



wwPDB EM Validation Summary Report ⓘ

Jul 19, 2026 – 04:34 pm BST

PDB ID : 9S1L / pdb_00009s1l
EMDB ID : EMD-54455
Title : Cryo-EM structure of Posidonia oceanica PSI-LHCI supercomplex
Authors : Capaldi, S.; Amelii, A.; Sanita, G.; Esposito, M.; Bassi, R.
Deposited on : 2025-07-18
Resolution : 2.83 Å(reported)
Based on initial model : 5ZJI

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

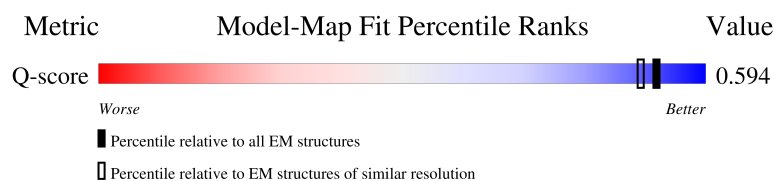
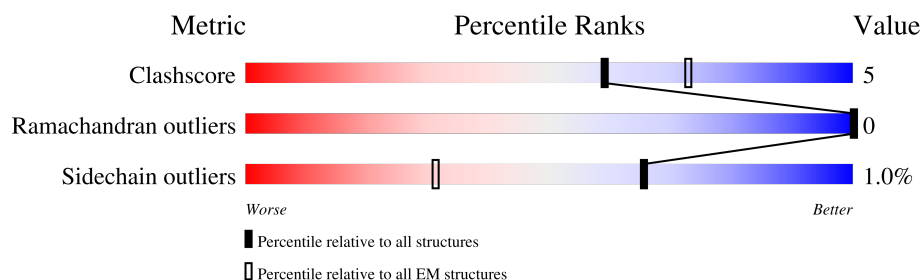
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

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



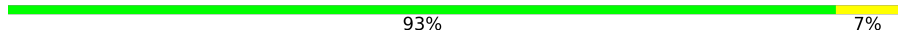
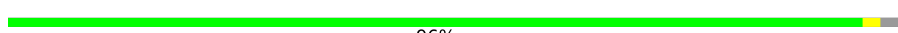
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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

Mol	Chain	Length	Quality of chain
1	1	200	
2	2	211	
3	3	232	
4	4	200	

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	155	
9	E	93	
10	F	159	
11	G	100	
12	H	95	
13	I	36	
14	J	42	
15	K	84	
16	L	170	

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 35475 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 6, chloroplastic (Lhca1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1504	981	252	266	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2 (Lhca2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1579	1031	257	285	6		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	213	Total	C	N	O	S	0	0
			1638	1074	263	295	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4 (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	724	Total	C	N	O	S	0	0
			5684	3726	968	972	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3847	996	1002	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			614	380	106	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-1 (PsaD).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1103	708	190	201	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A (PsaE1).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			519	333	92	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1224	794	209	217	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit V (PsaG).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			768	500	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1 (PsaH1).

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	94	Total	C	N	O	0	0
			736	483	114	139		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII (PsaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	32	Total	C	N	O	S	0	0
			246	167	39	39	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX (PsaJ).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	40	Total	C	N	O	0	0
			319	216	49	54		

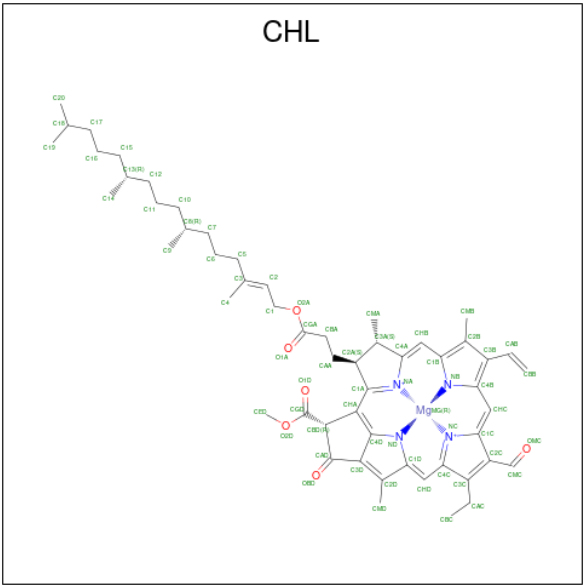
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK (PsaK).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	55	Total	C	N	O	S	0	0
			386	251	62	69	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI (PsaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	152	Total	C	N	O	S	0	0
			1141	755	179	204	3		

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



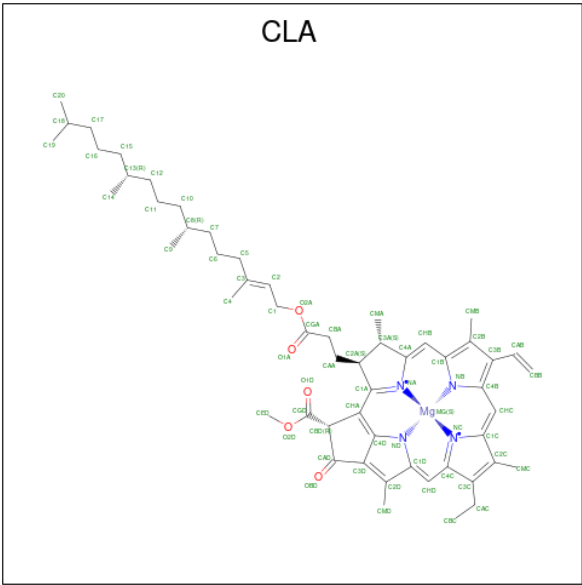
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	3	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0

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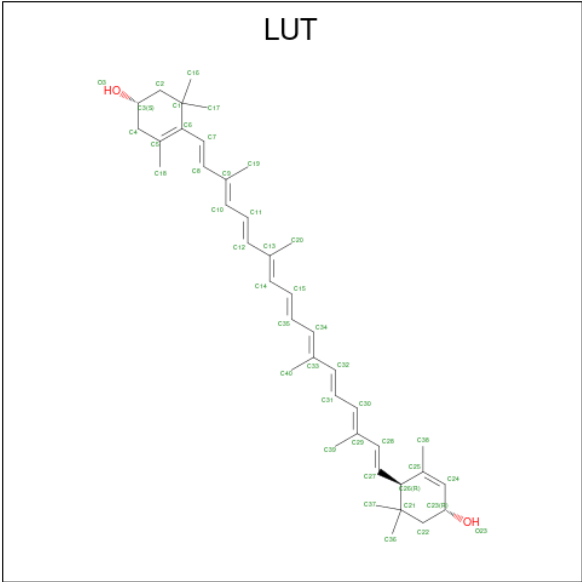
Mol	Chain	Residues	Atoms					AltConf
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			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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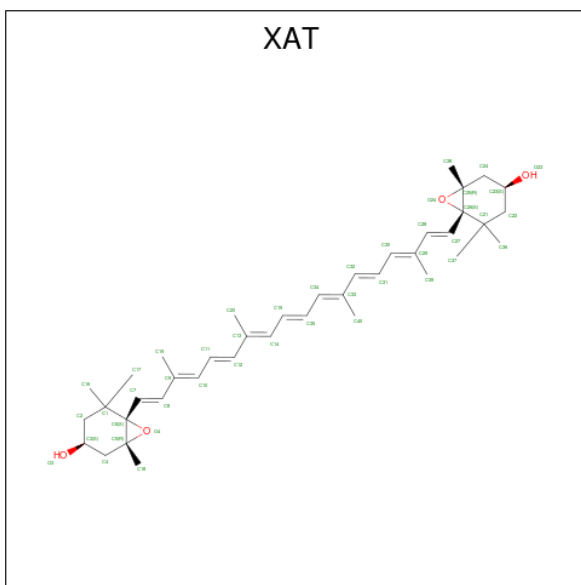
Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 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).



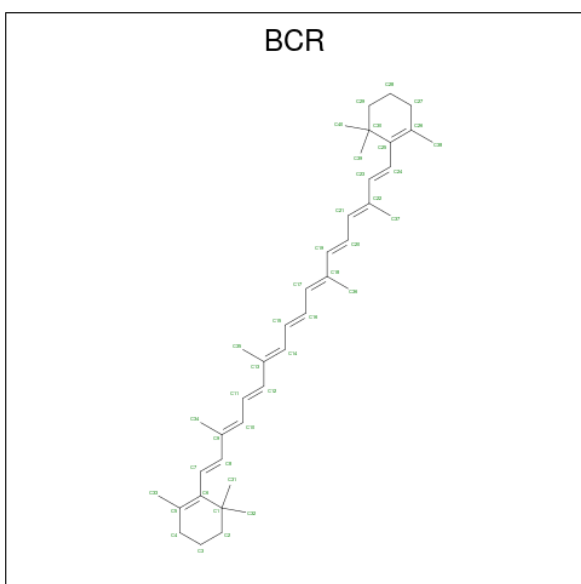
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			42	40	2	
19	1	1	Total	C	O	0
			42	40	2	
19	2	1	Total	C	O	0
			42	40	2	
19	3	1	Total	C	O	0
			42	40	2	
19	4	1	Total	C	O	0
			42	40	2	

- Molecule 20 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
20	1	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



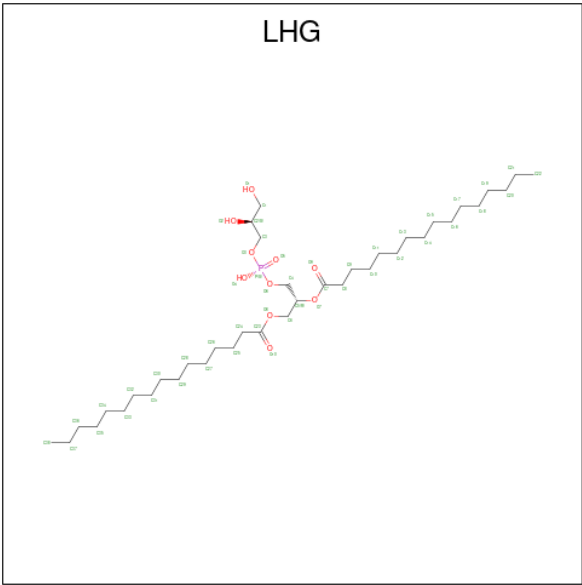
Mol	Chain	Residues	Atoms	AltConf
21	1	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

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



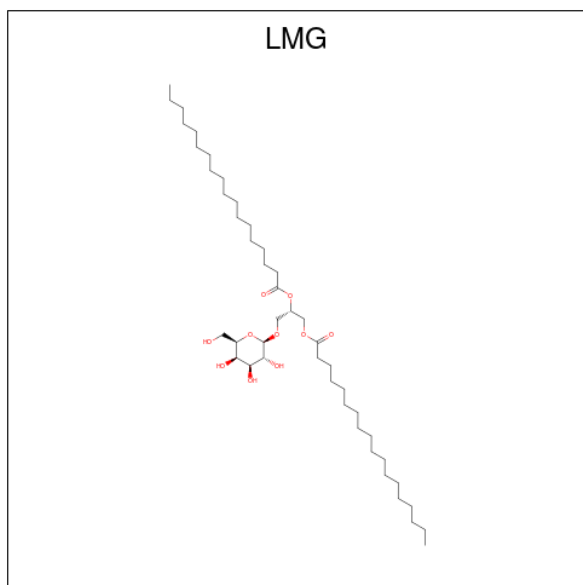
Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 38 27 10 1	0
22	2	1	Total C O P 37 26 10 1	0
22	A	1	Total C O P 49 38 10 1	0

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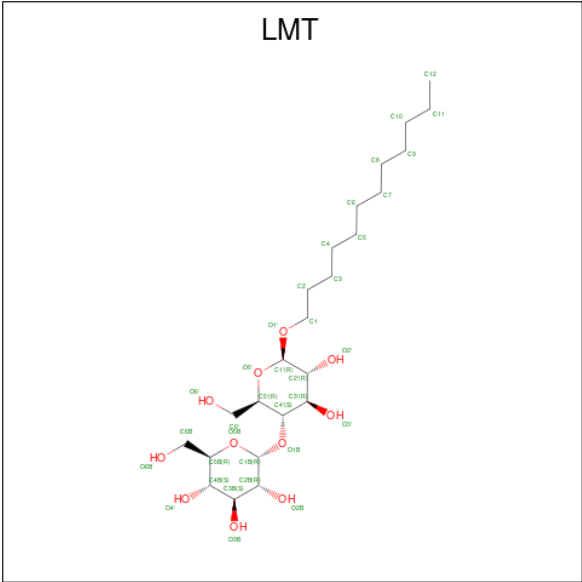
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			30	19	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



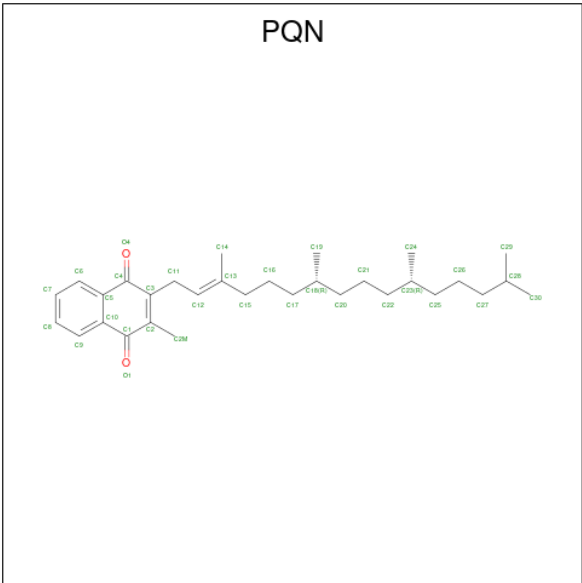
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			53	43	10	
23	1	1	Total	C	O	0
			50	40	10	
23	4	1	Total	C	O	0
			36	26	10	
23	4	1	Total	C	O	0
			49	39	10	
23	B	1	Total	C	O	0
			52	42	10	
23	F	1	Total	C	O	0
			47	37	10	
23	F	1	Total	C	O	0
			30	20	10	

- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



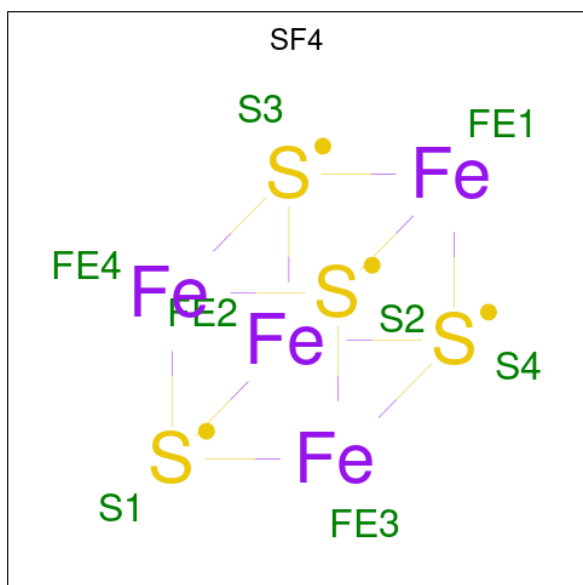
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	

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



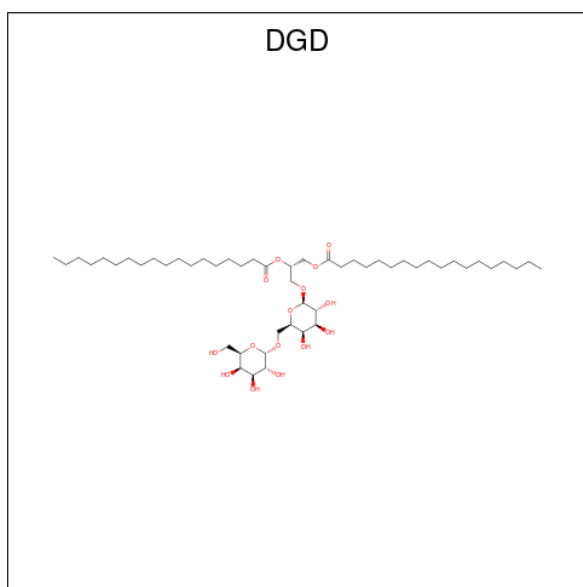
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- 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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).



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

3 Residue-property plots

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

- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic (Lhca1)

Chain 1: 



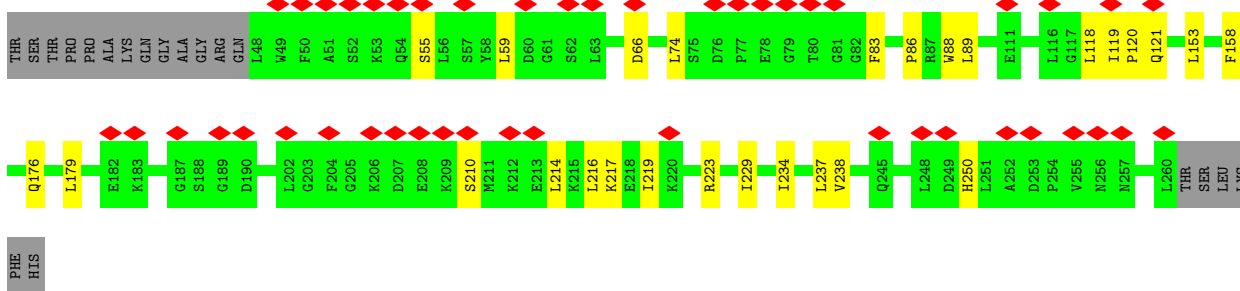
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2 (Lhca2)

Chain 2: 



- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3)

Chain 3: 

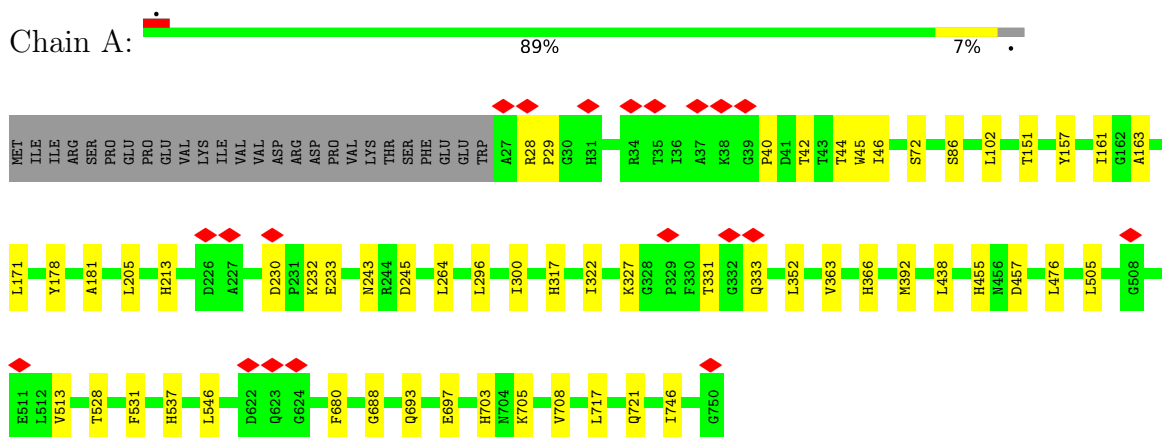


- Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)

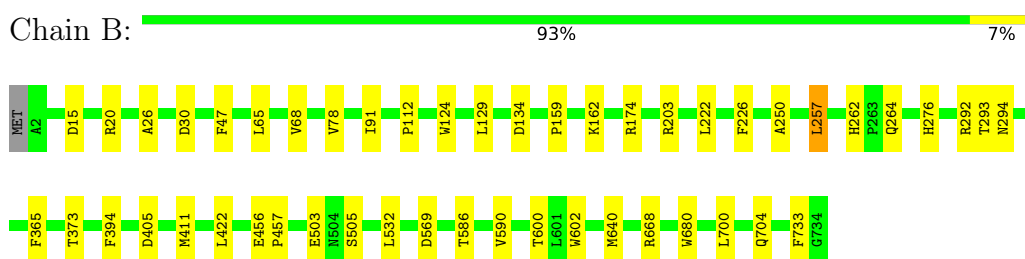
Chain 4: 



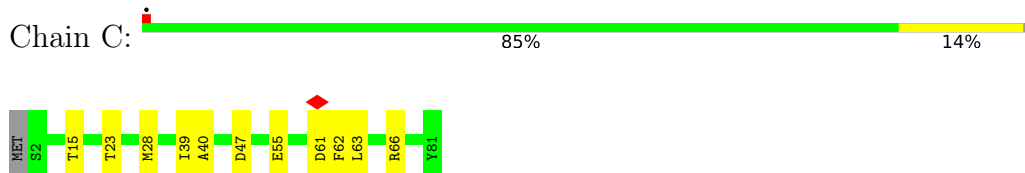
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1 (PsaA)



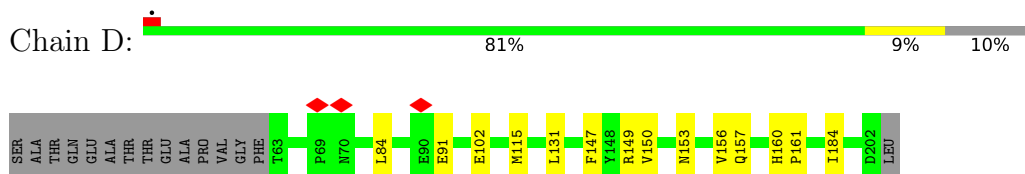
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 (PsaB)



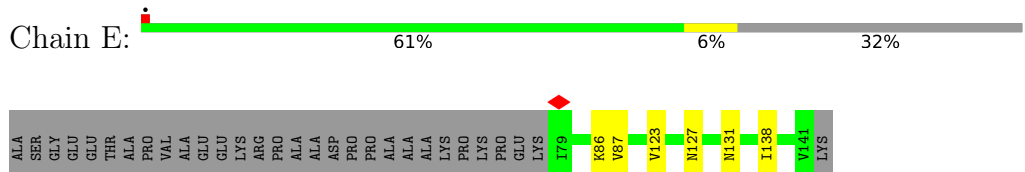
- Molecule 7: Photosystem I iron-sulfur center (PsaC)



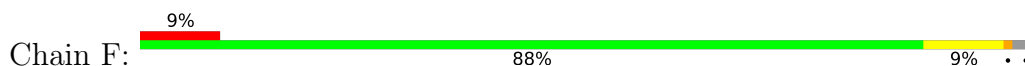
- Molecule 8: Photosystem I reaction center subunit II-1 (PsaD)



- Molecule 9: Photosystem I reaction center subunit IV A (PsaE1)



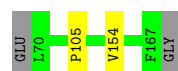
- Molecule 10: Photosystem I reaction center subunit III (PsaF)





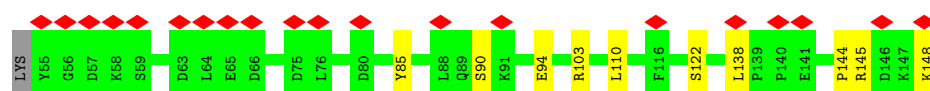
- Molecule 11: Photosystem I reaction center subunit V (PsaG)

Chain G: 96% ..



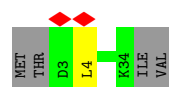
- Molecule 12: Photosystem I reaction center subunit VI-1 (PsaH1)

Chain H: 21% 88% 11% .



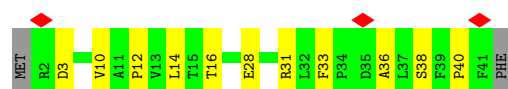
- Molecule 13: Photosystem I reaction center subunit VIII (PsaI)

Chain I: 6% 86% 11% .



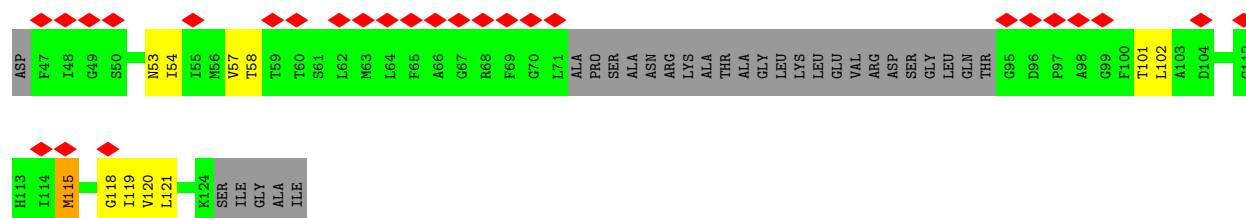
- Molecule 14: Photosystem I reaction center subunit IX (PsaJ)

Chain J: 7% 69% 26% 5%



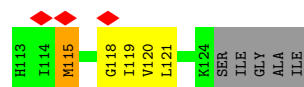
- Molecule 15: Photosystem I reaction center subunit psaK (PsaK)

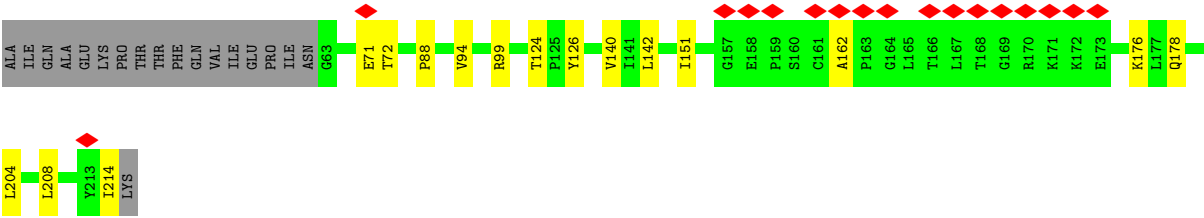
Chain K: 32% 52% 12% 35%



- Molecule 16: Photosystem I reaction center subunit XI (PsaL)

Chain L: 10% 80% 9% 11%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	40.986	Depositor
Minimum map value	-19.686	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.15	0/1553	0.29	0/2119
2	2	0.15	0/1634	0.29	0/2236
3	3	0.14	0/1690	0.31	0/2292
4	4	0.15	0/1606	0.30	0/2191
5	A	0.17	0/5878	0.32	0/8020
6	B	0.18	0/6070	0.33	0/8291
7	C	0.17	0/626	0.40	0/849
8	D	0.14	0/1131	0.38	0/1530
9	E	0.14	0/531	0.29	0/721
10	F	0.17	0/1253	0.36	0/1691
11	G	0.12	0/788	0.27	0/1069
12	H	0.11	0/759	0.28	0/1030
13	I	0.14	0/252	0.30	0/343
14	J	0.15	0/328	0.34	0/448
15	K	0.11	0/390	0.25	0/525
16	L	0.11	0/1176	0.27	0/1608
All	All	0.16	0/25665	0.32	0/34963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1504	0	1491	12	0
2	2	1579	0	1524	12	0
3	3	1638	0	1602	20	0
4	4	1557	0	1519	12	0
5	A	5684	0	5539	39	0
6	B	5858	0	5635	32	0
7	C	614	0	593	8	0
8	D	1103	0	1114	10	0
9	E	519	0	512	5	0
10	F	1224	0	1257	13	0
11	G	768	0	748	2	0
12	H	736	0	723	8	0
13	I	246	0	265	1	0
14	J	319	0	330	11	0
15	K	386	0	404	8	0
16	L	1141	0	1143	11	0
17	1	96	0	68	1	0
17	2	226	0	150	5	0
17	3	47	0	31	1	0
17	4	194	0	138	5	0
18	1	628	0	553	8	0
18	2	458	0	400	5	0
18	3	601	0	463	7	0
18	4	548	0	451	3	0
18	A	2510	0	2449	37	0
18	B	2282	0	2215	36	0
18	F	140	0	113	1	0
18	G	132	0	97	1	0
18	H	51	0	41	3	0
18	J	42	0	31	1	0
18	K	128	0	91	4	0
18	L	150	0	125	3	0
19	1	84	0	112	8	0
19	2	42	0	56	1	0
19	3	42	0	56	4	0
19	4	42	0	56	5	0
20	1	44	0	56	0	0
20	2	44	0	56	1	0
20	3	44	0	56	3	0
20	4	44	0	56	0	0
21	1	40	0	56	1	0
21	2	40	0	56	5	0
21	3	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	4	40	0	56	0	0
21	A	240	0	336	15	0
21	B	240	0	336	9	0
21	F	80	0	112	2	0
21	G	40	0	56	1	0
21	I	40	0	56	0	0
21	J	80	0	112	8	0
21	K	80	0	112	3	0
21	L	160	0	224	7	0
22	1	136	0	194	4	0
22	2	37	0	44	3	0
22	A	79	0	104	3	0
23	1	103	0	149	2	0
23	4	85	0	113	0	0
23	B	52	0	77	2	0
23	F	77	0	97	2	0
24	4	35	0	46	0	0
24	A	70	0	92	1	0
24	G	35	0	46	0	0
25	A	33	0	46	0	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	61	0	83	2	0
All	All	35475	0	35024	324	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.

The worst 5 of 324 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)
16:L:124:THR:HG22	16:L:126:TYR:H	1.43	0.82
6:B:262:HIS:HD2	6:B:264:GLN:H	1.30	0.81
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.67	0.76
19:3:614:LUT:H171	19:3:614:LUT:H8	1.68	0.75
6:B:411:MET:HE2	21:B:845:BCR:H292	1.68	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/200 (96%)	190 (99%)	2 (1%)	0	100	100
2	2	201/211 (95%)	196 (98%)	5 (2%)	0	100	100
3	3	211/232 (91%)	207 (98%)	4 (2%)	0	100	100
4	4	196/200 (98%)	189 (96%)	7 (4%)	0	100	100
5	A	722/750 (96%)	706 (98%)	16 (2%)	0	100	100
6	B	731/734 (100%)	712 (97%)	19 (3%)	0	100	100
7	C	78/81 (96%)	70 (90%)	8 (10%)	0	100	100
8	D	138/155 (89%)	128 (93%)	10 (7%)	0	100	100
9	E	61/93 (66%)	59 (97%)	2 (3%)	0	100	100
10	F	153/159 (96%)	147 (96%)	6 (4%)	0	100	100
11	G	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
12	H	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
13	I	30/36 (83%)	30 (100%)	0	0	100	100
14	J	38/42 (90%)	36 (95%)	2 (5%)	0	100	100
15	K	51/84 (61%)	51 (100%)	0	0	100	100
16	L	150/170 (88%)	145 (97%)	5 (3%)	0	100	100
All	All	3140/3342 (94%)	3048 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	155/160 (97%)	154 (99%)	1 (1%)	78	89
2	2	164/169 (97%)	161 (98%)	3 (2%)	51	74
3	3	166/181 (92%)	162 (98%)	4 (2%)	43	67
4	4	166/167 (99%)	165 (99%)	1 (1%)	78	89
5	A	582/608 (96%)	578 (99%)	4 (1%)	76	88
6	B	597/598 (100%)	591 (99%)	6 (1%)	68	83
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	119/130 (92%)	117 (98%)	2 (2%)	53	75
9	E	58/79 (73%)	58 (100%)	0	100	100
10	F	128/132 (97%)	127 (99%)	1 (1%)	73	86
11	G	82/83 (99%)	82 (100%)	0	100	100
12	H	79/80 (99%)	79 (100%)	0	100	100
13	I	28/32 (88%)	28 (100%)	0	100	100
14	J	35/37 (95%)	34 (97%)	1 (3%)	37	61
15	K	41/62 (66%)	40 (98%)	1 (2%)	43	67
16	L	118/134 (88%)	117 (99%)	1 (1%)	73	86
All	All	2588/2723 (95%)	2563 (99%)	25 (1%)	65	83

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	78	VAL
6	B	600	THR
16	L	214	ILE
6	B	394	PHE
6	B	640	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	196	HIS
6	B	467	HIS
6	B	210	ASN
6	B	299	HIS
6	B	627	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

215 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	$\# Z > 2$
18	CLA	F	301	-	61,65,73	1.30	7 (11%)	73,103,113	1.73	9 (12%)
21	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.32	0
18	CLA	B	830	6	47,51,73	1.41	8 (17%)	56,86,113	1.85	6 (10%)
18	CLA	B	812	6	69,73,73	1.24	8 (11%)	83,113,113	1.77	12 (14%)
18	CLA	4	612	4	61,65,73	1.30	8 (13%)	73,103,113	1.74	10 (13%)
18	CLA	B	835	-	54,58,73	1.40	7 (12%)	65,95,113	1.89	10 (15%)
18	CLA	A	815	5	46,50,73	1.42	8 (17%)	55,85,113	1.84	6 (10%)
18	CLA	1	608	1	69,73,73	1.22	7 (10%)	83,113,113	1.66	10 (12%)
18	CLA	B	825	6	66,70,73	1.28	8 (12%)	79,109,113	1.74	11 (13%)
18	CLA	H	201	12	55,59,73	1.37	9 (16%)	66,96,113	1.80	11 (16%)
18	CLA	B	814	6	59,63,73	1.34	8 (13%)	71,101,113	1.82	9 (12%)
21	BCR	K	204	-	41,41,41	0.25	0	56,56,56	0.46	0
22	LHG	2	617	-	36,36,48	0.34	0	39,42,54	0.31	0
19	LUT	3	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	A	836	5	49,53,73	1.40	8 (16%)	59,89,113	1.89	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	806	5	69,73,73	1.24	8 (11%)	83,113,113	1.75	8 (9%)
18	CLA	3	606	-	44,49,73	1.45	7 (15%)	52,84,113	1.83	4 (7%)
18	CLA	B	834	-	46,50,73	1.43	8 (17%)	55,85,113	1.92	7 (12%)
19	LUT	1	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.53	9 (17%)
17	CHL	2	606	-	42,51,74	2.49	14 (33%)	31,86,114	3.37	15 (48%)
18	CLA	1	603	1	59,63,73	1.32	8 (13%)	71,101,113	1.86	10 (14%)
18	CLA	4	614	4	54,58,73	1.39	8 (14%)	65,95,113	1.79	10 (15%)
18	CLA	A	817	5	64,68,73	1.29	8 (12%)	77,107,113	1.69	11 (14%)
21	BCR	A	846	-	41,41,41	0.15	0	56,56,56	0.60	2 (3%)
22	LHG	A	855	18	29,29,48	0.37	0	32,35,54	0.35	0
21	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.66	1 (1%)
18	CLA	B	829	6	47,51,73	1.42	8 (17%)	56,86,113	1.90	7 (12%)
18	CLA	G	204	11	49,53,73	1.42	7 (14%)	59,89,113	1.82	7 (11%)
21	BCR	L	306	-	41,41,41	0.11	0	56,56,56	0.26	0
18	CLA	A	826	-	69,73,73	1.26	8 (11%)	83,113,113	1.67	12 (14%)
21	BCR	A	845	-	41,41,41	0.14	0	56,56,56	0.25	0
18	CLA	B	840	22	69,73,73	1.25	8 (11%)	83,113,113	1.69	12 (14%)
18	CLA	3	610	3	47,51,73	1.42	7 (14%)	56,86,113	1.84	8 (14%)
18	CLA	A	839	5	54,58,73	1.40	8 (14%)	65,95,113	1.84	10 (15%)
18	CLA	4	602	4	64,68,73	1.28	8 (12%)	77,107,113	1.72	12 (15%)
18	CLA	B	826	6	64,68,73	1.27	8 (12%)	77,107,113	1.75	12 (15%)
18	CLA	A	842	-	69,73,73	1.24	7 (10%)	83,113,113	1.70	9 (10%)
23	LMG	4	621	-	49,49,55	0.19	0	57,57,63	0.14	0
26	SF4	C	101	7	0,12,12	-	-	-	-	-
23	LMG	1	620	-	53,53,55	0.18	0	61,61,63	0.16	0
18	CLA	3	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.81	8 (13%)
18	CLA	3	602	3	64,68,73	1.29	8 (12%)	77,107,113	1.73	12 (15%)
17	CHL	4	606	-	45,54,74	2.46	15 (33%)	35,90,114	3.19	16 (45%)
18	CLA	B	810	6	58,62,73	1.34	9 (15%)	73,100,113	2.05	11 (15%)
17	CHL	4	615	4	40,49,74	2.45	12 (30%)	31,84,114	3.27	14 (45%)
18	CLA	A	840	5	69,73,73	1.23	7 (10%)	83,113,113	1.71	11 (13%)
18	CLA	L	303	16	64,68,73	1.28	8 (12%)	77,107,113	1.73	12 (15%)
18	CLA	1	613	1	49,53,73	1.43	8 (16%)	59,89,113	1.88	10 (16%)
18	CLA	3	613	3	43,48,73	1.48	8 (18%)	51,83,113	1.87	8 (15%)
18	CLA	A	804	5	59,63,73	1.33	8 (13%)	71,101,113	1.85	12 (16%)
18	CLA	B	820	6	59,63,73	1.34	8 (13%)	71,101,113	1.74	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	819	6	54,58,73	1.39	8 (14%)	65,95,113	1.85	10 (15%)
17	CHL	2	614	2	42,51,74	2.46	12 (28%)	31,86,114	3.36	15 (48%)
18	CLA	2	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	12 (14%)
18	CLA	A	828	5	69,73,73	1.22	7 (10%)	83,113,113	1.72	9 (10%)
18	CLA	F	304	10	45,49,73	1.46	9 (20%)	54,84,113	1.99	10 (18%)
18	CLA	1	604	-	53,57,73	1.37	7 (13%)	62,93,113	1.86	7 (11%)
19	LUT	1	619	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	11 (21%)
20	XAT	3	615	-	39,47,47	0.09	0	54,74,74	0.79	3 (5%)
21	BCR	J	103	-	41,41,41	0.14	0	56,56,56	0.26	0
21	BCR	1	617	-	41,41,41	0.12	0	56,56,56	0.29	0
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.45	0
18	CLA	A	810	5	54,58,73	1.41	8 (14%)	65,95,113	1.75	11 (16%)
18	CLA	1	612	1	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)
18	CLA	K	202	-	49,53,73	1.42	7 (14%)	59,89,113	1.76	7 (11%)
24	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.18	0
23	LMG	1	623	-	50,50,55	0.19	0	58,58,63	0.17	0
21	BCR	4	618	-	41,41,41	0.13	0	56,56,56	0.33	0
17	CHL	4	607	-	50,59,74	2.34	14 (28%)	41,96,114	3.09	19 (46%)
18	CLA	A	832	5	60,64,73	1.32	8 (13%)	72,102,113	1.74	10 (13%)
18	CLA	J	102	-	46,50,73	1.42	7 (15%)	55,85,113	1.89	9 (16%)
18	CLA	A	841	5	69,73,73	1.24	8 (11%)	83,113,113	1.68	10 (12%)
18	CLA	4	613	4	49,53,73	1.42	8 (16%)	59,89,113	1.83	8 (13%)
18	CLA	B	833	6	64,68,73	1.28	8 (12%)	77,107,113	1.71	8 (10%)
18	CLA	3	607	3	49,53,73	1.42	8 (16%)	59,89,113	1.86	9 (15%)
18	CLA	A	831	5	54,58,73	1.41	8 (14%)	65,95,113	1.88	9 (13%)
18	CLA	A	838	5	59,63,73	1.34	8 (13%)	71,101,113	1.76	8 (11%)
24	LMT	4	620	-	36,36,36	0.11	0	47,47,47	0.16	0
18	CLA	3	608	3	49,53,73	1.42	8 (16%)	59,89,113	1.84	7 (11%)
18	CLA	B	836	6	69,73,73	1.24	8 (11%)	83,113,113	1.67	10 (12%)
18	CLA	A	816	-	49,53,73	1.42	8 (16%)	59,89,113	1.90	5 (8%)
18	CLA	B	839	6	69,73,73	1.23	8 (11%)	83,113,113	1.73	11 (13%)
18	CLA	A	834	5	69,73,73	1.24	8 (11%)	83,113,113	1.74	9 (10%)
18	CLA	B	801	6	69,73,73	1.23	8 (11%)	83,113,113	1.66	11 (13%)
21	BCR	F	305	-	41,41,41	0.12	0	56,56,56	0.31	0
18	CLA	A	854	22	54,58,73	1.41	7 (12%)	65,95,113	1.75	10 (15%)
23	LMG	F	306	-	47,47,55	0.21	0	55,55,63	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	613	2	47,51,73	1.41	8 (17%)	56,86,113	1.87	8 (14%)
18	CLA	B	813	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	9 (10%)
18	CLA	A	809	5	59,63,73	1.33	8 (13%)	71,101,113	1.77	10 (14%)
18	CLA	3	609	3	45,49,73	1.45	7 (15%)	54,84,113	1.84	9 (16%)
18	CLA	4	609	4	58,62,73	1.34	8 (13%)	69,99,113	1.80	10 (14%)
18	CLA	B	822	6	64,68,73	1.29	9 (14%)	77,107,113	1.63	13 (16%)
18	CLA	B	805	6	69,73,73	1.23	8 (11%)	83,113,113	1.77	9 (10%)
17	CHL	3	616	-	46,55,74	2.40	14 (30%)	36,91,114	3.27	17 (47%)
18	CLA	B	815	6	59,63,73	1.33	8 (13%)	71,101,113	1.80	9 (12%)
18	CLA	A	805	5	49,53,73	1.43	8 (16%)	59,89,113	1.92	7 (11%)
21	BCR	J	101	-	41,41,41	0.28	0	56,56,56	0.65	1 (1%)
17	CHL	2	607	-	50,59,74	2.34	15 (30%)	41,96,114	3.05	18 (43%)
21	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.28	0
18	CLA	1	609	1	63,67,73	1.30	7 (11%)	76,106,113	1.72	9 (11%)
18	CLA	A	807	5	69,73,73	1.24	8 (11%)	83,113,113	1.74	12 (14%)
18	CLA	B	823	-	69,73,73	1.23	8 (11%)	83,113,113	1.71	13 (15%)
18	CLA	3	605	-	51,55,73	1.39	7 (13%)	61,91,113	1.88	10 (16%)
18	CLA	B	806	6	56,60,73	1.38	8 (14%)	67,97,113	1.82	10 (14%)
18	CLA	B	838	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
20	XAT	1	616	-	39,47,47	0.11	0	54,74,74	0.81	3 (5%)
18	CLA	3	611	3	47,52,73	1.44	8 (17%)	56,88,113	1.75	7 (12%)
17	CHL	2	605	-	41,50,74	2.49	13 (31%)	30,85,114	3.33	13 (43%)
23	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.15	0
18	CLA	B	816	-	63,67,73	1.29	7 (11%)	75,105,113	1.71	9 (12%)
21	BCR	B	847	-	41,41,41	0.13	0	56,56,56	0.32	0
18	CLA	A	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.75	11 (13%)
23	LMG	4	619	-	36,36,55	0.20	0	44,44,63	0.17	0
18	CLA	F	303	-	46,50,73	1.43	7 (15%)	55,85,113	1.88	7 (12%)
18	CLA	B	817	6	64,68,73	1.28	8 (12%)	77,107,113	1.76	13 (16%)
18	CLA	A	833	5	69,73,73	1.23	8 (11%)	83,113,113	1.70	9 (10%)
18	CLA	2	612	-	59,63,73	1.33	8 (13%)	71,101,113	1.87	12 (16%)
21	BCR	K	205	-	41,41,41	0.11	0	56,56,56	0.21	0
18	CLA	A	843	-	69,73,73	1.23	7 (10%)	83,113,113	1.70	11 (13%)
18	CLA	2	611	2	49,53,73	1.42	8 (16%)	59,89,113	1.88	9 (15%)
21	BCR	F	302	-	41,41,41	0.16	0	56,56,56	0.36	0
27	DGD	B	848	-	62,62,67	0.16	0	76,76,81	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	803	6	45,49,73	1.45	7 (15%)	54,84,113	1.85	9 (16%)
21	BCR	2	618	-	41,41,41	0.27	0	56,56,56	0.59	1 (1%)
20	XAT	4	617	-	39,47,47	0.13	0	54,74,74	0.90	3 (5%)
18	CLA	A	824	5	59,63,73	1.34	8 (13%)	71,101,113	1.70	10 (14%)
21	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.35	0
18	CLA	G	203	11	46,50,73	1.41	8 (17%)	55,85,113	1.92	6 (10%)
18	CLA	1	607	-	47,52,73	1.44	8 (17%)	56,88,113	1.78	7 (12%)
18	CLA	2	608	2	49,53,73	1.43	8 (16%)	59,89,113	1.78	7 (11%)
21	BCR	L	301	-	41,41,41	0.13	0	56,56,56	0.26	0
18	CLA	3	612	-	43,48,73	1.49	8 (18%)	51,83,113	1.75	8 (15%)
18	CLA	K	203	15	50,54,73	1.40	7 (14%)	60,90,113	1.88	8 (13%)
18	CLA	B	832	6	49,53,73	1.42	6 (12%)	59,89,113	1.84	8 (13%)
25	PQN	A	844	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
21	BCR	G	205	-	41,41,41	0.11	0	56,56,56	0.34	0
18	CLA	A	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
18	CLA	L	304	-	49,53,73	1.43	8 (16%)	59,89,113	1.92	9 (15%)
18	CLA	A	811	5	69,73,73	1.24	8 (11%)	83,113,113	1.71	12 (14%)
18	CLA	A	837	5	55,59,73	1.37	8 (14%)	66,96,113	1.97	9 (13%)
24	LMT	A	856	-	36,36,36	0.13	0	47,47,47	0.52	0
24	LMT	A	853	-	36,36,36	0.11	0	47,47,47	0.24	0
18	CLA	B	831	-	69,73,73	1.26	9 (13%)	83,113,113	1.77	12 (14%)
18	CLA	B	824	-	54,58,73	1.40	8 (14%)	65,95,113	1.73	10 (15%)
21	BCR	3	601	-	41,41,41	0.11	0	56,56,56	0.27	0
18	CLA	A	813	5	69,73,73	1.24	8 (11%)	83,113,113	1.78	11 (13%)
18	CLA	4	610	-	64,68,73	1.29	7 (10%)	77,107,113	1.69	10 (12%)
18	CLA	1	610	22	59,63,73	1.34	7 (11%)	71,101,113	1.78	10 (14%)
18	CLA	B	811	6	47,51,73	1.40	7 (14%)	56,86,113	1.85	7 (12%)
18	CLA	B	828	6	60,64,73	1.34	8 (13%)	72,102,113	1.76	9 (12%)
18	CLA	2	609	2	59,63,73	1.32	8 (13%)	71,101,113	1.77	7 (9%)
18	CLA	B	837	6	51,55,73	1.38	7 (13%)	61,91,113	1.92	10 (16%)
18	CLA	A	822	5	46,50,73	1.43	8 (17%)	55,85,113	1.80	8 (14%)
19	LUT	2	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.52	10 (19%)
21	BCR	B	842	-	41,41,41	0.14	0	56,56,56	0.29	0
18	CLA	B	809	-	69,73,73	1.24	8 (11%)	83,113,113	1.61	10 (12%)
18	CLA	A	829	5	69,73,73	1.23	8 (11%)	83,113,113	1.70	10 (12%)
21	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	823	5	45,49,73	1.46	8 (17%)	54,84,113	1.92	9 (16%)
22	LHG	1	618	18	48,48,48	0.29	0	51,54,54	0.30	0
20	XAT	2	616	-	39,47,47	0.11	0	54,74,74	0.83	4 (7%)
17	CHL	2	601	2	46,55,74	2.44	14 (30%)	36,91,114	3.20	17 (47%)
18	CLA	4	608	4	49,53,73	1.42	8 (16%)	59,89,113	1.91	6 (10%)
17	CHL	1	601	1	54,63,74	2.24	15 (27%)	46,101,114	2.78	16 (34%)
21	BCR	L	307	-	41,41,41	0.12	0	56,56,56	0.25	0
25	PQN	B	841	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
18	CLA	A	827	5	69,73,73	1.24	8 (11%)	83,113,113	1.77	10 (12%)
22	LHG	1	621	-	48,48,48	0.30	0	51,54,54	0.31	0
18	CLA	2	610	-	45,49,73	1.46	7 (15%)	54,84,113	1.84	8 (14%)
18	CLA	A	818	5	63,67,73	1.29	7 (11%)	75,105,113	1.75	10 (13%)
18	CLA	B	827	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	11 (13%)
18	CLA	L	302	16	49,53,73	1.42	8 (16%)	59,89,113	1.84	8 (13%)
18	CLA	1	605	-	43,48,73	1.42	7 (16%)	52,82,113	1.92	7 (13%)
22	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.30	0
18	CLA	B	804	6	69,73,73	1.25	8 (11%)	83,113,113	1.77	13 (15%)
21	BCR	L	305	-	41,41,41	0.19	0	56,56,56	0.34	0
18	CLA	3	603	3	59,63,73	1.33	7 (11%)	71,101,113	1.80	10 (14%)
17	CHL	1	606	1	40,49,74	2.53	13 (32%)	29,84,114	3.33	13 (44%)
18	CLA	A	803	-	69,73,73	1.22	7 (10%)	83,113,113	1.70	11 (13%)
18	CLA	A	820	5	49,53,73	1.42	8 (16%)	59,89,113	1.88	7 (11%)
18	CLA	A	819	5	69,73,73	1.24	8 (11%)	83,113,113	1.68	13 (15%)
18	CLA	1	611	1	49,53,73	1.43	8 (16%)	59,89,113	1.91	7 (11%)
18	CLA	G	202	-	49,53,73	1.43	8 (16%)	59,89,113	1.85	7 (11%)
18	CLA	A	801	5	69,73,73	1.22	8 (11%)	83,113,113	1.72	11 (13%)
18	CLA	A	830	5	69,73,73	1.25	8 (11%)	83,113,113	1.68	10 (12%)
18	CLA	B	807	-	69,73,73	1.22	7 (10%)	83,113,113	1.71	11 (13%)
19	LUT	4	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.55	9 (17%)
18	CLA	4	601	4	50,54,73	1.40	8 (16%)	60,90,113	1.83	8 (13%)
26	SF4	C	102	7	0,12,12	-	-	-	-	-
18	CLA	4	603	4	49,53,73	1.41	7 (14%)	59,89,113	1.89	9 (15%)
18	CLA	K	201	15	42,45,73	1.53	8 (19%)	50,78,113	1.85	8 (16%)
18	CLA	A	814	5	49,53,73	1.44	8 (16%)	59,89,113	1.87	9 (15%)
18	CLA	B	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.83	13 (15%)
18	CLA	A	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.64	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	A	851	6,5	0,12,12	-	-	-		
18	CLA	A	808	5	54,58,73	1.41	8 (14%)	65,95,113	1.84	11 (16%)
21	BCR	B	845	-	41,41,41	0.12	0	56,56,56	0.35	0
23	LMG	B	849	-	52,52,55	0.20	0	60,60,63	0.15	0
18	CLA	B	818	-	59,63,73	1.34	7 (11%)	71,101,113	1.76	11 (15%)
18	CLA	B	821	6	59,63,73	1.34	8 (13%)	71,101,113	1.76	10 (14%)
17	CHL	4	605	-	55,64,74	2.26	15 (27%)	47,102,114	2.84	18 (38%)
21	BCR	B	843	-	41,41,41	0.20	0	56,56,56	0.45	0
18	CLA	B	808	6	59,63,73	1.34	8 (13%)	71,101,113	1.76	9 (12%)
18	CLA	3	617	5	59,63,73	1.34	8 (13%)	71,101,113	1.77	11 (15%)
21	BCR	I	101	-	41,41,41	0.13	0	56,56,56	0.25	0
18	CLA	2	603	2	47,52,73	1.44	8 (17%)	56,88,113	1.81	7 (12%)
22	LHG	1	622	18	37,37,48	0.33	0	40,43,54	0.31	0
18	CLA	4	611	4	44,49,73	1.45	8 (18%)	52,84,113	1.87	5 (9%)
18	CLA	2	602	2	69,73,73	1.24	8 (11%)	83,113,113	1.65	12 (14%)
18	CLA	1	602	1	65,69,73	1.29	8 (12%)	78,108,113	1.73	12 (15%)
18	CLA	1	614	1	49,53,73	1.42	8 (16%)	59,89,113	1.84	8 (13%)
18	CLA	A	812	5	58,62,73	1.35	8 (13%)	69,99,113	1.82	11 (15%)
18	CLA	4	604	-	49,53,73	1.42	7 (14%)	59,89,113	1.82	9 (15%)
18	CLA	A	835	5	49,53,73	1.41	8 (16%)	59,89,113	1.82	9 (15%)

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
18	CLA	F	301	-	-	11/30/106/115	-
21	BCR	B	846	-	-	3/29/63/63	0/2/2/2
18	CLA	B	830	6	-	3/13/89/115	-
18	CLA	B	812	6	-	19/39/115/115	-
18	CLA	4	612	4	-	17/30/106/115	-
18	CLA	B	835	-	-	5/21/97/115	-
18	CLA	A	815	5	-	5/12/88/115	-
18	CLA	1	608	1	-	18/39/115/115	-
18	CLA	B	825	6	-	12/36/112/115	-
18	CLA	H	201	12	-	14/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	814	6	-	10/27/103/115	-
21	BCR	K	204	-	-	3/29/63/63	0/2/2/2
22	LHG	2	617	-	-	6/41/41/53	-
19	LUT	3	614	-	-	2/29/67/67	0/2/2/2
18	CLA	A	836	5	-	6/15/91/115	-
18	CLA	A	806	5	-	22/39/115/115	-
18	CLA	3	606	-	-	3/10/86/115	-
18	CLA	B	834	-	-	1/12/88/115	-
19	LUT	1	615	-	-	1/29/67/67	0/2/2/2
17	CHL	2	606	-	-	4/12/110/137	-
18	CLA	1	603	1	-	6/27/103/115	-
18	CLA	4	614	4	-	8/21/97/115	-
18	CLA	A	817	5	-	16/33/109/115	-
21	BCR	A	846	-	-	5/29/63/63	0/2/2/2
22	LHG	A	855	18	-	6/34/34/53	-
21	BCR	A	850	-	-	7/29/63/63	0/2/2/2
18	CLA	B	829	6	-	6/13/89/115	-
18	CLA	G	204	11	-	5/15/91/115	-
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	A	826	-	-	11/39/115/115	-
21	BCR	A	845	-	-	4/29/63/63	0/2/2/2
18	CLA	B	840	22	-	25/39/115/115	-
18	CLA	3	610	3	-	6/13/89/115	-
18	CLA	A	839	5	-	10/21/97/115	-
18	CLA	4	602	4	-	8/33/109/115	-
18	CLA	B	826	6	-	14/33/109/115	-
18	CLA	A	842	-	-	17/39/115/115	-
23	LMG	4	621	-	-	9/44/64/70	0/1/1/1
26	SF4	C	101	7	-	-	0/6/5/5
23	LMG	1	620	-	-	11/48/68/70	0/1/1/1
18	CLA	3	604	-	-	4/15/91/115	-
18	CLA	3	602	3	-	14/33/109/115	-
17	CHL	4	606	-	-	6/15/113/137	-
18	CLA	B	810	6	-	6/25/101/115	-
17	CHL	4	615	4	-	2/10/106/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	840	5	-	18/39/115/115	-
18	CLA	L	303	16	-	16/33/109/115	-
18	CLA	1	613	1	-	6/15/91/115	-
18	CLA	3	613	3	-	0/8/84/115	-
18	CLA	A	804	5	-	14/27/103/115	-
18	CLA	B	820	6	-	12/27/103/115	-
18	CLA	B	819	6	-	7/21/97/115	-
17	CHL	2	614	2	-	5/12/110/137	-
18	CLA	2	604	-	-	18/39/115/115	-
18	CLA	A	828	5	-	14/39/115/115	-
18	CLA	F	304	10	-	2/10/86/115	-
18	CLA	1	604	-	-	3/20/96/115	-
19	LUT	1	619	-	-	2/29/67/67	0/2/2/2
20	XAT	3	615	-	-	0/31/93/93	0/4/4/4
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
21	BCR	1	617	-	-	2/29/63/63	0/2/2/2
21	BCR	A	849	-	-	4/29/63/63	0/2/2/2
18	CLA	A	810	5	-	6/21/97/115	-
18	CLA	1	612	1	-	16/39/115/115	-
18	CLA	K	202	-	-	6/15/91/115	-
24	LMT	G	201	-	-	2/21/61/61	0/2/2/2
23	LMG	1	623	-	-	10/45/65/70	0/1/1/1
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
17	CHL	4	607	-	-	5/21/119/137	-
18	CLA	A	832	5	-	3/29/105/115	-
18	CLA	J	102	-	-	6/12/88/115	-
18	CLA	A	841	5	-	13/39/115/115	-
18	CLA	4	613	4	-	4/15/91/115	-
18	CLA	B	833	6	-	13/33/109/115	-
18	CLA	3	607	3	-	6/15/91/115	-
18	CLA	A	831	5	-	11/21/97/115	-
18	CLA	A	838	5	-	6/27/103/115	-
24	LMT	4	620	-	-	3/21/61/61	0/2/2/2
18	CLA	3	608	3	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	836	6	-	10/39/115/115	-
18	CLA	A	816	-	-	4/15/91/115	-
18	CLA	B	839	6	-	15/39/115/115	-
18	CLA	A	834	5	-	15/39/115/115	-
18	CLA	B	801	6	-	19/39/115/115	-
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
18	CLA	A	854	22	-	4/21/97/115	-
23	LMG	F	306	-	-	10/42/62/70	0/1/1/1
18	CLA	2	613	2	-	4/13/89/115	-
18	CLA	B	813	6	-	18/39/115/115	-
18	CLA	A	809	5	-	8/27/103/115	-
18	CLA	3	609	3	-	4/10/86/115	-
18	CLA	4	609	4	-	5/26/102/115	-
18	CLA	B	822	6	-	22/33/109/115	-
18	CLA	B	805	6	-	21/39/115/115	-
17	CHL	3	616	-	-	6/17/115/137	-
18	CLA	B	815	6	-	5/27/103/115	-
18	CLA	A	805	5	-	7/15/91/115	-
21	BCR	J	101	-	-	6/29/63/63	0/2/2/2
17	CHL	2	607	-	-	5/21/119/137	-
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
18	CLA	1	609	1	-	7/31/107/115	-
18	CLA	A	807	5	-	16/39/115/115	-
18	CLA	B	823	-	-	13/39/115/115	-
18	CLA	3	605	-	-	6/18/94/115	-
18	CLA	B	806	6	-	1/24/100/115	-
18	CLA	B	838	-	-	12/39/115/115	-
20	XAT	1	616	-	-	0/31/93/93	0/4/4/4
18	CLA	3	611	3	-	4/13/89/115	-
17	CHL	2	605	-	-	2/10/108/137	-
23	LMG	F	307	-	-	0/25/45/70	0/1/1/1
18	CLA	B	816	-	-	16/32/108/115	-
21	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	CLA	A	802	-	-	13/39/115/115	-
23	LMG	4	619	-	-	5/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	303	-	-	1/12/88/115	-
18	CLA	B	817	6	-	16/33/109/115	-
18	CLA	A	833	5	-	17/39/115/115	-
18	CLA	2	612	-	-	12/27/103/115	-
21	BCR	K	205	-	-	4/29/63/63	0/2/2/2
18	CLA	A	843	-	-	15/39/115/115	-
18	CLA	2	611	2	-	4/15/91/115	-
21	BCR	F	302	-	-	0/29/63/63	0/2/2/2
27	DGD	B	848	-	-	7/50/90/95	0/2/2/2
18	CLA	B	803	6	-	2/10/86/115	-
21	BCR	2	618	-	-	14/29/63/63	0/2/2/2
20	XAT	4	617	-	-	0/31/93/93	0/4/4/4
18	CLA	A	824	5	-	12/27/103/115	-
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	G	203	11	-	1/12/88/115	-
18	CLA	1	607	-	-	0/13/89/115	-
18	CLA	2	608	2	-	4/15/91/115	-
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
18	CLA	3	612	-	-	2/8/84/115	-
18	CLA	K	203	15	-	7/17/93/115	-
18	CLA	B	832	6	-	5/15/91/115	-
25	PQN	A	844	-	-	7/23/43/43	0/2/2/2
21	BCR	G	205	-	-	0/29/63/63	0/2/2/2
18	CLA	A	821	-	-	14/39/115/115	-
18	CLA	L	304	-	-	9/15/91/115	-
18	CLA	A	811	5	-	11/39/115/115	-
18	CLA	A	837	5	-	10/23/99/115	-
24	LMT	A	856	-	-	5/21/61/61	0/2/2/2
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
18	CLA	B	831	-	-	16/39/115/115	-
18	CLA	B	824	-	-	5/21/97/115	-
21	BCR	3	601	-	-	0/29/63/63	0/2/2/2
18	CLA	A	813	5	-	17/39/115/115	-
18	CLA	4	610	-	-	11/33/109/115	-
18	CLA	1	610	22	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	811	6	-	2/13/89/115	-
18	CLA	B	828	6	-	11/29/105/115	-
18	CLA	2	609	2	-	3/27/103/115	-
18	CLA	B	837	6	-	6/18/94/115	-
18	CLA	A	822	5	-	4/12/88/115	-
19	LUT	2	615	-	-	1/29/67/67	0/2/2/2
21	BCR	B	842	-	-	0/29/63/63	0/2/2/2
18	CLA	B	809	-	-	18/39/115/115	-
18	CLA	A	829	5	-	16/39/115/115	-
21	BCR	A	847	-	-	3/29/63/63	0/2/2/2
18	CLA	A	823	5	-	3/10/86/115	-
22	LHG	1	618	18	-	11/53/53/53	-
20	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CHL	2	601	2	-	4/17/115/137	-
18	CLA	4	608	4	-	3/15/91/115	-
17	CHL	1	601	1	-	10/25/123/137	-
21	BCR	L	307	-	-	4/29/63/63	0/2/2/2
25	PQN	B	841	-	-	7/23/43/43	0/2/2/2
18	CLA	A	827	5	-	13/39/115/115	-
22	LHG	1	621	-	-	13/53/53/53	-
18	CLA	2	610	-	-	1/10/86/115	-
18	CLA	A	818	5	-	9/32/108/115	-
18	CLA	B	827	6	-	17/39/115/115	-
18	CLA	L	302	16	-	6/15/91/115	-
18	CLA	1	605	-	-	2/10/82/115	-
22	LHG	A	852	-	-	11/53/53/53	-
18	CLA	B	804	6	-	15/39/115/115	-
21	BCR	L	305	-	-	3/29/63/63	0/2/2/2
18	CLA	3	603	3	-	8/27/103/115	-
17	CHL	1	606	1	-	3/8/106/137	-
18	CLA	A	803	-	-	9/39/115/115	-
18	CLA	A	820	5	-	3/15/91/115	-
18	CLA	A	819	5	-	20/39/115/115	-
18	CLA	1	611	1	-	5/15/91/115	-
18	CLA	G	202	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	801	5	-	11/39/115/115	-
18	CLA	A	830	5	-	15/39/115/115	-
18	CLA	B	807	-	-	14/39/115/115	-
19	LUT	4	616	-	-	1/29/67/67	0/2/2/2
18	CLA	4	601	4	-	6/17/93/115	-
26	SF4	C	102	7	-	-	0/6/5/5
18	CLA	4	603	4	-	6/15/91/115	-
18	CLA	K	201	15	-	0/4/76/115	-
18	CLA	A	814	5	-	3/15/91/115	-
18	CLA	B	802	-	-	17/39/115/115	-
18	CLA	A	825	-	-	20/39/115/115	-
26	SF4	A	851	6,5	-	-	0/6/5/5
18	CLA	A	808	5	-	7/21/97/115	-
21	BCR	B	845	-	-	0/29/63/63	0/2/2/2
23	LMG	B	849	-	-	13/47/67/70	0/1/1/1
18	CLA	B	818	-	-	5/27/103/115	-
18	CLA	B	821	6	-	8/27/103/115	-
17	CHL	4	605	-	-	1/27/125/137	-
21	BCR	B	843	-	-	3/29/63/63	0/2/2/2
18	CLA	B	808	6	-	8/27/103/115	-
18	CLA	3	617	5	-	10/27/103/115	-
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	2	603	2	-	5/13/89/115	-
22	LHG	1	622	18	-	5/42/42/53	-
18	CLA	4	611	4	-	2/10/86/115	-
18	CLA	2	602	2	-	11/39/115/115	-
18	CLA	1	602	1	-	13/35/111/115	-
18	CLA	1	614	1	-	7/15/91/115	-
18	CLA	A	812	5	-	9/26/102/115	-
18	CLA	4	604	-	-	5/15/91/115	-
18	CLA	A	835	5	-	3/15/91/115	-

The worst 5 of 1319 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	CMC-C2C	7.16	1.56	1.44
17	2	601	CHL	C3B-C4B	7.12	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	605	CHL	CMC-C2C	7.10	1.56	1.44
17	3	616	CHL	CMC-C2C	7.04	1.56	1.44
17	1	606	CHL	CMC-C2C	7.04	1.56	1.44

The worst 5 of 1618 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	601	CHL	C1B-CHB-C4A	13.32	129.55	121.39
17	3	616	CHL	C1B-CHB-C4A	13.07	129.40	121.39
17	2	606	CHL	C1B-CHB-C4A	12.87	129.27	121.39
17	4	607	CHL	C1B-CHB-C4A	12.84	129.26	121.39
17	4	615	CHL	C1B-CHB-C4A	12.81	129.24	121.39

There are no chirality outliers.

5 of 1603 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	606	CHL	C4C-C3C-CAC-CBC
17	2	601	CHL	CBA-CGA-O2A-C1
17	2	606	CHL	C3A-C2A-CAA-CBA
17	2	607	CHL	C3C-C2C-CMC-OMC
17	2	614	CHL	C1A-C2A-CAA-CBA

There are no ring outliers.

124 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	301	CLA	1	0
21	B	846	BCR	1	0
18	B	812	CLA	3	0
18	1	608	CLA	1	0
18	B	825	CLA	1	0
18	H	201	CLA	3	0
21	K	204	BCR	3	0
22	2	617	LHG	3	0
19	3	614	LUT	4	0
18	A	836	CLA	1	0
18	A	806	CLA	1	0
19	1	615	LUT	3	0
17	2	606	CHL	1	0
18	1	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	614	CLA	1	0
18	A	817	CLA	4	0
21	A	846	BCR	2	0
22	A	855	LHG	3	0
21	A	850	BCR	5	0
18	B	829	CLA	2	0
21	L	306	BCR	2	0
21	A	845	BCR	3	0
18	B	840	CLA	3	0
18	4	602	CLA	2	0
18	B	826	CLA	3	0
18	A	842	CLA	1	0
23	1	620	LMG	1	0
18	3	602	CLA	1	0
17	4	606	CHL	2	0
18	1	613	CLA	1	0
18	A	804	CLA	1	0
17	2	614	CHL	1	0
18	2	604	CLA	1	0
18	A	828	CLA	1	0
19	1	619	LUT	5	0
20	3	615	XAT	3	0
21	J	103	BCR	2	0
21	1	617	BCR	1	0
21	A	849	BCR	3	0
18	A	810	CLA	2	0
18	1	612	CLA	2	0
18	K	202	CLA	3	0
23	1	623	LMG	1	0
17	4	607	CHL	1	0
18	A	832	CLA	1	0
18	J	102	CLA	1	0
18	A	841	CLA	1	0
18	A	831	CLA	1	0
18	B	839	CLA	3	0
18	A	834	CLA	1	0
18	B	801	CLA	1	0
21	F	305	BCR	1	0
18	A	854	CLA	2	0
23	F	306	LMG	1	0
18	B	813	CLA	2	0
18	A	809	CLA	2	0

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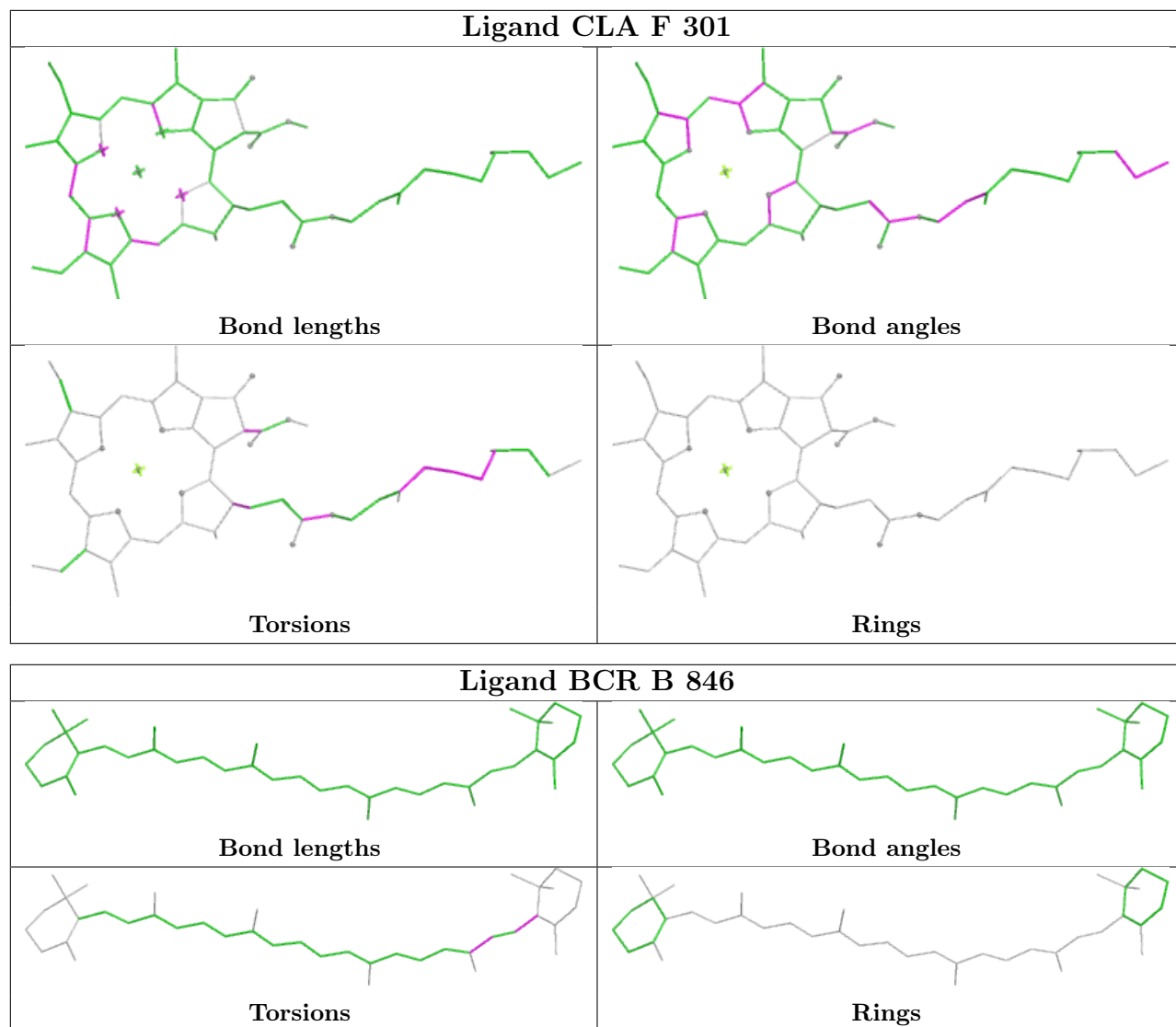
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	616	CHL	1	0
18	B	815	CLA	1	0
21	J	101	BCR	6	0
17	2	607	CHL	2	0
21	B	844	BCR	1	0
18	1	609	CLA	2	0
18	A	807	CLA	3	0
18	B	823	CLA	2	0
18	B	838	CLA	2	0
18	3	611	CLA	3	0
23	F	307	LMG	1	0
18	B	816	CLA	4	0
21	B	847	BCR	3	0
18	A	802	CLA	3	0
18	B	817	CLA	2	0
18	2	612	CLA	1	0
18	A	843	CLA	2	0
21	F	302	BCR	1	0
27	B	848	DGD	2	0
21	2	618	BCR	5	0
18	G	203	CLA	1	0
21	L	301	BCR	2	0
18	K	203	CLA	1	0
21	G	205	BCR	1	0
18	A	821	CLA	1	0
18	A	837	CLA	1	0
24	A	856	LMT	1	0
21	3	601	BCR	2	0
18	B	811	CLA	1	0
18	B	828	CLA	1	0
18	2	609	CLA	2	0
19	2	615	LUT	1	0
21	B	842	BCR	2	0
18	B	809	CLA	4	0
18	A	829	CLA	1	0
21	A	847	BCR	2	0
22	1	618	LHG	1	0
20	2	616	XAT	1	0
17	2	601	CHL	1	0
21	L	307	BCR	1	0
25	B	841	PQN	2	0
18	A	827	CLA	1	0

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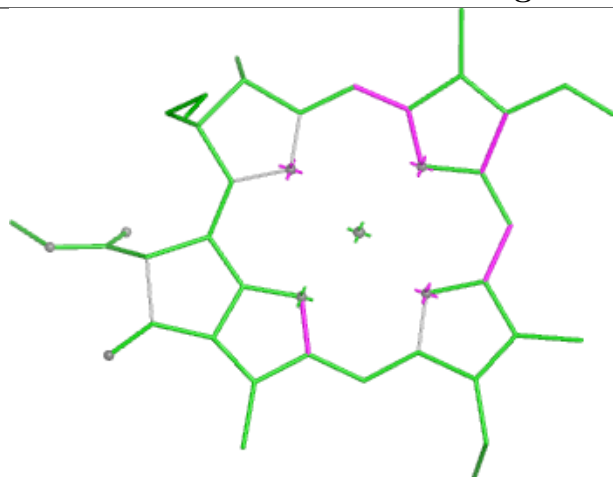
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	621	LHG	2	0
18	2	610	CLA	1	0
18	A	818	CLA	1	0
18	B	827	CLA	1	0
18	L	302	CLA	3	0
18	B	804	CLA	1	0
21	L	305	BCR	2	0
18	3	603	CLA	2	0
17	1	606	CHL	1	0
18	A	803	CLA	1	0
18	A	819	CLA	1	0
18	A	830	CLA	2	0
18	B	807	CLA	2	0
19	4	616	LUT	5	0
18	4	601	CLA	1	0
18	A	825	CLA	2	0
18	A	808	CLA	1	0
21	B	845	BCR	1	0
23	B	849	LMG	2	0
18	B	821	CLA	2	0
17	4	605	CHL	4	0
21	B	843	BCR	1	0
18	3	617	CLA	1	0
22	1	622	LHG	1	0
18	1	614	CLA	1	0
18	A	812	CLA	1	0

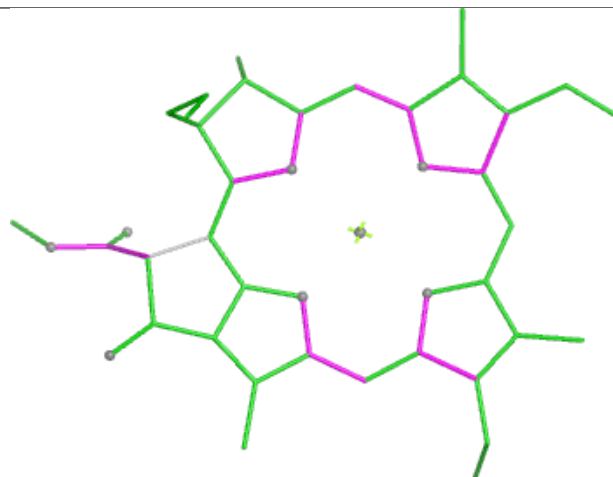
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



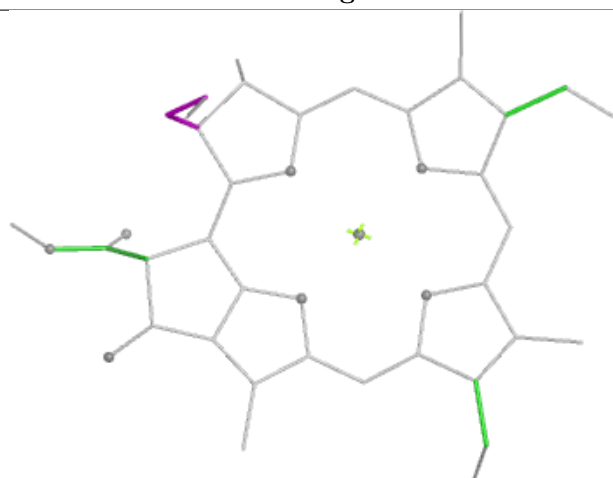
Ligand CLA B 830



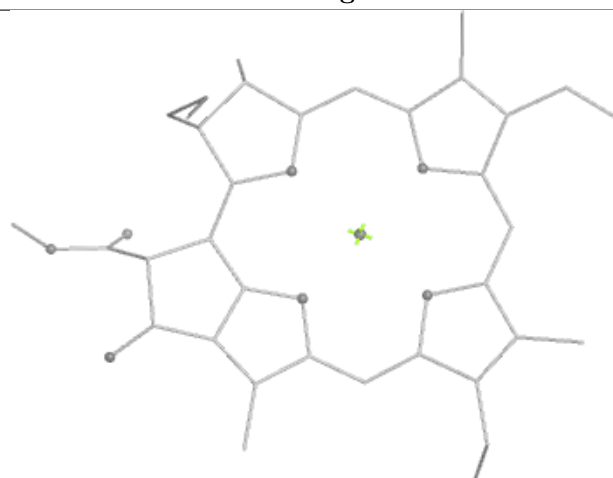
Bond lengths



Bond angles

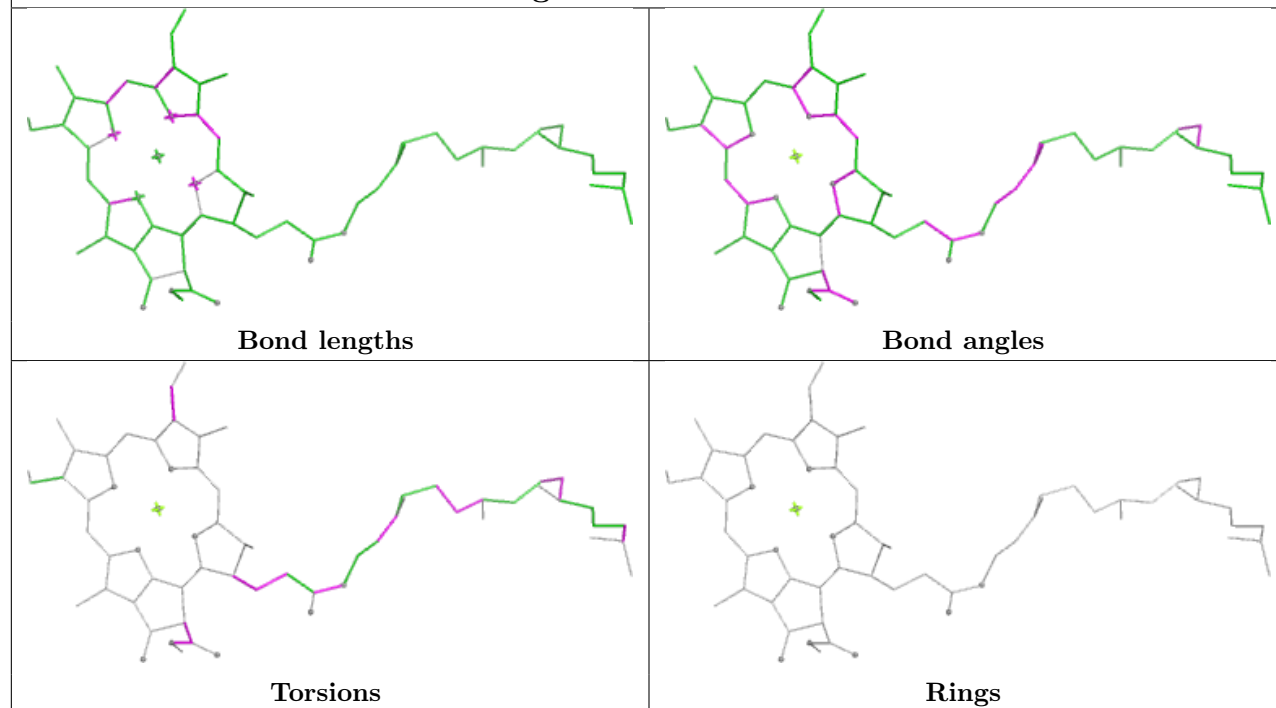


Torsions

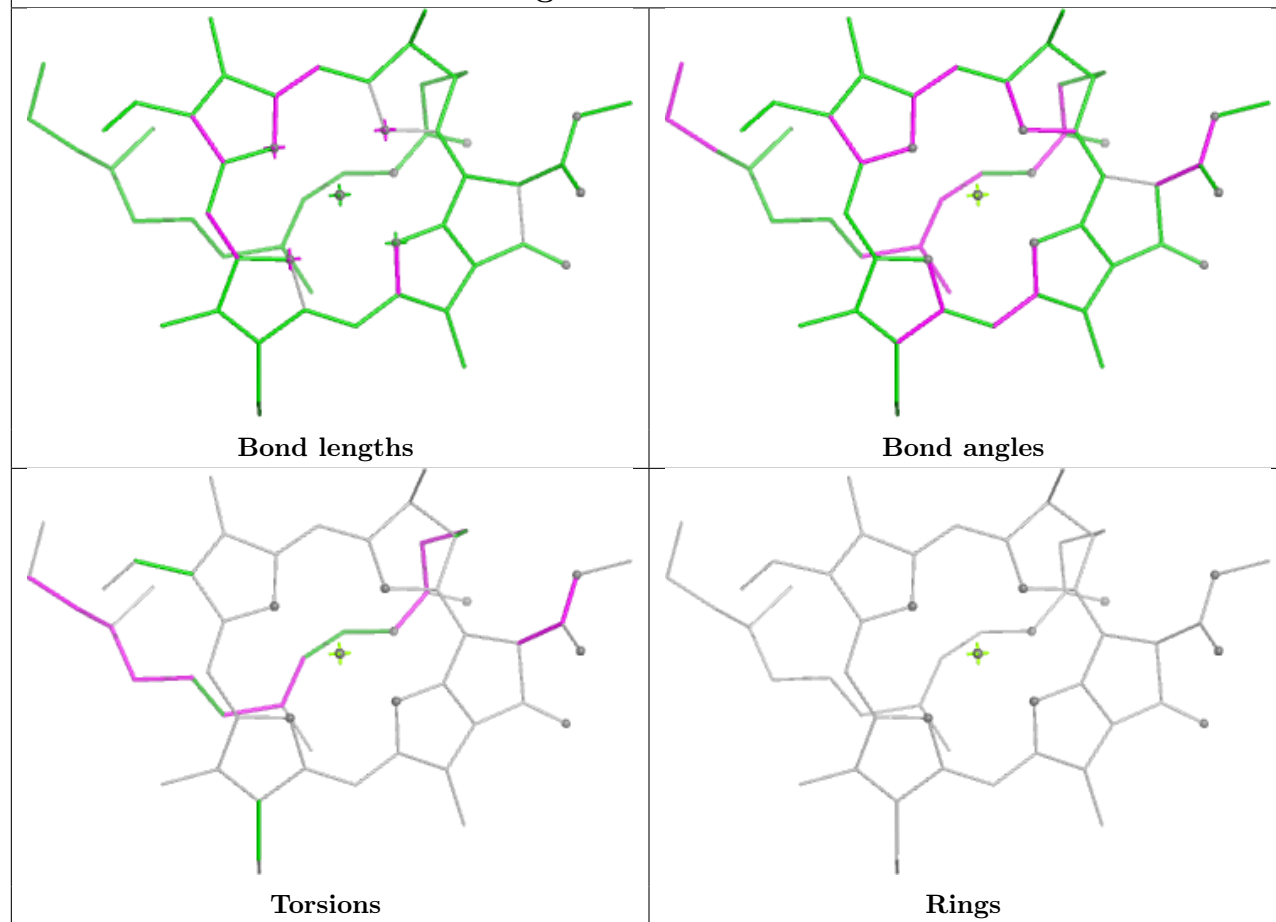


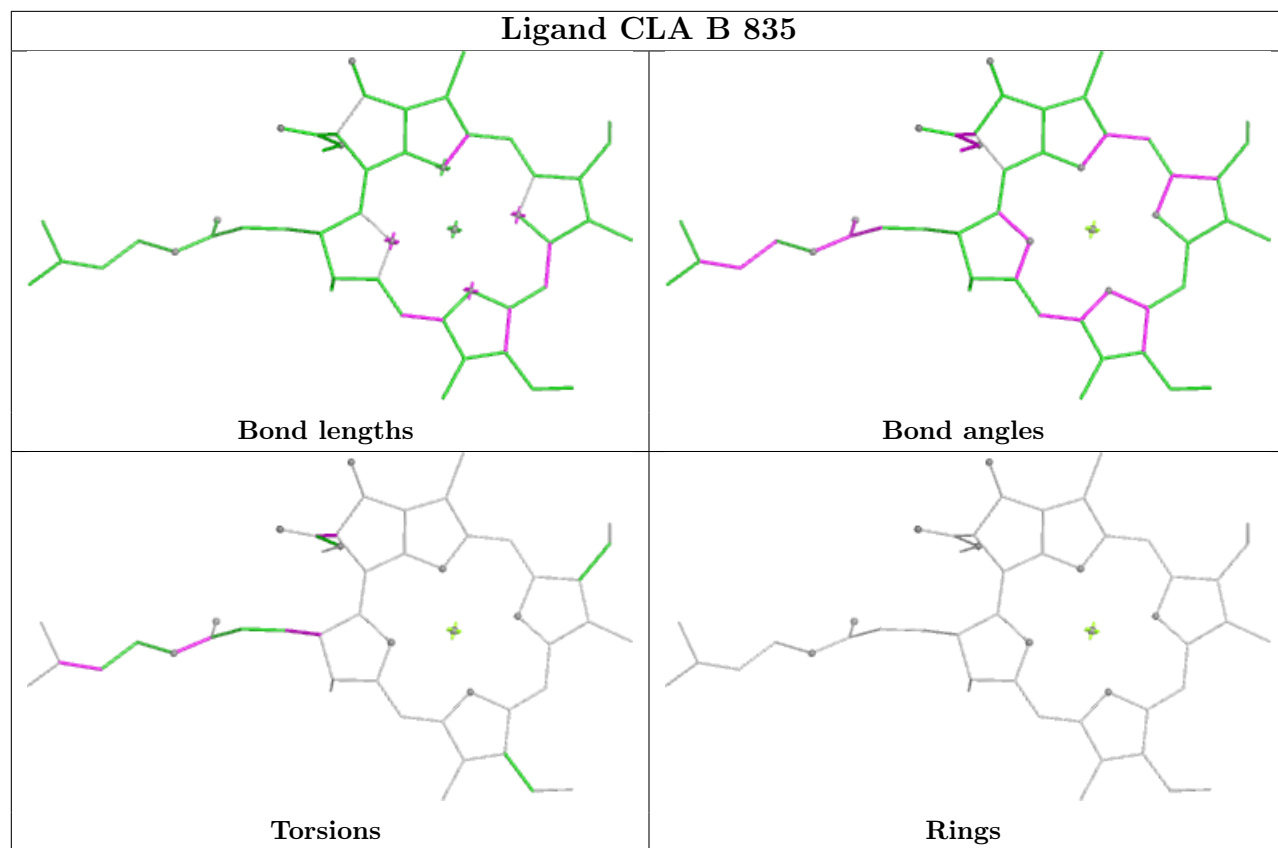
Rings

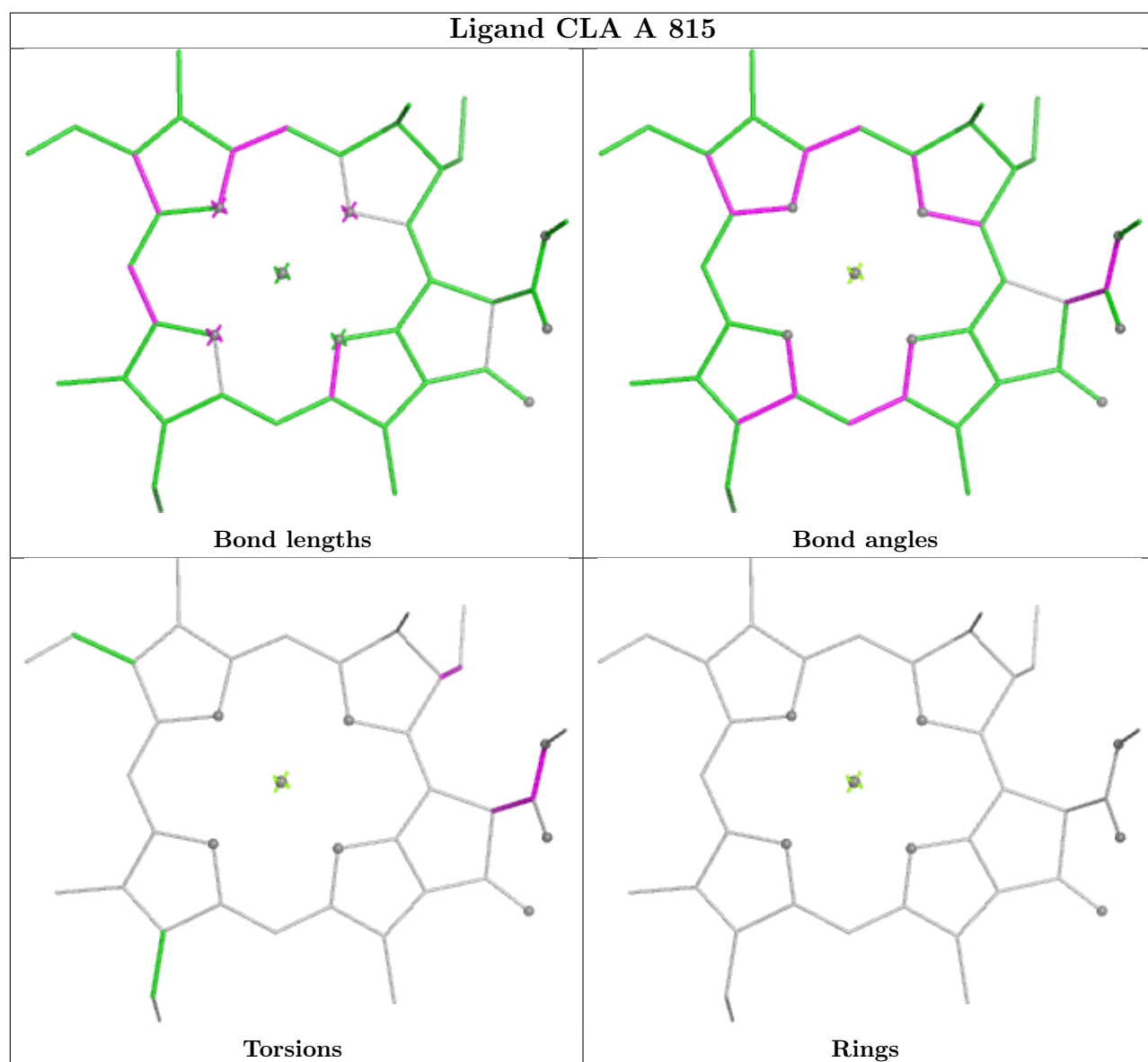
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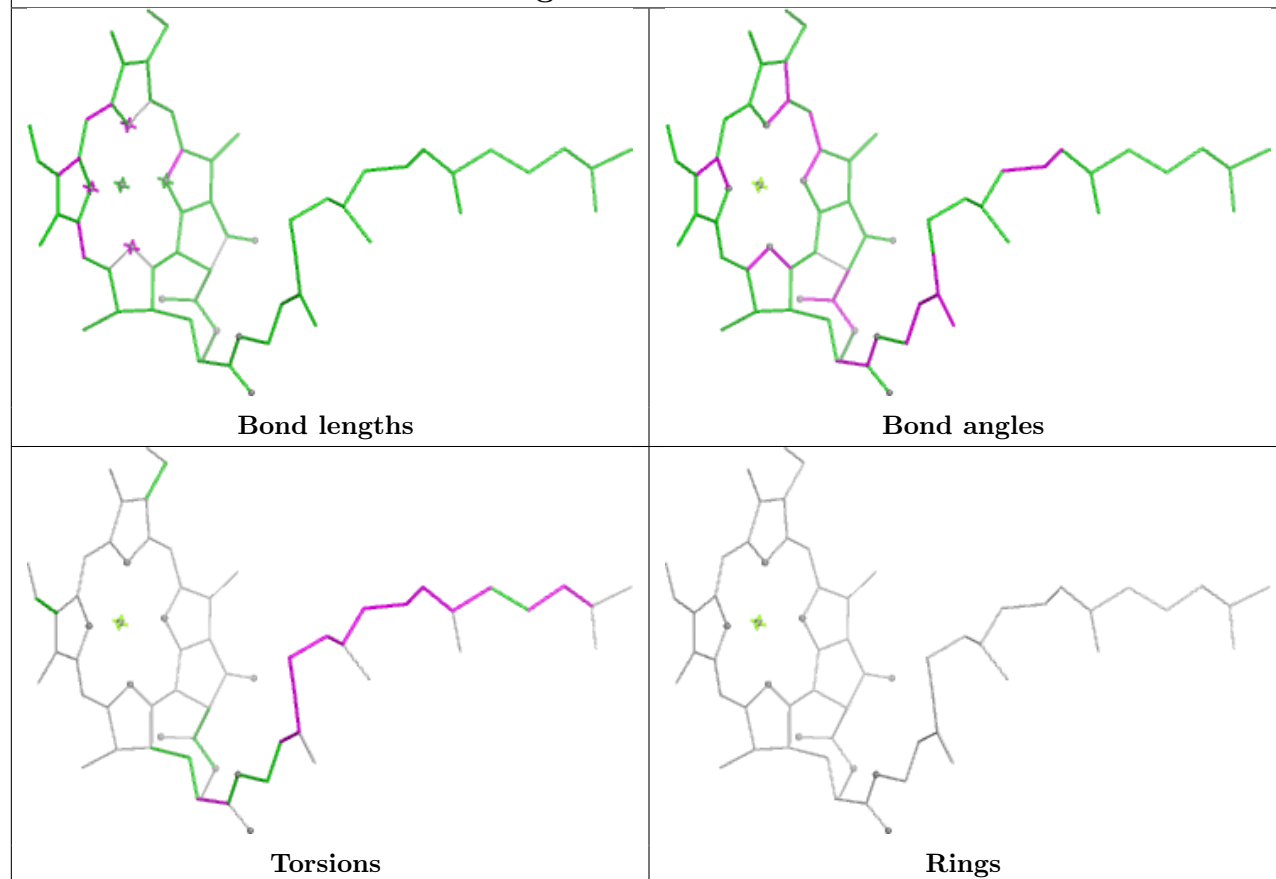
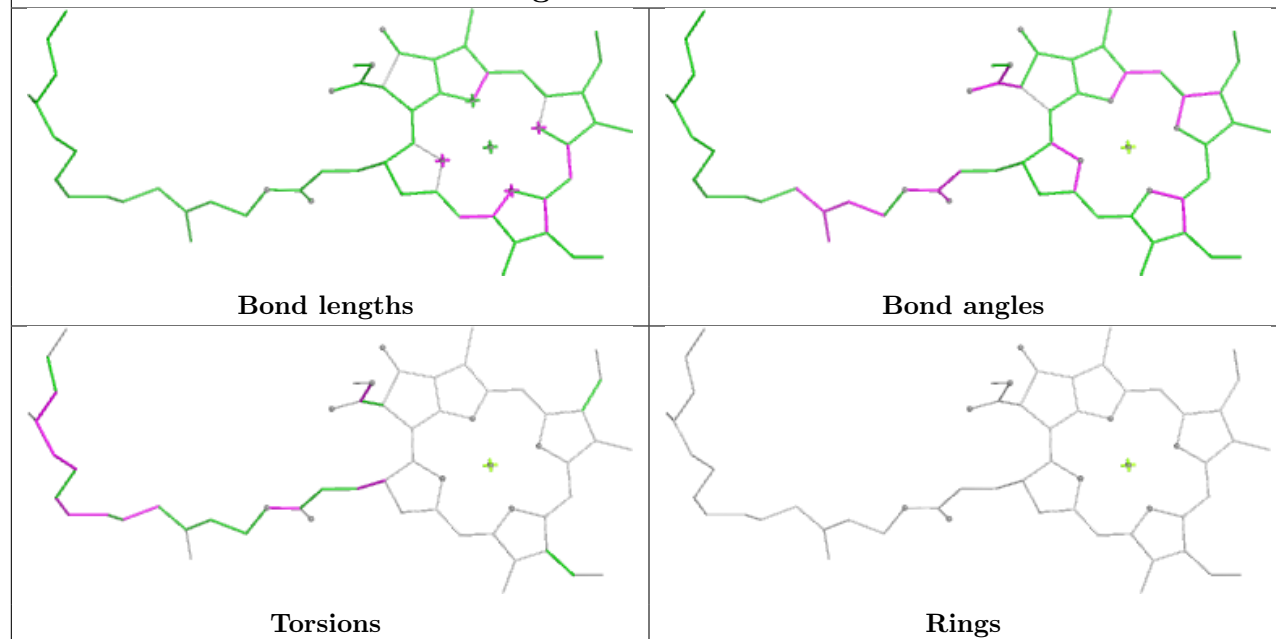


