



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 05:03 PM JST

PDB ID : 9XJ9 / pdb_00009xj9
EMDB ID : EMD-66932
Title : In situ structure of the PSI-LHCI-LHCII supercomplex from *Oryza sativa*
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-04
Resolution : 2.96 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

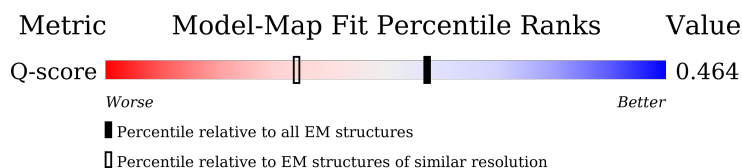
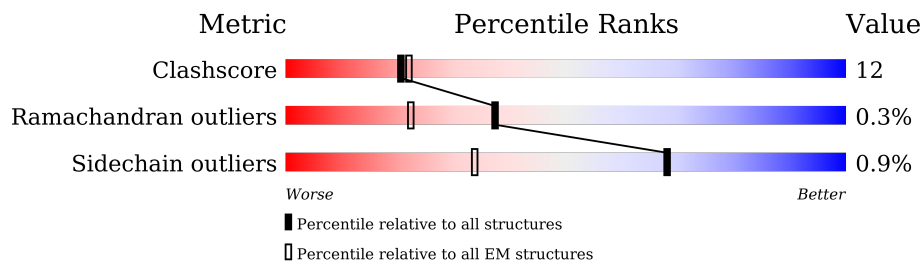
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



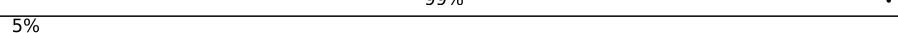
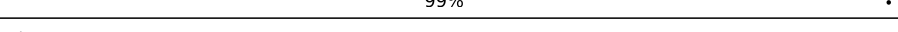
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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

Mol	Chain	Length	Quality of chain
1	1	200	78% 22%
2	2	207	75% 24% •
3	3	222	80% 20%
4	4	198	75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	742	 74%25%
6	B	732	 74%25%
7	C	80	 79%20%
8	D	143	 82%17%
9	E	66	 85%14%
10	F	158	 76%23%
11	G	97	 82%18%
12	H	93	 67%27%6%
13	I	30	 83%17%
14	J	44	 70%23%7%
15	K	88	 72%27%
16	L	163	 80%20%
17	N	84	 88%12%
18	O	92	 88%12%
19	X	218	 29%99%
19	Z	218	 5%99%
20	Y	222	 99%

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
22	CLA	1	307	X	-	-	-
22	CLA	1	317	X	-	-	-
22	CLA	1	318	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	318	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	312	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	844	X	-	-	-
22	CLA	A	846	X	-	-	-
22	CLA	A	849	X	-	-	-
22	CLA	A	850	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	A	857	X	-	-	-
22	CLA	A	858	X	-	-	-
22	CLA	A	859	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	845	X	-	-	-
22	CLA	B	847	X	-	-	-
22	CLA	B	848	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	B	851	X	-	-	-
22	CLA	B	852	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	L	306	X	-	-	-
22	CLA	O	207	X	-	-	-
22	CLA	O	208	X	-	-	-
22	CLA	Y	311	X	-	-	-
30	CL0	A	825	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 43745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	200	Total	C	N	O	S	0	0
			1560	1013	258	283	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	207	Total	C	N	O	S	0	0
			1612	1055	263	289	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	222	Total	C	N	O	S	0	0
			1723	1134	276	307	6		

- Molecule 4 is a protein called Chlorophyll A-B binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1570	1024	257	284	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5839	3824	992	1005	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	732	Total	C	N	O	S	0	0
			5856	3843	994	1006	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			602	371	104	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	726	197	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	65	Total	C	N	O	S	0	0
			518	329	92	97			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	158	Total	C	N	O	S	0	0
			1236	806	210	217	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	97	Total	C	N	O	S	0	0
			760	492	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	93	Total	C	N	O	S	0	0
			709	465	112	132			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	30	Total	C	N	O	S	0	0
			232	160	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	44	Total	C	N	O	S	0	0
			353	241	53	58	1		

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	88	Total	C	N	O	S	0	0
			620	392	107	117	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	163	Total	C	N	O	S	0	0
			1223	809	194	218	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			685	439	112	130	4		

- Molecule 18 is a protein called H0622F05.3 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	O	92	Total	C	N	O	0	0
			733	491	118	124		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	39	GLN	ARG	conflict	UNP Q01L93

