



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 02:07 PM UTC

PDB ID : 8ZWB / pdb_00008zwb
EMDB ID : EMD-60522
Title : 1.8 Å resolution structure of the Photosystem I assembly intermediate lacking stromal subunits.
Authors : Naschberger, A.; Komenda, J.
Deposited on : 2024-06-12
Resolution : 1.83 Å(reported)

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:

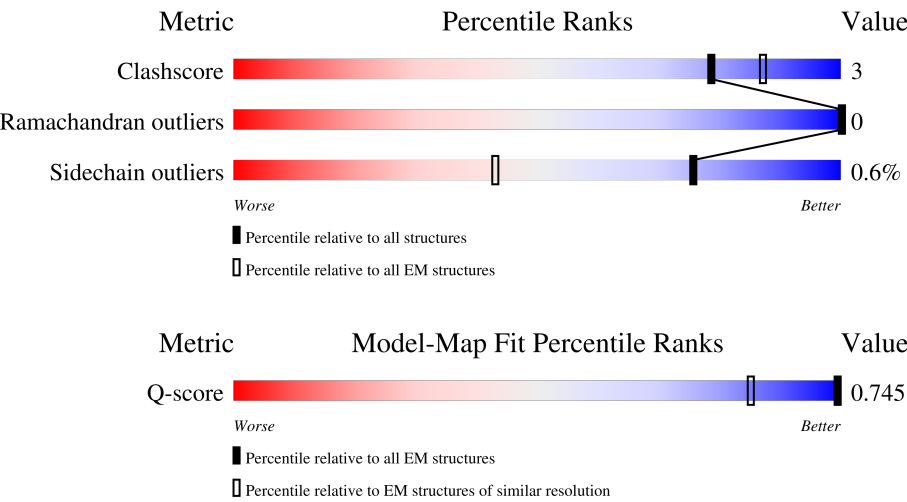
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.83 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	903 (1.33 - 2.33)

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	A	751	
2	B	731	
3	F	165	
4	I	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	40	
6	K	86	
7	M	31	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	804	X	-	-	-
10	CLA	A	805	X	-	-	-
10	CLA	A	807	X	-	-	-
10	CLA	A	808	X	-	-	-
10	CLA	A	809	X	-	-	-
10	CLA	A	810	X	-	-	-
10	CLA	A	811	X	-	-	-
10	CLA	A	812	X	-	-	-
10	CLA	A	813	X	-	-	-
10	CLA	A	814	X	-	-	-
10	CLA	A	815	X	-	-	-
10	CLA	A	816	X	-	-	-
10	CLA	A	817	X	-	-	-
10	CLA	A	818	X	-	-	-
10	CLA	A	819	X	-	-	-
10	CLA	A	820	X	-	-	-
10	CLA	A	821	X	-	-	-
10	CLA	A	822	X	-	-	-
10	CLA	A	823	X	-	-	-
10	CLA	A	824	X	-	-	-
10	CLA	A	825	X	-	-	-
10	CLA	A	826	X	-	-	-
10	CLA	A	827	X	-	-	-
10	CLA	A	828	X	-	-	-
10	CLA	A	829	X	-	-	-
10	CLA	A	830	X	-	-	-
10	CLA	A	831	X	-	-	-
10	CLA	A	832	X	-	-	-
10	CLA	A	833	X	-	-	-
10	CLA	A	834	X	-	-	-
10	CLA	A	835	X	-	-	-
10	CLA	A	836	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	837	X	-	-	-
10	CLA	A	838	X	-	-	-
10	CLA	A	839	X	-	-	-
10	CLA	A	840	X	-	-	-
10	CLA	A	841	X	-	-	-
10	CLA	A	842	X	-	-	-
10	CLA	A	843	X	-	-	-
10	CLA	A	844	X	-	-	-
10	CLA	A	845	X	-	-	-
10	CLA	A	846	X	-	-	-
10	CLA	A	861	X	-	-	-
10	CLA	A	863	X	-	-	-
10	CLA	B	801	X	-	-	-
10	CLA	B	802	X	-	-	-
10	CLA	B	803	X	-	-	-
10	CLA	B	806	X	-	-	-
10	CLA	B	807	X	-	-	-
10	CLA	B	808	X	-	-	-
10	CLA	B	809	X	-	-	-
10	CLA	B	810	X	-	-	-
10	CLA	B	811	X	-	-	-
10	CLA	B	812	X	-	-	-
10	CLA	B	813	X	-	-	-
10	CLA	B	814	X	-	-	-
10	CLA	B	815	X	-	-	-
10	CLA	B	816	X	-	-	-
10	CLA	B	817	X	-	-	-
10	CLA	B	818	X	-	-	-
10	CLA	B	819	X	-	-	-
10	CLA	B	820	X	-	-	-
10	CLA	B	821	X	-	-	-
10	CLA	B	822	X	-	-	-
10	CLA	B	823	X	-	-	-
10	CLA	B	824	X	-	-	-
10	CLA	B	825	X	-	-	-
10	CLA	B	826	X	-	-	-
10	CLA	B	827	X	-	-	-
10	CLA	B	828	X	-	-	-
10	CLA	B	829	X	-	-	-
10	CLA	B	830	X	-	-	-
10	CLA	B	831	X	-	-	-
10	CLA	B	832	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	B	833	X	-	-	-
10	CLA	B	834	X	-	-	-
10	CLA	B	835	X	-	-	-
10	CLA	B	836	X	-	-	-
10	CLA	B	837	X	-	-	-
10	CLA	B	838	X	-	-	-
10	CLA	B	839	X	-	-	-
10	CLA	B	840	X	-	-	-
10	CLA	B	841	X	-	-	-
10	CLA	B	842	X	-	-	-
10	CLA	B	843	X	-	-	-
10	CLA	F	203	X	-	-	-
10	CLA	F	204	X	-	-	-
10	CLA	J	101	X	-	-	-
10	CLA	J	102	X	-	-	-
10	CLA	K	101	X	-	-	-
10	CLA	K	102	X	-	-	-
10	CLA	K	103	X	-	-	-
17	SF4	B	805	-	-	X	-
9	CL0	A	803	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 41672 atoms, of which 20603 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	734	Total	C	H	N	O	S	0	0
			11352	3770	5602	973	980	27		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	729	Total	C	H	N	O	S	0	0
			11317	3798	5547	967	990	15		

- Molecule 3 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	137	Total	C	H	N	O	S	0	0
			2116	689	1051	175	196	5		

- Molecule 4 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	I	37	Total	C	H	N	O	S	0	0
			585	200	292	41	49	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	J	40	Total	C	H	N	O	S	0	0
			647	215	328	47	54	3		

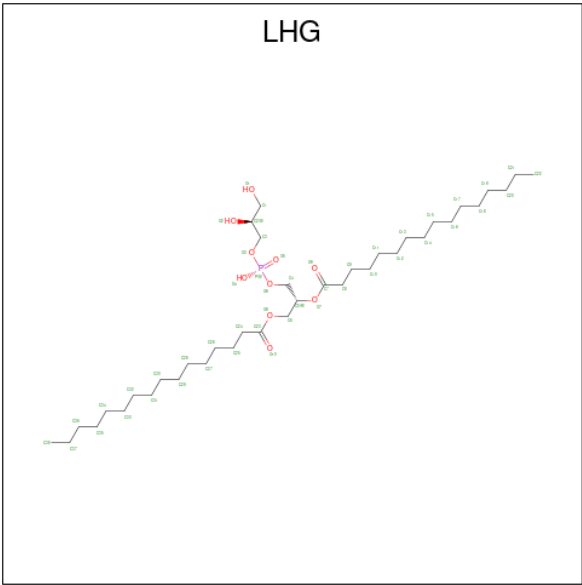
- Molecule 6 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	78	Total	C	H	N	O	S	0	0
			1114	356	570	90	94	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit XII.

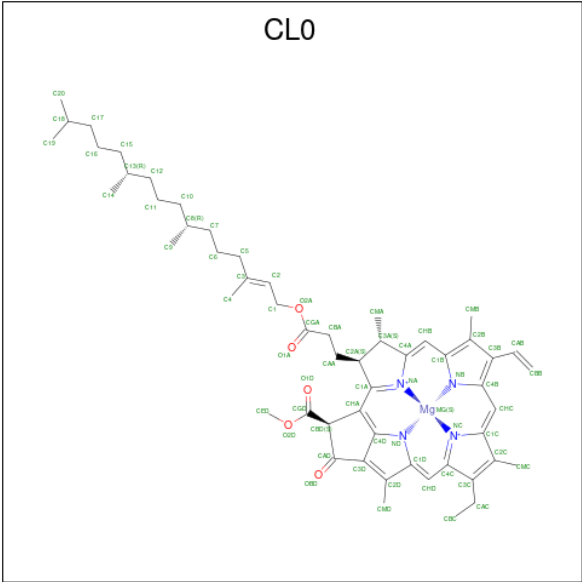
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	M	31	498	159	260	36	42	1	0	0

- Molecule 8 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



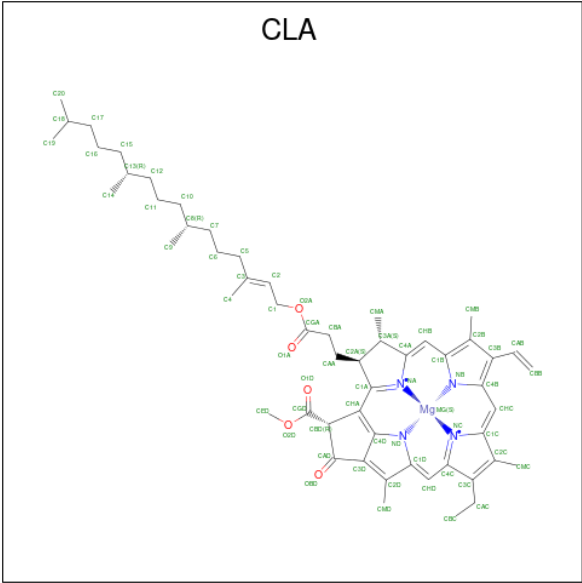
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
8	A	1	123	38	74	10	1	0
8	A	1	69	22	36	10	1	0
8	B	1	90	28	51	10	1	0

- Molecule 9 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			102	44	48	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			102	44	48	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			82	37	35	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

Continued on next page...

Continued from previous page...

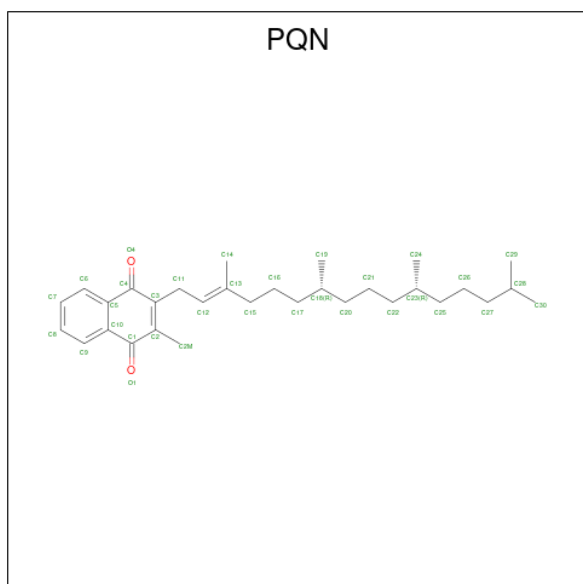
Mol	Chain	Residues	Atoms						AltConf
10	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	B	1	Total	C	H	Mg	N	O	0
			30	22	3	1	4		
10	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

Continued on next page...

Continued from previous page...

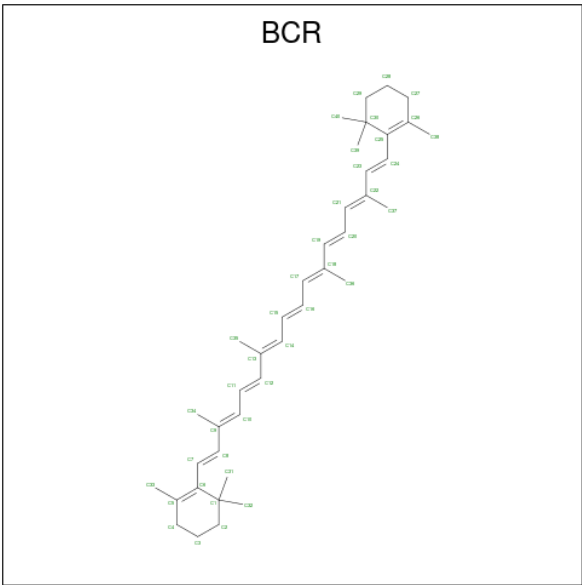
Mol	Chain	Residues	Atoms						AltConf
10	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	J	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	J	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
10	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

- Molecule 11 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



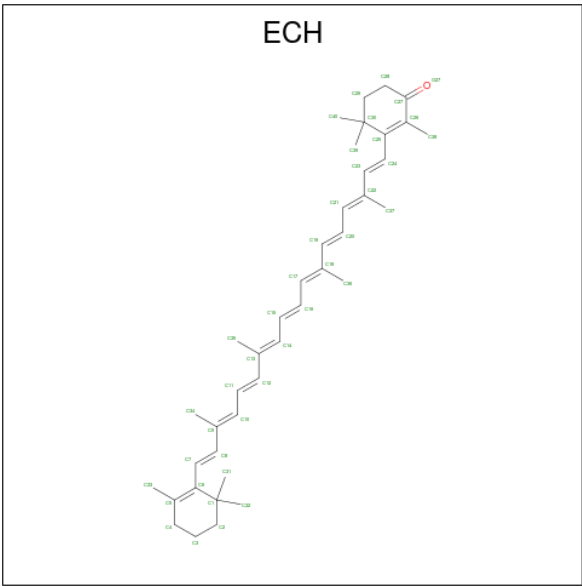
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	H	O	0
			79	31	46	2	
11	B	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



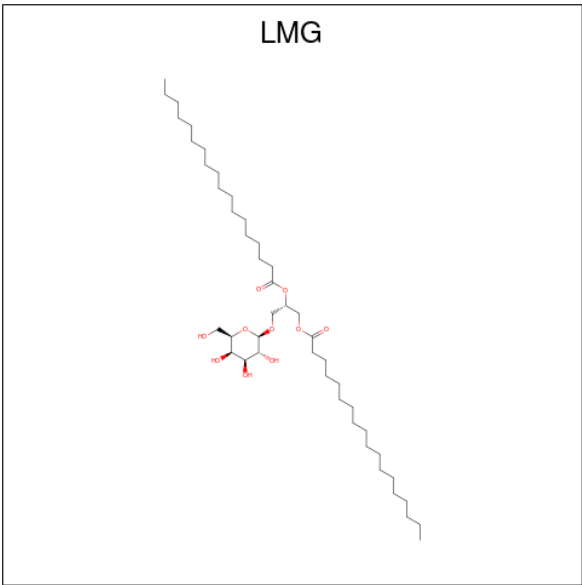
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	H	0
			96	40	56	
12	A	1	Total	C	H	0
			96	40	56	
12	A	1	Total	C	H	0
			96	40	56	
12	A	1	Total	C	H	0
			96	40	56	
12	A	1	Total	C	H	0
			96	40	56	
12	B	1	Total	C	H	0
			96	40	56	
12	B	1	Total	C	H	0
			96	40	56	
12	B	1	Total	C	H	0
			96	40	56	
12	B	1	Total	C	H	0
			96	40	56	
12	F	1	Total	C	H	0
			96	40	56	
12	I	1	Total	C	H	0
			96	40	56	
12	J	1	Total	C	H	0
			96	40	56	
12	K	1	Total	C	H	0
			96	40	56	

- Molecule 13 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



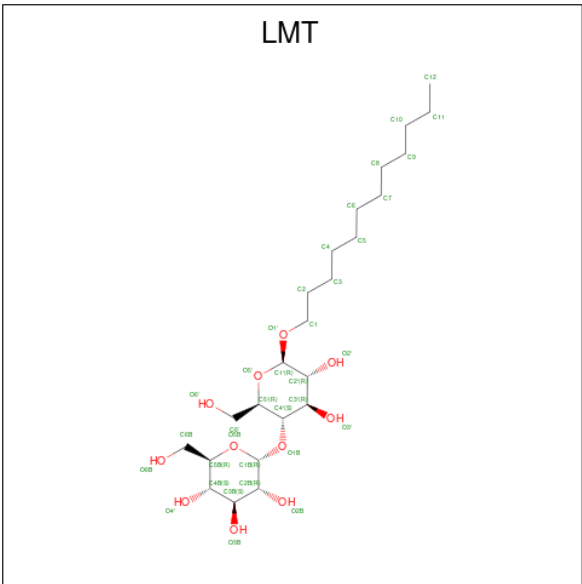
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	H	O	0
			95	40	54	1	
13	A	1	Total	C	H	O	0
			95	40	54	1	
13	B	1	Total	C	H	O	0
			95	40	54	1	
13	F	1	Total	C	H	O	0
			95	40	54	1	
13	M	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	H	O	0
			66	22	34	10	
14	B	1	Total	C	H	O	0
			114	38	66	10	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	H	O	0
			81	24	46	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	H	O	0
			31	10	15	6	
15	A	1	Total	C	H	O	0
			38	12	25	1	
15	A	1	Total	C	H	O	0
			29	10	18	1	
15	A	1	Total	C	H	O	0
			38	12	25	1	
15	A	1	Total	C	H	O	0
			57	18	33	6	
15	A	1	Total	C	H	O	0
			38	12	25	1	
15	A	1	Total	C	H	O	0
			57	18	33	6	
15	A	1	Total	C	H	O	0
			81	24	46	11	
15	B	1	Total	C	H	O	0
			58	18	34	6	
15	B	1	Total	C	H	O	0
			52	16	25	11	
15	B	1	Total	C	H	O	0
			64	20	33	11	
15	B	1	Total	C	H	O	0
			38	12	25	1	
15	B	1	Total	C	H	O	0
			38	12	25	1	
15	B	1	Total	C	H	O	0
			43	14	23	6	
15	B	1	Total	C	H	O	0
			38	12	25	1	
15	B	1	Total	C	H	O	0
			38	12	25	1	
15	B	1	Total	C	H	O	0
			38	12	25	1	
15	F	1	Total	C	H	O	0
			61	19	31	11	
15	F	1	Total	C	H	O	0
			38	12	25	1	
15	F	1	Total	C	H	O	0
			72	23	38	11	
15	I	1	Total	C	H	O	0
			51	15	25	11	

Continued on next page...

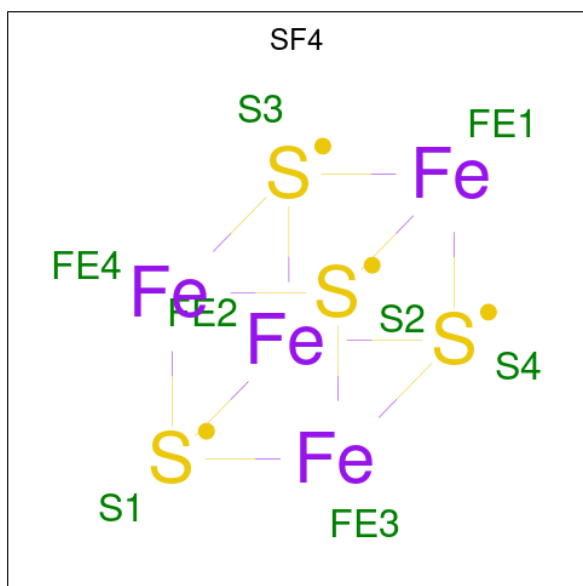
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
15	I	1	Total	C	H	O	0
			64	20	33	11	
15	J	1	Total	C	H	O	0
			38	12	25	1	
15	J	1	Total	C	H	O	0
			38	12	25	1	
15	M	1	Total	C	H	O	0
			38	12	25	1	

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

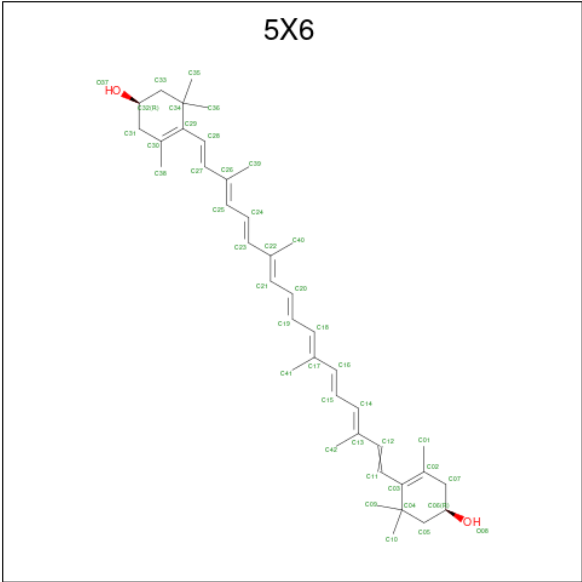
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Cl	0
			1	1	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	Fe	S	0
			6	2	4	

- Molecule 18 is Zeaxanthin (CCD ID: 5X6) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms				AltConf
18	B	1	Total	C	H	O	0
			98	40	56	2	

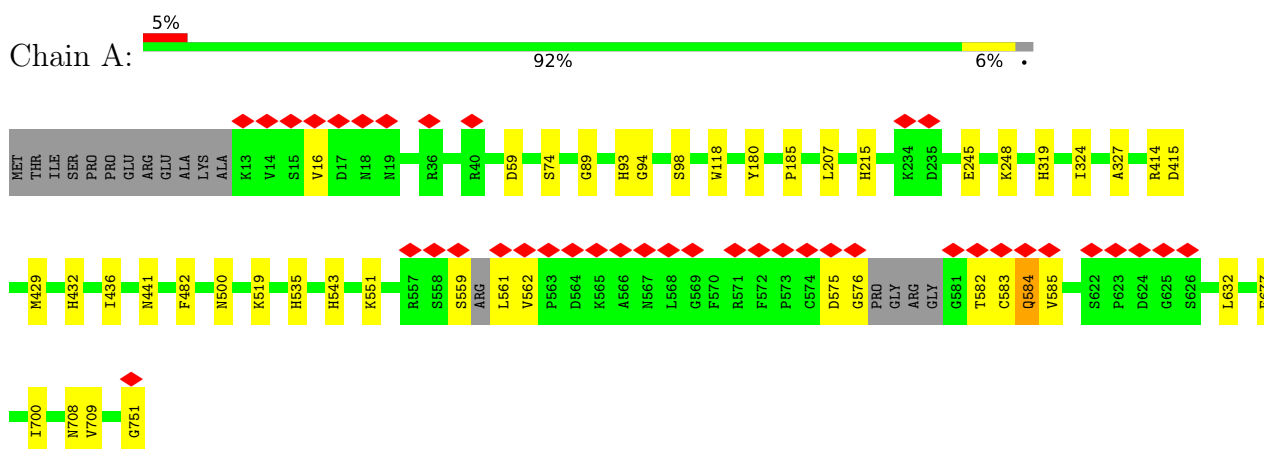
- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	A	171	Total	O	0
			171	171	
19	B	150	Total	O	0
			150	150	
19	F	17	Total	O	0
			17	17	
19	J	5	Total	O	0
			5	5	
19	K	11	Total	O	0
			11	11	
19	M	1	Total	O	0
			1	1	

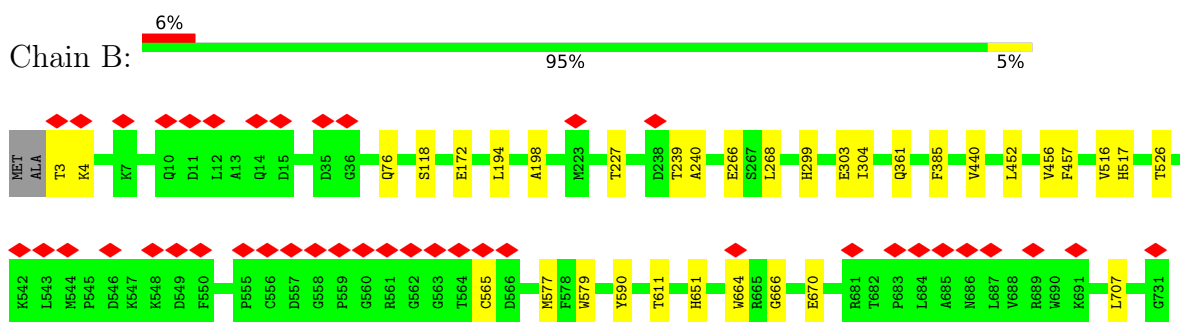
3 Residue-property plots [i](#)

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

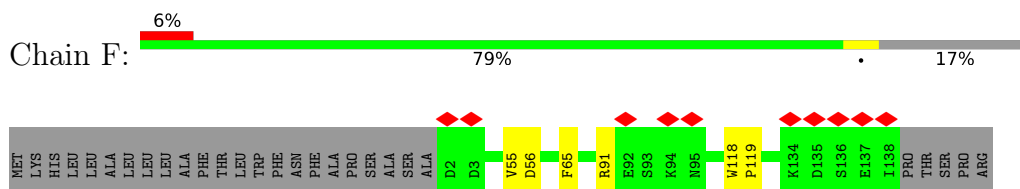
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



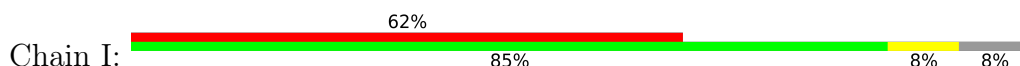
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

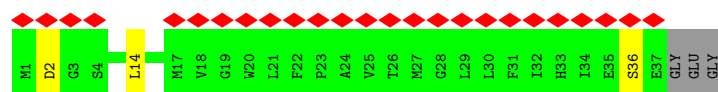


- Molecule 3: Photosystem I reaction center subunit III

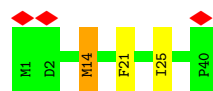


- Molecule 4: Photosystem I reaction center subunit VIII

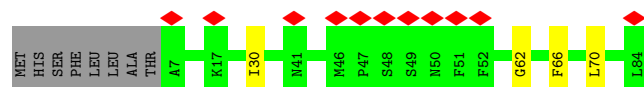
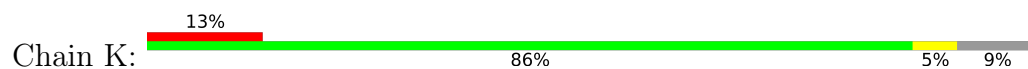




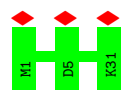
- Molecule 5: Photosystem I reaction center subunit IX



- Molecule 6: Photosystem I reaction center subunit PsaK 1



- Molecule 7: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	333941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	255.15, 255.15, 255.15	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LMT, BCR, CL, CLA, LHG, CL0, 5X6, ECH, PQN, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.09	0/5945	0.21	0/8102
2	B	0.08	0/5981	0.21	0/8178
3	F	0.08	0/1093	0.22	0/1486
4	I	0.07	0/304	0.21	0/416
5	J	0.08	0/328	0.21	0/443
6	K	0.07	0/555	0.18	0/752
7	M	0.06	0/241	0.15	0/326
All	All	0.08	0/14447	0.21	0/19703

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	A	5750	5602	5606	33	0
2	B	5770	5547	5549	25	0
3	F	1065	1051	1050	4	0
4	I	293	292	292	3	0
5	J	319	328	328	3	0
6	K	544	570	570	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	238	260	260	0	0
8	A	82	110	110	0	0
8	B	39	51	51	0	0
9	A	65	0	72	2	0
10	A	2466	2358	2358	20	0
10	B	2269	2142	2142	23	0
10	F	90	66	66	0	0
10	J	90	66	66	0	0
10	K	150	125	125	3	0
11	A	33	46	46	0	0
11	B	33	46	46	0	0
12	A	200	280	280	8	0
12	B	200	280	280	11	0
12	F	40	56	56	3	0
12	I	40	56	56	0	0
12	J	40	56	56	1	0
12	K	40	56	56	0	0
13	A	82	108	108	7	0
13	B	41	54	54	0	0
13	F	41	54	54	2	0
13	M	41	54	54	1	0
14	A	32	34	34	0	0
14	B	48	66	66	0	0
15	A	184	266	271	0	0
15	B	167	240	246	0	0
15	F	77	94	99	0	0
15	I	57	58	60	1	0
15	J	26	50	50	0	0
15	M	13	25	25	0	0
16	A	1	0	0	0	0
17	B	6	0	0	2	0
18	B	42	56	0	0	0
19	A	171	0	0	2	0
19	B	150	0	0	0	0
19	F	17	0	0	0	0
19	J	5	0	0	0	0
19	K	11	0	0	0	0
19	M	1	0	0	0	0
All	All	21069	20603	20642	116	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 3.

The worst 5 of 116 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)
1:A:575:ASP:O	1:A:582:THR:OG1	2.00	0.79
1:A:432:HIS:CE1	1:A:436:ILE:HD11	2.20	0.76
10:B:810:CLA:H43	10:B:829:CLA:H42	1.67	0.75
1:A:415:ASP:OD2	19:A:901:HOH:O	2.10	0.70
1:A:575:ASP:OD1	1:A:576:GLY:N	2.25	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	728/751 (97%)	713 (98%)	15 (2%)	0	100	100
2	B	727/731 (100%)	716 (98%)	11 (2%)	0	100	100
3	F	135/165 (82%)	134 (99%)	1 (1%)	0	100	100
4	I	35/40 (88%)	35 (100%)	0	0	100	100
5	J	38/40 (95%)	38 (100%)	0	0	100	100
6	K	76/86 (88%)	75 (99%)	1 (1%)	0	100	100
7	M	29/31 (94%)	29 (100%)	0	0	100	100
All	All	1768/1844 (96%)	1740 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/603 (98%)	585 (99%)	5 (1%)	73	65
2	B	582/583 (100%)	580 (100%)	2 (0%)	86	81
3	F	113/137 (82%)	113 (100%)	0	100	100
4	I	31/32 (97%)	31 (100%)	0	100	100
5	J	35/35 (100%)	34 (97%)	1 (3%)	37	20
6	K	55/62 (89%)	55 (100%)	0	100	100
7	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1431/1477 (97%)	1423 (99%)	8 (1%)	76	72

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	14	MET
2	B	651	HIS
1	A	585	VAL
1	A	584	GLN
2	B	517	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	701	GLN
3	F	31	ASN
4	I	33	HIS
3	F	99	GLN
2	B	34	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 1 is monoatomic - leaving 147 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
10	CLA	B	820	2	69,73,73	1.14	4 (5%)	82,113,113	0.81	3 (3%)
10	CLA	A	845	1	69,73,73	1.11	4 (5%)	82,113,113	0.82	3 (3%)
10	CLA	B	830	2	69,73,73	1.12	4 (5%)	82,113,113	0.80	3 (3%)
10	CLA	B	816	2	50,54,73	1.32	4 (8%)	59,90,113	0.95	3 (5%)
15	LMT	B	861	-	12,12,36	0.26	0	11,11,47	0.34	0
15	LMT	A	853	-	36,36,36	0.55	0	47,47,47	0.79	1 (2%)
9	CL0	A	803	1	58,73,73	1.34	7 (12%)	60,113,113	1.61	5 (8%)
14	LMG	B	850	-	48,48,55	0.18	0	56,56,63	0.13	0
13	ECH	B	846	-	42,42,42	0.11	0	55,58,58	0.28	0
10	CLA	A	839	1	58,62,73	1.25	4 (6%)	68,99,113	0.89	3 (4%)
10	CLA	B	802	19	69,73,73	1.20	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	A	804	19	69,73,73	1.22	4 (5%)	82,113,113	0.82	3 (3%)
10	CLA	A	834	1	69,73,73	1.14	4 (5%)	82,113,113	0.80	2 (2%)
15	LMT	I	102	-	27,27,36	0.59	0	38,38,47	0.76	0
15	LMT	A	857	-	12,12,36	0.26	0	11,11,47	0.32	0
10	CLA	A	835	1	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	813	2	49,53,73	1.33	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	A	824	1	69,73,73	1.12	4 (5%)	82,113,113	0.87	4 (4%)
15	LMT	F	206	-	12,12,36	0.26	0	11,11,47	0.32	0
10	CLA	B	825	2	59,63,73	1.25	4 (6%)	70,101,113	0.88	2 (2%)
14	LMG	A	852	-	32,32,55	0.20	0	40,40,63	0.17	0
12	BCR	B	849	-	41,41,41	0.11	0	56,56,56	0.48	0
12	BCR	A	847	-	41,41,41	0.12	0	56,56,56	0.27	0
10	CLA	A	830	19	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LMT	J	104	-	12,12,36	0.27	0	11,11,47	0.37	0
10	CLA	A	833	1	69,73,73	1.14	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	A	821	19	49,53,73	1.38	4 (8%)	58,89,113	0.99	3 (5%)
10	CLA	A	822	1	69,73,73	1.11	4 (5%)	82,113,113	0.82	3 (3%)
15	LMT	B	853	-	24,24,36	0.51	0	29,29,47	0.56	0
12	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.33	0
11	PQN	B	804	-	34,34,34	0.33	0	43,45,45	0.41	0
12	BCR	J	103	-	41,41,41	0.13	0	56,56,56	0.31	0
13	ECH	M	101	-	42,42,42	0.12	0	55,58,58	0.27	0
13	ECH	A	851	-	42,42,42	0.12	0	55,58,58	0.33	0
12	BCR	B	844	-	41,41,41	0.25	0	56,56,56	0.46	0
15	LMT	A	859	-	12,12,36	0.26	0	11,11,47	0.32	0
15	LMT	A	854	-	16,16,36	0.60	0	21,21,47	0.64	0
10	CLA	A	829	1	63,67,73	1.19	4 (6%)	74,105,113	0.86	2 (2%)
10	CLA	B	832	2	49,53,73	1.33	4 (8%)	58,89,113	0.99	4 (6%)
10	CLA	B	811	2	49,53,73	1.38	4 (8%)	58,89,113	0.94	2 (3%)
12	BCR	A	849	-	41,41,41	0.12	0	56,56,56	0.26	0
10	CLA	A	836	1	49,53,73	1.36	4 (8%)	58,89,113	0.97	4 (6%)
10	CLA	A	827	1	53,57,73	1.32	4 (7%)	61,93,113	0.96	3 (4%)
10	CLA	B	817	2	49,53,73	1.35	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	A	816	10,1	69,73,73	1.12	4 (5%)	82,113,113	0.79	2 (2%)
10	CLA	B	809	2	64,68,73	1.18	4 (6%)	76,107,113	0.84	3 (3%)
12	BCR	F	202	-	41,41,41	0.15	0	56,56,56	0.46	0
15	LMT	B	856	-	12,12,36	0.26	0	11,11,47	0.32	0
10	CLA	A	807	8	49,53,73	1.38	4 (8%)	58,89,113	0.94	3 (5%)
10	CLA	B	823	2	49,53,73	1.37	4 (8%)	58,89,113	0.97	2 (3%)
13	ECH	A	865	-	42,42,42	0.10	0	55,58,58	0.23	0
8	LHG	A	801	-	48,48,48	0.22	0	51,54,54	0.26	0
10	CLA	K	103	19	64,68,73	1.20	4 (6%)	76,107,113	0.86	3 (3%)
15	LMT	B	858	-	20,20,36	0.57	0	25,25,47	0.61	0
10	CLA	A	841	1	55,59,73	1.25	4 (7%)	64,96,113	0.93	2 (3%)
10	CLA	A	863	19	69,73,73	1.15	4 (5%)	82,113,113	0.81	2 (2%)
10	CLA	A	831	19	59,63,73	1.23	4 (6%)	70,101,113	0.87	3 (4%)
10	CLA	A	820	1	49,53,73	1.34	4 (8%)	58,89,113	0.96	3 (5%)
15	LMT	F	207	-	35,35,36	0.54	0	46,46,47	0.67	0
10	CLA	A	818	1	59,63,73	1.21	4 (6%)	70,101,113	0.86	2 (2%)
18	5X6	B	852	-	43,43,43	0.11	0	56,60,60	0.19	0
10	CLA	B	836	19	49,53,73	1.38	4 (8%)	58,89,113	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BCR	B	848	-	41,41,41	0.15	0	56,56,56	0.50	0
15	LMT	B	859	-	12,12,36	0.26	0	11,11,47	0.32	0
10	CLA	A	814	1	54,58,73	1.34	4 (7%)	64,95,113	0.92	2 (3%)
8	LHG	A	802	10	32,32,48	0.26	0	35,38,54	0.33	0
10	CLA	A	812	1	50,54,73	1.31	4 (8%)	59,90,113	0.95	3 (5%)
10	CLA	B	838	2	54,58,73	1.27	4 (7%)	64,95,113	0.90	3 (4%)
10	CLA	J	102	5	49,53,73	1.37	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	B	822	2	66,70,73	1.18	4 (6%)	78,109,113	0.86	3 (3%)
10	CLA	J	101	5	49,53,73	1.40	4 (8%)	58,89,113	0.97	2 (3%)
15	LMT	J	105	-	12,12,36	0.27	0	11,11,47	0.31	0
10	CLA	A	813	1	69,73,73	1.14	4 (5%)	82,113,113	0.79	2 (2%)
12	BCR	K	104	-	41,41,41	0.12	0	56,56,56	0.28	0
12	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.30	0
10	CLA	A	817	1	58,62,73	1.25	4 (6%)	68,99,113	0.88	3 (4%)
15	LMT	M	102	-	12,12,36	0.27	0	11,11,47	0.34	0
15	LMT	A	856	-	10,10,36	0.28	0	9,9,47	0.37	0
10	CLA	B	829	2	69,73,73	1.15	4 (5%)	82,113,113	0.83	2 (2%)
15	LMT	A	860	-	24,24,36	0.52	0	29,29,47	0.56	0
10	CLA	B	819	2	69,73,73	1.11	4 (5%)	82,113,113	0.81	3 (3%)
15	LMT	A	864	-	36,36,36	0.56	0	47,47,47	0.71	0
12	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.32	0
10	CLA	A	825	1	64,68,73	1.17	4 (6%)	76,107,113	0.83	4 (5%)
10	CLA	B	806	2	49,53,73	1.34	4 (8%)	58,89,113	0.95	3 (5%)
10	CLA	B	810	2	69,73,73	1.13	4 (5%)	82,113,113	0.84	2 (2%)
10	CLA	B	840	2	55,59,73	1.29	4 (7%)	64,96,113	0.91	2 (3%)
10	CLA	A	828	1	55,59,73	1.29	4 (7%)	64,96,113	0.93	2 (3%)
15	LMT	B	855	-	32,32,36	0.57	0	43,43,47	0.67	0
10	CLA	A	826	19	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)
10	CLA	B	815	2	69,73,73	1.14	4 (5%)	82,113,113	0.82	3 (3%)
10	CLA	B	843	8	27,35,73	1.91	6 (22%)	32,60,113	1.57	5 (15%)
10	CLA	A	844	1	69,73,73	1.12	4 (5%)	82,113,113	0.81	3 (3%)
10	CLA	B	803	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	814	2	49,53,73	1.37	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	B	841	19	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
8	LHG	B	851	10	38,38,48	0.25	0	41,44,54	0.29	0
10	CLA	A	819	1	49,53,73	1.34	4 (8%)	58,89,113	0.96	2 (3%)
15	LMT	F	201	-	31,31,36	0.58	0	42,42,47	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	B	821	19	69,73,73	1.17	4 (5%)	82,113,113	0.80	3 (3%)
10	CLA	A	810	-	69,73,73	1.11	4 (5%)	82,113,113	0.86	3 (3%)
10	CLA	A	837	1	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	A	843	1	51,55,73	1.33	4 (7%)	60,91,113	0.97	3 (5%)
15	LMT	A	855	-	12,12,36	0.26	0	11,11,47	0.32	0
10	CLA	A	823	1	69,73,73	1.15	4 (5%)	82,113,113	0.85	2 (2%)
10	CLA	A	842	1	59,63,73	1.24	4 (6%)	70,101,113	0.89	3 (4%)
15	LMT	A	858	-	24,24,36	0.51	0	29,29,47	0.62	0
17	SF4	B	805	1	0,6,12	-	-	-		
10	CLA	A	838	1	49,53,73	1.34	4 (8%)	58,89,113	0.96	4 (6%)
11	PQN	A	806	-	34,34,34	0.32	0	43,45,45	0.42	0
10	CLA	B	812	2	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	K	102	6	49,53,73	1.38	4 (8%)	58,89,113	0.95	3 (5%)
10	CLA	B	827	19	54,58,73	1.30	4 (7%)	64,95,113	0.90	2 (3%)
10	CLA	B	808	2	69,73,73	1.15	4 (5%)	82,113,113	0.79	2 (2%)
10	CLA	B	833	2	59,63,73	1.23	4 (6%)	70,101,113	0.86	3 (4%)
10	CLA	B	828	2	69,73,73	1.15	4 (5%)	82,113,113	0.84	3 (3%)
13	ECH	F	205	-	42,42,42	0.09	0	55,58,58	0.31	0
10	CLA	A	846	19	49,53,73	1.38	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	B	807	2	69,73,73	1.15	4 (5%)	82,113,113	0.83	3 (3%)
10	CLA	A	811	1	69,73,73	1.14	4 (5%)	82,113,113	0.79	3 (3%)
12	BCR	B	845	-	41,41,41	0.13	0	56,56,56	0.40	0
10	CLA	B	801	2	69,73,73	1.11	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	F	203	19	49,53,73	1.37	4 (8%)	58,89,113	0.95	2 (3%)
10	CLA	A	861	1	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	A	808	1	69,73,73	1.12	4 (5%)	82,113,113	0.82	3 (3%)
12	BCR	A	866	-	41,41,41	0.13	0	56,56,56	0.25	0
12	BCR	I	101	-	41,41,41	0.12	0	56,56,56	0.39	0
10	CLA	B	837	19	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
10	CLA	B	839	2	66,70,73	1.17	4 (6%)	78,109,113	0.83	3 (3%)
15	LMT	I	103	-	32,32,36	0.55	0	43,43,47	0.67	0
15	LMT	B	860	-	12,12,36	0.26	0	11,11,47	0.33	0
10	CLA	B	831	2	64,68,73	1.17	4 (6%)	76,107,113	0.84	2 (2%)
10	CLA	B	842	2	49,53,73	1.35	4 (8%)	58,89,113	0.96	2 (3%)
10	CLA	B	834	2	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	F	204	3	49,53,73	1.36	4 (8%)	58,89,113	0.96	3 (5%)
15	LMT	B	857	-	12,12,36	0.27	0	11,11,47	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	A	832	1	69,73,73	1.15	4 (5%)	82,113,113	0.79	2 (2%)
10	CLA	B	826	19	69,73,73	1.19	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	835	2	65,69,73	1.16	4 (6%)	77,108,113	0.85	3 (3%)
10	CLA	K	101	6	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
10	CLA	B	824	2	64,68,73	1.18	4 (6%)	76,107,113	0.83	2 (2%)
15	LMT	B	854	-	28,28,36	0.60	0	39,39,47	0.69	0
10	CLA	A	809	10,1	54,58,73	1.25	4 (7%)	64,95,113	0.92	3 (4%)
10	CLA	A	805	-	69,73,73	1.13	4 (5%)	82,113,113	0.78	2 (2%)
10	CLA	B	818	2	59,63,73	1.22	4 (6%)	70,101,113	0.94	4 (5%)
10	CLA	A	840	1	49,53,73	1.37	4 (8%)	58,89,113	0.95	3 (5%)
10	CLA	A	815	1	49,53,73	1.35	4 (8%)	58,89,113	0.95	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	820	2	1/1/20/20	4/39/115/115	-
10	CLA	A	845	1	1/1/20/20	4/39/115/115	-
10	CLA	B	830	2	1/1/20/20	2/39/115/115	-
10	CLA	B	816	2	1/1/15/20	0/17/93/115	-
15	LMT	B	861	-	-	0/10/10/61	-
15	LMT	A	853	-	-	4/21/61/61	0/2/2/2
9	CL0	A	803	1	3/3/20/25	4/37/135/135	-
14	LMG	B	850	-	-	4/43/63/70	0/1/1/1
13	ECH	B	846	-	-	4/29/66/66	0/2/2/2
10	CLA	A	839	1	1/1/17/20	3/26/102/115	-
10	CLA	B	802	19	1/1/20/20	5/39/115/115	-
10	CLA	A	804	19	1/1/20/20	2/39/115/115	-
10	CLA	A	834	1	1/1/20/20	2/39/115/115	-
15	LMT	I	102	-	-	3/12/52/61	0/2/2/2
15	LMT	A	857	-	-	0/10/10/61	-
10	CLA	A	835	1	1/1/20/20	3/39/115/115	-
10	CLA	B	813	2	1/1/15/20	1/15/91/115	-
10	CLA	A	824	1	1/1/20/20	2/39/115/115	-
15	LMT	F	206	-	-	0/10/10/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	825	2	1/1/18/20	3/27/103/115	-
14	LMG	A	852	-	-	5/27/47/70	0/1/1/1
12	BCR	B	849	-	-	0/29/63/63	0/2/2/2
12	BCR	A	847	-	-	0/29/63/63	0/2/2/2
10	CLA	A	830	19	1/1/20/20	8/39/115/115	-
15	LMT	J	104	-	-	2/10/10/61	-
10	CLA	A	833	1	1/1/20/20	1/39/115/115	-
10	CLA	A	821	19	1/1/15/20	2/15/91/115	-
10	CLA	A	822	1	1/1/20/20	1/39/115/115	-
15	LMT	B	853	-	-	2/15/35/61	0/1/1/2
12	BCR	A	850	-	-	2/29/63/63	0/2/2/2
11	PQN	B	804	-	-	0/23/43/43	0/2/2/2
12	BCR	J	103	-	-	2/29/63/63	0/2/2/2
13	ECH	M	101	-	-	4/29/66/66	0/2/2/2
13	ECH	A	851	-	-	6/29/66/66	0/2/2/2
12	BCR	B	844	-	-	0/29/63/63	0/2/2/2
15	LMT	A	859	-	-	0/10/10/61	-
15	LMT	A	854	-	-	1/7/27/61	0/1/1/2
10	CLA	A	829	1	1/1/18/20	4/32/108/115	-
10	CLA	B	832	2	1/1/15/20	0/15/91/115	-
10	CLA	B	811	2	1/1/15/20	2/15/91/115	-
12	BCR	A	849	-	-	2/29/63/63	0/2/2/2
10	CLA	A	836	1	1/1/15/20	2/15/91/115	-
10	CLA	A	827	1	1/1/16/20	3/20/96/115	-
10	CLA	B	817	2	1/1/15/20	0/15/91/115	-
10	CLA	A	816	10,1	1/1/20/20	7/39/115/115	-
10	CLA	B	809	2	1/1/19/20	2/33/109/115	-
12	BCR	F	202	-	-	0/29/63/63	0/2/2/2
15	LMT	B	856	-	-	0/10/10/61	-
10	CLA	A	807	8	1/1/15/20	0/15/91/115	-
10	CLA	B	823	2	1/1/15/20	5/15/91/115	-
13	ECH	A	865	-	-	0/29/66/66	0/2/2/2
10	CLA	K	103	19	1/1/19/20	5/33/109/115	-
8	LHG	A	801	-	-	14/53/53/53	-
15	LMT	B	858	-	-	1/11/31/61	0/1/1/2
10	CLA	A	841	1	1/1/17/20	0/23/99/115	-
10	CLA	A	863	19	1/1/20/20	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	831	19	1/1/18/20	0/27/103/115	-
10	CLA	A	820	1	1/1/15/20	2/15/91/115	-
15	LMT	F	207	-	-	5/20/60/61	0/2/2/2
10	CLA	A	818	1	1/1/18/20	1/27/103/115	-
18	5X6	B	852	-	-	2/29/67/67	0/2/2/2
10	CLA	B	836	19	1/1/15/20	0/15/91/115	-
12	BCR	B	848	-	-	2/29/63/63	0/2/2/2
15	LMT	B	859	-	-	1/10/10/61	-
10	CLA	A	814	1	1/1/17/20	1/21/97/115	-
8	LHG	A	802	10	-	10/37/37/53	-
10	CLA	A	812	1	1/1/15/20	0/17/93/115	-
10	CLA	B	838	2	1/1/17/20	0/21/97/115	-
10	CLA	J	102	5	1/1/15/20	2/15/91/115	-
10	CLA	B	822	2	1/1/19/20	6/36/112/115	-
10	CLA	J	101	5	1/1/15/20	4/15/91/115	-
15	LMT	J	105	-	-	2/10/10/61	-
10	CLA	A	813	1	1/1/20/20	4/39/115/115	-
12	BCR	K	104	-	-	0/29/63/63	0/2/2/2
12	BCR	A	848	-	-	2/29/63/63	0/2/2/2
10	CLA	A	817	1	1/1/17/20	0/26/102/115	-
15	LMT	M	102	-	-	0/10/10/61	-
15	LMT	A	856	-	-	0/8/8/61	-
10	CLA	B	829	2	1/1/20/20	7/39/115/115	-
15	LMT	A	860	-	-	3/15/35/61	0/1/1/2
10	CLA	B	819	2	1/1/20/20	4/39/115/115	-
15	LMT	A	864	-	-	2/21/61/61	0/2/2/2
12	BCR	B	847	-	-	2/29/63/63	0/2/2/2
10	CLA	A	825	1	1/1/19/20	2/33/109/115	-
10	CLA	B	806	2	1/1/15/20	5/15/91/115	-
10	CLA	B	810	2	1/1/20/20	5/39/115/115	-
10	CLA	B	840	2	1/1/17/20	2/23/99/115	-
10	CLA	A	828	1	1/1/17/20	2/23/99/115	-
15	LMT	B	855	-	-	0/17/57/61	0/2/2/2
10	CLA	A	826	19	1/1/20/20	1/39/115/115	-
10	CLA	B	815	2	1/1/20/20	3/39/115/115	-
10	CLA	B	843	8	1/1/8/20	-	-
10	CLA	A	844	1	1/1/20/20	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	803	-	1/1/20/20	3/39/115/115	-
10	CLA	B	814	2	1/1/15/20	2/15/91/115	-
10	CLA	B	841	19	1/1/15/20	3/15/91/115	-
8	LHG	B	851	10	-	7/43/43/53	-
10	CLA	A	819	1	1/1/15/20	2/15/91/115	-
15	LMT	F	201	-	-	0/16/56/61	0/2/2/2
10	CLA	B	821	19	1/1/20/20	2/39/115/115	-
10	CLA	A	810	-	1/1/20/20	3/39/115/115	-
10	CLA	A	837	1	1/1/15/20	4/15/91/115	-
10	CLA	A	843	1	1/1/15/20	2/18/94/115	-
15	LMT	A	855	-	-	1/10/10/61	-
10	CLA	A	823	1	1/1/20/20	6/39/115/115	-
10	CLA	A	842	1	1/1/18/20	2/27/103/115	-
15	LMT	A	858	-	-	6/15/35/61	0/1/1/2
17	SF4	B	805	1	-	-	0/1/1/5
10	CLA	A	838	1	1/1/15/20	2/15/91/115	-
11	PQN	A	806	-	-	0/23/43/43	0/2/2/2
10	CLA	B	812	2	1/1/15/20	4/15/91/115	-
10	CLA	K	102	6	1/1/15/20	6/15/91/115	-
10	CLA	B	827	19	1/1/17/20	2/21/97/115	-
10	CLA	B	808	2	1/1/20/20	2/39/115/115	-
10	CLA	B	833	2	1/1/18/20	2/27/103/115	-
10	CLA	B	828	2	1/1/20/20	2/39/115/115	-
13	ECH	F	205	-	-	2/29/66/66	0/2/2/2
10	CLA	A	846	19	1/1/15/20	3/15/91/115	-
10	CLA	B	807	2	1/1/20/20	7/39/115/115	-
10	CLA	A	811	1	1/1/20/20	2/39/115/115	-
12	BCR	B	845	-	-	2/29/63/63	0/2/2/2
10	CLA	B	801	2	1/1/20/20	2/39/115/115	-
10	CLA	F	203	19	1/1/15/20	2/15/91/115	-
10	CLA	A	861	1	1/1/15/20	0/15/91/115	-
10	CLA	A	808	1	1/1/20/20	2/39/115/115	-
12	BCR	A	866	-	-	0/29/63/63	0/2/2/2
12	BCR	I	101	-	-	0/29/63/63	0/2/2/2
10	CLA	B	837	19	1/1/15/20	2/15/91/115	-
10	CLA	B	839	2	1/1/19/20	0/36/112/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	I	103	-	-	4/17/57/61	0/2/2/2
15	LMT	B	860	-	-	0/10/10/61	-
10	CLA	B	831	2	1/1/19/20	5/33/109/115	-
10	CLA	B	842	2	1/1/15/20	5/15/91/115	-
10	CLA	B	834	2	1/1/20/20	1/39/115/115	-
10	CLA	F	204	3	1/1/15/20	2/15/91/115	-
15	LMT	B	857	-	-	1/10/10/61	-
10	CLA	A	832	1	1/1/20/20	2/39/115/115	-
10	CLA	B	826	19	1/1/20/20	2/39/115/115	-
10	CLA	B	835	2	1/1/19/20	2/35/111/115	-
10	CLA	K	101	6	1/1/15/20	4/15/91/115	-
10	CLA	B	824	2	1/1/19/20	5/33/109/115	-
15	LMT	B	854	-	-	1/13/53/61	0/2/2/2
10	CLA	A	809	10,1	1/1/17/20	0/21/97/115	-
10	CLA	A	805	-	1/1/20/20	5/39/115/115	-
10	CLA	B	818	2	1/1/18/20	4/27/103/115	-
10	CLA	A	840	1	1/1/15/20	5/15/91/115	-
10	CLA	A	815	1	1/1/15/20	1/15/91/115	-

The worst 5 of 377 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	804	CLA	MG-NB	-5.87	1.94	2.05
10	A	814	CLA	MG-NB	-5.41	1.95	2.05
10	B	802	CLA	MG-NB	-5.39	1.95	2.05
10	B	829	CLA	C1D-ND	5.36	1.44	1.37
10	A	841	CLA	C1D-ND	5.33	1.44	1.37

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	803	CL0	C1B-CHB-C4A	10.14	127.84	121.32
10	B	843	CLA	C1C-NC-C4C	-5.06	104.37	106.68
10	A	810	CLA	C1D-ND-C4D	-4.53	103.14	106.31
10	A	822	CLA	C1D-ND-C4D	-4.47	103.17	106.31
10	A	808	CLA	C1D-ND-C4D	-4.43	103.20	106.31

5 of 95 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	803	CL0	NA
9	A	803	CL0	NC
9	A	803	CL0	ND
10	A	804	CLA	ND
10	A	805	CLA	ND

5 of 359 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	LHG	C4-O6-P-O3
8	A	801	LHG	C4-O6-P-O4
8	A	802	LHG	C3-O3-P-O5
8	A	802	LHG	C4-O6-P-O4
8	B	851	LHG	C4-O6-P-O3

There are no ring outliers.

