



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:37 PM EDT

PDB ID : 9MGZ / pdb_00009mgz
EMDB ID : EMD-48264
Title : Dunaliella tertiolecta PSI-LHCI-TID1 supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 2.80 Å(reported)
Based on initial model : 6SL5

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:

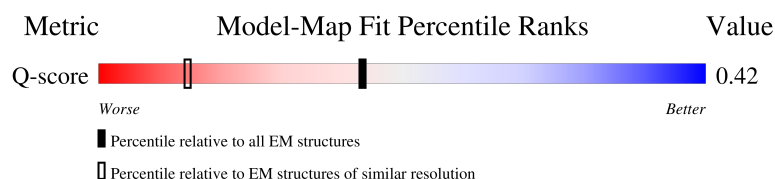
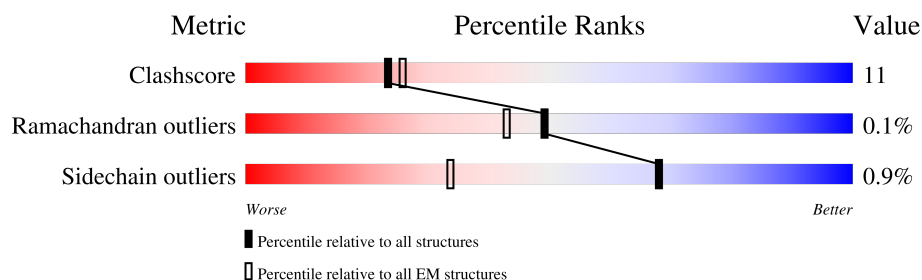
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



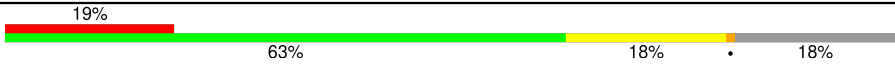
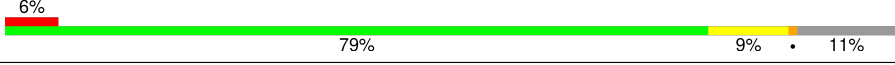
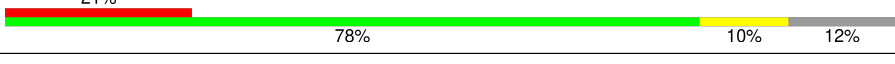
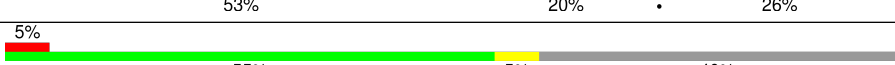
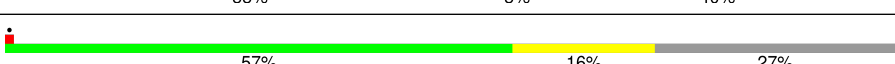
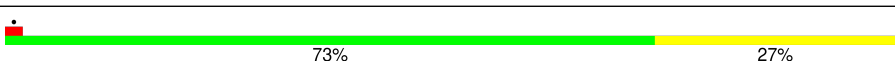
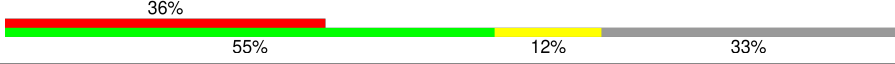
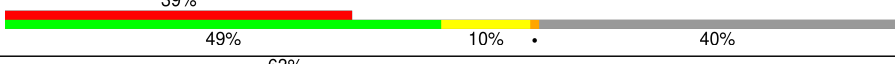
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1	228	
1	a	228	
2	3	286	
3	7	255	

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Mol	Chain	Length	Quality of chain
3	c	255	
4	8	254	
4	b	254	
5	A	751	
6	B	735	
7	C	81	
8	D	193	
9	E	111	
10	F	227	
11	J	41	
12	K	123	
13	T	350	
14	L	198	
15	I	108	

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
16	CHL	3	301	X	-	-	-
16	CHL	3	322	X	-	-	-
18	LUT	1	615	X	-	-	-
18	LUT	3	315	X	-	-	-
18	LUT	7	315	X	-	-	-
18	LUT	8	316	X	-	-	-
18	LUT	T	413	X	-	-	-
18	LUT	a	615	X	-	-	-
18	LUT	b	615	X	-	-	-
18	LUT	c	314	X	-	-	-

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 44202 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		
1	a	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	226	Total	C	N	O	S	0	0
			1719	1120	282	312	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	217	Total	C	N	O	S	0	0
			1669	1078	281	304	6		
3	c	209	Total	C	N	O	S	0	0
			1607	1037	271	293	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	226	Total	C	N	O	S	0	0
			1721	1108	286	320	7		
4	b	224	Total	C	N	O	S	0	0
			1710	1102	284	317	7		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	67	Total	C	N	O	0	0
			535	340	94	101		

- Molecule 10 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

- Molecule 13 is a protein called TIDI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	210	Total	C	N	O	S	0	0
			1639	1062	271	298	8		

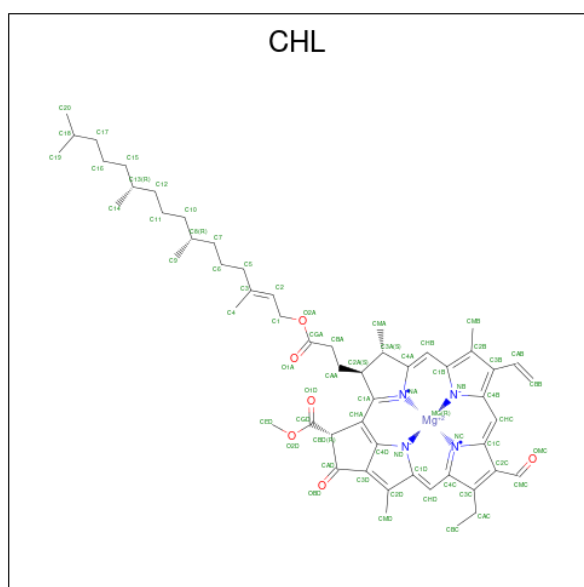
- Molecule 14 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	124	Total	C	N	O	S	0	0
			894	582	147	160	5		

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			274	191	40	42	1		

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



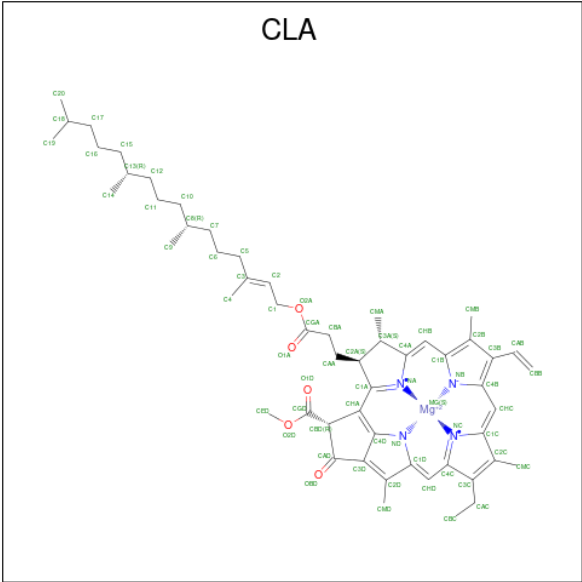
Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
16	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	T	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
17	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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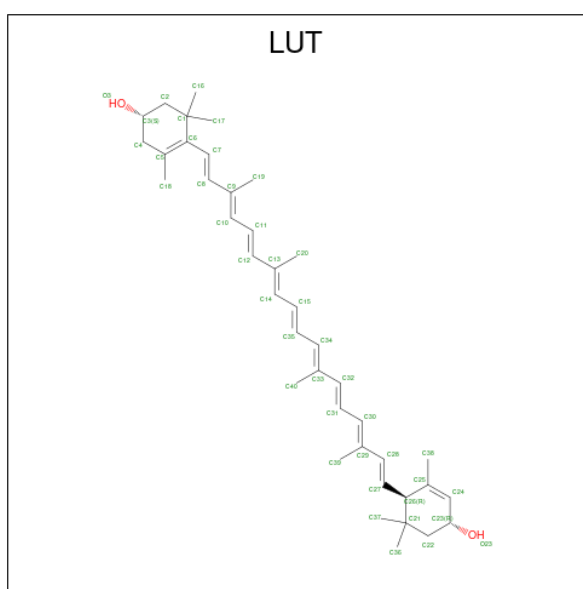
Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 18 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



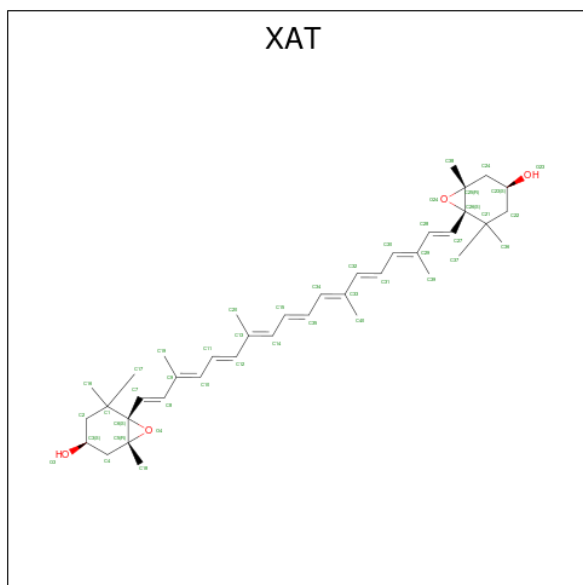
Mol	Chain	Residues	Atoms				AltConf
18	1	1	Total	C	O		0
			42	40	2		
18	3	1	Total	C	O		0
			42	40	2		
18	7	1	Total	C	O		0
			42	40	2		
18	8	1	Total	C	O		0
			42	40	2		
18	T	1	Total	C	O		0
			42	40	2		
18	a	1	Total	C	O		0
			42	40	2		
18	b	1	Total	C	O		0
			42	40	2		

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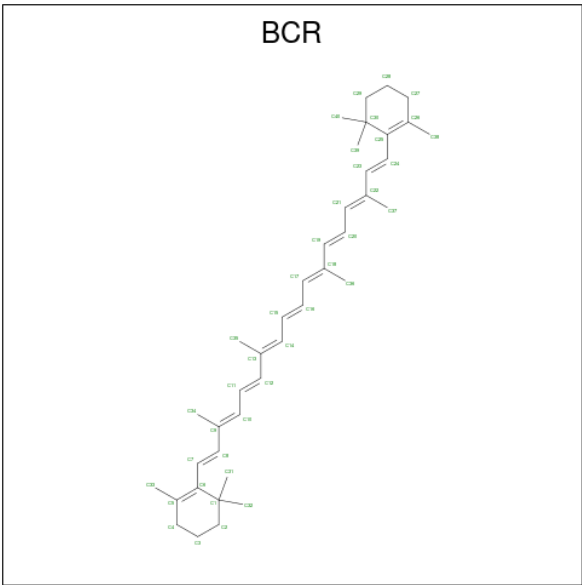
Mol	Chain	Residues	Atoms			AltConf
18	c	1	Total	C	O	0
			42	40	2	

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	3	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	T	1	Total	C	O	0
			44	40	4	
19	a	1	Total	C	O	0
			44	40	4	
19	b	1	Total	C	O	0
			44	40	4	
19	c	1	Total	C	O	0
			44	40	4	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



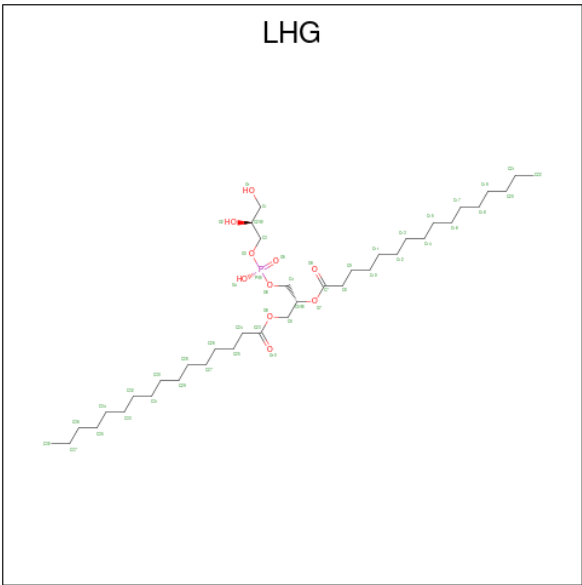
Mol	Chain	Residues	Atoms	AltConf
20	1	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	7	1	Total C 40 40	0
20	8	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0

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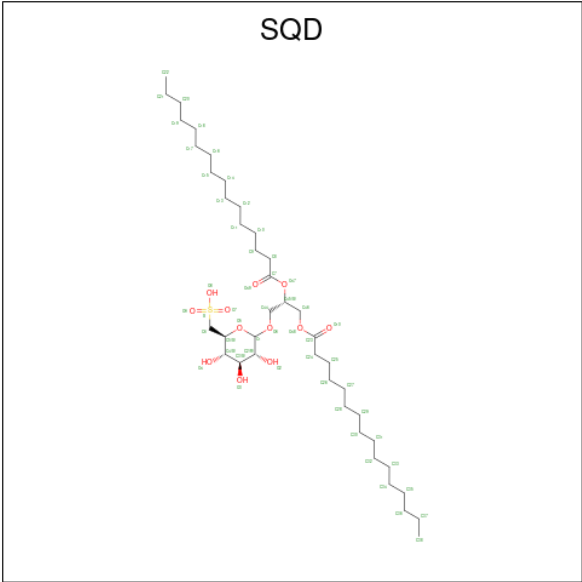
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	I	1	Total C 40 40	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



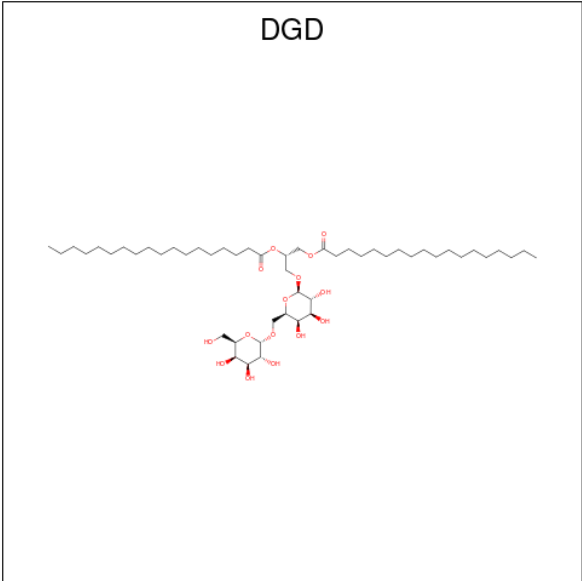
Mol	Chain	Residues	Atoms				AltConf
21	1	1	Total	C	O	P	0
			27	16	10	1	
21	1	1	Total	C	O	P	0
			31	20	10	1	
21	7	1	Total	C	O	P	0
			34	23	10	1	
21	8	1	Total	C	O	P	0
			30	19	10	1	
21	A	1	Total	C	O	P	0
			36	25	10	1	
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			30	20	9	1	
21	F	1	Total	C	O	P	0
			31	20	10	1	
21	a	1	Total	C	O	P	0
			23	13	9	1	
21	a	1	Total	C	O	P	0
			23	12	10	1	
21	b	1	Total	C	O	P	0
			21	10	10	1	
21	c	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
22	3	1	35	22	12	1	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



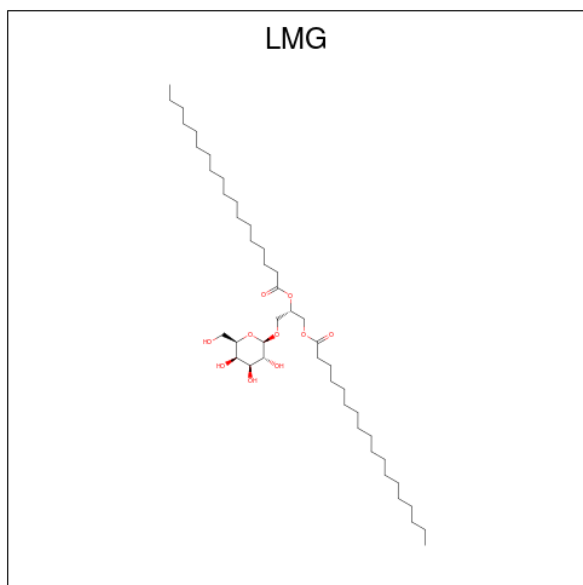
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	3	1	50	35	15	0
23	8	1	39	24	15	0

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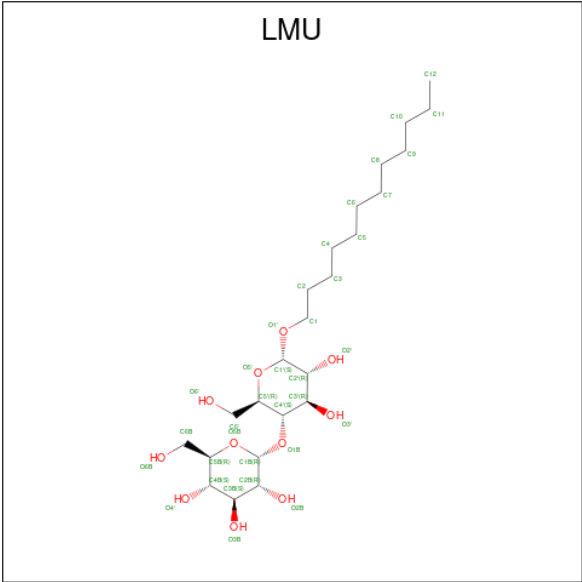
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			61	46	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



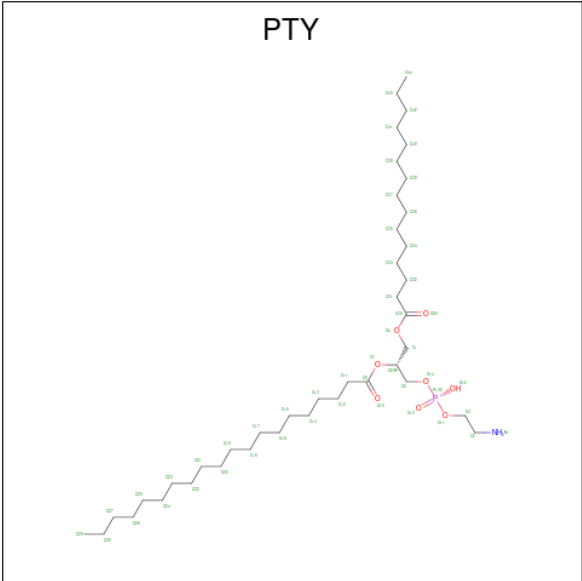
Mol	Chain	Residues	Atoms			AltConf
24	7	1	Total	C	O	0
			50	40	10	
24	A	1	Total	C	O	0
			32	22	10	
24	F	1	Total	C	O	0
			29	19	10	

- Molecule 25 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
25	7	1	Total	C	O	0
			35	24	11	
25	A	1	Total	C	O	0
			35	24	11	

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



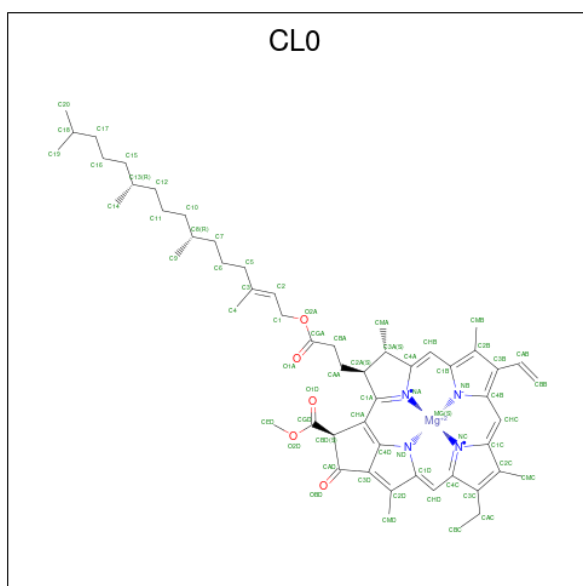
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	N	O	P	0
			21	11	1	8	1	

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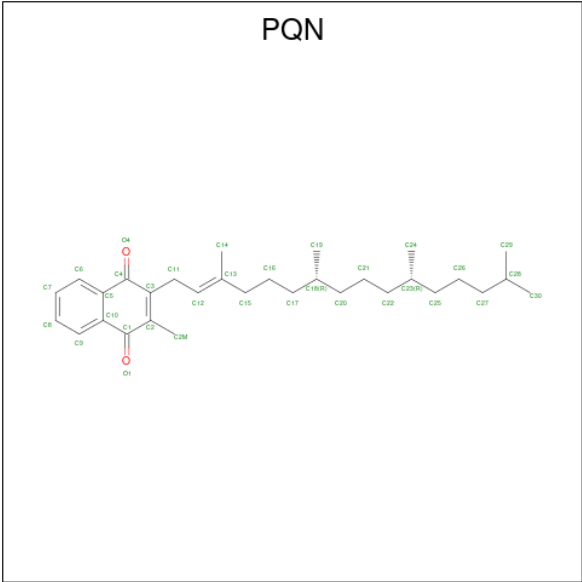
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
26	F	1	Total	C	N	O	P	0
			33	23	1	8	1	
26	F	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



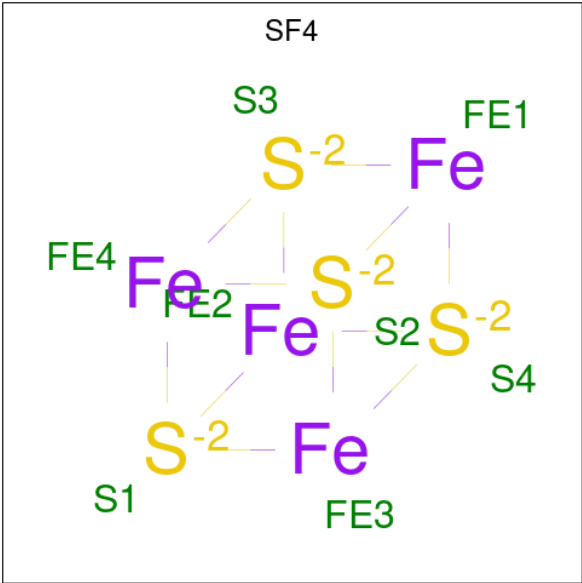
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			33	31	2	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



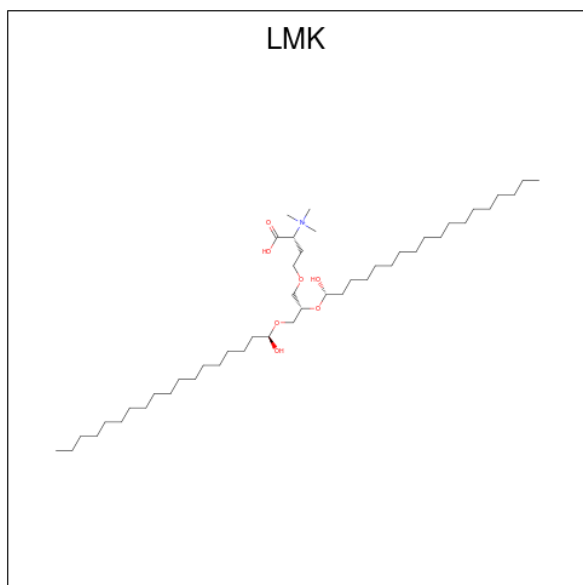
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: C₄₆H₉₄NO₇) (labeled as "Ligand of Interest" by depositor).

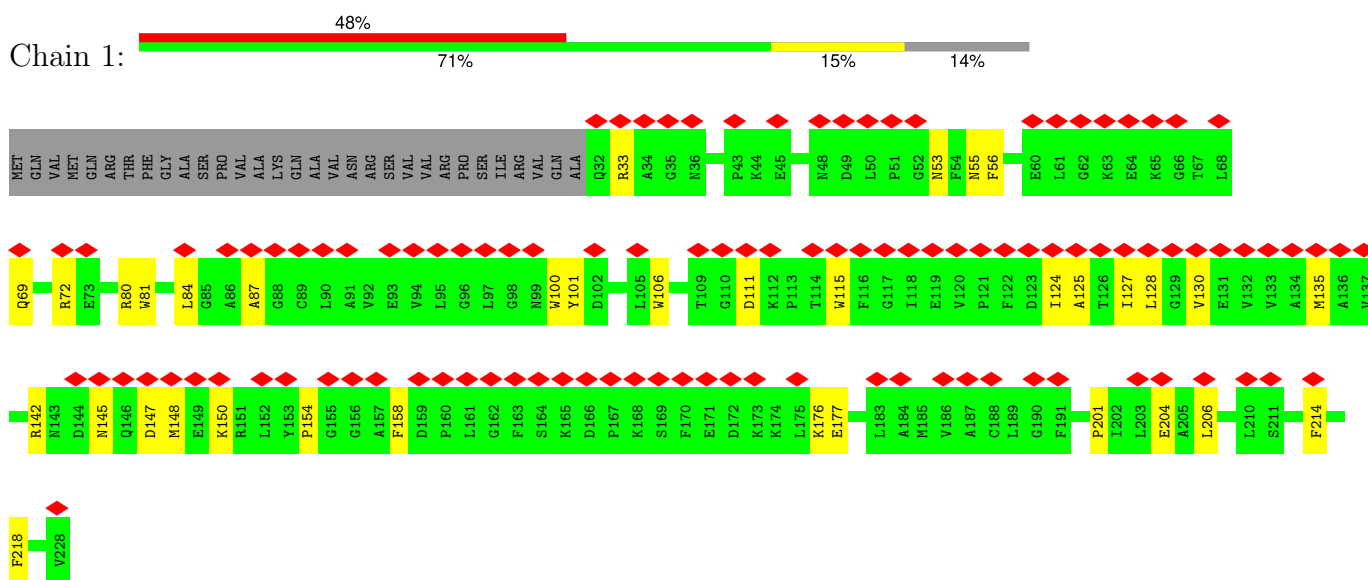


Mol	Chain	Residues	Atoms				AltConf
30	J	1	Total	C	N	O	0
			35	27	1	7	

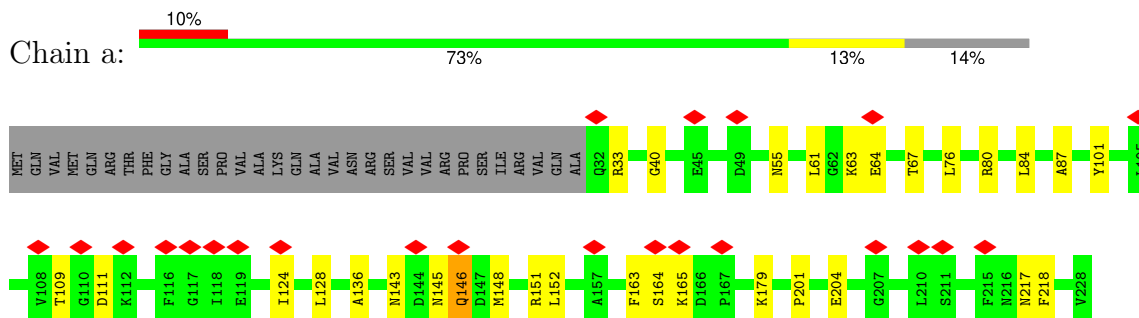
3 Residue-property plots

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.

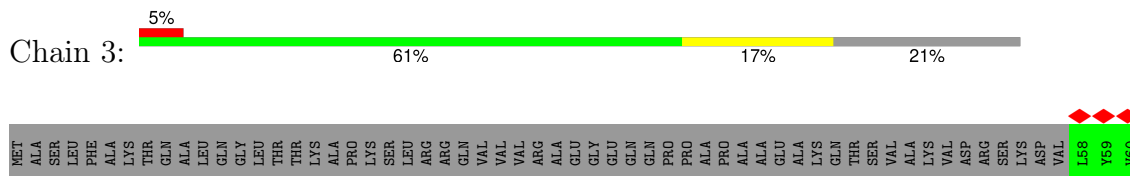
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

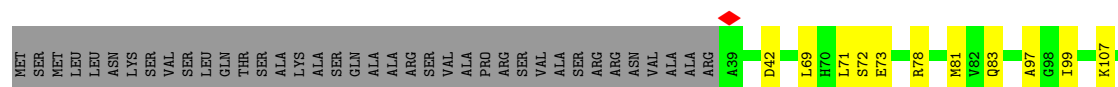


- Molecule 2: LHCA3

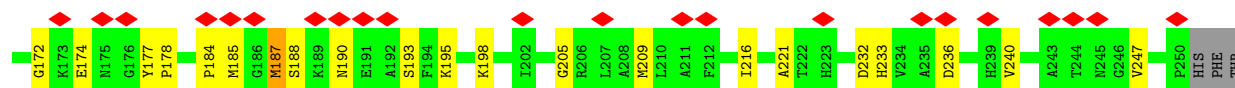
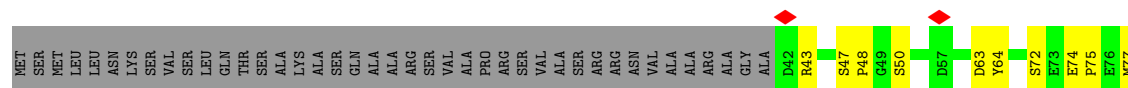




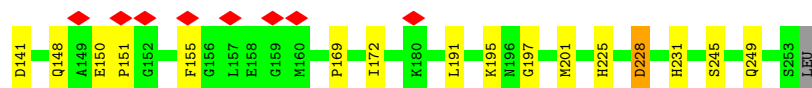
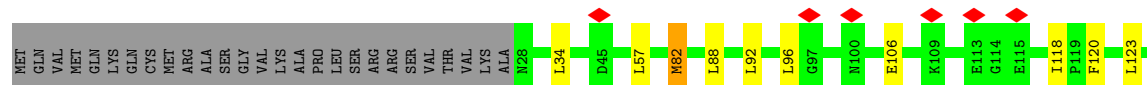
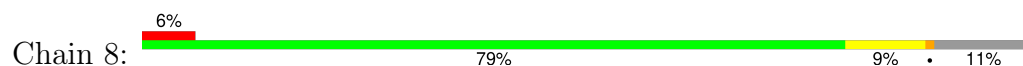
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



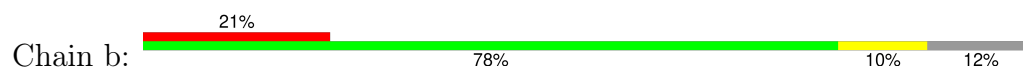
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

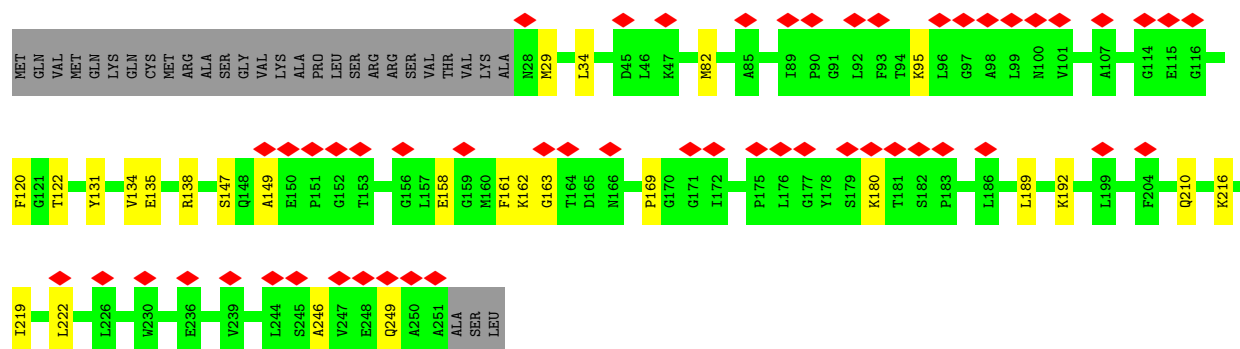


- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



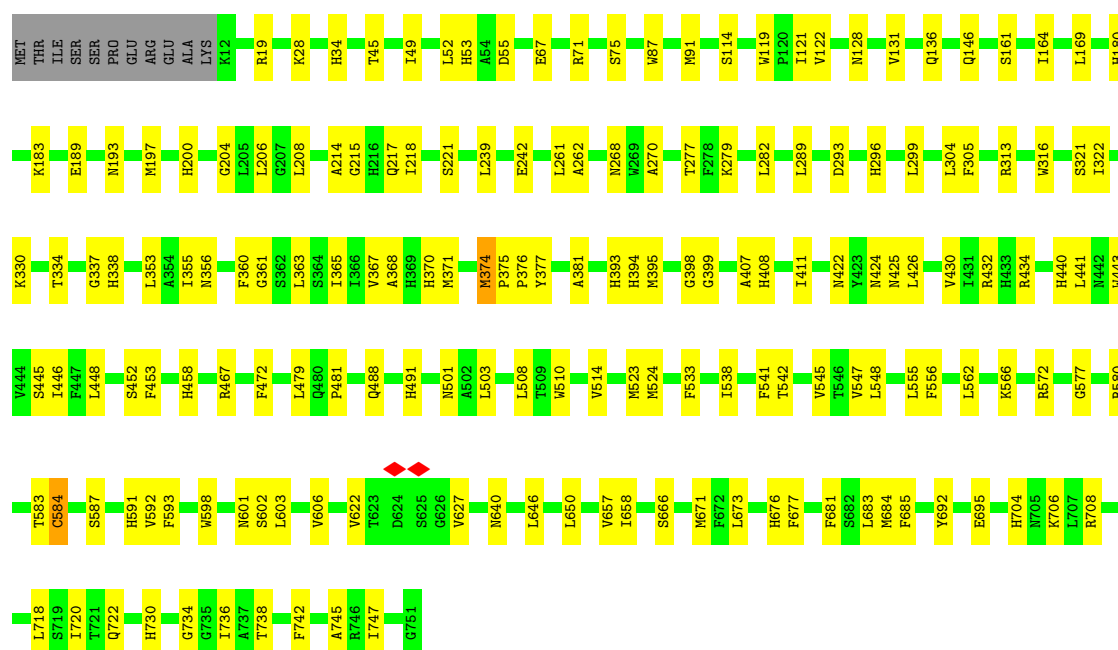
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic





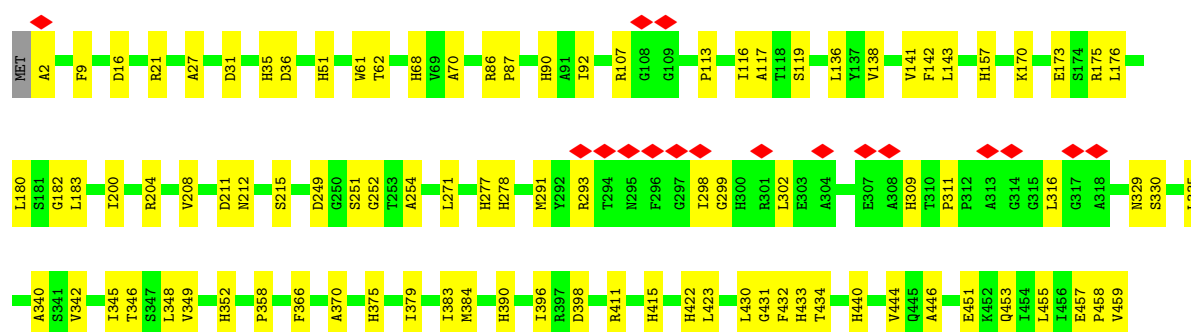
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

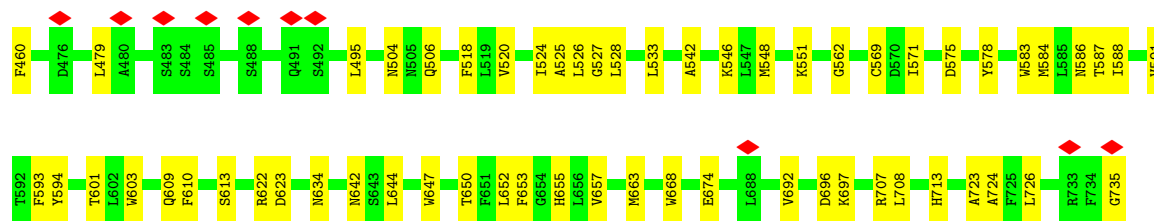
Chain A: 76% 23%



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 79% 21%





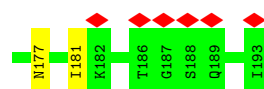
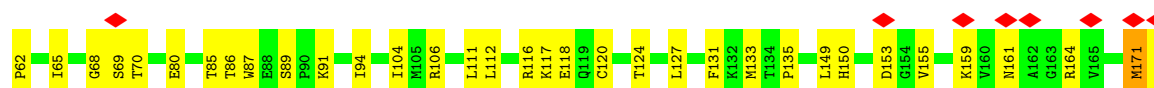
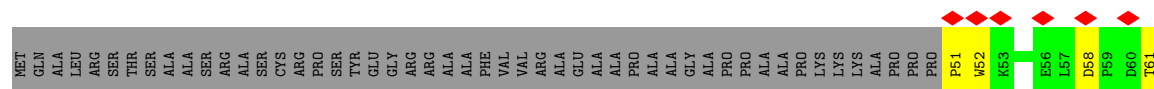
• Molecule 7: Photosystem I iron-sulfur center

Chain C: 80% 19%



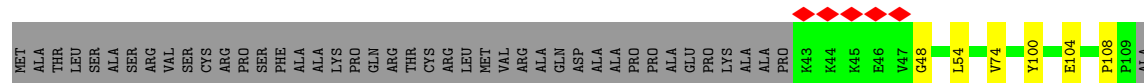
• Molecule 8: Photosystem I reaction center subunit II, chloroplastic

Chain D: 10% 53% 20% 26%



• Molecule 9: Photosystem I reaction center subunit IV

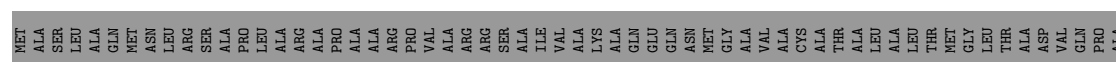
Chain E: 5% 55% 5% 40%

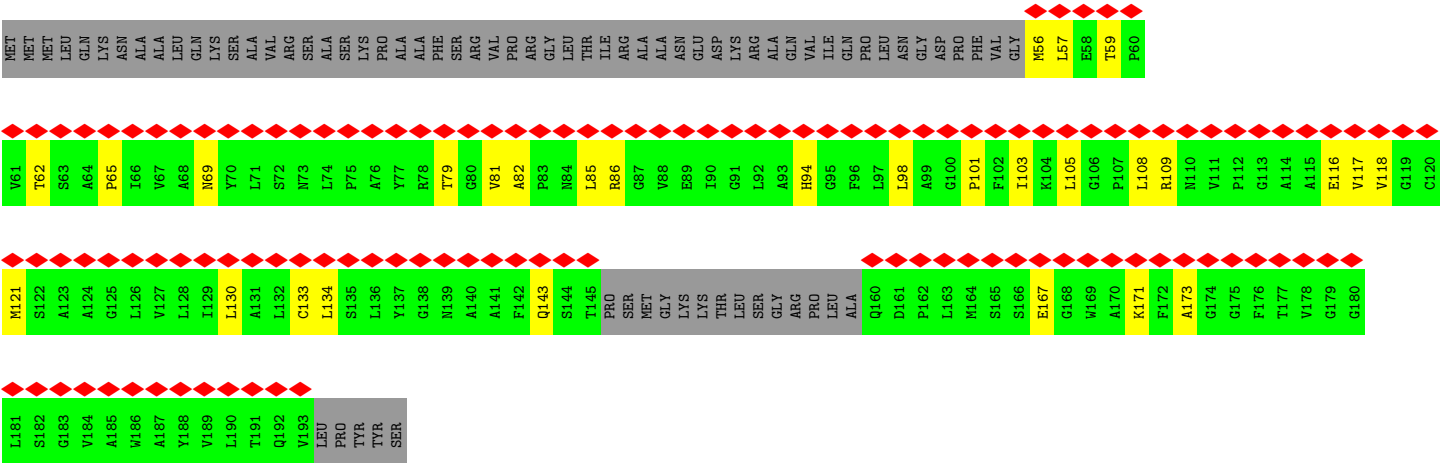


LYS

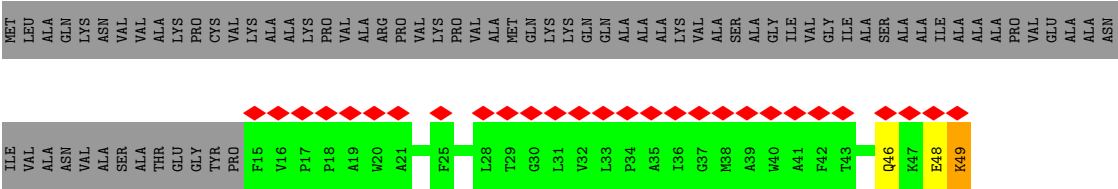
• Molecule 10: PSAF1

Chain F: 57% 16% 27%





● Molecule 15: Photosystem I reaction center subunit VIII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0151	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, SQD, LUT, SF4, LHG, DGD, LMK, PQN, BCR, CHL, LMG, LMU, CLA, PTY, CL0

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	1	0.19	0/1544	0.40	0/2093
1	a	0.16	0/1544	0.43	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.14	0/1722	0.36	0/2339
3	c	0.16	0/1657	0.41	1/2251 (0.0%)
4	8	0.15	0/1770	0.38	1/2401 (0.0%)
4	b	0.14	0/1759	0.33	0/2386
5	A	0.14	0/6004	0.30	0/8190
6	B	0.14	0/6026	0.33	0/8235
7	C	0.11	0/610	0.30	0/828
8	D	0.13	0/1163	0.41	1/1571 (0.1%)
9	E	0.19	0/547	0.37	0/743
10	F	0.16	0/1329	0.36	0/1797
11	J	0.18	0/338	0.46	0/461
12	K	0.19	0/587	0.52	0/795
13	T	0.18	0/1688	0.47	0/2292
14	L	0.18	0/914	0.39	0/1248
15	I	0.19	0/286	0.41	0/394
All	All	0.15	0/31256	0.37	3/42519 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8	82	MET	CB-CG-SD	5.25	128.45	112.70
3	c	81	MET	CB-CG-SD	5.23	128.40	112.70
8	D	171	MET	CB-CG-SD	5.06	127.89	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1470	31	0
1	a	1505	0	1469	35	0
2	3	1719	0	1671	48	0
3	7	1669	0	1615	35	0
3	c	1607	0	1563	49	0
4	8	1721	0	1662	22	0
4	b	1710	0	1652	21	0
5	A	5808	0	5637	148	0
6	B	5814	0	5560	132	0
7	C	600	0	582	15	0
8	D	1133	0	1138	31	0
9	E	535	0	534	3	0
10	F	1300	0	1322	26	0
11	J	327	0	328	12	0
12	K	579	0	608	14	0
13	T	1639	0	1590	29	0
14	L	894	0	908	27	0
15	I	274	0	282	3	0
16	1	98	0	68	4	0
16	3	123	0	114	16	0
16	7	141	0	95	10	0
16	8	144	0	99	10	0
16	T	97	0	68	11	0
16	a	94	0	62	3	0
16	b	145	0	99	12	0
16	c	144	0	101	22	0
17	1	614	0	522	23	0
17	3	773	0	655	27	0
17	7	510	0	423	18	0
17	8	546	0	431	18	0
17	A	2453	0	2473	140	0
17	B	2252	0	2113	107	0
17	F	263	0	230	8	0
17	J	49	0	39	3	0
17	K	181	0	132	7	0
17	L	110	0	101	4	0
17	T	531	0	401	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	578	0	441	15	0
17	b	551	0	440	14	0
17	c	526	0	457	27	0
18	1	42	0	56	6	0
18	3	42	0	56	3	0
18	7	42	0	56	3	0
18	8	42	0	56	1	0
18	T	42	0	47	4	0
18	a	42	0	56	4	0
18	b	42	0	56	1	0
18	c	42	0	56	0	0
19	1	44	0	56	1	0
19	3	44	0	56	4	0
19	7	44	0	56	6	0
19	8	44	0	56	1	0
19	T	44	0	56	2	0
19	a	44	0	56	1	0
19	b	44	0	56	0	0
19	c	44	0	55	1	0
20	1	40	0	54	8	0
20	3	120	0	163	9	0
20	7	40	0	56	3	0
20	8	40	0	56	5	0
20	A	240	0	336	24	0
20	B	280	0	391	21	0
20	F	80	0	112	9	0
20	I	40	0	53	2	0
20	J	80	0	112	6	0
20	K	40	0	55	5	0
20	L	80	0	110	6	0
20	T	40	0	56	3	0
20	a	40	0	56	4	0
20	b	40	0	56	6	0
20	c	40	0	56	2	0
21	1	58	0	56	2	0
21	7	34	0	37	0	0
21	8	30	0	30	2	0
21	A	115	0	143	9	0
21	F	31	0	31	0	0
21	a	46	0	29	2	0
21	b	21	0	12	0	0
21	c	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3	35	0	33	5	0
23	3	50	0	56	1	0
23	8	39	0	36	2	0
23	B	61	0	83	8	0
24	7	50	0	73	5	0
24	A	32	0	27	2	0
24	F	29	0	28	1	0
25	7	35	0	46	3	0
25	A	35	0	46	1	0
26	8	42	0	30	0	0
26	F	51	0	49	0	0
27	A	65	0	72	8	0
28	A	33	0	46	2	0
28	B	33	0	46	3	0
29	A	8	0	0	0	0
29	C	16	0	0	1	0
30	J	35	0	0	0	0
All	All	44202	0	42797	957	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (957) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:81:VAL:CG1	14:L:85:LEU:HD12	1.67	1.23
1:a:76:LEU:HD12	1:a:152:LEU:CD2	1.71	1.20
5:A:646:LEU:HD22	6:B:652:LEU:HD21	1.24	1.18
1:a:76:LEU:CD1	1:a:152:LEU:HD22	1.73	1.17
1:1:201:PRO:HD2	1:1:204:GLU:OE1	1.43	1.16
3:c:138:LEU:O	17:c:307:CLA:HBB2	1.43	1.16
14:L:81:VAL:HG13	14:L:85:LEU:HD12	1.35	1.07
1:a:76:LEU:HD12	1:a:152:LEU:HD22	1.31	1.05
16:c:304:CHL:C1C	16:c:305:CHL:HBC3	1.88	1.04
7:C:17:CYS:SG	7:C:26:LEU:CD2	2.49	1.01
14:L:81:VAL:HG11	14:L:85:LEU:HD12	1.47	0.92
16:7:305:CHL:HBC2	16:7:306:CHL:HHD	1.50	0.91
13:T:328:PRO:O	13:T:332:LEU:HG	1.71	0.89
1:a:76:LEU:CD1	1:a:152:LEU:CD2	2.43	0.88
7:C:17:CYS:SG	7:C:26:LEU:HD22	2.14	0.87
3:c:144:VAL:HG11	16:c:306:CHL:C1B	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:657:VAL:HG22	5:A:745:ALA:HB3	1.57	0.84
5:A:646:LEU:HD22	6:B:652:LEU:CD2	2.07	0.83
3:c:144:VAL:HG11	16:c:306:CHL:CHB	2.05	0.83
6:B:431:GLY:N	6:B:526:LEU:HD13	1.95	0.82
16:7:306:CHL:H2A	16:7:306:CHL:HED3	1.62	0.82
16:T:401:CHL:HHB	16:T:401:CHL:H2	1.64	0.79
17:K:203:CLA:H3A	20:K:205:BCR:H363	1.65	0.79
5:A:363:LEU:HD21	17:A:5020:CLA:H93	1.62	0.79
7:C:17:CYS:SG	7:C:26:LEU:HD23	2.21	0.78
20:T:415:BCR:HC32	16:T:416:CHL:HHD	1.66	0.77
11:J:16:LEU:O	11:J:20:ILE:HD12	1.85	0.77
16:T:416:CHL:HBB2	17:c:301:CLA:HHD	1.66	0.76
5:A:363:LEU:O	5:A:367:VAL:HG23	1.86	0.76
17:A:5021:CLA:HBB2	20:A:5048:BCR:H281	1.67	0.76
2:3:198:LEU:HD22	2:3:201:LEU:HD22	1.68	0.75
6:B:431:GLY:HA2	6:B:526:LEU:CD2	2.17	0.75
2:3:134:VAL:HG22	17:c:313:CLA:HAA1	1.67	0.75
20:3:317:BCR:HC22	16:3:322:CHL:HHD	1.67	0.75
17:3:305:CLA:HAB	24:7:301:LMG:H341	1.68	0.74
17:B:814:CLA:H12	20:B:845:BCR:H20C	1.69	0.74
3:c:144:VAL:HG22	16:c:306:CHL:C3B	2.17	0.74
6:B:440:HIS:HE1	17:B:832:CLA:NA	1.82	0.73
13:T:245:THR:HB	16:T:416:CHL:HED2	1.71	0.73
3:c:144:VAL:HG13	16:c:306:CHL:C4B	1.77	0.73
16:b:605:CHL:HBA1	20:b:617:BCR:H19C	1.72	0.72
5:A:121:ILE:HG13	5:A:122:VAL:HG13	1.71	0.72
17:F:5004:CLA:HBB1	20:F:5005:BCR:H23C	1.71	0.71
6:B:384:MET:HE3	17:B:825:CLA:C1C	2.13	0.71
1:a:76:LEU:HD11	1:a:152:LEU:HD22	1.69	0.71
1:1:201:PRO:CD	1:1:204:GLU:OE1	2.31	0.70
1:a:201:PRO:HD2	1:a:204:GLU:OE1	1.90	0.70
3:c:147:LYS:HD3	16:c:306:CHL:HHC	1.73	0.70
6:B:330:SER:CB	6:B:398:ASP:OD2	2.39	0.70
6:B:431:GLY:HA2	6:B:526:LEU:HD21	1.73	0.70
1:a:87:ALA:HB2	18:a:615:LUT:H15	1.73	0.70
1:a:84:LEU:HB3	17:a:604:CLA:HAB	1.73	0.70
5:A:684:MET:HE3	17:A:5004:CLA:NB	1.97	0.70
17:A:5008:CLA:H13	20:A:5049:BCR:H19C	1.72	0.69
1:1:87:ALA:HB2	18:1:615:LUT:H34	1.75	0.69
17:A:5004:CLA:HBB1	17:A:5044:CLA:C4B	2.22	0.69
6:B:157:HIS:HE1	17:B:811:CLA:NC	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:15:THR:O	7:C:15:THR:HG22	1.93	0.68
5:A:671:MET:HE1	20:A:5052:BCR:H352	1.76	0.68
6:B:204:ARG:HH12	6:B:254:ALA:H	1.39	0.68
17:c:303:CLA:HBB1	20:c:316:BCR:H24C	1.76	0.68
6:B:423:LEU:HG	17:B:837:CLA:HBB1	1.76	0.68
13:T:192:ILE:HD12	17:T:412:CLA:NC	2.05	0.68
10:F:204:LEU:HD12	17:F:5009:CLA:HBB2	1.75	0.67
17:b:601:CLA:HBB2	17:b:602:CLA:HHD	1.75	0.67
17:3:306:CLA:H42	18:3:315:LUT:H27	1.77	0.67
5:A:393:HIS:HE1	17:A:5029:CLA:ND	1.93	0.67
17:B:830:CLA:HBC1	20:B:846:BCR:H21C	1.77	0.67
6:B:390:HIS:HE1	17:B:829:CLA:NA	1.92	0.66
16:8:308:CHL:HMB3	20:8:318:BCR:H16C	1.78	0.66
20:B:849:BCR:H10C	11:J:39:PHE:HA	1.77	0.66
13:T:232:LEU:HD11	17:T:404:CLA:C4C	2.25	0.66
5:A:448:LEU:HB3	5:A:541:PHE:HB2	1.76	0.66
16:3:322:CHL:HBB2	17:7:302:CLA:HHD	1.76	0.65
14:L:81:VAL:HG12	14:L:82:ALA:N	2.11	0.65
16:T:401:CHL:HAB	19:T:414:XAT:H30	1.78	0.65
5:A:646:LEU:CD2	6:B:652:LEU:HD21	2.16	0.65
1:1:147:ASP:HB3	1:1:150:LYS:HB2	1.79	0.65
16:3:301:CHL:H43	17:3:302:CLA:HBA1	1.79	0.65
24:7:301:LMG:H182	17:A:5017:CLA:H52	1.78	0.65
6:B:309:HIS:HE1	17:B:822:CLA:ND	1.93	0.65
6:B:330:SER:HA	6:B:398:ASP:OD2	1.97	0.65
5:A:395:MET:HE2	5:A:606:VAL:HG11	1.79	0.64
16:c:304:CHL:H3A	20:c:316:BCR:H21C	1.79	0.64
17:B:806:CLA:H91	23:B:848:DGD:HBN1	1.79	0.64
14:L:59:THR:OG1	14:L:62:THR:OG1	2.16	0.64
17:A:5033:CLA:HBB2	20:L:204:BCR:H342	1.78	0.64
8:D:87:TRP:HB3	8:D:135:PRO:HB3	1.78	0.64
17:1:605:CLA:C1A	20:1:617:BCR:H383	2.22	0.63
20:3:318:BCR:H393	17:A:5016:CLA:H11	1.80	0.63
3:c:232:ASP:HB3	3:c:240:VAL:HG11	1.80	0.63
17:B:836:CLA:H72	17:B:836:CLA:HBB1	1.81	0.63
3:c:174:GLU:HB2	3:c:177:TYR:HB2	1.80	0.63
3:7:81:MET:HB3	17:7:302:CLA:H3A	1.80	0.63
7:C:73:SER:H	7:C:76:SER:HB3	1.64	0.62
17:1:605:CLA:HAA1	20:1:617:BCR:H24C	1.81	0.62
2:3:129:LEU:HD13	2:3:134:VAL:HG11	1.81	0.62
14:L:94:HIS:HE1	17:L:201:CLA:ND	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:323:CLA:NA	5:A:180:HIS:HE1	1.97	0.62
16:c:304:CHL:HBC2	16:c:305:CHL:HHD	1.81	0.62
17:1:608:CLA:HBA1	21:1:619:LHG:H101	1.82	0.62
3:7:170:LEU:HD22	16:7:307:CHL:HMC	1.81	0.62
2:3:134:VAL:CG2	17:c:313:CLA:HAA1	2.30	0.62
2:3:169:GLU:O	2:3:173:ILE:HG22	2.00	0.62
14:L:81:VAL:CG1	14:L:85:LEU:CD1	2.61	0.62
13:T:192:ILE:HD12	17:T:412:CLA:C4C	2.30	0.61
6:B:277:HIS:HE1	17:B:817:CLA:ND	1.92	0.61
17:a:611:CLA:HAB	18:a:615:LUT:H12	1.82	0.61
14:L:81:VAL:HG11	14:L:85:LEU:CD1	2.25	0.61
5:A:446:ILE:HG12	17:B:803:CLA:HBA1	1.82	0.61
3:c:172:GLY:HA2	3:c:178:PRO:HA	1.81	0.61
5:A:282:LEU:HD11	5:A:375:PRO:HD2	1.83	0.61
17:8:302:CLA:HBB2	17:8:303:CLA:HHD	1.82	0.61
6:B:208:VAL:HA	6:B:212:ASN:HD21	1.66	0.61
4:8:141:ASP:HB3	4:8:148:GLN:HG2	1.81	0.61
6:B:431:GLY:N	6:B:526:LEU:CD1	2.63	0.61
5:A:128:ASN:HB3	5:A:136:GLN:HB3	1.83	0.60
17:A:5025:CLA:HBB2	21:A:5055:LHG:H242	1.82	0.60
16:7:306:CHL:HBA1	23:8:301:DGD:HD61	1.84	0.60
5:A:217:GLN:HA	5:A:221:SER:HB2	1.82	0.60
5:A:296:HIS:HE1	17:A:5018:CLA:ND	1.99	0.60
4:b:134:VAL:HG11	16:b:607:CHL:HMA3	1.82	0.60
17:b:610:CLA:H2	17:b:611:CLA:HMD2	1.84	0.60
1:1:145:ASN:HD21	1:1:150:LYS:HB3	1.67	0.60
17:B:830:CLA:H62	17:B:840:CLA:H11	1.83	0.60
3:c:144:VAL:CG1	16:c:306:CHL:C1B	2.54	0.60
17:A:5025:CLA:H2	17:A:5036:CLA:H161	1.84	0.60
6:B:92:ILE:HB	6:B:113:PRO:HB2	1.82	0.60
6:B:119:SER:HA	17:B:827:CLA:HMA2	1.84	0.60
2:3:178:LEU:HD13	16:3:322:CHL:HMA2	1.83	0.60
5:A:356:ASN:HD21	17:A:5026:CLA:H101	1.66	0.59
1:1:177:GLU:HA	17:1:609:CLA:HBB1	1.84	0.59
2:3:178:LEU:HB3	16:3:322:CHL:HED2	1.84	0.59
5:A:279:LYS:HA	5:A:503:LEU:HB2	1.84	0.59
11:J:21:PHE:HA	17:J:102:CLA:HBB2	1.83	0.59
1:1:201:PRO:HD2	1:1:204:GLU:CD	2.24	0.59
2:3:113:ALA:HB1	2:3:239:GLY:HA3	1.85	0.59
12:K:57:ALA:HB1	17:K:204:CLA:HBB2	1.84	0.59
17:T:403:CLA:HMB3	17:T:404:CLA:HAB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:96:LEU:HD22	1:a:124:ILE:HD13	1.85	0.59
6:B:143:LEU:HD11	20:B:845:BCR:H292	1.84	0.59
17:J:102:CLA:H3A	17:J:102:CLA:H2	1.83	0.59
17:3:305:CLA:H12	24:7:301:LMG:H141	1.84	0.58
4:8:169:PRO:HD3	16:8:308:CHL:HMD2	1.85	0.58
16:3:301:CHL:H91	17:3:307:CLA:H172	1.84	0.58
12:K:69:SER:H	12:K:72:LYS:HB2	1.66	0.58
17:K:201:CLA:ND	20:K:205:BCR:H281	2.18	0.58
5:A:481:PRO:HG3	5:A:533:PHE:HB2	1.86	0.58
4:8:245:SER:O	4:8:249:GLN:NE2	2.36	0.58
5:A:657:VAL:HG21	5:A:742:PHE:HA	1.84	0.58
8:D:69:SER:H	14:L:56:MET:HG2	1.68	0.58
4:b:135:GLU:OE1	4:b:138:ARG:NH2	2.36	0.58
10:F:67:LEU:HB2	10:F:124:LEU:HD13	1.85	0.58
17:K:203:CLA:HBB1	20:K:205:BCR:H352	1.85	0.58
6:B:451:GLU:OE2	10:F:114:ARG:NH1	2.37	0.58
5:A:75:SER:OG	17:A:5013:CLA:HAC2	2.04	0.58
27:A:5003:CL0:H36	27:A:5003:CL0:H30	1.85	0.58
17:A:5035:CLA:H62	14:L:101:PRO:HG2	1.84	0.57
6:B:175:ARG:HB2	17:B:813:CLA:HBC2	1.85	0.57
17:8:311:CLA:C1C	21:8:321:LHG:HC61	2.23	0.57
17:7:302:CLA:HAB	19:7:316:XAT:H12	1.85	0.57
17:7:312:CLA:HED3	17:7:312:CLA:H2A	1.86	0.57
17:A:5015:CLA:HAC2	17:A:5016:CLA:HMB2	1.86	0.57
6:B:87:PRO:HB2	6:B:117:ALA:HB3	1.87	0.57
6:B:479:LEU:HD22	6:B:495:LEU:HD11	1.86	0.57
3:7:144:VAL:HG13	16:7:307:CHL:C4B	2.15	0.57
17:A:5041:CLA:H91	17:F:5007:CLA:HAC2	1.85	0.57
17:B:819:CLA:H43	20:B:846:BCR:H363	1.87	0.57
3:c:64:TYR:HB2	17:c:301:CLA:HMD1	1.86	0.57
1:a:164:SER:HB3	17:a:609:CLA:HBA1	1.86	0.57
3:c:72:SER:HB2	3:c:78:ARG:HA	1.85	0.57
17:3:302:CLA:H143	17:3:307:CLA:H42	1.86	0.57
16:b:605:CHL:HAA1	20:b:617:BCR:H21C	1.85	0.57
17:3:302:CLA:H52	17:A:5014:CLA:H191	1.87	0.57
5:A:708:ARG:HB2	10:F:168:ARG:HH21	1.70	0.57
6:B:422:HIS:HE1	17:B:831:CLA:NA	2.02	0.57
17:T:402:CLA:H2	17:T:402:CLA:H2A	1.87	0.57
17:A:5025:CLA:H2A	17:A:5025:CLA:HED3	1.85	0.57
17:A:5025:CLA:H42	20:A:5051:BCR:H352	1.87	0.57
5:A:91:MET:HE1	17:A:5011:CLA:H2A	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:838:CLA:HAB	28:B:842:PQN:H141	1.87	0.56
20:3:318:BCR:H17C	17:A:5016:CLA:H93	1.87	0.56
13:T:152:ARG:NH2	13:T:251:TYR:O	2.37	0.56
5:A:467:ARG:NH2	17:A:5035:CLA:OBD	2.38	0.56
6:B:142:PHE:HE2	20:B:845:BCR:H373	1.70	0.56
7:C:17:CYS:HB3	29:C:102:SF4:S2	2.45	0.56
5:A:87:TRP:HA	17:A:5010:CLA:HBB2	1.87	0.56
14:L:105:LEU:HA	14:L:109:ARG:HD3	1.88	0.56
2:3:74:LEU:HD12	16:3:301:CHL:HED3	1.88	0.56
12:K:76:PRO:HB2	12:K:77:LEU:HD22	1.88	0.56
5:A:53:HIS:HE1	17:A:5006:CLA:ND	2.04	0.56
6:B:433:HIS:HB3	20:B:849:BCR:H393	1.87	0.56
5:A:734:GLY:O	5:A:738:THR:OG1	2.21	0.56
8:D:85:THR:OG1	8:D:120:CYS:SG	2.64	0.56
6:B:2:ALA:O	15:I:49:LYS:NZ	2.39	0.55
6:B:431:GLY:HA2	6:B:526:LEU:HD22	1.88	0.55
16:a:601:CHL:HBB2	17:a:602:CLA:HHD	1.88	0.55
5:A:399:GLY:HA3	5:A:603:LEU:HD11	1.87	0.55
17:A:5004:CLA:H42	17:A:5044:CLA:HBB1	1.87	0.55
17:8:303:CLA:H2A	17:8:303:CLA:HED3	1.87	0.55
13:T:169:HIS:HB3	13:T:311:MET:HE1	1.88	0.55
6:B:524:ILE:HG12	6:B:591:VAL:HG12	1.89	0.55
14:L:81:VAL:CG1	14:L:82:ALA:N	2.70	0.55
2:3:142:ASP:HB2	2:3:145:ARG:HG3	1.87	0.55
5:A:657:VAL:HG22	5:A:745:ALA:CB	2.32	0.55
6:B:51:HIS:HB3	17:B:813:CLA:HED3	1.89	0.55
6:B:634:ASN:O	6:B:642:ASN:ND2	2.39	0.55
13:T:262:PHE:HE2	17:T:406:CLA:HBB2	1.71	0.55
5:A:718:LEU:HB3	5:A:722:GLN:HG2	1.88	0.55
17:A:5008:CLA:H171	20:A:5048:BCR:H342	1.87	0.55
17:A:5019:CLA:H41	17:A:5019:CLA:H92	1.88	0.55
6:B:459:VAL:HG11	10:F:134:ILE:HG23	1.89	0.55
5:A:488:GLN:HG2	5:A:510:TRP:HA	1.88	0.55
17:A:5004:CLA:H171	17:A:5044:CLA:H171	1.89	0.55
17:A:5033:CLA:H51	17:L:201:CLA:H43	1.89	0.55
20:A:5052:BCR:H291	20:F:5005:BCR:H17C	1.88	0.55
21:A:5002:LHG:H242	11:J:1:MET:HE2	1.89	0.55
17:B:828:CLA:HED3	17:B:828:CLA:H2A	1.89	0.55
5:A:441:LEU:HG	5:A:548:LEU:HB2	1.89	0.54
20:A:5050:BCR:H323	20:A:5051:BCR:H271	1.89	0.54
8:D:116:ARG:NH2	8:D:118:GLU:OE1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:40:GLY:HA3	4:b:147:SER:HB2	1.89	0.54
17:1:604:CLA:HBB1	20:1:617:BCR:H23C	1.88	0.54
4:8:195:LYS:HD3	21:8:321:LHG:HC42	1.89	0.54
16:8:308:CHL:HAA1	16:8:308:CHL:HED2	1.89	0.54
6:B:663:MET:HB2	17:B:803:CLA:C1C	2.36	0.54
17:B:806:CLA:H151	17:B:828:CLA:HBB2	1.89	0.54
5:A:441:LEU:HD21	5:A:547:VAL:HG12	1.89	0.54
17:3:306:CLA:HHB	20:3:319:BCR:H342	1.87	0.54
6:B:330:SER:CA	6:B:398:ASP:OD2	2.56	0.54
5:A:206:LEU:HD21	17:A:5030:CLA:H171	1.90	0.54
17:A:5029:CLA:H61	20:A:5052:BCR:H331	1.90	0.54
17:B:827:CLA:HBC3	23:B:848:DGD:HBV1	1.89	0.54
1:1:106:TRP:HB2	1:1:111:ASP:HB2	1.90	0.54
22:3:320:SQD:H281	24:A:5001:LMG:HC91	1.89	0.54
3:7:232:ASP:HB3	3:7:240:VAL:HG11	1.89	0.54
6:B:358:PRO:HG3	17:B:818:CLA:HBA1	1.90	0.54
13:T:288:LEU:O	13:T:291:LYS:NZ	2.40	0.54
1:1:81:TRP:CZ2	1:1:135:MET:HE1	2.42	0.54
16:1:606:CHL:HBB2	17:1:608:CLA:HBC1	1.90	0.54
6:B:330:SER:OG	6:B:398:ASP:OD2	2.25	0.54
16:b:605:CHL:HBC2	16:b:606:CHL:HHD	1.90	0.54
24:F:5011:LMG:H132	11:J:8:LEU:HB3	1.89	0.54
14:L:65:PRO:O	14:L:69:ASN:ND2	2.41	0.54
2:3:222:GLY:HA2	2:3:227:GLU:HB3	1.90	0.54
5:A:430:VAL:HG11	17:A:5022:CLA:H192	1.90	0.54
1:1:214:PHE:HB3	4:8:118:ILE:HG23	1.89	0.53
17:1:604:CLA:HBA1	20:1:617:BCR:H272	1.91	0.53
4:8:123:LEU:HD13	16:8:306:CHL:HHD	1.89	0.53
20:A:5047:BCR:H10C	20:A:5048:BCR:H382	1.90	0.53
12:K:88:THR:HG22	12:K:88:THR:O	2.07	0.53
3:7:245:ASN:ND2	17:7:312:CLA:OBD	2.40	0.53
20:A:5049:BCR:H371	20:A:5049:BCR:C26	2.38	0.53
2:3:109:GLU:HG2	2:3:236:ILE:HD11	1.90	0.53
5:A:45:THR:HG22	5:A:714:GLN:HB2	1.89	0.53
5:A:508:LEU:HD12	5:A:523:MET:HB3	1.89	0.53
4:8:197:GLY:O	4:8:201:MET:HG3	2.09	0.53
5:A:353:LEU:HD11	17:A:5031:CLA:HBB1	1.90	0.53
8:D:117:LYS:HE3	8:D:149:LEU:HD13	1.91	0.53
8:D:94:ILE:HG12	8:D:104:ILE:HG12	1.90	0.53
17:B:828:CLA:C4D	20:B:844:BCR:H282	2.39	0.53
8:D:124:THR:HG23	8:D:135:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:224:THR:HG23	2:3:227:GLU:H	1.73	0.53
5:A:268:ASN:OD1	12:K:118:LYS:NZ	2.41	0.53
17:B:806:CLA:H43	23:B:848:DGD:HB61	1.91	0.53
6:B:520:VAL:HG23	17:B:802:CLA:H141	1.90	0.53
10:F:185:ILE:HG23	10:F:186:ILE:HG13	1.90	0.53
5:A:640:ASN:OD1	5:A:640:ASN:N	2.40	0.52
10:F:177:ASP:OD1	10:F:177:ASP:N	2.41	0.52
19:3:316:XAT:H171	17:A:5016:CLA:H191	1.91	0.52
3:7:83:GLN:HG3	3:7:152:LEU:HD13	1.91	0.52
5:A:67:GLU:OE2	5:A:71:ARG:NH2	2.43	0.52
3:c:43:ARG:NH2	3:c:63:ASP:OD1	2.43	0.52
5:A:279:LYS:HB3	5:A:503:LEU:HD22	1.91	0.52
17:1:609:CLA:H102	18:1:615:LUT:H30	1.91	0.52
17:3:323:CLA:H72	17:A:5014:CLA:H18	1.91	0.52
5:A:572:ARG:NH1	21:A:5053:LHG:O10	2.43	0.52
6:B:107:ARG:HH21	6:B:116:ILE:HG12	1.73	0.52
6:B:298:ILE:HB	17:B:821:CLA:HMD1	1.92	0.52
17:B:809:CLA:H3A	17:B:810:CLA:HBB1	1.92	0.52
3:7:174:GLU:HB2	3:7:177:TYR:HB2	1.91	0.52
5:A:119:TRP:HB3	20:J:104:BCR:HC42	1.90	0.52
5:A:424:ASN:OD1	5:A:432:ARG:NH2	2.43	0.52
6:B:61:TRP:NE1	17:B:827:CLA:OBD	2.42	0.52
16:T:416:CHL:HED1	3:c:47:SER:HB3	1.90	0.52
4:b:169:PRO:HG2	16:b:607:CHL:HHB	1.92	0.52
4:b:246:ALA:HA	4:b:249:GLN:HE21	1.75	0.52
6:B:251:SER:OG	6:B:252:GLY:N	2.43	0.52
1:a:84:LEU:HG	17:a:604:CLA:HBB2	1.91	0.52
1:1:206:LEU:HD13	18:1:615:LUT:H21	1.92	0.52
5:A:440:HIS:HE1	17:A:5033:CLA:NA	2.07	0.52
7:C:32:ASP:OD1	7:C:32:ASP:N	2.43	0.52
11:J:28:GLU:OE1	11:J:31:ARG:NH2	2.42	0.52
3:c:144:VAL:CG2	16:c:306:CHL:C1B	2.87	0.52
17:A:5004:CLA:H3A	17:A:5004:CLA:H12	1.92	0.52
6:B:453:GLN:HE21	6:B:455:LEU:HD11	1.75	0.52
13:T:328:PRO:O	13:T:332:LEU:CG	2.54	0.52
1:1:80:ARG:NH1	17:1:607:CLA:OBD	2.43	0.51
17:A:5035:CLA:HMA2	14:L:105:LEU:HB3	1.91	0.51
7:C:29:VAL:HG12	8:D:164:ARG:HB2	1.92	0.51
13:T:244:GLU:OE2	13:T:247:ARG:NH2	2.39	0.51
4:8:228:ASP:OD2	4:8:231:HIS:ND1	2.40	0.51
17:B:818:CLA:H162	17:B:826:CLA:H3A	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:832:CLA:HAA2	20:J:103:BCR:HC42	1.91	0.51
17:F:5006:CLA:H12	11:J:14:VAL:HG23	1.92	0.51
3:7:69:LEU:HD12	19:7:316:XAT:H172	1.93	0.51
5:A:338:HIS:CD2	17:A:5025:CLA:ND	2.79	0.51
17:A:5005:CLA:HAC2	17:B:803:CLA:HBC3	1.92	0.51
17:A:5025:CLA:H11	20:A:5050:BCR:H15C	1.92	0.51
5:A:208:LEU:HD22	20:A:5048:BCR:H361	1.91	0.51
5:A:363:LEU:HD11	17:A:5020:CLA:H71	1.91	0.51
17:A:5006:CLA:H3A	21:A:5053:LHG:H152	1.91	0.51
17:A:5044:CLA:HAB	6:B:583:TRP:CH2	2.46	0.51
6:B:650:THR:HG23	6:B:724:ALA:HB2	1.92	0.51
6:B:697:LYS:NZ	8:D:80:GLU:OE2	2.41	0.51
17:1:609:CLA:H2	18:1:615:LUT:H382	1.92	0.51
3:7:172:GLY:HA2	3:7:178:PRO:HA	1.91	0.51
4:8:57:LEU:HD22	10:F:198:GLN:HA	1.91	0.51
17:A:5022:CLA:H18	20:A:5050:BCR:H322	1.92	0.51
17:A:5032:CLA:HBB2	17:A:5040:CLA:HHC	1.93	0.51
8:D:65:ILE:HG13	8:D:106:ARG:HE	1.75	0.51
2:3:162:PRO:HA	2:3:165:LEU:HD12	1.92	0.51
3:7:99:ILE:HG12	3:7:115:TRP:HB2	1.93	0.51
17:A:5005:CLA:H201	17:B:809:CLA:H2	1.92	0.51
17:A:5005:CLA:H203	20:B:801:BCR:H321	1.92	0.51
17:A:5044:CLA:HBC2	6:B:586:ASN:HB2	1.93	0.51
16:T:416:CHL:HMD1	3:c:48:PRO:HG3	1.93	0.51
5:A:355:ILE:HD11	20:A:5050:BCR:H342	1.93	0.51
2:3:254:VAL:HG23	23:3:321:DGD:HA21	1.93	0.51
25:7:319:LMU:H111	17:A:5017:CLA:H62	1.93	0.51
5:A:566:LYS:NZ	6:B:674:GLU:OE2	2.40	0.51
5:A:584:CYS:HB2	6:B:668:TRP:HB3	1.91	0.51
6:B:182:GLY:HA3	17:B:813:CLA:HBB1	1.93	0.51
8:D:155:VAL:HG11	8:D:161:ASN:HB2	1.92	0.51
12:K:52:VAL:HG22	17:K:203:CLA:HBA2	1.92	0.51
13:T:134:PRO:HB2	13:T:304:ILE:HG12	1.92	0.51
6:B:457:GLU:OE1	10:F:132:HIS:ND1	2.44	0.50
17:B:839:CLA:HAA2	23:B:848:DGD:HAW1	1.92	0.50
1:1:33:ARG:HA	1:1:53:ASN:HB3	1.93	0.50
5:A:683:LEU:HB2	17:A:5004:CLA:HMC2	1.93	0.50
6:B:27:ALA:HB1	23:B:848:DGD:HB21	1.92	0.50
1:a:63:LYS:O	1:a:67:THR:OG1	2.28	0.50
14:L:103:ILE:HG22	14:L:116:GLU:HA	1.92	0.50
17:A:5014:CLA:HAA2	17:A:5026:CLA:H51	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:504:ASN:HD21	6:B:506:GLN:HB2	1.76	0.50
1:1:158:PHE:HE2	17:1:607:CLA:NC	2.08	0.50
5:A:704:HIS:HE1	17:A:5041:CLA:ND	2.08	0.50
6:B:36:ASP:OD1	6:B:36:ASP:N	2.41	0.50
4:b:138:ARG:HG3	16:b:607:CHL:HMD3	1.94	0.50
16:7:305:CHL:HBB2	16:7:306:CHL:HBB1	1.93	0.50
6:B:396:ILE:HG13	6:B:542:ALA:HB1	1.94	0.50
13:T:175:LEU:O	17:T:403:CLA:HAB	2.12	0.50
13:T:291:LYS:HG3	13:T:295:GLN:HB3	1.94	0.50
2:3:100:VAL:HG23	17:3:323:CLA:HBD	1.92	0.50
5:A:270:ALA:HA	17:A:5018:CLA:HAA2	1.93	0.50
5:A:316:TRP:HD1	12:K:85:ILE:HD11	1.76	0.50
6:B:62:THR:HG23	6:B:143:LEU:HD13	1.93	0.50
4:b:163:GLY:HA2	4:b:169:PRO:HA	1.94	0.50
1:1:81:TRP:HZ2	1:1:135:MET:HE1	1.77	0.50
5:A:374:MET:HE2	17:A:5019:CLA:HBA2	1.93	0.50
27:A:5003:CL0:H2	17:B:802:CLA:NC	2.27	0.50
17:B:808:CLA:HAB	17:B:809:CLA:HAA2	1.93	0.50
3:7:72:SER:HB2	3:7:78:ARG:HA	1.93	0.50
6:B:384:MET:HG3	17:B:825:CLA:C4C	2.42	0.50
8:D:172:ARG:NE	8:D:177:ASN:OD1	2.43	0.50
1:a:145:ASN:HD21	17:a:607:CLA:HHH	1.77	0.50
1:a:201:PRO:HG2	1:a:204:GLU:CD	2.37	0.50
3:7:73:GLU:O	3:7:78:ARG:NH2	2.44	0.50
5:A:204:GLY:HA3	17:A:5014:CLA:HBB1	1.93	0.50
17:A:5011:CLA:H192	17:A:5042:CLA:H101	1.94	0.50
17:3:308:CLA:H12	18:3:315:LUT:H24	1.92	0.49
17:B:828:CLA:H8	20:B:844:BCR:H21C	1.92	0.49
4:b:34:LEU:HD13	17:b:601:CLA:HMA3	1.94	0.49
17:3:307:CLA:H203	20:A:5049:BCR:H321	1.93	0.49
3:7:247:VAL:HG12	3:7:248:SER:H	1.77	0.49
6:B:345:ILE:HG23	17:B:818:CLA:H71	1.93	0.49
3:7:236:ASP:HB3	3:7:240:VAL:HG23	1.94	0.49
17:B:805:CLA:H42	17:B:806:CLA:HBB2	1.94	0.49
5:A:556:PHE:O	5:A:566:LYS:NZ	2.44	0.49
17:A:5032:CLA:HMA2	14:L:59:THR:CG2	2.42	0.49
3:7:195:LYS:HA	3:7:198:LYS:HE2	1.94	0.49
5:A:407:ALA:HB2	5:A:592:VAL:HG11	1.93	0.49
5:A:472:PHE:HD1	5:A:479:LEU:HD22	1.77	0.49
5:A:501:ASN:ND2	17:A:5037:CLA:OBD	2.46	0.49
10:F:67:LEU:HD22	10:F:126:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:150:LYS:HG2	1:1:154:PRO:HA	1.94	0.49
2:3:119:GLY:HA2	19:3:316:XAT:H181	1.94	0.49
3:7:183:ASP:OD1	18:7:315:LUT:O3	2.27	0.49
20:A:5048:BCR:H362	20:A:5049:BCR:H10C	1.95	0.49
4:b:95:LYS:HG3	4:b:219:ILE:HG21	1.95	0.49
5:A:28:LYS:HD2	17:A:5013:CLA:HMA2	1.94	0.49
6:B:170:LYS:NZ	6:B:329:ASN:OD1	2.46	0.49
10:F:90:ARG:HH21	10:F:104:LEU:HD21	1.77	0.49
1:1:176:LYS:HD3	17:1:611:CLA:HBA1	1.94	0.49
17:1:605:CLA:H3A	20:1:617:BCR:H21C	1.94	0.49
3:c:195:LYS:HA	3:c:198:LYS:HE2	1.95	0.49
21:1:618:LHG:HC81	21:1:618:LHG:HC5	1.41	0.49
5:A:313:ARG:HH21	5:A:321:SER:HB2	1.77	0.49
17:A:5009:CLA:HED2	17:A:5009:CLA:H11	1.95	0.49
6:B:340:ALA:HB2	20:B:847:BCR:H372	1.94	0.49
6:B:211:ASP:OD1	6:B:211:ASP:N	2.46	0.48
6:B:609:GLN:O	6:B:613:SER:CB	2.61	0.48
3:c:147:LYS:NZ	16:c:306:CHL:OMC	2.46	0.48
2:3:129:LEU:HD13	2:3:134:VAL:CG1	2.42	0.48
3:7:147:LYS:HD3	16:7:307:CHL:HHC	1.94	0.48
5:A:580:ARG:NH2	8:D:118:GLU:OE2	2.45	0.48
17:A:5018:CLA:C1D	17:A:5019:CLA:HBB2	2.44	0.48
9:E:100:TYR:HB3	9:E:104:GLU:HG3	1.96	0.48
12:K:78:LYS:NZ	17:K:204:CLA:O1A	2.43	0.48
13:T:263:LEU:HD11	17:c:309:CLA:HBB2	1.95	0.48
17:1:610:CLA:HAB	4:8:155:PHE:HE1	1.78	0.48
5:A:587:SER:O	5:A:591:HIS:ND1	2.40	0.48
5:A:681:PHE:HZ	17:A:5042:CLA:HBC2	1.77	0.48
6:B:311:PRO:HG2	6:B:316:LEU:HG	1.95	0.48
17:c:303:CLA:HHB	16:c:304:CHL:HHC	1.95	0.48
2:3:206:ASP:OD1	2:3:206:ASP:N	2.44	0.48
3:7:115:TRP:O	19:7:316:XAT:O23	2.25	0.48
6:B:86:ARG:NH1	6:B:735:GLY:O	2.46	0.48
2:3:201:LEU:HA	2:3:214:PRO:HD2	1.96	0.48
6:B:90:HIS:CD2	17:B:808:CLA:NA	2.82	0.48
5:A:189:GLU:O	5:A:193:ASN:ND2	2.47	0.48
6:B:430:LEU:CB	6:B:526:LEU:HD13	2.44	0.48
17:B:832:CLA:H3A	20:B:849:BCR:H14C	1.95	0.48
4:b:189:LEU:HD22	17:b:609:CLA:HHB	1.94	0.48
3:c:144:VAL:HG21	16:c:306:CHL:C1B	2.43	0.48
14:L:81:VAL:HG11	14:L:85:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:837:CLA:H2A	17:B:837:CLA:HED2	1.96	0.48
12:K:84:VAL:HG12	12:K:85:ILE:HG13	1.95	0.48
4:b:149:ALA:HB2	4:b:162:LYS:HB2	1.96	0.48
4:b:210:GLN:HE21	17:b:612:CLA:C4D	1.82	0.48
14:L:143:GLN:NE2	15:I:46:GLN:O	2.47	0.48
6:B:370:ALA:HB1	6:B:726:LEU:HD11	1.95	0.48
6:B:423:LEU:HB3	6:B:533:LEU:HB2	1.95	0.48
12:K:83:GLU:O	12:K:85:ILE:N	2.47	0.48
3:7:42:ASP:OD1	3:7:42:ASP:N	2.38	0.47
5:A:214:ALA:O	5:A:218:ILE:HG13	2.14	0.47
5:A:356:ASN:O	5:A:360:PHE:HB2	2.14	0.47
17:A:5008:CLA:H161	17:A:5014:CLA:H41	1.95	0.47
6:B:430:LEU:O	6:B:434:THR:OG1	2.28	0.47
7:C:16:GLN:HB3	7:C:57:ALA:HB1	1.96	0.47
9:E:54:LEU:HB2	9:E:108:PRO:HG3	1.96	0.47
1:a:109:THR:OG1	1:a:111:ASP:OD1	2.32	0.47
3:c:144:VAL:HG22	16:c:306:CHL:C4B	2.44	0.47
3:7:241:THR:OG1	3:7:242:PHE:N	2.47	0.47
17:7:304:CLA:C1B	20:7:317:BCR:H281	2.19	0.47
4:8:34:LEU:HD13	17:8:302:CLA:HMA3	1.95	0.47
5:A:572:ARG:HD2	21:A:5053:LHG:HC61	1.96	0.47
6:B:430:LEU:C	6:B:526:LEU:HD13	2.40	0.47
3:c:233:HIS:HB2	17:c:311:CLA:HAA2	1.96	0.47
5:A:736:ILE:HG22	20:A:5052:BCR:HC32	1.96	0.47
17:A:5028:CLA:H112	17:A:5028:CLA:H72	1.48	0.47
6:B:548:MET:SD	7:C:66:ARG:NH2	2.82	0.47
17:B:803:CLA:H141	17:B:810:CLA:HBC1	1.96	0.47
14:L:79:THR:HA	14:L:86:ARG:HH12	1.79	0.47
17:L:201:CLA:H62	20:L:204:BCR:H323	1.96	0.47
6:B:713:HIS:HE1	17:B:839:CLA:ND	2.13	0.47
13:T:308:ARG:HB3	16:T:401:CHL:HAC1	1.96	0.47
4:b:222:LEU:HB2	18:b:615:LUT:H21	1.96	0.47
6:B:352:HIS:CD2	17:B:826:CLA:NC	2.83	0.47
17:B:830:CLA:H43	17:B:840:CLA:H8	1.96	0.47
13:T:225:TYR:HE2	17:T:404:CLA:HAC1	1.79	0.47
20:T:415:BCR:H313	21:c:317:LHG:HC92	1.95	0.47
5:A:408:HIS:HA	5:A:411:ILE:HD12	1.96	0.47
6:B:68:HIS:HE1	17:B:807:CLA:ND	2.12	0.47
8:D:58:ASP:HB3	8:D:61:THR:HG23	1.97	0.47
1:a:33:ARG:NH1	1:a:55:ASN:OD1	2.48	0.47
17:1:612:CLA:HBC2	17:1:614:CLA:HAB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:91:SER:O	5:A:19:ARG:NH1	2.48	0.47
17:A:5009:CLA:H152	17:A:5030:CLA:HBB2	1.96	0.47
7:C:26:LEU:HA	7:C:41:SER:O	2.15	0.47
8:D:127:LEU:HB3	8:D:133:MET:HB2	1.97	0.47
10:F:67:LEU:CB	10:F:124:LEU:HD13	2.45	0.47
10:F:188:ASP:HB3	10:F:191:LEU:HB3	1.96	0.47
1:a:179:LYS:HE2	21:a:619:LHG:HC61	1.95	0.47
3:c:47:SER:HB2	3:c:50:SER:HB3	1.95	0.47
17:A:5011:CLA:HAB	17:A:5029:CLA:H13	1.97	0.47
7:C:15:THR:O	7:C:15:THR:CG2	2.63	0.47
16:a:601:CHL:H3A	16:a:601:CHL:HBA2	1.65	0.47
5:A:367:VAL:O	5:A:371:MET:HB2	2.14	0.47
17:A:5044:CLA:H41	17:A:5044:CLA:H61	1.72	0.47
6:B:278:HIS:HE1	17:B:818:CLA:NA	2.10	0.47
7:C:24:ASP:OD2	8:D:150:HIS:ND1	2.45	0.47
10:F:133:LEU:HG	10:F:148:GLU:HB3	1.97	0.47
17:b:604:CLA:CGA	16:b:605:CHL:HMD2	2.45	0.47
5:A:370:HIS:CD2	17:A:5028:CLA:NC	2.83	0.47
6:B:16:ASP:HB3	6:B:21:ARG:HB2	1.97	0.47
6:B:650:THR:HA	6:B:653:PHE:HB3	1.97	0.47
10:F:208:GLN:O	10:F:212:ASN:ND2	2.48	0.47
17:F:5004:CLA:H121	20:F:5010:BCR:H402	1.97	0.47
17:B:841:CLA:H18	14:L:98:LEU:HD11	1.97	0.46
17:7:309:CLA:HBA2	17:7:309:CLA:H3A	1.51	0.46
17:B:812:CLA:HBB2	17:B:820:CLA:H8	1.97	0.46
3:c:236:ASP:HB3	3:c:240:VAL:HG23	1.97	0.46
14:L:167:GLU:OE2	14:L:167:GLU:N	2.48	0.46
5:A:541:PHE:HE2	27:A:5003:CL0:H67	1.80	0.46
6:B:70:ALA:HB2	6:B:136:LEU:HB2	1.96	0.46
17:a:613:CLA:HBA2	17:a:613:CLA:H3A	1.79	0.46
16:3:301:CHL:H41	16:3:301:CHL:H61	1.38	0.46
17:B:825:CLA:H42	17:B:833:CLA:HBB2	1.98	0.46
8:D:124:THR:HA	8:D:135:PRO:HG2	1.97	0.46
17:b:604:CLA:C1C	20:b:617:BCR:H281	2.33	0.46
14:L:117:VAL:O	14:L:121:MET:HG3	2.15	0.46
2:3:246:MET:HE2	19:3:316:XAT:H10	1.97	0.46
17:8:303:CLA:HBA2	17:8:303:CLA:H3A	1.54	0.46
5:A:334:THR:HB	5:A:426:LEU:HD11	1.98	0.46
5:A:708:ARG:NH1	10:F:214:SER:O	2.48	0.46
10:F:206:ALA:HB1	20:F:5010:BCR:H391	1.98	0.46
13:T:237:LEU:HD11	17:c:313:CLA:CBC	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:188:SER:HB3	17:c:308:CLA:HAA2	1.97	0.46
22:3:320:SQD:H241	22:3:320:SQD:H461	1.50	0.46
3:7:115:TRP:HE3	19:7:316:XAT:H242	1.81	0.46
24:A:5001:LMG:H112	24:A:5001:LMG:HC8	1.38	0.46
17:A:5011:CLA:H143	17:A:5011:CLA:H111	1.82	0.46
3:c:75:PRO:O	3:c:79:LYS:HG2	2.15	0.46
17:3:305:CLA:H2	24:7:301:LMG:H252	1.96	0.46
5:A:304:LEU:HD21	17:A:5028:CLA:H201	1.96	0.46
5:A:393:HIS:HE1	17:A:5029:CLA:C1D	2.28	0.46
5:A:458:HIS:HE1	17:A:5035:CLA:NA	2.10	0.46
17:B:805:CLA:H112	17:B:805:CLA:HBD	1.97	0.46
17:F:5004:CLA:HBA1	20:F:5005:BCR:H362	1.98	0.46
13:T:192:ILE:HG13	13:T:193:PRO:HD2	1.96	0.46
17:a:605:CLA:HBA1	20:a:617:BCR:H21C	1.98	0.46
3:c:64:TYR:N	17:c:301:CLA:OBD	2.48	0.46
20:7:317:BCR:HC42	17:8:302:CLA:HMD1	1.98	0.46
16:c:304:CHL:HBD	16:c:304:CHL:HED2	1.61	0.46
2:3:164:THR:HG23	17:7:313:CLA:HED3	1.98	0.46
2:3:170:VAL:O	2:3:174:GLN:HB2	2.16	0.46
4:8:96:LEU:HD11	1:a:128:LEU:HD22	1.98	0.46
17:A:5007:CLA:HAA1	17:A:5013:CLA:H51	1.96	0.46
6:B:430:LEU:HD11	17:B:836:CLA:HMB1	1.97	0.46
3:c:115:TRP:O	19:c:315:XAT:O23	2.28	0.46
3:c:184:PRO:HB2	3:c:185:MET:HE3	1.97	0.46
13:T:309:LEU:HD12	18:T:413:LUT:H403	1.98	0.46
20:3:318:BCR:H403	20:A:5048:BCR:H402	1.98	0.45
4:8:106:GLU:HA	16:8:307:CHL:HED2	1.98	0.45
17:A:5011:CLA:H61	17:A:5011:CLA:H101	1.72	0.45
17:A:5012:CLA:O1A	20:J:104:BCR:H14C	2.16	0.45
17:B:802:CLA:H161	17:B:802:CLA:H122	1.63	0.45
4:b:29:MET:SD	4:b:29:MET:N	2.83	0.45
4:b:120:PHE:CE1	16:b:606:CHL:HBC2	2.50	0.45
17:1:605:CLA:H3A	20:1:617:BCR:C21	2.47	0.45
2:3:78:TYR:HB2	16:3:301:CHL:HMD1	1.97	0.45
2:3:81:ASP:OD1	19:3:316:XAT:O23	2.34	0.45
17:A:5005:CLA:H122	20:B:801:BCR:H12C	1.98	0.45
3:c:190:ASN:HD21	3:c:193:SER:HB2	1.81	0.45
3:7:115:TRP:HH2	3:7:216:ILE:HG12	1.82	0.45
25:7:319:LMU:H82	5:A:161:SER:HA	1.98	0.45
5:A:239:LEU:N	5:A:242:GLU:OE1	2.49	0.45
6:B:183:LEU:HD21	17:B:813:CLA:HAA1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:335:LEU:HD11	17:B:829:CLA:HBB1	1.98	0.45
6:B:375:HIS:HB2	17:B:827:CLA:C1B	2.47	0.45
6:B:525:ALA:HB2	17:B:836:CLA:HMA1	1.98	0.45
6:B:653:PHE:O	6:B:657:VAL:HG23	2.15	0.45
17:B:806:CLA:HHB	17:B:829:CLA:HAB	1.99	0.45
17:B:826:CLA:H2A	17:B:826:CLA:HED2	1.98	0.45
13:T:263:LEU:HD12	20:T:415:BCR:H343	1.98	0.45
17:B:838:CLA:H8	17:B:839:CLA:H121	1.99	0.45
2:3:103:ARG:HH21	22:3:320:SQD:H62	1.82	0.45
17:3:305:CLA:HBB2	17:A:5017:CLA:CHD	2.46	0.45
5:A:368:ALA:HB2	5:A:394:HIS:HB2	1.97	0.45
16:T:416:CHL:HBB2	17:c:301:CLA:HAC2	1.97	0.45
1:a:80:ARG:O	1:a:84:LEU:HD22	2.16	0.45
2:3:159:TRP:NE1	17:3:304:CLA:OBD	2.48	0.45
17:7:303:CLA:HED3	17:7:303:CLA:H11	1.99	0.45
17:7:312:CLA:H152	17:7:312:CLA:H112	1.79	0.45
17:8:309:CLA:HBA2	17:8:309:CLA:H3A	1.57	0.45
17:A:5008:CLA:HBC2	17:A:5031:CLA:HMA1	1.99	0.45
8:D:89:SER:OG	8:D:91:LYS:O	2.34	0.45
1:1:218:PHE:HE1	17:1:613:CLA:HED3	1.82	0.45
8:D:89:SER:HA	8:D:133:MET:HE1	1.97	0.45
8:D:153:ASP:OD1	8:D:153:ASP:N	2.44	0.45
3:7:107:LYS:HZ1	3:7:228:ASP:HA	1.82	0.45
23:8:301:DGD:HA21	23:8:301:DGD:HG12	1.65	0.45
5:A:114:SER:HB2	5:A:131:VAL:HG11	1.99	0.45
17:A:5020:CLA:H92	17:A:5030:CLA:H91	1.98	0.45
17:A:5027:CLA:HMA1	20:A:5051:BCR:H16C	1.98	0.45
3:c:90:ARG:HA	3:c:93:MET:HE2	1.99	0.45
3:c:144:VAL:HG22	16:c:306:CHL:C2B	2.46	0.45
16:8:306:CHL:H3A	20:8:318:BCR:C21	2.47	0.45
6:B:588:ILE:HA	6:B:591:VAL:HG22	1.97	0.45
17:T:408:CLA:C3B	18:T:413:LUT:H10	2.47	0.45
17:A:5019:CLA:H102	17:A:5037:CLA:HBA1	1.98	0.45
17:A:5034:CLA:H193	28:B:842:PQN:H272	1.98	0.45
6:B:609:GLN:O	6:B:613:SER:HB3	2.17	0.45
3:c:81:MET:HA	3:c:81:MET:HE3	1.99	0.45
1:1:87:ALA:HB2	18:1:615:LUT:C34	2.46	0.44
16:1:601:CHL:HBA1	16:1:601:CHL:H3A	1.67	0.44
3:7:136:THR:HG23	17:8:314:CLA:HAA2	1.98	0.44
25:7:319:LMU:H71	5:A:164:ILE:HG21	1.98	0.44
5:A:657:VAL:CG2	5:A:745:ALA:HB3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:5003:CL0:H51	27:A:5003:CL0:H58	1.53	0.44
17:B:836:CLA:H121	20:F:5010:BCR:H323	1.98	0.44
13:T:168:ILE:HG21	13:T:247:ARG:HH12	1.82	0.44
3:c:138:LEU:O	17:c:307:CLA:CBB	2.37	0.44
5:A:650:LEU:HD22	27:A:5003:CL0:H26	2.00	0.44
6:B:212:ASN:O	6:B:215:SER:OG	2.34	0.44
17:B:811:CLA:H3A	17:B:811:CLA:HBA2	1.51	0.44
2:3:156:LYS:HE3	2:3:156:LYS:HB3	1.81	0.44
5:A:692:TYR:OH	17:A:5004:CLA:OBD	2.26	0.44
17:B:828:CLA:H3A	17:B:828:CLA:HBA2	1.40	0.44
4:b:95:LYS:HA	4:b:95:LYS:HD3	1.73	0.44
2:3:83:LEU:HD13	17:3:324:CLA:H52	2.00	0.44
5:A:695:GLU:OE2	6:B:551:LYS:NZ	2.37	0.44
17:A:5029:CLA:H193	20:J:103:BCR:H14C	1.99	0.44
17:B:803:CLA:H62	17:B:803:CLA:H41	1.54	0.44
7:C:7:ILE:HG21	7:C:40:ALA:HB3	1.98	0.44
10:F:169:GLN:HB3	10:F:195:LEU:HD22	1.99	0.44
5:A:169:LEU:HD21	17:A:5014:CLA:H62	1.99	0.44
17:A:5010:CLA:C4D	25:A:5054:LMU:H62	2.48	0.44
8:D:159:LYS:HA	8:D:159:LYS:HD2	1.77	0.44
3:7:178:PRO:HG3	16:7:307:CHL:HMD2	1.99	0.44
5:A:445:SER:HB3	5:A:545:VAL:HG22	1.98	0.44
17:A:5005:CLA:H93	17:B:839:CLA:HBB2	2.00	0.44
10:F:159:VAL:O	10:F:163:ILE:HG12	2.17	0.44
16:b:606:CHL:HMC	16:b:606:CHL:HBC3	2.00	0.44
17:1:604:CLA:C1B	20:1:617:BCR:H271	2.48	0.44
2:3:276:LEU:N	17:3:311:CLA:O1A	2.50	0.44
6:B:379:ILE:O	6:B:383:ILE:HG12	2.18	0.44
17:B:807:CLA:H2A	17:B:809:CLA:HED1	2.00	0.44
8:D:86:THR:HG22	8:D:111:LEU:HD12	1.99	0.44
10:F:156:PHE:HZ	17:F:5004:CLA:NA	2.12	0.44
1:a:165:LYS:HA	1:a:165:LYS:HD3	1.73	0.44
2:3:149:ILE:HG22	2:3:152:ALA:H	1.83	0.44
17:8:313:CLA:H11	17:8:313:CLA:H51	1.77	0.44
5:A:289:LEU:HD12	5:A:376:PRO:HB3	2.00	0.44
6:B:655:HIS:CD2	17:B:802:CLA:NB	2.86	0.44
17:B:807:CLA:H11	17:B:807:CLA:H51	1.84	0.44
13:T:318:MET:HE2	17:T:405:CLA:HMA1	2.00	0.44
1:a:201:PRO:HG2	1:a:204:GLU:CG	2.47	0.44
17:a:604:CLA:HBB1	20:a:617:BCR:H23C	2.00	0.44
17:1:612:CLA:H12	17:1:612:CLA:HBA1	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:91:MET:HE3	5:A:91:MET:HA	2.00	0.44
17:A:5036:CLA:H51	17:A:5036:CLA:H11	1.82	0.44
1:a:136:ALA:HA	17:a:608:CLA:HAB	2.00	0.44
3:c:144:VAL:CG2	16:c:306:CHL:C2B	2.95	0.44
2:3:193:GLN:NE2	16:3:322:CHL:HMD3	2.33	0.43
17:3:307:CLA:H122	17:3:307:CLA:H8	1.83	0.43
17:8:315:CLA:HBA1	17:8:315:CLA:H3A	1.61	0.43
5:A:206:LEU:HD11	17:A:5030:CLA:H192	2.00	0.43
5:A:375:PRO:HG2	5:A:381:ALA:HB2	1.99	0.43
5:A:598:TRP:HE1	17:B:803:CLA:C1D	2.31	0.43
5:A:685:PHE:HA	28:A:5045:PQN:H9	1.99	0.43
6:B:692:VAL:HG21	17:B:841:CLA:HMB1	2.00	0.43
8:D:131:PHE:HB2	8:D:133:MET:HG2	2.00	0.43
1:a:146:GLN:OE1	1:a:146:GLN:N	2.51	0.43
16:3:301:CHL:H102	17:3:324:CLA:H93	1.98	0.43
16:3:301:CHL:HBA2	16:3:301:CHL:H3A	1.61	0.43
6:B:342:VAL:O	6:B:346:THR:HG22	2.19	0.43
20:B:801:BCR:H14C	17:B:839:CLA:HBB1	2.00	0.43
17:c:301:CLA:H3A	17:c:301:CLA:HBA2	1.63	0.43
17:8:304:CLA:HBC3	19:8:317:XAT:H11	1.99	0.43
17:A:5042:CLA:HAC2	20:F:5005:BCR:H342	2.00	0.43
17:A:5044:CLA:H2	20:A:5052:BCR:H362	2.00	0.43
6:B:173:GLU:HG3	6:B:302:LEU:HD23	1.99	0.43
6:B:348:LEU:HG	17:B:818:CLA:H41	1.99	0.43
6:B:593:PHE:HE2	17:B:802:CLA:H72	1.81	0.43
5:A:658:ILE:HB	6:B:622:ARG:HB2	1.99	0.43
17:A:5012:CLA:HAB	17:B:832:CLA:HMD2	2.00	0.43
17:A:5019:CLA:H41	17:A:5019:CLA:H61	1.66	0.43
17:A:5029:CLA:H162	17:A:5029:CLA:H203	1.79	0.43
17:A:5035:CLA:H61	17:A:5035:CLA:H92	1.76	0.43
20:A:5050:BCR:H24C	20:A:5050:BCR:H371	1.87	0.43
6:B:411:ARG:O	6:B:415:HIS:ND1	2.51	0.43
6:B:696:ASP:OD1	6:B:696:ASP:N	2.42	0.43
20:K:205:BCR:H20C	20:K:205:BCR:H361	1.82	0.43
3:c:163:PHE:CZ	16:c:306:CHL:HBB2	2.53	0.43
3:c:205:GLY:O	3:c:209:MET:HG2	2.19	0.43
1:1:128:LEU:HD23	1:1:128:LEU:HA	1.87	0.43
5:A:34:HIS:CE1	17:A:5013:CLA:HAA1	2.53	0.43
21:A:5002:LHG:HC81	21:A:5002:LHG:HC5	1.72	0.43
20:A:5052:BCR:H20C	20:A:5052:BCR:H361	1.87	0.43
20:F:5010:BCR:H24C	20:F:5010:BCR:H371	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:95:LYS:CG	4:b:219:ILE:HG21	2.49	0.43
17:7:308:CLA:HBA1	17:7:308:CLA:H3A	1.79	0.43
4:8:172:ILE:HD12	4:8:172:ILE:HA	1.87	0.43
5:A:215:GLY:HA3	17:A:5016:CLA:HAB	2.01	0.43
27:A:5003:CL0:H8	17:B:802:CLA:CAB	2.49	0.43
17:A:5029:CLA:H13	17:A:5029:CLA:H102	1.63	0.43
6:B:430:LEU:HB2	6:B:526:LEU:HD13	1.99	0.43
17:c:308:CLA:H3A	17:c:308:CLA:HBA2	1.75	0.43
1:1:142:ARG:NH1	17:1:607:CLA:O1D	2.51	0.43
5:A:676:HIS:HD2	27:A:5003:CL0:H6	1.84	0.43
5:A:706:LYS:HE3	10:F:216:LEU:HD12	2.00	0.43
17:A:5015:CLA:H12	17:A:5017:CLA:HMB1	2.00	0.43
17:A:5019:CLA:HAC1	17:A:5036:CLA:H42	2.00	0.43
17:A:5028:CLA:H121	17:A:5036:CLA:H101	2.01	0.43
17:A:5029:CLA:H3A	17:A:5029:CLA:HBA2	1.75	0.43
17:A:5032:CLA:HBB1	21:A:5055:LHG:H301	2.00	0.43
17:B:804:CLA:HBC2	20:L:203:BCR:HC21	2.01	0.43
8:D:87:TRP:HH2	8:D:112:LEU:HD12	1.84	0.43
13:T:212:LEU:O	13:T:214:ALA:N	2.51	0.43
1:a:61:LEU:HD12	19:a:616:XAT:H163	2.00	0.43
3:c:94:LEU:HB3	17:c:303:CLA:HBB2	2.01	0.43
17:7:303:CLA:H12	17:7:303:CLA:H2A	2.01	0.43
5:A:183:LYS:HA	5:A:183:LYS:HD2	1.90	0.43
5:A:374:MET:HE1	17:A:5028:CLA:HHC	2.01	0.43
13:T:149:ASP:O	13:T:155:ASN:ND2	2.50	0.43
17:b:601:CLA:HBA2	17:b:601:CLA:H3A	1.76	0.43
17:b:602:CLA:H3A	17:b:602:CLA:HBA2	1.64	0.43
3:c:122:ALA:HB3	16:c:304:CHL:HAC1	2.01	0.43
17:3:324:CLA:NA	5:A:200:HIS:HE1	2.12	0.43
5:A:622:VAL:HG22	5:A:627:VAL:HG22	2.01	0.43
17:A:5010:CLA:H42	17:J:102:CLA:HAC1	1.99	0.43
17:A:5016:CLA:H92	17:A:5016:CLA:H61	1.83	0.43
8:D:51:PRO:HB2	8:D:52:TRP:H	1.67	0.43
10:F:95:GLU:HG2	10:F:98:SER:HB2	2.01	0.43
1:a:143:ASN:O	1:a:151:ARG:NH2	2.39	0.43
3:c:187:MET:HG2	17:c:308:CLA:HBA1	2.01	0.43
17:3:309:CLA:HHB	13:T:157:MET:HE2	2.00	0.43
5:A:197:MET:HB2	17:A:5014:CLA:HBC2	2.00	0.43
5:A:299:LEU:HG	17:A:5018:CLA:HAB	2.01	0.43
5:A:367:VAL:HG11	17:A:5030:CLA:HMD3	2.01	0.43
17:A:5011:CLA:H191	11:J:19:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:200:ILE:HG13	6:B:271:LEU:HB3	2.01	0.43
6:B:249:ASP:OD1	6:B:249:ASP:N	2.50	0.43
6:B:349:VAL:HA	17:B:818:CLA:H42	2.00	0.43
6:B:575:ASP:OD1	6:B:707:ARG:NH1	2.51	0.43
6:B:644:LEU:HA	6:B:647:TRP:HD1	1.84	0.43
22:3:320:SQD:H45	22:3:320:SQD:H81	1.51	0.42
5:A:49:ILE:O	5:A:52:LEU:HB3	2.19	0.42
6:B:601:THR:HG21	6:B:610:PHE:HB2	2.00	0.42
17:B:819:CLA:HMD3	17:B:822:CLA:HHD	2.00	0.42
10:F:133:LEU:HD23	10:F:149:VAL:HG13	1.99	0.42
21:a:618:LHG:HC81	21:a:618:LHG:HC5	1.38	0.42
2:3:264:LEU:HB2	18:3:315:LUT:H21	2.00	0.42
5:A:146:GLN:HB3	5:A:377:TYR:HB3	2.01	0.42
5:A:730:HIS:HE1	17:A:5042:CLA:ND	2.16	0.42
6:B:180:LEU:HD23	6:B:180:LEU:HA	1.90	0.42
17:B:820:CLA:H3A	17:B:820:CLA:HBA2	1.49	0.42
17:B:829:CLA:H141	17:B:829:CLA:H161	1.85	0.42
5:A:562:LEU:HD21	5:A:583:THR:HG22	2.01	0.42
6:B:613:SER:OG	6:B:623:ASP:OD2	2.36	0.42
17:B:829:CLA:H151	17:B:829:CLA:H111	1.77	0.42
8:D:68:GLY:HA3	14:L:57:LEU:HA	2.01	0.42
17:K:202:CLA:HBA1	17:K:202:CLA:H3A	1.70	0.42
17:T:410:CLA:HMB2	18:T:413:LUT:H382	2.00	0.42
3:c:144:VAL:CG1	16:c:306:CHL:C4B	2.64	0.42
3:c:185:MET:HE3	3:c:185:MET:H	1.84	0.42
14:L:134:LEU:HD23	14:L:173:ALA:HA	2.01	0.42
1:1:56:PHE:CZ	16:1:601:CHL:HAB	2.54	0.42
2:3:170:VAL:HG23	17:3:307:CLA:HBB2	2.02	0.42
20:3:318:BCR:H21C	17:A:5016:CLA:H62	2.02	0.42
5:A:75:SER:OG	17:A:5013:CLA:HHD	2.19	0.42
17:A:5018:CLA:H122	17:A:5018:CLA:H8	1.92	0.42
17:B:816:CLA:C1D	17:B:817:CLA:HBB2	2.50	0.42
20:B:849:BCR:HC42	11:J:36:PRO:HB3	2.01	0.42
20:F:5005:BCR:H20C	20:F:5005:BCR:H361	1.90	0.42
17:F:5007:CLA:HBA1	17:F:5007:CLA:H3A	1.63	0.42
17:a:604:CLA:CBB	20:a:617:BCR:H23C	2.49	0.42
17:c:301:CLA:H143	17:c:301:CLA:H161	1.89	0.42
2:3:268:LEU:HD22	17:3:312:CLA:HAB	2.02	0.42
5:A:407:ALA:HA	5:A:592:VAL:HG21	2.01	0.42
17:A:5004:CLA:H71	6:B:432:PHE:HE1	1.84	0.42
6:B:584:MET:HB3	6:B:584:MET:HE3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:809:CLA:HBA2	17:B:809:CLA:H12	1.74	0.42
17:B:818:CLA:H3A	17:B:818:CLA:HBA2	1.35	0.42
20:B:843:BCR:H20C	20:B:843:BCR:H361	1.87	0.42
16:c:304:CHL:CBC	16:c:305:CHL:HHD	2.48	0.42
2:3:167:PHE:HA	2:3:170:VAL:HG12	2.00	0.42
2:3:276:LEU:HD22	17:3:311:CLA:H2	2.00	0.42
3:7:123:ILE:HG23	16:7:305:CHL:HBC1	2.02	0.42
5:A:261:LEU:HD21	20:A:5047:BCR:HC42	2.01	0.42
5:A:432:ARG:O	8:D:70:THR:OG1	2.24	0.42
17:A:5034:CLA:H102	17:A:5034:CLA:H62	1.80	0.42
17:B:826:CLA:H192	17:B:826:CLA:H162	1.83	0.42
17:T:406:CLA:H3A	17:T:406:CLA:HBA2	1.72	0.42
1:a:61:LEU:HD23	1:a:61:LEU:HA	1.87	0.42
1:a:76:LEU:HD12	1:a:152:LEU:HD21	1.84	0.42
17:b:609:CLA:H11	17:b:609:CLA:H52	1.78	0.42
3:7:241:THR:HG23	3:7:243:ALA:H	1.83	0.42
17:7:312:CLA:H121	17:7:312:CLA:HAB	2.01	0.42
17:8:310:CLA:H12	18:8:316:LUT:H26	2.02	0.42
5:A:684:MET:HE1	17:A:5004:CLA:C4A	2.42	0.42
17:A:5013:CLA:H61	17:A:5013:CLA:H41	1.73	0.42
6:B:176:LEU:HD21	17:B:819:CLA:HMA3	2.01	0.42
6:B:398:ASP:HA	8:D:181:ILE:HB	2.01	0.42
17:B:829:CLA:H72	23:B:848:DGD:HA92	2.02	0.42
12:K:78:LYS:HE2	12:K:78:LYS:HB2	1.90	0.42
3:c:131:GLY:H	3:c:134:ILE:HD12	1.84	0.42
4:8:155:PHE:HE2	20:8:318:BCR:H343	1.84	0.42
5:A:577:GLY:HA2	6:B:562:GLY:HA2	2.01	0.42
6:B:460:PHE:HE1	10:F:136:ASP:HB2	1.85	0.42
17:B:807:CLA:H62	20:I:4001:BCR:H282	2.01	0.42
17:B:817:CLA:H12	17:B:817:CLA:H52	1.83	0.42
17:B:839:CLA:HHD	28:B:842:PQN:H171	2.00	0.42
16:b:605:CHL:HAA1	20:b:617:BCR:C21	2.49	0.42
2:3:243:MET:HE1	16:3:301:CHL:HHC	2.00	0.42
17:A:5018:CLA:CHD	17:A:5019:CLA:HBB2	2.49	0.42
6:B:527:GLY:HA2	6:B:583:TRP:HZ3	1.84	0.42
11:J:31:ARG:HD3	20:J:104:BCR:H332	2.01	0.42
1:a:152:LEU:HD23	1:a:152:LEU:HA	1.84	0.42
2:3:135:ILE:HD13	2:3:135:ILE:HA	1.96	0.42
2:3:243:MET:CE	16:3:301:CHL:HHC	2.50	0.42
5:A:434:ARG:NH1	5:A:555:LEU:O	2.45	0.42
5:A:514:VAL:HG22	5:A:524:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:5017:CLA:H2A	17:A:5017:CLA:HED2	2.02	0.42
20:B:846:BCR:H24C	20:B:846:BCR:H371	1.88	0.42
20:B:849:BCR:H361	20:B:849:BCR:H20C	1.86	0.42
3:c:89:ALA:O	3:c:93:MET:HG2	2.20	0.42
3:c:221:ALA:HA	3:c:247:VAL:HG12	2.01	0.42
17:c:301:CLA:HBB1	17:c:301:CLA:H51	2.01	0.42
15:I:48:GLU:O	15:I:49:LYS:C	2.63	0.42
1:1:84:LEU:HB3	17:1:604:CLA:HAB	2.01	0.41
17:1:604:CLA:HMA2	17:1:605:CLA:HBC3	2.01	0.41
3:7:97:ALA:HB2	18:7:315:LUT:H15	2.02	0.41
24:7:301:LMG:H321	17:A:5017:CLA:H2	2.01	0.41
4:8:191:LEU:HD11	4:8:195:LYS:HE3	2.02	0.41
5:A:361:GLY:HA2	5:A:398:GLY:HA2	2.02	0.41
5:A:422:ASN:OD1	5:A:425:ASN:ND2	2.51	0.41
5:A:542:THR:HB	5:A:602:SER:HB2	2.01	0.41
12:K:51:MET:HE3	12:K:51:MET:HB2	1.99	0.41
3:7:71:LEU:HD12	19:7:316:XAT:H3	2.01	0.41
5:A:452:SER:HB2	5:A:538:ILE:HG12	2.02	0.41
5:A:601:ASN:ND2	27:A:5003:CL0:H37	2.35	0.41
17:A:5008:CLA:H193	17:A:5014:CLA:H61	2.02	0.41
6:B:291:MET:HE2	6:B:291:MET:HB3	1.92	0.41
17:B:803:CLA:HED2	17:B:803:CLA:HBD	1.82	0.41
17:B:817:CLA:HBA2	17:B:817:CLA:H3A	1.82	0.41
17:B:826:CLA:H161	20:B:847:BCR:H17C	2.03	0.41
7:C:31:TRP:HZ2	8:D:171:MET:HE1	1.84	0.41
4:b:192:LYS:HG2	17:b:611:CLA:HBD	2.02	0.41
1:1:100:TRP:O	19:1:616:XAT:O23	2.34	0.41
16:7:305:CHL:H3A	20:7:317:BCR:C21	2.50	0.41
20:8:318:BCR:H24C	20:8:318:BCR:H371	1.94	0.41
5:A:747:ILE:HD12	5:A:747:ILE:HA	1.89	0.41
17:A:5004:CLA:H41	17:A:5004:CLA:H62	1.74	0.41
17:A:5007:CLA:HBA1	17:A:5007:CLA:H3A	1.80	0.41
17:A:5019:CLA:H141	17:A:5028:CLA:H203	2.01	0.41
6:B:708:LEU:HD23	23:B:848:DGD:HA21	2.02	0.41
17:b:613:CLA:H2A	3:c:136:THR:HG22	2.01	0.41
17:c:307:CLA:HBA2	17:c:307:CLA:H3A	1.51	0.41
17:c:308:CLA:H91	17:c:308:CLA:H111	1.86	0.41
20:3:319:BCR:H20C	20:3:319:BCR:H361	1.91	0.41
17:8:305:CLA:CGA	16:8:306:CHL:HMD2	2.50	0.41
17:8:310:CLA:CBB	17:8:312:CLA:H3A	2.51	0.41
8:D:159:LYS:O	8:D:164:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:16:LEU:HD11	20:J:104:BCR:H19C	2.03	0.41
13:T:260:GLN:NE2	16:T:416:CHL:HMD3	2.35	0.41
2:3:79:GLY:N	16:3:301:CHL:OBD	2.53	0.41
2:3:281:GLY:HA3	5:A:262:ALA:HB2	2.02	0.41
5:A:322:ILE:HG23	17:A:5022:CLA:HED3	2.02	0.41
17:B:823:CLA:O1A	20:B:846:BCR:H14C	2.21	0.41
12:K:107:HIS:CG	20:K:205:BCR:H12C	2.54	0.41
1:a:101:TYR:CZ	16:a:606:CHL:HMA2	2.56	0.41
1:a:217:ASN:ND2	4:b:122:THR:OG1	2.45	0.41
17:b:614:CLA:HBA1	17:b:614:CLA:H3A	1.71	0.41
20:L:203:BCR:H20C	20:L:203:BCR:H361	1.88	0.41
17:8:305:CLA:C4B	20:8:318:BCR:H281	2.29	0.41
17:A:5009:CLA:H43	21:A:5053:LHG:H282	2.01	0.41
17:A:5022:CLA:H162	17:A:5022:CLA:H141	1.88	0.41
6:B:138:VAL:HA	6:B:141:VAL:HG12	2.02	0.41
6:B:345:ILE:HG12	17:B:818:CLA:H71	2.03	0.41
6:B:366:PHE:HB3	6:B:603:TRP:CZ3	2.56	0.41
23:B:848:DGD:HB21	23:B:848:DGD:HG2	1.67	0.41
4:b:216:LYS:HE2	4:b:216:LYS:HB2	1.79	0.41
14:L:171:LYS:HD3	14:L:171:LYS:HA	1.82	0.41
2:3:195:PHE:HA	20:3:317:BCR:H333	1.68	0.41
3:7:231:VAL:HA	3:7:234:VAL:HG22	2.01	0.41
17:7:312:CLA:H3A	17:7:312:CLA:HBA2	1.88	0.41
17:8:305:CLA:HBA1	16:8:306:CHL:HMD2	2.01	0.41
5:A:277:THR:OG1	5:A:293:ASP:OD1	2.35	0.41
5:A:361:GLY:O	5:A:365:ILE:HG12	2.21	0.41
6:B:293:ARG:HA	6:B:299:GLY:HA3	2.01	0.41
14:L:108:LEU:HD23	14:L:118:VAL:HG11	2.03	0.41
14:L:130:LEU:HD23	14:L:130:LEU:HA	1.90	0.41
1:1:115:TRP:CD1	17:1:604:CLA:H12	2.55	0.41
20:1:617:BCR:H24C	20:1:617:BCR:H21C	1.88	0.41
16:3:322:CHL:H142	16:3:322:CHL:H111	1.86	0.41
5:A:491:HIS:HE1	17:A:5036:CLA:NB	2.18	0.41
5:A:673:LEU:HD23	5:A:673:LEU:HA	1.87	0.41
6:B:458:PRO:HB3	6:B:518:PHE:HB2	2.03	0.41
6:B:528:LEU:HD23	6:B:587:THR:HG21	2.03	0.41
6:B:548:MET:HG3	6:B:571:ILE:HD13	2.02	0.41
16:T:401:CHL:H11	19:T:414:XAT:H363	2.03	0.41
20:a:617:BCR:H20C	20:a:617:BCR:H361	1.89	0.41
1:1:127:ILE:HA	1:1:130:VAL:HG12	2.03	0.41
18:1:615:LUT:H31	18:1:615:LUT:H391	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:182:GLN:HA	2:3:185:LYS:HE2	2.02	0.41
3:7:184:PRO:HD2	18:7:315:LUT:H22	2.01	0.41
17:7:302:CLA:H72	19:7:316:XAT:H10	2.02	0.41
4:8:225:HIS:CG	17:8:313:CLA:HAA2	2.56	0.41
16:8:308:CHL:HED2	16:8:308:CHL:HBD	1.63	0.41
17:8:311:CLA:O2A	17:a:608:CLA:H3A	2.21	0.41
5:A:305:PHE:HZ	17:A:5020:CLA:H112	1.86	0.41
5:A:322:ILE:HG21	17:A:5026:CLA:HAC1	2.02	0.41
5:A:443:TRP:CE2	17:A:5033:CLA:HAB	2.56	0.41
17:A:5007:CLA:H11	17:A:5007:CLA:H52	1.79	0.41
17:A:5017:CLA:H51	17:A:5017:CLA:H8	1.93	0.41
17:A:5024:CLA:HHB	17:A:5043:CLA:HBC3	2.02	0.41
17:A:5029:CLA:H72	17:A:5029:CLA:H111	1.86	0.41
6:B:31:ASP:HB2	17:B:829:CLA:HAA2	2.03	0.41
6:B:398:ASP:OD1	6:B:398:ASP:O	2.39	0.41
6:B:444:VAL:HG11	6:B:453:GLN:N	2.36	0.41
6:B:520:VAL:HG21	6:B:594:TYR:HB2	2.03	0.41
6:B:723:ALA:HB2	17:B:827:CLA:HBB1	2.02	0.41
17:B:802:CLA:H2	17:B:802:CLA:H62	1.79	0.41
12:K:100:LEU:HD23	12:K:100:LEU:HA	1.90	0.41
13:T:234:PHE:HB3	17:c:312:CLA:HED3	2.02	0.41
1:a:148:MET:HA	1:a:148:MET:HE3	2.02	0.41
17:a:612:CLA:HBA1	17:a:612:CLA:H12	1.84	0.41
3:c:141:PHE:HB3	17:c:307:CLA:CHC	2.51	0.41
3:c:142:GLY:HA2	17:c:307:CLA:C2B	2.48	0.41
17:c:312:CLA:HED2	17:c:312:CLA:HBD	1.75	0.41
1:1:148:MET:HA	1:1:148:MET:HE3	2.02	0.41
2:3:181:LEU:HD21	22:3:320:SQD:H82	2.03	0.41
17:B:803:CLA:H8	17:B:803:CLA:H122	1.74	0.41
17:B:821:CLA:HAA2	20:B:843:BCR:H282	2.03	0.41
13:T:332:LEU:HD22	18:T:413:LUT:H24	1.64	0.41
16:b:607:CHL:HMA1	20:b:617:BCR:H362	2.03	0.41
1:1:69:GLN:HA	1:1:72:ARG:HD3	2.03	0.40
1:1:101:TYR:CZ	16:1:606:CHL:HED3	2.56	0.40
2:3:178:LEU:HD23	2:3:178:LEU:HA	1.92	0.40
3:7:121:GLU:HA	3:7:124:LYS:HB2	2.03	0.40
3:7:218:GLN:NE2	17:7:312:CLA:C4D	2.80	0.40
4:8:88:LEU:O	4:8:92:LEU:N	2.40	0.40
5:A:55:ASP:OD2	21:A:5053:LHG:O1	2.36	0.40
5:A:204:GLY:O	5:A:208:LEU:HB2	2.21	0.40
5:A:330:LYS:HA	5:A:337:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:666:SER:HB2	6:B:446:ALA:HB1	2.03	0.40
1:a:218:PHE:CD1	17:a:612:CLA:H2	2.56	0.40
17:b:602:CLA:H41	17:b:602:CLA:H62	1.86	0.40
16:b:605:CHL:HMB2	20:b:617:BCR:H373	2.03	0.40
3:c:74:GLU:HB3	3:c:77:MET:HB2	2.04	0.40
3:7:148:ARG:NH1	17:7:308:CLA:O1D	2.50	0.40
17:B:841:CLA:H151	20:L:204:BCR:H17C	2.03	0.40
4:b:82:MET:HA	4:b:82:MET:HE3	2.02	0.40
4:8:82:MET:HE3	4:8:82:MET:HA	2.04	0.40
4:8:120:PHE:CD1	16:8:307:CHL:HMD2	2.55	0.40
4:8:150:GLU:HA	4:8:151:PRO:HD3	1.98	0.40
5:A:261:LEU:HD12	5:A:261:LEU:HA	1.93	0.40
17:A:5004:CLA:H143	28:A:5045:PQN:H28	2.03	0.40
17:B:808:CLA:H3A	17:B:808:CLA:HBA2	1.75	0.40
10:F:187:LEU:HD12	11:J:14:VAL:HG21	2.02	0.40
18:a:615:LUT:H31	18:a:615:LUT:H391	1.92	0.40
20:I:4001:BCR:H20C	20:I:4001:BCR:H361	1.86	0.40
1:1:124:ILE:HD12	1:1:125:ALA:N	2.36	0.40
20:3:317:BCR:H20C	20:3:317:BCR:H361	1.95	0.40
3:7:233:HIS:CD2	17:7:313:CLA:NC	2.89	0.40
6:B:423:LEU:HD23	6:B:423:LEU:HA	1.93	0.40
17:B:818:CLA:H161	17:B:818:CLA:H141	1.89	0.40
8:D:62:PRO:HB2	8:D:106:ARG:HD2	2.03	0.40
9:E:48:GLY:HA3	9:E:74:VAL:HG11	2.04	0.40
17:T:409:CLA:H12	17:T:409:CLA:HBA1	1.77	0.40
1:a:87:ALA:HB2	18:a:615:LUT:H34	2.03	0.40
3:c:115:TRP:HH2	3:c:216:ILE:HG22	1.85	0.40
17:c:302:CLA:HBC1	16:c:305:CHL:HBB2	2.03	0.40
17:L:201:CLA:H51	20:L:204:BCR:HC21	2.03	0.40
1:1:124:ILE:H	1:1:124:ILE:HG13	1.71	0.40
2:3:124:ILE:HD13	2:3:124:ILE:HA	1.79	0.40
17:3:302:CLA:OBD	17:3:307:CLA:H2	2.21	0.40
17:3:307:CLA:HHB	17:3:314:CLA:HBC2	2.04	0.40
5:A:453:PHE:CE1	17:A:5005:CLA:HHB	2.56	0.40
5:A:677:PHE:CG	20:A:5052:BCR:H363	2.57	0.40
5:A:720:ILE:H	5:A:720:ILE:HG13	1.64	0.40
6:B:9:PHE:HB2	6:B:35:HIS:CG	2.57	0.40
10:F:217:GLU:HB3	10:F:222:ILE:HD11	2.04	0.40
1:a:163:PHE:N	17:a:609:CLA:O1A	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/228 (86%)	187 (96%)	7 (4%)	1 (0%)	24	55
1	a	195/228 (86%)	184 (94%)	9 (5%)	2 (1%)	12	38
2	3	224/286 (78%)	213 (95%)	11 (5%)	0	100	100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100	100
3	c	207/255 (81%)	201 (97%)	6 (3%)	0	100	100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100	100
4	b	222/254 (87%)	217 (98%)	5 (2%)	0	100	100
5	A	738/751 (98%)	715 (97%)	23 (3%)	0	100	100
6	B	732/735 (100%)	711 (97%)	21 (3%)	0	100	100
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	141/193 (73%)	131 (93%)	10 (7%)	0	100	100
9	E	65/111 (59%)	62 (95%)	3 (5%)	0	100	100
10	F	163/227 (72%)	154 (94%)	9 (6%)	0	100	100
11	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
12	K	81/123 (66%)	72 (89%)	9 (11%)	0	100	100
13	T	208/350 (59%)	200 (96%)	8 (4%)	0	100	100
14	L	120/198 (61%)	118 (98%)	2 (2%)	0	100	100
15	I	33/108 (31%)	33 (100%)	0	0	100	100
All	All	3880/4678 (83%)	3738 (96%)	139 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	146	GLN
1	a	64	GLU
1	1	55	ASN

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	1	153/179 (86%)	153 (100%)	0	100	100
1	a	153/179 (86%)	153 (100%)	0	100	100
2	3	170/217 (78%)	169 (99%)	1 (1%)	78	92
3	7	171/201 (85%)	168 (98%)	3 (2%)	51	82
3	c	166/201 (83%)	165 (99%)	1 (1%)	78	92
4	8	173/197 (88%)	172 (99%)	1 (1%)	78	92
4	b	172/197 (87%)	168 (98%)	4 (2%)	44	78
5	A	599/609 (98%)	596 (100%)	3 (0%)	81	93
6	B	595/596 (100%)	592 (100%)	3 (0%)	81	93
7	C	68/69 (99%)	68 (100%)	0	100	100
8	D	123/156 (79%)	123 (100%)	0	100	100
9	E	60/93 (64%)	60 (100%)	0	100	100
10	F	136/177 (77%)	135 (99%)	1 (1%)	76	91
11	J	36/36 (100%)	36 (100%)	0	100	100
12	K	58/88 (66%)	58 (100%)	0	100	100
13	T	169/280 (60%)	161 (95%)	8 (5%)	23	57
14	L	91/150 (61%)	90 (99%)	1 (1%)	65	87
15	I	28/76 (37%)	27 (96%)	1 (4%)	31	66
All	All	3121/3701 (84%)	3094 (99%)	27 (1%)	68	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	83	LEU
3	7	171	LYS
3	7	185	MET
3	7	255	PHE
4	8	228	ASP
5	A	374	MET

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Mol	Chain	Res	Type
5	A	584	CYS
5	A	593	PHE
6	B	546	LYS
6	B	569	CYS
6	B	578	TYR
10	F	174	SER
13	T	155	ASN
13	T	157	MET
13	T	174	MET
13	T	236	MET
13	T	240	MET
13	T	291	LYS
13	T	317	PHE
13	T	320	GLN
4	b	131	TYR
4	b	158	GLU
4	b	161	PHE
4	b	180	LYS
3	c	187	MET
14	L	133	CYS
15	I	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	145	ASN
1	1	180	ASN
2	3	106	GLN
2	3	220	ASN
2	3	238	ASN
3	7	204	ASN
4	8	166	ASN
5	A	311	GLN
5	A	544	HIS
6	B	99	GLN
6	B	115	ASN
6	B	325	HIS
6	B	351	GLN
6	B	404	ASN
6	B	631	GLN
6	B	705	GLN
8	D	189	GLN

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Mol	Chain	Res	Type
9	E	66	ASN
10	F	145	HIS
10	F	208	GLN
12	K	86	GLN
13	T	143	HIS
13	T	330	GLN
1	a	36	ASN
1	a	53	ASN
1	a	145	ASN
1	a	180	ASN
1	a	216	ASN
4	b	30	ASN
4	b	140	GLN
4	b	221	ASN
4	b	249	GLN
3	c	154	ASN
3	c	204	ASN
3	c	245	ASN
14	L	69	ASN
14	L	84	ASN
15	I	46	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

284 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5039	5	59,63,73	1.23	7 (11%)	70,101,113	1.21	6 (8%)
17	CLA	B	830	6,21	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
17	CLA	A	5027	-	61,65,73	1.31	8 (13%)	72,103,113	1.19	6 (8%)
17	CLA	A	5016	5	69,73,73	1.18	9 (13%)	82,113,113	1.25	8 (9%)
17	CLA	A	5036	5	68,72,73	1.19	8 (11%)	80,111,113	1.20	4 (5%)
21	LHG	A	5002	24	35,35,48	0.35	0	38,41,54	0.37	0
17	CLA	8	314	4	50,54,73	1.33	7 (14%)	59,90,113	1.29	4 (6%)
17	CLA	c	312	3	54,58,73	1.32	7 (12%)	64,95,113	1.24	6 (9%)
17	CLA	8	315	4	49,53,73	1.37	7 (14%)	58,89,113	1.27	4 (6%)
17	CLA	A	5022	-	69,73,73	1.15	7 (10%)	82,113,113	1.16	4 (4%)
17	CLA	L	201	14	69,73,73	1.14	7 (10%)	82,113,113	1.08	5 (6%)
16	CHL	8	306	-	50,54,74	1.62	3 (6%)	55,90,114	1.80	10 (18%)
17	CLA	T	407	13	54,58,73	1.27	8 (14%)	64,95,113	1.22	6 (9%)
17	CLA	A	5013	17,24,5	69,73,73	1.12	7 (10%)	82,113,113	1.12	7 (8%)
17	CLA	A	5043	21	49,53,73	1.35	8 (16%)	58,89,113	1.30	5 (8%)
17	CLA	8	312	4	54,58,73	1.37	10 (18%)	64,95,113	1.40	7 (10%)
17	CLA	8	310	4	64,68,73	1.18	7 (10%)	76,107,113	1.10	4 (5%)
17	CLA	T	402	13,17	54,58,73	1.30	8 (14%)	64,95,113	1.31	6 (9%)
17	CLA	b	608	-	49,53,73	1.37	6 (12%)	58,89,113	1.31	5 (8%)
17	CLA	B	815	-	54,58,73	1.31	7 (12%)	64,95,113	1.34	6 (9%)
17	CLA	b	603	4	54,58,73	1.33	9 (16%)	64,95,113	1.40	5 (7%)
17	CLA	c	313	3	49,53,73	1.35	7 (14%)	58,89,113	1.33	4 (6%)
17	CLA	B	826	6	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
24	LMG	F	5011	-	29,29,55	0.20	0	37,37,63	0.15	0
16	CHL	1	601	-	55,59,74	1.33	3 (5%)	61,96,114	1.80	12 (19%)
25	LMU	A	5054	-	36,36,36	0.13	0	47,47,47	0.19	0
17	CLA	c	307	3	54,58,73	1.31	8 (14%)	64,95,113	1.58	10 (15%)
17	CLA	A	5008	5	69,73,73	1.11	7 (10%)	82,113,113	1.11	7 (8%)
17	CLA	3	307	2	69,73,73	1.15	7 (10%)	82,113,113	1.11	6 (7%)
29	SF4	A	5046	6,5	0,12,12	-	-	-	-	-
20	BCR	A	5052	-	41,41,41	0.17	0	56,56,56	0.36	0
17	CLA	a	610	21	50,54,73	1.35	6 (12%)	59,90,113	1.25	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	DGD	3	321	2	51,51,67	0.17	0	65,65,81	0.16	0
17	CLA	a	605	-	49,53,73	1.37	8 (16%)	58,89,113	1.28	4 (6%)
19	XAT	1	616	-	41,47,47	0.15	0	54,74,74	0.97	3 (5%)
17	CLA	K	201	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	4 (6%)
17	CLA	c	310	3	49,53,73	1.41	9 (18%)	58,89,113	1.47	5 (8%)
17	CLA	A	5024	5	64,68,73	1.18	7 (10%)	76,107,113	1.09	4 (5%)
17	CLA	B	832	6	59,63,73	1.26	8 (13%)	70,101,113	1.15	7 (10%)
17	CLA	T	412	-	46,50,73	1.38	7 (15%)	53,85,113	1.18	4 (7%)
18	LUT	a	615	-	42,43,43	0.17	0	51,60,60	1.17	6 (11%)
21	LHG	a	619	1,16,17	22,22,48	0.40	0	25,28,54	0.38	0
17	CLA	K	203	12	49,53,73	1.37	8 (16%)	58,89,113	1.23	4 (6%)
17	CLA	B	805	-	69,73,73	1.13	6 (8%)	82,113,113	1.24	7 (8%)
17	CLA	A	5042	5	64,68,73	1.24	8 (12%)	76,107,113	1.21	5 (6%)
20	BCR	7	317	-	41,41,41	0.16	0	56,56,56	0.43	0
16	CHL	T	401	13	55,59,74	1.26	3 (5%)	61,96,114	2.41	14 (22%)
18	LUT	1	615	-	42,43,43	0.20	0	51,60,60	1.47	8 (15%)
17	CLA	B	804	6	52,56,73	1.31	8 (15%)	61,92,113	1.15	5 (8%)
17	CLA	3	311	2	59,63,73	1.26	7 (11%)	70,101,113	1.28	5 (7%)
20	BCR	J	103	-	41,41,41	0.15	0	56,56,56	0.27	0
17	CLA	7	304	17	54,58,73	1.35	8 (14%)	64,95,113	1.39	6 (9%)
19	XAT	a	616	-	41,47,47	0.15	0	54,74,74	0.77	2 (3%)
20	BCR	T	415	-	41,41,41	0.12	0	56,56,56	0.28	0
17	CLA	A	5033	5	59,63,73	1.26	8 (13%)	70,101,113	1.18	5 (7%)
17	CLA	B	806	6	69,73,73	1.15	9 (13%)	82,113,113	1.11	4 (4%)
17	CLA	c	309	3,21	64,68,73	1.20	7 (10%)	76,107,113	1.27	6 (7%)
20	BCR	B	849	-	41,41,41	0.22	0	56,56,56	1.03	4 (7%)
17	CLA	K	202	-	50,54,73	1.34	7 (14%)	59,90,113	1.22	5 (8%)
17	CLA	1	602	1	59,63,73	1.25	7 (11%)	70,101,113	1.32	7 (10%)
19	XAT	b	616	-	41,47,47	0.14	0	54,74,74	0.79	2 (3%)
20	BCR	B	846	-	41,41,41	0.15	0	56,56,56	0.21	0
17	CLA	B	835	6	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
19	XAT	8	317	-	41,47,47	0.15	0	54,74,74	0.88	1 (1%)
20	BCR	A	5049	-	41,41,41	0.29	0	56,56,56	0.83	2 (3%)
17	CLA	T	409	18	56,60,73	1.31	6 (10%)	65,97,113	1.49	8 (12%)
17	CLA	c	311	-	54,58,73	1.30	6 (11%)	64,95,113	1.32	5 (7%)
17	CLA	L	202	14	49,53,73	1.46	9 (18%)	58,89,113	1.34	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	816	6	54,58,73	1.30	8 (14%)	64,95,113	1.33	6 (9%)
18	LUT	T	413	17,13	42,43,43	0.37	0	51,60,60	0.63	2 (3%)
21	LHG	c	317	17	27,27,48	0.37	0	30,33,54	0.35	0
17	CLA	B	839	6	69,73,73	1.18	9 (13%)	82,113,113	1.11	6 (7%)
17	CLA	A	5021	5	54,58,73	1.29	8 (14%)	64,95,113	1.28	6 (9%)
17	CLA	1	610	21	50,54,73	1.34	6 (12%)	59,90,113	1.25	4 (6%)
18	LUT	b	615	-	42,43,43	0.23	0	51,60,60	0.42	0
20	BCR	B	844	-	41,41,41	0.21	0	56,56,56	0.44	0
17	CLA	B	833	6	64,68,73	1.19	7 (10%)	76,107,113	1.21	5 (6%)
19	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.78	2 (3%)
18	LUT	7	315	-	42,43,43	0.38	1 (2%)	51,60,60	0.52	1 (1%)
17	CLA	8	304	4	55,59,73	1.33	8 (14%)	64,96,113	1.41	6 (9%)
17	CLA	a	607	-	50,54,73	1.38	9 (18%)	59,90,113	1.39	4 (6%)
28	PQN	B	842	-	34,34,34	0.29	0	43,45,45	0.51	1 (2%)
17	CLA	A	5015	5	59,63,73	1.23	6 (10%)	70,101,113	1.37	6 (8%)
17	CLA	A	5018	5	64,68,73	1.18	8 (12%)	76,107,113	1.18	4 (5%)
17	CLA	A	5017	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	5 (7%)
22	SQD	3	320	2	33,35,54	0.27	0	43,46,65	0.52	0
17	CLA	a	608	1,17	49,53,73	1.36	7 (14%)	57,88,113	1.42	5 (8%)
17	CLA	B	824	-	54,58,73	1.33	8 (14%)	64,95,113	1.48	6 (9%)
17	CLA	A	5025	5	64,68,73	1.19	8 (12%)	76,107,113	1.22	5 (6%)
17	CLA	B	802	6	69,73,73	1.17	9 (13%)	82,113,113	1.02	5 (6%)
17	CLA	F	5004	6,10	69,73,73	1.27	11 (15%)	82,113,113	1.36	6 (7%)
17	CLA	B	808	6	69,73,73	1.14	9 (13%)	82,113,113	1.12	5 (6%)
20	BCR	J	104	-	41,41,41	0.16	0	56,56,56	0.33	0
17	CLA	B	837	6	54,58,73	1.27	7 (12%)	64,95,113	1.26	6 (9%)
17	CLA	A	5030	-	69,73,73	1.16	8 (11%)	82,113,113	1.19	5 (6%)
17	CLA	1	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.12	5 (6%)
17	CLA	3	310	2	50,54,73	1.34	8 (16%)	59,90,113	1.39	4 (6%)
17	CLA	7	303	3	59,63,73	1.28	9 (15%)	70,101,113	1.23	5 (7%)
17	CLA	7	311	3	50,54,73	1.37	8 (16%)	59,90,113	1.43	6 (10%)
17	CLA	T	405	13	49,53,73	1.37	7 (14%)	58,89,113	1.26	5 (8%)
19	XAT	c	315	3	41,47,47	0.16	0	54,74,74	0.76	2 (3%)
20	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.37	0
20	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.32	0
26	PTY	F	5002	10	32,32,49	0.56	0	35,37,54	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	I	4001	20	41,41,41	0.17	0	56,56,56	0.26	0
17	CLA	3	309	17,2	50,54,73	1.34	7 (14%)	59,90,113	1.14	4 (6%)
17	CLA	8	309	4	50,54,73	1.38	7 (14%)	59,90,113	1.30	4 (6%)
17	CLA	3	324	5,2	59,63,73	1.26	8 (13%)	70,101,113	1.21	4 (5%)
17	CLA	1	609	1	69,73,73	1.14	8 (11%)	82,113,113	1.20	4 (4%)
17	CLA	B	823	6	54,58,73	1.27	6 (11%)	64,95,113	1.19	5 (7%)
17	CLA	B	825	-	54,58,73	1.34	8 (14%)	64,95,113	1.18	7 (10%)
29	SF4	C	101	7	0,12,12	-	-	-	-	-
17	CLA	1	605	-	49,53,73	1.41	7 (14%)	58,89,113	1.45	4 (6%)
17	CLA	8	303	4	54,58,73	1.29	7 (12%)	64,95,113	1.18	5 (7%)
20	BCR	L	204	20	41,41,41	0.14	0	56,56,56	0.24	0
16	CHL	c	304	17	50,54,74	1.16	3 (6%)	55,90,114	2.16	8 (14%)
17	CLA	7	310	21	50,54,73	1.35	5 (10%)	59,90,113	1.22	4 (6%)
29	SF4	C	102	7	0,12,12	-	-	-	-	-
17	CLA	3	312	2	50,54,73	1.32	7 (14%)	59,90,113	1.15	4 (6%)
17	CLA	B	820	-	59,63,73	1.26	7 (11%)	70,101,113	1.30	5 (7%)
16	CHL	7	305	-	50,54,74	1.44	3 (6%)	55,90,114	1.49	11 (20%)
17	CLA	A	5006	5	69,73,73	1.14	8 (11%)	82,113,113	1.20	6 (7%)
16	CHL	T	416	-	50,54,74	1.25	4 (8%)	55,90,114	2.21	11 (20%)
17	CLA	B	810	6	59,63,73	1.26	7 (11%)	70,101,113	1.29	4 (5%)
20	BCR	a	617	-	41,41,41	0.18	0	56,56,56	0.34	0
23	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.23	0
20	BCR	A	5047	-	41,41,41	0.17	0	56,56,56	0.32	0
17	CLA	B	836	6	64,68,73	1.17	7 (10%)	76,107,113	1.23	5 (6%)
17	CLA	8	311	21,17	59,63,73	1.26	8 (13%)	70,101,113	1.22	5 (7%)
17	CLA	F	5009	10	50,54,73	1.37	7 (14%)	59,90,113	1.43	4 (6%)
17	CLA	3	305	2	54,58,73	1.31	9 (16%)	64,95,113	1.27	6 (9%)
17	CLA	A	5035	5	69,73,73	1.13	8 (11%)	82,113,113	1.16	5 (6%)
17	CLA	a	612	-	54,58,73	1.30	8 (14%)	64,95,113	1.25	5 (7%)
20	BCR	F	5005	-	41,41,41	0.15	0	56,56,56	0.26	0
20	BCR	F	5010	-	41,41,41	0.15	0	56,56,56	0.33	0
17	CLA	3	303	-	50,54,73	1.33	7 (14%)	59,90,113	1.33	4 (6%)
17	CLA	B	814	-	54,58,73	1.30	8 (14%)	64,95,113	1.36	6 (9%)
17	CLA	B	827	-	64,68,73	1.18	7 (10%)	76,107,113	1.13	4 (5%)
17	CLA	c	302	3	50,54,73	1.32	8 (16%)	59,90,113	1.21	4 (6%)
21	LHG	a	618	1	22,22,48	0.45	0	25,27,54	0.46	0
25	LMU	7	319	-	36,36,36	0.12	0	47,47,47	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CHL	3	301	2	66,70,74	1.12	3 (4%)	74,109,114	1.88	11 (14%)
20	BCR	3	319	2	41,41,41	0.19	0	56,56,56	0.29	0
16	CHL	b	607	-	55,59,74	1.16	4 (7%)	61,96,114	2.17	12 (19%)
17	CLA	A	5010	-	54,58,73	1.35	10 (18%)	64,95,113	1.35	6 (9%)
17	CLA	A	5004	-	69,73,73	1.14	8 (11%)	82,113,113	1.08	4 (4%)
17	CLA	1	612	-	64,68,73	1.21	6 (9%)	76,107,113	1.20	6 (7%)
17	CLA	B	818	6	69,73,73	1.14	8 (11%)	82,113,113	1.14	6 (7%)
16	CHL	8	308	-	55,59,74	1.14	3 (5%)	61,96,114	2.43	11 (18%)
17	CLA	B	829	6	69,73,73	1.15	6 (8%)	82,113,113	1.13	5 (6%)
20	BCR	K	205	-	41,41,41	0.27	0	56,56,56	0.76	2 (3%)
20	BCR	c	316	-	41,41,41	0.14	0	56,56,56	0.58	2 (3%)
21	LHG	1	618	17	26,26,48	0.40	0	29,32,54	0.43	0
18	LUT	c	314	-	42,43,43	0.40	1 (2%)	51,60,60	0.59	0
17	CLA	A	5044	-	69,73,73	1.15	7 (10%)	82,113,113	1.11	7 (8%)
17	CLA	A	5041	5	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
16	CHL	c	306	-	52,56,74	1.38	3 (5%)	57,92,114	1.96	10 (17%)
17	CLA	3	323	5,2	59,63,73	1.22	7 (11%)	70,101,113	1.23	5 (7%)
17	CLA	T	403	-	54,58,73	1.44	10 (18%)	64,95,113	1.28	11 (17%)
16	CHL	c	305	-	54,58,74	1.04	4 (7%)	58,94,114	2.15	11 (18%)
17	CLA	7	309	3	50,54,73	1.30	8 (16%)	59,90,113	1.14	3 (5%)
17	CLA	B	817	6	59,63,73	1.24	7 (11%)	70,101,113	1.18	5 (7%)
17	CLA	B	831	6	59,63,73	1.26	8 (13%)	70,101,113	1.22	6 (8%)
17	CLA	a	614	1,17	50,54,73	1.36	7 (14%)	59,90,113	1.36	4 (6%)
17	CLA	b	602	4	64,68,73	1.19	7 (10%)	76,107,113	1.10	5 (6%)
17	CLA	c	308	3	69,73,73	1.14	8 (11%)	82,113,113	1.17	5 (6%)
17	CLA	F	5008	10	49,53,73	1.37	7 (14%)	58,89,113	1.29	4 (6%)
17	CLA	3	313	-	46,50,73	1.38	7 (15%)	53,85,113	1.23	4 (7%)
21	LHG	F	5001	17	30,30,48	0.37	0	33,36,54	0.32	0
26	PTY	8	319	26	20,20,49	0.69	0	23,25,54	0.51	0
17	CLA	A	5019	5	65,69,73	1.25	10 (15%)	77,108,113	1.28	4 (5%)
26	PTY	F	5003	26	17,17,49	0.70	0	18,21,54	0.60	0
30	LMK	J	101	-	34,34,53	0.44	0	34,41,60	0.56	1 (2%)
17	CLA	B	807	6	59,63,73	1.22	7 (11%)	70,101,113	1.20	5 (7%)
17	CLA	7	308	3	50,54,73	1.33	6 (12%)	59,90,113	1.34	4 (6%)
17	CLA	8	302	4	50,54,73	1.34	6 (12%)	59,90,113	1.40	5 (8%)
17	CLA	7	312	3	69,73,73	1.23	8 (11%)	82,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5023	5	50,54,73	1.34	7 (14%)	59,90,113	1.35	4 (6%)
17	CLA	b	604	-	54,58,73	1.32	8 (14%)	64,95,113	1.42	5 (7%)
17	CLA	B	819	-	64,68,73	1.23	8 (12%)	76,107,113	1.27	4 (5%)
17	CLA	c	301	3	69,73,73	1.17	7 (10%)	82,113,113	1.10	6 (7%)
17	CLA	1	604	-	54,58,73	1.28	7 (12%)	64,95,113	1.32	5 (7%)
17	CLA	a	603	-	49,53,73	1.38	7 (14%)	58,89,113	1.40	4 (6%)
21	LHG	7	318	17	33,33,48	0.35	0	36,39,54	0.34	0
20	BCR	3	317	2	41,41,41	0.14	0	56,56,56	0.32	0
24	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
17	CLA	a	602	1	59,63,73	1.25	8 (13%)	70,101,113	1.19	5 (7%)
17	CLA	7	314	3	50,54,73	1.33	7 (14%)	59,90,113	1.29	4 (6%)
20	BCR	B	843	6	41,41,41	0.16	0	56,56,56	0.31	0
17	CLA	A	5012	5	59,63,73	1.27	9 (15%)	70,101,113	1.36	7 (10%)
17	CLA	A	5014	-	69,73,73	1.14	7 (10%)	82,113,113	1.25	5 (6%)
17	CLA	B	834	-	54,58,73	1.30	7 (12%)	64,95,113	1.31	6 (9%)
16	CHL	a	606	-	51,55,74	1.24	4 (7%)	56,91,114	2.21	14 (25%)
20	BCR	8	318	-	41,41,41	0.17	0	56,56,56	0.53	0
21	LHG	1	619	-	30,30,48	0.36	0	33,36,54	0.34	0
17	CLA	1	608	-	49,53,73	1.36	6 (12%)	58,89,113	1.32	4 (6%)
17	CLA	A	5026	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	4 (4%)
17	CLA	c	303	16	54,58,73	1.31	7 (12%)	64,95,113	1.32	5 (7%)
17	CLA	T	410	13	54,58,73	1.30	7 (12%)	64,95,113	1.29	6 (9%)
24	LMG	A	5001	17,21,5	32,32,55	0.23	0	40,40,63	0.25	0
17	CLA	T	404	-	50,54,73	1.41	7 (14%)	59,90,113	1.17	5 (8%)
17	CLA	F	5006	-	64,68,73	1.18	7 (10%)	76,107,113	1.11	5 (6%)
17	CLA	3	304	-	50,54,73	1.35	7 (14%)	59,90,113	1.28	4 (6%)
17	CLA	a	604	-	53,56,73	1.36	8 (15%)	62,92,113	1.29	6 (9%)
20	BCR	L	203	-	41,41,41	0.14	0	56,56,56	0.36	0
17	CLA	7	313	3	54,58,73	1.31	7 (12%)	64,95,113	1.29	6 (9%)
17	CLA	a	609	1	64,68,73	1.18	7 (10%)	76,107,113	1.09	5 (6%)
20	BCR	A	5048	-	41,41,41	0.29	0	56,56,56	0.58	0
17	CLA	A	5020	5	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
17	CLA	J	102	11	53,57,73	1.30	6 (11%)	61,93,113	1.36	5 (8%)
19	XAT	7	316	-	41,47,47	0.18	0	54,74,74	0.85	3 (5%)
17	CLA	B	822	6	49,53,73	1.36	7 (14%)	58,89,113	1.35	4 (6%)
26	PTY	8	320	-	20,20,49	0.66	0	21,24,54	0.55	0
16	CHL	3	322	-	65,69,74	1.31	3 (4%)	73,108,114	1.89	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	803	-	69,73,73	1.14	8 (11%)	82,113,113	1.14	4 (4%)
20	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.35	0
17	CLA	3	308	2	59,63,73	1.24	7 (11%)	70,101,113	1.12	6 (8%)
16	CHL	7	306	-	51,55,74	1.05	4 (7%)	56,91,114	2.37	12 (21%)
16	CHL	7	307	-	52,56,74	1.32	3 (5%)	57,92,114	1.96	10 (17%)
17	CLA	8	305	-	50,54,73	1.38	9 (18%)	59,90,113	1.43	4 (6%)
17	CLA	b	613	4	50,54,73	1.32	7 (14%)	59,90,113	1.18	5 (8%)
17	CLA	a	613	1	50,54,73	1.34	7 (14%)	59,90,113	1.19	4 (6%)
28	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.57	1 (2%)
17	CLA	A	5031	5	69,73,73	1.14	7 (10%)	82,113,113	1.20	5 (6%)
21	LHG	8	321	17	29,29,48	0.37	0	32,35,54	0.35	0
21	LHG	A	5055	17	29,29,48	0.37	0	33,35,54	0.33	0
18	LUT	8	316	-	42,43,43	0.26	0	51,60,60	0.45	0
27	CL0	A	5003	5	69,73,73	1.09	4 (5%)	82,113,113	1.85	10 (12%)
17	CLA	T	411	-	50,54,73	1.33	7 (14%)	59,90,113	1.20	4 (6%)
17	CLA	3	306	-	59,63,73	1.24	8 (13%)	70,101,113	1.24	6 (8%)
17	CLA	b	601	4	50,54,73	1.36	6 (12%)	59,90,113	1.27	4 (6%)
17	CLA	A	5028	5	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
18	LUT	3	315	-	42,43,43	0.20	0	51,60,60	0.35	0
17	CLA	3	314	2	50,54,73	1.33	8 (16%)	59,90,113	1.28	4 (6%)
21	LHG	A	5053	5	48,48,48	0.29	0	51,54,54	0.29	0
16	CHL	1	606	-	51,55,74	1.29	4 (7%)	56,91,114	2.17	11 (19%)
17	CLA	8	313	4	55,59,73	1.41	8 (14%)	64,96,113	1.22	5 (7%)
17	CLA	F	5007	-	51,55,73	1.31	8 (15%)	60,91,113	1.17	5 (8%)
17	CLA	B	840	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	4 (4%)
20	BCR	B	845	-	41,41,41	0.28	0	56,56,56	0.91	3 (5%)
16	CHL	8	307	-	51,55,74	1.07	4 (7%)	56,91,114	2.10	11 (19%)
16	CHL	a	601	21	51,55,74	1.33	4 (7%)	56,91,114	1.99	12 (21%)
17	CLA	K	204	-	49,53,73	1.36	7 (14%)	58,89,113	1.23	4 (6%)
17	CLA	A	5040	-	64,68,73	1.21	8 (12%)	76,107,113	1.15	4 (5%)
17	CLA	A	5011	5	69,73,73	1.17	8 (11%)	82,113,113	1.12	6 (7%)
20	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
17	CLA	1	614	1	50,54,73	1.35	6 (12%)	59,90,113	1.35	4 (6%)
17	CLA	1	611	1	50,54,73	1.39	10 (20%)	59,90,113	1.41	6 (10%)
17	CLA	B	812	6	50,54,73	1.34	7 (14%)	59,90,113	1.28	4 (6%)
17	CLA	b	609	4	64,68,73	1.17	8 (12%)	76,107,113	1.08	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	B	801	-	41,41,41	0.15	0	56,56,56	0.35	0
23	DGD	8	301	-	40,40,67	0.27	0	54,54,81	0.47	0
17	CLA	B	838	-	59,63,73	1.30	9 (15%)	70,101,113	1.27	5 (7%)
17	CLA	b	612	4	52,56,73	1.40	8 (15%)	61,92,113	1.27	5 (8%)
17	CLA	T	406	-	54,58,73	1.32	7 (12%)	64,95,113	1.33	6 (9%)
17	CLA	A	5038	5	54,58,73	1.34	8 (14%)	64,95,113	1.39	5 (7%)
19	XAT	T	414	-	41,47,47	0.15	0	54,74,74	0.72	1 (1%)
17	CLA	3	302	2	69,73,73	1.16	9 (13%)	82,113,113	1.21	4 (4%)
17	CLA	1	613	1	50,54,73	1.34	7 (14%)	59,90,113	1.33	4 (6%)
21	LHG	b	618	17	20,20,48	0.39	0	23,26,54	0.39	0
20	BCR	A	5050	-	41,41,41	0.17	0	56,56,56	0.29	0
16	CHL	b	606	-	51,55,74	1.08	4 (7%)	56,91,114	2.17	12 (21%)
17	CLA	A	5007	17	64,68,73	1.17	5 (7%)	76,107,113	1.12	4 (5%)
17	CLA	A	5032	5	49,53,73	1.40	8 (16%)	58,89,113	1.34	4 (6%)
17	CLA	B	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.16	5 (6%)
17	CLA	B	809	6	64,68,73	1.21	7 (10%)	76,107,113	1.19	5 (6%)
17	CLA	T	408	18,13	54,58,73	1.28	8 (14%)	64,95,113	1.24	6 (9%)
17	CLA	a	611	1	50,54,73	1.37	8 (16%)	59,90,113	1.42	6 (10%)
17	CLA	B	821	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	4 (7%)
17	CLA	1	603	1	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
17	CLA	A	5005	-	69,73,73	1.13	8 (11%)	82,113,113	1.10	5 (6%)
17	CLA	A	5009	5	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
17	CLA	b	610	21	54,58,73	1.29	6 (11%)	64,95,113	1.24	5 (7%)
17	CLA	7	302	3	64,68,73	1.20	8 (12%)	76,107,113	1.08	3 (3%)
20	BCR	1	617	1	41,41,41	0.24	0	56,56,56	0.46	0
17	CLA	A	5034	5	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
17	CLA	A	5037	5	54,58,73	1.31	8 (14%)	64,95,113	1.30	6 (9%)
17	CLA	B	811	6	54,58,73	1.31	7 (12%)	64,95,113	1.28	5 (7%)
17	CLA	A	5029	5	69,73,73	1.11	6 (8%)	82,113,113	1.24	6 (7%)
17	CLA	B	813	6	54,58,73	1.31	5 (9%)	64,95,113	1.35	6 (9%)
17	CLA	B	828	-	59,63,73	1.35	8 (13%)	70,101,113	1.29	5 (7%)
17	CLA	b	611	4	54,58,73	1.35	8 (14%)	64,95,113	1.41	7 (10%)
17	CLA	b	614	4	50,54,73	1.33	7 (14%)	59,90,113	1.25	4 (6%)
16	CHL	b	605	-	51,55,74	1.19	3 (5%)	56,91,114	2.21	11 (19%)