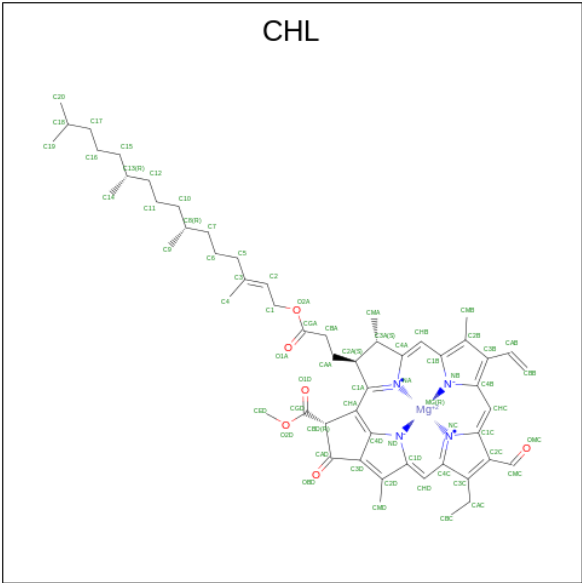
- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	218	Total	C	N	O	0	0
			1094	658	218	218		
19	Z	218	Total	C	N	O	0	0
			1094	658	218	218		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	222	Total	C	N	O	0	0
			1112	669	222	221		

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



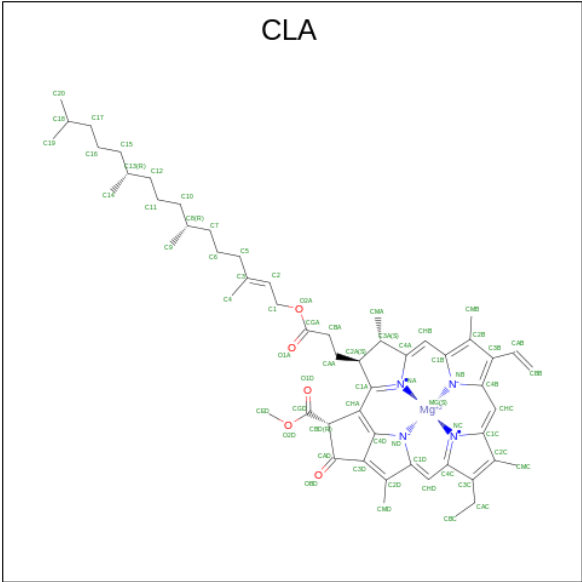
Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	4	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	X	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	X	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	X	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	X	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Z	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	Z	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	Z	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	Z	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 41	C 33	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

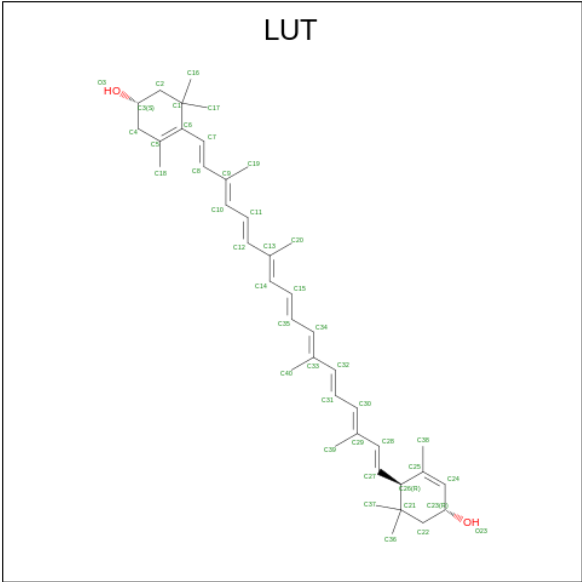
Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	O	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	X	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

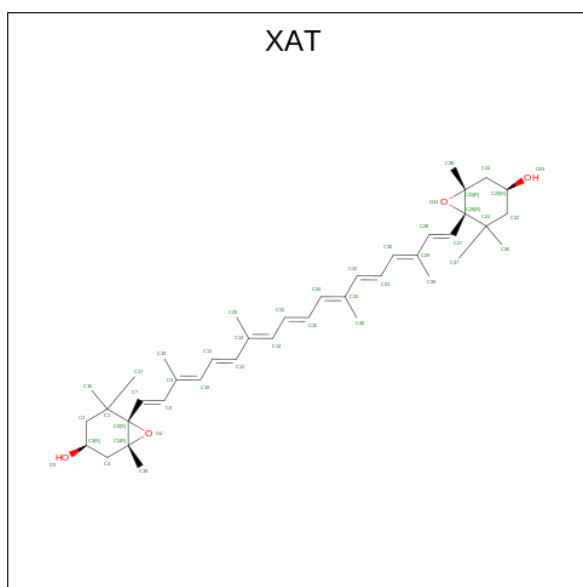
Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