47 monomers are involved in 73 short contacts:

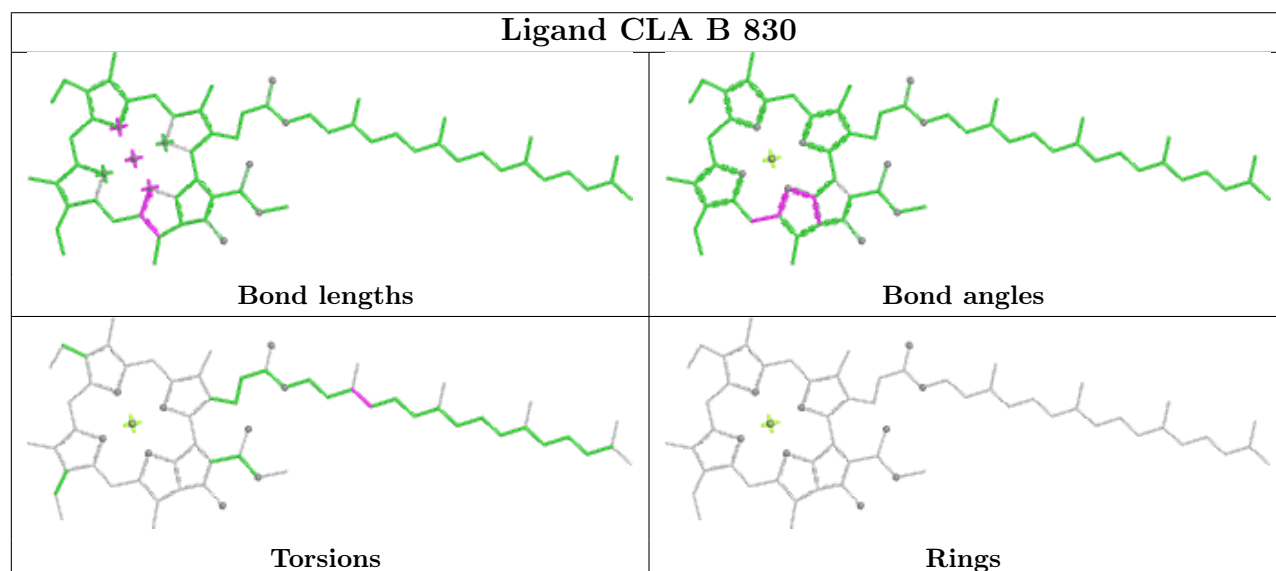
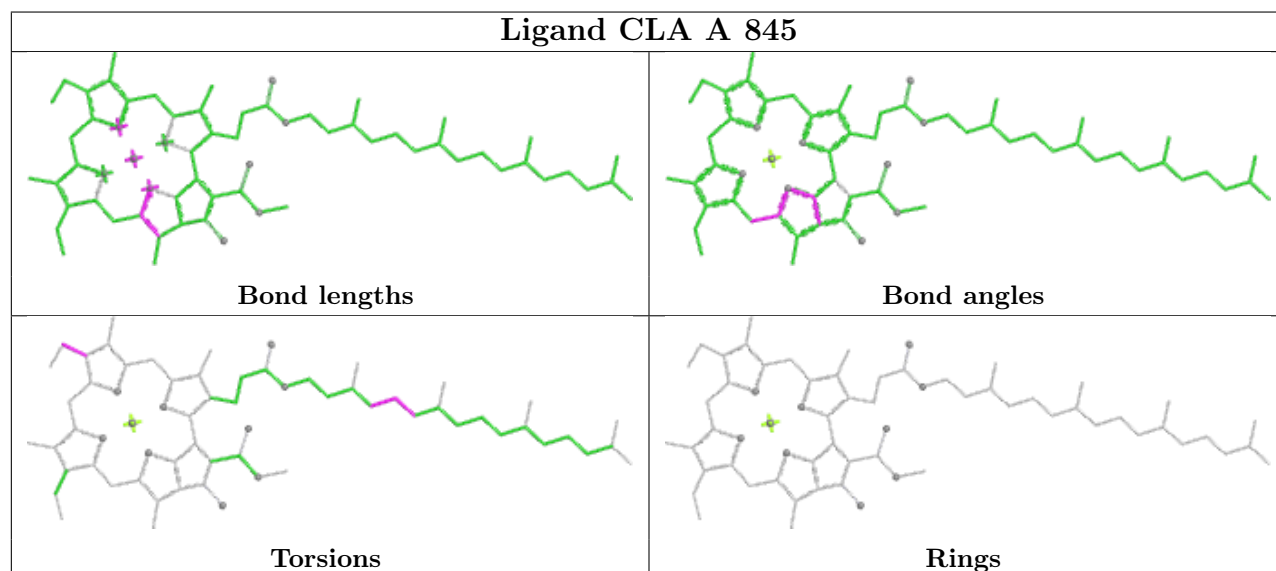
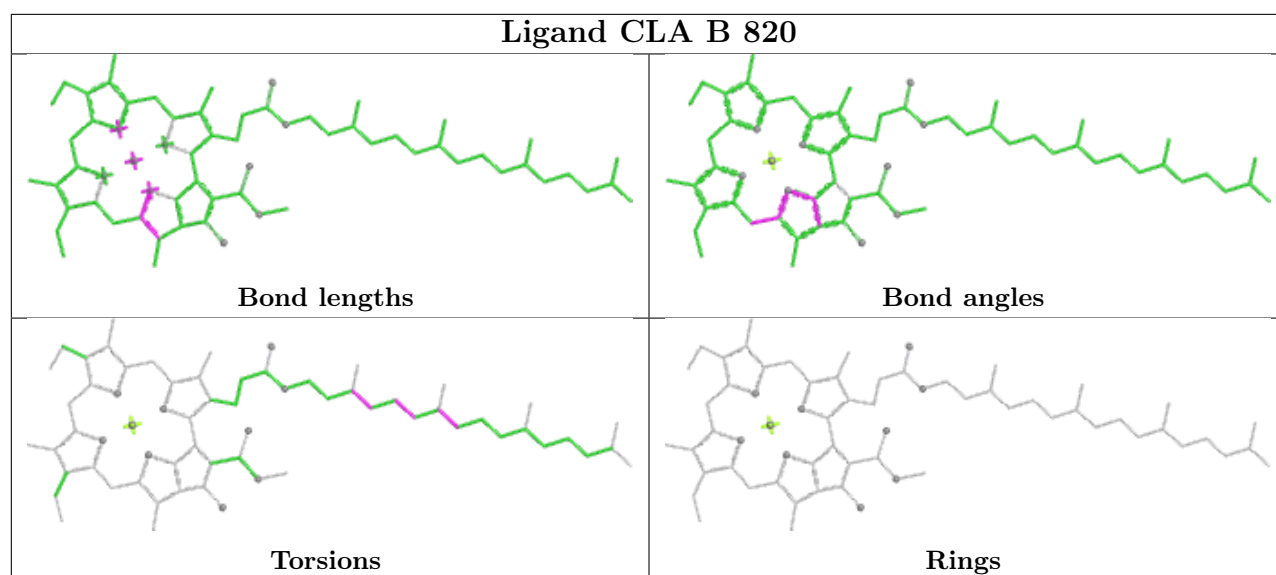
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	845	CLA	1	0
9	A	803	CL0	2	0
10	B	802	CLA	3	0
10	A	804	CLA	1	0
15	I	102	LMT	1	0
10	B	825	CLA	1	0
12	B	849	BCR	2	0
12	A	847	BCR	1	0
10	A	830	CLA	1	0
12	A	850	BCR	2	0
12	J	103	BCR	1	0
13	M	101	ECH	1	0
13	A	851	ECH	5	0
12	B	844	BCR	4	0
10	A	827	CLA	1	0
10	B	809	CLA	1	0
12	F	202	BCR	3	0
10	B	823	CLA	1	0
13	A	865	ECH	2	0
12	B	848	BCR	2	0
10	A	814	CLA	2	0
10	A	813	CLA	3	0
12	A	848	BCR	1	0
10	B	829	CLA	2	0

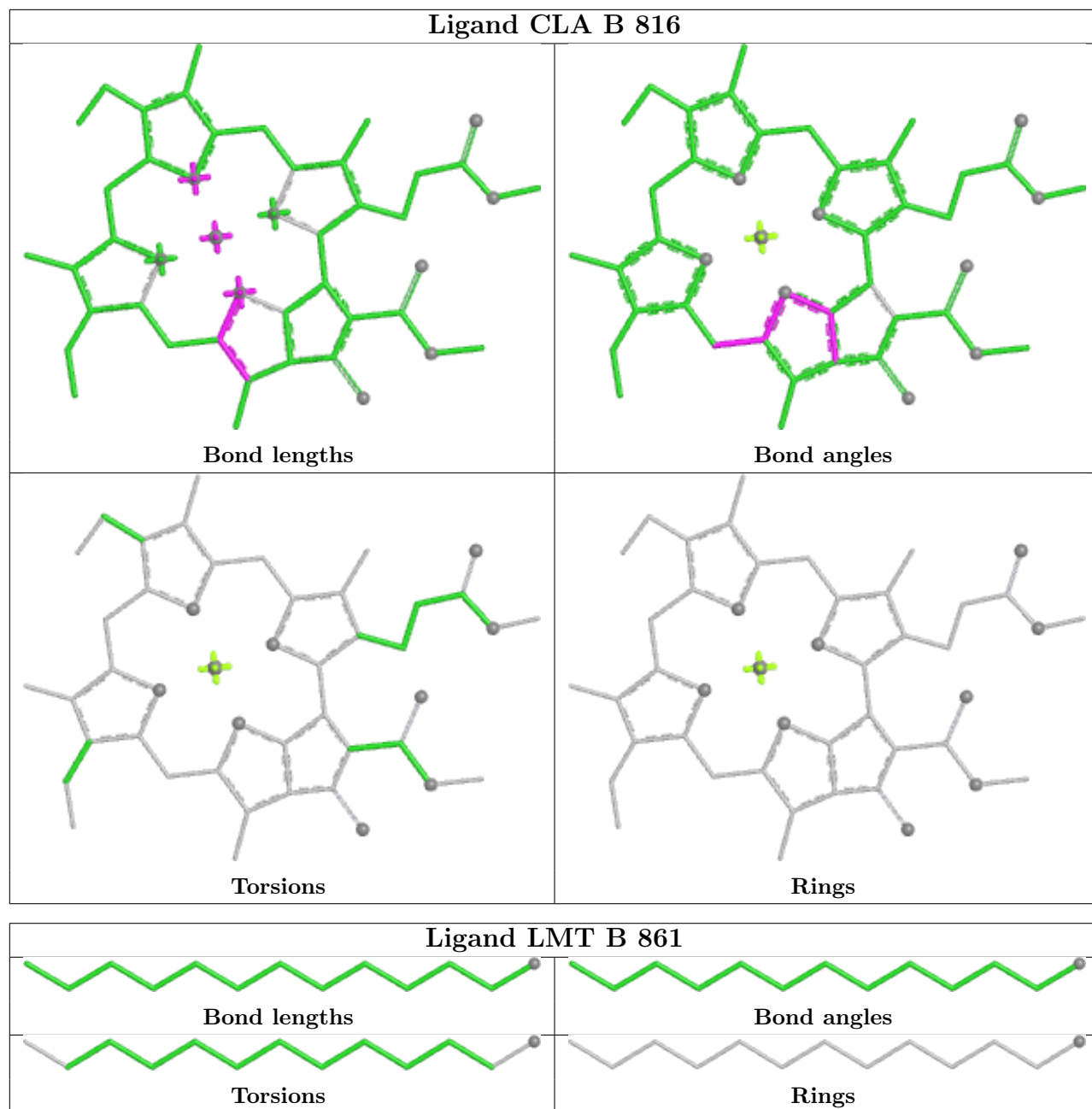
Continued on next page...

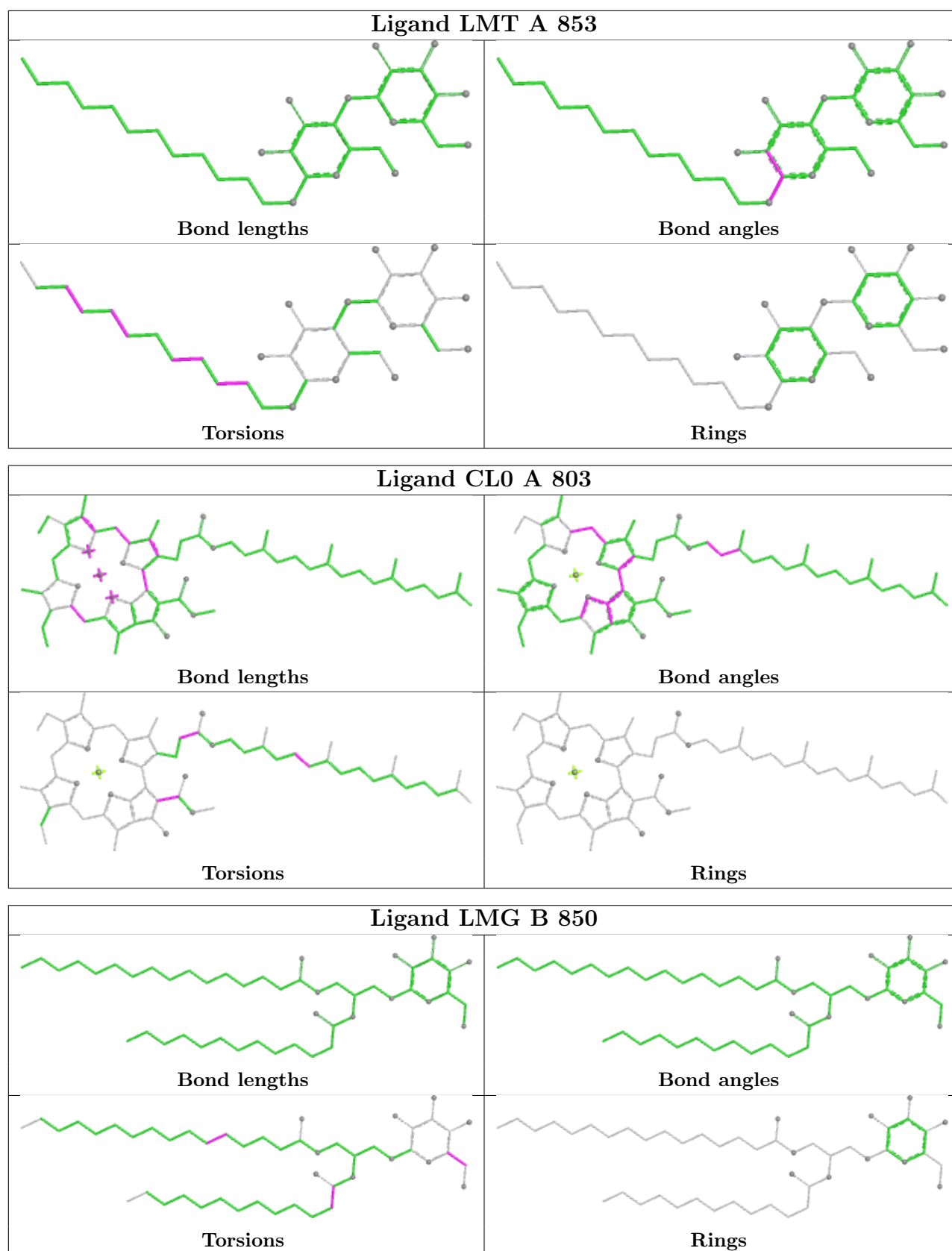
Continued from previous page...

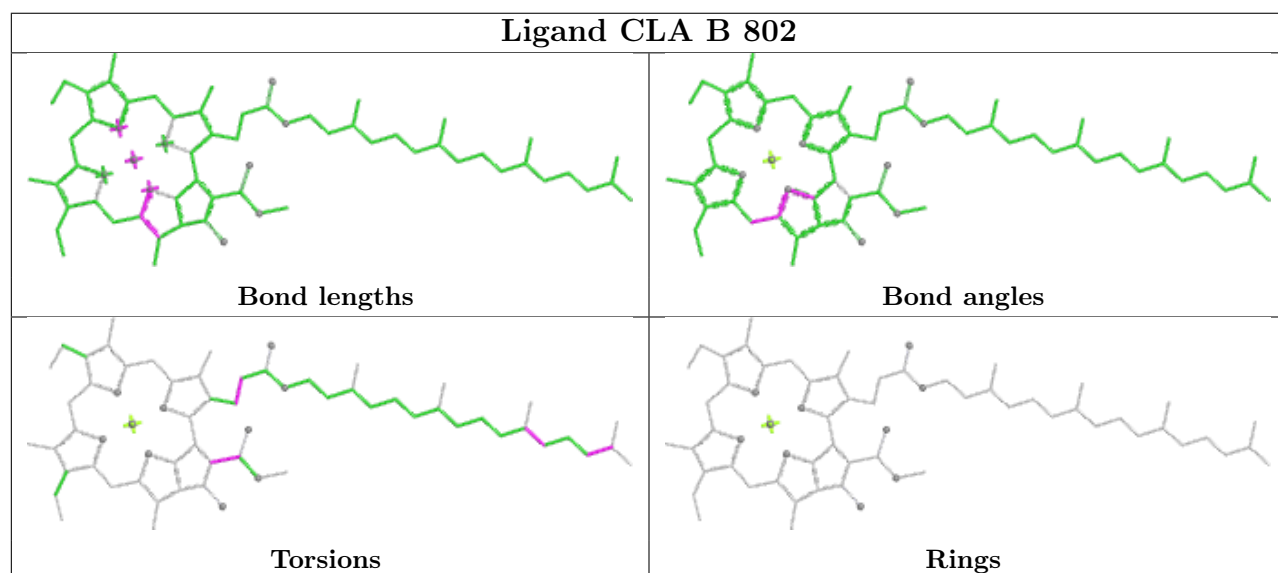
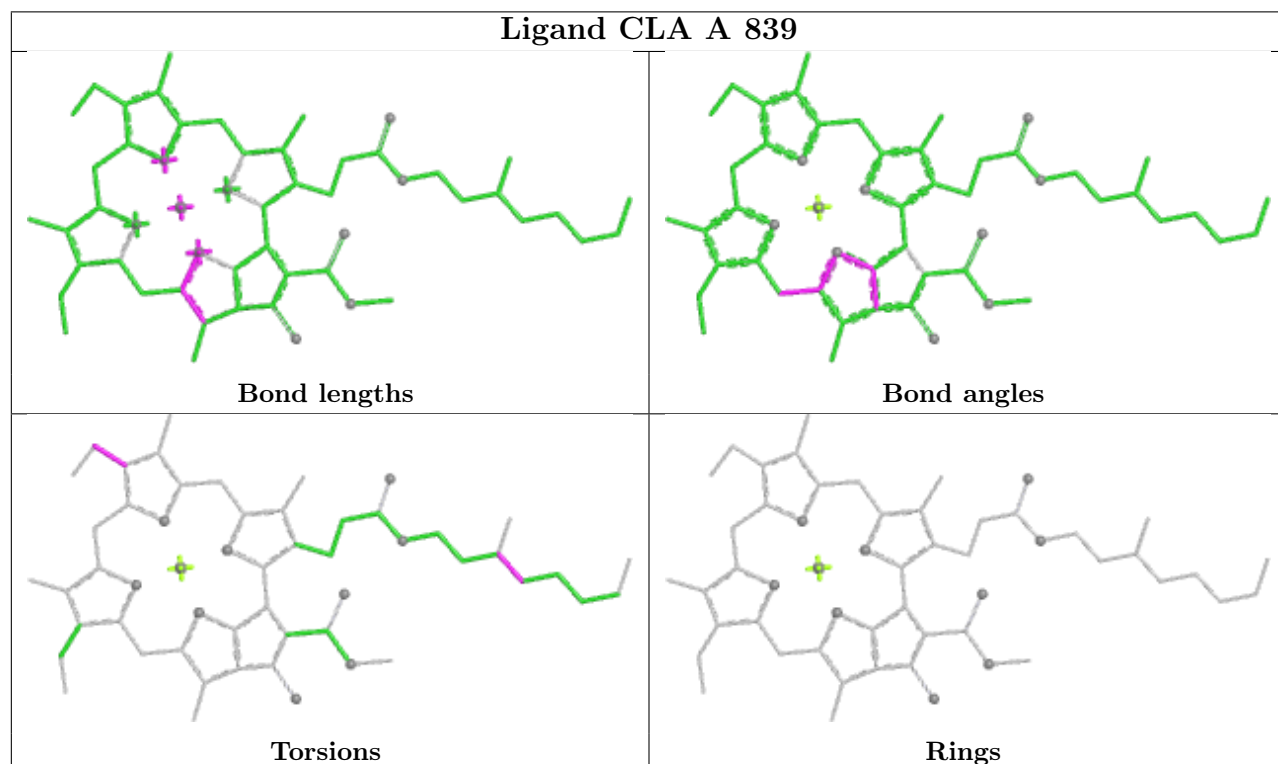
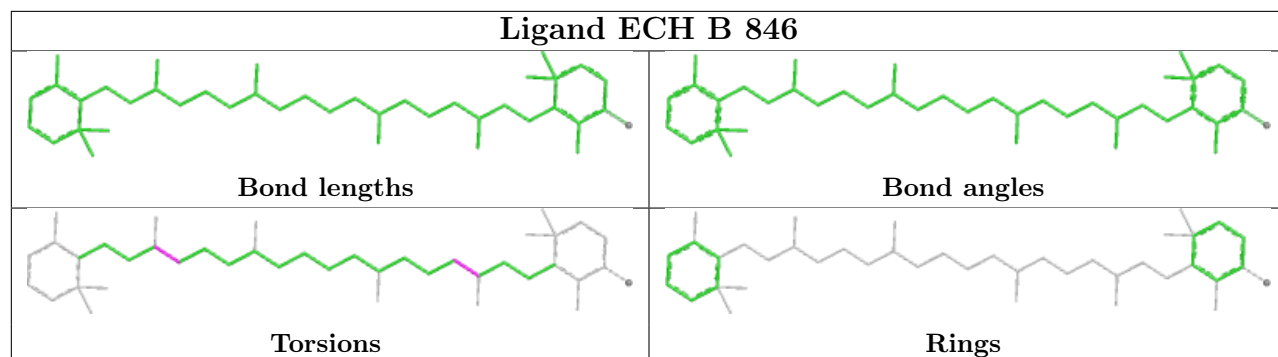
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	819	CLA	1	0
12	B	847	BCR	2	0
10	B	810	CLA	4	0
10	A	828	CLA	3	0
10	A	844	CLA	2	0
10	B	803	CLA	1	0
10	A	819	CLA	1	0
10	B	821	CLA	3	0
10	A	810	CLA	1	0
10	A	842	CLA	1	0
17	B	805	SF4	2	0
10	A	838	CLA	1	0
10	K	102	CLA	3	0
10	B	808	CLA	2	0
10	B	828	CLA	2	0
13	F	205	ECH	2	0
12	B	845	BCR	1	0
12	A	866	BCR	4	0
10	B	834	CLA	1	0
10	B	826	CLA	5	0
10	B	835	CLA	1	0
10	A	805	CLA	1	0
10	A	840	CLA	1	0

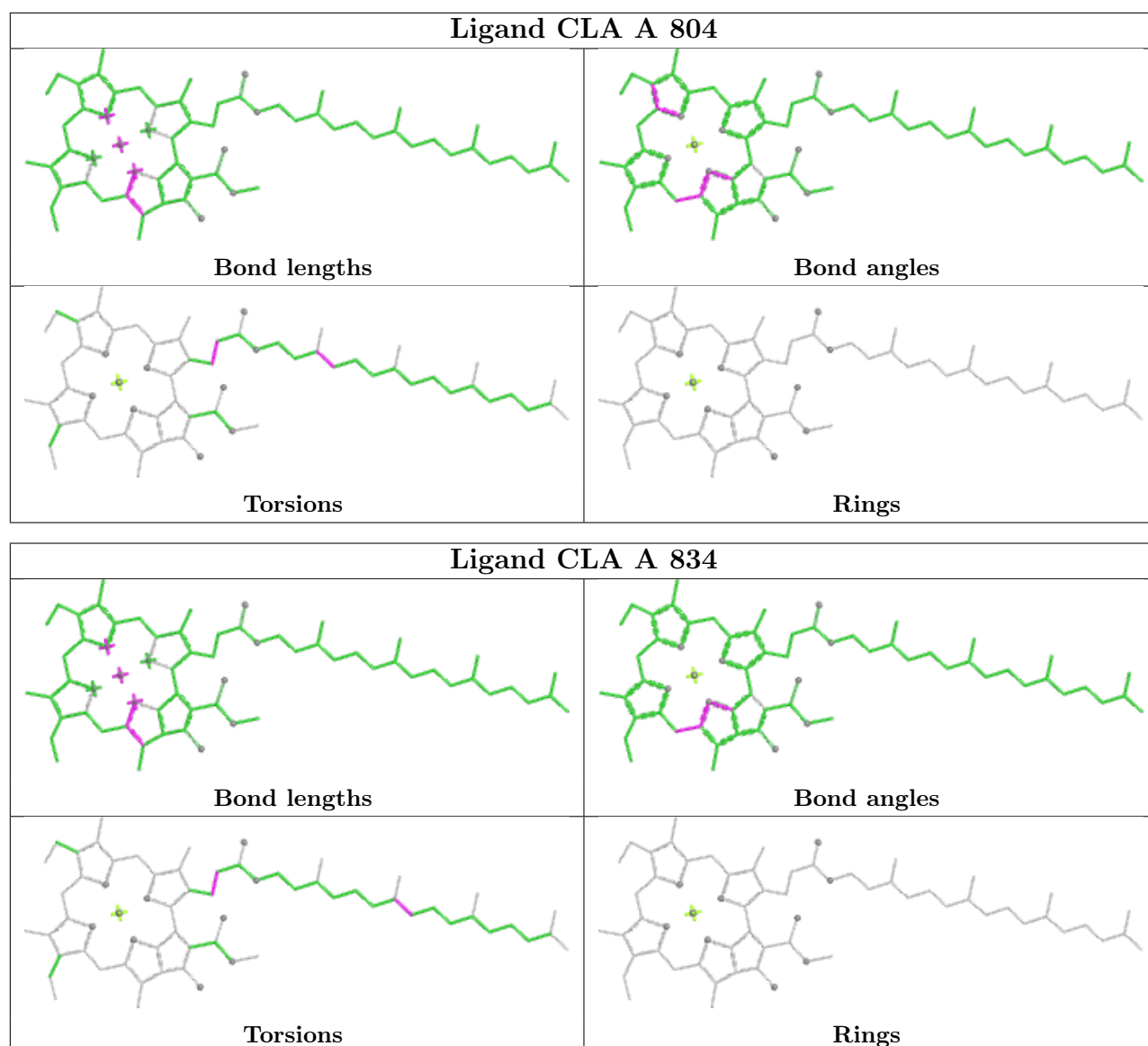
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

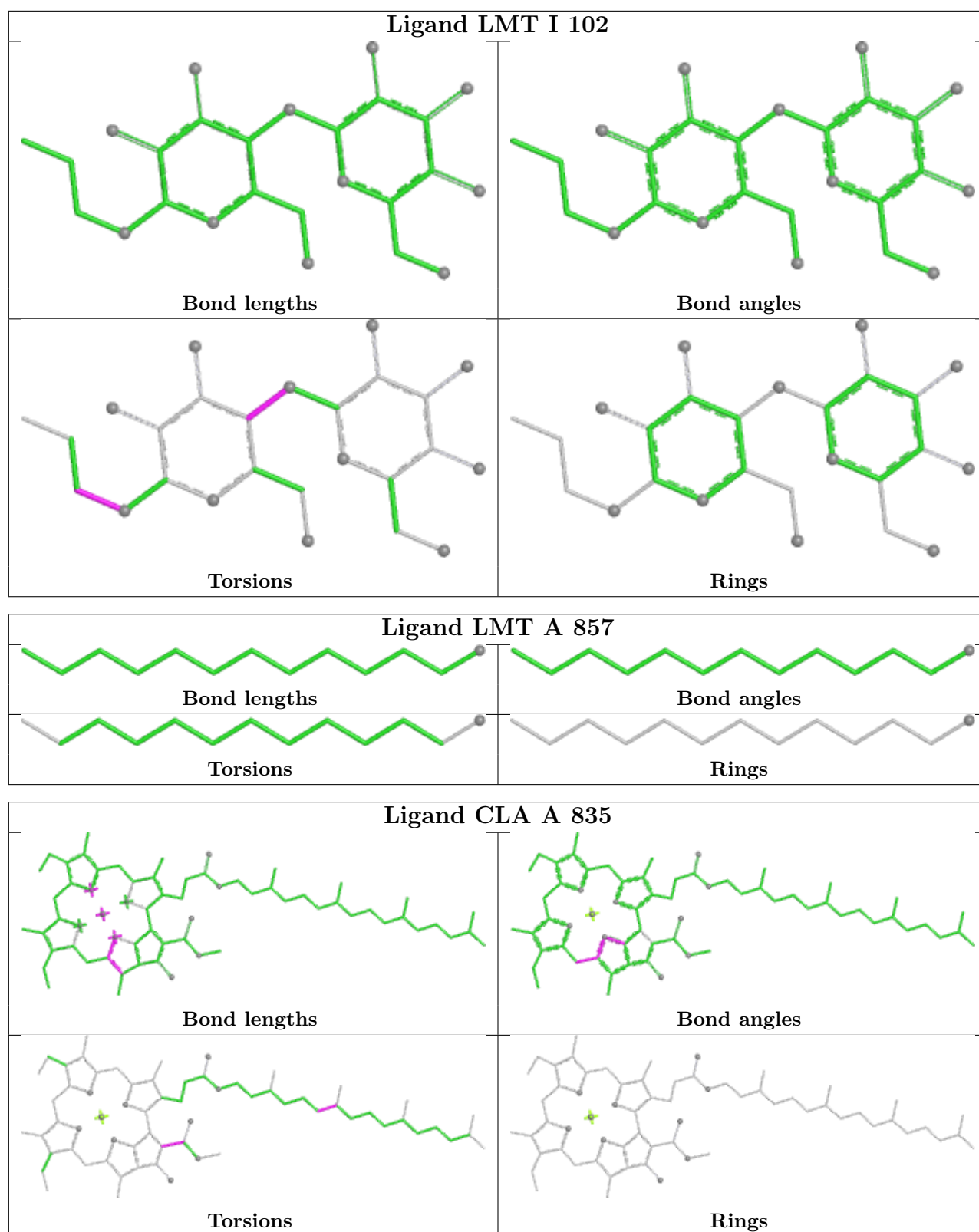




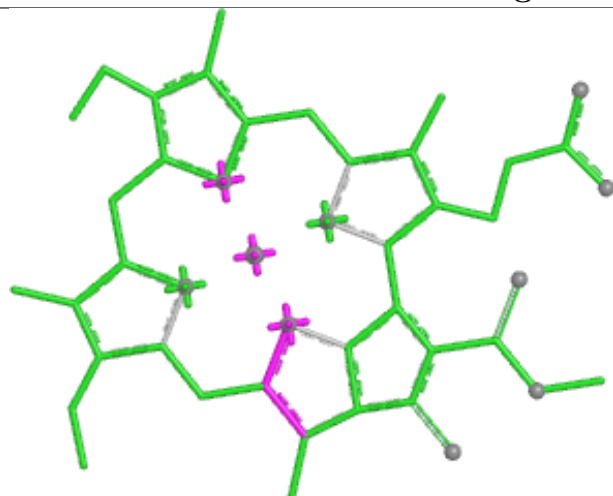




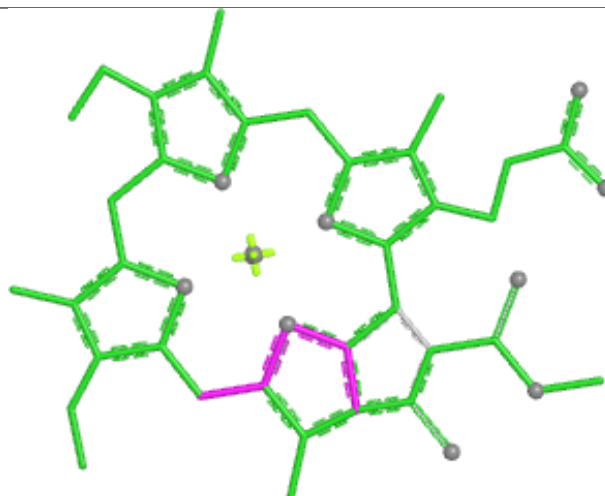




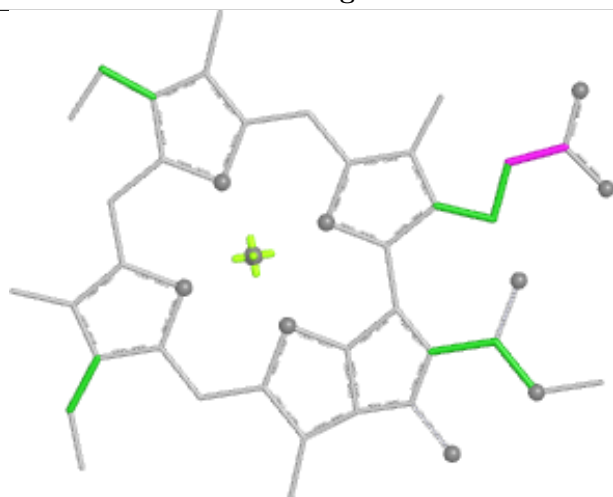
Ligand CLA B 813



Bond lengths



Bond angles

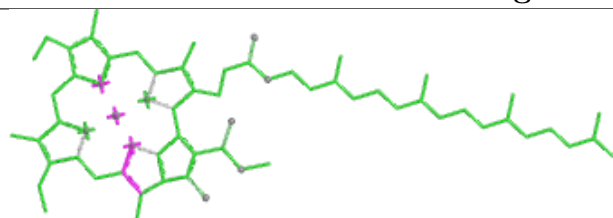


Torsions

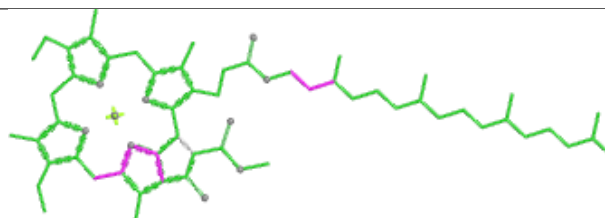


Rings

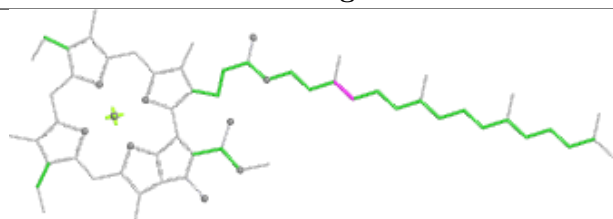
Ligand CLA A 824



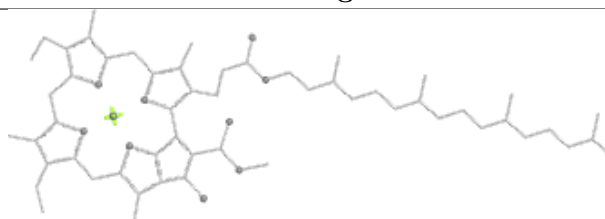
Bond lengths



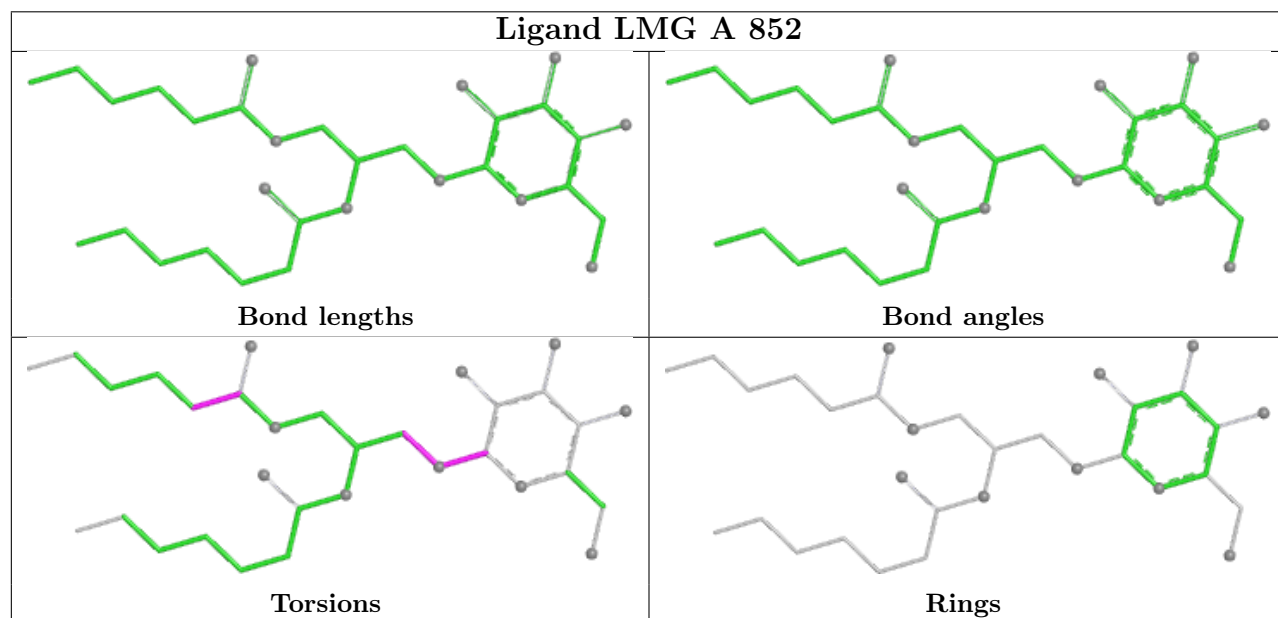
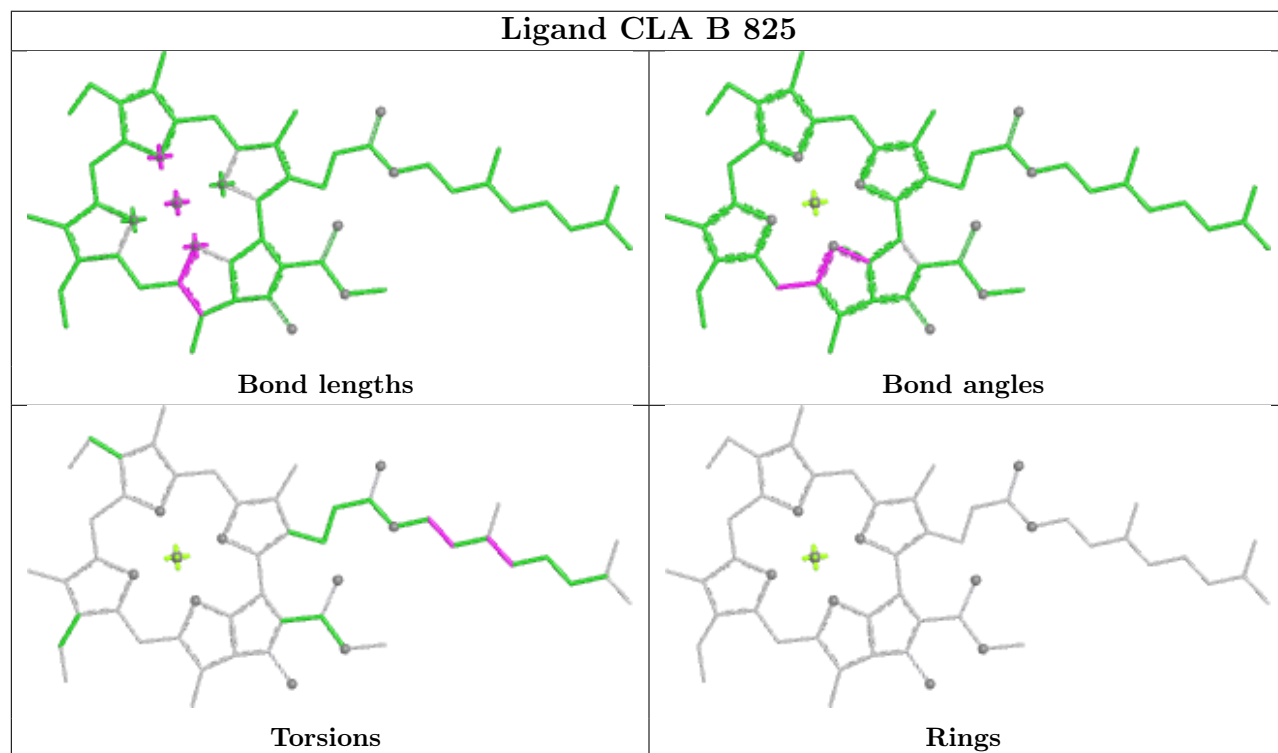
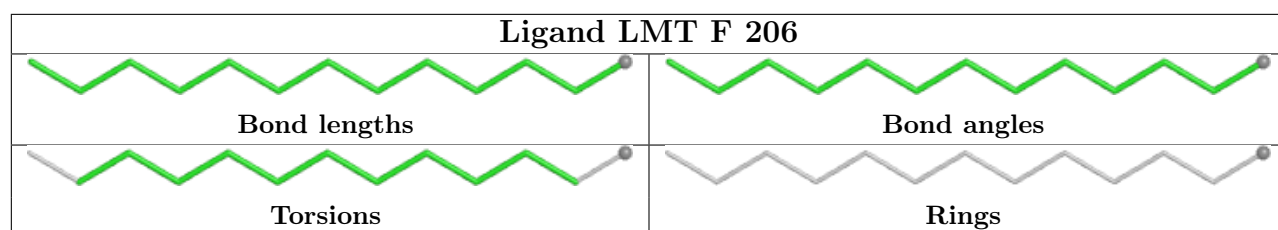
Bond angles

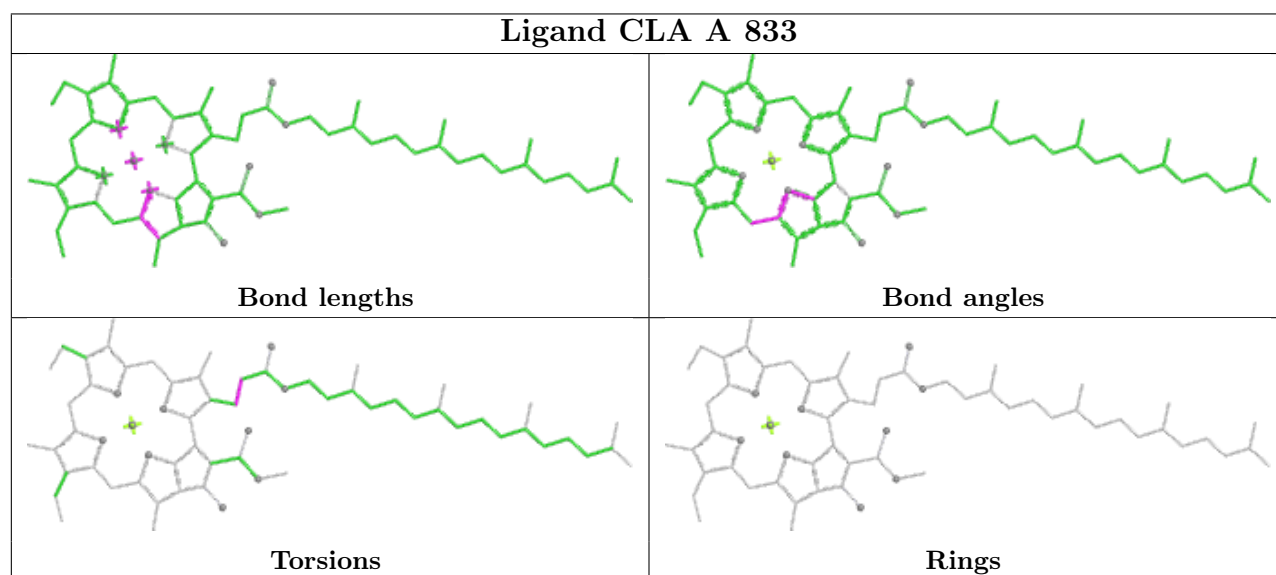
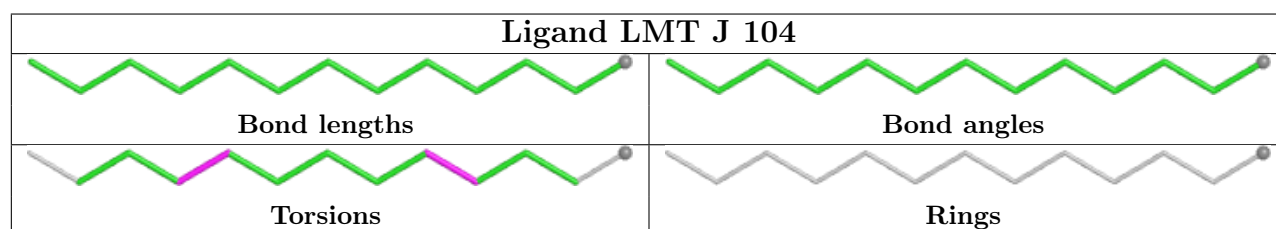
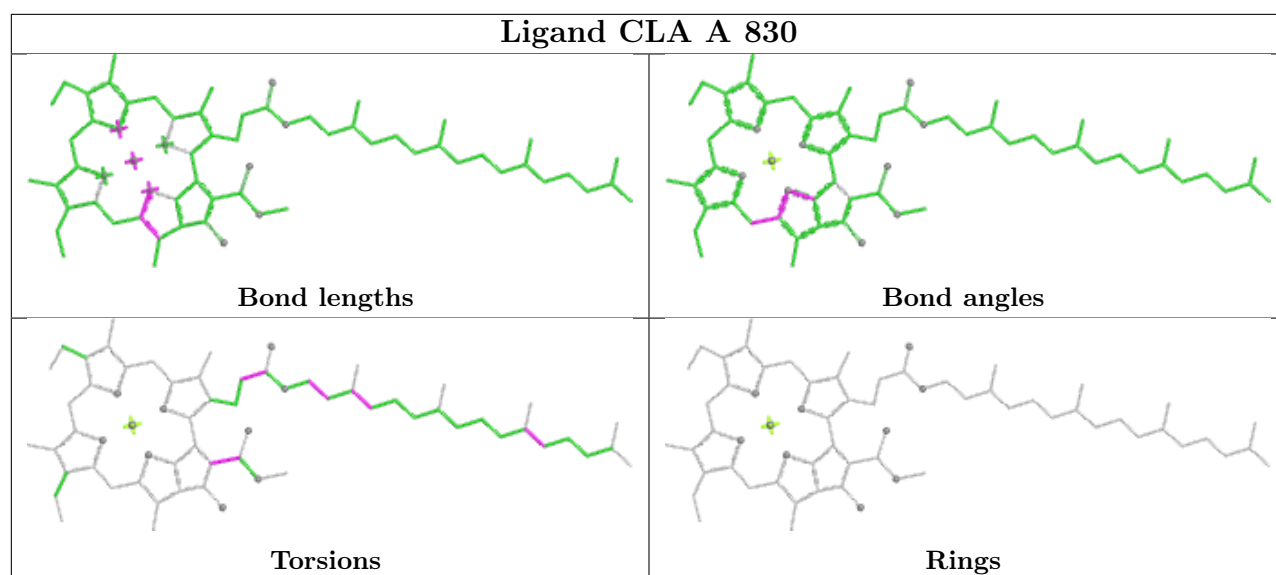


