



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 10:48 AM UTC

PDB ID : 9LUT / pdb_00009lut
EMDB ID : EMD-63404
Title : PSI-LHCI supercomplex binding with 4 Lhcas from M. polymorpha
Authors : Tsai, P.-C.; La Rocca, R.; Shen, J.-R.; Akita, F.
Deposited on : 2025-02-10
Resolution : 1.94 Å(reported)
Based on initial model : 6L35

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:

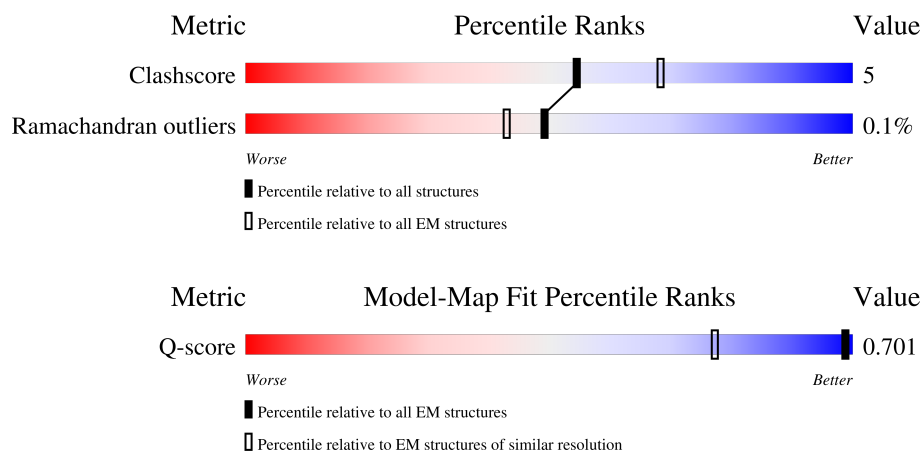
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 1.94 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	-
Q-score	-	25397	1283 (1.45 - 2.44)

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	6	243	
2	2	267	
3	3	279	
4	5	249	
5	A	750	

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	215	
9	E	132	
10	F	246	
11	G	161	
12	I	36	
13	J	42	
14	K	135	
15	M	32	
16	H	142	
17	L	221	

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
18	CHL	2	301	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	307	X	-	-	-
18	CHL	2	314	X	-	-	-
18	CHL	2	320	X	-	-	-
18	CHL	3	306	X	-	-	-
18	CHL	3	314	X	-	-	-
18	CHL	5	304	X	-	-	-
18	CHL	5	305	X	-	-	-
18	CHL	5	306	X	-	-	-
18	CHL	5	313	X	-	-	-
18	CHL	6	301	X	-	-	-
18	CHL	6	306	X	-	-	-
19	CLA	2	302	X	-	-	-
19	CLA	2	303	X	-	-	-
19	CLA	2	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	308	X	-	-	-
19	CLA	2	309	X	-	-	-
19	CLA	2	310	X	-	-	-
19	CLA	2	311	X	-	-	-
19	CLA	2	313	X	-	-	-
19	CLA	3	301	X	-	-	-
19	CLA	3	302	X	-	-	-
19	CLA	3	303	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	5	302	X	-	-	-
19	CLA	5	303	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	6	302	X	-	-	-
19	CLA	6	303	X	-	-	-
19	CLA	6	304	X	-	-	-
19	CLA	6	305	X	-	-	-
19	CLA	6	307	X	-	-	-
19	CLA	6	308	X	-	-	-
19	CLA	6	309	X	-	-	-
19	CLA	6	310	X	-	-	-
19	CLA	6	311	X	-	-	-
19	CLA	6	313	X	-	-	-
19	CLA	6	314	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	B	842	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	F	304	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	G	204	X	-	-	-
19	CLA	J	102	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	L	301	X	-	-	-
19	CLA	L	303	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36239 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	6	194	Total	C	N	O	S	0	0
			1496	977	248	268	3		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	201	Total	C	N	O	S	0	0
			1557	1025	253	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1705	1115	277	307	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	198	Total	C	N	O	S	0	0
			1549	1022	248	275	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5846	3837	988	1004	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		

- 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
			602	368	104	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1112	719	191	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O	S	0	0
			503	319	86	96	2		

- Molecule 10 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	90	Total	C	N	O	S	0	0
			673	432	117	123	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	35	Total	C	N	O	S	0	0
			274	187	36	49	2		

- Molecule 13 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			328	225	48	54	1		

- Molecule 14 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	80	Total	C	N	O	S	0	0
			561	354	97	106	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	30	Total	C	N	O		0	0
			235	155	36	44			

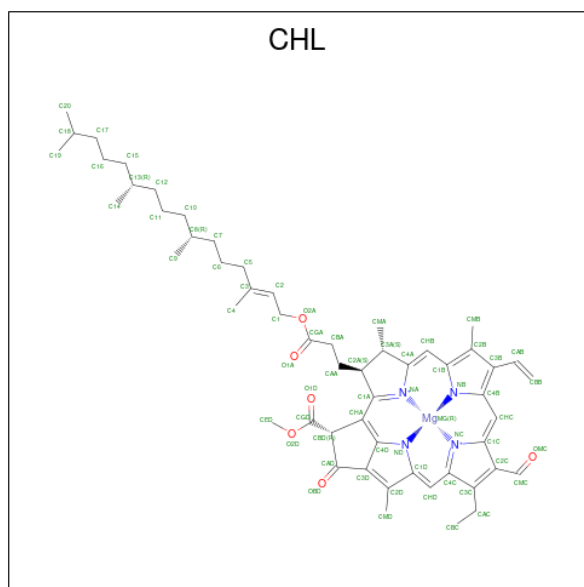
- Molecule 16 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	78	Total	C	N	O	S	0	0
			578	374	99	103	2		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	128	Total	C	N	O	S	0	0
			958	639	150	167	2		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



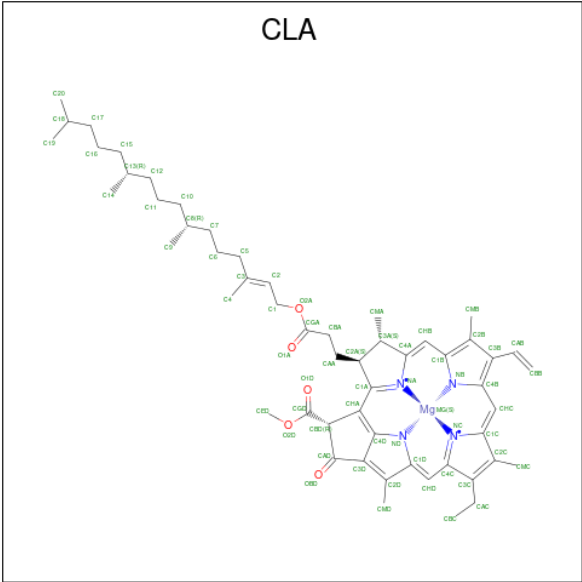
Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 19 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
19	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
19	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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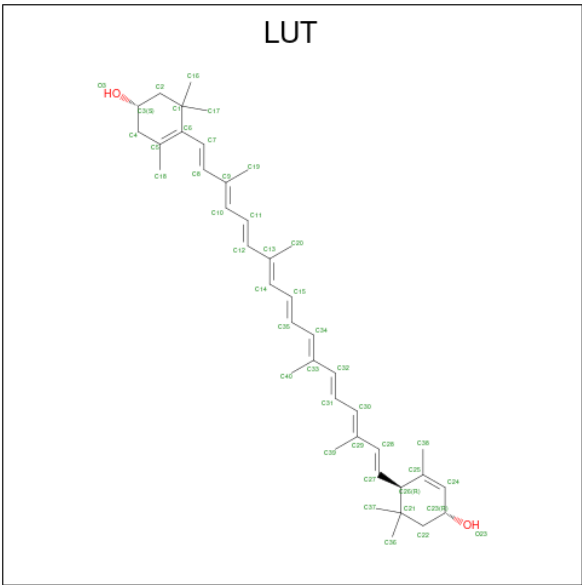
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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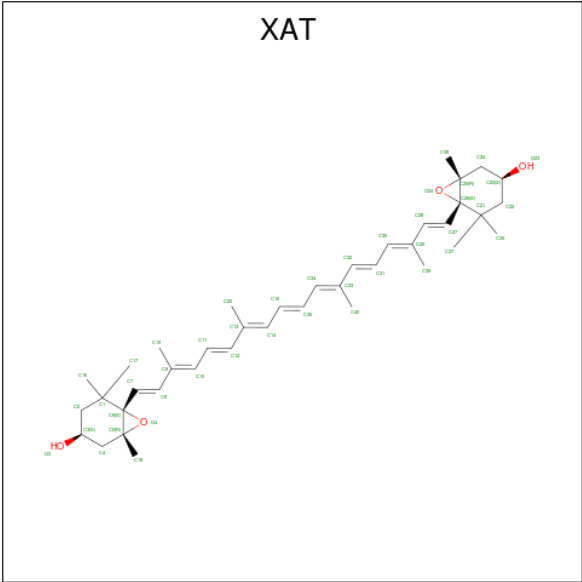
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	K	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 20 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



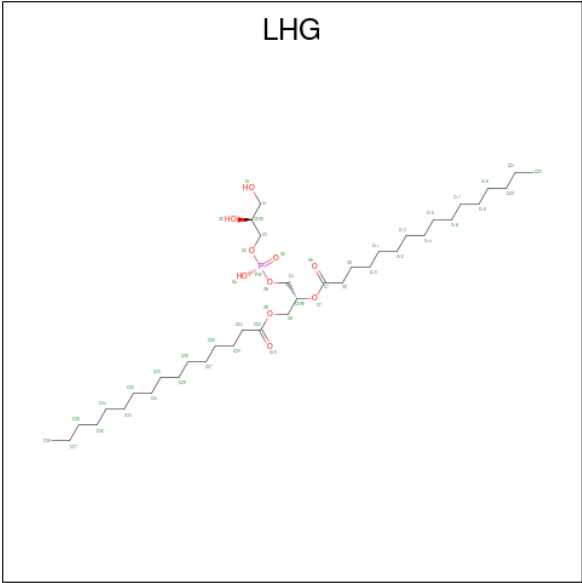
Mol	Chain	Residues	Atoms			AltConf
20	6	1	Total	C	O	0
			42	40	2	
20	6	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	5	1	Total	C	O	0
			42	40	2	
20	5	1	Total	C	O	0
			42	40	2	
20	J	1	Total	C	O	0
			42	40	2	

- Molecule 21 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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	6	1	Total	C	O	0
			44	40	4	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



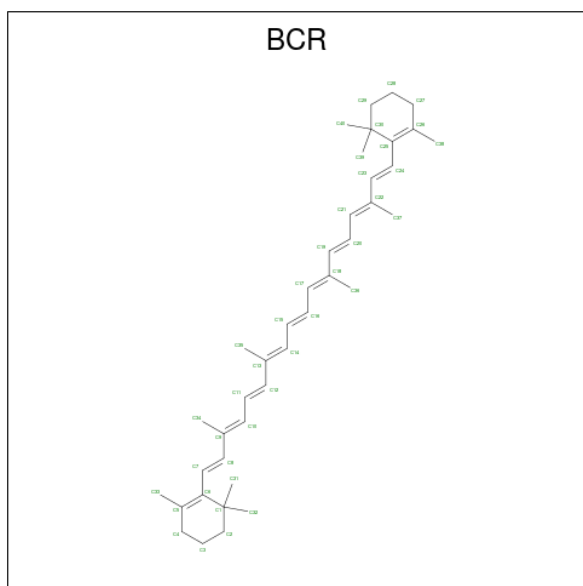
Mol	Chain	Residues	Atoms				AltConf
22	6	1	Total	C	O	P	0
			49	38	10	1	
22	6	1	Total	C	O	P	0
			27	16	10	1	

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Mol	Chain	Residues	Atoms				AltConf
22	2	1	Total	C	O	P	0
			38	27	10	1	
22	5	1	Total	C	O	P	0
			44	33	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	A	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



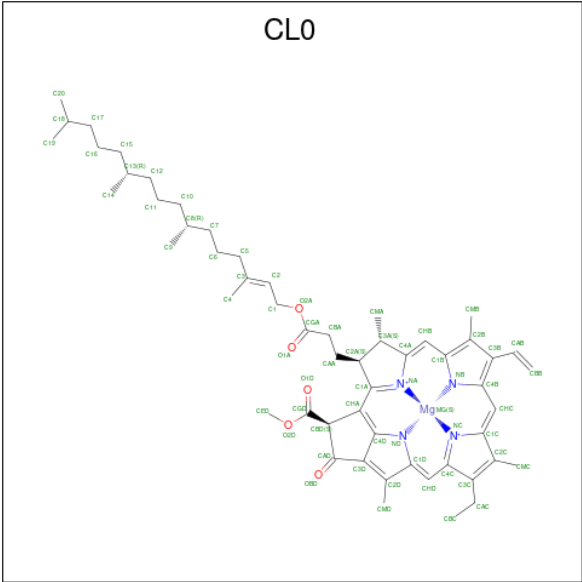
Mol	Chain	Residues	Atoms		AltConf
23	2	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	

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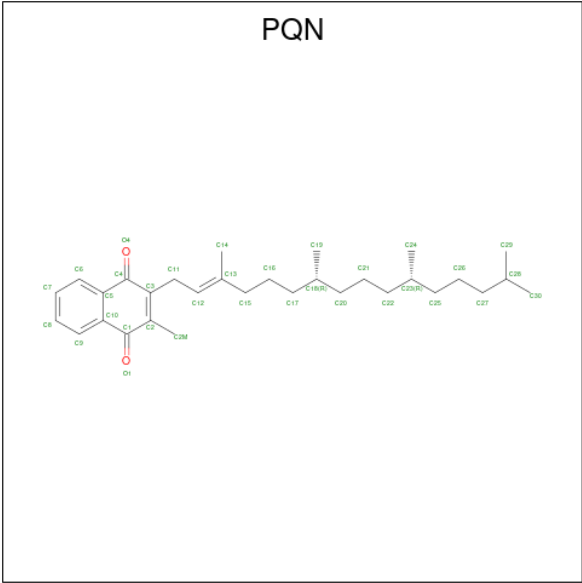
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	M	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



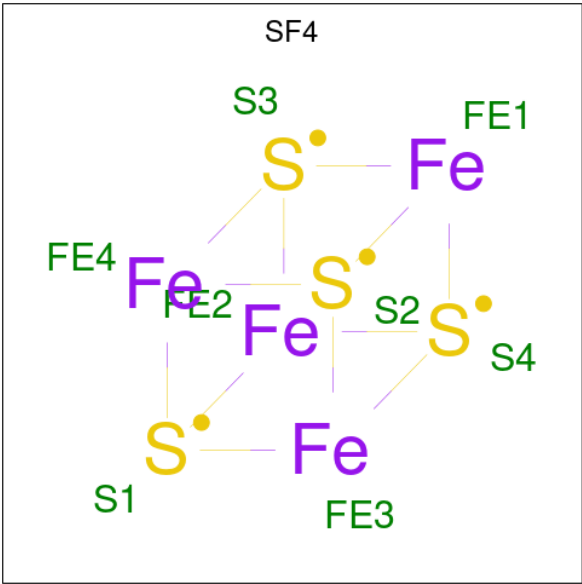
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



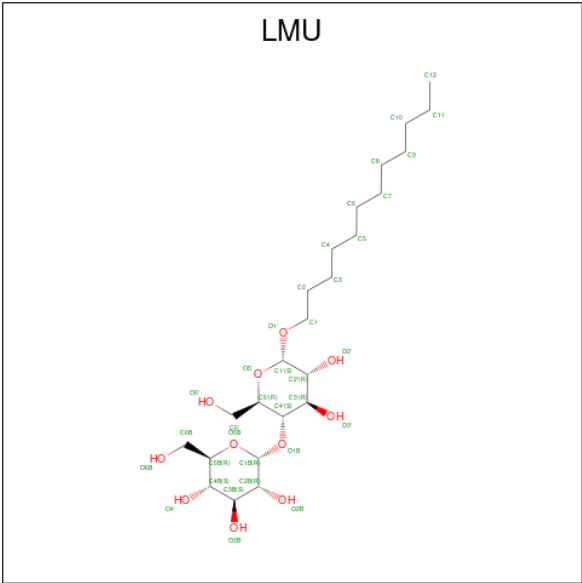
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



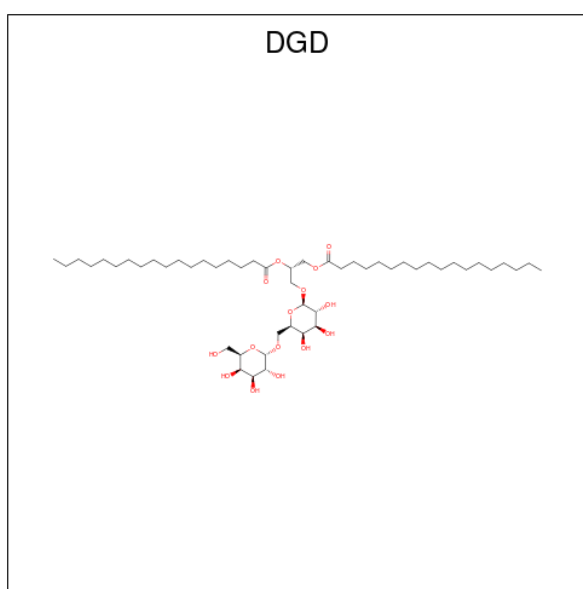
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).



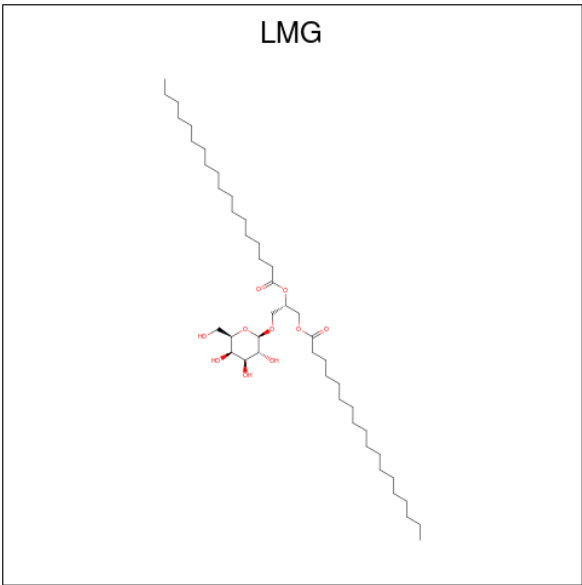
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	G	1	Total	C	O	0
			35	24	11	

- Molecule 28 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
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 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
29	J	1	Total	C	O	0
			30	20	10	
29	J	1	Total	C	O	0
			41	31	10	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	6	14	Total	O	0
			14	14	
30	2	25	Total	O	0
			25	25	
30	3	37	Total	O	0
			37	37	
30	5	17	Total	O	0
			17	17	
30	A	184	Total	O	0
			184	184	
30	B	205	Total	O	0
			205	205	
30	C	45	Total	O	0
			45	45	
30	D	20	Total	O	0
			20	20	
30	E	17	Total	O	0
			17	17	
30	F	20	Total	O	0
			20	20	

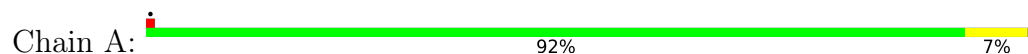
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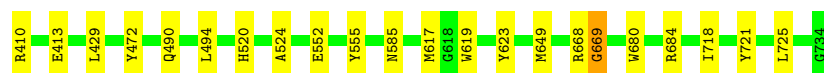
Mol	Chain	Residues	Atoms		AltConf
30	G	2	Total 2	O 2	0
30	I	3	Total 3	O 3	0
30	J	4	Total 4	O 4	0
30	K	2	Total 2	O 2	0
30	M	2	Total 2	O 2	0
30	L	9	Total 9	O 9	0



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center

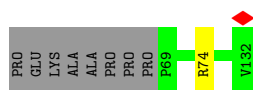


- Molecule 8: Photosystem I reaction center subunit II, chloroplastic



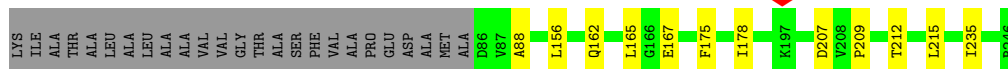
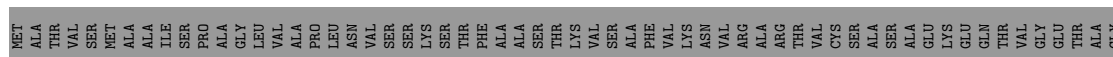
- Molecule 9: Photosystem I reaction centre subunit IV





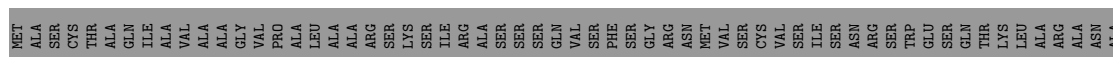
- Molecule 10: Photosystem I reaction center subunit III

Chain F: 61% 5% 35%



- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G: 55% 0% 44%



- Molecule 12: Photosystem I reaction center subunit VIII

Chain I: 89% 0% 8%



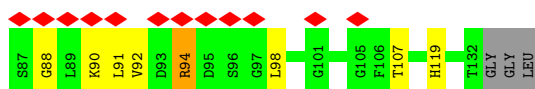
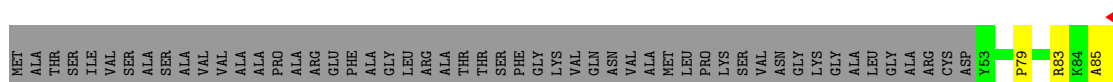
- Molecule 13: Photosystem I reaction center subunit IX

Chain J: 93% 5% 0%

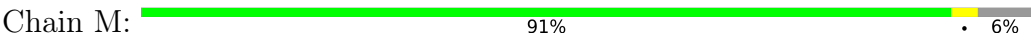


- Molecule 14: PSI-K

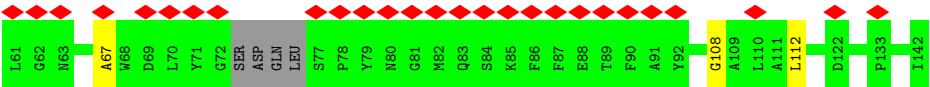
Chain K: 10% 50% 8% 41%



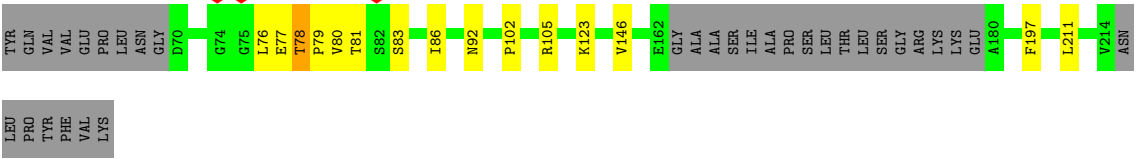
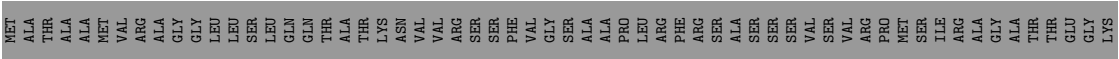
- Molecule 15: Photosystem I reaction center subunit XII



• Molecule 16: Photosystem I reaction center subunit VI, chloroplastic



• Molecule 17: PSI subunit V



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157685	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.674	Depositor
Minimum map value	-0.321	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	363.5, 363.5, 363.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

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

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	6	0.25	0/1546	0.48	0/2112
2	2	0.22	0/1612	0.40	0/2203
3	3	0.24	0/1755	0.46	0/2379
4	5	0.23	0/1600	0.45	0/2185
5	A	0.28	0/6044	0.50	0/8247
6	B	0.31	0/6066	0.56	0/8277
7	C	0.36	0/612	0.58	0/829
8	D	0.20	0/1141	0.47	0/1538
9	E	0.28	0/516	0.40	0/701
10	F	0.22	0/1275	0.49	0/1725
11	G	0.19	0/686	0.42	0/931
12	I	0.30	0/281	0.64	0/384
13	J	0.18	0/338	0.42	0/462
14	K	0.42	0/567	0.59	0/766
15	M	0.21	0/236	0.41	0/317
16	H	0.20	0/591	0.45	0/796
17	L	0.32	0/987	0.55	0/1348
All	All	0.28	0/25853	0.50	0/35200

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1
9	E	0	1
14	K	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	172	HIS	Peptide
9	E	74	ARG	Sidechain
14	K	94	ARG	Sidechain

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	6	1496	0	1474	11	0
2	2	1557	0	1510	9	0
3	3	1705	0	1672	14	0
4	5	1549	0	1528	16	0
5	A	5846	0	5712	39	0
6	B	5854	0	5632	36	0
7	C	602	0	575	1	0
8	D	1112	0	1128	6	0
9	E	503	0	490	0	0
10	F	1248	0	1291	9	0
11	G	673	0	678	1	0
12	I	274	0	285	2	0
13	J	328	0	339	2	0
14	K	561	0	581	11	0
15	M	235	0	259	1	0
16	H	578	0	590	2	0
17	L	958	0	956	11	0
18	2	302	0	234	11	0
18	3	112	0	101	4	0
18	5	178	0	120	1	0
18	6	97	0	68	6	0
19	2	482	0	433	12	0
19	3	618	0	535	15	0
19	5	549	0	501	11	0
19	6	626	0	548	18	0
19	A	2443	0	2417	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	2485	0	2516	57	0
19	F	146	0	121	4	0
19	G	90	0	66	1	0
19	J	42	0	31	1	0
19	K	140	0	104	1	0
19	L	147	0	123	4	0
20	2	126	0	168	8	0
20	3	84	0	112	11	0
20	5	84	0	112	7	0
20	6	84	0	112	4	0
20	J	42	0	56	4	0
21	6	44	0	56	3	0
22	2	38	0	46	0	0
22	5	44	0	58	5	0
22	6	76	0	98	6	0
22	A	83	0	112	3	0
23	2	40	0	56	2	0
23	3	40	0	56	2	0
23	5	40	0	56	2	0
23	A	200	0	280	17	0
23	B	200	0	280	13	0
23	F	80	0	112	6	0
23	G	80	0	112	6	0
23	I	40	0	56	2	0
23	J	40	0	56	6	0
23	K	80	0	112	4	0
23	L	80	0	112	4	0
23	M	40	0	56	3	0
24	A	65	0	72	2	0
25	A	33	0	46	2	0
25	B	33	0	46	1	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	A	35	0	46	0	0
27	B	70	0	92	4	0
27	G	35	0	46	2	0
28	B	66	0	96	4	0
29	J	71	0	85	3	0
30	2	25	0	0	0	0
30	3	37	0	0	0	0
30	5	17	0	0	0	0
30	6	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	184	0	0	0	0
30	B	205	0	0	2	0
30	C	45	0	0	0	0
30	D	20	0	0	0	0
30	E	17	0	0	0	0
30	F	20	0	0	0	0
30	G	2	0	0	0	0
30	I	3	0	0	0	0
30	J	4	0	0	0	0
30	K	2	0	0	0	0
30	L	9	0	0	0	0
30	M	2	0	0	0	0
All	All	36239	0	35421	364	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 5.

All (364) 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)
3:3:242:VAL:HG11	20:3:316:LUT:H32	1.69	0.74
3:3:191:PHE:HE2	18:3:306:CHL:HBB2	1.56	0.71
19:A:824:CLA:H2	14:K:88:GLY:HA3	1.73	0.71
19:A:811:CLA:HBB2	19:A:814:CLA:HMA3	1.75	0.68
1:6:98:VAL:HG11	20:6:315:LUT:H12	1.76	0.68
2:2:229:VAL:HG11	20:2:316:LUT:H32	1.76	0.66
19:B:812:CLA:HBA2	27:G:202:LMU:H41	1.79	0.63
4:5:231:LEU:HB2	20:5:315:LUT:H22	1.81	0.62
5:A:151:THR:H	5:A:155:GLN:HE22	1.46	0.62
15:M:16:VAL:HG23	23:M:101:BCR:H14C	1.82	0.62
5:A:214:GLN:HA	5:A:218:SER:HB2	1.81	0.61
1:6:237:ILE:HG22	1:6:238:ILE:HG13	1.81	0.61
19:A:837:CLA:HBA2	19:K:201:CLA:H2	1.83	0.61
13:J:12:PRO:HB2	20:J:101:LUT:H163	1.81	0.61
18:2:301:CHL:H71	18:3:314:CHL:H72	1.81	0.61
1:6:100:GLY:O	30:6:401:HOH:O	2.16	0.61
19:B:812:CLA:HBB2	19:B:814:CLA:HMA3	1.82	0.61
19:2:302:CLA:H51	19:2:303:CLA:H3A	1.83	0.60
19:A:822:CLA:H102	19:A:825:CLA:H71	1.83	0.60
19:A:821:CLA:HBB2	23:A:848:BCR:H402	1.84	0.60
14:K:86:LEU:HB2	14:K:90:LYS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:159:PRO:HA	6:B:162:LYS:HE2	1.83	0.59
17:L:92:ASN:HB3	19:L:301:CLA:HAC1	1.84	0.59
23:G:201:BCR:H362	23:G:205:BCR:H312	1.85	0.59
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.84	0.58
12:I:32:GLN:HE21	12:I:35:ILE:HG22	1.68	0.58
3:3:92:GLY:HA3	5:A:13:VAL:HA	1.85	0.58
5:A:505:LEU:HD21	5:A:513:ILE:HG13	1.85	0.57
27:B:850:LMU:H4'	27:G:202:LMU:H6D	1.86	0.57
14:K:92:VAL:HG13	14:K:94:ARG:HE	1.69	0.57
18:6:301:CHL:HBA1	19:5:314:CLA:HED1	1.87	0.56
6:B:191:THR:HG21	6:B:278:LEU:HB2	1.87	0.56
19:B:832:CLA:HBA1	10:F:235:ILE:HD12	1.88	0.56
19:6:312:CLA:H112	22:6:317:LHG:H301	1.87	0.55
8:D:100:GLN:HG2	16:H:67:ALA:HB2	1.89	0.55
5:A:398:LEU:HD21	19:A:808:CLA:H142	1.88	0.55
5:A:279:LEU:HB2	5:A:513:ILE:HD12	1.89	0.55
6:B:585:ASN:HB2	19:B:802:CLA:HBC2	1.89	0.55
14:K:83:ARG:HB3	14:K:91:LEU:HD22	1.88	0.55
19:A:810:CLA:H71	23:J:103:BCR:H343	1.89	0.55
19:B:818:CLA:HBA2	19:B:827:CLA:HBB2	1.89	0.55
5:A:476:LEU:HB2	5:A:528:THR:HG23	1.89	0.54
3:3:96:PHE:HB2	19:3:302:CLA:H43	1.89	0.54
19:6:305:CLA:HBA1	20:6:318:LUT:H30	1.89	0.54
4:5:148:HIS:HD2	19:5:307:CLA:HBB1	1.72	0.54
1:6:180:ASP:HB3	1:6:183:LYS:HB2	1.89	0.54
5:A:29:PRO:HB2	5:A:45:TRP:HH2	1.73	0.54
19:B:823:CLA:HBB2	23:B:846:BCR:H343	1.90	0.54
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.88	0.54
19:L:302:CLA:HAB	23:L:305:BCR:H352	1.90	0.53
17:L:102:PRO:HA	17:L:105:ARG:HD3	1.90	0.53
4:5:148:HIS:CD2	19:5:307:CLA:HBB1	2.44	0.53
18:6:301:CHL:H2	22:6:317:LHG:H302	1.91	0.53
19:2:308:CLA:HBA2	23:2:319:BCR:H381	1.91	0.53
19:L:302:CLA:H51	23:L:305:BCR:H323	1.91	0.53
20:3:315:LUT:H171	20:3:315:LUT:H8	1.91	0.53
4:5:233:THR:HG22	4:5:241:THR:HG21	1.91	0.52
5:A:125:ASN:HB3	5:A:133:GLN:HB3	1.91	0.52
3:3:111:ARG:HA	3:3:114:MET:HE3	1.91	0.52
3:3:224:MET:HG3	3:3:228:LYS:HE3	1.92	0.52
19:6:309:CLA:HAB	20:6:315:LUT:H32	1.90	0.52
10:F:209:PRO:HD3	29:J:104:LMG:HC71	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:302:CLA:HAB	21:6:316:XAT:H32	1.93	0.51
5:A:728:ALA:HA	22:A:846:LHG:H342	1.91	0.51
6:B:619:TRP:O	6:B:623:TYR:HB3	2.10	0.51
3:3:87:LEU:HD21	19:A:813:CLA:H12	1.93	0.51
19:3:302:CLA:H51	19:A:811:CLA:H92	1.93	0.50
19:5:301:CLA:HAB	20:5:316:LUT:H12	1.93	0.50
2:2:193:PRO:HB3	18:2:307:CHL:HBC2	1.93	0.50
5:A:522:LEU:HD11	5:A:616:VAL:HA	1.93	0.50
19:B:816:CLA:H2	23:G:201:BCR:H282	1.94	0.50
30:B:901:HOH:O	8:D:202:PRO:HD3	2.11	0.50
10:F:178:ILE:HG23	19:F:303:CLA:HAA1	1.94	0.50
6:B:472:TYR:HB3	10:F:88:ALA:HA	1.94	0.49
19:B:841:CLA:H193	12:I:23:MET:HE3	1.94	0.49
5:A:302:PHE:HE1	19:A:822:CLA:HAB	1.77	0.49
19:B:817:CLA:H193	19:B:820:CLA:HBC1	1.94	0.49
14:K:79:PRO:HG3	14:K:85:ALA:HB2	1.95	0.49
19:A:822:CLA:H101	23:A:851:BCR:H10C	1.94	0.49
5:A:346:TRP:HB3	19:A:807:CLA:HAC1	1.95	0.49
19:A:805:CLA:H201	19:B:802:CLA:H141	1.95	0.49
23:A:848:BCR:H321	23:A:848:BCR:HC8	1.95	0.49
6:B:721:TYR:HB2	19:B:803:CLA:HED2	1.94	0.49
5:A:405:HIS:HA	5:A:408:ILE:HD12	1.94	0.49
19:B:802:CLA:HHB	19:B:803:CLA:H202	1.94	0.49
18:2:320:CHL:HAA1	22:5:318:LHG:H292	1.95	0.49
8:D:210:ALA:HB1	8:D:214:GLU:HB2	1.95	0.49
5:A:536:ILE:HD12	24:A:802:CL0:H63	1.95	0.49
13:J:26:LEU:HB2	23:J:103:BCR:H371	1.94	0.49
19:2:312:CLA:H43	18:3:314:CHL:H121	1.94	0.49
18:2:314:CHL:HHC	18:2:314:CHL:HBB1	1.95	0.49
5:A:279:LEU:HD21	5:A:372:PRO:HD2	1.94	0.49
19:B:806:CLA:HBC2	19:B:830:CLA:HMA1	1.95	0.49
17:L:211:LEU:HG	19:L:303:CLA:HED3	1.95	0.48
23:F:302:BCR:HC32	29:J:105:LMG:H132	1.95	0.48
14:K:98:LEU:HB2	14:K:107:THR:HG21	1.95	0.48
19:3:302:CLA:H52	19:A:814:CLA:H193	1.95	0.48
5:A:286:LEU:HD13	19:A:819:CLA:HMA2	1.94	0.48
19:B:830:CLA:H143	19:B:841:CLA:HED3	1.95	0.48
1:6:90:HIS:HD2	21:6:316:XAT:H15	1.79	0.48
19:A:806:CLA:H2	19:A:812:CLA:H92	1.95	0.48
4:5:136:ALA:HA	4:5:139:LEU:HD12	1.96	0.48
5:A:327:LYS:HE3	5:A:327:LYS:HB2	1.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:807:CLA:H191	28:B:849:DGD:HAG3	1.95	0.48
6:B:299:HIS:HB3	6:B:304:ILE:HD11	1.95	0.48
6:B:429:LEU:HD11	19:B:838:CLA:HMB2	1.96	0.48
19:A:818:CLA:H101	23:K:205:BCR:HC22	1.95	0.48
2:2:145:ASP:HB2	23:2:319:BCR:H332	1.95	0.47
2:2:247:LEU:HB2	20:2:315:LUT:H222	1.95	0.47
5:A:200:ALA:HB2	5:A:306:GLY:HA3	1.96	0.47
19:A:841:CLA:H121	25:A:844:PQN:H272	1.96	0.47
14:K:91:LEU:HD23	14:K:91:LEU:HA	1.69	0.47
4:5:225:ALA:HB1	4:5:229:GLU:HG2	1.96	0.47
19:3:309:CLA:H2	19:3:310:CLA:HMD2	1.96	0.47
3:3:170:GLY:O	3:3:174:HIS:HB2	2.14	0.47
6:B:410:ARG:HA	6:B:413:GLU:HB2	1.95	0.47
19:B:838:CLA:H192	23:F:305:BCR:H272	1.97	0.47
19:6:310:CLA:H2	19:6:311:CLA:HMD2	1.97	0.47
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.95	0.47
6:B:718:ILE:HD12	19:B:828:CLA:HAB	1.97	0.47
19:B:812:CLA:H122	27:B:850:LMU:H92	1.97	0.47
19:A:810:CLA:H111	19:A:810:CLA:H152	1.79	0.47
6:B:257:PHE:HZ	19:B:818:CLA:H71	1.80	0.47
19:B:834:CLA:H51	23:F:302:BCR:H312	1.96	0.47
20:J:101:LUT:H7	20:J:101:LUT:H181	1.61	0.47
5:A:438:LEU:HD21	5:A:545:VAL:HG12	1.97	0.47
19:3:301:CLA:HAB	20:3:316:LUT:H12	1.97	0.46
4:5:231:LEU:HD22	20:5:315:LUT:H172	1.96	0.46
18:5:313:CHL:HHC	18:5:313:CHL:HBB1	1.97	0.46
19:A:823:CLA:HBB	19:A:824:CLA:H12	1.97	0.46
6:B:374:HIS:HE2	19:B:829:CLA:C1B	2.29	0.46
19:3:312:CLA:HBC1	20:3:315:LUT:H162	1.97	0.46
19:6:303:CLA:HBC1	18:6:306:CHL:HBB2	1.98	0.46
4:5:211:LEU:HD12	22:5:318:LHG:H101	1.97	0.46
6:B:317:ARG:HB3	6:B:320:LYS:HD2	1.96	0.46
3:3:278:ILE:HD12	19:A:816:CLA:HBD	1.98	0.46
6:B:231:ASN:HA	19:B:817:CLA:HAA2	1.98	0.46
19:B:816:CLA:H61	19:B:816:CLA:H41	1.70	0.46
19:B:826:CLA:HMA1	23:B:847:BCR:H14C	1.98	0.46
23:G:201:BCR:H311	23:G:201:BCR:HC7	1.74	0.46
19:A:823:CLA:HAA1	14:K:85:ALA:HB3	1.98	0.45
6:B:524:ALA:HB2	19:B:838:CLA:HMA1	1.97	0.45
18:6:301:CHL:H11	4:5:149:TYR:HB2	1.98	0.45
19:6:305:CLA:HBB2	18:6:306:CHL:CBB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:801:CLA:H152	23:L:305:BCR:H17C	1.97	0.45
19:B:811:CLA:HHC	19:B:811:CLA:HBB1	1.96	0.45
6:B:369:ALA:HB1	6:B:725:LEU:HD11	1.99	0.45
10:F:207:ASP:HA	29:J:104:LMG:HC61	1.98	0.45
19:A:821:CLA:HHC	19:A:821:CLA:HBB1	1.98	0.45
8:D:83:THR:HG23	8:D:131:PRO:HB2	1.99	0.45
19:2:302:CLA:H91	19:2:302:CLA:H112	1.77	0.45
6:B:53:GLN:HG2	19:B:806:CLA:H3A	1.99	0.45
19:5:308:CLA:H61	19:5:308:CLA:H41	1.66	0.45
19:6:308:CLA:HHC	19:6:308:CLA:HBB1	1.98	0.45
19:3:309:CLA:HHC	19:3:309:CLA:HBB1	1.99	0.45
23:3:317:BCR:HC7	23:3:317:BCR:H331	1.66	0.45
19:A:831:CLA:H62	22:A:846:LHG:H132	1.98	0.45
23:F:305:BCR:H11C	23:F:305:BCR:H341	1.85	0.45
19:6:307:CLA:H3A	19:6:307:CLA:HBA2	1.81	0.45
18:2:320:CHL:HHC	18:2:320:CHL:HBB1	1.99	0.45
6:B:301:ILE:HG23	19:B:820:CLA:HED3	1.98	0.45
6:B:668:ARG:O	6:B:669:GLY:C	2.60	0.45
19:B:801:CLA:H52	19:B:840:CLA:H43	1.99	0.45
19:B:810:CLA:H13	28:B:849:DGD:HAH2	1.99	0.45
14:K:83:ARG:HE	14:K:91:LEU:HD13	1.82	0.45
19:3:310:CLA:HHC	19:3:310:CLA:HBB1	1.99	0.44
19:3:311:CLA:HHC	19:3:311:CLA:HBB1	1.99	0.44
19:B:812:CLA:HAC1	27:B:850:LMU:H51	1.99	0.44
19:A:807:CLA:H203	23:A:848:BCR:H10C	1.99	0.44
19:B:806:CLA:H8	19:B:825:CLA:HBA2	1.98	0.44
19:B:824:CLA:H3A	19:B:842:CLA:HED3	1.98	0.44
23:B:845:BCR:H15C	23:B:845:BCR:H351	1.87	0.44
19:6:312:CLA:HHC	19:6:312:CLA:HBB1	1.99	0.44
4:5:70:GLY:HA2	22:5:318:LHG:HC11	1.98	0.44
19:A:833:CLA:HBB1	19:B:801:CLA:HAA2	1.99	0.44
6:B:26:ALA:HB2	28:B:849:DGD:HA42	1.99	0.44
2:2:192:TYR:HB3	19:2:309:CLA:HED2	2.00	0.44
19:3:305:CLA:HHC	19:3:305:CLA:HBB1	2.00	0.44
19:3:313:CLA:HHC	19:3:313:CLA:HBB1	2.00	0.44
19:5:311:CLA:HHC	19:5:311:CLA:HBB1	2.00	0.44
19:A:824:CLA:HHC	19:A:824:CLA:HBB1	1.99	0.44
19:B:812:CLA:H101	19:B:812:CLA:H61	1.84	0.44
20:2:315:LUT:H15	20:2:315:LUT:H201	1.80	0.44
19:A:836:CLA:HHC	19:A:836:CLA:HBB1	2.00	0.44
8:D:139:LYS:HE3	8:D:171:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:77:GLU:O	17:L:81:THR:OG1	2.36	0.44
19:A:825:CLA:HBB2	22:A:847:LHG:HC92	2.00	0.44
23:B:846:BCR:H361	23:B:846:BCR:H20C	1.77	0.44
23:B:848:BCR:H15C	23:B:848:BCR:H351	1.78	0.44
2:2:201:LEU:HD12	20:2:315:LUT:H22	1.98	0.44
5:A:29:PRO:HB3	19:A:805:CLA:HAC1	2.00	0.44
3:3:215:LEU:HD12	20:3:315:LUT:H222	1.99	0.44
23:5:317:BCR:H15C	23:5:317:BCR:H351	1.81	0.44
5:A:196:ASN:HB3	19:A:821:CLA:HMD2	2.00	0.44
19:A:837:CLA:HHC	19:A:837:CLA:HBB1	2.00	0.44
19:2:310:CLA:HBB1	19:2:310:CLA:HHC	1.99	0.44
19:A:808:CLA:HED2	19:A:808:CLA:H62	2.00	0.44
19:6:304:CLA:HHC	19:6:304:CLA:HBB1	1.99	0.43
19:6:310:CLA:HHC	19:6:310:CLA:HBB1	1.99	0.43
19:A:842:CLA:HHC	19:A:842:CLA:HBB1	2.00	0.43
19:A:808:CLA:H152	19:A:808:CLA:H111	1.76	0.43
10:F:212:THR:HA	10:F:215:LEU:HG	1.99	0.43
23:J:103:BCR:H403	23:J:103:BCR:H24C	1.82	0.43
18:6:306:CHL:HHC	18:6:306:CHL:HBB1	2.00	0.43
19:3:303:CLA:HAC1	19:3:308:CLA:H151	1.99	0.43
19:A:834:CLA:HHC	19:A:834:CLA:HBB1	2.01	0.43
23:A:849:BCR:H11C	23:A:849:BCR:H341	1.91	0.43
19:B:807:CLA:HHC	19:B:807:CLA:HBB1	2.01	0.43
23:J:103:BCR:HC8	23:J:103:BCR:H311	2.00	0.43
20:3:316:LUT:H7	20:3:316:LUT:H181	1.74	0.43
4:5:115:LYS:HE3	4:5:115:LYS:HB3	1.77	0.43
22:5:318:LHG:H242	22:5:318:LHG:H112	2.01	0.43
5:A:244:ARG:HG3	19:A:816:CLA:HED3	2.01	0.43
5:A:360:LEU:HD11	19:A:820:CLA:H71	2.00	0.43
5:A:405:HIS:HE1	19:A:831:CLA:NA	2.16	0.43
19:A:834:CLA:H8	25:B:843:PQN:H202	2.00	0.43
19:2:311:CLA:HAC2	19:2:312:CLA:H201	2.01	0.43
23:B:848:BCR:H24C	23:B:848:BCR:H403	1.82	0.43
23:G:205:BCR:H403	23:G:205:BCR:H23C	2.00	0.43
19:J:102:CLA:HHC	19:J:102:CLA:HBB1	2.00	0.43
14:K:119:HIS:CG	23:K:205:BCR:H12C	2.53	0.43
19:5:309:CLA:HHC	19:5:309:CLA:HBB1	2.00	0.43
19:B:842:CLA:H161	19:B:842:CLA:H141	1.79	0.43
19:A:812:CLA:HHC	19:A:812:CLA:HBB1	2.00	0.43
19:F:301:CLA:HMC2	23:F:302:BCR:H381	2.01	0.43
16:H:108:GLY:O	16:H:112:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:305:CHL:HBB1	19:2:308:CLA:HBC1	2.01	0.43
19:5:312:CLA:HHC	19:5:312:CLA:HBB1	2.01	0.43
6:B:395:ILE:HD13	6:B:555:TYR:HA	2.01	0.43
19:B:825:CLA:H62	19:B:825:CLA:H41	1.92	0.43
23:B:847:BCR:H15C	23:B:847:BCR:H351	1.81	0.43
10:F:162:GLN:HA	10:F:165:LEU:HG	2.00	0.43
1:6:237:ILE:HD12	1:6:237:ILE:HA	1.93	0.43
2:2:203:TRP:HB2	19:2:309:CLA:HBA1	1.99	0.43
5:A:498:ASN:HB2	19:A:837:CLA:HED2	2.00	0.43
10:F:156:LEU:HD22	10:F:167:GLU:HG2	2.01	0.43
17:L:123:LYS:HA	17:L:123:LYS:HD3	1.87	0.43
19:6:312:CLA:H72	22:6:317:LHG:H182	2.00	0.43
18:3:314:CHL:HED2	18:3:314:CHL:HBD	1.95	0.43
6:B:181:GLY:HA2	6:B:185:VAL:HB	2.01	0.43
6:B:680:TRP:CE2	6:B:684:ARG:HG3	2.54	0.43
19:F:304:CLA:HHC	19:F:304:CLA:HBB1	2.00	0.42
18:2:301:CHL:HHC	18:2:301:CHL:HBB1	2.01	0.42
19:5:307:CLA:H41	19:5:307:CLA:H61	1.68	0.42
5:A:534:HIS:CG	19:A:839:CLA:HED3	2.54	0.42
19:B:807:CLA:H72	19:B:807:CLA:H111	1.94	0.42
19:B:814:CLA:H92	19:B:825:CLA:H12	2.00	0.42
19:B:830:CLA:H91	28:B:849:DGD:HBW2	2.00	0.42
19:B:831:CLA:H3A	19:B:831:CLA:HBA2	1.85	0.42
19:F:301:CLA:HHC	19:F:301:CLA:HBB1	2.00	0.42
19:G:203:CLA:HHC	19:G:203:CLA:HBB1	2.00	0.42
1:6:152:VAL:HG11	20:6:318:LUT:H401	2.00	0.42
19:6:312:CLA:H202	23:5:317:BCR:H331	2.00	0.42
20:5:316:LUT:H191	20:5:316:LUT:H11	1.76	0.42
19:A:808:CLA:HAB	23:A:849:BCR:HC32	2.00	0.42
19:6:313:CLA:HBB1	19:6:313:CLA:HHC	2.00	0.42
5:A:403:ALA:HB2	23:A:851:BCR:H323	2.01	0.42
6:B:490:GLN:HA	6:B:494:LEU:HB2	2.00	0.42
8:D:83:THR:HB	8:D:133:LEU:HB2	2.01	0.42
4:5:190:LEU:HD12	20:5:315:LUT:H222	2.01	0.42
19:A:825:CLA:HBB1	19:A:825:CLA:HHC	2.01	0.42
6:B:552:GLU:OE2	30:B:901:HOH:O	2.22	0.42
20:J:101:LUT:H11	20:J:101:LUT:H191	1.89	0.42
19:3:311:CLA:HHB	19:3:312:CLA:HBC3	2.01	0.42
6:B:339:ALA:HB2	23:B:847:BCR:H372	2.01	0.42
4:5:99:TRP:CE2	19:5:307:CLA:HBC3	2.55	0.42
5:A:20:LYS:HA	5:A:20:LYS:HD2	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:LEU:HG	5:A:546:LEU:HB2	2.02	0.42
5:A:445:LEU:HB3	5:A:539:PHE:HB2	2.01	0.42
6:B:390:GLY:HA2	23:B:847:BCR:H393	2.01	0.42
23:B:844:BCR:H11C	23:B:844:BCR:H341	1.87	0.42
23:G:201:BCR:H11C	23:G:201:BCR:H341	1.86	0.42
2:2:250:HIS:CG	19:2:312:CLA:HAA2	2.55	0.42
19:5:302:CLA:HHC	19:5:302:CLA:HBB1	2.01	0.42
19:A:820:CLA:H111	19:A:822:CLA:HBB2	2.00	0.42
19:2:312:CLA:HHC	19:2:312:CLA:HBB1	2.01	0.42
17:L:78:THR:HG22	17:L:81:THR:H	1.85	0.42
23:A:851:BCR:H321	23:A:851:BCR:HC7	1.85	0.42
19:B:822:CLA:HMB1	19:B:823:CLA:H2	2.02	0.42
23:J:103:BCR:H341	23:J:103:BCR:H11C	1.81	0.42
17:L:77:GLU:H	17:L:77:GLU:HG2	1.73	0.42
22:5:318:LHG:H251	22:5:318:LHG:H282	1.84	0.41
19:A:822:CLA:H171	19:A:832:CLA:HBC1	2.02	0.41
19:B:809:CLA:HHC	19:B:809:CLA:HBB1	2.01	0.41
19:B:841:CLA:HHC	19:B:841:CLA:HBB1	2.01	0.41
2:2:113:GLY:HA2	20:2:316:LUT:H381	2.02	0.41
18:2:301:CHL:H2	18:2:301:CHL:H61	1.61	0.41
3:3:206:TYR:HB3	19:3:308:CLA:HED2	2.01	0.41
3:3:248:GLN:HE21	3:3:259:ASN:HD22	1.67	0.41
23:A:852:BCR:H321	23:A:852:BCR:HC7	1.86	0.41
23:A:852:BCR:H403	23:A:852:BCR:H24C	1.87	0.41
6:B:520:HIS:CG	19:B:838:CLA:HED3	2.55	0.41
6:B:649:MET:HE1	19:B:809:CLA:H41	2.01	0.41
20:J:101:LUT:H35	20:J:101:LUT:H401	1.83	0.41
17:L:83:SER:HB3	17:L:86:ILE:HB	2.02	0.41
23:L:305:BCR:H15C	23:L:305:BCR:H351	1.87	0.41
1:6:118:TRP:CE2	1:6:126:ALA:HB2	2.55	0.41
4:5:58:LEU:HD22	4:5:59:PRO:HD2	2.02	0.41
24:A:802:CL0:H14	24:A:802:CL0:H2	1.86	0.41
19:A:839:CLA:HHC	19:A:839:CLA:HAB	1.91	0.41
6:B:287:ALA:HB2	19:B:820:CLA:HBC2	2.02	0.41
19:B:840:CLA:HHC	19:B:840:CLA:HBB1	2.01	0.41
14:K:79:PRO:HA	14:K:91:LEU:HD21	2.01	0.41
17:L:76:LEU:HB3	17:L:77:GLU:H	1.67	0.41
17:L:146:VAL:HG22	17:L:197:PHE:HE1	1.84	0.41
19:A:818:CLA:HHC	19:A:818:CLA:HBB1	2.02	0.41
19:2:309:CLA:H12	20:2:315:LUT:H173	2.02	0.41
19:3:302:CLA:HHC	19:3:302:CLA:HBB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:316:LUT:H15	20:5:316:LUT:H201	1.83	0.41
19:A:819:CLA:HBB1	19:A:819:CLA:HHC	2.02	0.41
23:A:848:BCR:H11C	23:A:848:BCR:H341	1.93	0.41
19:B:816:CLA:H51	23:B:845:BCR:HC21	2.01	0.41
7:C:61:ASP:HA	7:C:62:PHE:HA	1.85	0.41
22:6:317:LHG:H342	22:6:317:LHG:H311	1.89	0.41
20:2:317:LUT:H15	20:2:317:LUT:H201	1.86	0.41
20:3:316:LUT:H11	20:3:316:LUT:H191	1.82	0.41
18:2:305:CHL:HBB2	18:2:306:CHL:HAB	2.02	0.41
3:3:237:LEU:HG	20:3:315:LUT:H191	2.02	0.41
23:A:852:BCR:H20C	23:A:852:BCR:H361	1.81	0.41
19:B:840:CLA:H93	23:I:101:BCR:H382	2.03	0.41
23:K:204:BCR:H311	23:K:204:BCR:HC7	1.73	0.41
23:M:101:BCR:H20C	23:M:101:BCR:H361	1.98	0.41
4:5:231:LEU:HD13	20:5:315:LUT:H163	2.01	0.41
5:A:304:VAL:HG21	19:A:818:CLA:H121	2.02	0.41
19:A:807:CLA:H151	23:A:848:BCR:H323	2.02	0.41
23:J:103:BCR:H20C	23:J:103:BCR:H361	1.89	0.41
1:6:237:ILE:HG23	19:6:314:CLA:C4B	2.51	0.41
3:3:116:GLY:HA2	20:3:316:LUT:H381	2.02	0.41
20:3:315:LUT:H7	20:3:315:LUT:H181	1.79	0.41
5:A:84:TRP:HZ3	23:A:849:BCR:H322	1.86	0.41
5:A:118:ILE:HG13	5:A:119:VAL:HG13	2.02	0.41
5:A:294:HIS:HB2	19:A:819:CLA:C1B	2.51	0.41
19:A:835:CLA:HMC2	19:B:804:CLA:H101	2.03	0.41
23:A:851:BCR:H20C	23:A:851:BCR:H361	1.93	0.41
23:K:204:BCR:H15C	23:K:204:BCR:H351	1.87	0.41
20:3:316:LUT:H15	20:3:316:LUT:H201	1.83	0.41
5:A:379:THR:HG21	5:A:515:VAL:HB	2.03	0.41
5:A:447:PHE:C	19:A:835:CLA:HBB2	2.46	0.41
19:A:842:CLA:H41	25:A:844:PQN:H18	2.02	0.41
6:B:180:SER:HB3	6:B:288:GLY:HA3	2.02	0.41
19:6:302:CLA:HBC1	22:6:317:LHG:H142	2.03	0.40
6:B:4:ARG:HB2	6:B:13:SER:HB2	2.02	0.40
19:6:308:CLA:H11	27:B:851:LMU:H41	2.03	0.40
22:6:317:LHG:H262	22:6:317:LHG:H132	2.01	0.40
5:A:672:LEU:HD11	6:B:617:MET:HB2	2.02	0.40
18:2:307:CHL:HMA1	20:2:317:LUT:H403	2.03	0.40
18:2:320:CHL:HMA3	4:5:55:LEU:HD13	2.03	0.40
19:A:811:CLA:H12	19:A:811:CLA:H52	1.94	0.40
19:A:819:CLA:H3A	19:A:819:CLA:HBA2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:828:CLA:H93	19:A:828:CLA:H112	1.86	0.40
23:A:851:BCR:H11C	23:A:851:BCR:H341	1.91	0.40
6:B:303:GLU:HG3	11:G:97:ALA:HA	2.03	0.40
19:B:829:CLA:H171	23:B:844:BCR:H352	2.03	0.40
19:B:832:CLA:HAB	19:B:833:CLA:H192	2.03	0.40
23:B:845:BCR:HC7	23:B:845:BCR:H311	1.92	0.40
23:3:317:BCR:H11C	23:3:317:BCR:H341	1.90	0.40
23:A:850:BCR:H24C	23:A:850:BCR:H371	1.94	0.40
19:B:816:CLA:HBA1	23:G:201:BCR:H281	2.02	0.40
10:F:175:PHE:HB2	23:F:302:BCR:H321	2.03	0.40
23:M:101:BCR:H15C	23:M:101:BCR:H351	1.91	0.40
17:L:79:PRO:O	17:L:80:VAL:C	2.65	0.40
1:6:104:PRO:HG2	30:6:401:HOH:O	2.21	0.40
1:6:202:PHE:CZ	21:6:316:XAT:H10	2.56	0.40
23:I:101:BCR:H20C	23:I:101:BCR:H361	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	192/243 (79%)	189 (98%)	3 (2%)	0	100	100
2	2	185/267 (69%)	182 (98%)	3 (2%)	0	100	100
3	3	218/279 (78%)	210 (96%)	8 (4%)	0	100	100
4	5	196/249 (79%)	191 (97%)	5 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	713 (98%)	17 (2%)	1 (0%)	48	41
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	140/215 (65%)	134 (96%)	5 (4%)	1 (1%)	18	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	62/132 (47%)	61 (98%)	1 (2%)	0	100	100
10	F	159/246 (65%)	156 (98%)	3 (2%)	0	100	100
11	G	88/161 (55%)	88 (100%)	0	0	100	100
12	I	33/36 (92%)	33 (100%)	0	0	100	100
13	J	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
14	K	78/135 (58%)	73 (94%)	5 (6%)	0	100	100
15	M	28/32 (88%)	28 (100%)	0	0	100	100
16	H	74/142 (52%)	72 (97%)	2 (3%)	0	100	100
17	L	124/221 (56%)	117 (94%)	6 (5%)	1 (1%)	16	7
All	All	3165/3965 (80%)	3083 (97%)	79 (2%)	3 (0%)	49	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	173	PRO
17	L	78	THR
6	B	669	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

207 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	$\# Z > 2$
19	CLA	J	102	13	46,50,73	1.44	7 (15%)	53,85,113	1.18	4 (7%)
19	CLA	B	840	30	69,73,73	1.14	6 (8%)	82,113,113	1.08	7 (8%)
20	LUT	J	101	-	42,43,43	1.31	8 (19%)	51,60,60	1.82	14 (27%)
19	CLA	G	203	11	49,53,73	1.47	8 (16%)	58,89,113	1.02	3 (5%)
19	CLA	B	823	6	59,63,73	1.35	8 (13%)	70,101,113	1.13	6 (8%)
19	CLA	5	310	4	48,52,73	1.36	6 (12%)	57,88,113	1.04	4 (7%)
19	CLA	B	831	6	49,53,73	1.46	7 (14%)	58,89,113	1.02	3 (5%)
23	BCR	L	304	-	41,41,41	1.46	9 (21%)	56,56,56	1.92	19 (33%)
28	DGD	B	849	-	67,67,67	0.53	0	81,81,81	0.73	1 (1%)
19	CLA	3	310	3	47,51,73	1.49	7 (14%)	55,86,113	1.14	4 (7%)
23	BCR	F	302	-	41,41,41	1.46	5 (12%)	56,56,56	1.75	15 (26%)
19	CLA	L	302	17	64,68,73	1.21	7 (10%)	76,107,113	0.88	3 (3%)
23	BCR	B	845	-	41,41,41	1.42	8 (19%)	56,56,56	1.73	16 (28%)
19	CLA	A	827	30	59,63,73	1.23	6 (10%)	70,101,113	0.96	4 (5%)
19	CLA	A	828	5	69,73,73	1.24	8 (11%)	82,113,113	0.99	6 (7%)
19	CLA	2	303	2	49,53,73	1.43	7 (14%)	58,89,113	1.02	5 (8%)
19	CLA	A	808	5	69,73,73	1.17	8 (11%)	82,113,113	0.92	3 (3%)
23	BCR	K	204	-	41,41,41	1.47	4 (9%)	56,56,56	1.74	17 (30%)
19	CLA	A	807	5	69,73,73	1.14	7 (10%)	82,113,113	0.94	4 (4%)
19	CLA	2	309	2	65,69,73	1.18	7 (10%)	77,108,113	1.06	6 (7%)
19	CLA	A	832	5	54,58,73	1.37	6 (11%)	64,95,113	0.95	3 (4%)
19	CLA	6	313	1	49,53,73	1.41	7 (14%)	58,89,113	1.12	4 (6%)
19	CLA	F	304	10	45,49,73	1.48	8 (17%)	54,84,113	1.15	4 (7%)
19	CLA	B	801	30	69,73,73	1.20	9 (13%)	82,113,113	0.96	5 (6%)
19	CLA	3	305	3	50,54,73	1.38	7 (14%)	59,90,113	1.10	5 (8%)
19	CLA	6	310	22	60,64,73	1.28	7 (11%)	71,102,113	0.99	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	6	304	30	53,57,73	1.33	7 (13%)	61,93,113	1.09	4 (6%)
19	CLA	6	311	1	49,53,73	1.43	7 (14%)	58,89,113	1.16	5 (8%)
20	LUT	2	316	-	42,43,43	1.33	6 (14%)	51,60,60	1.60	12 (23%)
19	CLA	B	807	6	69,73,73	1.21	7 (10%)	82,113,113	0.99	4 (4%)
19	CLA	B	836	30	49,53,73	1.39	8 (16%)	58,89,113	1.09	5 (8%)
19	CLA	B	832	6	69,73,73	1.19	8 (11%)	82,113,113	0.94	3 (3%)
19	CLA	B	815	6	69,73,73	1.19	7 (10%)	82,113,113	0.88	4 (4%)
19	CLA	2	302	2	69,73,73	1.15	7 (10%)	82,113,113	0.96	4 (4%)
19	CLA	A	842	5	69,73,73	1.21	7 (10%)	82,113,113	0.95	3 (3%)
19	CLA	K	202	14	48,52,73	1.47	9 (18%)	59,88,113	1.01	3 (5%)
19	CLA	5	301	4	64,68,73	1.21	7 (10%)	76,107,113	0.96	4 (5%)
19	CLA	B	822	6	50,54,73	1.40	7 (14%)	59,90,113	1.09	4 (6%)
19	CLA	A	824	5	69,73,73	1.19	6 (8%)	82,113,113	1.03	5 (6%)
19	CLA	2	312	2	69,73,73	1.20	8 (11%)	82,113,113	1.01	5 (6%)
19	CLA	B	805	6	49,53,73	1.45	7 (14%)	58,89,113	1.04	3 (5%)
22	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.38	0
23	BCR	B	847	-	41,41,41	1.47	4 (9%)	56,56,56	1.73	14 (25%)
19	CLA	5	303	30	49,53,73	1.38	7 (14%)	58,89,113	1.04	5 (8%)
19	CLA	B	803	6	69,73,73	1.24	7 (10%)	82,113,113	0.80	3 (3%)
18	CHL	5	305	30	37,51,74	1.20	3 (8%)	30,86,114	3.10	10 (33%)
29	LMG	J	104	-	30,30,55	0.62	0	38,38,63	0.70	0
19	CLA	3	303	30	51,55,73	1.35	8 (15%)	60,91,113	1.04	5 (8%)
19	CLA	B	814	6	69,73,73	1.21	8 (11%)	82,113,113	0.92	3 (3%)
22	LHG	6	319	-	26,26,48	0.37	0	29,32,54	0.48	0
19	CLA	2	304	30	54,58,73	1.31	8 (14%)	64,95,113	1.01	5 (7%)
22	LHG	A	847	19	33,33,48	0.31	0	36,39,54	0.40	0
19	CLA	A	805	5	69,73,73	1.16	7 (10%)	82,113,113	0.90	4 (4%)
23	BCR	A	848	-	41,41,41	1.45	8 (19%)	56,56,56	1.85	17 (30%)
19	CLA	5	308	4	64,68,73	1.17	7 (10%)	76,107,113	0.96	4 (5%)
21	XAT	6	316	-	41,47,47	0.73	2 (4%)	54,74,74	0.98	3 (5%)
19	CLA	L	303	30	46,50,73	1.42	8 (17%)	53,85,113	1.13	4 (7%)
18	CHL	5	304	30	40,54,74	1.29	3 (7%)	34,90,114	3.00	10 (29%)
26	SF4	A	845	5,6	0,12,12	-	-	-	-	-
18	CHL	6	306	1	40,54,74	1.15	2 (5%)	34,90,114	2.90	11 (32%)
19	CLA	6	314	1	49,53,73	1.39	7 (14%)	58,89,113	1.13	6 (10%)
19	CLA	5	309	30	64,68,73	1.21	7 (10%)	76,107,113	0.97	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	5	318	-	43,43,48	0.29	0	46,49,54	0.36	0
19	CLA	A	801	5	59,63,73	1.26	8 (13%)	70,101,113	0.98	4 (5%)
19	CLA	A	836	5	64,68,73	1.22	7 (10%)	76,107,113	0.94	3 (3%)
19	CLA	B	817	6	69,73,73	1.23	6 (8%)	82,113,113	0.89	5 (6%)
23	BCR	J	103	-	41,41,41	1.45	10 (24%)	56,56,56	2.20	20 (35%)
19	CLA	B	809	6	69,73,73	1.19	7 (10%)	82,113,113	0.90	3 (3%)
18	CHL	5	306	30	40,54,74	1.07	3 (7%)	34,90,114	2.98	10 (29%)
19	CLA	A	829	5	69,73,73	1.21	7 (10%)	82,113,113	0.95	3 (3%)
19	CLA	B	804	-	69,73,73	1.12	7 (10%)	82,113,113	0.97	6 (7%)
20	LUT	3	316	-	42,43,43	1.31	8 (19%)	51,60,60	1.79	15 (29%)
27	LMU	B	851	-	36,36,36	0.23	0	47,47,47	0.41	0
19	CLA	2	313	2	54,58,73	1.34	5 (9%)	64,95,113	1.05	5 (7%)
19	CLA	B	824	6	49,53,73	1.35	8 (16%)	58,89,113	1.07	5 (8%)
19	CLA	A	830	5	69,73,73	1.24	7 (10%)	82,113,113	0.89	2 (2%)
20	LUT	6	315	-	42,43,43	1.33	8 (19%)	51,60,60	1.55	12 (23%)
18	CHL	2	305	30	40,54,74	1.32	3 (7%)	34,90,114	2.93	9 (26%)
19	CLA	3	304	30	49,53,73	1.39	8 (16%)	58,89,113	1.10	5 (8%)
19	CLA	2	308	2	49,53,73	1.34	6 (12%)	58,89,113	1.06	4 (6%)
19	CLA	A	820	5	69,73,73	1.15	8 (11%)	82,113,113	0.94	4 (4%)
19	CLA	A	812	5	69,73,73	1.20	8 (11%)	82,113,113	0.92	3 (3%)
19	CLA	B	834	6	64,68,73	1.23	7 (10%)	76,107,113	0.92	4 (5%)
19	CLA	B	830	6	64,68,73	1.23	8 (12%)	76,107,113	0.98	5 (6%)
25	PQN	B	843	-	34,34,34	0.40	0	43,45,45	0.66	0
18	CHL	6	301	1	45,59,74	1.07	3 (6%)	40,96,114	2.81	11 (27%)
19	CLA	F	301	30	64,68,73	1.24	7 (10%)	76,107,113	1.02	5 (6%)
22	LHG	2	318	19	37,37,48	0.31	0	40,43,54	0.41	0
18	CHL	2	314	2	40,54,74	1.15	3 (7%)	34,90,114	2.84	11 (32%)
19	CLA	B	820	30	61,65,73	1.26	8 (13%)	72,103,113	1.03	5 (6%)
19	CLA	A	804	30	69,73,73	1.16	7 (10%)	82,113,113	0.95	5 (6%)
19	CLA	A	814	5	69,73,73	1.18	8 (11%)	82,113,113	0.96	5 (6%)
19	CLA	5	314	4	49,53,73	1.50	6 (12%)	58,89,113	1.37	7 (12%)
19	CLA	A	831	5	69,73,73	1.28	8 (11%)	82,113,113	0.85	3 (3%)
19	CLA	6	303	1	59,63,73	1.30	6 (10%)	70,101,113	0.93	4 (5%)
19	CLA	B	806	6	69,73,73	1.18	8 (11%)	82,113,113	0.90	4 (4%)
22	LHG	6	317	19	48,48,48	0.29	0	51,54,54	0.38	0
19	CLA	5	312	4	69,73,73	1.20	7 (10%)	82,113,113	1.02	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	L	305	-	41,41,41	1.43	4 (9%)	56,56,56	1.68	15 (26%)
24	CL0	A	802	5	58,73,73	0.87	4 (6%)	60,113,113	1.70	8 (13%)
19	CLA	3	301	3	64,68,73	1.20	7 (10%)	76,107,113	0.95	5 (6%)
19	CLA	B	812	6	64,68,73	1.28	6 (9%)	76,107,113	0.95	4 (5%)
23	BCR	B	848	-	41,41,41	1.45	8 (19%)	56,56,56	2.07	14 (25%)
23	BCR	A	852	-	41,41,41	1.47	7 (17%)	56,56,56	1.76	14 (25%)
23	BCR	K	205	-	41,41,41	1.37	8 (19%)	56,56,56	1.47	12 (21%)
27	LMU	A	853	-	36,36,36	0.25	0	47,47,47	0.73	3 (6%)
19	CLA	B	837	6	56,60,73	1.37	7 (12%)	65,97,113	1.04	4 (6%)
19	CLA	A	803	-	69,73,73	1.17	7 (10%)	82,113,113	0.91	4 (4%)
26	SF4	C	101	7	0,12,12	-	-	-	-	-
19	CLA	A	819	5	61,65,73	1.27	7 (11%)	72,103,113	1.06	6 (8%)
20	LUT	2	317	-	42,43,43	1.29	8 (19%)	51,60,60	1.87	13 (25%)
23	BCR	2	319	-	41,41,41	1.47	6 (14%)	56,56,56	2.11	19 (33%)
19	CLA	3	312	3	46,50,73	1.45	6 (13%)	53,85,113	1.09	4 (7%)
19	CLA	B	841	6	69,73,73	1.26	8 (11%)	82,113,113	0.89	3 (3%)
19	CLA	B	827	6	69,73,73	1.24	8 (11%)	82,113,113	0.91	3 (3%)
19	CLA	K	201	30	55,59,73	1.30	7 (12%)	64,96,113	1.10	6 (9%)
23	BCR	A	850	-	41,41,41	1.45	7 (17%)	56,56,56	1.61	13 (23%)
19	CLA	L	301	17	49,53,73	1.40	8 (16%)	58,89,113	1.11	5 (8%)
19	CLA	A	834	5	69,73,73	1.24	8 (11%)	82,113,113	0.93	3 (3%)
23	BCR	G	205	-	41,41,41	1.44	9 (21%)	56,56,56	1.69	14 (25%)
18	CHL	5	313	4	37,51,74	1.15	2 (5%)	30,86,114	3.04	11 (36%)
19	CLA	B	810	6	69,73,73	1.20	8 (11%)	82,113,113	0.95	6 (7%)
19	CLA	6	308	1	54,58,73	1.34	8 (14%)	64,95,113	1.04	3 (4%)
19	CLA	A	813	5	58,62,73	1.27	8 (13%)	68,99,113	0.96	4 (5%)
19	CLA	A	833	5	59,63,73	1.29	8 (13%)	70,101,113	0.99	5 (7%)
19	CLA	B	819	6	69,73,73	1.15	7 (10%)	82,113,113	0.93	4 (4%)
23	BCR	I	101	-	41,41,41	1.46	4 (9%)	56,56,56	1.63	14 (25%)
19	CLA	A	823	5	49,53,73	1.41	7 (14%)	58,89,113	1.10	5 (8%)
27	LMU	G	202	-	36,36,36	0.26	0	47,47,47	0.70	1 (2%)
19	CLA	B	829	6	69,73,73	1.20	6 (8%)	82,113,113	0.82	3 (3%)
19	CLA	3	313	30	49,53,73	1.38	8 (16%)	58,89,113	1.12	4 (6%)
19	CLA	B	813	6	49,53,73	1.39	7 (14%)	58,89,113	1.10	5 (8%)
23	BCR	F	305	-	41,41,41	1.43	7 (17%)	56,56,56	1.73	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	826	30	69,73,73	1.25	7 (10%)	82,113,113	0.98	5 (6%)
19	CLA	A	838	5	55,59,73	1.37	8 (14%)	64,96,113	1.09	6 (9%)
23	BCR	M	101	-	41,41,41	1.45	7 (17%)	56,56,56	1.68	15 (26%)
19	CLA	B	808	6	64,68,73	1.21	6 (9%)	76,107,113	0.96	4 (5%)
19	CLA	3	307	3	64,68,73	1.19	7 (10%)	76,107,113	1.13	6 (7%)
18	CHL	2	320	4	46,60,74	1.20	2 (4%)	40,97,114	2.63	8 (20%)
19	CLA	5	311	4	65,69,73	1.18	6 (9%)	77,108,113	1.03	5 (6%)
19	CLA	6	307	30	49,53,73	1.44	6 (12%)	58,89,113	1.19	6 (10%)
19	CLA	3	308	3	69,73,73	1.13	6 (8%)	82,113,113	0.98	4 (4%)
19	CLA	A	810	5	69,73,73	1.16	8 (11%)	82,113,113	0.92	4 (4%)
19	CLA	A	840	5	54,58,73	1.38	6 (11%)	64,95,113	1.05	4 (6%)
19	CLA	A	835	5	69,73,73	1.20	7 (10%)	82,113,113	0.90	4 (4%)
19	CLA	A	825	5	69,73,73	1.21	8 (11%)	82,113,113	1.00	6 (7%)
19	CLA	A	809	5	52,56,73	1.41	6 (11%)	61,92,113	1.01	4 (6%)
20	LUT	2	315	-	42,43,43	1.31	8 (19%)	51,60,60	1.72	13 (25%)
19	CLA	B	821	6	47,51,73	1.41	7 (14%)	55,86,113	1.07	4 (7%)
20	LUT	3	315	-	42,43,43	1.34	5 (11%)	51,60,60	1.72	14 (27%)
19	CLA	B	838	6	69,73,73	1.16	7 (10%)	82,113,113	0.93	4 (4%)
19	CLA	A	839	5	59,63,73	1.28	7 (11%)	70,101,113	0.95	3 (4%)
19	CLA	K	203	14	49,53,73	1.37	6 (12%)	58,89,113	1.04	4 (6%)
19	CLA	A	806	5	59,63,73	1.26	7 (11%)	70,101,113	0.95	4 (5%)
18	CHL	2	307	30	43,57,74	1.07	3 (6%)	37,93,114	2.86	10 (27%)
18	CHL	3	314	3	60,74,74	1.11	3 (5%)	58,114,114	2.20	12 (20%)
19	CLA	B	802	30	69,73,73	1.16	7 (10%)	82,113,113	0.91	5 (6%)
23	BCR	A	851	-	41,41,41	1.46	5 (12%)	56,56,56	1.72	15 (26%)
19	CLA	2	310	22	60,64,73	1.26	7 (11%)	71,102,113	0.98	4 (5%)
19	CLA	B	828	6	69,73,73	1.20	7 (10%)	82,113,113	0.92	4 (4%)
19	CLA	2	311	2	49,53,73	1.45	6 (12%)	58,89,113	1.06	4 (6%)
19	CLA	3	311	3	59,63,73	1.29	9 (15%)	70,101,113	1.12	5 (7%)
19	CLA	B	839	6	51,55,73	1.39	6 (11%)	60,91,113	1.04	5 (8%)
19	CLA	6	309	1	69,73,73	1.13	6 (8%)	82,113,113	0.94	5 (6%)
19	CLA	B	842	-	69,73,73	1.17	7 (10%)	82,113,113	0.89	5 (6%)
19	CLA	B	816	6	69,73,73	1.21	8 (11%)	82,113,113	0.98	5 (6%)
19	CLA	3	302	3	59,63,73	1.36	8 (13%)	70,101,113	0.97	4 (5%)
19	CLA	A	821	5	49,53,73	1.40	7 (14%)	58,89,113	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	309	30	59,63,73	1.28	7 (11%)	70,101,113	1.00	4 (5%)
19	CLA	A	822	30	69,73,73	1.16	8 (11%)	82,113,113	0.91	4 (4%)
25	PQN	A	844	-	34,34,34	0.36	0	43,45,45	0.69	1 (2%)
19	CLA	B	825	30	69,73,73	1.17	8 (11%)	82,113,113	1.02	6 (7%)
20	LUT	6	318	-	42,43,43	1.33	8 (19%)	51,60,60	2.03	19 (37%)
23	BCR	B	844	-	41,41,41	1.44	6 (14%)	56,56,56	1.74	17 (30%)
19	CLA	A	843	22	49,53,73	1.40	8 (16%)	58,89,113	1.04	4 (6%)
18	CHL	2	306	30	37,51,74	1.19	3 (8%)	30,86,114	3.20	12 (40%)
19	CLA	A	817	30	49,53,73	1.38	5 (10%)	58,89,113	1.17	5 (8%)
18	CHL	3	306	30	40,54,74	1.08	3 (7%)	34,90,114	2.88	11 (32%)
19	CLA	6	302	1	65,69,73	1.19	7 (10%)	77,108,113	0.95	4 (5%)
27	LMU	B	850	-	36,36,36	0.25	0	47,47,47	0.42	0
23	BCR	5	317	-	41,41,41	1.44	9 (21%)	56,56,56	1.94	18 (32%)
19	CLA	A	818	5	64,68,73	1.31	8 (12%)	76,107,113	1.06	6 (7%)
20	LUT	5	315	-	42,43,43	1.31	8 (19%)	51,60,60	1.54	9 (17%)
19	CLA	6	305	30	49,53,73	1.39	6 (12%)	58,89,113	1.04	3 (5%)
19	CLA	A	811	5	59,63,73	1.30	7 (11%)	70,101,113	0.94	3 (4%)
23	BCR	3	317	-	41,41,41	1.46	7 (17%)	56,56,56	1.82	19 (33%)
19	CLA	6	312	1	69,73,73	1.14	7 (10%)	82,113,113	1.10	5 (6%)
18	CHL	2	301	2	60,74,74	0.94	2 (3%)	58,114,114	2.38	11 (18%)
23	BCR	A	849	-	41,41,41	1.46	7 (17%)	56,56,56	1.69	16 (28%)
19	CLA	A	815	5	55,59,73	1.34	7 (12%)	64,96,113	1.03	6 (9%)
23	BCR	B	846	-	41,41,41	1.44	8 (19%)	56,56,56	2.10	18 (32%)
19	CLA	B	818	6	66,70,73	1.24	7 (10%)	78,109,113	1.08	6 (7%)
19	CLA	B	833	6	69,73,73	1.21	7 (10%)	82,113,113	0.96	5 (6%)
20	LUT	5	316	-	42,43,43	1.30	8 (19%)	51,60,60	1.80	13 (25%)
19	CLA	B	811	6	69,73,73	1.19	7 (10%)	82,113,113	0.91	3 (3%)
19	CLA	5	307	4	63,67,73	1.19	6 (9%)	74,105,113	1.04	5 (6%)
19	CLA	F	303	30	49,53,73	1.38	6 (12%)	58,89,113	1.06	3 (5%)
19	CLA	A	816	5	46,50,73	1.44	7 (15%)	53,85,113	1.10	5 (9%)
19	CLA	5	302	4	54,58,73	1.39	7 (12%)	64,95,113	1.00	3 (4%)
23	BCR	G	201	-	41,41,41	1.48	5 (12%)	56,56,56	1.71	15 (26%)
19	CLA	G	204	11	49,53,73	1.39	7 (14%)	58,89,113	1.04	5 (8%)
19	CLA	B	835	6	49,53,73	1.37	6 (12%)	58,89,113	1.05	4 (6%)
19	CLA	A	841	5	69,73,73	1.18	7 (10%)	82,113,113	0.89	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	J	105	-	41,41,55	0.53	0	49,49,63	0.69	0
26	SF4	C	102	7	0,12,12	-	-	-		
19	CLA	B	826	30	57,61,73	1.25	7 (12%)	67,98,113	0.98	4 (5%)
19	CLA	A	837	5	49,53,73	1.38	7 (14%)	58,89,113	1.14	4 (6%)

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
19	CLA	J	102	13	1/1/10/20	0/12/88/115	-
19	CLA	B	840	30	-	5/39/115/115	-
20	LUT	J	101	-	-	2/29/67/67	0/2/2/2
19	CLA	G	203	11	1/1/11/20	4/15/91/115	-
19	CLA	B	823	6	1/1/13/20	3/27/103/115	-
19	CLA	5	310	4	1/1/11/20	7/13/89/115	-
19	CLA	B	831	6	-	4/15/91/115	-
23	BCR	L	304	-	-	2/29/63/63	0/2/2/2
28	DGD	B	849	-	-	21/55/95/95	0/2/2/2
19	CLA	3	310	3	1/1/10/20	1/13/89/115	-
23	BCR	F	302	-	-	2/29/63/63	0/2/2/2
19	CLA	L	302	17	-	4/33/109/115	-
23	BCR	B	845	-	-	5/29/63/63	0/2/2/2
19	CLA	A	827	30	1/1/13/20	0/27/103/115	-
19	CLA	A	828	5	1/1/15/20	15/39/115/115	-
19	CLA	2	303	2	1/1/11/20	4/15/91/115	-
19	CLA	A	808	5	1/1/15/20	9/39/115/115	-
23	BCR	K	204	-	-	3/29/63/63	0/2/2/2
19	CLA	A	807	5	1/1/15/20	4/39/115/115	-
19	CLA	2	309	2	1/1/14/20	6/35/111/115	-
19	CLA	F	304	10	1/1/10/20	2/10/86/115	-
19	CLA	6	313	1	1/1/11/20	2/15/91/115	-
19	CLA	A	832	5	-	0/21/97/115	-
19	CLA	B	801	30	1/1/15/20	7/39/115/115	-
19	CLA	3	305	3	1/1/11/20	0/17/93/115	-
19	CLA	6	310	22	1/1/13/20	1/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	6	304	30	1/1/11/20	2/20/96/115	-
19	CLA	6	311	1	1/1/11/20	5/15/91/115	-
20	LUT	2	316	-	-	0/29/67/67	0/2/2/2
19	CLA	B	807	6	1/1/15/20	5/39/115/115	-
19	CLA	B	836	30	1/1/11/20	1/15/91/115	-
19	CLA	B	832	6	1/1/15/20	3/39/115/115	-
19	CLA	B	815	6	1/1/15/20	3/39/115/115	-
19	CLA	2	302	2	1/1/15/20	6/39/115/115	-
19	CLA	A	842	5	1/1/15/20	0/39/115/115	-
19	CLA	K	202	14	1/1/11/20	2/13/89/115	-
19	CLA	5	301	4	-	3/33/109/115	-
19	CLA	B	822	6	-	0/17/93/115	-
19	CLA	A	824	5	1/1/15/20	2/39/115/115	-
19	CLA	2	312	2	-	0/39/115/115	-
19	CLA	B	805	6	-	3/15/91/115	-
22	LHG	A	846	-	-	6/53/53/53	-
23	BCR	B	847	-	-	0/29/63/63	0/2/2/2
19	CLA	5	303	30	1/1/11/20	1/15/91/115	-
19	CLA	B	803	6	1/1/15/20	1/39/115/115	-
18	CHL	5	305	30	3/3/15/26	2/12/110/137	-
29	LMG	J	104	-	-	6/25/45/70	0/1/1/1
19	CLA	3	303	30	1/1/11/20	1/18/94/115	-
19	CLA	B	814	6	1/1/15/20	6/39/115/115	-
22	LHG	6	319	-	-	2/31/31/53	-
19	CLA	2	304	30	1/1/12/20	2/21/97/115	-
22	LHG	A	847	19	-	4/38/38/53	-
19	CLA	A	805	5	1/1/15/20	4/39/115/115	-
23	BCR	A	848	-	-	5/29/63/63	0/2/2/2
19	CLA	5	308	4	1/1/14/20	4/33/109/115	-
21	XAT	6	316	-	-	1/31/93/93	0/4/4/4
19	CLA	L	303	30	1/1/10/20	1/12/88/115	-
18	CHL	5	304	30	3/3/16/26	3/15/113/137	-
26	SF4	A	845	5,6	-	-	0/6/5/5
18	CHL	6	306	1	3/3/16/26	4/15/113/137	-
19	CLA	6	314	1	1/1/11/20	4/15/91/115	-
19	CLA	5	309	30	1/1/14/20	0/33/109/115	-
22	LHG	5	318	-	-	7/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	801	5	-	6/27/103/115	-
19	CLA	A	836	5	-	3/33/109/115	-
19	CLA	B	817	6	-	2/39/115/115	-
23	BCR	J	103	-	-	6/29/63/63	0/2/2/2
19	CLA	B	809	6	1/1/15/20	2/39/115/115	-
18	CHL	5	306	30	3/3/16/26	4/15/113/137	-
19	CLA	A	829	5	1/1/15/20	4/39/115/115	-
19	CLA	B	804	-	1/1/15/20	1/39/115/115	-
20	LUT	3	316	-	-	3/29/67/67	0/2/2/2
27	LMU	B	851	-	-	4/21/61/61	0/2/2/2
19	CLA	2	313	2	1/1/12/20	2/21/97/115	-
19	CLA	B	824	6	-	1/15/91/115	-
19	CLA	A	830	5	1/1/15/20	4/39/115/115	-
20	LUT	6	315	-	-	2/29/67/67	0/2/2/2
18	CHL	2	305	30	3/3/16/26	4/15/113/137	-
19	CLA	3	304	30	1/1/11/20	3/15/91/115	-
19	CLA	2	308	2	1/1/11/20	0/15/91/115	-
19	CLA	A	820	5	1/1/15/20	5/39/115/115	-
19	CLA	A	812	5	1/1/15/20	7/39/115/115	-
19	CLA	B	834	6	-	2/33/109/115	-
19	CLA	B	830	6	-	4/33/109/115	-
25	PQN	B	843	-	-	1/23/43/43	0/2/2/2
18	CHL	6	301	1	3/3/17/26	2/21/119/137	-
19	CLA	F	301	30	1/1/14/20	2/33/109/115	-
22	LHG	2	318	19	-	3/42/42/53	-
18	CHL	2	314	2	3/3/16/26	4/15/113/137	-
19	CLA	B	820	30	-	0/30/106/115	-
19	CLA	A	804	30	1/1/15/20	3/39/115/115	-
19	CLA	A	814	5	1/1/15/20	5/39/115/115	-
19	CLA	5	314	4	-	5/15/91/115	-
19	CLA	A	831	5	-	4/39/115/115	-
19	CLA	6	303	1	1/1/13/20	3/27/103/115	-
19	CLA	B	806	6	1/1/15/20	4/39/115/115	-
22	LHG	6	317	19	-	7/53/53/53	-
19	CLA	5	312	4	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	L	305	-	-	3/29/63/63	0/2/2/2
24	CL0	A	802	5	-	3/37/135/135	-
19	CLA	3	301	3	1/1/14/20	3/33/109/115	-
19	CLA	B	812	6	1/1/14/20	4/33/109/115	-
23	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	BCR	A	852	-	-	7/29/63/63	0/2/2/2
23	BCR	K	205	-	-	17/29/63/63	0/2/2/2
27	LMU	A	853	-	-	4/21/61/61	0/2/2/2
19	CLA	B	837	6	1/1/12/20	3/24/100/115	-
19	CLA	A	803	-	1/1/15/20	4/39/115/115	-
26	SF4	C	101	7	-	-	0/6/5/5
19	CLA	A	819	5	-	5/30/106/115	-
20	LUT	2	317	-	-	3/29/67/67	0/2/2/2
23	BCR	2	319	-	-	8/29/63/63	0/2/2/2
19	CLA	3	312	3	1/1/10/20	1/12/88/115	-
19	CLA	B	841	6	-	1/39/115/115	-
19	CLA	B	827	6	1/1/15/20	0/39/115/115	-
19	CLA	K	201	30	-	5/23/99/115	-
23	BCR	A	850	-	-	0/29/63/63	0/2/2/2
19	CLA	L	301	17	1/1/11/20	1/15/91/115	-
19	CLA	A	834	5	1/1/15/20	2/39/115/115	-
23	BCR	G	205	-	-	0/29/63/63	0/2/2/2
18	CHL	5	313	4	3/3/15/26	1/12/110/137	-
19	CLA	B	810	6	1/1/15/20	4/39/115/115	-
19	CLA	6	308	1	1/1/12/20	1/21/97/115	-
19	CLA	A	813	5	1/1/12/20	1/26/102/115	-
19	CLA	B	819	6	1/1/15/20	8/39/115/115	-
19	CLA	A	833	5	-	2/27/103/115	-
23	BCR	I	101	-	-	0/29/63/63	0/2/2/2
19	CLA	A	823	5	-	5/15/91/115	-
27	LMU	G	202	-	-	7/21/61/61	0/2/2/2
19	CLA	B	829	6	1/1/15/20	2/39/115/115	-
19	CLA	3	313	30	1/1/11/20	5/15/91/115	-
19	CLA	B	813	6	-	3/15/91/115	-
23	BCR	F	305	-	-	3/29/63/63	0/2/2/2
19	CLA	A	826	30	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	838	5	1/1/12/20	5/23/99/115	-
23	BCR	M	101	-	-	2/29/63/63	0/2/2/2
19	CLA	B	808	6	1/1/14/20	1/33/109/115	-
19	CLA	3	307	3	1/1/14/20	6/33/109/115	-
18	CHL	2	320	4	3/3/17/26	2/23/121/137	-
19	CLA	5	311	4	-	2/35/111/115	-
19	CLA	6	307	30	1/1/11/20	2/15/91/115	-
19	CLA	3	308	3	1/1/15/20	1/39/115/115	-
19	CLA	A	810	5	1/1/15/20	5/39/115/115	-
19	CLA	A	840	5	1/1/12/20	1/21/97/115	-
19	CLA	A	835	5	1/1/15/20	2/39/115/115	-
19	CLA	A	825	5	-	3/39/115/115	-
19	CLA	A	809	5	1/1/11/20	0/19/95/115	-
20	LUT	2	315	-	-	2/29/67/67	0/2/2/2
19	CLA	B	821	6	1/1/10/20	1/13/89/115	-
20	LUT	3	315	-	-	4/29/67/67	0/2/2/2
19	CLA	B	838	6	1/1/15/20	5/39/115/115	-
19	CLA	A	839	5	1/1/13/20	0/27/103/115	-
19	CLA	K	203	14	1/1/11/20	5/15/91/115	-
19	CLA	A	806	5	1/1/13/20	2/27/103/115	-
18	CHL	2	307	30	2/2/16/26	3/19/117/137	-
18	CHL	3	314	3	3/3/20/26	8/39/137/137	-
19	CLA	B	802	30	1/1/15/20	6/39/115/115	-
23	BCR	A	851	-	-	0/29/63/63	0/2/2/2
19	CLA	2	310	22	1/1/13/20	0/29/105/115	-
19	CLA	B	828	6	1/1/15/20	3/39/115/115	-
19	CLA	2	311	2	1/1/11/20	5/15/91/115	-
19	CLA	B	839	6	1/1/11/20	2/18/94/115	-
19	CLA	3	311	3	-	5/27/103/115	-
19	CLA	6	309	1	1/1/15/20	9/39/115/115	-
19	CLA	B	842	-	1/1/15/20	17/39/115/115	-
19	CLA	B	816	6	-	9/39/115/115	-
19	CLA	3	302	3	1/1/13/20	1/27/103/115	-
19	CLA	A	821	5	1/1/11/20	2/15/91/115	-
19	CLA	3	309	30	1/1/13/20	0/27/103/115	-
19	CLA	A	822	30	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PQN	A	844	-	-	4/23/43/43	0/2/2/2
19	CLA	B	825	30	1/1/15/20	7/39/115/115	-
20	LUT	6	318	-	-	6/29/67/67	0/2/2/2
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
19	CLA	A	843	22	1/1/11/20	3/15/91/115	-
18	CHL	2	306	30	3/3/15/26	4/12/110/137	-
19	CLA	A	817	30	1/1/11/20	3/15/91/115	-
18	CHL	3	306	30	2/2/16/26	2/15/113/137	-
19	CLA	6	302	1	1/1/14/20	5/35/111/115	-
27	LMU	B	850	-	-	7/21/61/61	0/2/2/2
23	BCR	5	317	-	-	6/29/63/63	0/2/2/2
19	CLA	A	818	5	-	7/33/109/115	-
20	LUT	5	315	-	-	2/29/67/67	0/2/2/2
19	CLA	6	305	30	1/1/11/20	2/15/91/115	-
19	CLA	A	811	5	-	1/27/103/115	-
23	BCR	3	317	-	-	3/29/63/63	0/2/2/2
19	CLA	6	312	1	-	4/39/115/115	-
18	CHL	2	301	2	3/3/20/26	3/39/137/137	-
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
19	CLA	A	815	5	1/1/12/20	0/23/99/115	-
23	BCR	B	846	-	-	5/29/63/63	0/2/2/2
19	CLA	B	818	6	1/1/14/20	2/36/112/115	-
19	CLA	B	833	6	1/1/15/20	2/39/115/115	-
20	LUT	5	316	-	-	3/29/67/67	0/2/2/2
19	CLA	B	811	6	1/1/15/20	5/39/115/115	-
19	CLA	5	307	4	1/1/13/20	10/32/108/115	-
19	CLA	F	303	30	1/1/11/20	1/15/91/115	-
19	CLA	A	816	5	1/1/10/20	0/12/88/115	-
19	CLA	5	302	4	1/1/12/20	2/21/97/115	-
23	BCR	G	201	-	-	4/29/63/63	0/2/2/2
19	CLA	G	204	11	1/1/11/20	6/15/91/115	-
19	CLA	B	835	6	1/1/11/20	2/15/91/115	-
19	CLA	A	841	5	1/1/15/20	4/39/115/115	-
29	LMG	J	105	-	-	9/36/56/70	0/1/1/1
26	SF4	C	102	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	826	30	1/1/12/20	4/25/101/115	-
19	CLA	A	837	5	1/1/11/20	2/15/91/115	-