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
17	CLA	A	5039	5	-	5/27/103/115	-
17	CLA	B	830	6,21	-	12/39/115/115	-
17	CLA	A	5027	-	-	9/30/106/115	-
17	CLA	A	5016	5	-	16/39/115/115	-
17	CLA	A	5036	5	-	9/39/115/115	-
21	LHG	A	5002	24	-	8/40/40/53	-
17	CLA	8	314	4	-	9/17/93/115	-
17	CLA	c	312	3	-	7/21/97/115	-
17	CLA	8	315	4	-	8/15/91/115	-
17	CLA	A	5022	-	-	14/39/115/115	-
17	CLA	L	201	14	-	10/39/115/115	-
16	CHL	8	306	-	-	9/17/93/117	-
17	CLA	T	407	13	-	11/21/97/115	-
17	CLA	A	5013	17,24,5	-	15/39/115/115	-
17	CLA	A	5043	21	-	8/15/91/115	-
17	CLA	8	312	4	-	8/21/97/115	-
17	CLA	8	310	4	-	11/33/109/115	-
17	CLA	T	402	13,17	-	6/21/97/115	-
17	CLA	b	608	-	-	6/15/91/115	-
17	CLA	B	815	-	-	6/21/97/115	-
17	CLA	b	603	4	-	10/21/97/115	-
17	CLA	c	313	3	-	6/15/91/115	-
17	CLA	B	826	6	-	9/39/115/115	-
24	LMG	F	5011	-	-	3/24/44/70	0/1/1/1
16	CHL	1	601	-	-	9/23/99/117	-
25	LMU	A	5054	-	-	5/21/61/61	0/2/2/2
17	CLA	c	307	3	-	6/21/97/115	-
17	CLA	A	5008	5	-	13/39/115/115	-
17	CLA	3	307	2	-	13/39/115/115	-
29	SF4	A	5046	6,5	-	-	0/6/5/5
20	BCR	A	5052	-	-	5/29/63/63	0/2/2/2
17	CLA	a	610	21	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DGD	3	321	2	-	10/39/79/95	0/2/2/2
17	CLA	a	605	-	-	6/15/91/115	-
19	XAT	1	616	-	-	2/31/93/93	0/4/4/4
17	CLA	K	201	-	-	7/15/91/115	-
17	CLA	c	310	3	-	7/15/91/115	-
17	CLA	A	5024	5	-	16/33/109/115	-
17	CLA	B	832	6	-	8/27/103/115	-
18	LUT	a	615	-	3/3/12/27	9/29/67/67	0/2/2/2
17	CLA	T	412	-	-	4/12/88/115	-
21	LHG	a	619	1,16,17	-	6/26/26/53	-
17	CLA	K	203	12	-	10/15/91/115	-
17	CLA	B	805	-	-	9/39/115/115	-
17	CLA	A	5042	5	-	8/33/109/115	-
20	BCR	7	317	-	-	4/29/63/63	0/2/2/2
16	CHL	T	401	13	-	10/23/99/117	-
18	LUT	1	615	-	3/3/12/27	10/29/67/67	0/2/2/2
17	CLA	B	804	6	-	9/19/95/115	-
17	CLA	3	311	2	-	10/27/103/115	-
20	BCR	J	103	-	-	4/29/63/63	0/2/2/2
17	CLA	7	304	17	-	7/21/97/115	-
19	XAT	a	616	-	-	3/31/93/93	0/4/4/4
20	BCR	T	415	-	-	4/29/63/63	0/2/2/2
17	CLA	A	5033	5	-	5/27/103/115	-
17	CLA	B	806	6	-	17/39/115/115	-
17	CLA	c	309	3,21	-	11/33/109/115	-
20	BCR	B	849	-	-	6/29/63/63	0/2/2/2
17	CLA	K	202	-	-	7/17/93/115	-
17	CLA	1	602	1	-	15/27/103/115	-
19	XAT	b	616	-	-	0/31/93/93	0/4/4/4
20	BCR	B	846	-	-	2/29/63/63	0/2/2/2
17	CLA	B	835	6	-	9/21/97/115	-
19	XAT	8	317	-	-	0/31/93/93	0/4/4/4
20	BCR	A	5049	-	-	3/29/63/63	0/2/2/2
17	CLA	T	409	18	-	13/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LUT	T	413	17,13	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	c	311	-	-	6/21/97/115	-
17	CLA	B	816	6	-	6/21/97/115	-
17	CLA	L	202	14	-	6/15/91/115	-
21	LHG	c	317	17	-	3/32/32/53	-
17	CLA	B	839	6	-	10/39/115/115	-
17	CLA	A	5021	5	-	5/21/97/115	-
18	LUT	b	615	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	1	610	21	-	9/17/93/115	-
20	BCR	B	844	-	-	2/29/63/63	0/2/2/2
17	CLA	B	833	6	-	11/33/109/115	-
19	XAT	3	316	-	-	3/31/93/93	0/4/4/4
18	LUT	7	315	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	8	304	4	-	10/23/99/115	-
17	CLA	a	607	-	-	4/17/93/115	-
28	PQN	B	842	-	-	1/23/43/43	0/2/2/2
17	CLA	A	5015	5	-	6/27/103/115	-
17	CLA	A	5018	5	-	13/33/109/115	-
17	CLA	A	5017	-	-	12/27/103/115	-
22	SQD	3	320	2	-	11/30/50/69	0/1/1/1
17	CLA	a	608	1,17	-	7/15/91/115	-
17	CLA	B	824	-	-	11/21/97/115	-
17	CLA	A	5025	5	-	9/33/109/115	-
17	CLA	B	802	6	-	15/39/115/115	-
17	CLA	F	5004	6,10	-	12/39/115/115	-
17	CLA	B	808	6	-	20/39/115/115	-
20	BCR	J	104	-	-	2/29/63/63	0/2/2/2
17	CLA	B	837	6	-	8/21/97/115	-
17	CLA	A	5030	-	-	10/39/115/115	-
17	CLA	1	607	-	-	13/39/115/115	-
17	CLA	3	310	2	-	8/17/93/115	-
17	CLA	7	303	3	-	4/27/103/115	-
17	CLA	7	311	3	-	7/17/93/115	-
17	CLA	T	405	13	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	XAT	c	315	3	-	3/31/93/93	0/4/4/4
20	BCR	b	617	-	-	4/29/63/63	0/2/2/2
20	BCR	3	318	-	-	4/29/63/63	0/2/2/2
26	PTY	F	5002	10	-	6/36/36/53	-
20	BCR	I	4001	20	-	2/29/63/63	0/2/2/2
17	CLA	3	309	17,2	-	9/17/93/115	-
17	CLA	8	309	4	-	5/17/93/115	-
17	CLA	3	324	5,2	-	6/27/103/115	-
17	CLA	1	609	1	-	11/39/115/115	-
17	CLA	B	823	6	-	9/21/97/115	-
17	CLA	B	825	-	-	4/21/97/115	-
29	SF4	C	101	7	-	-	0/6/5/5
17	CLA	1	605	-	-	6/15/91/115	-
17	CLA	8	303	4	-	8/21/97/115	-
20	BCR	L	204	20	-	4/29/63/63	0/2/2/2
16	CHL	c	304	17	-	7/17/93/117	-
17	CLA	7	310	21	-	7/17/93/115	-
29	SF4	C	102	7	-	-	0/6/5/5
17	CLA	3	312	2	-	8/17/93/115	-
17	CLA	B	820	-	-	10/27/103/115	-
16	CHL	7	305	-	-	5/17/93/117	-
17	CLA	A	5006	5	-	17/39/115/115	-
16	CHL	T	416	-	-	8/17/93/117	-
17	CLA	B	810	6	-	13/27/103/115	-
20	BCR	a	617	-	-	5/29/63/63	0/2/2/2
23	DGD	B	848	-	-	4/50/90/95	0/2/2/2
20	BCR	A	5047	-	-	4/29/63/63	0/2/2/2
17	CLA	B	836	6	-	7/33/109/115	-
17	CLA	8	311	21,17	-	6/27/103/115	-
17	CLA	F	5009	10	-	5/17/93/115	-
17	CLA	3	305	2	-	6/21/97/115	-
17	CLA	A	5035	5	-	15/39/115/115	-
17	CLA	a	612	-	-	8/21/97/115	-
20	BCR	F	5005	-	-	0/29/63/63	0/2/2/2
20	BCR	F	5010	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	303	-	-	8/17/93/115	-
17	CLA	B	814	-	-	12/21/97/115	-
17	CLA	B	827	-	-	10/33/109/115	-
17	CLA	c	302	3	-	4/17/93/115	-
21	LHG	a	618	1	-	14/26/26/53	-
25	LMU	7	319	-	-	9/21/61/61	0/2/2/2
16	CHL	3	301	2	1/1/14/21	21/37/113/117	-
20	BCR	3	319	2	-	4/29/63/63	0/2/2/2
16	CHL	b	607	-	-	8/23/99/117	-
17	CLA	A	5010	-	-	7/21/97/115	-
17	CLA	A	5004	-	-	15/39/115/115	-
17	CLA	1	612	-	-	11/33/109/115	-
17	CLA	B	818	6	-	14/39/115/115	-
16	CHL	8	308	-	-	10/23/99/117	-
17	CLA	B	829	6	-	16/39/115/115	-
20	BCR	K	205	-	-	10/29/63/63	0/2/2/2
20	BCR	c	316	-	-	9/29/63/63	0/2/2/2
21	LHG	1	618	17	-	11/31/31/53	-
18	LUT	c	314	-	3/3/12/27	5/29/67/67	0/2/2/2
17	CLA	A	5044	-	-	12/39/115/115	-
17	CLA	A	5041	5	-	8/39/115/115	-
16	CHL	c	306	-	-	6/20/96/117	-
18	LUT	8	316	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	3	323	5,2	-	10/27/103/115	-
16	CHL	c	305	-	-	14/22/98/117	-
17	CLA	7	309	3	-	7/17/93/115	-
17	CLA	B	817	6	-	9/27/103/115	-
17	CLA	B	831	6	-	10/27/103/115	-
17	CLA	T	403	-	-	10/21/97/115	-
17	CLA	a	614	1,17	-	8/17/93/115	-
17	CLA	b	602	4	-	11/33/109/115	-
17	CLA	F	5008	10	-	5/15/91/115	-
17	CLA	3	313	-	-	5/12/88/115	-
17	CLA	c	308	3	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LHG	F	5001	17	-	11/35/35/53	-
26	PTY	8	319	26	-	9/23/23/53	-
17	CLA	A	5019	5	-	10/35/111/115	-
26	PTY	F	5003	26	-	10/19/19/53	-
30	LMK	J	101	-	-	3/41/41/60	-
17	CLA	B	807	6	-	11/27/103/115	-
17	CLA	7	308	3	-	6/17/93/115	-
17	CLA	8	302	4	-	5/17/93/115	-
17	CLA	7	312	3	-	13/39/115/115	-
17	CLA	A	5023	5	-	7/17/93/115	-
17	CLA	b	604	-	-	8/21/97/115	-
17	CLA	B	819	-	-	9/33/109/115	-
17	CLA	c	301	3	-	14/39/115/115	-
17	CLA	1	604	-	-	9/21/97/115	-
17	CLA	a	603	-	-	8/15/91/115	-
21	LHG	7	318	17	-	2/38/38/53	-
20	BCR	3	317	2	-	4/29/63/63	0/2/2/2
24	LMG	7	301	-	-	12/45/65/70	0/1/1/1
17	CLA	a	602	1	-	6/27/103/115	-
17	CLA	7	314	3	-	7/17/93/115	-
20	BCR	B	843	6	-	5/29/63/63	0/2/2/2
17	CLA	A	5012	5	-	7/27/103/115	-
17	CLA	A	5014	-	-	14/39/115/115	-
17	CLA	B	834	-	-	13/21/97/115	-
16	CHL	a	606	-	-	6/19/95/117	-
20	BCR	8	318	-	-	6/29/63/63	0/2/2/2
21	LHG	1	619	-	-	7/35/35/53	-
17	CLA	1	608	-	-	8/15/91/115	-
17	CLA	A	5026	-	-	11/39/115/115	-
17	CLA	c	303	16	-	6/21/97/115	-
17	CLA	T	410	13	-	7/21/97/115	-
24	LMG	A	5001	17,21,5	-	4/26/46/70	0/1/1/1
17	CLA	T	404	-	-	9/17/93/115	-
17	CLA	F	5006	-	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	304	-	-	8/17/93/115	-
17	CLA	a	604	-	-	10/19/95/115	-
20	BCR	L	203	-	-	4/29/63/63	0/2/2/2
17	CLA	7	313	3	-	5/21/97/115	-
17	CLA	a	609	1	-	11/33/109/115	-
20	BCR	A	5048	-	-	7/29/63/63	0/2/2/2
17	CLA	A	5020	5	-	13/39/115/115	-
17	CLA	J	102	11	-	7/20/96/115	-
19	XAT	7	316	-	-	4/31/93/93	0/4/4/4
17	CLA	B	822	6	-	5/15/91/115	-
26	PTY	8	320	-	-	8/23/23/53	-
16	CHL	3	322	-	1/1/14/21	19/35/111/117	-
17	CLA	B	803	-	-	18/39/115/115	-
20	BCR	B	847	-	-	2/29/63/63	0/2/2/2
17	CLA	3	308	2	-	10/27/103/115	-
16	CHL	7	306	-	-	9/19/95/117	-
16	CHL	7	307	-	-	6/20/96/117	-
17	CLA	8	305	-	-	9/17/93/115	-
17	CLA	b	613	4	-	7/17/93/115	-
17	CLA	a	613	1	-	6/17/93/115	-
28	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
17	CLA	A	5031	5	-	9/39/115/115	-
21	LHG	8	321	17	-	9/34/34/53	-
21	LHG	A	5055	17	-	3/33/33/53	-
27	CL0	A	5003	5	-	16/39/115/115	-
17	CLA	T	411	-	-	10/17/93/115	-
17	CLA	3	306	-	-	8/27/103/115	-
18	LUT	3	315	-	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	A	5028	5	-	16/39/115/115	-
17	CLA	b	601	4	-	9/17/93/115	-
17	CLA	3	314	2	-	8/17/93/115	-
21	LHG	A	5053	5	-	11/53/53/53	-
16	CHL	1	606	-	-	4/19/95/117	-
17	CLA	8	313	4	-	8/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	F	5007	-	-	9/18/94/115	-
17	CLA	B	840	-	-	11/39/115/115	-
20	BCR	B	845	-	-	9/29/63/63	0/2/2/2
16	CHL	8	307	-	-	9/19/95/117	-
16	CHL	a	601	21	-	7/19/95/117	-
17	CLA	K	204	-	-	9/15/91/115	-
17	CLA	A	5040	-	-	10/33/109/115	-
17	CLA	A	5011	5	-	14/39/115/115	-
20	BCR	A	5051	-	-	2/29/63/63	0/2/2/2
17	CLA	1	614	1	-	9/17/93/115	-
17	CLA	1	611	1	-	8/17/93/115	-
17	CLA	B	812	6	-	6/17/93/115	-
17	CLA	b	609	4	-	11/33/109/115	-
20	BCR	B	801	-	-	2/29/63/63	0/2/2/2
23	DGD	8	301	-	-	14/28/68/95	0/2/2/2
17	CLA	B	838	-	-	9/27/103/115	-
17	CLA	b	612	4	-	8/19/95/115	-
17	CLA	T	406	-	-	10/21/97/115	-
17	CLA	A	5038	5	-	7/21/97/115	-
19	XAT	T	414	-	-	1/31/93/93	0/4/4/4
17	CLA	3	302	2	-	7/39/115/115	-
17	CLA	1	613	1	-	7/17/93/115	-
21	LHG	b	618	17	-	7/23/23/53	-
20	BCR	A	5050	-	-	2/29/63/63	0/2/2/2
16	CHL	b	606	-	-	8/19/95/117	-
17	CLA	A	5007	17	-	11/33/109/115	-
17	CLA	A	5032	5	-	6/15/91/115	-
17	CLA	B	841	-	-	13/39/115/115	-
17	CLA	B	809	6	-	12/33/109/115	-
17	CLA	T	408	18,13	-	7/21/97/115	-
17	CLA	a	611	1	-	8/17/93/115	-
17	CLA	B	821	-	-	8/13/89/115	-
17	CLA	1	603	1	-	6/15/91/115	-
17	CLA	A	5005	-	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	5009	5	-	15/39/115/115	-
17	CLA	b	610	21	-	8/21/97/115	-
17	CLA	7	302	3	-	13/33/109/115	-
20	BCR	1	617	1	-	5/29/63/63	0/2/2/2
17	CLA	A	5034	5	-	8/39/115/115	-
17	CLA	A	5037	5	-	9/21/97/115	-
17	CLA	B	811	6	-	8/21/97/115	-
17	CLA	A	5029	5	-	11/39/115/115	-
17	CLA	B	813	6	-	9/21/97/115	-
17	CLA	B	828	-	-	10/27/103/115	-
17	CLA	b	611	4	-	10/21/97/115	-
17	CLA	b	614	4	-	7/17/93/115	-
16	CHL	b	605	-	-	8/19/95/117	-

All (1460) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	8	306	CHL	MG-NA	7.52	2.24	2.06
16	3	322	CHL	MG-NA	7.12	2.23	2.06
16	8	306	CHL	MG-NC	7.00	2.22	2.06
16	7	305	CHL	MG-NA	6.62	2.22	2.06
16	1	606	CHL	MG-NA	6.60	2.21	2.06
16	T	401	CHL	MG-NC	6.58	2.21	2.06
16	a	606	CHL	MG-NA	6.50	2.21	2.06
16	c	306	CHL	MG-NA	6.32	2.21	2.06
16	1	601	CHL	MG-NA	6.25	2.21	2.06
16	7	305	CHL	MG-NC	6.23	2.21	2.06
16	7	307	CHL	MG-NA	6.20	2.21	2.06
16	3	301	CHL	MG-NC	6.16	2.20	2.06
16	8	308	CHL	MG-NA	6.14	2.20	2.06
16	3	322	CHL	MG-NC	6.04	2.20	2.06
16	b	607	CHL	MG-NA	6.02	2.20	2.06
16	1	601	CHL	MG-NC	5.97	2.20	2.06
16	a	601	CHL	MG-NC	5.96	2.20	2.06
16	c	306	CHL	MG-NC	5.94	2.20	2.06
16	c	304	CHL	MG-NA	5.93	2.20	2.06
27	A	5003	CL0	MG-NA	5.82	2.20	2.06
16	T	416	CHL	MG-NA	5.81	2.20	2.06
16	7	307	CHL	MG-NC	5.57	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	601	CHL	MG-NA	5.54	2.19	2.06
16	b	605	CHL	MG-NA	5.10	2.18	2.06
16	b	605	CHL	MG-NC	4.83	2.17	2.06
16	T	401	CHL	MG-NA	4.76	2.17	2.06
27	A	5003	CL0	MG-NC	4.75	2.17	2.06
16	8	307	CHL	MG-NA	4.61	2.17	2.06
16	c	305	CHL	MG-NA	4.59	2.17	2.06
16	7	306	CHL	MG-NA	4.55	2.17	2.06
16	T	416	CHL	MG-NC	4.53	2.17	2.06
16	b	606	CHL	MG-NA	4.49	2.16	2.06
17	B	828	CLA	MG-NA	4.42	2.16	2.06
17	8	313	CLA	MG-NC	4.37	2.16	2.06
16	3	301	CHL	MG-NA	4.23	2.16	2.06
16	b	606	CHL	MG-NC	4.22	2.16	2.06
16	c	305	CHL	MG-NC	4.01	2.15	2.06
16	8	307	CHL	MG-NC	3.98	2.15	2.06
16	1	606	CHL	MG-NC	3.97	2.15	2.06
16	b	607	CHL	MG-NC	3.94	2.15	2.06
17	F	5004	CLA	C1D-ND	3.79	1.42	1.37
17	T	405	CLA	C1D-ND	3.77	1.42	1.37
17	3	309	CLA	C1D-ND	3.76	1.42	1.37
17	T	409	CLA	C1D-ND	3.69	1.42	1.37
17	A	5019	CLA	C1D-ND	3.67	1.42	1.37
17	b	611	CLA	C1D-ND	3.67	1.42	1.37
17	a	612	CLA	C1D-ND	3.67	1.42	1.37
17	c	310	CLA	C1D-ND	3.65	1.42	1.37
17	8	305	CLA	C1D-ND	3.64	1.42	1.37
17	a	603	CLA	C1D-ND	3.63	1.42	1.37
17	8	313	CLA	C1D-ND	3.63	1.42	1.37
17	b	612	CLA	MG-ND	-3.63	1.98	2.05
17	b	601	CLA	C1D-ND	3.63	1.42	1.37
17	c	302	CLA	C1D-ND	3.62	1.42	1.37
17	a	608	CLA	C1D-ND	3.62	1.42	1.37
17	B	824	CLA	C1D-ND	3.61	1.42	1.37
17	B	822	CLA	C1D-ND	3.61	1.42	1.37
17	B	837	CLA	C1D-ND	3.60	1.42	1.37
17	b	603	CLA	C1D-ND	3.60	1.42	1.37
17	F	5009	CLA	C1D-ND	3.60	1.42	1.37
17	T	402	CLA	C1D-ND	3.60	1.42	1.37
17	a	610	CLA	C1D-ND	3.60	1.42	1.37
17	F	5007	CLA	C1D-ND	3.59	1.42	1.37
17	7	304	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	406	CLA	C1D-ND	3.59	1.42	1.37
16	7	306	CHL	MG-NC	3.58	2.14	2.06
17	A	5025	CLA	C1D-ND	3.58	1.42	1.37
17	1	605	CLA	C1D-ND	3.58	1.42	1.37
17	7	303	CLA	C1D-ND	3.58	1.42	1.37
17	1	611	CLA	C1D-ND	3.58	1.42	1.37
17	B	815	CLA	C1D-ND	3.58	1.42	1.37
17	K	201	CLA	C1D-ND	3.58	1.42	1.37
17	A	5009	CLA	C1D-ND	3.57	1.42	1.37
17	a	611	CLA	C1D-ND	3.57	1.42	1.37
17	B	825	CLA	MG-NA	3.57	2.14	2.06
17	3	302	CLA	C1D-ND	3.57	1.42	1.37
17	A	5038	CLA	C1D-ND	3.56	1.42	1.37
17	7	311	CLA	C1D-ND	3.56	1.42	1.37
17	L	202	CLA	C1D-ND	3.56	1.42	1.37
17	A	5029	CLA	C1D-ND	3.56	1.42	1.37
17	B	813	CLA	C1D-ND	3.55	1.42	1.37
17	3	303	CLA	C1D-ND	3.55	1.42	1.37
17	B	817	CLA	C1D-ND	3.55	1.42	1.37
17	B	816	CLA	C1D-ND	3.55	1.42	1.37
17	K	203	CLA	C1D-ND	3.55	1.42	1.37
17	a	607	CLA	C1D-ND	3.55	1.42	1.37
17	1	610	CLA	C1D-ND	3.55	1.42	1.37
17	8	312	CLA	C1D-ND	3.55	1.42	1.37
17	T	403	CLA	C1D-ND	3.55	1.42	1.37
16	8	308	CHL	MG-NC	3.55	2.14	2.06
17	B	821	CLA	C1D-ND	3.54	1.42	1.37
17	A	5014	CLA	C1D-ND	3.54	1.42	1.37
17	B	841	CLA	C1D-ND	3.54	1.42	1.37
17	8	304	CLA	C1D-ND	3.54	1.42	1.37
17	1	607	CLA	C1D-ND	3.54	1.42	1.37
17	b	610	CLA	C1D-ND	3.54	1.42	1.37
17	b	612	CLA	C1D-ND	3.54	1.42	1.37
17	7	310	CLA	C1D-ND	3.54	1.42	1.37
17	A	5032	CLA	C1D-ND	3.54	1.42	1.37
17	a	614	CLA	C1D-ND	3.54	1.42	1.37
17	A	5034	CLA	C1D-ND	3.53	1.42	1.37
17	B	811	CLA	C1D-ND	3.53	1.42	1.37
17	T	410	CLA	C1D-ND	3.53	1.42	1.37
17	3	313	CLA	C1D-ND	3.52	1.42	1.37
17	1	603	CLA	C1D-ND	3.52	1.42	1.37
17	c	313	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	608	CLA	C1D-ND	3.52	1.42	1.37
17	b	604	CLA	C1D-ND	3.52	1.42	1.37
17	B	820	CLA	C1D-ND	3.52	1.42	1.37
17	7	308	CLA	C1D-ND	3.52	1.42	1.37
17	7	312	CLA	C1D-ND	3.52	1.42	1.37
17	c	303	CLA	C1D-ND	3.51	1.42	1.37
17	A	5028	CLA	C1D-ND	3.51	1.42	1.37
17	T	411	CLA	C1D-ND	3.51	1.42	1.37
16	a	606	CHL	MG-NC	3.51	2.14	2.06
17	B	819	CLA	C1D-ND	3.51	1.42	1.37
17	7	313	CLA	C1D-ND	3.51	1.42	1.37
17	a	609	CLA	C1D-ND	3.51	1.42	1.37
17	1	612	CLA	C1D-ND	3.51	1.42	1.37
17	c	307	CLA	C1D-ND	3.51	1.42	1.37
17	c	301	CLA	C1D-ND	3.50	1.42	1.37
17	J	102	CLA	C1D-ND	3.50	1.42	1.37
17	B	835	CLA	C1D-ND	3.50	1.42	1.37
17	B	826	CLA	C1D-ND	3.50	1.42	1.37
17	A	5036	CLA	C1D-ND	3.50	1.42	1.37
17	a	604	CLA	C1D-ND	3.50	1.42	1.37
17	a	605	CLA	C1D-ND	3.50	1.42	1.37
17	8	309	CLA	C1D-ND	3.50	1.42	1.37
17	1	614	CLA	C1D-ND	3.49	1.42	1.37
17	A	5026	CLA	C1D-ND	3.49	1.42	1.37
17	7	312	CLA	MG-ND	-3.49	1.98	2.05
17	B	814	CLA	C1D-ND	3.49	1.42	1.37
17	8	302	CLA	C1D-ND	3.49	1.42	1.37
17	A	5012	CLA	C1D-ND	3.49	1.42	1.37
17	T	404	CLA	C1D-ND	3.49	1.42	1.37
17	T	412	CLA	C1D-ND	3.49	1.42	1.37
17	A	5010	CLA	C1D-ND	3.48	1.42	1.37
17	K	204	CLA	C1D-ND	3.48	1.42	1.37
17	a	613	CLA	C1D-ND	3.48	1.42	1.37
17	1	613	CLA	C1D-ND	3.48	1.42	1.37
17	8	303	CLA	C1D-ND	3.48	1.42	1.37
17	3	307	CLA	C1D-ND	3.48	1.42	1.37
17	F	5008	CLA	C1D-ND	3.48	1.42	1.37
17	B	830	CLA	C1D-ND	3.48	1.42	1.37
17	A	5042	CLA	C1D-ND	3.48	1.42	1.37
17	B	810	CLA	C1D-ND	3.48	1.42	1.37
17	3	308	CLA	C1D-ND	3.47	1.42	1.37
17	b	602	CLA	C1D-ND	3.47	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	314	CLA	C1D-ND	3.47	1.42	1.37
17	A	5023	CLA	C1D-ND	3.47	1.42	1.37
17	3	305	CLA	C1D-ND	3.47	1.42	1.37
17	8	311	CLA	C1D-ND	3.47	1.42	1.37
17	B	834	CLA	C1D-ND	3.47	1.42	1.37
17	A	5022	CLA	C1D-ND	3.47	1.42	1.37
17	A	5040	CLA	C1D-ND	3.46	1.42	1.37
17	7	314	CLA	C1D-ND	3.46	1.42	1.37
17	K	202	CLA	C1D-ND	3.46	1.42	1.37
17	A	5020	CLA	C1D-ND	3.46	1.42	1.37
17	B	812	CLA	C1D-ND	3.46	1.42	1.37
17	T	407	CLA	C1D-ND	3.45	1.42	1.37
17	B	806	CLA	C1D-ND	3.45	1.42	1.37
17	B	809	CLA	C1D-ND	3.45	1.42	1.37
17	B	828	CLA	C1D-ND	3.45	1.42	1.37
17	A	5033	CLA	C1D-ND	3.45	1.42	1.37
17	B	838	CLA	C1D-ND	3.45	1.42	1.37
17	c	309	CLA	C1D-ND	3.44	1.42	1.37
17	B	840	CLA	C1D-ND	3.44	1.42	1.37
17	B	832	CLA	C1D-ND	3.44	1.42	1.37
17	A	5031	CLA	C1D-ND	3.44	1.42	1.37
17	A	5017	CLA	C1D-ND	3.44	1.42	1.37
17	3	312	CLA	C1D-ND	3.43	1.42	1.37
17	A	5030	CLA	C1D-ND	3.43	1.42	1.37
17	c	311	CLA	C1D-ND	3.43	1.42	1.37
17	A	5007	CLA	C1D-ND	3.43	1.42	1.37
17	8	314	CLA	C1D-ND	3.43	1.42	1.37
17	a	602	CLA	C1D-ND	3.43	1.42	1.37
17	A	5037	CLA	C1D-ND	3.42	1.42	1.37
17	B	802	CLA	C1D-ND	3.42	1.42	1.37
17	T	408	CLA	C1D-ND	3.42	1.42	1.37
17	1	604	CLA	C1D-ND	3.42	1.42	1.37
17	8	310	CLA	C1D-ND	3.42	1.42	1.37
17	F	5006	CLA	C1D-ND	3.42	1.42	1.37
17	B	833	CLA	C1D-ND	3.41	1.42	1.37
17	B	818	CLA	C1D-ND	3.41	1.42	1.37
17	b	613	CLA	C1D-ND	3.41	1.42	1.37
17	c	312	CLA	C1D-ND	3.41	1.42	1.37
17	A	5024	CLA	C1D-ND	3.40	1.42	1.37
17	b	608	CLA	C1D-ND	3.40	1.42	1.37
17	c	308	CLA	C1D-ND	3.40	1.42	1.37
17	1	602	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5005	CLA	C1D-ND	3.40	1.42	1.37
17	A	5016	CLA	C1D-ND	3.40	1.42	1.37
17	1	609	CLA	C1D-ND	3.39	1.42	1.37
17	3	306	CLA	C1D-ND	3.39	1.42	1.37
17	B	827	CLA	C1D-ND	3.39	1.42	1.37
17	A	5041	CLA	C1D-ND	3.39	1.42	1.37
17	A	5035	CLA	C1D-ND	3.39	1.42	1.37
17	B	831	CLA	C1D-ND	3.39	1.42	1.37
17	3	304	CLA	C1D-ND	3.39	1.42	1.37
17	A	5011	CLA	C1D-ND	3.39	1.42	1.37
17	B	826	CLA	MG-NA	3.38	2.14	2.06
17	B	829	CLA	C1D-ND	3.38	1.42	1.37
17	8	315	CLA	C1D-ND	3.38	1.42	1.37
17	B	805	CLA	C1D-ND	3.37	1.42	1.37
17	7	302	CLA	C1D-ND	3.37	1.42	1.37
17	b	614	CLA	C1D-ND	3.37	1.42	1.37
17	B	823	CLA	C1D-ND	3.37	1.42	1.37
17	A	5043	CLA	C1D-ND	3.37	1.42	1.37
17	B	808	CLA	C1D-ND	3.37	1.42	1.37
17	B	839	CLA	C1D-ND	3.36	1.42	1.37
17	A	5039	CLA	C1D-ND	3.36	1.42	1.37
17	3	310	CLA	C1D-ND	3.35	1.42	1.37
17	A	5044	CLA	C1D-ND	3.35	1.42	1.37
17	b	609	CLA	C1D-ND	3.35	1.42	1.37
17	3	311	CLA	C1D-ND	3.35	1.42	1.37
17	A	5018	CLA	C1D-ND	3.34	1.42	1.37
17	A	5013	CLA	C1D-ND	3.34	1.42	1.37
17	B	804	CLA	C1D-ND	3.33	1.42	1.37
17	B	836	CLA	C1D-ND	3.33	1.42	1.37
17	3	324	CLA	C1D-ND	3.33	1.42	1.37
17	B	807	CLA	C1D-ND	3.33	1.42	1.37
17	7	309	CLA	C1D-ND	3.32	1.42	1.37
17	T	403	CLA	C4B-NB	3.31	1.42	1.37
17	A	5027	CLA	C1D-ND	3.30	1.42	1.37
17	A	5006	CLA	C1D-ND	3.28	1.42	1.37
17	A	5021	CLA	C1D-ND	3.25	1.42	1.37
17	B	825	CLA	C1D-ND	3.24	1.42	1.37
17	L	201	CLA	C1D-ND	3.24	1.42	1.37
17	A	5015	CLA	C1D-ND	3.24	1.42	1.37
17	B	839	CLA	C4B-NB	3.18	1.42	1.37
17	T	410	CLA	C4B-NB	3.18	1.42	1.37
17	A	5004	CLA	C1D-ND	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	611	CLA	C4B-NB	3.17	1.42	1.37
16	3	322	CHL	C1D-C2D	-3.17	1.39	1.45
17	a	610	CLA	C4B-NB	3.16	1.42	1.37
17	A	5042	CLA	C4B-NB	3.15	1.42	1.37
17	3	323	CLA	C1D-ND	3.15	1.42	1.37
16	c	304	CHL	MG-NC	3.15	2.13	2.06
17	b	601	CLA	C4B-NB	3.14	1.42	1.37
17	A	5027	CLA	MG-ND	-3.13	1.99	2.05
17	a	612	CLA	C4B-NB	3.13	1.42	1.37
17	A	5008	CLA	C1D-ND	3.13	1.42	1.37
17	b	612	CLA	C4B-NB	3.13	1.42	1.37
17	b	603	CLA	C4B-NB	3.12	1.42	1.37
17	7	311	CLA	C4B-NB	3.12	1.42	1.37
17	3	313	CLA	C4B-NB	3.12	1.42	1.37
17	a	614	CLA	C4B-NB	3.12	1.42	1.37
17	1	613	CLA	C4B-NB	3.11	1.42	1.37
17	B	841	CLA	C4B-NB	3.11	1.42	1.37
17	A	5004	CLA	C4B-NB	3.11	1.41	1.37
17	B	803	CLA	C1D-ND	3.11	1.41	1.37
17	F	5004	CLA	MG-ND	-3.11	1.99	2.05
17	7	304	CLA	C4B-NB	3.10	1.41	1.37
17	B	822	CLA	C4B-NB	3.10	1.41	1.37
17	L	202	CLA	C4B-NB	3.10	1.41	1.37
17	B	820	CLA	C4B-NB	3.10	1.41	1.37
17	c	309	CLA	C4B-NB	3.10	1.41	1.37
17	B	815	CLA	C4B-NB	3.10	1.41	1.37
17	A	5031	CLA	C1B-C2B	3.10	1.50	1.43
17	a	611	CLA	C4B-NB	3.10	1.41	1.37
17	A	5017	CLA	C4B-NB	3.08	1.41	1.37
17	1	607	CLA	C4B-NB	3.08	1.41	1.37
17	a	605	CLA	C4B-NB	3.08	1.41	1.37
17	8	305	CLA	C4B-NB	3.08	1.41	1.37
17	A	5010	CLA	C4B-NB	3.08	1.41	1.37
17	b	608	CLA	C4B-NB	3.08	1.41	1.37
17	T	409	CLA	C4B-NB	3.08	1.41	1.37
17	1	605	CLA	C4B-NB	3.08	1.41	1.37
17	F	5006	CLA	C4B-NB	3.08	1.41	1.37
17	T	411	CLA	C4B-NB	3.08	1.41	1.37
17	a	607	CLA	C4B-NB	3.07	1.41	1.37
17	1	612	CLA	C4B-NB	3.07	1.41	1.37
17	B	811	CLA	C4B-NB	3.07	1.41	1.37
17	1	610	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	201	CLA	C4B-NB	3.07	1.41	1.37
17	c	310	CLA	C4B-NB	3.07	1.41	1.37
17	8	312	CLA	C4B-NB	3.07	1.41	1.37
17	T	406	CLA	C4B-NB	3.07	1.41	1.37
17	T	403	CLA	MG-NB	-3.06	1.99	2.05
16	T	416	CHL	C1D-C2D	-3.06	1.39	1.45
17	1	603	CLA	C4B-NB	3.06	1.41	1.37
17	8	304	CLA	C4B-NB	3.06	1.41	1.37
17	B	833	CLA	C4B-NB	3.06	1.41	1.37
17	3	324	CLA	C4B-NB	3.05	1.41	1.37
17	A	5009	CLA	C4B-NB	3.05	1.41	1.37
17	A	5027	CLA	C4B-NB	3.05	1.41	1.37
17	c	313	CLA	C4B-NB	3.05	1.41	1.37
17	A	5036	CLA	C4B-NB	3.05	1.41	1.37
17	8	315	CLA	C4B-NB	3.05	1.41	1.37
17	A	5037	CLA	C4B-NB	3.05	1.41	1.37
17	b	604	CLA	C4B-NB	3.05	1.41	1.37
17	c	311	CLA	C4B-NB	3.05	1.41	1.37
17	7	314	CLA	C4B-NB	3.04	1.41	1.37
17	B	834	CLA	C4B-NB	3.04	1.41	1.37
17	B	829	CLA	C1B-C2B	3.04	1.50	1.43
17	1	602	CLA	C4B-NB	3.04	1.41	1.37
17	1	614	CLA	C4B-NB	3.04	1.41	1.37
17	8	311	CLA	C4B-NB	3.04	1.41	1.37
17	8	302	CLA	C4B-NB	3.04	1.41	1.37
17	3	309	CLA	C4B-NB	3.04	1.41	1.37
17	8	313	CLA	C4B-NB	3.04	1.41	1.37
17	A	5034	CLA	C4B-NB	3.03	1.41	1.37
16	a	601	CHL	C1D-C2D	-3.03	1.39	1.45
17	8	309	CLA	C4B-NB	3.03	1.41	1.37
17	F	5008	CLA	C4B-NB	3.03	1.41	1.37
17	c	303	CLA	C4B-NB	3.03	1.41	1.37
17	B	838	CLA	C4B-NB	3.03	1.41	1.37
17	c	307	CLA	C4B-NB	3.03	1.41	1.37
17	A	5032	CLA	C4B-NB	3.03	1.41	1.37
17	A	5023	CLA	C4B-NB	3.02	1.41	1.37
17	b	614	CLA	C4B-NB	3.02	1.41	1.37
17	F	5009	CLA	C4B-NB	3.02	1.41	1.37
17	A	5041	CLA	C4B-NB	3.02	1.41	1.37
17	B	802	CLA	MG-NC	3.02	2.13	2.06
17	7	308	CLA	C4B-NB	3.02	1.41	1.37
17	B	807	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5040	CLA	C4B-NB	3.02	1.41	1.37
17	a	602	CLA	C4B-NB	3.02	1.41	1.37
17	F	5004	CLA	MG-NA	3.02	2.13	2.06
27	A	5003	CL0	C1D-C2D	-3.02	1.39	1.45
17	A	5039	CLA	C4B-NB	3.01	1.41	1.37
17	B	837	CLA	C4B-NB	3.01	1.41	1.37
17	A	5012	CLA	C4B-NB	3.01	1.41	1.37
17	7	312	CLA	C4B-NB	3.01	1.41	1.37
17	B	809	CLA	C4B-NB	3.01	1.41	1.37
17	b	610	CLA	C4B-NB	3.01	1.41	1.37
17	L	201	CLA	C4B-NB	3.01	1.41	1.37
17	a	603	CLA	C4B-NB	3.00	1.41	1.37
17	A	5019	CLA	C4B-NB	3.00	1.41	1.37
17	7	303	CLA	MG-NA	3.00	2.13	2.06
17	A	5018	CLA	C4B-NB	3.00	1.41	1.37
17	T	407	CLA	C4B-NB	3.00	1.41	1.37
17	b	613	CLA	C4B-NB	3.00	1.41	1.37
17	B	824	CLA	C4B-NB	3.00	1.41	1.37
17	3	312	CLA	C4B-NB	3.00	1.41	1.37
17	A	5043	CLA	C4B-NB	2.99	1.41	1.37
17	T	412	CLA	C4B-NB	2.99	1.41	1.37
17	c	302	CLA	C4B-NB	2.99	1.41	1.37
17	B	812	CLA	C4B-NB	2.99	1.41	1.37
17	K	204	CLA	C4B-NB	2.99	1.41	1.37
17	K	202	CLA	C4B-NB	2.99	1.41	1.37
17	7	310	CLA	C4B-NB	2.99	1.41	1.37
17	B	830	CLA	C4B-NB	2.99	1.41	1.37
17	c	307	CLA	C3B-C4B	2.99	1.51	1.42
17	B	832	CLA	C4B-NB	2.99	1.41	1.37
17	B	818	CLA	C4B-NB	2.99	1.41	1.37
17	b	609	CLA	C4B-NB	2.99	1.41	1.37
17	B	816	CLA	C4B-NB	2.99	1.41	1.37
17	B	825	CLA	C4B-NB	2.99	1.41	1.37
17	3	306	CLA	C4B-NB	2.99	1.41	1.37
17	3	302	CLA	C4B-NB	2.98	1.41	1.37
17	3	311	CLA	C4B-NB	2.98	1.41	1.37
17	J	102	CLA	C4B-NB	2.98	1.41	1.37
17	a	613	CLA	C4B-NB	2.98	1.41	1.37
16	3	301	CHL	C1D-C2D	-2.98	1.39	1.45
17	B	804	CLA	C4B-NB	2.97	1.41	1.37
17	1	611	CLA	C4B-NB	2.97	1.41	1.37
17	B	826	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	304	CLA	C4B-NB	2.97	1.41	1.37
17	B	821	CLA	C4B-NB	2.97	1.41	1.37
17	B	810	CLA	C4B-NB	2.97	1.41	1.37
17	B	831	CLA	C4B-NB	2.97	1.41	1.37
17	A	5028	CLA	C4B-NB	2.96	1.41	1.37
17	A	5026	CLA	C4B-NB	2.96	1.41	1.37
17	B	828	CLA	C4B-NB	2.96	1.41	1.37
17	8	314	CLA	C4B-NB	2.95	1.41	1.37
17	7	313	CLA	C4B-NB	2.95	1.41	1.37
17	A	5007	CLA	C4B-NB	2.95	1.41	1.37
17	B	814	CLA	C4B-NB	2.95	1.41	1.37
17	T	408	CLA	C4B-NB	2.95	1.41	1.37
17	7	302	CLA	C4B-NB	2.95	1.41	1.37
17	A	5030	CLA	C4B-NB	2.95	1.41	1.37
17	A	5021	CLA	C4B-NB	2.95	1.41	1.37
17	B	819	CLA	C4B-NB	2.95	1.41	1.37
17	A	5005	CLA	C4B-NB	2.95	1.41	1.37
17	A	5033	CLA	C4B-NB	2.95	1.41	1.37
17	a	609	CLA	C4B-NB	2.94	1.41	1.37
17	A	5031	CLA	C4B-NB	2.94	1.41	1.37
17	3	314	CLA	C4B-NB	2.94	1.41	1.37
17	B	817	CLA	C4B-NB	2.94	1.41	1.37
17	T	402	CLA	C4B-NB	2.94	1.41	1.37
17	A	5022	CLA	C4B-NB	2.94	1.41	1.37
17	3	305	CLA	C4B-NB	2.93	1.41	1.37
17	c	301	CLA	C4B-NB	2.93	1.41	1.37
17	a	604	CLA	C3C-C4C	2.93	1.46	1.40
17	3	310	CLA	C4B-NB	2.93	1.41	1.37
17	A	5016	CLA	C4B-NB	2.92	1.41	1.37
17	A	5020	CLA	C4B-NB	2.92	1.41	1.37
17	A	5015	CLA	C4B-NB	2.92	1.41	1.37
16	7	305	CHL	C1D-C2D	-2.92	1.39	1.45
17	c	312	CLA	C4B-NB	2.92	1.41	1.37
17	1	608	CLA	C4B-NB	2.92	1.41	1.37
17	B	835	CLA	C4B-NB	2.92	1.41	1.37
17	F	5004	CLA	C4B-NB	2.92	1.41	1.37
17	A	5008	CLA	C4B-NB	2.92	1.41	1.37
17	A	5044	CLA	C4B-NB	2.92	1.41	1.37
17	A	5038	CLA	C4B-NB	2.92	1.41	1.37
17	1	604	CLA	C4B-NB	2.91	1.41	1.37
17	B	802	CLA	C4B-NB	2.91	1.41	1.37
17	b	602	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	840	CLA	C4B-NB	2.91	1.41	1.37
17	a	608	CLA	C4B-NB	2.91	1.41	1.37
17	1	605	CLA	MG-NC	2.91	2.13	2.06
17	A	5011	CLA	C4B-NB	2.91	1.41	1.37
17	A	5014	CLA	C4B-NB	2.90	1.41	1.37
16	8	306	CHL	C1D-C2D	-2.90	1.39	1.45
17	7	303	CLA	C4B-NB	2.90	1.41	1.37
17	7	309	CLA	C4B-NB	2.90	1.41	1.37
17	3	303	CLA	C4B-NB	2.90	1.41	1.37
17	F	5007	CLA	C4B-NB	2.90	1.41	1.37
17	A	5025	CLA	C4B-NB	2.89	1.41	1.37
17	a	604	CLA	C4B-NB	2.88	1.41	1.37
17	K	203	CLA	C4B-NB	2.88	1.41	1.37
16	7	307	CHL	C1D-C2D	-2.88	1.39	1.45
17	A	5029	CLA	C4B-NB	2.88	1.41	1.37
17	T	404	CLA	MG-NB	2.88	2.11	2.05
17	A	5024	CLA	C4B-NB	2.88	1.41	1.37
17	1	609	CLA	C4B-NB	2.88	1.41	1.37
16	b	605	CHL	C1D-C2D	-2.87	1.39	1.45
17	A	5036	CLA	C2C-C1C	2.87	1.46	1.40
17	8	310	CLA	C4B-NB	2.87	1.41	1.37
17	A	5006	CLA	C4B-NB	2.86	1.41	1.37
17	7	304	CLA	C1B-C2B	2.86	1.49	1.43
17	L	202	CLA	C1B-C2B	2.86	1.49	1.43
17	3	323	CLA	C4B-NB	2.86	1.41	1.37
17	c	313	CLA	C1B-C2B	2.86	1.49	1.43
17	8	303	CLA	C4B-NB	2.86	1.41	1.37
17	B	806	CLA	C4B-NB	2.86	1.41	1.37
17	c	311	CLA	C1B-C2B	2.86	1.49	1.43
17	A	5035	CLA	C4B-NB	2.85	1.41	1.37
17	B	805	CLA	C4B-NB	2.85	1.41	1.37
17	3	307	CLA	C4B-NB	2.85	1.41	1.37
17	T	404	CLA	C4B-NB	2.85	1.41	1.37
17	B	836	CLA	C4B-NB	2.85	1.41	1.37
17	3	308	CLA	C4B-NB	2.84	1.41	1.37
17	B	813	CLA	C4B-NB	2.84	1.41	1.37
17	B	823	CLA	C4B-NB	2.84	1.41	1.37
17	B	803	CLA	C4B-NB	2.84	1.41	1.37
17	K	201	CLA	C1B-C2B	2.84	1.49	1.43
17	c	308	CLA	C4B-NB	2.83	1.41	1.37
17	c	303	CLA	C1B-C2B	2.83	1.49	1.43
17	T	412	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	822	CLA	C1B-C2B	2.82	1.49	1.43
17	A	5035	CLA	C1B-C2B	2.82	1.49	1.43
17	3	323	CLA	C1B-C2B	2.82	1.49	1.43
17	B	823	CLA	C1B-C2B	2.82	1.49	1.43
17	B	811	CLA	C1B-C2B	2.82	1.49	1.43
17	a	603	CLA	C1B-C2B	2.82	1.49	1.43
17	B	808	CLA	C4B-NB	2.81	1.41	1.37
17	B	827	CLA	C4B-NB	2.81	1.41	1.37
17	T	405	CLA	C4B-NB	2.81	1.41	1.37
17	1	605	CLA	C1B-C2B	2.81	1.49	1.43
16	1	606	CHL	C1D-C2D	-2.81	1.39	1.45
17	b	611	CLA	C1B-C2B	2.80	1.49	1.43
17	A	5018	CLA	C1B-C2B	2.80	1.49	1.43
17	K	203	CLA	C1B-C2B	2.80	1.49	1.43
17	B	814	CLA	C1B-C2B	2.79	1.49	1.43
17	B	821	CLA	C1B-C2B	2.79	1.49	1.43
17	T	408	CLA	C1B-C2B	2.79	1.49	1.43
17	3	311	CLA	C1B-C2B	2.79	1.49	1.43
17	A	5017	CLA	C1B-C2B	2.79	1.49	1.43
17	3	313	CLA	C1B-C2B	2.79	1.49	1.43
17	A	5043	CLA	C1B-C2B	2.79	1.49	1.43
17	B	815	CLA	C1B-C2B	2.79	1.49	1.43
17	A	5006	CLA	C1B-C2B	2.79	1.49	1.43
17	b	614	CLA	C1B-C2B	2.79	1.49	1.43
17	T	409	CLA	C1B-C2B	2.78	1.49	1.43
17	F	5008	CLA	C1B-C2B	2.78	1.49	1.43
17	8	309	CLA	C1B-C2B	2.78	1.49	1.43
17	a	610	CLA	C1B-C2B	2.78	1.49	1.43
17	b	601	CLA	C1B-C2B	2.78	1.49	1.43
17	b	604	CLA	C1B-C2B	2.78	1.49	1.43
17	A	5025	CLA	C1B-C2B	2.78	1.49	1.43
17	L	202	CLA	MG-NA	2.77	2.12	2.06
17	8	312	CLA	C1B-C2B	2.77	1.49	1.43
17	B	810	CLA	C1B-C2B	2.77	1.49	1.43
17	B	812	CLA	C1B-C2B	2.77	1.49	1.43
16	b	607	CHL	C1D-C2D	-2.77	1.39	1.45
17	T	411	CLA	C1B-C2B	2.77	1.49	1.43
17	b	612	CLA	C1B-C2B	2.77	1.49	1.43
17	B	802	CLA	C1B-C2B	2.77	1.49	1.43
17	8	313	CLA	C1B-C2B	2.77	1.49	1.43
17	F	5009	CLA	C1B-C2B	2.76	1.49	1.43
17	B	807	CLA	C1B-C2B	2.76	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	611	CLA	C1B-C2B	2.76	1.49	1.43
17	a	613	CLA	C1B-C2B	2.76	1.49	1.43
17	B	813	CLA	C1B-C2B	2.76	1.49	1.43
17	K	204	CLA	C1B-C2B	2.76	1.49	1.43
17	8	304	CLA	MG-NA	2.76	2.12	2.06
17	B	820	CLA	C1B-C2B	2.76	1.49	1.43
17	7	312	CLA	C1B-C2B	2.76	1.49	1.43
17	c	312	CLA	C1B-C2B	2.75	1.49	1.43
17	B	808	CLA	C1B-C2B	2.75	1.49	1.43
17	3	303	CLA	C1B-C2B	2.75	1.49	1.43
17	c	309	CLA	C1B-C2B	2.75	1.49	1.43
17	B	835	CLA	C1B-C2B	2.75	1.49	1.43
16	c	306	CHL	C1D-C2D	-2.75	1.39	1.45
17	B	829	CLA	C4B-NB	2.75	1.41	1.37
17	a	611	CLA	C1B-C2B	2.75	1.49	1.43
17	1	612	CLA	C1B-C2B	2.75	1.49	1.43
17	7	311	CLA	C1B-C2B	2.75	1.49	1.43
17	b	610	CLA	C1B-C2B	2.75	1.49	1.43
17	A	5037	CLA	C1B-C2B	2.75	1.49	1.43
16	8	308	CHL	C1D-C2D	-2.75	1.39	1.45
17	a	612	CLA	C1B-C2B	2.74	1.49	1.43
16	c	304	CHL	C1D-C2D	-2.74	1.39	1.45
17	J	102	CLA	C1B-C2B	2.74	1.49	1.43
17	A	5026	CLA	C1B-C2B	2.74	1.49	1.43
17	A	5012	CLA	C1B-C2B	2.74	1.49	1.43
16	1	601	CHL	C1D-C2D	-2.74	1.39	1.45
17	B	809	CLA	C1B-C2B	2.74	1.49	1.43
17	T	406	CLA	C1B-C2B	2.74	1.49	1.43
17	T	402	CLA	C1B-C2B	2.74	1.49	1.43
17	1	607	CLA	C1B-C2B	2.74	1.49	1.43
16	T	401	CHL	C1D-C2D	-2.74	1.39	1.45
17	A	5023	CLA	C1B-C2B	2.73	1.49	1.43
17	F	5007	CLA	C1B-C2B	2.73	1.49	1.43
17	1	610	CLA	C1B-C2B	2.73	1.49	1.43
17	b	613	CLA	C1B-C2B	2.73	1.49	1.43
17	B	805	CLA	C1B-C2B	2.73	1.49	1.43
17	3	314	CLA	C1B-C2B	2.73	1.49	1.43
17	b	603	CLA	C1B-C2B	2.73	1.49	1.43
17	a	607	CLA	C1B-C2B	2.73	1.49	1.43
17	B	833	CLA	C1B-C2B	2.73	1.49	1.43
17	c	310	CLA	C1B-C2B	2.73	1.49	1.43
17	A	5036	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	608	CLA	C1B-C2B	2.73	1.49	1.43
17	8	304	CLA	C1B-C2B	2.72	1.49	1.43
17	8	315	CLA	C1B-C2B	2.72	1.49	1.43
17	T	407	CLA	C1B-C2B	2.72	1.49	1.43
17	7	308	CLA	C1B-C2B	2.72	1.49	1.43
17	7	303	CLA	C1B-C2B	2.72	1.49	1.43
17	8	305	CLA	C1B-C2B	2.72	1.49	1.43
17	B	830	CLA	C1B-C2B	2.72	1.49	1.43
17	K	202	CLA	C1B-C2B	2.72	1.49	1.43
17	A	5028	CLA	MG-NA	2.71	2.12	2.06
17	8	311	CLA	C1B-C2B	2.71	1.49	1.43
17	c	302	CLA	C1B-C2B	2.71	1.49	1.43
17	A	5016	CLA	C1B-C2B	2.71	1.49	1.43
17	T	405	CLA	C1B-C2B	2.71	1.49	1.43
17	B	826	CLA	C1B-C2B	2.71	1.49	1.43
17	1	608	CLA	C1B-C2B	2.71	1.49	1.43
17	7	310	CLA	C1B-C2B	2.71	1.49	1.43
17	b	602	CLA	C1B-C2B	2.71	1.49	1.43
17	A	5024	CLA	C1B-C2B	2.71	1.49	1.43
17	B	806	CLA	C1B-C2B	2.71	1.49	1.43
17	3	308	CLA	C1B-C2B	2.71	1.49	1.43
17	1	603	CLA	C1B-C2B	2.71	1.49	1.43
17	B	817	CLA	C1B-C2B	2.71	1.49	1.43
17	1	613	CLA	C1B-C2B	2.71	1.49	1.43
17	A	5008	CLA	C1B-C2B	2.71	1.49	1.43
17	A	5010	CLA	C1B-C2B	2.71	1.49	1.43
17	7	314	CLA	C1B-C2B	2.70	1.49	1.43
17	3	304	CLA	C1B-C2B	2.70	1.49	1.43
17	B	816	CLA	C1B-C2B	2.70	1.49	1.43
17	A	5034	CLA	C1B-C2B	2.70	1.49	1.43
17	b	608	CLA	C1B-C2B	2.70	1.49	1.43
17	1	602	CLA	C1B-C2B	2.70	1.49	1.43
17	a	609	CLA	C1B-C2B	2.70	1.49	1.43
17	A	5009	CLA	C1B-C2B	2.70	1.49	1.43
17	T	403	CLA	CMB-C2B	-2.70	1.45	1.50
17	B	827	CLA	C1B-C2B	2.70	1.49	1.43
17	T	404	CLA	C1B-C2B	2.70	1.49	1.43
17	A	5013	CLA	C4B-NB	2.70	1.41	1.37
17	3	302	CLA	C1B-C2B	2.69	1.49	1.43
17	A	5005	CLA	C1B-C2B	2.69	1.49	1.43
17	a	602	CLA	C1B-C2B	2.69	1.49	1.43
17	a	605	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	314	CLA	C1B-C2B	2.69	1.49	1.43
17	A	5040	CLA	C1B-C2B	2.69	1.49	1.43
17	B	819	CLA	C1B-C2B	2.69	1.49	1.43
17	c	301	CLA	C1B-C2B	2.69	1.49	1.43
17	3	312	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5027	CLA	C1B-C2B	2.68	1.49	1.43
17	B	838	CLA	MG-ND	-2.68	2.00	2.05
17	7	313	CLA	C1B-C2B	2.68	1.49	1.43
17	3	309	CLA	C1B-C2B	2.68	1.49	1.43
17	3	306	CLA	C1B-C2B	2.68	1.49	1.43
17	B	804	CLA	C1B-C2B	2.68	1.49	1.43
17	B	838	CLA	C1B-C2B	2.68	1.49	1.43
17	F	5004	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5032	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5029	CLA	C1B-C2B	2.68	1.49	1.43
17	B	834	CLA	C1B-C2B	2.68	1.49	1.43
17	8	302	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5014	CLA	C1B-C2B	2.68	1.49	1.43
17	B	818	CLA	C1B-C2B	2.68	1.49	1.43
17	B	832	CLA	C1B-C2B	2.68	1.49	1.43
17	B	837	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5013	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5038	CLA	C1B-C2B	2.68	1.49	1.43
17	A	5041	CLA	C1B-C2B	2.67	1.49	1.43
17	7	302	CLA	C1B-C2B	2.67	1.49	1.43
17	c	312	CLA	MG-NA	2.67	2.12	2.06
17	B	840	CLA	C1B-C2B	2.67	1.49	1.43
17	3	310	CLA	C1B-C2B	2.67	1.49	1.43
16	7	306	CHL	C1D-C2D	-2.67	1.40	1.45
17	1	604	CLA	C1B-C2B	2.67	1.49	1.43
17	B	841	CLA	C1B-C2B	2.67	1.49	1.43
17	A	5015	CLA	C1B-C2B	2.66	1.49	1.43
17	B	828	CLA	C1B-C2B	2.66	1.49	1.43
17	F	5006	CLA	C1B-C2B	2.66	1.49	1.43
17	A	5019	CLA	C1B-C2B	2.66	1.49	1.43
17	A	5022	CLA	C1B-C2B	2.66	1.49	1.43
17	A	5021	CLA	C1B-C2B	2.66	1.49	1.43
16	b	606	CHL	C1D-C2D	-2.66	1.40	1.45
16	a	606	CHL	C1D-C2D	-2.65	1.40	1.45
17	1	614	CLA	C1B-C2B	2.65	1.49	1.43
17	a	614	CLA	C1B-C2B	2.65	1.49	1.43
17	T	410	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5039	CLA	C1B-C2B	2.64	1.49	1.43
17	L	201	CLA	C1B-C2B	2.64	1.49	1.43
17	B	824	CLA	C1B-C2B	2.64	1.49	1.43
17	A	5028	CLA	C1B-C2B	2.63	1.49	1.43
17	1	609	CLA	C1B-C2B	2.63	1.49	1.43
17	A	5033	CLA	C1B-C2B	2.63	1.49	1.43
17	3	305	CLA	C1B-C2B	2.63	1.49	1.43
17	3	324	CLA	C1B-C2B	2.63	1.49	1.43
17	B	836	CLA	C1B-C2B	2.63	1.49	1.43
17	A	5007	CLA	C1B-C2B	2.63	1.49	1.43
17	T	403	CLA	MG-NA	2.62	2.12	2.06
17	8	303	CLA	C1B-C2B	2.62	1.49	1.43
17	A	5027	CLA	CMD-C2D	-2.62	1.45	1.50
17	A	5030	CLA	C1B-C2B	2.61	1.49	1.43
17	b	609	CLA	C1B-C2B	2.61	1.49	1.43
17	B	803	CLA	C1B-C2B	2.60	1.49	1.43
16	8	307	CHL	C1D-C2D	-2.60	1.40	1.45
17	B	831	CLA	C1B-C2B	2.60	1.49	1.43
16	c	305	CHL	C1D-C2D	-2.60	1.40	1.45
17	A	5044	CLA	C1B-C2B	2.59	1.49	1.43
17	B	825	CLA	C1B-C2B	2.58	1.49	1.43
17	c	308	CLA	C1B-C2B	2.58	1.49	1.43
17	1	609	CLA	CMC-C2C	-2.58	1.45	1.50
17	3	307	CLA	C1B-C2B	2.58	1.49	1.43
17	A	5004	CLA	C1B-C2B	2.57	1.49	1.43
17	A	5042	CLA	C1B-C2B	2.57	1.49	1.43
17	B	839	CLA	CMB-C2B	-2.56	1.45	1.50
17	B	839	CLA	C1B-C2B	2.56	1.49	1.43
17	A	5011	CLA	C1B-C2B	2.55	1.49	1.43
17	T	403	CLA	MG-ND	-2.55	2.00	2.05
17	A	5020	CLA	C1B-C2B	2.54	1.49	1.43
17	a	604	CLA	C1B-C2B	2.54	1.49	1.43
17	A	5027	CLA	MG-NB	-2.53	2.00	2.05
17	A	5010	CLA	MG-ND	-2.51	2.00	2.05
17	T	404	CLA	C3B-C4B	2.51	1.50	1.42
17	c	308	CLA	CHC-C1C	2.49	1.43	1.38
17	8	310	CLA	C1B-C2B	2.49	1.49	1.43
17	7	309	CLA	C1B-C2B	2.49	1.49	1.43
17	8	312	CLA	MG-ND	-2.48	2.00	2.05
17	1	603	CLA	MG-NA	2.47	2.12	2.06
17	A	5044	CLA	CHC-C1C	2.47	1.43	1.38
17	A	5032	CLA	MG-ND	-2.46	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5042	CLA	MG-NB	-2.45	2.00	2.05
17	8	311	CLA	MG-NA	2.44	2.12	2.06
17	c	308	CLA	C3B-C4B	2.44	1.49	1.42
17	B	824	CLA	C3B-C4B	2.43	1.49	1.42
17	7	309	CLA	C3B-C4B	2.42	1.49	1.42
17	A	5007	CLA	C3B-C4B	2.42	1.49	1.42
17	8	303	CLA	C3B-C4B	2.42	1.49	1.42
17	B	805	CLA	C3B-C4B	2.42	1.49	1.42
17	7	302	CLA	CHC-C1C	2.41	1.43	1.38
17	T	404	CLA	CHC-C1C	2.41	1.43	1.38
17	A	5008	CLA	CHC-C1C	2.41	1.43	1.38
17	A	5015	CLA	C3B-C4B	2.41	1.49	1.42
17	A	5010	CLA	MG-NA	2.40	2.12	2.06
17	A	5029	CLA	C3B-C4B	2.40	1.49	1.42
17	T	402	CLA	MG-NA	2.40	2.12	2.06
17	B	825	CLA	C3B-C4B	2.39	1.49	1.42
17	A	5021	CLA	MG-ND	-2.39	2.01	2.05
17	A	5016	CLA	C3B-C4B	2.39	1.49	1.42
17	b	601	CLA	C3B-C4B	2.38	1.49	1.42
17	A	5044	CLA	C3B-C4B	2.38	1.49	1.42
17	1	614	CLA	C3B-C4B	2.38	1.49	1.42
17	1	611	CLA	C3B-C4B	2.38	1.49	1.42
17	1	604	CLA	C3B-C4B	2.38	1.49	1.42
17	A	5004	CLA	C3B-C4B	2.38	1.49	1.42
17	1	608	CLA	C3B-C4B	2.38	1.49	1.42
17	3	312	CLA	C3B-C4B	2.38	1.49	1.42
17	B	807	CLA	C3B-C4B	2.38	1.49	1.42
17	3	309	CLA	C3B-C4B	2.38	1.49	1.42
17	B	804	CLA	C3B-C4B	2.38	1.49	1.42
17	b	609	CLA	CHC-C1C	2.37	1.43	1.38
17	b	609	CLA	C3B-C4B	2.37	1.49	1.42
17	a	609	CLA	C3B-C4B	2.37	1.49	1.42
17	A	5038	CLA	MG-ND	-2.37	2.01	2.05
17	A	5042	CLA	CMB-C2B	-2.37	1.45	1.50
17	b	603	CLA	MG-NA	2.37	2.11	2.06
17	8	303	CLA	CHC-C1C	2.37	1.43	1.38
17	T	412	CLA	C3B-C4B	2.37	1.49	1.42
17	1	602	CLA	CHC-C1C	2.37	1.43	1.38
17	3	312	CLA	CHC-C1C	2.37	1.43	1.38
17	B	816	CLA	C3B-C4B	2.36	1.49	1.42
17	B	838	CLA	CHC-C1C	2.36	1.43	1.38
17	K	201	CLA	C3B-C4B	2.36	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	201	CLA	CHC-C1C	2.36	1.43	1.38
17	7	302	CLA	C3B-C4B	2.36	1.49	1.42
17	B	836	CLA	C3B-C4B	2.36	1.49	1.42
17	B	824	CLA	CHC-C1C	2.36	1.43	1.38
17	1	607	CLA	C3B-C4B	2.36	1.49	1.42
17	B	833	CLA	CHC-C1C	2.36	1.43	1.38
17	8	311	CLA	C3B-C4B	2.35	1.49	1.42
17	T	403	CLA	C3B-C4B	2.35	1.49	1.42
17	1	612	CLA	C3B-C4B	2.35	1.49	1.42
17	8	305	CLA	C3B-C4B	2.35	1.49	1.42
17	8	310	CLA	C3B-C4B	2.35	1.49	1.42
17	A	5037	CLA	C3B-C4B	2.35	1.49	1.42
17	B	804	CLA	CHC-C1C	2.35	1.43	1.38
17	B	829	CLA	CHC-C1C	2.35	1.43	1.38
17	a	602	CLA	C3B-C4B	2.35	1.49	1.42
17	F	5007	CLA	C3B-C4B	2.35	1.49	1.42
17	K	202	CLA	C3B-C4B	2.35	1.49	1.42
17	1	608	CLA	CHC-C1C	2.35	1.43	1.38
17	3	304	CLA	C3B-C4B	2.35	1.49	1.42
17	F	5008	CLA	C3B-C4B	2.35	1.49	1.42
17	A	5008	CLA	C3B-C4B	2.34	1.49	1.42
17	B	805	CLA	CHC-C1C	2.34	1.43	1.38
17	A	5019	CLA	C3B-C4B	2.34	1.49	1.42
17	B	828	CLA	C3B-C4B	2.34	1.49	1.42
17	B	837	CLA	C3B-C4B	2.34	1.49	1.42
17	8	309	CLA	C3B-C4B	2.34	1.49	1.42
17	8	309	CLA	CHC-C1C	2.34	1.43	1.38
17	1	613	CLA	C3B-C4B	2.34	1.49	1.42
17	B	840	CLA	C3B-C4B	2.34	1.49	1.42
17	A	5030	CLA	C3B-C4B	2.34	1.49	1.42
17	3	304	CLA	CMD-C2D	-2.34	1.46	1.50
17	c	301	CLA	CHC-C1C	2.34	1.43	1.38
17	A	5034	CLA	C3B-C4B	2.34	1.49	1.42
17	a	603	CLA	C3B-C4B	2.34	1.49	1.42
17	T	409	CLA	C3B-C4B	2.34	1.49	1.42
17	A	5022	CLA	C3B-C4B	2.34	1.49	1.42
17	T	405	CLA	C3B-C4B	2.34	1.49	1.42
17	B	831	CLA	C3B-C4B	2.34	1.49	1.42
17	a	609	CLA	CHC-C1C	2.34	1.43	1.38
17	B	831	CLA	MG-ND	-2.34	2.01	2.05
17	K	204	CLA	CHC-C1C	2.33	1.43	1.38
17	b	611	CLA	MG-NC	2.33	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	825	CLA	CHC-C1C	2.33	1.43	1.38
17	A	5010	CLA	C3B-C4B	2.33	1.49	1.42
17	8	302	CLA	C3B-C4B	2.33	1.49	1.42
17	b	611	CLA	C3B-C4B	2.33	1.49	1.42
17	B	820	CLA	CHC-C1C	2.33	1.43	1.38
17	8	305	CLA	CHC-C1C	2.33	1.43	1.38
17	c	303	CLA	C3B-C4B	2.33	1.49	1.42
17	B	827	CLA	C3B-C4B	2.33	1.49	1.42
17	a	611	CLA	C3B-C4B	2.33	1.49	1.42
17	A	5040	CLA	C3B-C4B	2.33	1.49	1.42
17	1	614	CLA	CHC-C1C	2.33	1.43	1.38
17	A	5009	CLA	C3B-C4B	2.33	1.49	1.42
17	B	828	CLA	CHC-C1C	2.32	1.43	1.38
17	B	803	CLA	C3B-C4B	2.32	1.49	1.42
17	a	613	CLA	C3B-C4B	2.32	1.49	1.42
17	J	102	CLA	C3B-C4B	2.32	1.49	1.42
17	A	5036	CLA	CHC-C1C	2.32	1.43	1.38
17	A	5028	CLA	C3B-C4B	2.32	1.49	1.42
17	A	5012	CLA	MG-ND	-2.32	2.01	2.05
17	F	5006	CLA	C3B-C4B	2.32	1.49	1.42
17	8	305	CLA	MG-NA	2.32	2.11	2.06
17	7	304	CLA	MG-NA	2.32	2.11	2.06
17	b	603	CLA	C3B-C4B	2.32	1.49	1.42
17	b	604	CLA	C3B-C4B	2.32	1.49	1.42
17	B	833	CLA	C3B-C4B	2.32	1.49	1.42
17	8	312	CLA	C3B-C4B	2.32	1.49	1.42
17	7	313	CLA	CHC-C1C	2.32	1.43	1.38
17	A	5024	CLA	C3B-C4B	2.32	1.49	1.42
17	1	604	CLA	CHC-C1C	2.32	1.43	1.38
17	3	304	CLA	CHC-C1C	2.32	1.43	1.38
17	1	603	CLA	C3B-C4B	2.32	1.49	1.42
17	A	5005	CLA	C3B-C4B	2.32	1.49	1.42
17	B	814	CLA	CMB-C2B	-2.32	1.46	1.50
17	A	5011	CLA	C3B-C4B	2.32	1.49	1.42
17	B	813	CLA	C3B-C4B	2.32	1.49	1.42
17	b	610	CLA	C3B-C4B	2.32	1.49	1.42
17	1	609	CLA	CHC-C1C	2.32	1.43	1.38
17	T	412	CLA	CHC-C1C	2.32	1.43	1.38
17	c	307	CLA	C1B-C2B	2.32	1.48	1.43
17	T	410	CLA	C3B-C4B	2.32	1.49	1.42
17	A	5015	CLA	CHC-C1C	2.32	1.43	1.38
17	B	803	CLA	CHC-C1C	2.32	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	602	CLA	C3B-C4B	2.32	1.49	1.42
17	F	5004	CLA	C3B-C4B	2.32	1.49	1.42
17	1	607	CLA	CHC-C1C	2.32	1.43	1.38
17	c	307	CLA	CHC-C1C	2.32	1.43	1.38
17	1	609	CLA	C3B-C4B	2.32	1.49	1.42
17	B	816	CLA	CHC-C1C	2.32	1.43	1.38
17	7	309	CLA	CHC-C1C	2.31	1.43	1.38
17	3	324	CLA	C3B-C4B	2.31	1.49	1.42
17	B	826	CLA	CHC-C1C	2.31	1.43	1.38
17	B	838	CLA	C3B-C4B	2.31	1.49	1.42
17	c	309	CLA	C3B-C4B	2.31	1.49	1.42
17	3	302	CLA	MG-NA	2.31	2.11	2.06
17	a	605	CLA	C3B-C4B	2.31	1.49	1.42
17	c	302	CLA	C3B-C4B	2.31	1.49	1.42
17	B	810	CLA	C3B-C4B	2.31	1.49	1.42
17	1	610	CLA	CHC-C1C	2.31	1.43	1.38
17	A	5030	CLA	CHC-C1C	2.31	1.43	1.38
17	8	313	CLA	C3B-C4B	2.31	1.49	1.42
17	A	5019	CLA	MG-ND	-2.31	2.01	2.05
17	B	821	CLA	C3B-C4B	2.31	1.49	1.42
17	B	815	CLA	C3B-C4B	2.31	1.49	1.42
17	K	204	CLA	C3B-C4B	2.31	1.49	1.42
17	A	5007	CLA	CHC-C1C	2.31	1.43	1.38
17	A	5016	CLA	CHC-C1C	2.31	1.43	1.38
17	A	5043	CLA	C3B-C4B	2.31	1.49	1.42
17	c	310	CLA	C3B-C4B	2.31	1.49	1.42
17	7	308	CLA	CHC-C1C	2.31	1.43	1.38
17	8	314	CLA	C3B-C4B	2.30	1.49	1.42
17	T	402	CLA	C3B-C4B	2.30	1.49	1.42
17	T	408	CLA	C3B-C4B	2.30	1.49	1.42
17	A	5010	CLA	CHC-C1C	2.30	1.43	1.38
17	B	823	CLA	C3B-C4B	2.30	1.49	1.42
17	b	602	CLA	C3B-C4B	2.30	1.49	1.42
17	3	314	CLA	C3B-C4B	2.30	1.49	1.42
17	B	817	CLA	C3B-C4B	2.30	1.49	1.42
17	B	830	CLA	C3B-C4B	2.30	1.49	1.42
17	c	301	CLA	C3B-C4B	2.30	1.49	1.42
17	B	811	CLA	C3B-C4B	2.30	1.49	1.42
17	F	5009	CLA	C3B-C4B	2.30	1.49	1.42
17	A	5024	CLA	CHC-C1C	2.30	1.43	1.38
17	T	403	CLA	CHC-C1C	2.30	1.43	1.38
17	A	5014	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	612	CLA	C3B-C4B	2.30	1.49	1.42
17	7	310	CLA	CHC-C1C	2.30	1.43	1.38
17	T	411	CLA	C3B-C4B	2.30	1.49	1.42
17	b	603	CLA	CHC-C1C	2.30	1.43	1.38
17	7	311	CLA	C3B-C4B	2.30	1.49	1.42
17	B	826	CLA	C3B-C4B	2.30	1.49	1.42
17	T	407	CLA	C3B-C4B	2.29	1.49	1.42
17	a	607	CLA	C3B-C4B	2.29	1.49	1.42
17	B	834	CLA	C3B-C4B	2.29	1.49	1.42
17	3	308	CLA	C3B-C4B	2.29	1.49	1.42
17	A	5023	CLA	C3B-C4B	2.29	1.49	1.42
17	a	614	CLA	C3B-C4B	2.29	1.49	1.42
17	L	202	CLA	C3B-C4B	2.29	1.49	1.42
17	A	5026	CLA	MG-ND	-2.29	2.01	2.05
17	7	310	CLA	C3B-C4B	2.29	1.49	1.42
17	B	821	CLA	CHC-C1C	2.29	1.43	1.38
17	F	5006	CLA	CHC-C1C	2.29	1.43	1.38
17	7	303	CLA	C3B-C4B	2.29	1.49	1.42
17	a	612	CLA	C3B-C4B	2.29	1.49	1.42
17	B	831	CLA	CHC-C1C	2.29	1.43	1.38
17	B	829	CLA	C3B-C4B	2.29	1.49	1.42
17	A	5006	CLA	C3B-C4B	2.29	1.49	1.42
17	A	5020	CLA	C3B-C4B	2.29	1.49	1.42
17	B	841	CLA	C3B-C4B	2.29	1.49	1.42
17	a	608	CLA	C3B-C4B	2.29	1.49	1.42
17	B	818	CLA	C3B-C4B	2.29	1.49	1.42
17	8	304	CLA	C3B-C4B	2.29	1.49	1.42
17	a	604	CLA	C3B-C4B	2.29	1.49	1.42
17	b	608	CLA	CHC-C1C	2.29	1.43	1.38
17	1	605	CLA	C3B-C4B	2.29	1.49	1.42
17	1	610	CLA	C3B-C4B	2.29	1.49	1.42
17	A	5014	CLA	CHC-C1C	2.29	1.43	1.38
17	B	836	CLA	CHC-C1C	2.29	1.43	1.38
17	K	203	CLA	C3B-C4B	2.29	1.49	1.42
17	c	309	CLA	CHC-C1C	2.29	1.43	1.38
17	A	5027	CLA	C3B-C4B	2.29	1.49	1.42
17	K	202	CLA	CHC-C1C	2.28	1.43	1.38
17	A	5035	CLA	C3B-C4B	2.28	1.49	1.42
17	a	613	CLA	CHC-C1C	2.28	1.43	1.38
17	T	410	CLA	CHC-C1C	2.28	1.43	1.38
17	a	614	CLA	CHC-C1C	2.28	1.43	1.38
17	b	611	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	314	CLA	C3B-C4B	2.28	1.49	1.42
17	F	5007	CLA	CHC-C1C	2.28	1.43	1.38
17	A	5041	CLA	C3B-C4B	2.28	1.49	1.42
17	B	812	CLA	C3B-C4B	2.28	1.49	1.42
17	T	406	CLA	C3B-C4B	2.28	1.49	1.42
17	7	308	CLA	C3B-C4B	2.28	1.49	1.42
17	A	5028	CLA	CHC-C1C	2.28	1.43	1.38
17	3	313	CLA	C3B-C4B	2.28	1.49	1.42
17	3	323	CLA	C3B-C4B	2.28	1.49	1.42
17	3	307	CLA	C3B-C4B	2.28	1.49	1.42
17	a	604	CLA	CHC-C1C	2.28	1.43	1.38
17	b	613	CLA	C3B-C4B	2.28	1.49	1.42
17	b	604	CLA	CHC-C1C	2.28	1.43	1.38
17	c	312	CLA	CHC-C1C	2.28	1.43	1.38
17	B	822	CLA	C3B-C4B	2.28	1.49	1.42
17	F	5008	CLA	CHC-C1C	2.28	1.43	1.38
17	a	610	CLA	CHC-C1C	2.28	1.43	1.38
17	a	607	CLA	CHC-C1C	2.28	1.43	1.38
17	T	407	CLA	CHC-C1C	2.27	1.43	1.38
17	B	820	CLA	C3B-C4B	2.27	1.49	1.42
17	c	312	CLA	CMD-C2D	-2.27	1.46	1.50
17	3	310	CLA	C3B-C4B	2.27	1.49	1.42
17	8	315	CLA	CHC-C1C	2.27	1.43	1.38
17	b	608	CLA	C3B-C4B	2.27	1.49	1.42
17	8	311	CLA	CHC-C1C	2.27	1.43	1.38
17	8	310	CLA	CHC-C1C	2.27	1.43	1.38
17	b	602	CLA	CHC-C1C	2.27	1.43	1.38
17	b	613	CLA	CHC-C1C	2.27	1.43	1.38
17	1	613	CLA	CHC-C1C	2.27	1.43	1.38
17	b	610	CLA	CHC-C1C	2.27	1.43	1.38
17	b	609	CLA	CMC-C2C	-2.27	1.46	1.50
17	3	302	CLA	C3B-C4B	2.27	1.49	1.42
17	7	313	CLA	C3B-C4B	2.27	1.49	1.42
17	J	102	CLA	CHC-C1C	2.27	1.43	1.38
17	3	311	CLA	C3B-C4B	2.27	1.49	1.42
17	B	835	CLA	C3B-C4B	2.27	1.49	1.42
17	c	311	CLA	C3B-C4B	2.27	1.49	1.42
17	c	312	CLA	C3B-C4B	2.27	1.49	1.42
17	B	806	CLA	CHC-C1C	2.27	1.43	1.38
17	A	5019	CLA	CHC-C1C	2.27	1.43	1.38
17	a	610	CLA	C3B-C4B	2.26	1.49	1.42
17	8	312	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5013	CLA	C3B-C4B	2.26	1.49	1.42
17	B	808	CLA	C3B-C4B	2.26	1.49	1.42
17	A	5040	CLA	CHC-C1C	2.26	1.43	1.38
17	B	832	CLA	C3B-C4B	2.26	1.49	1.42
17	b	614	CLA	CHC-C1C	2.26	1.43	1.38
17	A	5039	CLA	C3B-C4B	2.26	1.49	1.42
17	B	817	CLA	CHC-C1C	2.26	1.43	1.38
17	T	406	CLA	CHC-C1C	2.26	1.43	1.38
17	8	315	CLA	C3B-C4B	2.26	1.49	1.42
17	B	829	CLA	CMD-C2D	-2.26	1.46	1.50
17	B	806	CLA	C3B-C4B	2.26	1.49	1.42
17	3	311	CLA	CHC-C1C	2.26	1.43	1.38
17	3	324	CLA	CHC-C1C	2.26	1.43	1.38
17	A	5011	CLA	CHC-C1C	2.26	1.43	1.38
17	1	612	CLA	CHC-C1C	2.26	1.43	1.38
17	A	5041	CLA	CHC-C1C	2.26	1.43	1.38
17	A	5025	CLA	C3B-C4B	2.26	1.49	1.42
17	A	5026	CLA	C3B-C4B	2.26	1.49	1.42
17	1	611	CLA	CHC-C1C	2.26	1.43	1.38
17	B	834	CLA	CHC-C1C	2.26	1.43	1.38
17	T	409	CLA	CHC-C1C	2.25	1.43	1.38
17	1	603	CLA	CHC-C1C	2.25	1.43	1.38
17	A	5039	CLA	CHC-C1C	2.25	1.43	1.38
17	A	5022	CLA	CHC-C1C	2.25	1.43	1.38
17	A	5034	CLA	CHC-C1C	2.25	1.43	1.38
17	A	5012	CLA	CHC-C1C	2.25	1.43	1.38
17	B	838	CLA	MG-NA	2.25	2.11	2.06
17	3	303	CLA	C3B-C4B	2.25	1.49	1.42
17	8	304	CLA	CHC-C1C	2.25	1.43	1.38
17	B	811	CLA	CHC-C1C	2.25	1.43	1.38
17	B	808	CLA	MG-ND	-2.25	2.01	2.05
17	7	312	CLA	C3B-C4B	2.25	1.49	1.42
17	A	5026	CLA	CHC-C1C	2.25	1.43	1.38
17	T	408	CLA	CHC-C1C	2.25	1.43	1.38
17	A	5037	CLA	CHC-C1C	2.25	1.43	1.38
17	T	411	CLA	CHC-C1C	2.25	1.43	1.38
17	c	303	CLA	CHC-C1C	2.25	1.43	1.38
17	a	602	CLA	CHC-C1C	2.24	1.43	1.38
17	a	611	CLA	CHC-C1C	2.24	1.43	1.38
17	b	614	CLA	C3B-C4B	2.24	1.49	1.42
17	B	819	CLA	CMB-C2B	-2.24	1.46	1.50
17	3	306	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	302	CLA	CHC-C1C	2.24	1.43	1.38
17	A	5012	CLA	C3B-C4B	2.24	1.49	1.42
17	B	809	CLA	CMB-C2B	-2.24	1.46	1.50
17	a	605	CLA	CHC-C1C	2.24	1.43	1.38
17	3	313	CLA	CHC-C1C	2.24	1.43	1.38
17	A	5033	CLA	C3B-C4B	2.24	1.49	1.42
17	B	822	CLA	CHC-C1C	2.24	1.43	1.38
17	T	405	CLA	MG-NA	2.24	2.11	2.06
17	A	5006	CLA	CMD-C2D	-2.24	1.46	1.50
17	B	815	CLA	CHC-C1C	2.24	1.43	1.38
17	8	314	CLA	CHC-C1C	2.23	1.43	1.38
17	T	405	CLA	CHC-C1C	2.23	1.43	1.38
17	8	310	CLA	CMB-C2B	-2.23	1.46	1.50
17	3	309	CLA	CHC-C1C	2.23	1.43	1.38
17	B	824	CLA	CMD-C2D	-2.23	1.46	1.50
17	A	5029	CLA	CHC-C1C	2.23	1.43	1.38
17	A	5032	CLA	C3B-C4B	2.23	1.49	1.42
17	c	310	CLA	CHC-C1C	2.23	1.43	1.38
17	A	5036	CLA	C3B-C4B	2.23	1.49	1.42
17	K	201	CLA	MG-NA	2.23	2.11	2.06
17	A	5042	CLA	C3B-C4B	2.23	1.49	1.42
17	8	313	CLA	CHC-C1C	2.23	1.43	1.38
17	B	839	CLA	MG-NC	2.23	2.11	2.06
17	B	823	CLA	CHC-C1C	2.23	1.42	1.38
17	1	605	CLA	CHC-C1C	2.23	1.42	1.38
17	F	5004	CLA	CHC-C1C	2.23	1.42	1.38
17	c	302	CLA	CHC-C1C	2.23	1.42	1.38
17	A	5031	CLA	C3B-C4B	2.22	1.49	1.42
17	B	819	CLA	MG-ND	-2.22	2.01	2.05
17	A	5031	CLA	CHC-C1C	2.22	1.42	1.38
17	a	609	CLA	CMC-C2C	-2.22	1.46	1.50
17	B	812	CLA	CHC-C1C	2.22	1.42	1.38
17	A	5020	CLA	CMB-C2B	-2.22	1.46	1.50
17	A	5018	CLA	C3B-C4B	2.22	1.49	1.42
17	B	840	CLA	CHC-C1C	2.22	1.42	1.38
17	A	5043	CLA	CHC-C1C	2.22	1.42	1.38
17	A	5023	CLA	CHC-C1C	2.22	1.42	1.38
17	b	612	CLA	CHC-C1C	2.22	1.42	1.38
17	1	611	CLA	MG-NA	2.22	2.11	2.06
17	A	5033	CLA	CHC-C1C	2.22	1.42	1.38
17	a	612	CLA	CHC-C1C	2.22	1.42	1.38
17	A	5017	CLA	C3B-C4B	2.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5004	CLA	CMB-C2B	-2.21	1.46	1.50
17	3	314	CLA	CHC-C1C	2.21	1.42	1.38
17	c	311	CLA	CHC-C1C	2.21	1.42	1.38
17	A	5004	CLA	CHC-C1C	2.21	1.42	1.38
17	A	5020	CLA	CHC-C1C	2.21	1.42	1.38
17	b	601	CLA	CHC-C1C	2.21	1.42	1.38
17	a	608	CLA	CHC-C1C	2.21	1.42	1.38
17	L	201	CLA	C3B-C4B	2.21	1.49	1.42
17	A	5008	CLA	CMC-C2C	-2.21	1.46	1.50
17	F	5009	CLA	CHC-C1C	2.21	1.42	1.38
17	B	819	CLA	C3B-C4B	2.21	1.49	1.42
17	B	835	CLA	MG-ND	-2.21	2.01	2.05
17	A	5021	CLA	C3B-C4B	2.21	1.49	1.42
17	B	814	CLA	C3B-C4B	2.21	1.49	1.42
17	c	313	CLA	C3B-C4B	2.20	1.49	1.42
17	B	813	CLA	CHC-C1C	2.20	1.42	1.38
17	A	5035	CLA	CHC-C1C	2.20	1.42	1.38
17	B	832	CLA	CMB-C2B	-2.20	1.46	1.50
17	3	307	CLA	CHC-C1C	2.20	1.42	1.38
17	8	312	CLA	MG-NA	2.20	2.11	2.06
17	B	837	CLA	CHC-C1C	2.20	1.42	1.38
18	c	314	LUT	C22-C23	-2.20	1.50	1.52
17	c	307	CLA	C1B-NB	-2.20	1.35	1.37
17	A	5023	CLA	MG-ND	-2.20	2.01	2.05
17	B	838	CLA	CMD-C2D	-2.20	1.46	1.50
17	7	304	CLA	CHC-C1C	2.20	1.42	1.38
17	B	827	CLA	CHC-C1C	2.19	1.42	1.38
17	b	612	CLA	CMD-C2D	-2.19	1.46	1.50
17	a	604	CLA	C1C-C2C	2.19	1.46	1.42
17	B	802	CLA	C3B-C4B	2.19	1.49	1.42
17	L	201	CLA	CHC-C1C	2.19	1.42	1.38
17	A	5027	CLA	CHC-C1C	2.19	1.42	1.38
17	7	303	CLA	CHC-C1C	2.19	1.42	1.38
17	A	5011	CLA	CMB-C2B	-2.19	1.46	1.50
17	B	824	CLA	MG-ND	-2.19	2.01	2.05
27	A	5003	CL0	C4B-NB	2.19	1.40	1.37
17	A	5004	CLA	CMC-C2C	-2.19	1.46	1.50
17	8	313	CLA	CMD-C2D	-2.19	1.46	1.50
17	B	808	CLA	CMC-C2C	-2.19	1.46	1.50
17	B	809	CLA	C3B-C4B	2.18	1.49	1.42
17	A	5004	CLA	CMD-C2D	-2.18	1.46	1.50
17	B	825	CLA	CMC-C2C	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	311	CLA	CHC-C1C	2.18	1.42	1.38
17	B	825	CLA	CMD-C2D	-2.18	1.46	1.50
17	a	602	CLA	CMD-C2D	-2.18	1.46	1.50
17	c	311	CLA	CMD-C2D	-2.18	1.46	1.50
17	7	304	CLA	C3B-C4B	2.18	1.49	1.42
17	A	5022	CLA	CMB-C2B	-2.18	1.46	1.50
17	B	830	CLA	CHC-C1C	2.18	1.42	1.38
17	B	834	CLA	CMB-C2B	-2.18	1.46	1.50
17	a	608	CLA	CMB-C2B	-2.18	1.46	1.50
17	B	807	CLA	CHC-C1C	2.17	1.42	1.38
17	B	841	CLA	CHC-C1C	2.17	1.42	1.38
17	B	810	CLA	CHC-C1C	2.17	1.42	1.38
17	3	305	CLA	C3B-C4B	2.17	1.49	1.42
17	A	5038	CLA	C3B-C4B	2.17	1.49	1.42
17	A	5006	CLA	CHC-C1C	2.17	1.42	1.38
17	A	5018	CLA	CHC-C1C	2.17	1.42	1.38
17	3	323	CLA	CMD-C2D	-2.17	1.46	1.50
17	7	309	CLA	CMB-C2B	-2.16	1.46	1.50
17	8	302	CLA	CHC-C1C	2.16	1.42	1.38
17	K	203	CLA	CHC-C1C	2.16	1.42	1.38
17	3	306	CLA	CMB-C2B	-2.16	1.46	1.50
17	A	5032	CLA	CHC-C1C	2.16	1.42	1.38
17	A	5036	CLA	CMB-C2B	-2.16	1.46	1.50
17	A	5037	CLA	MG-ND	-2.16	2.01	2.05
17	7	304	CLA	CMB-C2B	-2.16	1.46	1.50
17	3	303	CLA	CHC-C1C	2.16	1.42	1.38
17	b	611	CLA	CMD-C2D	-2.16	1.46	1.50
17	3	310	CLA	CHC-C1C	2.15	1.42	1.38
17	B	809	CLA	MG-ND	-2.15	2.01	2.05
17	B	818	CLA	CHC-C1C	2.15	1.42	1.38
17	7	314	CLA	CHC-C1C	2.15	1.42	1.38
17	B	832	CLA	CHC-C1C	2.15	1.42	1.38
17	c	310	CLA	MG-ND	-2.15	2.01	2.05
16	1	606	CHL	C1C-NC	-2.15	1.34	1.37
17	F	5006	CLA	CMD-C2D	-2.15	1.46	1.50
17	7	314	CLA	CMD-C2D	-2.15	1.46	1.50
17	3	323	CLA	CHC-C1C	2.15	1.42	1.38
17	B	832	CLA	CMD-C2D	-2.15	1.46	1.50
17	3	306	CLA	CHC-C1C	2.14	1.42	1.38
17	T	402	CLA	CHC-C1C	2.14	1.42	1.38
17	A	5019	CLA	MG-NB	-2.14	2.01	2.05
17	b	613	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	841	CLA	CMB-C2B	-2.14	1.46	1.50
17	3	309	CLA	CMB-C2B	-2.14	1.46	1.50
17	A	5009	CLA	CHC-C1C	2.14	1.42	1.38
17	A	5017	CLA	CMB-C2B	-2.14	1.46	1.50
17	B	827	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	5016	CLA	MG-ND	-2.14	2.01	2.05
17	a	603	CLA	CHC-C1C	2.14	1.42	1.38
17	A	5017	CLA	CHC-C1C	2.14	1.42	1.38
17	7	313	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	802	CLA	CHC-C1C	2.13	1.42	1.38
17	A	5032	CLA	CMB-C2B	-2.13	1.46	1.50
17	A	5009	CLA	MG-ND	-2.13	2.01	2.05
17	a	607	CLA	MG-ND	-2.13	2.01	2.05
17	7	302	CLA	CMD-C2D	-2.13	1.46	1.50
16	T	416	CHL	C1C-NC	-2.13	1.34	1.37
17	T	404	CLA	CMD-C2D	-2.13	1.46	1.50
17	3	324	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	808	CLA	CMD-C2D	-2.13	1.46	1.50
17	7	312	CLA	CHC-C1C	2.13	1.42	1.38
17	B	802	CLA	CMD-C2D	-2.13	1.46	1.50
17	A	5005	CLA	CHC-C1C	2.13	1.42	1.38
17	L	201	CLA	MG-NA	2.13	2.11	2.06
17	F	5004	CLA	MG-NC	2.13	2.11	2.06
17	3	305	CLA	MG-ND	-2.13	2.01	2.05
17	B	828	CLA	CMB-C2B	-2.13	1.46	1.50
17	A	5019	CLA	CMC-C2C	-2.13	1.46	1.50
17	A	5021	CLA	CMD-C2D	-2.13	1.46	1.50
17	B	819	CLA	CHC-C1C	2.12	1.42	1.38
17	T	408	CLA	CMB-C2B	-2.12	1.46	1.50
18	7	315	LUT	C22-C23	-2.12	1.50	1.52
17	B	810	CLA	MG-ND	-2.12	2.01	2.05
17	B	835	CLA	CHC-C1C	2.12	1.42	1.38
17	3	305	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	5032	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	5017	CLA	CMD-C2D	-2.12	1.46	1.50
17	c	310	CLA	MG-NA	2.12	2.11	2.06
17	8	312	CLA	CMD-C2D	-2.12	1.46	1.50
17	3	302	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	5026	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	5033	CLA	MG-NB	-2.12	2.01	2.05
17	B	831	CLA	CMD-C2D	-2.12	1.46	1.50
17	B	817	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	605	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	5025	CLA	CHC-C1C	2.12	1.42	1.38
17	7	311	CLA	CMC-C2C	-2.12	1.46	1.50
17	B	841	CLA	CMD-C2D	-2.11	1.46	1.50
17	1	605	CLA	CMB-C2B	-2.11	1.46	1.50
17	A	5014	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	839	CLA	CMD-C2D	-2.11	1.46	1.50
17	3	308	CLA	CHC-C1C	2.11	1.42	1.38
17	L	202	CLA	CHC-C1C	2.11	1.42	1.38
17	A	5044	CLA	CMD-C2D	-2.11	1.46	1.50
17	c	313	CLA	CHC-C1C	2.11	1.42	1.38
17	A	5013	CLA	CMD-C2D	-2.11	1.46	1.50
17	A	5014	CLA	CMC-C2C	-2.11	1.46	1.50
17	c	313	CLA	CMD-C2D	-2.11	1.46	1.50
16	7	306	CHL	C1C-NC	-2.11	1.34	1.37
17	B	803	CLA	CMD-C2D	-2.11	1.46	1.50
17	B	839	CLA	C3B-C4B	2.10	1.48	1.42
17	A	5033	CLA	CMD-C2D	-2.10	1.46	1.50
17	b	603	CLA	CMD-C2D	-2.10	1.46	1.50
17	8	305	CLA	CMB-C2B	-2.10	1.46	1.50
17	A	5012	CLA	CMD-C2D	-2.10	1.46	1.50
17	c	313	CLA	CMB-C2B	-2.10	1.46	1.50
17	T	410	CLA	MG-NC	2.10	2.11	2.06
17	1	609	CLA	CMB-C2B	-2.10	1.46	1.50
17	A	5042	CLA	CMD-C2D	-2.10	1.46	1.50
17	3	311	CLA	CMB-C2B	-2.10	1.46	1.50
17	3	310	CLA	MG-NA	2.10	2.11	2.06
17	B	806	CLA	MG-ND	-2.10	2.01	2.05
17	B	835	CLA	CMD-C2D	-2.10	1.46	1.50
17	c	308	CLA	CMD-C2D	-2.10	1.46	1.50
17	3	305	CLA	MG-NB	-2.10	2.01	2.05
17	F	5004	CLA	CMD-C2D	-2.10	1.46	1.50
17	c	302	CLA	CMD-C2D	-2.10	1.46	1.50
17	A	5040	CLA	CMD-C2D	-2.10	1.46	1.50
17	c	308	CLA	CMC-C2C	-2.10	1.46	1.50
17	B	830	CLA	CMD-C2D	-2.10	1.46	1.50
17	3	302	CLA	CMB-C2B	-2.10	1.46	1.50
17	b	608	CLA	CMD-C2D	-2.10	1.46	1.50
17	A	5024	CLA	CMD-C2D	-2.09	1.46	1.50
17	c	303	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	5013	CLA	CMB-C2B	-2.09	1.46	1.50
16	a	601	CHL	C1C-NC	-2.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	302	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	5008	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	5018	CLA	CMB-C2B	-2.09	1.46	1.50
17	A	5028	CLA	CMC-C2C	-2.09	1.46	1.50
17	B	808	CLA	CHC-C1C	2.09	1.42	1.38
17	A	5037	CLA	CMB-C2B	-2.09	1.46	1.50
17	B	803	CLA	CMB-C2B	-2.09	1.46	1.50
17	B	814	CLA	CHC-C1C	2.09	1.42	1.38
17	A	5030	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	837	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	804	CLA	CMB-C2B	-2.09	1.46	1.50
17	T	408	CLA	CMD-C2D	-2.09	1.46	1.50
17	3	308	CLA	CMD-C2D	-2.09	1.46	1.50
17	3	303	CLA	CMB-C2B	-2.09	1.46	1.50
17	3	307	CLA	CMD-C2D	-2.09	1.46	1.50
17	8	311	CLA	CMD-C2D	-2.09	1.46	1.50
17	1	612	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	5018	CLA	CMC-C2C	-2.09	1.46	1.50
17	T	403	CLA	CMD-C2D	-2.09	1.46	1.50
17	A	5040	CLA	MG-ND	-2.09	2.01	2.05
17	K	201	CLA	CMB-C2B	-2.09	1.46	1.50
17	B	828	CLA	CMD-C2D	-2.09	1.46	1.50
17	B	807	CLA	CMB-C2B	-2.09	1.46	1.50
17	1	611	CLA	CMD-C2D	-2.08	1.46	1.50
17	c	309	CLA	CMB-C2B	-2.08	1.46	1.50
17	A	5021	CLA	CHC-C1C	2.08	1.42	1.38
17	A	5019	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	836	CLA	CMD-C2D	-2.08	1.46	1.50
17	a	607	CLA	CMD-C2D	-2.08	1.46	1.50
16	b	607	CHL	C1C-NC	-2.08	1.34	1.37
17	B	839	CLA	MG-NB	-2.08	2.01	2.05
17	L	201	CLA	CMD-C2D	-2.08	1.46	1.50
17	A	5038	CLA	CHC-C1C	2.08	1.42	1.38
17	7	303	CLA	CMD-C2D	-2.08	1.46	1.50
17	a	611	CLA	CMC-C2C	-2.08	1.46	1.50
17	8	311	CLA	CMB-C2B	-2.08	1.46	1.50
17	8	315	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	806	CLA	CMB-C2B	-2.08	1.46	1.50
17	8	304	CLA	CMD-C2D	-2.08	1.46	1.50
17	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
17	b	602	CLA	CMD-C2D	-2.08	1.46	1.50
17	3	314	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	5006	CLA	CMB-C2B	-2.08	1.46	1.50
17	B	822	CLA	CMB-C2B	-2.08	1.46	1.50
17	a	609	CLA	CMD-C2D	-2.08	1.46	1.50
17	T	411	CLA	CMB-C2B	-2.08	1.46	1.50
17	A	5025	CLA	CMB-C2B	-2.08	1.46	1.50
17	B	806	CLA	CMC-C2C	-2.08	1.46	1.50
17	B	809	CLA	CHC-C1C	2.08	1.42	1.38
17	B	818	CLA	CMD-C2D	-2.08	1.46	1.50
17	F	5009	CLA	CMD-C2D	-2.08	1.46	1.50
17	b	614	CLA	CMD-C2D	-2.08	1.46	1.50
17	T	412	CLA	CMB-C2B	-2.08	1.46	1.50
17	B	836	CLA	CMB-C2B	-2.08	1.46	1.50
17	3	324	CLA	CMB-C2B	-2.08	1.46	1.50
17	A	5005	CLA	CMB-C2B	-2.08	1.46	1.50
17	c	303	CLA	CMB-C2B	-2.08	1.46	1.50
17	8	314	CLA	CMD-C2D	-2.07	1.46	1.50
17	a	612	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5011	CLA	MG-ND	-2.07	2.01	2.05
17	A	5021	CLA	CMB-C2B	-2.07	1.46	1.50
17	7	312	CLA	CMD-C2D	-2.07	1.46	1.50
17	c	310	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5038	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	803	CLA	CMC-C2C	-2.07	1.46	1.50
17	b	604	CLA	MG-NA	2.07	2.11	2.06
17	3	310	CLA	CMB-C2B	-2.07	1.46	1.50
17	A	5011	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5019	CLA	CMB-C2B	-2.07	1.46	1.50
17	K	202	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5005	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5012	CLA	CMB-C2B	-2.07	1.46	1.50
17	A	5041	CLA	CMB-C2B	-2.07	1.46	1.50
17	a	607	CLA	CMB-C2B	-2.07	1.46	1.50
17	A	5029	CLA	CMD-C2D	-2.07	1.46	1.50
17	A	5030	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	823	CLA	CMB-C2B	-2.07	1.46	1.50
17	A	5020	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	807	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	830	CLA	CMB-C2B	-2.07	1.46	1.50
16	b	606	CHL	C1C-NC	-2.07	1.34	1.37
17	A	5042	CLA	CHC-C1C	2.07	1.42	1.38
17	3	311	CLA	CMD-C2D	-2.07	1.46	1.50
17	7	311	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	311	CLA	CMB-C2B	-2.07	1.46	1.50
17	7	312	CLA	CMB-C2B	-2.07	1.46	1.50
17	B	818	CLA	CMC-C2C	-2.07	1.46	1.50
17	3	324	CLA	MG-ND	-2.07	2.01	2.05
17	b	601	CLA	CMD-C2D	-2.07	1.46	1.50
17	B	819	CLA	CMD-C2D	-2.06	1.46	1.50
17	c	302	CLA	CMC-C2C	-2.06	1.46	1.50
17	1	608	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	811	CLA	CMB-C2B	-2.06	1.46	1.50
17	A	5013	CLA	CHC-C1C	2.06	1.42	1.38
17	a	612	CLA	CMB-C2B	-2.06	1.46	1.50
17	1	602	CLA	CMB-C2B	-2.06	1.46	1.50
17	3	309	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	806	CLA	CMD-C2D	-2.06	1.46	1.50
17	B	824	CLA	CMC-C2C	-2.06	1.46	1.50
17	3	305	CLA	CMD-C2D	-2.06	1.46	1.50
17	8	309	CLA	CMB-C2B	-2.06	1.46	1.50
17	b	612	CLA	CMB-C2B	-2.06	1.46	1.50
17	8	309	CLA	CMD-C2D	-2.06	1.46	1.50
17	3	310	CLA	CMC-C2C	-2.06	1.46	1.50
17	A	5025	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	5034	CLA	CMB-C2B	-2.06	1.46	1.50
17	7	303	CLA	CMC-C2C	-2.06	1.46	1.50
17	A	5028	CLA	CMB-C2B	-2.06	1.46	1.50
17	A	5024	CLA	CMB-C2B	-2.06	1.46	1.50
17	8	303	CLA	CMB-C2B	-2.06	1.46	1.50
17	L	202	CLA	CMD-C2D	-2.06	1.46	1.50
17	c	307	CLA	MG-NA	2.06	2.11	2.06
17	3	302	CLA	CMC-C2C	-2.06	1.46	1.50
17	T	406	CLA	CMD-C2D	-2.06	1.46	1.50
17	a	610	CLA	CMD-C2D	-2.06	1.46	1.50
17	A	5009	CLA	CMD-C2D	-2.05	1.46	1.50
17	8	312	CLA	MG-NC	2.05	2.11	2.06
17	B	810	CLA	CMB-C2B	-2.05	1.46	1.50
17	a	603	CLA	CMB-C2B	-2.05	1.46	1.50
17	A	5041	CLA	CMD-C2D	-2.05	1.46	1.50
17	3	314	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	5016	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	831	CLA	CMB-C2B	-2.05	1.46	1.50
16	a	606	CHL	C1C-NC	-2.05	1.34	1.37
17	3	305	CLA	CHC-C1C	2.05	1.42	1.38
17	8	313	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	602	CLA	CMB-C2B	-2.05	1.46	1.50
17	a	614	CLA	CMD-C2D	-2.05	1.46	1.50
17	3	313	CLA	CMD-C2D	-2.05	1.46	1.50
17	b	604	CLA	CMB-C2B	-2.05	1.46	1.50
17	a	604	CLA	CMD-C2D	-2.05	1.46	1.50
17	L	202	CLA	CMB-C2B	-2.05	1.46	1.50
17	3	312	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	5018	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	5040	CLA	CMB-C2B	-2.05	1.46	1.50
17	B	815	CLA	CMD-C2D	-2.05	1.46	1.50
17	a	602	CLA	CMC-C2C	-2.05	1.46	1.50
17	a	614	CLA	CMB-C2B	-2.05	1.46	1.50
17	b	614	CLA	CMB-C2B	-2.05	1.46	1.50
17	B	812	CLA	CMB-C2B	-2.05	1.46	1.50
17	B	818	CLA	CMB-C2B	-2.05	1.46	1.50
17	a	611	CLA	CMB-C2B	-2.05	1.46	1.50
17	b	611	CLA	CMB-C2B	-2.05	1.46	1.50
17	3	313	CLA	CMB-C2B	-2.05	1.46	1.50
17	c	301	CLA	CMB-C2B	-2.05	1.46	1.50
17	K	204	CLA	CMB-C2B	-2.05	1.46	1.50
17	7	308	CLA	CMB-C2B	-2.05	1.46	1.50
17	T	406	CLA	CMB-C2B	-2.05	1.46	1.50
17	B	802	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	5043	CLA	CMB-C2B	-2.05	1.46	1.50
17	7	309	CLA	CMD-C2D	-2.05	1.46	1.50
17	B	820	CLA	CMD-C2D	-2.05	1.46	1.50
17	8	305	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	5015	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	5028	CLA	CMD-C2D	-2.05	1.46	1.50
17	A	5012	CLA	CMC-C2C	-2.05	1.46	1.50
17	A	5026	CLA	CMB-C2B	-2.05	1.46	1.50
17	A	5031	CLA	CMD-C2D	-2.05	1.46	1.50
17	J	102	CLA	CMD-C2D	-2.05	1.46	1.50
17	3	303	CLA	CMD-C2D	-2.05	1.46	1.50
17	3	308	CLA	CMB-C2B	-2.04	1.46	1.50
17	A	5009	CLA	CMB-C2B	-2.04	1.46	1.50
17	B	804	CLA	CMD-C2D	-2.04	1.46	1.50
17	F	5007	CLA	CMC-C2C	-2.04	1.46	1.50
17	B	838	CLA	CMB-C2B	-2.04	1.46	1.50
17	A	5035	CLA	CMD-C2D	-2.04	1.46	1.50
17	7	304	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	840	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	609	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	5010	CLA	CMB-C2B	-2.04	1.46	1.50
17	a	613	CLA	CMB-C2B	-2.04	1.46	1.50
17	b	603	CLA	CMB-C2B	-2.04	1.46	1.50
17	1	614	CLA	CMD-C2D	-2.04	1.46	1.50
17	K	203	CLA	CMC-C2C	-2.04	1.46	1.50
17	a	603	CLA	CMD-C2D	-2.04	1.46	1.50
17	1	604	CLA	CMB-C2B	-2.04	1.46	1.50
17	c	309	CLA	CMD-C2D	-2.04	1.46	1.50
17	7	314	CLA	CMB-C2B	-2.04	1.46	1.50
17	A	5010	CLA	CMC-C2C	-2.04	1.46	1.50
17	K	203	CLA	CMD-C2D	-2.04	1.46	1.50
17	8	314	CLA	CMB-C2B	-2.04	1.46	1.50
17	B	833	CLA	CMB-C2B	-2.04	1.46	1.50
17	T	402	CLA	CMD-C2D	-2.04	1.46	1.50
17	b	609	CLA	CMD-C2D	-2.04	1.46	1.50
17	7	302	CLA	CMB-C2B	-2.04	1.46	1.50
17	F	5008	CLA	CMB-C2B	-2.04	1.46	1.50
17	A	5016	CLA	CMB-C2B	-2.03	1.46	1.50
17	A	5033	CLA	CMB-C2B	-2.03	1.46	1.50
17	b	613	CLA	CMB-C2B	-2.03	1.46	1.50
17	7	302	CLA	CMC-C2C	-2.03	1.46	1.50
17	A	5035	CLA	CMB-C2B	-2.03	1.46	1.50
17	F	5006	CLA	CMB-C2B	-2.03	1.46	1.50
17	b	604	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	816	CLA	CMD-C2D	-2.03	1.46	1.50
17	b	603	CLA	CMC-C2C	-2.03	1.46	1.50
17	1	610	CLA	CMD-C2D	-2.03	1.46	1.50
17	8	303	CLA	CMD-C2D	-2.03	1.46	1.50
17	b	609	CLA	CMB-C2B	-2.03	1.46	1.50
17	B	808	CLA	CMB-C2B	-2.03	1.46	1.50
17	c	308	CLA	CMB-C2B	-2.03	1.46	1.50
17	A	5037	CLA	CMD-C2D	-2.03	1.46	1.50
17	A	5006	CLA	CMC-C2C	-2.03	1.46	1.50
17	T	405	CLA	CMB-C2B	-2.03	1.46	1.50
17	A	5039	CLA	CMB-C2B	-2.03	1.46	1.50
17	A	5016	CLA	CMC-C2C	-2.03	1.46	1.50
17	A	5022	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	805	CLA	CMC-C2C	-2.03	1.46	1.50
16	8	307	CHL	C1C-NC	-2.03	1.34	1.37
17	7	303	CLA	CMB-C2B	-2.03	1.46	1.50
17	K	204	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	613	CLA	CMD-C2D	-2.03	1.46	1.50
17	3	306	CLA	CMC-C2C	-2.03	1.46	1.50
16	c	305	CHL	C1C-NC	-2.03	1.34	1.37
17	7	313	CLA	CMB-C2B	-2.03	1.46	1.50
17	F	5007	CLA	CMD-C2D	-2.03	1.46	1.50
17	c	302	CLA	CMB-C2B	-2.02	1.46	1.50
17	1	603	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	820	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	816	CLA	CMB-C2B	-2.02	1.46	1.50
17	b	610	CLA	CMD-C2D	-2.02	1.46	1.50
17	K	202	CLA	CMB-C2B	-2.02	1.46	1.50
17	a	613	CLA	CMD-C2D	-2.02	1.46	1.50
17	F	5008	CLA	CMD-C2D	-2.02	1.46	1.50
17	c	301	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	839	CLA	CHC-C1C	2.02	1.42	1.38
17	c	307	CLA	CMD-C2D	-2.02	1.46	1.50
17	3	307	CLA	CMB-C2B	-2.02	1.46	1.50
17	A	5043	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	822	CLA	CMD-C2D	-2.02	1.46	1.50
17	8	312	CLA	CMB-C2B	-2.02	1.46	1.50
17	A	5044	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	814	CLA	CMC-C2C	-2.02	1.46	1.50
17	F	5007	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	802	CLA	CMB-C2B	-2.02	1.46	1.50
17	B	814	CLA	CMD-C2D	-2.02	1.46	1.50
17	7	309	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	840	CLA	CMB-C2B	-2.02	1.46	1.50
17	T	410	CLA	CMB-C2B	-2.02	1.46	1.50
17	a	608	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	5010	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	812	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	5020	CLA	MG-ND	-2.02	2.01	2.05
17	a	605	CLA	CMD-C2D	-2.02	1.46	1.50
17	1	613	CLA	CMB-C2B	-2.02	1.46	1.50
17	1	603	CLA	CMD-C2D	-2.02	1.46	1.50
17	1	607	CLA	CMD-C2D	-2.02	1.46	1.50
17	1	611	CLA	CMC-C2C	-2.02	1.46	1.50
17	A	5035	CLA	CMC-C2C	-2.02	1.46	1.50
17	8	305	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
17	T	402	CLA	CMB-C2B	-2.02	1.46	1.50
17	T	409	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	202	CLA	MG-NB	-2.02	2.01	2.05
17	1	604	CLA	CMD-C2D	-2.02	1.46	1.50
17	A	5023	CLA	CMD-C2D	-2.02	1.46	1.50
17	F	5009	CLA	CMB-C2B	-2.02	1.46	1.50
17	A	5036	CLA	CMD-C2D	-2.01	1.46	1.50
17	3	306	CLA	CMD-C2D	-2.01	1.46	1.50
17	8	304	CLA	CMB-C2B	-2.01	1.46	1.50
17	A	5009	CLA	CMC-C2C	-2.01	1.46	1.50
17	A	5043	CLA	CMC-C2C	-2.01	1.46	1.50
17	T	412	CLA	CMD-C2D	-2.01	1.46	1.50
17	3	323	CLA	CMB-C2B	-2.01	1.46	1.50
17	A	5038	CLA	CMB-C2B	-2.01	1.46	1.50
17	a	611	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	611	CLA	CMB-C2B	-2.01	1.46	1.50
17	a	612	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	826	CLA	CMC-C2C	-2.01	1.46	1.50
17	8	315	CLA	CMB-C2B	-2.01	1.46	1.50
17	8	310	CLA	CMD-C2D	-2.01	1.46	1.50
17	3	304	CLA	CMC-C2C	-2.01	1.46	1.50
17	T	408	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	804	CLA	CMC-C2C	-2.01	1.46	1.50
17	1	602	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	827	CLA	CMB-C2B	-2.01	1.46	1.50
17	T	407	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	832	CLA	MG-NA	2.01	2.11	2.06
17	A	5025	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	821	CLA	CMB-C2B	-2.01	1.46	1.50
17	c	310	CLA	CMB-C2B	-2.01	1.46	1.50
17	F	5004	CLA	CMB-C2B	-2.01	1.46	1.50
17	B	833	CLA	CMD-C2D	-2.01	1.46	1.50
17	A	5031	CLA	CMC-C2C	-2.01	1.46	1.50
17	B	811	CLA	CMD-C2D	-2.01	1.46	1.50
17	T	407	CLA	CMD-C2D	-2.01	1.46	1.50
17	1	611	CLA	MG-NC	2.01	2.11	2.06
17	a	607	CLA	MG-NA	2.01	2.11	2.06
17	T	411	CLA	CMD-C2D	-2.01	1.46	1.50
17	T	403	CLA	C1B-C2B	2.01	1.47	1.43
17	B	834	CLA	CMD-C2D	-2.01	1.46	1.50
17	A	5005	CLA	CMC-C2C	-2.01	1.46	1.50
17	A	5030	CLA	CMC-C2C	-2.01	1.46	1.50
17	F	5004	CLA	CMC-C2C	-2.00	1.46	1.50
17	K	201	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	407	CLA	CMB-C2B	-2.00	1.46	1.50
17	A	5039	CLA	CMD-C2D	-2.00	1.46	1.50
17	B	815	CLA	CMB-C2B	-2.00	1.46	1.50
17	B	816	CLA	CMC-C2C	-2.00	1.46	1.50
17	B	837	CLA	CMB-C2B	-2.00	1.46	1.50
17	K	203	CLA	CMB-C2B	-2.00	1.46	1.50
17	b	602	CLA	CMB-C2B	-2.00	1.46	1.50
17	a	605	CLA	CMC-C2C	-2.00	1.46	1.50
17	3	314	CLA	CMC-C2C	-2.00	1.46	1.50
17	3	312	CLA	CMC-C2C	-2.00	1.46	1.50

All (1224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	8	308	CHL	C4A-NA-C1A	15.65	113.82	106.68
16	T	401	CHL	C4A-NA-C1A	15.40	113.71	106.68
16	7	306	CHL	C4A-NA-C1A	14.52	113.31	106.68
16	b	607	CHL	C4A-NA-C1A	13.23	112.72	106.68
27	A	5003	CL0	C4A-NA-C1A	13.04	112.63	106.68
16	b	605	CHL	C4A-NA-C1A	12.82	112.53	106.68
16	T	416	CHL	C4A-NA-C1A	12.79	112.51	106.68
16	c	304	CHL	C4A-NA-C1A	12.79	112.51	106.68
16	c	305	CHL	C4A-NA-C1A	12.74	112.49	106.68
16	3	322	CHL	C4A-NA-C1A	12.30	112.29	106.68
16	3	301	CHL	C4A-NA-C1A	12.30	112.29	106.68
16	b	606	CHL	C4A-NA-C1A	12.18	112.24	106.68
16	a	606	CHL	C4A-NA-C1A	12.16	112.22	106.68
16	1	606	CHL	C4A-NA-C1A	12.15	112.22	106.68
16	8	307	CHL	C4A-NA-C1A	12.06	112.18	106.68
16	c	306	CHL	C4A-NA-C1A	11.33	111.85	106.68
16	7	307	CHL	C4A-NA-C1A	11.28	111.83	106.68
16	a	601	CHL	C4A-NA-C1A	11.01	111.70	106.68
16	8	306	CHL	C4A-NA-C1A	9.34	110.94	106.68
16	1	601	CHL	C4A-NA-C1A	8.54	110.57	106.68
17	T	409	CLA	C4A-NA-C1A	7.32	110.02	106.68
17	7	304	CLA	C4A-NA-C1A	6.92	109.83	106.68
17	F	5009	CLA	C4A-NA-C1A	6.89	109.82	106.68
17	8	305	CLA	C4A-NA-C1A	6.83	109.80	106.68
17	8	304	CLA	C4A-NA-C1A	6.81	109.78	106.68
17	A	5026	CLA	C4A-NA-C1A	6.80	109.78	106.68
17	A	5012	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	B	824	CLA	C4A-NA-C1A	6.77	109.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	5017	CLA	C4A-NA-C1A	6.74	109.75	106.68
17	c	310	CLA	C4A-NA-C1A	6.69	109.73	106.68
17	b	603	CLA	C4A-NA-C1A	6.68	109.73	106.68
17	F	5004	CLA	C4A-NA-C1A	6.68	109.73	106.68
17	b	604	CLA	C4A-NA-C1A	6.67	109.72	106.68
17	1	605	CLA	C4A-NA-C1A	6.62	109.70	106.68
17	a	611	CLA	C4A-NA-C1A	6.59	109.69	106.68
17	7	311	CLA	C4A-NA-C1A	6.54	109.66	106.68
17	A	5015	CLA	C4A-NA-C1A	6.49	109.64	106.68
17	3	310	CLA	C4A-NA-C1A	6.46	109.63	106.68
17	L	202	CLA	C4A-NA-C1A	6.45	109.62	106.68
17	b	611	CLA	C4A-NA-C1A	6.44	109.61	106.68
17	B	835	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	a	607	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	1	611	CLA	C4A-NA-C1A	6.42	109.61	106.68
17	A	5009	CLA	C4A-NA-C1A	6.39	109.59	106.68
17	8	312	CLA	C4A-NA-C1A	6.36	109.58	106.68
17	a	603	CLA	C4A-NA-C1A	6.35	109.57	106.68
17	A	5028	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	B	840	CLA	C4A-NA-C1A	6.34	109.57	106.68
17	J	102	CLA	C4A-NA-C1A	6.25	109.53	106.68
17	B	819	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	3	311	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	B	826	CLA	C4A-NA-C1A	6.20	109.51	106.68
17	B	820	CLA	C4A-NA-C1A	6.18	109.50	106.68
17	a	608	CLA	C4A-NA-C1A	6.18	109.50	106.68
17	8	302	CLA	C4A-NA-C1A	6.14	109.48	106.68
17	A	5038	CLA	C4A-NA-C1A	6.13	109.48	106.68
17	A	5019	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	c	309	CLA	C4A-NA-C1A	6.08	109.45	106.68
17	B	810	CLA	C4A-NA-C1A	6.07	109.45	106.68
17	1	602	CLA	C4A-NA-C1A	6.06	109.45	106.68
17	A	5023	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	c	313	CLA	C4A-NA-C1A	6.03	109.43	106.68
17	B	813	CLA	C4A-NA-C1A	6.01	109.42	106.68
17	3	303	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	c	311	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	7	312	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	A	5014	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	A	5010	CLA	C4A-NA-C1A	5.94	109.39	106.68
17	1	614	CLA	C4A-NA-C1A	5.91	109.37	106.68
17	T	406	CLA	C4A-NA-C1A	5.90	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	816	CLA	C4A-NA-C1A	5.88	109.36	106.68
17	B	814	CLA	C4A-NA-C1A	5.87	109.36	106.68
17	A	5029	CLA	C4A-NA-C1A	5.82	109.33	106.68
17	B	815	CLA	C4A-NA-C1A	5.82	109.33	106.68
17	1	603	CLA	C4A-NA-C1A	5.82	109.33	106.68
17	A	5031	CLA	C4A-NA-C1A	5.81	109.33	106.68
17	B	822	CLA	C4A-NA-C1A	5.75	109.30	106.68
17	a	614	CLA	C4A-NA-C1A	5.73	109.29	106.68
17	c	307	CLA	CMB-C2B-C1B	-5.72	116.70	125.42
17	B	805	CLA	C4A-NA-C1A	5.72	109.29	106.68
17	1	613	CLA	C4A-NA-C1A	5.71	109.28	106.68
17	7	314	CLA	C4A-NA-C1A	5.69	109.28	106.68
17	T	402	CLA	C4A-NA-C1A	5.67	109.27	106.68
17	A	5034	CLA	C4A-NA-C1A	5.65	109.26	106.68
17	A	5032	CLA	C4A-NA-C1A	5.65	109.26	106.68
17	7	308	CLA	C4A-NA-C1A	5.65	109.26	106.68
17	1	609	CLA	C4A-NA-C1A	5.65	109.25	106.68
17	3	302	CLA	C4A-NA-C1A	5.62	109.25	106.68
17	B	838	CLA	C4A-NA-C1A	5.58	109.22	106.68
17	A	5030	CLA	C4A-NA-C1A	5.57	109.22	106.68
17	B	836	CLA	C4A-NA-C1A	5.56	109.22	106.68
17	c	303	CLA	C4A-NA-C1A	5.56	109.21	106.68
17	T	410	CLA	C4A-NA-C1A	5.54	109.21	106.68
17	A	5025	CLA	C4A-NA-C1A	5.53	109.20	106.68
17	B	833	CLA	C4A-NA-C1A	5.48	109.18	106.68
17	B	828	CLA	C4A-NA-C1A	5.47	109.17	106.68
17	A	5006	CLA	C4A-NA-C1A	5.46	109.17	106.68
17	A	5018	CLA	C4A-NA-C1A	5.43	109.16	106.68
17	A	5036	CLA	C4A-NA-C1A	5.40	109.14	106.68
17	8	309	CLA	C4A-NA-C1A	5.37	109.13	106.68
17	K	201	CLA	C4A-NA-C1A	5.37	109.13	106.68
17	3	314	CLA	C4A-NA-C1A	5.34	109.12	106.68
17	b	612	CLA	C4A-NA-C1A	5.34	109.11	106.68
17	A	5042	CLA	C4A-NA-C1A	5.33	109.11	106.68
17	A	5037	CLA	C4A-NA-C1A	5.32	109.11	106.68
17	7	303	CLA	C4A-NA-C1A	5.31	109.10	106.68
17	8	314	CLA	C4A-NA-C1A	5.31	109.10	106.68
17	B	830	CLA	C4A-NA-C1A	5.26	109.08	106.68
17	1	608	CLA	C4A-NA-C1A	5.25	109.08	106.68
17	B	834	CLA	C4A-NA-C1A	5.24	109.07	106.68
17	3	306	CLA	C4A-NA-C1A	5.21	109.06	106.68
17	B	841	CLA	C4A-NA-C1A	5.20	109.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	812	CLA	C4A-NA-C1A	5.20	109.05	106.68
17	7	313	CLA	C4A-NA-C1A	5.17	109.04	106.68
17	c	307	CLA	C4A-NA-C1A	5.17	109.04	106.68
17	B	811	CLA	C4A-NA-C1A	5.15	109.03	106.68
17	A	5041	CLA	C4A-NA-C1A	5.14	109.02	106.68
17	B	809	CLA	C4A-NA-C1A	5.11	109.01	106.68
17	B	837	CLA	C4A-NA-C1A	5.11	109.01	106.68
17	b	601	CLA	C4A-NA-C1A	5.08	109.00	106.68
17	B	807	CLA	C4A-NA-C1A	5.07	108.99	106.68
17	1	612	CLA	C4A-NA-C1A	5.07	108.99	106.68
17	F	5008	CLA	C4A-NA-C1A	5.05	108.98	106.68
17	B	831	CLA	C4A-NA-C1A	5.03	108.97	106.68
16	7	305	CHL	C4A-NA-C1A	5.01	108.96	106.68
17	b	608	CLA	C4A-NA-C1A	4.99	108.96	106.68
17	b	610	CLA	C4A-NA-C1A	4.99	108.96	106.68
17	3	304	CLA	C4A-NA-C1A	4.98	108.95	106.68
17	8	311	CLA	C4A-NA-C1A	4.97	108.95	106.68
17	B	829	CLA	C4A-NA-C1A	4.94	108.94	106.68
17	a	612	CLA	C4A-NA-C1A	4.93	108.93	106.68
17	1	604	CLA	C4A-NA-C1A	4.92	108.92	106.68
17	A	5027	CLA	C4A-NA-C1A	4.92	108.92	106.68
17	A	5022	CLA	C4A-NA-C1A	4.91	108.92	106.68
17	A	5039	CLA	C4A-NA-C1A	4.85	108.89	106.68
17	c	308	CLA	C4A-NA-C1A	4.83	108.88	106.68
17	A	5021	CLA	C4A-NA-C1A	4.82	108.88	106.68
18	1	615	LUT	C35-C15-C14	4.81	133.37	123.52
17	3	323	CLA	C4A-NA-C1A	4.81	108.87	106.68
17	a	602	CLA	C4A-NA-C1A	4.80	108.87	106.68
17	3	324	CLA	C4A-NA-C1A	4.76	108.85	106.68
17	a	605	CLA	C4A-NA-C1A	4.71	108.83	106.68
17	A	5035	CLA	C4A-NA-C1A	4.70	108.82	106.68
17	1	610	CLA	C4A-NA-C1A	4.68	108.82	106.68
17	b	614	CLA	C4A-NA-C1A	4.68	108.81	106.68
17	a	610	CLA	C4A-NA-C1A	4.67	108.81	106.68
17	3	305	CLA	C4A-NA-C1A	4.66	108.81	106.68
17	B	821	CLA	C4A-NA-C1A	4.66	108.81	106.68
17	8	315	CLA	C4A-NA-C1A	4.61	108.78	106.68
18	1	615	LUT	C15-C35-C34	-4.59	114.14	123.52
17	A	5016	CLA	C4A-NA-C1A	4.57	108.76	106.68
17	T	408	CLA	C4A-NA-C1A	4.50	108.73	106.68
17	7	310	CLA	C4A-NA-C1A	4.46	108.71	106.68
17	A	5020	CLA	C4A-NA-C1A	4.45	108.71	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	317	XAT	C7-C8-C9	4.38	132.32	125.53
17	A	5043	CLA	C4A-NA-C1A	4.37	108.67	106.68
19	1	616	XAT	C27-C28-C29	4.32	132.23	125.53
17	A	5033	CLA	C4A-NA-C1A	4.31	108.65	106.68
18	a	615	LUT	C35-C15-C14	4.31	132.34	123.52
20	B	845	BCR	C21-C20-C19	4.27	135.57	123.20
20	A	5049	BCR	C24-C23-C22	4.27	132.55	126.23
17	B	818	CLA	C4A-NA-C1A	4.26	108.62	106.68
17	A	5040	CLA	C4A-NA-C1A	4.26	108.62	106.68
17	c	312	CLA	C4A-NA-C1A	4.25	108.62	106.68
16	T	401	CHL	C1-C2-C3	-4.24	119.90	126.76
17	c	302	CLA	C4A-NA-C1A	4.20	108.59	106.68
16	8	308	CHL	C1-C2-C3	-4.19	119.98	126.76
17	1	607	CLA	C4A-NA-C1A	4.18	108.59	106.68
17	B	806	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	b	607	CHL	C1-C2-C3	-4.14	120.07	126.76
16	1	601	CHL	C1-C2-C3	-4.12	120.09	126.76
17	B	827	CLA	C4A-NA-C1A	4.10	108.55	106.68
17	3	313	CLA	C4A-NA-C1A	4.09	108.55	106.68
17	8	313	CLA	C4A-NA-C1A	4.04	108.52	106.68
17	A	5005	CLA	C4A-NA-C1A	4.03	108.52	106.68
17	T	411	CLA	C4A-NA-C1A	3.97	108.49	106.68
17	B	808	CLA	C4A-NA-C1A	3.94	108.48	106.68
16	a	606	CHL	CHD-C4C-C3C	3.93	130.51	124.77
16	b	606	CHL	CHD-C4C-C3C	3.92	130.49	124.77
16	3	301	CHL	C1-C2-C3	-3.92	119.77	126.20
27	A	5003	CL0	CHD-C4C-C3C	3.89	130.44	124.77
17	A	5011	CLA	C4A-NA-C1A	3.87	108.45	106.68
17	B	817	CLA	C4A-NA-C1A	3.86	108.44	106.68
17	T	407	CLA	C4A-NA-C1A	3.85	108.44	106.68
16	T	416	CHL	CHD-C4C-C3C	3.85	130.39	124.77
17	K	204	CLA	C4A-NA-C1A	3.84	108.43	106.68
27	A	5003	CL0	C1-C2-C3	-3.82	119.94	126.20
16	1	606	CHL	CHD-C4C-C3C	3.78	130.29	124.77
17	a	613	CLA	C4A-NA-C1A	3.75	108.39	106.68
17	A	5007	CLA	C4A-NA-C1A	3.75	108.39	106.68
17	c	301	CLA	C4A-NA-C1A	3.74	108.39	106.68
16	c	304	CHL	CHD-C4C-C3C	3.73	130.22	124.77
16	3	322	CHL	C1-C2-C3	-3.72	120.11	126.20
17	3	307	CLA	C4A-NA-C1A	3.71	108.37	106.68
17	K	203	CLA	C4A-NA-C1A	3.69	108.36	106.68
19	b	616	XAT	C7-C8-C9	3.69	131.25	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	202	CLA	C4A-NA-C1A	3.67	108.35	106.68
17	c	307	CLA	CMB-C2B-C3B	3.66	135.15	126.55
17	B	823	CLA	C4A-NA-C1A	3.65	108.34	106.68
20	A	5049	BCR	C23-C24-C25	3.65	136.75	127.00
17	A	5016	CLA	CAC-C3C-C4C	3.62	129.50	124.79
16	b	605	CHL	CHD-C4C-C3C	3.61	130.04	124.77
19	T	414	XAT	C7-C8-C9	3.57	131.08	125.53
17	B	839	CLA	C4A-NA-C1A	3.56	108.30	106.68
16	8	308	CHL	CHD-C4C-C3C	3.55	129.95	124.77
16	c	305	CHL	CHD-C4C-C3C	3.54	129.94	124.77
16	b	605	CHL	C2D-C1D-ND	-3.53	106.63	110.13
16	3	322	CHL	CHD-C4C-C3C	3.53	129.92	124.77
16	7	306	CHL	CHD-C4C-C3C	3.52	129.90	124.77
17	B	803	CLA	C4A-NA-C1A	3.52	108.28	106.68
16	a	606	CHL	C3B-C4B-NB	-3.51	107.40	110.53
17	A	5043	CLA	O2D-CGD-O1D	-3.48	117.06	123.85
16	1	601	CHL	C2A-C1A-CHA	3.48	129.91	123.87
16	a	601	CHL	CHD-C4C-C3C	3.48	129.85	124.77
16	8	307	CHL	CHD-C4C-C3C	3.48	129.84	124.77
16	8	306	CHL	C2D-C1D-ND	-3.45	106.71	110.13
16	1	606	CHL	C3B-C4B-NB	-3.44	107.46	110.53
17	A	5035	CLA	CHB-C4A-NA	3.43	129.36	124.40
17	8	302	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
17	b	613	CLA	C4A-NA-C1A	3.43	108.24	106.68
17	A	5006	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
17	B	824	CLA	CHB-C4A-NA	3.34	129.22	124.40
16	b	607	CHL	CHD-C4C-C3C	3.33	129.63	124.77
16	c	306	CHL	C2A-C1A-CHA	3.33	129.64	123.87
17	F	5007	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	3	322	CHL	C3B-C4B-NB	-3.32	107.57	110.53
16	T	416	CHL	C2D-C1D-ND	-3.32	106.84	110.13
16	a	606	CHL	C2A-C1A-CHA	3.31	129.60	123.87
17	B	808	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
16	b	606	CHL	C3B-C4B-NB	-3.29	107.59	110.53
16	1	601	CHL	CHD-C4C-C3C	3.28	129.56	124.77
17	a	604	CLA	CHB-C4A-NA	3.27	129.12	124.40
17	A	5019	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	b	605	CHL	C3B-C4B-NB	-3.27	107.61	110.53
17	T	409	CLA	CHB-C4A-NA	3.26	129.11	124.40
17	1	604	CLA	C3B-C4B-NB	-3.26	107.62	110.53
16	c	305	CHL	C3D-C2D-C1D	3.24	110.25	105.83
16	b	606	CHL	C2A-C1A-CHA	3.23	129.48	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	303	CLA	C3B-C4B-NB	-3.23	107.65	110.53
17	a	608	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
17	7	309	CLA	CHB-C4A-NA	3.22	129.05	124.40
17	a	604	CLA	C3B-C4B-NB	-3.22	107.65	110.53
16	a	606	CHL	C1D-CHD-C4C	-3.22	119.17	126.02
17	A	5013	CLA	CHB-C4A-NA	3.22	129.05	124.40
17	3	323	CLA	CHB-C4A-NA	3.22	129.04	124.40
17	7	302	CLA	CHB-C4A-NA	3.21	129.04	124.40
17	L	201	CLA	C4A-NA-C1A	3.21	108.14	106.68
17	8	310	CLA	CHB-C4A-NA	3.21	129.04	124.40
17	B	820	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
16	7	305	CHL	CHD-C4C-C3C	3.18	129.42	124.77
17	b	602	CLA	CHB-C4A-NA	3.18	128.99	124.40
17	K	202	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
16	1	606	CHL	C2D-C1D-ND	-3.16	107.00	110.13
17	A	5014	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
17	A	5033	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	1	606	CHL	C2A-C1A-CHA	3.15	129.33	123.87
17	a	609	CLA	CHB-C4A-NA	3.15	128.94	124.40
17	c	307	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
17	1	604	CLA	CHB-C4A-NA	3.14	128.93	124.40
16	1	606	CHL	C1D-CHD-C4C	-3.14	119.36	126.02
17	a	604	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
16	7	305	CHL	C2A-C1A-CHA	3.13	129.30	123.87
16	8	308	CHL	C3D-C2D-C1D	3.13	110.10	105.83
17	1	602	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
17	A	5035	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
18	T	413	LUT	C7-C8-C9	3.13	130.86	126.23
18	a	615	LUT	C15-C35-C34	-3.13	117.12	123.52
16	a	601	CHL	C2D-C1D-ND	-3.12	107.03	110.13
17	3	307	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
17	1	604	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
17	8	303	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
17	b	608	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
17	A	5044	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
17	a	614	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
28	A	5045	PQN	C11-C3-C4	-3.10	115.31	118.58
20	B	849	BCR	C15-C16-C17	3.10	129.86	123.52
17	B	834	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
16	7	306	CHL	C3B-C4B-NB	-3.08	107.78	110.53
17	3	308	CLA	C4A-NA-C1A	3.08	108.08	106.68
16	c	305	CHL	C3B-C4B-NB	-3.07	107.79	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	322	CHL	C2D-C1D-ND	-3.07	107.09	110.13
17	B	804	CLA	C3B-C4B-NB	-3.06	107.79	110.53
17	F	5006	CLA	C4A-NA-C1A	3.06	108.08	106.68
16	7	307	CHL	CHD-C4C-C3C	3.06	129.24	124.77
17	7	311	CLA	CHB-C4A-NA	3.06	128.82	124.40
17	T	407	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
17	T	403	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
16	b	605	CHL	C1D-ND-C4D	-3.06	104.17	106.31
16	7	307	CHL	C1C-C2C-C3C	-3.05	104.47	107.28
17	7	309	CLA	C3B-C4B-NB	-3.05	107.80	110.53
17	8	312	CLA	CHB-C4A-NA	3.05	128.80	124.40
17	T	403	CLA	CMB-C2B-C1B	-3.05	120.78	125.42
17	A	5028	CLA	C3B-C4B-NB	-3.05	107.81	110.53
17	A	5011	CLA	C3B-C4B-NB	-3.05	107.81	110.53
16	3	301	CHL	CHD-C4C-C3C	3.04	129.21	124.77
17	c	308	CLA	CHB-C4A-NA	3.04	128.79	124.40
17	A	5009	CLA	CHB-C4A-NA	3.04	128.78	124.40
17	A	5020	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
17	A	5037	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
17	b	601	CLA	C3B-C4B-NB	-3.03	107.83	110.53
16	1	601	CHL	C2D-C1D-ND	-3.03	107.13	110.13
17	8	312	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	3	316	XAT	C27-C28-C29	3.03	130.23	125.53
17	A	5007	CLA	C3B-C4B-NB	-3.03	107.83	110.53
17	T	403	CLA	C3B-C4B-NB	-3.03	107.83	110.53
16	T	416	CHL	C3B-C4B-NB	-3.02	107.83	110.53
17	T	409	CLA	C3B-C4B-NB	-3.02	107.83	110.53
17	B	838	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
17	B	836	CLA	C3B-C4B-NB	-3.01	107.84	110.53
17	A	5031	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
17	B	818	CLA	C1-C2-C3	-3.01	121.27	126.20
16	T	401	CHL	C2D-C1D-ND	-3.01	107.15	110.13
17	7	310	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	8	308	CHL	C3B-C4B-NB	-3.00	107.85	110.53
17	1	614	CLA	C3B-C4B-NB	-3.00	107.85	110.53
16	c	304	CHL	C3B-C4B-NB	-3.00	107.85	110.53
17	A	5024	CLA	CHB-C4A-NA	3.00	128.73	124.40
17	B	836	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
16	8	307	CHL	C3D-C2D-C1D	3.00	109.92	105.83
16	c	304	CHL	C2D-C1D-ND	-3.00	107.16	110.13
17	1	605	CLA	C3B-C4B-NB	-2.99	107.86	110.53
17	T	404	CLA	C3B-C4B-NB	-2.99	107.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	609	CLA	CHB-C4A-NA	2.99	128.71	124.40
17	B	833	CLA	C3B-C4B-NB	-2.99	107.86	110.53
16	7	306	CHL	C2D-C1D-ND	-2.98	107.17	110.13
17	A	5041	CLA	CHB-C4A-NA	2.98	128.70	124.40
17	7	302	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	B	803	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	B	840	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	3	309	CLA	C3B-C4B-NB	-2.98	107.87	110.53
17	a	614	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	3	301	CHL	C2A-C1A-CHA	2.98	129.03	123.87
17	b	611	CLA	CHB-C4A-NA	2.97	128.69	124.40
17	1	610	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
17	1	602	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	a	610	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	A	5007	CLA	CHB-C4A-NA	2.97	128.69	124.40
17	B	808	CLA	CHB-C4A-NA	2.97	128.69	124.40
17	J	102	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	c	308	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	B	824	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
17	3	307	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	J	102	CLA	CHB-C4A-NA	2.97	128.68	124.40
17	L	201	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
17	1	610	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	8	311	CLA	C3B-C4B-NB	-2.97	107.88	110.53
17	A	5024	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
17	B	825	CLA	C3B-C4B-NB	-2.96	107.88	110.53
17	1	605	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
17	3	323	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
17	b	602	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
16	1	601	CHL	C1C-C2C-C3C	-2.96	104.56	107.28
16	c	306	CHL	CHD-C4C-C3C	2.96	129.09	124.77
17	a	609	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	F	5006	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	T	412	CLA	C3B-C4B-NB	-2.96	107.89	110.53
17	F	5004	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
17	8	310	CLA	C3B-C4B-NB	-2.95	107.90	110.53
17	8	309	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	b	607	CHL	C3B-C4B-NB	-2.95	107.90	110.53
17	K	202	CLA	C3B-C4B-NB	-2.95	107.90	110.53
17	A	5010	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	b	608	CLA	C3B-C4B-NB	-2.94	107.90	110.53
17	A	5041	CLA	C3B-C4B-NB	-2.94	107.90	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	825	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	A	5004	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	B	810	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
17	8	310	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
17	B	840	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
17	T	403	CLA	CHB-C1B-NB	2.94	128.46	124.05
17	8	313	CLA	CHB-C4A-NA	2.94	128.64	124.40
28	B	842	PQN	C11-C3-C4	-2.94	115.49	118.58
17	B	816	CLA	C3B-C4B-NB	-2.94	107.91	110.53
17	1	612	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
17	B	828	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
17	3	324	CLA	C3B-C4B-NB	-2.93	107.91	110.53
16	T	401	CHL	C2A-C1A-CHA	2.93	128.96	123.87
17	8	309	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
18	1	615	LUT	C30-C31-C32	2.93	131.70	123.20
17	A	5021	CLA	CHB-C4A-NA	2.93	128.63	124.40
17	1	608	CLA	C3B-C4B-NB	-2.93	107.91	110.53
17	A	5021	CLA	C3B-C4B-NB	-2.93	107.91	110.53
17	A	5026	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
17	A	5030	CLA	C3B-C4B-NB	-2.93	107.92	110.53
17	a	602	CLA	C3B-C4B-NB	-2.93	107.92	110.53
17	3	308	CLA	CHB-C4A-NA	2.93	128.62	124.40
17	3	307	CLA	CHB-C4A-NA	2.93	128.62	124.40
17	A	5036	CLA	CHB-C4A-NA	2.92	128.62	124.40
16	3	301	CHL	C3D-C2D-C1D	2.92	109.82	105.83
17	8	304	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
17	8	302	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	A	5015	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
17	b	609	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	A	5007	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	K	202	CLA	CHB-C4A-NA	2.92	128.61	124.40
17	1	613	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	K	201	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	b	604	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
17	b	611	CLA	C3B-C4B-NB	-2.91	107.93	110.53
17	7	308	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	7	313	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	B	829	CLA	CHB-C4A-NA	2.91	128.60	124.40
17	A	5040	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	B	819	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
17	A	5044	CLA	C4A-NA-C1A	2.91	108.01	106.68
19	a	616	XAT	C27-C28-C29	2.91	130.04	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	609	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	c	310	CLA	CHB-C4A-NA	2.91	128.60	124.40
17	1	603	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	A	5004	CLA	C4A-NA-C1A	2.91	108.01	106.68
17	8	315	CLA	C3B-C4B-NB	-2.91	107.93	110.53
17	B	815	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	B	817	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	B	823	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
16	8	307	CHL	C3B-C4B-NB	-2.90	107.94	110.53
17	b	604	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	B	830	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	1	607	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	a	613	CLA	C3B-C4B-NB	-2.90	107.94	110.53
27	A	5003	CL0	C3B-C4B-NB	-2.90	107.94	110.53
17	A	5042	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	a	603	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
17	T	407	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	B	830	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	3	324	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	8	313	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	a	612	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	B	812	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	B	813	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	7	308	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	B	837	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	B	826	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	1	609	CLA	CHB-C4A-NA	2.89	128.57	124.40
17	b	614	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	7	310	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	B	802	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	B	814	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
17	A	5013	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
20	B	849	BCR	C16-C15-C14	-2.89	117.61	123.52
17	L	201	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	1	608	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
17	8	315	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
16	7	305	CHL	C3D-C2D-C1D	2.88	109.76	105.83
17	A	5008	CLA	CHB-C4A-NA	2.88	128.56	124.40
17	A	5029	CLA	CHB-C4A-NA	2.88	128.56	124.40
17	8	314	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	T	408	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	A	5017	CLA	O2D-CGD-O1D	-2.88	118.24	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	809	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	A	5023	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	a	610	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	7	313	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	3	312	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	T	411	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	B	817	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	c	313	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
17	T	410	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
17	B	814	CLA	CHB-C4A-NA	2.87	128.55	124.40
20	c	316	BCR	C24-C23-C22	2.87	130.49	126.23
17	K	201	CLA	C3B-C4B-NB	-2.87	107.96	110.53
17	A	5022	CLA	CHB-C4A-NA	2.87	128.55	124.40
17	T	411	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	A	5039	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	A	5018	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	F	5008	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	F	5007	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	1	611	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
17	B	804	CLA	C4A-NA-C1A	2.87	107.99	106.68
17	b	610	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
16	b	607	CHL	C3D-C2D-C1D	2.87	109.75	105.83
19	c	315	XAT	C38-C25-C24	-2.87	111.02	114.24
17	T	406	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	A	5008	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	7	312	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
17	A	5024	CLA	C3B-C4B-NB	-2.87	107.97	110.53
17	c	309	CLA	C3B-C4B-NB	-2.86	107.97	110.53
17	c	303	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	8	306	CHL	CHD-C1D-C2D	2.86	131.44	125.49
17	A	5029	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	A	5037	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	T	412	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	B	822	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	K	203	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
17	A	5040	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	B	827	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	B	803	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
17	A	5022	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
17	c	308	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
17	A	5009	CLA	C3B-C4B-NB	-2.86	107.98	110.53
17	T	407	CLA	CHB-C4A-NA	2.85	128.52	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	807	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
17	3	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	B	805	CLA	CHB-C4A-NA	2.85	128.52	124.40
17	T	405	CLA	CHB-C4A-NA	2.85	128.52	124.40
17	A	5016	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	b	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	B	802	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	3	308	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	c	310	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
17	7	312	CLA	CHB-C4A-NA	2.85	128.51	124.40
17	1	614	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	3	313	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	J	102	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	B	834	CLA	C3B-C4B-NB	-2.85	107.99	110.53
17	8	305	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
27	A	5003	CL0	C2D-C1D-ND	-2.84	107.31	110.13
17	B	835	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
16	a	606	CHL	C2D-C1D-ND	-2.84	107.31	110.13
17	7	309	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
17	a	613	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
17	7	308	CLA	CHB-C4A-NA	2.84	128.50	124.40
17	1	612	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	a	607	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	1	609	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	A	5038	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	B	831	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	K	204	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	8	313	CLA	C3B-C4B-NB	-2.84	107.99	110.53
17	A	5027	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	c	311	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	8	303	CLA	CHB-C4A-NA	2.84	128.50	124.40
16	b	606	CHL	C2D-C1D-ND	-2.84	107.31	110.13
16	8	307	CHL	C2A-C1A-CHA	2.84	128.79	123.87
17	B	829	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	A	5008	CLA	C4A-NA-C1A	2.84	107.97	106.68
17	B	806	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	7	304	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
17	3	304	CLA	C3B-C4B-NB	-2.84	108.00	110.53
17	b	614	CLA	C3B-C4B-NB	-2.83	108.00	110.53
16	T	401	CHL	CHD-C4C-C3C	2.83	128.91	124.77
16	7	305	CHL	C2D-C1D-ND	-2.83	107.32	110.13
19	a	616	XAT	O24-C25-C24	-2.83	110.84	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	302	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
17	B	819	CLA	C3B-C4B-NB	-2.83	108.00	110.53
17	B	811	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
18	1	615	LUT	C35-C34-C33	2.83	131.25	127.28
17	K	204	CLA	C3B-C4B-NB	-2.83	108.01	110.53
17	a	611	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
17	A	5017	CLA	C3B-C4B-NB	-2.83	108.01	110.53
18	a	615	LUT	C26-C27-C28	2.82	128.97	124.58
17	B	827	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
17	B	804	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
17	1	605	CLA	CHB-C4A-NA	2.82	128.47	124.40
17	B	816	CLA	CHB-C4A-NA	2.82	128.47	124.40
17	B	832	CLA	CHB-C4A-NA	2.82	128.47	124.40
17	3	311	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
17	F	5009	CLA	CHB-C4A-NA	2.82	128.47	124.40
17	3	303	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
17	B	815	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	a	601	CHL	C2A-C1A-CHA	2.82	128.76	123.87
20	B	845	BCR	C20-C19-C18	2.82	134.09	126.36
17	8	305	CLA	C3B-C4B-NB	-2.82	108.02	110.53
17	A	5009	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
17	B	841	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
17	F	5008	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
17	b	601	CLA	CHB-C4A-NA	2.82	128.46	124.40
17	c	311	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	c	301	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
17	K	203	CLA	CHB-C4A-NA	2.81	128.46	124.40
17	7	311	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
17	A	5032	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
17	A	5025	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
17	3	309	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
17	B	821	CLA	C3B-C4B-NB	-2.81	108.02	110.53
17	B	833	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
17	B	815	CLA	CHB-C4A-NA	2.81	128.45	124.40
17	T	402	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
17	F	5006	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
17	b	603	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
17	A	5010	CLA	C3B-C4B-NB	-2.80	108.03	110.53
17	B	821	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
17	F	5009	CLA	C3B-C4B-NB	-2.80	108.03	110.53
17	3	306	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
17	F	5006	CLA	CHB-C4A-NA	2.80	128.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	803	CLA	CHB-C4A-NA	2.80	128.44	124.40
17	A	5036	CLA	C3B-C4B-NB	-2.80	108.03	110.53
18	1	615	LUT	C26-C27-C28	2.80	128.93	124.58
17	B	824	CLA	C3B-C4B-NB	-2.80	108.03	110.53
17	A	5023	CLA	CHB-C4A-NA	2.80	128.44	124.40
17	A	5019	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
17	3	313	CLA	C3B-C4B-NB	-2.79	108.03	110.53
17	A	5027	CLA	C3B-C4B-NB	-2.79	108.03	110.53
17	b	609	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
17	c	302	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	7	303	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	3	312	CLA	CHB-C4A-NA	2.79	128.43	124.40
17	A	5032	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	B	820	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	T	406	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	A	5028	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	b	611	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	3	305	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	B	817	CLA	CHB-C4A-NA	2.79	128.42	124.40
17	7	314	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
17	A	5006	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	c	306	CHL	C2D-C1D-ND	-2.79	107.37	110.13
17	B	807	CLA	C3B-C4B-NB	-2.78	108.04	110.53
17	b	610	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	b	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	3	311	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	c	303	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	A	5043	CLA	CHB-C4A-NA	2.78	128.41	124.40
17	3	314	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	a	605	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	3	302	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	A	5033	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	B	839	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	b	612	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
27	A	5003	CL0	C3D-C2D-C1D	2.78	109.62	105.83
17	A	5025	CLA	CHB-C4A-NA	2.78	128.41	124.40
17	A	5034	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	T	409	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	T	408	CLA	CHB-C4A-NA	2.78	128.41	124.40
17	F	5009	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	1	613	CLA	C3B-C4B-NB	-2.78	108.05	110.53
17	1	608	CLA	CHB-C4A-NA	2.78	128.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	412	CLA	C4A-NA-C1A	2.77	107.94	106.68
17	A	5015	CLA	C3B-C4B-NB	-2.77	108.05	110.53
17	B	826	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	8	308	CHL	C2D-C1D-ND	-2.77	107.38	110.13
17	b	612	CLA	CHB-C4A-NA	2.77	128.40	124.40
17	3	308	CLA	C3B-C4B-NB	-2.77	108.06	110.53
17	B	838	CLA	C3B-C4B-NB	-2.77	108.06	110.53
17	B	823	CLA	CHB-C4A-NA	2.77	128.40	124.40
16	7	306	CHL	C2A-C1A-CHA	2.77	128.67	123.87
17	A	5014	CLA	C3B-C4B-NB	-2.77	108.06	110.53
17	1	610	CLA	CHB-C4A-NA	2.77	128.39	124.40
17	B	811	CLA	CHB-C4A-NA	2.77	128.39	124.40
17	c	312	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
20	K	205	BCR	C10-C11-C12	2.76	131.21	123.20
17	A	5023	CLA	C3B-C4B-NB	-2.76	108.06	110.53
17	a	605	CLA	C3B-C4B-NB	-2.76	108.06	110.53
17	c	301	CLA	C3B-C4B-NB	-2.76	108.06	110.53
17	a	607	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
17	B	838	CLA	CHB-C4A-NA	2.76	128.39	124.40
17	3	314	CLA	C3B-C4B-NB	-2.76	108.06	110.53
17	8	311	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
16	b	607	CHL	C2D-C1D-ND	-2.76	107.39	110.13
16	7	307	CHL	C3D-C2D-C1D	2.76	109.60	105.83
17	3	304	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
16	8	306	CHL	C2A-C1A-CHA	2.76	128.66	123.87
17	B	816	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	8	315	CLA	CHB-C4A-NA	2.76	128.38	124.40
17	T	405	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	B	831	CLA	C3B-C4B-NB	-2.76	108.07	110.53
17	B	807	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	7	307	CHL	C2D-C1D-ND	-2.76	107.40	110.13
17	A	5012	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	A	5041	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	b	603	CLA	C3B-C4B-NB	-2.76	108.07	110.53
17	3	313	CLA	CHB-C4A-NA	2.76	128.38	124.40
16	c	306	CHL	C3D-C2D-C1D	2.75	109.59	105.83
17	B	835	CLA	C3B-C4B-NB	-2.75	108.07	110.53
17	F	5007	CLA	C3B-C4B-NB	-2.75	108.07	110.53
17	A	5036	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
17	8	314	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
16	c	305	CHL	C2A-C1A-CHA	2.75	128.64	123.87
17	B	806	CLA	CHB-C4A-NA	2.75	128.37	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	401	CHL	CHD-C1D-C2D	2.75	131.20	125.49
17	K	204	CLA	CHB-C4A-NA	2.75	128.37	124.40
17	3	311	CLA	CHB-C4A-NA	2.75	128.36	124.40
17	A	5037	CLA	CHB-C4A-NA	2.74	128.36	124.40
17	3	306	CLA	CHB-C4A-NA	2.74	128.36	124.40
17	A	5031	CLA	C3B-C4B-NB	-2.74	108.08	110.53
17	A	5006	CLA	CHB-C4A-NA	2.74	128.36	124.40
17	b	608	CLA	CHB-C4A-NA	2.74	128.36	124.40
17	1	607	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	3	310	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	A	5021	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
17	K	203	CLA	C3B-C4B-NB	-2.74	108.08	110.53
17	A	5040	CLA	CHB-C4A-NA	2.74	128.35	124.40
17	T	408	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	a	603	CLA	C3B-C4B-NB	-2.74	108.08	110.53
17	B	832	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	A	5016	CLA	CHB-C4A-NA	2.74	128.35	124.40
17	B	812	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
17	B	841	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	B	827	CLA	CHB-C4A-NA	2.73	128.34	124.40
17	A	5042	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	3	312	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	1	607	CLA	CHB-C4A-NA	2.73	128.34	124.40
17	B	805	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
17	a	604	CLA	CHC-C1C-C2C	-2.73	123.97	129.94
17	A	5012	CLA	CHB-C4A-NA	2.72	128.33	124.40
17	8	304	CLA	C3B-C4B-NB	-2.72	108.10	110.53
17	A	5031	CLA	CHB-C4A-NA	2.72	128.32	124.40
16	8	306	CHL	CHD-C4C-C3C	2.72	128.74	124.77
17	1	611	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	B	804	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	A	5015	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	b	614	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	A	5044	CLA	C3B-C4B-NB	-2.72	108.11	110.53
17	a	602	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
17	A	5012	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	8	312	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	b	613	CLA	CHB-C4A-NA	2.71	128.31	124.40
16	T	416	CHL	C2A-C1A-CHA	2.71	128.57	123.87
17	8	314	CLA	CHB-C4A-NA	2.71	128.31	124.40
17	3	314	CLA	CHB-C4A-NA	2.71	128.31	124.40
17	B	818	CLA	O2D-CGD-O1D	-2.71	118.58	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	202	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
17	a	608	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	c	310	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	c	312	CLA	C3B-C4B-NB	-2.71	108.11	110.53
17	7	310	CLA	CHB-C4A-NA	2.70	128.30	124.40
19	7	316	XAT	C38-C25-C24	-2.70	111.21	114.24
17	3	302	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	b	612	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	A	5030	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
17	T	411	CLA	CHB-C4A-NA	2.70	128.29	124.40
17	B	835	CLA	CHB-C4A-NA	2.70	128.29	124.40
17	c	309	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
17	3	303	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	8	304	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	B	811	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	T	404	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
17	A	5034	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	1	614	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	7	304	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	A	5004	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	B	833	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	B	836	CLA	CHB-C4A-NA	2.69	128.28	124.40
17	1	609	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	A	5018	CLA	CHB-C4A-NA	2.68	128.27	124.40
17	3	310	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	c	305	CHL	C1D-ND-C4D	2.68	108.19	106.31
17	A	5039	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	B	805	CLA	CMB-C2B-C1B	-2.68	121.34	125.42
17	a	611	CLA	CHB-C4A-NA	2.68	128.26	124.40
16	a	601	CHL	C3B-C4B-NB	-2.68	108.14	110.53
17	a	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
17	8	302	CLA	CHB-C4A-NA	2.68	128.26	124.40
17	L	201	CLA	CHB-C4A-NA	2.68	128.26	124.40
17	A	5022	CLA	C3B-C4B-NB	-2.67	108.14	110.53
17	a	602	CLA	CHB-C4A-NA	2.67	128.25	124.40
17	7	314	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	B	825	CLA	CHB-C4A-NA	2.67	128.25	124.40
17	1	603	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	7	311	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	T	405	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	b	602	CLA	C3B-C4B-NB	-2.67	108.15	110.53
17	A	5010	CLA	CHB-C4A-NA	2.66	128.25	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	601	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
17	B	829	CLA	C3B-C4B-NB	-2.66	108.15	110.53
17	A	5011	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	a	608	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	A	5038	CLA	C3B-C4B-NB	-2.66	108.15	110.53
17	B	834	CLA	CHB-C4A-NA	2.66	128.24	124.40
16	c	305	CHL	C2D-C1D-ND	-2.66	107.49	110.13
17	3	305	CLA	CHB-C4A-NA	2.66	128.24	124.40
17	B	806	CLA	C3B-C4B-NB	-2.66	108.16	110.53
17	3	306	CLA	C3B-C4B-NB	-2.66	108.16	110.53
17	B	832	CLA	C3B-C4B-NB	-2.66	108.16	110.53
17	L	202	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	A	5005	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
17	B	830	CLA	C1-C2-C3	-2.65	121.85	126.20
17	B	813	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	a	612	CLA	CHB-C4A-NA	2.65	128.23	124.40
16	1	606	CHL	CHD-C1D-C2D	2.65	131.00	125.49
17	c	308	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
17	B	810	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	F	5004	CLA	C3B-C4B-NB	-2.65	108.16	110.53
17	c	301	CLA	CHB-C4A-NA	2.65	128.23	124.40
17	A	5004	CLA	CHB-C4A-NA	2.65	128.22	124.40
18	1	615	LUT	C22-C23-C24	2.65	115.12	111.18
17	A	5026	CLA	C3B-C4B-NB	-2.65	108.17	110.53
17	8	309	CLA	CHB-C4A-NA	2.65	128.22	124.40
17	A	5017	CLA	CHB-C4A-NA	2.65	128.22	124.40
17	B	822	CLA	C3B-C4B-NB	-2.65	108.17	110.53
19	1	616	XAT	O24-C25-C24	-2.64	111.01	113.49
17	B	820	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	3	310	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	a	610	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	T	406	CLA	CHB-C4A-NA	2.64	128.21	124.40
17	B	823	CLA	C3B-C4B-NB	-2.64	108.18	110.53
17	A	5028	CLA	CHB-C4A-NA	2.64	128.20	124.40
16	7	305	CHL	C3B-C4B-NB	-2.64	108.18	110.53
16	8	307	CHL	C2D-C1D-ND	-2.64	107.52	110.13
17	B	808	CLA	C3B-C4B-NB	-2.63	108.18	110.53
17	3	309	CLA	CHB-C4A-NA	2.63	128.20	124.40
17	B	828	CLA	CHB-C4A-NA	2.63	128.20	124.40
17	B	826	CLA	C3B-C4B-NB	-2.63	108.18	110.53
17	B	813	CLA	CHB-C4A-NA	2.63	128.20	124.40
17	a	607	CLA	CHB-C4A-NA	2.63	128.20	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	311	CLA	CHB-C4A-NA	2.63	128.19	124.40
17	c	302	CLA	C3B-C4B-NB	-2.63	108.18	110.53
17	a	614	CLA	CHB-C4A-NA	2.63	128.19	124.40
17	A	5018	CLA	C3B-C4B-NB	-2.62	108.19	110.53
17	A	5033	CLA	CHB-C4A-NA	2.62	128.19	124.40
17	B	819	CLA	CHB-C4A-NA	2.62	128.19	124.40
17	7	312	CLA	C3B-C4B-NB	-2.62	108.19	110.53
17	F	5007	CLA	CHB-C4A-NA	2.62	128.18	124.40
17	B	837	CLA	C3B-C4B-NB	-2.61	108.20	110.53
17	T	412	CLA	CHB-C4A-NA	2.61	128.17	124.40
17	A	5020	CLA	C3B-C4B-NB	-2.61	108.20	110.53
17	7	313	CLA	CHB-C4A-NA	2.61	128.16	124.40
17	A	5020	CLA	C1-C2-C3	-2.61	121.93	126.20
17	1	612	CLA	CHB-C4A-NA	2.61	128.16	124.40
16	b	606	CHL	C3D-C2D-C1D	2.61	109.39	105.83
19	3	316	XAT	C7-C8-C9	2.61	129.57	125.53
17	b	604	CLA	CHB-C4A-NA	2.61	128.16	124.40
27	A	5003	CL0	C2A-C1A-CHA	2.60	128.39	123.87
17	c	309	CLA	CHB-C4A-NA	2.60	128.16	124.40
17	A	5008	CLA	C3B-C4B-NB	-2.60	108.21	110.53
17	B	814	CLA	C3B-C4B-NB	-2.60	108.21	110.53
17	B	812	CLA	CHB-C4A-NA	2.60	128.15	124.40
17	a	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
17	c	303	CLA	CHB-C4A-NA	2.60	128.15	124.40
17	B	830	CLA	CHB-C4A-NA	2.59	128.14	124.40
17	1	611	CLA	C3B-C4B-NB	-2.59	108.22	110.53
17	8	311	CLA	CHB-C4A-NA	2.59	128.14	124.40
17	B	818	CLA	CHB-C4A-NA	2.59	128.13	124.40
17	a	611	CLA	C2A-C1A-CHA	2.59	128.35	123.87
17	3	302	CLA	CHB-C4A-NA	2.59	128.13	124.40
17	A	5035	CLA	C3B-C4B-NB	-2.58	108.22	110.53
17	A	5026	CLA	CHB-C4A-NA	2.58	128.13	124.40
17	1	603	CLA	CHB-C4A-NA	2.57	128.12	124.40
17	a	613	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	1	602	CLA	C1-C2-C3	-2.57	121.98	126.20
17	A	5025	CLA	C3B-C4B-NB	-2.57	108.23	110.53
17	c	307	CLA	C4B-C3B-C2B	-2.57	104.10	107.30
17	A	5039	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	3	324	CLA	CHB-C4A-NA	2.57	128.11	124.40
17	3	323	CLA	C3B-C4B-NB	-2.57	108.24	110.53
17	1	611	CLA	C2A-C1A-CHA	2.57	128.32	123.87
16	7	307	CHL	C3B-C4B-NB	-2.57	108.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	201	CLA	CHB-C4A-NA	2.56	128.10	124.40
17	3	303	CLA	C3B-C4B-NB	-2.56	108.24	110.53
17	3	309	CLA	C4A-NA-C1A	2.56	107.85	106.68
16	T	401	CHL	C1D-CHD-C4C	-2.56	120.58	126.02
17	7	311	CLA	C2A-C1A-CHA	2.56	128.31	123.87
17	B	810	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	F	5008	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	b	610	CLA	CHB-C4A-NA	2.56	128.09	124.40
17	T	409	CLA	C2A-C1A-CHA	2.55	128.30	123.87
17	A	5014	CLA	CHB-C4A-NA	2.55	128.09	124.40
17	B	821	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	A	5043	CLA	C3B-C4B-NB	-2.55	108.25	110.53
17	3	304	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	A	5038	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	B	809	CLA	C3B-C4B-NB	-2.55	108.25	110.53
17	1	604	CLA	C1-C2-C3	-2.55	122.64	126.76
17	B	818	CLA	C3B-C4B-NB	-2.55	108.26	110.53
17	A	5020	CLA	CHB-C4A-NA	2.55	128.07	124.40
17	7	303	CLA	C3B-C4B-NB	-2.54	108.26	110.53
17	A	5030	CLA	CHB-C4A-NA	2.54	128.07	124.40
16	a	606	CHL	CHD-C1D-C2D	2.54	130.77	125.49
16	1	601	CHL	CHC-C4B-NB	-2.54	120.24	124.05
17	1	613	CLA	CHB-C4A-NA	2.54	128.06	124.40
16	a	606	CHL	C1D-ND-C4D	2.53	108.09	106.31
17	T	405	CLA	C1D-ND-C4D	-2.53	104.53	106.31
16	1	601	CHL	CHD-C1D-C2D	2.53	130.75	125.49
20	K	205	BCR	C11-C12-C13	2.53	133.30	126.36
16	a	606	CHL	C3D-C2D-C1D	2.53	109.28	105.83
17	A	5029	CLA	C3B-C4B-NB	-2.53	108.27	110.53
16	3	322	CHL	C1D-CHD-C4C	-2.52	120.65	126.02
17	A	5014	CLA	O2D-CGD-CBD	2.52	115.64	111.23
17	a	605	CLA	CHB-C4A-NA	2.52	128.04	124.40
17	B	809	CLA	CHB-C4A-NA	2.52	128.03	124.40
17	b	609	CLA	C4A-NA-C1A	2.52	107.83	106.68
17	1	602	CLA	CHB-C4A-NA	2.51	128.03	124.40
17	B	840	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	3	322	CHL	CHD-C1D-C2D	2.51	130.71	125.49
16	T	416	CHL	CHD-C1D-C2D	2.51	130.71	125.49
19	1	616	XAT	C7-C8-C9	2.51	129.42	125.53
17	T	404	CLA	CHB-C4A-NA	2.51	128.02	124.40
17	c	312	CLA	CHB-C4A-NA	2.50	128.01	124.40
16	T	401	CHL	C3B-C4B-NB	-2.50	108.30	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	5004	CLA	CHB-C4A-NA	2.50	128.00	124.40
18	T	413	LUT	C8-C7-C6	2.50	133.67	127.00
17	b	603	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	8	305	CLA	CHB-C4A-NA	2.50	128.00	124.40
17	B	805	CLA	C3B-C4B-NB	-2.49	108.31	110.53
17	T	402	CLA	CHB-C4A-NA	2.49	127.99	124.40
17	B	822	CLA	CHB-C4A-NA	2.48	127.98	124.40
17	B	828	CLA	C3B-C4B-NB	-2.48	108.31	110.53
17	T	402	CLA	C3B-C4B-NB	-2.48	108.31	110.53
17	B	837	CLA	CHB-C4A-NA	2.48	127.98	124.40
16	7	306	CHL	C3D-C2D-C1D	2.48	109.22	105.83
17	A	5005	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
17	A	5044	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
16	b	605	CHL	CHD-C1D-C2D	2.48	130.64	125.49
17	c	311	CLA	C1-C2-C3	-2.47	122.76	126.76
17	A	5034	CLA	CHB-C4A-NA	2.47	127.96	124.40
17	T	403	CLA	C4A-NA-C1A	2.47	107.80	106.68
17	T	410	CLA	C3B-C4B-NB	-2.47	108.33	110.53
20	B	849	BCR	C23-C24-C25	2.46	133.58	127.00
16	b	606	CHL	CHD-C1D-C2D	2.46	130.61	125.49
16	7	306	CHL	CHD-C1D-C2D	2.46	130.60	125.49
17	B	841	CLA	CHB-C4A-NA	2.46	127.94	124.40
17	7	314	CLA	CHB-C4A-NA	2.45	127.94	124.40
17	c	302	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	c	306	CHL	C3B-C4B-NB	-2.45	108.34	110.53
16	a	601	CHL	C1D-CHD-C4C	-2.45	120.82	126.02
17	T	406	CLA	C1-C2-C3	-2.45	122.81	126.76
16	b	606	CHL	C1D-CHD-C4C	-2.44	120.82	126.02
17	3	312	CLA	C4A-NA-C1A	2.44	107.79	106.68
17	B	839	CLA	CHB-C4A-NA	2.44	127.92	124.40
16	b	607	CHL	CHB-C1B-NB	-2.43	120.40	124.05
16	c	304	CHL	CHB-C1B-NB	-2.43	120.40	124.05
17	A	5019	CLA	CHB-C4A-NA	2.43	127.91	124.40
17	B	809	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
16	a	601	CHL	C1C-C2C-C3C	-2.43	105.04	107.28
17	a	608	CLA	O2D-CGD-CBD	2.43	115.48	111.23
17	B	811	CLA	C1-C2-C3	-2.43	122.83	126.76
16	3	301	CHL	C2D-C1D-ND	-2.43	107.72	110.13
17	A	5013	CLA	C4A-NA-C1A	2.43	107.79	106.68
16	b	607	CHL	C2A-C1A-CHA	2.43	128.08	123.87
17	a	603	CLA	CHB-C4A-NA	2.42	127.90	124.40
16	7	307	CHL	CHC-C4B-NB	-2.41	120.44	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	830	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
17	A	5042	CLA	CHB-C4A-NA	2.40	127.86	124.40
20	c	316	BCR	C23-C24-C25	2.40	133.41	127.00
16	8	308	CHL	CHB-C1B-NB	-2.40	120.45	124.05
17	A	5016	CLA	C3B-C4B-NB	-2.40	108.39	110.53
17	B	813	CLA	C1-C2-C3	-2.40	122.88	126.76
16	8	306	CHL	C3B-C4B-NB	-2.40	108.39	110.53
16	3	301	CHL	CHC-C4B-NB	-2.39	120.47	124.05
16	c	304	CHL	C4B-CHC-C1C	-2.39	120.63	126.25
17	8	303	CLA	C1-C2-C3	-2.39	122.90	126.76
18	a	615	LUT	C21-C26-C27	2.38	115.56	112.83
17	A	5032	CLA	CHB-C4A-NA	2.38	127.84	124.40
17	8	302	CLA	O2D-CGD-CBD	2.38	115.40	111.23
16	a	601	CHL	CHD-C1D-C2D	2.38	130.44	125.49
17	B	837	CLA	C1-C2-C3	-2.38	122.91	126.76
17	A	5044	CLA	CHB-C4A-NA	2.38	127.83	124.40
17	A	5016	CLA	CBC-CAC-C3C	2.37	118.86	112.42
17	A	5030	CLA	C1-C2-C3	-2.37	122.31	126.20
16	c	304	CHL	CHC-C1C-NC	-2.37	120.74	124.31
16	b	605	CHL	CHC-C4B-NB	-2.37	120.49	124.05
16	T	416	CHL	CHB-C1B-NB	-2.37	120.50	124.05
17	c	313	CLA	CHB-C4A-NA	2.37	127.82	124.40
17	B	839	CLA	C3B-C4B-NB	-2.37	108.42	110.53
16	8	308	CHL	CHC-C1C-NC	-2.36	120.76	124.31
16	T	401	CHL	CHC-C4B-NB	-2.36	120.51	124.05
17	B	816	CLA	C1-C2-C3	-2.36	122.95	126.76
16	1	606	CHL	C1C-C2C-C3C	-2.36	105.11	107.28
16	c	305	CHL	CHB-C1B-NB	-2.36	120.52	124.05
17	A	5011	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
18	1	615	LUT	C32-C33-C34	2.35	122.71	119.01
17	B	831	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	T	416	CHL	C1D-CHD-C4C	-2.35	121.03	126.02
17	7	304	CLA	CHB-C4A-NA	2.35	127.79	124.40
17	c	309	CLA	C1-C2-C3	-2.34	122.36	126.20
16	a	601	CHL	CHC-C4B-NB	-2.34	120.54	124.05
17	a	609	CLA	C4A-NA-C1A	2.34	107.75	106.68
17	B	824	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
16	3	322	CHL	C2A-C1A-CHA	2.34	127.93	123.87
17	c	303	CLA	C1-C2-C3	-2.34	122.98	126.76
16	7	305	CHL	CHC-C4B-NB	-2.34	120.54	124.05
17	B	805	CLA	CMB-C2B-C3B	2.34	132.05	126.55
17	B	835	CLA	C1-C2-C3	-2.33	122.99	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	7	303	CLA	CHB-C4A-NA	2.33	127.77	124.40
16	8	306	CHL	C1D-CHD-C4C	-2.33	121.08	126.02
17	A	5034	CLA	C1-C2-C3	-2.32	122.39	126.20
18	1	615	LUT	C21-C26-C27	2.32	115.49	112.83
16	7	305	CHL	CHD-C1D-C2D	2.32	130.31	125.49
16	c	306	CHL	CHC-C1C-NC	-2.32	120.81	124.31
17	T	410	CLA	CHB-C4A-NA	2.32	127.75	124.40
16	b	606	CHL	CHB-C1B-NB	-2.32	120.57	124.05
17	B	815	CLA	C1-C2-C3	-2.32	123.02	126.76
16	3	301	CHL	C1C-C2C-C3C	-2.32	105.15	107.28
17	8	312	CLA	C1-C2-C3	-2.31	123.02	126.76
17	b	611	CLA	C1-C2-C3	-2.31	123.02	126.76
17	b	611	CLA	C2A-C1A-CHA	2.31	127.87	123.87
16	8	307	CHL	CHB-C1B-NB	-2.31	120.59	124.05
17	7	304	CLA	C1-C2-C3	-2.30	123.03	126.76
16	1	601	CHL	C3D-C2D-C1D	2.30	108.98	105.83
16	8	306	CHL	CHC-C4B-NB	-2.30	120.59	124.05
16	8	308	CHL	CHC-C4B-NB	-2.30	120.60	124.05
18	a	615	LUT	C30-C31-C32	2.30	129.85	123.20
16	a	601	CHL	CHB-C1B-NB	-2.29	120.61	124.05
17	c	313	CLA	C3B-C4B-NB	-2.29	108.48	110.53
30	J	101	LMK	O2-C4-C3	2.29	117.18	111.88
17	B	802	CLA	CHB-C4A-NA	2.29	127.70	124.40
18	7	315	LUT	C21-C26-C27	2.29	115.45	112.83
19	7	316	XAT	C36-C21-C26	2.29	116.22	110.05
17	B	823	CLA	C1-C2-C3	-2.29	123.06	126.76
17	T	407	CLA	C1-C2-C3	-2.29	123.06	126.76
17	F	5004	CLA	C2A-C1A-CHA	2.28	127.83	123.87
16	7	306	CHL	CHB-C1B-NB	-2.28	120.63	124.05
17	A	5012	CLA	C1-C2-C3	-2.28	122.46	126.20
16	c	304	CHL	CHC-C4B-NB	-2.28	120.63	124.05
16	8	307	CHL	CHC-C4B-NB	-2.28	120.63	124.05
17	A	5013	CLA	C3B-C4B-NB	-2.28	108.50	110.53
16	7	305	CHL	CHB-C1B-NB	-2.27	120.64	124.05
17	c	312	CLA	C1-C2-C3	-2.27	123.09	126.76
16	7	307	CHL	CHB-C1B-NB	-2.27	120.65	124.05
16	8	308	CHL	C4B-CHC-C1C	-2.27	120.92	126.25
16	a	606	CHL	C1C-C2C-C3C	-2.27	105.20	107.28
16	c	306	CHL	CHC-C4B-NB	-2.27	120.65	124.05
17	T	404	CLA	CHD-C1D-ND	-2.26	121.62	124.80
17	A	5016	CLA	CMB-C2B-C1B	-2.26	121.97	125.42
16	c	306	CHL	C4B-CHC-C1C	-2.26	120.93	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	410	CLA	C1-C2-C3	-2.26	123.10	126.76
16	a	606	CHL	CHB-C1B-NB	-2.26	120.66	124.05
17	A	5037	CLA	C1-C2-C3	-2.26	123.11	126.76
16	8	307	CHL	CHC-C1C-NC	-2.26	120.91	124.31
16	b	607	CHL	CHC-C1C-NC	-2.26	120.91	124.31
17	T	409	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
17	c	307	CLA	C1-C2-C3	-2.26	123.11	126.76
18	a	615	LUT	C35-C34-C33	2.25	130.44	127.28
16	7	305	CHL	C1D-CHD-C4C	-2.25	121.23	126.02
17	A	5006	CLA	O2D-CGD-CBD	2.25	115.17	111.23
17	7	313	CLA	C1-C2-C3	-2.25	123.12	126.76
17	A	5021	CLA	C1-C2-C3	-2.25	123.12	126.76
17	B	834	CLA	C1-C2-C3	-2.25	123.12	126.76
16	b	606	CHL	CHC-C4B-NB	-2.25	120.68	124.05
17	B	808	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	a	606	CHL	CHD-C4C-NC	-2.25	120.75	124.23
17	b	602	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
16	7	306	CHL	CHC-C4B-NB	-2.24	120.68	124.05
16	c	305	CHL	CHC-C4B-NB	-2.24	120.68	124.05
16	1	601	CHL	C3B-C4B-NB	-2.24	108.53	110.53
17	c	307	CLA	CHB-C1B-NB	2.24	127.41	124.05
16	T	401	CHL	CHD-C1D-ND	-2.24	121.65	124.80
17	A	5044	CLA	CMB-C2B-C3B	2.24	131.82	126.55
17	T	404	CLA	CHD-C1D-C2D	2.24	130.15	125.49
20	B	845	BCR	C10-C11-C12	2.24	129.68	123.20
17	B	814	CLA	C1-C2-C3	-2.23	123.15	126.76
16	1	601	CHL	C1D-CHD-C4C	-2.23	121.27	126.02
16	3	301	CHL	C3B-C4B-NB	-2.23	108.54	110.53
17	B	805	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	7	306	CHL	C1D-CHD-C4C	-2.22	121.30	126.02
17	a	604	CLA	C1-C2-C3	-2.22	123.17	126.76
16	b	607	CHL	CHC-C4B-NB	-2.22	120.72	124.05
17	A	5013	CLA	CHD-C1D-ND	-2.22	121.68	124.80
17	3	305	CLA	C1-C2-C3	-2.22	123.17	126.76
16	1	606	CHL	CHC-C1C-NC	-2.21	120.98	124.31
17	T	408	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
17	c	307	CLA	O2D-CGD-CBD	2.21	115.10	111.23
17	A	5041	CLA	C1-C2-C3	-2.21	122.58	126.20
16	b	605	CHL	C1D-CHD-C4C	-2.21	121.32	126.02
17	A	5043	CLA	O2D-CGD-CBD	2.21	115.09	111.23
17	A	5027	CLA	CHB-C4A-NA	2.21	127.59	124.40
17	A	5005	CLA	CMB-C2B-C3B	2.21	131.74	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	607	CHL	C4B-CHC-C1C	-2.21	121.06	126.25
17	c	307	CLA	CHB-C4A-NA	2.20	127.58	124.40
17	T	403	CLA	CMB-C2B-C3B	2.20	131.73	126.55
16	T	401	CHL	C1C-C2C-C3C	-2.20	105.26	107.28
17	A	5011	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
17	B	813	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	c	305	CHL	CHD-C1D-C2D	2.19	130.04	125.49
16	1	606	CHL	CHB-C1B-NB	-2.19	120.76	124.05
16	b	605	CHL	CHC-C1C-NC	-2.19	121.01	124.31
17	A	5031	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
16	a	601	CHL	C4B-CHC-C1C	-2.19	121.10	126.25
17	A	5037	CLA	O2D-CGD-CBD	2.19	115.05	111.23
17	A	5008	CLA	CHD-C1D-ND	-2.19	121.73	124.80
17	T	403	CLA	C1-C2-C3	-2.19	123.23	126.76
17	T	408	CLA	C1-C2-C3	-2.19	123.23	126.76
17	1	611	CLA	CHA-C1A-NA	-2.18	121.44	126.39
17	A	5015	CLA	C1-C2-C3	-2.18	122.62	126.20
16	a	601	CHL	CHC-C1C-NC	-2.18	121.02	124.31
17	A	5039	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	B	839	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
17	B	825	CLA	C1-C2-C3	-2.18	123.23	126.76
16	b	605	CHL	CHB-C1B-NB	-2.18	120.78	124.05
27	A	5003	CL0	CHB-C1B-NB	-2.18	120.78	124.05
17	1	612	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
17	A	5010	CLA	C1-C2-C3	-2.18	123.24	126.76
17	A	5010	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	7	307	CHL	C2A-C1A-CHA	2.17	127.64	123.87
17	a	604	CLA	C1C-NC-C4C	2.17	107.67	106.68
16	c	305	CHL	CHC-C1C-NC	-2.17	121.04	124.31
17	T	409	CLA	C1-C2-C3	-2.17	122.64	126.20
17	A	5015	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
17	a	609	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
16	8	306	CHL	CHB-C1B-NB	-2.17	120.80	124.05
17	T	406	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
17	c	309	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
16	b	606	CHL	CHD-C4C-NC	-2.17	120.87	124.23
16	7	306	CHL	CHC-C1C-NC	-2.17	121.05	124.31
16	8	307	CHL	C4B-CHC-C1C	-2.17	121.16	126.25
17	T	402	CLA	C1-C2-C3	-2.17	123.26	126.76
19	c	315	XAT	C36-C21-C26	2.16	115.89	110.05
16	1	601	CHL	CHB-C1B-NB	-2.16	120.80	124.05
17	B	832	CLA	O2A-CGA-O1A	-2.16	118.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	403	CLA	CHA-C1A-NA	-2.16	121.50	126.39
17	3	306	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	8	311	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	a	611	CLA	CHA-C1A-NA	-2.16	121.50	126.39
17	B	829	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	B	818	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
17	8	310	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
17	B	831	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	b	606	CHL	CHC-C1C-NC	-2.15	121.07	124.31
17	A	5009	CLA	C1-C2-C3	-2.15	122.67	126.20
17	B	832	CLA	C2A-C1A-CHA	2.15	127.60	123.87
17	T	403	CLA	O2D-CGD-CBD	2.15	114.98	111.23
17	B	814	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
16	a	606	CHL	CHC-C1C-NC	-2.14	121.08	124.31
17	b	610	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	T	401	CHL	CHB-C1B-NB	-2.14	120.84	124.05
17	B	832	CLA	C1-C2-C3	-2.14	122.69	126.20
16	3	322	CHL	CHB-C1B-NB	-2.14	120.84	124.05
17	A	5039	CLA	C1-C2-C3	-2.14	122.70	126.20
17	b	604	CLA	C1-C2-C3	-2.13	123.31	126.76
17	8	313	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
17	A	5012	CLA	CAA-CBA-CGA	-2.13	107.15	113.21
17	3	311	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
17	B	837	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	T	416	CHL	CHC-C1C-NC	-2.12	121.11	124.31
16	c	306	CHL	CHB-C1B-NB	-2.12	120.86	124.05
17	F	5004	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
17	F	5007	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
17	A	5017	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
17	B	824	CLA	C2A-C1A-CHA	2.12	127.55	123.87
17	b	602	CLA	C1-C2-C3	-2.12	122.73	126.20
17	3	305	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
17	A	5008	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
17	8	303	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	T	401	CHL	CHC-C1C-NC	-2.12	121.12	124.31
17	A	5009	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
17	T	405	CLA	C4D-C3D-CAD	-2.11	105.81	108.11
17	A	5021	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
17	A	5034	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
17	7	311	CLA	CHA-C1A-NA	-2.11	121.62	126.39
17	A	5025	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
17	B	825	CLA	O2A-CGA-O1A	-2.10	118.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	804	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
19	b	616	XAT	C27-C28-C29	2.10	128.79	125.53
17	B	828	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
16	8	307	CHL	CHD-C1D-C2D	2.10	129.86	125.49
17	A	5005	CLA	C3B-C4B-NB	-2.10	108.65	110.53
16	8	306	CHL	CHD-C1D-ND	-2.10	121.85	124.80
17	c	312	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
27	A	5003	CL0	CHC-C1C-NC	-2.10	121.15	124.31
16	1	606	CHL	CHD-C4C-NC	-2.10	120.98	124.23
17	A	5006	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
17	7	313	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
17	B	831	CLA	C1-C2-C3	-2.09	122.77	126.20
17	B	825	CLA	O2D-CGD-CBD	2.09	114.89	111.23
17	A	5041	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	3	301	CHL	CHB-C1B-NB	-2.09	120.91	124.05
17	3	306	CLA	C1-C2-C3	-2.09	122.77	126.20
17	T	402	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
17	A	5013	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
17	A	5008	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
16	3	322	CHL	C4B-C3B-C2B	-2.08	104.71	107.30
17	1	607	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	B	817	CLA	CHD-C1D-ND	-2.08	121.88	124.80
16	7	306	CHL	C1D-ND-C4D	2.08	107.77	106.31
17	B	807	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
17	T	407	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
17	8	304	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	7	316	XAT	O4-C5-C4	-2.07	111.55	113.49
17	3	307	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	3	308	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	B	834	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
17	A	5016	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	B	838	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	A	5027	CLA	C1-C2-C3	-2.07	122.81	126.20
17	A	5029	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
17	a	612	CLA	C1-C2-C3	-2.07	123.42	126.76
17	T	403	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
17	7	312	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
17	c	301	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
16	8	308	CHL	C2A-C1A-CHA	2.06	127.45	123.87
17	B	820	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
17	B	835	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
17	B	816	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	c	310	CLA	C2A-C1A-CHA	2.06	127.44	123.87
17	7	312	CLA	C1-C2-C3	-2.06	122.82	126.20
16	T	401	CHL	C3D-C2D-C1D	2.06	108.64	105.83
16	7	305	CHL	CHC-C1C-NC	-2.06	121.21	124.31
17	T	409	CLA	CHA-C1A-NA	-2.06	121.73	126.39
20	B	849	BCR	C7-C8-C9	2.06	129.28	126.23
17	K	202	CLA	O2D-CGD-CBD	2.05	114.82	111.23
17	A	5038	CLA	C1-C2-C3	-2.05	123.44	126.76
17	8	304	CLA	C2A-C1A-CHA	2.05	127.43	123.87
17	A	5028	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	T	416	CHL	CHD-C4C-NC	-2.05	121.05	124.23
16	T	416	CHL	CHC-C4B-NB	-2.05	120.97	124.05
16	3	301	CHL	CHC-C1C-NC	-2.05	121.22	124.31
17	b	612	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
17	3	307	CLA	O2D-CGD-CBD	2.05	114.82	111.23
17	1	602	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	a	606	CHL	CHD-C1D-ND	-2.05	121.92	124.80
17	A	5012	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
17	b	608	CLA	O2D-CGD-CBD	2.04	114.81	111.23
17	1	602	CLA	O1D-CGD-CBD	2.04	128.55	124.52
17	A	5020	CLA	O2A-CGA-O1A	-2.04	118.51	123.63
16	7	307	CHL	C4B-CHC-C1C	-2.04	121.44	126.25
17	B	832	CLA	CHA-C1A-NA	-2.04	121.77	126.39
17	a	602	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
17	T	403	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
17	3	323	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
17	c	301	CLA	C1-C2-C3	-2.03	122.86	126.20
17	A	5024	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	b	605	CHL	CHD-C4C-NC	-2.03	121.08	124.23
17	A	5042	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
17	T	410	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
17	A	5011	CLA	O1D-CGD-CBD	2.03	128.52	124.52
17	1	612	CLA	C1-C2-C3	-2.03	122.88	126.20
17	7	303	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
17	b	603	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
17	B	826	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	B	815	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	3	308	CLA	C1-C2-C3	-2.02	122.89	126.20
17	8	312	CLA	C2A-C1A-CHA	2.02	127.37	123.87
17	L	201	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
17	B	839	CLA	C1-C2-C3	-2.01	122.90	126.20
17	B	836	CLA	O2D-CGD-CBD	2.01	114.75	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	841	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	b	611	CLA	CHA-C1A-NA	-2.01	121.84	126.39
27	A	5003	CL0	CHD-C4C-NC	-2.01	121.11	124.23
17	A	5044	CLA	C1-C2-C3	-2.01	122.90	126.20
17	B	833	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
17	A	5013	CLA	CHC-C1C-NC	2.01	127.33	124.31
17	B	825	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
17	A	5035	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	B	802	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	A	5029	CLA	CHD-C1D-ND	-2.01	121.98	124.80
17	b	613	CLA	CHD-C1D-ND	-2.01	121.98	124.80
17	F	5006	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	J	102	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	8	312	CLA	O2D-CGD-CBD	2.00	114.73	111.23
16	b	607	CHL	CHD-C1D-C2D	2.00	129.65	125.49
17	A	5033	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	B	802	CLA	C4A-NA-C1A	2.00	107.59	106.68
17	A	5027	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	7	304	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
17	c	307	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	3	301	CHL	C8
16	3	322	CHL	C8
18	1	615	LUT	C3
18	1	615	LUT	C26
18	1	615	LUT	C23
18	3	315	LUT	C3
18	3	315	LUT	C26
18	3	315	LUT	C23
18	7	315	LUT	C3
18	7	315	LUT	C26
18	7	315	LUT	C23
18	8	316	LUT	C3
18	8	316	LUT	C26
18	8	316	LUT	C23
18	T	413	LUT	C3
18	T	413	LUT	C26
18	T	413	LUT	C23
18	a	615	LUT	C3