Torsions

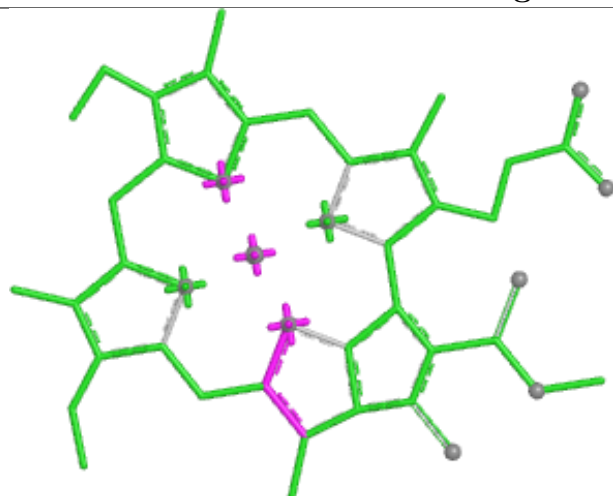


Rings

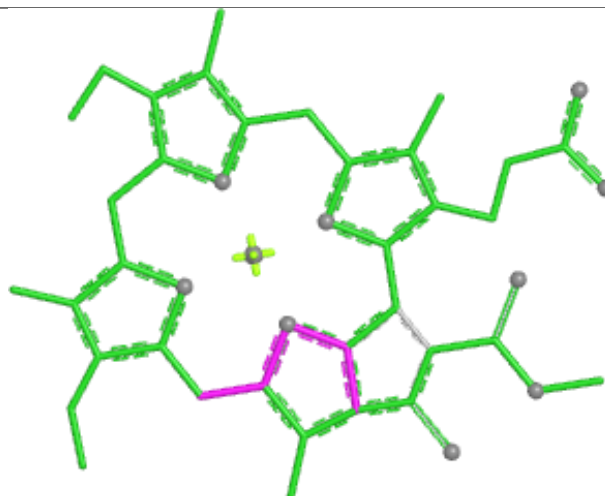




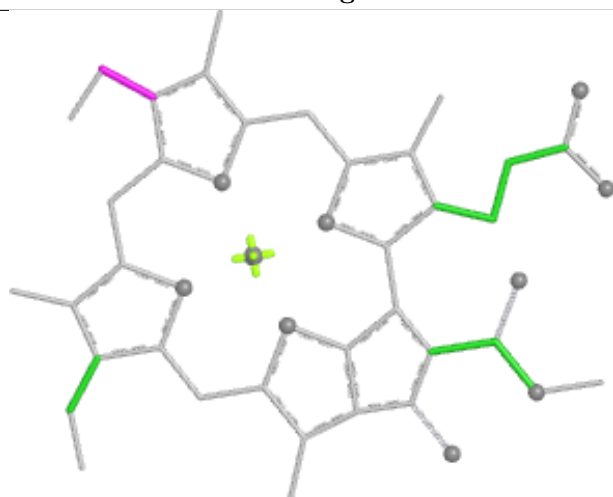
Ligand CLA A 821



Bond lengths



Bond angles

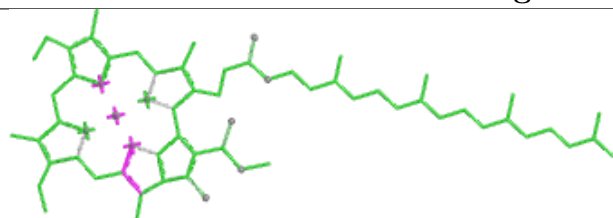


Torsions

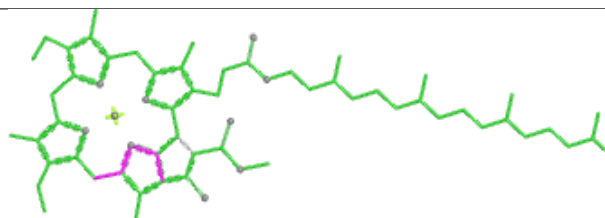


Rings

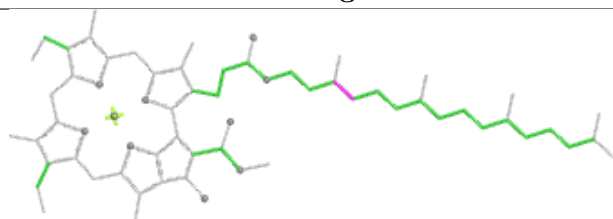
Ligand CLA A 822



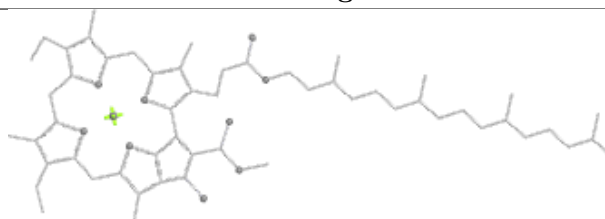
Bond lengths



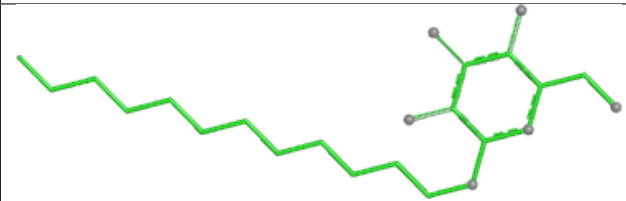
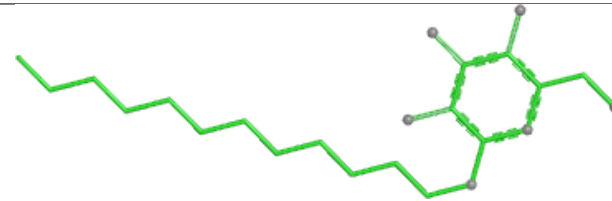
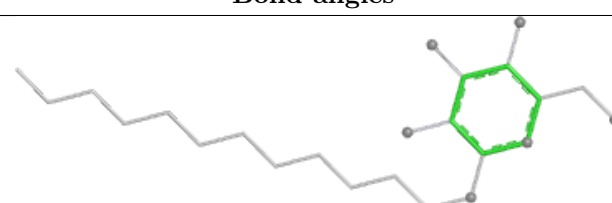
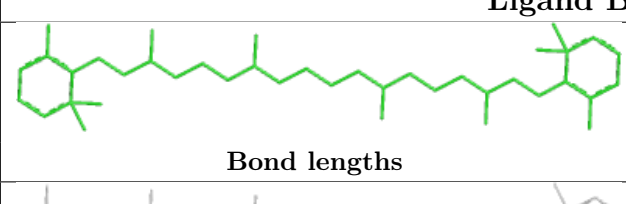
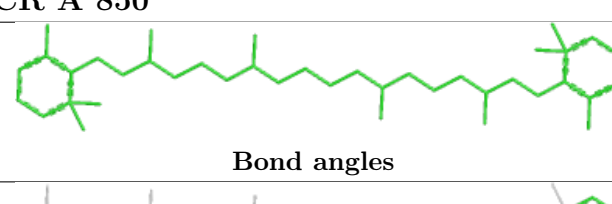
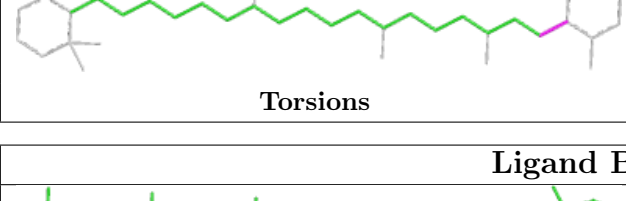
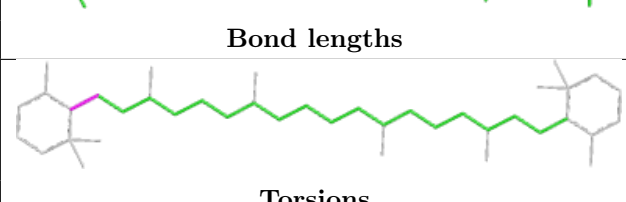
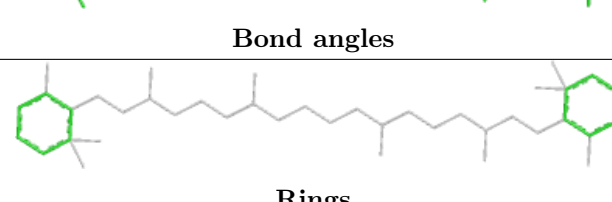
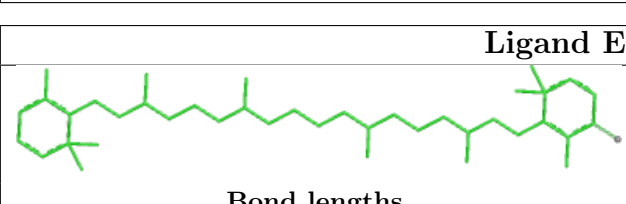
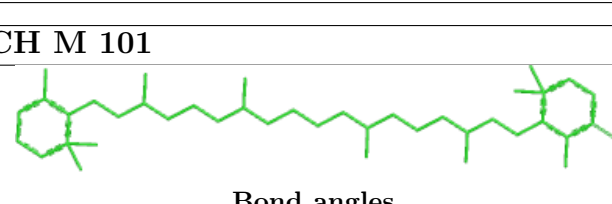
Bond angles

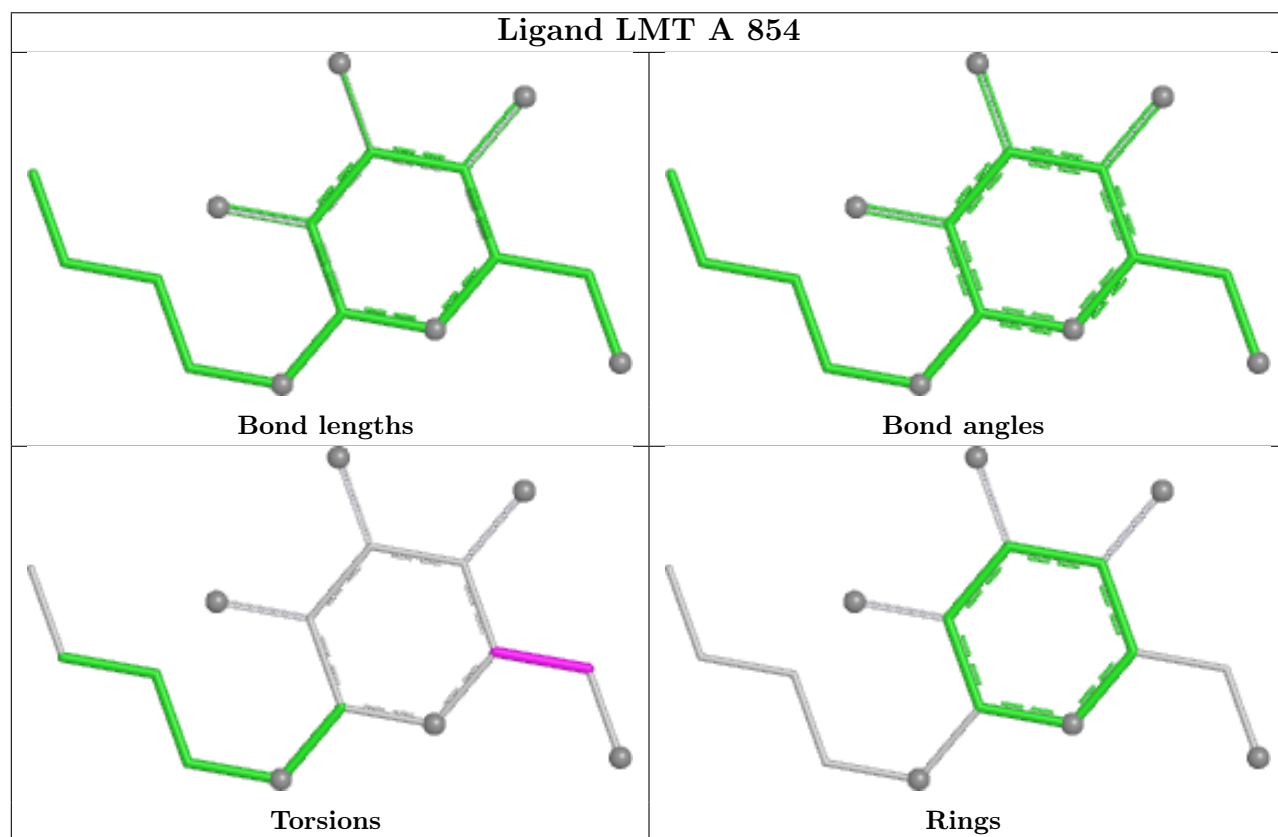
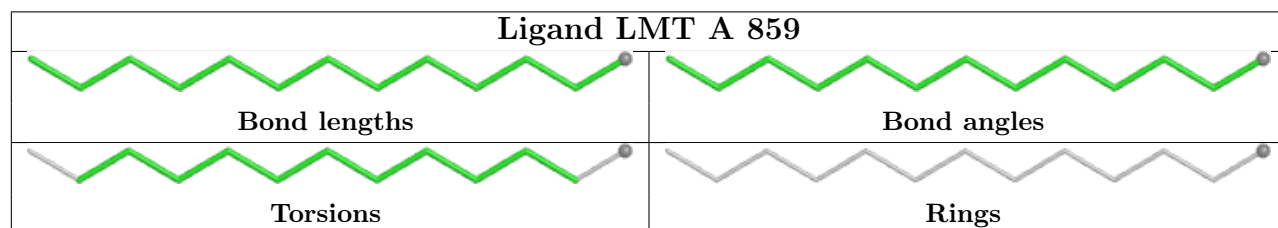
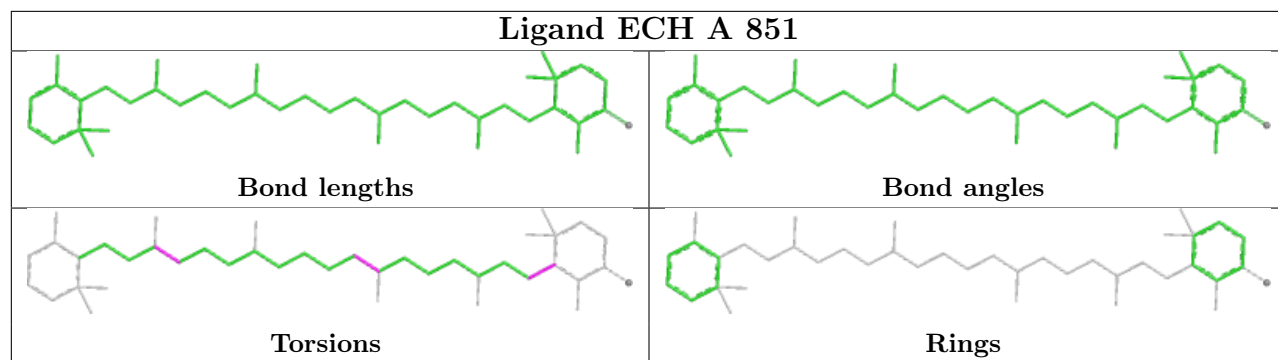


Torsions

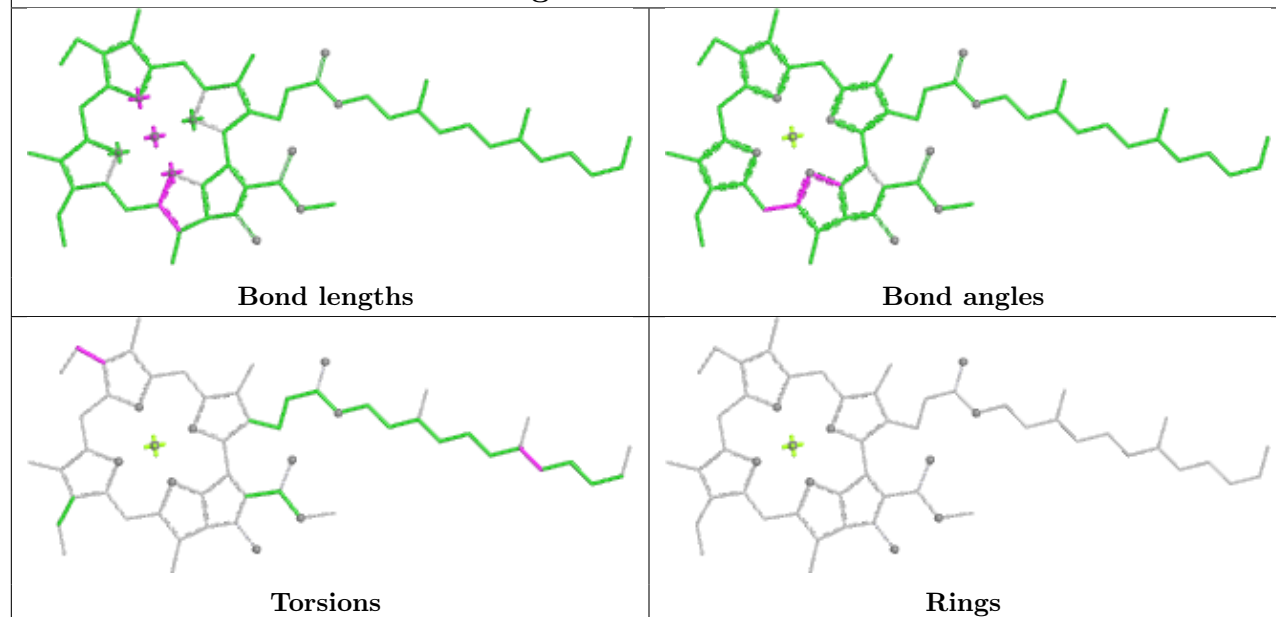


Rings

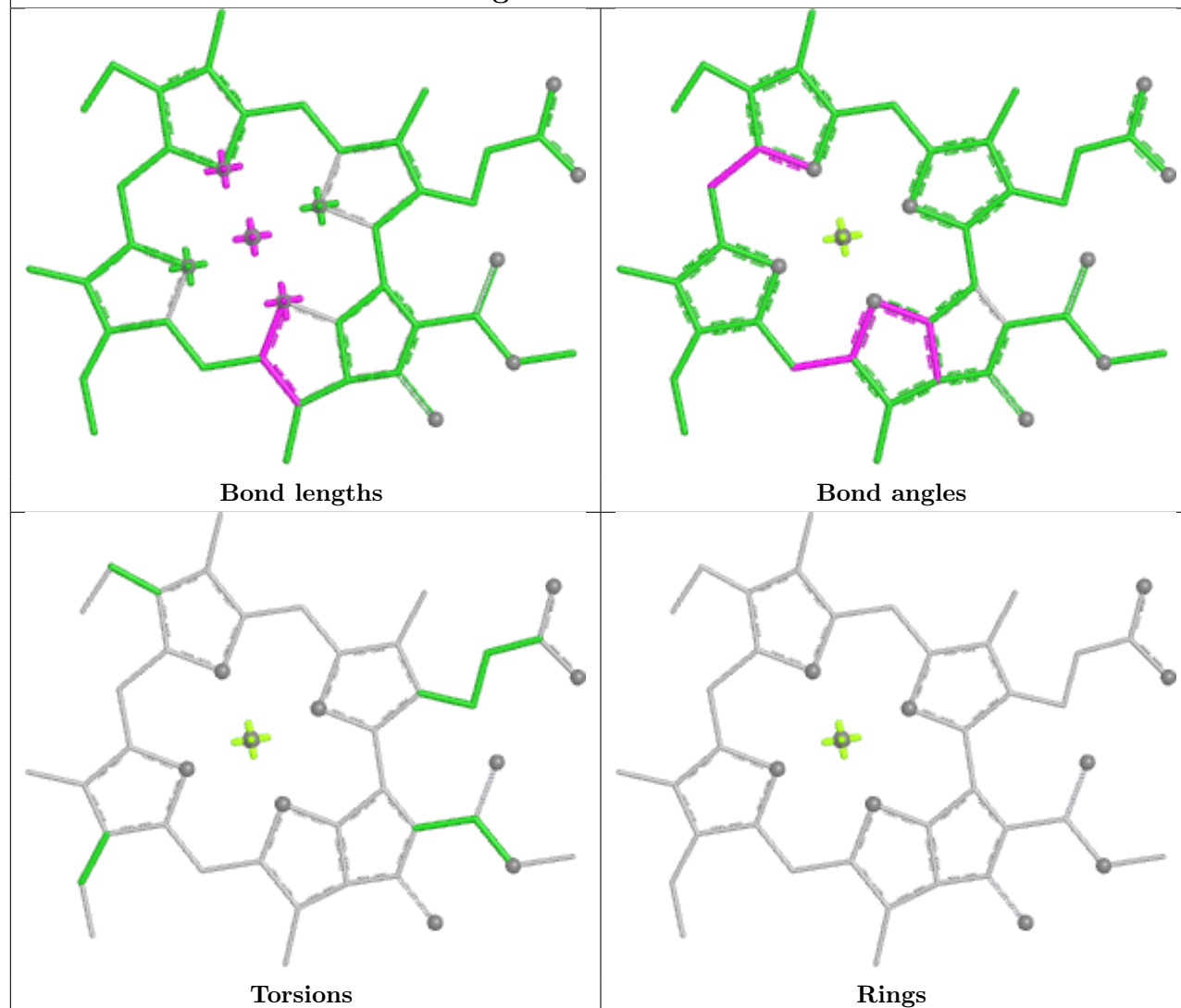
Ligand LMT B 853	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ECH M 101	
 Bond lengths	 Bond angles
Torsions	Rings

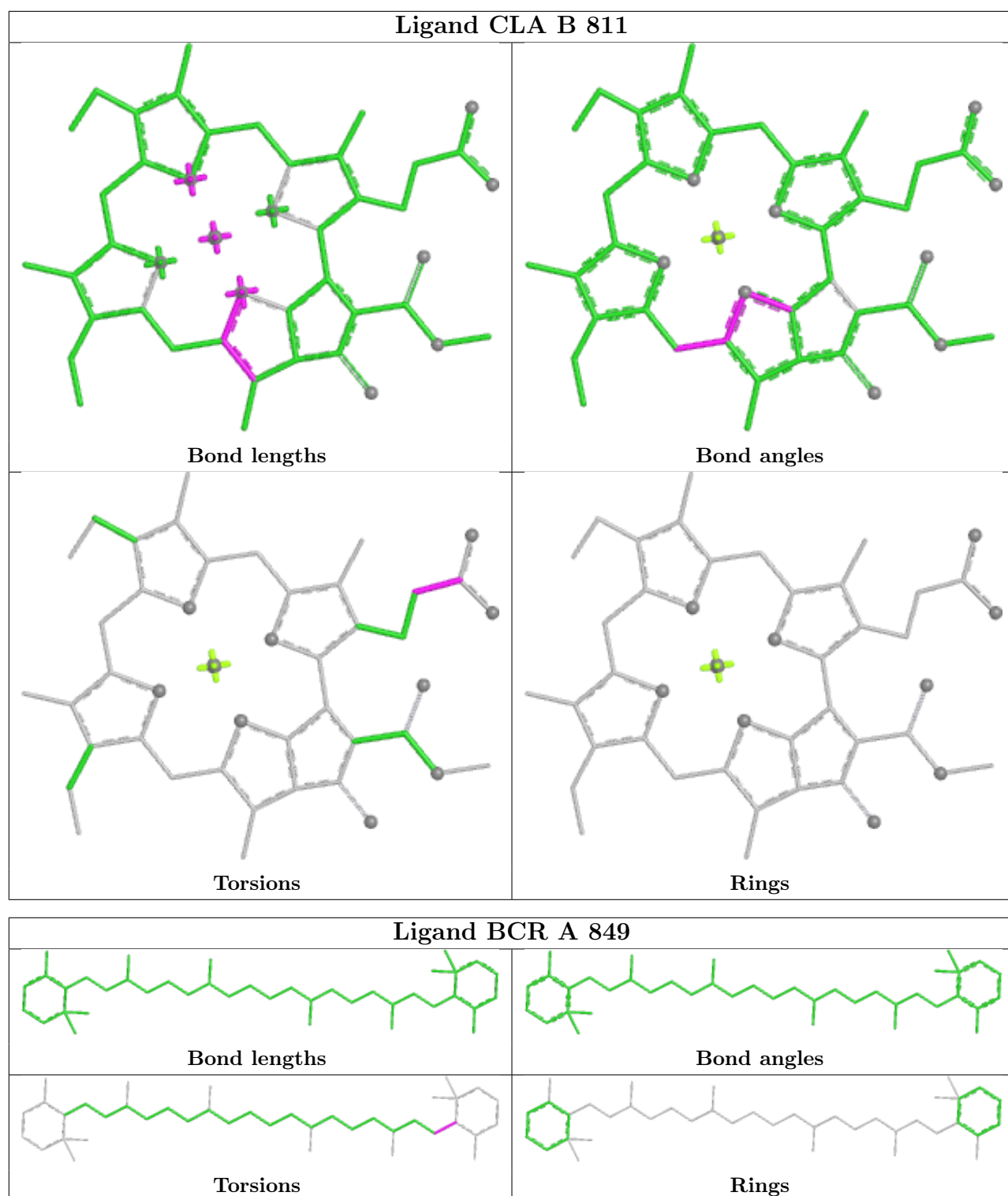


Ligand CLA A 829

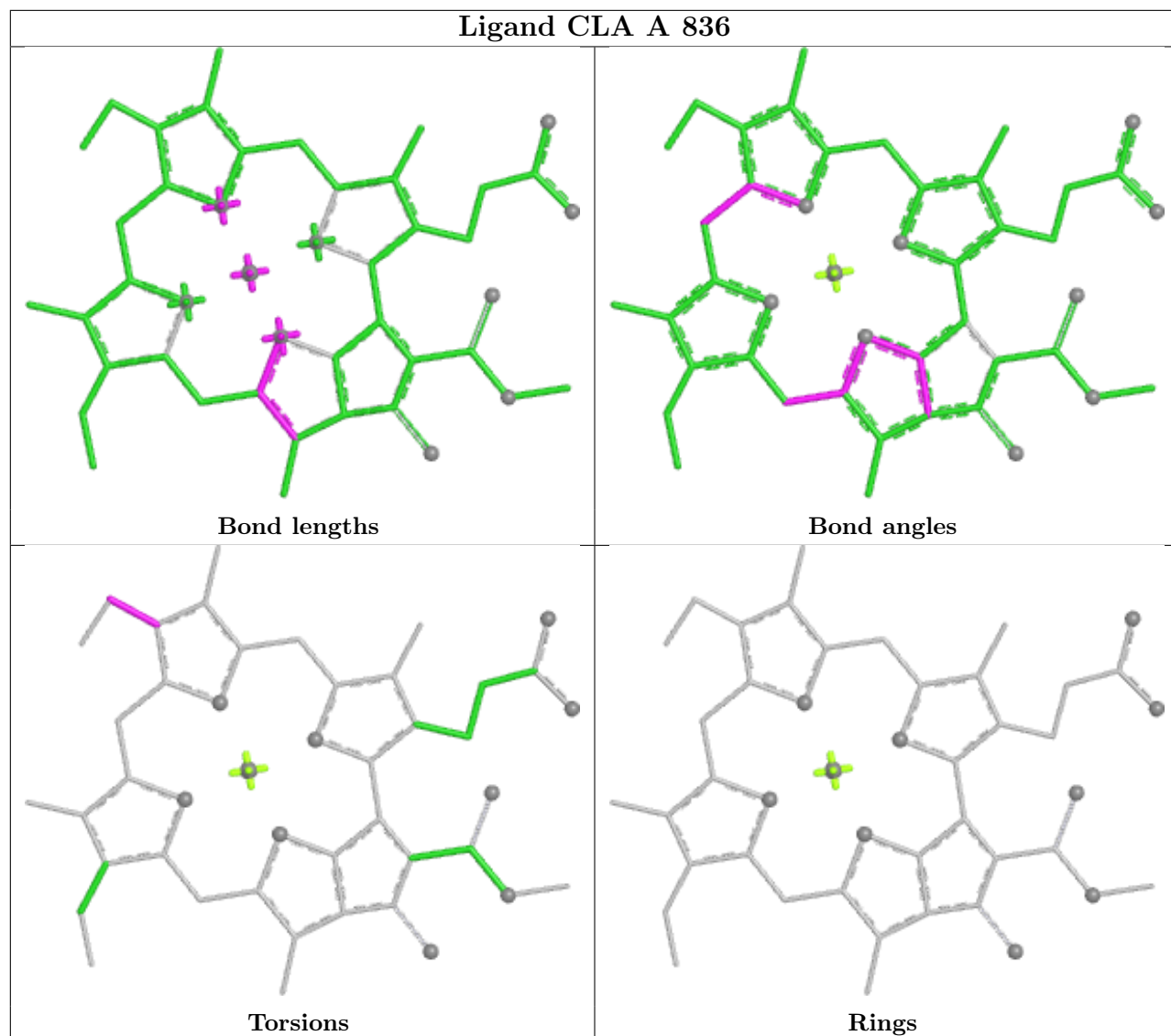


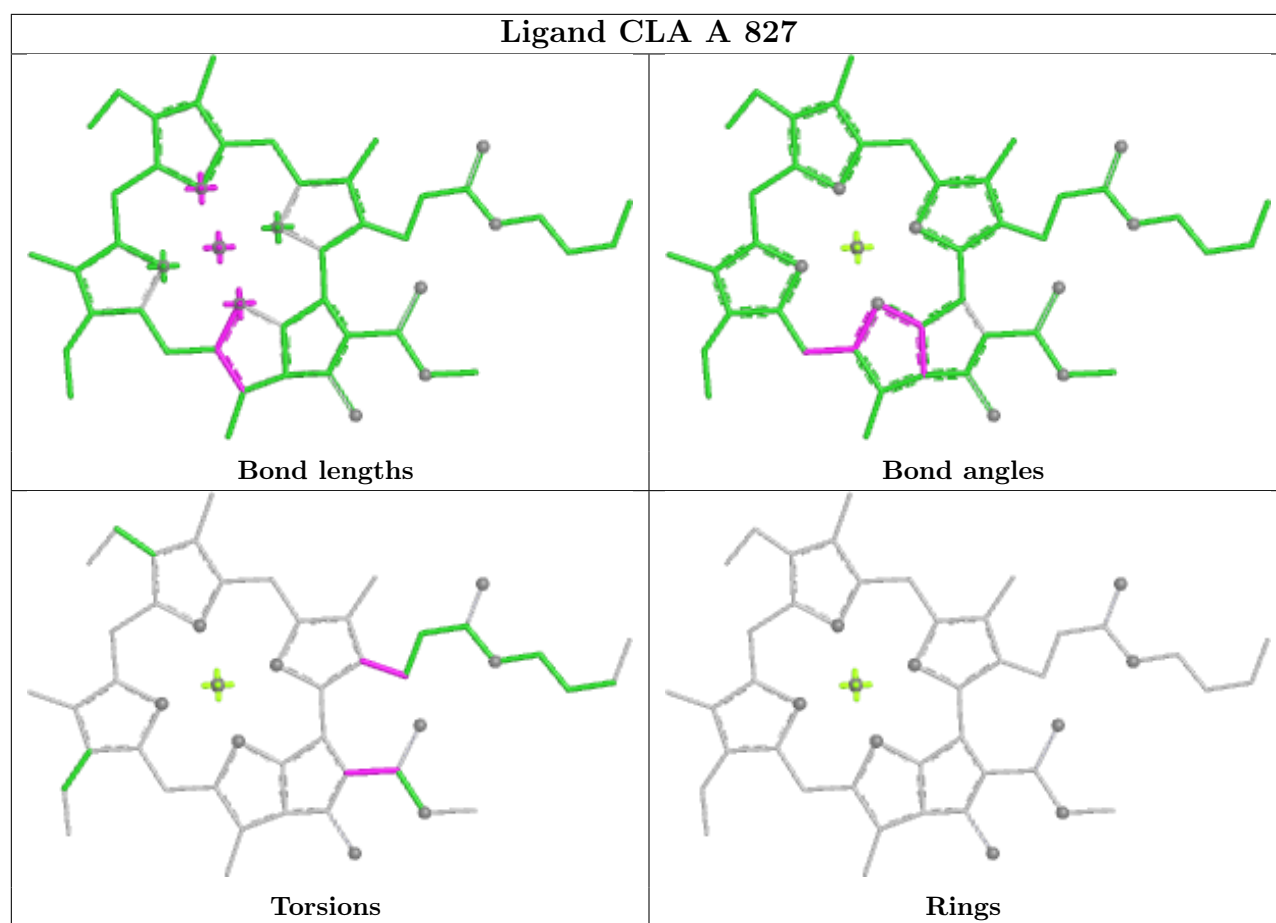
Ligand CLA B 832



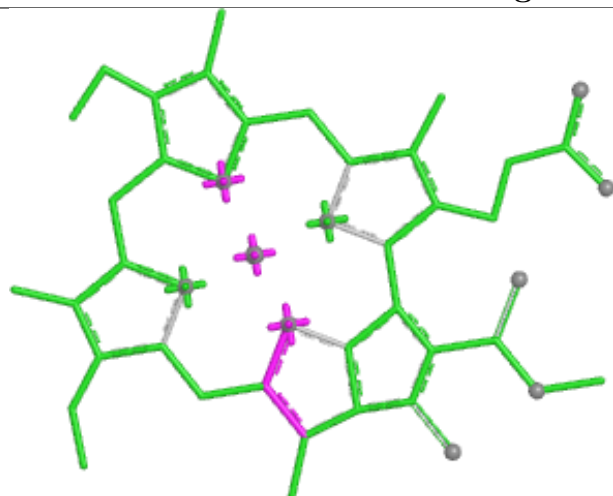


Ligand CLA A 836

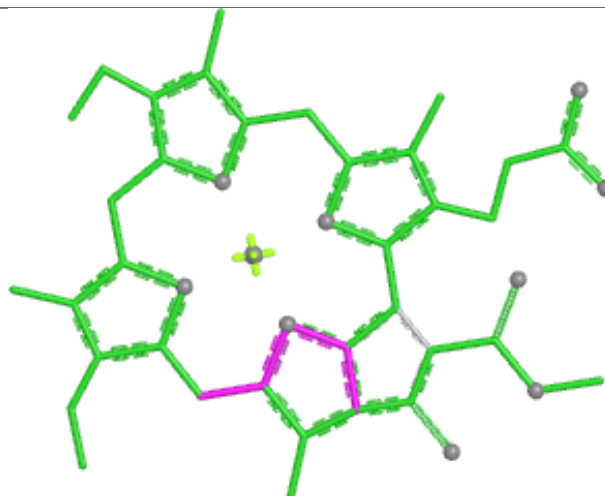




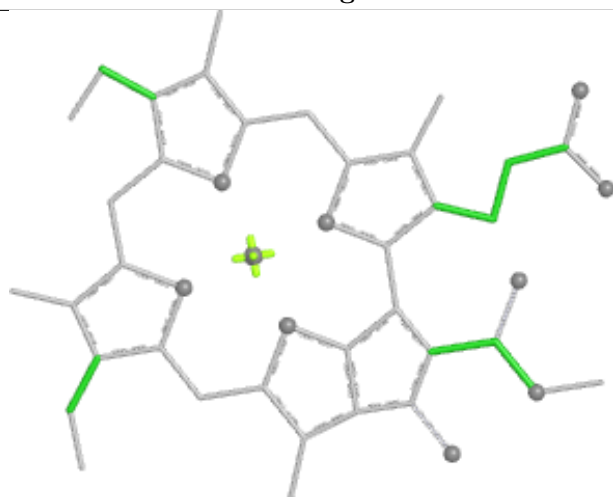
Ligand CLA B 817



Bond lengths



Bond angles

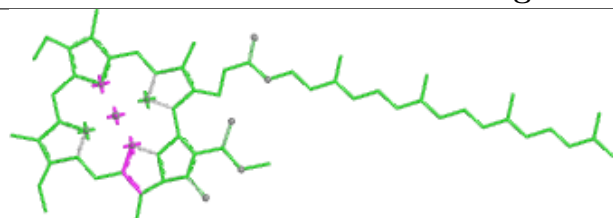


Torsions

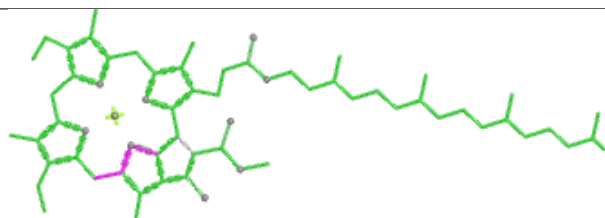


Rings

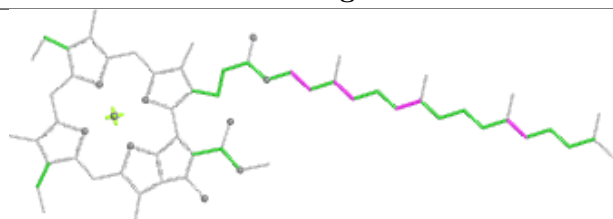
Ligand CLA A 816



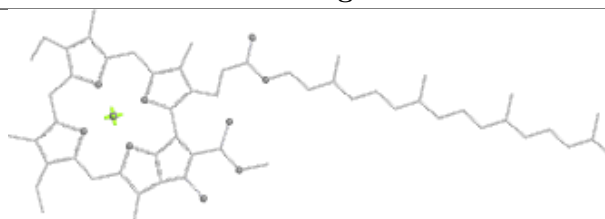
Bond lengths



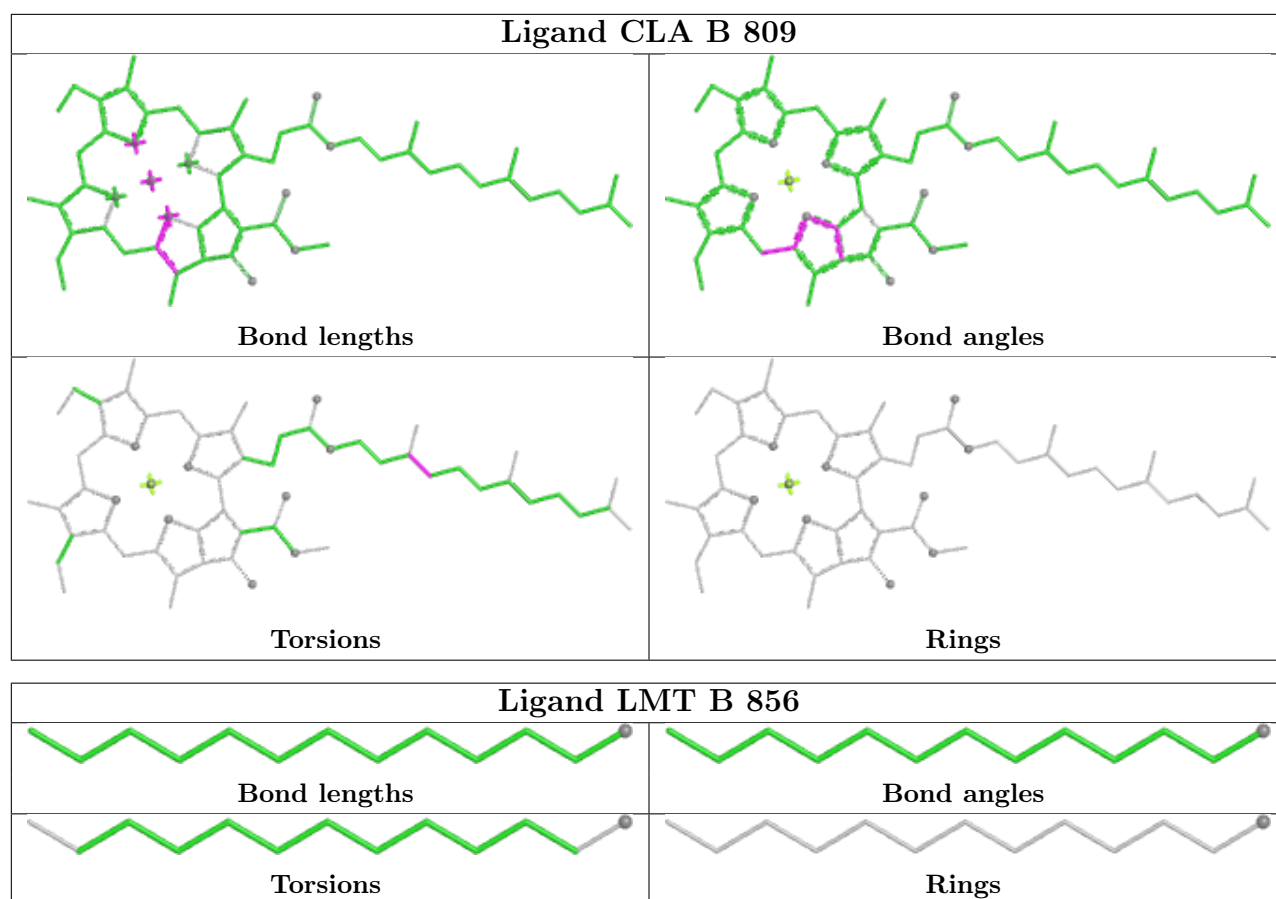
Bond angles

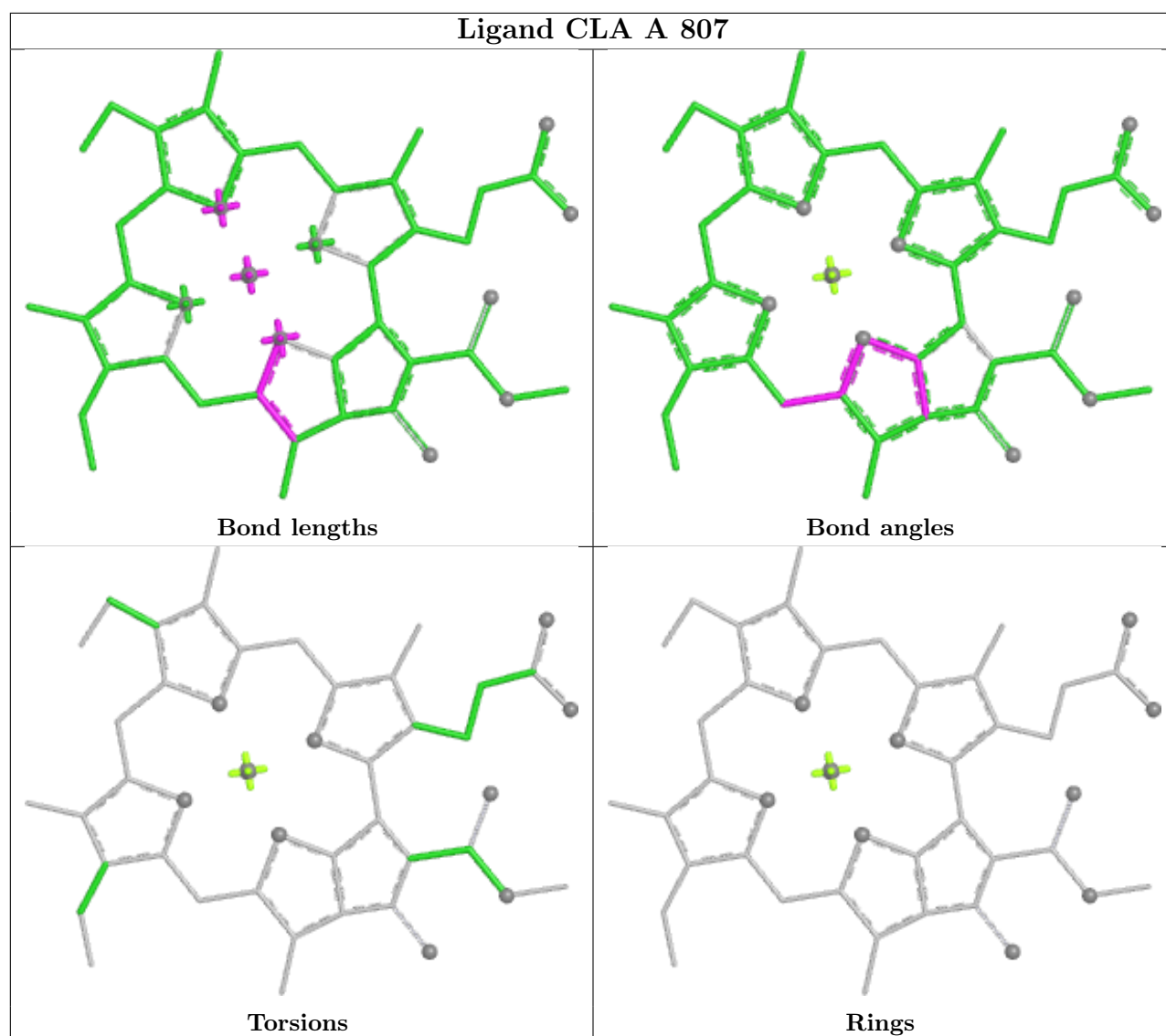


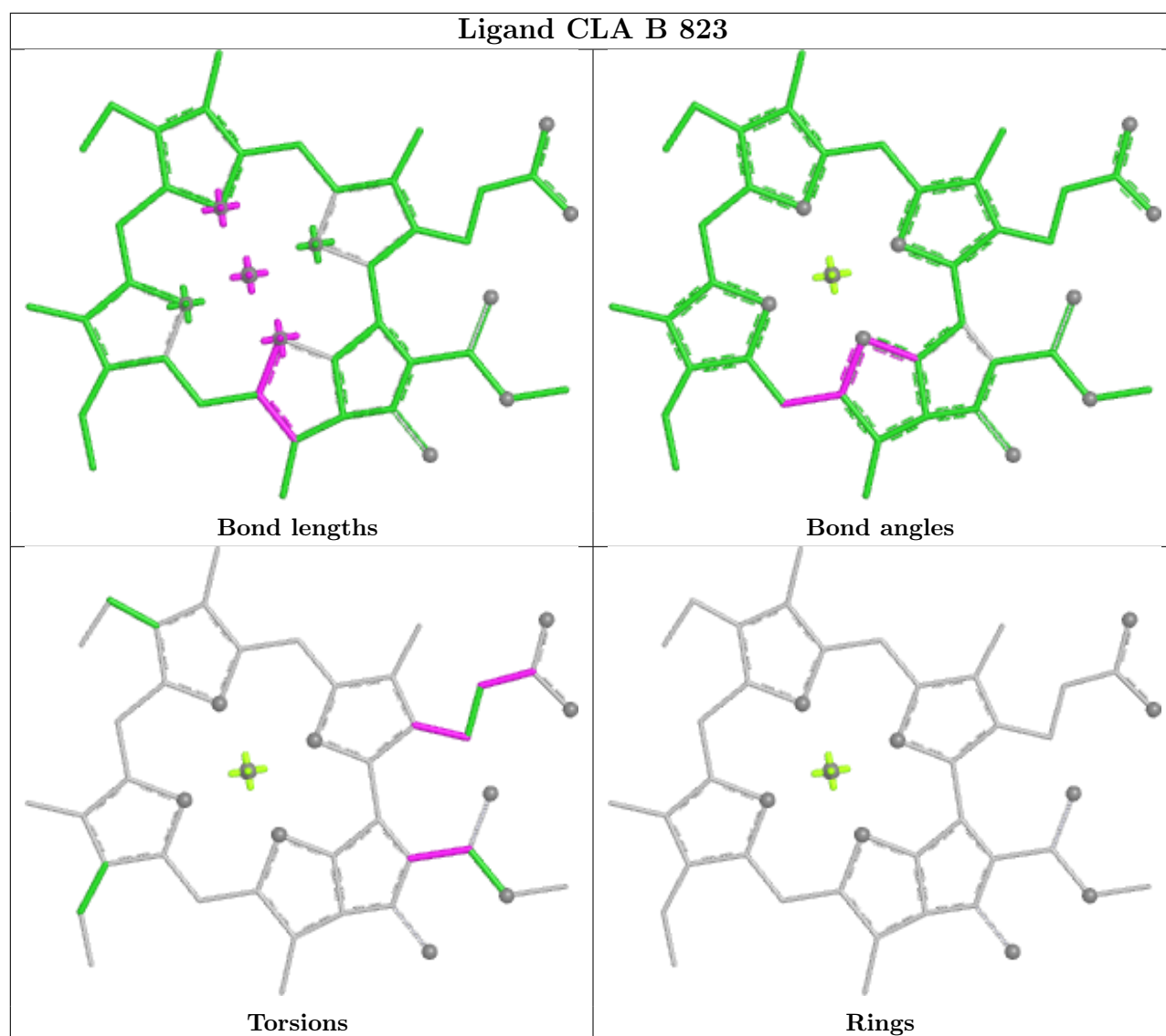
Torsions

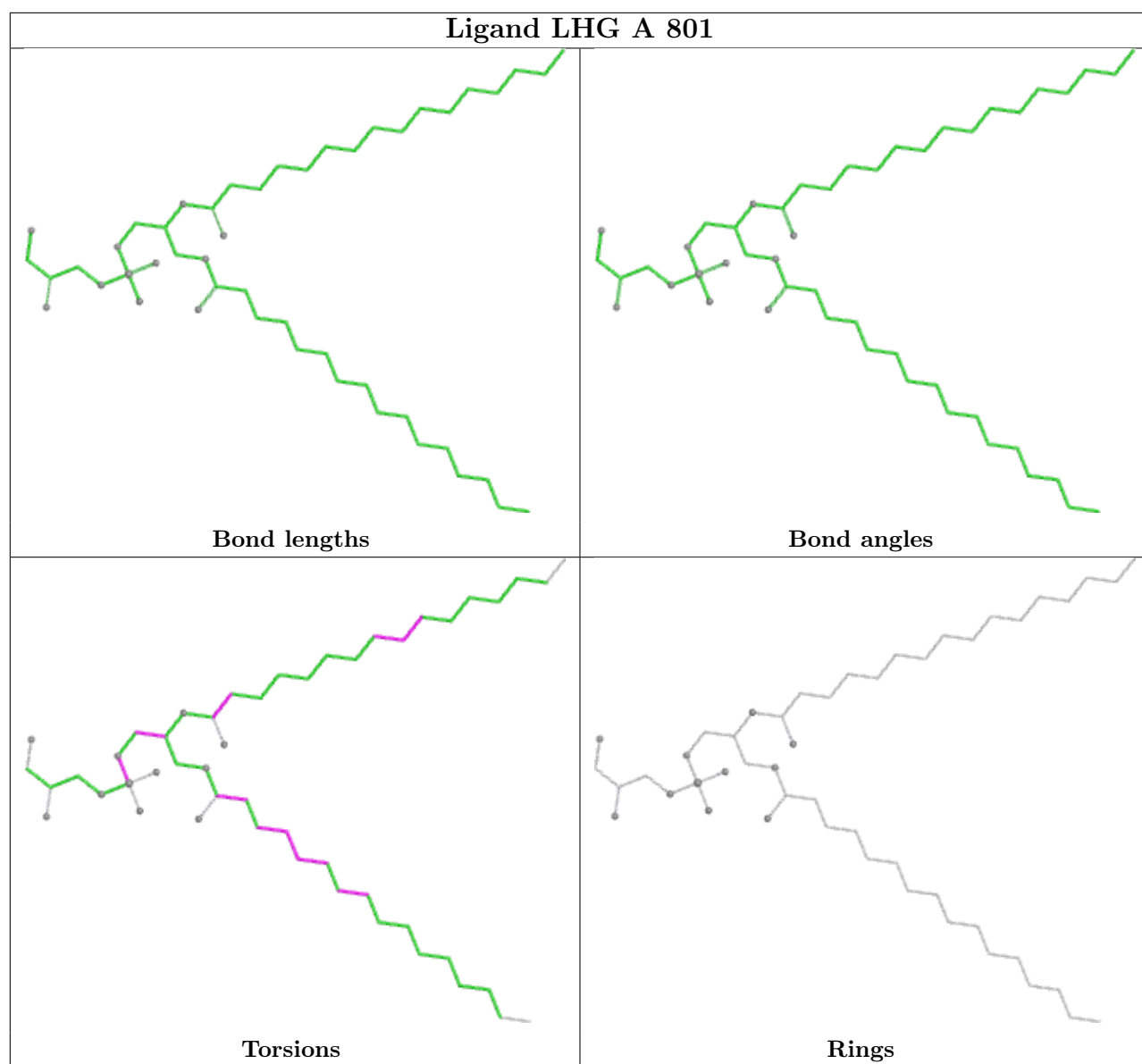


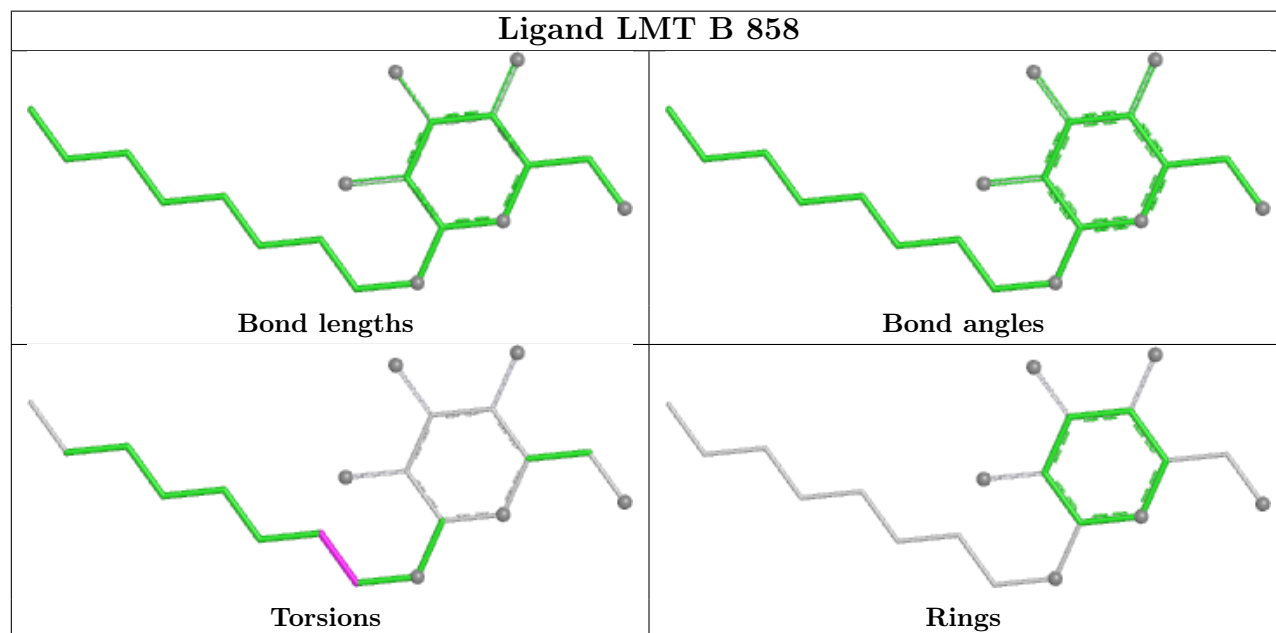
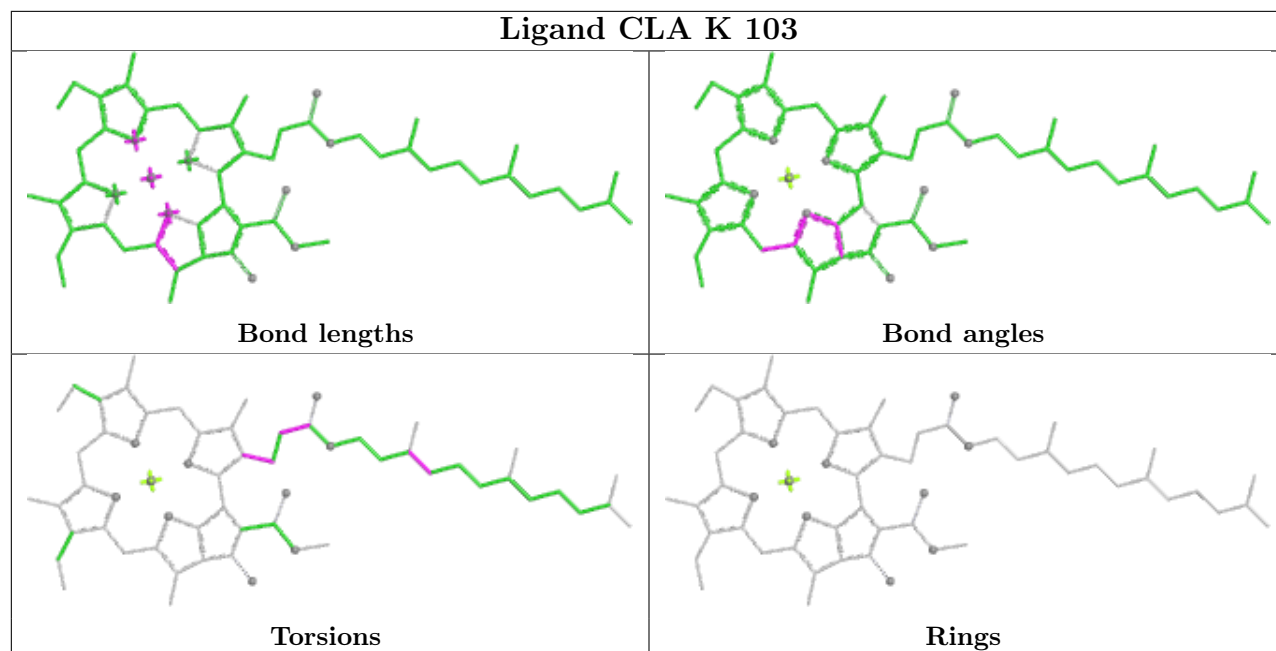
Rings