All (1270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	314	CHL	C2C-C3C	5.79	1.42	1.36
18	2	320	CHL	C2C-C3C	5.73	1.41	1.36
18	2	305	CHL	C2C-C3C	5.62	1.41	1.36
18	5	304	CHL	C2C-C3C	5.62	1.41	1.36
19	A	831	CLA	MG-NA	4.93	2.18	2.06
19	B	823	CLA	MG-NA	4.88	2.17	2.06
19	B	837	CLA	MG-NA	4.79	2.17	2.06
19	B	827	CLA	MG-NA	4.78	2.17	2.06
19	A	830	CLA	MG-NA	4.77	2.17	2.06
19	3	302	CLA	MG-NA	4.73	2.17	2.06
19	5	302	CLA	C4C-C3C	-4.73	1.37	1.45
19	A	838	CLA	MG-NA	4.72	2.17	2.06
19	A	826	CLA	MG-NA	4.66	2.17	2.06
19	3	310	CLA	MG-NA	4.62	2.17	2.06
19	5	314	CLA	MG-NA	4.61	2.17	2.06
19	B	821	CLA	C4C-C3C	-4.60	1.37	1.45
19	A	809	CLA	MG-NA	4.59	2.17	2.06
19	B	829	CLA	C4C-C3C	-4.57	1.37	1.45
19	B	807	CLA	C4C-C3C	-4.57	1.37	1.45
19	B	831	CLA	C4C-C3C	-4.57	1.37	1.45
19	B	819	CLA	C4C-C3C	-4.57	1.37	1.45
19	B	842	CLA	C4C-C3C	-4.56	1.37	1.45
19	A	833	CLA	C4C-C3C	-4.56	1.37	1.45
19	B	805	CLA	MG-NA	4.56	2.17	2.06
19	A	828	CLA	C4C-C3C	-4.56	1.37	1.45
19	B	827	CLA	C4C-C3C	-4.56	1.37	1.45
19	B	833	CLA	MG-NA	4.56	2.17	2.06
19	G	203	CLA	MG-NA	4.54	2.17	2.06
19	A	806	CLA	C4C-C3C	-4.54	1.37	1.45
19	2	311	CLA	MG-NA	4.54	2.17	2.06
19	5	308	CLA	C4C-C3C	-4.54	1.37	1.45
19	A	836	CLA	C4C-C3C	-4.54	1.37	1.45
19	B	812	CLA	MG-NA	4.53	2.17	2.06
19	B	841	CLA	C4C-C3C	-4.53	1.37	1.45
19	B	803	CLA	C4C-C3C	-4.52	1.37	1.45
19	A	818	CLA	MG-NA	4.52	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	803	CLA	C4C-C3C	-4.52	1.37	1.45
19	2	311	CLA	C4C-C3C	-4.51	1.37	1.45
19	3	310	CLA	C4C-C3C	-4.51	1.37	1.45
19	B	809	CLA	C4C-C3C	-4.51	1.37	1.45
19	L	302	CLA	C4C-C3C	-4.51	1.37	1.45
19	B	818	CLA	C4C-C3C	-4.50	1.37	1.45
19	6	309	CLA	C4C-C3C	-4.50	1.37	1.45
19	6	311	CLA	C4C-C3C	-4.50	1.37	1.45
19	A	827	CLA	C4C-C3C	-4.50	1.37	1.45
19	A	810	CLA	C4C-C3C	-4.49	1.37	1.45
19	L	301	CLA	C4C-C3C	-4.49	1.37	1.45
19	F	301	CLA	C4C-C3C	-4.49	1.37	1.45
19	3	301	CLA	C4C-C3C	-4.49	1.37	1.45
19	B	838	CLA	C4C-C3C	-4.49	1.37	1.45
19	A	811	CLA	C4C-C3C	-4.49	1.37	1.45
19	5	303	CLA	C4C-C3C	-4.49	1.37	1.45
19	B	826	CLA	C4C-C3C	-4.49	1.37	1.45
19	B	805	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	812	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	829	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	815	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	826	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	805	CLA	C4C-C3C	-4.48	1.37	1.45
19	2	309	CLA	C4C-C3C	-4.48	1.37	1.45
19	K	201	CLA	C4C-C3C	-4.48	1.37	1.45
19	6	303	CLA	C4C-C3C	-4.48	1.37	1.45
19	2	303	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	813	CLA	C4C-C3C	-4.48	1.37	1.45
19	A	832	CLA	C4C-C3C	-4.48	1.37	1.45
19	2	310	CLA	C4C-C3C	-4.47	1.37	1.45
19	A	834	CLA	C4C-C3C	-4.47	1.37	1.45
19	F	303	CLA	C4C-C3C	-4.47	1.37	1.45
19	A	809	CLA	C4C-C3C	-4.47	1.37	1.45
19	5	301	CLA	C4C-C3C	-4.47	1.37	1.45
19	B	811	CLA	C4C-C3C	-4.46	1.37	1.45
19	5	314	CLA	C4C-C3C	-4.46	1.37	1.45
19	A	842	CLA	C4C-C3C	-4.46	1.37	1.45
19	5	309	CLA	C4C-C3C	-4.46	1.37	1.45
19	A	818	CLA	C4C-C3C	-4.46	1.37	1.45
19	6	313	CLA	C4C-C3C	-4.46	1.37	1.45
19	K	202	CLA	C4C-C3C	-4.46	1.37	1.45
19	2	304	CLA	C4C-C3C	-4.46	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	813	CLA	C4C-C3C	-4.46	1.37	1.45
19	A	823	CLA	C4C-C3C	-4.45	1.37	1.45
19	6	310	CLA	C4C-C3C	-4.45	1.37	1.45
19	A	807	CLA	C4C-C3C	-4.45	1.37	1.45
19	B	810	CLA	C4C-C3C	-4.45	1.37	1.45
19	2	308	CLA	C4C-C3C	-4.45	1.37	1.45
19	B	825	CLA	C4C-C3C	-4.45	1.37	1.45
19	B	817	CLA	C4C-C3C	-4.44	1.37	1.45
19	K	203	CLA	C4C-C3C	-4.44	1.37	1.45
19	B	828	CLA	C4C-C3C	-4.44	1.37	1.45
19	A	801	CLA	C4C-C3C	-4.44	1.37	1.45
19	6	307	CLA	MG-NA	4.44	2.16	2.06
19	6	304	CLA	C4C-C3C	-4.44	1.37	1.45
19	2	312	CLA	C4C-C3C	-4.43	1.37	1.45
19	3	303	CLA	C4C-C3C	-4.43	1.37	1.45
19	B	839	CLA	C4C-C3C	-4.43	1.37	1.45
19	A	821	CLA	C4C-C3C	-4.43	1.37	1.45
19	A	835	CLA	C4C-C3C	-4.43	1.37	1.45
19	A	830	CLA	C4C-C3C	-4.43	1.37	1.45
19	A	841	CLA	C4C-C3C	-4.43	1.37	1.45
19	3	304	CLA	C4C-C3C	-4.43	1.37	1.45
19	B	840	CLA	C4C-C3C	-4.42	1.37	1.45
19	6	308	CLA	C4C-C3C	-4.42	1.37	1.45
19	3	309	CLA	C4C-C3C	-4.42	1.37	1.45
19	A	808	CLA	C4C-C3C	-4.42	1.37	1.45
19	B	835	CLA	C4C-C3C	-4.42	1.37	1.45
19	3	312	CLA	C4C-C3C	-4.42	1.37	1.45
19	F	304	CLA	C4C-C3C	-4.42	1.37	1.45
19	B	814	CLA	MG-NA	4.42	2.16	2.06
19	3	308	CLA	C4C-C3C	-4.42	1.37	1.45
19	3	305	CLA	C4C-C3C	-4.42	1.37	1.45
19	B	832	CLA	C4C-C3C	-4.41	1.37	1.45
19	B	834	CLA	C4C-C3C	-4.41	1.37	1.45
19	J	102	CLA	C4C-C3C	-4.41	1.37	1.45
19	6	312	CLA	C4C-C3C	-4.41	1.37	1.45
19	A	831	CLA	C4C-C3C	-4.41	1.37	1.45
19	A	843	CLA	C4C-C3C	-4.41	1.37	1.45
19	B	822	CLA	C4C-C3C	-4.41	1.37	1.45
19	B	824	CLA	C4C-C3C	-4.41	1.37	1.45
19	B	815	CLA	C4C-C3C	-4.41	1.37	1.45
19	3	313	CLA	C4C-C3C	-4.40	1.37	1.45
19	A	837	CLA	C4C-C3C	-4.40	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	302	CLA	C4C-C3C	-4.40	1.37	1.45
19	5	312	CLA	C4C-C3C	-4.39	1.37	1.45
19	G	203	CLA	C4C-C3C	-4.39	1.37	1.45
19	A	816	CLA	C4C-C3C	-4.39	1.37	1.45
19	A	840	CLA	MG-NA	4.39	2.16	2.06
19	B	801	CLA	C4C-C3C	-4.39	1.37	1.45
19	A	838	CLA	C4C-C3C	-4.39	1.37	1.45
19	B	836	CLA	C4C-C3C	-4.38	1.37	1.45
19	G	204	CLA	C4C-C3C	-4.38	1.37	1.45
19	A	840	CLA	C4C-C3C	-4.38	1.37	1.45
19	6	307	CLA	C4C-C3C	-4.38	1.37	1.45
19	B	804	CLA	C4C-C3C	-4.38	1.37	1.45
19	3	311	CLA	C4C-C3C	-4.37	1.37	1.45
19	A	820	CLA	C4C-C3C	-4.37	1.37	1.45
19	B	816	CLA	C4C-C3C	-4.37	1.37	1.45
19	A	822	CLA	C4C-C3C	-4.37	1.37	1.45
19	B	830	CLA	C4C-C3C	-4.37	1.37	1.45
19	B	812	CLA	C4C-C3C	-4.37	1.37	1.45
19	6	302	CLA	C4C-C3C	-4.37	1.37	1.45
19	B	808	CLA	C4C-C3C	-4.36	1.37	1.45
19	B	823	CLA	C4C-C3C	-4.36	1.37	1.45
19	B	817	CLA	MG-NA	4.36	2.16	2.06
19	A	804	CLA	C4C-C3C	-4.36	1.37	1.45
19	A	839	CLA	C4C-C3C	-4.36	1.37	1.45
19	B	837	CLA	C4C-C3C	-4.35	1.37	1.45
19	2	313	CLA	C4C-C3C	-4.35	1.37	1.45
19	B	832	CLA	MG-NA	4.35	2.16	2.06
19	5	311	CLA	C4C-C3C	-4.35	1.37	1.45
19	A	814	CLA	C4C-C3C	-4.35	1.37	1.45
19	B	806	CLA	C4C-C3C	-4.34	1.37	1.45
19	6	305	CLA	C4C-C3C	-4.34	1.37	1.45
19	A	825	CLA	C4C-C3C	-4.34	1.37	1.45
19	2	313	CLA	MG-NA	4.34	2.16	2.06
19	3	302	CLA	C4C-C3C	-4.34	1.37	1.45
19	3	307	CLA	C4C-C3C	-4.33	1.37	1.45
19	B	816	CLA	MG-NA	4.33	2.16	2.06
19	2	303	CLA	MG-NA	4.32	2.16	2.06
19	B	833	CLA	C4C-C3C	-4.32	1.37	1.45
19	A	824	CLA	C4C-C3C	-4.32	1.37	1.45
19	B	820	CLA	C4C-C3C	-4.32	1.37	1.45
19	B	831	CLA	MG-NA	4.32	2.16	2.06
19	6	314	CLA	C4C-C3C	-4.31	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	MG-NA	4.31	2.16	2.06
19	6	311	CLA	MG-NA	4.30	2.16	2.06
19	B	818	CLA	MG-NA	4.29	2.16	2.06
19	B	802	CLA	C4C-C3C	-4.28	1.37	1.45
19	B	810	CLA	C1C-C2C	-4.28	1.35	1.44
19	3	307	CLA	C1C-C2C	-4.27	1.35	1.44
19	5	307	CLA	C1C-C2C	-4.27	1.35	1.44
19	5	302	CLA	MG-NA	4.27	2.16	2.06
19	A	835	CLA	C1C-C2C	-4.27	1.35	1.44
19	3	312	CLA	MG-NA	4.26	2.16	2.06
19	5	307	CLA	C4C-C3C	-4.26	1.37	1.45
19	A	815	CLA	MG-NA	4.25	2.16	2.06
19	A	817	CLA	C4C-C3C	-4.25	1.37	1.45
19	B	814	CLA	C4C-C3C	-4.24	1.37	1.45
19	B	804	CLA	C1C-C2C	-4.23	1.35	1.44
19	A	839	CLA	MG-NA	4.22	2.16	2.06
19	L	303	CLA	C4C-C3C	-4.22	1.37	1.45
19	A	811	CLA	MG-NA	4.21	2.16	2.06
19	B	827	CLA	C1C-C2C	-4.21	1.36	1.44
19	6	303	CLA	MG-NA	4.21	2.16	2.06
19	B	807	CLA	MG-NA	4.21	2.16	2.06
19	B	809	CLA	C1C-C2C	-4.20	1.36	1.44
18	2	306	CHL	C2C-C3C	4.20	1.40	1.36
19	2	312	CLA	MG-NA	4.19	2.16	2.06
18	5	305	CHL	C2C-C3C	4.19	1.40	1.36
19	B	822	CLA	MG-NA	4.18	2.16	2.06
19	B	839	CLA	MG-NA	4.18	2.16	2.06
19	B	815	CLA	MG-NA	4.18	2.16	2.06
19	3	302	CLA	C1C-C2C	-4.17	1.36	1.44
19	A	807	CLA	C1C-C2C	-4.17	1.36	1.44
19	A	842	CLA	MG-NA	4.17	2.16	2.06
19	A	819	CLA	C4C-C3C	-4.17	1.38	1.45
19	B	816	CLA	C1C-C2C	-4.17	1.36	1.44
19	A	819	CLA	MG-NA	4.16	2.16	2.06
18	6	306	CHL	C2C-C3C	4.16	1.40	1.36
19	A	831	CLA	C1C-C2C	-4.16	1.36	1.44
19	A	828	CLA	C1C-C2C	-4.15	1.36	1.44
19	B	841	CLA	C1C-C2C	-4.15	1.36	1.44
19	A	830	CLA	C1C-C2C	-4.14	1.36	1.44
19	L	301	CLA	MG-NA	4.14	2.16	2.06
19	A	825	CLA	MG-NA	4.13	2.16	2.06
19	B	828	CLA	MG-NA	4.13	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	829	CLA	C1C-C2C	-4.13	1.36	1.44
19	B	801	CLA	MG-NA	4.13	2.16	2.06
18	2	301	CHL	C2C-C3C	4.13	1.40	1.36
19	F	301	CLA	MG-NA	4.13	2.16	2.06
19	5	312	CLA	MG-NA	4.13	2.16	2.06
18	6	301	CHL	C2C-C3C	4.12	1.40	1.36
19	6	313	CLA	MG-NA	4.12	2.16	2.06
19	A	805	CLA	C1C-C2C	-4.12	1.36	1.44
19	A	816	CLA	MG-NA	4.11	2.16	2.06
19	B	834	CLA	C1C-C2C	-4.11	1.36	1.44
19	A	817	CLA	C1C-C2C	-4.11	1.36	1.44
19	B	831	CLA	C1C-C2C	-4.11	1.36	1.44
19	A	840	CLA	C1C-C2C	-4.10	1.36	1.44
19	A	814	CLA	C1C-C2C	-4.10	1.36	1.44
19	B	814	CLA	C1C-C2C	-4.10	1.36	1.44
19	F	304	CLA	MG-NA	4.10	2.16	2.06
19	3	304	CLA	C1C-C2C	-4.10	1.36	1.44
19	K	202	CLA	C1C-C2C	-4.10	1.36	1.44
19	A	820	CLA	C1C-C2C	-4.10	1.36	1.44
19	B	824	CLA	C1C-C2C	-4.10	1.36	1.44
19	A	843	CLA	C1C-C2C	-4.09	1.36	1.44
19	2	313	CLA	C1C-C2C	-4.09	1.36	1.44
19	A	832	CLA	C1C-C2C	-4.09	1.36	1.44
19	F	303	CLA	C1C-C2C	-4.09	1.36	1.44
19	A	825	CLA	C1C-C2C	-4.09	1.36	1.44
19	B	801	CLA	C1C-C2C	-4.09	1.36	1.44
19	B	836	CLA	C1C-C2C	-4.09	1.36	1.44
19	5	310	CLA	C1C-C2C	-4.09	1.36	1.44
19	5	302	CLA	C1C-C2C	-4.09	1.36	1.44
19	A	811	CLA	C1C-C2C	-4.08	1.36	1.44
19	A	839	CLA	C1C-C2C	-4.08	1.36	1.44
19	A	832	CLA	MG-NA	4.08	2.16	2.06
19	A	824	CLA	C1C-C2C	-4.08	1.36	1.44
19	5	314	CLA	C1C-C2C	-4.07	1.36	1.44
19	A	824	CLA	MG-NA	4.07	2.15	2.06
19	B	823	CLA	C1C-C2C	-4.07	1.36	1.44
19	A	829	CLA	MG-NA	4.07	2.15	2.06
19	B	811	CLA	C1C-C2C	-4.07	1.36	1.44
19	J	102	CLA	MG-NA	4.07	2.15	2.06
19	A	813	CLA	C1C-C2C	-4.07	1.36	1.44
19	6	303	CLA	C1C-C2C	-4.07	1.36	1.44
18	2	314	CHL	C2C-C3C	4.07	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	307	CLA	C1C-C2C	-4.06	1.36	1.44
19	A	834	CLA	C1C-C2C	-4.06	1.36	1.44
19	B	819	CLA	C1C-C2C	-4.06	1.36	1.44
19	A	835	CLA	MG-NA	4.05	2.15	2.06
19	A	812	CLA	MG-NA	4.05	2.15	2.06
19	B	808	CLA	C1C-C2C	-4.05	1.36	1.44
19	A	819	CLA	C1C-C2C	-4.05	1.36	1.44
19	6	310	CLA	MG-NA	4.05	2.15	2.06
19	A	842	CLA	C1C-C2C	-4.05	1.36	1.44
19	3	308	CLA	C1C-C2C	-4.05	1.36	1.44
19	A	803	CLA	C1C-C2C	-4.04	1.36	1.44
19	2	304	CLA	C1C-C2C	-4.04	1.36	1.44
19	A	826	CLA	C1C-C2C	-4.04	1.36	1.44
19	B	832	CLA	C1C-C2C	-4.04	1.36	1.44
19	B	803	CLA	C1C-C2C	-4.04	1.36	1.44
19	6	310	CLA	C1C-C2C	-4.04	1.36	1.44
19	B	812	CLA	C1C-C2C	-4.04	1.36	1.44
19	A	804	CLA	C1C-C2C	-4.04	1.36	1.44
19	6	314	CLA	C1C-C2C	-4.04	1.36	1.44
19	2	310	CLA	C1C-C2C	-4.04	1.36	1.44
19	3	301	CLA	C1C-C2C	-4.04	1.36	1.44
19	B	835	CLA	C1C-C2C	-4.04	1.36	1.44
19	B	829	CLA	MG-NA	4.03	2.15	2.06
19	5	303	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	818	CLA	C1C-C2C	-4.03	1.36	1.44
19	5	310	CLA	MG-NA	4.03	2.15	2.06
19	A	823	CLA	MG-NA	4.03	2.15	2.06
19	A	838	CLA	C1C-C2C	-4.03	1.36	1.44
19	B	842	CLA	C1C-C2C	-4.03	1.36	1.44
19	2	308	CLA	C1C-C2C	-4.03	1.36	1.44
19	5	312	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	827	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	822	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	823	CLA	C1C-C2C	-4.03	1.36	1.44
19	G	204	CLA	MG-NA	4.03	2.15	2.06
19	B	839	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	816	CLA	C1C-C2C	-4.03	1.36	1.44
19	B	830	CLA	C1C-C2C	-4.03	1.36	1.44
19	A	841	CLA	C1C-C2C	-4.02	1.36	1.44
19	2	303	CLA	C1C-C2C	-4.02	1.36	1.44
19	2	311	CLA	C1C-C2C	-4.02	1.36	1.44
19	B	830	CLA	MG-NA	4.02	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	201	CLA	C1C-C2C	-4.02	1.36	1.44
19	6	304	CLA	C1C-C2C	-4.02	1.36	1.44
19	3	303	CLA	C1C-C2C	-4.02	1.36	1.44
19	L	301	CLA	C1C-C2C	-4.02	1.36	1.44
19	3	313	CLA	C1C-C2C	-4.02	1.36	1.44
19	L	303	CLA	MG-NA	4.02	2.15	2.06
19	A	821	CLA	C1C-C2C	-4.02	1.36	1.44
19	3	309	CLA	MG-NA	4.02	2.15	2.06
19	L	303	CLA	C1C-C2C	-4.02	1.36	1.44
19	6	305	CLA	MG-NA	4.01	2.15	2.06
19	B	817	CLA	C1C-C2C	-4.01	1.36	1.44
19	6	311	CLA	C1C-C2C	-4.01	1.36	1.44
19	A	808	CLA	C1C-C2C	-4.01	1.36	1.44
19	A	837	CLA	C1C-C2C	-4.01	1.36	1.44
19	3	309	CLA	C1C-C2C	-4.01	1.36	1.44
19	A	821	CLA	MG-NA	4.01	2.15	2.06
19	6	308	CLA	C1C-C2C	-4.01	1.36	1.44
19	B	818	CLA	C1C-C2C	-4.01	1.36	1.44
19	A	814	CLA	MG-NA	4.00	2.15	2.06
19	B	813	CLA	C1C-C2C	-4.00	1.36	1.44
19	A	806	CLA	C1C-C2C	-4.00	1.36	1.44
19	5	309	CLA	C1C-C2C	-4.00	1.36	1.44
19	A	815	CLA	C1C-C2C	-4.00	1.36	1.44
19	B	825	CLA	C1C-C2C	-4.00	1.36	1.44
19	A	812	CLA	C1C-C2C	-3.99	1.36	1.44
19	A	836	CLA	C1C-C2C	-3.99	1.36	1.44
19	5	308	CLA	C1C-C2C	-3.99	1.36	1.44
19	B	815	CLA	C1C-C2C	-3.99	1.36	1.44
19	B	826	CLA	C1C-C2C	-3.99	1.36	1.44
19	3	312	CLA	C1C-C2C	-3.99	1.36	1.44
19	J	102	CLA	C1C-C2C	-3.99	1.36	1.44
19	G	203	CLA	C1C-C2C	-3.99	1.36	1.44
19	L	302	CLA	C1C-C2C	-3.99	1.36	1.44
19	G	204	CLA	C1C-C2C	-3.98	1.36	1.44
19	3	310	CLA	C1C-C2C	-3.98	1.36	1.44
19	5	301	CLA	C1C-C2C	-3.98	1.36	1.44
19	B	822	CLA	C1C-C2C	-3.98	1.36	1.44
19	A	810	CLA	C1C-C2C	-3.98	1.36	1.44
19	2	312	CLA	C1C-C2C	-3.98	1.36	1.44
19	2	302	CLA	C1C-C2C	-3.98	1.36	1.44
19	3	311	CLA	C1C-C2C	-3.98	1.36	1.44
19	6	309	CLA	C1C-C2C	-3.97	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	305	CLA	C1C-C2C	-3.97	1.36	1.44
19	3	305	CLA	C1C-C2C	-3.97	1.36	1.44
19	B	821	CLA	C1C-C2C	-3.97	1.36	1.44
19	B	833	CLA	C1C-C2C	-3.97	1.36	1.44
19	3	305	CLA	MG-NA	3.97	2.15	2.06
19	A	801	CLA	C1C-C2C	-3.97	1.36	1.44
19	6	302	CLA	C1C-C2C	-3.97	1.36	1.44
19	B	802	CLA	MG-NA	3.96	2.15	2.06
19	B	837	CLA	C1C-C2C	-3.96	1.36	1.44
19	5	311	CLA	C1C-C2C	-3.96	1.36	1.44
19	B	840	CLA	C1C-C2C	-3.96	1.36	1.44
19	A	833	CLA	MG-NA	3.95	2.15	2.06
19	B	828	CLA	C1C-C2C	-3.95	1.36	1.44
19	B	806	CLA	C1C-C2C	-3.95	1.36	1.44
19	K	203	CLA	C1C-C2C	-3.95	1.36	1.44
19	3	311	CLA	MG-NA	3.95	2.15	2.06
19	6	312	CLA	C1C-C2C	-3.95	1.36	1.44
18	2	307	CHL	C2C-C3C	3.94	1.40	1.36
19	B	813	CLA	MG-NA	3.94	2.15	2.06
19	2	309	CLA	C1C-C2C	-3.94	1.36	1.44
19	B	838	CLA	C1C-C2C	-3.94	1.36	1.44
19	B	834	CLA	MG-NA	3.94	2.15	2.06
19	6	313	CLA	C1C-C2C	-3.94	1.36	1.44
19	A	809	CLA	C1C-C2C	-3.93	1.36	1.44
19	A	833	CLA	C1C-C2C	-3.93	1.36	1.44
19	6	308	CLA	MG-NA	3.93	2.15	2.06
19	B	807	CLA	C1C-C2C	-3.93	1.36	1.44
19	A	817	CLA	MG-NA	3.92	2.15	2.06
19	A	843	CLA	MG-NA	3.92	2.15	2.06
19	B	803	CLA	MG-NA	3.91	2.15	2.06
19	F	304	CLA	C1C-C2C	-3.91	1.36	1.44
19	B	808	CLA	MG-NA	3.91	2.15	2.06
19	B	825	CLA	MG-NA	3.90	2.15	2.06
19	B	836	CLA	MG-NA	3.90	2.15	2.06
19	B	821	CLA	MG-NA	3.90	2.15	2.06
19	B	810	CLA	MG-NA	3.90	2.15	2.06
19	B	806	CLA	MG-NA	3.89	2.15	2.06
19	A	829	CLA	C1C-C2C	-3.89	1.36	1.44
19	B	820	CLA	MG-NA	3.89	2.15	2.06
19	2	310	CLA	MG-NA	3.89	2.15	2.06
19	A	841	CLA	MG-NA	3.89	2.15	2.06
18	5	313	CHL	C2C-C3C	3.89	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	202	CLA	MG-NA	3.89	2.15	2.06
19	B	802	CLA	C1C-C2C	-3.89	1.36	1.44
19	B	820	CLA	C1C-C2C	-3.88	1.36	1.44
19	B	805	CLA	C1C-C2C	-3.88	1.36	1.44
19	B	838	CLA	MG-NA	3.87	2.15	2.06
19	3	304	CLA	MG-NA	3.86	2.15	2.06
19	A	813	CLA	MG-NA	3.86	2.15	2.06
19	F	301	CLA	C1C-C2C	-3.85	1.36	1.44
19	A	804	CLA	MG-NA	3.84	2.15	2.06
19	6	314	CLA	MG-NA	3.83	2.15	2.06
19	B	841	CLA	MG-NA	3.83	2.15	2.06
19	5	309	CLA	MG-NA	3.83	2.15	2.06
19	K	201	CLA	MG-NA	3.82	2.15	2.06
19	6	304	CLA	MG-NA	3.82	2.15	2.06
19	B	811	CLA	MG-NA	3.82	2.15	2.06
19	5	303	CLA	MG-NA	3.81	2.15	2.06
19	A	808	CLA	MG-NA	3.81	2.15	2.06
19	A	828	CLA	MG-NA	3.81	2.15	2.06
19	6	302	CLA	MG-NA	3.80	2.15	2.06
19	2	304	CLA	MG-NA	3.80	2.15	2.06
19	3	303	CLA	MG-NA	3.79	2.15	2.06
19	A	801	CLA	MG-NA	3.78	2.15	2.06
19	5	301	CLA	MG-NA	3.77	2.15	2.06
19	3	313	CLA	MG-NA	3.77	2.15	2.06
19	L	302	CLA	MG-NA	3.74	2.15	2.06
19	F	303	CLA	MG-NA	3.74	2.15	2.06
19	A	806	CLA	MG-NA	3.73	2.15	2.06
19	A	836	CLA	MG-NA	3.72	2.15	2.06
19	K	203	CLA	MG-NA	3.72	2.15	2.06
19	A	837	CLA	MG-NA	3.71	2.15	2.06
19	B	809	CLA	MG-NA	3.67	2.15	2.06
19	A	822	CLA	MG-NA	3.67	2.15	2.06
19	B	803	CLA	MG-NC	3.65	2.14	2.06
19	2	302	CLA	MG-NA	3.64	2.14	2.06
19	B	835	CLA	MG-NA	3.62	2.14	2.06
19	A	810	CLA	MG-NA	3.62	2.14	2.06
19	B	842	CLA	MG-NA	3.57	2.14	2.06
19	A	805	CLA	MG-NA	3.55	2.14	2.06
19	5	311	CLA	MG-NA	3.55	2.14	2.06
19	3	301	CLA	MG-NA	3.54	2.14	2.06
19	B	819	CLA	MG-NA	3.53	2.14	2.06
20	3	315	LUT	C8-C9	-3.52	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	309	CLA	MG-NA	3.51	2.14	2.06
19	5	310	CLA	C4C-C3C	-3.51	1.37	1.44
18	3	306	CHL	C2C-C3C	3.51	1.39	1.36
19	A	820	CLA	MG-NA	3.50	2.14	2.06
23	B	847	BCR	C8-C9	-3.50	1.38	1.46
19	A	803	CLA	MG-NA	3.49	2.14	2.06
23	B	847	BCR	C23-C22	-3.47	1.38	1.46
19	5	307	CLA	MG-NA	3.44	2.14	2.06
23	A	850	BCR	C23-C22	-3.40	1.38	1.46
19	6	312	CLA	MG-NA	3.40	2.14	2.06
19	3	307	CLA	MG-NA	3.35	2.14	2.06
23	A	851	BCR	C23-C22	-3.33	1.38	1.46
23	I	101	BCR	C23-C22	-3.33	1.38	1.46
19	A	827	CLA	MG-NA	3.31	2.14	2.06
19	B	826	CLA	MG-NA	3.30	2.14	2.06
23	A	852	BCR	C23-C22	-3.30	1.38	1.46
19	B	840	CLA	MG-NA	3.29	2.14	2.06
19	6	309	CLA	MG-NA	3.29	2.14	2.06
23	G	201	BCR	C23-C22	-3.28	1.38	1.46
19	5	308	CLA	MG-NA	3.27	2.14	2.06
20	2	316	LUT	C8-C9	-3.26	1.39	1.46
19	A	840	CLA	MG-NC	3.26	2.14	2.06
19	2	308	CLA	MG-NA	3.25	2.14	2.06
19	3	308	CLA	MG-NA	3.24	2.14	2.06
19	B	841	CLA	MG-NC	3.24	2.14	2.06
19	B	824	CLA	MG-NA	3.24	2.14	2.06
23	3	317	BCR	C23-C22	-3.23	1.39	1.46
23	A	851	BCR	C8-C9	-3.23	1.39	1.46
23	2	319	BCR	C21-C22	3.21	1.43	1.35
23	3	317	BCR	C8-C9	-3.21	1.39	1.46
19	A	831	CLA	MG-NC	3.20	2.13	2.06
23	F	302	BCR	C23-C22	-3.20	1.39	1.46
19	B	823	CLA	MG-NC	3.19	2.13	2.06
18	5	306	CHL	C2C-C3C	3.19	1.39	1.36
23	L	305	BCR	C23-C22	-3.18	1.39	1.46
19	A	807	CLA	MG-NA	3.18	2.13	2.06
23	I	101	BCR	C8-C9	-3.18	1.39	1.46
23	G	201	BCR	C8-C9	-3.16	1.39	1.46
23	K	204	BCR	C8-C9	-3.15	1.39	1.46
23	M	101	BCR	C23-C22	-3.15	1.39	1.46
23	A	849	BCR	C8-C9	-3.15	1.39	1.46
19	3	302	CLA	MG-NC	3.13	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	844	BCR	C23-C22	-3.13	1.39	1.46
20	6	315	LUT	C8-C9	-3.12	1.39	1.46
23	L	304	BCR	C23-C22	-3.12	1.39	1.46
19	A	826	CLA	MG-NC	3.09	2.13	2.06
23	F	302	BCR	C8-C9	-3.08	1.39	1.46
20	J	101	LUT	C8-C9	-3.08	1.39	1.46
19	5	314	CLA	MG-NC	3.07	2.13	2.06
19	B	837	CLA	MG-NC	3.06	2.13	2.06
19	B	831	CLA	MG-NC	3.06	2.13	2.06
23	K	204	BCR	C23-C22	-3.05	1.39	1.46
19	A	809	CLA	MG-NC	3.05	2.13	2.06
23	A	848	BCR	C23-C22	-3.04	1.39	1.46
19	B	817	CLA	MG-NC	3.04	2.13	2.06
23	G	205	BCR	C8-C9	-3.04	1.39	1.46
23	A	852	BCR	C8-C9	-3.02	1.39	1.46
23	B	847	BCR	C12-C13	-3.01	1.39	1.46
19	B	812	CLA	MG-NC	3.01	2.13	2.06
20	2	315	LUT	C8-C9	-3.00	1.39	1.46
19	A	832	CLA	MG-NC	2.99	2.13	2.06
20	2	317	LUT	C8-C9	-2.99	1.39	1.46
23	F	305	BCR	C23-C22	-2.99	1.39	1.46
20	5	316	LUT	C8-C9	-2.98	1.39	1.46
23	F	305	BCR	C8-C9	-2.98	1.39	1.46
24	A	802	CL0	CHB-C1B	2.98	1.44	1.39
23	K	205	BCR	C8-C9	-2.97	1.39	1.46
23	2	319	BCR	C8-C9	-2.97	1.39	1.46
23	L	305	BCR	C8-C9	-2.96	1.39	1.46
20	3	316	LUT	C8-C9	-2.95	1.39	1.46
23	A	849	BCR	C23-C22	-2.95	1.39	1.46
23	G	201	BCR	C19-C18	-2.95	1.39	1.46
23	A	848	BCR	C8-C9	-2.93	1.39	1.46
23	B	848	BCR	C8-C9	-2.93	1.39	1.46
20	5	315	LUT	C8-C9	-2.93	1.39	1.46
23	L	304	BCR	C8-C9	-2.93	1.39	1.46
23	A	851	BCR	C12-C13	-2.92	1.39	1.46
19	A	830	CLA	MG-NC	2.91	2.13	2.06
19	6	307	CLA	MG-NC	2.91	2.13	2.06
23	I	101	BCR	C19-C18	-2.91	1.39	1.46
23	B	845	BCR	C23-C22	-2.91	1.39	1.46
23	5	317	BCR	C23-C22	-2.91	1.39	1.46
19	A	838	CLA	MG-NC	2.90	2.13	2.06
23	A	852	BCR	C19-C18	-2.90	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	839	CLA	MG-NC	2.88	2.13	2.06
23	2	319	BCR	C23-C22	-2.87	1.39	1.46
23	B	847	BCR	C19-C18	-2.87	1.39	1.46
19	B	804	CLA	MG-NA	2.87	2.13	2.06
23	G	201	BCR	C12-C13	-2.86	1.39	1.46
19	A	829	CLA	MG-NC	2.86	2.13	2.06
23	K	205	BCR	C23-C22	-2.86	1.39	1.46
23	5	317	BCR	C8-C9	-2.86	1.39	1.46
23	G	205	BCR	C23-C22	-2.85	1.39	1.46
23	B	848	BCR	C23-C22	-2.85	1.39	1.46
23	B	845	BCR	C8-C9	-2.85	1.39	1.46
19	B	814	CLA	MG-NC	2.85	2.13	2.06
23	A	850	BCR	C8-C9	-2.85	1.39	1.46
19	A	828	CLA	C3D-C4D	-2.84	1.37	1.44
19	B	820	CLA	C1B-C2B	-2.84	1.36	1.43
19	B	839	CLA	MG-NC	2.83	2.13	2.06
19	A	811	CLA	MG-NC	2.82	2.13	2.06
23	A	851	BCR	C19-C18	-2.82	1.39	1.46
23	B	848	BCR	C10-C9	2.82	1.42	1.35
19	A	834	CLA	MG-NC	2.81	2.13	2.06
23	M	101	BCR	C8-C9	-2.81	1.39	1.46
23	A	850	BCR	C19-C18	-2.79	1.40	1.46
19	A	818	CLA	MG-NC	2.79	2.12	2.06
19	2	311	CLA	MG-NC	2.78	2.12	2.06
19	B	828	CLA	MG-NC	2.78	2.12	2.06
23	B	844	BCR	C8-C9	-2.78	1.40	1.46
23	J	103	BCR	C8-C9	-2.78	1.40	1.46
20	3	315	LUT	C12-C13	-2.78	1.40	1.46
19	B	830	CLA	C3D-C4D	-2.77	1.38	1.44
23	I	101	BCR	C12-C13	-2.75	1.40	1.46
23	J	103	BCR	C23-C22	-2.74	1.40	1.46
21	6	316	XAT	O24-C25	-2.74	1.42	1.46
23	3	317	BCR	C19-C18	-2.74	1.40	1.46
23	A	849	BCR	C12-C13	-2.73	1.40	1.46
23	B	846	BCR	C8-C9	-2.73	1.40	1.46
24	A	802	CL0	C3B-C4B	-2.72	1.38	1.41
23	B	844	BCR	C19-C18	-2.72	1.40	1.46
20	6	318	LUT	C8-C9	-2.72	1.40	1.46
19	A	828	CLA	MG-NC	2.71	2.12	2.06
19	B	808	CLA	MG-NC	2.70	2.12	2.06
23	L	305	BCR	C19-C18	-2.70	1.40	1.46
23	3	317	BCR	C12-C13	-2.70	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K	204	BCR	C19-C18	-2.69	1.40	1.46
21	6	316	XAT	O4-C5	-2.68	1.42	1.46
19	6	303	CLA	MG-NC	2.67	2.12	2.06
20	2	316	LUT	C12-C13	-2.67	1.40	1.46
19	A	833	CLA	C3D-C4D	-2.66	1.38	1.44
19	B	833	CLA	MG-NC	2.66	2.12	2.06
19	3	310	CLA	MG-NC	2.66	2.12	2.06
23	F	302	BCR	C19-C18	-2.66	1.40	1.46
23	K	204	BCR	C12-C13	-2.65	1.40	1.46
20	3	315	LUT	C32-C33	-2.65	1.40	1.46
19	B	815	CLA	MG-NC	2.65	2.12	2.06
19	B	805	CLA	MG-NC	2.65	2.12	2.06
18	2	305	CHL	CHB-C1B	2.64	1.43	1.39
19	G	203	CLA	MG-NC	2.64	2.12	2.06
19	6	311	CLA	MG-NC	2.64	2.12	2.06
23	F	302	BCR	C12-C13	-2.64	1.40	1.46
19	A	803	CLA	C1D-C2D	-2.63	1.40	1.45
19	A	827	CLA	C3D-C4D	-2.62	1.38	1.44
20	2	316	LUT	C32-C33	-2.62	1.40	1.46
19	A	824	CLA	C3D-C4D	-2.62	1.38	1.44
20	6	318	LUT	C32-C33	-2.62	1.40	1.46
19	B	801	CLA	MG-NC	2.62	2.12	2.06
23	M	101	BCR	C19-C18	-2.61	1.40	1.46
19	A	841	CLA	MG-NC	2.61	2.12	2.06
19	A	816	CLA	MG-NC	2.60	2.12	2.06
23	L	304	BCR	C19-C18	-2.60	1.40	1.46
19	A	835	CLA	MG-NC	2.60	2.12	2.06
19	B	841	CLA	C3D-C4D	-2.60	1.38	1.44
18	2	314	CHL	CHB-C1B	2.60	1.43	1.39
20	3	315	LUT	C28-C29	-2.59	1.40	1.46
19	B	803	CLA	C1D-C2D	-2.59	1.40	1.45
23	L	304	BCR	C12-C13	-2.59	1.40	1.46
19	2	303	CLA	C3D-C4D	-2.59	1.38	1.44
19	B	829	CLA	C3D-C4D	-2.59	1.38	1.44
23	B	846	BCR	C23-C22	-2.58	1.40	1.46
19	B	807	CLA	C3D-C4D	-2.58	1.38	1.44
19	B	840	CLA	C3D-C4D	-2.58	1.38	1.44
19	A	815	CLA	MG-NC	2.57	2.12	2.06
20	5	315	LUT	C28-C29	-2.57	1.40	1.46
20	5	315	LUT	C32-C33	-2.57	1.40	1.46
23	A	848	BCR	C19-C18	-2.56	1.40	1.46
23	A	848	BCR	C12-C13	-2.56	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	6	315	LUT	C32-C33	-2.56	1.40	1.46
19	B	826	CLA	C3D-C4D	-2.56	1.38	1.44
19	A	808	CLA	C3D-C4D	-2.56	1.38	1.44
23	L	305	BCR	C12-C13	-2.55	1.40	1.46
19	B	824	CLA	C3D-C4D	-2.55	1.38	1.44
19	A	837	CLA	C1B-C2B	-2.55	1.37	1.43
19	A	832	CLA	C3D-C4D	-2.55	1.38	1.44
19	B	832	CLA	MG-NC	2.55	2.12	2.06
20	2	316	LUT	C28-C29	-2.55	1.40	1.46
19	A	828	CLA	C1D-C2D	-2.55	1.40	1.45
18	5	306	CHL	CHB-C1B	2.54	1.43	1.39
19	B	808	CLA	C3D-C4D	-2.54	1.38	1.44
19	B	820	CLA	C3D-C4D	-2.54	1.38	1.44
19	A	842	CLA	C3D-C4D	-2.54	1.38	1.44
19	A	822	CLA	C3D-C4D	-2.54	1.38	1.44
23	A	849	BCR	C19-C18	-2.53	1.40	1.46
19	6	305	CLA	MG-NC	2.53	2.12	2.06
23	2	319	BCR	C12-C13	-2.52	1.40	1.46
19	A	811	CLA	C3D-C4D	-2.52	1.38	1.44
19	A	805	CLA	C3D-C4D	-2.52	1.38	1.44
19	B	831	CLA	C3D-C4D	-2.52	1.38	1.44
19	3	312	CLA	MG-NC	2.52	2.12	2.06
19	B	817	CLA	C3D-C4D	-2.52	1.38	1.44
18	2	307	CHL	CHB-C1B	2.52	1.43	1.39
19	3	301	CLA	C3D-C4D	-2.52	1.38	1.44
19	6	303	CLA	C3D-C4D	-2.51	1.38	1.44
19	B	806	CLA	MG-NC	2.51	2.12	2.06
19	B	821	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	814	CLA	C3D-C4D	-2.51	1.38	1.44
19	B	842	CLA	C3D-C4D	-2.51	1.38	1.44
19	G	203	CLA	C3D-C4D	-2.51	1.38	1.44
19	L	302	CLA	C3D-C4D	-2.51	1.38	1.44
18	5	313	CHL	CHB-C1B	2.51	1.43	1.39
19	A	831	CLA	C1D-C2D	-2.50	1.40	1.45
19	B	828	CLA	C3D-C4D	-2.50	1.38	1.44
23	F	305	BCR	C19-C18	-2.50	1.40	1.46
23	J	103	BCR	C17-C18	2.50	1.41	1.35
20	6	315	LUT	C28-C29	-2.50	1.40	1.46
19	B	827	CLA	C1D-C2D	-2.50	1.40	1.45
19	A	834	CLA	C3D-C4D	-2.50	1.38	1.44
23	B	846	BCR	C21-C22	2.49	1.41	1.35
19	5	301	CLA	C3D-C4D	-2.49	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	841	CLA	MG-NB	2.49	2.10	2.05
23	K	205	BCR	C12-C13	-2.49	1.40	1.46
23	F	305	BCR	C12-C13	-2.49	1.40	1.46
19	A	841	CLA	C3D-C4D	-2.49	1.38	1.44
19	A	806	CLA	C3D-C4D	-2.49	1.38	1.44
19	B	811	CLA	C3D-C4D	-2.49	1.38	1.44
20	6	318	LUT	C28-C29	-2.49	1.40	1.46
19	A	803	CLA	C1B-NB	-2.49	1.34	1.37
19	B	818	CLA	C3D-C4D	-2.49	1.38	1.44
19	A	818	CLA	C3D-C4D	-2.48	1.38	1.44
18	5	305	CHL	CHB-C1B	2.48	1.43	1.39
20	J	101	LUT	C12-C13	-2.48	1.40	1.46
19	2	302	CLA	C3D-C4D	-2.48	1.38	1.44
23	A	850	BCR	C12-C13	-2.48	1.40	1.46
19	B	835	CLA	C3D-C4D	-2.48	1.38	1.44
19	A	801	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	806	CLA	C3D-C4D	-2.48	1.38	1.44
19	6	305	CLA	C3D-C4D	-2.48	1.38	1.44
18	5	304	CHL	CHB-C1B	2.48	1.43	1.39
19	A	807	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	813	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	813	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	812	CLA	C3D-C4D	-2.47	1.38	1.44
19	K	202	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	816	CLA	MG-NC	2.47	2.12	2.06
19	5	310	CLA	MG-NC	2.47	2.12	2.06
19	A	819	CLA	MG-NC	2.47	2.12	2.06
19	B	833	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	838	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	825	CLA	C3D-C4D	-2.46	1.38	1.44
19	B	837	CLA	C3D-C4D	-2.46	1.38	1.44
19	3	307	CLA	C3D-C4D	-2.46	1.38	1.44
19	A	836	CLA	C3D-C4D	-2.46	1.38	1.44
19	B	827	CLA	C3D-C4D	-2.46	1.38	1.44
19	6	302	CLA	C3D-C4D	-2.46	1.38	1.44
18	2	306	CHL	C3B-C4B	-2.46	1.39	1.41
19	6	312	CLA	C3D-C4D	-2.46	1.38	1.44
19	2	313	CLA	MG-NC	2.46	2.12	2.06
19	6	308	CLA	C3D-C4D	-2.46	1.38	1.44
18	2	305	CHL	C3B-C4B	-2.46	1.39	1.41
19	B	818	CLA	C1B-C2B	-2.46	1.37	1.43
19	A	816	CLA	C3D-C4D	-2.46	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	836	CLA	C3D-C4D	-2.46	1.38	1.44
19	B	812	CLA	C3D-C4D	-2.46	1.38	1.44
19	A	825	CLA	MG-NC	2.45	2.12	2.06
19	5	311	CLA	C3D-C4D	-2.45	1.38	1.44
19	A	819	CLA	C3D-C4D	-2.45	1.38	1.44
19	L	302	CLA	C1D-C2D	-2.45	1.40	1.45
19	B	819	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	840	CLA	C1B-C2B	-2.45	1.37	1.43
19	A	832	CLA	C1D-C2D	-2.45	1.40	1.45
20	5	316	LUT	C32-C33	-2.45	1.40	1.46
23	B	844	BCR	C12-C13	-2.45	1.40	1.46
19	B	829	CLA	MG-NC	2.45	2.12	2.06
20	2	315	LUT	C32-C33	-2.45	1.40	1.46
19	A	835	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	807	CLA	MG-NC	2.45	2.12	2.06
19	A	821	CLA	C3D-C4D	-2.44	1.38	1.44
19	2	303	CLA	MG-NC	2.44	2.12	2.06
19	A	825	CLA	C3D-C4D	-2.44	1.38	1.44
19	3	308	CLA	C3D-C4D	-2.44	1.38	1.44
19	A	830	CLA	C1D-C2D	-2.44	1.40	1.45
23	J	103	BCR	C21-C22	2.44	1.41	1.35
19	A	821	CLA	C1D-C2D	-2.44	1.40	1.45
19	B	831	CLA	C1D-C2D	-2.44	1.40	1.45
19	A	817	CLA	MG-NC	2.44	2.12	2.06
23	A	852	BCR	C12-C13	-2.43	1.40	1.46
19	B	834	CLA	C3D-C4D	-2.43	1.38	1.44
19	L	303	CLA	MG-NC	2.43	2.12	2.06
19	A	820	CLA	C3D-C4D	-2.43	1.38	1.44
19	A	822	CLA	C1B-C2B	-2.43	1.37	1.43
19	B	814	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	846	BCR	C14-C13	2.43	1.41	1.35
23	B	846	BCR	C17-C18	2.43	1.41	1.35
19	5	302	CLA	C1D-C2D	-2.43	1.40	1.45
19	5	302	CLA	C3D-C4D	-2.43	1.38	1.44
19	A	829	CLA	C3D-C4D	-2.43	1.38	1.44
19	F	304	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	845	BCR	C19-C18	-2.43	1.40	1.46
20	6	318	LUT	C14-C13	2.42	1.41	1.35
19	A	819	CLA	C1B-C2B	-2.42	1.37	1.43
19	B	804	CLA	C1D-C2D	-2.42	1.40	1.45
19	B	839	CLA	C3D-C4D	-2.42	1.38	1.44
19	6	307	CLA	C1D-C2D	-2.42	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	810	CLA	C1D-C2D	-2.42	1.40	1.45
19	A	818	CLA	MG-NB	2.42	2.10	2.05
19	G	204	CLA	MG-NC	2.42	2.12	2.06
20	3	316	LUT	C28-C29	-2.42	1.40	1.46
20	3	316	LUT	C32-C33	-2.42	1.40	1.46
19	3	313	CLA	C3D-C4D	-2.42	1.38	1.44
19	A	817	CLA	C3D-C4D	-2.42	1.38	1.44
19	A	809	CLA	C3D-C4D	-2.41	1.38	1.44
19	B	809	CLA	C3D-C4D	-2.41	1.38	1.44
19	6	310	CLA	C3D-C4D	-2.41	1.38	1.44
19	3	303	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	848	BCR	C12-C13	-2.41	1.40	1.46
19	5	307	CLA	C3D-C4D	-2.41	1.38	1.44
19	A	824	CLA	MG-NC	2.41	2.12	2.06
23	G	205	BCR	C12-C13	-2.41	1.40	1.46
19	6	313	CLA	C3D-C4D	-2.41	1.38	1.44
19	B	815	CLA	C3D-C4D	-2.41	1.38	1.44
19	B	807	CLA	C1B-C2B	-2.41	1.37	1.43
18	2	301	CHL	CHB-C1B	2.41	1.43	1.39
23	M	101	BCR	C12-C13	-2.41	1.40	1.46
19	6	314	CLA	C3D-C4D	-2.41	1.38	1.44
19	5	308	CLA	C3D-C4D	-2.41	1.38	1.44
23	5	317	BCR	C19-C18	-2.41	1.40	1.46
19	A	826	CLA	C1D-C2D	-2.41	1.40	1.45
19	3	311	CLA	C3D-C4D	-2.41	1.38	1.44
19	5	309	CLA	C3D-C4D	-2.41	1.38	1.44
19	3	311	CLA	MG-NC	2.41	2.12	2.06
19	A	823	CLA	C3D-C4D	-2.41	1.38	1.44
19	2	308	CLA	C3D-C4D	-2.40	1.38	1.44
19	A	801	CLA	C1D-C2D	-2.40	1.40	1.45
18	3	314	CHL	CHB-C1B	2.40	1.43	1.39
23	B	846	BCR	C10-C9	2.40	1.41	1.35
19	B	802	CLA	MG-NC	2.40	2.12	2.06
19	A	837	CLA	C3D-C4D	-2.40	1.38	1.44
19	A	833	CLA	C1B-C2B	-2.40	1.37	1.43
18	6	301	CHL	C3B-C4B	-2.40	1.39	1.41
19	F	301	CLA	C3D-C4D	-2.40	1.38	1.44
18	2	320	CHL	CHB-C1B	2.40	1.43	1.39
23	B	848	BCR	C19-C18	-2.40	1.40	1.46
19	F	301	CLA	C1D-C2D	-2.40	1.40	1.45
19	A	833	CLA	MG-NC	2.39	2.12	2.06
18	5	305	CHL	C3B-C4B	-2.39	1.39	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	304	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	842	CLA	MG-NC	2.39	2.12	2.06
19	2	304	CLA	C3D-C4D	-2.39	1.38	1.44
20	5	316	LUT	C28-C29	-2.39	1.40	1.46
19	B	823	CLA	C3D-C4D	-2.39	1.38	1.44
20	2	315	LUT	C28-C29	-2.39	1.40	1.46
23	G	205	BCR	C19-C18	-2.39	1.40	1.46
19	3	302	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	815	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	843	CLA	C3D-C4D	-2.39	1.38	1.44
19	B	824	CLA	C1D-C2D	-2.39	1.40	1.45
19	L	303	CLA	C3D-C4D	-2.39	1.38	1.44
19	B	822	CLA	C3D-C4D	-2.39	1.38	1.44
19	6	304	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	838	CLA	C3D-C4D	-2.39	1.38	1.44
19	B	807	CLA	C1D-C2D	-2.39	1.40	1.45
19	A	810	CLA	C3D-C4D	-2.39	1.38	1.44
19	B	816	CLA	C3D-C4D	-2.39	1.38	1.44
20	2	315	LUT	C12-C13	-2.39	1.40	1.46
19	A	833	CLA	C1D-C2D	-2.39	1.40	1.45
19	2	310	CLA	C3D-C4D	-2.38	1.38	1.44
19	6	309	CLA	C3D-C4D	-2.38	1.38	1.44
19	B	834	CLA	MG-NC	2.38	2.11	2.06
19	5	302	CLA	MG-NC	2.38	2.11	2.06
19	F	301	CLA	MG-NC	2.38	2.11	2.06
18	6	306	CHL	CHB-C1B	2.38	1.43	1.39
19	A	814	CLA	MG-NC	2.38	2.11	2.06
23	J	103	BCR	C14-C13	2.38	1.41	1.35
19	A	808	CLA	MG-NC	2.38	2.11	2.06
19	6	307	CLA	C3D-C4D	-2.38	1.38	1.44
19	B	820	CLA	C1D-C2D	-2.38	1.40	1.45
19	5	312	CLA	C3D-C4D	-2.38	1.38	1.44
19	F	303	CLA	C3D-C4D	-2.38	1.38	1.44
19	B	809	CLA	C1D-C2D	-2.38	1.40	1.45
23	B	845	BCR	C12-C13	-2.38	1.40	1.46
19	A	823	CLA	MG-NC	2.38	2.11	2.06
18	5	306	CHL	C3B-C4B	-2.38	1.39	1.41
20	5	316	LUT	C12-C13	-2.38	1.40	1.46
19	3	312	CLA	C3D-C4D	-2.38	1.38	1.44
18	3	306	CHL	C3B-C4B	-2.38	1.39	1.41
19	B	801	CLA	C1D-C2D	-2.37	1.40	1.45
19	B	830	CLA	MG-NC	2.37	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	204	CLA	C3D-C4D	-2.37	1.38	1.44
19	B	805	CLA	C3D-C4D	-2.37	1.38	1.44
19	B	832	CLA	C3D-C4D	-2.37	1.38	1.44
19	5	303	CLA	C3D-C4D	-2.37	1.38	1.44
19	A	830	CLA	C3D-C4D	-2.37	1.38	1.44
19	B	803	CLA	C3D-C4D	-2.37	1.38	1.44
19	2	313	CLA	C3D-C4D	-2.36	1.38	1.44
20	5	315	LUT	C12-C13	-2.36	1.40	1.46
18	6	301	CHL	CHB-C1B	2.36	1.43	1.39
19	J	102	CLA	C3D-C4D	-2.36	1.38	1.44
19	K	203	CLA	C3D-C4D	-2.36	1.38	1.44
19	A	839	CLA	C3D-C4D	-2.36	1.38	1.44
19	B	810	CLA	C3D-C4D	-2.36	1.38	1.44
19	K	201	CLA	C3D-C4D	-2.36	1.38	1.44
19	A	825	CLA	C1B-C2B	-2.36	1.37	1.43
19	5	310	CLA	C3D-C4D	-2.36	1.38	1.44
19	A	828	CLA	C1B-C2B	-2.36	1.37	1.43
19	3	305	CLA	C3D-C4D	-2.36	1.38	1.44
19	3	309	CLA	C3D-C4D	-2.35	1.38	1.44
19	B	821	CLA	C1D-C2D	-2.35	1.40	1.45
19	A	803	CLA	C1B-C2B	-2.35	1.37	1.43
19	2	312	CLA	MG-NC	2.35	2.11	2.06
19	6	308	CLA	C1D-C2D	-2.35	1.40	1.45
19	B	829	CLA	C1D-C2D	-2.35	1.40	1.45
19	A	831	CLA	C3D-C4D	-2.35	1.38	1.44
19	A	801	CLA	MG-NC	2.34	2.11	2.06
19	A	804	CLA	MG-NC	2.34	2.11	2.06
23	J	103	BCR	C10-C9	2.34	1.41	1.35
19	B	811	CLA	MG-NC	2.34	2.11	2.06
19	L	301	CLA	MG-NC	2.34	2.11	2.06
19	B	836	CLA	C1B-C2B	-2.34	1.37	1.43
19	A	838	CLA	C1B-C2B	-2.34	1.37	1.43
19	2	309	CLA	C3D-C4D	-2.34	1.38	1.44
20	6	318	LUT	C34-C33	2.33	1.41	1.35
19	2	311	CLA	C3D-C4D	-2.33	1.38	1.44
19	6	314	CLA	MG-NC	2.33	2.11	2.06
19	F	301	CLA	C1B-C2B	-2.33	1.37	1.43
19	A	814	CLA	C1D-C2D	-2.33	1.40	1.45
19	B	822	CLA	MG-NC	2.33	2.11	2.06
19	B	801	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	818	CLA	C1D-C2D	-2.33	1.40	1.45
19	3	310	CLA	C3D-C4D	-2.33	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	818	CLA	MG-NC	2.33	2.11	2.06
19	B	813	CLA	MG-NC	2.33	2.11	2.06
19	B	809	CLA	C1B-C2B	-2.33	1.37	1.43
19	6	311	CLA	C3D-C4D	-2.33	1.39	1.44
19	F	304	CLA	MG-NC	2.33	2.11	2.06
19	B	828	CLA	C1D-C2D	-2.32	1.40	1.45
18	2	307	CHL	C3B-C4B	-2.32	1.39	1.41
23	5	317	BCR	C10-C9	2.32	1.41	1.35
19	5	312	CLA	MG-NC	2.32	2.11	2.06
23	K	205	BCR	C19-C18	-2.32	1.41	1.46
19	L	301	CLA	C3D-C4D	-2.32	1.39	1.44
19	2	312	CLA	C1D-C2D	-2.32	1.40	1.45
19	5	314	CLA	C1D-C2D	-2.31	1.40	1.45
19	K	202	CLA	C1D-C2D	-2.31	1.40	1.45
19	A	840	CLA	C3D-C4D	-2.31	1.39	1.44
23	L	304	BCR	C29-C28	-2.31	1.47	1.52
19	B	809	CLA	MG-NC	2.31	2.11	2.06
19	2	312	CLA	C3D-C4D	-2.31	1.39	1.44
19	A	813	CLA	C1D-C2D	-2.31	1.40	1.45
19	A	819	CLA	C1D-C2D	-2.31	1.40	1.45
19	A	836	CLA	C1B-C2B	-2.30	1.37	1.43
20	5	315	LUT	C10-C9	2.30	1.41	1.35
19	B	842	CLA	C1D-C2D	-2.30	1.40	1.45
19	B	814	CLA	C1D-C2D	-2.30	1.40	1.45
19	A	842	CLA	C1B-C2B	-2.30	1.37	1.43
20	2	317	LUT	C30-C29	2.30	1.41	1.35
20	J	101	LUT	C30-C29	2.30	1.41	1.35
20	2	317	LUT	C10-C9	2.30	1.41	1.35
19	A	829	CLA	C1D-C2D	-2.30	1.40	1.45
19	3	310	CLA	C1D-C2D	-2.30	1.40	1.45
18	3	306	CHL	CHB-C1B	2.29	1.43	1.39
19	B	816	CLA	C1D-C2D	-2.29	1.40	1.45
19	A	843	CLA	MG-NC	2.29	2.11	2.06
19	B	837	CLA	C1D-C2D	-2.29	1.40	1.45
19	B	827	CLA	MG-NC	2.29	2.11	2.06
23	2	319	BCR	C19-C18	-2.29	1.41	1.46
19	K	202	CLA	CAB-C3B	-2.29	1.46	1.50
19	J	102	CLA	MG-NC	2.29	2.11	2.06
19	B	823	CLA	C1D-C2D	-2.29	1.40	1.45
23	5	317	BCR	C12-C13	-2.29	1.41	1.46
19	6	308	CLA	MG-NC	2.29	2.11	2.06
19	B	836	CLA	MG-NC	2.29	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	302	CLA	C1B-C2B	-2.29	1.37	1.43
19	A	838	CLA	C1D-C2D	-2.28	1.40	1.45
18	2	306	CHL	CHB-C1B	2.28	1.43	1.39
19	B	833	CLA	C1D-C2D	-2.28	1.40	1.45
19	A	820	CLA	C1B-C2B	-2.28	1.37	1.43
19	A	843	CLA	C1D-C2D	-2.28	1.40	1.45
19	3	313	CLA	C1B-C2B	-2.28	1.37	1.43
19	A	826	CLA	C3D-C4D	-2.28	1.39	1.44
20	6	315	LUT	C12-C13	-2.28	1.41	1.46
19	B	810	CLA	C1B-NB	-2.28	1.34	1.37
20	2	317	LUT	C14-C13	2.28	1.41	1.35
19	B	808	CLA	C1D-C2D	-2.28	1.40	1.45
19	A	811	CLA	C1D-C2D	-2.28	1.40	1.45
20	3	316	LUT	C12-C13	-2.28	1.41	1.46
19	F	304	CLA	C1D-C2D	-2.28	1.40	1.45
19	B	822	CLA	C1B-C2B	-2.28	1.37	1.43
19	3	305	CLA	MG-NC	2.27	2.11	2.06
20	J	101	LUT	C28-C29	-2.27	1.41	1.46
20	6	315	LUT	C34-C33	2.27	1.41	1.35
19	G	203	CLA	C1D-C2D	-2.27	1.40	1.45
19	B	834	CLA	C1D-C2D	-2.27	1.40	1.45
23	G	205	BCR	C17-C18	2.27	1.41	1.35
18	5	304	CHL	C3B-C4B	-2.27	1.39	1.41
19	A	818	CLA	C1B-C2B	-2.27	1.37	1.43
19	2	309	CLA	C1D-C2D	-2.27	1.40	1.45
19	B	837	CLA	C1B-C2B	-2.26	1.37	1.43
23	5	317	BCR	C14-C13	2.26	1.41	1.35
20	3	316	LUT	C10-C9	2.26	1.41	1.35
19	6	312	CLA	C1B-C2B	-2.26	1.37	1.43
19	A	812	CLA	MG-NC	2.26	2.11	2.06
19	A	836	CLA	C1D-C2D	-2.26	1.40	1.45
20	2	315	LUT	C10-C9	2.26	1.41	1.35
19	B	802	CLA	C1D-C2D	-2.26	1.40	1.45
19	3	309	CLA	MG-NC	2.26	2.11	2.06
19	3	305	CLA	C1B-C2B	-2.26	1.37	1.43
23	G	205	BCR	C21-C22	2.26	1.41	1.35
23	K	205	BCR	C21-C22	2.26	1.41	1.35
19	B	803	CLA	CHB-C1B	2.26	1.44	1.39
19	A	834	CLA	C1D-C2D	-2.25	1.40	1.45
20	5	315	LUT	C34-C33	2.25	1.41	1.35
19	A	808	CLA	C1D-C2D	-2.25	1.40	1.45
19	K	202	CLA	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	317	LUT	C34-C33	2.25	1.41	1.35
19	A	842	CLA	C1D-C2D	-2.25	1.40	1.45
19	J	102	CLA	C1B-C2B	-2.25	1.37	1.43
19	B	825	CLA	MG-NC	2.25	2.11	2.06
20	2	317	LUT	C12-C13	-2.25	1.41	1.46
20	6	315	LUT	C10-C9	2.25	1.41	1.35
19	6	310	CLA	MG-NC	2.24	2.11	2.06
19	A	815	CLA	C1D-C2D	-2.24	1.40	1.45
19	6	313	CLA	C1B-C2B	-2.24	1.37	1.43
19	3	308	CLA	C1B-C2B	-2.24	1.37	1.43
19	5	311	CLA	CHB-C1B	2.24	1.44	1.39
19	B	804	CLA	C3D-C4D	-2.24	1.39	1.44
20	6	318	LUT	C10-C9	2.24	1.41	1.35
19	2	311	CLA	C1D-C2D	-2.24	1.40	1.45
19	5	301	CLA	MG-NC	2.24	2.11	2.06
23	5	317	BCR	C17-C18	2.24	1.41	1.35
19	6	304	CLA	C1B-C2B	-2.24	1.37	1.43
19	2	309	CLA	C1B-C2B	-2.23	1.37	1.43
20	J	101	LUT	C34-C33	2.23	1.41	1.35
19	B	810	CLA	MG-NC	2.23	2.11	2.06
19	5	302	CLA	C1B-C2B	-2.23	1.37	1.43
19	A	804	CLA	C1B-C2B	-2.22	1.37	1.43
19	6	310	CLA	C1B-C2B	-2.22	1.37	1.43
19	B	841	CLA	C1B-C2B	-2.22	1.37	1.43
20	3	316	LUT	C34-C33	2.22	1.40	1.35
19	2	310	CLA	C1B-C2B	-2.22	1.37	1.43
19	K	203	CLA	MG-NC	2.22	2.11	2.06
19	5	310	CLA	C1D-C2D	-2.22	1.40	1.45
19	A	821	CLA	MG-NC	2.22	2.11	2.06
19	A	812	CLA	C1B-C2B	-2.22	1.37	1.43
19	6	302	CLA	MG-NC	2.22	2.11	2.06
20	J	101	LUT	C32-C33	-2.22	1.41	1.46
19	5	309	CLA	C1B-C2B	-2.22	1.37	1.43
20	3	316	LUT	C14-C13	2.22	1.40	1.35
19	B	836	CLA	C1B-NB	-2.22	1.34	1.37
20	J	101	LUT	C14-C13	2.22	1.40	1.35
19	A	809	CLA	C1D-C2D	-2.22	1.41	1.45
23	3	317	BCR	C29-C28	-2.22	1.47	1.52
19	F	304	CLA	C1B-C2B	-2.21	1.37	1.43
20	3	316	LUT	C30-C29	2.21	1.40	1.35
19	5	312	CLA	C1B-C2B	-2.21	1.37	1.43
19	3	302	CLA	C1D-C2D	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	805	CLA	C1D-C2D	-2.21	1.41	1.45
19	A	803	CLA	C3D-C4D	-2.21	1.39	1.44
19	A	810	CLA	C1D-C2D	-2.21	1.41	1.45
19	B	838	CLA	MG-NC	2.21	2.11	2.06
19	3	310	CLA	C1B-C2B	-2.21	1.37	1.43
19	A	821	CLA	C1B-C2B	-2.21	1.37	1.43
18	3	314	CHL	C3B-C4B	-2.21	1.39	1.41
20	6	318	LUT	C12-C13	-2.21	1.41	1.46
19	B	823	CLA	C1B-NB	-2.21	1.35	1.37
19	B	842	CLA	C1B-C2B	-2.21	1.37	1.43
19	A	804	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	848	BCR	C14-C13	2.21	1.40	1.35
19	B	835	CLA	MG-NC	2.21	2.11	2.06
19	A	828	CLA	C1B-NB	-2.20	1.35	1.37
19	B	830	CLA	C1D-C2D	-2.20	1.41	1.45
19	5	309	CLA	C1D-C2D	-2.20	1.41	1.45
20	2	315	LUT	C30-C29	2.20	1.40	1.35
19	A	807	CLA	C1B-C2B	-2.20	1.38	1.43
19	B	805	CLA	C1D-C2D	-2.20	1.41	1.45
19	A	834	CLA	C1B-C2B	-2.20	1.38	1.43
19	5	314	CLA	C3D-C4D	-2.20	1.39	1.44
20	6	315	LUT	C14-C13	2.20	1.40	1.35
19	3	304	CLA	MG-NC	2.20	2.11	2.06
19	A	812	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	813	CLA	C1D-C2D	-2.20	1.41	1.45
20	5	316	LUT	C10-C9	2.20	1.40	1.35
19	B	806	CLA	C1B-C2B	-2.20	1.38	1.43
19	B	811	CLA	C1B-C2B	-2.20	1.38	1.43
19	5	307	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	806	CLA	C1D-C2D	-2.20	1.41	1.45
19	B	826	CLA	C1D-C2D	-2.20	1.41	1.45
19	6	313	CLA	MG-NC	2.20	2.11	2.06
19	2	310	CLA	C1D-C2D	-2.20	1.41	1.45
19	2	312	CLA	C1B-C2B	-2.20	1.38	1.43
20	2	315	LUT	C34-C33	2.20	1.40	1.35
19	6	305	CLA	C1D-C2D	-2.19	1.41	1.45
19	6	310	CLA	C1D-C2D	-2.19	1.41	1.45
23	A	851	BCR	C29-C28	-2.19	1.47	1.52
19	A	841	CLA	C1D-C2D	-2.19	1.41	1.45
19	6	308	CLA	C1B-C2B	-2.19	1.38	1.43
23	B	848	BCR	C17-C18	2.19	1.40	1.35
19	A	823	CLA	C1D-C2D	-2.19	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	309	CLA	C1B-C2B	-2.18	1.38	1.43
23	G	205	BCR	C14-C13	2.18	1.40	1.35
19	L	303	CLA	C1D-C2D	-2.18	1.41	1.45
19	3	304	CLA	C1D-C2D	-2.18	1.41	1.45
20	2	315	LUT	C14-C13	2.18	1.40	1.35
19	A	822	CLA	C1D-C2D	-2.18	1.41	1.45
19	K	201	CLA	C1D-C2D	-2.18	1.41	1.45
23	K	205	BCR	C17-C18	2.18	1.40	1.35
19	B	821	CLA	MG-NC	2.18	2.11	2.06
19	B	804	CLA	C1B-NB	-2.18	1.35	1.37
19	A	806	CLA	C1B-C2B	-2.18	1.38	1.43
19	B	822	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	810	CLA	C1B-C2B	-2.18	1.38	1.43
19	3	309	CLA	C1D-C2D	-2.18	1.41	1.45
19	A	824	CLA	C1B-C2B	-2.18	1.38	1.43
19	3	301	CLA	C1D-C2D	-2.18	1.41	1.45
19	G	203	CLA	C1B-C2B	-2.18	1.38	1.43
19	B	815	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	804	CLA	C1B-C2B	-2.18	1.38	1.43
19	L	301	CLA	C1D-C2D	-2.17	1.41	1.45
19	3	311	CLA	C1B-C2B	-2.17	1.38	1.43
23	M	101	BCR	C10-C9	2.17	1.40	1.35
23	L	304	BCR	C17-C18	2.17	1.40	1.35
20	2	317	LUT	C32-C33	-2.17	1.41	1.46
19	2	302	CLA	C1D-C2D	-2.17	1.41	1.45
19	B	811	CLA	C1D-C2D	-2.17	1.41	1.45
19	A	810	CLA	MG-NC	2.17	2.11	2.06
19	B	841	CLA	C1D-C2D	-2.16	1.41	1.45
19	5	301	CLA	C1D-C2D	-2.16	1.41	1.45
23	M	101	BCR	C14-C13	2.16	1.40	1.35
19	B	819	CLA	C1B-C2B	-2.16	1.38	1.43
19	A	831	CLA	C1B-NB	-2.16	1.35	1.37
19	2	303	CLA	C1D-C2D	-2.16	1.41	1.45
23	B	846	BCR	C12-C13	-2.16	1.41	1.46
19	A	818	CLA	C1D-C2D	-2.16	1.41	1.45
23	K	205	BCR	C10-C9	2.16	1.40	1.35
19	3	305	CLA	C1D-C2D	-2.16	1.41	1.45
19	B	802	CLA	C1B-C2B	-2.16	1.38	1.43
19	A	838	CLA	C1B-NB	-2.16	1.35	1.37
19	F	303	CLA	C1D-C2D	-2.16	1.41	1.45
19	5	312	CLA	C1D-C2D	-2.15	1.41	1.45
19	B	835	CLA	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	315	LUT	C30-C29	2.15	1.40	1.35
23	A	850	BCR	C10-C9	2.15	1.40	1.35
23	3	317	BCR	C2-C3	-2.15	1.47	1.52
19	G	203	CLA	MG-NB	2.15	2.10	2.05
19	B	802	CLA	C3D-C4D	-2.15	1.39	1.44
19	3	312	CLA	C1D-C2D	-2.15	1.41	1.45
23	M	101	BCR	C17-C18	2.15	1.40	1.35
19	6	309	CLA	C1D-C2D	-2.15	1.41	1.45
19	A	840	CLA	C1D-C2D	-2.15	1.41	1.45
19	A	822	CLA	C1B-NB	-2.15	1.35	1.37
19	A	826	CLA	CHB-C1B	2.15	1.44	1.39
19	A	807	CLA	C1B-NB	-2.15	1.35	1.37
23	B	845	BCR	C14-C13	2.15	1.40	1.35
19	5	308	CLA	C1B-C2B	-2.14	1.38	1.43
19	2	304	CLA	MG-NC	2.14	2.11	2.06
20	5	315	LUT	C14-C13	2.14	1.40	1.35
19	B	819	CLA	C1D-C2D	-2.14	1.41	1.45
19	K	201	CLA	MG-NC	2.14	2.11	2.06
19	B	832	CLA	C1D-C2D	-2.14	1.41	1.45
23	B	848	BCR	C21-C22	2.14	1.40	1.35
19	5	303	CLA	MG-NC	2.14	2.11	2.06
19	A	835	CLA	C1B-C2B	-2.14	1.38	1.43
19	A	815	CLA	C1B-C2B	-2.14	1.38	1.43
19	3	311	CLA	MG-NB	2.14	2.10	2.05
19	B	839	CLA	C1D-C2D	-2.14	1.41	1.45
19	6	313	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	825	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	840	CLA	C1D-C2D	-2.13	1.41	1.45
19	3	301	CLA	C1B-C2B	-2.13	1.38	1.43
19	A	801	CLA	C1B-C2B	-2.13	1.38	1.43
19	A	816	CLA	C1D-C2D	-2.13	1.41	1.45
20	2	317	LUT	C28-C29	-2.13	1.41	1.46
19	5	311	CLA	C1B-C2B	-2.13	1.38	1.43
19	A	833	CLA	C1B-NB	-2.13	1.35	1.37
20	J	101	LUT	C10-C9	2.13	1.40	1.35
19	A	813	CLA	MG-NC	2.13	2.11	2.06
20	5	316	LUT	C34-C33	2.13	1.40	1.35
19	6	311	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	820	CLA	MG-NC	2.13	2.11	2.06
19	J	102	CLA	C1D-C2D	-2.13	1.41	1.45
19	B	842	CLA	MG-NC	2.12	2.11	2.06
19	A	841	CLA	C1B-C2B	-2.12	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	307	CLA	MG-NC	2.12	2.11	2.06
19	3	303	CLA	MG-NC	2.12	2.11	2.06
23	F	305	BCR	C17-C18	2.12	1.40	1.35
23	L	304	BCR	C14-C13	2.12	1.40	1.35
19	B	838	CLA	C1B-C2B	-2.12	1.38	1.43
19	L	302	CLA	C1B-C2B	-2.12	1.38	1.43
19	5	308	CLA	C1D-C2D	-2.12	1.41	1.45
20	5	316	LUT	C14-C13	2.12	1.40	1.35
19	B	828	CLA	CHB-C1B	2.12	1.44	1.39
19	B	817	CLA	C1D-C2D	-2.12	1.41	1.45
23	K	205	BCR	C14-C13	2.11	1.40	1.35
20	2	316	LUT	C34-C33	2.11	1.40	1.35
19	3	304	CLA	C1B-NB	-2.11	1.35	1.37
19	3	311	CLA	C1D-C2D	-2.11	1.41	1.45
23	B	845	BCR	C17-C18	2.11	1.40	1.35
19	A	836	CLA	MG-NC	2.11	2.11	2.06
19	K	203	CLA	C1D-C2D	-2.11	1.41	1.45
19	2	308	CLA	C1D-C2D	-2.11	1.41	1.45
23	A	848	BCR	C17-C18	2.11	1.40	1.35
19	F	303	CLA	MG-NC	2.11	2.11	2.06
19	A	806	CLA	MG-NC	2.11	2.11	2.06
23	5	317	BCR	C21-C22	2.11	1.40	1.35
19	A	827	CLA	C1D-C2D	-2.11	1.41	1.45
19	2	304	CLA	C1D-C2D	-2.11	1.41	1.45
19	2	310	CLA	MG-NC	2.11	2.11	2.06
19	L	302	CLA	MG-NC	2.10	2.11	2.06
23	G	205	BCR	C10-C9	2.10	1.40	1.35
19	G	204	CLA	C1D-C2D	-2.10	1.41	1.45
19	A	825	CLA	MG-NB	2.10	2.10	2.05
23	F	305	BCR	C21-C22	2.10	1.40	1.35
19	5	303	CLA	C1D-C2D	-2.10	1.41	1.45
23	B	845	BCR	C21-C22	2.10	1.40	1.35
19	A	837	CLA	C1D-C2D	-2.10	1.41	1.45
19	B	805	CLA	C1B-C2B	-2.10	1.38	1.43
23	B	844	BCR	C10-C9	2.10	1.40	1.35
23	A	849	BCR	C17-C18	2.10	1.40	1.35
23	J	103	BCR	C12-C13	-2.10	1.41	1.46
19	A	839	CLA	C1D-C2D	-2.10	1.41	1.45
23	A	852	BCR	C14-C13	2.10	1.40	1.35
19	A	811	CLA	C1B-C2B	-2.09	1.38	1.43
20	5	316	LUT	C30-C29	2.09	1.40	1.35
19	B	806	CLA	C1B-NB	-2.09	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	848	BCR	C21-C22	2.09	1.40	1.35
19	A	831	CLA	CHB-C1B	2.09	1.44	1.39
19	A	812	CLA	MG-NB	2.09	2.09	2.05
19	A	807	CLA	C1D-C2D	-2.09	1.41	1.45
19	B	830	CLA	C1B-C2B	-2.09	1.38	1.43
19	A	816	CLA	C1B-C2B	-2.09	1.38	1.43
19	6	302	CLA	C1D-C2D	-2.09	1.41	1.45
23	J	103	BCR	C2-C3	-2.09	1.47	1.52
19	6	309	CLA	C1B-C2B	-2.08	1.38	1.43
19	B	819	CLA	C1B-NB	-2.08	1.35	1.37
19	2	309	CLA	C1B-NB	-2.08	1.35	1.37
23	A	849	BCR	C21-C22	2.08	1.40	1.35
19	3	307	CLA	C1B-NB	-2.08	1.35	1.37
23	A	848	BCR	C14-C13	2.08	1.40	1.35
23	A	848	BCR	C10-C9	2.08	1.40	1.35
23	A	852	BCR	C17-C18	2.08	1.40	1.35
19	L	301	CLA	C1B-C2B	-2.08	1.38	1.43
23	2	319	BCR	C10-C9	2.07	1.40	1.35
19	B	801	CLA	CHB-C1B	2.07	1.44	1.39
19	A	822	CLA	MG-NC	2.07	2.11	2.06
23	B	845	BCR	C10-C9	2.07	1.40	1.35
19	3	303	CLA	C1D-C2D	-2.07	1.41	1.45
19	6	304	CLA	C1D-C2D	-2.07	1.41	1.45
19	6	312	CLA	CHB-C1B	2.07	1.44	1.39
19	B	814	CLA	C1B-C2B	-2.07	1.38	1.43
20	2	316	LUT	C14-C13	2.07	1.40	1.35
19	A	835	CLA	C1D-C2D	-2.07	1.41	1.45
19	3	304	CLA	C1B-C2B	-2.07	1.38	1.43
23	A	850	BCR	C14-C13	2.07	1.40	1.35
19	B	838	CLA	C1D-C2D	-2.06	1.41	1.45
19	B	832	CLA	C1B-C2B	-2.06	1.38	1.43
18	2	314	CHL	C3B-C4B	-2.06	1.39	1.41
19	3	302	CLA	C1B-NB	-2.06	1.35	1.37
19	B	812	CLA	C1D-C2D	-2.06	1.41	1.45
19	B	833	CLA	C1B-C2B	-2.06	1.38	1.43
19	3	311	CLA	CHB-C1B	2.06	1.44	1.39
23	L	304	BCR	C21-C22	2.06	1.40	1.35
19	A	843	CLA	C1B-NB	-2.06	1.35	1.37
19	6	304	CLA	MG-NC	2.06	2.11	2.06
19	B	827	CLA	C1B-C2B	-2.06	1.38	1.43
19	B	827	CLA	C1B-NB	-2.06	1.35	1.37
20	3	315	LUT	C34-C33	2.06	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	830	CLA	C1B-C2B	-2.06	1.38	1.43
19	B	823	CLA	C1B-C2B	-2.06	1.38	1.43
23	F	305	BCR	C10-C9	2.05	1.40	1.35
19	A	805	CLA	MG-NC	2.05	2.11	2.06
19	6	303	CLA	C1D-C2D	-2.05	1.41	1.45
19	3	301	CLA	CHB-C1B	2.05	1.44	1.39
23	F	302	BCR	C17-C18	2.05	1.40	1.35
19	A	810	CLA	C1B-C2B	-2.05	1.38	1.43
19	B	836	CLA	C1D-C2D	-2.05	1.41	1.45
19	B	832	CLA	C1B-NB	-2.05	1.35	1.37
19	A	839	CLA	C1B-C2B	-2.05	1.38	1.43
23	L	304	BCR	C10-C9	2.05	1.40	1.35
19	2	302	CLA	MG-NC	2.05	2.11	2.06
24	A	802	CL0	MG-ND	-2.05	2.01	2.05
19	B	826	CLA	C1B-C2B	-2.05	1.38	1.43
19	A	808	CLA	C1B-NB	-2.04	1.35	1.37
19	K	201	CLA	C1B-NB	-2.04	1.35	1.37
19	5	303	CLA	CHB-C1B	2.04	1.44	1.39
19	A	843	CLA	CHB-C1B	2.04	1.44	1.39
19	6	314	CLA	C1D-C2D	-2.04	1.41	1.45
19	A	827	CLA	C1B-C2B	-2.04	1.38	1.43
19	3	303	CLA	C1B-C2B	-2.04	1.38	1.43
19	A	806	CLA	C1D-C2D	-2.04	1.41	1.45
19	5	308	CLA	C1B-NB	-2.04	1.35	1.37
19	B	816	CLA	C1B-NB	-2.04	1.35	1.37
23	J	103	BCR	C19-C18	-2.04	1.41	1.46
19	3	307	CLA	C1D-C2D	-2.04	1.41	1.45
19	L	301	CLA	C1B-NB	-2.04	1.35	1.37
19	A	820	CLA	MG-NC	2.04	2.11	2.06
20	6	315	LUT	C30-C29	2.03	1.40	1.35
19	3	313	CLA	MG-NC	2.03	2.11	2.06
19	3	313	CLA	C1D-C2D	-2.03	1.41	1.45
19	A	808	CLA	C1B-C2B	-2.03	1.38	1.43
19	B	834	CLA	C1B-C2B	-2.03	1.38	1.43
19	A	813	CLA	C1B-C2B	-2.03	1.38	1.43
19	L	303	CLA	CHB-C1B	2.03	1.44	1.39
19	B	820	CLA	C1B-NB	-2.03	1.35	1.37
19	B	824	CLA	C1B-C2B	-2.03	1.38	1.43
23	B	844	BCR	C14-C13	2.03	1.40	1.35
19	A	820	CLA	C1D-C2D	-2.03	1.41	1.45
19	A	820	CLA	C1B-NB	-2.03	1.35	1.37
19	2	302	CLA	CHB-C1B	2.03	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	308	CLA	C1D-C2D	-2.03	1.41	1.45
19	5	309	CLA	MG-NC	2.03	2.11	2.06
19	B	816	CLA	C1B-C2B	-2.03	1.38	1.43
19	K	202	CLA	C1B-C2B	-2.02	1.38	1.43
23	3	317	BCR	C17-C18	2.02	1.40	1.35
23	A	850	BCR	C17-C18	2.02	1.40	1.35
19	A	837	CLA	MG-NC	2.02	2.11	2.06
19	5	301	CLA	C1B-C2B	-2.02	1.38	1.43
19	K	202	CLA	CHB-C1B	2.02	1.44	1.39
23	A	852	BCR	C10-C9	2.02	1.40	1.35
23	5	317	BCR	C29-C28	-2.02	1.47	1.52
19	A	813	CLA	C1B-NB	-2.02	1.35	1.37
19	B	825	CLA	C1B-NB	-2.02	1.35	1.37
19	2	304	CLA	C1B-C2B	-2.02	1.38	1.43
19	A	834	CLA	MG-NB	2.02	2.09	2.05
19	B	831	CLA	CHB-C1B	2.02	1.43	1.39
23	G	201	BCR	C29-C28	-2.02	1.47	1.52
19	6	302	CLA	CHB-C1B	2.02	1.43	1.39
19	F	304	CLA	CHB-C1B	2.02	1.43	1.39
19	B	801	CLA	C1B-NB	-2.02	1.35	1.37
19	3	313	CLA	CHB-C1B	2.02	1.43	1.39
23	J	103	BCR	C29-C28	-2.02	1.47	1.52
19	2	304	CLA	CHB-C1B	2.02	1.43	1.39
23	A	849	BCR	C14-C13	2.01	1.40	1.35
19	B	821	CLA	CHB-C1B	2.01	1.43	1.39
19	B	825	CLA	C1B-C2B	-2.01	1.38	1.43
19	3	303	CLA	C1B-NB	-2.01	1.35	1.37
19	2	303	CLA	C1B-C2B	-2.01	1.38	1.43
19	B	801	CLA	C1B-C2B	-2.01	1.38	1.43
19	A	801	CLA	CHB-C1B	2.01	1.43	1.39
19	6	311	CLA	CHB-C1B	2.01	1.43	1.39
19	6	312	CLA	C1D-C2D	-2.01	1.41	1.45
19	6	308	CLA	CHB-C1B	2.01	1.43	1.39
19	L	303	CLA	C1B-C2B	-2.01	1.38	1.43
23	B	846	BCR	C19-C18	-2.01	1.41	1.46
19	B	814	CLA	C1B-NB	-2.01	1.35	1.37
19	A	814	CLA	C1B-NB	-2.01	1.35	1.37
19	A	825	CLA	C1D-C2D	-2.01	1.41	1.45
19	3	307	CLA	C1B-C2B	-2.01	1.38	1.43
23	G	205	BCR	C29-C28	-2.01	1.47	1.52
19	G	204	CLA	CHB-C1B	2.01	1.43	1.39
19	A	804	CLA	C1D-C2D	-2.01	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	824	CLA	C1B-NB	-2.01	1.35	1.37
19	A	805	CLA	C1B-C2B	-2.01	1.38	1.43
19	A	829	CLA	C1B-C2B	-2.01	1.38	1.43
19	6	314	CLA	C1B-C2B	-2.01	1.38	1.43
19	B	813	CLA	C1B-C2B	-2.01	1.38	1.43
19	2	312	CLA	CHB-C1B	2.01	1.43	1.39
19	A	823	CLA	CHB-C1B	2.01	1.43	1.39
19	A	814	CLA	C1B-C2B	-2.01	1.38	1.43
19	B	815	CLA	C1B-C2B	-2.01	1.38	1.43
19	B	826	CLA	C1B-NB	-2.00	1.35	1.37
19	B	830	CLA	CHB-C1B	2.00	1.43	1.39
24	A	802	CL0	MG-NB	-2.00	2.01	2.05
19	A	810	CLA	C1B-NB	-2.00	1.35	1.37
20	6	318	LUT	C30-C29	2.00	1.40	1.35
19	2	308	CLA	CHB-C1B	2.00	1.43	1.39
19	B	824	CLA	MG-NC	2.00	2.11	2.06