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Mol	Chain	Res	Type	Atom
18	a	615	LUT	C26
18	a	615	LUT	C23
18	b	615	LUT	C3
18	b	615	LUT	C26
18	b	615	LUT	C23
18	c	314	LUT	C3
18	c	314	LUT	C26
18	c	314	LUT	C23

All (2283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CHL	C1A-C2A-CAA-CBA
16	1	601	CHL	C3A-C2A-CAA-CBA
16	1	601	CHL	C1C-C2C-CMC-OMC
16	1	601	CHL	C3C-C2C-CMC-OMC
16	1	601	CHL	CHA-CBD-CGD-O1D
16	1	601	CHL	CHA-CBD-CGD-O2D
16	1	601	CHL	CBD-CGD-O2D-CED
16	1	606	CHL	C2B-C3B-CAB-CBB
16	1	606	CHL	C4B-C3B-CAB-CBB
16	3	301	CHL	C3A-C2A-CAA-CBA
16	3	301	CHL	C1C-C2C-CMC-OMC
16	3	322	CHL	C1A-C2A-CAA-CBA
16	3	322	CHL	C3A-C2A-CAA-CBA
16	3	322	CHL	C3C-C2C-CMC-OMC
16	7	305	CHL	C1C-C2C-CMC-OMC
16	7	306	CHL	C2B-C3B-CAB-CBB
16	7	306	CHL	C4B-C3B-CAB-CBB
16	7	307	CHL	C3A-C2A-CAA-CBA
16	7	307	CHL	C1C-C2C-CMC-OMC
16	8	306	CHL	C3C-C2C-CMC-OMC
16	8	306	CHL	CHA-CBD-CGD-O2D
16	8	306	CHL	CBD-CGD-O2D-CED
16	8	307	CHL	C1A-C2A-CAA-CBA
16	8	307	CHL	C3A-C2A-CAA-CBA
16	8	307	CHL	C2B-C3B-CAB-CBB
16	8	307	CHL	C4B-C3B-CAB-CBB
16	8	308	CHL	C1C-C2C-CMC-OMC
16	8	308	CHL	CBD-CGD-O2D-CED
16	T	401	CHL	C1C-C2C-CMC-OMC
16	T	401	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	T	401	CHL	C1-C2-C3-C4
16	T	401	CHL	C1-C2-C3-C5
16	T	416	CHL	C1A-C2A-CAA-CBA
16	T	416	CHL	C3A-C2A-CAA-CBA
16	T	416	CHL	C3C-C2C-CMC-OMC
16	T	416	CHL	CHA-CBD-CGD-O1D
16	T	416	CHL	CHA-CBD-CGD-O2D
16	a	601	CHL	C1A-C2A-CAA-CBA
16	a	601	CHL	C3A-C2A-CAA-CBA
16	a	601	CHL	C3C-C2C-CMC-OMC
16	a	606	CHL	C1C-C2C-CMC-OMC
16	a	606	CHL	C3C-C2C-CMC-OMC
16	a	606	CHL	CBD-CGD-O2D-CED
16	b	605	CHL	C1C-C2C-CMC-OMC
16	b	605	CHL	CHA-CBD-CGD-O1D
16	b	605	CHL	CHA-CBD-CGD-O2D
16	b	607	CHL	C1A-C2A-CAA-CBA
16	b	607	CHL	C3C-C2C-CMC-OMC
16	c	304	CHL	C1C-C2C-CMC-OMC
16	c	304	CHL	CBD-CGD-O2D-CED
16	c	305	CHL	C2B-C3B-CAB-CBB
16	c	305	CHL	C4B-C3B-CAB-CBB
16	c	306	CHL	CBD-CGD-O2D-CED
17	1	602	CLA	CHA-CBD-CGD-O2D
17	1	603	CLA	CBD-CGD-O2D-CED
17	1	604	CLA	C2B-C3B-CAB-CBB
17	1	604	CLA	C4B-C3B-CAB-CBB
17	1	604	CLA	CAD-CBD-CGD-O1D
17	1	604	CLA	CAD-CBD-CGD-O2D
17	1	605	CLA	C2B-C3B-CAB-CBB
17	1	605	CLA	C4B-C3B-CAB-CBB
17	1	607	CLA	C3A-C2A-CAA-CBA
17	1	607	CLA	C4B-C3B-CAB-CBB
17	1	608	CLA	C1A-C2A-CAA-CBA
17	1	608	CLA	C3A-C2A-CAA-CBA
17	1	608	CLA	CHA-CBD-CGD-O2D
17	1	610	CLA	C2B-C3B-CAB-CBB
17	1	610	CLA	C4B-C3B-CAB-CBB
17	1	611	CLA	C1A-C2A-CAA-CBA
17	1	611	CLA	C3A-C2A-CAA-CBA
17	1	611	CLA	CBA-CGA-O2A-C1
17	1	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	1	612	CLA	C4B-C3B-CAB-CBB
17	1	612	CLA	CBD-CGD-O2D-CED
17	1	613	CLA	CBA-CGA-O2A-C1
17	1	614	CLA	C4B-C3B-CAB-CBB
17	3	302	CLA	CBD-CGD-O2D-CED
17	3	303	CLA	CBA-CGA-O2A-C1
17	3	303	CLA	O1A-CGA-O2A-C1
17	3	304	CLA	CBA-CGA-O2A-C1
17	3	304	CLA	O1A-CGA-O2A-C1
17	3	306	CLA	C1A-C2A-CAA-CBA
17	3	306	CLA	C3A-C2A-CAA-CBA
17	3	307	CLA	C3A-C2A-CAA-CBA
17	3	307	CLA	CHA-CBD-CGD-O1D
17	3	307	CLA	CHA-CBD-CGD-O2D
17	3	308	CLA	C2B-C3B-CAB-CBB
17	3	308	CLA	C4B-C3B-CAB-CBB
17	3	308	CLA	CBD-CGD-O2D-CED
17	3	309	CLA	C2B-C3B-CAB-CBB
17	3	309	CLA	C4B-C3B-CAB-CBB
17	3	309	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	C4B-C3B-CAB-CBB
17	3	311	CLA	C2B-C3B-CAB-CBB
17	3	311	CLA	C4B-C3B-CAB-CBB
17	3	312	CLA	CBD-CGD-O2D-CED
17	3	313	CLA	CBD-CGD-O2D-CED
17	3	314	CLA	CBA-CGA-O2A-C1
17	3	314	CLA	C2B-C3B-CAB-CBB
17	3	314	CLA	C4B-C3B-CAB-CBB
17	3	323	CLA	C1A-C2A-CAA-CBA
17	3	323	CLA	C3A-C2A-CAA-CBA
17	3	324	CLA	C1A-C2A-CAA-CBA
17	3	324	CLA	C3A-C2A-CAA-CBA
17	7	302	CLA	C1A-C2A-CAA-CBA
17	7	302	CLA	C3A-C2A-CAA-CBA
17	7	302	CLA	CBD-CGD-O2D-CED
17	7	303	CLA	C2B-C3B-CAB-CBB
17	7	303	CLA	C4B-C3B-CAB-CBB
17	7	304	CLA	CBD-CGD-O2D-CED
17	7	308	CLA	C1A-C2A-CAA-CBA
17	7	308	CLA	C3A-C2A-CAA-CBA
17	7	308	CLA	CBA-CGA-O2A-C1
17	7	309	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	7	309	CLA	C4B-C3B-CAB-CBB
17	7	310	CLA	C2B-C3B-CAB-CBB
17	7	310	CLA	C4B-C3B-CAB-CBB
17	7	311	CLA	C2B-C3B-CAB-CBB
17	7	311	CLA	C4B-C3B-CAB-CBB
17	7	312	CLA	C2B-C3B-CAB-CBB
17	7	312	CLA	C4B-C3B-CAB-CBB
17	7	313	CLA	C2B-C3B-CAB-CBB
17	7	313	CLA	C4B-C3B-CAB-CBB
17	7	314	CLA	C2B-C3B-CAB-CBB
17	7	314	CLA	C4B-C3B-CAB-CBB
17	8	303	CLA	C1A-C2A-CAA-CBA
17	8	303	CLA	C3A-C2A-CAA-CBA
17	8	303	CLA	C2B-C3B-CAB-CBB
17	8	303	CLA	C4B-C3B-CAB-CBB
17	8	304	CLA	C2B-C3B-CAB-CBB
17	8	304	CLA	C4B-C3B-CAB-CBB
17	8	309	CLA	C1A-C2A-CAA-CBA
17	8	309	CLA	C3A-C2A-CAA-CBA
17	8	310	CLA	C1A-C2A-CAA-CBA
17	8	310	CLA	C2B-C3B-CAB-CBB
17	8	310	CLA	C4B-C3B-CAB-CBB
17	8	311	CLA	C2B-C3B-CAB-CBB
17	8	311	CLA	C4B-C3B-CAB-CBB
17	8	312	CLA	CHA-CBD-CGD-O1D
17	8	312	CLA	CHA-CBD-CGD-O2D
17	8	313	CLA	C2B-C3B-CAB-CBB
17	8	313	CLA	C4B-C3B-CAB-CBB
17	8	313	CLA	CBD-CGD-O2D-CED
17	8	314	CLA	C1A-C2A-CAA-CBA
17	8	314	CLA	C3A-C2A-CAA-CBA
17	8	314	CLA	C2B-C3B-CAB-CBB
17	8	314	CLA	C4B-C3B-CAB-CBB
17	8	315	CLA	C2B-C3B-CAB-CBB
17	8	315	CLA	C4B-C3B-CAB-CBB
17	A	5004	CLA	CBD-CGD-O2D-CED
17	A	5006	CLA	C1A-C2A-CAA-CBA
17	A	5006	CLA	C3A-C2A-CAA-CBA
17	A	5006	CLA	C2B-C3B-CAB-CBB
17	A	5006	CLA	C4B-C3B-CAB-CBB
17	A	5007	CLA	C3A-C2A-CAA-CBA
17	A	5008	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	A	5008	CLA	C3A-C2A-CAA-CBA
17	A	5008	CLA	CAD-CBD-CGD-O1D
17	A	5008	CLA	CAD-CBD-CGD-O2D
17	A	5011	CLA	C3A-C2A-CAA-CBA
17	A	5012	CLA	C2B-C3B-CAB-CBB
17	A	5012	CLA	C4B-C3B-CAB-CBB
17	A	5013	CLA	C1A-C2A-CAA-CBA
17	A	5013	CLA	C2B-C3B-CAB-CBB
17	A	5013	CLA	C4B-C3B-CAB-CBB
17	A	5013	CLA	CBD-CGD-O2D-CED
17	A	5016	CLA	C1A-C2A-CAA-CBA
17	A	5016	CLA	C3A-C2A-CAA-CBA
17	A	5017	CLA	C2-C3-C5-C6
17	A	5017	CLA	C4-C3-C5-C6
17	A	5019	CLA	C4B-C3B-CAB-CBB
17	A	5020	CLA	CHA-CBD-CGD-O1D
17	A	5020	CLA	CHA-CBD-CGD-O2D
17	A	5021	CLA	C2B-C3B-CAB-CBB
17	A	5021	CLA	C4B-C3B-CAB-CBB
17	A	5023	CLA	C2B-C3B-CAB-CBB
17	A	5023	CLA	C4B-C3B-CAB-CBB
17	A	5024	CLA	C2B-C3B-CAB-CBB
17	A	5024	CLA	C4B-C3B-CAB-CBB
17	A	5025	CLA	C2B-C3B-CAB-CBB
17	A	5025	CLA	C4B-C3B-CAB-CBB
17	A	5025	CLA	CBD-CGD-O2D-CED
17	A	5026	CLA	CBD-CGD-O2D-CED
17	A	5027	CLA	C4B-C3B-CAB-CBB
17	A	5027	CLA	CHA-CBD-CGD-O1D
17	A	5027	CLA	CHA-CBD-CGD-O2D
17	A	5027	CLA	CBD-CGD-O2D-CED
17	A	5029	CLA	C1A-C2A-CAA-CBA
17	A	5029	CLA	C3A-C2A-CAA-CBA
17	A	5031	CLA	CHA-CBD-CGD-O1D
17	A	5031	CLA	CHA-CBD-CGD-O2D
17	A	5032	CLA	C2B-C3B-CAB-CBB
17	A	5032	CLA	C4B-C3B-CAB-CBB
17	A	5034	CLA	C4B-C3B-CAB-CBB
17	A	5035	CLA	CHA-CBD-CGD-O1D
17	A	5035	CLA	CHA-CBD-CGD-O2D
17	A	5036	CLA	C2B-C3B-CAB-CBB
17	A	5036	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	A	5037	CLA	C1A-C2A-CAA-CBA
17	A	5037	CLA	C3A-C2A-CAA-CBA
17	A	5037	CLA	C2B-C3B-CAB-CBB
17	A	5037	CLA	C4B-C3B-CAB-CBB
17	A	5037	CLA	CHA-CBD-CGD-O1D
17	A	5037	CLA	CHA-CBD-CGD-O2D
17	A	5039	CLA	C2B-C3B-CAB-CBB
17	A	5039	CLA	C4B-C3B-CAB-CBB
17	A	5040	CLA	C1A-C2A-CAA-CBA
17	A	5040	CLA	C4B-C3B-CAB-CBB
17	A	5041	CLA	C1A-C2A-CAA-CBA
17	A	5041	CLA	C3A-C2A-CAA-CBA
17	A	5042	CLA	C2B-C3B-CAB-CBB
17	A	5042	CLA	C4B-C3B-CAB-CBB
17	A	5043	CLA	CAD-CBD-CGD-O1D
17	A	5043	CLA	CAD-CBD-CGD-O2D
17	B	802	CLA	C2B-C3B-CAB-CBB
17	B	802	CLA	C4B-C3B-CAB-CBB
17	B	802	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	CBD-CGD-O2D-CED
17	B	804	CLA	C1A-C2A-CAA-CBA
17	B	804	CLA	C3A-C2A-CAA-CBA
17	B	806	CLA	CBD-CGD-O2D-CED
17	B	807	CLA	C2B-C3B-CAB-CBB
17	B	807	CLA	C4B-C3B-CAB-CBB
17	B	808	CLA	C1A-C2A-CAA-CBA
17	B	808	CLA	C3A-C2A-CAA-CBA
17	B	808	CLA	C4B-C3B-CAB-CBB
17	B	808	CLA	CBD-CGD-O2D-CED
17	B	809	CLA	C2B-C3B-CAB-CBB
17	B	809	CLA	C4B-C3B-CAB-CBB
17	B	811	CLA	C1A-C2A-CAA-CBA
17	B	811	CLA	C3A-C2A-CAA-CBA
17	B	812	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	O1A-CGA-O2A-C1
17	B	812	CLA	C2B-C3B-CAB-CBB
17	B	812	CLA	C4B-C3B-CAB-CBB
17	B	813	CLA	CBD-CGD-O2D-CED
17	B	813	CLA	O1D-CGD-O2D-CED
17	B	814	CLA	O1A-CGA-O2A-C1
17	B	814	CLA	C4B-C3B-CAB-CBB
17	B	818	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	B	819	CLA	C1A-C2A-CAA-CBA
17	B	819	CLA	C4B-C3B-CAB-CBB
17	B	819	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C3A-C2A-CAA-CBA
17	B	820	CLA	C2B-C3B-CAB-CBB
17	B	820	CLA	C4B-C3B-CAB-CBB
17	B	821	CLA	C2B-C3B-CAB-CBB
17	B	821	CLA	C4B-C3B-CAB-CBB
17	B	821	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	C2B-C3B-CAB-CBB
17	B	822	CLA	C4B-C3B-CAB-CBB
17	B	824	CLA	CHA-CBD-CGD-O1D
17	B	824	CLA	CHA-CBD-CGD-O2D
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	826	CLA	CBD-CGD-O2D-CED
17	B	828	CLA	C1A-C2A-CAA-CBA
17	B	828	CLA	C3A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C3A-C2A-CAA-CBA
17	B	829	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	C4B-C3B-CAB-CBB
17	B	832	CLA	C1A-C2A-CAA-CBA
17	B	832	CLA	C2B-C3B-CAB-CBB
17	B	832	CLA	C4B-C3B-CAB-CBB
17	B	833	CLA	C1A-C2A-CAA-CBA
17	B	833	CLA	C3A-C2A-CAA-CBA
17	B	833	CLA	C4B-C3B-CAB-CBB
17	B	833	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	C2B-C3B-CAB-CBB
17	B	834	CLA	C4B-C3B-CAB-CBB
17	B	834	CLA	CAD-CBD-CGD-O1D
17	B	834	CLA	CAD-CBD-CGD-O2D
17	B	834	CLA	CBD-CGD-O2D-CED
17	B	835	CLA	CBD-CGD-O2D-CED
17	B	837	CLA	CBD-CGD-O2D-CED
17	B	839	CLA	C3A-C2A-CAA-CBA
17	B	840	CLA	C2B-C3B-CAB-CBB
17	B	840	CLA	C4B-C3B-CAB-CBB
17	B	841	CLA	C2B-C3B-CAB-CBB
17	B	841	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	F	5006	CLA	CBD-CGD-O2D-CED
17	F	5007	CLA	C2B-C3B-CAB-CBB
17	F	5007	CLA	C4B-C3B-CAB-CBB
17	F	5008	CLA	C2B-C3B-CAB-CBB
17	F	5008	CLA	C4B-C3B-CAB-CBB
17	F	5008	CLA	CBD-CGD-O2D-CED
17	J	102	CLA	C2B-C3B-CAB-CBB
17	J	102	CLA	C4B-C3B-CAB-CBB
17	K	202	CLA	CBA-CGA-O2A-C1
17	K	202	CLA	O1A-CGA-O2A-C1
17	K	204	CLA	C1A-C2A-CAA-CBA
17	K	204	CLA	C4B-C3B-CAB-CBB
17	T	402	CLA	CBD-CGD-O2D-CED
17	T	402	CLA	O1D-CGD-O2D-CED
17	T	404	CLA	C1A-C2A-CAA-CBA
17	T	405	CLA	C2B-C3B-CAB-CBB
17	T	405	CLA	C4B-C3B-CAB-CBB
17	T	406	CLA	C1A-C2A-CAA-CBA
17	T	406	CLA	C3A-C2A-CAA-CBA
17	T	406	CLA	C4B-C3B-CAB-CBB
17	T	407	CLA	C1A-C2A-CAA-CBA
17	T	407	CLA	C3A-C2A-CAA-CBA
17	T	407	CLA	CHA-CBD-CGD-O1D
17	T	407	CLA	CHA-CBD-CGD-O2D
17	T	408	CLA	C2B-C3B-CAB-CBB
17	T	408	CLA	C4B-C3B-CAB-CBB
17	T	408	CLA	CBD-CGD-O2D-CED
17	T	409	CLA	C2B-C3B-CAB-CBB
17	T	409	CLA	C4B-C3B-CAB-CBB
17	T	410	CLA	C2B-C3B-CAB-CBB
17	T	410	CLA	C4B-C3B-CAB-CBB
17	T	411	CLA	C2B-C3B-CAB-CBB
17	T	411	CLA	C4B-C3B-CAB-CBB
17	T	412	CLA	CBD-CGD-O2D-CED
17	a	602	CLA	C4B-C3B-CAB-CBB
17	a	602	CLA	CBD-CGD-O2D-CED
17	a	603	CLA	C2B-C3B-CAB-CBB
17	a	603	CLA	C4B-C3B-CAB-CBB
17	a	603	CLA	CHA-CBD-CGD-O2D
17	a	603	CLA	CBD-CGD-O2D-CED
17	a	604	CLA	C1A-C2A-CAA-CBA
17	a	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	a	604	CLA	CAD-CBD-CGD-O2D
17	a	604	CLA	CBD-CGD-O2D-CED
17	a	605	CLA	C4B-C3B-CAB-CBB
17	a	607	CLA	C2B-C3B-CAB-CBB
17	a	607	CLA	C4B-C3B-CAB-CBB
17	a	608	CLA	C2B-C3B-CAB-CBB
17	a	608	CLA	C4B-C3B-CAB-CBB
17	a	608	CLA	CHA-CBD-CGD-O1D
17	a	608	CLA	CHA-CBD-CGD-O2D
17	a	609	CLA	C1A-C2A-CAA-CBA
17	a	609	CLA	C3A-C2A-CAA-CBA
17	a	609	CLA	O1A-CGA-O2A-C1
17	a	610	CLA	C2B-C3B-CAB-CBB
17	a	610	CLA	C4B-C3B-CAB-CBB
17	a	611	CLA	CBA-CGA-O2A-C1
17	a	612	CLA	CBD-CGD-O2D-CED
17	a	613	CLA	CBA-CGA-O2A-C1
17	a	613	CLA	O1A-CGA-O2A-C1
17	a	613	CLA	C2B-C3B-CAB-CBB
17	a	613	CLA	C4B-C3B-CAB-CBB
17	a	614	CLA	C4B-C3B-CAB-CBB
17	b	601	CLA	C1A-C2A-CAA-CBA
17	b	601	CLA	C3A-C2A-CAA-CBA
17	b	601	CLA	CBD-CGD-O2D-CED
17	b	602	CLA	C1A-C2A-CAA-CBA
17	b	602	CLA	C3A-C2A-CAA-CBA
17	b	603	CLA	C2B-C3B-CAB-CBB
17	b	603	CLA	C4B-C3B-CAB-CBB
17	b	603	CLA	CBD-CGD-O2D-CED
17	b	608	CLA	C3A-C2A-CAA-CBA
17	b	609	CLA	C2B-C3B-CAB-CBB
17	b	609	CLA	C4B-C3B-CAB-CBB
17	b	610	CLA	C2B-C3B-CAB-CBB
17	b	610	CLA	C4B-C3B-CAB-CBB
17	b	611	CLA	C2B-C3B-CAB-CBB
17	b	611	CLA	C4B-C3B-CAB-CBB
17	b	611	CLA	CHA-CBD-CGD-O1D
17	b	611	CLA	CHA-CBD-CGD-O2D
17	b	612	CLA	O1A-CGA-O2A-C1
17	b	612	CLA	C2B-C3B-CAB-CBB
17	b	612	CLA	C4B-C3B-CAB-CBB
17	b	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	b	614	CLA	C2B-C3B-CAB-CBB
17	b	614	CLA	C4B-C3B-CAB-CBB
17	b	614	CLA	CBD-CGD-O2D-CED
17	c	301	CLA	C1A-C2A-CAA-CBA
17	c	301	CLA	C3A-C2A-CAA-CBA
17	c	303	CLA	CBD-CGD-O2D-CED
17	c	307	CLA	C1A-C2A-CAA-CBA
17	c	307	CLA	C3A-C2A-CAA-CBA
17	c	308	CLA	C1A-C2A-CAA-CBA
17	c	308	CLA	C3A-C2A-CAA-CBA
17	c	308	CLA	CBA-CGA-O2A-C1
17	c	308	CLA	O1A-CGA-O2A-C1
17	c	308	CLA	CBD-CGD-O2D-CED
17	c	309	CLA	C2B-C3B-CAB-CBB
17	c	309	CLA	C4B-C3B-CAB-CBB
17	c	310	CLA	C2B-C3B-CAB-CBB
17	c	310	CLA	C4B-C3B-CAB-CBB
17	c	311	CLA	C2B-C3B-CAB-CBB
17	c	311	CLA	C4B-C3B-CAB-CBB
17	c	311	CLA	CBD-CGD-O2D-CED
17	c	312	CLA	C2B-C3B-CAB-CBB
17	c	312	CLA	C4B-C3B-CAB-CBB
17	c	312	CLA	CBD-CGD-O2D-CED
17	c	313	CLA	C2B-C3B-CAB-CBB
17	c	313	CLA	C4B-C3B-CAB-CBB
17	L	202	CLA	C2B-C3B-CAB-CBB
17	L	202	CLA	C4B-C3B-CAB-CBB
18	1	615	LUT	C1-C6-C7-C8
18	1	615	LUT	C5-C6-C7-C8
18	1	615	LUT	C11-C12-C13-C14
18	1	615	LUT	C13-C14-C15-C35
18	1	615	LUT	C21-C26-C27-C28
18	1	615	LUT	C25-C26-C27-C28
18	3	315	LUT	C25-C26-C27-C28
18	7	315	LUT	C21-C26-C27-C28
18	7	315	LUT	C25-C26-C27-C28
18	a	615	LUT	C11-C12-C13-C14
18	a	615	LUT	C13-C14-C15-C35
18	a	615	LUT	C21-C26-C27-C28
18	a	615	LUT	C25-C26-C27-C28
18	c	314	LUT	C13-C14-C15-C35
18	c	314	LUT	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
18	c	314	LUT	C33-C34-C35-C15
19	1	616	XAT	O4-C6-C7-C8
19	7	316	XAT	C25-C26-C27-C28
19	T	414	XAT	O24-C26-C27-C28
19	a	616	XAT	C6-C7-C8-C9
19	a	616	XAT	O24-C26-C27-C28
19	a	616	XAT	C26-C27-C28-C29
20	8	318	BCR	C13-C14-C15-C16
20	8	318	BCR	C15-C16-C17-C18
20	A	5047	BCR	C5-C6-C7-C8
20	A	5047	BCR	C21-C22-C23-C24
20	A	5048	BCR	C5-C6-C7-C8
20	A	5048	BCR	C15-C16-C17-C18
20	B	843	BCR	C5-C6-C7-C8
20	B	843	BCR	C19-C20-C21-C22
20	B	845	BCR	C11-C12-C13-C14
20	B	845	BCR	C11-C12-C13-C35
20	B	845	BCR	C19-C20-C21-C22
20	B	849	BCR	C7-C8-C9-C10
20	B	849	BCR	C7-C8-C9-C34
20	B	849	BCR	C17-C18-C19-C20
20	K	205	BCR	C1-C6-C7-C8
20	K	205	BCR	C5-C6-C7-C8
20	K	205	BCR	C11-C12-C13-C14
20	K	205	BCR	C11-C12-C13-C35
20	c	316	BCR	C21-C22-C23-C24
20	c	316	BCR	C37-C22-C23-C24
20	c	316	BCR	C22-C23-C24-C25
20	L	203	BCR	C21-C22-C23-C24
20	L	203	BCR	C23-C24-C25-C26
20	L	203	BCR	C23-C24-C25-C30
21	1	618	LHG	C3-O3-P-O4
21	1	618	LHG	C3-O3-P-O6
21	1	618	LHG	C4-O6-P-O3
21	1	618	LHG	O9-C7-O7-C5
21	1	618	LHG	C8-C7-O7-C5
21	1	619	LHG	C3-O3-P-O4
21	1	619	LHG	C3-O3-P-O5
21	1	619	LHG	C3-O3-P-O6
21	8	321	LHG	C3-O3-P-O5
21	8	321	LHG	C4-O6-P-O3
21	8	321	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
21	8	321	LHG	C4-O6-P-O5
21	A	5002	LHG	O7-C5-C6-O8
21	A	5002	LHG	O9-C7-O7-C5
21	A	5002	LHG	C8-C7-O7-C5
21	A	5053	LHG	O7-C5-C6-O8
21	A	5055	LHG	C4-O6-P-O3
21	A	5055	LHG	C4-O6-P-O5
21	F	5001	LHG	C3-O3-P-O4
21	F	5001	LHG	C3-O3-P-O5
21	F	5001	LHG	C3-O3-P-O6
21	F	5001	LHG	C4-O6-P-O3
21	F	5001	LHG	C5-C4-O6-P
21	F	5001	LHG	O7-C5-C6-O8
21	a	618	LHG	C3-O3-P-O4
21	a	618	LHG	C3-O3-P-O6
21	a	618	LHG	C4-O6-P-O3
21	a	618	LHG	C4-O6-P-O4
21	a	618	LHG	O9-C7-O7-C5
21	a	618	LHG	C8-C7-O7-C5
21	a	619	LHG	C4-O6-P-O3
21	a	619	LHG	C4-O6-P-O4
21	a	619	LHG	C4-O6-P-O5
21	b	618	LHG	C4-O6-P-O3
21	b	618	LHG	C4-O6-P-O4
21	b	618	LHG	C4-O6-P-O5
21	c	317	LHG	C4-O6-P-O4
22	3	320	SQD	O49-C7-O47-C45
22	3	320	SQD	C8-C7-O47-C45
22	3	320	SQD	O10-C23-O48-C46
22	3	320	SQD	C24-C23-O48-C46
22	3	320	SQD	O5-C5-C6-S
23	8	301	DGD	C2A-C1A-O1G-C1G
23	8	301	DGD	O1A-C1A-O1G-C1G
23	8	301	DGD	O6E-C1E-O5D-C6D
23	B	848	DGD	C2B-C1B-O2G-C2G
23	B	848	DGD	O1B-C1B-O2G-C2G
23	B	848	DGD	O6D-C1D-O3G-C3G
24	7	301	LMG	O1-C7-C8-O7
24	A	5001	LMG	C2-C1-O1-C7
24	A	5001	LMG	O6-C1-O1-C7
24	A	5001	LMG	O9-C10-O7-C8
24	A	5001	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	F	5011	LMG	O6-C1-O1-C7
26	8	319	PTY	C3-O11-P1-O12
26	8	319	PTY	C3-O11-P1-O14
26	8	319	PTY	C5-O14-P1-O11
26	8	319	PTY	C5-O14-P1-O13
26	8	320	PTY	O30-C30-O4-C1
26	8	320	PTY	C3-O11-P1-O12
26	8	320	PTY	C3-O11-P1-O14
26	8	320	PTY	C5-O14-P1-O11
26	8	320	PTY	C5-O14-P1-O12
26	F	5002	PTY	O10-C8-O7-C6
26	F	5003	PTY	N1-C2-C3-O11
26	F	5003	PTY	O30-C30-O4-C1
26	F	5003	PTY	C3-O11-P1-O14
26	F	5003	PTY	C5-O14-P1-O11
26	F	5003	PTY	C5-O14-P1-O12
26	F	5003	PTY	C5-O14-P1-O13
27	A	5003	CL0	C1A-C2A-CAA-CBA
27	A	5003	CL0	C3A-C2A-CAA-CBA
16	7	306	CHL	O1D-CGD-O2D-CED
16	8	306	CHL	O1D-CGD-O2D-CED
17	1	612	CLA	O1D-CGD-O2D-CED
17	3	302	CLA	O1D-CGD-O2D-CED
17	3	309	CLA	O1D-CGD-O2D-CED
17	7	304	CLA	O1D-CGD-O2D-CED
17	B	802	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	O1D-CGD-O2D-CED
17	B	806	CLA	O1D-CGD-O2D-CED
17	T	412	CLA	O1D-CGD-O2D-CED
17	a	603	CLA	O1D-CGD-O2D-CED
17	b	612	CLA	O1D-CGD-O2D-CED
17	c	308	CLA	O1D-CGD-O2D-CED
26	F	5003	PTY	C11-C8-O7-C6
16	8	308	CHL	O1D-CGD-O2D-CED
16	c	304	CHL	O1D-CGD-O2D-CED
17	1	614	CLA	O1D-CGD-O2D-CED
17	3	313	CLA	O1D-CGD-O2D-CED
17	8	305	CLA	O1D-CGD-O2D-CED
17	A	5016	CLA	O1D-CGD-O2D-CED
17	A	5029	CLA	O1D-CGD-O2D-CED
17	A	5034	CLA	O1D-CGD-O2D-CED
17	A	5036	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	F	5006	CLA	O1D-CGD-O2D-CED
17	F	5008	CLA	O1D-CGD-O2D-CED
17	K	203	CLA	O1D-CGD-O2D-CED
17	b	604	CLA	O1D-CGD-O2D-CED
17	c	312	CLA	O1D-CGD-O2D-CED
16	7	306	CHL	CBD-CGD-O2D-CED
16	c	305	CHL	CBD-CGD-O2D-CED
17	1	602	CLA	CBD-CGD-O2D-CED
17	1	605	CLA	CBD-CGD-O2D-CED
17	1	609	CLA	CBD-CGD-O2D-CED
17	1	613	CLA	CBD-CGD-O2D-CED
17	1	614	CLA	CBD-CGD-O2D-CED
17	3	310	CLA	CBD-CGD-O2D-CED
17	3	311	CLA	CBD-CGD-O2D-CED
17	3	323	CLA	CBD-CGD-O2D-CED
17	7	312	CLA	CBD-CGD-O2D-CED
17	8	303	CLA	CBD-CGD-O2D-CED
17	8	304	CLA	CBD-CGD-O2D-CED
17	8	305	CLA	CBD-CGD-O2D-CED
17	8	314	CLA	CBD-CGD-O2D-CED
17	A	5015	CLA	CBD-CGD-O2D-CED
17	A	5016	CLA	CBD-CGD-O2D-CED
17	A	5017	CLA	CBD-CGD-O2D-CED
17	A	5023	CLA	CBD-CGD-O2D-CED
17	A	5029	CLA	CBD-CGD-O2D-CED
17	A	5032	CLA	CBD-CGD-O2D-CED
17	A	5034	CLA	CBD-CGD-O2D-CED
17	A	5036	CLA	CBD-CGD-O2D-CED
17	A	5042	CLA	CBD-CGD-O2D-CED
17	A	5043	CLA	CBD-CGD-O2D-CED
17	B	807	CLA	CBD-CGD-O2D-CED
17	B	811	CLA	CBD-CGD-O2D-CED
17	B	822	CLA	CBD-CGD-O2D-CED
17	B	828	CLA	CBD-CGD-O2D-CED
17	F	5009	CLA	CBD-CGD-O2D-CED
17	J	102	CLA	CBD-CGD-O2D-CED
17	K	201	CLA	CBD-CGD-O2D-CED
17	K	203	CLA	CBD-CGD-O2D-CED
17	K	204	CLA	CBD-CGD-O2D-CED
17	T	410	CLA	CBD-CGD-O2D-CED
17	b	604	CLA	CBD-CGD-O2D-CED
17	b	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	c	301	CLA	CBD-CGD-O2D-CED
17	c	309	CLA	CBD-CGD-O2D-CED
17	c	313	CLA	CBD-CGD-O2D-CED
17	1	609	CLA	O1A-CGA-O2A-C1
17	1	612	CLA	O1A-CGA-O2A-C1
17	3	306	CLA	O1A-CGA-O2A-C1
17	3	307	CLA	O1A-CGA-O2A-C1
17	A	5015	CLA	O1A-CGA-O2A-C1
17	B	809	CLA	O1A-CGA-O2A-C1
17	B	824	CLA	O1A-CGA-O2A-C1
17	B	830	CLA	O1A-CGA-O2A-C1
17	T	409	CLA	O1A-CGA-O2A-C1
17	T	410	CLA	O1A-CGA-O2A-C1
17	1	611	CLA	O1A-CGA-O2A-C1
17	1	613	CLA	O1A-CGA-O2A-C1
17	a	611	CLA	O1A-CGA-O2A-C1
16	T	401	CHL	O1D-CGD-O2D-CED
17	8	313	CLA	O1D-CGD-O2D-CED
17	a	612	CLA	O1D-CGD-O2D-CED
16	8	307	CHL	CBA-CGA-O2A-C1
17	7	311	CLA	CBA-CGA-O2A-C1
17	b	614	CLA	CBA-CGA-O2A-C1
17	1	613	CLA	O1D-CGD-O2D-CED
17	A	5023	CLA	O1D-CGD-O2D-CED
17	B	811	CLA	O1D-CGD-O2D-CED
17	J	102	CLA	O1D-CGD-O2D-CED
17	K	204	CLA	O1D-CGD-O2D-CED
17	1	612	CLA	CBA-CGA-O2A-C1
17	3	307	CLA	CBA-CGA-O2A-C1
17	B	809	CLA	CBA-CGA-O2A-C1
17	B	820	CLA	CBA-CGA-O2A-C1
17	B	834	CLA	CBA-CGA-O2A-C1
17	F	5007	CLA	CBA-CGA-O2A-C1
17	T	407	CLA	CBA-CGA-O2A-C1
17	T	409	CLA	CBA-CGA-O2A-C1
17	b	612	CLA	CBA-CGA-O2A-C1
17	8	315	CLA	CBD-CGD-O2D-CED
17	3	305	CLA	O1A-CGA-O2A-C1
17	3	311	CLA	O1A-CGA-O2A-C1
17	3	323	CLA	O1A-CGA-O2A-C1
17	3	324	CLA	O1A-CGA-O2A-C1
17	8	303	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	8	311	CLA	O1A-CGA-O2A-C1
17	8	313	CLA	O1A-CGA-O2A-C1
17	A	5004	CLA	O1A-CGA-O2A-C1
17	A	5006	CLA	O1A-CGA-O2A-C1
17	A	5009	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	O1A-CGA-O2A-C1
17	B	804	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	O1A-CGA-O2A-C1
17	B	820	CLA	O1A-CGA-O2A-C1
17	B	834	CLA	O1A-CGA-O2A-C1
17	B	837	CLA	O1A-CGA-O2A-C1
17	F	5004	CLA	O1A-CGA-O2A-C1
17	F	5007	CLA	O1A-CGA-O2A-C1
17	T	406	CLA	O1A-CGA-O2A-C1
17	T	407	CLA	O1A-CGA-O2A-C1
17	T	408	CLA	O1A-CGA-O2A-C1
17	a	612	CLA	O1A-CGA-O2A-C1
17	b	602	CLA	O1A-CGA-O2A-C1
17	b	610	CLA	O1A-CGA-O2A-C1
17	b	611	CLA	O1A-CGA-O2A-C1
17	c	301	CLA	O1A-CGA-O2A-C1
17	c	309	CLA	O1A-CGA-O2A-C1
17	3	314	CLA	O1A-CGA-O2A-C1
17	7	308	CLA	O1A-CGA-O2A-C1
17	3	308	CLA	O1D-CGD-O2D-CED
17	7	302	CLA	O1D-CGD-O2D-CED
17	B	821	CLA	O1D-CGD-O2D-CED
17	B	829	CLA	O1D-CGD-O2D-CED
17	B	834	CLA	O1D-CGD-O2D-CED
17	F	5009	CLA	O1D-CGD-O2D-CED
17	T	410	CLA	O1D-CGD-O2D-CED
17	a	602	CLA	O1D-CGD-O2D-CED
16	1	601	CHL	O1D-CGD-O2D-CED
16	a	606	CHL	O1D-CGD-O2D-CED
16	c	306	CHL	O1D-CGD-O2D-CED
17	1	603	CLA	O1D-CGD-O2D-CED
17	A	5004	CLA	O1D-CGD-O2D-CED
17	A	5025	CLA	O1D-CGD-O2D-CED
17	A	5026	CLA	O1D-CGD-O2D-CED
17	A	5027	CLA	O1D-CGD-O2D-CED
17	B	808	CLA	O1D-CGD-O2D-CED
17	B	826	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	833	CLA	O1D-CGD-O2D-CED
17	B	835	CLA	O1D-CGD-O2D-CED
17	B	837	CLA	O1D-CGD-O2D-CED
17	b	603	CLA	O1D-CGD-O2D-CED
17	b	614	CLA	O1D-CGD-O2D-CED
17	7	309	CLA	CBD-CGD-O2D-CED
17	B	827	CLA	CBD-CGD-O2D-CED
17	B	831	CLA	CBD-CGD-O2D-CED
17	B	832	CLA	CBD-CGD-O2D-CED
17	c	311	CLA	O1D-CGD-O2D-CED
16	b	605	CHL	CBA-CGA-O2A-C1
17	T	411	CLA	CBA-CGA-O2A-C1
17	b	601	CLA	CBA-CGA-O2A-C1
17	3	310	CLA	O1A-CGA-O2A-C1
17	b	601	CLA	O1A-CGA-O2A-C1
17	c	302	CLA	O1A-CGA-O2A-C1
17	1	607	CLA	C3-C5-C6-C7
17	A	5016	CLA	C3-C5-C6-C7
17	B	803	CLA	C3-C5-C6-C7
17	B	805	CLA	C3-C5-C6-C7
17	B	806	CLA	C3-C5-C6-C7
17	B	808	CLA	C3-C5-C6-C7
17	B	810	CLA	C3-C5-C6-C7
17	B	827	CLA	C3-C5-C6-C7
17	B	831	CLA	C3-C5-C6-C7
17	b	609	CLA	C3-C5-C6-C7
17	A	5013	CLA	O1D-CGD-O2D-CED
17	B	819	CLA	O1D-CGD-O2D-CED
17	1	609	CLA	CBA-CGA-O2A-C1
17	3	306	CLA	CBA-CGA-O2A-C1
17	3	311	CLA	CBA-CGA-O2A-C1
17	8	303	CLA	CBA-CGA-O2A-C1
17	8	304	CLA	CBA-CGA-O2A-C1
17	8	311	CLA	CBA-CGA-O2A-C1
17	8	313	CLA	CBA-CGA-O2A-C1
17	A	5006	CLA	CBA-CGA-O2A-C1
17	A	5009	CLA	CBA-CGA-O2A-C1
17	A	5012	CLA	CBA-CGA-O2A-C1
17	A	5015	CLA	CBA-CGA-O2A-C1
17	B	803	CLA	CBA-CGA-O2A-C1
17	B	804	CLA	CBA-CGA-O2A-C1
17	B	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	824	CLA	CBA-CGA-O2A-C1
17	B	825	CLA	CBA-CGA-O2A-C1
17	B	830	CLA	CBA-CGA-O2A-C1
17	B	837	CLA	CBA-CGA-O2A-C1
17	T	406	CLA	CBA-CGA-O2A-C1
17	T	408	CLA	CBA-CGA-O2A-C1
17	T	410	CLA	CBA-CGA-O2A-C1
17	a	609	CLA	CBA-CGA-O2A-C1
17	a	612	CLA	CBA-CGA-O2A-C1
17	b	602	CLA	CBA-CGA-O2A-C1
17	b	610	CLA	CBA-CGA-O2A-C1
17	c	309	CLA	CBA-CGA-O2A-C1
26	8	319	PTY	O30-C30-O4-C1
16	7	307	CHL	CBD-CGD-O2D-CED
17	1	608	CLA	CBD-CGD-O2D-CED
17	3	303	CLA	CBD-CGD-O2D-CED
17	3	307	CLA	CBD-CGD-O2D-CED
17	7	311	CLA	CBD-CGD-O2D-CED
17	8	312	CLA	CBD-CGD-O2D-CED
17	A	5006	CLA	CBD-CGD-O2D-CED
17	A	5010	CLA	CBD-CGD-O2D-CED
17	A	5020	CLA	CBD-CGD-O2D-CED
17	B	810	CLA	CBD-CGD-O2D-CED
17	B	814	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	CBD-CGD-O2D-CED
17	B	820	CLA	CBD-CGD-O2D-CED
17	B	840	CLA	CBD-CGD-O2D-CED
17	K	202	CLA	CBD-CGD-O2D-CED
17	T	411	CLA	CBD-CGD-O2D-CED
17	a	611	CLA	CBD-CGD-O2D-CED
17	a	614	CLA	CBD-CGD-O2D-CED
17	b	602	CLA	CBD-CGD-O2D-CED
26	F	5002	PTY	C11-C8-O7-C6
17	T	408	CLA	O1D-CGD-O2D-CED
17	a	604	CLA	O1D-CGD-O2D-CED
17	b	601	CLA	O1D-CGD-O2D-CED
17	c	303	CLA	O1D-CGD-O2D-CED
17	T	404	CLA	O1A-CGA-O2A-C1
17	T	411	CLA	O1A-CGA-O2A-C1
17	3	312	CLA	O1D-CGD-O2D-CED
26	F	5003	PTY	O10-C8-O7-C6
17	3	310	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	T	404	CLA	CBA-CGA-O2A-C1
17	c	302	CLA	CBA-CGA-O2A-C1
17	B	823	CLA	CBD-CGD-O2D-CED
17	T	407	CLA	CBD-CGD-O2D-CED
16	c	305	CHL	O1D-CGD-O2D-CED
17	1	605	CLA	O1D-CGD-O2D-CED
17	7	312	CLA	O1D-CGD-O2D-CED
17	A	5042	CLA	O1D-CGD-O2D-CED
17	c	301	CLA	O1D-CGD-O2D-CED
17	c	309	CLA	O1D-CGD-O2D-CED
16	8	306	CHL	C2A-CAA-CBA-CGA
17	B	814	CLA	C2A-CAA-CBA-CGA
17	8	310	CLA	C3-C5-C6-C7
17	8	311	CLA	C3-C5-C6-C7
17	A	5013	CLA	C3-C5-C6-C7
17	A	5022	CLA	C3-C5-C6-C7
17	B	809	CLA	C3-C5-C6-C7
17	B	830	CLA	C3-C5-C6-C7
17	c	308	CLA	C3-C5-C6-C7
17	1	604	CLA	CBA-CGA-O2A-C1
17	3	305	CLA	CBA-CGA-O2A-C1
17	3	323	CLA	CBA-CGA-O2A-C1
17	3	324	CLA	CBA-CGA-O2A-C1
17	8	312	CLA	CBA-CGA-O2A-C1
17	A	5004	CLA	CBA-CGA-O2A-C1
17	A	5013	CLA	CBA-CGA-O2A-C1
17	B	807	CLA	CBA-CGA-O2A-C1
17	B	810	CLA	CBA-CGA-O2A-C1
17	B	817	CLA	CBA-CGA-O2A-C1
17	B	832	CLA	CBA-CGA-O2A-C1
17	F	5004	CLA	CBA-CGA-O2A-C1
17	T	403	CLA	CBA-CGA-O2A-C1
17	b	611	CLA	CBA-CGA-O2A-C1
17	c	301	CLA	CBA-CGA-O2A-C1
26	8	319	PTY	C31-C30-O4-C1
20	A	5048	BCR	C13-C14-C15-C16
20	a	617	BCR	C13-C14-C15-C16
17	1	604	CLA	O1A-CGA-O2A-C1
17	A	5012	CLA	O1A-CGA-O2A-C1
17	A	5025	CLA	O1A-CGA-O2A-C1
17	B	825	CLA	O1A-CGA-O2A-C1
17	B	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	833	CLA	O1A-CGA-O2A-C1
17	B	840	CLA	O1A-CGA-O2A-C1
17	a	604	CLA	O1A-CGA-O2A-C1
17	b	604	CLA	O1A-CGA-O2A-C1
17	c	307	CLA	O1A-CGA-O2A-C1
17	3	310	CLA	O1D-CGD-O2D-CED
17	3	311	CLA	O1D-CGD-O2D-CED
17	3	323	CLA	O1D-CGD-O2D-CED
17	B	828	CLA	O1D-CGD-O2D-CED
16	8	307	CHL	O1A-CGA-O2A-C1
16	b	605	CHL	O1A-CGA-O2A-C1
17	7	311	CLA	O1A-CGA-O2A-C1
17	b	614	CLA	O1A-CGA-O2A-C1
17	A	5015	CLA	O1D-CGD-O2D-CED
17	K	201	CLA	O1D-CGD-O2D-CED
16	3	301	CHL	C3-C5-C6-C7
17	1	602	CLA	C3-C5-C6-C7
17	A	5011	CLA	C3-C5-C6-C7
17	A	5028	CLA	C3-C5-C6-C7
17	F	5004	CLA	C3-C5-C6-C7
17	F	5007	CLA	CBD-CGD-O2D-CED
17	T	403	CLA	CBD-CGD-O2D-CED
17	T	405	CLA	CBD-CGD-O2D-CED
17	b	610	CLA	CBD-CGD-O2D-CED
17	A	5017	CLA	O1D-CGD-O2D-CED
17	A	5032	CLA	O1D-CGD-O2D-CED
17	A	5043	CLA	O1D-CGD-O2D-CED
17	B	807	CLA	O1D-CGD-O2D-CED
17	3	308	CLA	CBA-CGA-O2A-C1
17	7	303	CLA	CBA-CGA-O2A-C1
17	A	5019	CLA	CBA-CGA-O2A-C1
17	B	818	CLA	CBA-CGA-O2A-C1
17	B	829	CLA	CBA-CGA-O2A-C1
17	B	833	CLA	CBA-CGA-O2A-C1
17	a	604	CLA	CBA-CGA-O2A-C1
17	b	609	CLA	CBA-CGA-O2A-C1
27	A	5003	CL0	CBA-CGA-O2A-C1
23	8	301	DGD	C4D-C5D-C6D-O5D
17	7	303	CLA	O1A-CGA-O2A-C1
17	8	304	CLA	O1A-CGA-O2A-C1
17	A	5035	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	829	CLA	O1A-CGA-O2A-C1
17	8	304	CLA	O1D-CGD-O2D-CED
17	A	5038	CLA	CBD-CGD-O2D-CED
17	B	817	CLA	CBD-CGD-O2D-CED
17	a	609	CLA	CBD-CGD-O2D-CED
17	1	610	CLA	CBA-CGA-O2A-C1
17	c	313	CLA	O1D-CGD-O2D-CED
17	T	403	CLA	O1A-CGA-O2A-C1
17	1	609	CLA	O1D-CGD-O2D-CED
17	8	314	CLA	O1D-CGD-O2D-CED
17	8	310	CLA	CBD-CGD-O2D-CED
17	A	5024	CLA	CBD-CGD-O2D-CED
17	B	809	CLA	CBD-CGD-O2D-CED
17	T	409	CLA	CBD-CGD-O2D-CED
17	a	613	CLA	CBD-CGD-O2D-CED
17	1	602	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1D-CGD-O2D-CED
17	A	5007	CLA	CBA-CGA-O2A-C1
17	A	5025	CLA	CBA-CGA-O2A-C1
17	A	5035	CLA	CBA-CGA-O2A-C1
17	B	840	CLA	CBA-CGA-O2A-C1
17	b	604	CLA	CBA-CGA-O2A-C1
17	c	307	CLA	CBA-CGA-O2A-C1
16	3	301	CHL	C4-C3-C5-C6
17	A	5019	CLA	C4-C3-C5-C6
16	3	301	CHL	C2-C3-C5-C6
17	8	312	CLA	O1A-CGA-O2A-C1
17	A	5013	CLA	O1A-CGA-O2A-C1
17	A	5019	CLA	O1A-CGA-O2A-C1
17	B	810	CLA	O1A-CGA-O2A-C1
27	A	5003	CL0	O1A-CGA-O2A-C1
17	T	404	CLA	CBD-CGD-O2D-CED
17	8	303	CLA	O1D-CGD-O2D-CED
21	a	618	LHG	C5-C4-O6-P
16	c	304	CHL	C2A-CAA-CBA-CGA
17	3	306	CLA	C2A-CAA-CBA-CGA
17	8	310	CLA	C2A-CAA-CBA-CGA
17	A	5007	CLA	O1A-CGA-O2A-C1
22	3	320	SQD	O5-C1-O6-C44
23	3	321	DGD	O6E-C1E-O5D-C6D
23	8	301	DGD	O6D-C1D-O3G-C3G
25	7	319	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
16	3	322	CHL	CBA-CGA-O2A-C1
17	A	5011	CLA	CBA-CGA-O2A-C1
17	A	5018	CLA	CBA-CGA-O2A-C1
17	B	823	CLA	CBA-CGA-O2A-C1
17	1	610	CLA	CBD-CGD-O2D-CED
17	A	5011	CLA	CBD-CGD-O2D-CED
17	A	5022	CLA	CBD-CGD-O2D-CED
17	A	5035	CLA	CBD-CGD-O2D-CED
17	A	5044	CLA	CBD-CGD-O2D-CED
17	T	406	CLA	CBD-CGD-O2D-CED
17	a	605	CLA	CBD-CGD-O2D-CED
17	a	608	CLA	CBD-CGD-O2D-CED
17	a	610	CLA	CBD-CGD-O2D-CED
17	8	305	CLA	CBA-CGA-O2A-C1
17	b	613	CLA	CBA-CGA-O2A-C1
17	3	308	CLA	O1A-CGA-O2A-C1
17	B	818	CLA	O1A-CGA-O2A-C1
17	b	609	CLA	O1A-CGA-O2A-C1
17	F	5007	CLA	C2-C1-O2A-CGA
17	8	315	CLA	O1D-CGD-O2D-CED
17	1	604	CLA	CBD-CGD-O2D-CED
17	A	5012	CLA	CBD-CGD-O2D-CED
17	B	824	CLA	CBD-CGD-O2D-CED
17	A	5011	CLA	O1A-CGA-O2A-C1
17	B	823	CLA	O1A-CGA-O2A-C1
16	c	305	CHL	CBA-CGA-O2A-C1
17	7	302	CLA	CBA-CGA-O2A-C1
17	7	304	CLA	CBA-CGA-O2A-C1
17	8	310	CLA	CBA-CGA-O2A-C1
17	A	5037	CLA	CBA-CGA-O2A-C1
17	B	838	CLA	CBA-CGA-O2A-C1
17	B	841	CLA	CBA-CGA-O2A-C1
17	b	603	CLA	CBA-CGA-O2A-C1
17	8	314	CLA	CBA-CGA-O2A-C1
17	1	611	CLA	CBD-CGD-O2D-CED
17	A	5019	CLA	CBD-CGD-O2D-CED
17	B	830	CLA	CBD-CGD-O2D-CED
16	c	304	CHL	C2C-C3C-CAC-CBC
17	3	303	CLA	O1D-CGD-O2D-CED
17	7	309	CLA	O1D-CGD-O2D-CED
17	B	827	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	832	CLA	O1D-CGD-O2D-CED
17	T	411	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	C4-C3-C5-C6
17	A	5019	CLA	C2-C3-C5-C6
17	B	803	CLA	C2-C3-C5-C6
17	3	311	CLA	C3-C5-C6-C7
17	A	5019	CLA	C3-C5-C6-C7
27	A	5003	CL0	C3-C5-C6-C7
16	3	301	CHL	C11-C12-C13-C14
16	3	322	CHL	C11-C10-C8-C9
17	B	808	CLA	C11-C10-C8-C9
27	A	5003	CL0	C14-C13-C15-C16
17	B	814	CLA	O1D-CGD-O2D-CED
17	b	602	CLA	O1D-CGD-O2D-CED
22	3	320	SQD	C2-C1-O6-C44
23	3	321	DGD	C2E-C1E-O5D-C6D
23	8	301	DGD	C2D-C1D-O3G-C3G
23	8	301	DGD	C2E-C1E-O5D-C6D
25	7	319	LMU	C2'-C1'-O1'-C1
17	A	5020	CLA	O1D-CGD-O2D-CED
16	8	307	CHL	CBD-CGD-O2D-CED
17	1	608	CLA	O1D-CGD-O2D-CED
19	3	316	XAT	C27-C28-C29-C39
20	1	617	BCR	C37-C22-C23-C24
20	A	5048	BCR	C37-C22-C23-C24
20	A	5049	BCR	C36-C18-C19-C20
20	a	617	BCR	C37-C22-C23-C24
20	c	316	BCR	C7-C8-C9-C34
20	L	203	BCR	C37-C22-C23-C24
19	3	316	XAT	C27-C28-C29-C30
20	1	617	BCR	C21-C22-C23-C24
20	A	5048	BCR	C21-C22-C23-C24
20	B	845	BCR	C21-C22-C23-C24
20	a	617	BCR	C21-C22-C23-C24
20	c	316	BCR	C7-C8-C9-C10
17	A	5038	CLA	C2A-CAA-CBA-CGA
17	B	818	CLA	C2A-CAA-CBA-CGA
17	K	204	CLA	C2A-CAA-CBA-CGA
16	c	305	CHL	O1A-CGA-O2A-C1
17	7	302	CLA	O1A-CGA-O2A-C1
17	7	304	CLA	O1A-CGA-O2A-C1
17	b	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	a	601	CHL	CBA-CGA-O2A-C1
17	3	312	CLA	CBA-CGA-O2A-C1
21	b	618	LHG	O7-C5-C6-O8
17	a	614	CLA	O1D-CGD-O2D-CED
17	A	5016	CLA	CBA-CGA-O2A-C1
17	F	5004	CLA	C2-C1-O2A-CGA
16	7	307	CHL	O1D-CGD-O2D-CED
17	8	312	CLA	O1D-CGD-O2D-CED
17	A	5010	CLA	O1D-CGD-O2D-CED
17	B	840	CLA	O1D-CGD-O2D-CED
17	3	314	CLA	CBD-CGD-O2D-CED
17	A	5007	CLA	CBD-CGD-O2D-CED
17	A	5031	CLA	CBD-CGD-O2D-CED
17	A	5035	CLA	C8-C10-C11-C12
17	B	820	CLA	O1D-CGD-O2D-CED
17	B	838	CLA	CBD-CGD-O2D-CED
17	c	310	CLA	CBD-CGD-O2D-CED
17	A	5028	CLA	C11-C10-C8-C7
27	A	5003	CL0	C11-C12-C13-C15
17	A	5013	CLA	C4-C3-C5-C6
17	A	5035	CLA	C5-C6-C7-C8
17	K	202	CLA	O1D-CGD-O2D-CED
17	A	5006	CLA	O1D-CGD-O2D-CED
17	B	815	CLA	O1D-CGD-O2D-CED
16	3	322	CHL	C8-C10-C11-C12
17	A	5029	CLA	C15-C16-C17-C18
17	3	307	CLA	O1D-CGD-O2D-CED
17	A	5037	CLA	O1A-CGA-O2A-C1
17	A	5008	CLA	CBD-CGD-O2D-CED
17	1	610	CLA	O1A-CGA-O2A-C1
17	7	311	CLA	O1D-CGD-O2D-CED
17	a	611	CLA	O1D-CGD-O2D-CED
16	3	301	CHL	C2A-CAA-CBA-CGA
16	T	401	CHL	C2A-CAA-CBA-CGA
16	b	605	CHL	C2A-CAA-CBA-CGA
16	c	305	CHL	C2A-CAA-CBA-CGA
17	3	308	CLA	C2A-CAA-CBA-CGA
17	7	304	CLA	C2A-CAA-CBA-CGA
17	A	5004	CLA	C2A-CAA-CBA-CGA
17	A	5037	CLA	C2A-CAA-CBA-CGA
17	B	809	CLA	C2A-CAA-CBA-CGA
17	B	811	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	B	816	CLA	C2A-CAA-CBA-CGA
17	B	823	CLA	C2A-CAA-CBA-CGA
17	B	838	CLA	C2A-CAA-CBA-CGA
17	B	841	CLA	C2A-CAA-CBA-CGA
27	A	5003	CL0	C2A-CAA-CBA-CGA
17	8	310	CLA	O1A-CGA-O2A-C1
17	B	838	CLA	O1A-CGA-O2A-C1
17	B	841	CLA	O1A-CGA-O2A-C1
17	A	5013	CLA	C15-C16-C17-C18
17	A	5024	CLA	C5-C6-C7-C8
17	A	5026	CLA	C5-C6-C7-C8
17	B	809	CLA	C5-C6-C7-C8
17	B	818	CLA	C5-C6-C7-C8
17	B	829	CLA	C8-C10-C11-C12
17	B	839	CLA	C5-C6-C7-C8
17	B	840	CLA	C15-C16-C17-C18
27	A	5003	CL0	C15-C16-C17-C18
17	B	810	CLA	O1D-CGD-O2D-CED
16	3	322	CHL	O1A-CGA-O2A-C1
17	A	5018	CLA	O1A-CGA-O2A-C1
17	B	823	CLA	O1D-CGD-O2D-CED
17	a	607	CLA	CBA-CGA-O2A-C1
23	8	301	DGD	O6D-C5D-C6D-O5D
17	T	403	CLA	O1D-CGD-O2D-CED
17	T	407	CLA	O1D-CGD-O2D-CED
17	A	5020	CLA	C8-C10-C11-C12
17	B	802	CLA	C13-C15-C16-C17
16	8	308	CHL	CBA-CGA-O2A-C1
17	B	808	CLA	CBA-CGA-O2A-C1
17	B	816	CLA	CBA-CGA-O2A-C1
17	7	310	CLA	CBD-CGD-O2D-CED
17	F	5007	CLA	O1D-CGD-O2D-CED
17	T	405	CLA	O1D-CGD-O2D-CED
17	b	610	CLA	O1D-CGD-O2D-CED
17	7	310	CLA	CBA-CGA-O2A-C1
17	A	5036	CLA	C13-C15-C16-C17
17	A	5040	CLA	C3-C5-C6-C7
20	A	5048	BCR	C9-C10-C11-C12
16	8	308	CHL	C2A-CAA-CBA-CGA
17	8	305	CLA	C2A-CAA-CBA-CGA
17	A	5023	CLA	C2A-CAA-CBA-CGA
17	A	5041	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	B	834	CLA	C2A-CAA-CBA-CGA
17	J	102	CLA	C2A-CAA-CBA-CGA
17	T	406	CLA	C2A-CAA-CBA-CGA
17	7	313	CLA	CBA-CGA-O2A-C1
17	A	5021	CLA	CBA-CGA-O2A-C1
17	A	5027	CLA	CBA-CGA-O2A-C1
16	3	322	CHL	C10-C11-C12-C13
17	B	829	CLA	C10-C11-C12-C13
17	A	5038	CLA	O1D-CGD-O2D-CED
17	B	826	CLA	C15-C16-C17-C18
17	a	608	CLA	CAA-CBA-CGA-O2A
17	A	5009	CLA	C13-C15-C16-C17
17	A	5011	CLA	C5-C6-C7-C8
17	A	5014	CLA	C15-C16-C17-C18
17	A	5024	CLA	C8-C10-C11-C12
17	A	5028	CLA	C10-C11-C12-C13
17	B	803	CLA	C5-C6-C7-C8
17	B	808	CLA	C10-C11-C12-C13
17	c	308	CLA	C10-C11-C12-C13
17	L	201	CLA	C8-C10-C11-C12
17	B	817	CLA	O1D-CGD-O2D-CED
17	a	609	CLA	O1D-CGD-O2D-CED
17	A	5017	CLA	CBA-CGA-O2A-C1
17	B	836	CLA	CBA-CGA-O2A-C1
17	a	613	CLA	O1D-CGD-O2D-CED
16	b	607	CHL	C1-C2-C3-C5
17	A	5029	CLA	C3-C5-C6-C7
17	1	612	CLA	C6-C7-C8-C9
17	B	809	CLA	O1D-CGD-O2D-CED
23	3	321	DGD	C2D-C1D-O3G-C3G
17	1	607	CLA	C10-C11-C12-C13
17	L	201	CLA	C5-C6-C7-C8
16	7	306	CHL	CBA-CGA-O2A-C1
17	A	5034	CLA	CBA-CGA-O2A-C1
18	T	413	LUT	C7-C8-C9-C19
20	B	845	BCR	C37-C22-C23-C24
16	8	308	CHL	O1A-CGA-O2A-C1
17	A	5016	CLA	O1A-CGA-O2A-C1
17	1	614	CLA	C2A-CAA-CBA-CGA
17	3	311	CLA	C2A-CAA-CBA-CGA
17	7	309	CLA	C2A-CAA-CBA-CGA
17	8	309	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	A	5044	CLA	C2A-CAA-CBA-CGA
17	B	808	CLA	C2A-CAA-CBA-CGA
17	c	308	CLA	C2A-CAA-CBA-CGA
17	A	5024	CLA	O1D-CGD-O2D-CED
17	A	5022	CLA	C16-C17-C18-C20
17	B	839	CLA	C16-C17-C18-C19
17	c	301	CLA	C16-C17-C18-C19
17	T	409	CLA	O1D-CGD-O2D-CED
17	1	609	CLA	C10-C11-C12-C13
18	1	615	LUT	C12-C13-C14-C15
18	a	615	LUT	C12-C13-C14-C15
20	B	849	BCR	C16-C17-C18-C19
23	3	321	DGD	O6D-C1D-O3G-C3G
16	b	606	CHL	C2C-C3C-CAC-CBC
17	8	310	CLA	O1D-CGD-O2D-CED
17	A	5018	CLA	CBD-CGD-O2D-CED
17	T	404	CLA	O1D-CGD-O2D-CED
17	3	307	CLA	C2-C1-O2A-CGA
17	A	5027	CLA	C2-C1-O2A-CGA
17	B	816	CLA	C2-C1-O2A-CGA
17	B	820	CLA	C2-C1-O2A-CGA
17	T	407	CLA	C2-C1-O2A-CGA
17	b	610	CLA	C2-C1-O2A-CGA
17	3	308	CLA	C6-C7-C8-C9
17	A	5008	CLA	C16-C17-C18-C20
17	A	5017	CLA	C6-C7-C8-C9
17	A	5024	CLA	C11-C12-C13-C15
17	B	810	CLA	C6-C7-C8-C10
17	B	828	CLA	C6-C7-C8-C10
17	B	808	CLA	O1A-CGA-O2A-C1
17	A	5016	CLA	C2C-C3C-CAC-CBC
17	T	406	CLA	O1D-CGD-O2D-CED
17	A	5016	CLA	C15-C16-C17-C18
17	8	305	CLA	O1A-CGA-O2A-C1
17	b	613	CLA	O1A-CGA-O2A-C1
17	B	816	CLA	O1A-CGA-O2A-C1
30	J	101	LMK	O9-C10-C11-C12
17	1	610	CLA	O1D-CGD-O2D-CED
16	b	606	CHL	C4B-C3B-CAB-CBB
16	c	306	CHL	C4B-C3B-CAB-CBB
17	1	602	CLA	C4B-C3B-CAB-CBB
17	1	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	1	608	CLA	C4B-C3B-CAB-CBB
17	1	609	CLA	C4B-C3B-CAB-CBB
17	1	611	CLA	C4B-C3B-CAB-CBB
17	1	613	CLA	C4B-C3B-CAB-CBB
17	3	302	CLA	C4B-C3B-CAB-CBB
17	3	303	CLA	C4B-C3B-CAB-CBB
17	3	305	CLA	C4B-C3B-CAB-CBB
17	3	307	CLA	C4B-C3B-CAB-CBB
17	3	313	CLA	C4B-C3B-CAB-CBB
17	3	323	CLA	C4B-C3B-CAB-CBB
17	7	302	CLA	C4B-C3B-CAB-CBB
17	7	304	CLA	C4B-C3B-CAB-CBB
17	7	308	CLA	C4B-C3B-CAB-CBB
17	8	302	CLA	C4B-C3B-CAB-CBB
17	8	309	CLA	C4B-C3B-CAB-CBB
17	8	312	CLA	C4B-C3B-CAB-CBB
17	A	5004	CLA	C4B-C3B-CAB-CBB
17	A	5007	CLA	C4B-C3B-CAB-CBB
17	A	5009	CLA	C4B-C3B-CAB-CBB
17	A	5017	CLA	C4B-C3B-CAB-CBB
17	A	5031	CLA	C4B-C3B-CAB-CBB
17	A	5033	CLA	C4B-C3B-CAB-CBB
17	A	5035	CLA	C4B-C3B-CAB-CBB
17	A	5041	CLA	C4B-C3B-CAB-CBB
17	B	804	CLA	C4B-C3B-CAB-CBB
17	B	806	CLA	C4B-C3B-CAB-CBB
17	B	810	CLA	C4B-C3B-CAB-CBB
17	B	811	CLA	C4B-C3B-CAB-CBB
17	B	815	CLA	C4B-C3B-CAB-CBB
17	B	816	CLA	C4B-C3B-CAB-CBB
17	B	817	CLA	C4B-C3B-CAB-CBB
17	B	826	CLA	C4B-C3B-CAB-CBB
17	B	831	CLA	C4B-C3B-CAB-CBB
17	B	836	CLA	C4B-C3B-CAB-CBB
17	B	837	CLA	C4B-C3B-CAB-CBB
17	B	838	CLA	C4B-C3B-CAB-CBB
17	B	839	CLA	C4B-C3B-CAB-CBB
17	K	202	CLA	C4B-C3B-CAB-CBB
17	K	203	CLA	C4B-C3B-CAB-CBB
17	T	402	CLA	C4B-C3B-CAB-CBB
17	T	403	CLA	C4B-C3B-CAB-CBB
17	T	407	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	T	412	CLA	C4B-C3B-CAB-CBB
17	a	609	CLA	C4B-C3B-CAB-CBB
17	a	611	CLA	C4B-C3B-CAB-CBB
17	a	612	CLA	C4B-C3B-CAB-CBB
17	b	601	CLA	C4B-C3B-CAB-CBB
17	b	608	CLA	C4B-C3B-CAB-CBB
17	c	301	CLA	C4B-C3B-CAB-CBB
17	c	302	CLA	C4B-C3B-CAB-CBB
17	L	201	CLA	C4B-C3B-CAB-CBB
21	A	5053	LHG	C17-C18-C19-C20
17	A	5008	CLA	C16-C17-C18-C19
17	A	5015	CLA	C6-C7-C8-C9
17	A	5018	CLA	C11-C12-C13-C15
17	A	5022	CLA	C16-C17-C18-C19
17	B	810	CLA	C6-C7-C8-C9
17	B	828	CLA	C6-C7-C8-C9
17	B	839	CLA	C16-C17-C18-C20
17	c	301	CLA	C16-C17-C18-C20
17	7	314	CLA	C2A-CAA-CBA-CGA
17	B	827	CLA	C2A-CAA-CBA-CGA
17	B	805	CLA	C11-C10-C8-C7
17	b	609	CLA	C6-C7-C8-C10
24	7	301	LMG	C19-C20-C21-C22
17	8	314	CLA	O1A-CGA-O2A-C1
17	A	5027	CLA	O1A-CGA-O2A-C1
16	7	306	CHL	C3A-C2A-CAA-CBA
16	b	607	CHL	C3A-C2A-CAA-CBA
16	c	305	CHL	C3A-C2A-CAA-CBA
17	1	614	CLA	C3A-C2A-CAA-CBA
17	3	304	CLA	C3A-C2A-CAA-CBA
17	3	312	CLA	C3A-C2A-CAA-CBA
17	8	304	CLA	C3A-C2A-CAA-CBA
17	8	310	CLA	C3A-C2A-CAA-CBA
17	A	5005	CLA	C3A-C2A-CAA-CBA
17	A	5009	CLA	C3A-C2A-CAA-CBA
17	A	5038	CLA	C3A-C2A-CAA-CBA
17	A	5040	CLA	C3A-C2A-CAA-CBA
17	B	802	CLA	C3A-C2A-CAA-CBA
17	B	810	CLA	C3A-C2A-CAA-CBA
17	B	821	CLA	C3A-C2A-CAA-CBA
17	B	826	CLA	C3A-C2A-CAA-CBA
17	B	835	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	K	203	CLA	C3A-C2A-CAA-CBA
17	K	204	CLA	C3A-C2A-CAA-CBA
17	T	404	CLA	C3A-C2A-CAA-CBA
17	a	611	CLA	C3A-C2A-CAA-CBA
17	a	614	CLA	C3A-C2A-CAA-CBA
17	b	603	CLA	C3A-C2A-CAA-CBA
17	c	313	CLA	C3A-C2A-CAA-CBA
17	A	5022	CLA	O1D-CGD-O2D-CED
17	A	5013	CLA	C2-C3-C5-C6
17	A	5006	CLA	C8-C10-C11-C12
27	A	5003	CL0	C10-C11-C12-C13
17	3	308	CLA	C6-C7-C8-C10
17	A	5014	CLA	C16-C17-C18-C20
17	A	5024	CLA	C11-C12-C13-C14
17	7	313	CLA	O1A-CGA-O2A-C1
17	A	5017	CLA	O1A-CGA-O2A-C1
17	A	5021	CLA	O1A-CGA-O2A-C1
17	A	5024	CLA	CBA-CGA-O2A-C1
17	B	802	CLA	CBA-CGA-O2A-C1
17	c	303	CLA	CBA-CGA-O2A-C1
17	A	5011	CLA	O1D-CGD-O2D-CED
17	A	5034	CLA	O1A-CGA-O2A-C1
17	B	836	CLA	O1A-CGA-O2A-C1
17	A	5035	CLA	O1D-CGD-O2D-CED
17	A	5044	CLA	O1D-CGD-O2D-CED
16	c	304	CHL	C4C-C3C-CAC-CBC
17	a	610	CLA	O1D-CGD-O2D-CED
17	A	5017	CLA	C6-C7-C8-C10
17	A	5042	CLA	C11-C12-C13-C15
17	B	838	CLA	C6-C7-C8-C9
16	b	606	CHL	C2B-C3B-CAB-CBB
17	1	607	CLA	C2B-C3B-CAB-CBB
17	1	611	CLA	C2B-C3B-CAB-CBB
17	1	614	CLA	C2B-C3B-CAB-CBB
17	3	310	CLA	C2B-C3B-CAB-CBB
17	7	309	CLA	C2B-C3B-CAB-CBB
17	8	302	CLA	C2B-C3B-CAB-CBB
17	A	5009	CLA	C2B-C3B-CAB-CBB
17	A	5019	CLA	C2B-C3B-CAB-CBB
17	A	5031	CLA	C2B-C3B-CAB-CBB
17	A	5034	CLA	C2B-C3B-CAB-CBB
17	A	5040	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	B	808	CLA	C2B-C3B-CAB-CBB
17	B	810	CLA	C2B-C3B-CAB-CBB
17	B	814	CLA	C2B-C3B-CAB-CBB
17	B	819	CLA	C2B-C3B-CAB-CBB
17	B	830	CLA	C2B-C3B-CAB-CBB
17	B	833	CLA	C2B-C3B-CAB-CBB
17	B	836	CLA	C2B-C3B-CAB-CBB
17	B	837	CLA	C2B-C3B-CAB-CBB
17	K	202	CLA	C2B-C3B-CAB-CBB
17	K	203	CLA	C2B-C3B-CAB-CBB
17	K	204	CLA	C2B-C3B-CAB-CBB
17	T	406	CLA	C2B-C3B-CAB-CBB
17	a	602	CLA	C2B-C3B-CAB-CBB
17	a	605	CLA	C2B-C3B-CAB-CBB
17	a	614	CLA	C2B-C3B-CAB-CBB
17	b	601	CLA	C2B-C3B-CAB-CBB
17	b	613	CLA	C2B-C3B-CAB-CBB
20	3	317	BCR	C1-C6-C7-C8
20	7	317	BCR	C23-C24-C25-C26
20	7	317	BCR	C23-C24-C25-C30
20	8	318	BCR	C1-C6-C7-C8
20	8	318	BCR	C5-C6-C7-C8
20	8	318	BCR	C23-C24-C25-C26
20	8	318	BCR	C23-C24-C25-C30
20	A	5047	BCR	C1-C6-C7-C8
20	A	5048	BCR	C1-C6-C7-C8
20	B	843	BCR	C1-C6-C7-C8
20	B	845	BCR	C1-C6-C7-C8
20	B	845	BCR	C5-C6-C7-C8
20	B	846	BCR	C23-C24-C25-C26
20	B	846	BCR	C23-C24-C25-C30
20	J	103	BCR	C1-C6-C7-C8
20	J	103	BCR	C5-C6-C7-C8
20	J	103	BCR	C23-C24-C25-C26
20	J	103	BCR	C23-C24-C25-C30
20	J	104	BCR	C23-C24-C25-C26
20	J	104	BCR	C23-C24-C25-C30
20	T	415	BCR	C1-C6-C7-C8
20	T	415	BCR	C5-C6-C7-C8
20	T	415	BCR	C23-C24-C25-C26
20	T	415	BCR	C23-C24-C25-C30
20	b	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	b	617	BCR	C23-C24-C25-C26
20	b	617	BCR	C23-C24-C25-C30
20	c	316	BCR	C1-C6-C7-C8
26	8	320	PTY	C11-C8-O7-C6
17	A	5014	CLA	CBA-CGA-O2A-C1
17	B	807	CLA	C3-C5-C6-C7
17	B	817	CLA	C3-C5-C6-C7
17	a	605	CLA	O1D-CGD-O2D-CED
17	a	608	CLA	O1D-CGD-O2D-CED
17	3	303	CLA	C2A-CAA-CBA-CGA
17	3	309	CLA	C2A-CAA-CBA-CGA
17	B	837	CLA	C2A-CAA-CBA-CGA
17	T	403	CLA	C2A-CAA-CBA-CGA
22	3	320	SQD	C23-C24-C25-C26
18	T	413	LUT	C6-C7-C8-C9
17	3	312	CLA	O1A-CGA-O2A-C1
17	B	831	CLA	CBA-CGA-O2A-C1
16	a	601	CHL	O1A-CGA-O2A-C1
17	A	5012	CLA	O1D-CGD-O2D-CED
17	B	836	CLA	C5-C6-C7-C8
20	A	5047	BCR	C37-C22-C23-C24
17	7	312	CLA	C3-C5-C6-C7
17	b	602	CLA	C3-C5-C6-C7
18	c	314	LUT	C27-C28-C29-C30
16	3	322	CHL	C11-C12-C13-C15
17	B	838	CLA	C6-C7-C8-C10
17	A	5018	CLA	C4-C3-C5-C6
17	F	5004	CLA	C4-C3-C5-C6
17	A	5024	CLA	O1A-CGA-O2A-C1
21	A	5053	LHG	C13-C14-C15-C16
17	B	802	CLA	O1A-CGA-O2A-C1
17	c	303	CLA	O1A-CGA-O2A-C1
24	7	301	LMG	O6-C5-C6-O5
17	A	5007	CLA	C8-C10-C11-C12
17	B	806	CLA	C10-C11-C12-C13
26	8	320	PTY	O10-C8-O7-C6
23	3	321	DGD	O6E-C5E-C6E-O5E
25	7	319	LMU	O5B-C5B-C6B-O6B
25	A	5054	LMU	O5B-C5B-C6B-O6B
17	A	5015	CLA	C6-C7-C8-C10
17	A	5042	CLA	C11-C12-C13-C14
25	A	5054	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
17	B	805	CLA	C13-C15-C16-C17
23	3	321	DGD	O2G-C2G-C3G-O3G
17	1	604	CLA	O1D-CGD-O2D-CED
17	c	312	CLA	CBA-CGA-O2A-C1
26	F	5002	PTY	C31-C32-C33-C34
17	B	830	CLA	O1D-CGD-O2D-CED
25	7	319	LMU	O1'-C1-C2-C3
25	7	319	LMU	O5'-C5'-C6'-O6'
17	1	612	CLA	C11-C12-C13-C15
17	A	5014	CLA	C16-C17-C18-C19
17	A	5018	CLA	C11-C12-C13-C14
17	A	5034	CLA	C4-C3-C5-C6
17	B	819	CLA	C3-C5-C6-C7
17	B	818	CLA	C2-C3-C5-C6
17	F	5004	CLA	C2-C3-C5-C6
16	a	601	CHL	C2A-CAA-CBA-CGA
17	1	602	CLA	C2A-CAA-CBA-CGA
17	1	605	CLA	C2A-CAA-CBA-CGA
17	7	312	CLA	C2A-CAA-CBA-CGA
17	8	313	CLA	C2A-CAA-CBA-CGA
17	B	828	CLA	C2A-CAA-CBA-CGA
17	b	612	CLA	C2A-CAA-CBA-CGA
24	7	301	LMG	C17-C18-C19-C20
17	1	611	CLA	O1D-CGD-O2D-CED
17	A	5019	CLA	O1D-CGD-O2D-CED
17	B	824	CLA	O1D-CGD-O2D-CED
17	A	5028	CLA	C8-C10-C11-C12
17	A	5014	CLA	O1A-CGA-O2A-C1
16	3	301	CHL	C1A-C2A-CAA-CBA
16	7	307	CHL	C1A-C2A-CAA-CBA
16	8	308	CHL	C1A-C2A-CAA-CBA
16	T	401	CHL	C1A-C2A-CAA-CBA
17	1	604	CLA	C1A-C2A-CAA-CBA
17	1	607	CLA	C1A-C2A-CAA-CBA
17	1	610	CLA	C1A-C2A-CAA-CBA
17	1	612	CLA	C1A-C2A-CAA-CBA
17	1	614	CLA	C1A-C2A-CAA-CBA
17	3	304	CLA	C1A-C2A-CAA-CBA
17	3	307	CLA	C1A-C2A-CAA-CBA
17	3	308	CLA	C1A-C2A-CAA-CBA
17	3	309	CLA	C1A-C2A-CAA-CBA
17	7	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	7	310	CLA	C1A-C2A-CAA-CBA
17	7	312	CLA	C1A-C2A-CAA-CBA
17	8	304	CLA	C1A-C2A-CAA-CBA
17	8	311	CLA	C1A-C2A-CAA-CBA
17	8	315	CLA	C1A-C2A-CAA-CBA
17	A	5005	CLA	C1A-C2A-CAA-CBA
17	A	5007	CLA	C1A-C2A-CAA-CBA
17	A	5009	CLA	C1A-C2A-CAA-CBA
17	A	5011	CLA	C1A-C2A-CAA-CBA
17	A	5031	CLA	C1A-C2A-CAA-CBA
17	A	5033	CLA	C1A-C2A-CAA-CBA
17	A	5035	CLA	C1A-C2A-CAA-CBA
17	A	5036	CLA	C1A-C2A-CAA-CBA
17	A	5038	CLA	C1A-C2A-CAA-CBA
17	B	802	CLA	C1A-C2A-CAA-CBA
17	B	810	CLA	C1A-C2A-CAA-CBA
17	B	814	CLA	C1A-C2A-CAA-CBA
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	818	CLA	C1A-C2A-CAA-CBA
17	B	821	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	B	826	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	C1A-C2A-CAA-CBA
17	B	835	CLA	C1A-C2A-CAA-CBA
17	B	839	CLA	C1A-C2A-CAA-CBA
17	F	5004	CLA	C1A-C2A-CAA-CBA
17	F	5008	CLA	C1A-C2A-CAA-CBA
17	K	203	CLA	C1A-C2A-CAA-CBA
17	T	403	CLA	C1A-C2A-CAA-CBA
17	T	408	CLA	C1A-C2A-CAA-CBA
17	a	610	CLA	C1A-C2A-CAA-CBA
17	a	611	CLA	C1A-C2A-CAA-CBA
17	a	612	CLA	C1A-C2A-CAA-CBA
17	a	614	CLA	C1A-C2A-CAA-CBA
17	b	603	CLA	C1A-C2A-CAA-CBA
17	b	604	CLA	C1A-C2A-CAA-CBA
17	b	608	CLA	C1A-C2A-CAA-CBA
17	b	609	CLA	C1A-C2A-CAA-CBA
17	b	610	CLA	C1A-C2A-CAA-CBA
17	b	613	CLA	C1A-C2A-CAA-CBA
17	c	313	CLA	C1A-C2A-CAA-CBA
17	L	201	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	L	202	CLA	C1A-C2A-CAA-CBA
21	a	618	LHG	O6-C4-C5-C6
26	F	5002	PTY	O14-C5-C6-C1
23	8	301	DGD	O6E-C5E-C6E-O5E
16	3	301	CHL	C11-C10-C8-C7
17	1	607	CLA	C12-C13-C15-C16
17	A	5009	CLA	C12-C13-C15-C16
17	A	5022	CLA	C6-C7-C8-C10
17	A	5022	CLA	C11-C12-C13-C15
17	A	5028	CLA	C6-C7-C8-C10
17	A	5041	CLA	C11-C10-C8-C7
17	B	802	CLA	C6-C7-C8-C10
17	B	803	CLA	C12-C13-C15-C16
17	B	830	CLA	C11-C10-C8-C7
17	B	840	CLA	C11-C12-C13-C15
27	A	5003	CL0	C12-C13-C15-C16
28	B	842	PQN	C22-C23-C25-C26
17	B	831	CLA	C6-C7-C8-C9
17	B	828	CLA	C5-C6-C7-C8
17	B	805	CLA	C4-C3-C5-C6
17	A	5034	CLA	C2-C3-C5-C6
17	B	805	CLA	C2-C3-C5-C6
17	B	806	CLA	C2-C3-C5-C6
17	B	831	CLA	O1A-CGA-O2A-C1
17	A	5018	CLA	C2A-CAA-CBA-CGA
17	B	807	CLA	C2A-CAA-CBA-CGA
17	T	410	CLA	C2A-CAA-CBA-CGA
16	3	301	CHL	C11-C10-C8-C9
17	A	5016	CLA	C14-C13-C15-C16
17	A	5028	CLA	C6-C7-C8-C9
17	A	5030	CLA	C14-C13-C15-C16
17	A	5041	CLA	C11-C10-C8-C9
17	B	803	CLA	C6-C7-C8-C9
17	B	806	CLA	C14-C13-C15-C16
28	A	5045	PQN	C24-C23-C25-C26
17	A	5031	CLA	O1D-CGD-O2D-CED
17	1	607	CLA	CBA-CGA-O2A-C1
17	B	813	CLA	CBA-CGA-O2A-C1
16	8	307	CHL	O1D-CGD-O2D-CED
21	F	5001	LHG	C9-C10-C11-C12
17	b	612	CLA	O2A-C1-C2-C3
21	A	5002	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
21	A	5053	LHG	C4-C5-C6-O8
21	F	5001	LHG	C4-C5-C6-O8
21	b	618	LHG	C4-C5-C6-O8
17	A	5007	CLA	O1D-CGD-O2D-CED
17	c	309	CLA	C5-C6-C7-C8
17	3	314	CLA	O1D-CGD-O2D-CED
17	A	5028	CLA	CBA-CGA-O2A-C1
17	A	5029	CLA	CBA-CGA-O2A-C1
17	1	612	CLA	C11-C12-C13-C14
17	B	838	CLA	O1D-CGD-O2D-CED
17	7	310	CLA	O1A-CGA-O2A-C1
17	a	607	CLA	O1A-CGA-O2A-C1
17	c	310	CLA	O1D-CGD-O2D-CED
17	A	5004	CLA	C4-C3-C5-C6
17	B	818	CLA	C4-C3-C5-C6
17	c	312	CLA	O1A-CGA-O2A-C1
17	B	810	CLA	C5-C6-C7-C8
17	A	5030	CLA	C2A-CAA-CBA-CGA
17	B	820	CLA	C2A-CAA-CBA-CGA
21	1	618	LHG	C11-C10-C9-C8
17	A	5044	CLA	C13-C15-C16-C17
16	3	301	CHL	C3C-C2C-CMC-OMC
16	7	305	CHL	C3C-C2C-CMC-OMC
16	7	307	CHL	C3C-C2C-CMC-OMC
16	8	308	CHL	C3C-C2C-CMC-OMC
16	T	401	CHL	C3C-C2C-CMC-OMC
16	b	605	CHL	C3C-C2C-CMC-OMC
16	c	304	CHL	C3C-C2C-CMC-OMC
17	B	831	CLA	C6-C7-C8-C10
20	A	5049	BCR	C22-C23-C24-C25
17	A	5044	CLA	C4-C3-C5-C6
24	F	5011	LMG	O1-C7-C8-O7
17	1	612	CLA	C2A-CAA-CBA-CGA
17	b	604	CLA	C2A-CAA-CBA-CGA
17	A	5025	CLA	C5-C6-C7-C8
16	7	306	CHL	O1A-CGA-O2A-C1
23	3	321	DGD	C9B-CAB-CBB-CCB
19	3	316	XAT	C26-C27-C28-C29
19	c	315	XAT	C26-C27-C28-C29
17	7	312	CLA	CBA-CGA-O2A-C1
17	1	607	CLA	O1A-CGA-O2A-C1
17	7	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	5013	CLA	C10-C11-C12-C13
17	b	609	CLA	C11-C12-C13-C14
16	3	322	CHL	C4-C3-C5-C6
17	B	806	CLA	C4-C3-C5-C6
17	B	808	CLA	C2-C3-C5-C6
17	A	5008	CLA	O1D-CGD-O2D-CED
25	7	319	LMU	C2-C1-O1'-C1'
17	1	607	CLA	C14-C13-C15-C16
17	A	5009	CLA	C14-C13-C15-C16
17	A	5020	CLA	C11-C12-C13-C14
17	A	5022	CLA	C6-C7-C8-C9
17	A	5022	CLA	C11-C12-C13-C14
17	B	802	CLA	C6-C7-C8-C9
17	B	803	CLA	C14-C13-C15-C16
17	B	805	CLA	C11-C10-C8-C9
17	B	827	CLA	C11-C10-C8-C9
17	B	830	CLA	C11-C10-C8-C9
17	B	830	CLA	C14-C13-C15-C16
17	B	833	CLA	C11-C10-C8-C9
17	B	840	CLA	C11-C12-C13-C14
17	b	609	CLA	C6-C7-C8-C9
17	3	306	CLA	C4B-C3B-CAB-CBB
17	3	324	CLA	C4B-C3B-CAB-CBB
17	A	5010	CLA	C4B-C3B-CAB-CBB
17	A	5011	CLA	C4B-C3B-CAB-CBB
17	A	5014	CLA	C4B-C3B-CAB-CBB
17	A	5018	CLA	C4B-C3B-CAB-CBB
17	A	5020	CLA	C4B-C3B-CAB-CBB
17	A	5028	CLA	C4B-C3B-CAB-CBB
17	A	5030	CLA	C4B-C3B-CAB-CBB
17	A	5043	CLA	C4B-C3B-CAB-CBB
17	B	803	CLA	C4B-C3B-CAB-CBB
17	B	818	CLA	C4B-C3B-CAB-CBB
17	B	823	CLA	C4B-C3B-CAB-CBB
17	B	835	CLA	C4B-C3B-CAB-CBB
17	F	5006	CLA	C4B-C3B-CAB-CBB
17	F	5009	CLA	C4B-C3B-CAB-CBB
17	K	201	CLA	C4B-C3B-CAB-CBB
17	a	604	CLA	C4B-C3B-CAB-CBB
17	b	602	CLA	C4B-C3B-CAB-CBB
17	b	604	CLA	C4B-C3B-CAB-CBB
17	c	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	c	308	CLA	C4B-C3B-CAB-CBB
23	B	848	DGD	C2D-C1D-O3G-C3G
17	B	829	CLA	C3-C5-C6-C7
16	3	301	CHL	C6-C7-C8-C10
17	1	607	CLA	C11-C12-C13-C15
17	A	5016	CLA	C12-C13-C15-C16
17	A	5020	CLA	C11-C12-C13-C15
17	A	5024	CLA	C11-C10-C8-C7
17	A	5030	CLA	C12-C13-C15-C16
17	A	5035	CLA	C11-C12-C13-C15
17	B	803	CLA	C11-C10-C8-C7
17	B	808	CLA	C11-C12-C13-C15
17	B	827	CLA	C11-C10-C8-C7
17	B	830	CLA	C12-C13-C15-C16
17	B	833	CLA	C11-C10-C8-C7
17	c	301	CLA	C11-C12-C13-C15
17	c	308	CLA	C12-C13-C15-C16
28	A	5045	PQN	C22-C23-C25-C26
17	7	314	CLA	CBA-CGA-O2A-C1
17	A	5029	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	O1A-CGA-O2A-C1
17	8	315	CLA	C3A-C2A-CAA-CBA
17	A	5013	CLA	C3A-C2A-CAA-CBA
17	B	808	CLA	C4-C3-C5-C6
17	B	817	CLA	C3A-C2A-CAA-CBA
17	B	819	CLA	C3A-C2A-CAA-CBA
17	B	827	CLA	C3A-C2A-CAA-CBA
17	7	312	CLA	C2-C3-C5-C6
17	A	5028	CLA	O1A-CGA-O2A-C1
20	1	617	BCR	C13-C14-C15-C16
20	1	617	BCR	C11-C12-C13-C35
21	a	618	LHG	C2-C3-O3-P
17	A	5018	CLA	O1D-CGD-O2D-CED
17	A	5023	CLA	CBA-CGA-O2A-C1
16	b	606	CHL	C4C-C3C-CAC-CBC
17	B	804	CLA	O2A-C1-C2-C3
17	J	102	CLA	O2A-C1-C2-C3
21	1	618	LHG	C4-C5-C6-O8
24	7	301	LMG	O1-C7-C8-C9
24	7	301	LMG	C7-C8-C9-O8
17	7	312	CLA	C4-C3-C5-C6
17	c	309	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	c	309	CLA	C2-C3-C5-C6
17	A	5004	CLA	C5-C6-C7-C8
17	7	302	CLA	C11-C12-C13-C15
26	8	319	PTY	O14-C5-C6-O7
26	F	5002	PTY	O14-C5-C6-O7
17	3	307	CLA	C2B-C3B-CAB-CBB
17	A	5017	CLA	C2B-C3B-CAB-CBB
17	A	5027	CLA	C2B-C3B-CAB-CBB
18	8	316	LUT	C1-C6-C7-C8
18	a	615	LUT	C1-C6-C7-C8
18	b	615	LUT	C1-C6-C7-C8
20	3	317	BCR	C5-C6-C7-C8
20	3	317	BCR	C23-C24-C25-C30
20	3	318	BCR	C23-C24-C25-C30
20	A	5050	BCR	C1-C6-C7-C8
20	B	843	BCR	C23-C24-C25-C30
20	B	844	BCR	C1-C6-C7-C8
20	B	847	BCR	C23-C24-C25-C30
20	F	5010	BCR	C23-C24-C25-C30
20	a	617	BCR	C23-C24-C25-C30
20	c	316	BCR	C5-C6-C7-C8
20	c	316	BCR	C23-C24-C25-C30
16	1	606	CHL	CBA-CGA-O2A-C1
21	1	618	LHG	O7-C5-C6-O8
21	a	618	LHG	O7-C5-C6-O8
24	7	301	LMG	O7-C8-C9-O8
17	A	5004	CLA	C3-C5-C6-C7
21	7	318	LHG	C10-C11-C12-C13
16	3	322	CHL	C2-C3-C5-C6
16	3	301	CHL	C1-C2-C3-C5
16	3	322	CHL	C1-C2-C3-C5
17	B	836	CLA	C11-C12-C13-C14
17	A	5028	CLA	C5-C6-C7-C8
17	a	610	CLA	CBA-CGA-O2A-C1
16	b	607	CHL	C1-C2-C3-C4
17	B	803	CLA	C11-C10-C8-C9
16	b	606	CHL	CBA-CGA-O2A-C1
24	7	301	LMG	C2-C1-O1-C7
17	B	839	CLA	CAA-CBA-CGA-O2A
16	3	322	CHL	C11-C12-C13-C14
17	b	609	CLA	C11-C12-C13-C15
17	A	5013	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	T	402	CLA	CBA-CGA-O2A-C1
26	8	319	PTY	O14-C5-C6-C1
21	A	5053	LHG	C26-C27-C28-C29
17	3	309	CLA	CBA-CGA-O2A-C1
16	3	322	CHL	C11-C10-C8-C7
17	A	5004	CLA	C6-C7-C8-C10
17	A	5006	CLA	C11-C10-C8-C7
17	A	5044	CLA	C12-C13-C15-C16
17	B	806	CLA	C12-C13-C15-C16
19	7	316	XAT	C27-C28-C29-C30
20	1	617	BCR	C11-C12-C13-C14
20	A	5049	BCR	C17-C18-C19-C20
17	B	829	CLA	C2A-CAA-CBA-CGA
17	3	311	CLA	C6-C7-C8-C10
17	b	613	CLA	CBD-CGD-O2D-CED
17	A	5014	CLA	C10-C11-C12-C13
16	c	305	CHL	C2C-C3C-CAC-CBC
17	7	312	CLA	O1A-CGA-O2A-C1
17	A	5035	CLA	C10-C11-C12-C13
25	A	5054	LMU	C3'-C4'-O1B-C1B
17	3	302	CLA	C5-C6-C7-C8
17	B	806	CLA	C8-C10-C11-C12
21	a	618	LHG	C4-C5-C6-O8
17	1	609	CLA	C3-C5-C6-C7
17	1	602	CLA	C4-C3-C5-C6
17	L	201	CLA	C4-C3-C5-C6
17	A	5024	CLA	C2A-CAA-CBA-CGA
17	A	5029	CLA	C2A-CAA-CBA-CGA
17	B	824	CLA	C2A-CAA-CBA-CGA
17	B	835	CLA	C2A-CAA-CBA-CGA
17	A	5016	CLA	C5-C6-C7-C8
17	T	402	CLA	O1A-CGA-O2A-C1
17	1	609	CLA	C6-C7-C8-C9
17	A	5004	CLA	C6-C7-C8-C9
17	A	5006	CLA	C6-C7-C8-C9
17	c	308	CLA	C14-C13-C15-C16
17	1	610	CLA	CAA-CBA-CGA-O2A
17	A	5006	CLA	C10-C11-C12-C13
17	B	841	CLA	C2-C1-O2A-CGA
17	T	406	CLA	C2-C1-O2A-CGA
21	1	619	LHG	C5-C4-O6-P
16	3	322	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
17	B	836	CLA	C11-C12-C13-C15
25	A	5054	LMU	C5'-C4'-O1B-C1B
17	7	302	CLA	C11-C12-C13-C14
17	A	5020	CLA	C15-C16-C17-C18
18	c	314	LUT	C27-C28-C29-C39
16	3	322	CHL	C4B-C3B-CAB-CBB
16	7	306	CHL	C1A-C2A-CAA-CBA
16	8	308	CHL	C4B-C3B-CAB-CBB
16	a	606	CHL	C4B-C3B-CAB-CBB
16	b	607	CHL	C4B-C3B-CAB-CBB
16	c	305	CHL	C1A-C2A-CAA-CBA
17	3	312	CLA	C1A-C2A-CAA-CBA
17	3	314	CLA	C1A-C2A-CAA-CBA
17	7	313	CLA	C1A-C2A-CAA-CBA
17	A	5042	CLA	C1A-C2A-CAA-CBA
17	B	812	CLA	C1A-C2A-CAA-CBA
17	B	827	CLA	C1A-C2A-CAA-CBA
17	c	307	CLA	C4B-C3B-CAB-CBB
17	1	607	CLA	C8-C10-C11-C12
17	L	201	CLA	C2-C3-C5-C6
18	T	413	LUT	C7-C8-C9-C10
19	c	315	XAT	C27-C28-C29-C30
17	A	5014	CLA	C2A-CAA-CBA-CGA
17	A	5022	CLA	C2A-CAA-CBA-CGA
17	a	602	CLA	C2A-CAA-CBA-CGA
17	3	307	CLA	C11-C10-C8-C7
17	A	5006	CLA	C6-C7-C8-C10
17	A	5008	CLA	C12-C13-C15-C16
17	A	5009	CLA	C11-C12-C13-C15
17	A	5014	CLA	C11-C10-C8-C7
17	A	5026	CLA	C11-C12-C13-C15
17	A	5031	CLA	C11-C12-C13-C15
17	A	5036	CLA	C12-C13-C15-C16
17	B	806	CLA	C6-C7-C8-C10
17	B	829	CLA	C6-C7-C8-C10
17	B	841	CLA	C6-C7-C8-C10
17	3	311	CLA	C6-C7-C8-C9
21	1	619	LHG	C2-C3-O3-P
21	A	5002	LHG	C2-C3-O3-P
17	7	312	CLA	C3A-C2A-CAA-CBA
17	A	5028	CLA	C4-C3-C5-C6
17	A	5009	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
17	A	5018	CLA	C2-C3-C5-C6
21	a	618	LHG	O6-C4-C5-O7
17	A	5019	CLA	C2A-CAA-CBA-CGA
17	F	5009	CLA	C2A-CAA-CBA-CGA
17	A	5006	CLA	C11-C10-C8-C9
17	A	5024	CLA	C11-C10-C8-C9
17	A	5044	CLA	C14-C13-C15-C16
17	c	301	CLA	C11-C12-C13-C14
17	B	802	CLA	C8-C10-C11-C12
16	3	322	CHL	C1C-C2C-CMC-OMC
16	8	306	CHL	C1C-C2C-CMC-OMC
16	T	416	CHL	C1C-C2C-CMC-OMC
16	a	601	CHL	C1C-C2C-CMC-OMC
16	b	607	CHL	C1C-C2C-CMC-OMC
16	c	305	CHL	C1-C2-C3-C4
17	c	309	CLA	C3-C5-C6-C7
21	8	321	LHG	O7-C5-C6-O8
21	8	321	LHG	C4-C5-C6-O8
23	3	321	DGD	C1G-C2G-C3G-O3G
17	A	5004	CLA	C2-C3-C5-C6
17	F	5004	CLA	CBD-CGD-O2D-CED
17	7	302	CLA	CAD-CBD-CGD-O2D
17	8	302	CLA	CAD-CBD-CGD-O2D
17	8	305	CLA	CAD-CBD-CGD-O2D
17	B	805	CLA	CAD-CBD-CGD-O2D
17	B	821	CLA	CAD-CBD-CGD-O2D
17	K	203	CLA	CAD-CBD-CGD-O2D
17	K	204	CLA	CAD-CBD-CGD-O2D
17	A	5030	CLA	CBA-CGA-O2A-C1
17	B	841	CLA	C5-C6-C7-C8
17	3	302	CLA	C15-C16-C17-C18
17	B	809	CLA	C8-C10-C11-C12
17	A	5030	CLA	O1A-CGA-O2A-C1
16	8	306	CHL	CHA-CBD-CGD-O1D
17	1	602	CLA	CHA-CBD-CGD-O1D
17	1	608	CLA	CHA-CBD-CGD-O1D
17	7	302	CLA	CAD-CBD-CGD-O1D
17	8	302	CLA	CAD-CBD-CGD-O1D
17	8	304	CLA	CHA-CBD-CGD-O1D
17	8	304	CLA	CHA-CBD-CGD-O2D
17	8	305	CLA	CAD-CBD-CGD-O1D
17	A	5011	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	A	5011	CLA	CHA-CBD-CGD-O2D
17	A	5017	CLA	CHA-CBD-CGD-O1D
17	A	5017	CLA	CHA-CBD-CGD-O2D
17	A	5018	CLA	CHA-CBD-CGD-O1D
17	A	5018	CLA	CHA-CBD-CGD-O2D
17	A	5026	CLA	CHA-CBD-CGD-O1D
17	A	5026	CLA	CHA-CBD-CGD-O2D
17	A	5038	CLA	CHA-CBD-CGD-O1D
17	A	5038	CLA	CHA-CBD-CGD-O2D
17	B	805	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O2D
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	814	CLA	CHA-CBD-CGD-O1D
17	B	814	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	CHA-CBD-CGD-O1D
17	B	815	CLA	CHA-CBD-CGD-O2D
17	B	821	CLA	CAD-CBD-CGD-O1D
17	K	203	CLA	CAD-CBD-CGD-O1D
17	K	204	CLA	CAD-CBD-CGD-O1D
17	a	603	CLA	CHA-CBD-CGD-O1D
21	1	618	LHG	C4-O6-P-O5
21	8	321	LHG	C3-O3-P-O4
21	8	321	LHG	C3-O3-P-O6
21	A	5002	LHG	C4-O6-P-O5
21	A	5055	LHG	C4-O6-P-O4
21	F	5001	LHG	C4-O6-P-O5
21	b	618	LHG	C3-O3-P-O5
21	c	317	LHG	C3-O3-P-O6
21	c	317	LHG	C4-O6-P-O3
26	8	319	PTY	C5-O14-P1-O12
26	F	5003	PTY	C3-O11-P1-O13
17	a	609	CLA	C4-C3-C5-C6
16	3	322	CHL	C2B-C3B-CAB-CBB
16	c	306	CHL	C2B-C3B-CAB-CBB
17	1	602	CLA	C2B-C3B-CAB-CBB
17	1	603	CLA	C2B-C3B-CAB-CBB
17	1	608	CLA	C2B-C3B-CAB-CBB
17	1	609	CLA	C2B-C3B-CAB-CBB
17	1	613	CLA	C2B-C3B-CAB-CBB
17	3	302	CLA	C2B-C3B-CAB-CBB
17	3	303	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	3	305	CLA	C2B-C3B-CAB-CBB
17	3	313	CLA	C2B-C3B-CAB-CBB
17	3	323	CLA	C2B-C3B-CAB-CBB
17	7	302	CLA	C2B-C3B-CAB-CBB
17	7	304	CLA	C2B-C3B-CAB-CBB
17	7	308	CLA	C2B-C3B-CAB-CBB
17	8	309	CLA	C2B-C3B-CAB-CBB
17	8	312	CLA	C2B-C3B-CAB-CBB
17	A	5004	CLA	C2B-C3B-CAB-CBB
17	A	5007	CLA	C2B-C3B-CAB-CBB
17	A	5010	CLA	C2B-C3B-CAB-CBB
17	A	5033	CLA	C2B-C3B-CAB-CBB
17	A	5035	CLA	C2B-C3B-CAB-CBB
17	A	5041	CLA	C2B-C3B-CAB-CBB
17	B	804	CLA	C2B-C3B-CAB-CBB
17	B	806	CLA	C2B-C3B-CAB-CBB
17	B	811	CLA	C2B-C3B-CAB-CBB
17	B	815	CLA	C2B-C3B-CAB-CBB
17	B	816	CLA	C2B-C3B-CAB-CBB
17	B	817	CLA	C2B-C3B-CAB-CBB
17	B	826	CLA	C2B-C3B-CAB-CBB
17	B	831	CLA	C2B-C3B-CAB-CBB
17	B	838	CLA	C2B-C3B-CAB-CBB
17	B	839	CLA	C2B-C3B-CAB-CBB
17	T	402	CLA	C2B-C3B-CAB-CBB
17	T	403	CLA	C2B-C3B-CAB-CBB
17	T	407	CLA	C2B-C3B-CAB-CBB
17	T	412	CLA	C2B-C3B-CAB-CBB
17	a	609	CLA	C2B-C3B-CAB-CBB
17	a	611	CLA	C2B-C3B-CAB-CBB
17	a	612	CLA	C2B-C3B-CAB-CBB
17	b	608	CLA	C2B-C3B-CAB-CBB
17	c	301	CLA	C2B-C3B-CAB-CBB
17	c	302	CLA	C2B-C3B-CAB-CBB
17	c	303	CLA	C2B-C3B-CAB-CBB
17	c	307	CLA	C2B-C3B-CAB-CBB
17	L	201	CLA	C2B-C3B-CAB-CBB
20	3	318	BCR	C1-C6-C7-C8
20	B	801	BCR	C23-C24-C25-C30
18	1	615	LUT	C11-C12-C13-C20
17	T	409	CLA	C3-C5-C6-C7
17	B	841	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	5053	LHG	C24-C25-C26-C27
20	B	845	BCR	C10-C11-C12-C13
20	B	845	BCR	C18-C19-C20-C21
20	K	205	BCR	C10-C11-C12-C13
17	A	5044	CLA	C2-C3-C5-C6
17	1	602	CLA	C6-C7-C8-C10
17	c	308	CLA	C16-C17-C18-C20
16	3	301	CHL	C6-C7-C8-C9
17	1	607	CLA	C11-C12-C13-C14
17	A	5035	CLA	C11-C12-C13-C14
17	B	808	CLA	C11-C12-C13-C14
17	B	841	CLA	C6-C7-C8-C9
17	A	5014	CLA	C6-C7-C8-C10
17	B	808	CLA	C11-C10-C8-C7
17	A	5016	CLA	C4C-C3C-CAC-CBC
23	3	321	DGD	C3B-C4B-C5B-C6B
17	b	613	CLA	O1D-CGD-O2D-CED
21	8	321	LHG	O8-C23-C24-C25
17	A	5009	CLA	C16-C17-C18-C19
17	3	314	CLA	C2A-CAA-CBA-CGA
17	B	814	CLA	C2-C1-O2A-CGA
17	8	314	CLA	CAA-CBA-CGA-O2A
17	a	610	CLA	CAA-CBA-CGA-O2A
24	F	5011	LMG	O1-C7-C8-C9
30	J	101	LMK	C8-C7-O1-C1
17	F	5006	CLA	CBA-CGA-O2A-C1
17	A	5041	CLA	CAA-CBA-CGA-O2A
23	8	301	DGD	C2G-C3G-O3G-C1D
17	A	5020	CLA	C2A-CAA-CBA-CGA
17	A	5026	CLA	C2A-CAA-CBA-CGA
17	B	803	CLA	C2A-CAA-CBA-CGA
17	B	813	CLA	C2A-CAA-CBA-CGA
17	c	310	CLA	C2A-CAA-CBA-CGA
17	c	311	CLA	C2A-CAA-CBA-CGA
17	A	5033	CLA	C6-C7-C8-C10
17	B	827	CLA	CAA-CBA-CGA-O2A
17	A	5008	CLA	C11-C12-C13-C14
17	A	5026	CLA	C11-C12-C13-C14
17	B	829	CLA	C6-C7-C8-C9
21	F	5001	LHG	C2-C3-O3-P
17	F	5006	CLA	O1A-CGA-O2A-C1
17	3	304	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	B	813	CLA	C4B-C3B-CAB-CBB
17	A	5042	CLA	C5-C6-C7-C8
17	B	809	CLA	C4-C3-C5-C6
17	A	5028	CLA	C2-C3-C5-C6
17	7	312	CLA	C5-C6-C7-C8
17	B	803	CLA	C8-C10-C11-C12
17	F	5004	CLA	O1D-CGD-O2D-CED
17	A	5023	CLA	O1A-CGA-O2A-C1
16	3	301	CHL	C11-C12-C13-C15
17	A	5008	CLA	C11-C12-C13-C15
17	A	5011	CLA	C6-C7-C8-C10
17	B	802	CLA	C12-C13-C15-C16
17	7	314	CLA	O1A-CGA-O2A-C1
17	1	602	CLA	C6-C7-C8-C9
17	c	308	CLA	C16-C17-C18-C19
16	c	305	CHL	C4C-C3C-CAC-CBC
17	3	323	CLA	C4-C3-C5-C6
17	A	5022	CLA	C3A-C2A-CAA-CBA
17	A	5040	CLA	C4-C3-C5-C6
21	7	318	LHG	O8-C23-C24-C25
18	1	615	LUT	C40-C33-C34-C35
18	a	615	LUT	C40-C33-C34-C35
20	3	319	BCR	C35-C13-C14-C15
20	3	319	BCR	C16-C17-C18-C36
20	A	5052	BCR	C11-C10-C9-C34
20	A	5052	BCR	C16-C17-C18-C36
20	B	849	BCR	C35-C13-C14-C15
20	F	5010	BCR	C16-C17-C18-C36
20	K	205	BCR	C11-C10-C9-C34
20	L	204	BCR	C11-C10-C9-C34
20	I	4001	BCR	C35-C13-C14-C15
17	B	806	CLA	C2-C1-O2A-CGA
26	F	5002	PTY	C6-C5-O14-P1
17	a	603	CLA	CAA-CBA-CGA-O1A
21	A	5053	LHG	C11-C10-C9-C8
17	A	5035	CLA	C15-C16-C17-C18
17	1	603	CLA	CAA-CBA-CGA-O1A
17	K	203	CLA	CAA-CBA-CGA-O2A
17	A	5039	CLA	C4-C3-C5-C6
16	T	416	CHL	CAA-CBA-CGA-O1A
17	3	307	CLA	C11-C10-C8-C9
17	A	5028	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
17	B	805	CLA	C6-C7-C8-C9
25	7	319	LMU	C5'-C4'-O1B-C1B
16	3	301	CHL	C1-C2-C3-C4
16	3	322	CHL	C1-C2-C3-C4
16	8	306	CHL	CAA-CBA-CGA-O2A
16	T	416	CHL	CAA-CBA-CGA-O2A
17	a	603	CLA	CAA-CBA-CGA-O2A
25	7	319	LMU	C3'-C4'-O1B-C1B
17	1	613	CLA	C1A-C2A-CAA-CBA
17	3	303	CLA	C1A-C2A-CAA-CBA
17	A	5010	CLA	C1A-C2A-CAA-CBA
17	A	5022	CLA	C1A-C2A-CAA-CBA
17	A	5025	CLA	C1A-C2A-CAA-CBA
17	B	841	CLA	C1A-C2A-CAA-CBA
17	T	409	CLA	C1A-C2A-CAA-CBA
17	T	411	CLA	C1A-C2A-CAA-CBA
17	b	611	CLA	C1A-C2A-CAA-CBA
17	c	309	CLA	C1A-C2A-CAA-CBA
17	c	312	CLA	C1A-C2A-CAA-CBA
18	1	615	LUT	C32-C33-C34-C35
18	a	615	LUT	C32-C33-C34-C35
20	3	319	BCR	C12-C13-C14-C15
20	3	319	BCR	C16-C17-C18-C19
20	A	5052	BCR	C11-C10-C9-C8
20	A	5052	BCR	C16-C17-C18-C19
20	B	849	BCR	C12-C13-C14-C15
20	F	5010	BCR	C16-C17-C18-C19
20	K	205	BCR	C11-C10-C9-C8
20	L	204	BCR	C11-C10-C9-C8
20	I	4001	BCR	C12-C13-C14-C15
17	1	603	CLA	CAA-CBA-CGA-O2A
16	3	301	CHL	C2B-C3B-CAB-CBB
16	8	308	CHL	C2B-C3B-CAB-CBB
16	T	401	CHL	C2B-C3B-CAB-CBB
16	a	606	CHL	C2B-C3B-CAB-CBB
16	b	607	CHL	C2B-C3B-CAB-CBB
17	3	306	CLA	C2B-C3B-CAB-CBB
17	3	324	CLA	C2B-C3B-CAB-CBB
17	A	5011	CLA	C2B-C3B-CAB-CBB
17	A	5018	CLA	C2B-C3B-CAB-CBB
17	A	5028	CLA	C2B-C3B-CAB-CBB
17	A	5030	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	B	803	CLA	C2B-C3B-CAB-CBB
17	B	823	CLA	C2B-C3B-CAB-CBB
17	B	824	CLA	C2B-C3B-CAB-CBB
17	B	835	CLA	C2B-C3B-CAB-CBB
17	F	5006	CLA	C2B-C3B-CAB-CBB
18	8	316	LUT	C5-C6-C7-C8
18	a	615	LUT	C5-C6-C7-C8
18	b	615	LUT	C5-C6-C7-C8
20	3	317	BCR	C23-C24-C25-C26
20	3	318	BCR	C23-C24-C25-C26
20	7	317	BCR	C1-C6-C7-C8
20	A	5050	BCR	C5-C6-C7-C8
20	A	5051	BCR	C1-C6-C7-C8
20	B	843	BCR	C23-C24-C25-C26
20	B	844	BCR	C5-C6-C7-C8
20	B	847	BCR	C23-C24-C25-C26
20	F	5010	BCR	C23-C24-C25-C26
20	K	205	BCR	C23-C24-C25-C30
20	a	617	BCR	C23-C24-C25-C26
20	b	617	BCR	C5-C6-C7-C8
20	c	316	BCR	C23-C24-C25-C26
20	L	204	BCR	C1-C6-C7-C8
17	K	203	CLA	CAA-CBA-CGA-O1A
17	K	201	CLA	CAA-CBA-CGA-O1A
17	T	405	CLA	CAA-CBA-CGA-O2A
30	J	101	LMK	N4-C3-C4-O2
16	8	306	CHL	CAA-CBA-CGA-O1A
16	1	606	CHL	O1A-CGA-O2A-C1
17	A	5004	CLA	C11-C12-C13-C15
17	B	829	CLA	C11-C12-C13-C15
17	F	5004	CLA	C11-C10-C8-C7
17	T	409	CLA	C2A-CAA-CBA-CGA
16	b	606	CHL	O1A-CGA-O2A-C1
17	a	610	CLA	O1A-CGA-O2A-C1
17	3	309	CLA	O1A-CGA-O2A-C1
17	A	5044	CLA	C3-C5-C6-C7
17	B	809	CLA	C2-C3-C5-C6
17	K	201	CLA	CAA-CBA-CGA-O2A
17	A	5011	CLA	C2A-CAA-CBA-CGA
17	A	5016	CLA	C11-C12-C13-C14
17	B	802	CLA	C5-C6-C7-C8
17	A	5044	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	F	5006	CLA	C5-C6-C7-C8
25	7	319	LMU	C5-C6-C7-C8
17	1	602	CLA	C2-C3-C5-C6
17	a	609	CLA	C2-C3-C5-C6
17	8	315	CLA	CAA-CBA-CGA-O2A
17	b	608	CLA	CAA-CBA-CGA-O2A
17	A	5024	CLA	CAA-CBA-CGA-O2A
17	T	405	CLA	CAA-CBA-CGA-O1A
17	A	5008	CLA	C2A-CAA-CBA-CGA
17	A	5009	CLA	C2A-CAA-CBA-CGA
17	L	201	CLA	C2A-CAA-CBA-CGA
17	A	5033	CLA	C6-C7-C8-C9
16	3	301	CHL	C4B-C3B-CAB-CBB
16	T	401	CHL	C4B-C3B-CAB-CBB
17	8	305	CLA	C4B-C3B-CAB-CBB
17	B	824	CLA	C4B-C3B-CAB-CBB
27	A	5003	CL0	C4B-C3B-CAB-CBB
23	3	321	DGD	C4D-C5D-C6D-O5D
27	A	5003	CL0	C16-C17-C18-C19
17	A	5040	CLA	O1D-CGD-O2D-CED
17	A	5040	CLA	CBD-CGD-O2D-CED
17	B	806	CLA	C15-C16-C17-C18
17	a	605	CLA	CAA-CBA-CGA-O1A
17	A	5039	CLA	C2-C3-C5-C6
21	a	619	LHG	C5-C4-O6-P
17	A	5029	CLA	C11-C12-C13-C15
24	7	301	LMG	C12-C13-C14-C15
17	a	605	CLA	CAA-CBA-CGA-O2A
17	A	5006	CLA	C14-C13-C15-C16
17	A	5008	CLA	C14-C13-C15-C16
17	A	5009	CLA	C11-C12-C13-C14
17	A	5030	CLA	C11-C12-C13-C14
17	A	5036	CLA	C14-C13-C15-C16
17	B	819	CLA	C6-C7-C8-C9
17	B	803	CLA	C2-C1-O2A-CGA
17	B	829	CLA	C2-C1-O2A-CGA
17	B	834	CLA	C2-C1-O2A-CGA
17	B	808	CLA	C8-C10-C11-C12
17	A	5024	CLA	C3A-C2A-CAA-CBA
17	T	411	CLA	C3A-C2A-CAA-CBA
17	a	612	CLA	C3A-C2A-CAA-CBA
17	b	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	b	614	CLA	CAA-CBA-CGA-O2A
17	A	5032	CLA	CAA-CBA-CGA-O2A
17	A	5043	CLA	CAA-CBA-CGA-O2A
17	b	608	CLA	CAA-CBA-CGA-O1A
17	L	202	CLA	CAA-CBA-CGA-O2A
17	8	302	CLA	CAA-CBA-CGA-O2A
17	c	310	CLA	CAA-CBA-CGA-O2A
17	8	315	CLA	CAA-CBA-CGA-O1A
17	A	5030	CLA	C15-C16-C17-C18
19	7	316	XAT	O24-C26-C27-C28
19	c	315	XAT	O24-C26-C27-C28
24	7	301	LMG	C11-C12-C13-C14
17	L	201	CLA	CBD-CGD-O2D-CED
27	A	5003	CL0	C5-C6-C7-C8
16	1	601	CHL	C2A-CAA-CBA-CGA
26	F	5003	PTY	C6-C1-O4-C30
17	c	310	CLA	CAA-CBA-CGA-O1A
17	L	202	CLA	CAA-CBA-CGA-O1A
16	3	301	CHL	C14-C13-C15-C16
17	a	614	CLA	CAA-CBA-CGA-O2A
17	F	5004	CLA	C13-C15-C16-C17
22	3	320	SQD	O47-C45-C46-O48
17	A	5043	CLA	CAA-CBA-CGA-O1A
17	3	302	CLA	C6-C7-C8-C9
17	A	5014	CLA	C11-C10-C8-C9
17	A	5028	CLA	C11-C10-C8-C9
17	A	5031	CLA	C11-C12-C13-C14
17	B	806	CLA	C6-C7-C8-C9
17	B	818	CLA	C16-C17-C18-C20
17	3	305	CLA	CAA-CBA-CGA-O2A
17	b	611	CLA	CAA-CBA-CGA-O2A
21	a	619	LHG	O8-C23-C24-C25
23	8	301	DGD	O2G-C1B-C2B-C3B
21	A	5053	LHG	C9-C10-C11-C12
17	B	839	CLA	CAA-CBA-CGA-O1A
17	1	609	CLA	C2A-CAA-CBA-CGA
17	B	802	CLA	C2A-CAA-CBA-CGA
17	A	5016	CLA	C11-C12-C13-C15
17	B	819	CLA	C6-C7-C8-C10
17	B	830	CLA	C6-C7-C8-C10
17	3	304	CLA	C2B-C3B-CAB-CBB
17	8	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	A	5014	CLA	C2B-C3B-CAB-CBB
17	A	5020	CLA	C2B-C3B-CAB-CBB
17	A	5022	CLA	C2B-C3B-CAB-CBB
17	A	5043	CLA	C2B-C3B-CAB-CBB
17	B	813	CLA	C2B-C3B-CAB-CBB
17	B	818	CLA	C2B-C3B-CAB-CBB
17	B	829	CLA	C2B-C3B-CAB-CBB
17	F	5009	CLA	C2B-C3B-CAB-CBB
17	K	201	CLA	C2B-C3B-CAB-CBB
17	a	604	CLA	C2B-C3B-CAB-CBB
17	b	602	CLA	C2B-C3B-CAB-CBB
17	b	604	CLA	C2B-C3B-CAB-CBB
17	c	308	CLA	C2B-C3B-CAB-CBB
18	3	315	LUT	C1-C6-C7-C8
18	3	315	LUT	C5-C6-C7-C8
20	3	318	BCR	C5-C6-C7-C8
20	7	317	BCR	C5-C6-C7-C8
20	A	5051	BCR	C5-C6-C7-C8
20	B	801	BCR	C23-C24-C25-C26
20	K	205	BCR	C23-C24-C25-C26
20	L	204	BCR	C5-C6-C7-C8
17	3	306	CLA	C2-C1-O2A-CGA
17	8	313	CLA	C2-C1-O2A-CGA
17	A	5006	CLA	C2-C1-O2A-CGA
17	A	5021	CLA	C2-C1-O2A-CGA
17	B	808	CLA	C2-C1-O2A-CGA
17	B	824	CLA	C2-C1-O2A-CGA
17	B	837	CLA	C2-C1-O2A-CGA
17	A	5020	CLA	C16-C17-C18-C20
19	1	616	XAT	C6-C7-C8-C9
19	7	316	XAT	C26-C27-C28-C29
16	b	606	CHL	CAA-CBA-CGA-O2A
17	T	403	CLA	CAA-CBA-CGA-O2A
21	a	618	LHG	O8-C23-C24-C25
17	L	201	CLA	O1D-CGD-O2D-CED
24	7	301	LMG	C15-C16-C17-C18
25	A	5054	LMU	C1-C2-C3-C4
17	B	806	CLA	CAA-CBA-CGA-O2A
17	A	5005	CLA	C2A-CAA-CBA-CGA
17	F	5006	CLA	C2A-CAA-CBA-CGA
17	A	5032	CLA	CAA-CBA-CGA-O1A
16	c	305	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
17	3	310	CLA	CAA-CBA-CGA-O2A
17	7	314	CLA	CAA-CBA-CGA-O2A
17	B	813	CLA	CAA-CBA-CGA-O2A
17	A	5026	CLA	CAA-CBA-CGA-O2A
17	B	834	CLA	CAA-CBA-CGA-O2A
17	3	312	CLA	CAA-CBA-CGA-O2A
17	A	5010	CLA	CAA-CBA-CGA-O2A
17	B	818	CLA	CAA-CBA-CGA-O2A
21	A	5053	LHG	O8-C23-C24-C25
17	3	323	CLA	C2-C3-C5-C6
17	A	5040	CLA	C2-C3-C5-C6
17	b	603	CLA	C2A-CAA-CBA-CGA
21	1	619	LHG	O8-C23-C24-C25
17	A	5004	CLA	C11-C12-C13-C14
17	F	5004	CLA	C11-C10-C8-C9
16	b	605	CHL	C2C-C3C-CAC-CBC
17	T	409	CLA	CAA-CBA-CGA-O2A
17	T	411	CLA	CAA-CBA-CGA-O2A
16	7	305	CHL	C1A-C2A-CAA-CBA
17	7	311	CLA	C1A-C2A-CAA-CBA
17	A	5014	CLA	C1A-C2A-CAA-CBA
17	A	5022	CLA	C4B-C3B-CAB-CBB
17	A	5024	CLA	C1A-C2A-CAA-CBA
17	A	5028	CLA	C1A-C2A-CAA-CBA
17	A	5044	CLA	C1A-C2A-CAA-CBA
17	B	823	CLA	C1A-C2A-CAA-CBA
17	B	831	CLA	C1A-C2A-CAA-CBA
17	K	201	CLA	C1A-C2A-CAA-CBA
17	K	202	CLA	C1A-C2A-CAA-CBA
17	T	404	CLA	C4B-C3B-CAB-CBB
21	A	5002	LHG	C27-C28-C29-C30
17	3	304	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	CAA-CBA-CGA-O2A
17	B	841	CLA	CAA-CBA-CGA-O2A
17	1	602	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	CAA-CBA-CGA-O2A
17	T	404	CLA	CAA-CBA-CGA-O2A
21	1	618	LHG	O7-C7-C8-C9
16	8	307	CHL	C2A-CAA-CBA-CGA
17	A	5039	CLA	C2A-CAA-CBA-CGA
17	c	301	CLA	C2A-CAA-CBA-CGA
17	B	827	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	1	609	CLA	C2-C1-O2A-CGA
17	A	5007	CLA	C2-C1-O2A-CGA
17	1	614	CLA	CAA-CBA-CGA-O2A
17	B	835	CLA	CAA-CBA-CGA-O2A
17	A	5006	CLA	C12-C13-C15-C16
17	A	5013	CLA	C11-C10-C8-C7
17	A	5030	CLA	C11-C12-C13-C15
17	B	840	CLA	C11-C10-C8-C7
17	b	602	CLA	C6-C7-C8-C10
27	A	5003	CL0	C6-C7-C8-C10
17	A	5016	CLA	C13-C15-C16-C17
17	c	301	CLA	C13-C15-C16-C17
23	8	301	DGD	C3G-C2G-O2G-C1B
26	8	320	PTY	C1-C6-O7-C8
17	a	614	CLA	CAA-CBA-CGA-O1A
16	3	301	CHL	C8-C10-C11-C12
17	3	313	CLA	C3A-C2A-CAA-CBA
17	7	302	CLA	C2A-CAA-CBA-CGA
17	F	5007	CLA	C2A-CAA-CBA-CGA
17	c	308	CLA	C8-C10-C11-C12
17	B	828	CLA	CAA-CBA-CGA-O2A
17	7	314	CLA	CAA-CBA-CGA-O1A
17	J	102	CLA	O1A-CGA-O2A-C1
17	B	808	CLA	C15-C16-C17-C18
21	b	618	LHG	C5-C4-O6-P
16	7	305	CHL	C3A-C2A-CAA-CBA
17	A	5044	CLA	C3A-C2A-CAA-CBA
17	B	823	CLA	C3A-C2A-CAA-CBA
17	B	832	CLA	C3A-C2A-CAA-CBA
17	T	409	CLA	C3A-C2A-CAA-CBA
17	a	604	CLA	C3A-C2A-CAA-CBA
17	b	602	CLA	C5-C6-C7-C8
22	3	320	SQD	O47-C7-C8-C9
16	b	606	CHL	CAA-CBA-CGA-O1A
17	1	610	CLA	CAA-CBA-CGA-O1A
17	3	310	CLA	CAA-CBA-CGA-O1A
17	3	312	CLA	CAA-CBA-CGA-O1A
17	B	813	CLA	CAA-CBA-CGA-O1A
17	T	403	CLA	CAA-CBA-CGA-O1A
17	B	824	CLA	CAA-CBA-CGA-O2A
17	F	5007	CLA	CAA-CBA-CGA-O2A
17	3	305	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	B	834	CLA	CAA-CBA-CGA-O1A
21	a	618	LHG	O10-C23-C24-C25
21	F	5001	LHG	C10-C11-C12-C13
17	A	5014	CLA	C6-C7-C8-C9
17	B	840	CLA	C11-C10-C8-C9
17	b	611	CLA	CAA-CBA-CGA-O1A
21	a	619	LHG	O10-C23-C24-C25
17	B	828	CLA	C4-C3-C5-C6
17	3	304	CLA	CAA-CBA-CGA-O1A
17	B	826	CLA	CBA-CGA-O2A-C1
17	A	5012	CLA	C2-C3-C5-C6
17	B	826	CLA	O1A-CGA-O2A-C1
17	B	839	CLA	O1A-CGA-O2A-C1
17	T	411	CLA	CAA-CBA-CGA-O1A
24	7	301	LMG	C33-C34-C35-C36
21	A	5002	LHG	O8-C23-C24-C25
20	A	5052	BCR	C21-C22-C23-C24
20	K	205	BCR	C7-C8-C9-C10
17	T	409	CLA	CAA-CBA-CGA-O1A
23	8	301	DGD	O1B-C1B-C2B-C3B
23	8	301	DGD	C5D-C6D-O5D-C1E
16	c	306	CHL	O1A-CGA-O2A-C1
17	B	818	CLA	CAA-CBA-CGA-O1A
17	A	5025	CLA	CAA-CBA-CGA-O2A
17	B	814	CLA	CAA-CBA-CGA-O2A
17	b	609	CLA	C2A-CAA-CBA-CGA
21	A	5053	LHG	C32-C33-C34-C35
17	1	614	CLA	CAA-CBA-CGA-O1A
17	A	5036	CLA	C4-C3-C5-C6
17	A	5029	CLA	CAA-CBA-CGA-O2A
17	1	605	CLA	CAA-CBA-CGA-O2A
16	c	305	CHL	CAA-CBA-CGA-O1A
17	1	602	CLA	CAA-CBA-CGA-O1A
17	A	5010	CLA	CAA-CBA-CGA-O1A
17	A	5026	CLA	CAA-CBA-CGA-O1A
17	B	806	CLA	CAA-CBA-CGA-O1A
17	B	835	CLA	CAA-CBA-CGA-O1A
21	A	5053	LHG	O10-C23-C24-C25
17	8	310	CLA	C11-C12-C13-C14
17	A	5020	CLA	C16-C17-C18-C19
16	7	305	CHL	CAD-CBD-CGD-O2D
17	A	5007	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	812	CLA	CAD-CBD-CGD-O2D
17	B	829	CLA	CAD-CBD-CGD-O2D
17	B	833	CLA	CAD-CBD-CGD-O2D
17	T	409	CLA	CAD-CBD-CGD-O2D
17	L	202	CLA	CAD-CBD-CGD-O2D
17	3	309	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	CAA-CBA-CGA-O1A
17	B	841	CLA	CAA-CBA-CGA-O1A
21	1	619	LHG	O10-C23-C24-C25
17	A	5009	CLA	C8-C10-C11-C12
17	A	5026	CLA	O1A-CGA-O2A-C1
17	B	807	CLA	C2-C1-O2A-CGA
17	A	5040	CLA	CAA-CBA-CGA-O2A
17	b	601	CLA	CAA-CBA-CGA-O2A
27	A	5003	CL0	C1-C2-C3-C4
17	1	602	CLA	C5-C6-C7-C8
16	3	301	CHL	CAA-CBA-CGA-O2A
17	a	609	CLA	CAA-CBA-CGA-O2A
17	c	311	CLA	CAA-CBA-CGA-O2A
17	B	818	CLA	C16-C17-C18-C19
17	T	404	CLA	CAA-CBA-CGA-O1A
17	a	602	CLA	C5-C6-C7-C8
16	7	306	CHL	C2C-C3C-CAC-CBC
17	b	603	CLA	CAA-CBA-CGA-O2A
16	c	306	CHL	CBA-CGA-O2A-C1
21	1	618	LHG	O9-C7-C8-C9
22	3	320	SQD	O49-C7-C8-C9

There are no ring outliers.