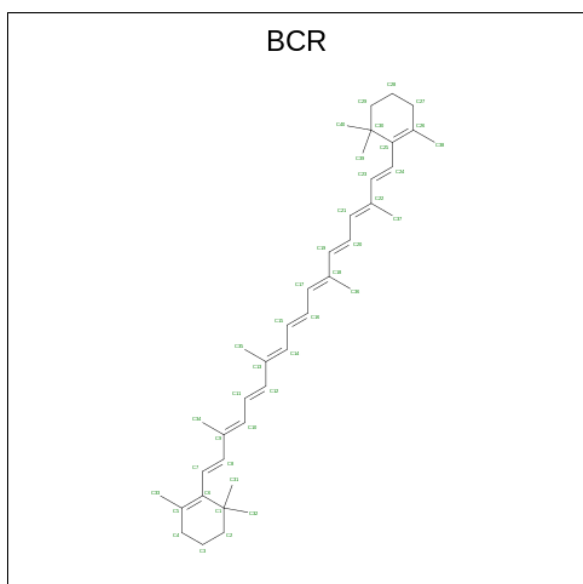
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			44	40	4	
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



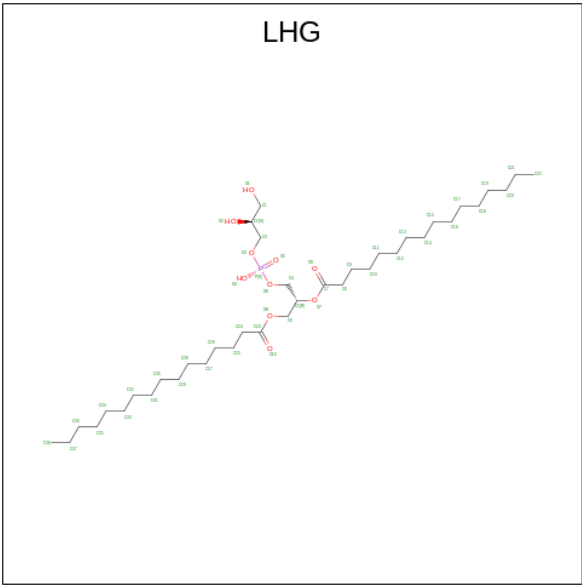
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 39 39	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 30 30	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



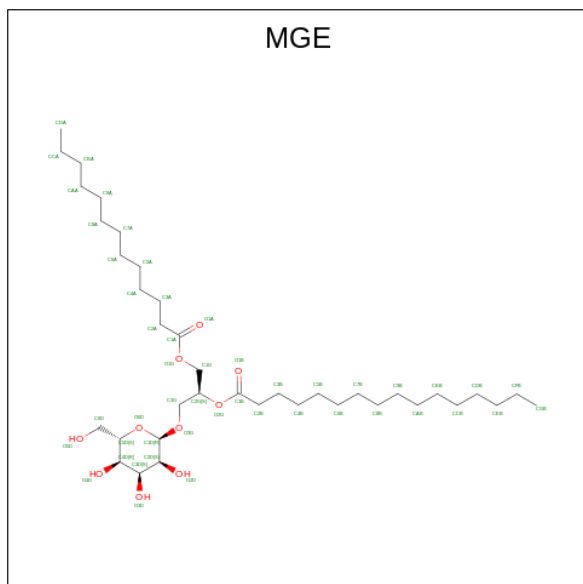
Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C O P 42 31 10 1	0
26	1	1	Total C O 29 25 4	0
26	1	1	Total C O 33 28 5	0

Continued on next page...

Continued from previous page...

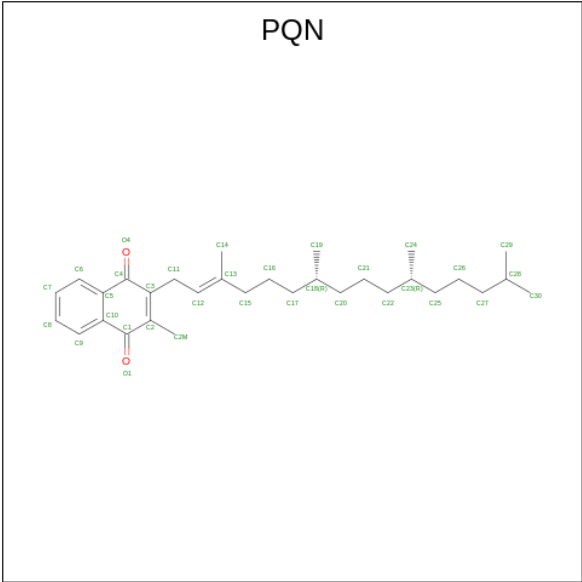
Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	P	0
			26	17	8	1	
26	2	1	Total	C	O	P	0
			29	20	8	1	
26	2	1	Total	C	O	P	0
			32	21	10	1	
26	2	1	Total	C	O	P	0
			36	27	8	1	
26	3	1	Total	C	O	P	0
			38	27	10	1	
26	4	1	Total	C	O	P	0
			29	20	8	1	
26	4	1	Total	C	O	P	0
			27	16	10	1	
26	4	1	Total	C	O	P	0
			36	27	8	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			24	15	8	1	
26	A	1	Total	C	O	P	0
			30	21	8	1	
26	A	1	Total	C	O	P	0
			33	22	10	1	
26	A	1	Total	C	O	P	0
			40	31	8	1	
26	B	1	Total	C	O	P	0
			30	19	10	1	
26	B	1	Total	C	O	P	0
			41	32	8	1	
26	F	1	Total	C	O	P	0
			31	22	8	1	
26	G	1	Total	C	O	P	0
			36	25	10	1	
26	G	1	Total	C	O	P	0
			25	16	8	1	
26	O	1	Total	C	O	P	0
			29	20	8	1	
26	O	1	Total	C	O	P	0
			28	19	8	1	
26	X	1	Total	C	O	P	0
			22	11	10	1	

- Molecule 27 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $C_{38}H_{72}O_{10}$) (labeled as "Ligand of Interest" by depositor).