All (1279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	301	CHL	C1B-CHB-C4A	14.50	130.65	121.32
18	6	301	CHL	C1B-CHB-C4A	14.10	130.40	121.32
18	5	304	CHL	C1B-CHB-C4A	14.04	130.35	121.32
18	2	307	CHL	C1B-CHB-C4A	13.87	130.24	121.32
18	5	306	CHL	C1B-CHB-C4A	13.83	130.22	121.32
18	2	305	CHL	C1B-CHB-C4A	13.52	130.02	121.32
18	5	305	CHL	C1B-CHB-C4A	13.26	129.85	121.32
18	6	306	CHL	C1B-CHB-C4A	13.23	129.83	121.32
18	2	320	CHL	C1B-CHB-C4A	13.11	129.75	121.32
18	2	306	CHL	C1B-CHB-C4A	13.05	129.72	121.32
18	3	306	CHL	C1B-CHB-C4A	12.90	129.62	121.32
18	5	313	CHL	C1B-CHB-C4A	12.89	129.62	121.32
18	2	314	CHL	C1B-CHB-C4A	12.77	129.54	121.32
18	3	314	CHL	C1B-CHB-C4A	12.12	129.12	121.32
24	A	802	CL0	C1B-CHB-C4A	9.65	127.53	121.32
23	B	848	BCR	C11-C10-C9	6.18	135.94	127.28
23	B	848	BCR	C10-C11-C12	5.92	140.34	123.20
23	2	319	BCR	C21-C20-C19	5.74	139.83	123.20
23	B	848	BCR	C16-C15-C14	5.59	134.95	123.52
23	A	852	BCR	C15-C16-C17	5.40	134.58	123.52
23	2	319	BCR	C20-C21-C22	5.39	134.84	127.28
20	2	317	LUT	C28-C29-C30	5.30	127.34	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	315	LUT	C35-C15-C14	5.18	134.11	123.52
20	6	318	LUT	C39-C29-C28	5.13	125.93	118.09
23	J	103	BCR	C23-C22-C21	5.06	126.96	119.01
19	5	314	CLA	O2D-CGD-CBD	4.99	119.96	111.23
20	3	316	LUT	C35-C15-C14	4.94	133.62	123.52
23	B	846	BCR	C23-C22-C21	4.71	126.41	119.01
23	F	305	BCR	C16-C15-C14	4.70	133.15	123.52
23	B	847	BCR	C16-C15-C14	4.68	133.10	123.52
23	5	317	BCR	C16-C15-C14	4.61	132.94	123.52
23	B	846	BCR	C16-C15-C14	4.54	132.81	123.52
20	6	318	LUT	C35-C15-C14	4.51	132.74	123.52
23	J	103	BCR	C24-C23-C22	4.47	132.84	126.23
20	5	316	LUT	C35-C15-C14	4.43	132.58	123.52
20	5	315	LUT	C35-C15-C14	4.42	132.56	123.52
18	3	314	CHL	O2D-CGD-CBD	4.32	115.69	110.95
20	2	316	LUT	C39-C29-C28	4.29	124.64	118.09
20	2	317	LUT	C39-C29-C30	-4.26	115.92	122.82
18	6	301	CHL	C3D-C4D-CHA	4.26	115.01	108.54
18	5	313	CHL	C1C-CHC-C4B	4.25	131.27	116.07
20	J	101	LUT	C15-C35-C34	4.25	132.21	123.52
20	J	101	LUT	C28-C29-C30	4.24	125.67	119.01
23	A	848	BCR	C15-C16-C17	4.21	132.14	123.52
18	2	306	CHL	O2D-CGD-CBD	4.19	115.56	110.95
18	2	314	CHL	C1C-CHC-C4B	4.19	131.07	116.07
23	K	204	BCR	C38-C26-C25	4.18	129.04	124.48
18	5	306	CHL	C3D-C4D-CHA	4.16	114.87	108.54
18	2	301	CHL	C3D-C4D-CHA	4.16	114.86	108.54
18	2	305	CHL	C3D-C4D-CHA	4.15	114.85	108.54
18	3	306	CHL	C3D-C4D-CHA	4.15	114.85	108.54
18	5	313	CHL	C3D-C4D-CHA	4.14	114.83	108.54
23	J	103	BCR	C8-C9-C10	4.13	125.50	119.01
20	5	315	LUT	C15-C35-C34	4.12	131.96	123.52
18	5	304	CHL	C3D-C4D-CHA	4.12	114.81	108.54
18	2	314	CHL	C3D-C4D-CHA	4.12	114.80	108.54
18	6	306	CHL	C3D-C4D-CHA	4.12	114.80	108.54
23	F	302	BCR	C15-C16-C17	4.12	131.94	123.52
18	5	305	CHL	C3D-C4D-CHA	4.11	114.78	108.54
19	A	828	CLA	C4D-CHA-C1A	4.10	126.14	121.24
23	2	319	BCR	C38-C26-C25	4.10	128.96	124.48
18	6	306	CHL	C1C-CHC-C4B	4.10	130.74	116.07
18	2	320	CHL	C3D-C4D-CHA	4.10	114.77	108.54
23	B	846	BCR	C19-C18-C17	4.08	125.43	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	314	CHL	C3D-C4D-CHA	4.07	114.73	108.54
18	2	307	CHL	C3D-C4D-CHA	4.07	114.73	108.54
23	B	846	BCR	C24-C23-C22	4.06	132.24	126.23
20	6	318	LUT	C18-C5-C6	4.05	128.90	124.48
18	2	306	CHL	C3D-C4D-CHA	4.04	114.68	108.54
18	2	301	CHL	C1C-CHC-C4B	4.02	130.46	116.07
18	2	320	CHL	C1C-CHC-C4B	4.02	130.45	116.07
23	B	847	BCR	C1-C6-C5	-4.01	117.16	122.64
23	B	846	BCR	C37-C22-C21	-4.01	116.33	122.82
20	2	317	LUT	C15-C35-C34	4.00	131.71	123.52
20	6	318	LUT	C31-C30-C29	4.00	132.88	127.28
23	B	846	BCR	C21-C20-C19	3.98	134.74	123.20
19	A	804	CLA	C4D-CHA-C1A	3.96	125.97	121.24
23	B	847	BCR	C7-C8-C9	3.95	132.08	126.23
23	J	103	BCR	C37-C22-C21	-3.94	116.43	122.82
18	5	313	CHL	C1A-CHA-C4D	3.94	125.56	118.98
18	2	305	CHL	C1A-CHA-C4D	3.93	125.54	118.98
19	3	307	CLA	C1-O2A-CGA	3.93	126.17	116.65
19	B	808	CLA	C4D-CHA-C1A	3.92	125.92	121.24
23	2	319	BCR	C16-C15-C14	3.92	131.54	123.52
23	J	103	BCR	C15-C16-C17	3.91	131.53	123.52
18	5	305	CHL	C1A-CHA-C4D	3.91	125.50	118.98
23	K	205	BCR	C15-C16-C17	3.90	131.50	123.52
18	2	306	CHL	C1A-CHA-C4D	3.90	125.49	118.98
20	6	318	LUT	C27-C28-C29	3.89	134.69	126.32
19	5	312	CLA	C1-O2A-CGA	3.88	126.04	116.65
23	A	850	BCR	C15-C16-C17	3.88	131.46	123.52
18	2	307	CHL	C1C-CHC-C4B	3.88	129.95	116.07
23	B	847	BCR	C34-C9-C8	3.88	124.01	118.09
19	6	312	CLA	CAA-C2A-C3A	-3.87	102.54	113.00
23	B	844	BCR	C38-C26-C25	3.86	128.69	124.48
18	5	305	CHL	C1C-CHC-C4B	3.85	129.85	116.07
18	3	306	CHL	C1A-CHA-C4D	3.84	125.39	118.98
18	2	306	CHL	C1C-CHC-C4B	3.83	129.79	116.07
18	6	301	CHL	C1C-CHC-C4B	3.83	129.78	116.07
19	6	311	CLA	C4D-CHA-C1A	3.82	125.81	121.24
19	A	807	CLA	C4D-CHA-C1A	3.82	125.81	121.24
20	3	315	LUT	C19-C9-C8	3.81	123.91	118.09
18	2	314	CHL	C1A-CHA-C4D	3.80	125.33	118.98
19	B	819	CLA	C4D-CHA-C1A	3.80	125.78	121.24
20	J	101	LUT	C39-C29-C30	-3.80	116.66	122.82
20	6	318	LUT	C19-C9-C10	-3.79	116.67	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	839	CLA	C4D-CHA-C1A	3.79	125.76	121.24
20	5	316	LUT	C19-C9-C10	-3.78	116.70	122.82
19	B	839	CLA	C4D-CHA-C1A	3.77	125.74	121.24
19	A	837	CLA	C4D-CHA-C1A	3.77	125.74	121.24
19	A	835	CLA	C4D-CHA-C1A	3.76	125.73	121.24
23	J	103	BCR	C34-C9-C10	-3.75	116.74	122.82
23	L	305	BCR	C38-C26-C25	3.74	128.57	124.48
18	2	307	CHL	C4D-CHA-CBD	-3.73	105.20	108.97
18	3	314	CHL	C1A-CHA-C4D	3.73	125.21	118.98
19	B	842	CLA	C4D-CHA-C1A	3.73	125.69	121.24
19	A	805	CLA	C4D-CHA-C1A	3.73	125.69	121.24
23	I	101	BCR	C37-C22-C23	3.72	123.78	118.09
18	3	314	CHL	C1C-CHC-C4B	3.72	129.38	116.07
23	A	851	BCR	C30-C25-C24	3.71	125.72	115.65
23	F	302	BCR	C38-C26-C25	3.71	128.53	124.48
19	B	837	CLA	C4D-CHA-C1A	3.71	125.66	121.24
18	2	305	CHL	C1C-CHC-C4B	3.70	129.31	116.07
23	J	103	BCR	C1-C6-C7	3.70	125.69	115.65
23	3	317	BCR	C30-C25-C24	3.70	125.68	115.65
23	G	205	BCR	C15-C16-C17	3.69	131.08	123.52
20	2	317	LUT	C35-C15-C14	3.69	131.07	123.52
19	A	816	CLA	C4D-CHA-C1A	3.69	125.65	121.24
23	5	317	BCR	C34-C9-C10	-3.69	116.84	122.82
20	3	316	LUT	C39-C29-C28	3.69	123.72	118.09
19	B	833	CLA	C4D-CHA-C1A	3.68	125.64	121.24
23	G	201	BCR	C38-C26-C25	3.67	128.49	124.48
18	2	320	CHL	C1A-CHA-C4D	3.67	125.10	118.98
18	5	304	CHL	C1A-CHA-C4D	3.66	125.08	118.98
18	6	301	CHL	C1A-CHA-C4D	3.65	125.08	118.98
19	B	823	CLA	C1-O2A-CGA	3.65	125.50	116.65
20	2	317	LUT	C30-C31-C32	3.65	133.76	123.20
18	5	306	CHL	C1A-CHA-C4D	3.64	125.06	118.98
23	B	844	BCR	C34-C9-C10	-3.64	116.92	122.82
23	J	103	BCR	C16-C15-C14	3.63	130.95	123.52
18	5	306	CHL	C1C-CHC-C4B	3.63	129.06	116.07
23	G	201	BCR	C34-C9-C10	-3.63	116.94	122.82
19	6	304	CLA	C4D-CHA-C1A	3.62	125.56	121.24
23	L	304	BCR	C30-C25-C24	3.62	125.47	115.65
18	5	304	CHL	C1C-CHC-C4B	3.62	129.01	116.07
23	L	304	BCR	C29-C30-C25	3.61	115.69	110.44
23	3	317	BCR	C37-C22-C23	3.61	123.60	118.09
23	3	317	BCR	C1-C6-C7	3.61	125.43	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	845	BCR	C15-C16-C17	3.60	130.89	123.52
23	K	204	BCR	C37-C22-C21	-3.60	116.98	122.82
23	5	317	BCR	C30-C25-C24	3.60	125.40	115.65
23	3	317	BCR	C16-C15-C14	3.59	130.86	123.52
19	B	838	CLA	C4D-CHA-C1A	3.58	125.52	121.24
23	B	846	BCR	C15-C16-C17	3.58	130.85	123.52
19	A	823	CLA	C4D-CHA-C1A	3.57	125.51	121.24
19	5	314	CLA	CED-O2D-CGD	3.57	124.01	115.92
23	L	304	BCR	C24-C23-C22	3.57	131.51	126.23
23	F	305	BCR	C34-C9-C10	-3.56	117.04	122.82
18	6	306	CHL	C1A-CHA-C4D	3.56	124.93	118.98
19	B	811	CLA	C4D-CHA-C1A	3.56	125.49	121.24
20	2	315	LUT	C19-C9-C10	-3.56	117.05	122.82
23	A	852	BCR	C38-C26-C25	3.55	128.36	124.48
20	J	101	LUT	C1-C6-C7	3.55	125.29	115.65
19	A	817	CLA	C4D-CHA-C1A	3.55	125.48	121.24
23	J	103	BCR	C1-C6-C5	-3.55	117.78	122.64
19	A	841	CLA	C4D-CHA-C1A	3.54	125.47	121.24
23	5	317	BCR	C12-C13-C14	3.54	124.58	119.01
23	G	201	BCR	C33-C5-C6	3.54	128.34	124.48
23	2	319	BCR	C34-C9-C10	-3.54	117.09	122.82
19	F	303	CLA	C4D-CHA-C1A	3.53	125.46	121.24
19	B	822	CLA	C4D-CHA-C1A	3.53	125.45	121.24
19	B	841	CLA	C4D-CHA-C1A	3.52	125.45	121.24
23	A	851	BCR	C37-C22-C23	3.52	123.47	118.09
23	J	103	BCR	C38-C26-C25	3.51	128.32	124.48
19	5	310	CLA	C4D-CHA-C1A	3.51	125.43	121.24
20	3	316	LUT	C19-C9-C10	-3.51	117.13	122.82
19	3	305	CLA	C4D-CHA-C1A	3.51	125.43	121.24
23	G	201	BCR	C15-C16-C17	3.51	130.70	123.52
18	3	306	CHL	C1C-CHC-C4B	3.51	128.62	116.07
19	6	305	CLA	C4D-CHA-C1A	3.51	125.43	121.24
23	5	317	BCR	C33-C5-C6	3.51	128.31	124.48
23	B	844	BCR	C16-C15-C14	3.50	130.69	123.52
20	5	316	LUT	C39-C29-C28	3.50	123.43	118.09
19	A	842	CLA	C4D-CHA-C1A	3.50	125.41	121.24
20	2	317	LUT	C19-C9-C10	-3.49	117.16	122.82
23	A	849	BCR	C37-C22-C21	-3.49	117.16	122.82
23	B	846	BCR	C34-C9-C10	-3.49	117.16	122.82
20	3	315	LUT	C1-C6-C7	3.49	125.11	115.65
18	2	307	CHL	C1A-CHA-C4D	3.49	124.80	118.98
19	A	827	CLA	C4D-CHA-C1A	3.49	125.40	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	817	CLA	C4D-CHA-C1A	3.49	125.40	121.24
23	A	848	BCR	C2-C1-C6	3.48	115.50	110.44
19	5	307	CLA	C4D-CHA-C1A	3.48	125.40	121.24
19	B	812	CLA	C4D-CHA-C1A	3.47	125.39	121.24
19	A	814	CLA	C4D-CHA-C1A	3.47	125.38	121.24
23	B	846	BCR	C36-C18-C17	-3.47	117.20	122.82
20	3	315	LUT	C39-C29-C28	3.46	123.37	118.09
23	A	848	BCR	C1-C6-C7	3.46	125.03	115.65
23	A	848	BCR	C34-C9-C10	-3.46	117.22	122.82
24	A	802	CL0	C1C-CHC-C4B	3.45	128.43	116.07
19	A	840	CLA	C4D-CHA-C1A	3.45	125.36	121.24
23	L	304	BCR	C33-C5-C6	3.45	128.25	124.48
23	K	205	BCR	C37-C22-C21	-3.45	117.23	122.82
19	B	834	CLA	C4D-CHA-C1A	3.45	125.36	121.24
20	2	317	LUT	C32-C33-C34	3.45	124.43	119.01
19	K	202	CLA	C4D-CHA-C1A	3.44	125.35	121.24
20	2	315	LUT	C12-C13-C14	3.44	124.42	119.01
23	2	319	BCR	C1-C6-C5	-3.44	117.93	122.64
23	L	304	BCR	C37-C22-C23	3.44	123.34	118.09
23	G	205	BCR	C37-C22-C21	-3.44	117.25	122.82
19	B	836	CLA	C4D-CHA-C1A	3.44	125.34	121.24
19	A	825	CLA	C4D-CHA-C1A	3.43	125.34	121.24
19	L	302	CLA	C4D-CHA-C1A	3.43	125.34	121.24
23	G	205	BCR	C30-C25-C24	3.43	124.94	115.65
23	A	851	BCR	C29-C30-C25	3.42	115.41	110.44
23	K	205	BCR	C34-C9-C10	-3.42	117.28	122.82
19	A	833	CLA	C4D-CHA-C1A	3.42	125.32	121.24
19	L	303	CLA	C4D-CHA-C1A	3.42	125.32	121.24
19	A	809	CLA	C4D-CHA-C1A	3.41	125.31	121.24
20	2	315	LUT	C39-C29-C28	3.41	123.30	118.09
18	2	301	CHL	C4D-CHA-CBD	-3.41	105.53	108.97
23	M	101	BCR	C33-C5-C6	3.41	128.20	124.48
23	K	204	BCR	C16-C15-C14	3.40	130.48	123.52
19	3	304	CLA	C4D-CHA-C1A	3.40	125.30	121.24
20	3	316	LUT	C1-C6-C7	3.40	124.87	115.65
19	2	313	CLA	C4D-CHA-C1A	3.40	125.29	121.24
19	6	302	CLA	C4D-CHA-C1A	3.39	125.29	121.24
19	3	311	CLA	C4D-CHA-C1A	3.39	125.28	121.24
19	2	304	CLA	C4D-CHA-C1A	3.39	125.28	121.24
23	B	845	BCR	C37-C22-C21	-3.38	117.33	122.82
20	6	315	LUT	C15-C35-C34	3.38	130.44	123.52
19	A	820	CLA	C4D-CHA-C1A	3.38	125.28	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	312	CLA	C4D-CHA-C1A	3.38	125.28	121.24
19	5	311	CLA	C4D-CHA-C1A	3.38	125.28	121.24
19	3	301	CLA	C4D-CHA-C1A	3.38	125.27	121.24
19	3	310	CLA	C4D-CHA-C1A	3.38	125.27	121.24
19	A	819	CLA	C4D-CHA-C1A	3.38	125.27	121.24
23	L	304	BCR	C30-C25-C26	-3.37	118.03	122.64
23	I	101	BCR	C15-C16-C17	3.37	130.42	123.52
19	A	815	CLA	C4D-CHA-C1A	3.37	125.26	121.24
19	A	818	CLA	C4D-CHA-C1A	3.36	125.26	121.24
20	6	315	LUT	C19-C9-C10	-3.36	117.37	122.82
23	M	101	BCR	C15-C16-C17	3.36	130.40	123.52
23	B	846	BCR	C12-C13-C14	3.36	124.30	119.01
20	J	101	LUT	C32-C33-C34	3.36	124.30	119.01
19	B	835	CLA	C4D-CHA-C1A	3.36	125.25	121.24
18	5	306	CHL	C4D-CHA-CBD	-3.36	105.58	108.97
19	G	204	CLA	C4D-CHA-C1A	3.36	125.25	121.24
23	A	849	BCR	C38-C26-C25	3.35	128.14	124.48
19	3	313	CLA	C4D-CHA-C1A	3.35	125.24	121.24
19	B	818	CLA	C4D-CHA-C1A	3.35	125.24	121.24
23	F	305	BCR	C38-C26-C25	3.35	128.14	124.48
18	6	301	CHL	C4D-CHA-CBD	-3.34	105.60	108.97
19	A	824	CLA	C4D-CHA-C1A	3.34	125.22	121.24
19	K	201	CLA	C4D-CHA-C1A	3.34	125.22	121.24
19	5	301	CLA	C4D-CHA-C1A	3.34	125.22	121.24
23	M	101	BCR	C34-C9-C10	-3.33	117.41	122.82
23	2	319	BCR	C12-C13-C14	3.33	124.25	119.01
23	B	848	BCR	C12-C13-C14	3.33	124.25	119.01
20	J	101	LUT	C19-C9-C10	-3.33	117.42	122.82
23	2	319	BCR	C33-C5-C6	3.33	128.12	124.48
23	B	845	BCR	C16-C15-C14	3.33	130.33	123.52
23	A	851	BCR	C34-C9-C10	-3.33	117.43	122.82
19	6	314	CLA	C4D-CHA-C1A	3.33	125.21	121.24
23	B	848	BCR	C37-C22-C21	-3.32	117.43	122.82
19	A	811	CLA	C4D-CHA-C1A	3.32	125.21	121.24
23	L	305	BCR	C16-C15-C14	3.32	130.32	123.52
19	A	810	CLA	C4D-CHA-C1A	3.32	125.20	121.24
19	2	302	CLA	C4D-CHA-C1A	3.32	125.20	121.24
19	B	813	CLA	C4D-CHA-C1A	3.32	125.20	121.24
23	K	205	BCR	C16-C15-C14	3.31	130.30	123.52
19	B	801	CLA	C4D-CHA-C1A	3.31	125.19	121.24
20	5	316	LUT	C1-C6-C7	3.31	124.62	115.65
19	F	304	CLA	C4D-CHA-C1A	3.30	125.19	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	802	CL0	C3D-C4D-CHA	3.30	113.56	108.54
18	2	301	CHL	C1A-CHA-C4D	3.30	124.49	118.98
19	J	102	CLA	C4D-CHA-C1A	3.30	125.18	121.24
23	F	305	BCR	C1-C6-C5	-3.30	118.13	122.64
23	A	852	BCR	C34-C9-C10	-3.29	117.48	122.82
23	5	317	BCR	C8-C9-C10	3.29	124.19	119.01
19	B	831	CLA	C4D-CHA-C1A	3.29	125.17	121.24
23	A	849	BCR	C15-C16-C17	3.29	130.26	123.52
19	5	303	CLA	C4D-CHA-C1A	3.29	125.17	121.24
23	K	204	BCR	C34-C9-C10	-3.29	117.48	122.82
20	5	315	LUT	C19-C9-C10	-3.29	117.48	122.82
18	3	306	CHL	C4D-CHA-CBD	-3.29	105.65	108.97
19	B	814	CLA	C4D-CHA-C1A	3.29	125.17	121.24
23	3	317	BCR	C34-C9-C10	-3.29	117.49	122.82
23	K	204	BCR	C33-C5-C6	3.28	128.07	124.48
19	5	309	CLA	C4D-CHA-C1A	3.28	125.16	121.24
23	F	305	BCR	C37-C22-C21	-3.28	117.50	122.82
23	L	304	BCR	C34-C9-C8	3.28	123.10	118.09
19	3	303	CLA	C4D-CHA-C1A	3.28	125.16	121.24
23	A	848	BCR	C7-C8-C9	3.28	131.09	126.23
23	A	848	BCR	C37-C22-C21	-3.28	117.51	122.82
23	A	849	BCR	C34-C9-C10	-3.26	117.53	122.82
18	3	306	CHL	C4D-ND-C1D	3.26	107.69	105.22
23	A	850	BCR	C37-C22-C21	-3.26	117.53	122.82
19	B	806	CLA	C4D-CHA-C1A	3.26	125.13	121.24
19	B	821	CLA	C4D-CHA-C1A	3.26	125.13	121.24
23	A	848	BCR	C1-C6-C5	-3.26	118.19	122.64
19	6	312	CLA	C4D-CHA-C1A	3.26	125.13	121.24
23	A	850	BCR	C34-C9-C10	-3.25	117.54	122.82
23	5	317	BCR	C37-C22-C21	-3.25	117.55	122.82
23	A	852	BCR	C37-C22-C21	-3.25	117.55	122.82
23	B	847	BCR	C37-C22-C23	3.24	123.04	118.09
19	6	303	CLA	C4D-CHA-C1A	3.24	125.11	121.24
20	3	316	LUT	C12-C13-C14	3.24	124.10	119.01
20	5	316	LUT	C12-C13-C14	3.24	124.10	119.01
18	5	304	CHL	C4D-ND-C1D	3.23	107.67	105.22
19	A	838	CLA	C4D-CHA-C1A	3.23	125.10	121.24
23	A	851	BCR	C30-C25-C26	-3.23	118.22	122.64
19	6	310	CLA	C4D-CHA-C1A	3.23	125.10	121.24
23	F	302	BCR	C37-C22-C21	-3.23	117.58	122.82
19	B	832	CLA	C4D-CHA-C1A	3.23	125.10	121.24
23	B	845	BCR	C34-C9-C10	-3.23	117.58	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	813	CLA	C4D-CHA-C1A	3.23	125.09	121.24
19	A	826	CLA	CHA-C1A-NA	-3.23	119.08	126.39
23	B	848	BCR	C38-C26-C25	3.23	128.01	124.48
19	6	307	CLA	CAA-C2A-C1A	3.23	122.55	111.97
18	2	307	CHL	C4D-ND-C1D	3.22	107.66	105.22
23	B	846	BCR	C38-C26-C25	3.22	128.00	124.48
23	L	305	BCR	C34-C9-C10	-3.22	117.60	122.82
23	L	304	BCR	C15-C16-C17	3.22	130.10	123.52
19	2	311	CLA	C4D-CHA-C1A	3.22	125.08	121.24
23	M	101	BCR	C37-C22-C23	3.22	123.00	118.09
23	A	852	BCR	C33-C5-C6	3.21	127.99	124.48
18	2	320	CHL	C4D-ND-C1D	3.20	107.65	105.22
23	I	101	BCR	C34-C9-C8	3.20	122.98	118.09
23	B	845	BCR	C33-C5-C6	3.20	127.98	124.48
19	A	801	CLA	C4D-CHA-C1A	3.20	125.06	121.24
20	2	316	LUT	C19-C9-C10	-3.19	117.64	122.82
20	2	317	LUT	C12-C13-C14	3.19	124.03	119.01
19	3	307	CLA	C4D-CHA-C1A	3.19	125.05	121.24
19	B	825	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
19	A	829	CLA	C4D-CHA-C1A	3.19	125.05	121.24
23	G	201	BCR	C37-C22-C23	3.19	122.95	118.09
19	A	834	CLA	C4D-CHA-C1A	3.18	125.04	121.24
23	J	103	BCR	C7-C8-C9	3.18	130.94	126.23
23	L	305	BCR	C37-C22-C23	3.18	122.95	118.09
20	5	316	LUT	C8-C9-C10	3.18	124.01	119.01
19	B	810	CLA	C4D-CHA-C1A	3.18	125.04	121.24
19	B	840	CLA	C4D-CHA-C1A	3.18	125.03	121.24
23	3	317	BCR	C1-C6-C5	-3.18	118.30	122.64
23	B	848	BCR	C35-C13-C14	-3.17	117.68	122.82
18	2	305	CHL	C4D-CHA-CBD	-3.17	105.77	108.97
19	5	302	CLA	C4D-CHA-C1A	3.17	125.03	121.24
18	6	306	CHL	C4D-CHA-CBD	-3.17	105.77	108.97
19	F	301	CLA	C4D-CHA-C1A	3.17	125.02	121.24
23	5	317	BCR	C35-C13-C14	-3.17	117.69	122.82
19	2	310	CLA	C4D-CHA-C1A	3.17	125.02	121.24
19	A	821	CLA	C4D-CHA-C1A	3.16	125.02	121.24
19	2	312	CLA	C4D-CHA-C1A	3.16	125.02	121.24
18	2	306	CHL	C4D-CHA-CBD	-3.16	105.78	108.97
23	3	317	BCR	C30-C25-C26	-3.16	118.32	122.64
20	5	315	LUT	C39-C29-C30	-3.16	117.70	122.82
23	G	205	BCR	C34-C9-C10	-3.16	117.70	122.82
19	K	203	CLA	C4D-CHA-C1A	3.15	125.01	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	844	BCR	C37-C22-C23	3.15	122.91	118.09
23	G	205	BCR	C30-C25-C26	-3.15	118.33	122.64
19	2	312	CLA	C4A-NA-C1A	3.14	108.11	106.68
23	B	848	BCR	C7-C8-C9	3.14	130.88	126.23
19	3	309	CLA	C4D-CHA-C1A	3.14	124.99	121.24
23	F	302	BCR	C33-C5-C6	3.14	127.91	124.48
23	L	305	BCR	C37-C22-C21	-3.14	117.73	122.82
18	2	320	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
18	5	304	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
23	2	319	BCR	C15-C16-C17	3.14	129.94	123.52
23	B	844	BCR	C37-C22-C21	-3.14	117.73	122.82
23	I	101	BCR	C37-C22-C21	-3.14	117.73	122.82
23	5	317	BCR	C30-C25-C26	-3.13	118.35	122.64
23	F	302	BCR	C34-C9-C10	-3.13	117.74	122.82
20	J	101	LUT	C40-C33-C34	-3.13	117.74	122.82
23	A	848	BCR	C38-C26-C25	3.13	127.90	124.48
18	5	305	CHL	C4D-ND-C1D	3.13	107.59	105.22
23	F	302	BCR	C34-C9-C8	3.13	122.86	118.09
23	L	304	BCR	C34-C9-C10	-3.13	117.75	122.82
19	B	829	CLA	C4D-CHA-C1A	3.13	124.97	121.24
19	B	816	CLA	C4D-CHA-C1A	3.12	124.97	121.24
23	B	844	BCR	C24-C25-C26	3.12	128.74	121.56
20	3	315	LUT	C11-C10-C9	3.12	131.65	127.28
19	A	806	CLA	C4D-CHA-C1A	3.12	124.96	121.24
19	A	843	CLA	C4D-CHA-C1A	3.12	124.96	121.24
19	A	832	CLA	C4D-CHA-C1A	3.12	124.96	121.24
19	L	301	CLA	C4D-CHA-C1A	3.12	124.96	121.24
19	A	803	CLA	CHA-C1A-NA	-3.12	119.33	126.39
19	A	826	CLA	C4A-NA-C1A	3.11	108.10	106.68
20	2	317	LUT	C40-C33-C34	-3.11	117.77	122.82
20	2	315	LUT	C20-C13-C14	-3.11	117.77	122.82
19	A	822	CLA	C4D-CHA-C1A	3.11	124.95	121.24
19	3	308	CLA	C4D-CHA-C1A	3.11	124.95	121.24
19	5	314	CLA	C4D-CHA-C1A	3.11	124.95	121.24
20	6	315	LUT	C39-C29-C30	-3.10	117.79	122.82
19	5	312	CLA	C4D-CHA-C1A	3.10	124.94	121.24
19	6	307	CLA	C4A-NA-C1A	3.10	108.09	106.68
23	G	201	BCR	C37-C22-C21	-3.10	117.80	122.82
23	G	205	BCR	C29-C30-C25	3.09	114.93	110.44
23	L	305	BCR	C34-C9-C8	3.09	122.81	118.09
19	6	307	CLA	CHA-C1A-NA	-3.09	119.39	126.39
23	I	101	BCR	C34-C9-C10	-3.09	117.81	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	C4D-CHA-C1A	3.09	124.93	121.24
19	6	313	CLA	C4D-CHA-C1A	3.09	124.93	121.24
18	5	305	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
19	B	828	CLA	C4D-CHA-C1A	3.09	124.93	121.24
19	6	307	CLA	C4D-CHA-C1A	3.09	124.92	121.24
19	B	823	CLA	C4D-CHA-C1A	3.09	124.92	121.24
23	L	304	BCR	C37-C22-C21	-3.09	117.82	122.82
18	6	301	CHL	C4D-ND-C1D	3.08	107.56	105.22
18	6	306	CHL	C4D-ND-C1D	3.08	107.56	105.22
19	2	308	CLA	C4D-CHA-C1A	3.08	124.92	121.24
19	A	830	CLA	C4D-CHA-C1A	3.07	124.91	121.24
18	2	306	CHL	C4D-ND-C1D	3.07	107.55	105.22
23	B	847	BCR	C33-C5-C6	3.07	127.83	124.48
23	5	317	BCR	C10-C11-C12	3.07	132.09	123.20
23	A	851	BCR	C15-C16-C17	3.07	129.79	123.52
23	2	319	BCR	C35-C13-C14	-3.06	117.85	122.82
19	K	201	CLA	C4A-NA-C1A	3.06	108.08	106.68
19	3	311	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
19	2	303	CLA	C4D-CHA-C1A	3.06	124.89	121.24
19	B	807	CLA	C4D-CHA-C1A	3.06	124.89	121.24
23	L	304	BCR	C7-C8-C9	3.05	130.75	126.23
23	3	317	BCR	C37-C22-C21	-3.05	117.87	122.82
23	A	851	BCR	C37-C22-C21	-3.05	117.87	122.82
20	5	316	LUT	C39-C29-C30	-3.05	117.88	122.82
20	2	316	LUT	C15-C35-C34	3.05	129.76	123.52
20	6	315	LUT	C8-C9-C10	3.05	123.80	119.01
19	5	308	CLA	C4D-CHA-C1A	3.04	124.87	121.24
19	A	808	CLA	C4D-CHA-C1A	3.04	124.87	121.24
18	2	301	CHL	C4D-ND-C1D	3.03	107.52	105.22
23	2	319	BCR	C36-C18-C17	-3.03	117.91	122.82
23	B	846	BCR	C35-C13-C14	-3.02	117.92	122.82
23	2	319	BCR	C24-C25-C26	3.02	128.52	121.56
20	J	101	LUT	C30-C31-C32	3.02	131.96	123.20
23	G	205	BCR	C16-C15-C14	3.02	129.70	123.52
23	B	846	BCR	C33-C5-C6	3.02	127.78	124.48
19	A	836	CLA	C4D-CHA-C1A	3.02	124.84	121.24
23	M	101	BCR	C38-C26-C25	3.02	127.78	124.48
23	A	849	BCR	C33-C5-C6	3.02	127.77	124.48
18	2	305	CHL	C4D-ND-C1D	3.01	107.51	105.22
19	B	823	CLA	CHA-C1A-NA	-3.01	119.56	126.39
18	5	306	CHL	C1C-C2C-CMC	3.01	132.23	126.80
20	2	315	LUT	C39-C29-C30	-3.01	117.93	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	825	CLA	C4D-CHA-C1A	3.01	124.83	121.24
20	3	316	LUT	C20-C13-C14	-3.00	117.95	122.82
23	M	101	BCR	C16-C15-C14	3.00	129.66	123.52
23	A	849	BCR	C34-C9-C8	3.00	122.67	118.09
23	K	204	BCR	C24-C25-C26	3.00	128.46	121.56
19	A	838	CLA	CHA-C1A-NA	-3.00	119.61	126.39
23	K	205	BCR	C19-C18-C17	3.00	123.72	119.01
20	6	318	LUT	C8-C9-C10	2.99	123.72	119.01
20	3	315	LUT	C39-C29-C30	-2.99	117.97	122.82
19	5	314	CLA	CGD-CBD-CAD	2.99	120.52	110.85
20	5	316	LUT	C20-C13-C14	-2.99	117.97	122.82
19	B	810	CLA	CHA-C1A-NA	-2.99	119.63	126.39
20	2	317	LUT	C20-C13-C14	-2.98	117.98	122.82
23	A	852	BCR	C37-C22-C23	2.98	122.64	118.09
23	I	101	BCR	C33-C5-C6	2.98	127.73	124.48
20	3	315	LUT	C15-C35-C34	2.98	129.61	123.52
20	6	318	LUT	C10-C11-C12	2.98	131.83	123.20
20	2	316	LUT	C31-C30-C29	2.98	131.45	127.28
19	B	820	CLA	C4D-CHA-C1A	2.97	124.79	121.24
23	F	302	BCR	C7-C8-C9	2.97	130.63	126.23
18	2	314	CHL	C4D-ND-C1D	2.97	107.47	105.22
20	6	315	LUT	C35-C15-C14	2.97	129.60	123.52
23	B	847	BCR	C37-C22-C21	-2.97	118.01	122.82
19	K	201	CLA	CHA-C1A-NA	-2.97	119.67	126.39
23	A	848	BCR	C34-C9-C8	2.97	122.62	118.09
20	6	315	LUT	C39-C29-C28	2.97	122.62	118.09
23	B	845	BCR	C38-C26-C25	2.97	127.72	124.48
19	A	830	CLA	CHA-C1A-NA	-2.96	119.68	126.39
23	5	317	BCR	C29-C30-C25	2.96	114.73	110.44
23	J	103	BCR	C19-C18-C17	2.95	123.65	119.01
19	A	825	CLA	CHD-C1D-ND	-2.95	120.65	124.80
20	3	315	LUT	C7-C8-C9	2.95	130.60	126.23
19	L	301	CLA	CHA-C1A-NA	-2.95	119.72	126.39
23	A	849	BCR	C16-C15-C14	2.94	129.54	123.52
18	5	313	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
19	6	309	CLA	C4D-CHA-C1A	2.94	124.75	121.24
19	6	308	CLA	C4D-CHA-C1A	2.94	124.75	121.24
20	2	315	LUT	C8-C9-C10	2.93	123.62	119.01
20	3	316	LUT	C39-C29-C30	-2.93	118.07	122.82
18	2	301	CHL	C4C-CHD-C1D	2.93	126.55	116.07
19	B	828	CLA	CHA-C1A-NA	-2.92	119.77	126.39
20	5	316	LUT	C10-C11-C12	2.92	131.67	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	CHA-C1A-NA	-2.92	119.78	126.39
19	2	309	CLA	CHA-C1A-NA	-2.92	119.79	126.39
24	A	802	CL0	C1A-CHA-C4D	2.91	123.84	118.98
19	A	840	CLA	CHA-C1A-NA	-2.91	119.80	126.39
19	B	802	CLA	CHA-C1A-NA	-2.91	119.80	126.39
23	M	101	BCR	C37-C22-C21	-2.91	118.10	122.82
23	A	850	BCR	C38-C26-C25	2.91	127.66	124.48
23	B	847	BCR	C34-C9-C10	-2.91	118.11	122.82
23	B	845	BCR	C12-C13-C14	2.90	123.58	119.01
19	B	804	CLA	CHA-C1A-NA	-2.90	119.82	126.39
23	K	205	BCR	C36-C18-C17	-2.90	118.11	122.82
19	B	825	CLA	CHA-C1A-NA	-2.90	119.82	126.39
19	A	833	CLA	CHA-C1A-NA	-2.89	119.84	126.39
19	B	823	CLA	C4A-NA-C1A	2.89	108.00	106.68
19	A	817	CLA	C4A-NA-C1A	2.89	108.00	106.68
19	2	312	CLA	CHA-C1A-NA	-2.89	119.84	126.39
19	3	304	CLA	CHA-C1A-NA	-2.89	119.84	126.39
23	L	305	BCR	C15-C16-C17	2.89	129.43	123.52
20	2	316	LUT	C27-C28-C29	2.89	132.53	126.32
18	3	314	CHL	CHA-C1A-C2A	-2.89	126.53	133.31
20	2	316	LUT	C39-C29-C30	-2.88	118.14	122.82
20	6	318	LUT	C7-C6-C5	2.88	128.19	121.56
19	A	821	CLA	CHA-C1A-NA	-2.88	119.87	126.39
18	3	314	CHL	C4D-ND-C1D	2.88	107.40	105.22
19	A	815	CLA	CHA-C1A-NA	-2.88	119.87	126.39
19	B	833	CLA	CHA-C1A-NA	-2.87	119.88	126.39
19	A	806	CLA	CHD-C1D-ND	-2.87	120.76	124.80
19	B	803	CLA	CHA-C1A-NA	-2.87	119.88	126.39
23	J	103	BCR	C36-C18-C17	-2.87	118.16	122.82
19	3	307	CLA	CHD-C1D-ND	-2.87	120.76	124.80
19	6	308	CLA	CHA-C1A-NA	-2.87	119.89	126.39
23	A	852	BCR	C24-C25-C26	2.87	128.17	121.56
18	2	314	CHL	C4D-CHA-CBD	-2.87	106.07	108.97
23	B	848	BCR	C34-C9-C8	2.87	122.47	118.09
19	A	834	CLA	CHA-C1A-NA	-2.87	119.90	126.39
20	5	315	LUT	C32-C33-C34	2.87	123.52	119.01
19	B	840	CLA	CAA-CBA-CGA	2.87	121.35	113.21
23	B	845	BCR	C35-C13-C14	-2.87	118.17	122.82
19	F	301	CLA	CHA-C1A-NA	-2.86	119.91	126.39
23	B	844	BCR	C33-C5-C6	2.86	127.61	124.48
19	3	308	CLA	CHD-C1D-ND	-2.86	120.78	124.80
19	B	816	CLA	CHA-C1A-NA	-2.86	119.92	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	305	CHL	CHA-C1A-C2A	-2.86	126.59	133.31
19	G	203	CLA	C4D-CHA-C1A	2.86	124.65	121.24
18	5	306	CHL	C4D-ND-C1D	2.86	107.39	105.22
18	2	306	CHL	CHA-C1A-C2A	-2.86	126.60	133.31
18	2	305	CHL	CHA-C1A-C2A	-2.86	126.60	133.31
18	2	314	CHL	CHA-C1A-C2A	-2.85	126.61	133.31
19	B	818	CLA	CHA-C1A-NA	-2.85	119.93	126.39
19	B	832	CLA	CHA-C1A-NA	-2.85	119.94	126.39
19	B	826	CLA	C4D-CHA-C1A	2.85	124.64	121.24
19	3	310	CLA	CHA-C1A-NA	-2.85	119.94	126.39
19	A	801	CLA	CHA-C1A-NA	-2.85	119.94	126.39
19	A	817	CLA	CHA-C1A-NA	-2.85	119.94	126.39
19	B	801	CLA	CHA-C1A-NA	-2.84	119.95	126.39
19	3	302	CLA	CHA-C1A-NA	-2.84	119.95	126.39
23	I	101	BCR	C38-C26-C25	2.84	127.58	124.48
19	B	837	CLA	CHA-C1A-NA	-2.84	119.97	126.39
19	B	839	CLA	CHA-C1A-NA	-2.84	119.97	126.39
19	B	821	CLA	CHA-C1A-NA	-2.83	119.97	126.39
19	2	311	CLA	CHA-C1A-NA	-2.83	119.97	126.39
19	6	311	CLA	O2D-CGD-CBD	2.83	116.18	111.23
19	A	828	CLA	CHD-C1D-ND	-2.83	120.82	124.80
18	5	313	CHL	CHA-C1A-C2A	-2.83	126.67	133.31
19	A	804	CLA	CHA-C1A-NA	-2.83	119.99	126.39
19	2	303	CLA	CHD-C1D-ND	-2.83	120.83	124.80
23	5	317	BCR	C15-C16-C17	2.82	129.30	123.52
19	B	838	CLA	CHD-C1D-ND	-2.82	120.83	124.80
19	B	836	CLA	CHA-C1A-NA	-2.82	120.00	126.39
19	A	820	CLA	CHD-C1D-ND	-2.82	120.83	124.80
19	A	829	CLA	CHA-C1A-NA	-2.82	120.00	126.39
20	6	318	LUT	C20-C13-C14	-2.82	118.25	122.82
19	B	813	CLA	CHA-C1A-NA	-2.82	120.01	126.39
18	5	313	CHL	C4D-ND-C1D	2.82	107.36	105.22
19	B	824	CLA	CHA-C1A-NA	-2.82	120.01	126.39
19	2	313	CLA	CHA-C1A-NA	-2.82	120.02	126.39
19	J	102	CLA	CHA-C1A-NA	-2.81	120.02	126.39
18	6	301	CHL	C4C-CHD-C1D	2.81	126.13	116.07
23	L	305	BCR	C35-C13-C14	-2.81	118.26	122.82
23	G	201	BCR	C7-C6-C5	2.81	128.03	121.56
19	A	818	CLA	O2A-C1-C2	2.81	118.92	108.11
19	B	809	CLA	C4D-CHA-C1A	2.81	124.59	121.24
19	A	814	CLA	CHA-C1A-NA	-2.81	120.03	126.39
19	L	303	CLA	CHA-C1A-NA	-2.81	120.03	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	807	CLA	CHA-C1A-NA	-2.81	120.03	126.39
23	B	845	BCR	C36-C18-C17	-2.81	118.27	122.82
23	J	103	BCR	C2-C1-C6	2.81	114.52	110.44
23	J	103	BCR	C12-C13-C14	2.80	123.42	119.01
18	5	304	CHL	C4C-CHD-C1D	2.80	126.10	116.07
19	A	843	CLA	CHA-C1A-NA	-2.80	120.05	126.39
23	A	848	BCR	C36-C18-C17	-2.80	118.28	122.82
19	3	312	CLA	CHA-C1A-NA	-2.80	120.06	126.39
20	2	316	LUT	C18-C5-C6	2.80	127.54	124.48
19	B	805	CLA	C4D-CHA-C1A	2.80	124.58	121.24
23	3	317	BCR	C15-C16-C17	2.79	129.24	123.52
19	B	814	CLA	CHA-C1A-NA	-2.79	120.06	126.39
19	B	819	CLA	CHD-C1D-ND	-2.79	120.87	124.80
19	A	819	CLA	CHA-C1A-NA	-2.79	120.07	126.39
19	A	824	CLA	CHA-C1A-NA	-2.79	120.08	126.39
19	5	314	CLA	CHA-C1A-NA	-2.79	120.08	126.39
18	2	306	CHL	C4C-CHD-C1D	2.78	126.03	116.07
23	K	205	BCR	C35-C13-C14	-2.78	118.31	122.82
19	A	824	CLA	CHD-C1D-ND	-2.78	120.89	124.80
19	3	309	CLA	CHA-C1A-NA	-2.78	120.09	126.39
18	3	306	CHL	C1C-C2C-CMC	2.78	131.81	126.80
20	2	315	LUT	C10-C11-C12	2.78	131.25	123.20
19	B	815	CLA	CHA-C1A-NA	-2.78	120.10	126.39
23	A	848	BCR	C19-C18-C17	2.78	123.38	119.01
18	5	305	CHL	C4C-CHD-C1D	2.78	126.01	116.07
20	3	316	LUT	C31-C30-C29	2.78	131.17	127.28
23	J	103	BCR	C24-C25-C26	2.78	127.95	121.56
20	6	318	LUT	C12-C13-C14	2.78	123.37	119.01
19	A	832	CLA	CHA-C1A-NA	-2.77	120.11	126.39
19	A	840	CLA	C4A-NA-C1A	2.77	107.94	106.68
19	B	812	CLA	CHA-C1A-NA	-2.77	120.12	126.39
19	6	310	CLA	CHA-C1A-NA	-2.77	120.12	126.39
23	J	103	BCR	C35-C13-C14	-2.77	118.33	122.82
19	A	809	CLA	CHA-C1A-NA	-2.77	120.12	126.39
23	F	302	BCR	C37-C22-C23	2.77	122.32	118.09
23	B	848	BCR	C24-C25-C26	2.77	127.93	121.56
23	J	103	BCR	C21-C20-C19	2.77	131.22	123.20
19	3	305	CLA	CHA-C1A-NA	-2.77	120.13	126.39
19	B	827	CLA	C4D-CHA-C1A	2.77	124.54	121.24
19	B	820	CLA	CHA-C1A-NA	-2.76	120.13	126.39
19	B	806	CLA	CHA-C1A-NA	-2.76	120.14	126.39
19	6	312	CLA	CHD-C1D-ND	-2.76	120.92	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	837	CLA	CHD-C1D-ND	-2.76	120.92	124.80
19	5	303	CLA	CHA-C1A-NA	-2.76	120.14	126.39
19	3	303	CLA	CHA-C1A-NA	-2.76	120.14	126.39
19	B	822	CLA	CHA-C1A-NA	-2.76	120.14	126.39
19	5	309	CLA	CHA-C1A-NA	-2.76	120.15	126.39
19	A	807	CLA	CHD-C1D-ND	-2.76	120.92	124.80
19	B	830	CLA	C4D-CHA-C1A	2.76	124.53	121.24
19	6	311	CLA	CHA-C1A-NA	-2.76	120.15	126.39
19	B	817	CLA	CHA-C1A-NA	-2.75	120.15	126.39
19	F	303	CLA	CHA-C1A-NA	-2.75	120.16	126.39
18	3	314	CHL	C4C-CHD-C1D	2.75	125.91	116.07
19	A	842	CLA	CHA-C1A-NA	-2.75	120.16	126.39
19	B	805	CLA	CHA-C1A-NA	-2.75	120.16	126.39
19	A	825	CLA	CHA-C1A-NA	-2.75	120.16	126.39
23	B	845	BCR	C19-C18-C17	2.75	123.33	119.01
18	2	305	CHL	C4C-CHD-C1D	2.75	125.91	116.07
19	A	823	CLA	CHA-C1A-NA	-2.75	120.17	126.39
19	6	302	CLA	CHA-C1A-NA	-2.75	120.17	126.39
23	A	852	BCR	C19-C18-C17	2.75	123.33	119.01
19	6	305	CLA	CHA-C1A-NA	-2.75	120.17	126.39
19	5	301	CLA	CHA-C1A-NA	-2.75	120.17	126.39
23	A	850	BCR	C19-C18-C17	2.75	123.33	119.01
23	L	304	BCR	C16-C15-C14	2.74	129.13	123.52
19	A	836	CLA	CHA-C1A-NA	-2.74	120.18	126.39
19	B	840	CLA	CHD-C1D-ND	-2.74	120.94	124.80
18	2	314	CHL	C4C-CHD-C1D	2.74	125.89	116.07
20	5	315	LUT	C40-C33-C34	-2.74	118.37	122.82
19	5	307	CLA	CHA-C1A-NA	-2.74	120.18	126.39
19	2	310	CLA	CHA-C1A-NA	-2.74	120.18	126.39
19	5	311	CLA	CHD-C1D-ND	-2.74	120.94	124.80
19	2	309	CLA	C4D-CHA-C1A	2.74	124.51	121.24
18	5	313	CHL	C4C-CHD-C1D	2.74	125.86	116.07
18	5	304	CHL	CHA-C1A-C2A	-2.74	126.88	133.31
19	A	813	CLA	CHA-C1A-NA	-2.74	120.20	126.39
23	5	317	BCR	C7-C6-C5	2.73	127.85	121.56
19	A	831	CLA	CHA-C1A-NA	-2.73	120.20	126.39
19	G	204	CLA	CHA-C1A-NA	-2.73	120.21	126.39
19	B	804	CLA	C4D-CHA-C1A	2.73	124.50	121.24
23	G	201	BCR	C24-C25-C26	2.72	127.83	121.56
19	2	302	CLA	CHA-C1A-NA	-2.72	120.22	126.39
20	2	317	LUT	C8-C9-C10	2.72	123.29	119.01
18	2	320	CHL	CHA-C1A-C2A	-2.72	126.91	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	837	CLA	CHA-C1A-NA	-2.72	120.23	126.39
19	2	304	CLA	CHA-C1A-NA	-2.72	120.23	126.39
19	A	816	CLA	CHA-C1A-NA	-2.72	120.23	126.39
19	A	812	CLA	C4D-CHA-C1A	2.72	124.49	121.24
19	A	811	CLA	CHA-C1A-NA	-2.72	120.24	126.39
19	B	831	CLA	CHA-C1A-NA	-2.72	120.24	126.39
19	B	830	CLA	CHA-C1A-NA	-2.71	120.24	126.39
23	K	205	BCR	C12-C13-C14	2.71	123.28	119.01
19	5	302	CLA	CHA-C1A-NA	-2.71	120.24	126.39
27	A	853	LMU	O1B-C4'-C3'	2.71	114.13	107.23
19	G	203	CLA	CHA-C1A-NA	-2.71	120.25	126.39
19	2	313	CLA	CHD-C1D-ND	-2.71	120.98	124.80
19	A	818	CLA	CHA-C1A-NA	-2.71	120.26	126.39
23	B	845	BCR	C34-C9-C8	2.71	122.22	118.09
19	3	301	CLA	CHA-C1A-NA	-2.70	120.27	126.39
19	A	827	CLA	CHD-C1D-ND	-2.70	121.00	124.80
18	3	306	CHL	C4C-CHD-C1D	2.70	125.74	116.07
19	6	304	CLA	CHA-C1A-NA	-2.70	120.27	126.39
19	A	828	CLA	CHA-C1A-NA	-2.70	120.27	126.39
19	6	309	CLA	CHA-C1A-NA	-2.70	120.28	126.39
23	A	851	BCR	C34-C9-C8	2.70	122.21	118.09
19	A	822	CLA	CHA-C1A-NA	-2.70	120.28	126.39
19	6	304	CLA	CHD-C1D-ND	-2.70	121.01	124.80
19	3	313	CLA	CHA-C1A-NA	-2.69	120.29	126.39
19	A	808	CLA	CHA-C1A-NA	-2.69	120.30	126.39
19	K	203	CLA	CHA-C1A-NA	-2.69	120.30	126.39
19	2	308	CLA	CHA-C1A-NA	-2.69	120.30	126.39
23	F	305	BCR	C33-C5-C6	2.69	127.42	124.48
23	G	205	BCR	C36-C18-C17	-2.69	118.46	122.82
23	A	849	BCR	C24-C25-C26	2.69	127.74	121.56
19	B	835	CLA	CHA-C1A-NA	-2.68	120.31	126.39
23	A	851	BCR	C16-C15-C14	2.68	129.01	123.52
18	6	306	CHL	C4C-CHD-C1D	2.68	125.67	116.07
23	L	305	BCR	C12-C13-C14	2.68	123.23	119.01
19	5	310	CLA	CHA-C1A-NA	-2.68	120.32	126.39
19	F	304	CLA	CHA-C1A-NA	-2.68	120.32	126.39
18	6	306	CHL	CHA-C1A-C2A	-2.68	127.02	133.31
19	A	817	CLA	CHD-C1D-ND	-2.68	121.03	124.80
19	6	314	CLA	CHA-C1A-NA	-2.68	120.33	126.39
19	K	202	CLA	CHA-C1A-NA	-2.68	120.33	126.39
20	3	315	LUT	C7-C6-C5	-2.68	115.39	121.56
19	A	804	CLA	CHD-C1D-ND	-2.68	121.04	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	844	BCR	C35-C13-C14	-2.68	118.48	122.82
19	B	830	CLA	CHD-C1D-ND	-2.67	121.04	124.80
18	5	306	CHL	CHA-C1A-C2A	-2.67	127.03	133.31
19	B	818	CLA	C1-O2A-CGA	2.67	123.12	116.65
19	3	311	CLA	CHA-C1A-NA	-2.67	120.34	126.39
19	A	841	CLA	CHA-C1A-NA	-2.67	120.35	126.39
20	5	315	LUT	C39-C29-C28	2.67	122.16	118.09
18	6	301	CHL	CHA-C1A-C2A	-2.67	127.04	133.31
19	3	308	CLA	CHA-C1A-NA	-2.67	120.36	126.39
23	3	317	BCR	C35-C13-C14	-2.66	118.50	122.82
19	6	313	CLA	CHA-C1A-NA	-2.66	120.36	126.39
19	A	839	CLA	CHA-C1A-NA	-2.66	120.36	126.39
23	I	101	BCR	C24-C23-C22	2.66	130.18	126.23
18	2	307	CHL	C4C-CHD-C1D	2.66	125.60	116.07
19	B	829	CLA	CHA-C1A-NA	-2.66	120.36	126.39
19	5	308	CLA	CHA-C1A-NA	-2.66	120.37	126.39
23	A	850	BCR	C36-C18-C17	-2.66	118.51	122.82
23	A	850	BCR	C33-C5-C6	2.66	127.38	124.48
19	L	301	CLA	C4A-NA-C1A	2.66	107.89	106.68
23	L	305	BCR	C36-C18-C17	-2.66	118.51	122.82
18	5	306	CHL	C4C-CHD-C1D	2.65	125.57	116.07
19	A	819	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	B	819	CLA	CHA-C1A-NA	-2.65	120.39	126.39
19	3	311	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	K	203	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	A	812	CLA	CHA-C1A-NA	-2.65	120.40	126.39
23	M	101	BCR	C35-C13-C14	-2.65	118.53	122.82
19	B	811	CLA	CHA-C1A-NA	-2.64	120.40	126.39
23	B	847	BCR	C35-C13-C14	-2.64	118.53	122.82
18	3	306	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
19	3	307	CLA	CHA-C1A-NA	-2.64	120.41	126.39
19	L	302	CLA	CHA-C1A-NA	-2.64	120.41	126.39
19	B	841	CLA	CHA-C1A-NA	-2.64	120.41	126.39
19	B	839	CLA	CHD-C1D-ND	-2.64	121.08	124.80
19	B	808	CLA	CHA-C1A-NA	-2.64	120.41	126.39
19	2	309	CLA	O2A-C1-C2	2.64	118.27	108.11
19	B	842	CLA	CHA-C1A-NA	-2.64	120.41	126.39
19	3	310	CLA	C4A-NA-C1A	2.64	107.88	106.68
20	J	101	LUT	C35-C15-C14	2.64	128.91	123.52
19	A	835	CLA	CHD-C1D-ND	-2.64	121.09	124.80
23	K	204	BCR	C35-C13-C14	-2.63	118.56	122.82
23	A	849	BCR	C36-C18-C17	-2.63	118.56	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	L	304	BCR	C36-C18-C17	-2.63	118.56	122.82
20	J	101	LUT	C7-C6-C5	-2.63	115.50	121.56
19	B	842	CLA	CHD-C1D-ND	-2.63	121.11	124.80
19	A	810	CLA	CHA-C1A-NA	-2.63	120.45	126.39
18	3	314	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
20	J	101	LUT	C12-C13-C14	2.62	123.14	119.01
23	B	847	BCR	C12-C13-C14	2.62	123.13	119.01
19	2	302	CLA	CHD-C1D-ND	-2.62	121.11	124.80
19	F	301	CLA	C4A-NA-C1A	2.62	107.88	106.68
20	6	318	LUT	C39-C29-C30	-2.62	118.57	122.82
19	5	308	CLA	CHD-C1D-ND	-2.62	121.12	124.80
19	B	834	CLA	CHA-C1A-NA	-2.62	120.47	126.39
23	L	305	BCR	C29-C30-C25	2.61	114.23	110.44
20	5	316	LUT	C31-C30-C29	2.61	130.94	127.28
19	6	303	CLA	CHD-C1D-ND	-2.61	121.13	124.80
19	A	810	CLA	CHD-C1D-ND	-2.61	121.13	124.80
19	6	312	CLA	CHA-C1A-NA	-2.61	120.49	126.39
19	B	820	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	B	826	CLA	CHD-C1D-ND	-2.60	121.14	124.80
19	J	102	CLA	C4A-NA-C1A	2.60	107.87	106.68
19	B	802	CLA	C4D-CHA-C1A	2.60	124.35	121.24
19	B	838	CLA	CHA-C1A-NA	-2.60	120.50	126.39
19	5	312	CLA	CHA-C1A-NA	-2.60	120.50	126.39
19	B	817	CLA	CHD-C1D-ND	-2.60	121.14	124.80
19	A	805	CLA	CHA-C1A-NA	-2.60	120.51	126.39
19	B	825	CLA	CHD-C1D-ND	-2.60	121.15	124.80
20	6	315	LUT	C20-C13-C14	-2.60	118.61	122.82
19	5	311	CLA	CAA-C2A-C3A	-2.59	105.99	113.00
23	K	204	BCR	C36-C18-C17	-2.59	118.61	122.82
18	2	301	CHL	CHA-C1A-C2A	-2.59	127.22	133.31
18	2	320	CHL	C4C-CHD-C1D	2.59	125.35	116.07
19	A	835	CLA	CHA-C1A-NA	-2.59	120.52	126.39
23	F	302	BCR	C24-C25-C26	2.59	127.52	121.56
23	F	305	BCR	C36-C18-C17	-2.59	118.62	122.82
23	M	101	BCR	C7-C6-C5	2.59	127.51	121.56
23	F	302	BCR	C36-C18-C17	-2.58	118.63	122.82
19	6	303	CLA	CHA-C1A-NA	-2.58	120.54	126.39
19	A	818	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	A	826	CLA	C4D-CHA-C1A	2.58	124.32	121.24
19	A	805	CLA	CHD-C1D-ND	-2.58	121.17	124.80
23	A	851	BCR	C36-C18-C17	-2.58	118.64	122.82
19	B	841	CLA	CHD-C1D-ND	-2.58	121.18	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	205	BCR	C35-C13-C14	-2.58	118.64	122.82
23	A	848	BCR	C35-C13-C14	-2.58	118.64	122.82
19	A	831	CLA	C4D-CHA-C1A	2.57	124.31	121.24
19	5	314	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	5	311	CLA	CHA-C1A-NA	-2.57	120.58	126.39
19	A	807	CLA	CHA-C1A-NA	-2.57	120.58	126.39
19	A	829	CLA	CHD-C1D-ND	-2.56	121.19	124.80
23	A	851	BCR	C35-C13-C14	-2.56	118.66	122.82
19	2	303	CLA	CHA-C1A-NA	-2.56	120.59	126.39
19	B	826	CLA	CHA-C1A-NA	-2.56	120.59	126.39
19	3	305	CLA	CHD-C1D-ND	-2.56	121.20	124.80
19	2	308	CLA	CHD-C1D-ND	-2.56	121.20	124.80
20	3	316	LUT	C8-C9-C10	2.56	123.03	119.01
23	G	205	BCR	C19-C18-C17	2.56	123.03	119.01
19	B	833	CLA	C4A-NA-C1A	2.56	107.84	106.68
19	6	309	CLA	CHD-C1D-ND	-2.56	121.21	124.80
19	B	836	CLA	CHD-C1D-ND	-2.55	121.21	124.80
20	5	316	LUT	C1-C6-C5	-2.55	119.15	122.64
19	A	806	CLA	CHA-C1A-NA	-2.55	120.61	126.39
23	K	205	BCR	C30-C25-C26	-2.55	119.15	122.64
20	J	101	LUT	C20-C13-C14	-2.55	118.68	122.82
24	A	802	CL0	CHA-C1A-C2A	-2.55	127.32	133.31
19	2	311	CLA	C4A-NA-C1A	2.55	107.84	106.68
19	B	808	CLA	CHD-C1D-ND	-2.55	121.22	124.80
23	L	304	BCR	C7-C6-C5	2.55	127.42	121.56
23	L	305	BCR	C24-C23-C22	2.55	130.00	126.23
23	A	850	BCR	C34-C9-C8	2.54	121.97	118.09
19	B	812	CLA	CHD-C1D-ND	-2.54	121.22	124.80
23	I	101	BCR	C36-C18-C17	-2.54	118.70	122.82
19	3	303	CLA	CHD-C1D-ND	-2.54	121.23	124.80
20	2	315	LUT	C31-C30-C29	2.54	130.84	127.28
19	A	820	CLA	CHA-C1A-NA	-2.54	120.65	126.39
19	A	819	CLA	CAC-C3C-C4C	2.54	128.09	124.79
19	K	201	CLA	CHD-C1D-ND	-2.53	121.23	124.80
19	B	840	CLA	CHA-C1A-NA	-2.53	120.65	126.39
19	A	823	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	B	801	CLA	C4A-NA-C1A	2.53	107.83	106.68
19	B	821	CLA	C4A-NA-C1A	2.53	107.83	106.68
19	6	314	CLA	O2D-CGD-CBD	2.53	115.66	111.23
23	L	304	BCR	C35-C13-C14	-2.53	118.72	122.82
20	3	315	LUT	C19-C9-C10	-2.53	118.72	122.82
19	3	301	CLA	CHD-C1D-ND	-2.53	121.24	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	301	CLA	CHD-C1D-ND	-2.53	121.24	124.80
20	5	315	LUT	C20-C13-C14	-2.53	118.72	122.82
23	2	319	BCR	C19-C18-C17	2.52	122.98	119.01
23	3	317	BCR	C12-C13-C14	2.52	122.98	119.01
19	5	303	CLA	CHD-C1D-ND	-2.52	121.25	124.80
20	3	316	LUT	C1-C6-C5	-2.52	119.19	122.64
20	3	316	LUT	C7-C6-C5	-2.52	115.75	121.56
18	6	306	CHL	C1C-C2C-CMC	2.52	131.34	126.80
23	A	849	BCR	C35-C13-C14	-2.51	118.74	122.82
23	A	848	BCR	C24-C25-C26	2.51	127.34	121.56
23	B	844	BCR	C1-C6-C5	-2.51	119.20	122.64
23	A	852	BCR	C35-C13-C14	-2.51	118.75	122.82
18	2	307	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
19	B	818	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	B	835	CLA	CHD-C1D-ND	-2.51	121.27	124.80
20	J	101	LUT	C1-C6-C5	-2.51	119.21	122.64
19	3	313	CLA	CHD-C1D-ND	-2.51	121.27	124.80
19	3	304	CLA	C4A-NA-C1A	2.51	107.82	106.68
23	K	204	BCR	C7-C6-C5	2.51	127.33	121.56
23	3	317	BCR	C29-C30-C25	2.51	114.08	110.44
19	L	302	CLA	CHD-C1D-ND	-2.51	121.28	124.80
23	B	848	BCR	C36-C18-C17	-2.51	118.76	122.82
20	3	316	LUT	C27-C28-C29	2.51	131.71	126.32
21	6	316	XAT	C11-C10-C9	2.50	130.78	127.28
23	L	304	BCR	C19-C18-C17	2.50	122.94	119.01
23	G	201	BCR	C35-C13-C14	-2.50	118.77	122.82
23	M	101	BCR	C36-C18-C17	-2.50	118.77	122.82
19	A	821	CLA	C4A-NA-C1A	2.50	107.82	106.68
19	B	834	CLA	CHD-C1D-ND	-2.50	121.29	124.80
23	G	201	BCR	C36-C18-C17	-2.49	118.78	122.82
23	F	305	BCR	C37-C22-C23	2.49	121.89	118.09
23	B	846	BCR	C29-C30-C25	2.49	114.06	110.44
23	B	845	BCR	C7-C6-C5	2.49	127.29	121.56
23	B	846	BCR	C8-C9-C10	2.49	122.93	119.01
23	A	849	BCR	C7-C8-C9	2.48	129.91	126.23
19	F	303	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	B	840	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
19	2	313	CLA	C4A-NA-C1A	2.48	107.81	106.68
19	A	838	CLA	C4A-NA-C1A	2.48	107.81	106.68
19	L	303	CLA	C4A-NA-C1A	2.48	107.81	106.68
20	2	317	LUT	C27-C28-C29	2.48	131.65	126.32
23	K	204	BCR	C29-C30-C25	2.47	114.03	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	312	CLA	CHD-C1D-ND	-2.47	121.32	124.80
23	M	101	BCR	C12-C13-C14	2.47	122.90	119.01
19	A	827	CLA	CHA-C1A-NA	-2.47	120.79	126.39
23	A	849	BCR	C19-C18-C17	2.47	122.90	119.01
19	B	809	CLA	CHA-C1A-NA	-2.47	120.79	126.39
19	B	824	CLA	C4D-CHA-C1A	2.47	124.19	121.24
19	A	839	CLA	CHD-C1D-ND	-2.47	121.33	124.80
19	2	304	CLA	CHD-C1D-ND	-2.47	121.33	124.80
20	6	318	LUT	C15-C35-C34	2.47	128.56	123.52
21	6	316	XAT	C8-C9-C10	-2.47	115.13	119.01
19	B	825	CLA	C4A-NA-C1A	2.47	107.80	106.68
19	A	822	CLA	CHD-C1D-ND	-2.46	121.33	124.80
23	L	305	BCR	C19-C18-C17	2.46	122.88	119.01
20	2	316	LUT	C35-C15-C14	2.46	128.55	123.52
19	L	303	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	G	204	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	A	826	CLA	C1D-ND-C4D	2.46	108.04	106.31
19	A	840	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	A	803	CLA	C2A-C1A-CHA	2.45	128.12	123.87
23	B	844	BCR	C12-C13-C14	2.45	122.86	119.01
19	A	816	CLA	CHD-C1D-ND	-2.45	121.35	124.80
18	2	314	CHL	C1C-C2C-CMC	2.45	131.21	126.80
23	5	317	BCR	C37-C22-C23	2.45	121.83	118.09
19	A	825	CLA	CHD-C1D-C2D	2.45	130.58	125.49
19	6	313	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	A	809	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	B	820	CLA	CHD-C1D-ND	-2.44	121.36	124.80
19	A	828	CLA	C1D-ND-C4D	2.44	108.03	106.31
19	A	803	CLA	C4A-NA-C1A	2.44	107.79	106.68
23	F	305	BCR	C15-C16-C17	2.44	128.51	123.52
23	B	848	BCR	C37-C22-C23	2.44	121.82	118.09
19	B	822	CLA	CHD-C1D-ND	-2.44	121.37	124.80
23	K	204	BCR	C12-C13-C14	2.44	122.85	119.01
23	5	317	BCR	C36-C18-C17	-2.44	118.86	122.82
19	B	804	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	B	806	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	A	815	CLA	C4A-NA-C1A	2.44	107.79	106.68
19	6	302	CLA	CHD-C1D-ND	-2.43	121.38	124.80
23	A	850	BCR	C35-C13-C14	-2.43	118.88	122.82
18	2	301	CHL	C1C-C2C-CMC	2.43	131.18	126.80
20	3	315	LUT	C35-C15-C14	2.43	128.49	123.52
23	K	204	BCR	C34-C9-C8	2.43	121.80	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	319	BCR	C23-C24-C25	2.43	133.49	127.00
19	6	314	CLA	CHD-C1D-ND	-2.43	121.38	124.80
23	F	302	BCR	C29-C30-C25	2.43	113.97	110.44
20	3	315	LUT	C1-C6-C5	-2.43	119.32	122.64
19	A	812	CLA	CHD-C1D-ND	-2.43	121.39	124.80
19	5	312	CLA	CHD-C1D-ND	-2.42	121.39	124.80
19	B	811	CLA	CHD-C1D-ND	-2.42	121.39	124.80
23	B	845	BCR	C10-C11-C12	2.42	130.22	123.20
19	A	828	CLA	C4A-NA-C1A	2.42	107.78	106.68
19	B	813	CLA	C4A-NA-C1A	2.42	107.78	106.68
19	3	304	CLA	CHD-C1D-ND	-2.42	121.40	124.80
18	5	305	CHL	C1C-C2C-CMC	2.42	131.16	126.80
23	A	848	BCR	C16-C15-C14	2.42	128.46	123.52
23	F	305	BCR	C35-C13-C14	-2.42	118.90	122.82
23	3	317	BCR	C24-C25-C26	-2.41	115.99	121.56
19	J	102	CLA	CHD-C1D-ND	-2.41	121.41	124.80
23	A	849	BCR	C12-C13-C14	2.41	122.80	119.01
23	K	204	BCR	C15-C16-C17	2.41	128.45	123.52
19	B	824	CLA	C2A-C1A-CHA	2.41	128.05	123.87
23	3	317	BCR	C36-C18-C17	-2.41	118.91	122.82
23	A	851	BCR	C24-C25-C26	-2.41	116.01	121.56
23	L	305	BCR	C24-C25-C26	2.41	127.10	121.56
19	A	838	CLA	CAA-C2A-C1A	2.41	119.86	111.97
19	A	815	CLA	CHD-C1D-ND	-2.40	121.42	124.80
23	F	302	BCR	C19-C18-C17	2.40	122.79	119.01
23	A	851	BCR	C19-C18-C17	2.40	122.78	119.01
19	A	811	CLA	CHD-C1D-ND	-2.40	121.43	124.80
18	5	313	CHL	C1C-C2C-CMC	2.39	131.12	126.80
19	L	301	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	B	833	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	F	304	CLA	CHD-C1D-ND	-2.39	121.44	124.80
20	6	315	LUT	C40-C33-C34	-2.39	118.95	122.82
19	A	841	CLA	CHD-C1D-ND	-2.39	121.44	124.80
19	5	307	CLA	CHD-C1D-ND	-2.39	121.45	124.80
19	B	821	CLA	CHD-C1D-ND	-2.38	121.45	124.80
23	2	319	BCR	C8-C9-C10	2.38	122.75	119.01
19	A	808	CLA	CHD-C1D-ND	-2.38	121.46	124.80
19	B	832	CLA	CHD-C1D-ND	-2.38	121.46	124.80
19	B	827	CLA	C4A-NA-C1A	2.37	107.76	106.68
19	2	309	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	A	844	PQN	C11-C3-C4	-2.37	116.08	118.58
20	5	316	LUT	C7-C6-C5	-2.37	116.09	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	301	CHL	C1C-C2C-CMC	2.37	131.07	126.80
19	B	804	CLA	C2A-C1A-CHA	2.37	127.98	123.87
23	A	850	BCR	C29-C30-C25	2.37	113.88	110.44
18	2	307	CHL	C1C-C2C-CMC	2.37	131.07	126.80
19	6	313	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
19	2	310	CLA	CHD-C1D-ND	-2.36	121.48	124.80
20	6	318	LUT	C8-C7-C6	2.36	133.30	127.00
19	A	826	CLA	C2A-C1A-CHA	2.36	127.96	123.87
20	6	315	LUT	C12-C13-C14	2.36	122.71	119.01
23	A	852	BCR	C7-C6-C5	2.35	126.98	121.56
23	I	101	BCR	C19-C18-C17	2.35	122.71	119.01
19	3	307	CLA	CHD-C1D-C2D	2.35	130.38	125.49
19	B	810	CLA	C4A-NA-C1A	2.35	107.75	106.68
23	2	319	BCR	C10-C11-C12	2.35	130.00	123.20
19	A	843	CLA	C4A-NA-C1A	2.35	107.75	106.68
19	6	307	CLA	C1D-ND-C4D	2.34	107.96	106.31
19	B	805	CLA	CHD-C1D-ND	-2.34	121.50	124.80
23	B	844	BCR	C15-C16-C17	2.34	128.31	123.52
19	A	836	CLA	CHD-C1D-ND	-2.34	121.51	124.80
20	3	316	LUT	C10-C11-C12	2.34	129.98	123.20
23	A	851	BCR	C12-C13-C14	2.34	122.69	119.01
20	2	316	LUT	C20-C13-C14	-2.34	119.03	122.82
23	K	204	BCR	C19-C18-C17	2.33	122.68	119.01
23	B	848	BCR	C33-C5-C6	2.33	127.03	124.48
23	B	846	BCR	C7-C6-C5	2.33	126.92	121.56
19	3	308	CLA	CHD-C1D-C2D	2.33	130.34	125.49
23	5	317	BCR	C24-C25-C26	-2.33	116.19	121.56
19	B	813	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	6	311	CLA	CHD-C1D-ND	-2.33	121.53	124.80
20	3	315	LUT	C40-C33-C34	-2.32	119.05	122.82
23	3	317	BCR	C7-C6-C5	-2.32	116.20	121.56
19	3	302	CLA	C4D-CHA-C1A	2.32	124.01	121.24
19	A	824	CLA	CHD-C1D-C2D	2.32	130.31	125.49
19	B	829	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	B	824	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	A	833	CLA	CHD-C1D-ND	-2.31	121.55	124.80
23	I	101	BCR	C35-C13-C14	-2.31	119.07	122.82
23	A	852	BCR	C34-C9-C8	2.31	121.62	118.09
19	5	310	CLA	CHD-C1D-ND	-2.31	121.56	124.80
23	A	852	BCR	C36-C18-C17	-2.31	119.08	122.82
27	A	853	LMU	O1B-C4'-C5'	-2.31	103.43	109.48
19	B	840	CLA	CHD-C1D-C2D	2.30	130.28	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	820	CLA	CHD-C1D-C2D	2.30	130.28	125.49
19	A	843	CLA	CHD-C1D-ND	-2.30	121.56	124.80
23	F	305	BCR	C19-C18-C17	2.30	122.63	119.01
23	M	101	BCR	C24-C25-C26	2.30	126.85	121.56
23	2	319	BCR	C29-C30-C25	2.30	113.78	110.44
19	B	815	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	A	807	CLA	CHD-C1D-C2D	2.30	130.26	125.49
23	B	847	BCR	C29-C30-C25	2.30	113.77	110.44
23	A	848	BCR	C12-C13-C14	2.29	122.61	119.01
19	B	810	CLA	C1D-ND-C4D	2.29	107.92	106.31
19	2	309	CLA	C1D-ND-C4D	2.29	107.92	106.31
19	B	830	CLA	CHD-C1D-C2D	2.29	130.25	125.49
19	2	312	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	K	202	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	B	807	CLA	C3B-C4B-NB	-2.29	108.49	110.53
20	3	315	LUT	C31-C30-C29	2.29	130.49	127.28
23	L	304	BCR	C12-C13-C14	2.28	122.60	119.01
23	F	302	BCR	C11-C10-C9	2.28	130.47	127.28
19	F	301	CLA	C3B-C4B-NB	-2.28	108.50	110.53
19	3	309	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	A	817	CLA	CHD-C1D-C2D	2.27	130.22	125.49
23	3	317	BCR	C34-C9-C8	2.27	121.56	118.09
23	K	204	BCR	C23-C24-C25	2.27	133.07	127.00
20	6	315	LUT	C32-C33-C34	2.27	122.58	119.01
19	6	305	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	A	828	CLA	CHD-C1D-C2D	2.27	130.21	125.49
19	B	831	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	G	203	CLA	CHD-C1D-ND	-2.27	121.61	124.80
23	2	319	BCR	C7-C6-C5	2.26	126.77	121.56
23	M	101	BCR	C19-C18-C17	2.26	122.57	119.01
19	6	310	CLA	CHD-C1D-ND	-2.26	121.62	124.80
23	B	844	BCR	C36-C18-C17	-2.26	119.15	122.82
19	A	823	CLA	C4A-NA-C1A	2.26	107.71	106.68
23	B	845	BCR	C24-C25-C26	2.26	126.76	121.56
23	G	205	BCR	C24-C25-C26	-2.26	116.35	121.56
20	6	318	LUT	C40-C33-C34	-2.26	119.16	122.82
19	5	309	CLA	CHD-C1D-ND	-2.26	121.63	124.80
23	F	305	BCR	C24-C25-C26	2.25	126.75	121.56
23	K	205	BCR	C23-C22-C21	2.25	122.56	119.01
19	B	803	CLA	C2A-C1A-CHA	2.25	127.77	123.87
20	2	316	LUT	C19-C9-C8	2.25	121.52	118.09
19	3	309	CLA	C4A-NA-C1A	2.25	107.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	CMD-C2D-C1D	2.24	128.68	124.73
19	6	312	CLA	CHD-C1D-C2D	2.24	130.16	125.49
20	6	315	LUT	C31-C30-C29	2.24	130.42	127.28
19	A	814	CLA	C4A-NA-C1A	2.24	107.70	106.68
23	B	844	BCR	C30-C25-C24	-2.24	109.57	115.65
19	5	310	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	B	839	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	B	840	CLA	C3B-C4B-NB	-2.24	108.53	110.53
19	A	813	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	A	806	CLA	CHD-C1D-C2D	2.24	130.14	125.49
19	A	837	CLA	CHD-C1D-C2D	2.23	130.13	125.49
20	6	318	LUT	C28-C29-C30	-2.23	115.50	119.01
23	J	103	BCR	C10-C11-C12	2.23	129.66	123.20
23	L	305	BCR	C10-C11-C12	2.23	129.66	123.20
19	A	834	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	B	825	CLA	CHD-C1D-C2D	2.23	130.12	125.49
20	5	316	LUT	C40-C33-C34	-2.23	119.21	122.82
19	A	842	CLA	CHD-C1D-ND	-2.23	121.67	124.80
23	G	201	BCR	C19-C18-C17	2.23	122.51	119.01
19	5	307	CLA	C7-C6-C5	2.22	119.19	113.26
19	2	303	CLA	CHD-C1D-C2D	2.22	130.11	125.49
19	B	837	CLA	CHD-C1D-ND	-2.22	121.67	124.80
23	A	851	BCR	C33-C5-C6	2.22	126.91	124.48
19	2	313	CLA	CHD-C1D-C2D	2.22	130.10	125.49
19	B	804	CLA	C1D-ND-C4D	2.22	107.87	106.31
19	A	838	CLA	C1D-ND-C4D	2.22	107.87	106.31
19	B	816	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	5	311	CLA	CHD-C1D-C2D	2.21	130.08	125.49
20	2	315	LUT	C27-C28-C29	2.20	131.07	126.32
19	B	838	CLA	CHD-C1D-C2D	2.20	130.07	125.49
23	G	201	BCR	C12-C13-C14	2.20	122.48	119.01
20	3	316	LUT	C40-C33-C34	-2.20	119.25	122.82
23	A	852	BCR	C12-C13-C14	2.20	122.47	119.01
19	A	827	CLA	CHD-C1D-C2D	2.20	130.06	125.49
19	B	828	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	B	826	CLA	CHD-C1D-C2D	2.20	130.06	125.49
20	2	315	LUT	C35-C34-C33	2.20	130.36	127.28
23	B	848	BCR	C19-C18-C17	2.19	122.46	119.01
23	J	103	BCR	C7-C6-C5	-2.19	116.50	121.56
23	L	304	BCR	C24-C25-C26	-2.19	116.50	121.56
20	2	316	LUT	C40-C33-C34	-2.19	119.27	122.82
18	2	306	CHL	C1C-C2C-CMC	2.19	130.75	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	307	CLA	C1D-ND-C4D	2.19	107.85	106.31
19	B	807	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	6	304	CLA	CHD-C1D-C2D	2.19	130.04	125.49
24	A	802	CL0	C4D-CHA-CBD	-2.19	106.76	108.97
19	A	813	CLA	C4A-NA-C1A	2.19	107.68	106.68
19	A	801	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	F	301	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	5	314	CLA	CHD-C1D-ND	-2.19	121.73	124.80
24	A	802	CL0	C3C-C4C-NC	-2.18	109.31	114.65
19	A	819	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	A	809	CLA	C4A-NA-C1A	2.18	107.67	106.68
20	6	315	LUT	C18-C5-C6	2.18	126.86	124.48
19	5	303	CLA	C4A-NA-C1A	2.18	107.67	106.68
23	B	844	BCR	C8-C9-C10	2.18	122.44	119.01
19	F	304	CLA	CAA-C2A-C3A	-2.18	111.24	116.23
24	A	802	CL0	C4C-CHD-C1D	2.17	123.83	116.07
23	G	205	BCR	C12-C13-C14	2.17	122.42	119.01
19	2	309	CLA	C2A-C1A-CHA	2.17	127.63	123.87
23	F	305	BCR	C12-C13-C14	2.17	122.42	119.01
27	A	853	LMU	O3'-C3'-C2'	-2.16	105.27	110.38
20	3	315	LUT	C20-C13-C14	-2.16	119.31	122.82
19	6	314	CLA	CED-O2D-CGD	2.16	120.81	115.92
19	A	833	CLA	C1D-ND-C4D	2.16	107.83	106.31
20	5	315	LUT	C12-C13-C14	2.16	122.40	119.01
23	G	205	BCR	C29-C28-C27	-2.16	106.53	111.28
19	B	803	CLA	C4D-CHA-C1A	2.16	123.82	121.24
20	3	316	LUT	C35-C34-C33	2.16	130.30	127.28
20	2	315	LUT	C40-C33-C34	-2.16	119.32	122.82
23	B	847	BCR	C4-C5-C6	-2.16	119.79	122.70
18	3	314	CHL	CED-O2D-CGD	2.16	120.81	115.92
19	B	819	CLA	CHD-C1D-C2D	2.15	129.97	125.49
19	2	310	CLA	C4A-NA-C1A	2.15	107.66	106.68
23	F	305	BCR	C24-C23-C22	2.15	129.42	126.23
19	A	803	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	A	835	CLA	CHD-C1D-C2D	2.15	129.96	125.49
19	A	821	CLA	CHD-C1D-ND	-2.15	121.78	124.80
23	3	317	BCR	C2-C1-C6	2.15	113.56	110.44
19	B	836	CLA	CHD-C1D-C2D	2.15	129.95	125.49
19	3	311	CLA	CHD-C1D-C2D	2.15	129.95	125.49
23	B	844	BCR	C2-C1-C6	2.15	113.56	110.44
19	A	819	CLA	C1C-C2C-C3C	2.14	109.24	106.98
19	A	831	CLA	C4A-NA-C1A	2.14	107.66	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	308	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	A	822	CLA	CHD-C1D-C2D	2.14	129.94	125.49
28	B	849	DGD	C1E-O6E-C5E	2.14	117.91	113.72
19	A	832	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	K	201	CLA	CAA-C2A-C1A	2.14	118.99	111.97
23	A	852	BCR	C30-C25-C24	-2.14	109.85	115.65
19	A	818	CLA	C1-O2A-CGA	2.14	121.83	116.65
23	G	205	BCR	C33-C5-C6	2.14	126.82	124.48
23	I	101	BCR	C7-C6-C5	2.14	126.48	121.56
19	B	818	CLA	C3B-C4B-NB	-2.14	108.62	110.53
23	K	204	BCR	C30-C25-C24	-2.14	109.86	115.65
23	G	201	BCR	C1-C6-C7	-2.14	109.86	115.65
19	3	303	CLA	C4A-NA-C1A	2.13	107.65	106.68
19	B	837	CLA	C4A-NA-C1A	2.13	107.65	106.68
19	2	302	CLA	CHD-C1D-C2D	2.13	129.93	125.49
23	A	849	BCR	C7-C6-C5	2.13	126.47	121.56
23	A	850	BCR	C16-C15-C14	2.13	127.88	123.52
23	A	848	BCR	C7-C6-C5	-2.13	116.65	121.56
19	3	303	CLA	CHD-C1D-C2D	2.13	129.92	125.49
23	I	101	BCR	C24-C25-C26	2.13	126.45	121.56
23	F	302	BCR	C35-C13-C14	-2.13	119.37	122.82
19	A	804	CLA	C1D-ND-C4D	2.13	107.80	106.31
19	2	311	CLA	CHD-C1D-ND	-2.13	121.81	124.80
23	3	317	BCR	C19-C18-C17	2.12	122.35	119.01
23	B	847	BCR	C36-C18-C17	-2.12	119.38	122.82
19	6	303	CLA	CHD-C1D-C2D	2.12	129.90	125.49
19	3	307	CLA	C1D-ND-C4D	2.12	107.80	106.31
23	F	302	BCR	C7-C6-C5	2.12	126.44	121.56
19	B	842	CLA	C3B-C4B-NB	-2.12	108.64	110.53
19	B	814	CLA	C4A-NA-C1A	2.12	107.64	106.68
23	B	844	BCR	C23-C24-C25	2.12	132.65	127.00
23	F	305	BCR	C34-C9-C8	2.12	121.32	118.09
19	6	309	CLA	CHD-C1D-C2D	2.11	129.88	125.49
19	5	301	CLA	CHD-C1D-C2D	2.11	129.88	125.49
19	B	802	CLA	C1D-ND-C4D	2.11	107.79	106.31
19	K	203	CLA	CHD-C1D-C2D	2.11	129.87	125.49
23	B	846	BCR	C24-C25-C26	2.11	126.41	121.56
19	3	301	CLA	CHD-C1D-C2D	2.10	129.86	125.49
20	J	101	LUT	C19-C9-C8	2.10	121.30	118.09
19	2	312	CLA	CAA-C2A-C1A	2.10	118.86	111.97
19	B	830	CLA	CMD-C2D-C1D	2.10	128.43	124.73
20	2	317	LUT	C10-C11-C12	2.10	129.28	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	316	XAT	C6-C7-C8	-2.10	121.56	125.99
19	A	810	CLA	CHD-C1D-C2D	2.10	129.85	125.49
19	B	801	CLA	CAA-C2A-C1A	2.10	118.84	111.97
19	B	810	CLA	CHD-C1D-ND	-2.10	121.85	124.80
19	B	801	CLA	C1D-ND-C4D	2.10	107.78	106.31
20	2	316	LUT	C12-C13-C14	2.09	122.30	119.01
23	2	319	BCR	C4-C5-C6	-2.09	119.88	122.70
19	L	301	CLA	CAA-C2A-C1A	2.09	118.83	111.97
19	6	307	CLA	C2A-C1A-CHA	2.09	127.50	123.87
19	B	820	CLA	CHD-C1D-C2D	2.09	129.84	125.49
23	A	849	BCR	C37-C22-C23	2.09	121.28	118.09
20	2	315	LUT	C18-C5-C6	2.09	126.76	124.48
23	B	844	BCR	C20-C21-C22	2.09	130.21	127.28
23	5	317	BCR	C19-C18-C17	2.09	122.29	119.01
19	B	823	CLA	CHD-C1D-ND	-2.09	121.87	124.80
23	B	845	BCR	C29-C30-C25	2.09	113.47	110.44
23	A	850	BCR	C1-C6-C5	-2.09	119.79	122.64
18	3	306	CHL	C3C-C4C-NC	-2.08	109.56	114.65
19	6	311	CLA	CED-O2D-CGD	2.08	120.64	115.92
19	3	313	CLA	CHD-C1D-C2D	2.08	129.82	125.49
19	B	822	CLA	C4A-NA-C1A	2.08	107.63	106.68
19	B	812	CLA	CHD-C1D-C2D	2.08	129.82	125.49
18	2	306	CHL	CED-O2D-CGD	2.08	120.63	115.92
18	2	301	CHL	OBD-CAD-CBD	-2.08	122.77	125.82
19	A	814	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	6	302	CLA	CHD-C1D-C2D	2.08	129.81	125.49
19	A	804	CLA	CHD-C1D-C2D	2.08	129.81	125.49
19	6	314	CLA	CHD-C1D-C2D	2.07	129.80	125.49
19	A	825	CLA	C1D-ND-C4D	2.07	107.77	106.31
19	B	842	CLA	CHD-C1D-C2D	2.07	129.80	125.49
23	B	846	BCR	C1-C6-C5	-2.07	119.80	122.64
19	B	802	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	3	305	CLA	CHD-C1D-C2D	2.07	129.80	125.49
19	5	308	CLA	CHD-C1D-C2D	2.07	129.79	125.49
23	B	847	BCR	C24-C23-C22	2.07	129.30	126.23
23	5	317	BCR	C29-C28-C27	-2.07	106.73	111.28
19	3	302	CLA	C4A-NA-C1A	2.07	107.62	106.68
19	B	804	CLA	CAC-C3C-C4C	2.07	127.48	124.79
18	5	306	CHL	C3C-C4C-NC	-2.07	109.60	114.65
19	5	303	CLA	CHD-C1D-C2D	2.07	129.78	125.49
19	2	308	CLA	CHD-C1D-C2D	2.06	129.78	125.49
19	B	824	CLA	CHD-C1D-C2D	2.06	129.76	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	849	BCR	C1-C6-C5	-2.06	119.83	122.64
18	2	301	CHL	C3C-C4C-NC	-2.06	109.62	114.65
23	K	204	BCR	C37-C22-C23	2.06	121.23	118.09
18	2	314	CHL	C3C-C4C-NC	-2.06	109.62	114.65
19	3	312	CLA	C4A-NA-C1A	2.06	107.62	106.68
19	B	835	CLA	CHD-C1D-C2D	2.05	129.76	125.49
18	5	313	CHL	C3C-C4C-NC	-2.05	109.63	114.65
19	B	816	CLA	C1D-ND-C4D	2.05	107.75	106.31
19	2	304	CLA	CHD-C1D-C2D	2.05	129.76	125.49
19	A	801	CLA	C2A-C1A-CHA	2.05	127.43	123.87
19	B	828	CLA	C2A-C1A-CHA	2.05	127.43	123.87
20	6	318	LUT	C32-C33-C34	2.05	122.23	119.01
19	A	815	CLA	C1D-ND-C4D	2.05	107.75	106.31
19	A	805	CLA	CHD-C1D-C2D	2.05	129.75	125.49
18	2	306	CHL	C3C-C4C-NC	-2.05	109.64	114.65
18	6	306	CHL	C3C-C4C-NC	-2.05	109.64	114.65
19	B	839	CLA	CHD-C1D-C2D	2.05	129.75	125.49
19	B	802	CLA	C2A-C1A-CHA	2.05	127.42	123.87
19	A	816	CLA	C4A-NA-C1A	2.05	107.61	106.68
19	B	817	CLA	C4A-NA-C1A	2.05	107.61	106.68
19	G	204	CLA	C4A-NA-C1A	2.05	107.61	106.68
19	5	302	CLA	CHD-C1D-ND	-2.05	121.92	124.80
23	G	201	BCR	C34-C9-C8	2.05	121.21	118.09
19	3	304	CLA	CHD-C1D-C2D	2.05	129.74	125.49
19	3	305	CLA	C4A-NA-C1A	2.05	107.61	106.68
19	A	838	CLA	CHD-C1D-ND	-2.04	121.93	124.80
18	3	306	CHL	OBD-CAD-CBD	-2.04	122.83	125.82
23	K	205	BCR	C2-C1-C6	2.04	113.40	110.44
19	A	833	CLA	C4A-NA-C1A	2.04	107.61	106.68
19	B	816	CLA	C4A-NA-C1A	2.04	107.61	106.68
19	B	809	CLA	CHD-C1D-ND	-2.04	121.93	124.80
18	6	301	CHL	C3C-C4C-NC	-2.04	109.67	114.65
18	6	306	CHL	OBD-CAD-CBD	-2.04	122.83	125.82
19	A	823	CLA	CHD-C1D-C2D	2.03	129.72	125.49
19	6	309	CLA	C2A-C1A-CHA	2.03	127.40	123.87
23	M	101	BCR	C20-C21-C22	2.03	130.13	127.28
19	B	836	CLA	C1D-ND-C4D	2.03	107.74	106.31
18	3	314	CHL	C3C-C4C-NC	-2.03	109.68	114.65
19	B	813	CLA	C1D-ND-C4D	2.03	107.74	106.31
18	6	301	CHL	OBD-CAD-CBD	-2.03	122.84	125.82
18	3	314	CHL	OBD-CAD-CBD	-2.03	122.84	125.82
19	2	304	CLA	C4A-NA-C1A	2.03	107.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	314	CHL	OBD-CAD-CBD	-2.03	122.84	125.82
19	A	814	CLA	C1D-ND-C4D	2.03	107.73	106.31
19	K	201	CLA	CHD-C1D-C2D	2.03	129.70	125.49
18	5	305	CHL	C3C-C4C-NC	-2.03	109.69	114.65
19	B	818	CLA	CHD-C1D-C2D	2.03	129.70	125.49
19	2	303	CLA	CMD-C2D-C1D	2.03	128.30	124.73
23	M	101	BCR	C24-C23-C22	2.03	129.23	126.23
23	A	850	BCR	C7-C8-C9	2.02	129.23	126.23
23	K	205	BCR	C8-C9-C10	2.02	122.19	119.01
18	5	304	CHL	C3C-C4C-NC	-2.02	109.71	114.65
19	B	834	CLA	CHD-C1D-C2D	2.02	129.69	125.49
19	B	810	CLA	C2A-C1A-CHA	2.02	127.37	123.87
23	B	845	BCR	C37-C22-C23	2.02	121.17	118.09
19	B	815	CLA	C4A-NA-C1A	2.02	107.60	106.68
27	G	202	LMU	O1B-C4'-C3'	-2.02	102.10	107.23
23	L	304	BCR	C11-C10-C9	2.02	130.11	127.28
18	2	305	CHL	C3C-C4C-NC	-2.02	109.72	114.65
18	5	313	CHL	OBD-CAD-CBD	-2.02	122.86	125.82
18	2	307	CHL	C3C-C4C-NC	-2.01	109.73	114.65
19	3	302	CLA	CHD-C1D-ND	-2.01	121.97	124.80
19	A	825	CLA	C4A-NA-C1A	2.01	107.60	106.68
19	A	815	CLA	CHD-C1D-C2D	2.01	129.67	125.49
19	B	817	CLA	CHD-C1D-C2D	2.01	129.67	125.49
23	3	317	BCR	C2-C3-C4	-2.01	106.86	111.28
20	6	318	LUT	C35-C34-C33	2.01	130.09	127.28
20	6	318	LUT	C30-C31-C32	-2.01	117.38	123.20
23	A	848	BCR	C37-C22-C23	2.01	121.16	118.09
19	A	818	CLA	C4A-NA-C1A	2.01	107.59	106.68
19	B	833	CLA	CAA-C2A-C1A	2.01	118.55	111.97
19	A	816	CLA	CHD-C1D-C2D	2.00	129.66	125.49
19	B	823	CLA	C2A-C1A-CHA	2.00	127.35	123.87
23	I	101	BCR	C16-C15-C14	2.00	127.62	123.52
19	B	806	CLA	CHD-C1D-C2D	2.00	129.65	125.49
18	5	304	CHL	OBD-CAD-CBD	-2.00	122.89	125.82
19	G	204	CLA	CHD-C1D-C2D	2.00	129.65	125.49
19	3	301	CLA	C1D-ND-C4D	2.00	107.72	106.31
23	G	201	BCR	C16-C15-C14	2.00	127.61	123.52
19	3	310	CLA	CHD-C1D-ND	-2.00	121.99	124.80
19	B	808	CLA	CHD-C1D-C2D	2.00	129.65	125.49

All (148) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	6	301	CHL	ND
18	6	301	CHL	NA
18	6	301	CHL	NC
18	6	306	CHL	ND
18	6	306	CHL	NA
18	6	306	CHL	NC
18	2	301	CHL	ND
18	2	301	CHL	NA
18	2	301	CHL	NC
18	2	305	CHL	ND
18	2	305	CHL	NA
18	2	305	CHL	NC
18	2	306	CHL	ND
18	2	306	CHL	NA
18	2	306	CHL	NC
18	2	307	CHL	NA
18	2	307	CHL	NC
18	2	314	CHL	ND
18	2	314	CHL	NA
18	2	314	CHL	NC
18	2	320	CHL	ND
18	2	320	CHL	NA
18	2	320	CHL	NC
18	3	306	CHL	NA
18	3	306	CHL	NC
18	3	314	CHL	ND
18	3	314	CHL	NA
18	3	314	CHL	NC
18	5	304	CHL	ND
18	5	304	CHL	NA
18	5	304	CHL	NC
18	5	305	CHL	ND
18	5	305	CHL	NA
18	5	305	CHL	NC
18	5	306	CHL	ND
18	5	306	CHL	NA
18	5	306	CHL	NC
18	5	313	CHL	ND
18	5	313	CHL	NA
18	5	313	CHL	NC
19	6	302	CLA	ND
19	6	303	CLA	ND
19	6	304	CLA	ND

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Mol	Chain	Res	Type	Atom
19	6	305	CLA	ND
19	6	307	CLA	ND
19	6	308	CLA	ND
19	6	309	CLA	ND
19	6	310	CLA	ND
19	6	311	CLA	ND
19	6	313	CLA	ND
19	6	314	CLA	ND
19	2	302	CLA	ND
19	2	303	CLA	ND
19	2	304	CLA	ND
19	2	308	CLA	ND
19	2	309	CLA	ND
19	2	310	CLA	ND
19	2	311	CLA	ND
19	2	313	CLA	ND
19	3	301	CLA	ND
19	3	302	CLA	ND
19	3	303	CLA	ND
19	3	304	CLA	ND
19	3	305	CLA	ND
19	3	307	CLA	ND
19	3	308	CLA	ND
19	3	309	CLA	ND
19	3	310	CLA	ND
19	3	312	CLA	ND
19	3	313	CLA	ND
19	5	302	CLA	ND
19	5	303	CLA	ND
19	5	307	CLA	ND
19	5	308	CLA	ND
19	5	309	CLA	ND
19	5	310	CLA	ND
19	5	312	CLA	ND
19	A	803	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	812	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	817	CLA	ND
19	A	820	CLA	ND
19	A	821	CLA	ND
19	A	824	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	834	CLA	ND
19	A	835	CLA	ND
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	841	CLA	ND
19	A	842	CLA	ND
19	A	843	CLA	ND
19	B	801	CLA	ND
19	B	802	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	821	CLA	ND
19	B	823	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	827	CLA	ND
19	B	828	CLA	ND
19	B	829	CLA	ND
19	B	832	CLA	ND
19	B	833	CLA	ND
19	B	835	CLA	ND
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	838	CLA	ND
19	B	839	CLA	ND
19	B	842	CLA	ND
19	F	301	CLA	ND
19	F	303	CLA	ND
19	F	304	CLA	ND
19	G	203	CLA	ND
19	G	204	CLA	ND
19	J	102	CLA	ND
19	K	202	CLA	ND
19	K	203	CLA	ND
19	L	301	CLA	ND
19	L	303	CLA	ND

All (712) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	2	306	CHL	CBD-CGD-O2D-CED
18	2	306	CHL	O1D-CGD-O2D-CED
18	3	314	CHL	CBD-CGD-O2D-CED
18	3	314	CHL	O1D-CGD-O2D-CED
19	6	311	CLA	CBD-CGD-O2D-CED
19	6	311	CLA	O1D-CGD-O2D-CED
19	6	314	CLA	CBD-CGD-O2D-CED
19	6	314	CLA	O1D-CGD-O2D-CED
19	2	302	CLA	CHA-CBD-CGD-O1D
19	2	302	CLA	CHA-CBD-CGD-O2D
19	2	309	CLA	C1A-C2A-CAA-CBA
19	2	309	CLA	C3A-C2A-CAA-CBA
19	2	311	CLA	CHA-CBD-CGD-O1D
19	2	311	CLA	CHA-CBD-CGD-O2D
19	3	301	CLA	CHA-CBD-CGD-O1D
19	3	301	CLA	CHA-CBD-CGD-O2D
19	3	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	3	307	CLA	O1A-CGA-O2A-C1
19	3	313	CLA	CAD-CBD-CGD-O1D
19	3	313	CLA	CAD-CBD-CGD-O2D
19	5	301	CLA	CHA-CBD-CGD-O2D
19	5	307	CLA	C1A-C2A-CAA-CBA
19	5	307	CLA	C3A-C2A-CAA-CBA
19	5	308	CLA	C4-C3-C5-C6
19	5	310	CLA	C1A-C2A-CAA-CBA
19	5	310	CLA	C3A-C2A-CAA-CBA
19	5	310	CLA	CHA-CBD-CGD-O1D
19	5	310	CLA	CHA-CBD-CGD-O2D
19	5	312	CLA	CBA-CGA-O2A-C1
19	5	312	CLA	O1A-CGA-O2A-C1
19	5	314	CLA	CBD-CGD-O2D-CED
19	5	314	CLA	O1D-CGD-O2D-CED
19	A	801	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	810	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	CHA-CBD-CGD-O2D
19	A	812	CLA	CHA-CBD-CGD-O2D
19	A	819	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C1-C2-C3-C4
19	A	828	CLA	C1-C2-C3-C5
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	835	CLA	CHA-CBD-CGD-O1D
19	A	835	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	C4-C3-C5-C6
19	A	843	CLA	CAD-CBD-CGD-O1D
19	A	843	CLA	CAD-CBD-CGD-O2D
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C3A-C2A-CAA-CBA
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	B	840	CLA	C1A-C2A-CAA-CBA
19	F	304	CLA	CHA-CBD-CGD-O1D
19	F	304	CLA	CHA-CBD-CGD-O2D
19	G	203	CLA	CHA-CBD-CGD-O1D
19	G	203	CLA	CHA-CBD-CGD-O2D
19	K	201	CLA	C2-C3-C5-C6
19	K	203	CLA	CHA-CBD-CGD-O1D
19	K	203	CLA	CHA-CBD-CGD-O2D
20	6	318	LUT	C1-C6-C7-C8
20	6	318	LUT	C5-C6-C7-C8
22	6	317	LHG	O10-C23-O8-C6
22	6	317	LHG	C24-C23-O8-C6
22	6	319	LHG	O10-C23-O8-C6
22	6	319	LHG	C24-C23-O8-C6
22	5	318	LHG	C3-O3-P-O5
23	2	319	BCR	C17-C18-C19-C20
23	2	319	BCR	C36-C18-C19-C20
23	2	319	BCR	C18-C19-C20-C21
23	2	319	BCR	C19-C20-C21-C22
23	2	319	BCR	C23-C24-C25-C26
23	2	319	BCR	C23-C24-C25-C30
23	3	317	BCR	C21-C22-C23-C24
23	B	844	BCR	C23-C24-C25-C26
23	K	205	BCR	C7-C8-C9-C10
23	K	205	BCR	C7-C8-C9-C34
23	K	205	BCR	C18-C19-C20-C21
23	K	205	BCR	C19-C20-C21-C22
23	K	205	BCR	C20-C21-C22-C23
23	K	205	BCR	C20-C21-C22-C37
23	K	205	BCR	C21-C22-C23-C24
23	K	205	BCR	C37-C22-C23-C24
23	K	205	BCR	C22-C23-C24-C25
27	B	850	LMU	O5'-C1'-O1'-C1
27	G	202	LMU	O5'-C1'-O1'-C1
27	G	202	LMU	C2-C1-O1'-C1'
28	B	849	DGD	O1B-C1B-O2G-C2G
29	J	104	LMG	C2-C1-O1-C7
27	G	202	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
29	J	104	LMG	O10-C28-O8-C9
19	B	819	CLA	C3-C5-C6-C7
29	J	104	LMG	C29-C28-O8-C9
28	B	849	DGD	C2B-C1B-O2G-C2G
19	3	307	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	B	842	CLA	C4-C3-C5-C6
19	3	307	CLA	C2-C3-C5-C6
19	5	308	CLA	C2-C3-C5-C6
19	B	842	CLA	C2-C3-C5-C6
19	6	309	CLA	C3-C5-C6-C7
19	B	810	CLA	C3-C5-C6-C7
23	B	848	BCR	C9-C10-C11-C12
27	B	851	LMU	C5'-C4'-O1B-C1B
28	B	849	DGD	O6E-C5E-C6E-O5E
19	A	833	CLA	C3-C5-C6-C7
19	A	831	CLA	C4-C3-C5-C6
19	B	825	CLA	C4-C3-C5-C6
19	A	831	CLA	C2-C3-C5-C6
19	B	801	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	A	810	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
29	J	104	LMG	O6-C1-O1-C7
19	A	803	CLA	C3-C5-C6-C7
19	A	828	CLA	CBA-CGA-O2A-C1
19	5	307	CLA	C4-C3-C5-C6
19	A	818	CLA	C4-C3-C5-C6
19	B	801	CLA	C4-C3-C5-C6
19	5	307	CLA	C2-C3-C5-C6
19	A	818	CLA	C2-C3-C5-C6
19	A	828	CLA	C11-C10-C8-C9
19	B	842	CLA	C11-C10-C8-C9
20	6	318	LUT	C11-C12-C13-C20
20	2	317	LUT	C27-C28-C29-C39
20	J	101	LUT	C27-C28-C29-C39
23	3	317	BCR	C37-C22-C23-C24
23	5	317	BCR	C7-C8-C9-C34
23	5	317	BCR	C37-C22-C23-C24
23	A	848	BCR	C7-C8-C9-C34
23	B	846	BCR	C37-C22-C23-C24
23	J	103	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	2	317	LUT	C27-C28-C29-C30
20	J	101	LUT	C27-C28-C29-C30
23	5	317	BCR	C7-C8-C9-C10
23	J	103	BCR	C21-C22-C23-C24
19	A	828	CLA	O1A-CGA-O2A-C1
19	5	307	CLA	C3-C5-C6-C7
28	B	849	DGD	C4E-C5E-C6E-O5E
19	B	806	CLA	C10-C11-C12-C13
19	A	808	CLA	C15-C16-C17-C18
19	B	814	CLA	C15-C16-C17-C18
23	K	205	BCR	C13-C14-C15-C16
23	K	205	BCR	C15-C16-C17-C18
19	5	307	CLA	C2A-CAA-CBA-CGA
19	A	803	CLA	C2A-CAA-CBA-CGA
28	B	849	DGD	C1A-C2A-C3A-C4A
28	B	849	DGD	C1B-C2B-C3B-C4B
23	K	205	BCR	C6-C7-C8-C9
19	A	808	CLA	C5-C6-C7-C8
19	A	819	CLA	C8-C10-C11-C12
19	2	302	CLA	C8-C10-C11-C12
19	B	814	CLA	C13-C15-C16-C17
19	B	842	CLA	C15-C16-C17-C18
19	6	309	CLA	C5-C6-C7-C8
19	B	812	CLA	C5-C6-C7-C8
19	B	842	CLA	C3-C5-C6-C7
27	B	850	LMU	C2'-C1'-O1'-C1
20	6	318	LUT	C11-C10-C9-C19
23	K	205	BCR	C11-C10-C9-C34
20	6	315	LUT	C7-C8-C9-C19
20	2	315	LUT	C7-C8-C9-C19
20	2	317	LUT	C7-C8-C9-C19
20	3	316	LUT	C7-C8-C9-C19
20	5	316	LUT	C7-C8-C9-C19
23	B	848	BCR	C11-C12-C13-C35
23	J	103	BCR	C7-C8-C9-C34
20	6	315	LUT	C7-C8-C9-C10
20	6	318	LUT	C11-C12-C13-C14
20	2	315	LUT	C7-C8-C9-C10
20	3	316	LUT	C7-C8-C9-C10
20	5	316	LUT	C7-C8-C9-C10
23	B	846	BCR	C21-C22-C23-C24
23	B	848	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	J	103	BCR	C7-C8-C9-C10
18	6	306	CHL	C2A-CAA-CBA-CGA
19	2	304	CLA	C2A-CAA-CBA-CGA
19	A	818	CLA	C8-C10-C11-C12
19	A	828	CLA	O2A-C1-C2-C3
23	K	205	BCR	C11-C10-C9-C8
19	B	825	CLA	C2-C3-C5-C6
25	A	844	PQN	C26-C27-C28-C29
19	B	842	CLA	C10-C11-C12-C13
28	B	849	DGD	C3A-C4A-C5A-C6A
22	6	317	LHG	C30-C31-C32-C33
19	B	842	CLA	C4B-C3B-CAB-CBB
19	B	840	CLA	C2A-CAA-CBA-CGA
19	5	312	CLA	C13-C15-C16-C17
27	A	853	LMU	C5'-C4'-O1B-C1B
19	A	834	CLA	C3A-C2A-CAA-CBA
22	A	847	LHG	C13-C14-C15-C16
29	J	105	LMG	C18-C19-C20-C21
19	6	312	CLA	C10-C11-C12-C13
28	B	849	DGD	C5A-C6A-C7A-C8A
19	B	842	CLA	C2B-C3B-CAB-CBB
23	2	319	BCR	C1-C6-C7-C8
23	5	317	BCR	C1-C6-C7-C8
23	5	317	BCR	C5-C6-C7-C8
23	A	849	BCR	C23-C24-C25-C26
23	A	852	BCR	C23-C24-C25-C26
23	B	844	BCR	C23-C24-C25-C30
23	B	845	BCR	C1-C6-C7-C8
23	B	848	BCR	C23-C24-C25-C26
23	F	302	BCR	C23-C24-C25-C26
23	G	201	BCR	C23-C24-C25-C26
23	J	103	BCR	C23-C24-C25-C26
23	K	204	BCR	C23-C24-C25-C26
23	K	204	BCR	C23-C24-C25-C30
23	M	101	BCR	C1-C6-C7-C8
23	M	101	BCR	C5-C6-C7-C8
23	L	304	BCR	C1-C6-C7-C8
19	A	814	CLA	C16-C17-C18-C19
22	A	846	LHG	C27-C28-C29-C30
27	A	853	LMU	O5B-C1B-O1B-C4'
27	B	851	LMU	C3'-C4'-O1B-C1B
27	G	202	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
19	B	842	CLA	C13-C15-C16-C17
27	A	853	LMU	C3'-C4'-O1B-C1B
27	B	850	LMU	C11-C10-C9-C8
19	6	310	CLA	C3-C5-C6-C7
19	A	814	CLA	C16-C17-C18-C20
19	A	836	CLA	C10-C11-C12-C13
25	A	844	PQN	C25-C26-C27-C28
29	J	104	LMG	C28-C29-C30-C31
19	A	828	CLA	C10-C11-C12-C13
27	B	851	LMU	O5B-C5B-C6B-O6B
27	G	202	LMU	O5B-C5B-C6B-O6B
27	G	202	LMU	O5'-C5'-C6'-O6'
19	A	825	CLA	C2-C3-C5-C6
18	2	301	CHL	C3-C5-C6-C7
19	3	302	CLA	C3-C5-C6-C7
19	3	313	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	819	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	C1A-C2A-CAA-CBA
19	B	816	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	6	309	CLA	C12-C13-C15-C16
19	A	829	CLA	C6-C7-C8-C10
19	B	816	CLA	C6-C7-C8-C10
19	F	301	CLA	C11-C10-C8-C7
19	6	309	CLA	C16-C17-C18-C20
29	J	105	LMG	O6-C5-C6-O5
19	A	829	CLA	C5-C6-C7-C8
19	B	816	CLA	C6-C7-C8-C9
19	B	838	CLA	C6-C7-C8-C9
22	5	318	LHG	C11-C10-C9-C8
18	5	305	CHL	CHA-CBD-CGD-O1D
18	5	306	CHL	CHA-CBD-CGD-O1D
18	5	306	CHL	CHA-CBD-CGD-O2D
19	A	825	CLA	C4-C3-C5-C6
29	J	104	LMG	O6-C5-C6-O5
19	B	842	CLA	CBA-CGA-O2A-C1
19	2	309	CLA	O2A-C1-C2-C3
19	A	828	CLA	C16-C17-C18-C19
20	6	318	LUT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	J	105	LMG	C17-C18-C19-C20
19	5	312	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C2A-CAA-CBA-CGA
19	A	820	CLA	C8-C10-C11-C12
28	B	849	DGD	CFA-CGA-CHA-CIA
25	B	843	PQN	C13-C15-C16-C17
19	B	830	CLA	C4-C3-C5-C6
19	6	309	CLA	C14-C13-C15-C16
19	A	829	CLA	C6-C7-C8-C9
19	B	801	CLA	C6-C7-C8-C9
19	F	301	CLA	C11-C10-C8-C9
19	3	311	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	C11-C10-C8-C7
19	B	838	CLA	C6-C7-C8-C10
27	B	850	LMU	C7-C8-C9-C10
19	A	808	CLA	C4-C3-C5-C6
19	B	807	CLA	C10-C11-C12-C13
19	A	828	CLA	C5-C6-C7-C8
20	3	315	LUT	C7-C8-C9-C19
19	K	201	CLA	C4-C3-C5-C6
18	2	307	CHL	O2A-C1-C2-C3
28	B	849	DGD	O1G-C1G-C2G-C3G
29	J	105	LMG	C7-C8-C9-O8
19	6	309	CLA	C16-C17-C18-C19
19	B	842	CLA	C1-C2-C3-C4
19	A	841	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	B	830	CLA	C2-C3-C5-C6
19	B	842	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	CBA-CCA-CDA-CEA
20	3	315	LUT	C5-C6-C7-C8
23	A	848	BCR	C5-C6-C7-C8
23	A	848	BCR	C23-C24-C25-C26
23	A	849	BCR	C23-C24-C25-C30
23	A	852	BCR	C1-C6-C7-C8
23	A	852	BCR	C23-C24-C25-C30
23	B	846	BCR	C1-C6-C7-C8
23	F	302	BCR	C23-C24-C25-C30
23	F	305	BCR	C23-C24-C25-C26
23	G	201	BCR	C1-C6-C7-C8
23	G	201	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	J	103	BCR	C23-C24-C25-C30
23	L	304	BCR	C5-C6-C7-C8
25	A	844	PQN	C26-C27-C28-C30
19	B	825	CLA	C10-C11-C12-C13
28	B	849	DGD	O2G-C2G-C3G-O3G
22	5	318	LHG	C24-C25-C26-C27
19	A	803	CLA	C1-C2-C3-C5
19	B	842	CLA	C1-C2-C3-C5
22	A	847	LHG	C11-C12-C13-C14
23	K	205	BCR	C36-C18-C19-C20
18	3	314	CHL	C11-C12-C13-C15
19	B	819	CLA	C12-C13-C15-C16
19	B	816	CLA	C15-C16-C17-C18
23	K	205	BCR	C17-C18-C19-C20
19	A	804	CLA	C2A-CAA-CBA-CGA
19	B	801	CLA	C2A-CAA-CBA-CGA
19	B	832	CLA	C2A-CAA-CBA-CGA
27	B	850	LMU	C5-C6-C7-C8
18	3	314	CHL	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	B	812	CLA	C4-C3-C5-C6
19	A	841	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	A	828	CLA	C16-C17-C18-C20
19	B	807	CLA	C3-C5-C6-C7
28	B	849	DGD	O1G-C1G-C2G-O2G
19	2	302	CLA	C11-C10-C8-C9
19	B	819	CLA	C14-C13-C15-C16
19	B	842	CLA	C16-C17-C18-C19
22	6	317	LHG	C28-C29-C30-C31
19	L	302	CLA	C3-C5-C6-C7
19	B	814	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C4-C3-C5-C6
23	5	317	BCR	C21-C22-C23-C24
22	5	318	LHG	C9-C10-C11-C12
19	A	838	CLA	C2-C3-C5-C6
19	5	312	CLA	C3-C5-C6-C7
19	6	312	CLA	C11-C10-C8-C7
19	A	808	CLA	C12-C13-C15-C16
19	A	810	CLA	C12-C13-C15-C16
19	A	820	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	817	CLA	C6-C7-C8-C10
19	B	819	CLA	C11-C10-C8-C7
25	A	844	PQN	C17-C18-C20-C21
19	B	837	CLA	C4-C3-C5-C6
19	B	842	CLA	C5-C6-C7-C8
19	6	304	CLA	C1-C2-C3-C4
29	J	105	LMG	O7-C8-C9-O8
19	3	311	CLA	CAA-CBA-CGA-O2A
18	3	314	CHL	C2-C3-C5-C6
18	2	320	CHL	CAD-CBD-CGD-O2D
19	A	807	CLA	CAD-CBD-CGD-O2D
19	B	802	CLA	CAD-CBD-CGD-O2D
19	A	818	CLA	C11-C12-C13-C14
18	2	306	CHL	CHA-CBD-CGD-O2D
18	2	314	CHL	CHA-CBD-CGD-O2D
18	2	320	CHL	CAD-CBD-CGD-O1D
18	5	305	CHL	CHA-CBD-CGD-O2D
19	6	302	CLA	CHA-CBD-CGD-O1D
19	6	302	CLA	CHA-CBD-CGD-O2D
19	5	301	CLA	CHA-CBD-CGD-O1D
19	A	807	CLA	CAD-CBD-CGD-O1D
19	A	812	CLA	CHA-CBD-CGD-O1D
19	A	823	CLA	CHA-CBD-CGD-O1D
19	A	823	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CAD-CBD-CGD-O1D
19	B	816	CLA	CHA-CBD-CGD-O1D
19	G	204	CLA	CHA-CBD-CGD-O1D
19	G	204	CLA	CHA-CBD-CGD-O2D
22	6	317	LHG	C4-O6-P-O5
22	A	847	LHG	C3-O3-P-O5
19	A	841	CLA	C8-C10-C11-C12
19	A	830	CLA	C4-C3-C5-C6
19	B	814	CLA	C4-C3-C5-C6
23	K	204	BCR	C1-C6-C7-C8
19	B	812	CLA	C2-C3-C5-C6
19	B	816	CLA	C3-C5-C6-C7
19	B	828	CLA	C8-C10-C11-C12
19	A	825	CLA	C8-C10-C11-C12
19	A	808	CLA	C2-C3-C5-C6
19	B	826	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	846	LHG	C24-C25-C26-C27
29	J	105	LMG	C29-C28-O8-C9
29	J	105	LMG	O10-C28-O8-C9
18	2	301	CHL	C11-C12-C13-C15
19	B	801	CLA	C6-C7-C8-C10
29	J	105	LMG	C12-C13-C14-C15
19	G	204	CLA	C2A-CAA-CBA-CGA
22	2	318	LHG	C23-C24-C25-C26
22	6	317	LHG	C5-C4-O6-P
24	A	802	CL0	CAA-CBA-CGA-O2A
19	A	819	CLA	CAA-CBA-CGA-O2A
28	B	849	DGD	C5D-C6D-O5D-C1E
19	B	804	CLA	C2A-CAA-CBA-CGA
19	B	818	CLA	C2A-CAA-CBA-CGA
19	2	309	CLA	C4-C3-C5-C6
19	A	806	CLA	C4-C3-C5-C6
19	2	309	CLA	C2-C3-C5-C6
19	A	818	CLA	C11-C12-C13-C15
18	3	314	CHL	C11-C12-C13-C14
19	A	808	CLA	C14-C13-C15-C16
19	B	819	CLA	C11-C10-C8-C9
19	6	312	CLA	C8-C10-C11-C12
19	A	804	CLA	C4-C3-C5-C6
19	B	810	CLA	C4-C3-C5-C6
19	B	819	CLA	C4-C3-C5-C6
19	B	842	CLA	CAA-CBA-CGA-O2A
19	6	304	CLA	O2A-C1-C2-C3
19	5	311	CLA	C3A-C2A-CAA-CBA
19	A	801	CLA	C4-C3-C5-C6
19	B	802	CLA	C3A-C2A-CAA-CBA
19	B	814	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	C4-C3-C5-C6
19	B	807	CLA	C2-C3-C5-C6
19	K	203	CLA	CAA-CBA-CGA-O1A
20	5	315	LUT	C20-C13-C14-C15
23	3	317	BCR	C20-C21-C22-C37
23	A	852	BCR	C11-C10-C9-C34
23	A	852	BCR	C16-C17-C18-C36
23	B	845	BCR	C11-C10-C9-C34
23	B	845	BCR	C20-C21-C22-C37
23	B	846	BCR	C16-C17-C18-C36
23	F	305	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	L	305	BCR	C11-C10-C9-C34
19	B	830	CLA	C3-C5-C6-C7
19	6	311	CLA	CAA-CBA-CGA-O1A
19	A	830	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	B	837	CLA	C2-C3-C5-C6
27	B	850	LMU	C3-C4-C5-C6
19	6	307	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	C10-C11-C12-C13
19	6	313	CLA	CAA-CBA-CGA-O1A
19	6	309	CLA	C11-C10-C8-C9
19	3	307	CLA	C6-C7-C8-C9
19	5	307	CLA	C6-C7-C8-C9
19	B	828	CLA	C11-C10-C8-C9
19	B	842	CLA	C14-C13-C15-C16
19	A	812	CLA	C16-C17-C18-C19
28	B	849	DGD	C8B-C9B-CAB-CBB
19	B	812	CLA	C3-C5-C6-C7
19	A	806	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
18	5	306	CHL	CAA-CBA-CGA-O1A
19	6	307	CLA	CAA-CBA-CGA-O1A
19	K	202	CLA	CAA-CBA-CGA-O1A
19	K	202	CLA	CAA-CBA-CGA-O2A
19	A	805	CLA	C2A-CAA-CBA-CGA
19	3	311	CLA	C1A-C2A-CAA-CBA
19	B	802	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
20	5	315	LUT	C12-C13-C14-C15
23	A	852	BCR	C11-C10-C9-C8
23	A	852	BCR	C16-C17-C18-C19
23	B	845	BCR	C11-C10-C9-C8
23	B	845	BCR	C20-C21-C22-C23
23	B	846	BCR	C16-C17-C18-C19
23	F	305	BCR	C12-C13-C14-C15
19	A	817	CLA	CAA-CBA-CGA-O1A
23	2	319	BCR	C5-C6-C7-C8
23	K	205	BCR	C1-C6-C7-C8
23	L	305	BCR	C23-C24-C25-C26
19	B	819	CLA	C8-C10-C11-C12
27	B	850	LMU	C4-C5-C6-C7
19	6	311	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	6	313	CLA	CAA-CBA-CGA-O2A
19	A	805	CLA	C4-C3-C5-C6
19	B	808	CLA	C4-C3-C5-C6
19	B	832	CLA	C4-C3-C5-C6
19	B	838	CLA	C4-C3-C5-C6
19	L	302	CLA	C4-C3-C5-C6
19	2	311	CLA	CAA-CBA-CGA-O1A
19	K	203	CLA	CAA-CBA-CGA-O2A
19	A	812	CLA	C13-C15-C16-C17
19	G	204	CLA	CAA-CBA-CGA-O2A
22	A	847	LHG	C10-C11-C12-C13
19	2	303	CLA	CAA-CBA-CGA-O2A
19	A	828	CLA	C13-C15-C16-C17
19	A	801	CLA	C2-C3-C5-C6
19	A	804	CLA	C2-C3-C5-C6
19	B	819	CLA	C2-C3-C5-C6
19	A	824	CLA	C2-C1-O2A-CGA
18	3	306	CHL	CAA-CBA-CGA-O2A
19	2	311	CLA	CAA-CBA-CGA-O2A
18	2	314	CHL	CAA-CBA-CGA-O1A
19	G	204	CLA	CAA-CBA-CGA-O1A
27	B	851	LMU	C5-C6-C7-C8
21	6	316	XAT	C29-C30-C31-C32
18	5	306	CHL	CAA-CBA-CGA-O2A
19	6	314	CLA	CAA-CBA-CGA-O2A
19	B	813	CLA	CAA-CBA-CGA-O2A
19	2	302	CLA	C4-C3-C5-C6
19	A	829	CLA	C4-C3-C5-C6
19	A	817	CLA	CAA-CBA-CGA-O2A
19	A	821	CLA	CAA-CBA-CGA-O2A
29	J	105	LMG	C20-C21-C22-C23
19	A	823	CLA	CAA-CBA-CGA-O2A
22	2	318	LHG	C27-C28-C29-C30
18	2	305	CHL	CAA-CBA-CGA-O2A
18	5	304	CHL	CAA-CBA-CGA-O2A
19	B	840	CLA	C16-C17-C18-C20
18	6	306	CHL	CAA-CBA-CGA-O1A
19	A	812	CLA	C4-C3-C5-C6
19	2	303	CLA	CAA-CBA-CGA-O1A
19	5	310	CLA	CAA-CBA-CGA-O2A
18	2	314	CHL	CAA-CBA-CGA-O2A
19	6	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	2	305	CHL	CHA-CBD-CGD-O1D
18	2	305	CHL	CHA-CBD-CGD-O2D
18	2	306	CHL	CHA-CBD-CGD-O1D
18	2	307	CHL	CHA-CBD-CGD-O1D
18	2	307	CHL	CHA-CBD-CGD-O2D
18	2	314	CHL	CHA-CBD-CGD-O1D
24	A	802	CL0	CHA-CBD-CGD-O1D
24	A	802	CL0	CHA-CBD-CGD-O2D
18	3	314	CHL	C10-C11-C12-C13
18	3	306	CHL	CAA-CBA-CGA-O1A
19	B	831	CLA	CAA-CBA-CGA-O2A
19	3	313	CLA	CAA-CBA-CGA-O2A
19	B	813	CLA	CAA-CBA-CGA-O1A
19	5	312	CLA	C11-C12-C13-C14
19	A	810	CLA	C14-C13-C15-C16
19	A	826	CLA	C11-C10-C8-C9
19	A	828	CLA	C6-C7-C8-C9
18	5	304	CHL	CAA-CBA-CGA-O1A
19	6	314	CLA	CAA-CBA-CGA-O1A
19	3	304	CLA	CAA-CBA-CGA-O2A
19	A	808	CLA	C2-C1-O2A-CGA
19	A	812	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C3A-C2A-CAA-CBA
19	B	831	CLA	CAA-CBA-CGA-O1A
19	L	302	CLA	C2-C3-C5-C6
19	5	308	CLA	C3-C5-C6-C7
19	6	305	CLA	CAA-CBA-CGA-O1A
27	A	853	LMU	C2B-C1B-O1B-C4'
19	5	310	CLA	CAA-CBA-CGA-O1A
19	A	837	CLA	CAA-CBA-CGA-O2A
22	A	846	LHG	C28-C29-C30-C31
18	2	305	CHL	CAA-CBA-CGA-O1A
19	A	821	CLA	CAA-CBA-CGA-O1A
19	B	835	CLA	CAA-CBA-CGA-O2A
27	G	202	LMU	C2-C3-C4-C5
19	A	820	CLA	C10-C11-C12-C13
23	L	305	BCR	C11-C10-C9-C8
19	A	823	CLA	CAA-CBA-CGA-O1A
19	3	304	CLA	CAA-CBA-CGA-O1A
19	A	837	CLA	CAA-CBA-CGA-O1A
28	B	849	DGD	C1G-C2G-C3G-O3G
28	B	849	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	808	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	CAA-CBA-CGA-O1A
19	6	312	CLA	C11-C10-C8-C9
19	A	841	CLA	C14-C13-C15-C16
19	A	826	CLA	C11-C10-C8-C7
19	B	811	CLA	C11-C12-C13-C15
19	3	313	CLA	CAA-CBA-CGA-O1A
19	6	302	CLA	C2B-C3B-CAB-CBB
19	6	303	CLA	C2B-C3B-CAB-CBB
19	6	309	CLA	C2B-C3B-CAB-CBB
19	6	311	CLA	C2B-C3B-CAB-CBB
19	2	302	CLA	C2B-C3B-CAB-CBB
19	2	304	CLA	C2B-C3B-CAB-CBB
19	2	309	CLA	C2B-C3B-CAB-CBB
19	2	311	CLA	C2B-C3B-CAB-CBB
19	2	313	CLA	C2B-C3B-CAB-CBB
19	3	301	CLA	C2B-C3B-CAB-CBB
19	3	303	CLA	C2B-C3B-CAB-CBB
19	3	304	CLA	C2B-C3B-CAB-CBB
19	3	308	CLA	C2B-C3B-CAB-CBB
19	3	312	CLA	C2B-C3B-CAB-CBB
19	5	301	CLA	C2B-C3B-CAB-CBB
19	5	303	CLA	C2B-C3B-CAB-CBB
19	5	308	CLA	C2B-C3B-CAB-CBB
19	5	310	CLA	C2B-C3B-CAB-CBB
19	5	314	CLA	C2B-C3B-CAB-CBB
19	A	801	CLA	C2B-C3B-CAB-CBB
19	A	813	CLA	C2B-C3B-CAB-CBB
19	A	814	CLA	C2B-C3B-CAB-CBB
19	A	817	CLA	C2B-C3B-CAB-CBB
19	A	822	CLA	C2B-C3B-CAB-CBB
19	A	826	CLA	C2B-C3B-CAB-CBB
19	A	830	CLA	C2B-C3B-CAB-CBB
19	A	833	CLA	C2B-C3B-CAB-CBB
19	A	838	CLA	C2B-C3B-CAB-CBB
19	A	840	CLA	C2B-C3B-CAB-CBB
19	A	843	CLA	C2B-C3B-CAB-CBB
19	B	802	CLA	C2B-C3B-CAB-CBB
19	B	813	CLA	C2B-C3B-CAB-CBB
19	B	821	CLA	C2B-C3B-CAB-CBB
19	B	829	CLA	C2B-C3B-CAB-CBB
19	B	832	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	B	836	CLA	C2B-C3B-CAB-CBB
19	B	837	CLA	C2B-C3B-CAB-CBB
19	B	838	CLA	C2B-C3B-CAB-CBB
19	B	839	CLA	C2B-C3B-CAB-CBB
19	F	303	CLA	C2B-C3B-CAB-CBB
19	G	204	CLA	C2B-C3B-CAB-CBB
19	K	201	CLA	C2B-C3B-CAB-CBB
19	K	203	CLA	C2B-C3B-CAB-CBB
19	L	301	CLA	C2B-C3B-CAB-CBB
19	L	303	CLA	C2B-C3B-CAB-CBB
20	3	315	LUT	C1-C6-C7-C8
20	3	316	LUT	C5-C6-C7-C8
20	5	316	LUT	C5-C6-C7-C8
23	A	848	BCR	C1-C6-C7-C8
23	A	849	BCR	C1-C6-C7-C8
23	G	201	BCR	C23-C24-C25-C30
19	A	818	CLA	C2-C1-O2A-CGA
19	A	828	CLA	C2-C1-O2A-CGA
19	B	841	CLA	C2-C1-O2A-CGA
19	B	811	CLA	CAA-CBA-CGA-O2A
19	G	203	CLA	CAA-CBA-CGA-O2A
19	A	836	CLA	C5-C6-C7-C8
19	A	814	CLA	CAA-CBA-CGA-O2A
19	B	840	CLA	CAA-CBA-CGA-O2A
19	B	815	CLA	C2-C3-C5-C6
18	6	306	CHL	CAA-CBA-CGA-O2A
19	K	201	CLA	CAA-CBA-CGA-O2A
19	3	307	CLA	C3-C5-C6-C7
22	5	318	LHG	C16-C17-C18-C19
28	B	849	DGD	O6D-C5D-C6D-O5D
28	B	849	DGD	C4B-C5B-C6B-C7B
19	5	307	CLA	CAA-CBA-CGA-O2A
19	B	833	CLA	C15-C16-C17-C18
19	B	807	CLA	CAA-CBA-CGA-O2A
19	2	303	CLA	C1A-C2A-CAA-CBA
19	3	310	CLA	C4B-C3B-CAB-CBB
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	806	CLA	C1A-C2A-CAA-CBA
19	3	311	CLA	C4-C3-C5-C6
22	6	317	LHG	C31-C32-C33-C34
19	5	314	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	5	314	CLA	CAA-CBA-CGA-O2A
20	3	315	LUT	C7-C8-C9-C10
23	A	848	BCR	C7-C8-C9-C10
19	5	307	CLA	C5-C6-C7-C8
19	6	303	CLA	CAA-CBA-CGA-O2A
19	5	302	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	C2A-CAA-CBA-CGA
22	A	846	LHG	C10-C11-C12-C13
18	2	301	CHL	C2-C1-O2A-CGA
19	A	801	CLA	C2-C1-O2A-CGA
19	B	801	CLA	C2-C1-O2A-CGA
19	B	803	CLA	C2-C1-O2A-CGA
18	6	301	CHL	CAA-CBA-CGA-O2A
19	A	820	CLA	C6-C7-C8-C10
19	B	838	CLA	C2-C3-C5-C6
19	G	203	CLA	CAA-CBA-CGA-O1A
19	B	823	CLA	O2A-C1-C2-C3
19	B	839	CLA	CAA-CBA-CGA-O2A
22	5	318	LHG	C10-C11-C12-C13
19	6	302	CLA	C2A-CAA-CBA-CGA
22	2	318	LHG	C12-C13-C14-C15
19	6	309	CLA	C15-C16-C17-C18
19	B	811	CLA	CAA-CBA-CGA-O1A
19	2	303	CLA	C3A-C2A-CAA-CBA
19	3	311	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
28	B	849	DGD	C5B-C6B-C7B-C8B
28	B	849	DGD	CCB-CDB-CEB-CFB
19	K	201	CLA	CAA-CBA-CGA-O1A
19	B	840	CLA	CAA-CBA-CGA-O1A
19	L	302	CLA	C5-C6-C7-C8
19	A	820	CLA	C11-C12-C13-C14
19	B	817	CLA	C6-C7-C8-C9
22	A	846	LHG	C11-C10-C9-C8
19	A	808	CLA	CAA-CBA-CGA-O1A
19	A	814	CLA	CAA-CBA-CGA-O1A
22	A	846	LHG	C13-C14-C15-C16
19	5	312	CLA	C10-C11-C12-C13
19	5	302	CLA	CAA-CBA-CGA-O1A
19	A	807	CLA	C2A-CAA-CBA-CGA
19	A	836	CLA	C8-C10-C11-C12
18	6	306	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	5	304	CHL	CAD-CBD-CGD-O2D
18	5	313	CHL	CAD-CBD-CGD-O2D
19	6	308	CLA	CAD-CBD-CGD-O2D
19	2	313	CLA	CAD-CBD-CGD-O2D
19	5	311	CLA	CAD-CBD-CGD-O2D
19	A	801	CLA	CAD-CBD-CGD-O2D
19	B	815	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	B	833	CLA	CAD-CBD-CGD-O2D
19	A	803	CLA	CAA-CBA-CGA-O2A
19	A	826	CLA	CAA-CBA-CGA-O2A
22	5	318	LHG	O8-C23-C24-C25
19	6	303	CLA	CAA-CBA-CGA-O1A
19	5	307	CLA	CAA-CBA-CGA-O1A
19	A	807	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
19	B	830	CLA	CAA-CBA-CGA-O2A
18	6	301	CHL	CAA-CBA-CGA-O1A
19	A	828	CLA	CAA-CBA-CGA-O2A
19	B	825	CLA	CAA-CBA-CGA-O2A
18	3	314	CHL	CAA-CBA-CGA-O2A
19	6	302	CLA	CAA-CBA-CGA-O2A
19	B	806	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

165 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	J	102	CLA	1	0
19	B	840	CLA	3	0
20	J	101	LUT	4	0
19	G	203	CLA	1	0
19	B	823	CLA	2	0
19	B	831	CLA	1	0
28	B	849	DGD	4	0
19	3	310	CLA	2	0
23	F	302	BCR	4	0
19	L	302	CLA	2	0
23	B	845	BCR	3	0
19	A	828	CLA	1	0
19	2	303	CLA	1	0
19	A	808	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	204	BCR	2	0
19	A	807	CLA	3	0
19	2	309	CLA	3	0
19	A	832	CLA	1	0
19	6	313	CLA	1	0
19	F	304	CLA	1	0
19	B	801	CLA	3	0
19	3	305	CLA	1	0
19	6	310	CLA	2	0
19	6	304	CLA	1	0
19	6	311	CLA	1	0
20	2	316	LUT	2	0
19	B	807	CLA	3	0
19	B	832	CLA	2	0
19	2	302	CLA	2	0
19	A	842	CLA	2	0
19	5	301	CLA	1	0
19	B	822	CLA	1	0
19	A	824	CLA	3	0
19	2	312	CLA	4	0
22	A	846	LHG	2	0
23	B	847	BCR	4	0
19	B	803	CLA	2	0
29	J	104	LMG	2	0
19	3	303	CLA	1	0
19	B	814	CLA	2	0
22	A	847	LHG	1	0
19	A	805	CLA	2	0
23	A	848	BCR	5	0
19	5	308	CLA	1	0
21	6	316	XAT	3	0
19	L	303	CLA	1	0
18	6	306	CHL	3	0
19	6	314	CLA	1	0
19	5	309	CLA	1	0
22	5	318	LHG	5	0
19	A	836	CLA	1	0
19	B	817	CLA	2	0
23	J	103	BCR	6	0
19	B	809	CLA	2	0
19	B	804	CLA	1	0
20	3	316	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	851	LMU	1	0
19	B	824	CLA	1	0
20	6	315	LUT	2	0
18	2	305	CHL	2	0
19	2	308	CLA	2	0
19	A	820	CLA	2	0
19	A	812	CLA	2	0
19	B	834	CLA	1	0
19	B	830	CLA	3	0
25	B	843	PQN	1	0
18	6	301	CHL	3	0
19	F	301	CLA	2	0
18	2	314	CHL	1	0
19	B	820	CLA	3	0
19	A	814	CLA	2	0
19	5	314	CLA	1	0
19	A	831	CLA	2	0
19	6	303	CLA	1	0
19	B	806	CLA	3	0
22	6	317	LHG	6	0
19	5	312	CLA	1	0
23	L	305	BCR	4	0
24	A	802	CL0	2	0
19	3	301	CLA	1	0
19	B	812	CLA	5	0
23	B	848	BCR	2	0
23	A	852	BCR	3	0
23	K	205	BCR	2	0
19	A	819	CLA	4	0
20	2	317	LUT	2	0
23	2	319	BCR	2	0
19	3	312	CLA	2	0
19	B	841	CLA	3	0
19	B	827	CLA	1	0
19	K	201	CLA	1	0
23	A	850	BCR	1	0
19	L	301	CLA	1	0
19	A	834	CLA	2	0
23	G	205	BCR	2	0
18	5	313	CHL	1	0
19	B	810	CLA	1	0
19	6	308	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	813	CLA	1	0
19	A	833	CLA	1	0
23	I	101	BCR	2	0
19	A	823	CLA	2	0
27	G	202	LMU	2	0
19	B	829	CLA	2	0
19	3	313	CLA	1	0
23	F	305	BCR	2	0
23	M	101	BCR	3	0
18	2	320	CHL	3	0
19	5	311	CLA	1	0
19	6	307	CLA	1	0
19	3	308	CLA	2	0
19	A	810	CLA	2	0
19	A	835	CLA	2	0
19	A	825	CLA	3	0
20	2	315	LUT	4	0
20	3	315	LUT	5	0
19	B	838	CLA	4	0
19	A	839	CLA	2	0
19	A	806	CLA	1	0
18	2	307	CHL	2	0
18	3	314	CHL	3	0
19	B	802	CLA	3	0
23	A	851	BCR	5	0
19	2	310	CLA	1	0
19	B	828	CLA	1	0
19	2	311	CLA	1	0
19	3	311	CLA	2	0
19	6	309	CLA	1	0
19	B	842	CLA	2	0
19	B	816	CLA	4	0
19	3	302	CLA	4	0
19	A	821	CLA	3	0
19	3	309	CLA	2	0
19	A	822	CLA	5	0
25	A	844	PQN	2	0
19	B	825	CLA	3	0
20	6	318	LUT	2	0
23	B	844	BCR	2	0
18	2	306	CHL	1	0
18	3	306	CHL	1	0

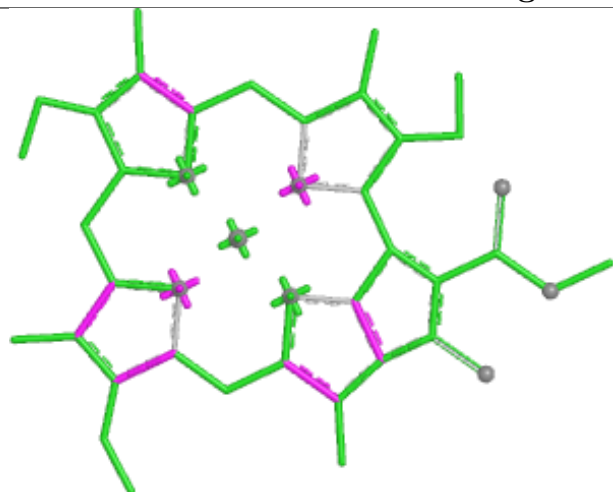
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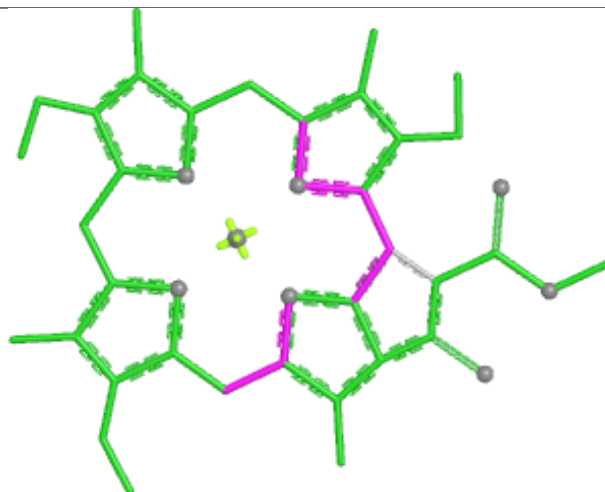
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	302	CLA	2	0
27	B	850	LMU	3	0
23	5	317	BCR	2	0
19	A	818	CLA	3	0
20	5	315	LUT	4	0
19	6	305	CLA	2	0
19	A	811	CLA	3	0
23	3	317	BCR	2	0
19	6	312	CLA	4	0
18	2	301	CHL	3	0
23	A	849	BCR	3	0
23	B	846	BCR	2	0
19	B	818	CLA	2	0
19	B	833	CLA	1	0
20	5	316	LUT	3	0
19	B	811	CLA	1	0
19	5	307	CLA	4	0
19	F	303	CLA	1	0
19	A	816	CLA	2	0
19	5	302	CLA	1	0
23	G	201	BCR	5	0
19	A	841	CLA	1	0
29	J	105	LMG	1	0
19	B	826	CLA	1	0
19	A	837	CLA	3	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.