247 monomers are involved in 585 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	830	CLA	3	0
17	A	5027	CLA	1	0
17	A	5016	CLA	7	0
17	A	5036	CLA	5	0
21	A	5002	LHG	2	0
17	8	314	CLA	1	0
17	c	312	CLA	2	0
17	8	315	CLA	1	0
17	A	5022	CLA	4	0
17	L	201	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	8	306	CHL	4	0
17	A	5013	CLA	6	0
17	A	5043	CLA	1	0
17	8	312	CLA	1	0
17	8	310	CLA	2	0
17	T	402	CLA	1	0
17	c	313	CLA	3	0
17	B	826	CLA	5	0
24	F	5011	LMG	1	0
16	1	601	CHL	2	0
25	A	5054	LMU	1	0
17	c	307	CLA	5	0
17	A	5008	CLA	5	0
17	3	307	CLA	7	0
20	A	5052	BCR	7	0
23	3	321	DGD	1	0
17	a	605	CLA	1	0
19	1	616	XAT	1	0
17	K	201	CLA	1	0
17	A	5024	CLA	1	0
17	B	832	CLA	4	0
17	T	412	CLA	2	0
18	a	615	LUT	4	0
21	a	619	LHG	1	0
17	K	203	CLA	3	0
17	B	805	CLA	2	0
17	A	5042	CLA	4	0
20	7	317	BCR	3	0
16	T	401	CHL	4	0
18	1	615	LUT	6	0
17	B	804	CLA	1	0
17	3	311	CLA	2	0
20	J	103	BCR	2	0
17	7	304	CLA	1	0
19	a	616	XAT	1	0
20	T	415	BCR	3	0
17	A	5033	CLA	4	0
17	B	806	CLA	5	0
17	c	309	CLA	1	0
20	B	849	BCR	5	0
17	K	202	CLA	1	0
20	B	846	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	8	317	XAT	1	0
20	A	5049	BCR	4	0
17	T	409	CLA	1	0
17	c	311	CLA	1	0
17	B	816	CLA	1	0
18	T	413	LUT	4	0
21	c	317	LHG	1	0
17	B	839	CLA	6	0
17	A	5021	CLA	1	0
17	1	610	CLA	1	0
18	b	615	LUT	1	0
20	B	844	BCR	2	0
17	B	833	CLA	1	0
19	3	316	XAT	4	0
18	7	315	LUT	3	0
17	8	304	CLA	1	0
17	a	607	CLA	1	0
28	B	842	PQN	3	0
17	A	5015	CLA	2	0
17	A	5018	CLA	6	0
17	A	5017	CLA	7	0
22	3	320	SQD	5	0
17	a	608	CLA	2	0
17	A	5025	CLA	6	0
17	B	802	CLA	7	0
17	F	5004	CLA	4	0
17	B	808	CLA	3	0
20	J	104	BCR	4	0
17	B	837	CLA	2	0
17	A	5030	CLA	5	0
17	1	607	CLA	3	0
17	7	303	CLA	2	0
17	T	405	CLA	1	0
19	c	315	XAT	1	0
20	b	617	BCR	6	0
20	3	318	BCR	4	0
20	I	4001	BCR	2	0
17	3	309	CLA	1	0
17	8	309	CLA	1	0
17	3	324	CLA	3	0
17	1	609	CLA	3	0
17	B	823	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	825	CLA	3	0
17	1	605	CLA	5	0
17	8	303	CLA	3	0
20	L	204	BCR	4	0
16	c	304	CHL	7	0
29	C	102	SF4	1	0
17	3	312	CLA	1	0
17	B	820	CLA	2	0
16	7	305	CHL	4	0
17	A	5006	CLA	2	0
16	T	416	CHL	7	0
17	B	810	CLA	2	0
20	a	617	BCR	4	0
23	B	848	DGD	8	0
20	A	5047	BCR	2	0
17	B	836	CLA	4	0
17	8	311	CLA	2	0
17	F	5009	CLA	1	0
17	3	305	CLA	4	0
17	A	5035	CLA	5	0
17	a	612	CLA	2	0
20	F	5005	BCR	5	0
20	F	5010	BCR	4	0
17	B	814	CLA	1	0
17	B	827	CLA	5	0
17	c	302	CLA	1	0
21	a	618	LHG	1	0
25	7	319	LMU	3	0
16	3	301	CHL	10	0
20	3	319	BCR	2	0
16	b	607	CHL	4	0
17	A	5010	CLA	3	0
17	A	5004	CLA	11	0
17	1	612	CLA	2	0
17	B	818	CLA	9	0
16	8	308	CHL	4	0
17	B	829	CLA	7	0
20	K	205	BCR	5	0
20	c	316	BCR	2	0
21	1	618	LHG	1	0
17	A	5044	CLA	7	0
17	A	5041	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	c	306	CHL	14	0
17	3	323	CLA	3	0
17	T	403	CLA	2	0
16	c	305	CHL	4	0
17	7	309	CLA	1	0
17	B	817	CLA	4	0
17	B	831	CLA	1	0
17	b	602	CLA	3	0
17	c	308	CLA	4	0
17	A	5019	CLA	8	0
17	B	807	CLA	4	0
17	7	308	CLA	2	0
17	8	302	CLA	3	0
17	7	312	CLA	6	0
17	b	604	CLA	2	0
17	B	819	CLA	3	0
17	c	301	CLA	7	0
17	1	604	CLA	6	0
20	3	317	BCR	3	0
24	7	301	LMG	5	0
17	a	602	CLA	1	0
20	B	843	BCR	2	0
17	A	5012	CLA	2	0
17	A	5014	CLA	8	0
16	a	606	CHL	1	0
20	8	318	BCR	5	0
21	1	619	LHG	1	0
17	1	608	CLA	2	0
17	A	5026	CLA	3	0
17	c	303	CLA	3	0
17	T	410	CLA	1	0
24	A	5001	LMG	2	0
17	T	404	CLA	3	0
17	F	5006	CLA	1	0
17	3	304	CLA	1	0
17	a	604	CLA	4	0
20	L	203	BCR	2	0
17	7	313	CLA	2	0
17	a	609	CLA	2	0
20	A	5048	BCR	6	0
17	A	5020	CLA	4	0
17	J	102	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	7	316	XAT	6	0
17	B	822	CLA	2	0
16	3	322	CHL	6	0
17	B	803	CLA	8	0
20	B	847	BCR	2	0
17	3	308	CLA	1	0
16	7	306	CHL	4	0
16	7	307	CHL	4	0
17	8	305	CLA	3	0
17	b	613	CLA	1	0
17	a	613	CLA	1	0
28	A	5045	PQN	2	0
17	A	5031	CLA	2	0
21	8	321	LHG	2	0
21	A	5055	LHG	2	0
18	8	316	LUT	1	0
27	A	5003	CL0	8	0
17	3	306	CLA	2	0
17	b	601	CLA	3	0
17	A	5028	CLA	6	0
18	3	315	LUT	3	0
17	3	314	CLA	1	0
21	A	5053	LHG	5	0
16	1	606	CHL	2	0
17	8	313	CLA	2	0
17	F	5007	CLA	2	0
17	B	840	CLA	2	0
20	B	845	BCR	3	0
16	8	307	CHL	2	0
16	a	601	CHL	2	0
17	K	204	CLA	2	0
17	A	5040	CLA	1	0
17	A	5011	CLA	6	0
20	A	5051	BCR	3	0
17	1	614	CLA	1	0
17	1	611	CLA	1	0
17	B	812	CLA	1	0
17	b	609	CLA	2	0
20	B	801	BCR	3	0
23	8	301	DGD	2	0
17	B	838	CLA	2	0
17	b	612	CLA	1	0

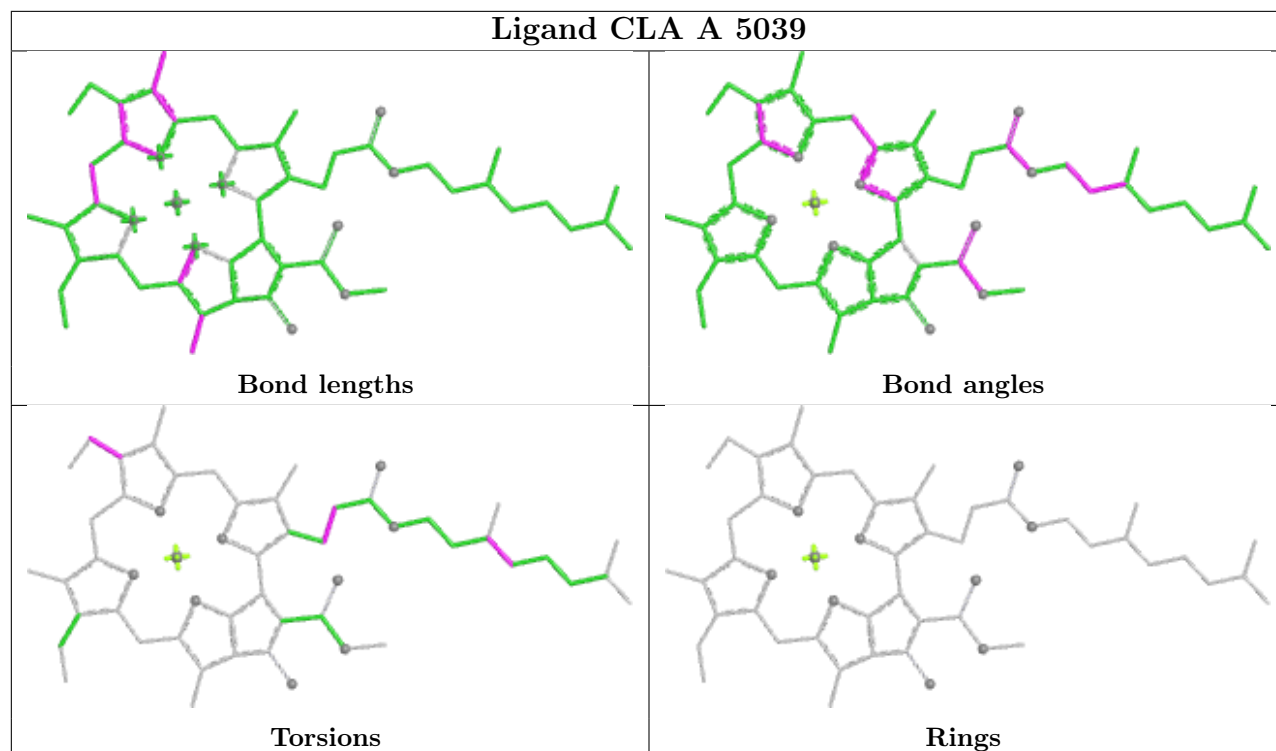
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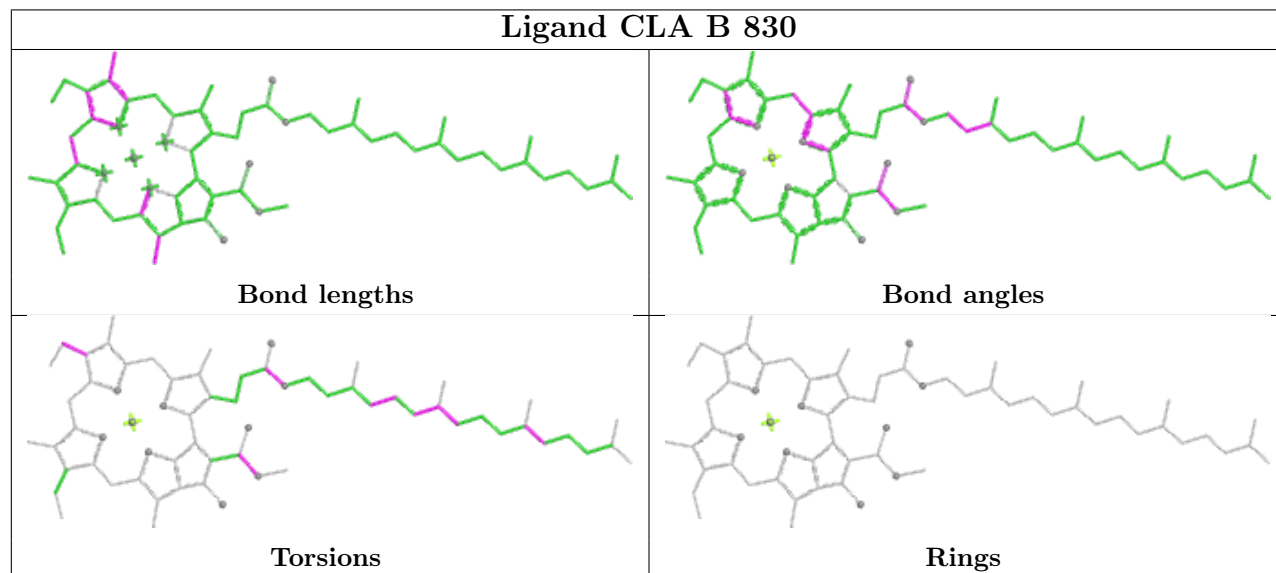
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	406	CLA	2	0
19	T	414	XAT	2	0
17	3	302	CLA	4	0
17	1	613	CLA	1	0
20	A	5050	BCR	5	0
16	b	606	CHL	3	0
17	A	5007	CLA	3	0
17	A	5032	CLA	3	0
17	B	841	CLA	3	0
17	B	809	CLA	5	0
17	T	408	CLA	1	0
17	a	611	CLA	1	0
17	B	821	CLA	2	0
17	A	5005	CLA	6	0
17	A	5009	CLA	3	0
17	b	610	CLA	1	0
17	7	302	CLA	4	0
20	1	617	BCR	8	0
17	A	5034	CLA	2	0
17	A	5037	CLA	2	0
17	B	811	CLA	2	0
17	A	5029	CLA	9	0
17	B	813	CLA	4	0
17	B	828	CLA	5	0
17	b	611	CLA	2	0
17	b	614	CLA	1	0
16	b	605	CHL	6	0

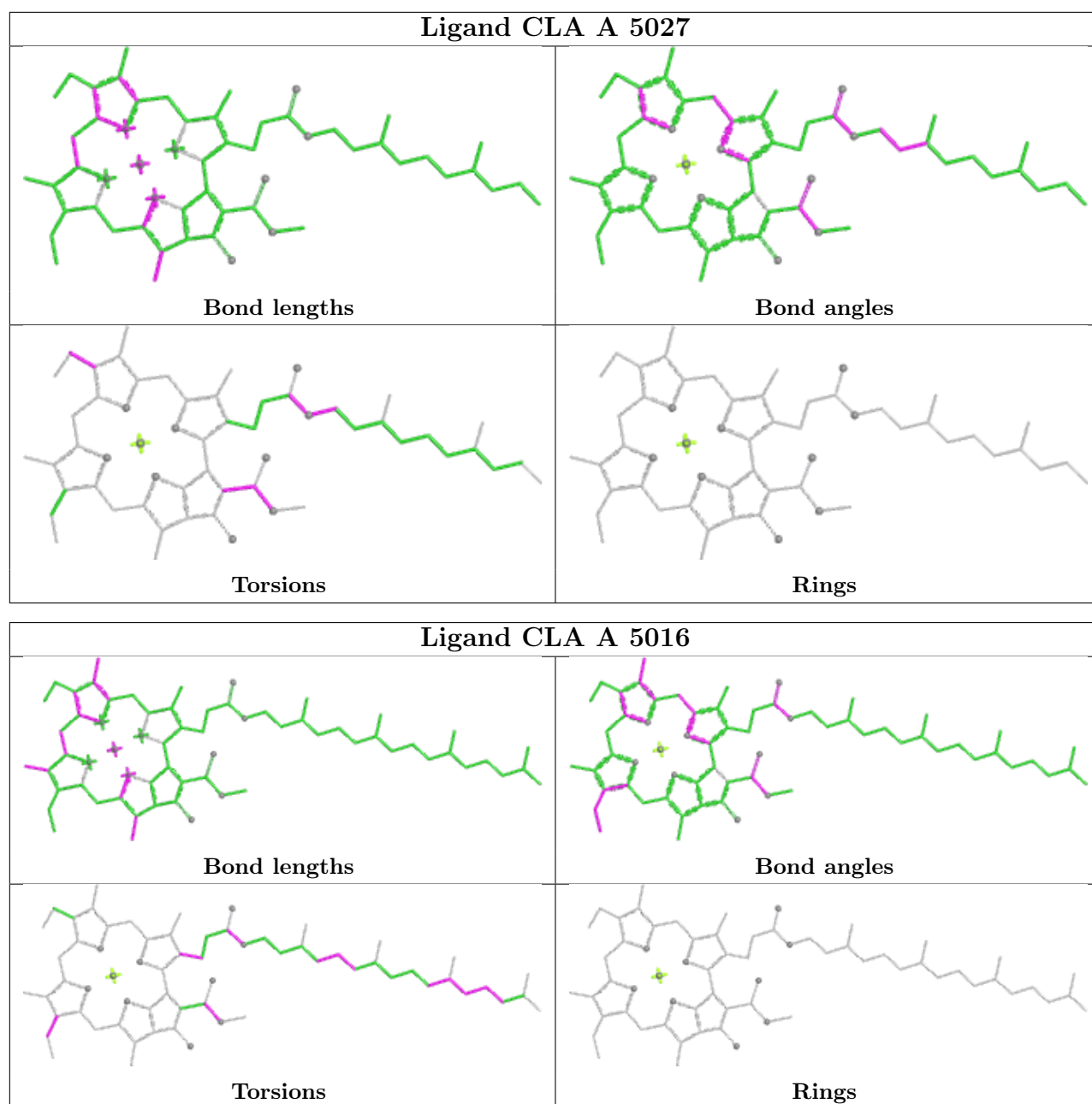
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

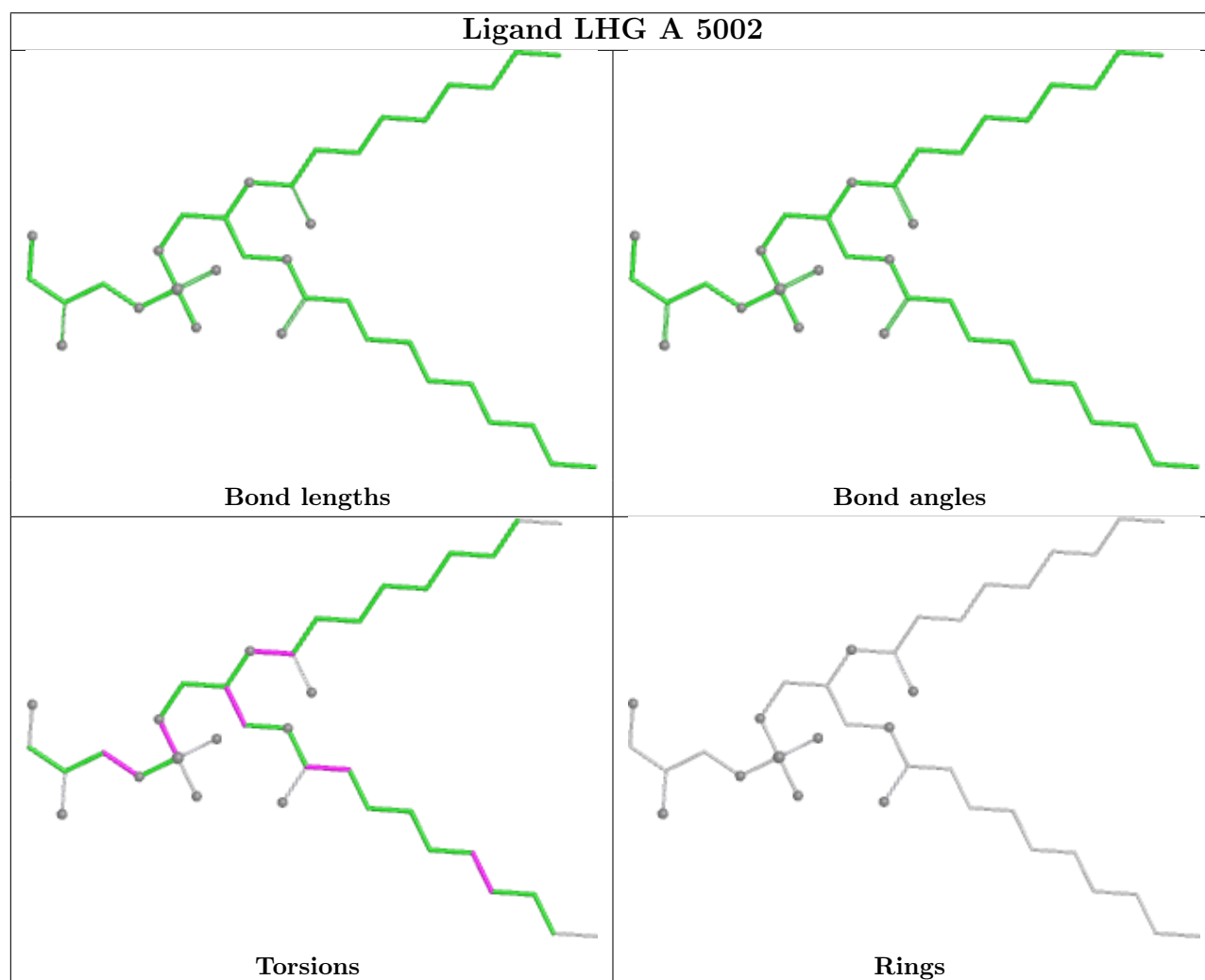
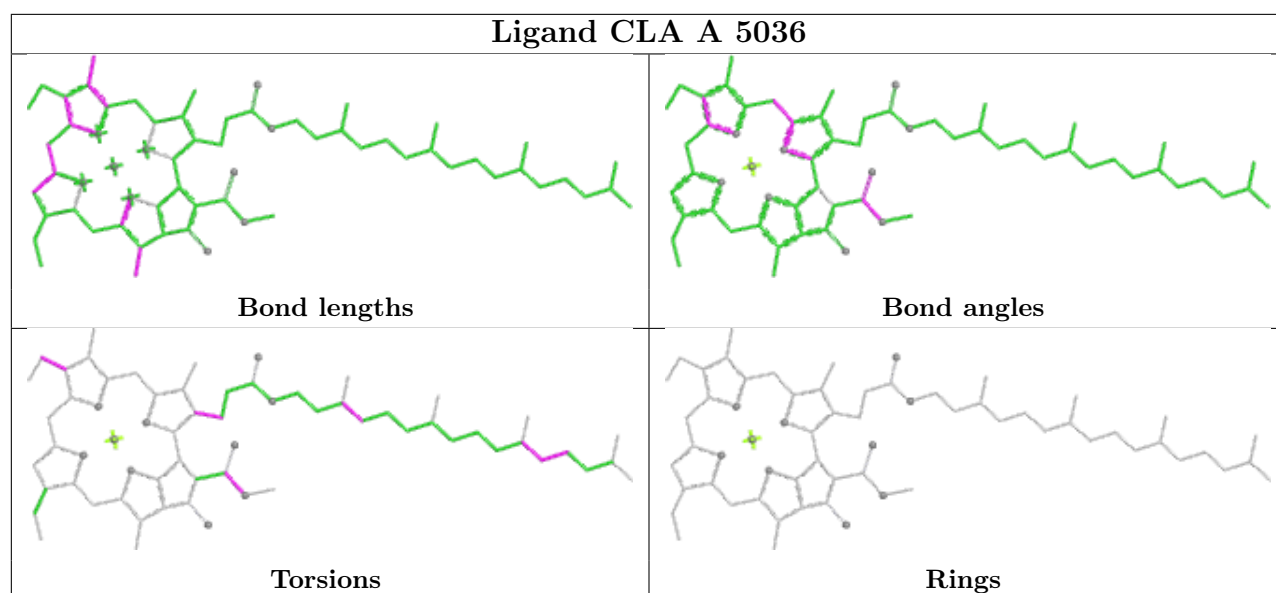
Ligand CLA A 5039



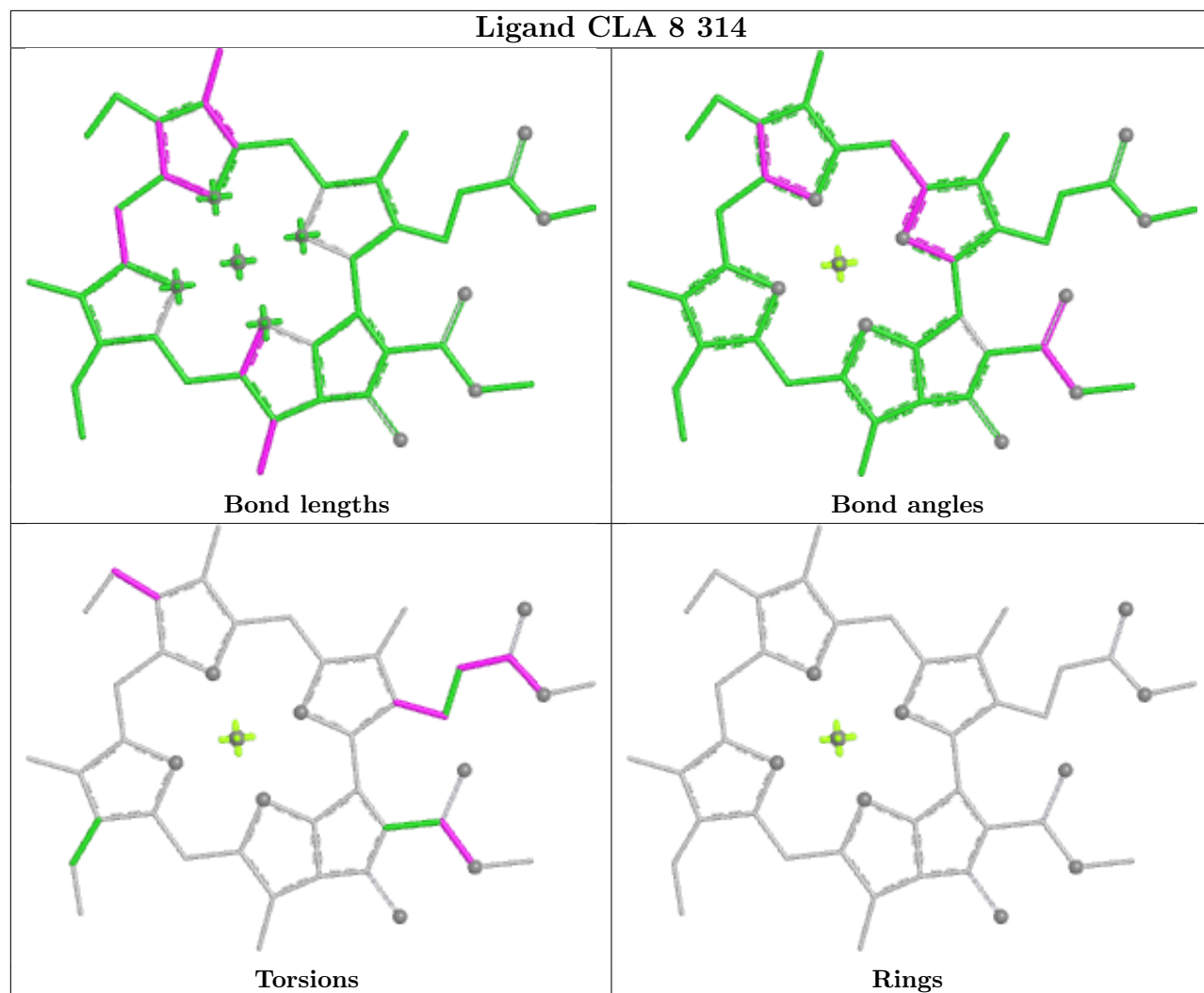
Ligand CLA B 830

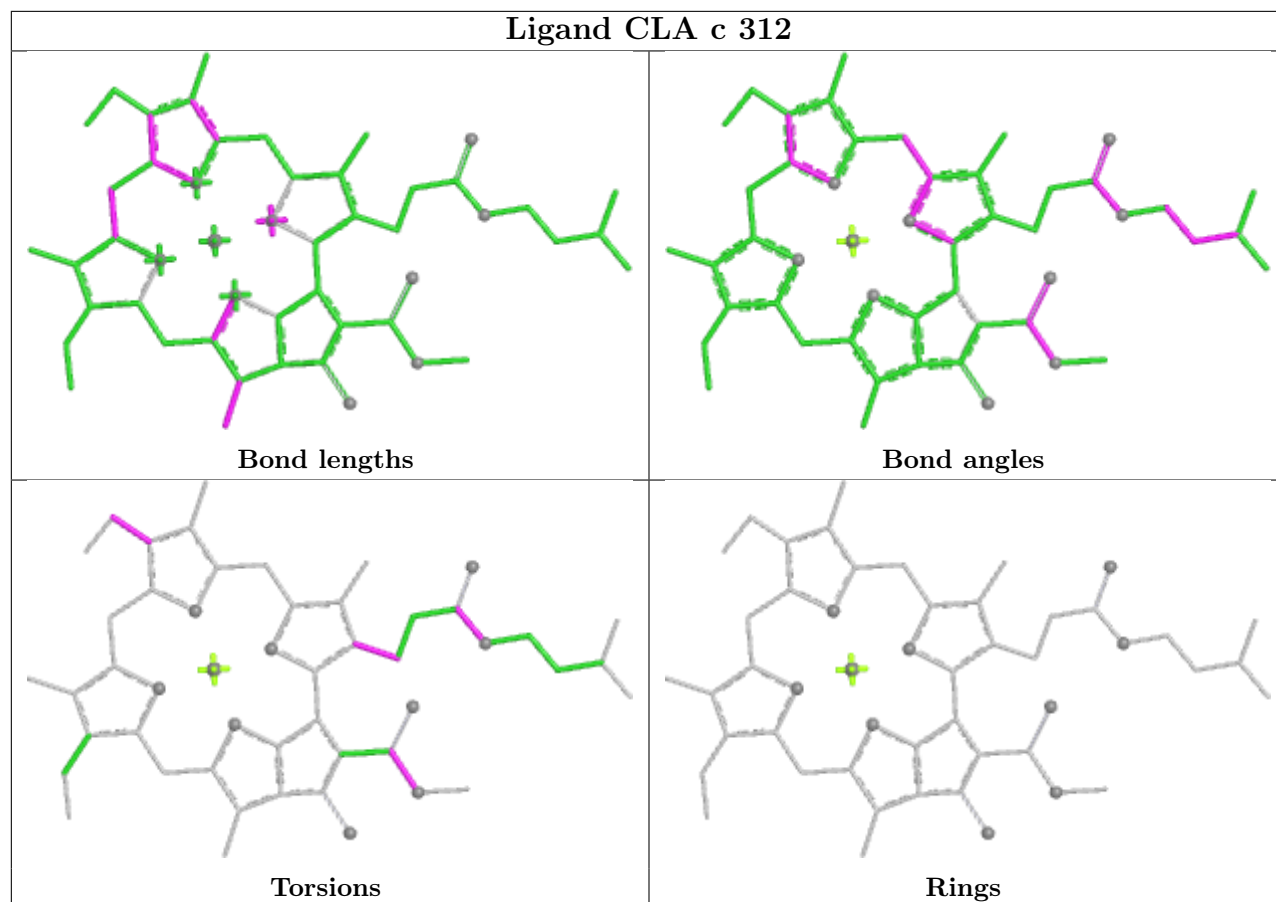




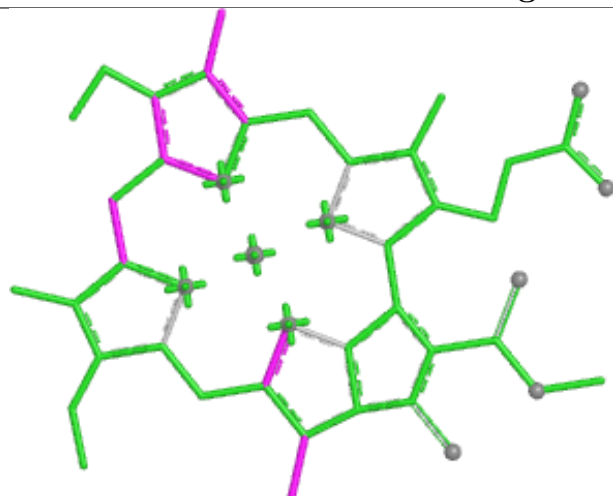


Ligand CLA 8 314

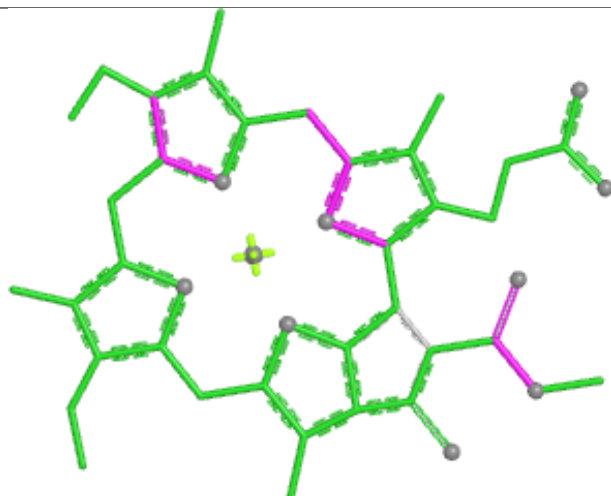




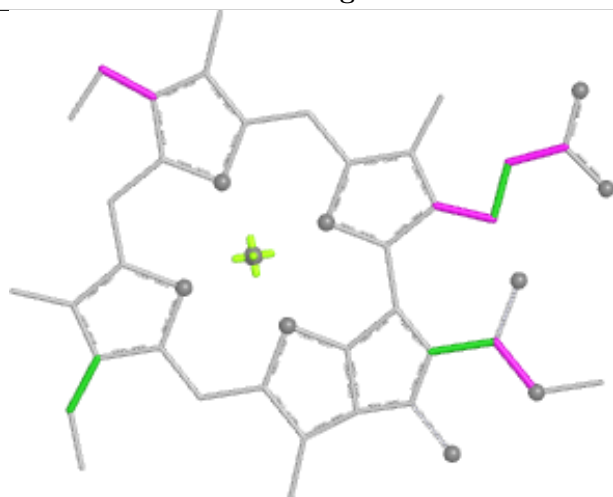
Ligand CLA 8 315



Bond lengths



Bond angles

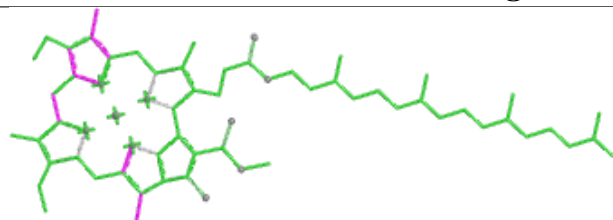


Torsions

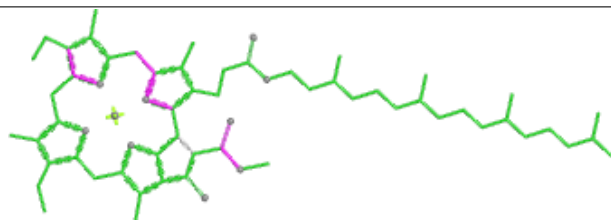


Rings

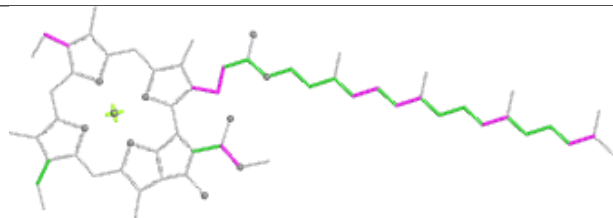
Ligand CLA A 5022



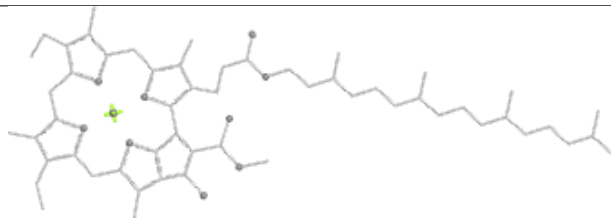
Bond lengths



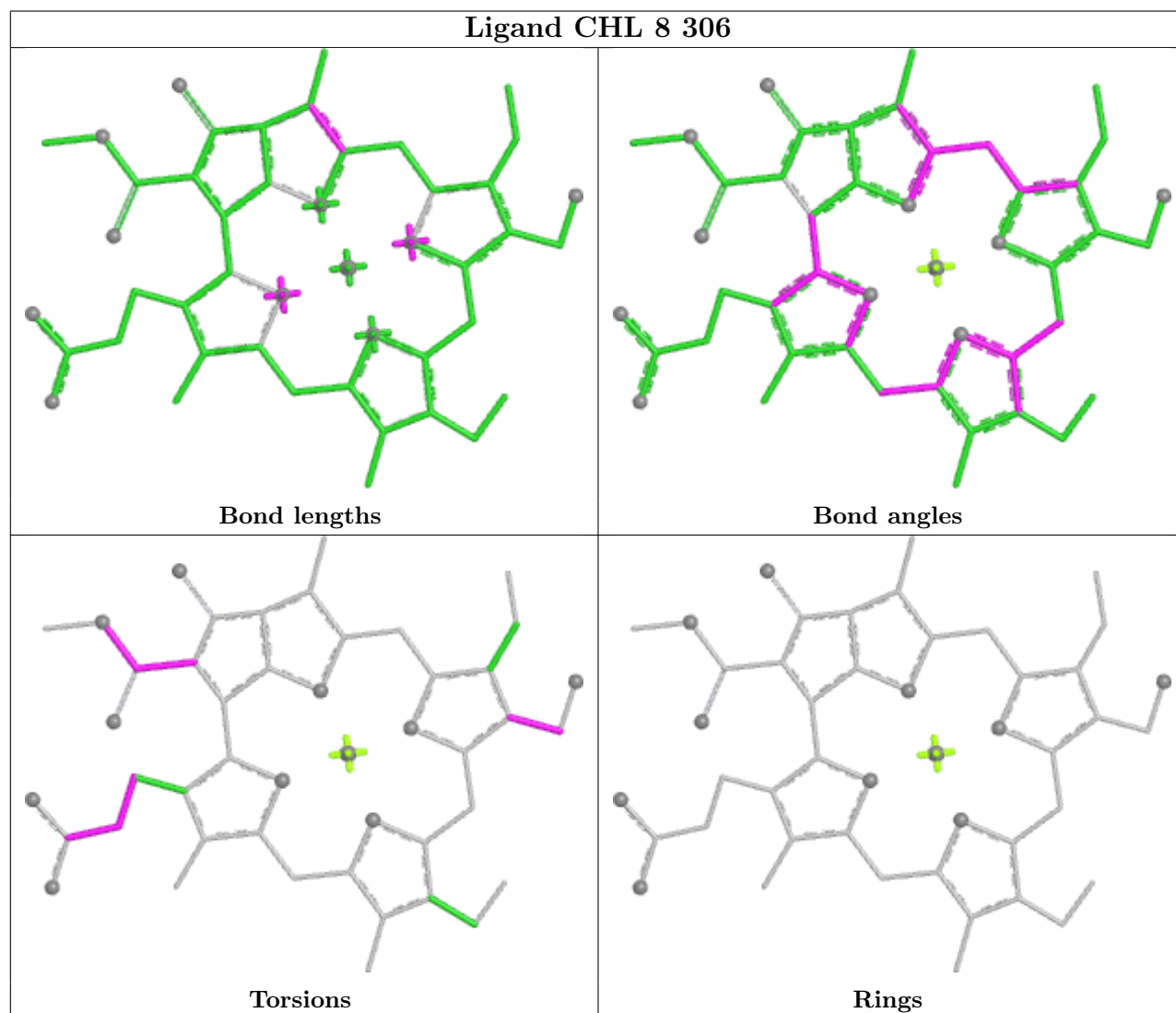
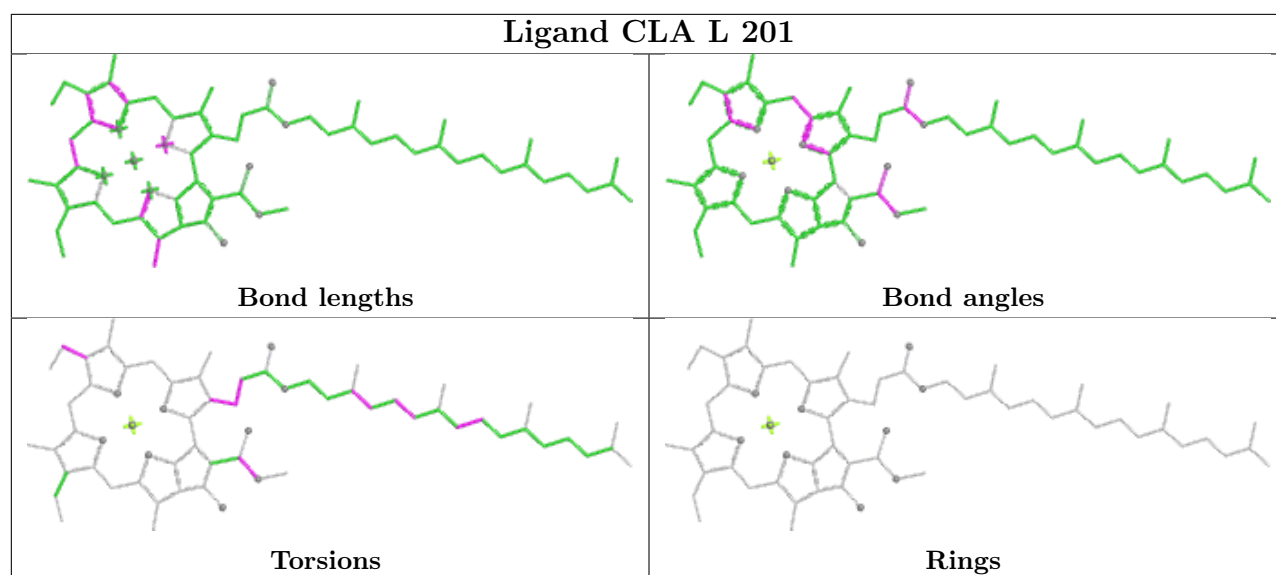
Bond angles



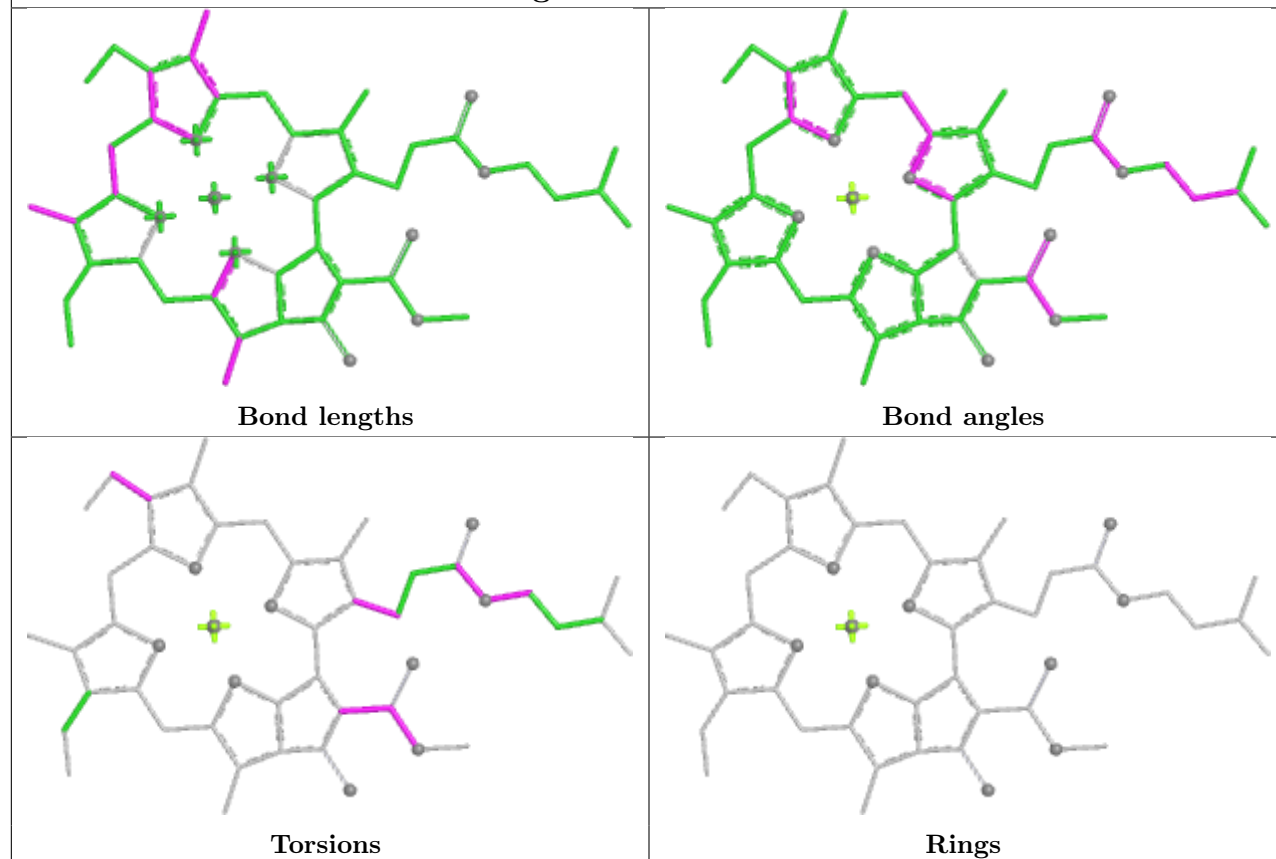
Torsions



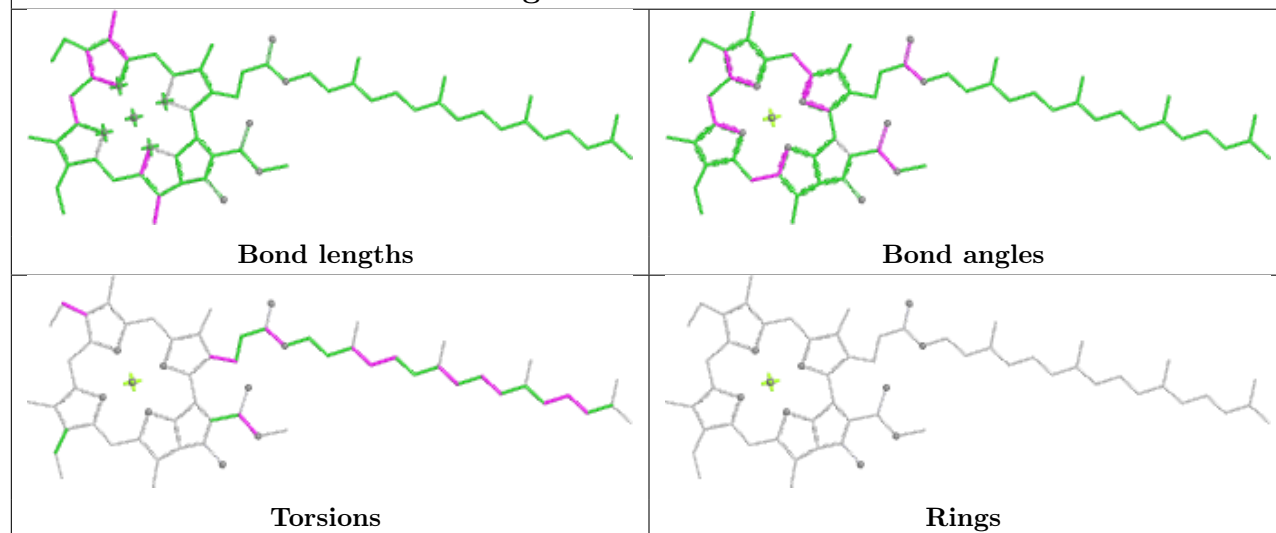
Rings



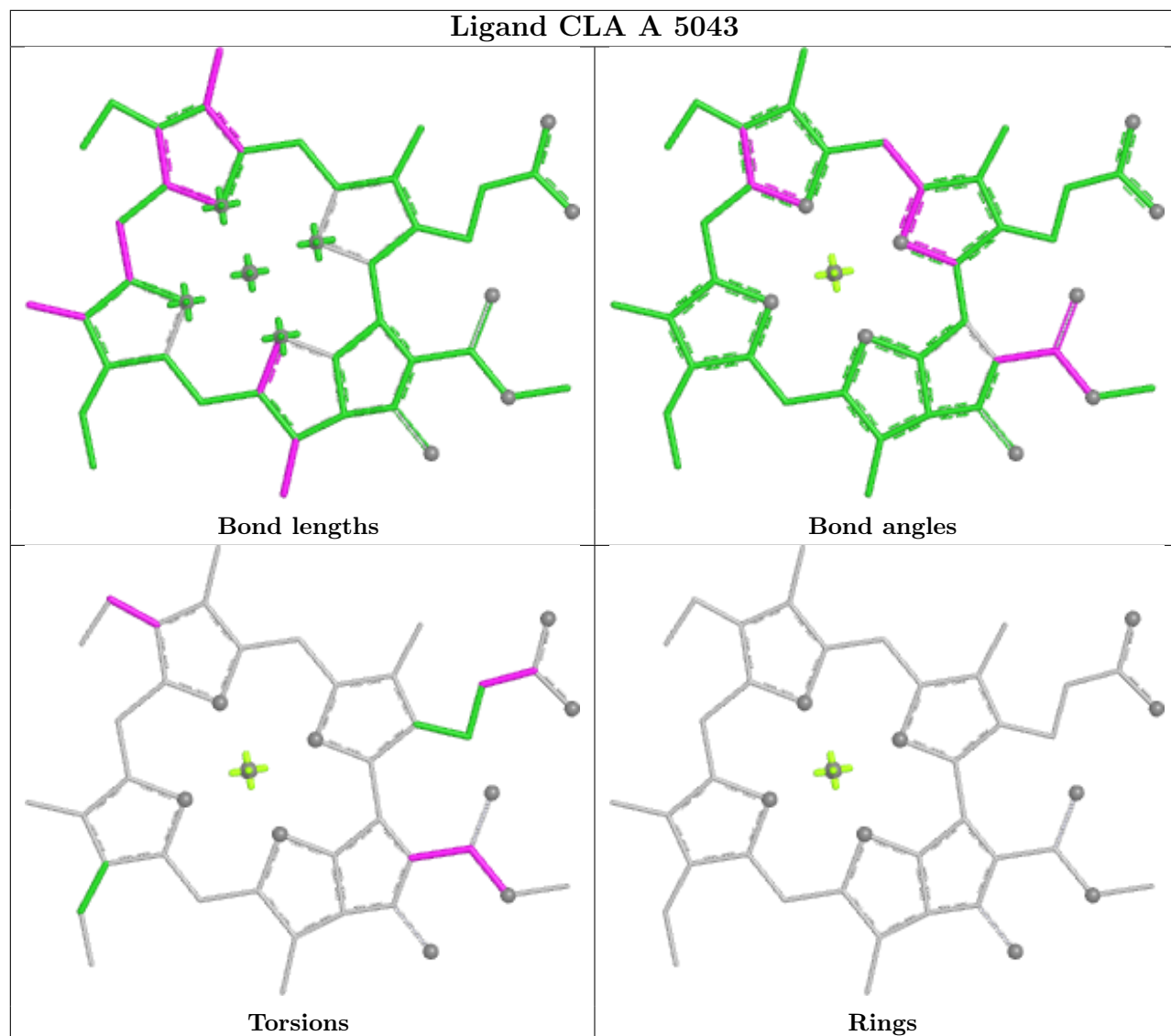
Ligand CLA T 407



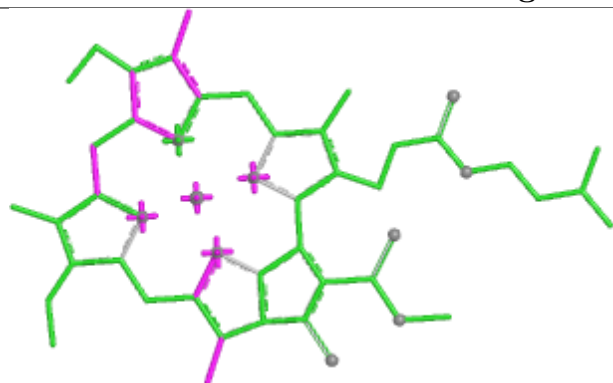
Ligand CLA A 5013



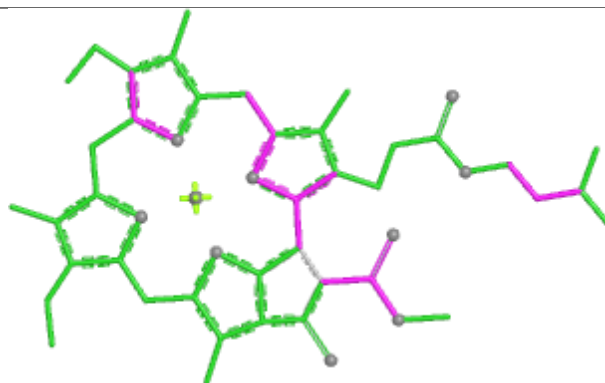
Ligand CLA A 5043



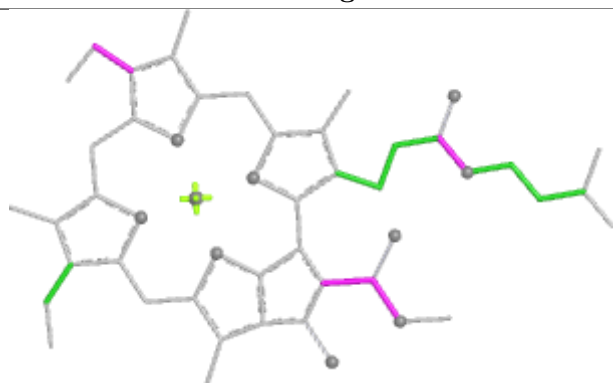
Ligand CLA 8 312



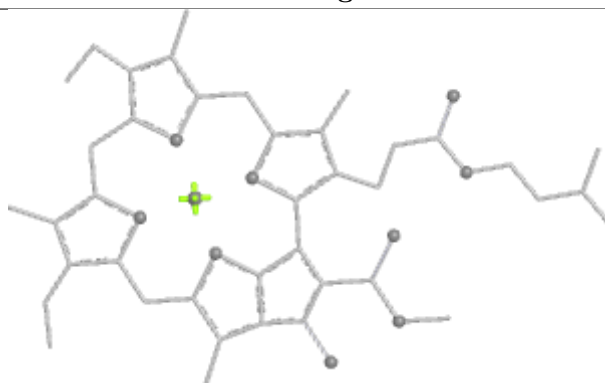
Bond lengths



Bond angles

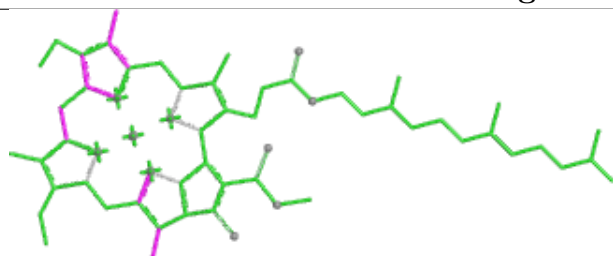


Torsions

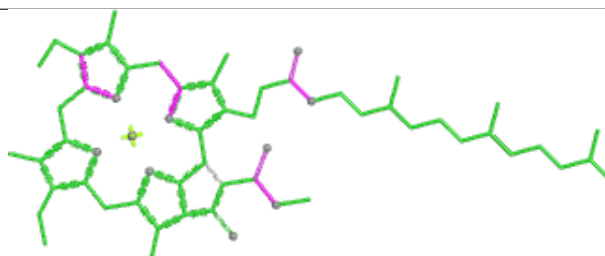


Rings

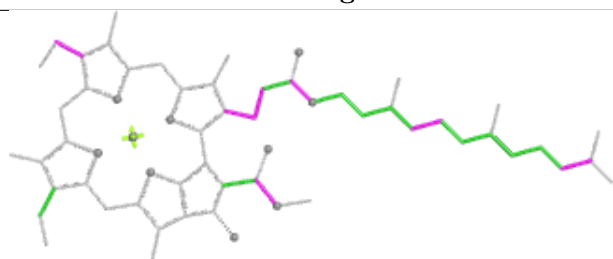
Ligand CLA 8 310



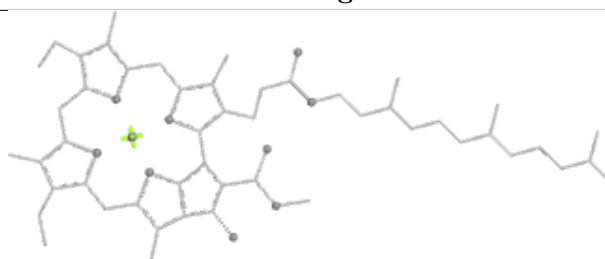
Bond lengths



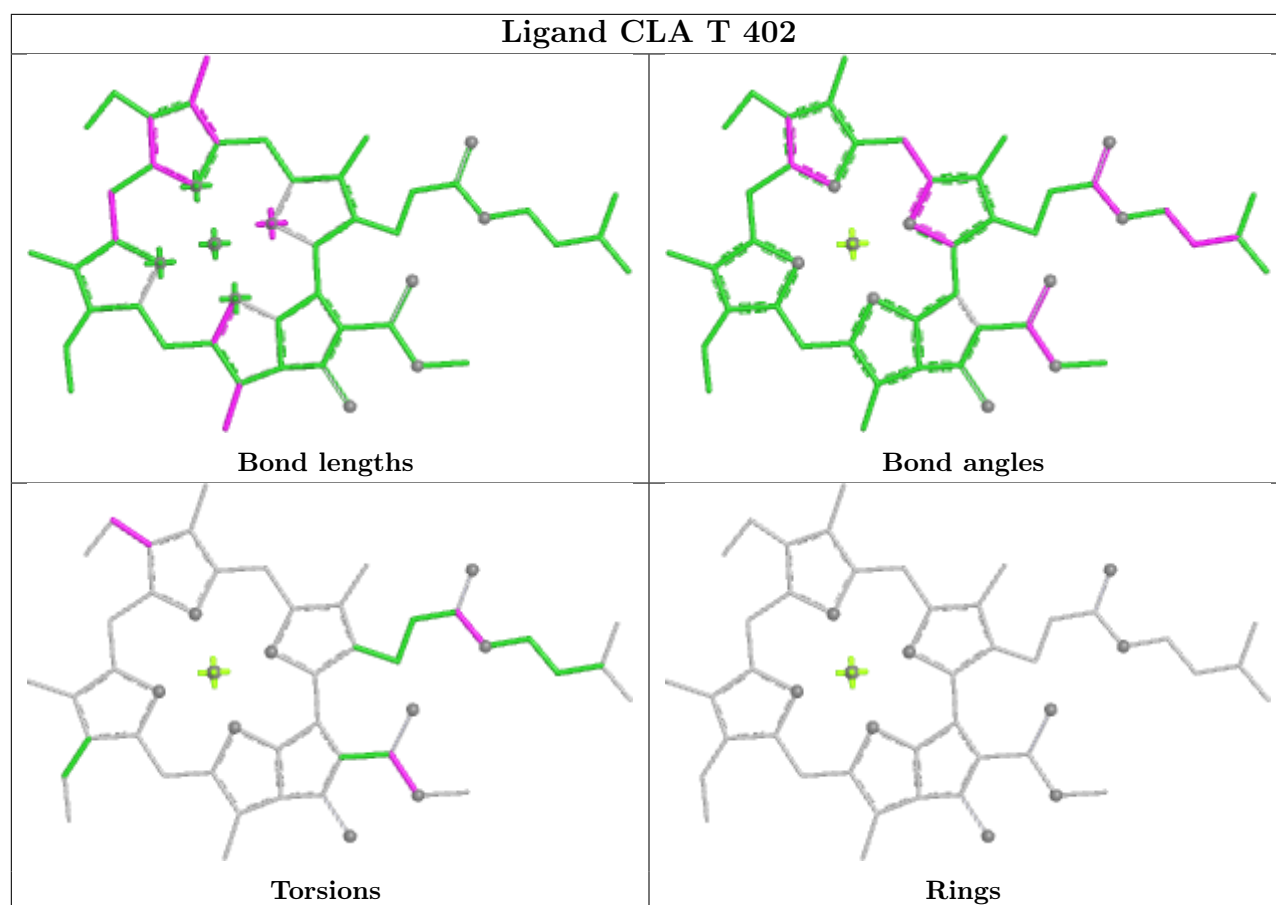
Bond angles



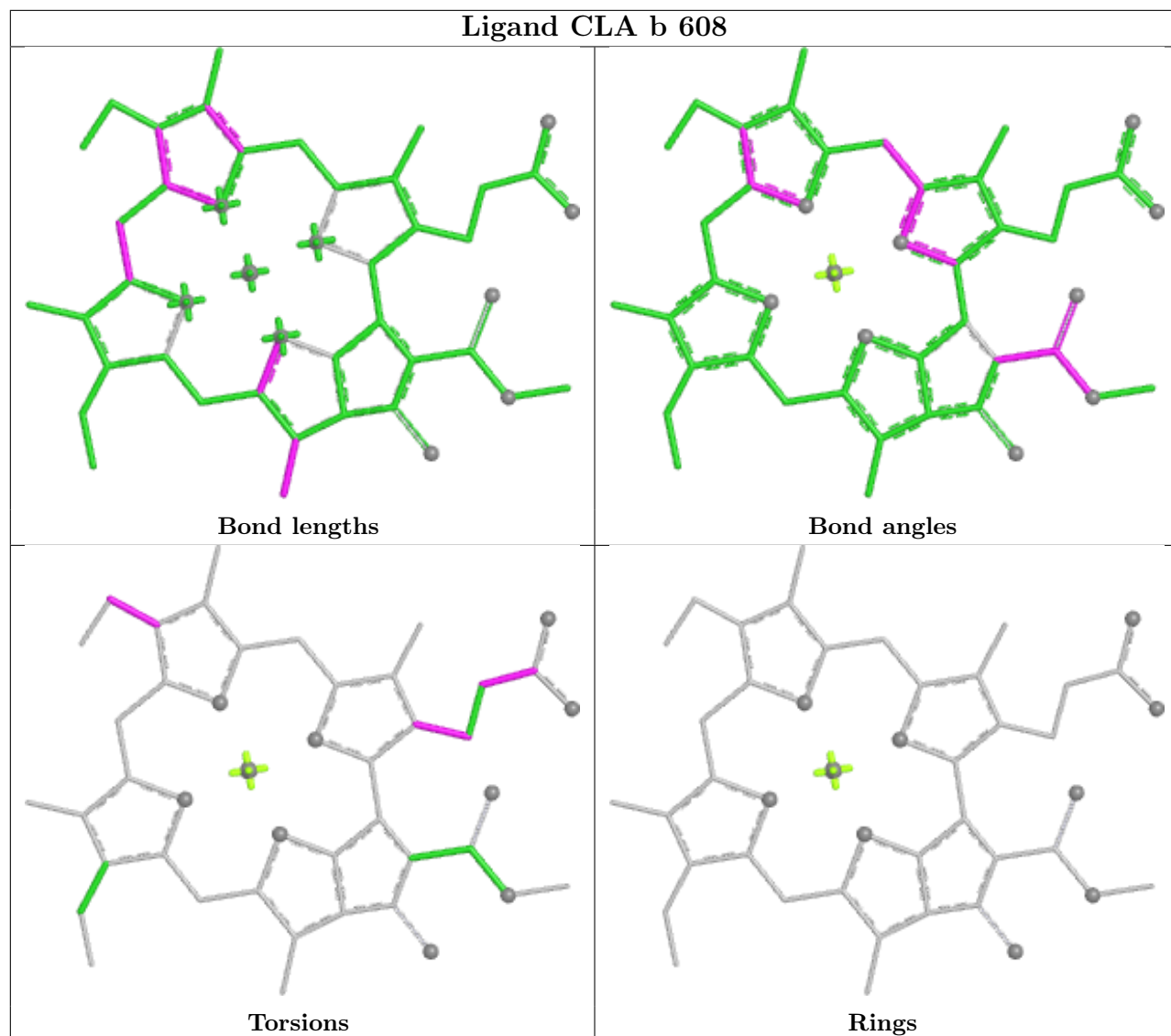
Torsions

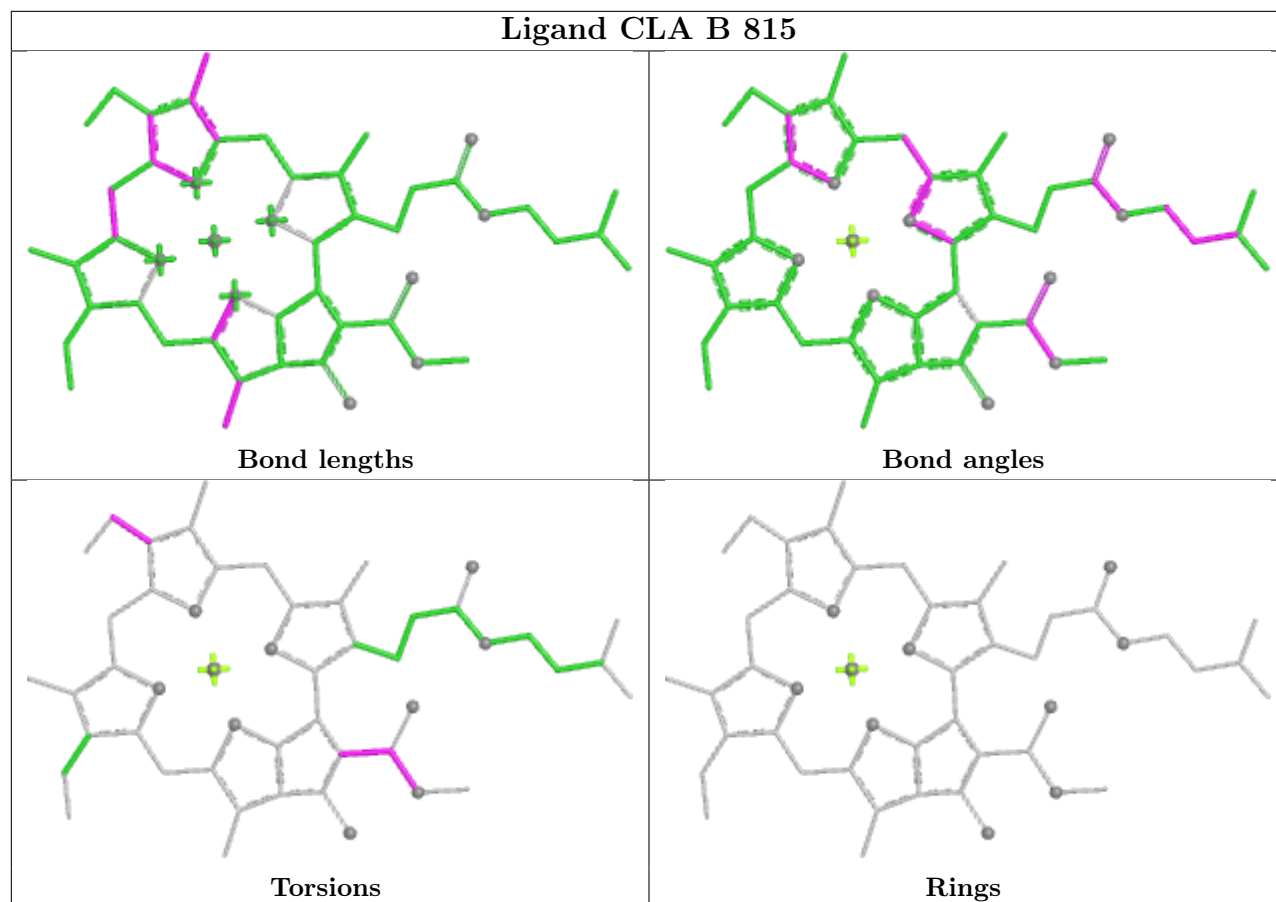


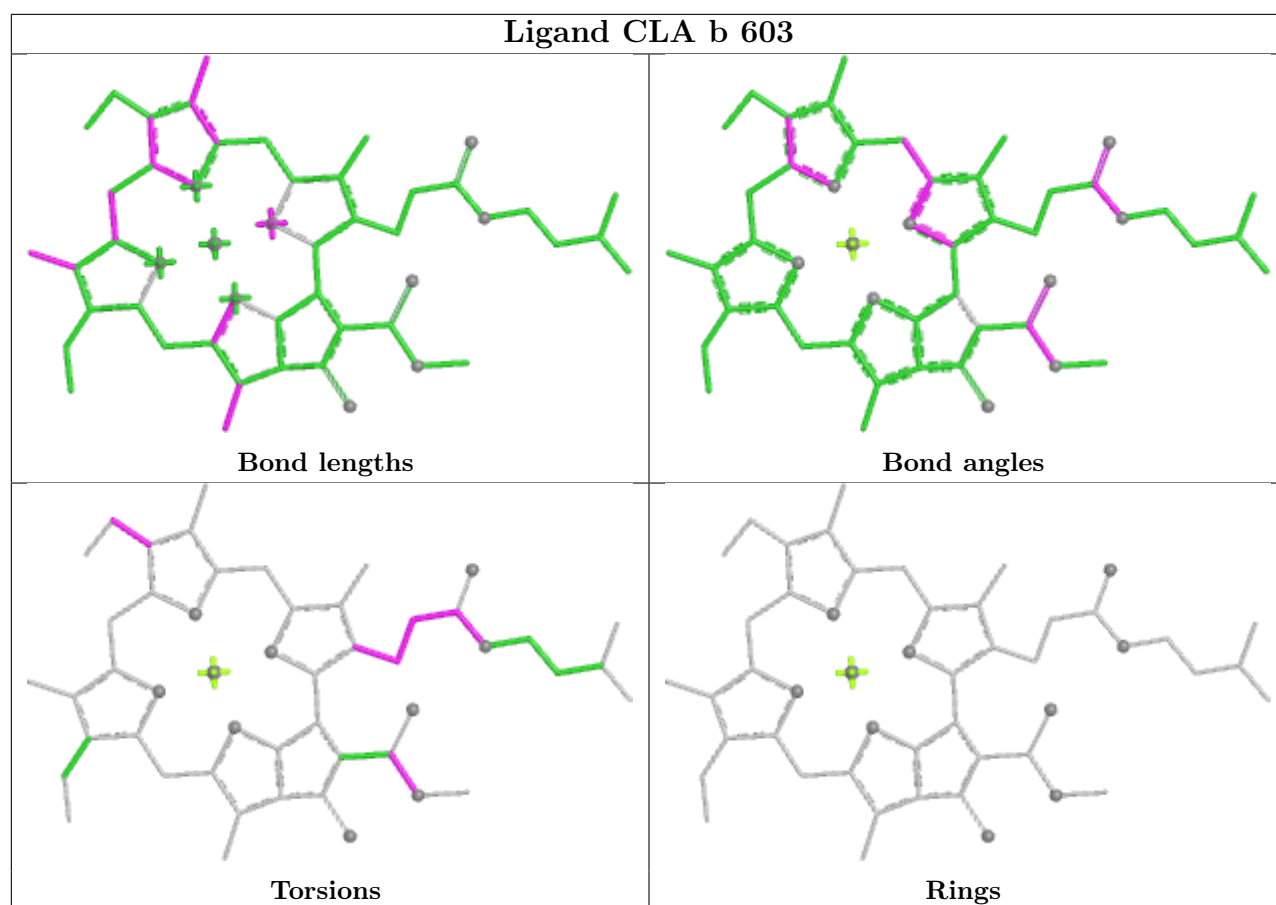
Rings



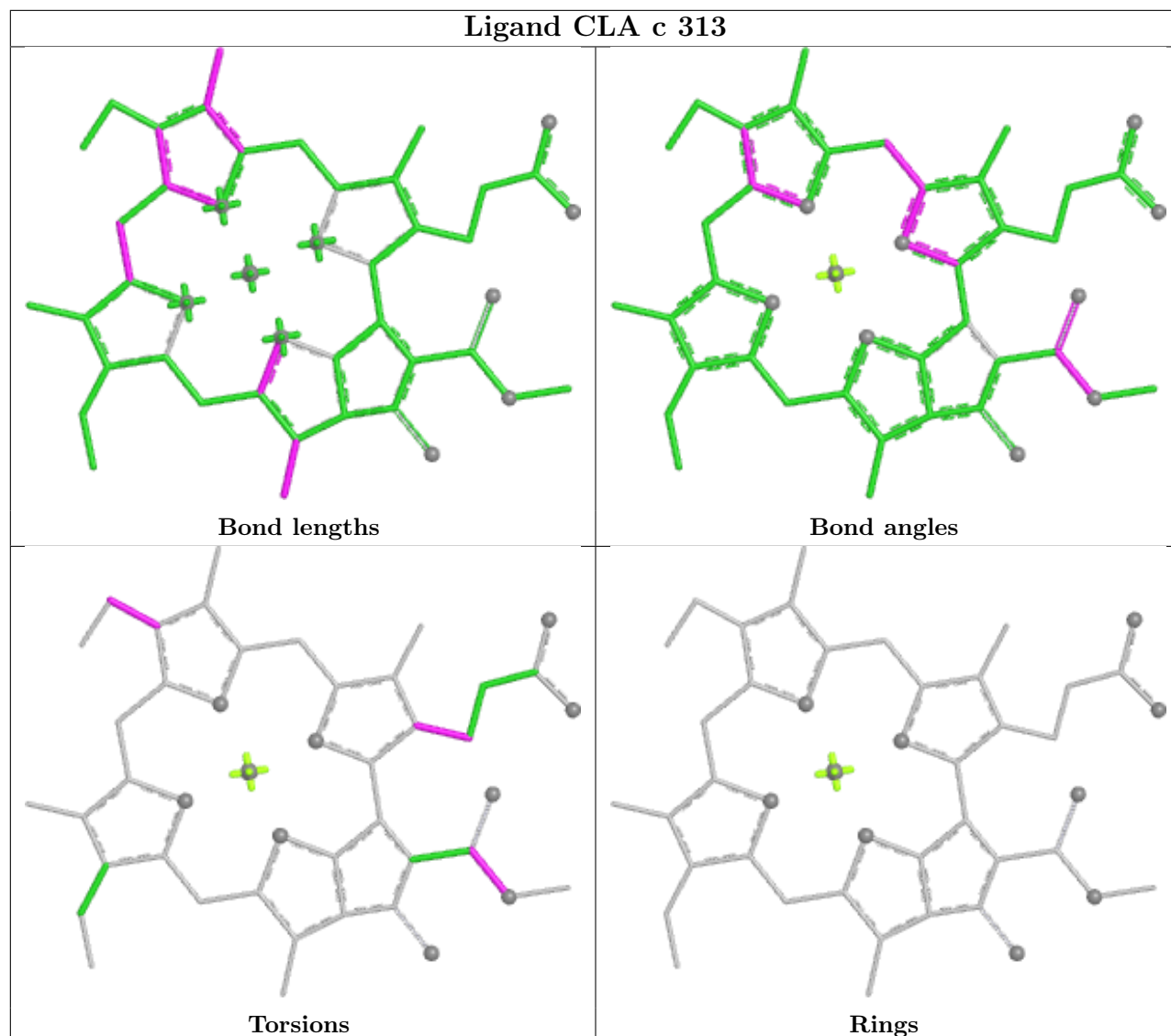
Ligand CLA b 608



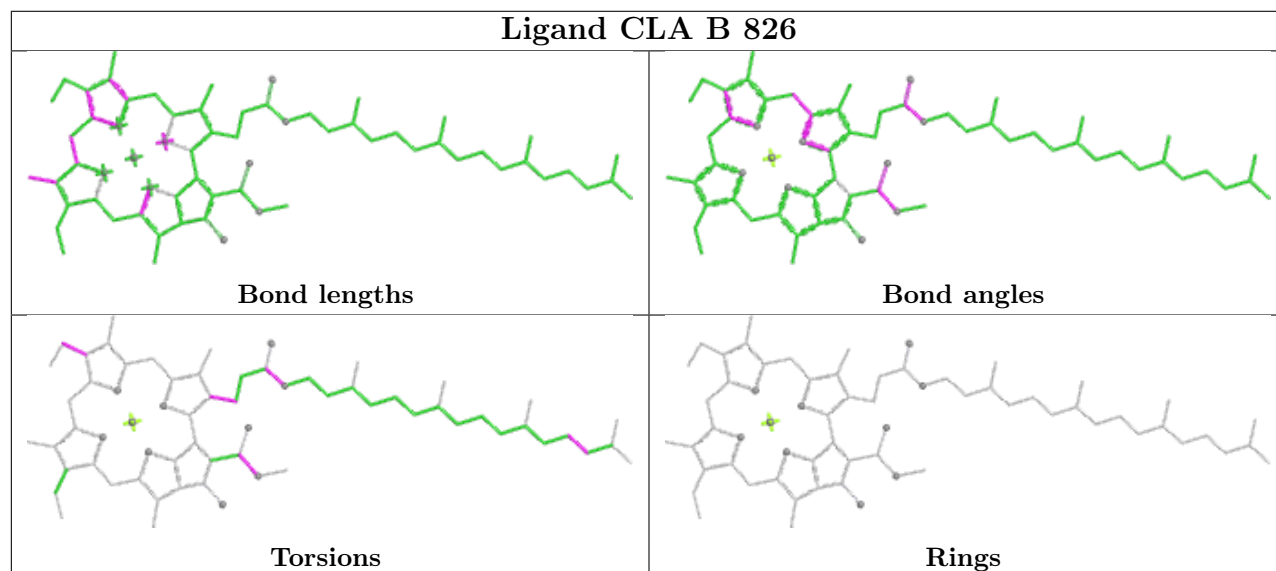


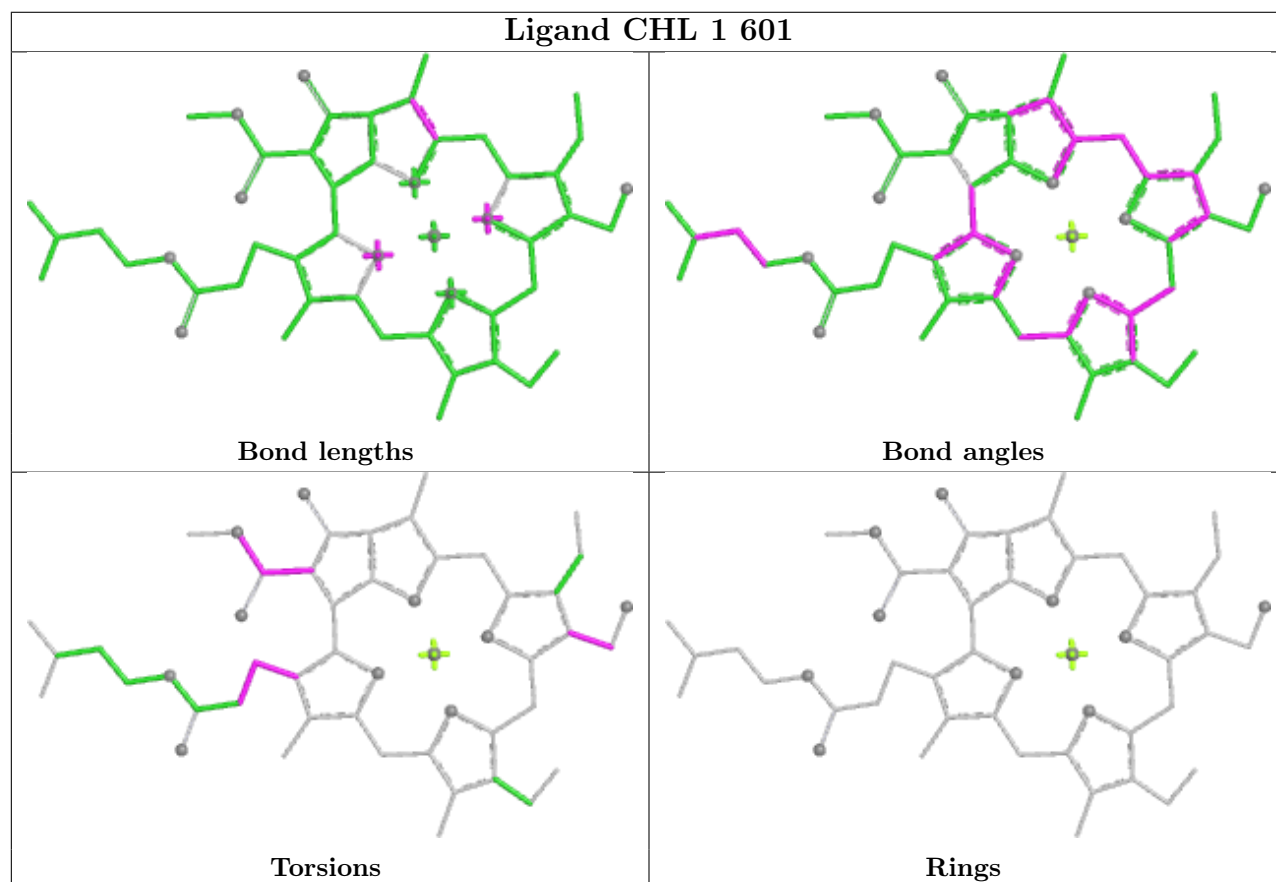
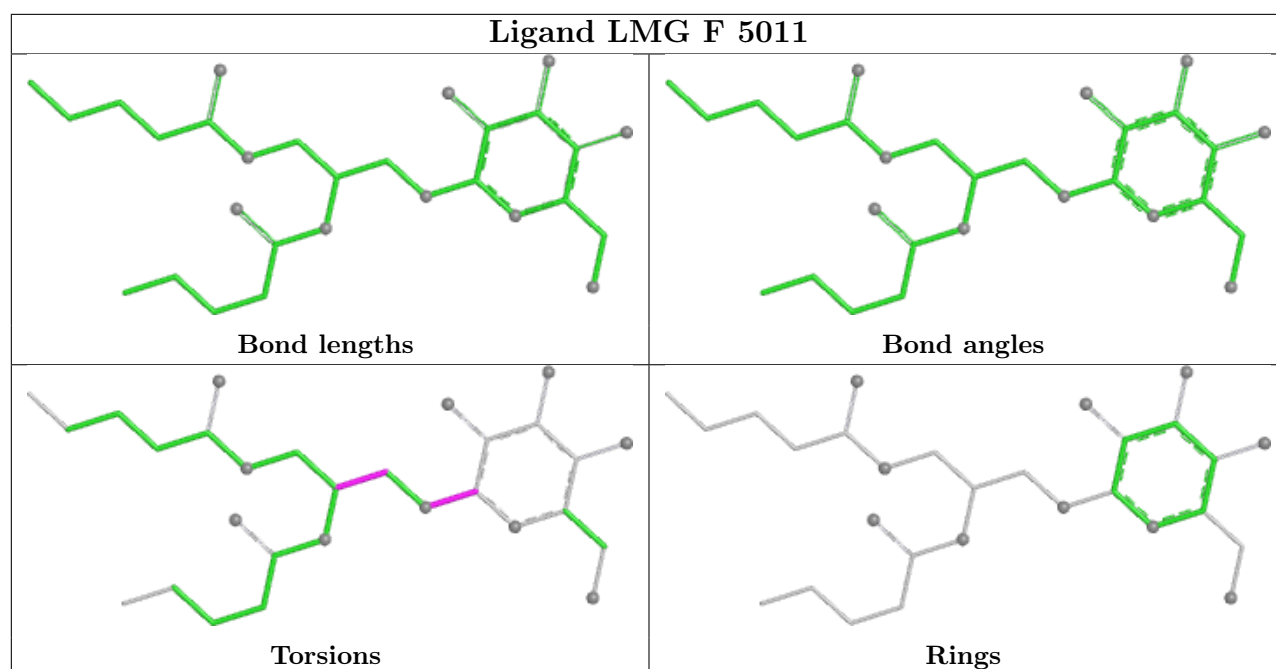


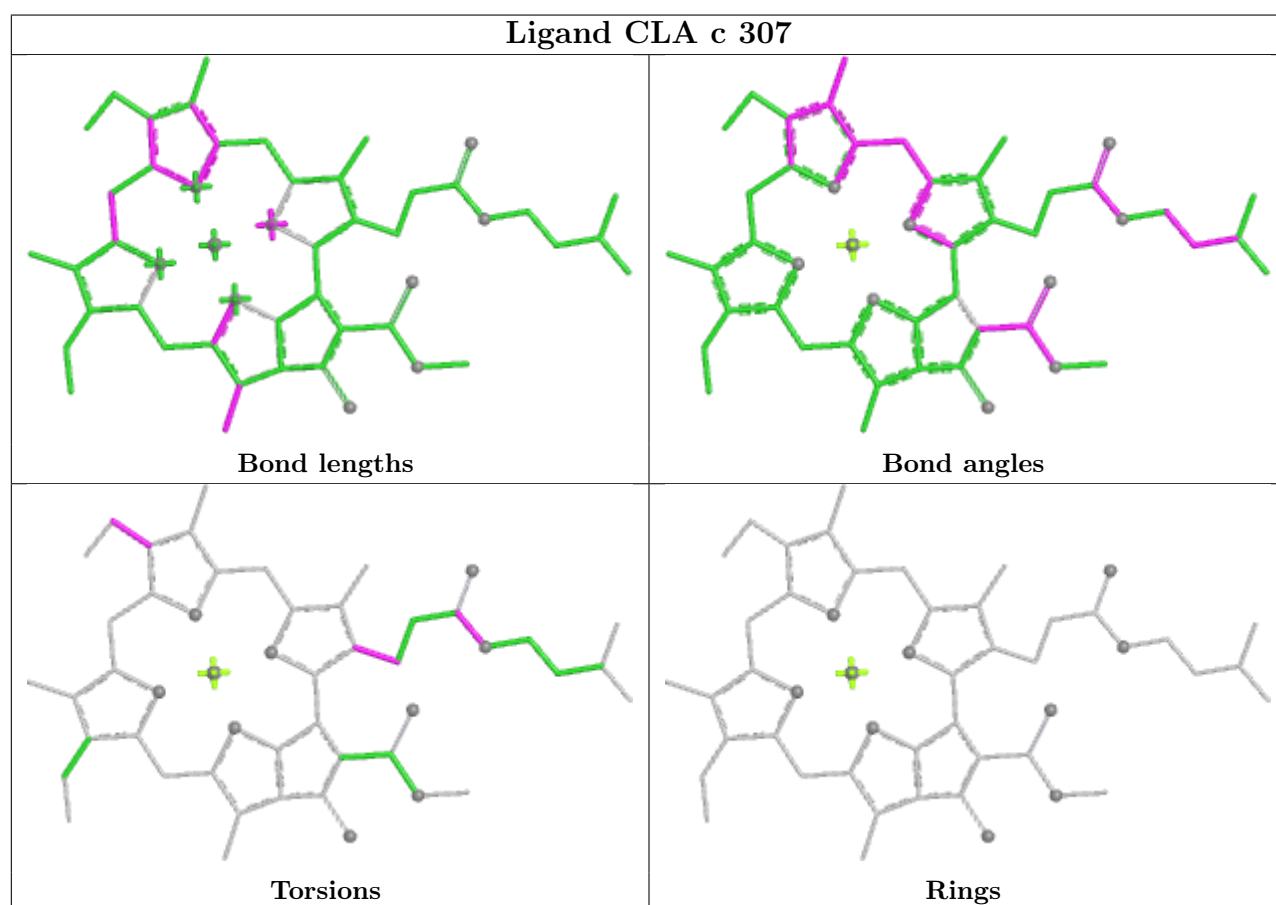
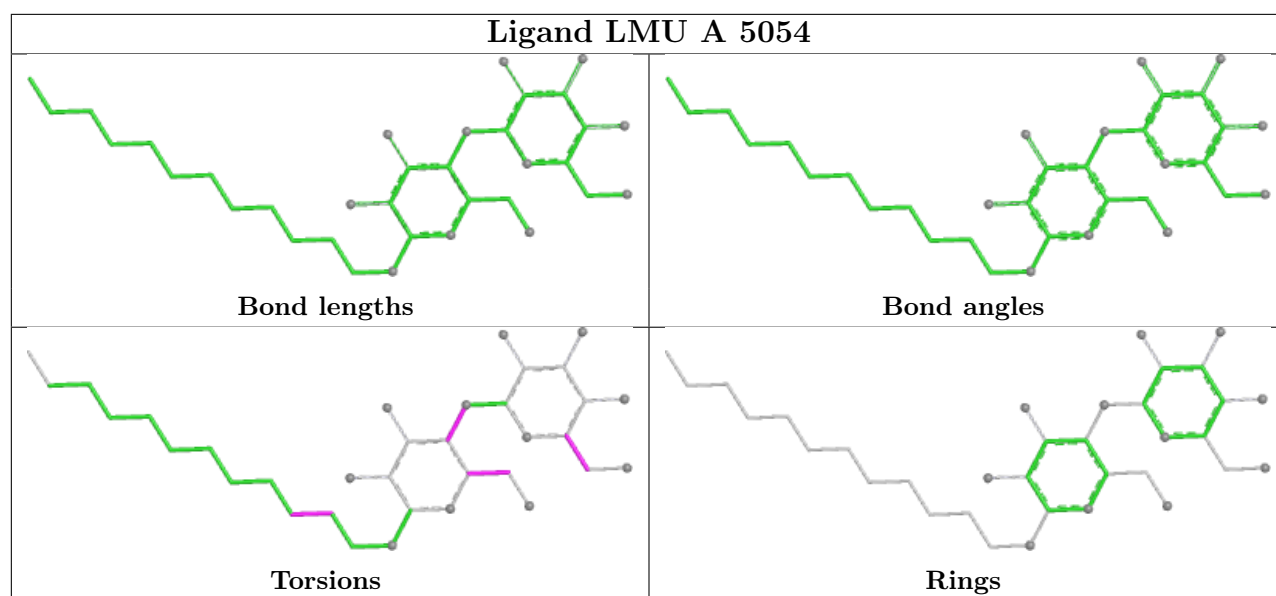
Ligand CLA c 313

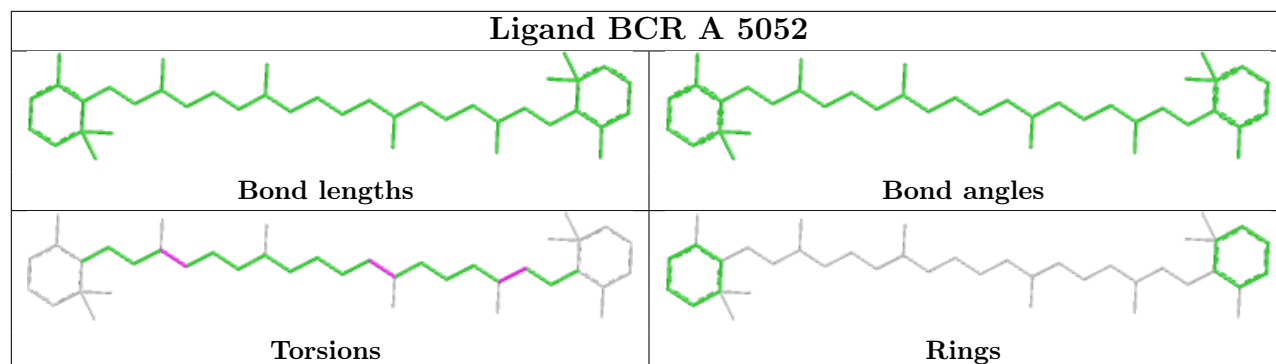
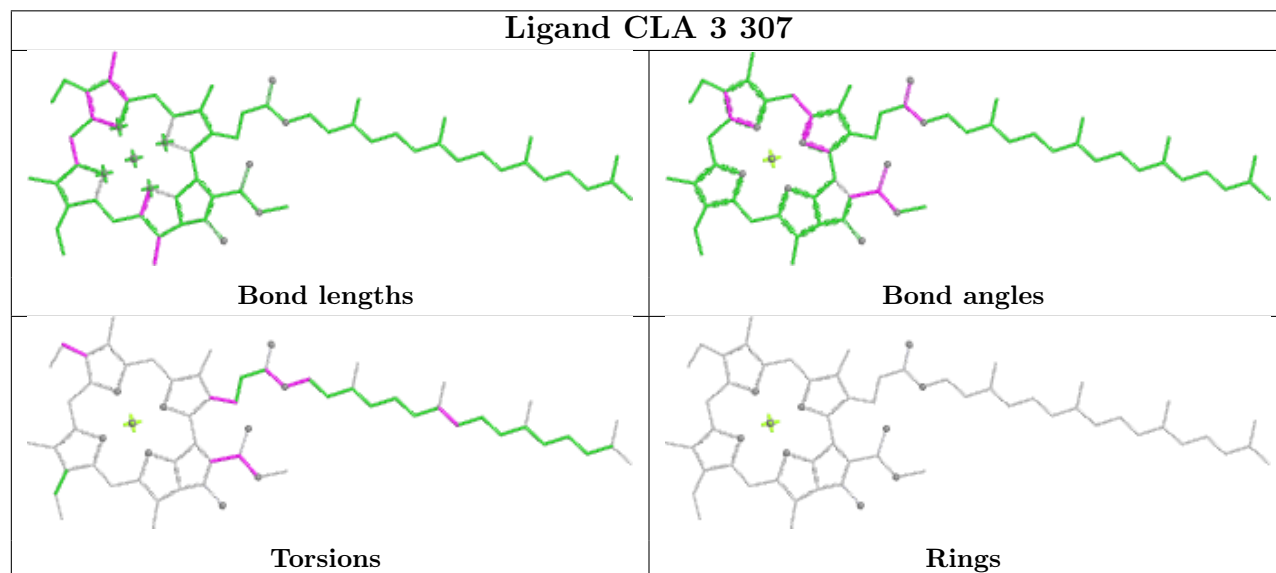
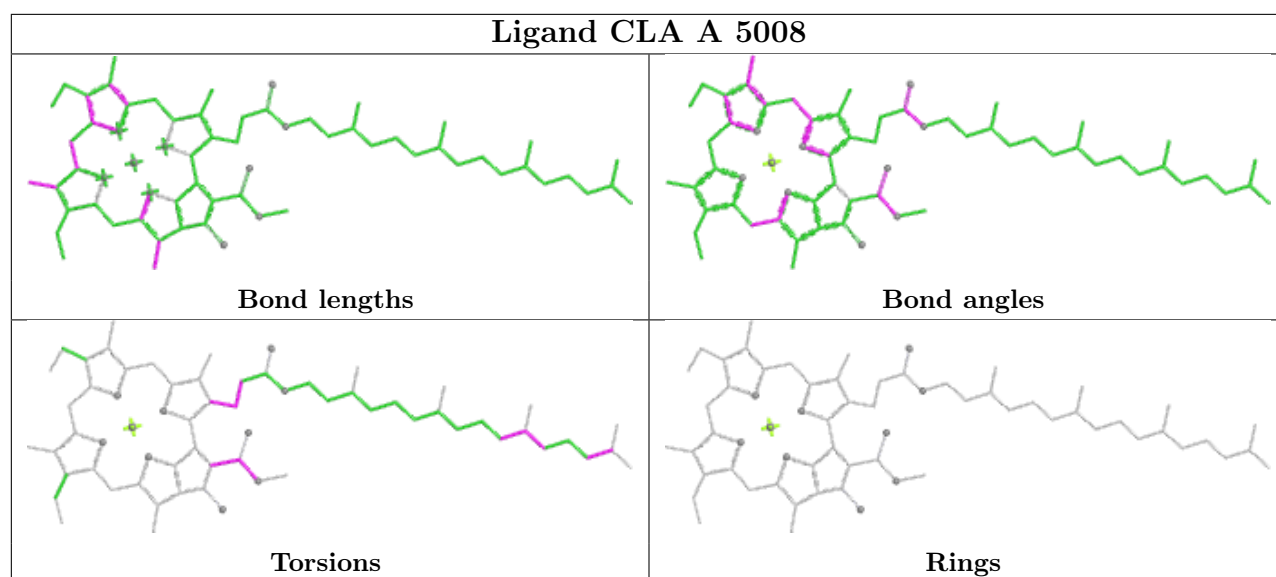


Ligand CLA B 826

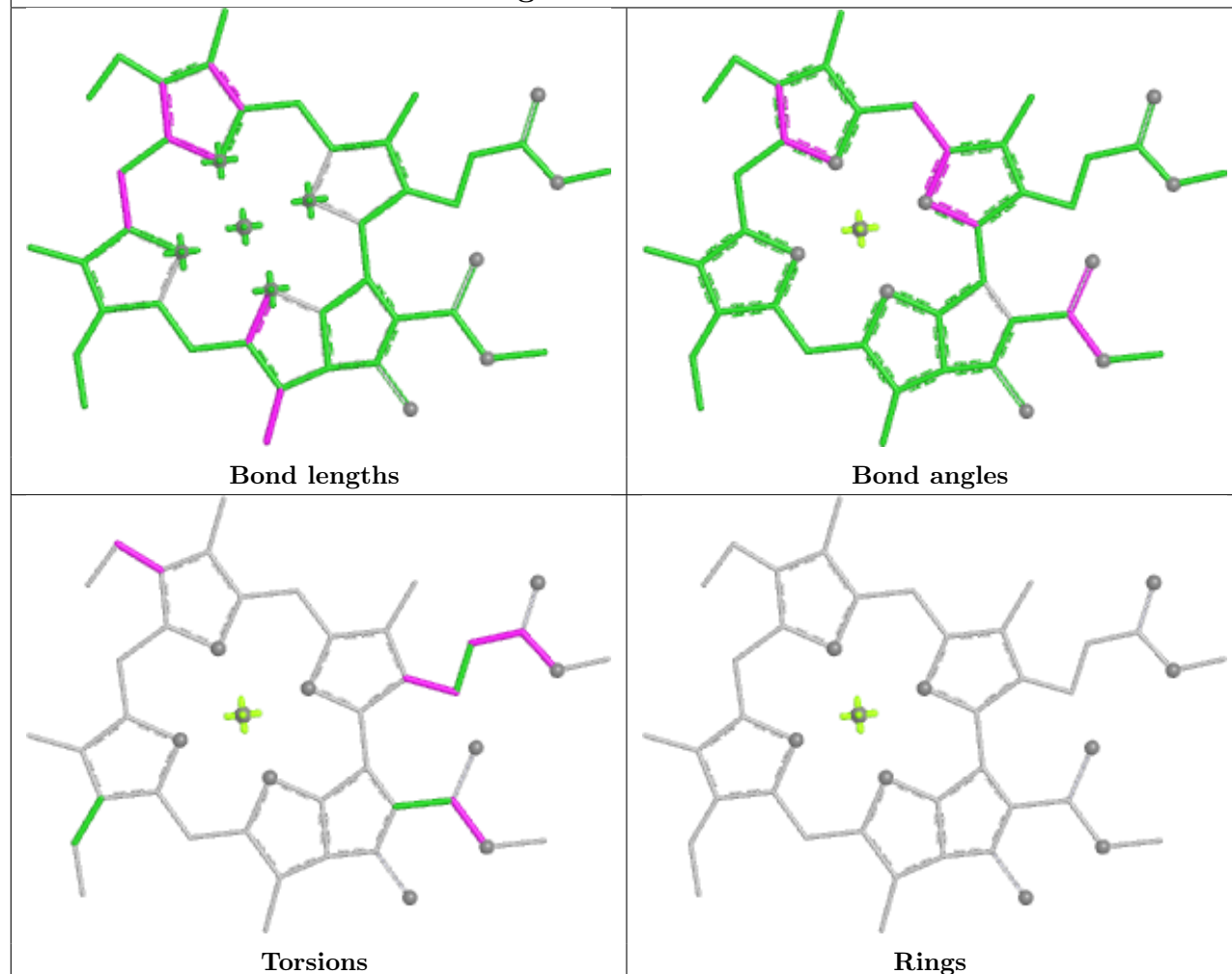




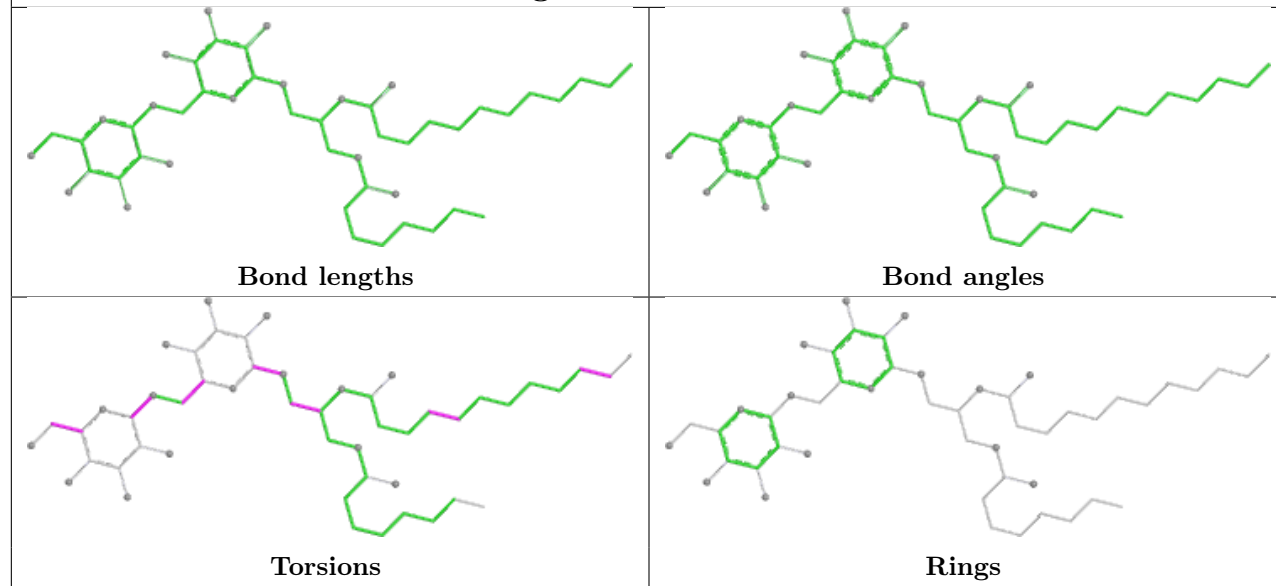




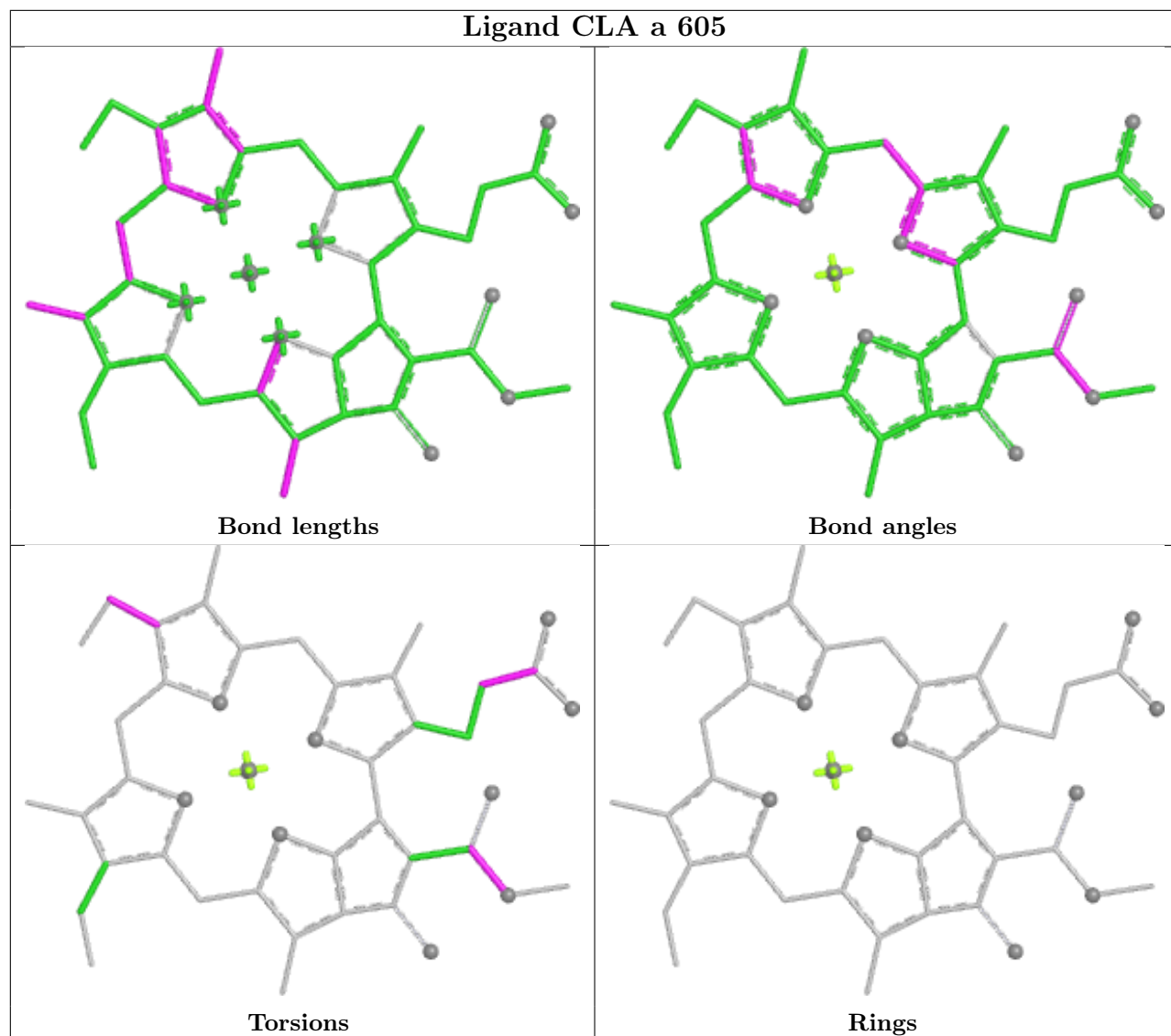
Ligand CLA a 610



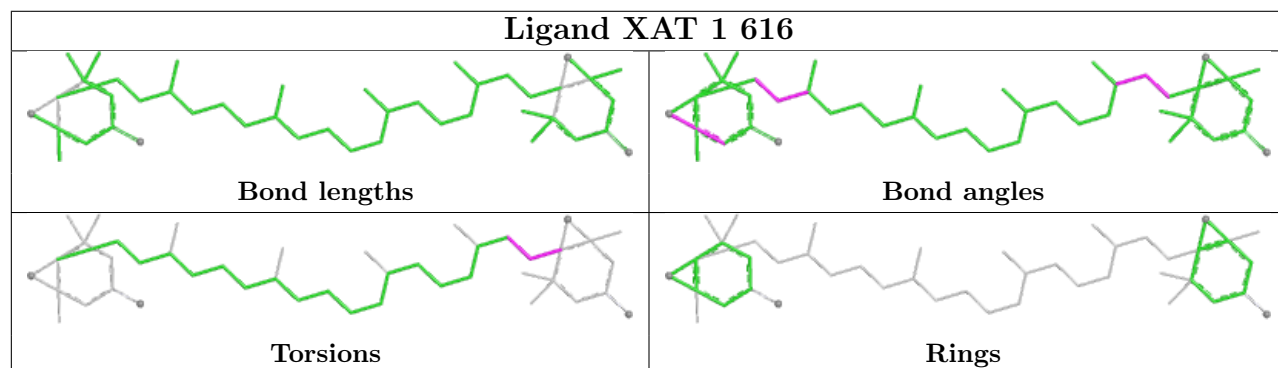
Ligand DGD 3 321

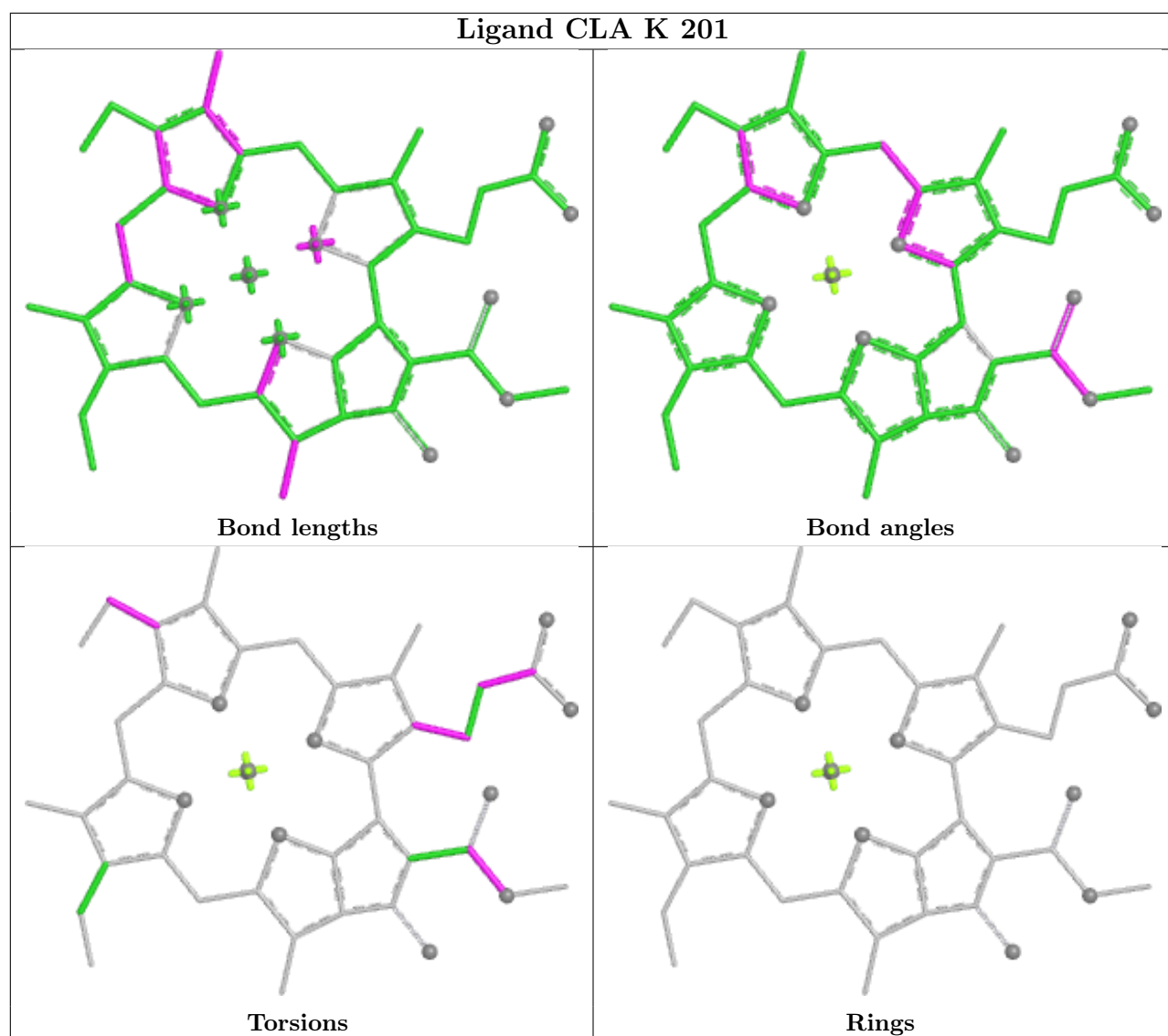


Ligand CLA a 605

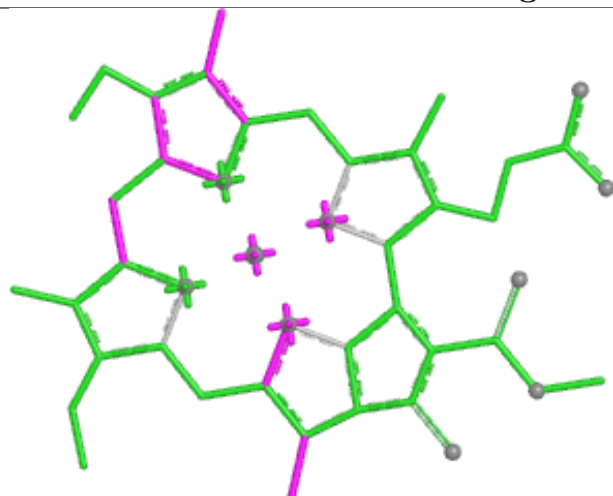


Ligand XAT 1 616

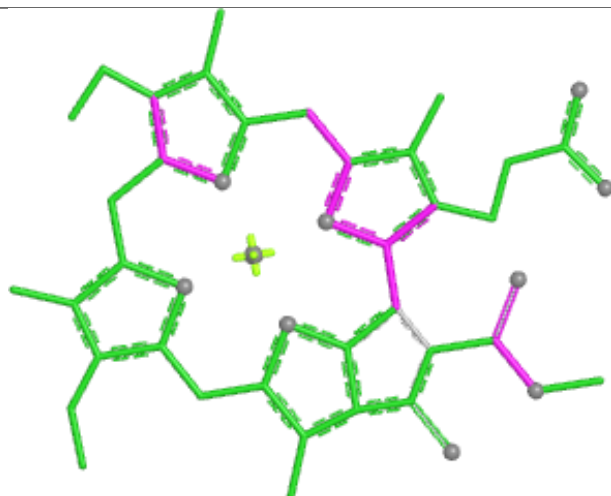




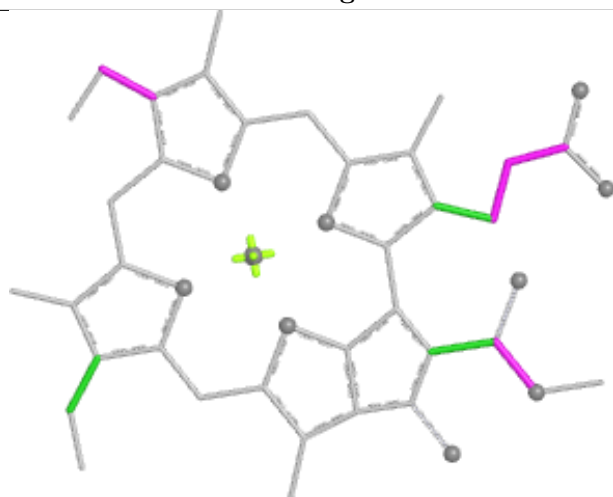
Ligand CLA c 310



Bond lengths



Bond angles

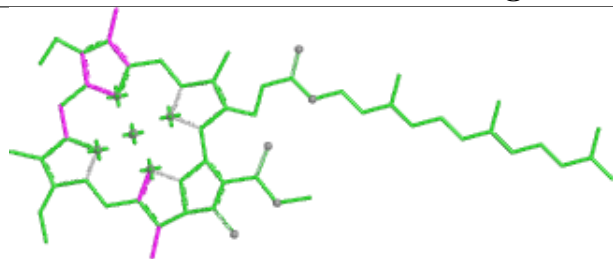


Torsions

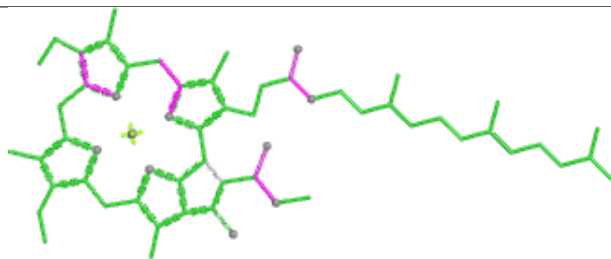


Rings

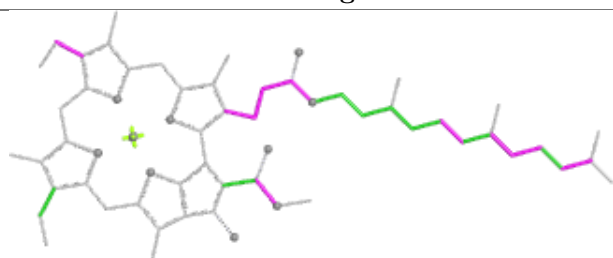
Ligand CLA A 5024



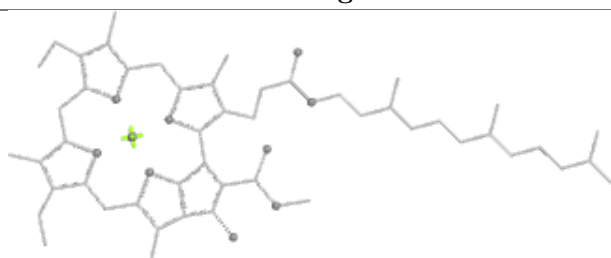
Bond lengths



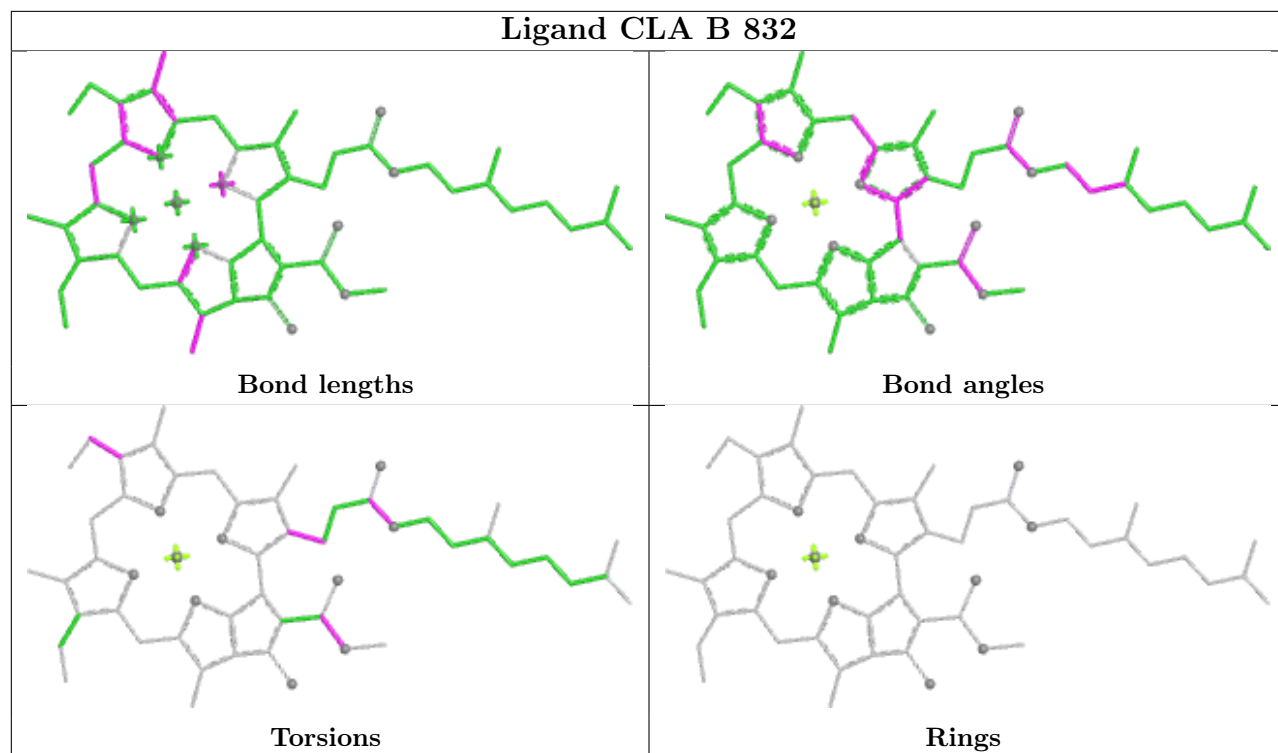
Bond angles



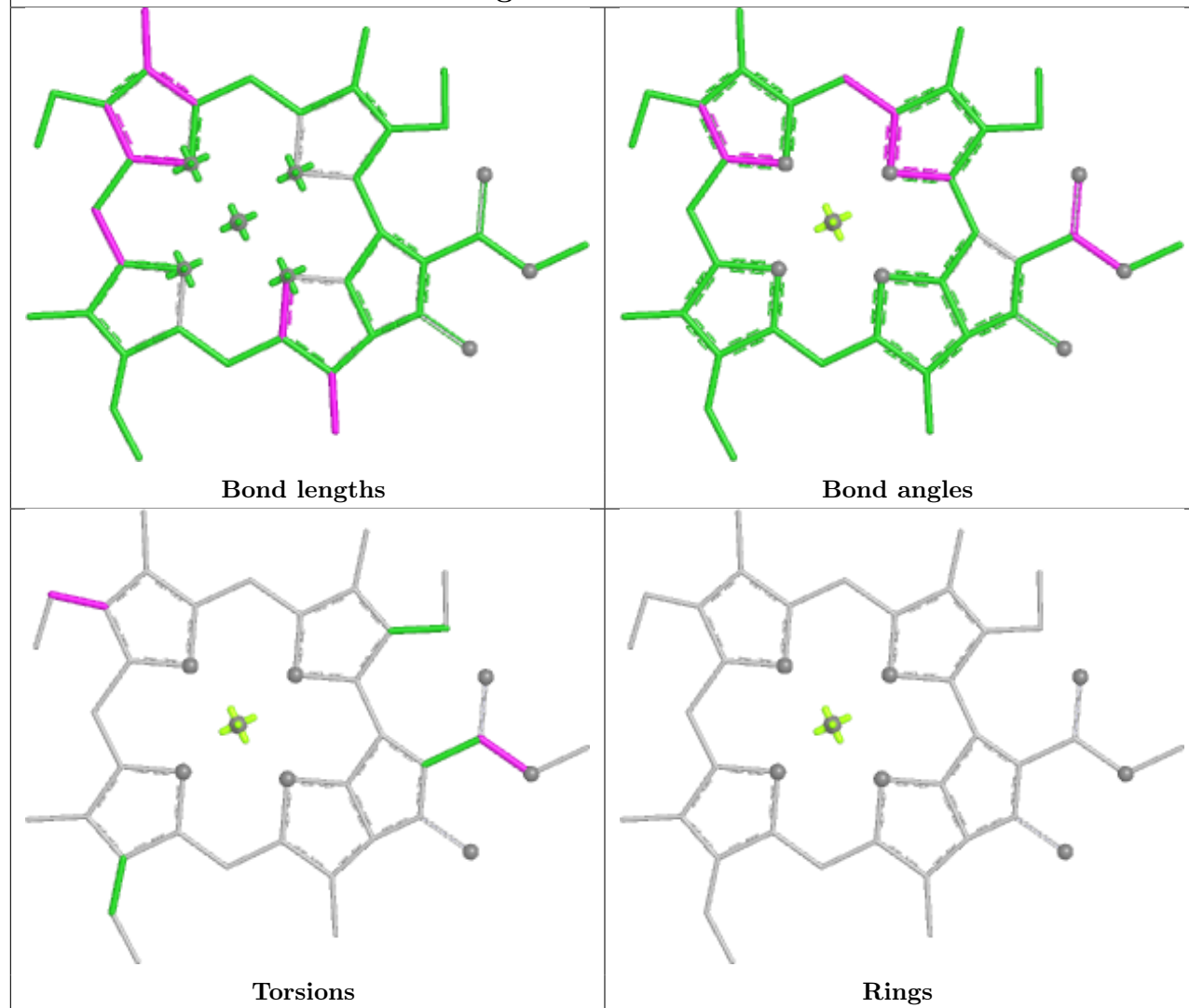
Torsions



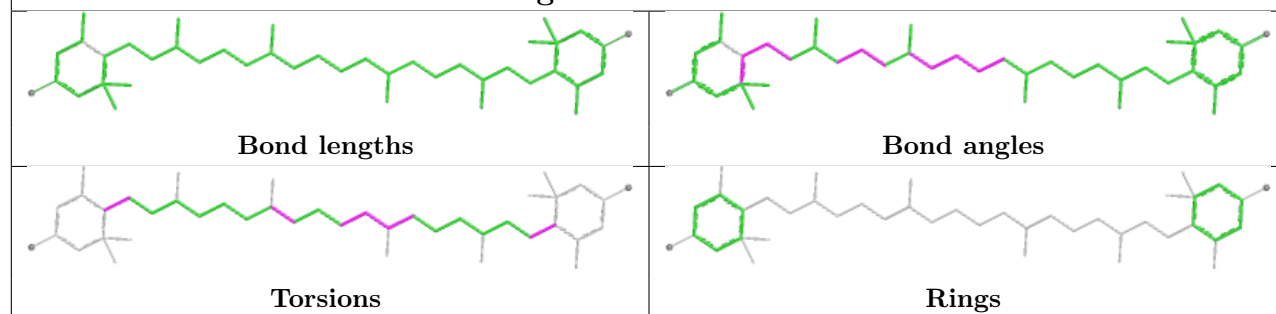
Rings

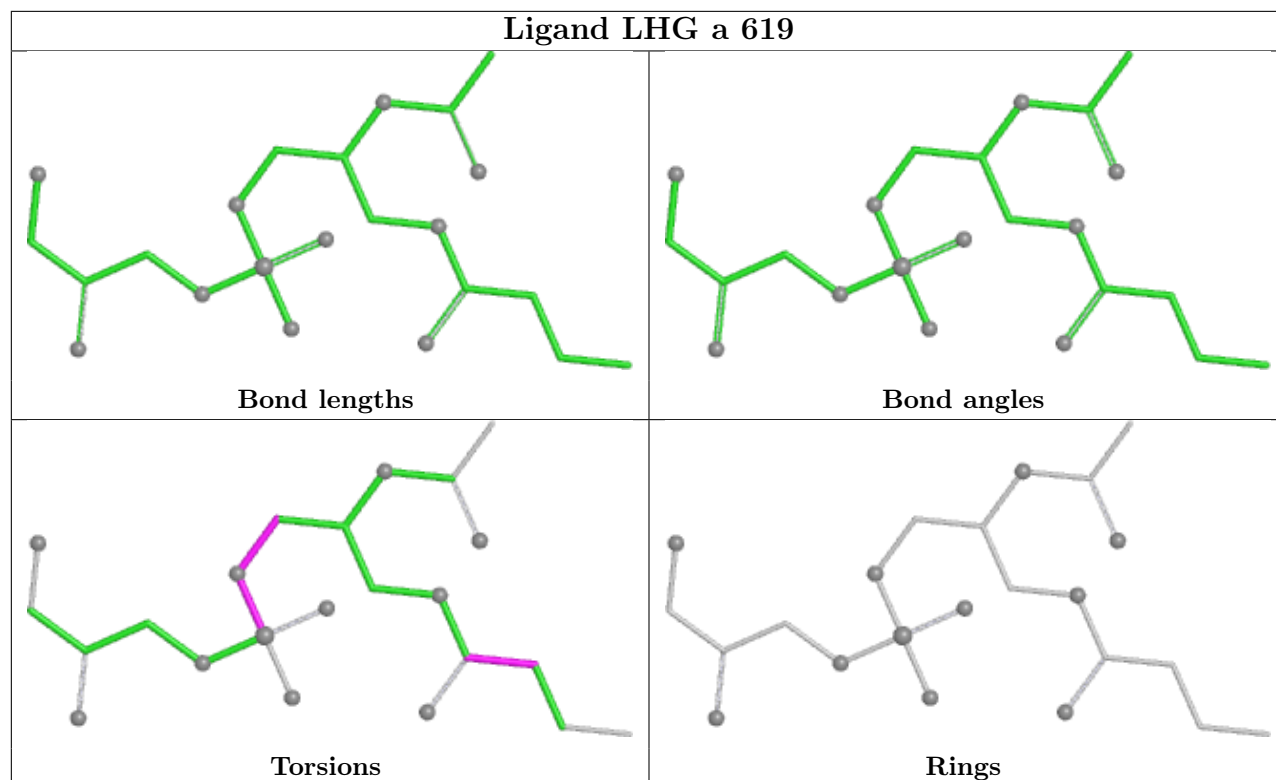


Ligand CLA T 412

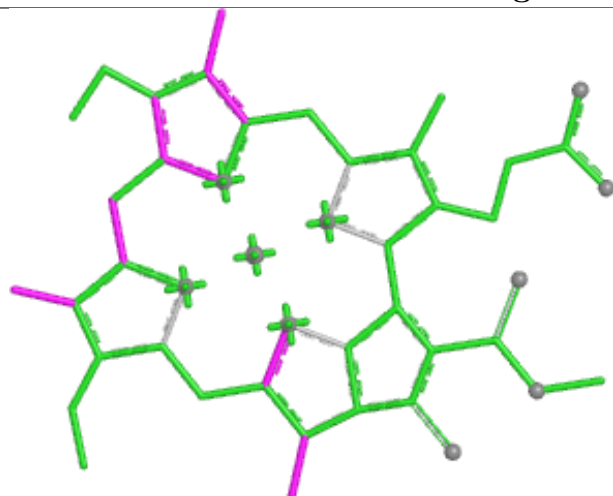


Ligand LUT a 615

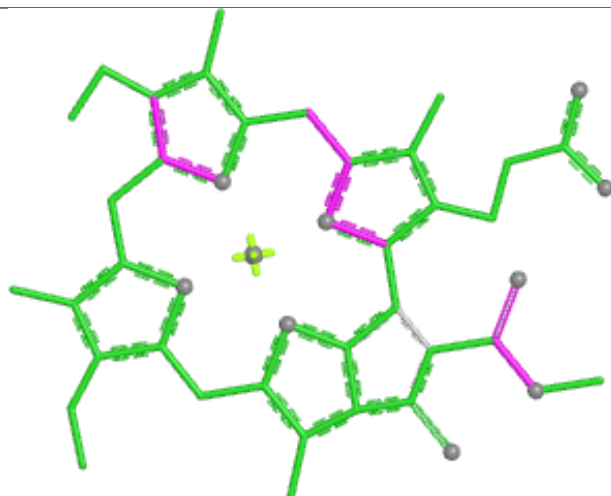




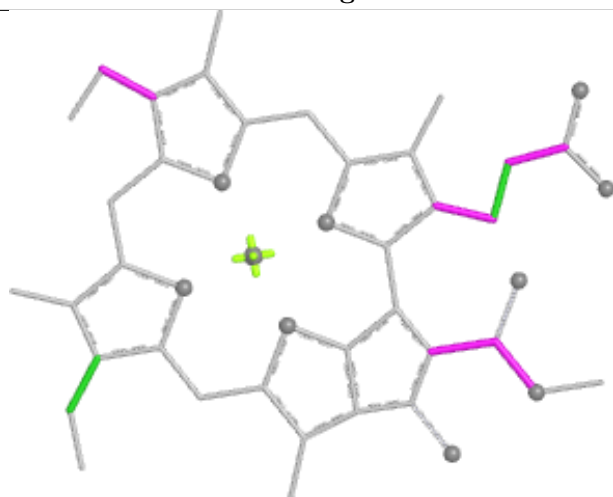
Ligand CLA K 203



Bond lengths



Bond angles

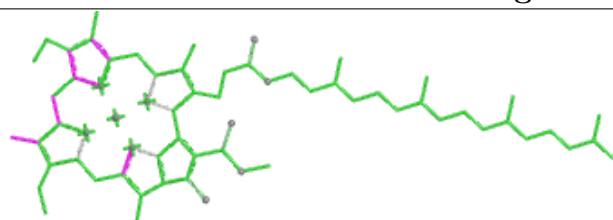


Torsions

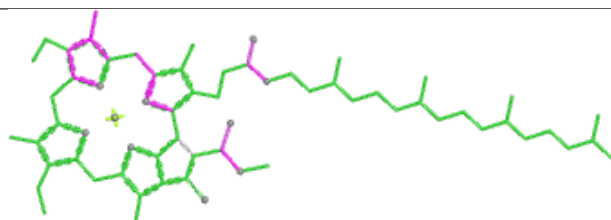


Rings

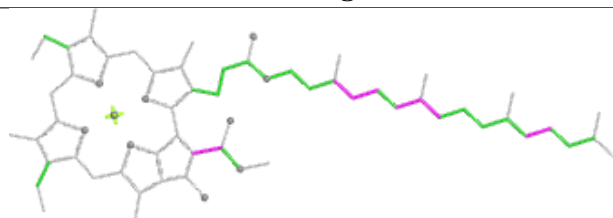
Ligand CLA B 805



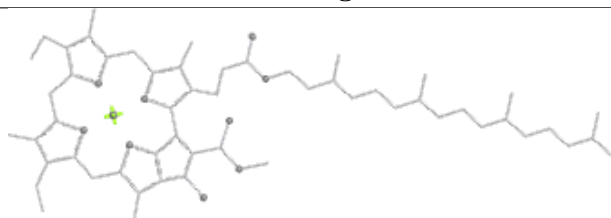
Bond lengths



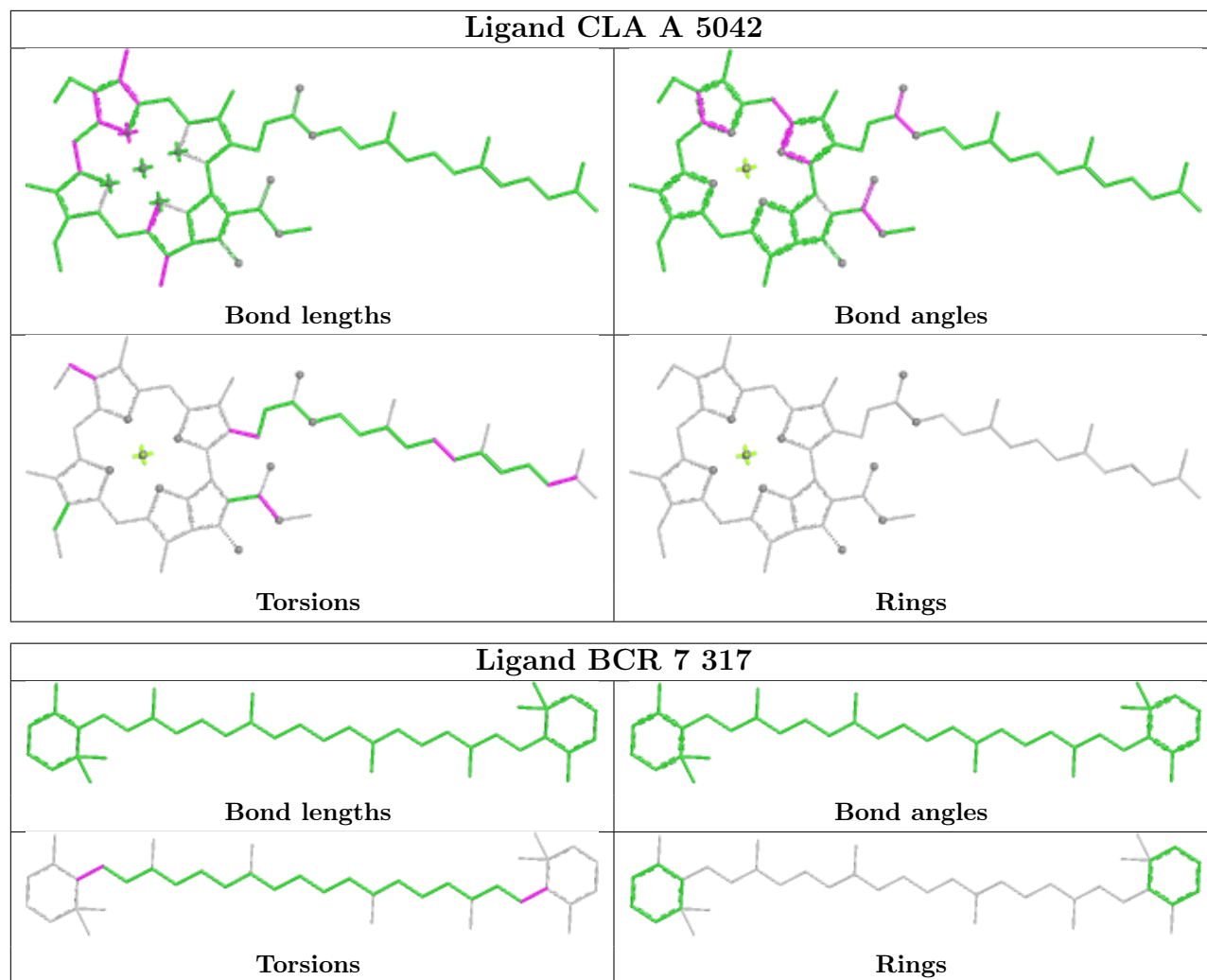
Bond angles

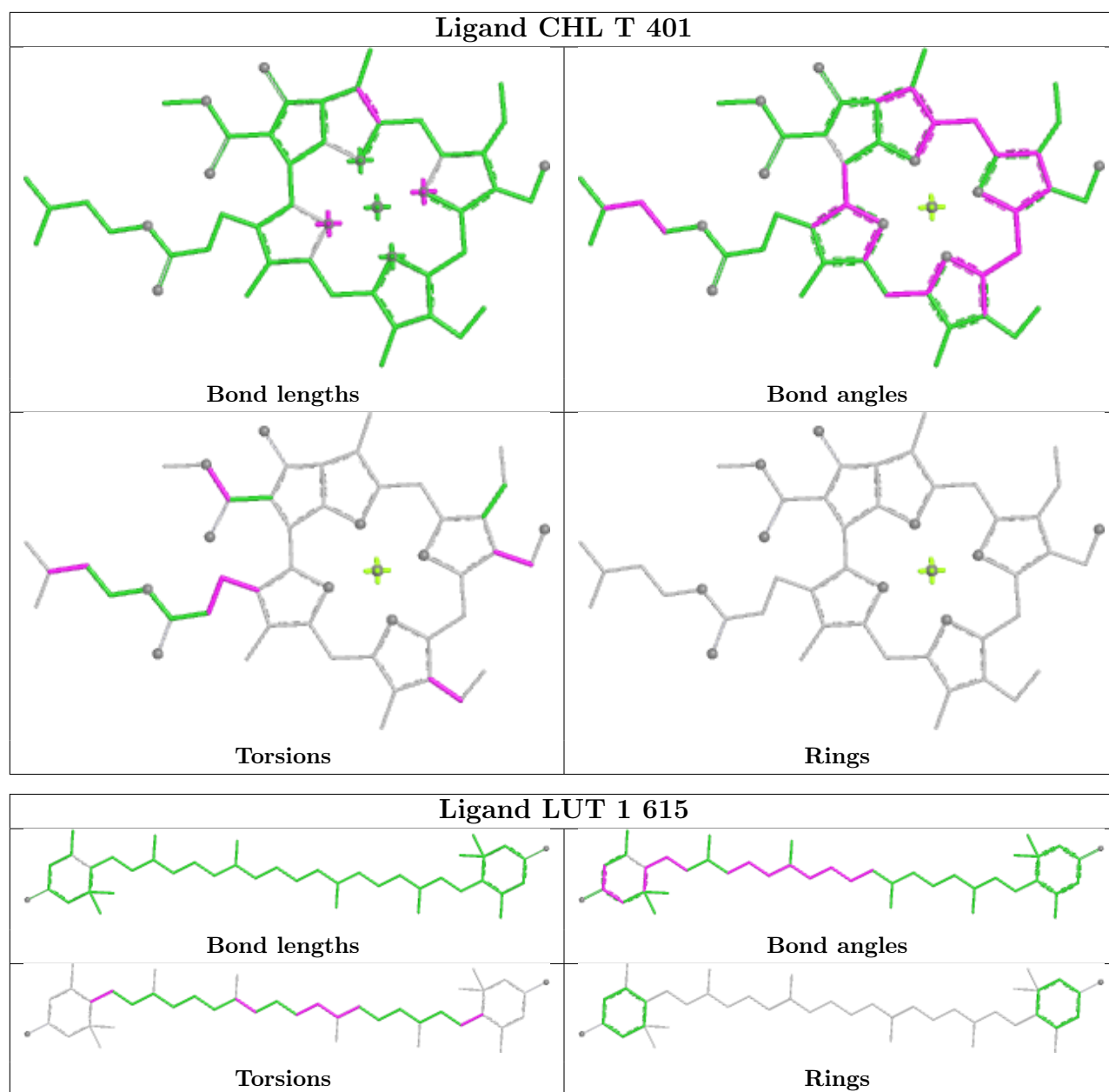


Torsions

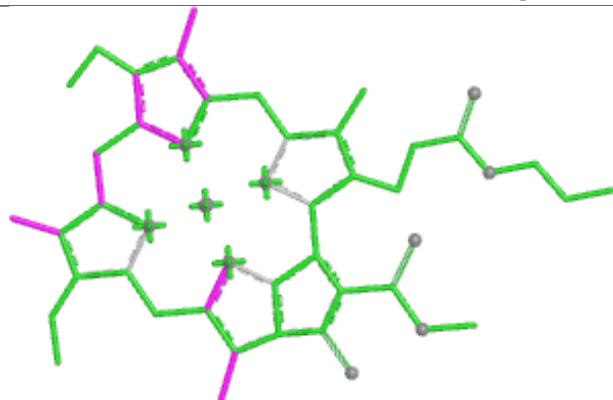


Rings

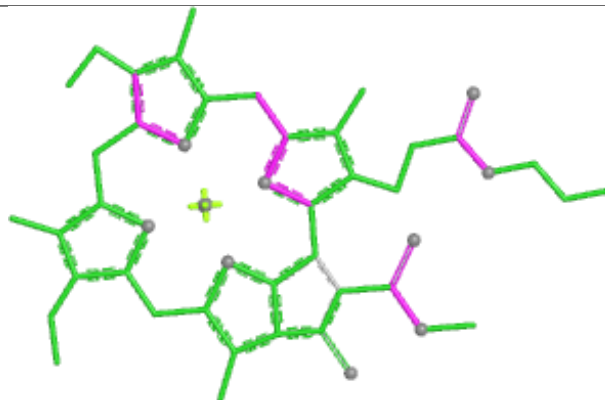




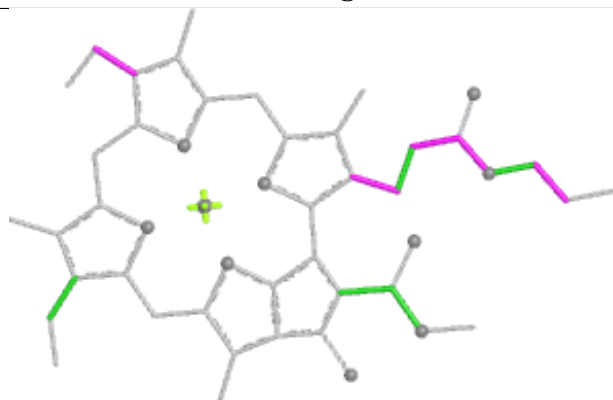
Ligand CLA B 804



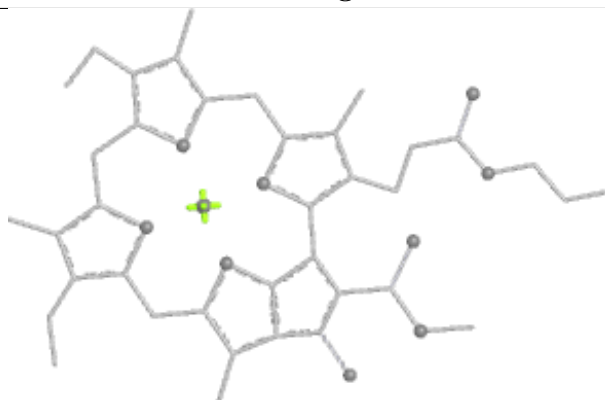
Bond lengths



Bond angles

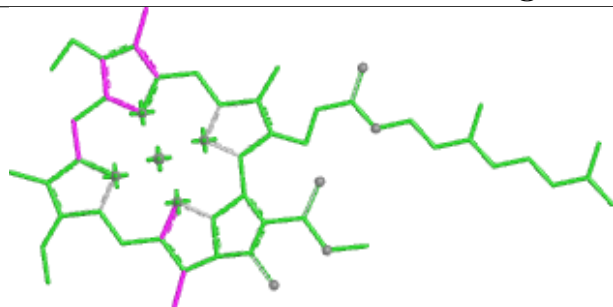


Torsions

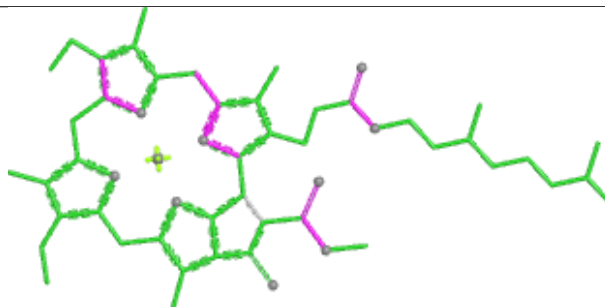


Rings

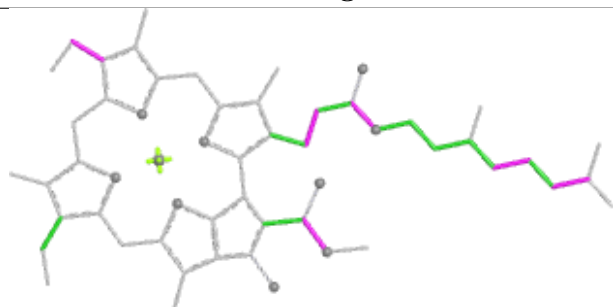
Ligand CLA 3 311



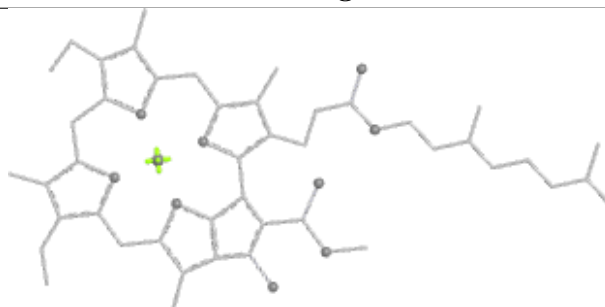
Bond lengths



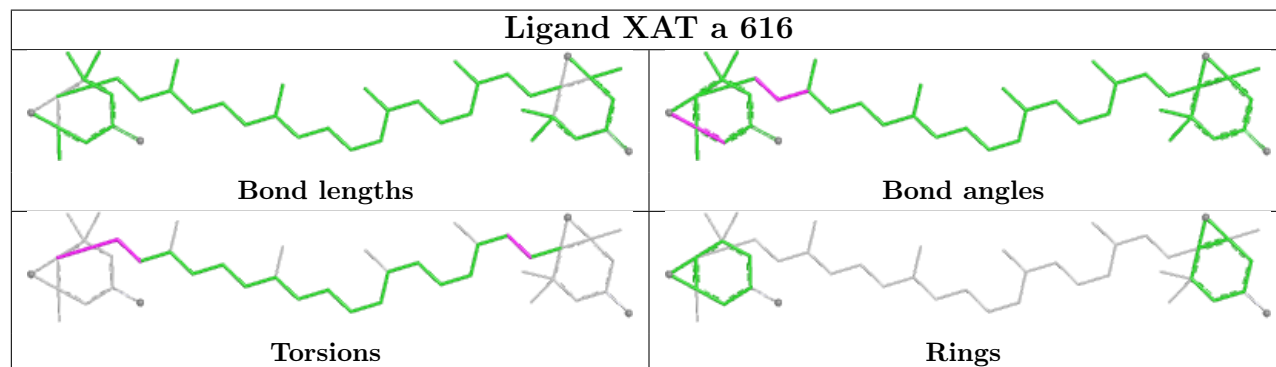
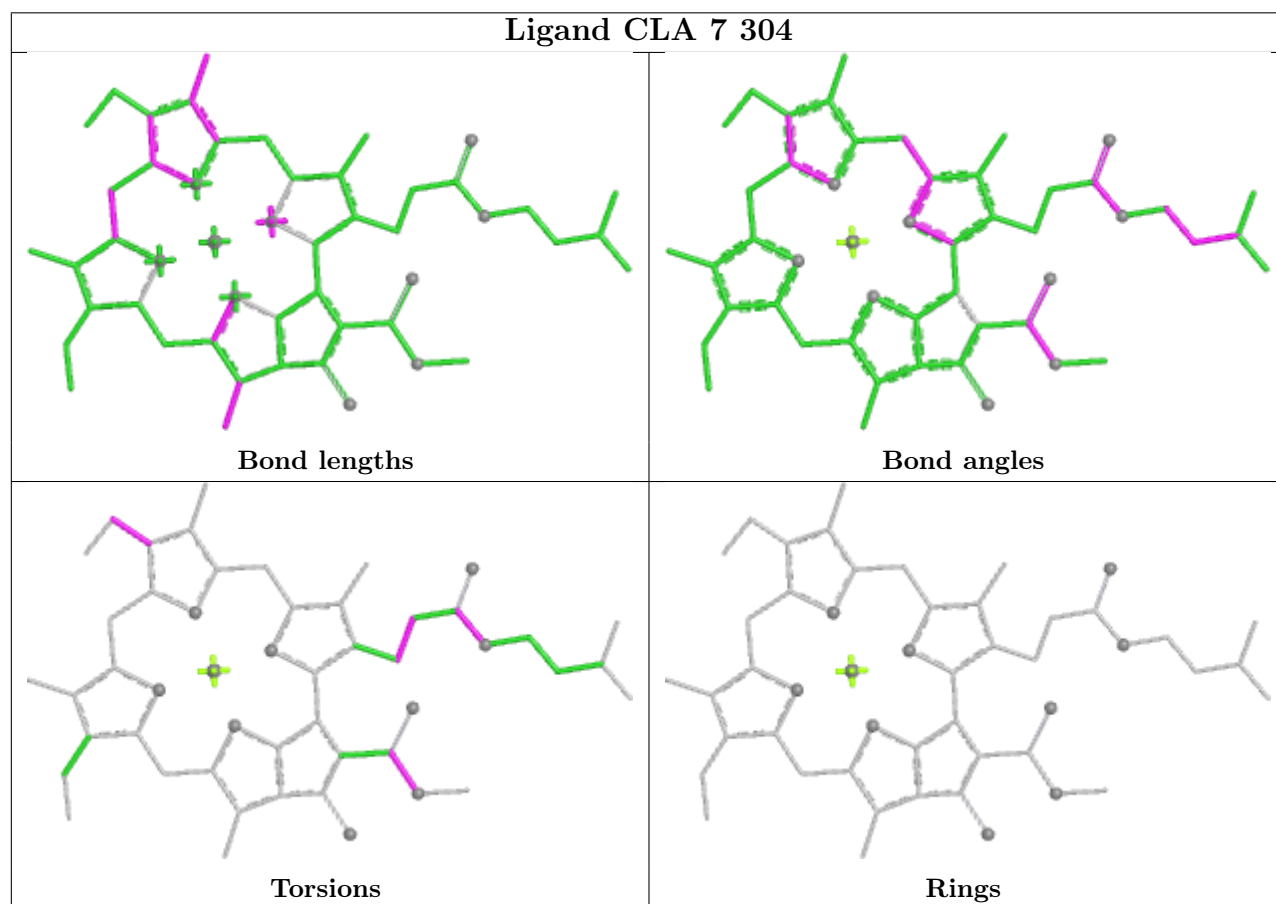
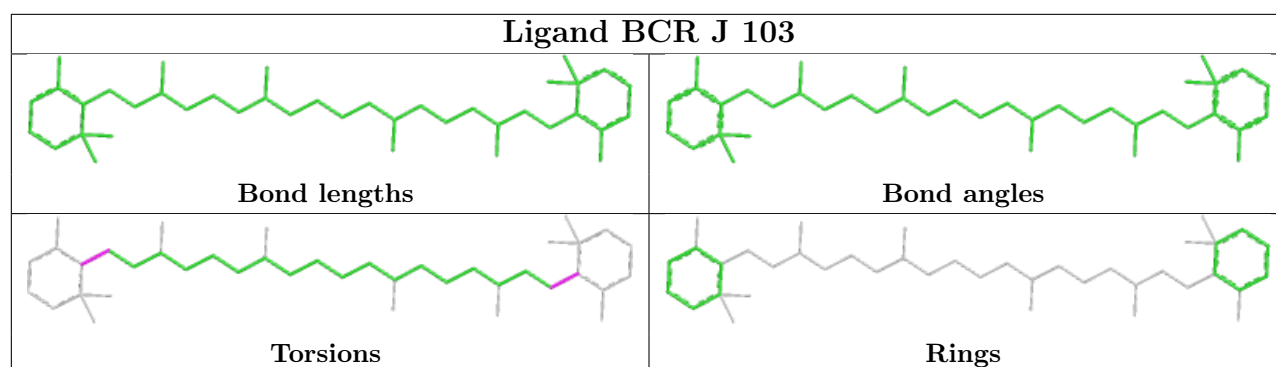
Bond angles

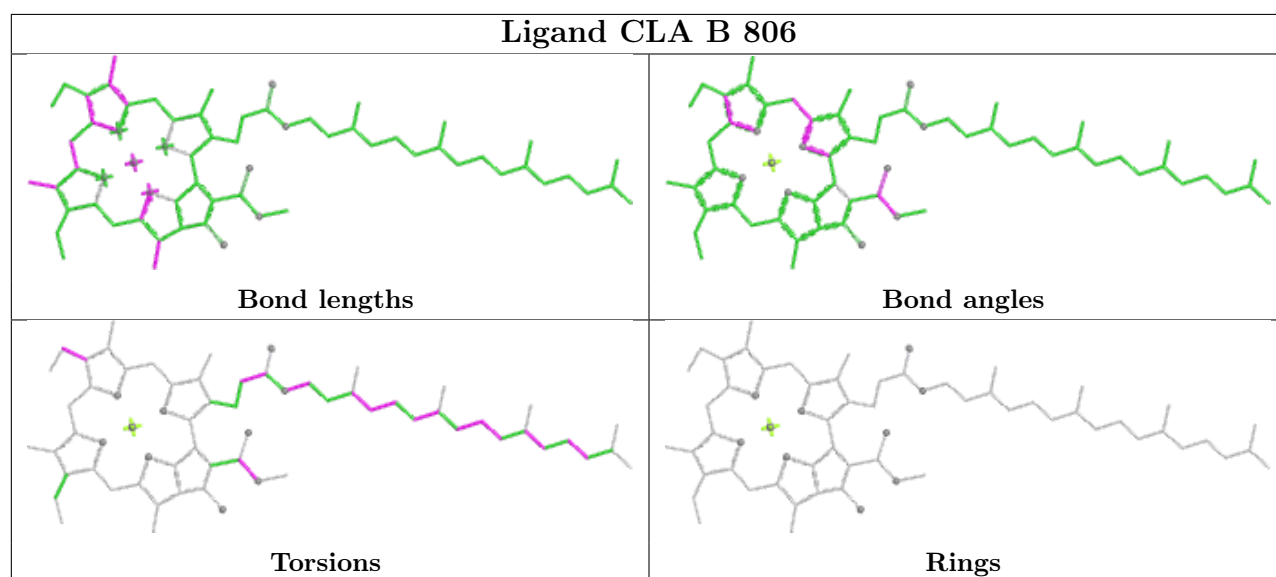
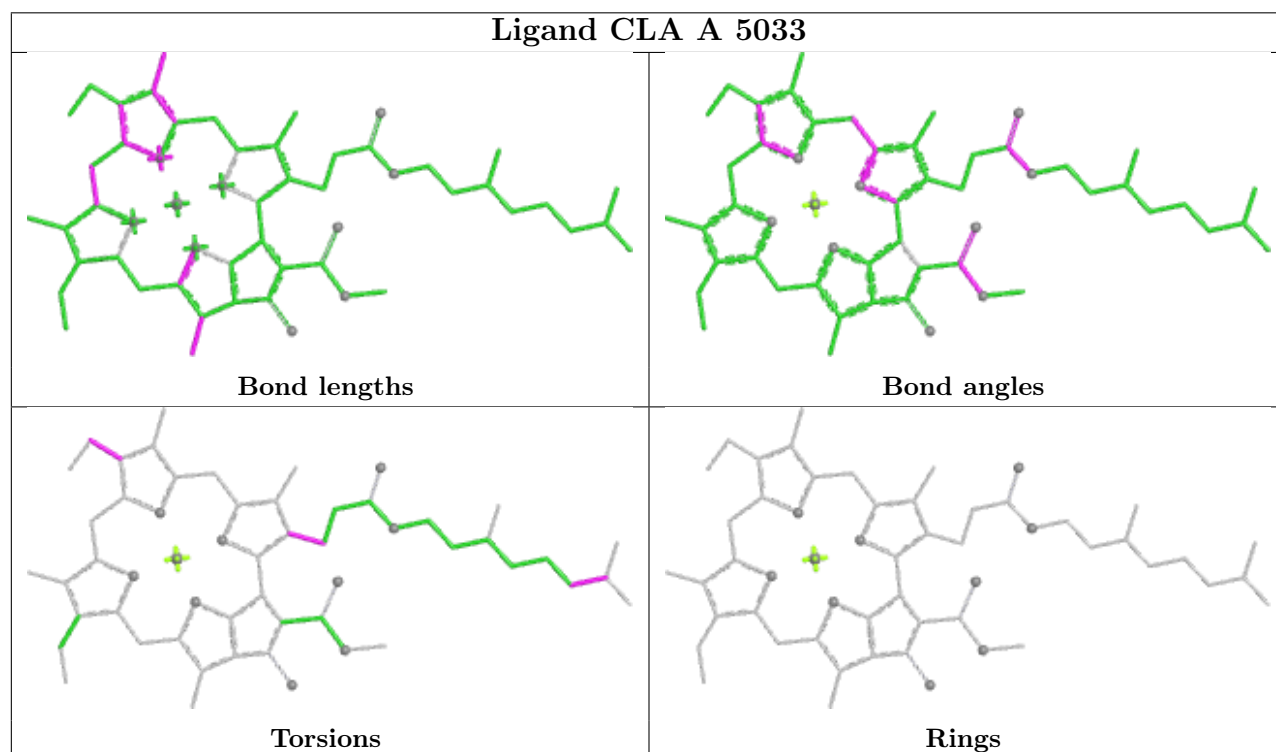
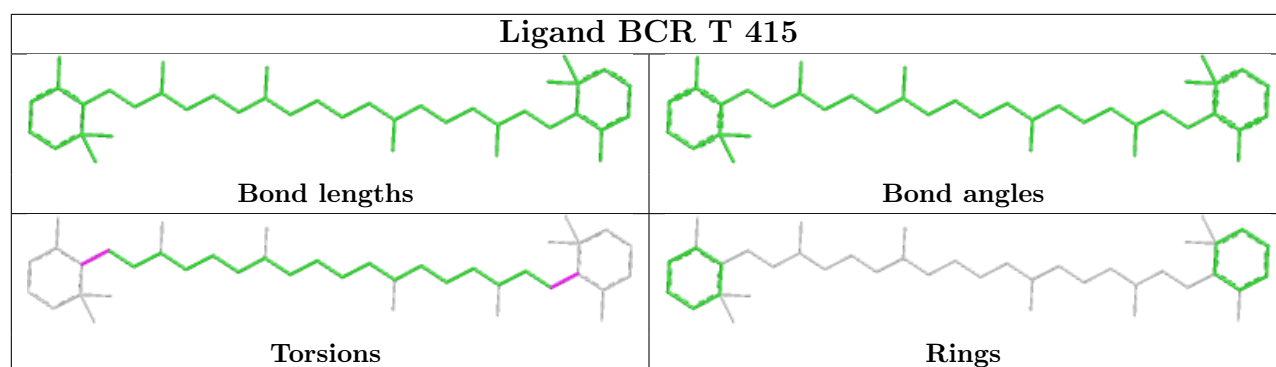