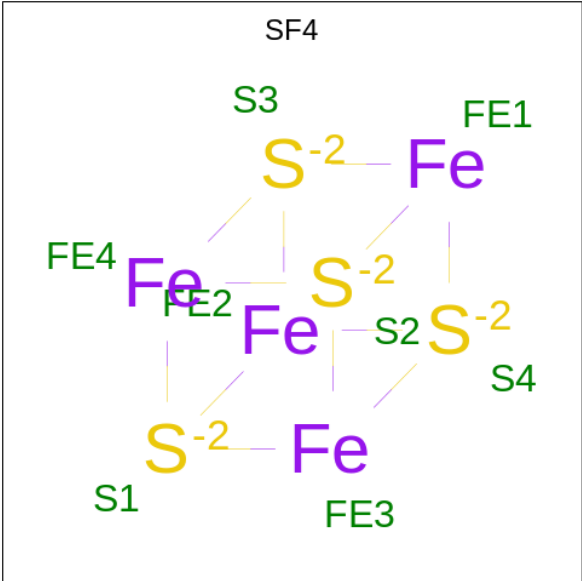
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			37	27	10	
27	3	1	Total	C	O	0
			32	22	10	
27	3	1	Total	C	O	0
			26	16	10	
27	F	1	Total	C	O	0
			37	27	10	
27	F	1	Total	C	O	0
			28	18	10	
27	N	1	Total	C	O	0
			32	22	10	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			33	31	2	
28	B	1	Total	C	O	0
			30	28	2	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



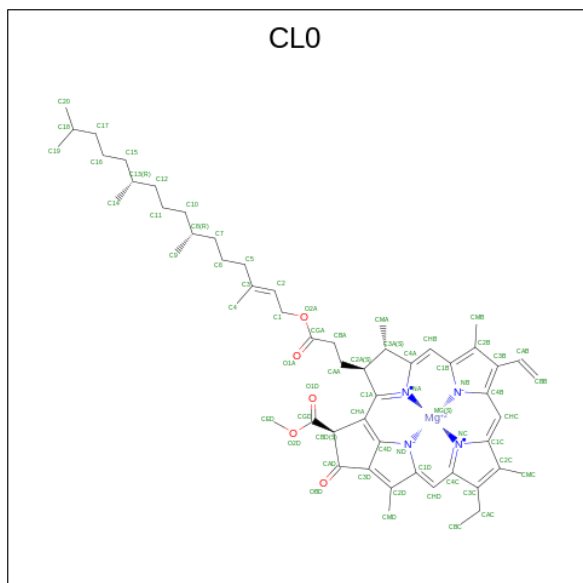
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

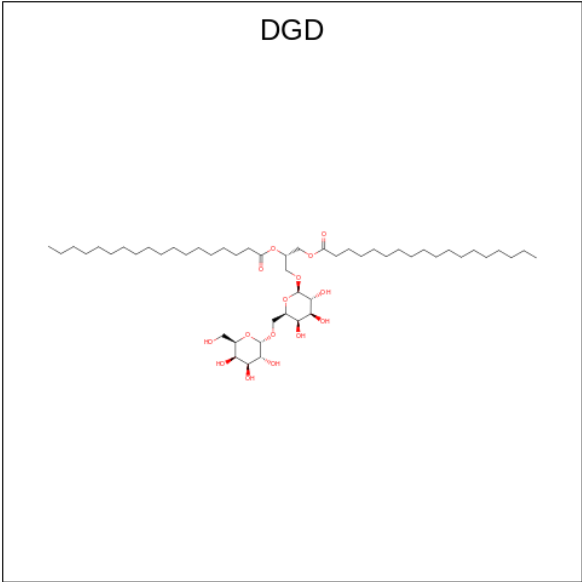
Mol	Chain	Residues	Atoms			AltConf
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