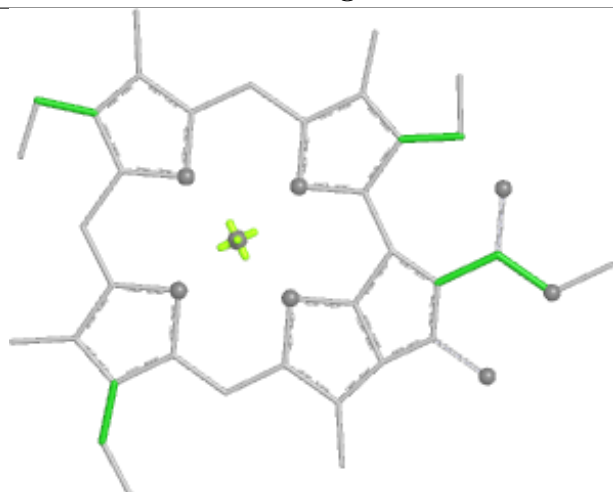
Ligand CLA J 102



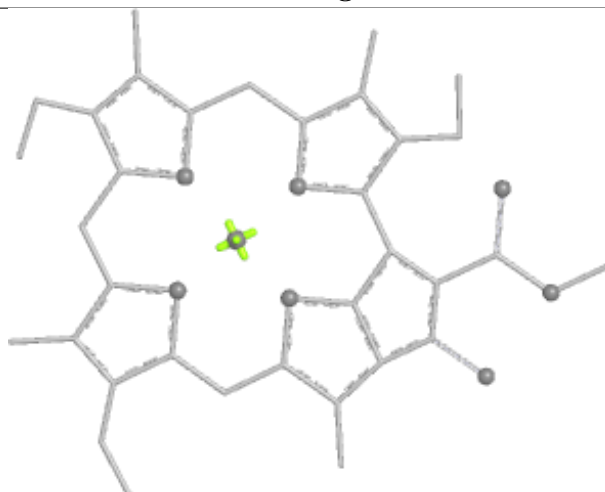
Bond lengths



Bond angles

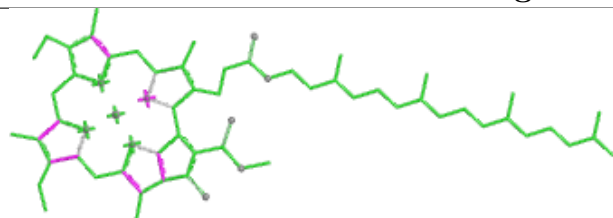


Torsions

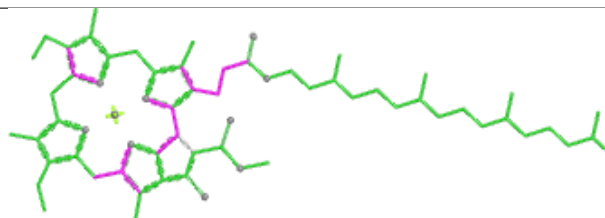


Rings

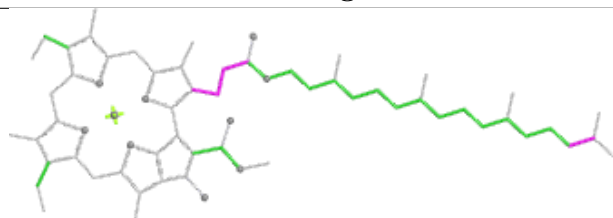
Ligand CLA B 840



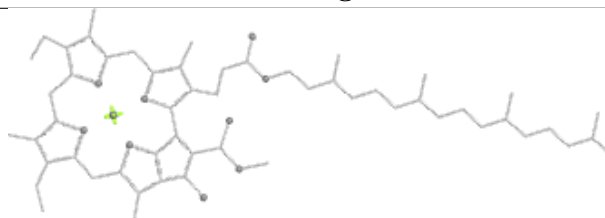
Bond lengths



Bond angles

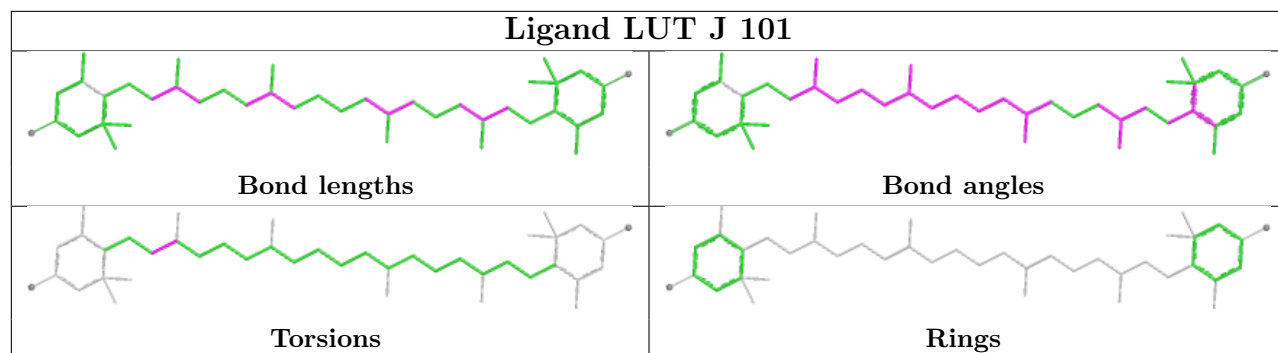


Torsions

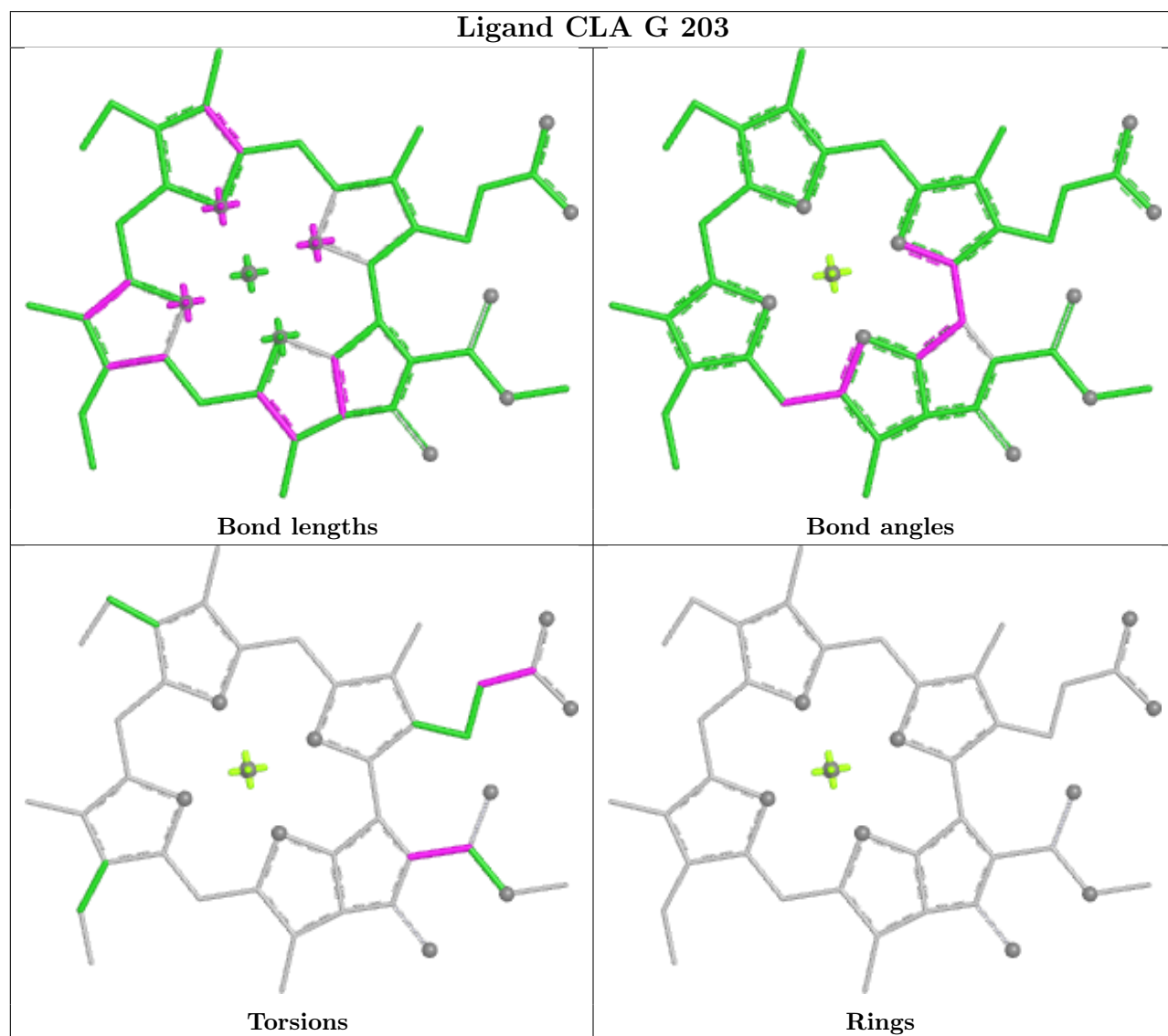


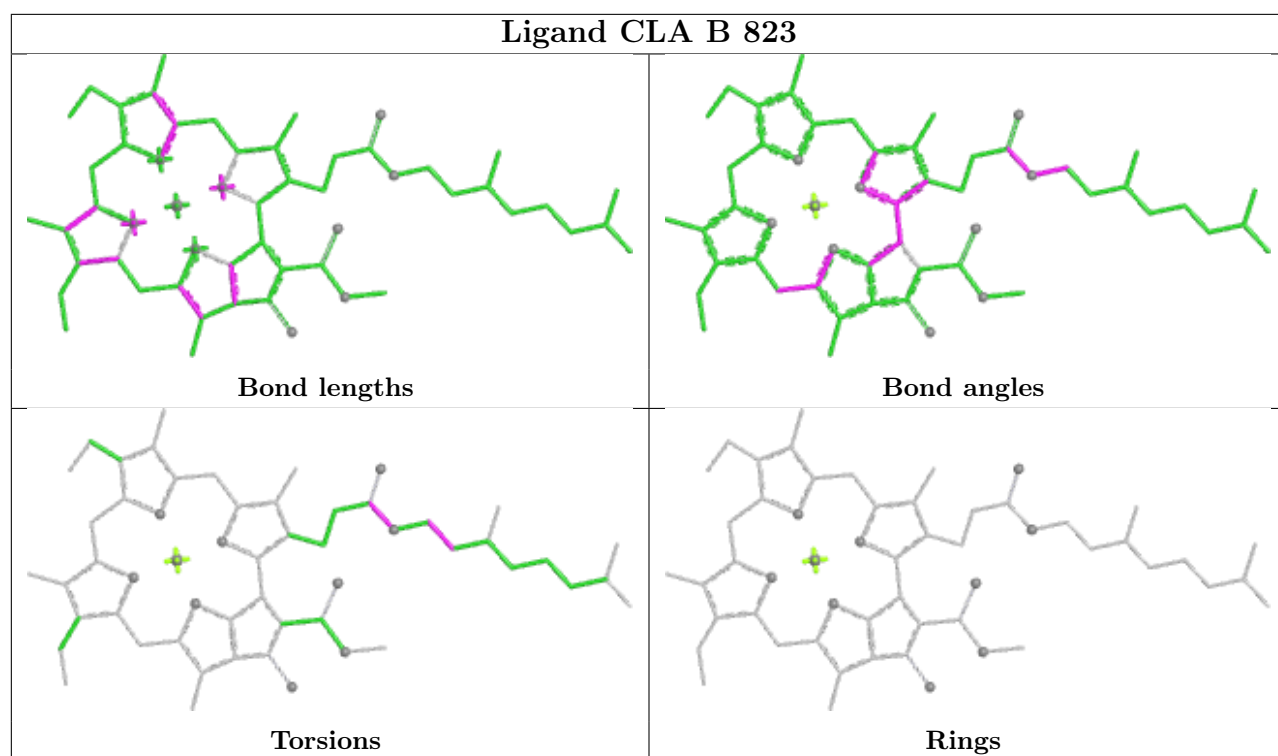
Rings

Ligand LUT J 101

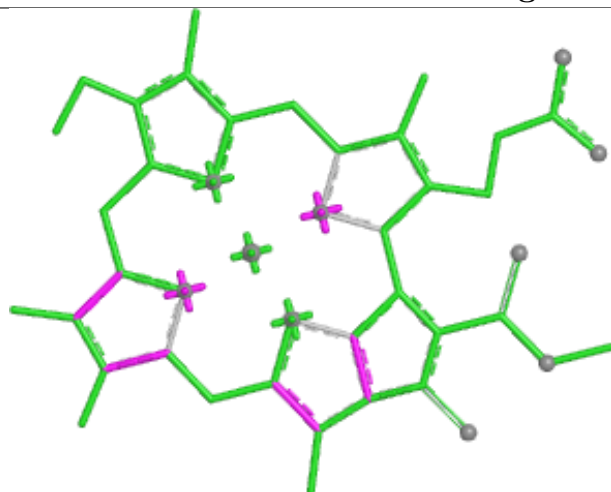


Ligand CLA G 203

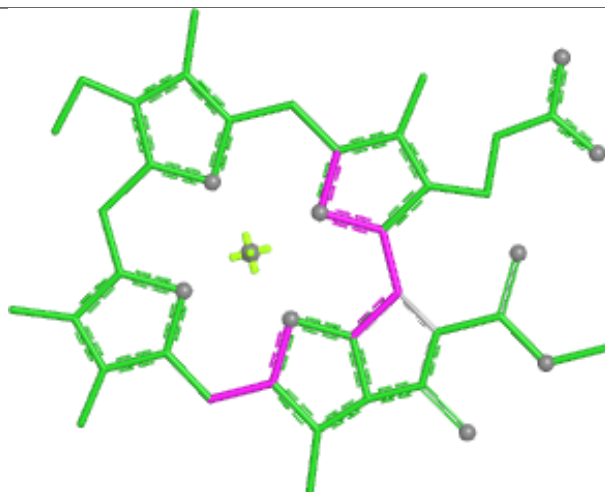




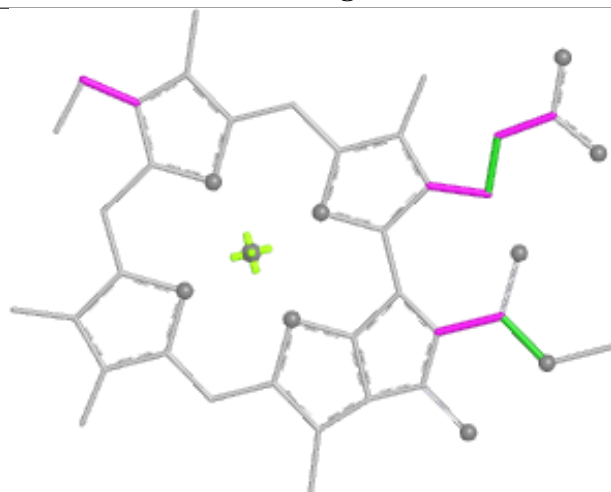
Ligand CLA 5 310



Bond lengths



Bond angles

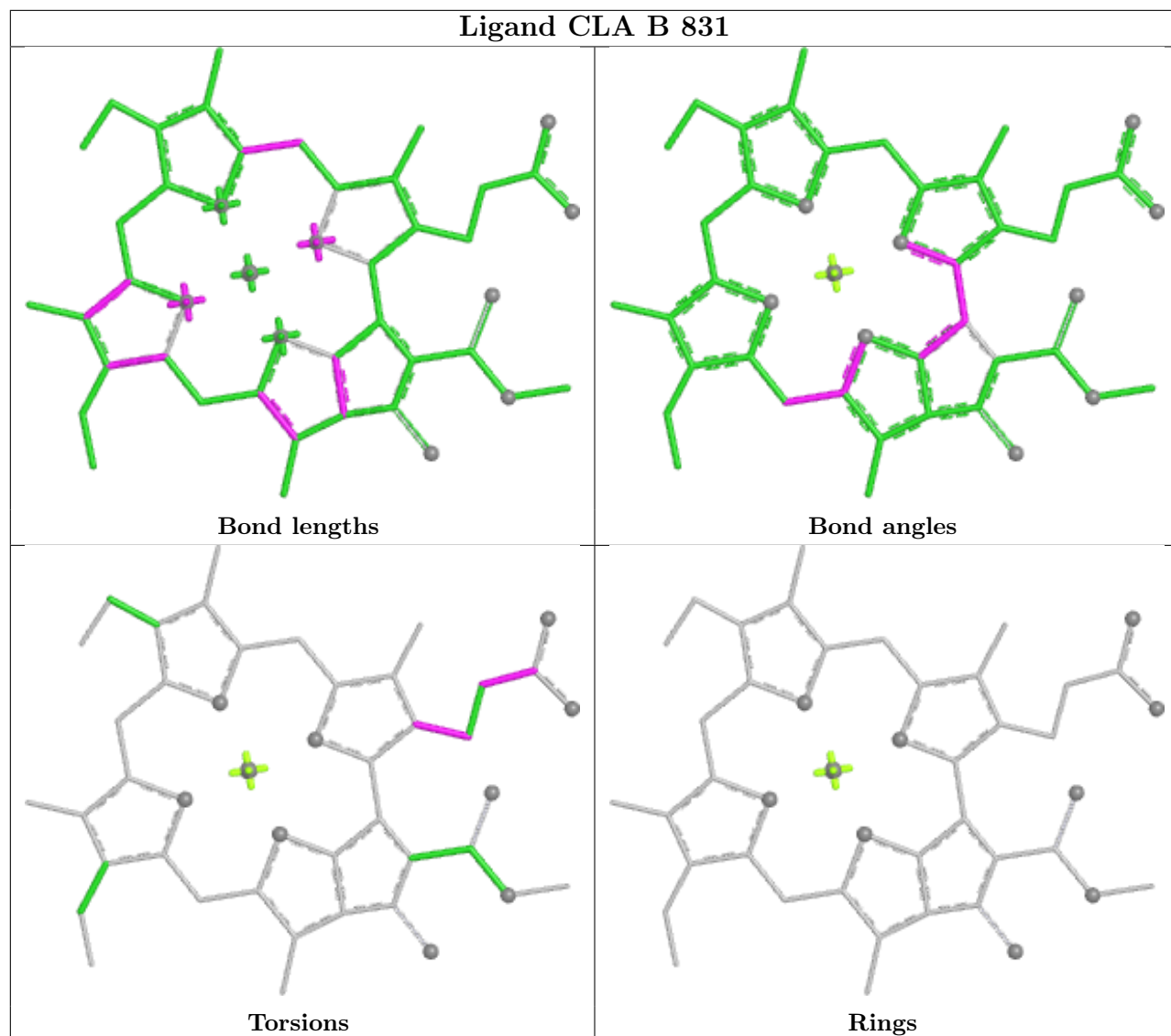


Torsions

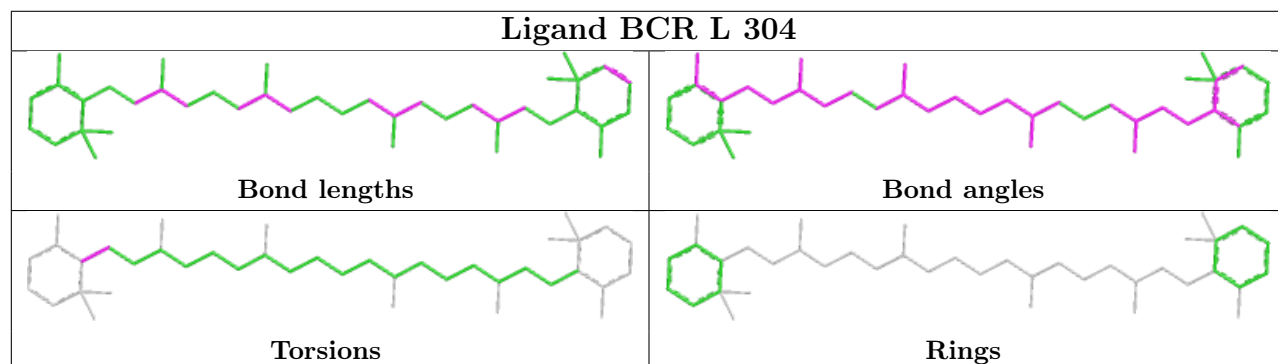


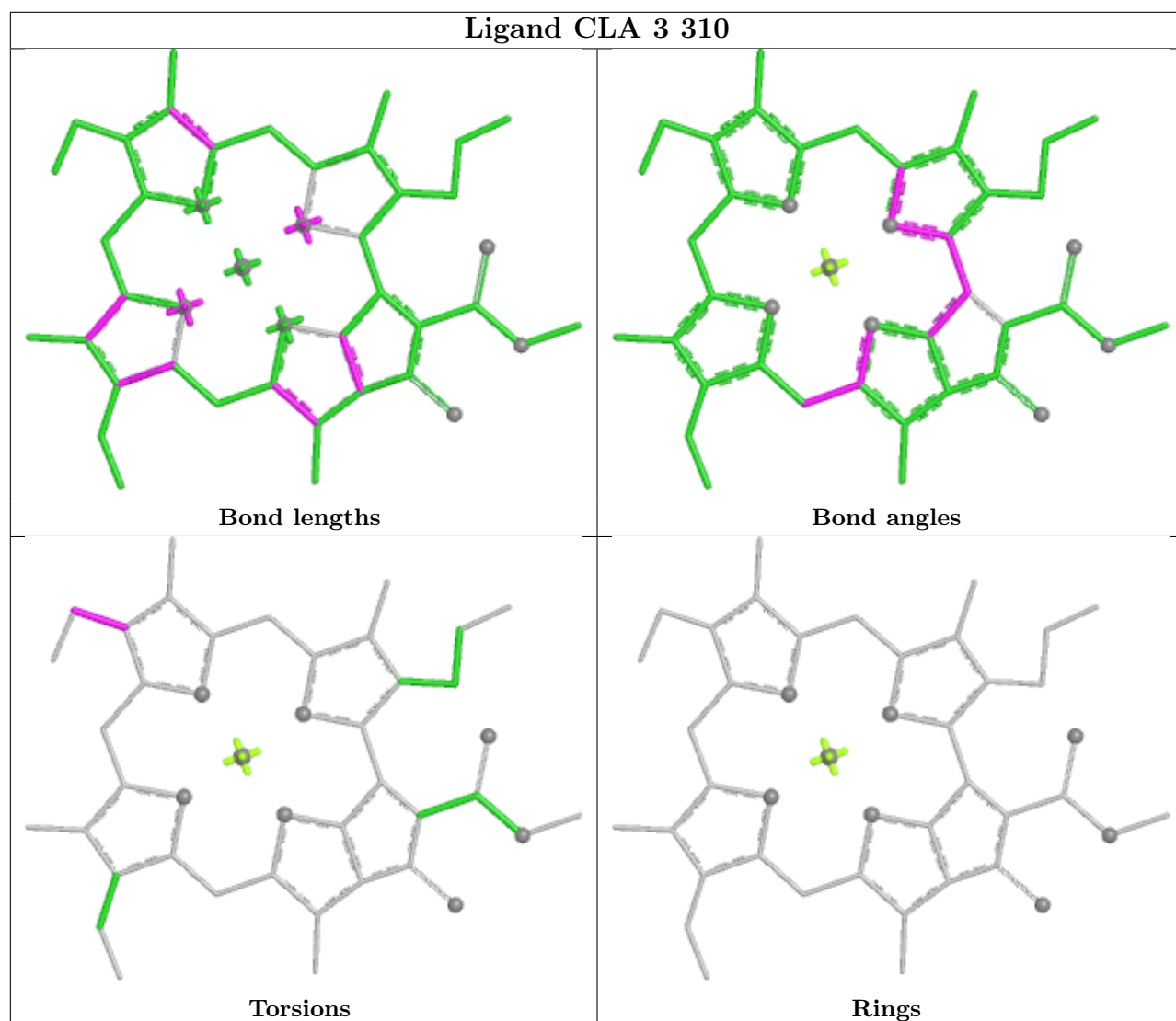
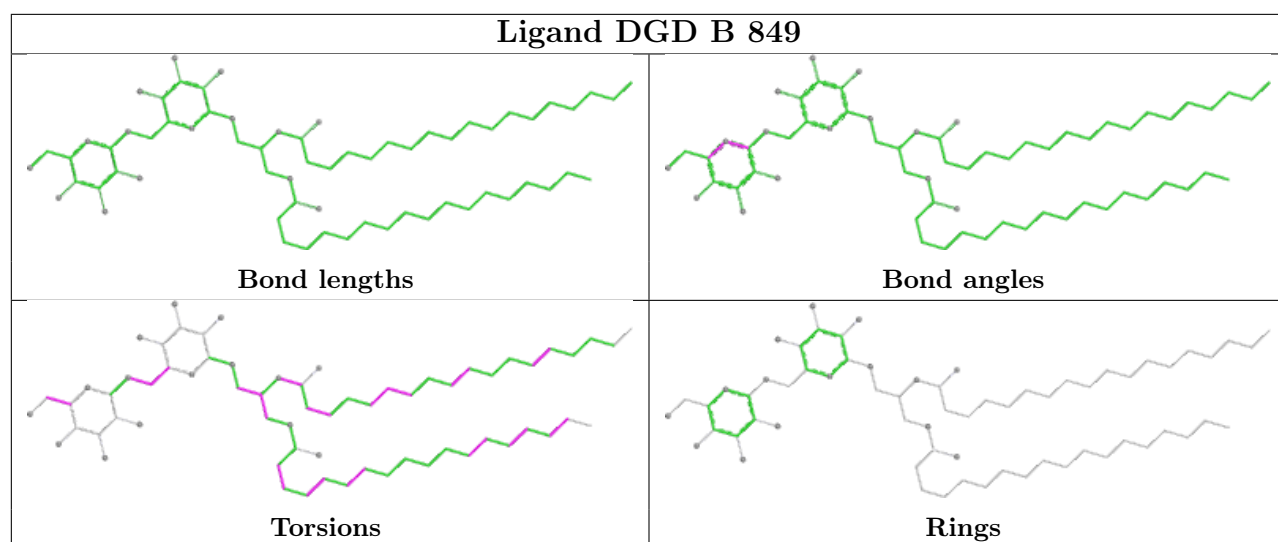
Rings

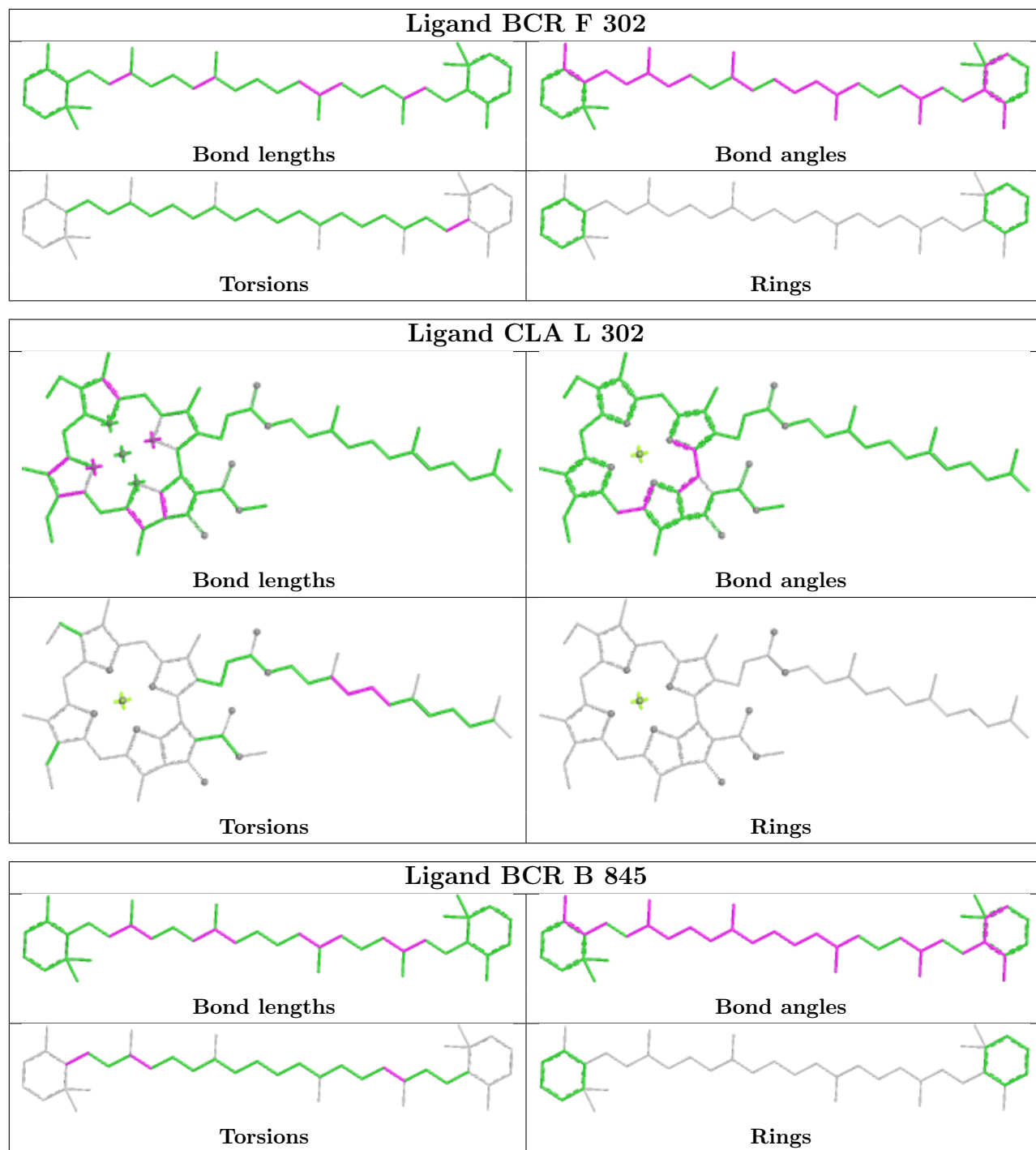
Ligand CLA B 831



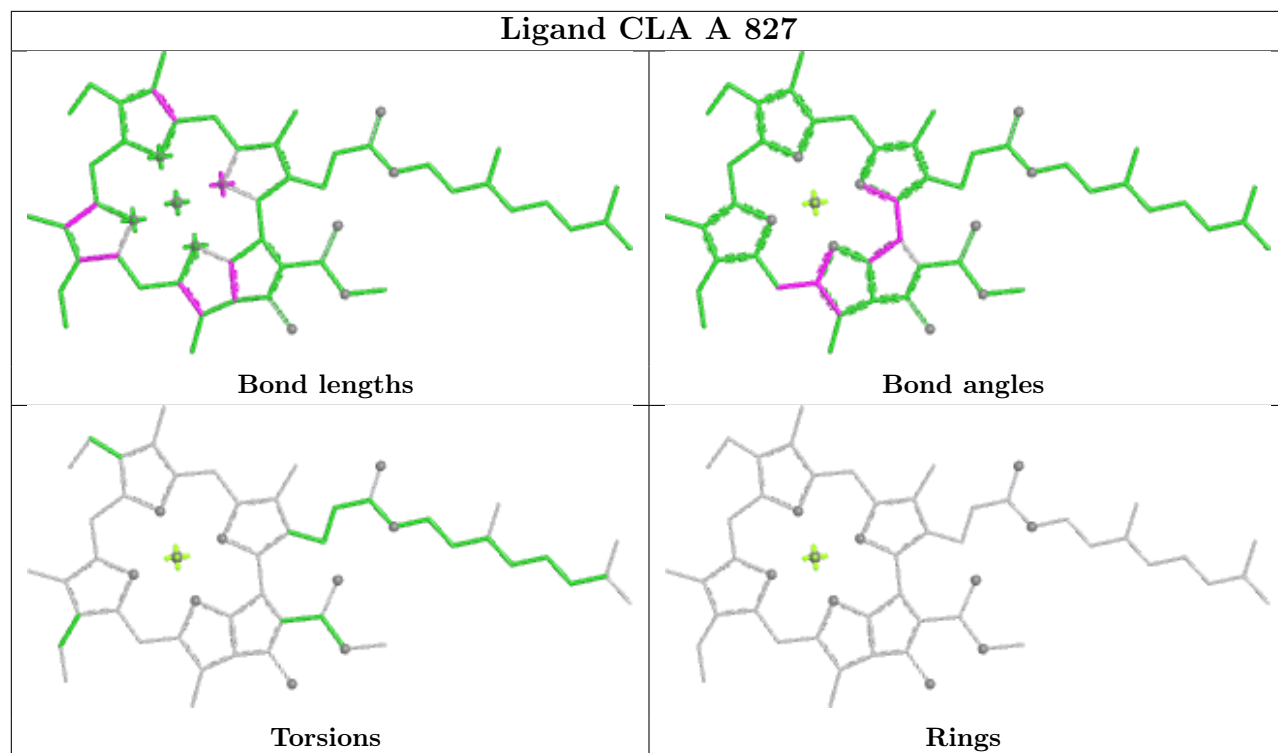
Ligand BCR L 304



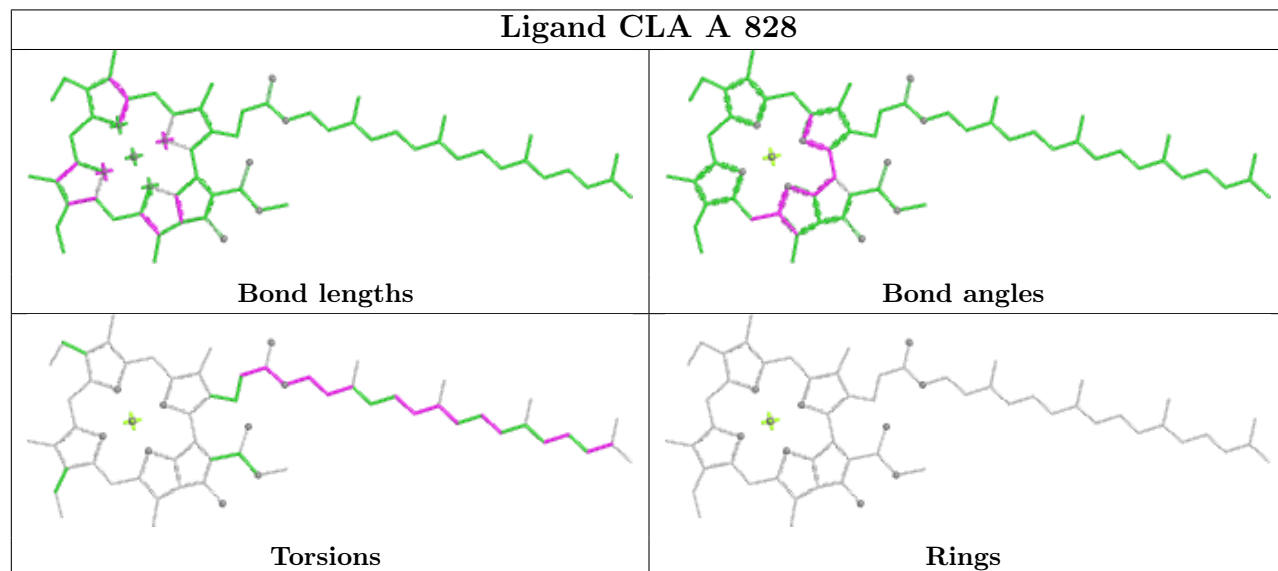




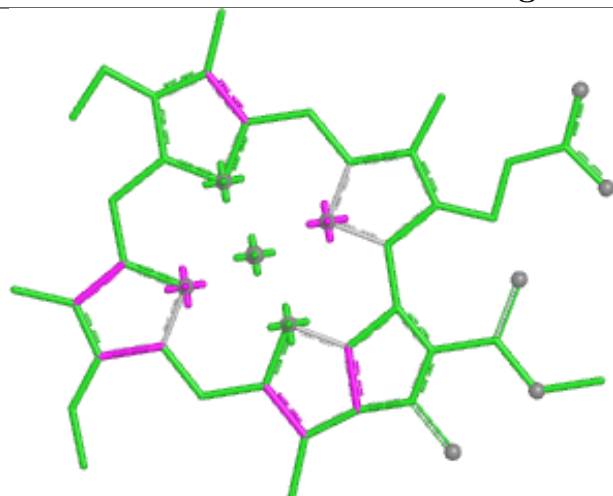
Ligand CLA A 827



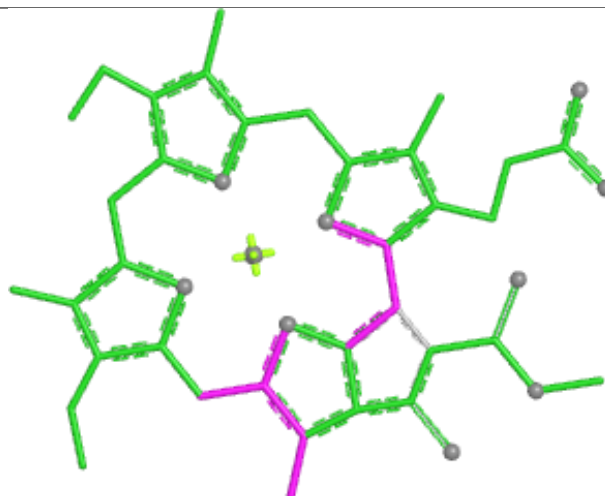
Ligand CLA A 828



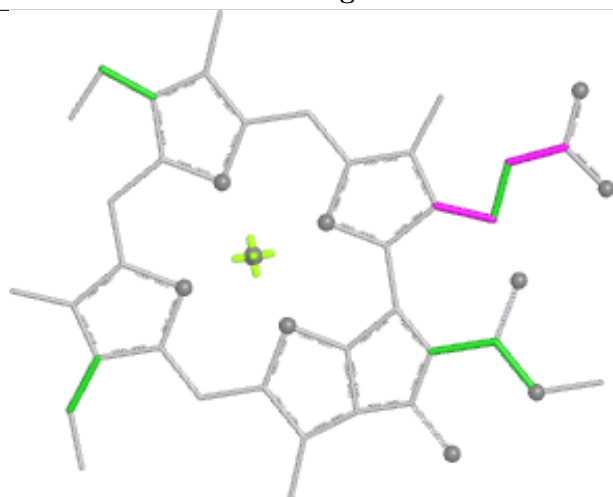
Ligand CLA 2 303



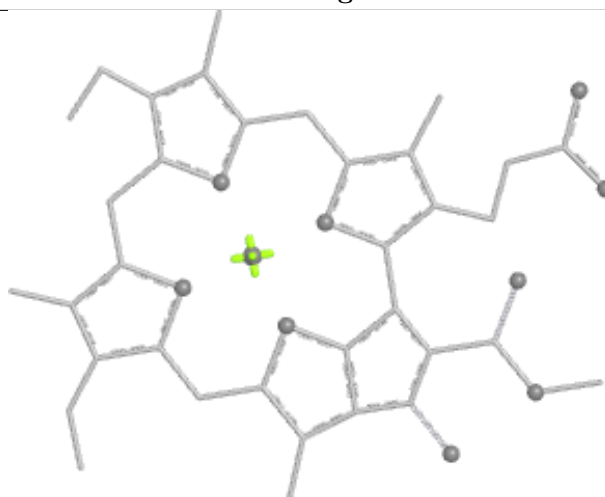
Bond lengths



Bond angles

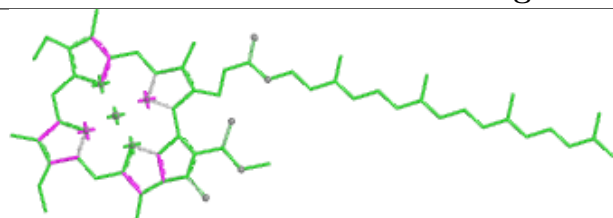


Torsions

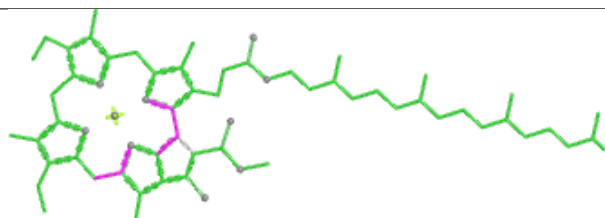


Rings

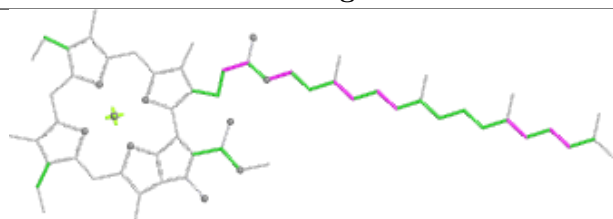
Ligand CLA A 808



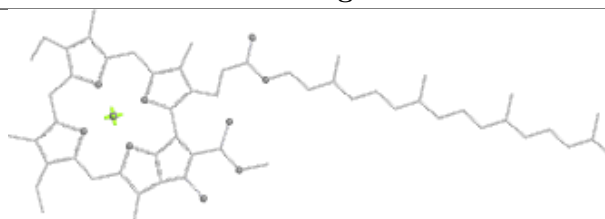
Bond lengths



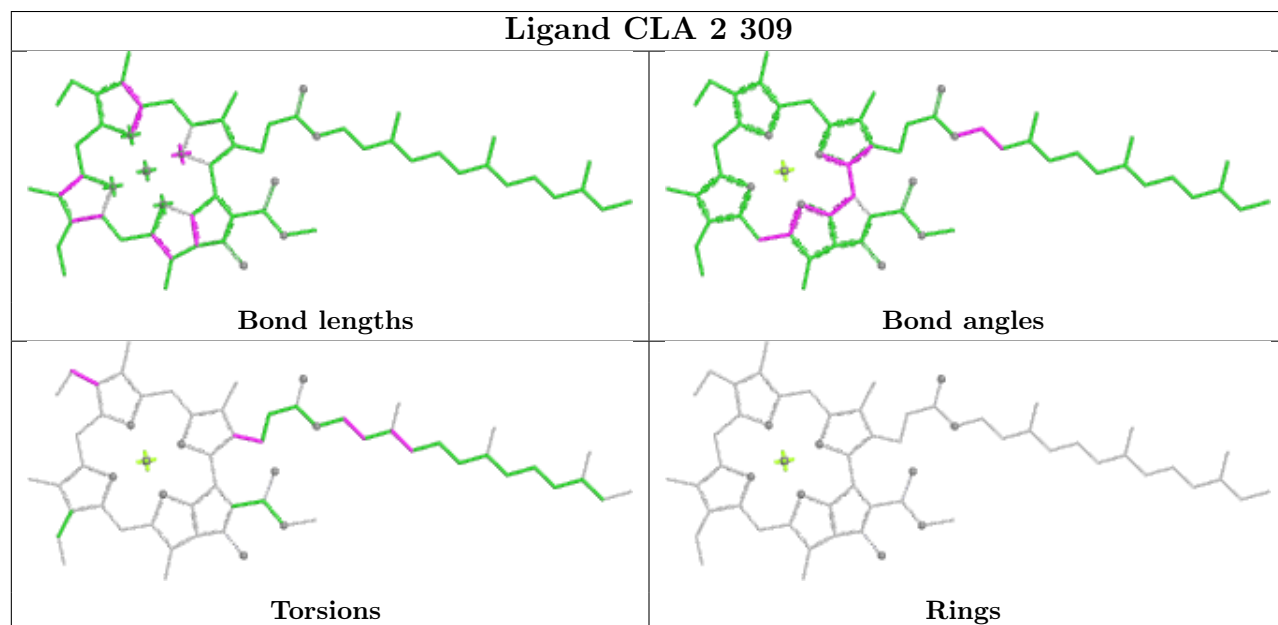
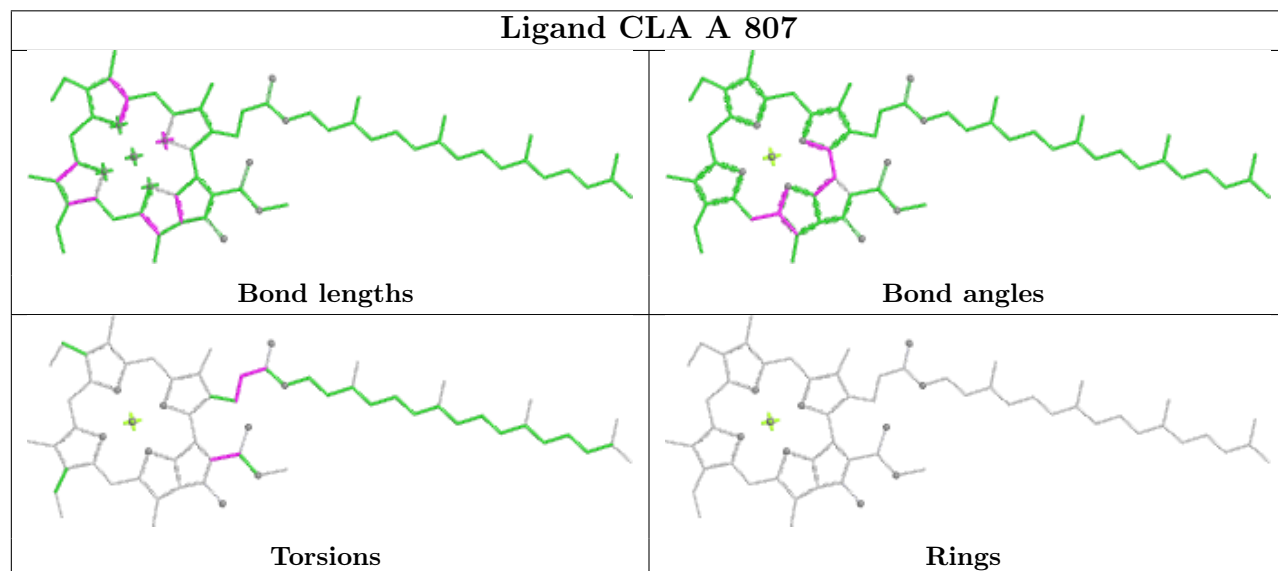
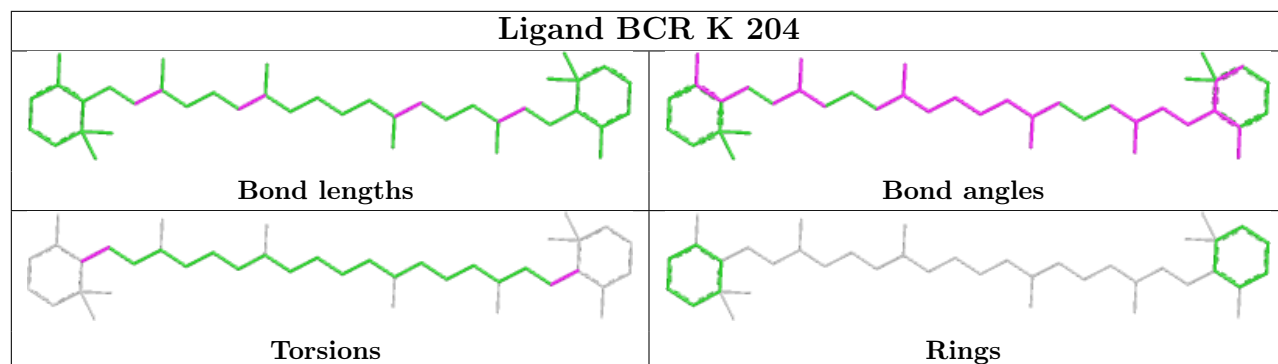
Bond angles

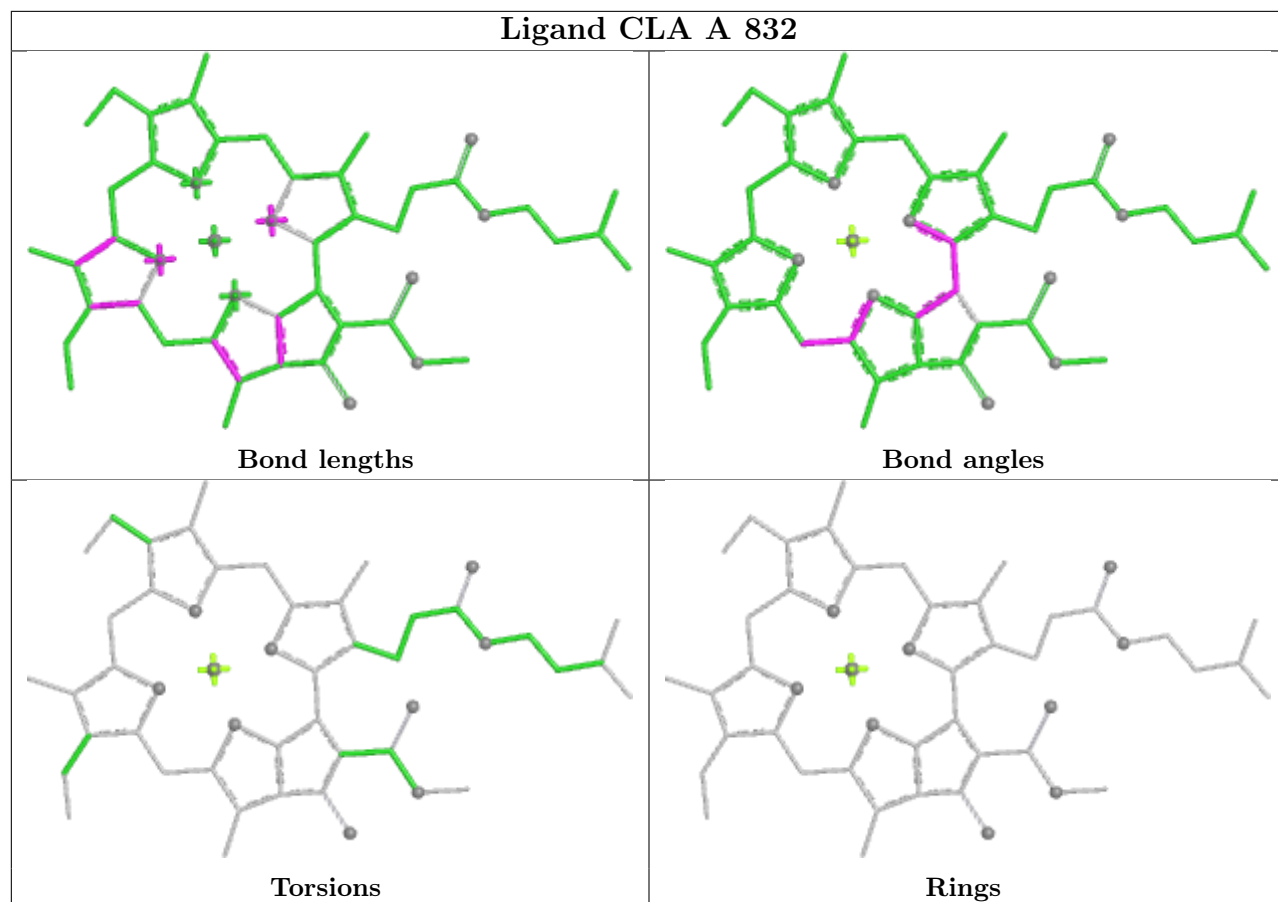


Torsions

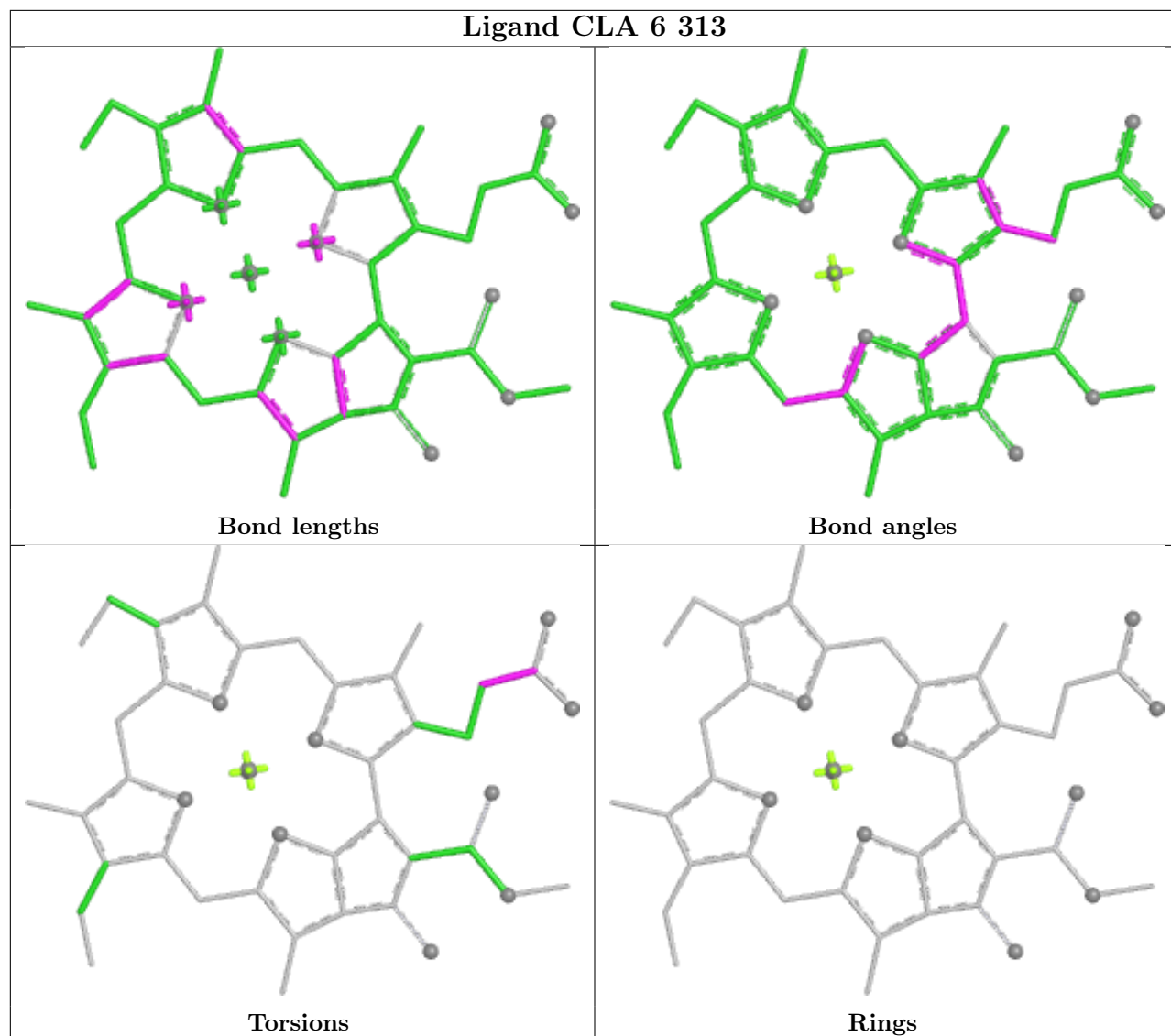


Rings

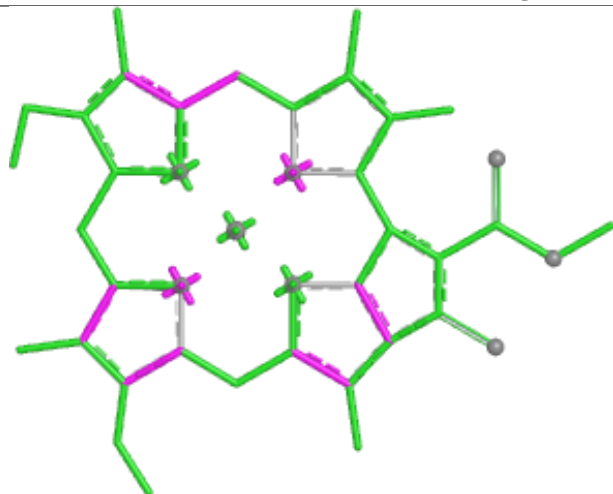




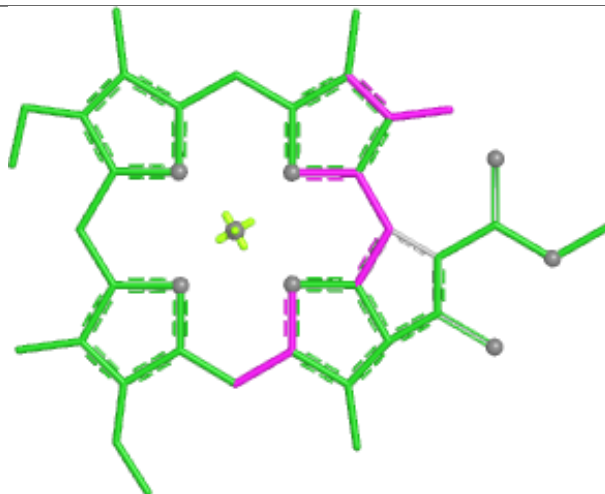
Ligand CLA 6 313



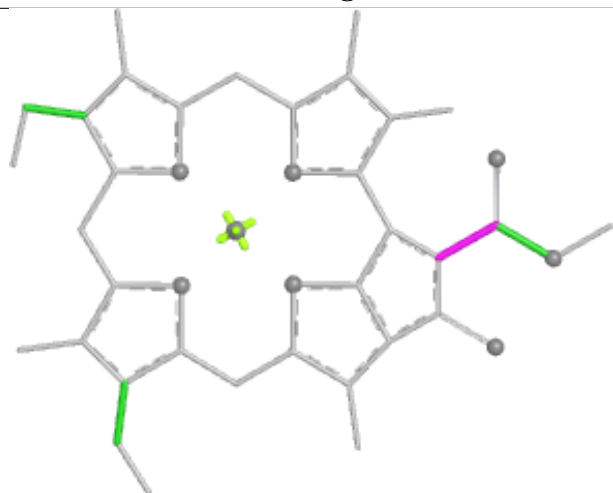
Ligand CLA F 304



Bond lengths



Bond angles

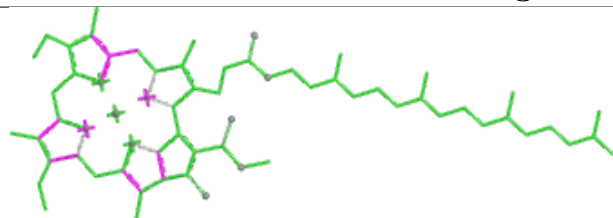


Torsions

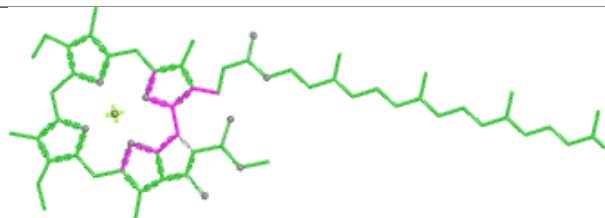


Rings

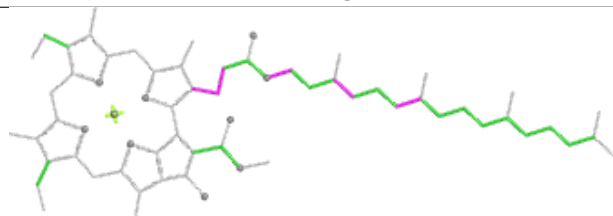
Ligand CLA B 801



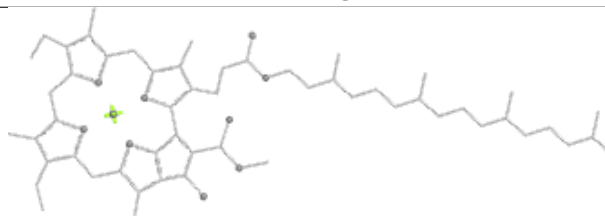
Bond lengths



Bond angles

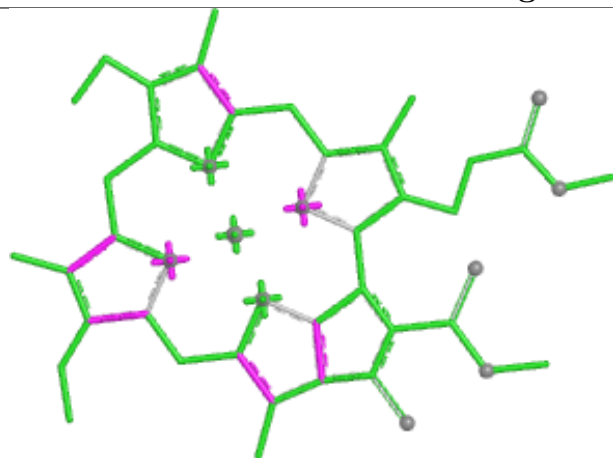


Torsions

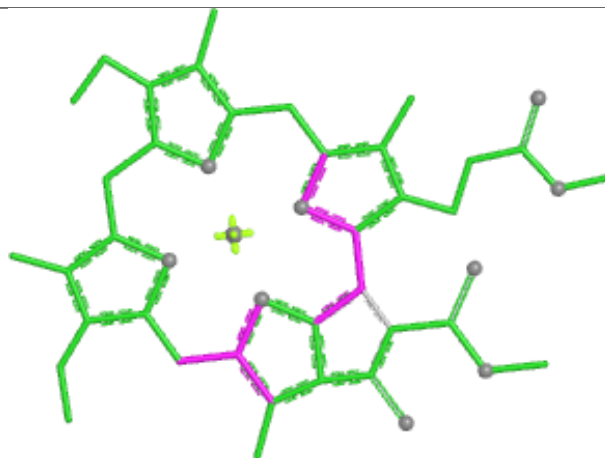


Rings

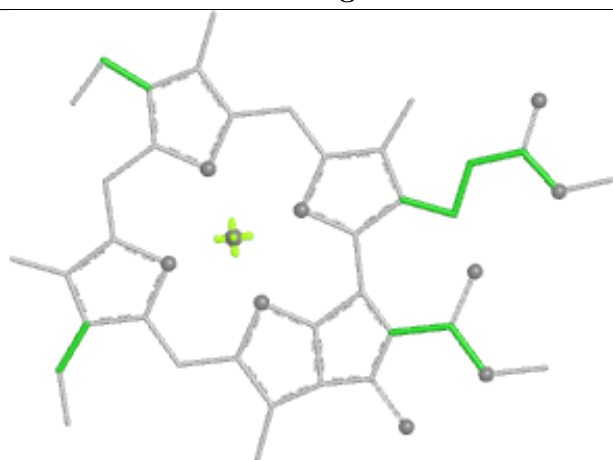
Ligand CLA 3 305



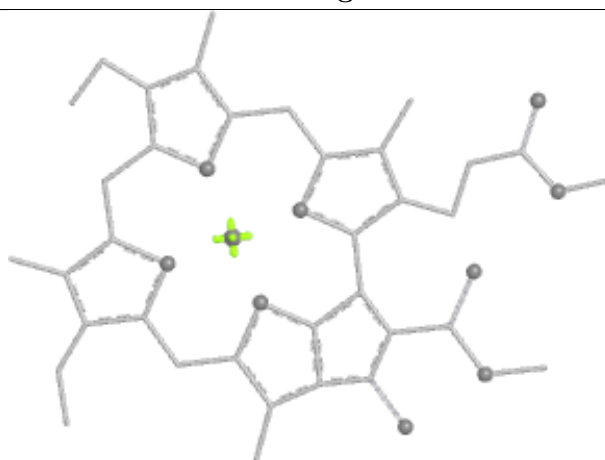
Bond lengths



Bond angles

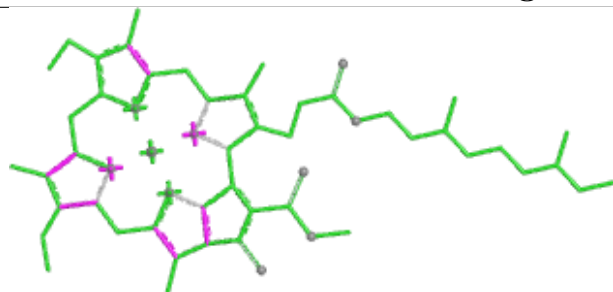


Torsions

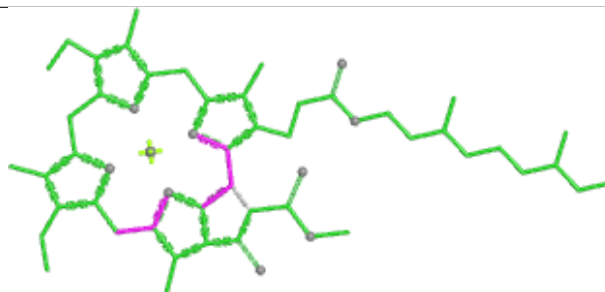


Rings

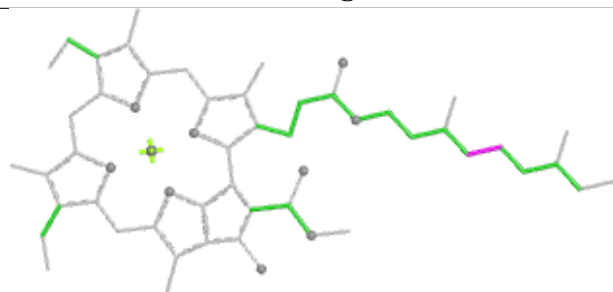
Ligand CLA 6 310



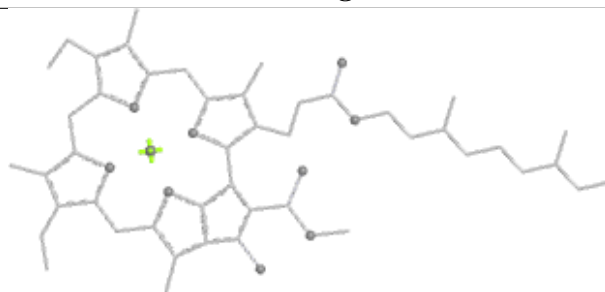
Bond lengths



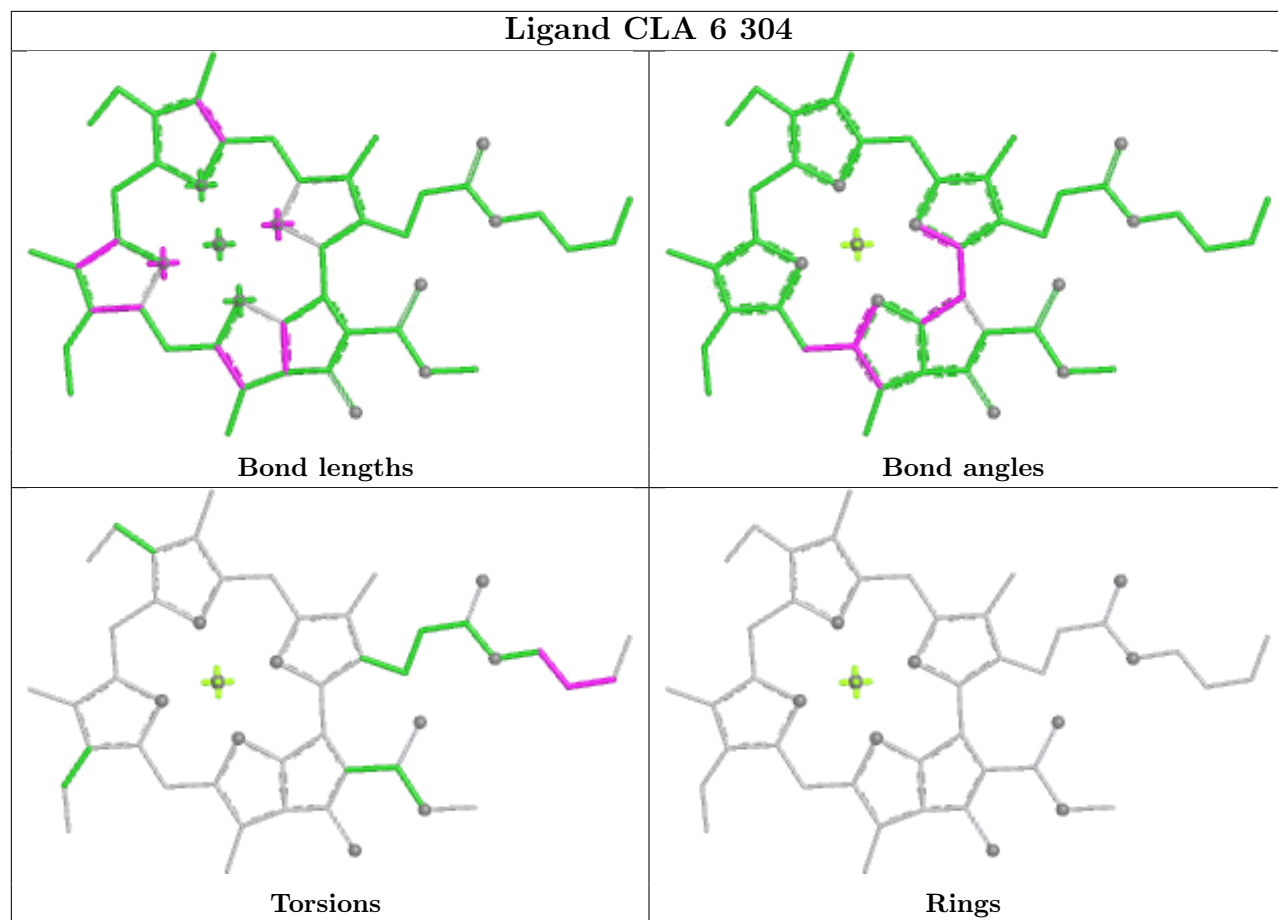
Bond angles



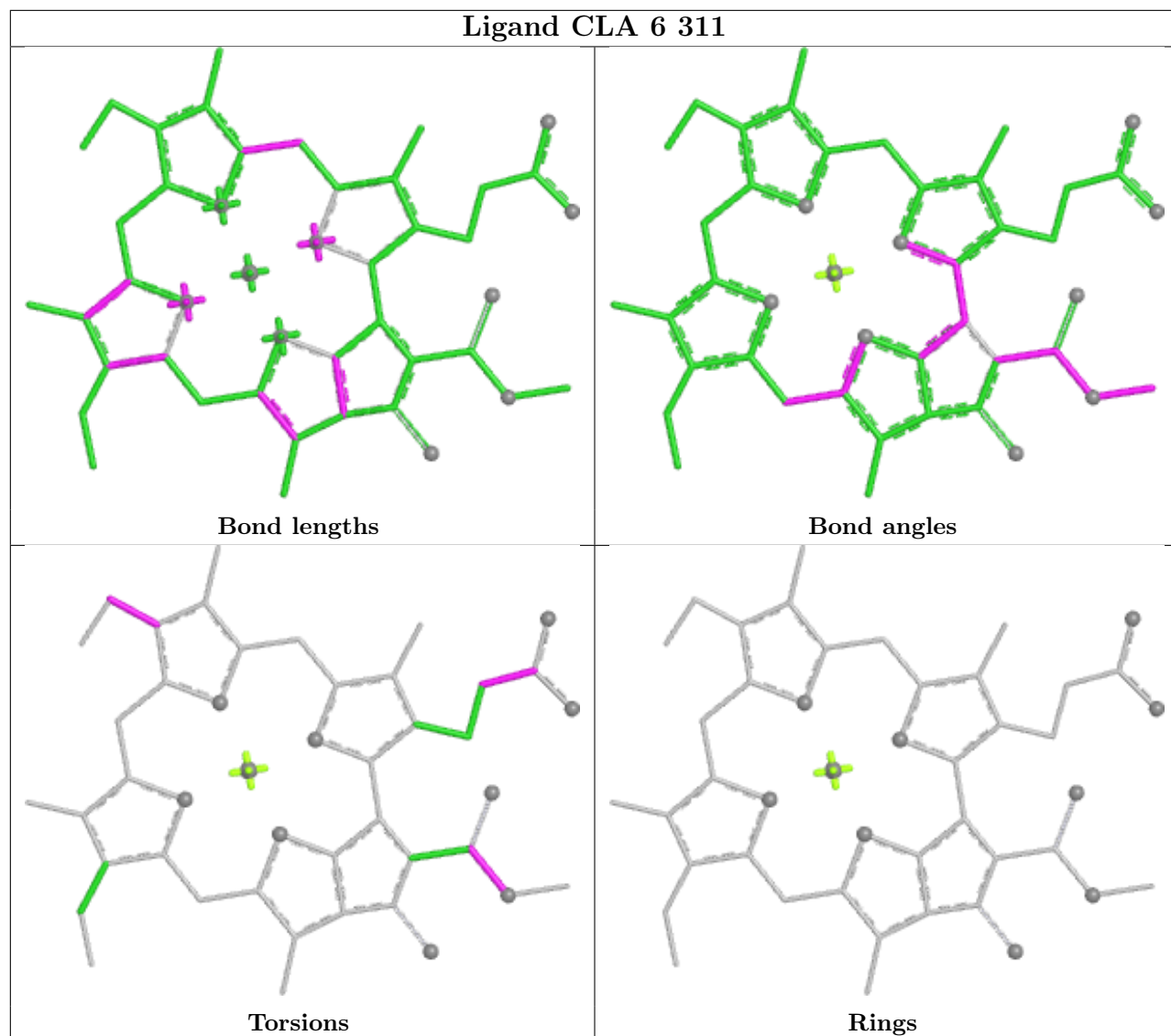
Torsions



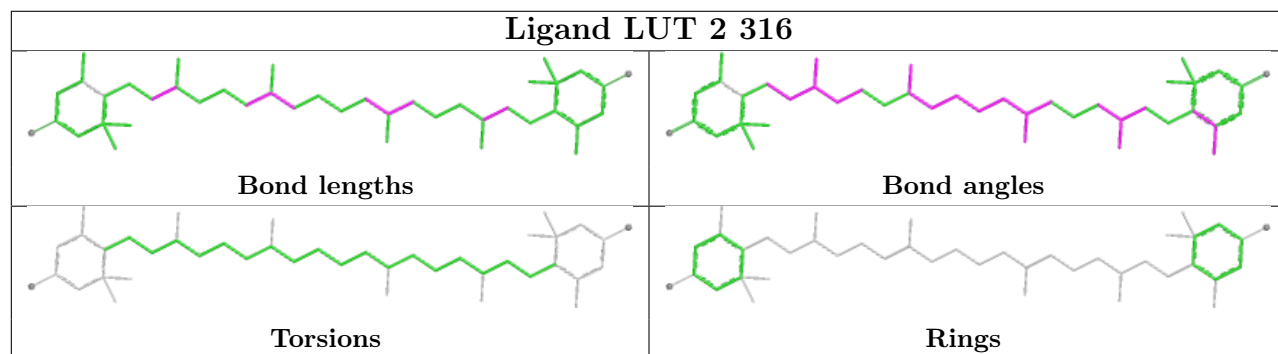
Rings

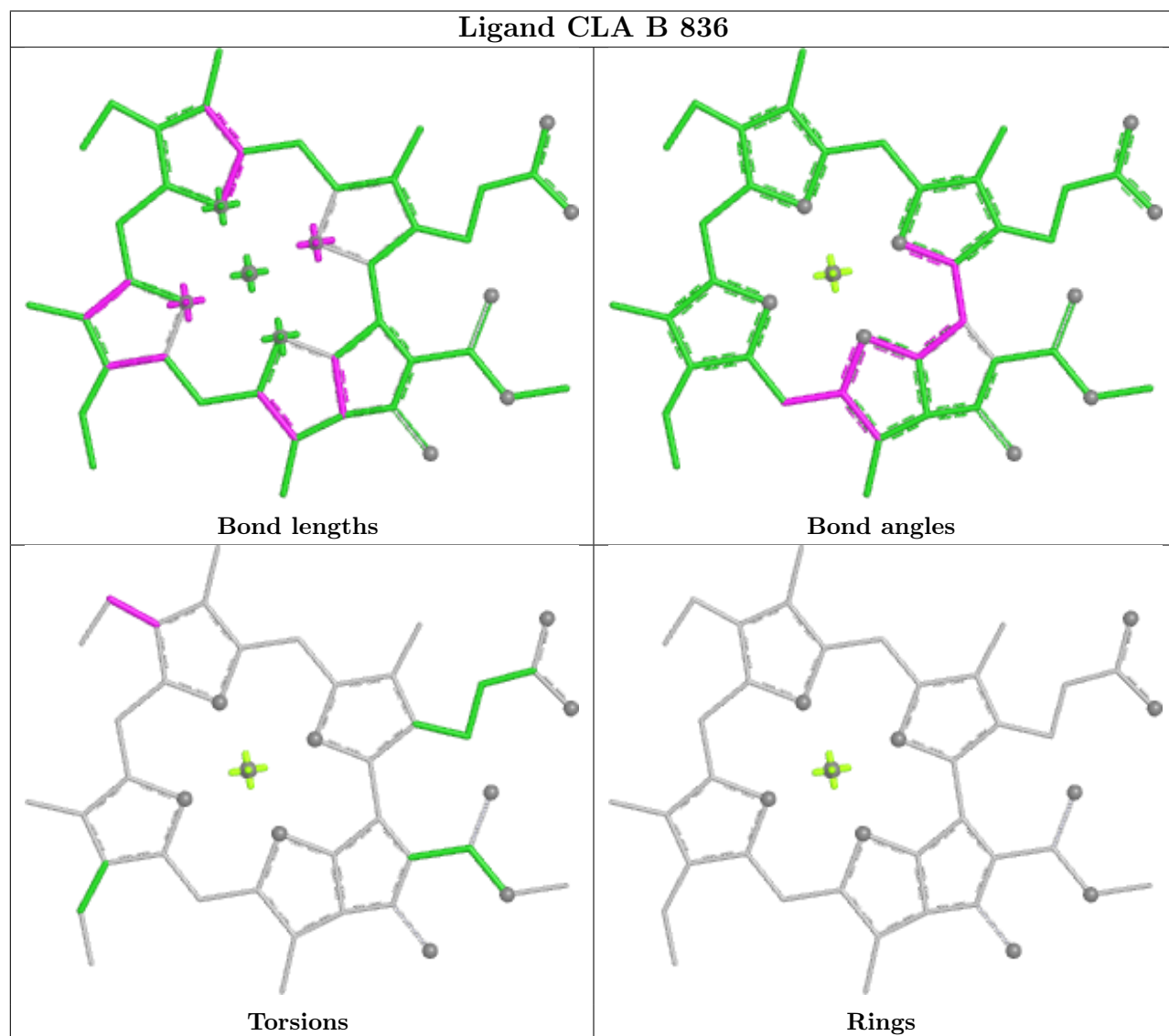
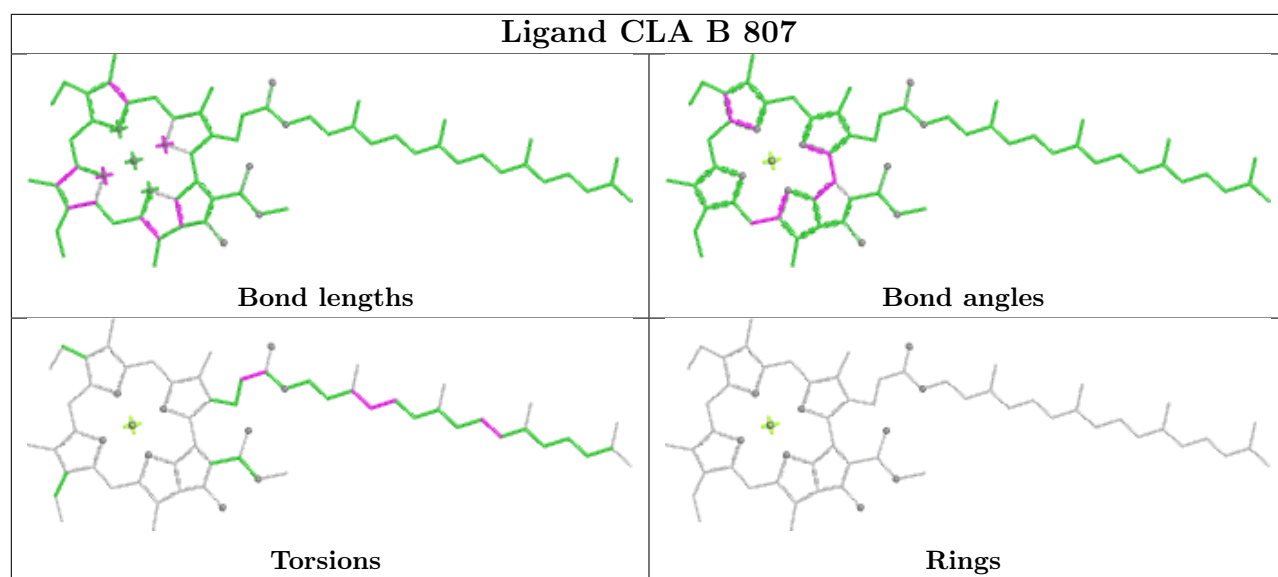


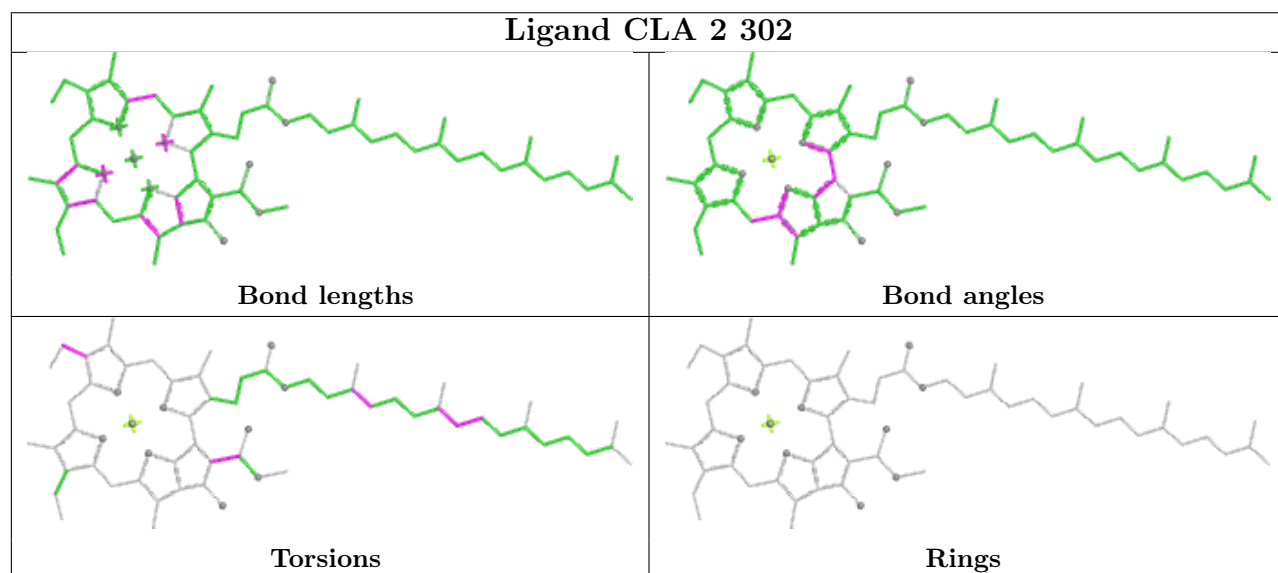
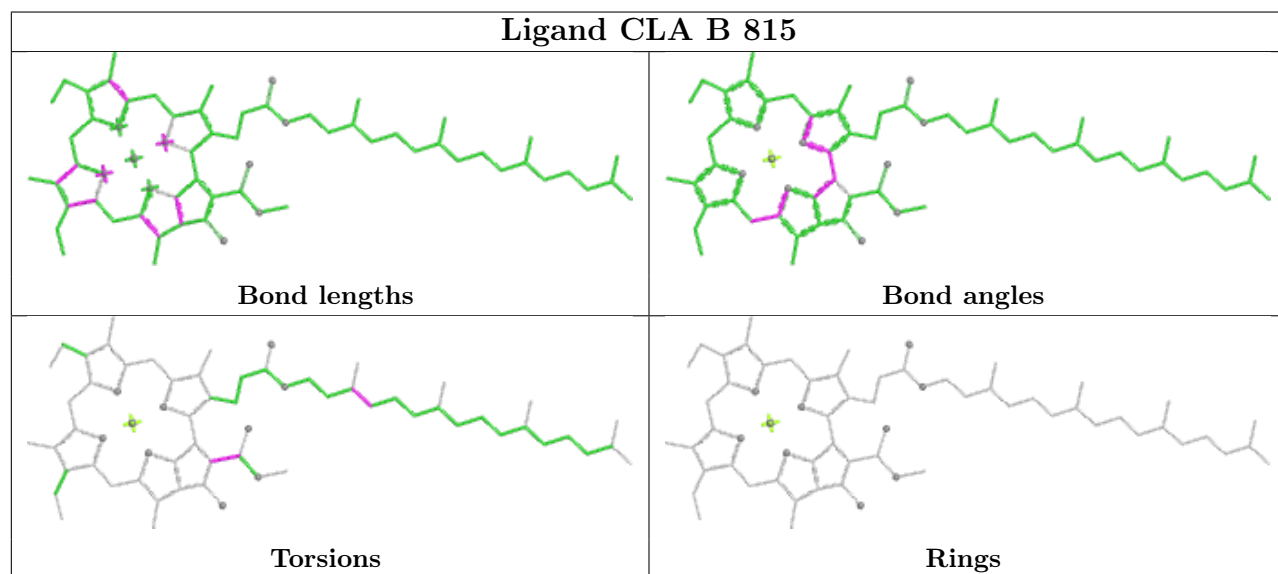
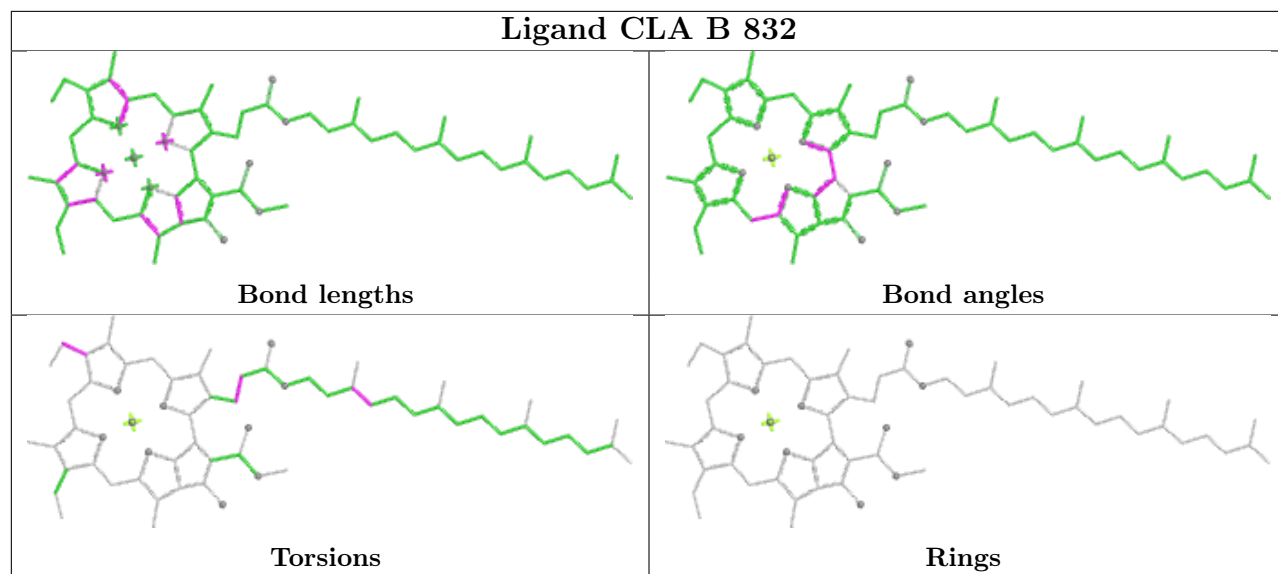
Ligand CLA 6 311

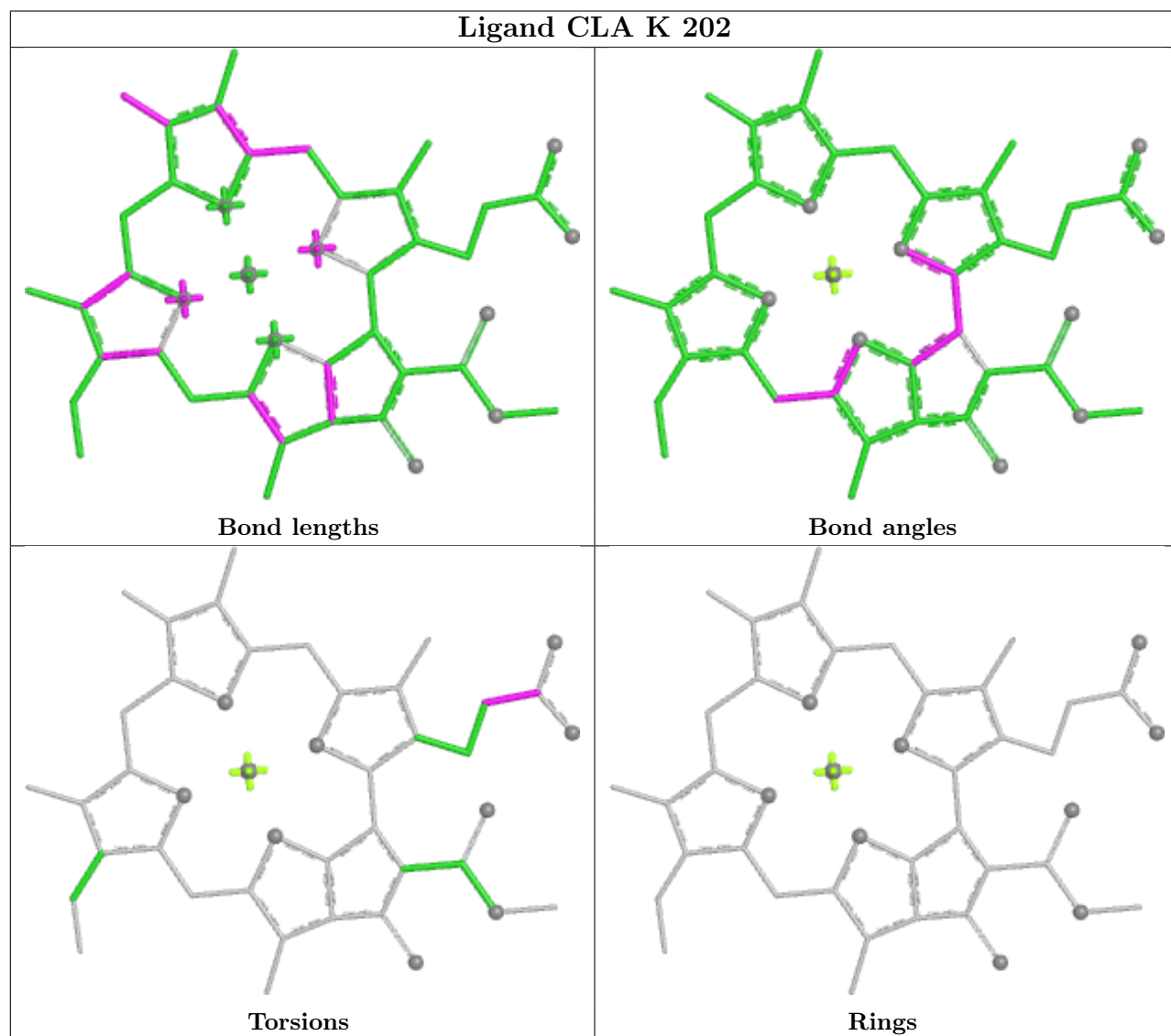
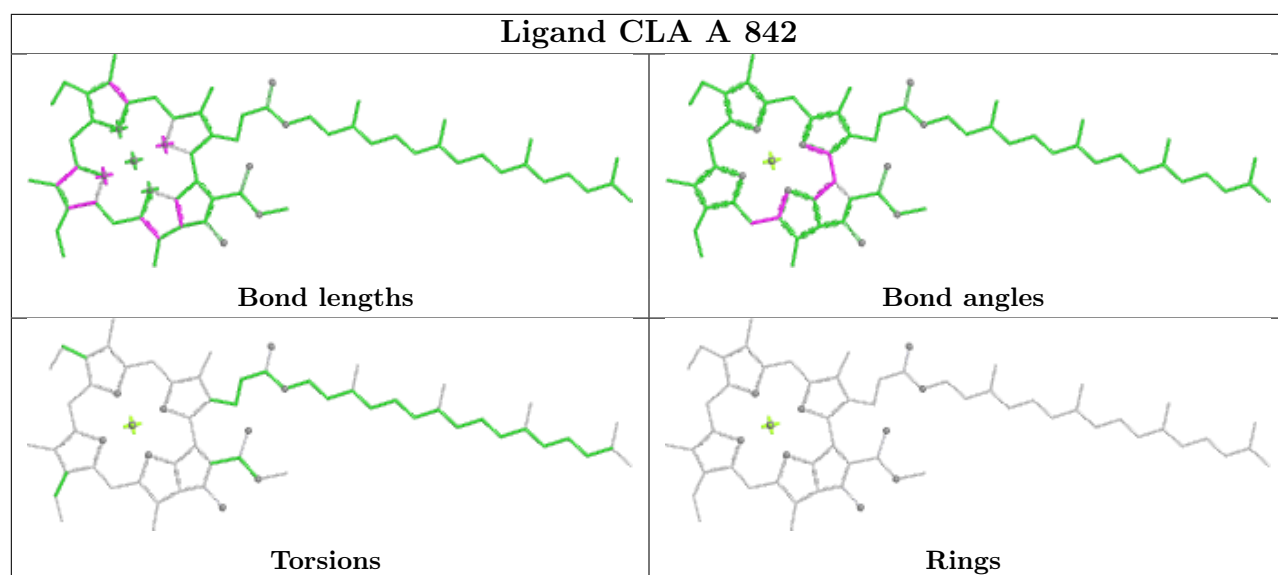


Ligand LUT 2 316

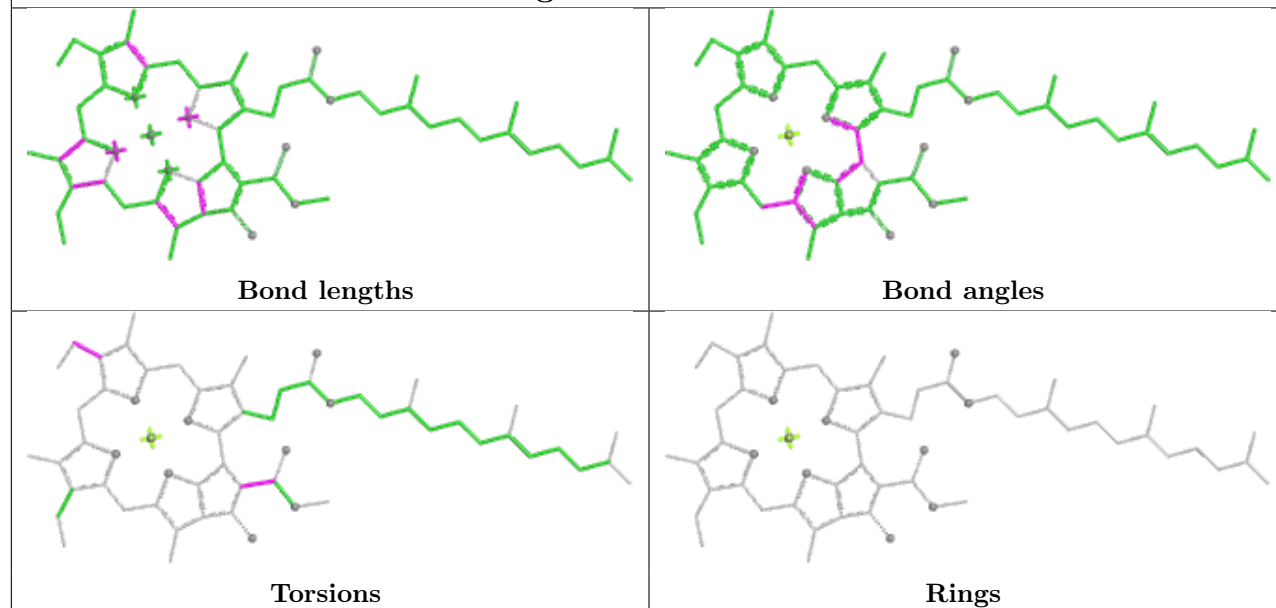




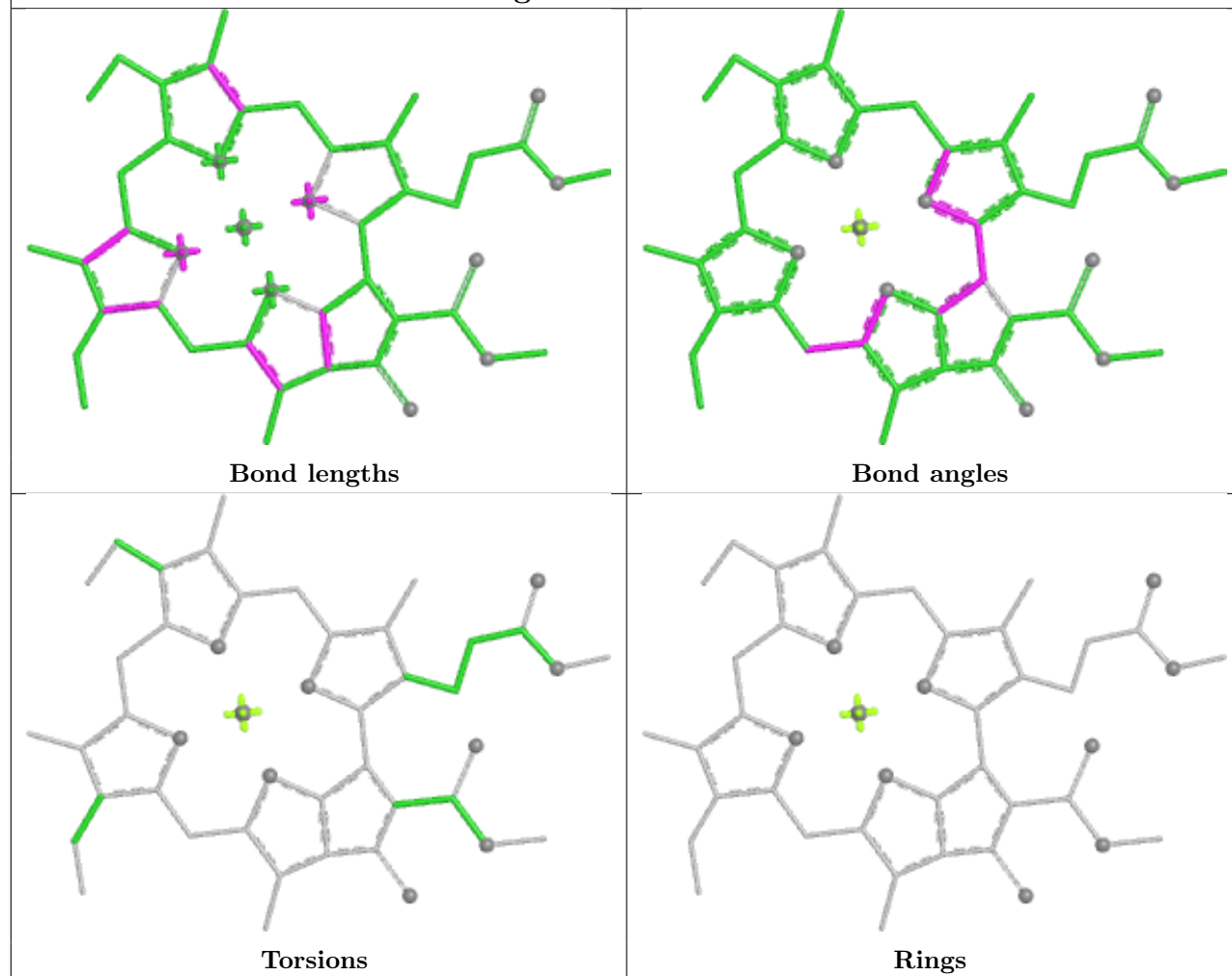


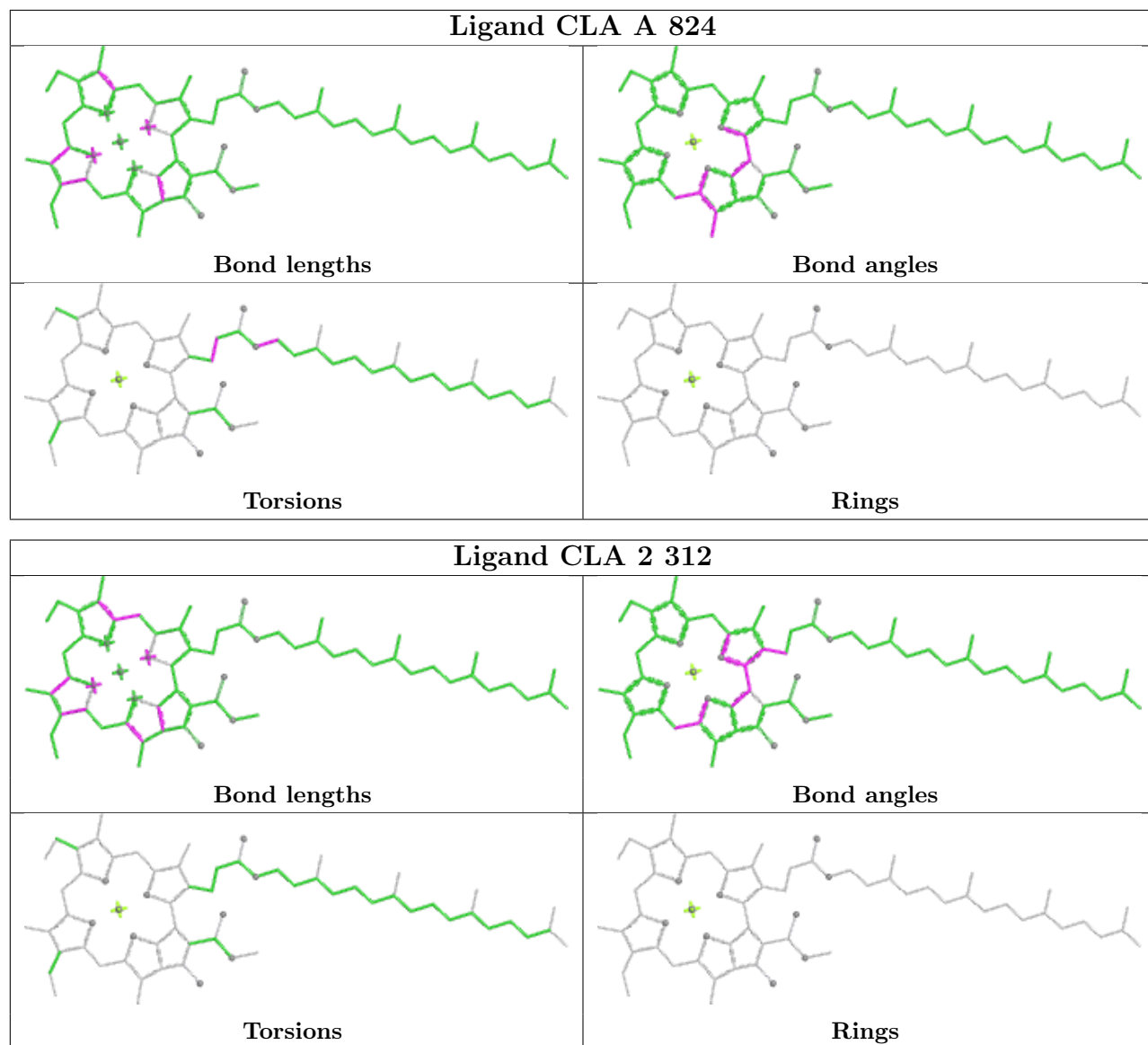


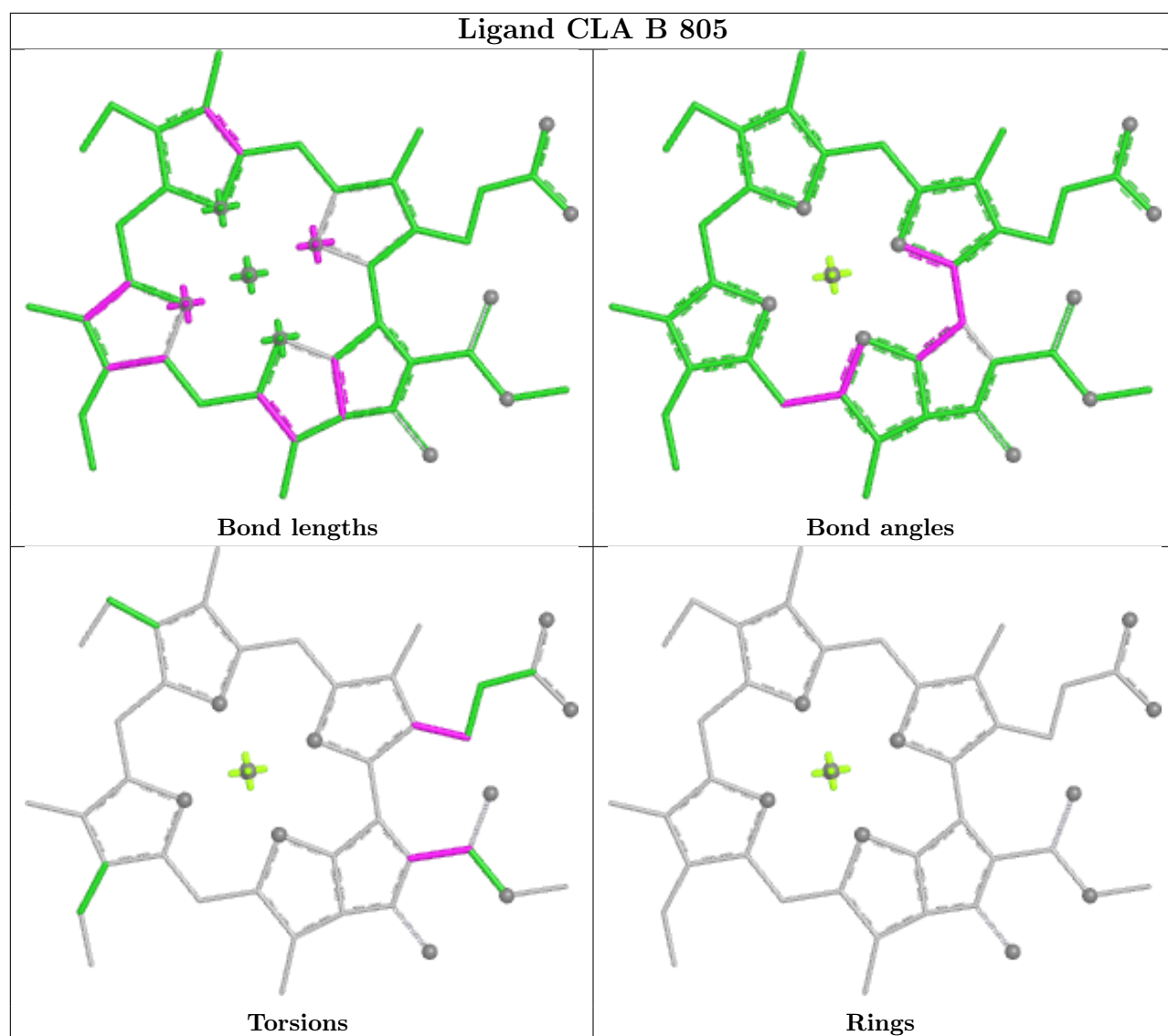
Ligand CLA 5 301

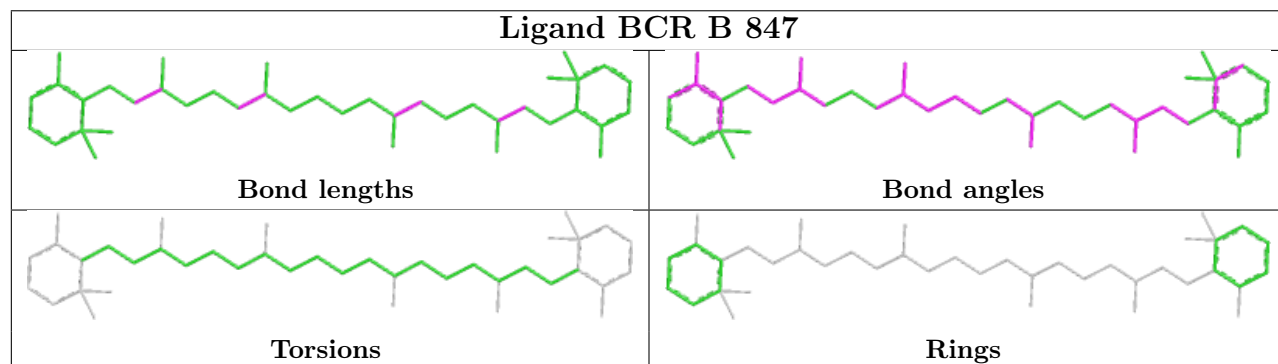
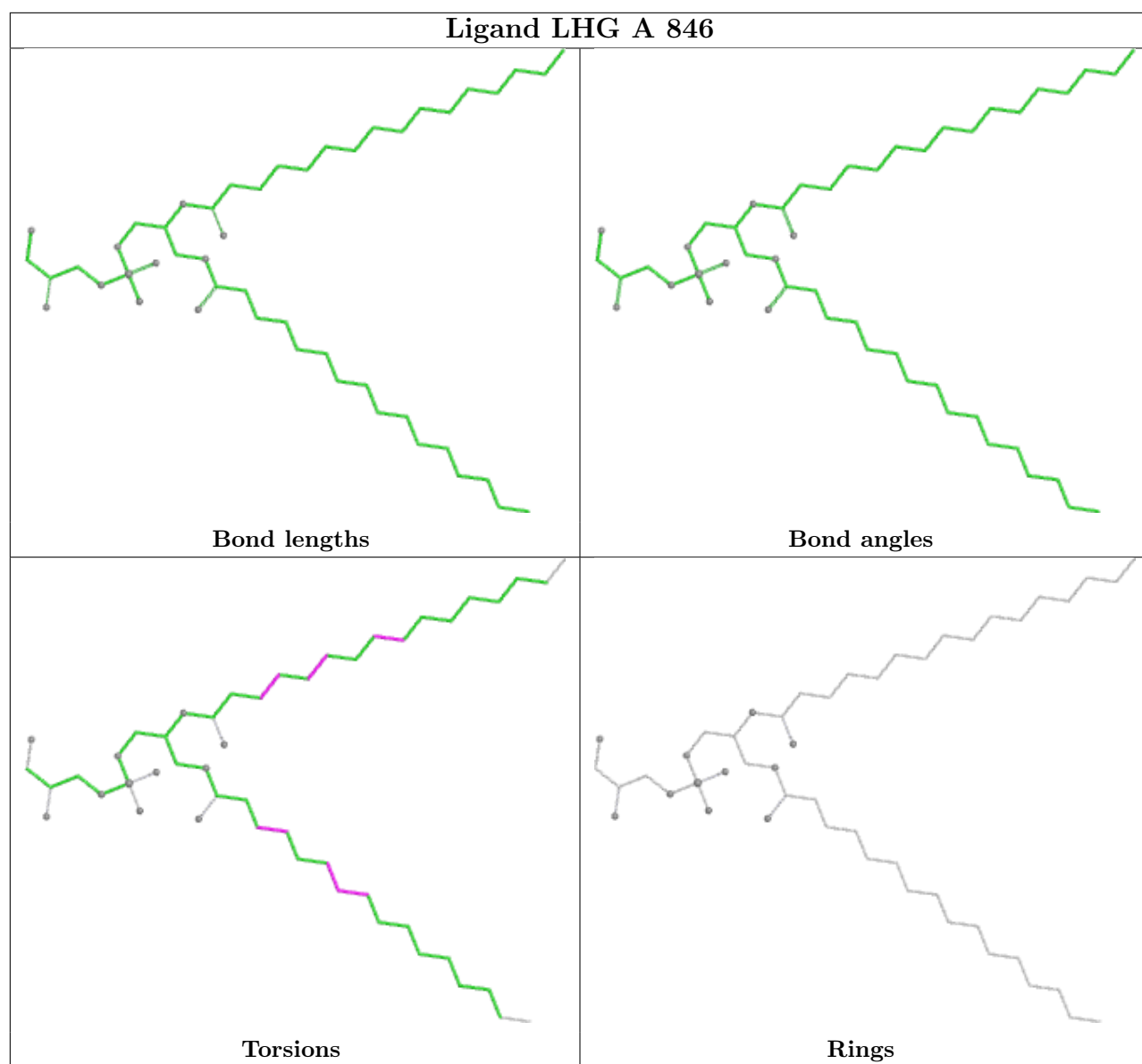