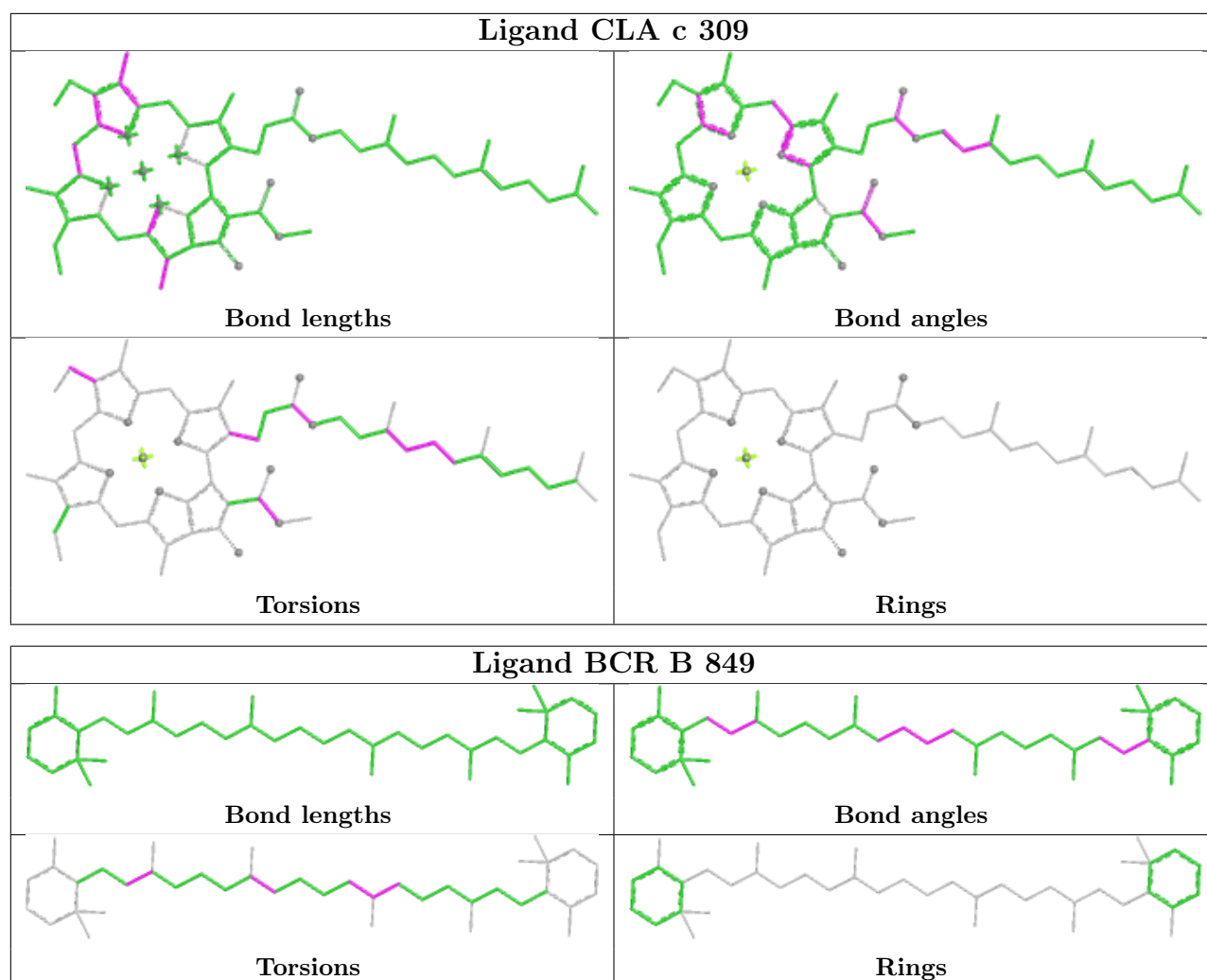
Torsions

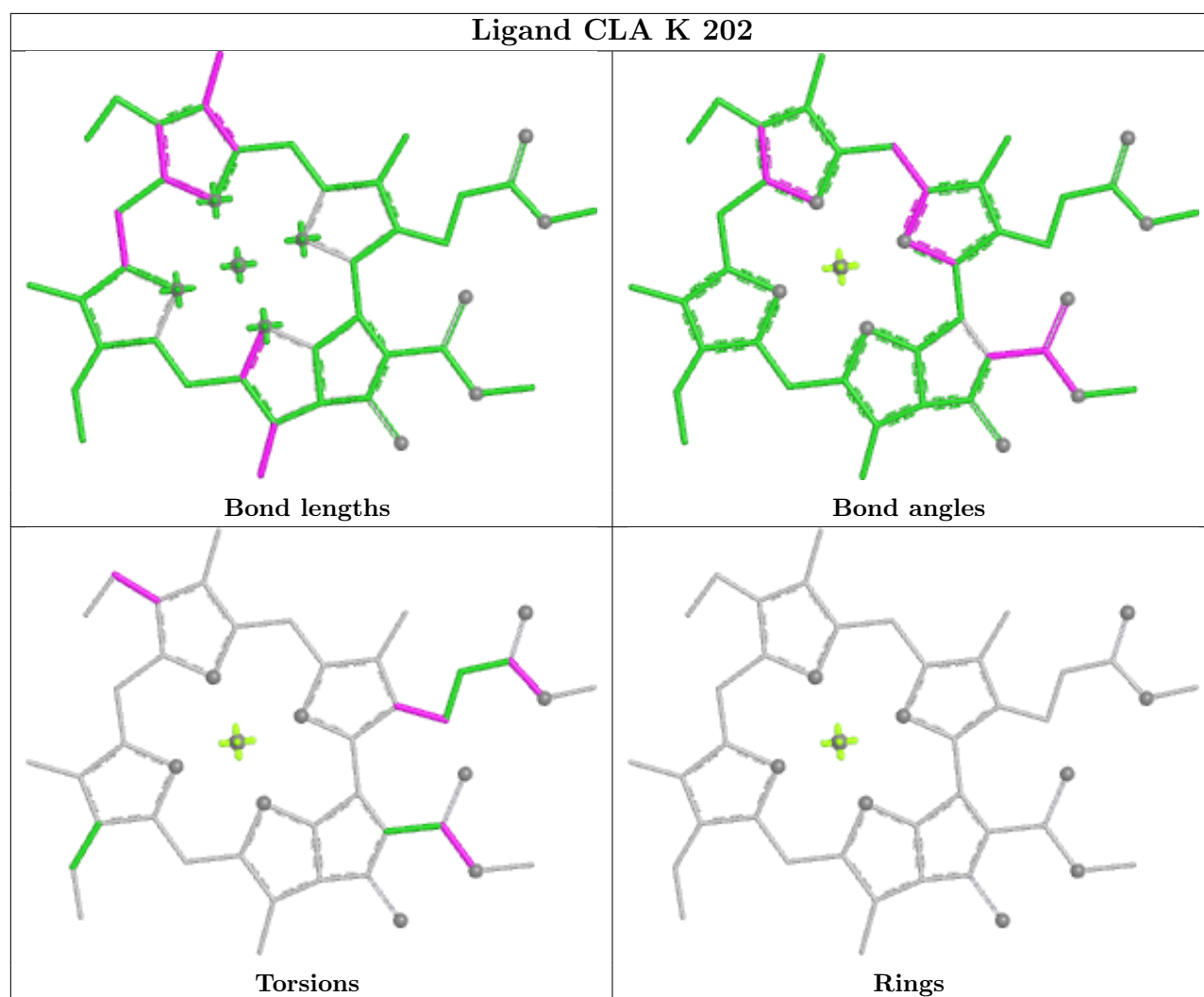


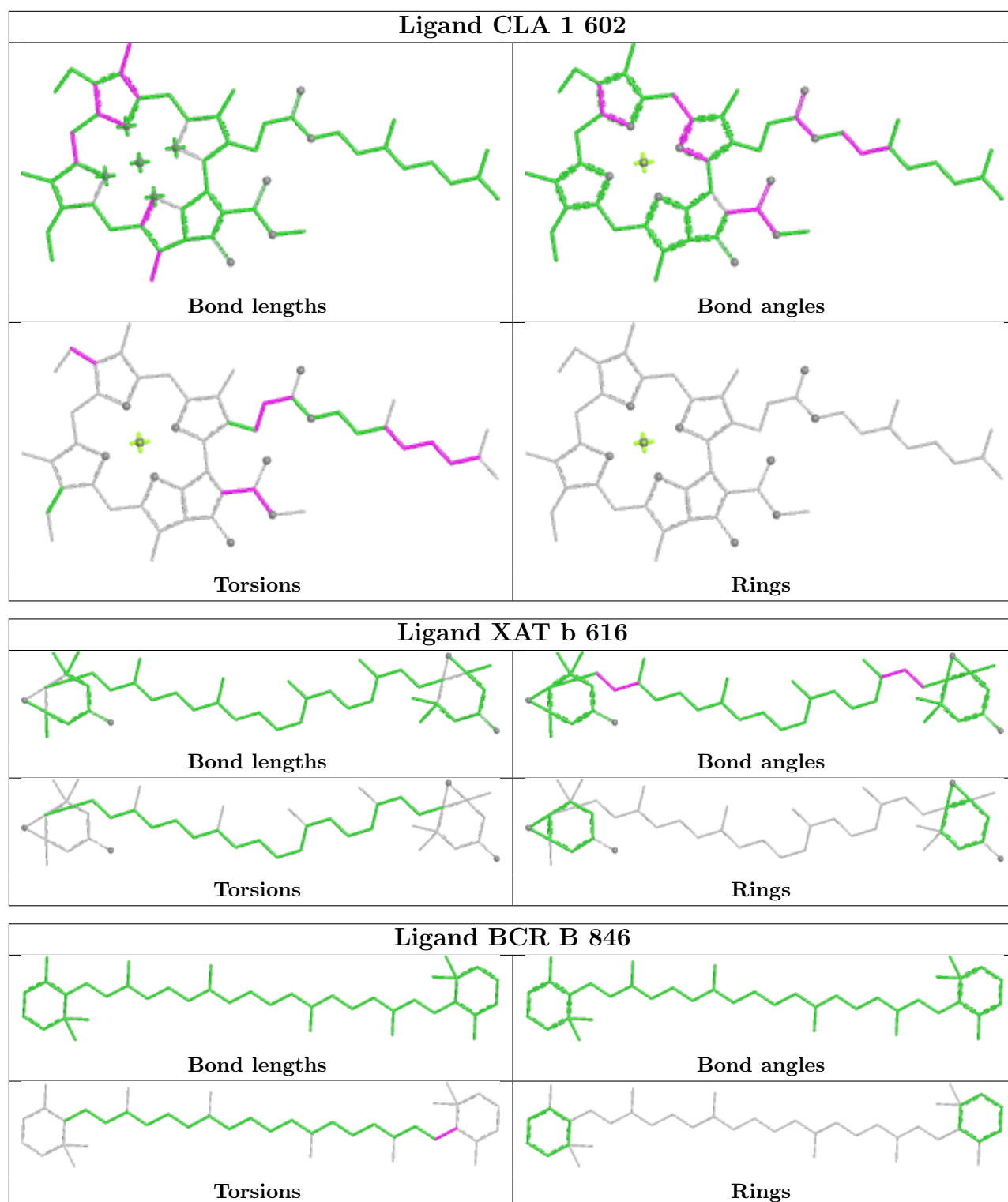
Rings



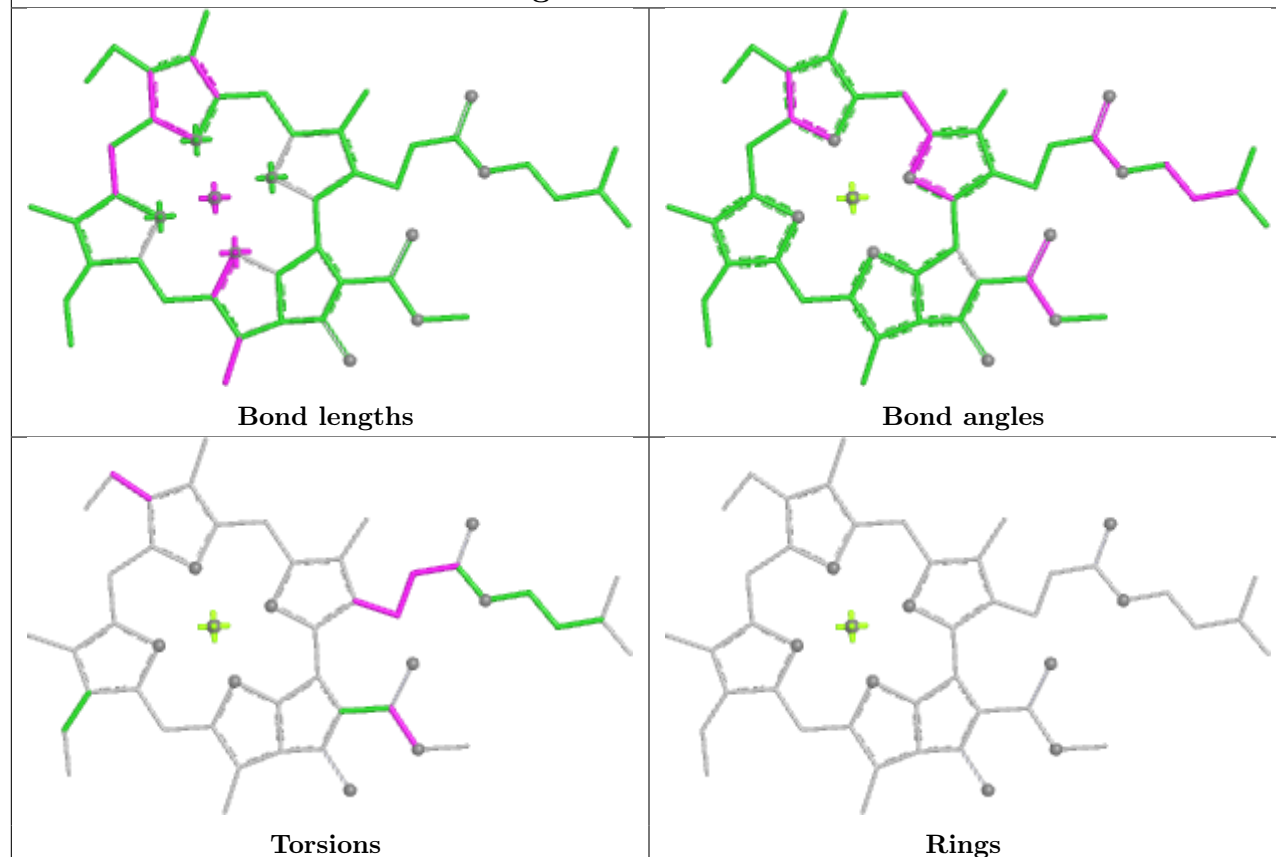




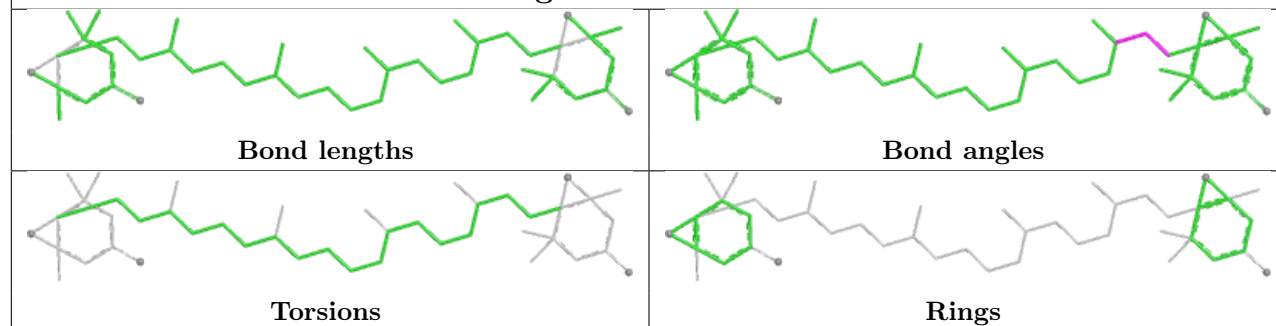




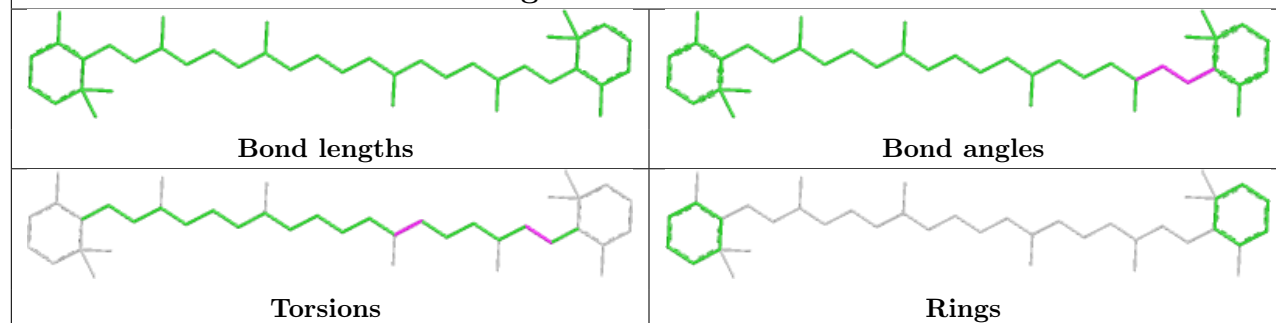
Ligand CLA B 835



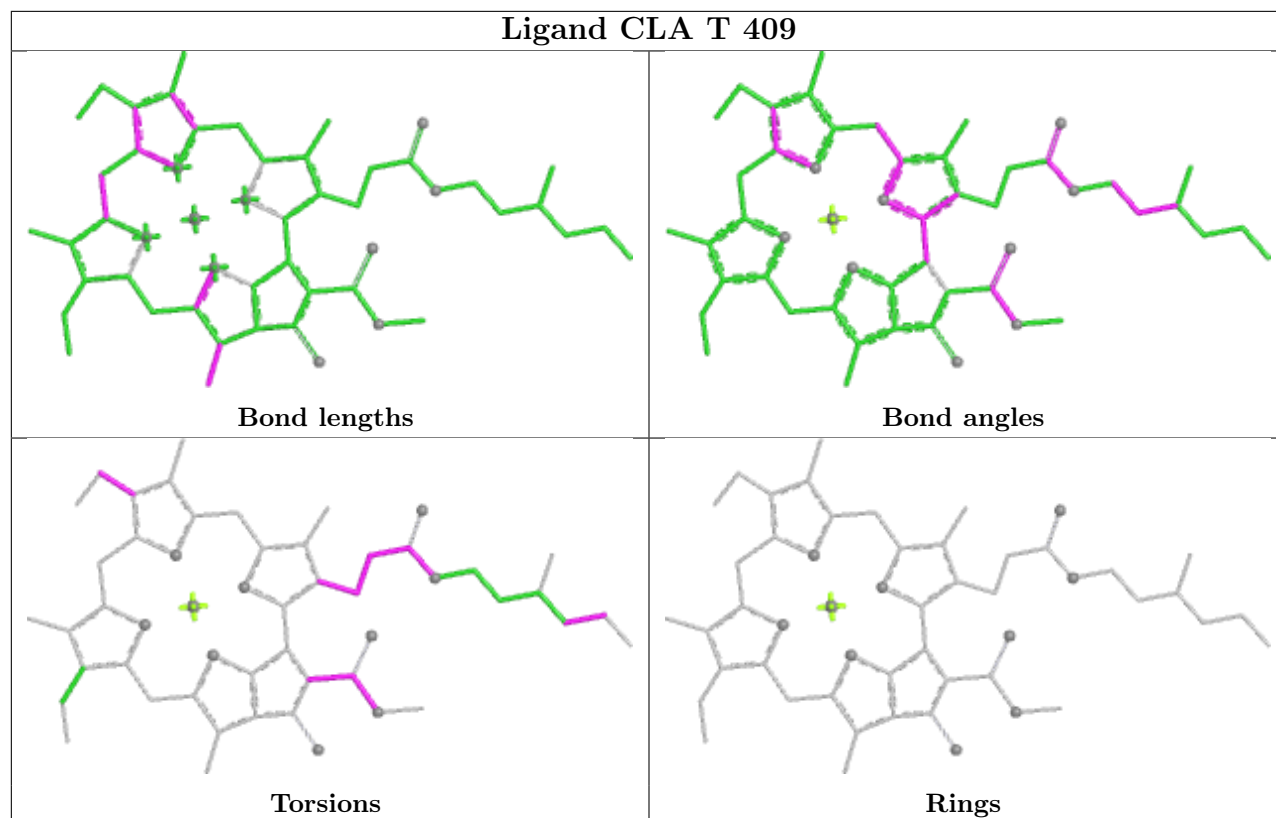
Ligand XAT 8 317



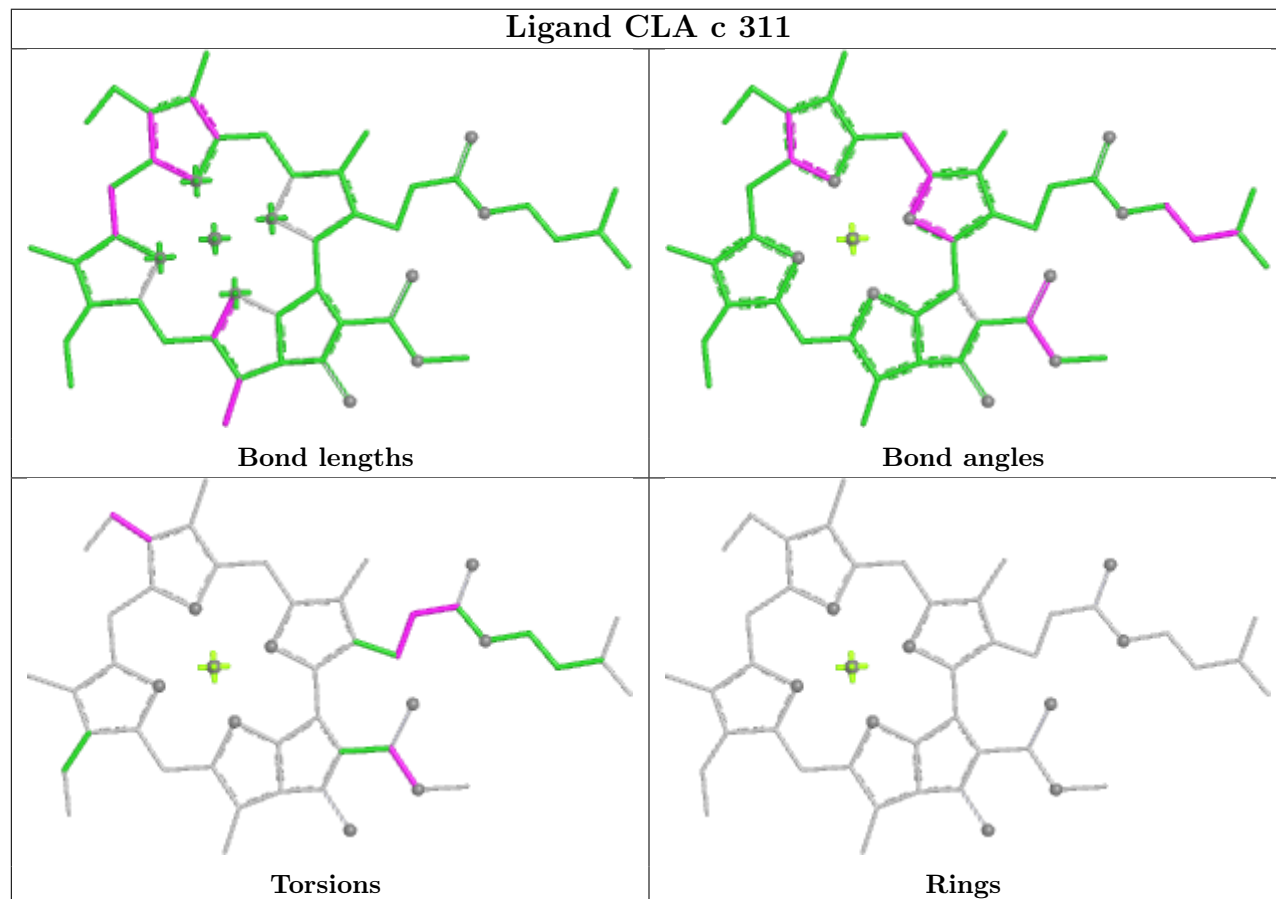
Ligand BCR A 5049



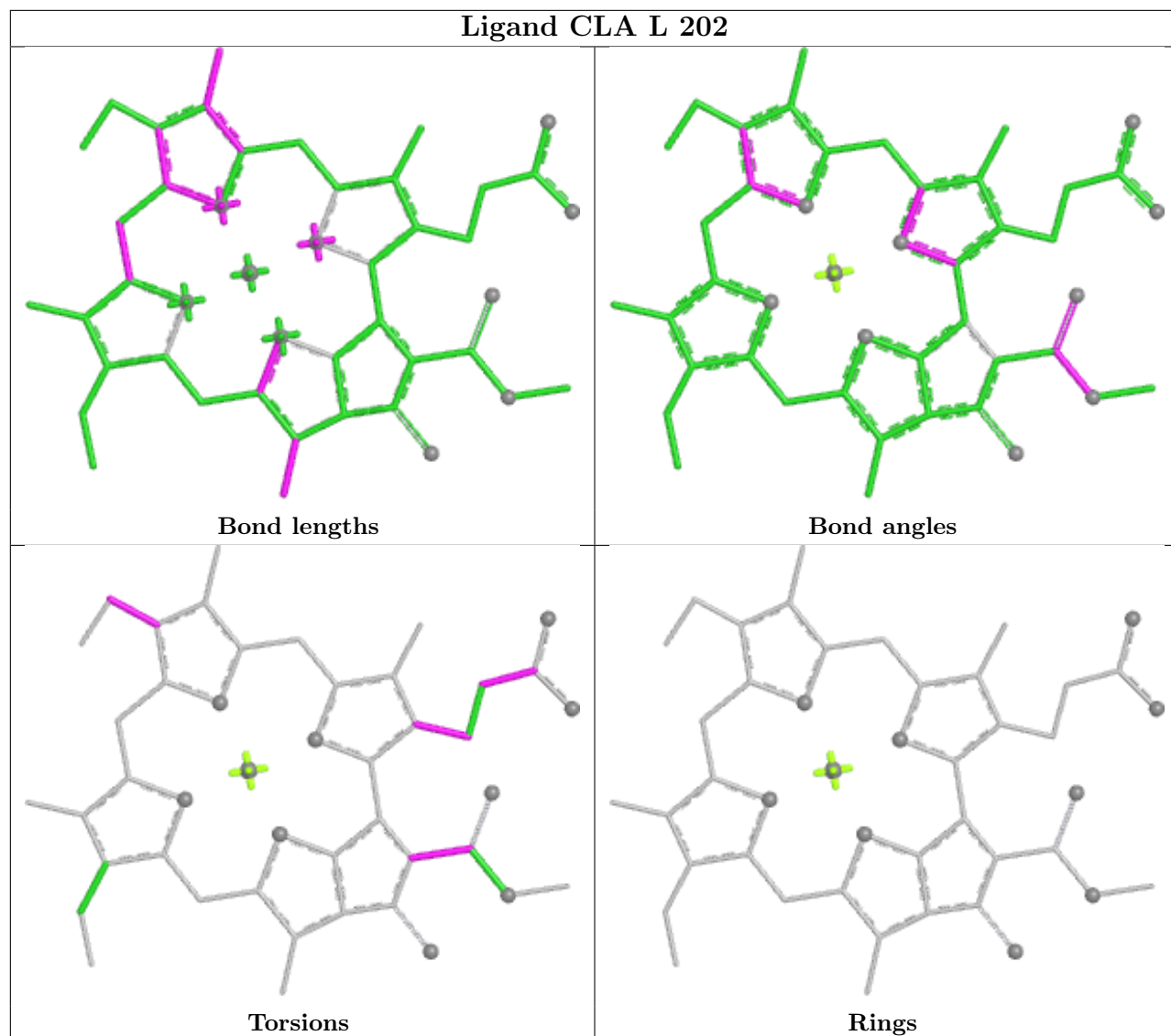
Ligand CLA T 409



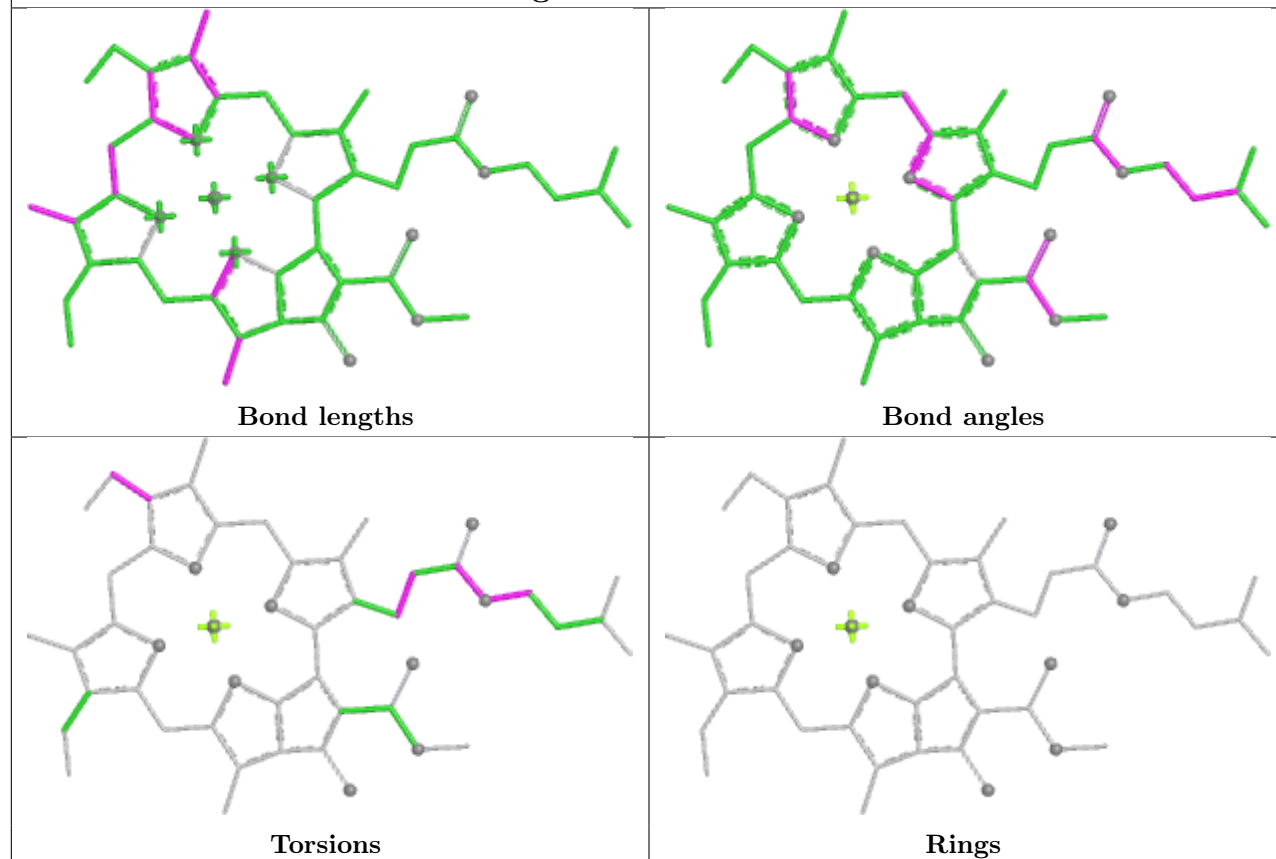
Ligand CLA c 311



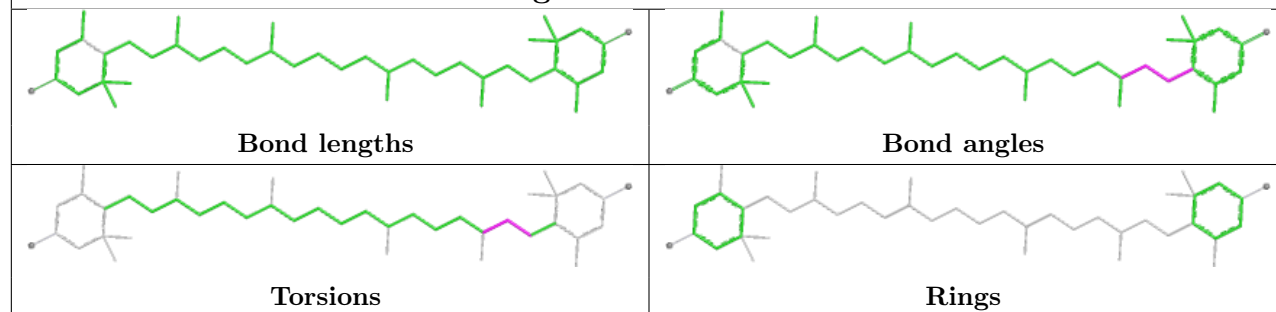
Ligand CLA L 202

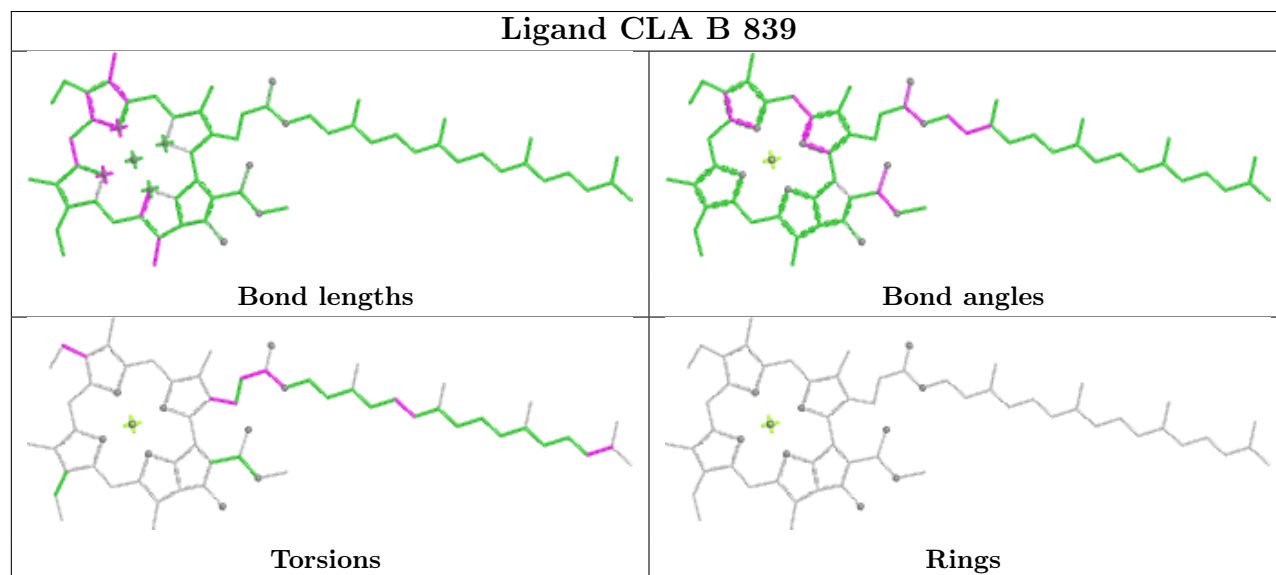
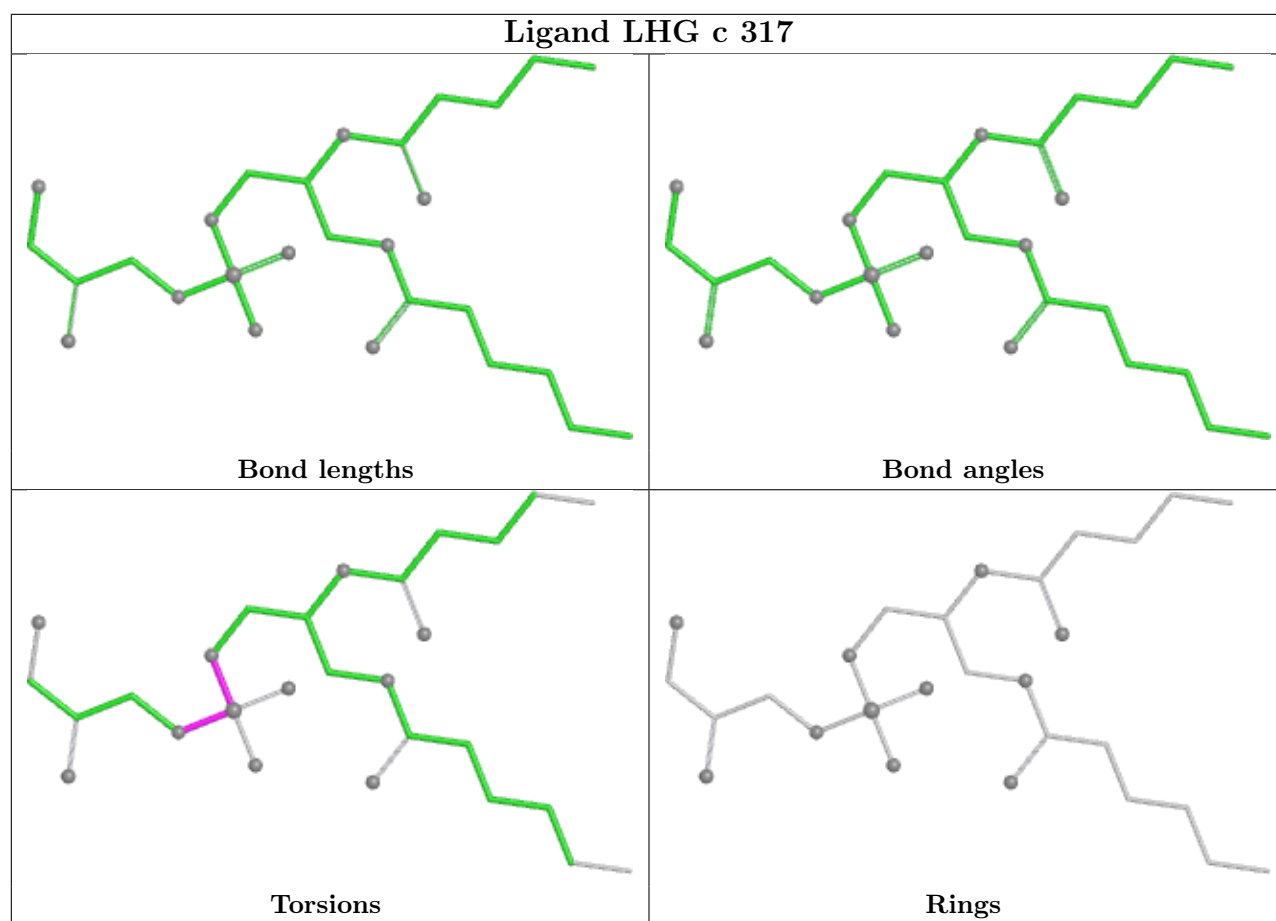


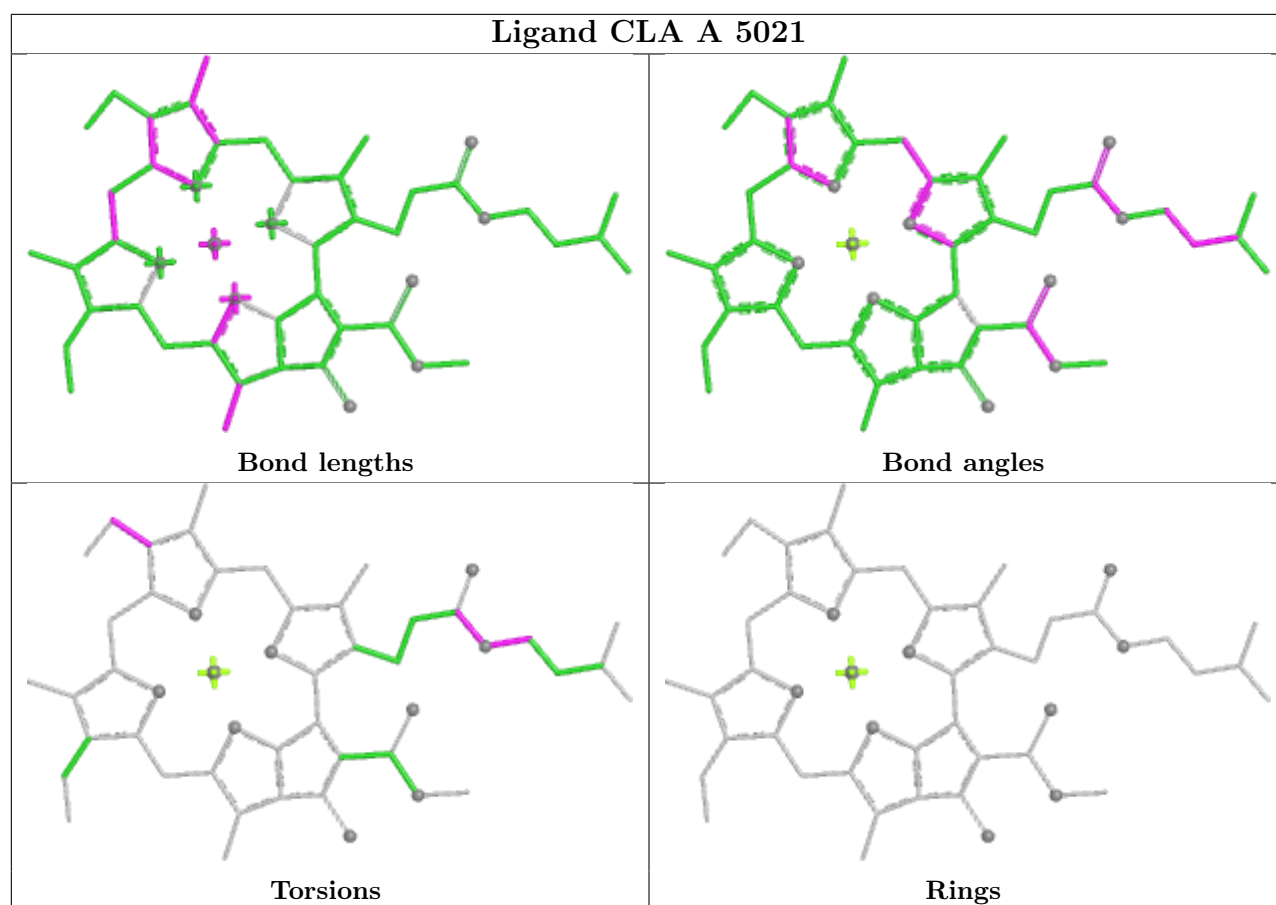
Ligand CLA B 816



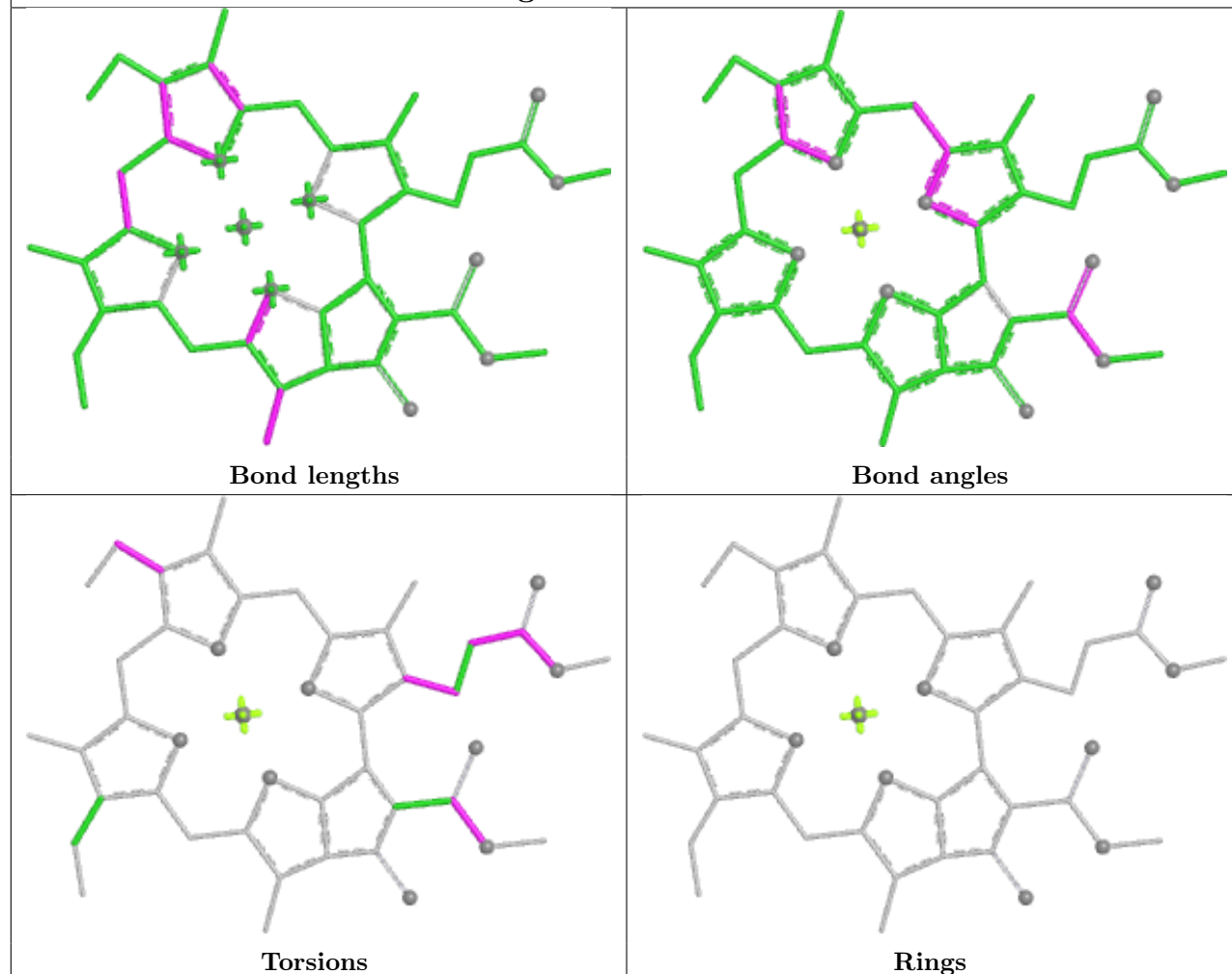
Ligand LUT T 413



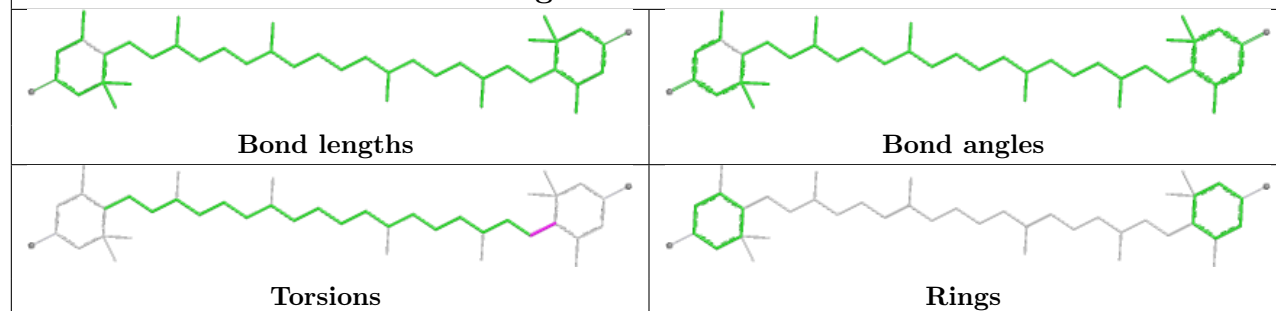




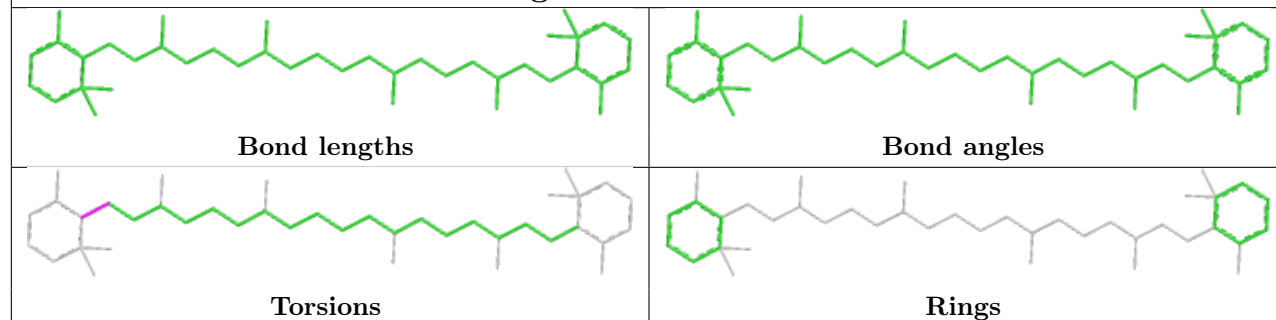
Ligand CLA 1 610

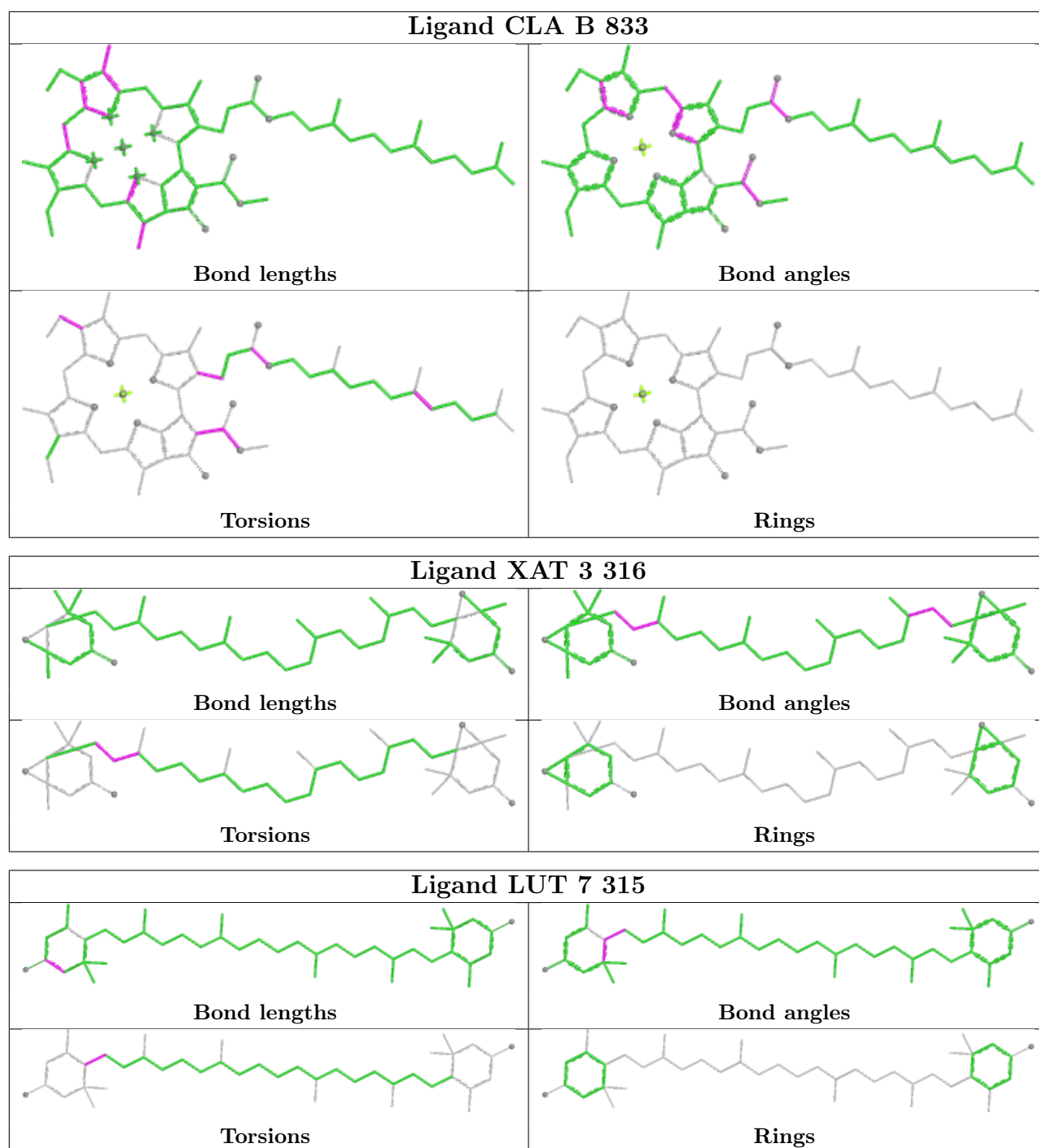


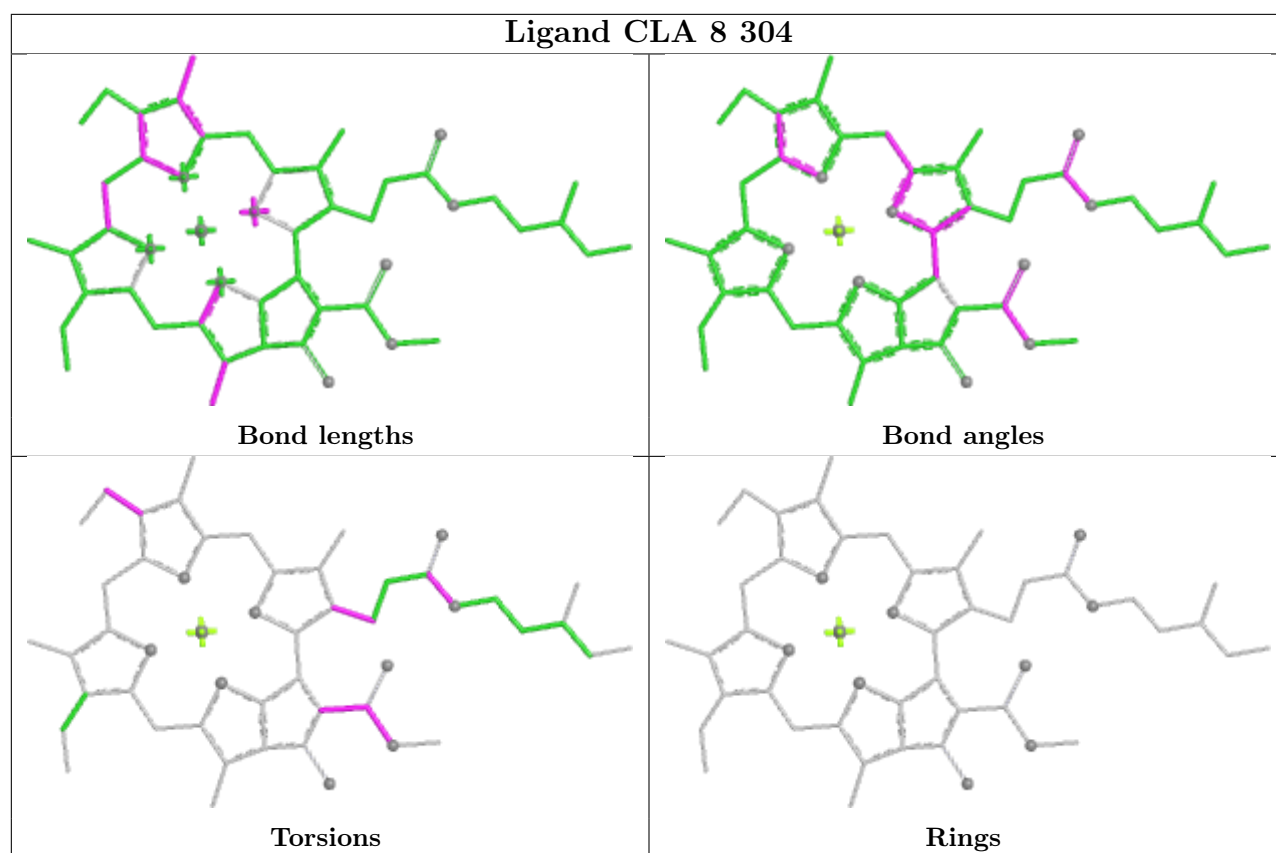
Ligand LUT b 615



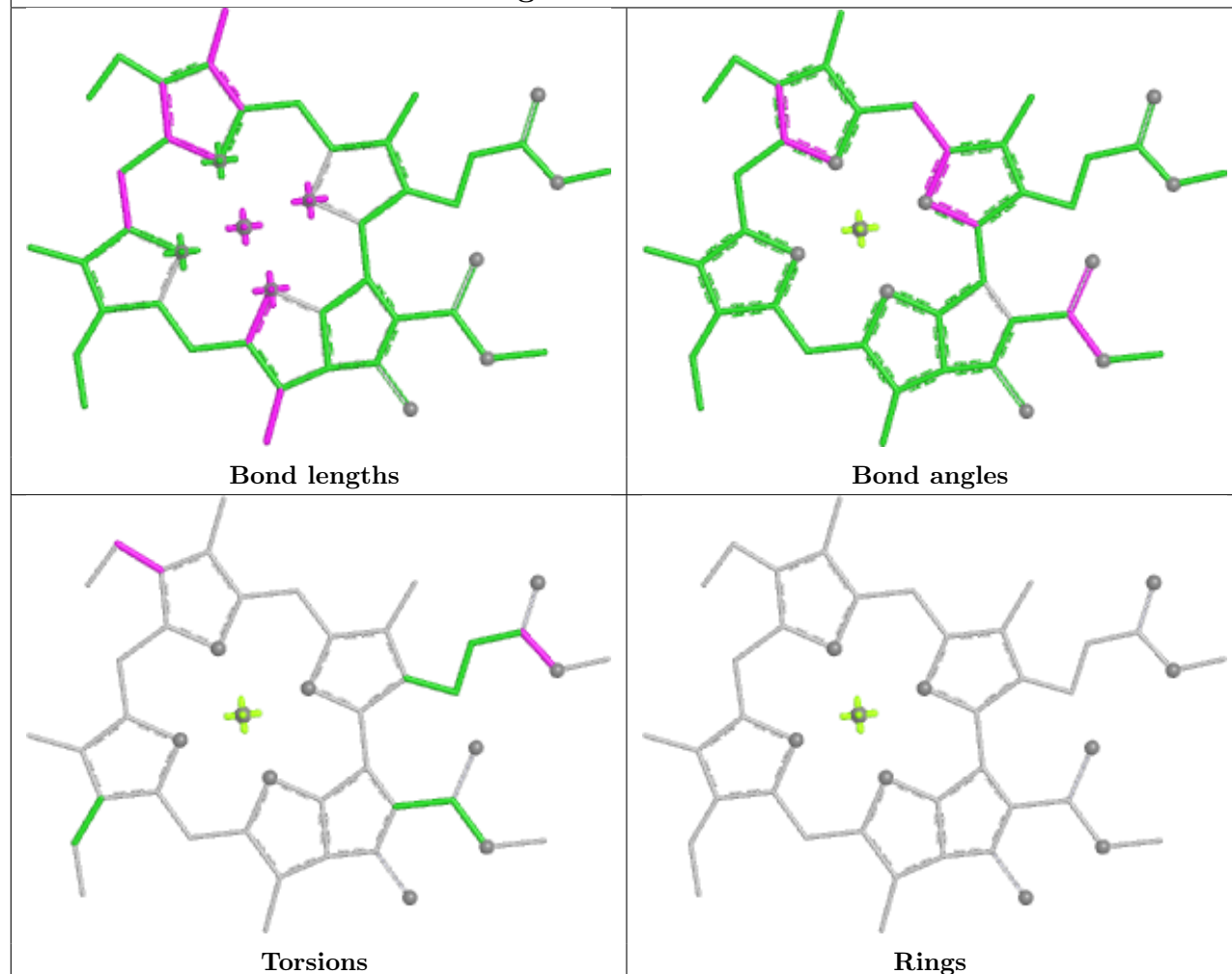
Ligand BCR B 844



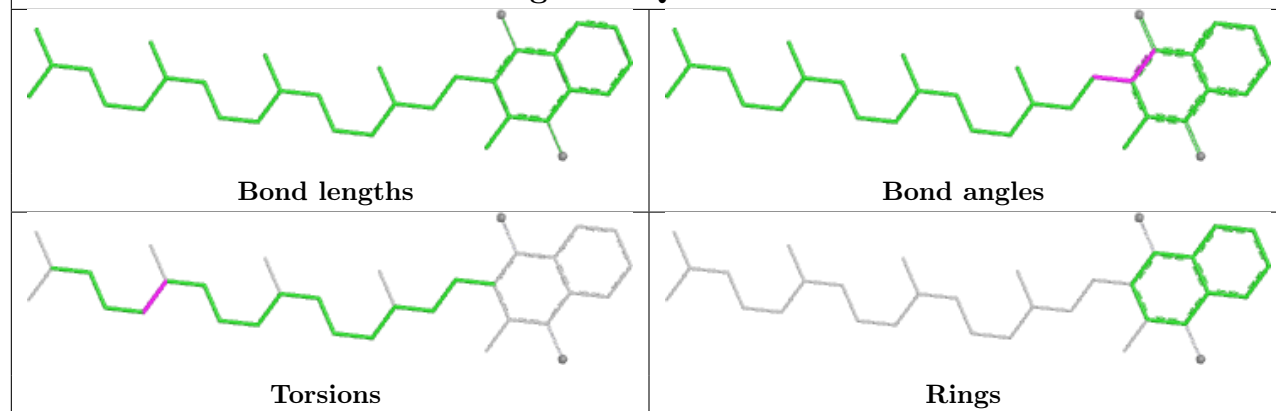




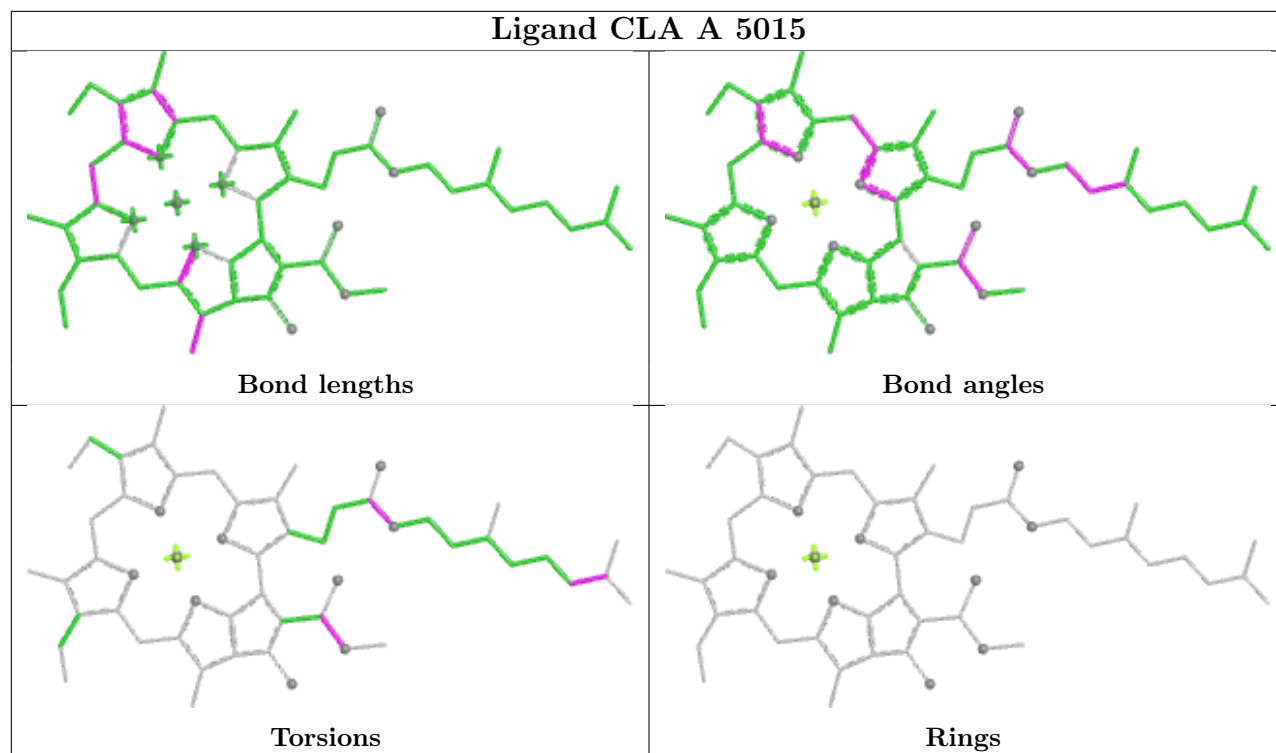
Ligand CLA a 607



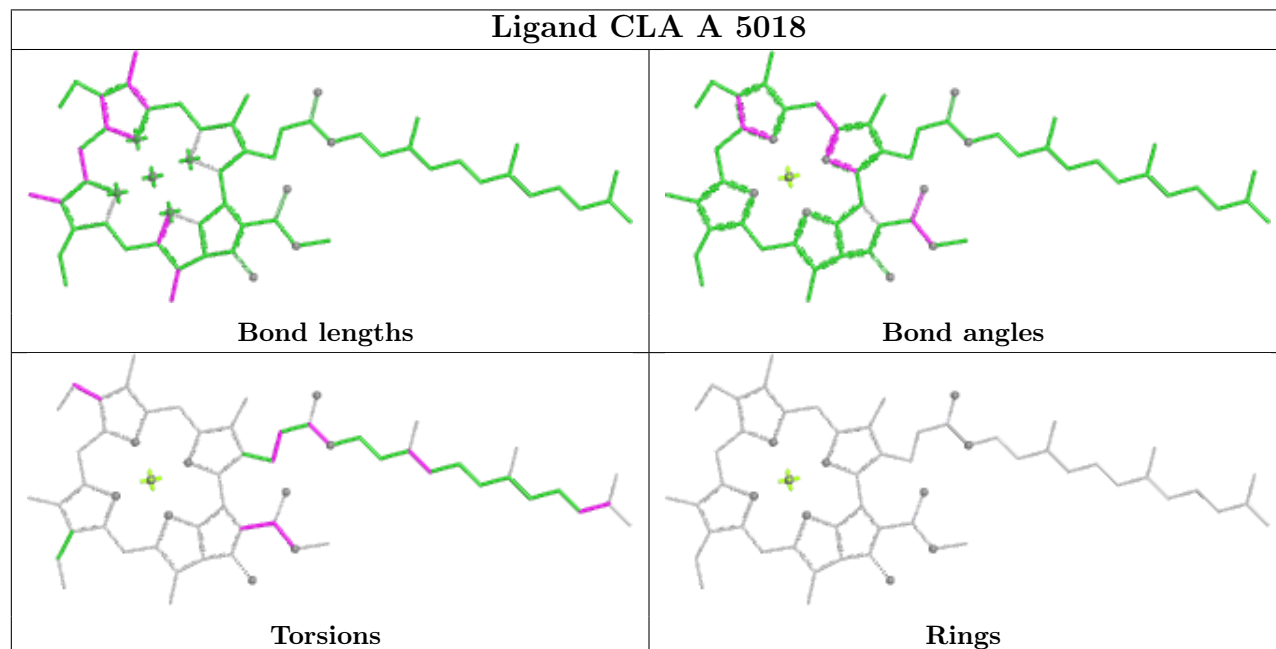
Ligand PQN B 842



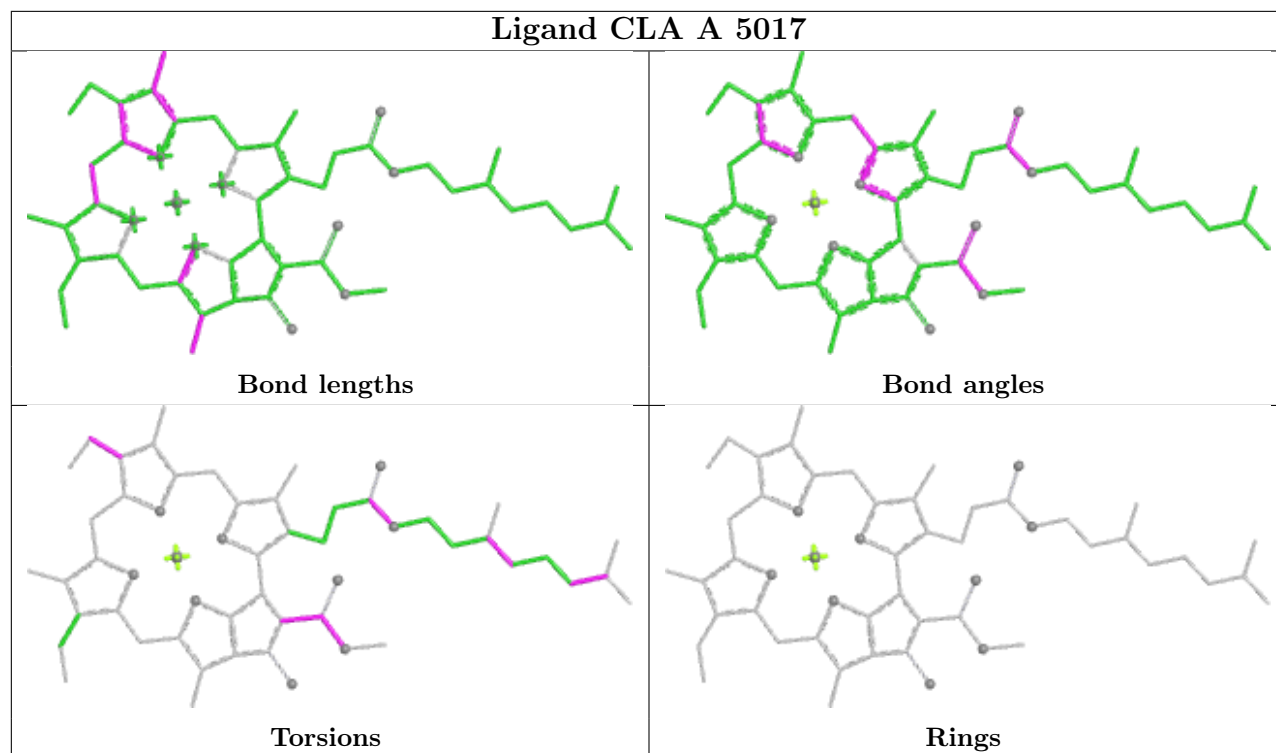
Ligand CLA A 5015



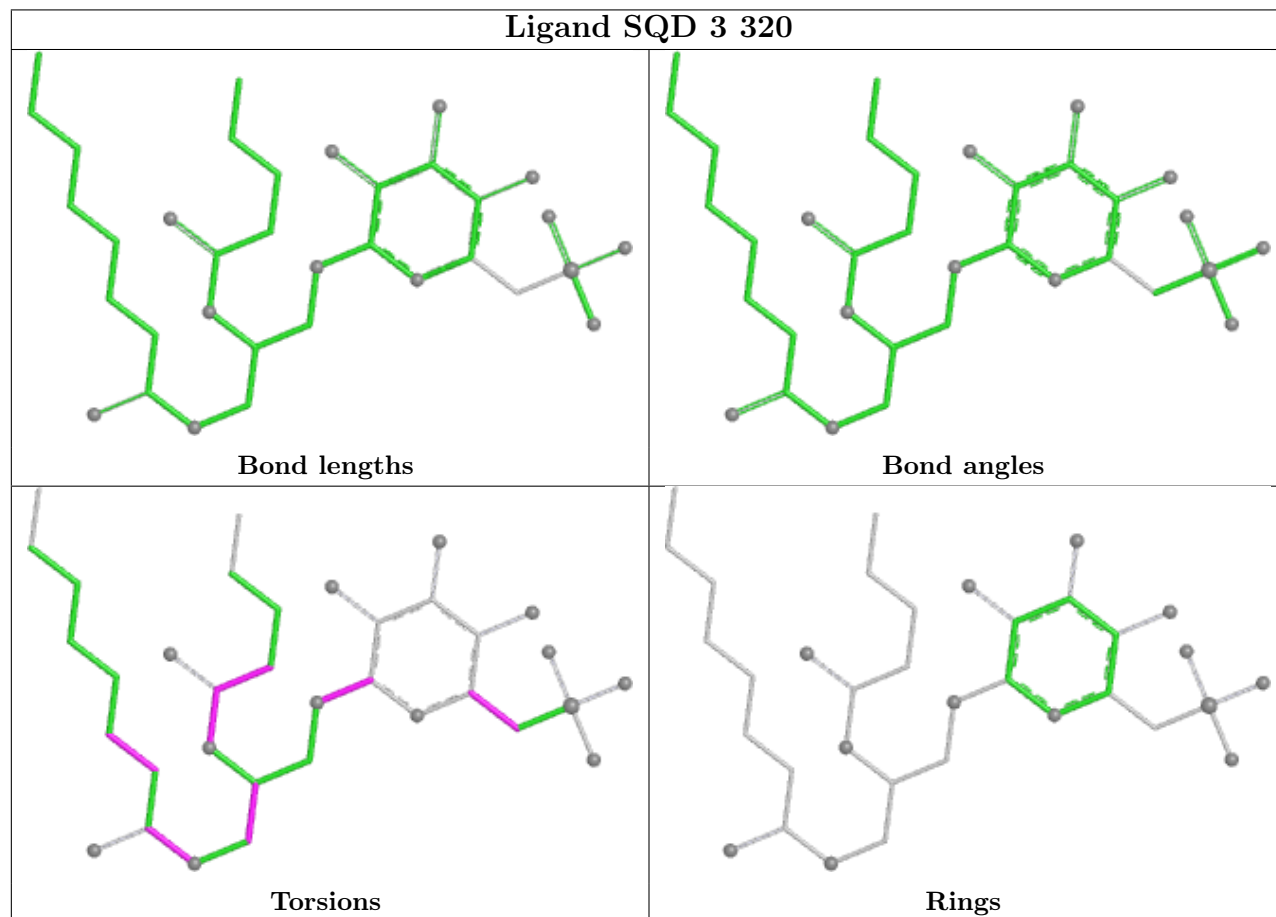
Ligand CLA A 5018



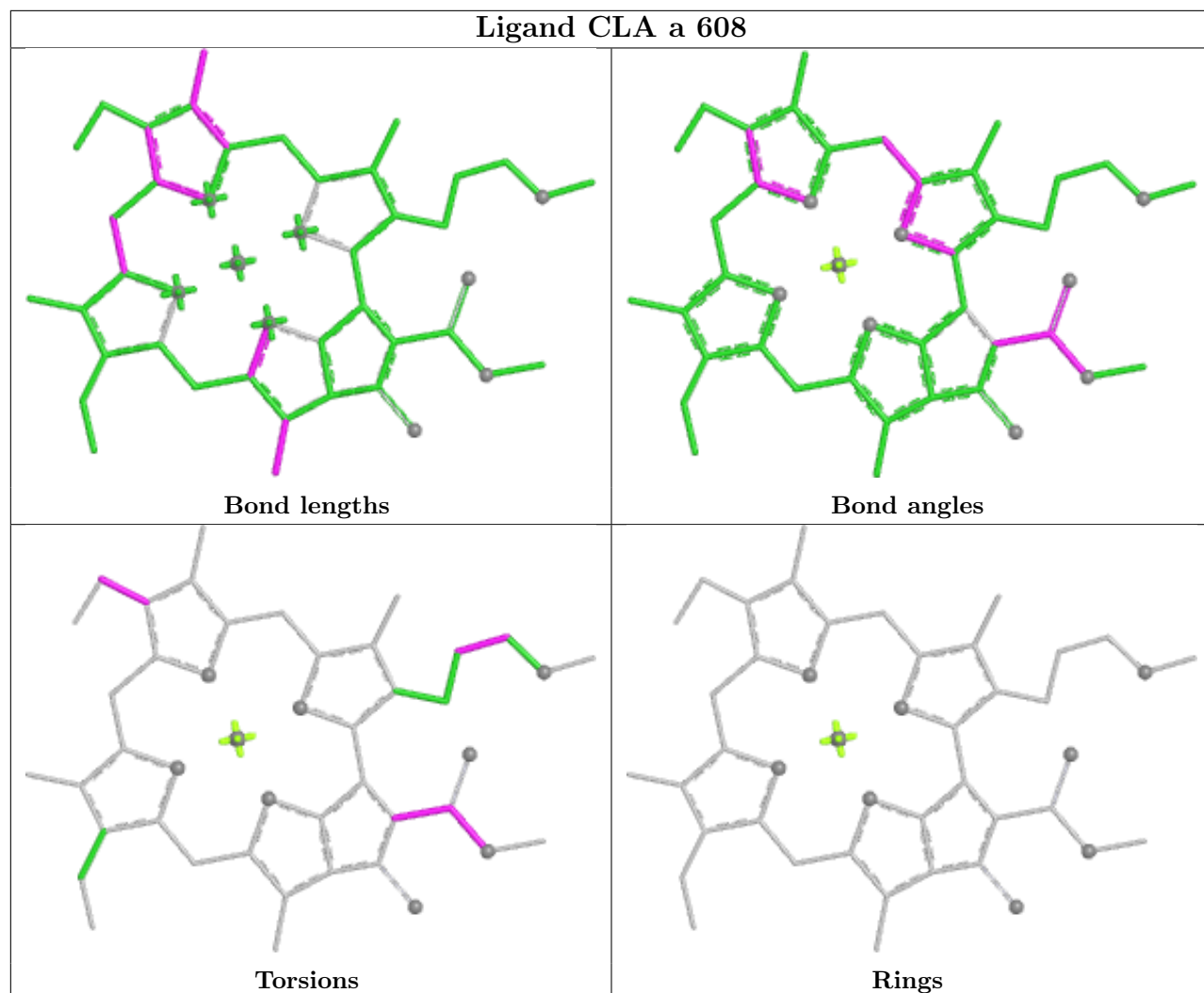
Ligand CLA A 5017



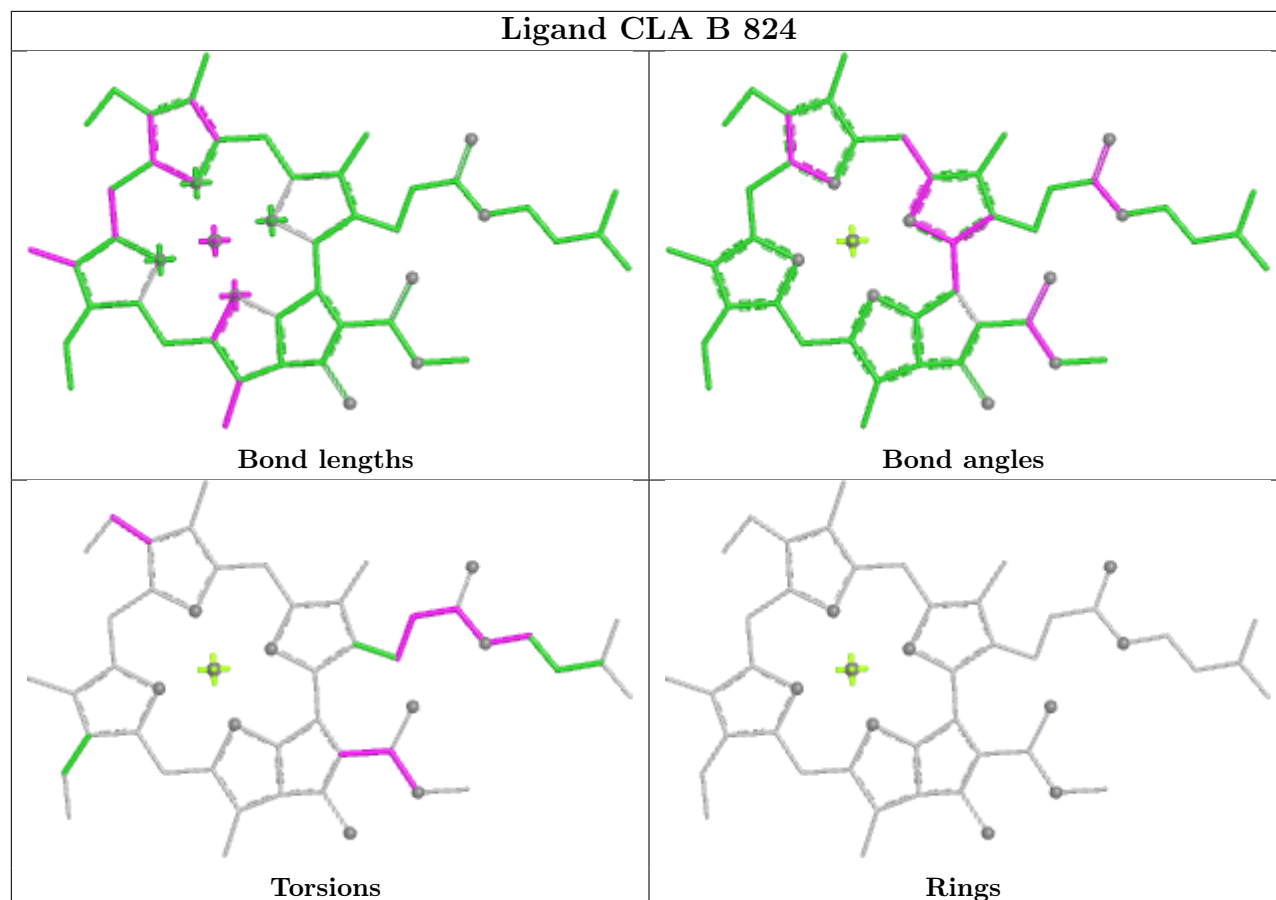
Ligand SQD 3 320



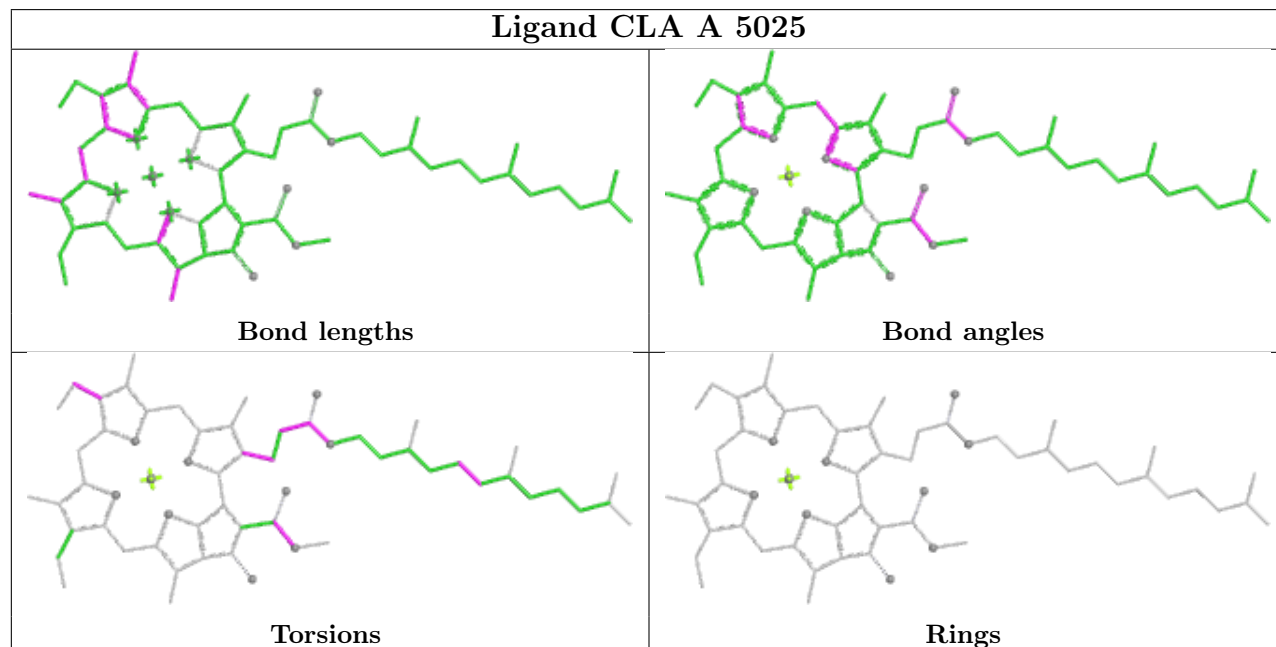
Ligand CLA a 608

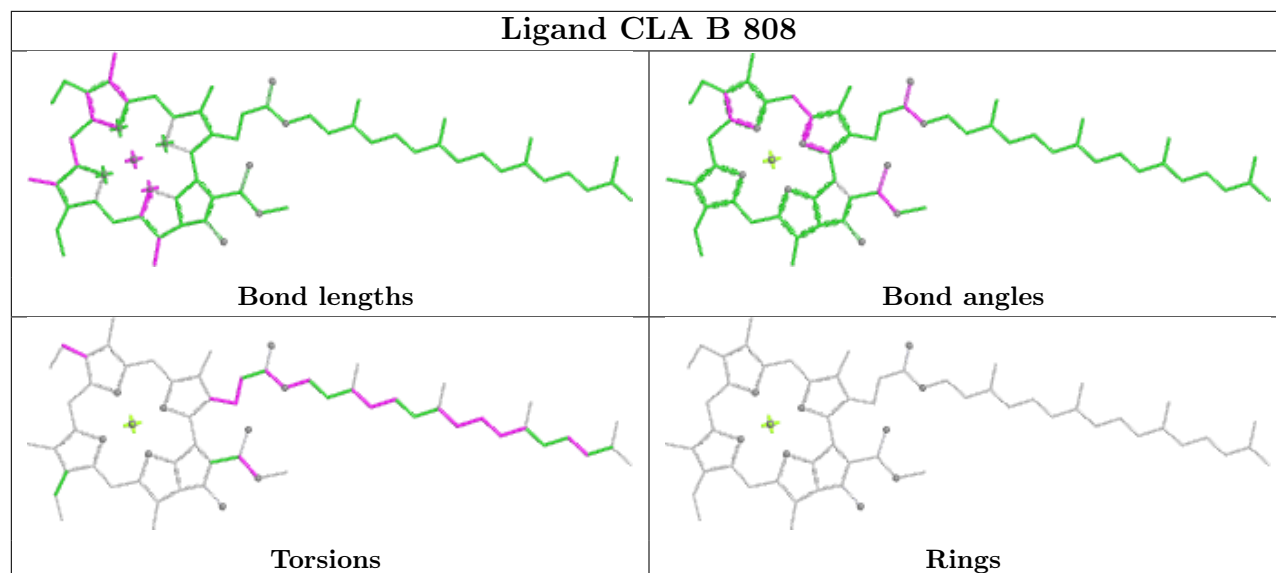
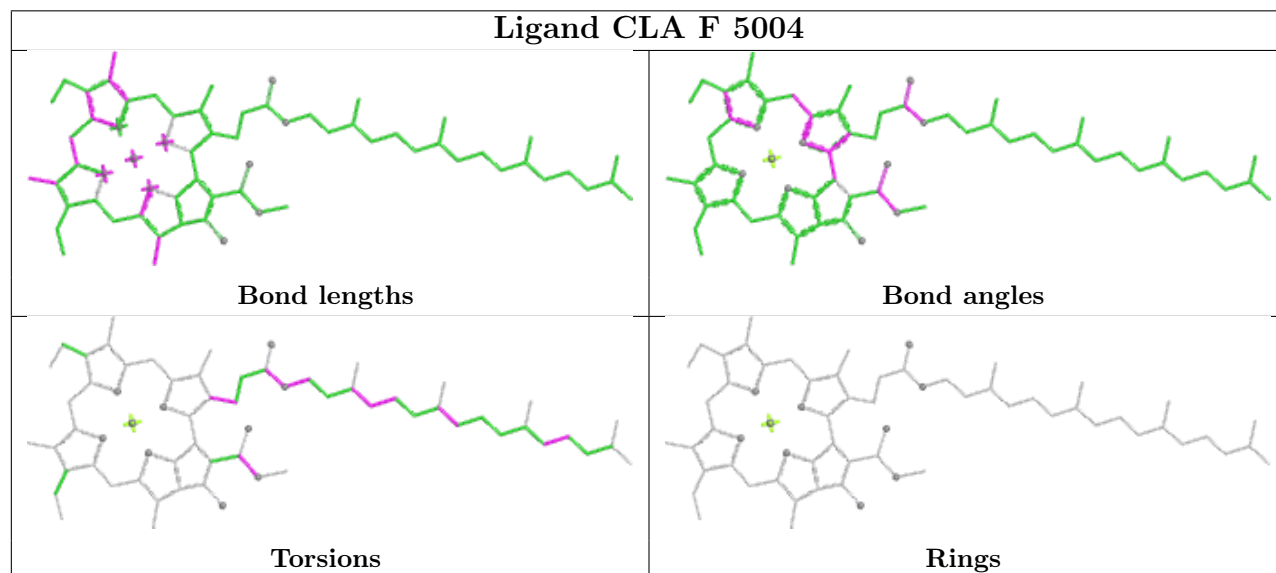
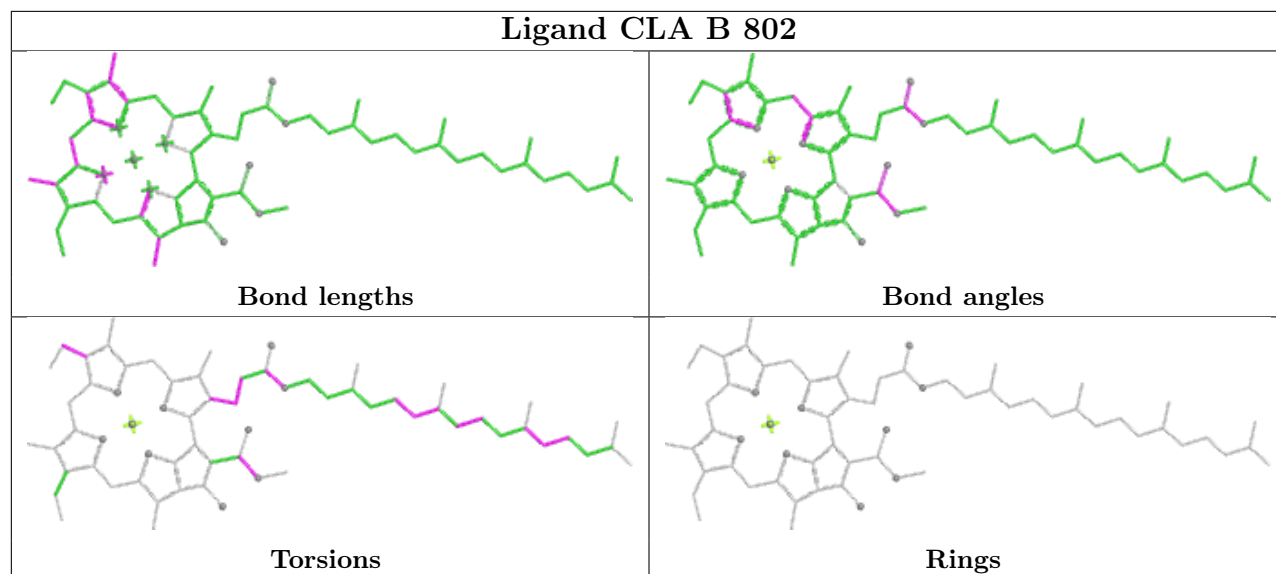


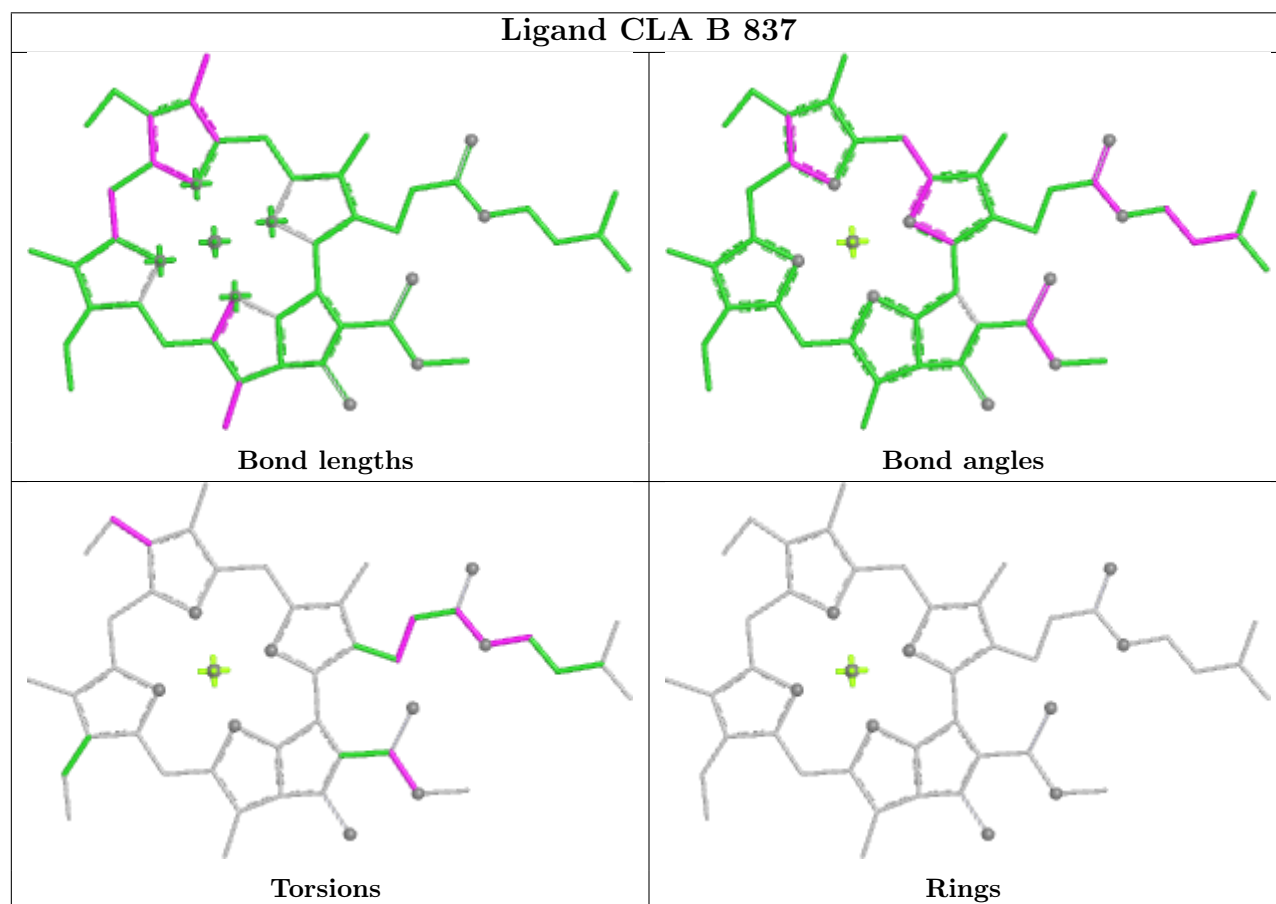
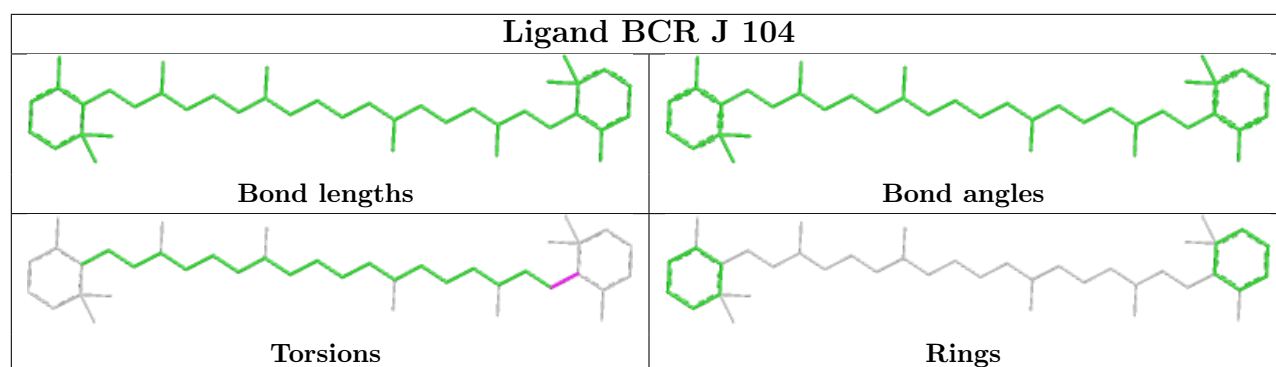
Ligand CLA B 824

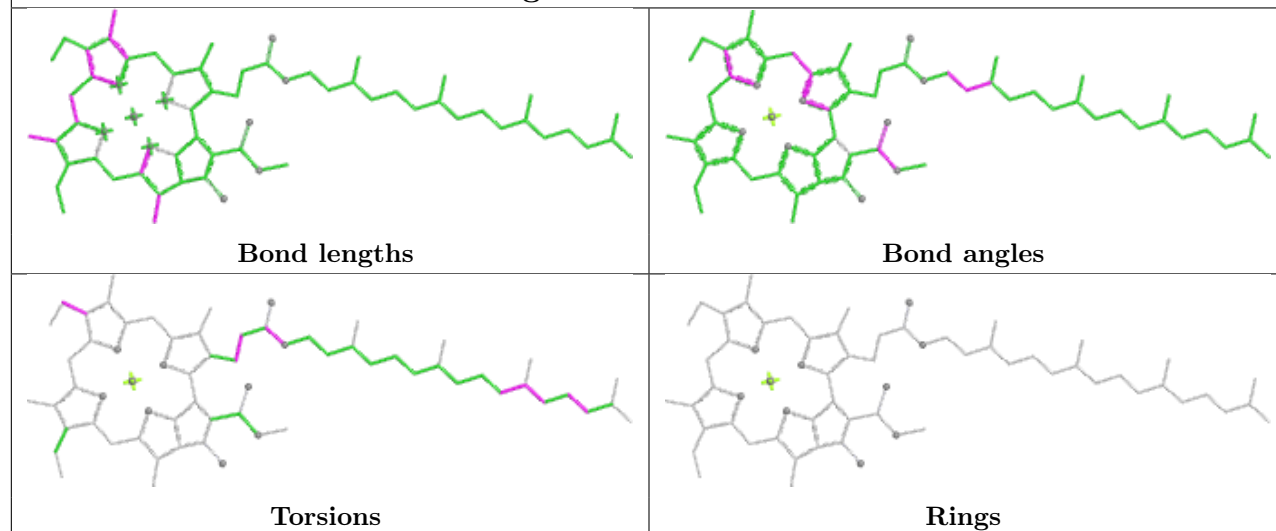
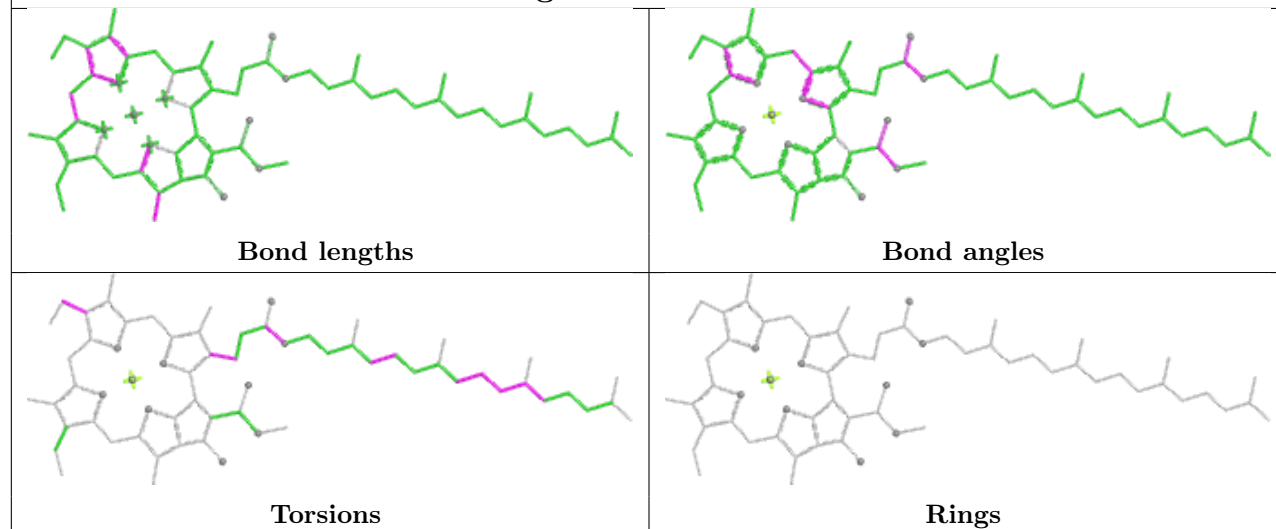


Ligand CLA A 5025

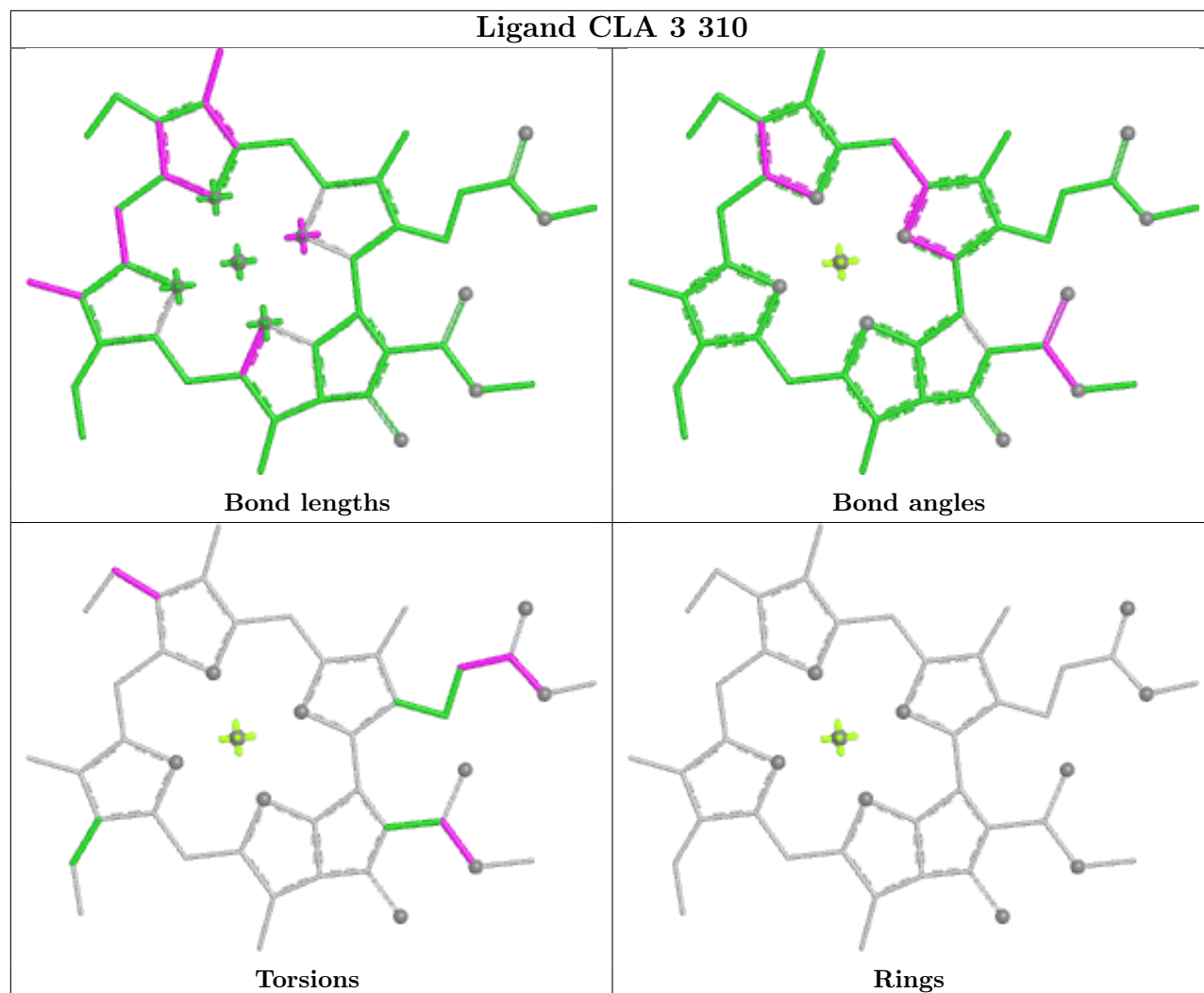


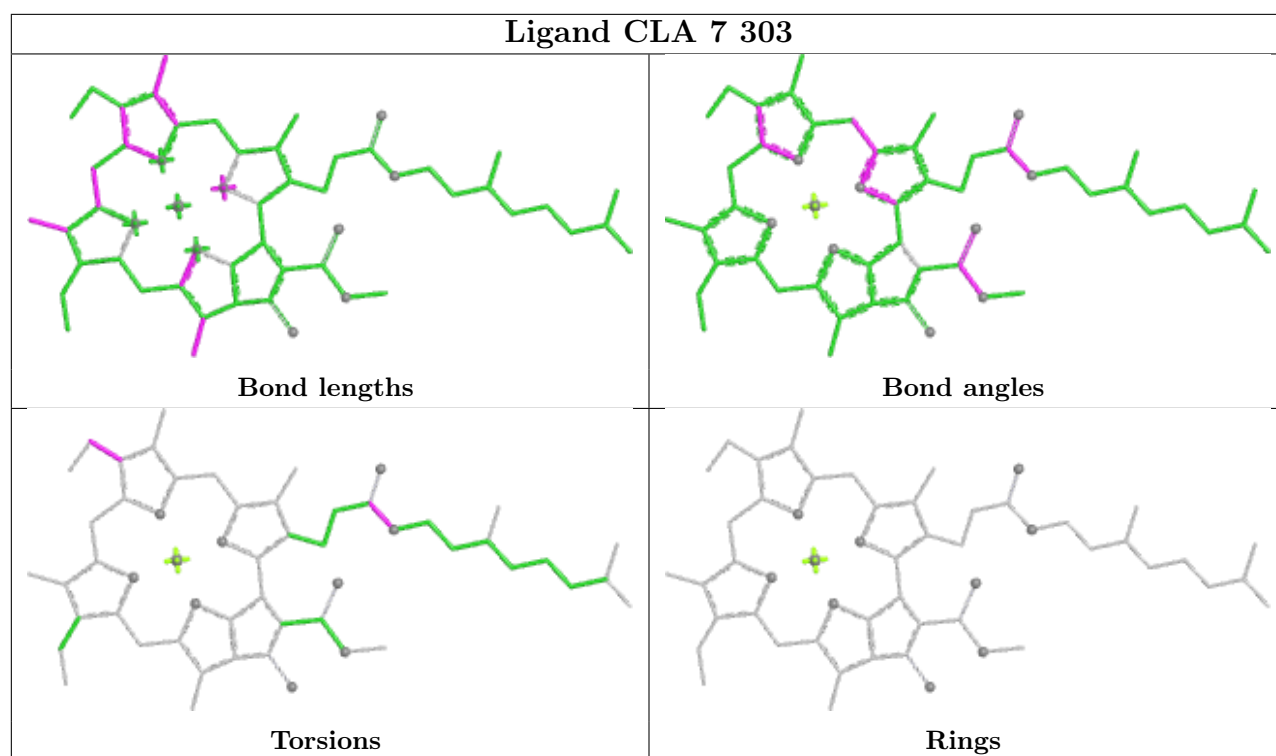




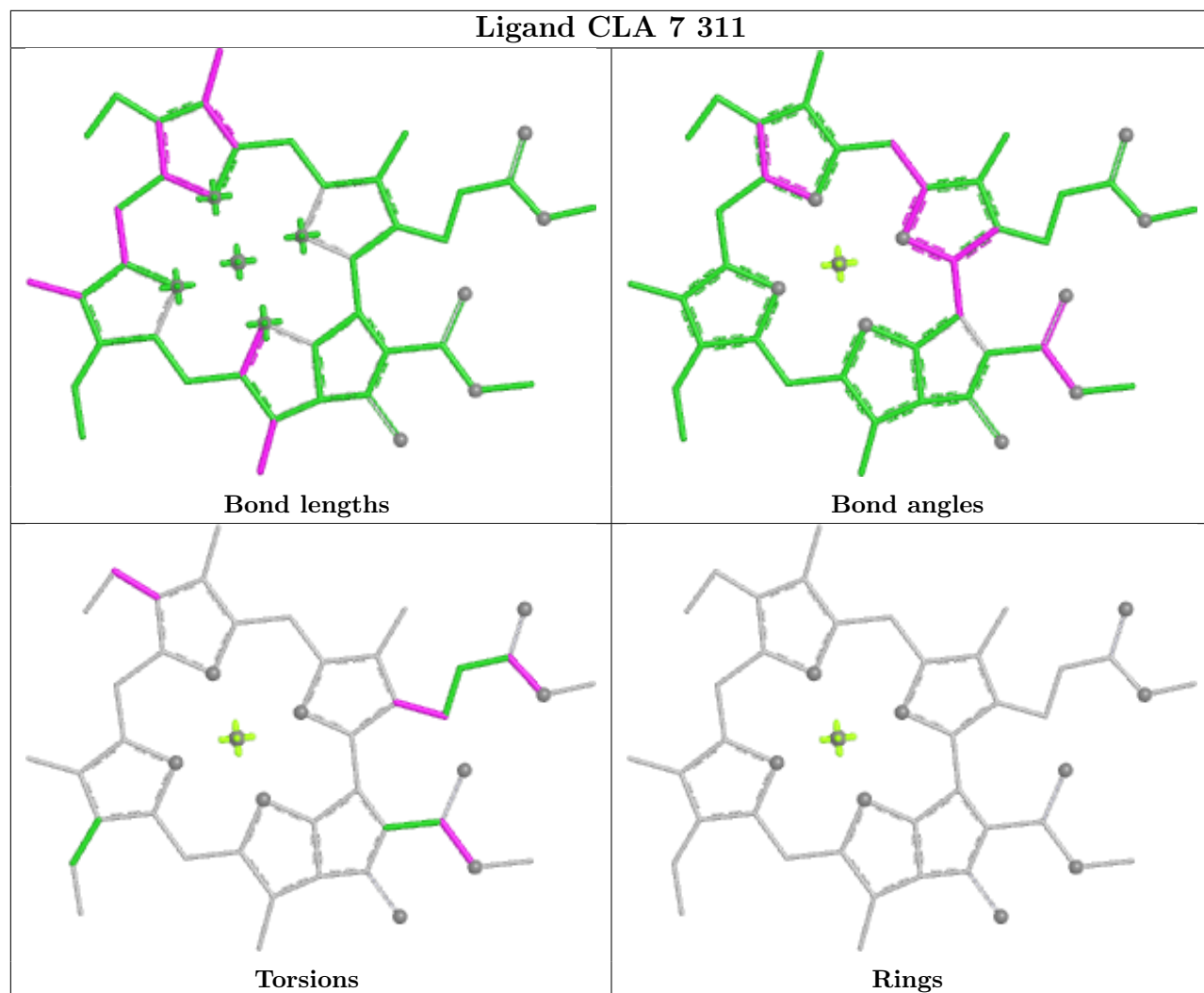
Ligand CLA A 5030**Ligand CLA 1 607**

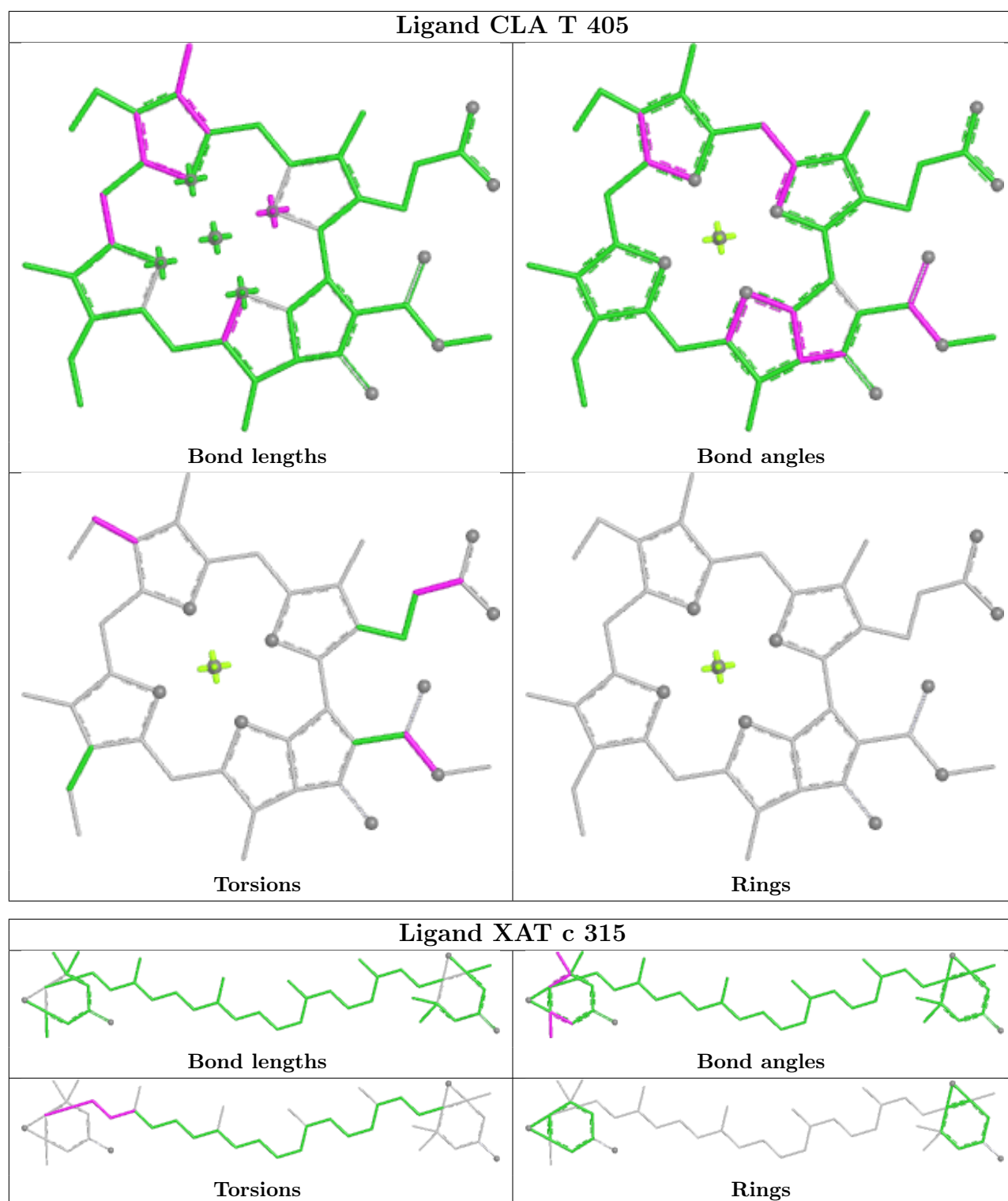
Ligand CLA 3 310

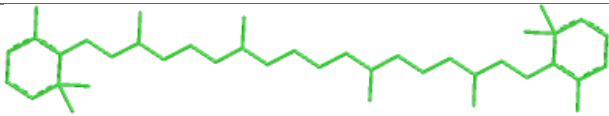
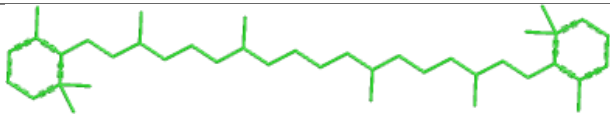
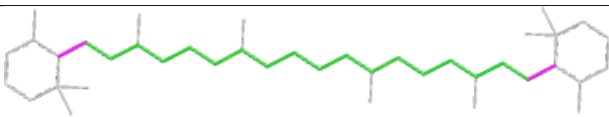
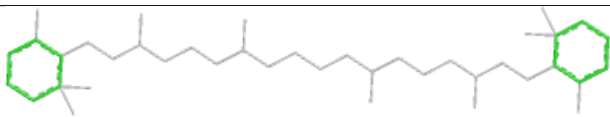


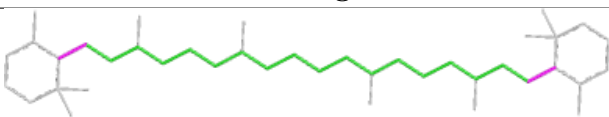
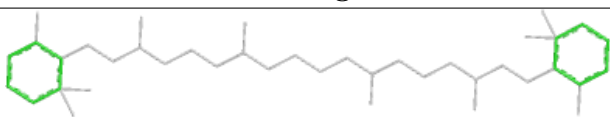


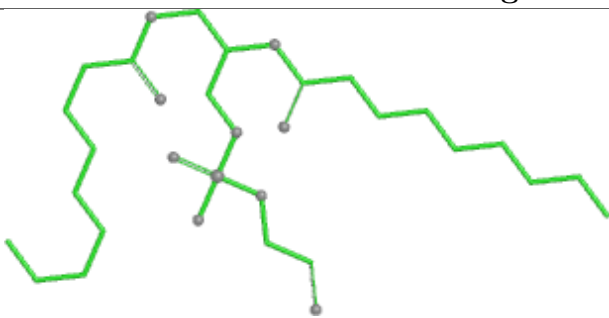
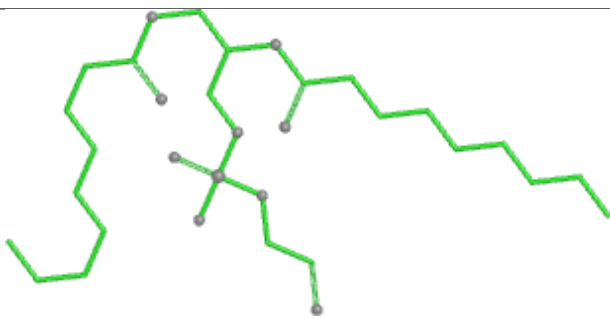
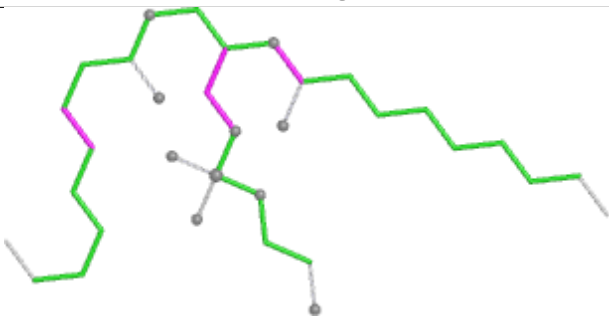
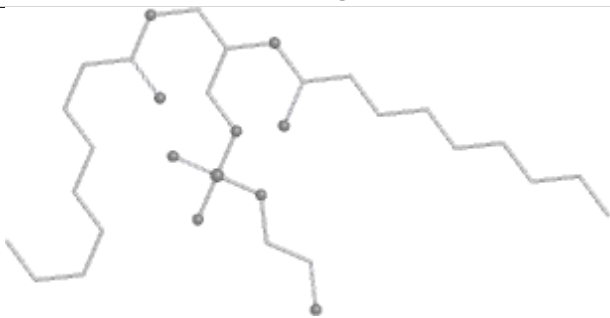
Ligand CLA 7 311

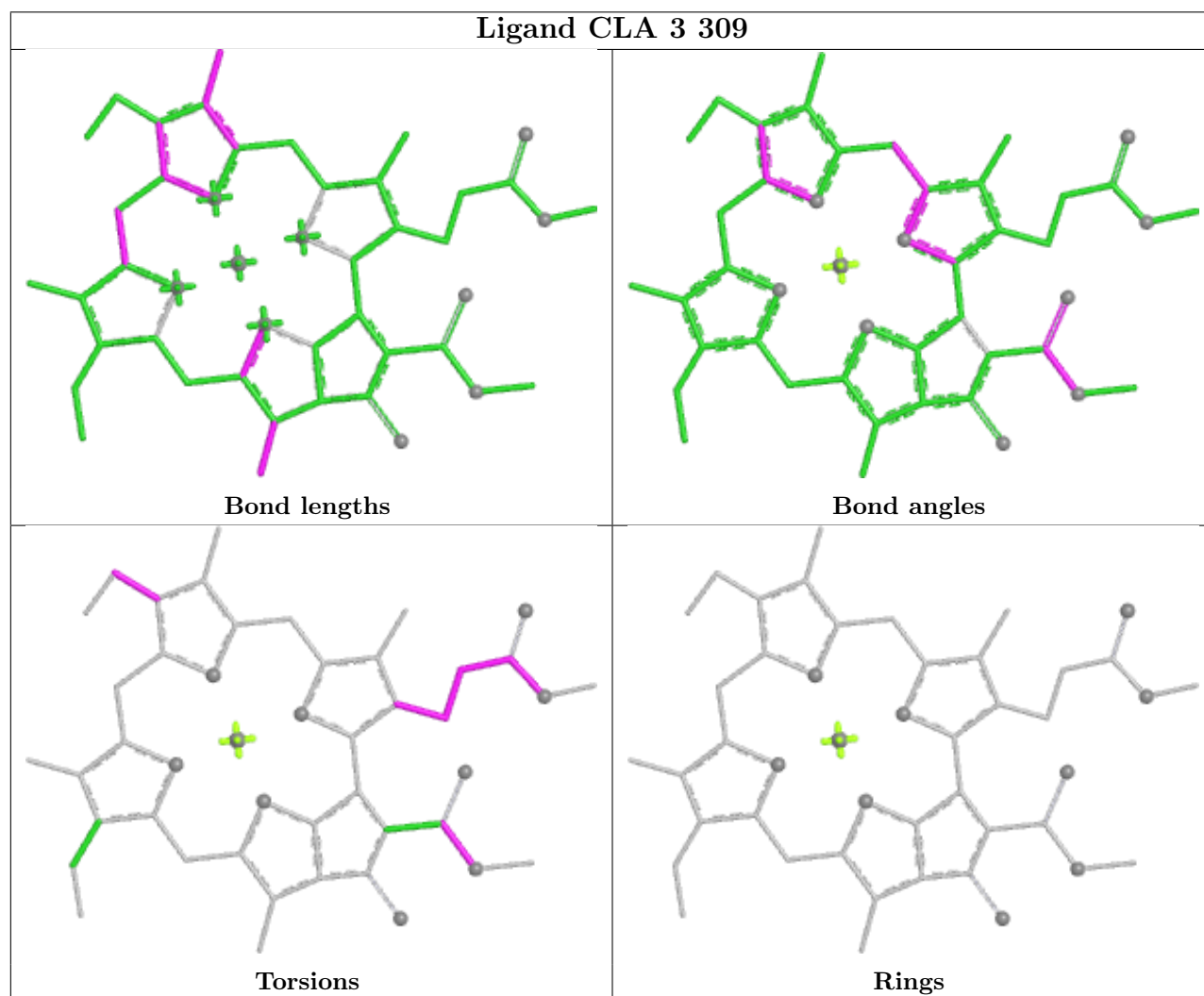
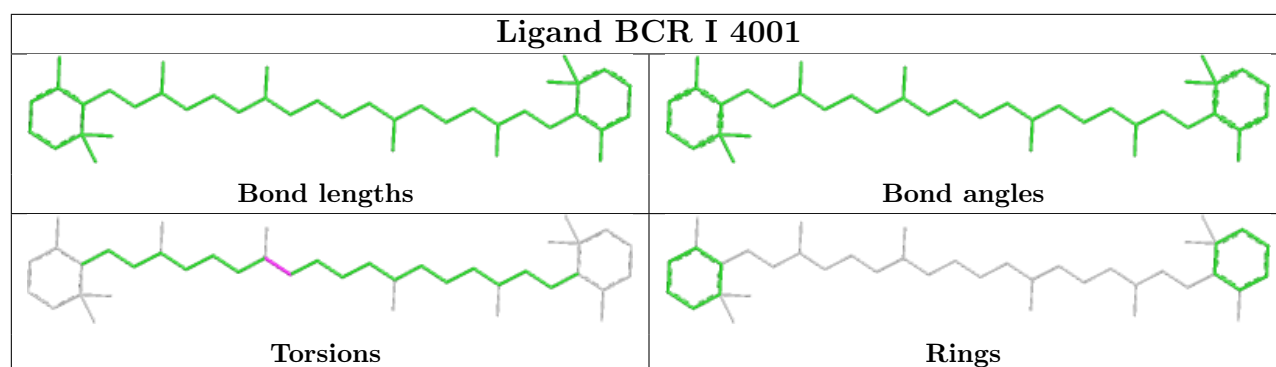




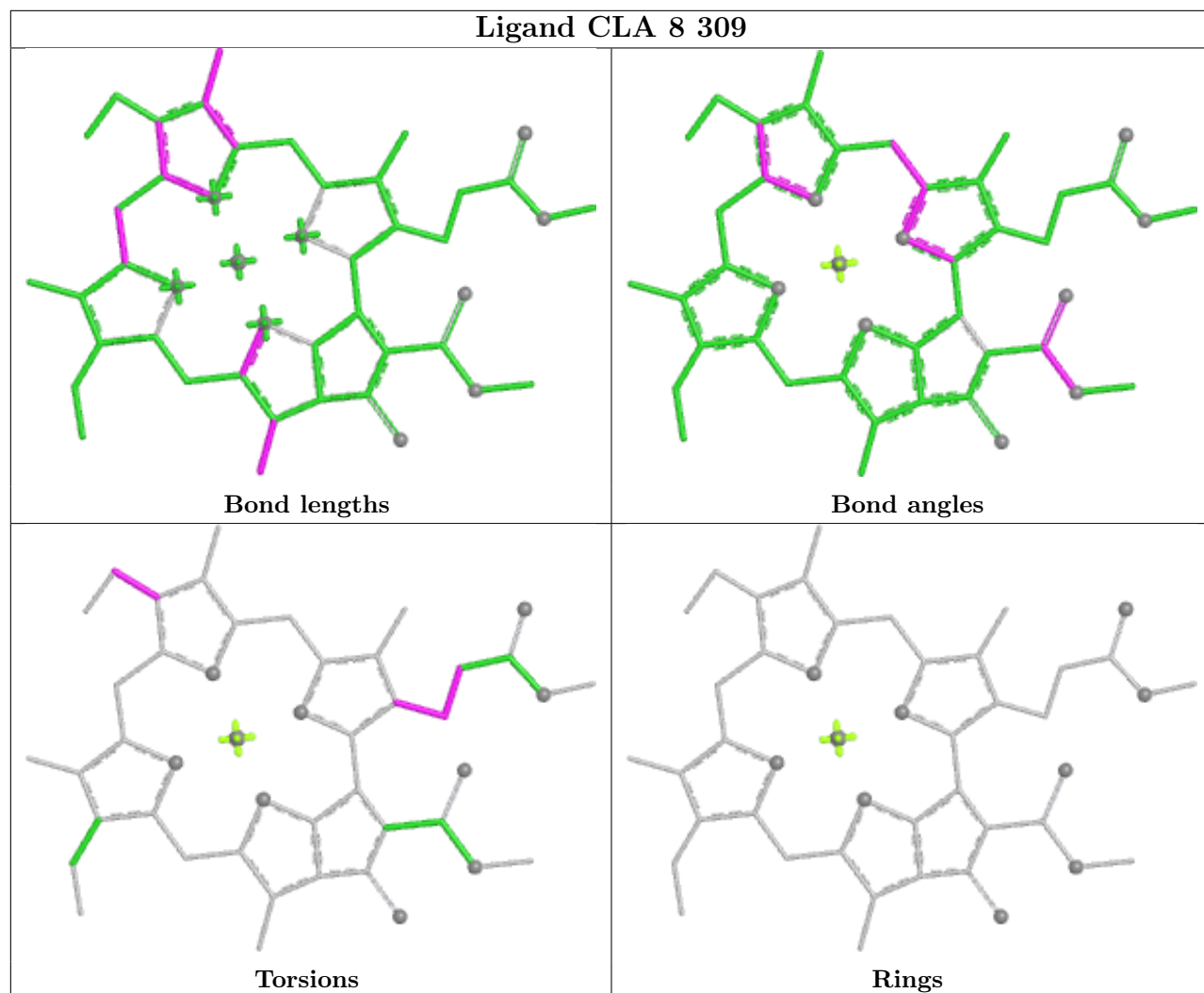
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 3 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

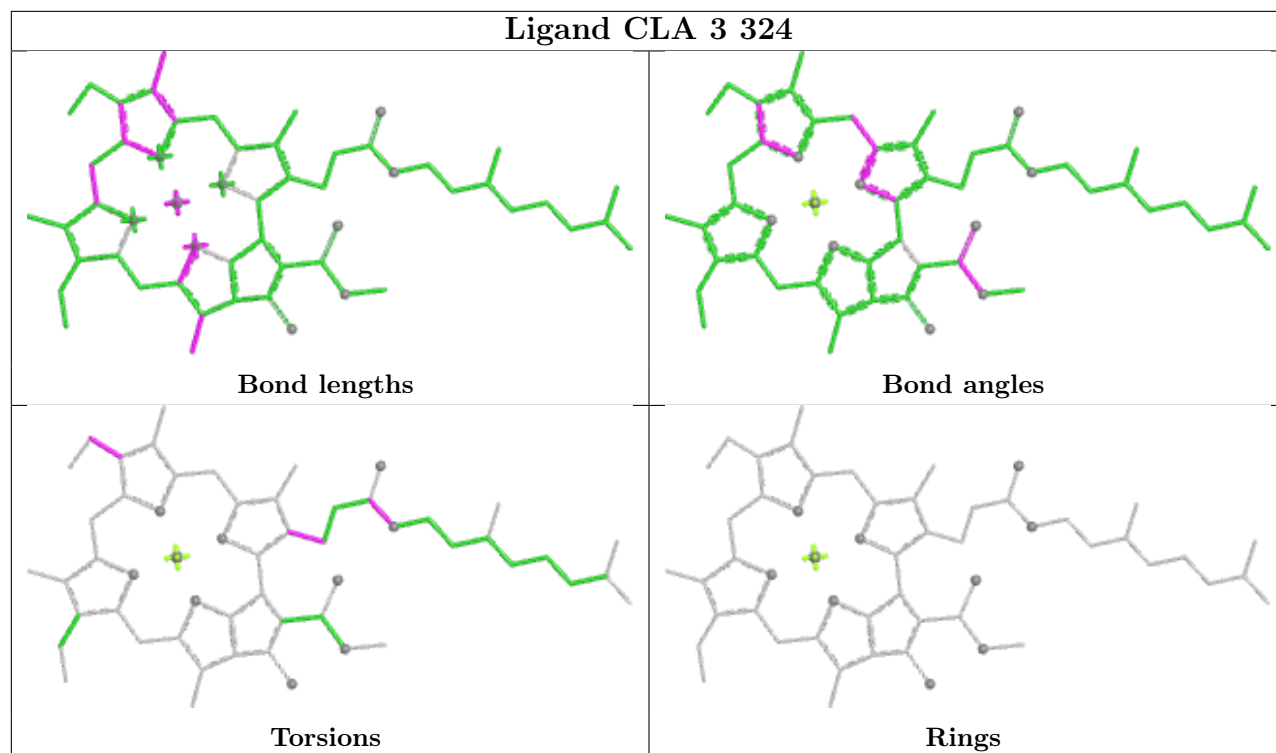
Ligand PTY F 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings