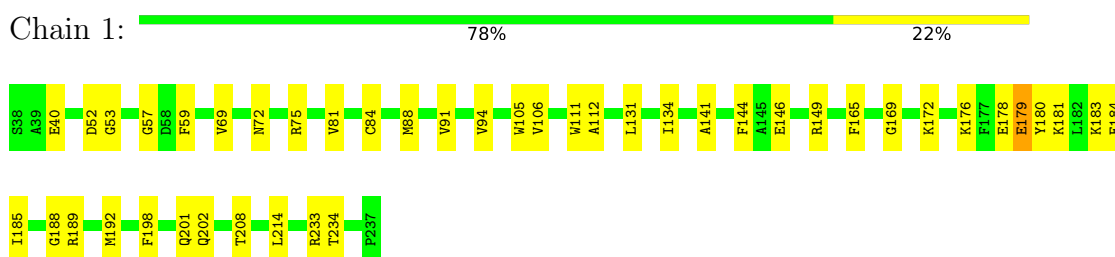


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			59	44	15	
31	G	1	Total	C	O	0
			39	30	9	
31	J	1	Total	C	O	0
			58	43	15	
31	O	1	Total	C	O	0
			53	38	15	

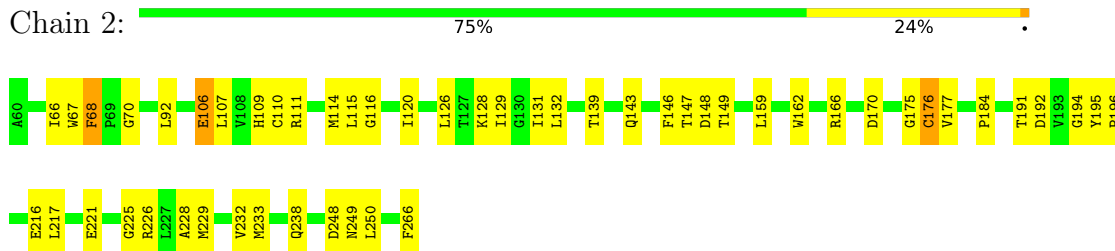
3 Residue-property plots

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

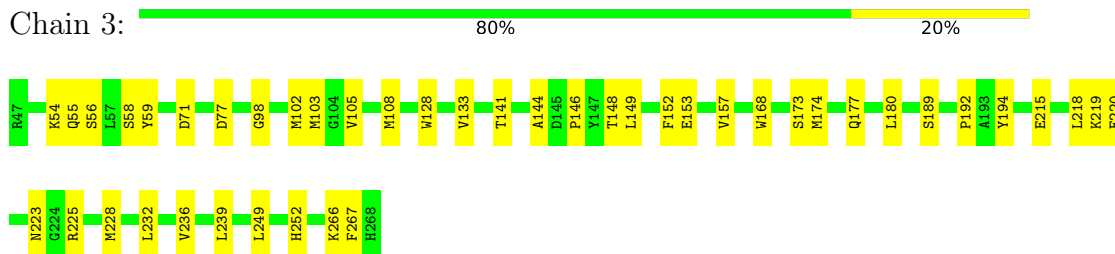
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



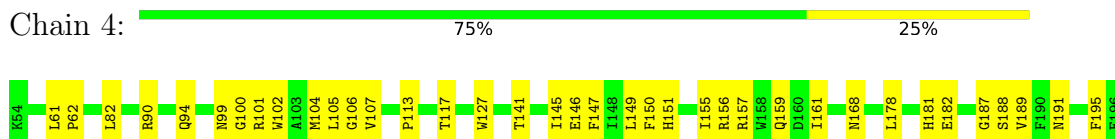
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



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



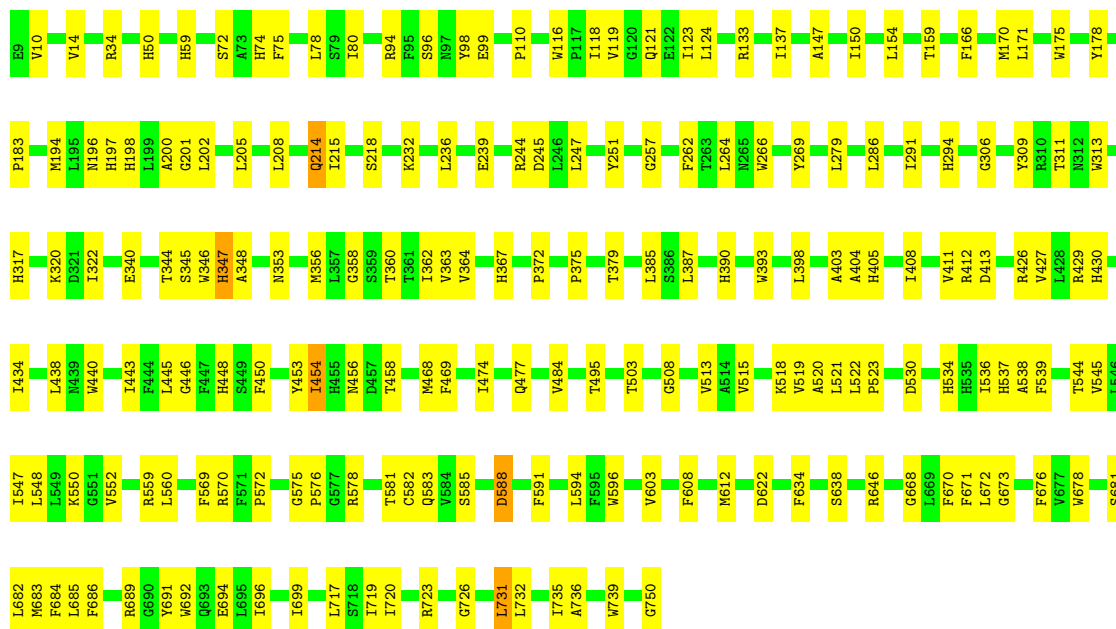
- Molecule 4: Chlorophyll A-B binding protein