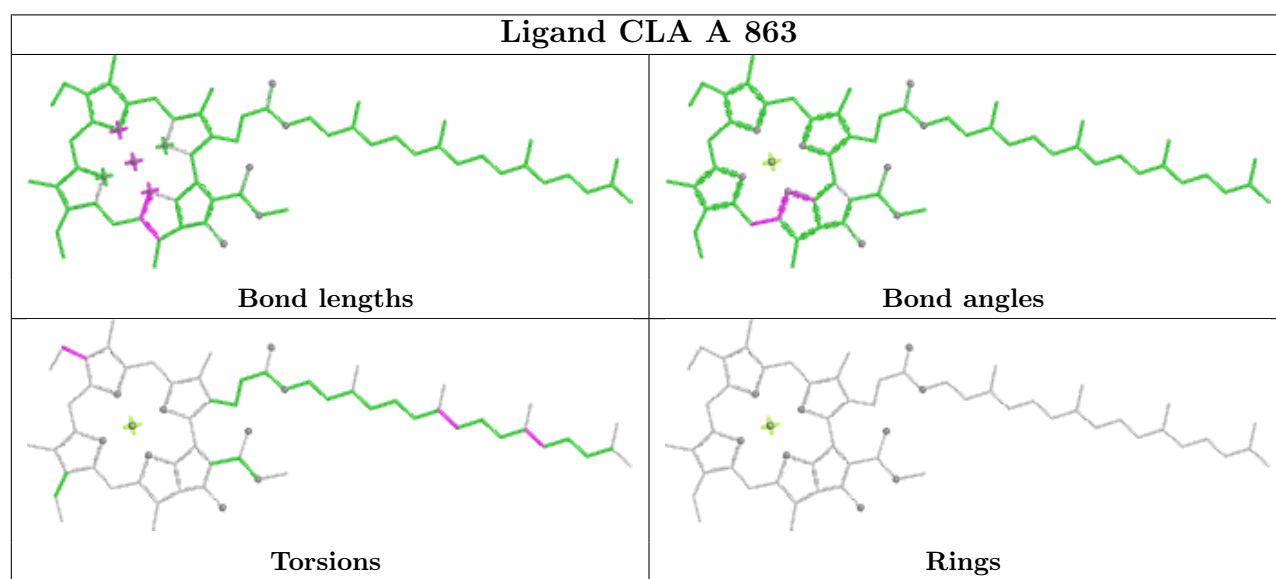
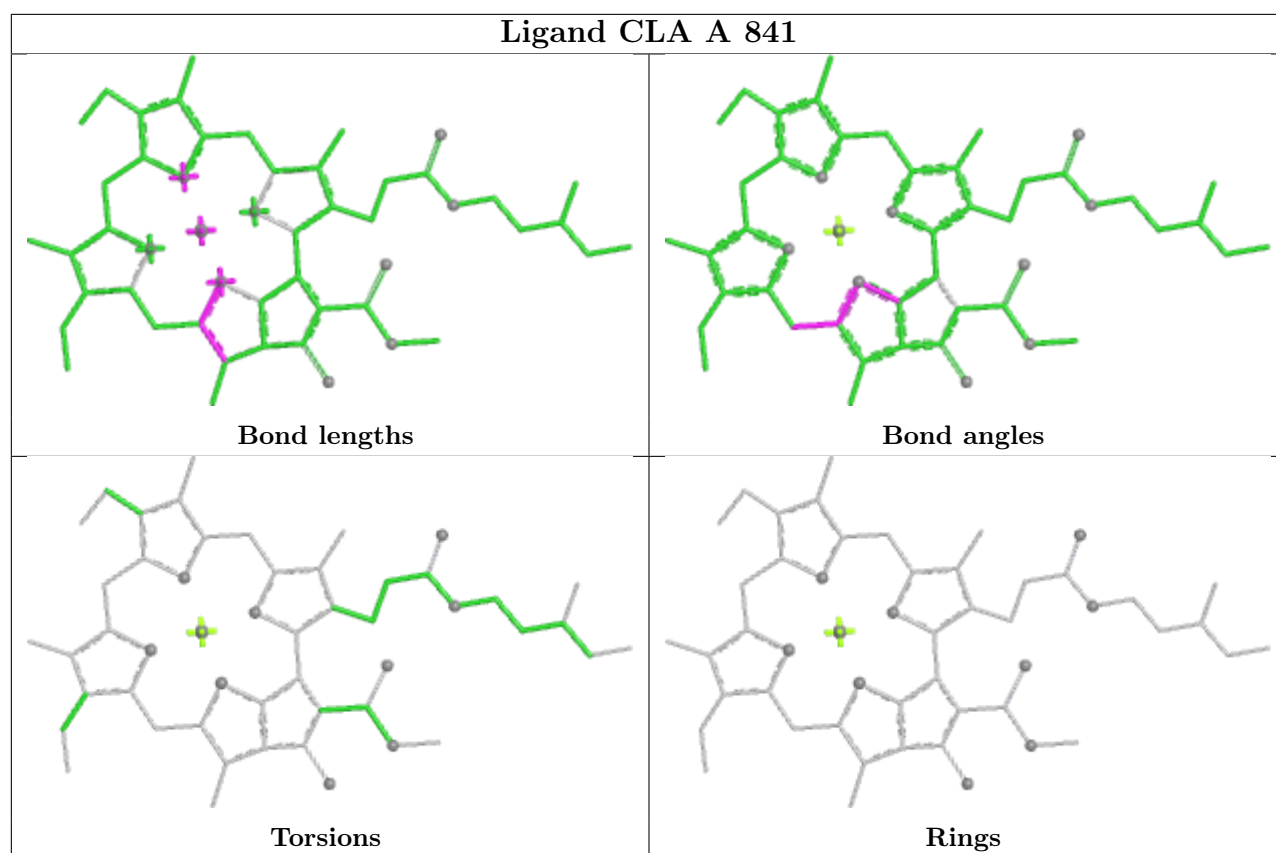


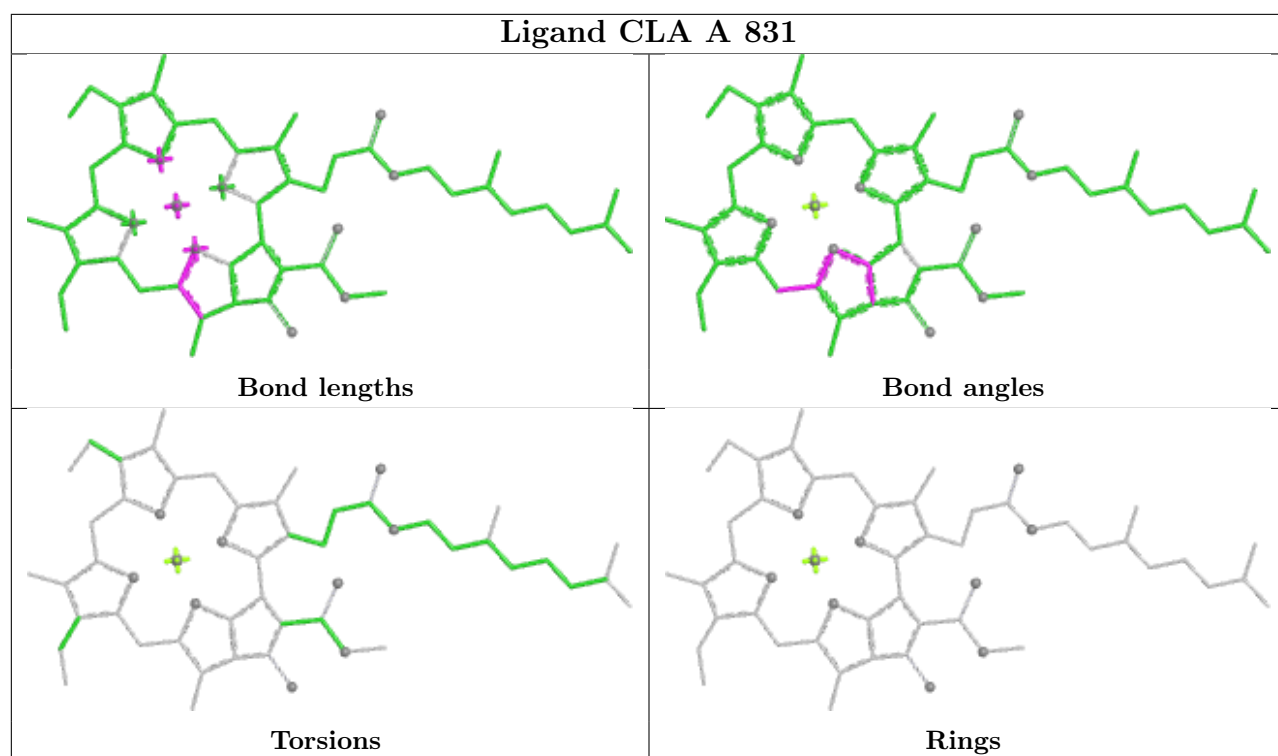


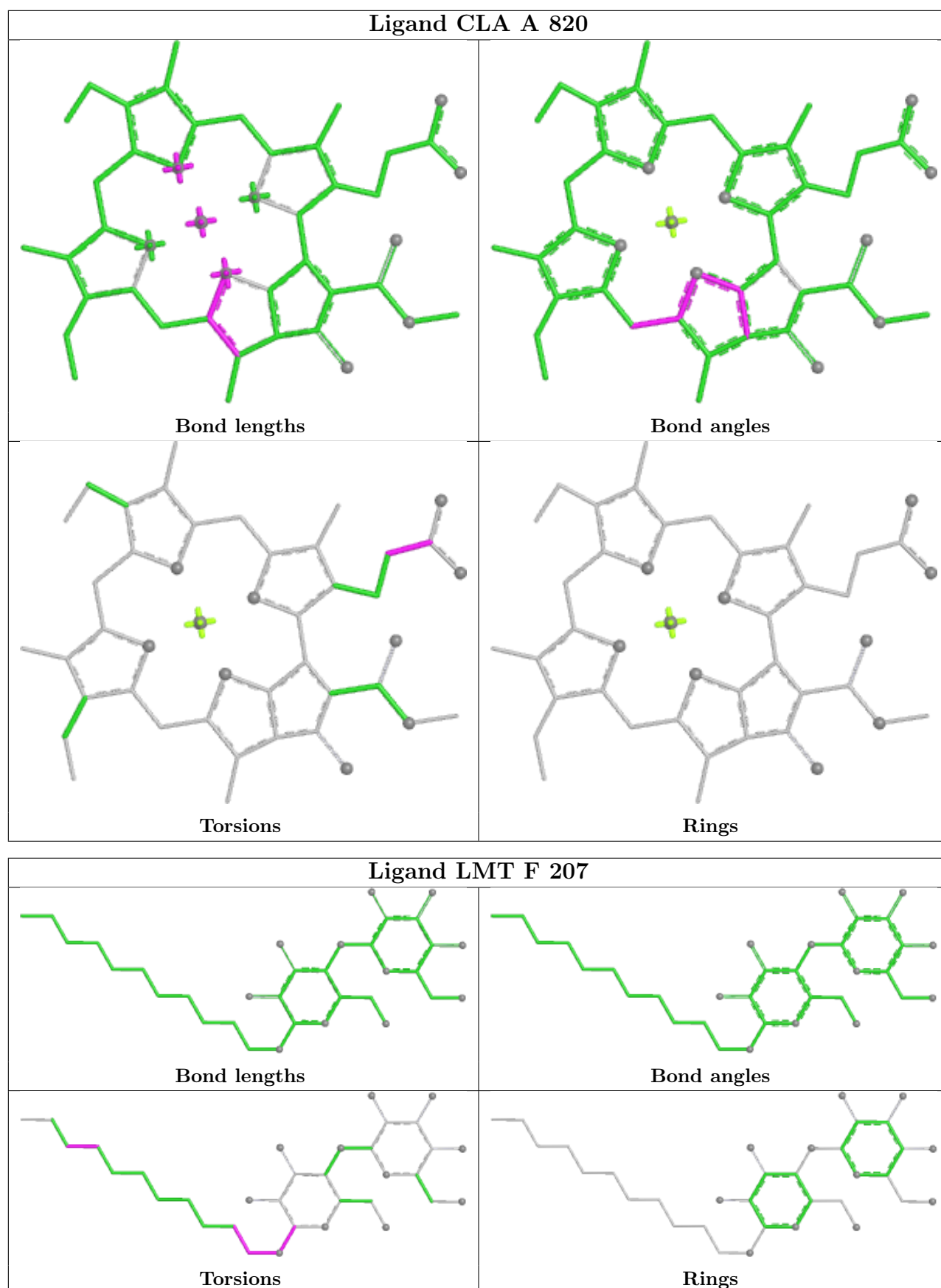


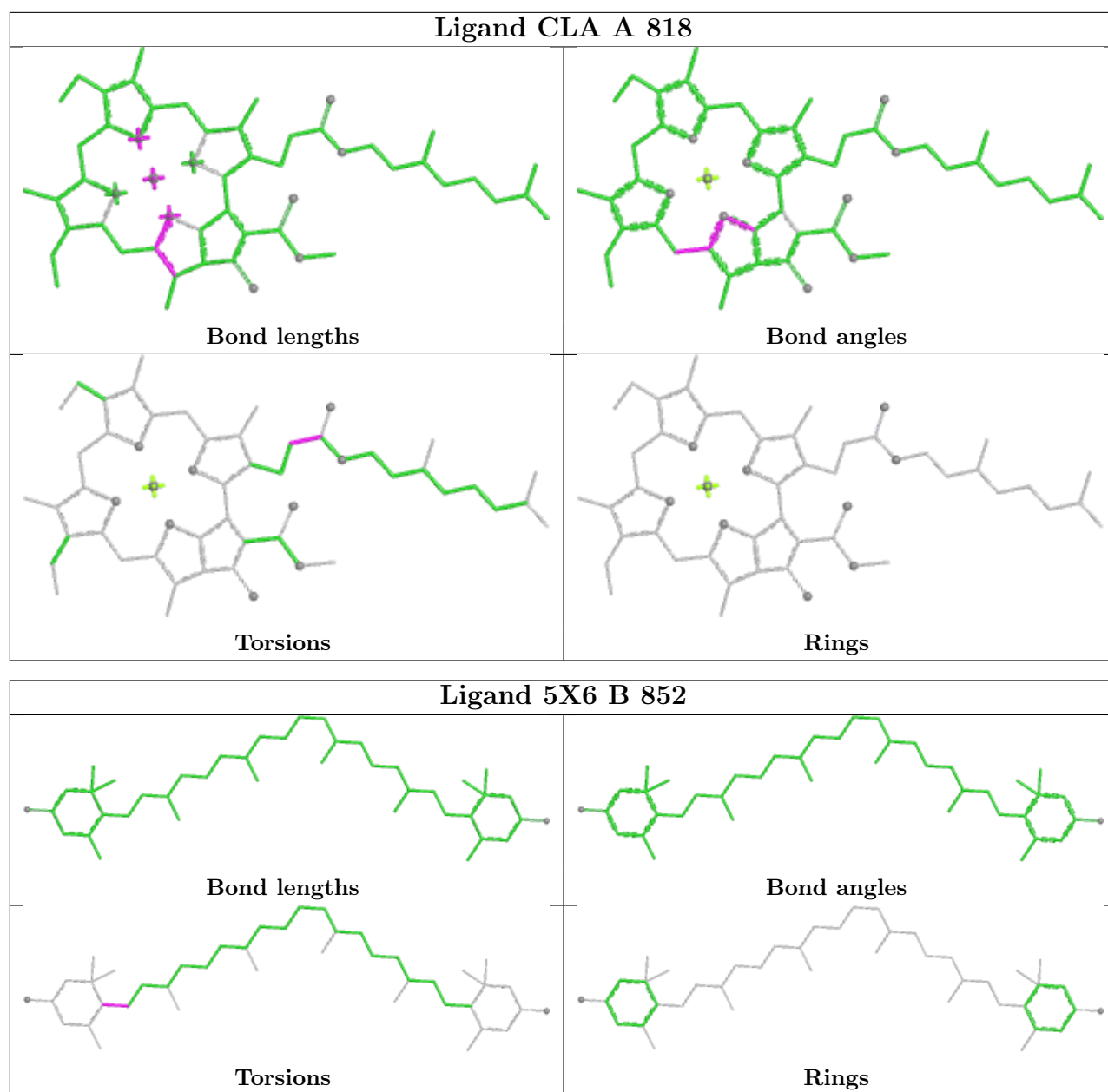


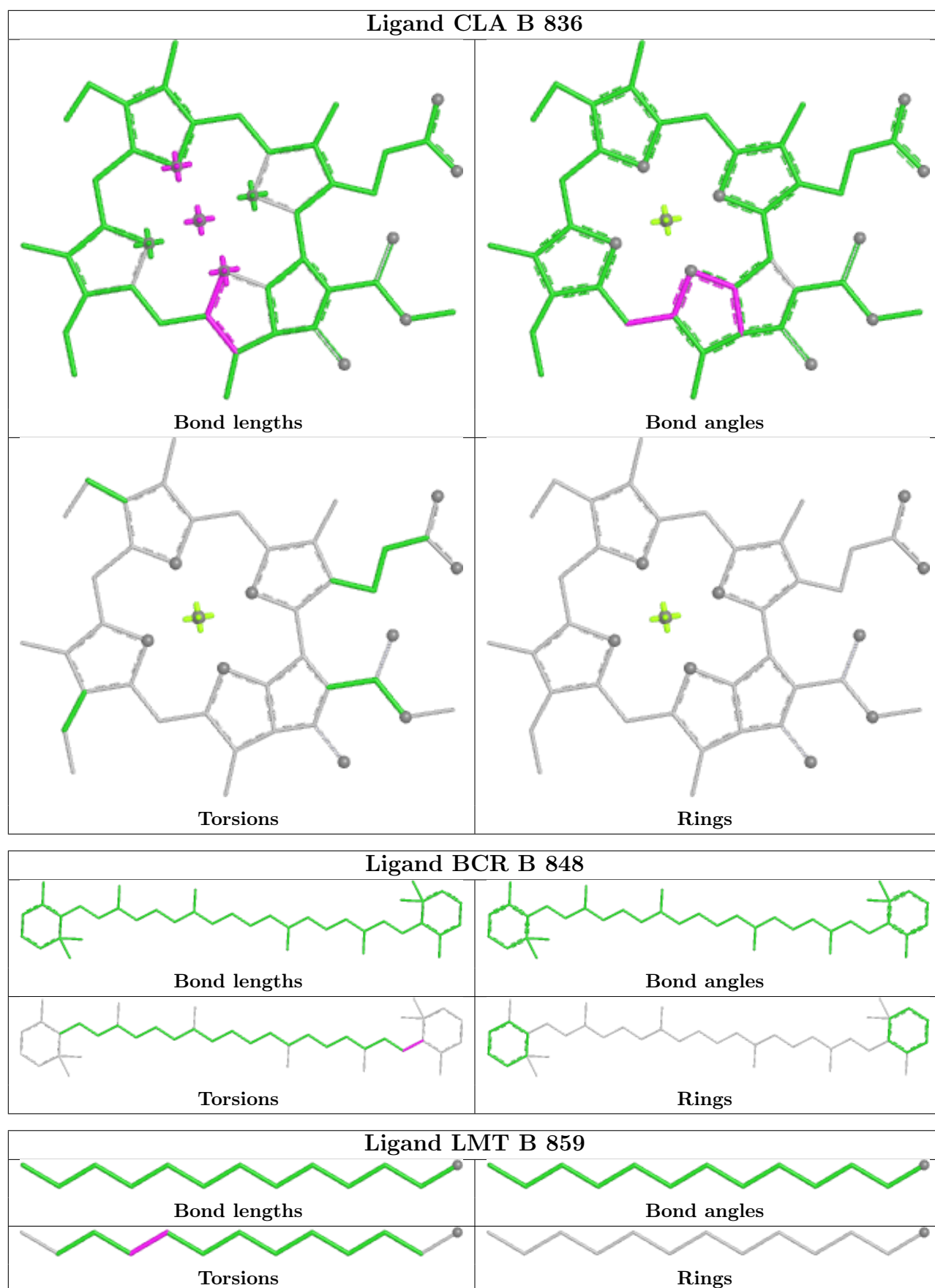




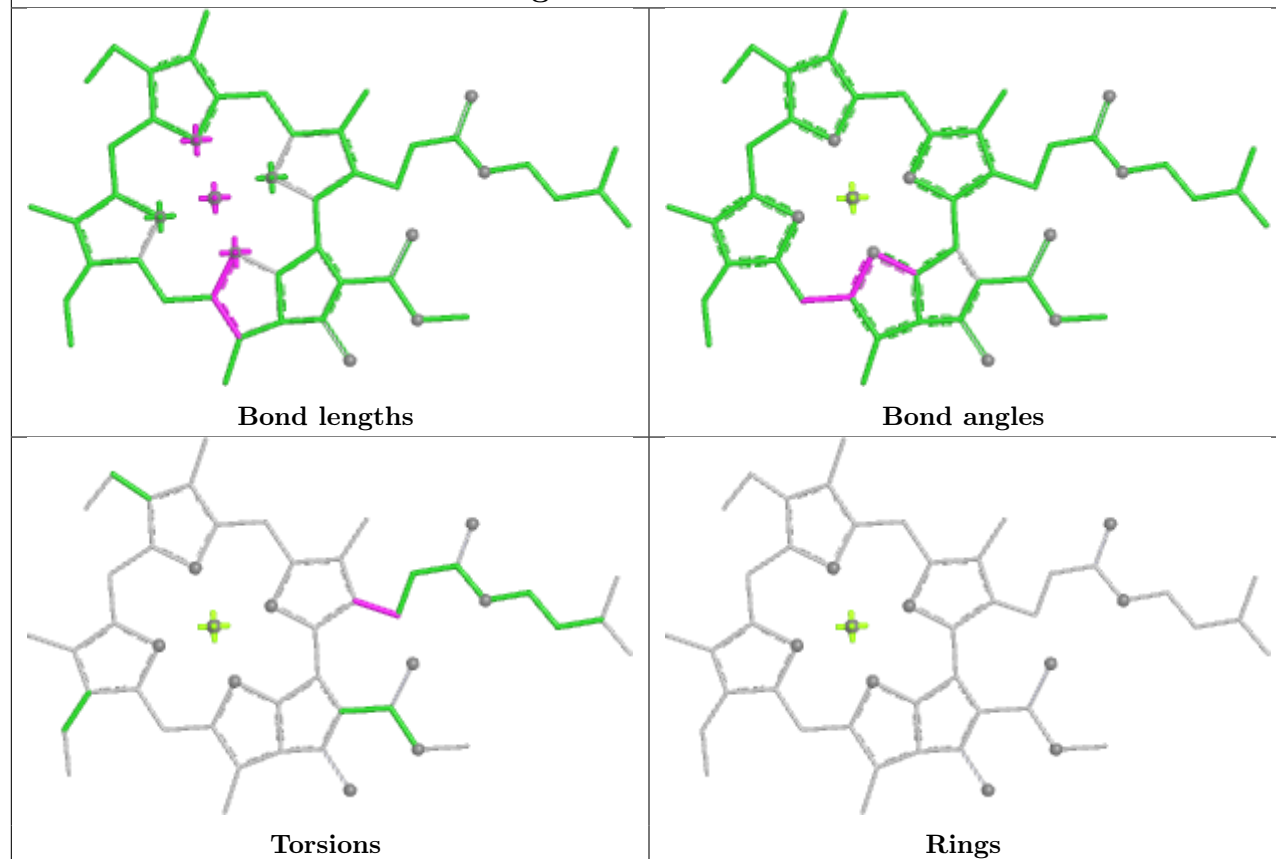




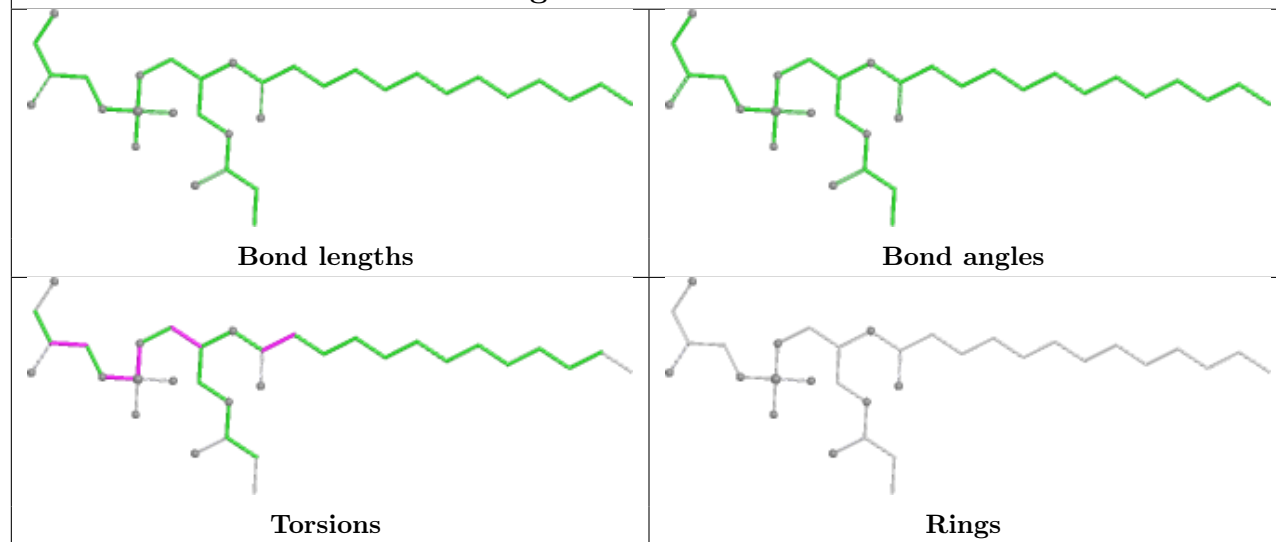


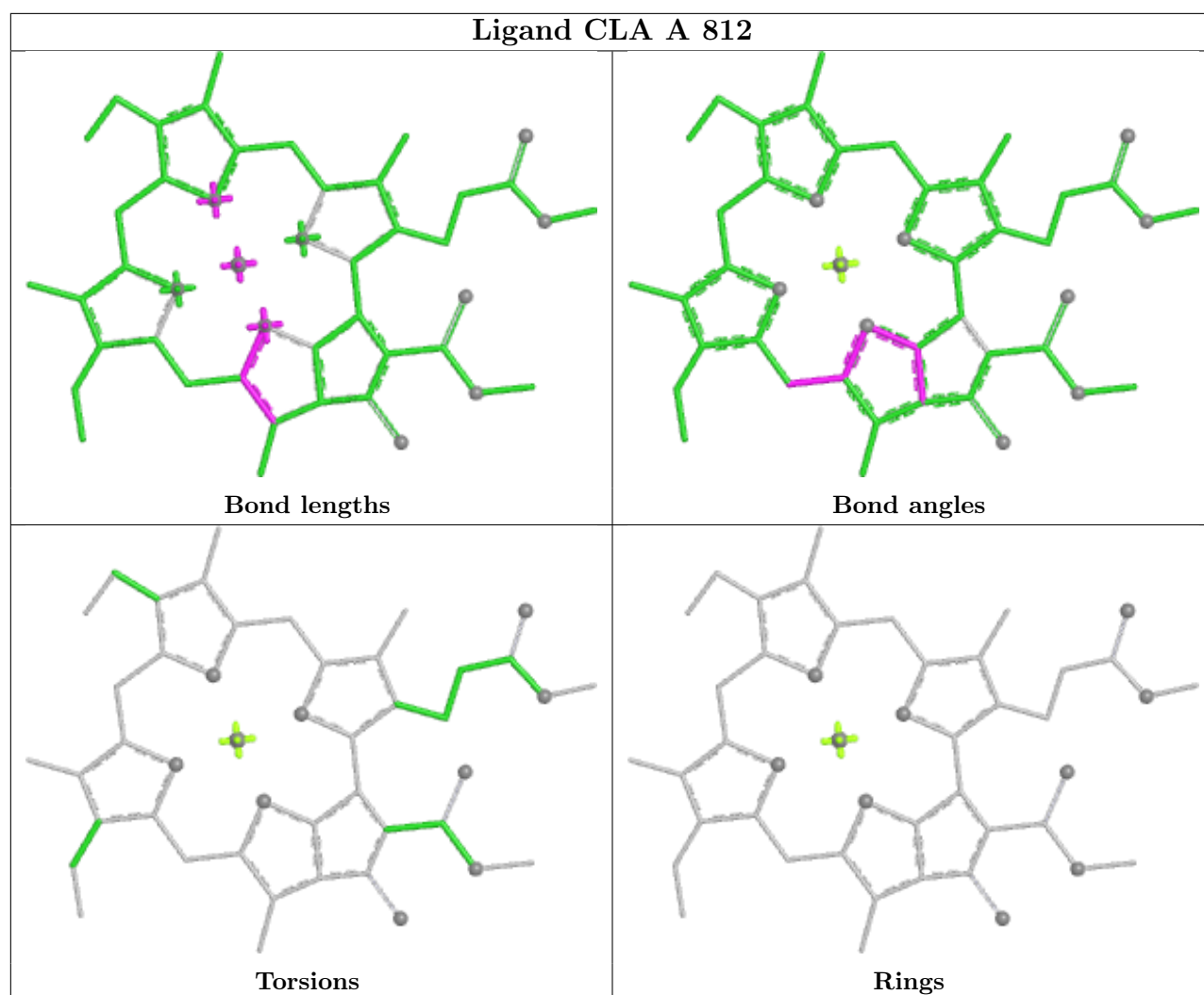


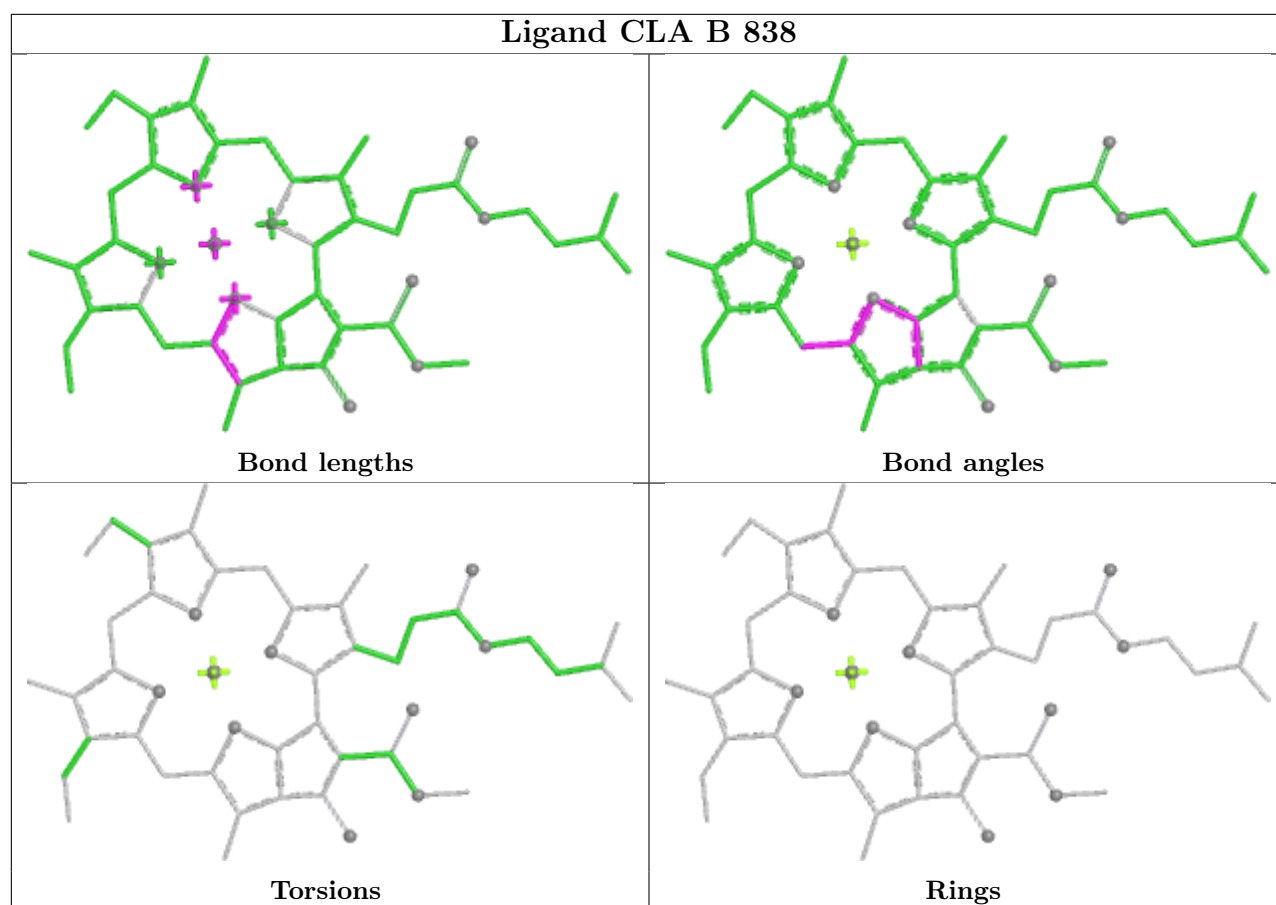
Ligand CLA A 814



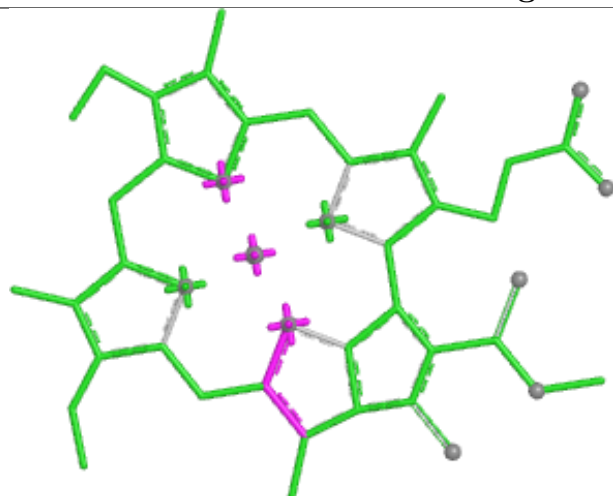
Ligand LHG A 802



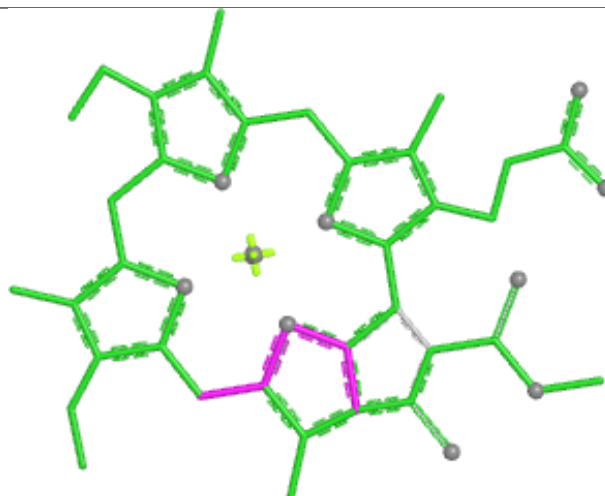




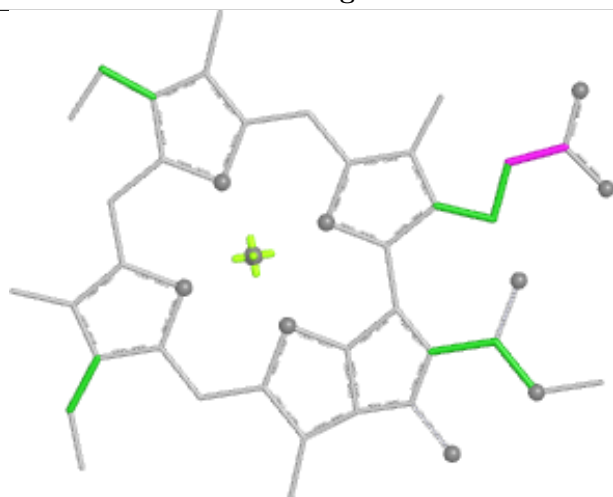
Ligand CLA J 102



Bond lengths



Bond angles

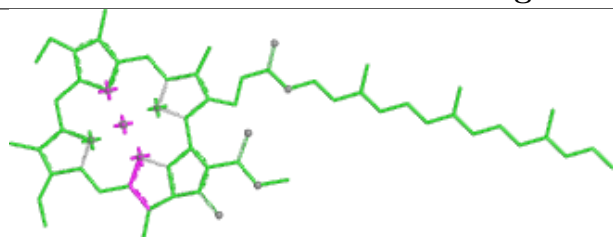


Torsions

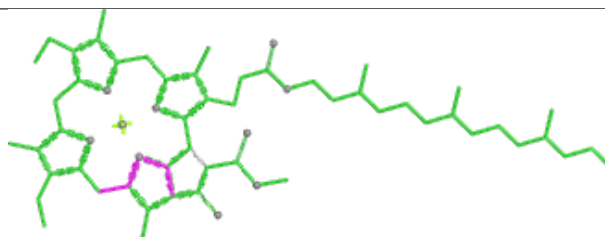


Rings

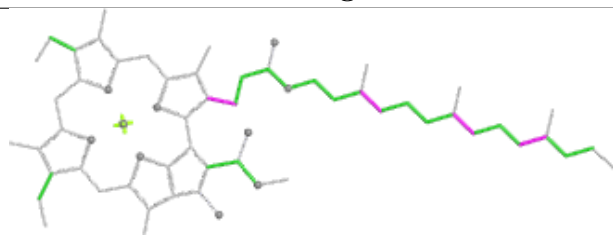
Ligand CLA B 822



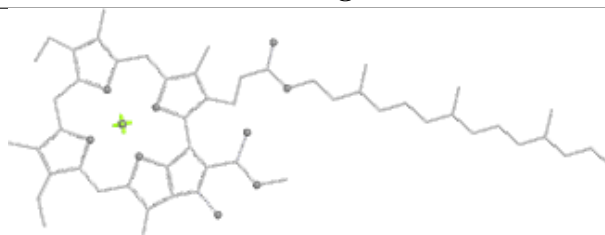
Bond lengths



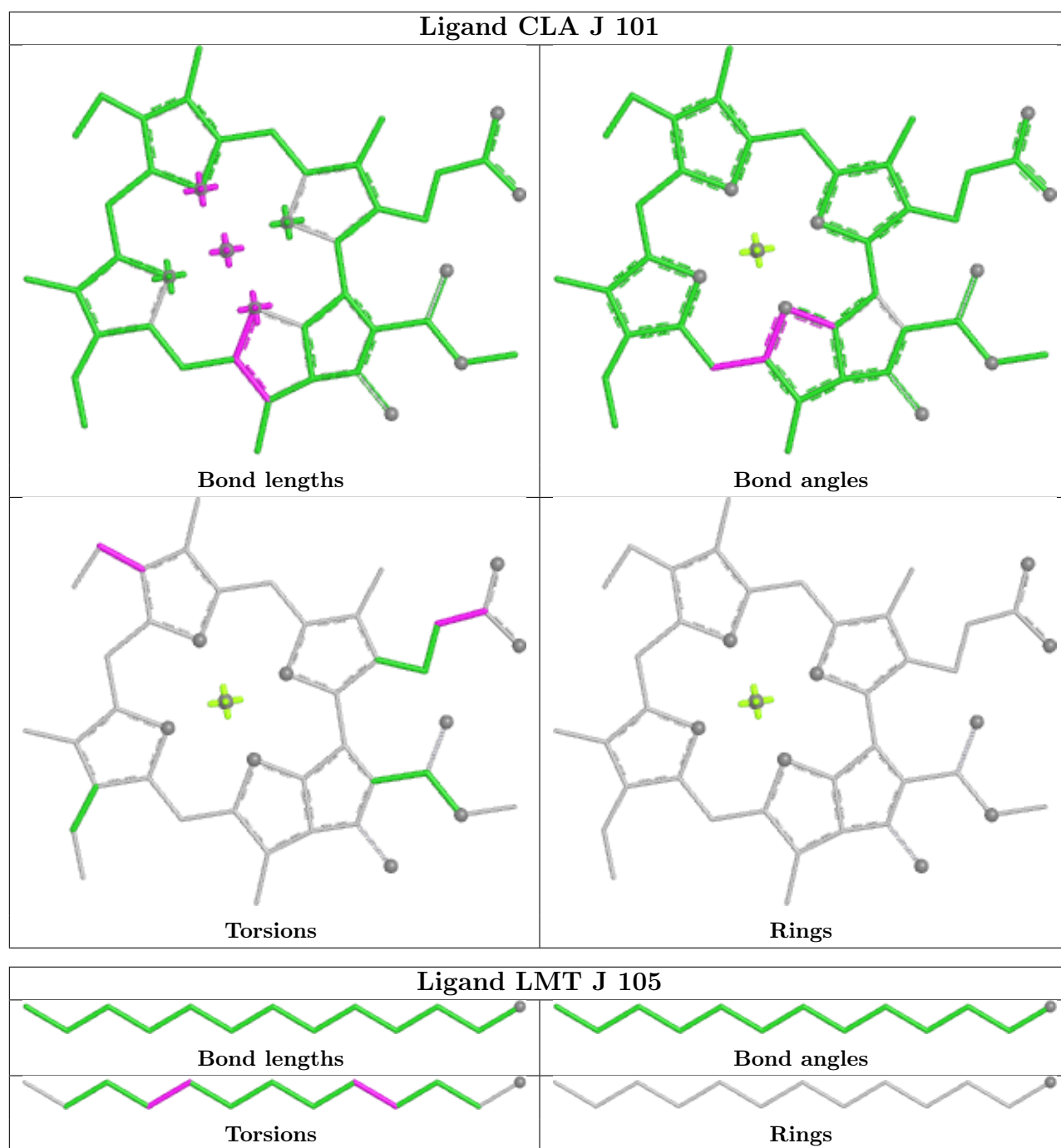
Bond angles

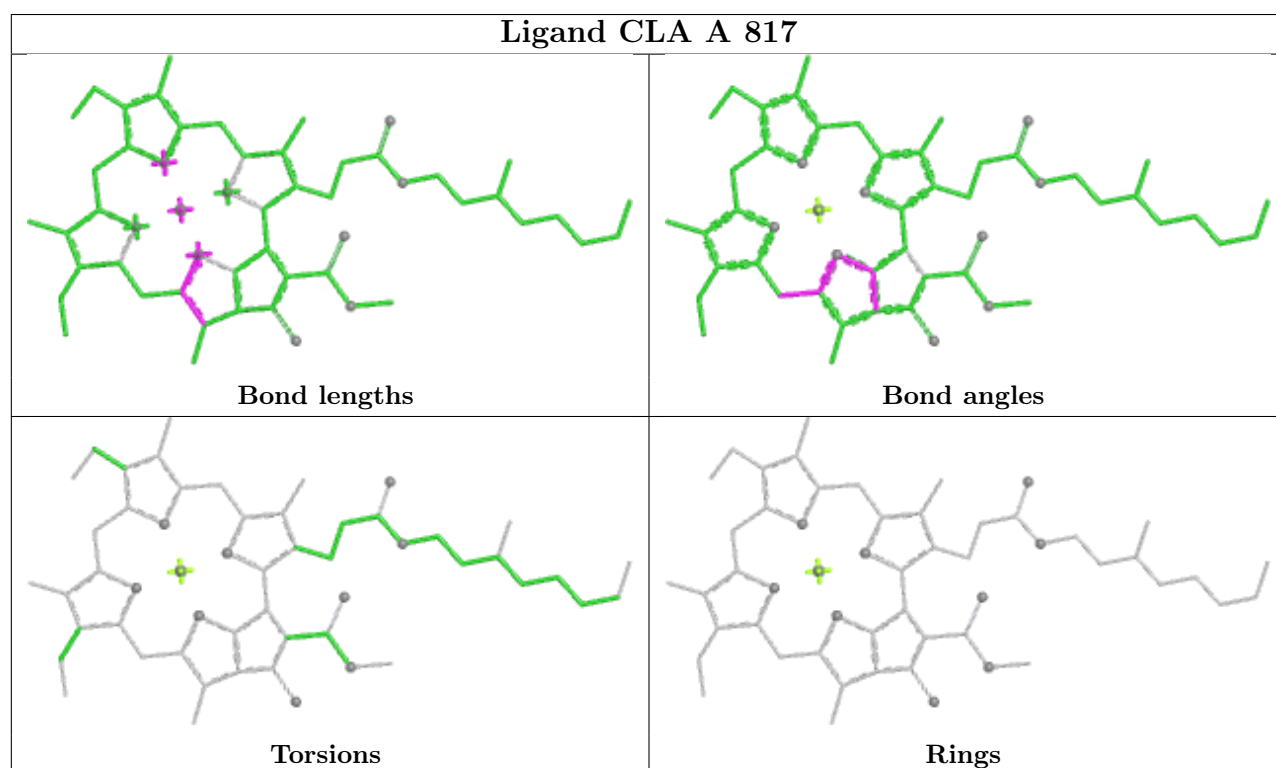
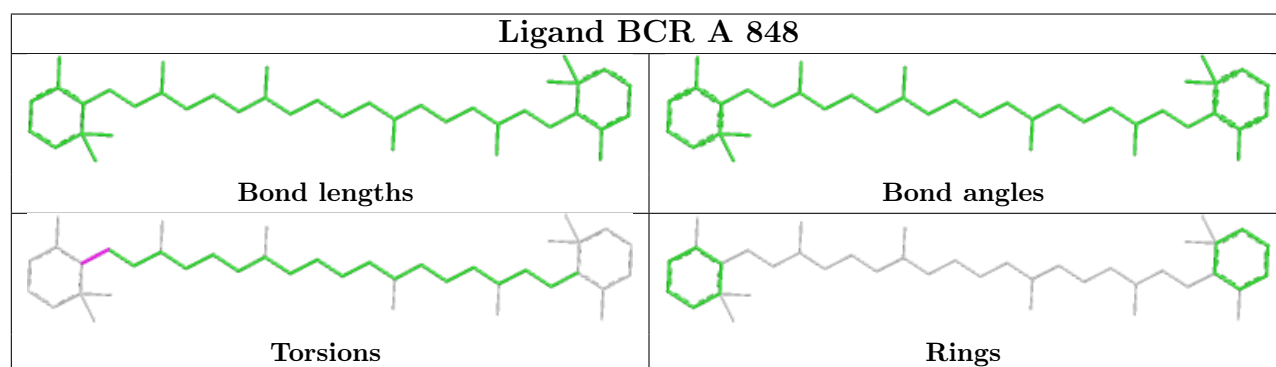
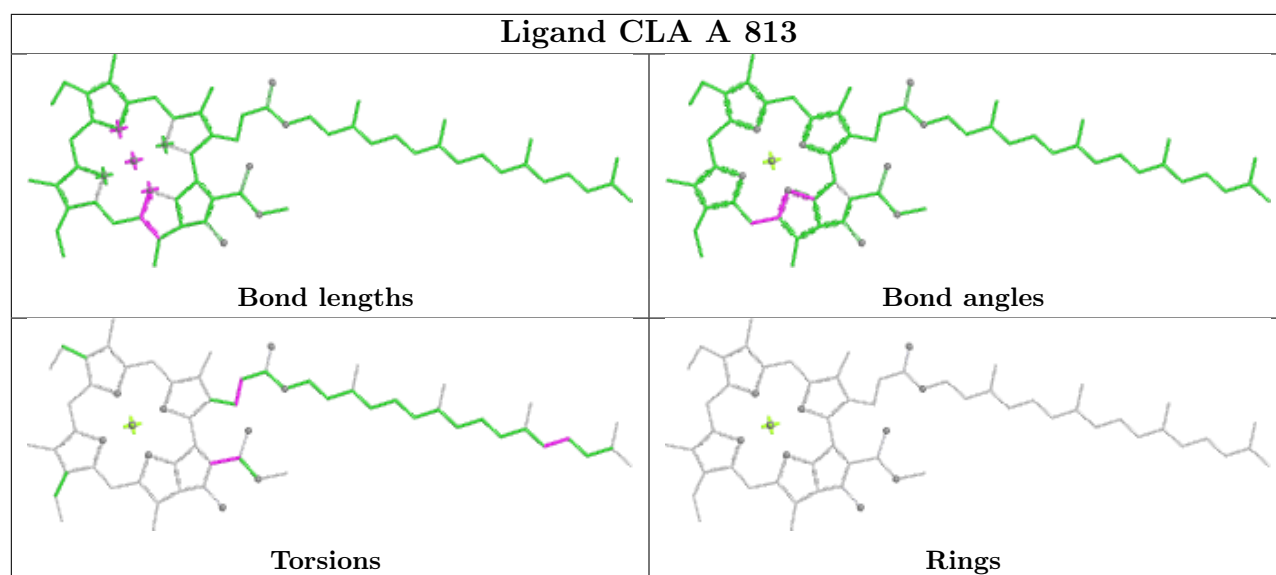