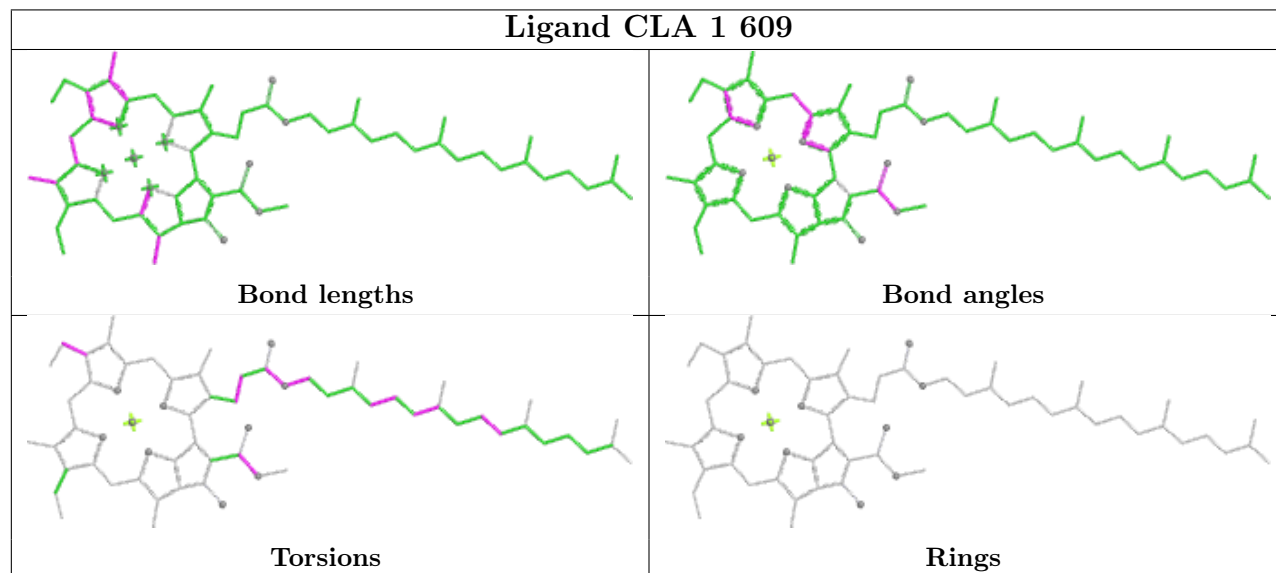
Ligand CLA 8 309

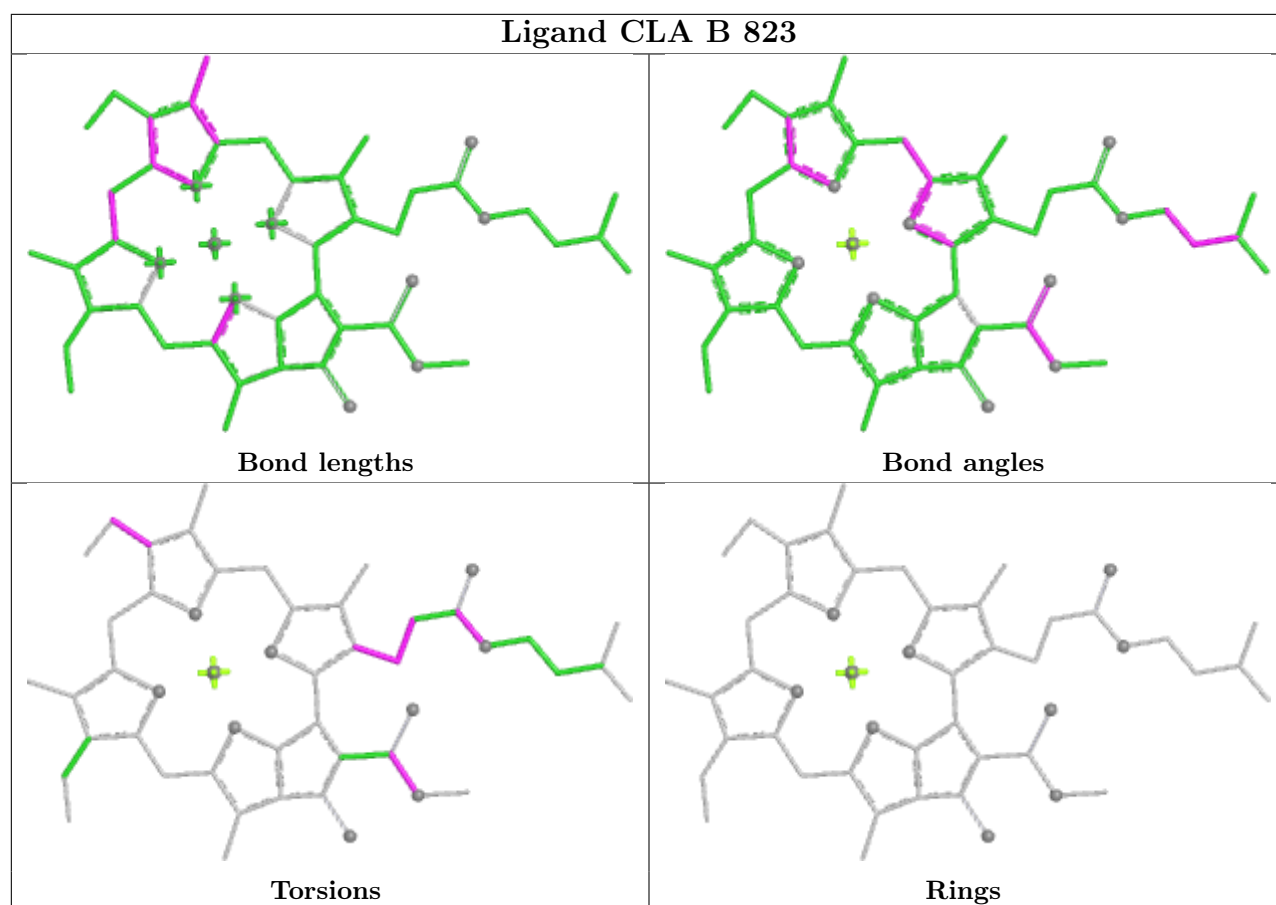


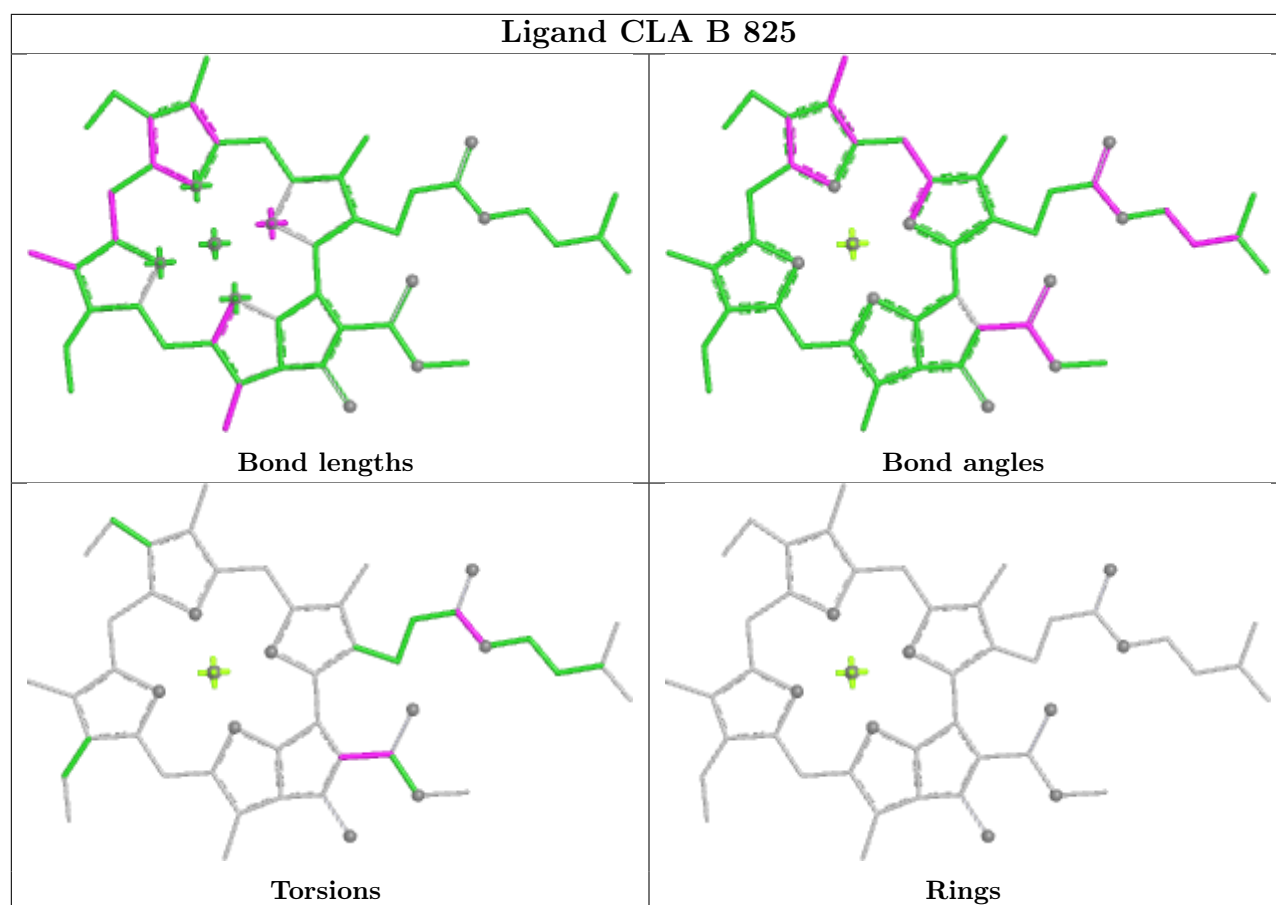
Ligand CLA 3 324



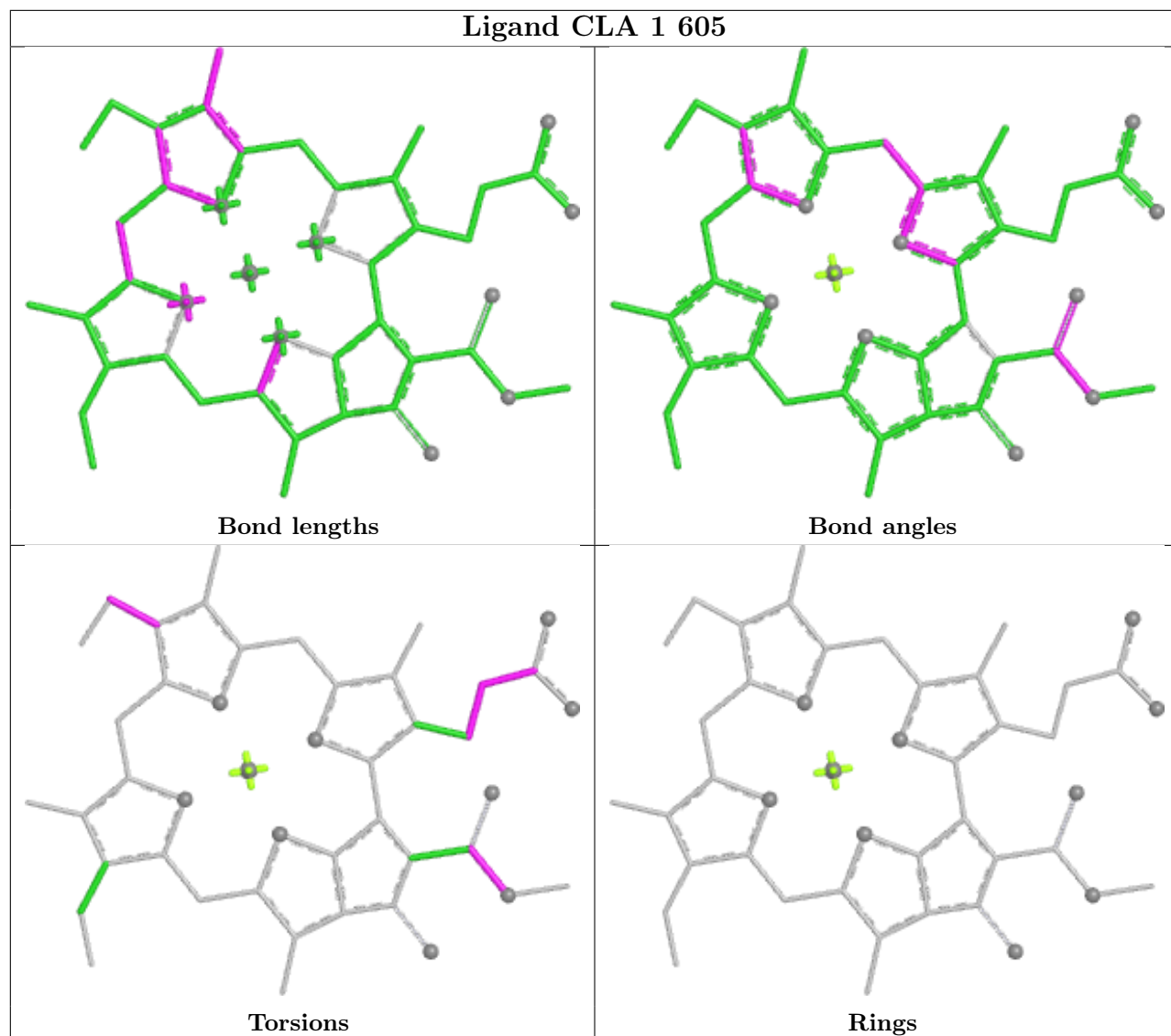
Ligand CLA 1 609



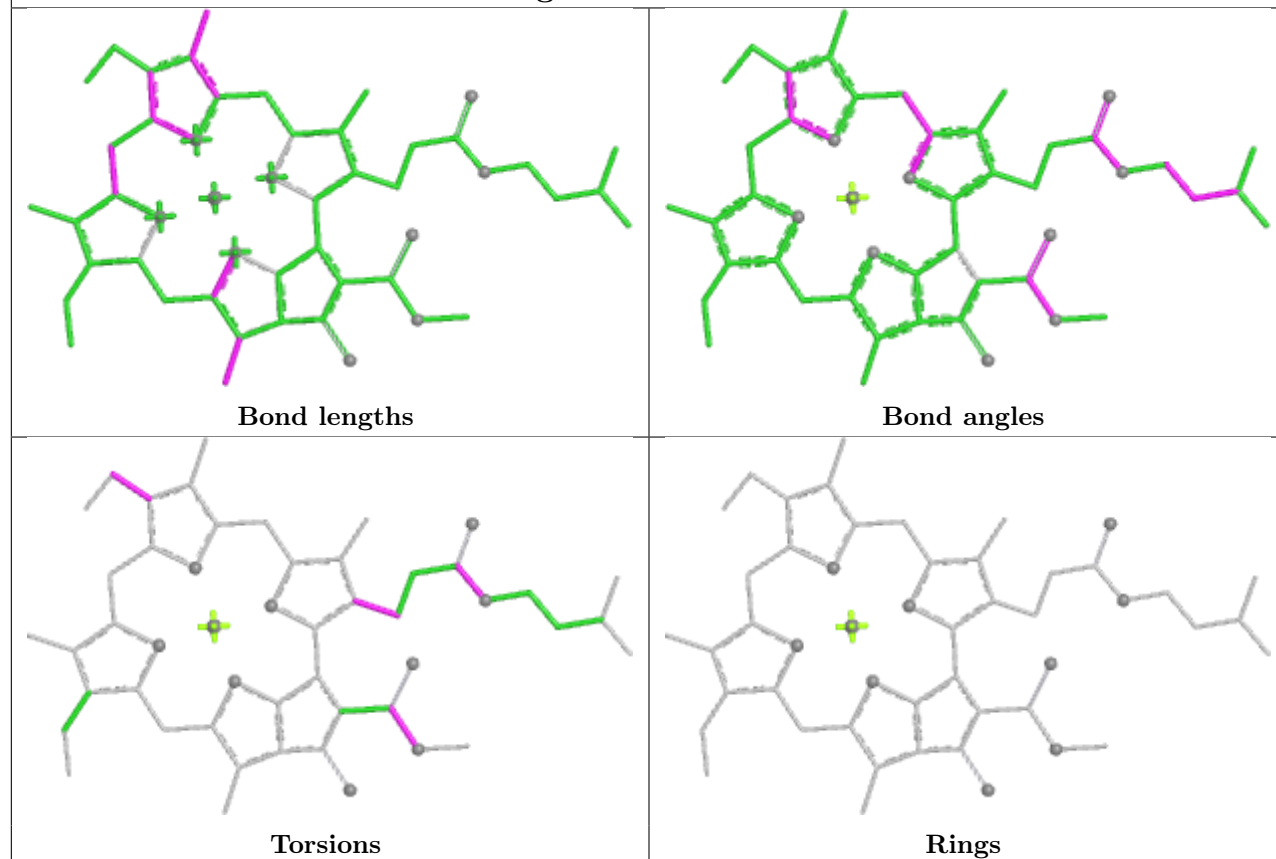




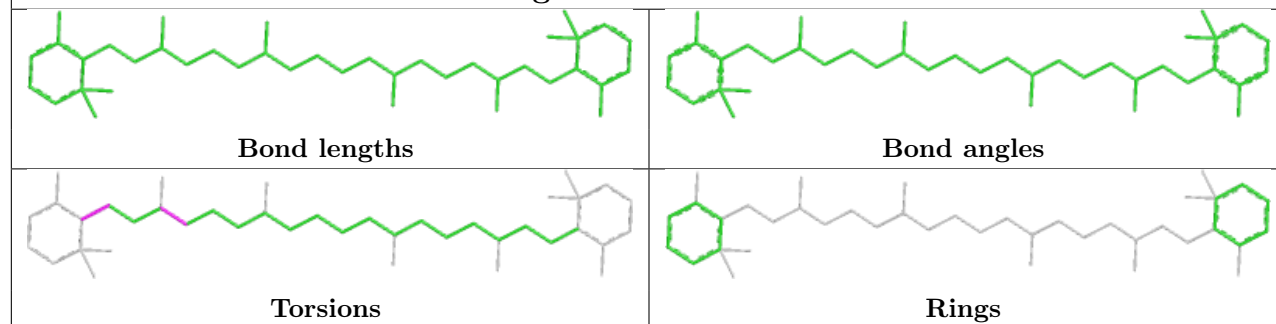
Ligand CLA 1 605



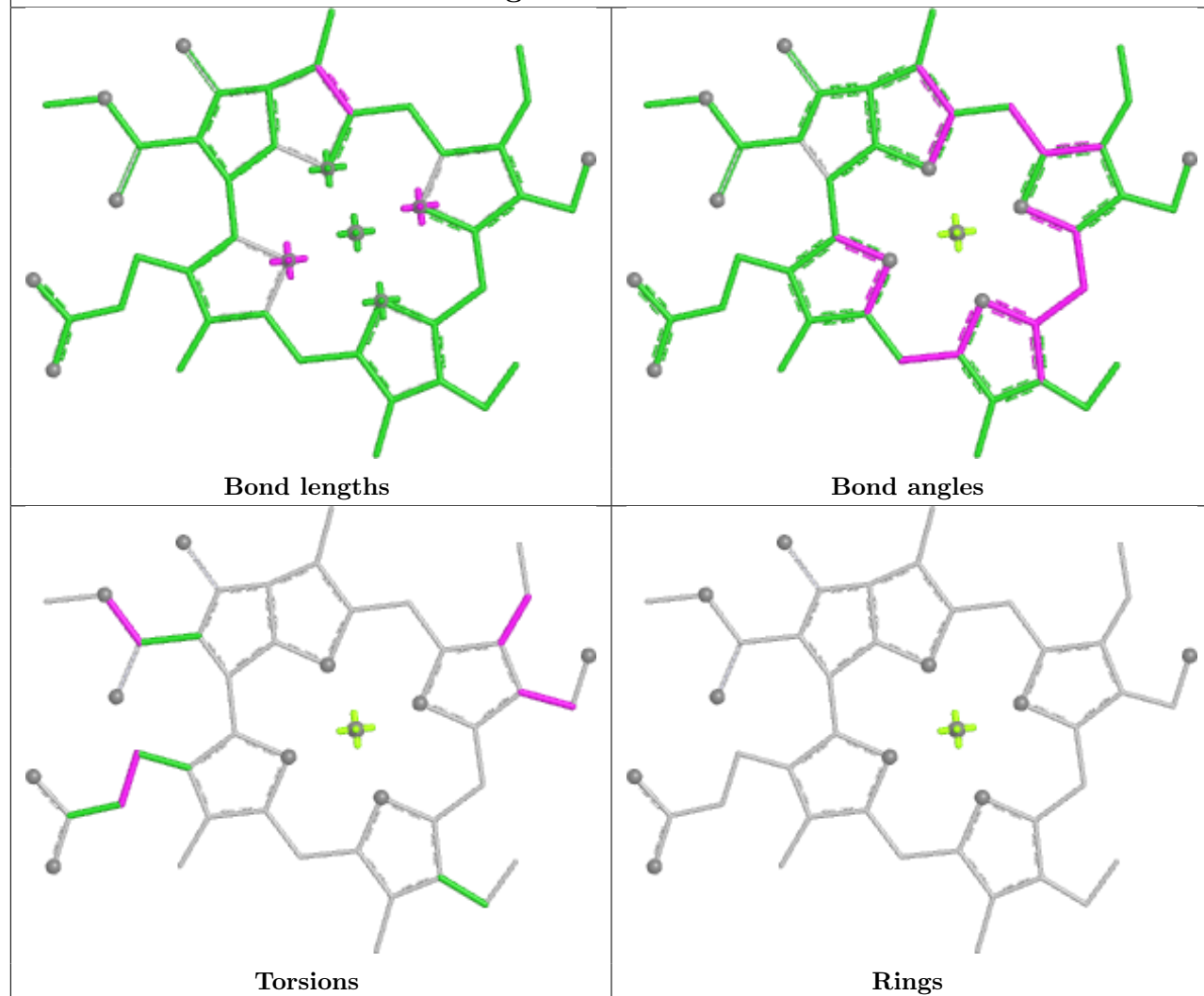
Ligand CLA 8 303



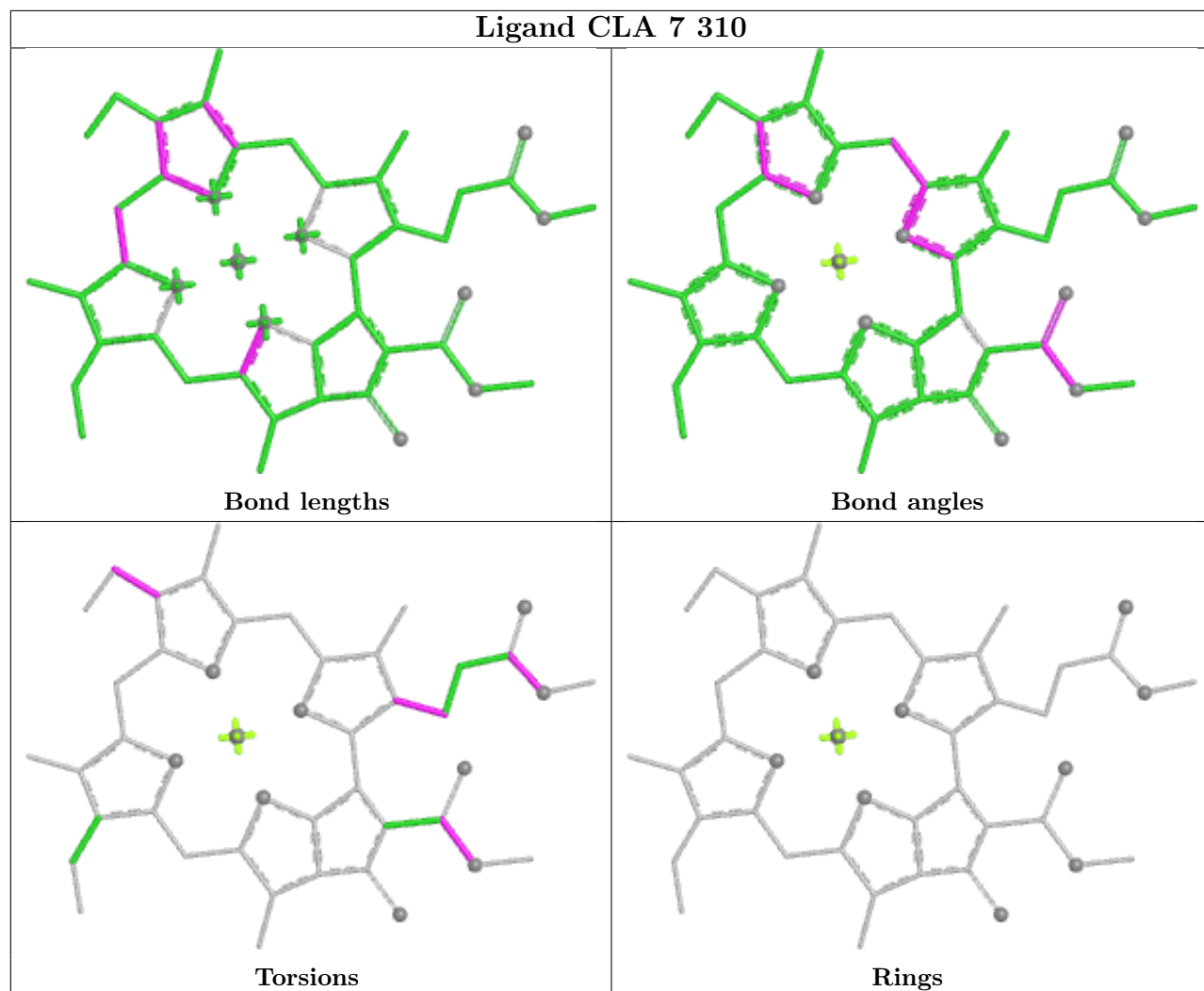
Ligand BCR L 204



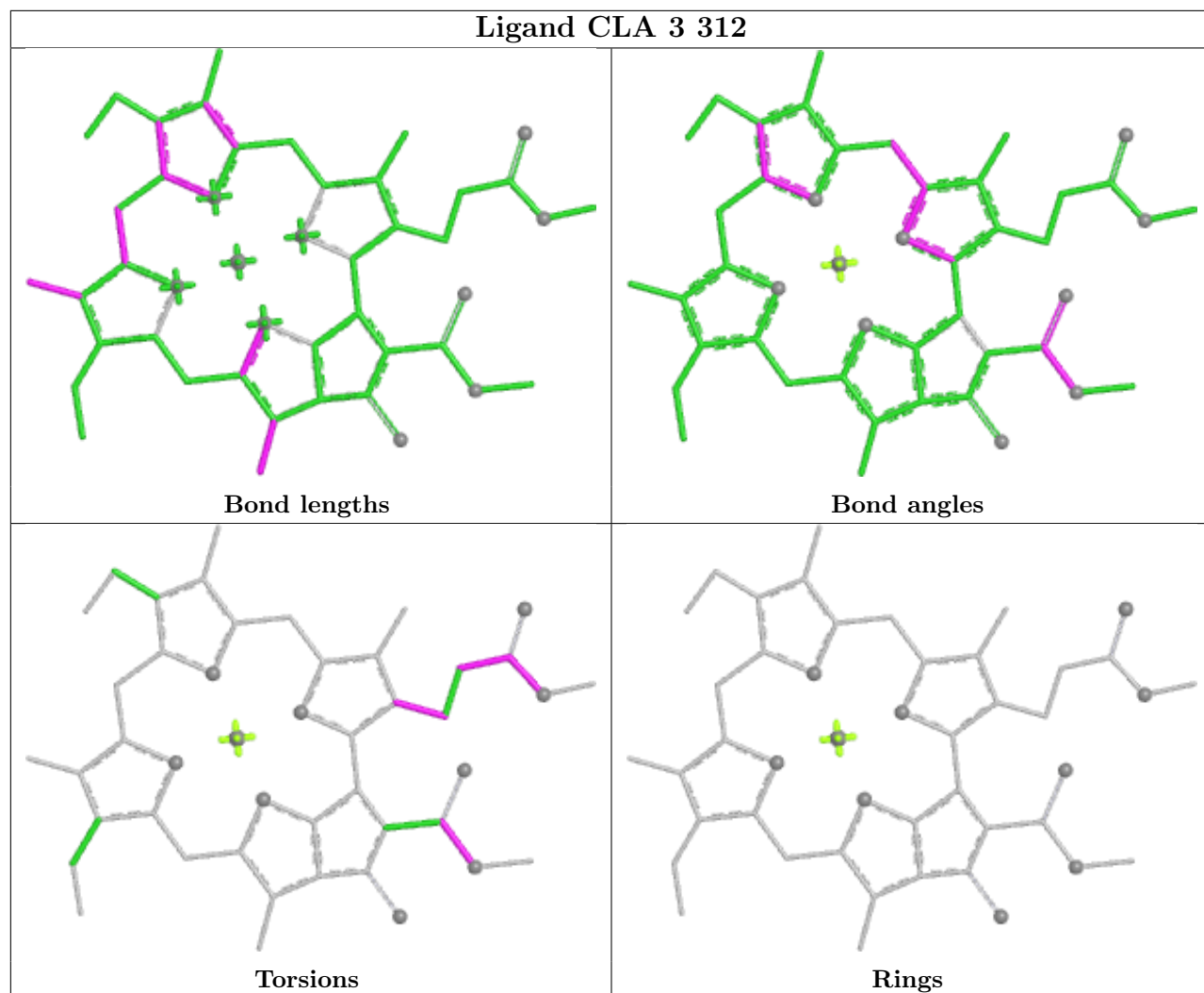
Ligand CHL c 304

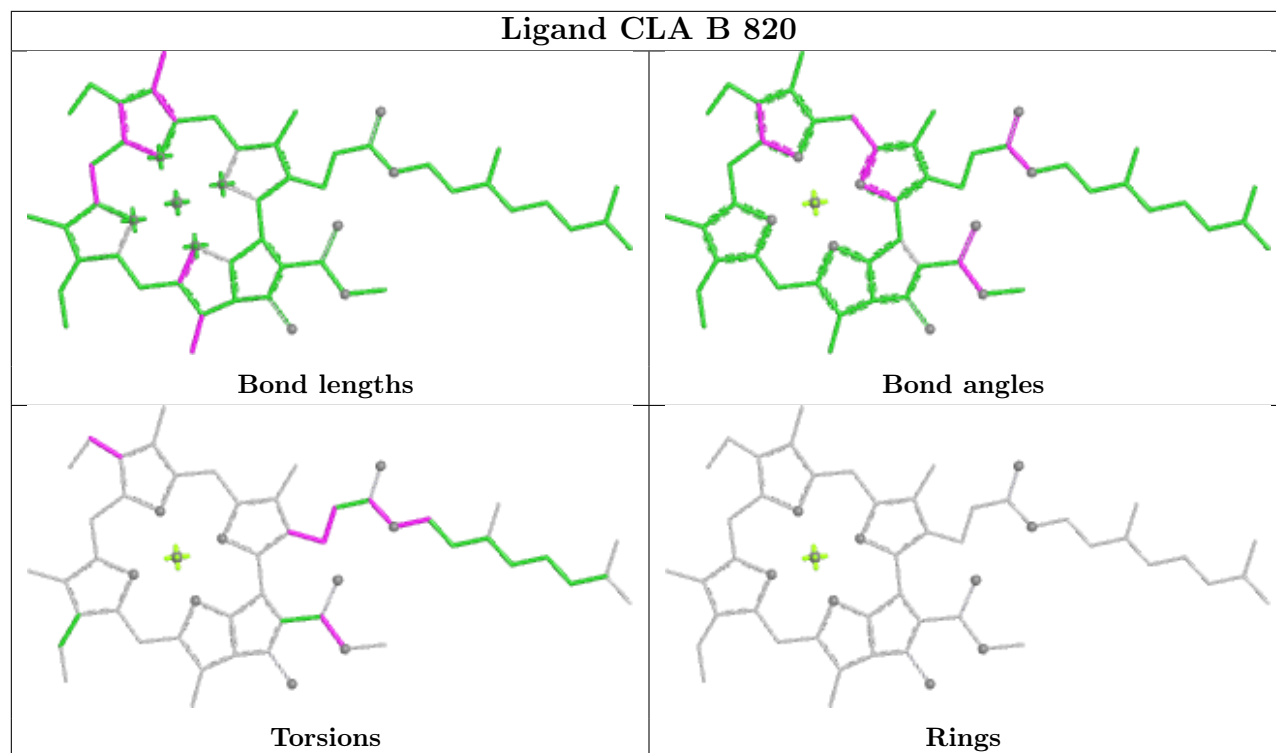


Ligand CLA 7 310

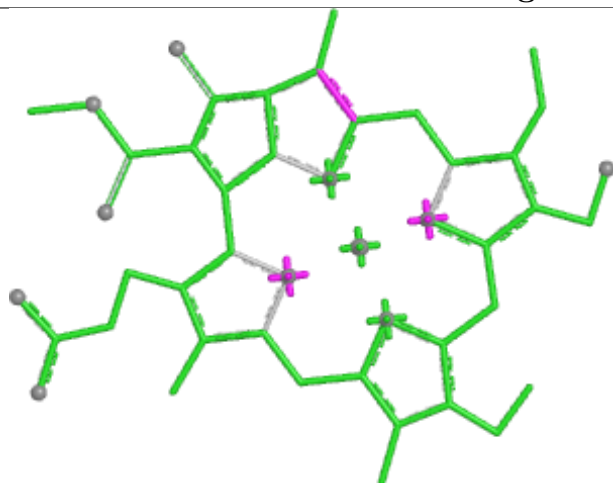


Ligand CLA 3 312

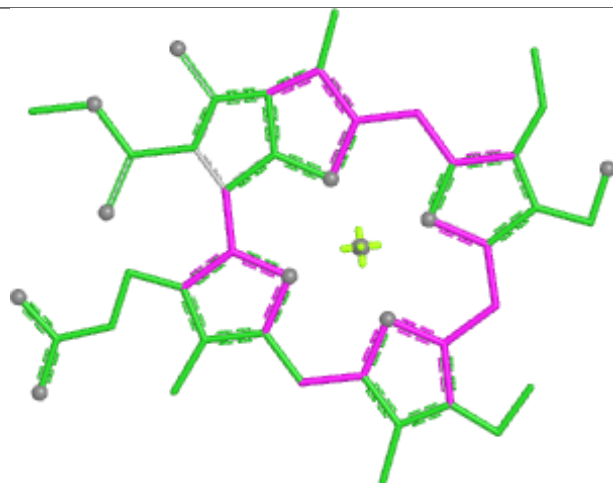




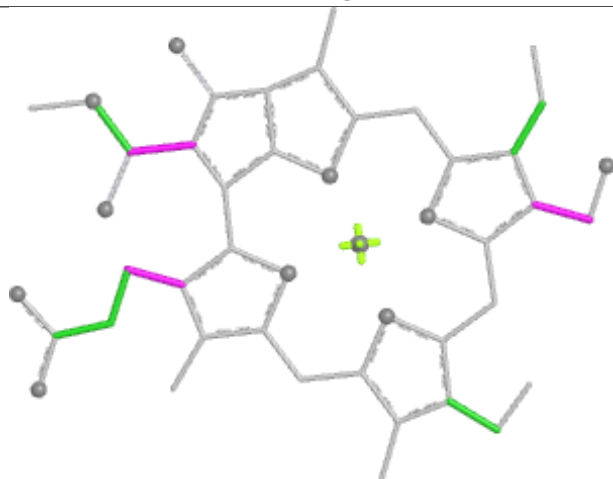
Ligand CHL 7 305



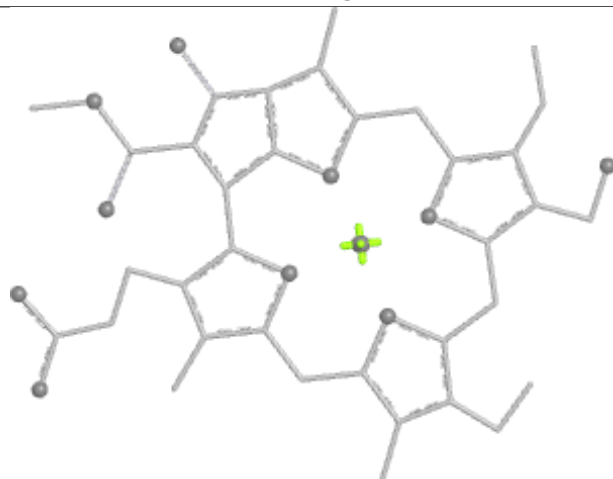
Bond lengths



Bond angles

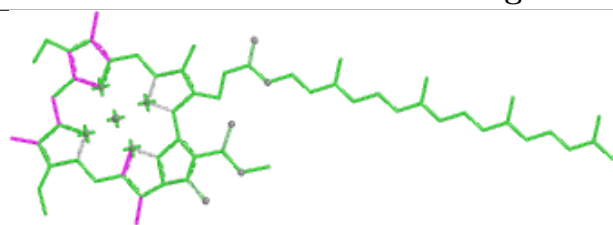


Torsions

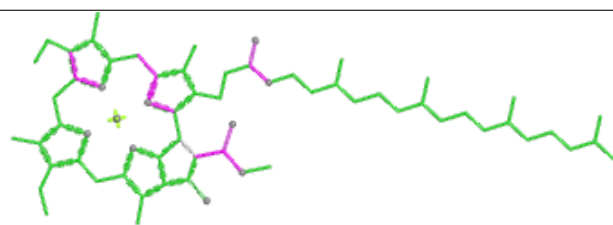


Rings

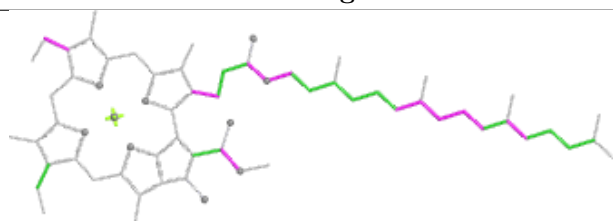
Ligand CLA A 5006



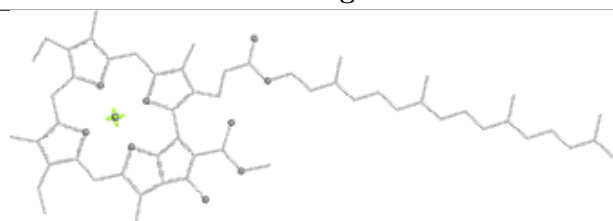
Bond lengths



Bond angles

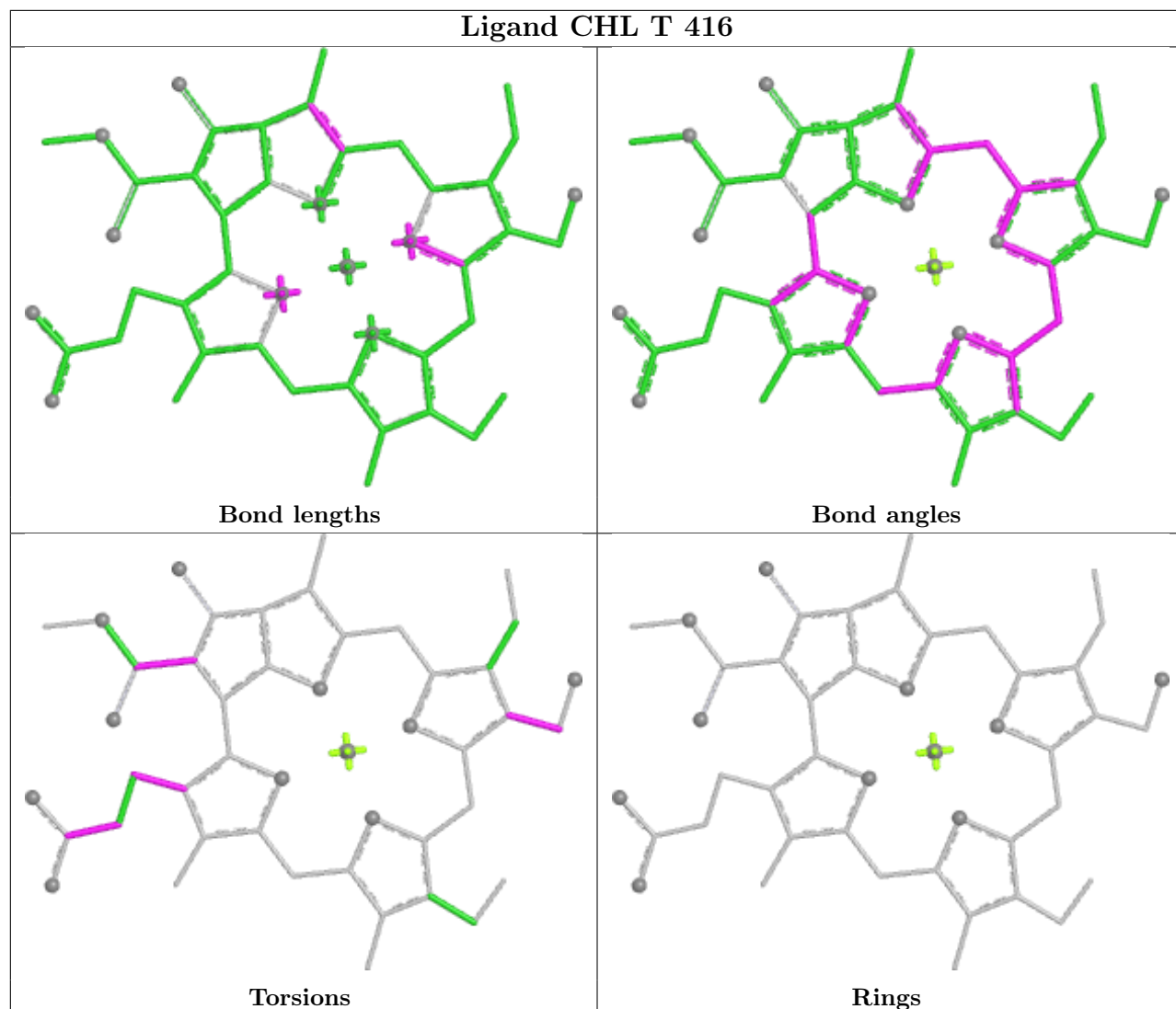


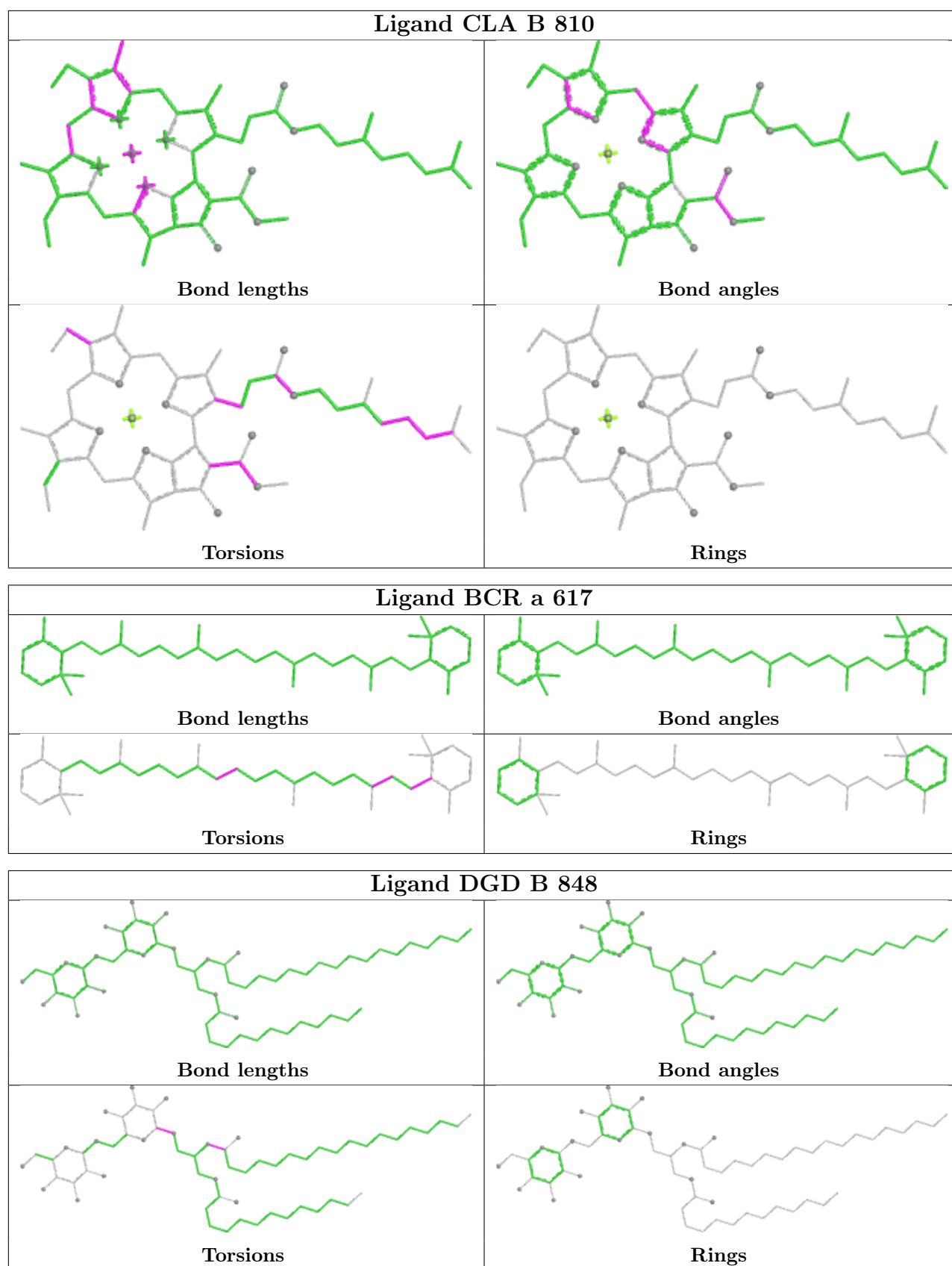
Torsions



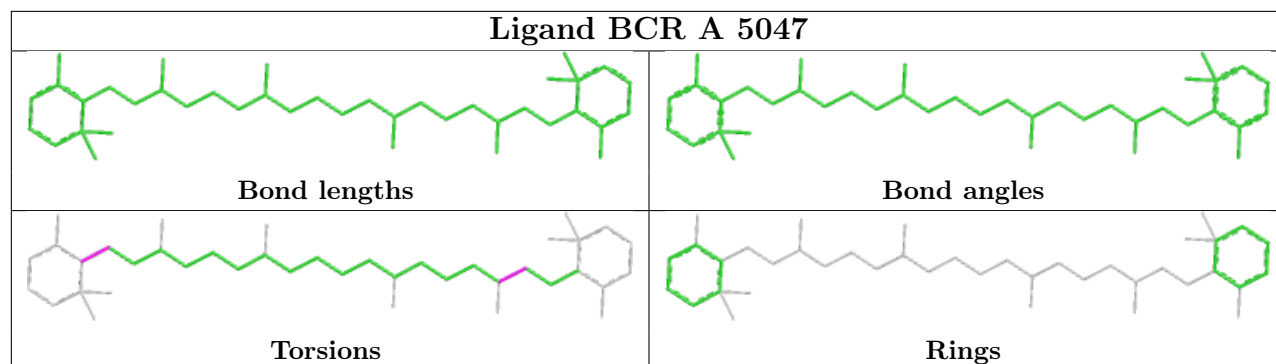
Rings

Ligand CHL T 416

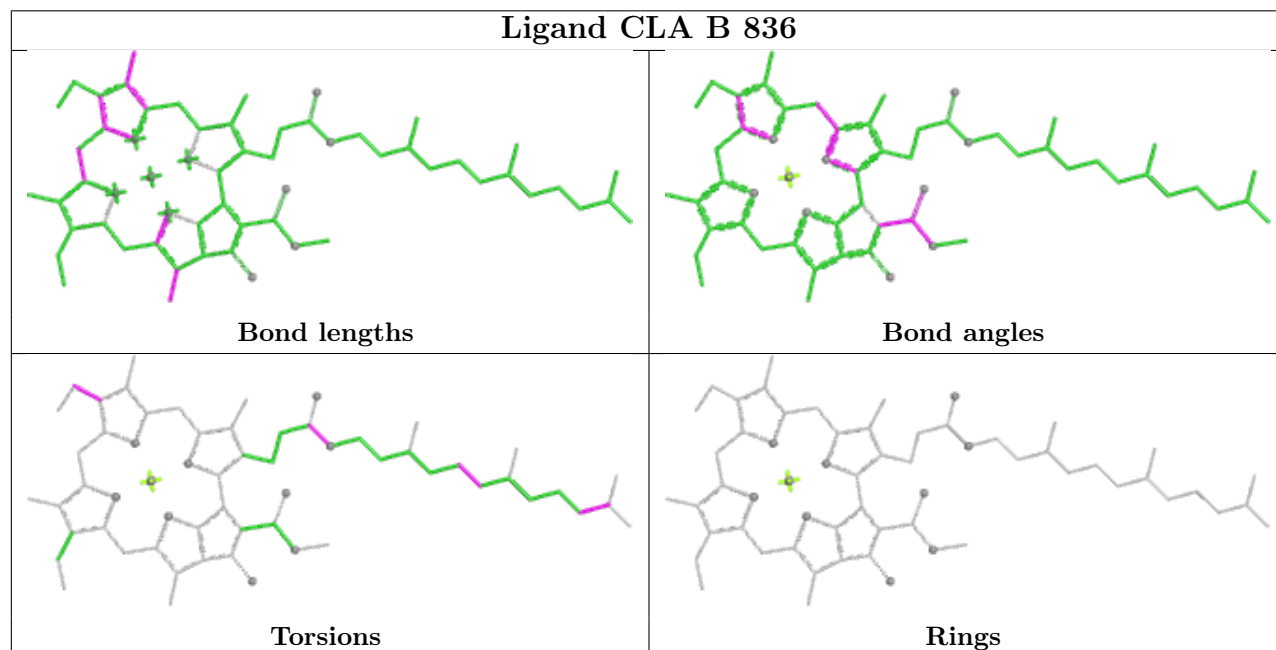




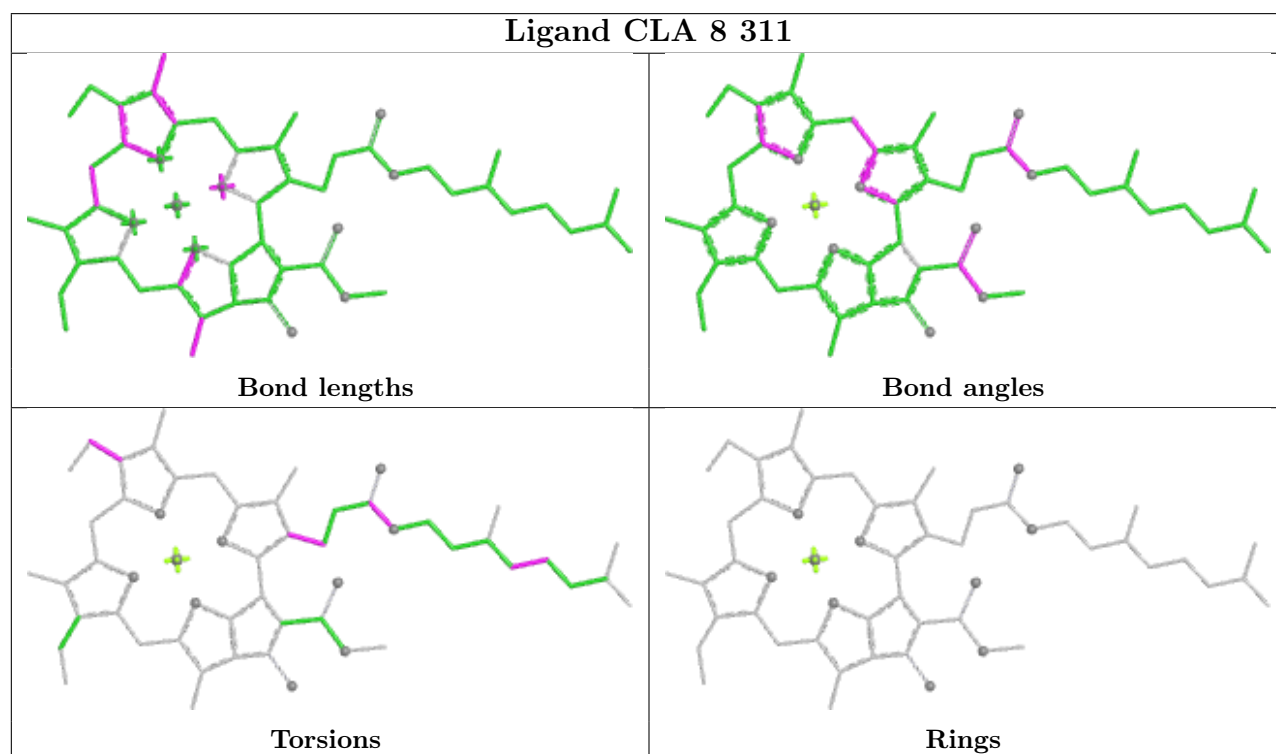
Ligand BCR A 5047

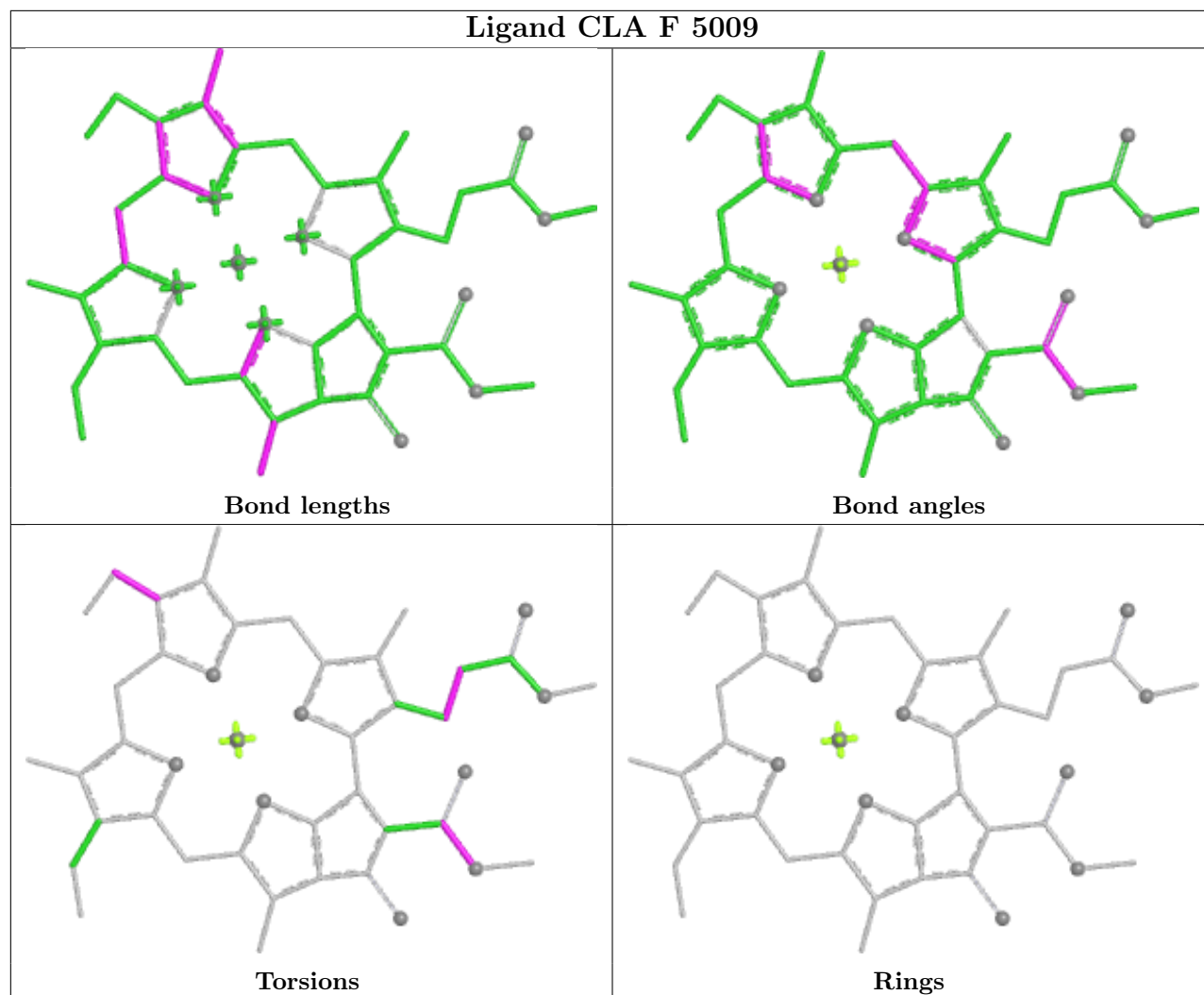


Ligand CLA B 836

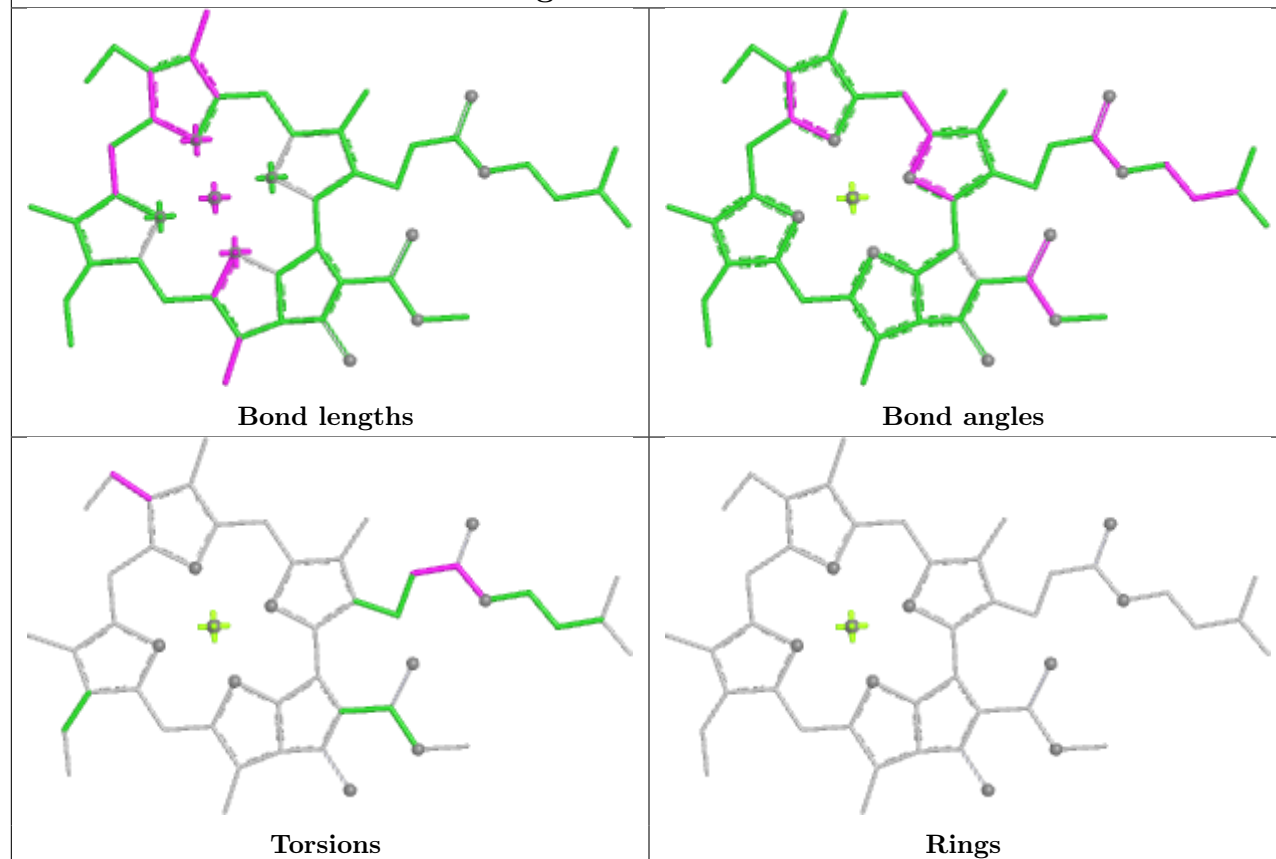


Ligand CLA 8 311

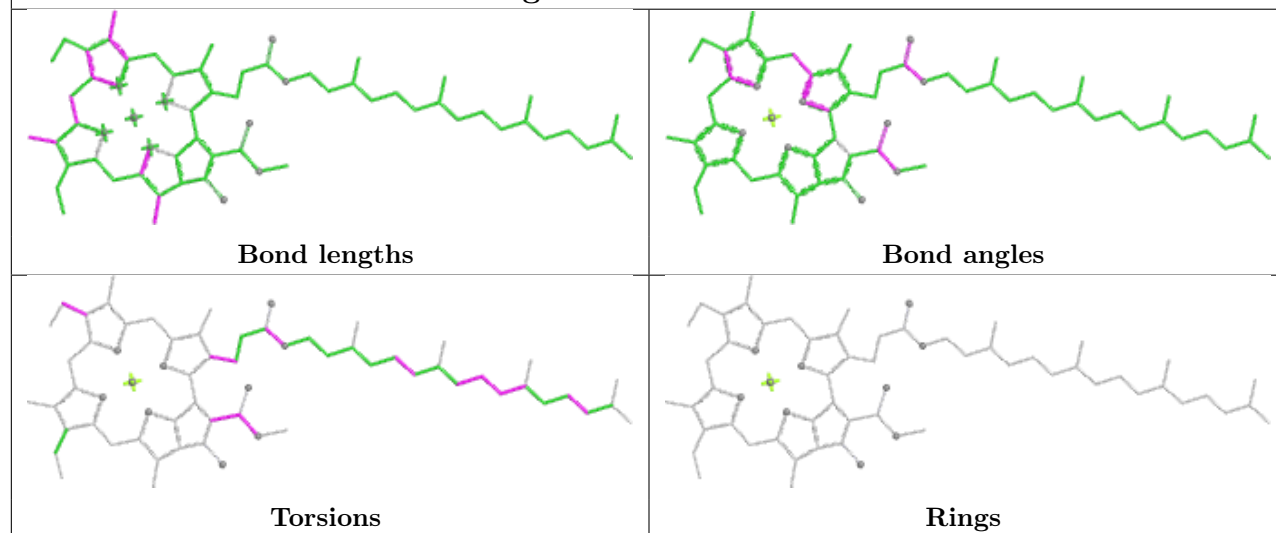


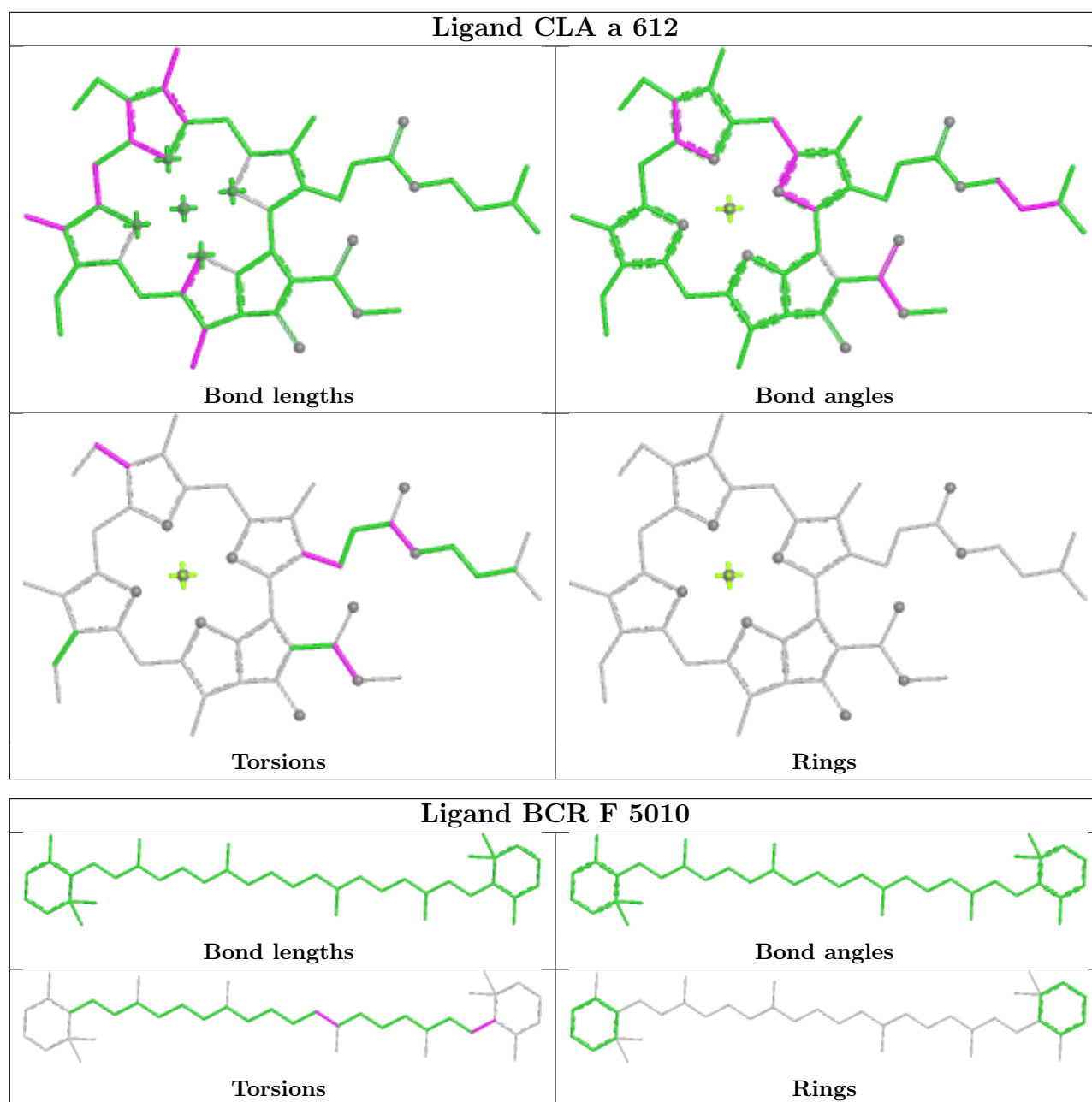


Ligand CLA 3 305

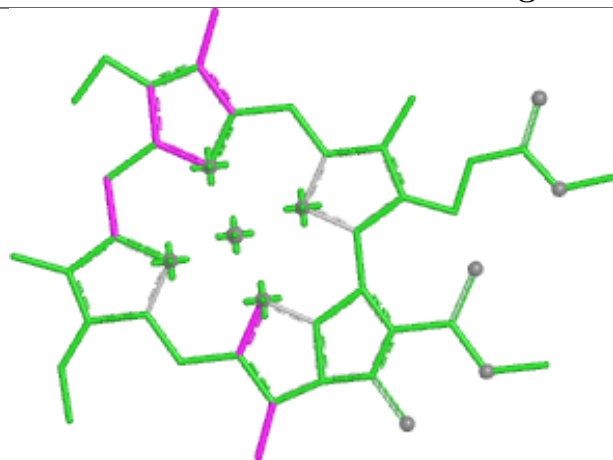


Ligand CLA A 5035

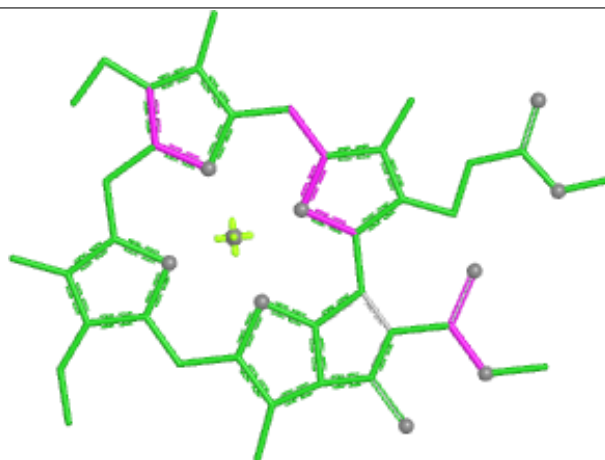




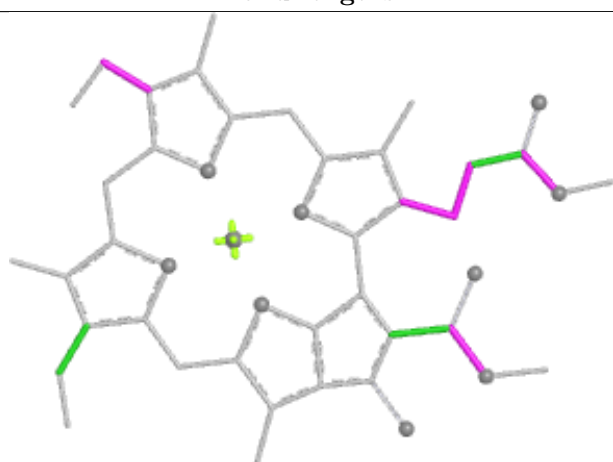
Ligand CLA 3 303



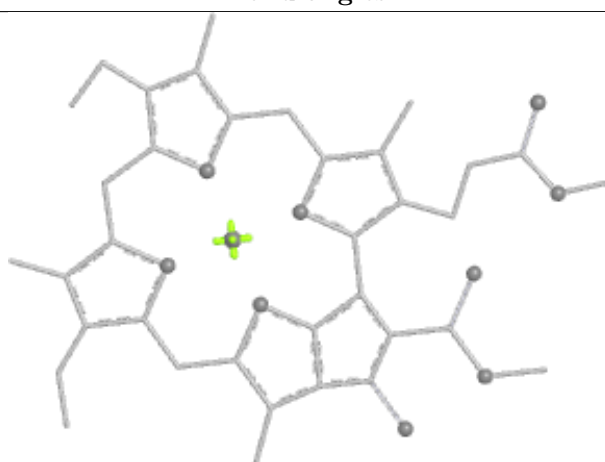
Bond lengths



Bond angles

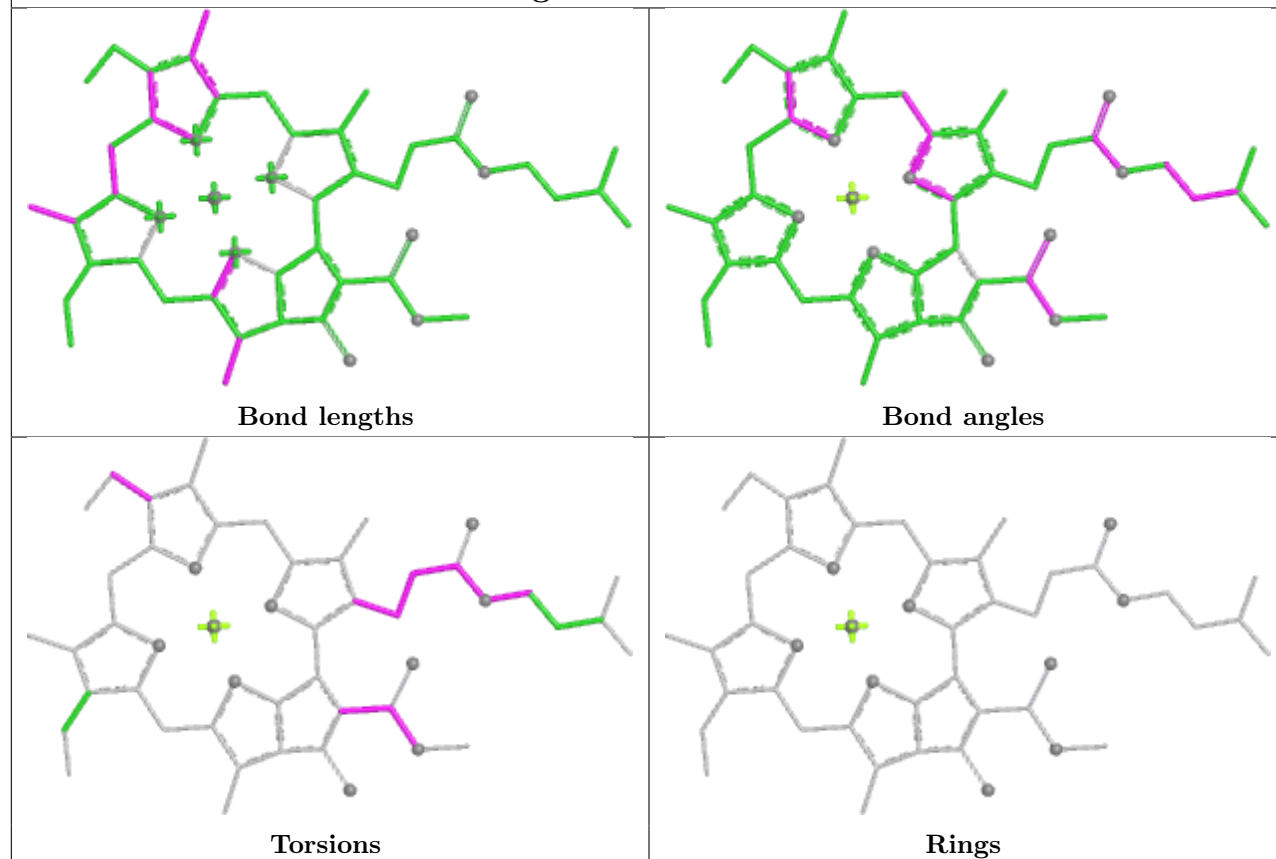


Torsions

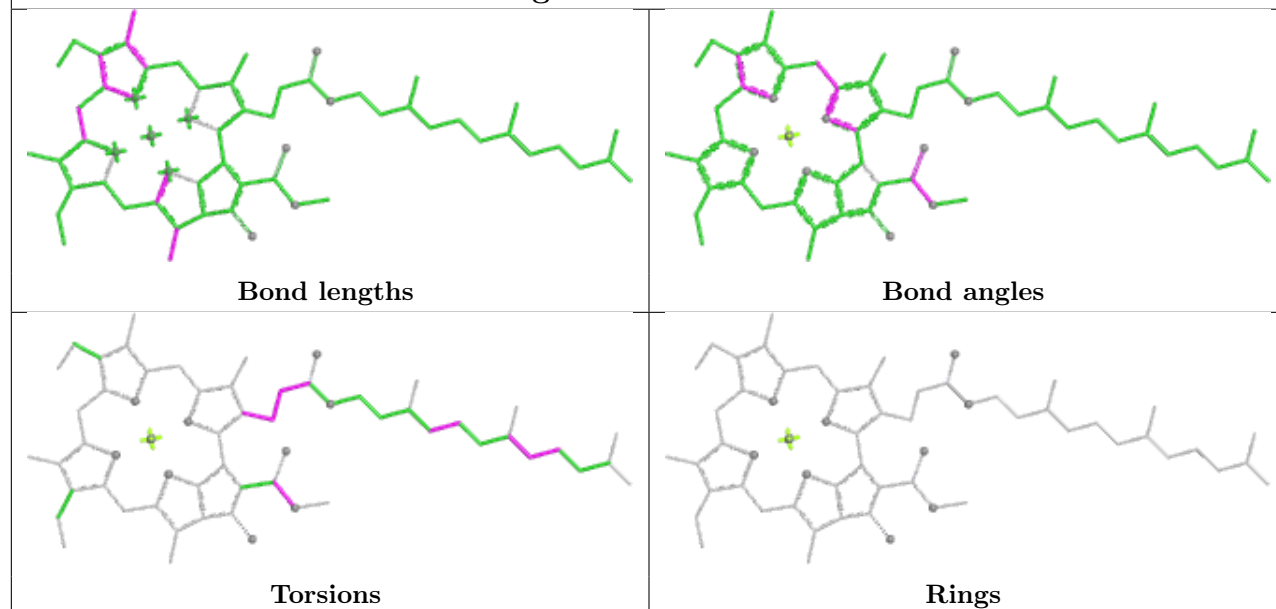


Rings

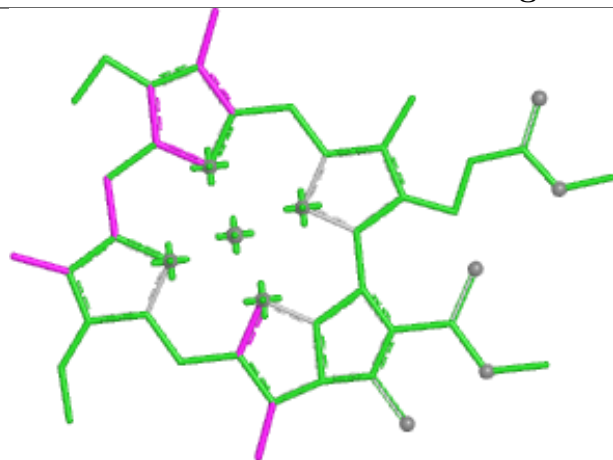
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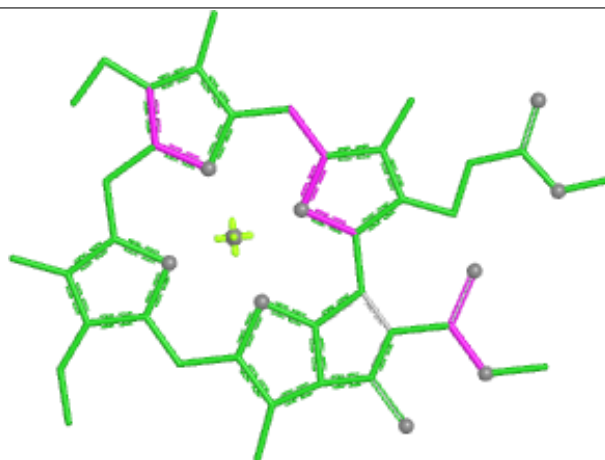
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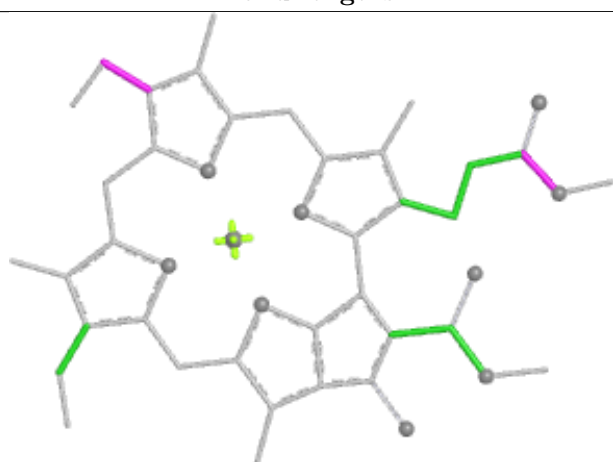
Ligand CLA c 302



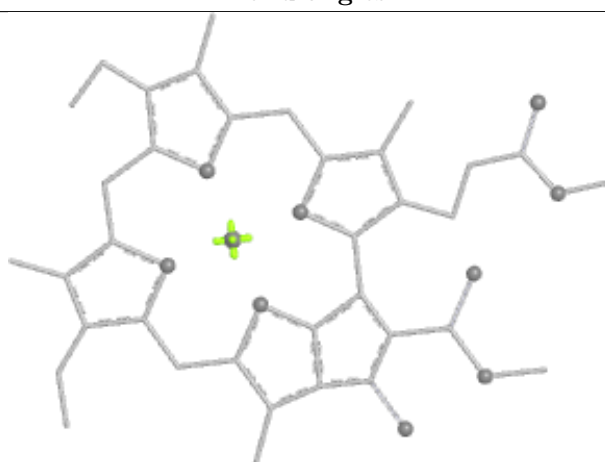
Bond lengths



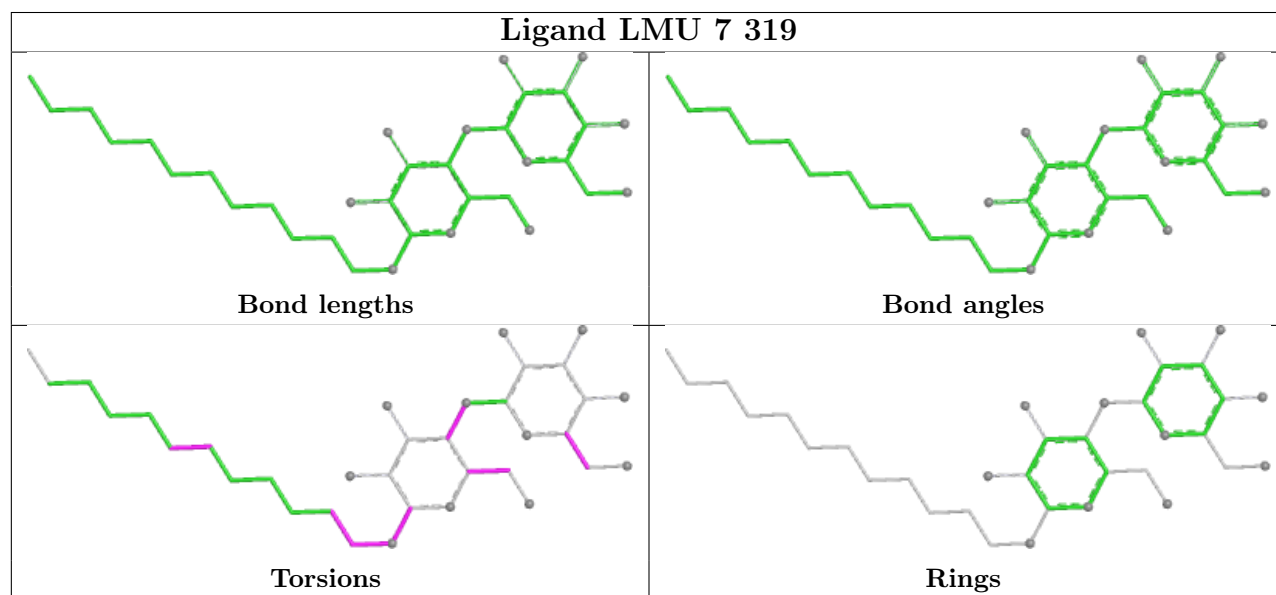
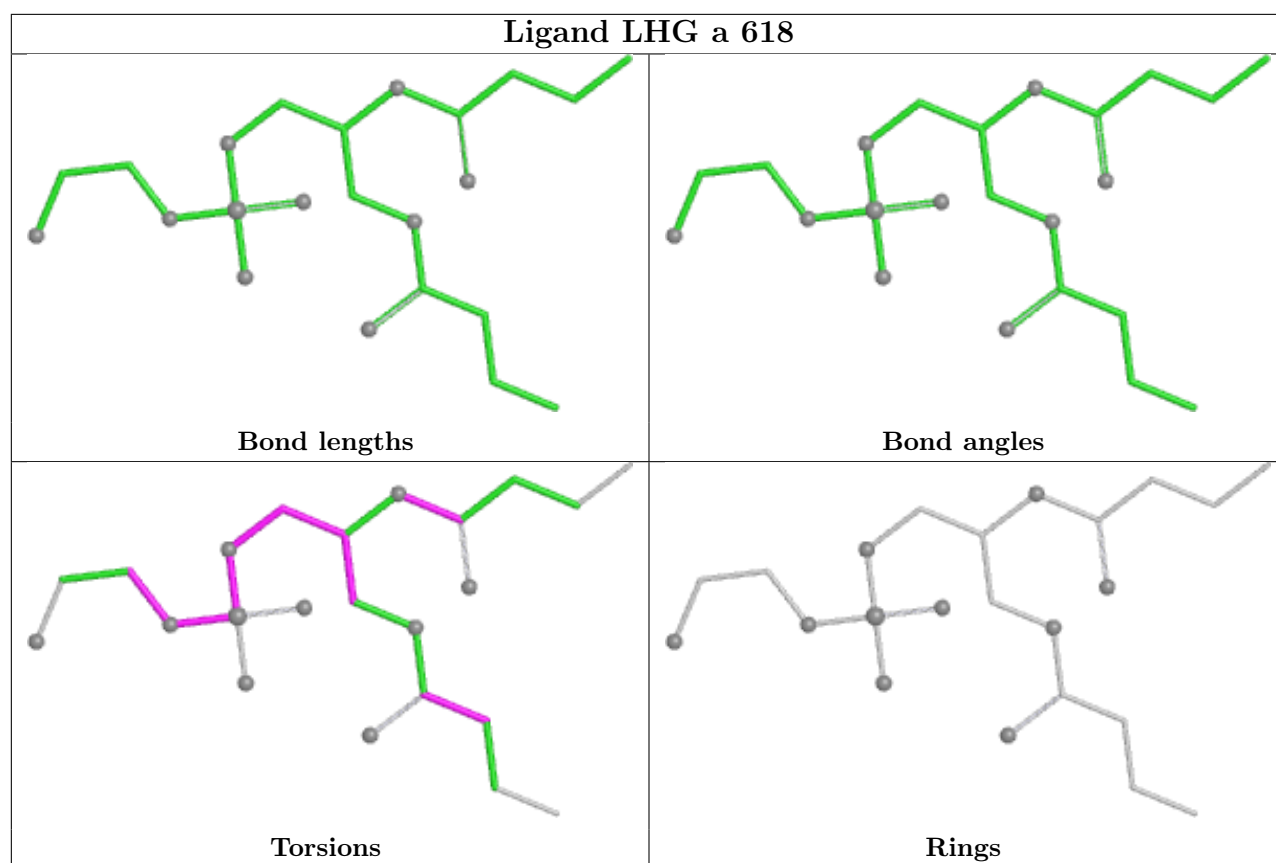
Bond angles

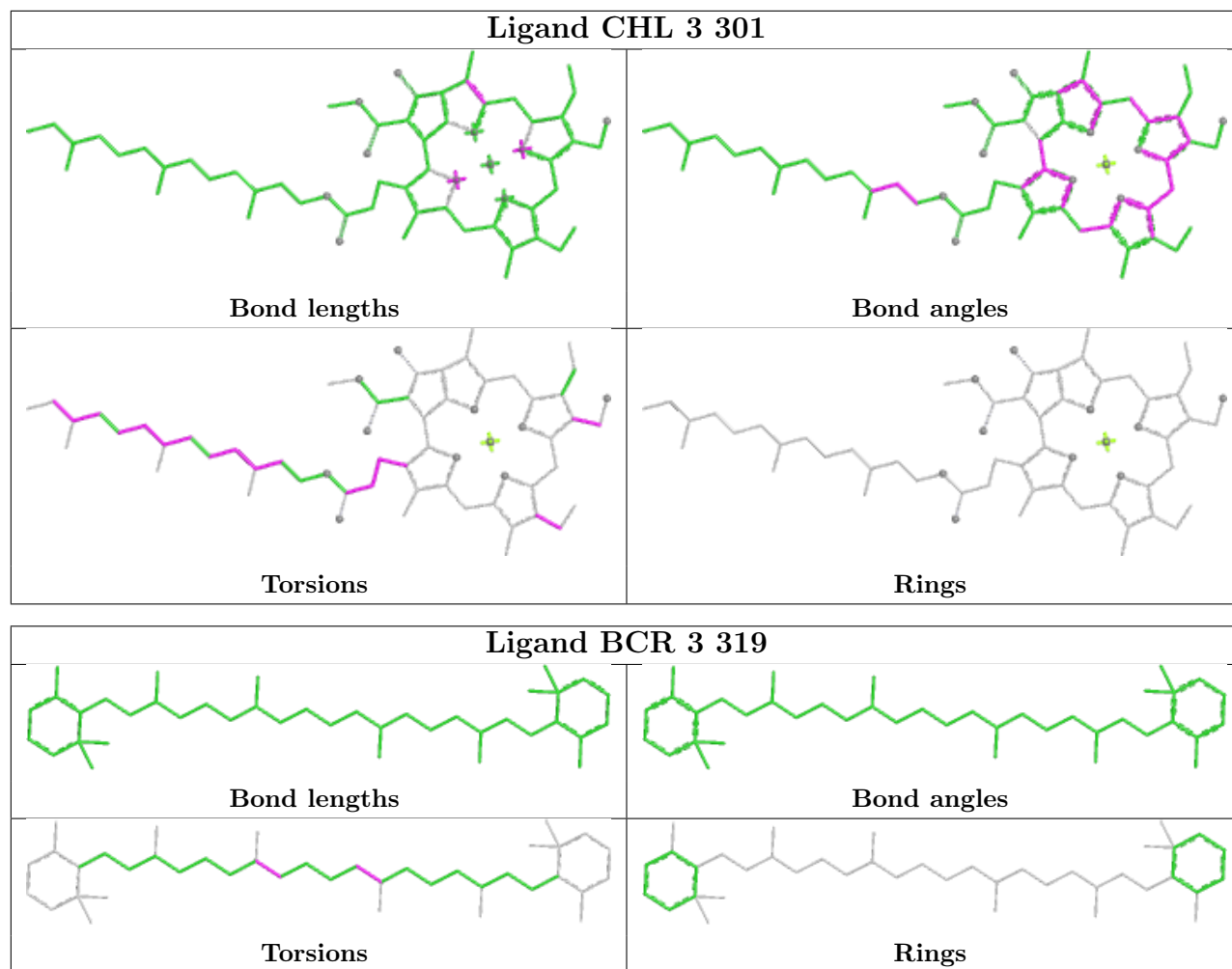


Torsions

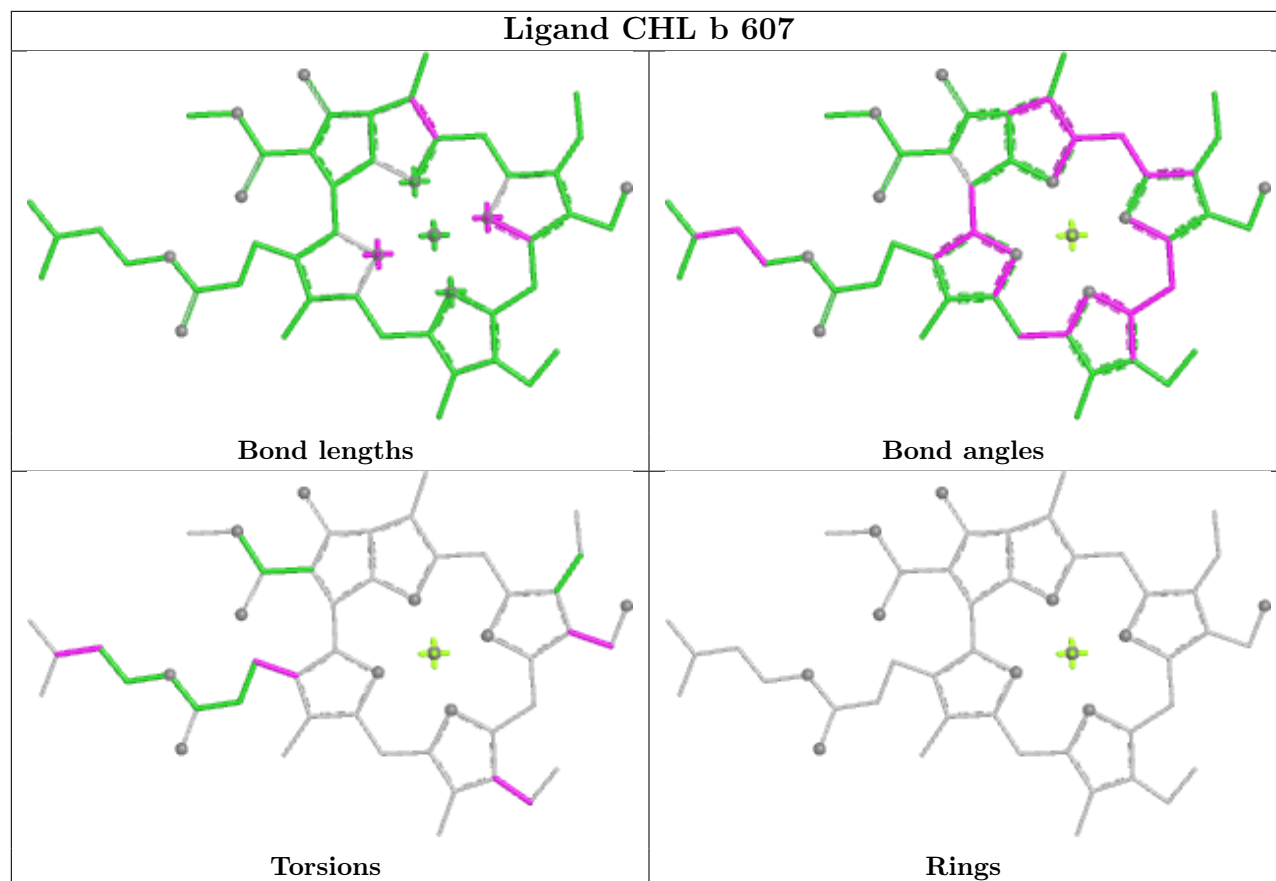


Rings

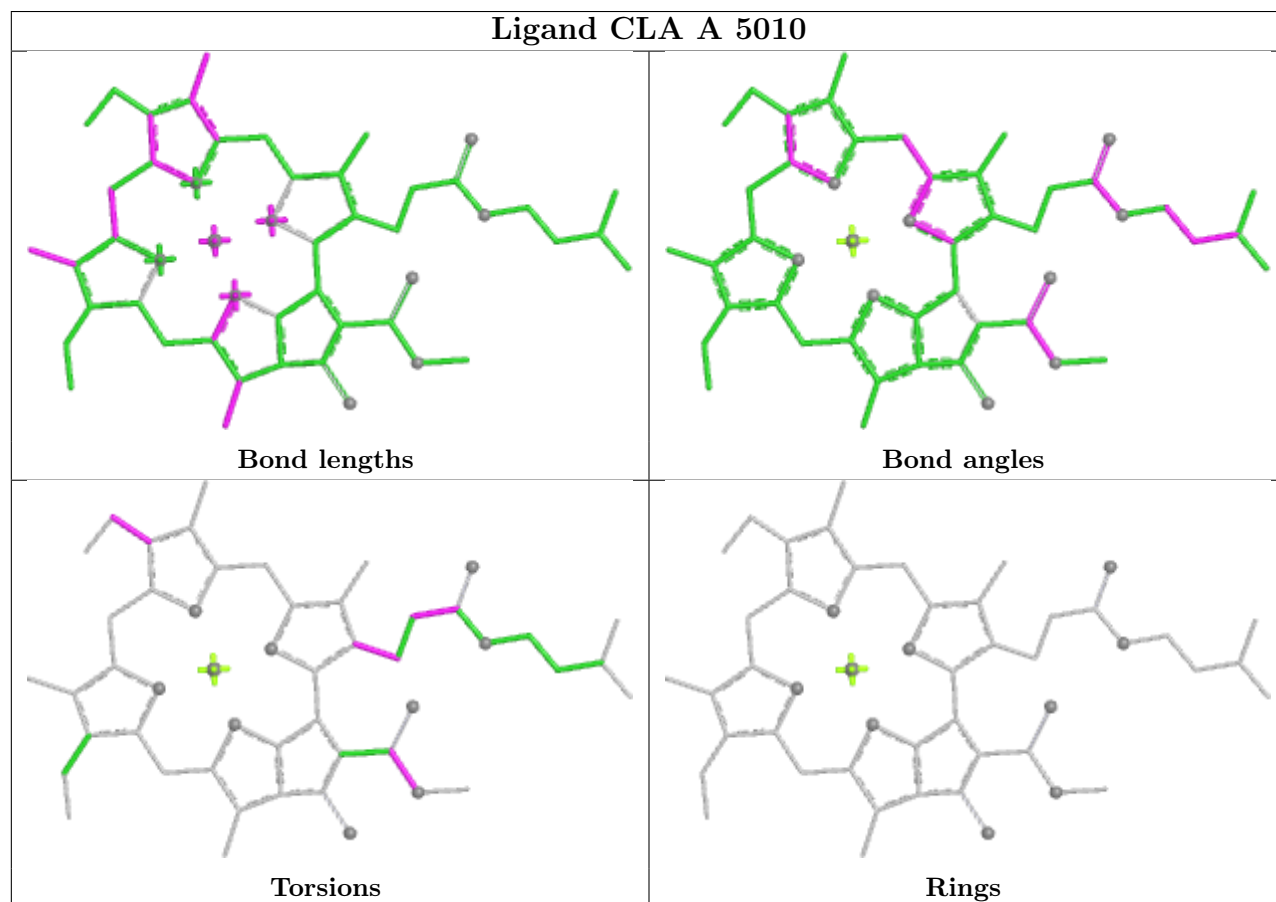


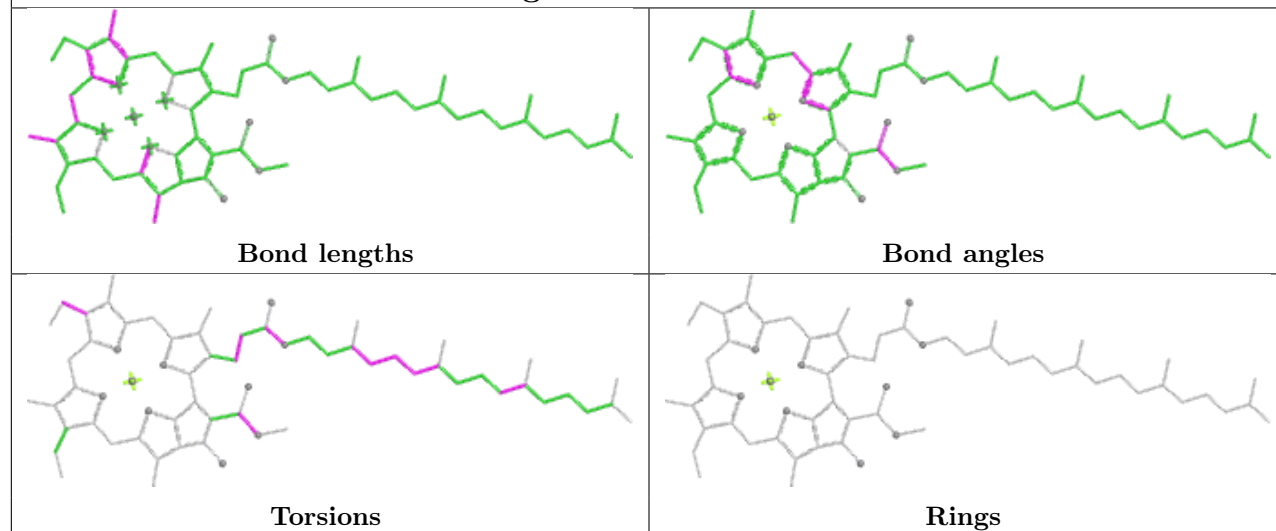
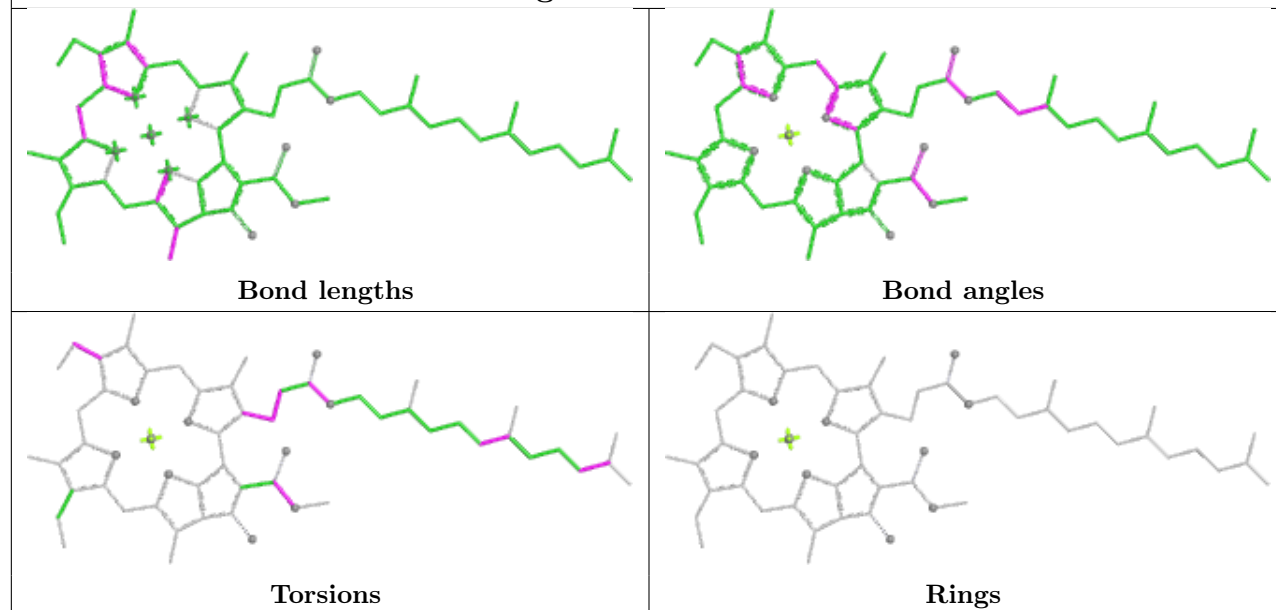


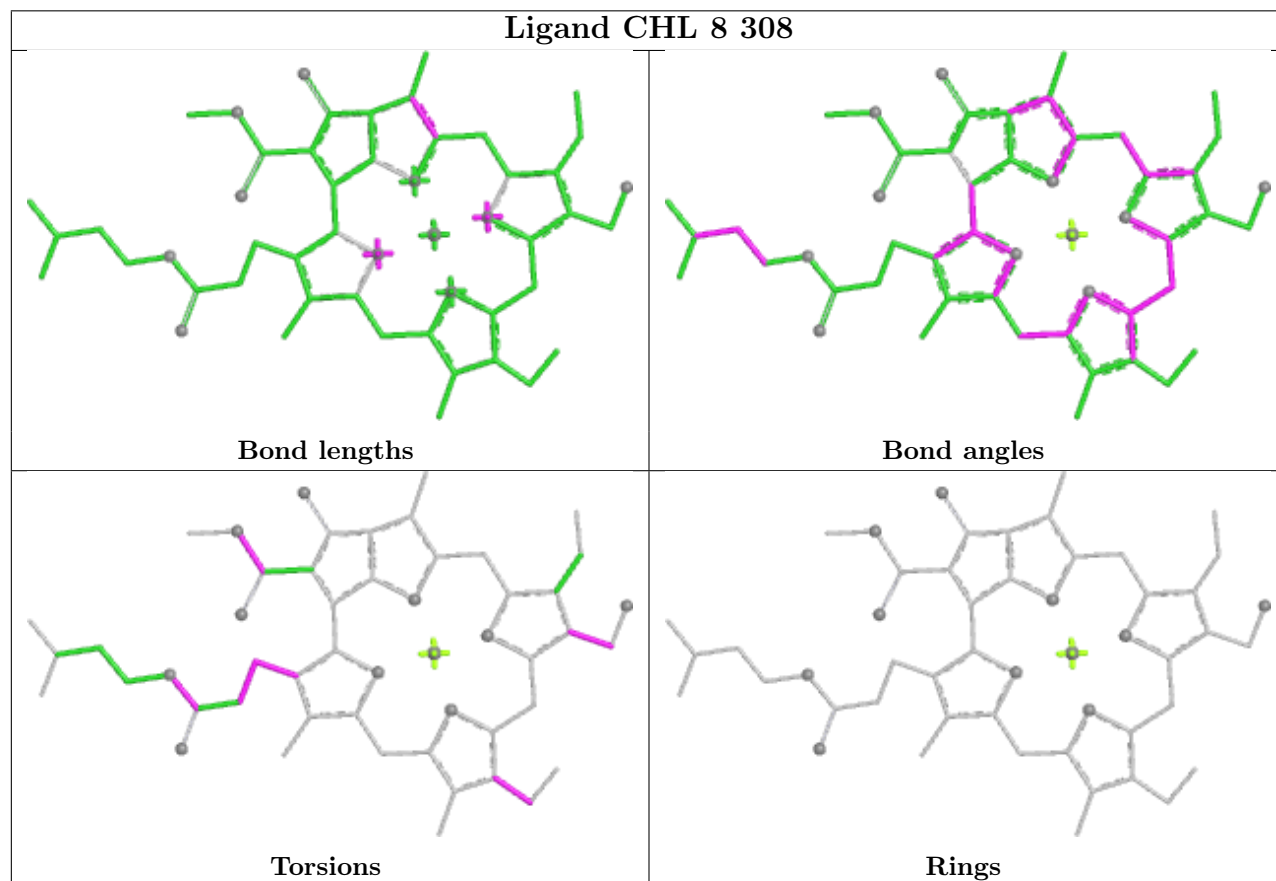
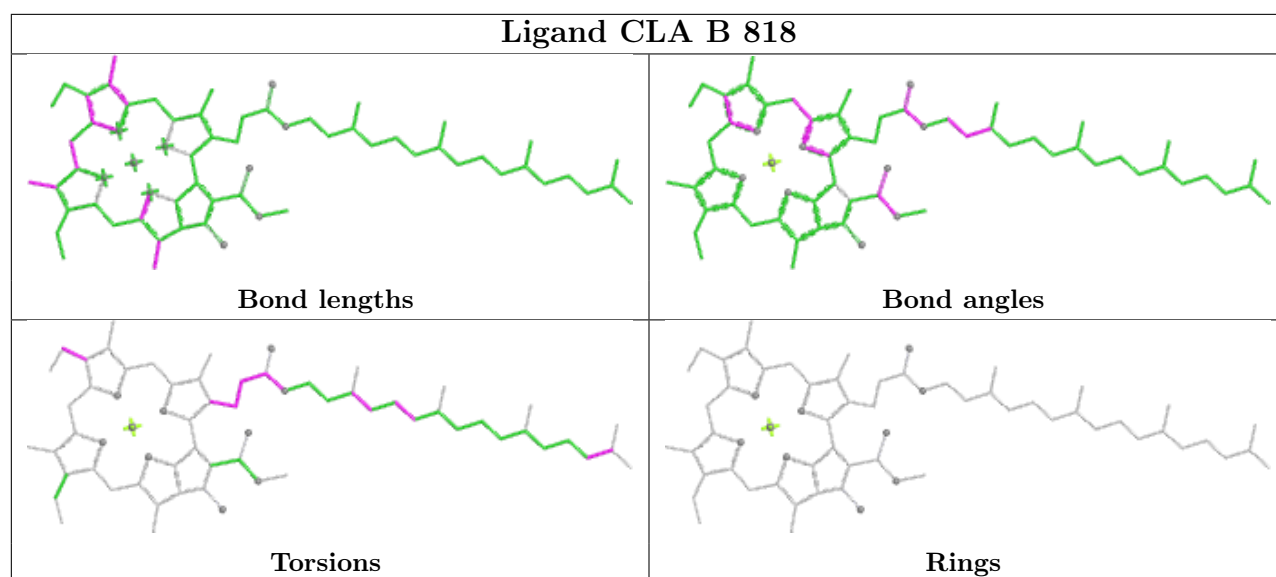
Ligand CHL b 607

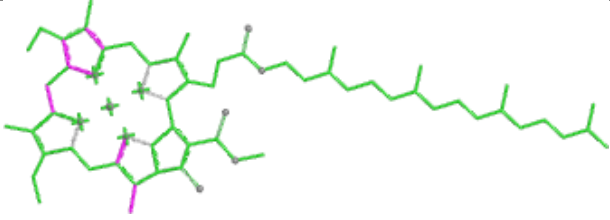
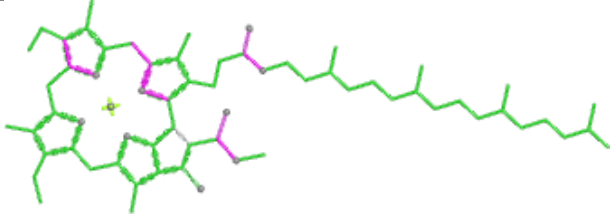
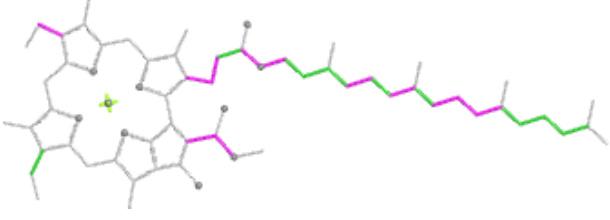
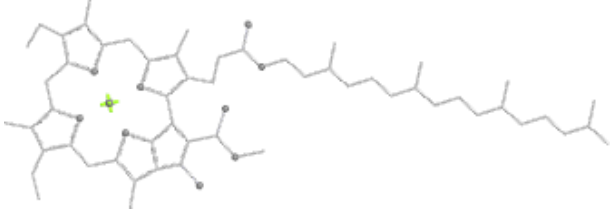
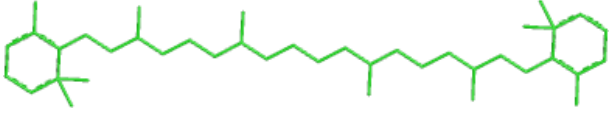
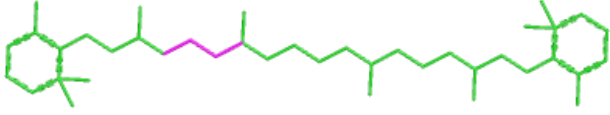
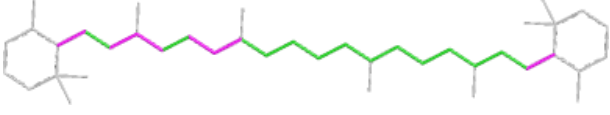
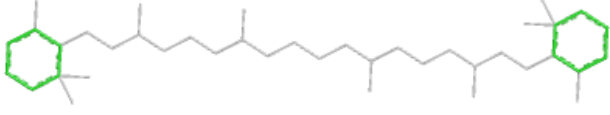
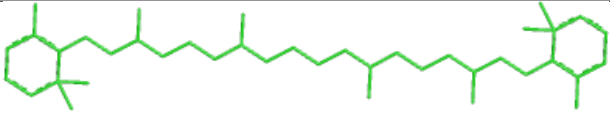
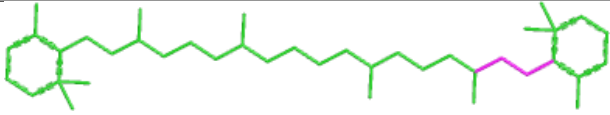
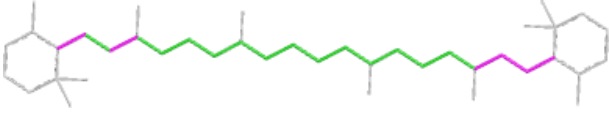
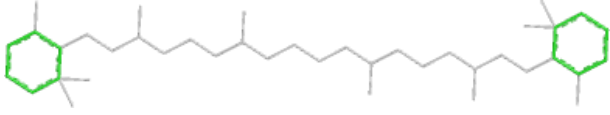


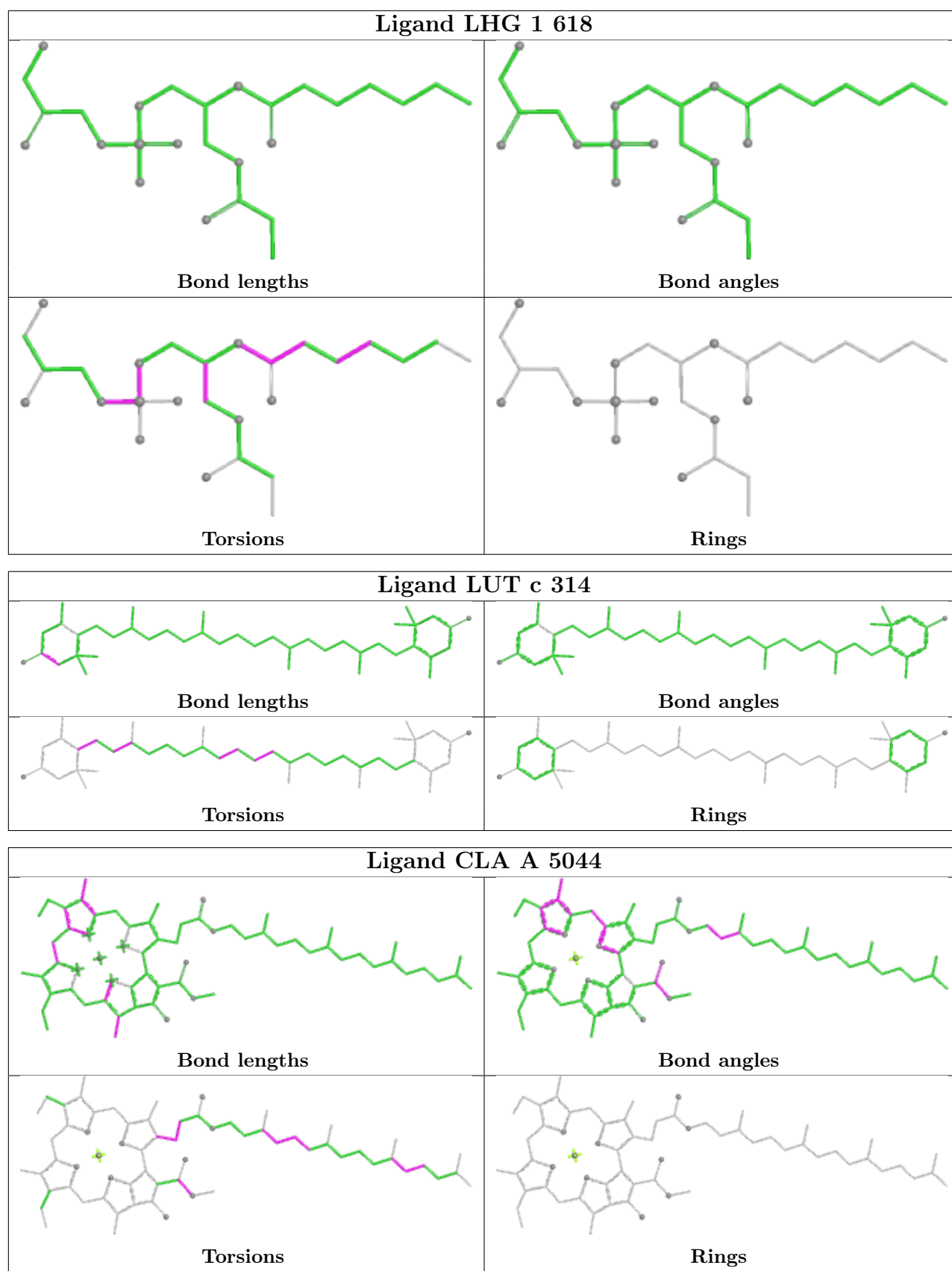
Ligand CLA A 5010

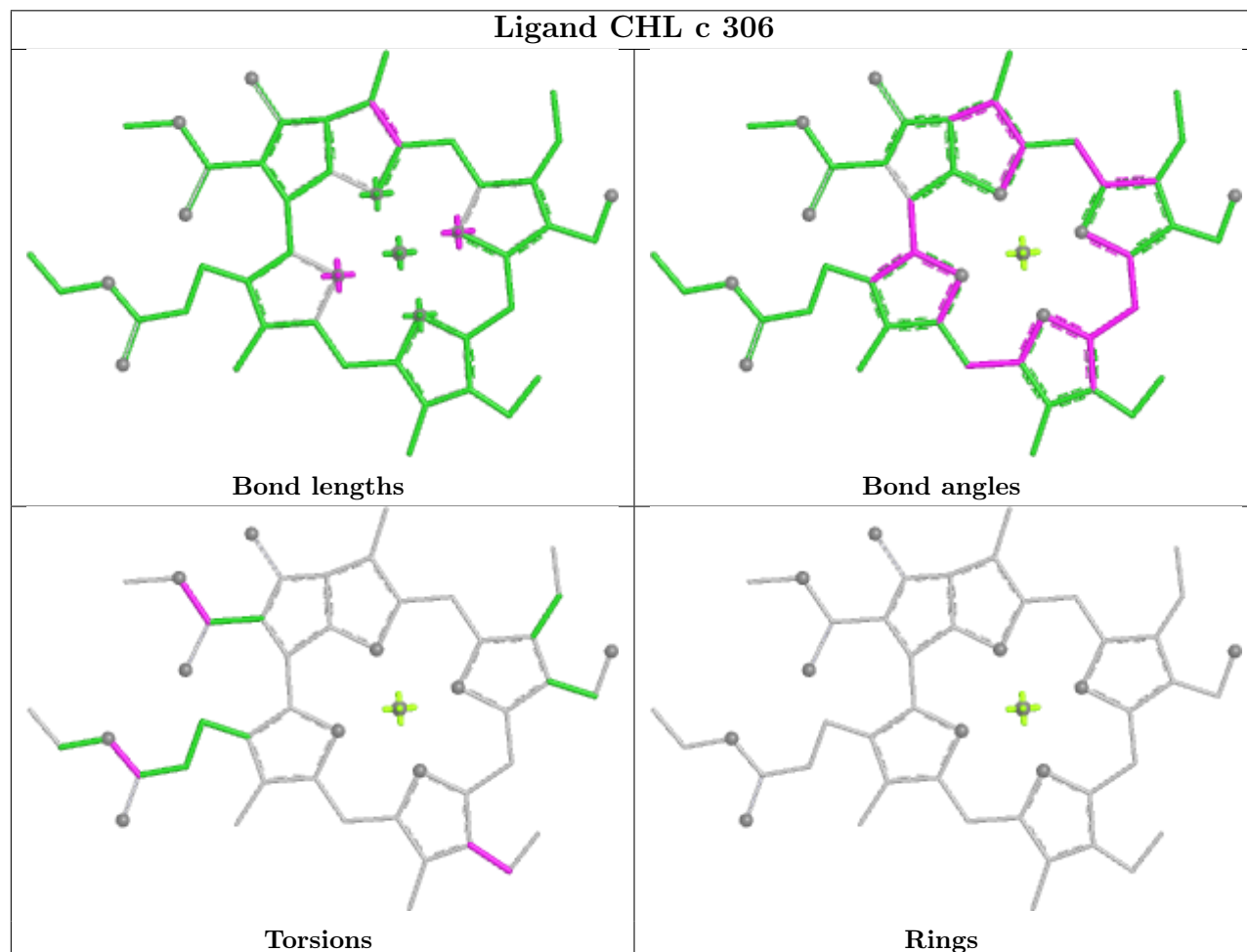
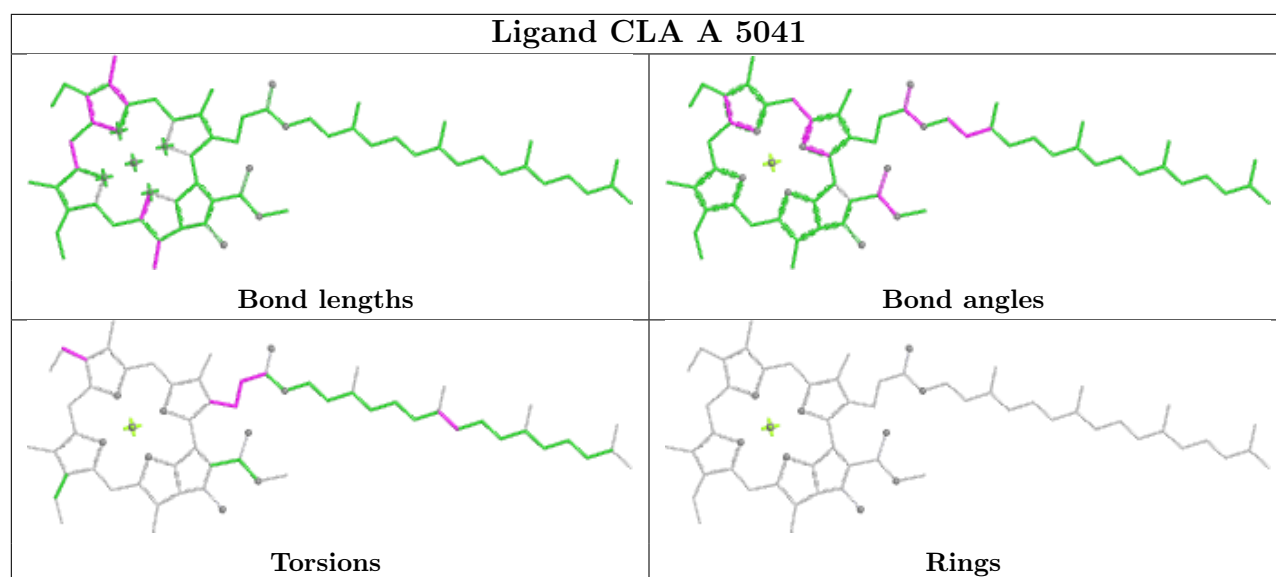


Ligand CLA A 5004**Ligand CLA 1 612**

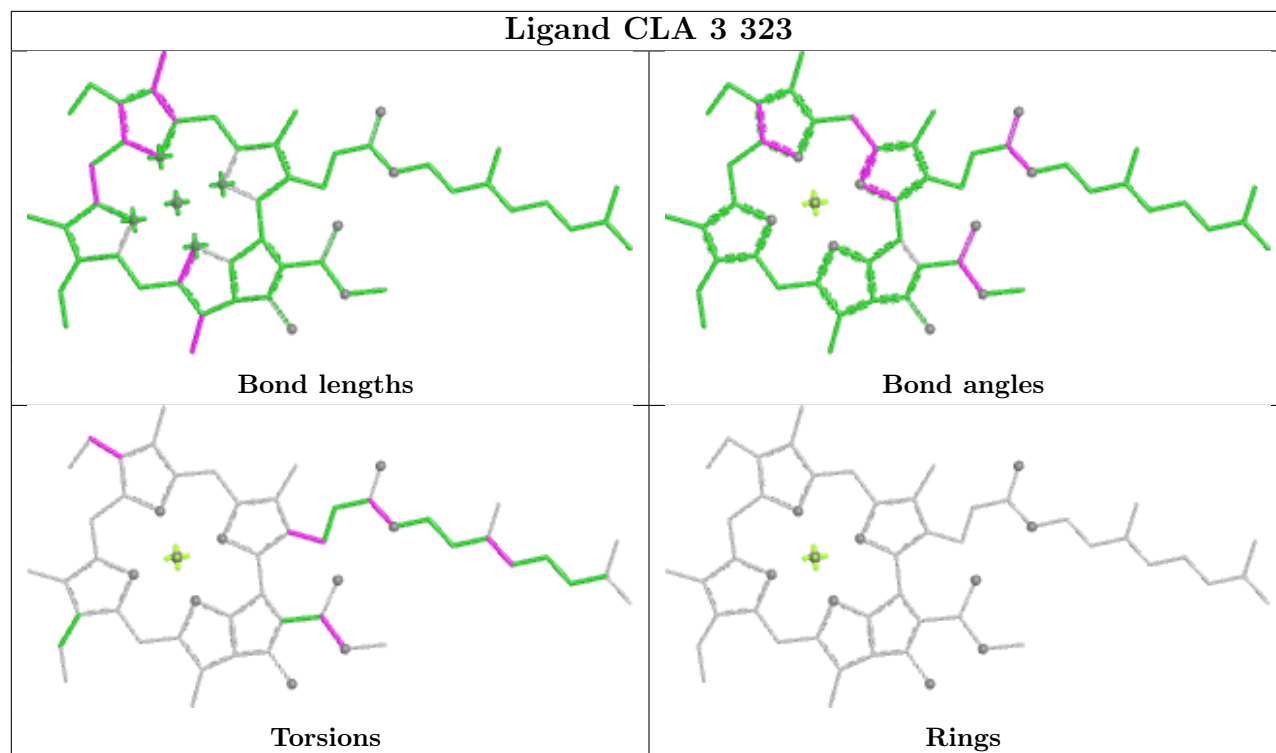


Ligand CLA B 829	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

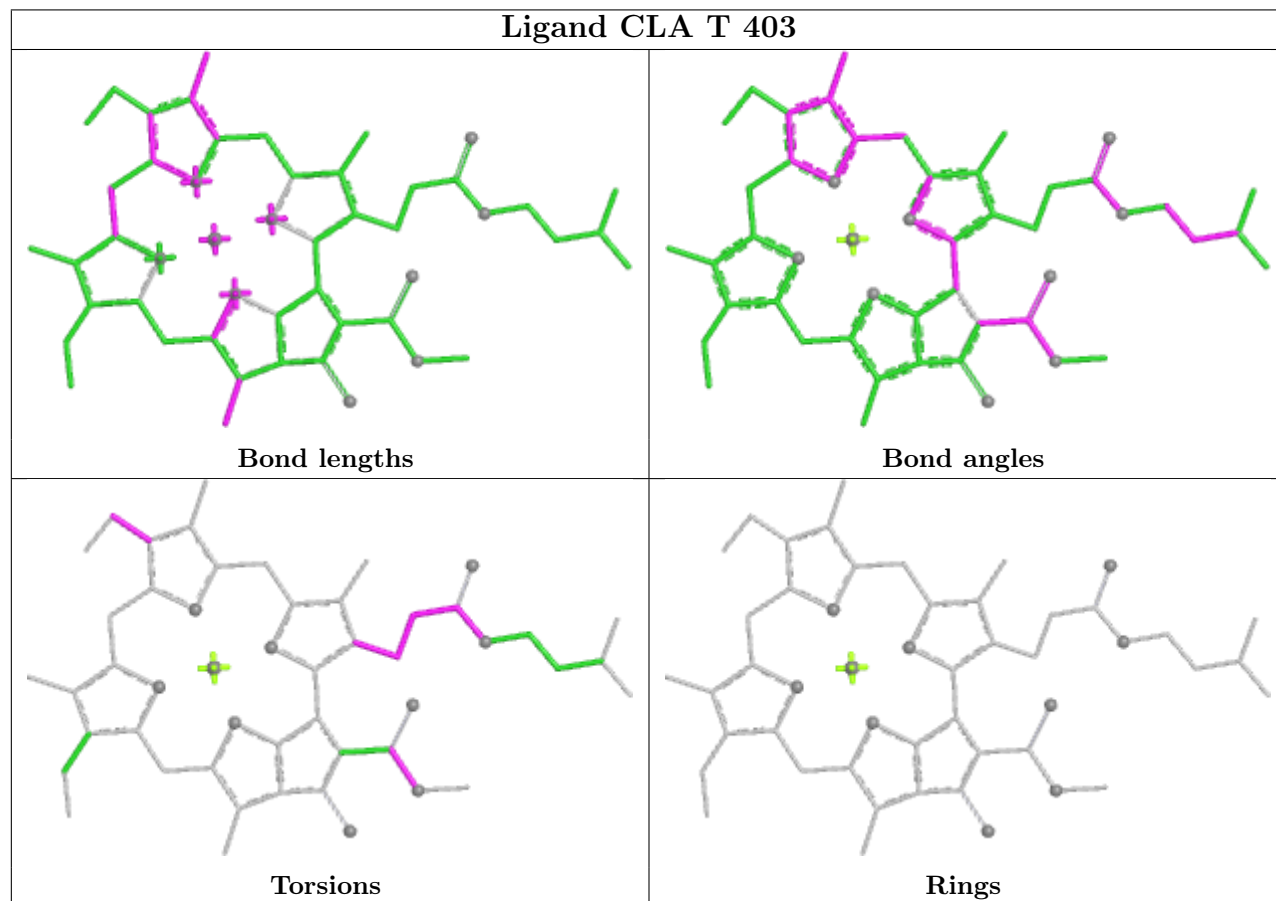


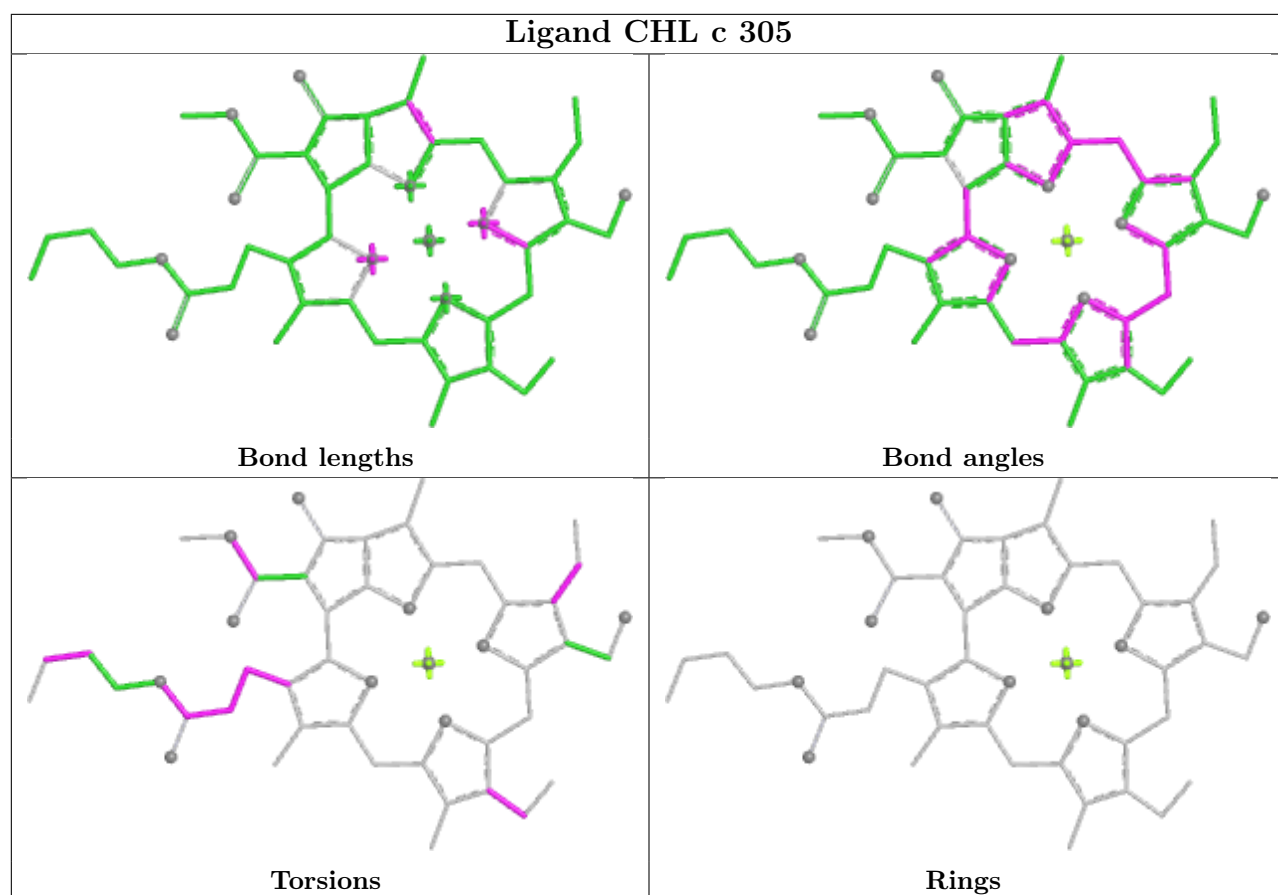


Ligand CLA 3 323

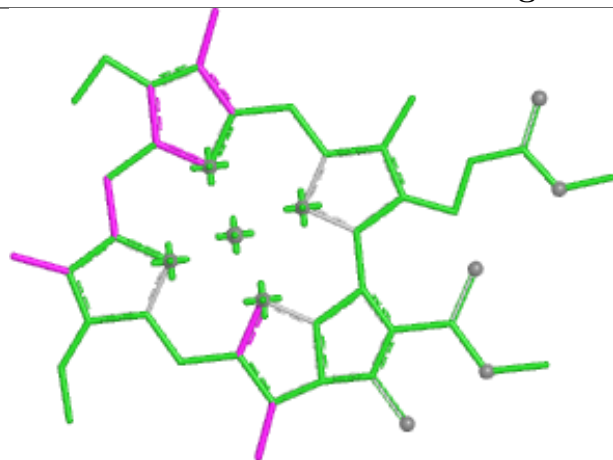


Ligand CLA T 403

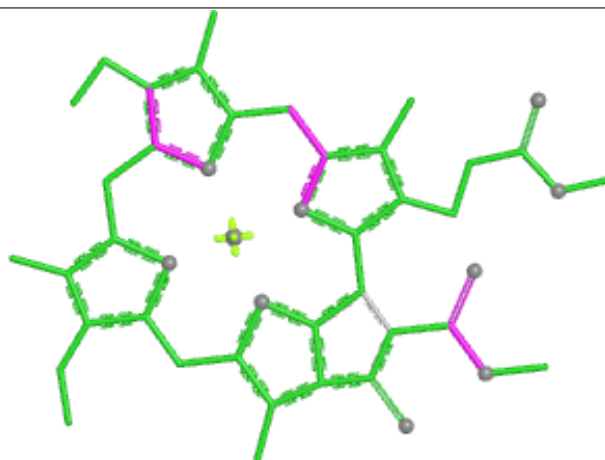




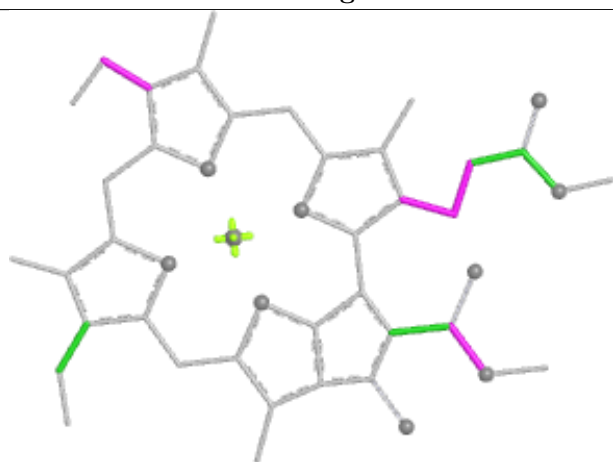
Ligand CLA 7 309



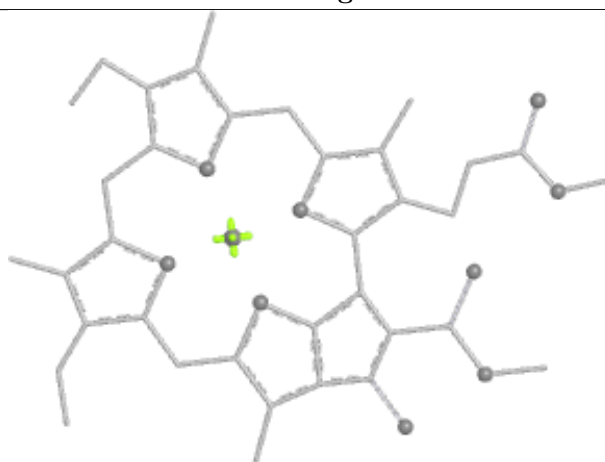
Bond lengths



Bond angles

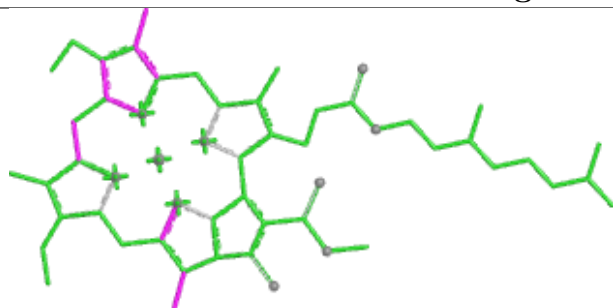


Torsions

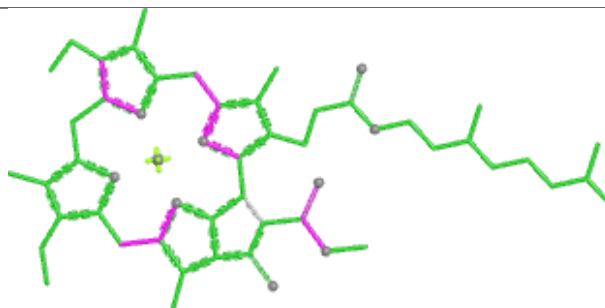


Rings

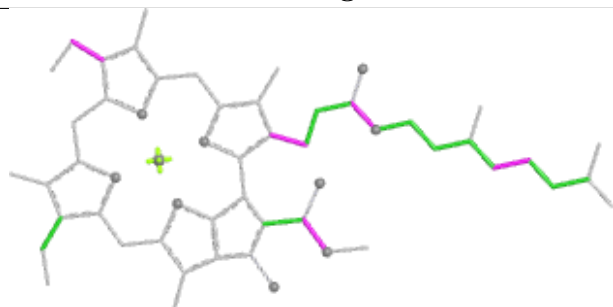
Ligand CLA B 817



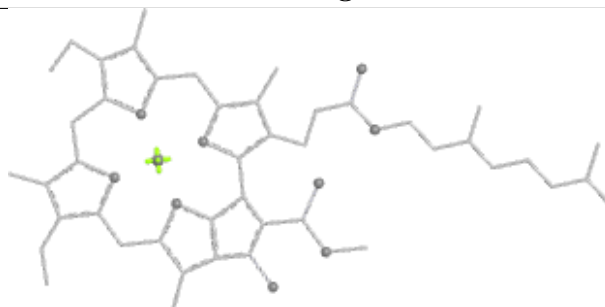
Bond lengths



Bond angles

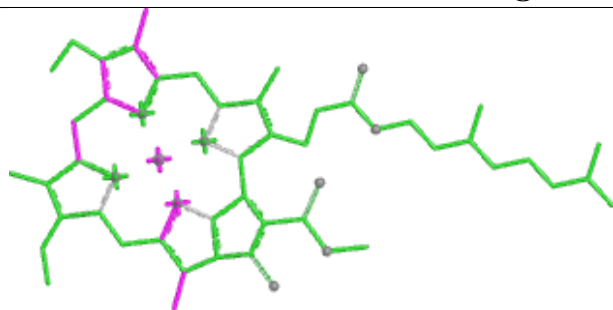


Torsions

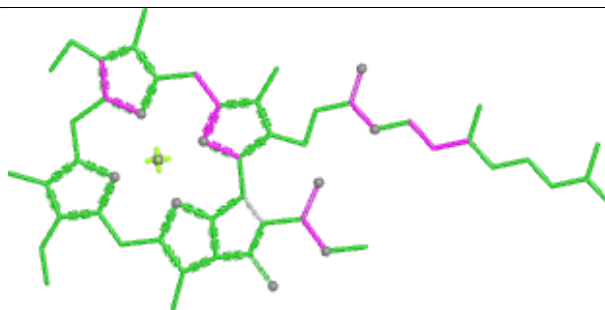


Rings

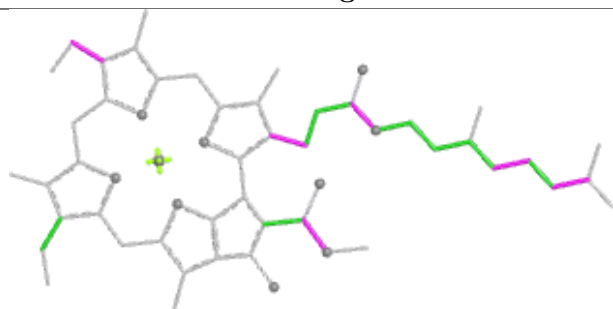
Ligand CLA B 831



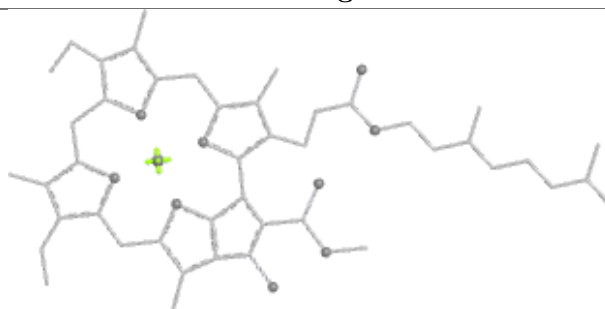
Bond lengths



Bond angles

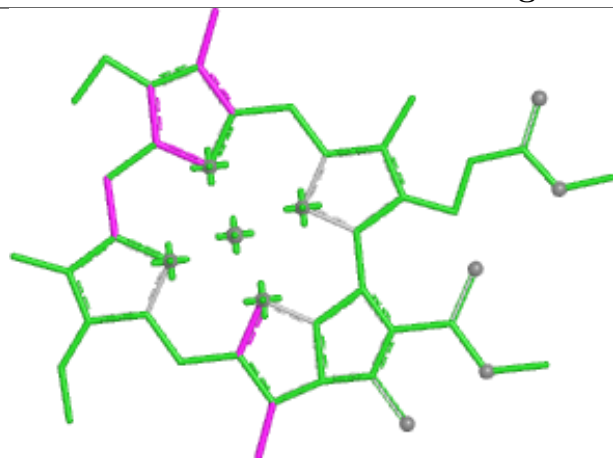


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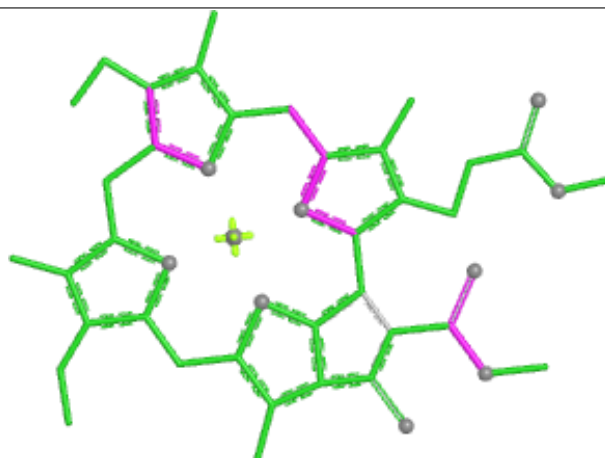


Rings

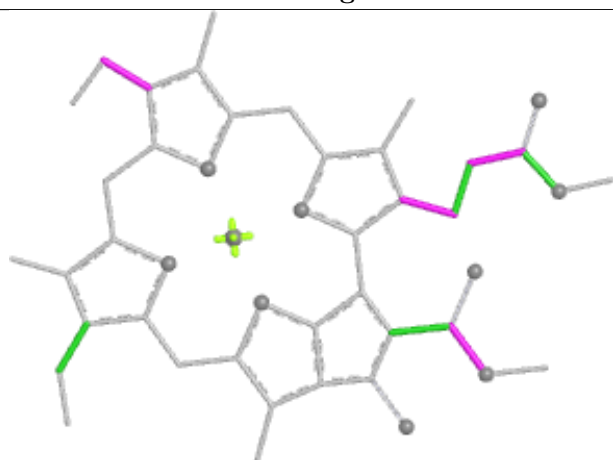
Ligand CLA a 614



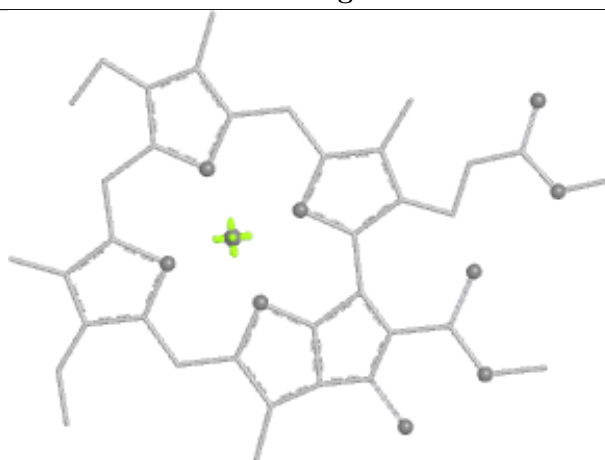
Bond lengths



Bond angles

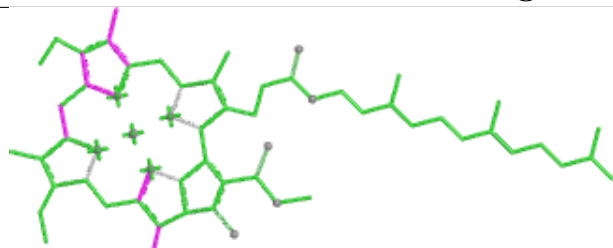


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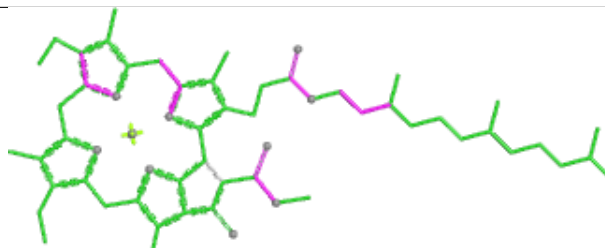


Rings

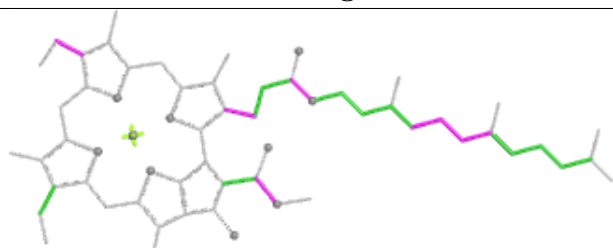
Ligand CLA b 602



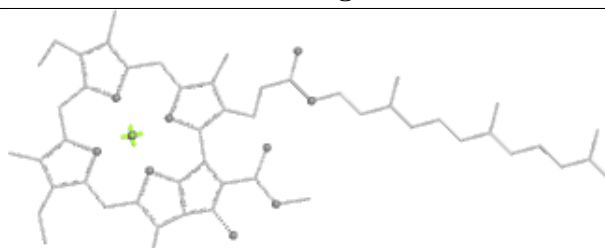
Bond lengths



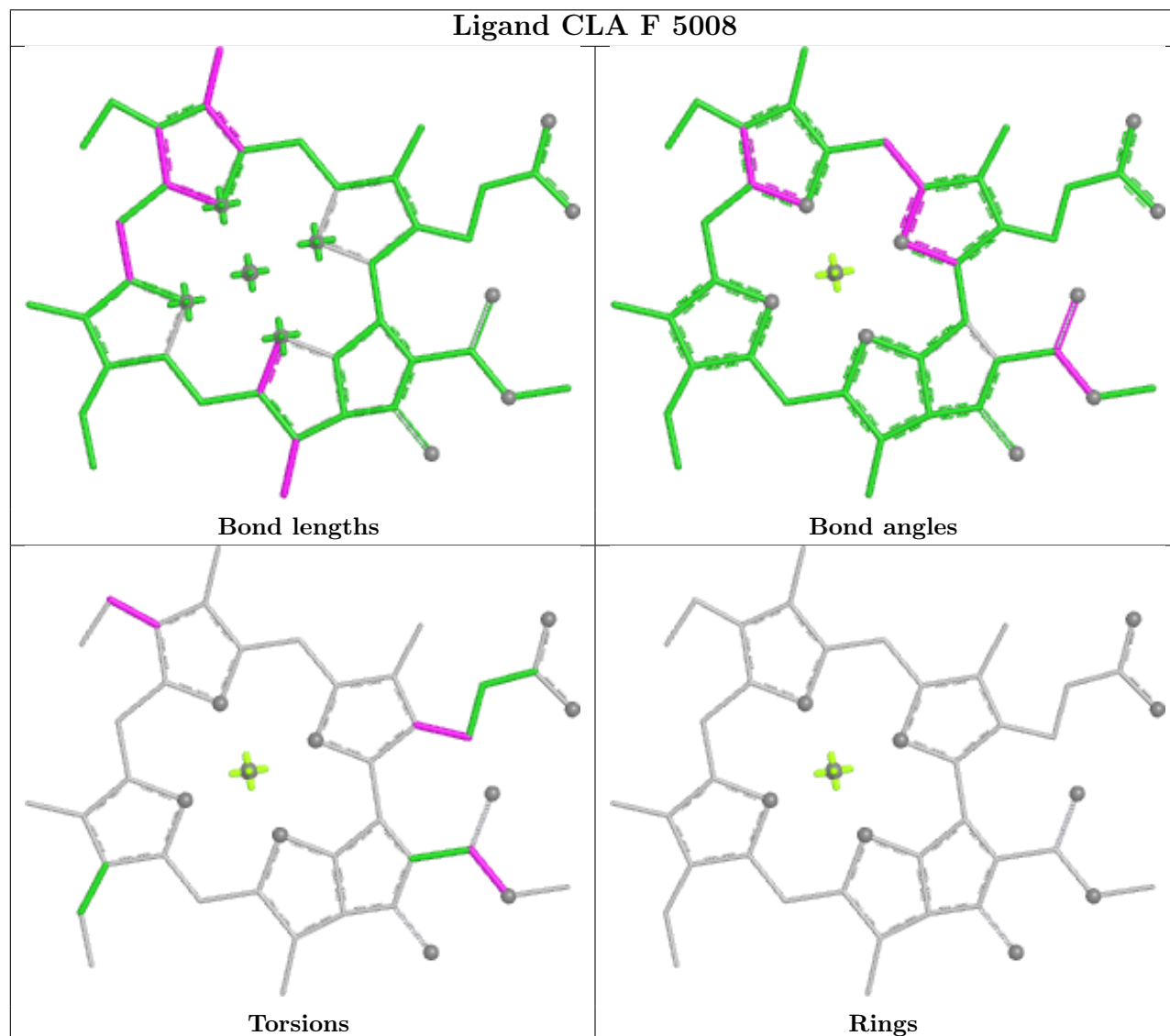
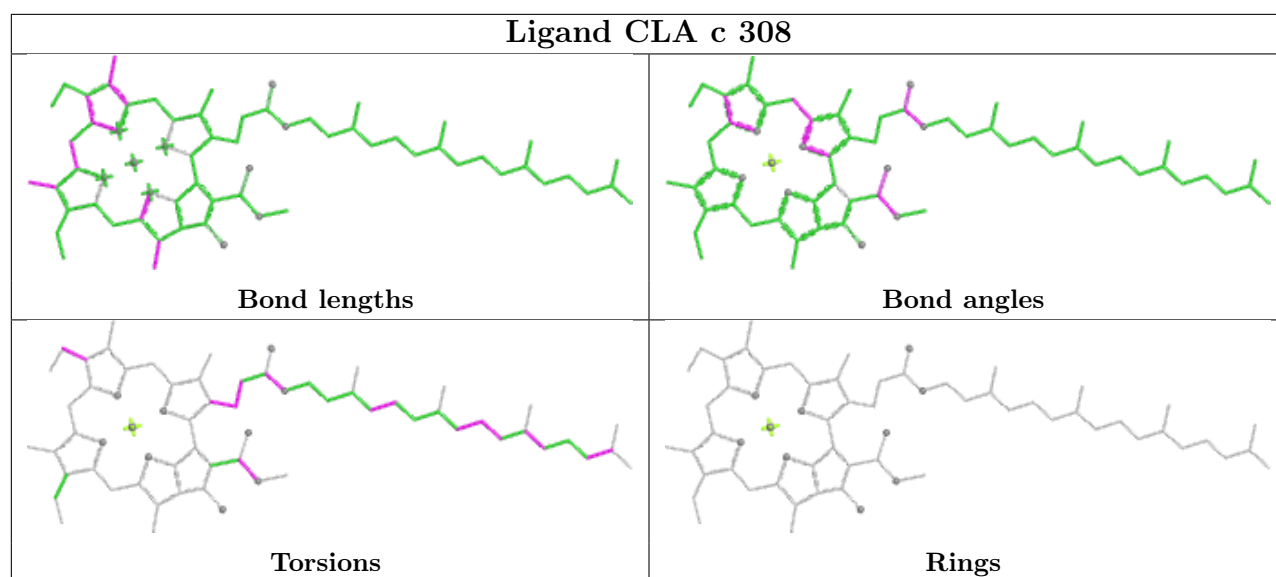
Bond angles



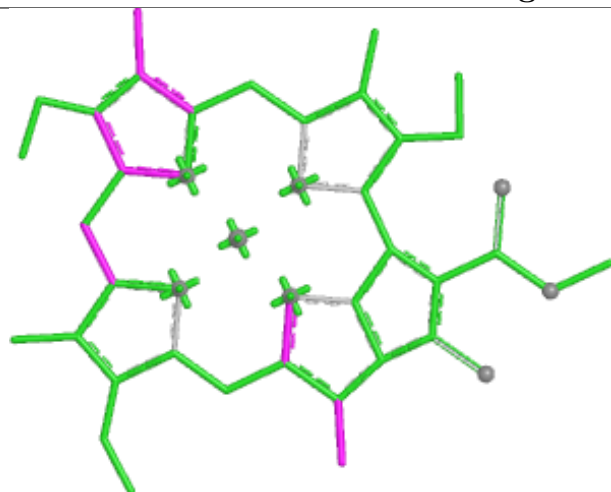
Torsions



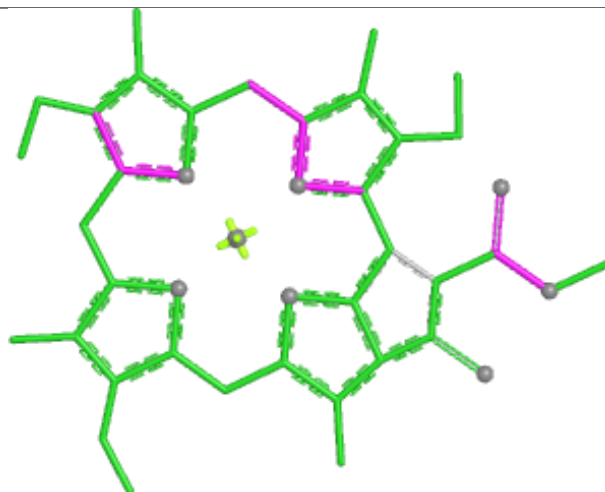
Rings



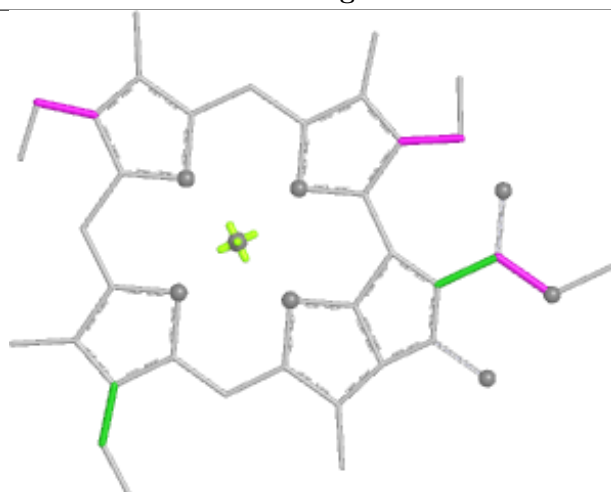
Ligand CLA 3 313



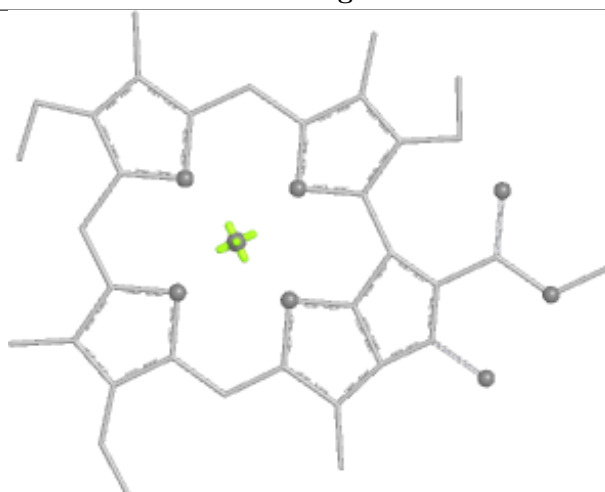
Bond lengths



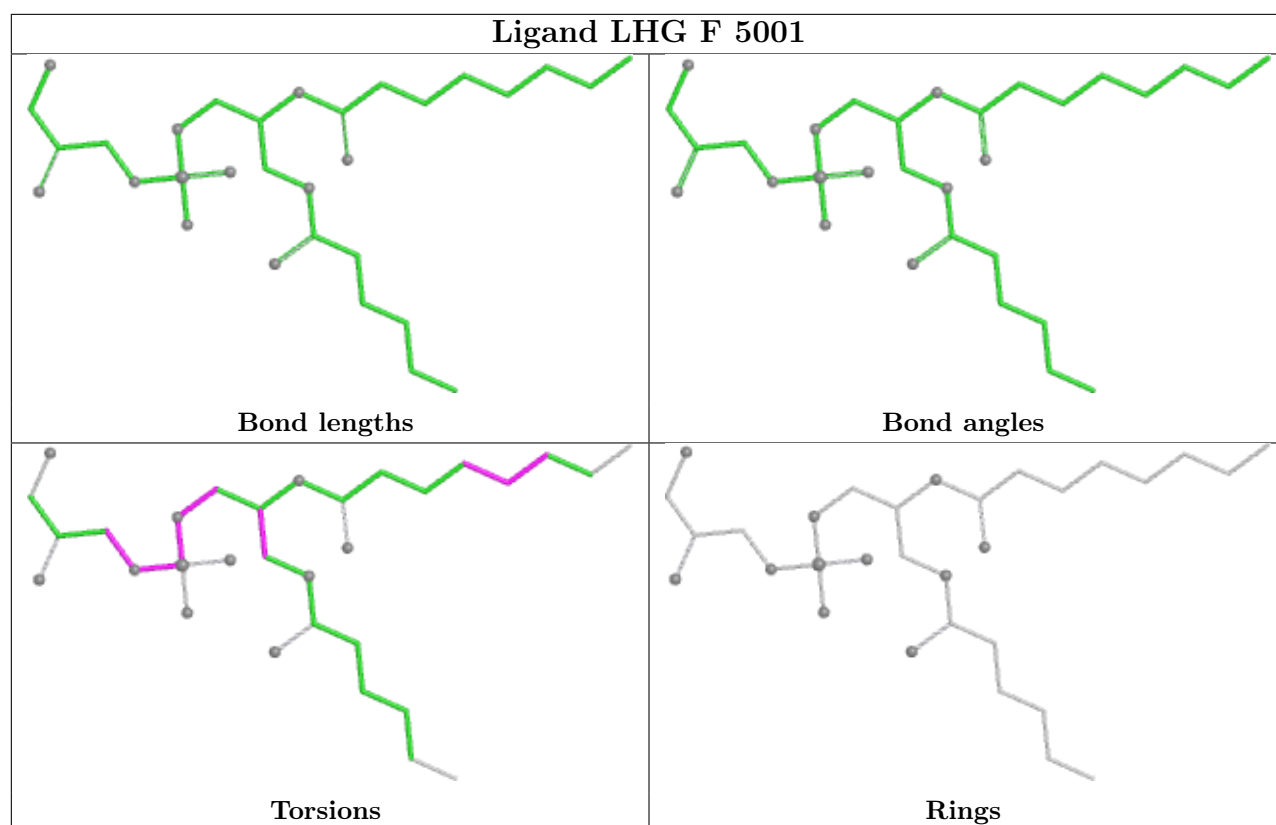
Bond angles



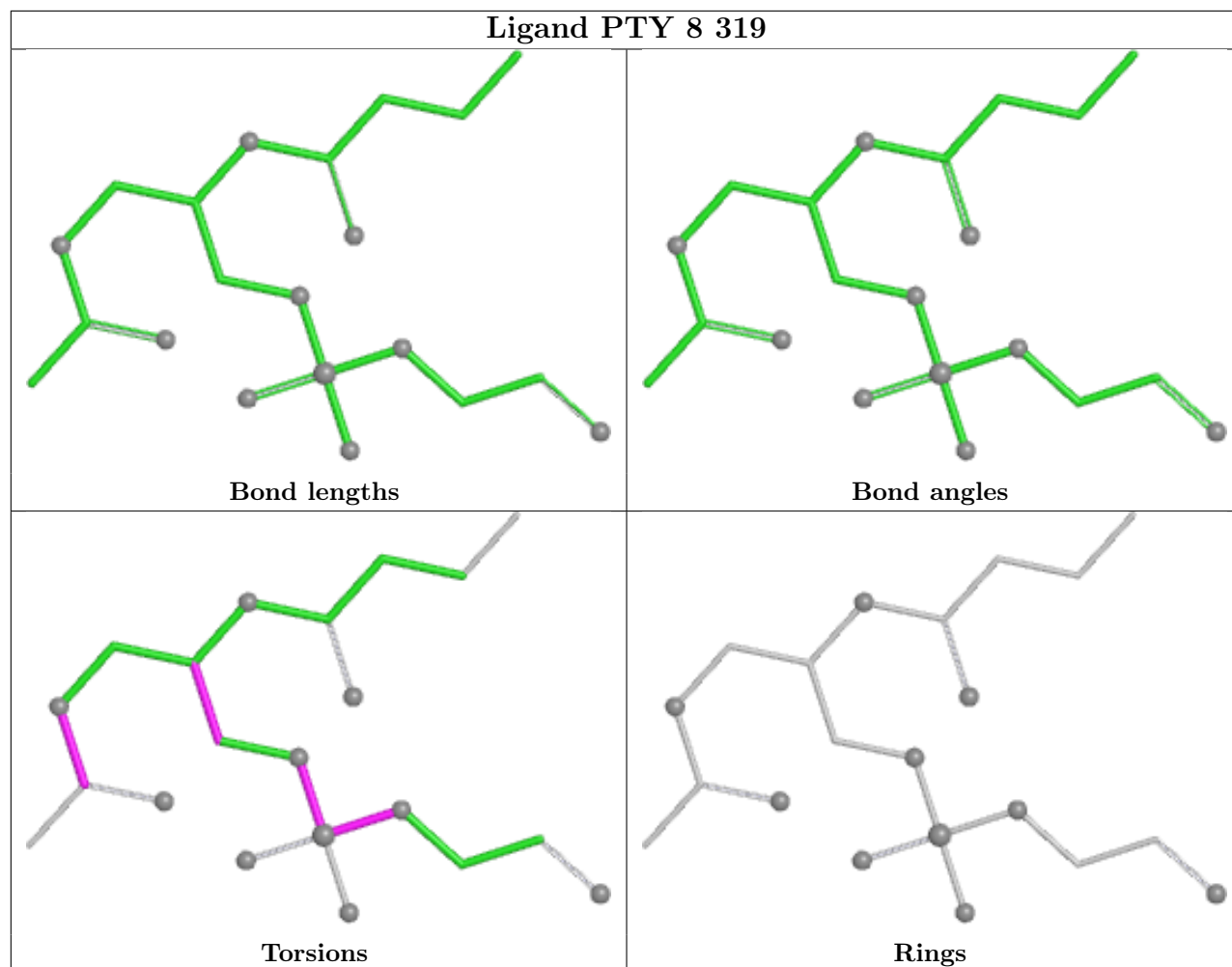
Torsions



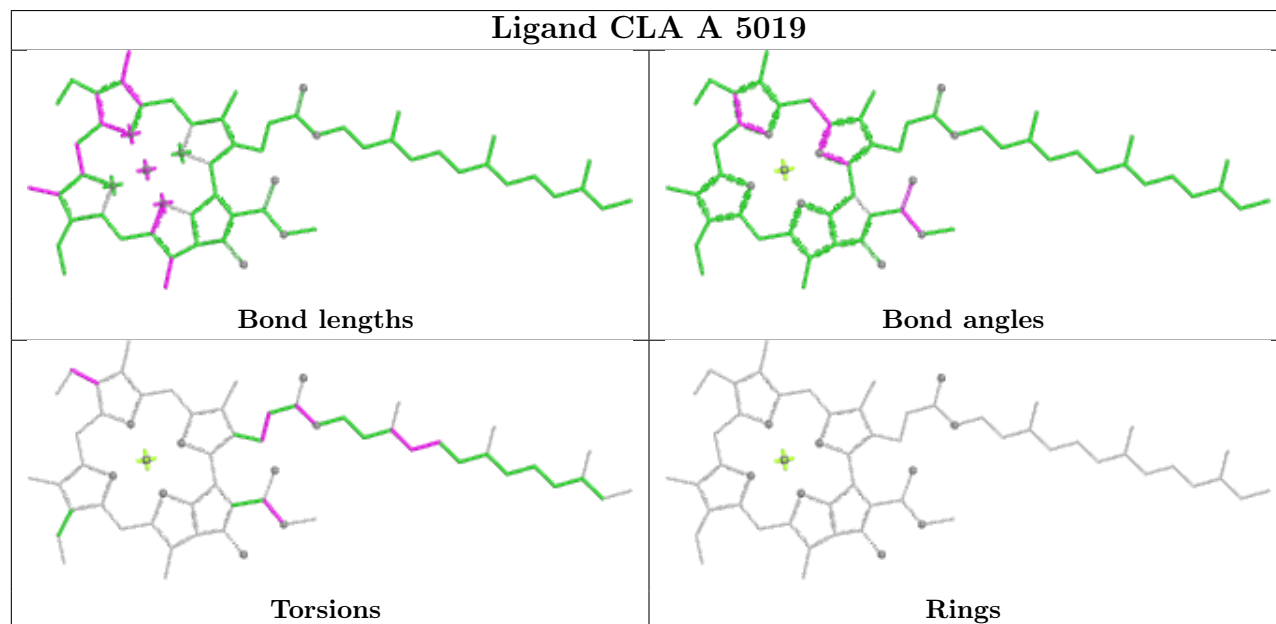
Rings

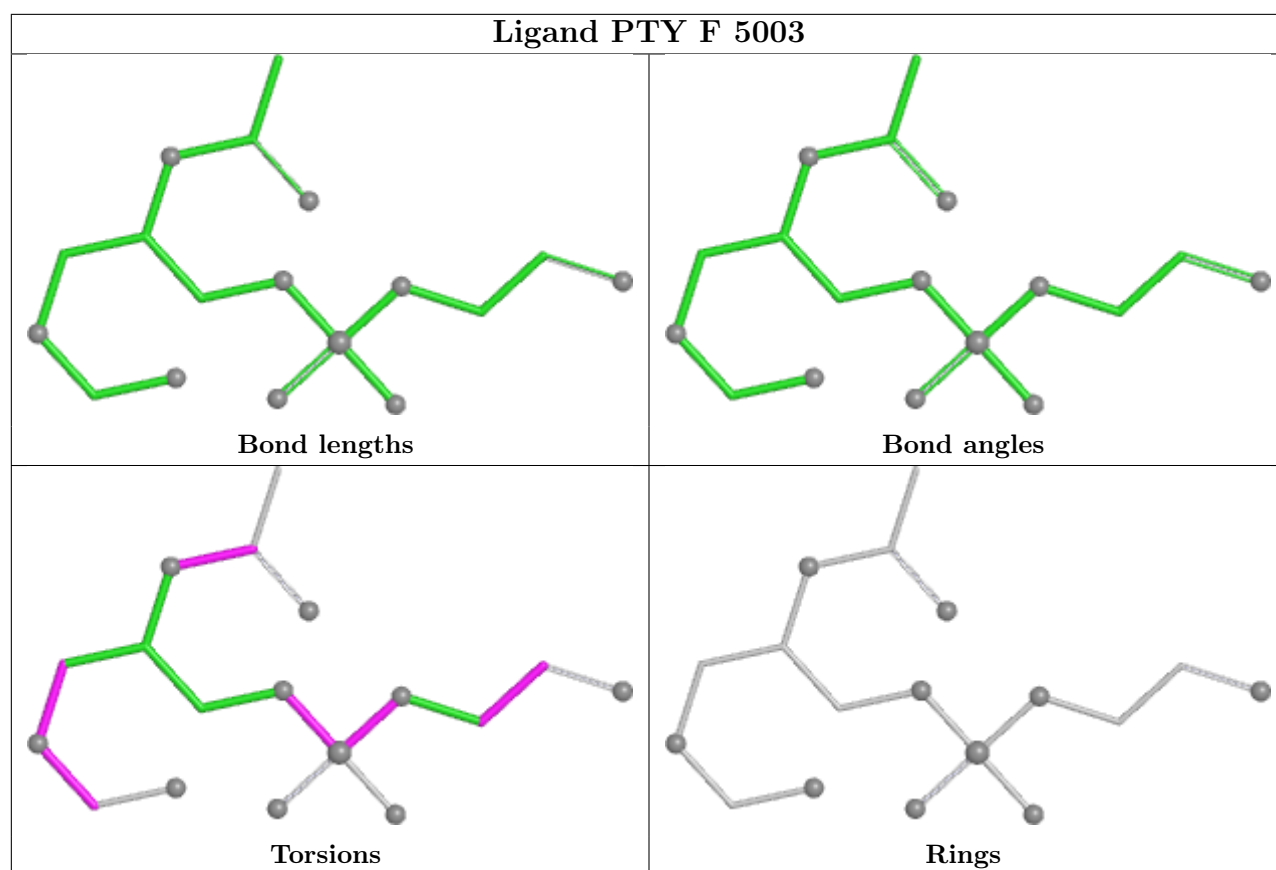


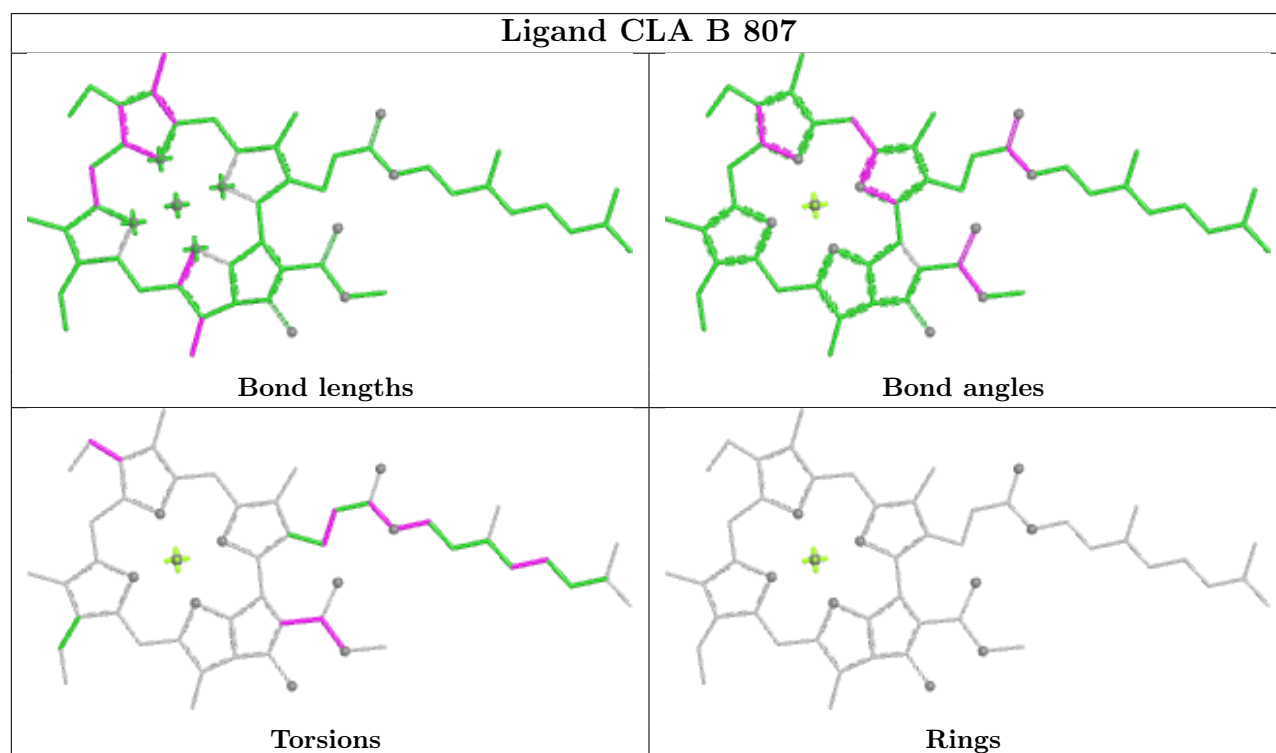
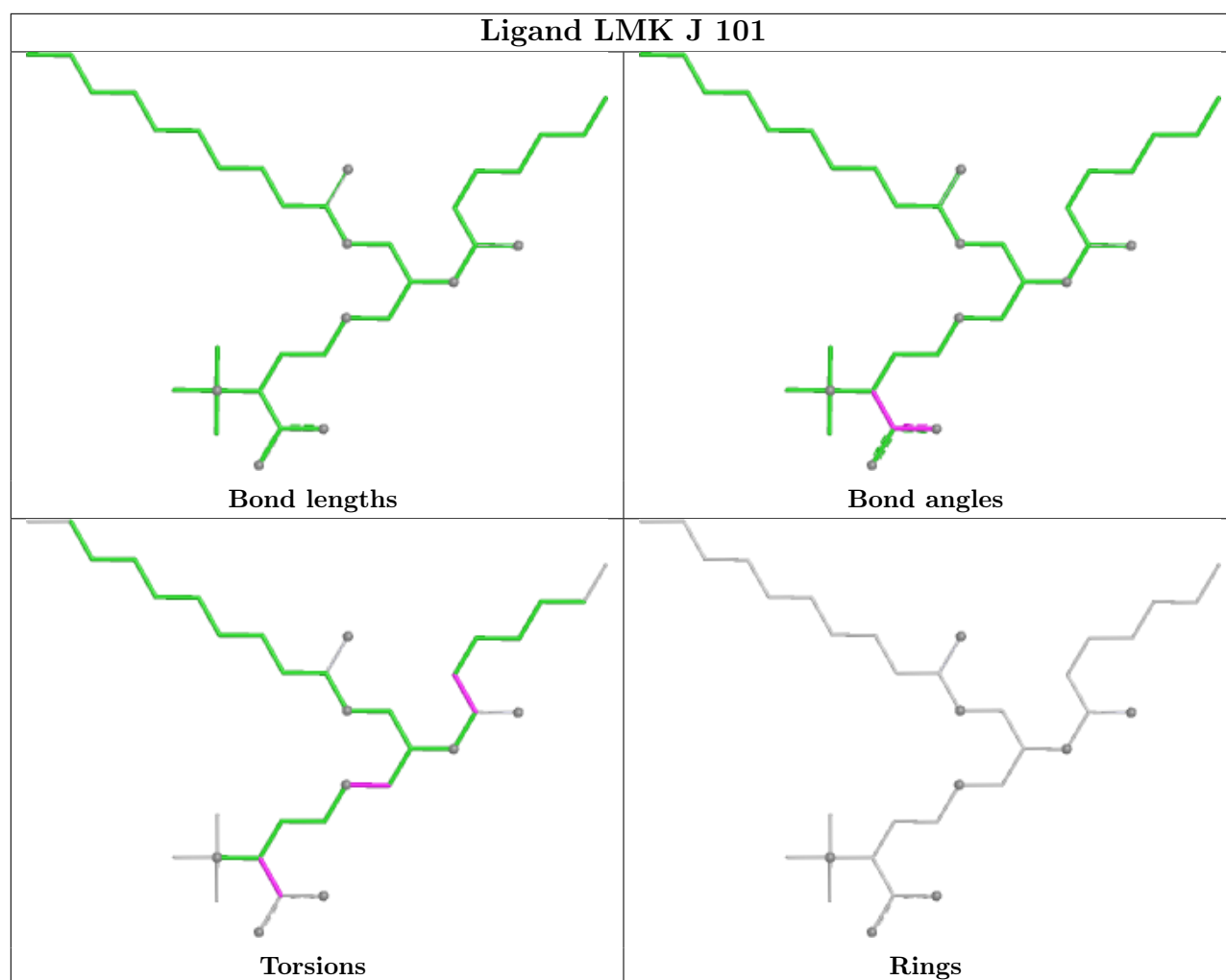
Ligand PTY 8 319



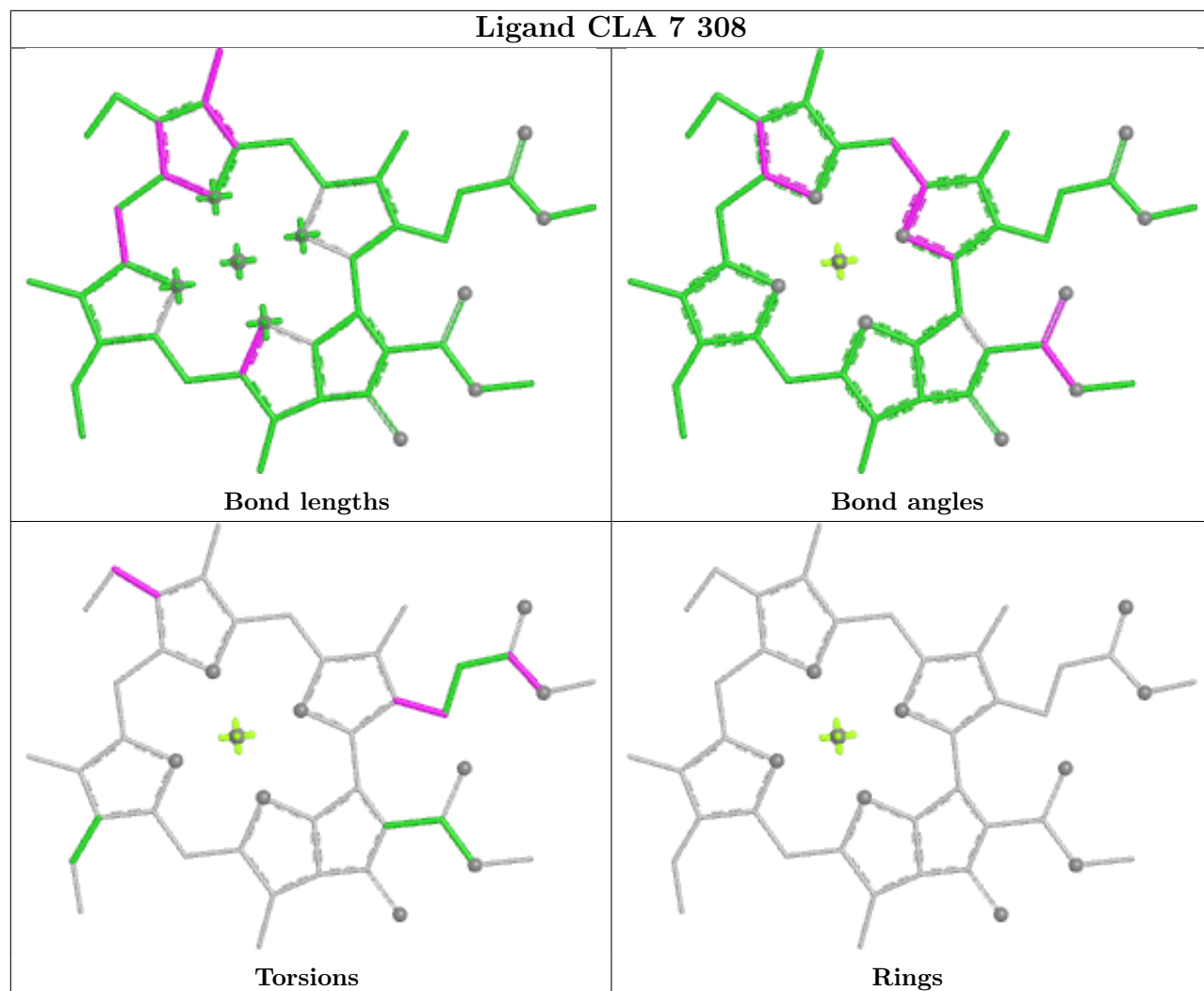
Ligand CLA A 5019



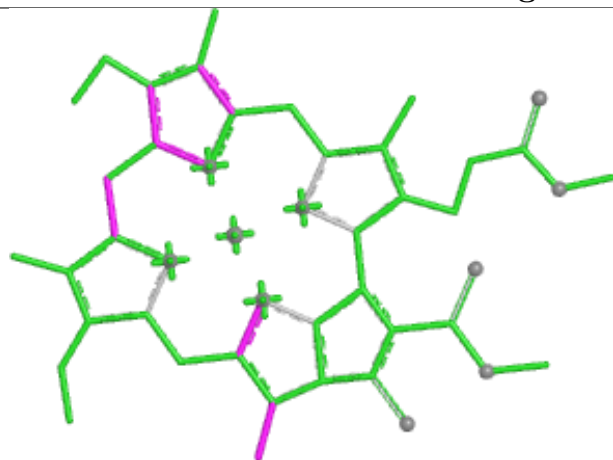




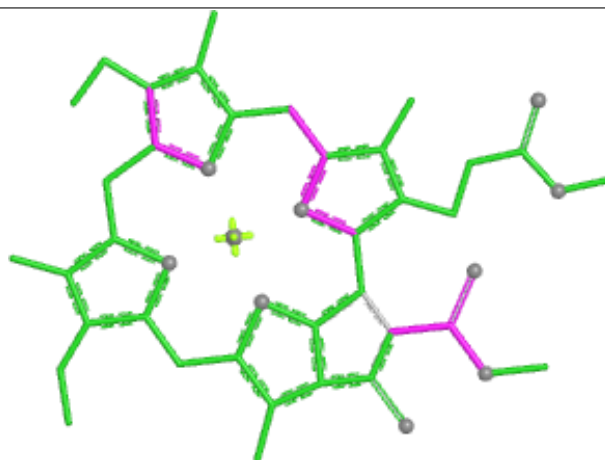
Ligand CLA 7 308



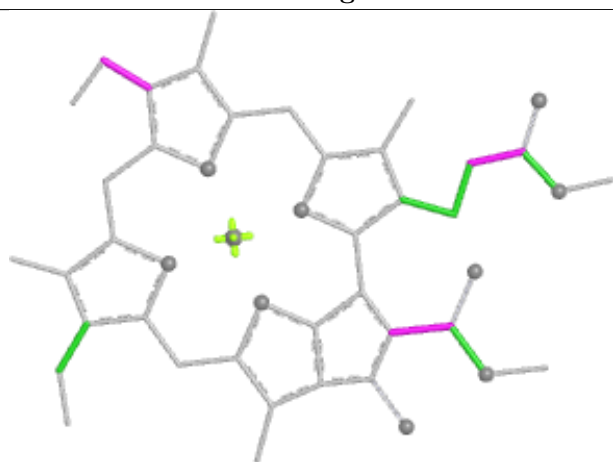
Ligand CLA 8 302



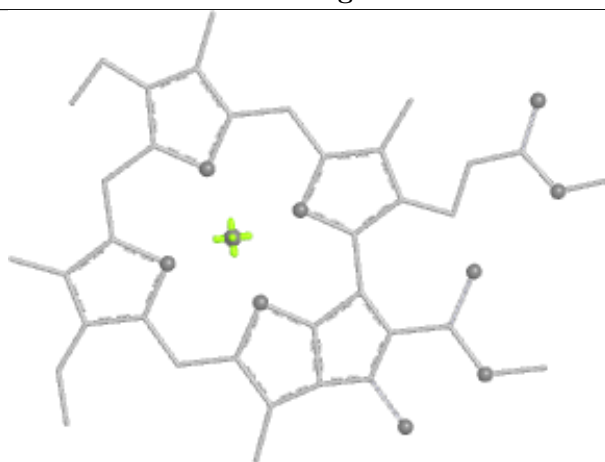
Bond lengths



Bond angles

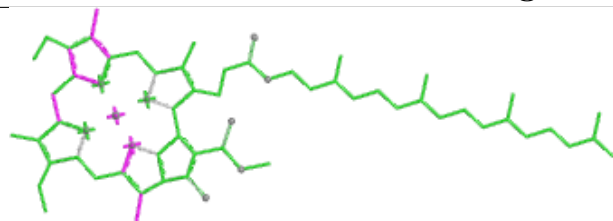


Torsions

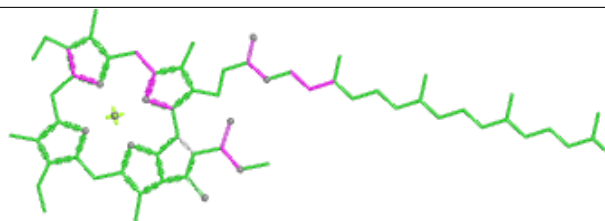


Rings

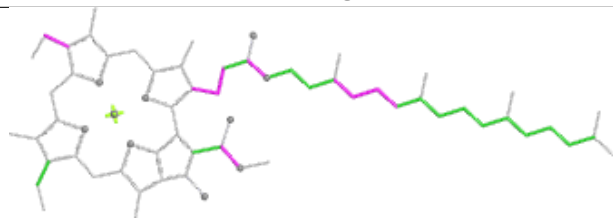
Ligand CLA 7 312



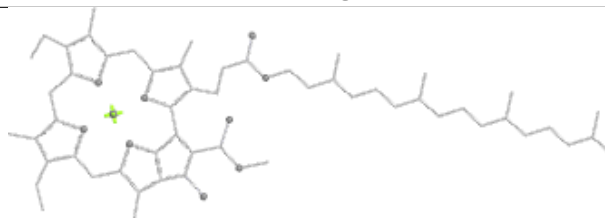
Bond lengths



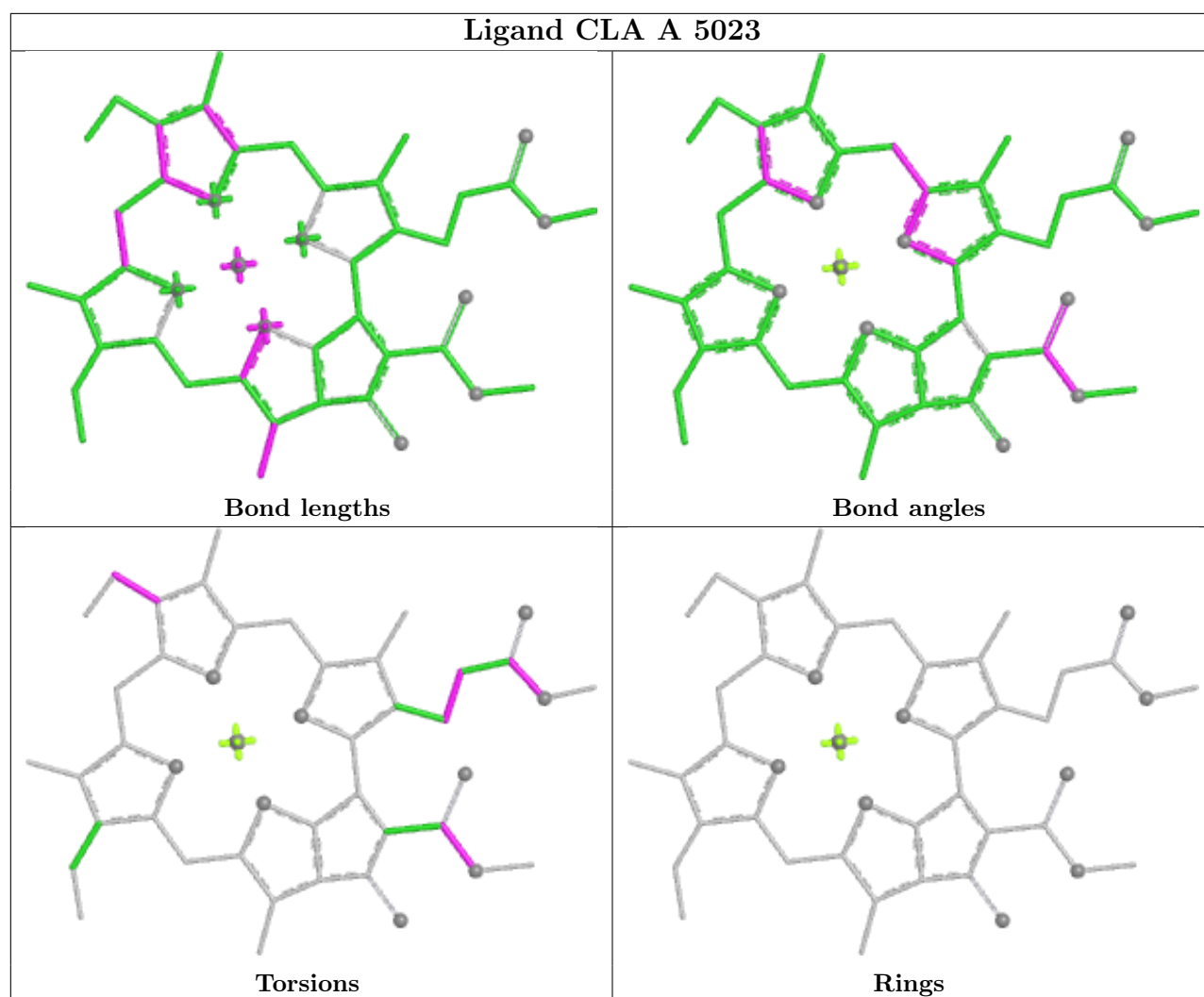
Bond angles



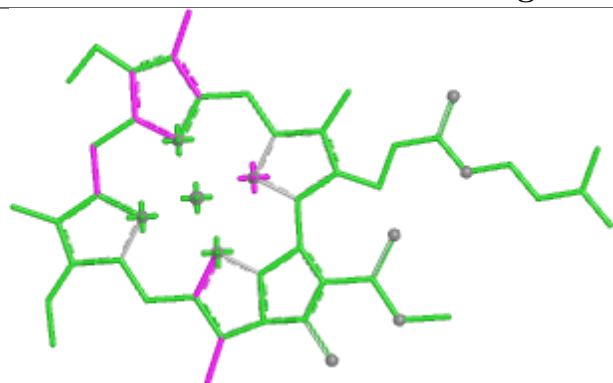
Torsions



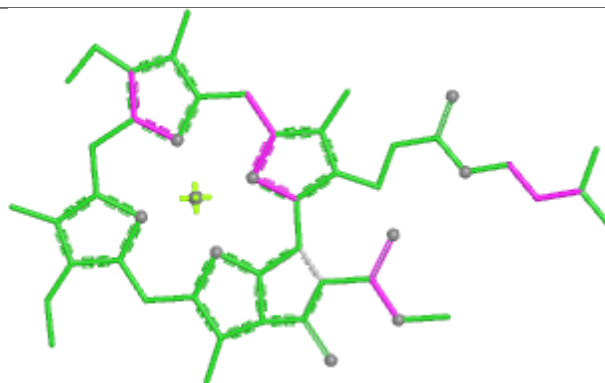
Rings



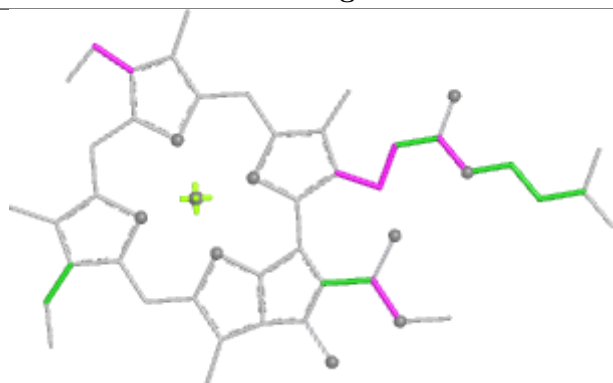
Ligand CLA b 604



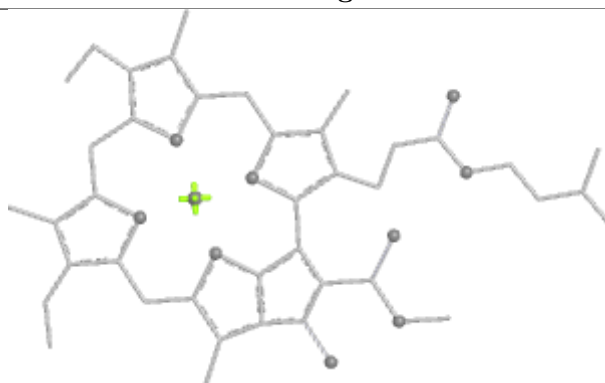
Bond lengths



Bond angles

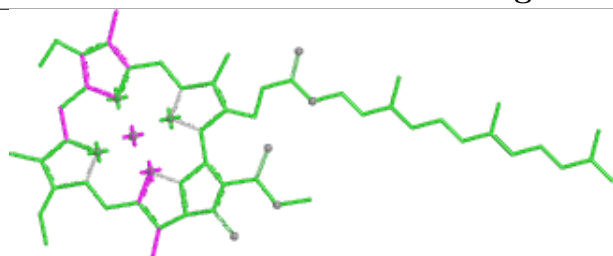


Torsions

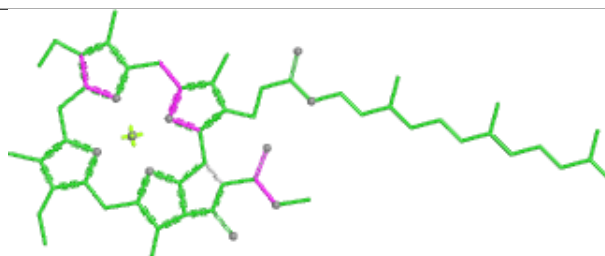


Rings

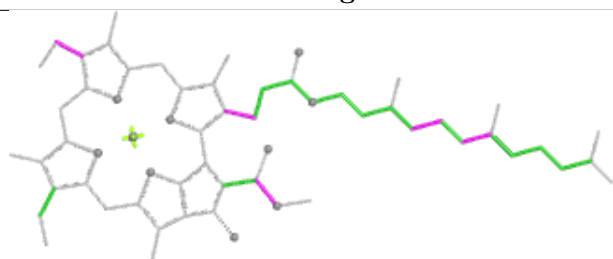
Ligand CLA B 819



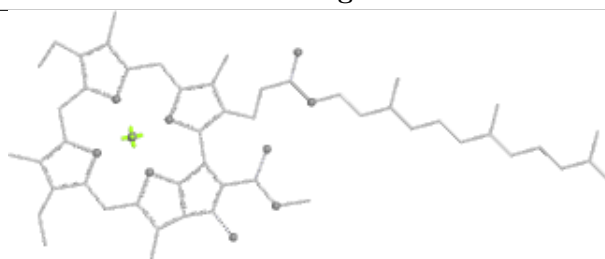
Bond lengths



Bond angles

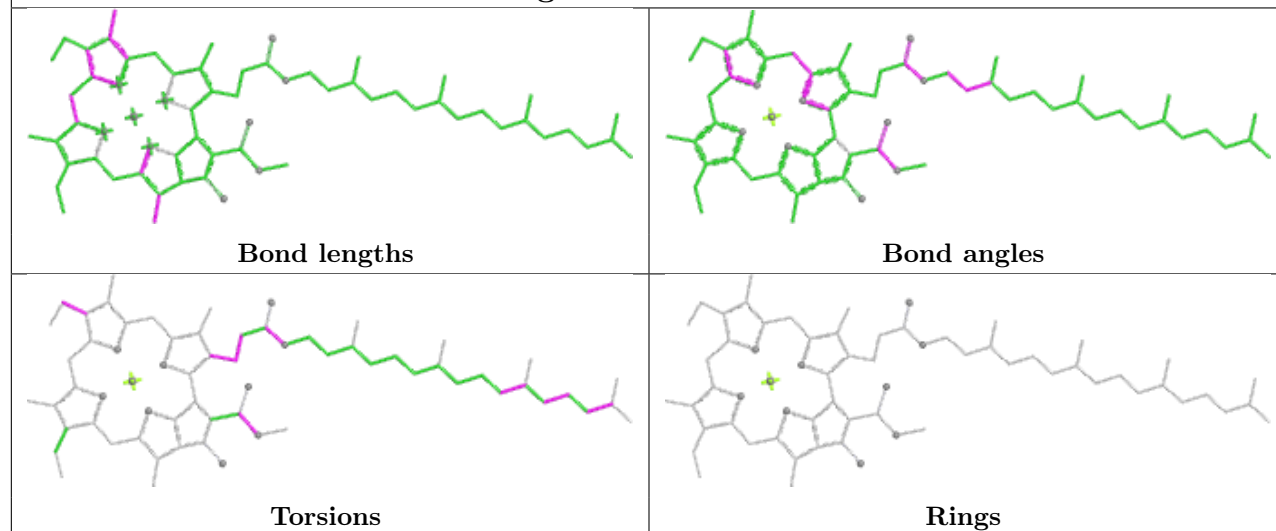


Torsions

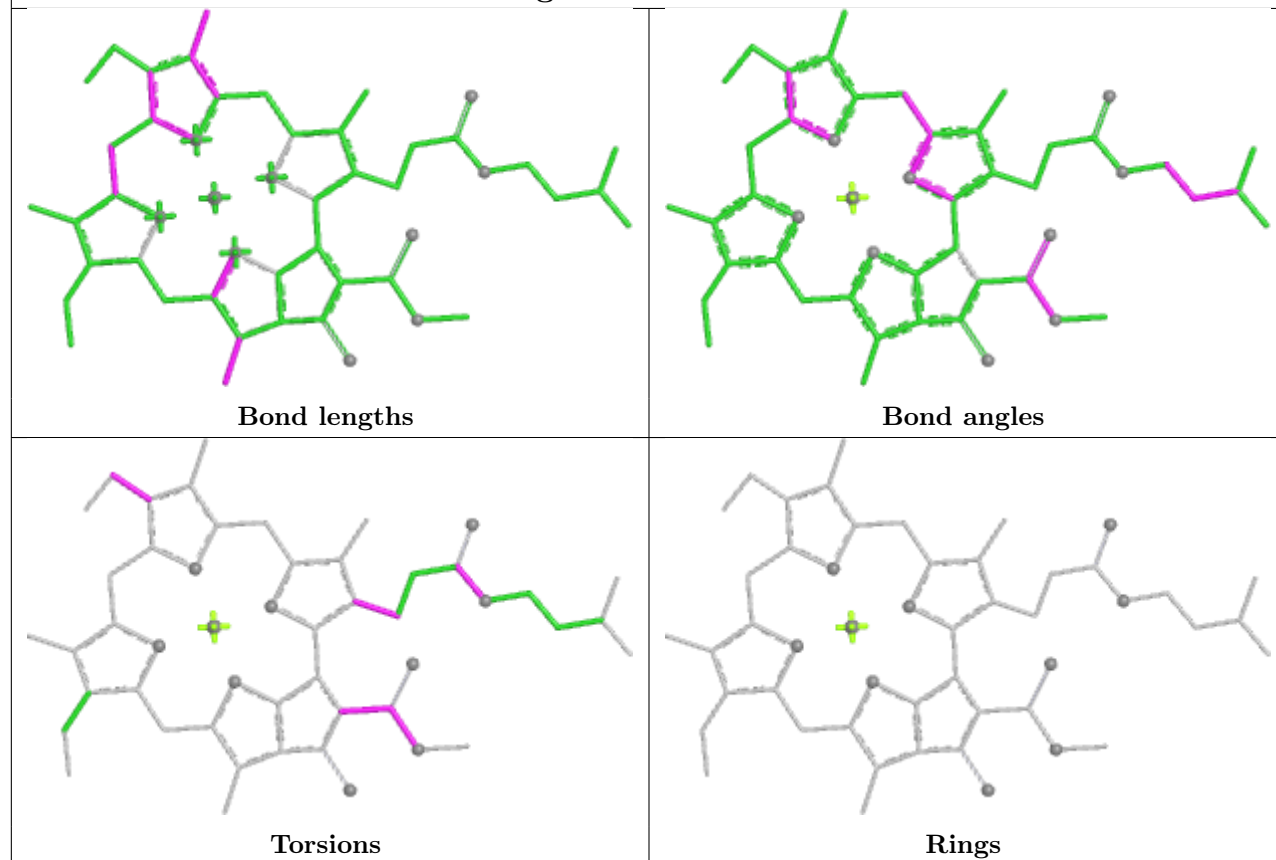


Rings

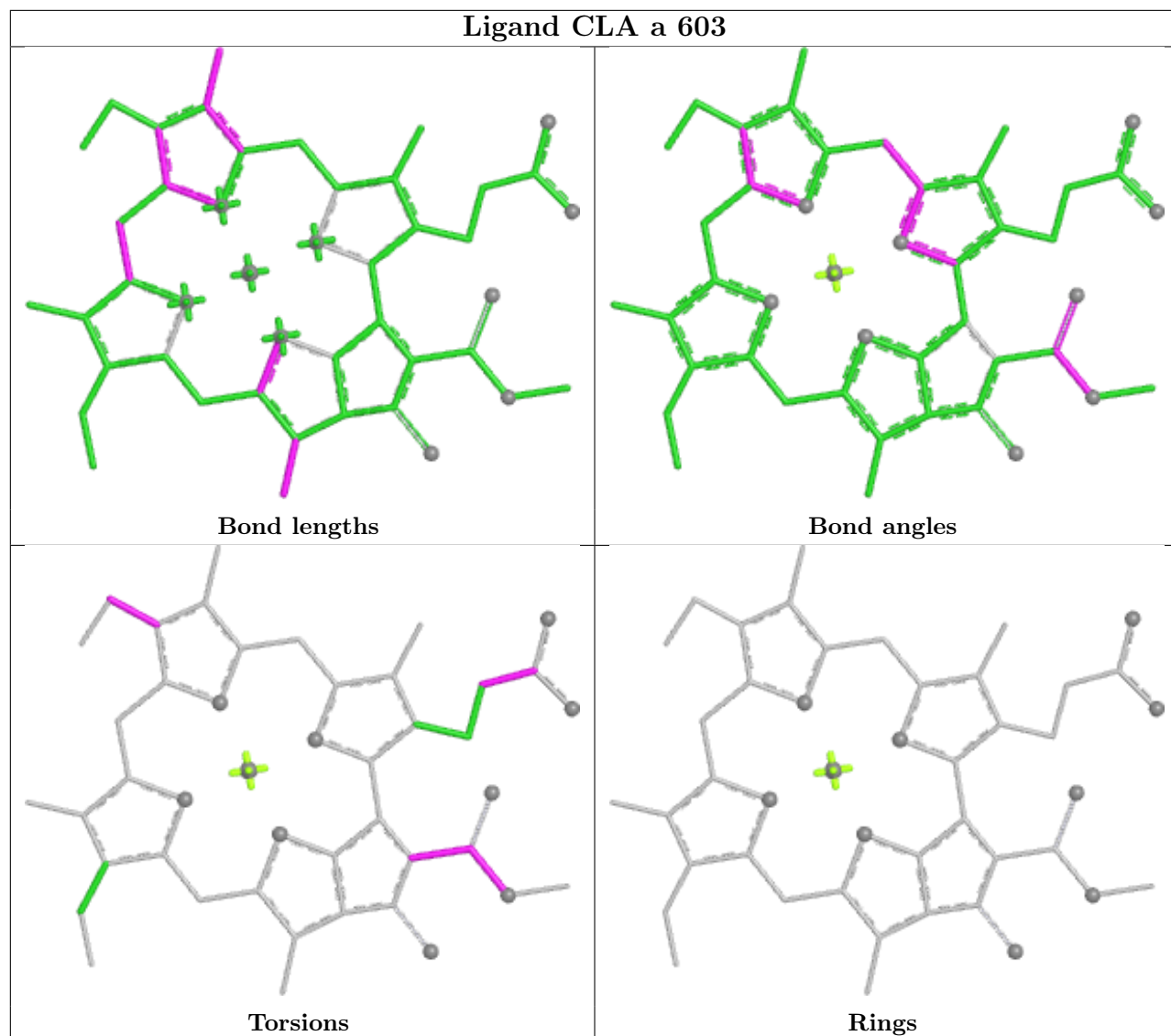
Ligand CLA c 301



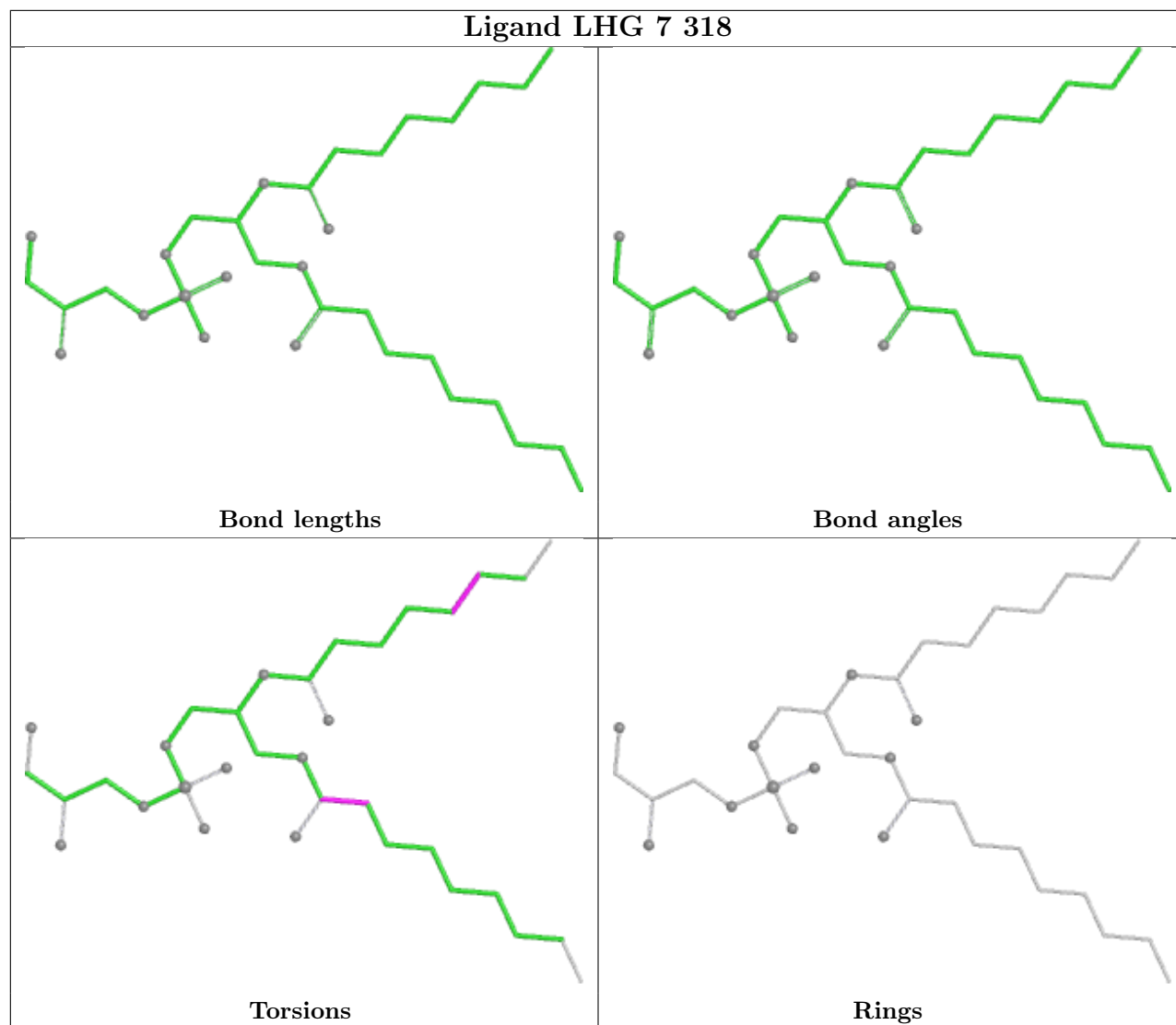
Ligand CLA 1 604



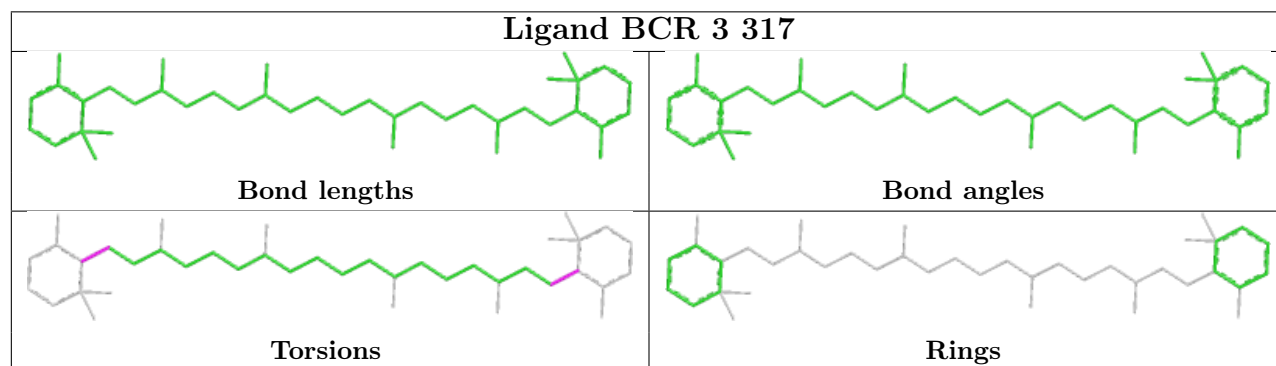
Ligand CLA a 603

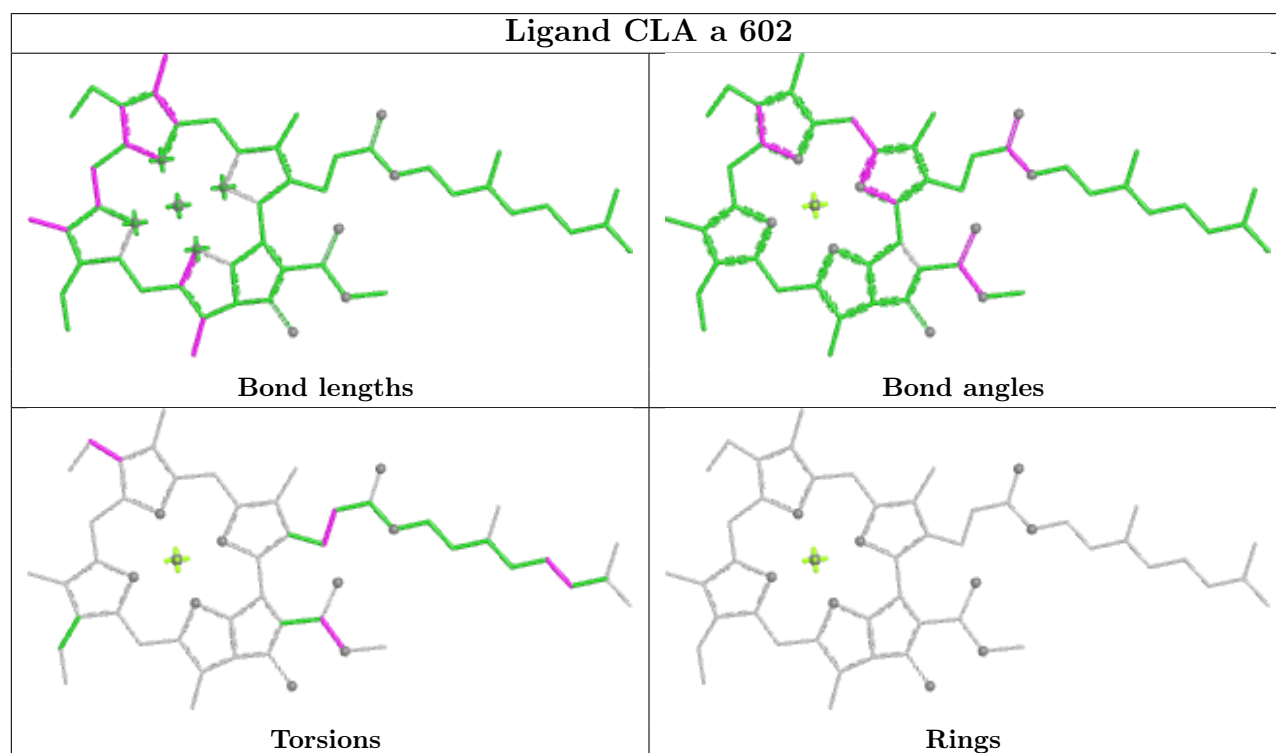
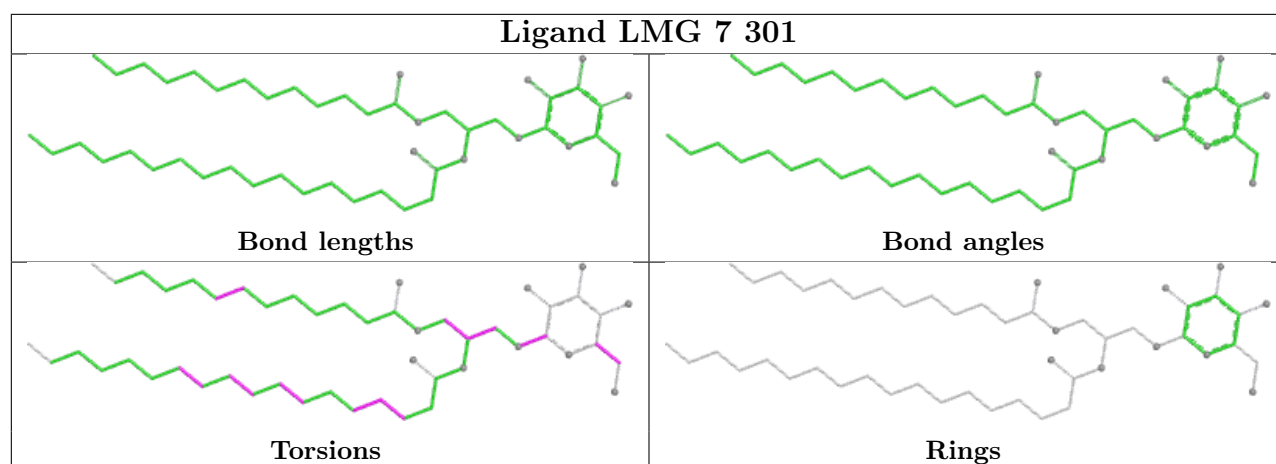