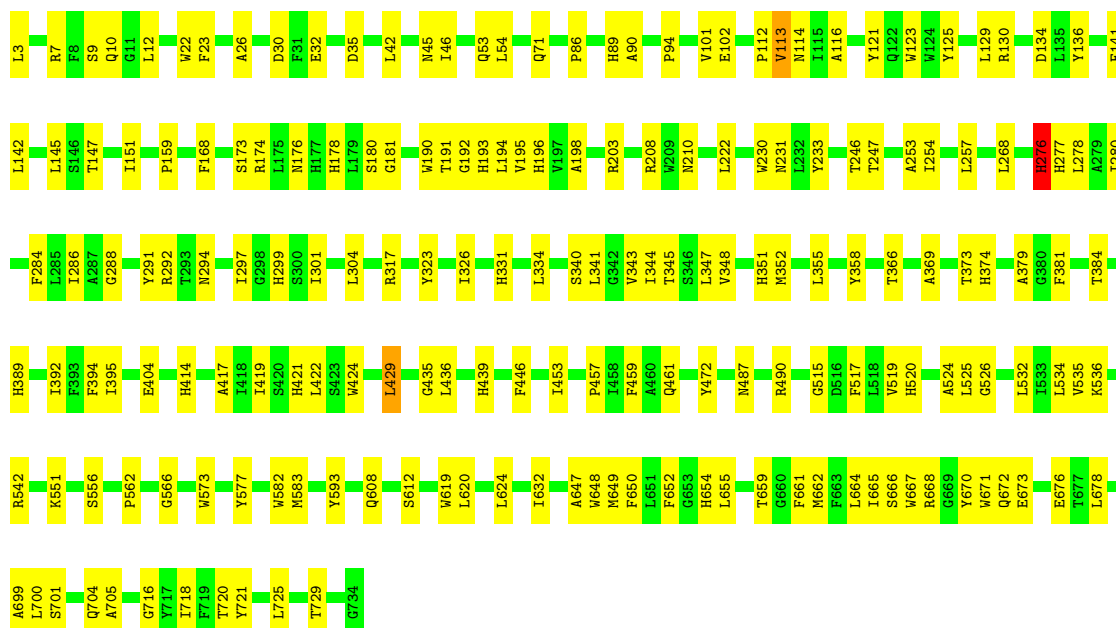
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 74% 25%



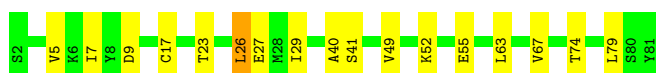
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 74% 25%



• Molecule 7: Photosystem I iron-sulfur center

Chain C:  79% 20% .



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

Chain D:  82% 17% .



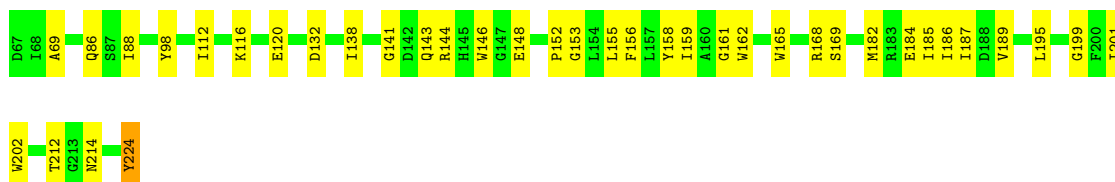
- Molecule 9: Photosystem I reaction center subunit IV

Chain E:  85% 14% .



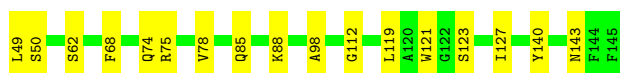
- Molecule 10: Photosystem I reaction center subunit III

Chain F:  76% 23% .



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

Chain G:  82% 18% .



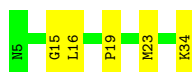
- Molecule 12: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  67% 27% 6% .



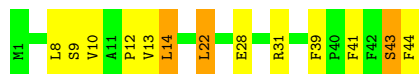
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  83% 17% .



- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  70% 23% 7%



- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  72% 27% .



- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic

Chain L:  80% 20% .