Ligand CLA B 822

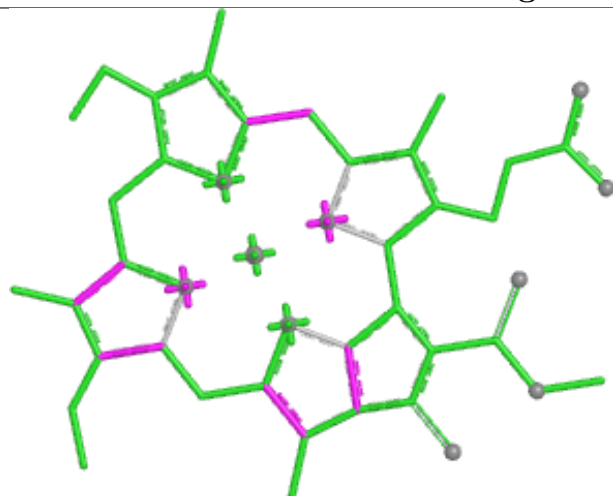




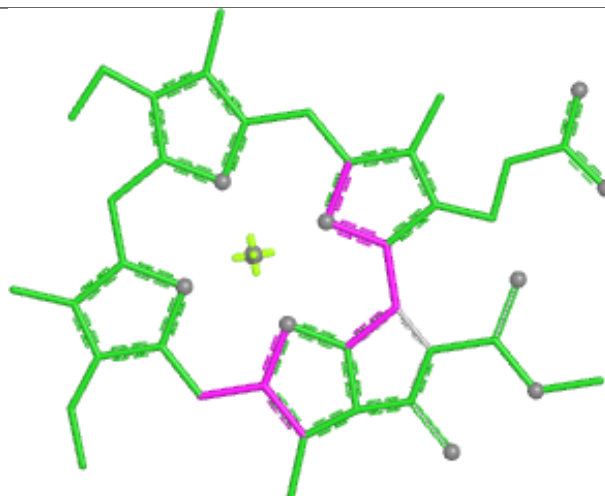




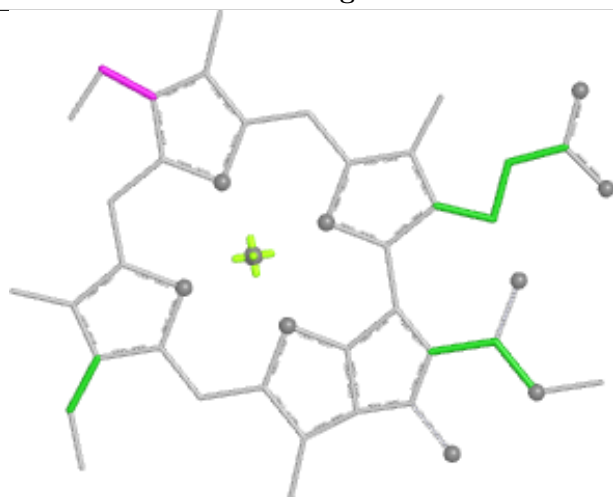
Ligand CLA 5 303



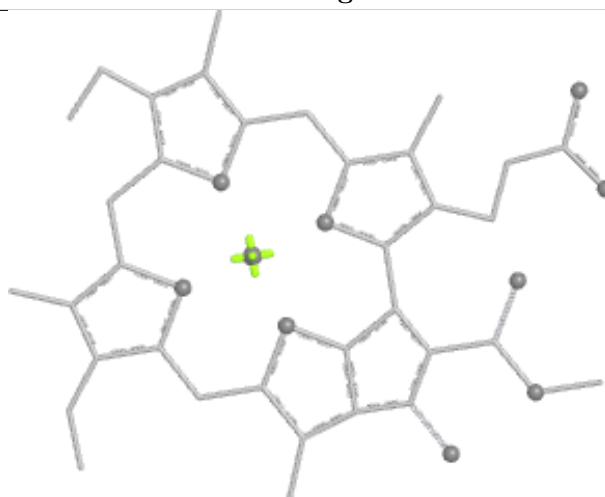
Bond lengths



Bond angles

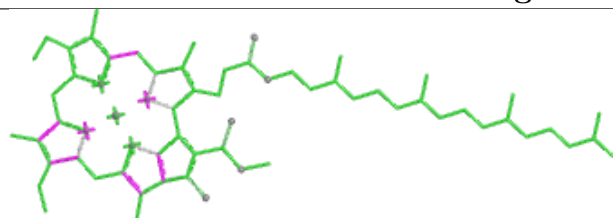


Torsions

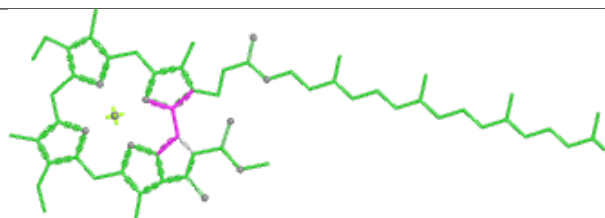


Rings

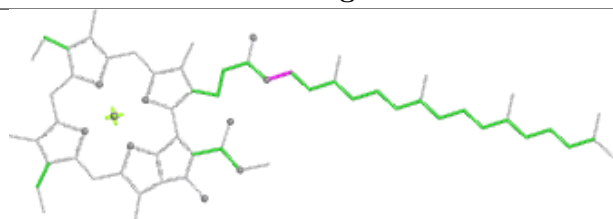
Ligand CLA B 803



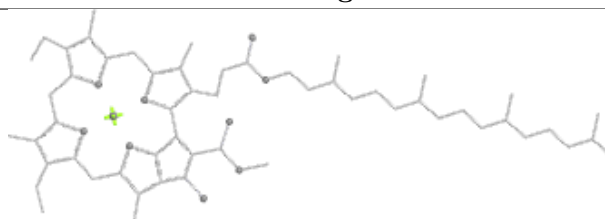
Bond lengths



Bond angles

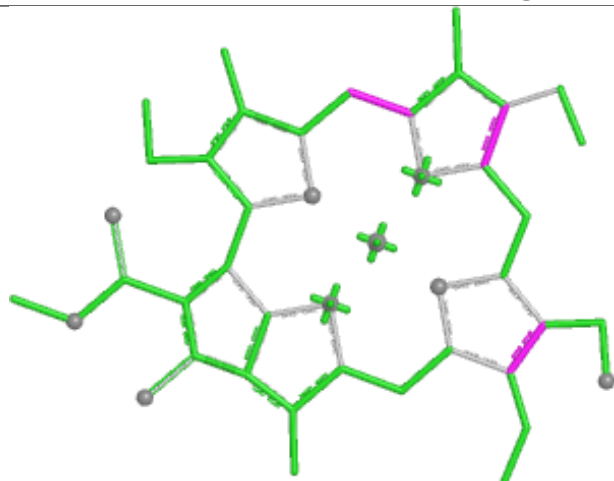


Torsions

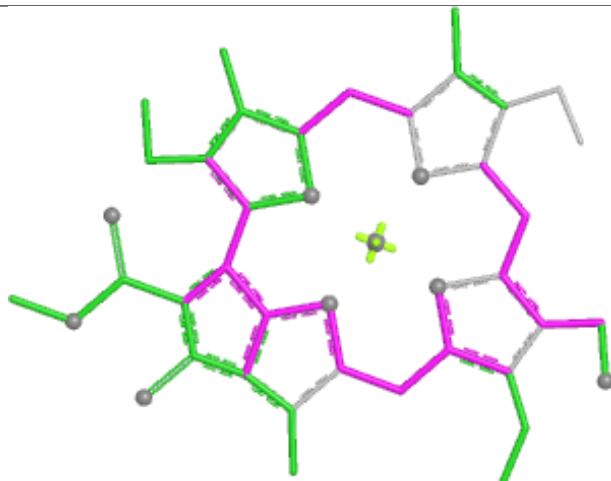


Rings

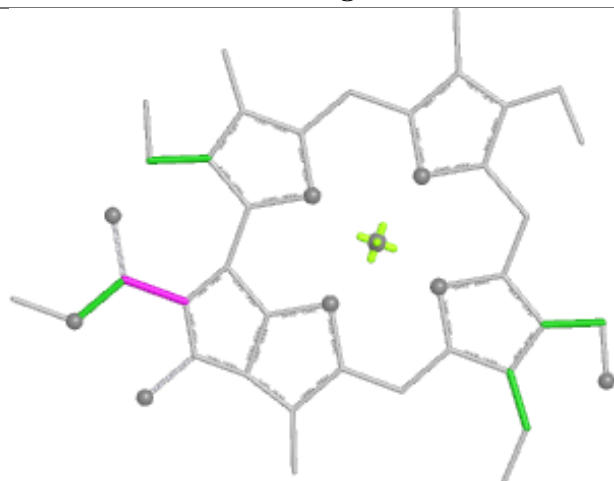
Ligand CHL 5 305



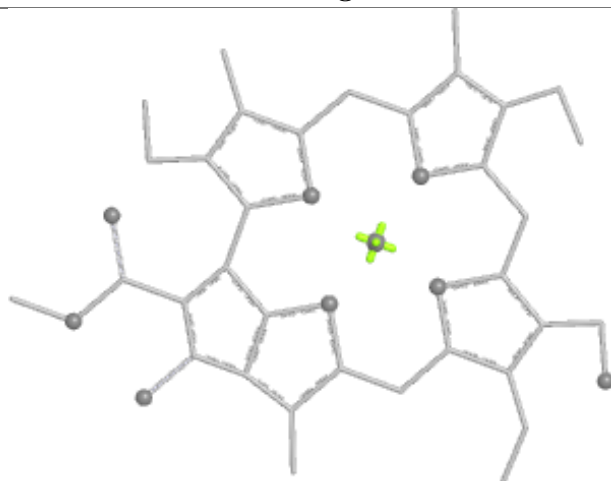
Bond lengths



Bond angles

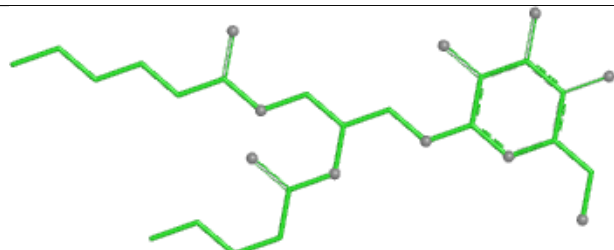


Torsions

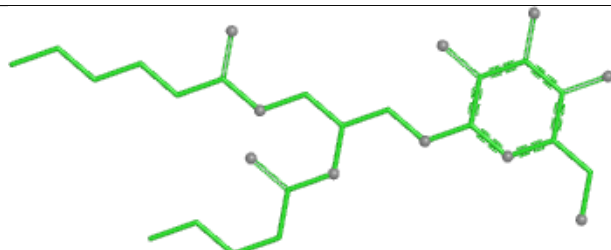


Rings

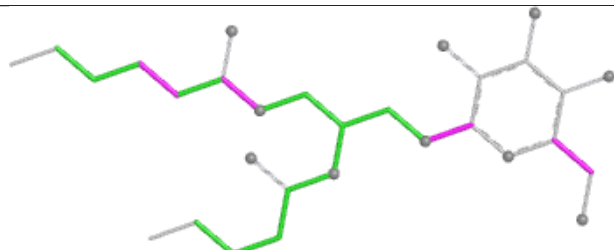
Ligand LMG J 104



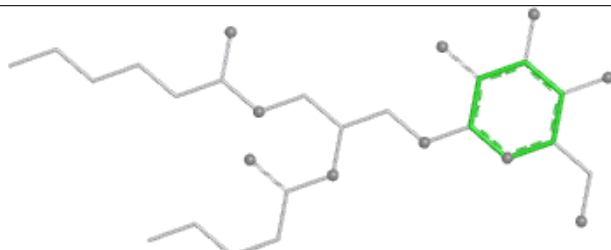
Bond lengths



Bond angles

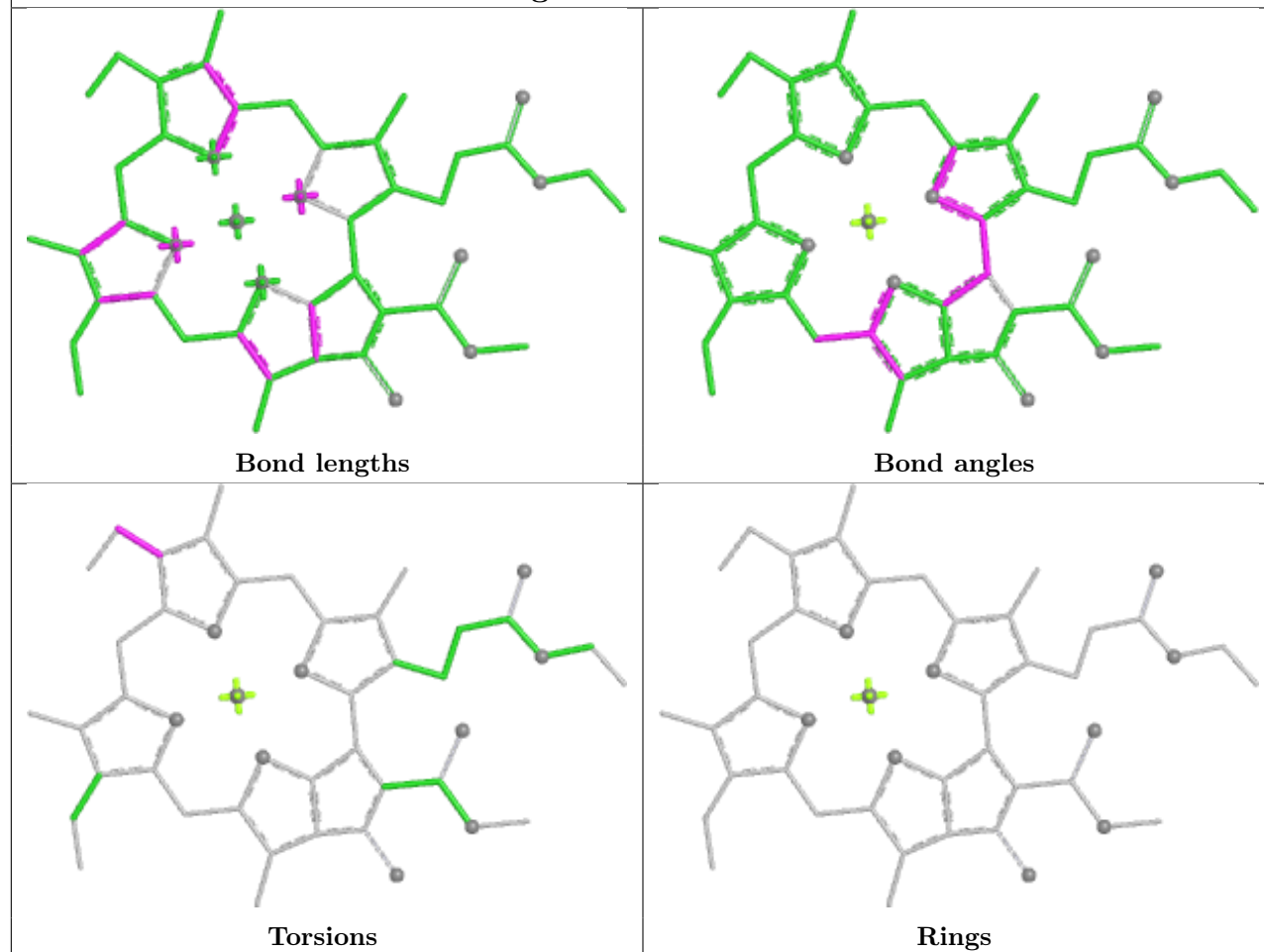


Torsions

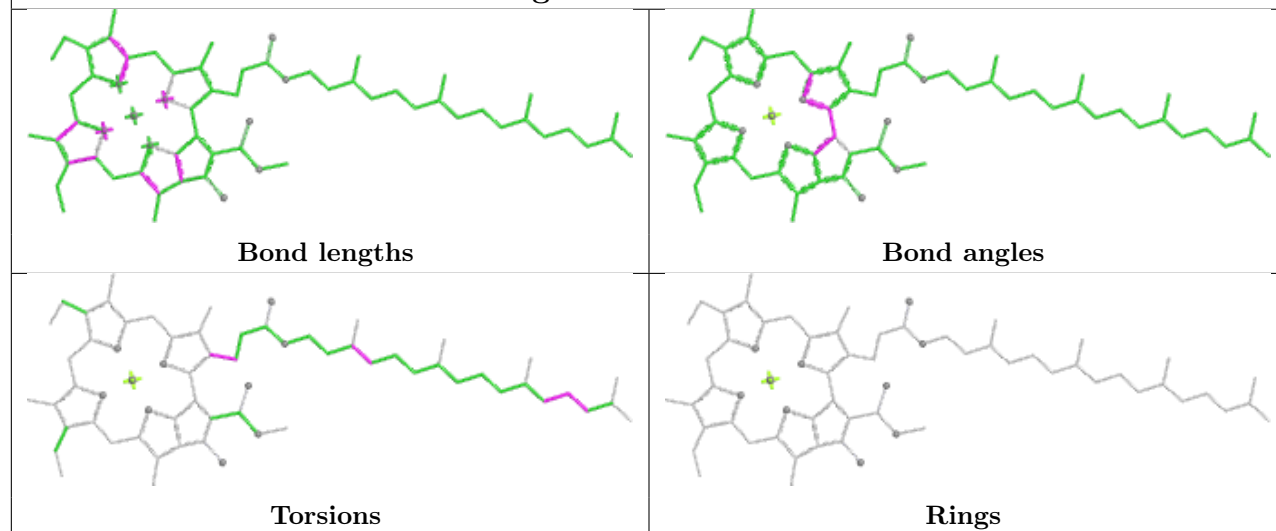


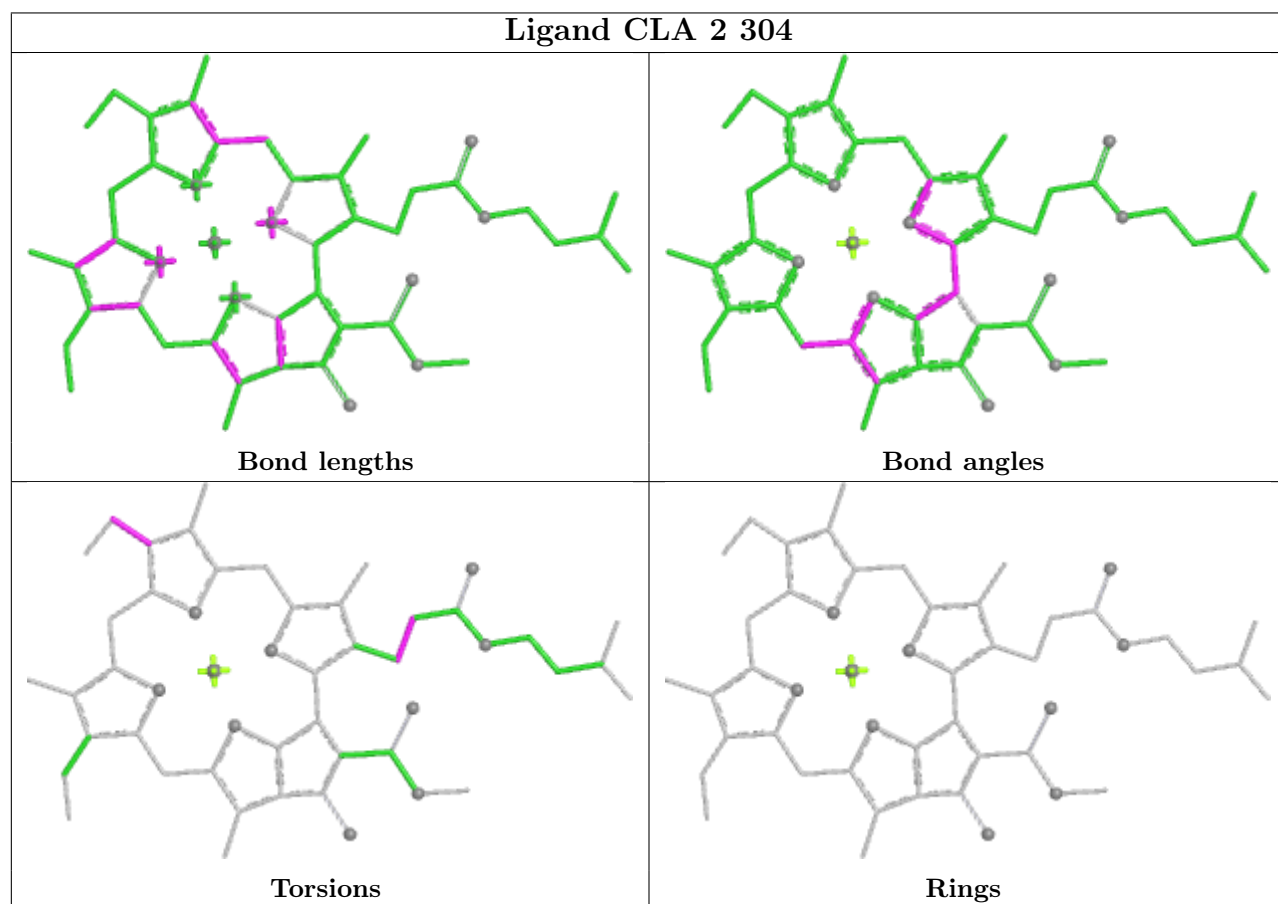
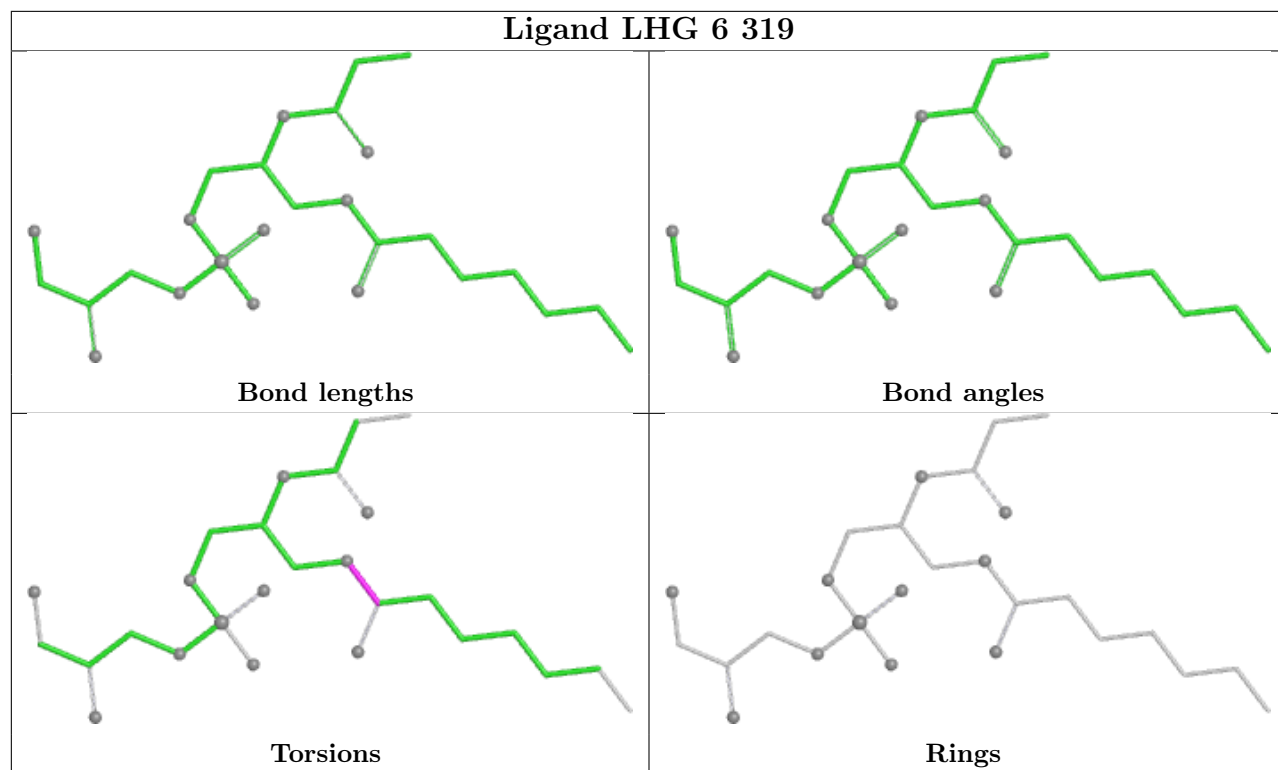
Rings

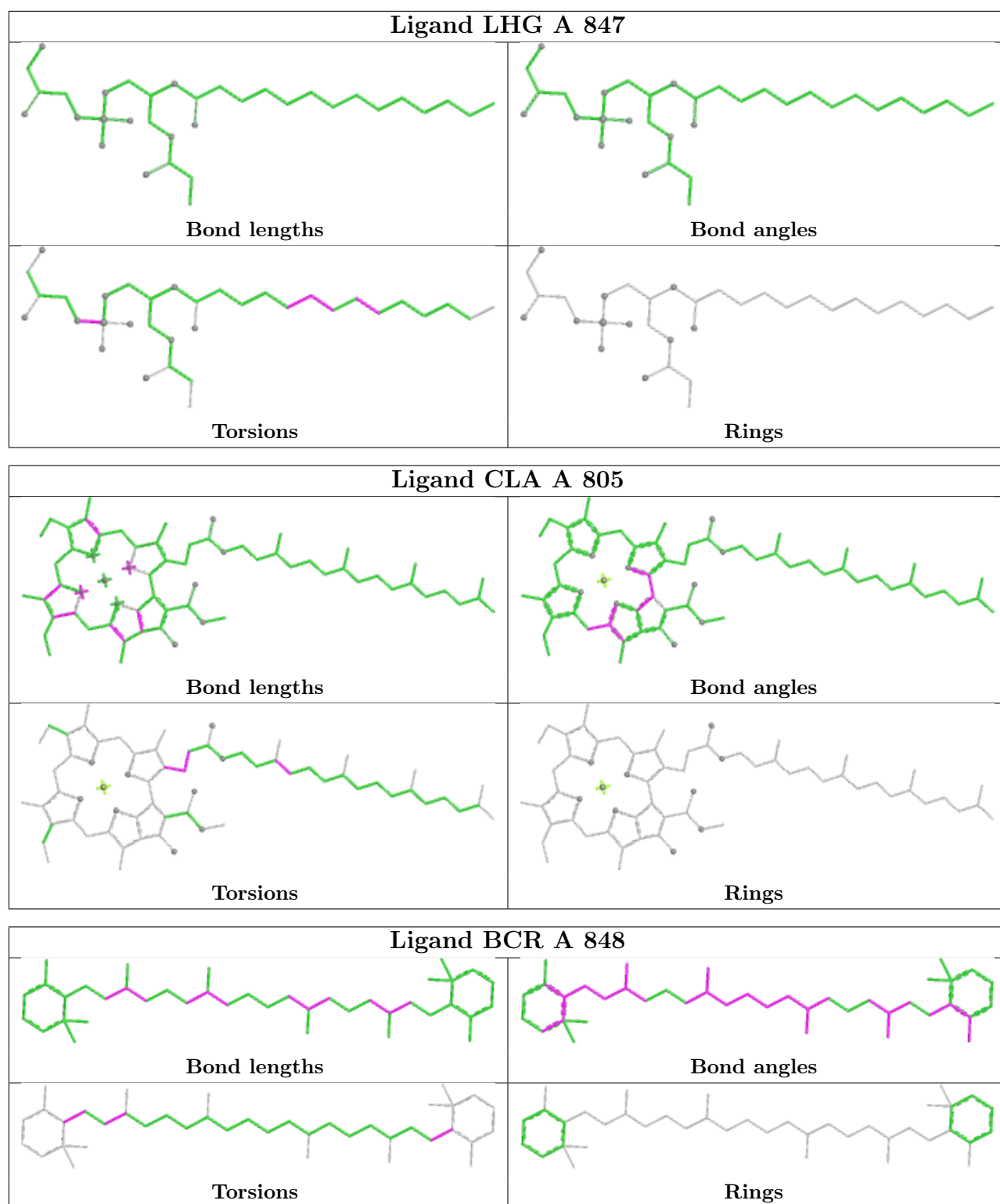
Ligand CLA 3 303

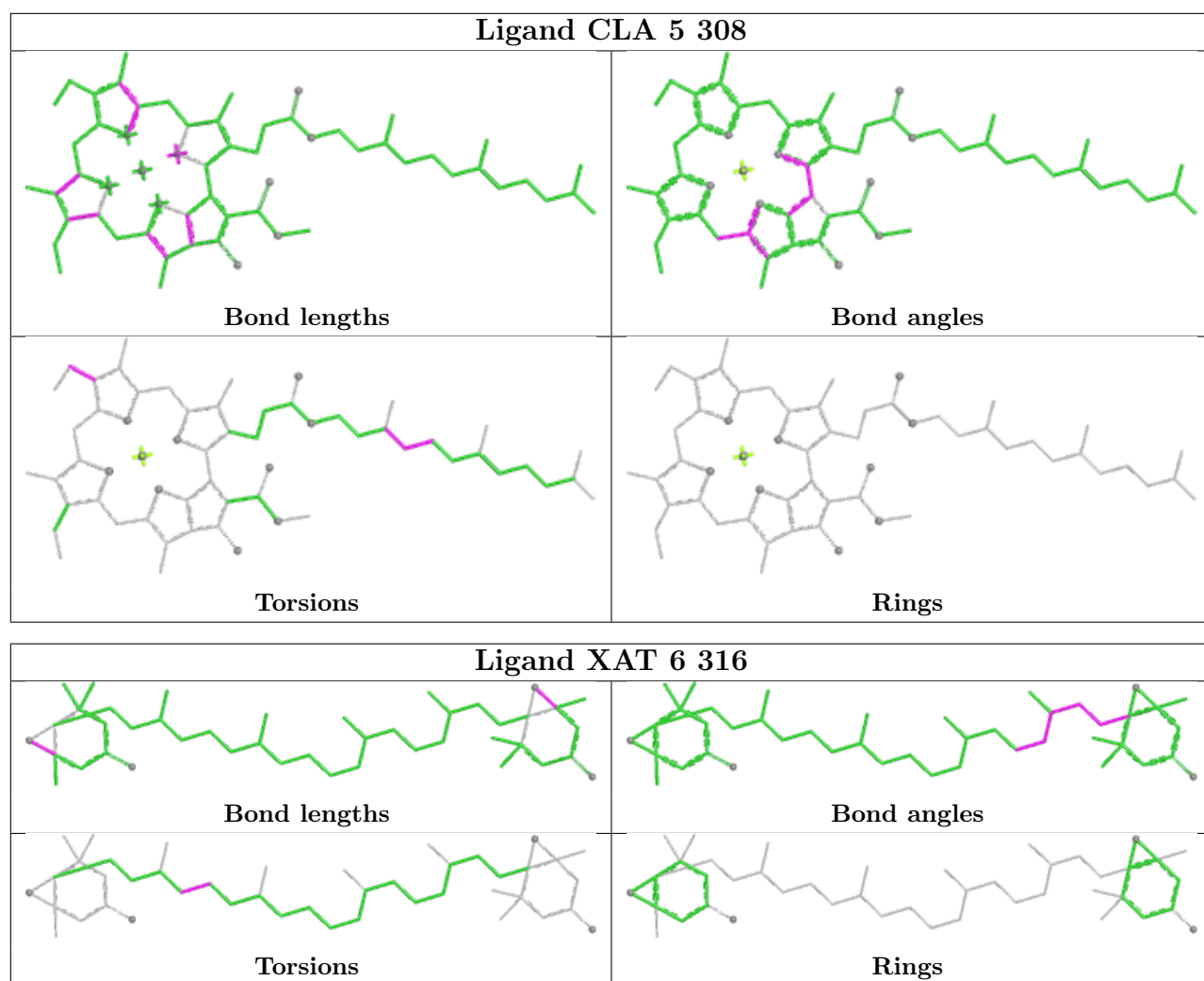


Ligand CLA B 814

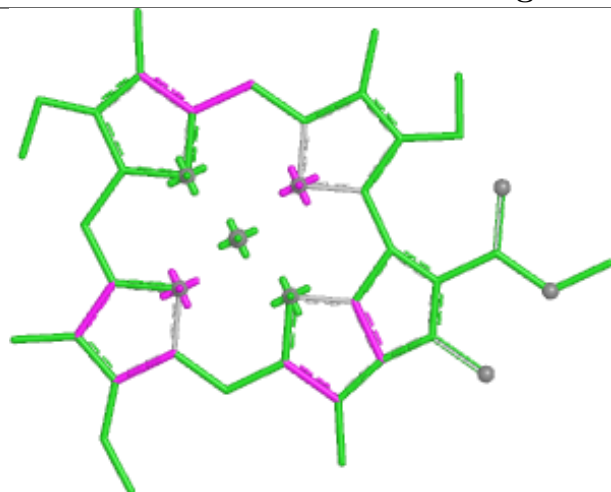




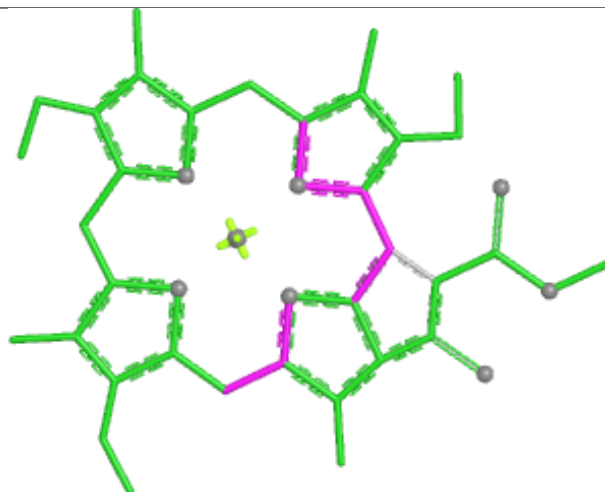




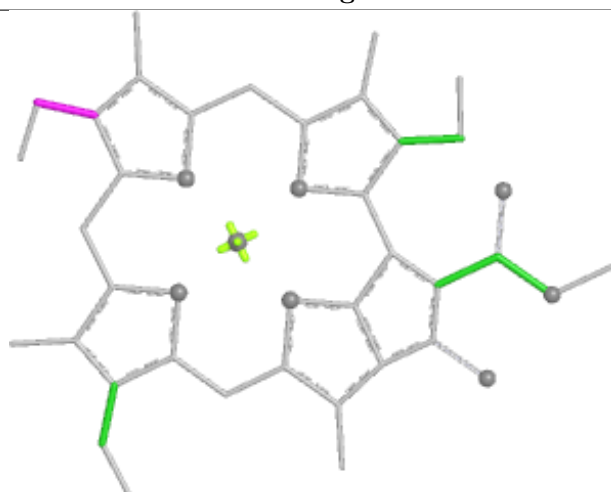
Ligand CLA L 303



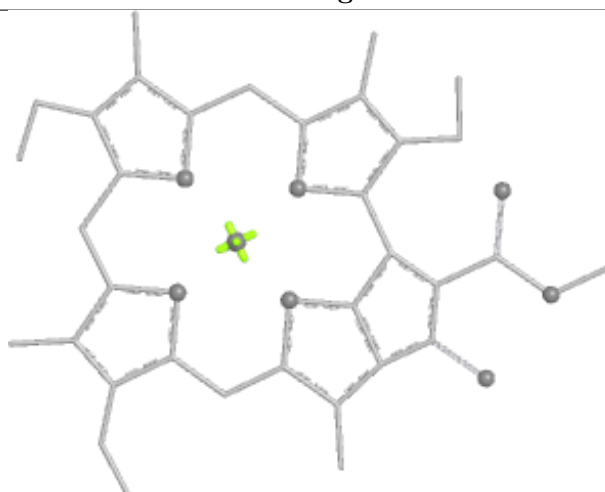
Bond lengths



Bond angles

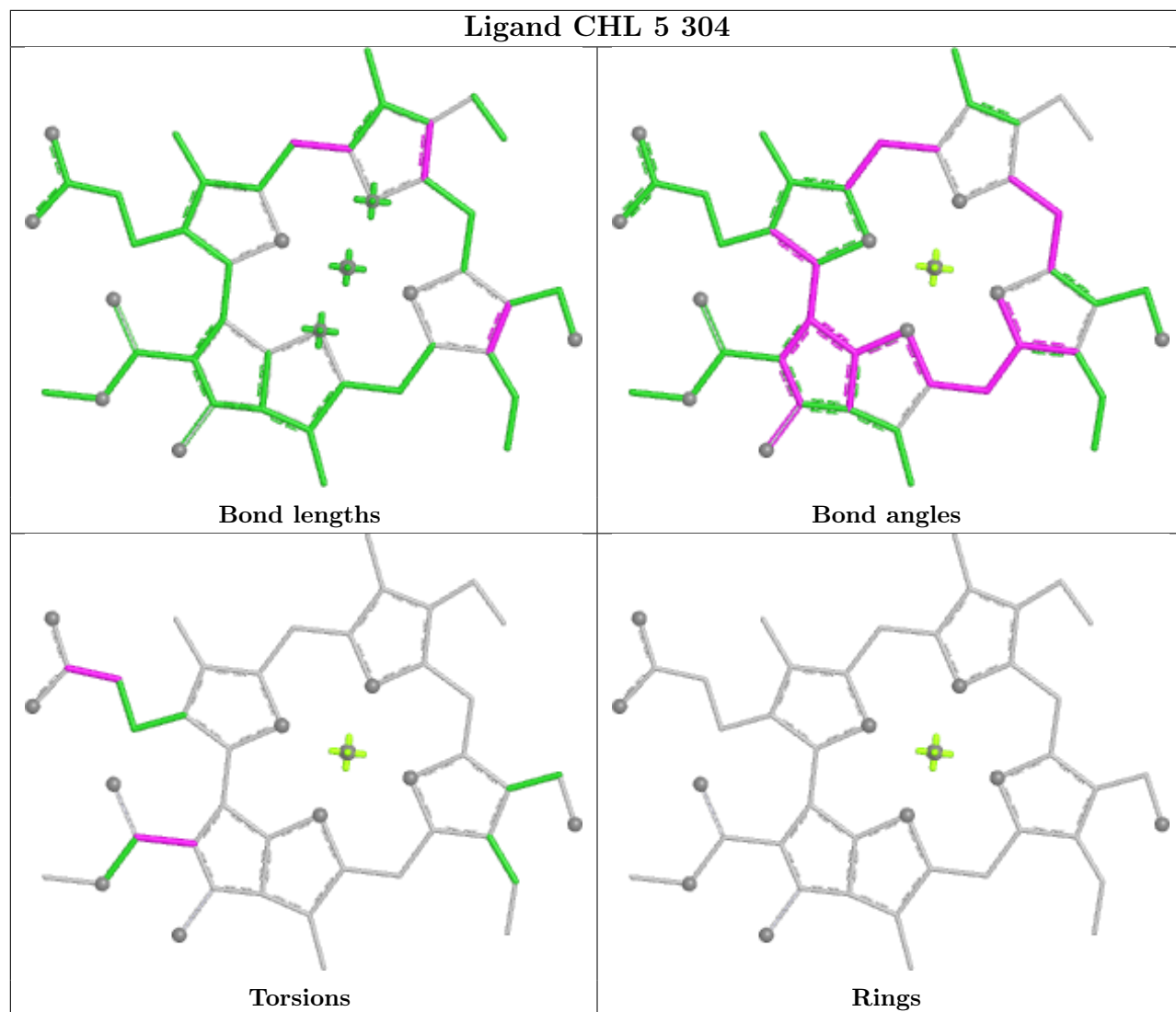


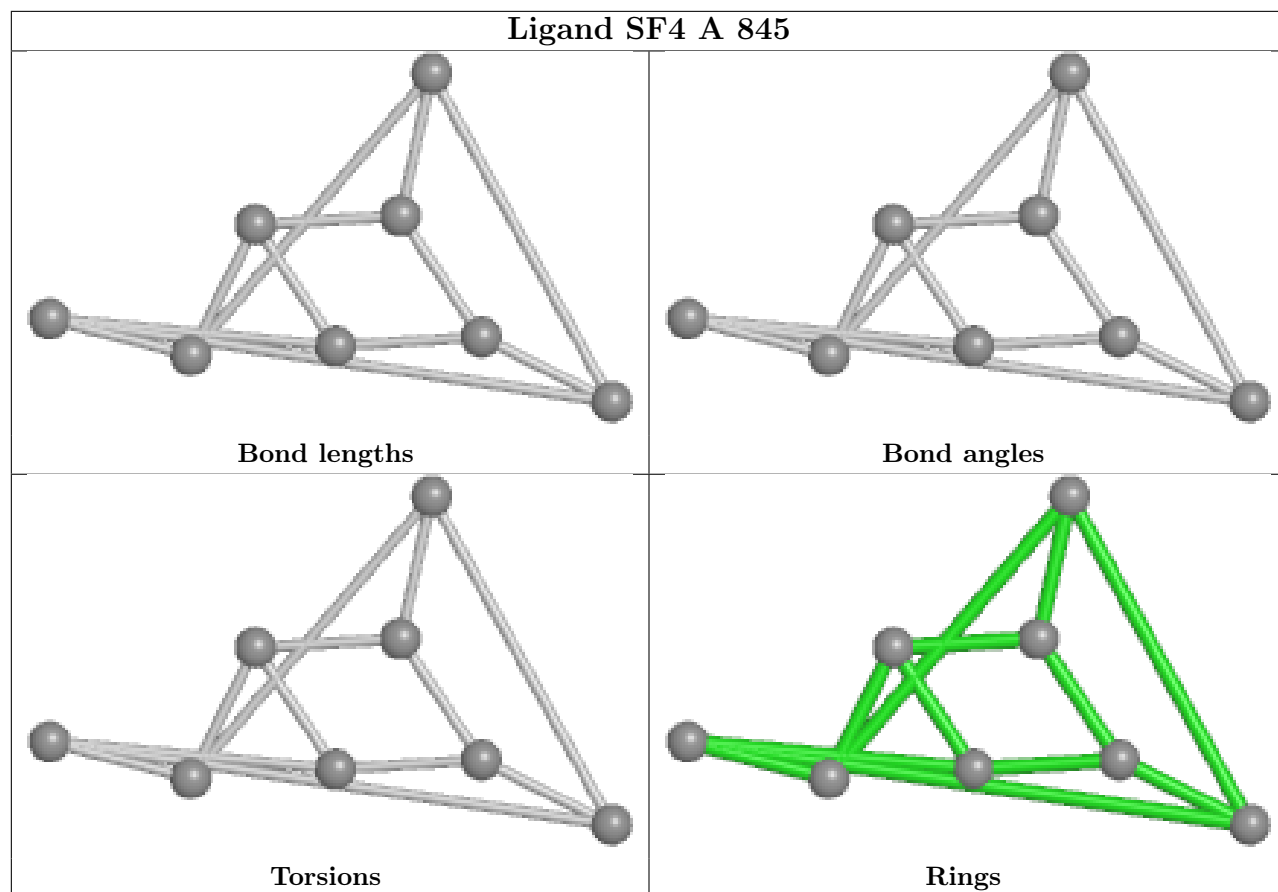
Torsions



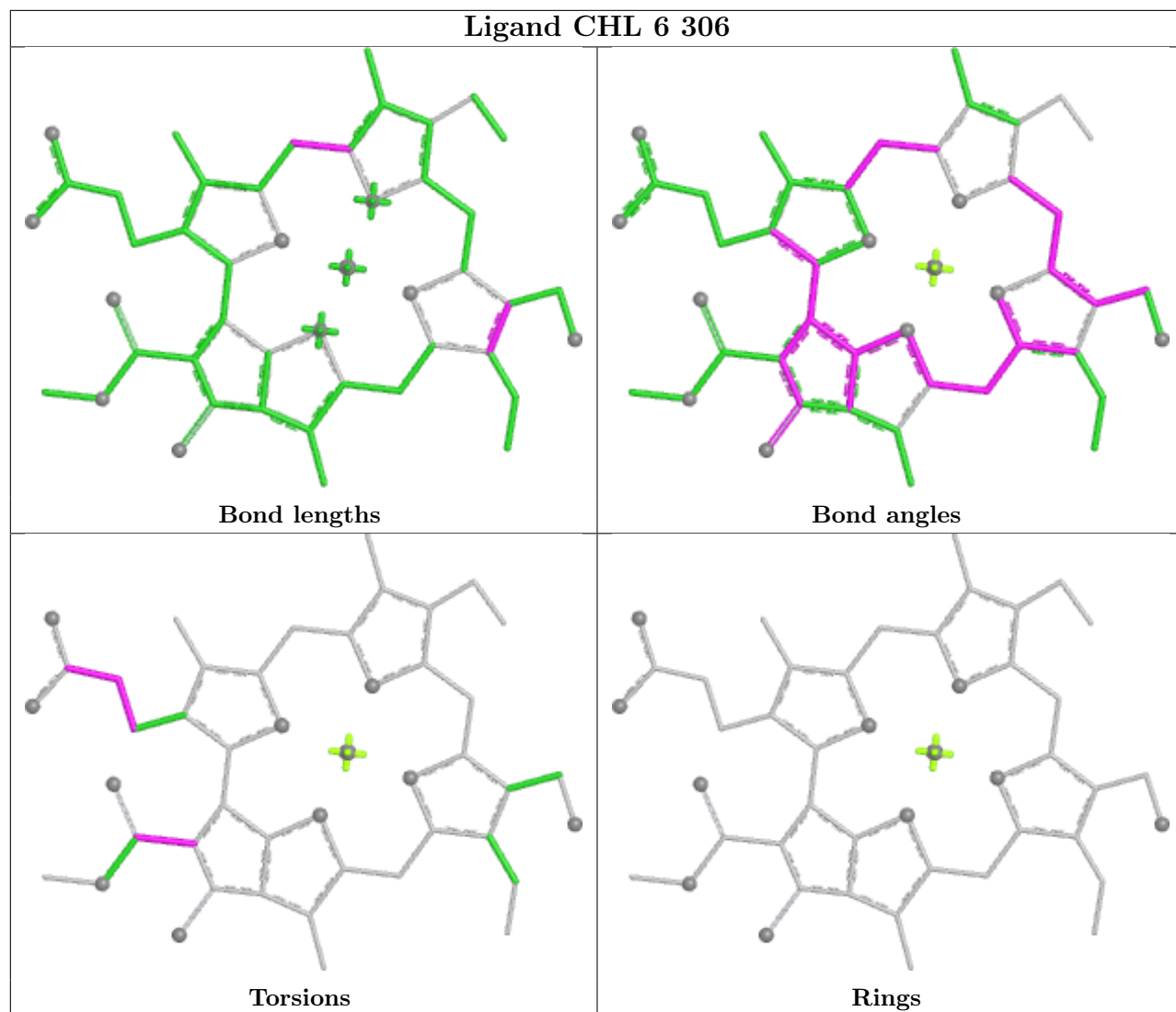
Rings

Ligand CHL 5 304

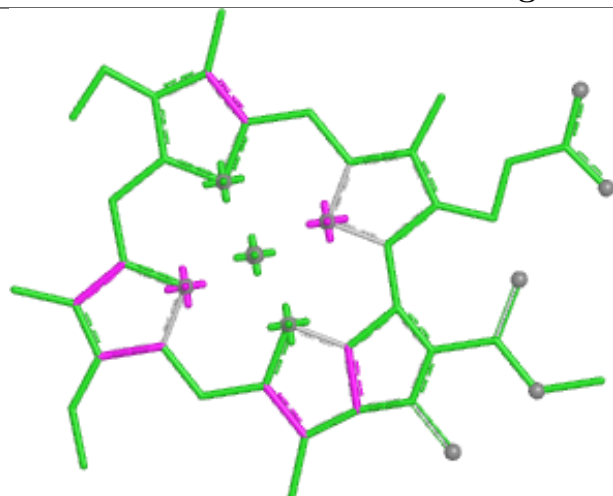




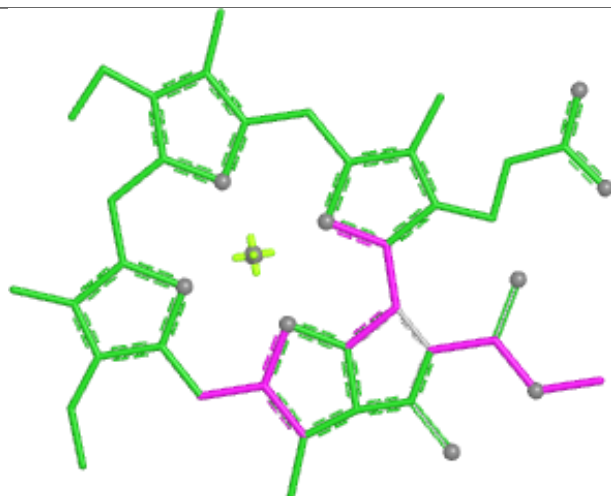
Ligand CHL 6 306



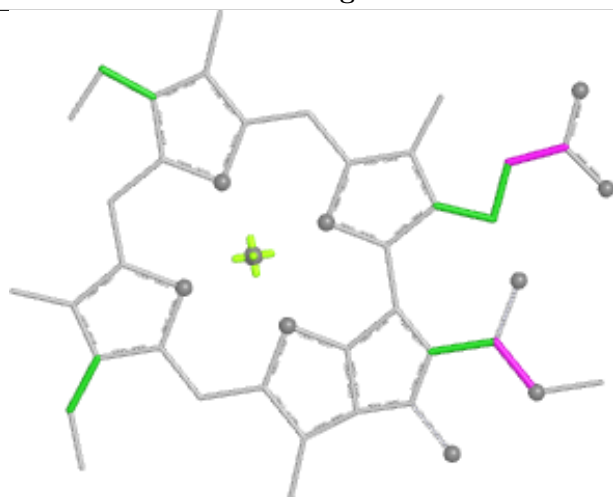
Ligand CLA 6 314



Bond lengths



Bond angles

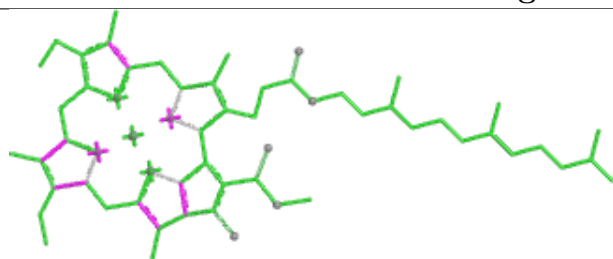


Torsions

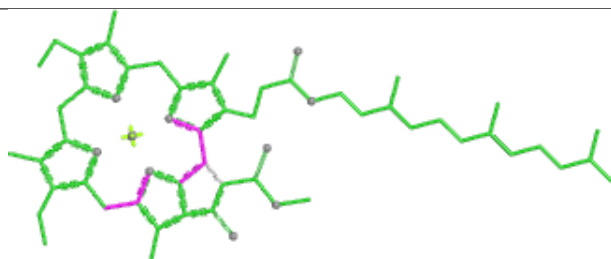


Rings

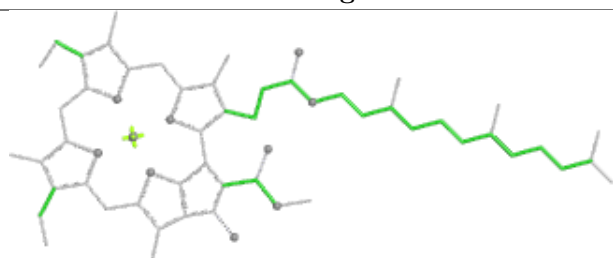
Ligand CLA 5 309



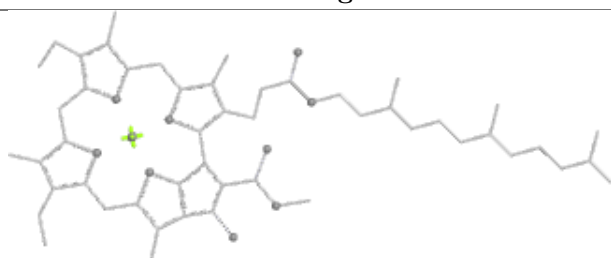
Bond lengths



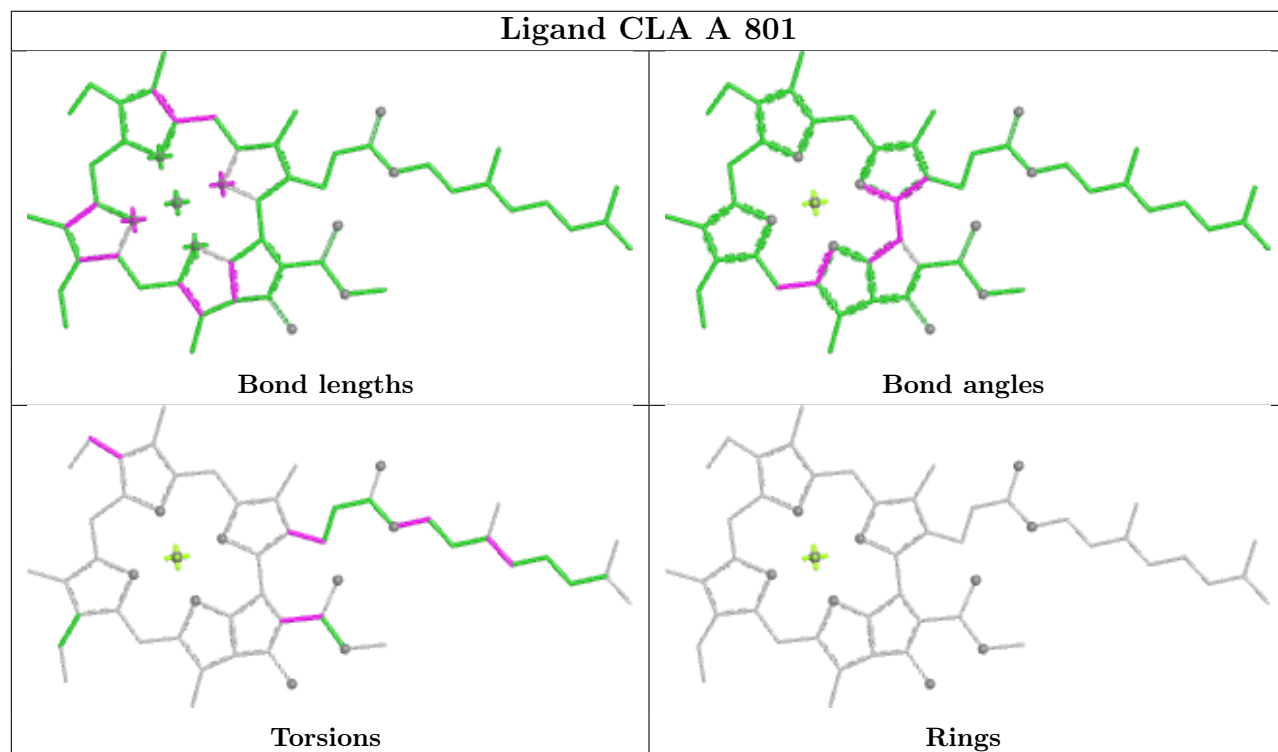
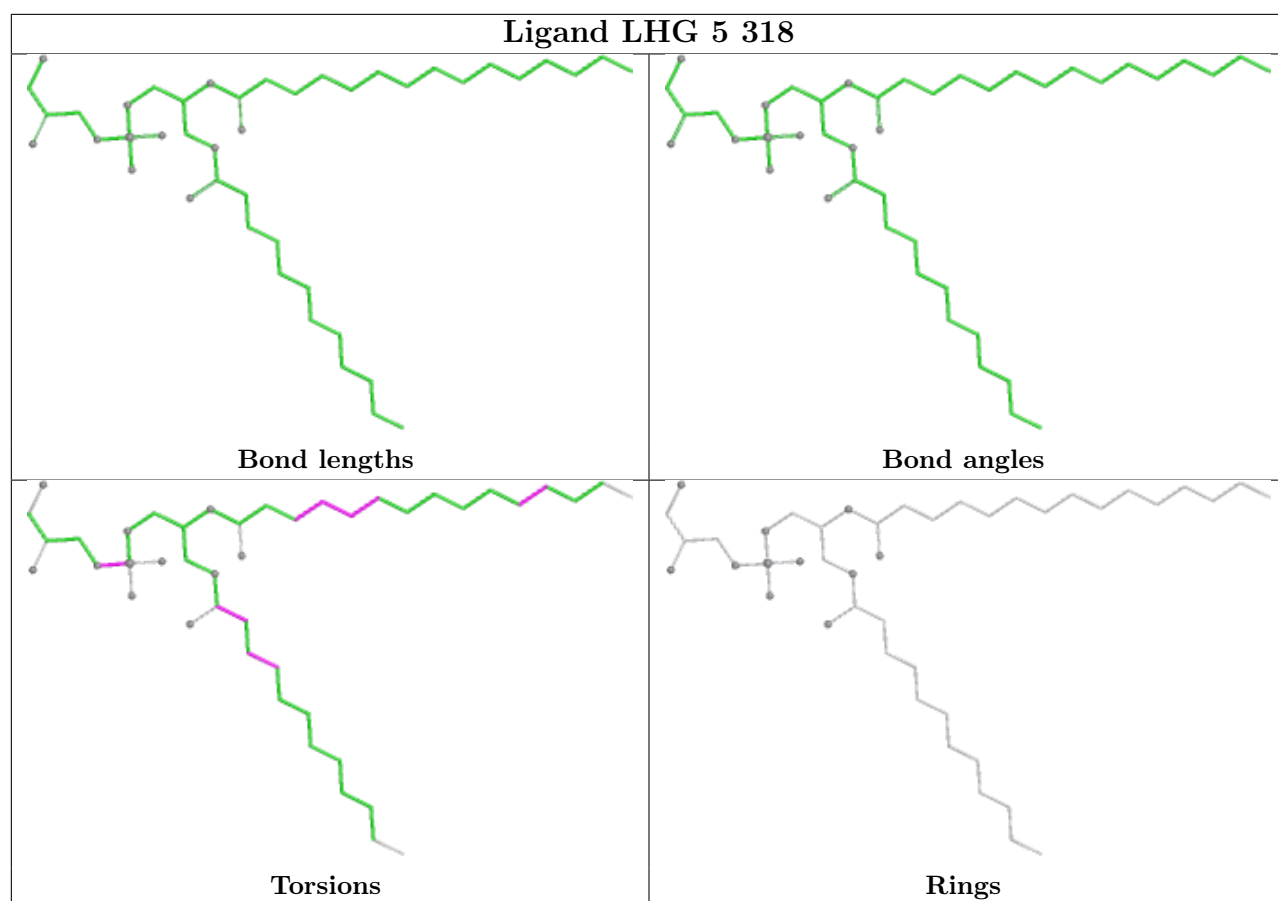
Bond angles

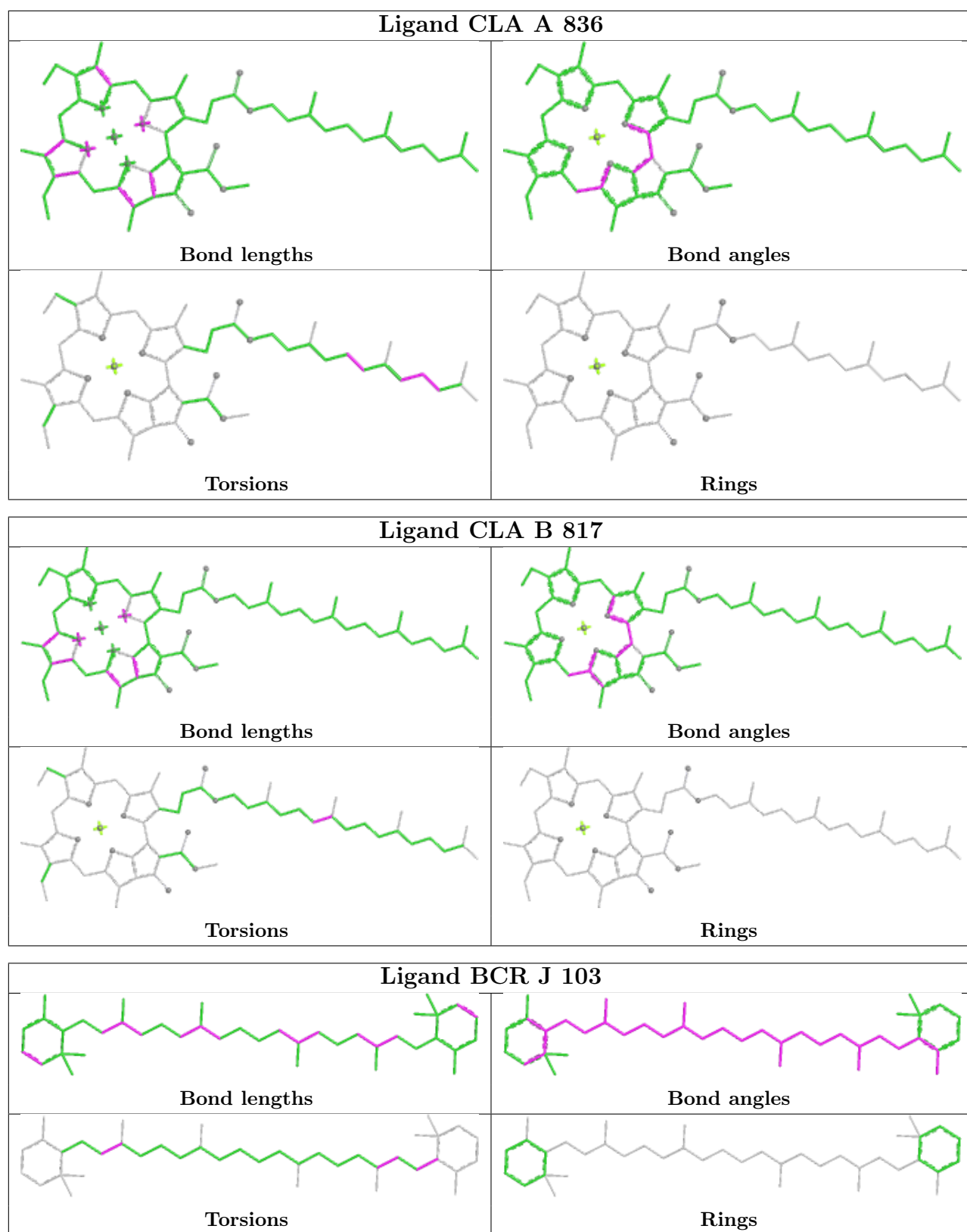


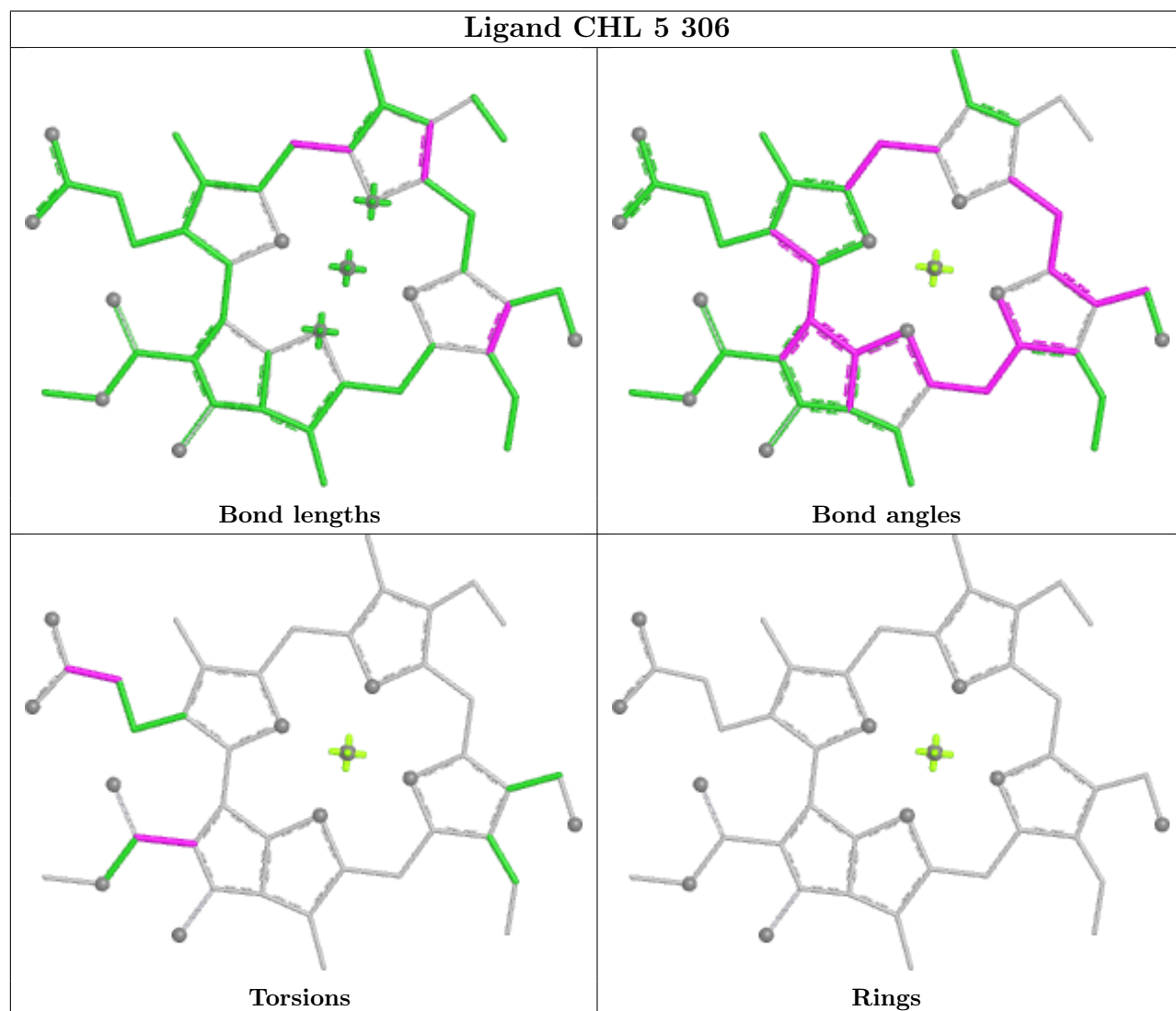
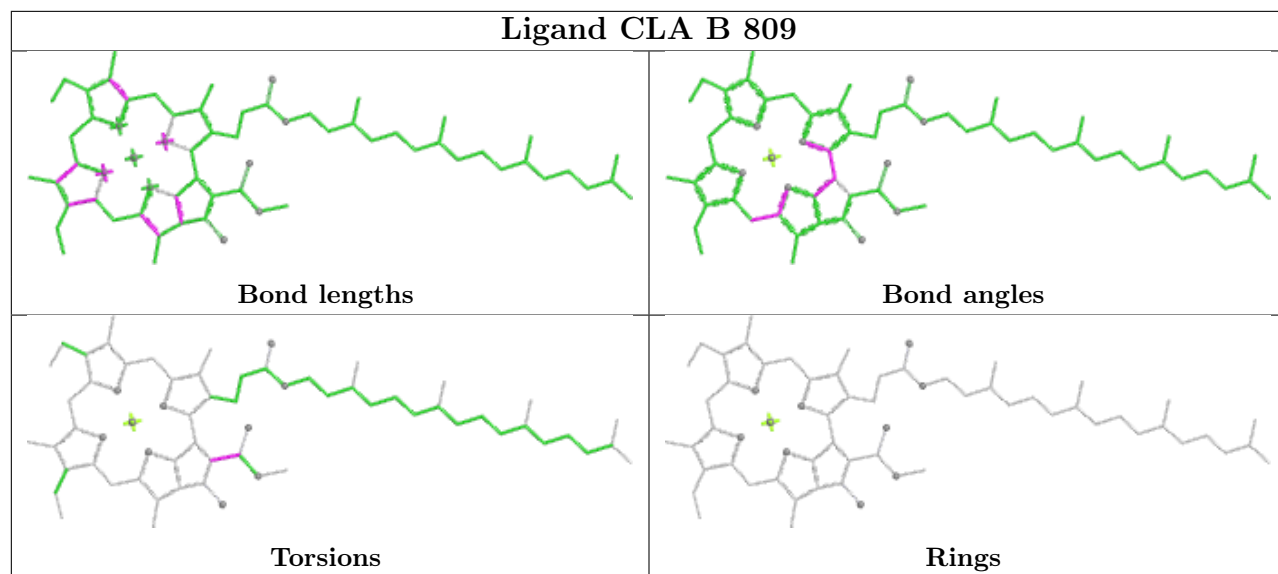
Torsions

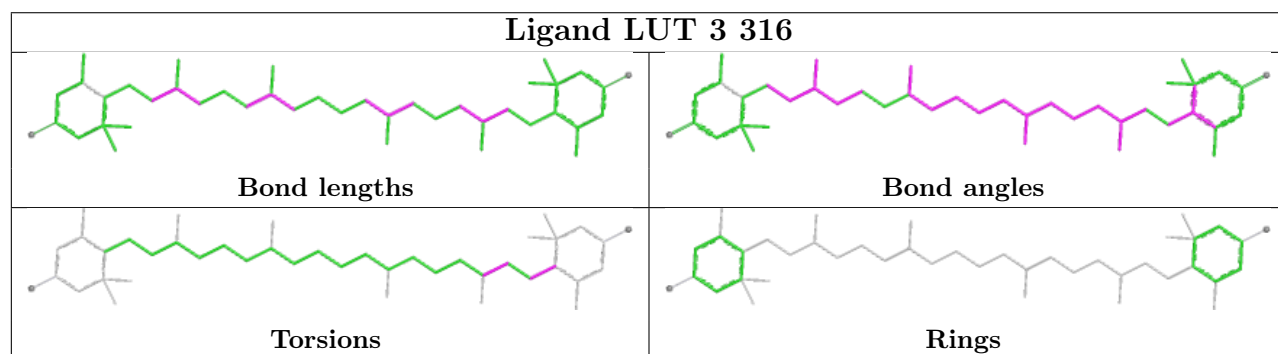
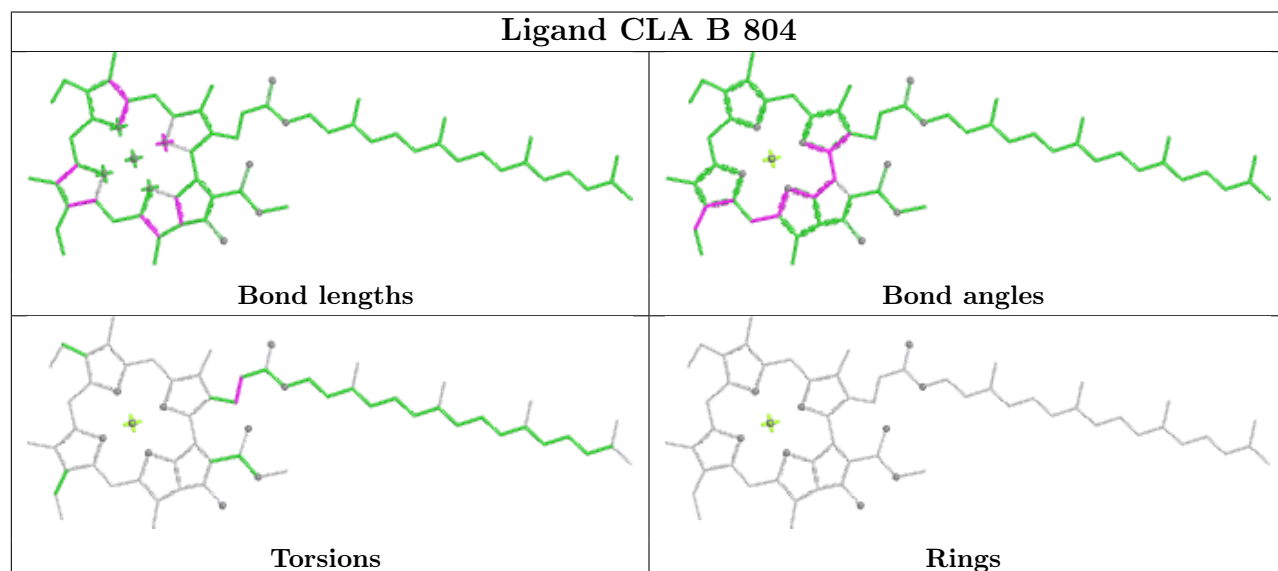
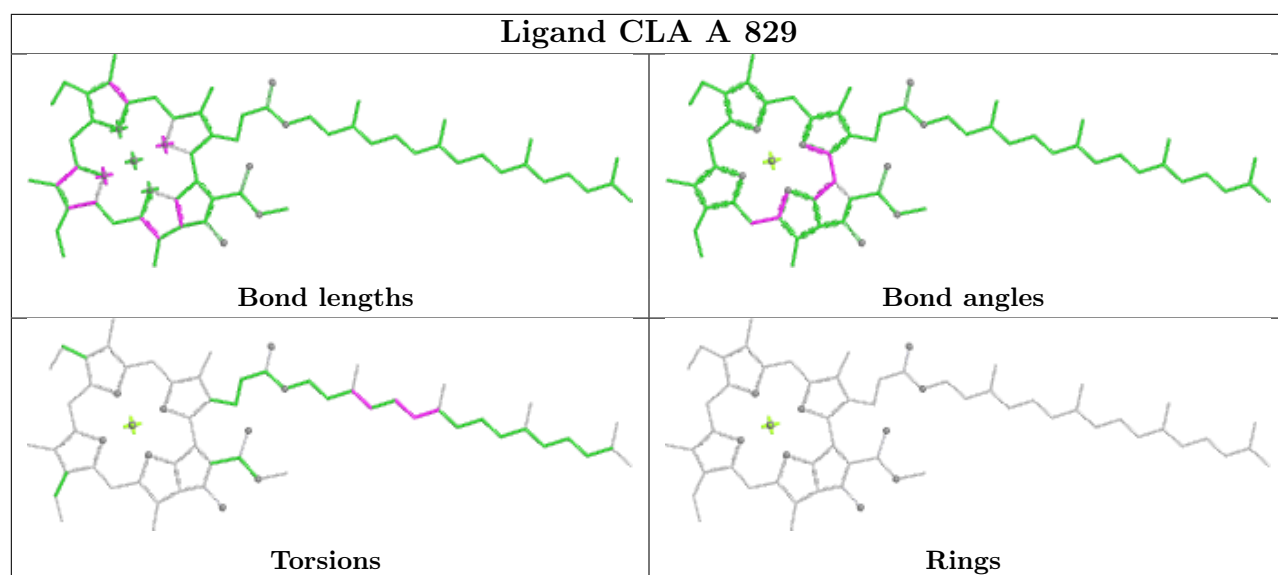


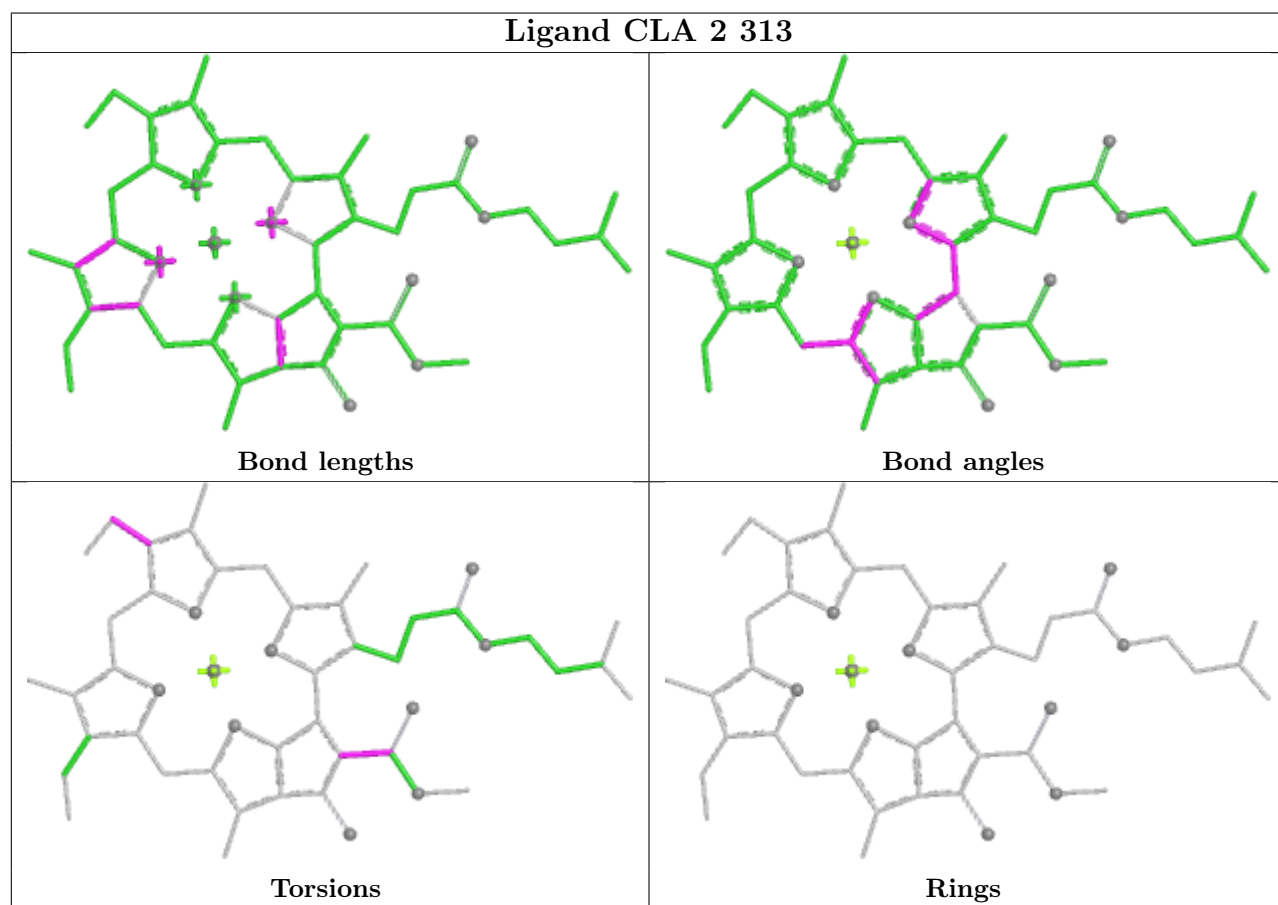
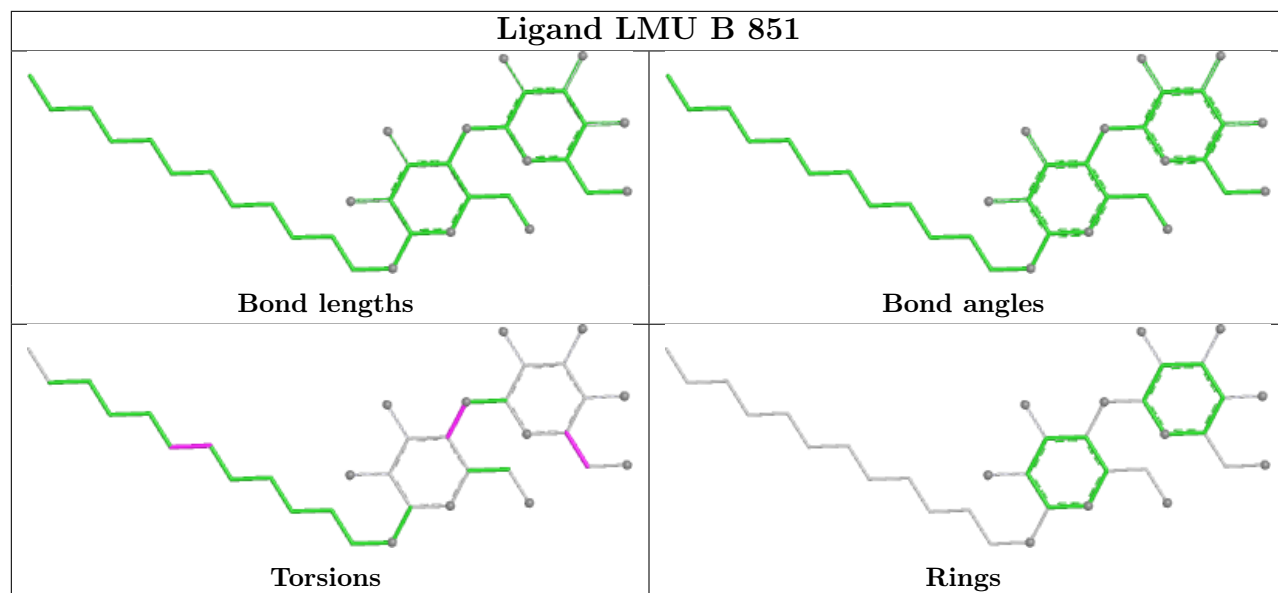
Rings



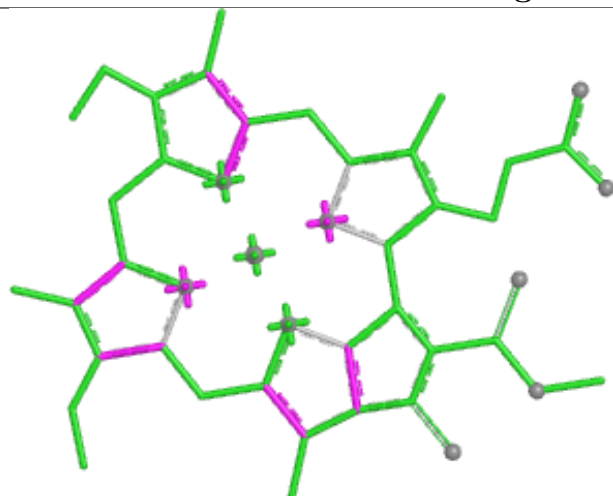




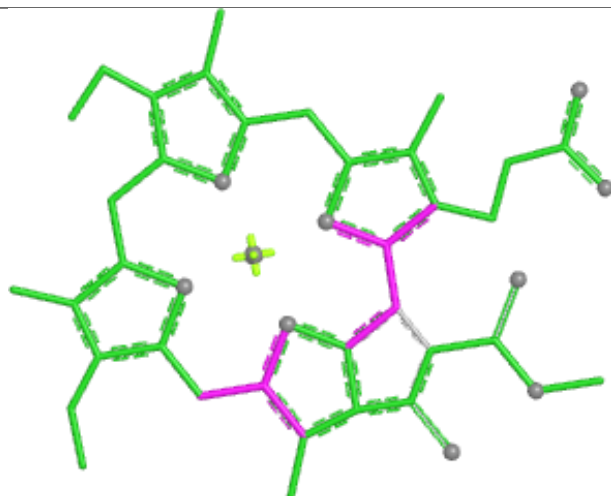




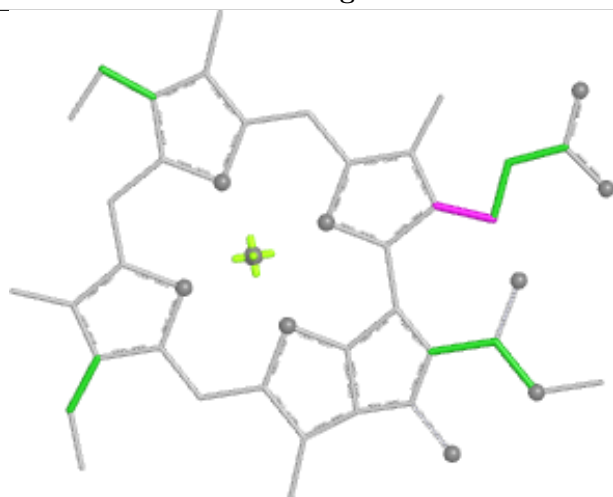
Ligand CLA B 824



Bond lengths



Bond angles

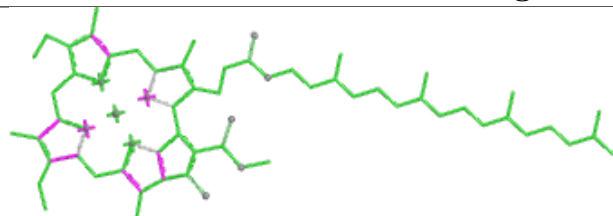


Torsions

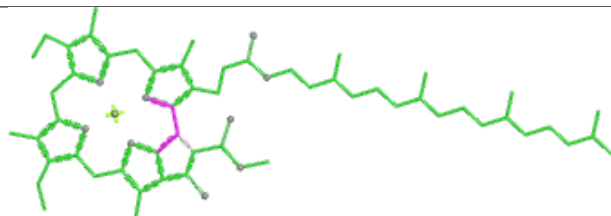


Rings

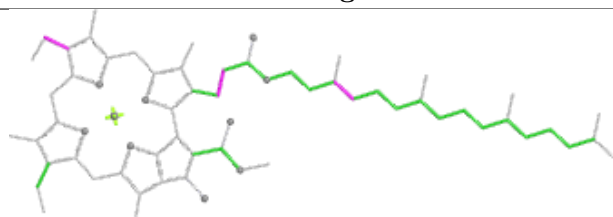
Ligand CLA A 830



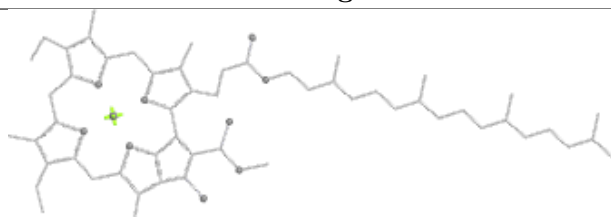
Bond lengths



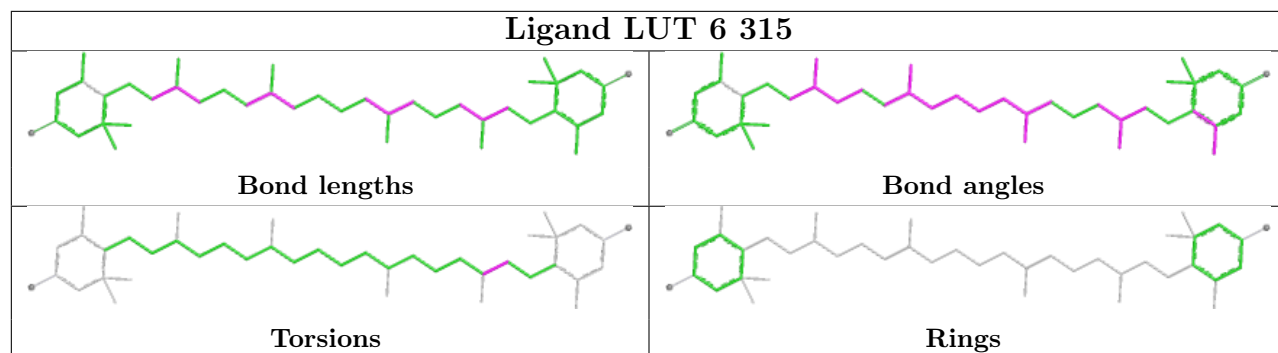
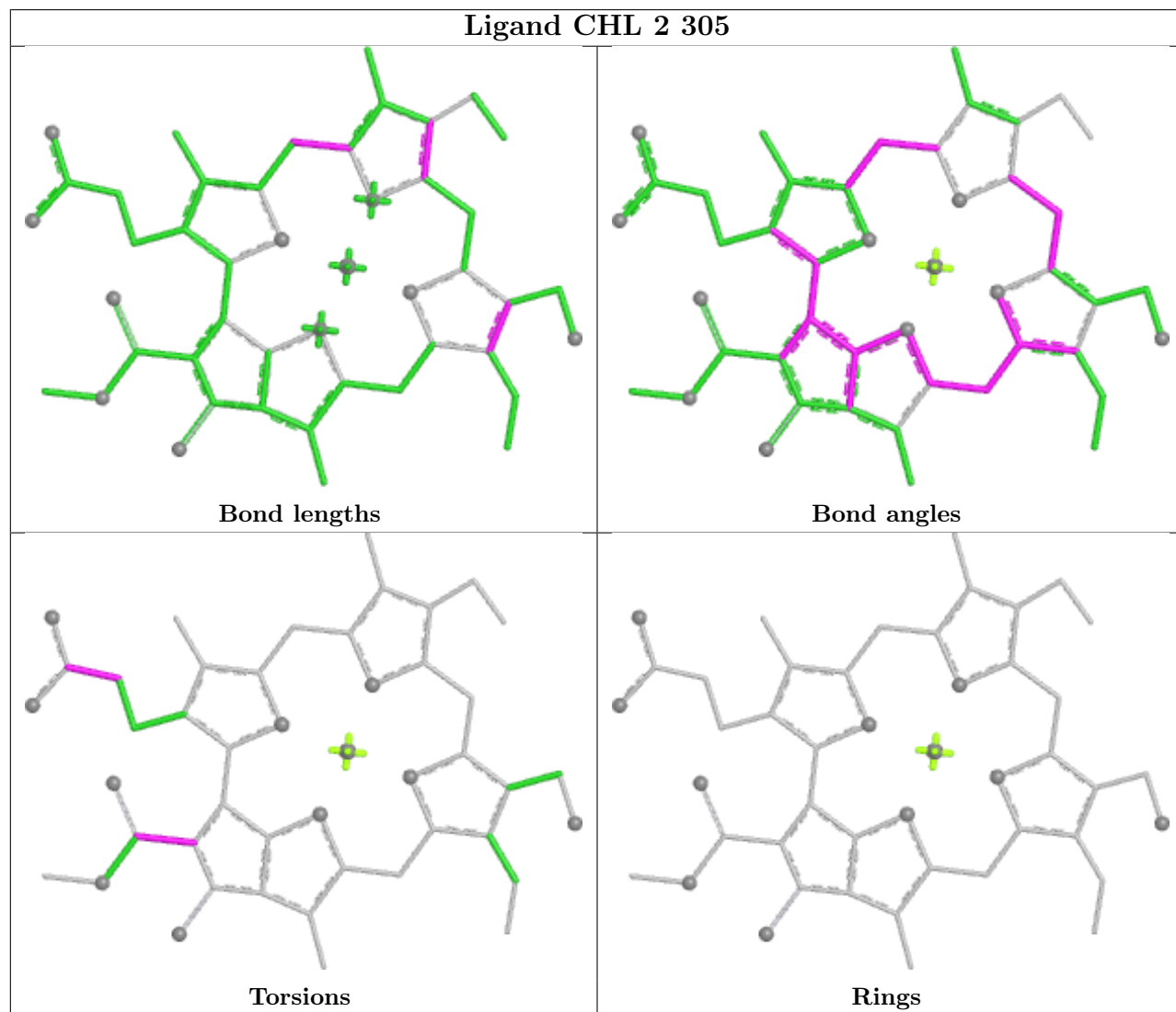
Bond angles



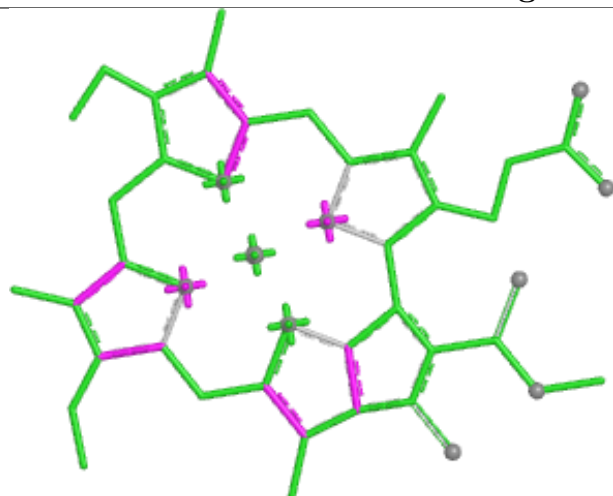
Torsions



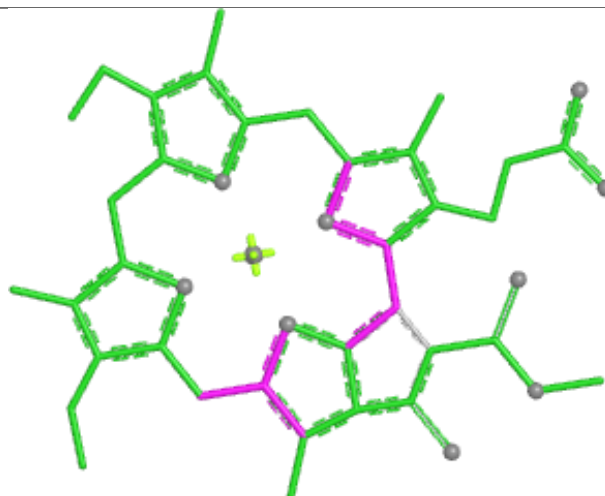
Rings

Ligand LUT 6 315**Ligand CHL 2 305**

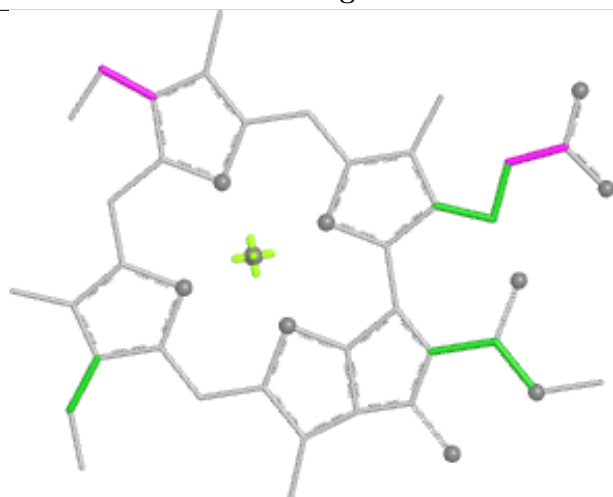
Ligand CLA 3 304



Bond lengths



Bond angles

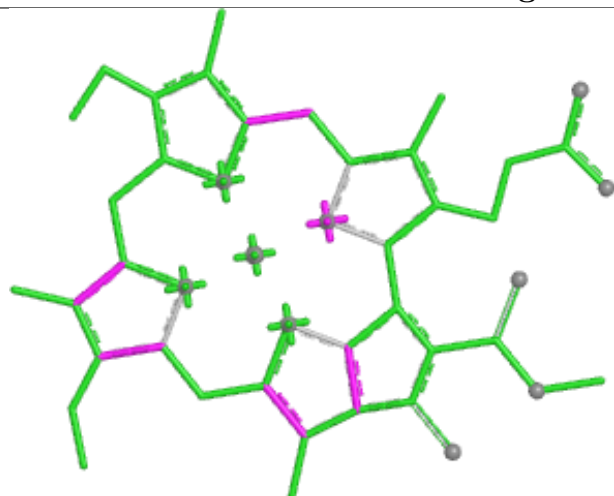


Torsions

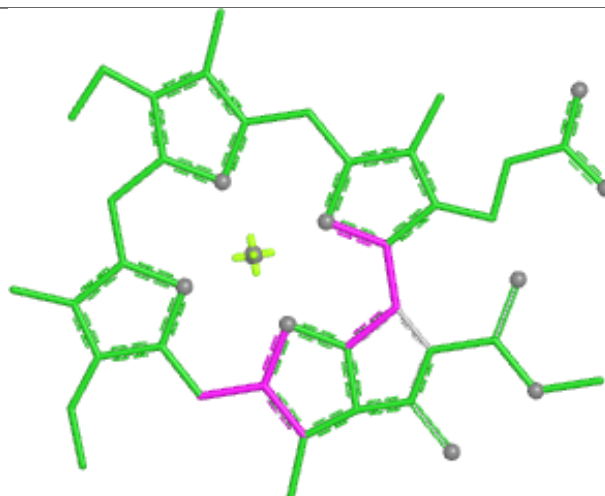


Rings

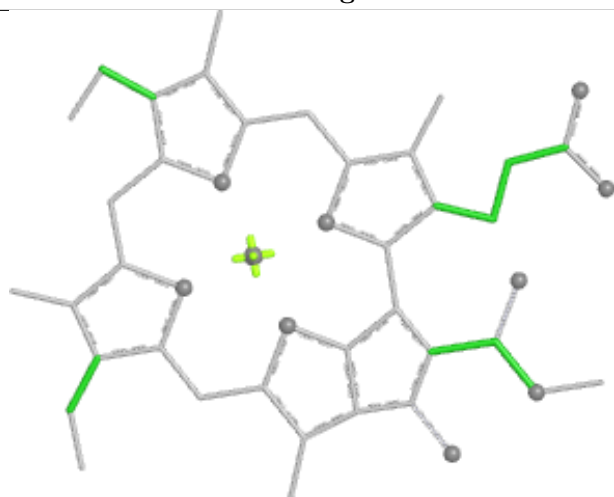
Ligand CLA 2 308



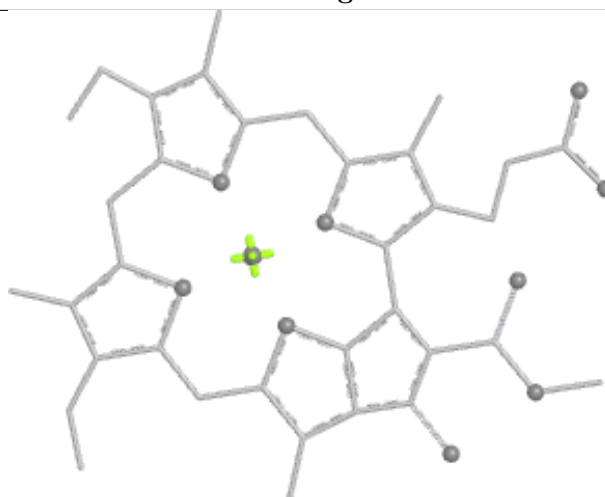
Bond lengths



Bond angles

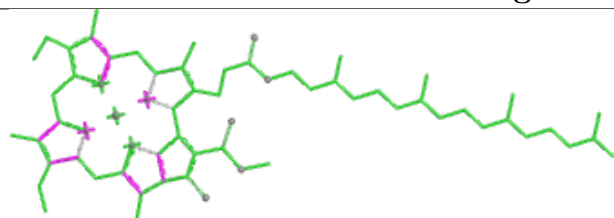


Torsions

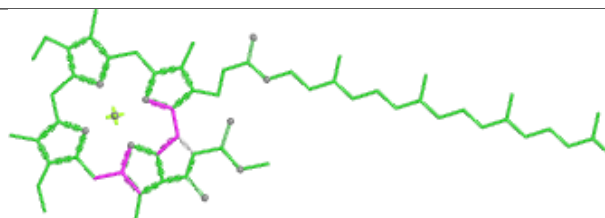


Rings

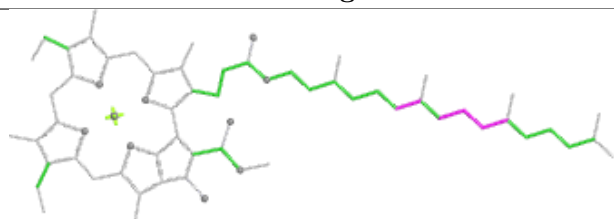
Ligand CLA A 820



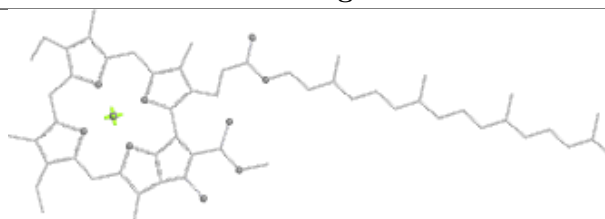
Bond lengths



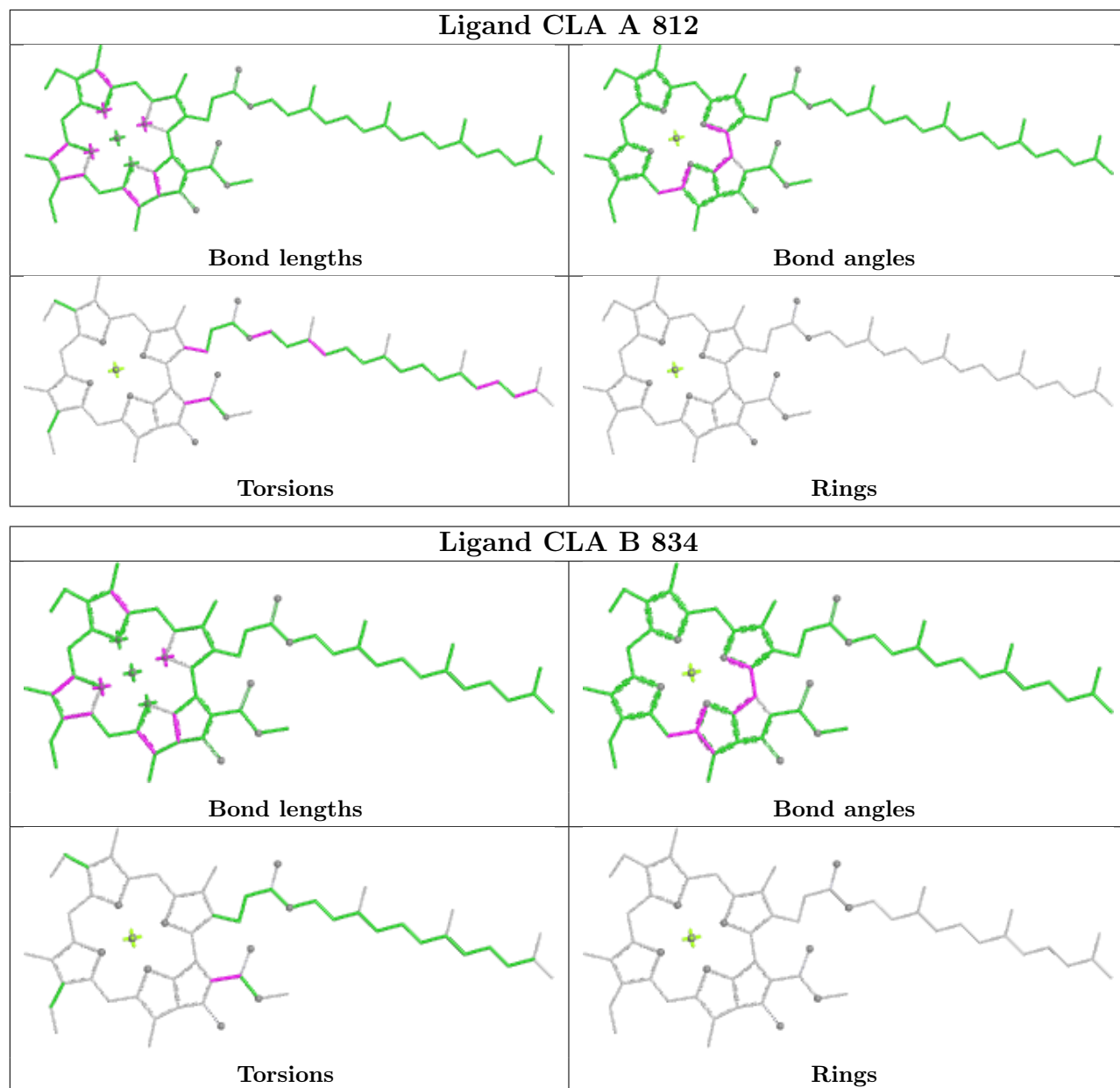
Bond angles

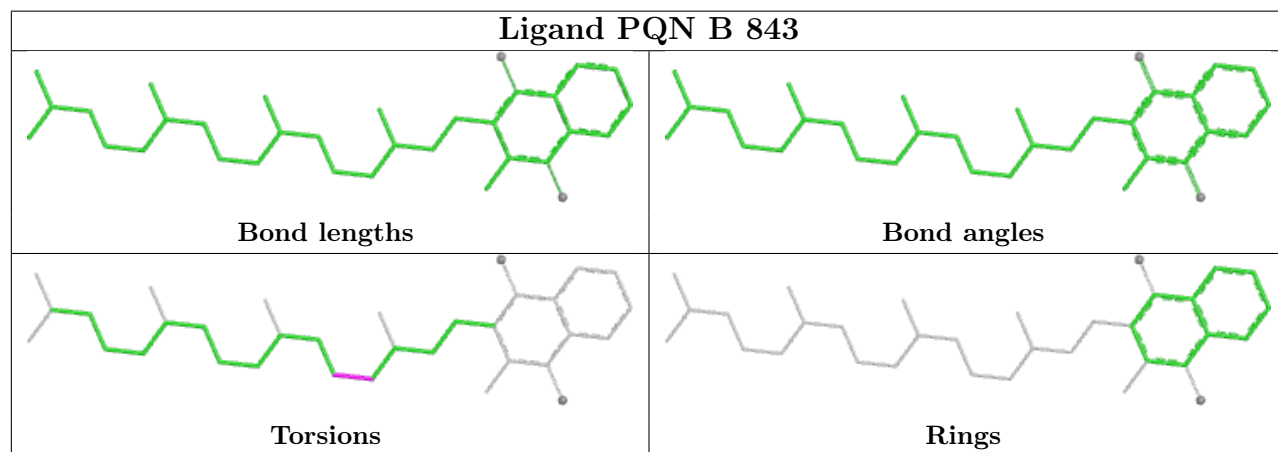
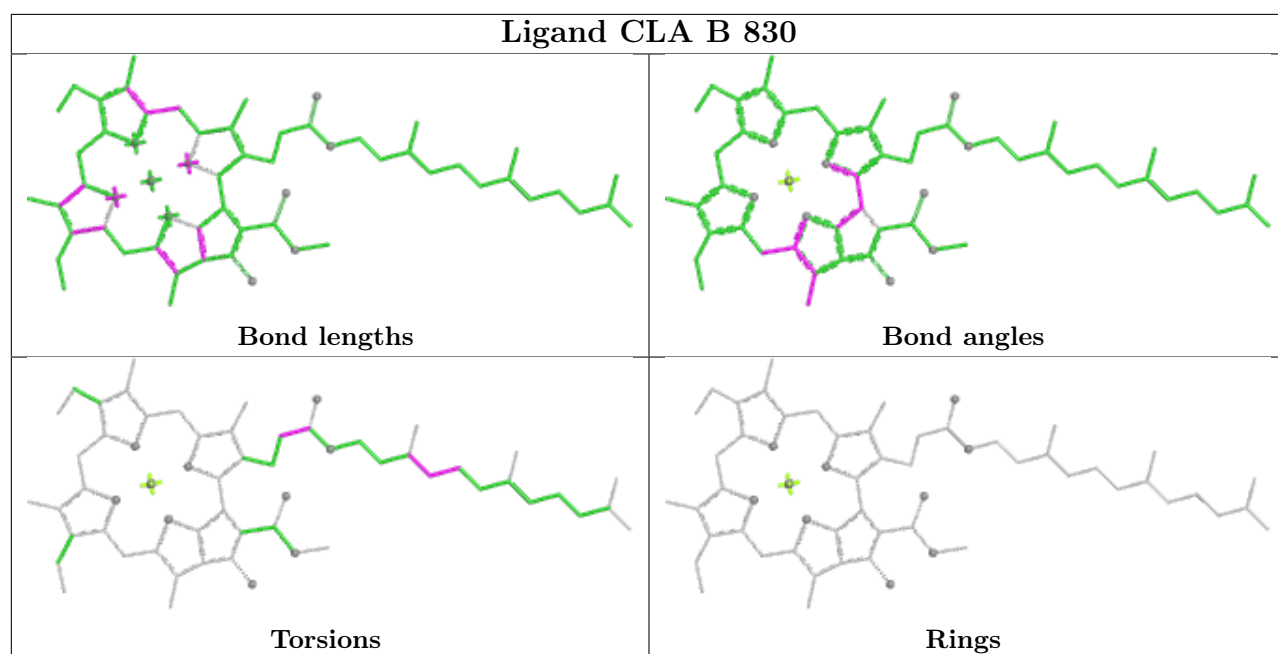