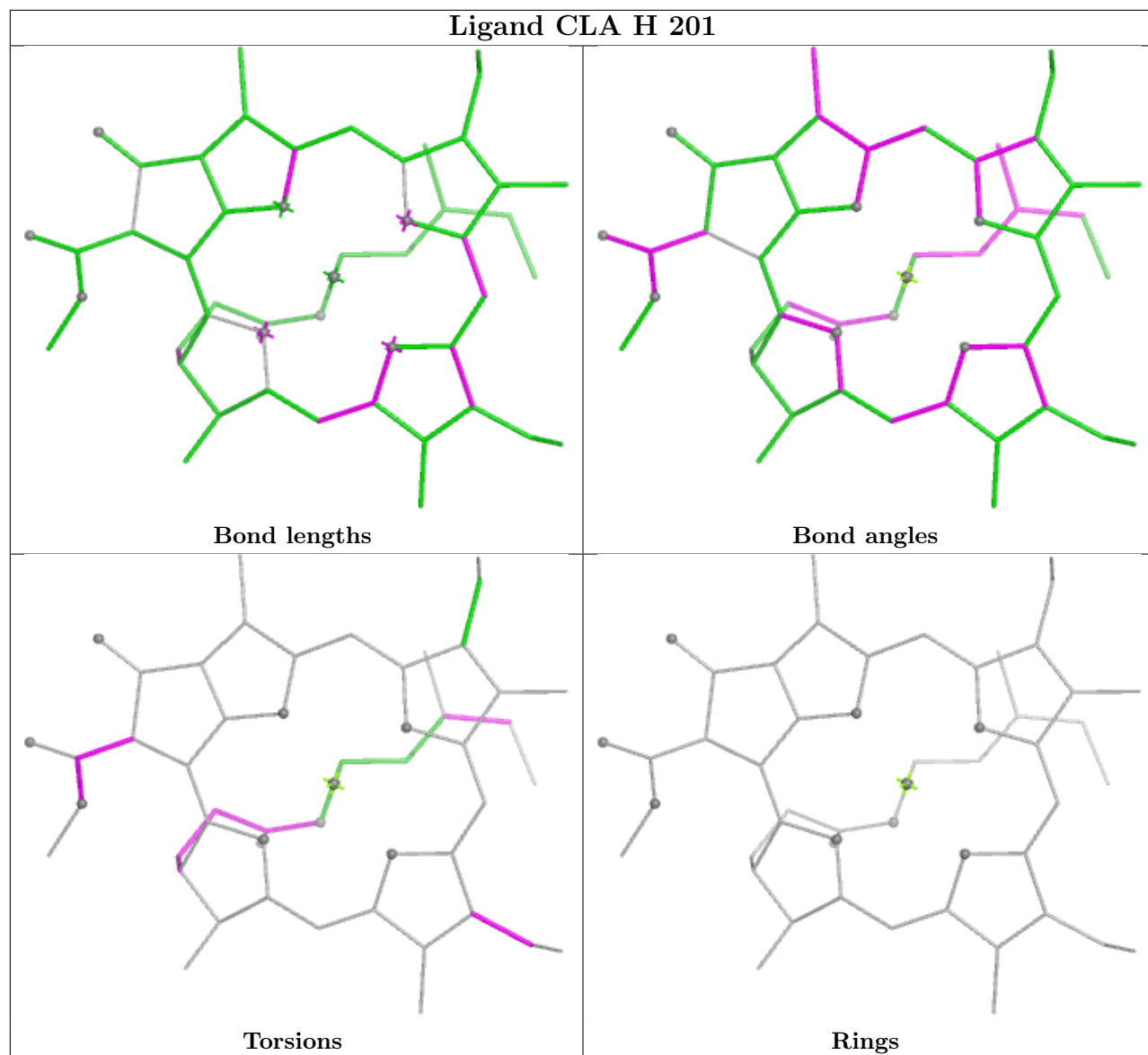
Ligand CLA 4 612



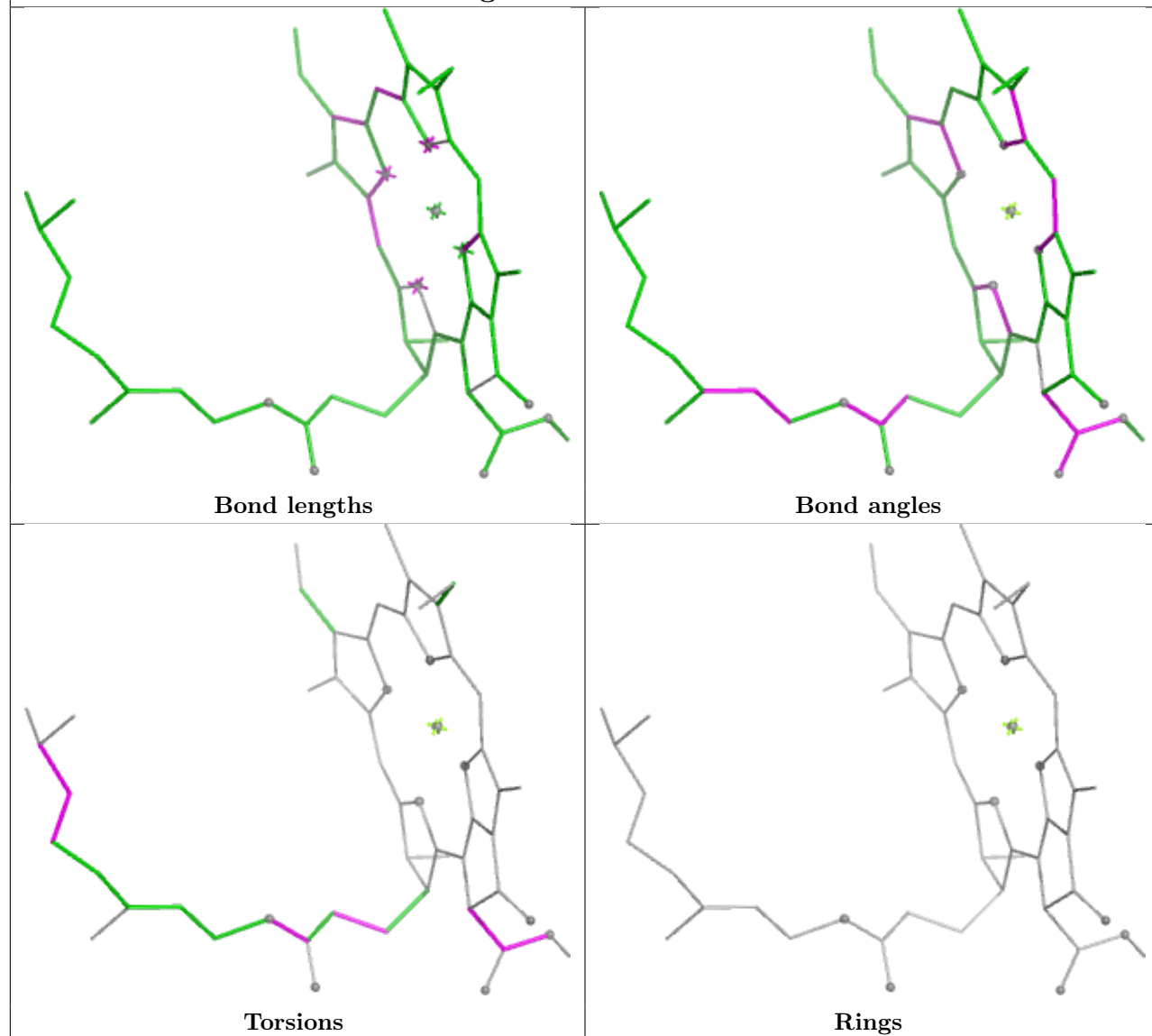




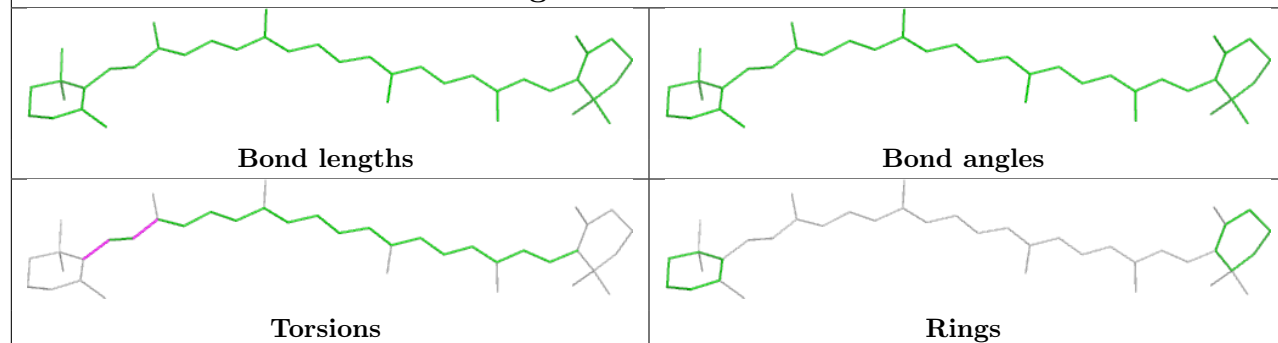
Ligand CLA 1 608**Ligand CLA B 825**

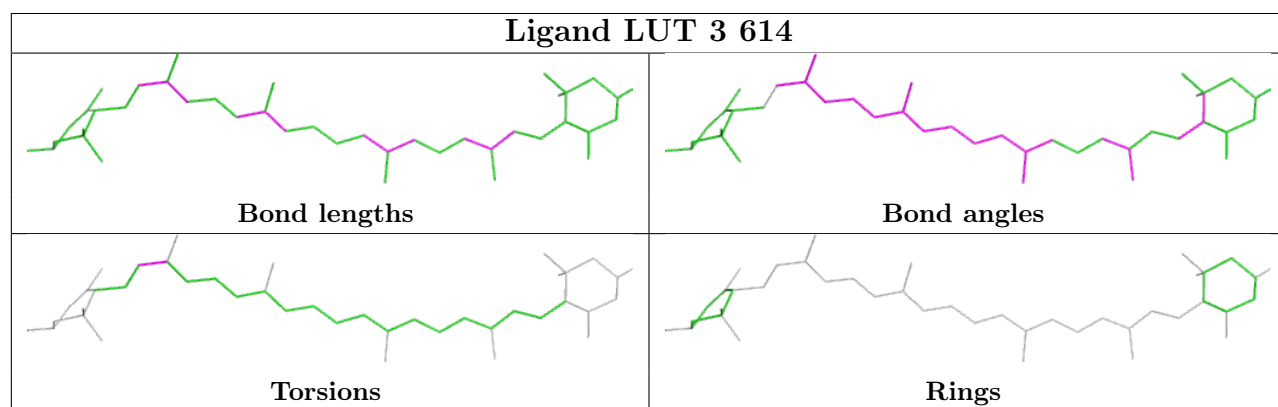
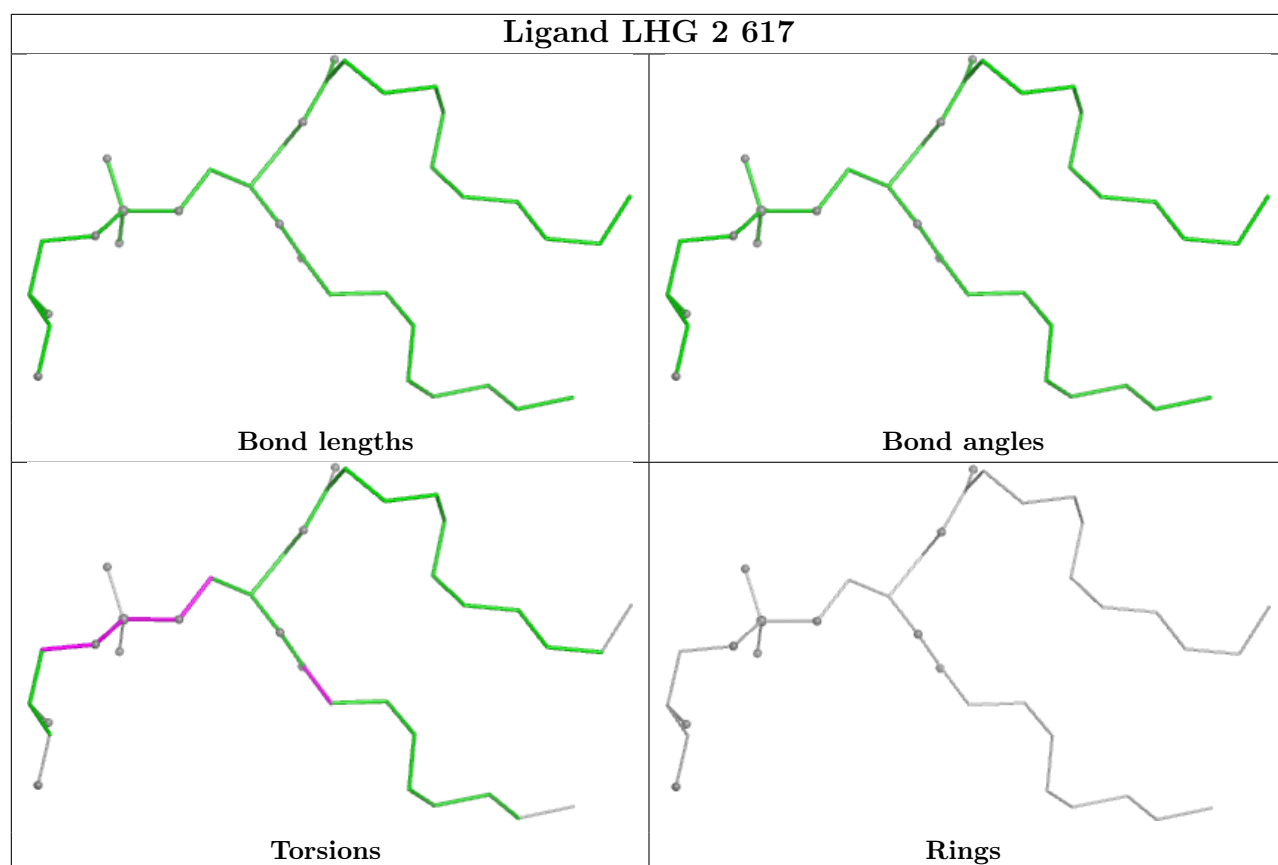


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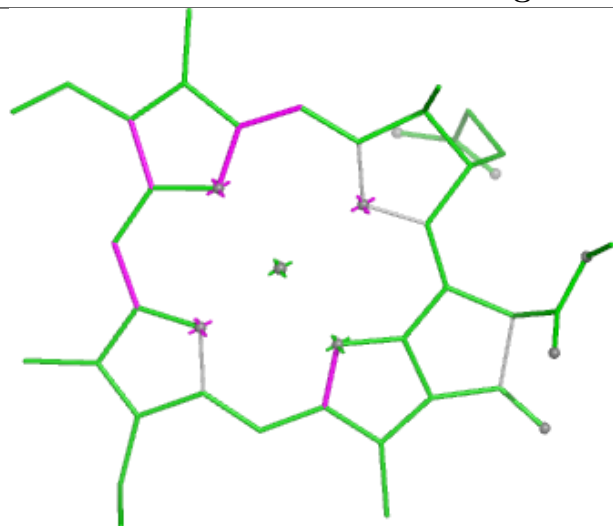


Ligand BCR K 204

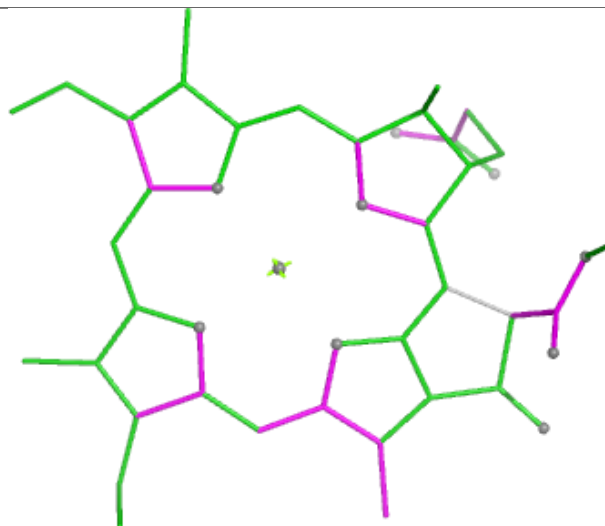




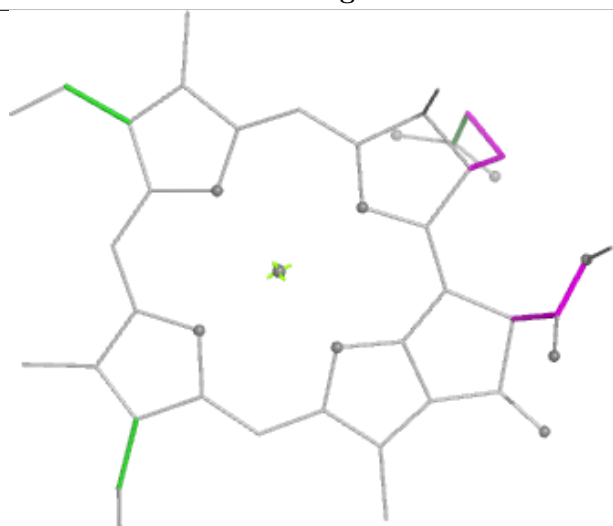
Ligand CLA A 836



Bond lengths



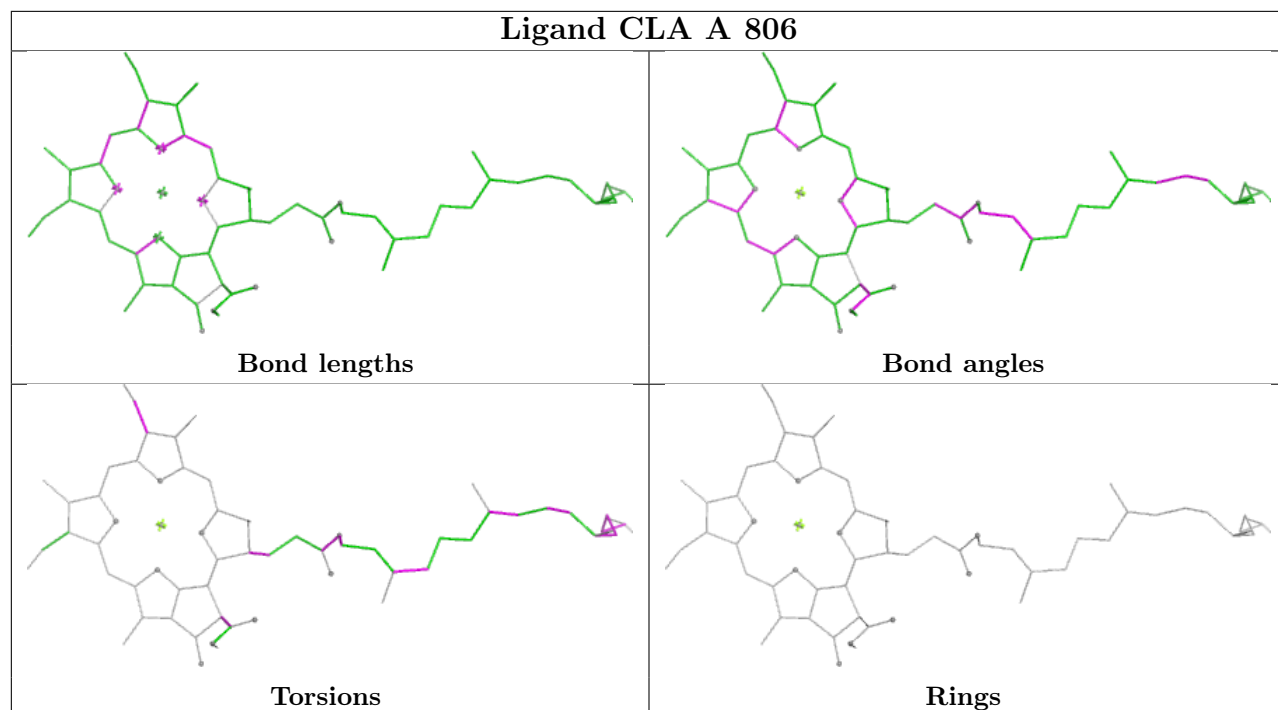
Bond angles



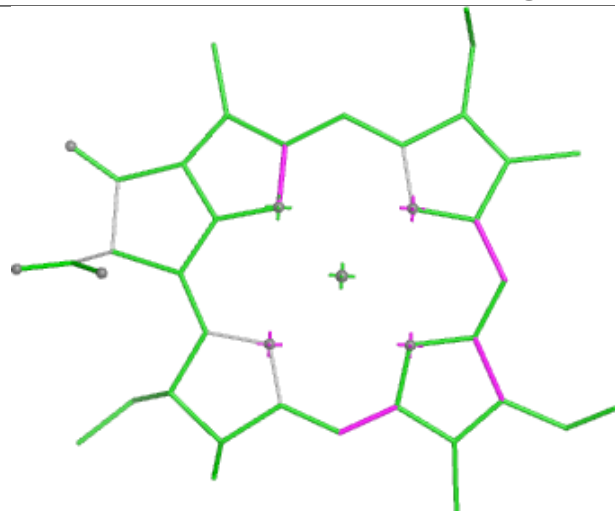
Torsions



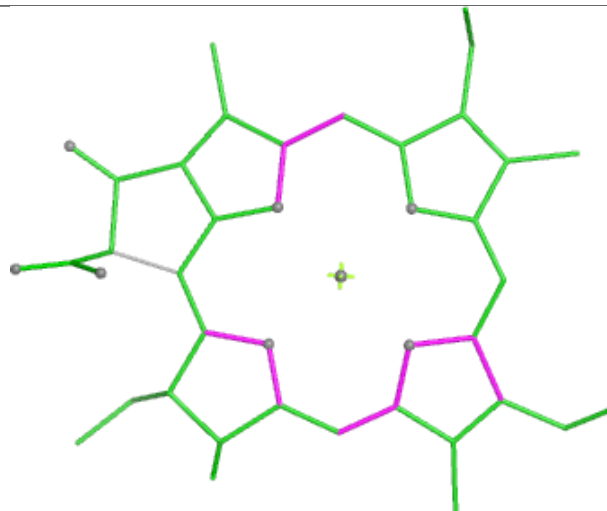
Rings



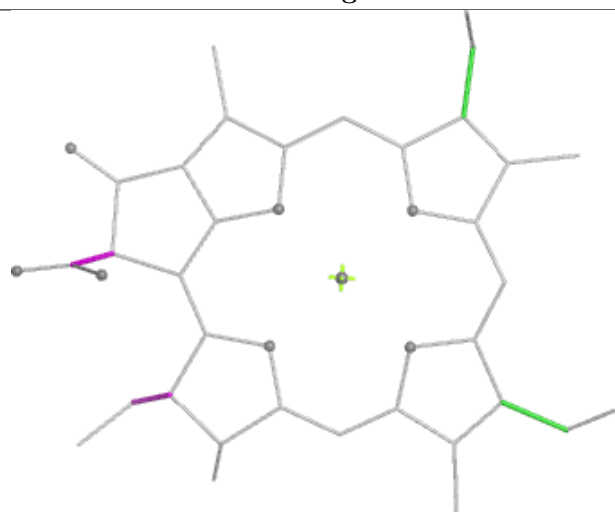
Ligand CLA 3 606



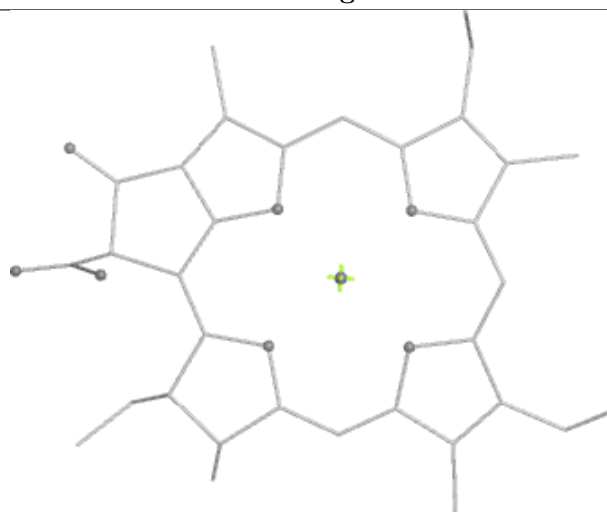
Bond lengths



Bond angles

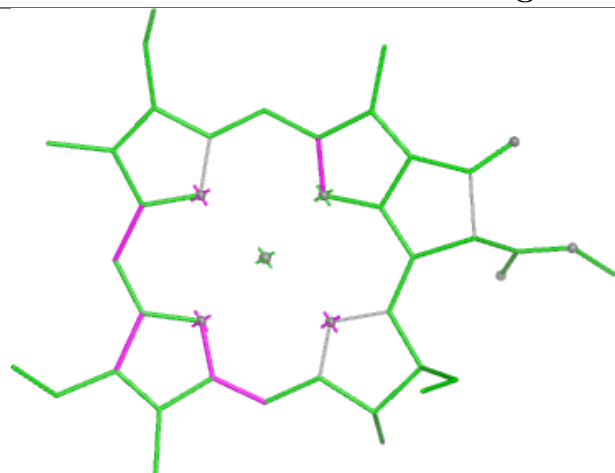


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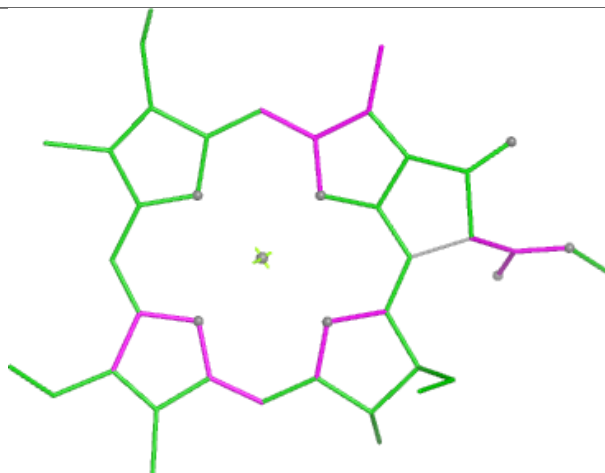


Rings

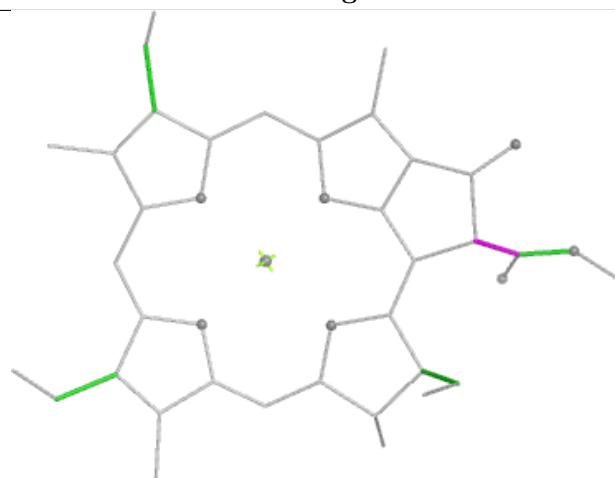
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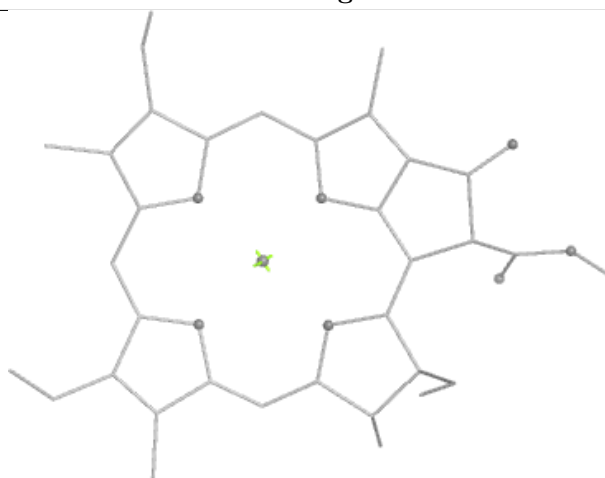
Bond lengths



Bond angles

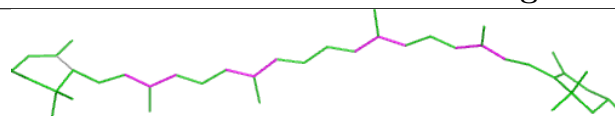


Torsions

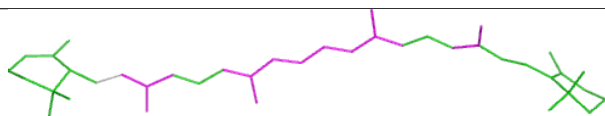


Rings

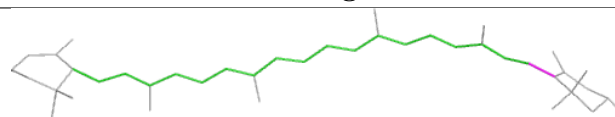
Ligand LUT 1 615



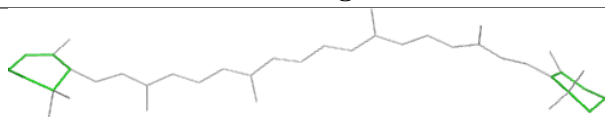
Bond lengths



Bond angles

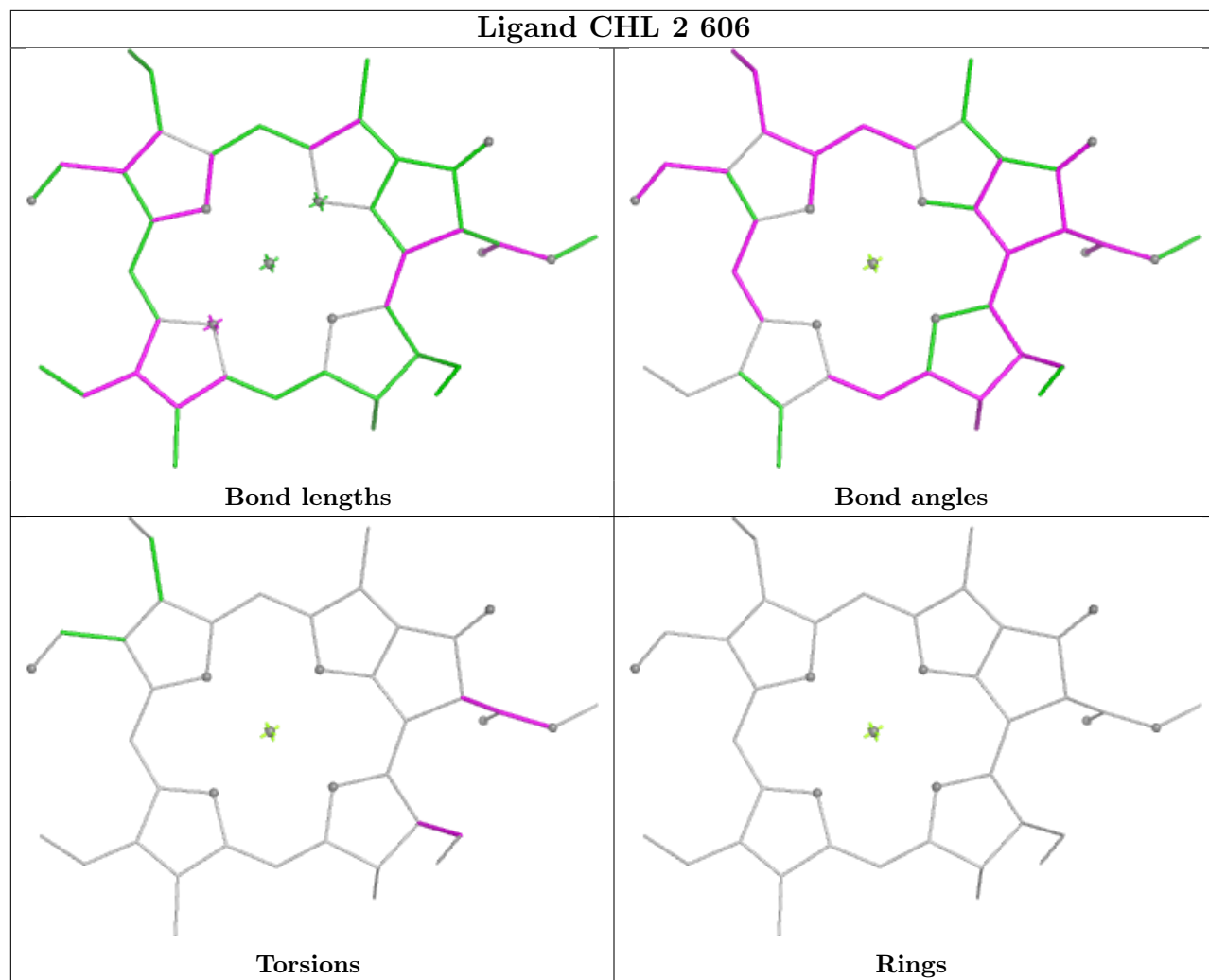


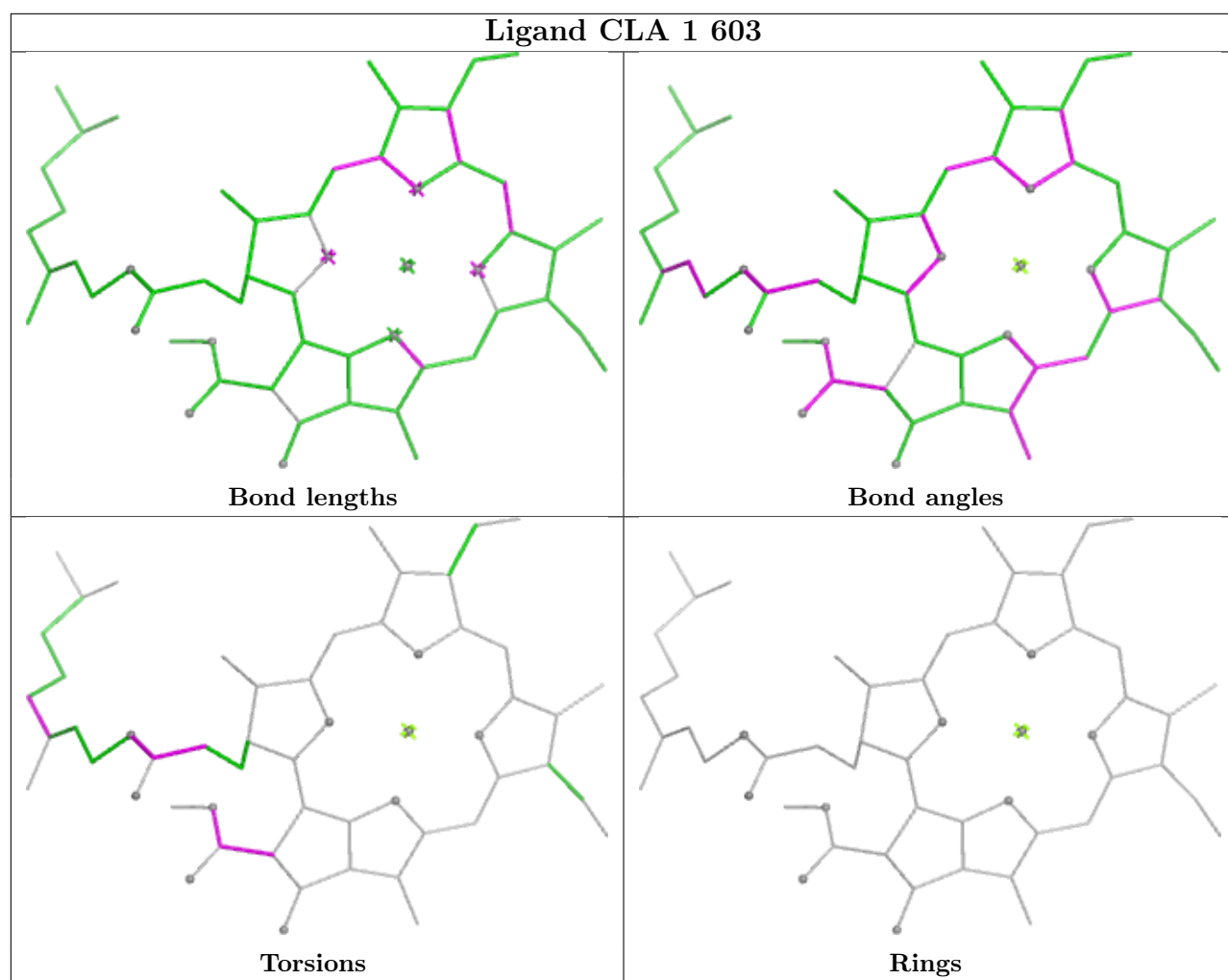
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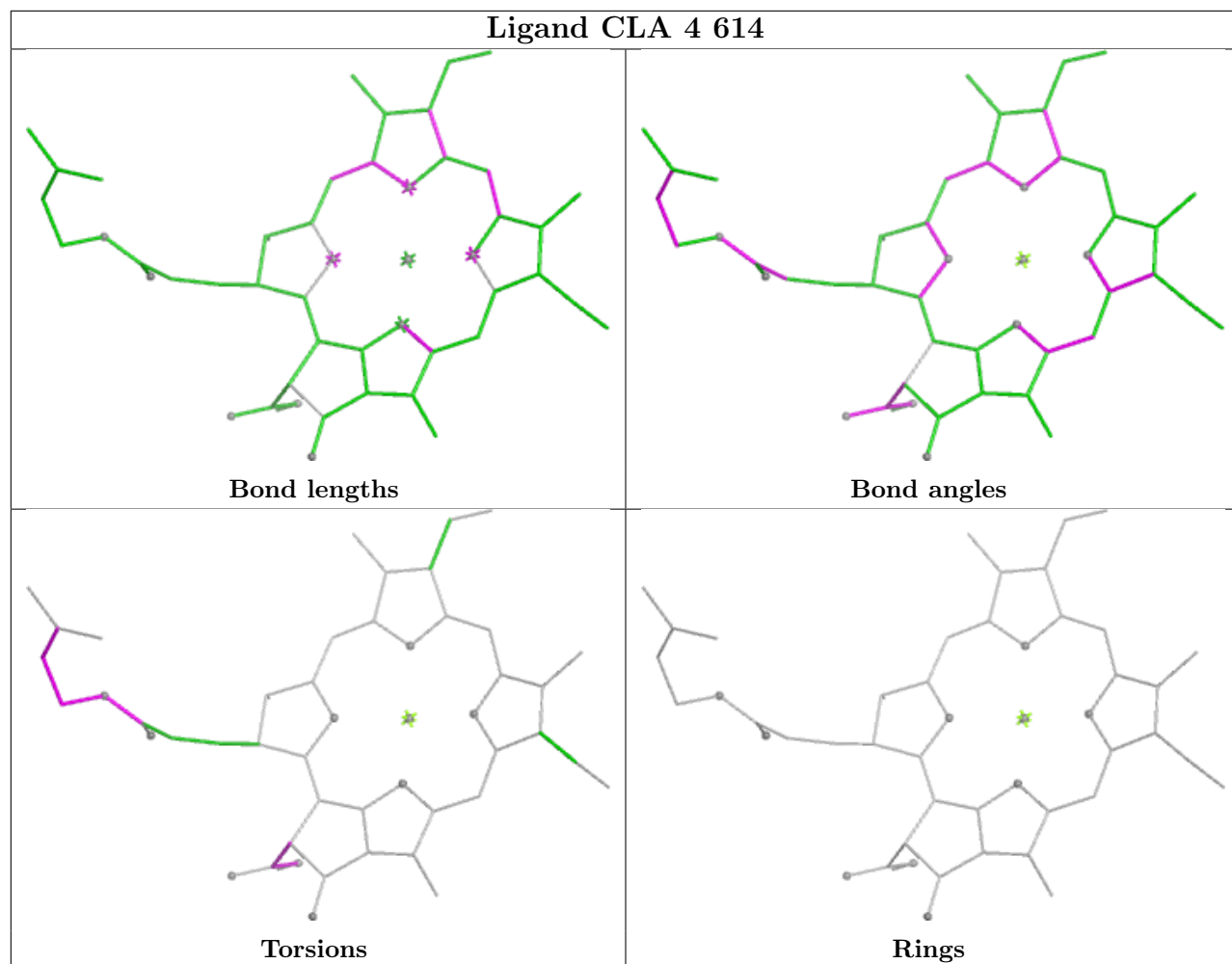
Rings

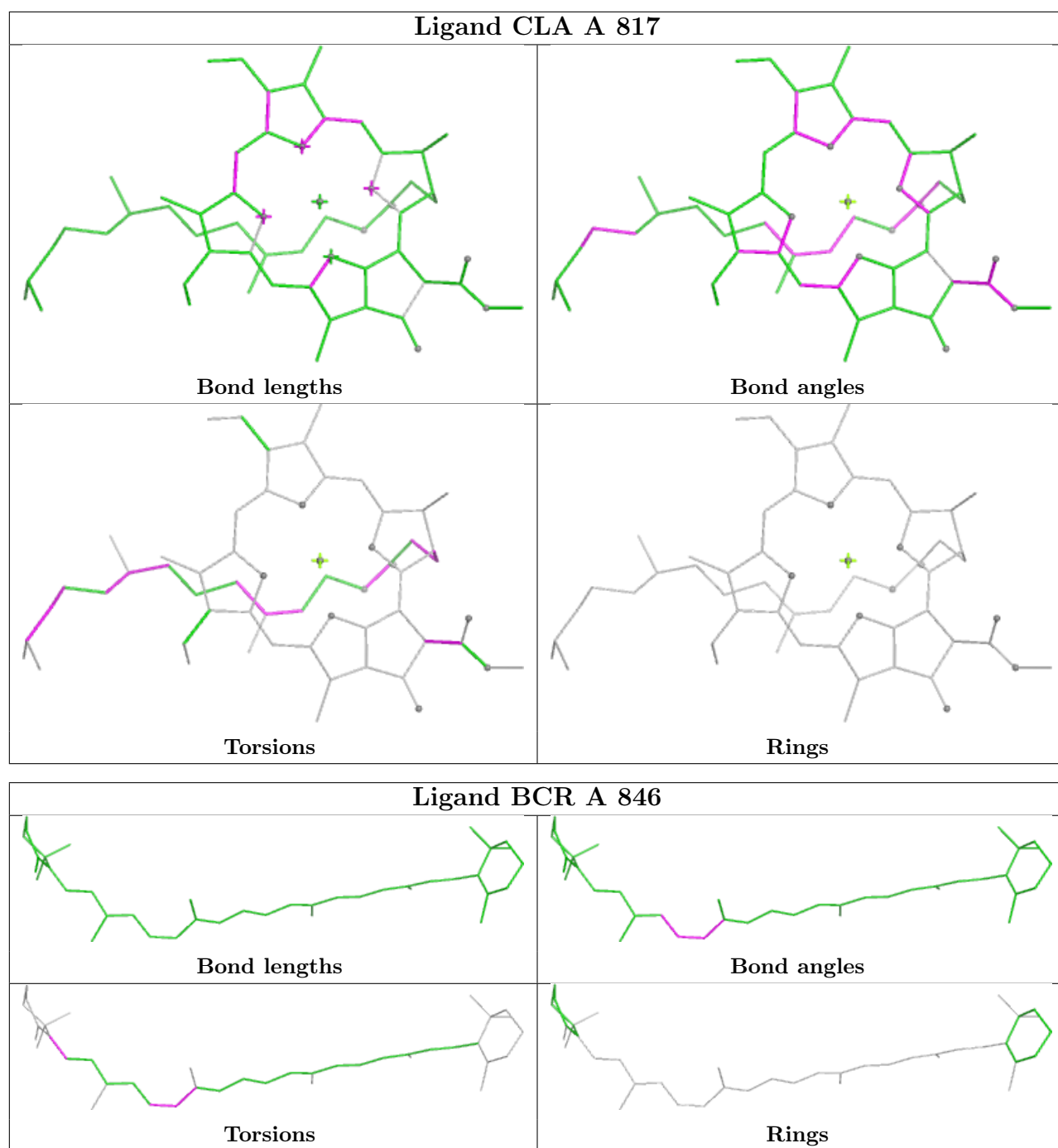
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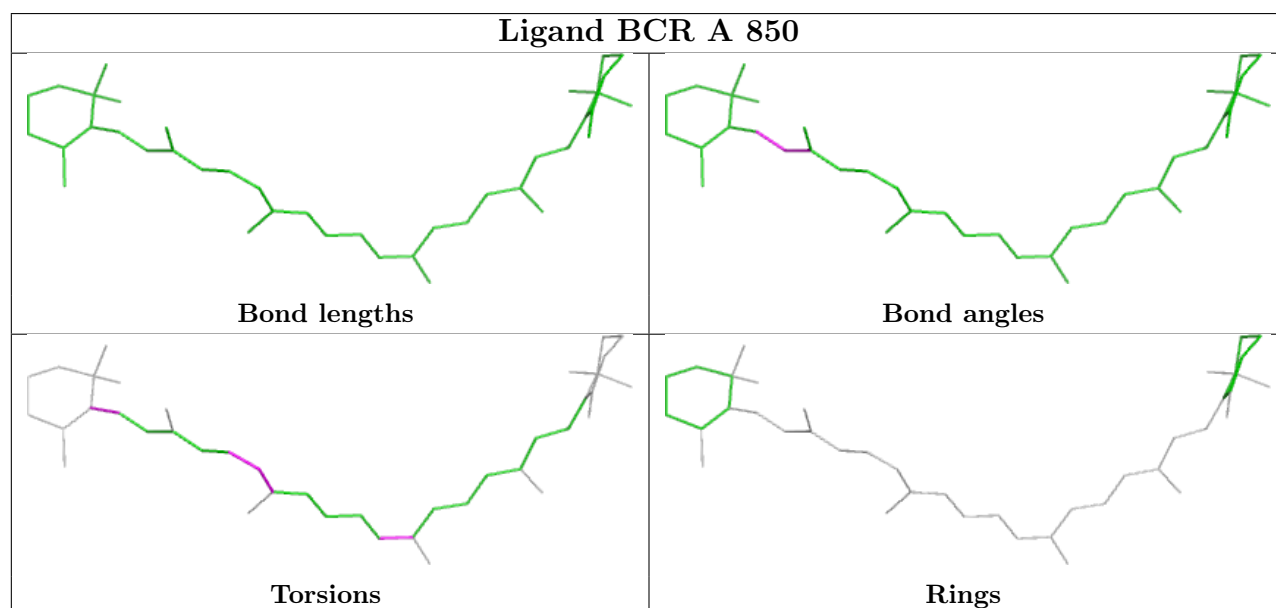
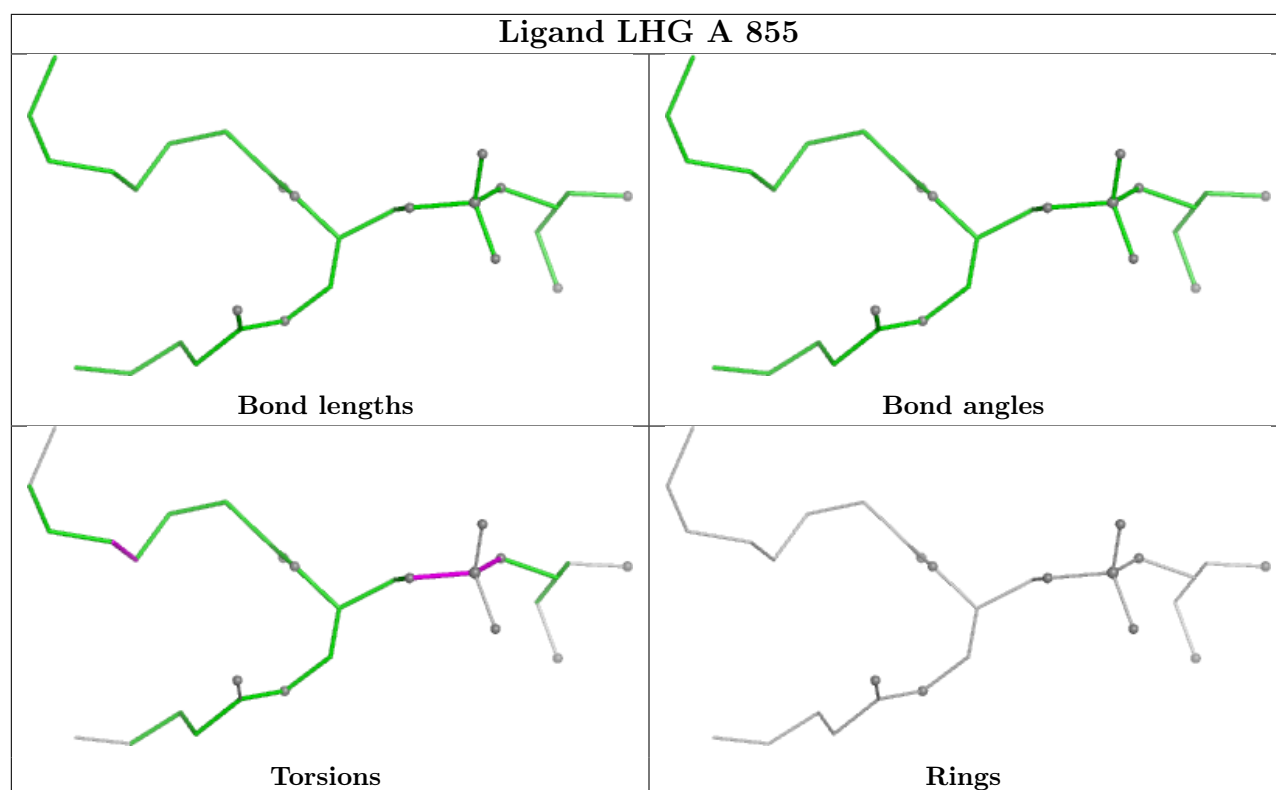




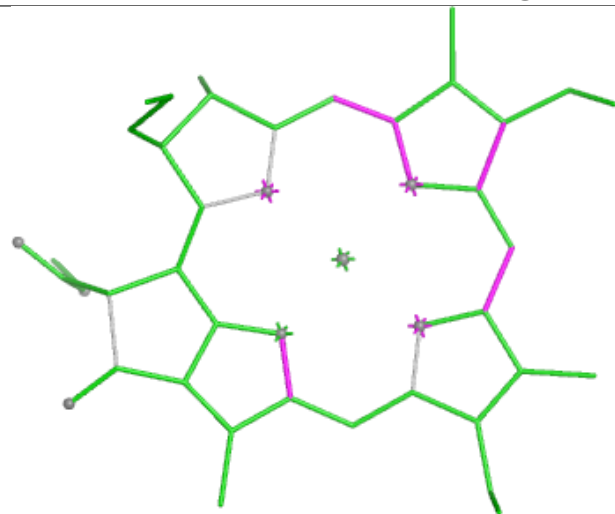
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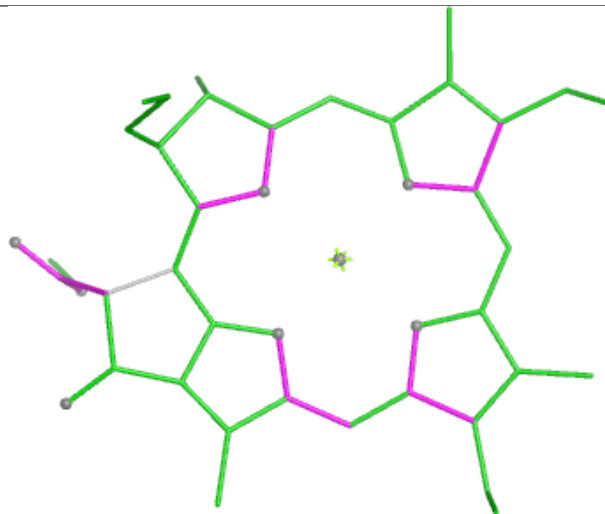




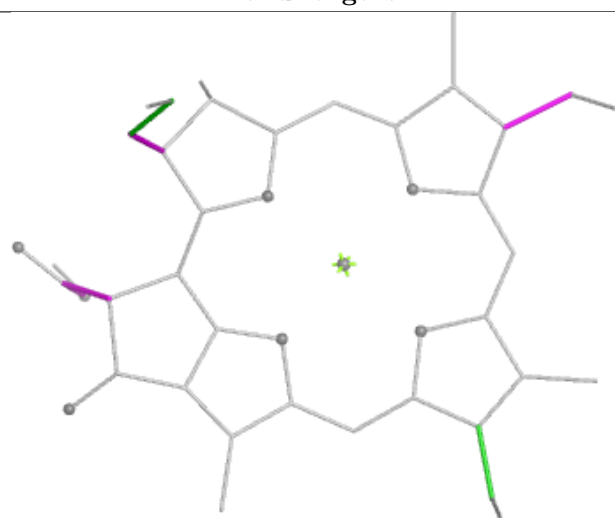
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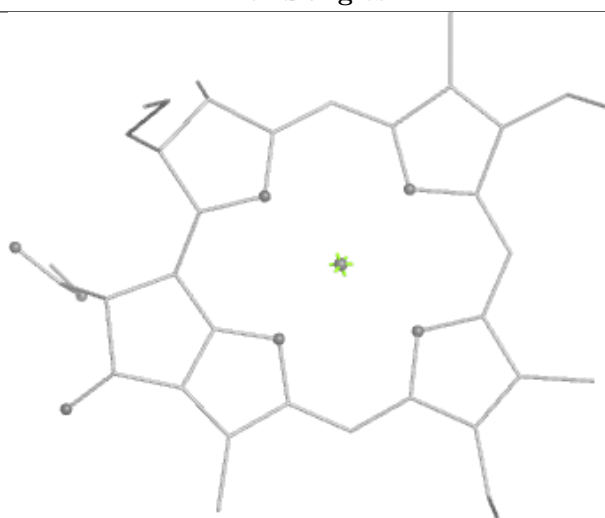
Bond lengths



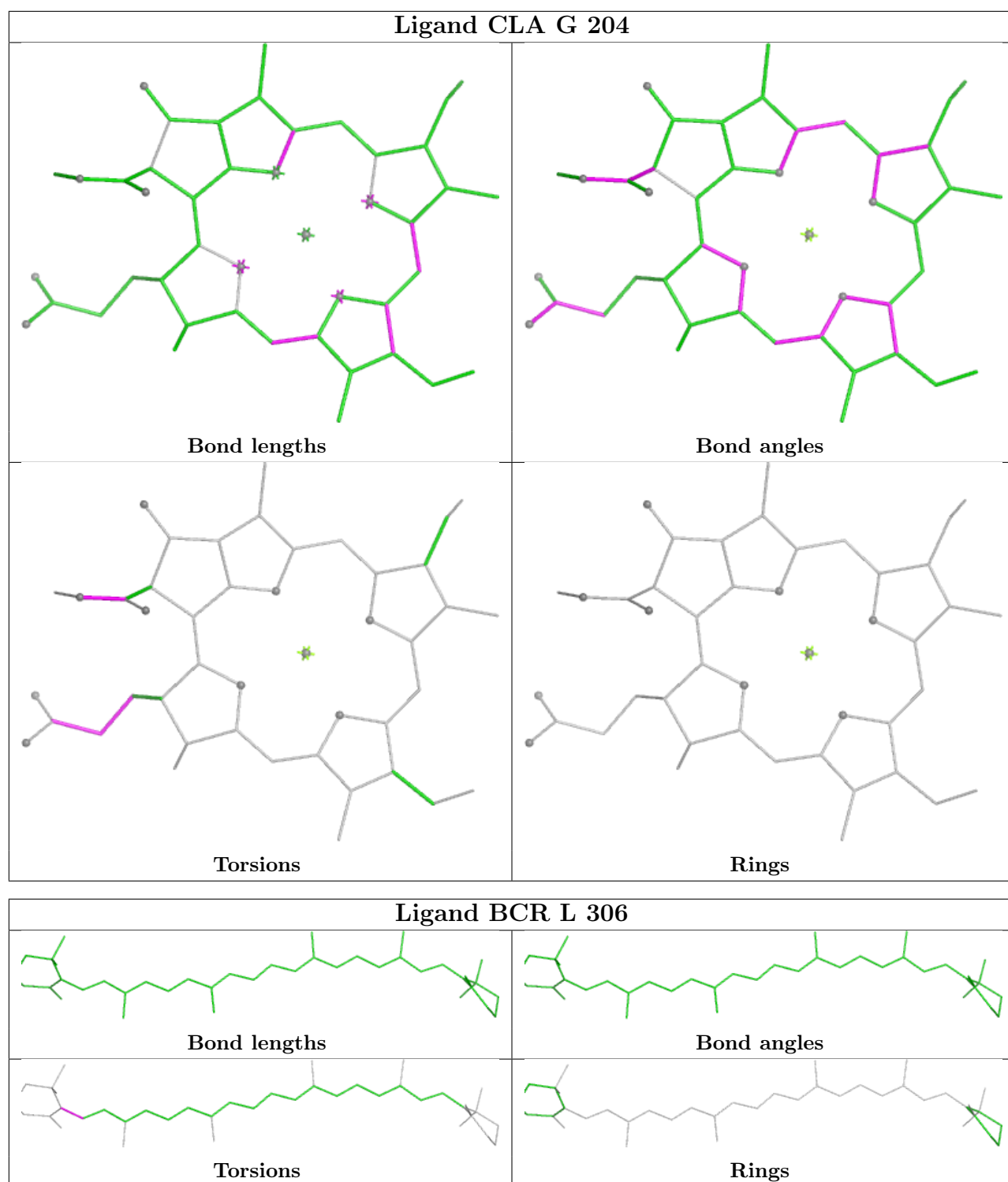
Bond angles

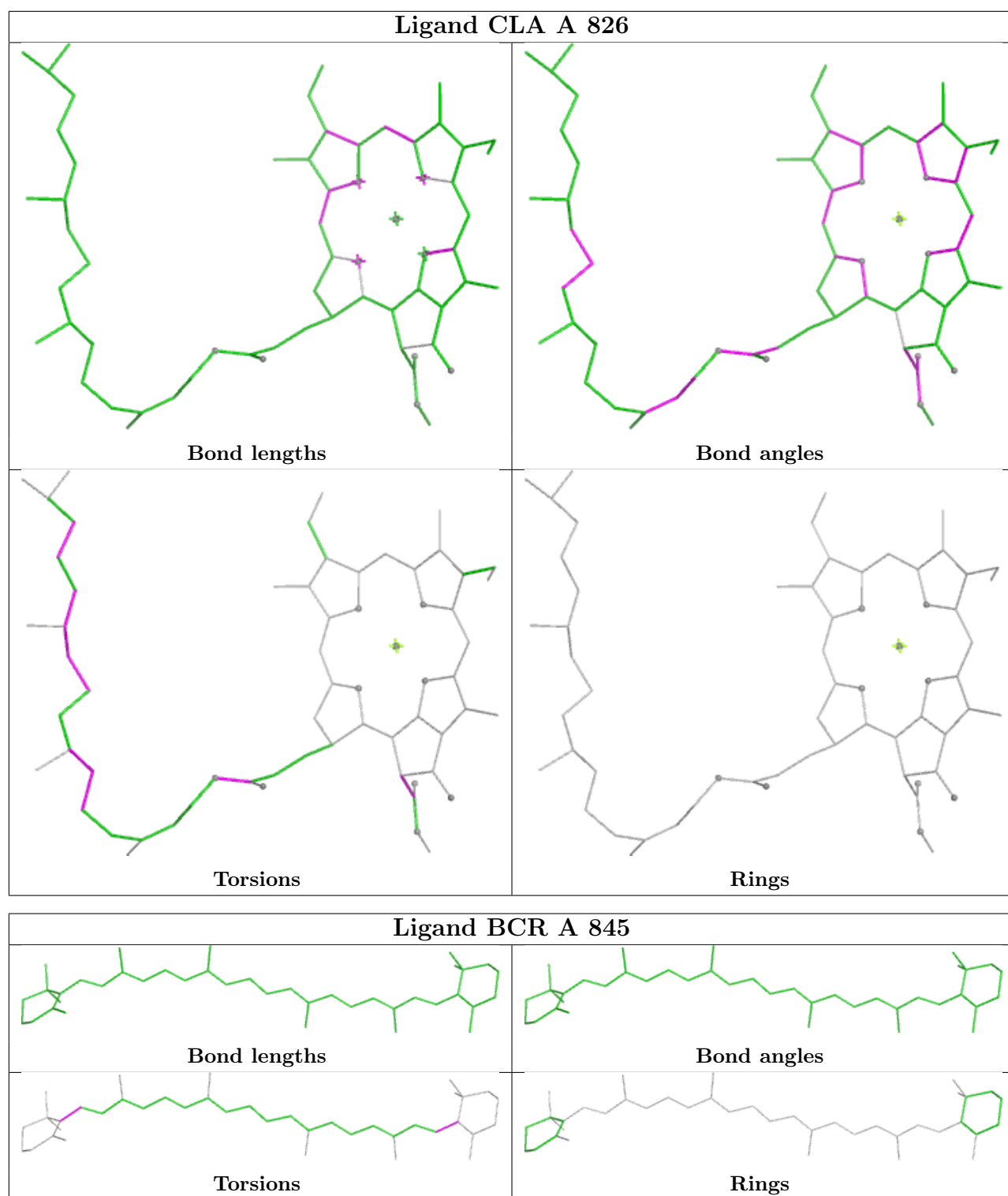


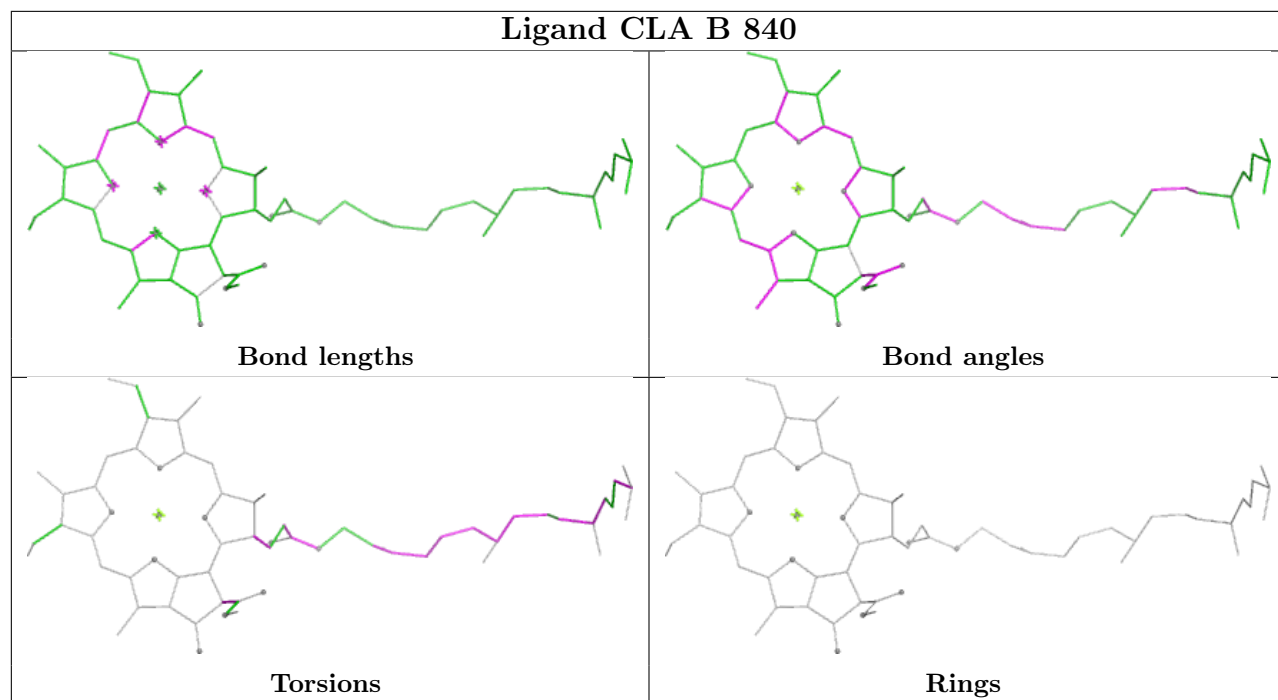
Torsions



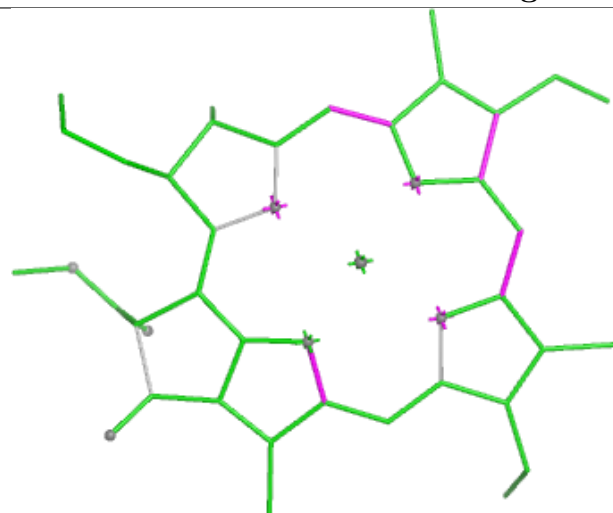
Rings



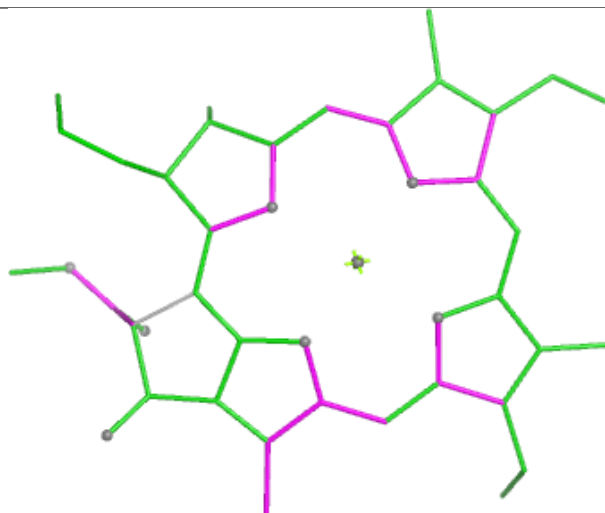




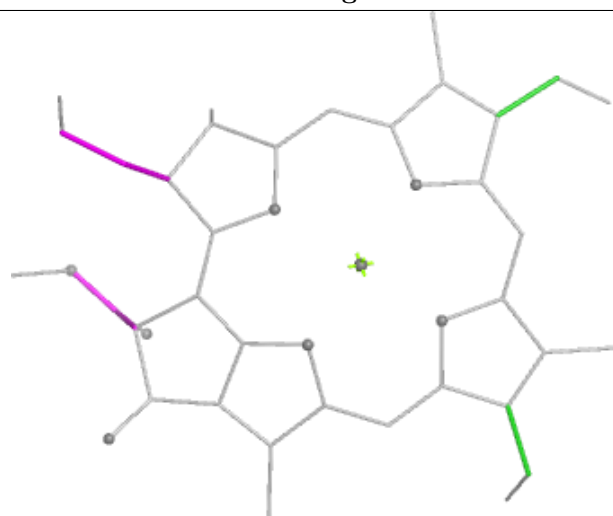
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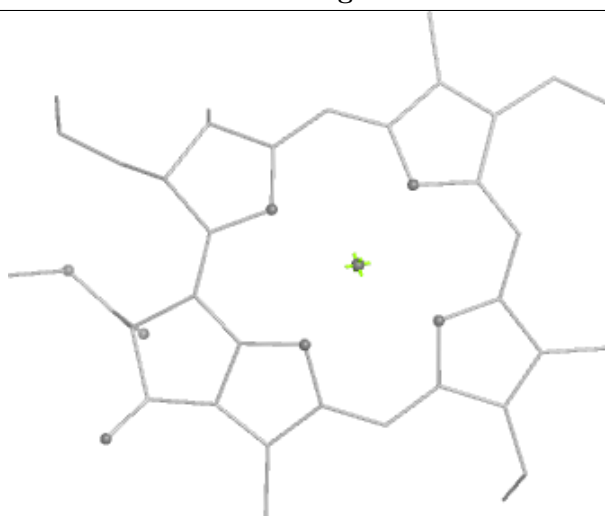
Bond lengths



Bond angles

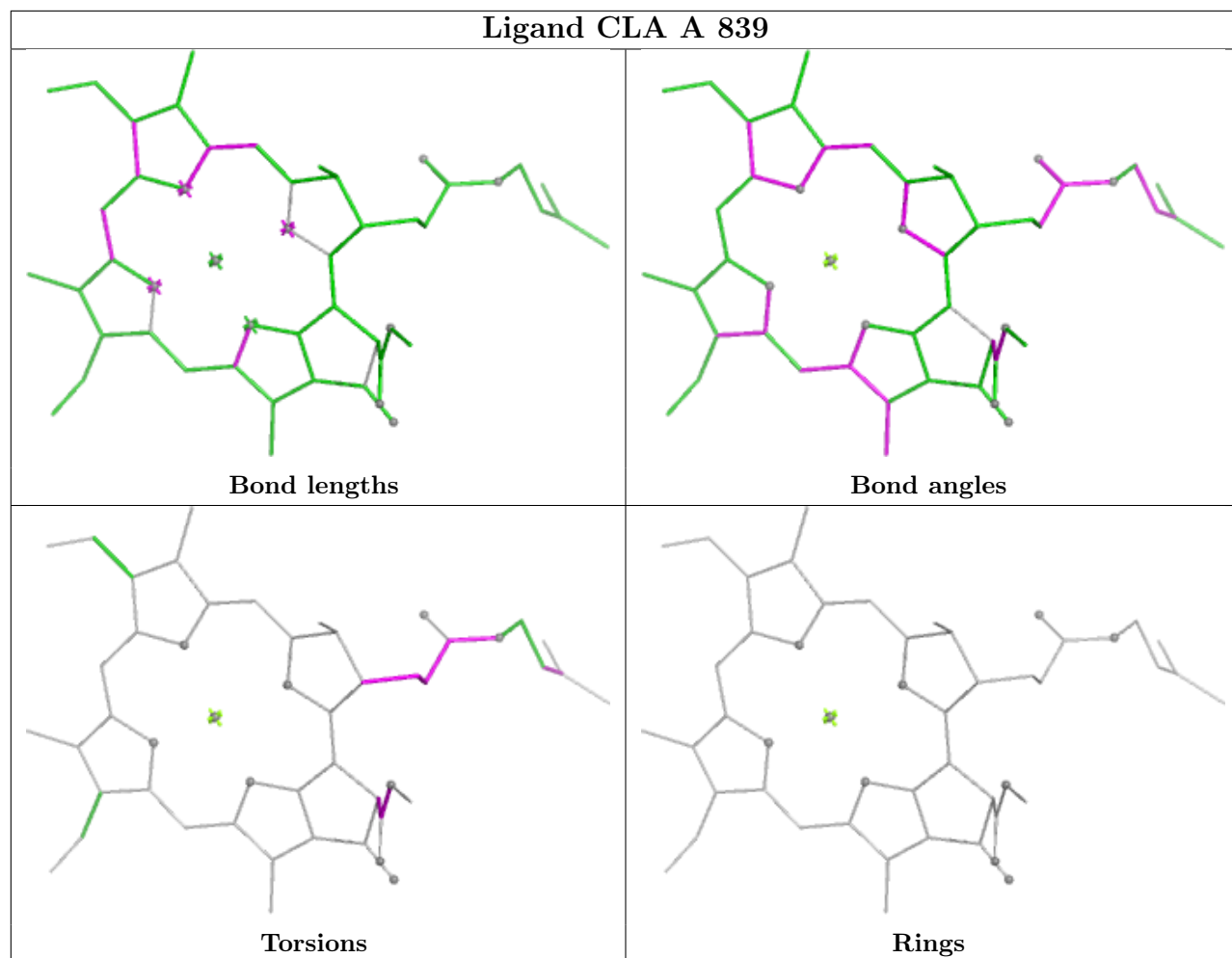


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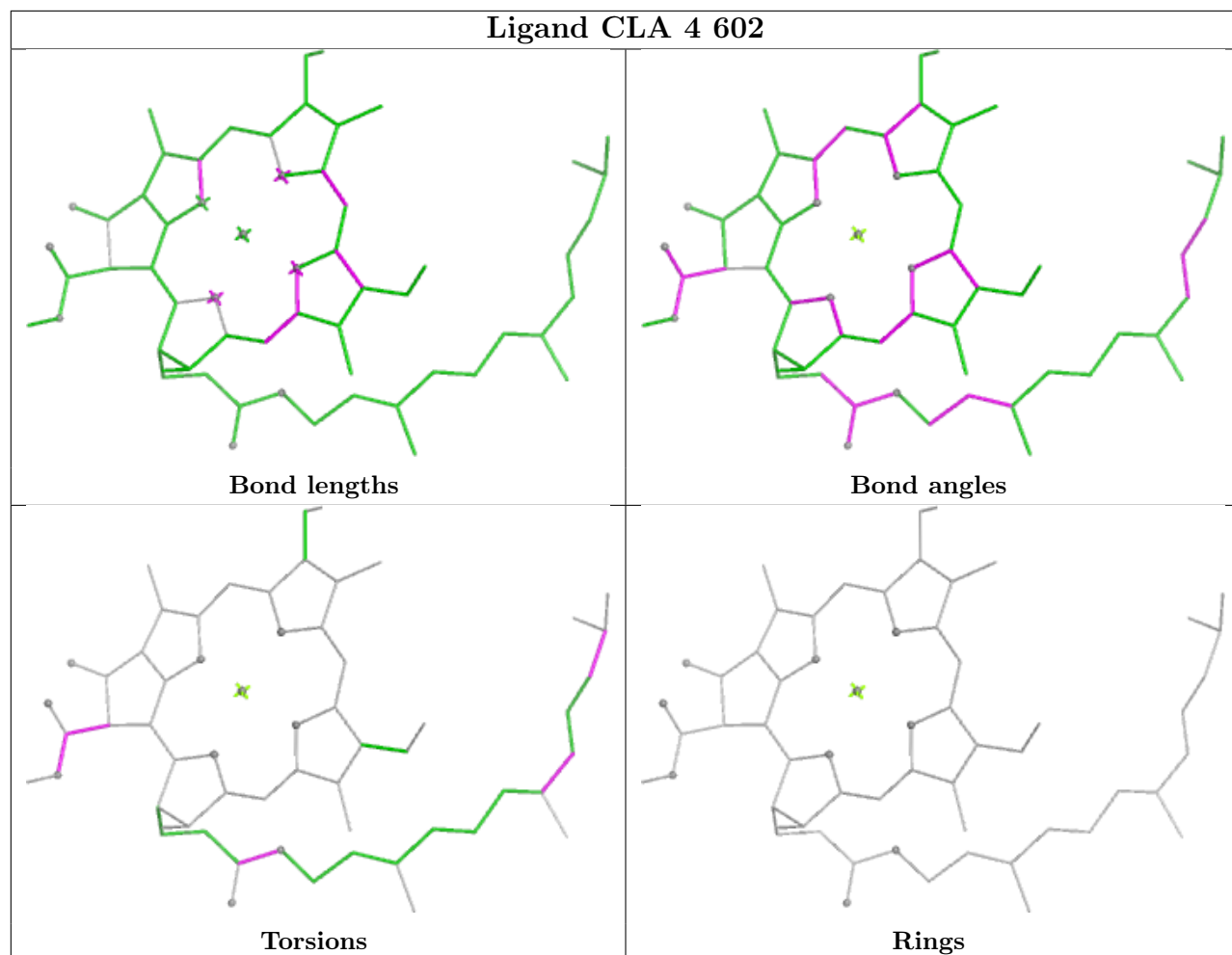


Rings

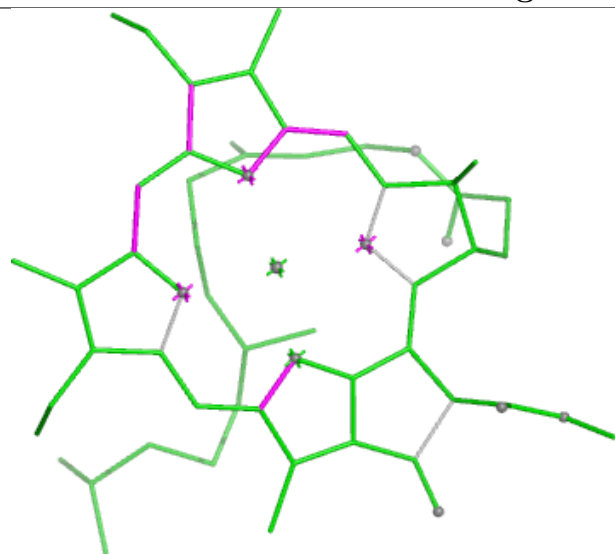
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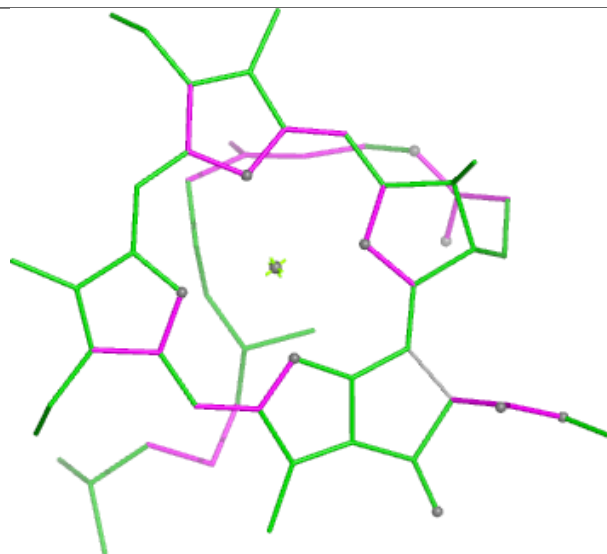
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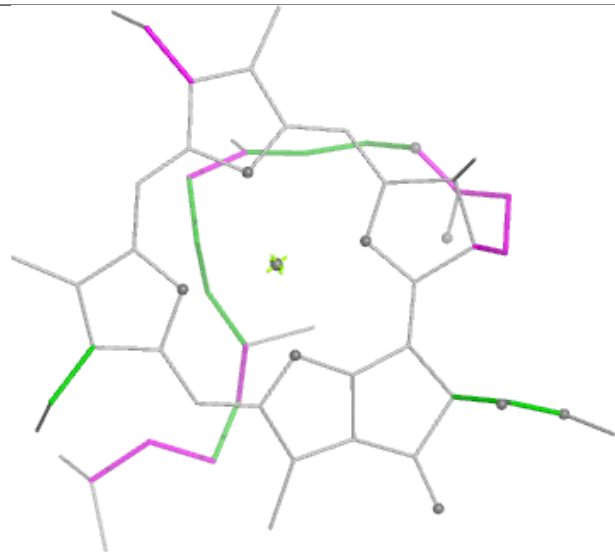
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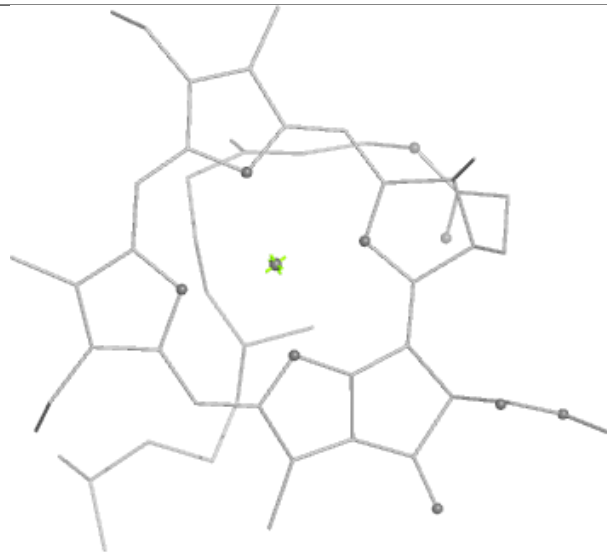
Bond lengths



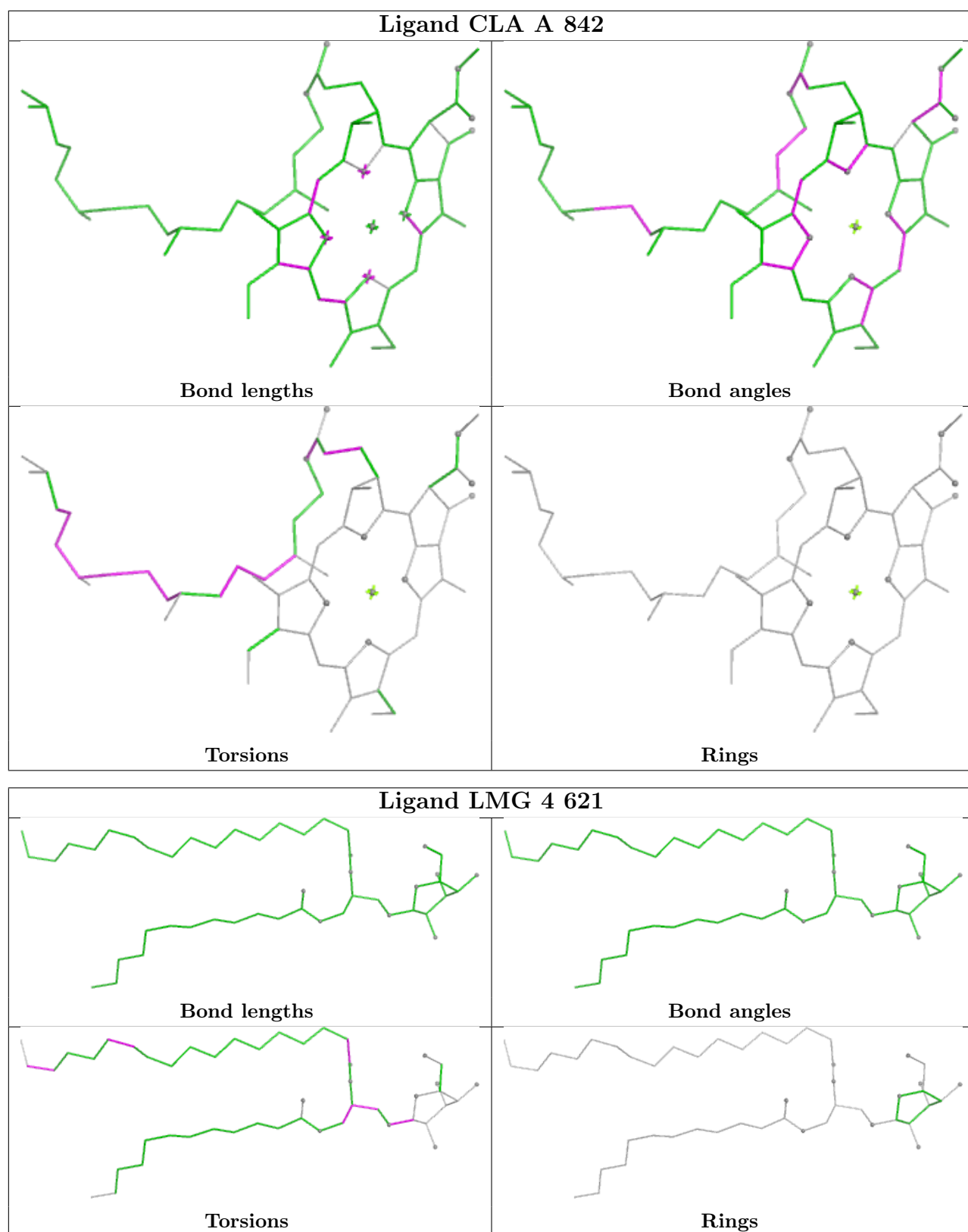
Bond angles

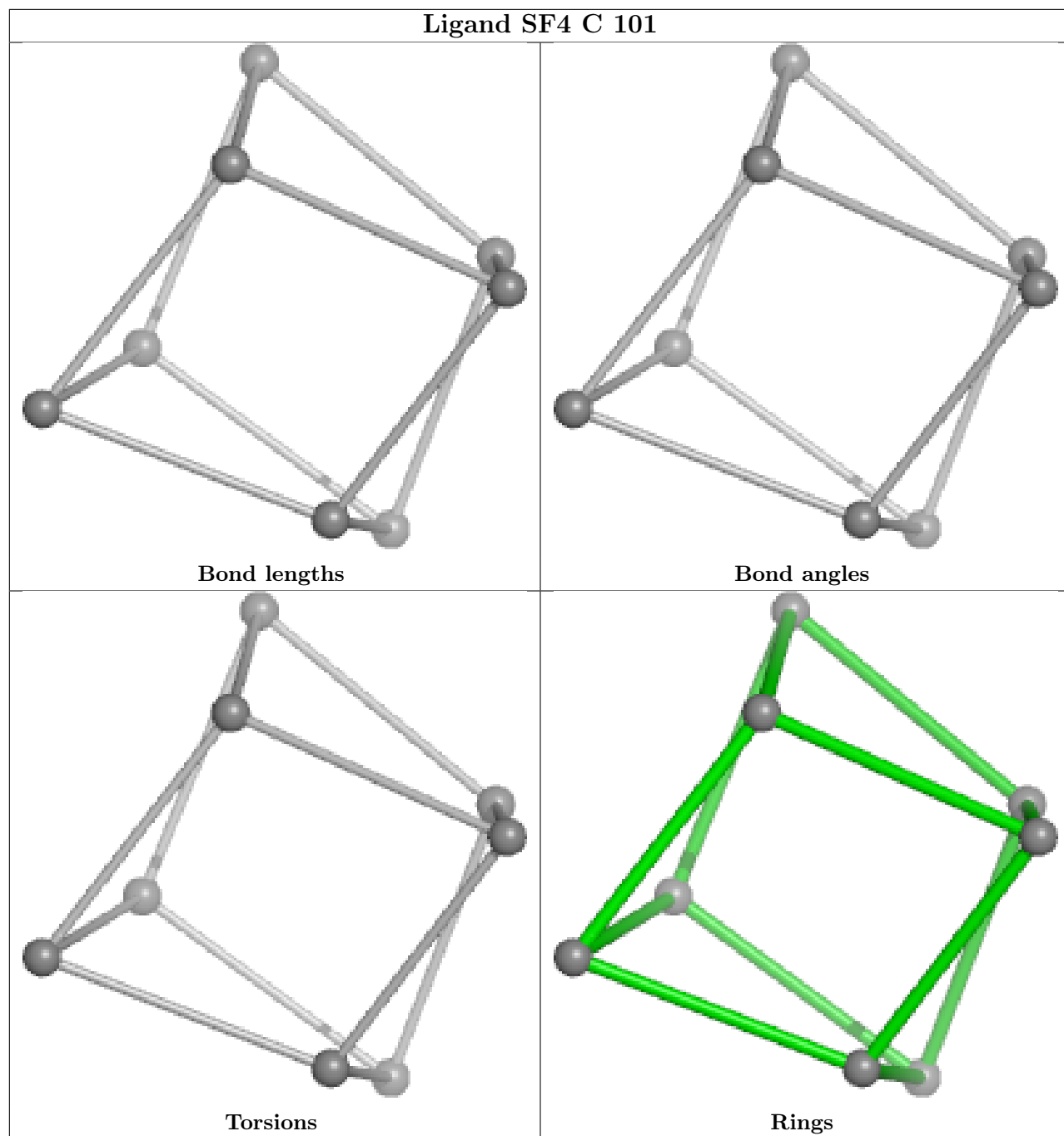


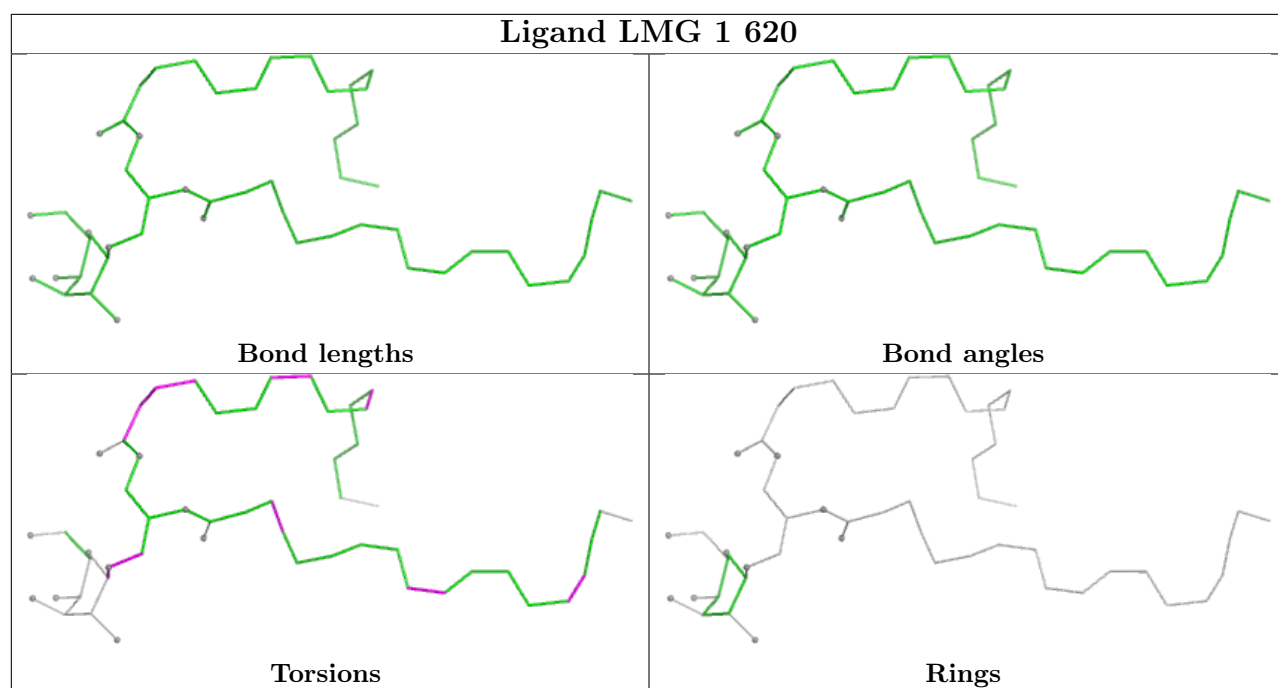
Torsions



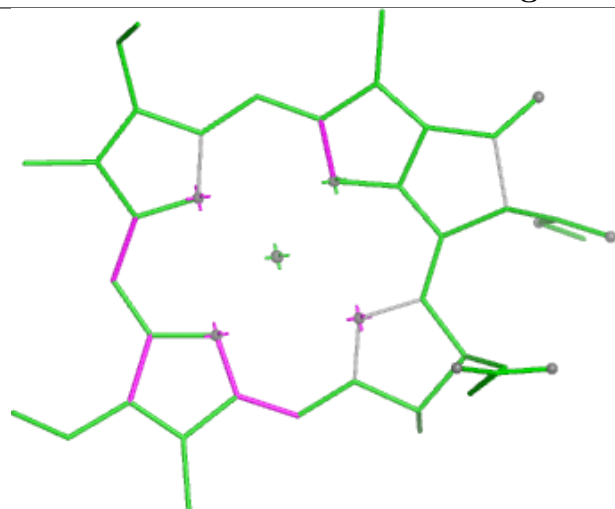
Rings



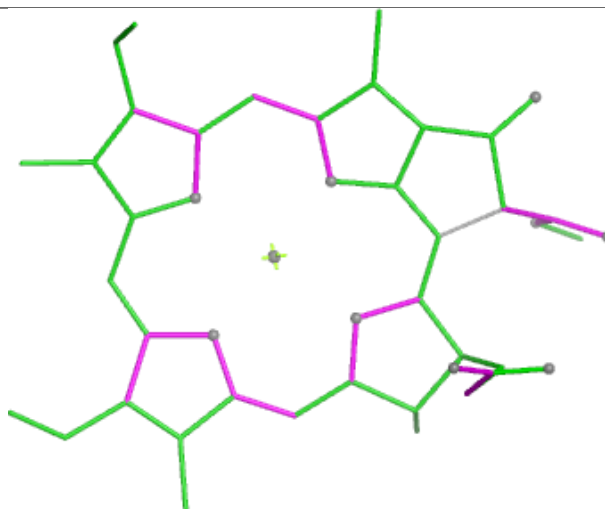




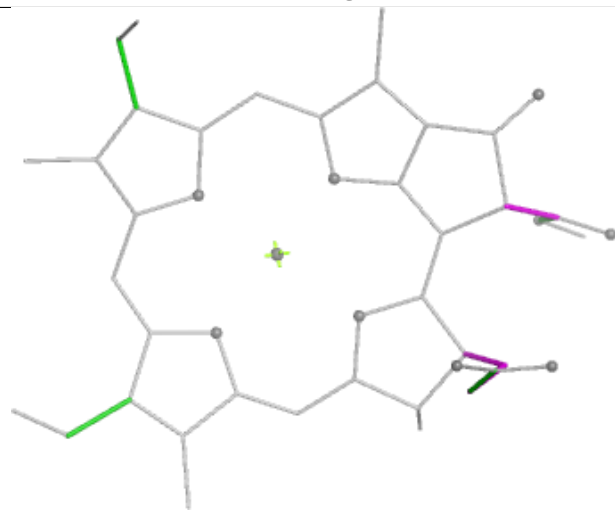
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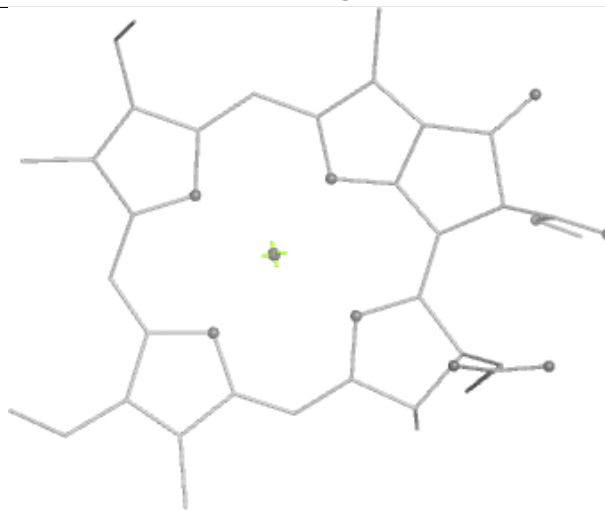
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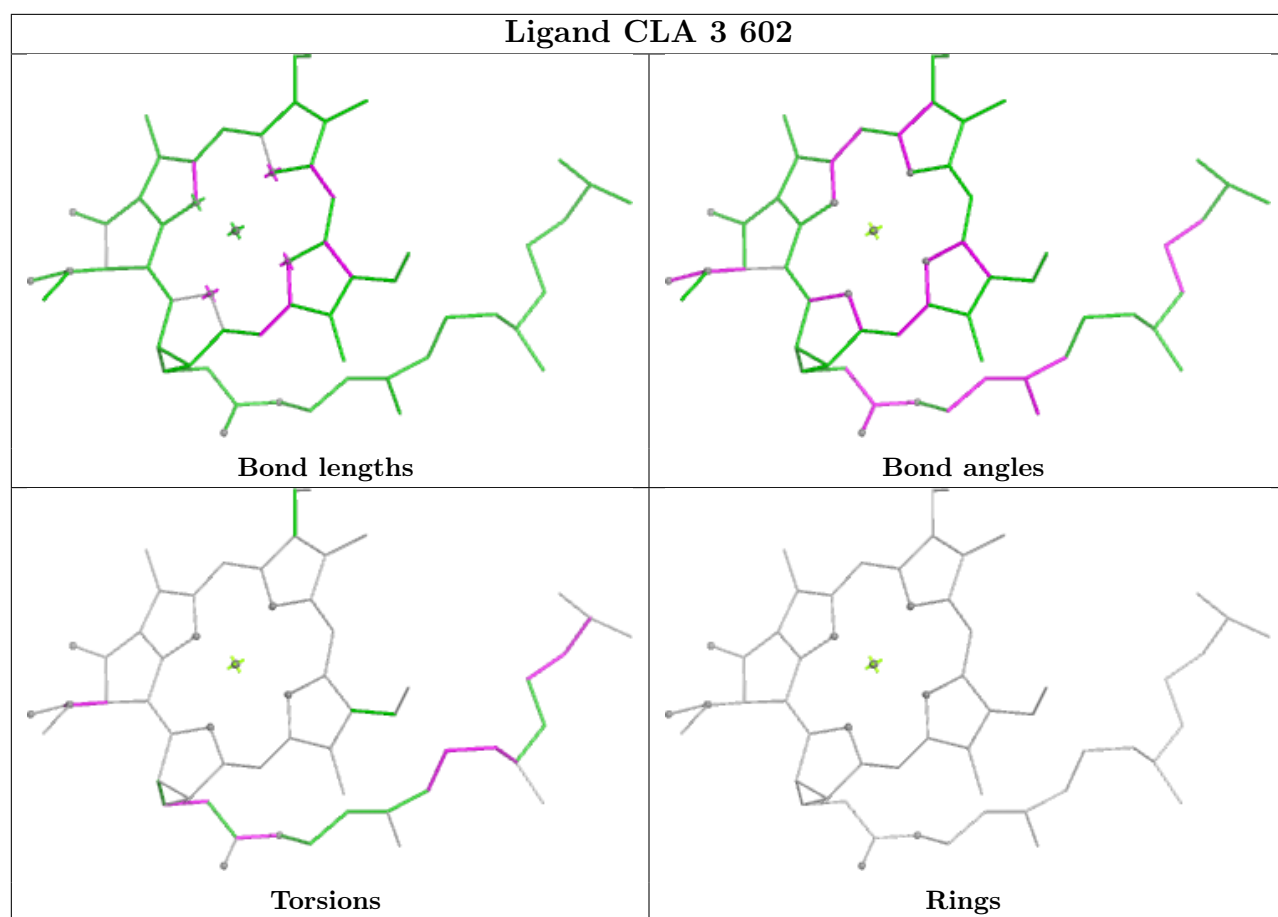
Bond angles