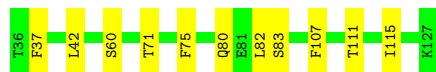
- Molecule 17: Photosystem I reaction center subunit N, chloroplastic

Chain N:  88% 12%

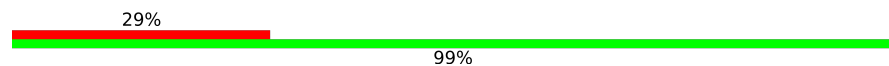


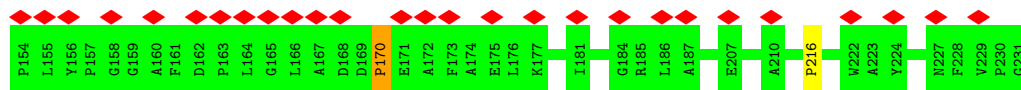
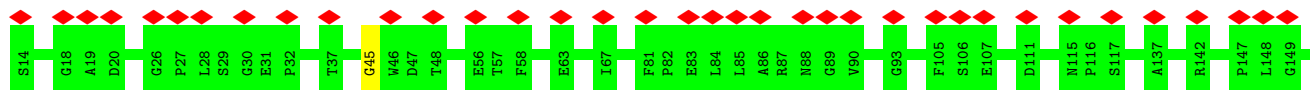
- Molecule 18: H0622F05.3 protein

Chain O:  88% 12%

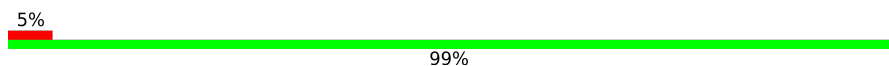


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain X:  29% 99% .

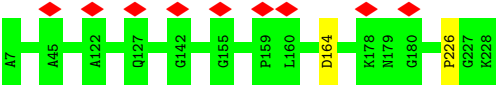


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain Z:  5% 99% .



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124514	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 ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.622	Depositor
Minimum map value	-0.191	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.30	0/1614	0.65	1/2203 (0.0%)
2	2	0.30	0/1670	0.67	2/2286 (0.1%)
3	3	0.28	0/1779	0.59	0/2419
4	4	0.27	0/1621	0.62	2/2214 (0.1%)
5	A	0.28	0/6037	0.55	6/8234 (0.1%)
6	B	0.27	0/6067	0.57	7/8285 (0.1%)
7	C	0.23	0/613	0.55	0/830
8	D	0.24	0/1157	0.53	0/1564
9	E	0.24	0/530	0.55	0/722
10	F	0.25	0/1265	0.56	1/1710 (0.1%)
11	G	0.29	0/780	0.69	0/1057
12	H	0.37	0/732	0.70	1/996 (0.1%)
13	I	0.36	0/238	0.84	0/324
14	J	0.35	0/364	0.70	0/495
15	K	0.23	0/626	0.56	0/847
16	L	0.26	0/1261	0.59	0/1726
17	N	0.19	0/701	0.49	0/939
18	O	0.26	0/762	0.65	0/1041
19	X	0.53	3/1109 (0.3%)	1.13	7/1547 (0.5%)
19	Z	0.17	0/1109	0.42	1/1547 (0.1%)
20	Y	0.17	0/1127	0.45	0/1571
All	All	0.28	3/31162 (0.0%)	0.61	28/42557 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B	0	1
7	C	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	1
14	J	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	216	PRO	CG-CD	-9.81	1.17	1.50
19	X	216	PRO	CB-CG	-8.18	1.08	1.49
19	X	170	PRO	CG-CD	-7.20	1.26	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	X	216	PRO	CB-CG-CD	23.09	179.97	106.10
19	X	216	PRO	N-CD-CG	-19.72	73.62	103.20
19	X	216	PRO	CA-CB-CG	-15.99	74.12	104.50
19	X	170	PRO	N-CD-CG	-14.10	82.05	103.20
19	X	170	PRO	CA-CB-CG	-10.22	85.08	104.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	276	HIS	Sidechain
7	C	26	LEU	Peptide
8	D	162	HIS	Peptide
14	J	41	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1560	0	1507	37	0
2	2	1612	0	1552	42	0
3	3	1723	0	1688	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	1570	0	1527	38	0
5	A	5839	0	5687	183	0
6	B	5856	0	5634	152	0
7	C	602	0	585	13	0
8	D	1128	0	1135	19	0
9	E	518	0	517	6	0
10	F	1236	0	1274	30	0
11	G	760	0	734	17	0
12	H	709	0	704	26	0
13	I	232	0	252	4	0
14	J	353	0	363	15	0
15	K	620	0	647	21	0
16	L	1223	0	1228	25	0
17	N	685	0	658	10	0
18	O	733	0	710	9	0
19	X	1094	0	618	1	0
19	Z	1094	0	618	1	0
20	Y	1112	0	618	1	0
21	1	89	0	60	2	0
21	2	188	0	127	11	0
21	3	97	0	67	3	0
21	4	177	0	111	5	0
21	X	281	0	188	0	0
21	Y	276	0	186	3	0
21	Z	280	0	186	5	0
22	1	614	0	477	30	0
22	2	544	0	437	21	0
22	3	628	0	508	24	0
22	4	487	0	352	17	0
22	A	2512	0	2384	161	0
22	B	2368	0	2303	159	0
22	F	92	0	66	4	0
22	G	143	0	111	11	0
22	H	41	0	29	0	0
22	J	41	0	28	1	0
22	K	191	0	151	9	0
22	L	155	0	138	16	0
22	N	44	0	30	0	0
22	O	258	0	224	6	0
22	X	322	0	230	4	0
22	Y	387	0	303	3	0
22	Z	368	0	264	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	1	42	0	56	4	0
23	2	42	0	56	4	0
23	3	42	0	56	5	0
23	4	84	0	112	9	0
24	1	44	0	56	4	0
24	2	44	0	56	9	0
24	3	44	0	56	7	0
24	4	44	0	56	5	0
25	1	40	0	56	6	0
25	2	40	0	56	12	0
25	3	40	0	56	2	0
25	4	40	0	56	1	0
25	A	239	0	333	34	0
25	B	310	0	431	44	0
25	F	40	0	56	6	0
25	G	40	0	56	4	0
25	I	40	0	56	5	0
25	J	80	0	112	11	0
25	K	40	0	56	5	0
25	L	160	0	223	12	0
25	O	80	0	112	9	0
26	1	104	0	147	4	0
26	2	123	0	135	10	0
26	3	38	0	46	3	0
26	4	92	0	96	5	0
26	A	176	0	215	29	0
26	B	71	0	86	10	0
26	F	31	0	35	3	0
26	G	61	0	65	2	0
26	O	57	0	60	2	0
26	X	22	0	16	0	0
27	1	37	0	43	3	0
27	3	58	0	58	3	0
27	F	65	0	70	3	0
27	N	32	0	34	2	0
28	A	33	0	46	4	0
28	B	30	0	37	7	0
29	A	8	0	0	0	0
29	C	16	0	0	2	0
30	A	65	0	71	4	0
31	B	59	0	79	4	0
31	G	39	0	47	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	J	58	0	77	0	0
31	O	53	0	64	4	0
All	All	43745	0	40906	1027	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 12.