Torsions

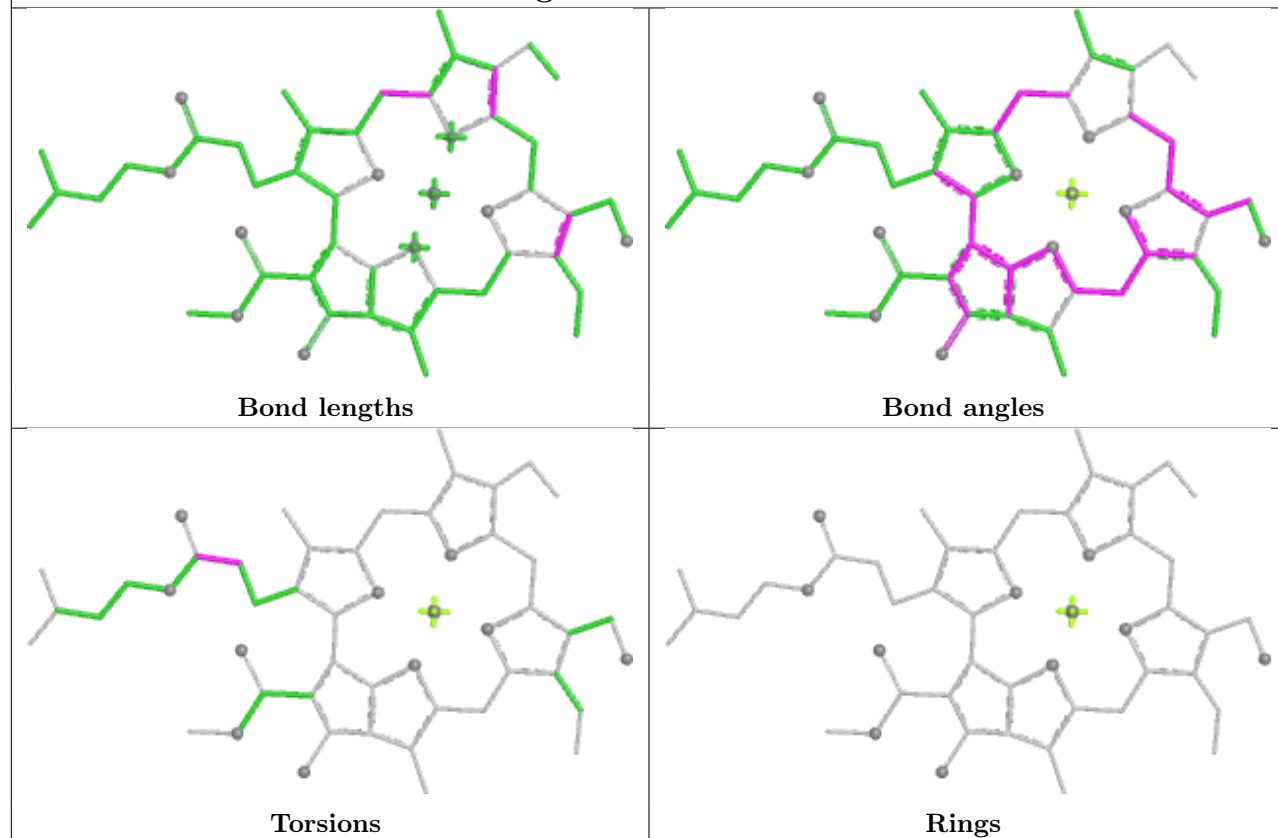


Rings

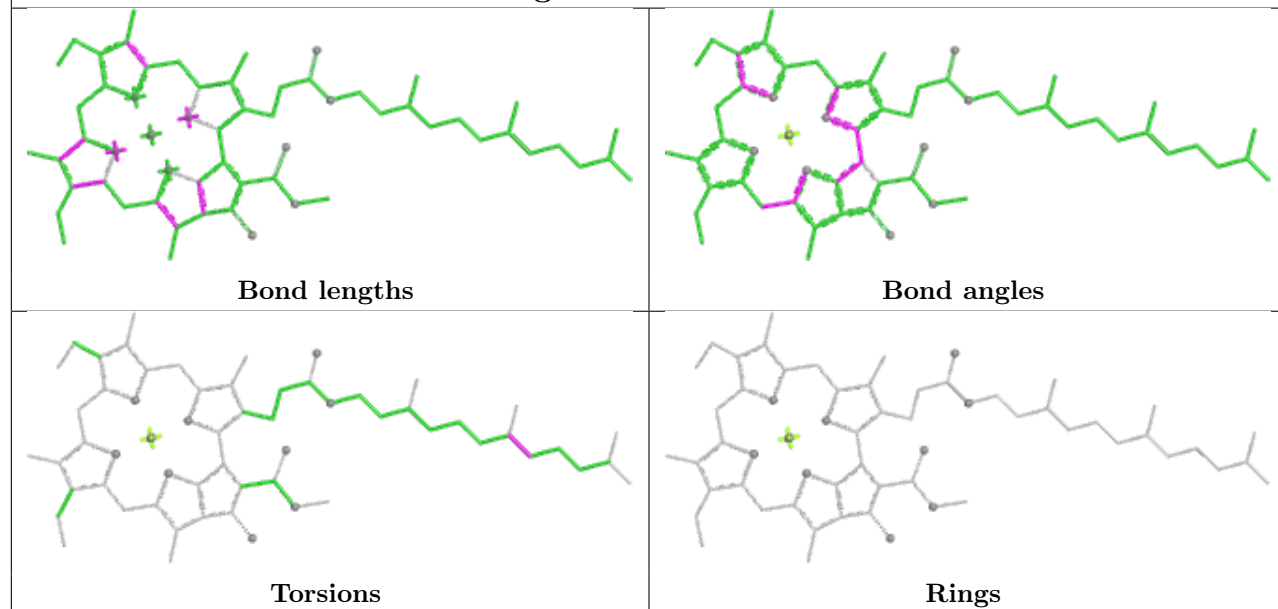


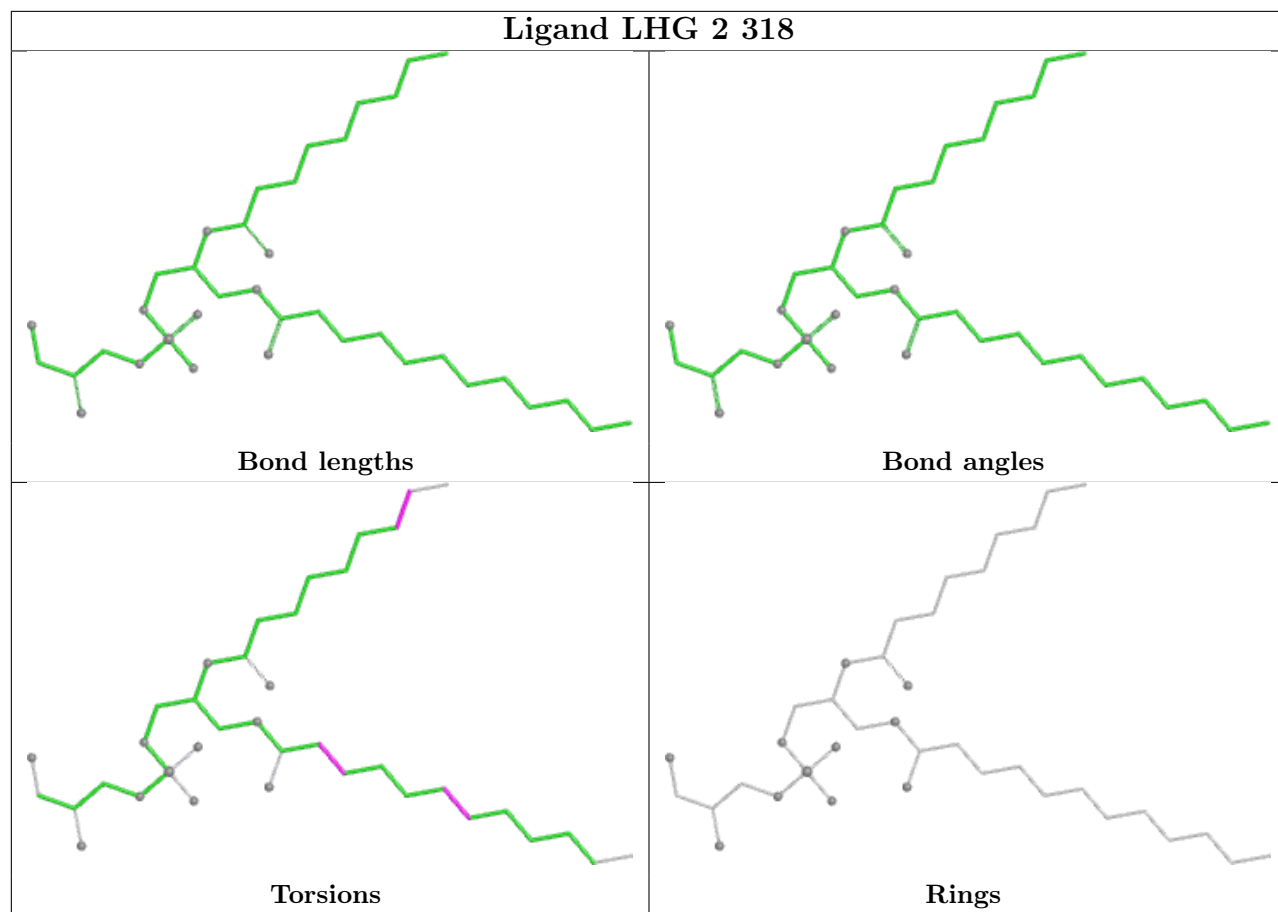


Ligand CHL 6 301

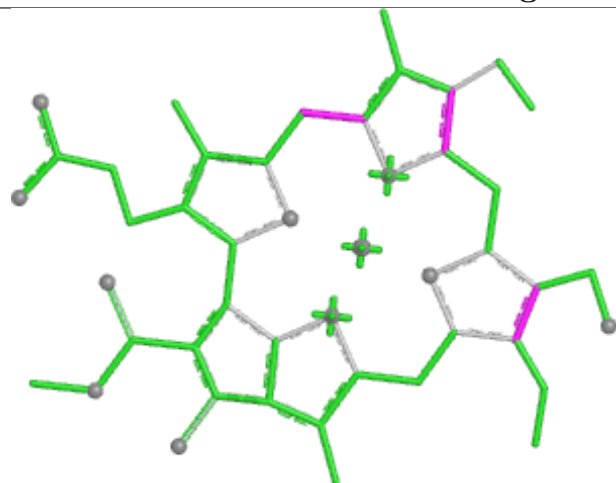


Ligand CLA F 301

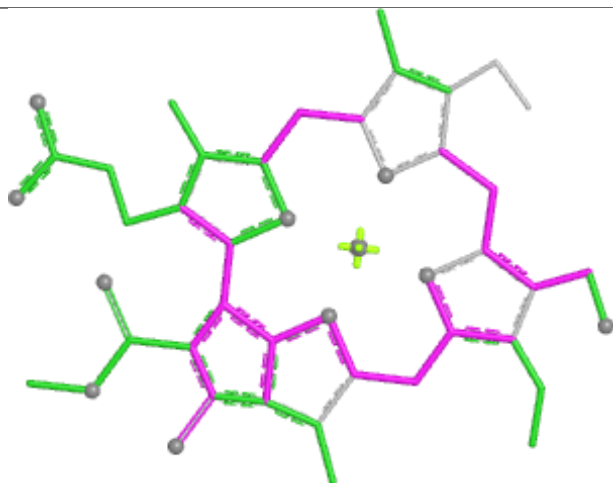




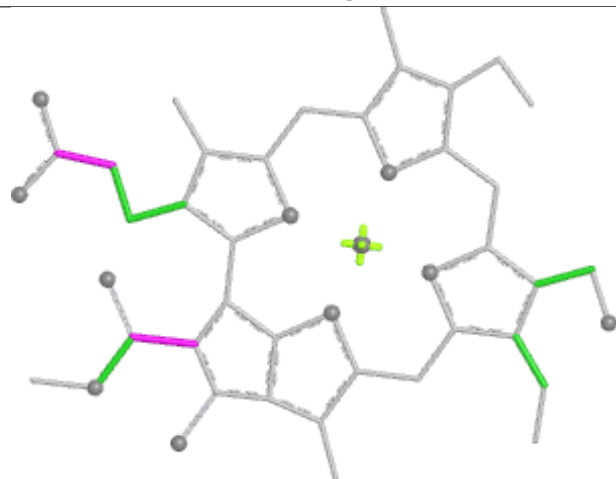
Ligand CHL 2 314



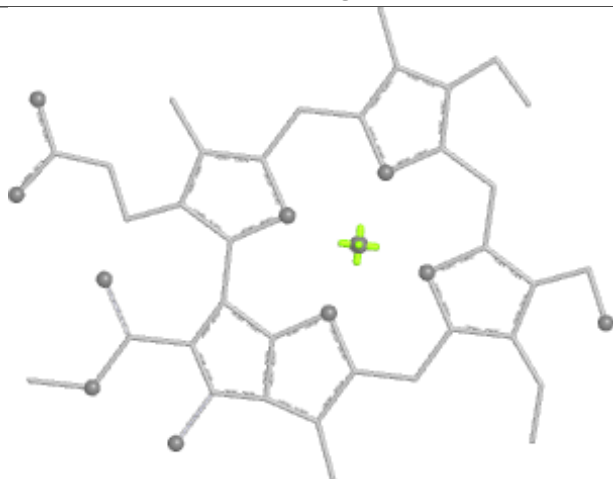
Bond lengths



Bond angles

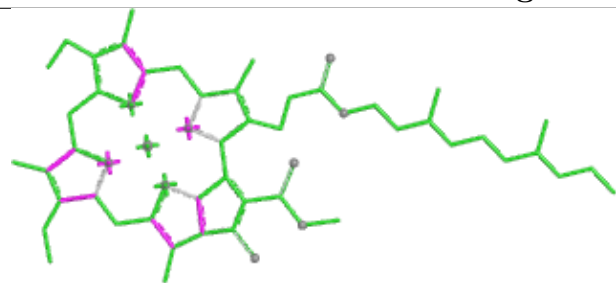


Torsions

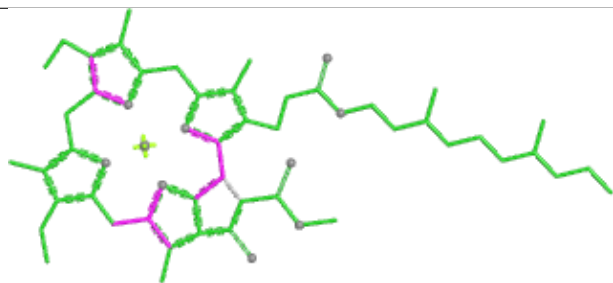


Rings

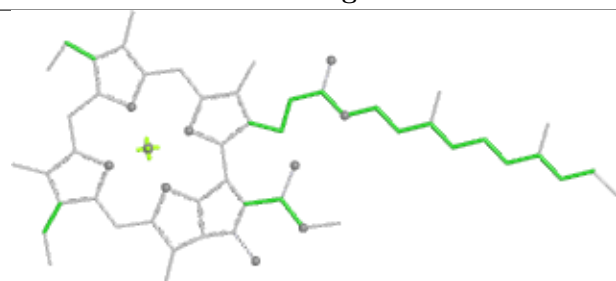
Ligand CLA B 820



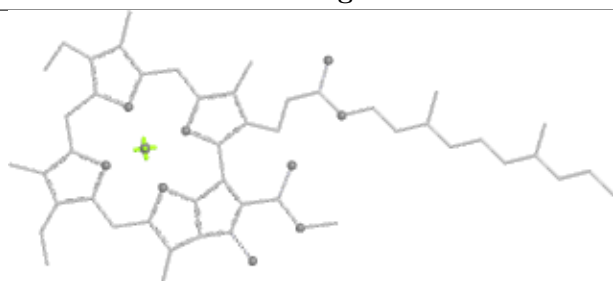
Bond lengths



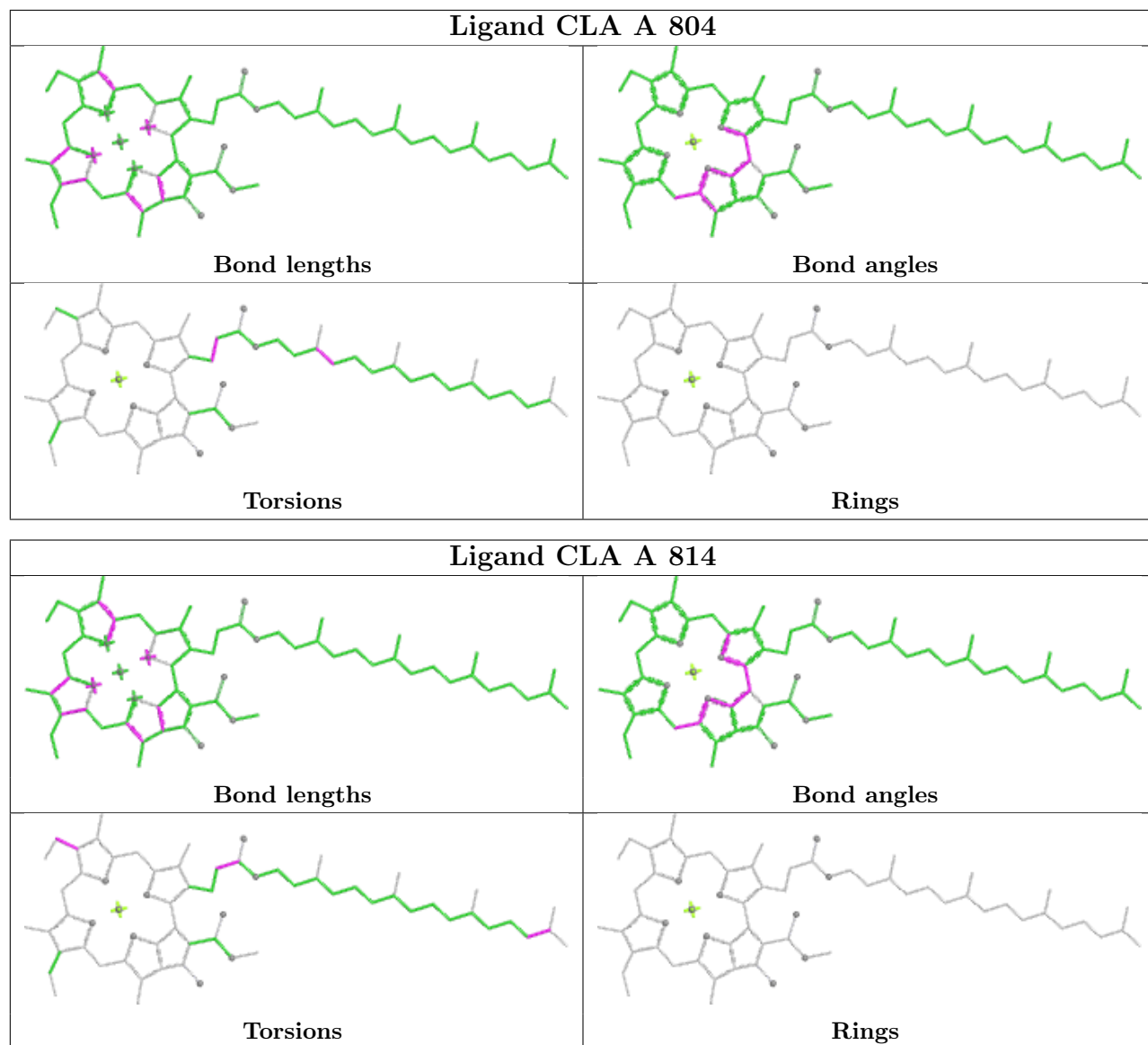
Bond angles



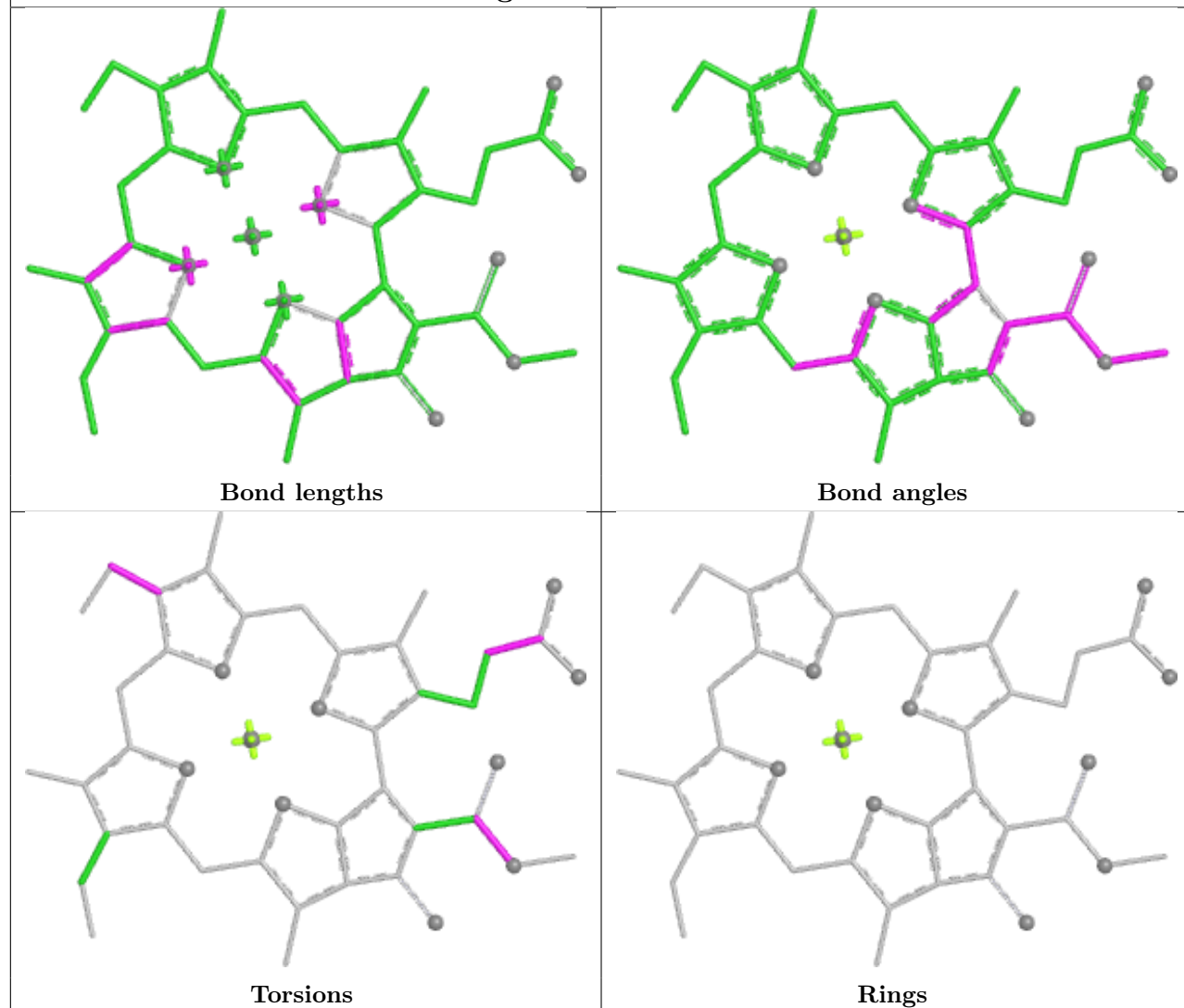
Torsions



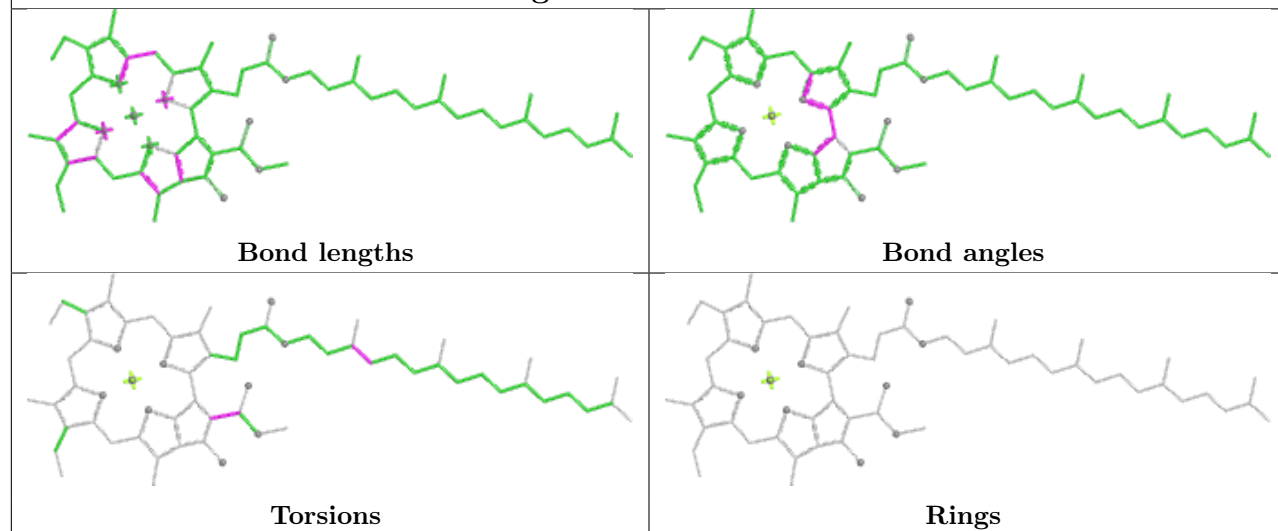
Rings

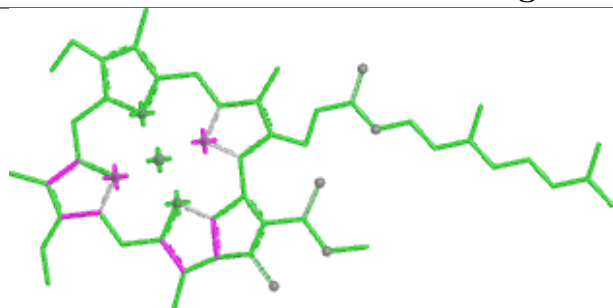


Ligand CLA 5 314

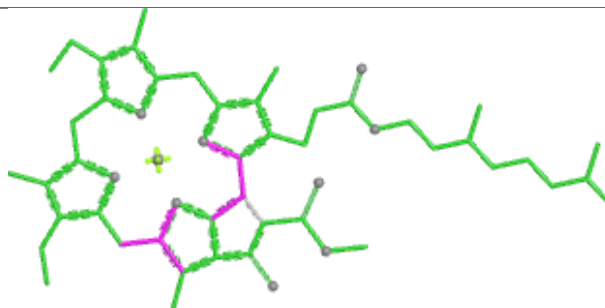


Ligand CLA A 831

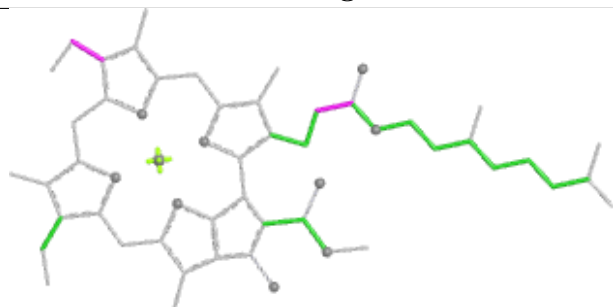


Ligand CLA 6 303

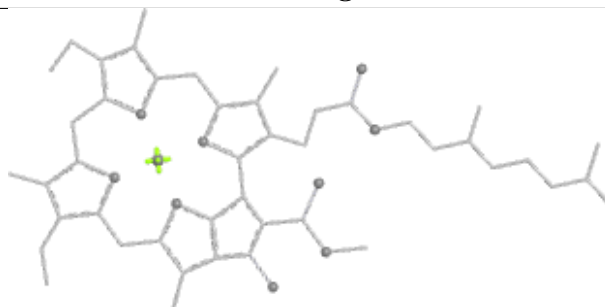
Bond lengths



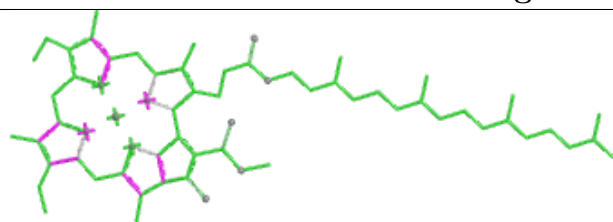
Bond angles



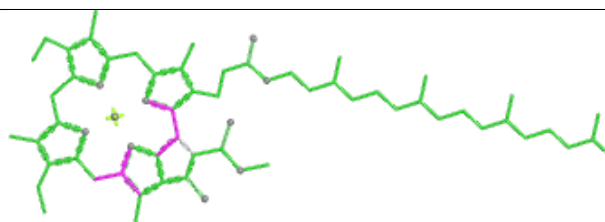
Torsions



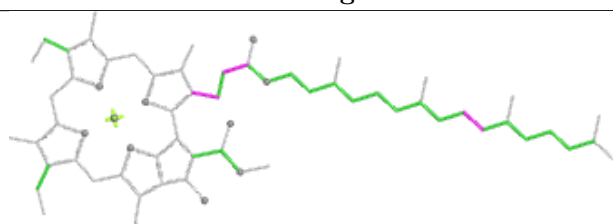
Rings

Ligand CLA B 806

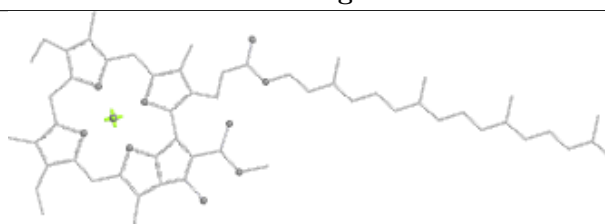
Bond lengths



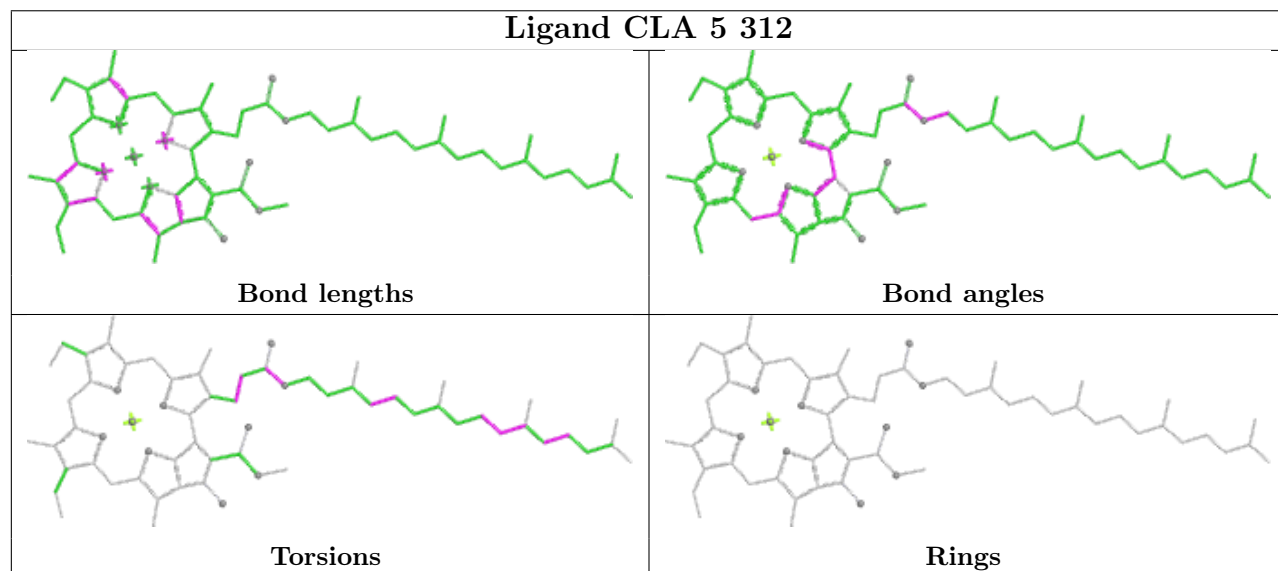
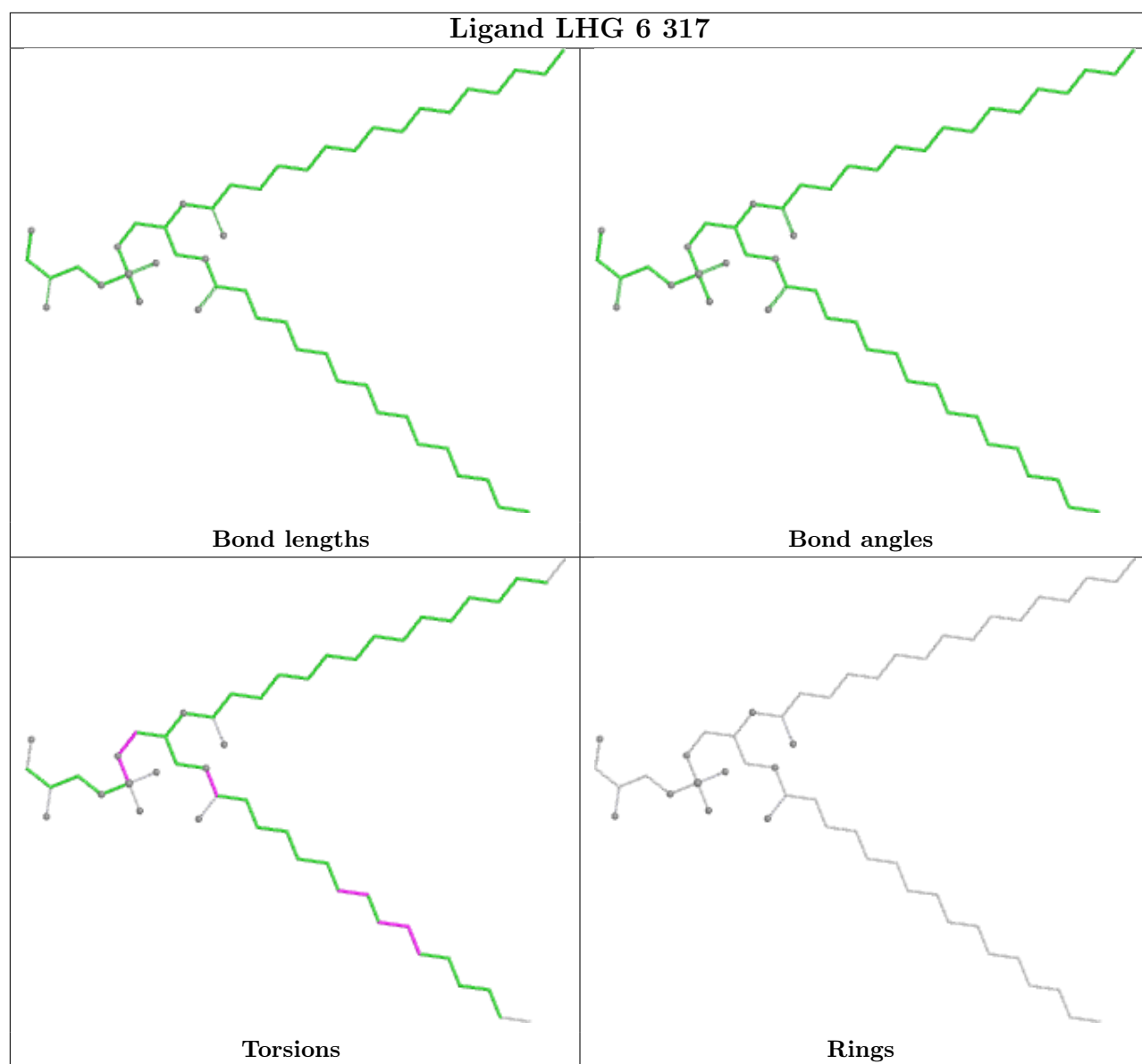
Bond angles

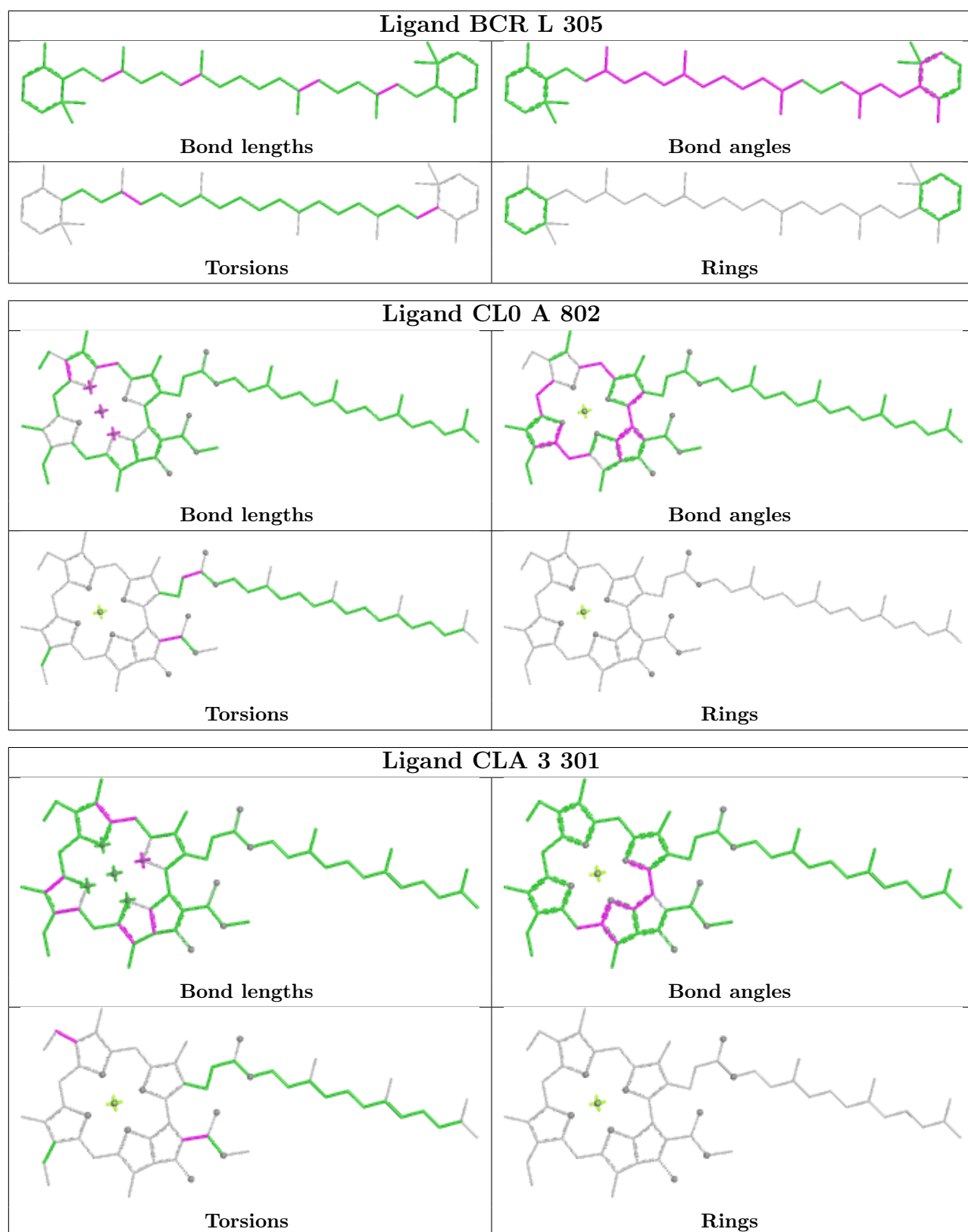


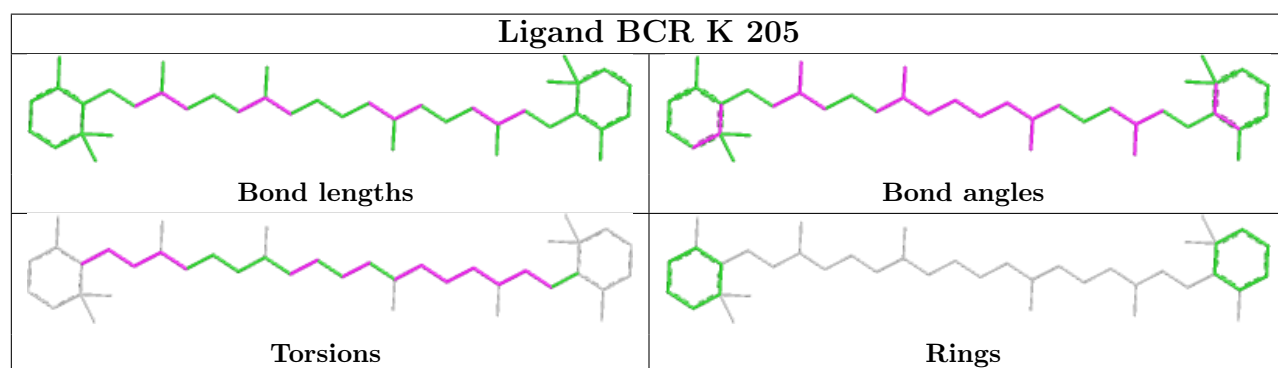
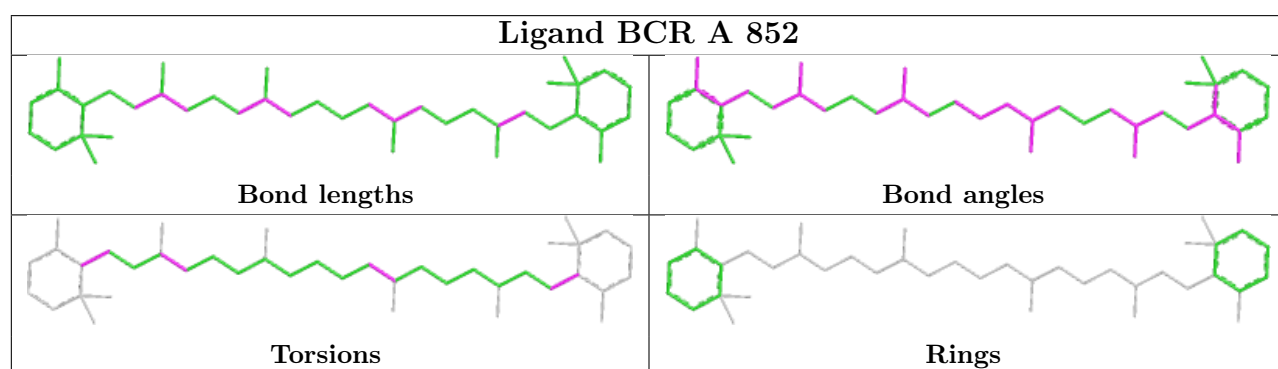
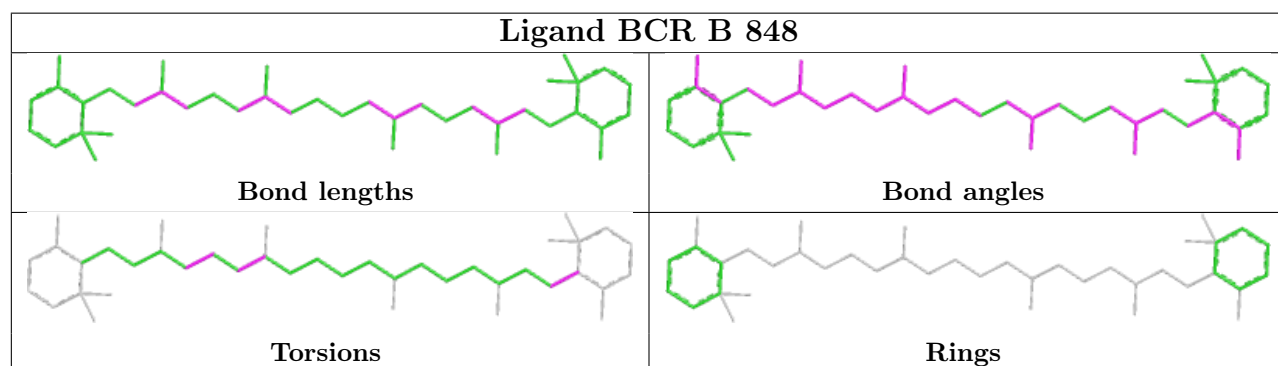
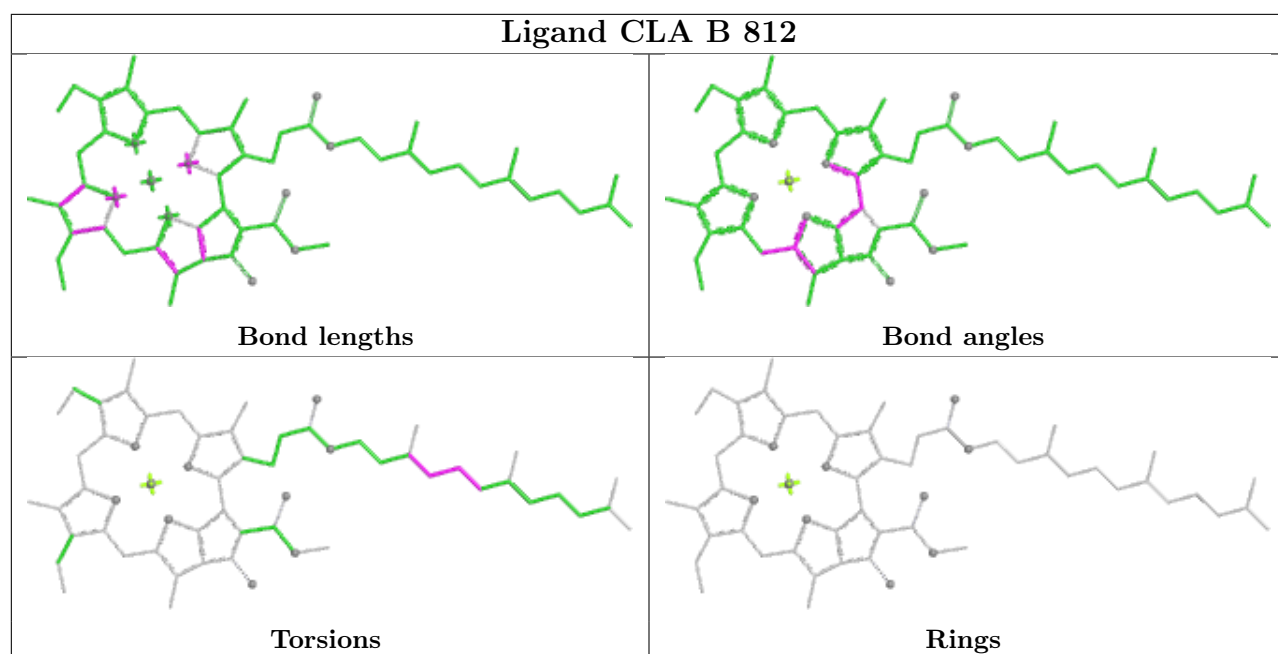
Torsions

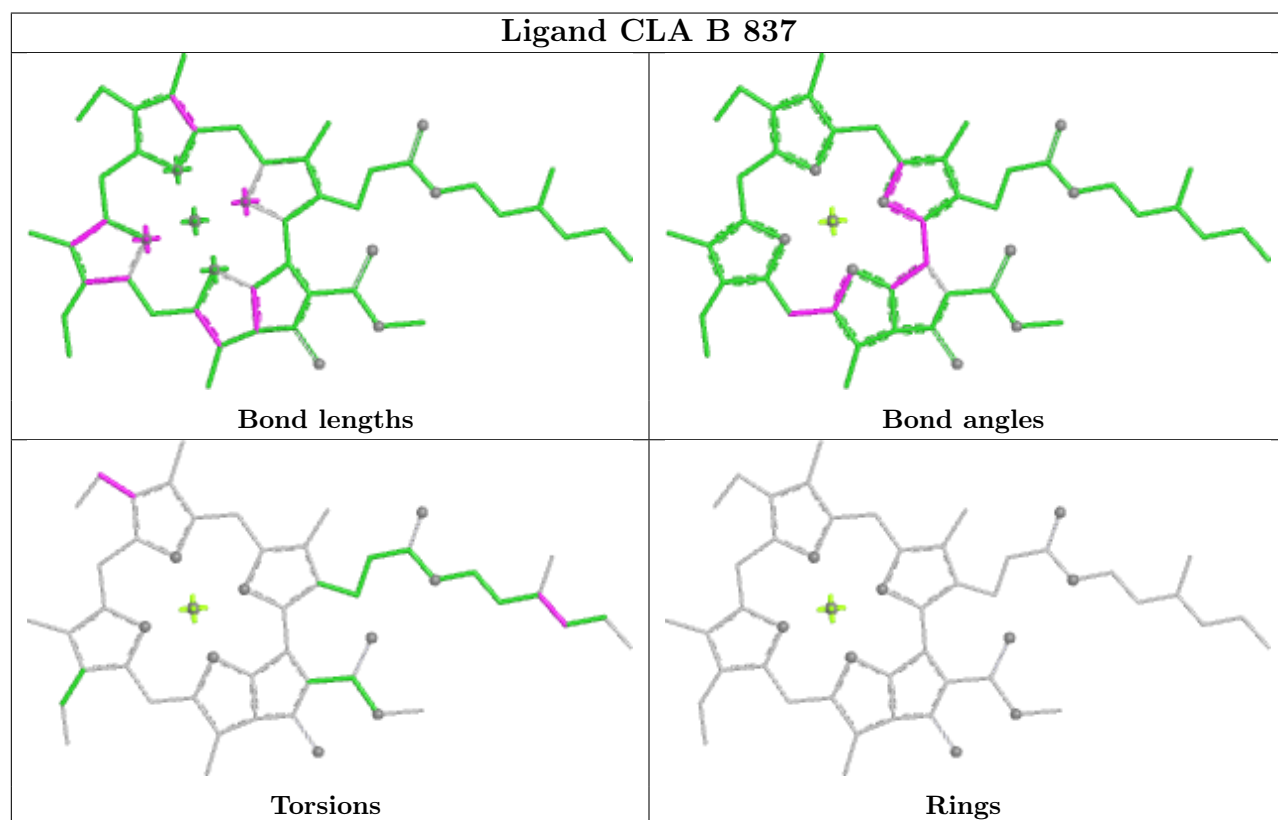
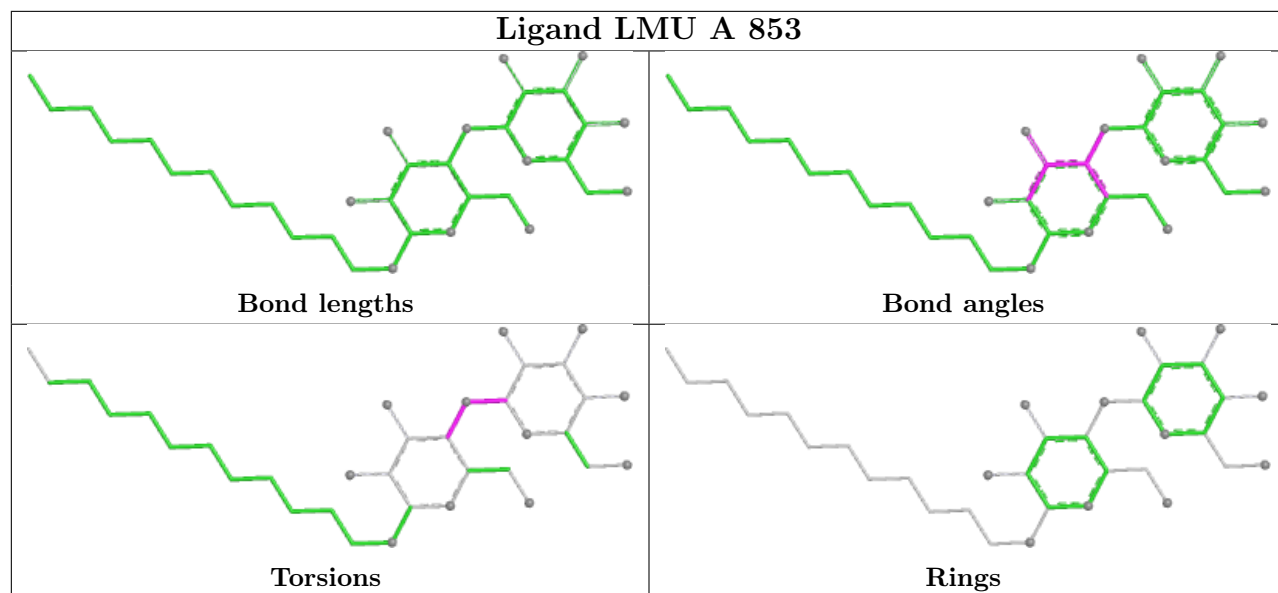


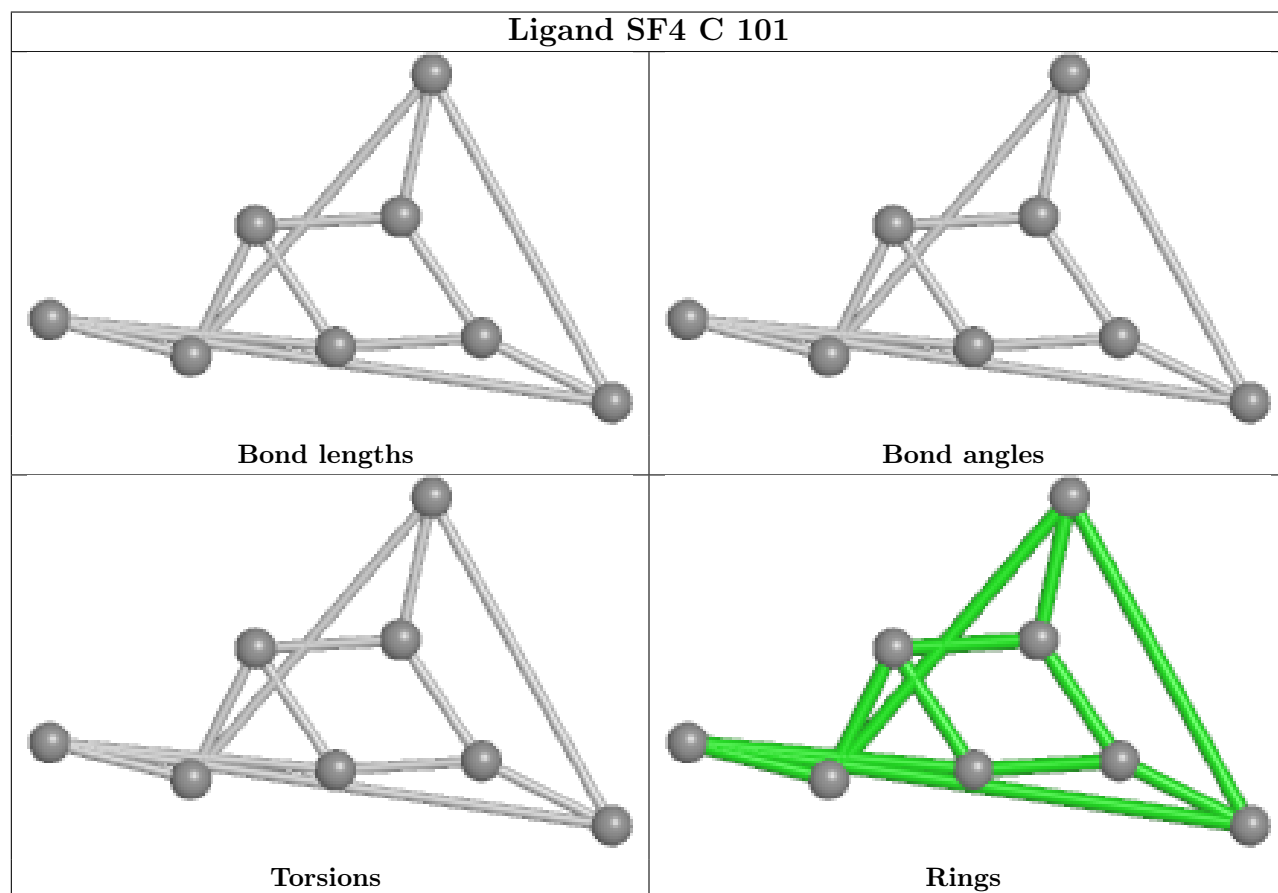
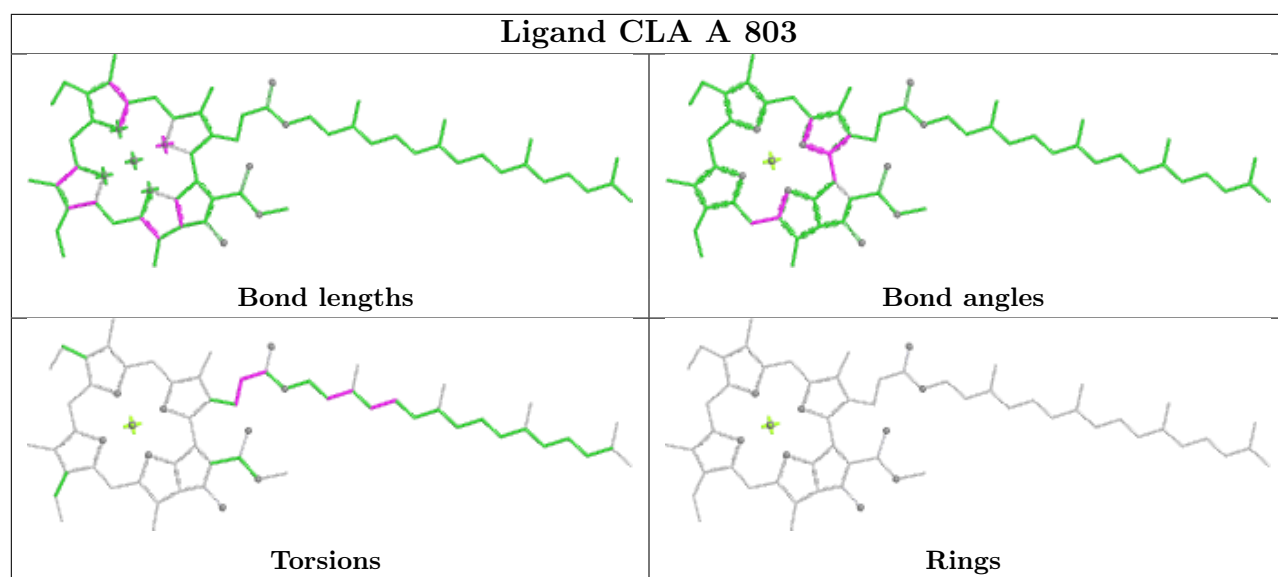
Rings

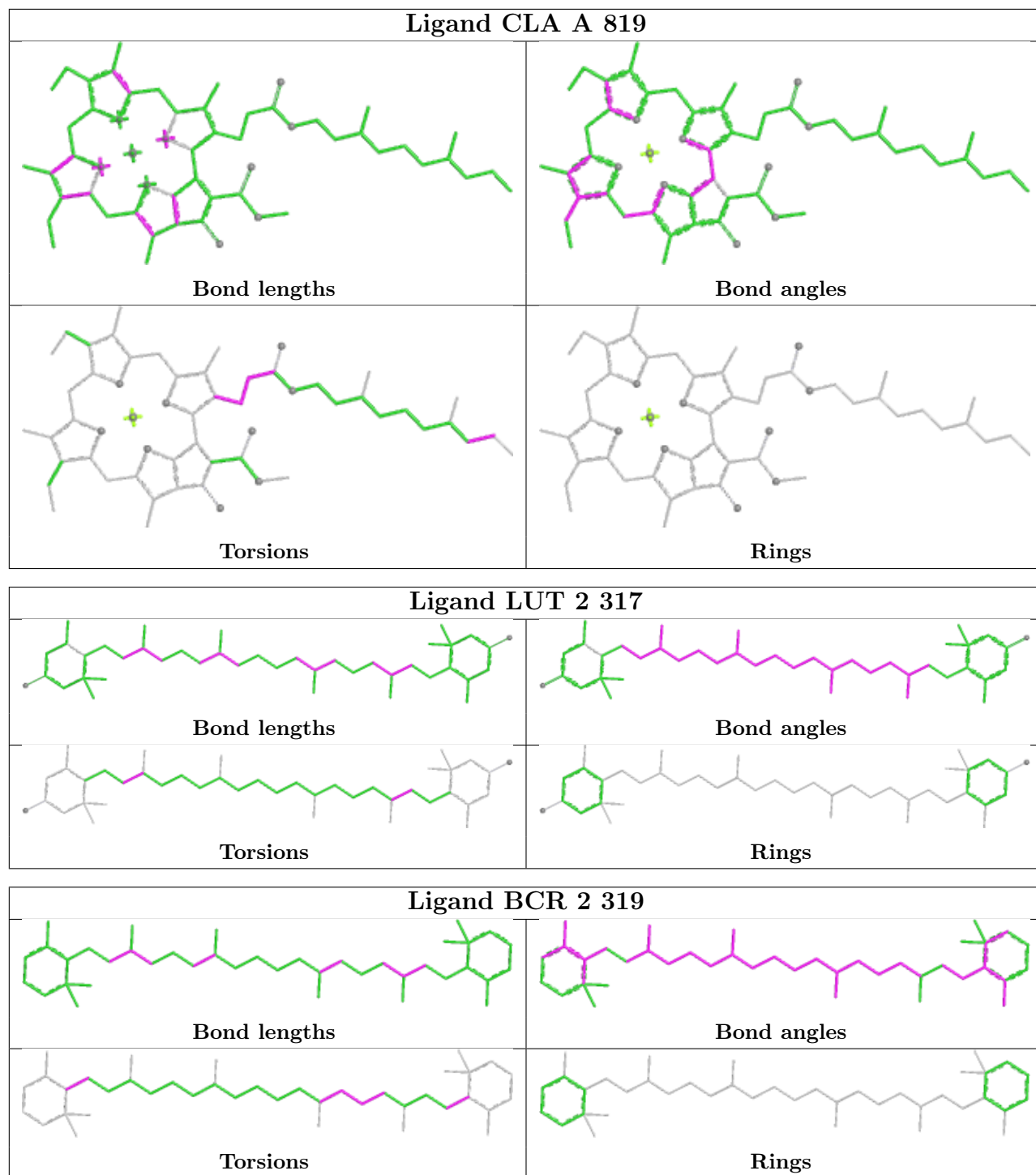




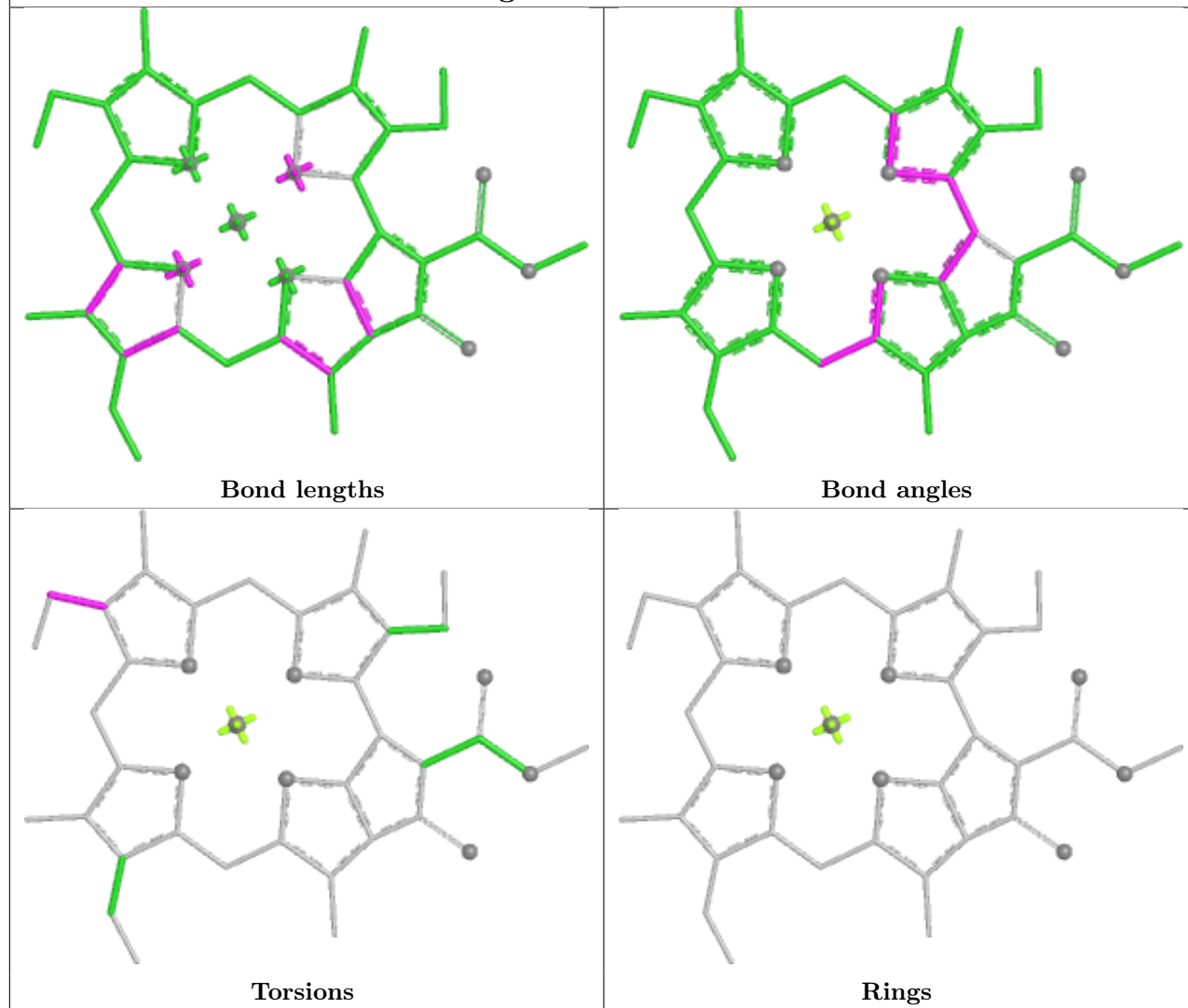




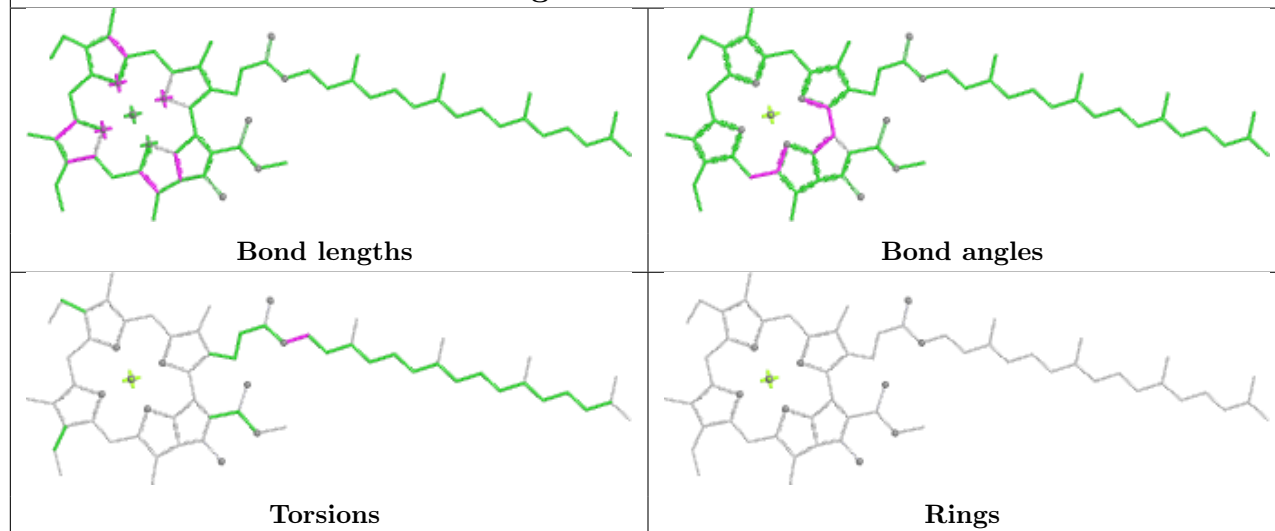


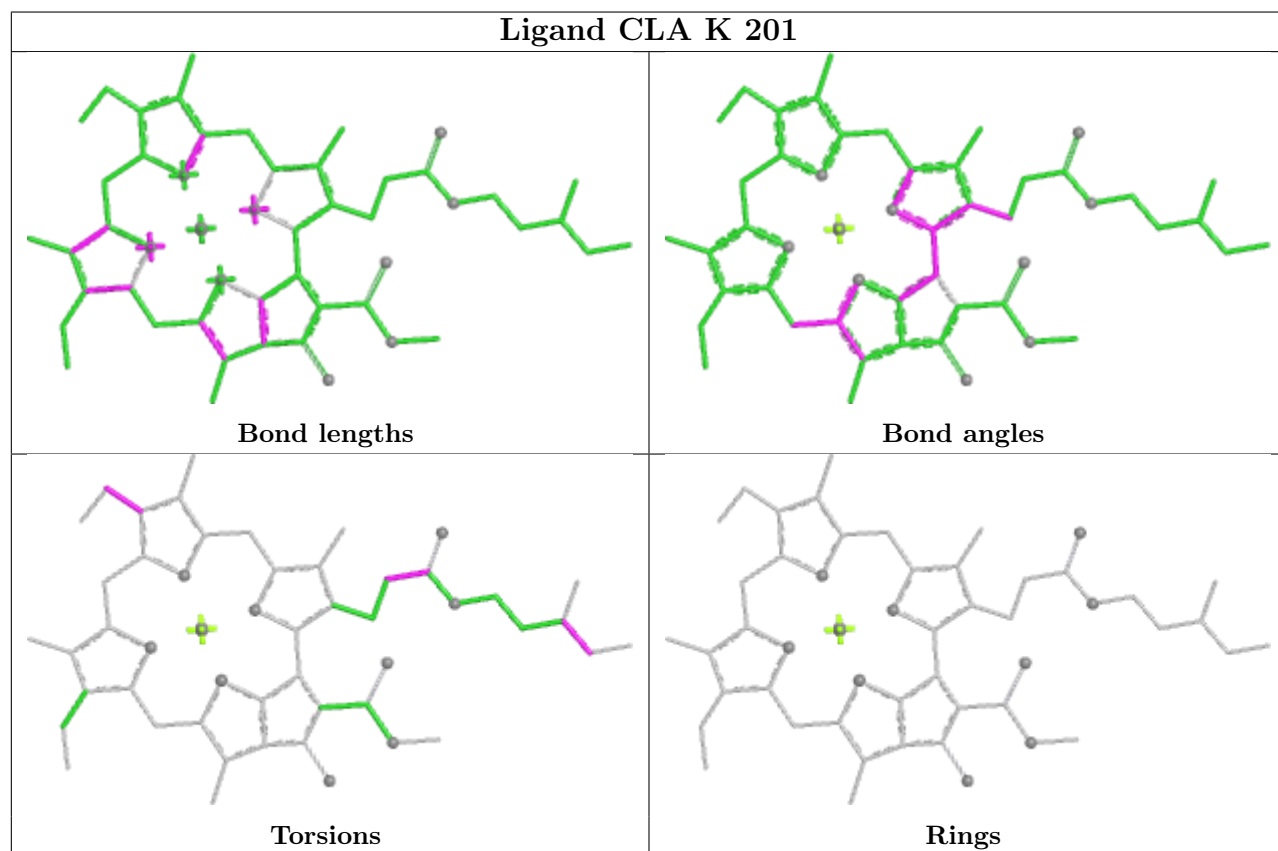
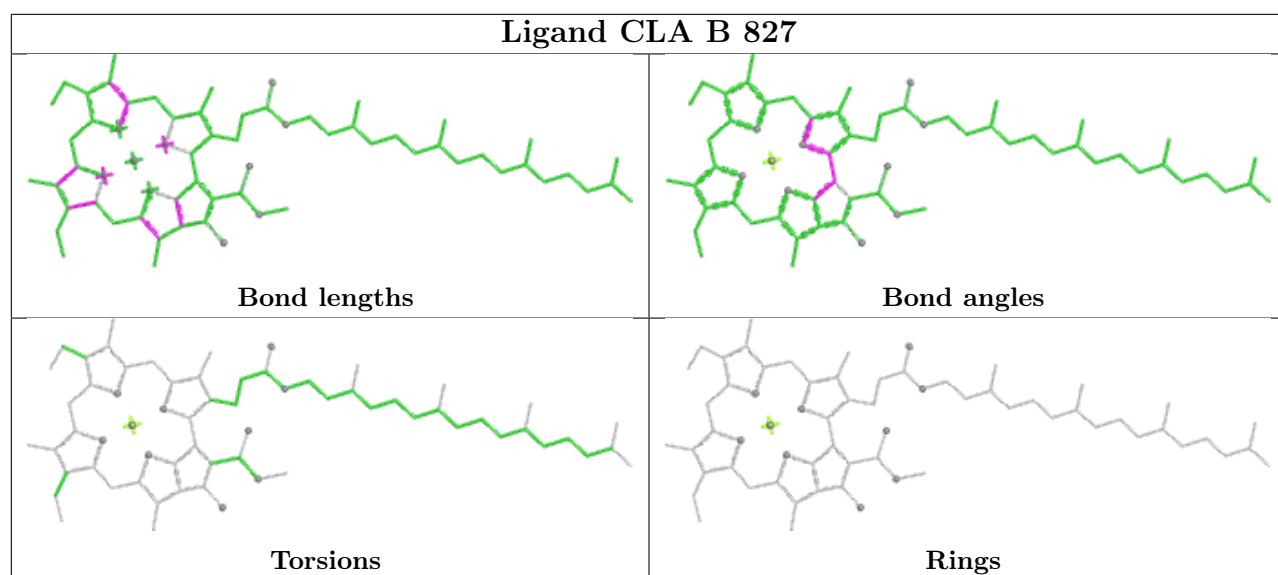


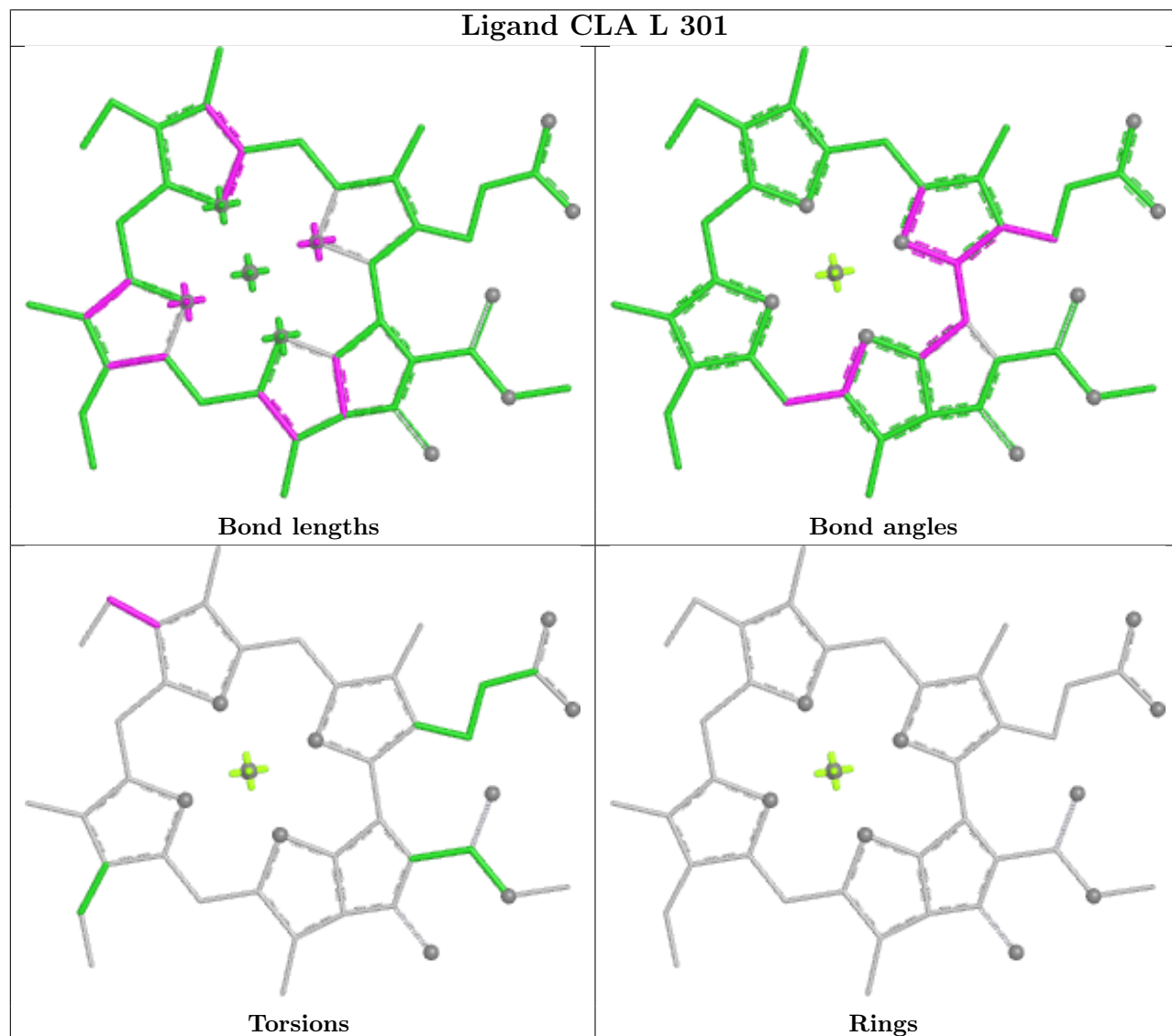
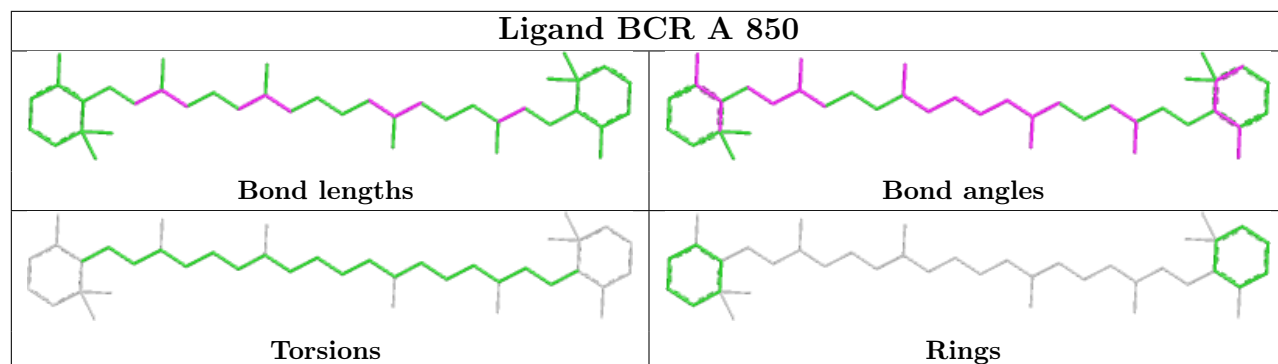
Ligand CLA 3 312

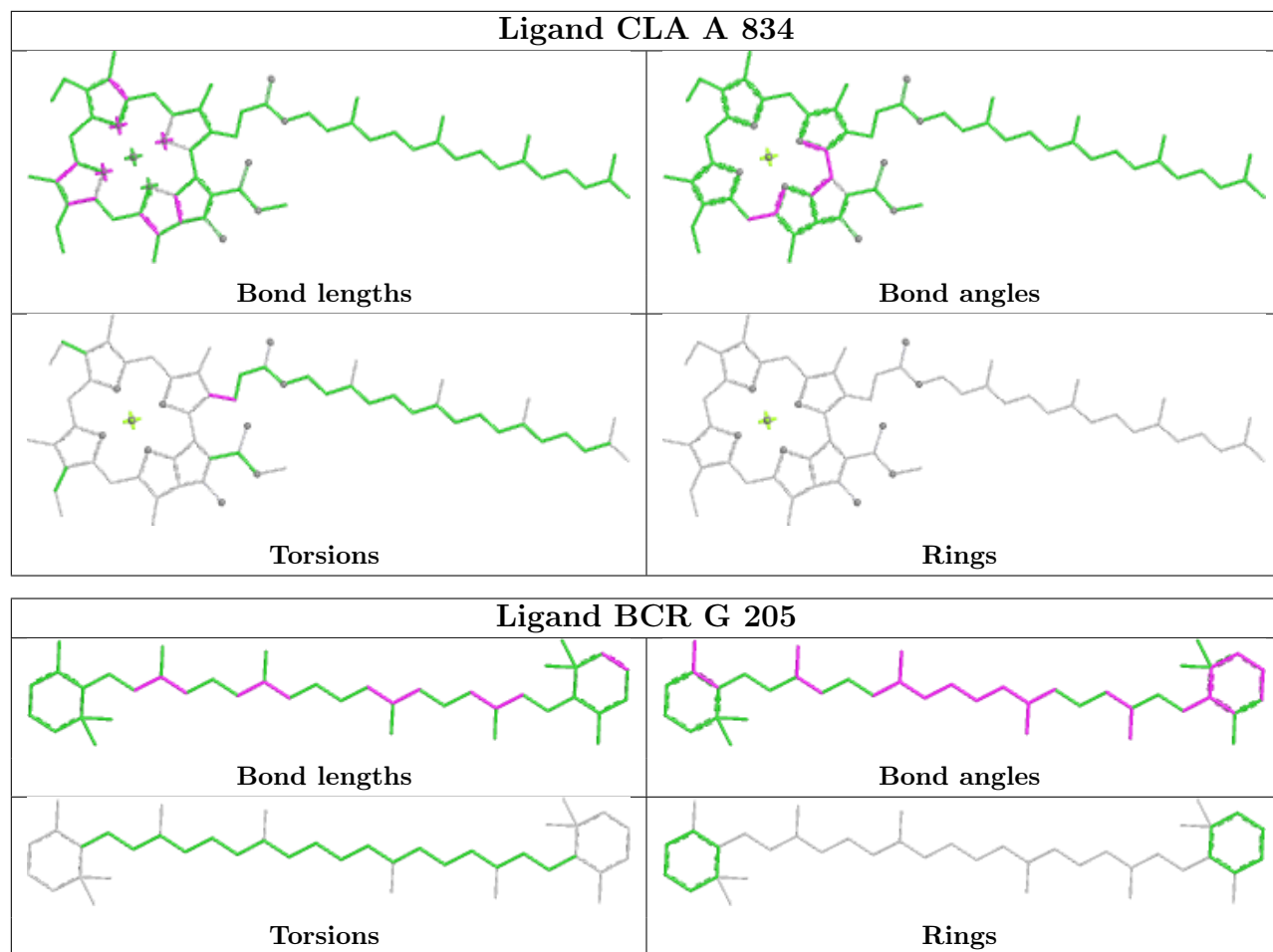


Ligand CLA B 841

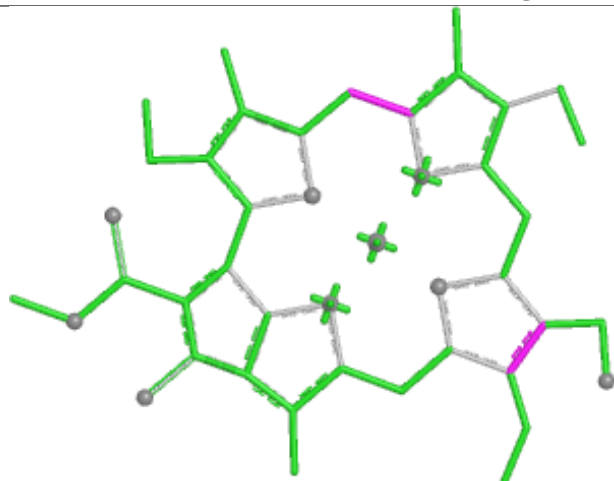




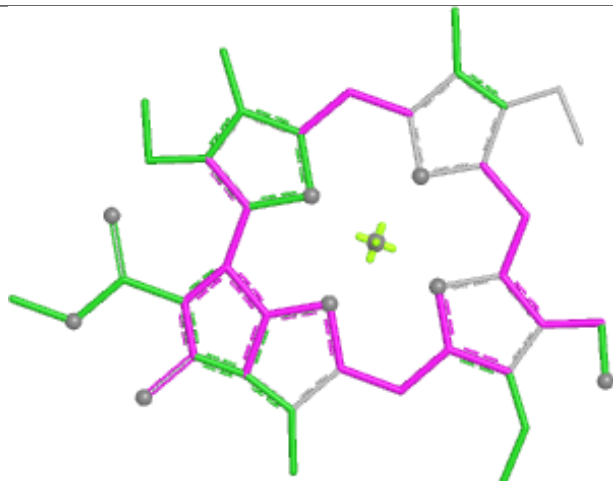




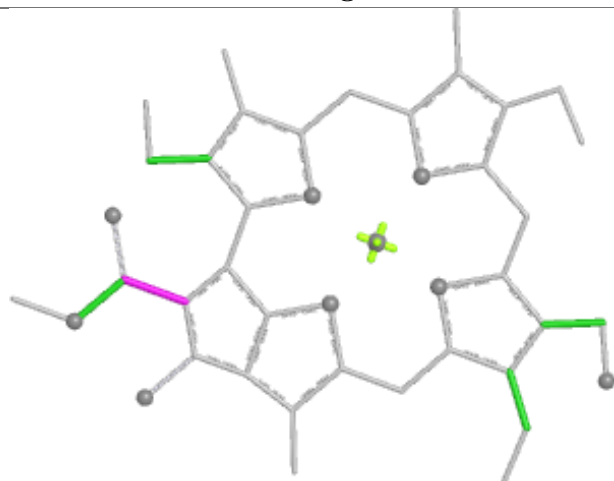
Ligand CHL 5 313



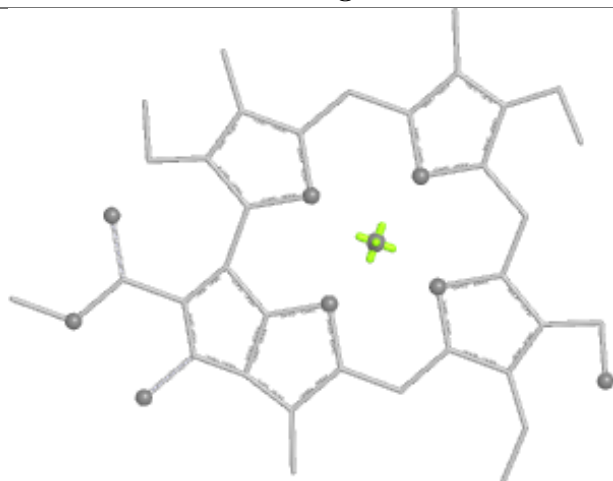
Bond lengths



Bond angles

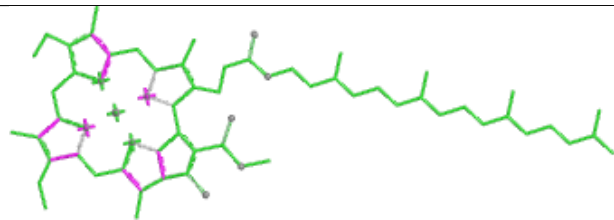


Torsions

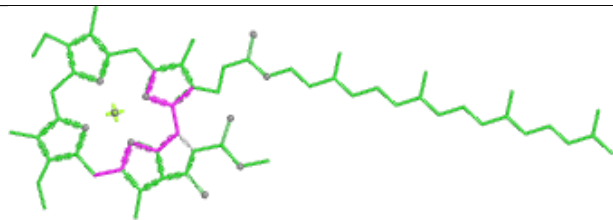


Rings

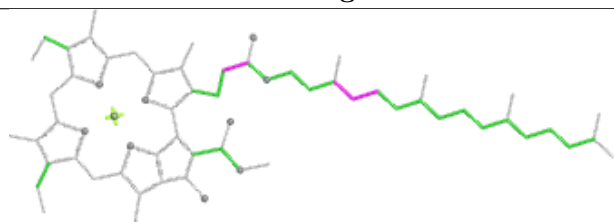
Ligand CLA B 810



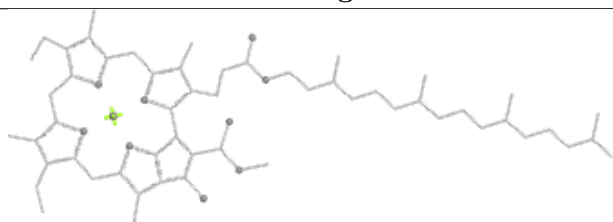
Bond lengths



Bond angles

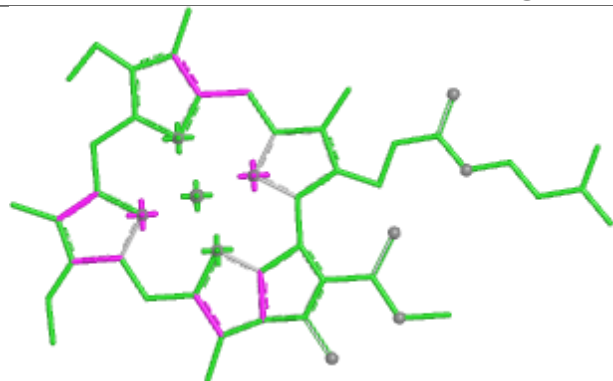


Torsions

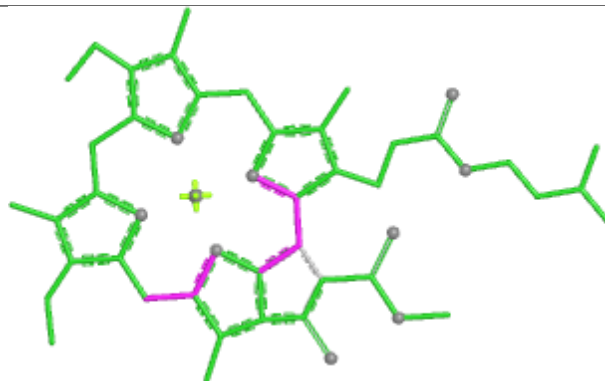


Rings

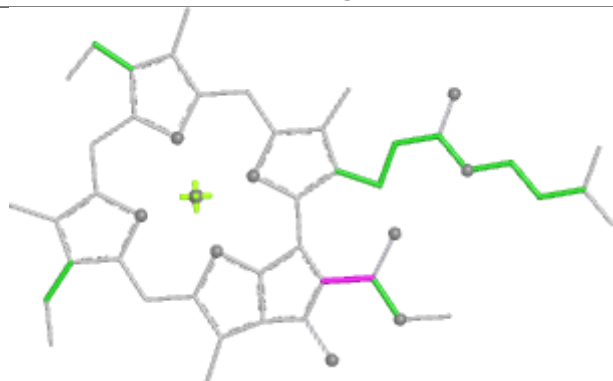
Ligand CLA 6 308



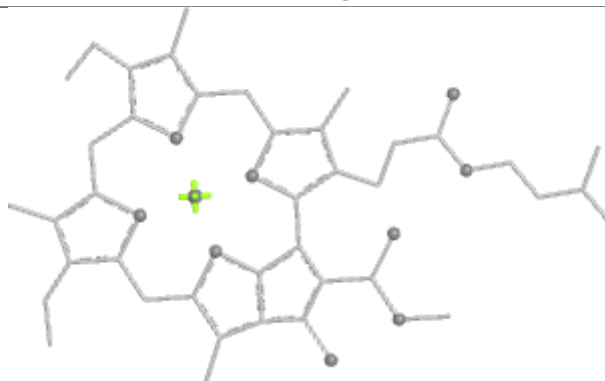
Bond lengths



Bond angles

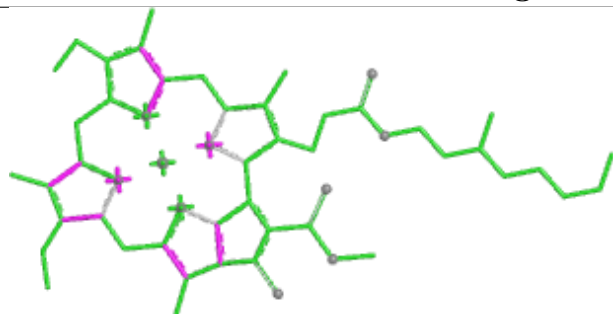


Torsions

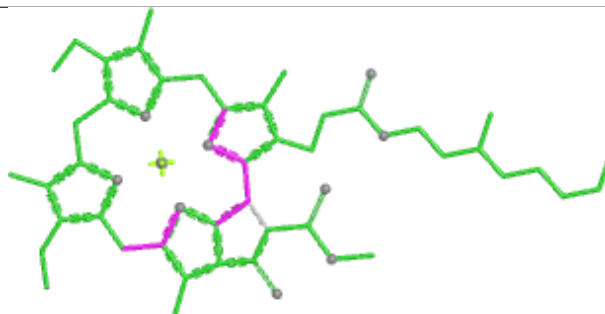


Rings

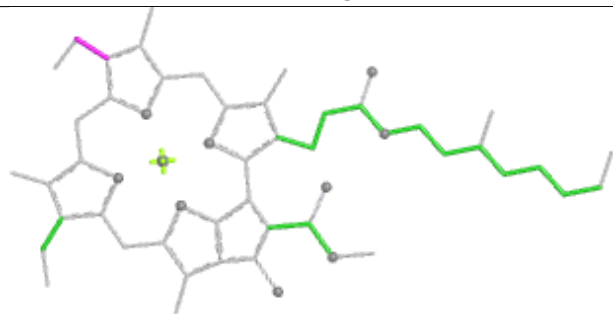
Ligand CLA A 813



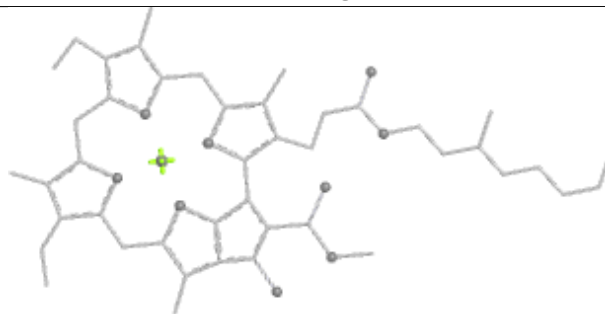
Bond lengths



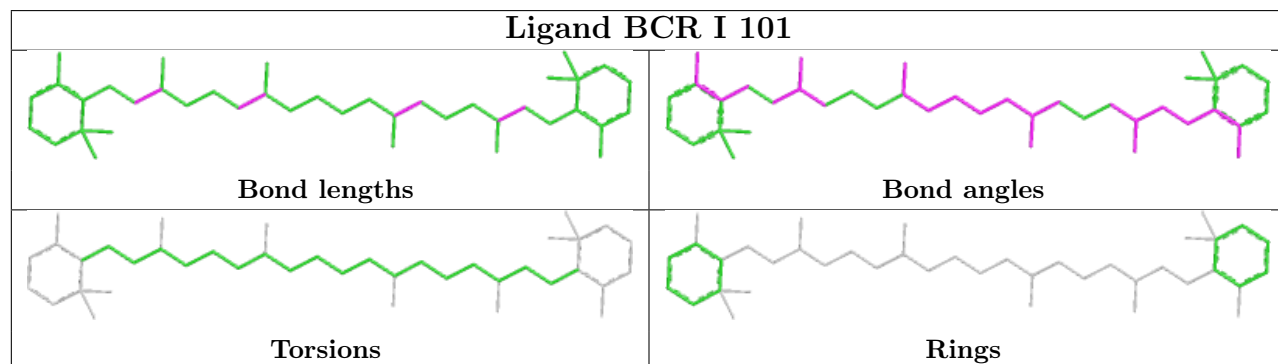
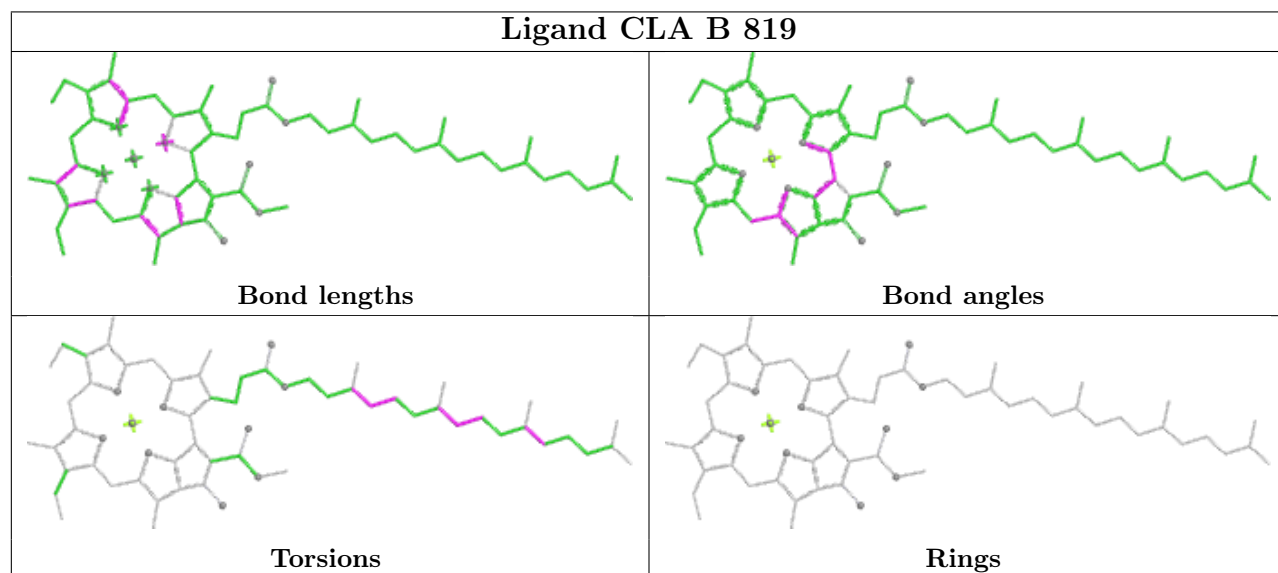
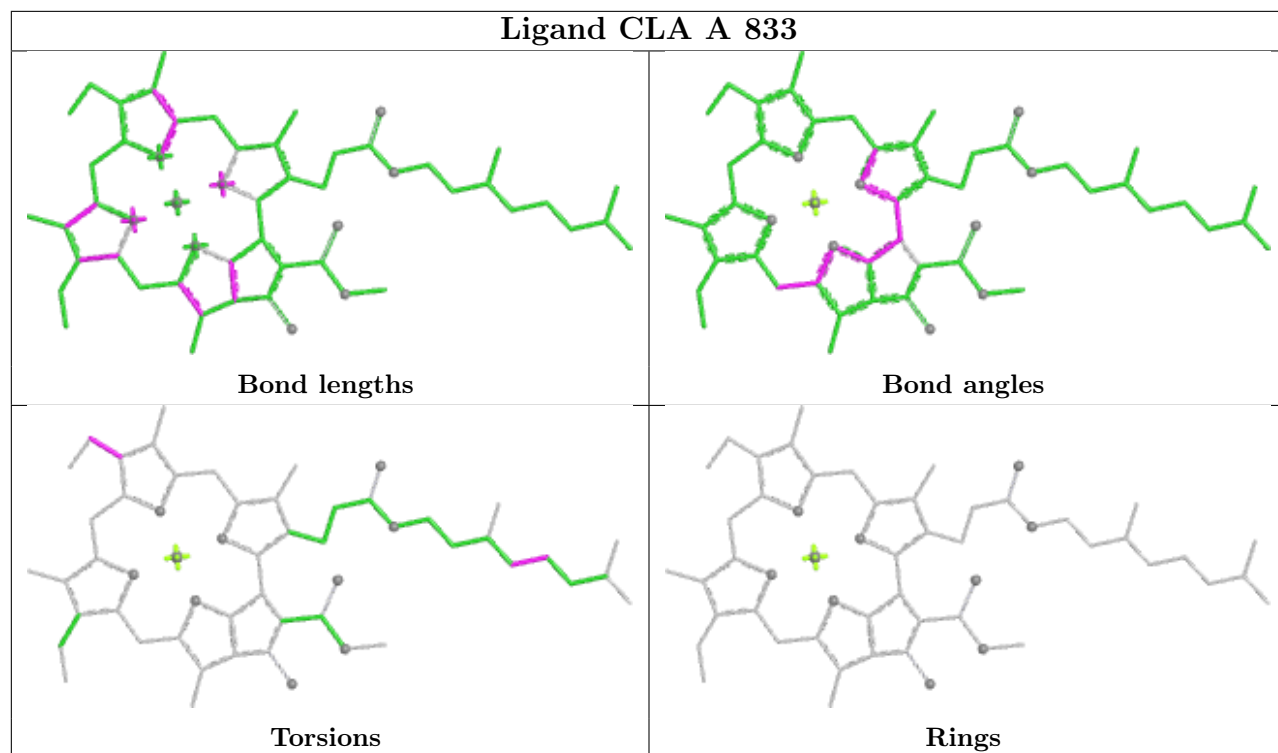
Bond angles



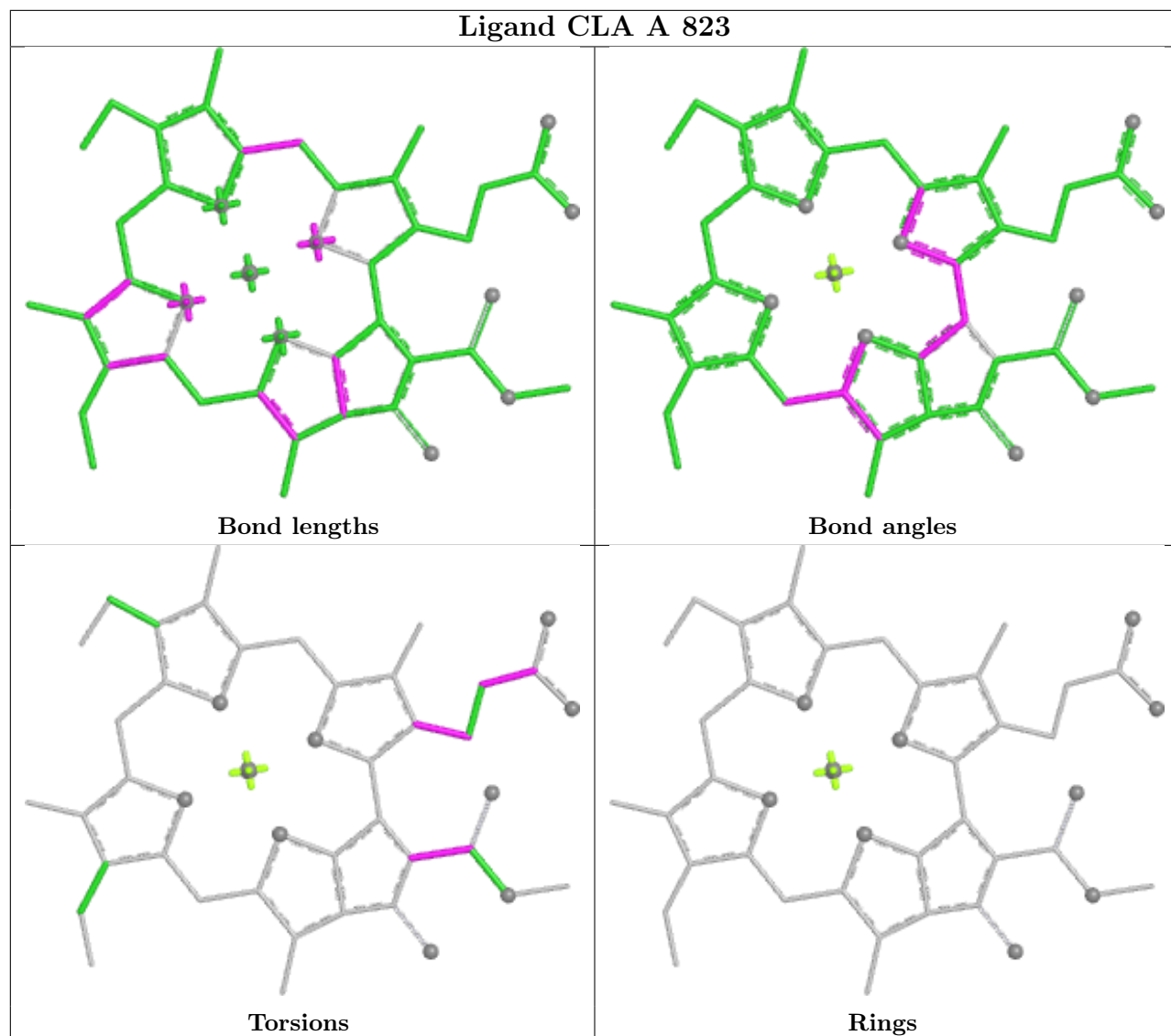
Torsions



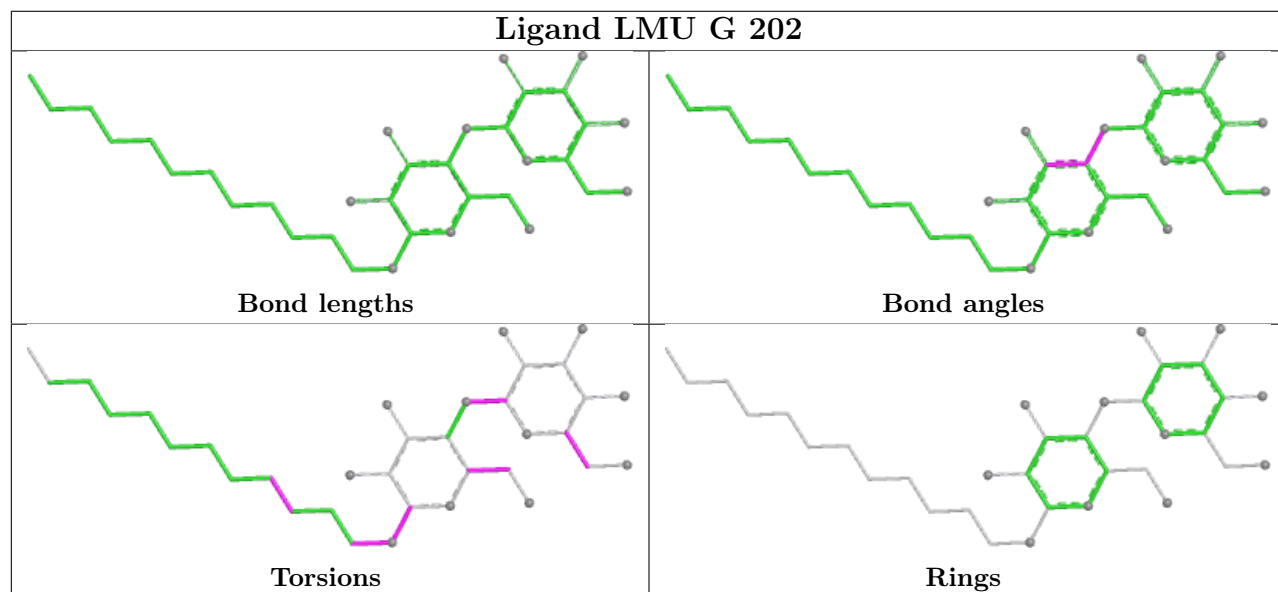
Rings

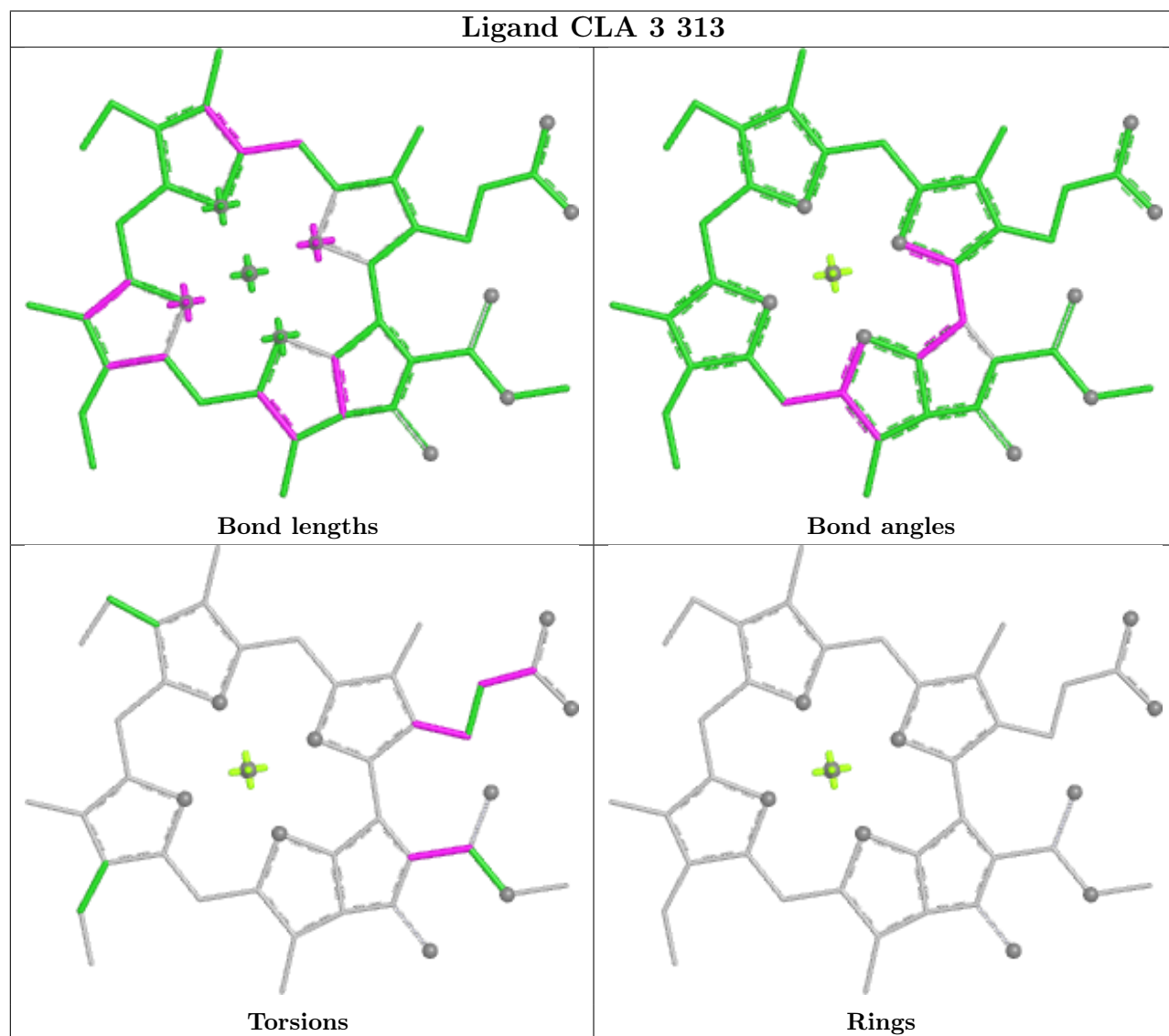
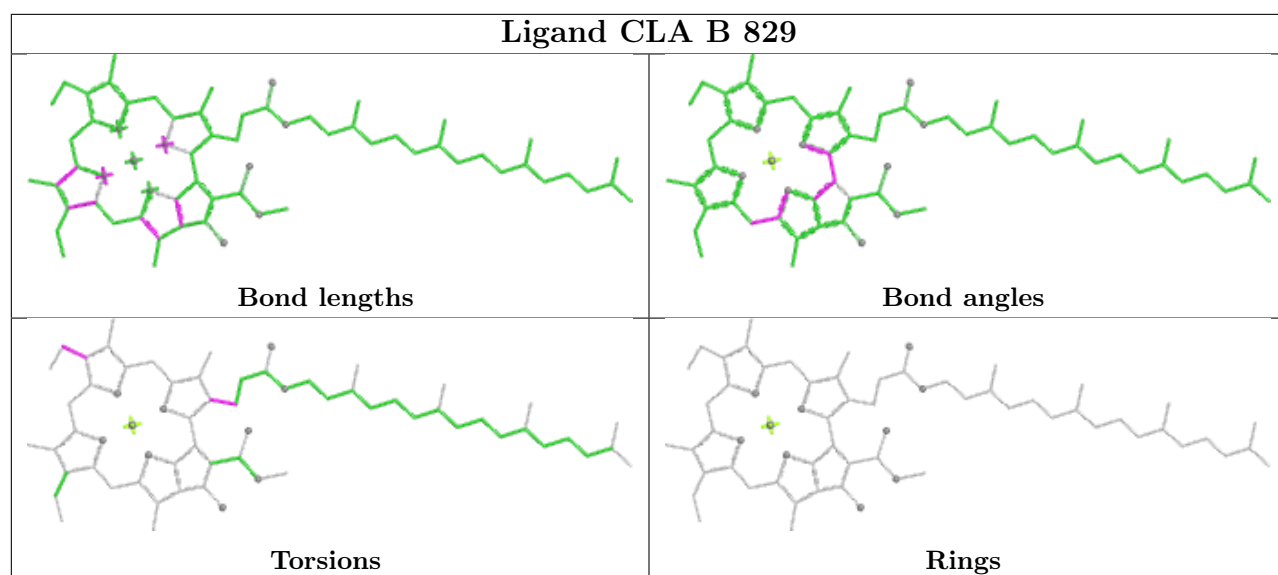