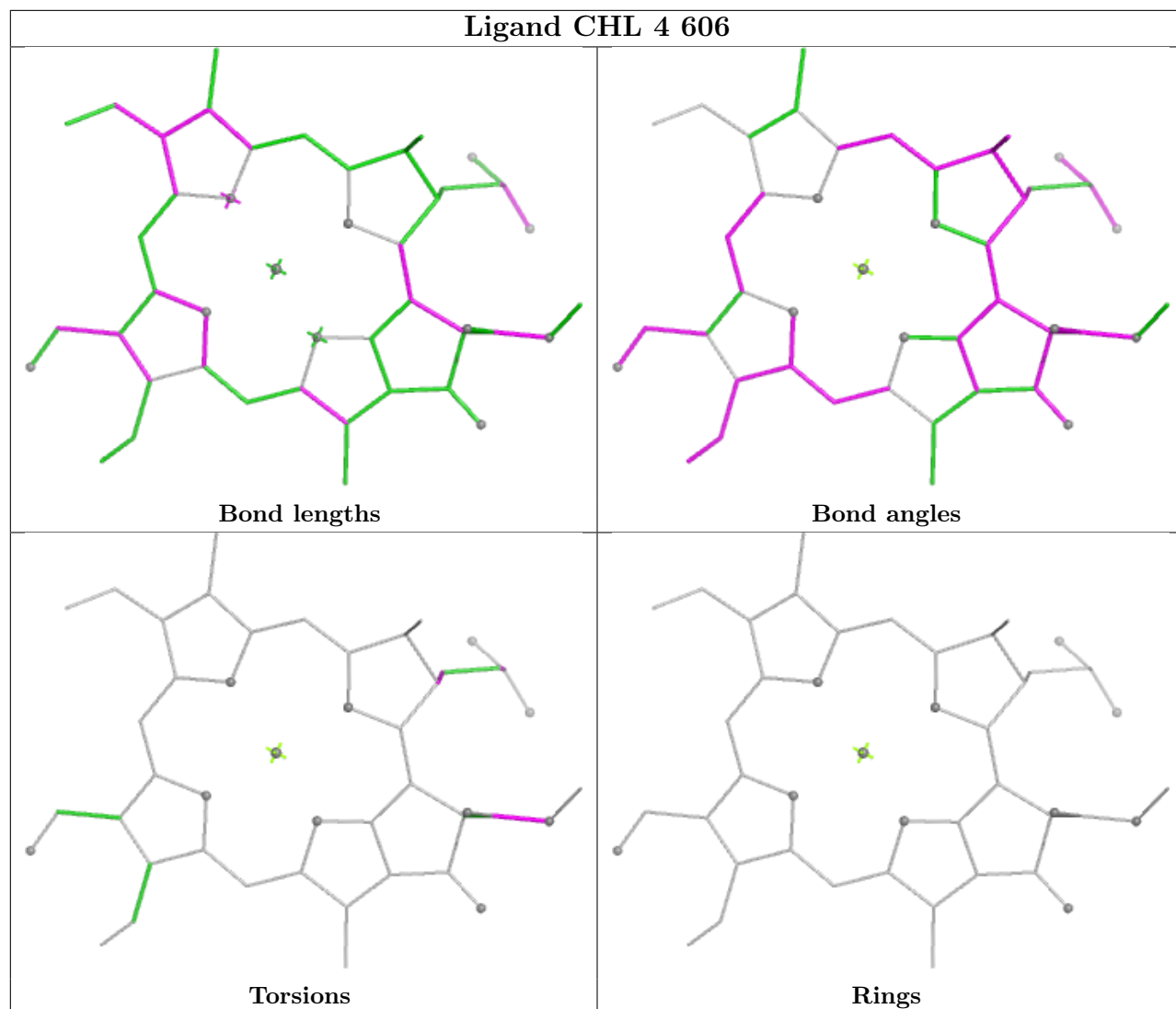
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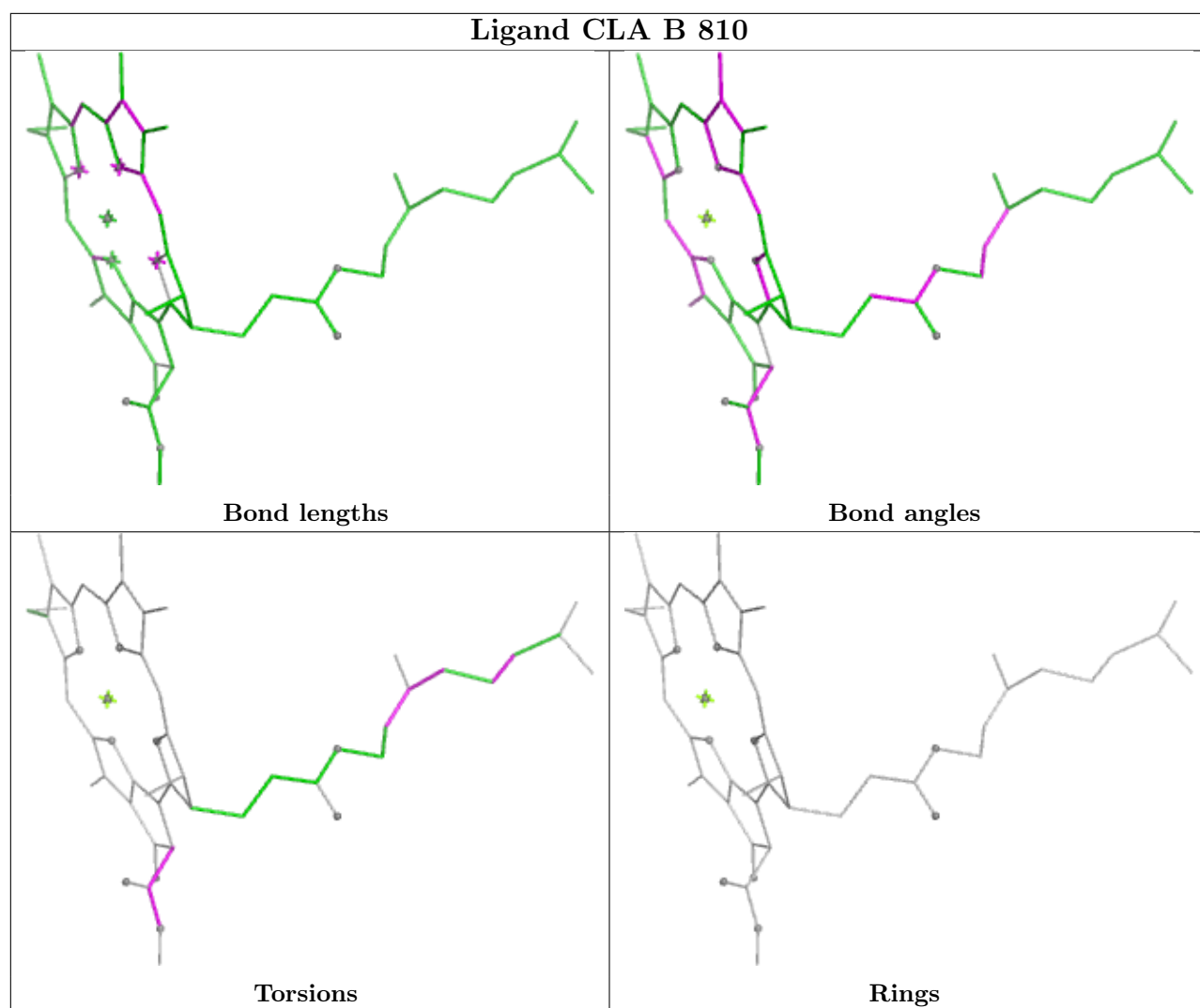


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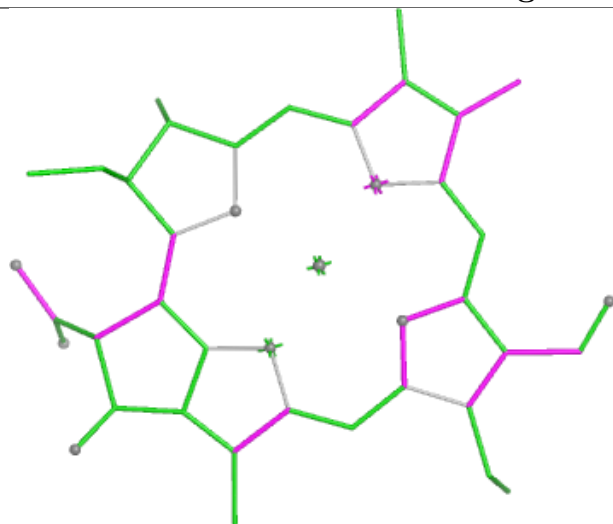


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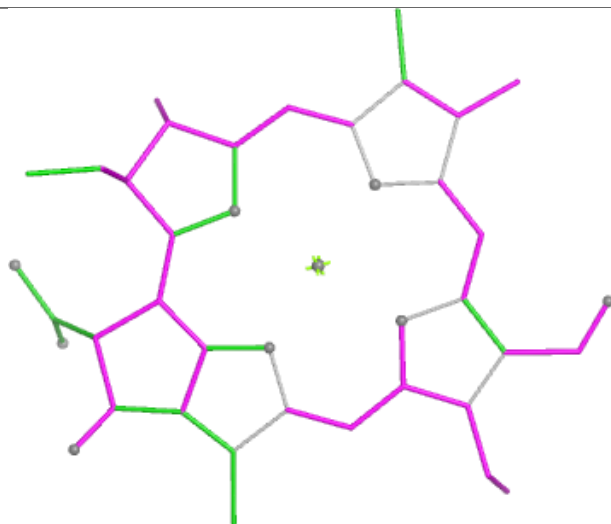




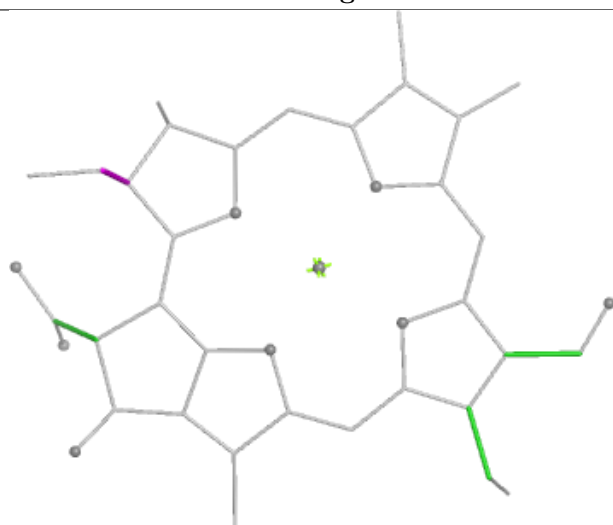
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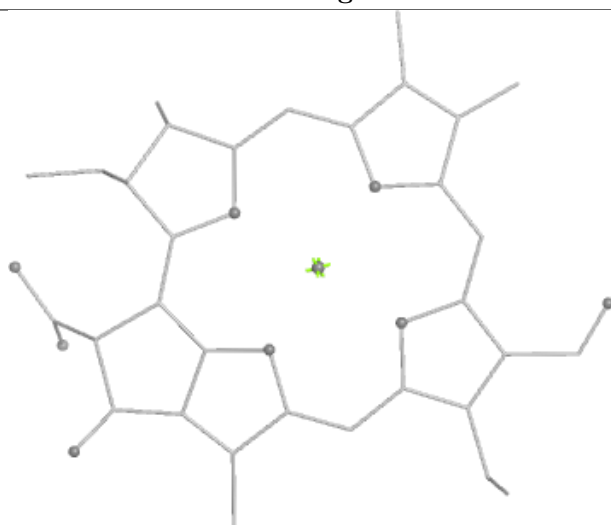
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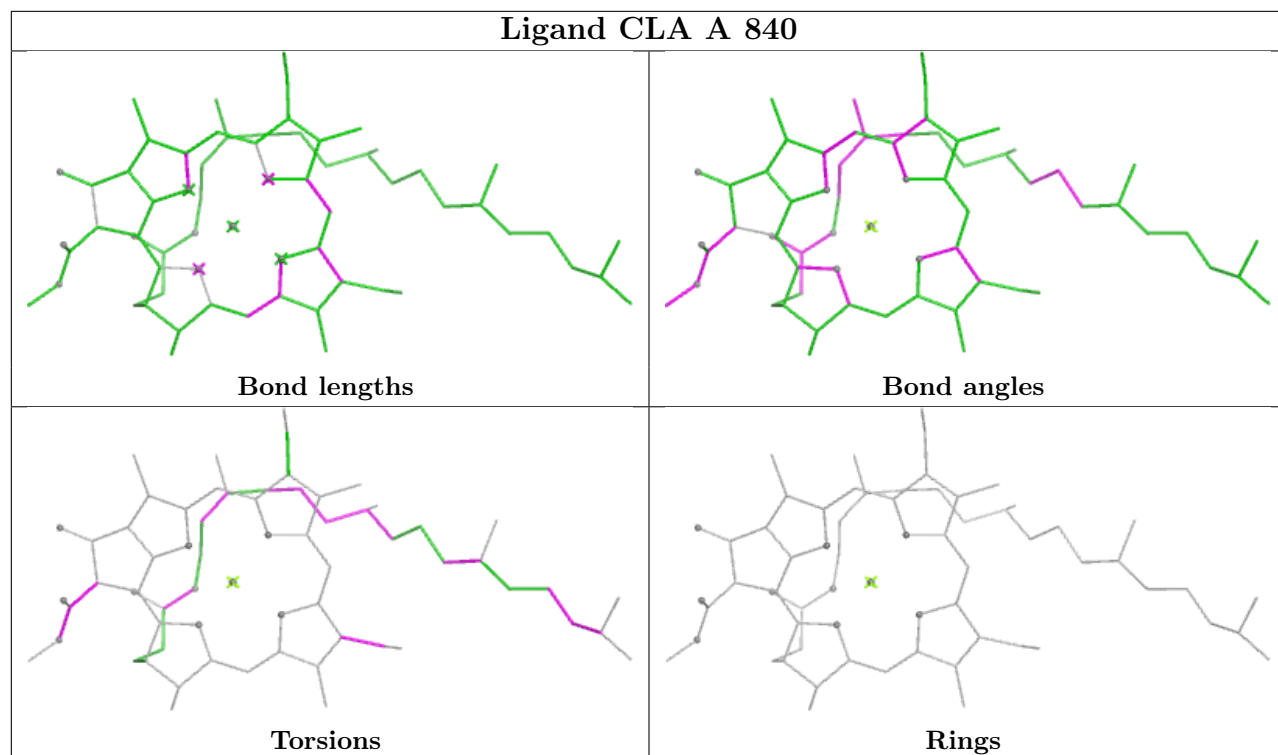
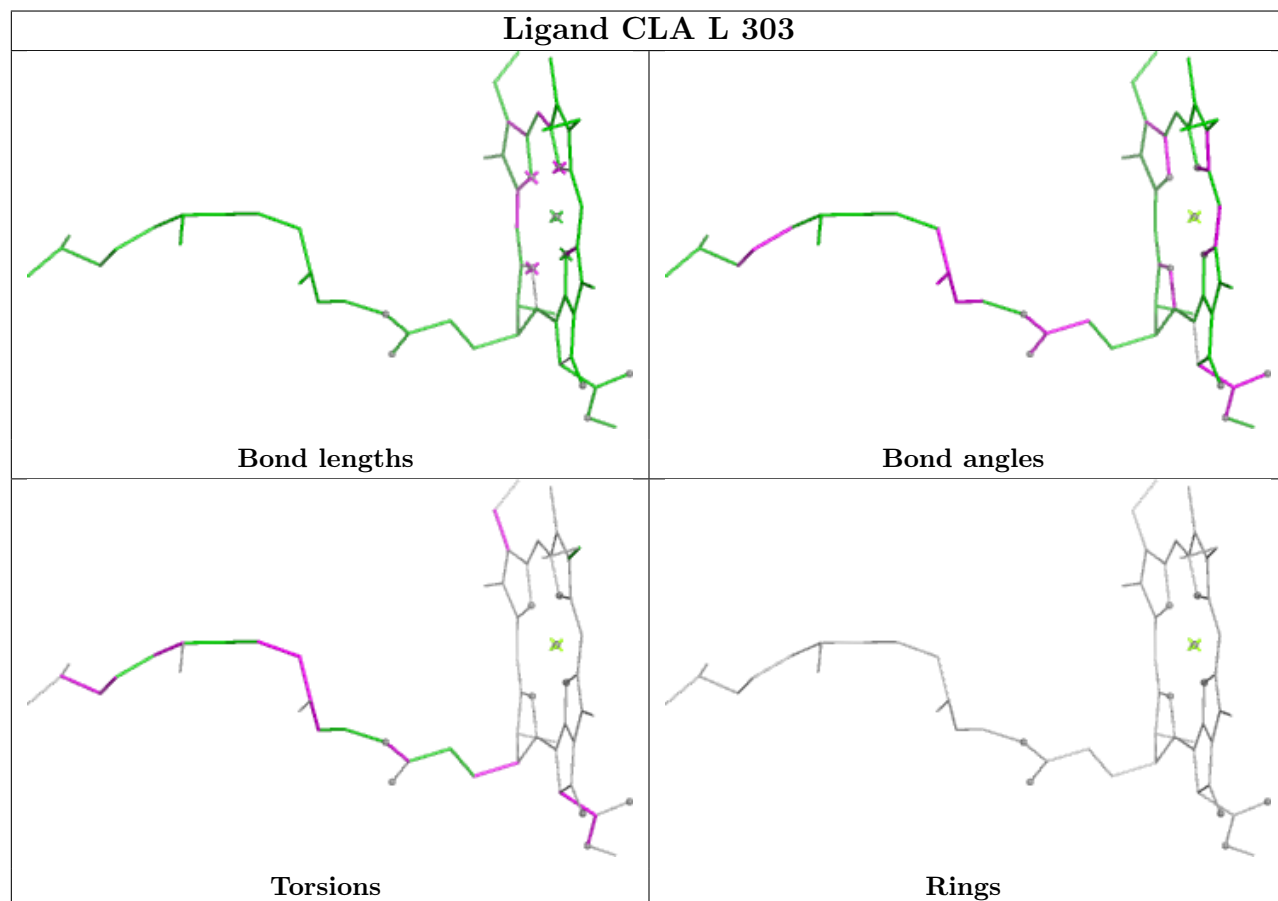
Bond angles



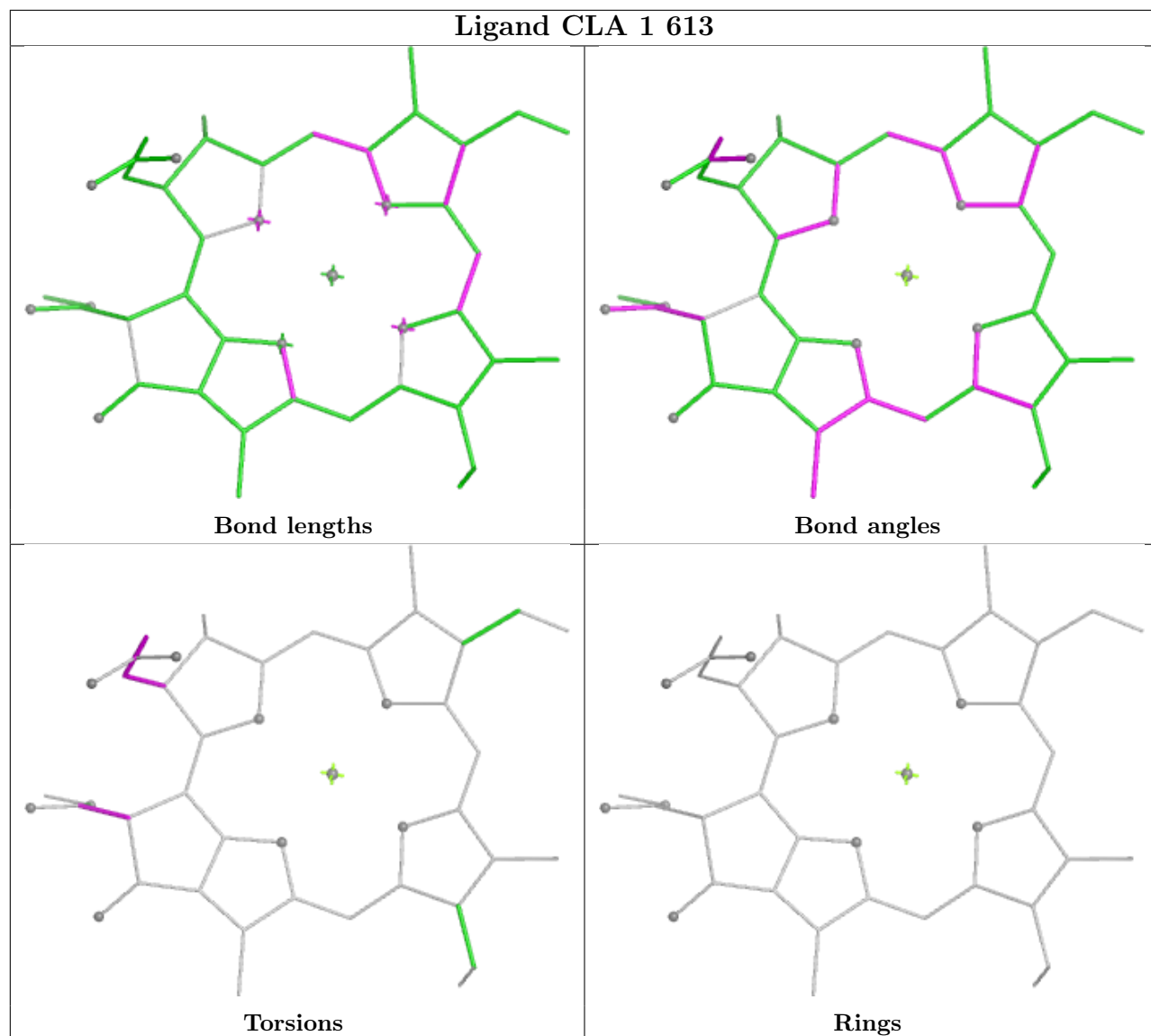
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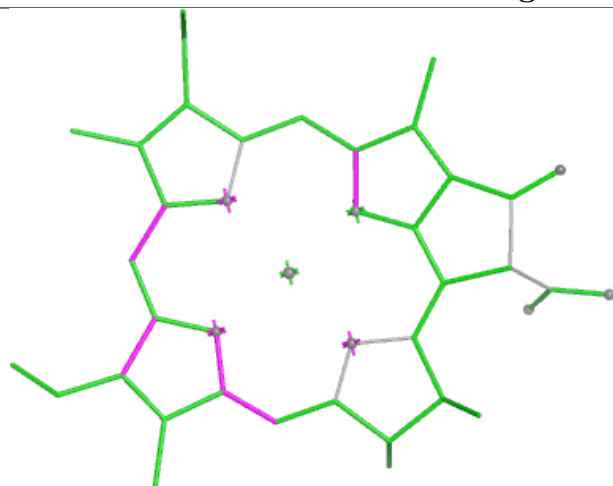
Rings

Ligand CLA A 840**Ligand CLA L 303**

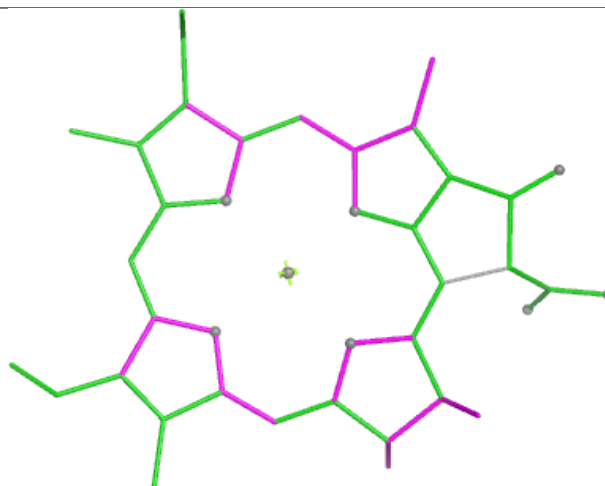
Ligand CLA 1 613



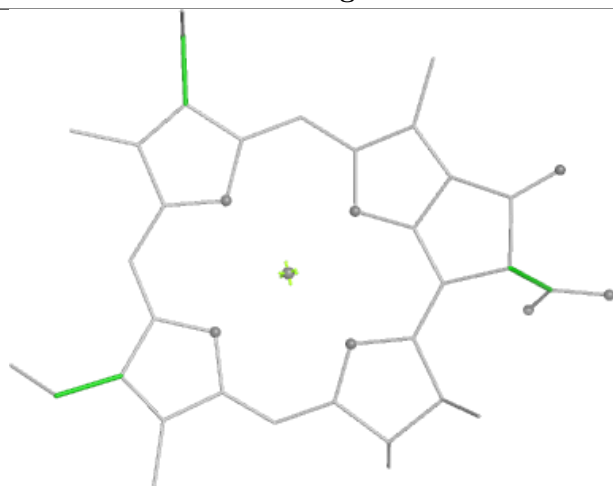
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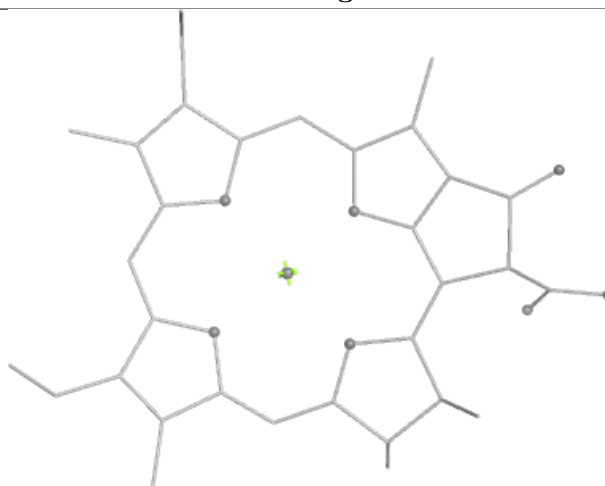
Bond lengths



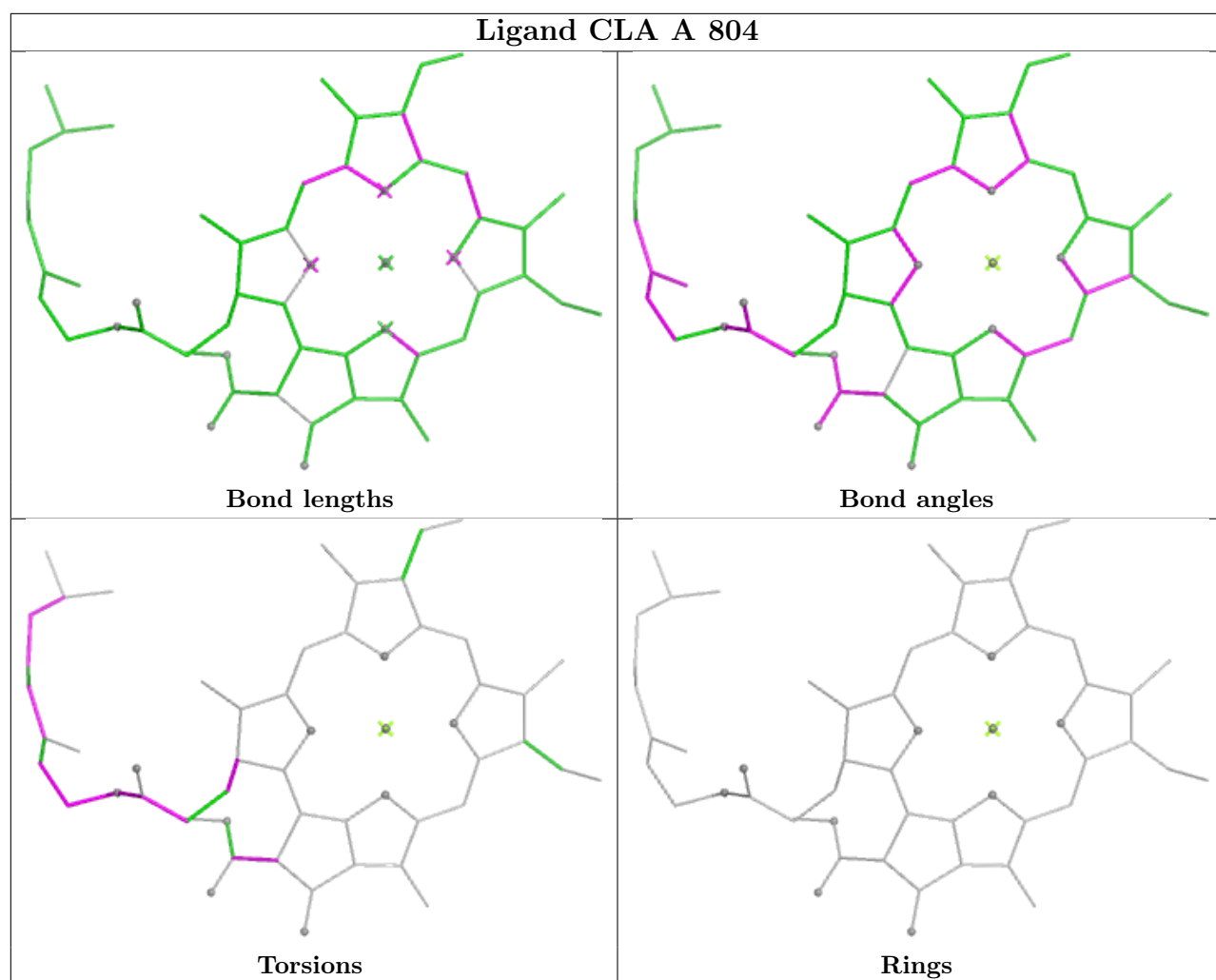
Bond angles

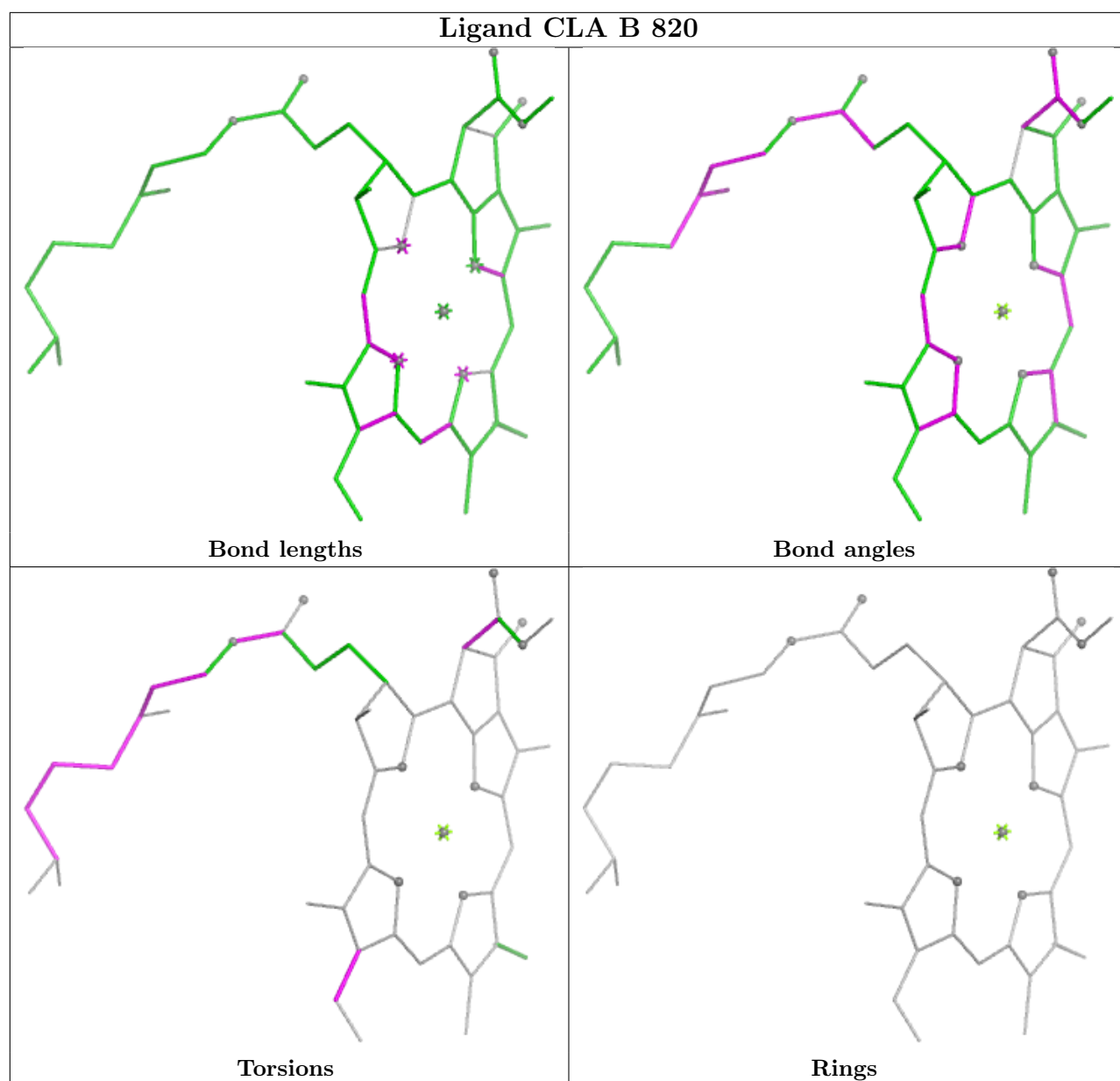


Torsions

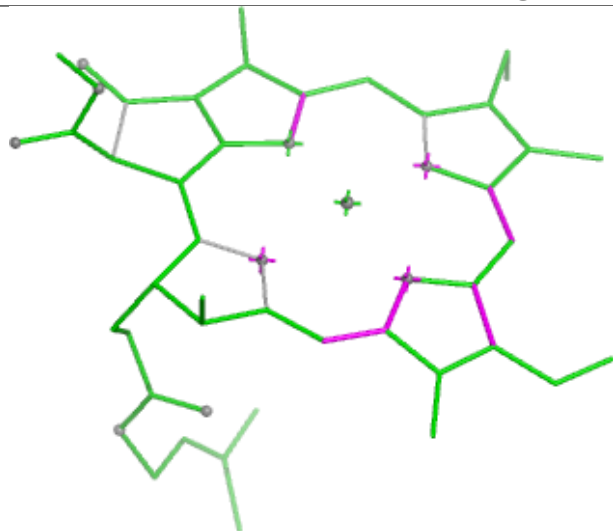


Rings

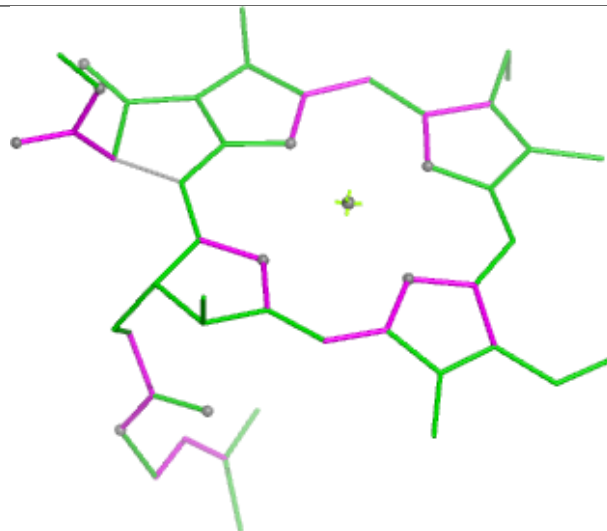




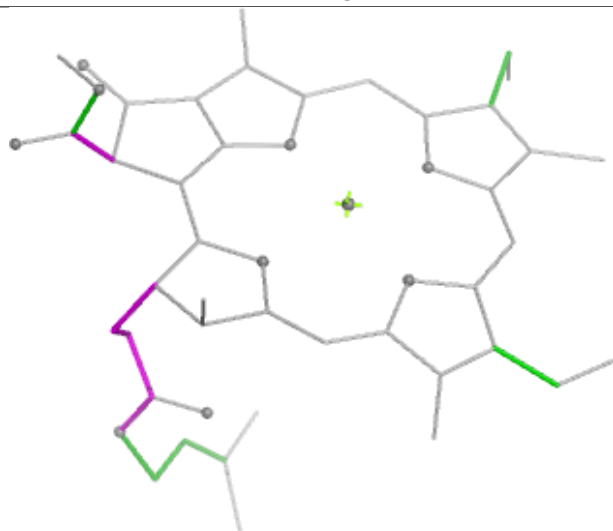
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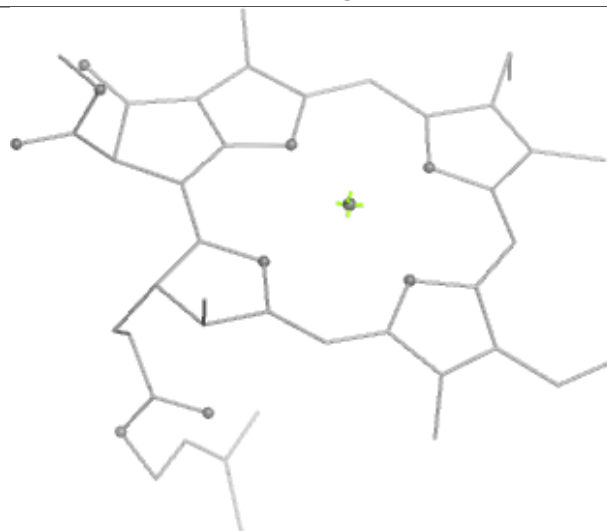
Bond lengths



Bond angles

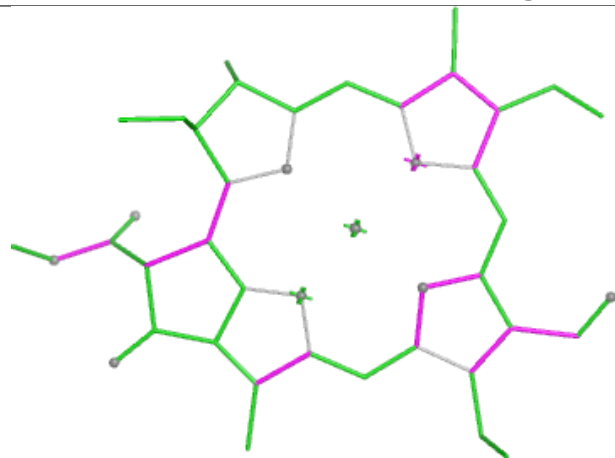


Torsions

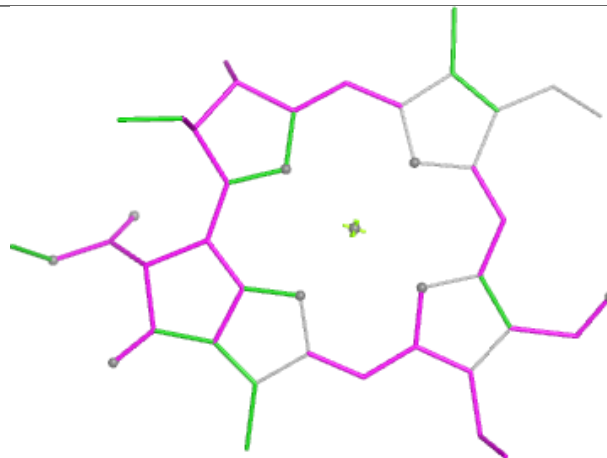


Rings

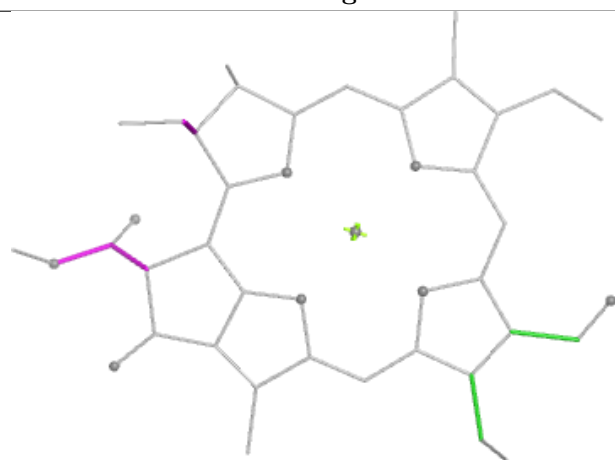
Ligand CHL 2 614



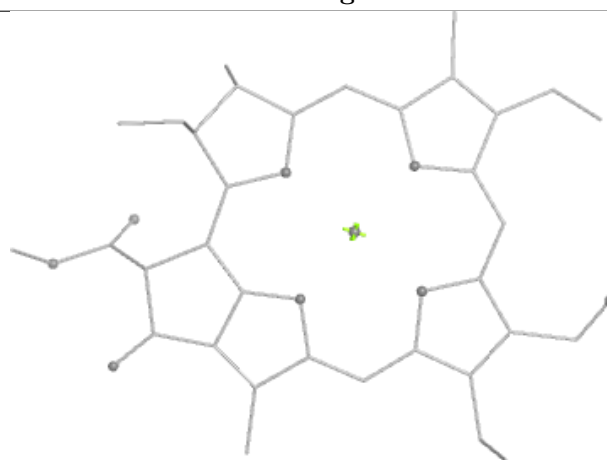
Bond lengths



Bond angles

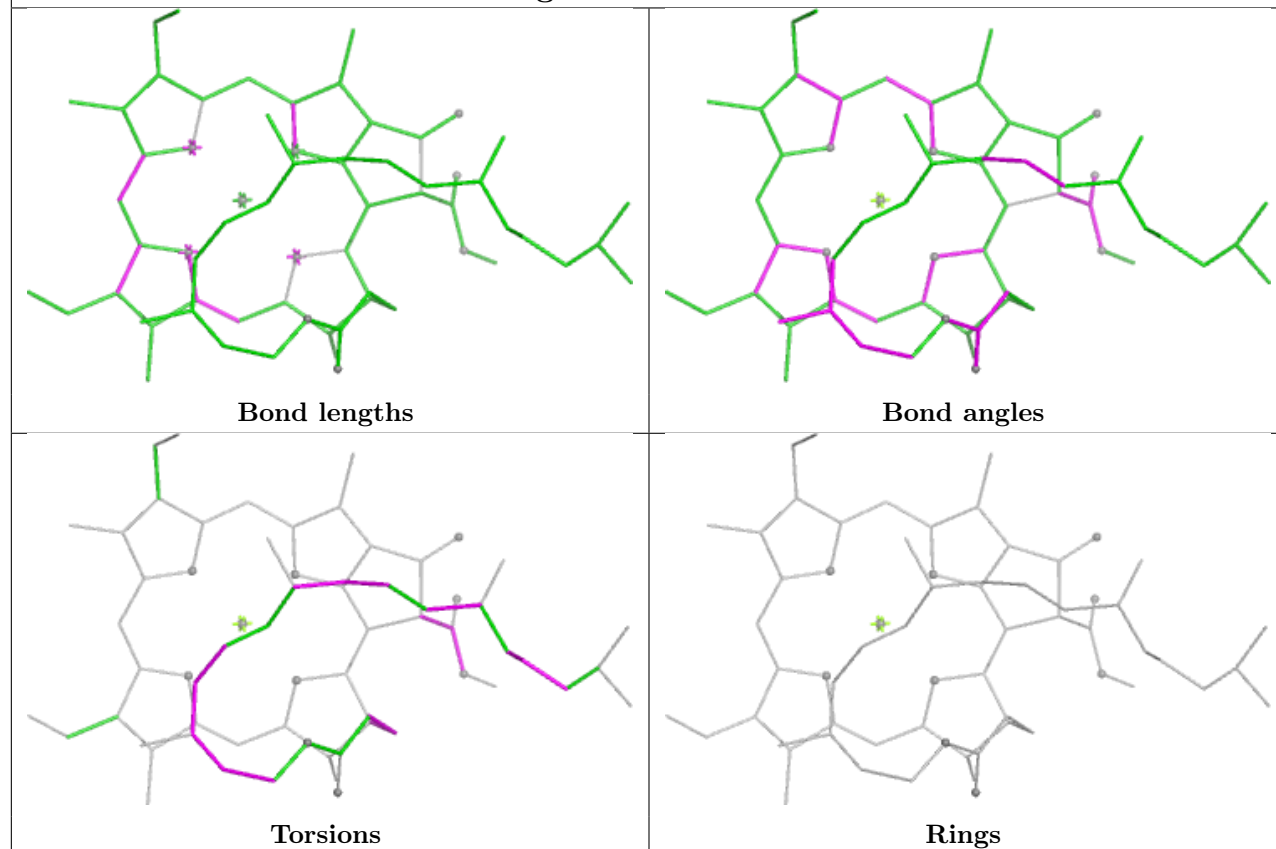


Torsions

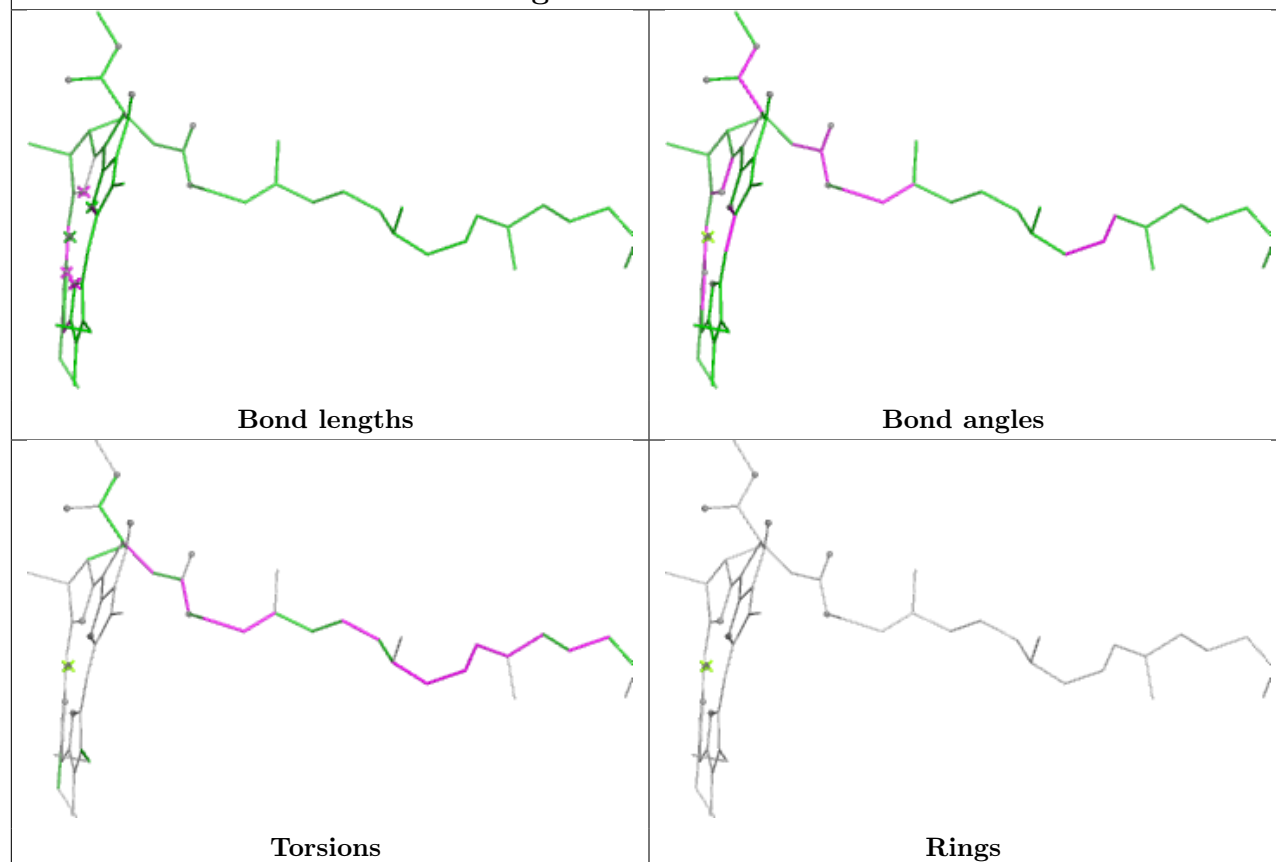


Rings

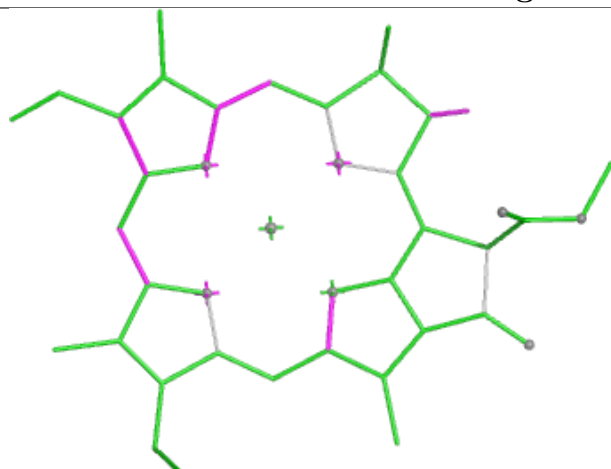
Ligand CLA 2 604



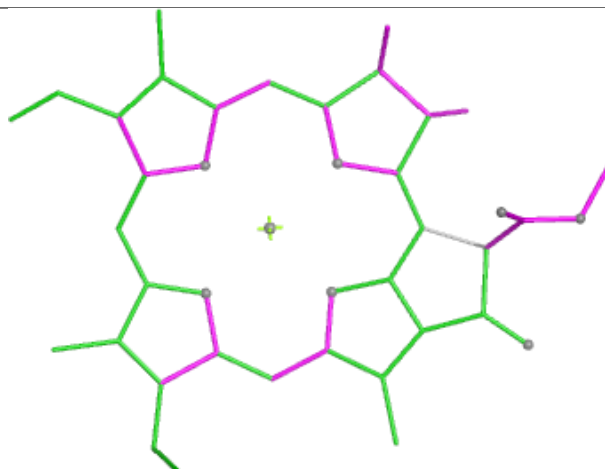
Ligand CLA A 828



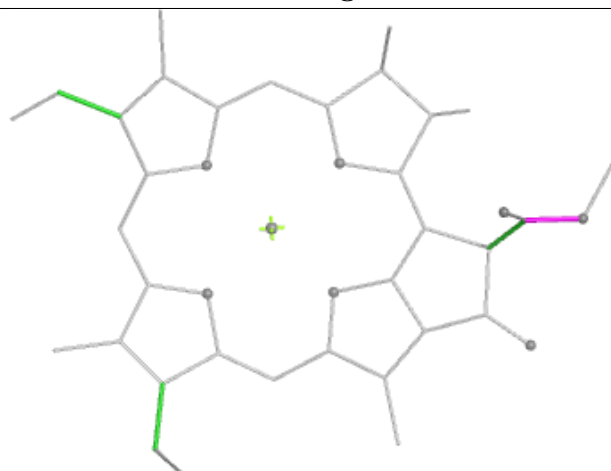
Ligand CLA F 304



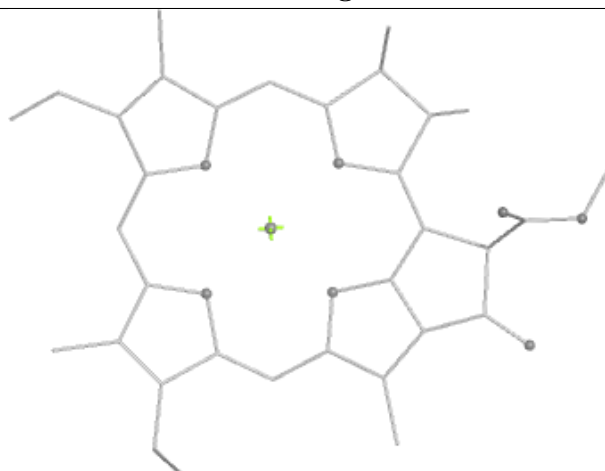
Bond lengths



Bond angles

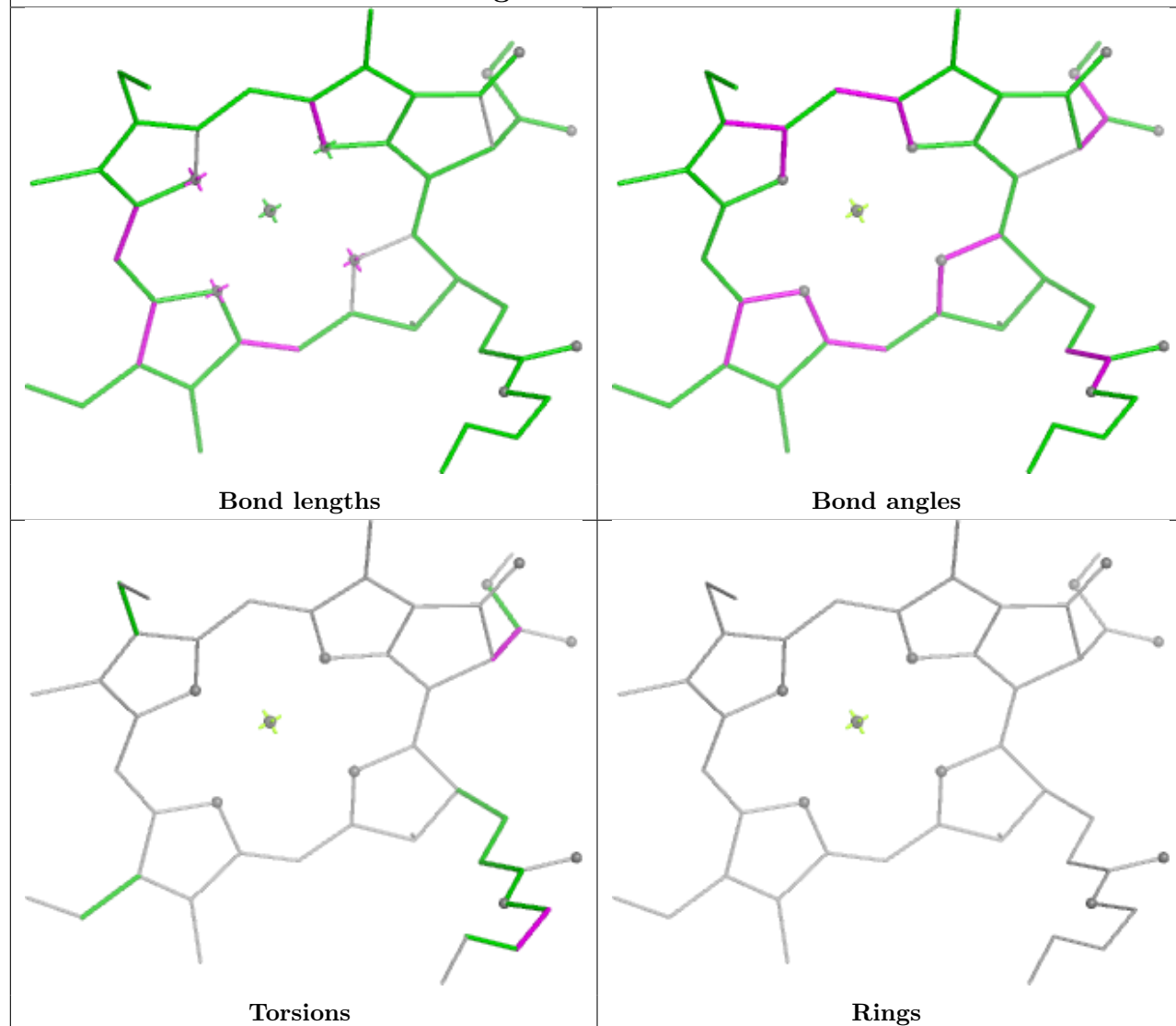


Torsions

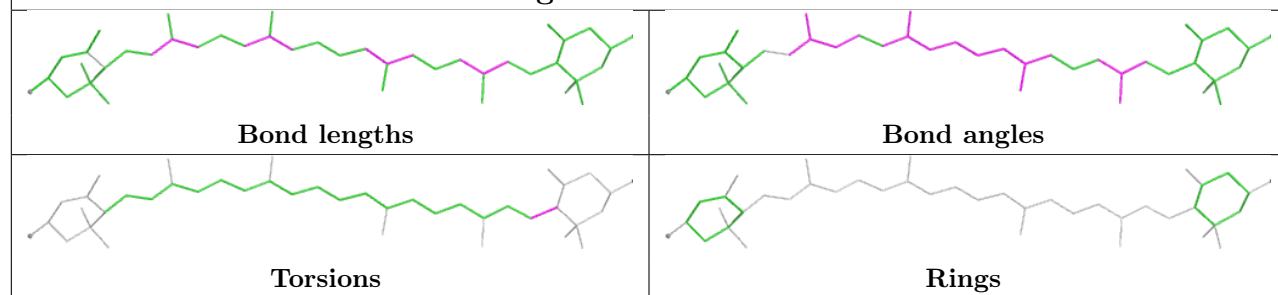


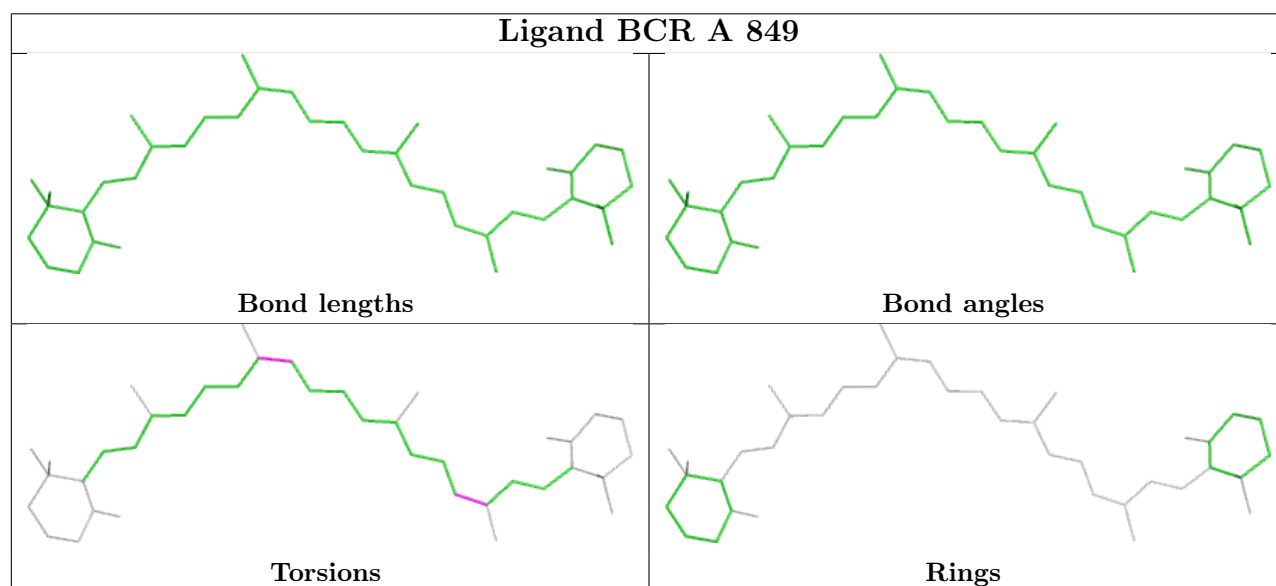
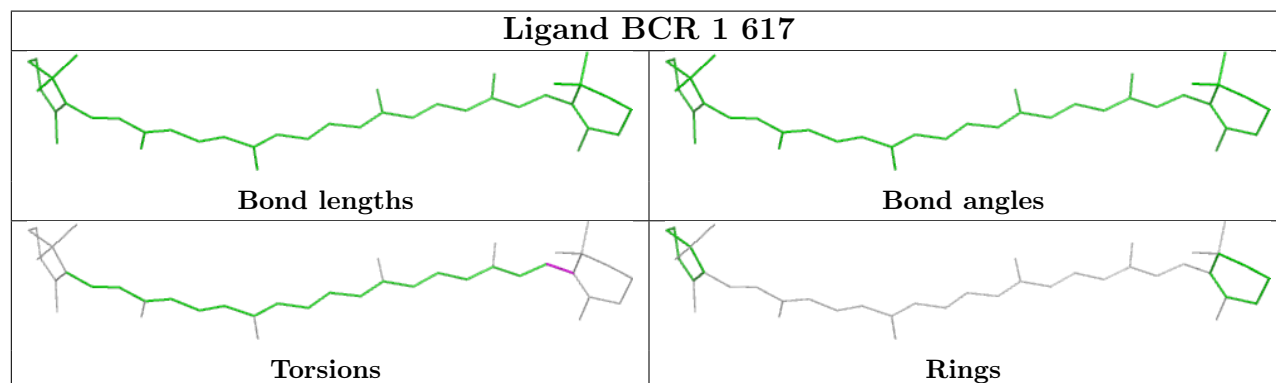
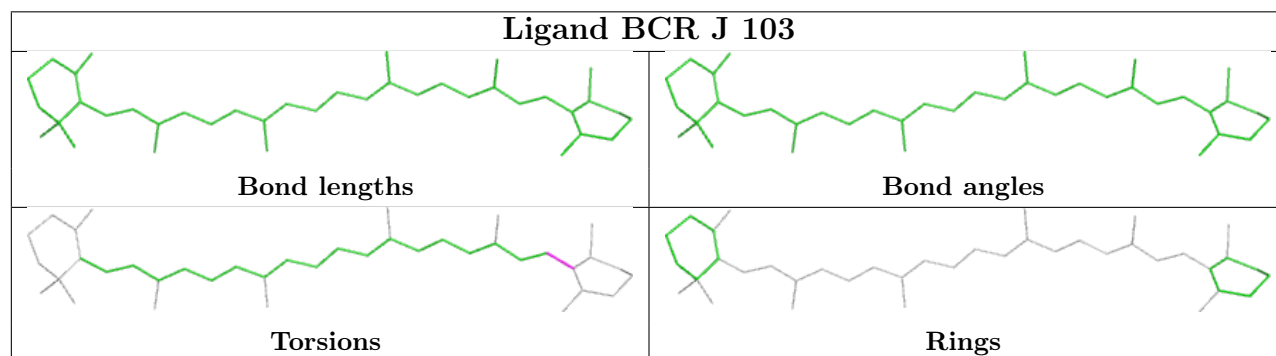
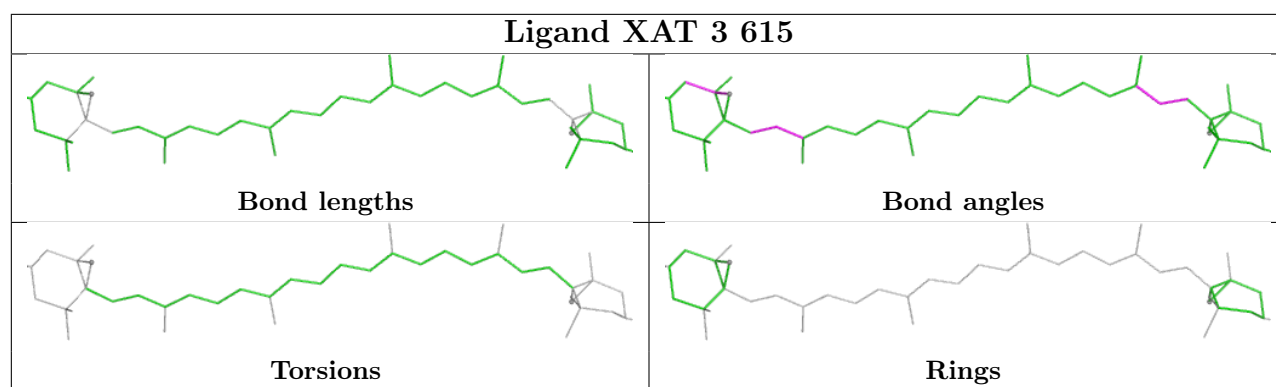
Rings

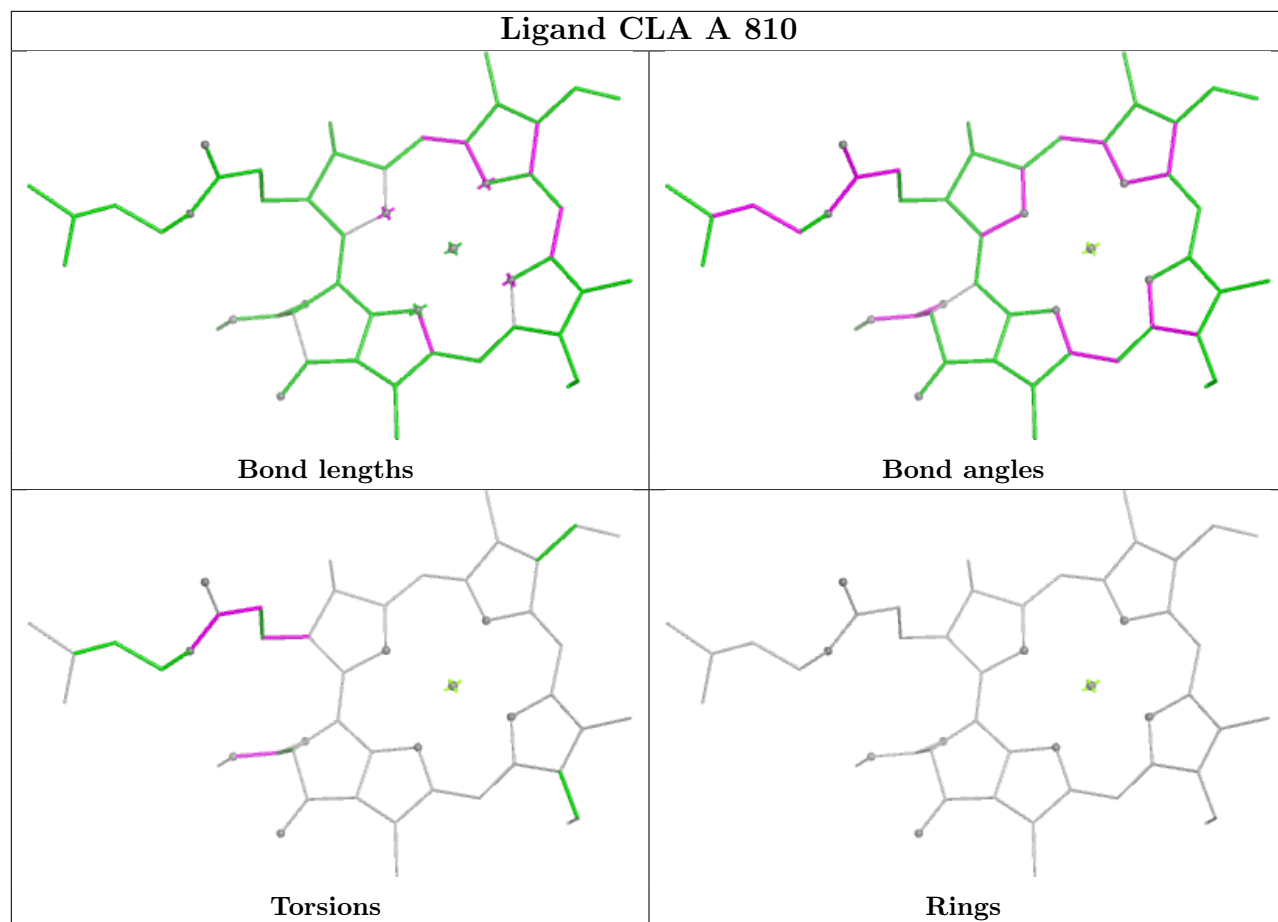
Ligand CLA 1 604

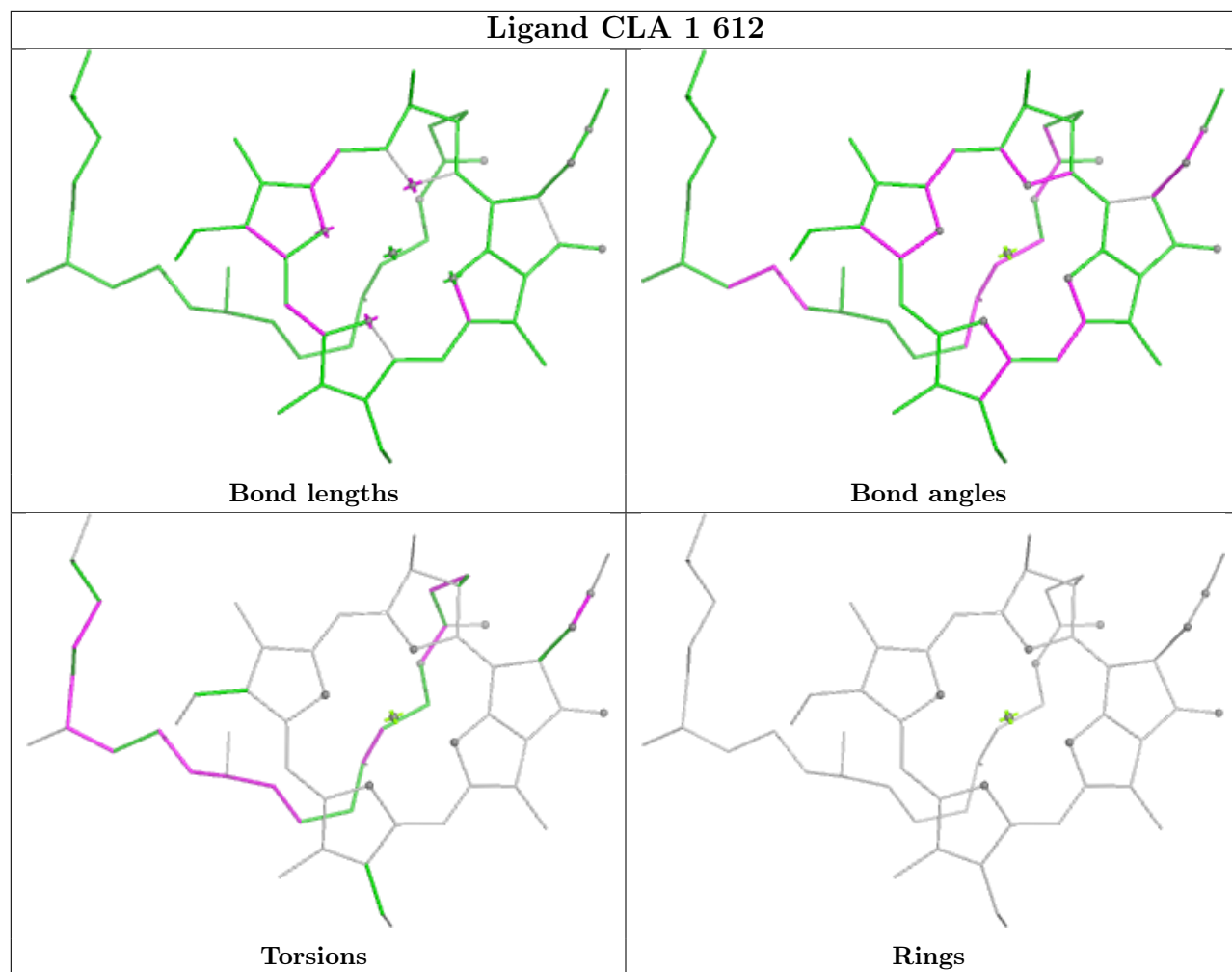


Ligand LUT 1 619

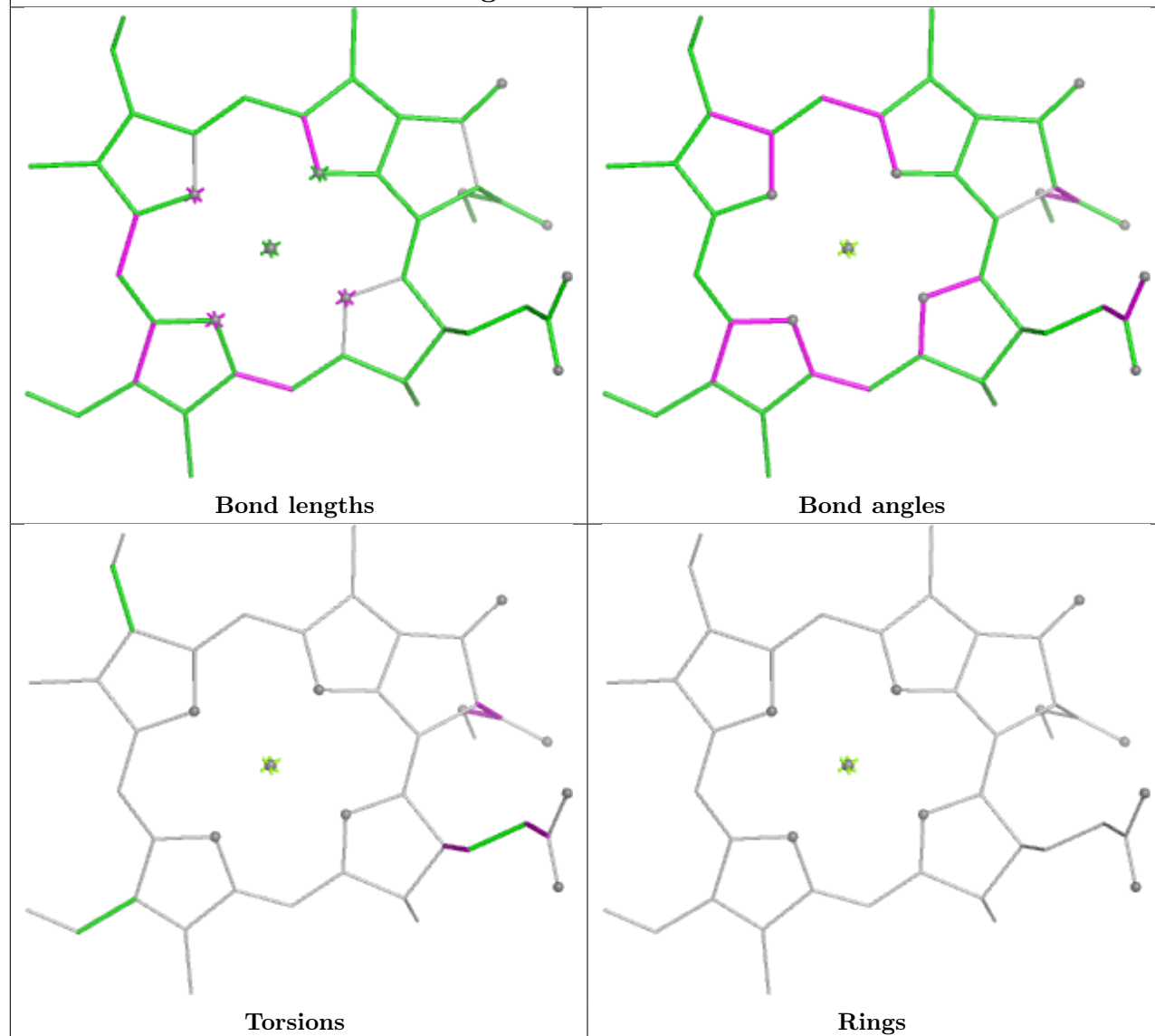




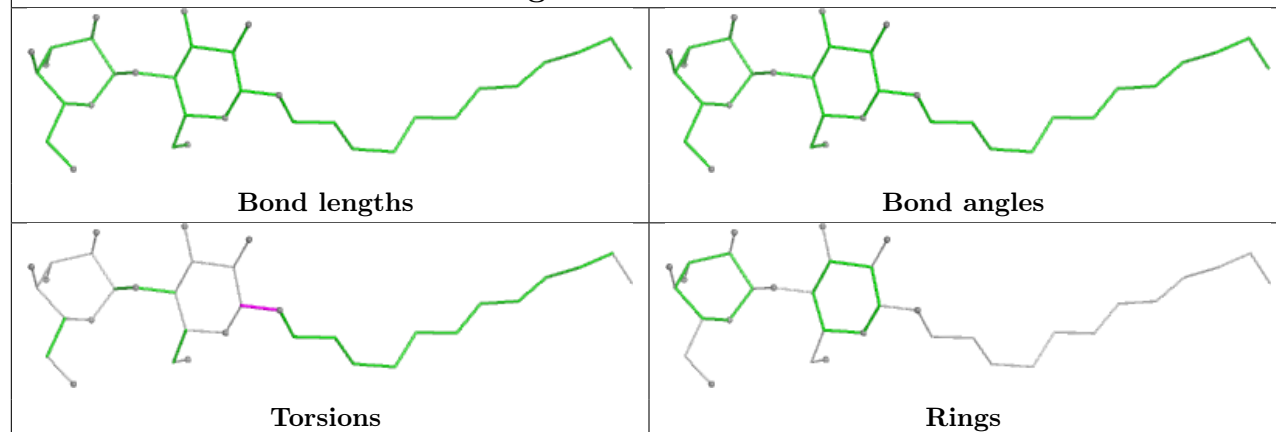


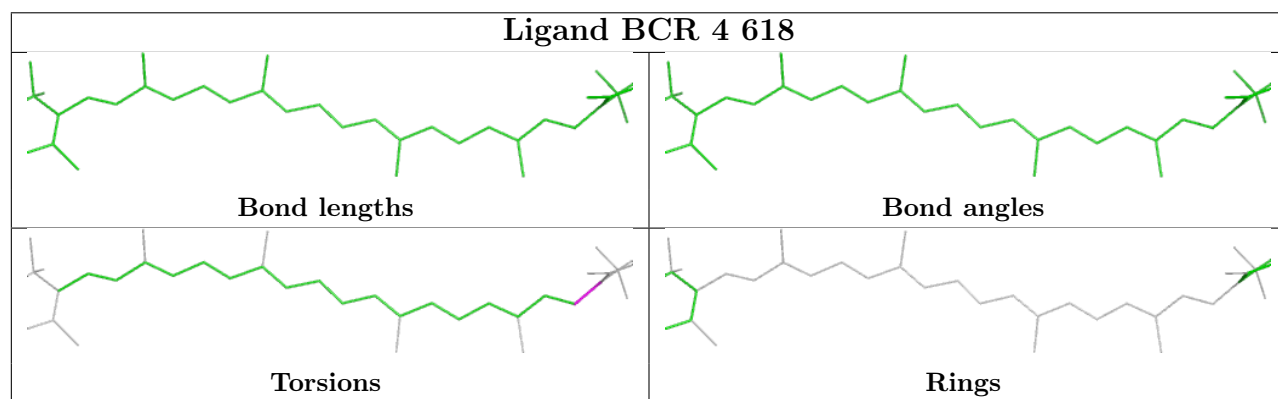
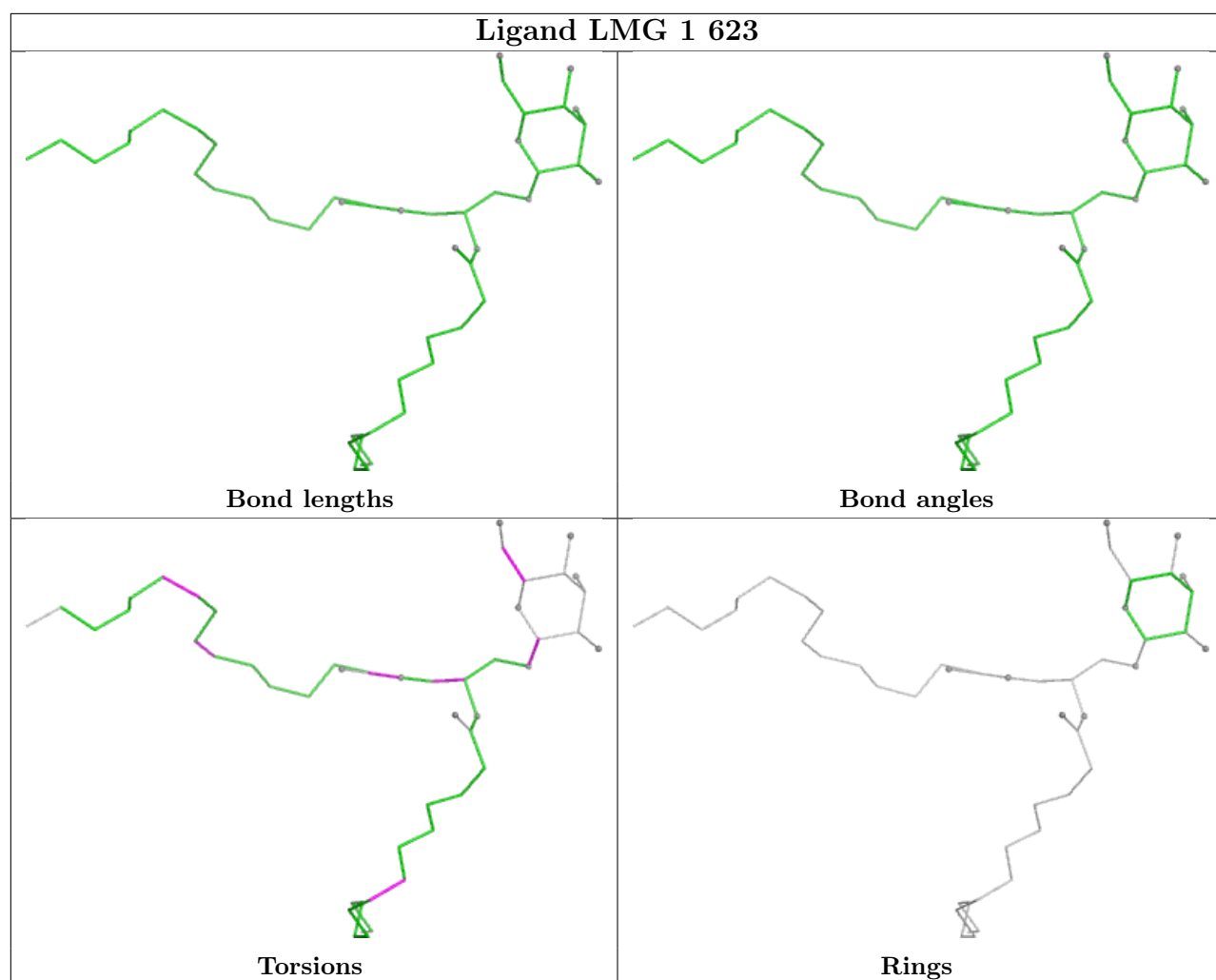