Ligand LHG 7 318

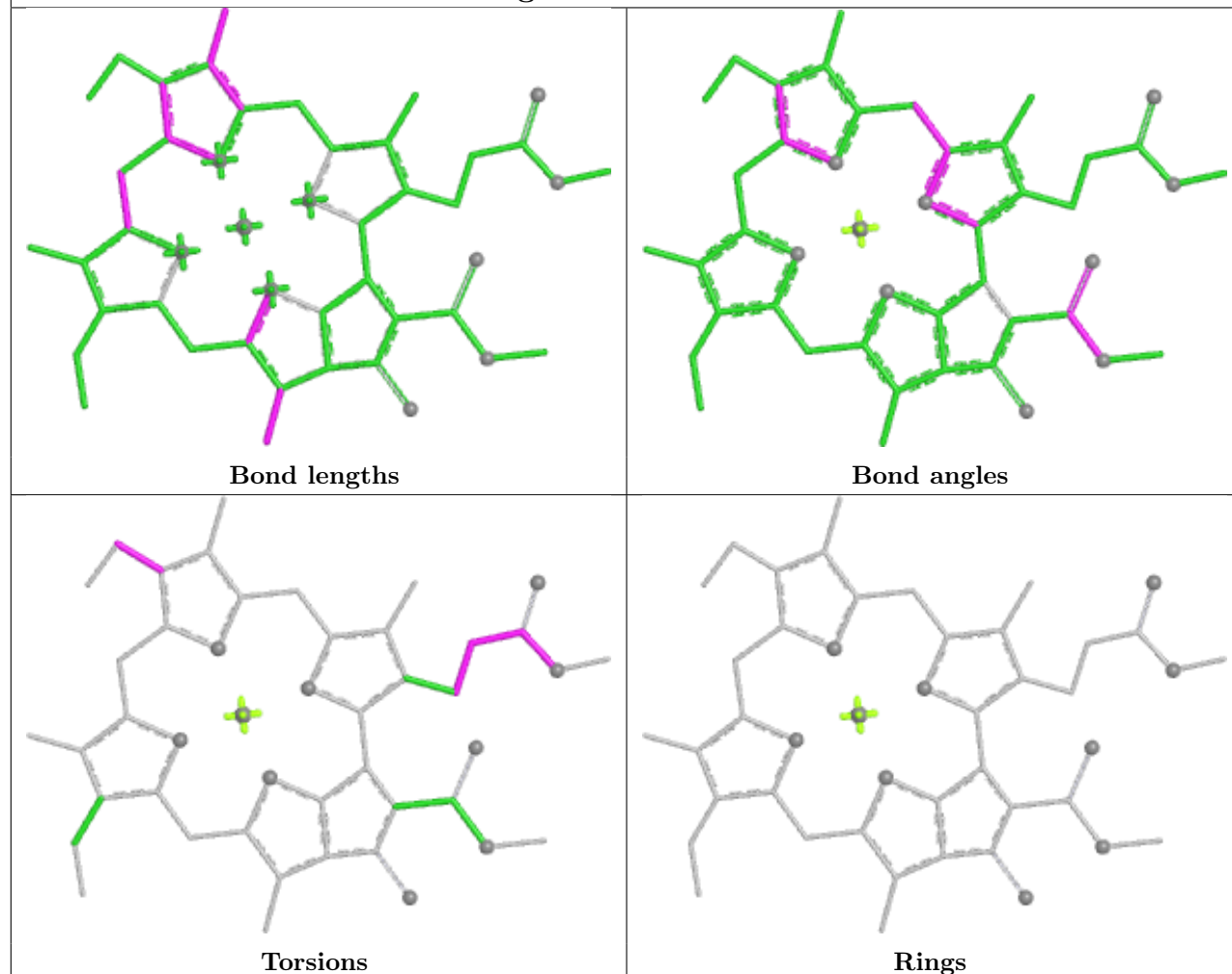


Ligand BCR 3 317

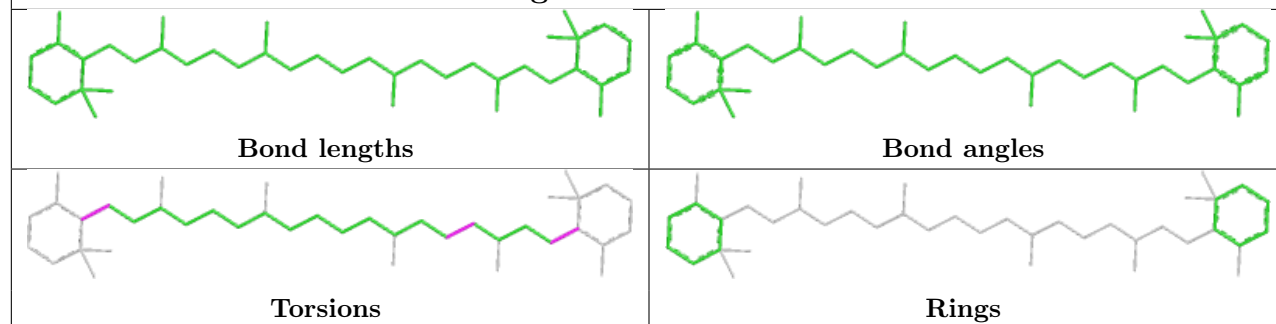




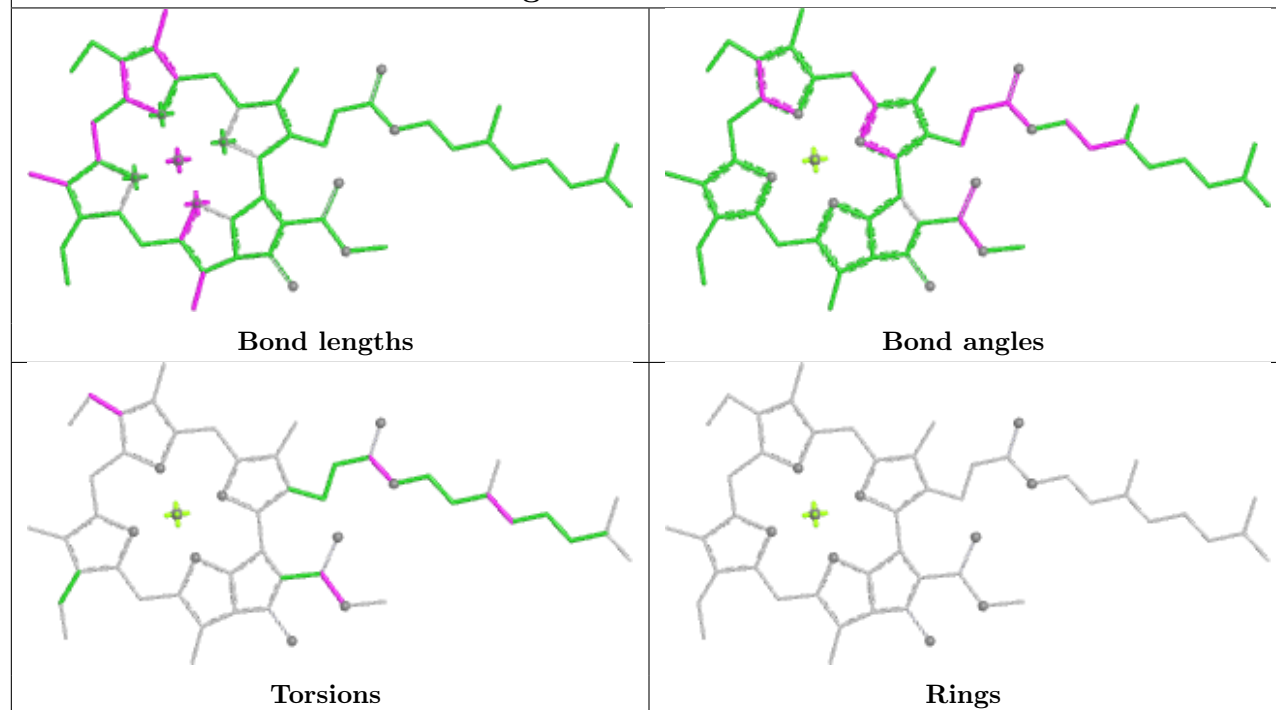
Ligand CLA 7 314



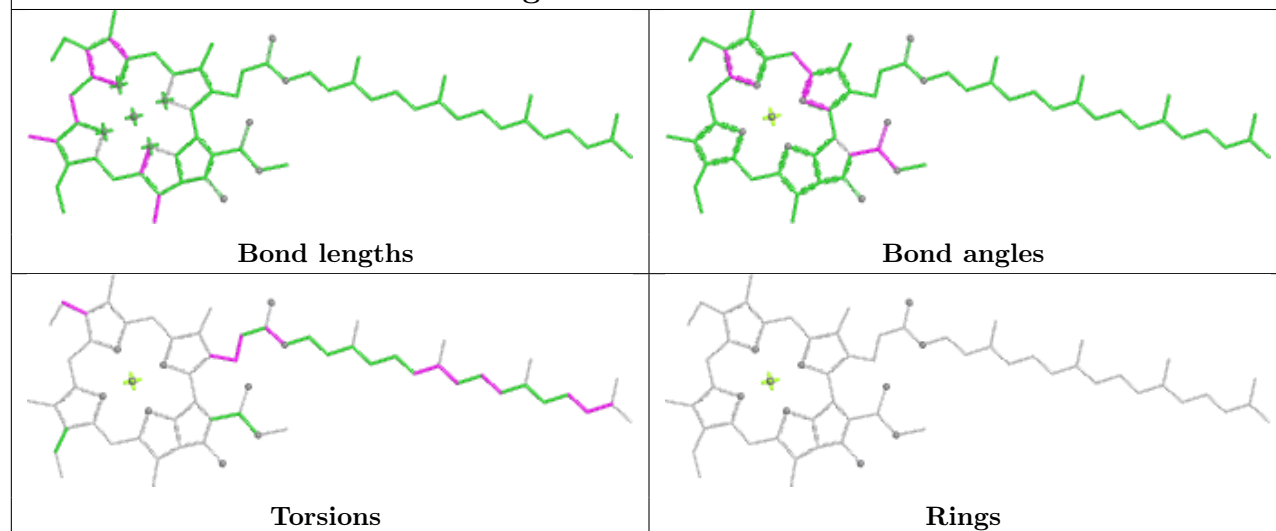
Ligand BCR B 843

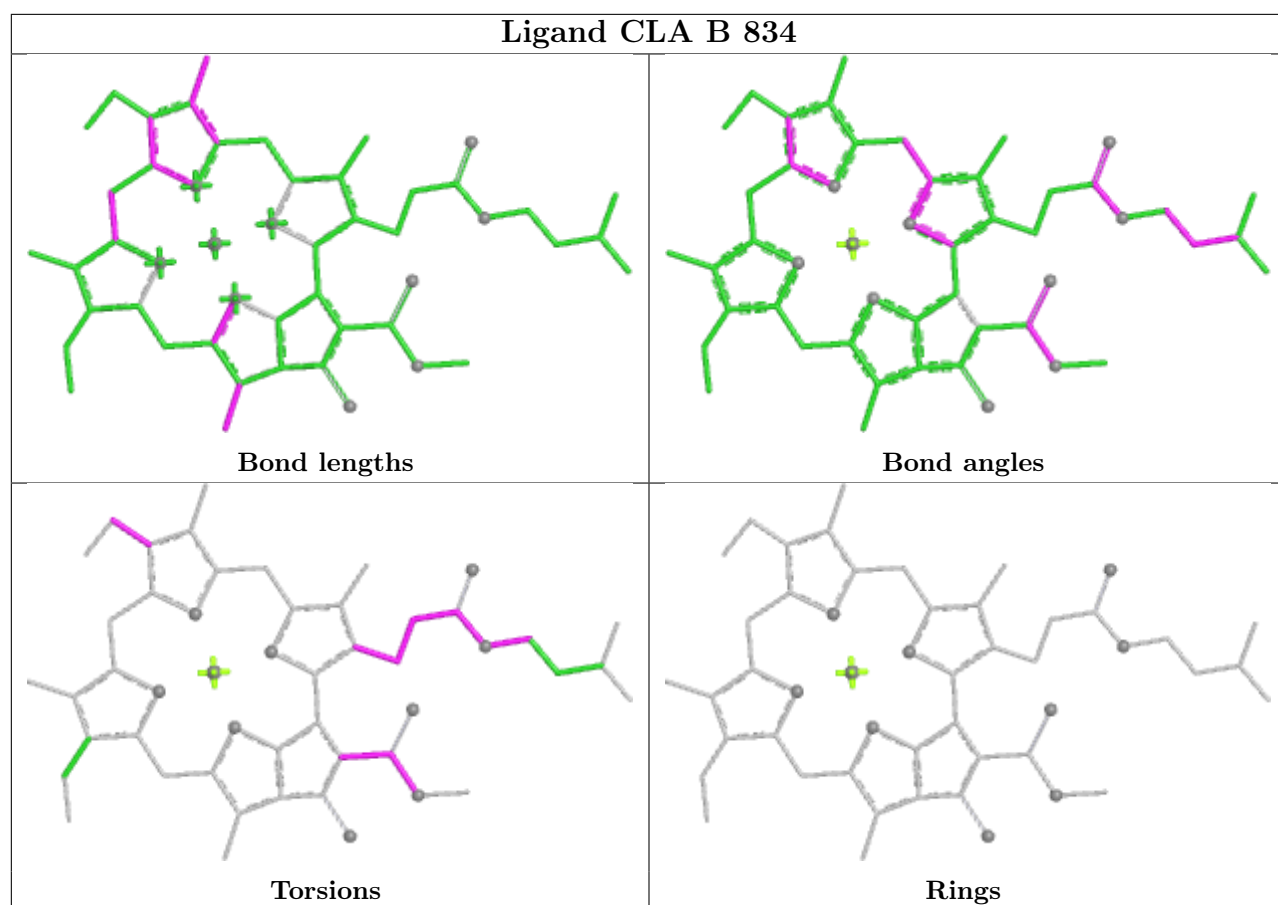


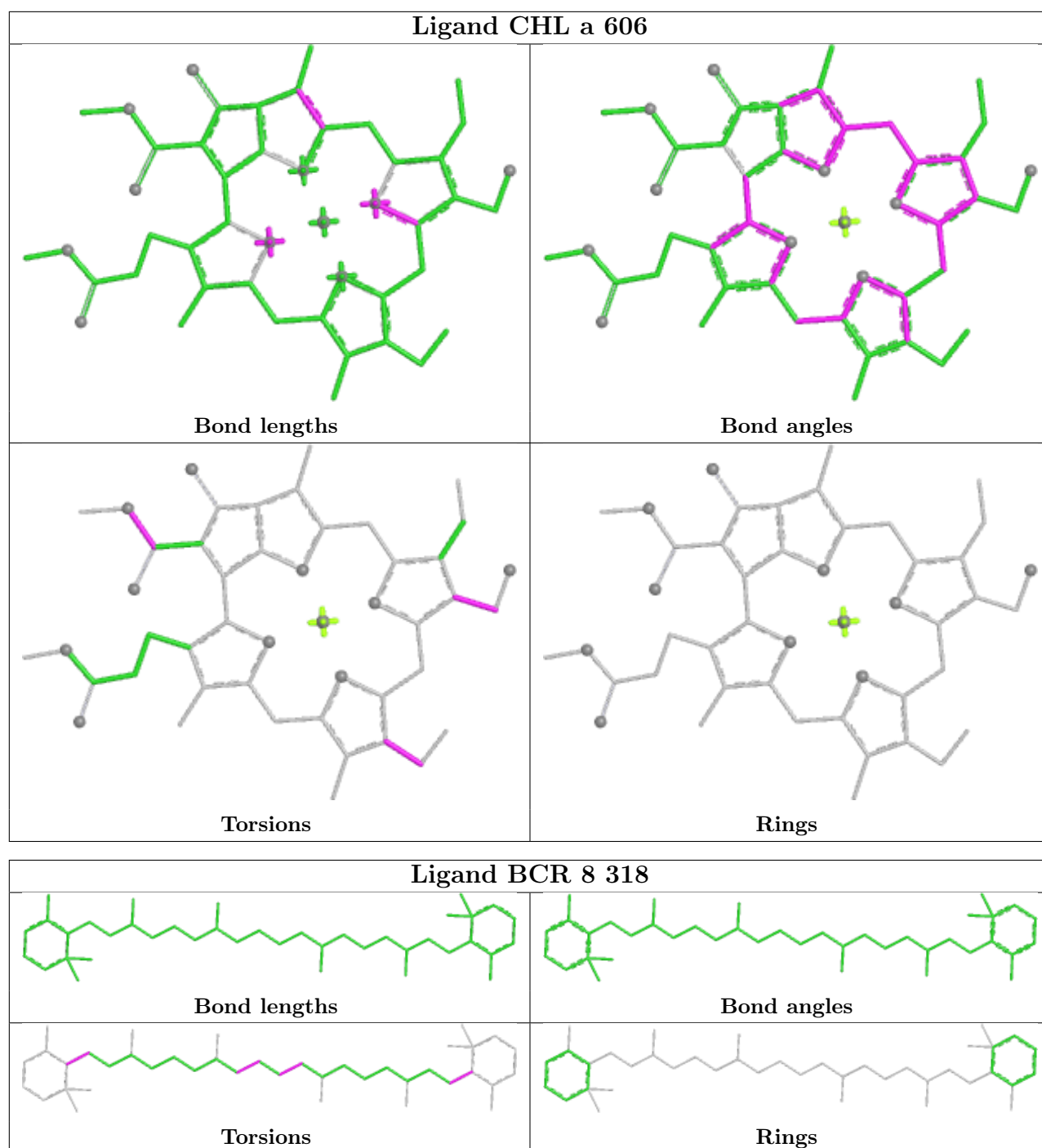
Ligand CLA A 5012

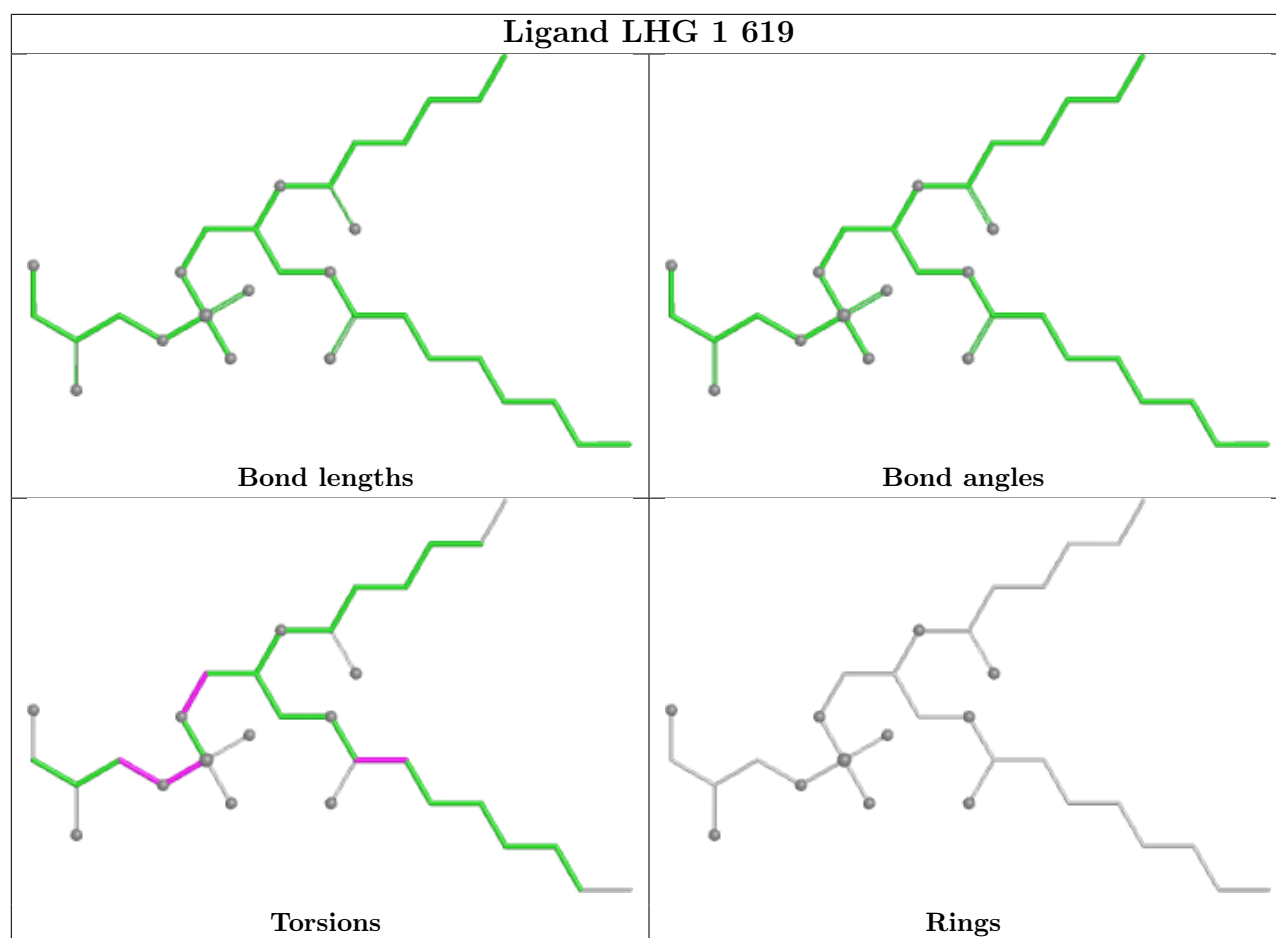


Ligand CLA A 5014

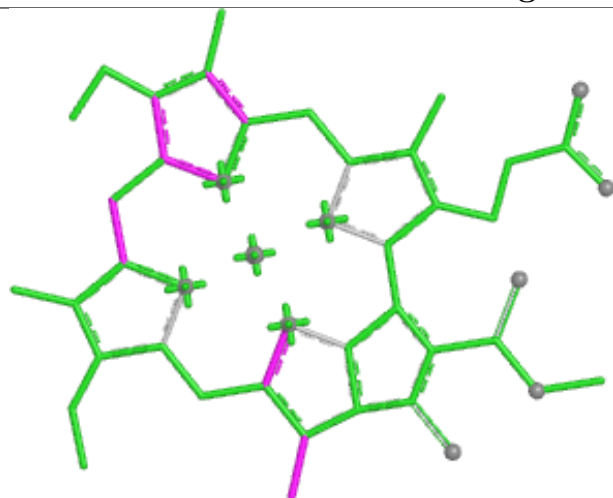




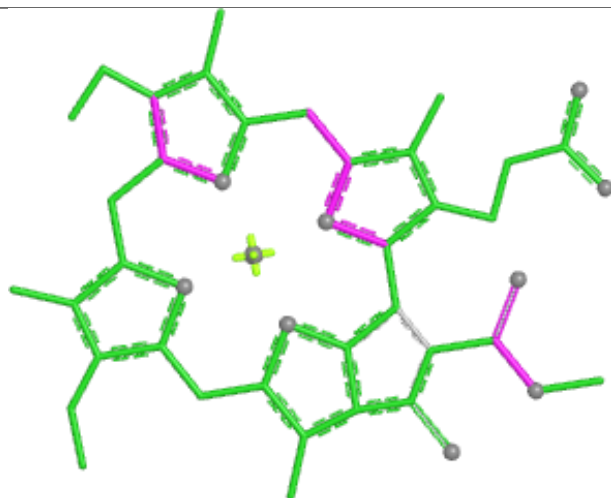




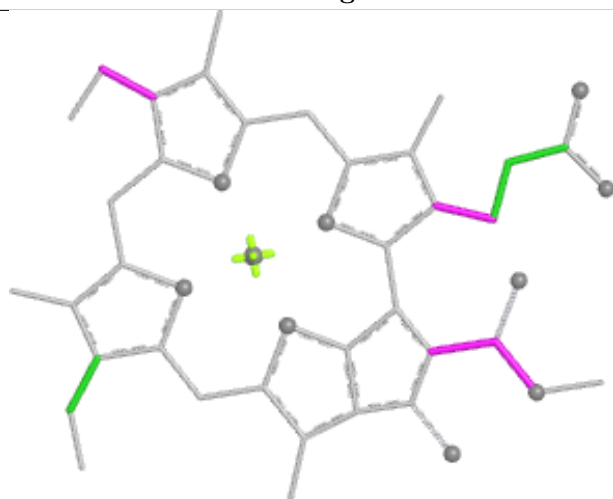
Ligand CLA 1 608



Bond lengths



Bond angles

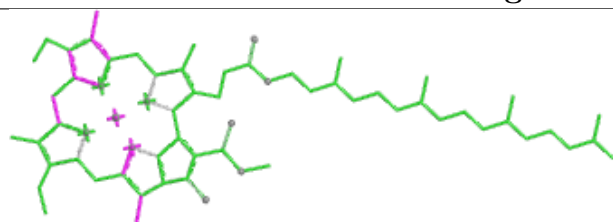


Torsions

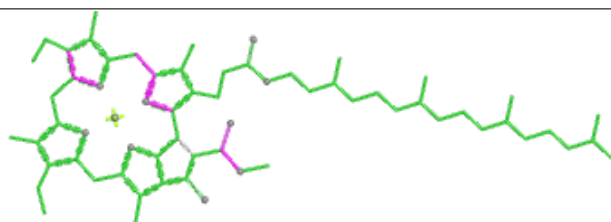


Rings

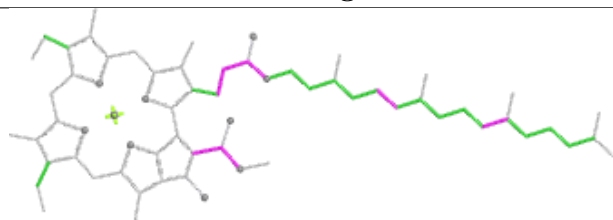
Ligand CLA A 5026



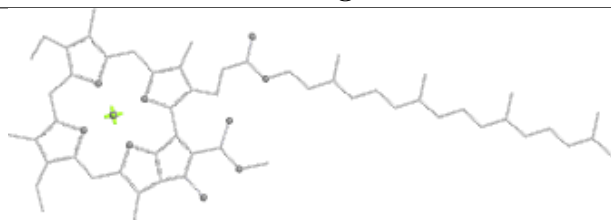
Bond lengths



Bond angles

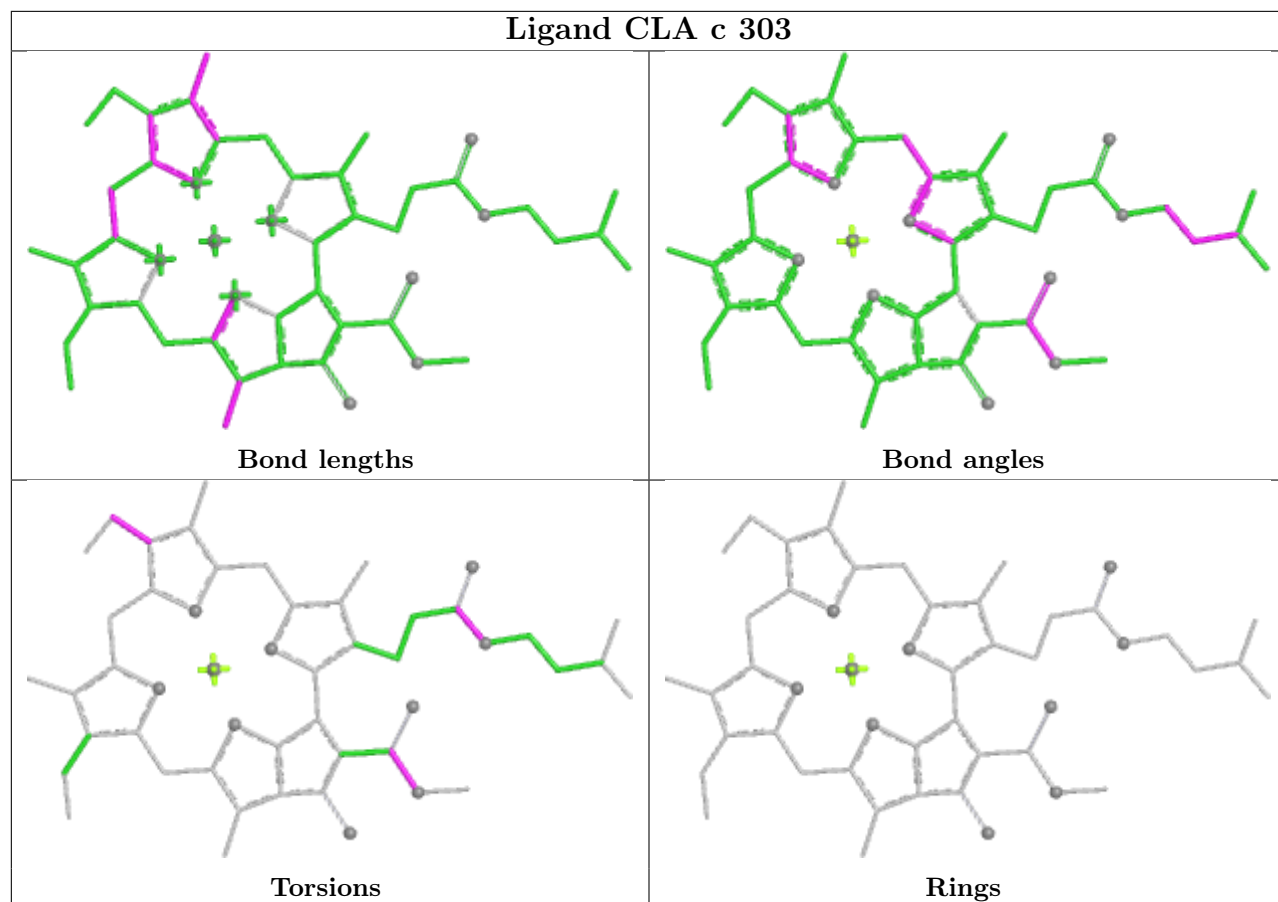


Torsions

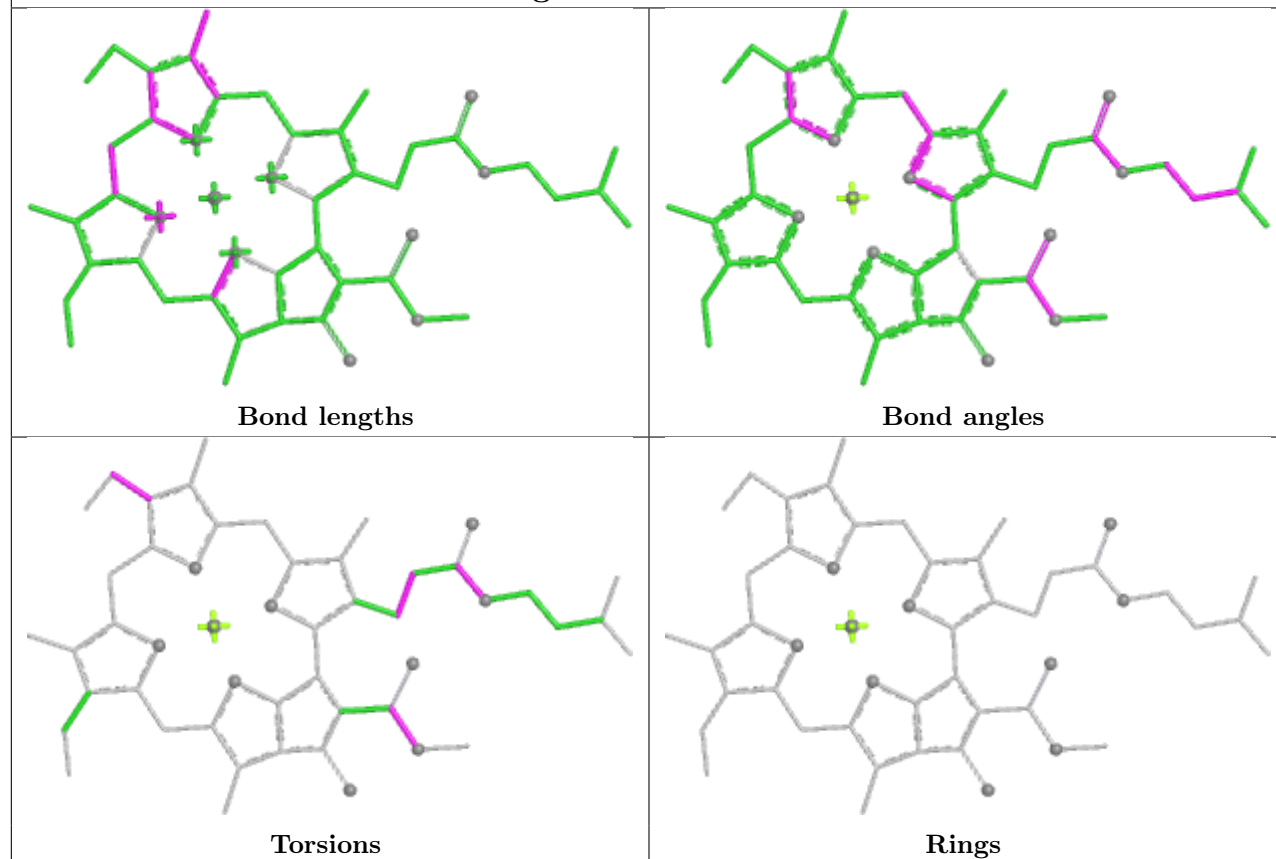


Rings

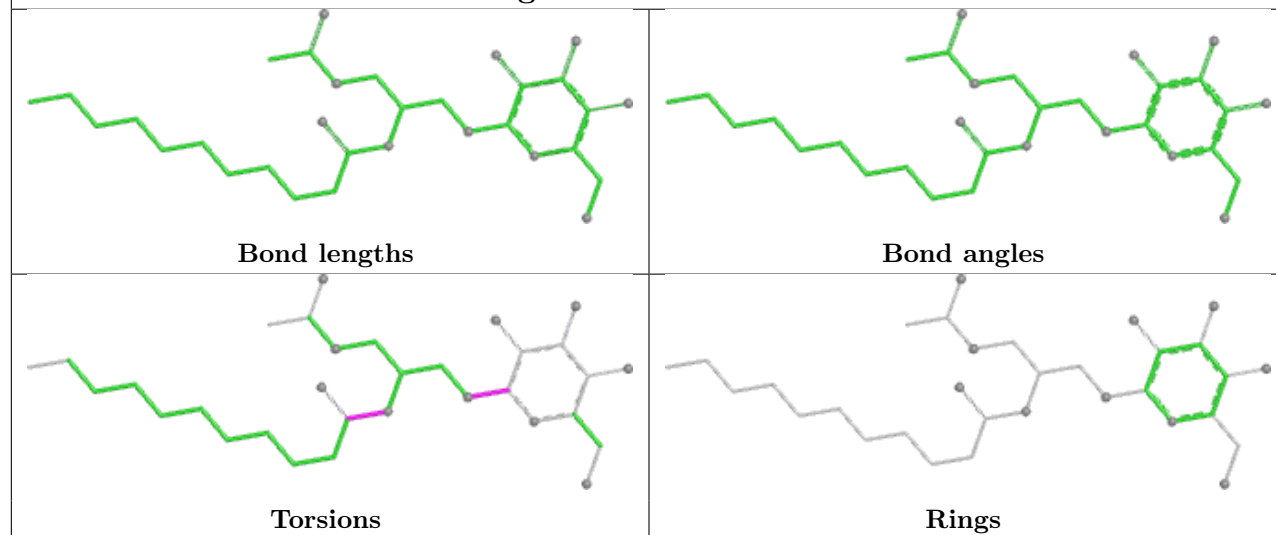
Ligand CLA c 303



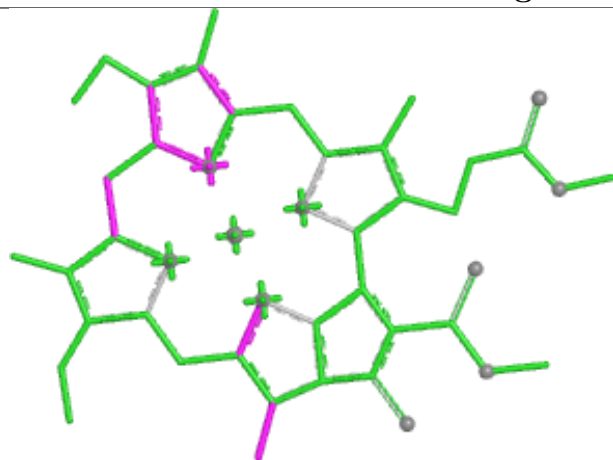
Ligand CLA T 410



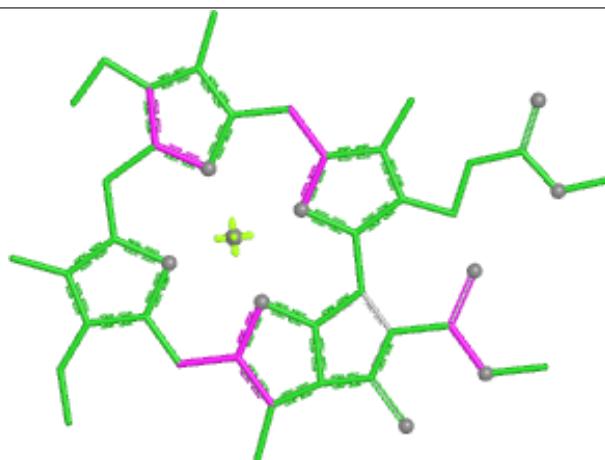
Ligand LMG A 5001



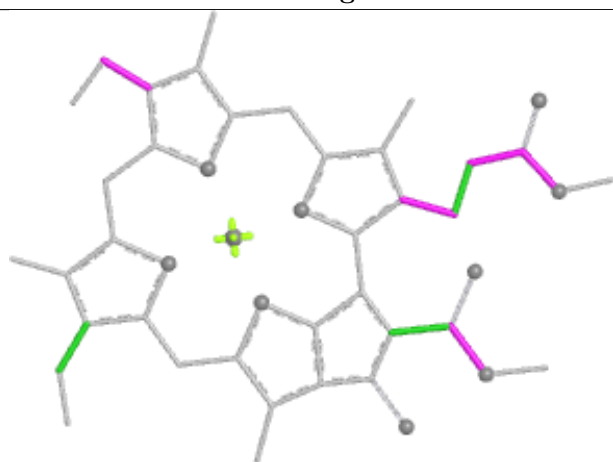
Ligand CLA T 404



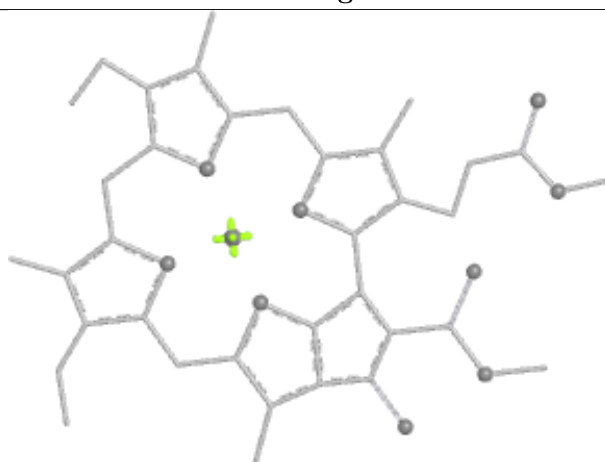
Bond lengths



Bond angles

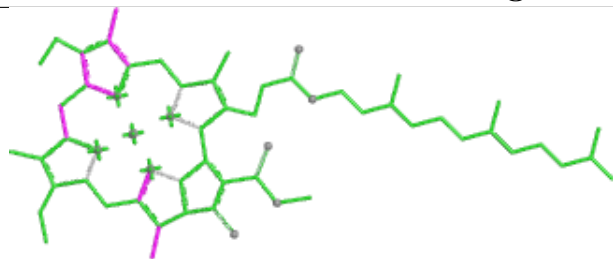


Torsions

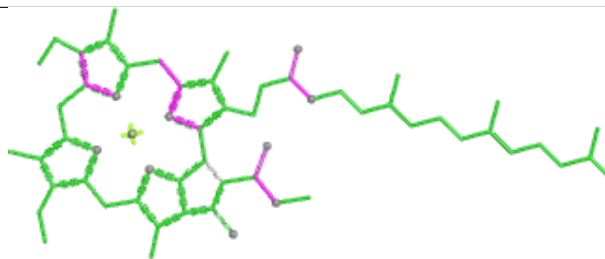


Rings

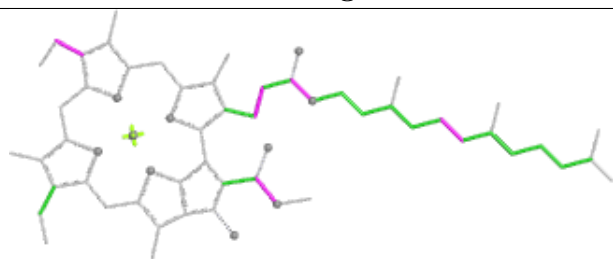
Ligand CLA F 5006



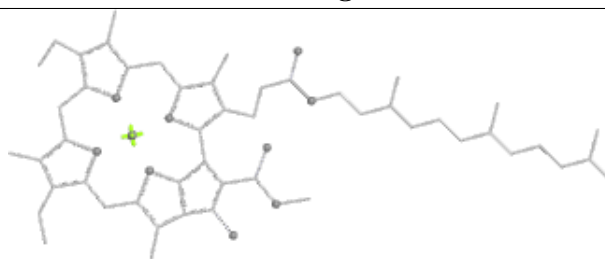
Bond lengths



Bond angles

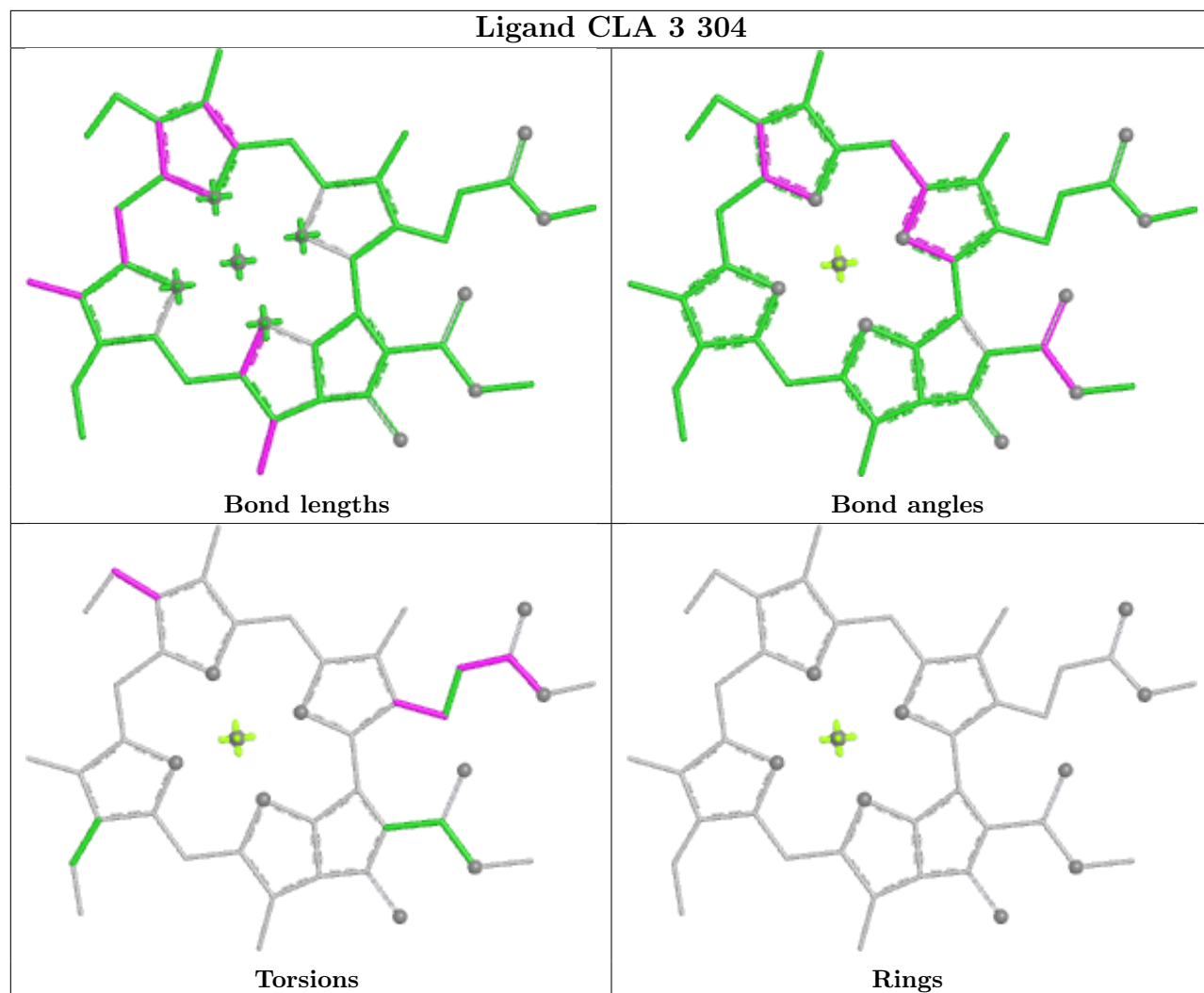


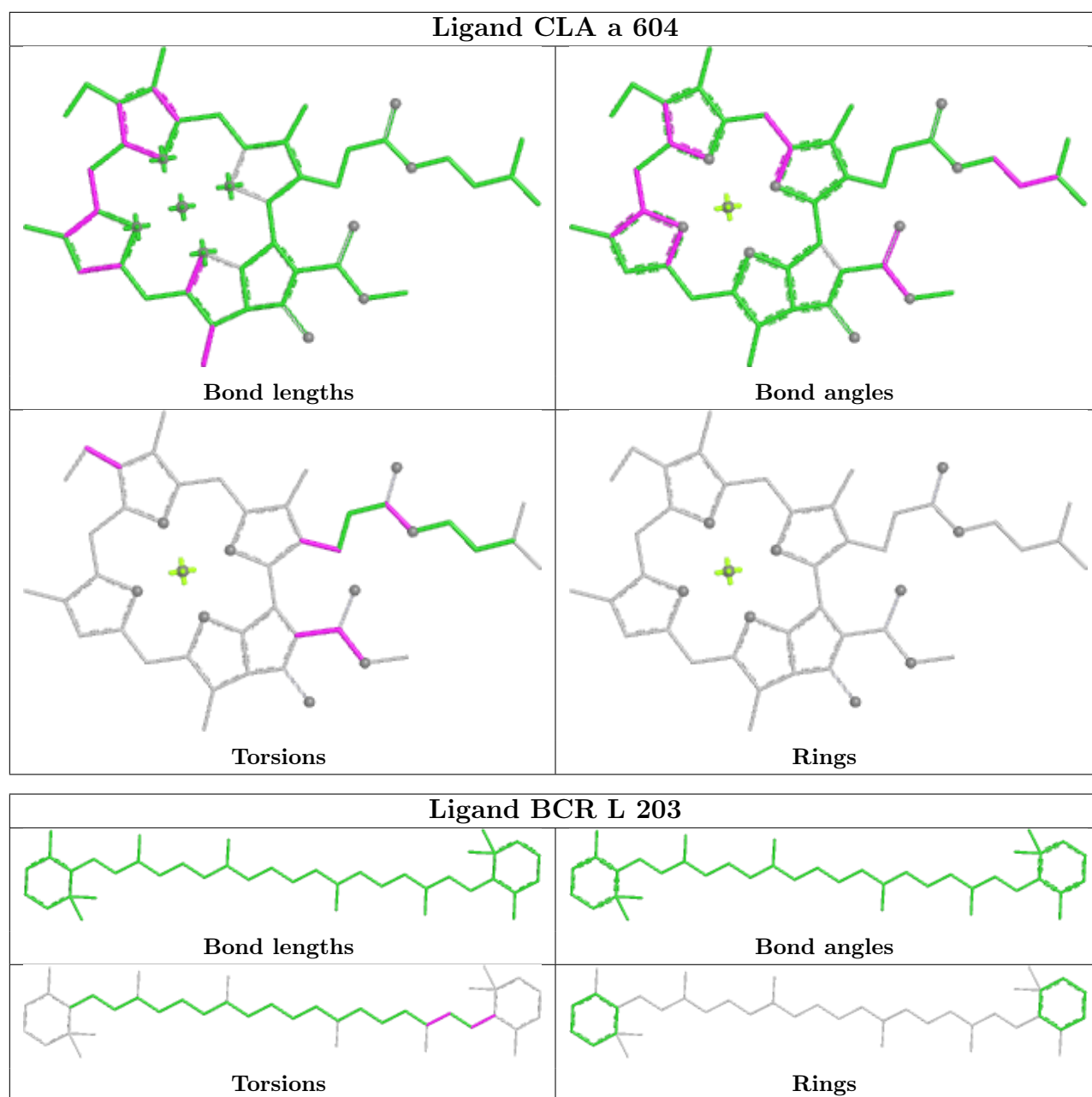
Torsions



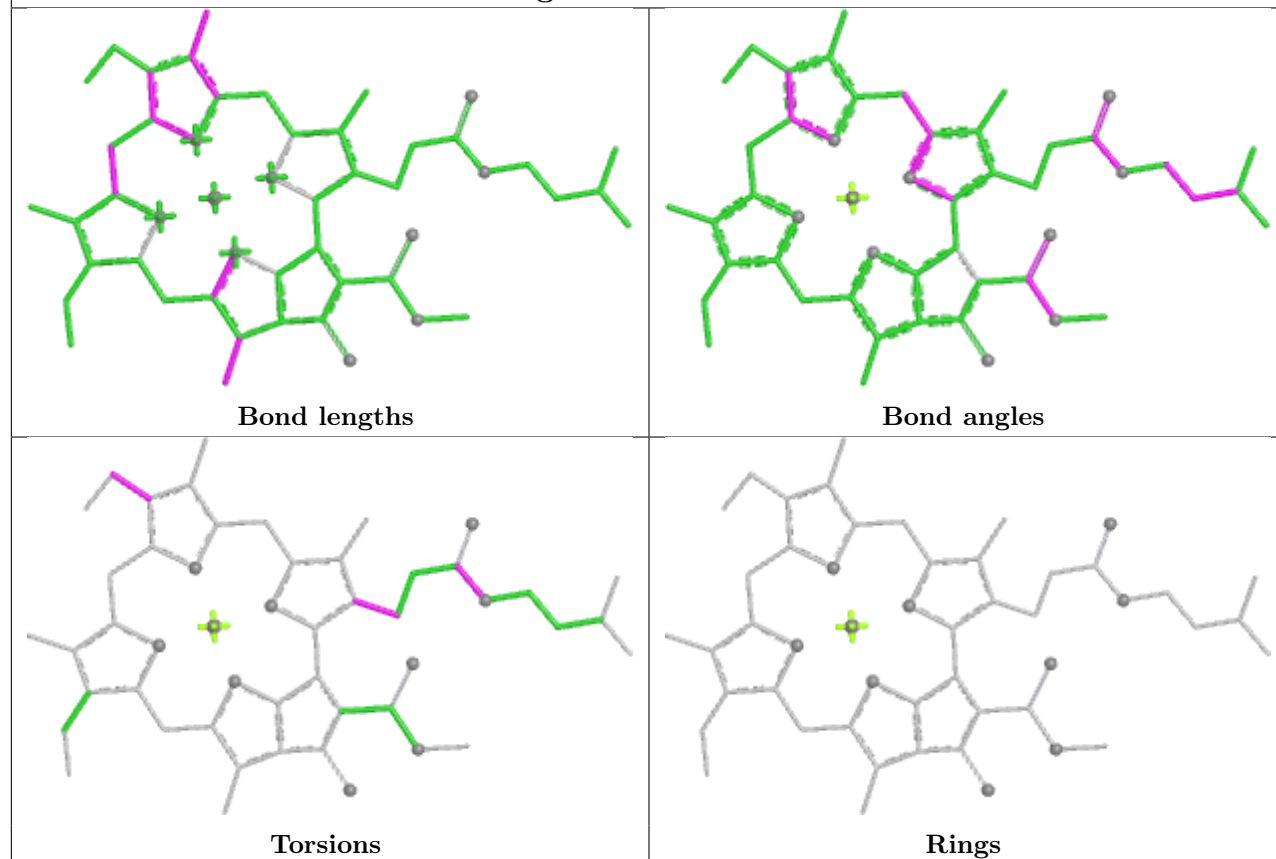
Rings

Ligand CLA 3 304

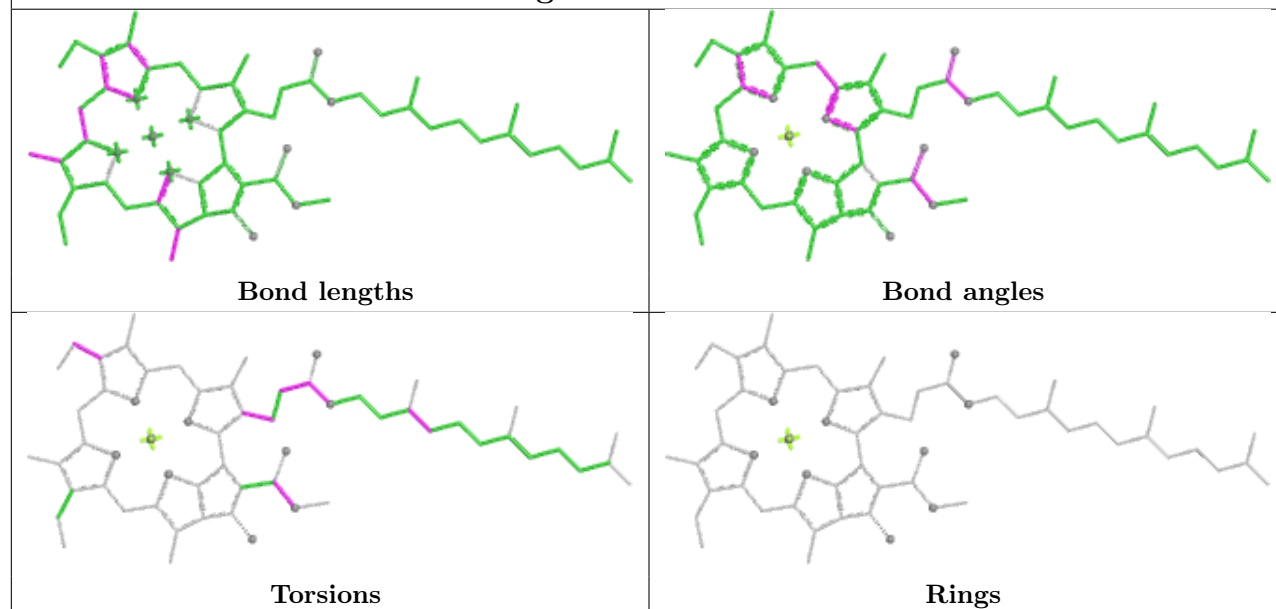


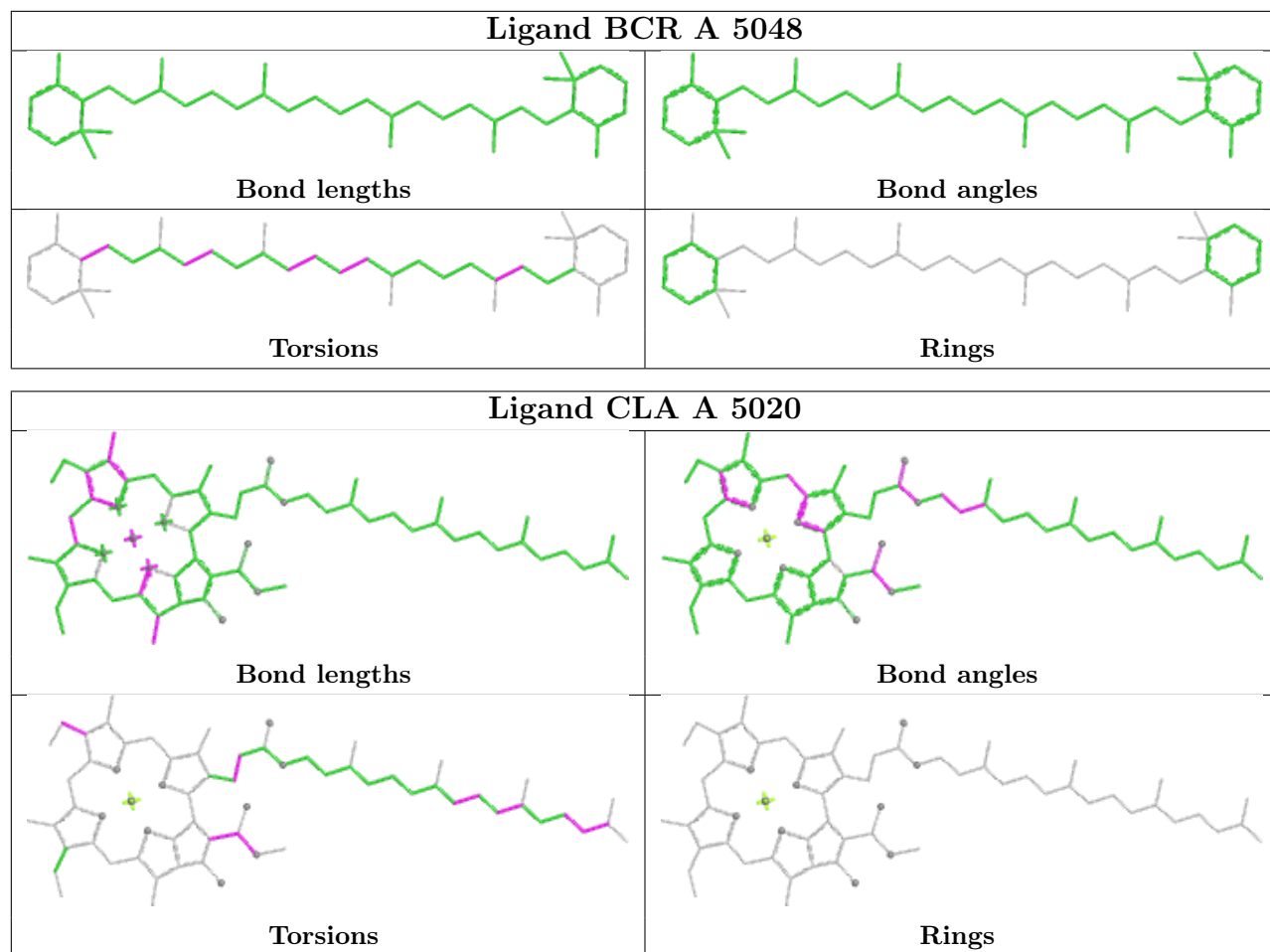


Ligand CLA 7 313

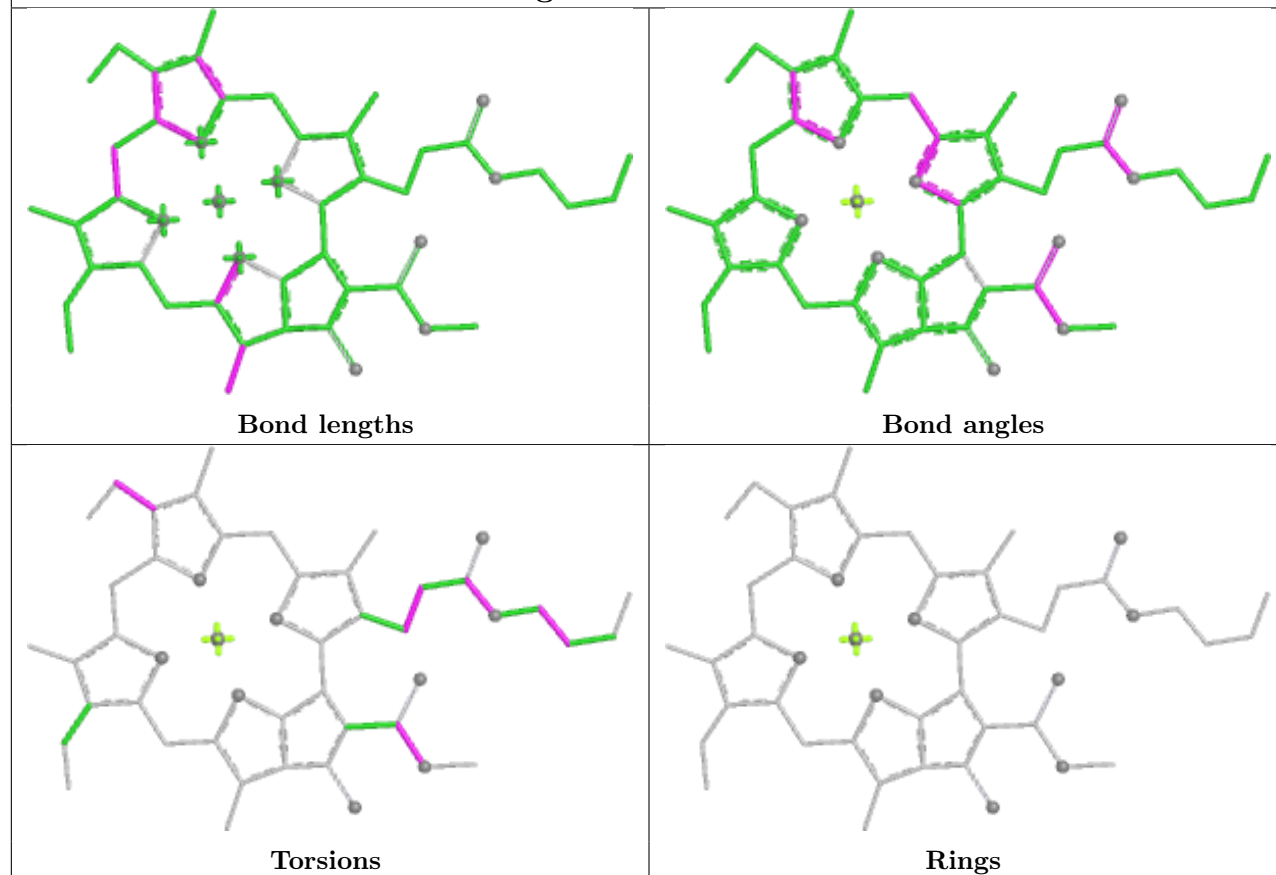


Ligand CLA a 609

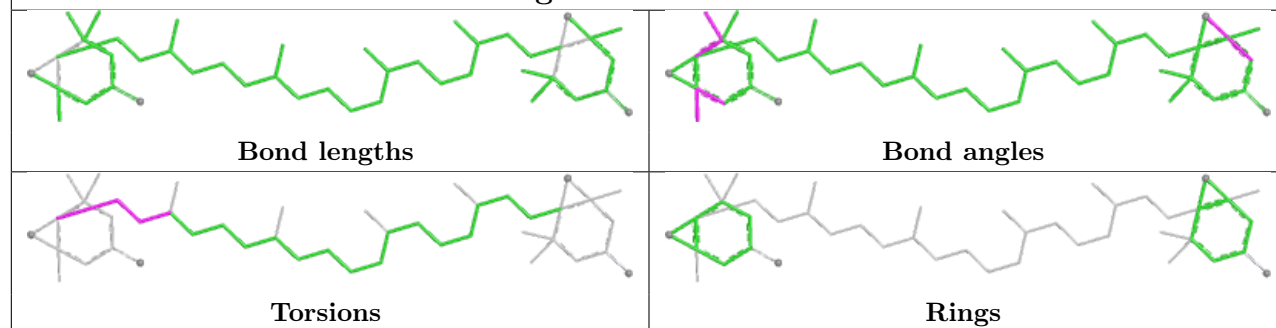




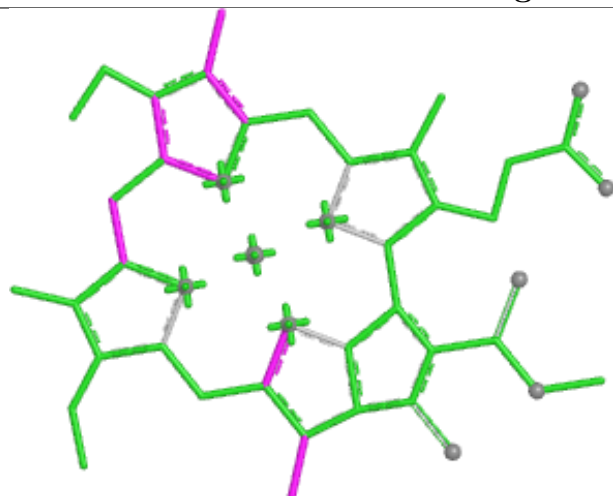
Ligand CLA J 102



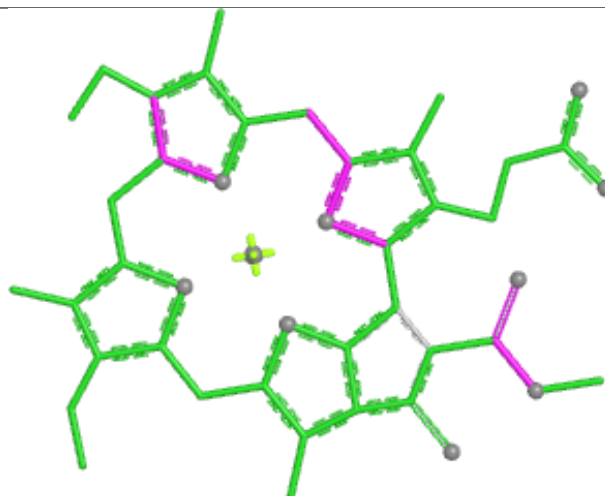
Ligand XAT 7 316



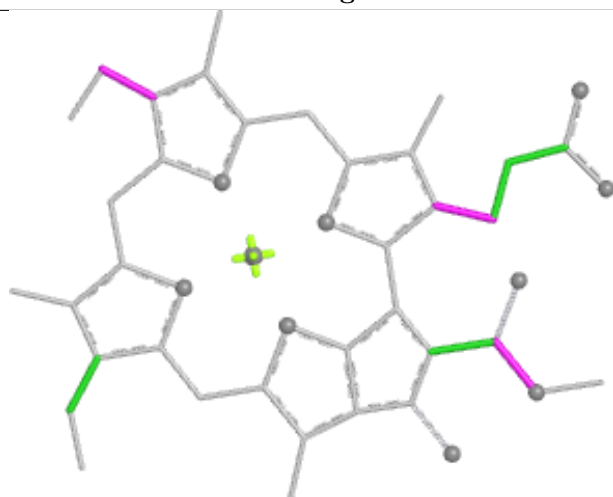
Ligand CLA B 822



Bond lengths



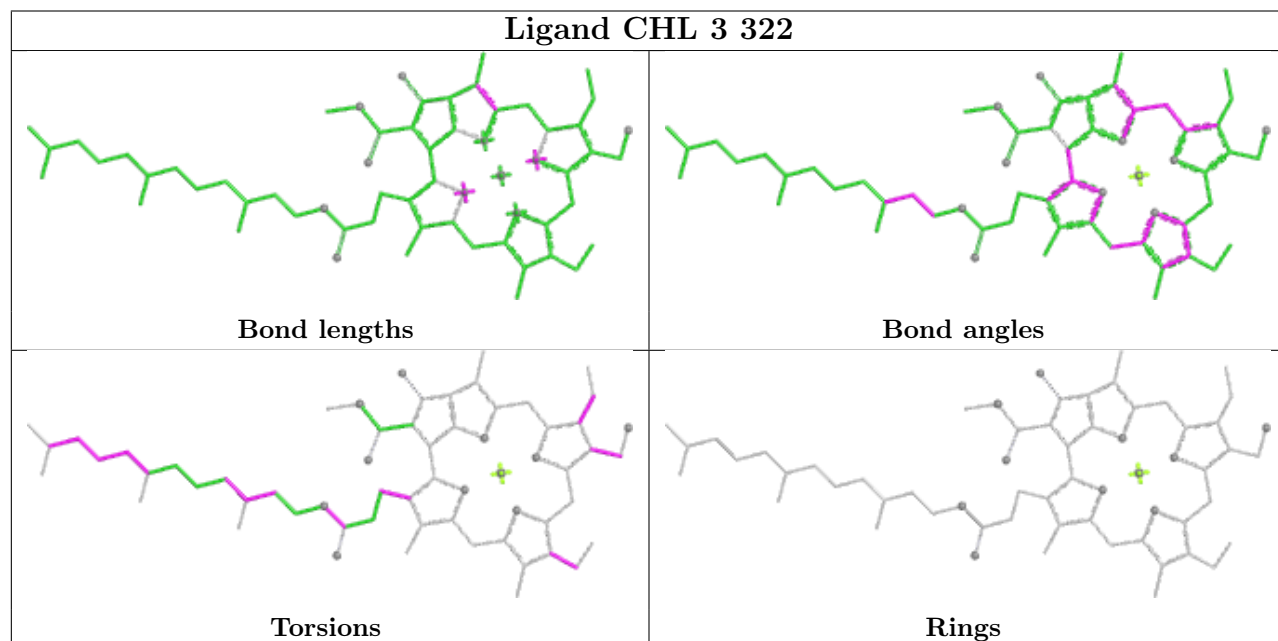
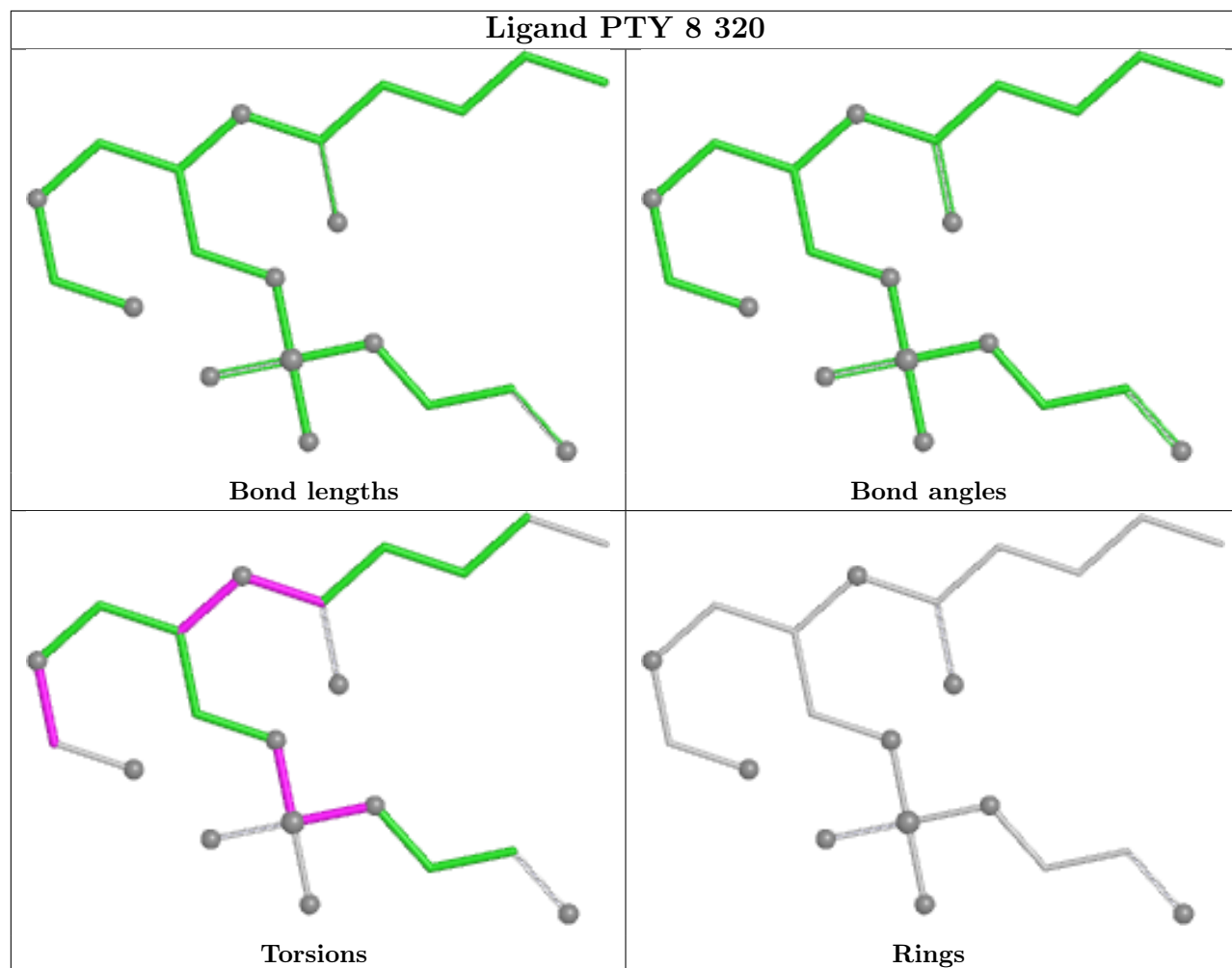
Bond angles



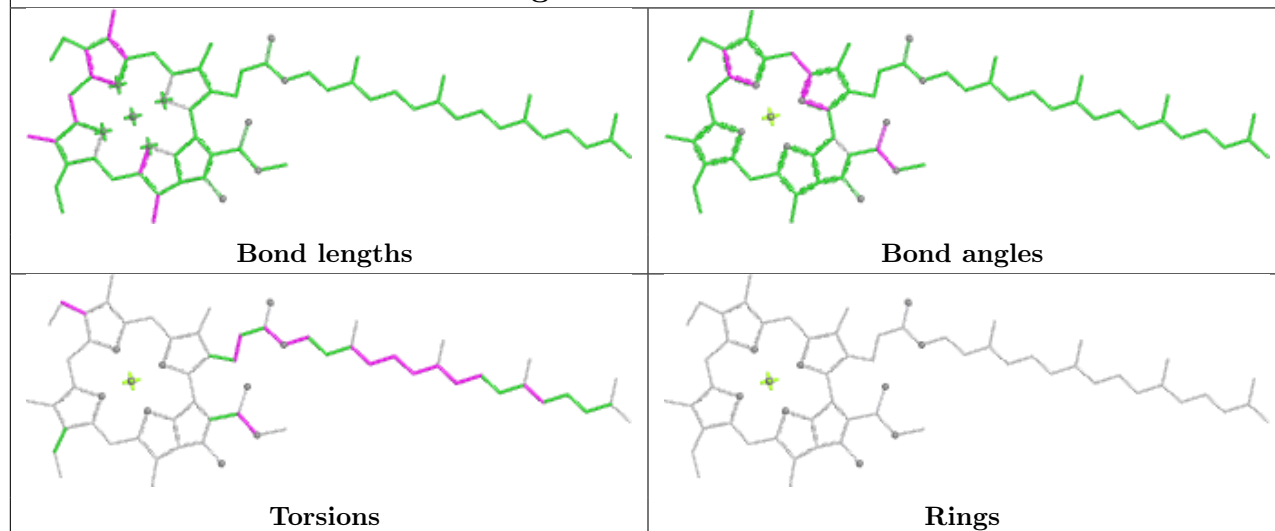
Torsions



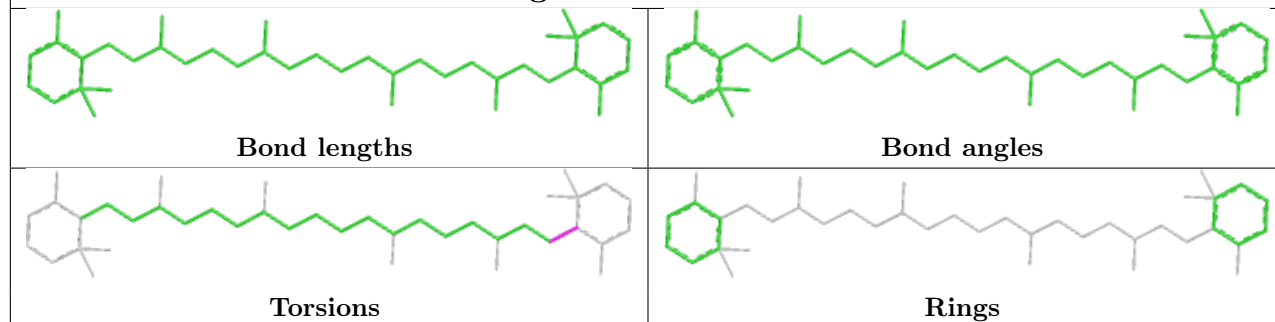
Rings



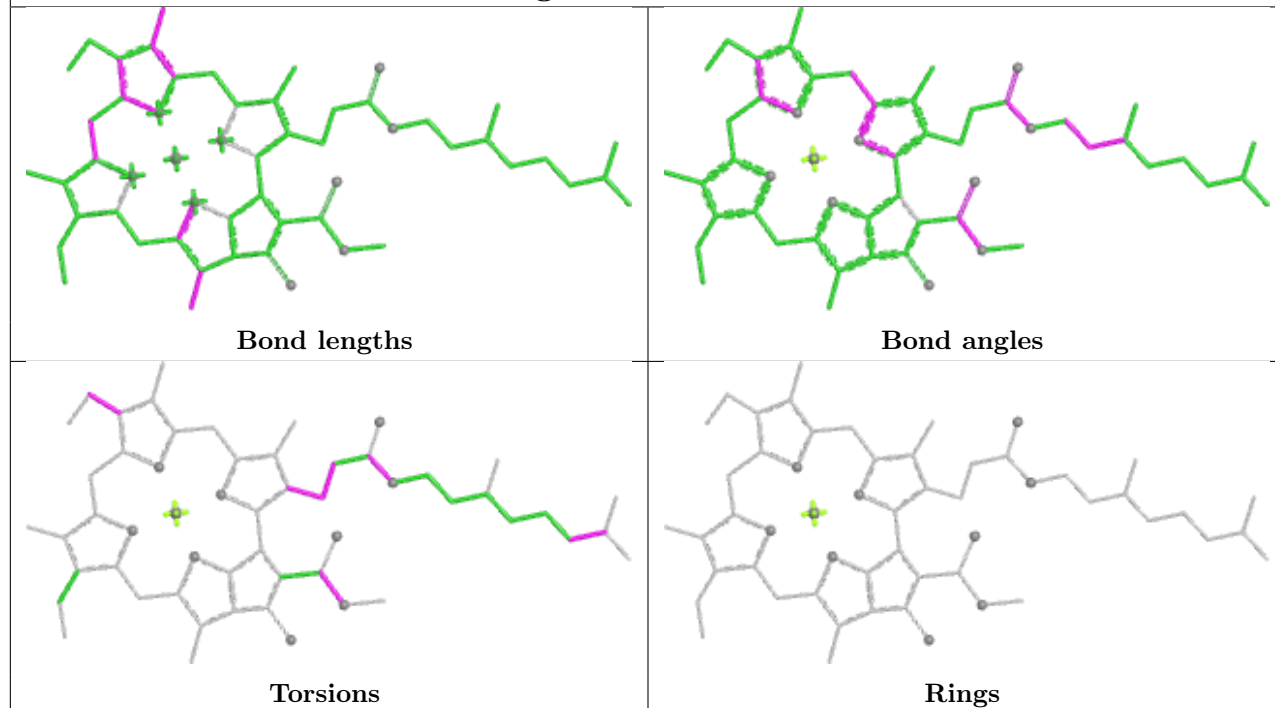
Ligand CLA B 803



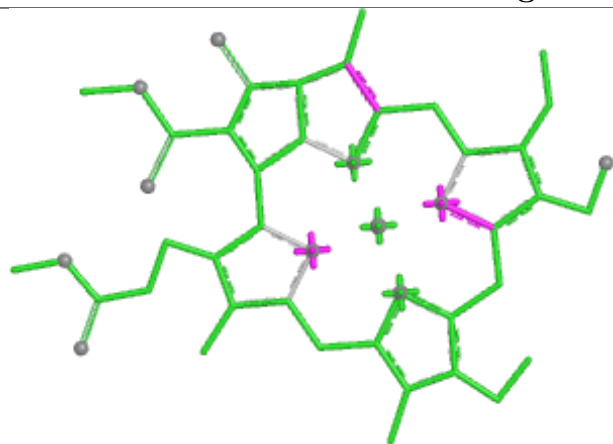
Ligand BCR B 847



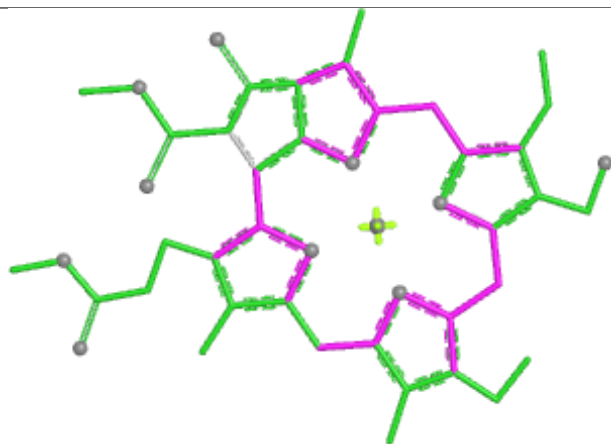
Ligand CLA 3 308



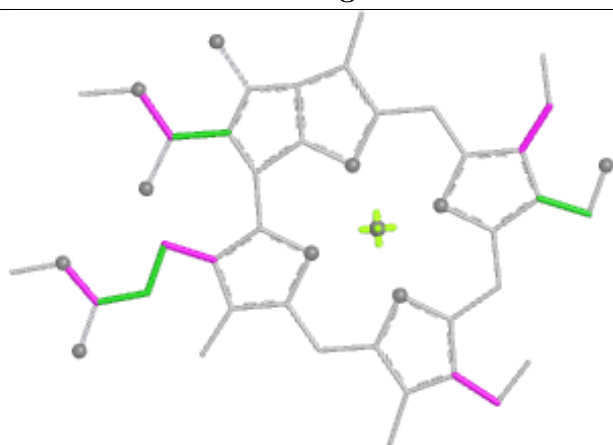
Ligand CHL 7 306



Bond lengths



Bond angles

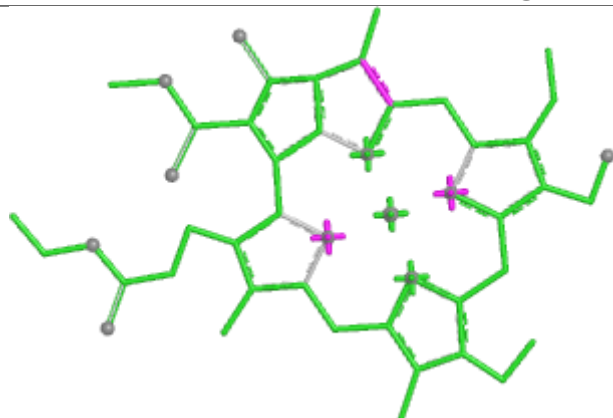


Torsions

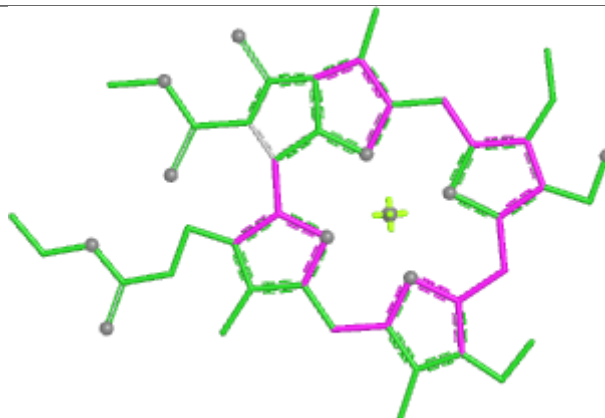


Rings

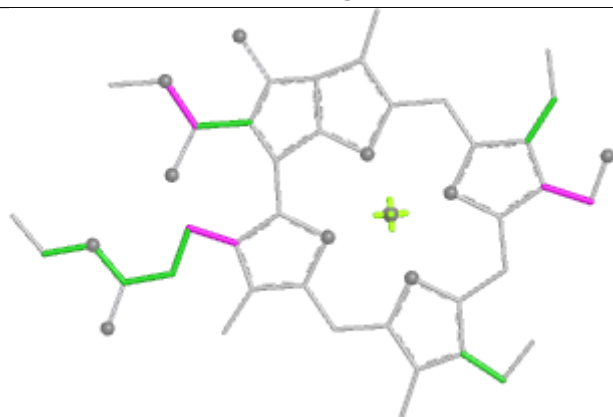
Ligand CHL 7 307



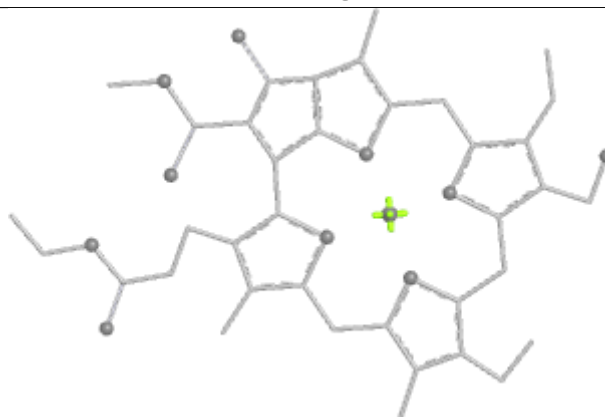
Bond lengths



Bond angles

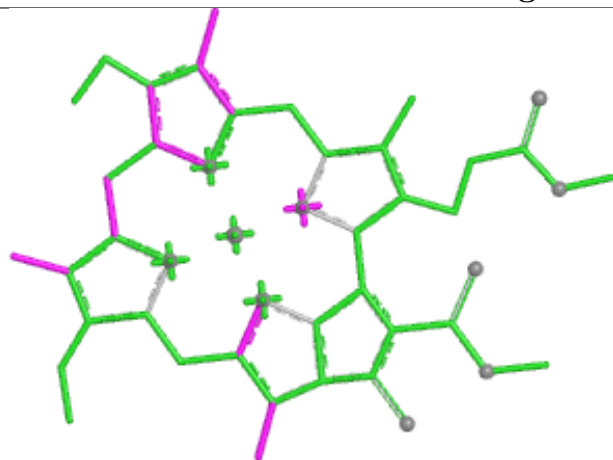


Torsions

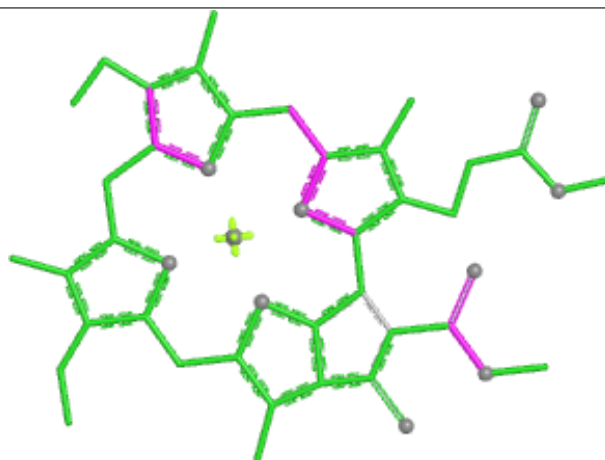


Rings

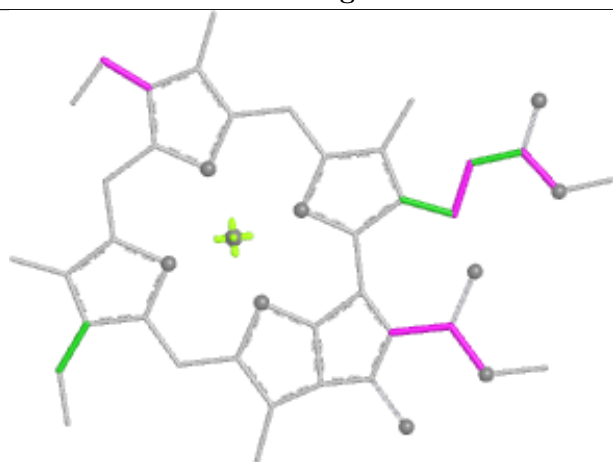
Ligand CLA 8 305



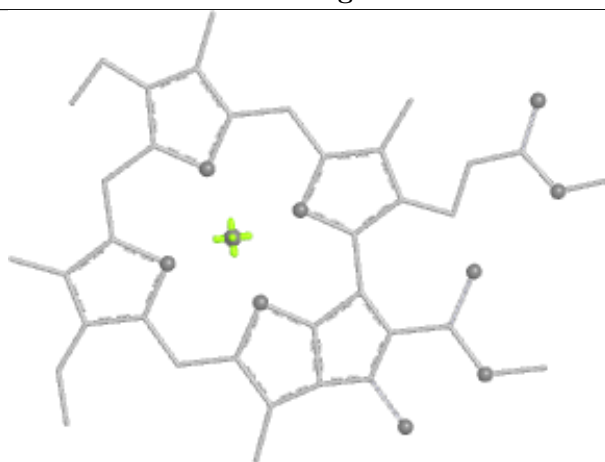
Bond lengths



Bond angles

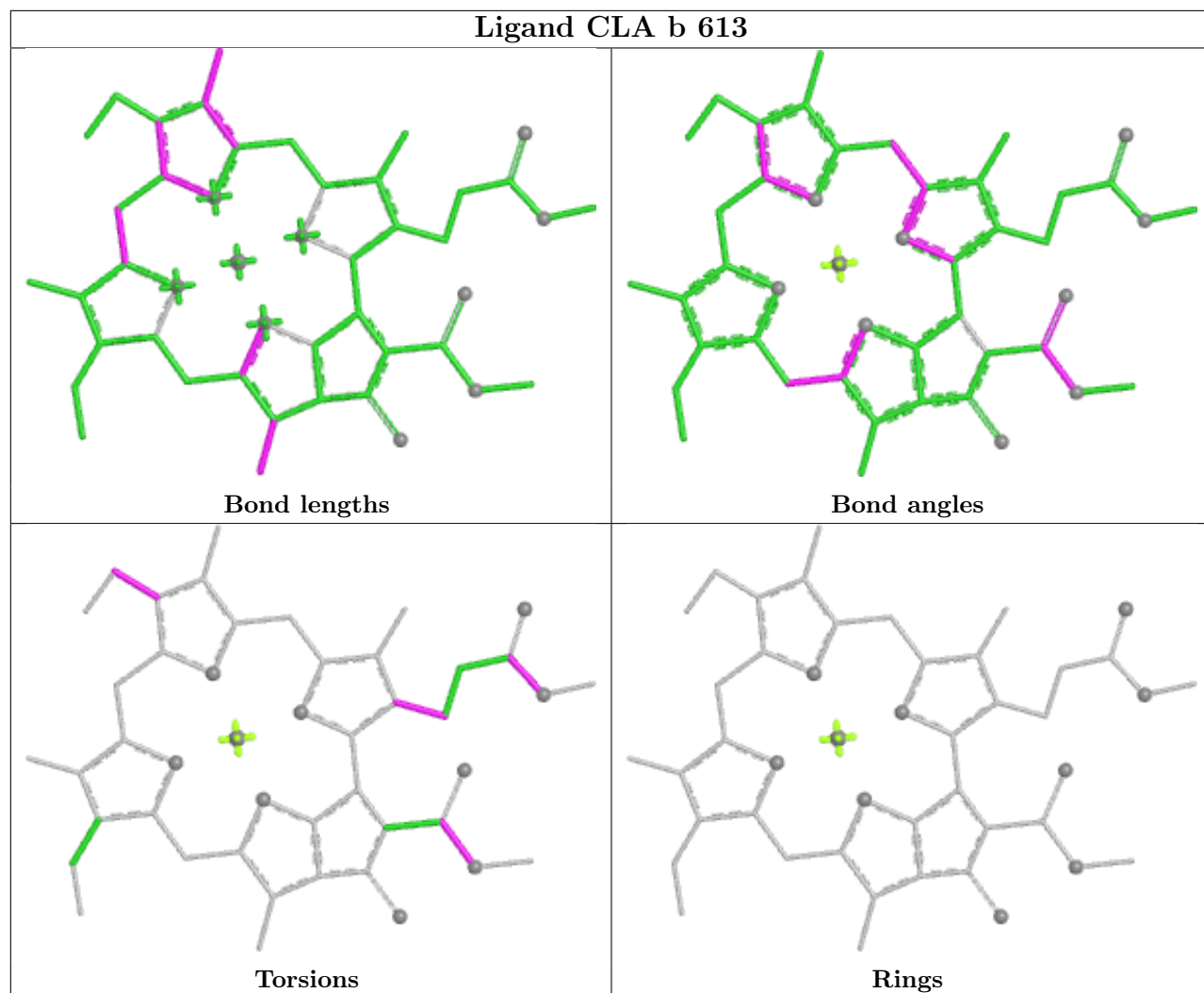


Torsions

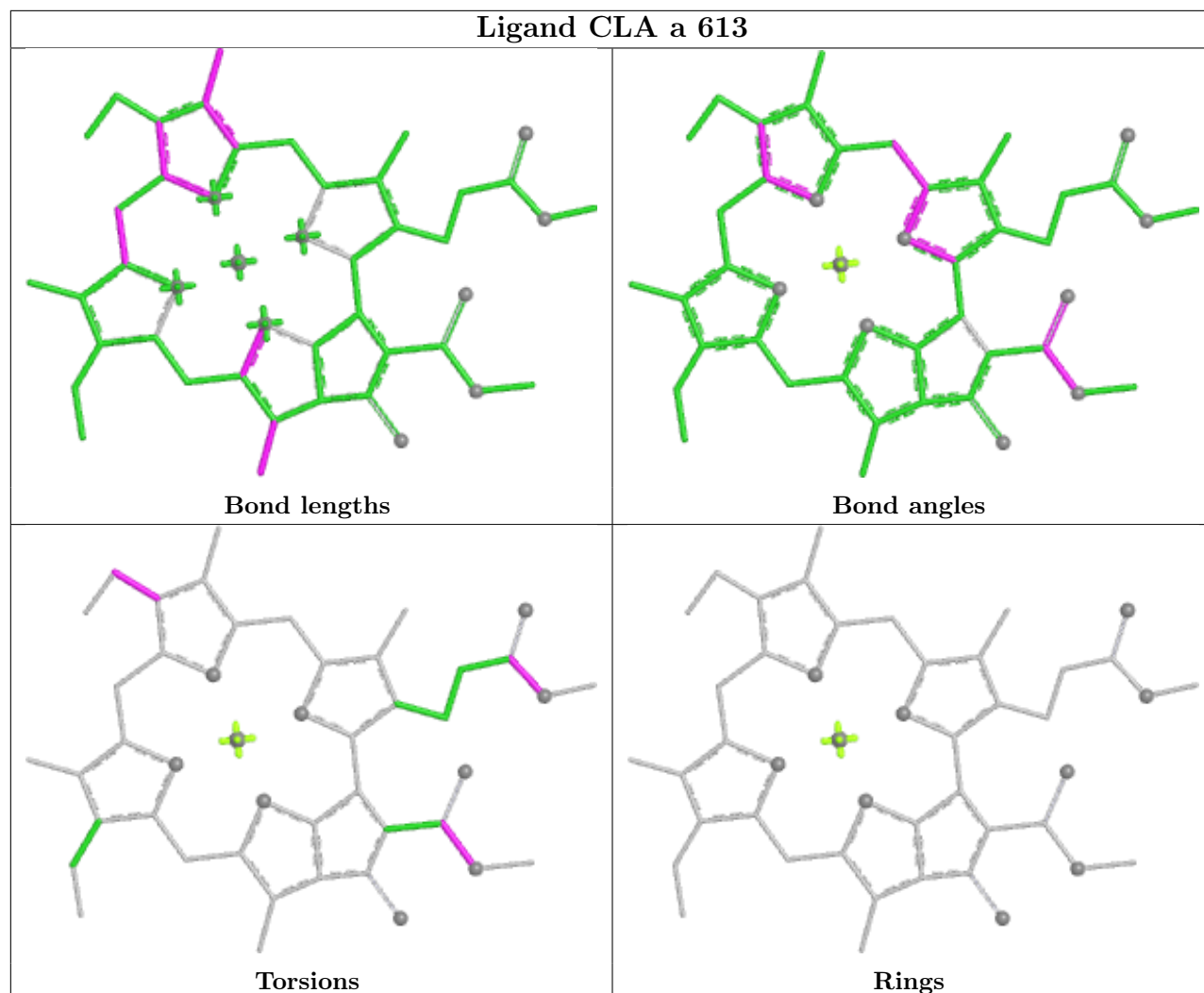


Rings

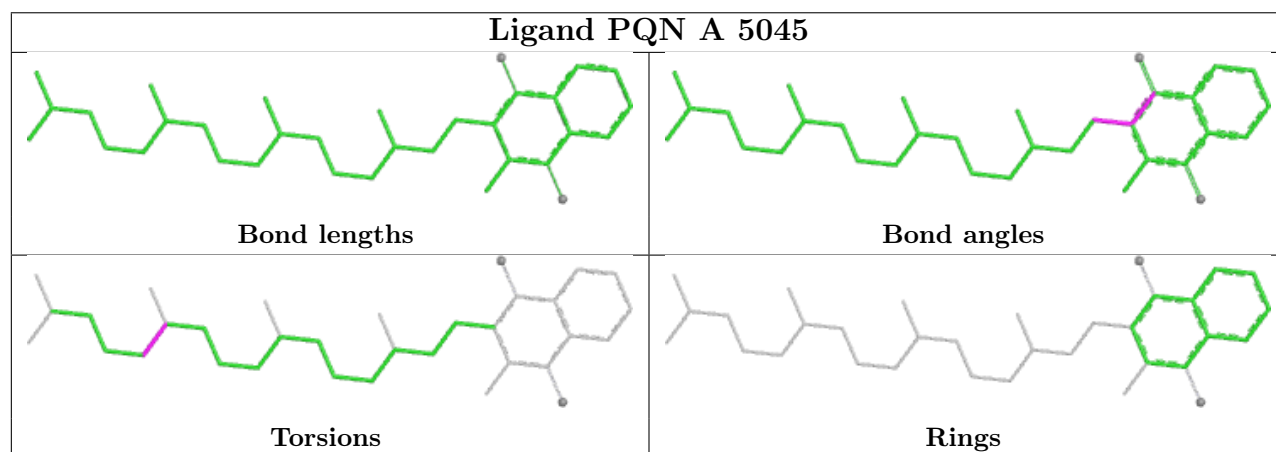
Ligand CLA b 613

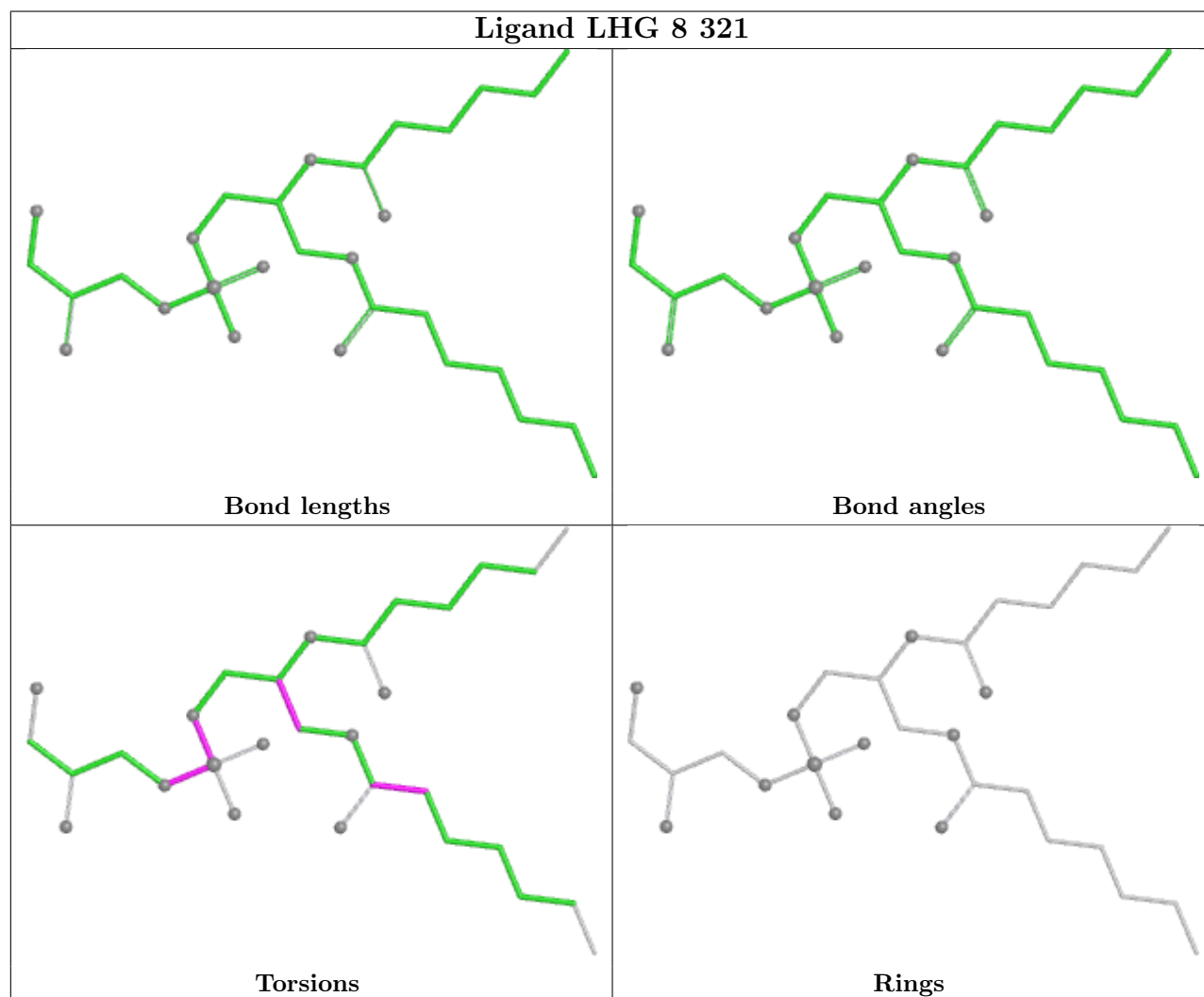
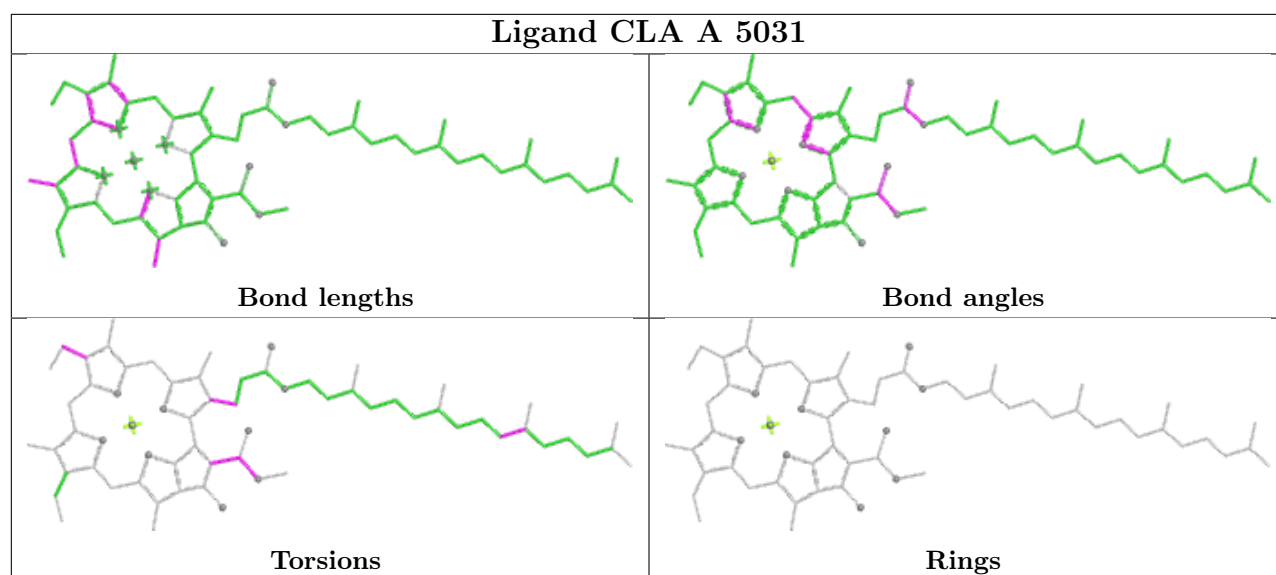


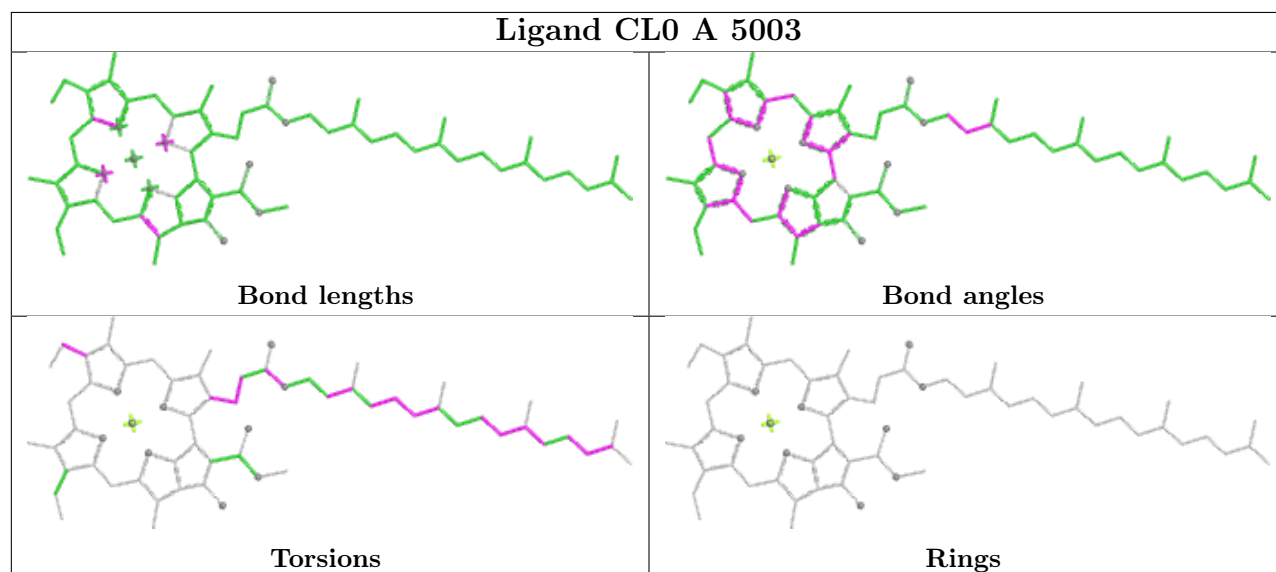
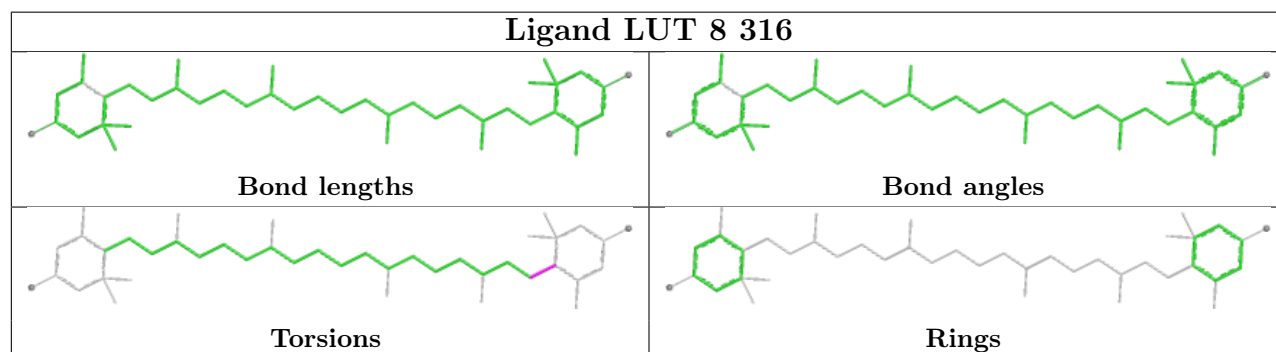
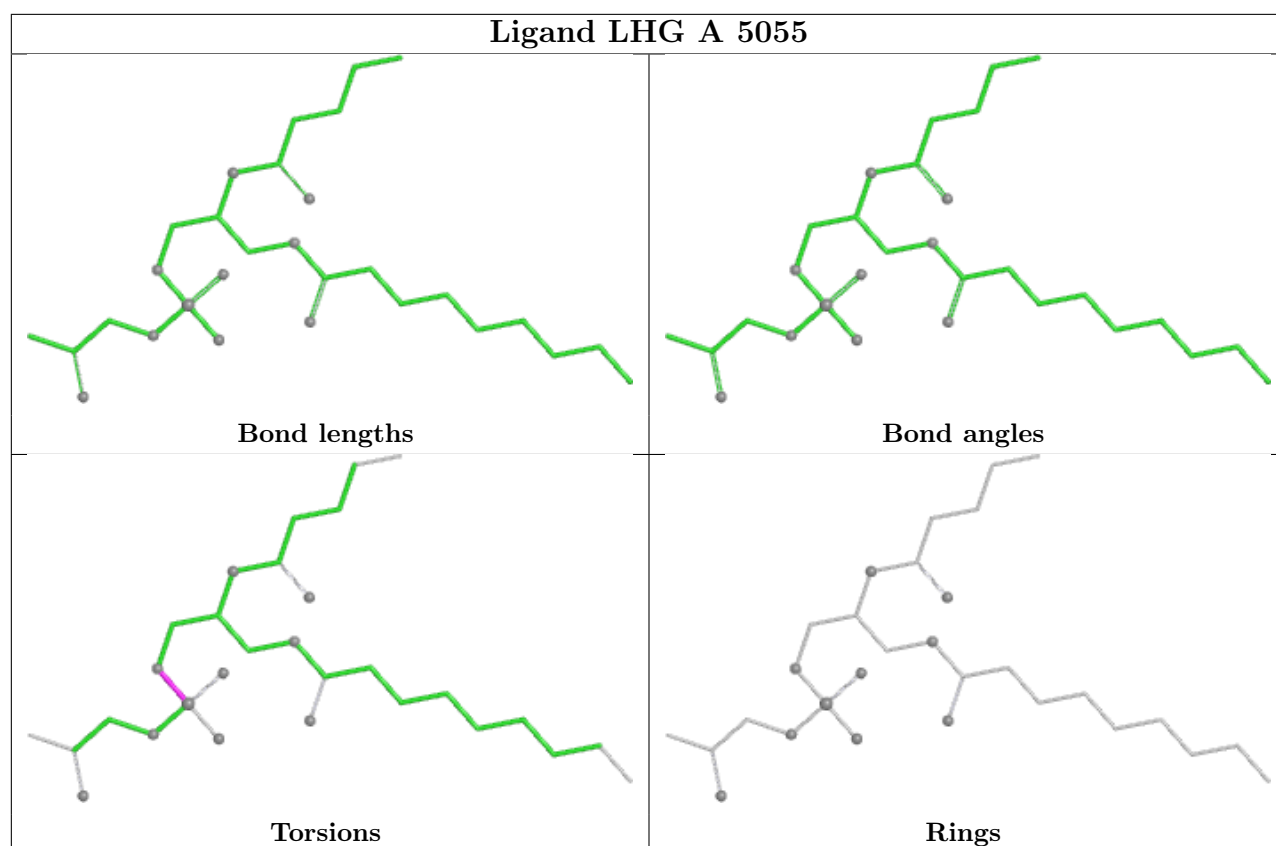
Ligand CLA a 613



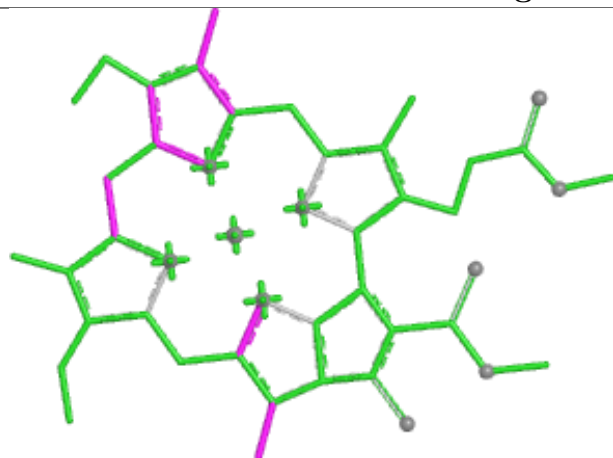
Ligand PQN A 5045



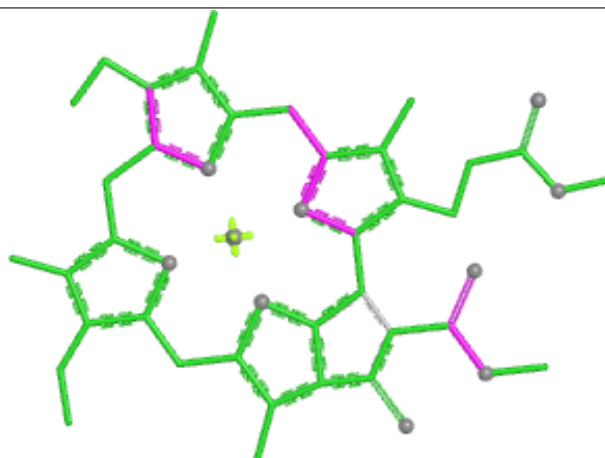




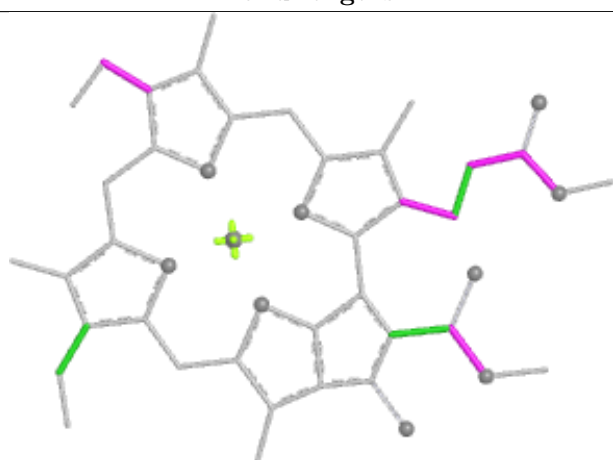
Ligand CLA T 411



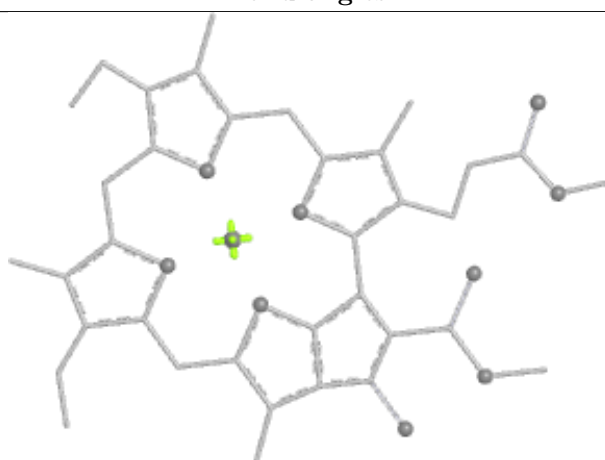
Bond lengths



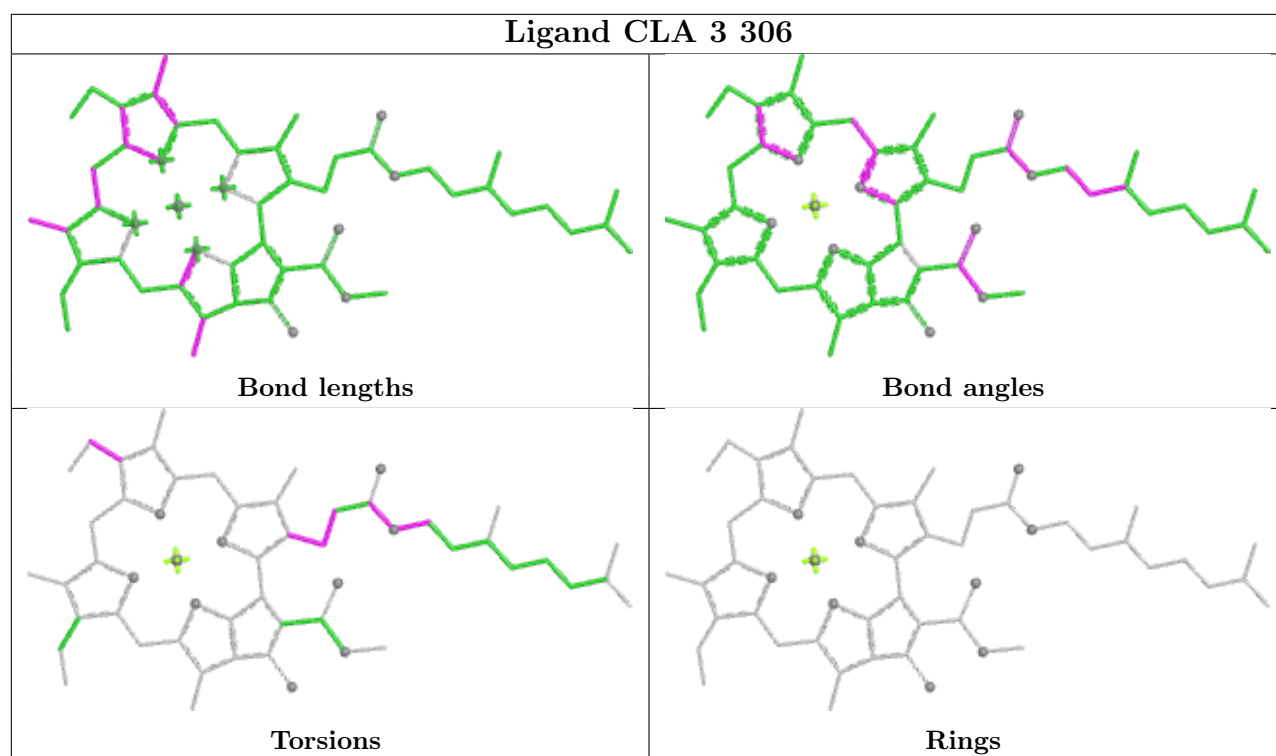
Bond angles



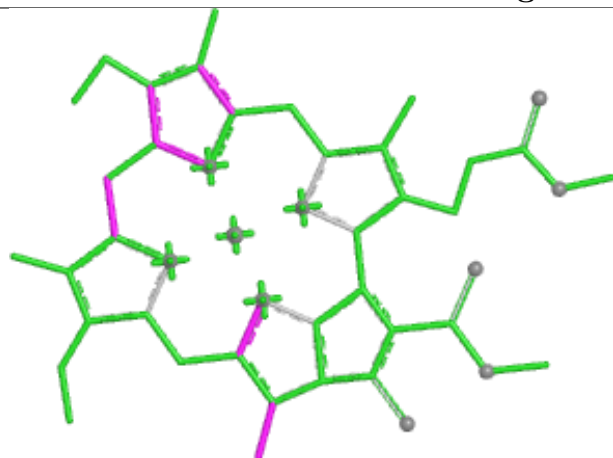
Torsions



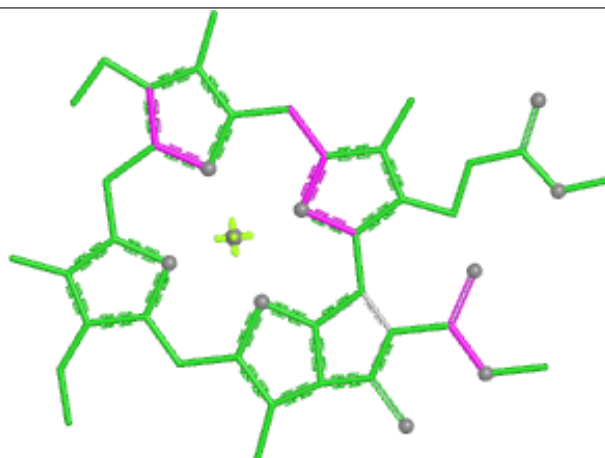
Rings



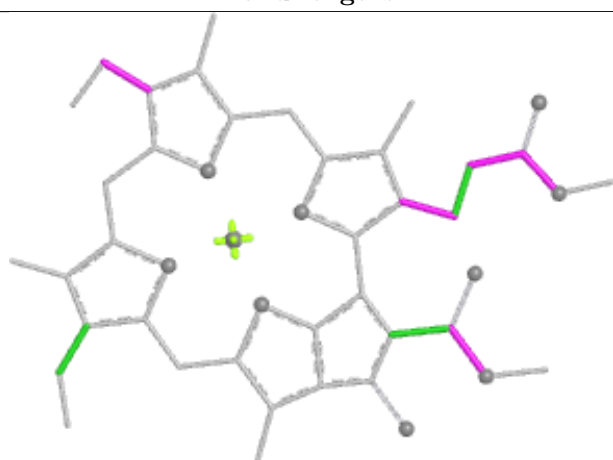
Ligand CLA b 601



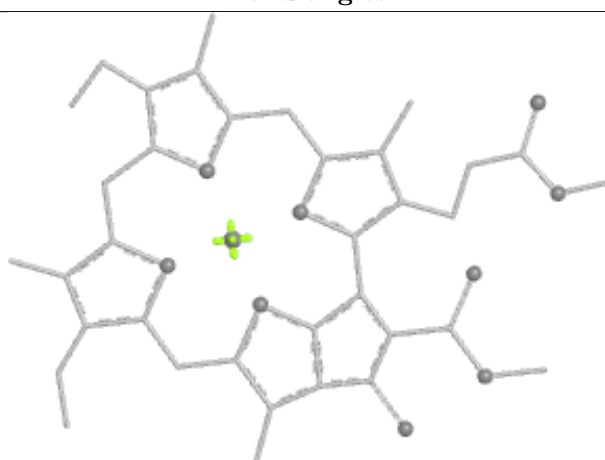
Bond lengths



Bond angles

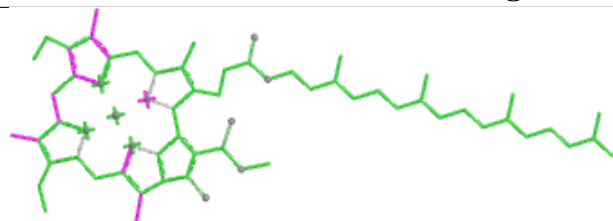


Torsions

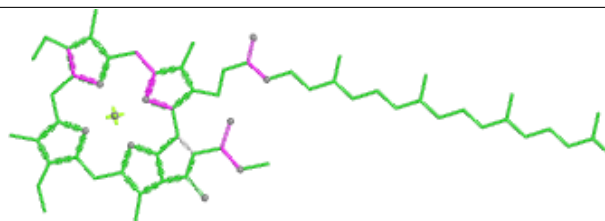


Rings

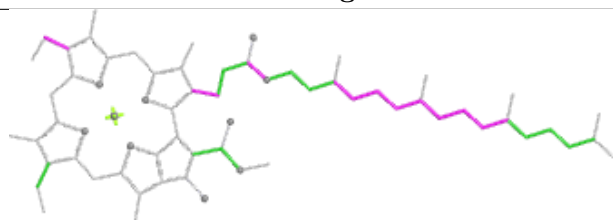
Ligand CLA A 5028



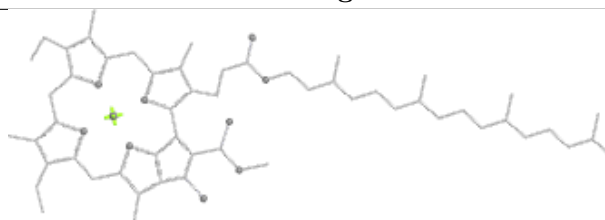
Bond lengths



Bond angles

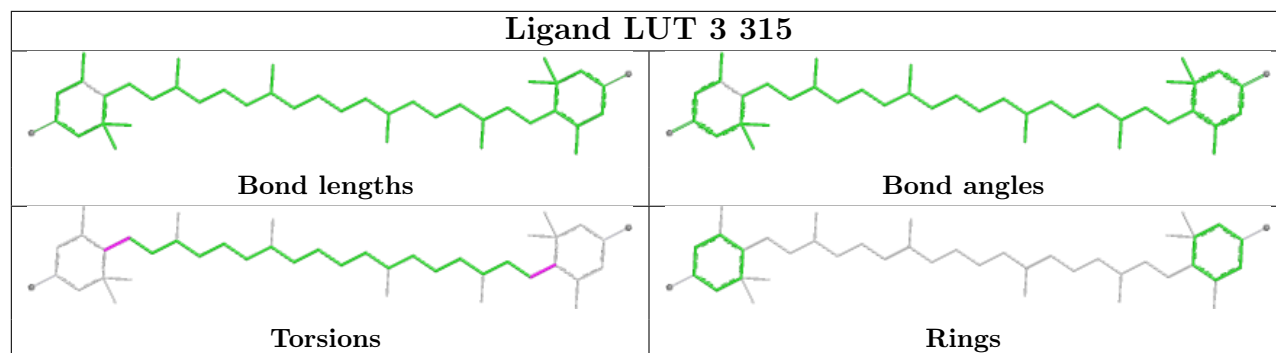


Torsions

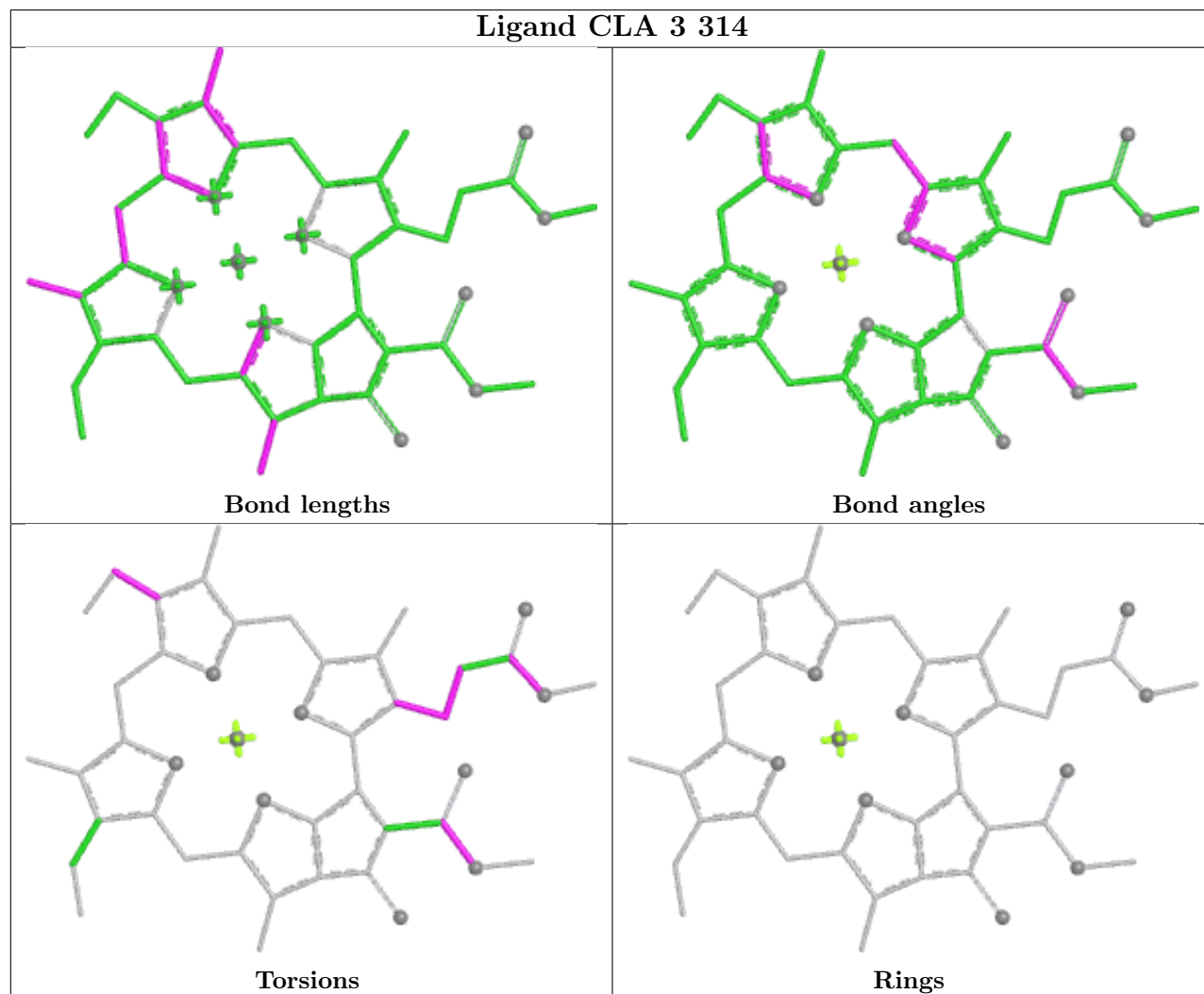


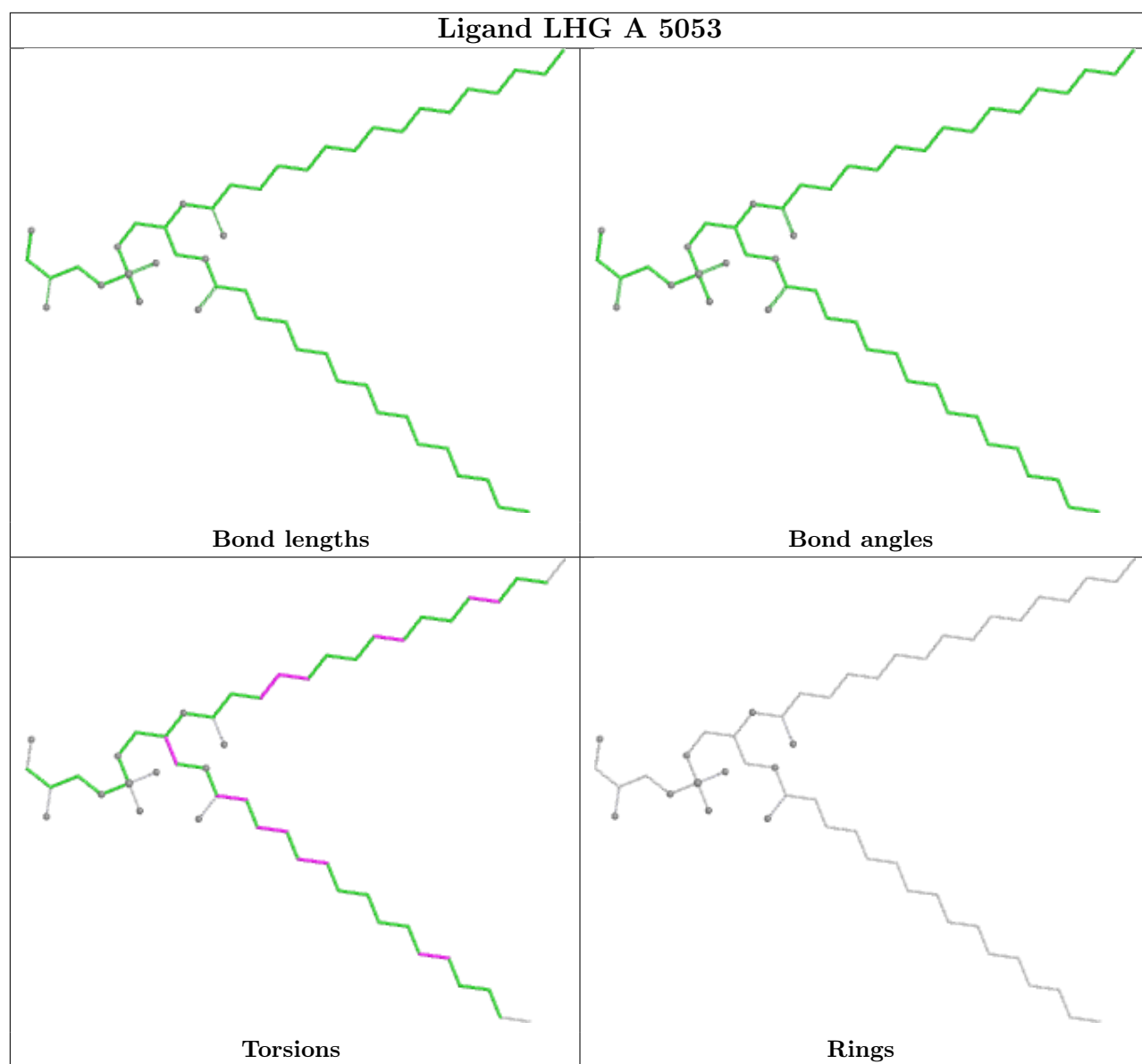
Rings

Ligand LUT 3 315

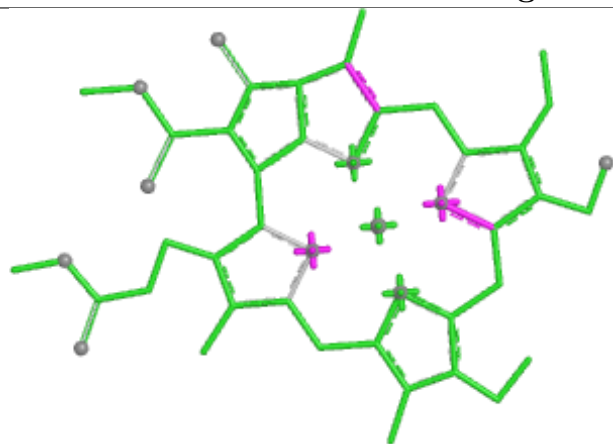


Ligand CLA 3 314

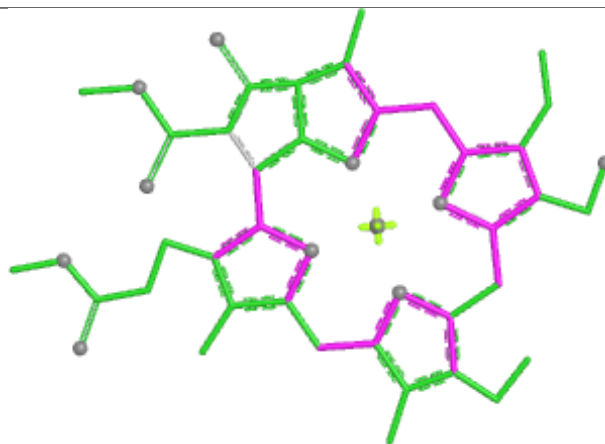




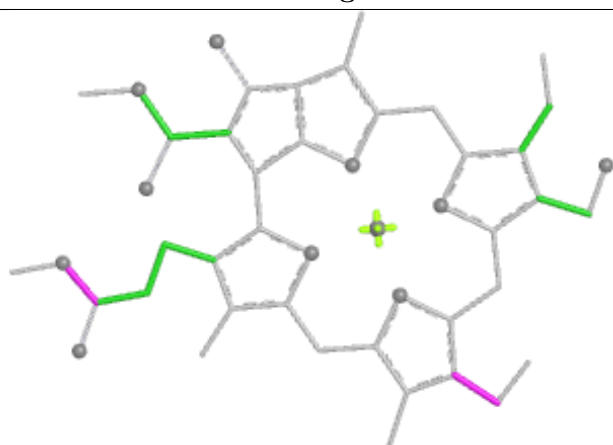
Ligand CHL 1 606



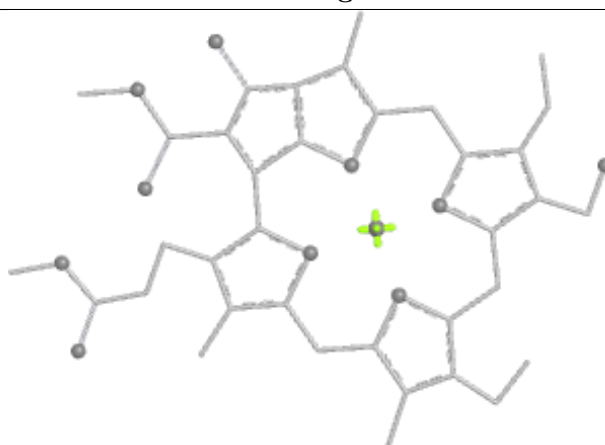
Bond lengths



Bond angles

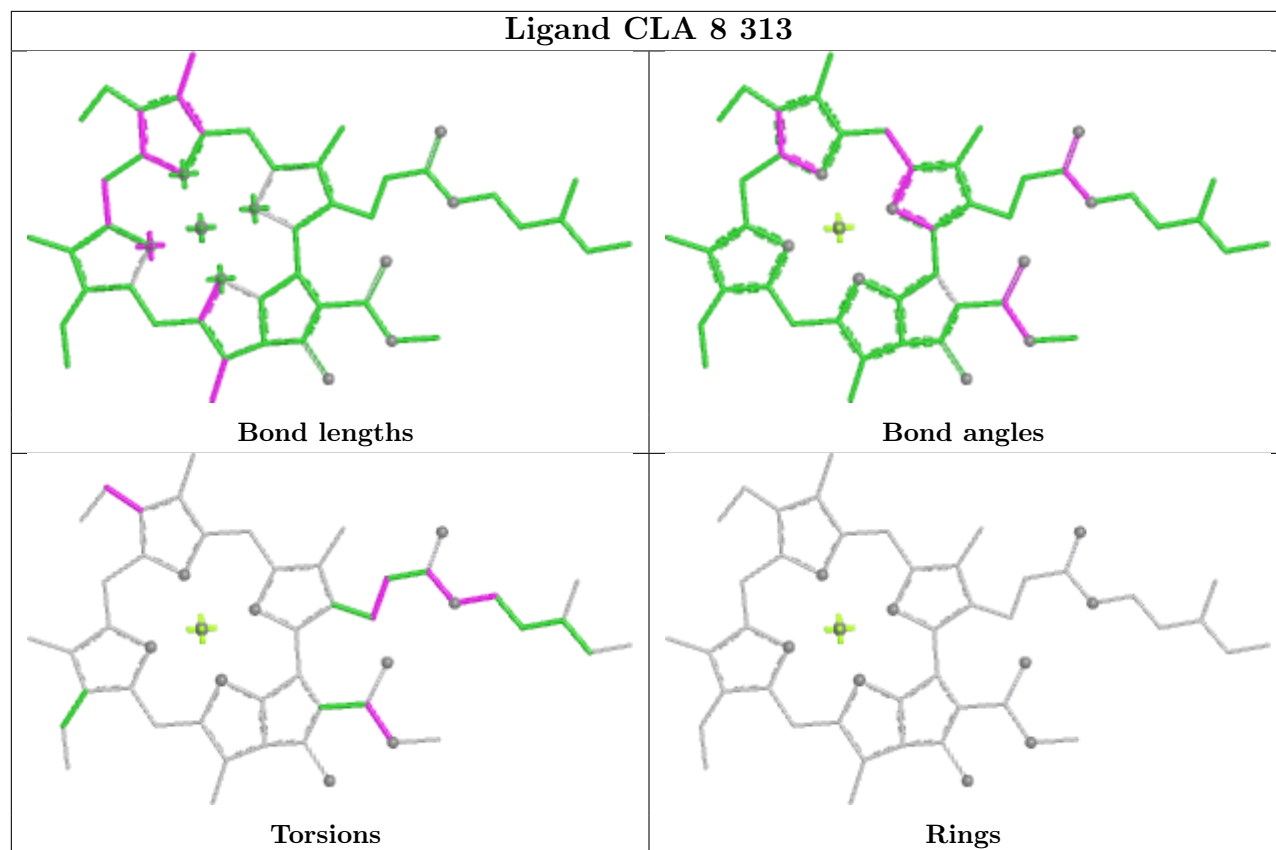


Torsions

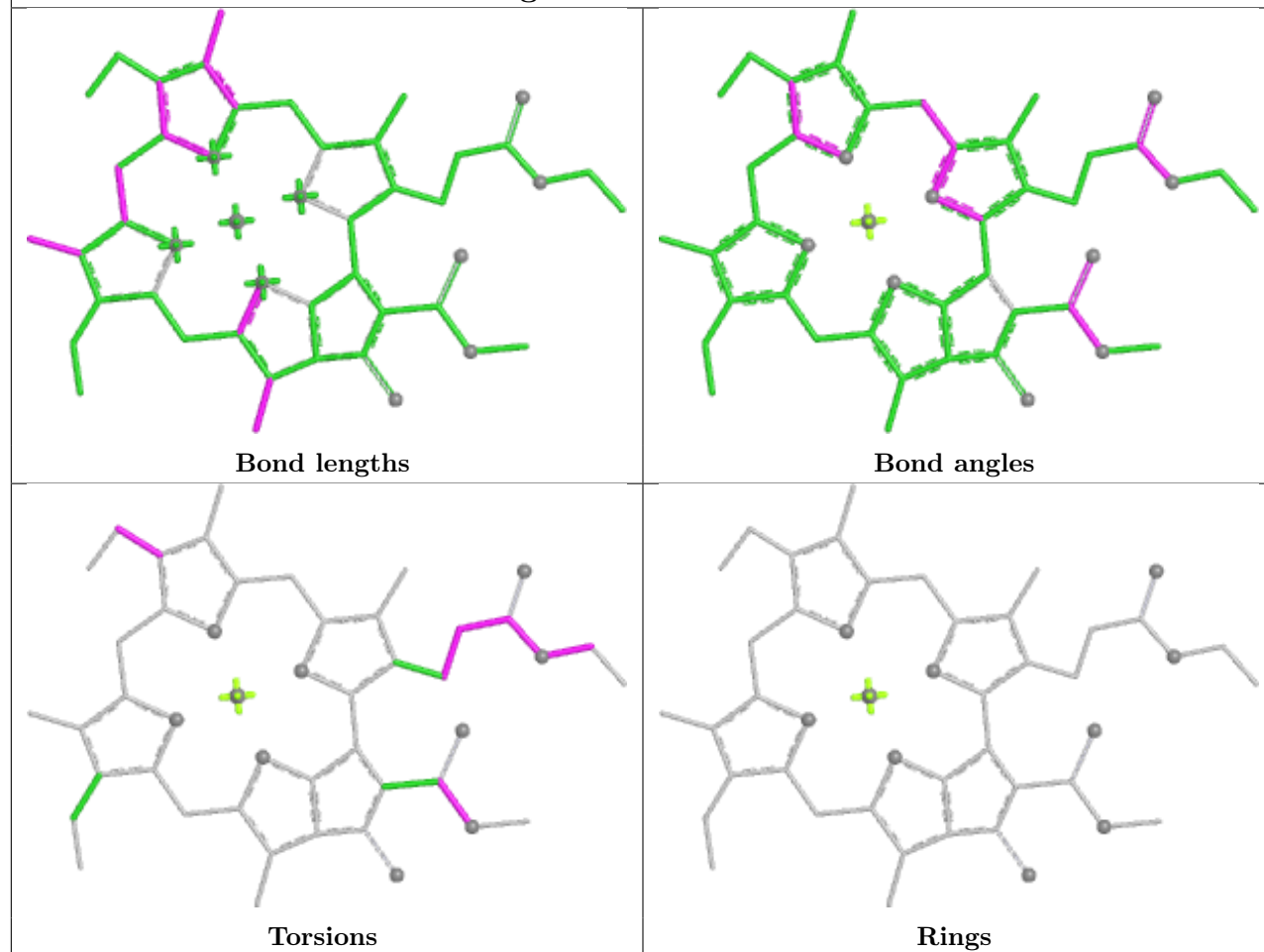


Rings

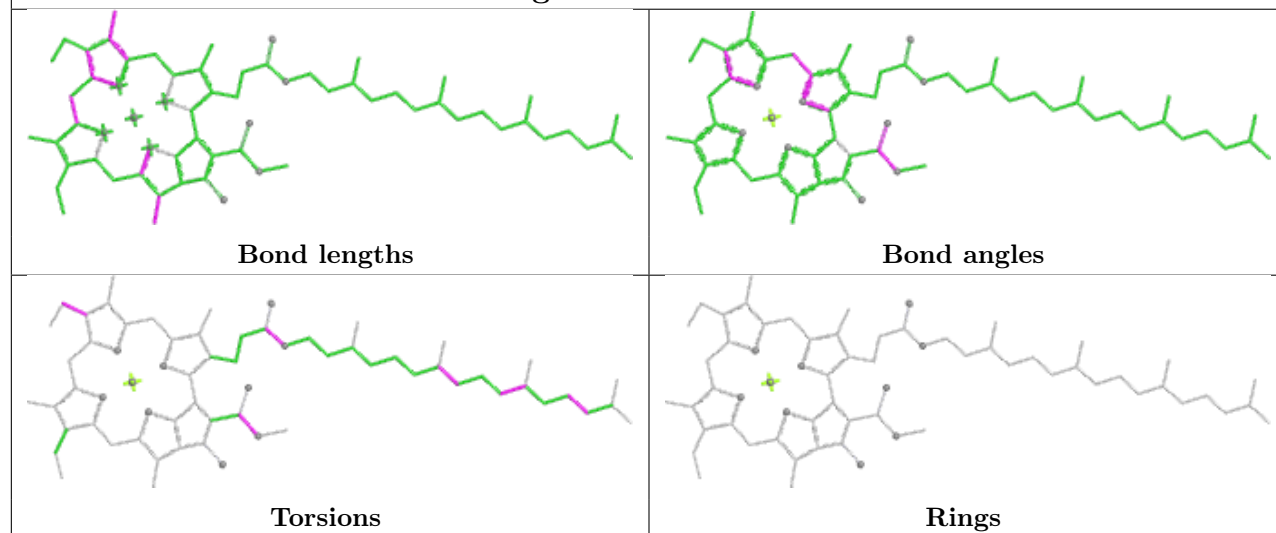
Ligand CLA 8 313

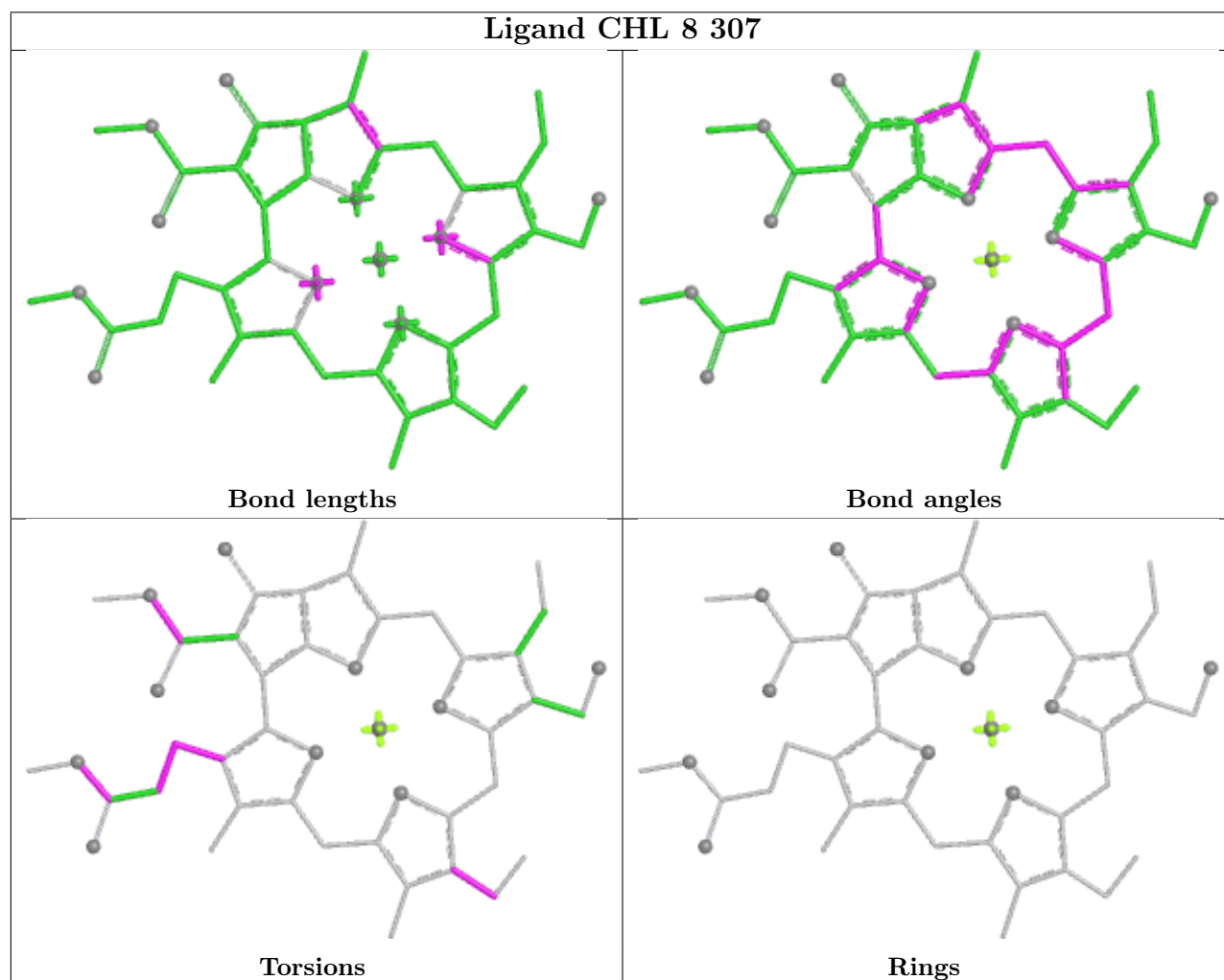
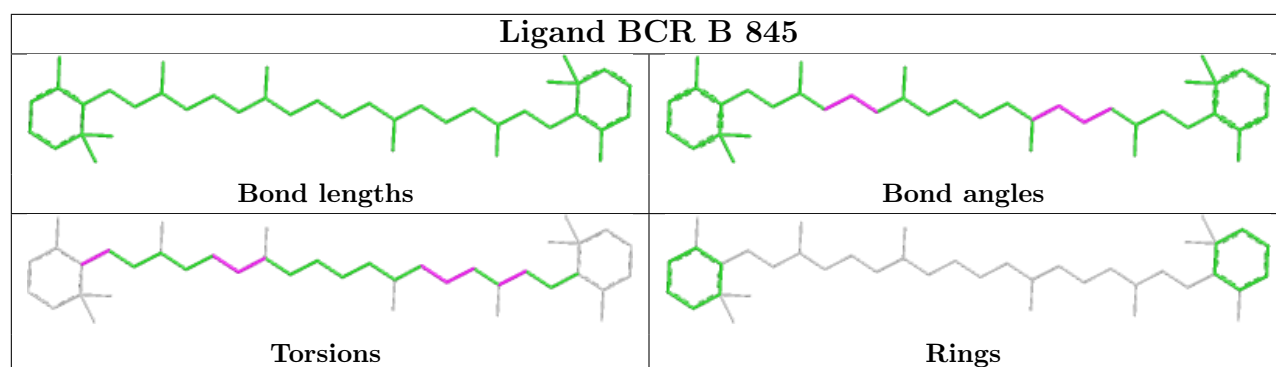