Ligand CLA A 823

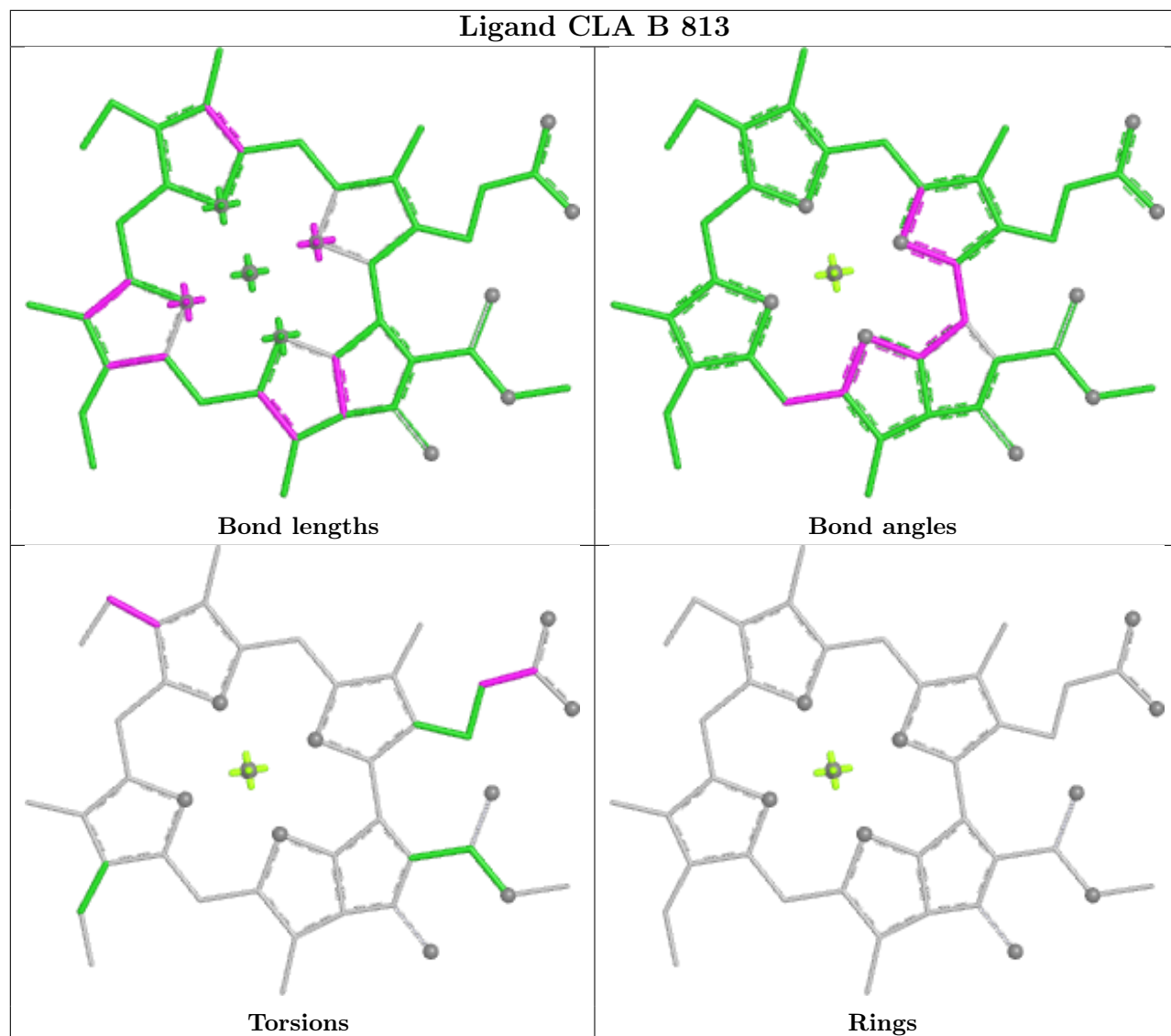


Ligand LMU G 202

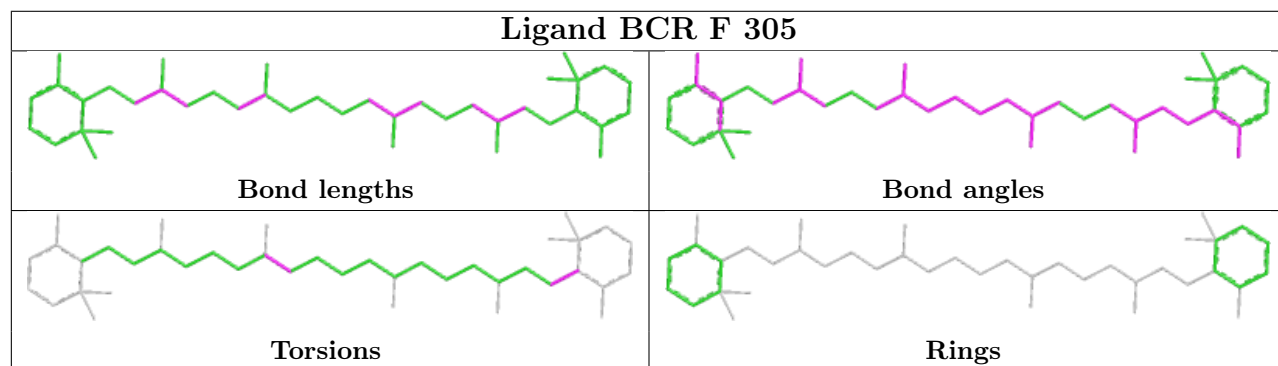


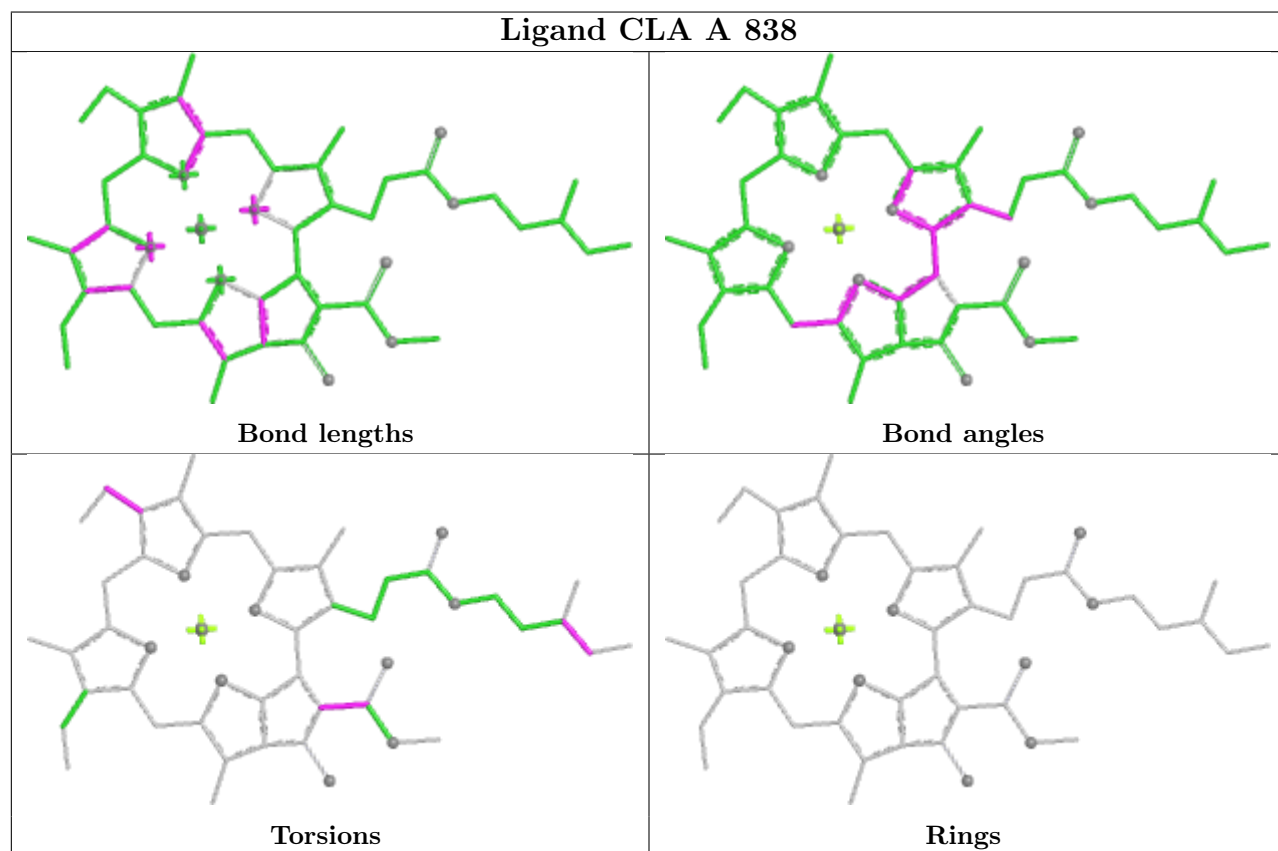
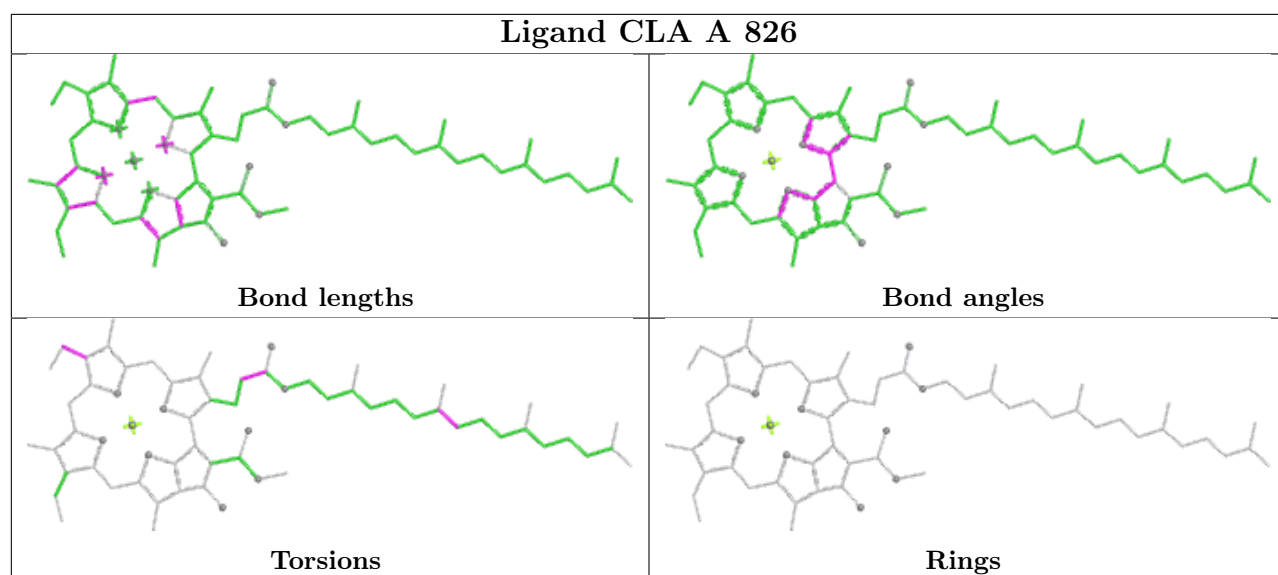


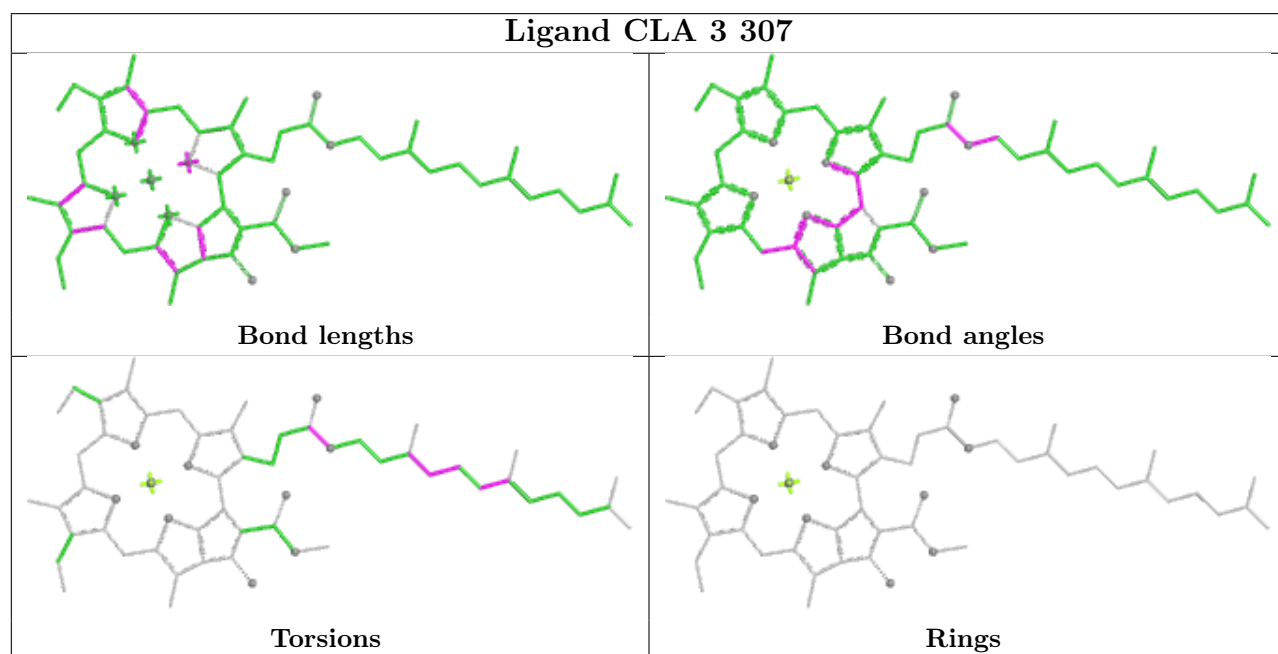
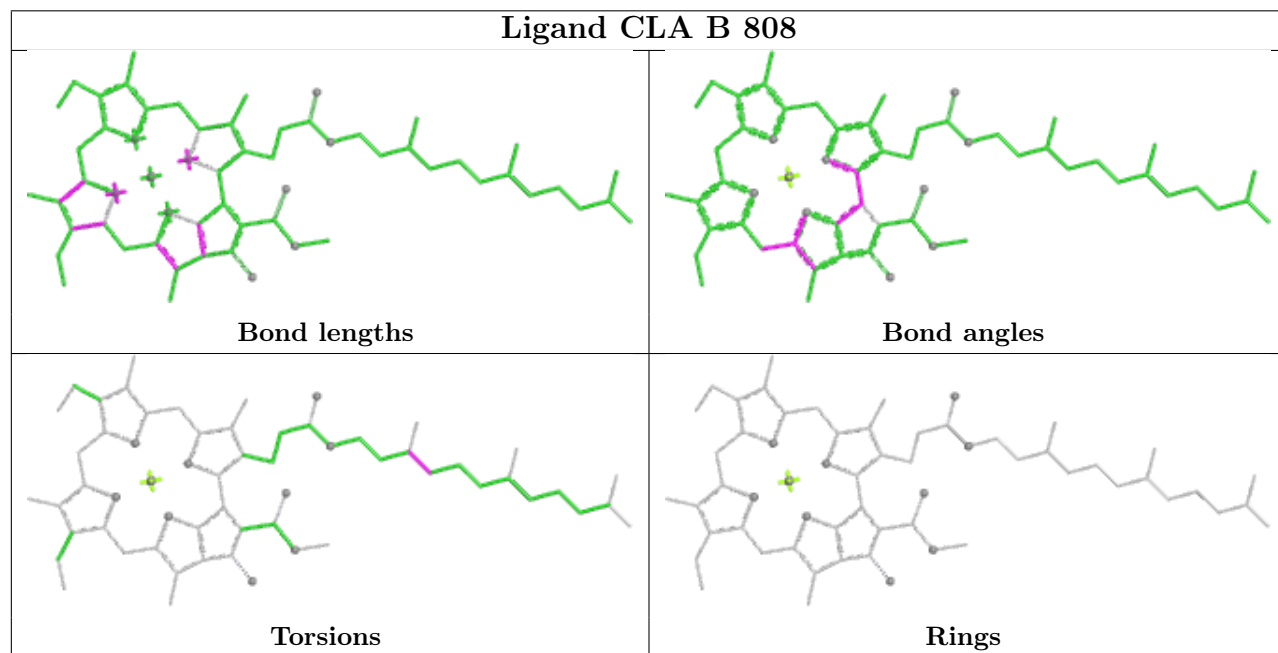
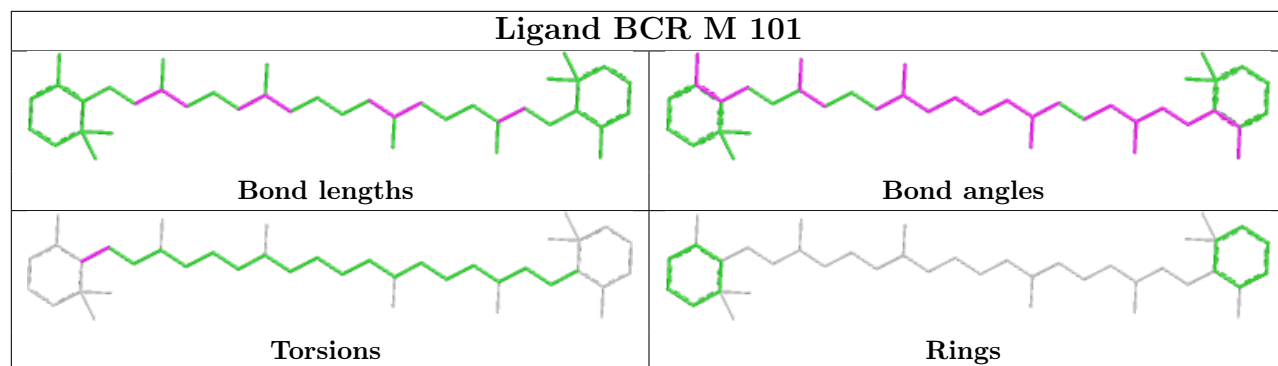
Ligand CLA B 813

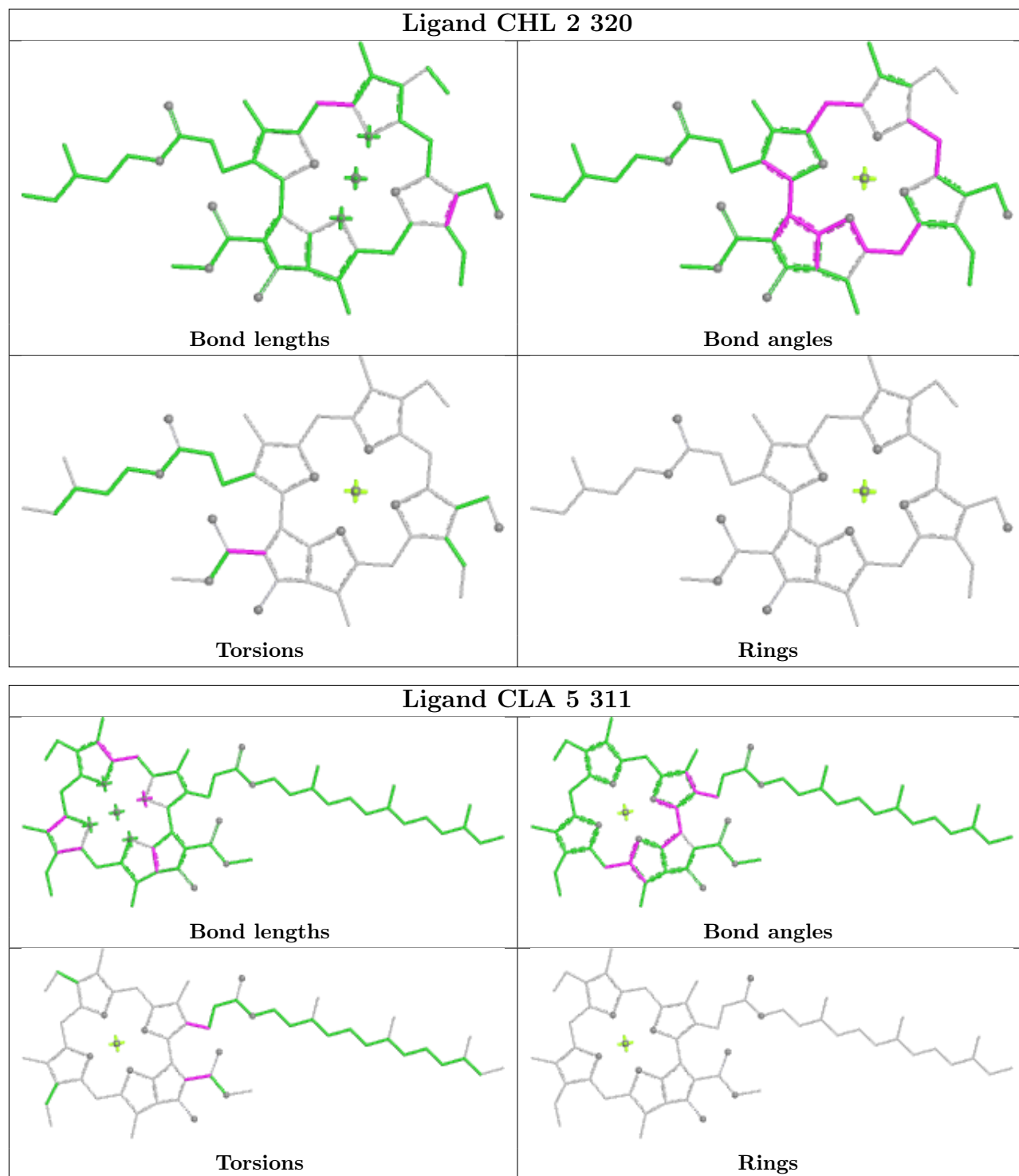


Ligand BCR F 305

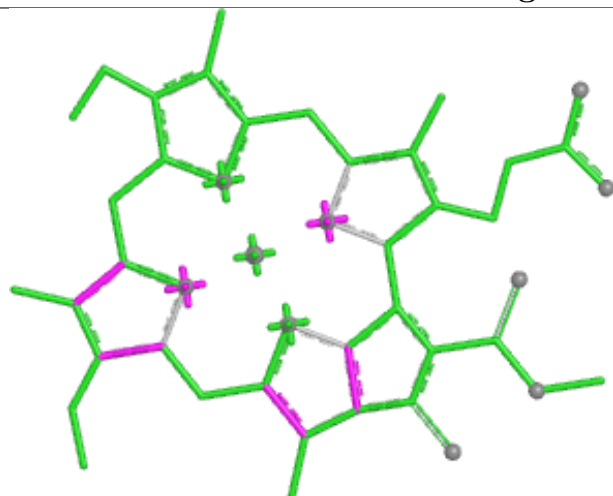




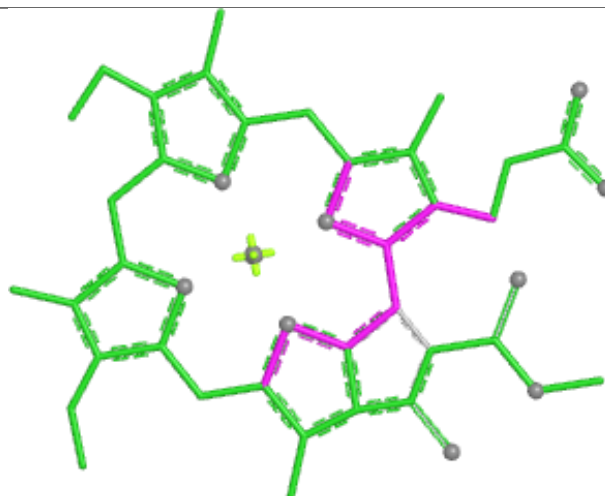




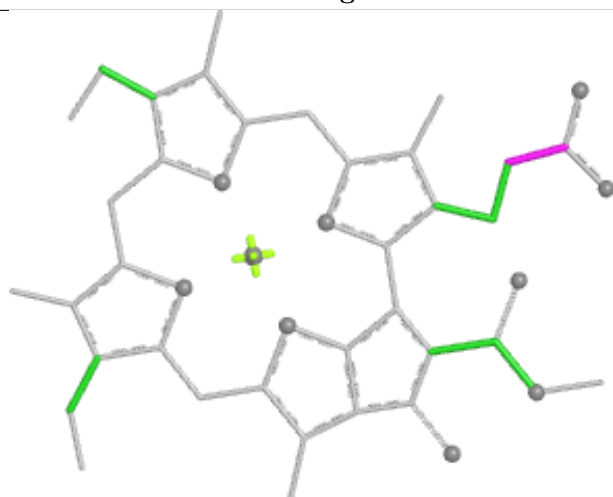
Ligand CLA 6 307



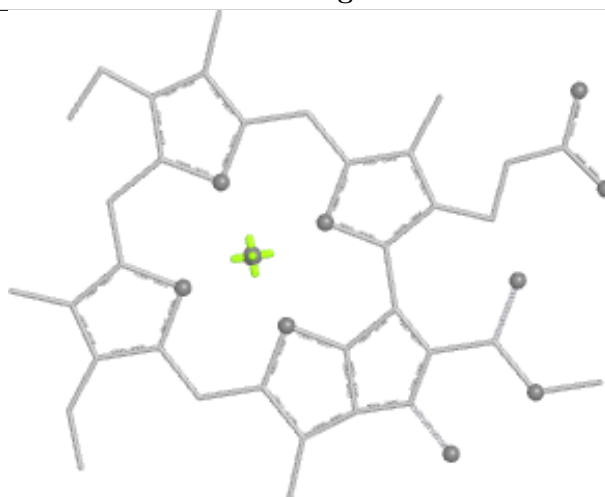
Bond lengths



Bond angles

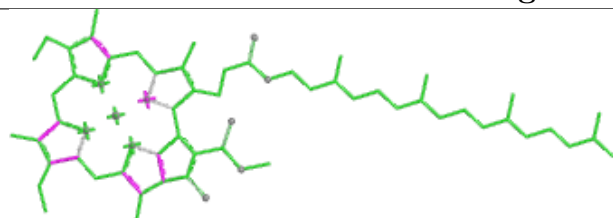


Torsions

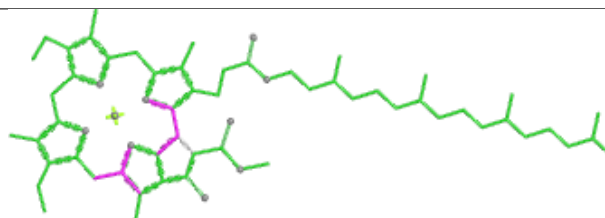


Rings

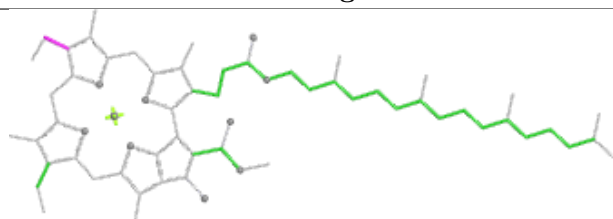
Ligand CLA 3 308



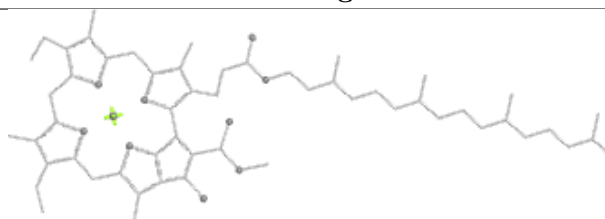
Bond lengths



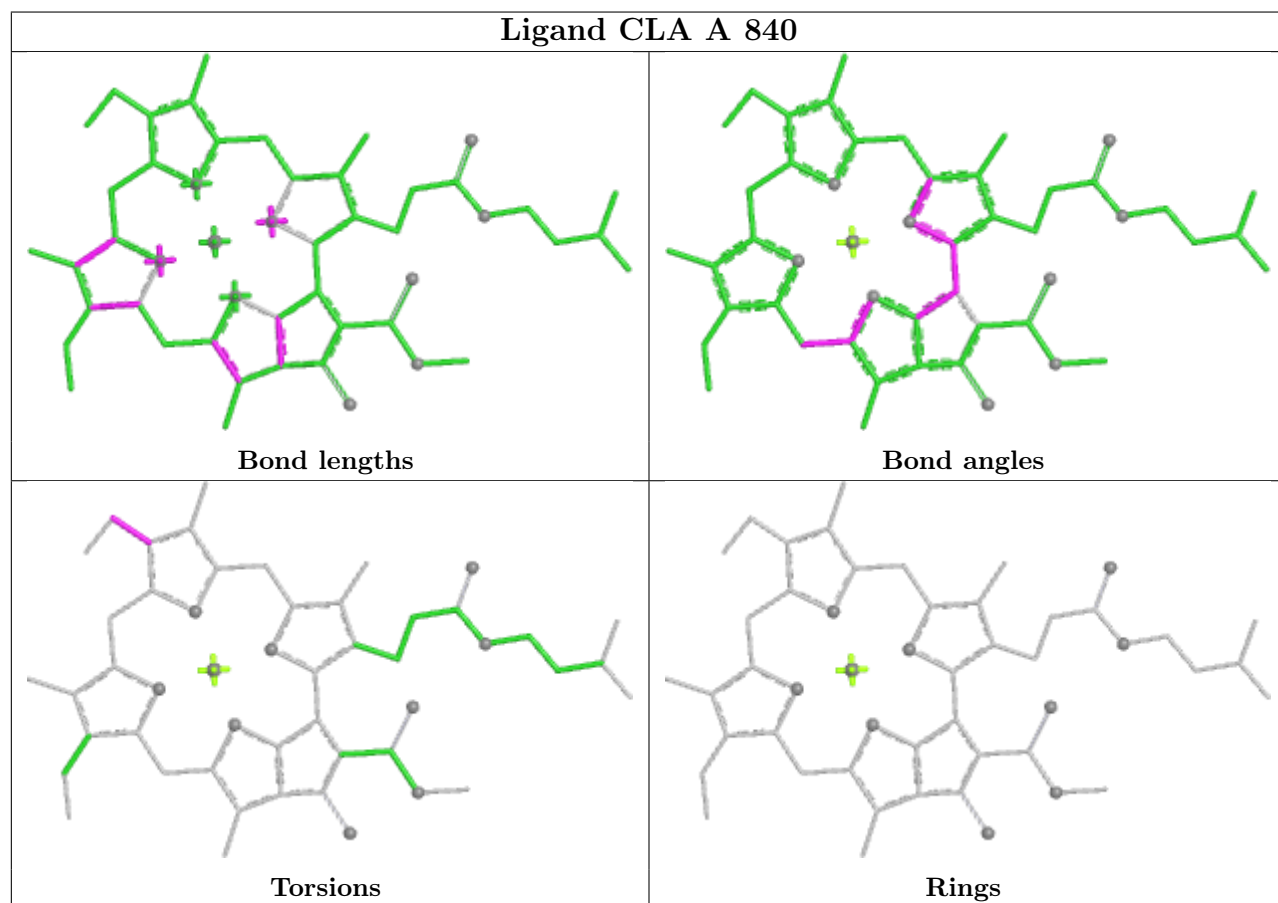
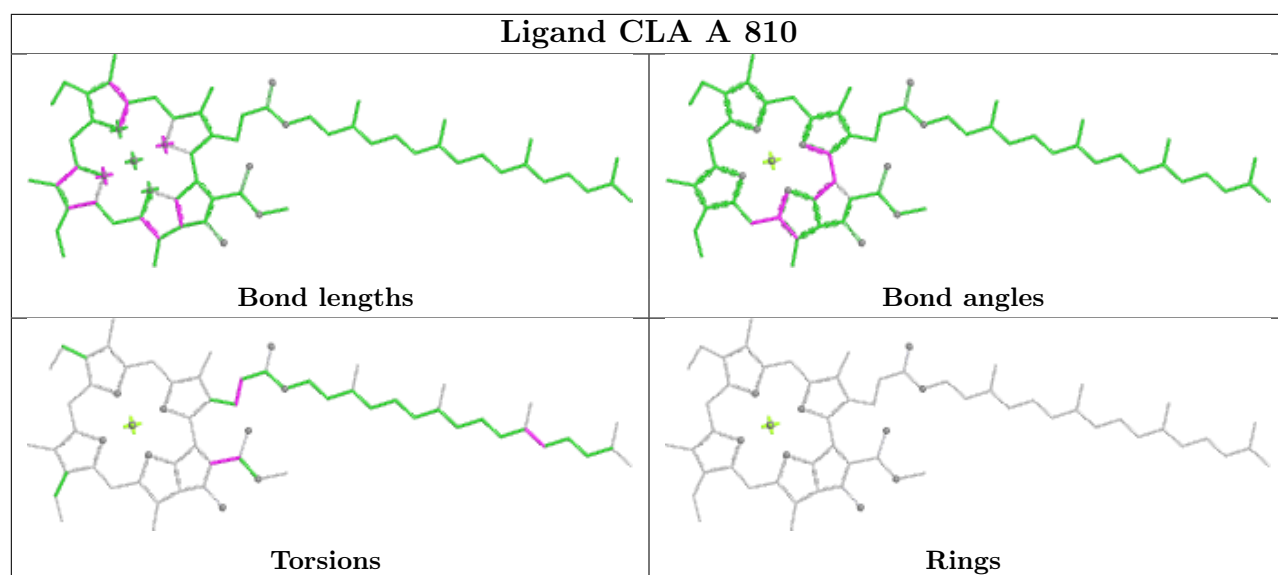
Bond angles

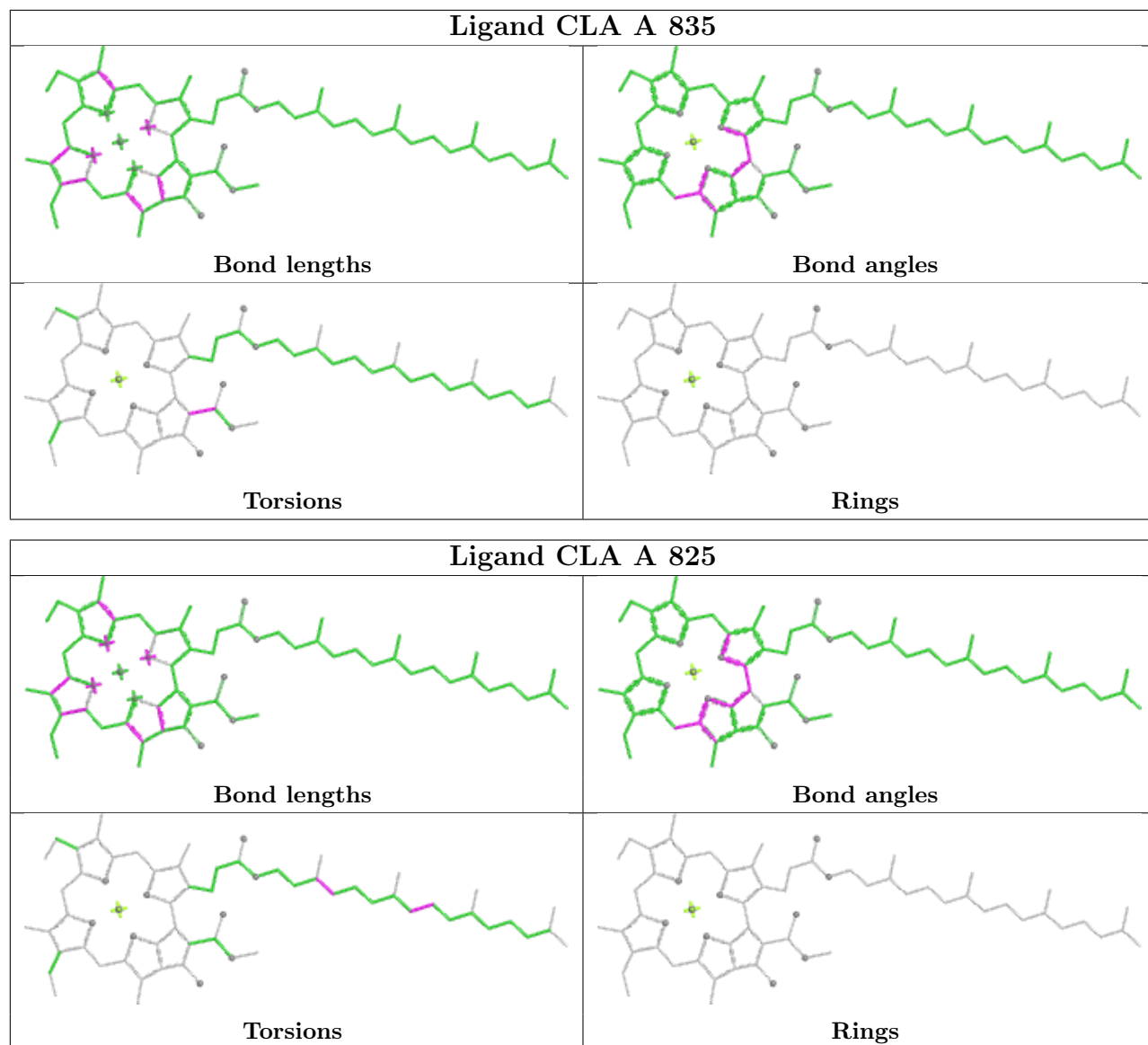


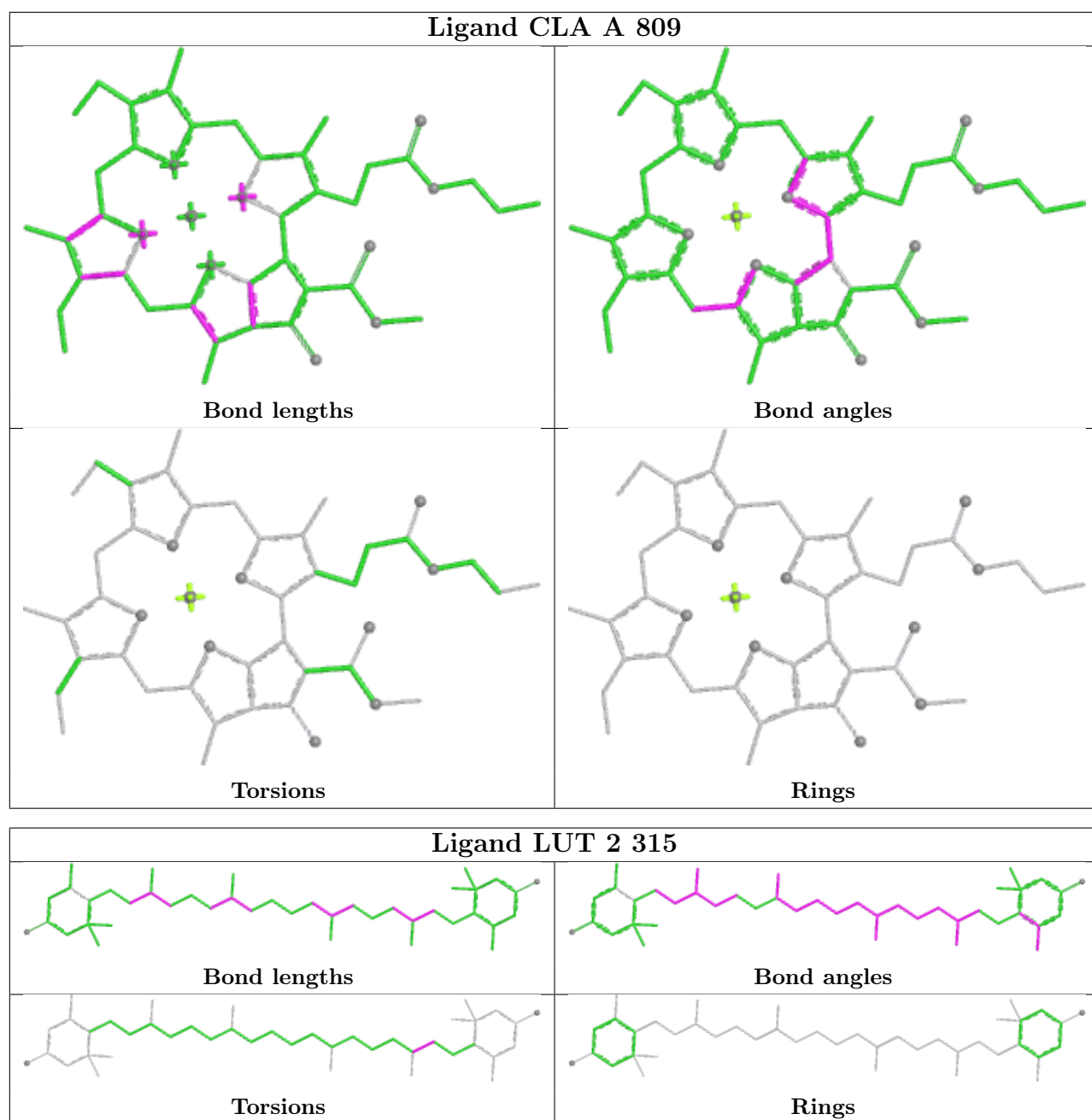
Torsions



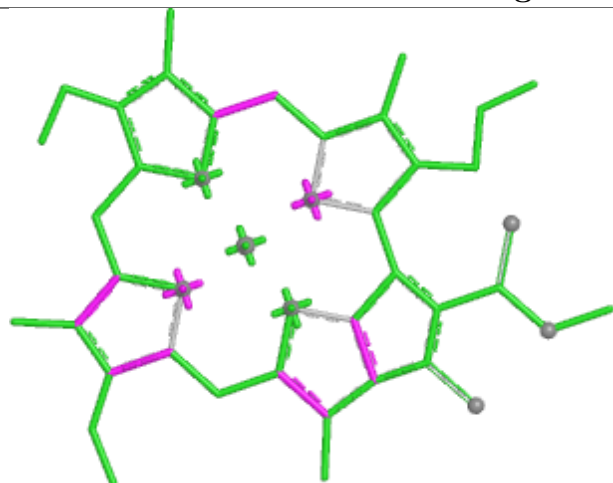
Rings



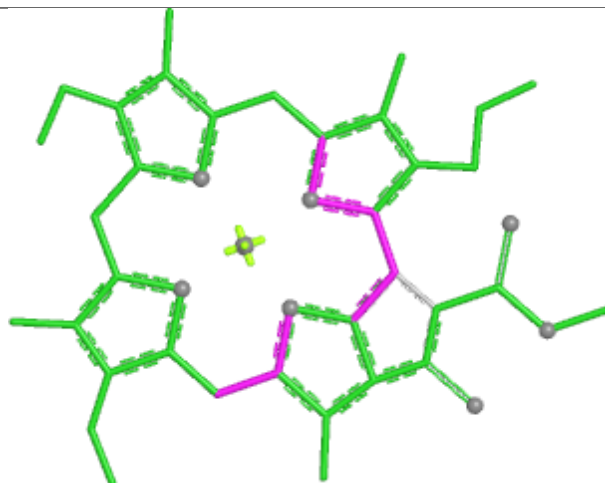




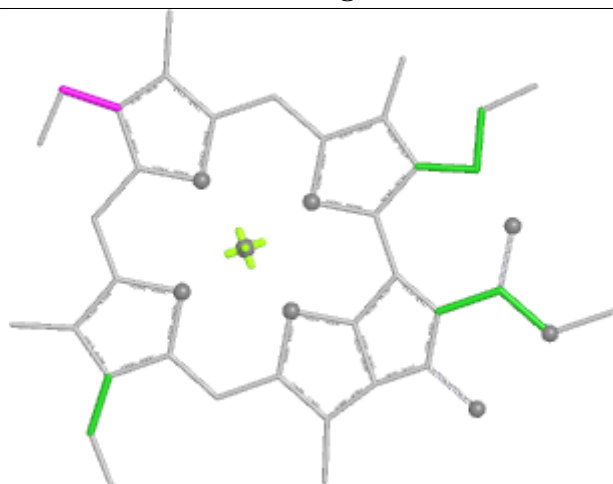
Ligand CLA B 821



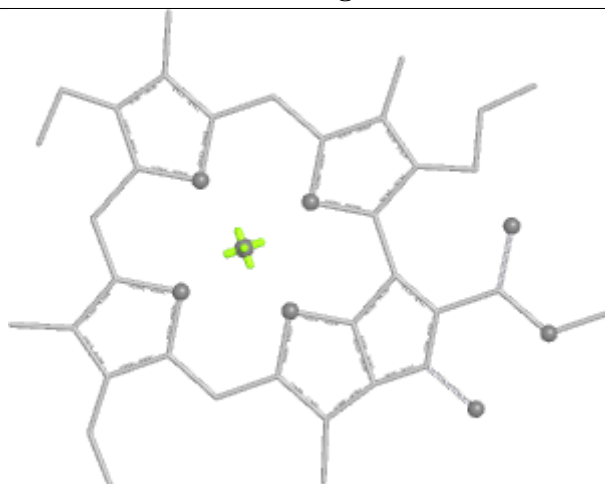
Bond lengths



Bond angles

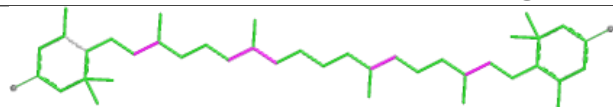


Torsions

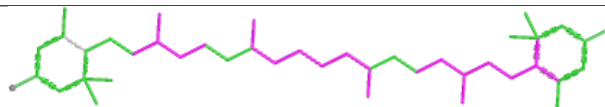


Rings

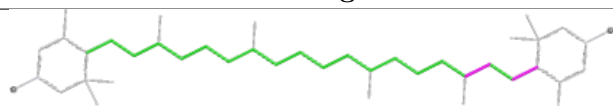
Ligand LUT 3 315



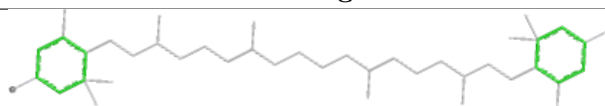
Bond lengths



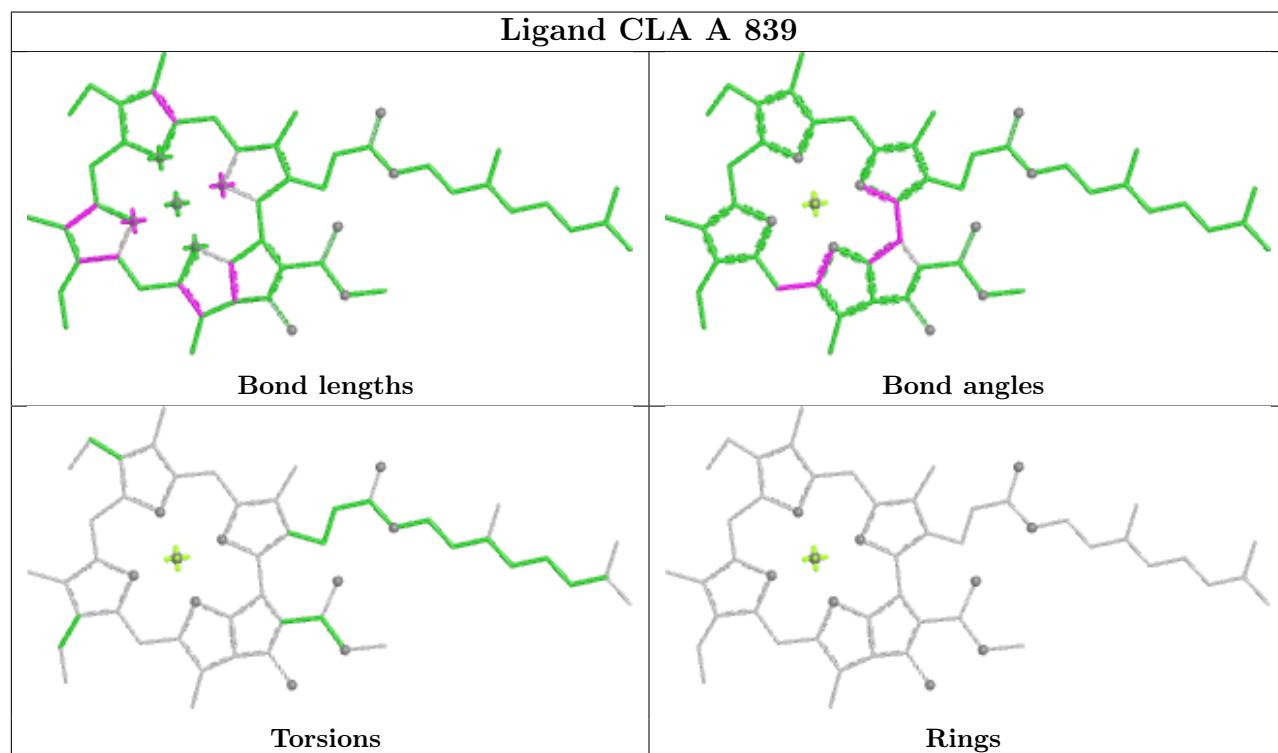
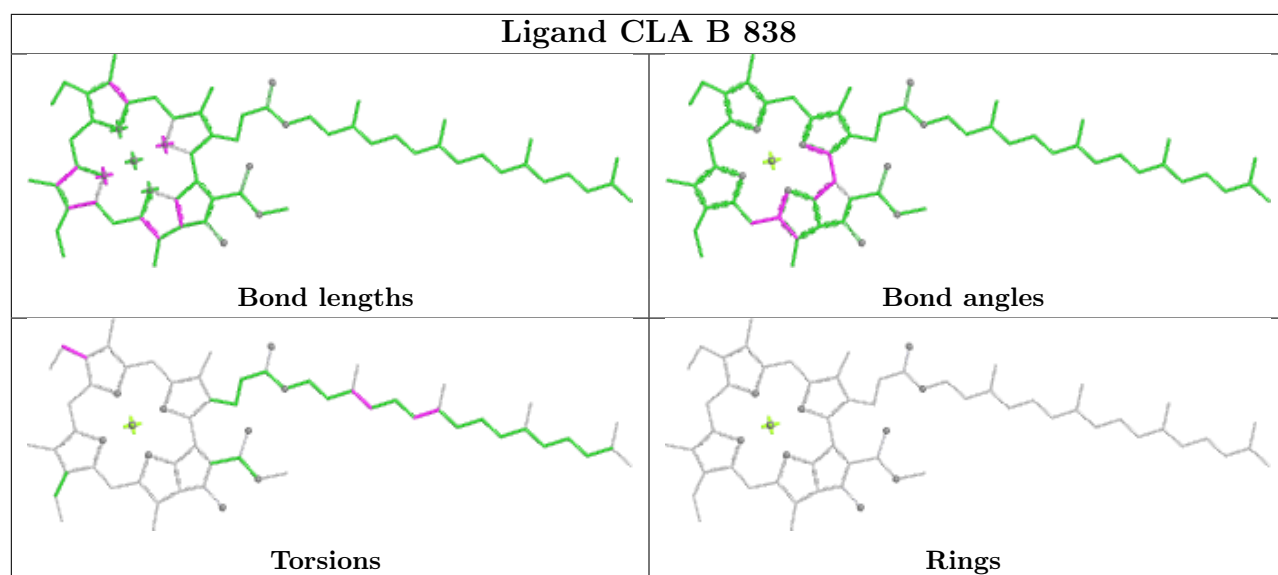
Bond angles

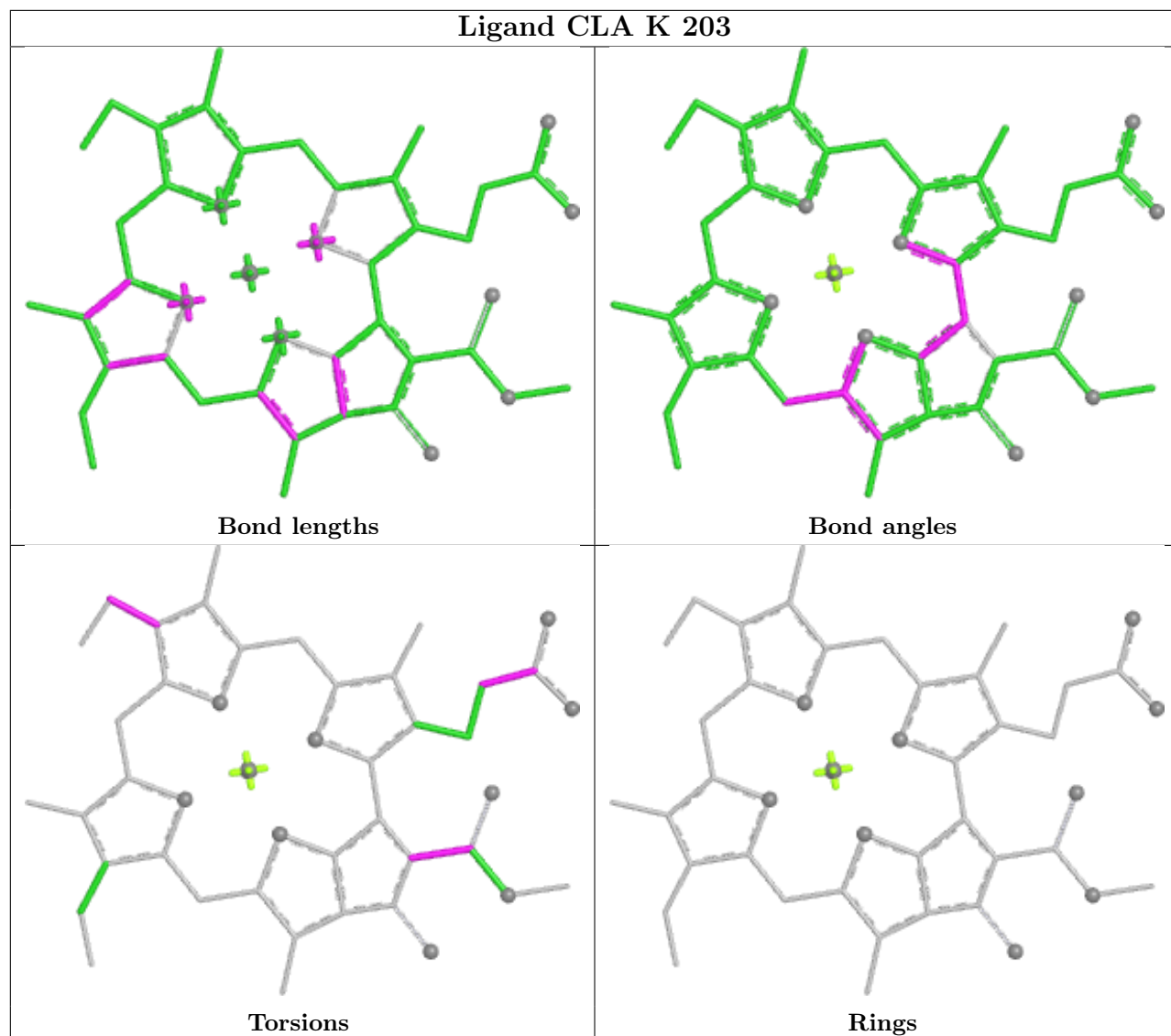


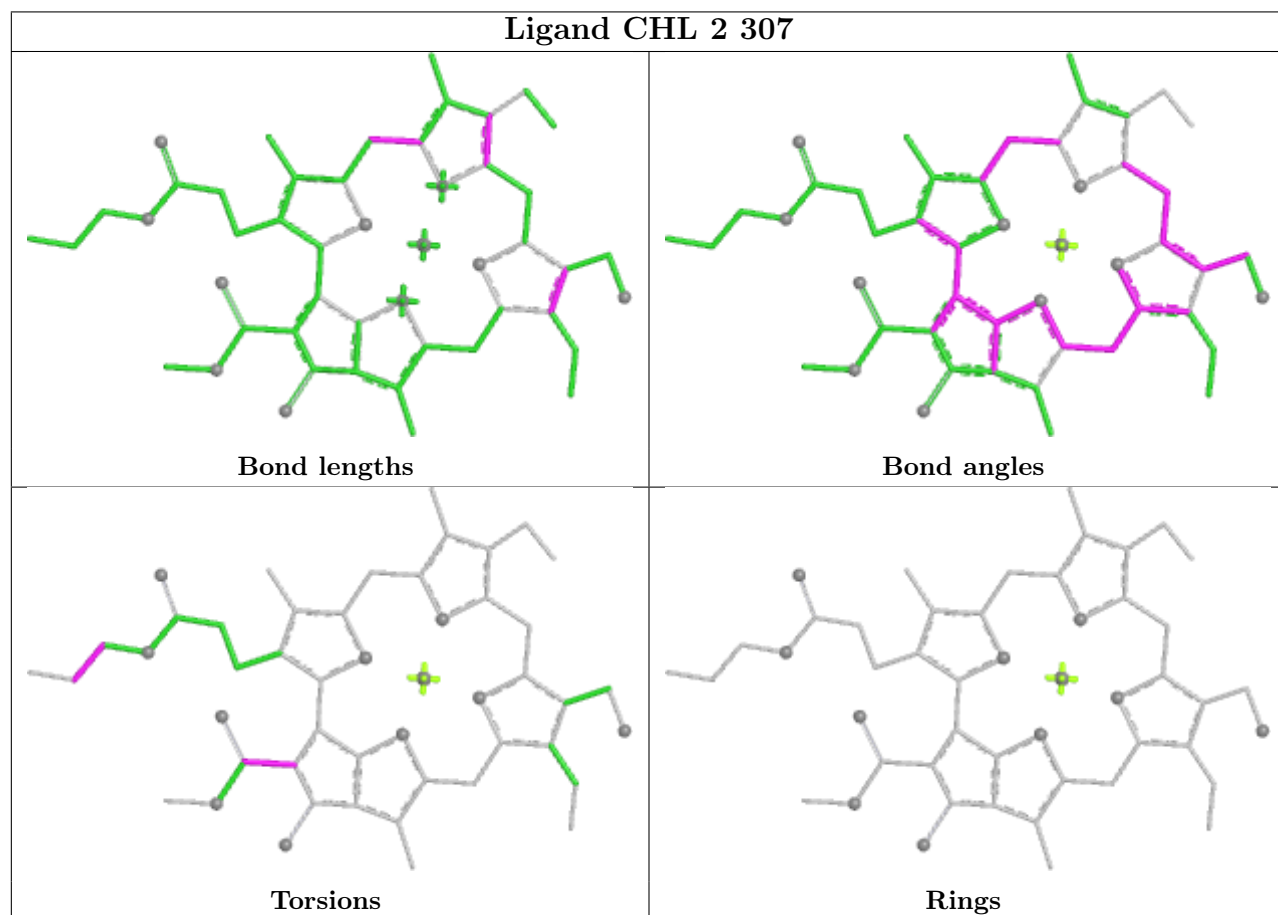
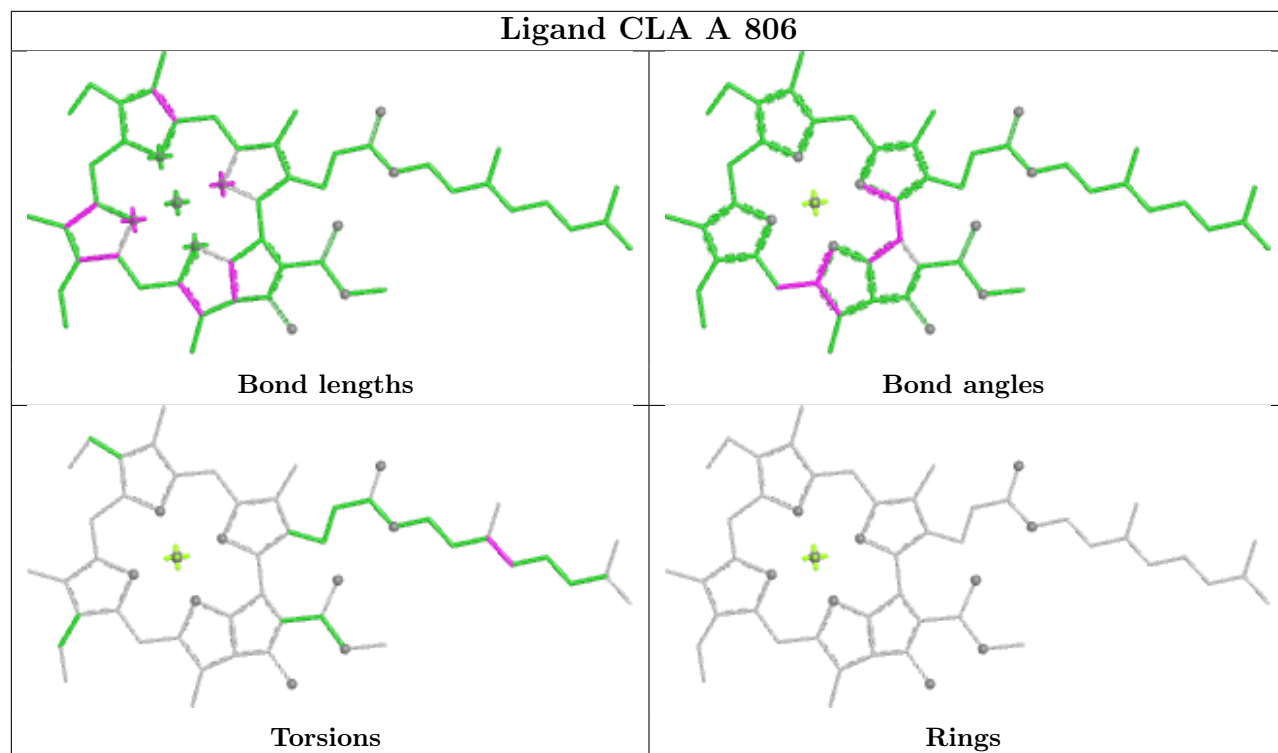
Torsions

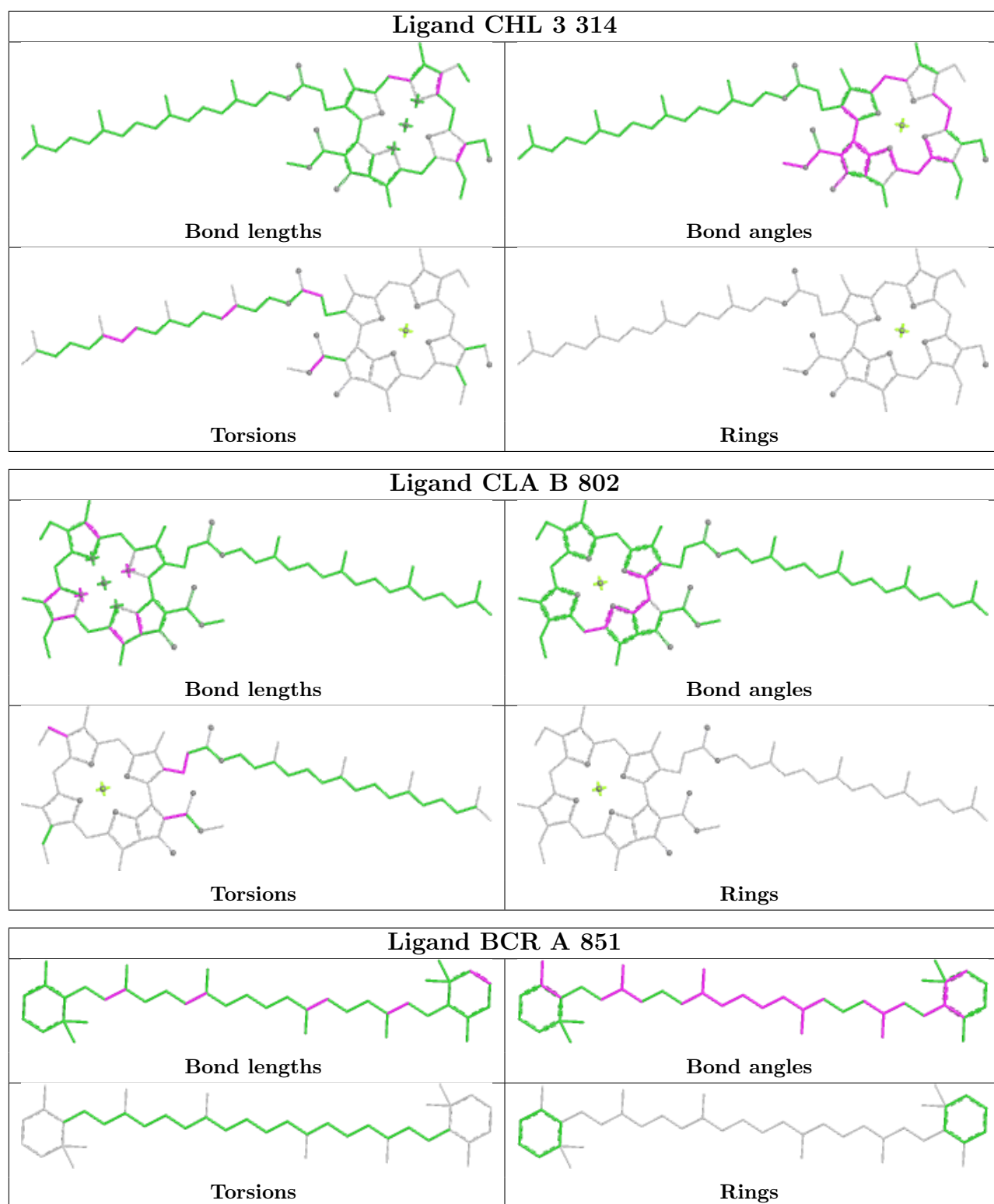


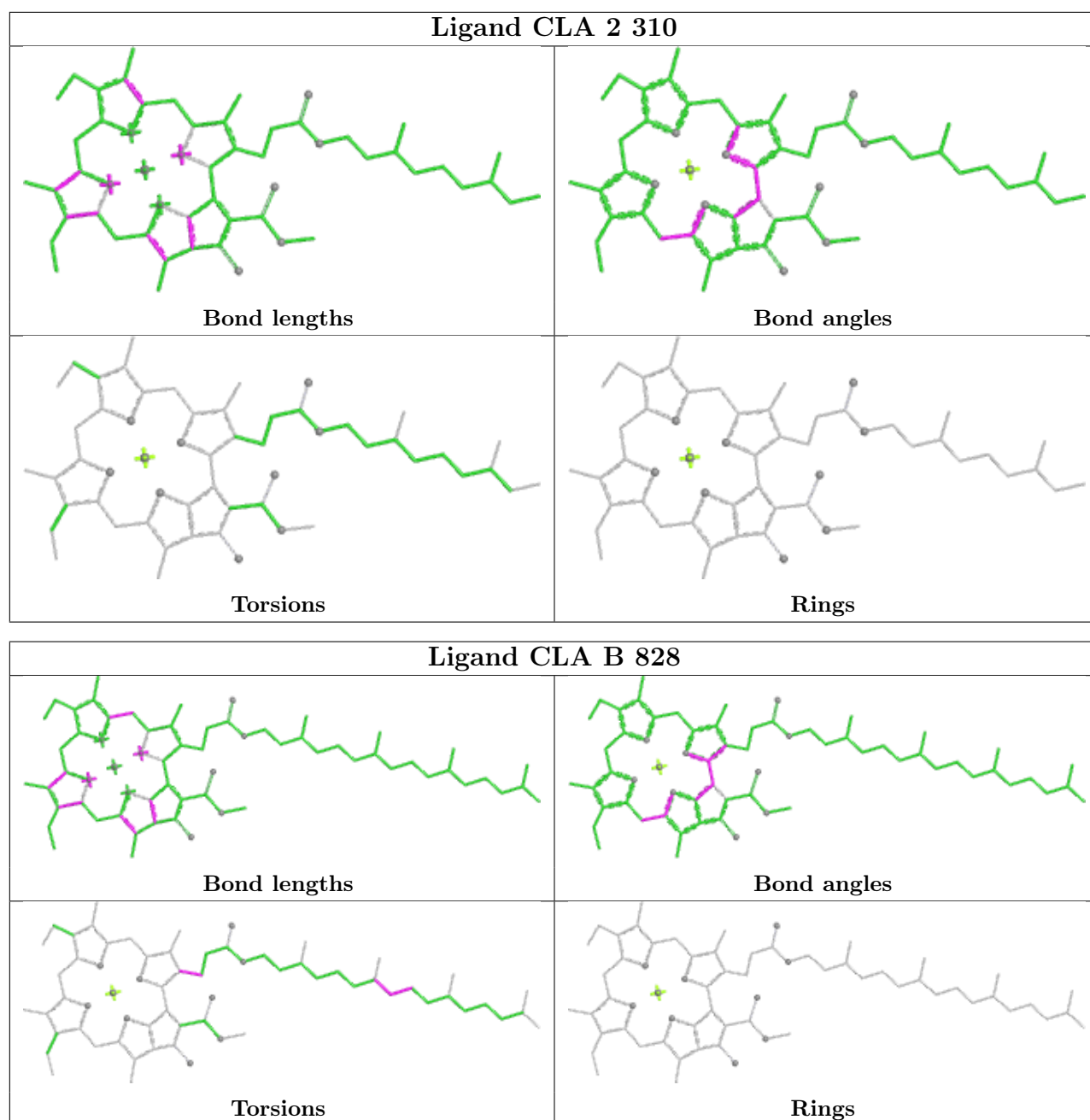
Rings



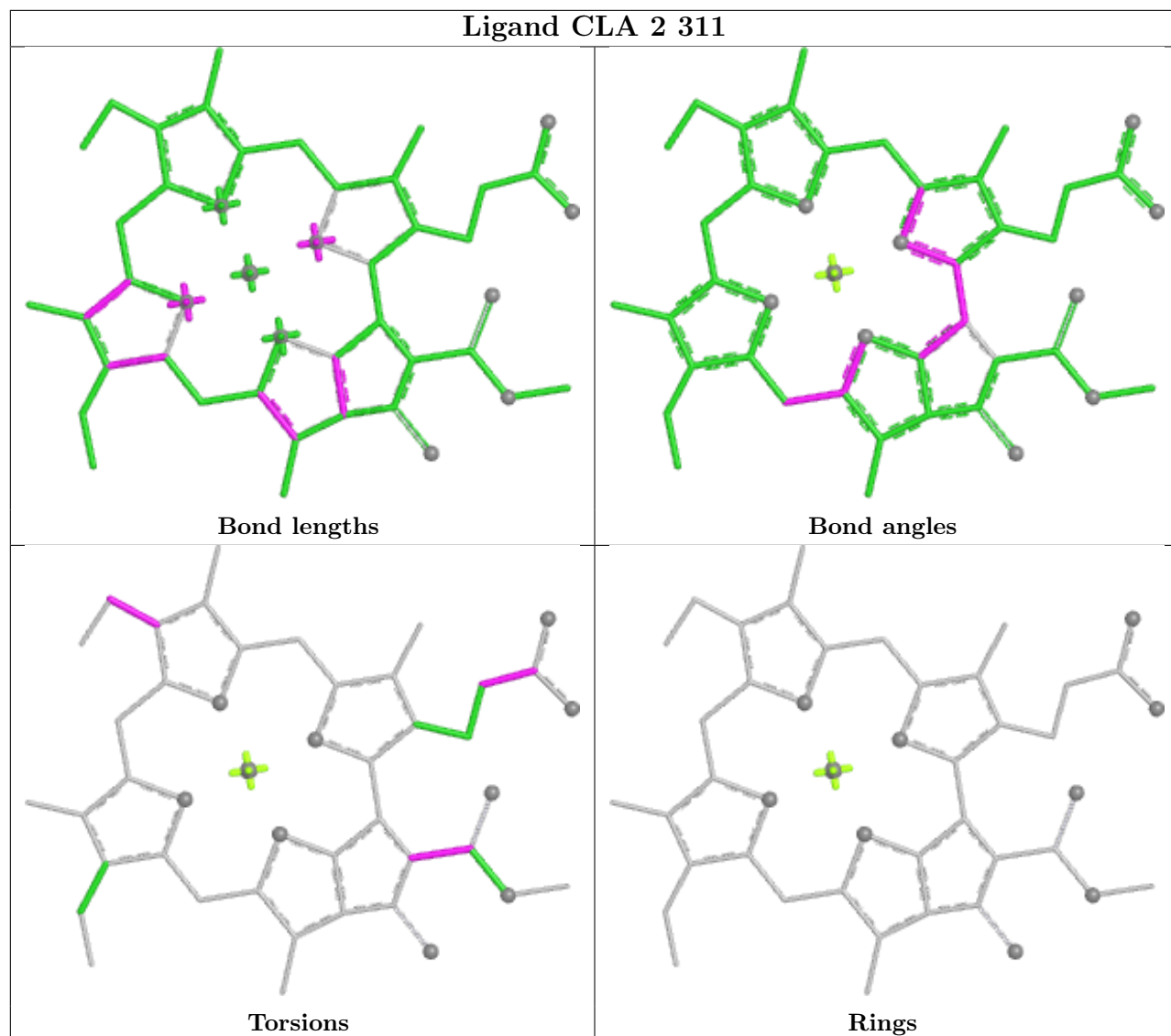




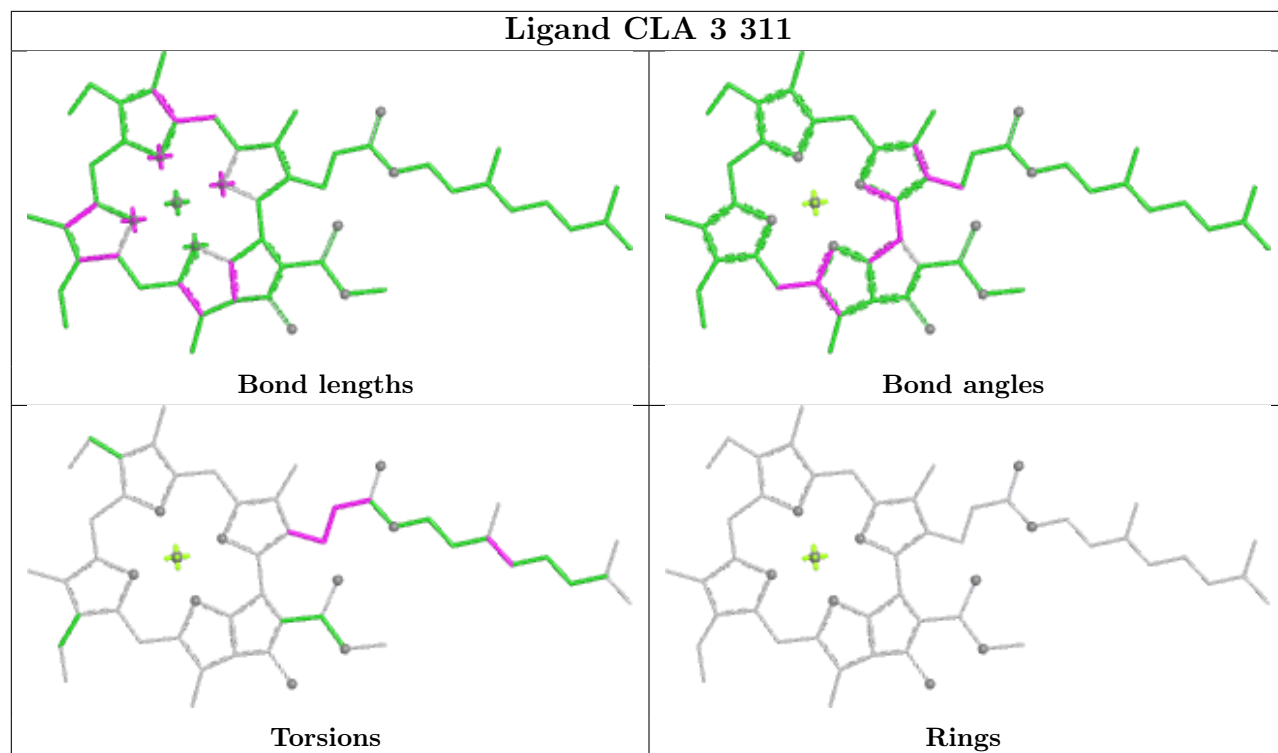




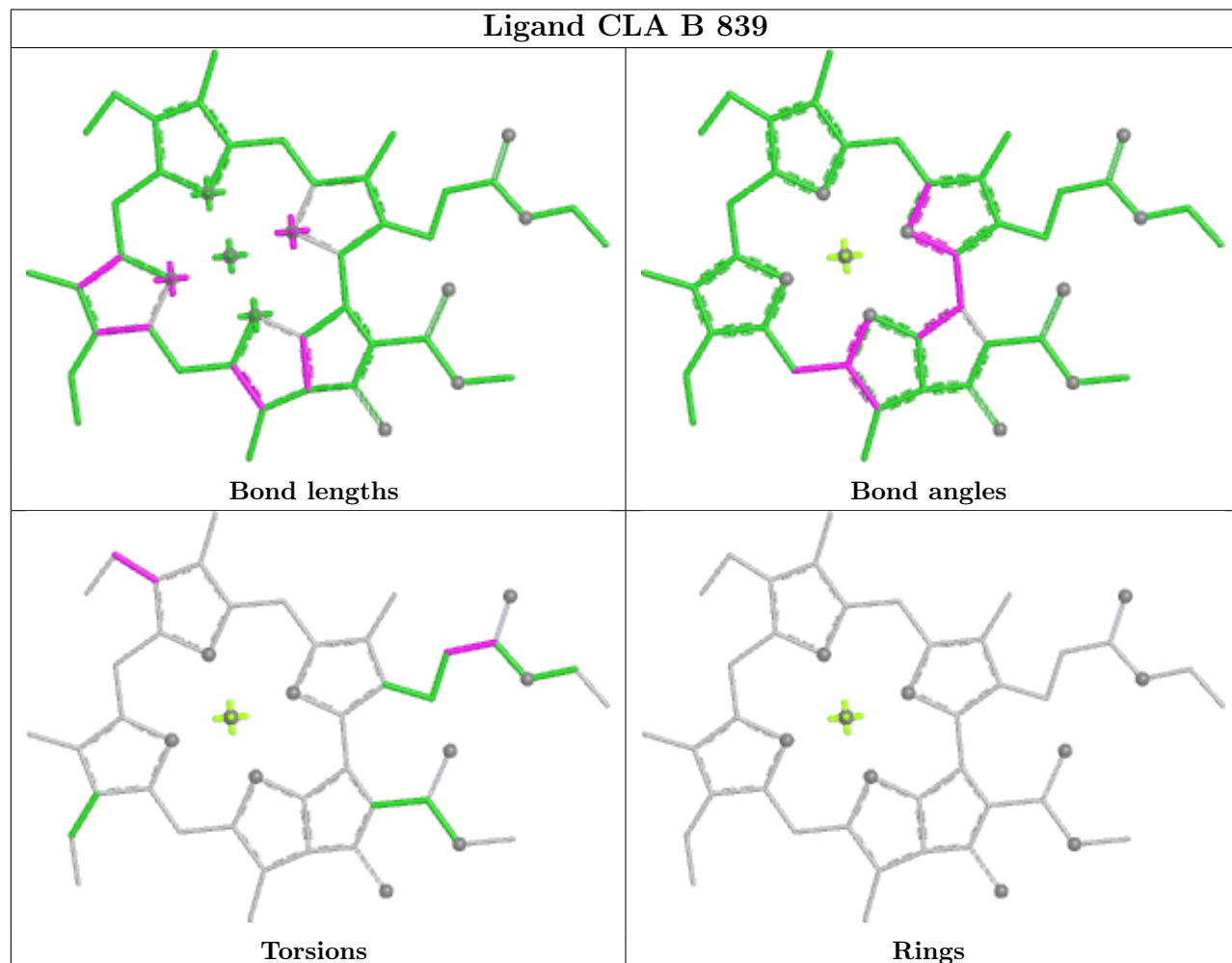
Ligand CLA 2 311

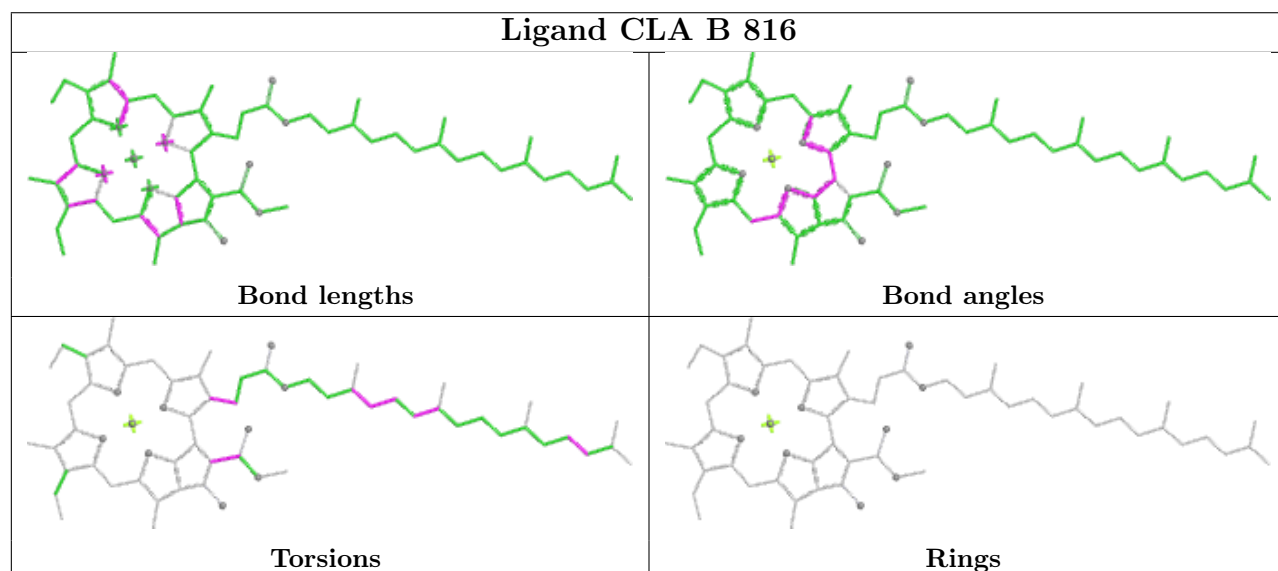
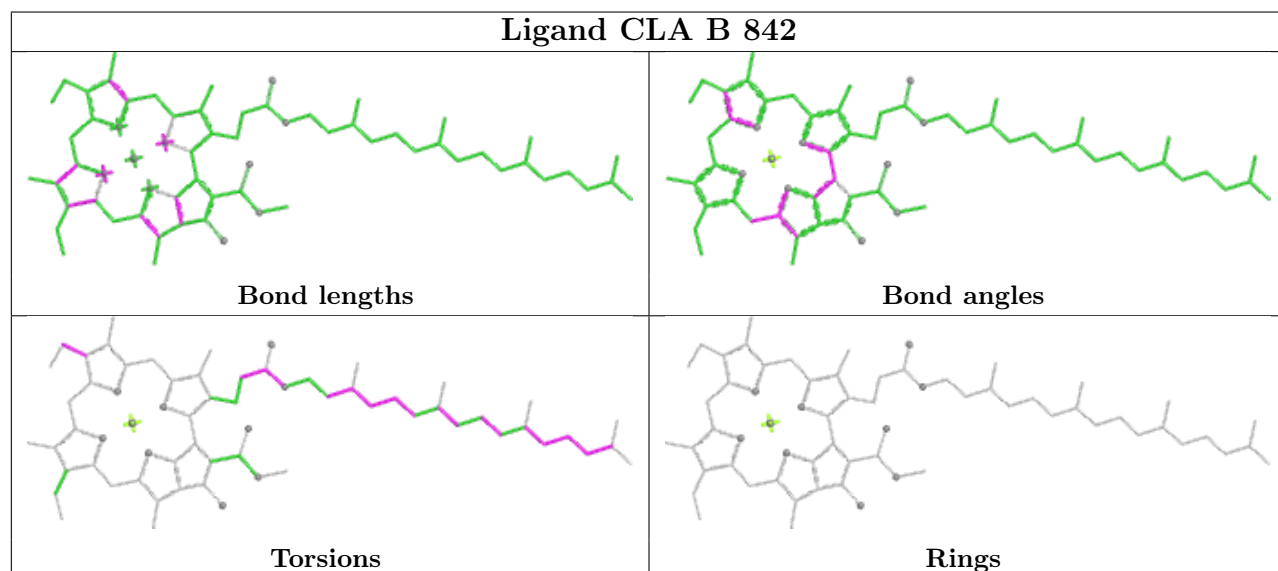
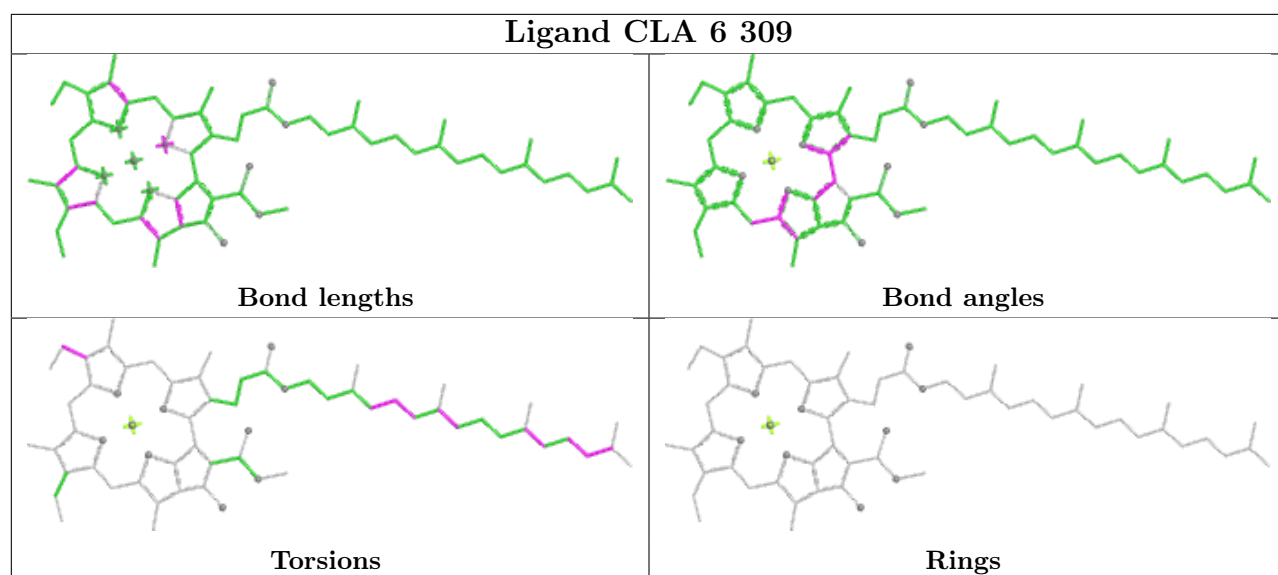