Ligand CLA K 202

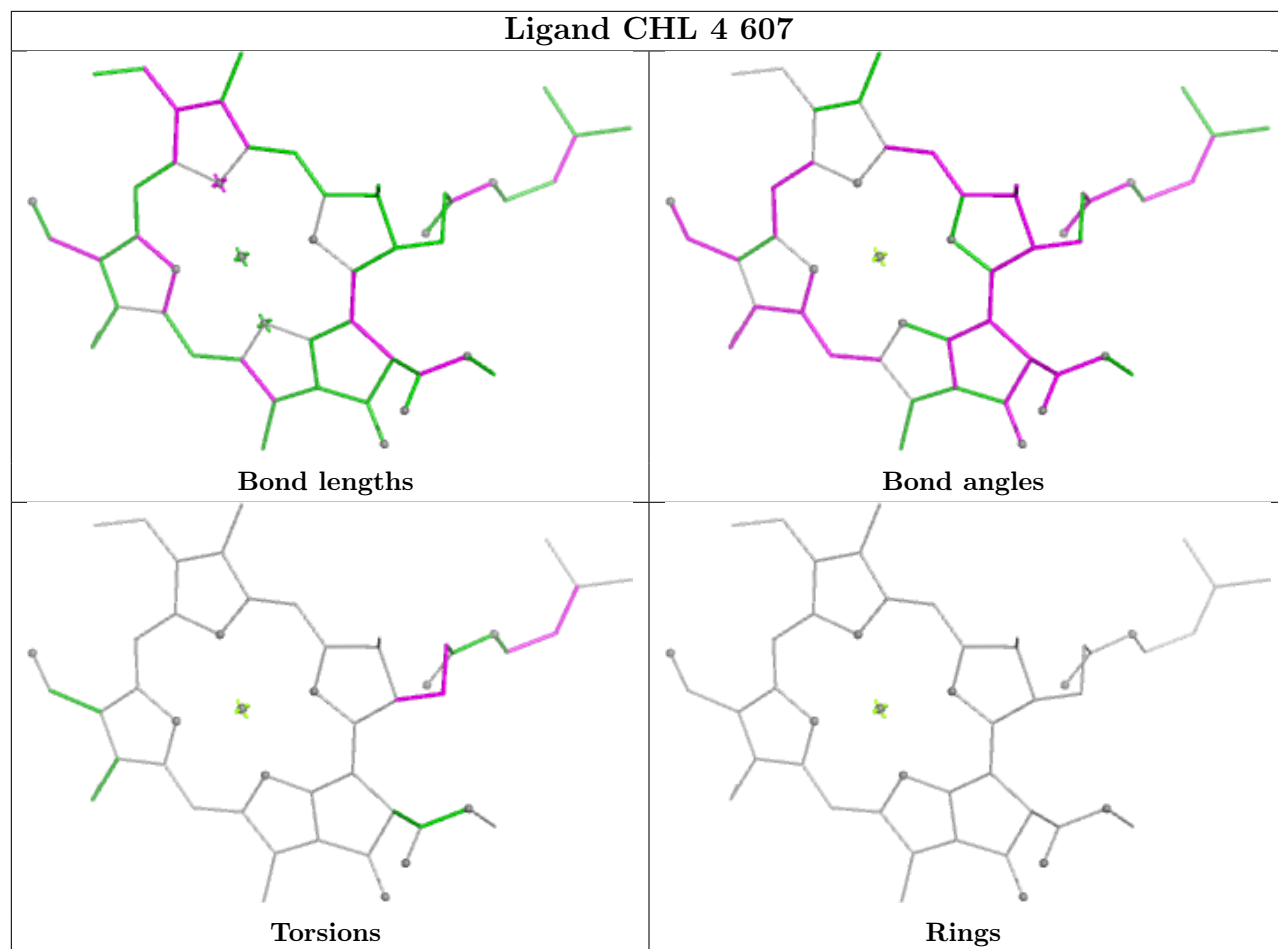


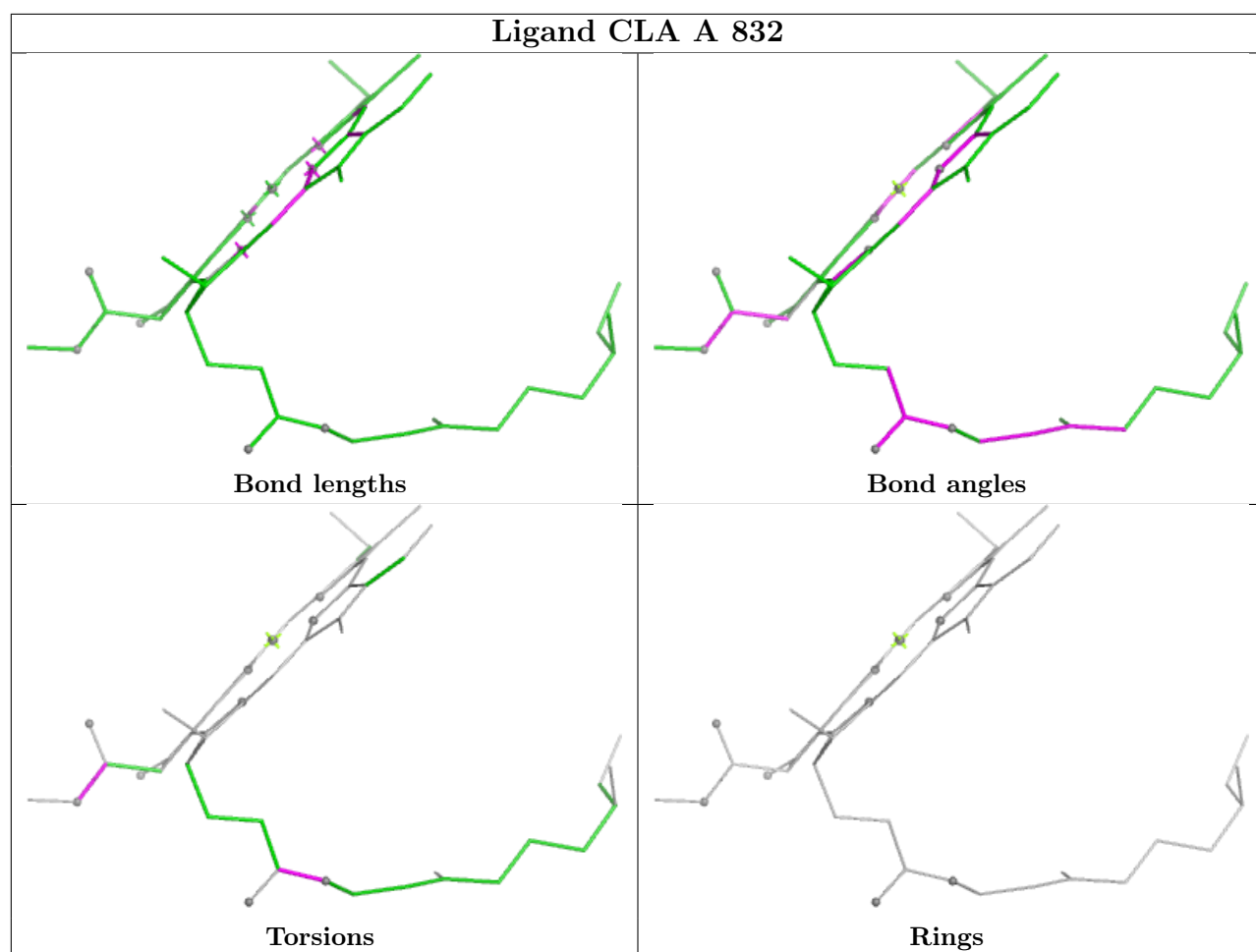
Ligand LMT G 201



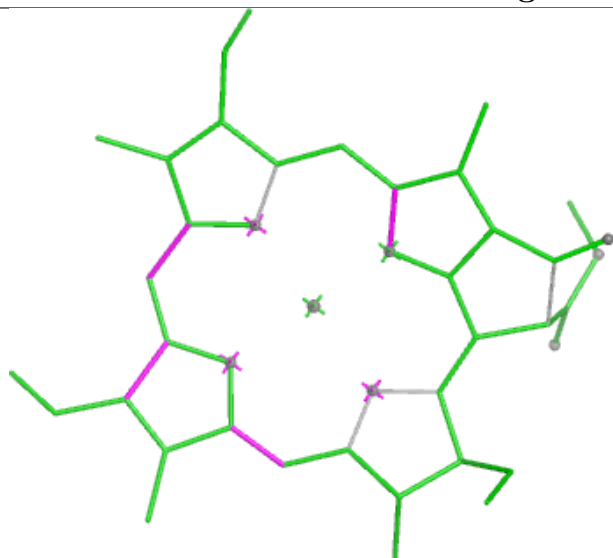


Ligand CHL 4 607

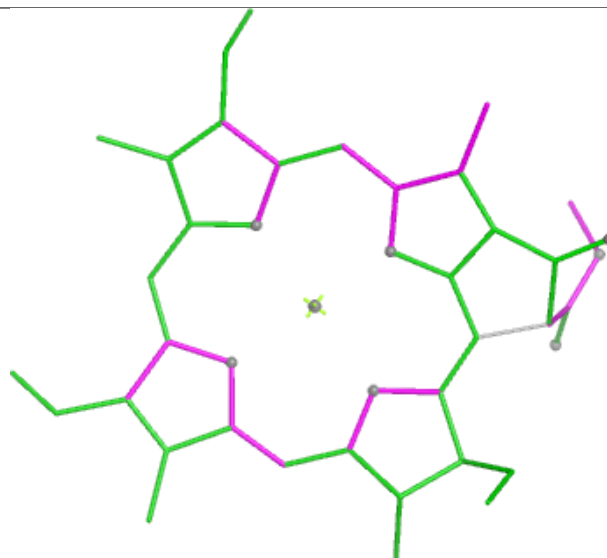




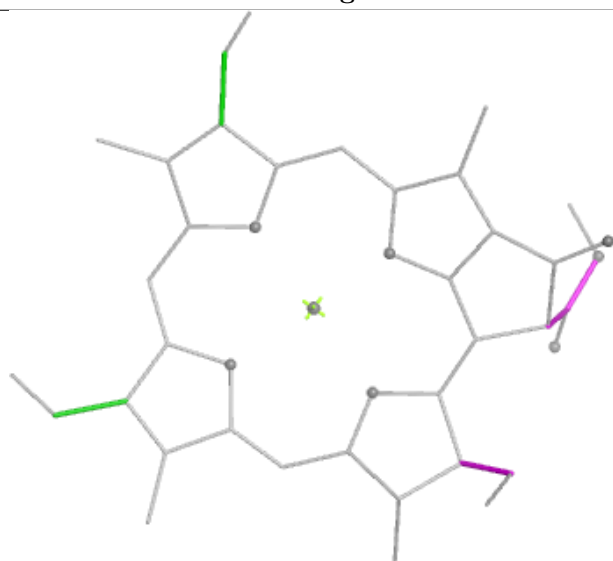
Ligand CLA J 102



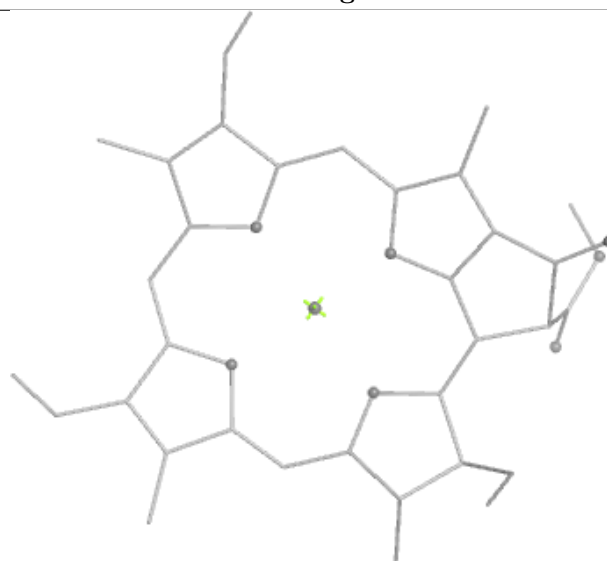
Bond lengths



Bond angles

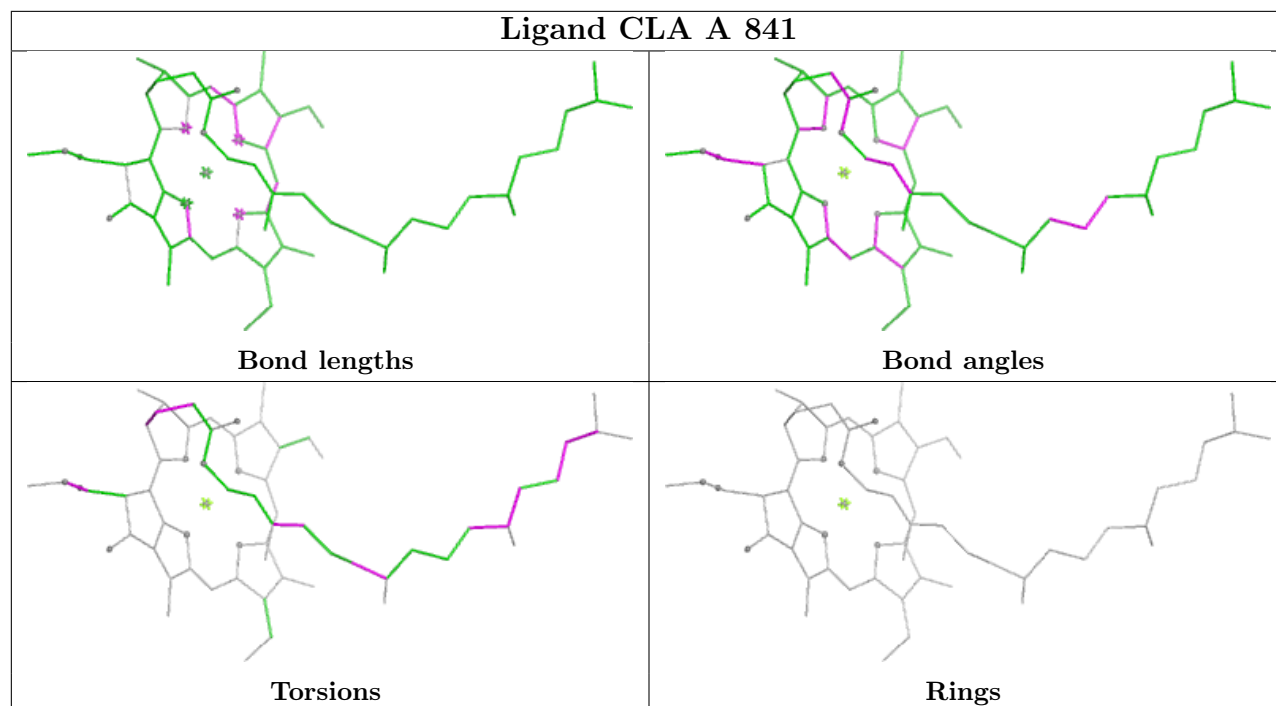


Torsions

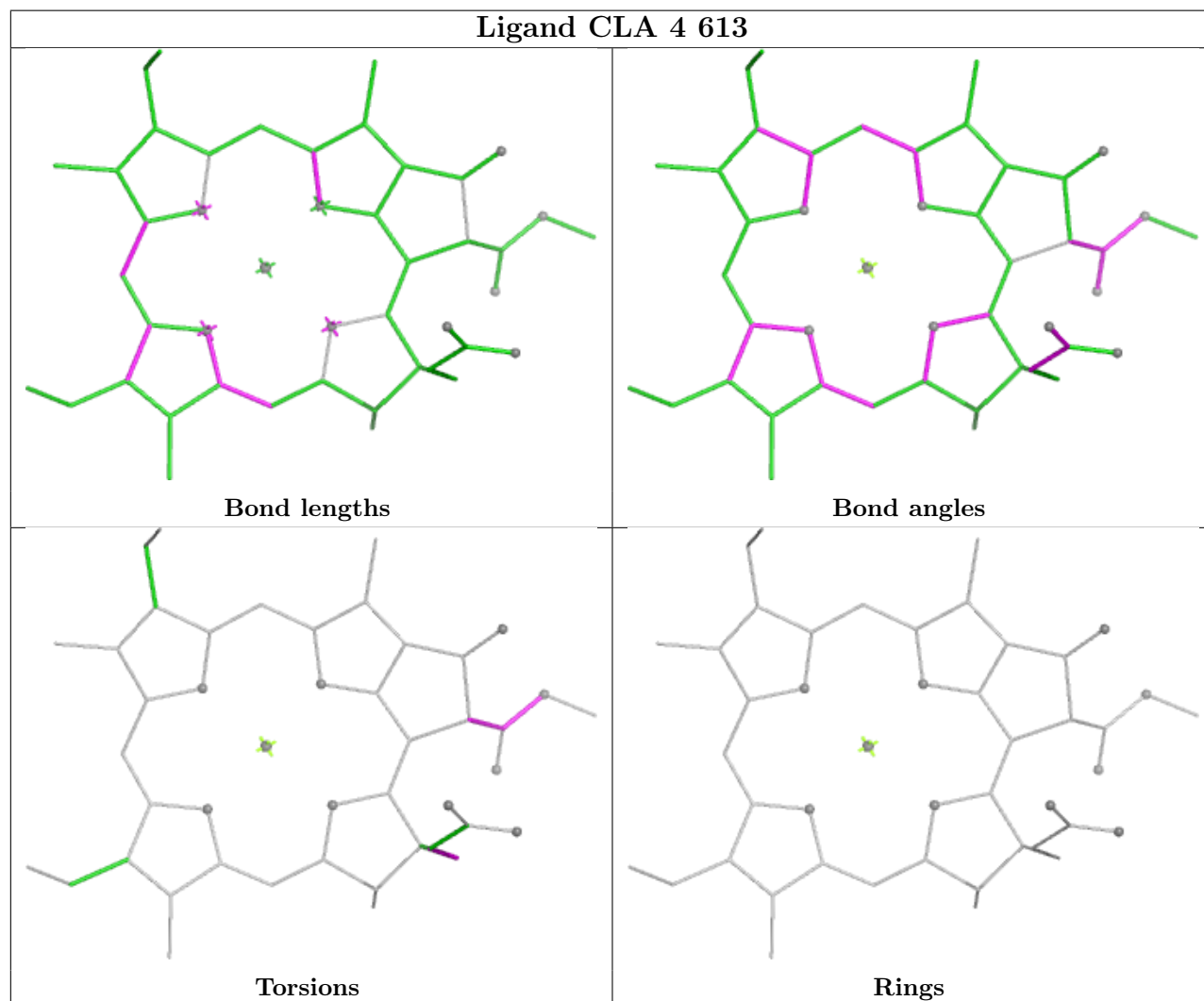


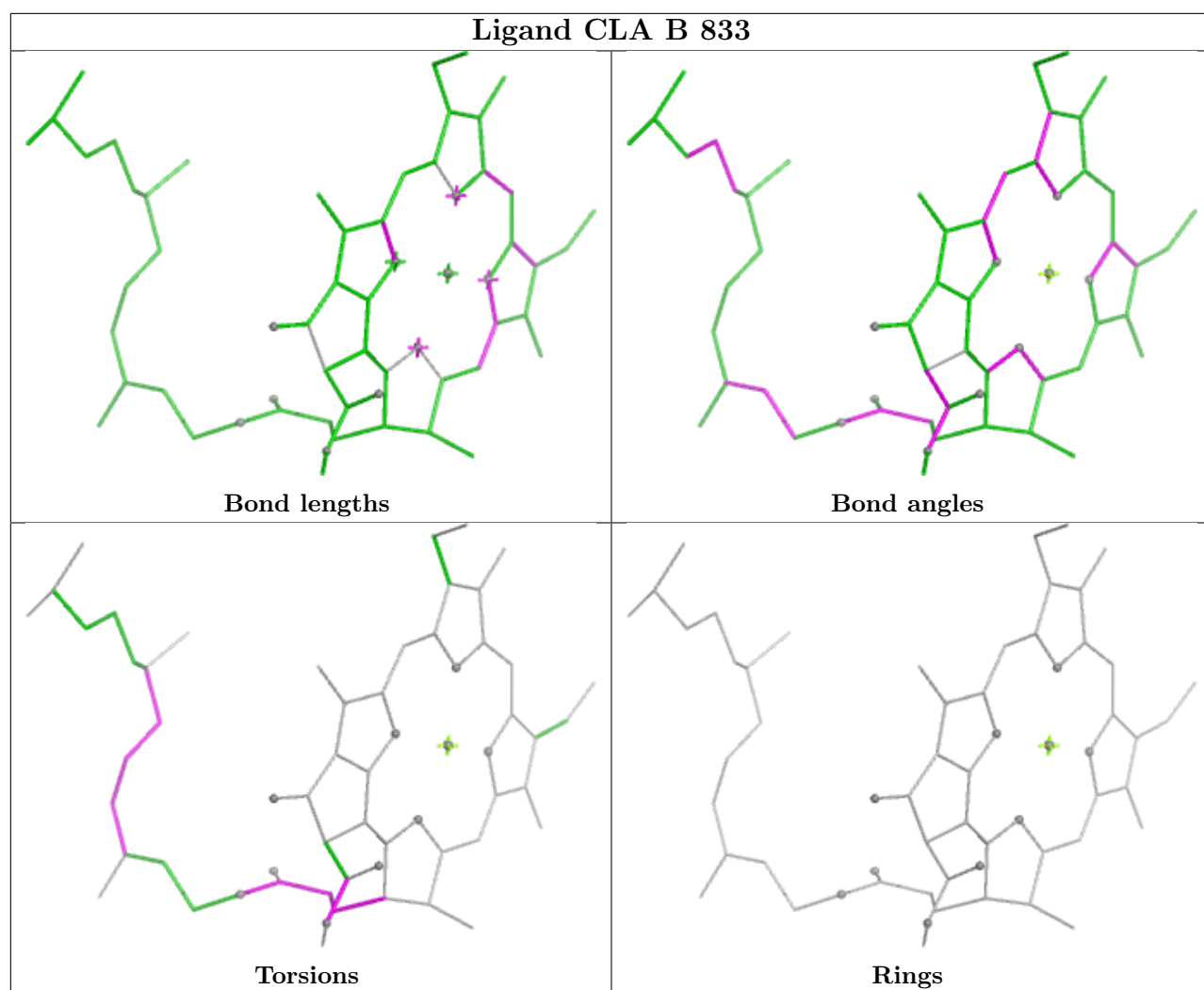
Rings

Ligand CLA A 841

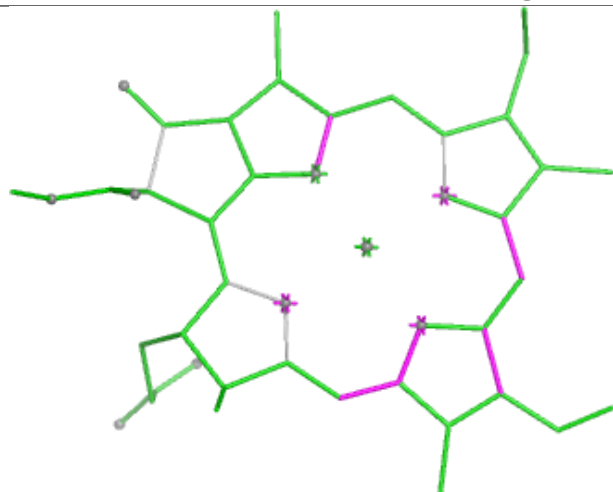


Ligand CLA 4 613

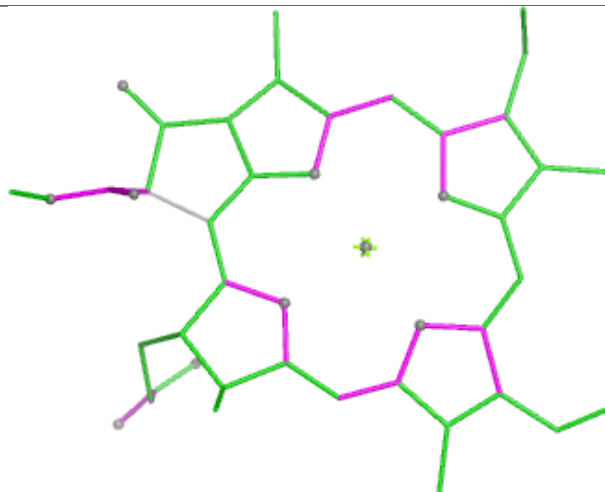




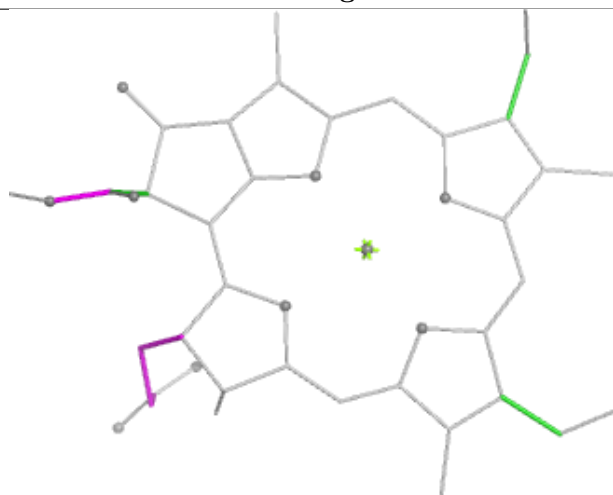
Ligand CLA 3 607



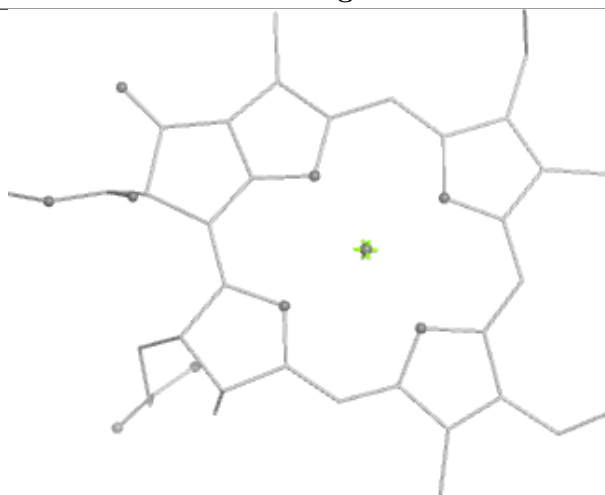
Bond lengths



Bond angles

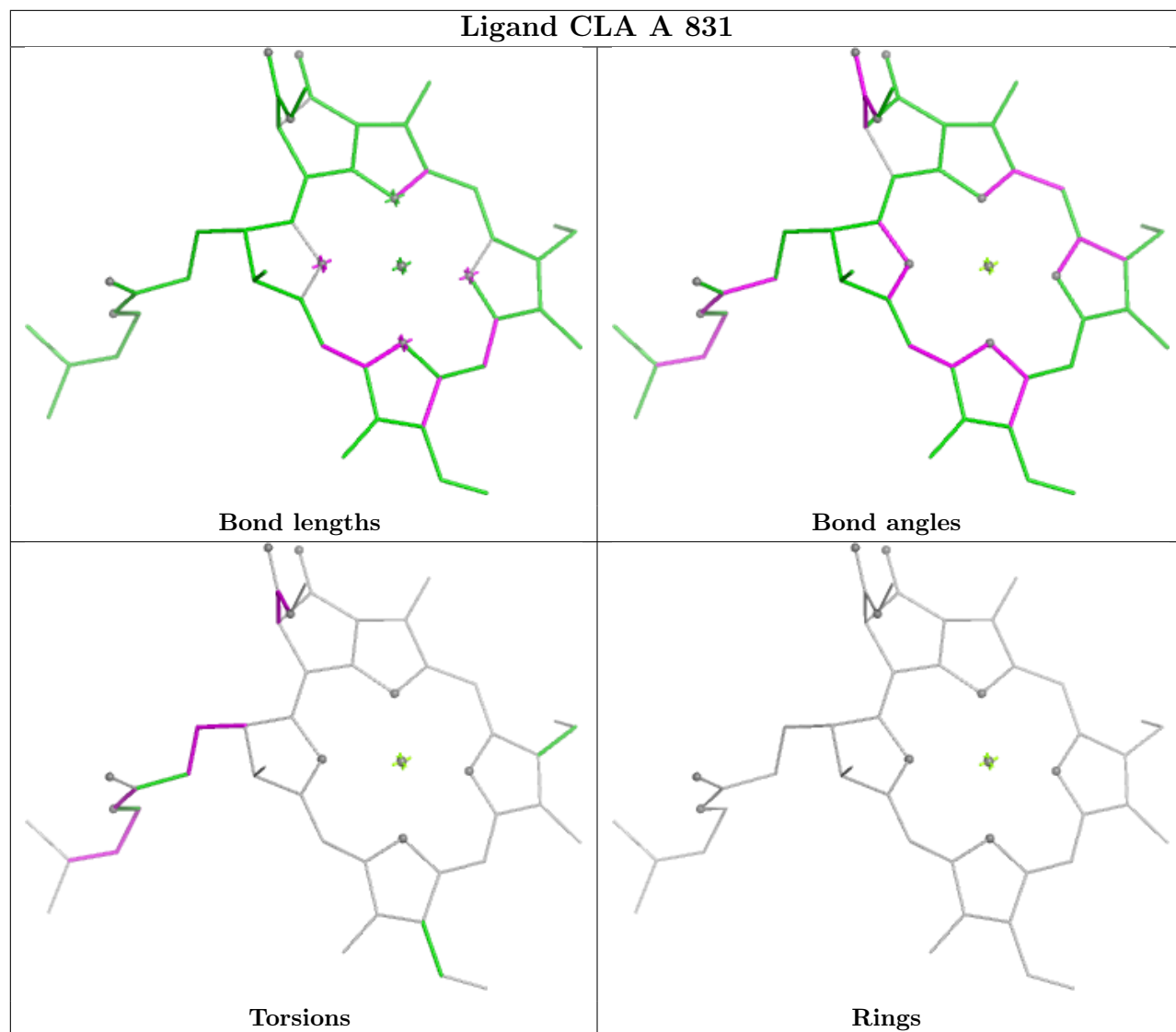


Torsions

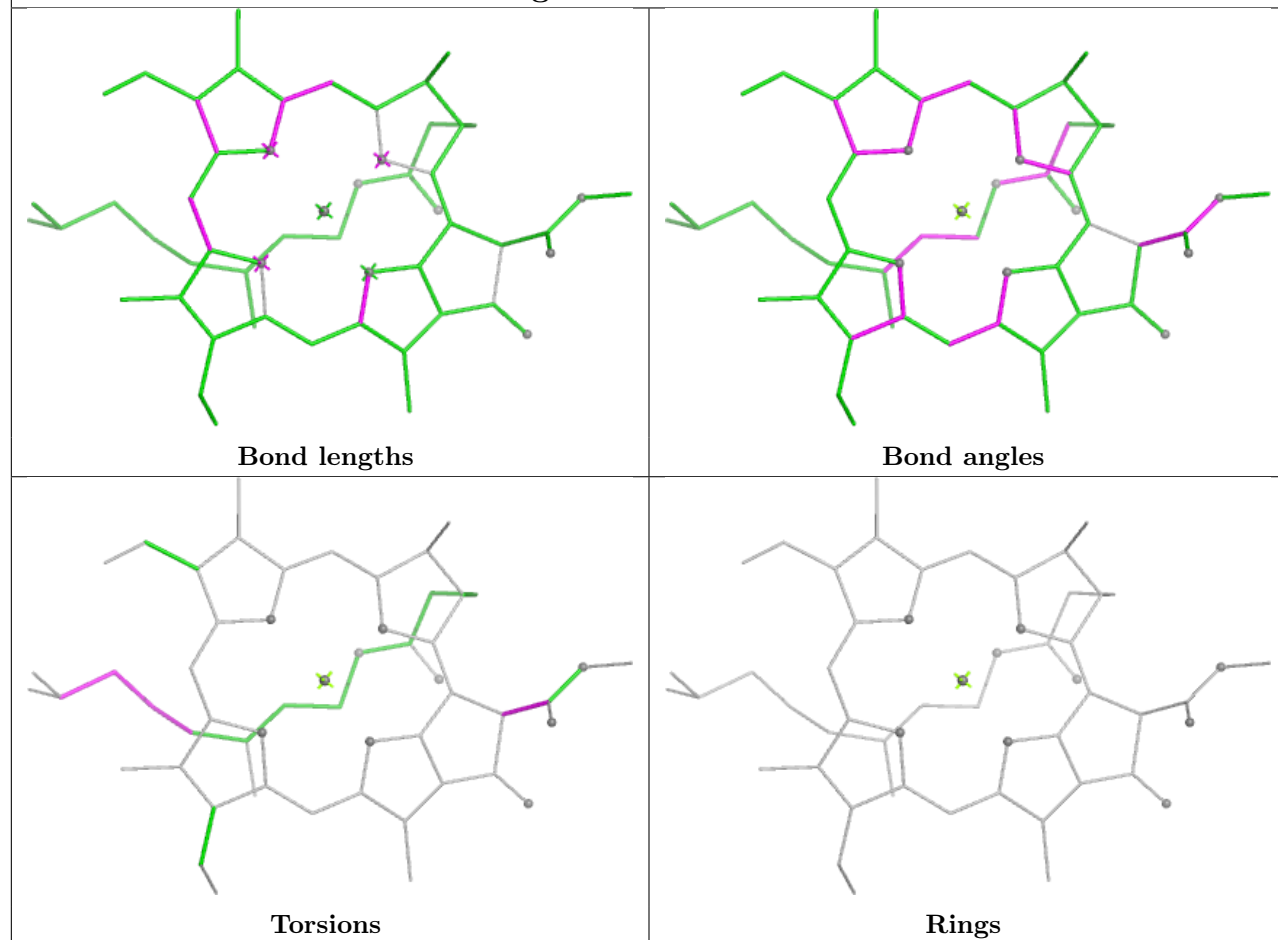


Rings

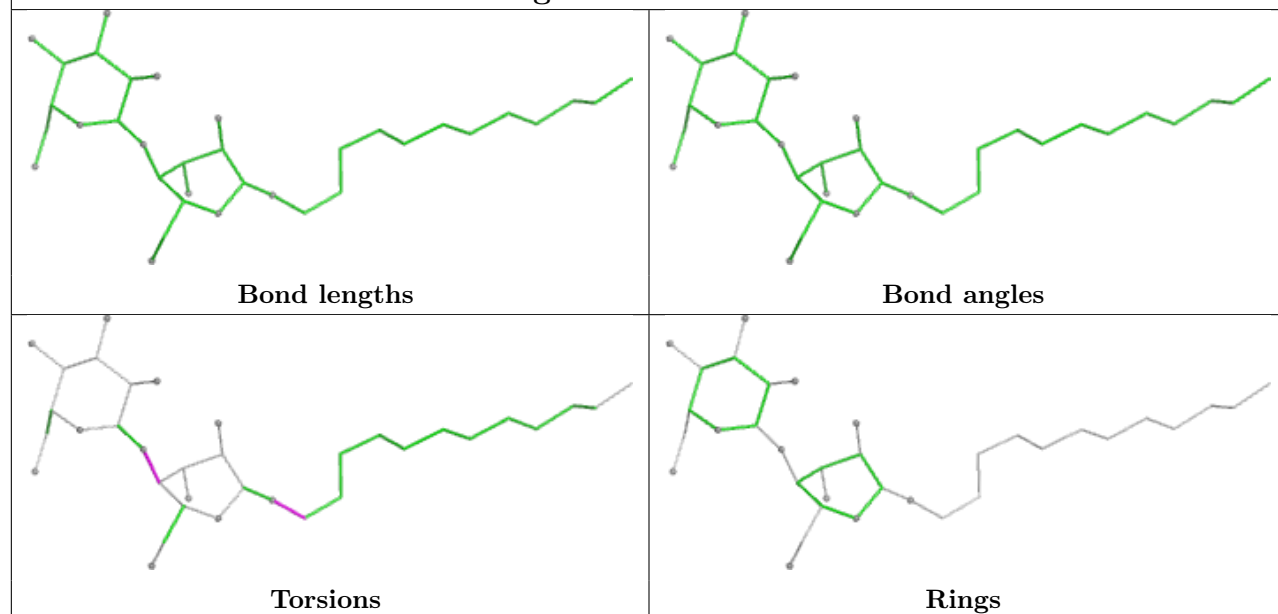
Ligand CLA A 831



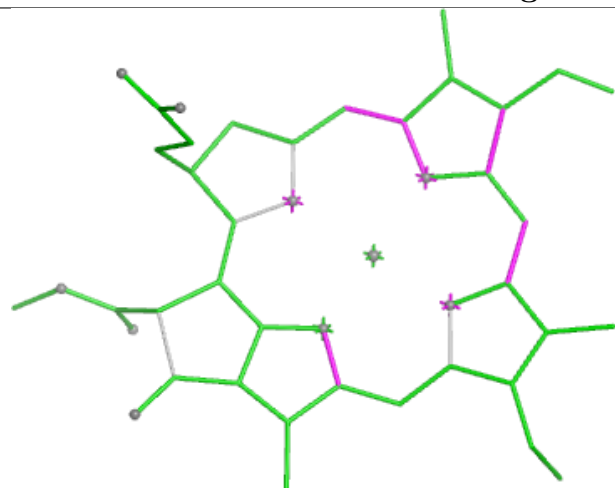
Ligand CLA A 838



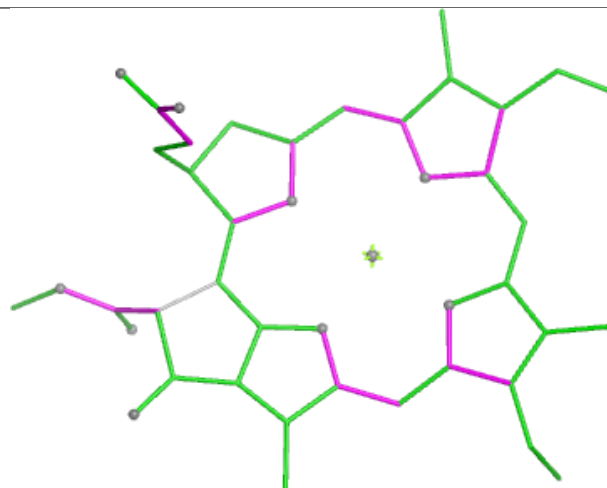
Ligand LMT 4 620



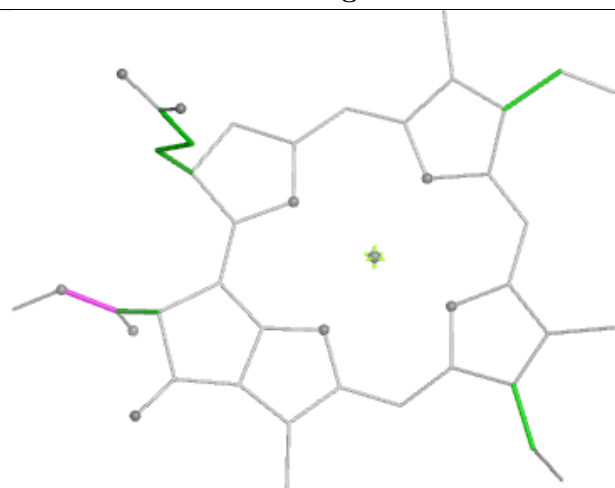
Ligand CLA 3 608



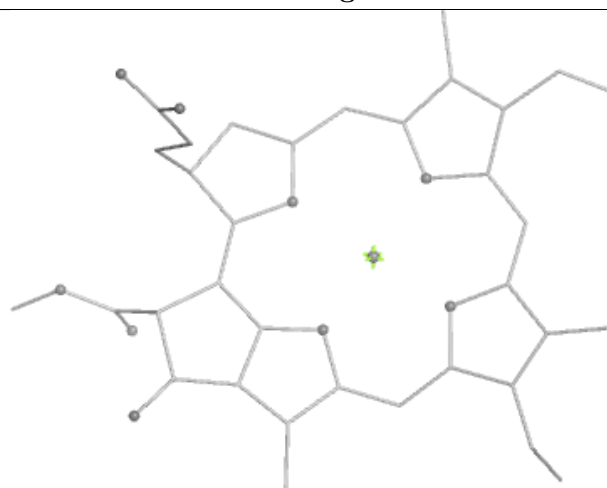
Bond lengths



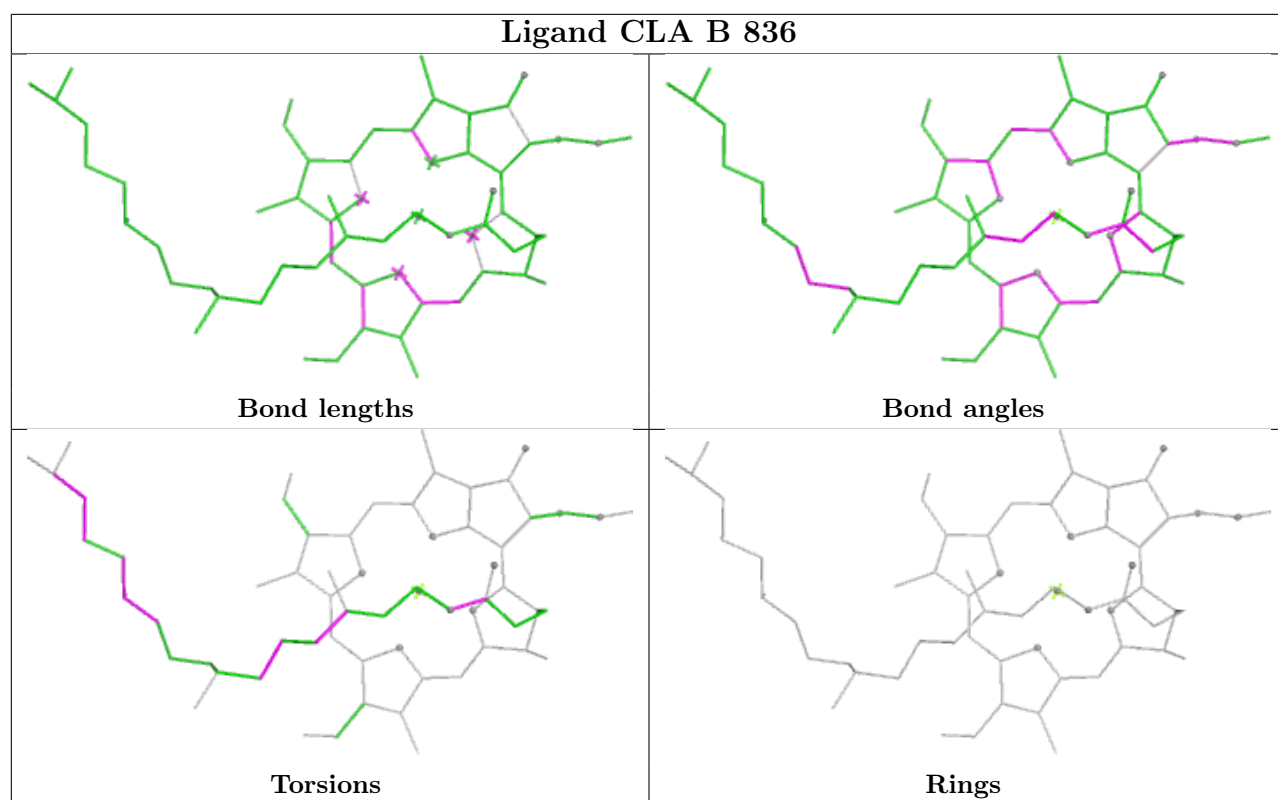
Bond angles



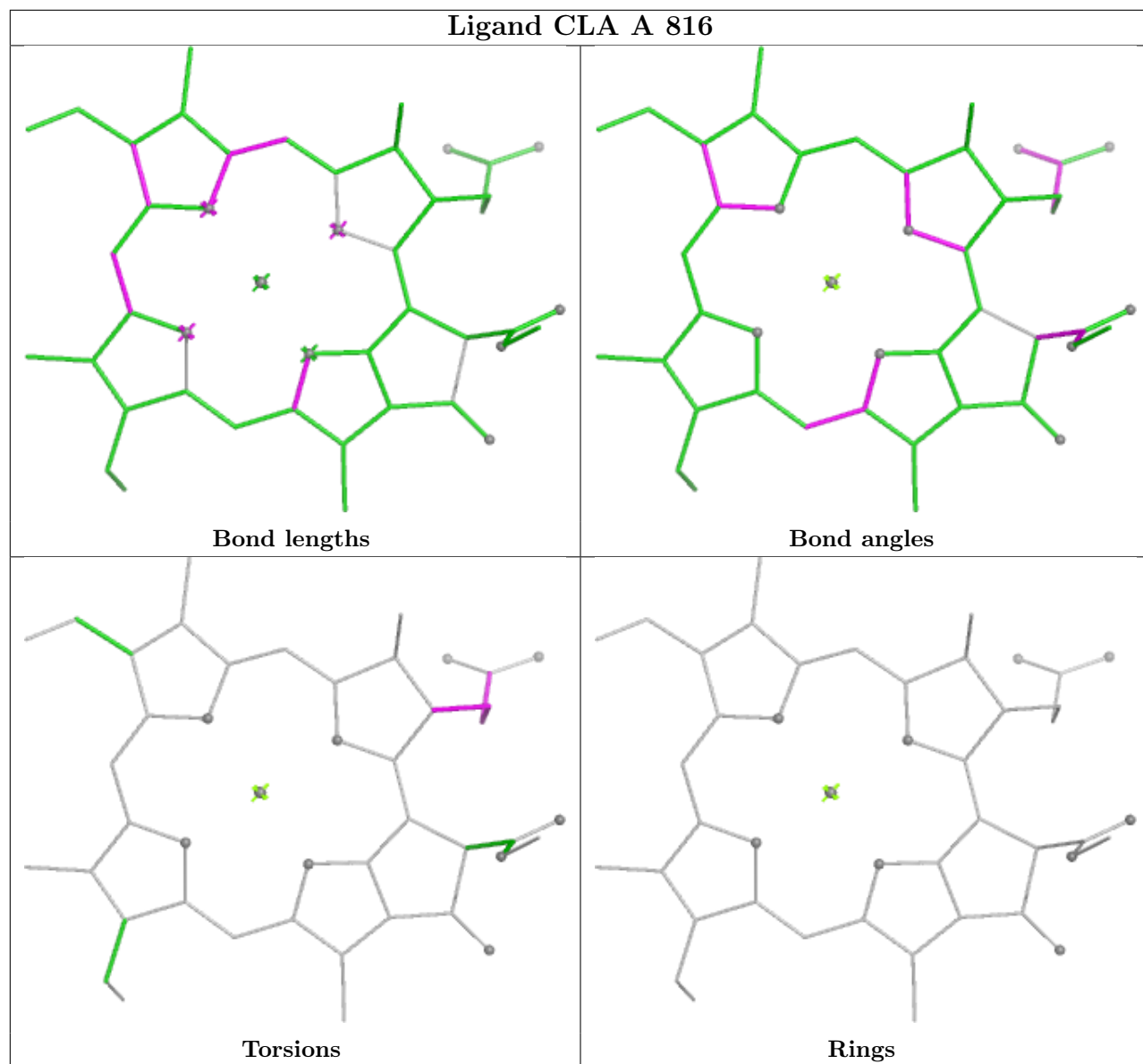
Torsions

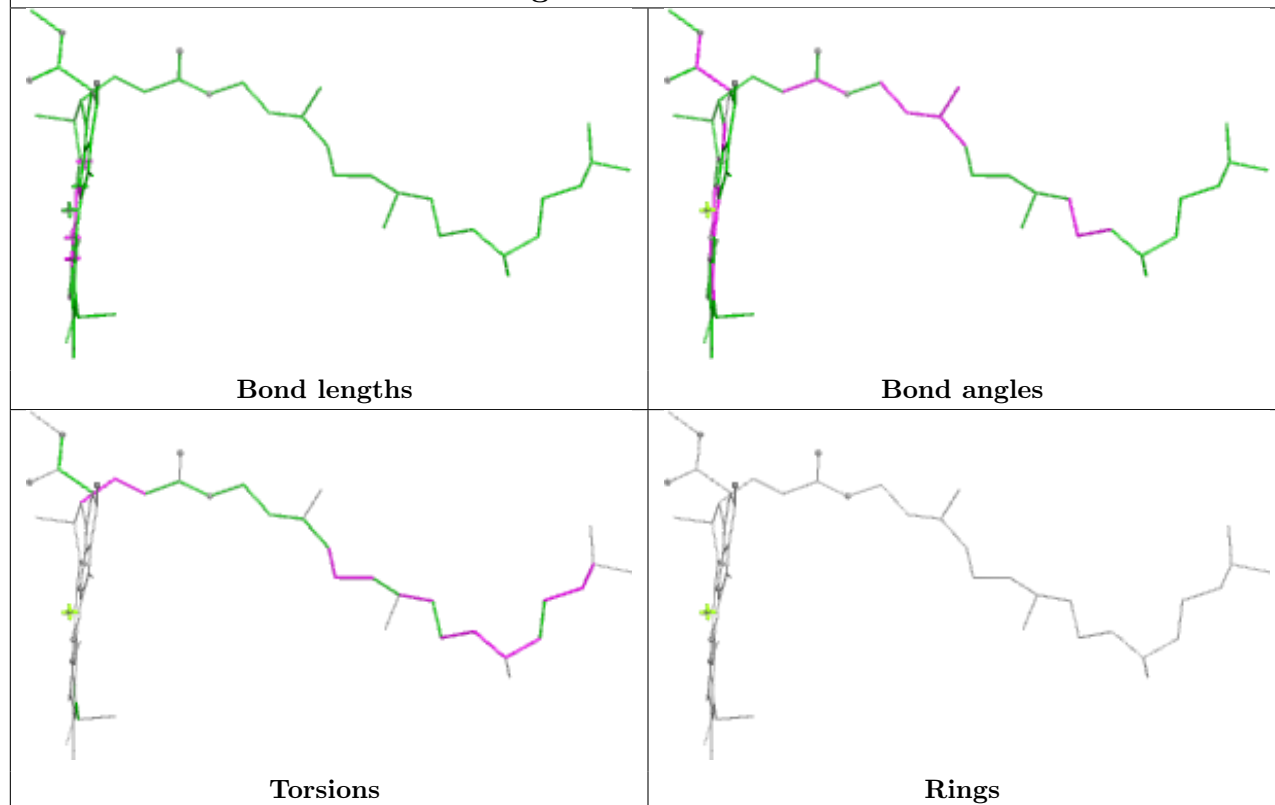
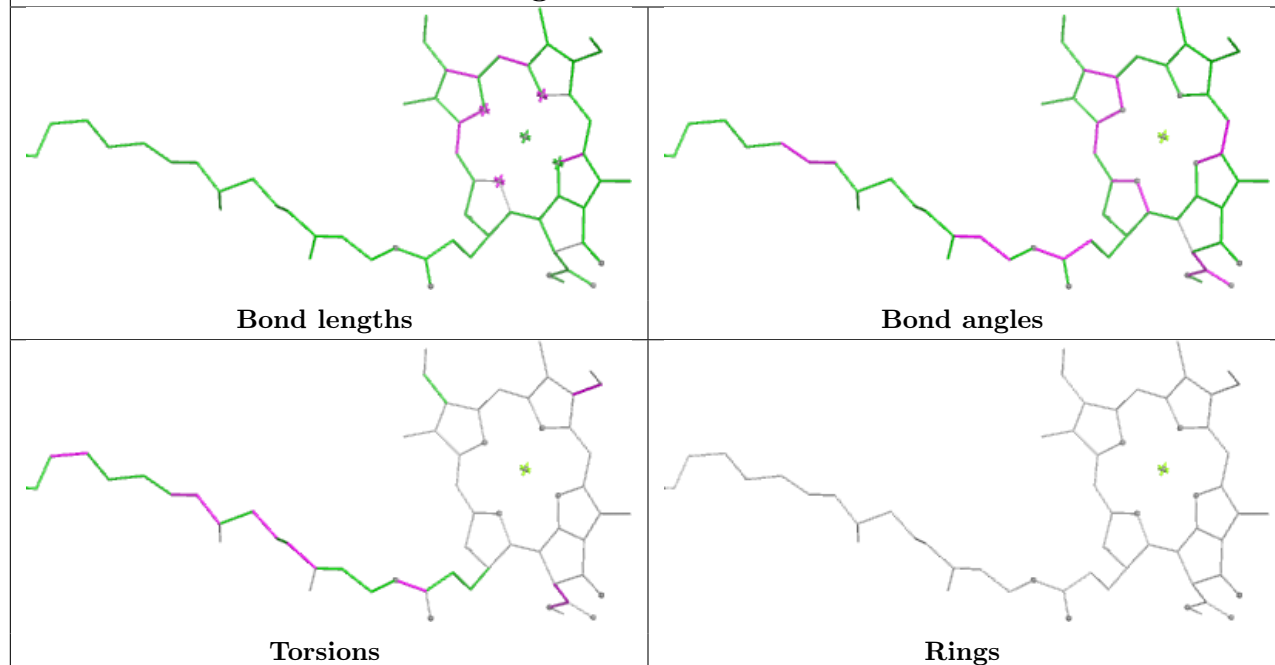


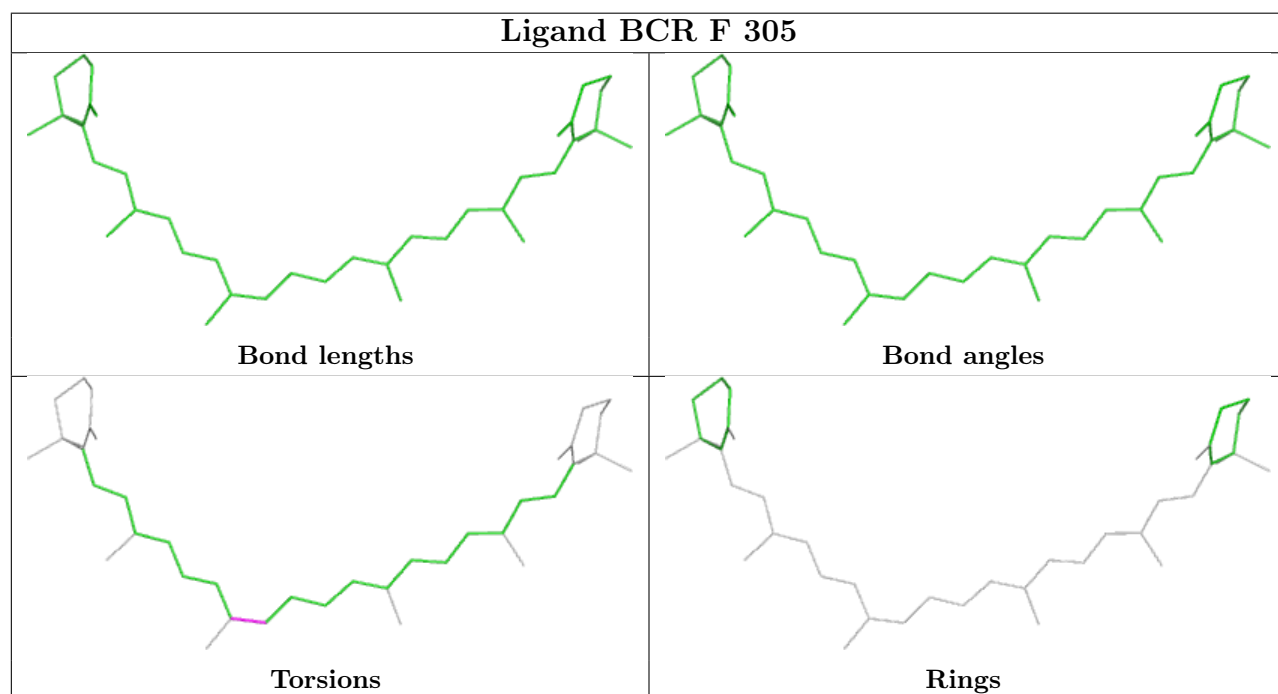
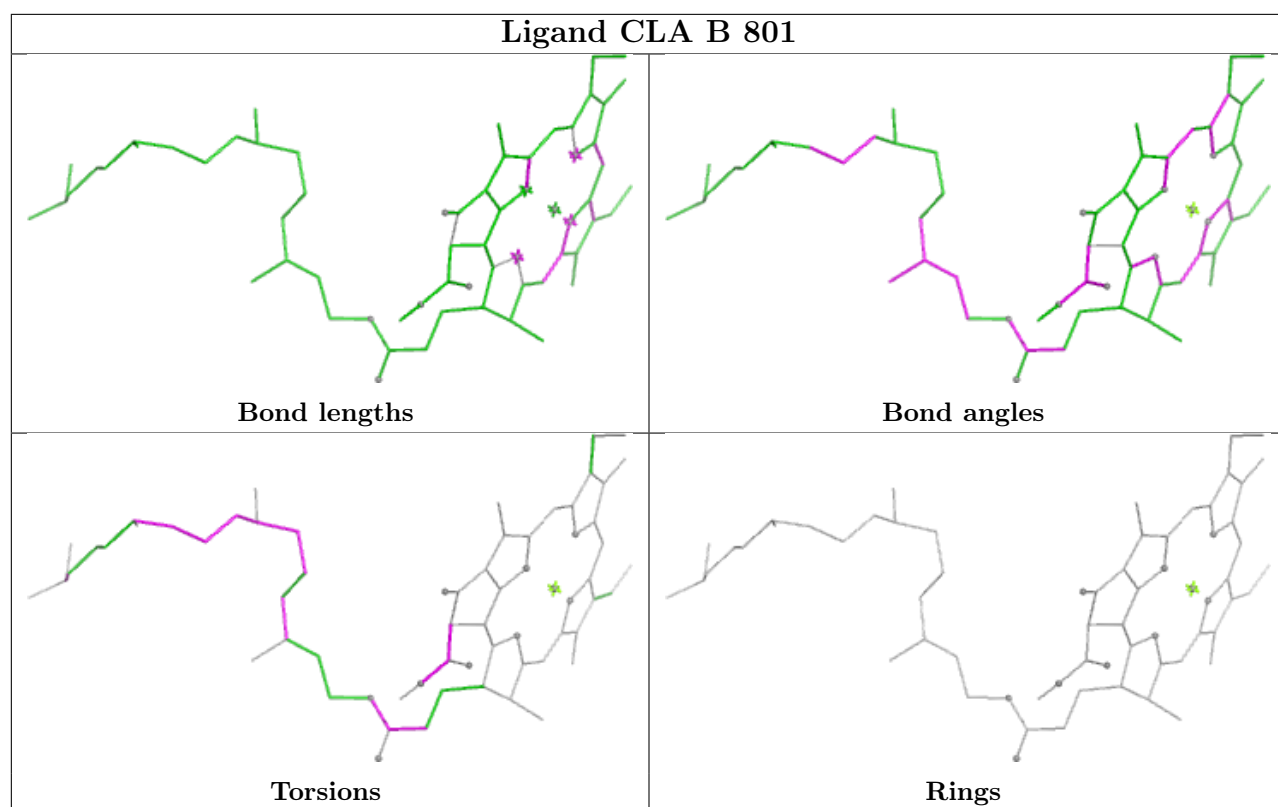
Rings

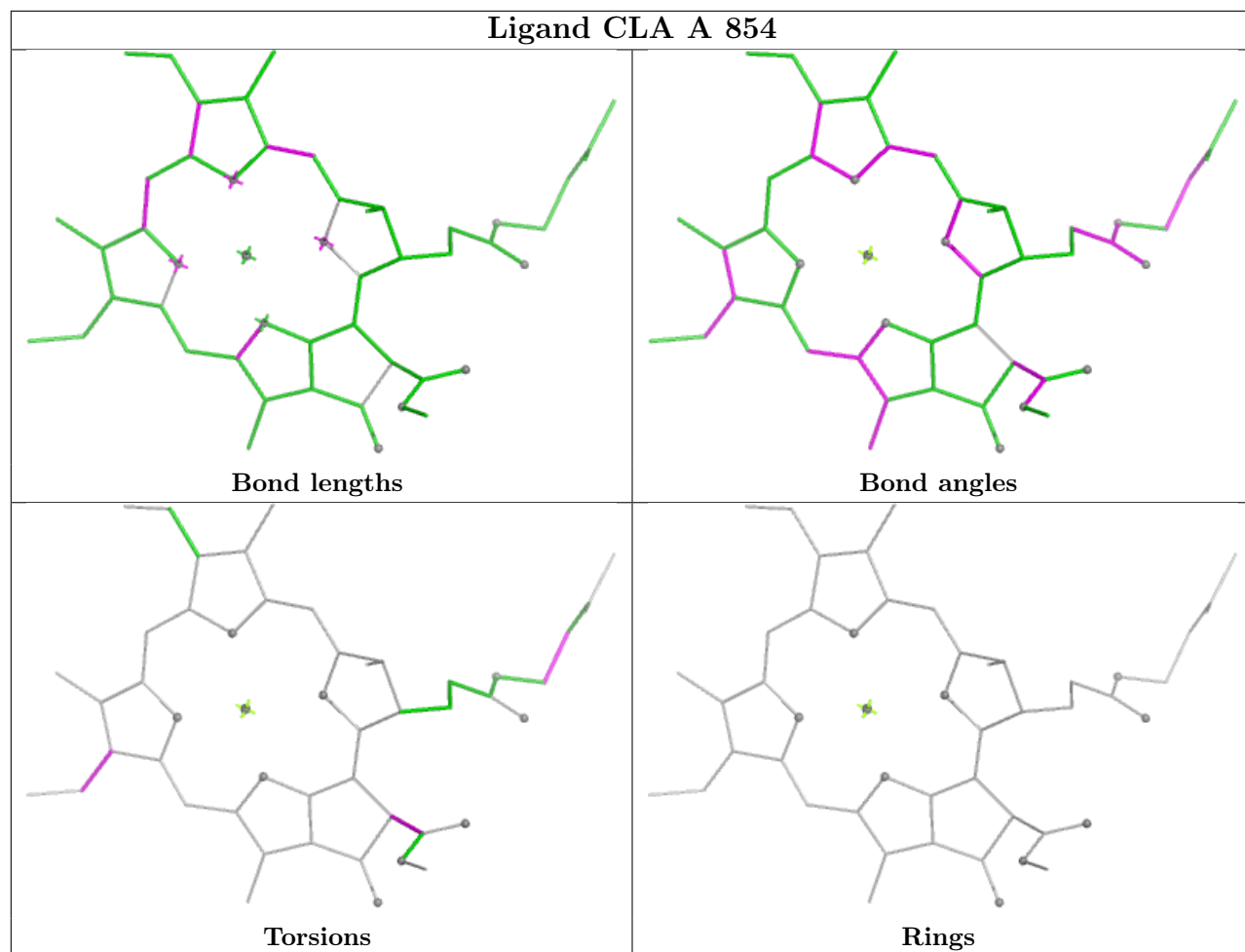


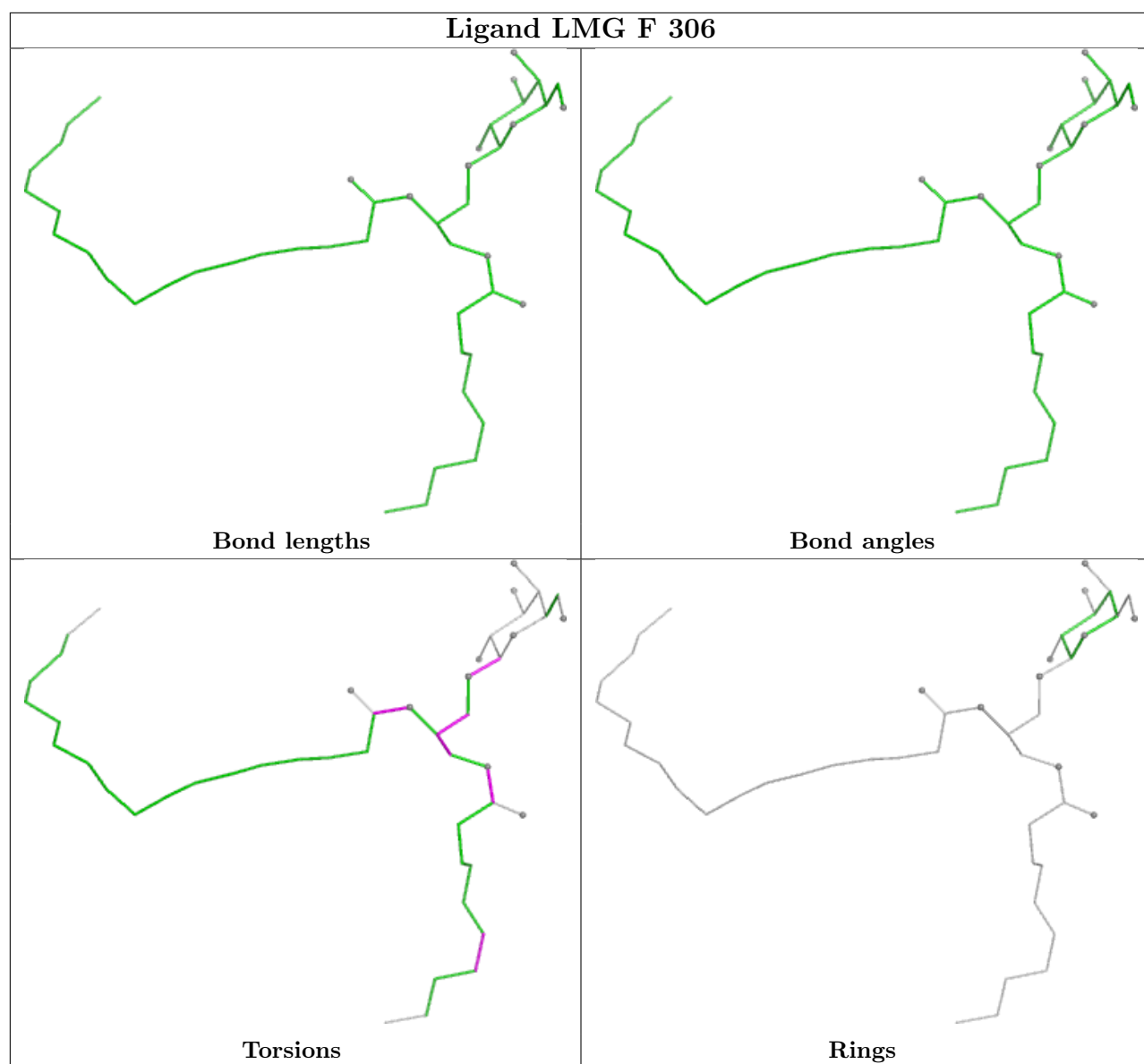
Ligand CLA A 816



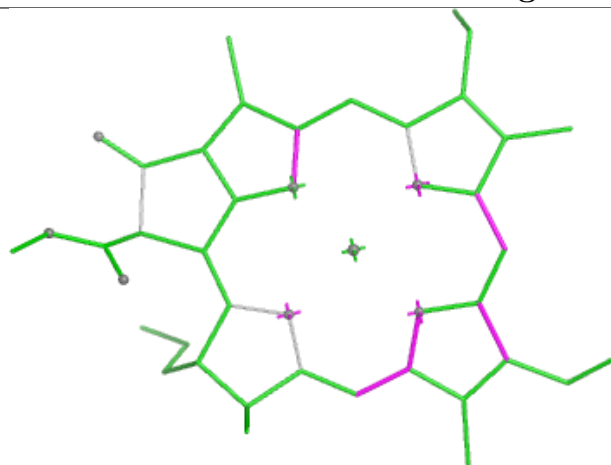
Ligand CLA B 839**Ligand CLA A 834**



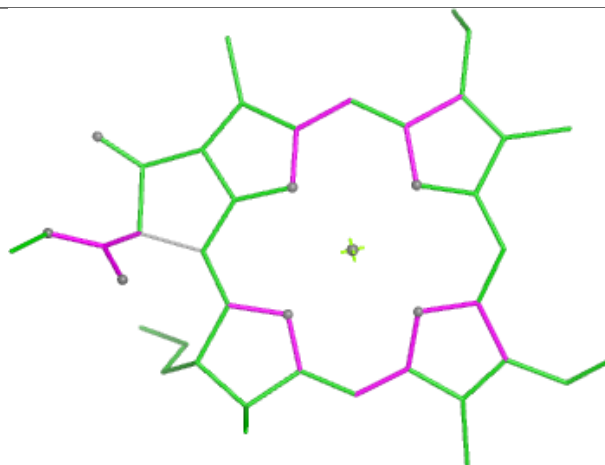




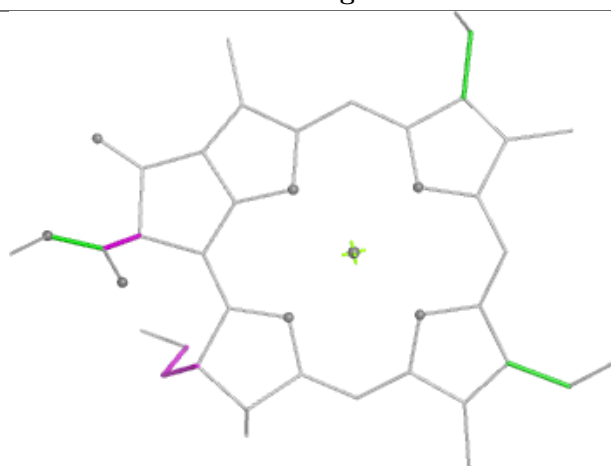
Ligand CLA 2 613



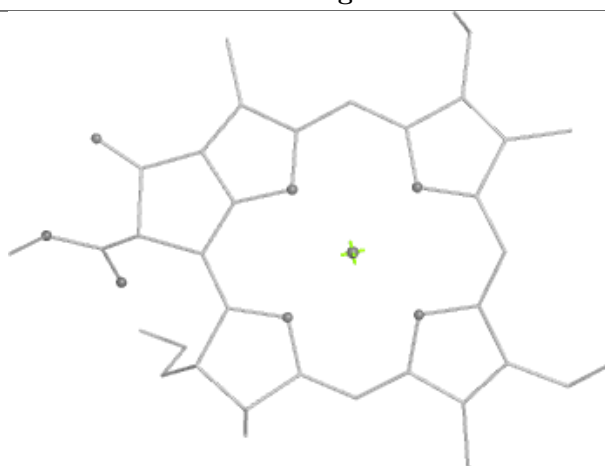
Bond lengths



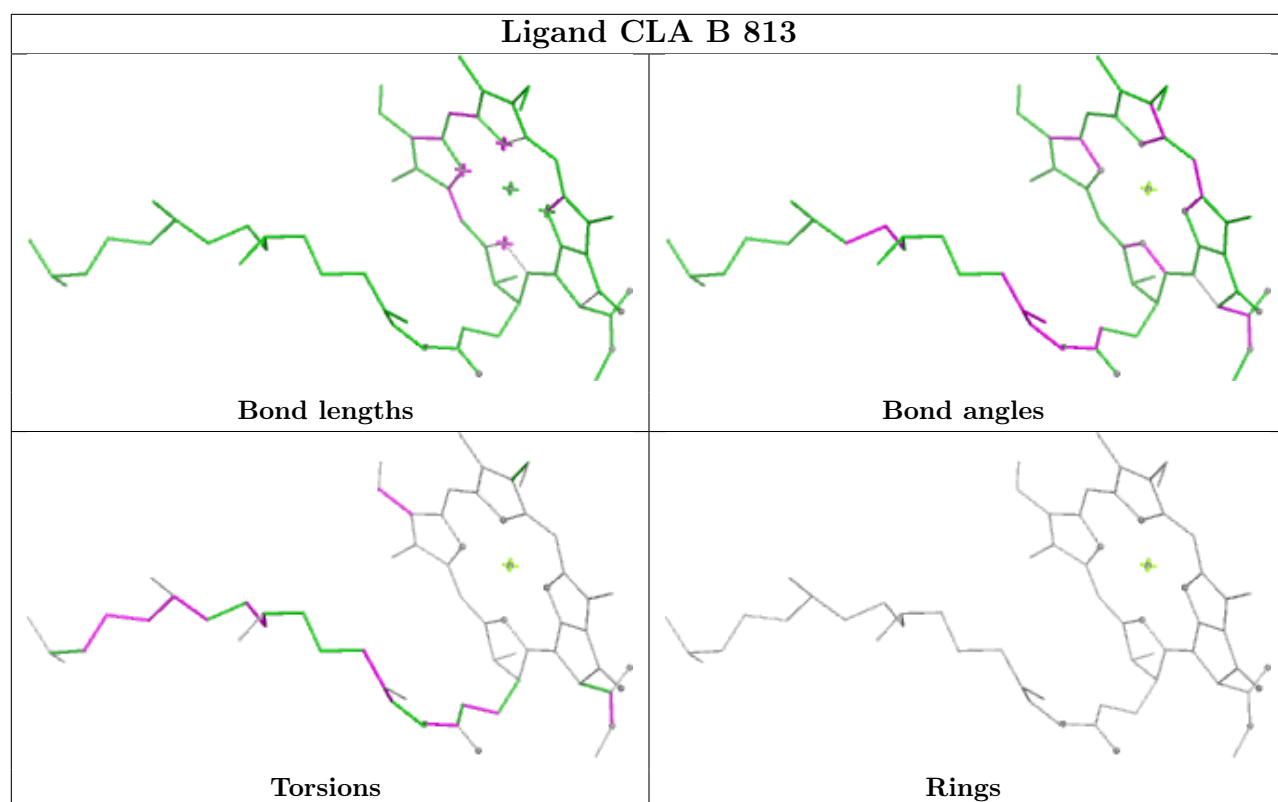
Bond angles

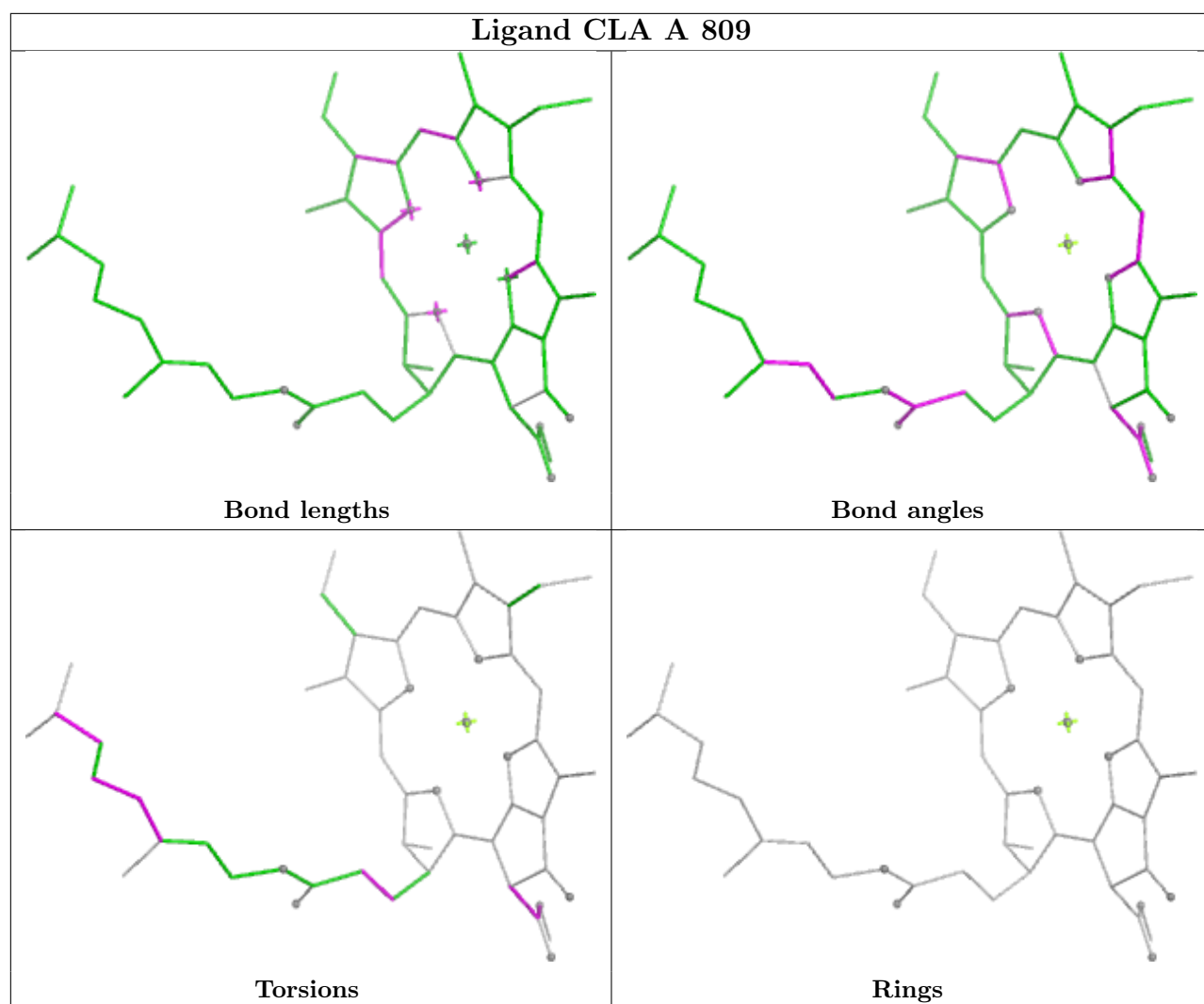


Torsions

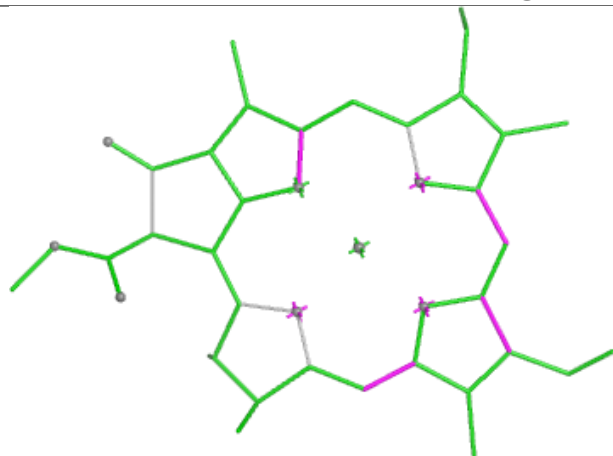


Rings

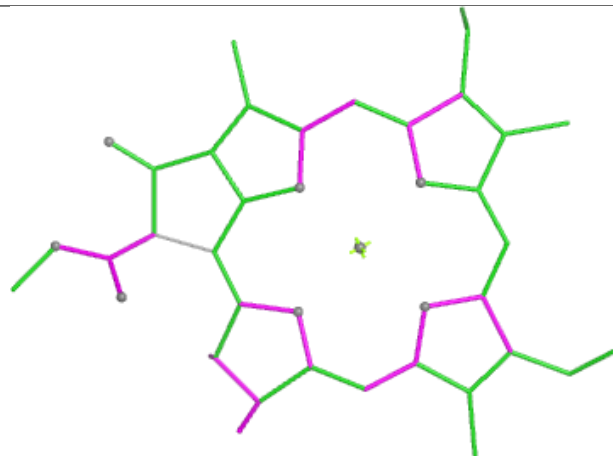




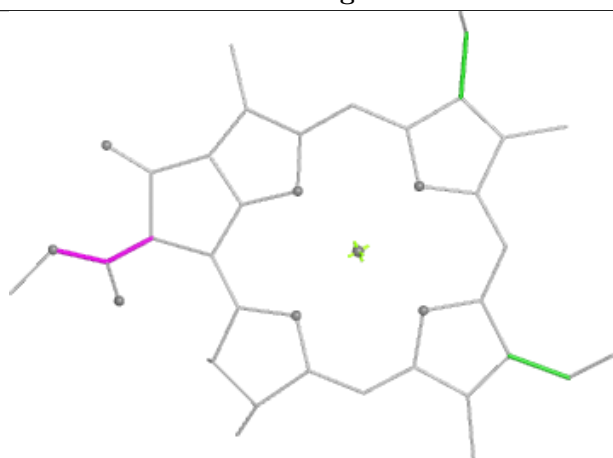
Ligand CLA 3 609



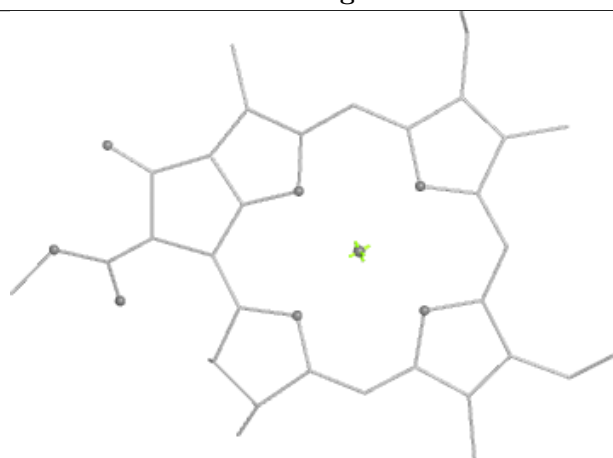
Bond lengths



Bond angles

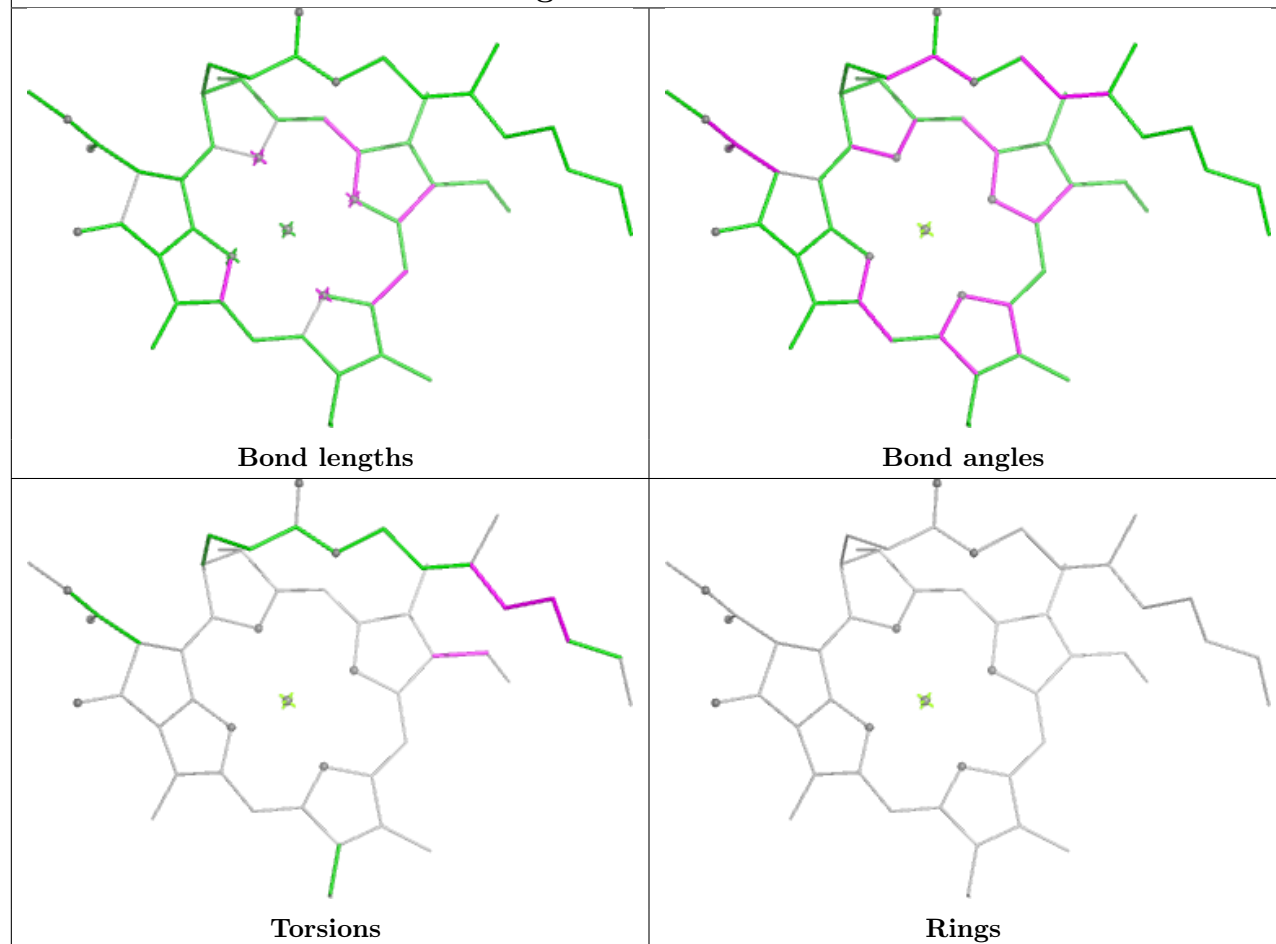


Torsions

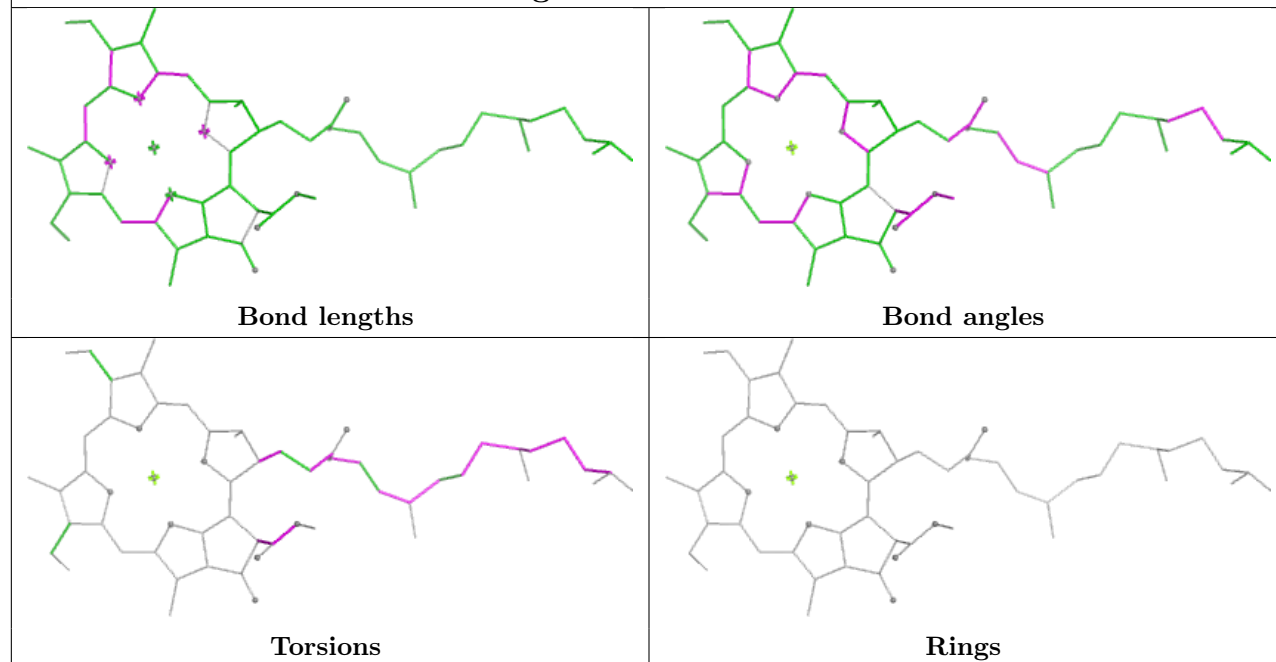


Rings

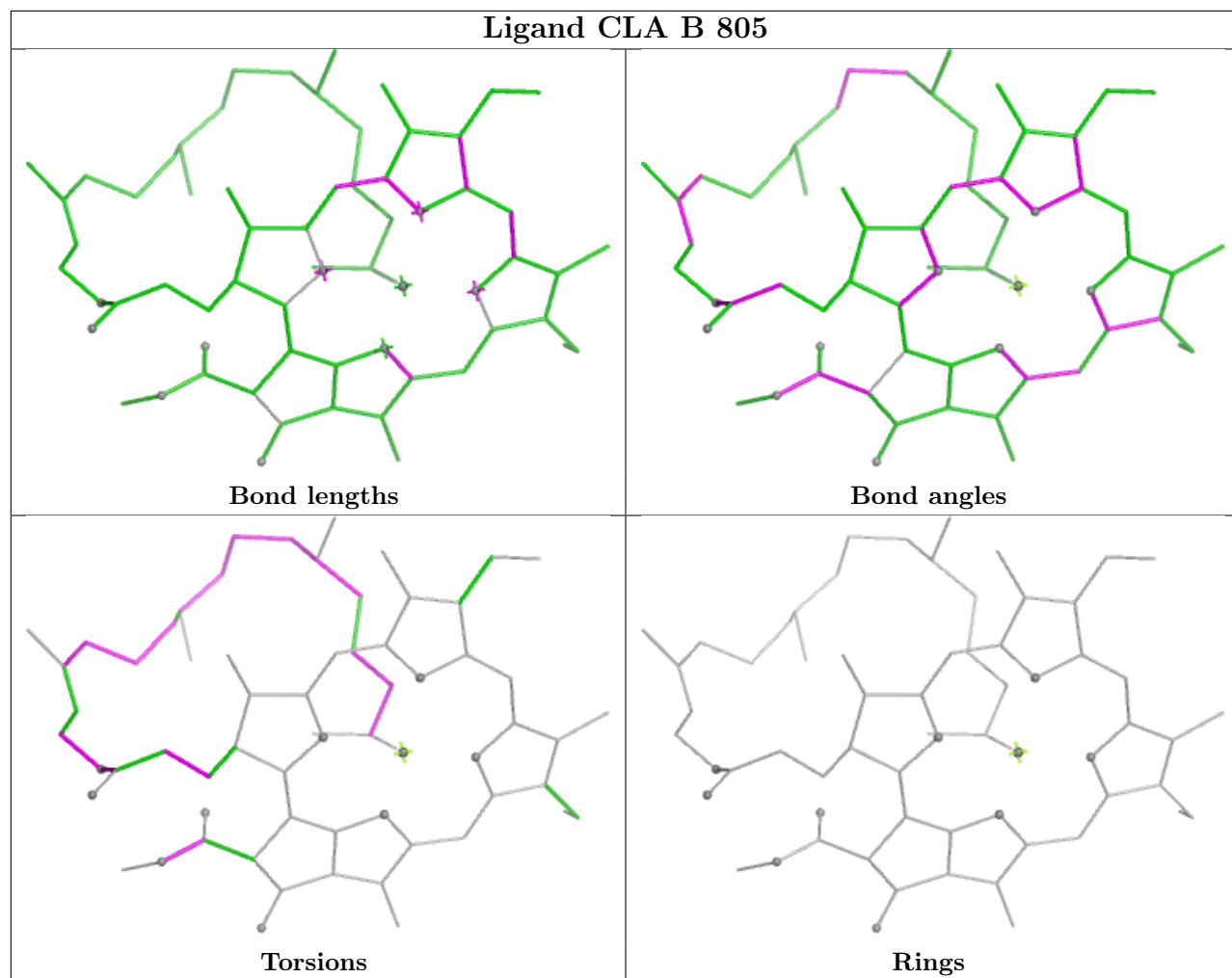
Ligand CLA 4 609



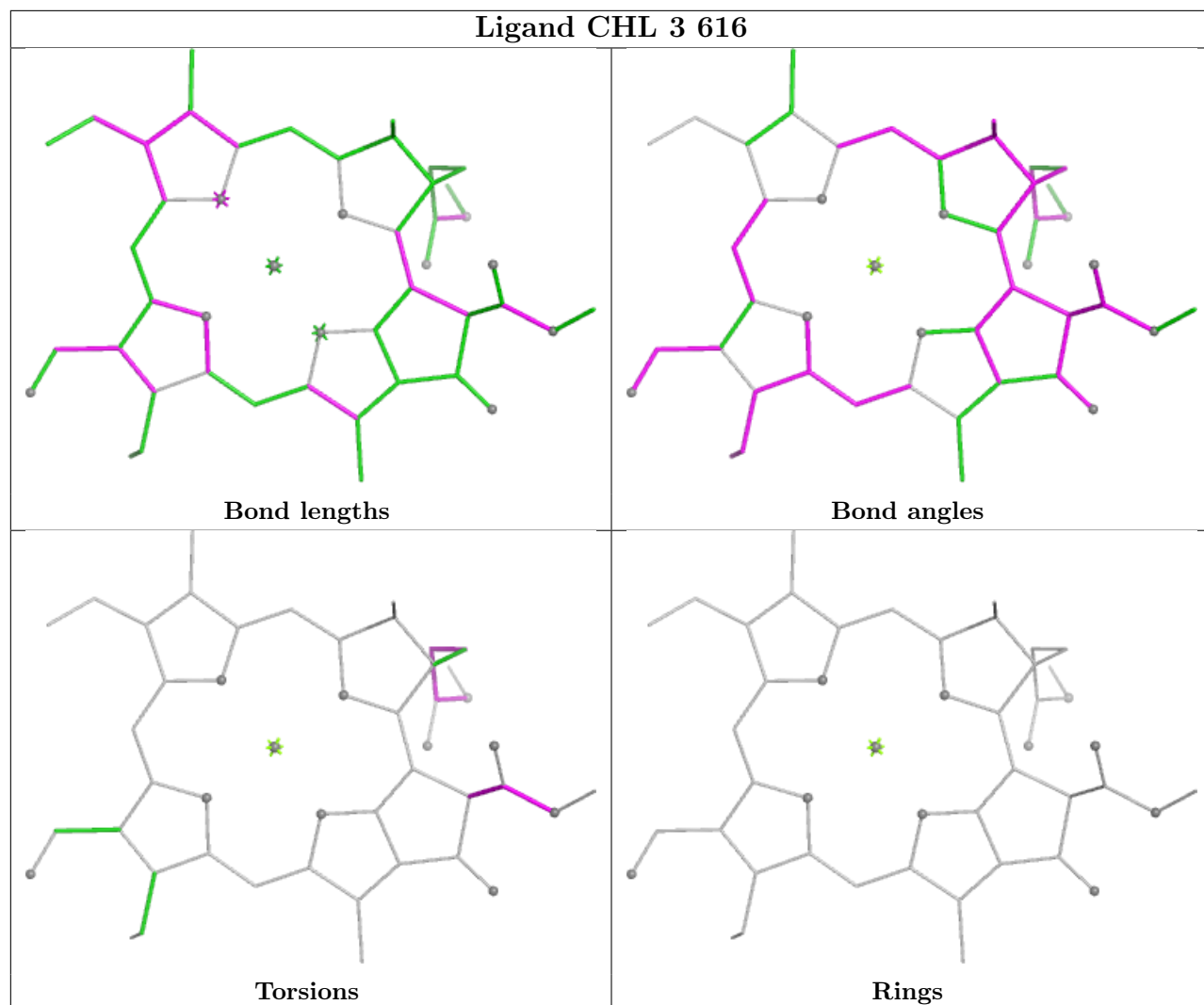
Ligand CLA B 822



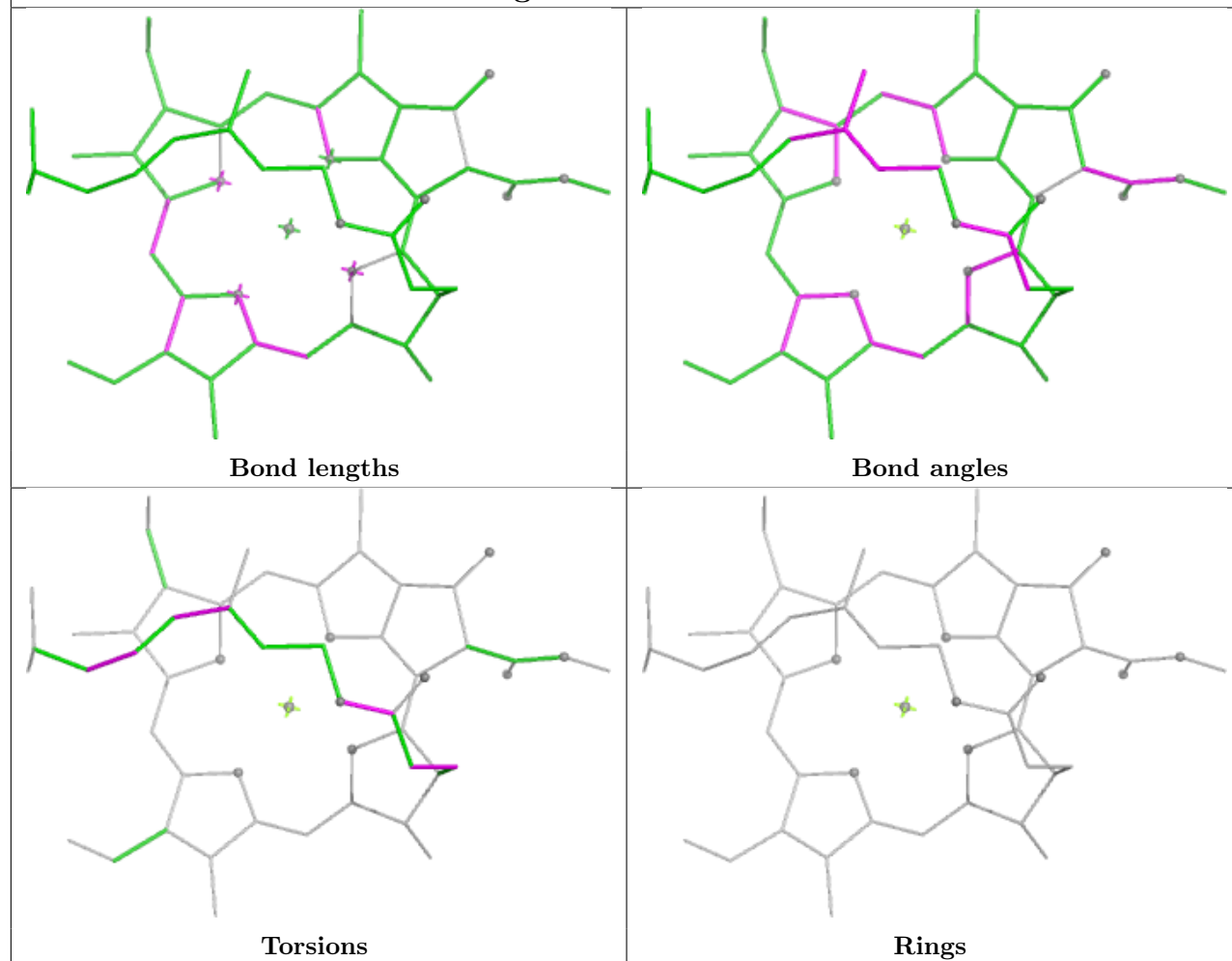
Ligand CLA B 805

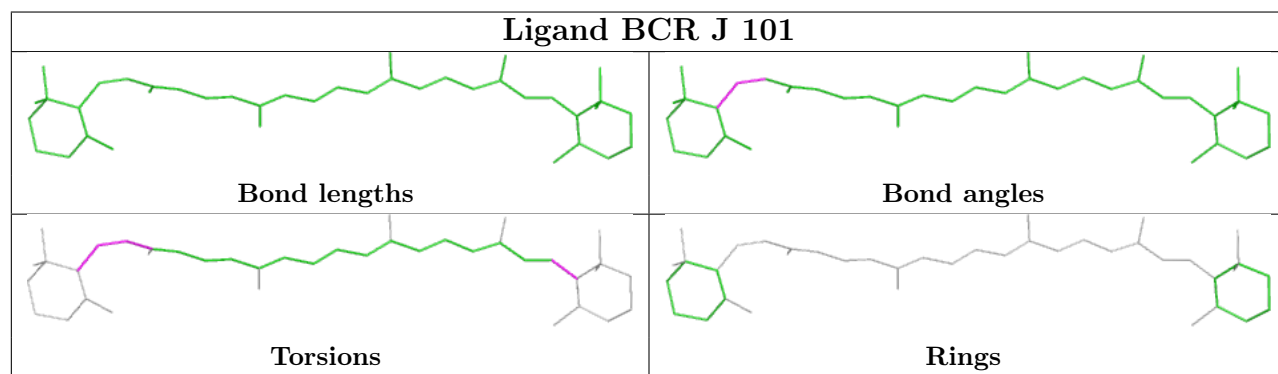
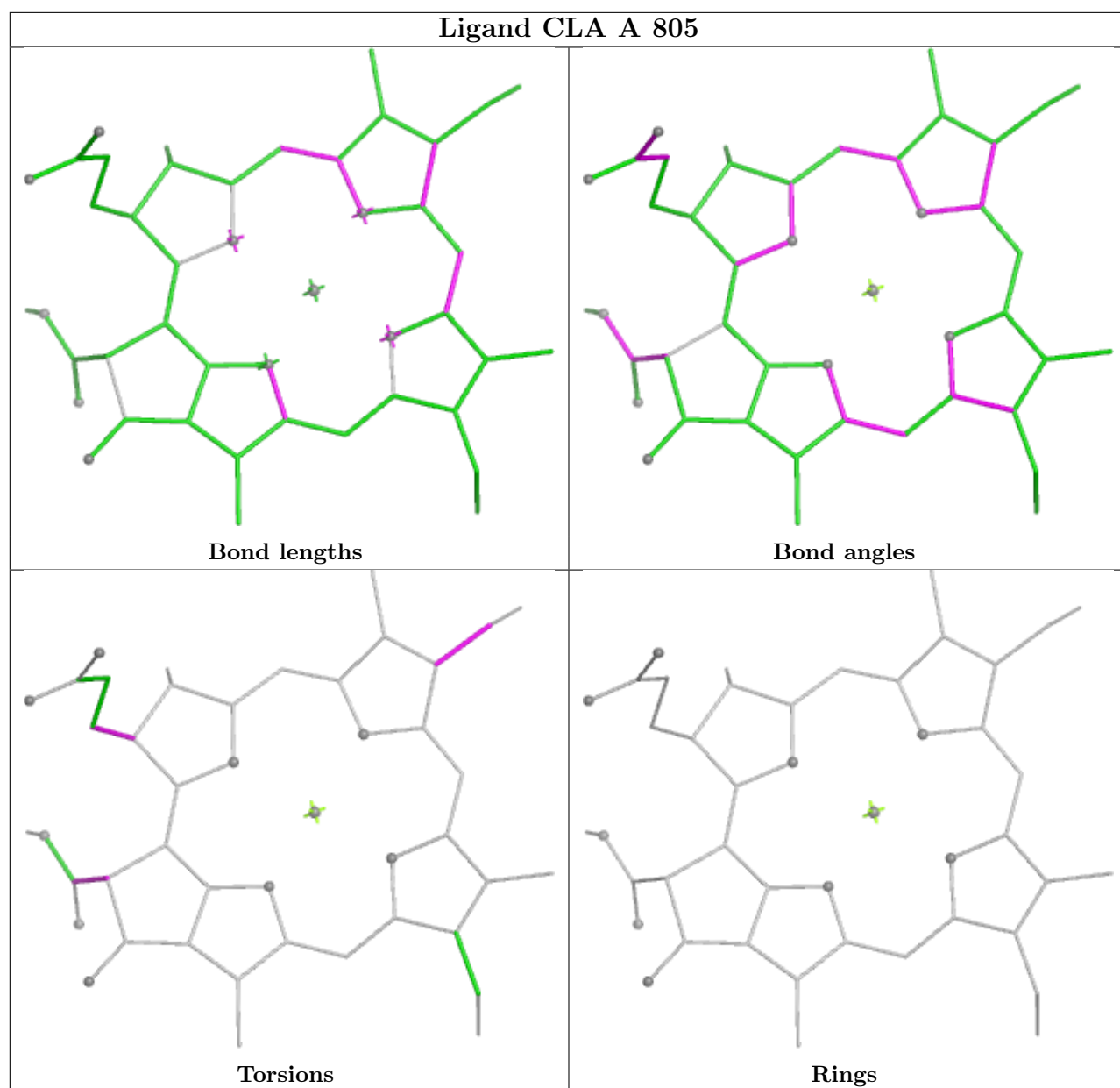