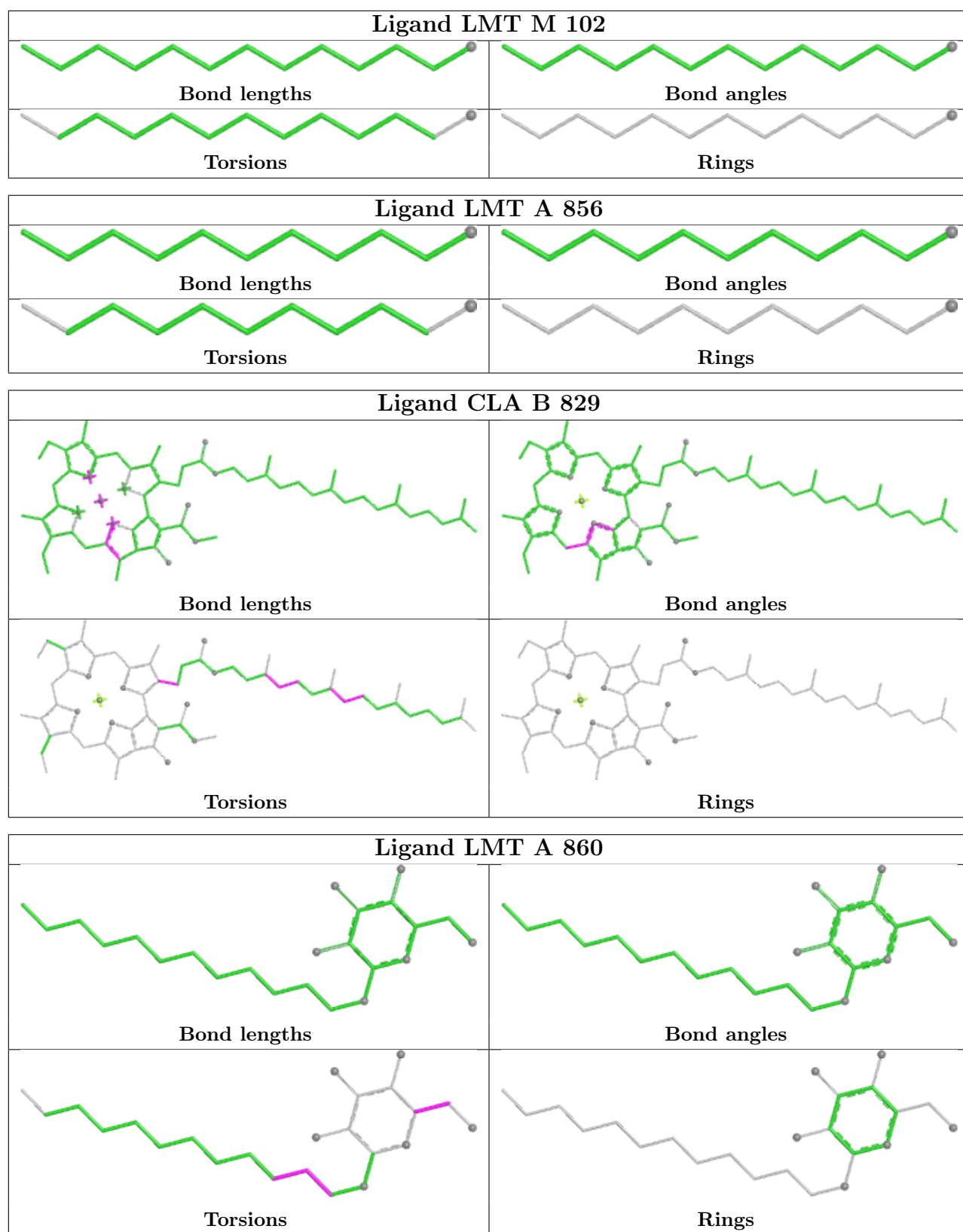
Torsions

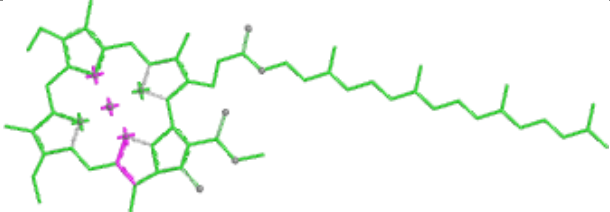
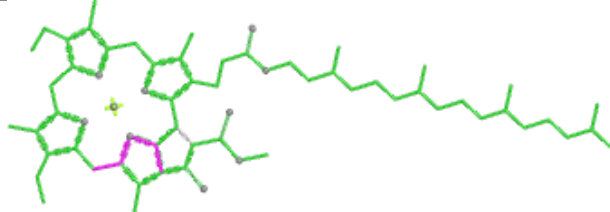
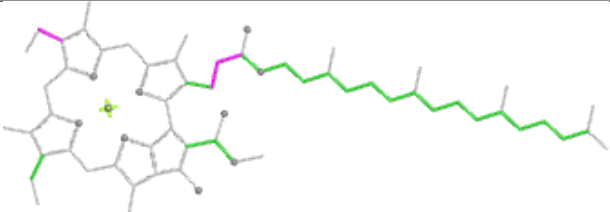
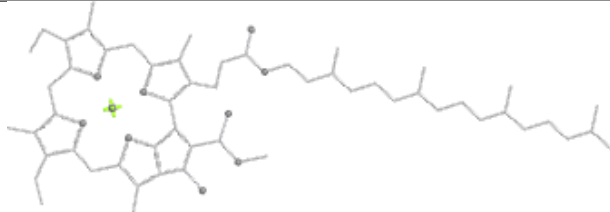
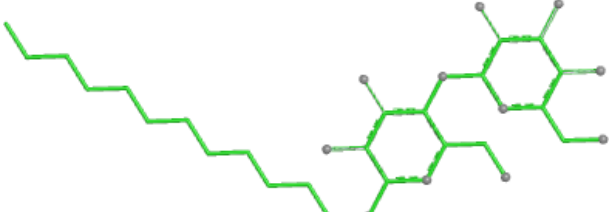
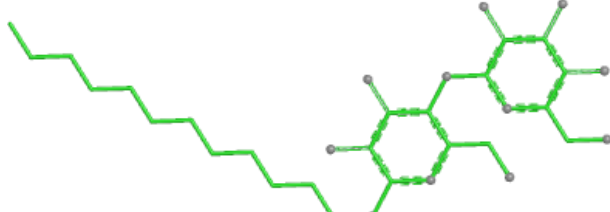
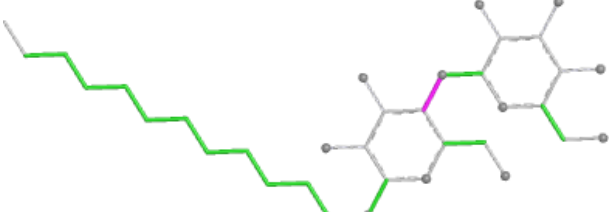
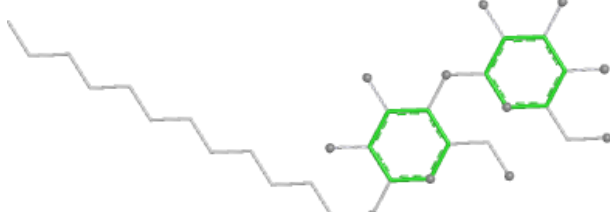
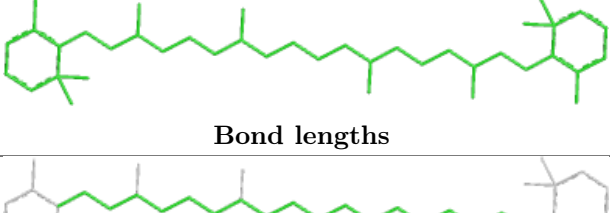
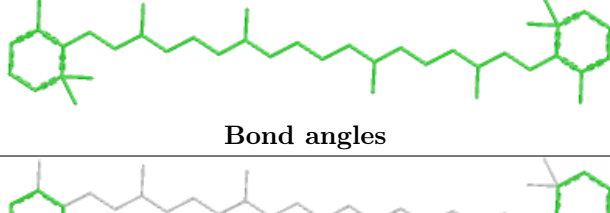
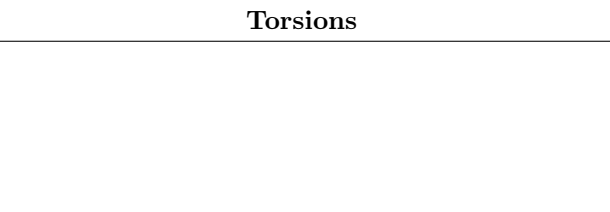
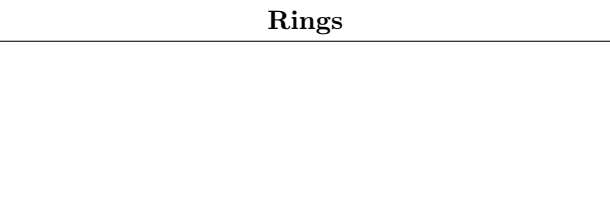


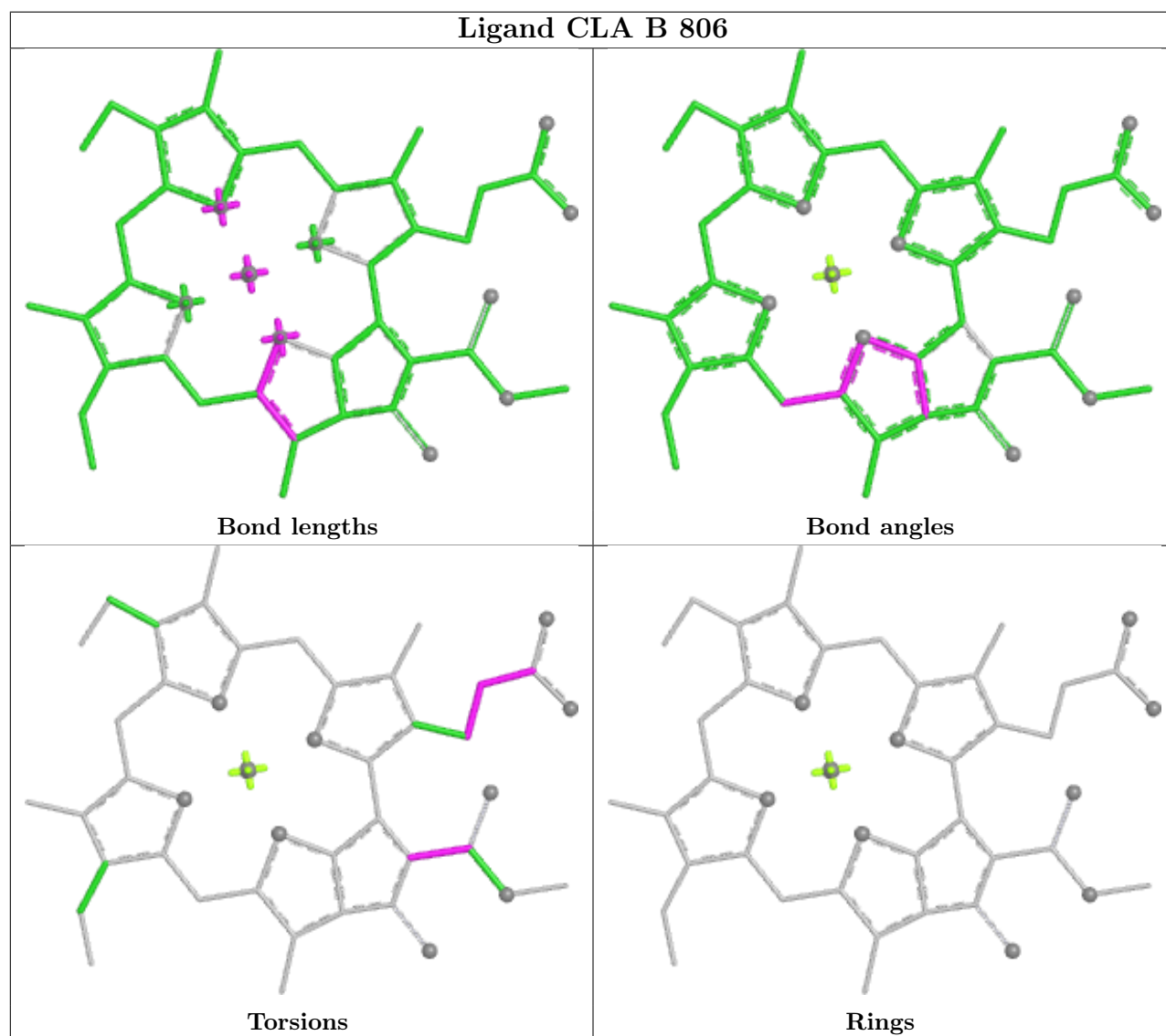
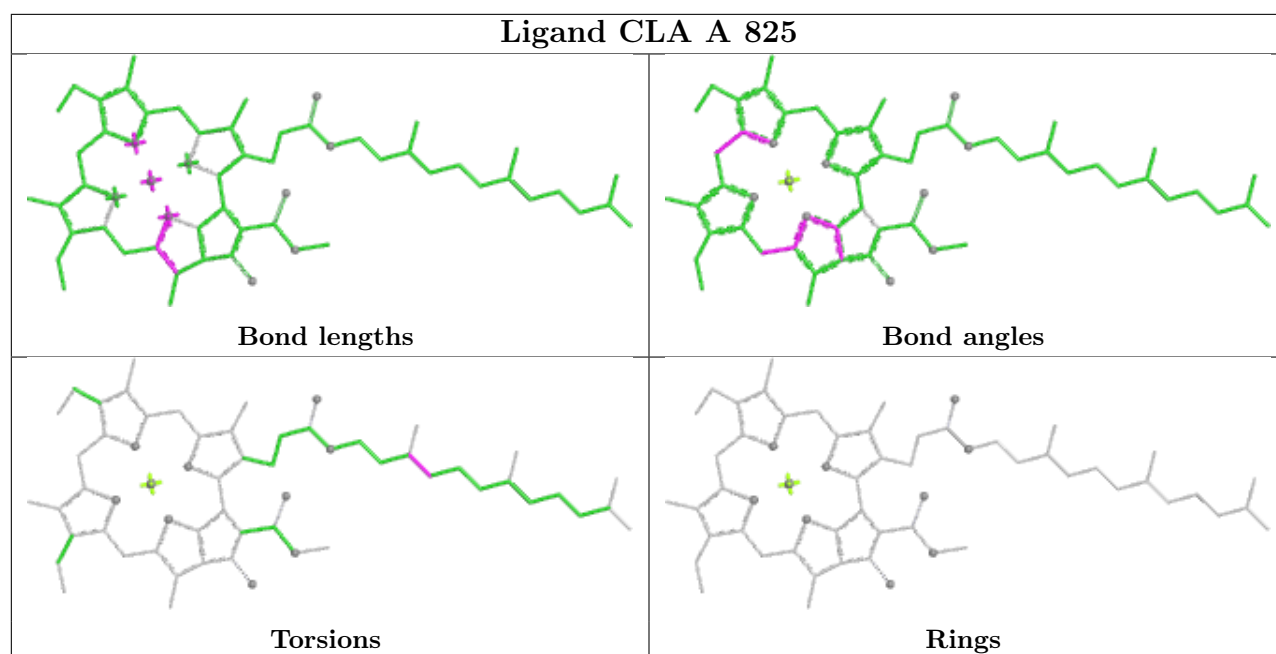
Rings

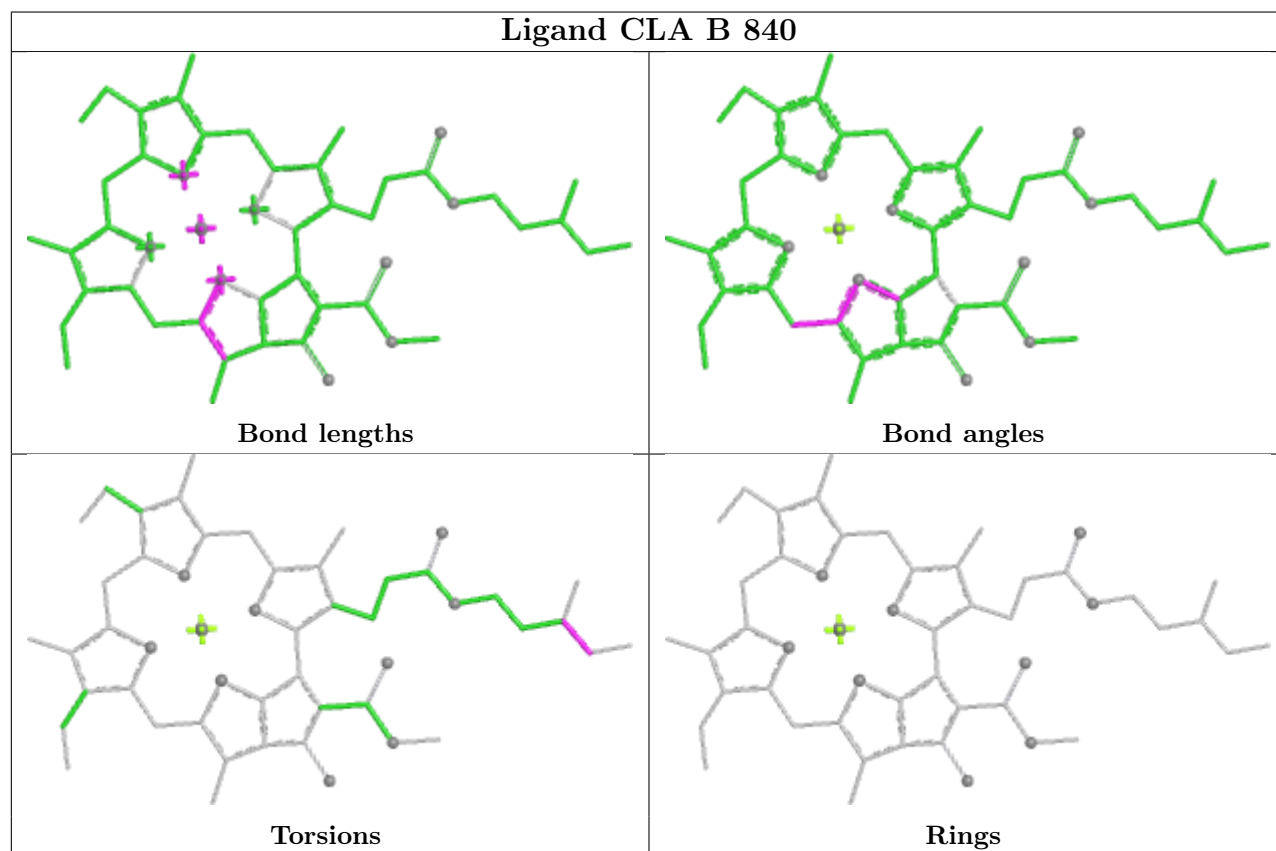
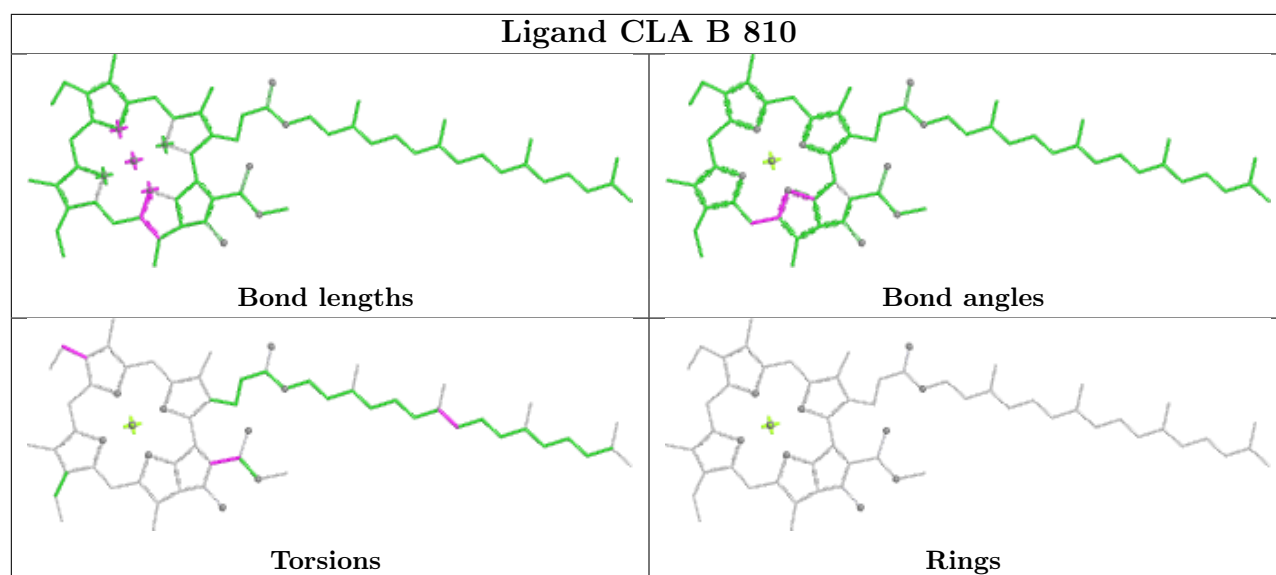


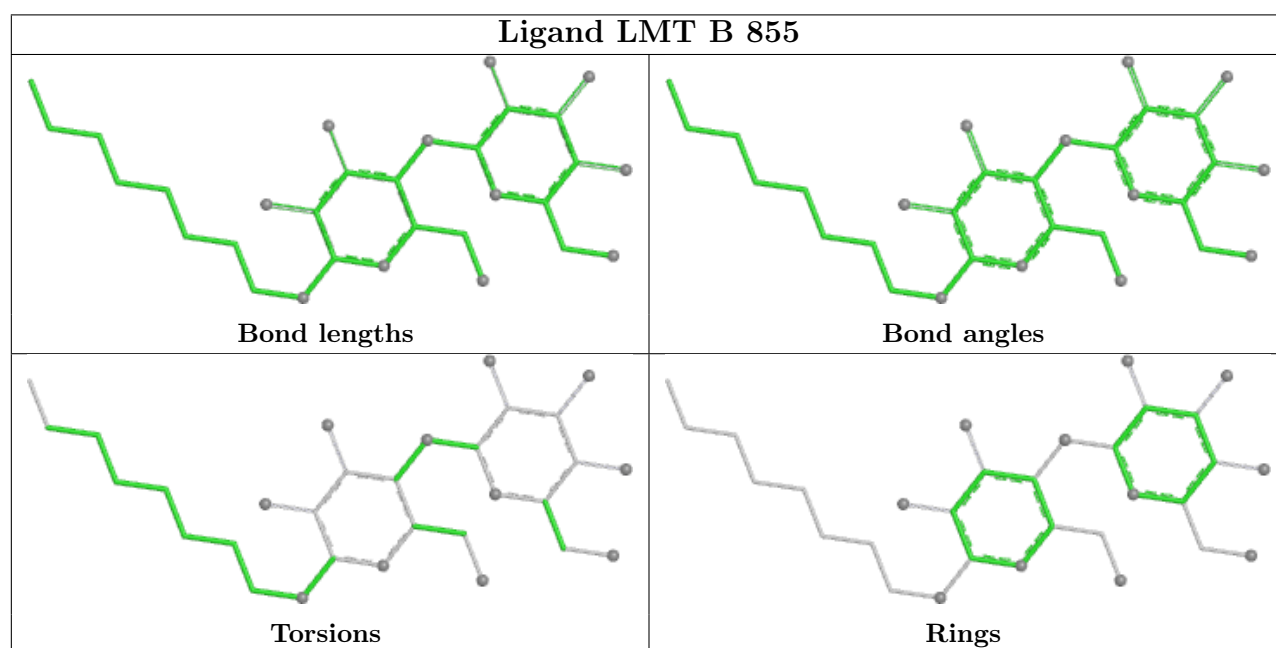
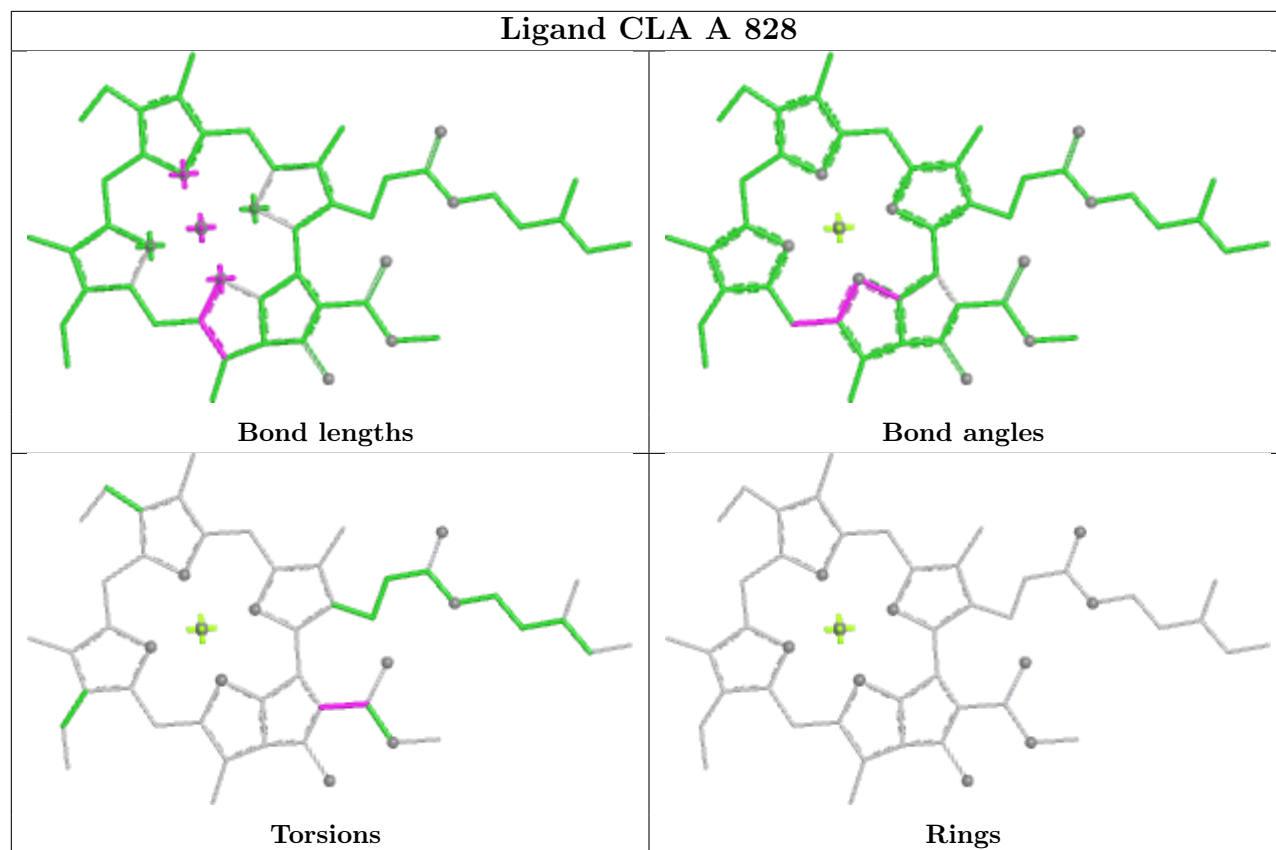


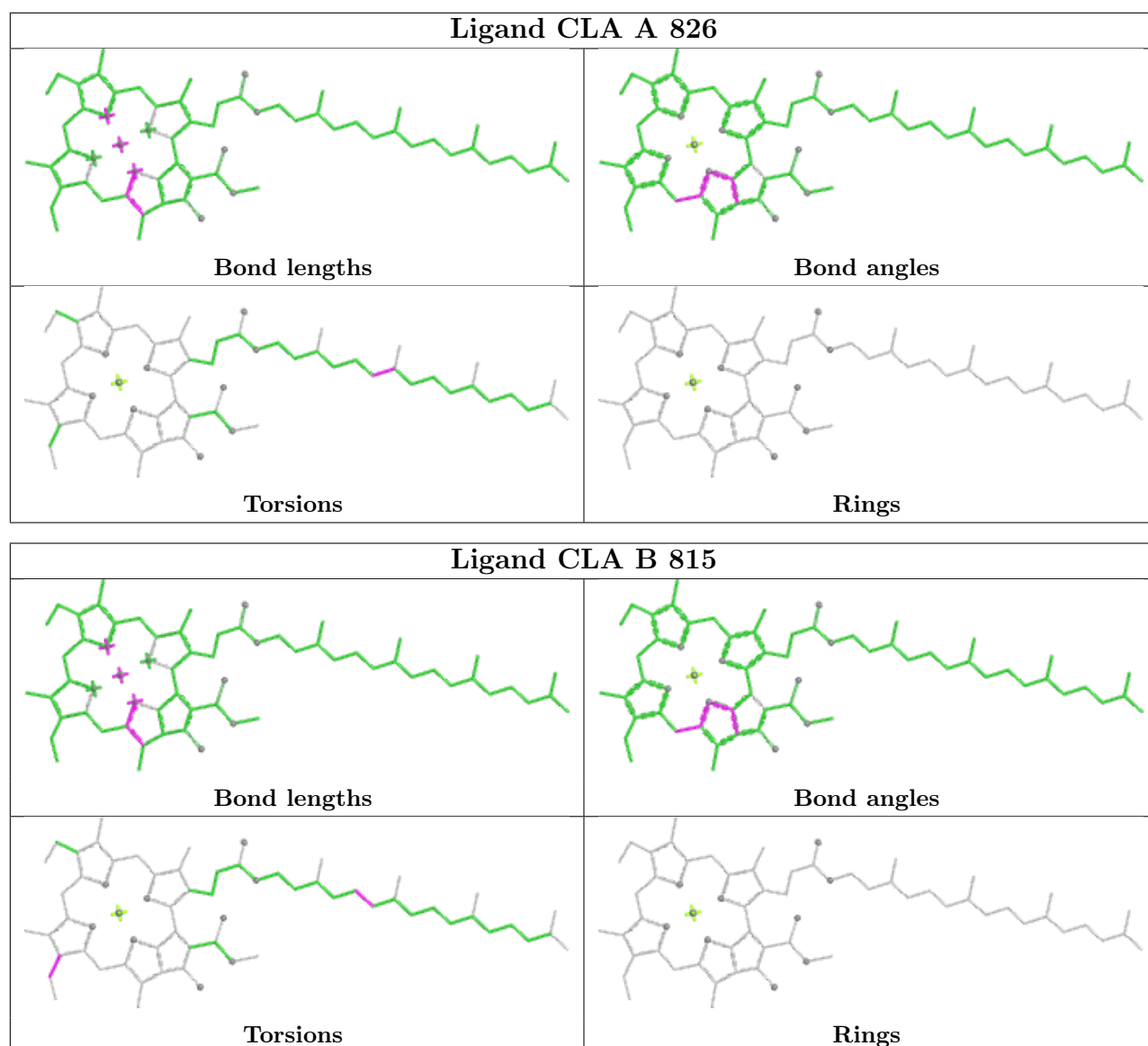


Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT A 864	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