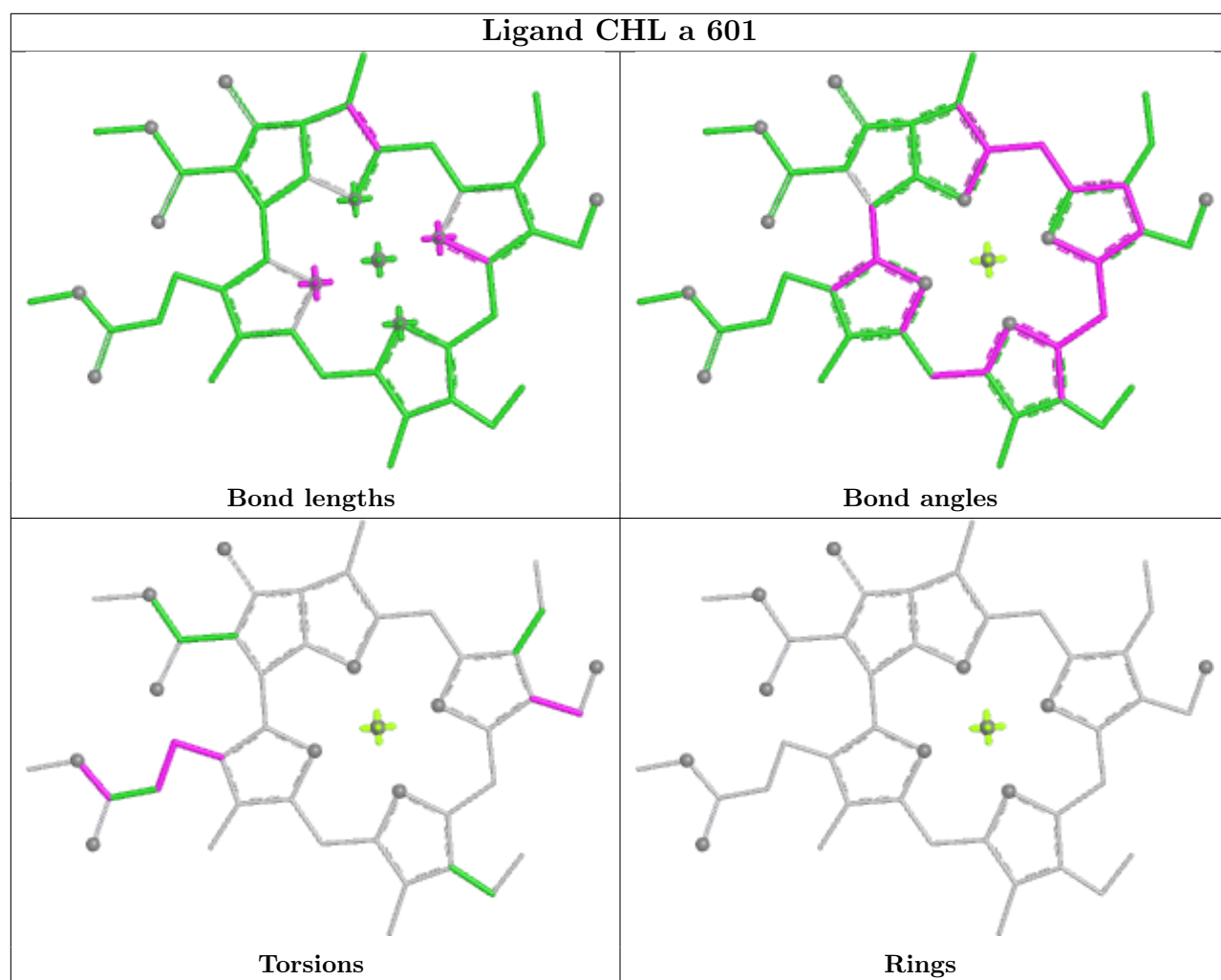
Ligand CLA F 5007



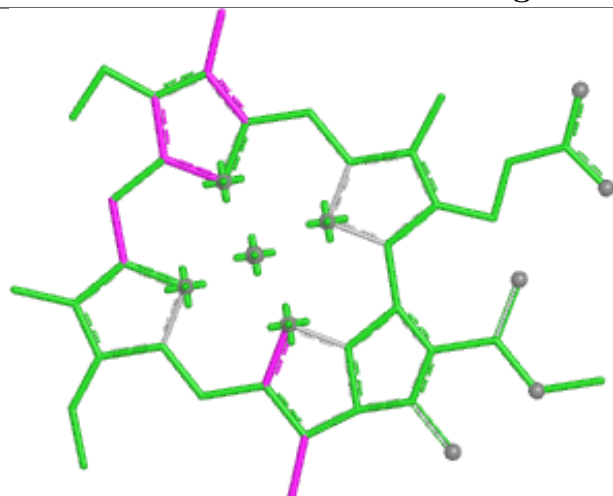
Ligand CLA B 840



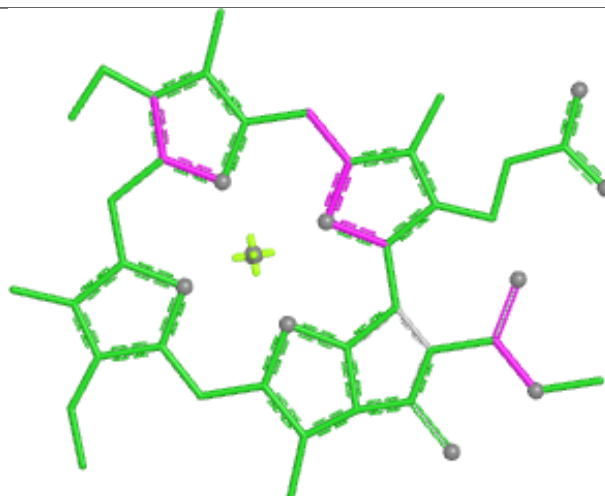




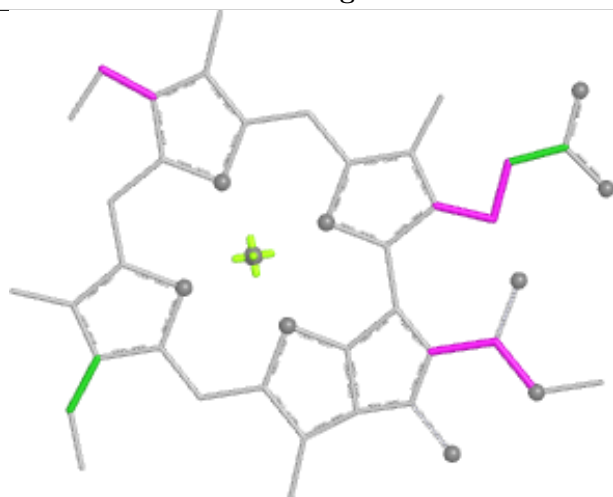
Ligand CLA K 204



Bond lengths



Bond angles

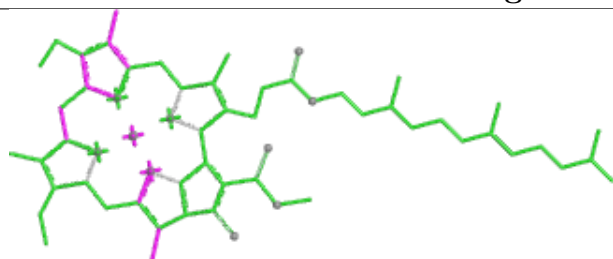


Torsions

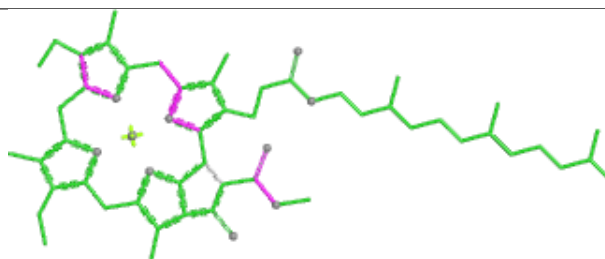


Rings

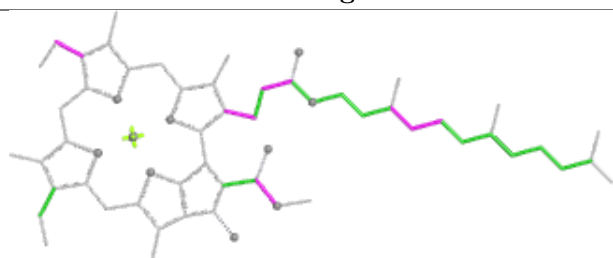
Ligand CLA A 5040



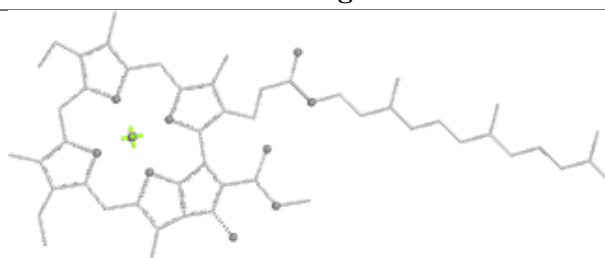
Bond lengths



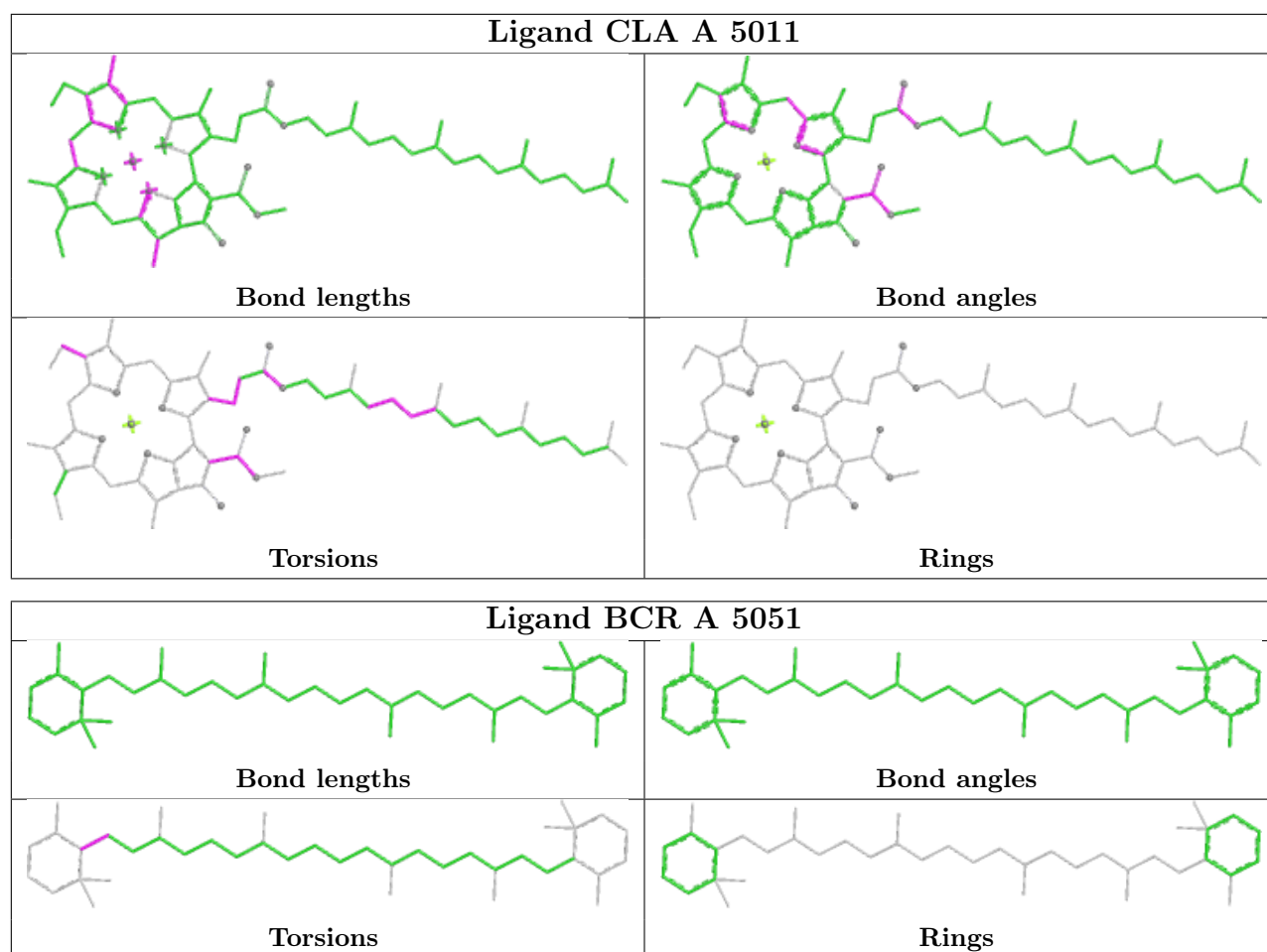
Bond angles



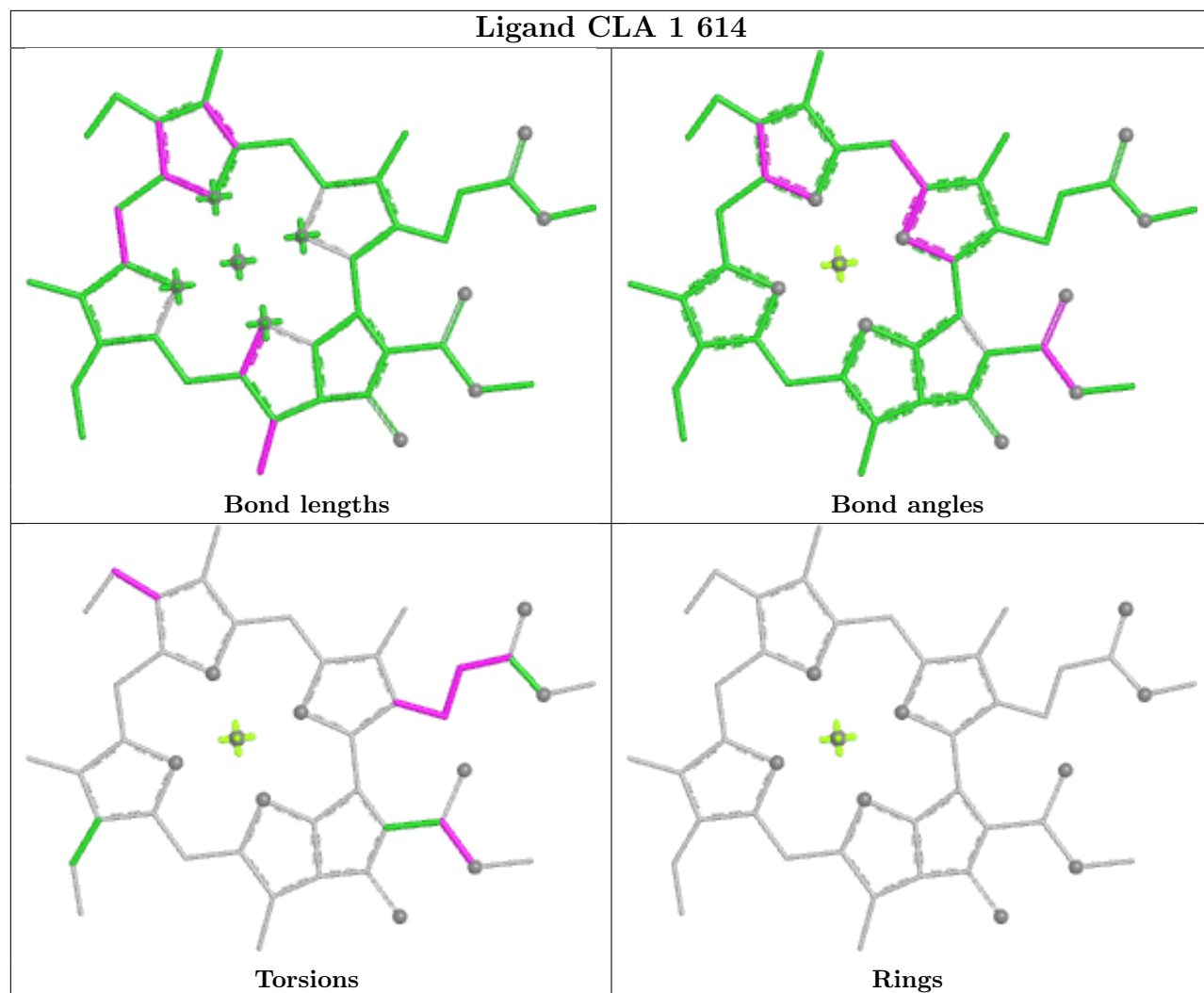
Torsions



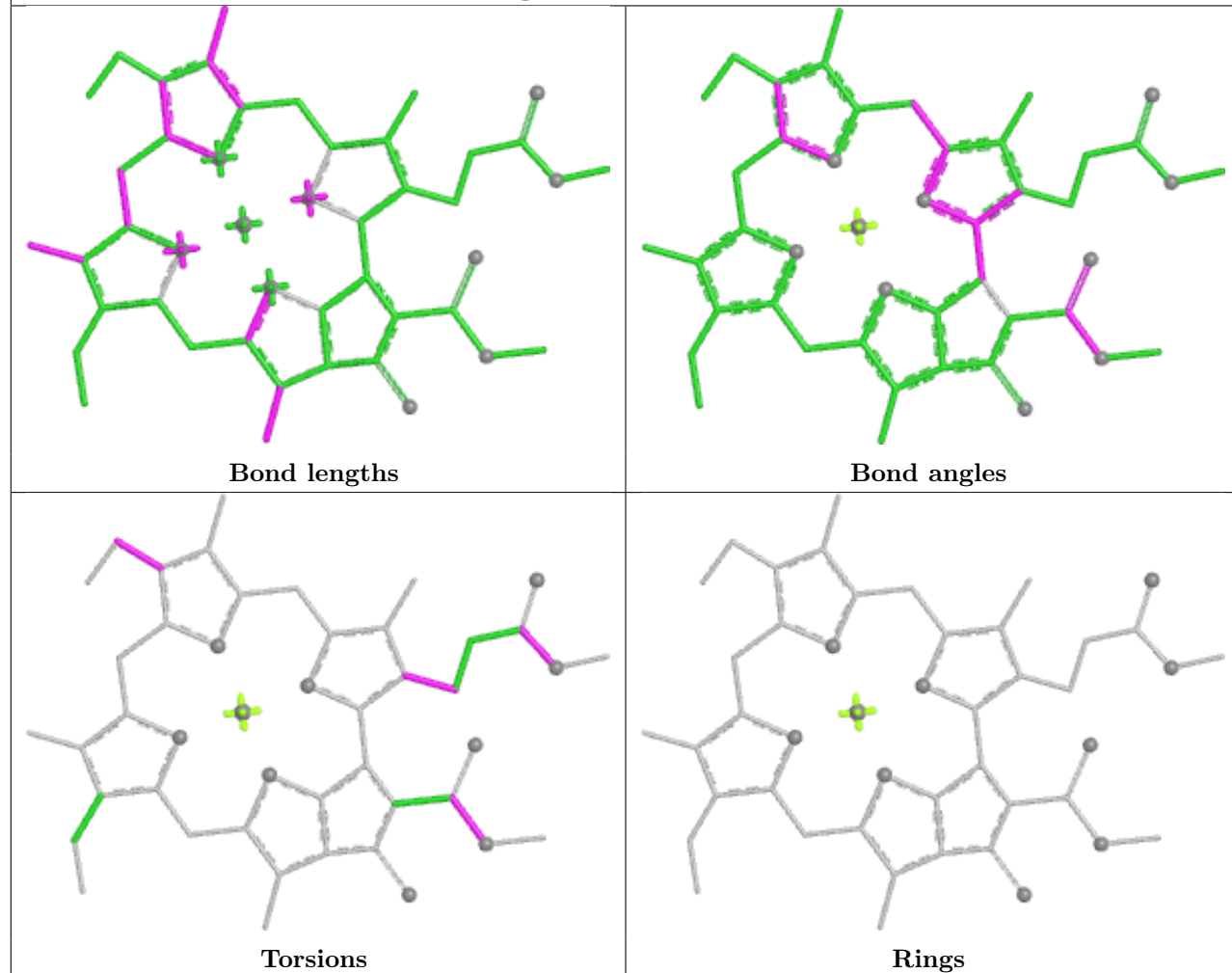
Rings



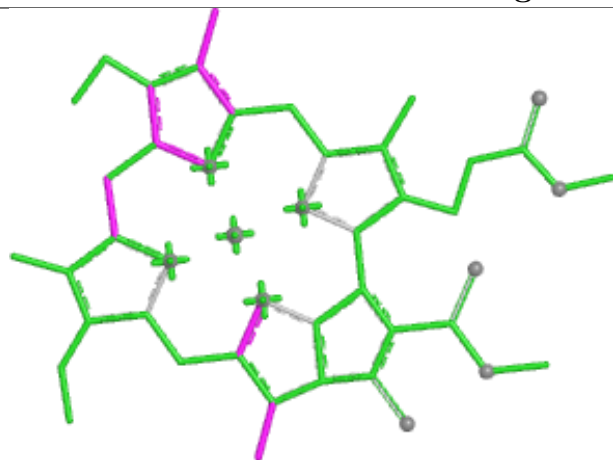
Ligand CLA 1 614



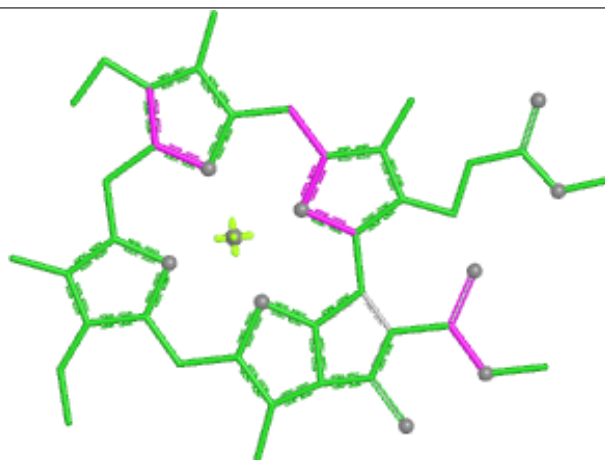
Ligand CLA 1 611



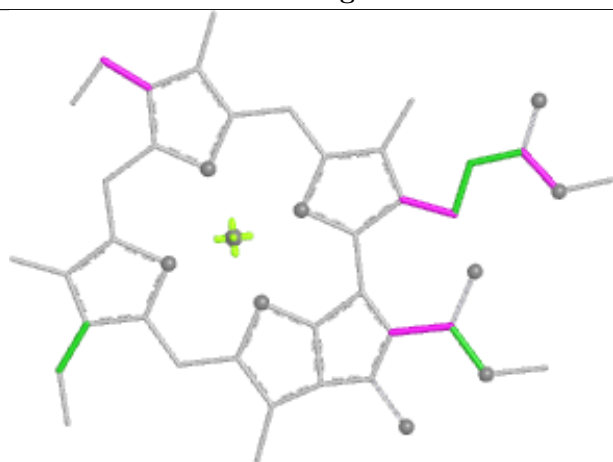
Ligand CLA B 812



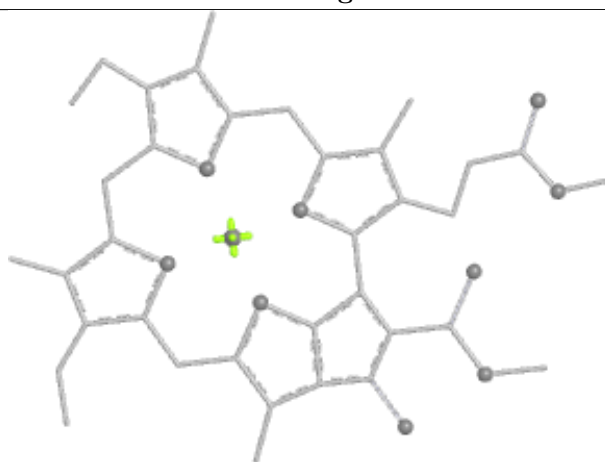
Bond lengths



Bond angles

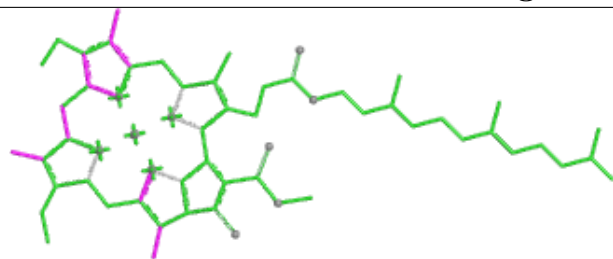


Torsions

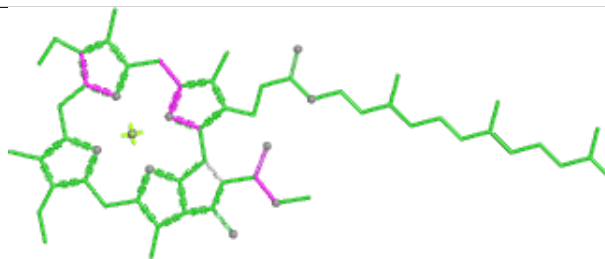


Rings

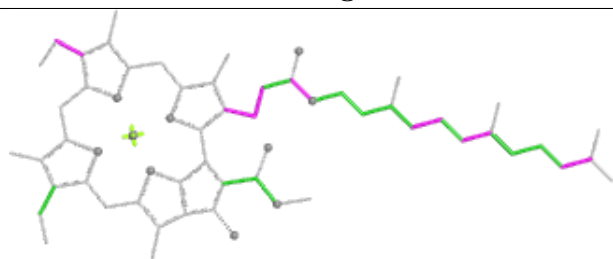
Ligand CLA b 609



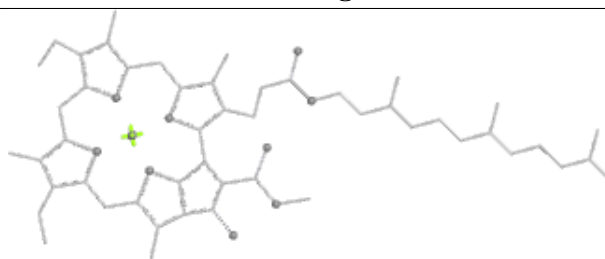
Bond lengths



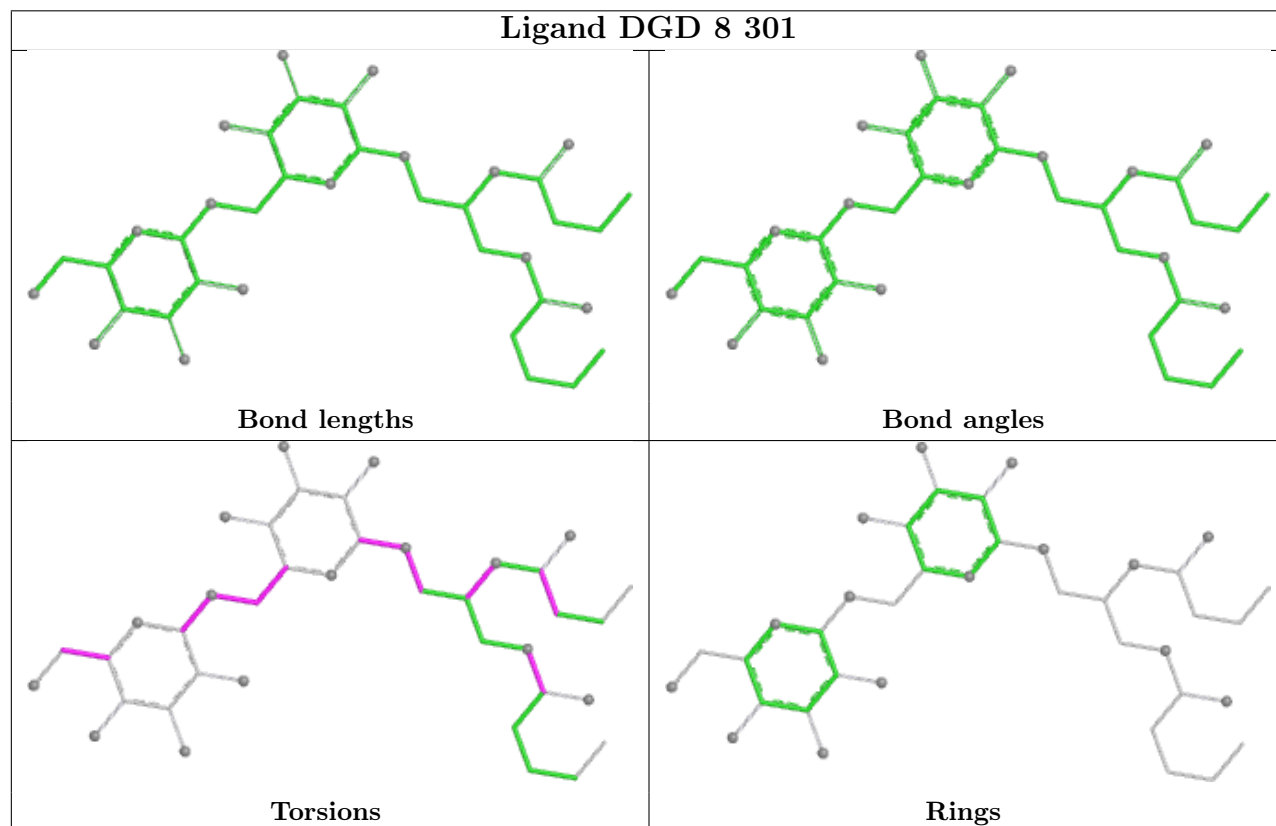
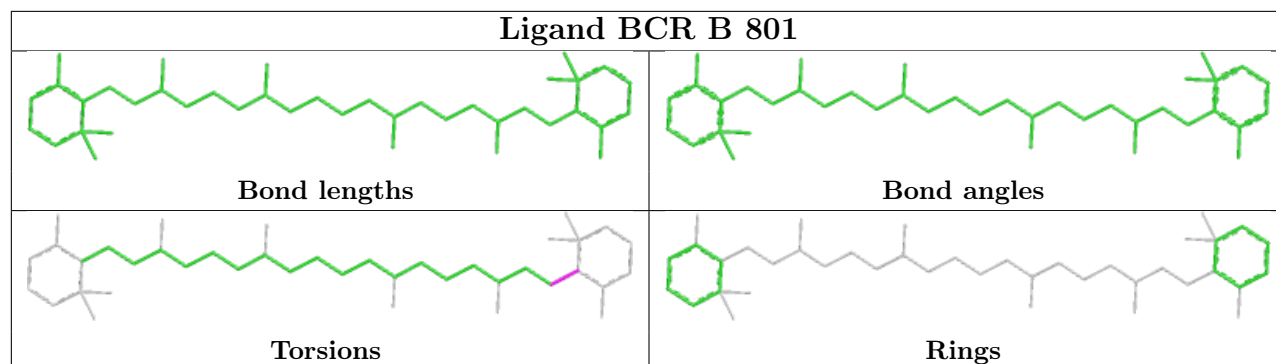
Bond angles



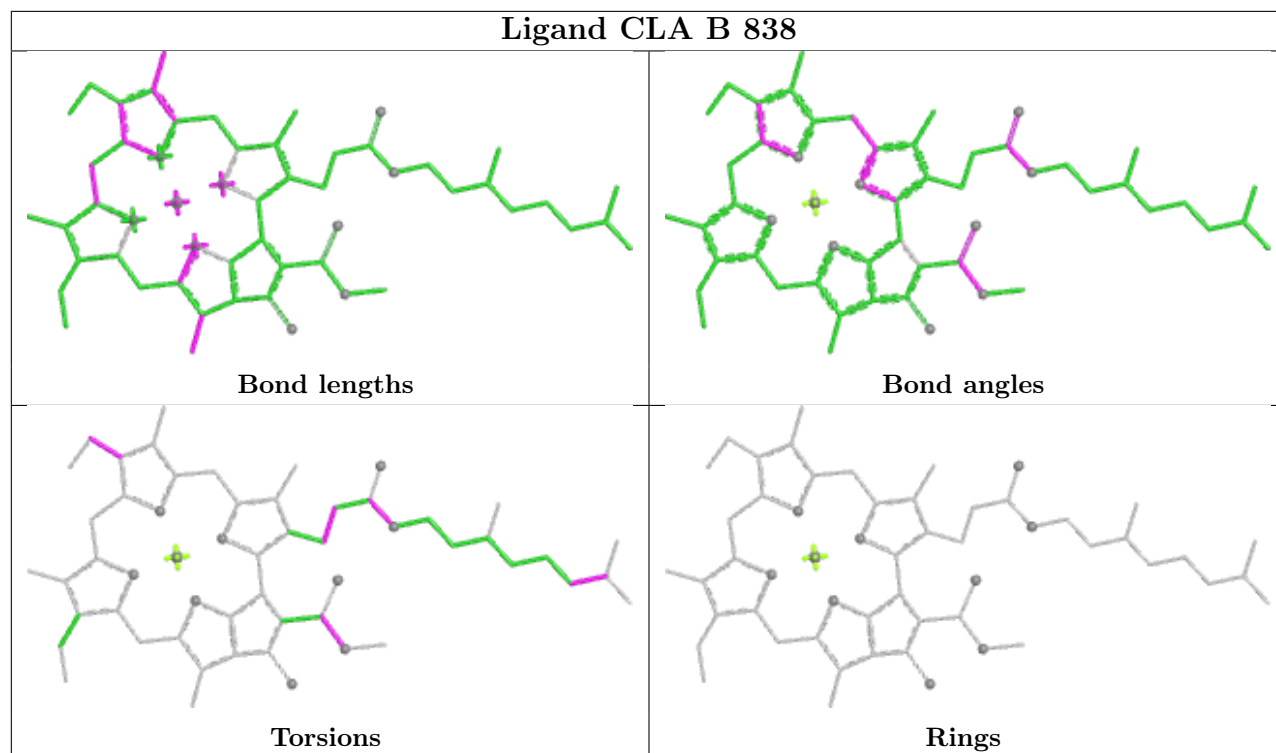
Torsions



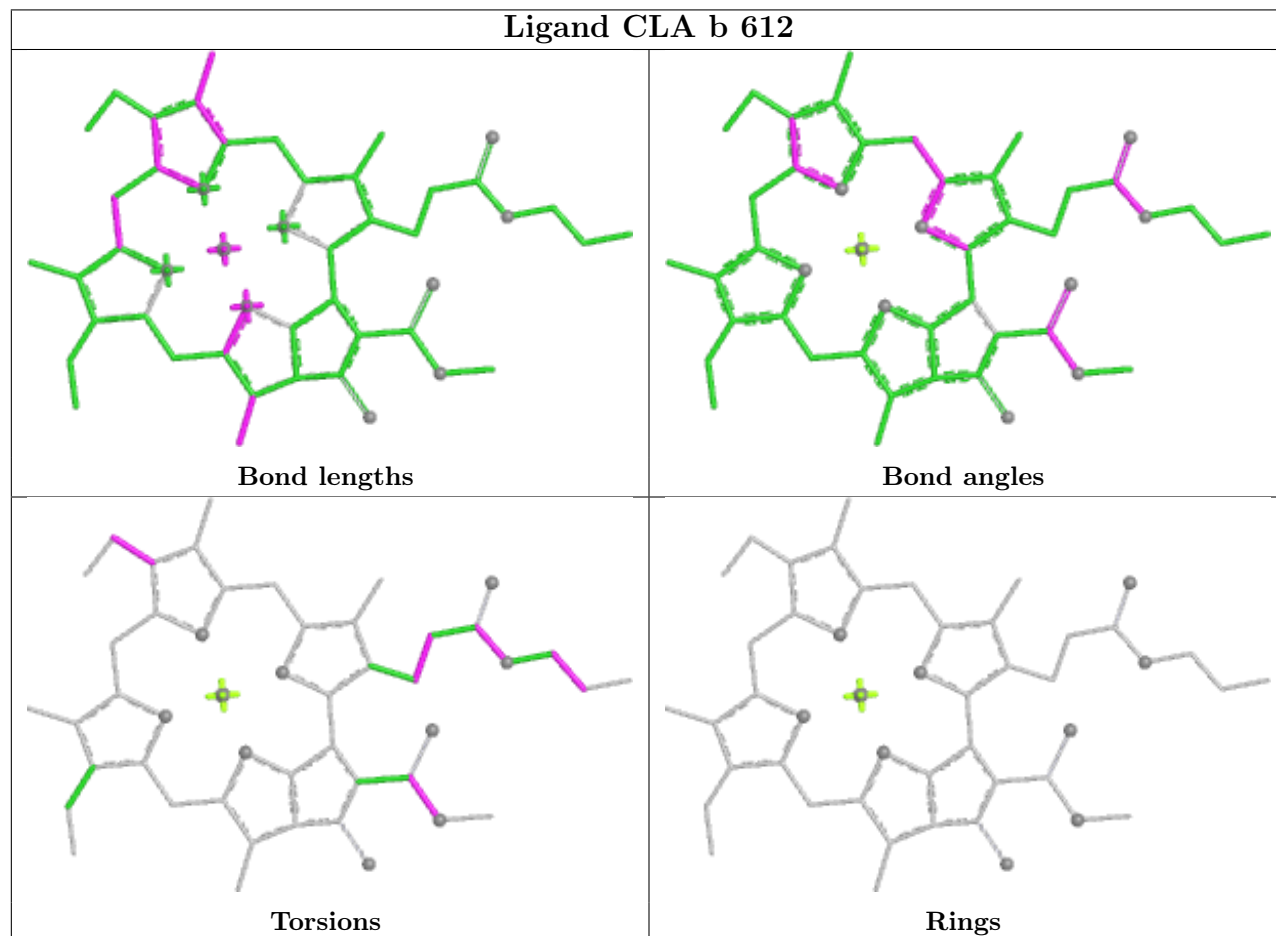
Rings

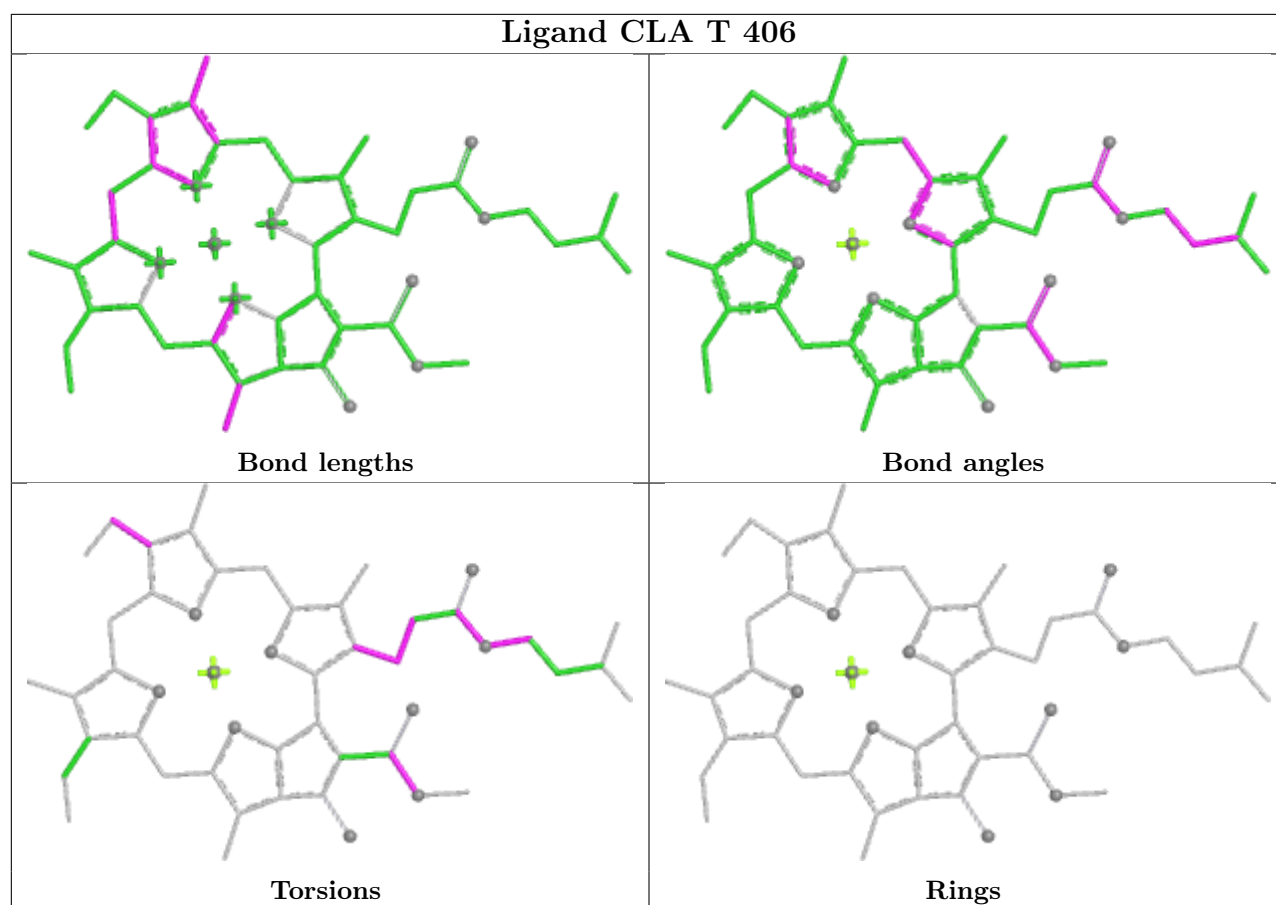


Ligand CLA B 838

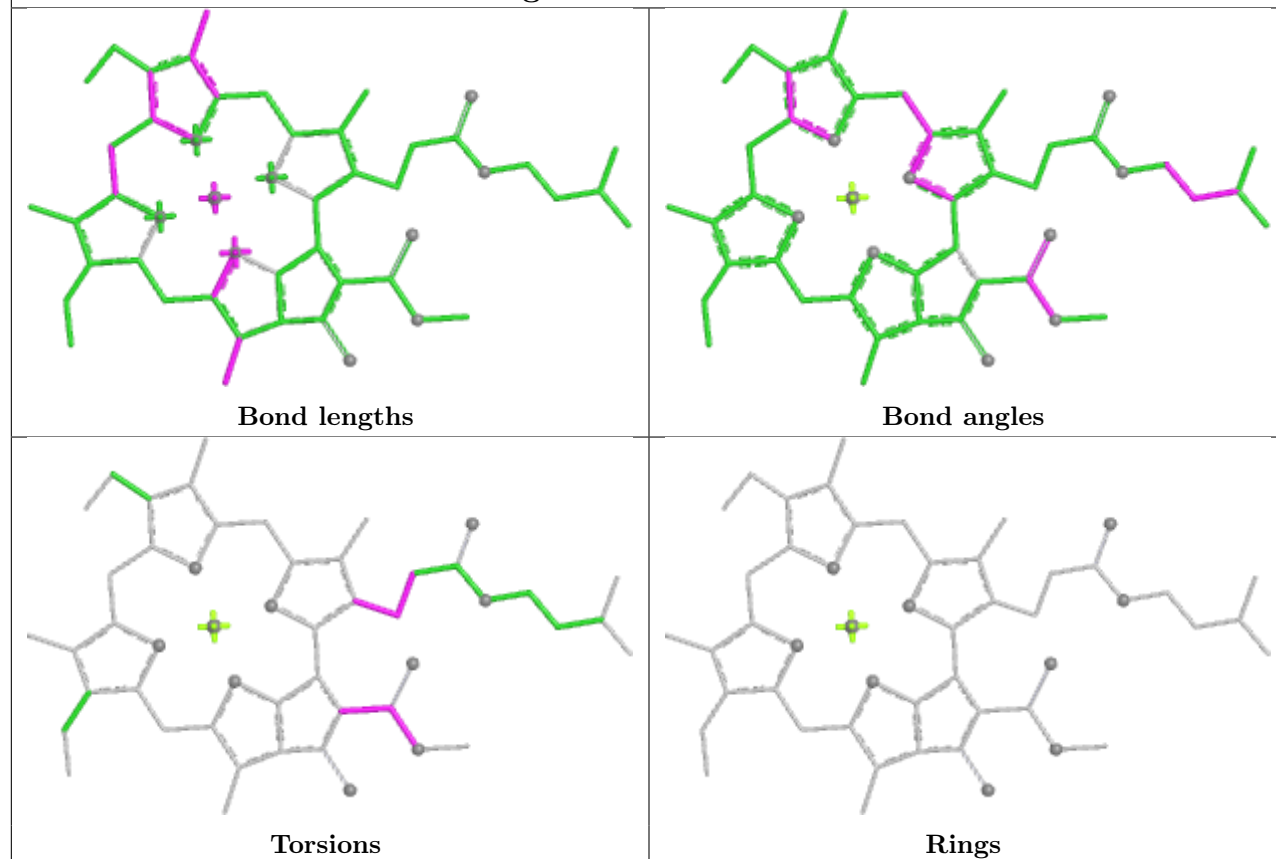


Ligand CLA b 612

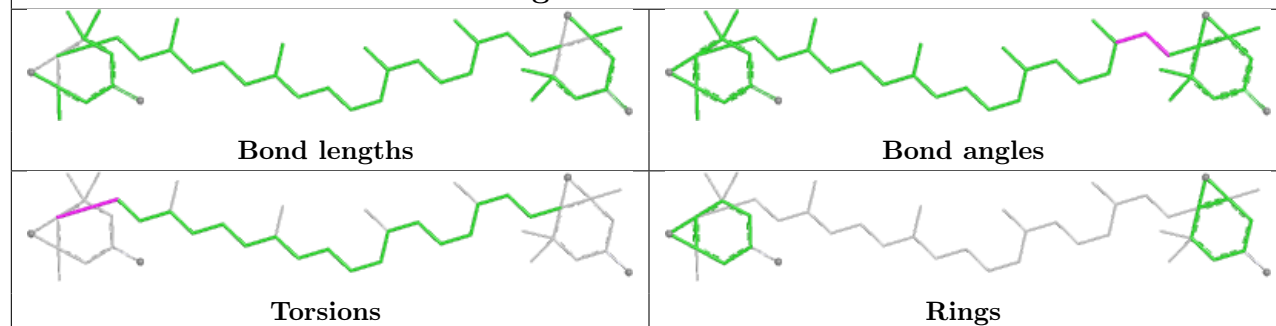




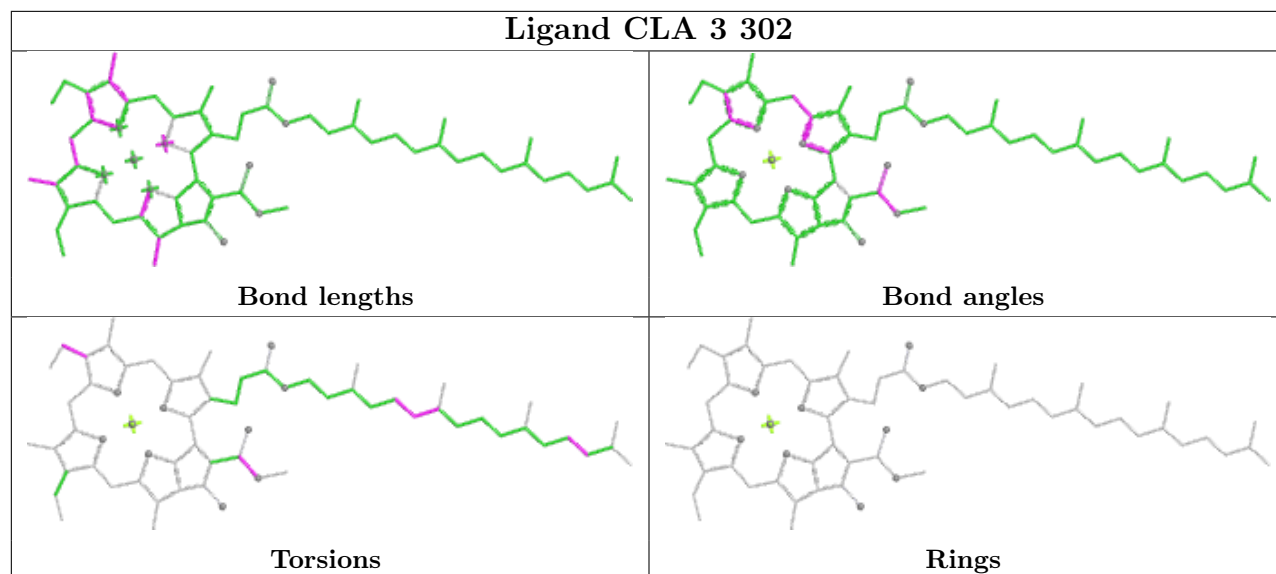
Ligand CLA A 5038



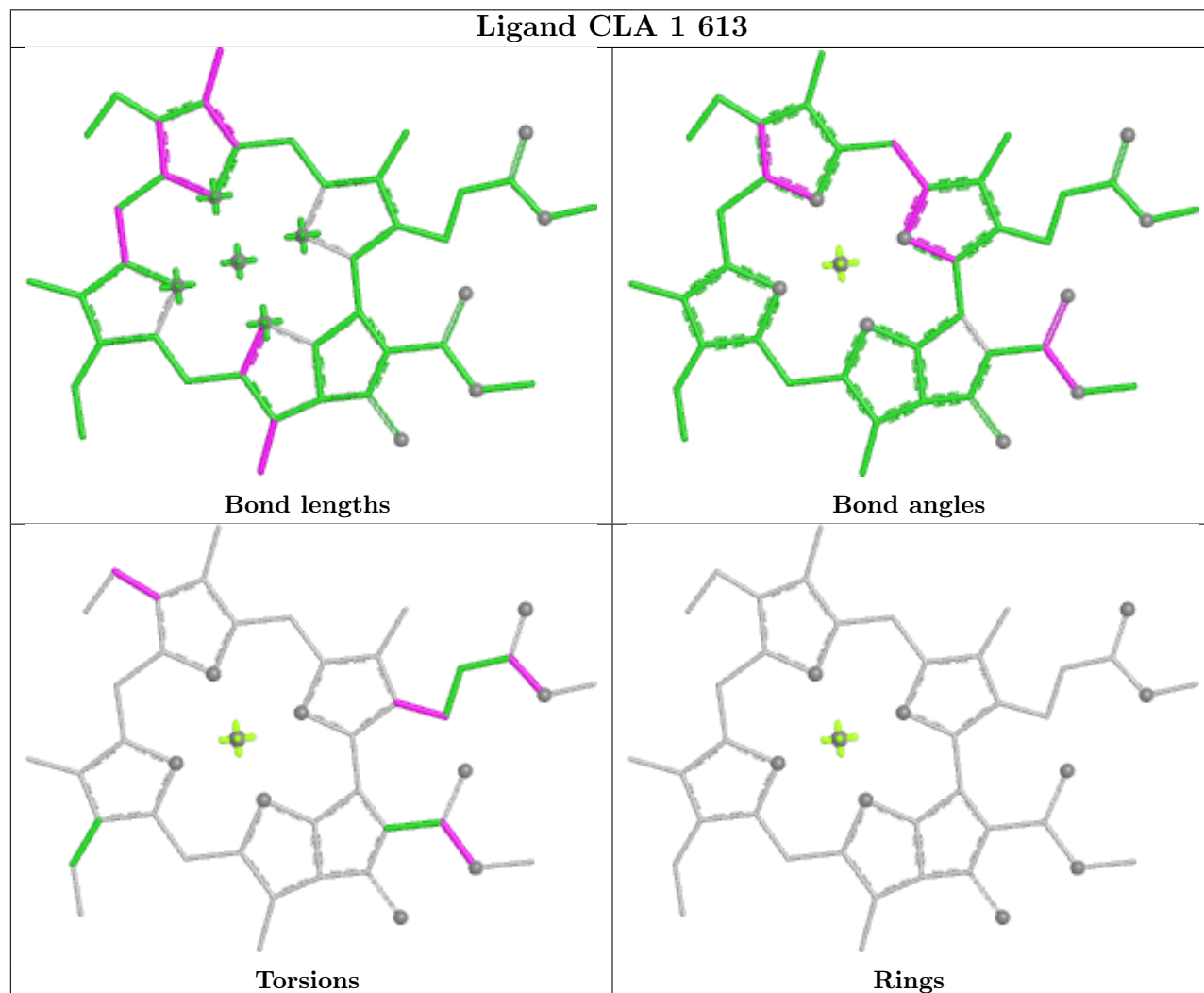
Ligand XAT T 414

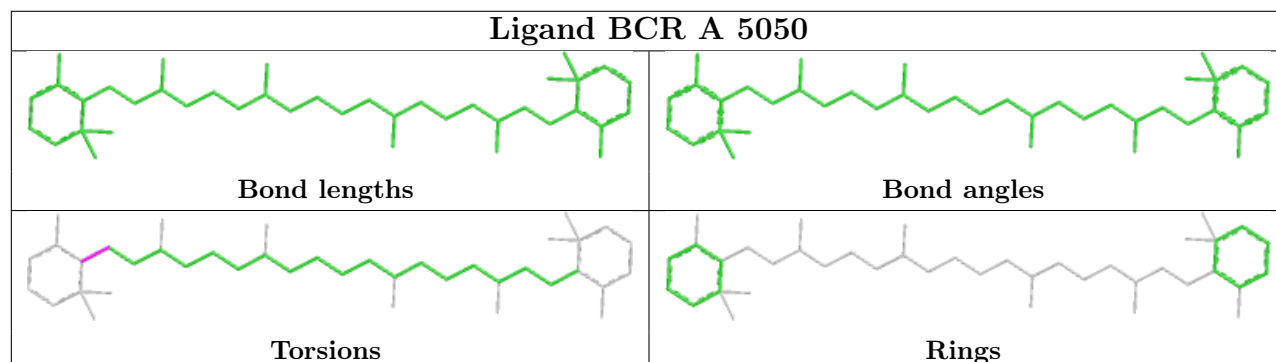
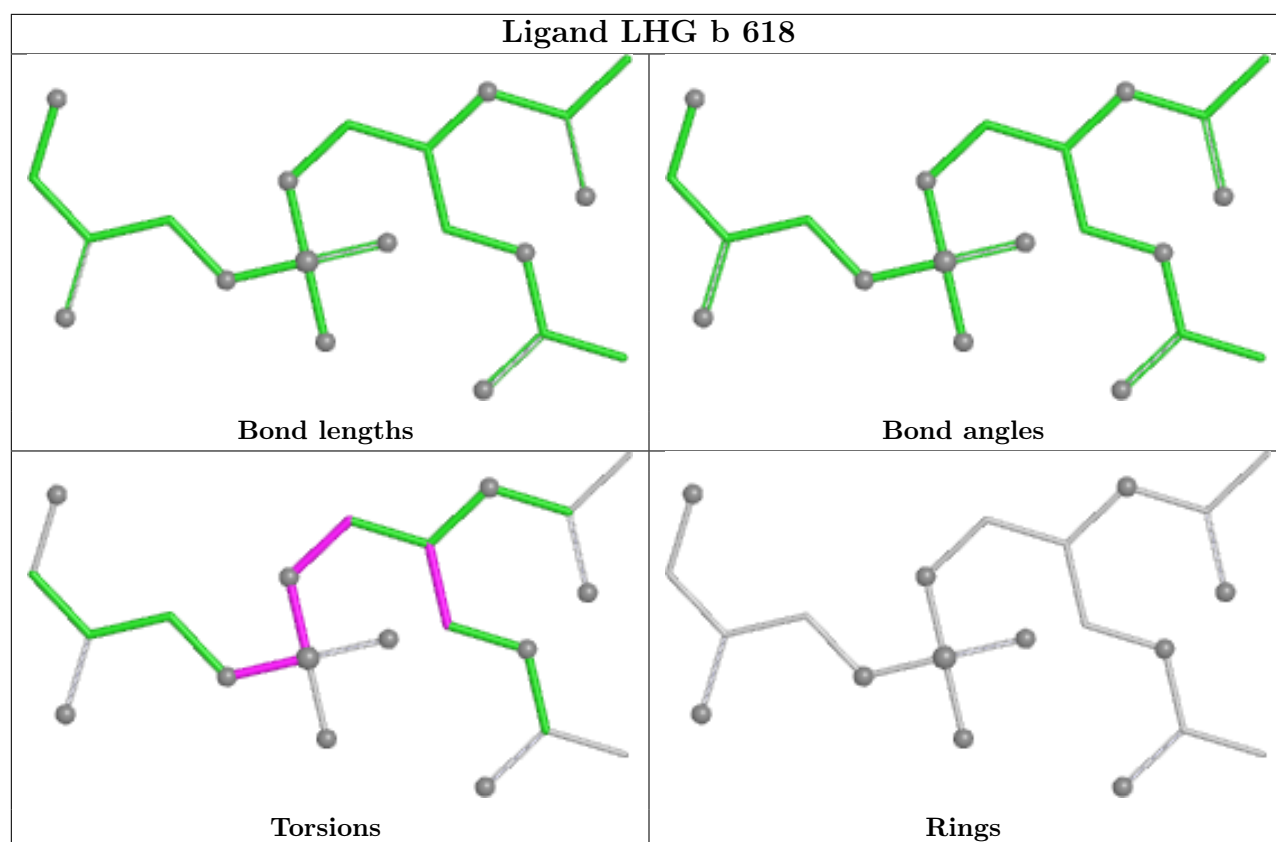


Ligand CLA 3 302

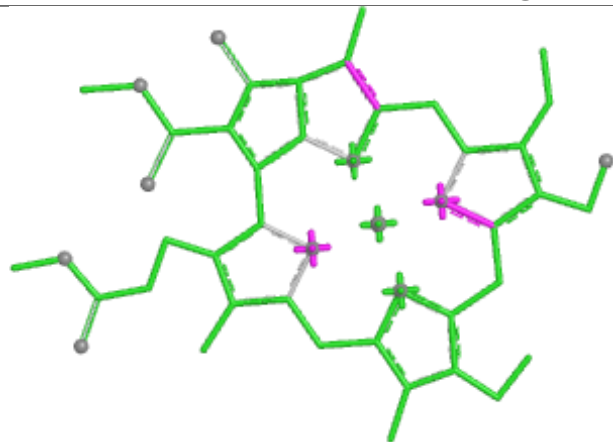


Ligand CLA 1 613

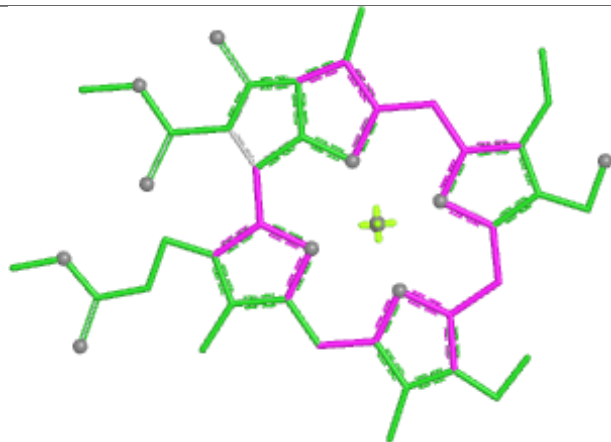




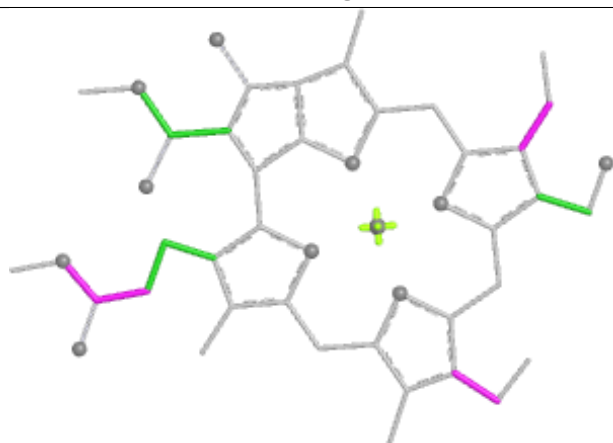
Ligand CHL b 606



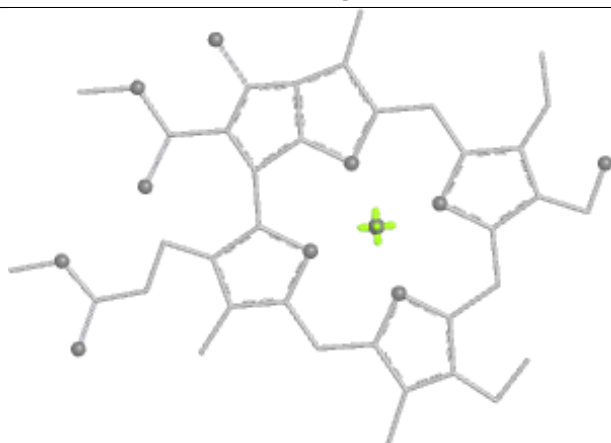
Bond lengths



Bond angles

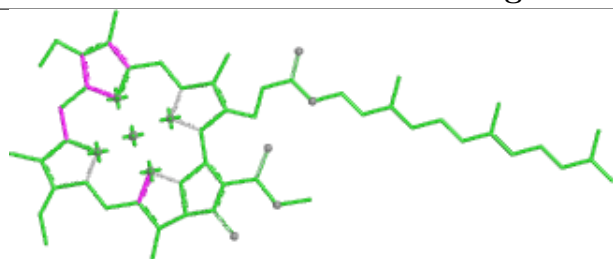


Torsions

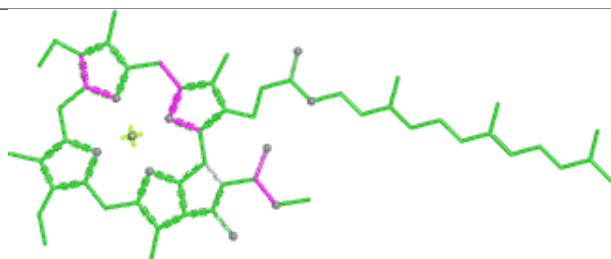


Rings

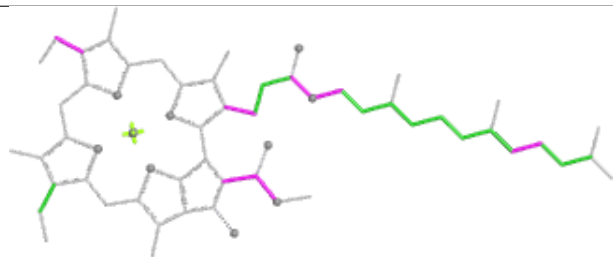
Ligand CLA A 5007



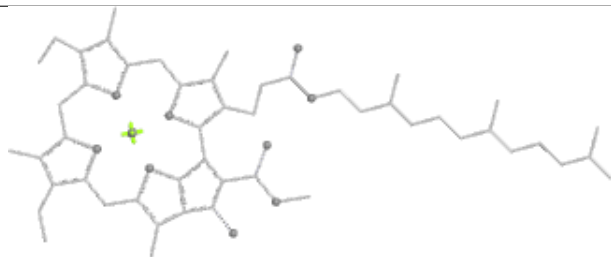
Bond lengths



Bond angles

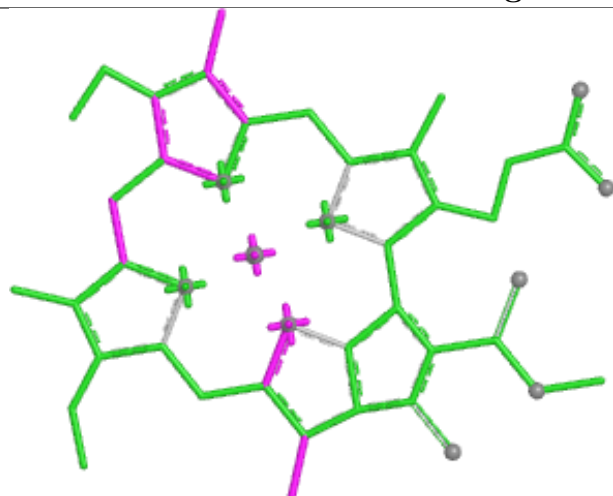


Torsions

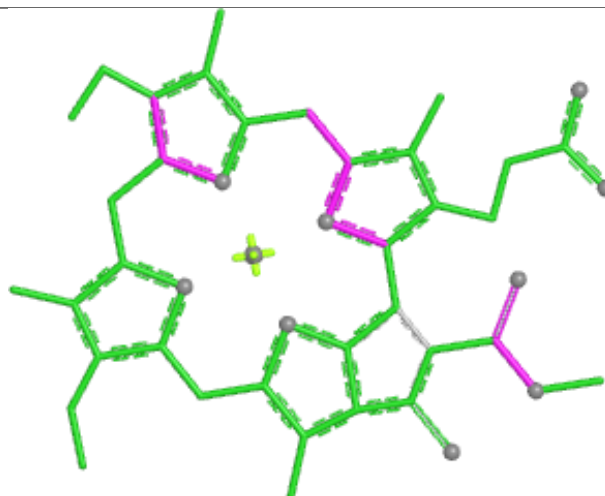


Rings

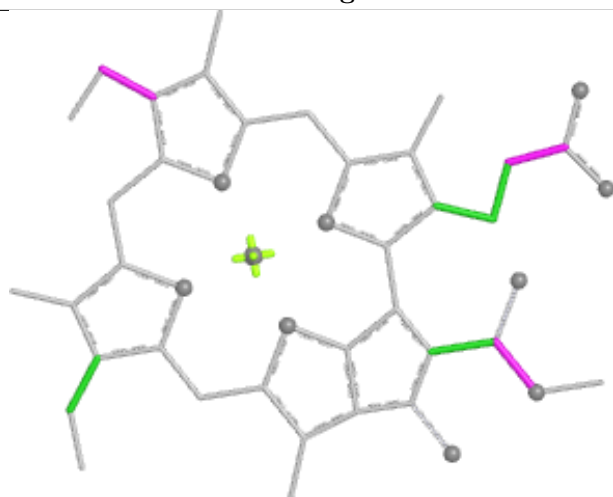
Ligand CLA A 5032



Bond lengths



Bond angles

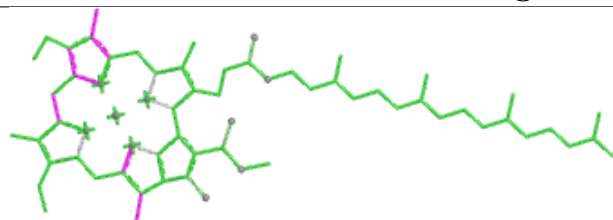


Torsions

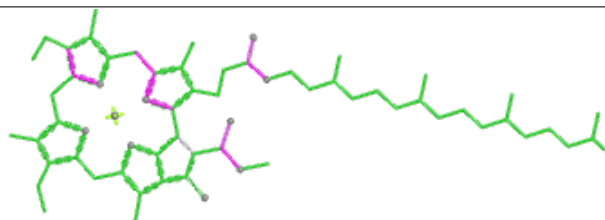


Rings

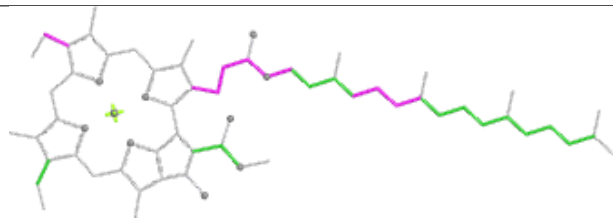
Ligand CLA B 841



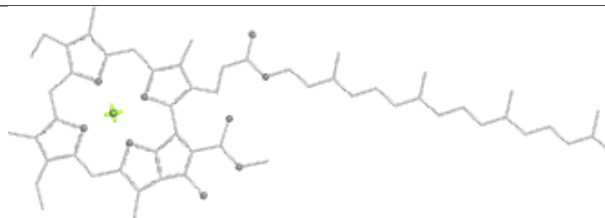
Bond lengths



Bond angles

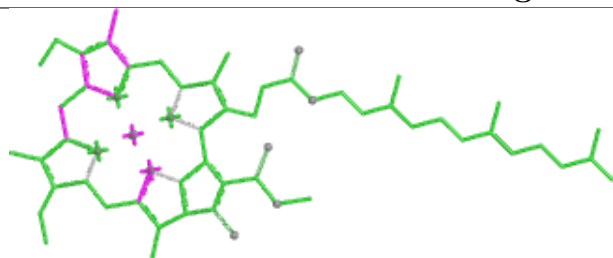


Torsions

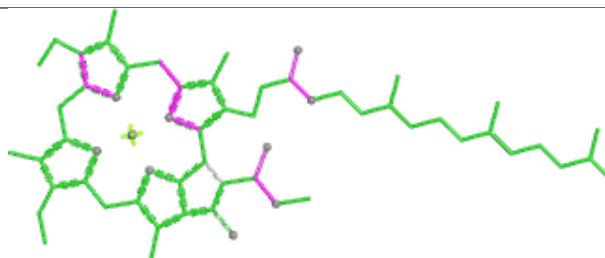


Rings

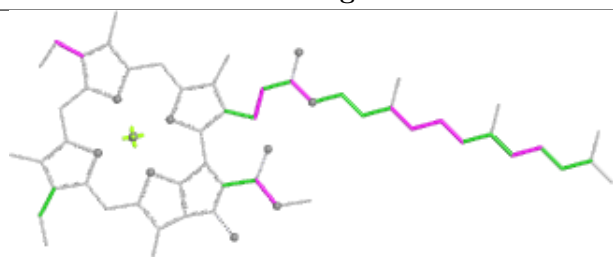
Ligand CLA B 809



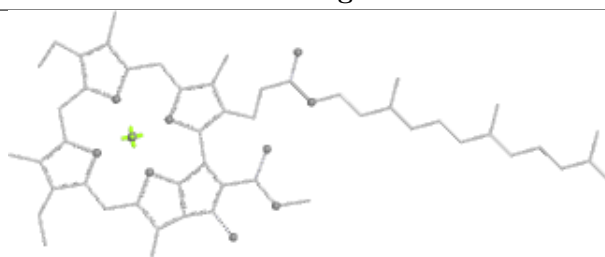
Bond lengths



Bond angles

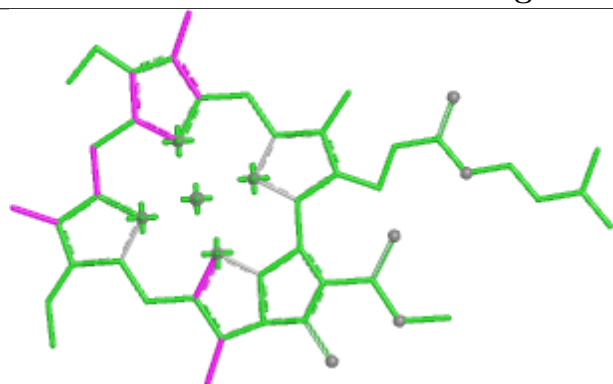


Torsions

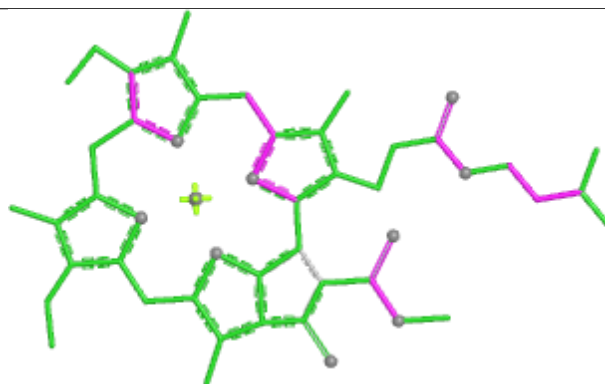


Rings

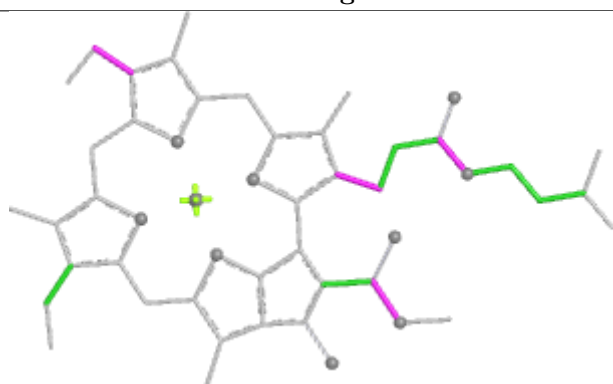
Ligand CLA T 408



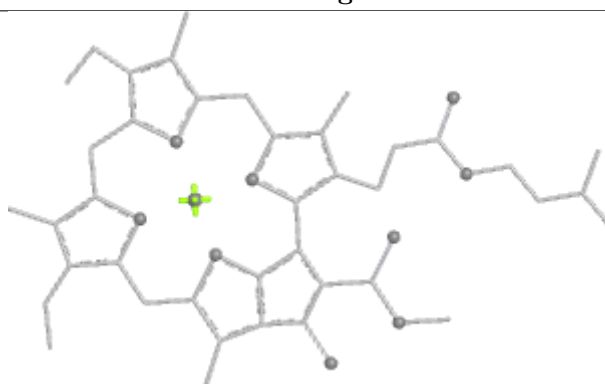
Bond lengths



Bond angles

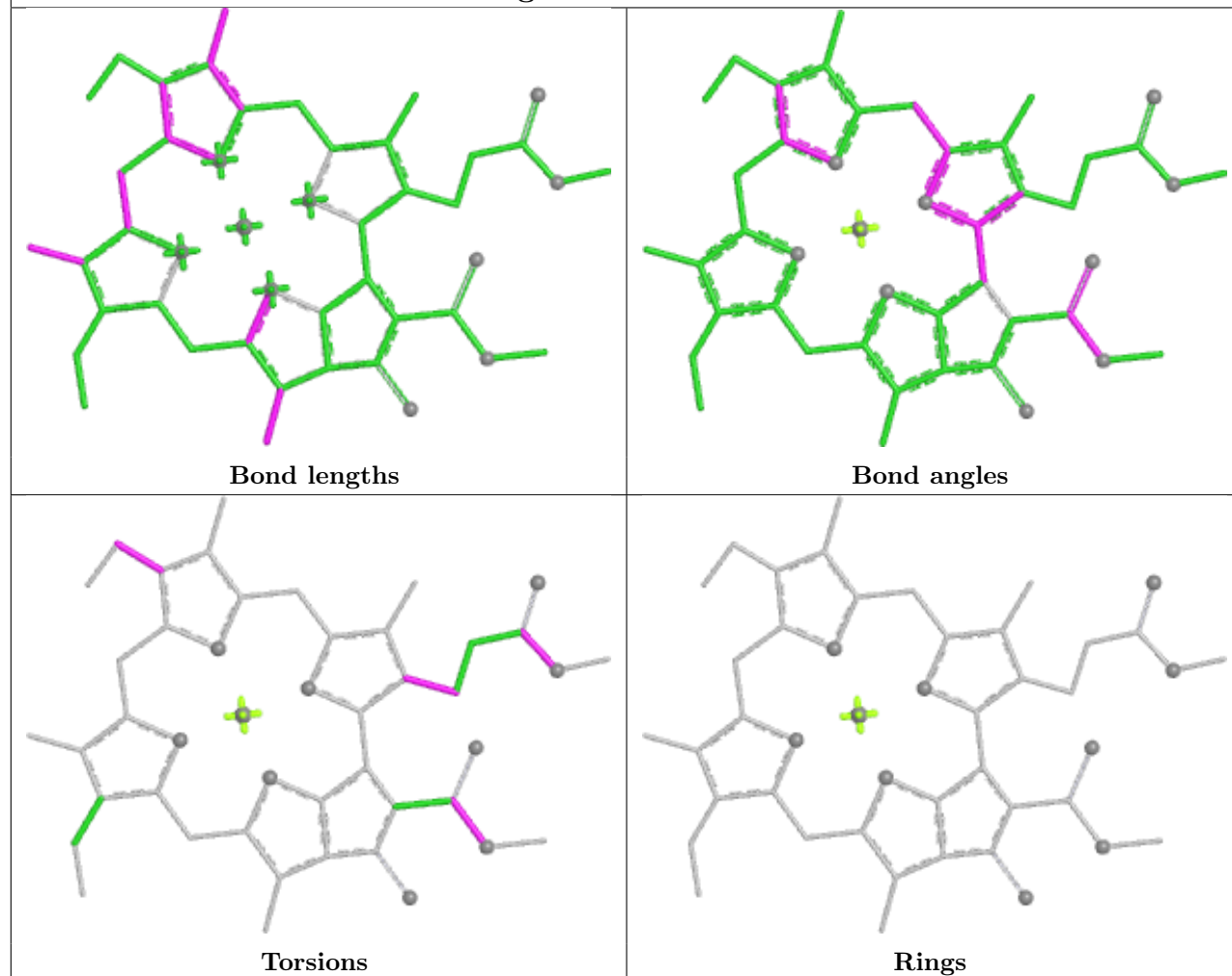


Torsions

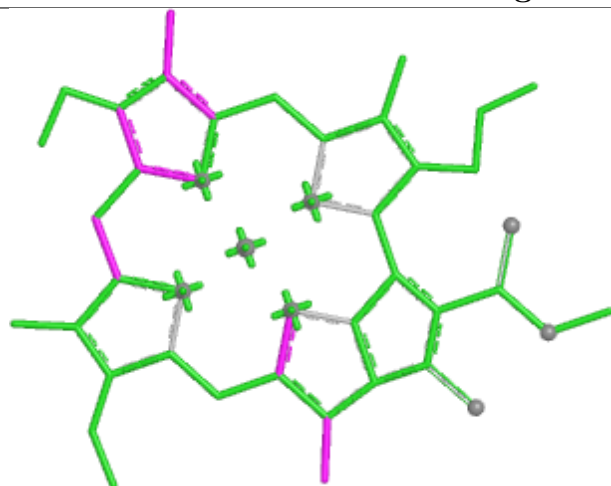


Rings

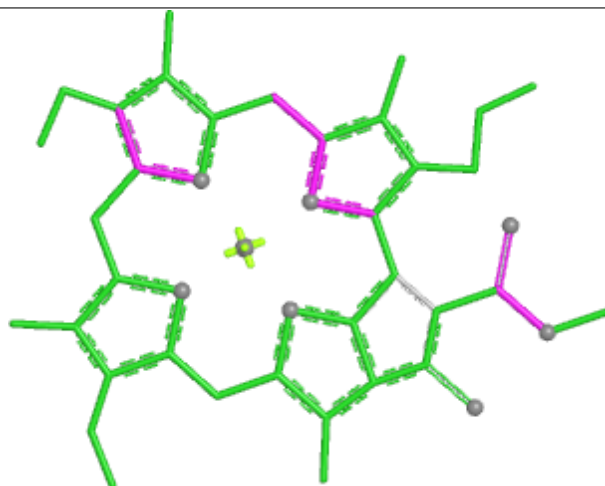
Ligand CLA a 611



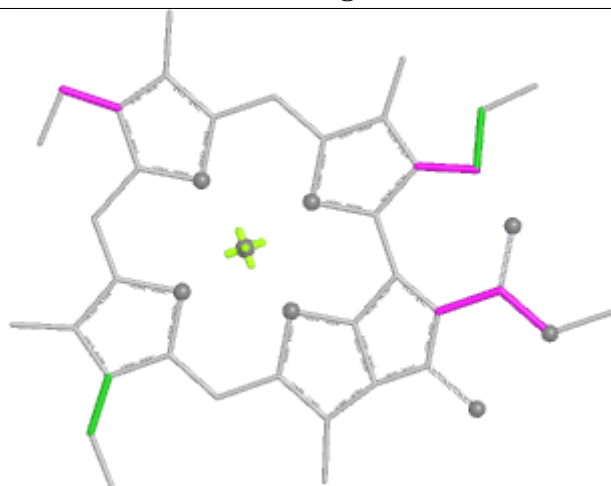
Ligand CLA B 821



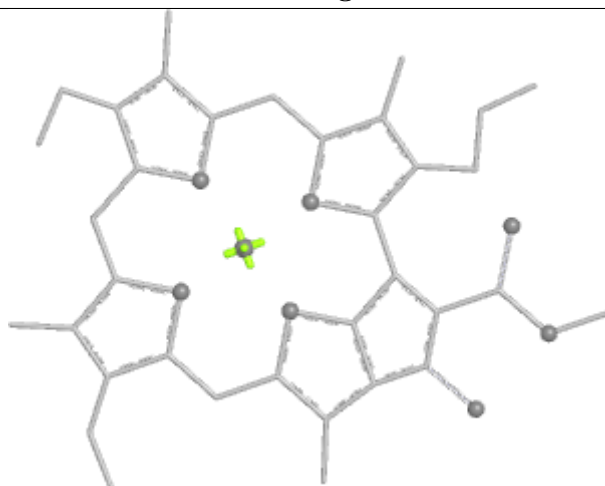
Bond lengths



Bond angles

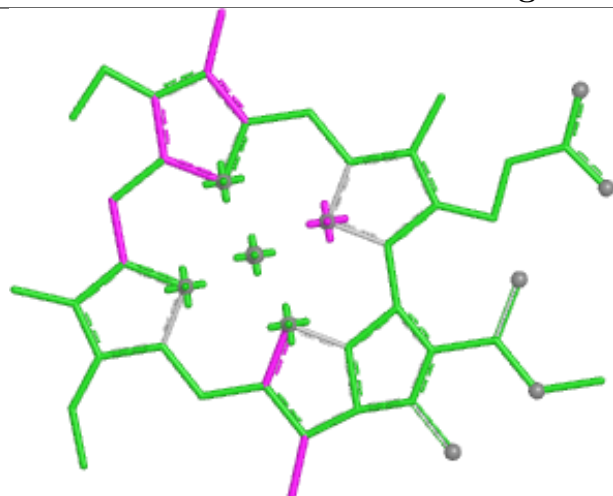


Torsions

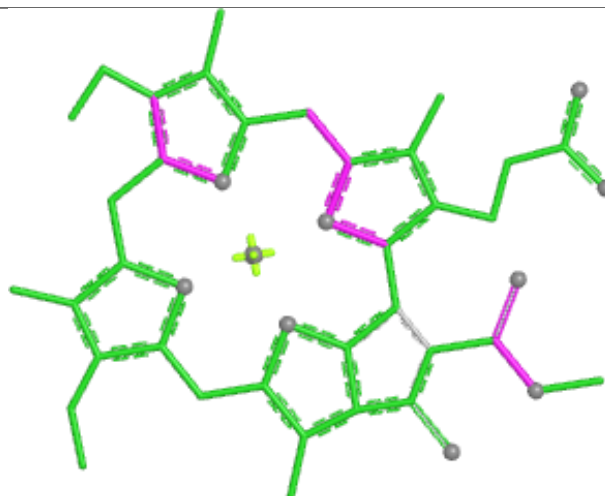


Rings

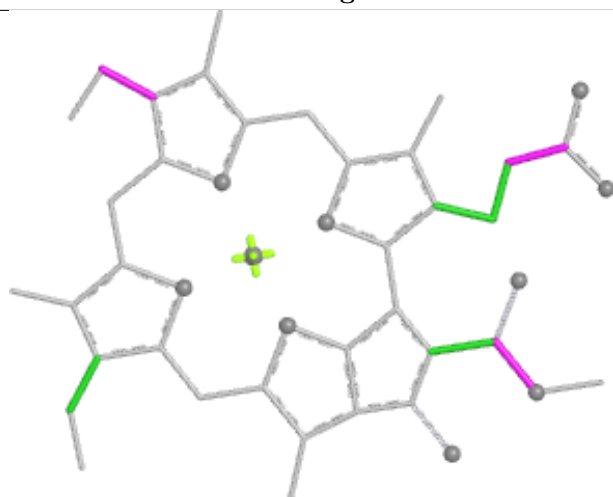
Ligand CLA 1 603



Bond lengths



Bond angles

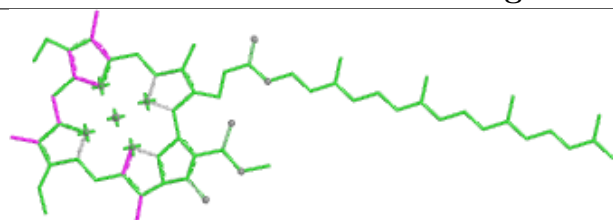


Torsions

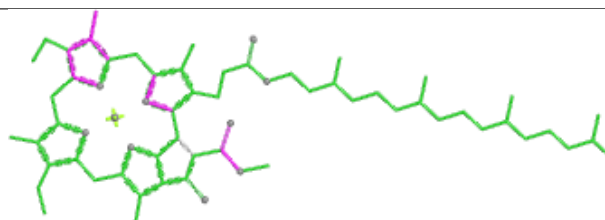


Rings

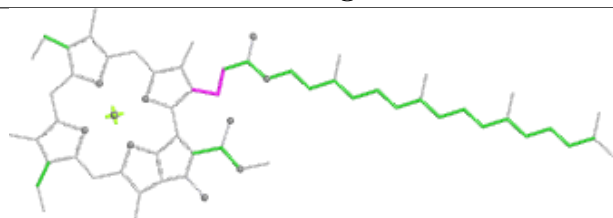
Ligand CLA A 5005



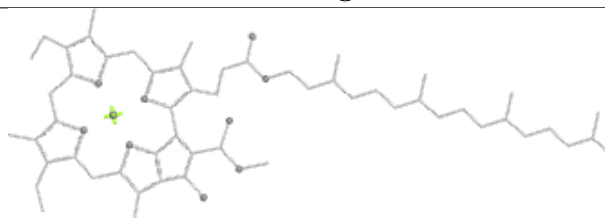
Bond lengths



Bond angles

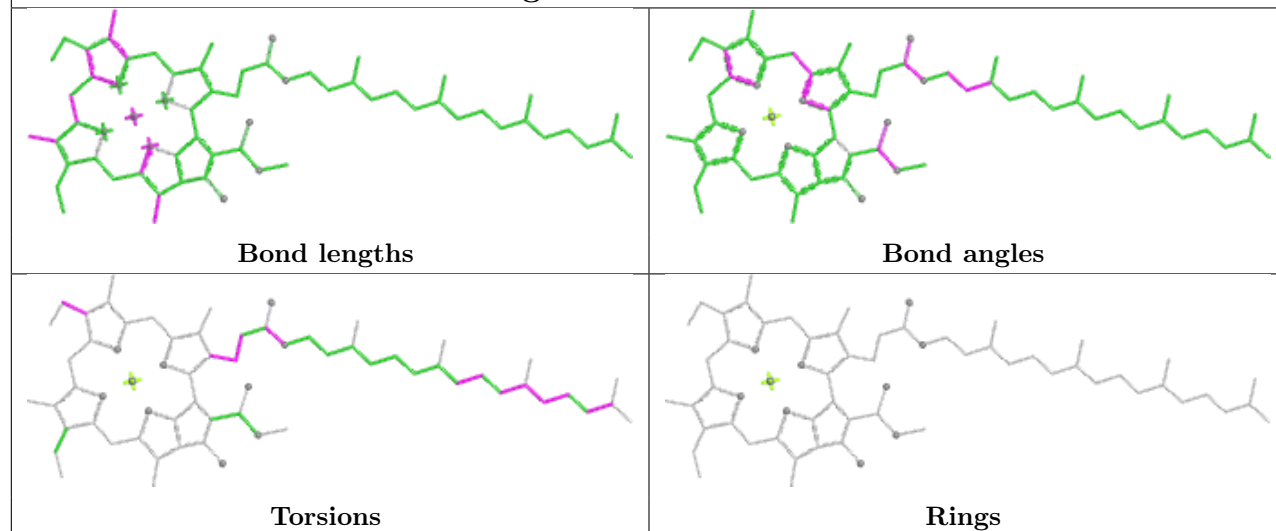


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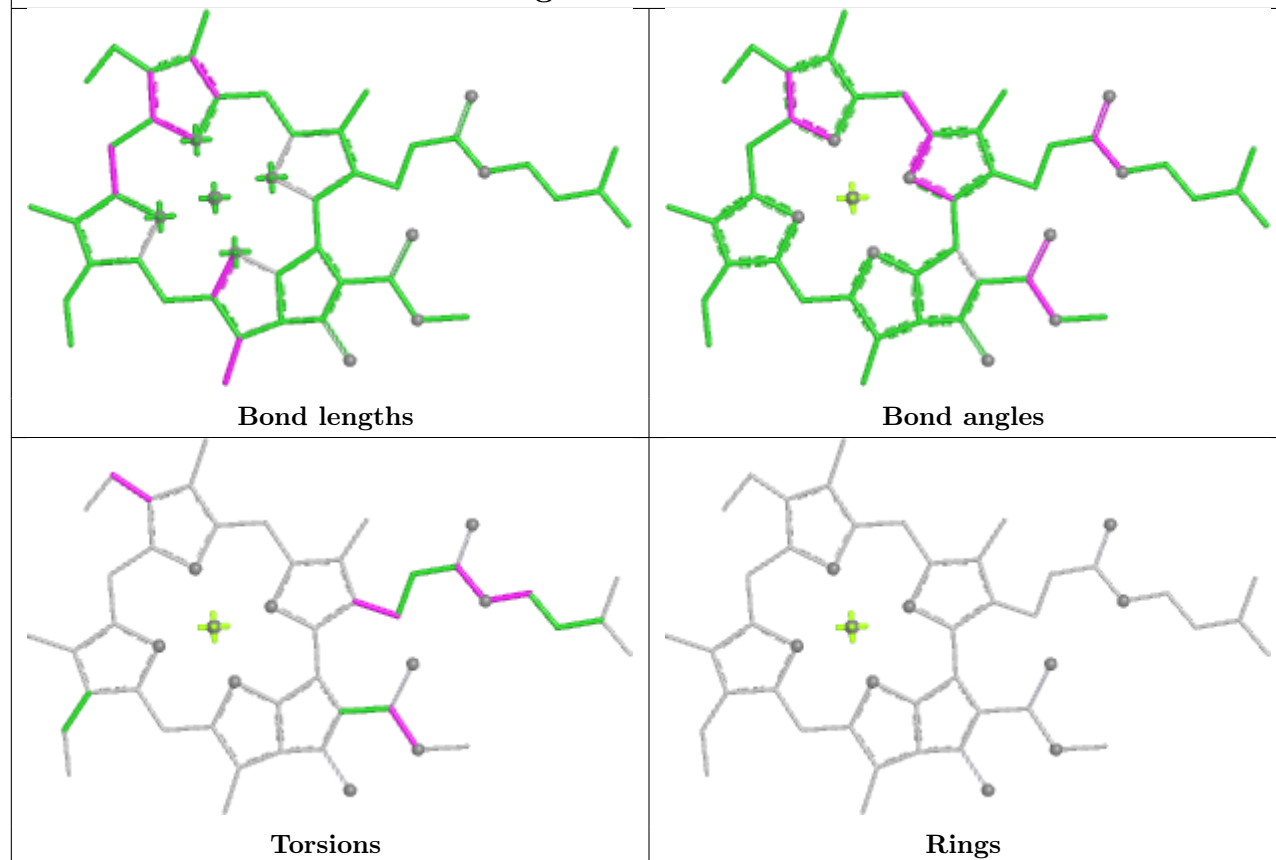


Rings

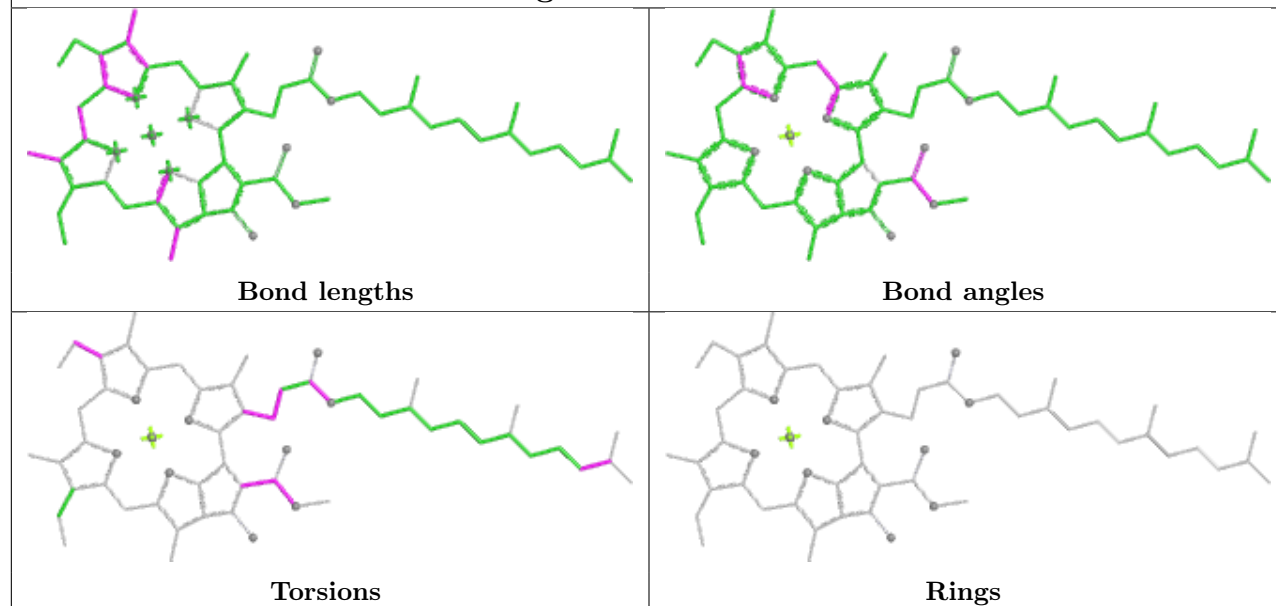
Ligand CLA A 5009



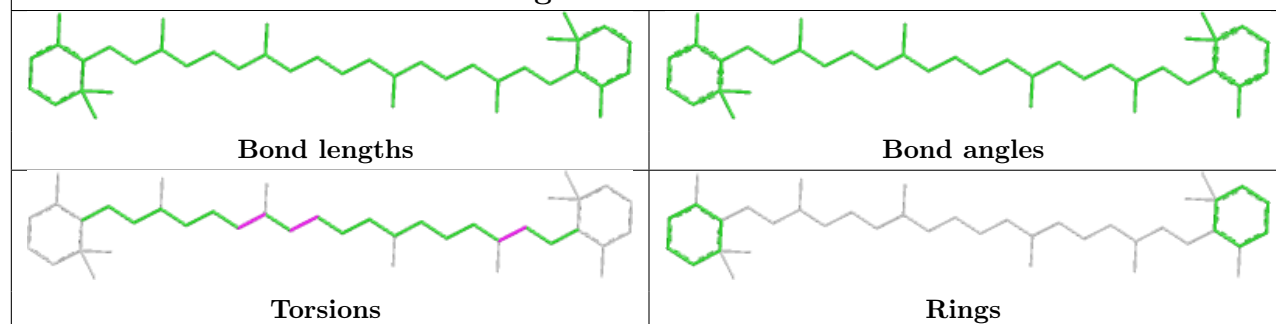
Ligand CLA b 610



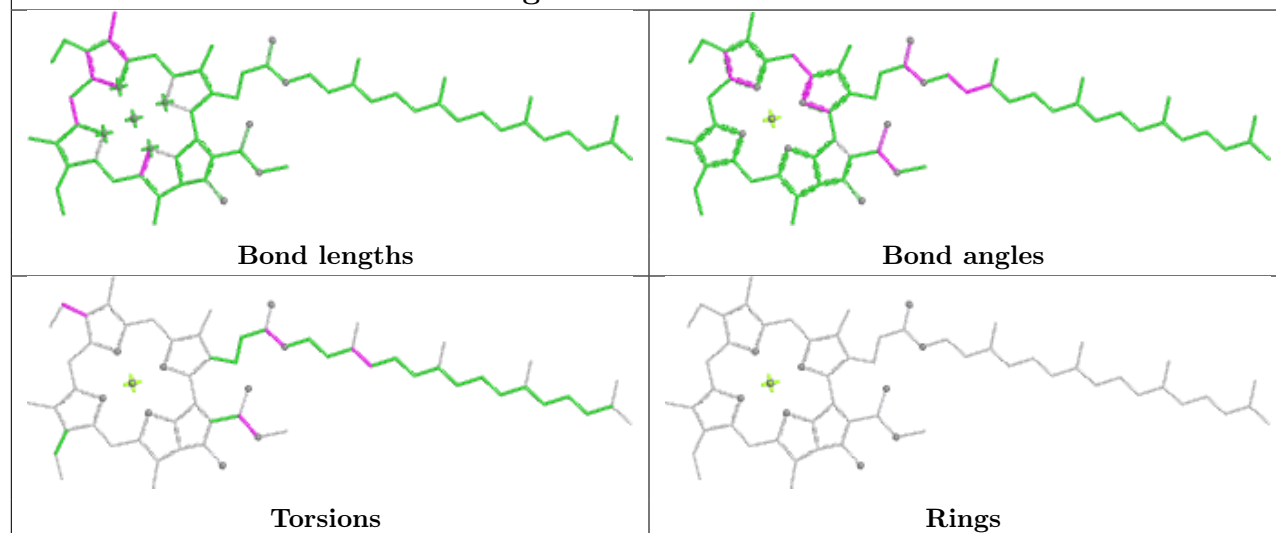
Ligand CLA 7 302

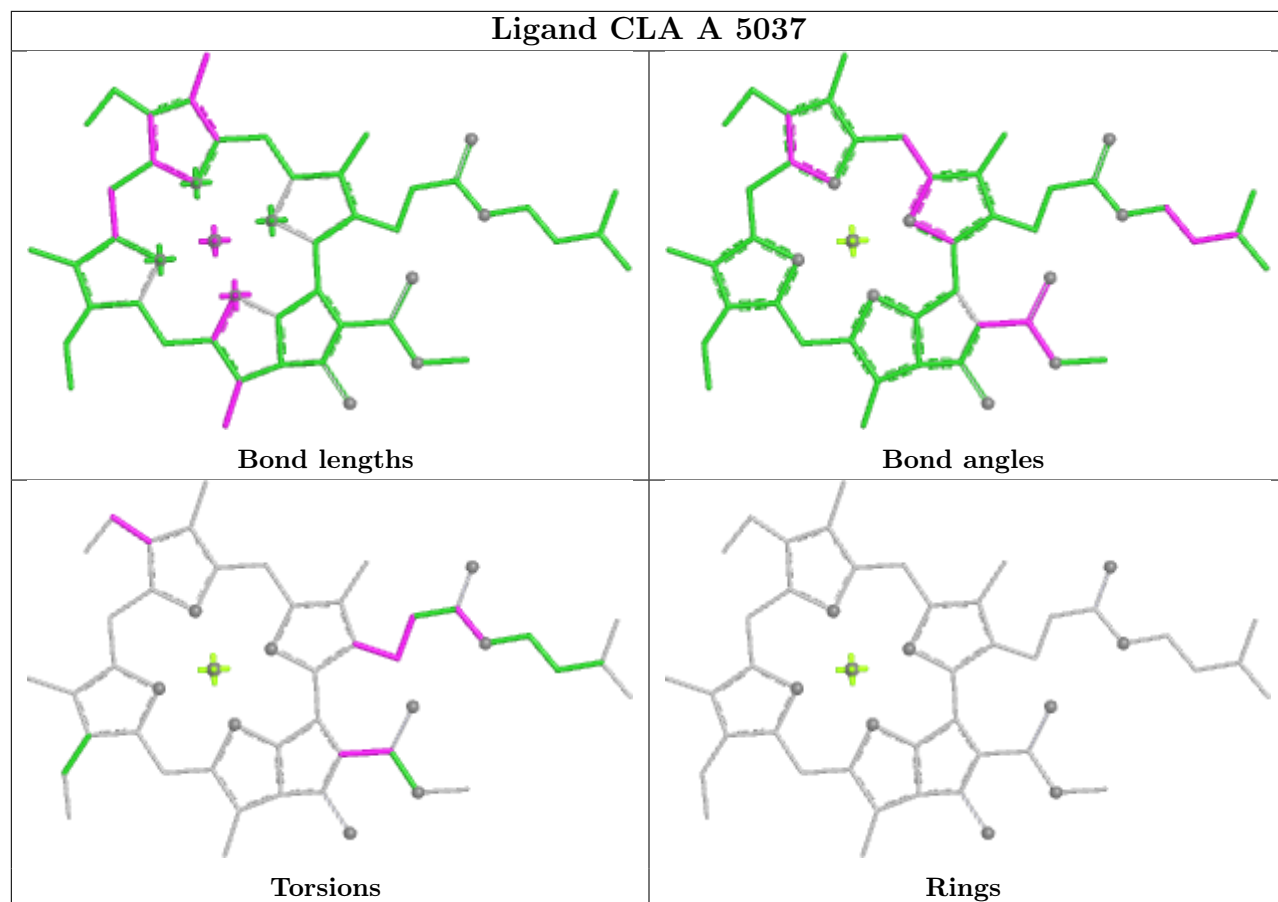


Ligand BCR 1 617

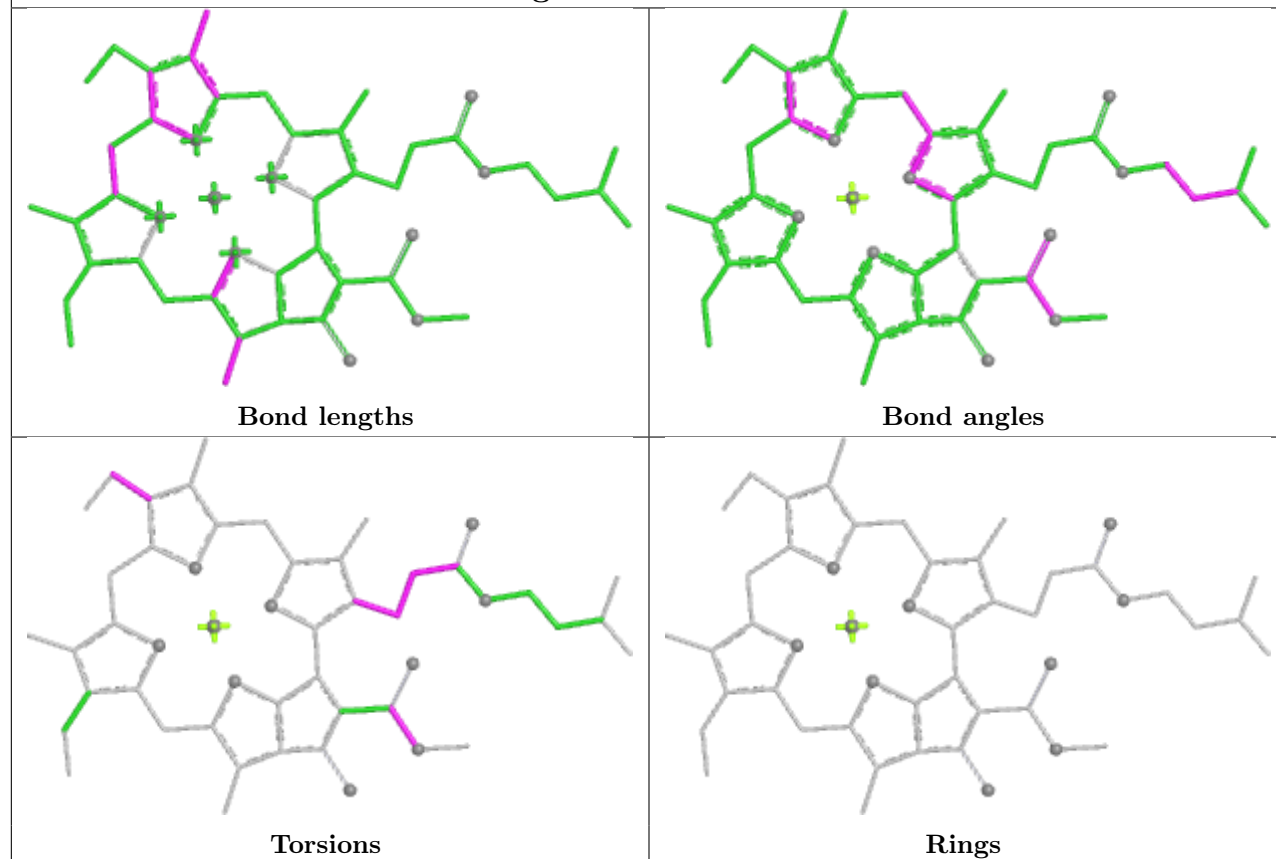


Ligand CLA A 5034

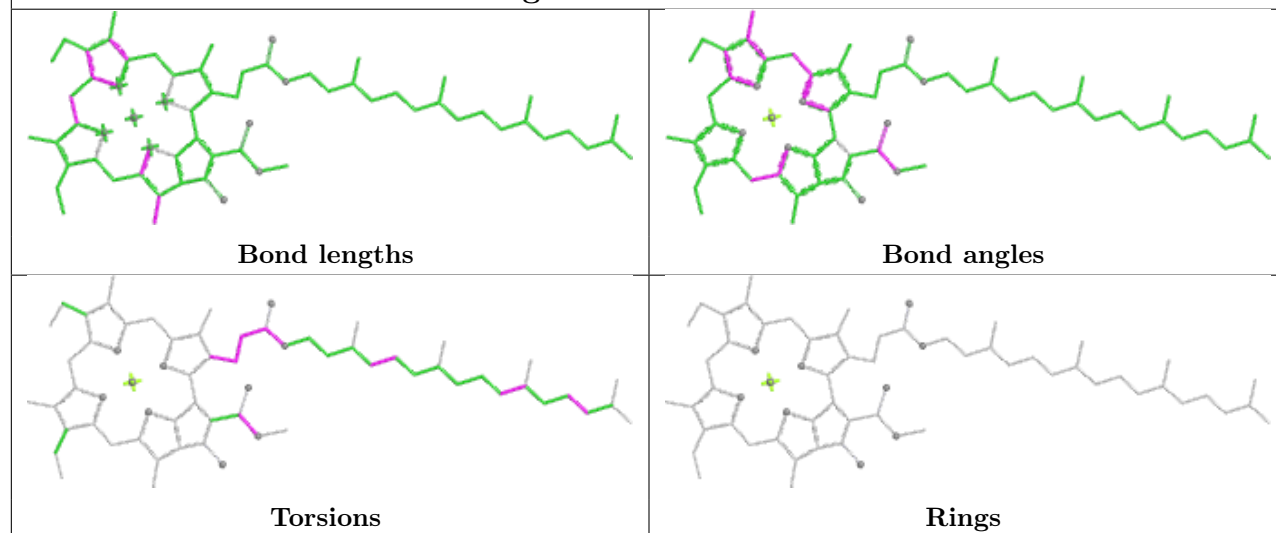




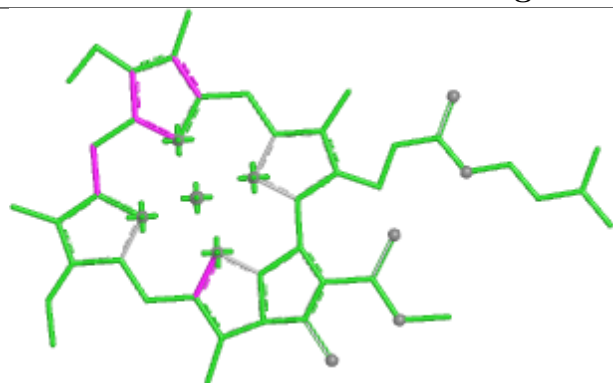
Ligand CLA B 811



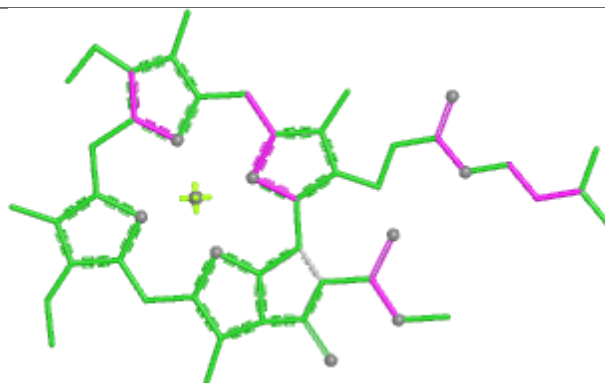
Ligand CLA A 5029



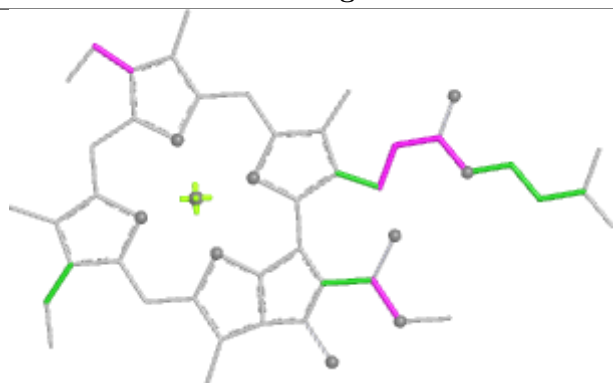
Ligand CLA B 813



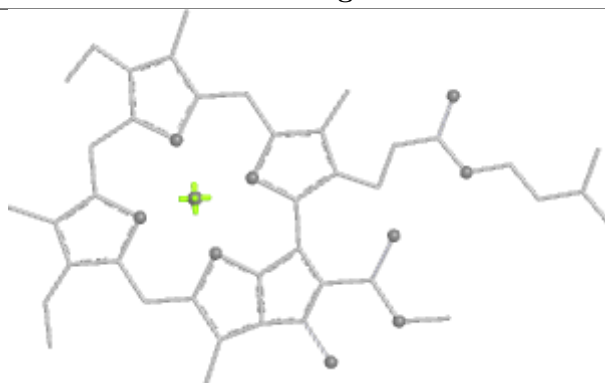
Bond lengths



Bond angles

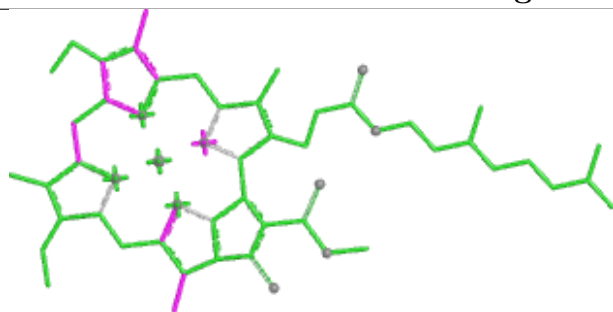


Torsions

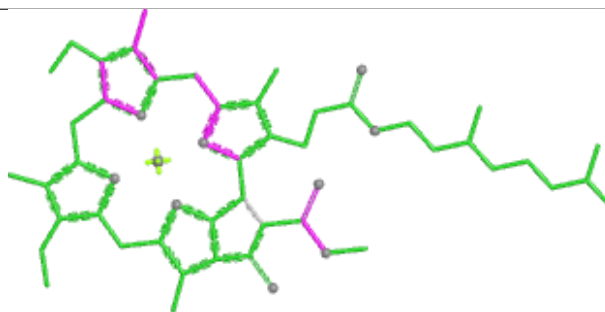


Rings

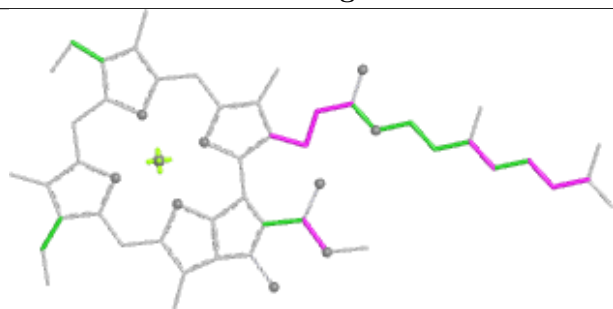
Ligand CLA B 828



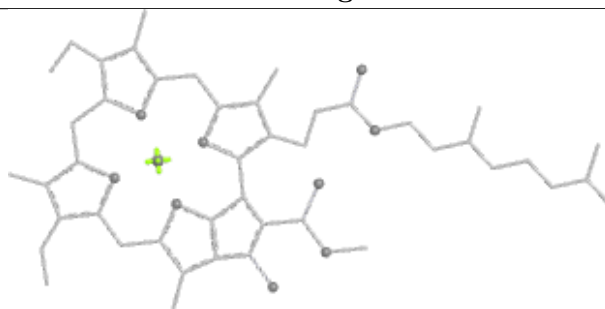
Bond lengths



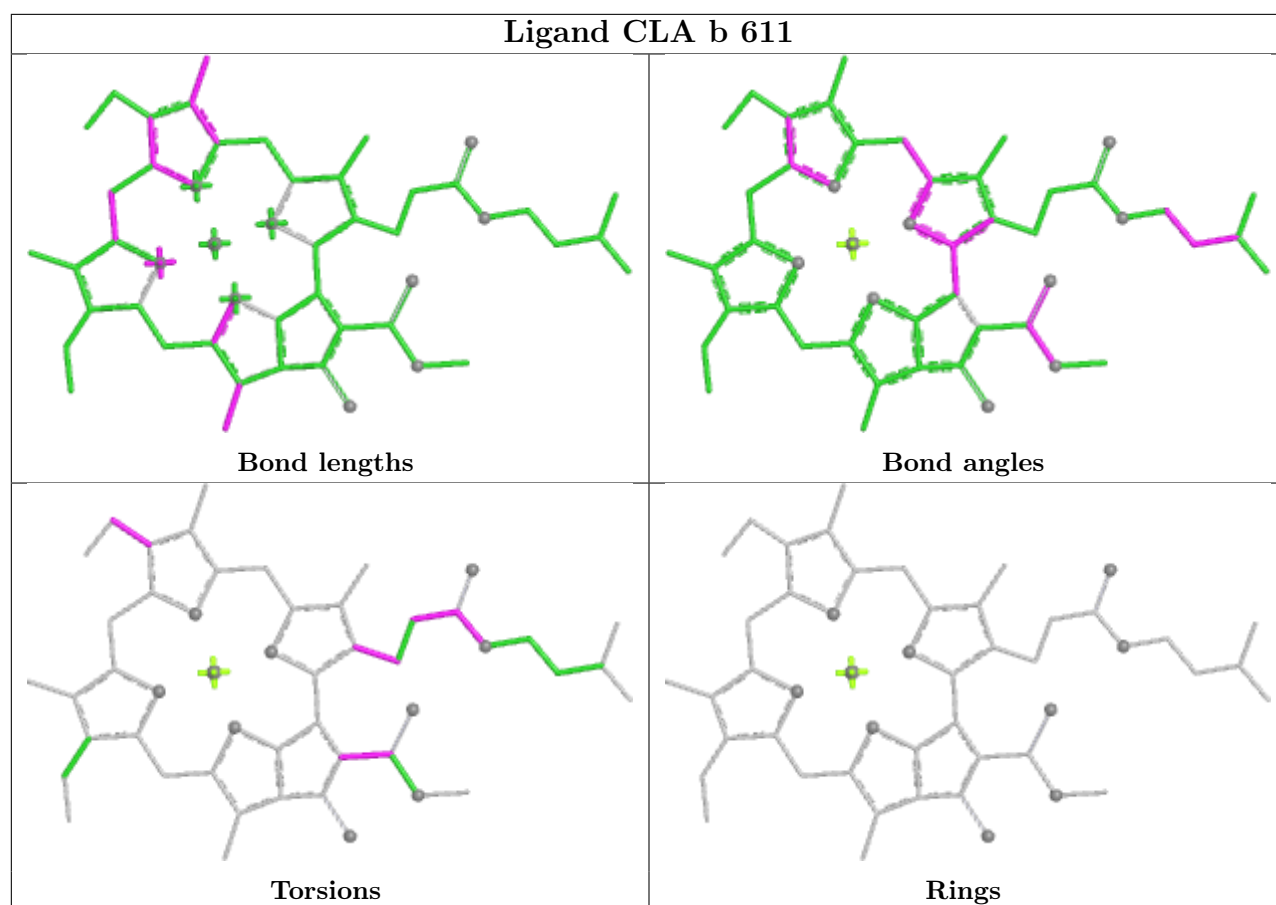
Bond angles



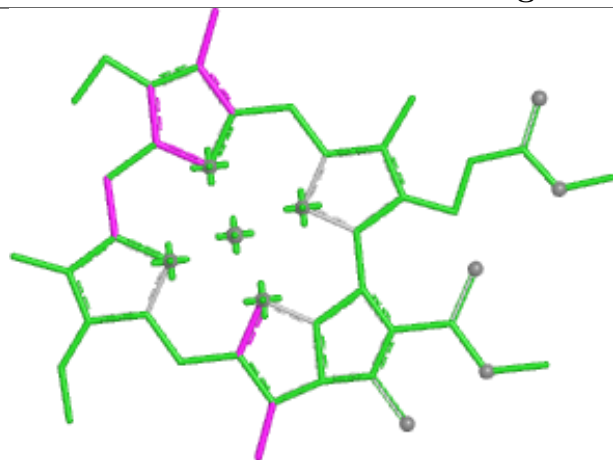
Torsions



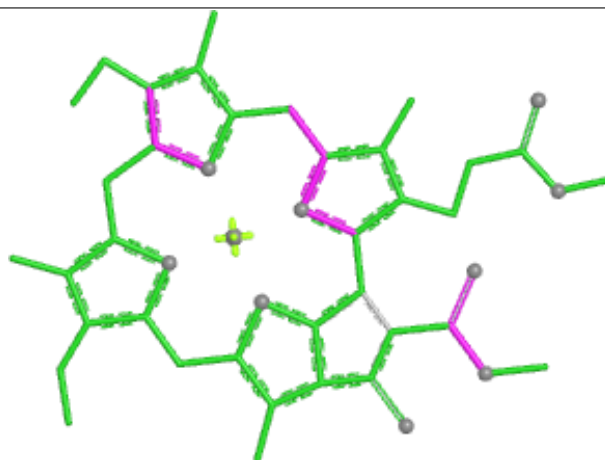
Rings



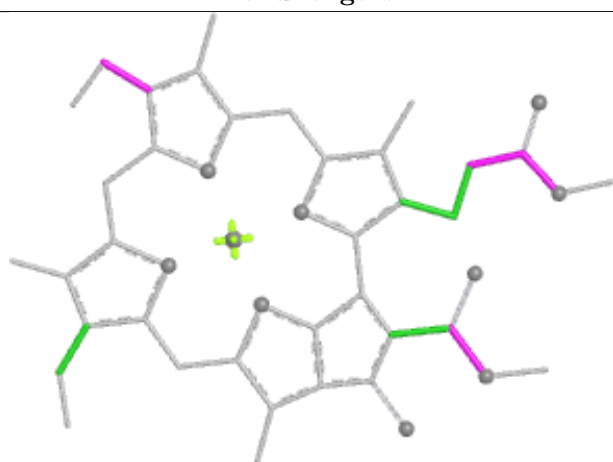
Ligand CLA b 614



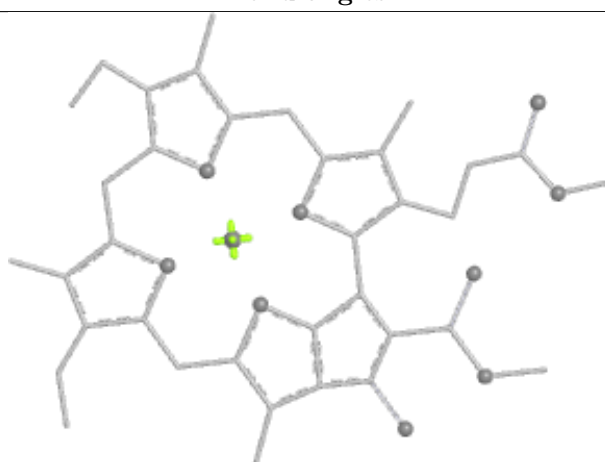
Bond lengths



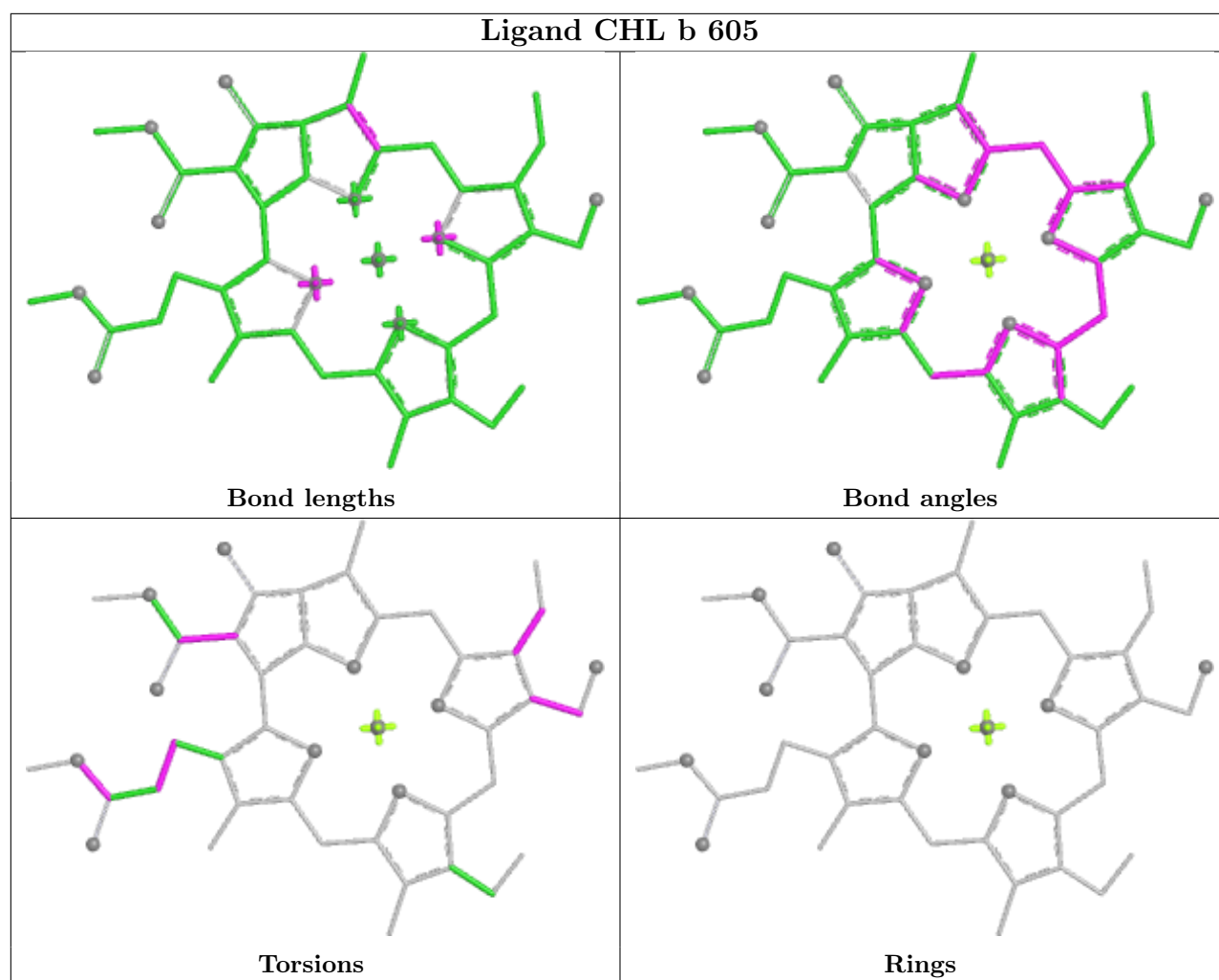
Bond angles



Torsions



Rings



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.

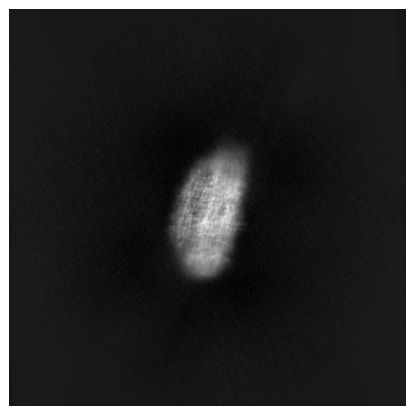
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48264. These allow visual inspection of the internal detail of the map and identification of artifacts.

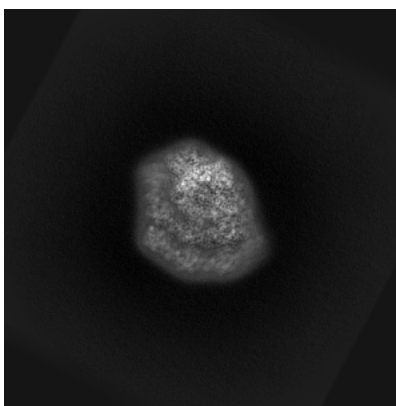
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

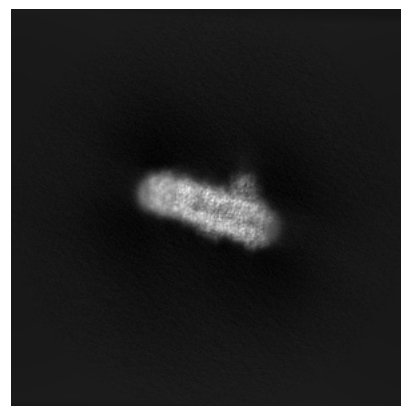
6.1.1 Primary map



X

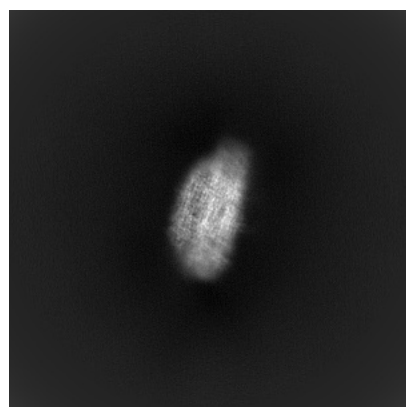


Y

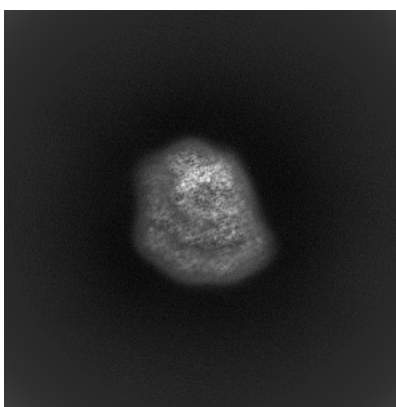


Z

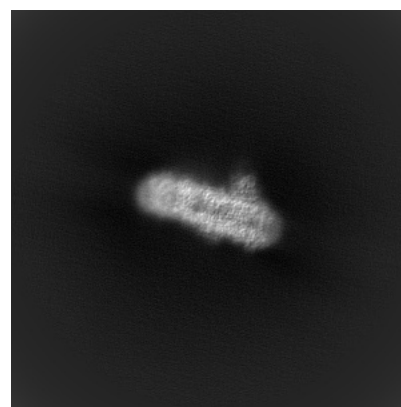
6.1.2 Raw map



X



Y

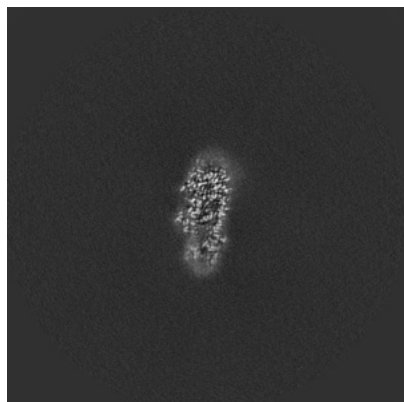


Z

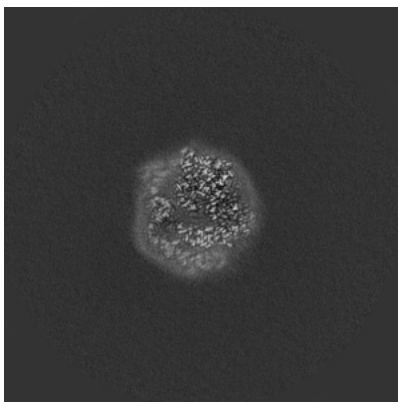
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

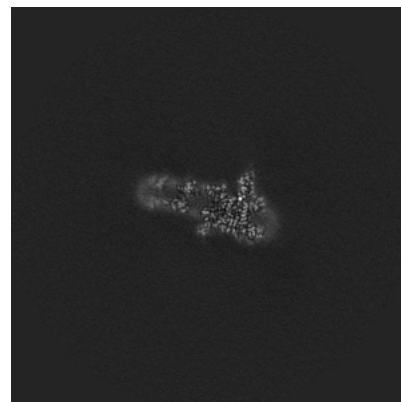
6.2.1 Primary map



X Index: 240

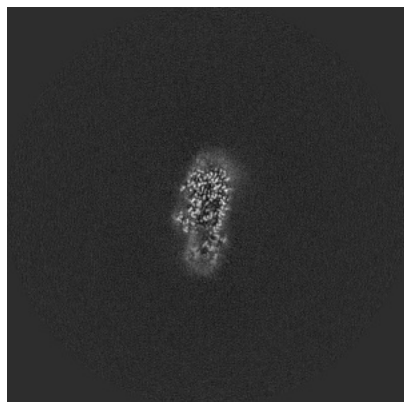


Y Index: 240

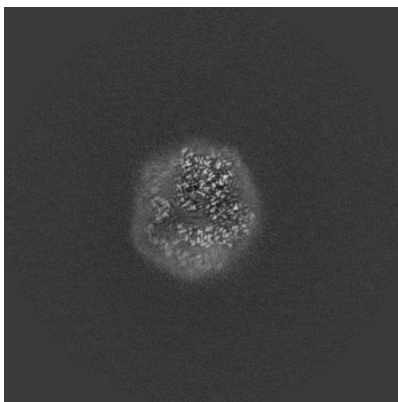


Z Index: 240

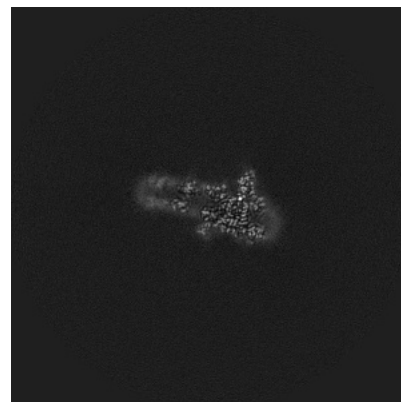
6.2.2 Raw map



X Index: 240



Y Index: 240

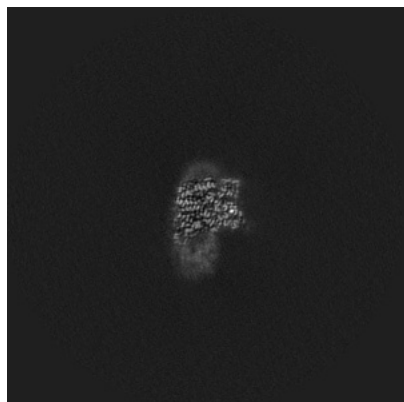


Z Index: 240

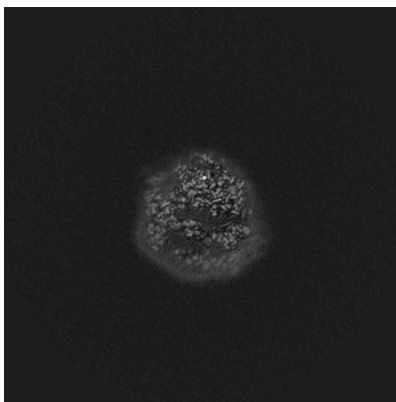
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

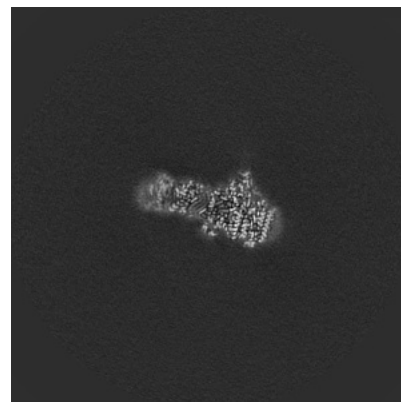
6.3.1 Primary map



X Index: 277

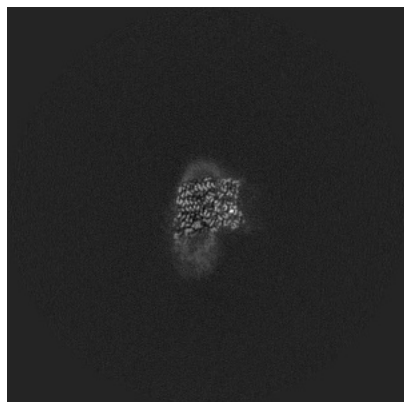


Y Index: 249

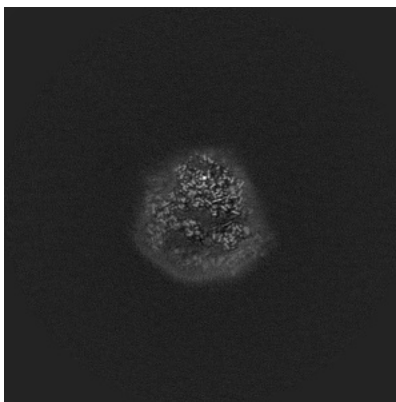


Z Index: 228

6.3.2 Raw map



X Index: 277



Y Index: 249

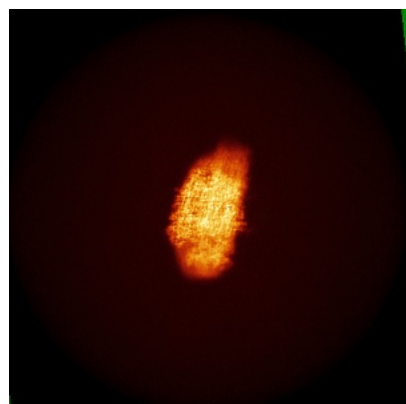


Z Index: 228

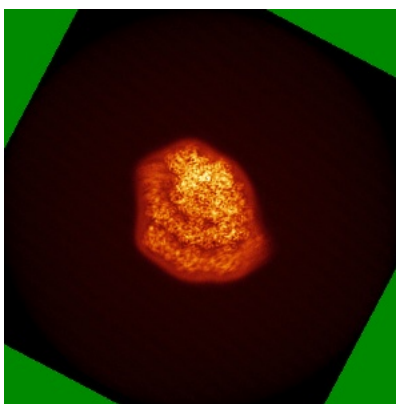
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

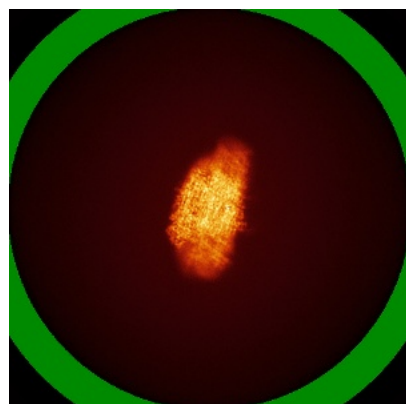


Y

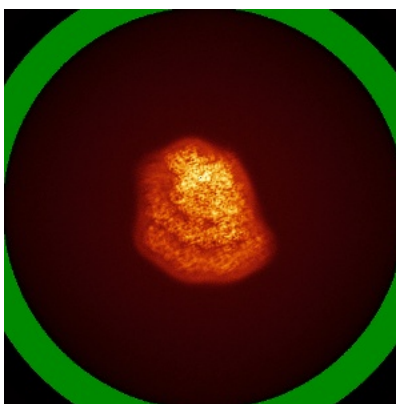


Z

6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

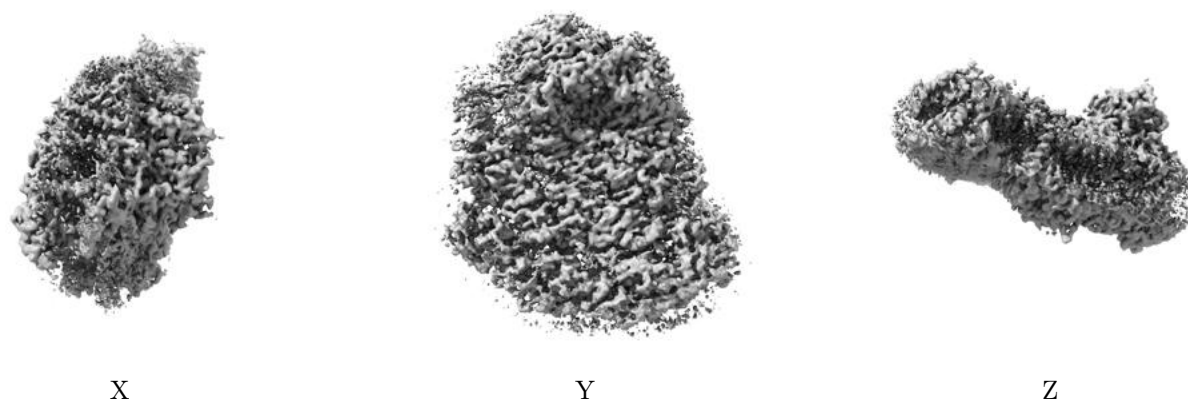
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0151. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

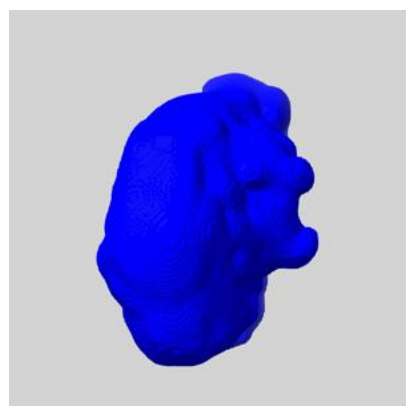
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

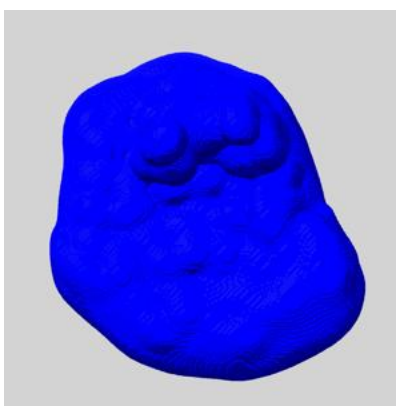
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

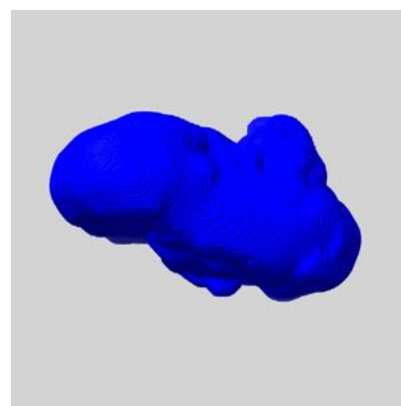
6.6.1 emd_48264_msk_1.map [i](#)



X



Y

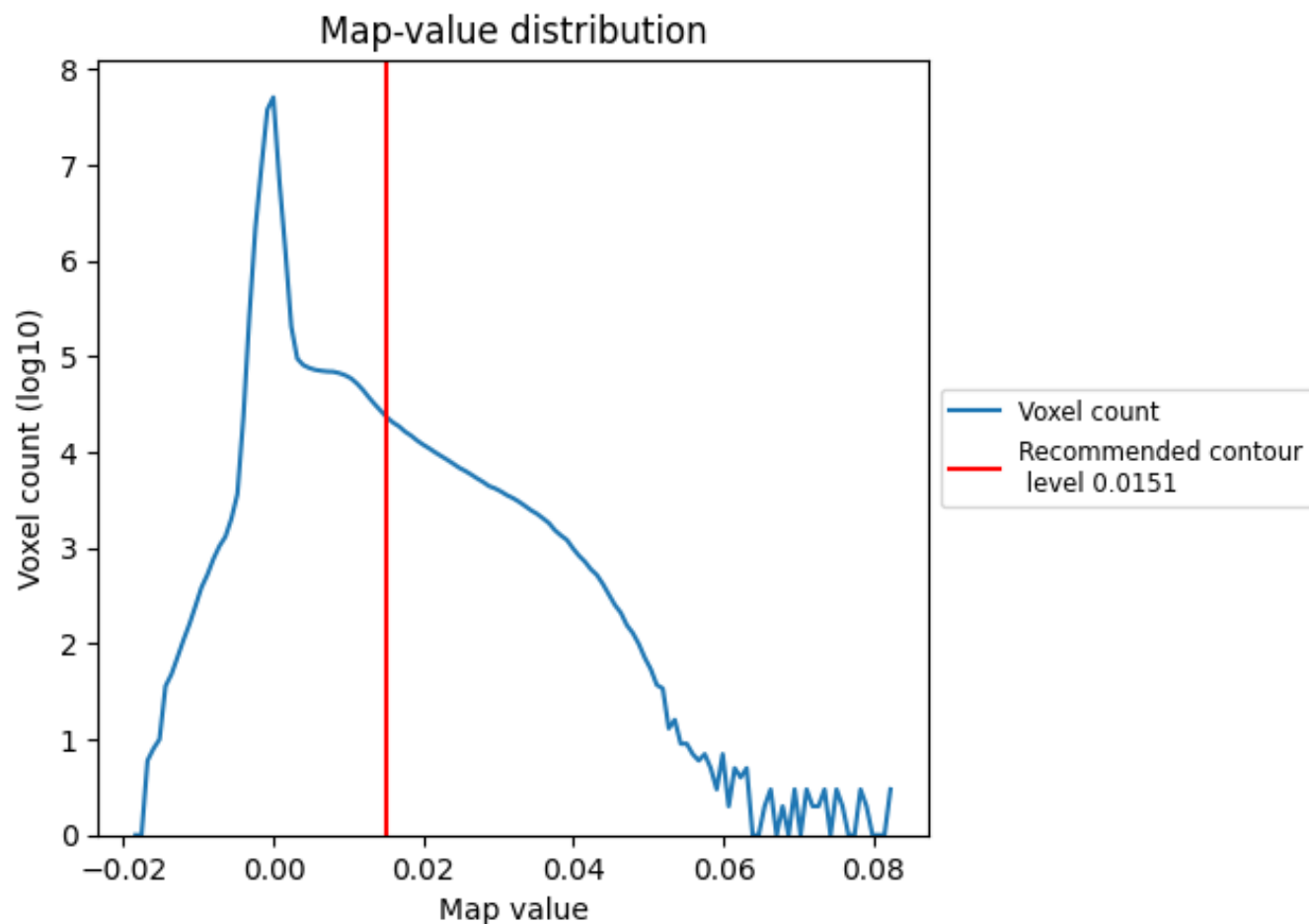


Z

7 Map analysis [i](#)

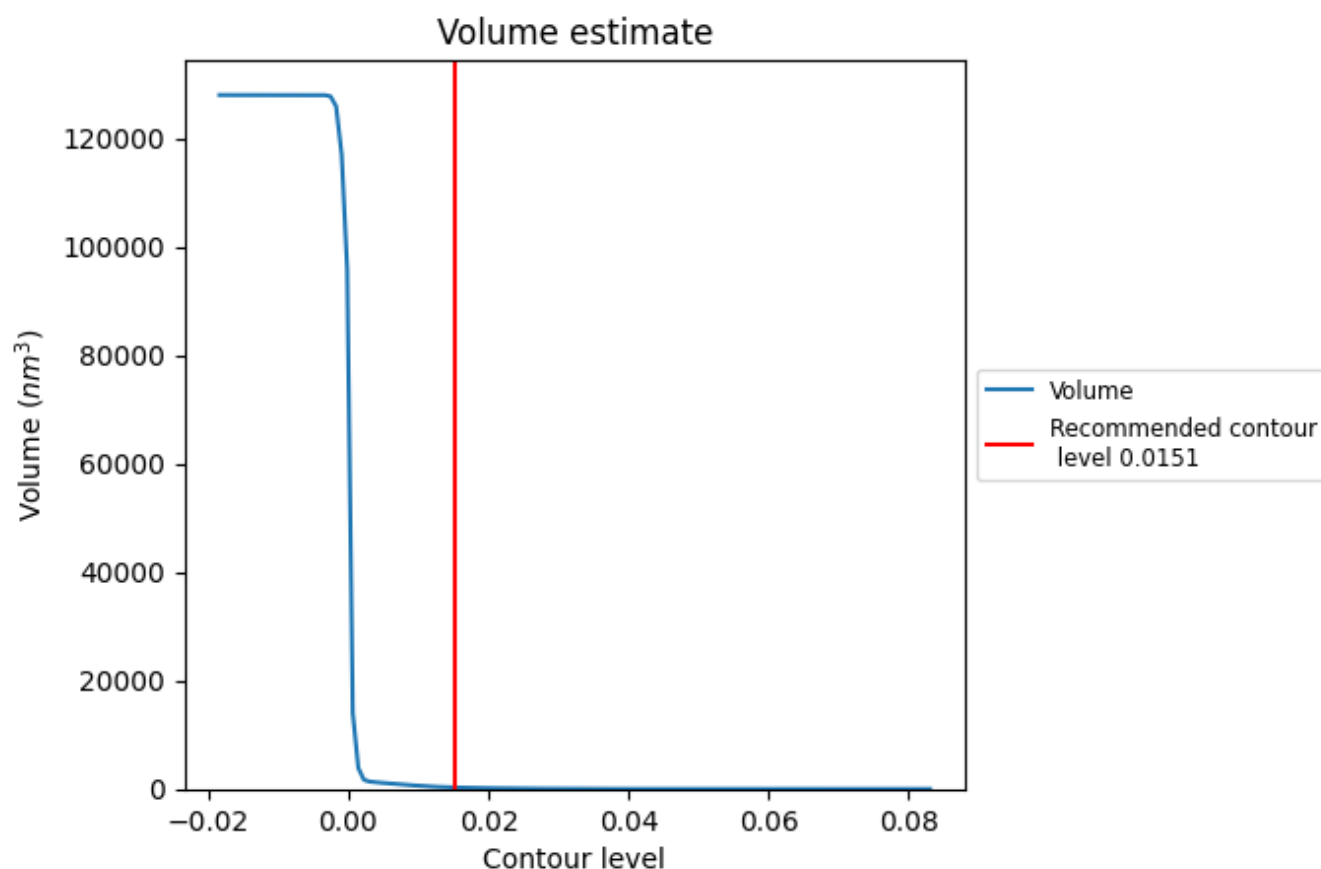
This section contains the results of statistical analysis of the map.

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.

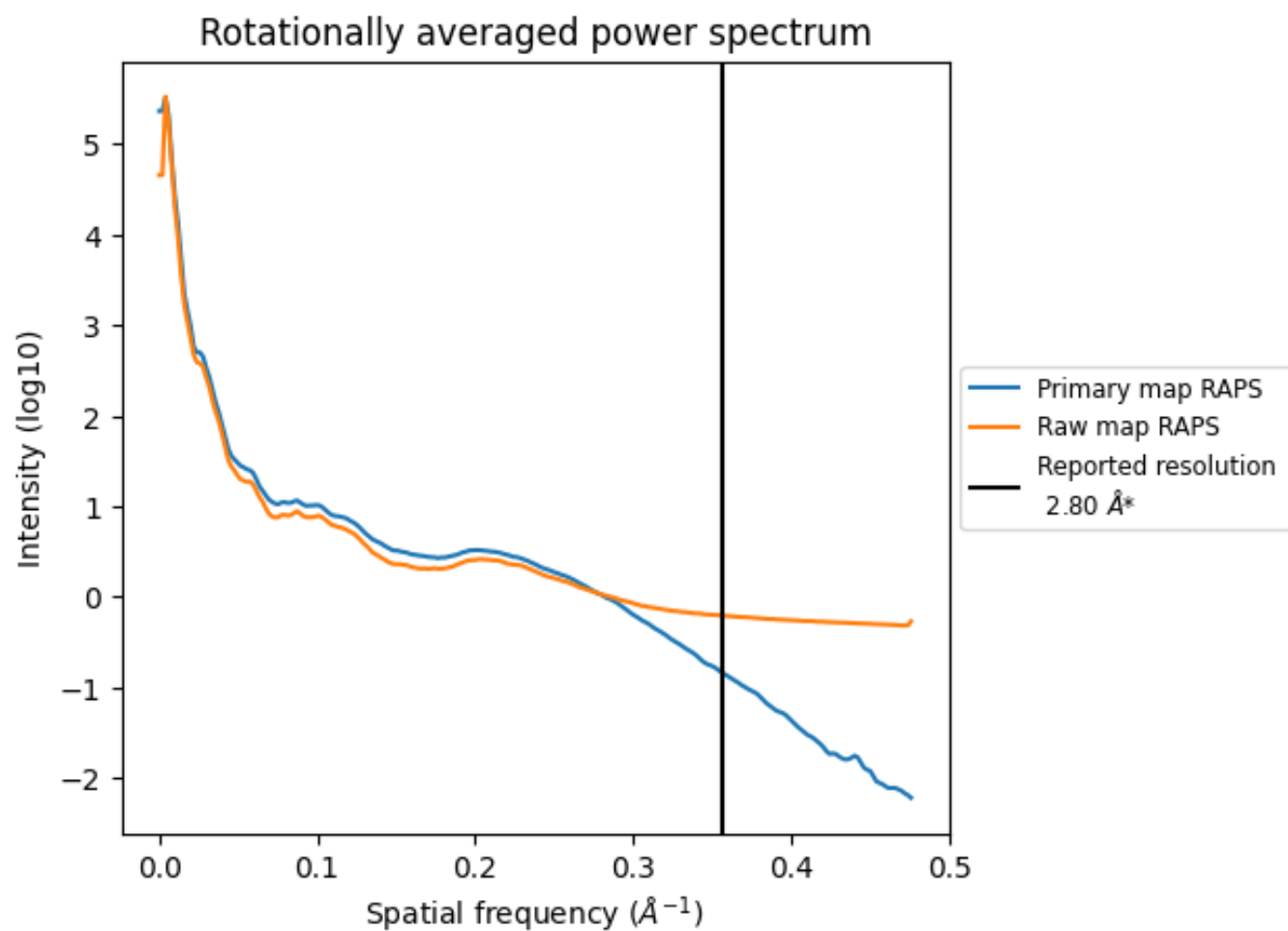
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm^3 ; this corresponds to an approximate mass of 251 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 ⓘ

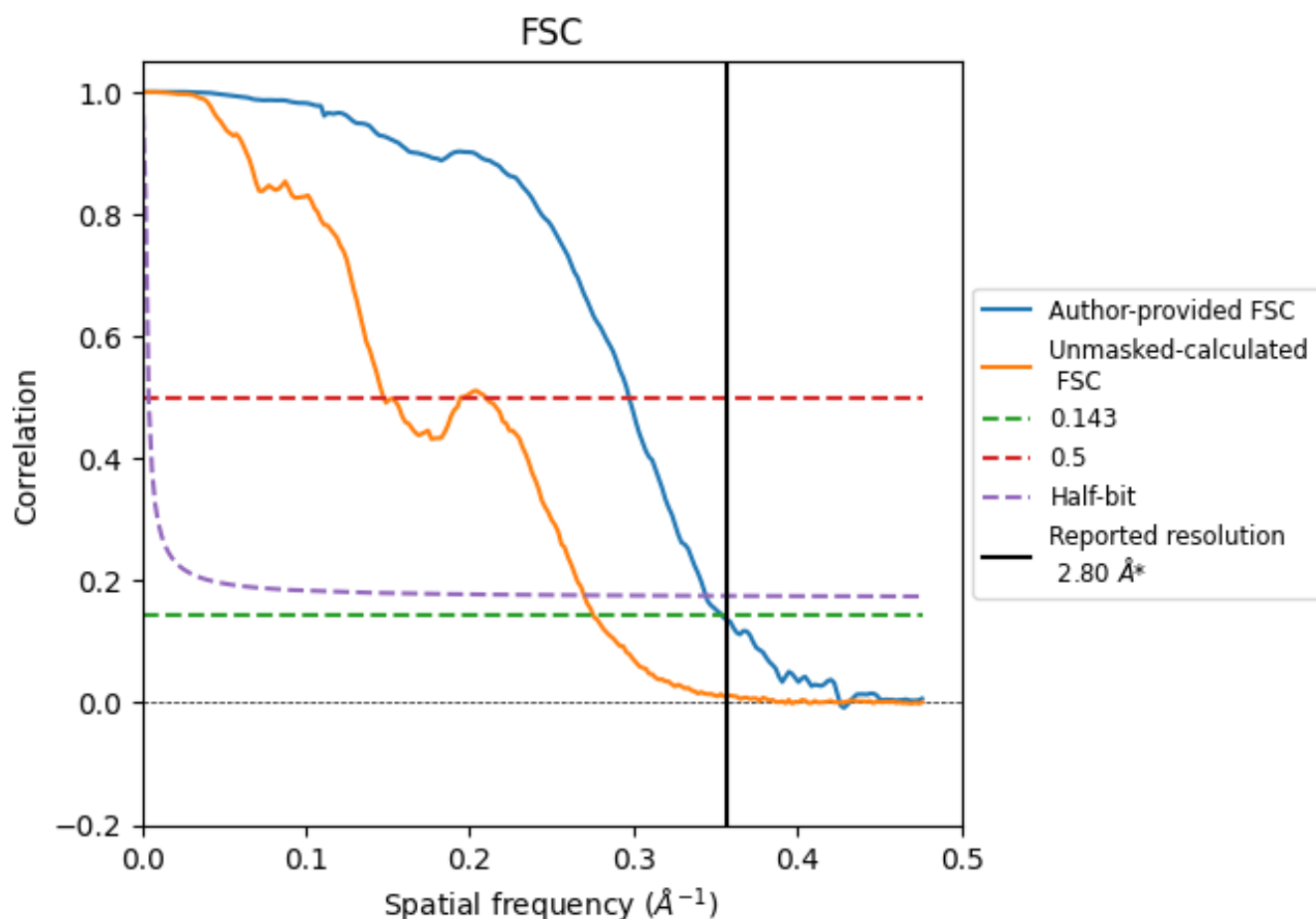


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

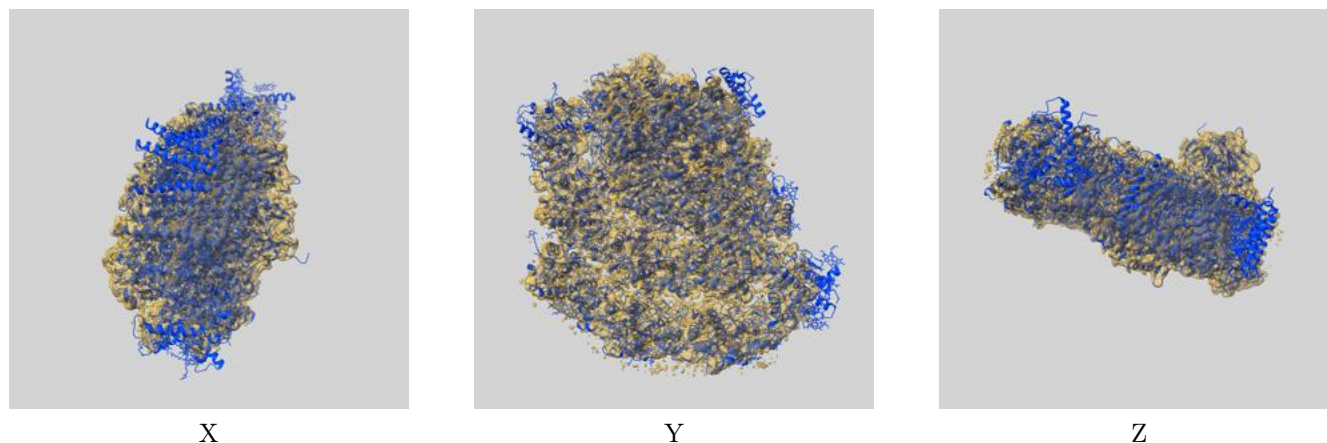
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.36	2.91
Unmasked-calculated*	3.63	6.78	3.71

*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 3.63 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

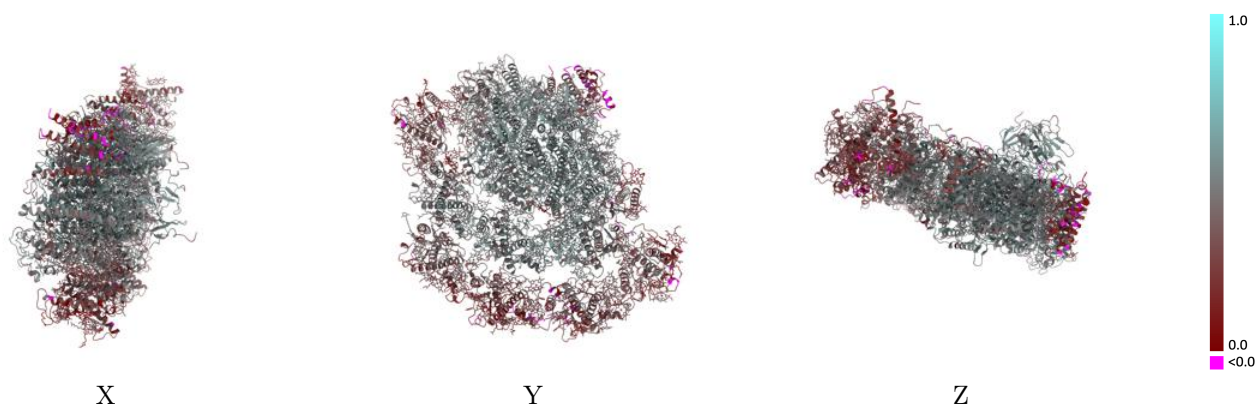
This section contains information regarding the fit between EMDB map EMD-48264 and PDB model 9MGZ. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



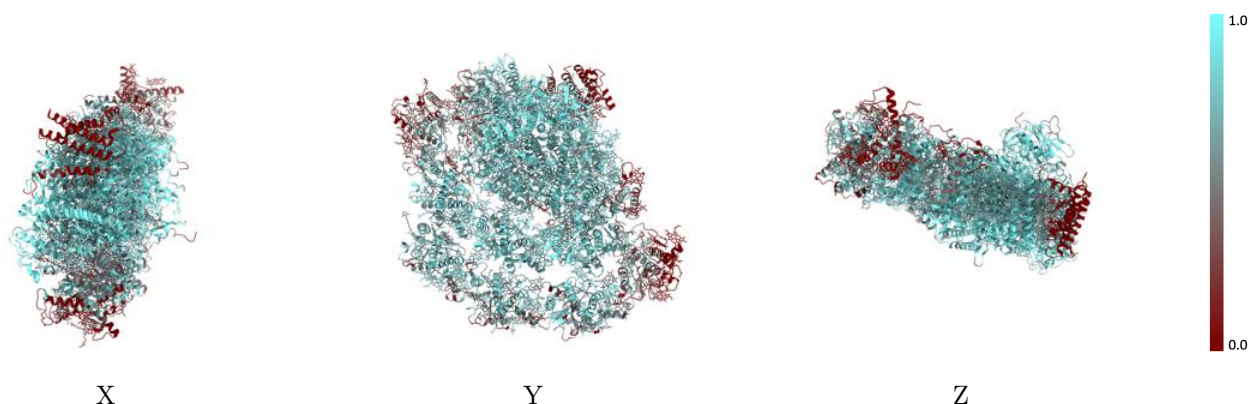
The images above show the 3D surface view of the map at the recommended contour level 0.0151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



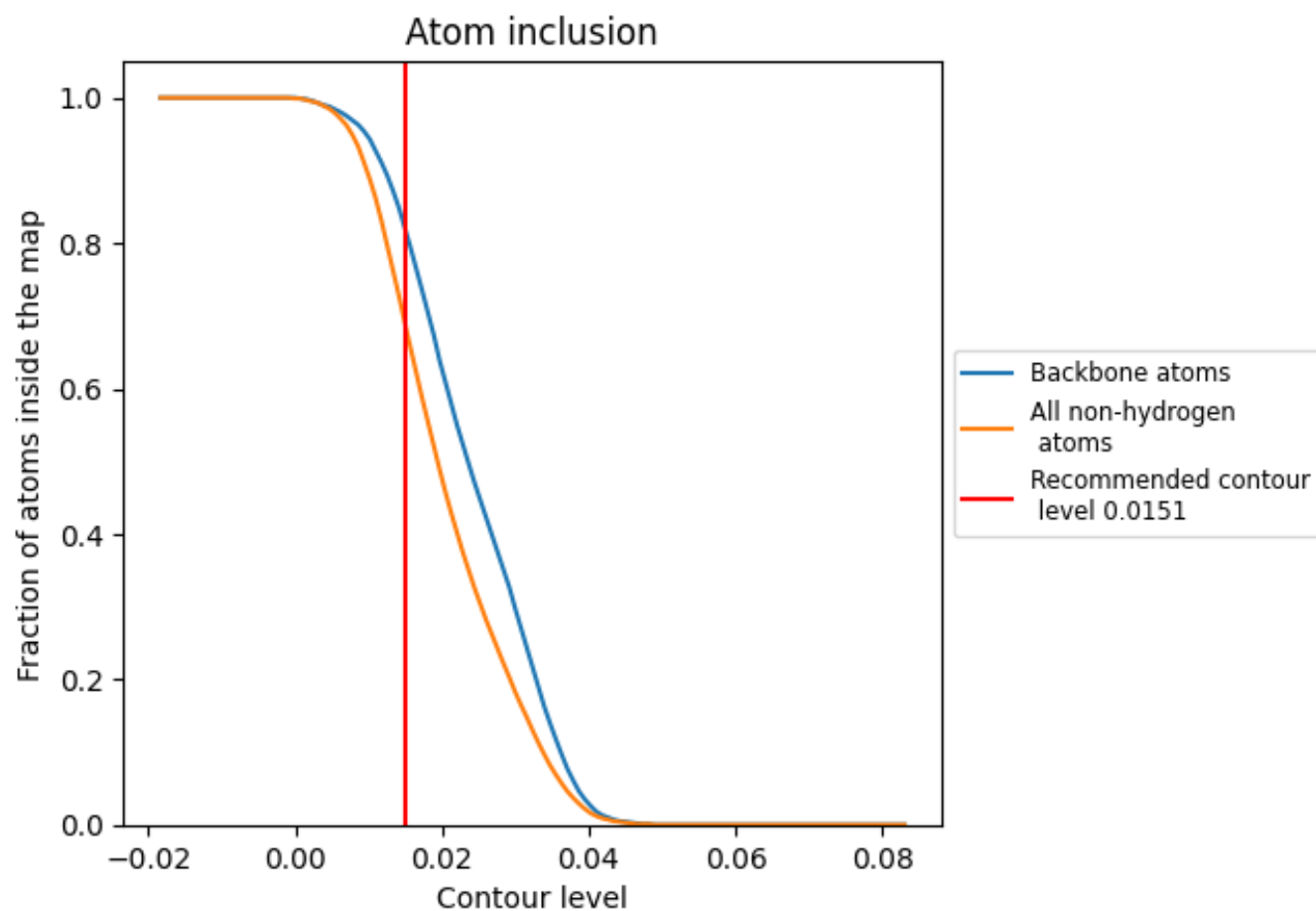
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0151).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.0151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4200
1	0.3730	0.2550
3	0.7700	0.4760
7	0.7960	0.4870
8	0.7280	0.4340
A	0.8310	0.5250
B	0.7930	0.4920
C	0.9220	0.5250
D	0.7140	0.4830
E	0.7810	0.4970
F	0.7440	0.4650
I	0.1160	0.2330
J	0.7660	0.4970
K	0.3510	0.3060
L	0.0170	0.1430
T	0.2980	0.2780
a	0.6690	0.3280
b	0.5940	0.2330
c	0.6130	0.2830