Ligand CHL 3 616

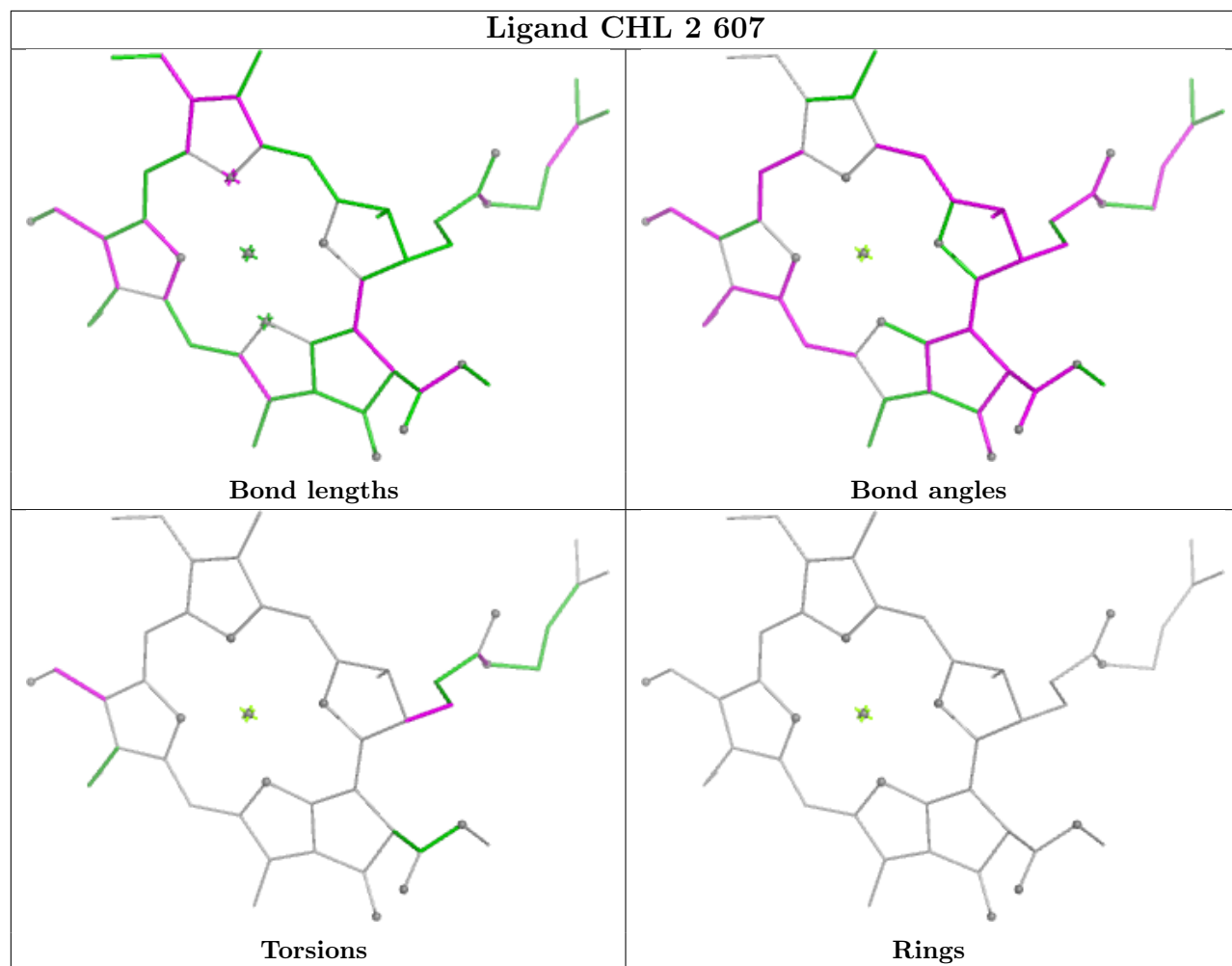


Ligand CLA B 815

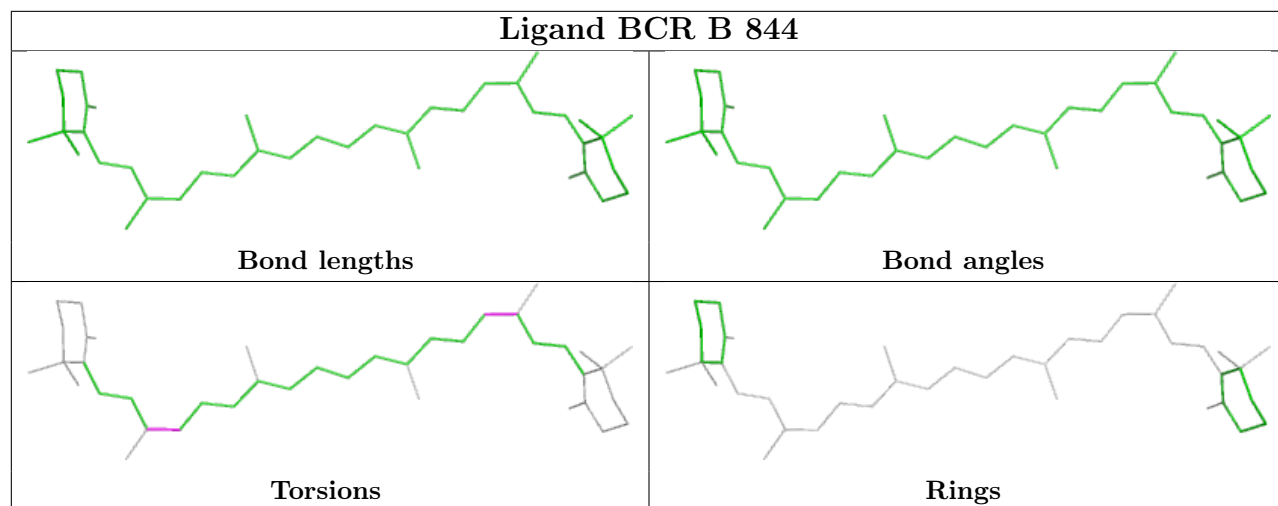


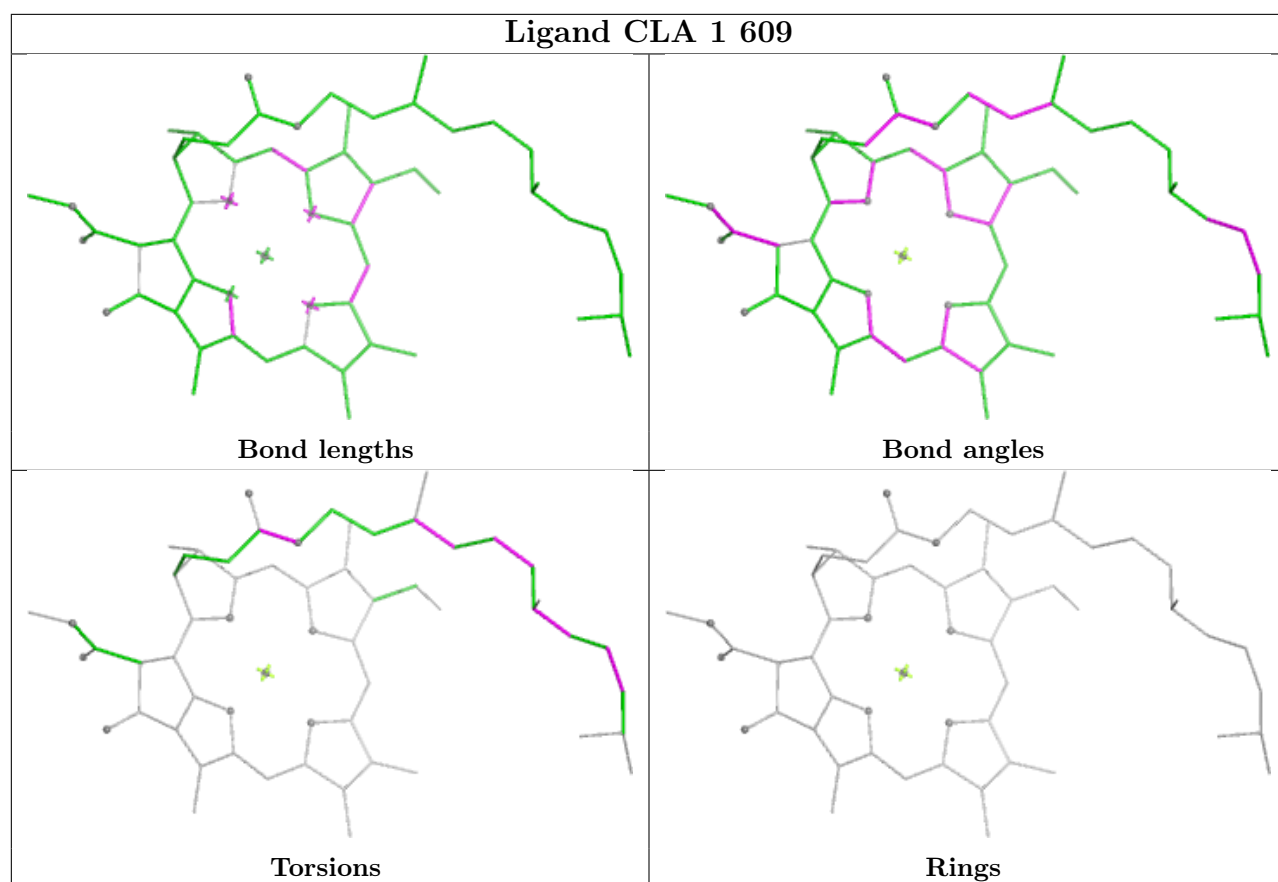


Ligand CHL 2 607

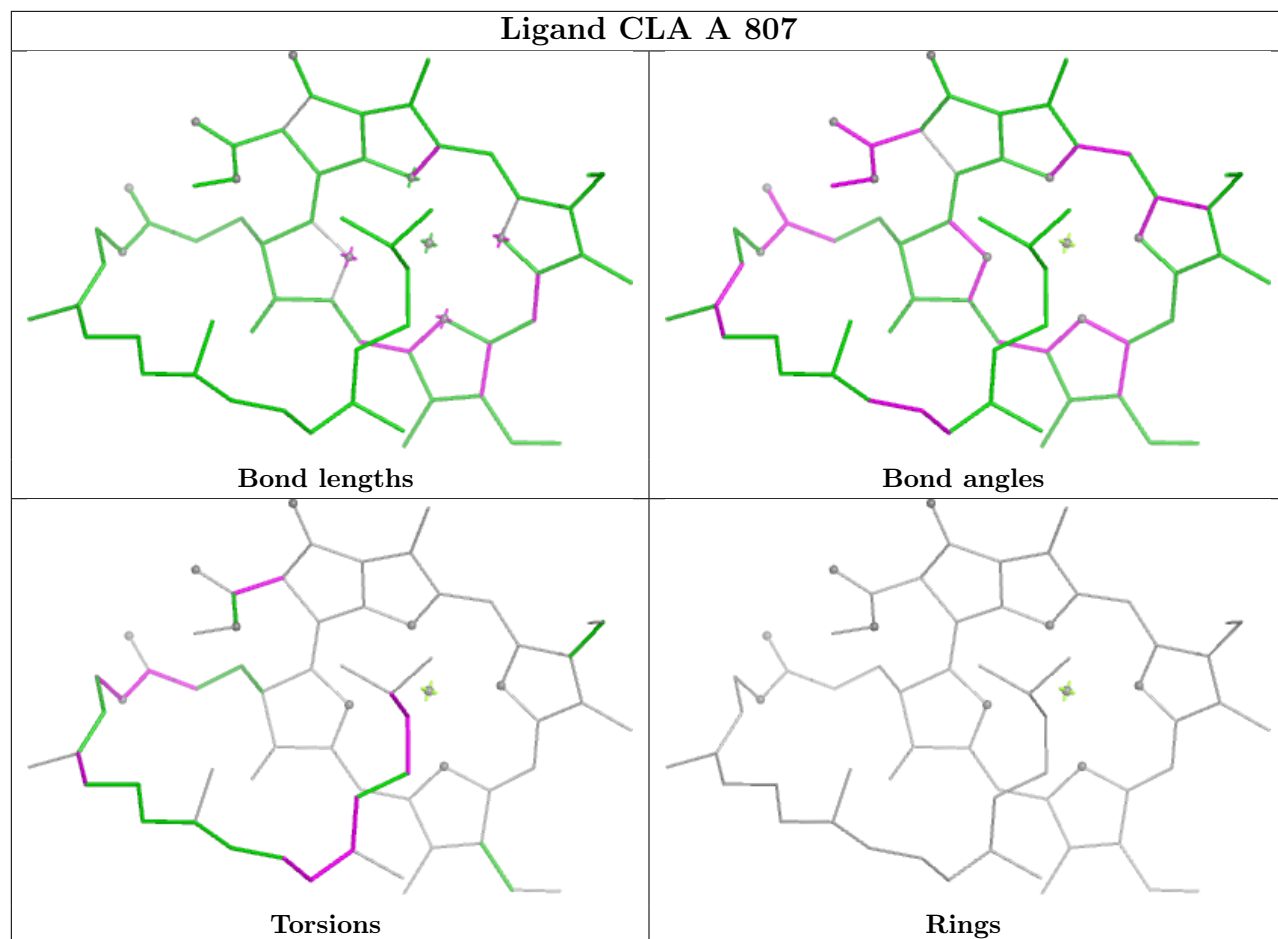


Ligand BCR B 844

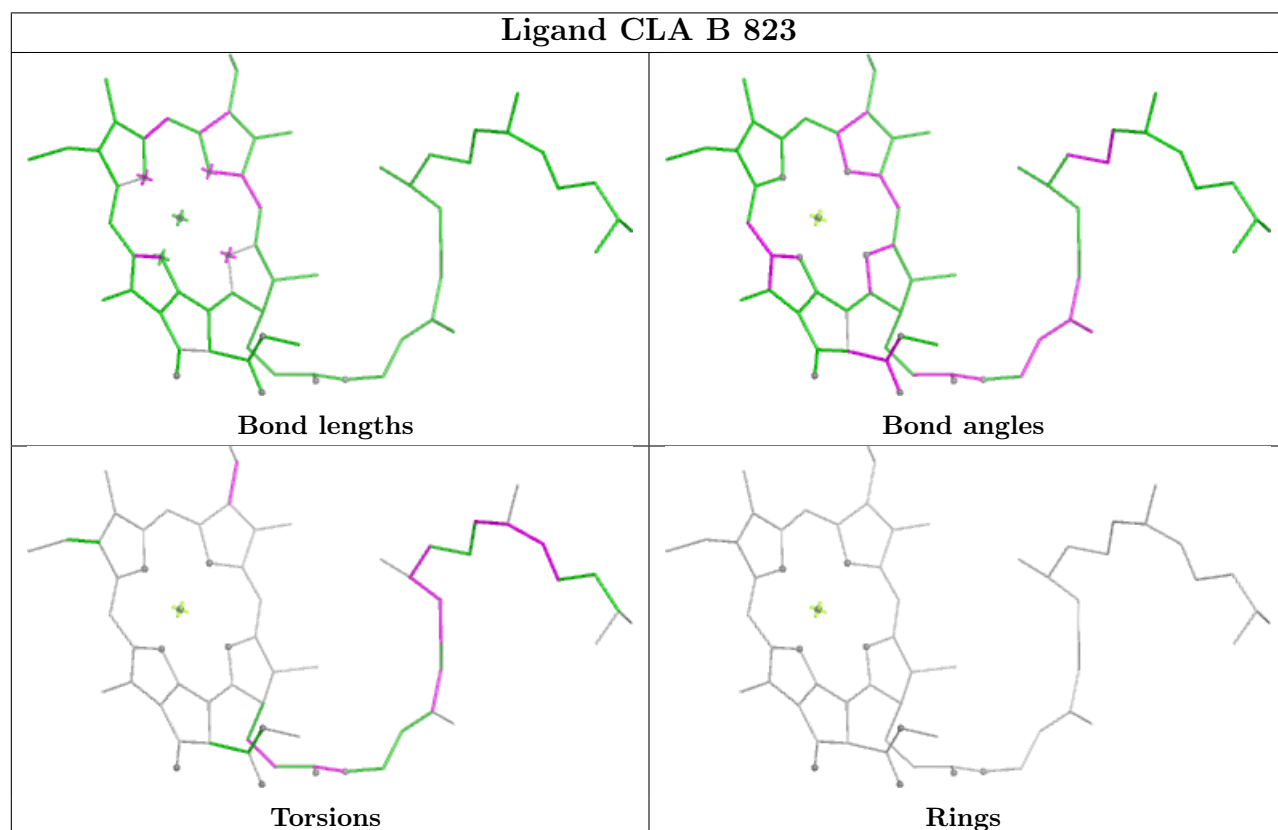




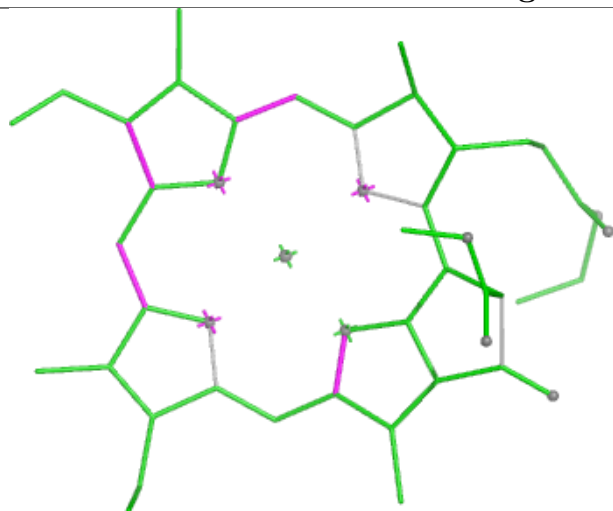
Ligand CLA A 807



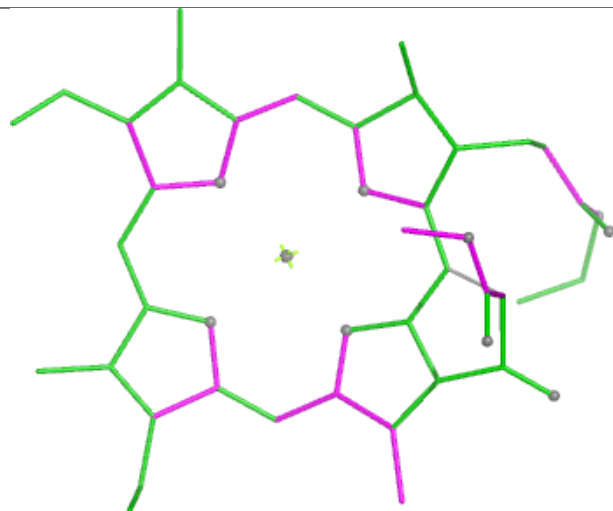
Ligand CLA B 823



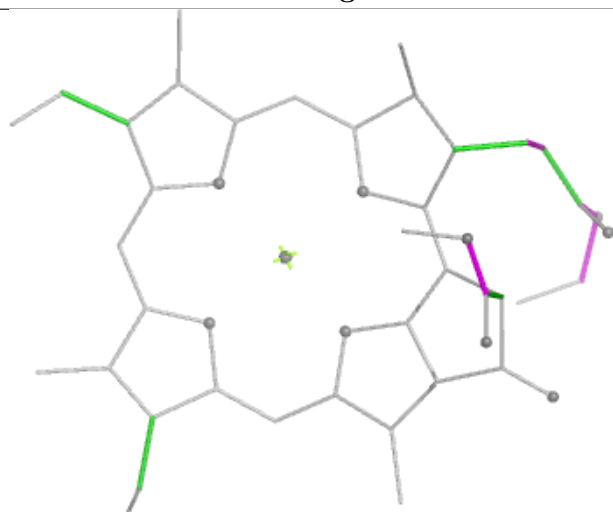
Ligand CLA 3 605



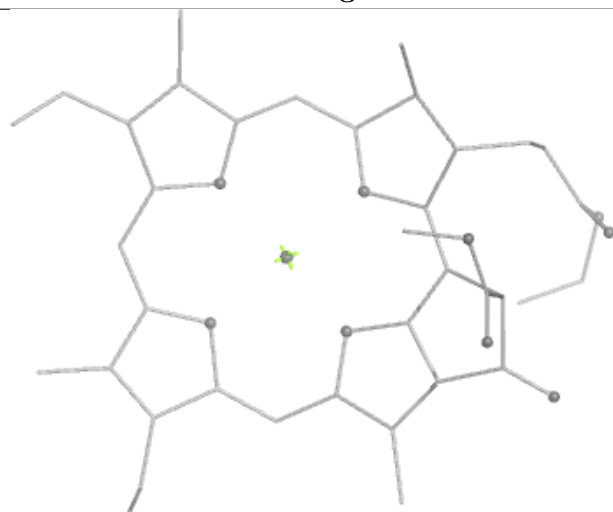
Bond lengths



Bond angles

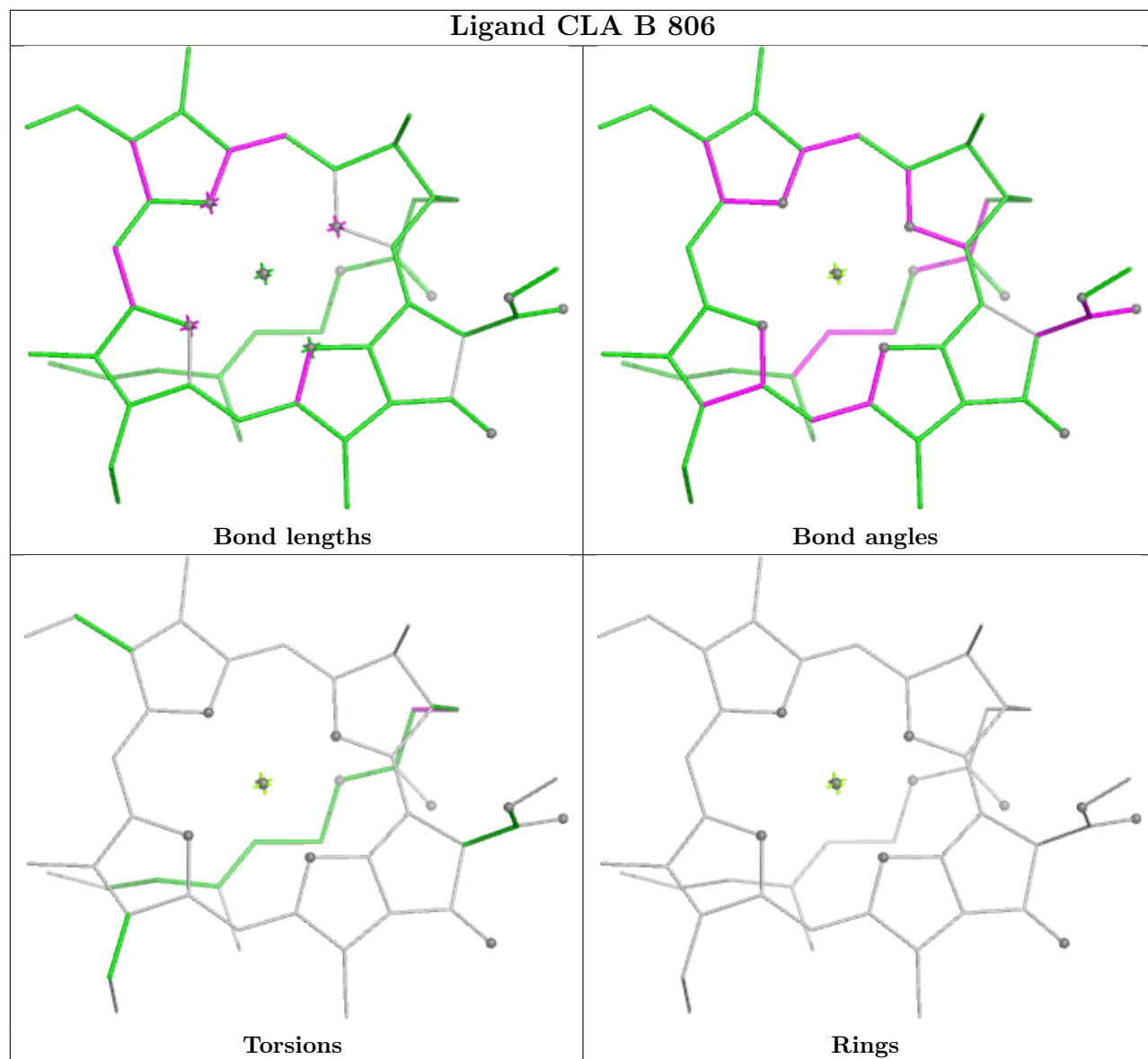


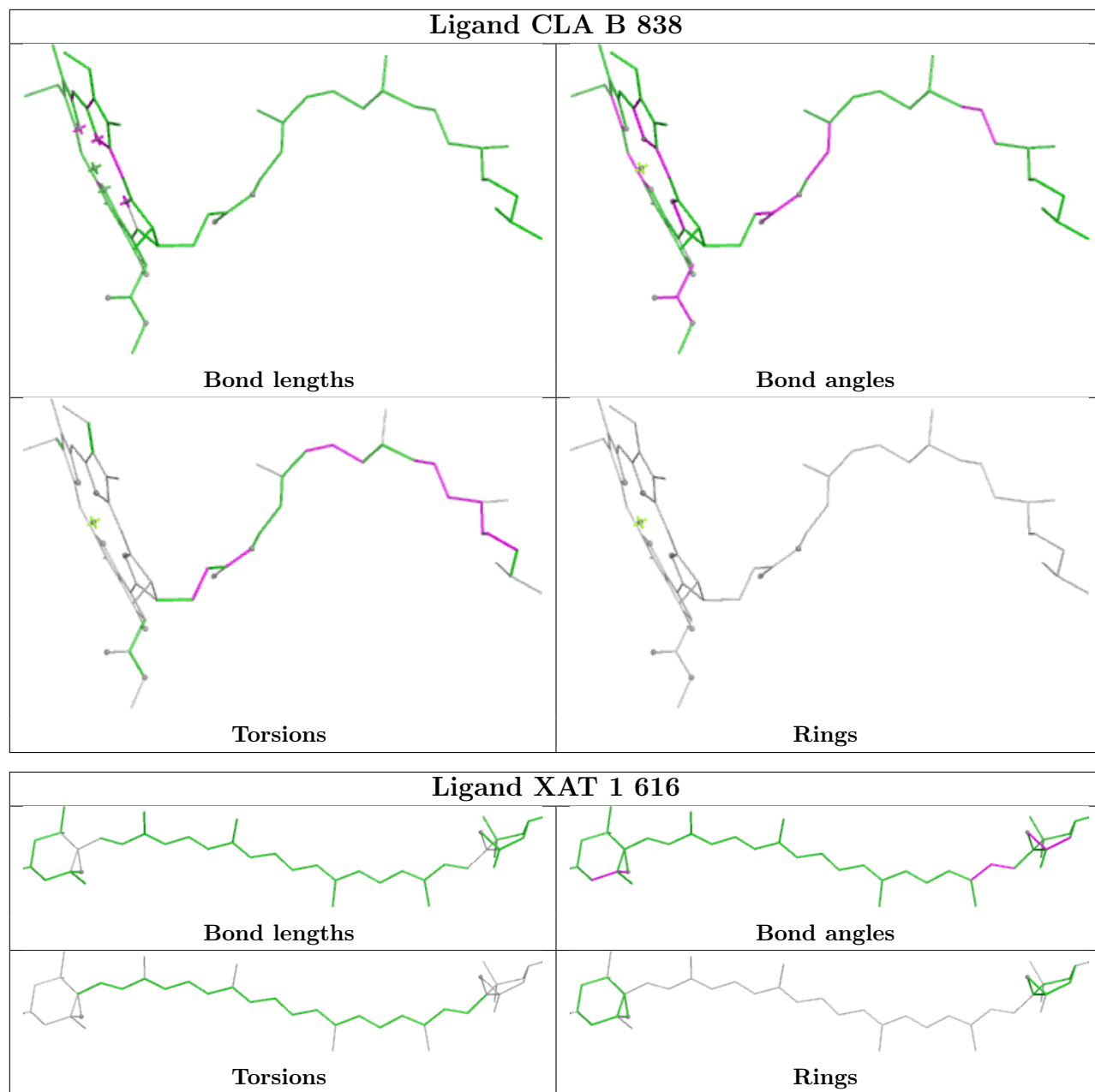
Torsions



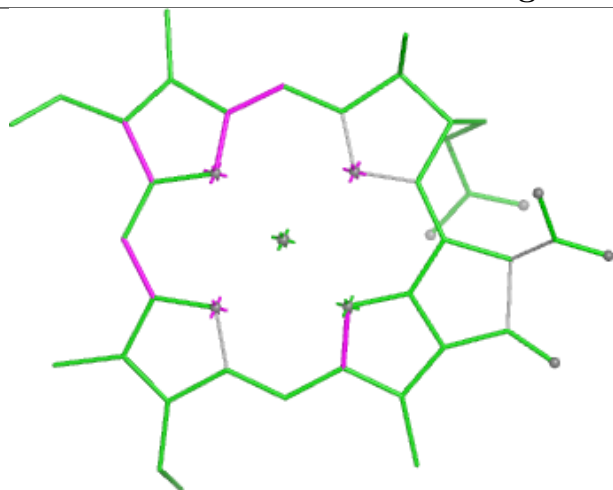
Rings

Ligand CLA B 806

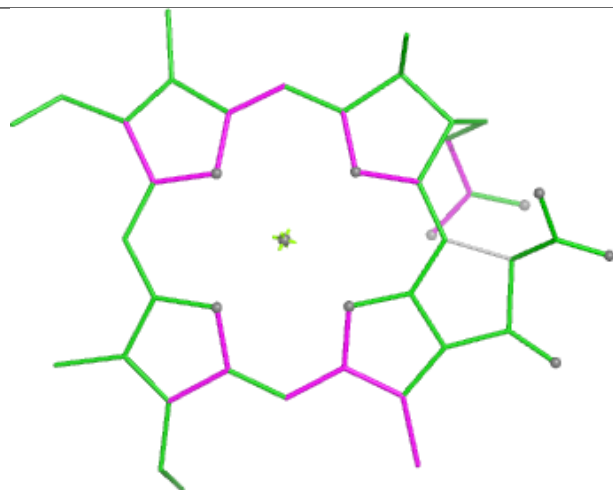




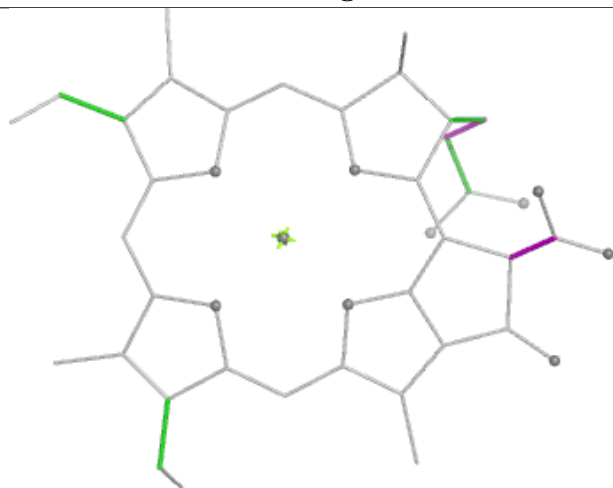
Ligand CLA 3 611



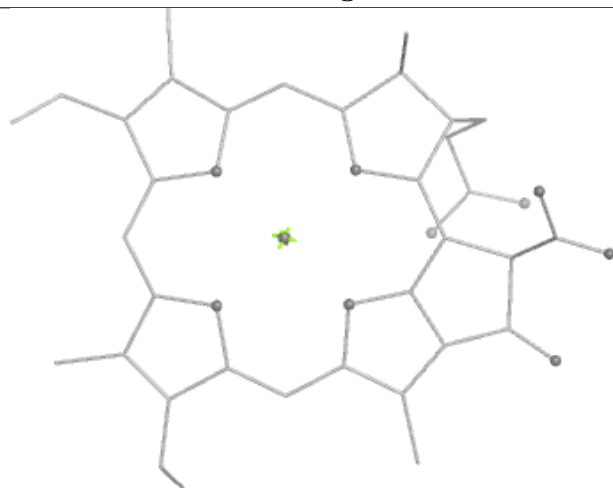
Bond lengths



Bond angles

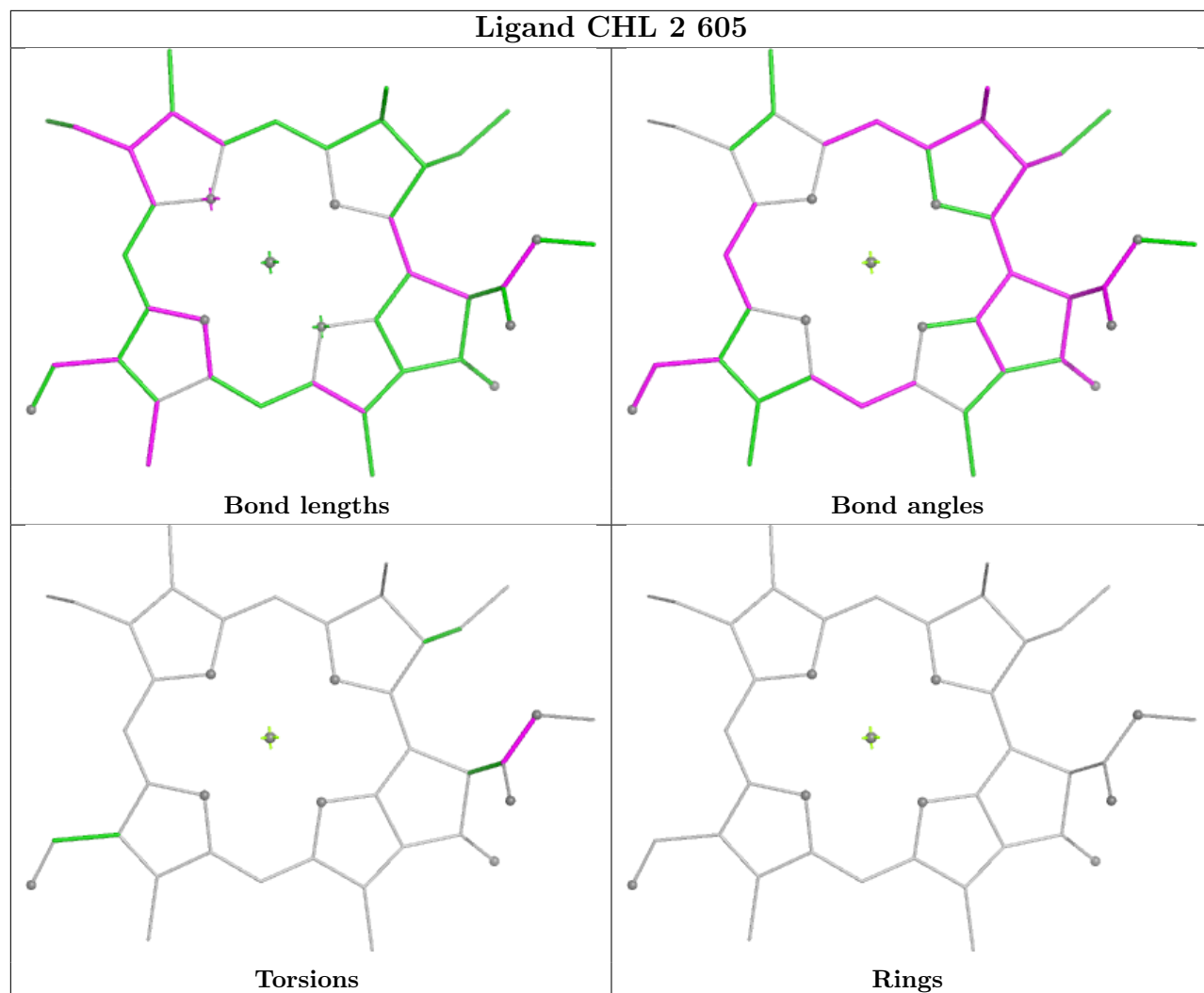


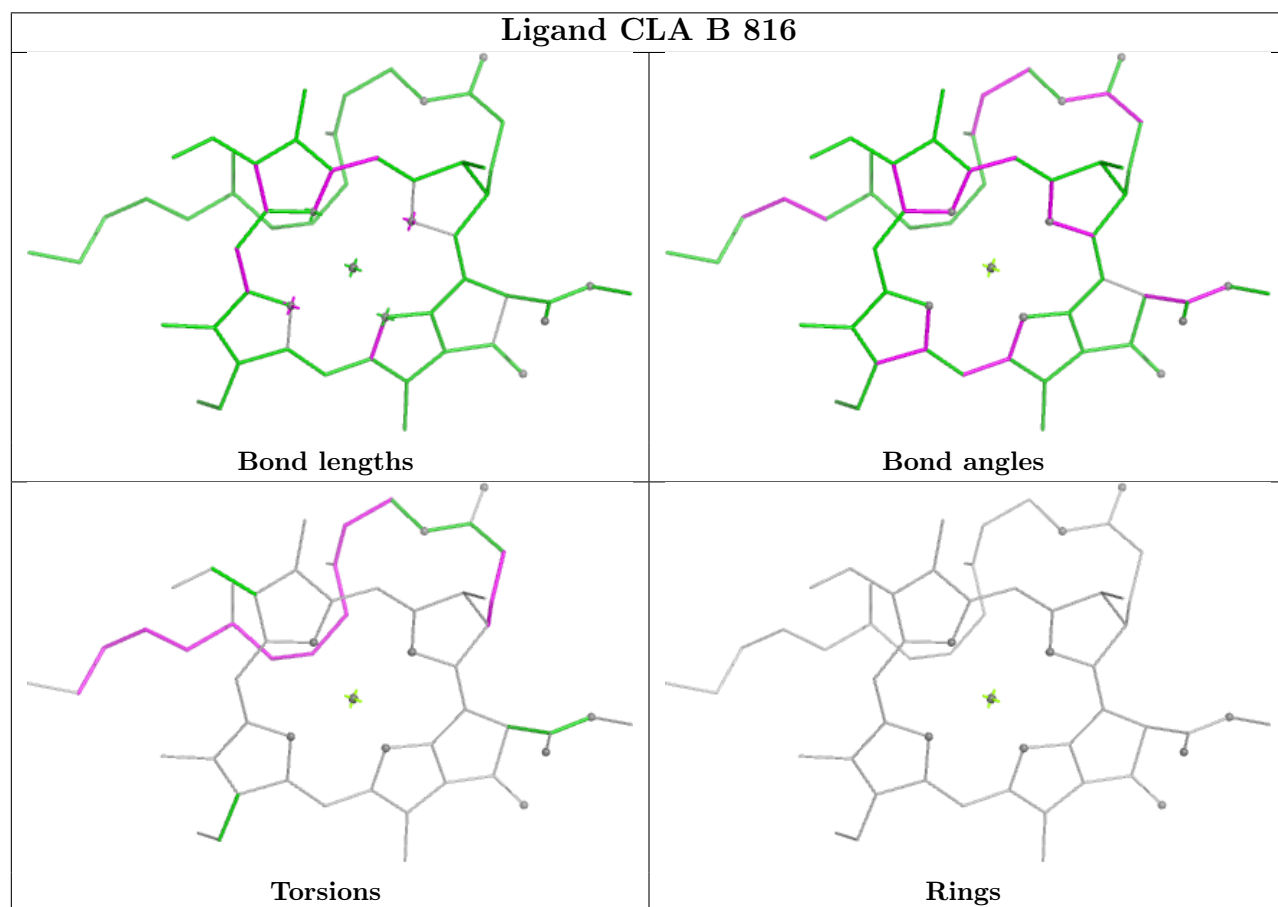
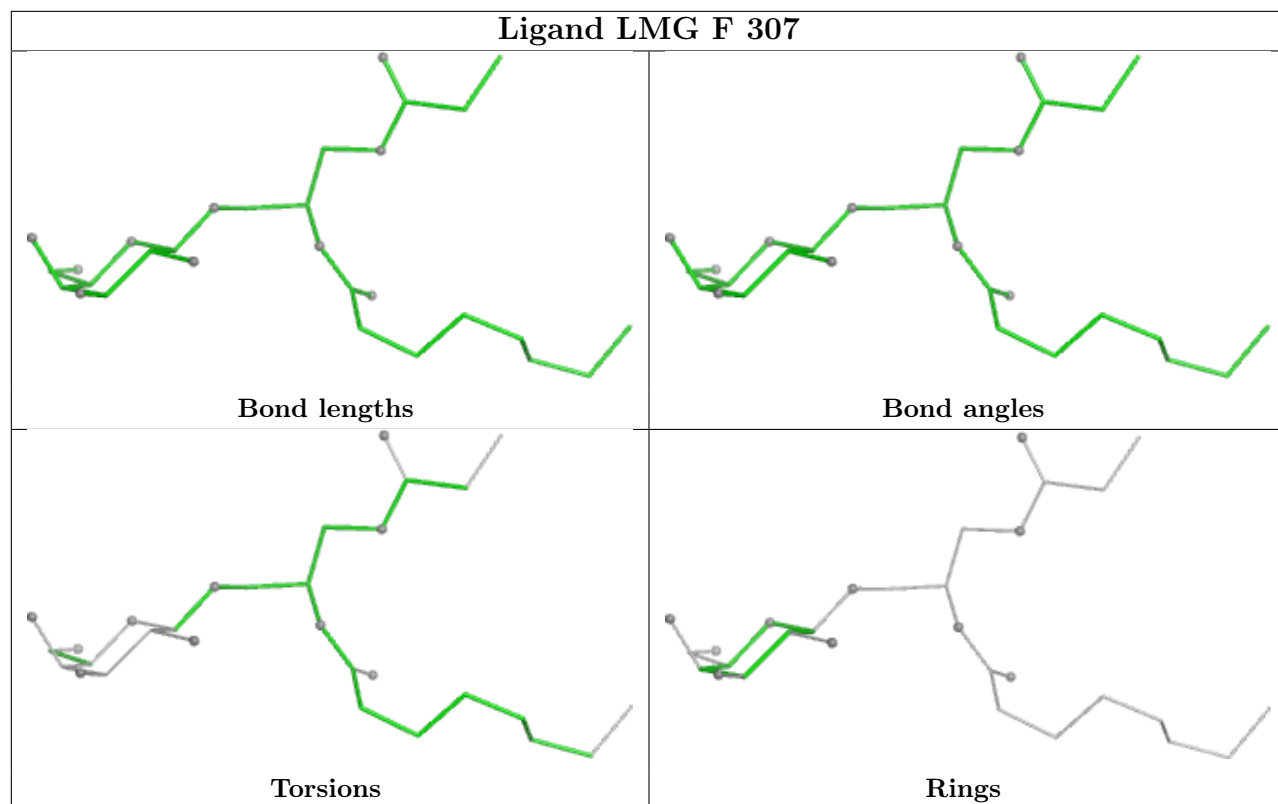
Torsions

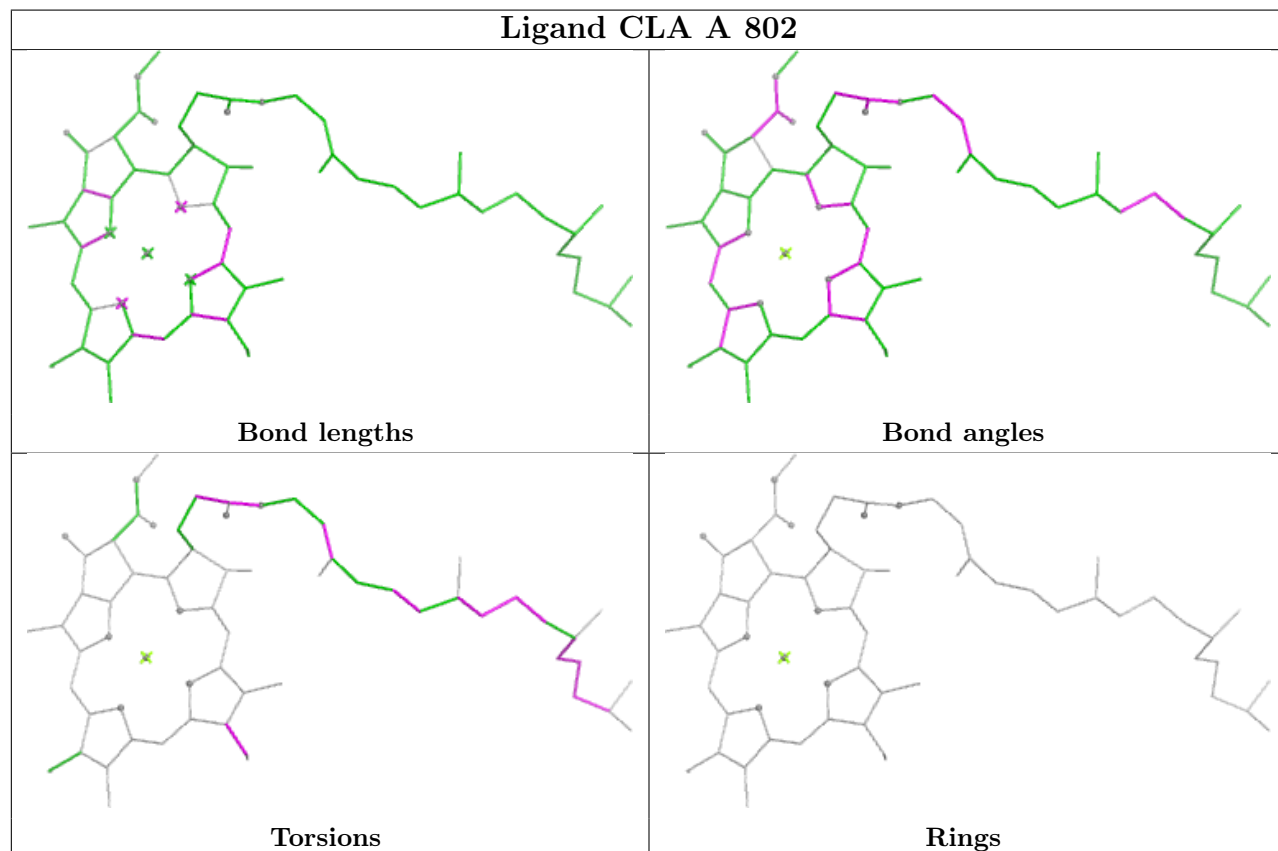
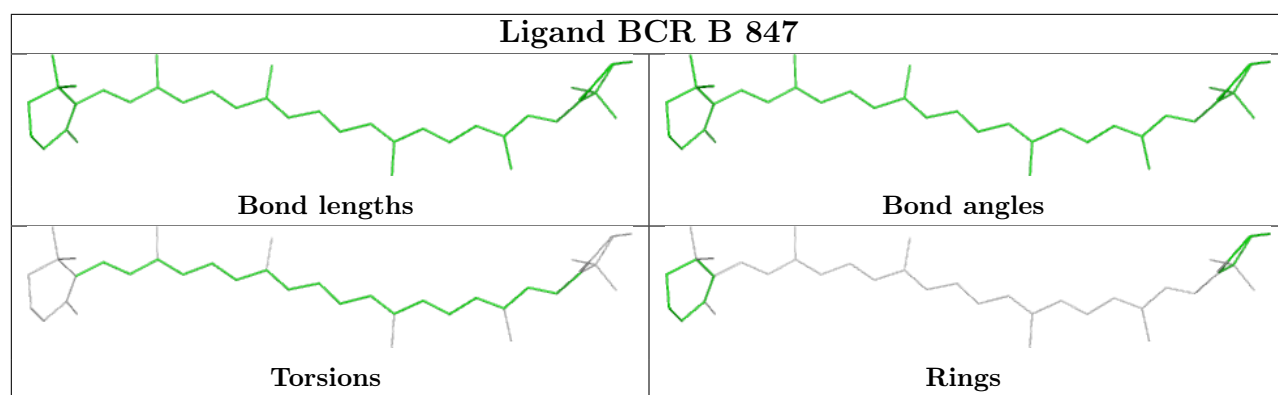


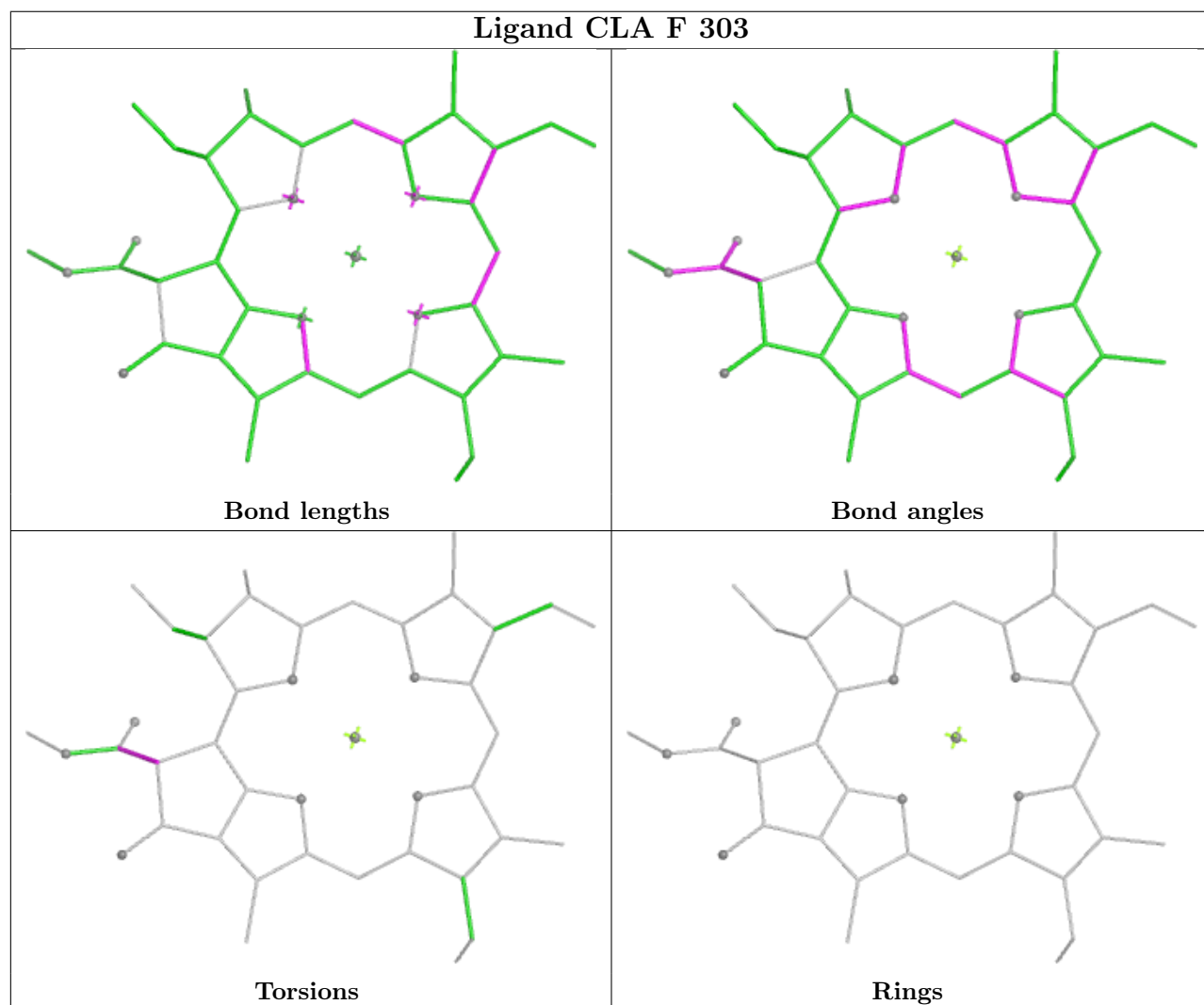
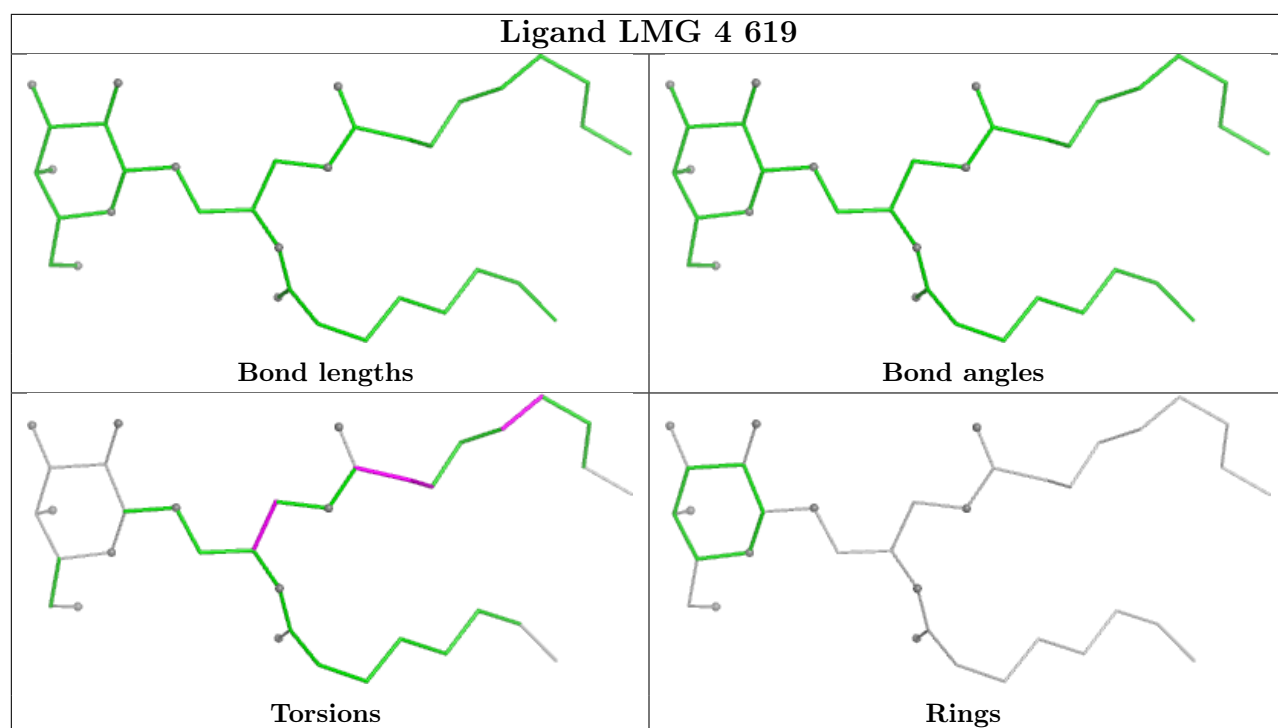
Rings

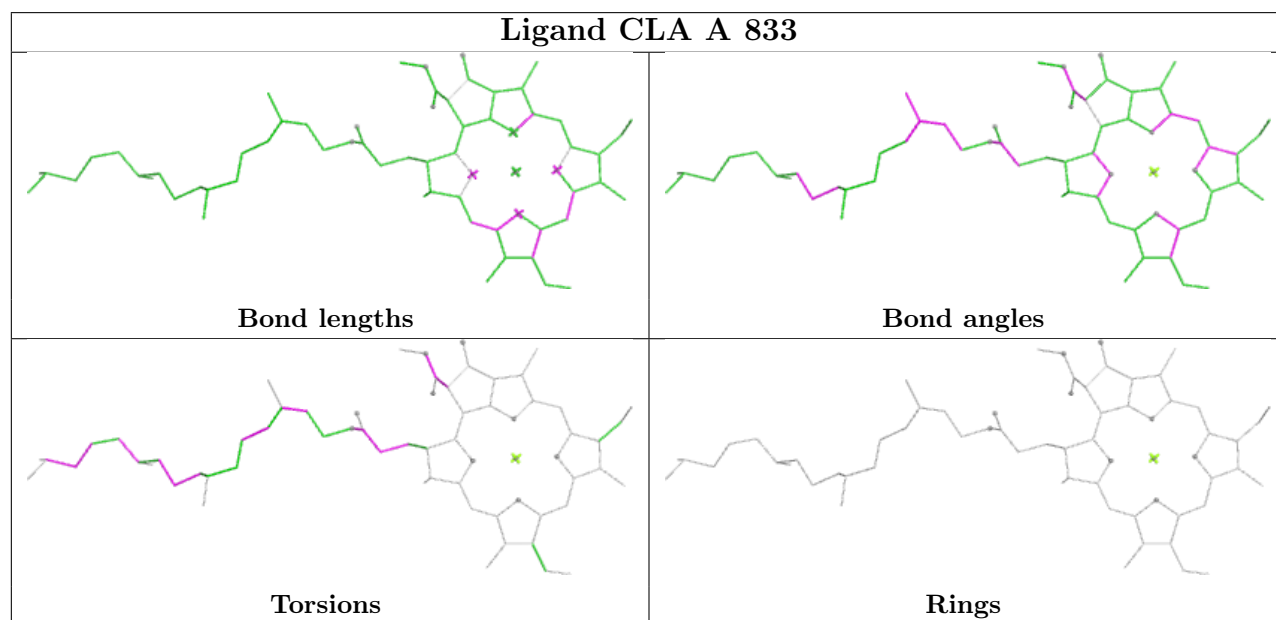
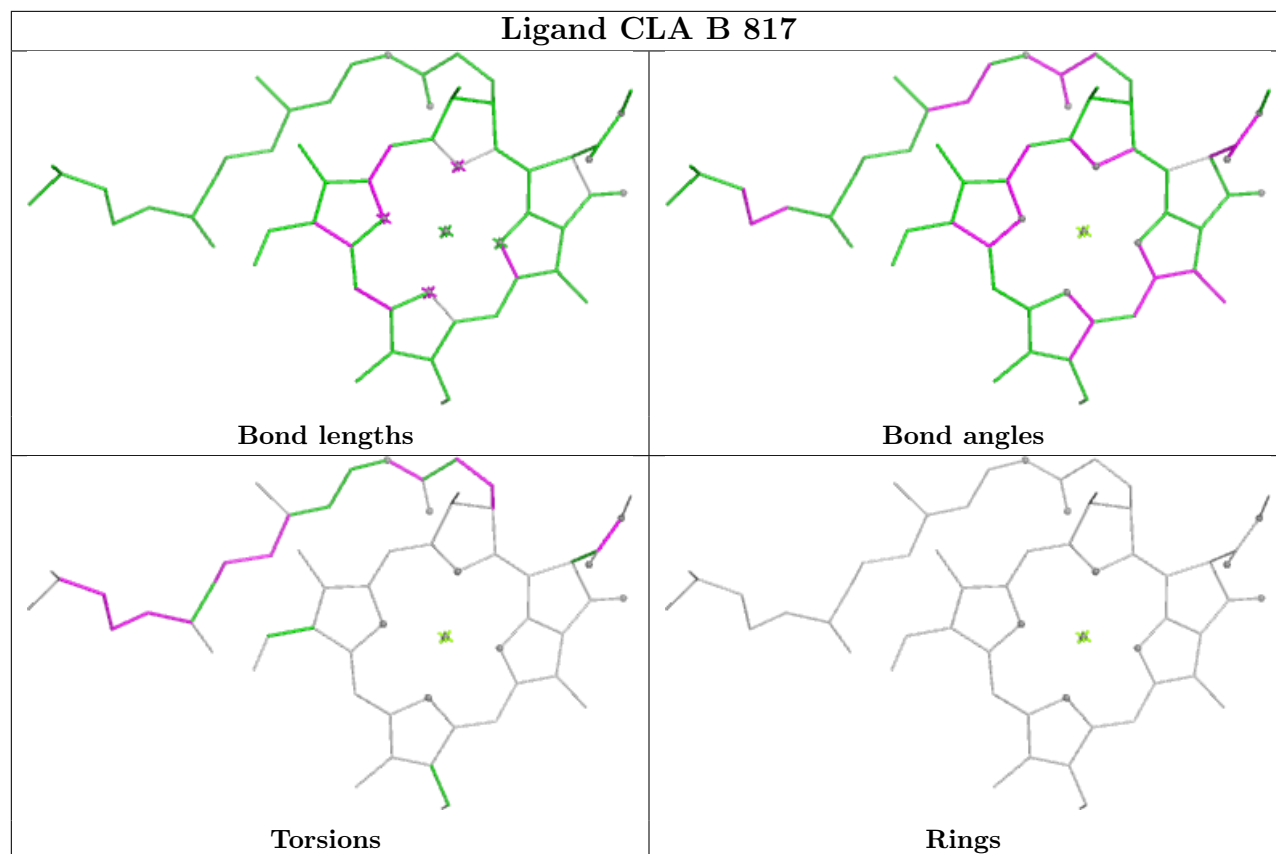
Ligand CHL 2 605



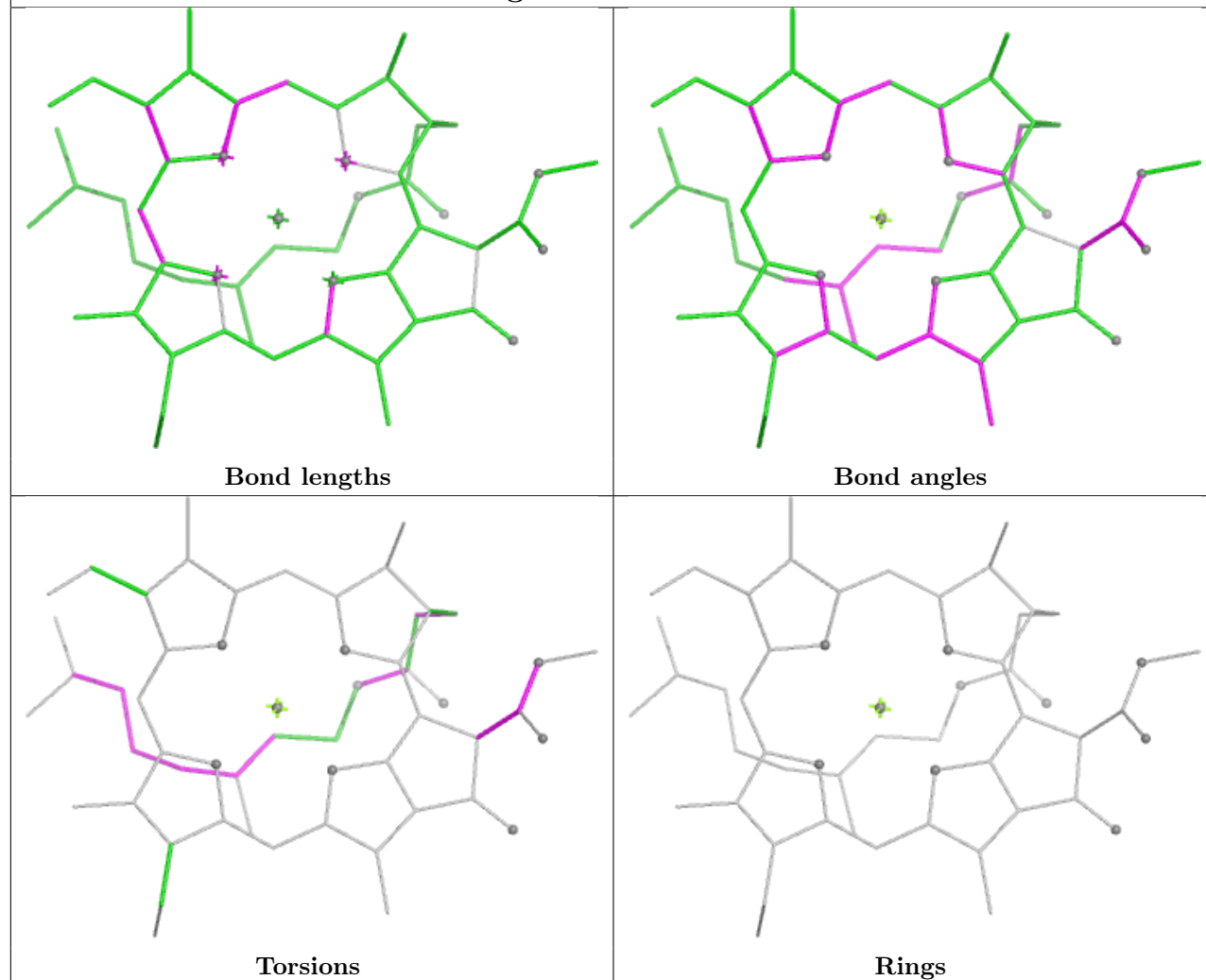




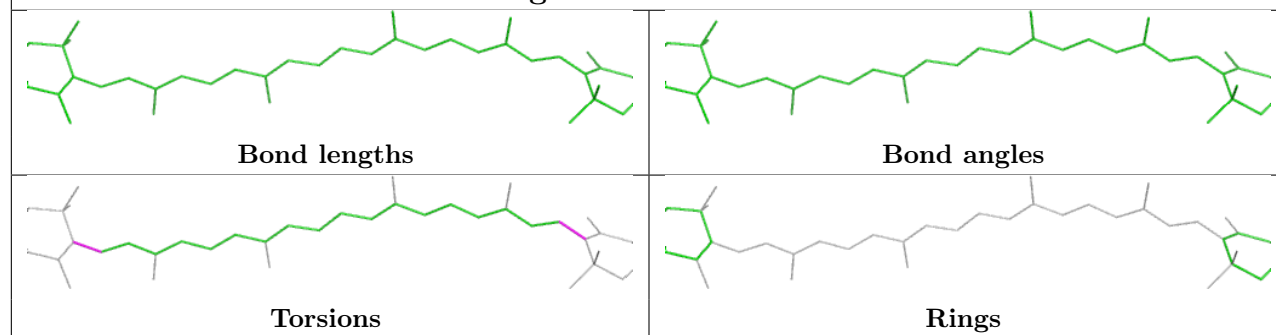


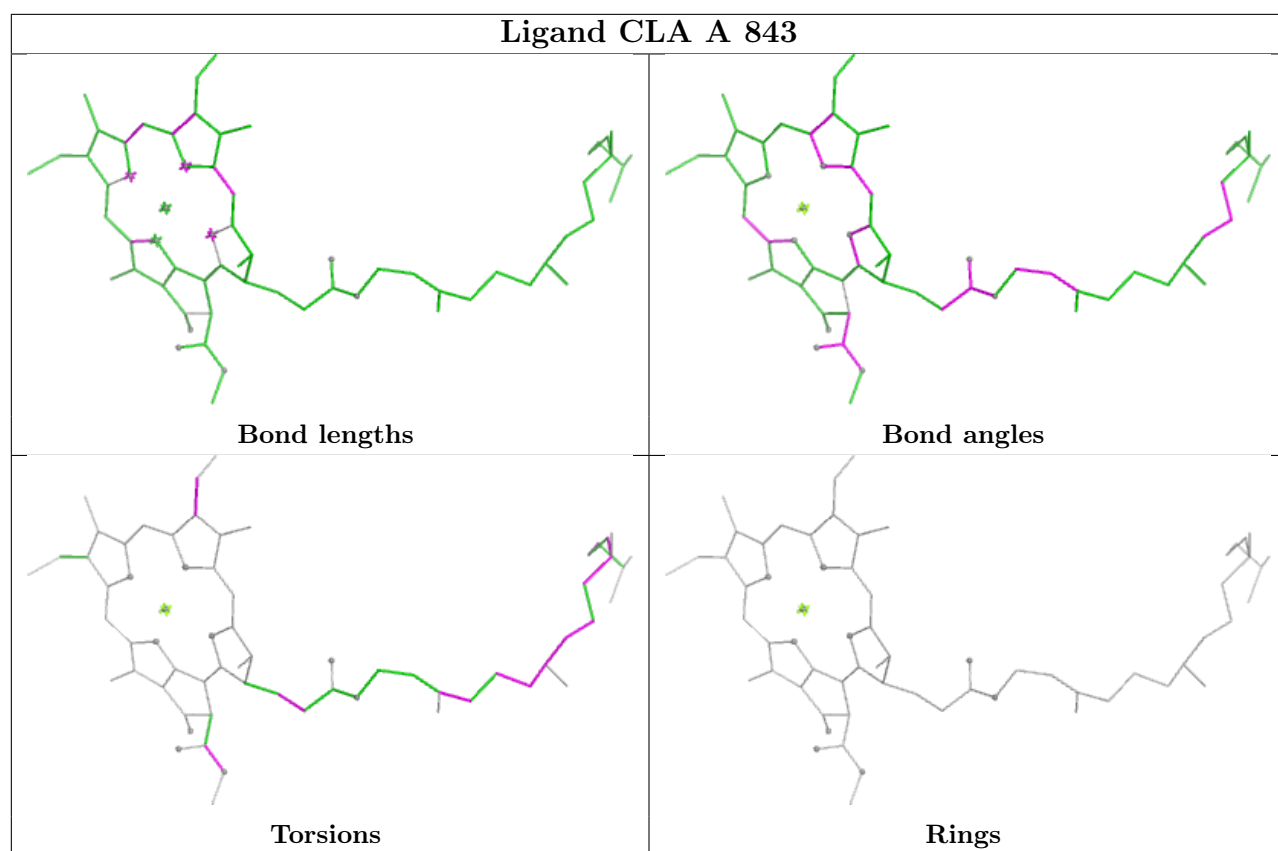


Ligand CLA 2 612

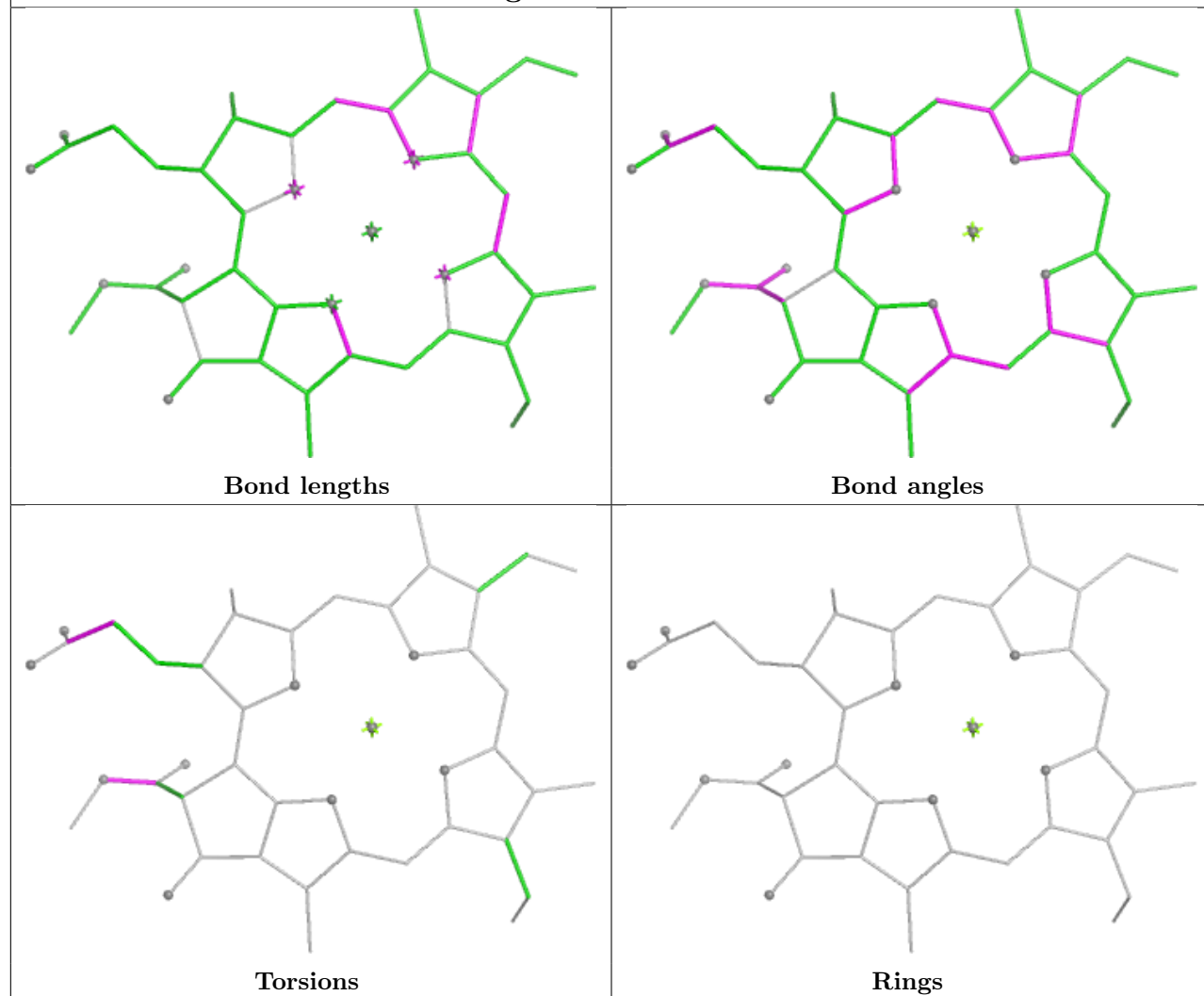


Ligand BCR K 205

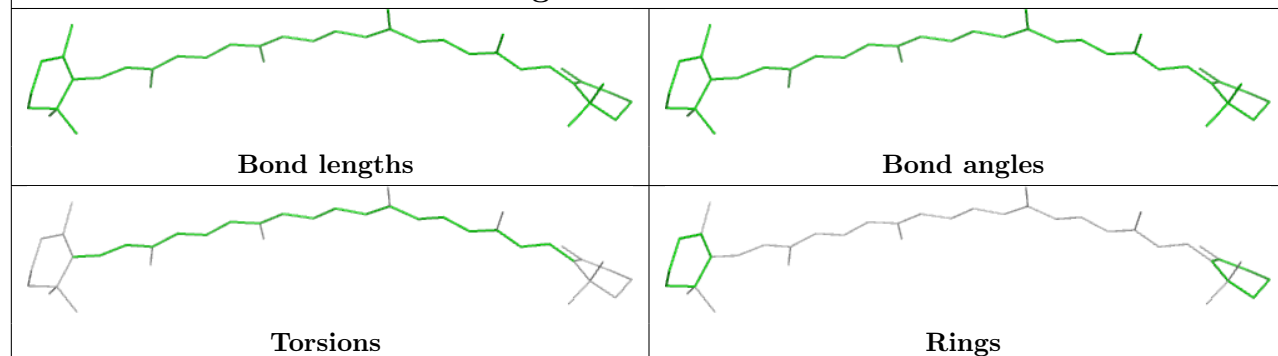


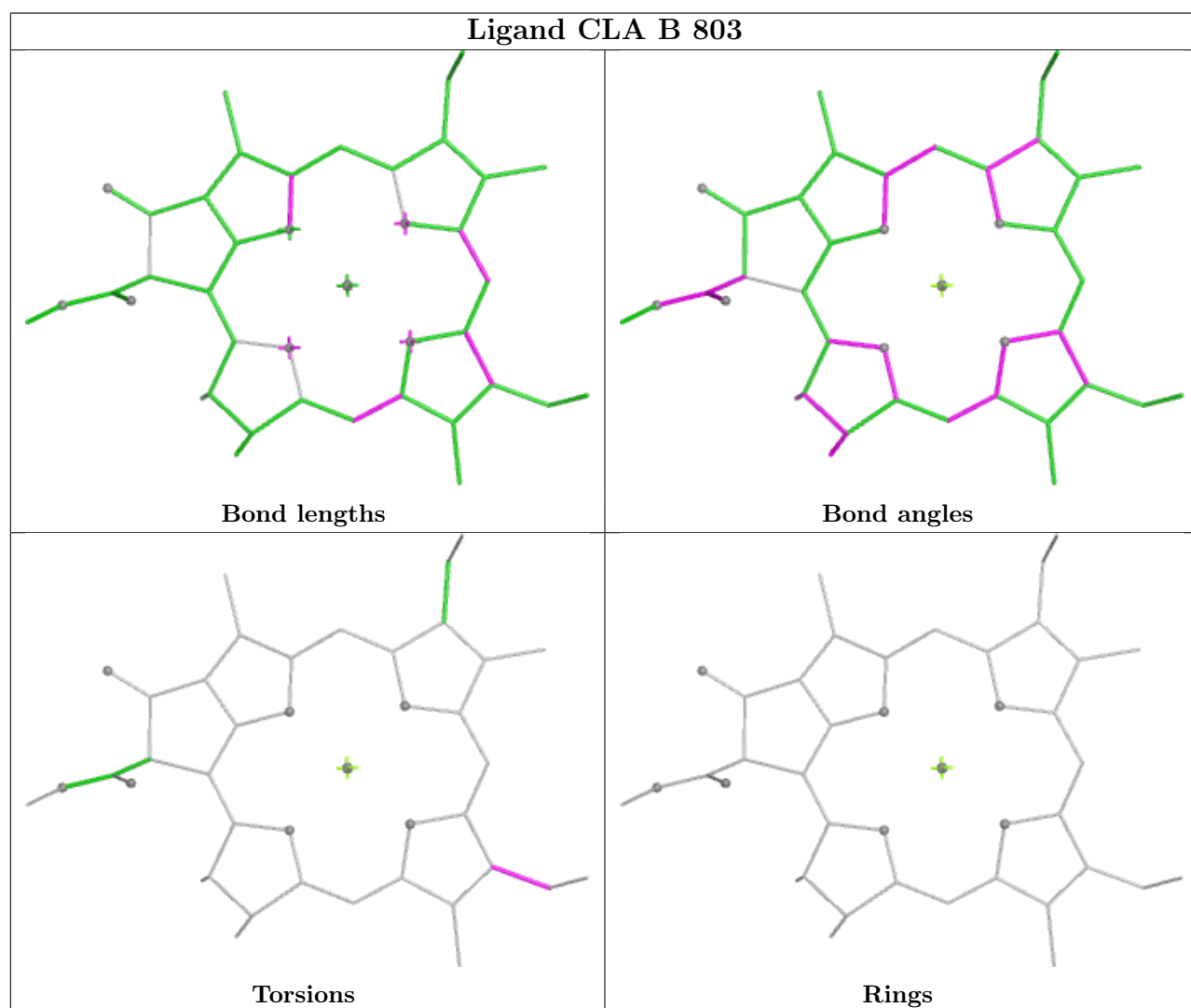
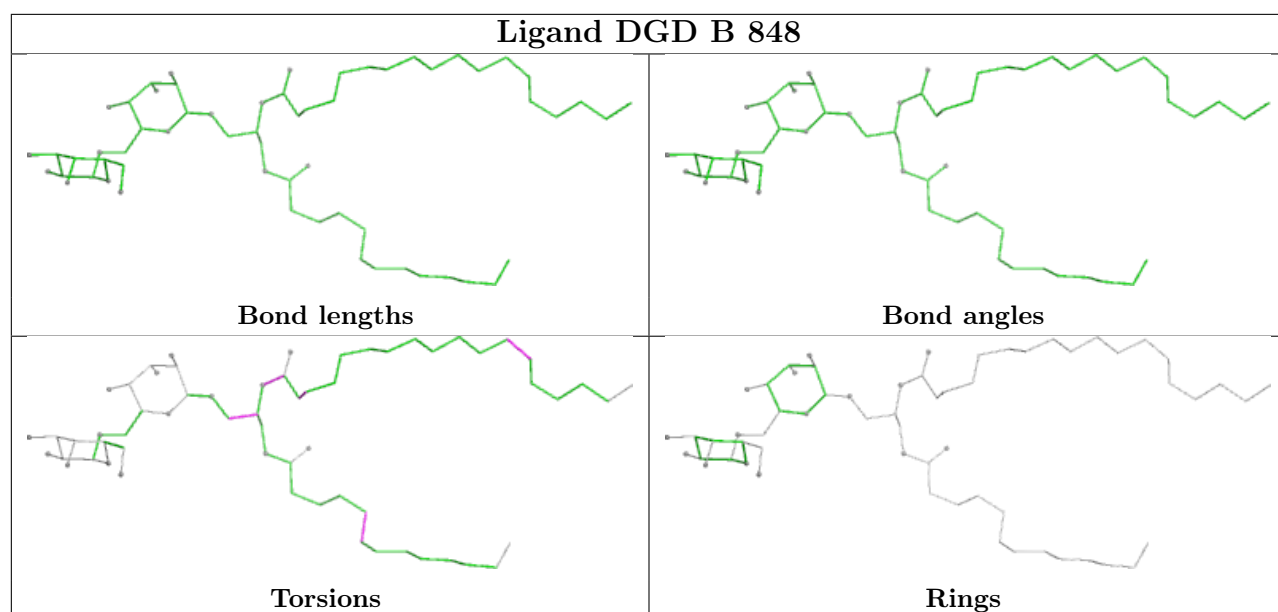


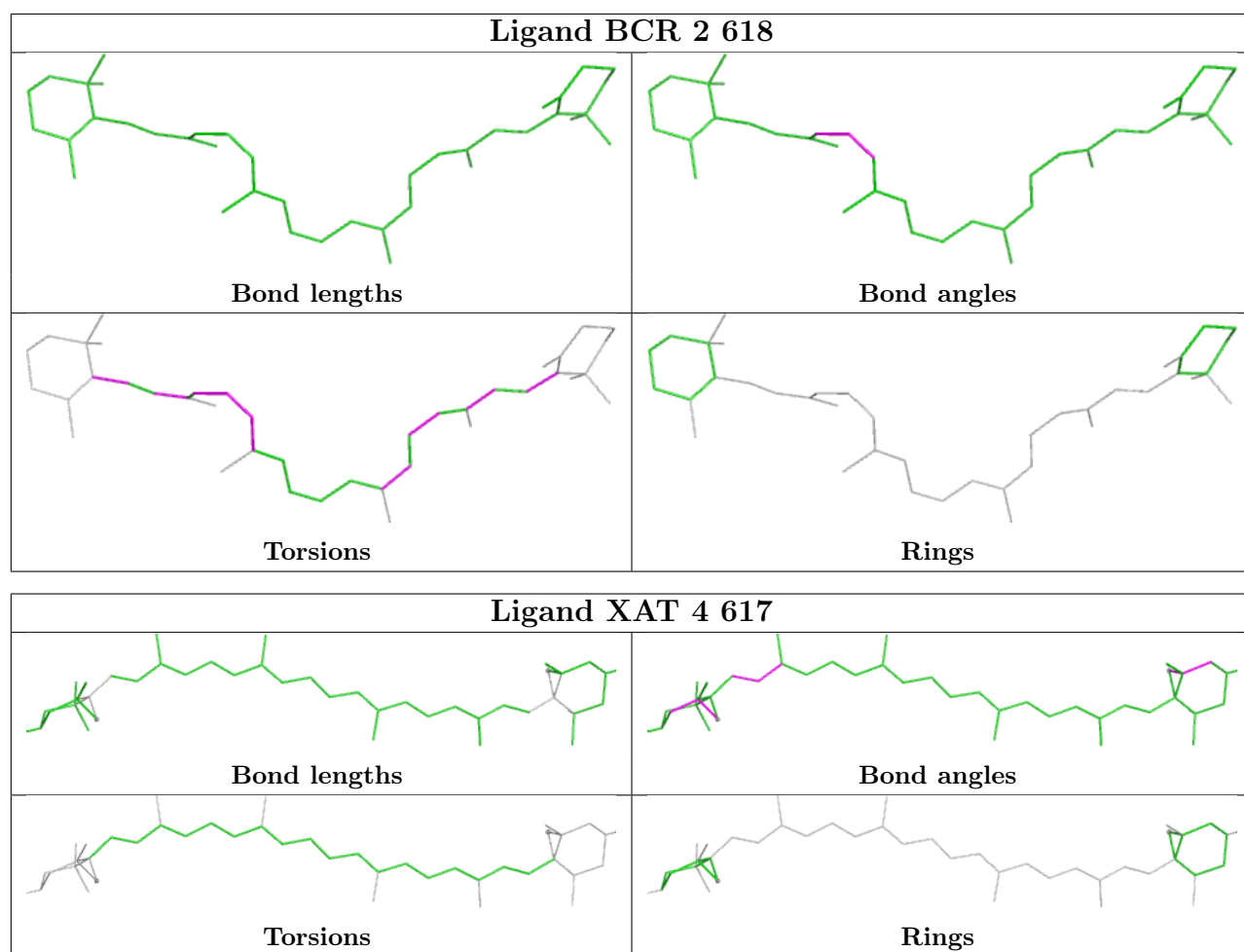
Ligand CLA 2 611

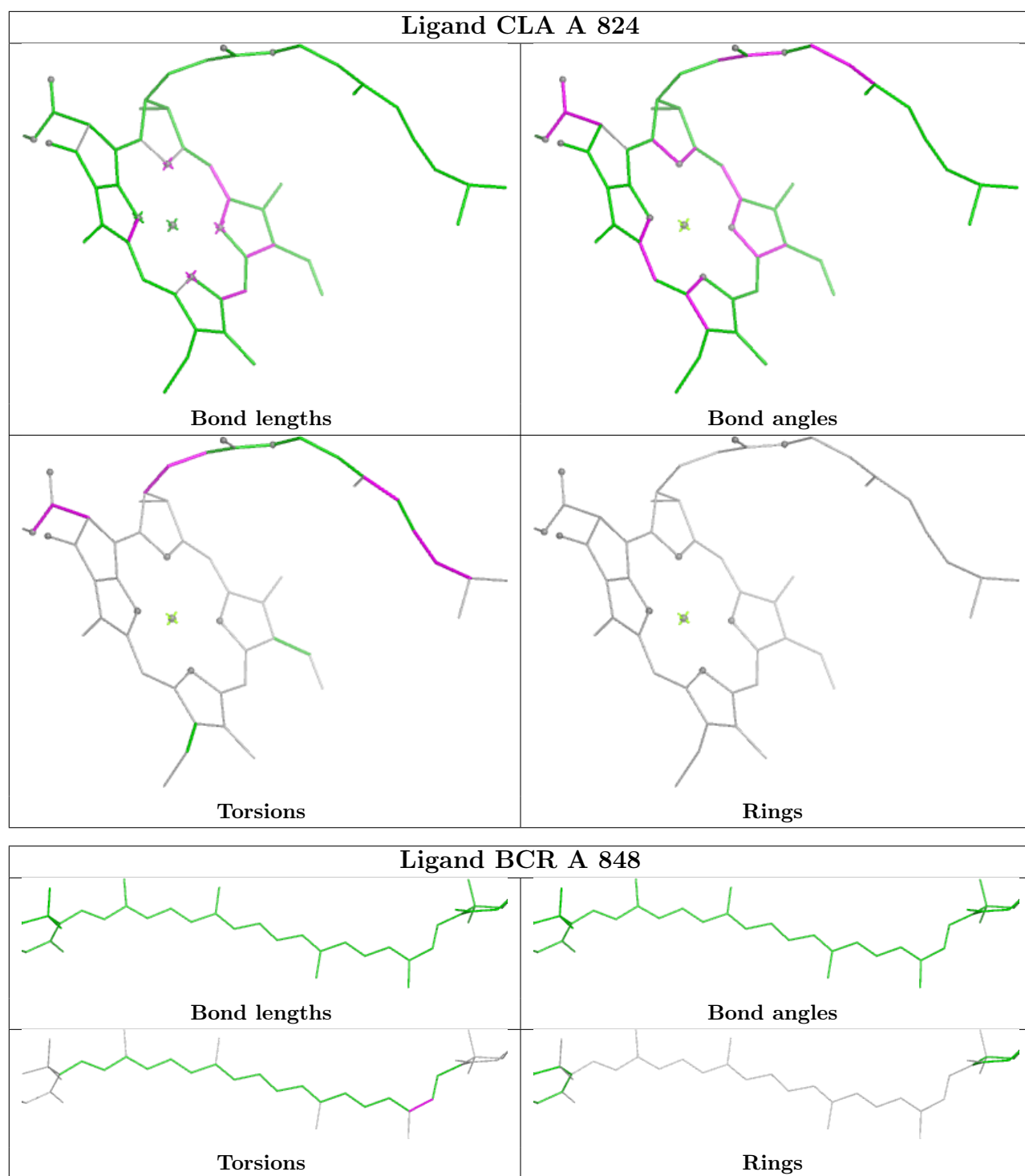


Ligand BCR F 302

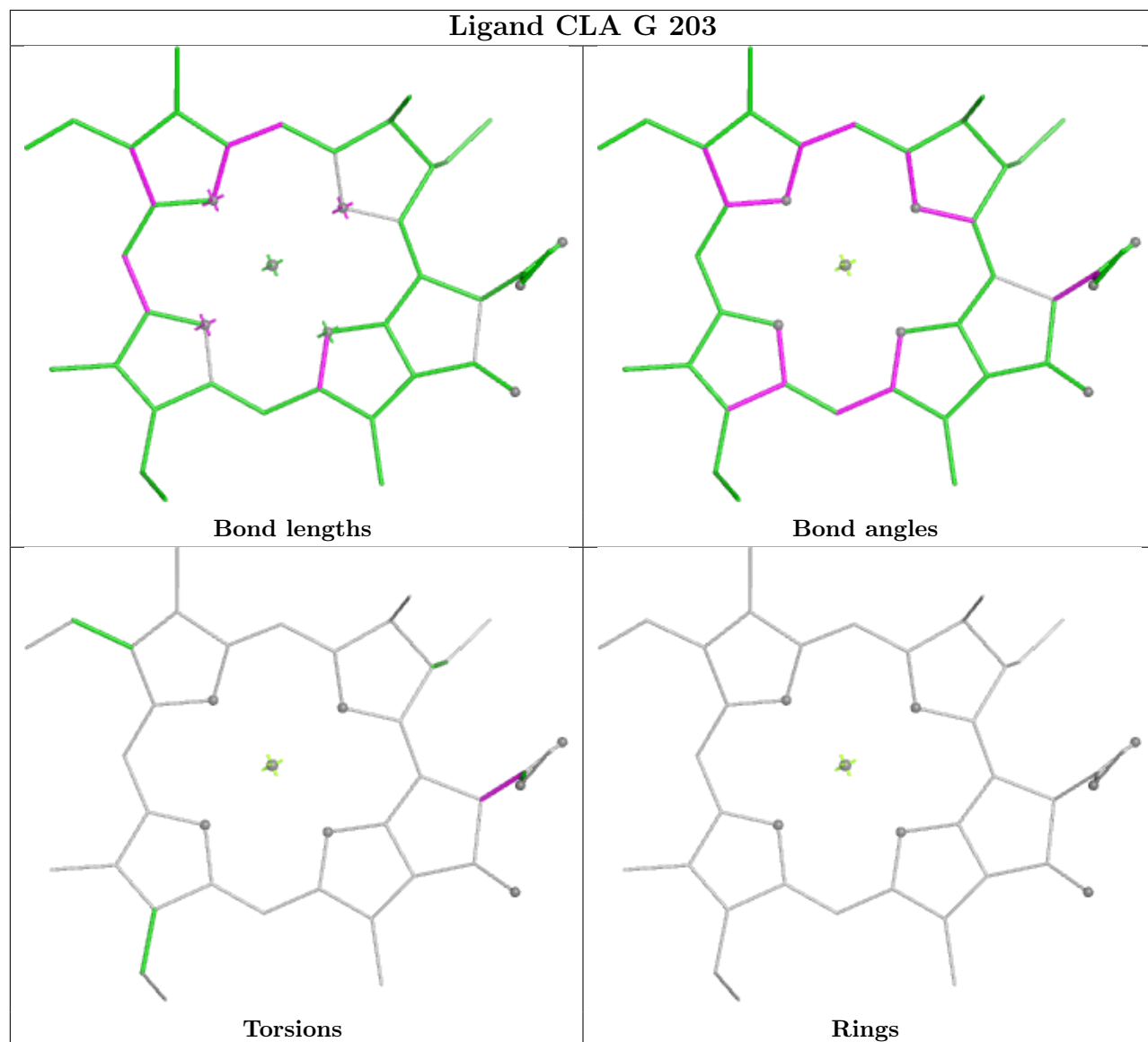




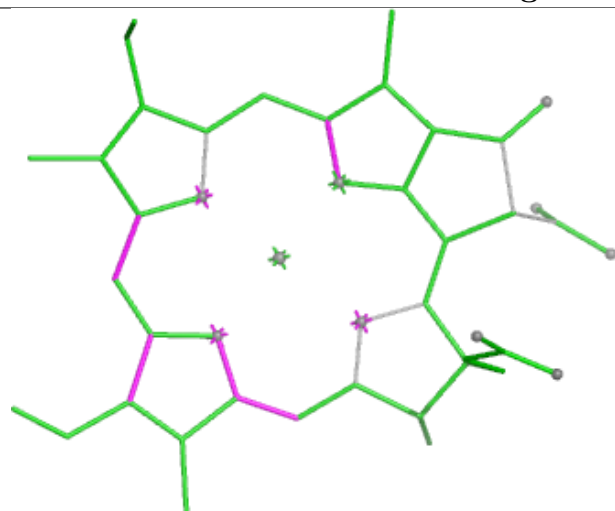




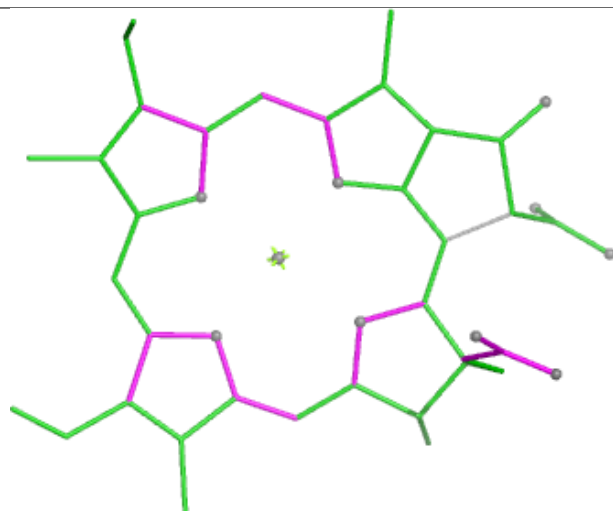
Ligand CLA G 203



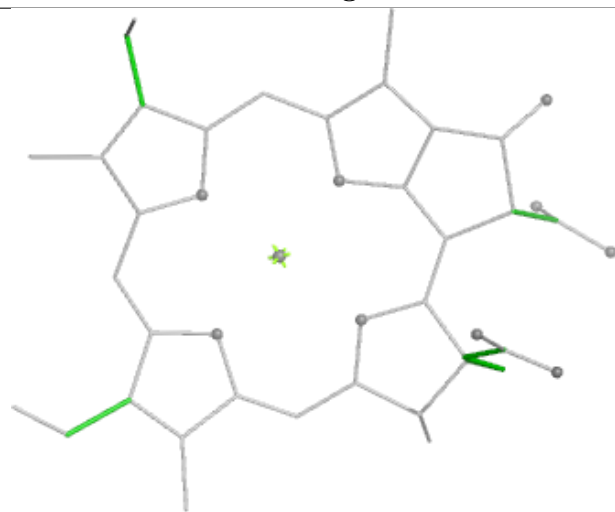
Ligand CLA 1 607



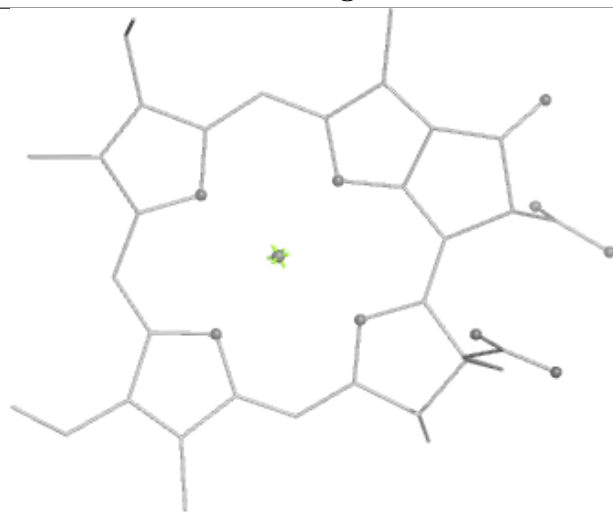
Bond lengths



Bond angles

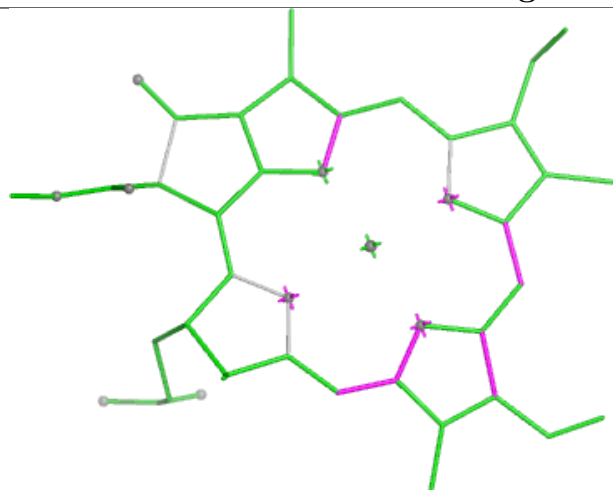


Torsions

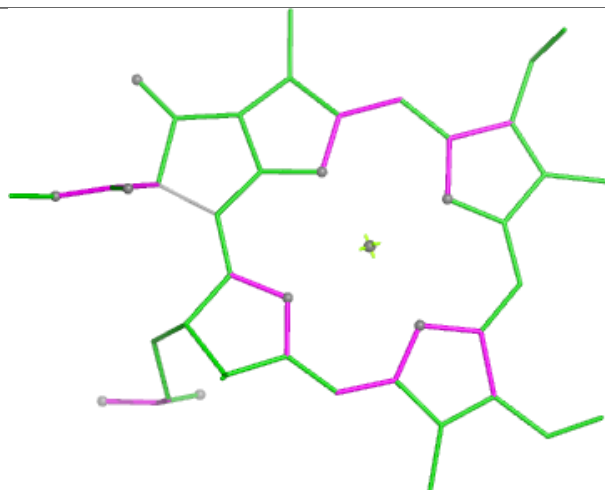


Rings

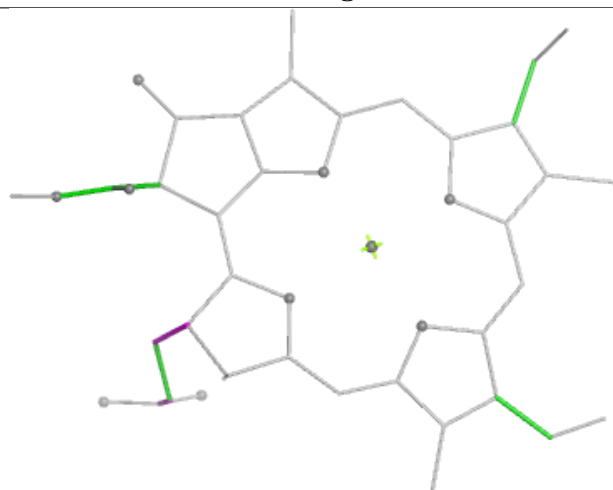
Ligand CLA 2 608



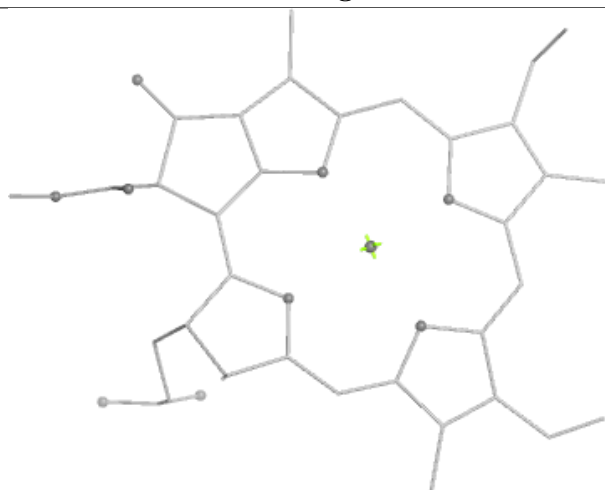
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR L 301