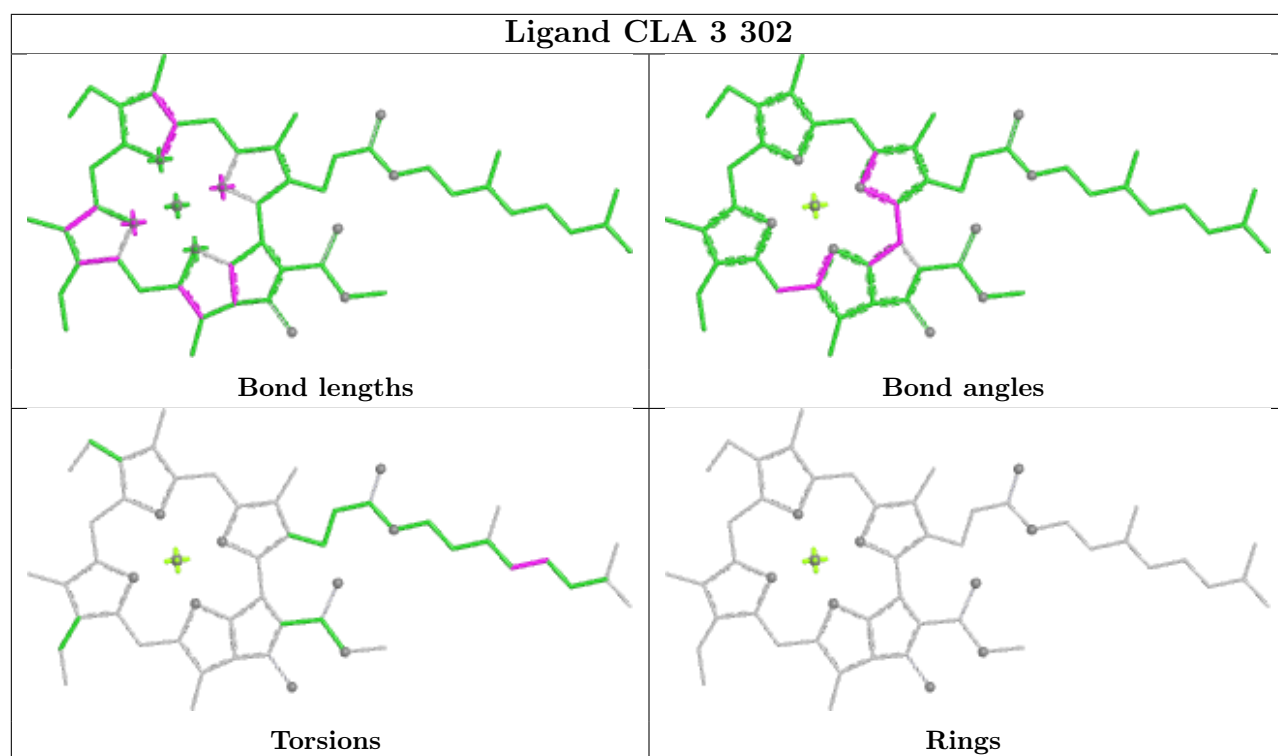
Ligand CLA 3 311

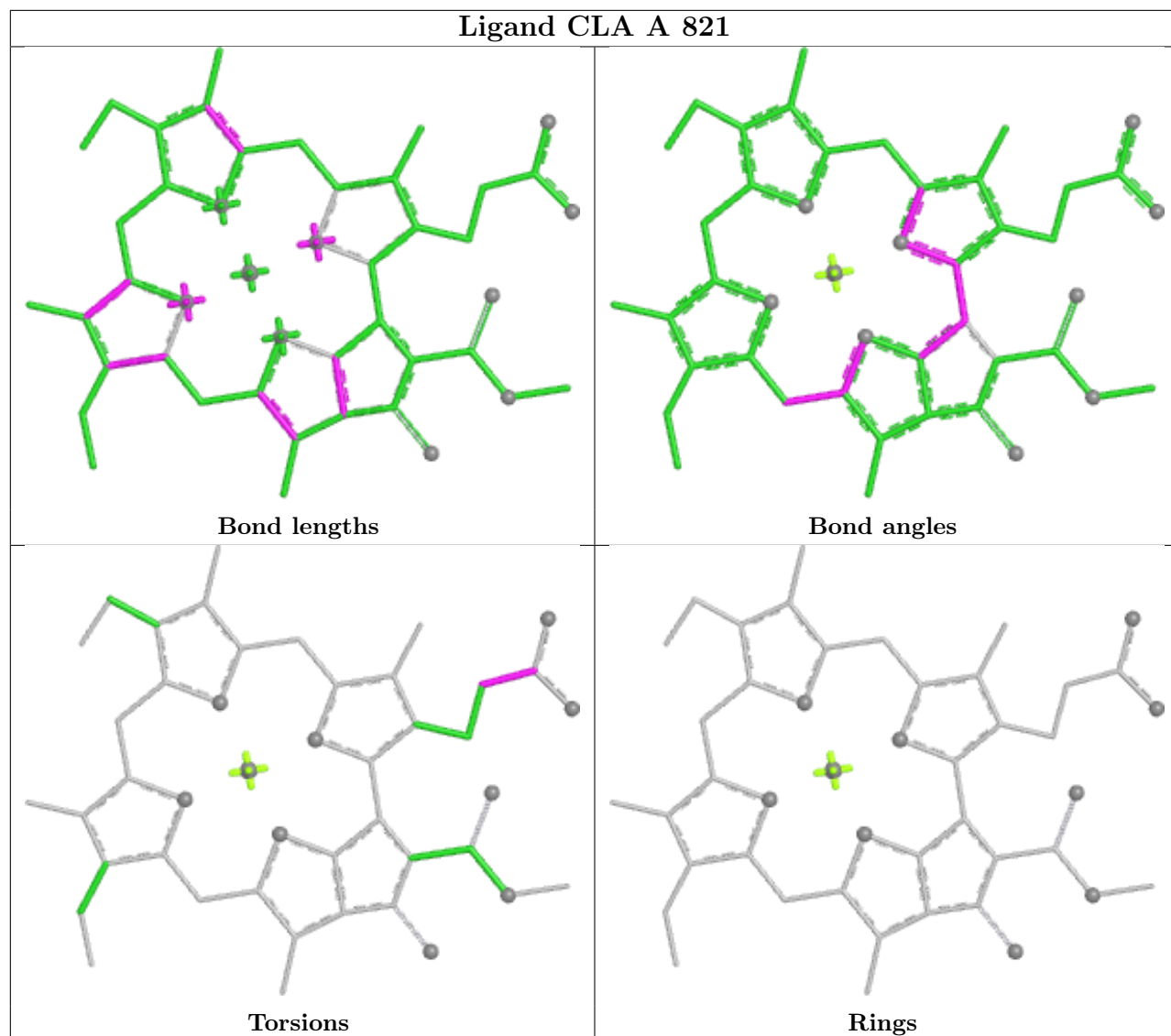


Ligand CLA B 839

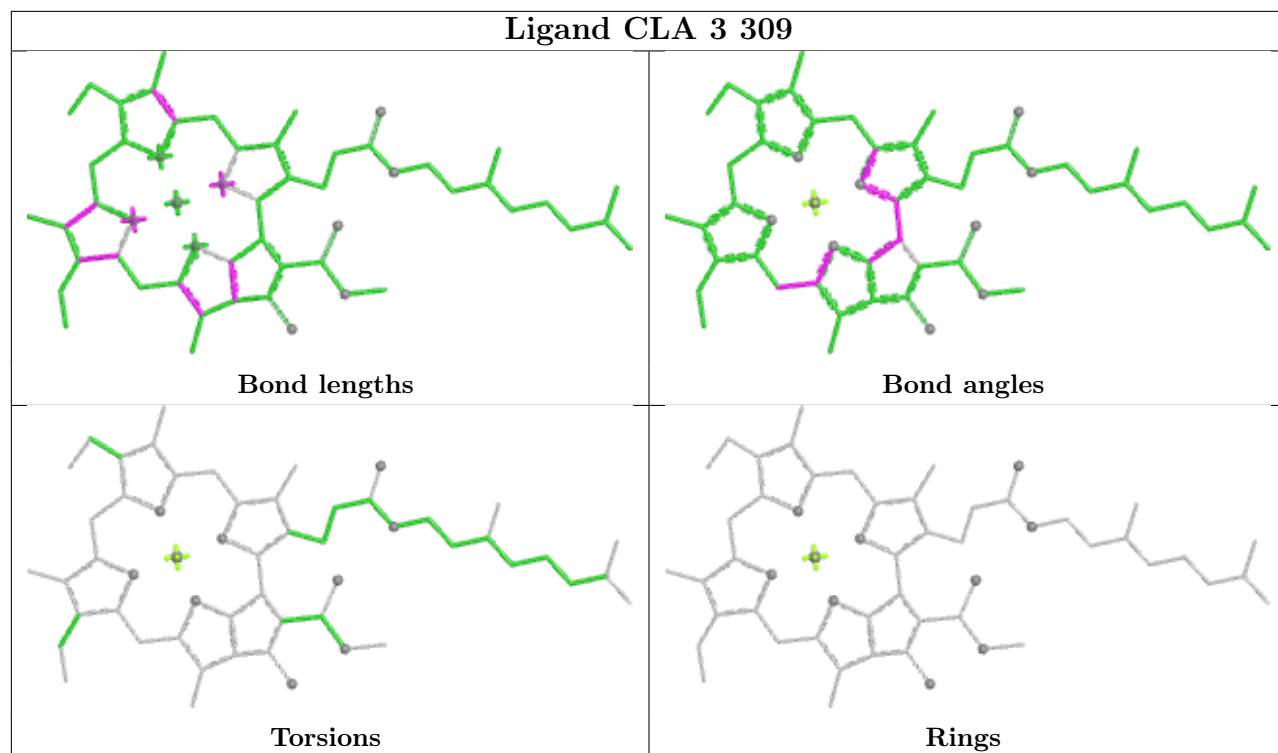




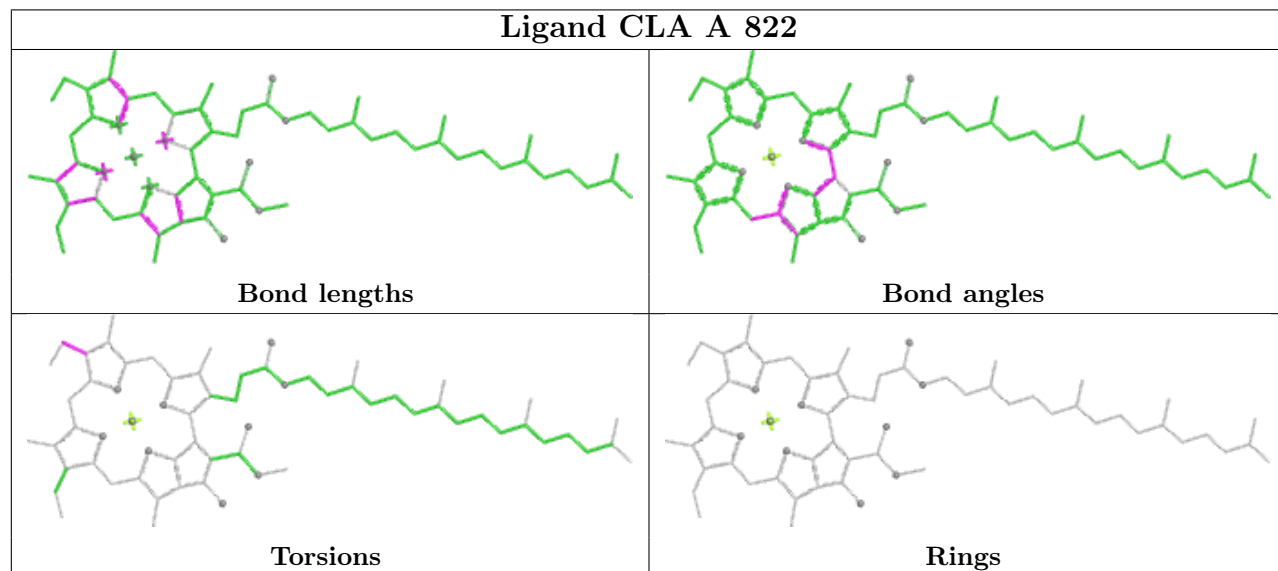




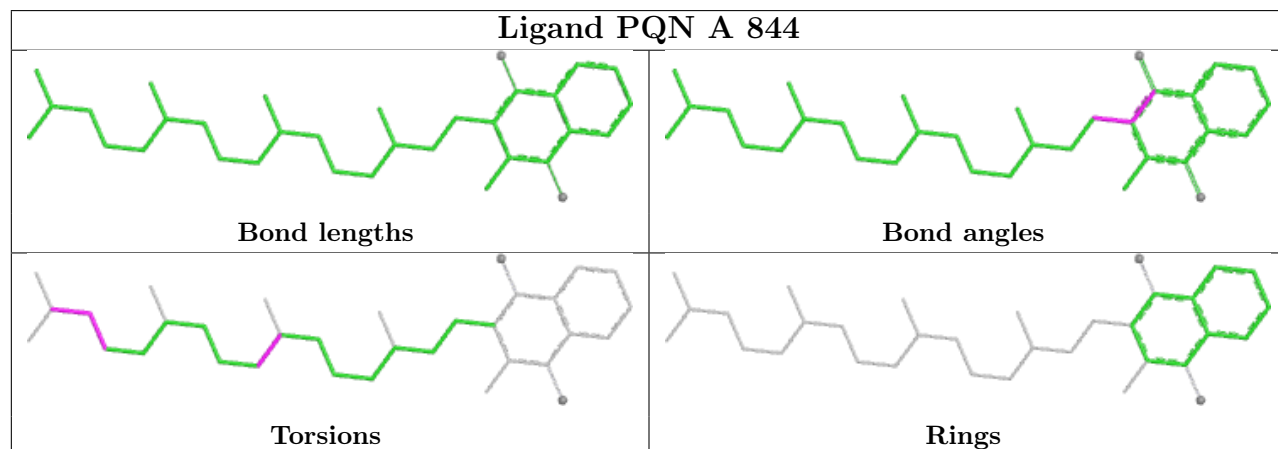
Ligand CLA 3 309

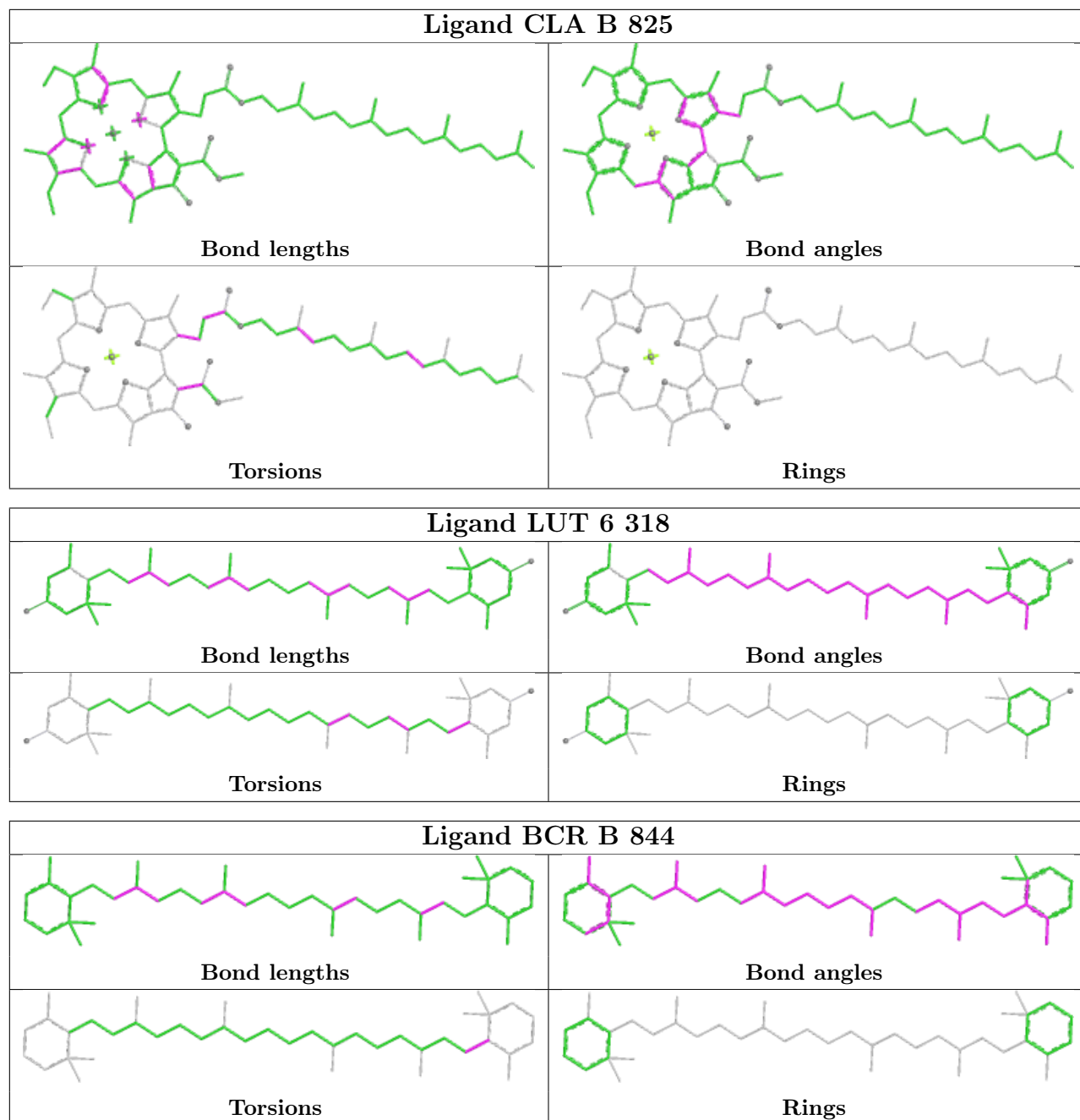


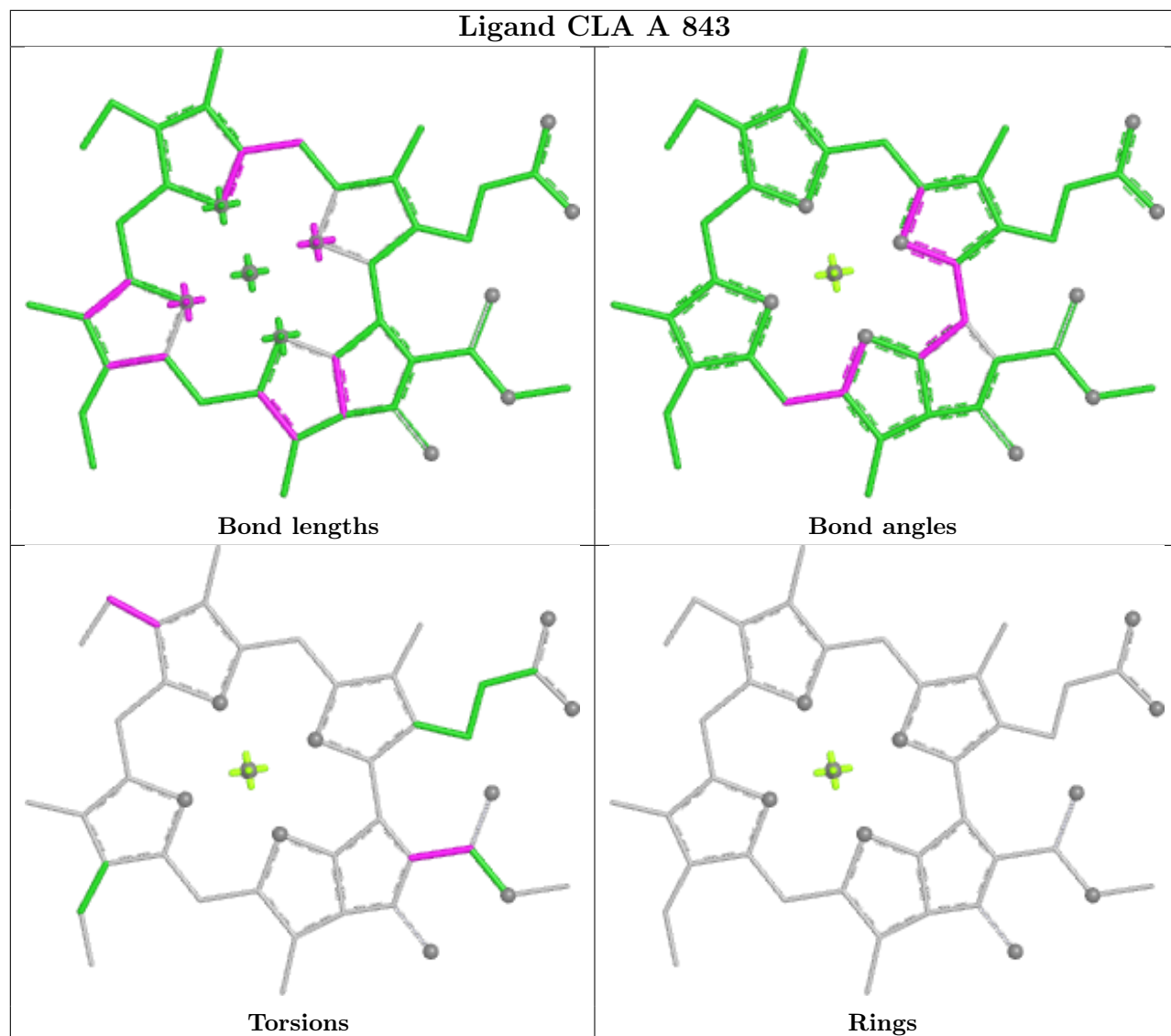
Ligand CLA A 822



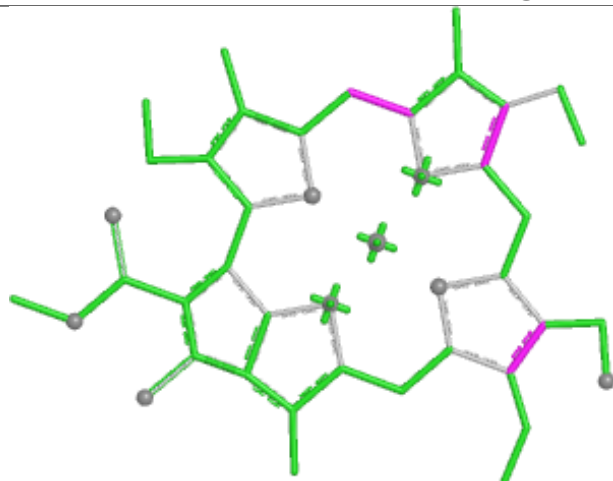
Ligand PQN A 844



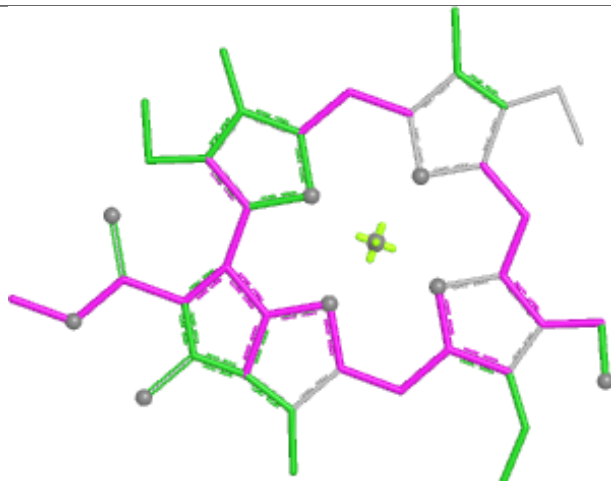




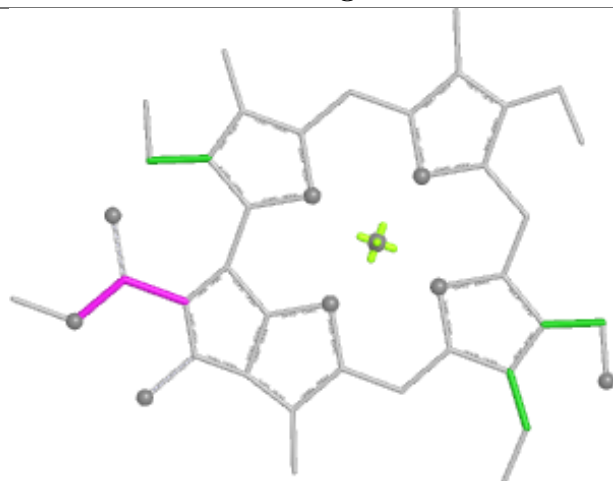
Ligand CHL 2 306



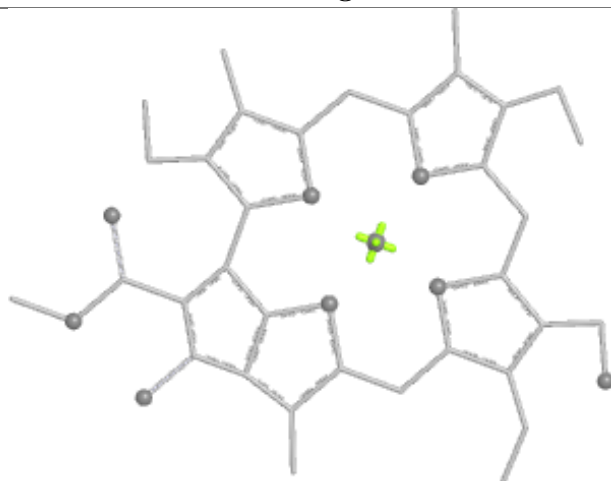
Bond lengths



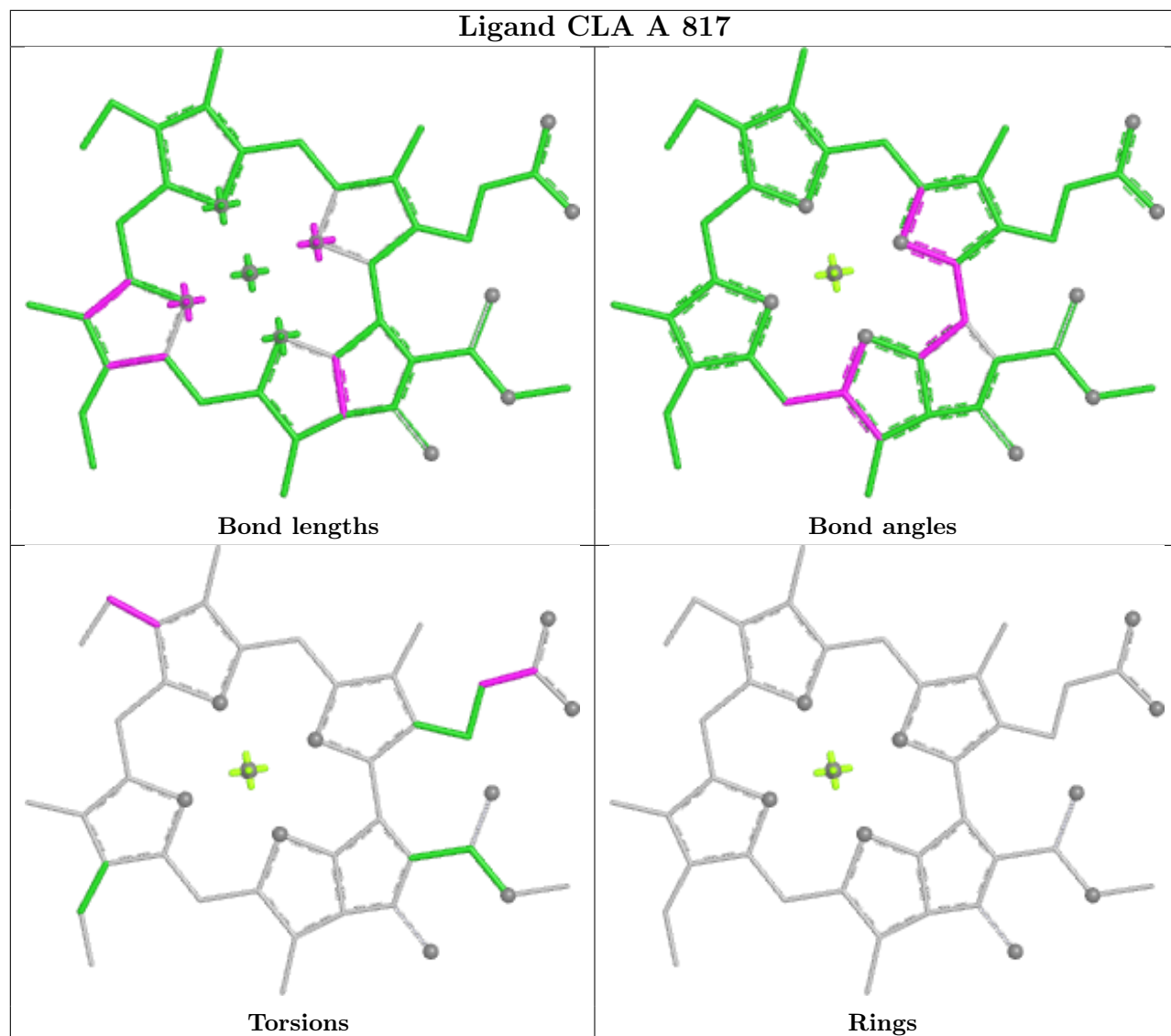
Bond angles



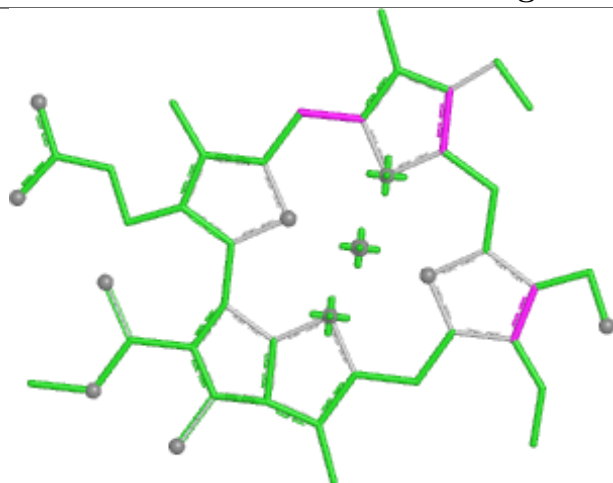
Torsions



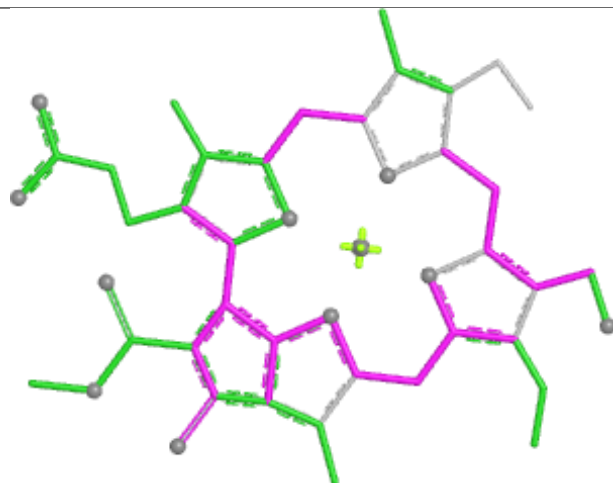
Rings



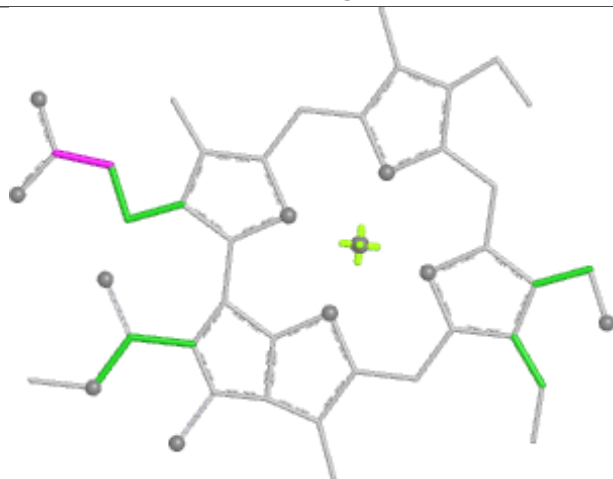
Ligand CHL 3 306



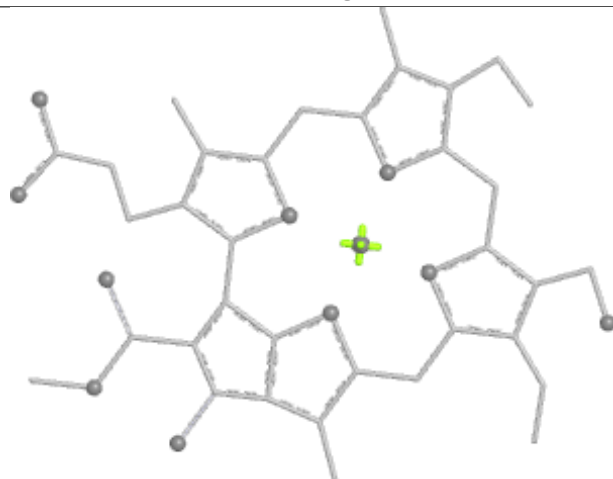
Bond lengths



Bond angles

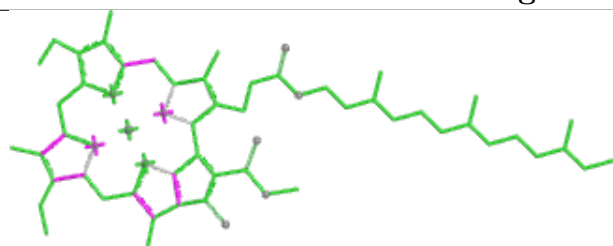


Torsions

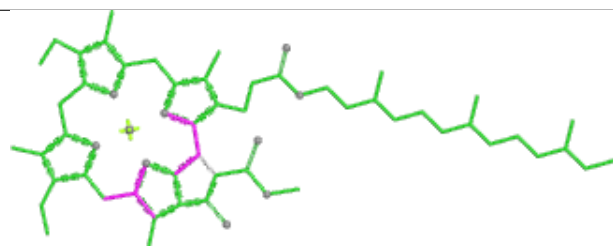


Rings

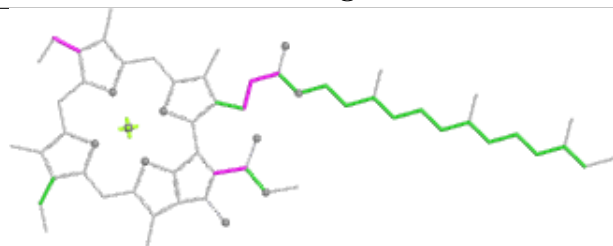
Ligand CLA 6 302



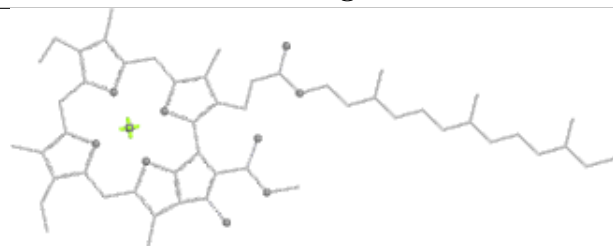
Bond lengths



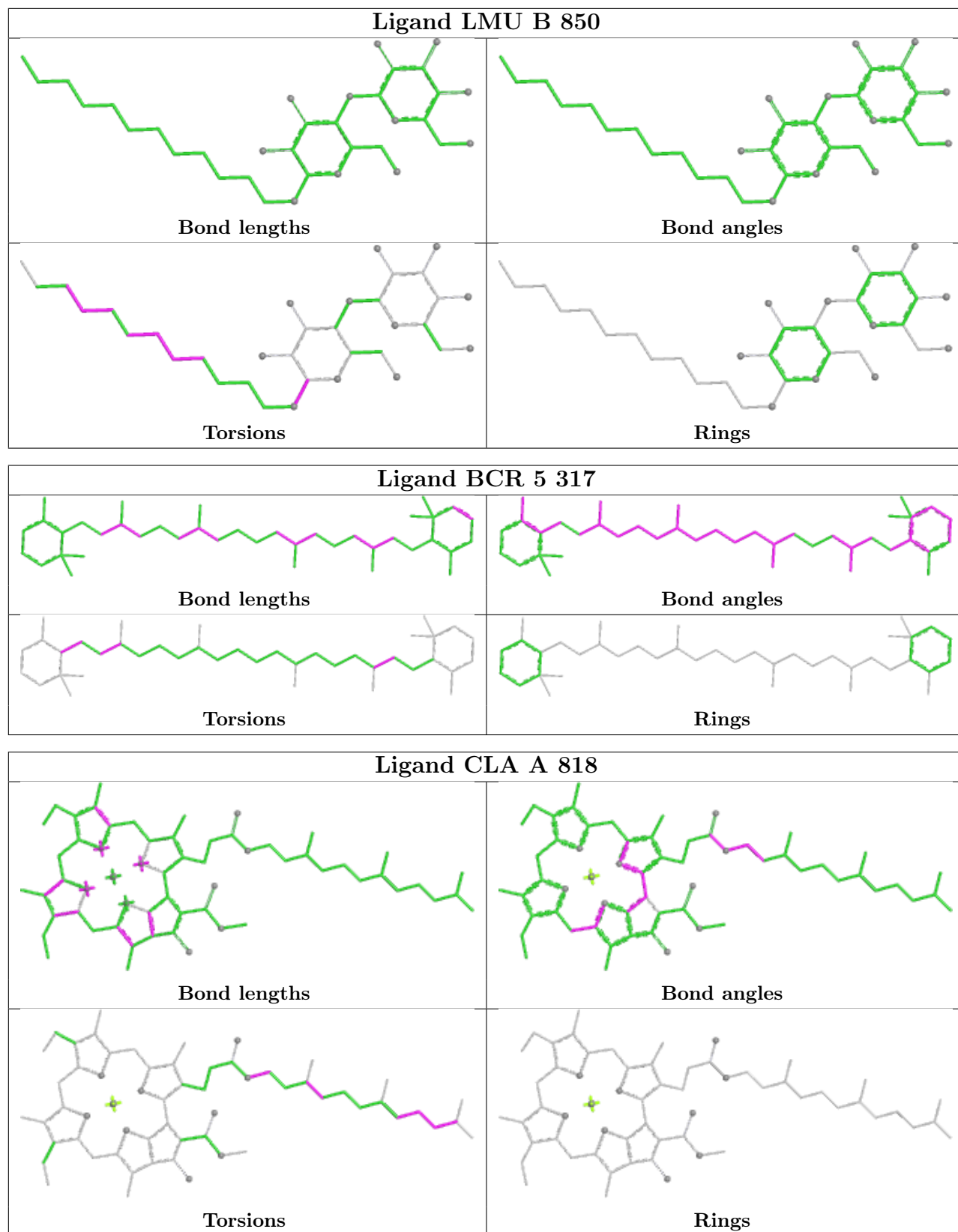
Bond angles



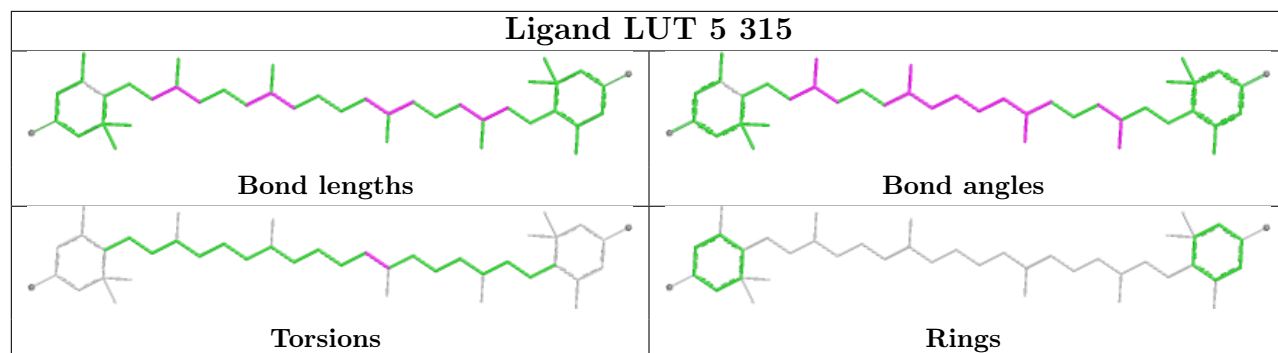
Torsions



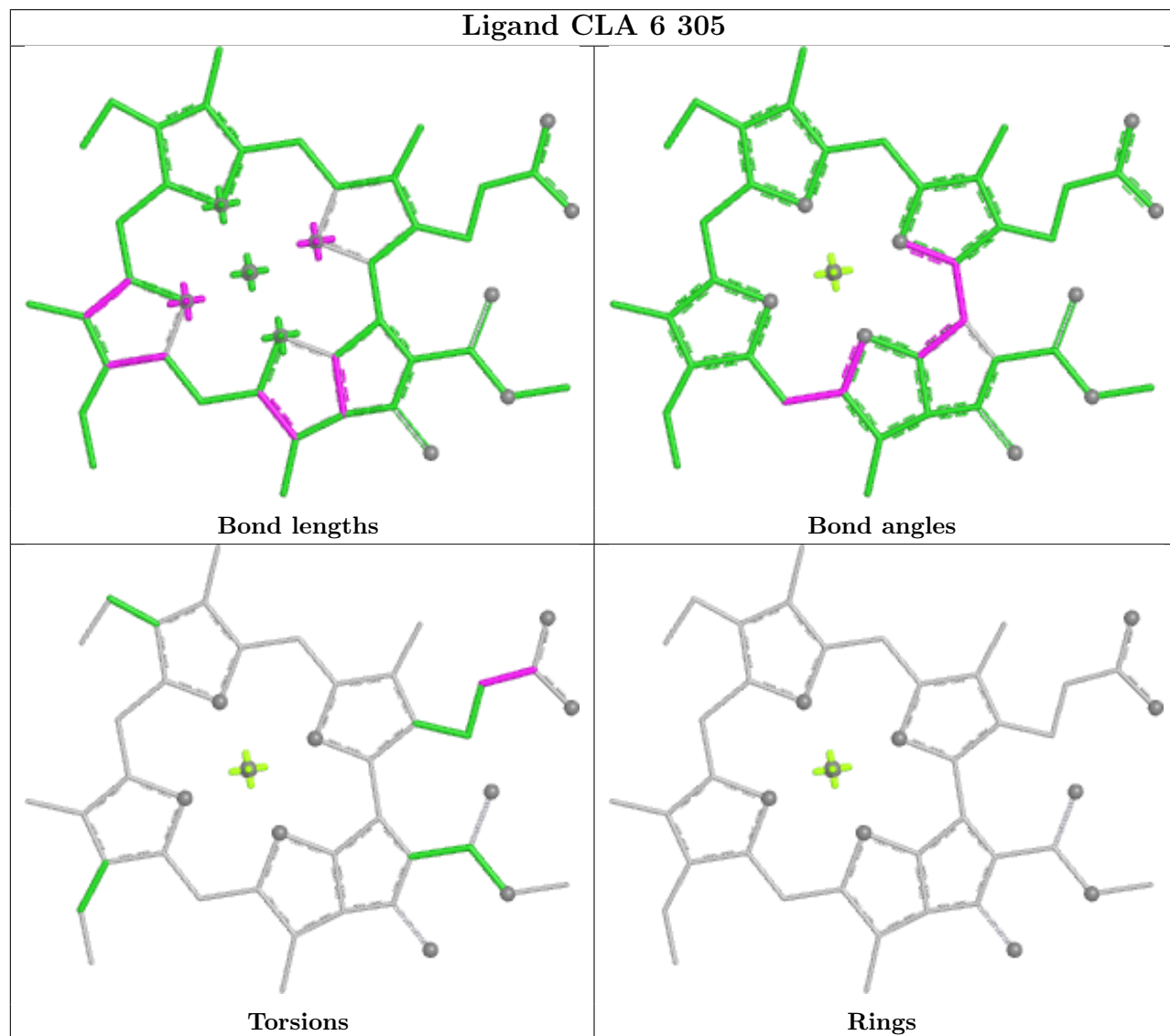
Rings

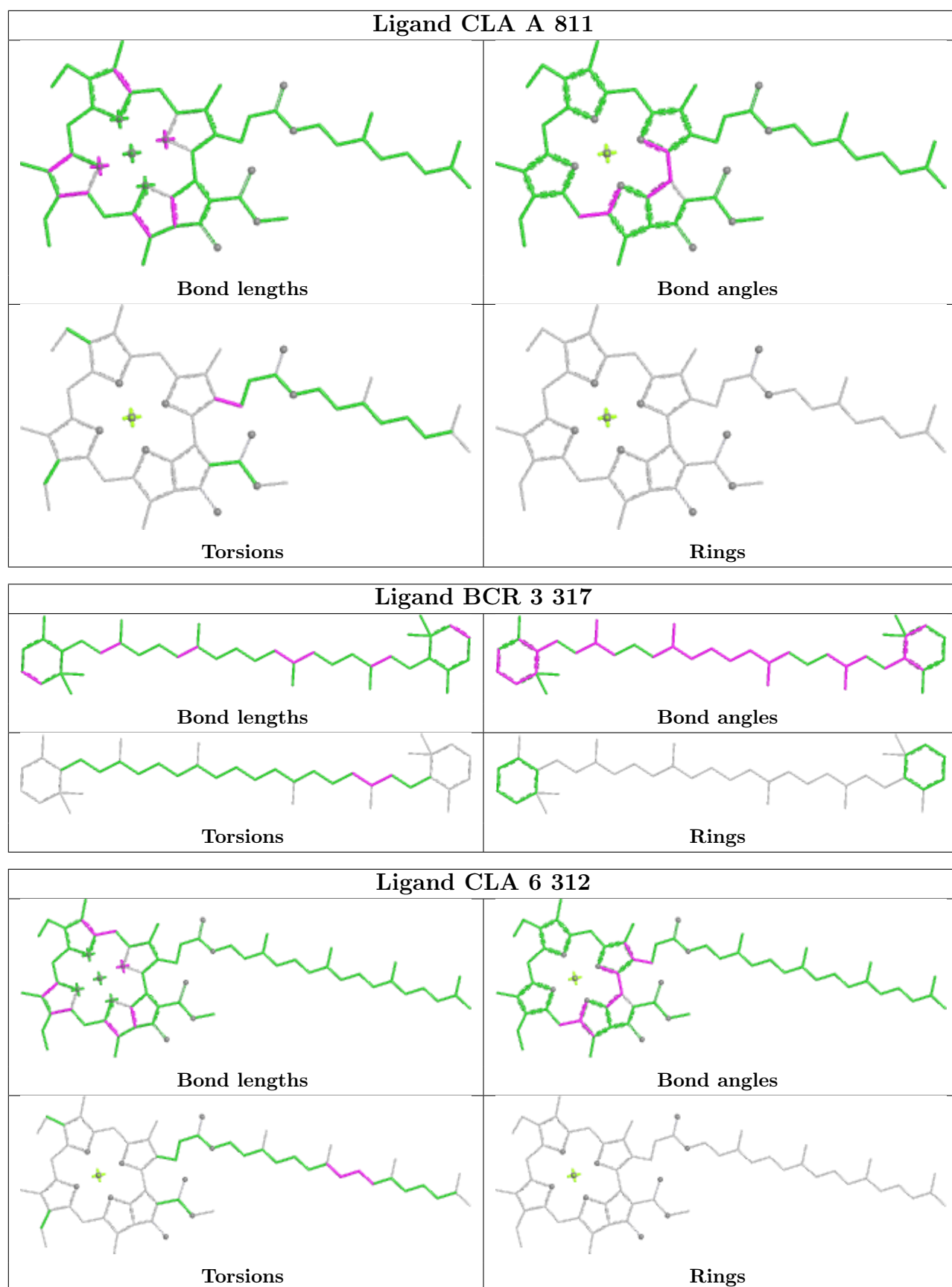


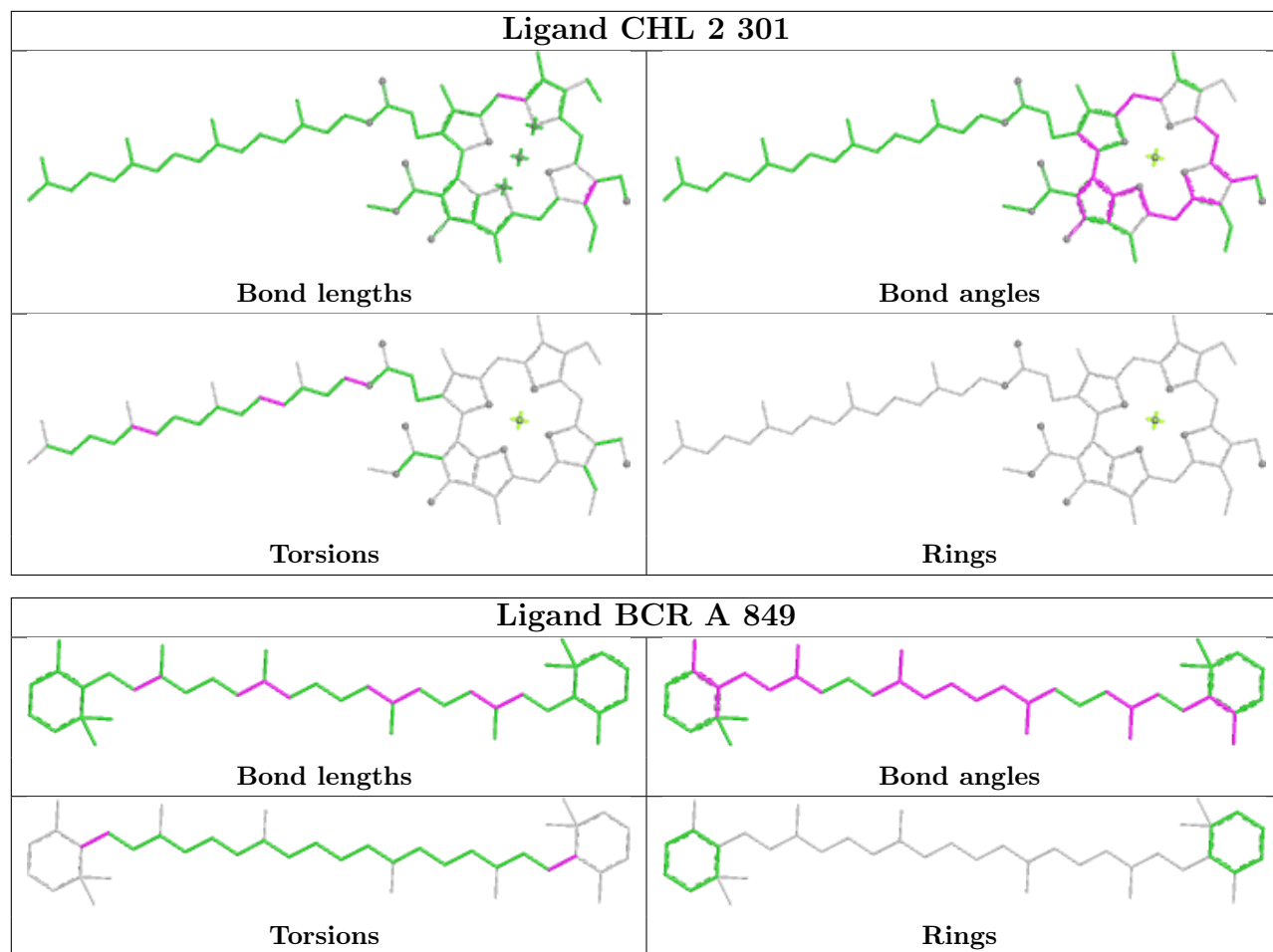
Ligand LUT 5 315



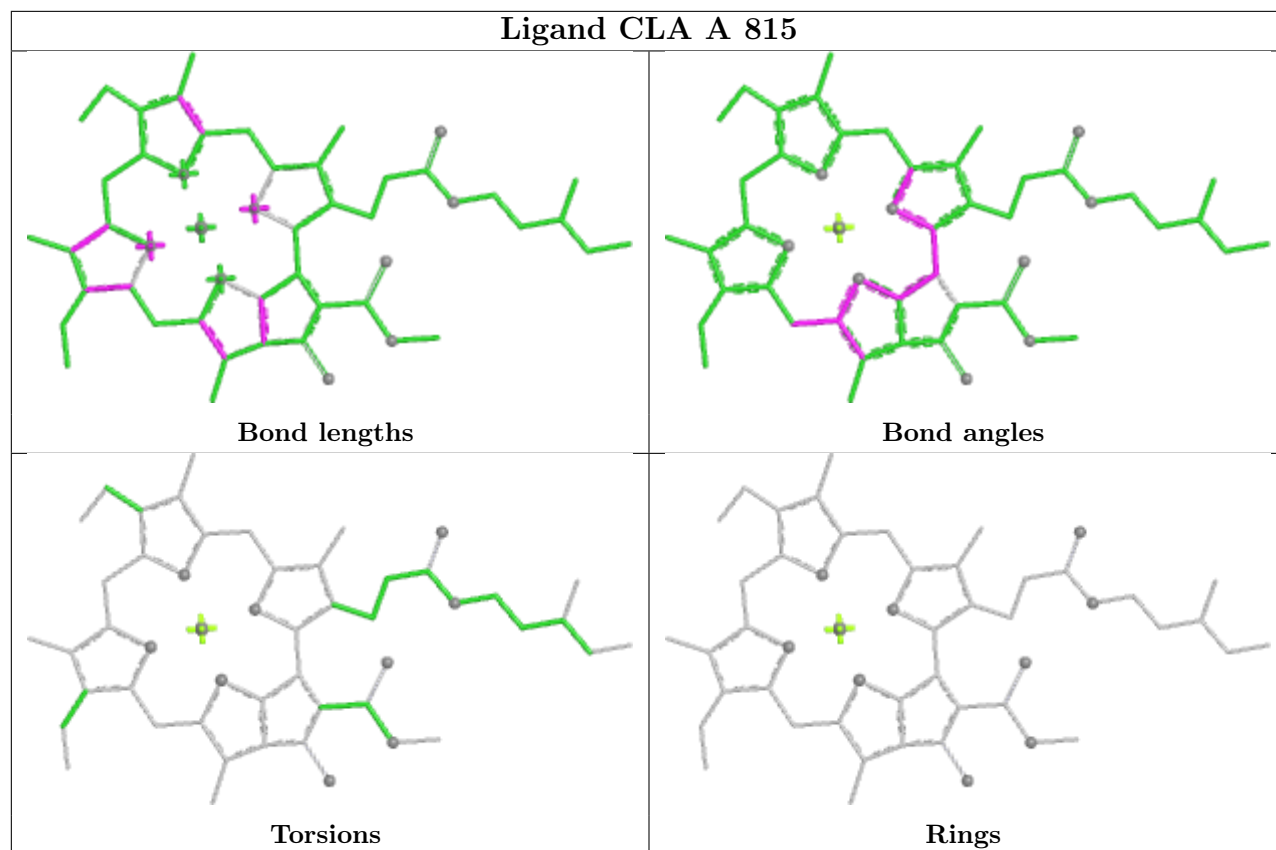
Ligand CLA 6 305



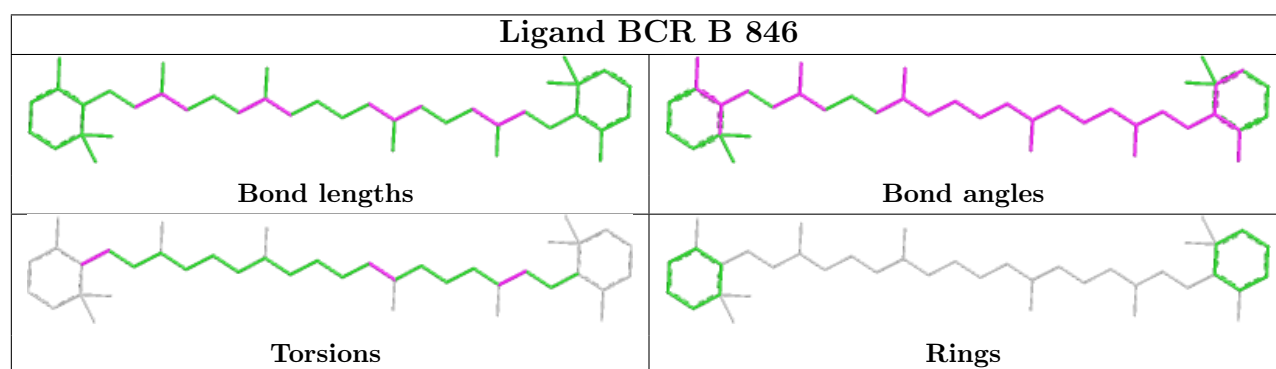


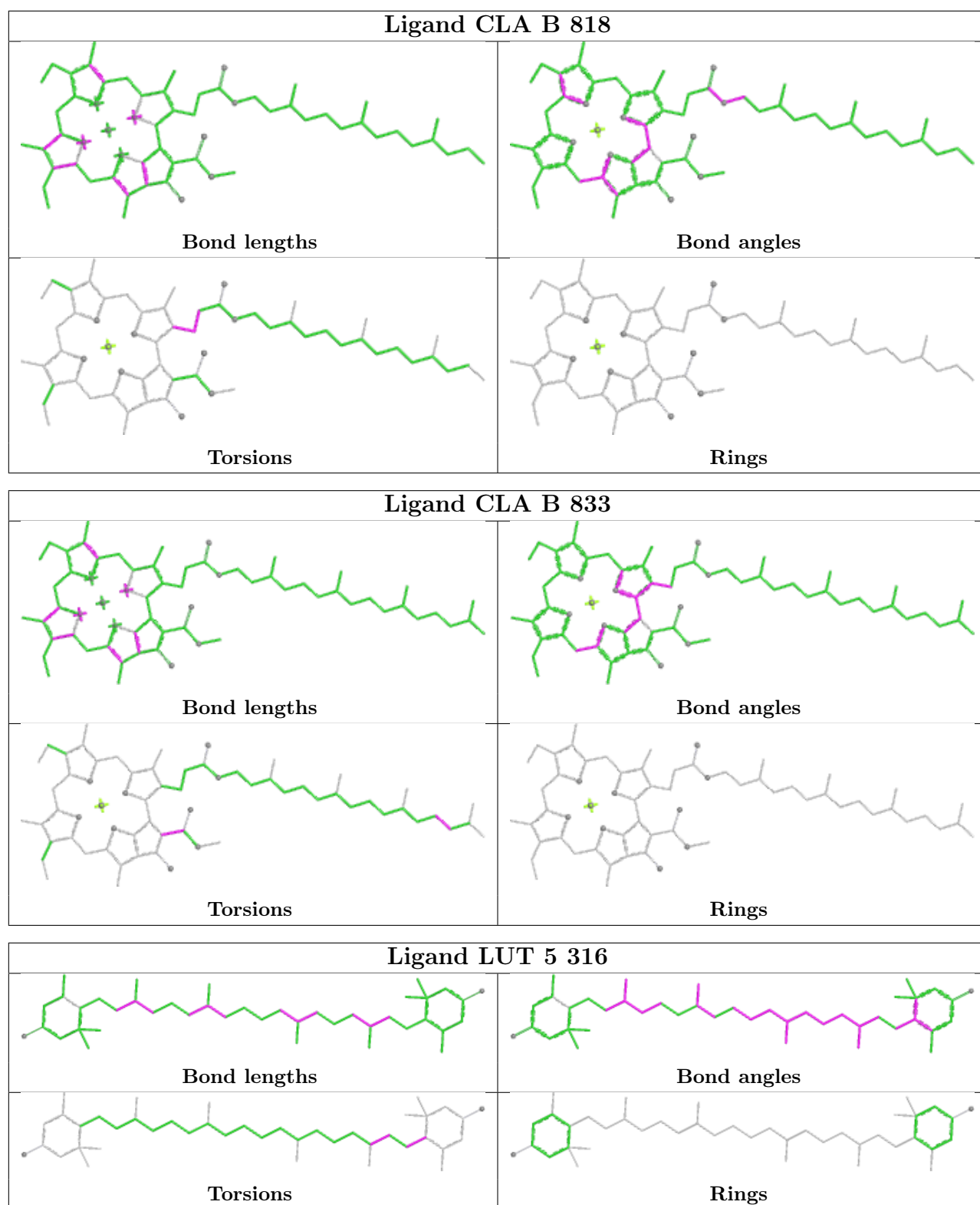


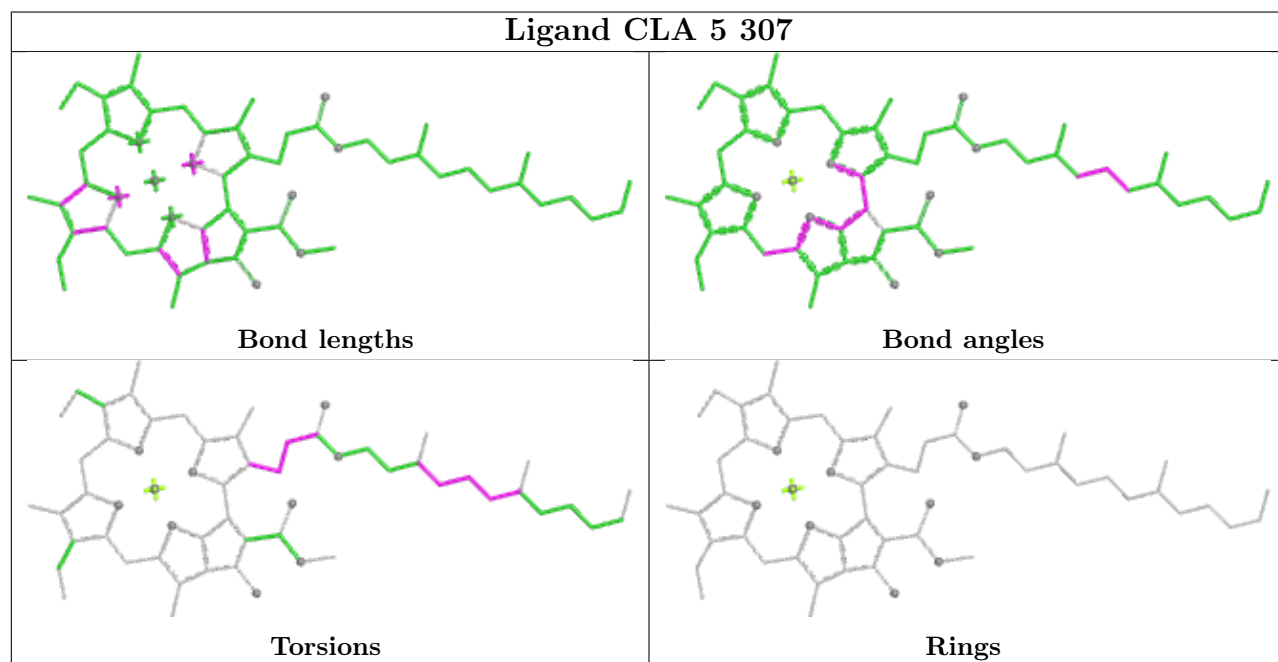
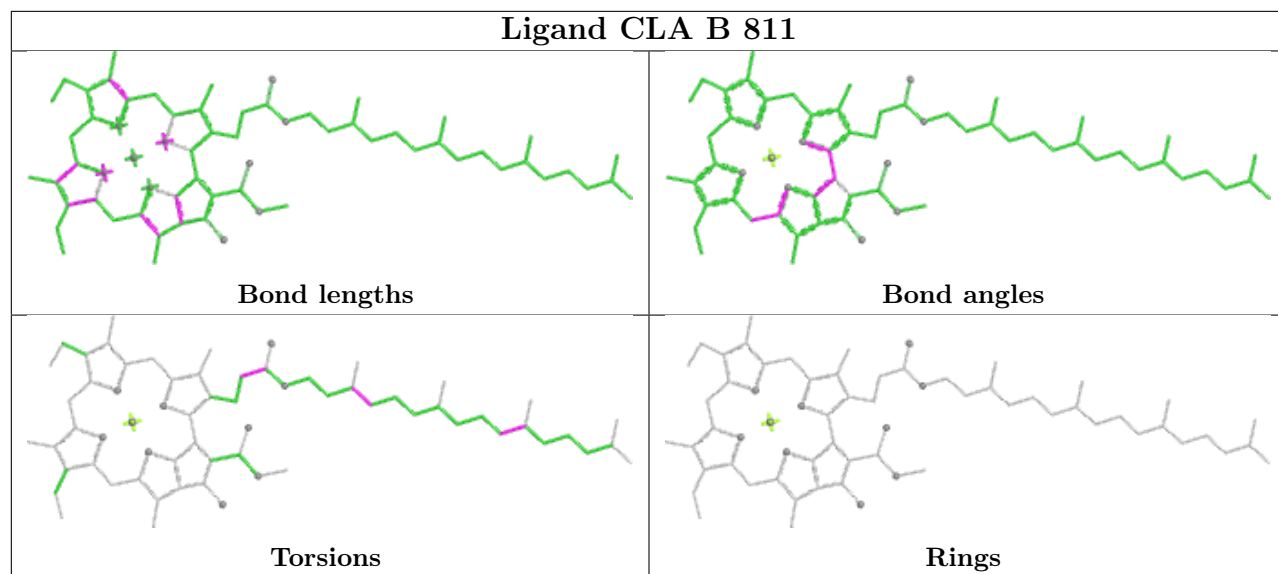
Ligand CLA A 815



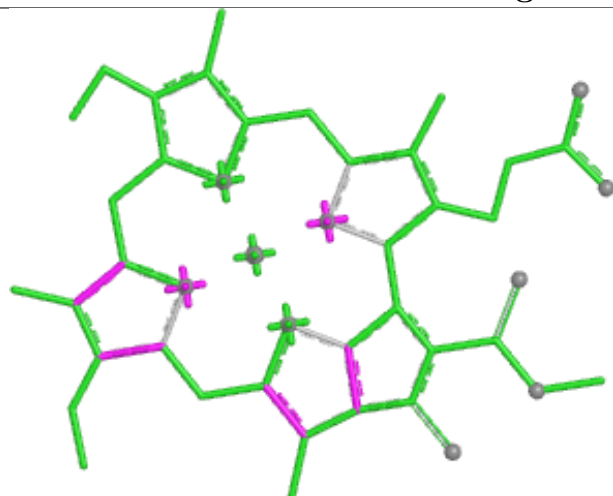
Ligand BCR B 846



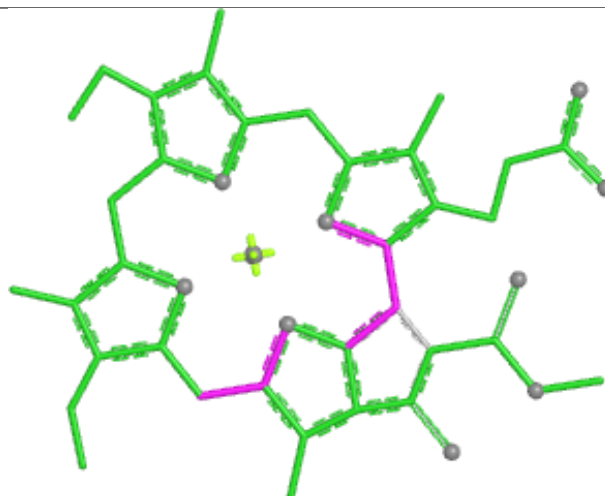




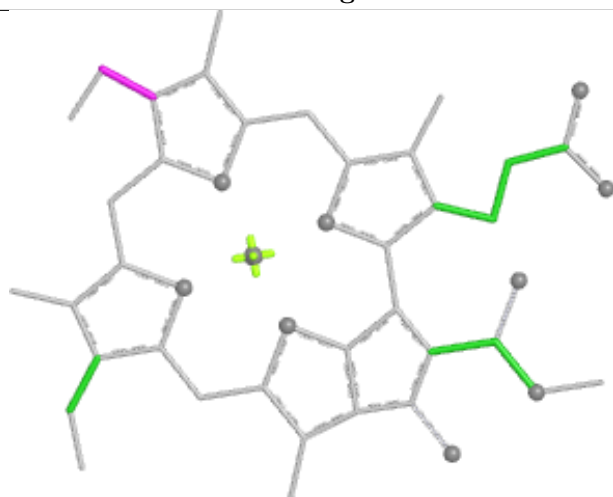
Ligand CLA F 303



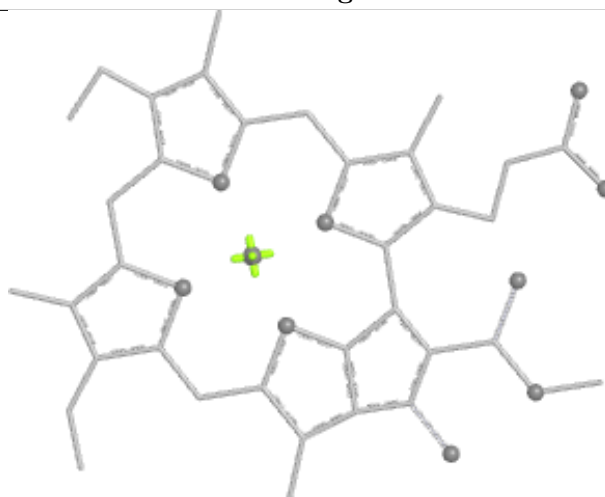
Bond lengths



Bond angles

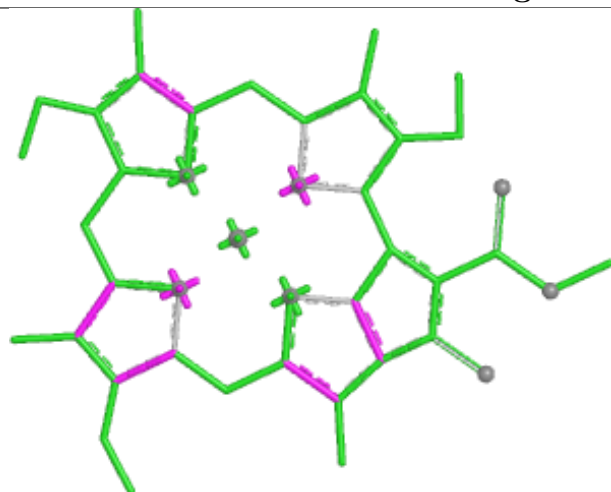


Torsions



Rings

Ligand CLA A 816



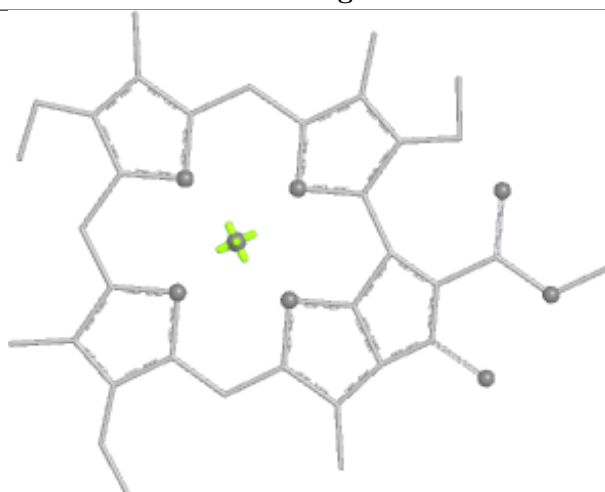
Bond lengths



Bond angles

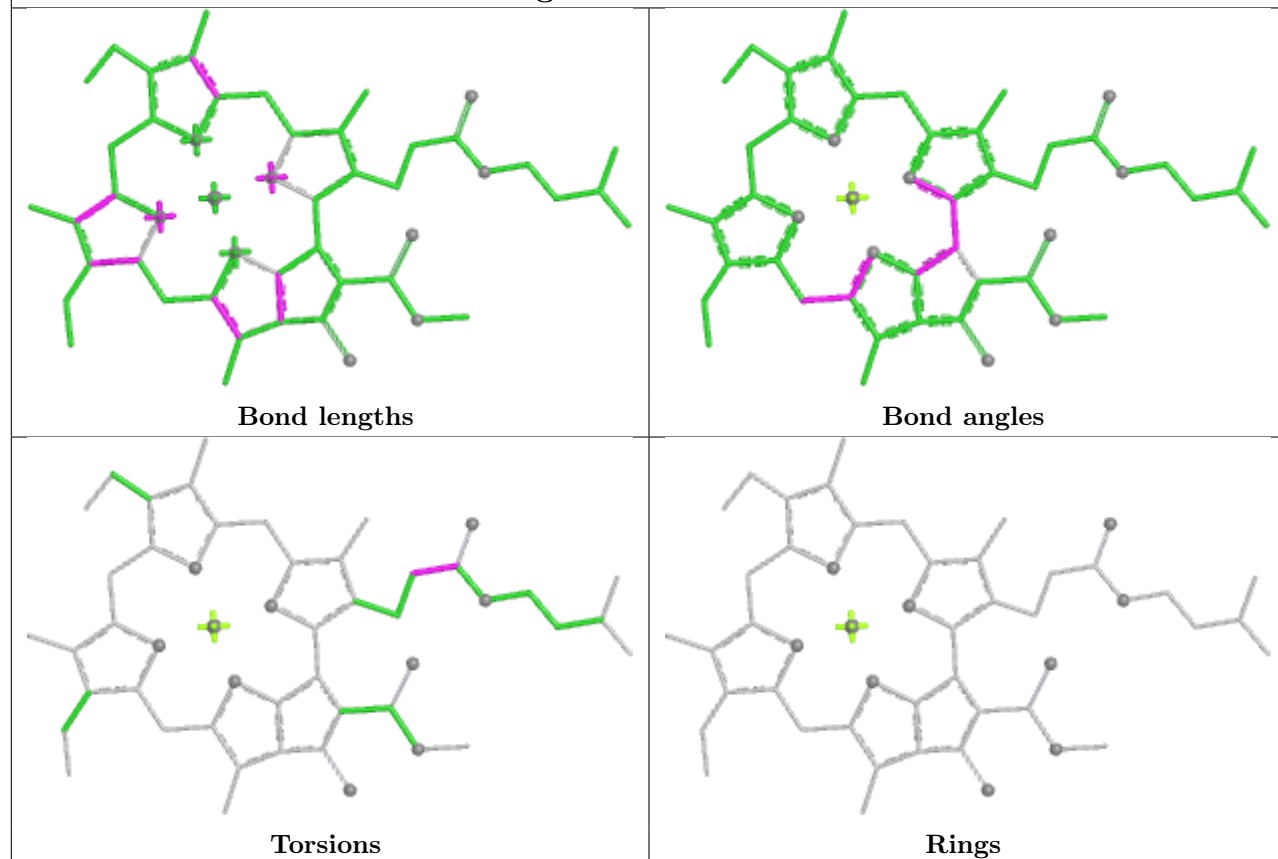


Torsions

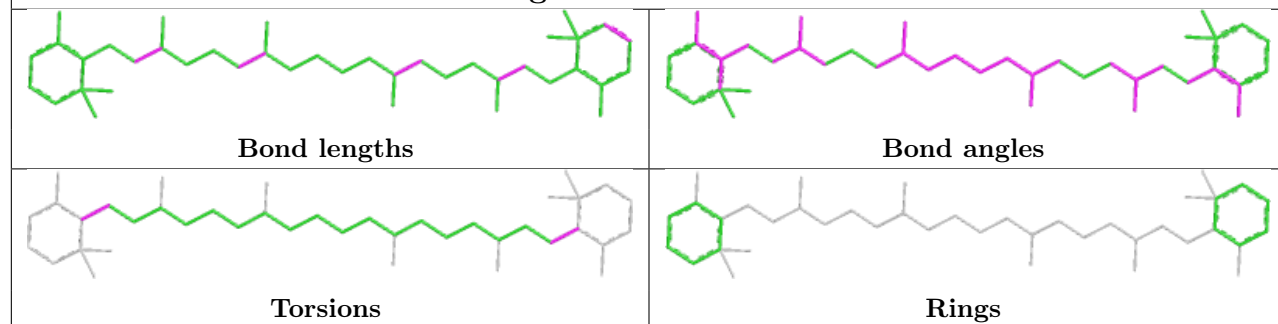


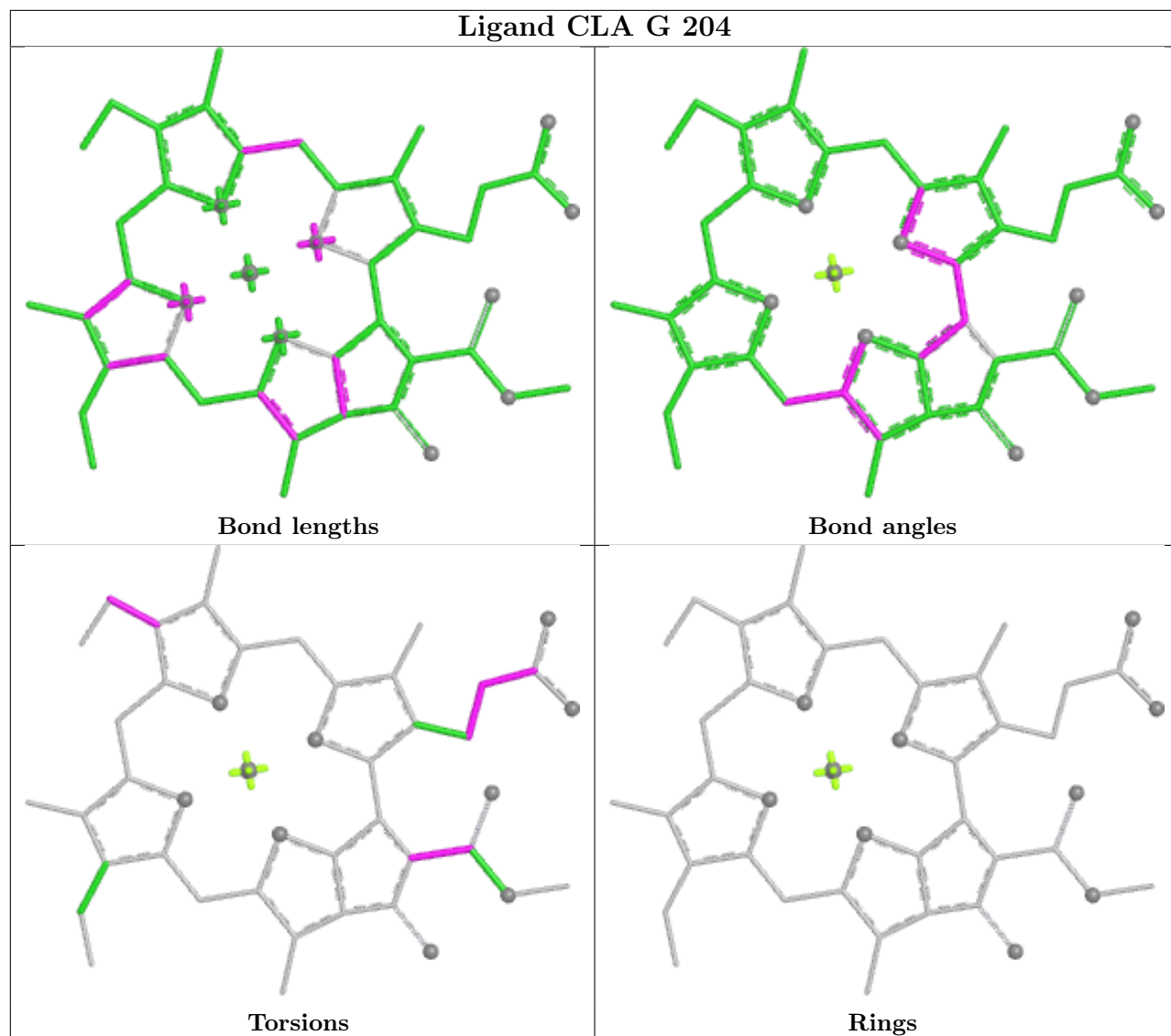
Rings

Ligand CLA 5 302

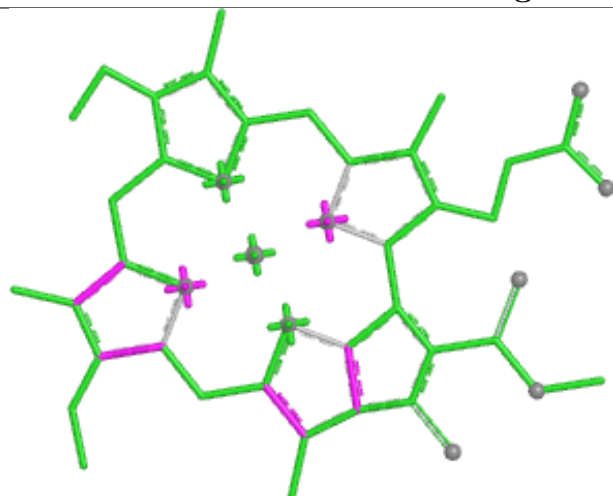


Ligand BCR G 201

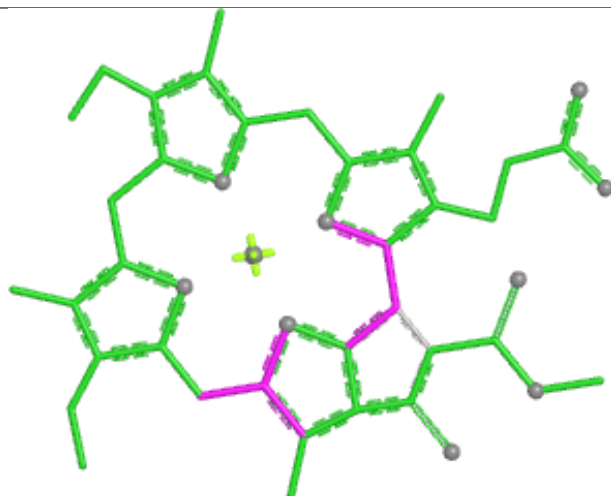




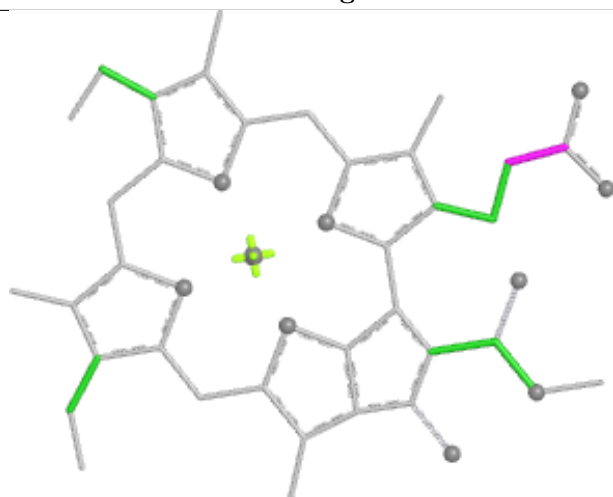
Ligand CLA B 835



Bond lengths



Bond angles

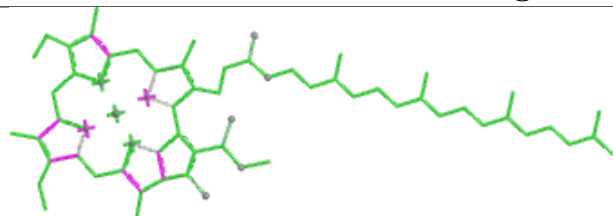


Torsions

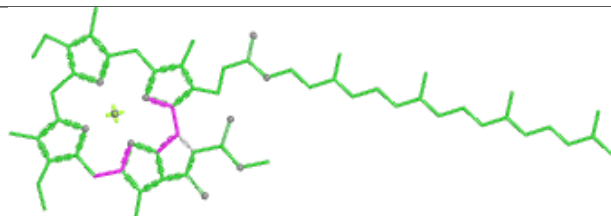


Rings

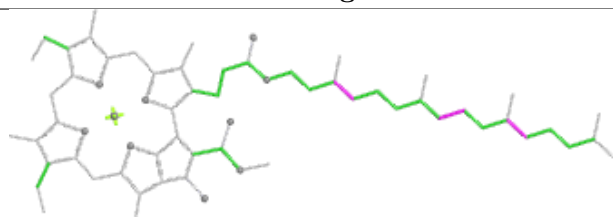
Ligand CLA A 841



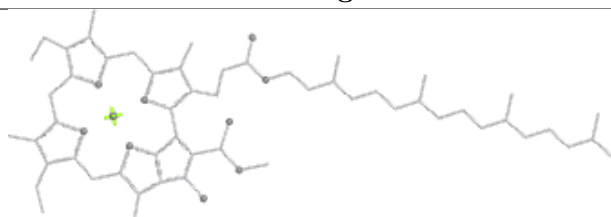
Bond lengths



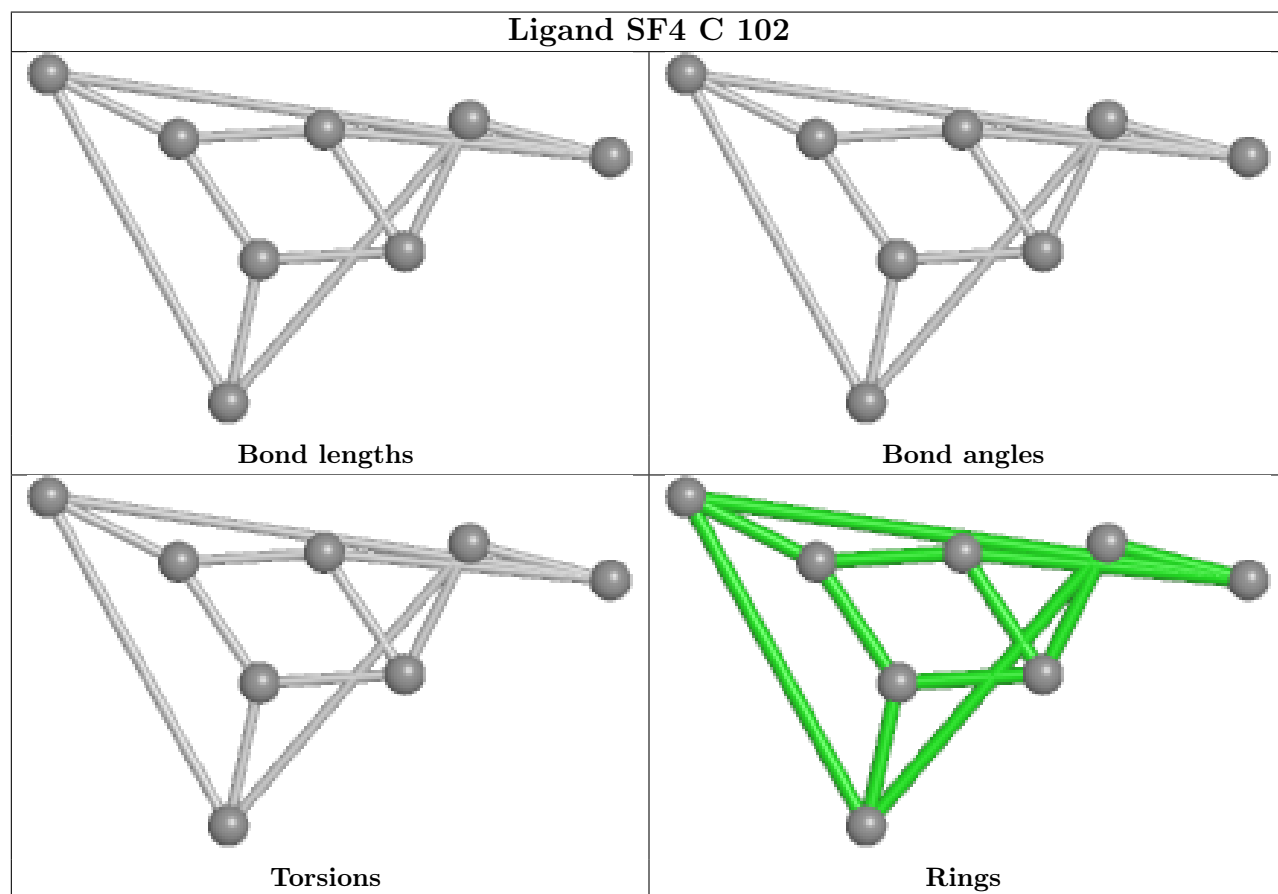
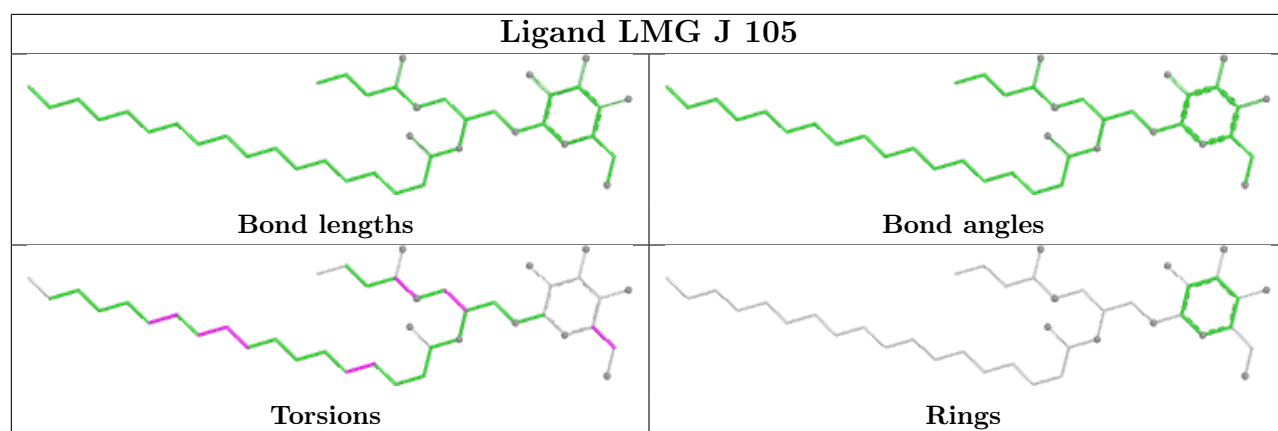
Bond angles

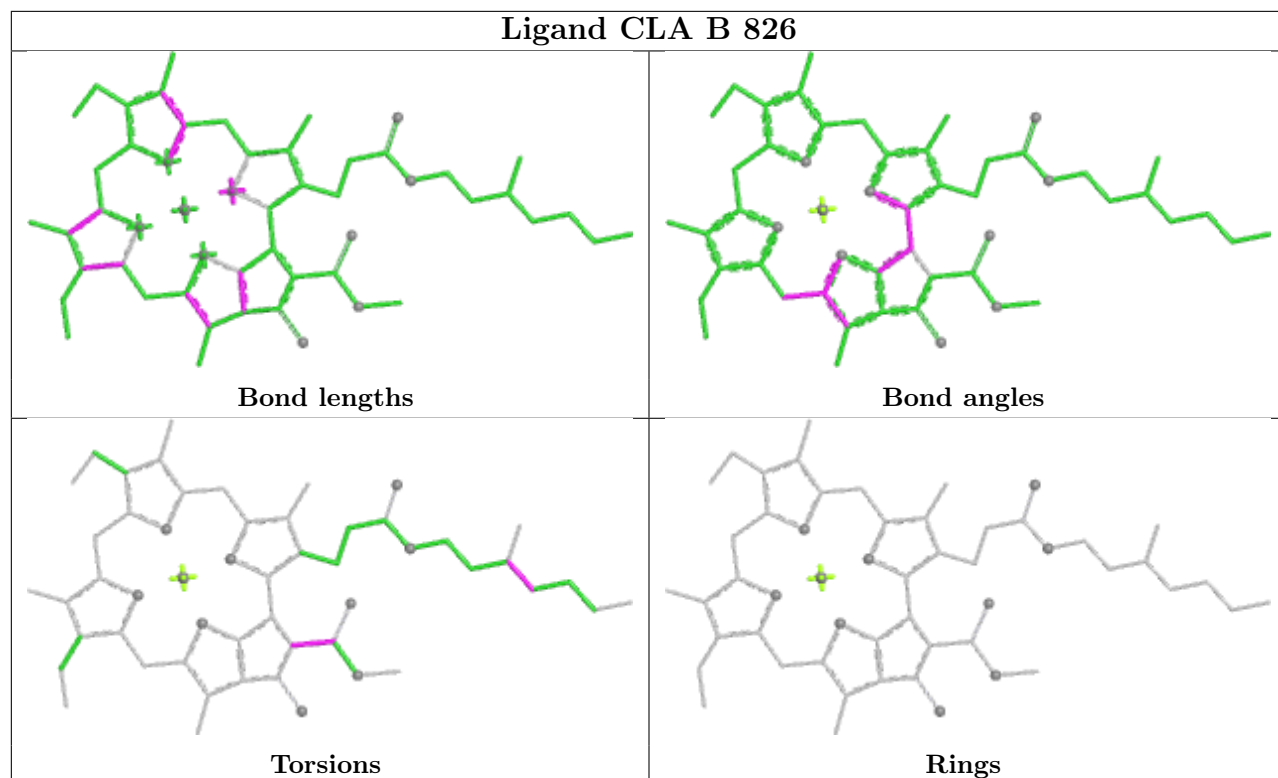


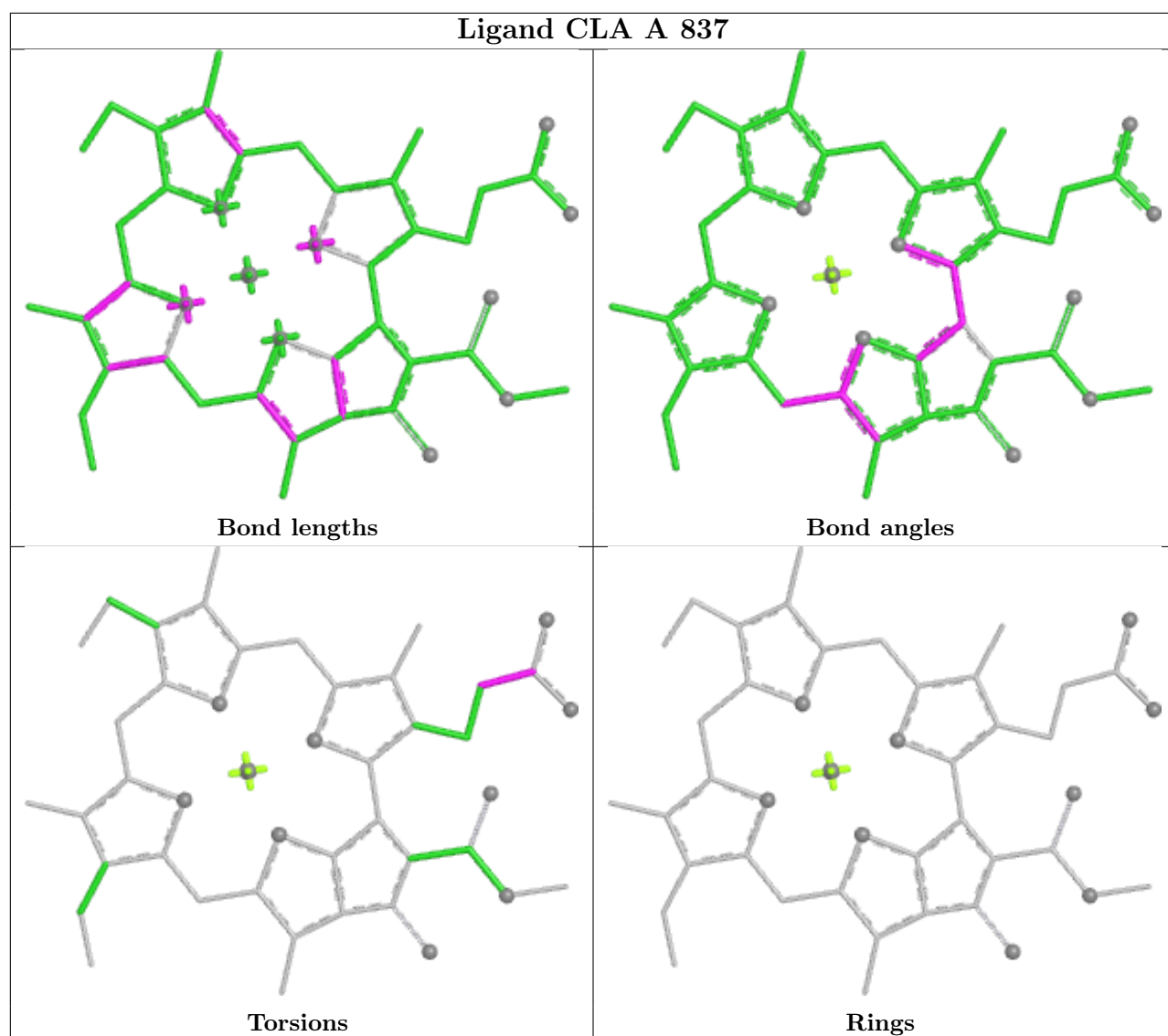
Torsions



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.

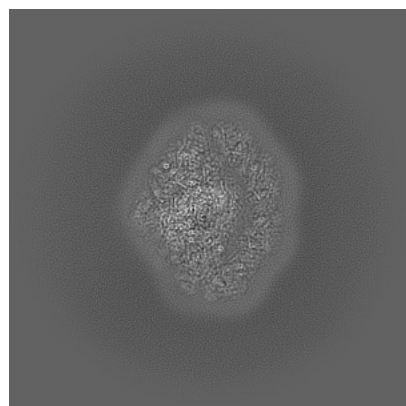
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63404. These allow visual inspection of the internal detail of the map and identification of artifacts.

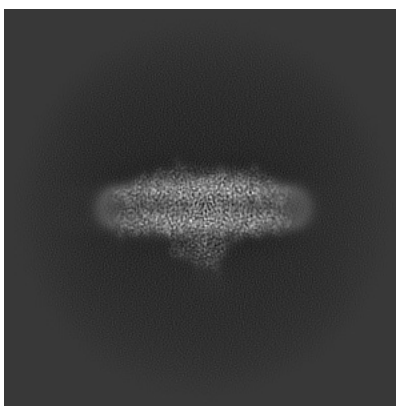
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

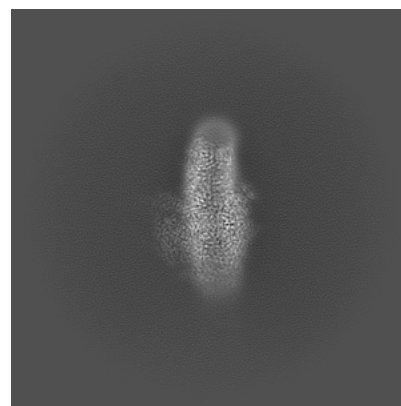
6.1.1 Primary map



X

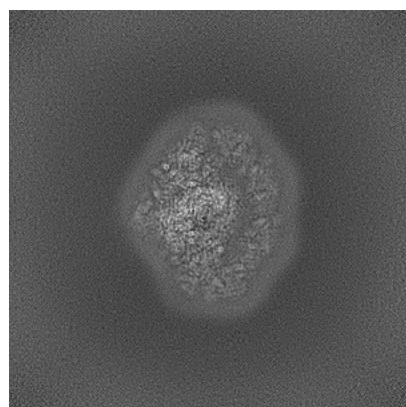


Y

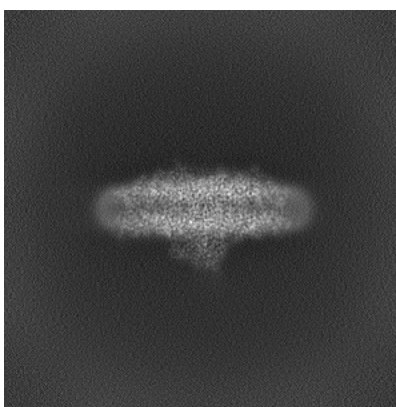


Z

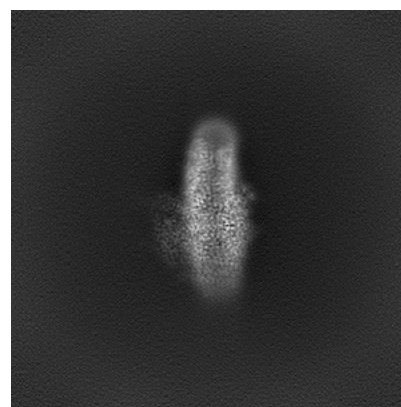
6.1.2 Raw map



X



Y

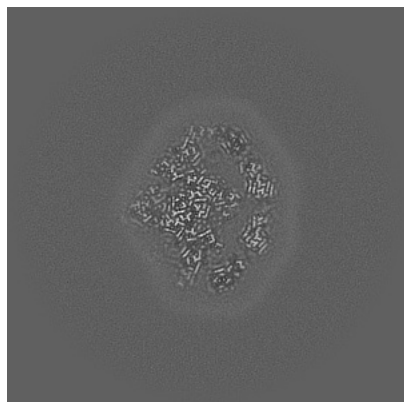


Z

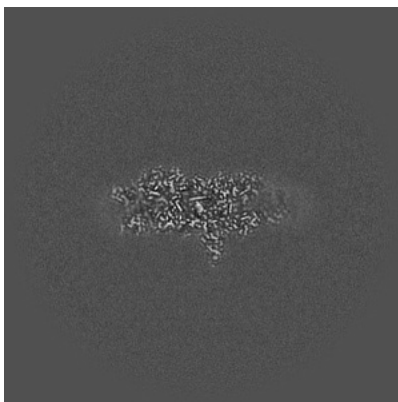
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

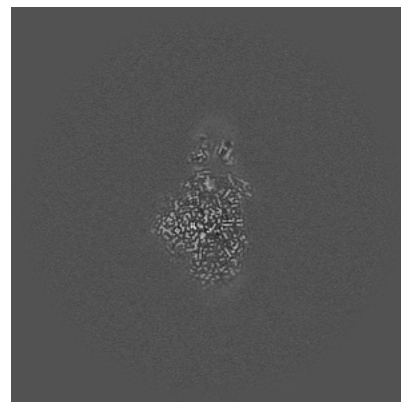
6.2.1 Primary map



X Index: 250

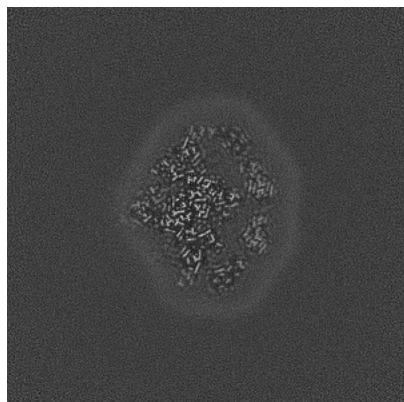


Y Index: 250

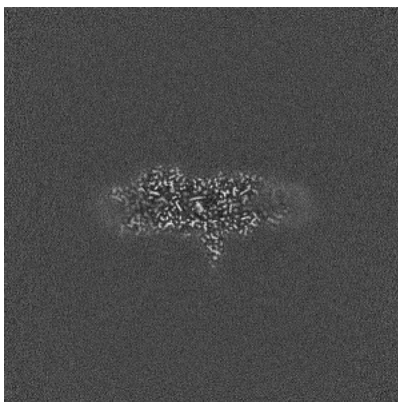


Z Index: 250

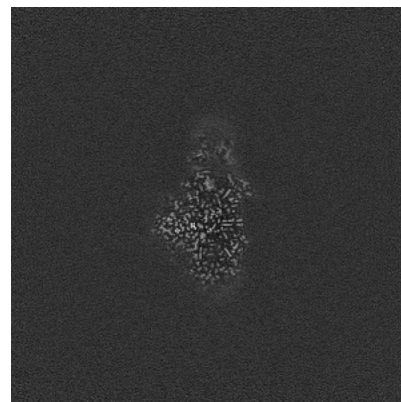
6.2.2 Raw map



X Index: 250



Y Index: 250

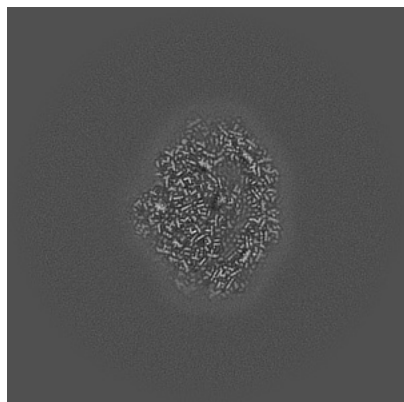


Z Index: 250

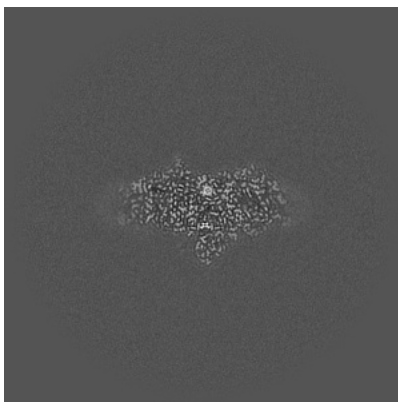
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

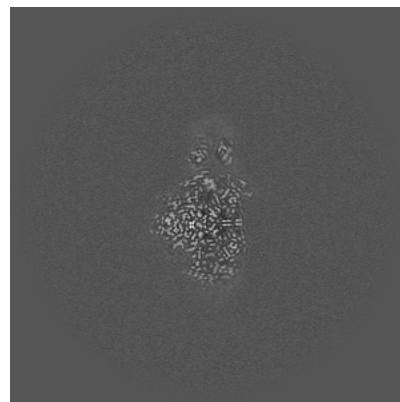
6.3.1 Primary map



X Index: 236

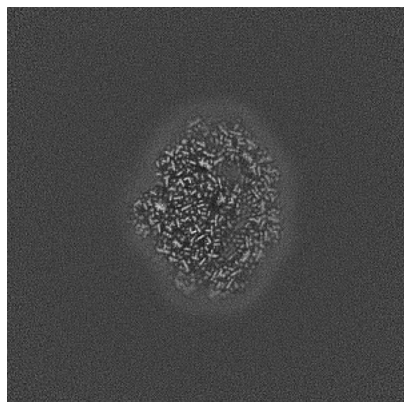


Y Index: 227

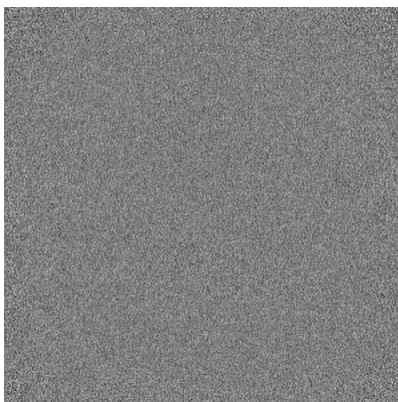


Z Index: 251

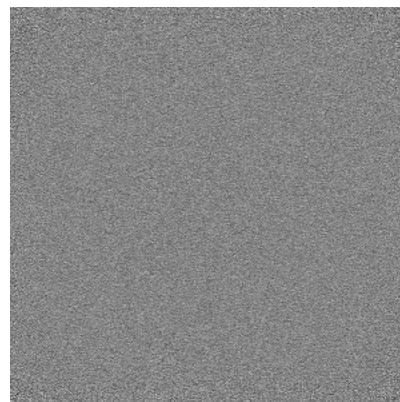
6.3.2 Raw map



X Index: 236



Y Index: 0

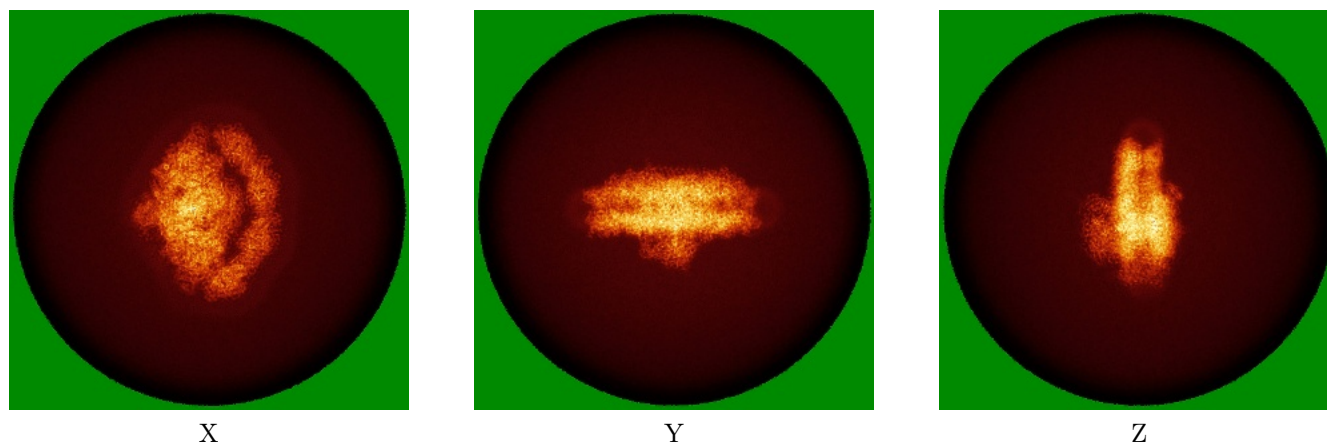


Z Index: 0

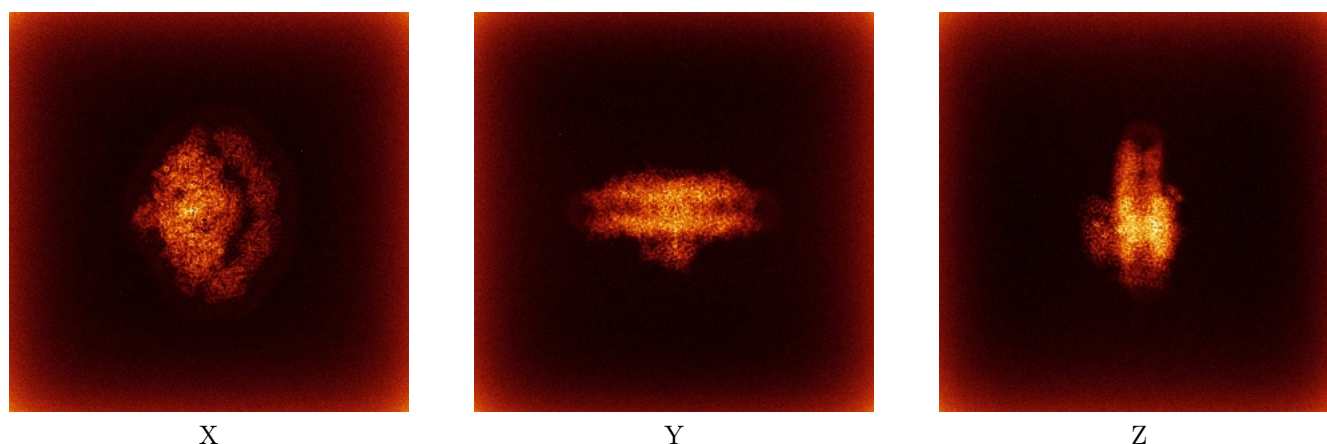
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

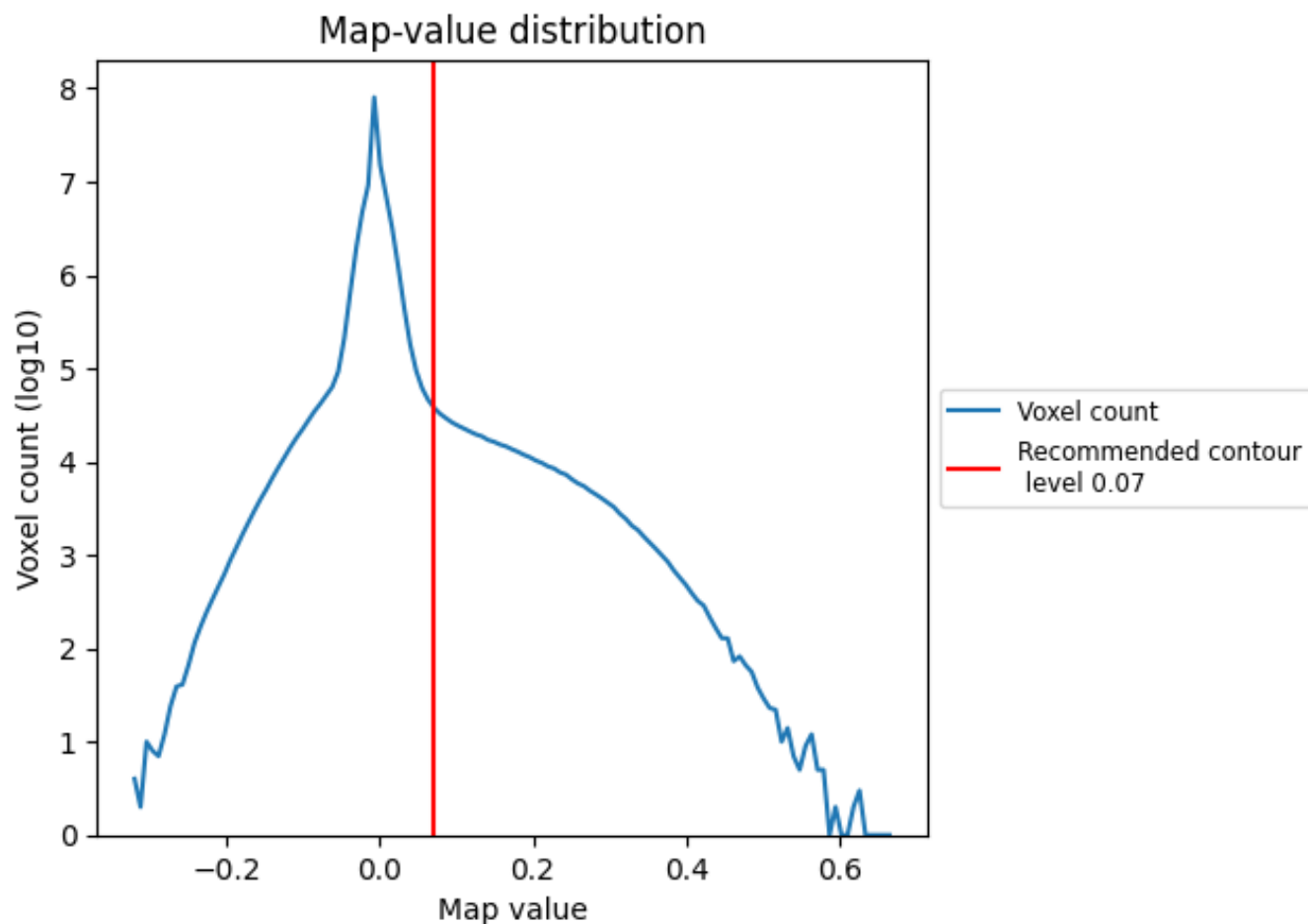
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

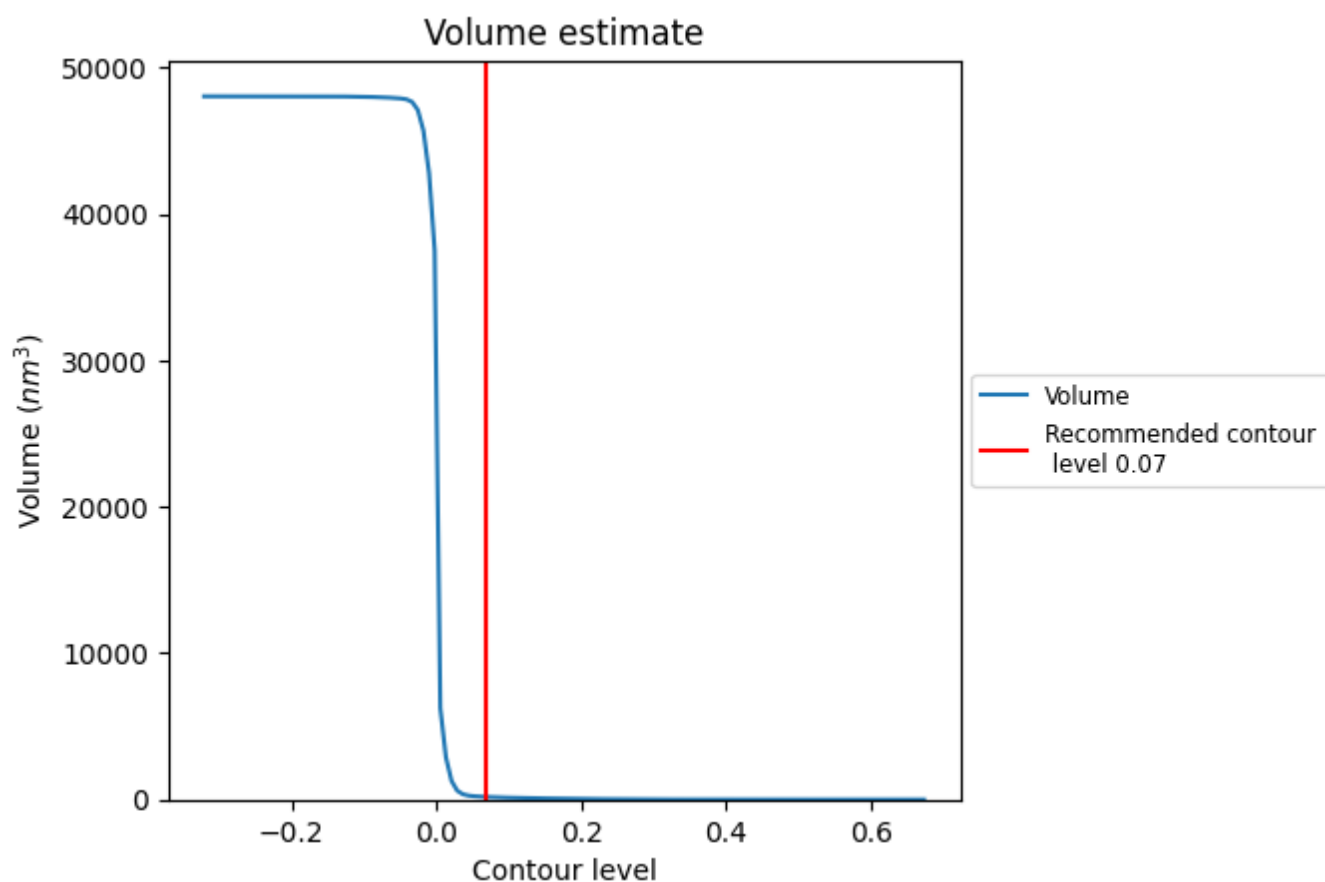
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

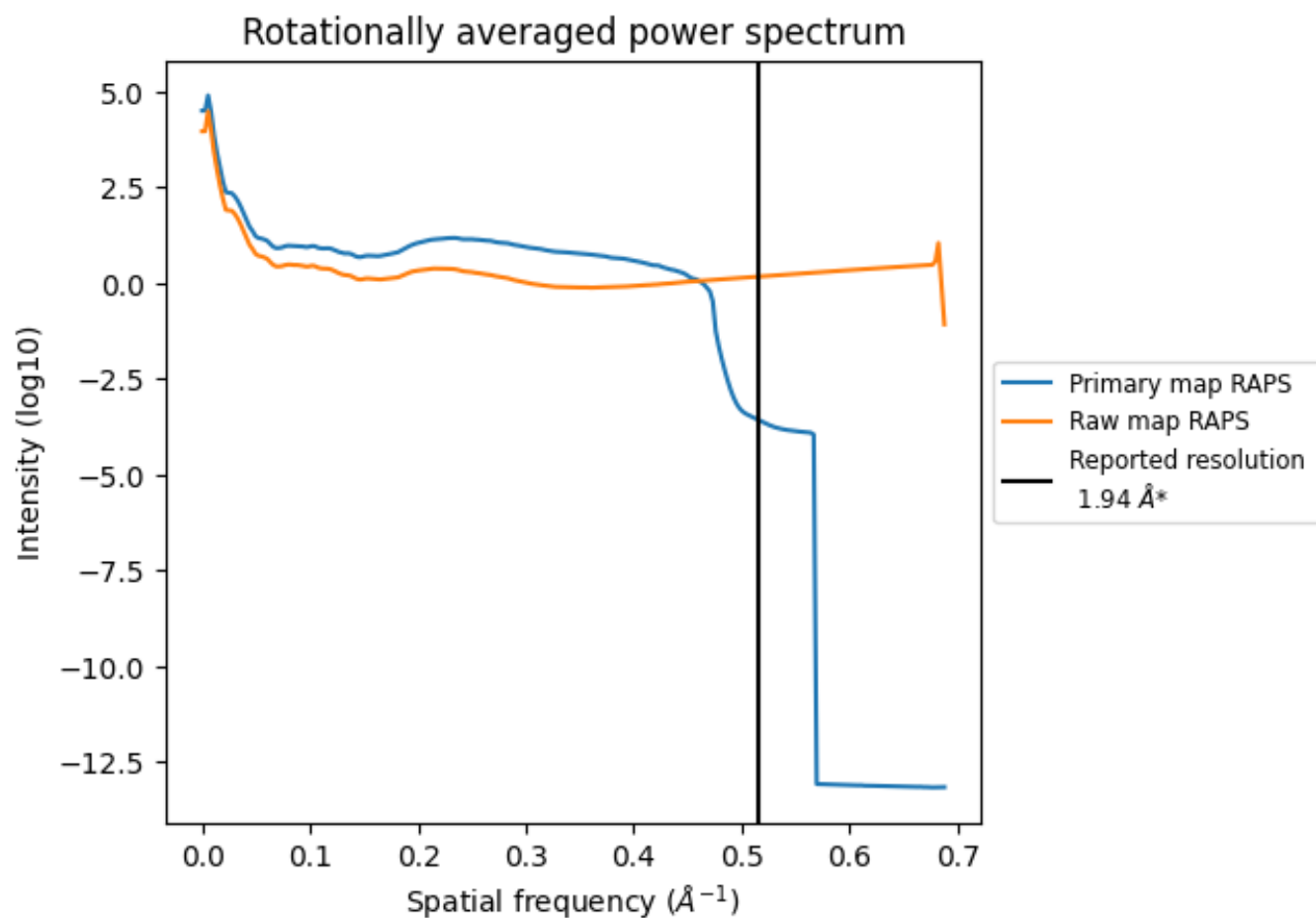
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 159 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 ⓘ

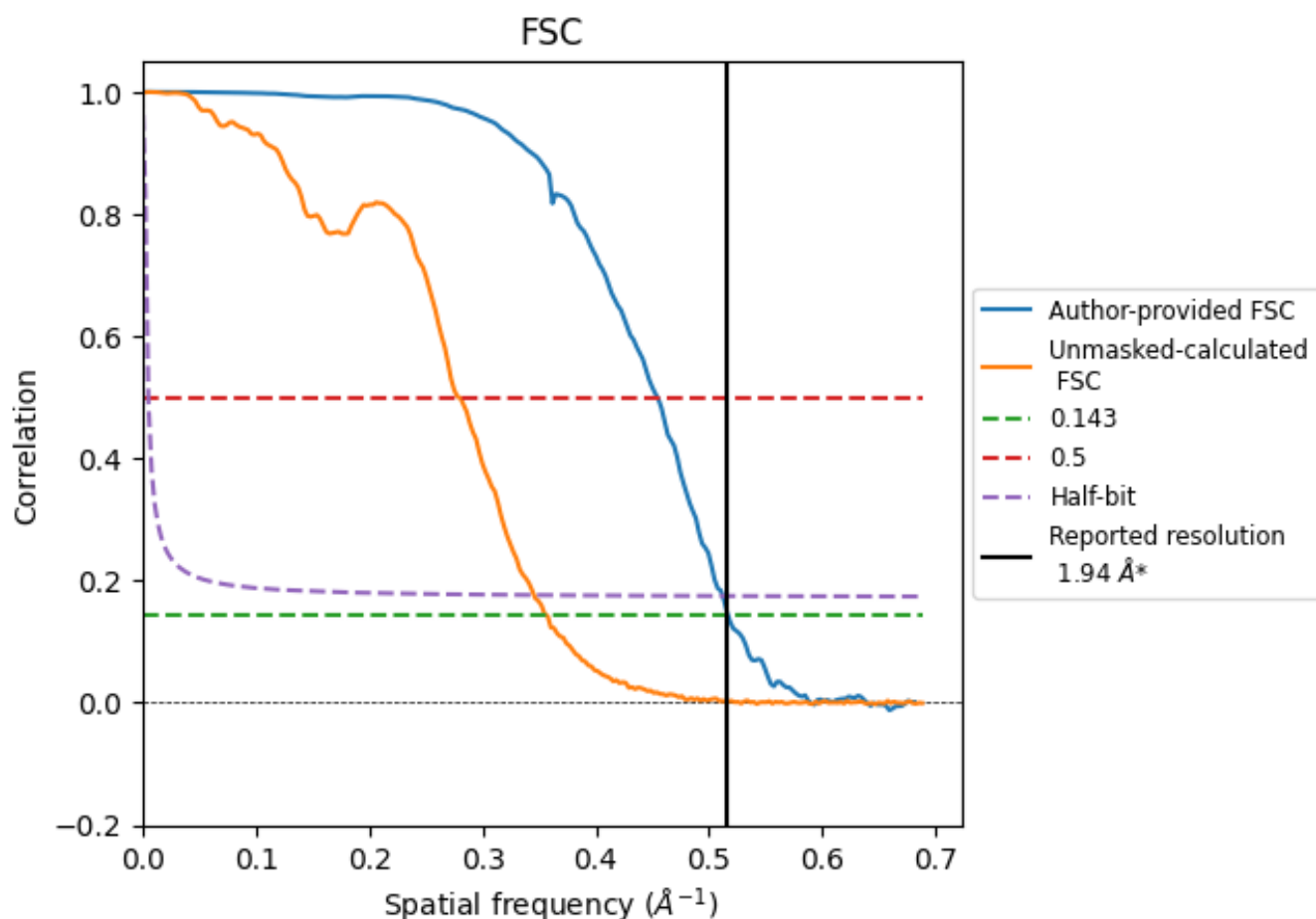


*Reported resolution corresponds to spatial frequency of 0.515 Å⁻¹

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 0.515 \AA^{-1}

8.2 Resolution estimates [i](#)

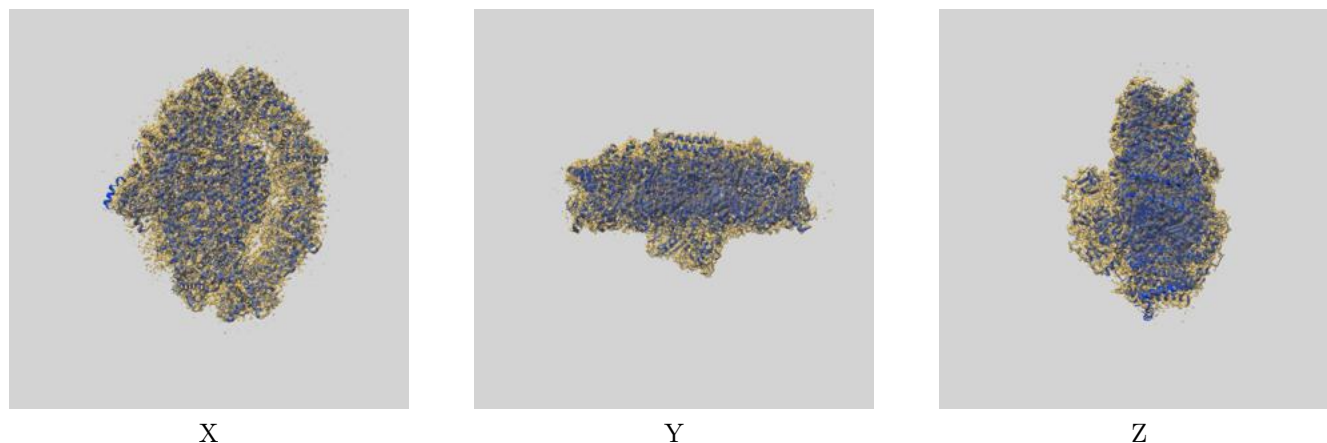
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.94	-	-
Author-provided FSC curve	1.94	2.20	1.95
Unmasked-calculated*	2.80	3.58	2.89

*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 2.80 differs from the reported value 1.94 by more than 10 %

9 Map-model fit [i](#)

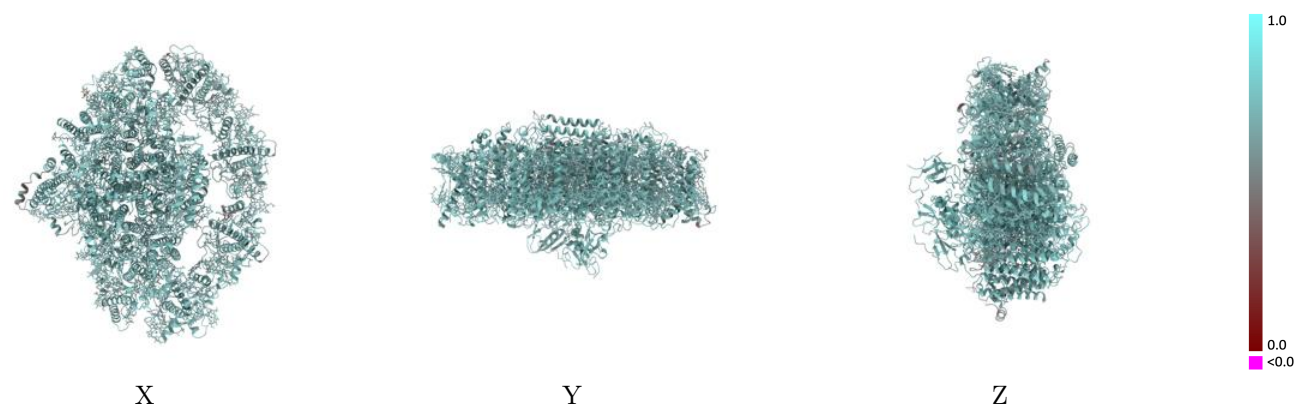
This section contains information regarding the fit between EMDB map EMD-63404 and PDB model 9LUT. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



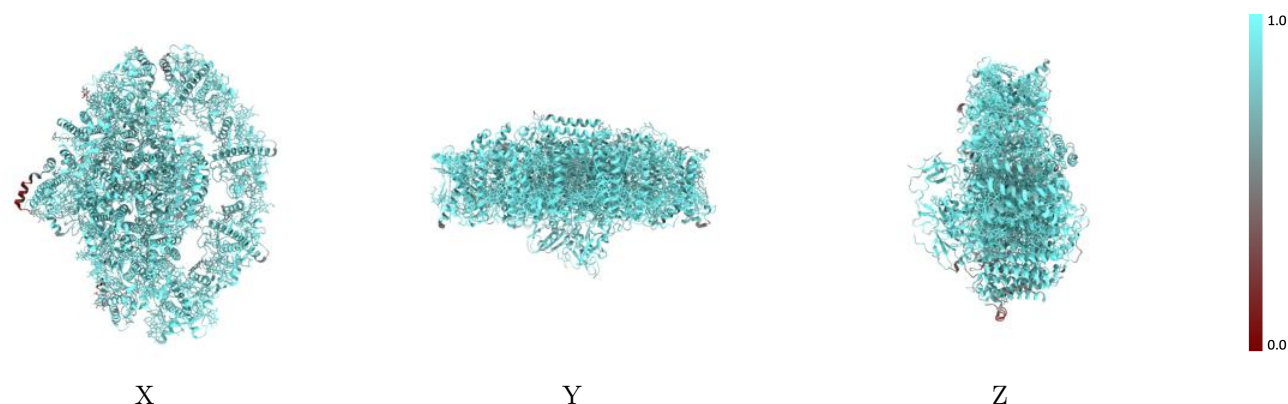
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



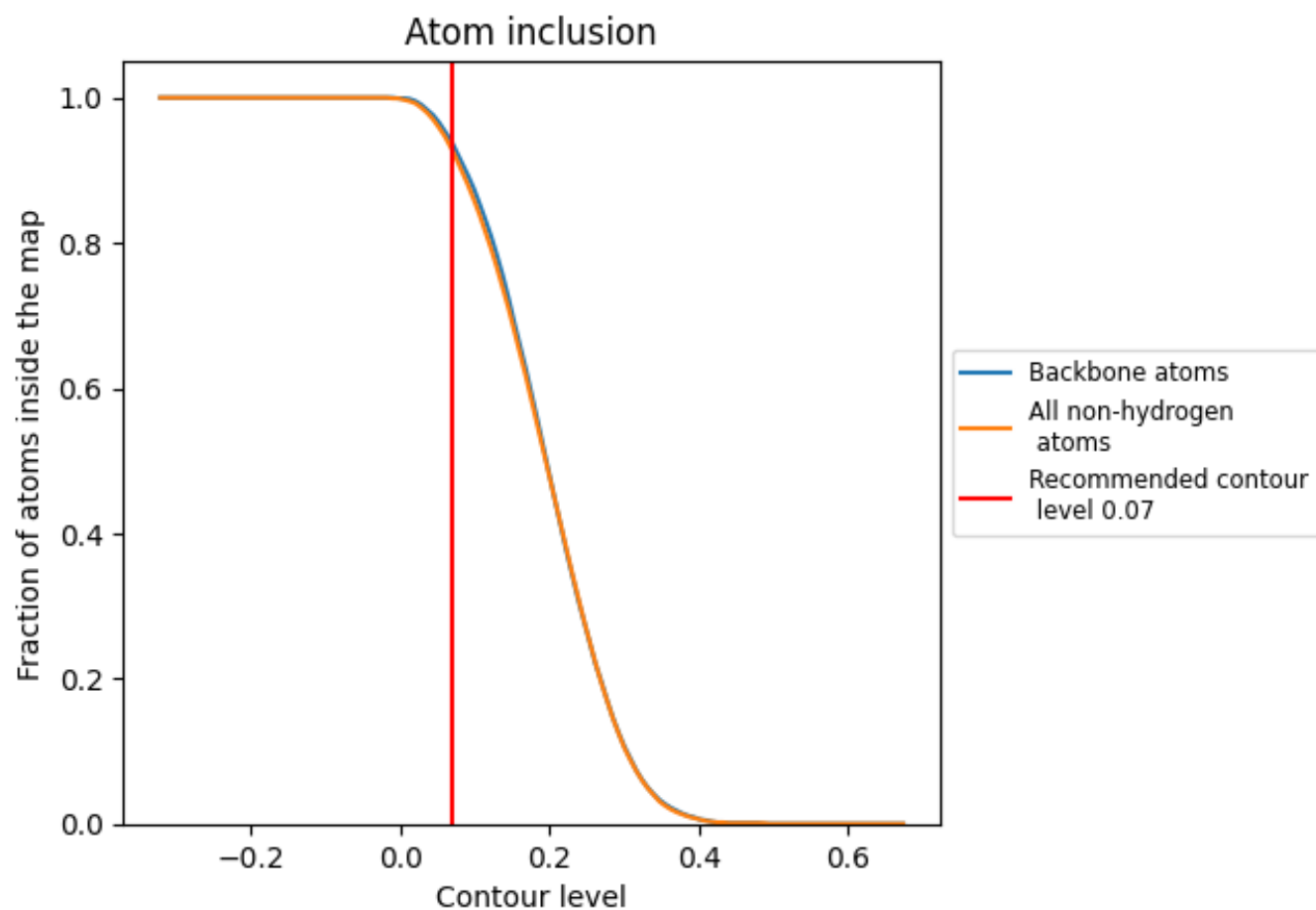
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9280	<div></div> 0.7010
2	<div></div> 0.9240	<div></div> 0.6830
3	<div></div> 0.9280	<div></div> 0.6930
5	<div></div> 0.9090	<div></div> 0.6680
6	<div></div> 0.8820	<div></div> 0.6520
A	<div></div> 0.9680	<div></div> 0.7270
B	<div></div> 0.9610	<div></div> 0.7210
C	<div></div> 0.9830	<div></div> 0.7350
D	<div></div> 0.9250	<div></div> 0.7020
E	<div></div> 0.9100	<div></div> 0.6980
F	<div></div> 0.9190	<div></div> 0.7020
G	<div></div> 0.8640	<div></div> 0.6730
H	<div></div> 0.5090	<div></div> 0.6040
I	<div></div> 0.9620	<div></div> 0.7000
J	<div></div> 0.9460	<div></div> 0.6980
K	<div></div> 0.7170	<div></div> 0.6180
L	<div></div> 0.9140	<div></div> 0.6820
M	<div></div> 0.8680	<div></div> 0.6720