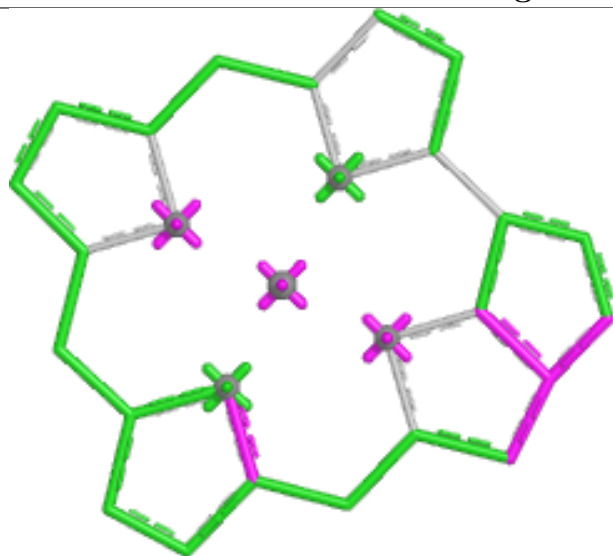




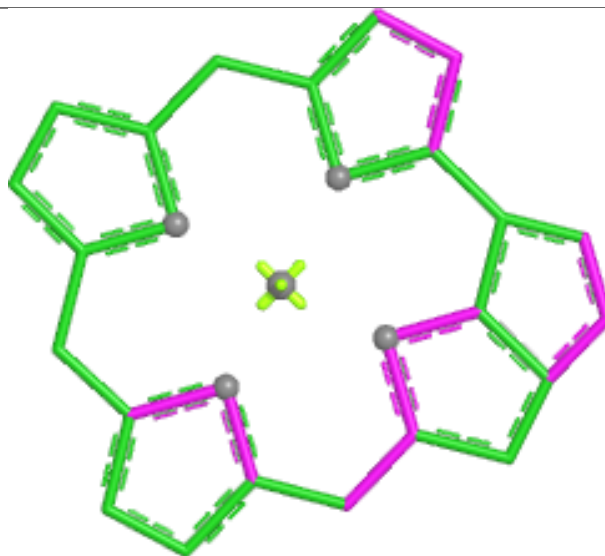




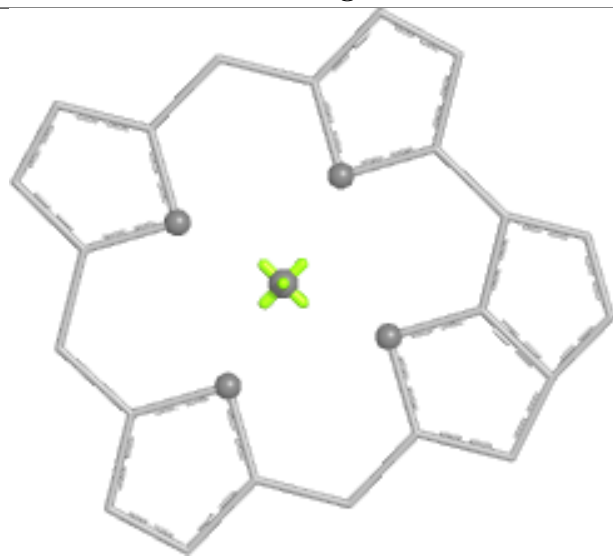
Ligand CLA B 843



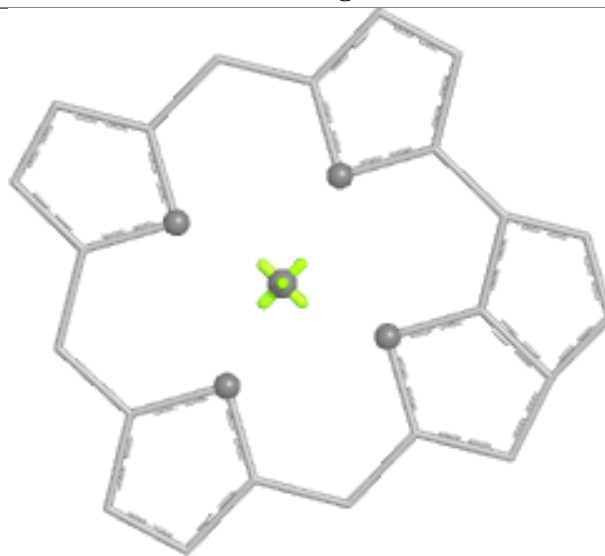
Bond lengths



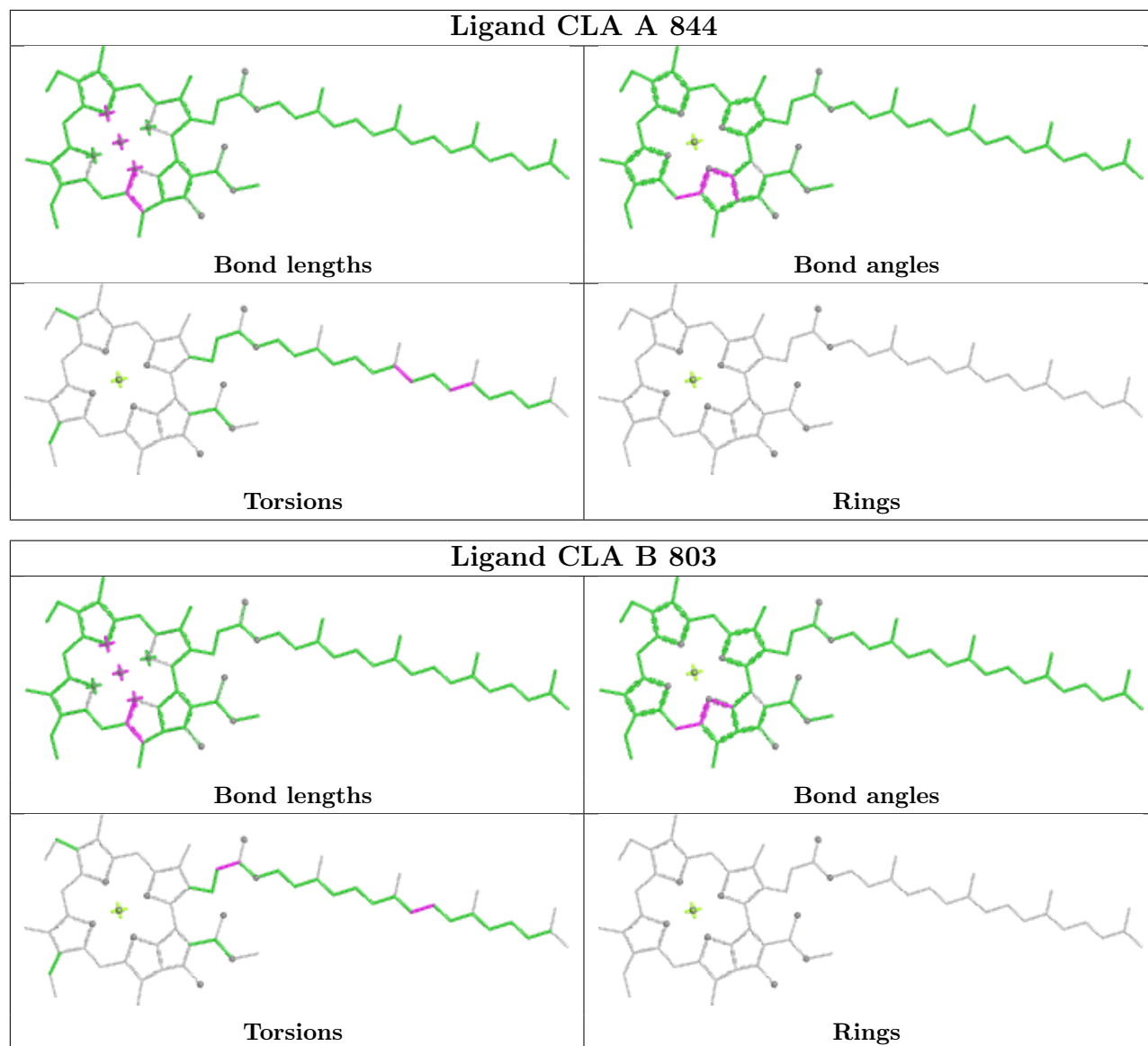
Bond angles



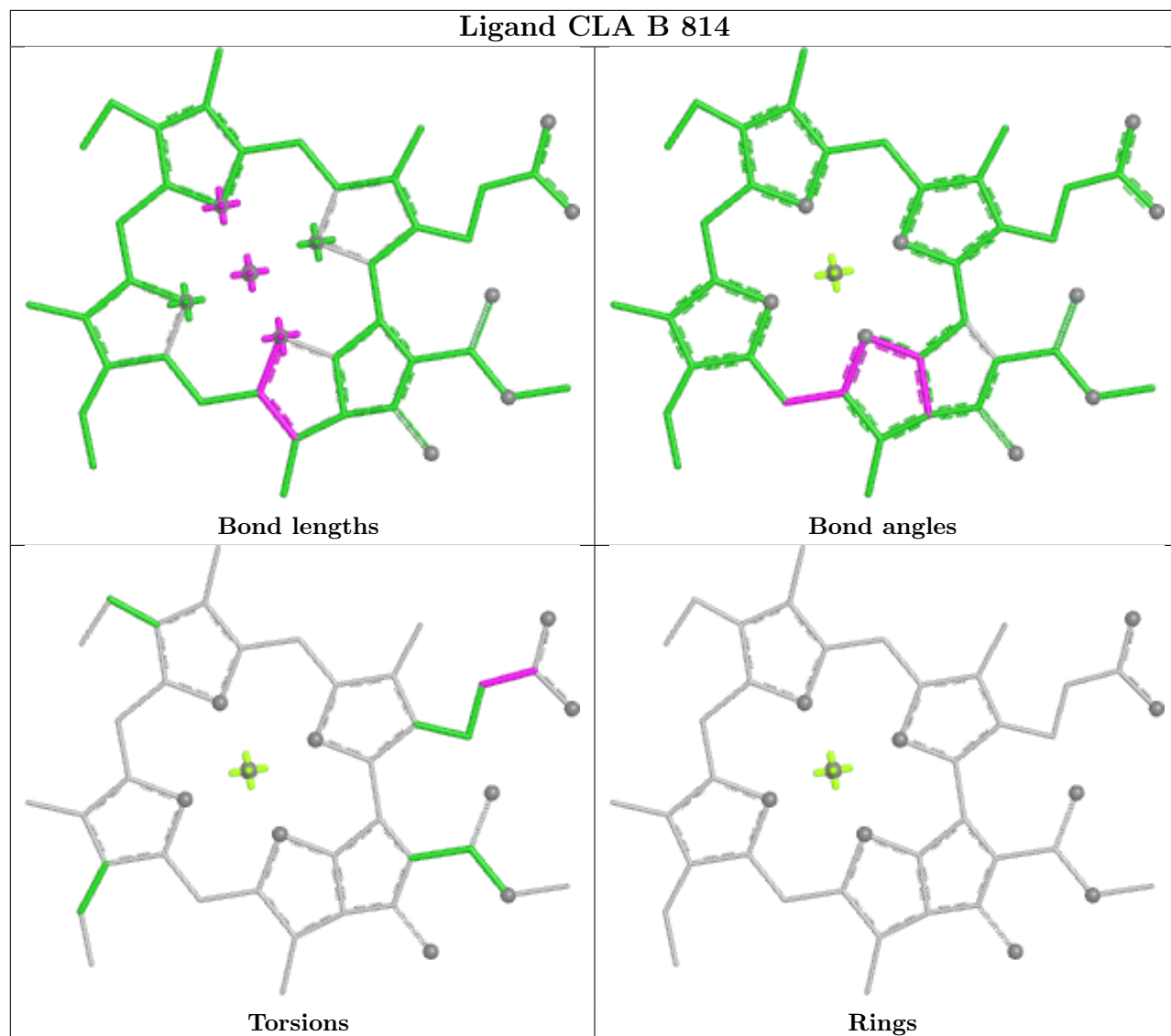
Torsions



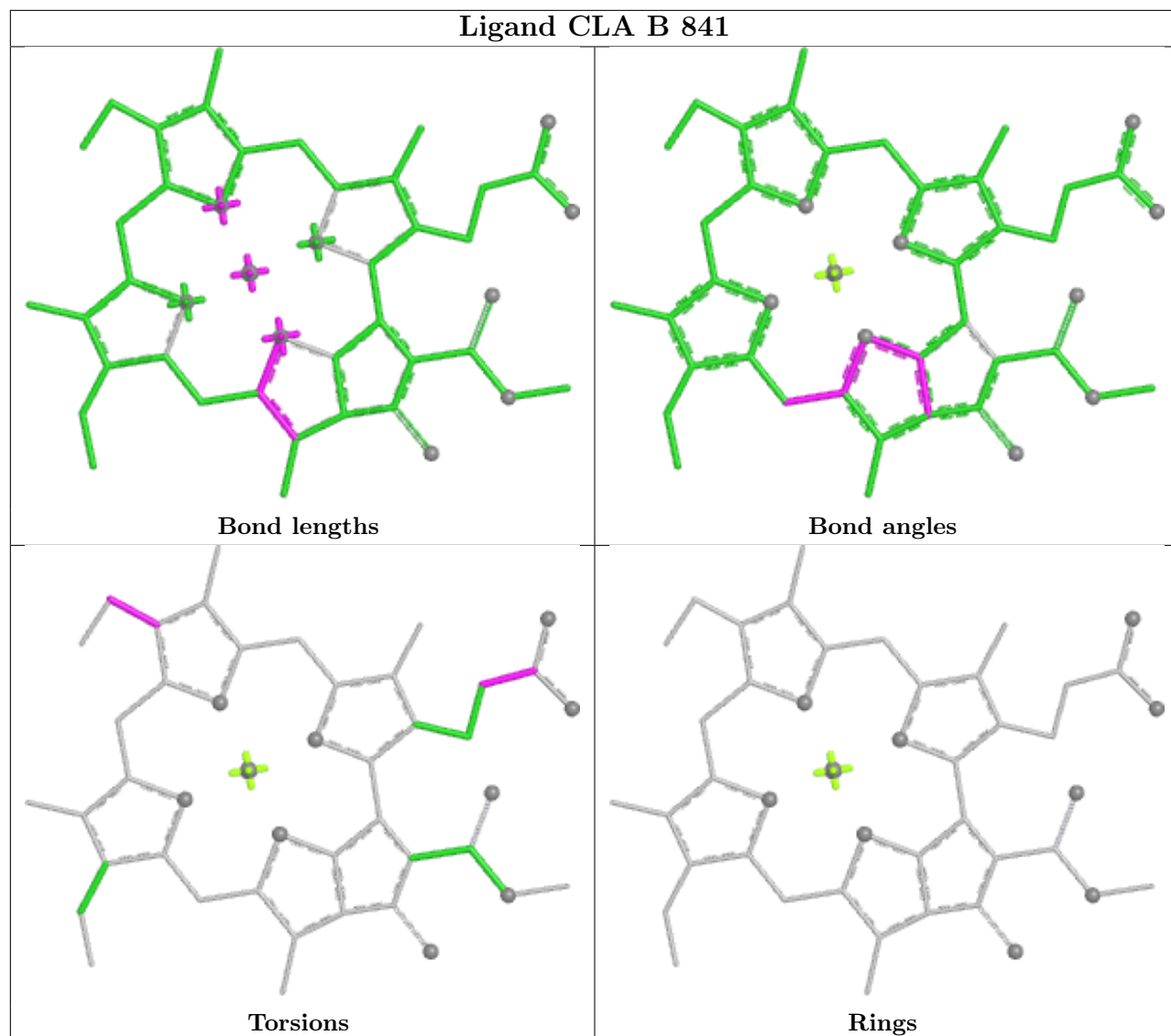
Rings

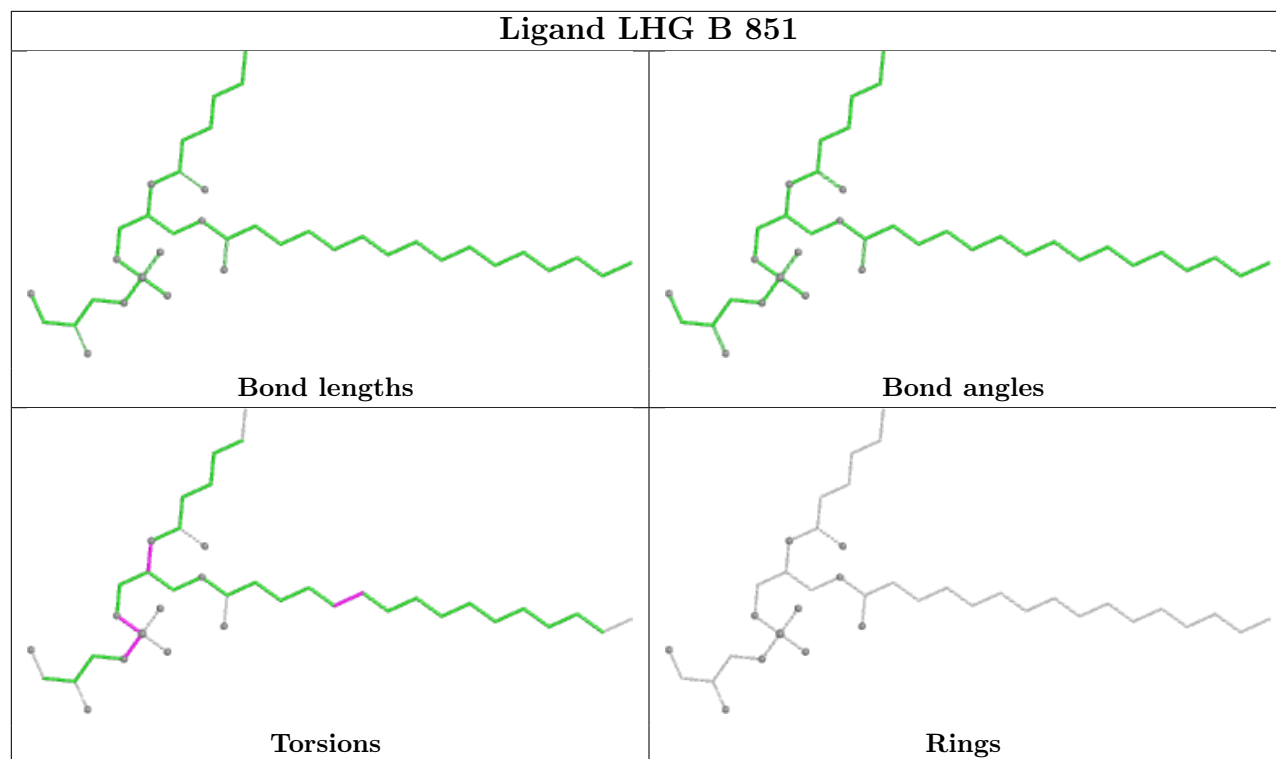


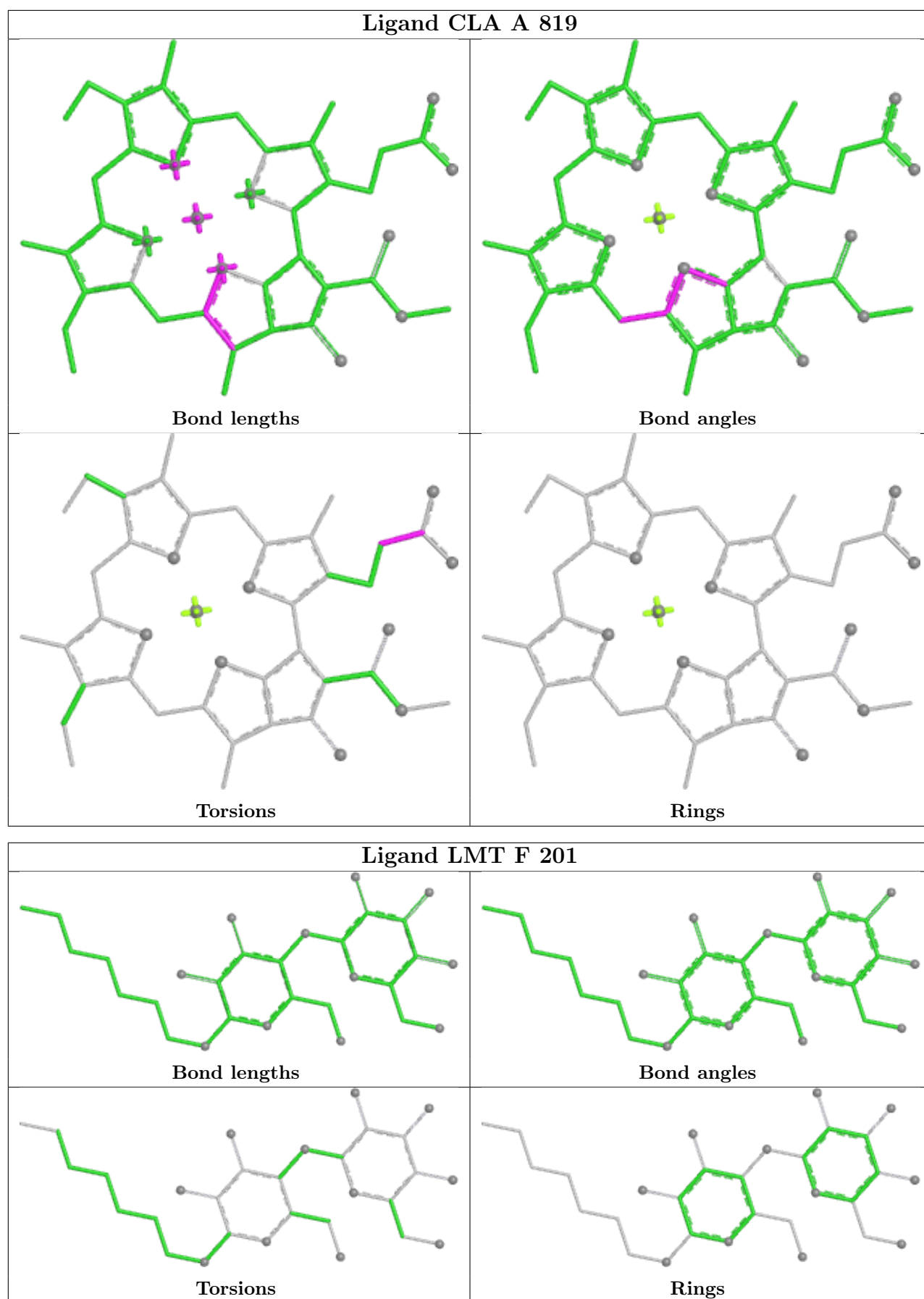
Ligand CLA B 814

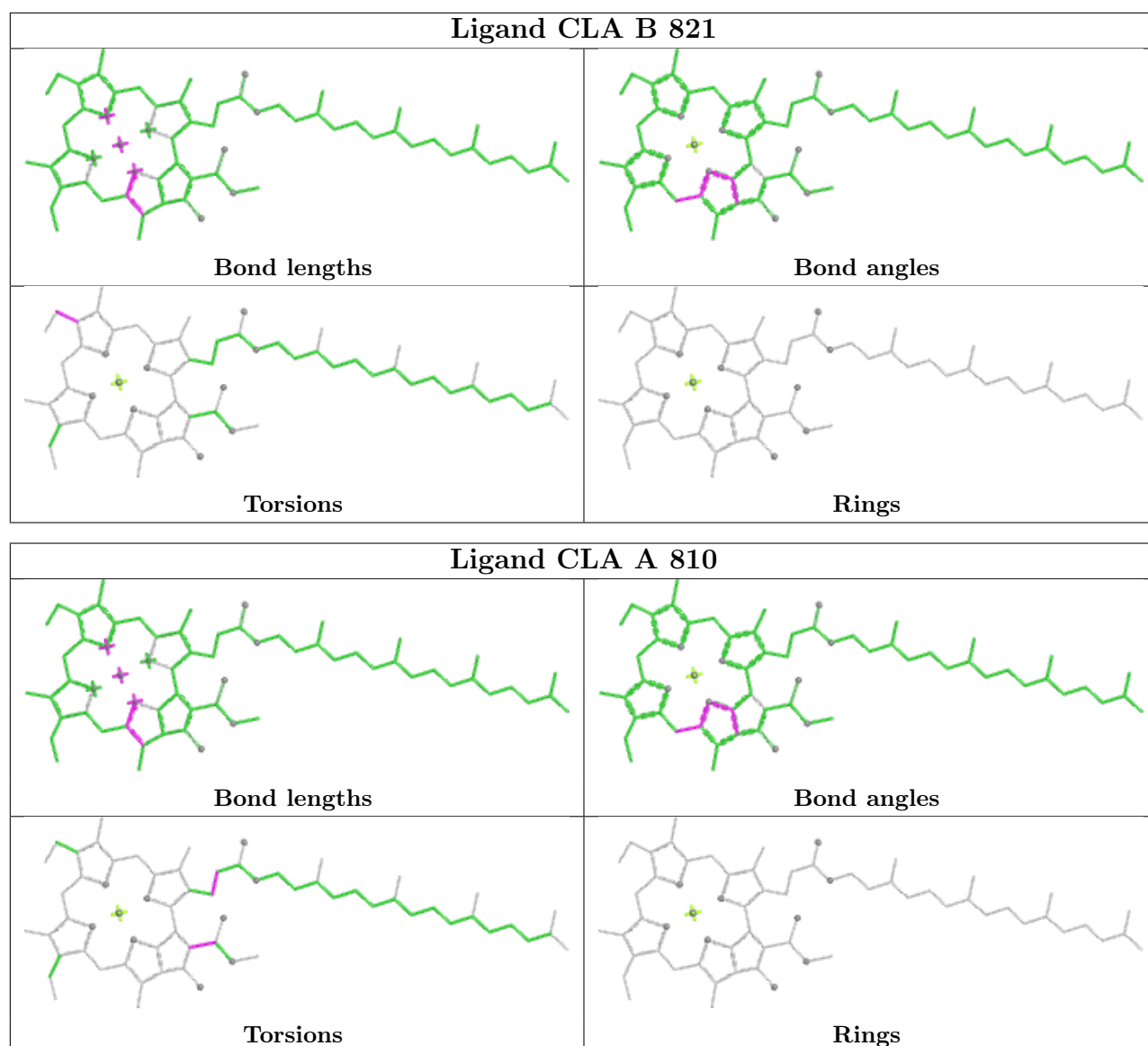


Ligand CLA B 841

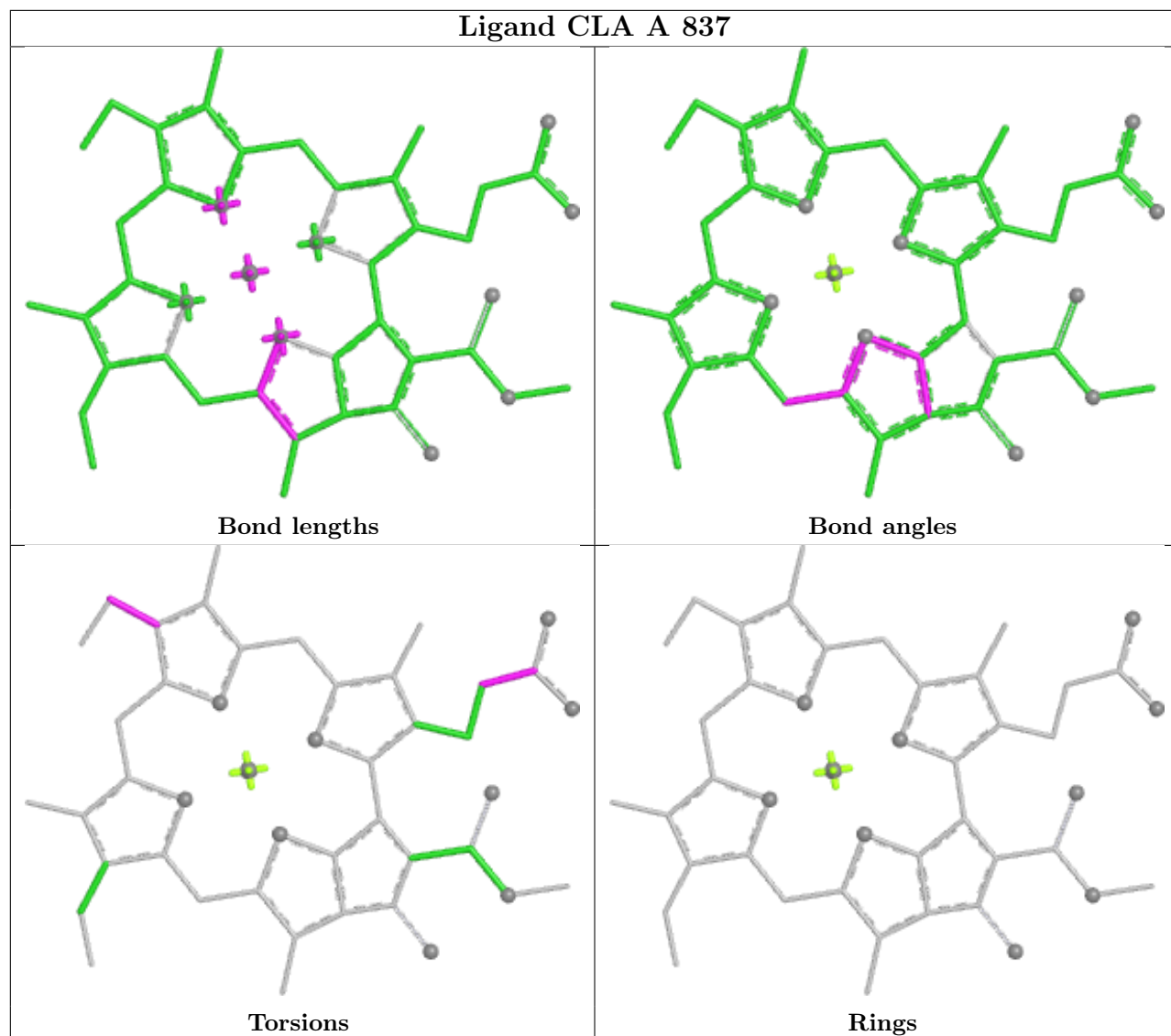


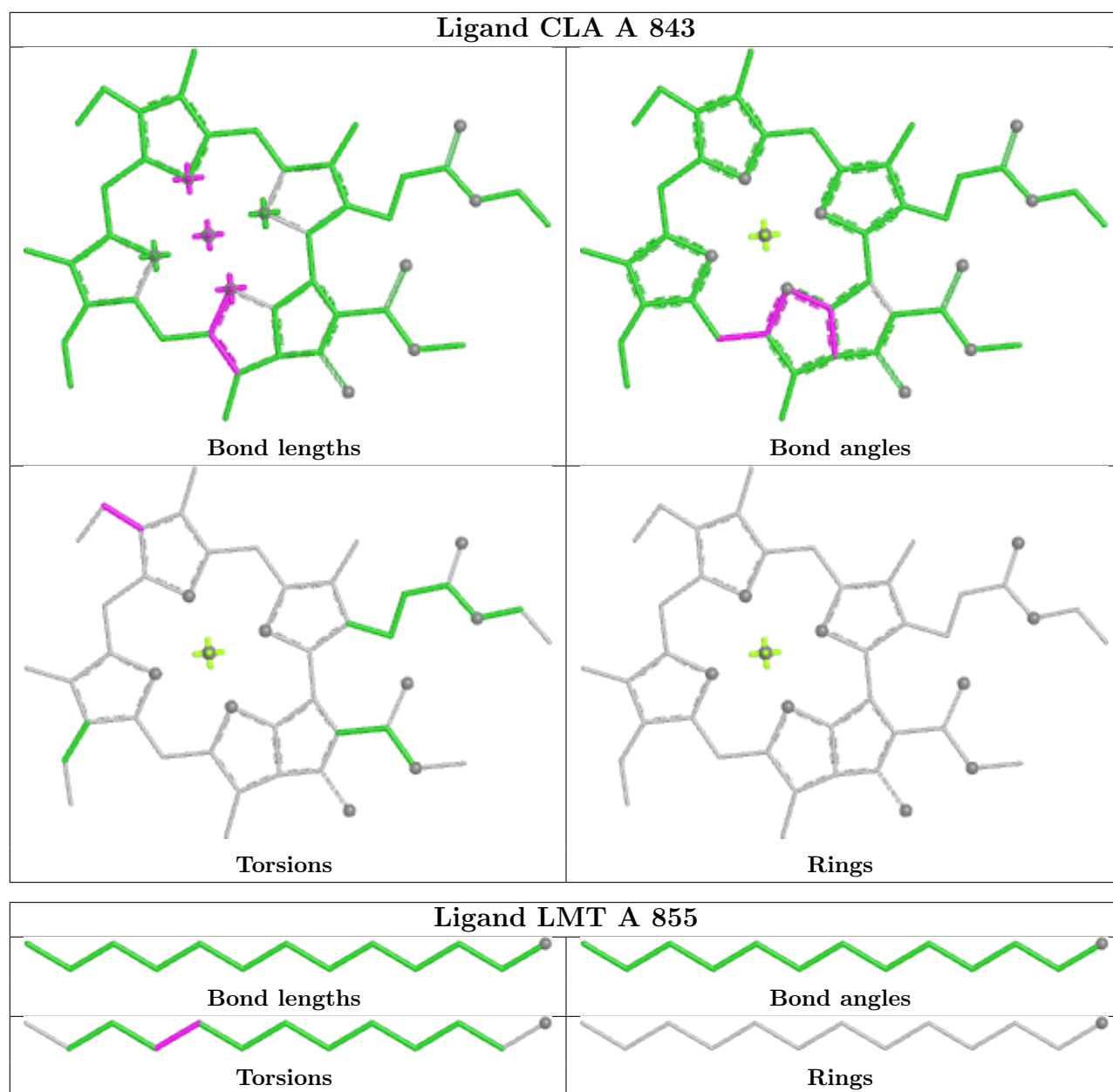


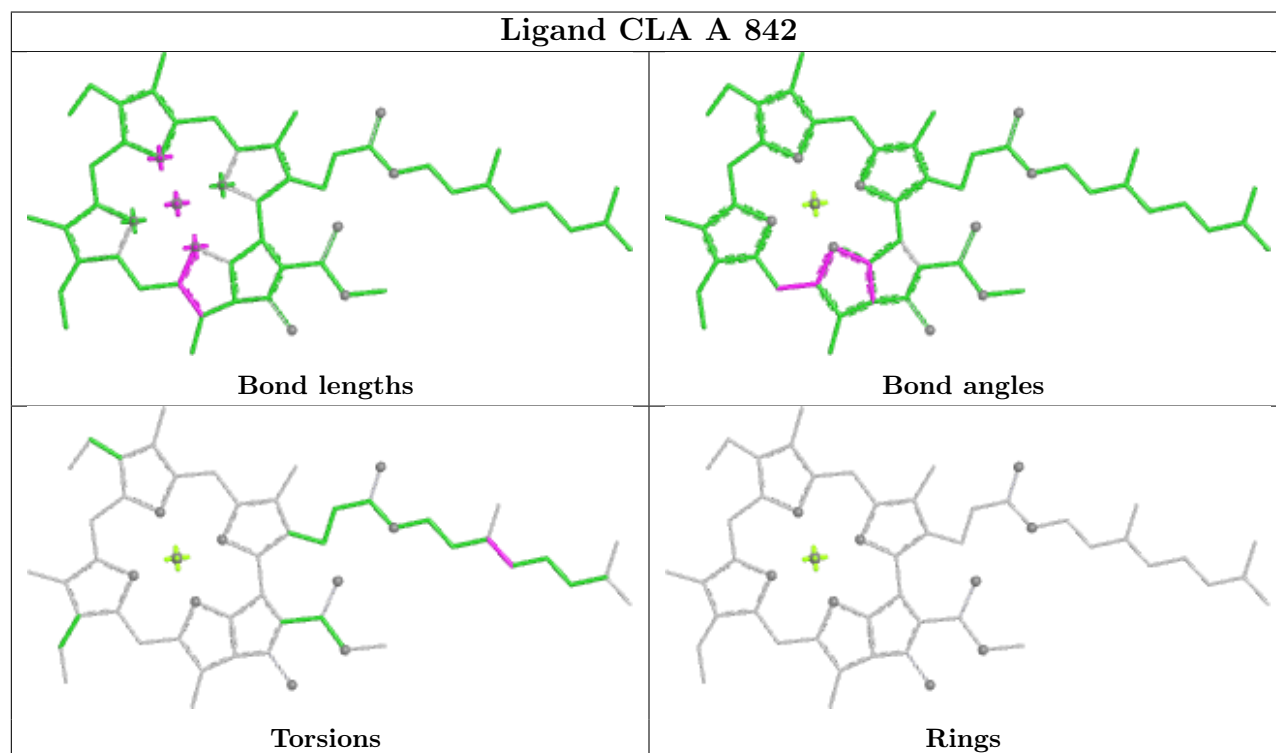
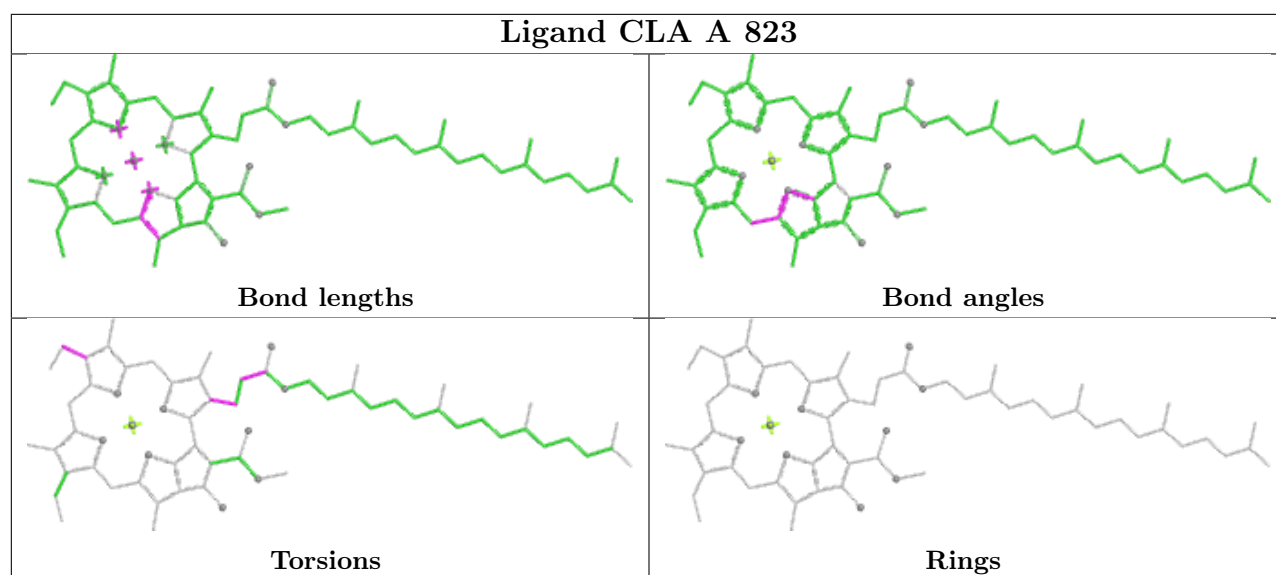


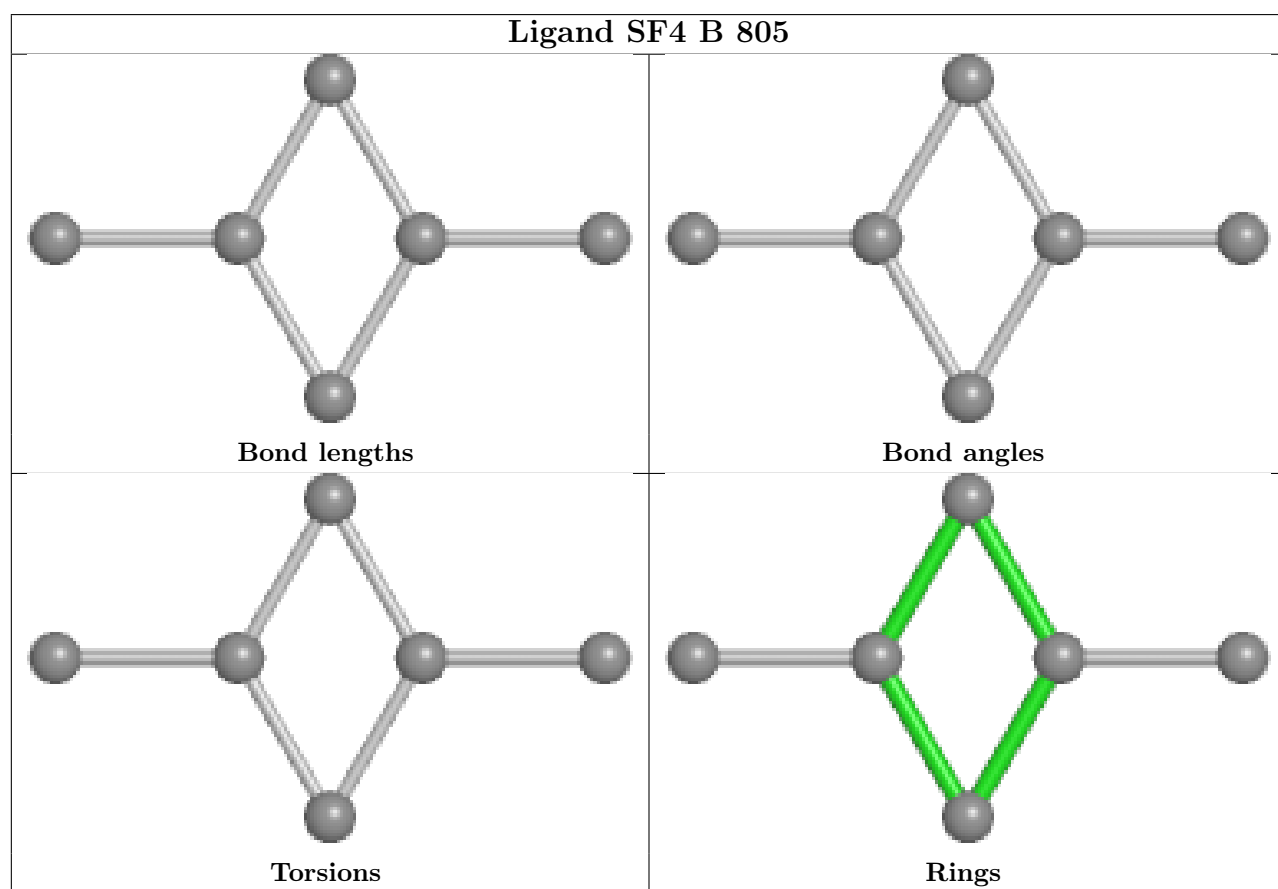
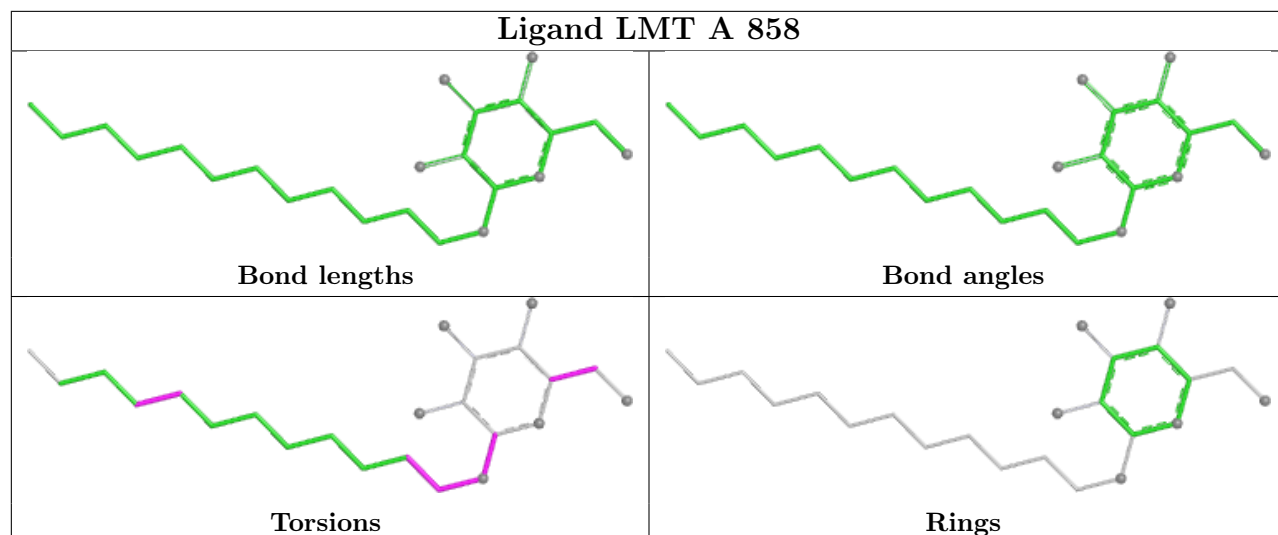


Ligand CLA A 837

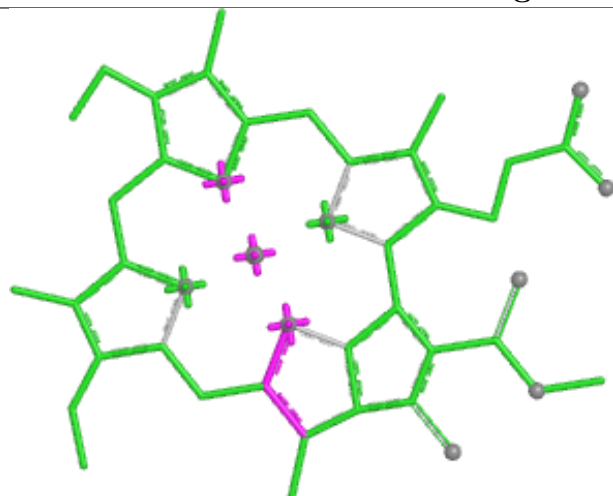




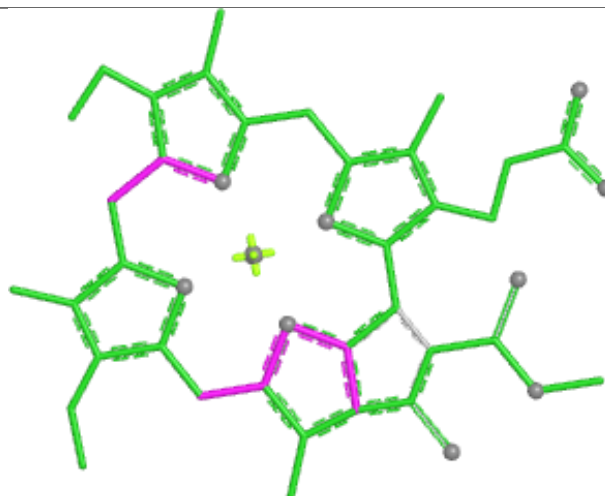




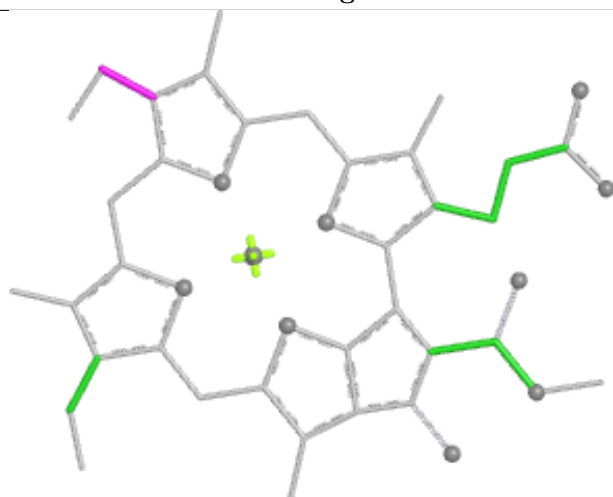
Ligand CLA A 838



Bond lengths



Bond angles

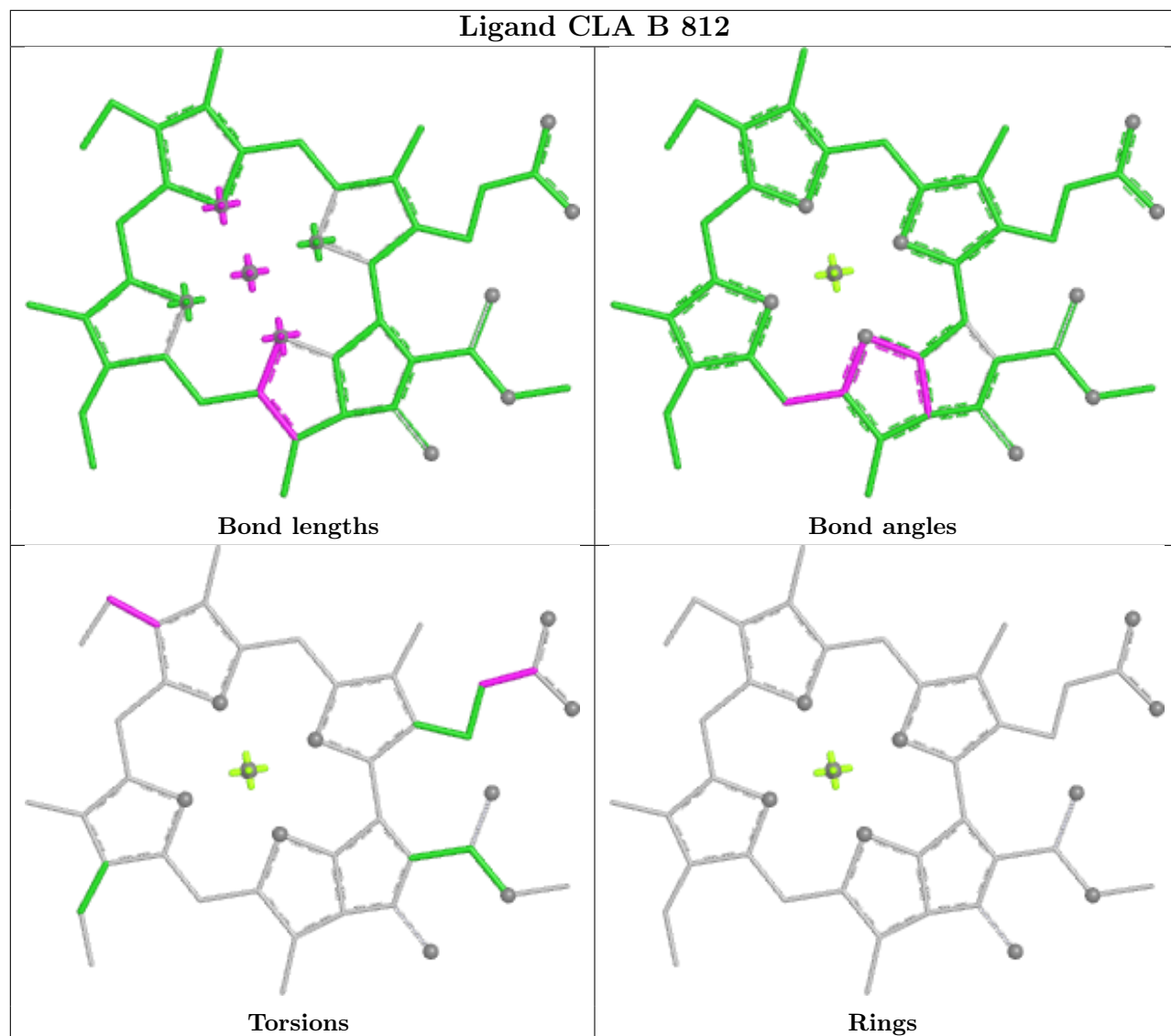


Torsions

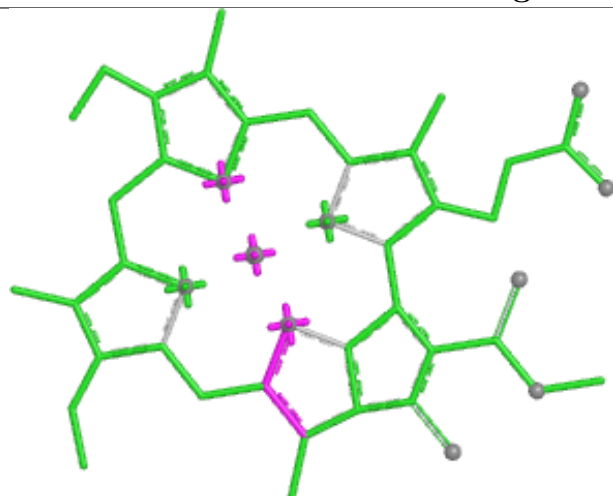


Rings

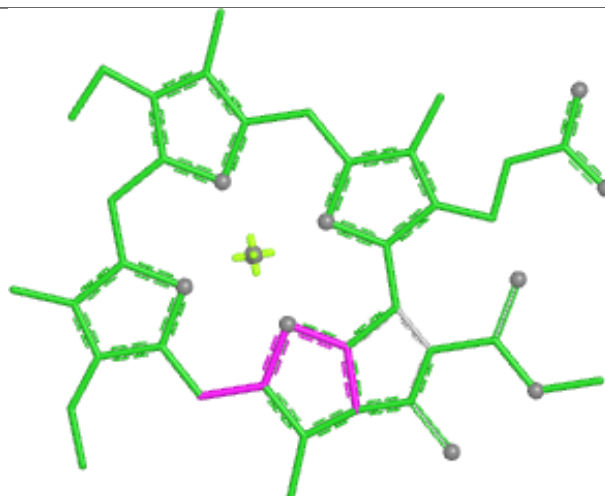
Ligand CLA B 812



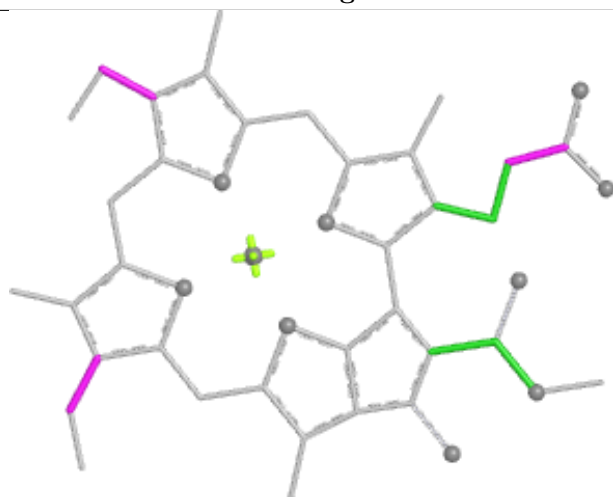
Ligand CLA K 102



Bond lengths



Bond angles

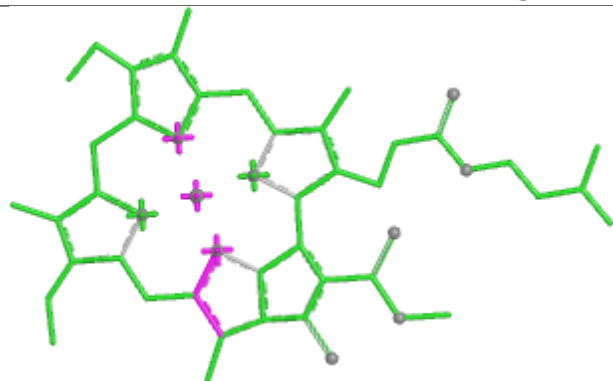


Torsions

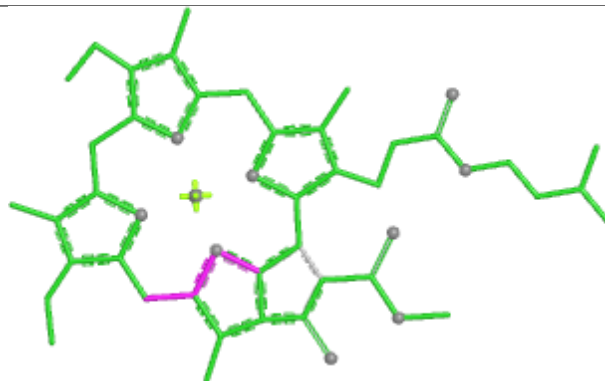


Rings

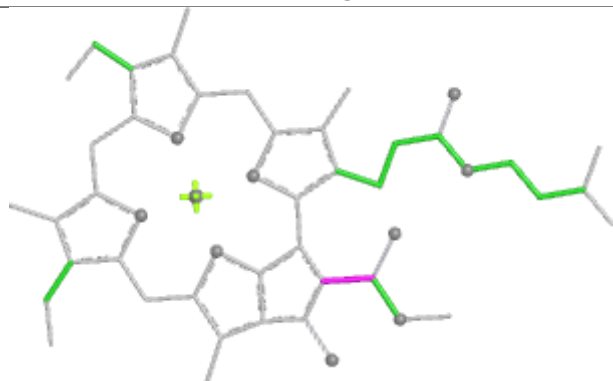
Ligand CLA B 827



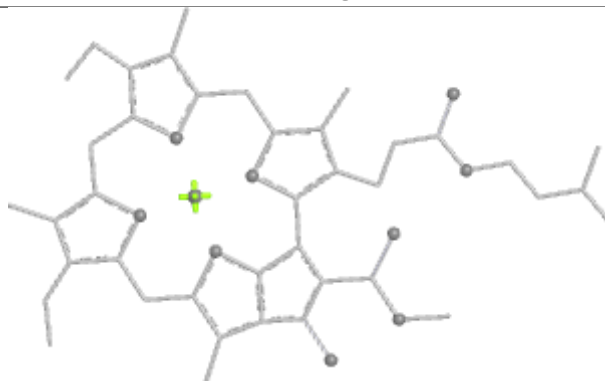
Bond lengths



Bond angles

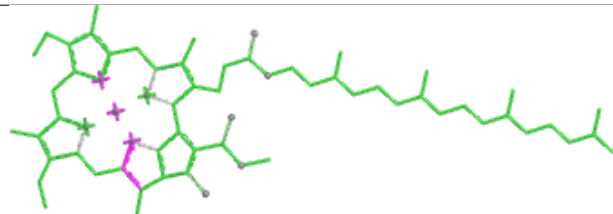


Torsions

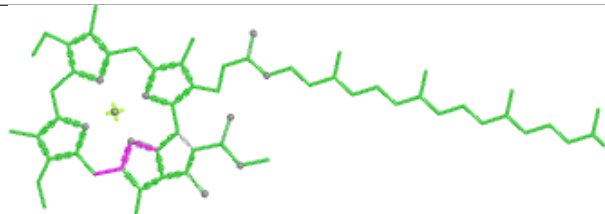


Rings

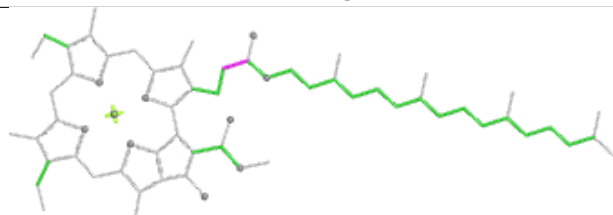
Ligand CLA B 808



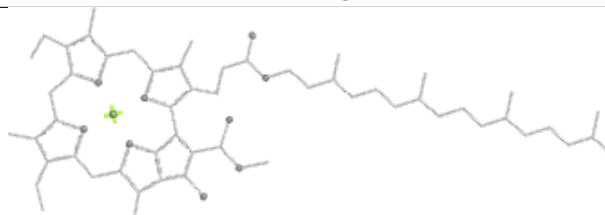
Bond lengths



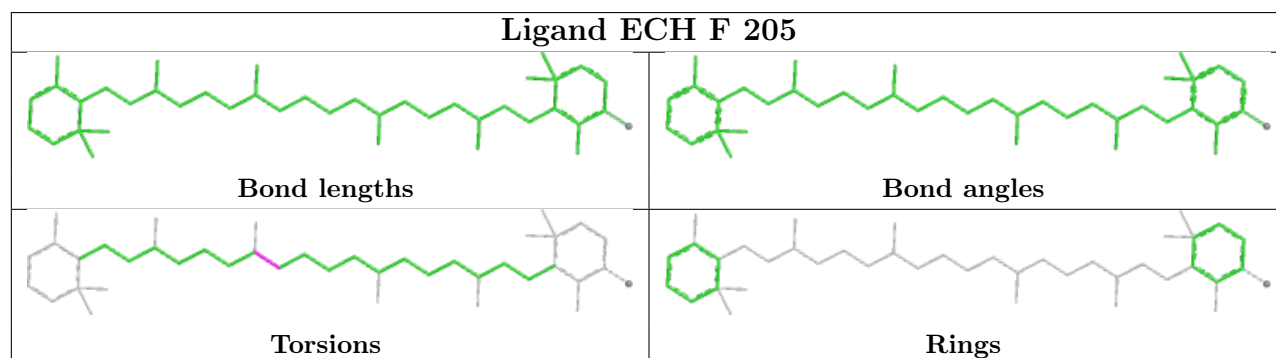
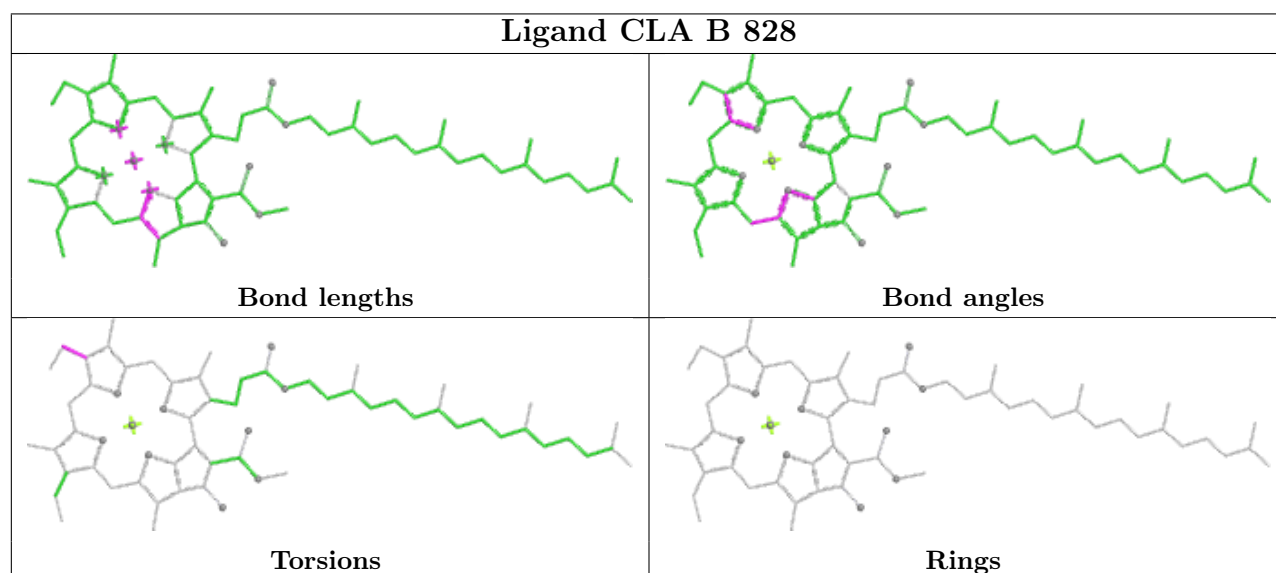
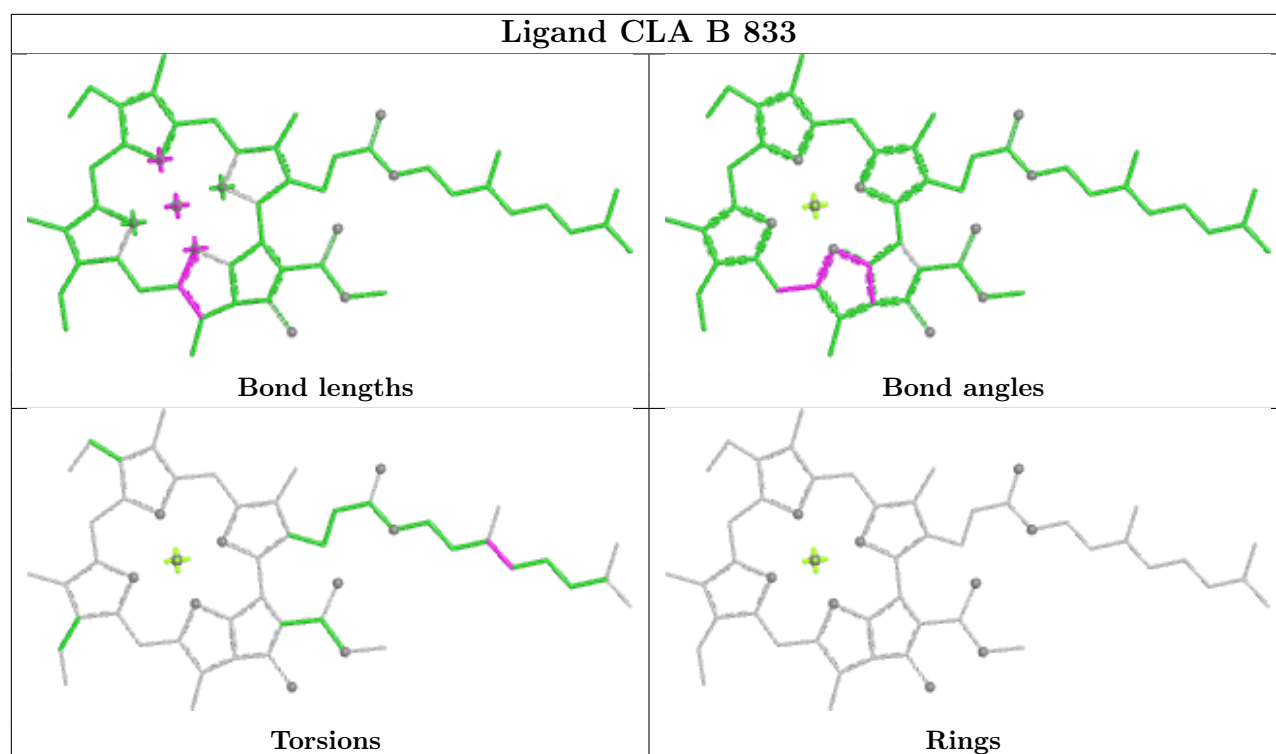
Bond angles



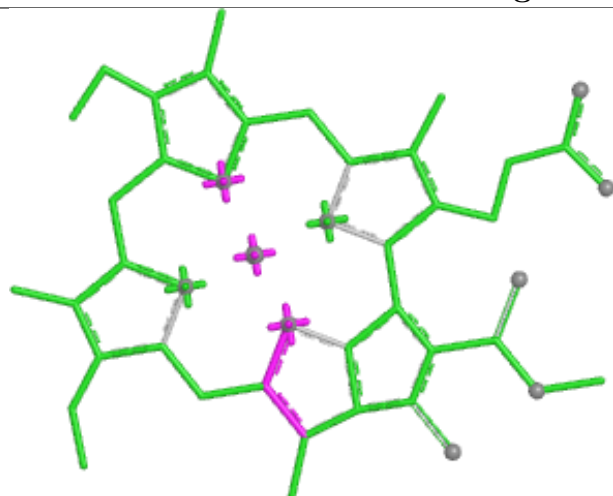
Torsions



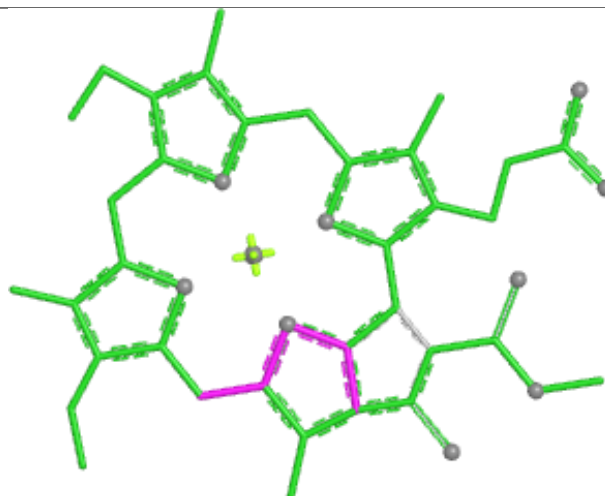
Rings



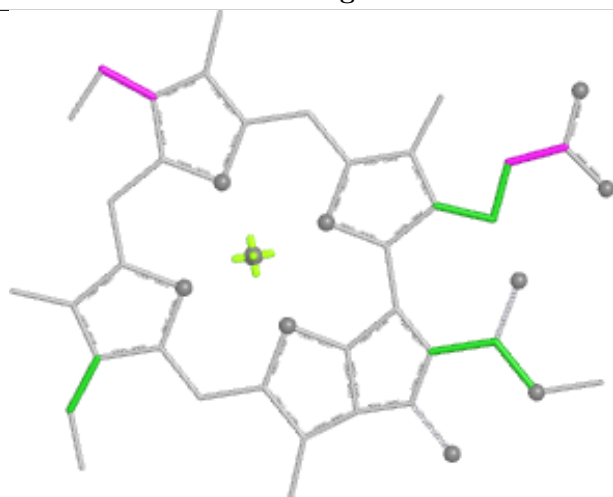
Ligand CLA A 846



Bond lengths



Bond angles

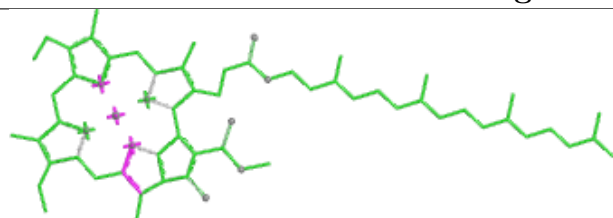


Torsions

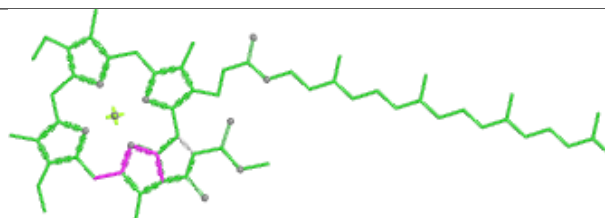


Rings

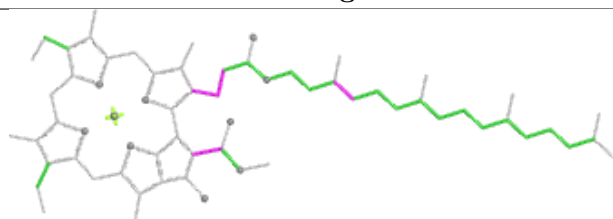
Ligand CLA B 807



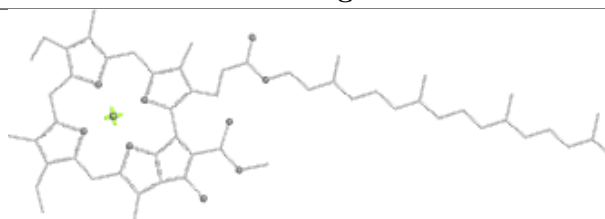
Bond lengths



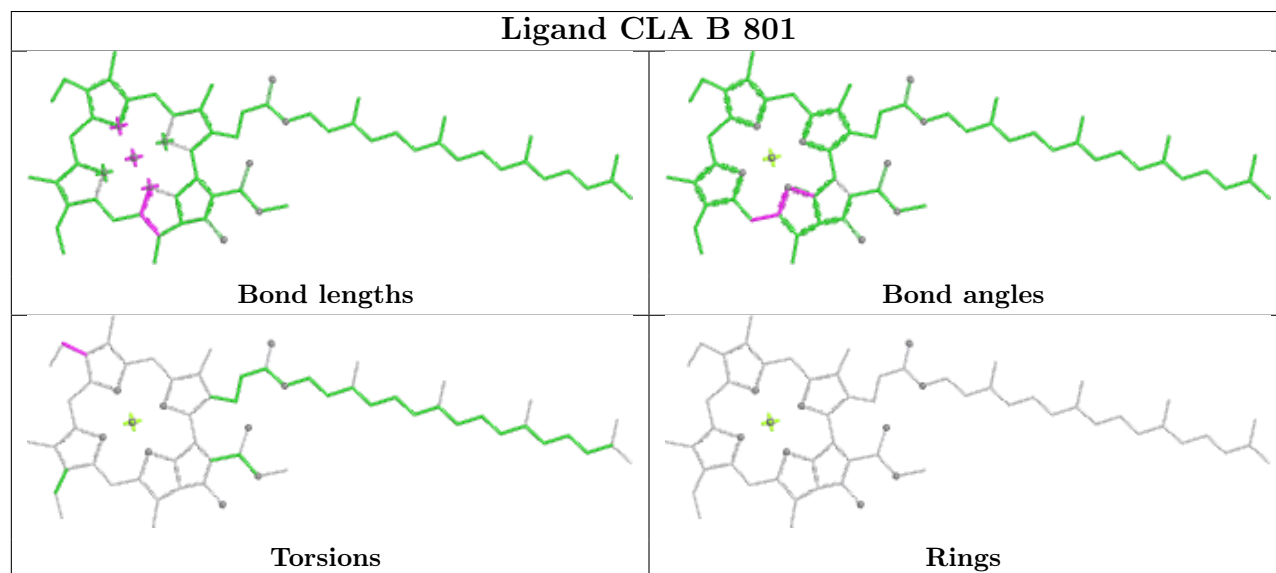
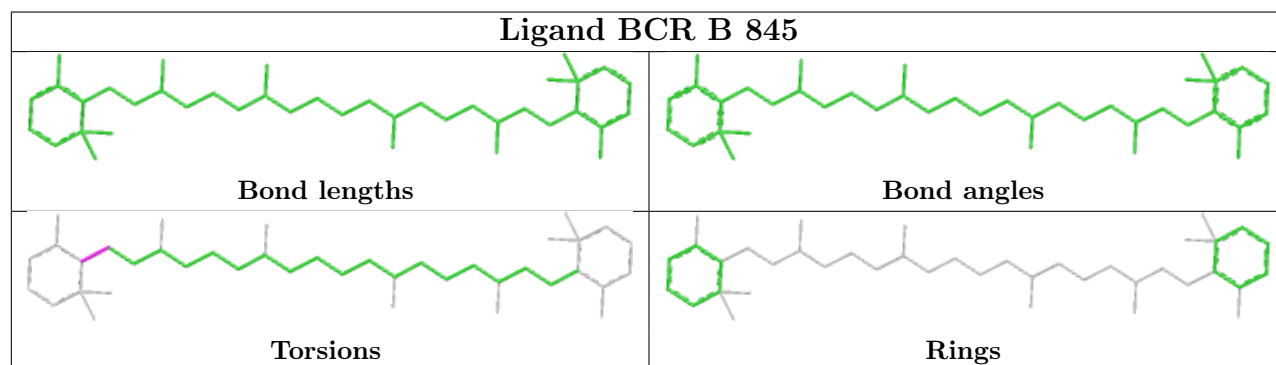
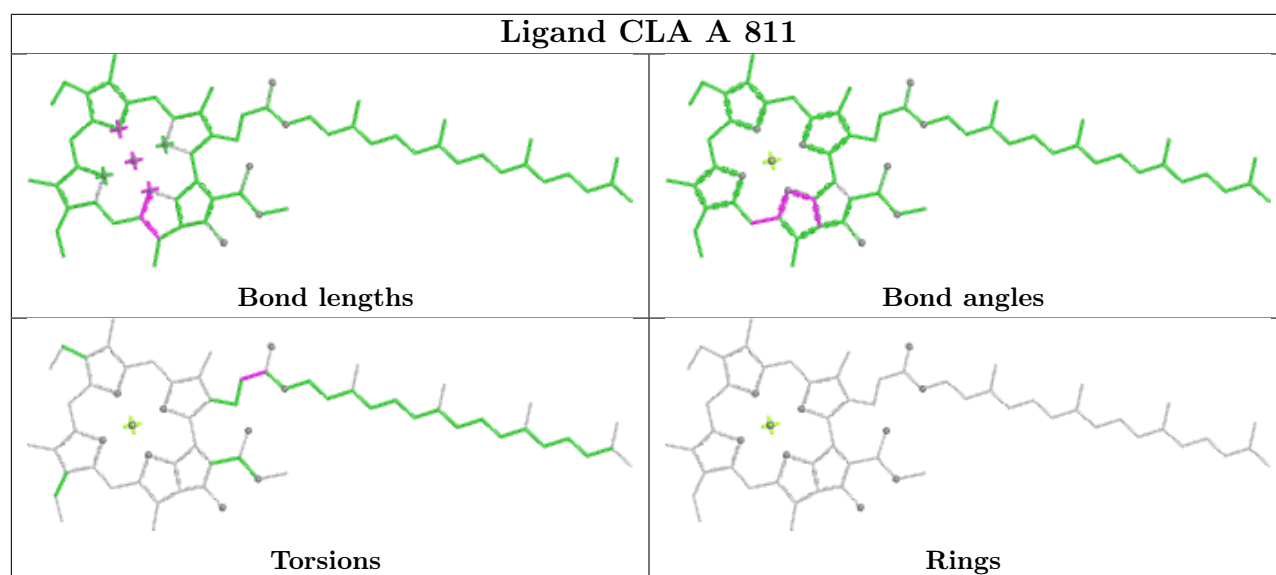
Bond angles