Bond lengths



Bond angles

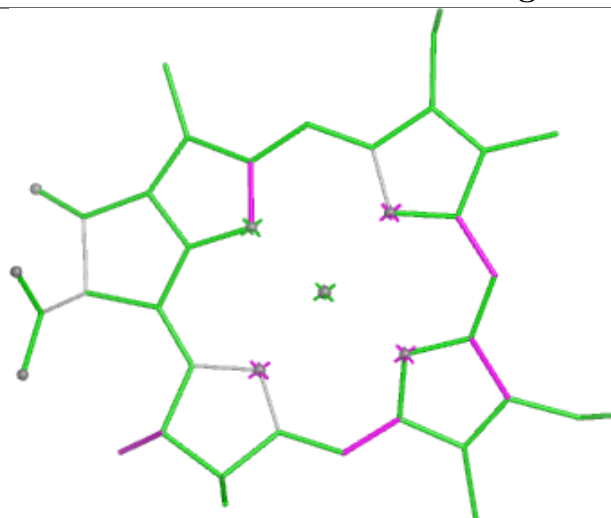


Torsions

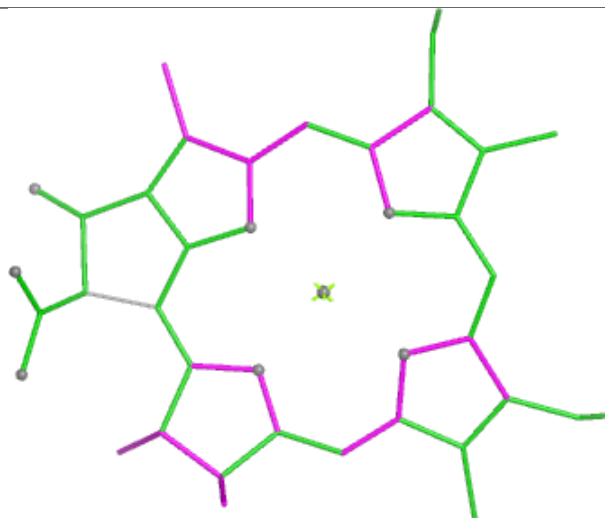


Rings

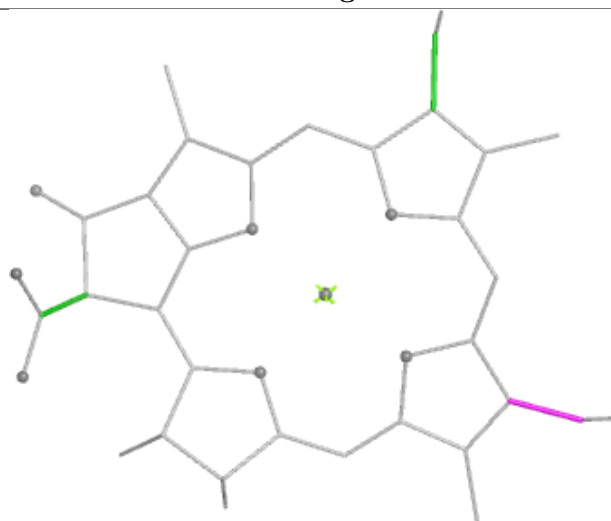
Ligand CLA 3 612



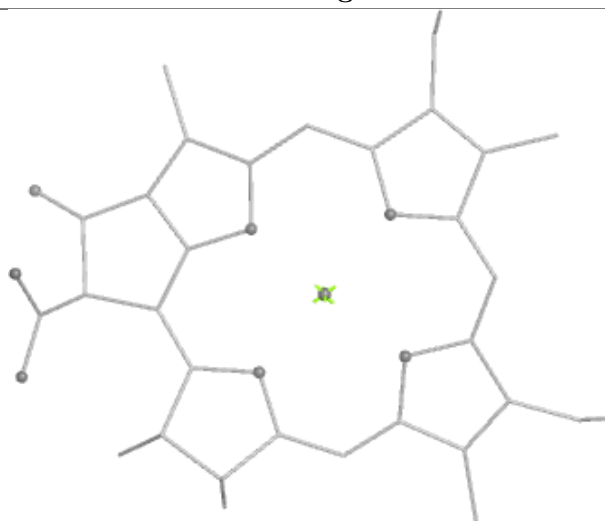
Bond lengths



Bond angles

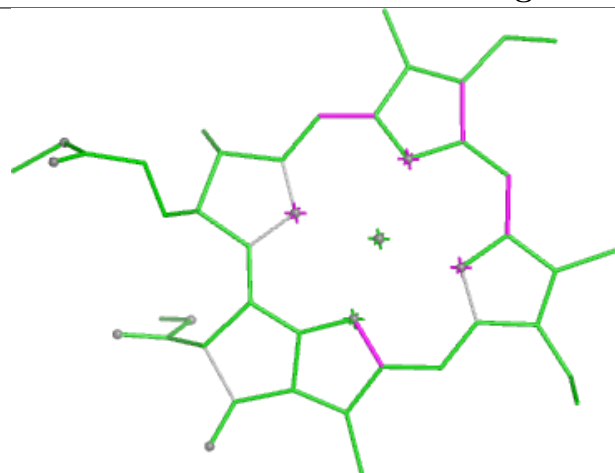


Torsions

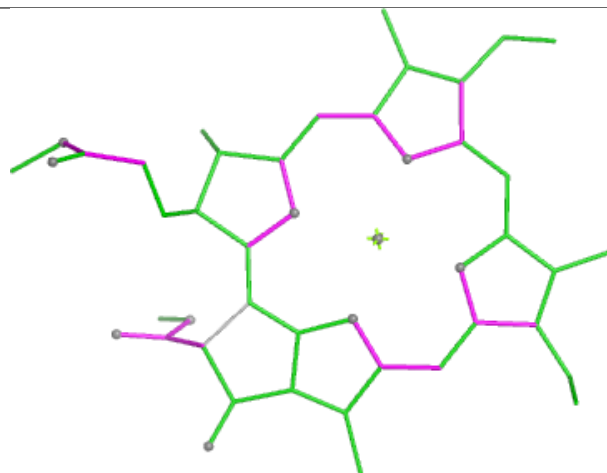


Rings

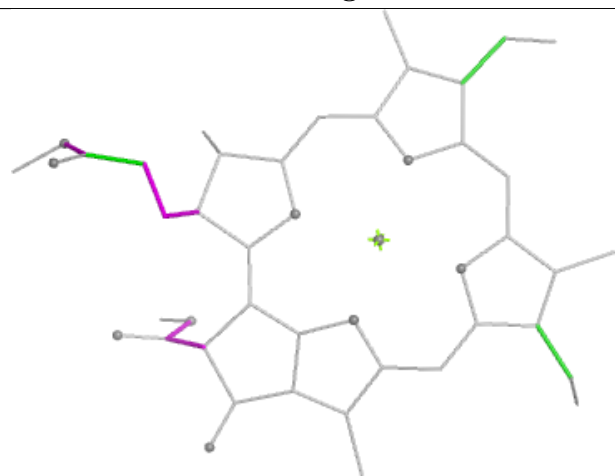
Ligand CLA K 203



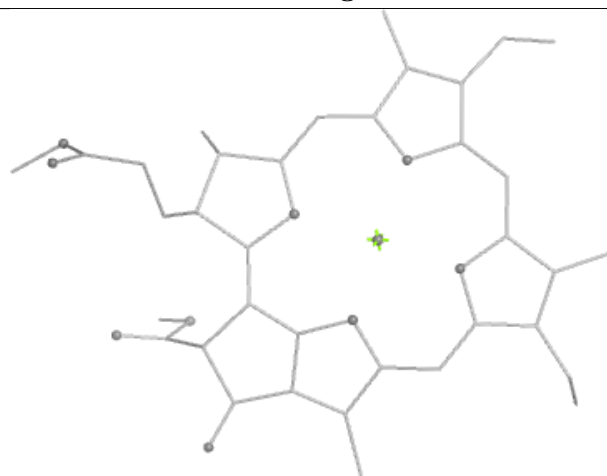
Bond lengths



Bond angles

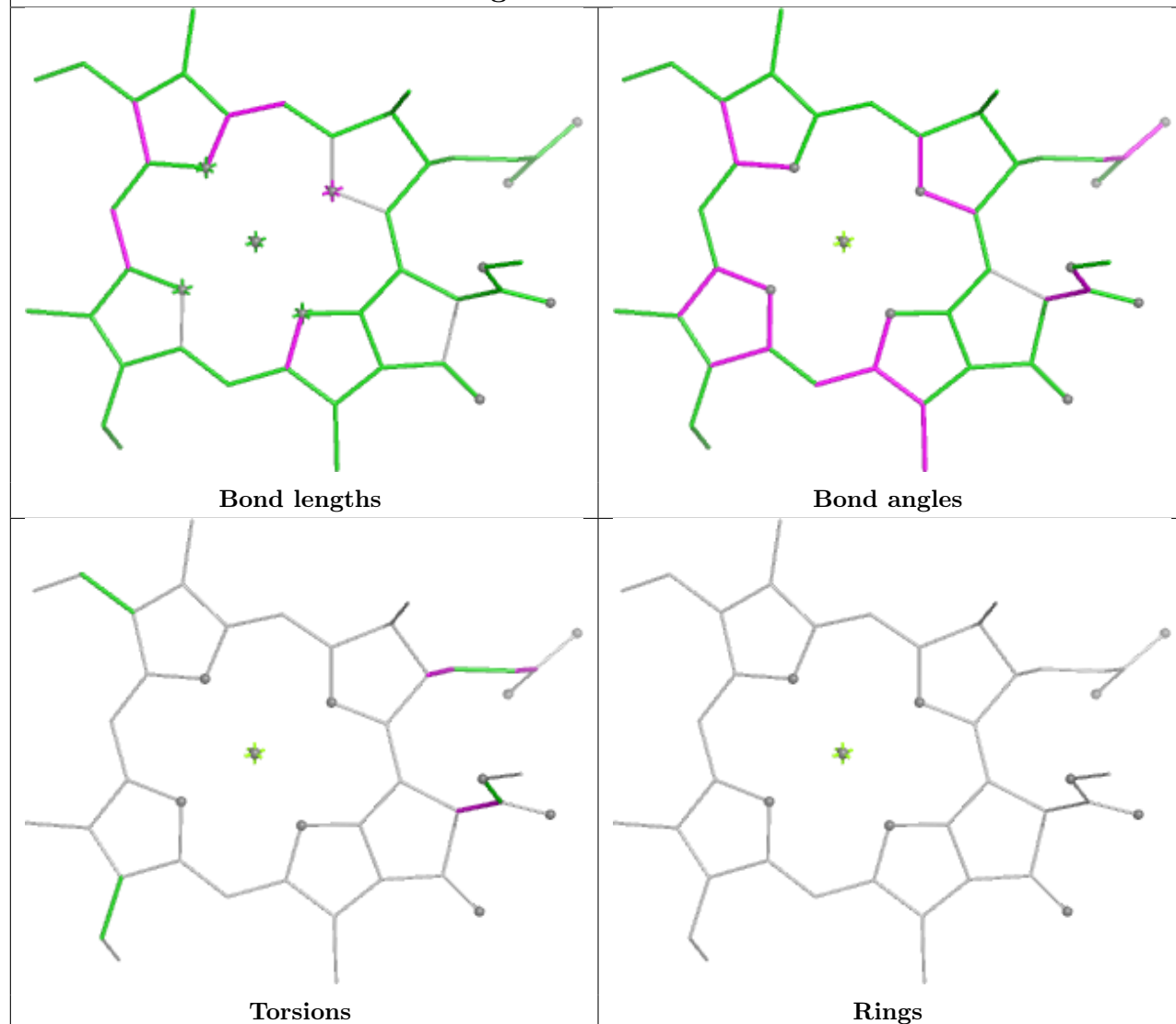


Torsions

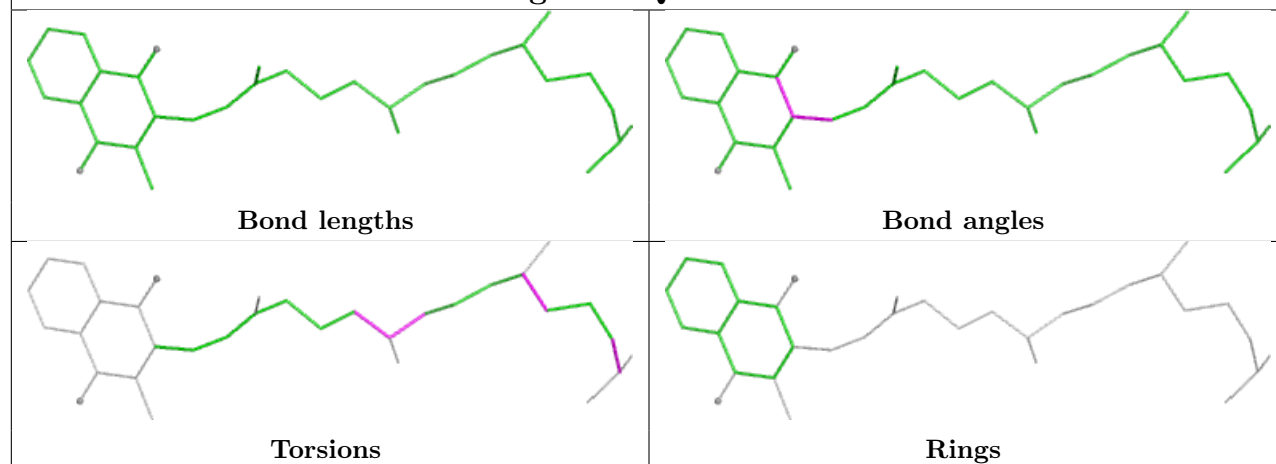


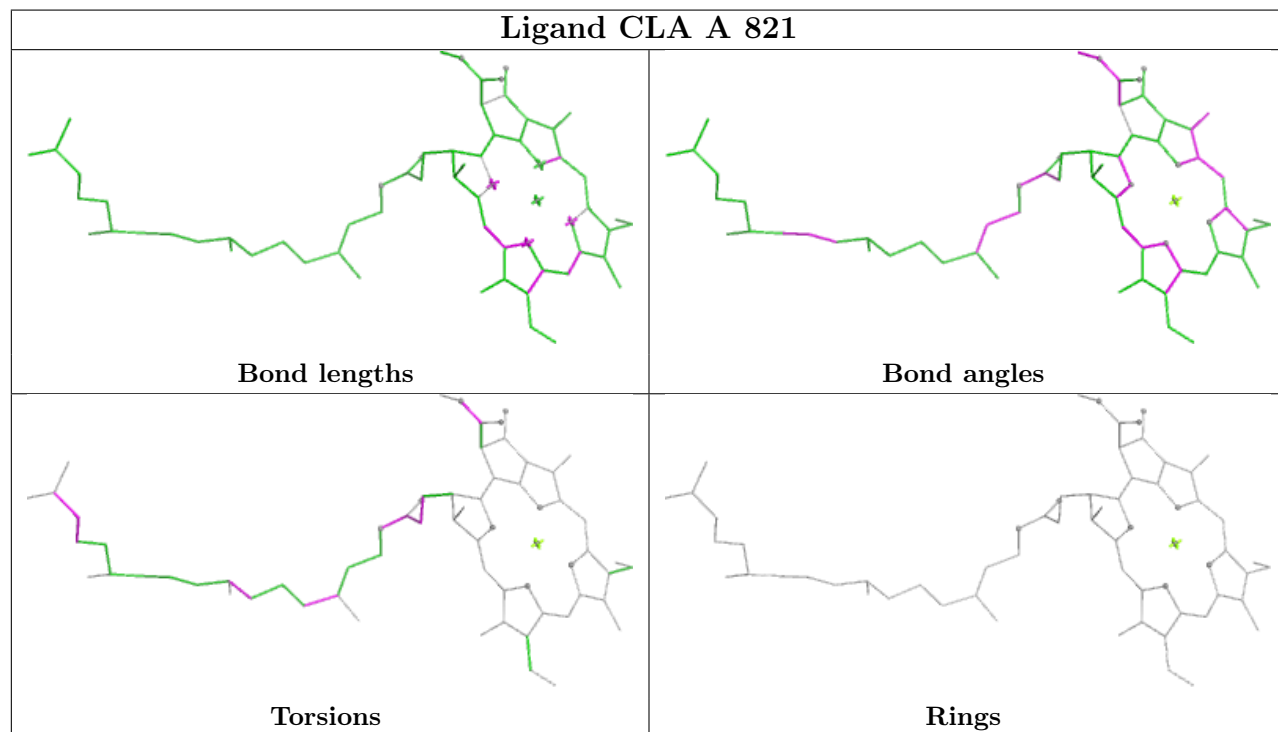
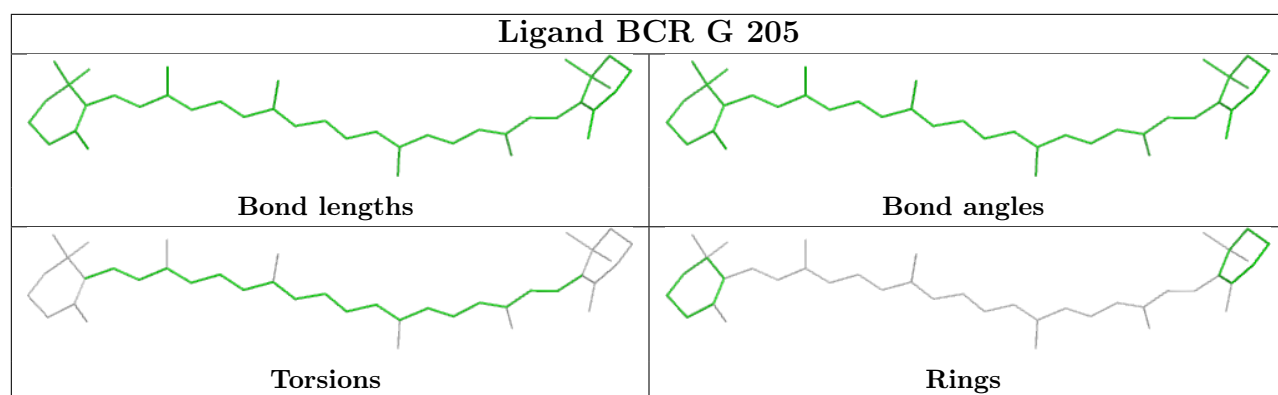
Rings

Ligand CLA B 832

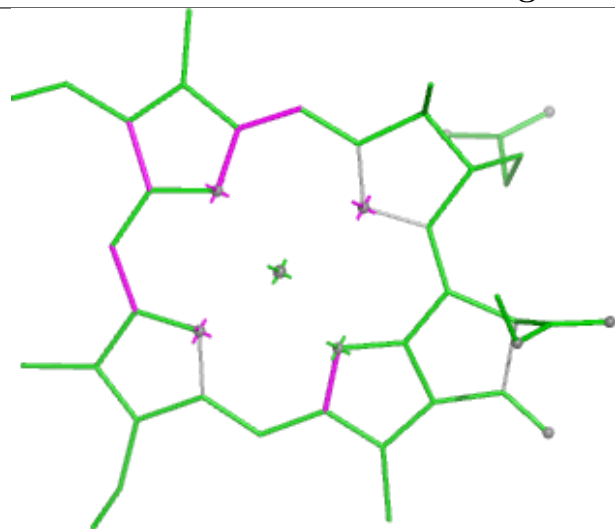


Ligand PQN A 844

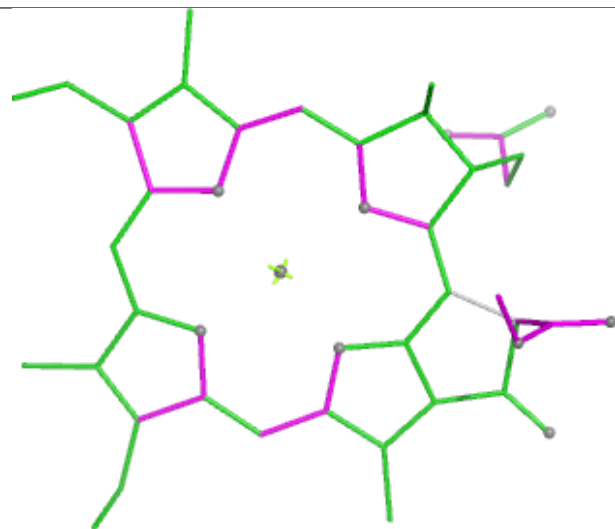




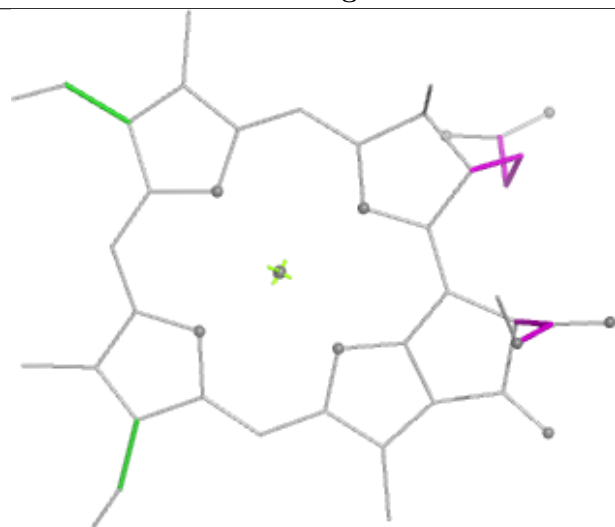
Ligand CLA L 304



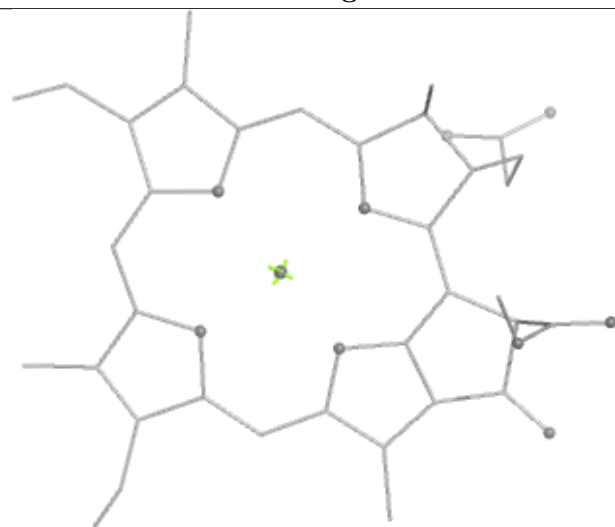
Bond lengths



Bond angles

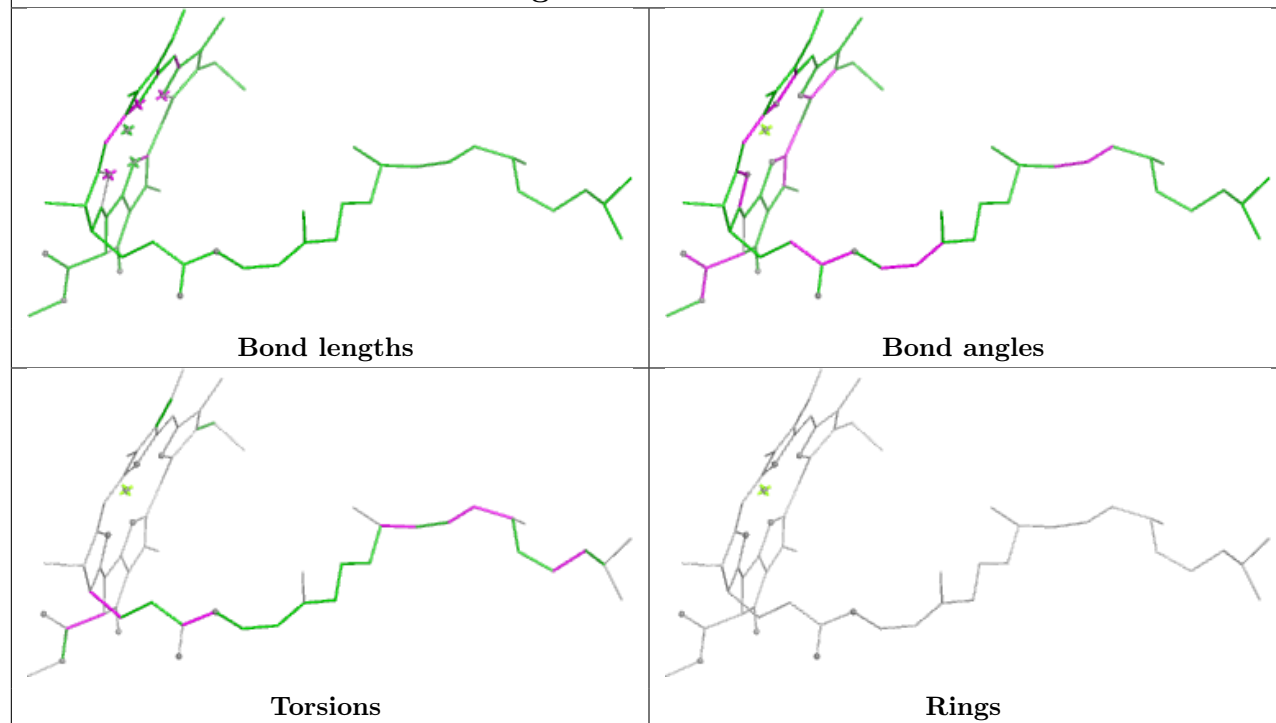


Torsions

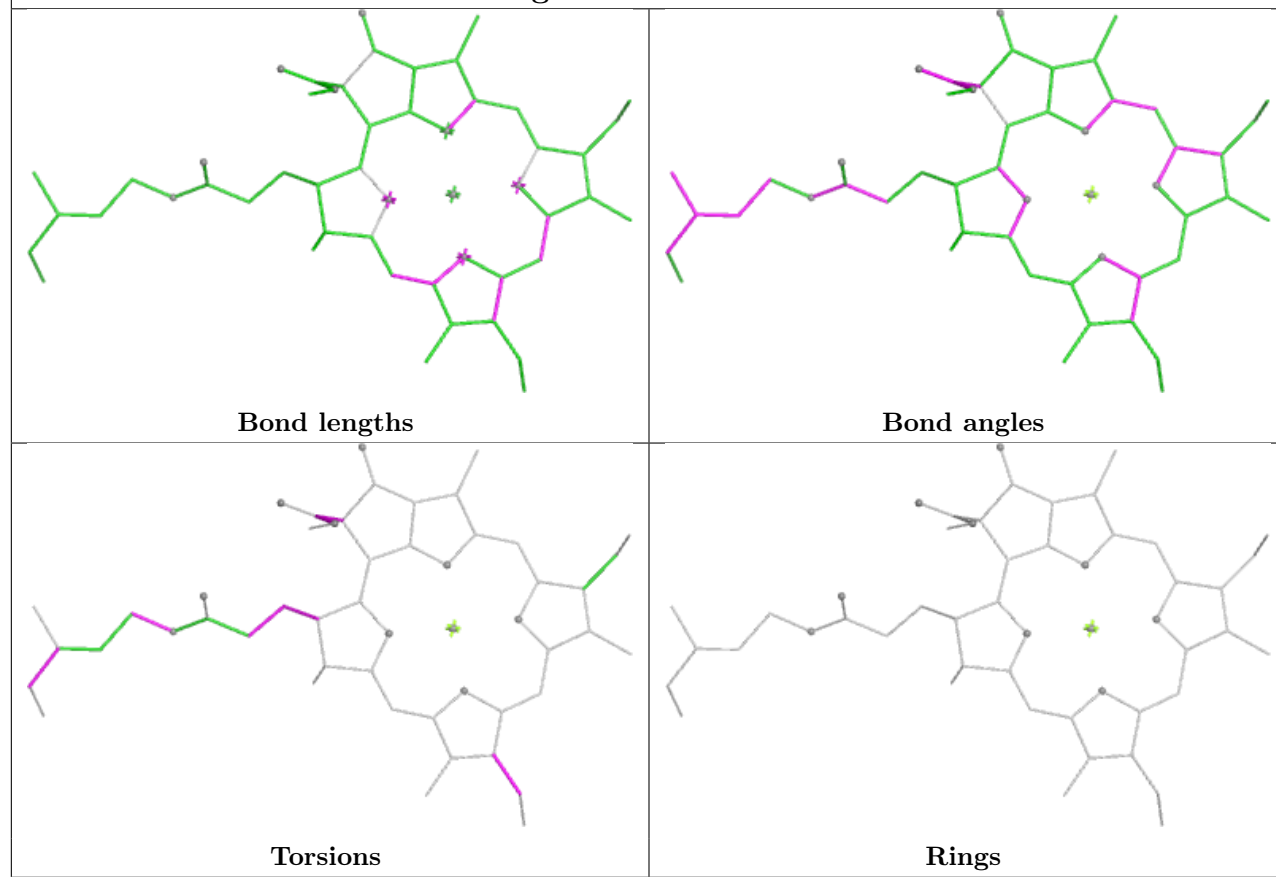


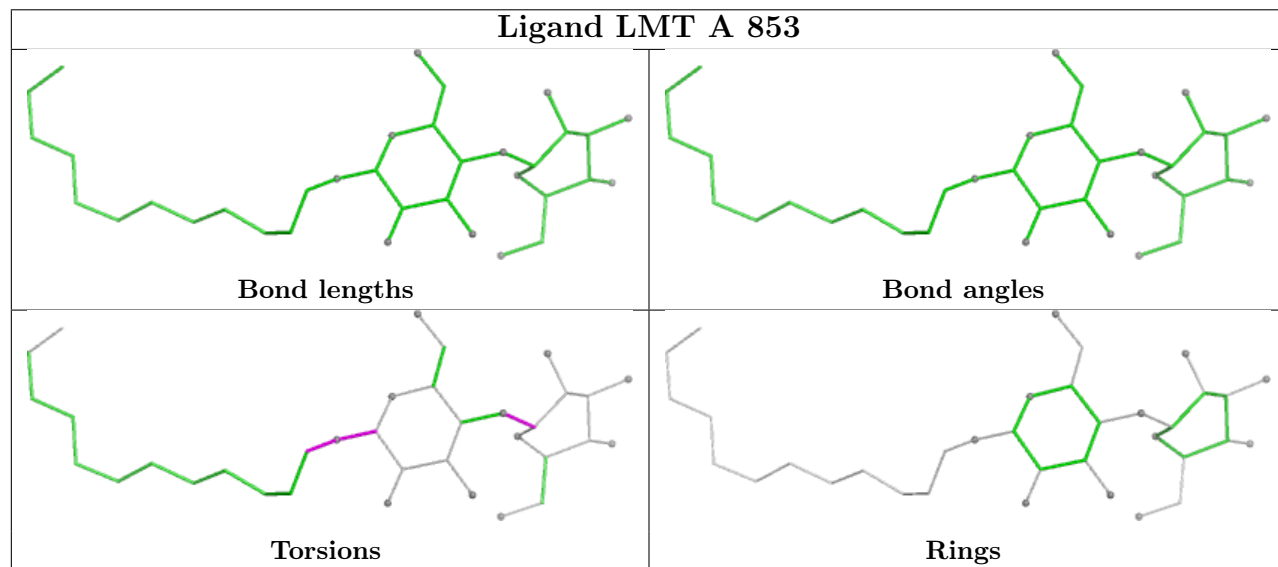
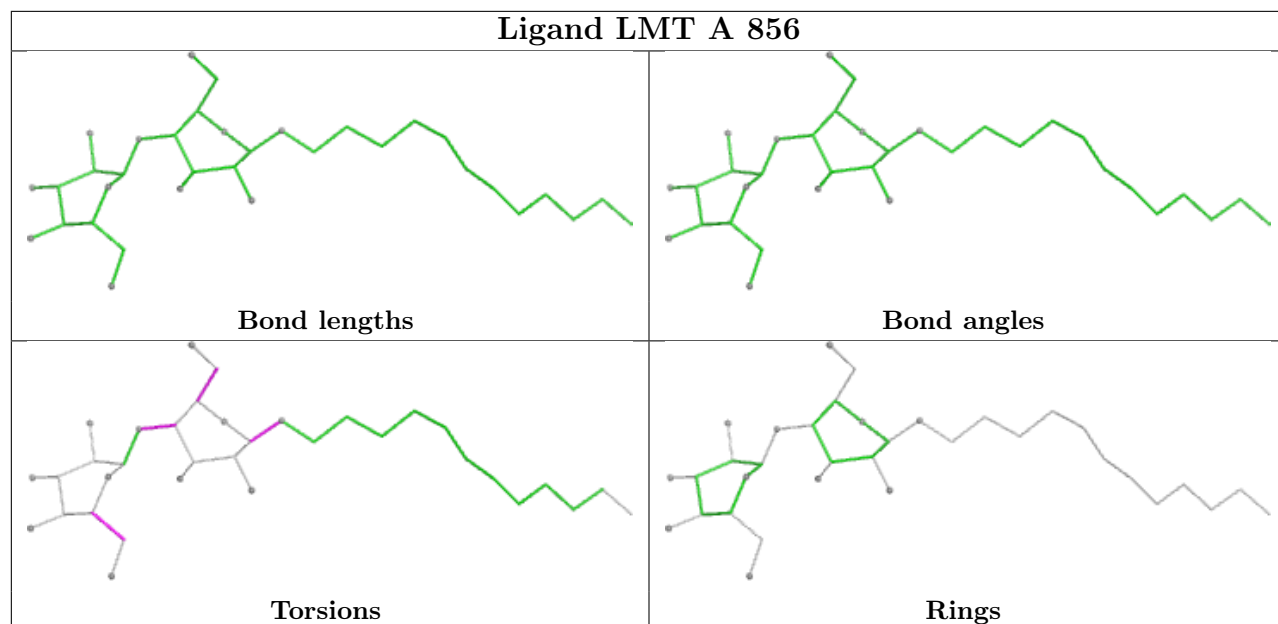
Rings

Ligand CLA A 811

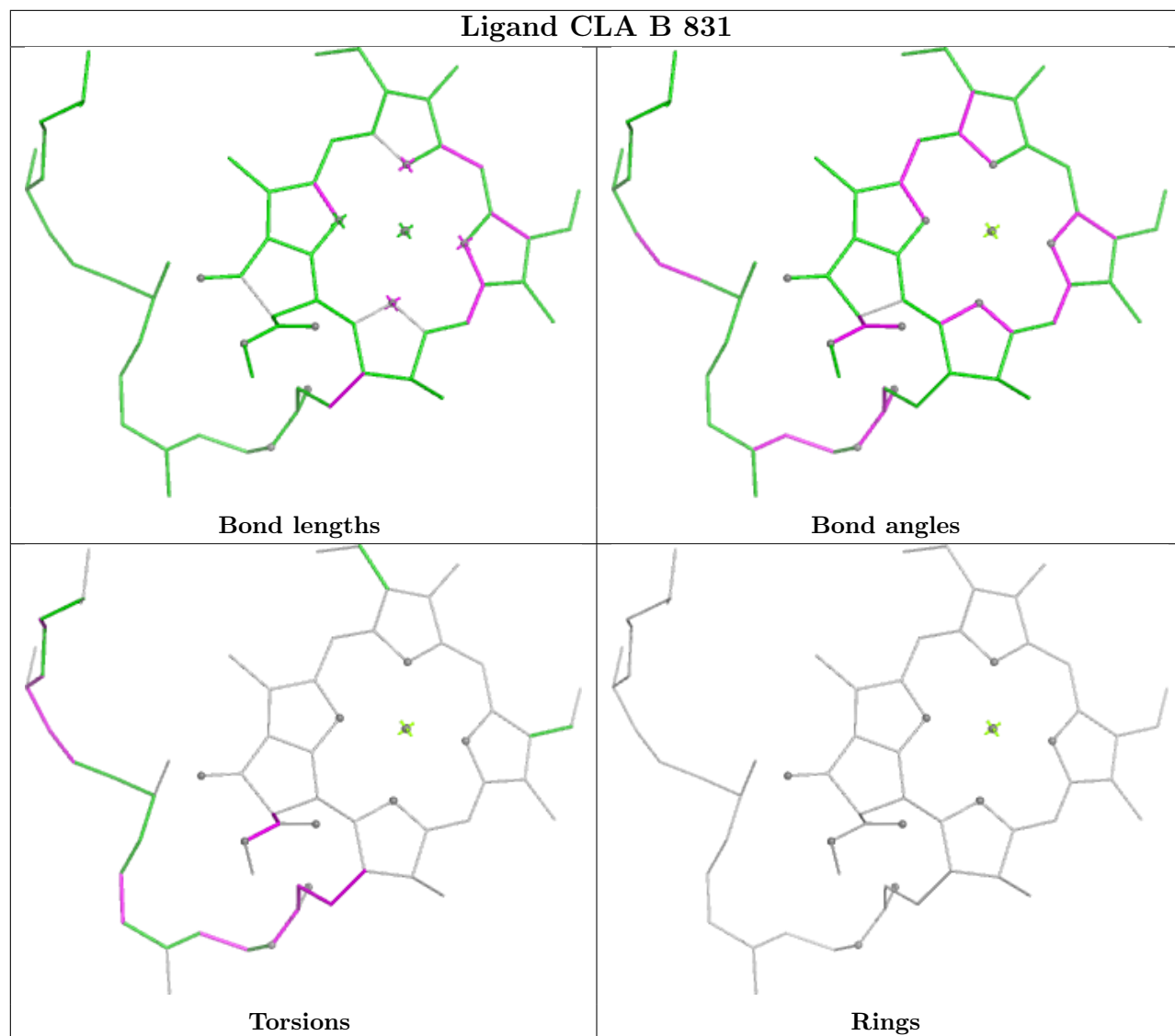


Ligand CLA A 837

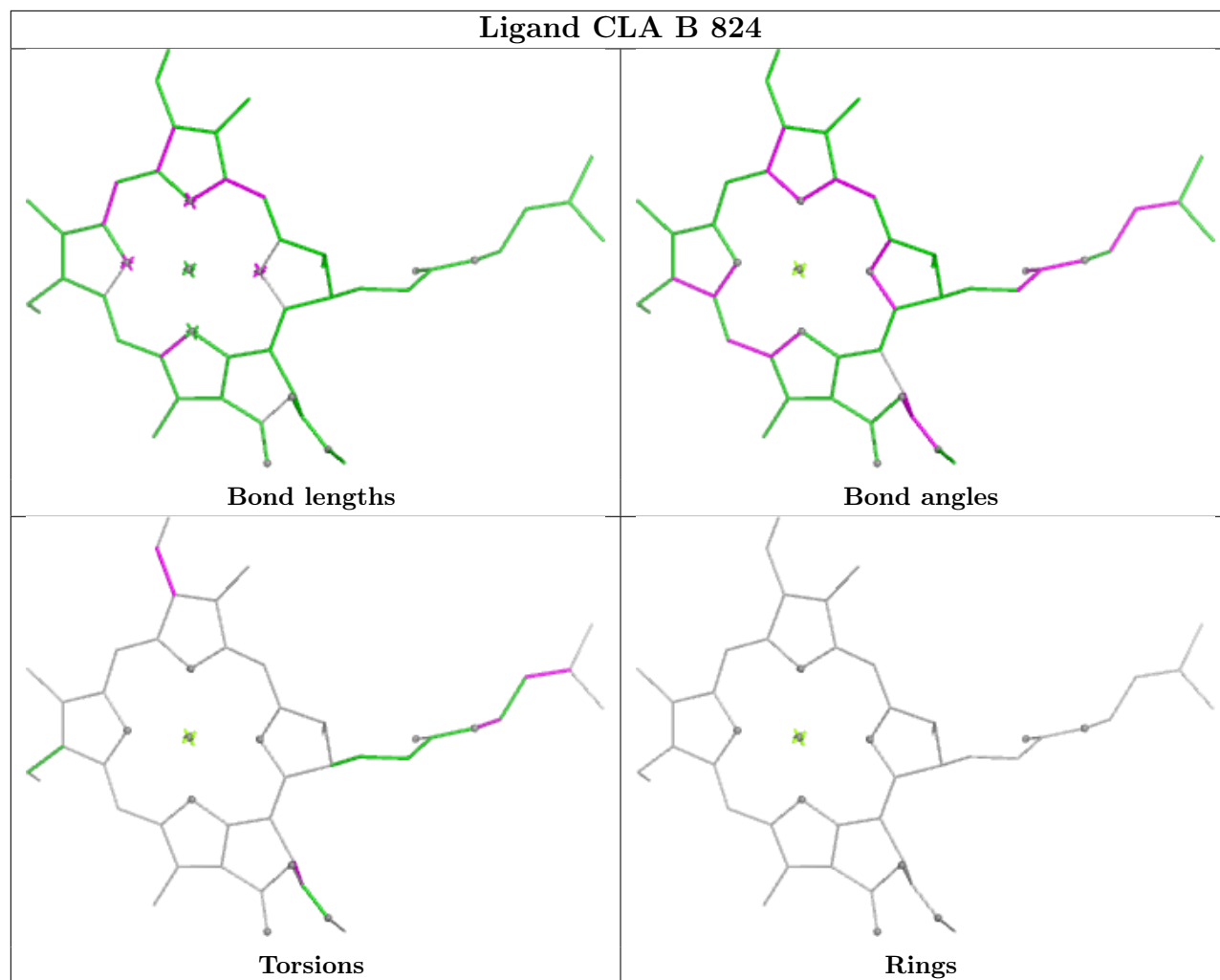




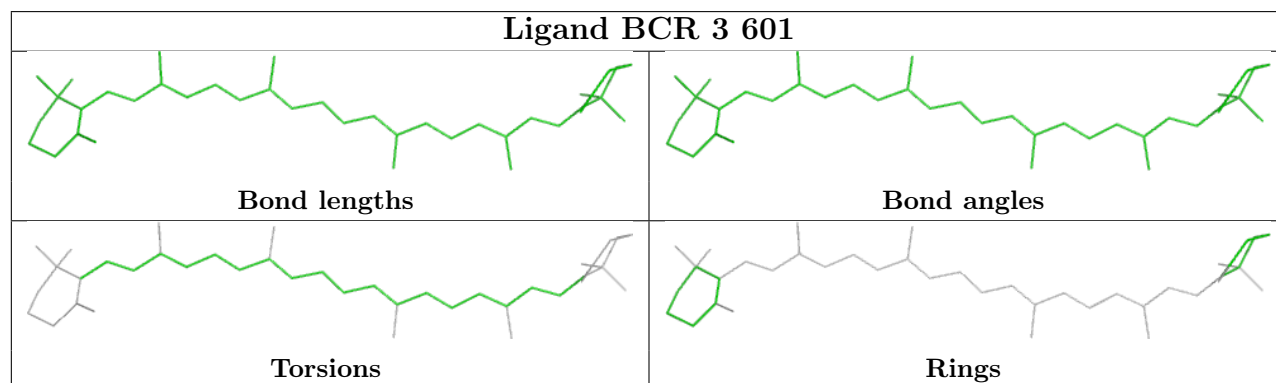
Ligand CLA B 831



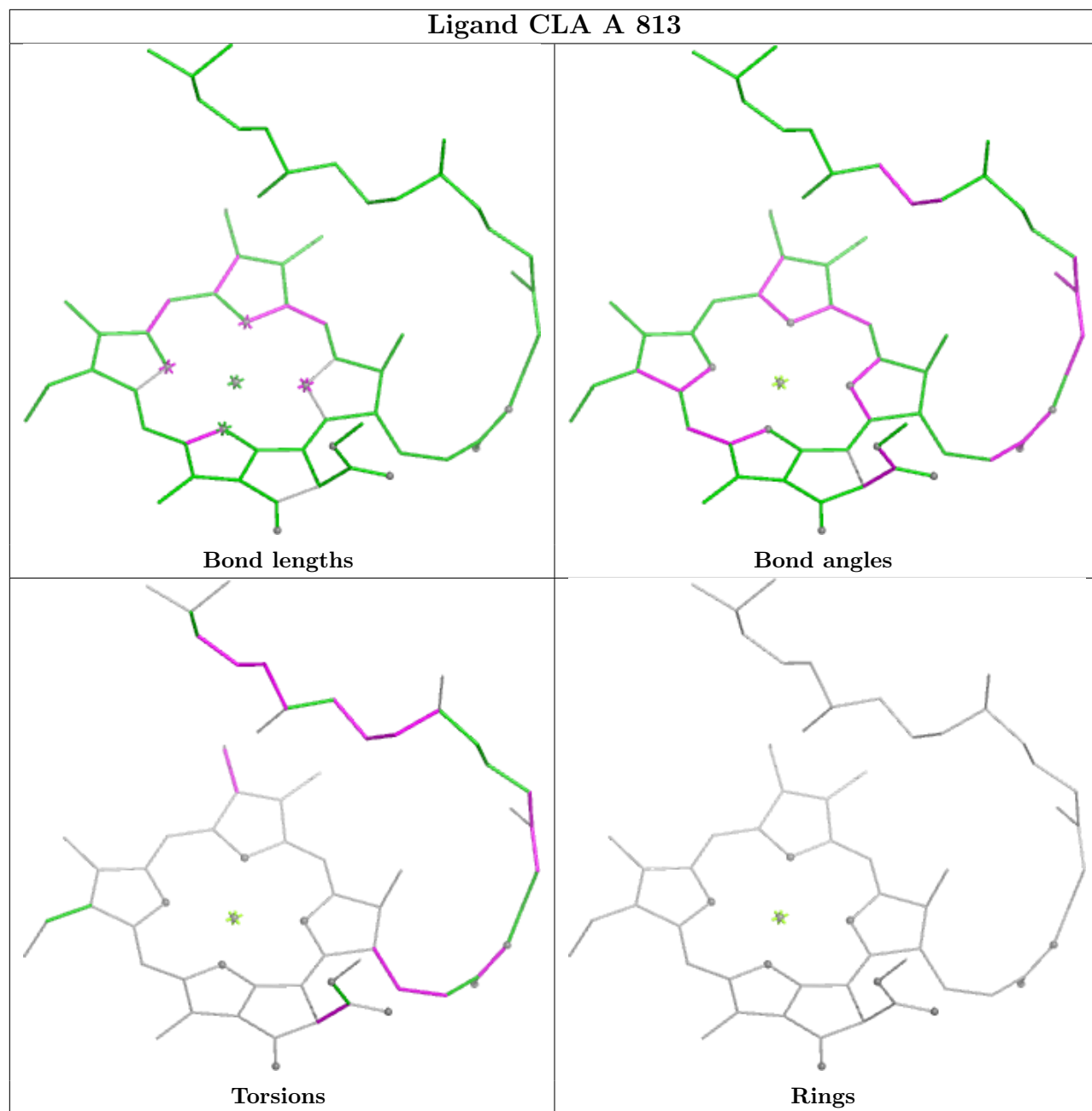
Ligand CLA B 824

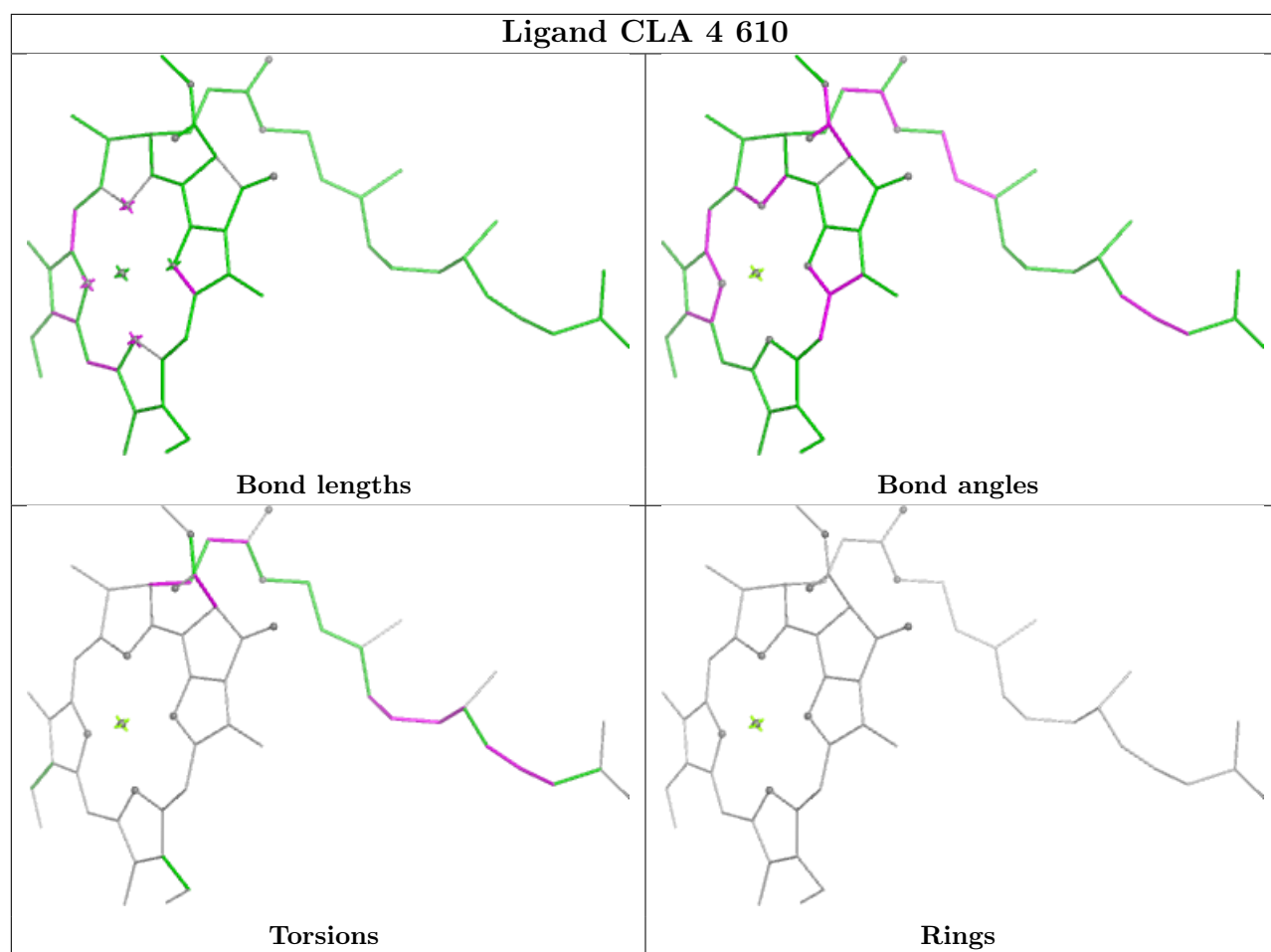


Ligand BCR 3 601

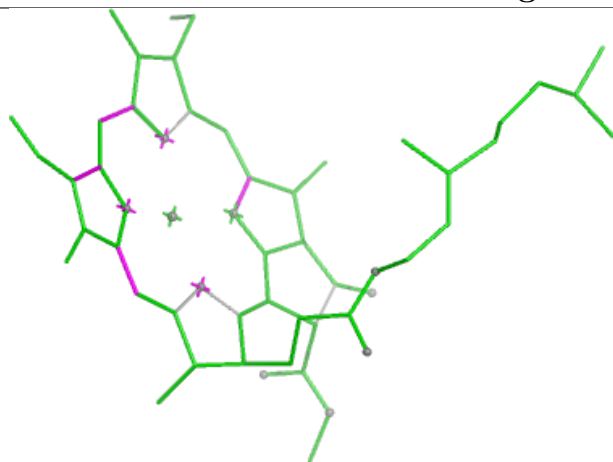


Ligand CLA A 813

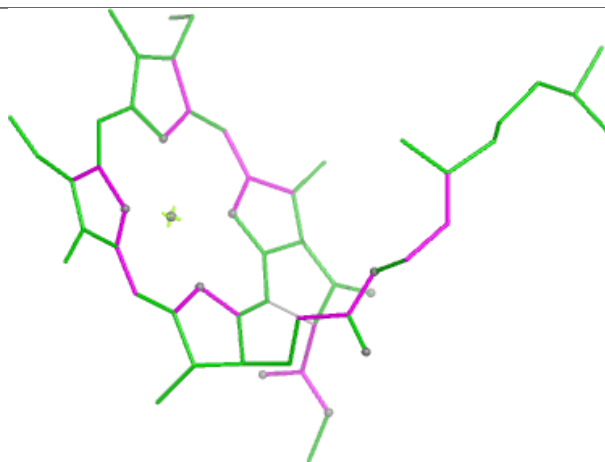




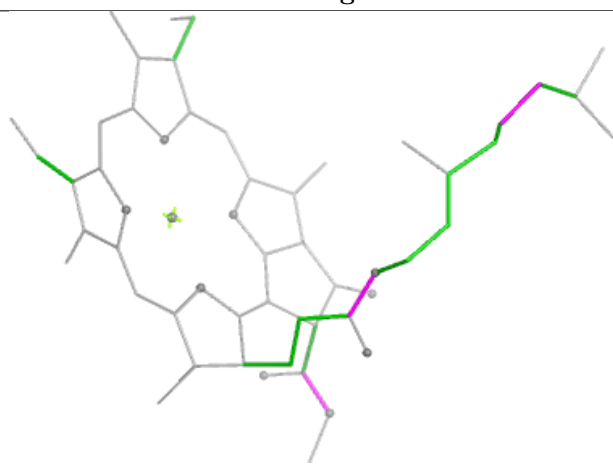
Ligand CLA 1 610



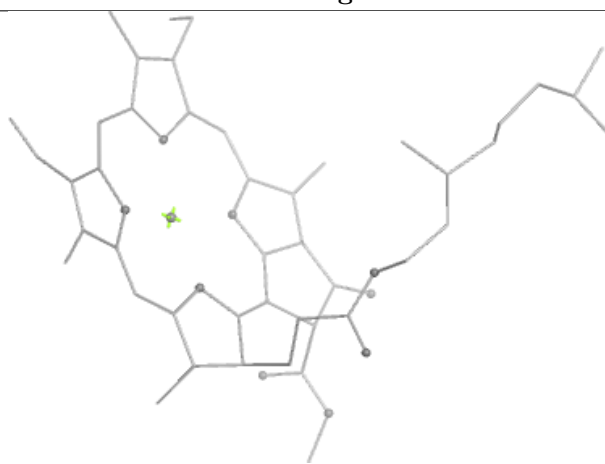
Bond lengths



Bond angles

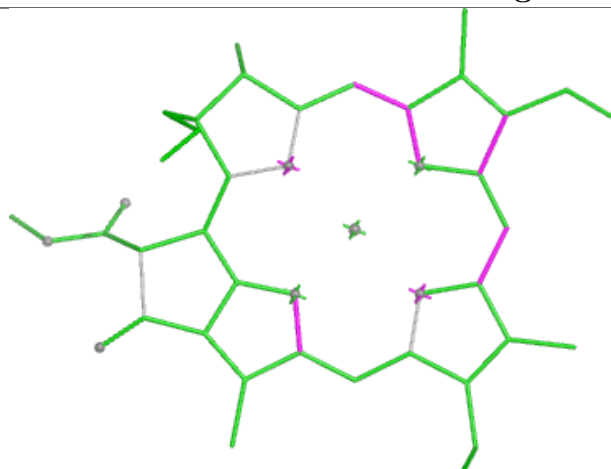


Torsions

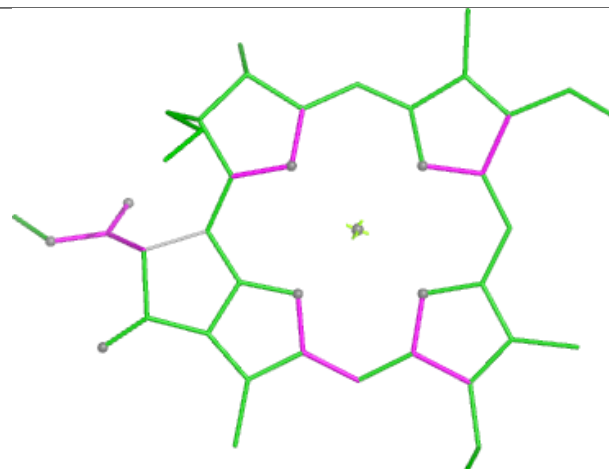


Rings

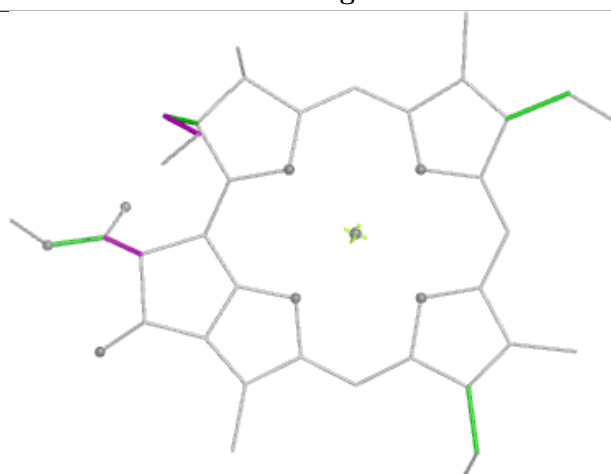
Ligand CLA B 811



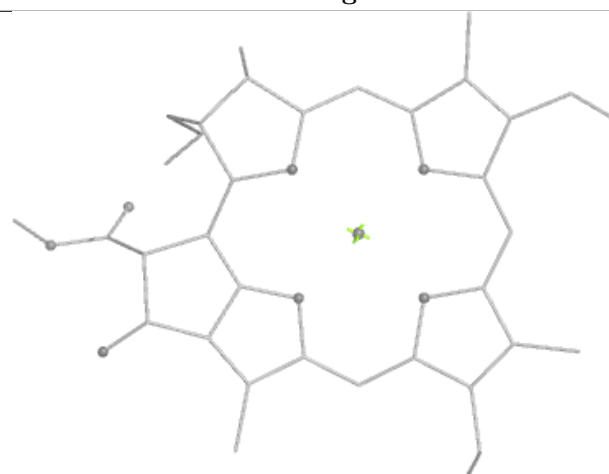
Bond lengths



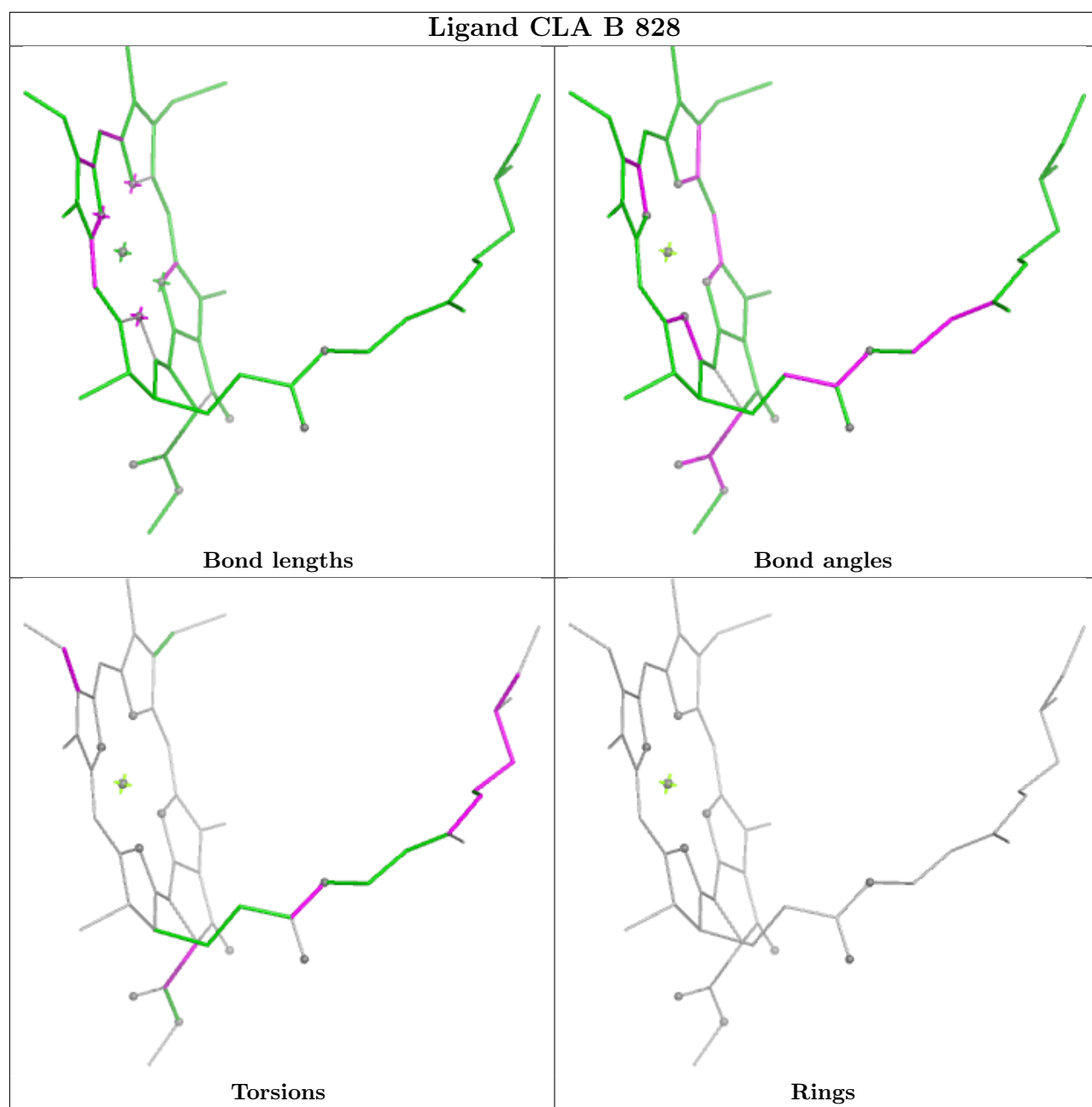
Bond angles



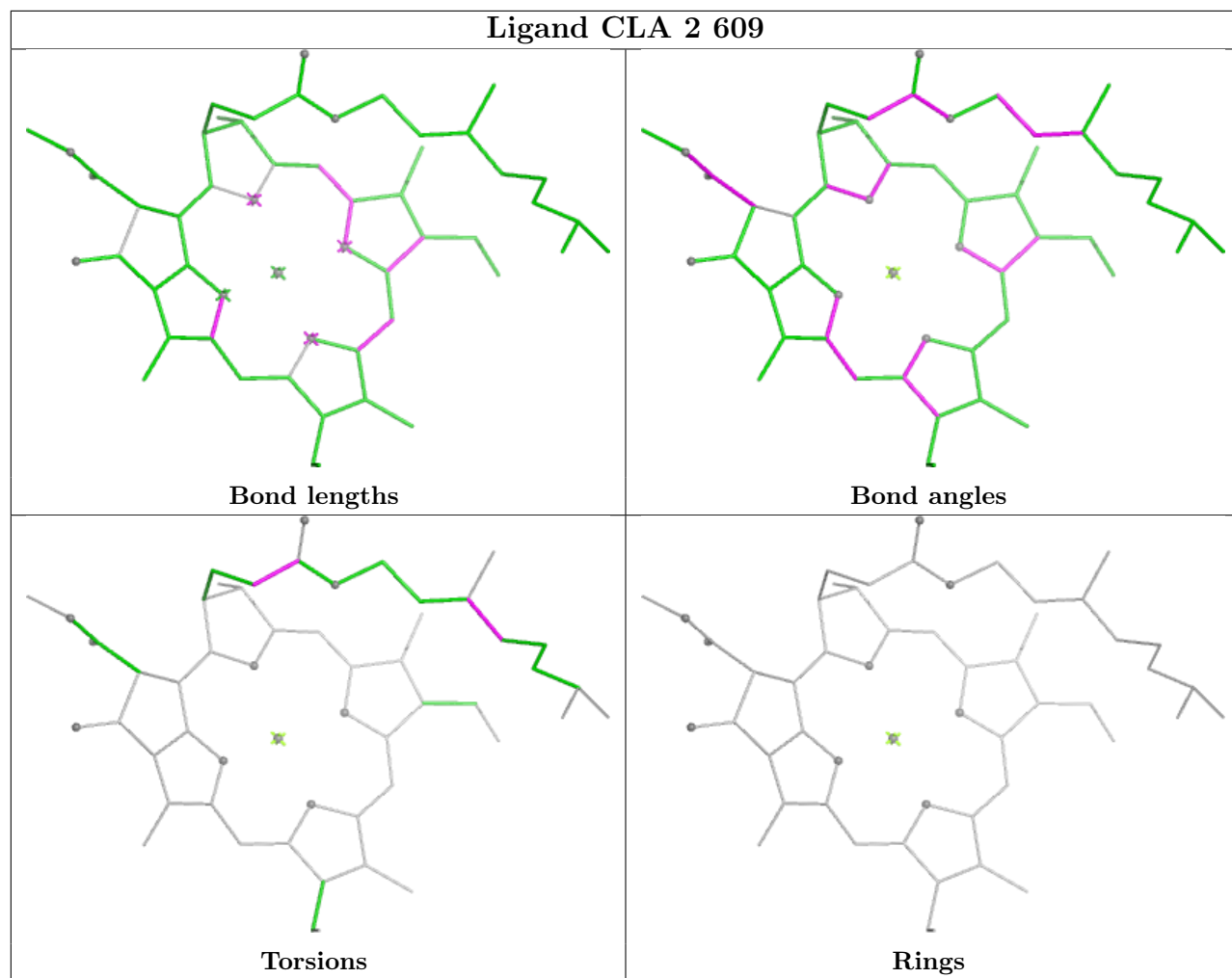
Torsions



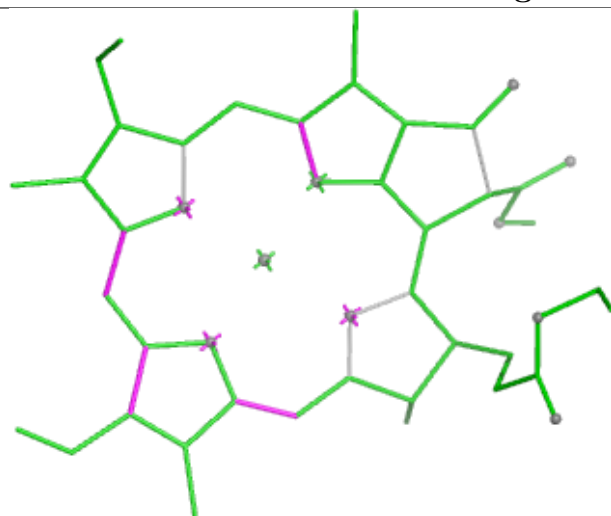
Rings



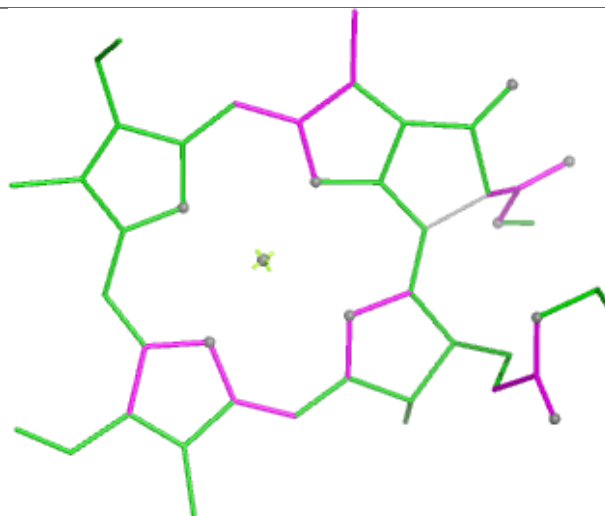
Ligand CLA 2 609



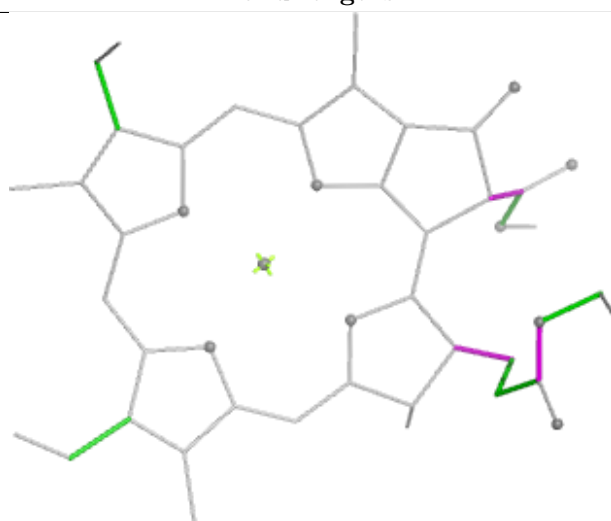
Ligand CLA B 837



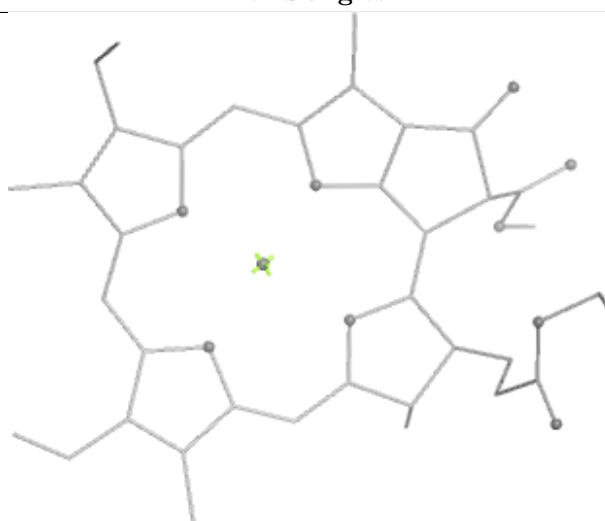
Bond lengths



Bond angles

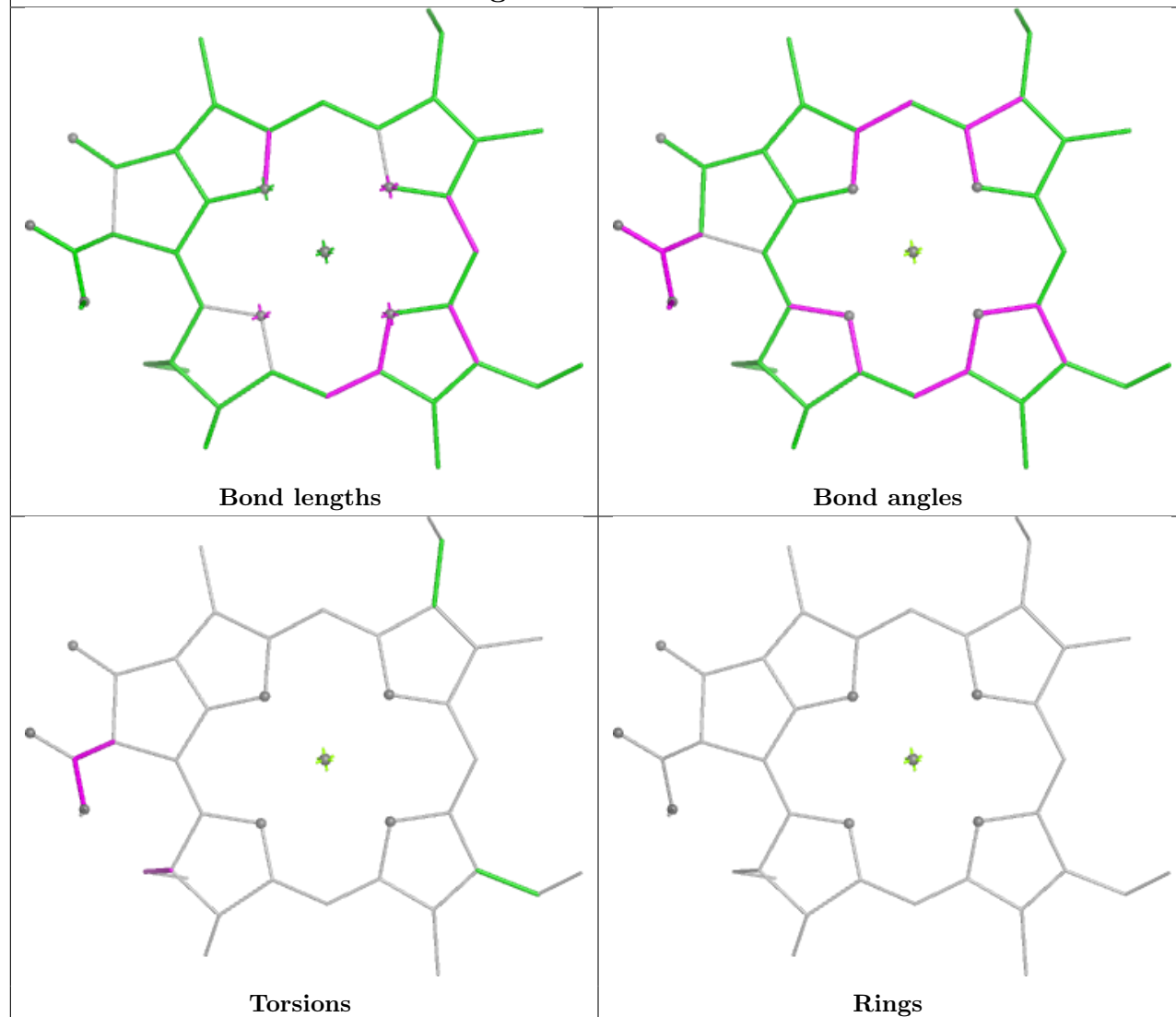


Torsions

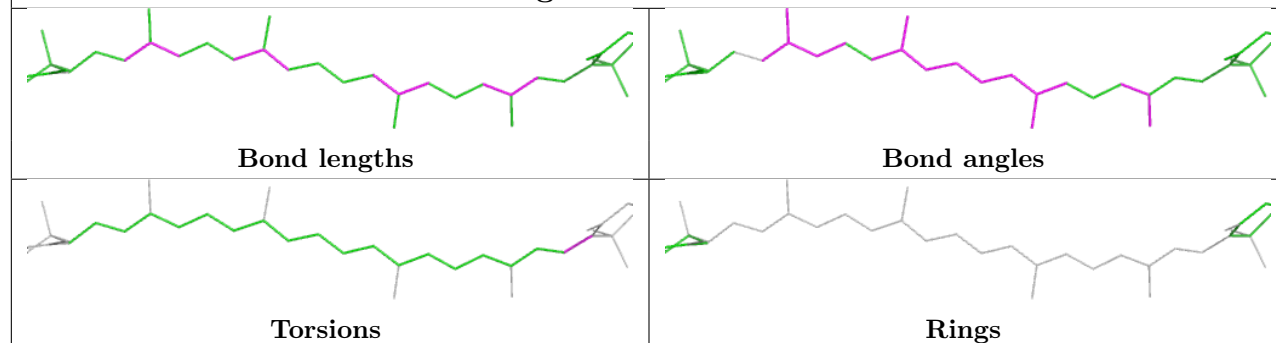


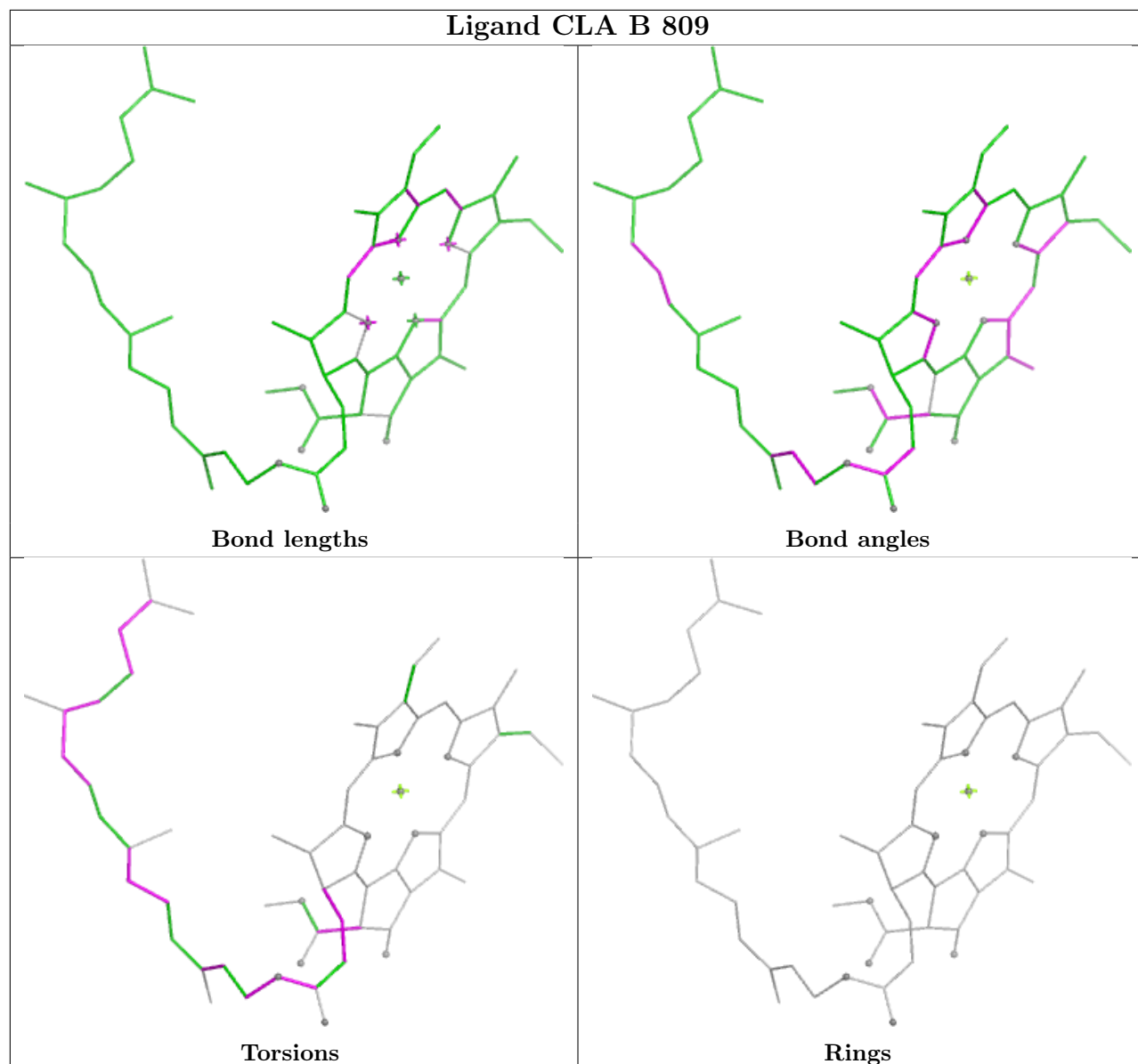
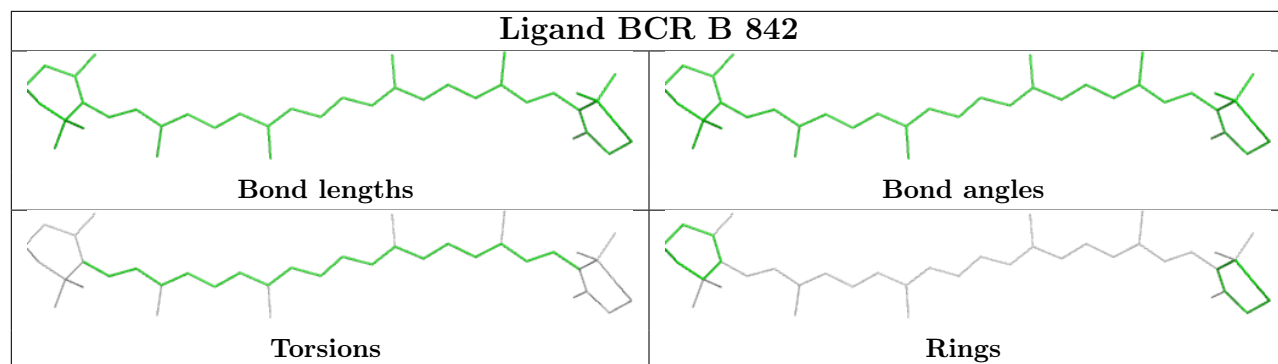
Rings

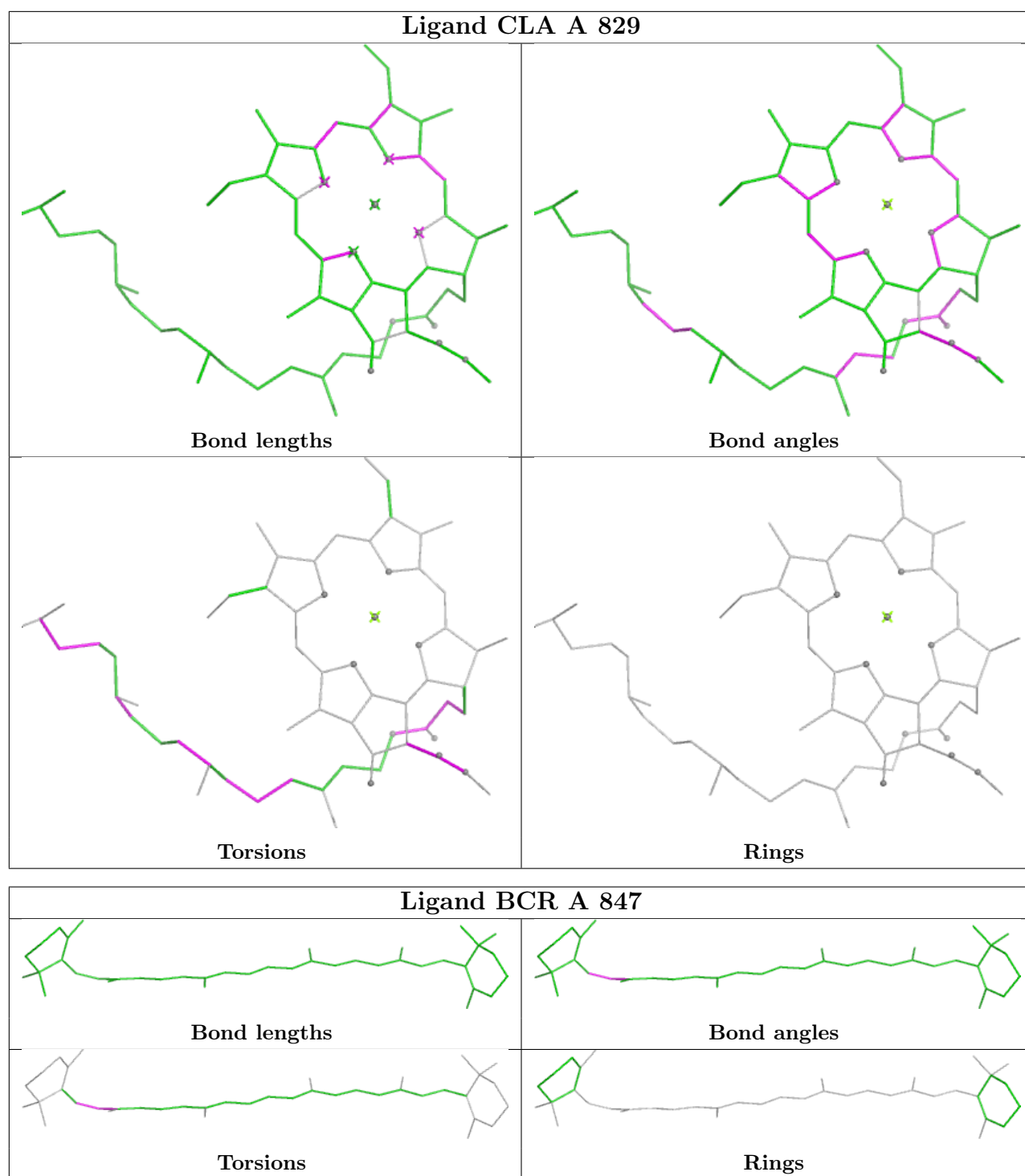
Ligand CLA A 822



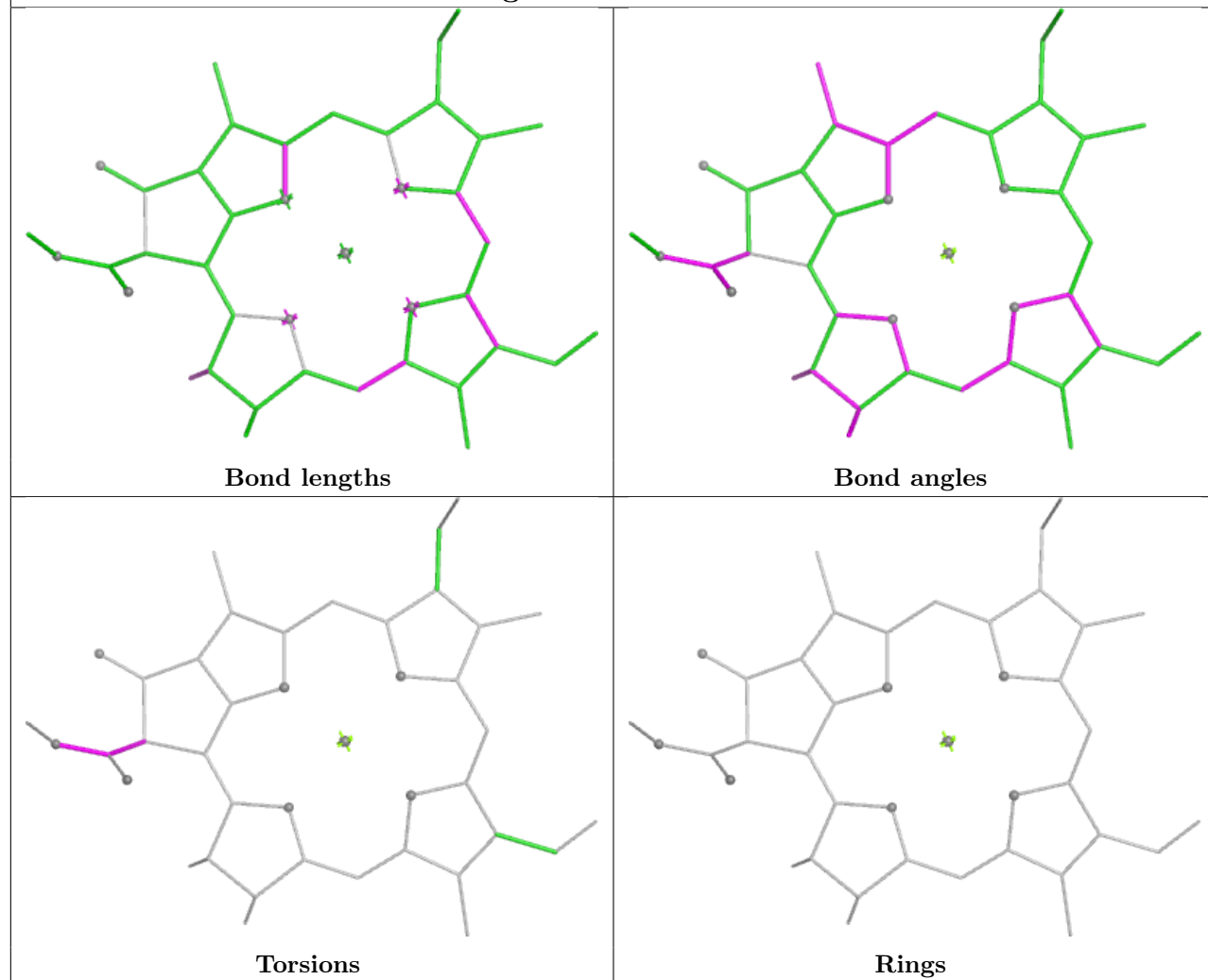
Ligand LUT 2 615



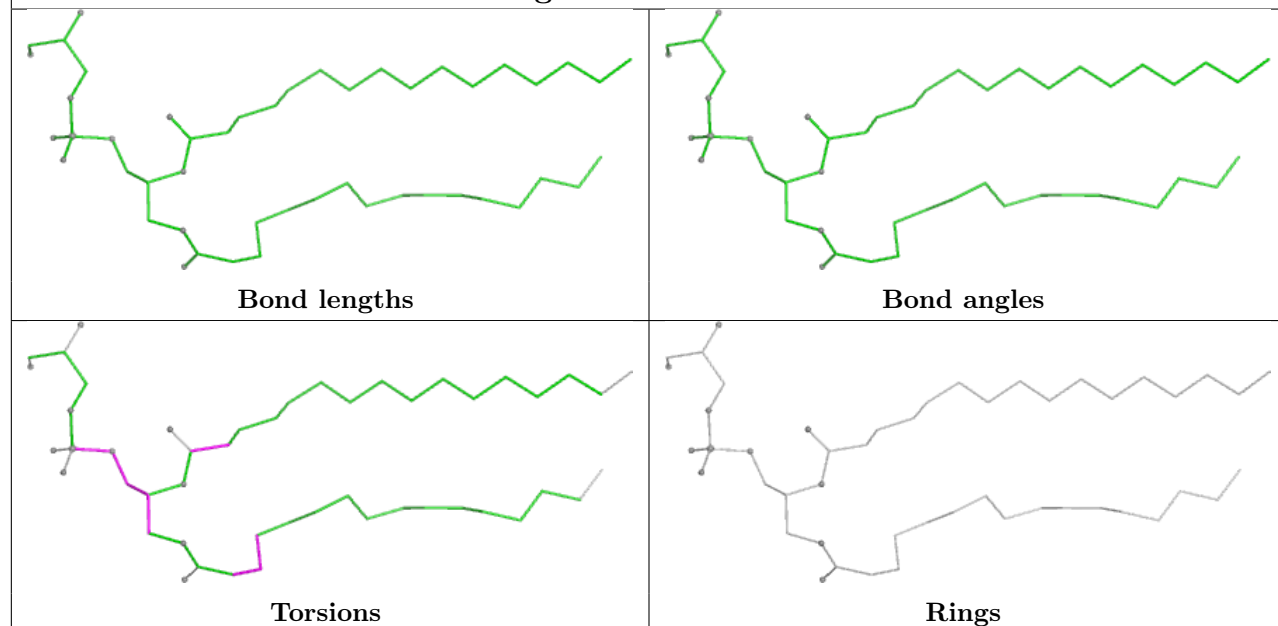


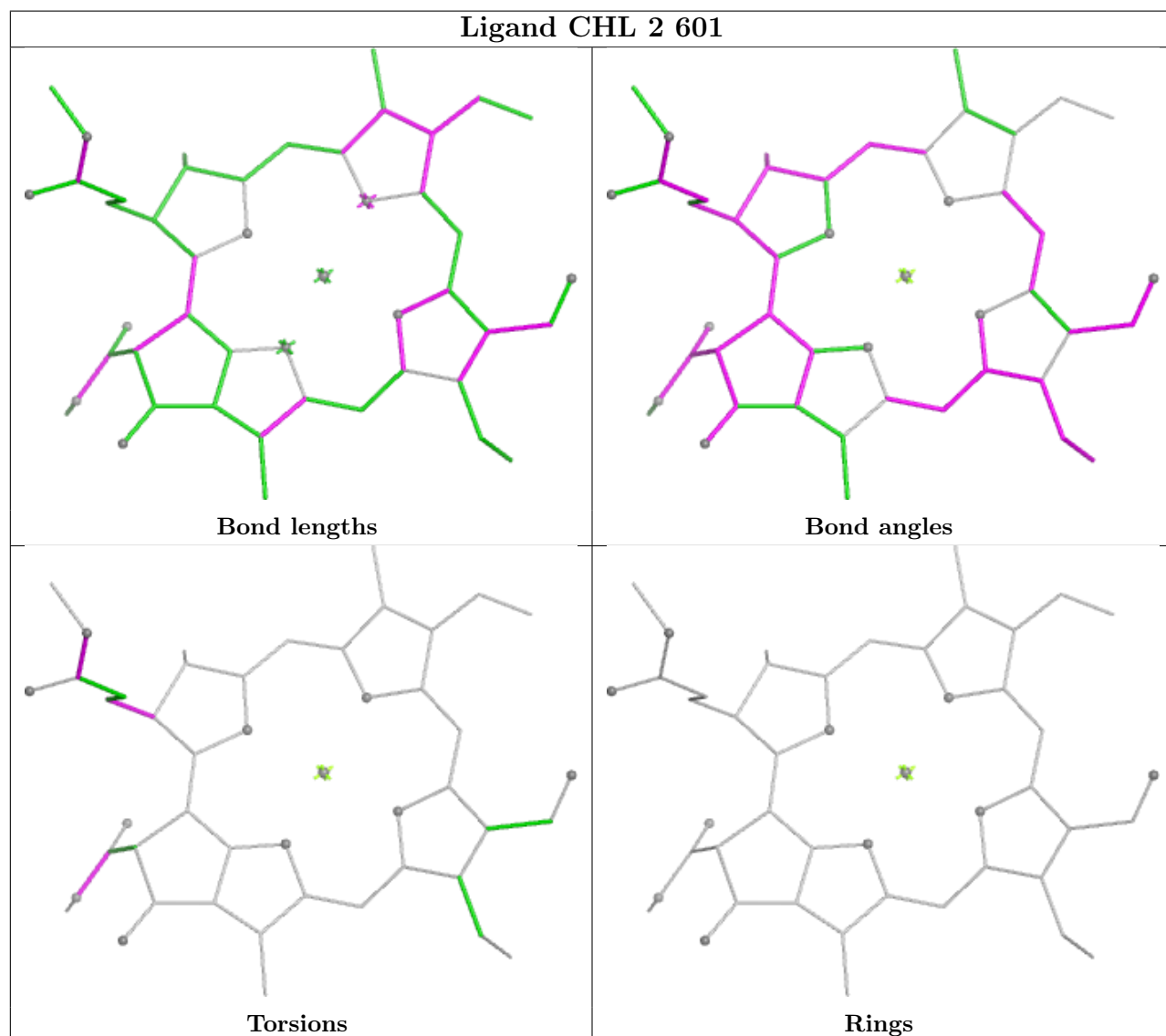
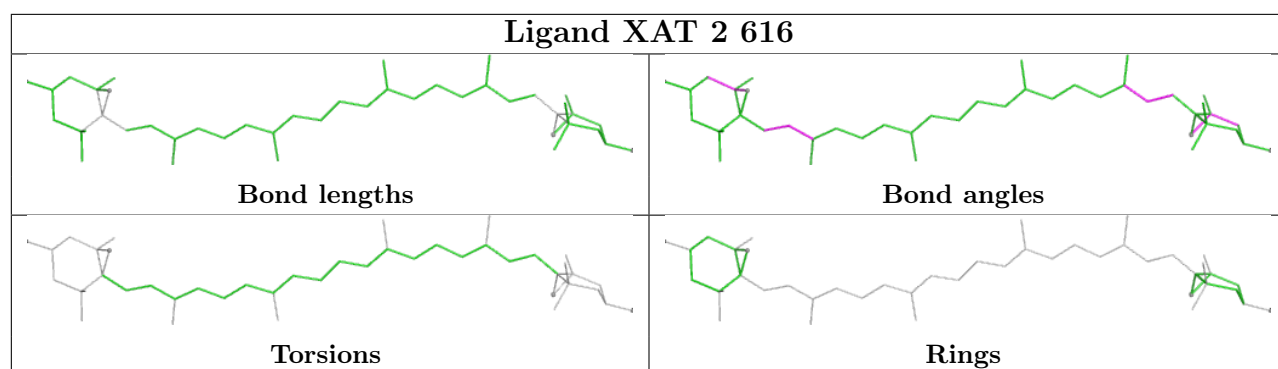


Ligand CLA A 823

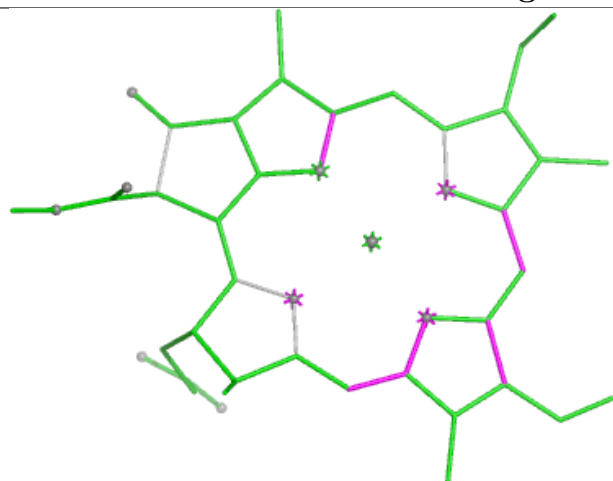


Ligand LHG 1 618

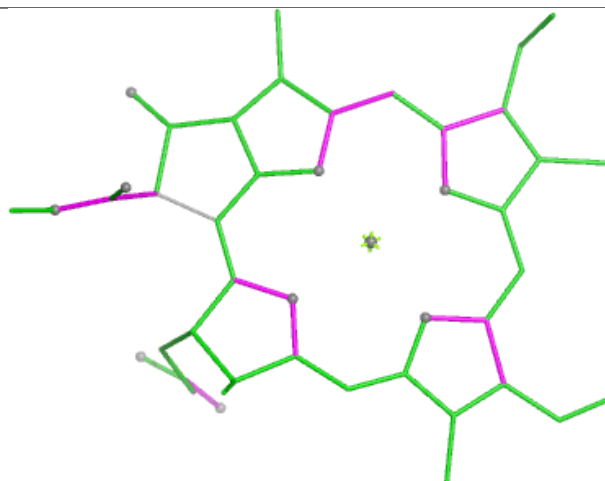




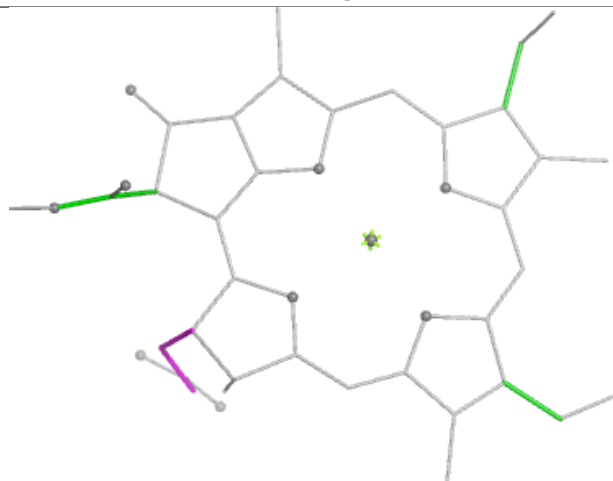
Ligand CLA 4 608



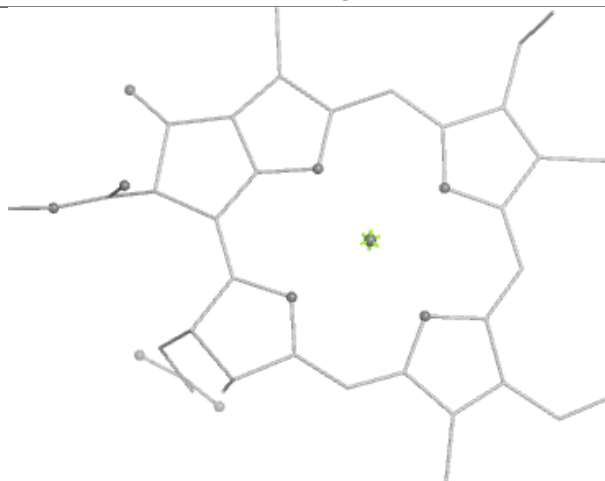
Bond lengths



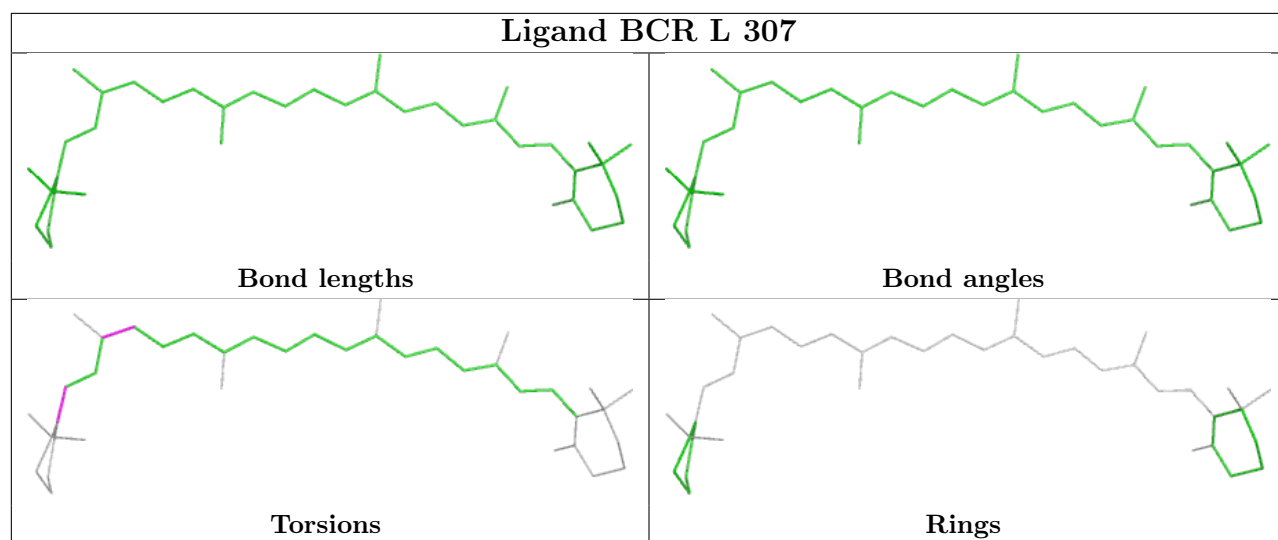
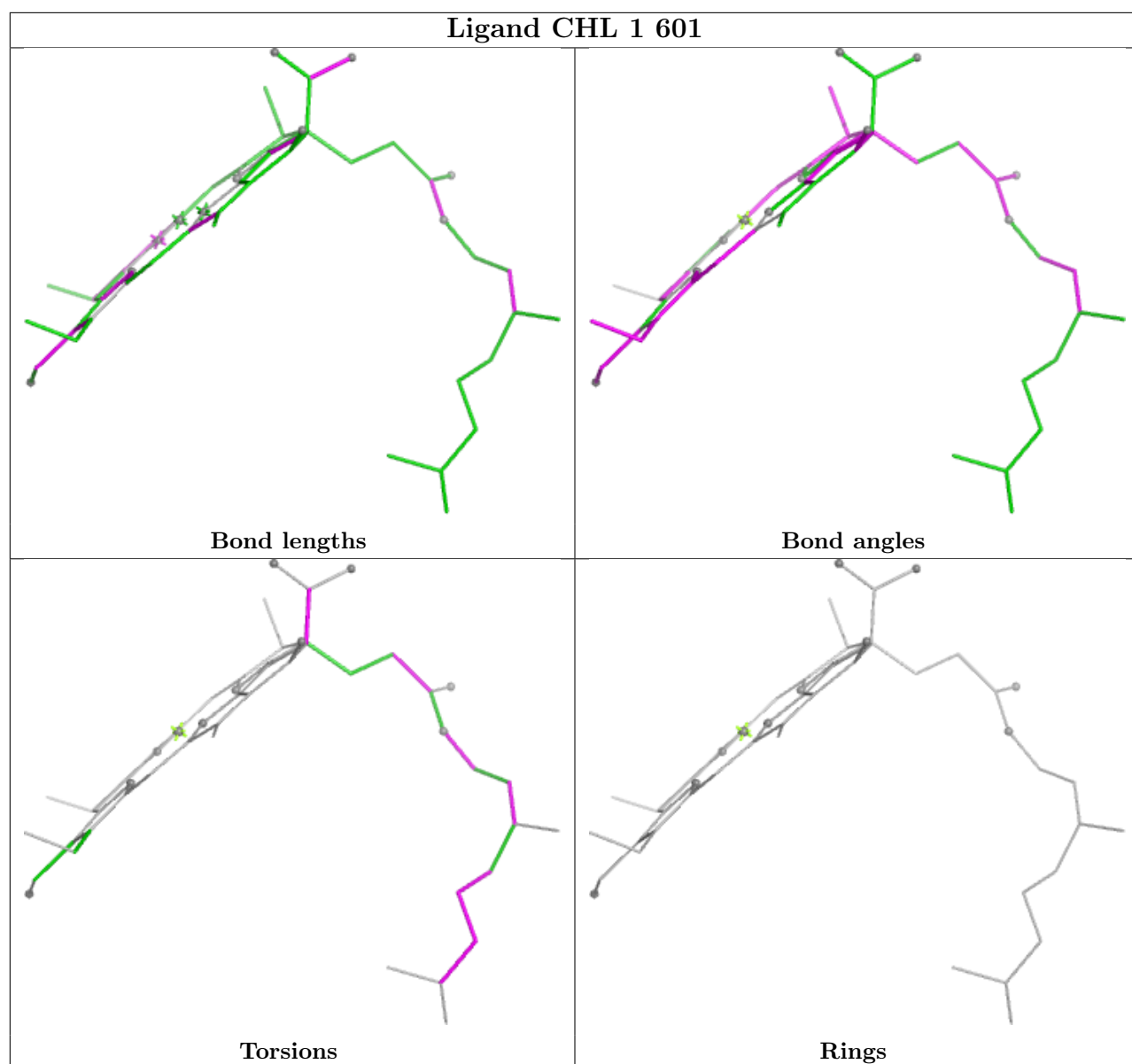
Bond angles

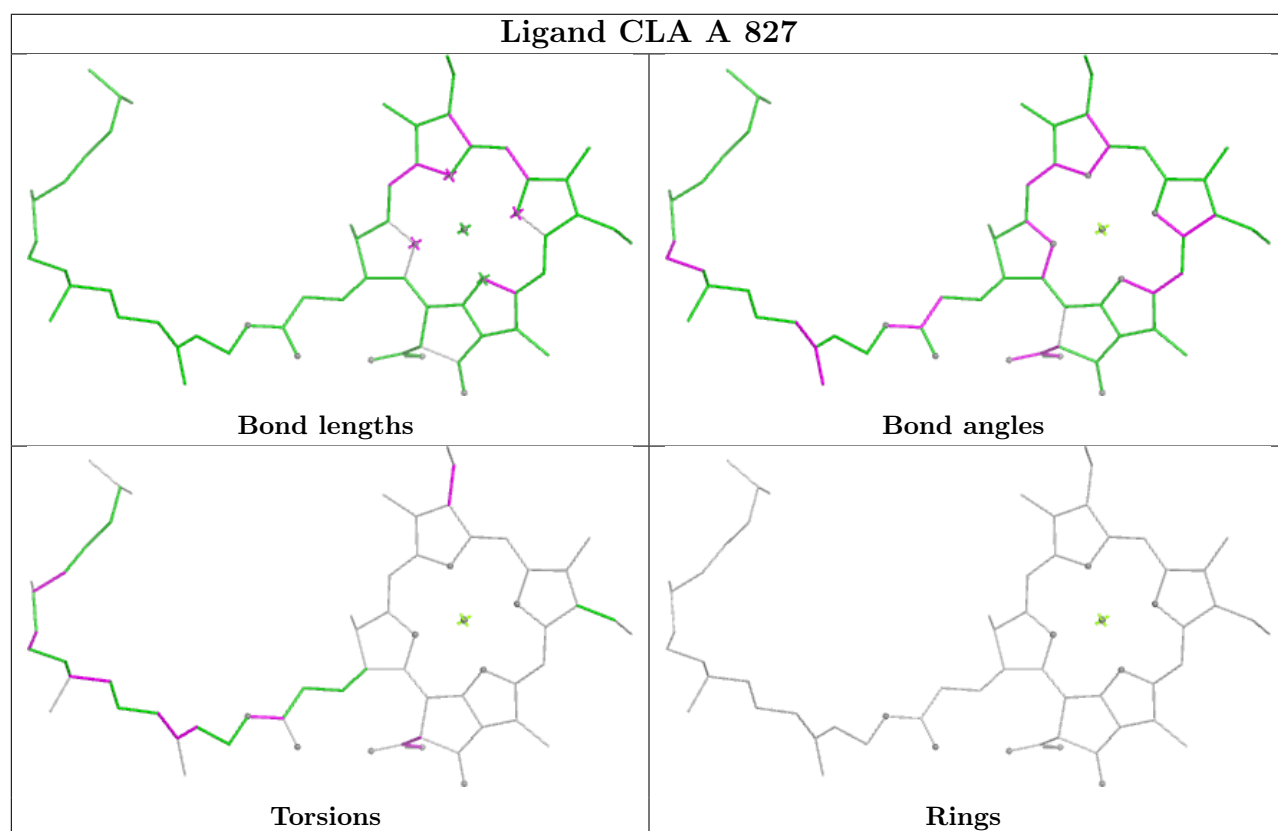
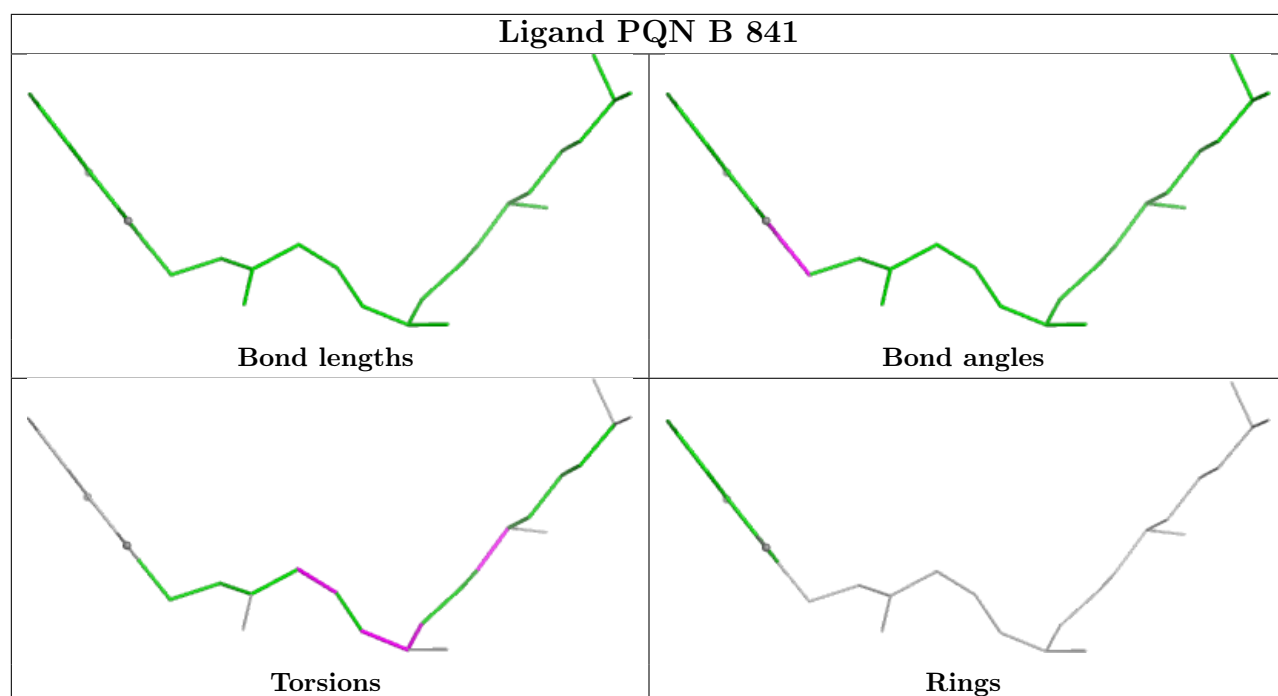


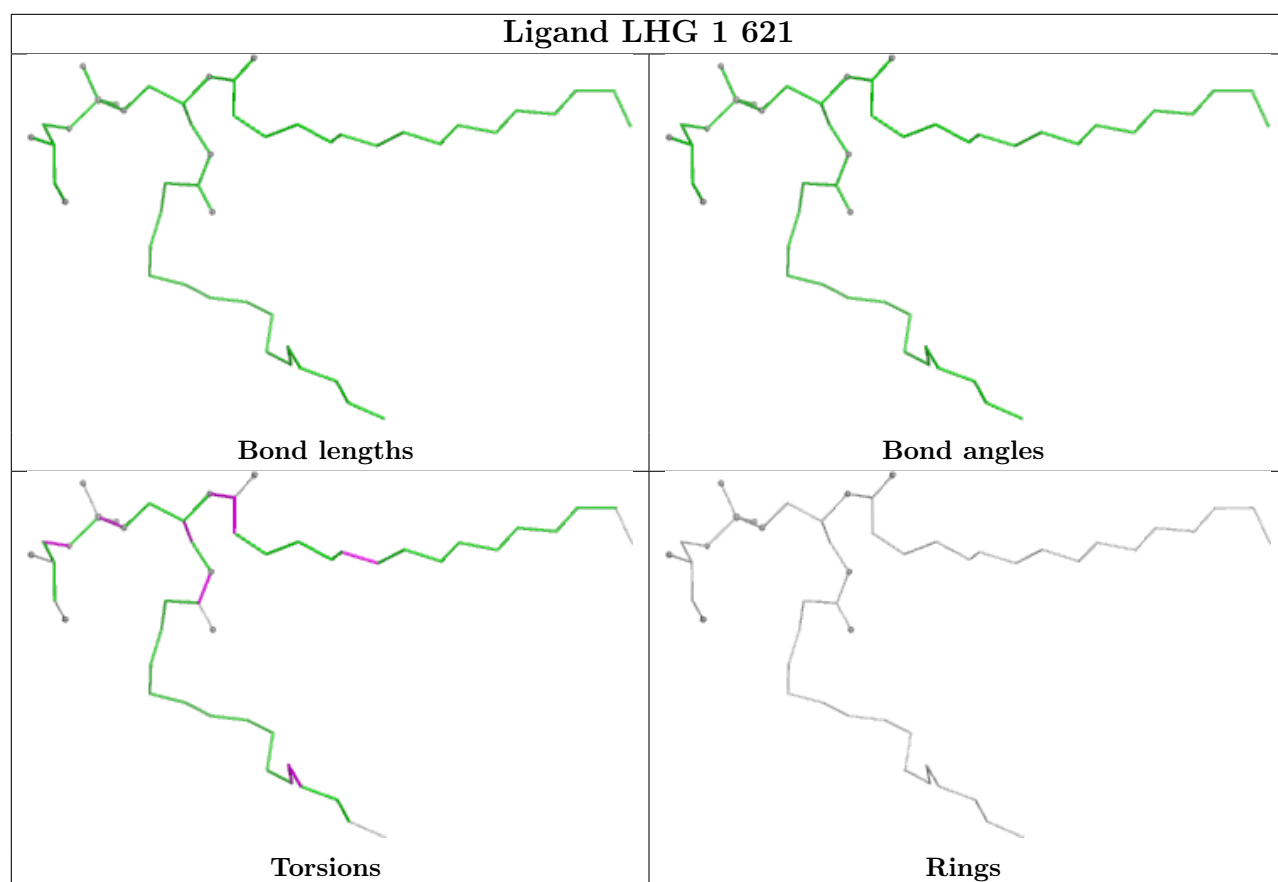
Torsions



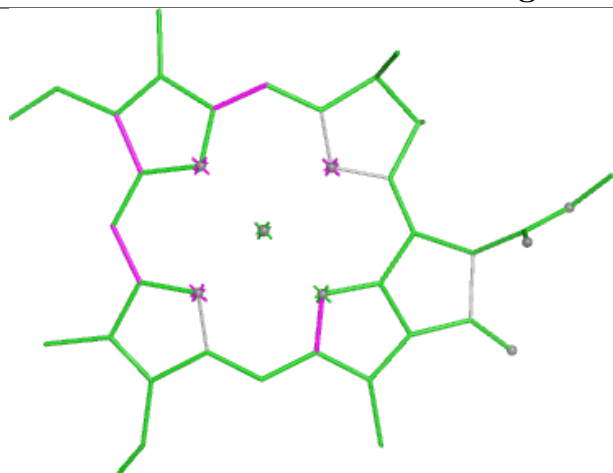
Rings



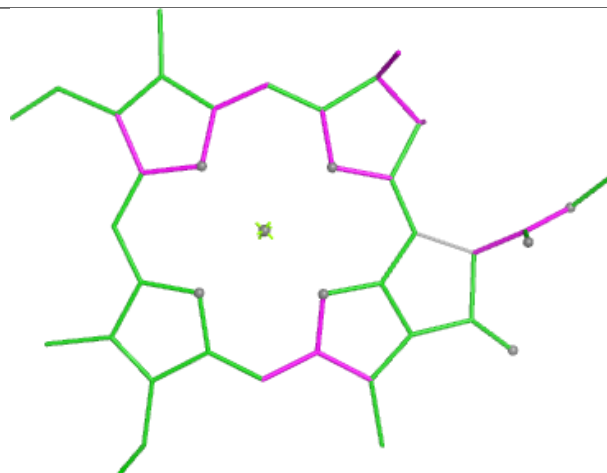




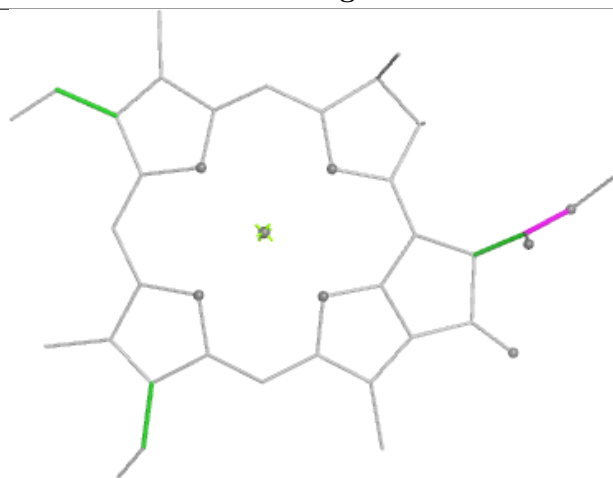
Ligand CLA 2 610



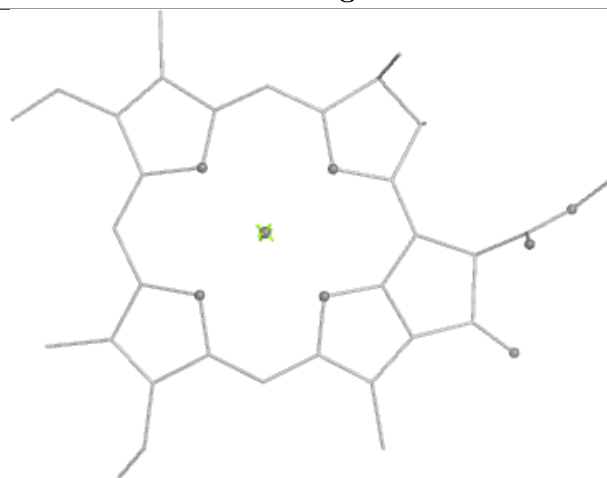
Bond lengths



Bond angles

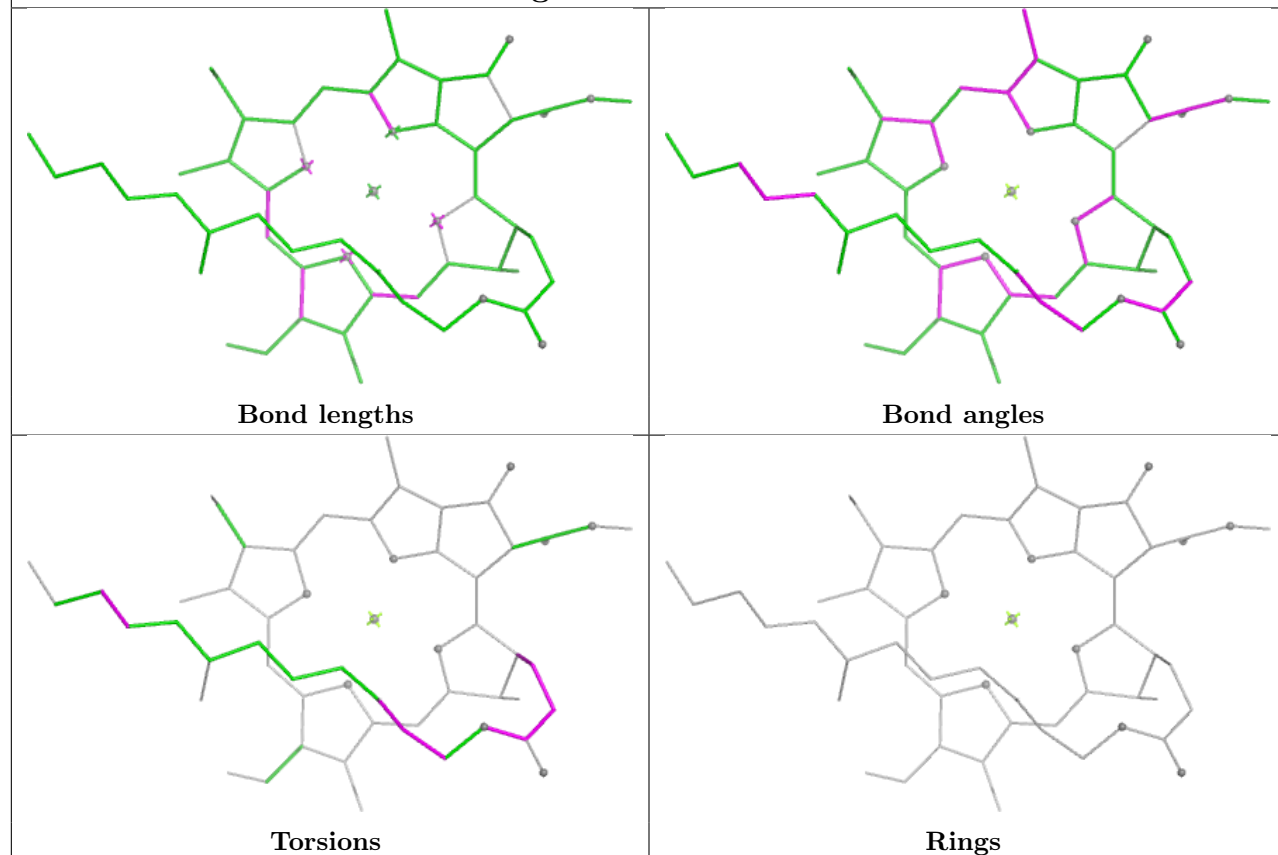


Torsions

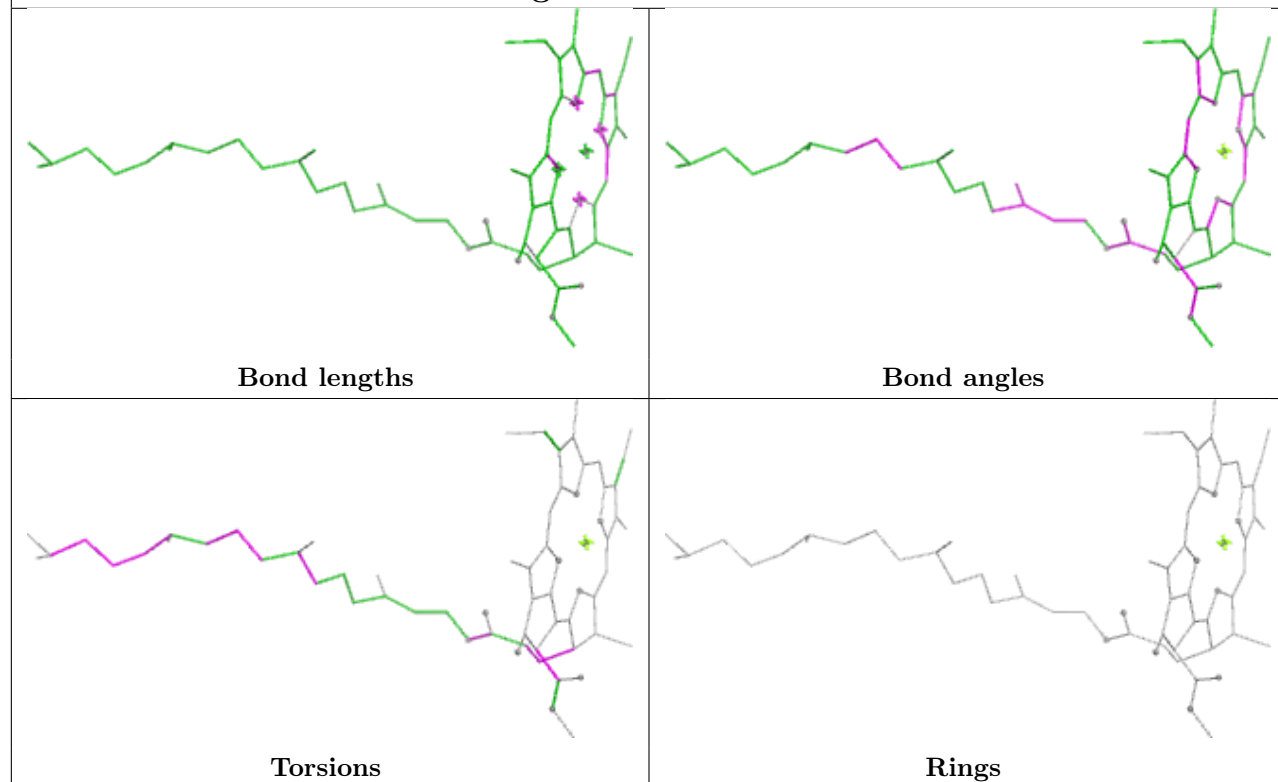


Rings

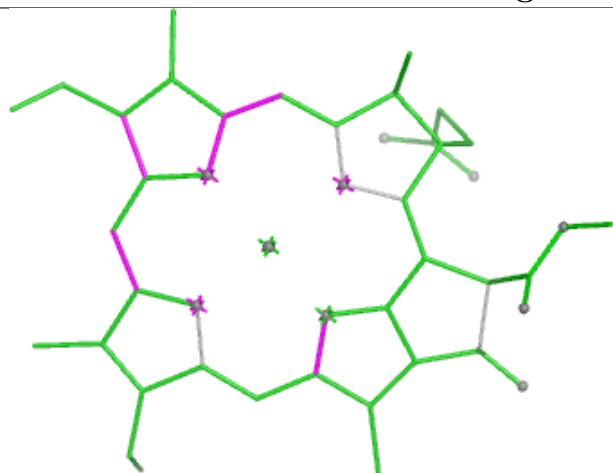
Ligand CLA A 818



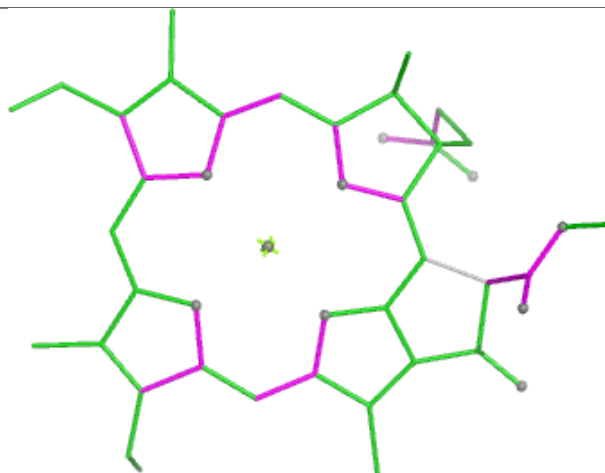
Ligand CLA B 827



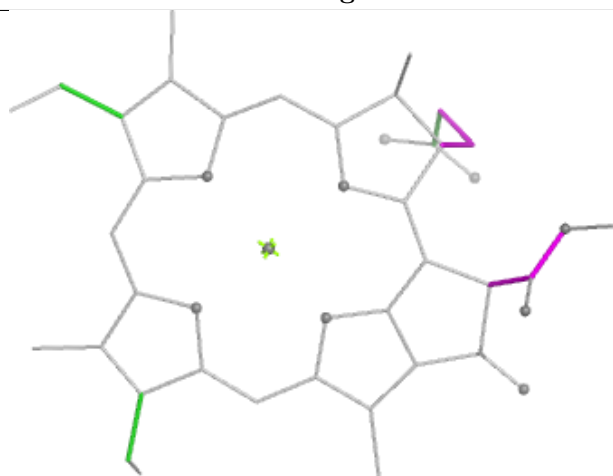
Ligand CLA L 302



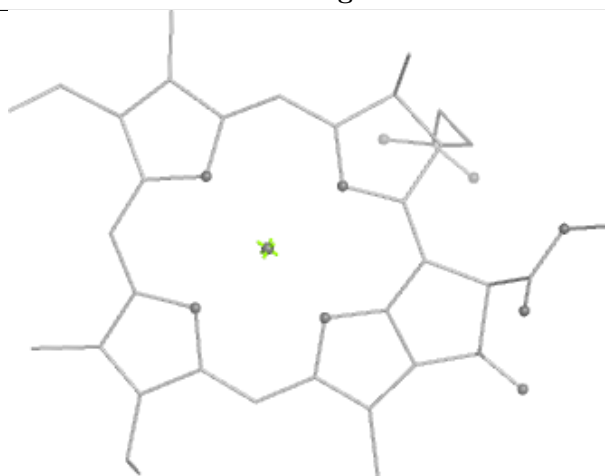
Bond lengths



Bond angles

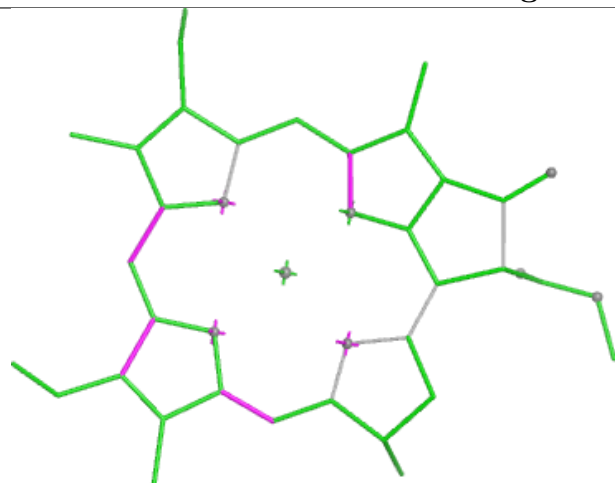


Torsions

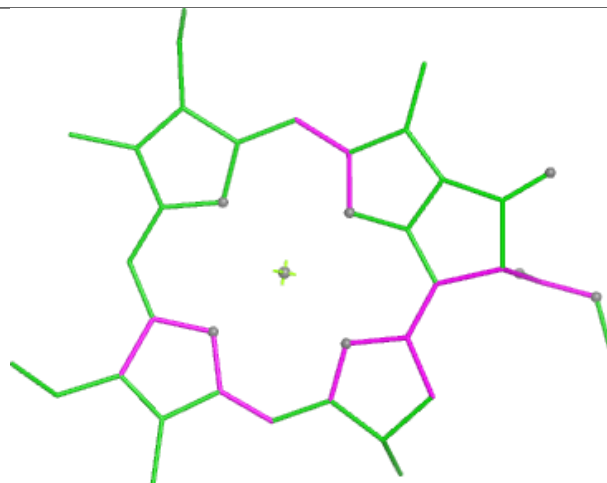


Rings

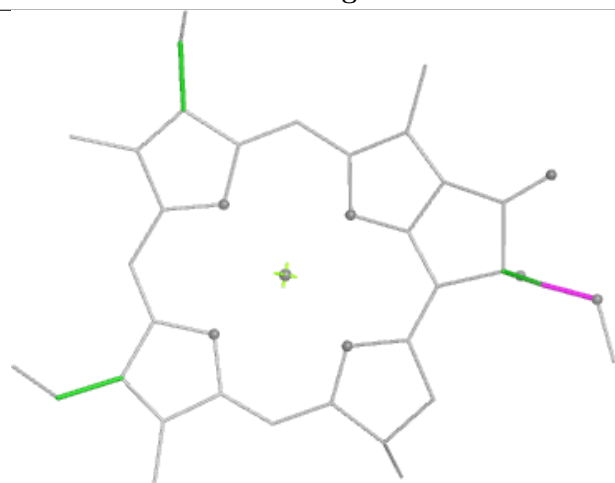
Ligand CLA 1 605



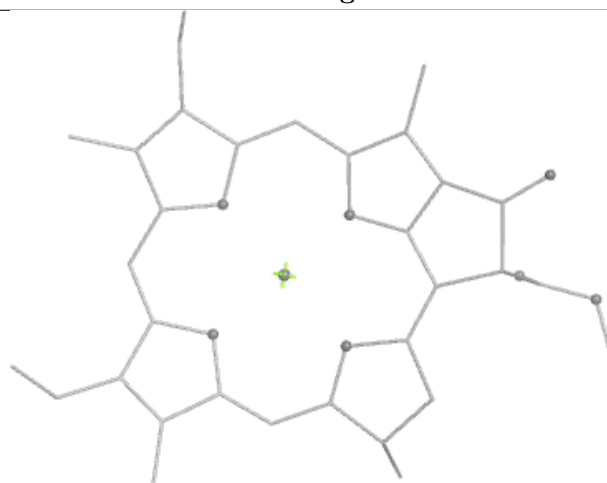
Bond lengths



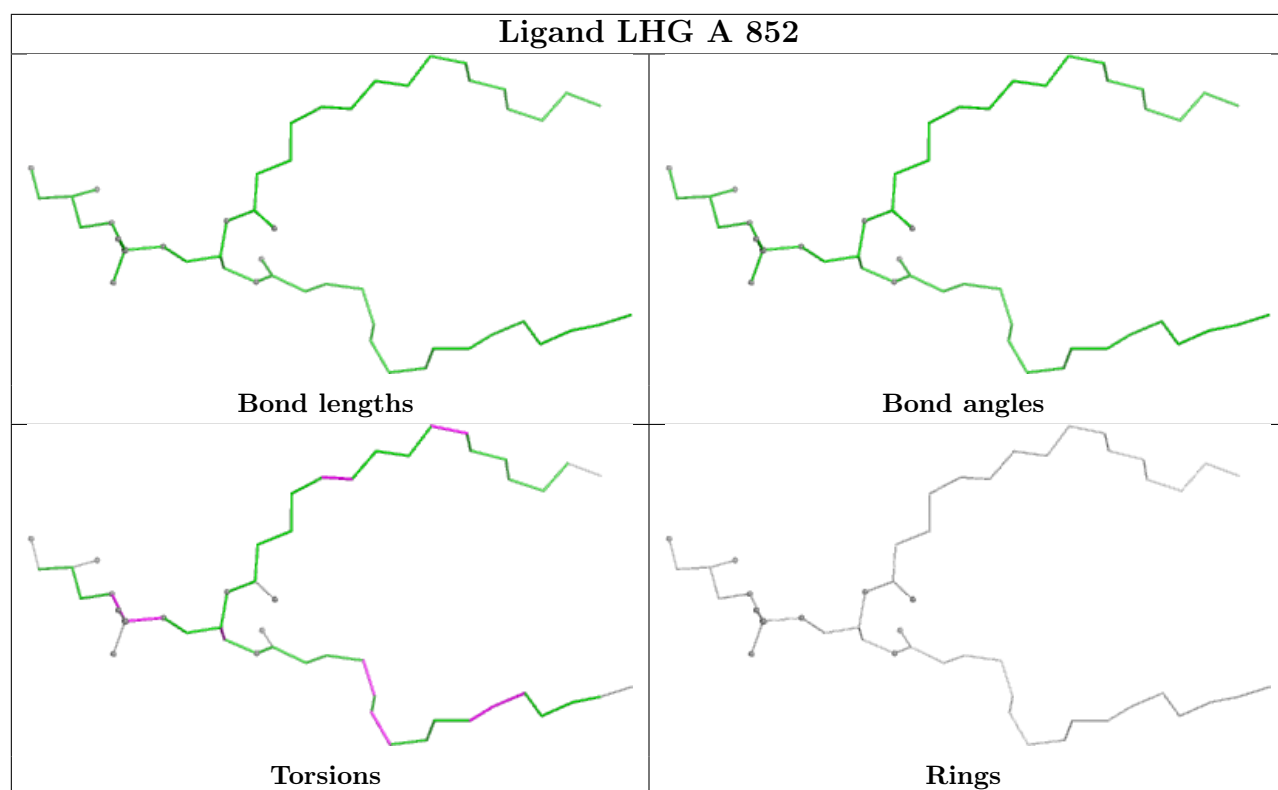
Bond angles



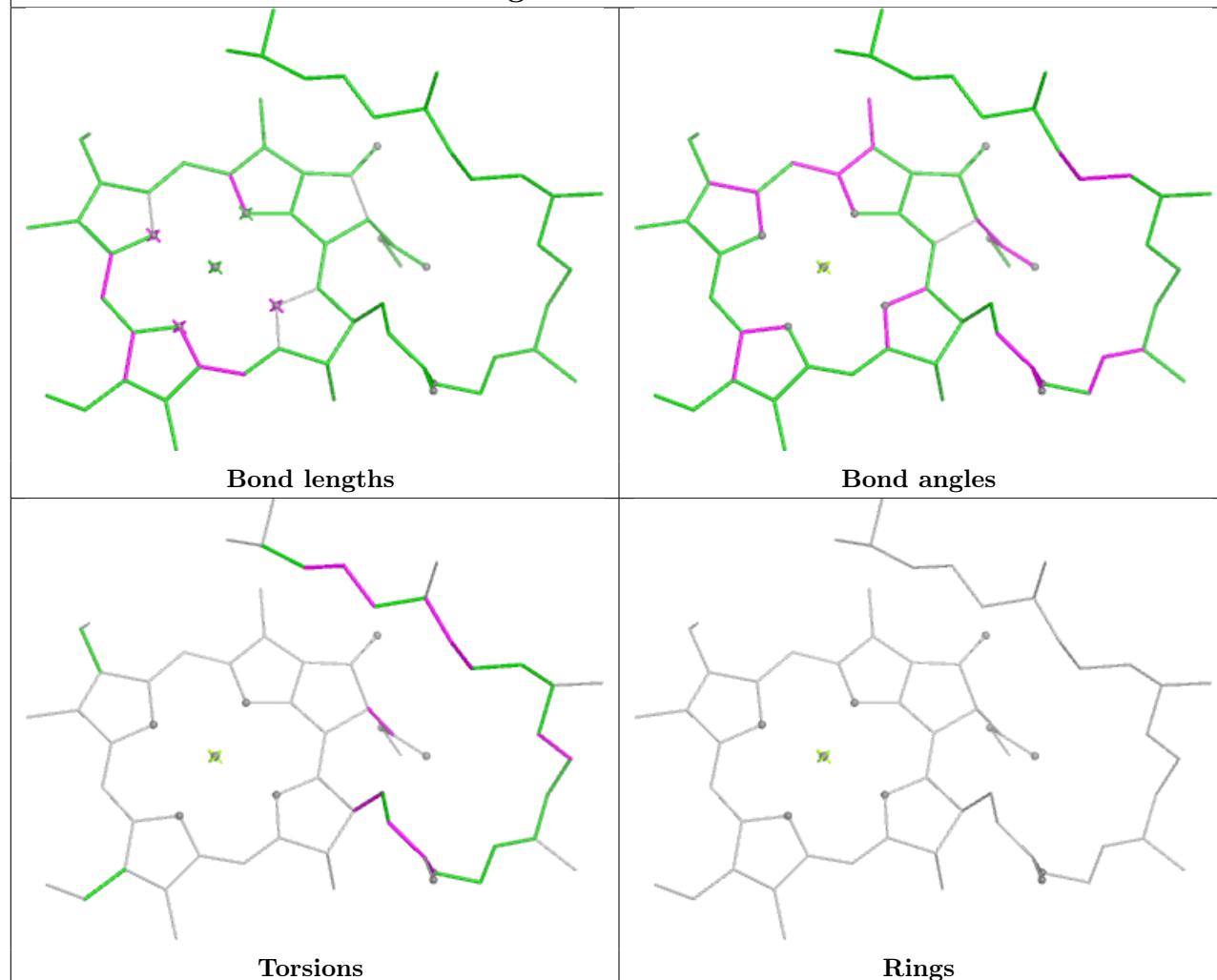
Torsions



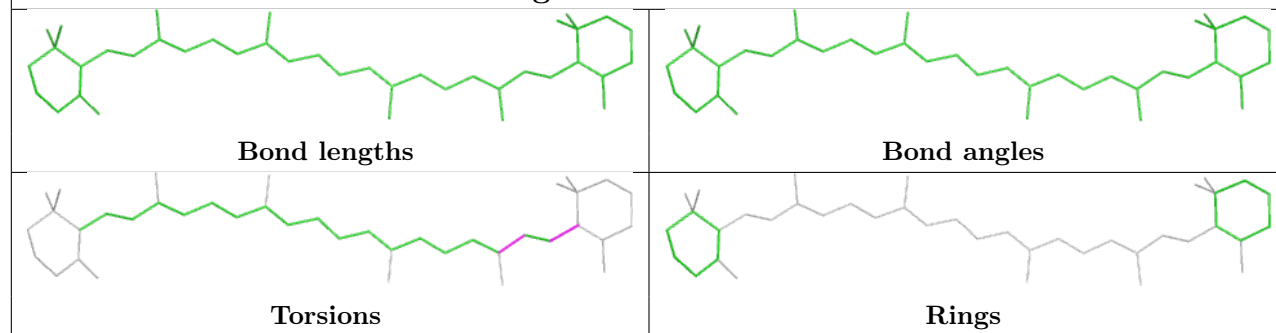
Rings



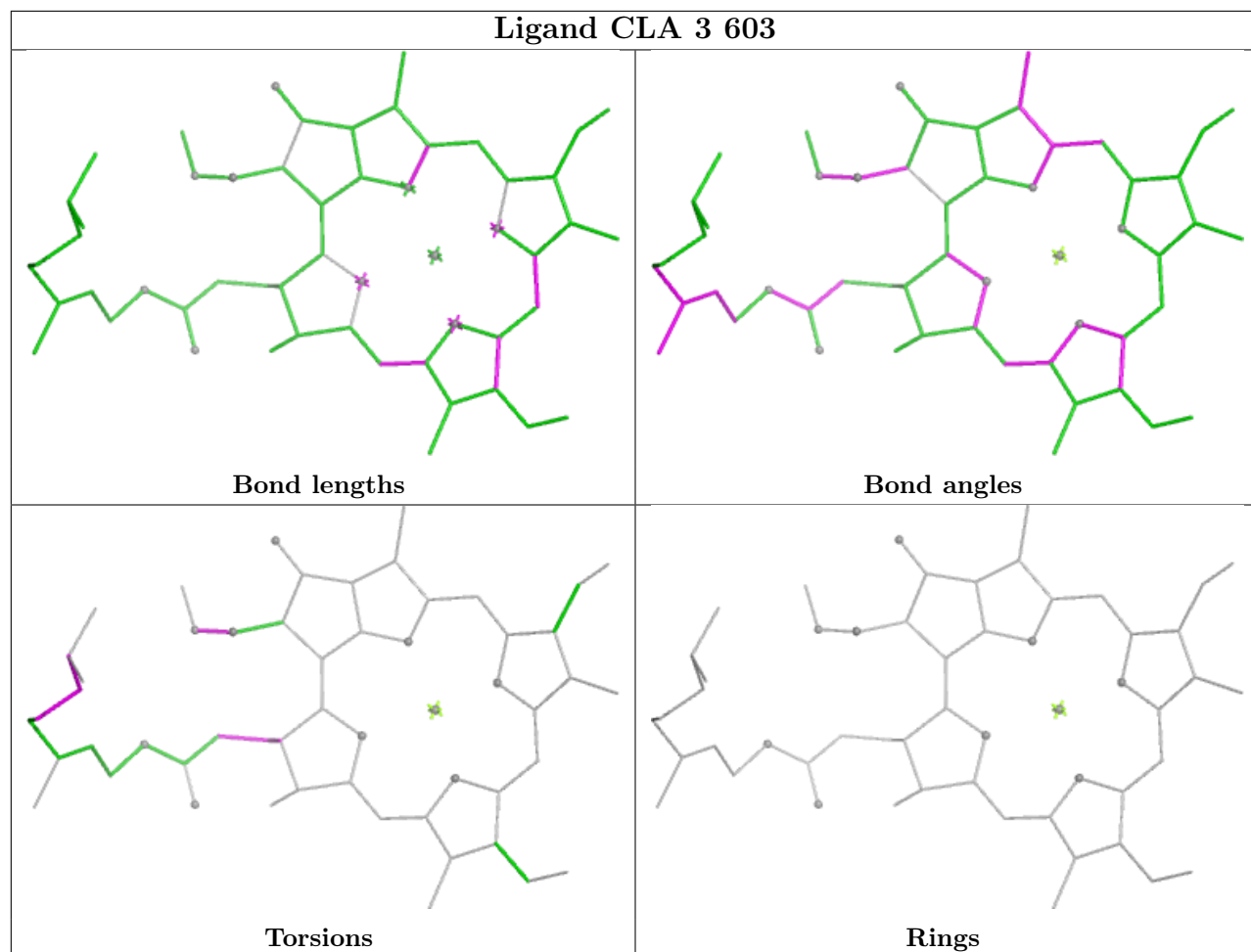
Ligand CLA B 804



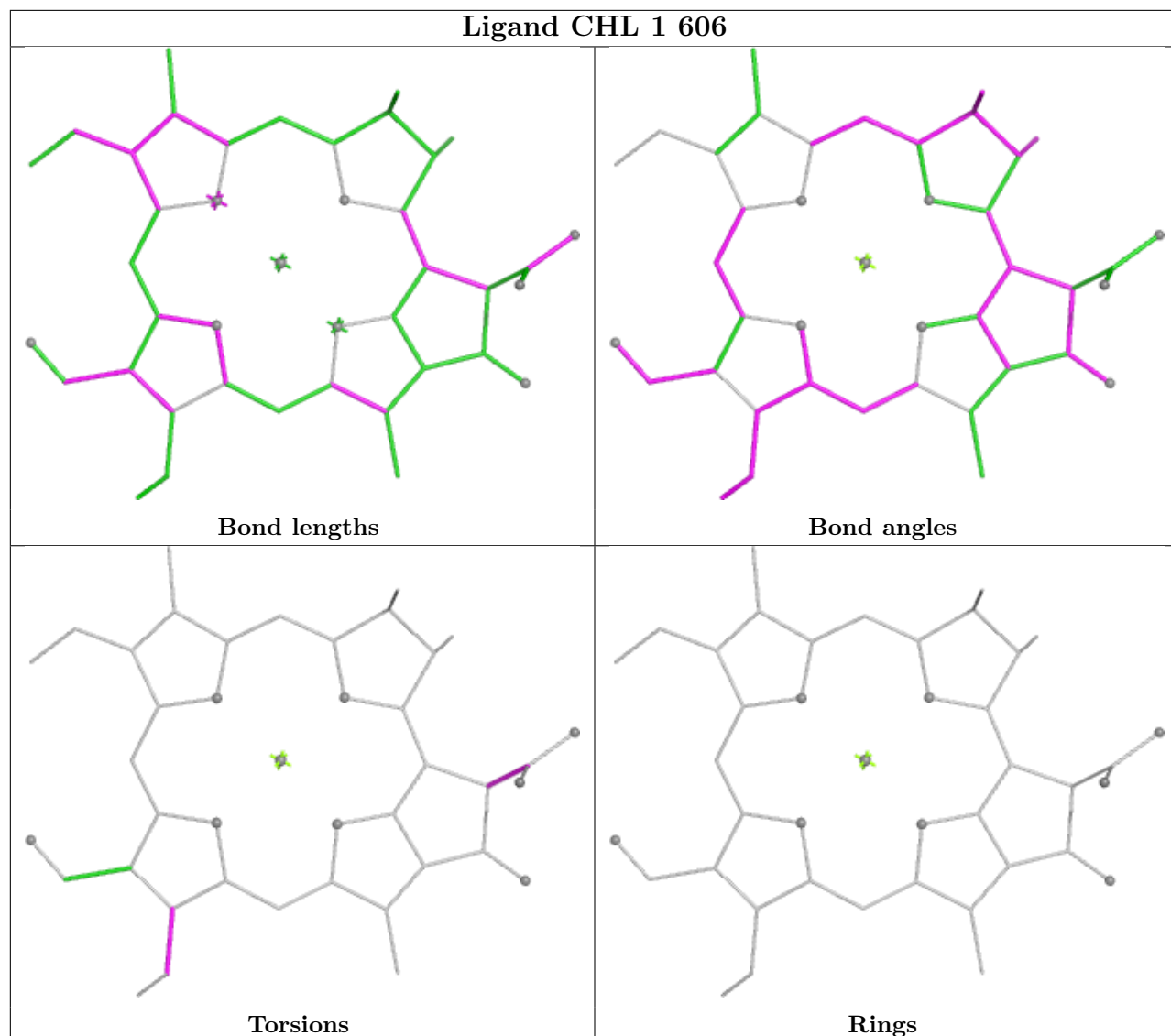
Ligand BCR L 305

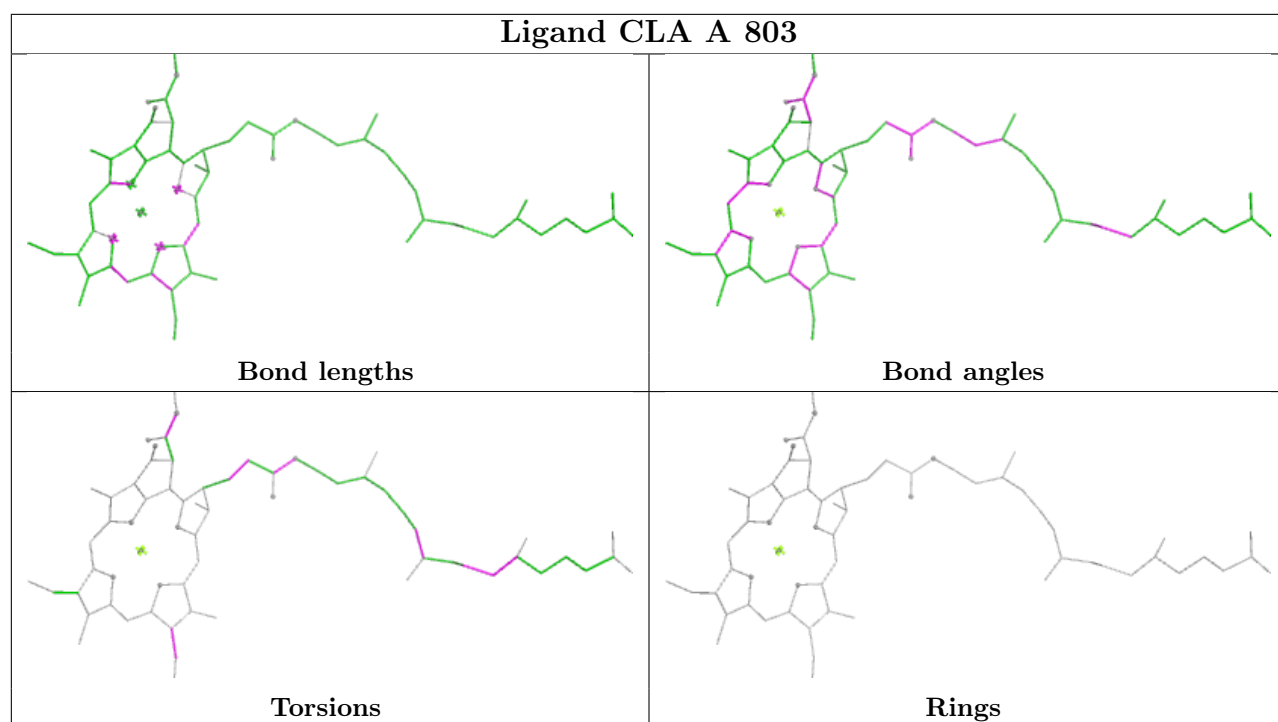


Ligand CLA 3 603

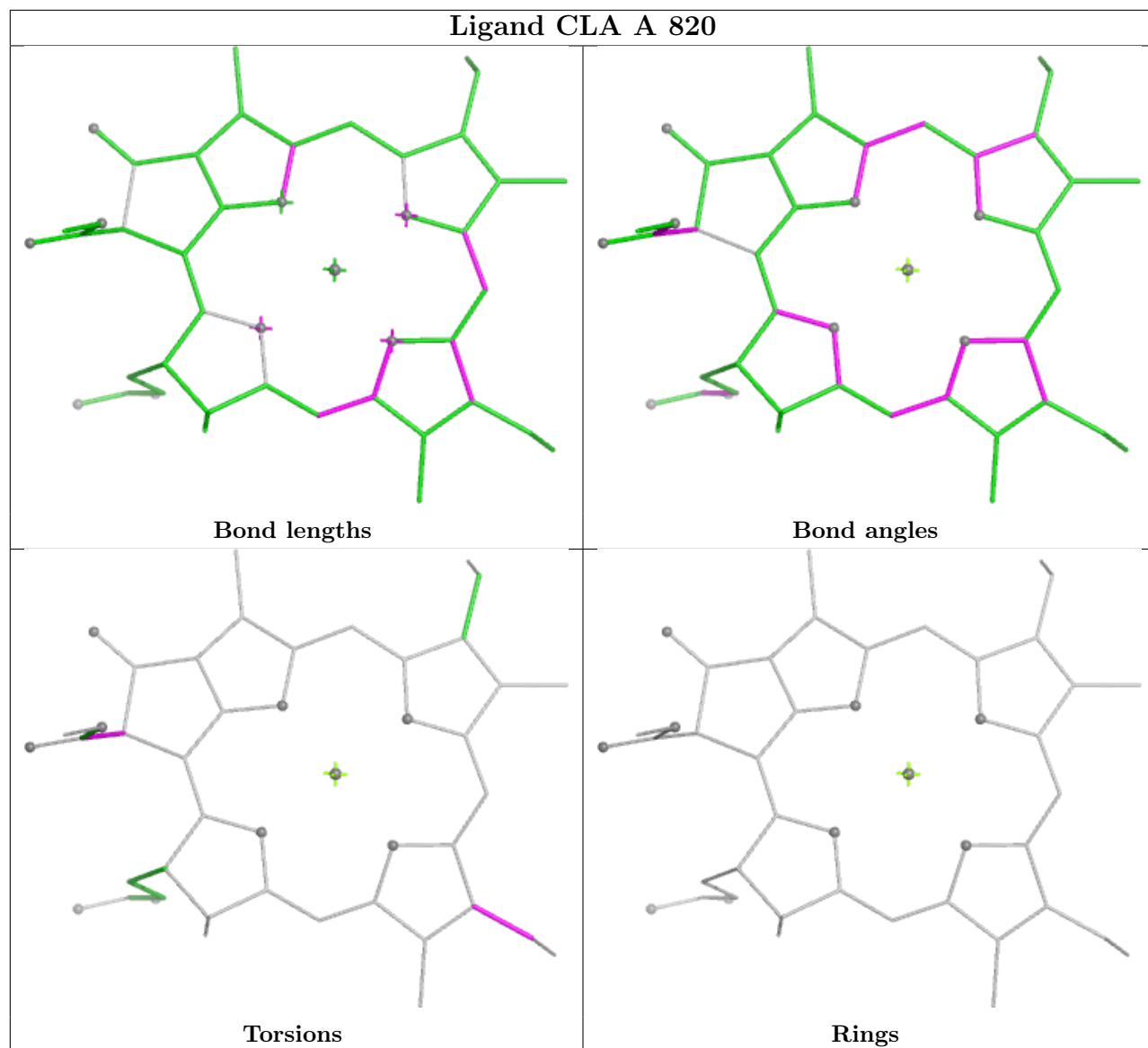


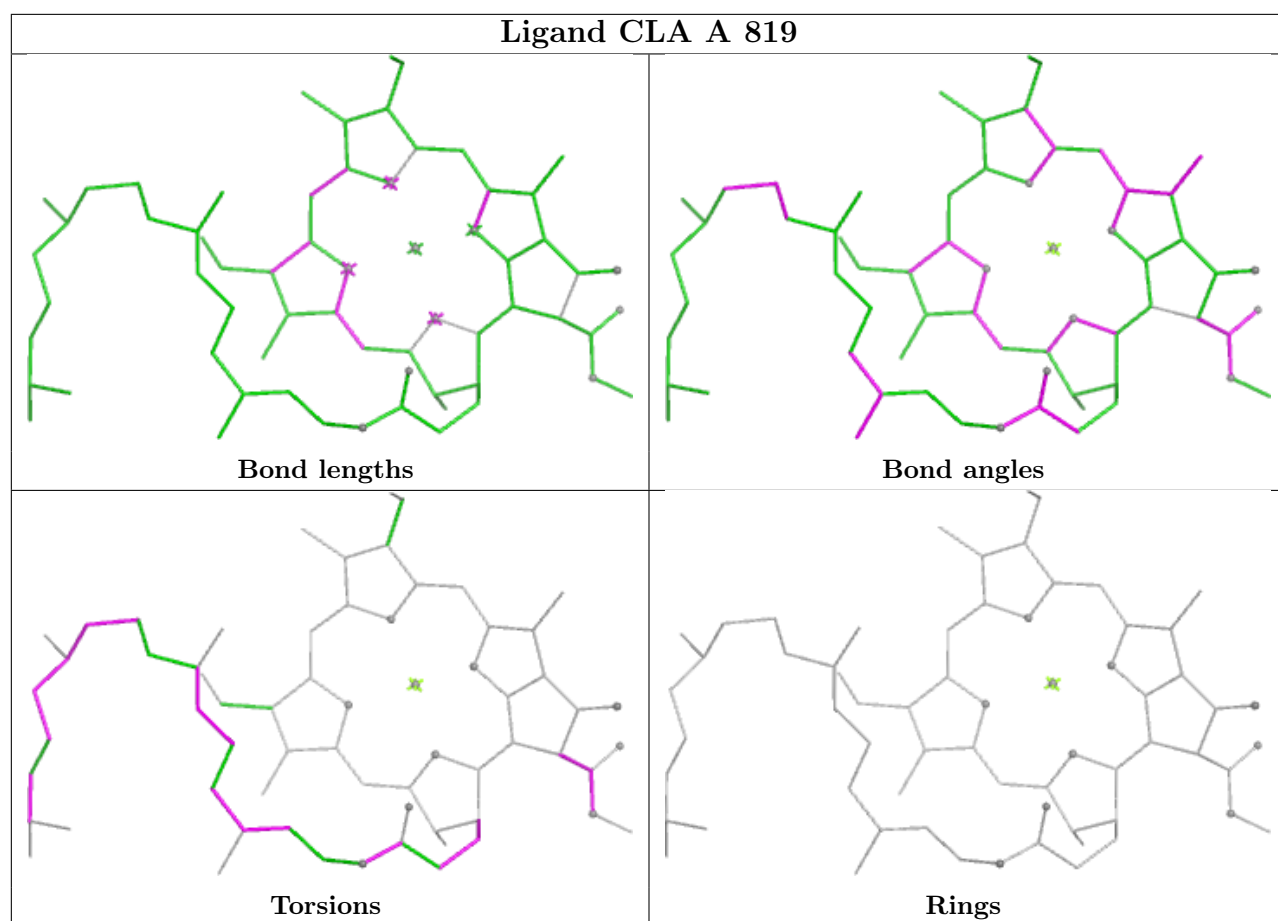
Ligand CHL 1 606



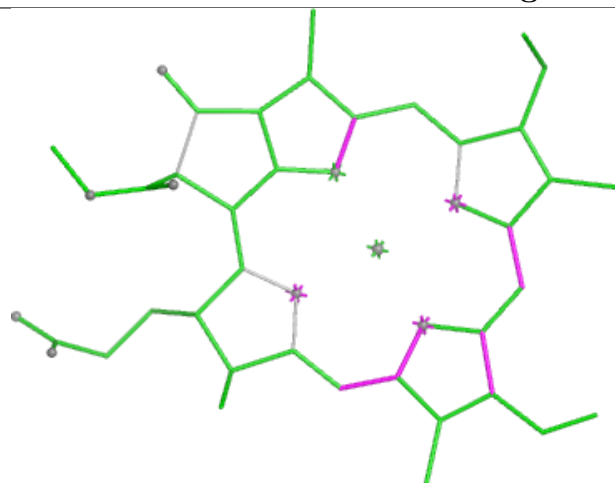


Ligand CLA A 820

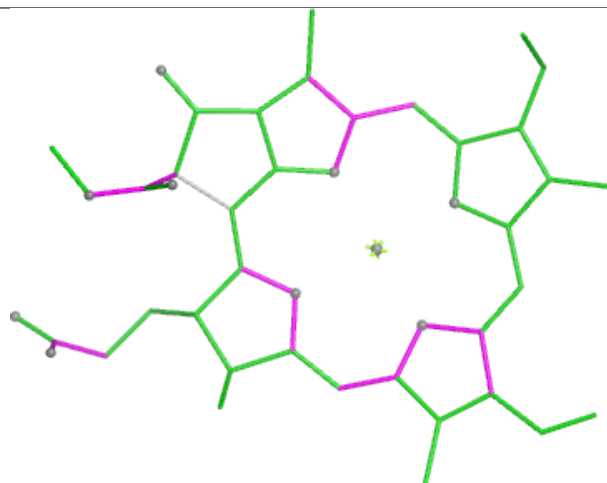




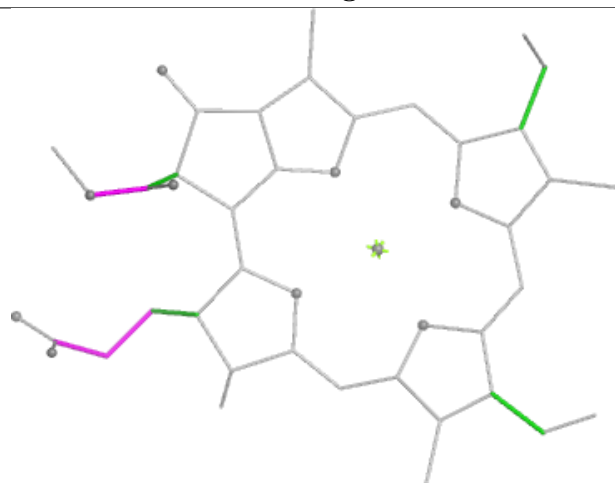
Ligand CLA 1 611



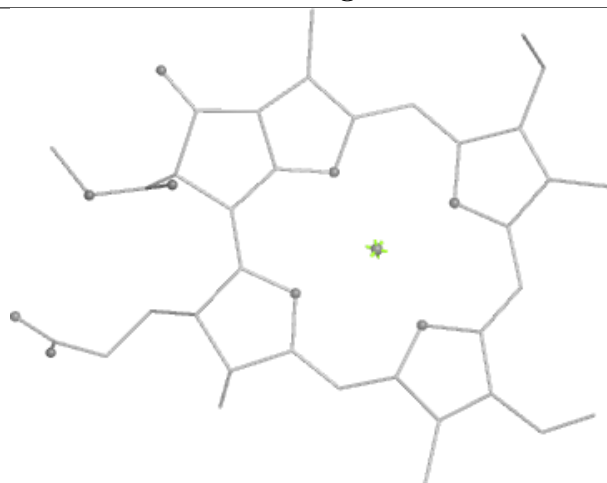
Bond lengths



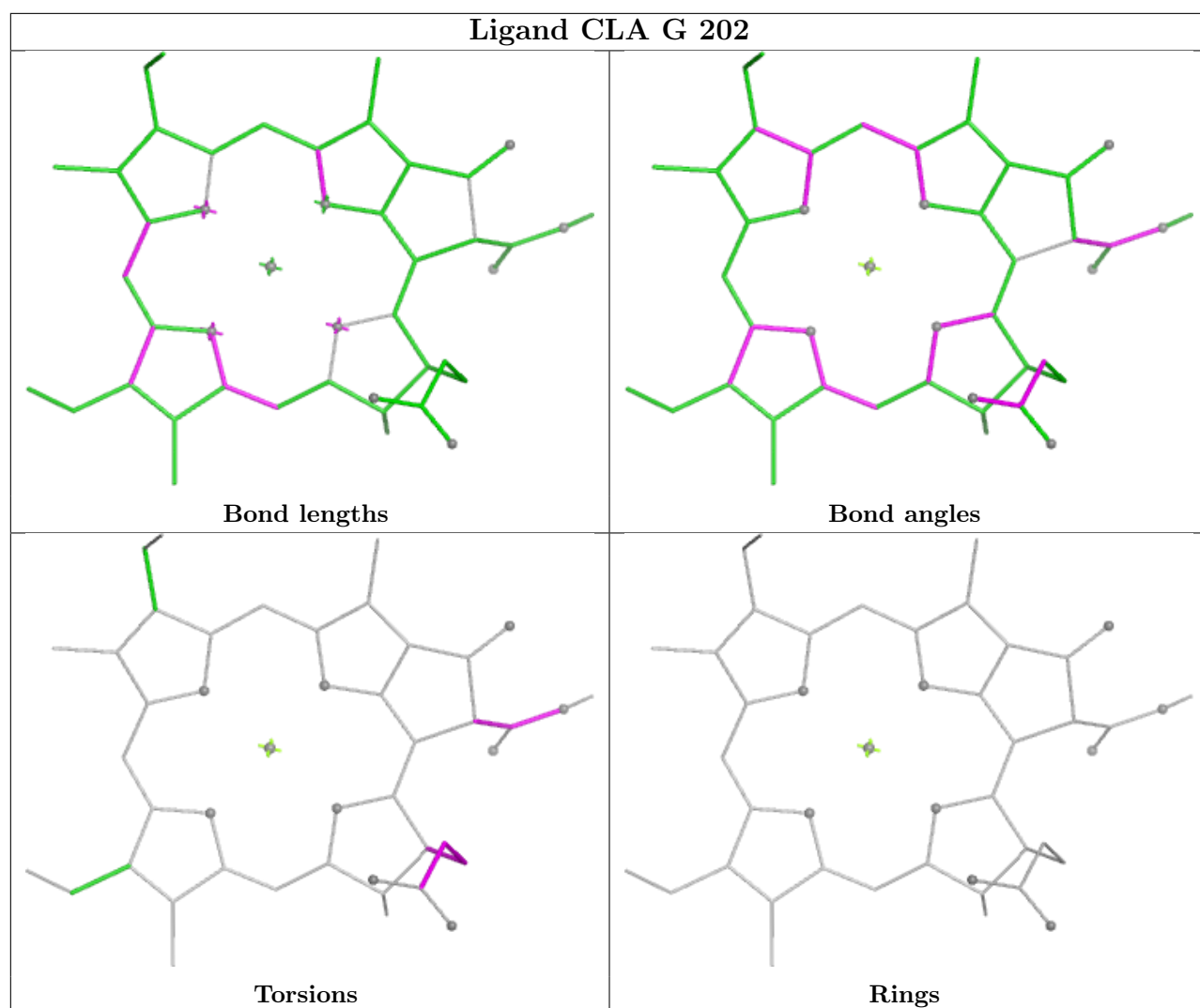
Bond angles

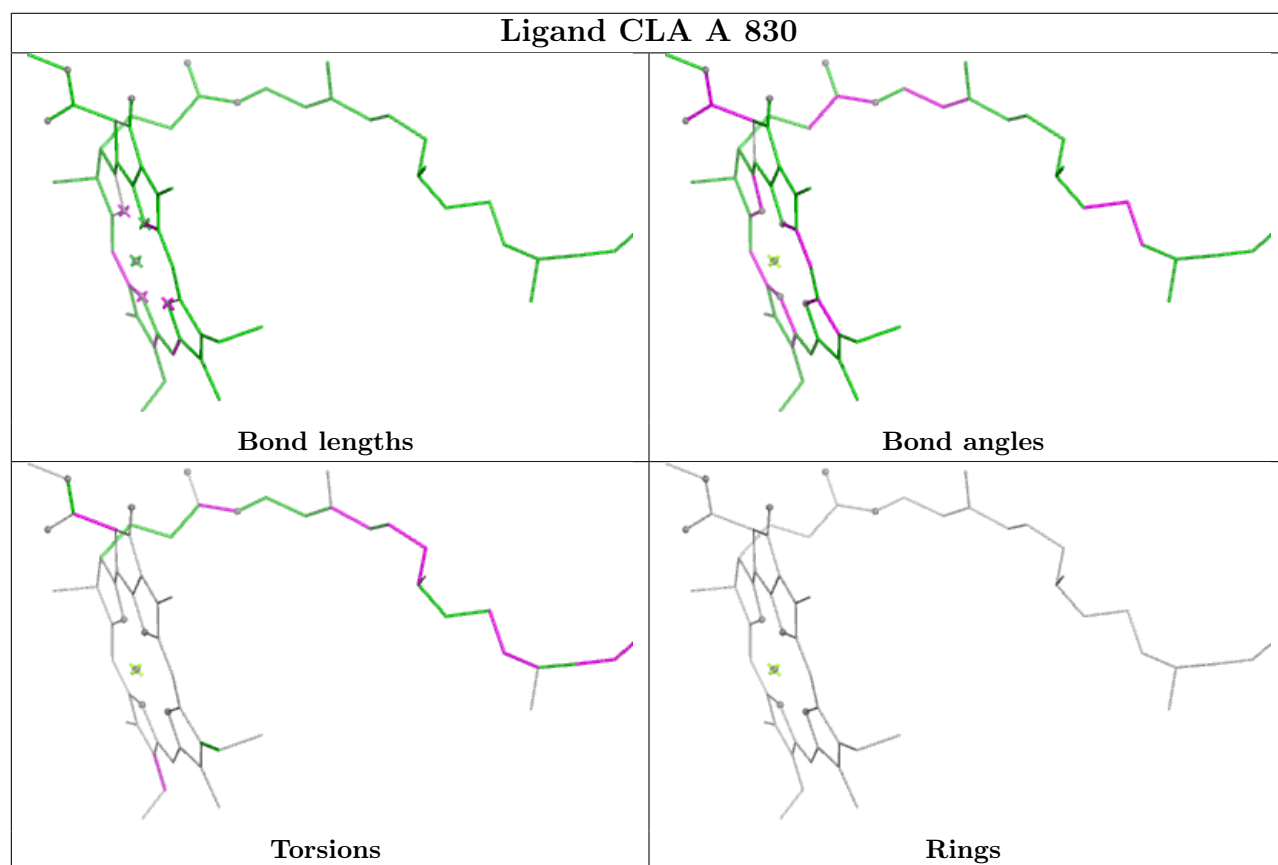
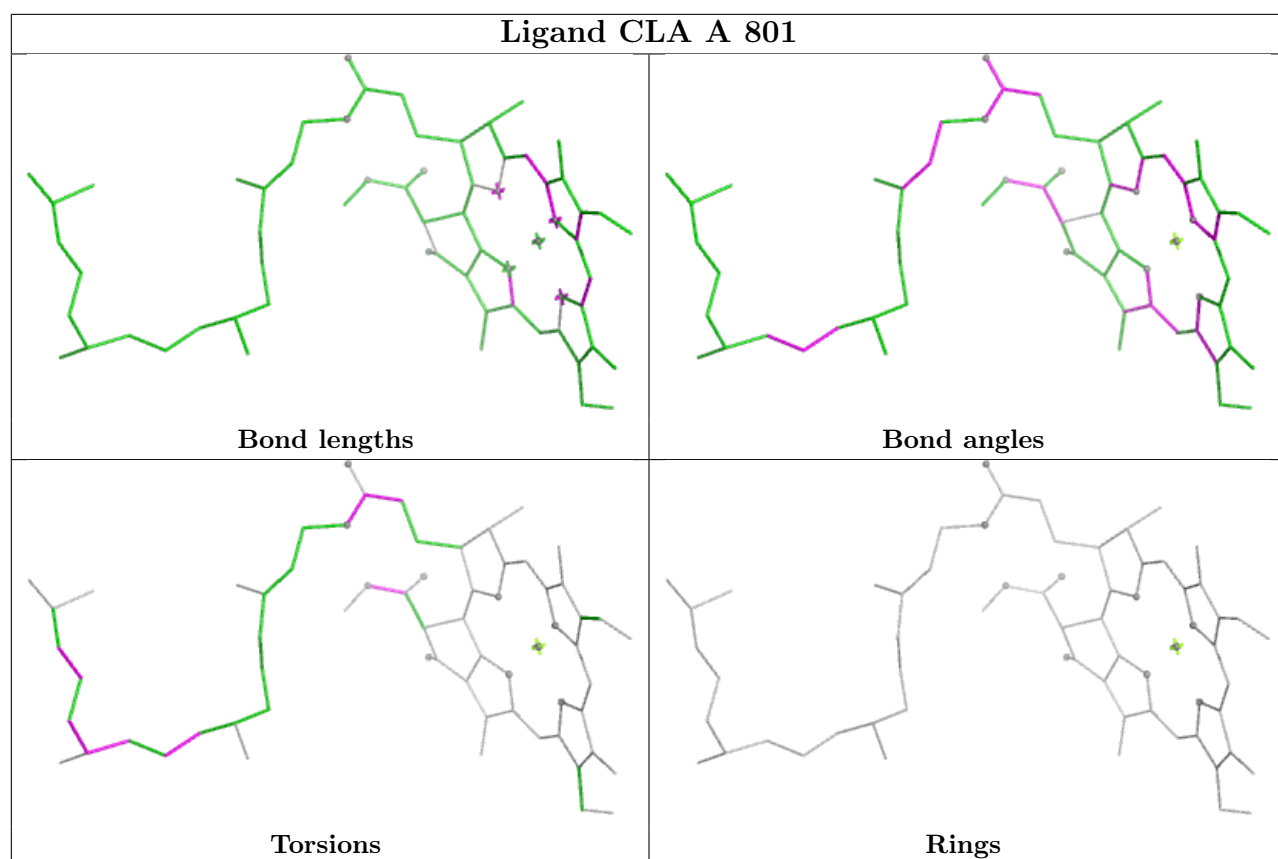