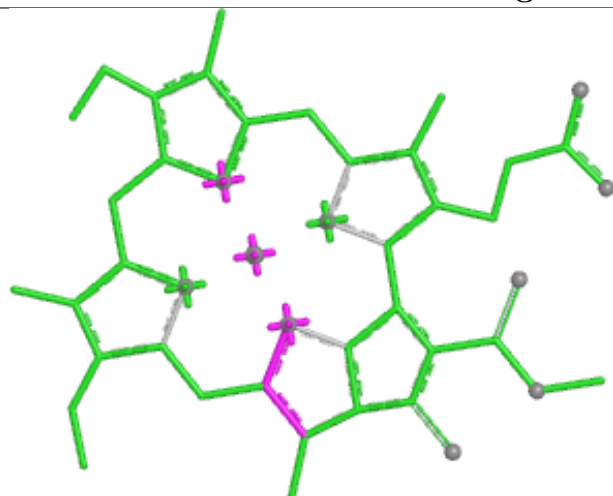
Torsions



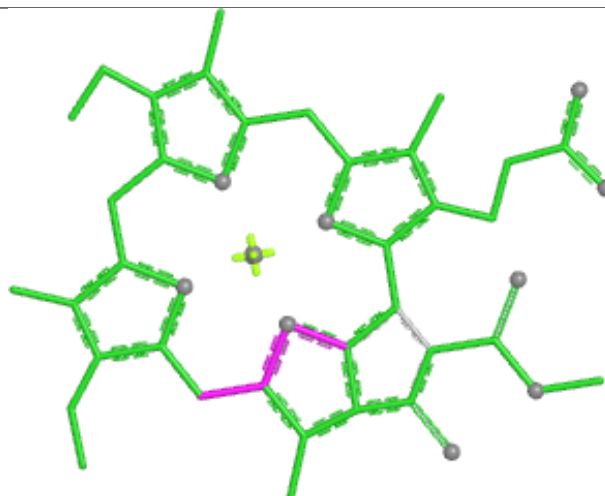
Rings



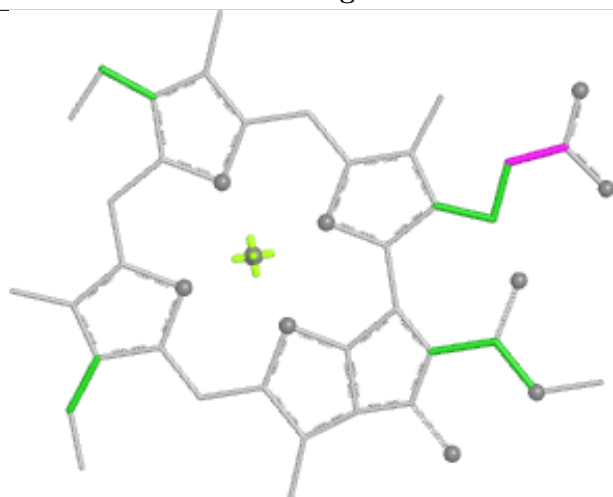
Ligand CLA F 203



Bond lengths



Bond angles

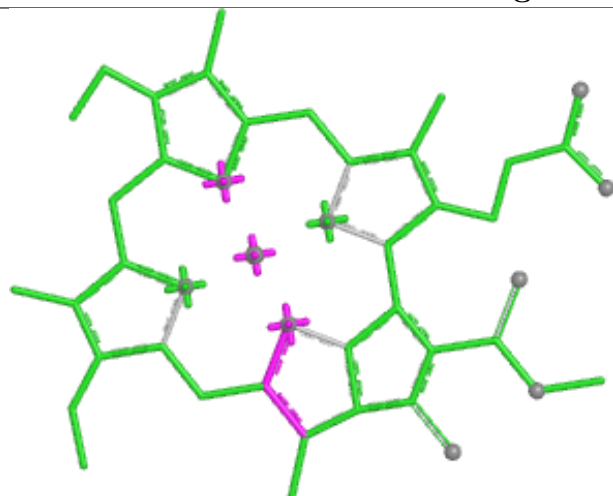


Torsions

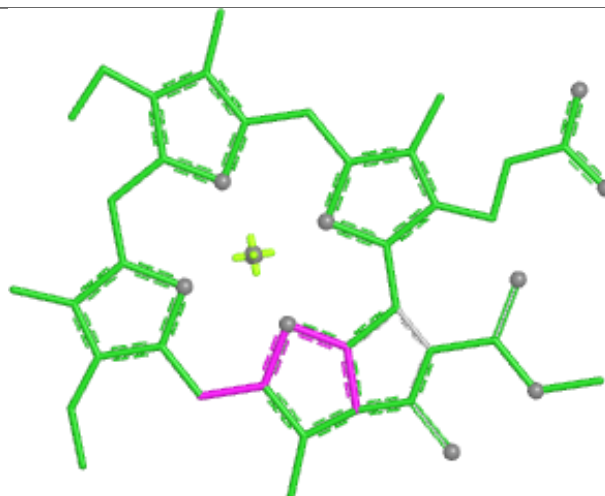


Rings

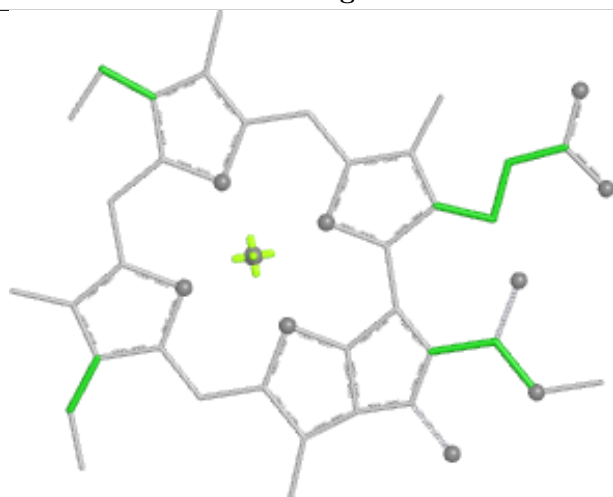
Ligand CLA A 861



Bond lengths



Bond angles

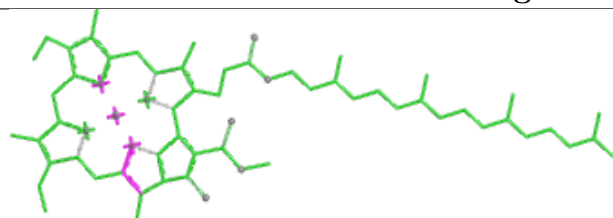


Torsions

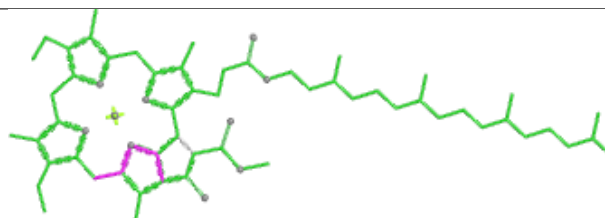


Rings

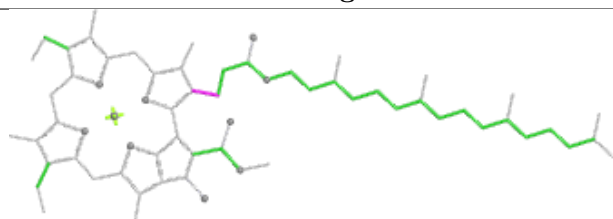
Ligand CLA A 808



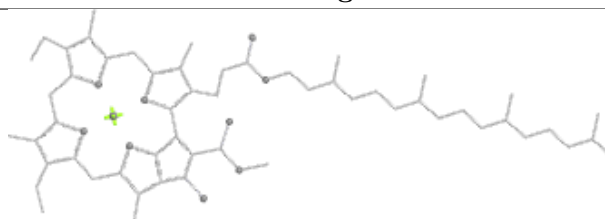
Bond lengths



Bond angles

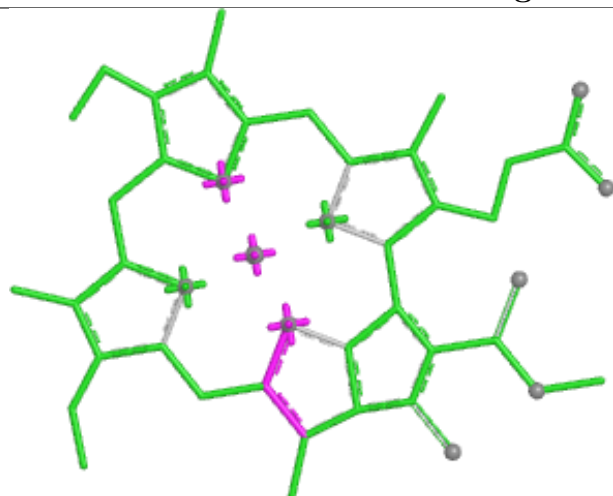


Torsions

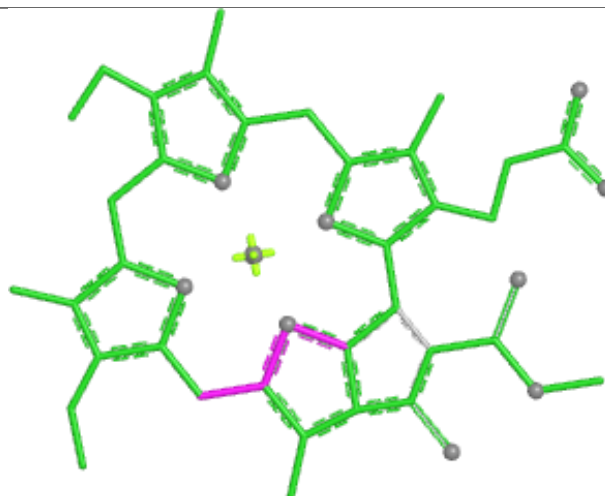


Rings

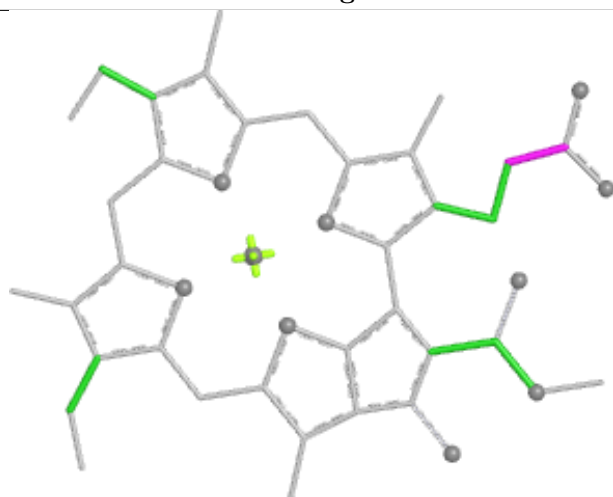
Ligand CLA B 837



Bond lengths



Bond angles

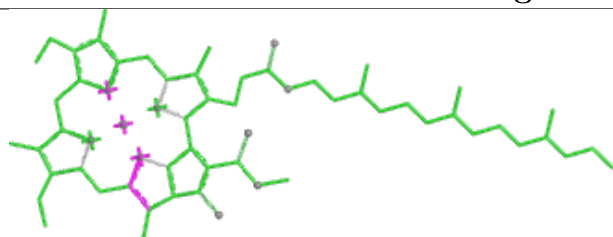


Torsions

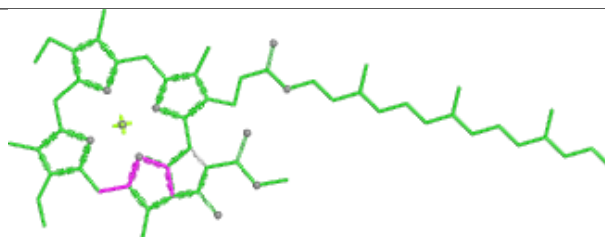


Rings

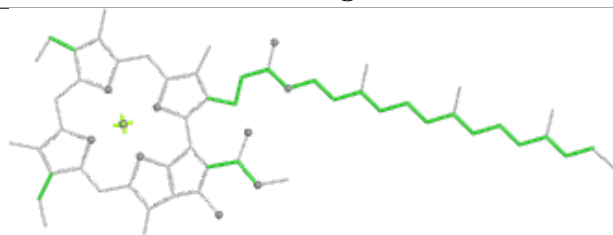
Ligand CLA B 839



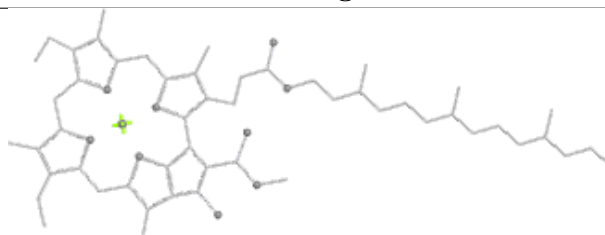
Bond lengths



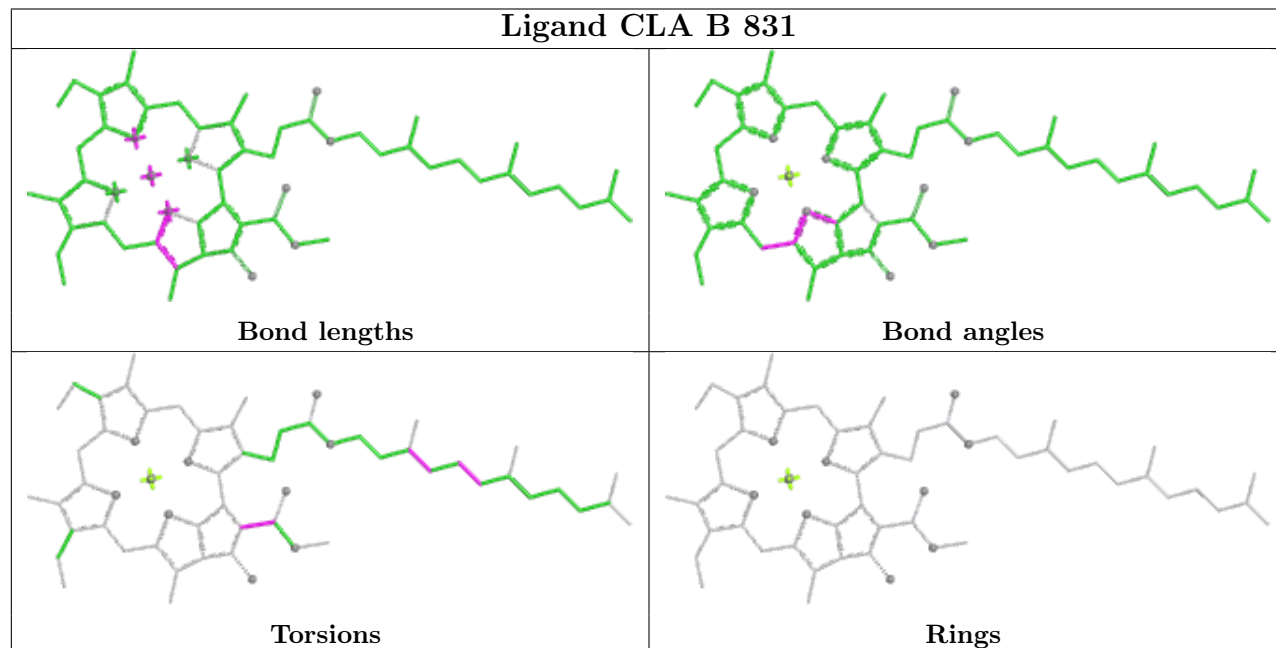
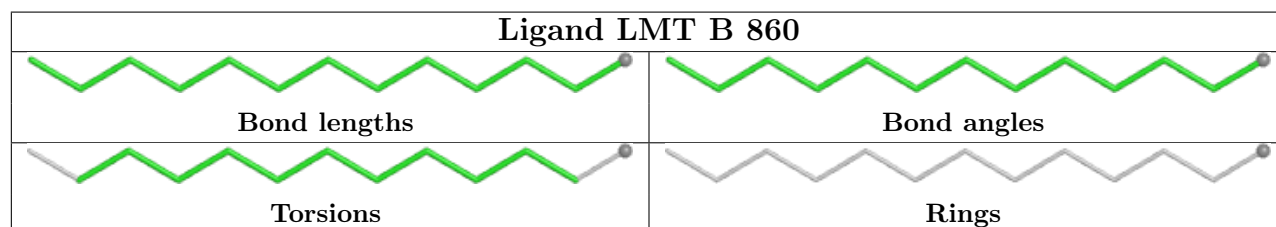
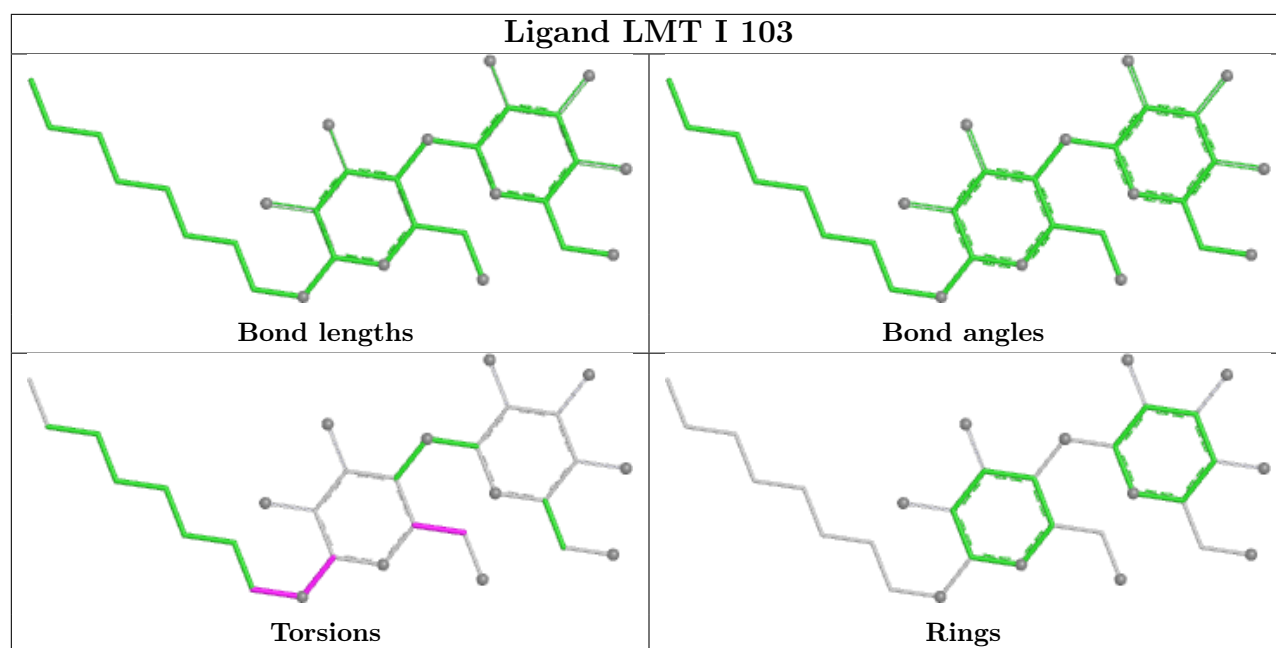
Bond angles



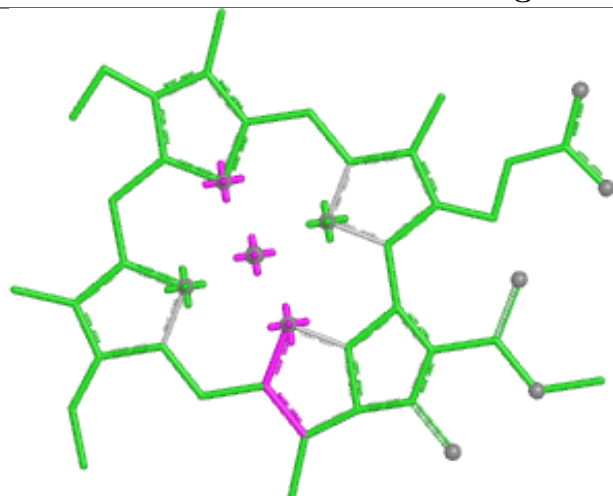
Torsions



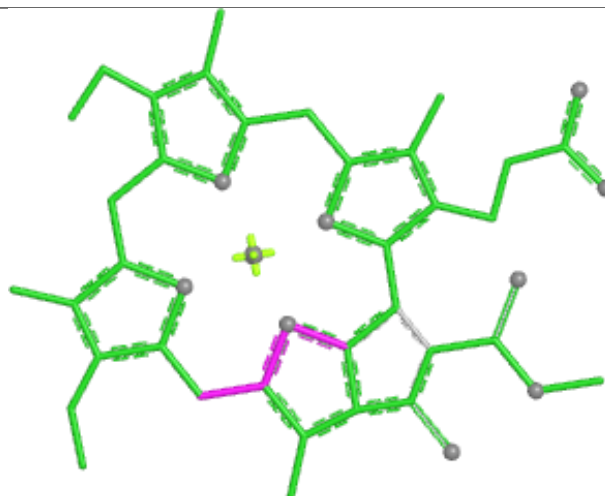
Rings



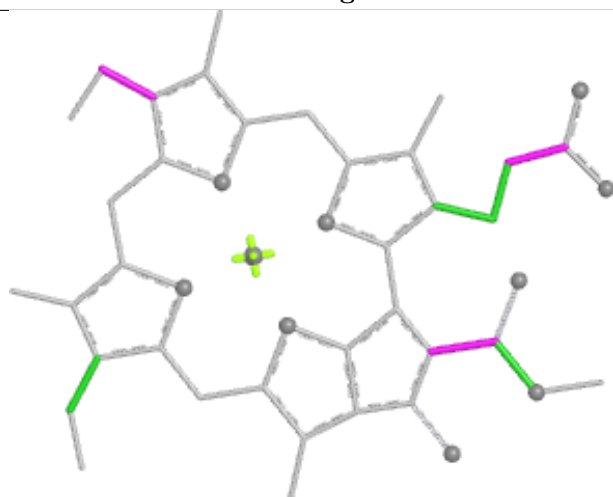
Ligand CLA B 842



Bond lengths



Bond angles

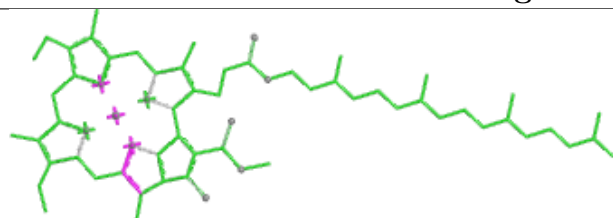


Torsions

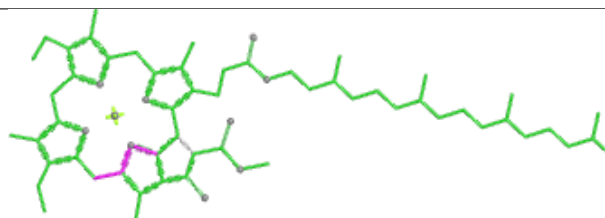


Rings

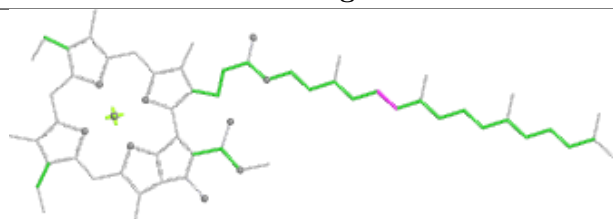
Ligand CLA B 834



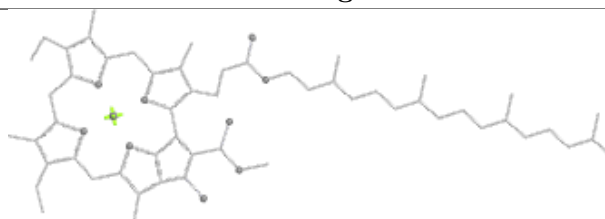
Bond lengths



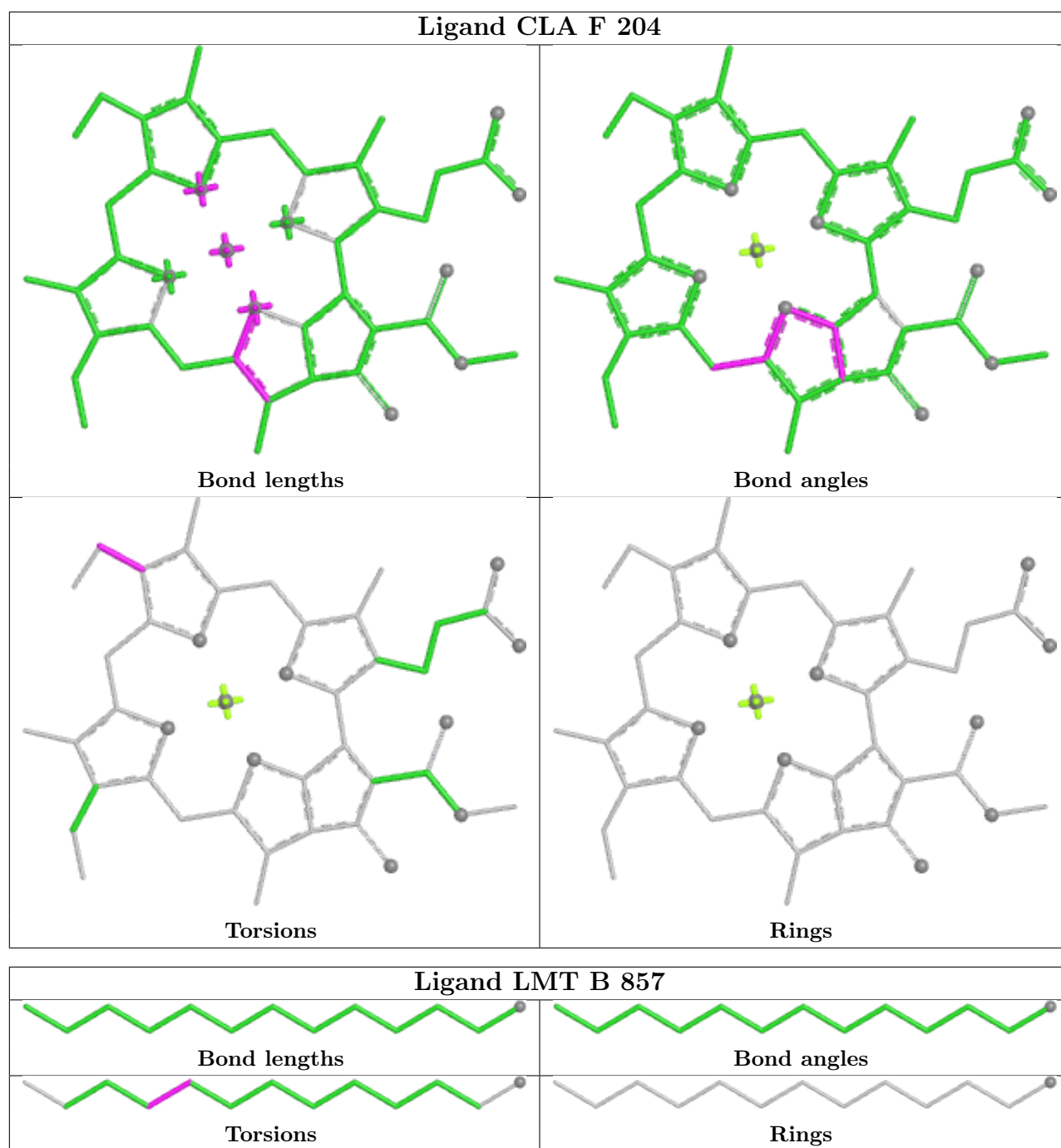
Bond angles

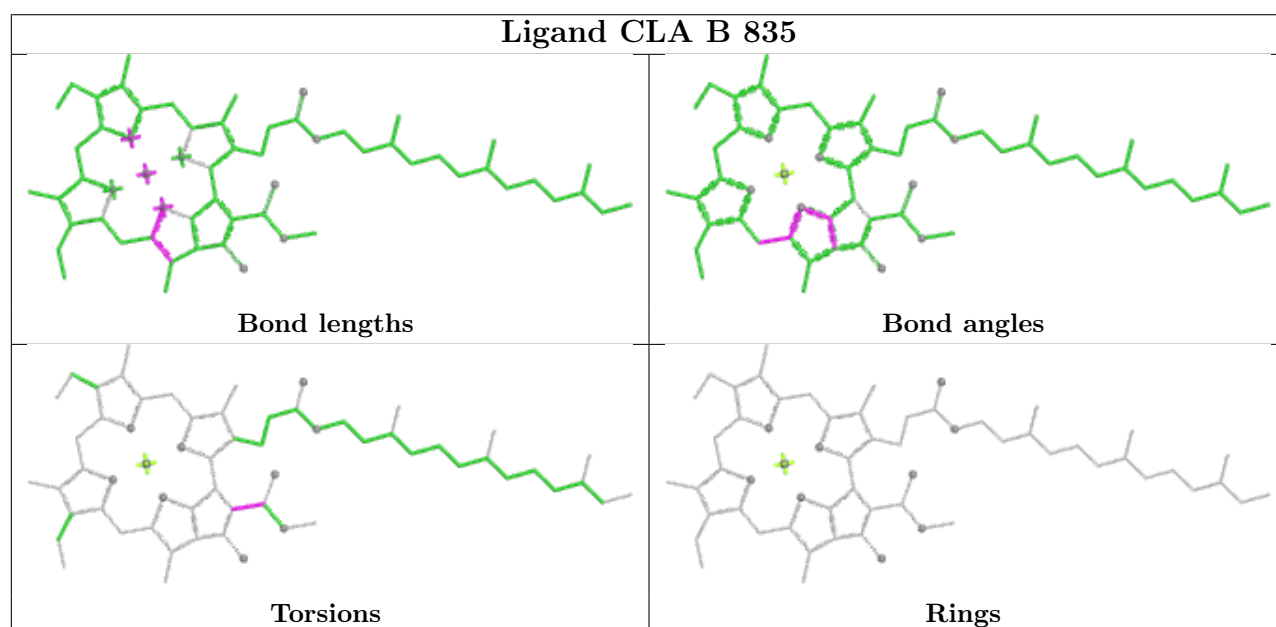
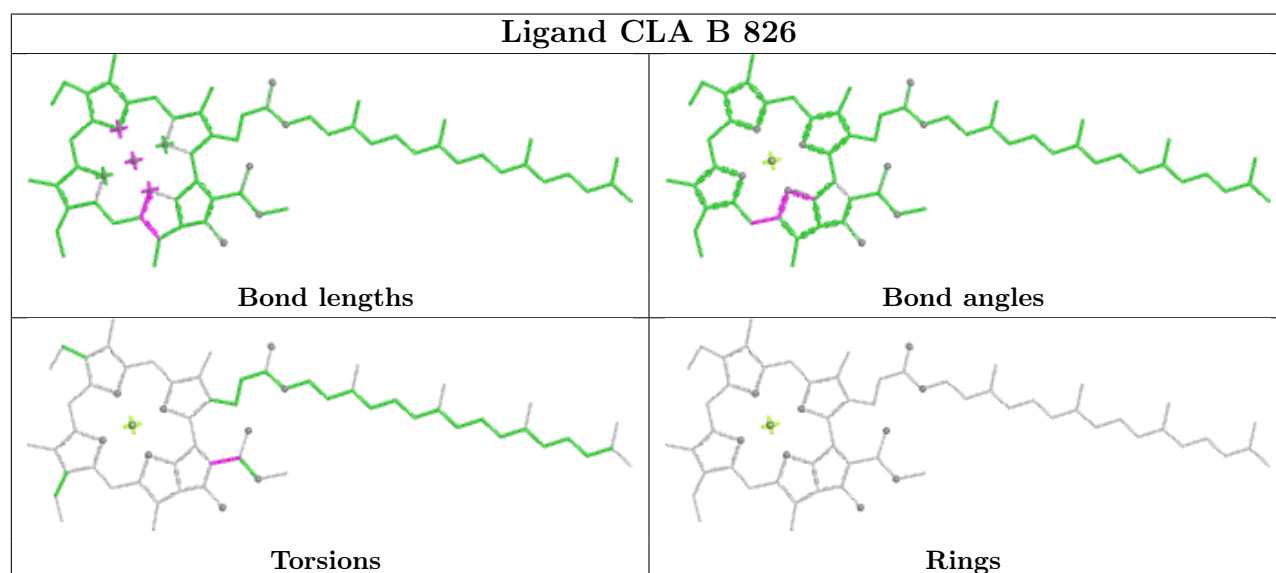
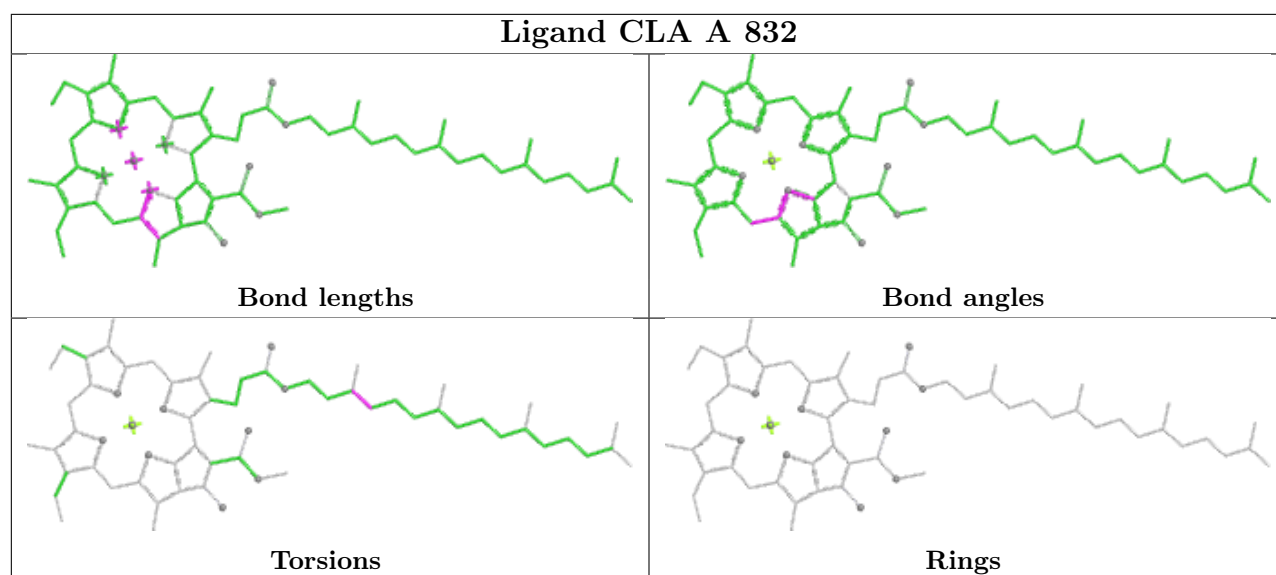


Torsions

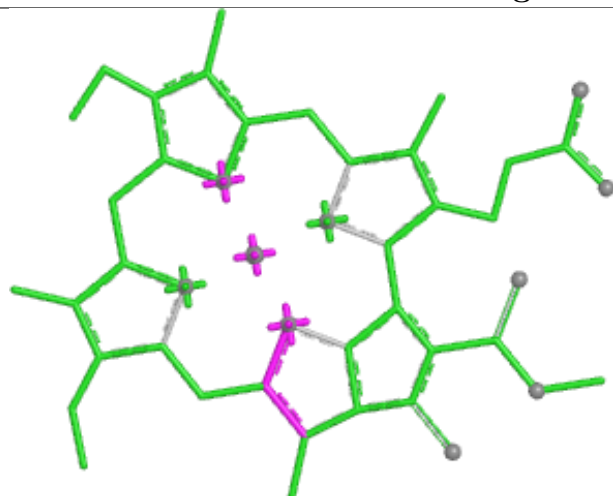


Rings

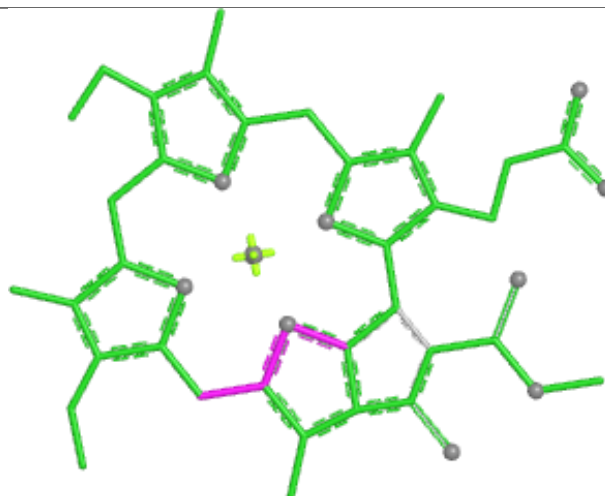




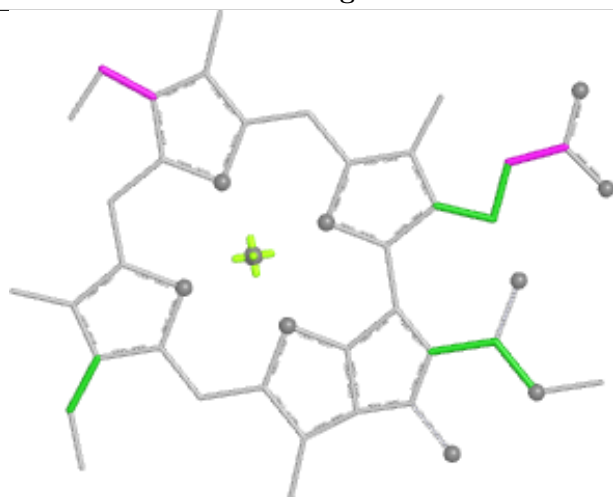
Ligand CLA K 101



Bond lengths



Bond angles

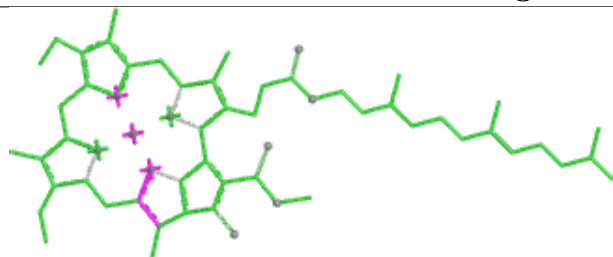


Torsions

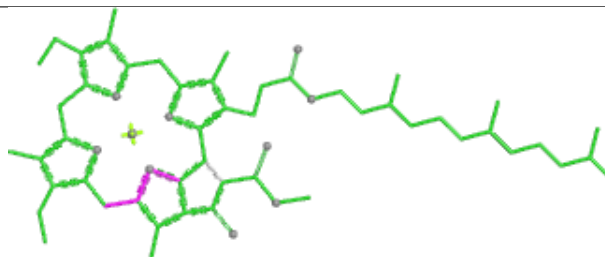


Rings

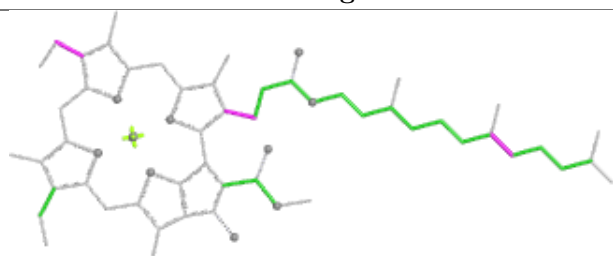
Ligand CLA B 824



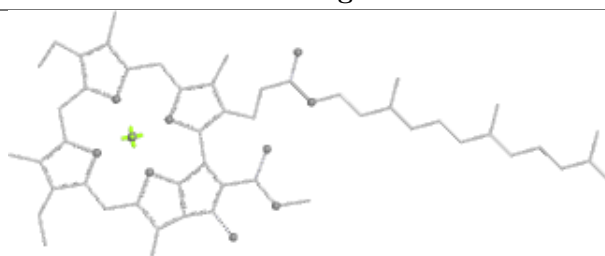
Bond lengths



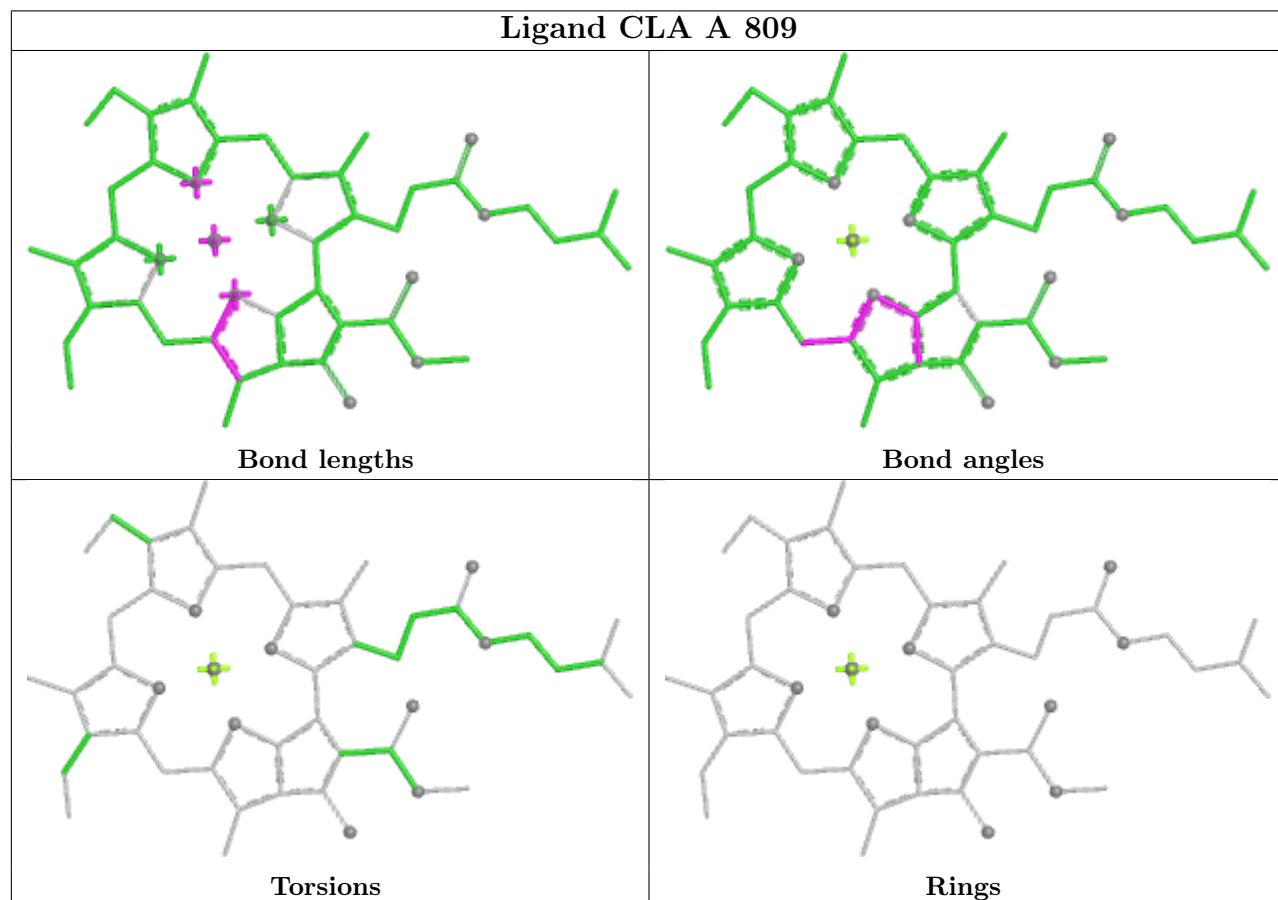
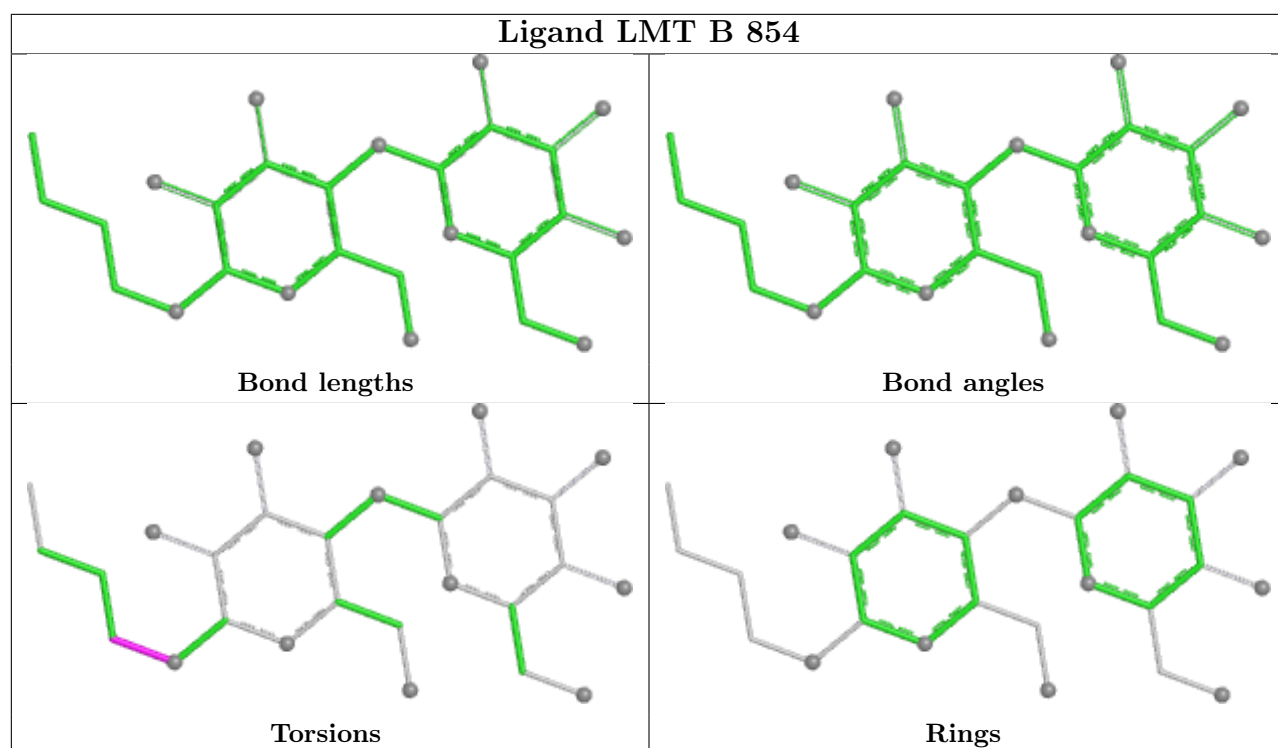
Bond angles