Torsions

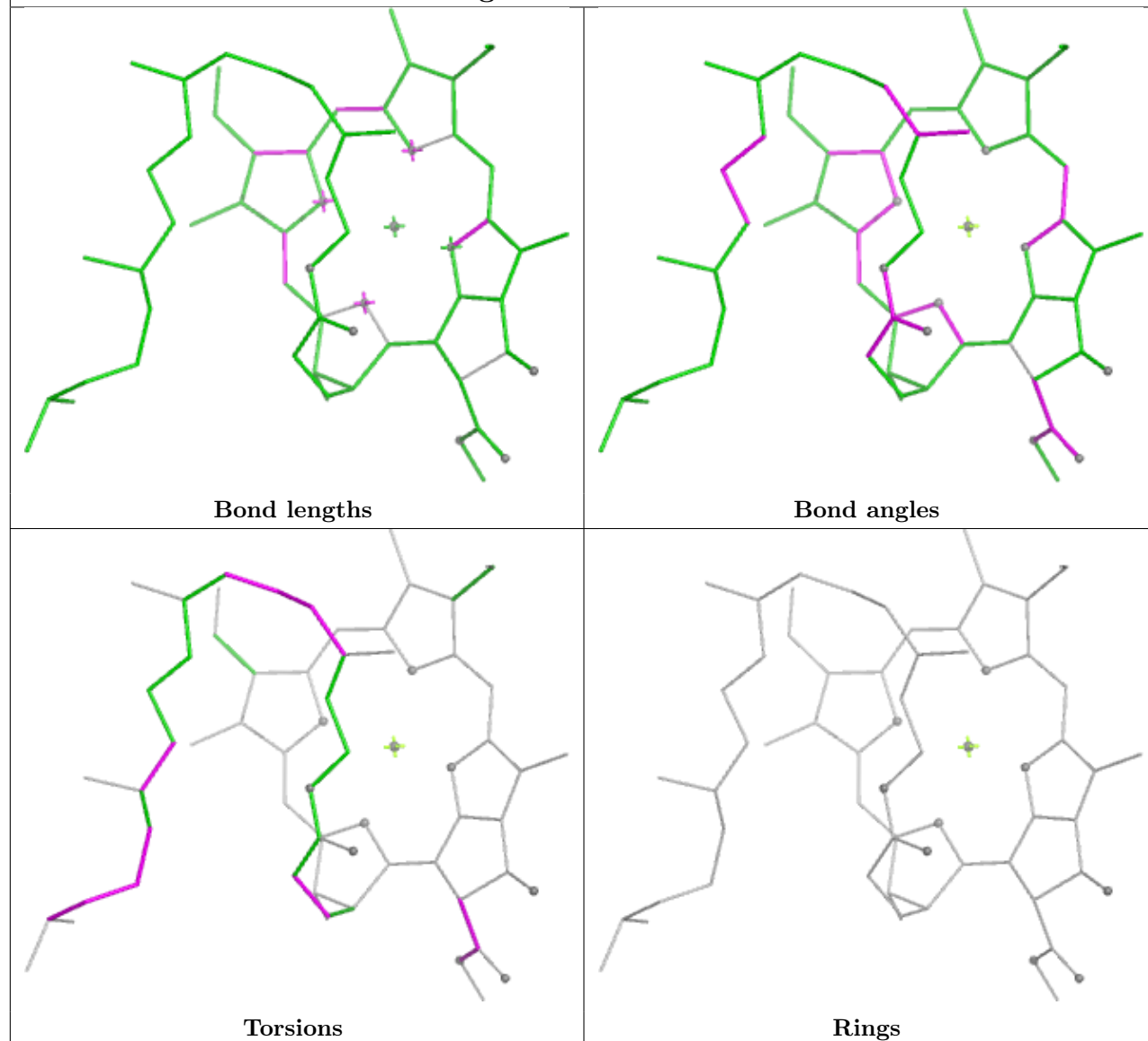


Rings

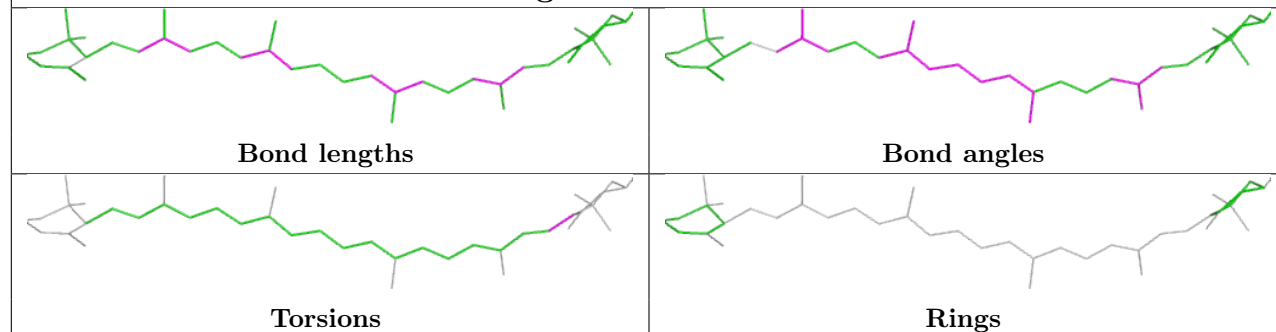




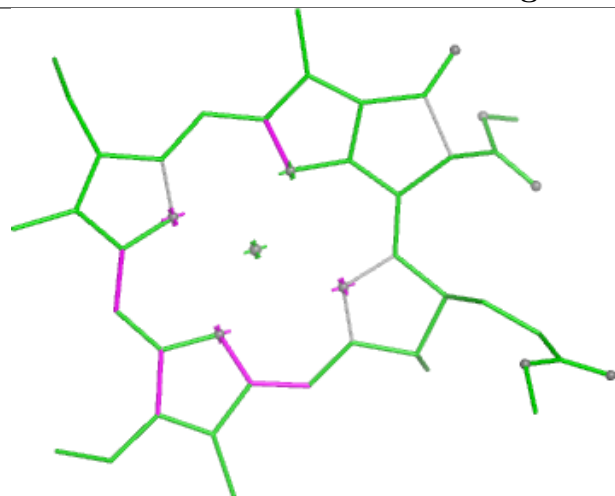
Ligand CLA B 807



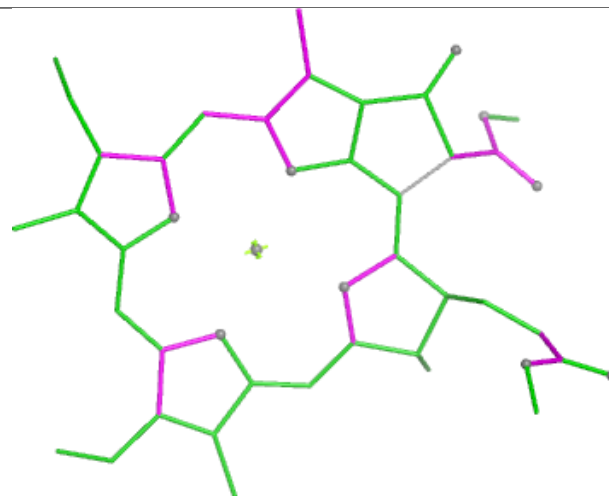
Ligand LUT 4 616



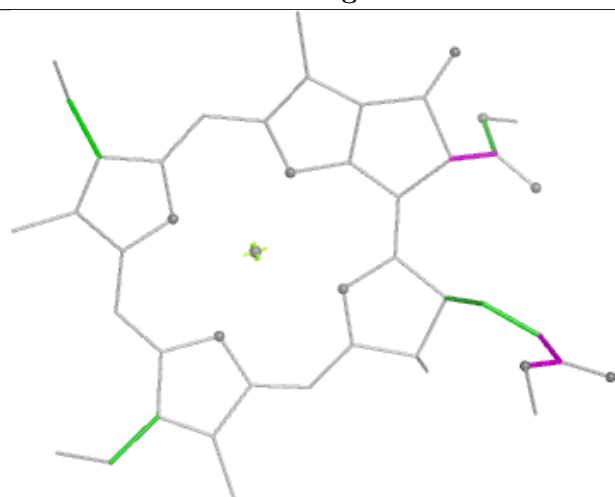
Ligand CLA 4 601



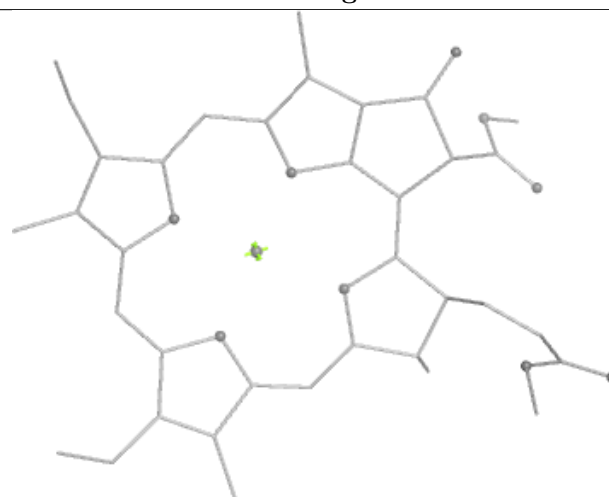
Bond lengths



Bond angles

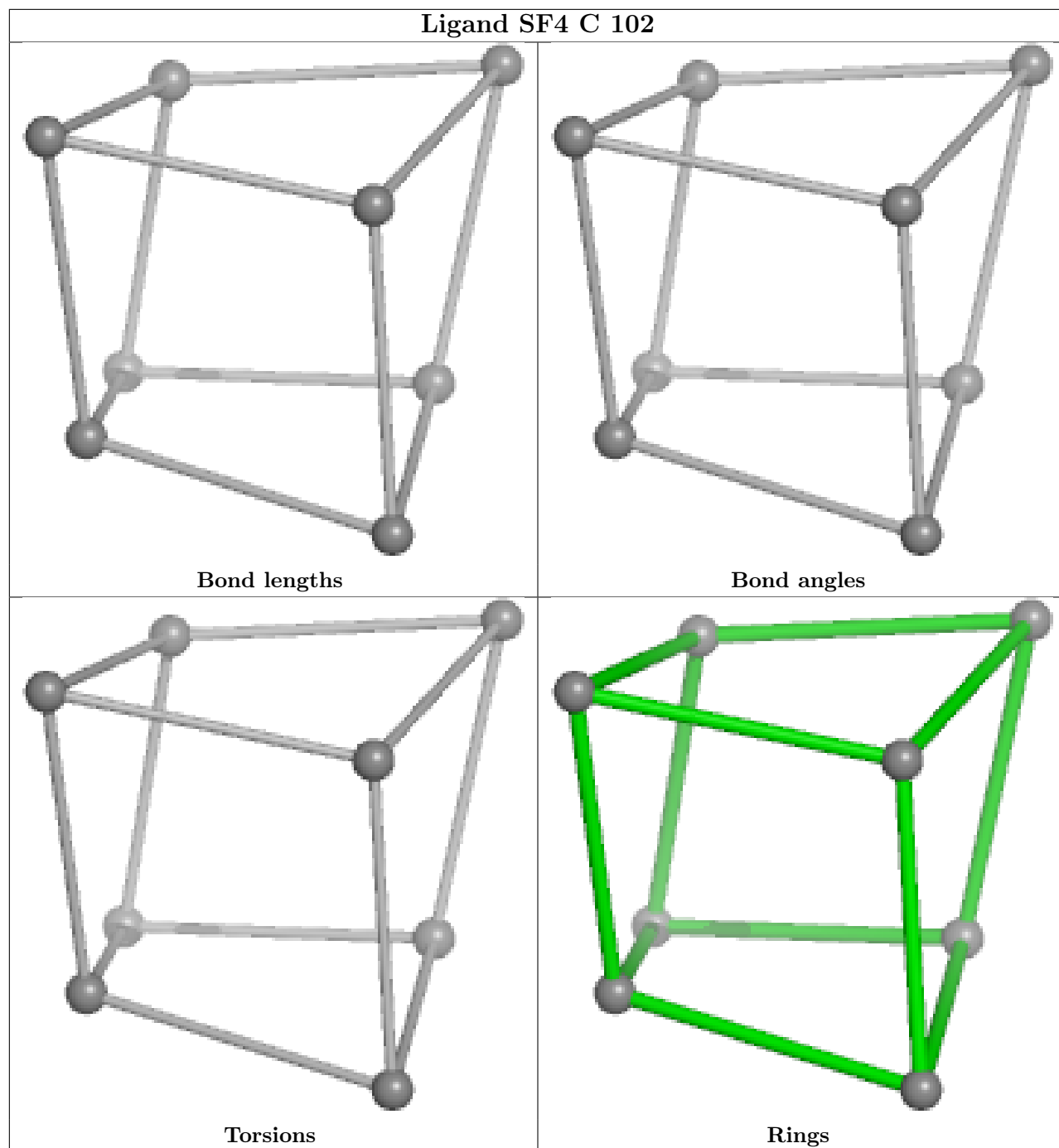


Torsions

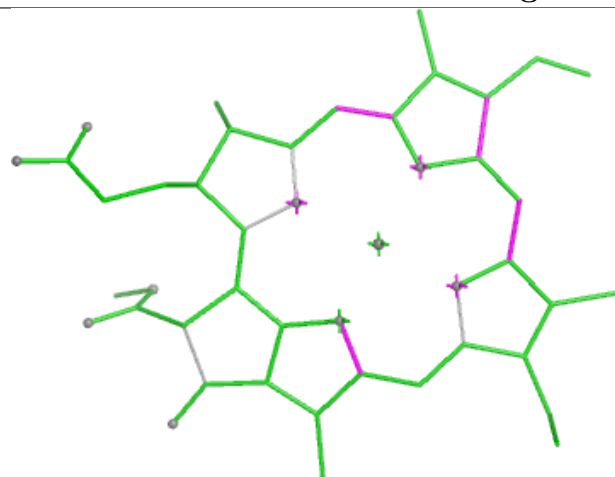


Rings

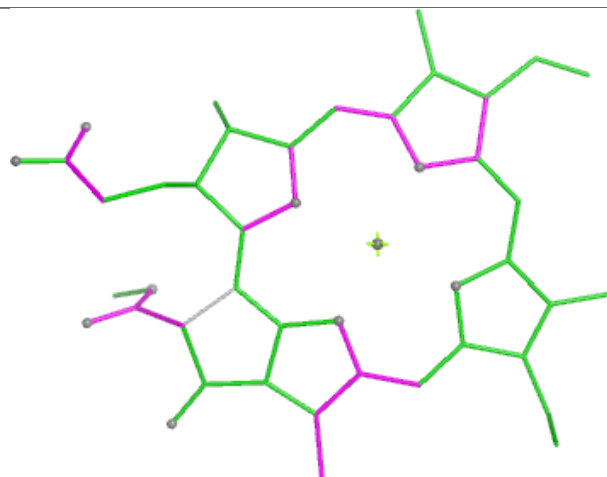
Ligand SF4 C 102



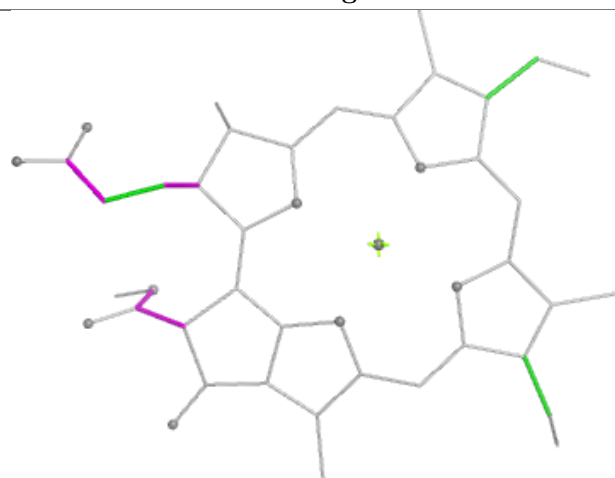
Ligand CLA 4 603



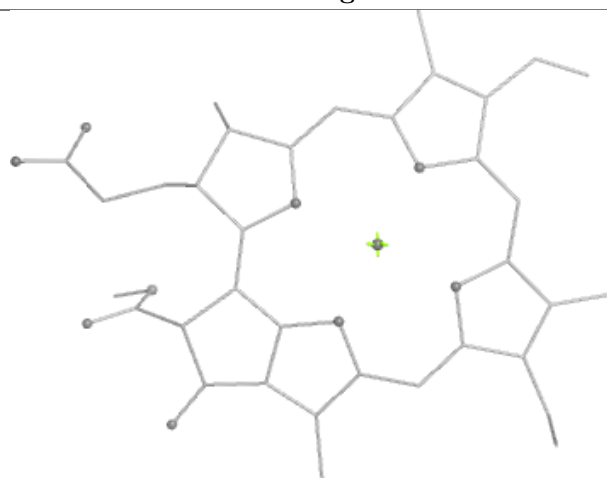
Bond lengths



Bond angles

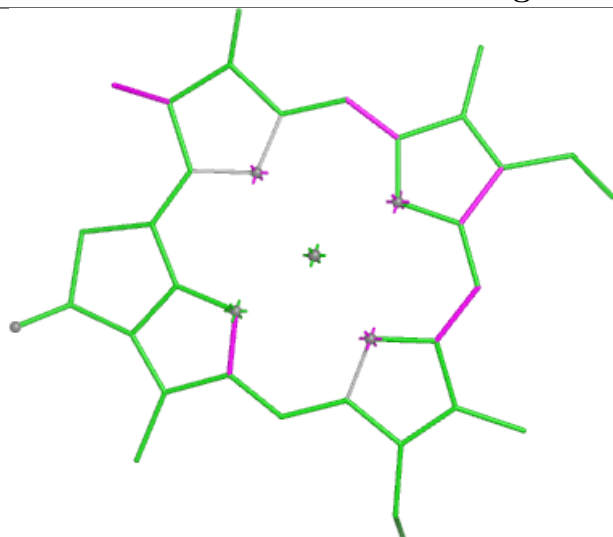


Torsions

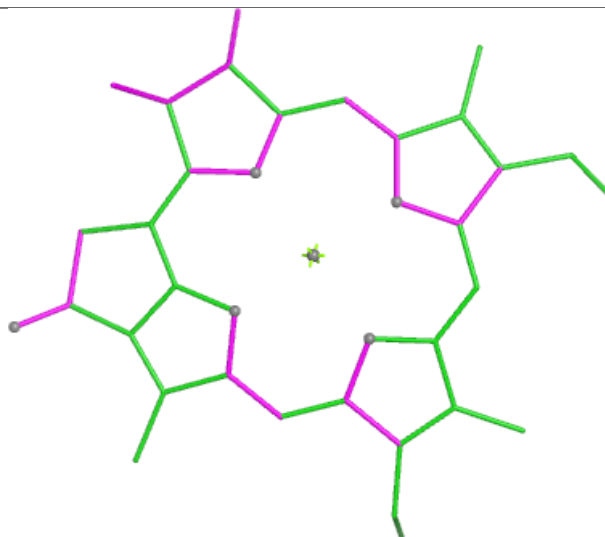


Rings

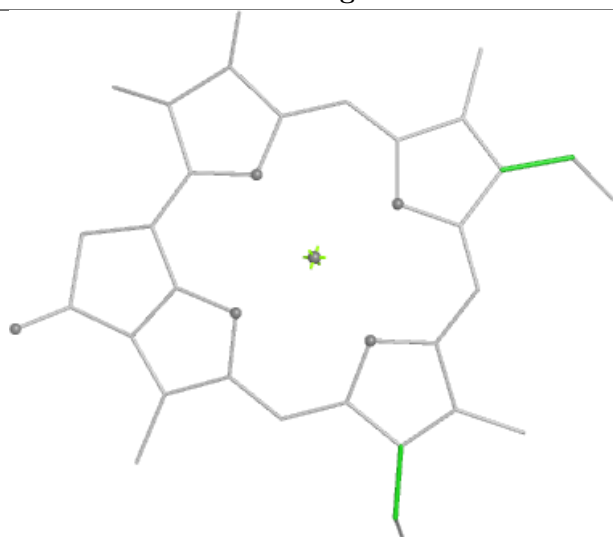
Ligand CLA K 201



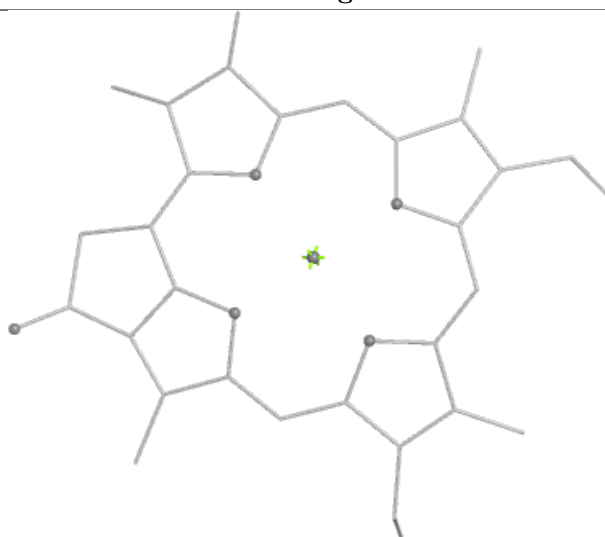
Bond lengths



Bond angles

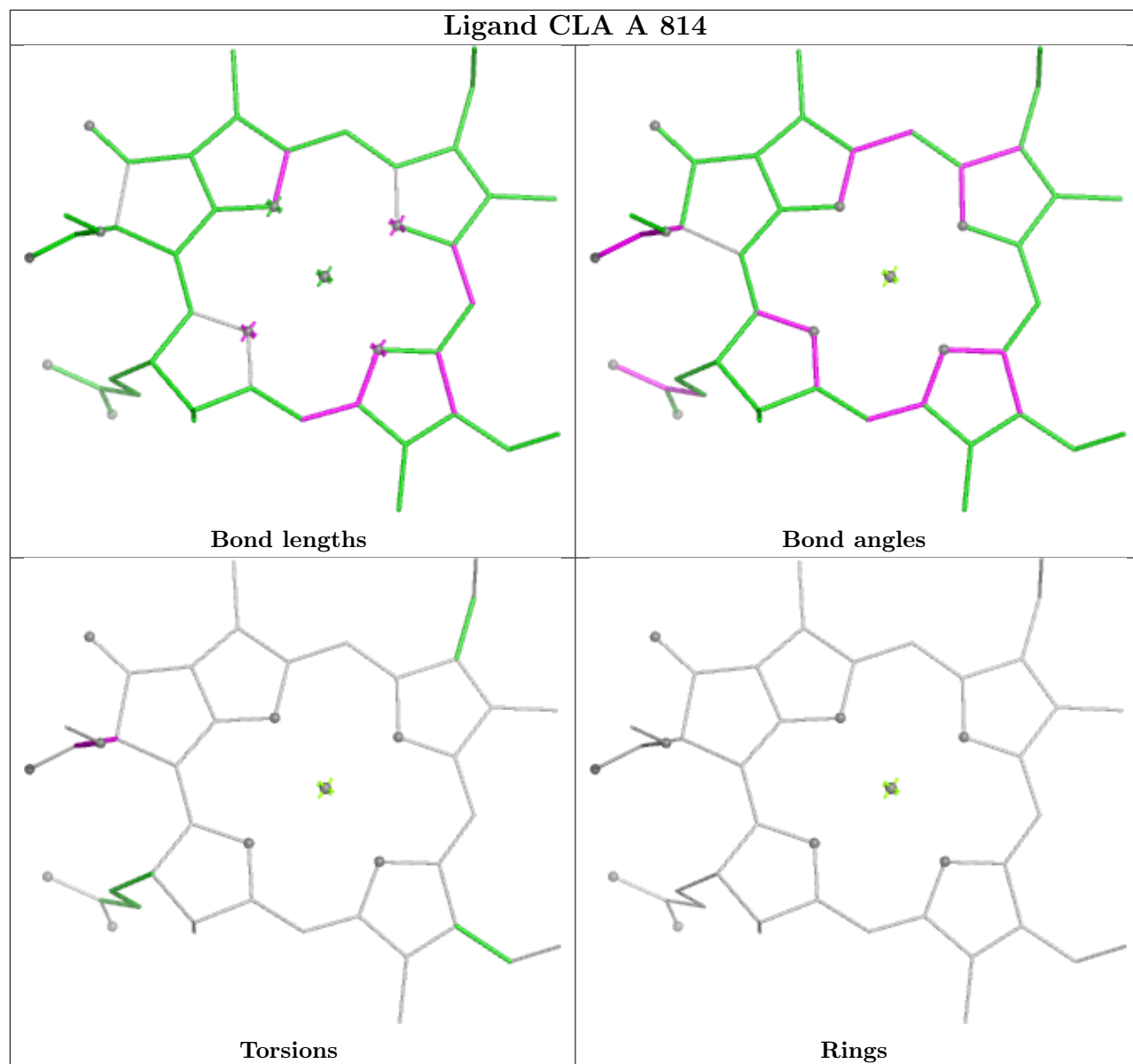


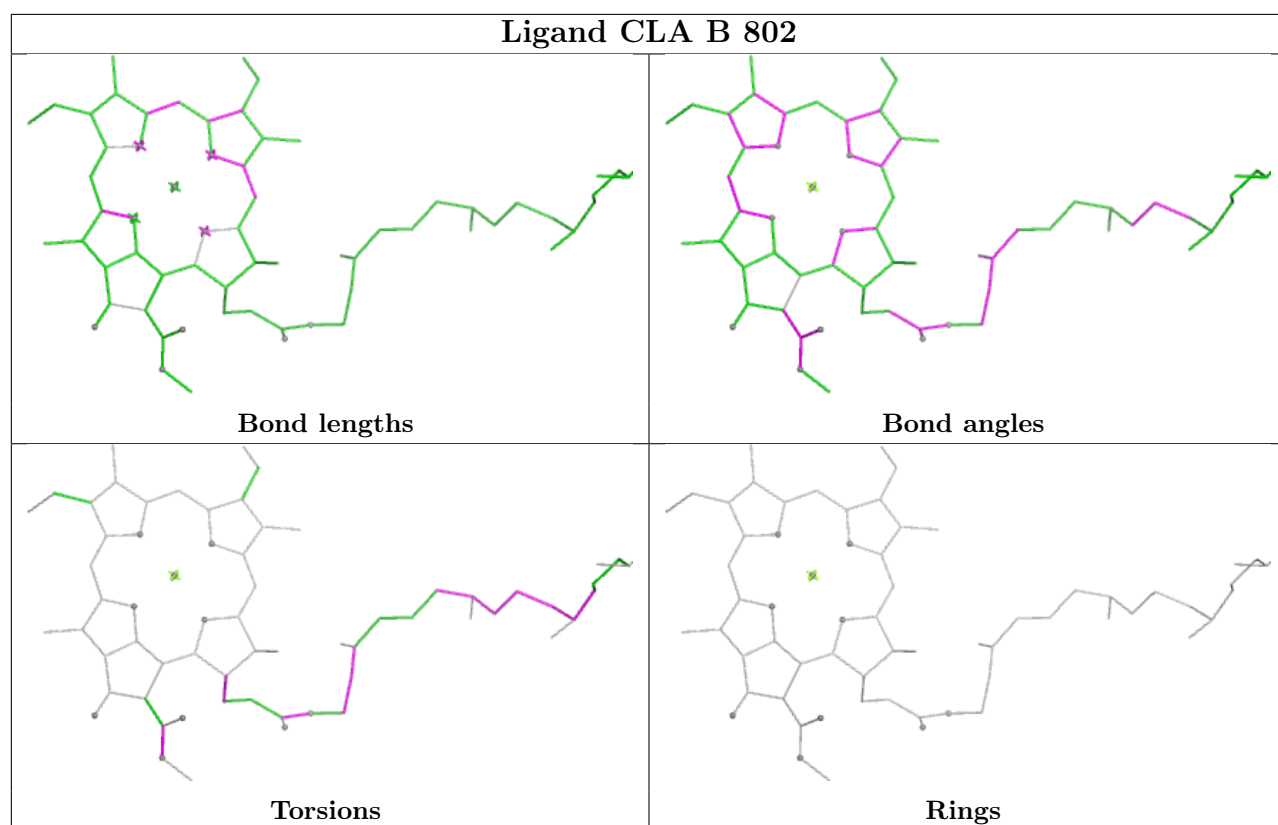
Torsions

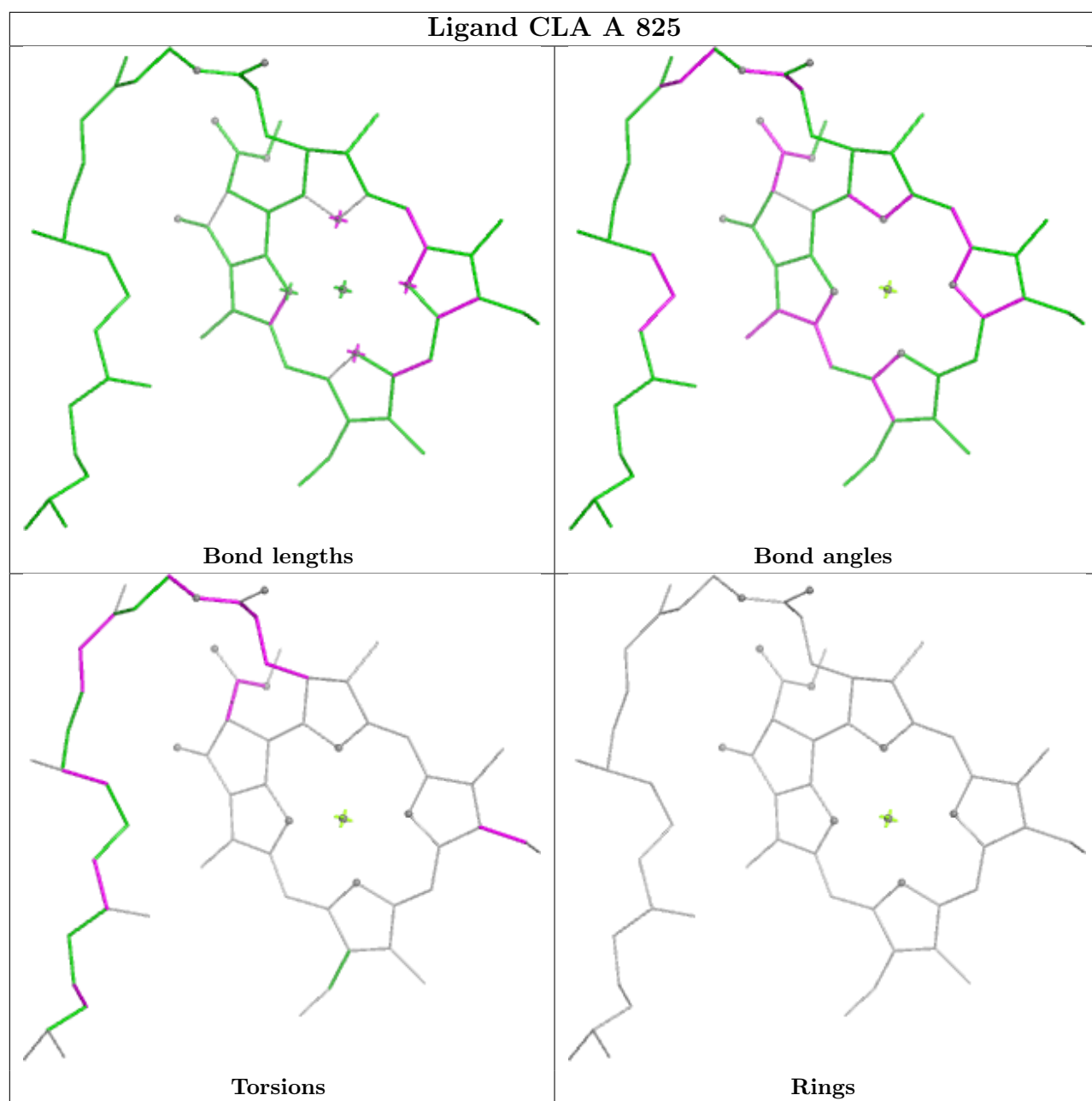


Rings

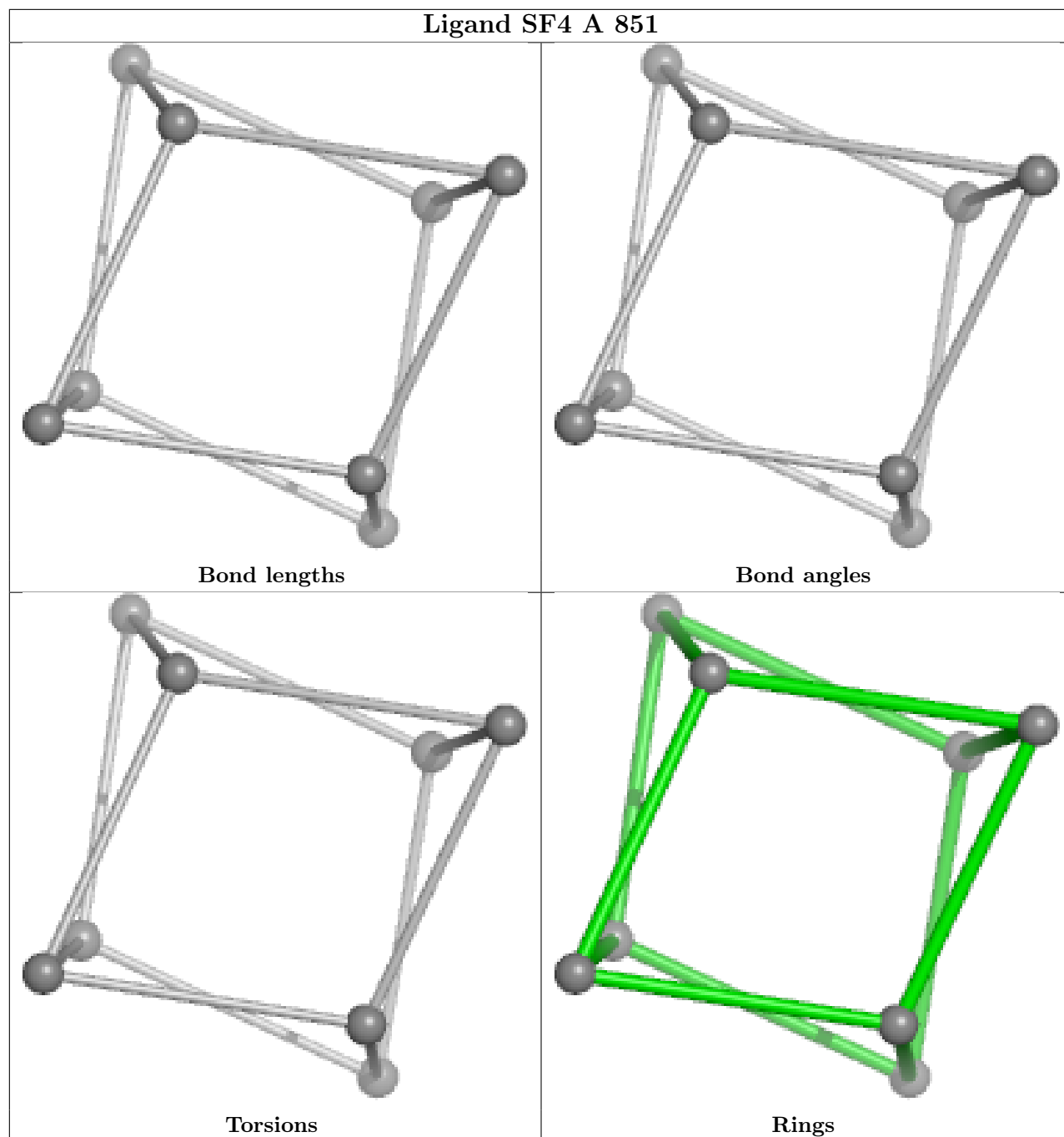
Ligand CLA A 814



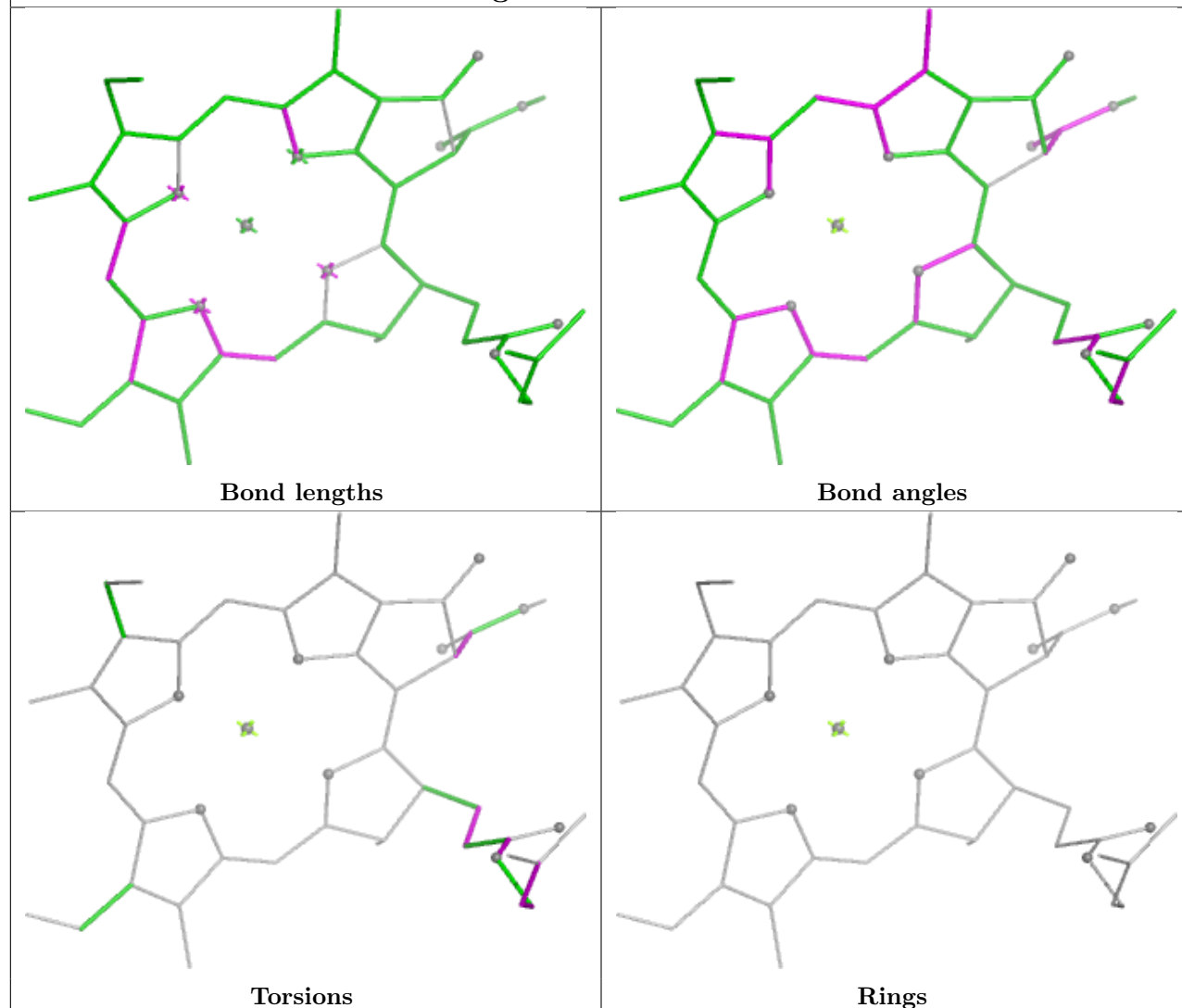




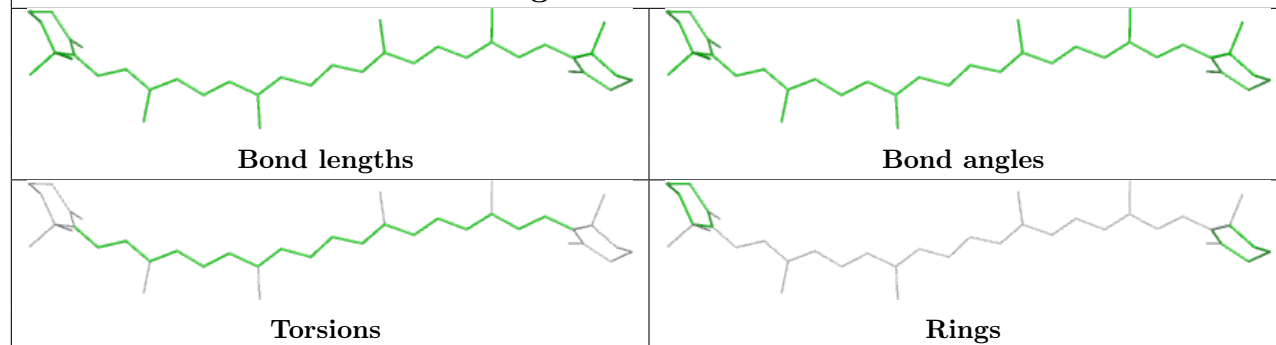
Ligand SF4 A 851

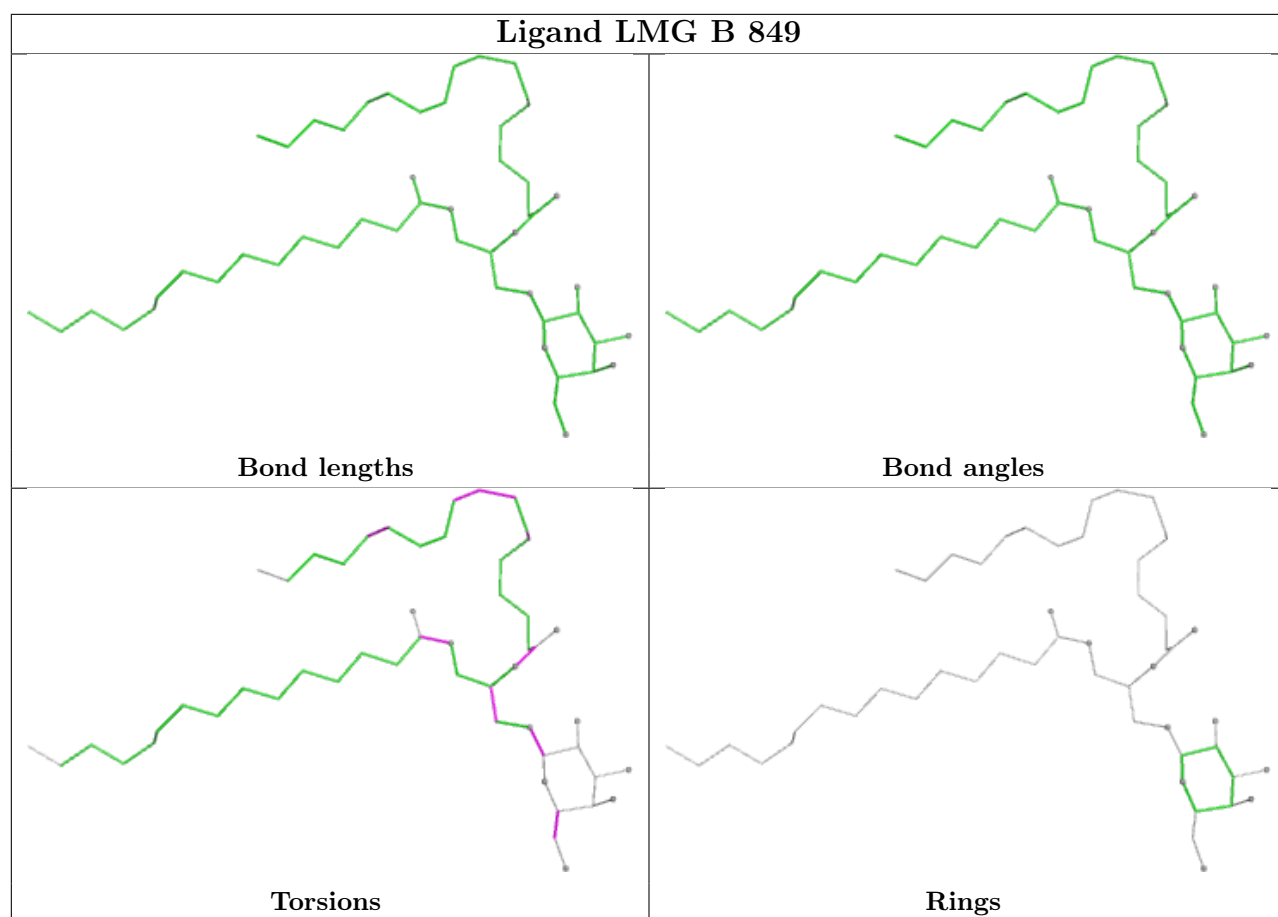


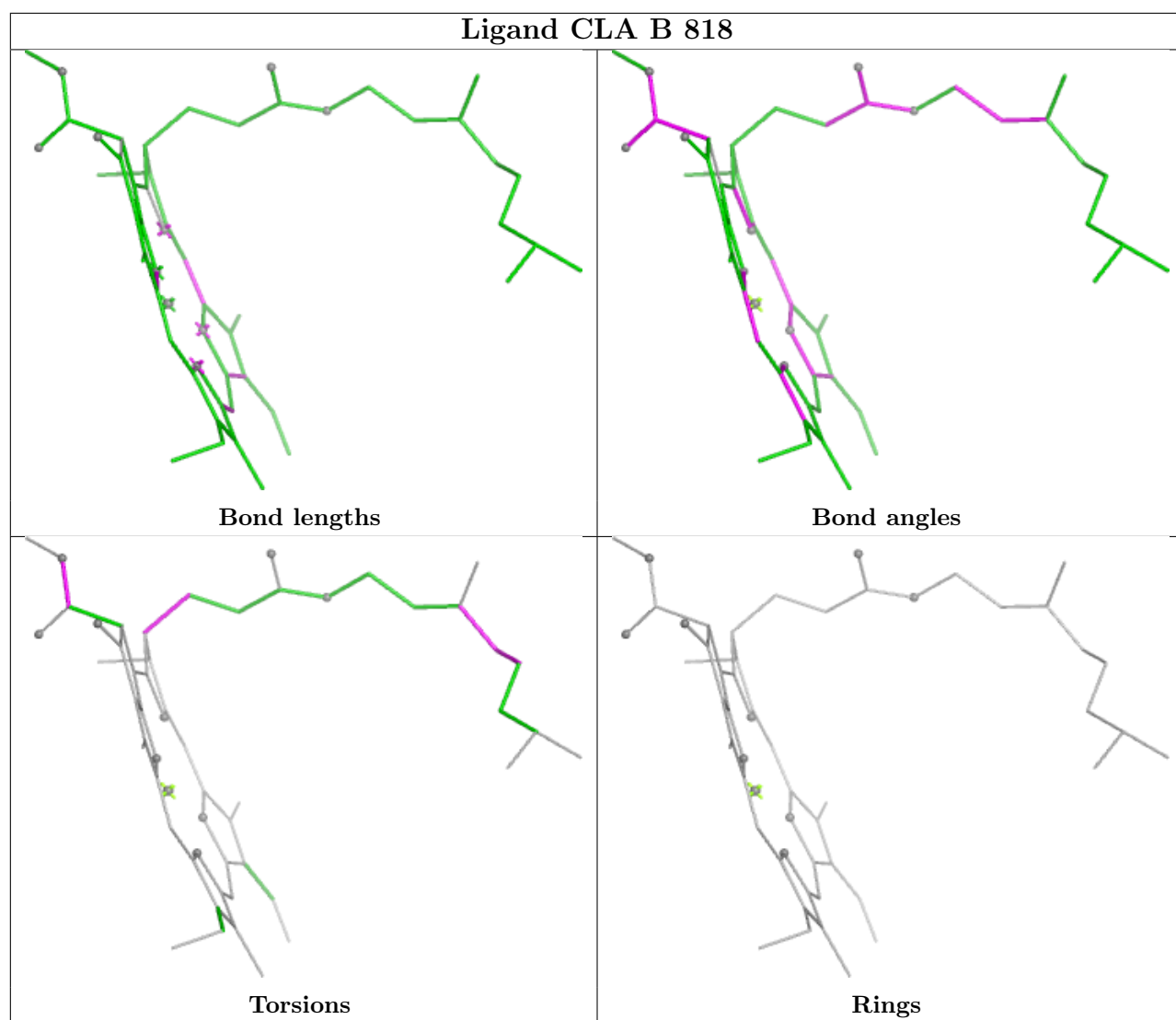
Ligand CLA A 808



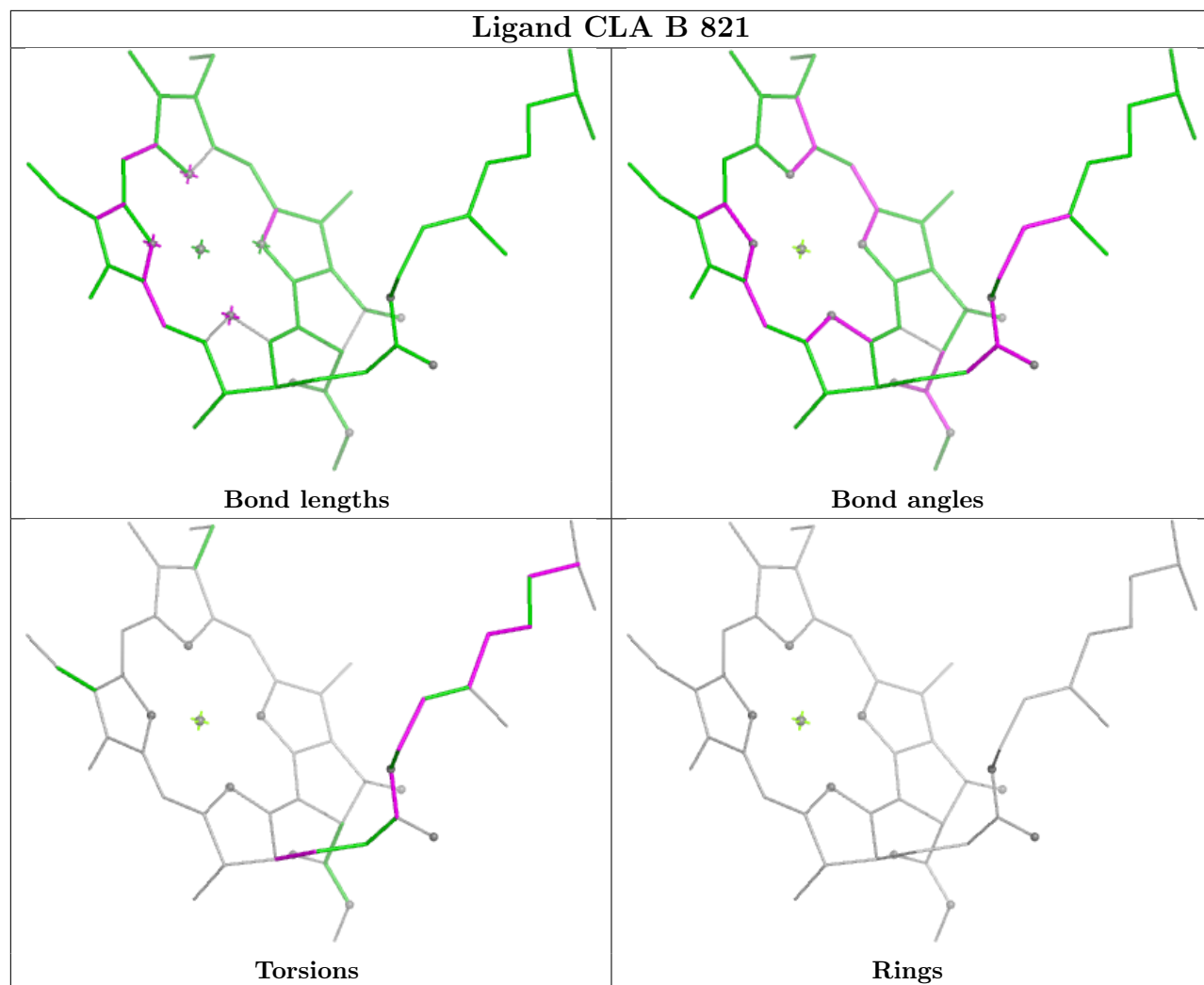
Ligand BCR B 845

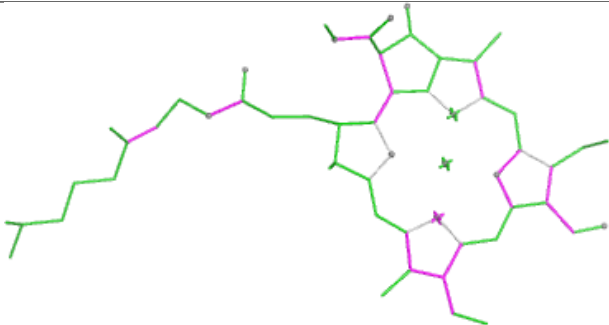
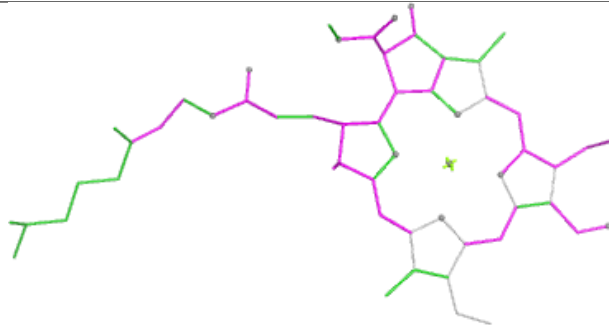
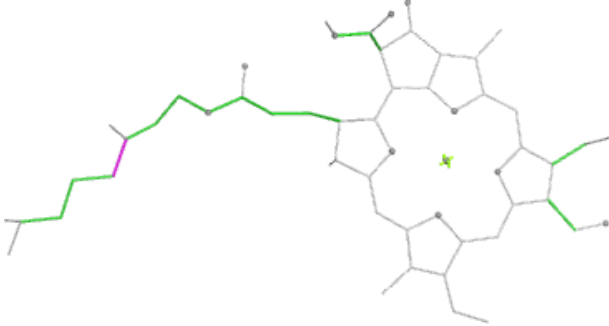
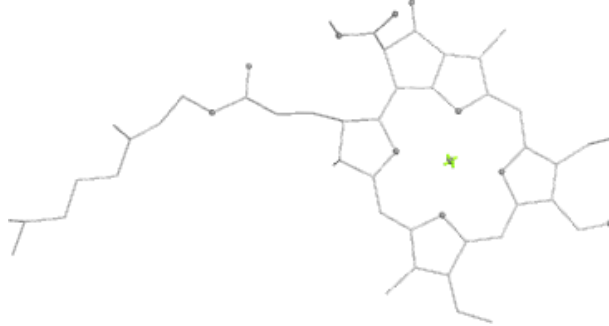


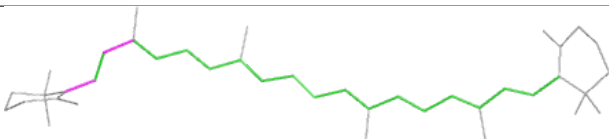
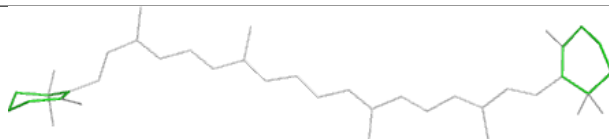


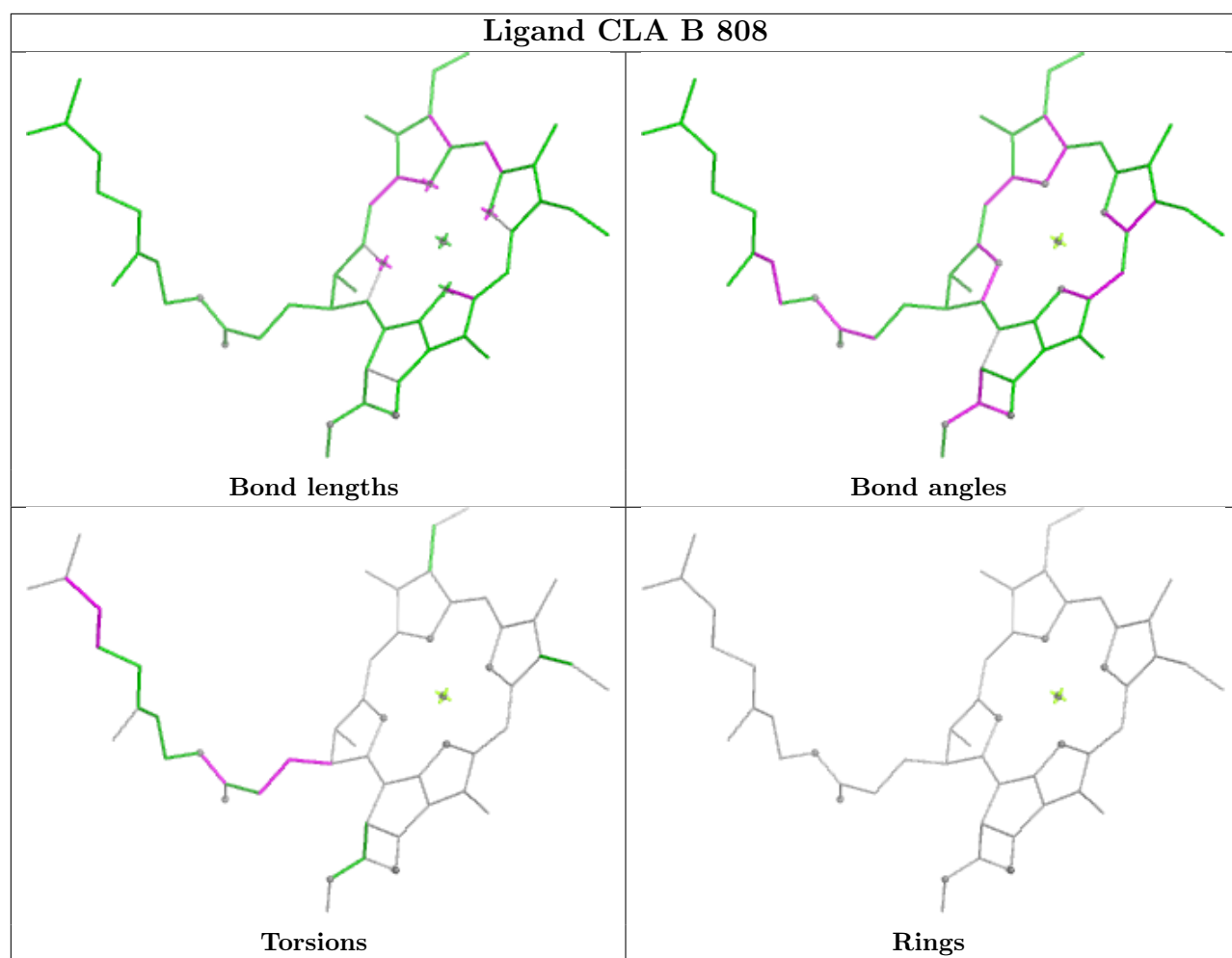


Ligand CLA B 821

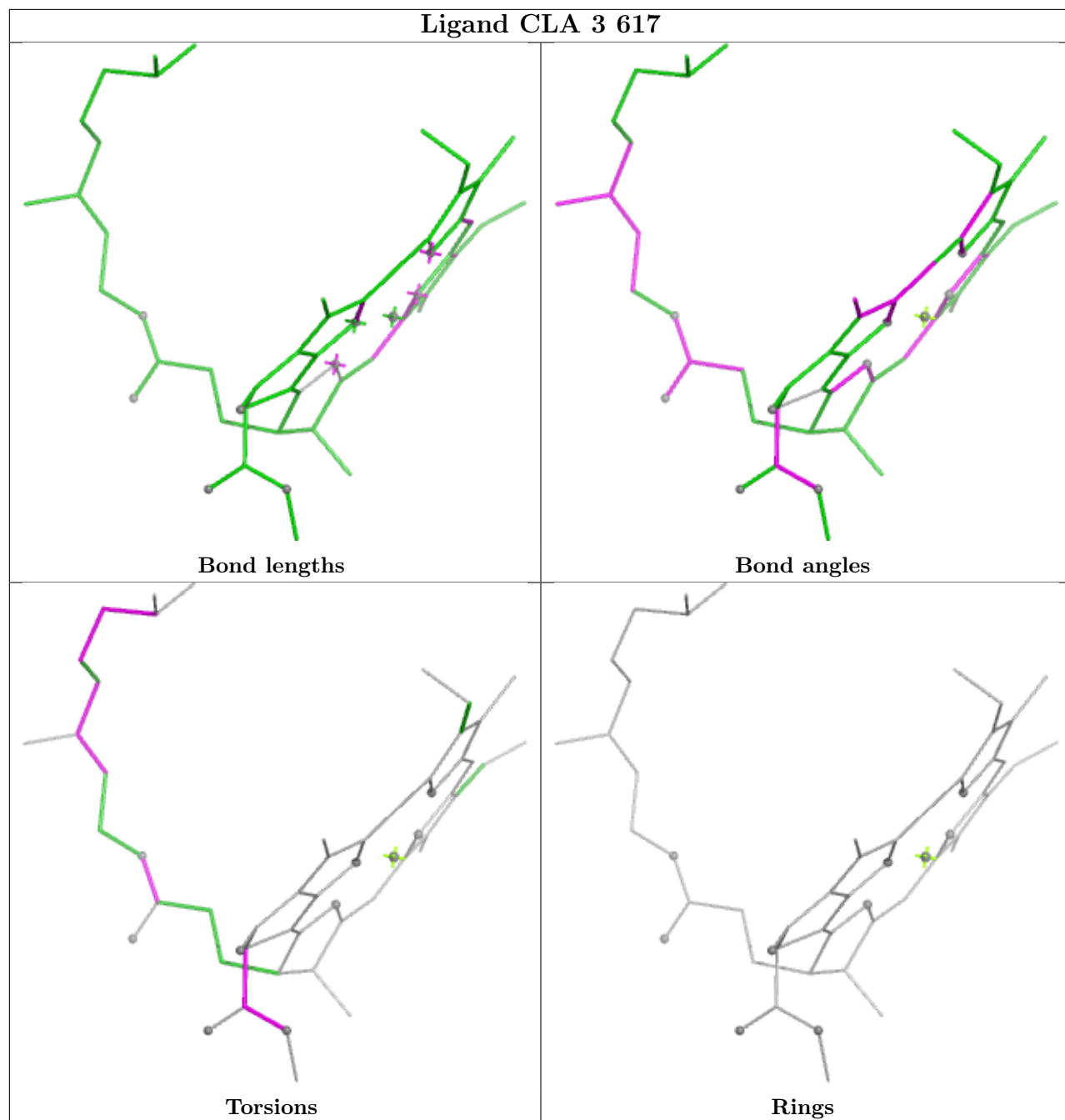


Ligand CHL 4 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

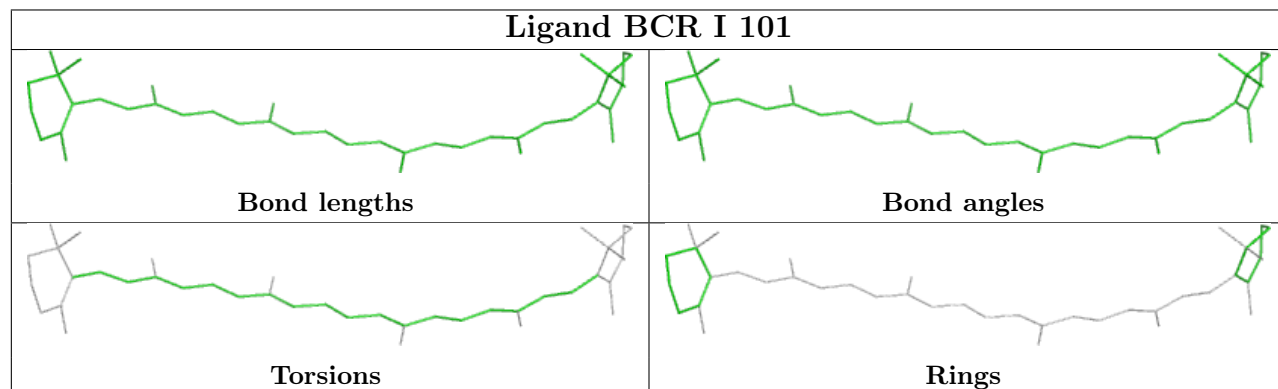
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings



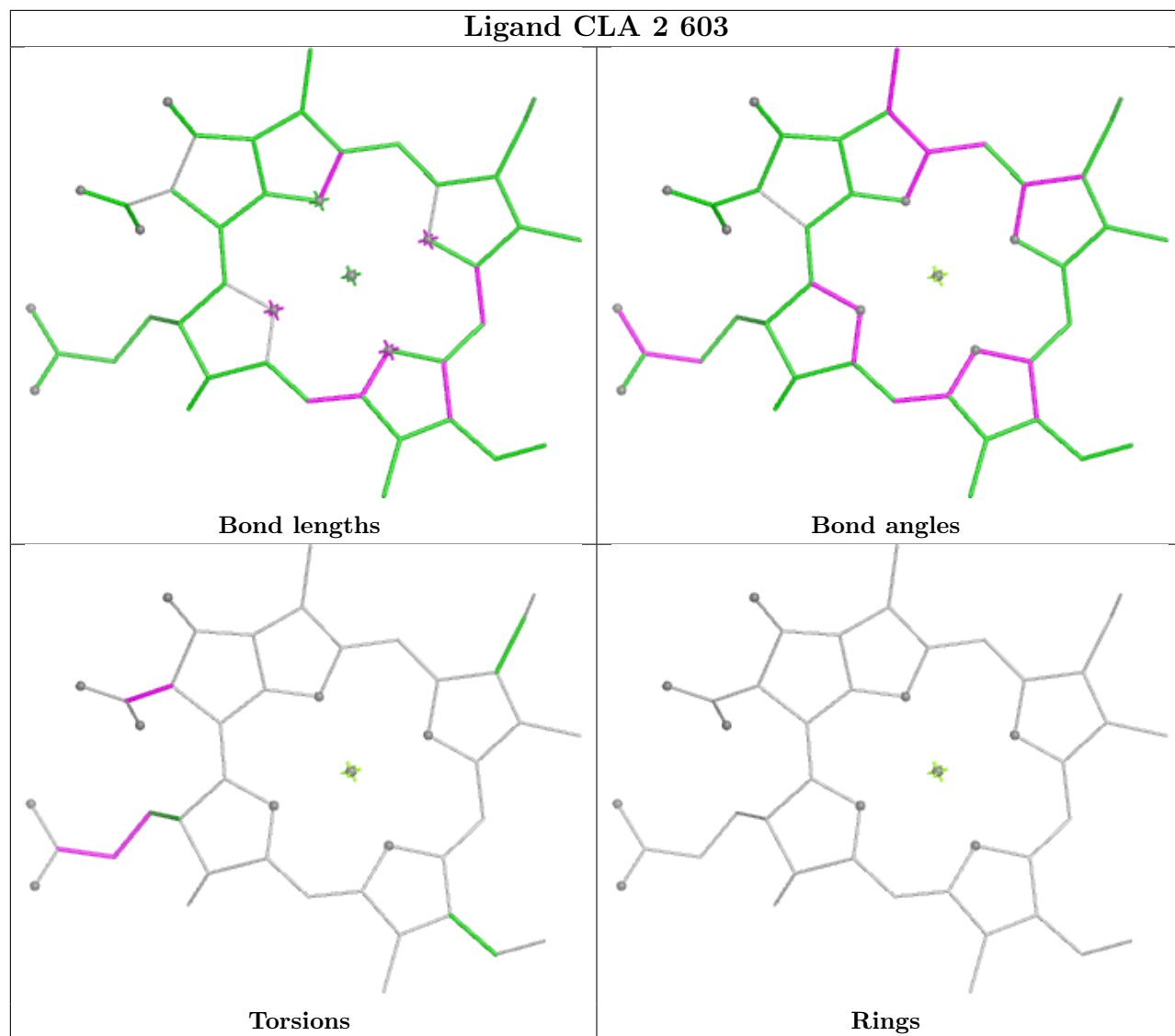
Ligand CLA 3 617

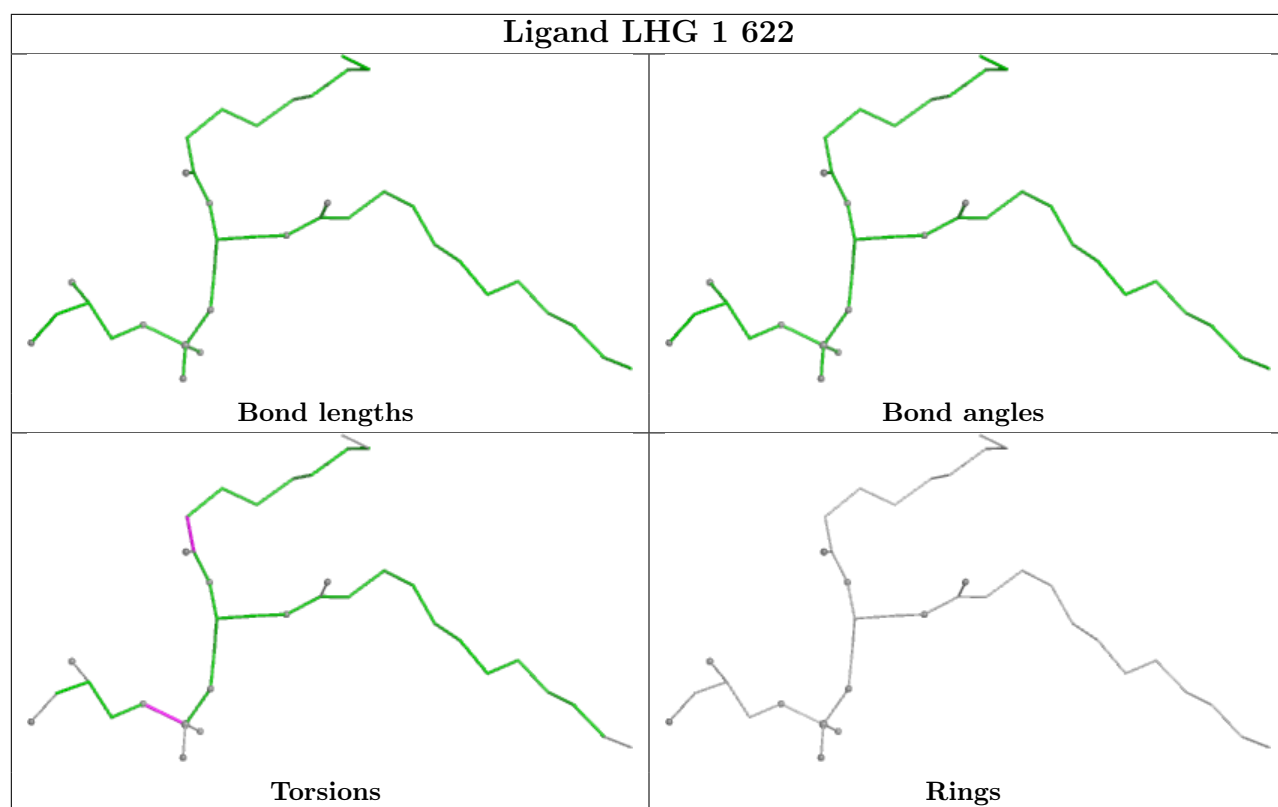


Ligand BCR I 101

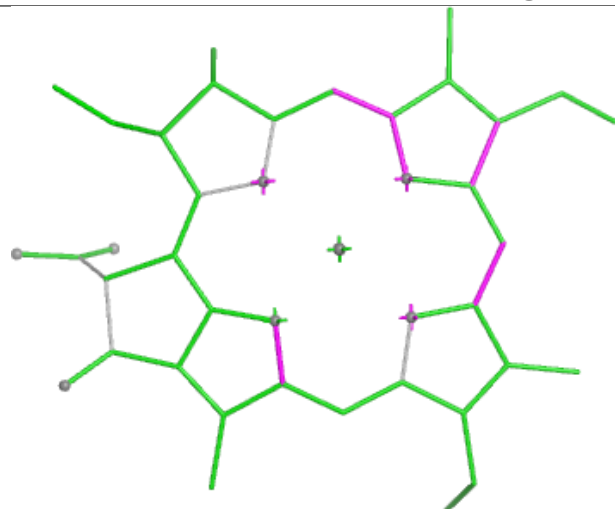


Ligand CLA 2 603

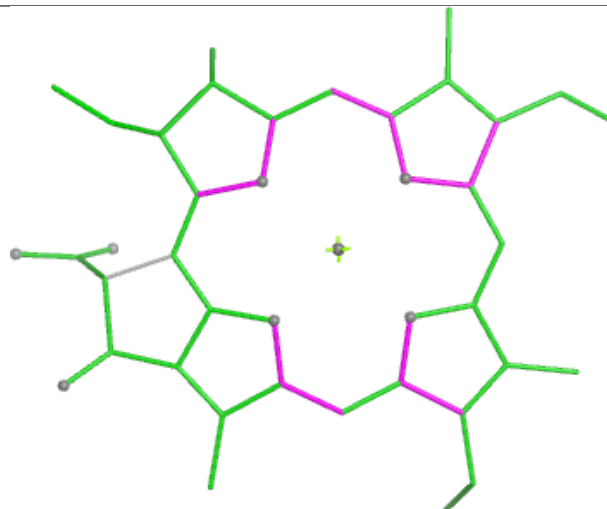




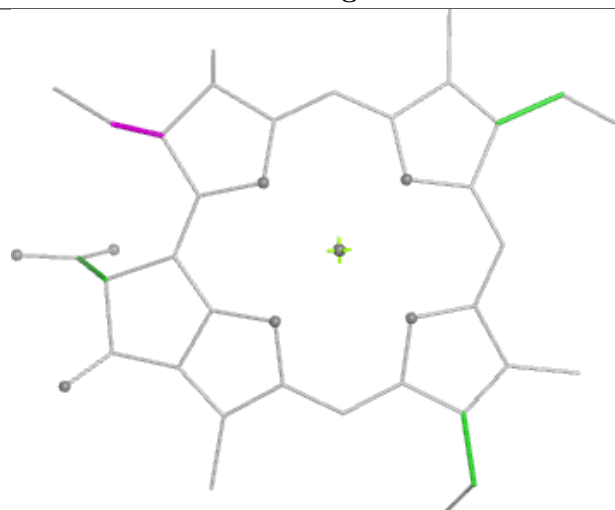
Ligand CLA 4 611



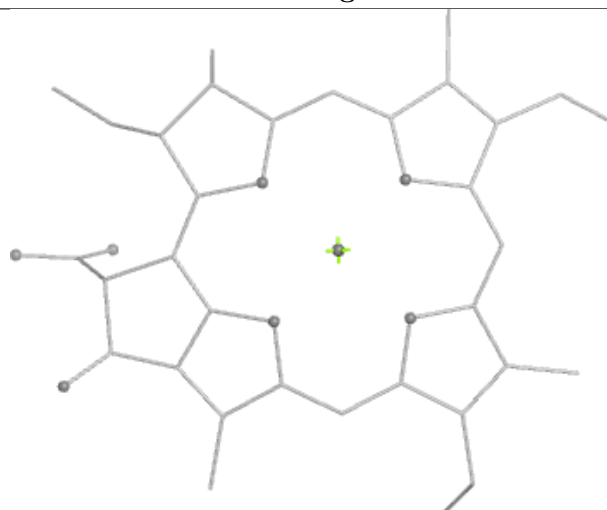
Bond lengths



Bond angles

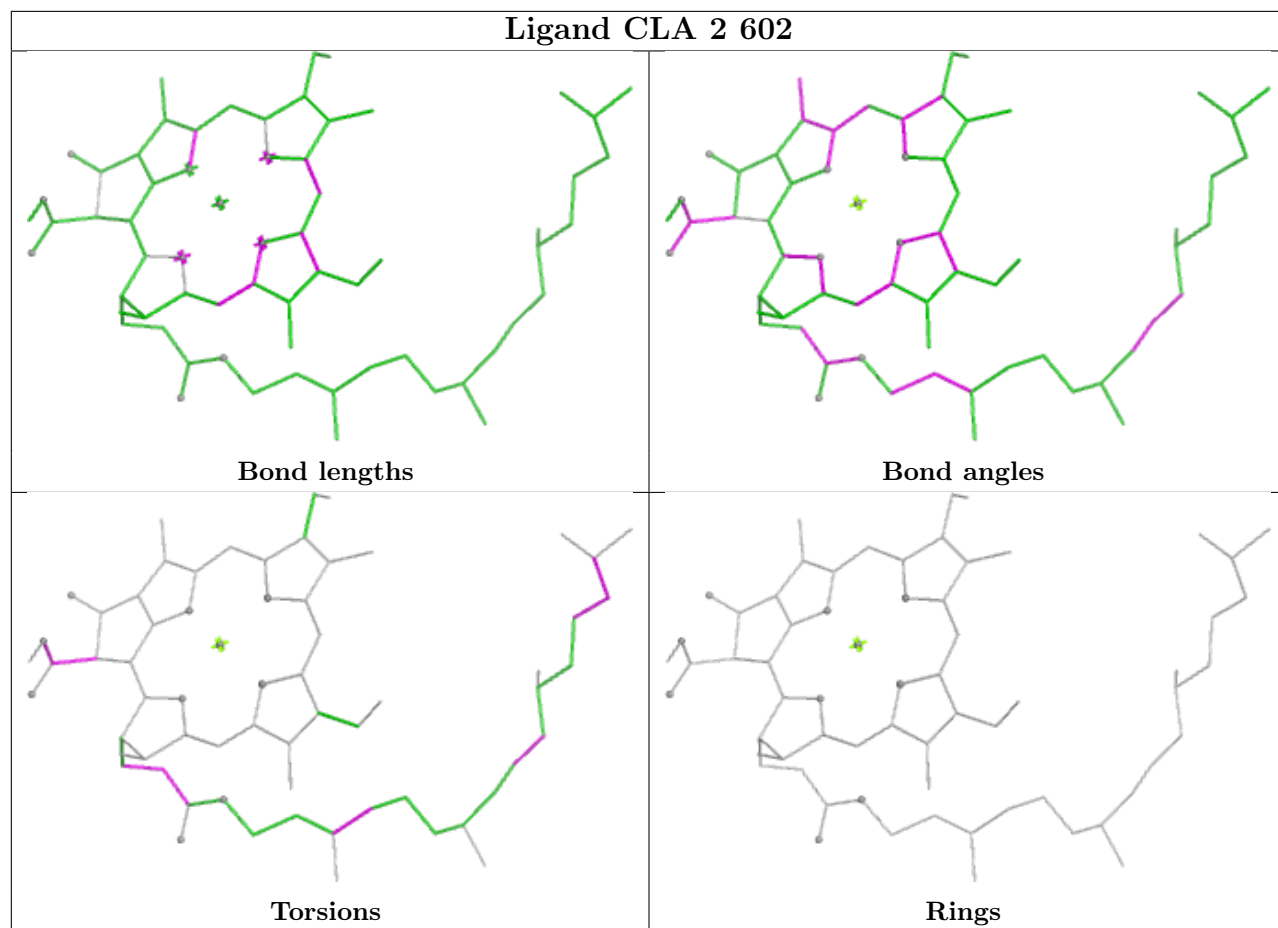


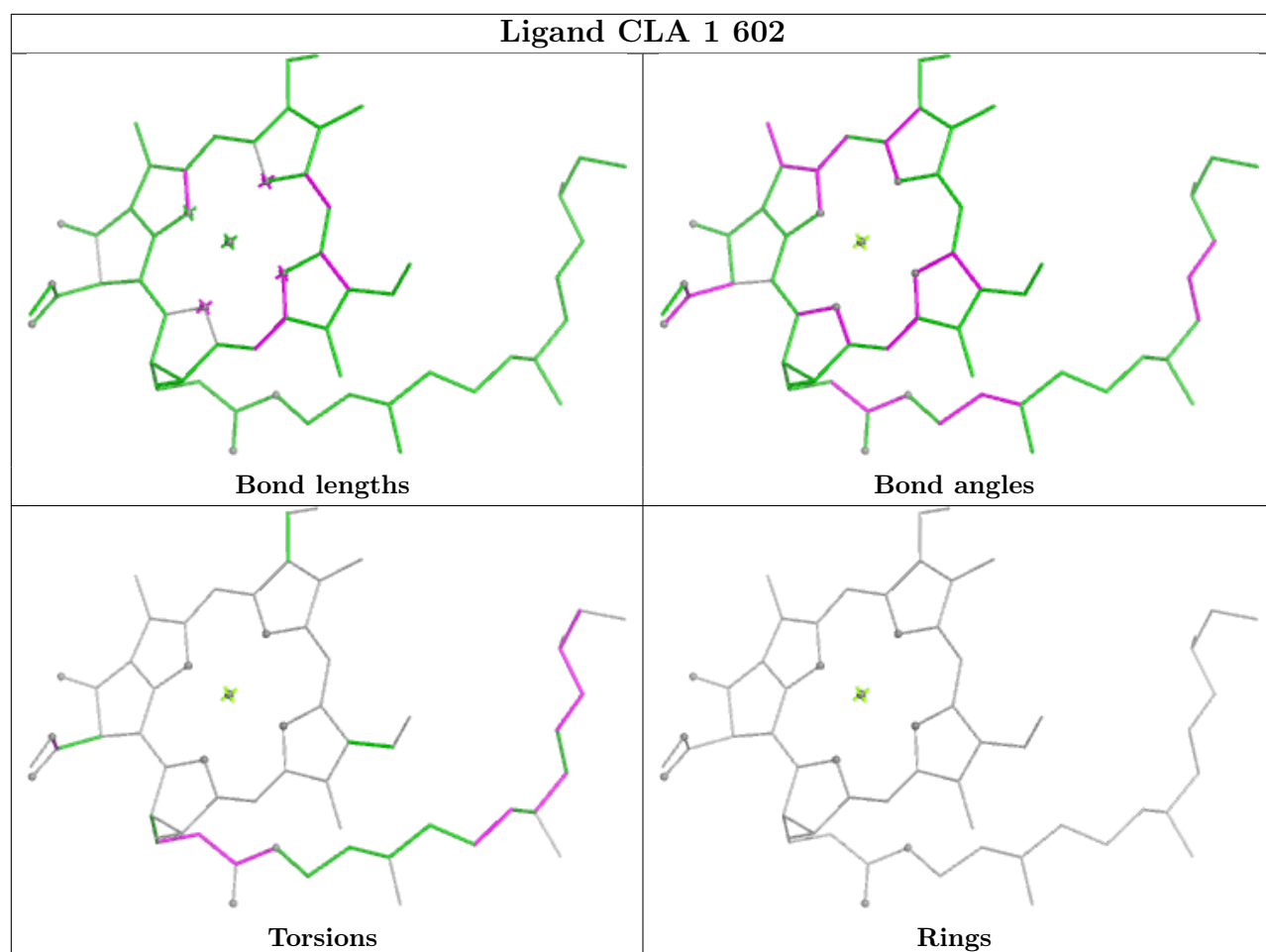
Torsions



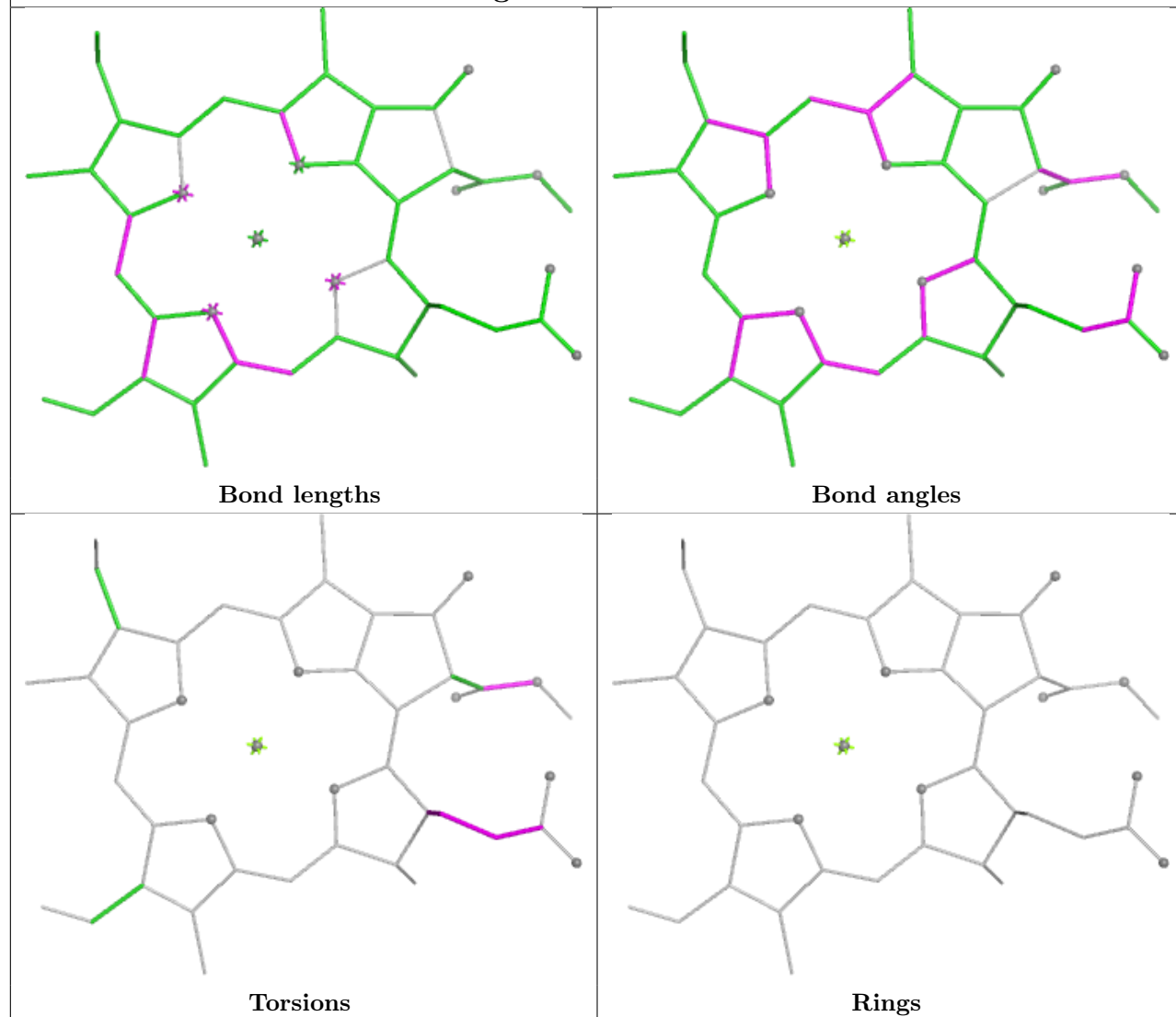
Rings

Ligand CLA 2 602

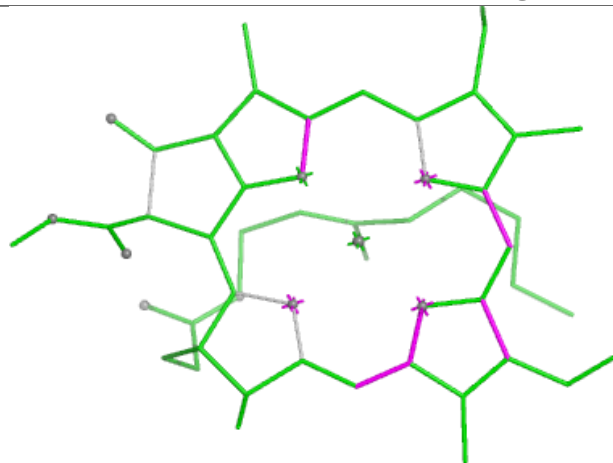




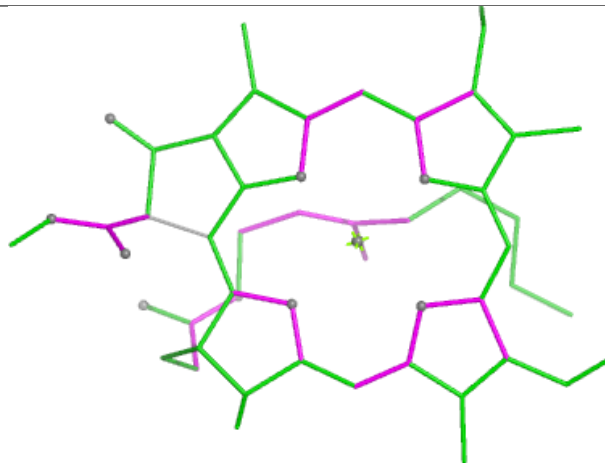
Ligand CLA 1 614



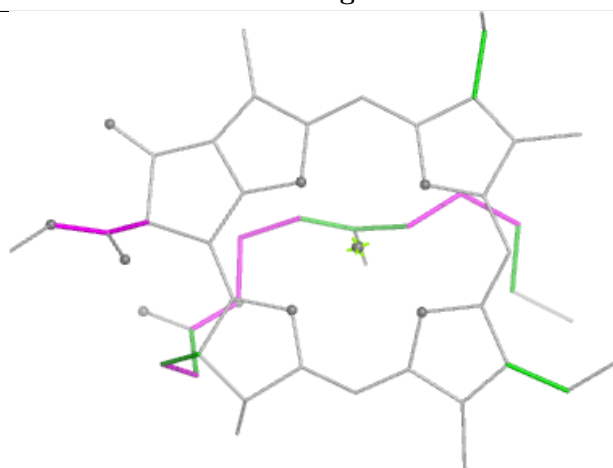
Ligand CLA A 812



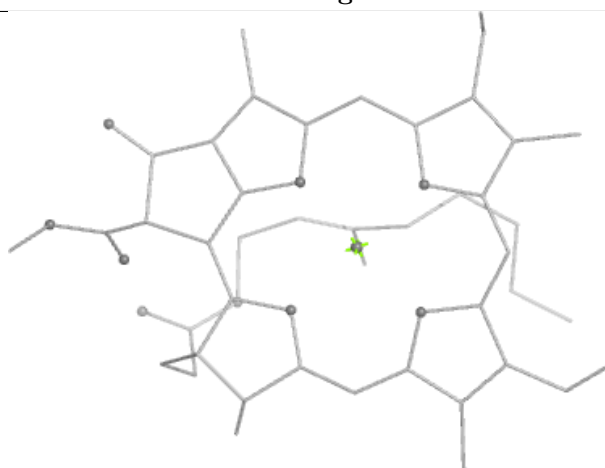
Bond lengths



Bond angles

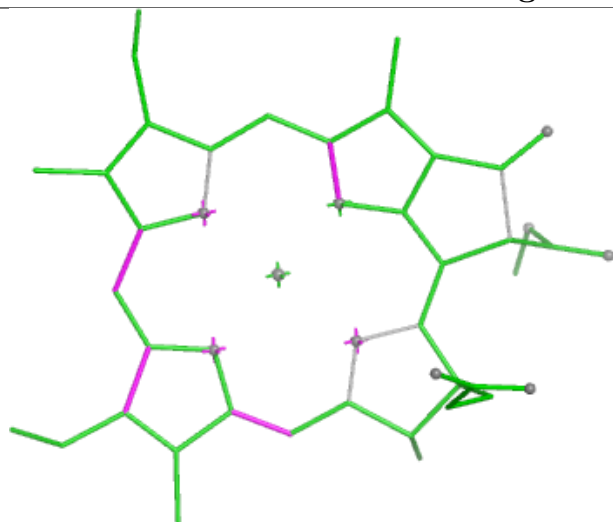


Torsions

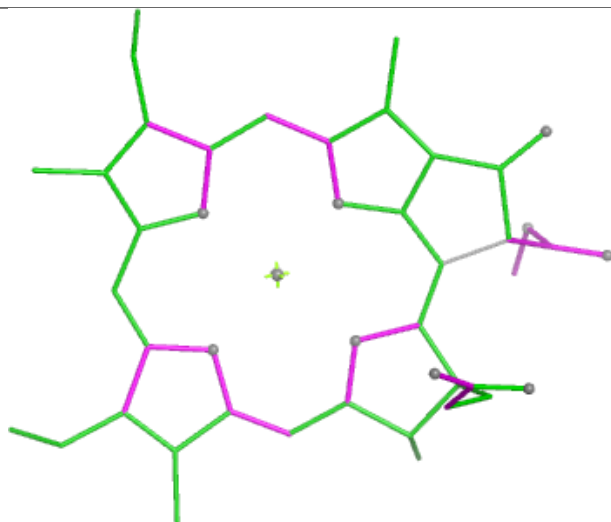


Rings

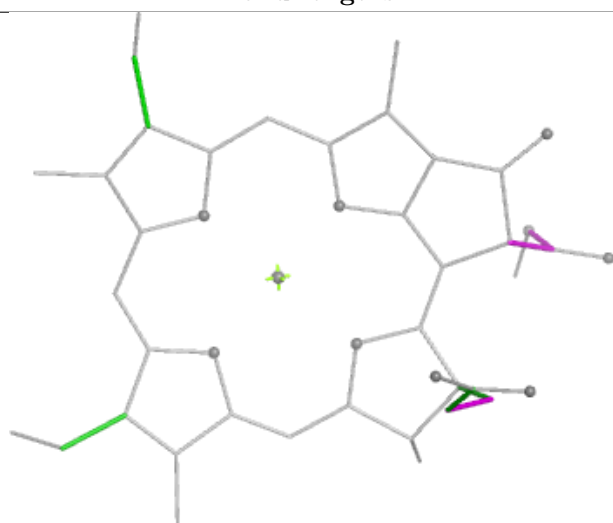
Ligand CLA 4 604



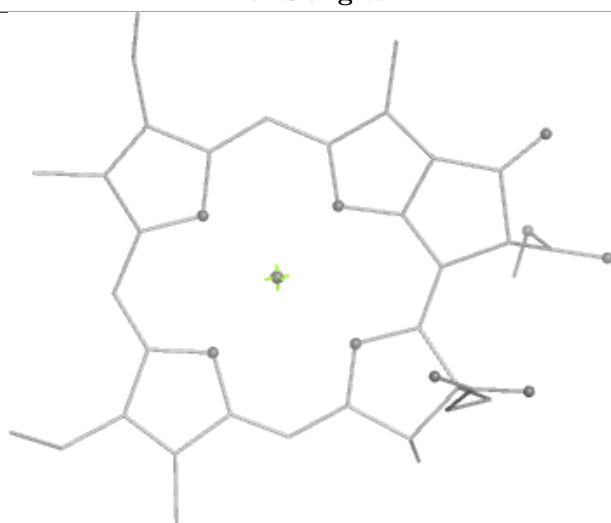
Bond lengths



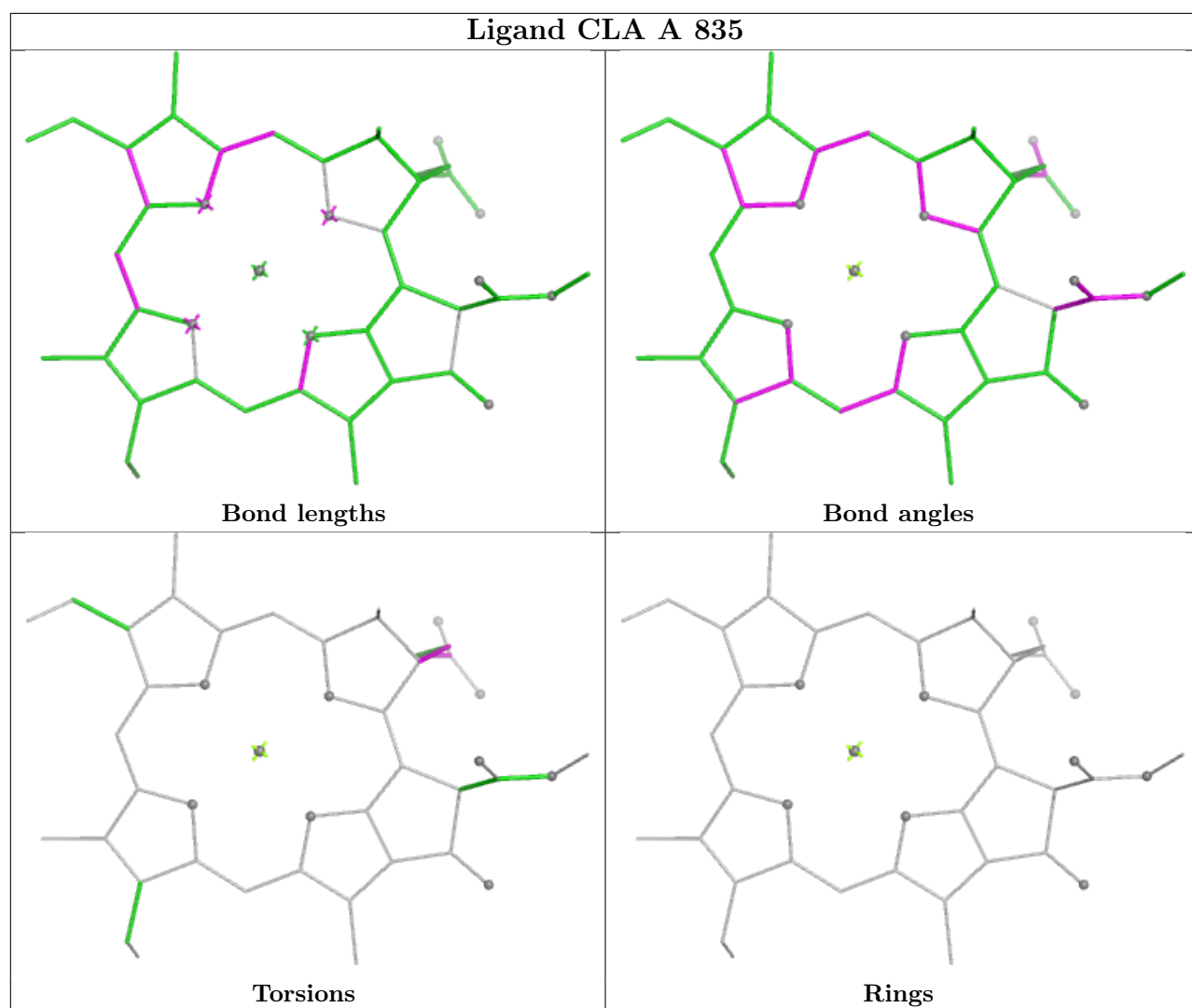
Bond angles



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.

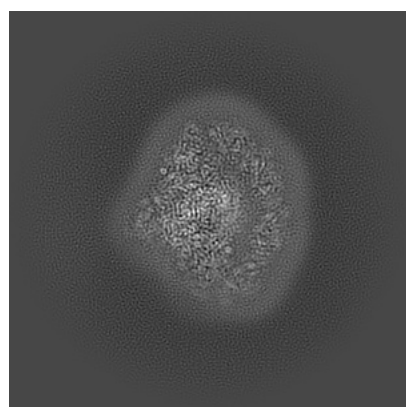
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54455. These allow visual inspection of the internal detail of the map and identification of artifacts.

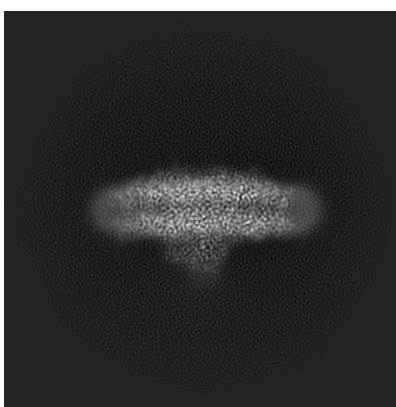
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

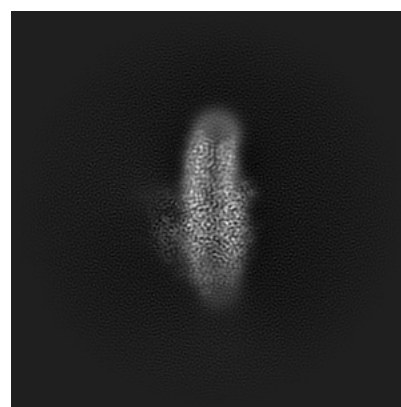
6.1.1 Primary map



X



Y

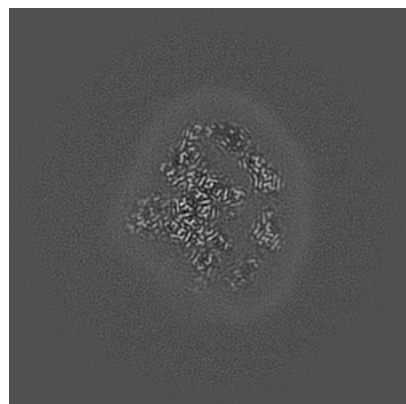


Z

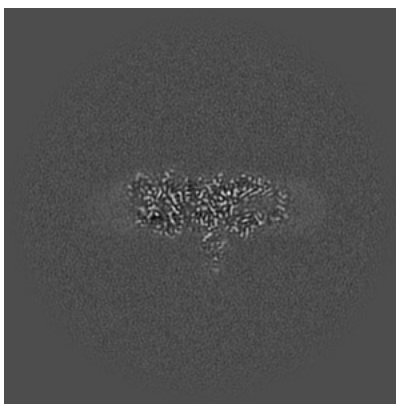
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

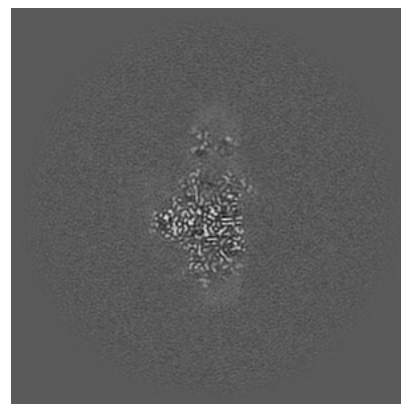
6.2.1 Primary map



X Index: 200



Y Index: 200

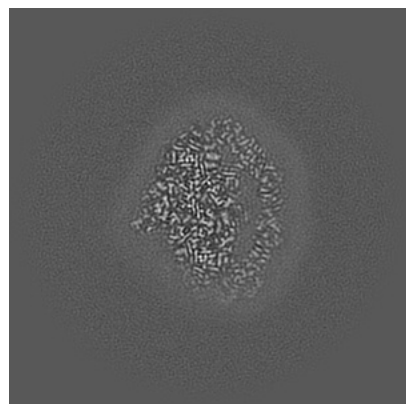


Z Index: 200

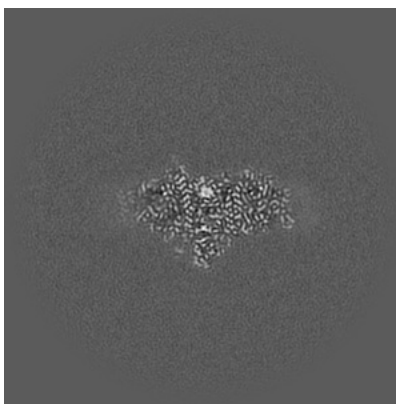
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

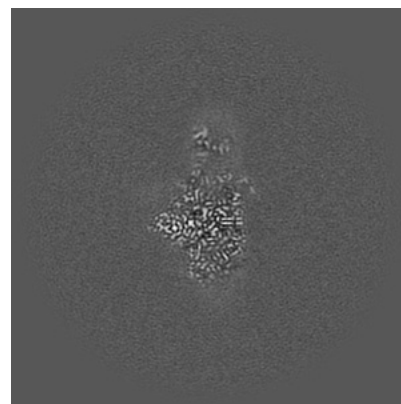
6.3.1 Primary map



X Index: 215



Y Index: 184

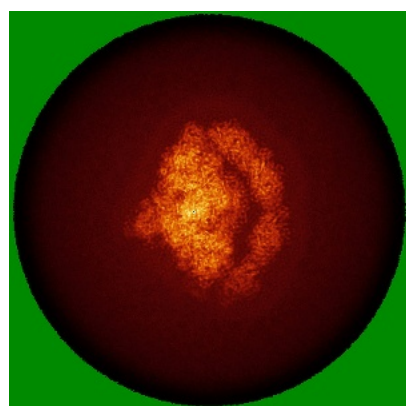


Z Index: 198

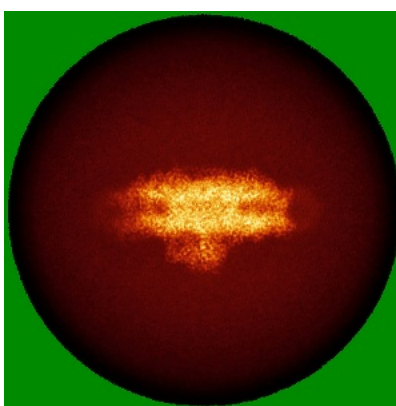
The images above show the largest variance slices of the map in three orthogonal directions.

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

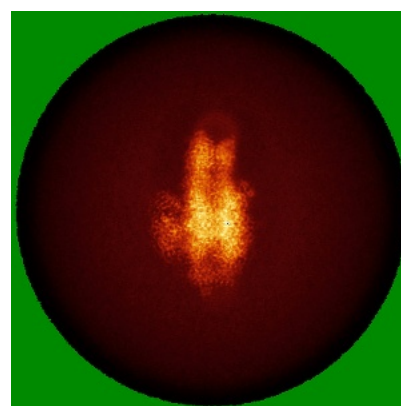
6.4.1 Primary map



X



Y

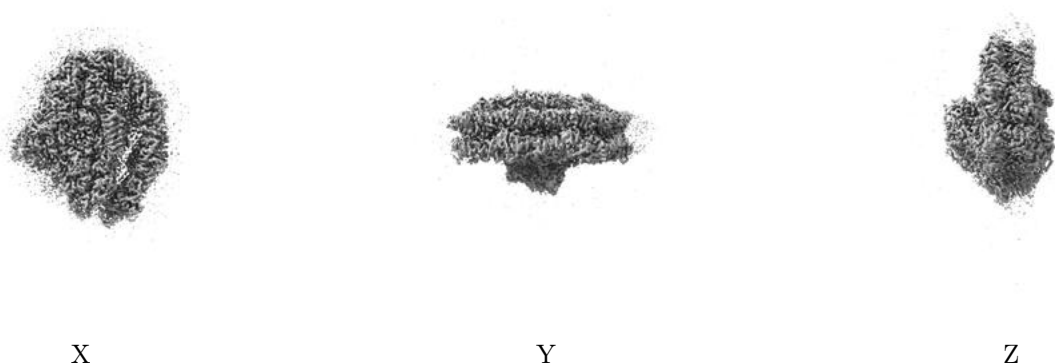


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

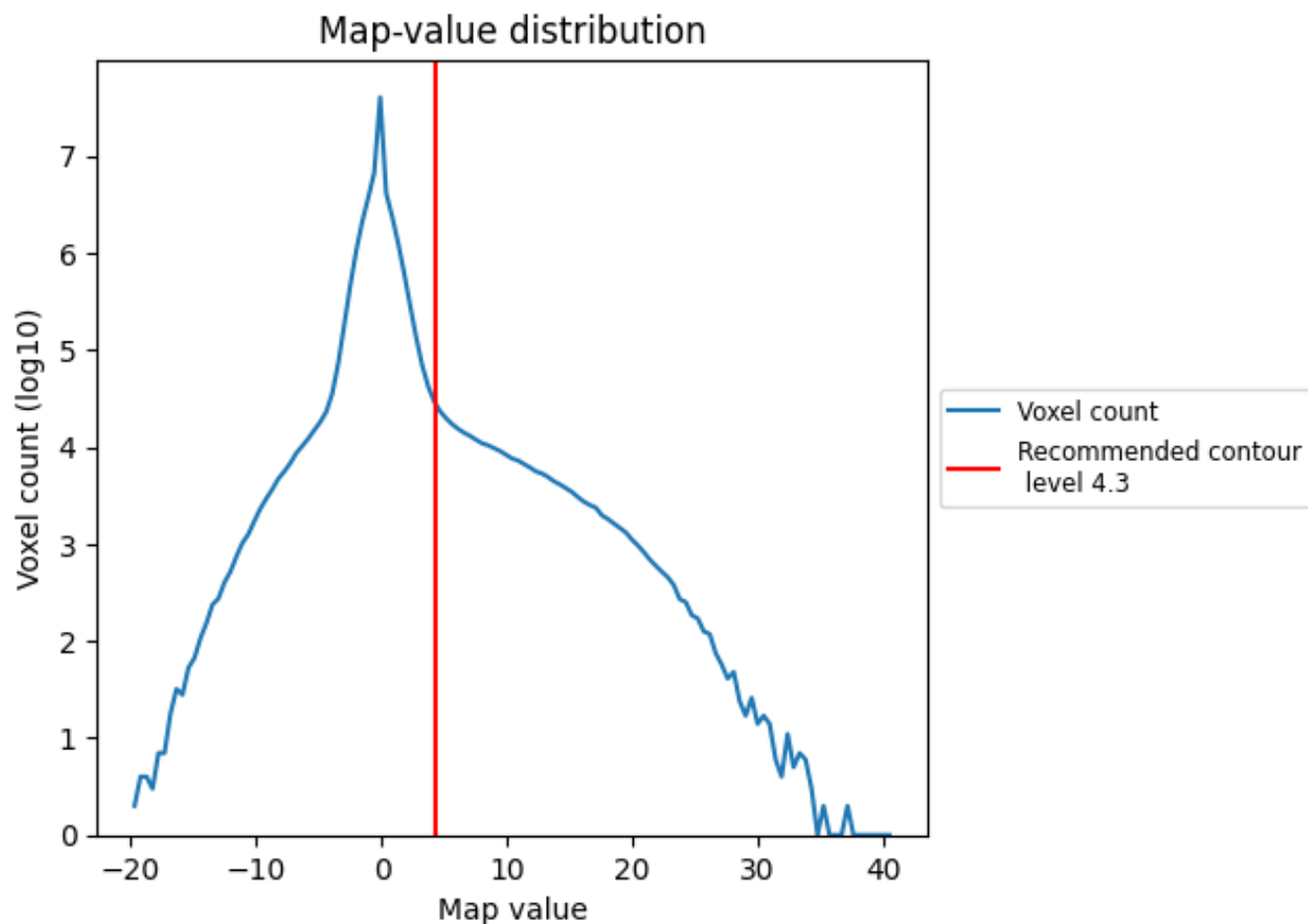
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

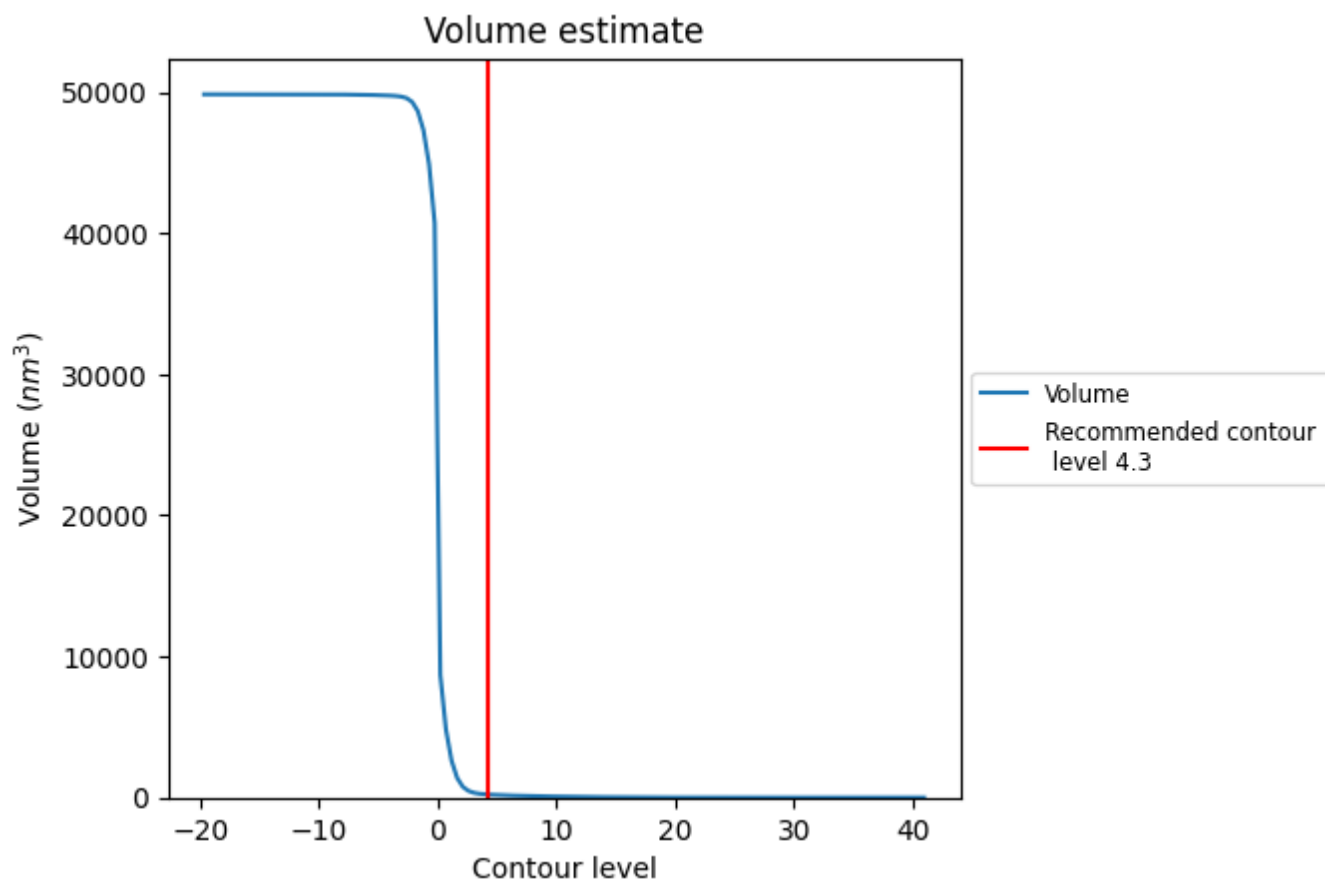
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

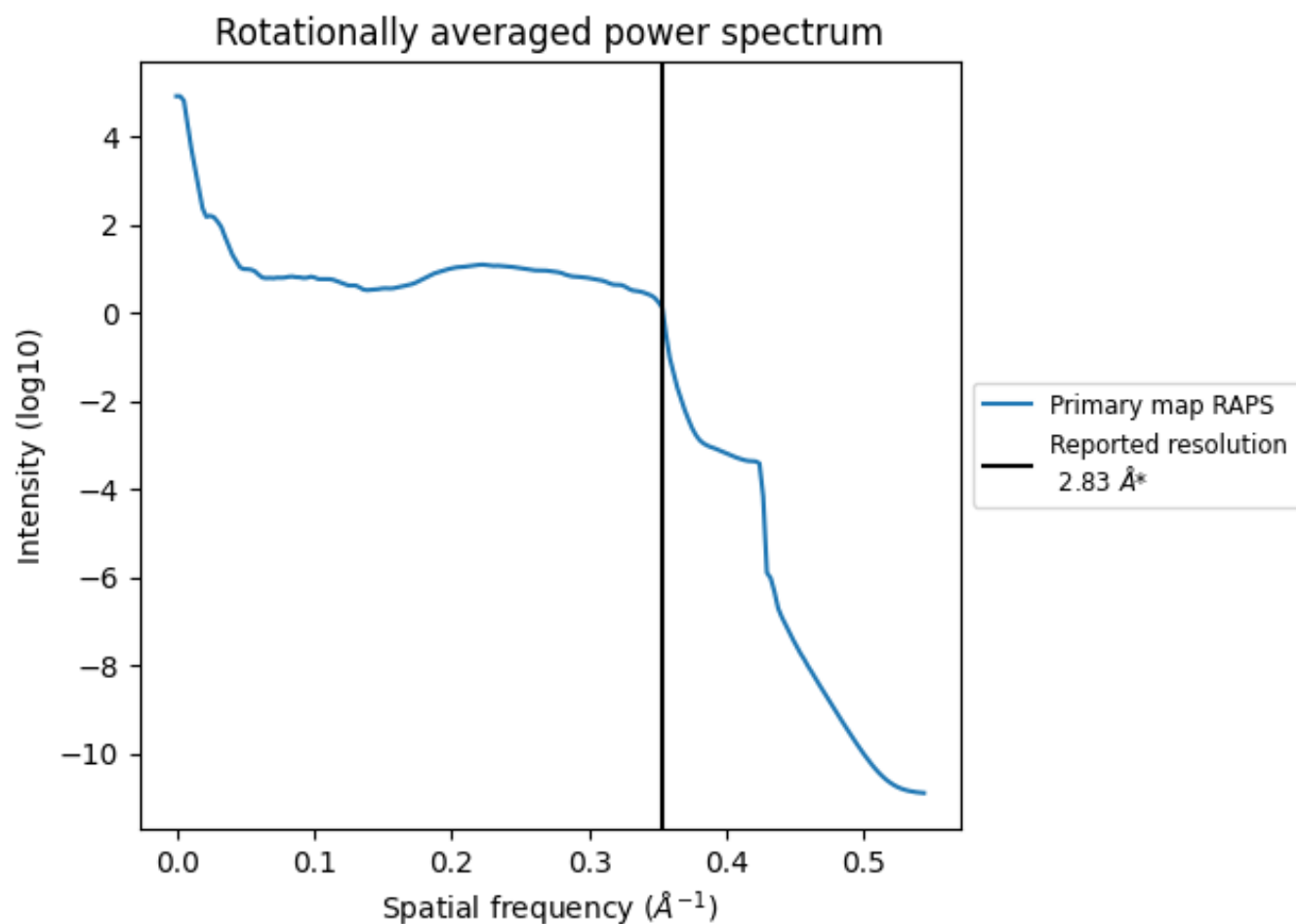
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 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 0.353 Å⁻¹

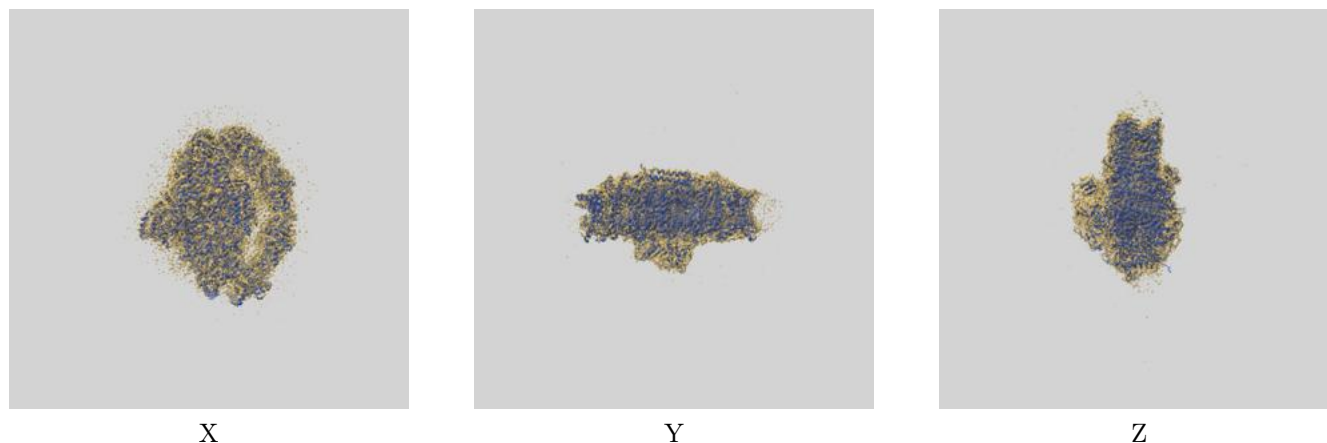
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

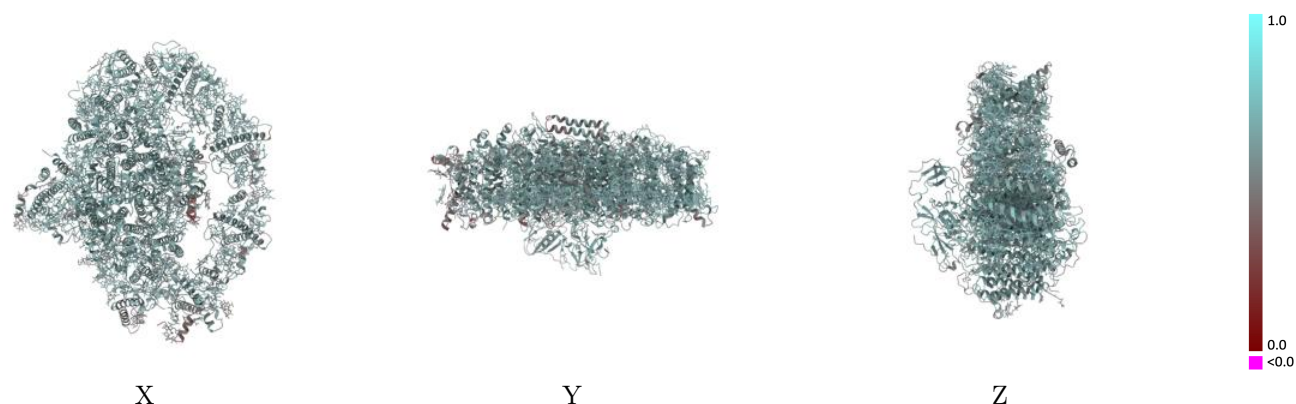
This section contains information regarding the fit between EMDB map EMD-54455 and PDB model 9S1L. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



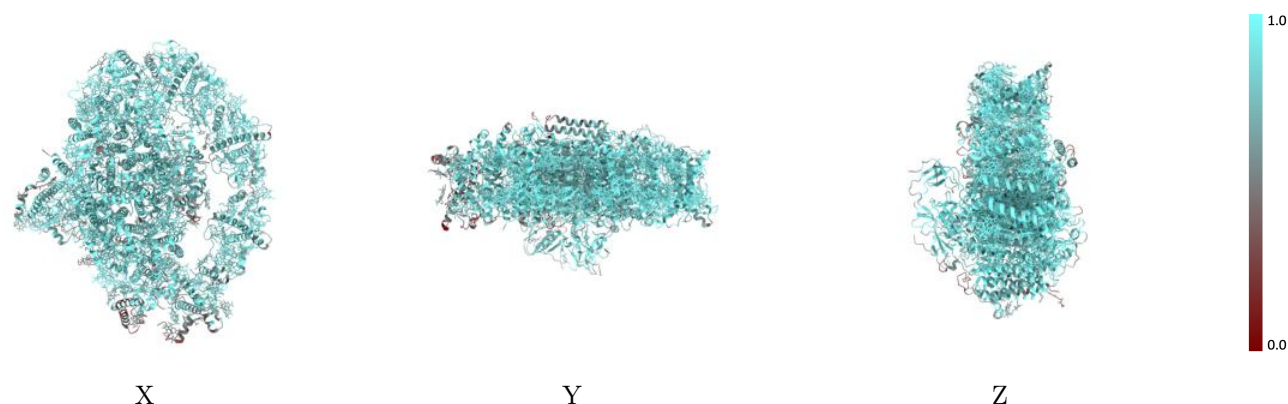
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



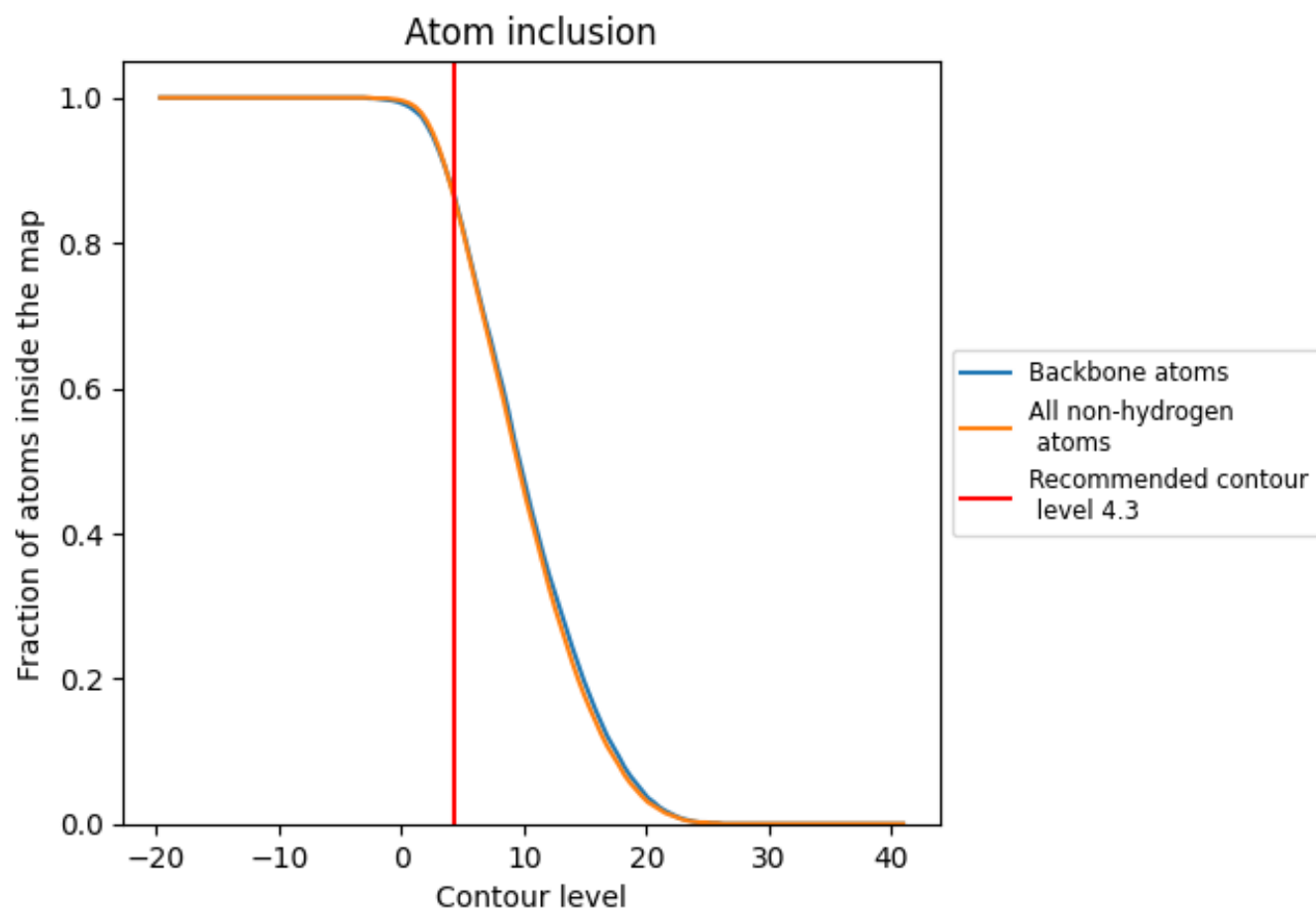
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.5940
1	0.8810	0.5940
2	0.8480	0.5650
3	0.6900	0.5240
4	0.8740	0.5890
A	0.9050	0.6120
B	0.9380	0.6240
C	0.9280	0.6080
D	0.8550	0.5960
E	0.8450	0.5930
F	0.7980	0.5730
G	0.8770	0.5950
H	0.6370	0.5330
I	0.8880	0.5990
J	0.7290	0.5240
K	0.4710	0.4880
L	0.7980	0.5810