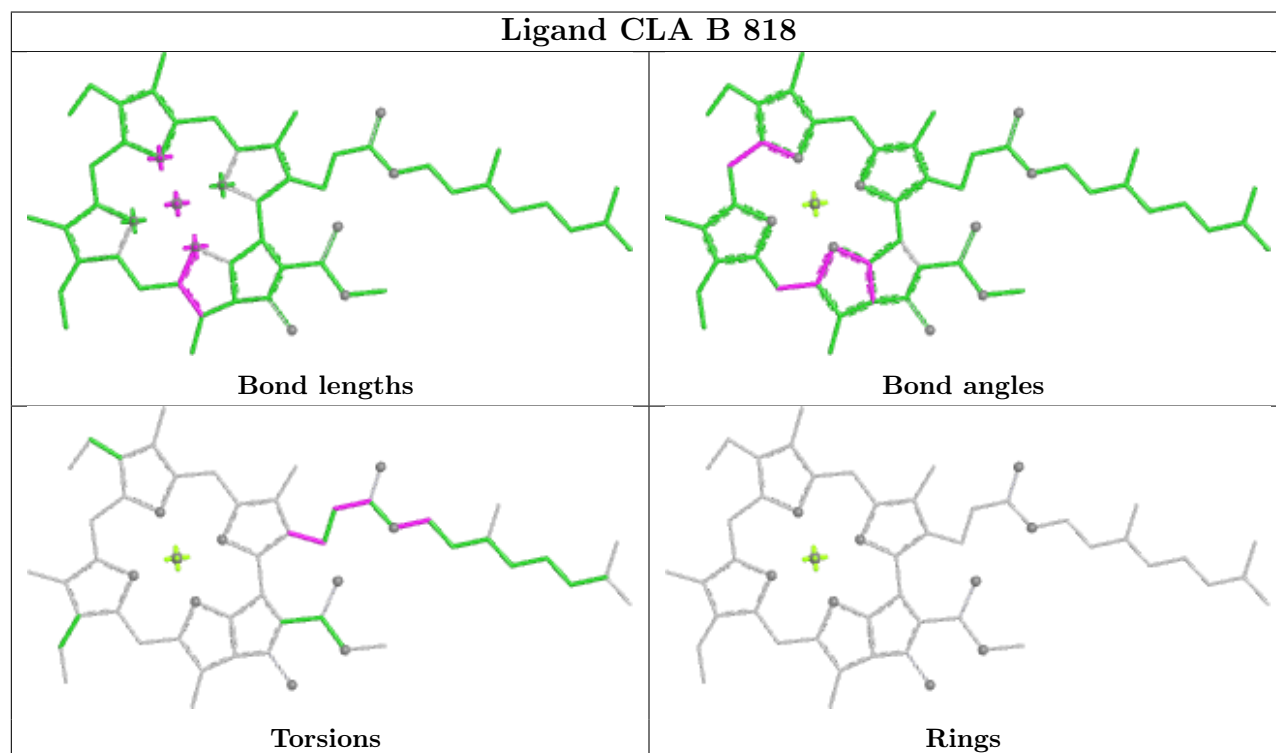
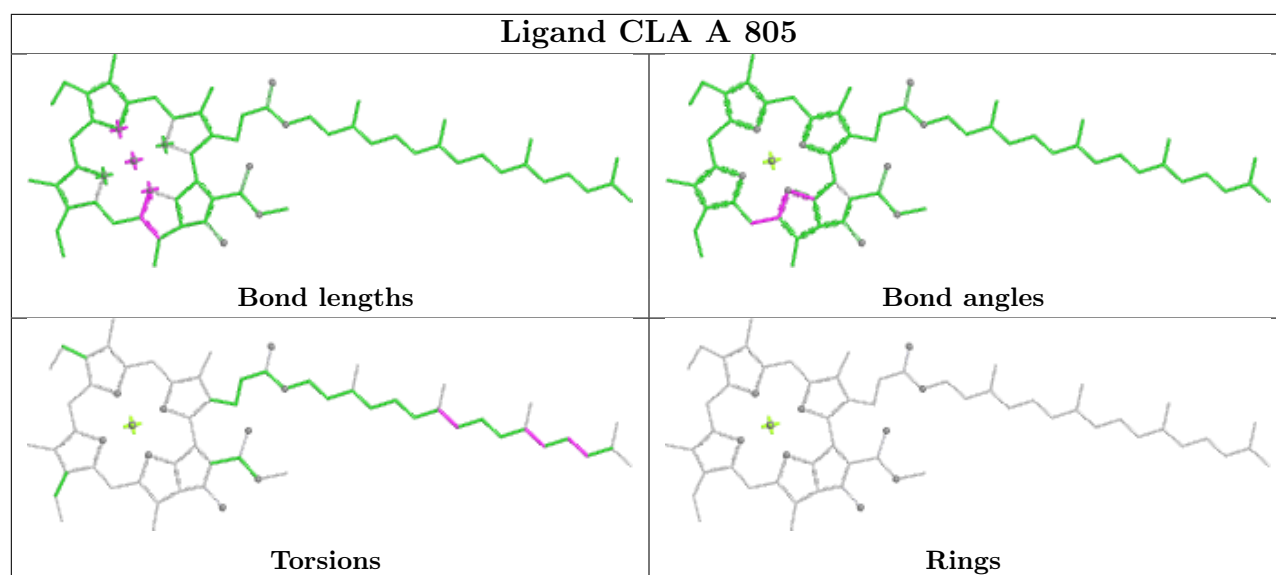


Torsions

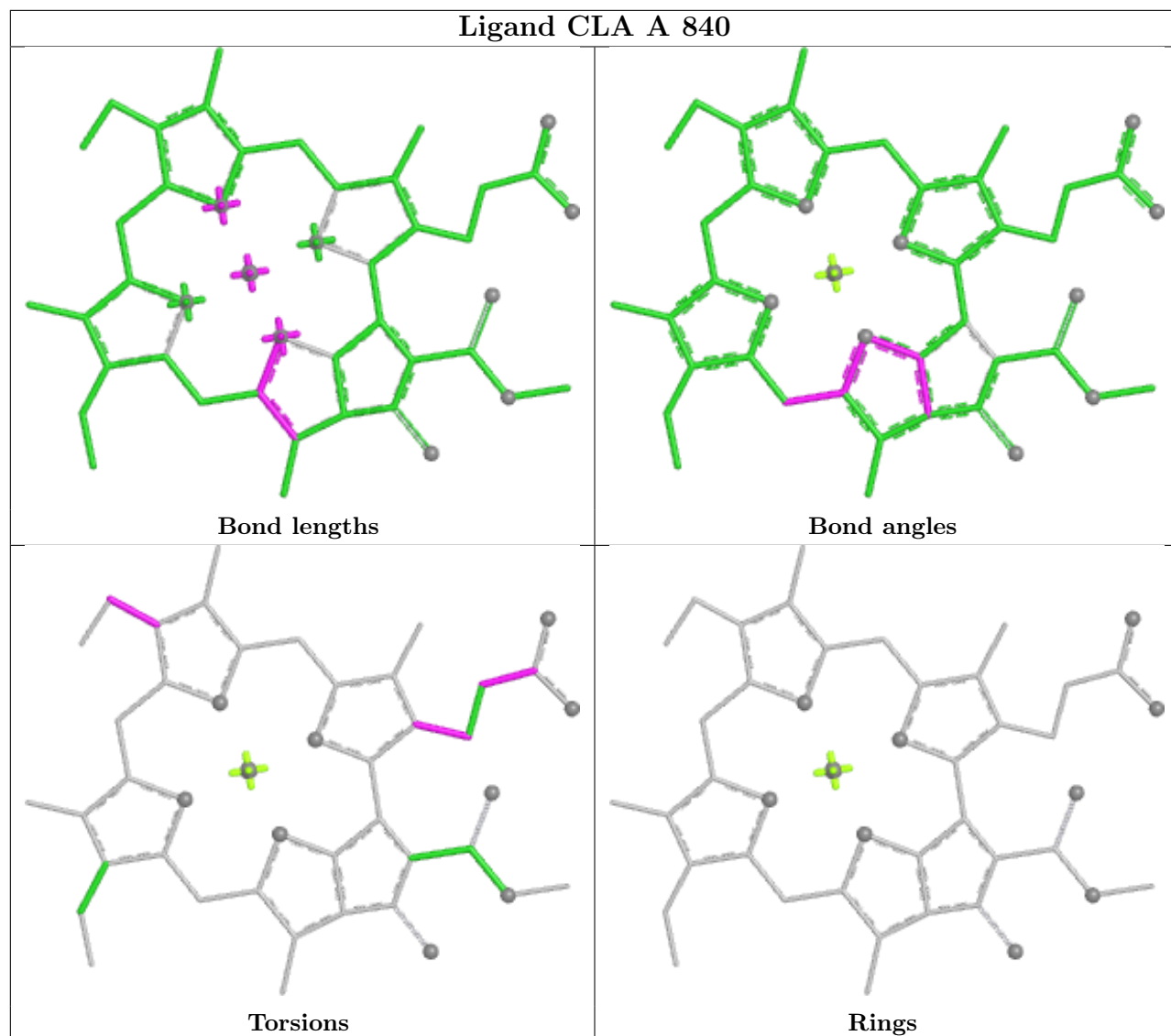


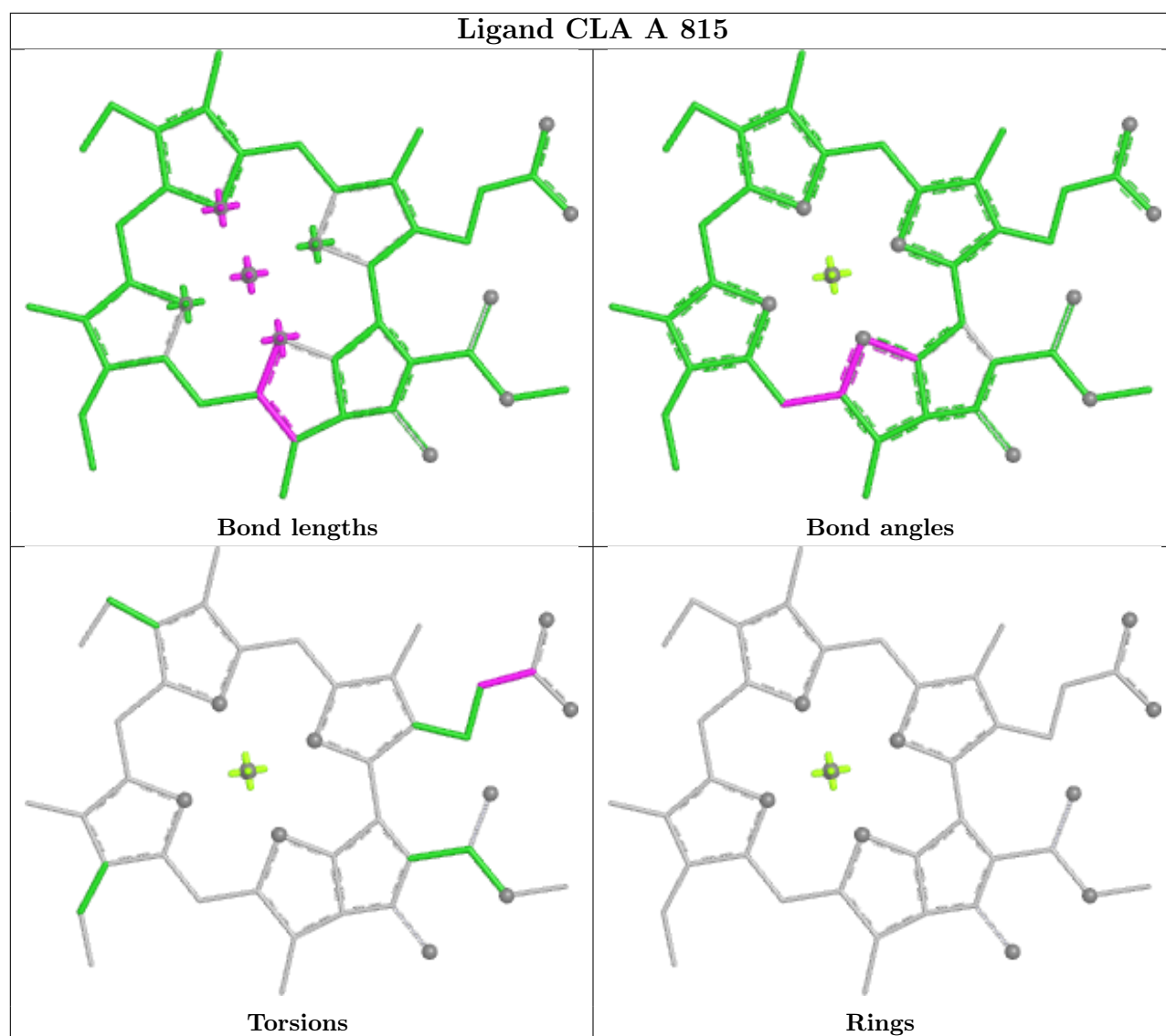
Rings





Ligand CLA A 840





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.

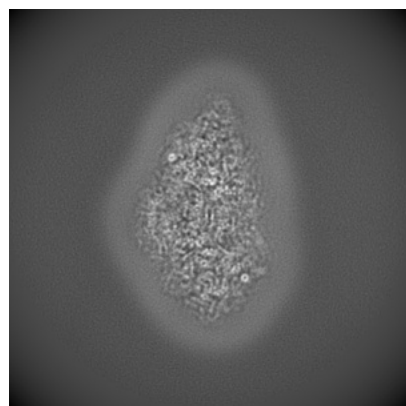
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60522. These allow visual inspection of the internal detail of the map and identification of artifacts.

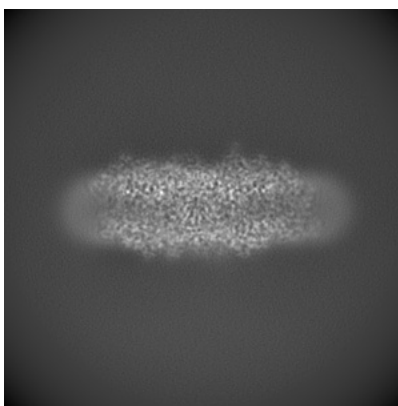
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

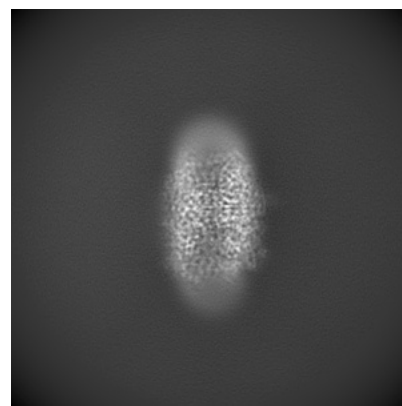
6.1.1 Primary map



X

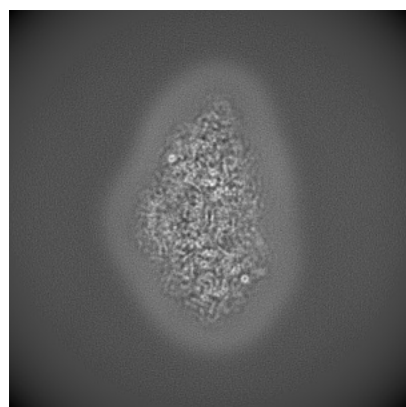


Y

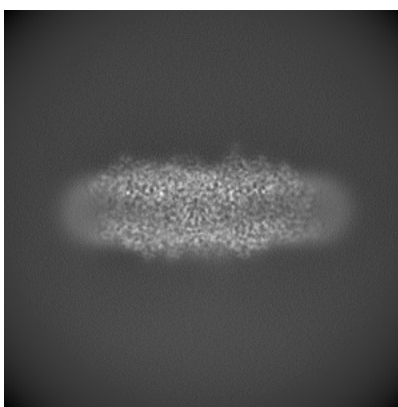


Z

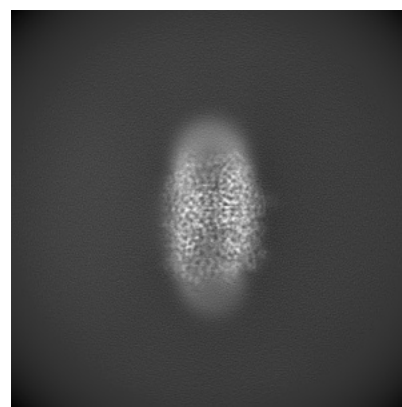
6.1.2 Raw map



X



Y

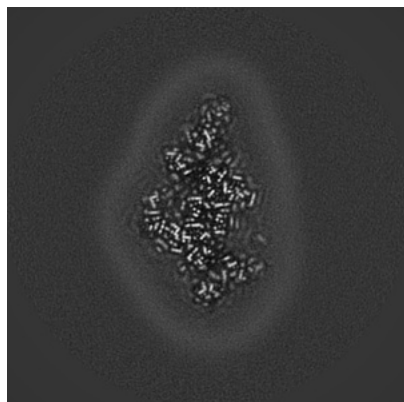


Z

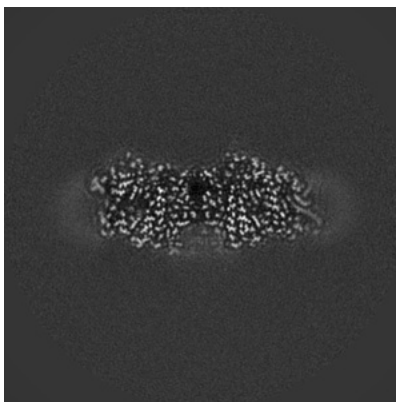
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

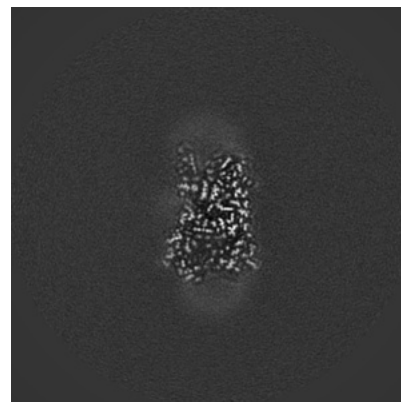
6.2.1 Primary map



X Index: 175

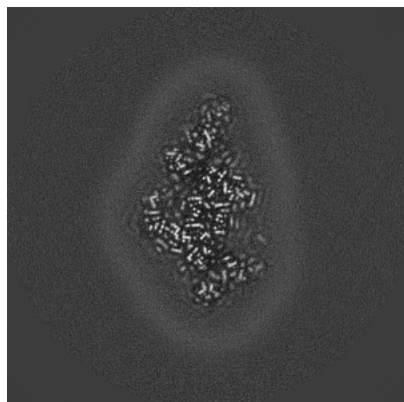


Y Index: 175

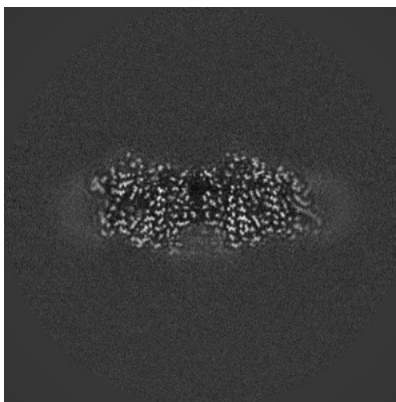


Z Index: 175

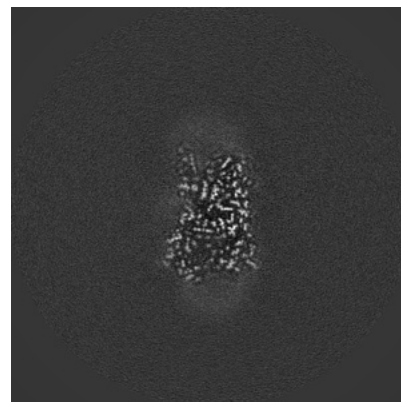
6.2.2 Raw map



X Index: 175



Y Index: 175

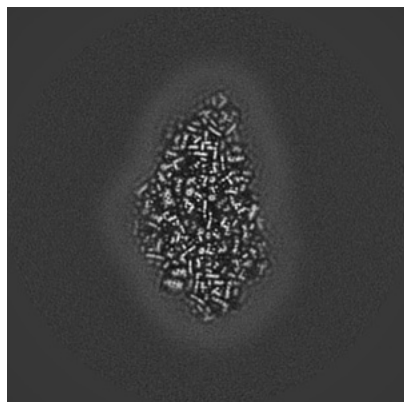


Z Index: 175

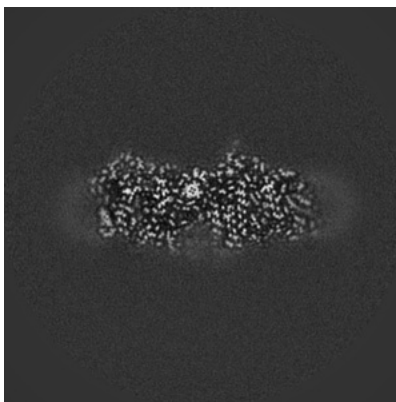
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

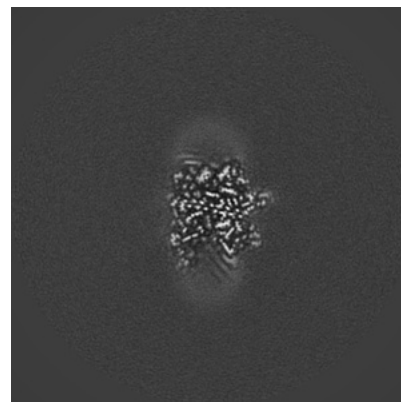
6.3.1 Primary map



X Index: 190

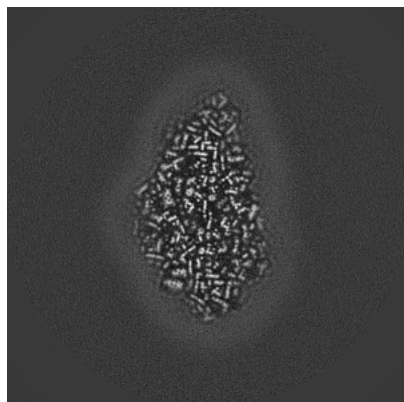


Y Index: 177

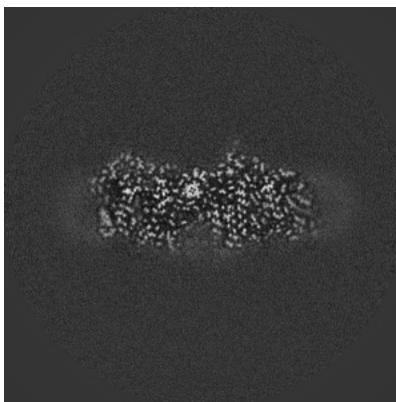


Z Index: 198

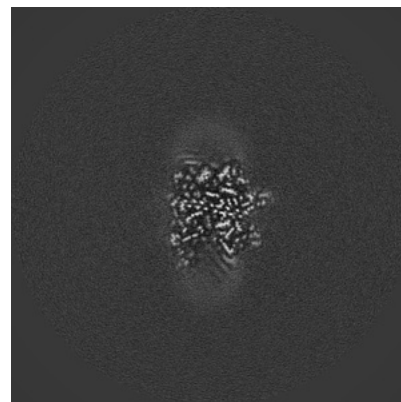
6.3.2 Raw map



X Index: 190



Y Index: 177

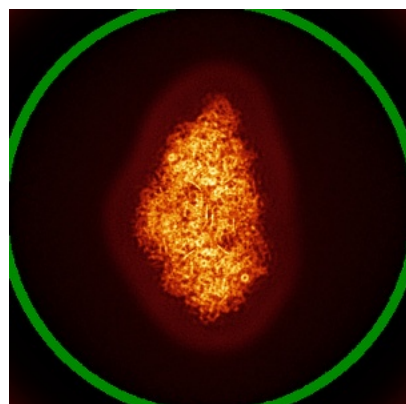


Z Index: 198

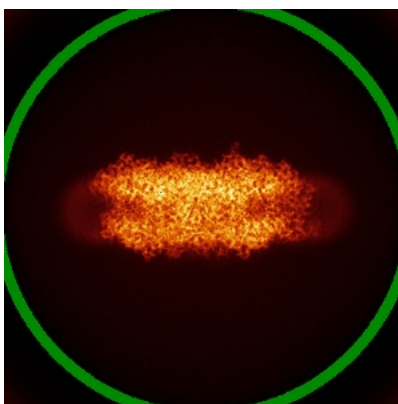
The images above show the largest variance slices of the map in three orthogonal directions.

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

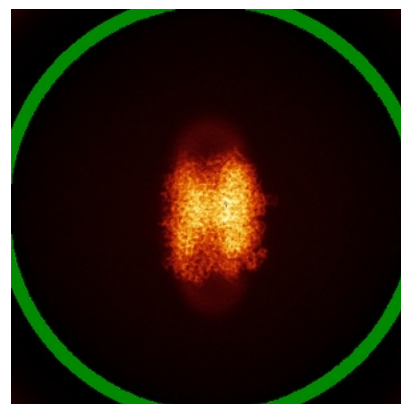
6.4.1 Primary map



X

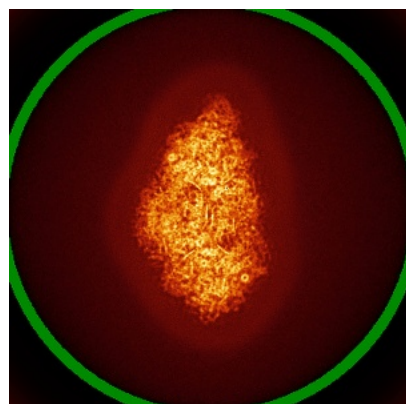


Y

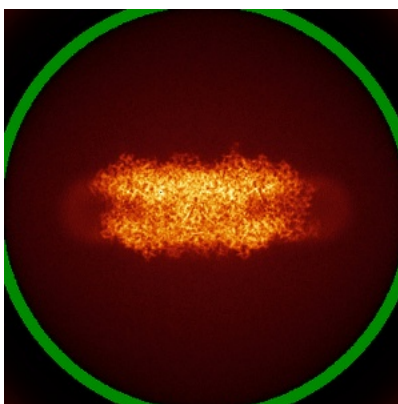


Z

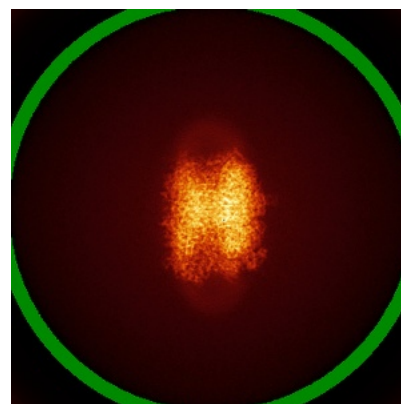
6.4.2 Raw map



X



Y



Z

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

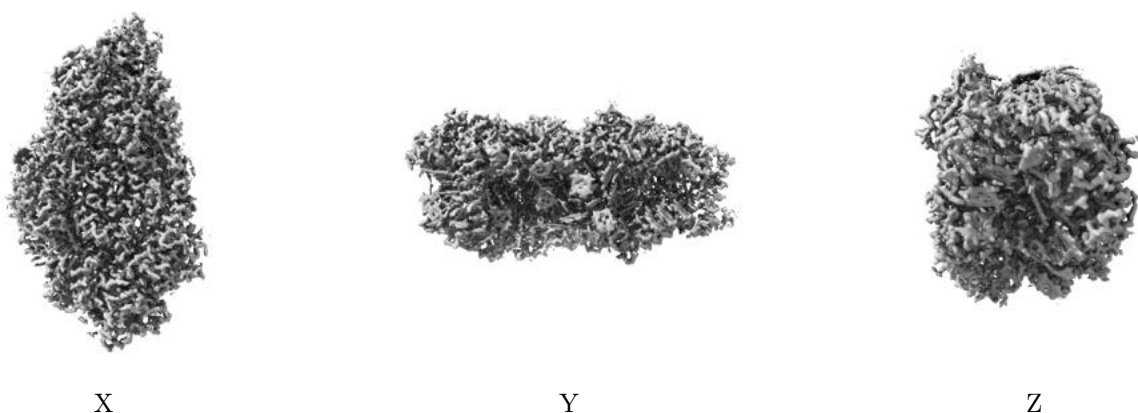
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

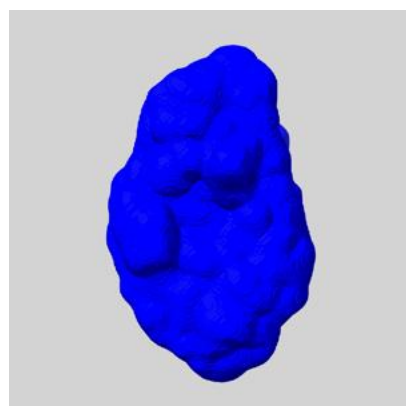
6.6 Mask visualisation [i](#)

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

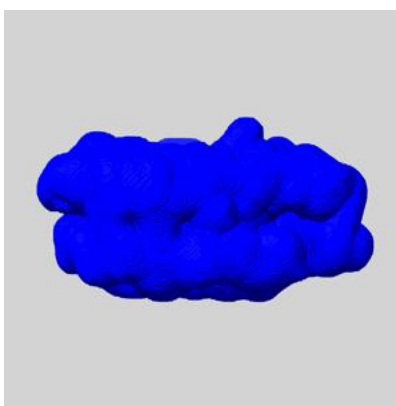
A mask typically either:

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

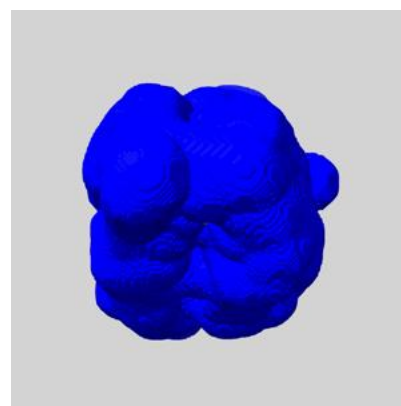
6.6.1 emd_60522_msk_1.map [i](#)



X



Y

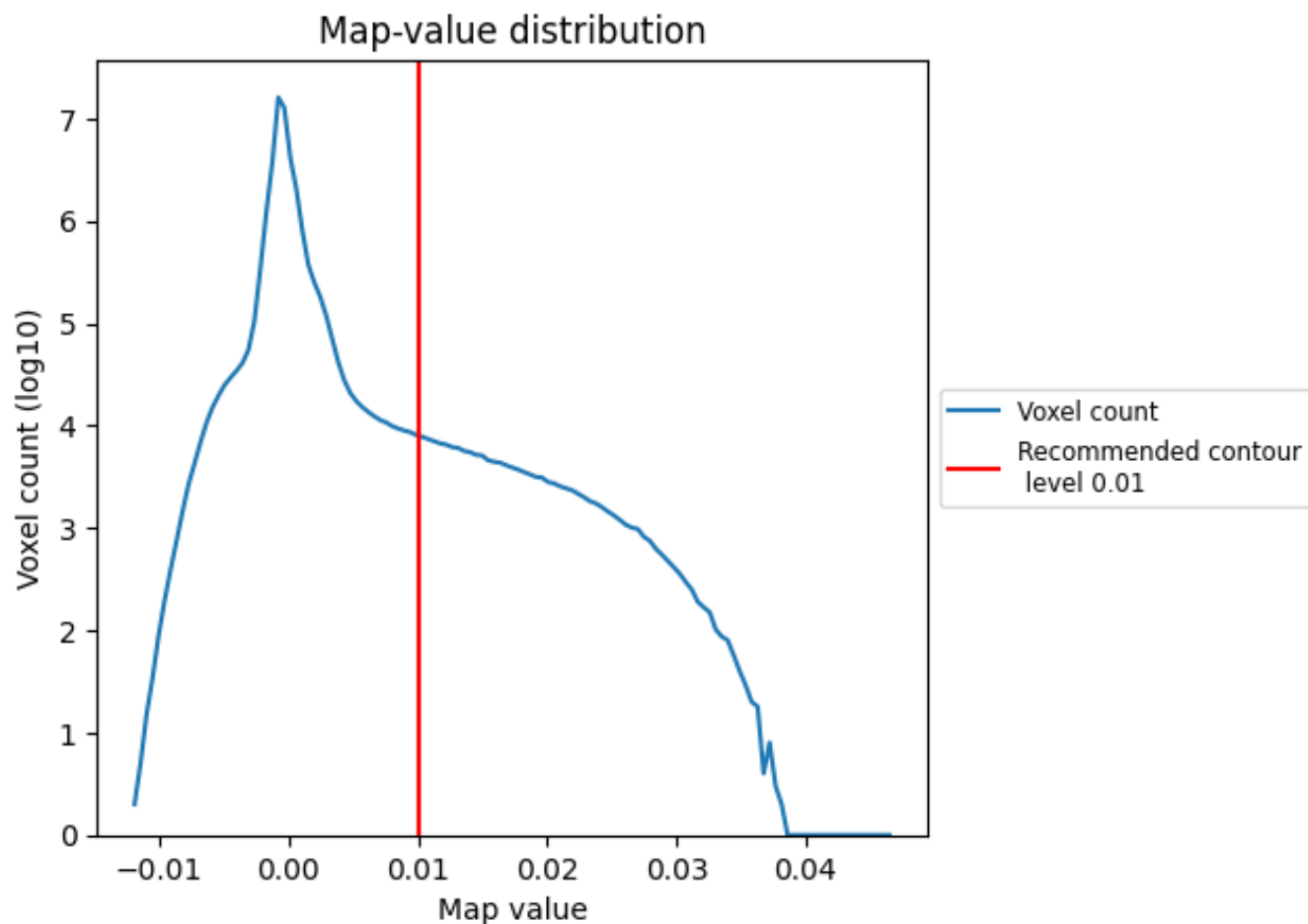


Z

7 Map analysis [i](#)

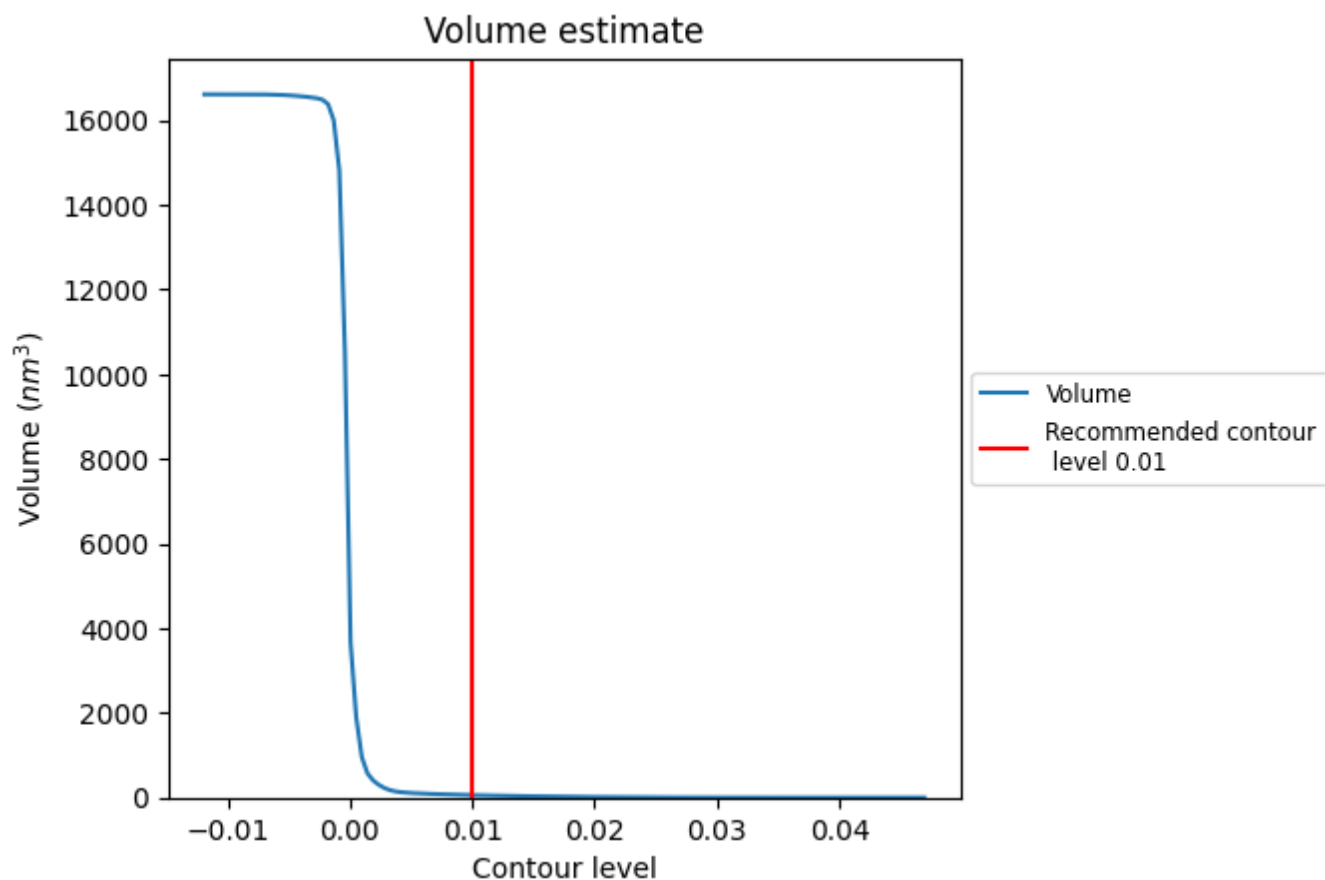
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

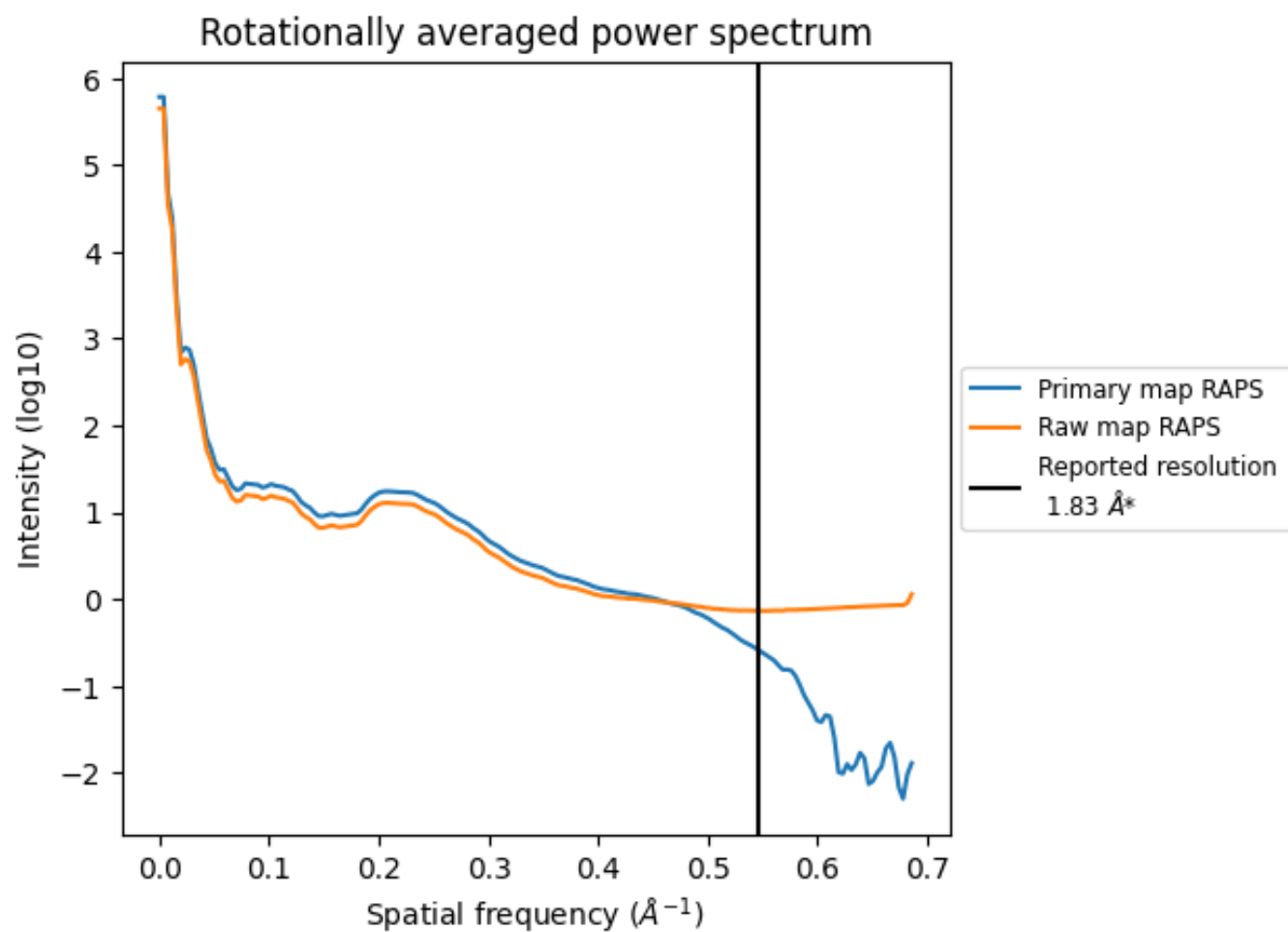
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm³; this corresponds to an approximate mass of 52 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

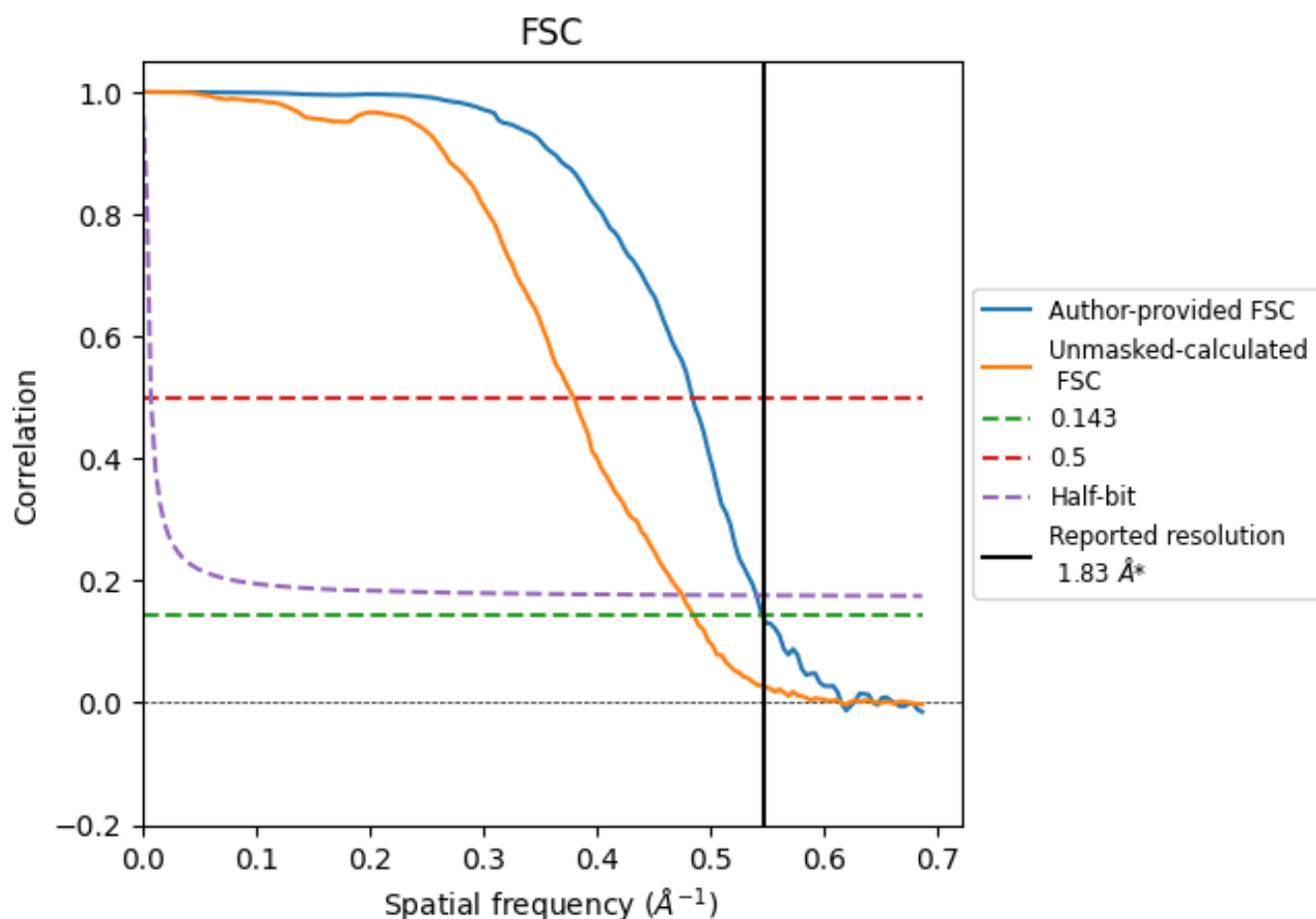


*Reported resolution corresponds to spatial frequency of 0.546 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.546 Å⁻¹

8.2 Resolution estimates [i](#)

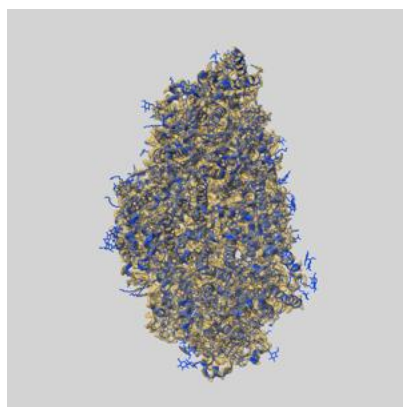
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	1.83	2.07	1.85
Unmasked-calculated*	2.06	2.64	2.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.06 differs from the reported value 1.83 by more than 10 %

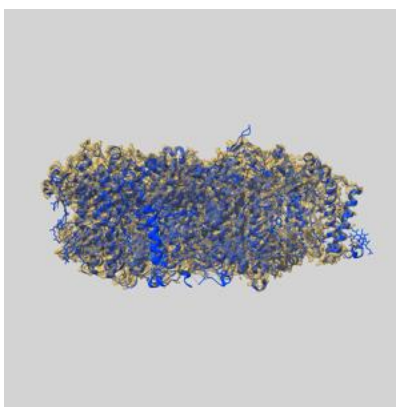
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60522 and PDB model 8ZWB. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

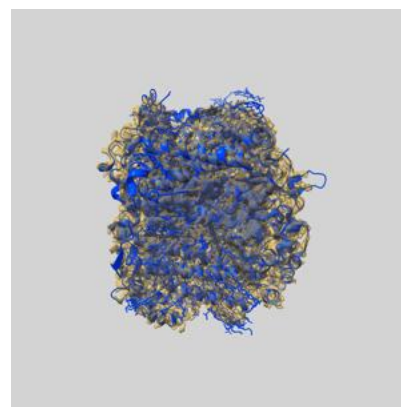
9.1 Map-model overlay [i](#)



X



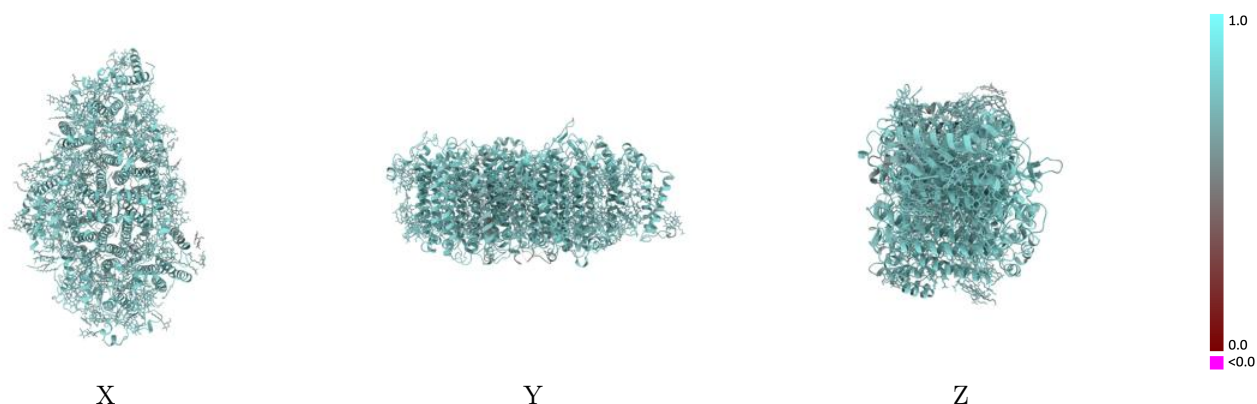
Y



Z

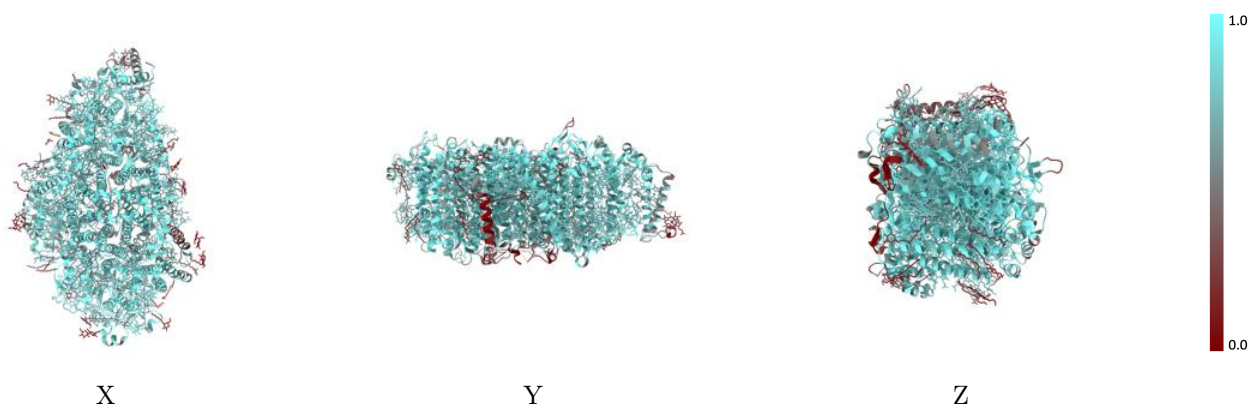
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



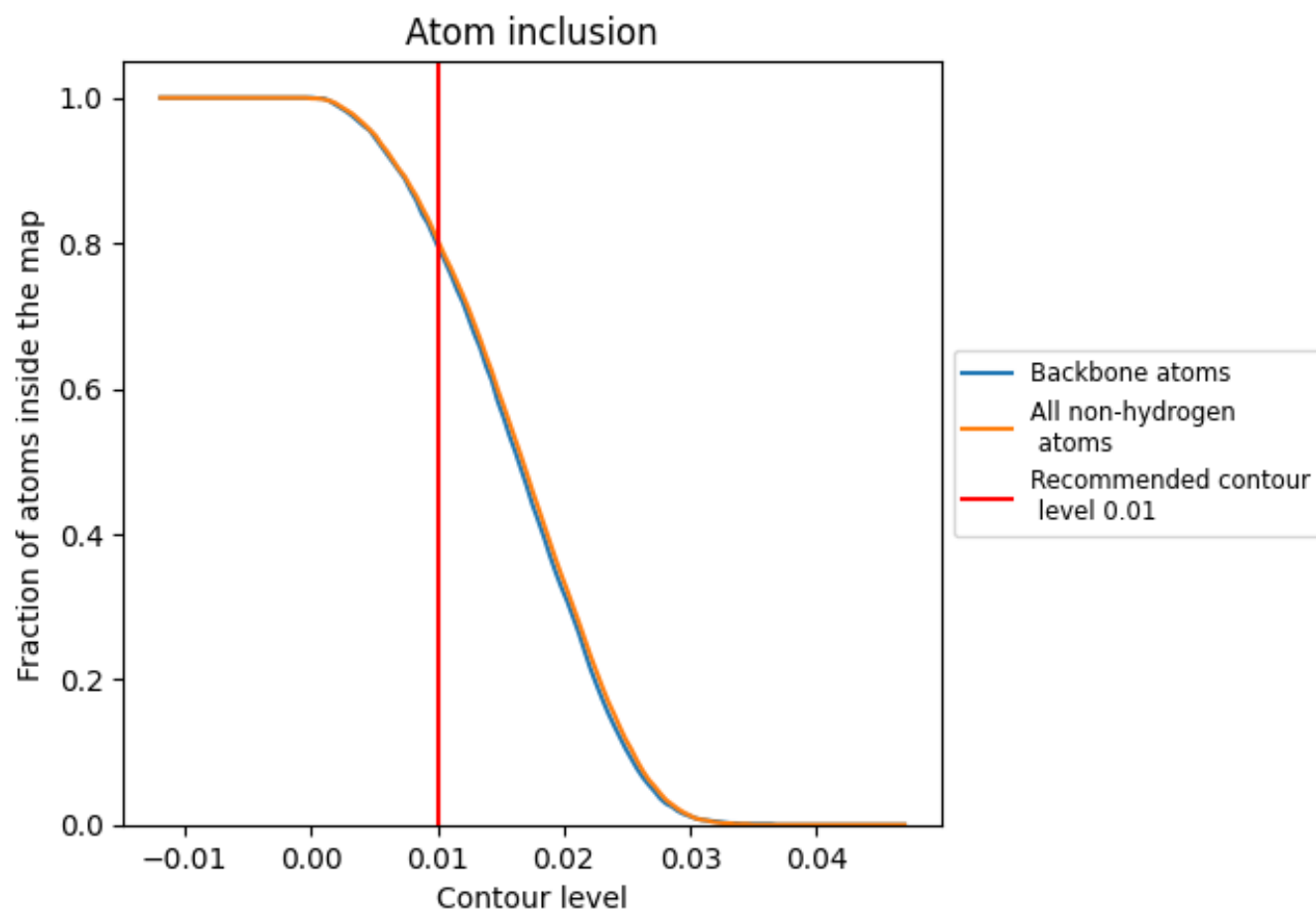
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.7450
A	0.8480	0.7550
B	0.8240	0.7490
F	0.7400	0.7330
I	0.2070	0.6250
J	0.7130	0.7220
K	0.5660	0.7020
M	0.5810	0.7170

1.0

0.0

<0.0