The worst 5 of 1027 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)
6:B:659:THR:O	6:B:662:MET:HB2	1.56	1.05
5:A:50:HIS:HE1	22:A:828:CLA:ND	1.55	1.03
22:1:303:CLA:HHB	31:G:201:DGD:HA22	1.45	0.97
5:A:198:HIS:HE1	22:A:838:CLA:ND	1.71	0.87
22:B:819:CLA:HAB	22:B:848:CLA:HHB	1.57	0.86

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	1	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
2	2	205/207 (99%)	187 (91%)	17 (8%)	1 (0%)	24	49
3	3	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
4	4	196/198 (99%)	190 (97%)	5 (3%)	1 (0%)	24	49
5	A	740/742 (100%)	705 (95%)	34 (5%)	1 (0%)	48	72
6	B	730/732 (100%)	707 (97%)	23 (3%)	0	100	100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	D	141/143 (99%)	133 (94%)	6 (4%)	2 (1%)	9	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
10	F	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
11	G	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	11	29
12	H	91/93 (98%)	77 (85%)	10 (11%)	4 (4%)	2	4
13	I	28/30 (93%)	28 (100%)	0	0	100	100
14	J	42/44 (96%)	36 (86%)	5 (12%)	1 (2%)	4	13
15	K	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
16	L	161/163 (99%)	153 (95%)	7 (4%)	1 (1%)	21	45
17	N	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
18	O	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
19	X	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
19	Z	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
20	Y	220/222 (99%)	202 (92%)	17 (8%)	1 (0%)	24	49
All	All	4054/4097 (99%)	3831 (94%)	210 (5%)	13 (0%)	37	59

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	176	CYS
4	4	189	VAL
5	A	348	ALA
8	D	163	PRO
12	H	76	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/162 (100%)	162 (100%)	0	100	100
2	2	165/165 (100%)	160 (97%)	5 (3%)	36	60
3	3	176/176 (100%)	176 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	169/169 (100%)	168 (99%)	1 (1%)	78	89
5	A	602/602 (100%)	598 (99%)	4 (1%)	76	87
6	B	599/599 (100%)	594 (99%)	5 (1%)	73	85
7	C	69/70 (99%)	69 (100%)	0	100	100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73	85
9	E	57/58 (98%)	57 (100%)	0	100	100
10	F	127/127 (100%)	125 (98%)	2 (2%)	55	75
11	G	81/81 (100%)	81 (100%)	0	100	100
12	H	76/76 (100%)	73 (96%)	3 (4%)	28	54
13	I	26/26 (100%)	26 (100%)	0	100	100
14	J	38/38 (100%)	36 (95%)	2 (5%)	20	45
15	K	64/64 (100%)	63 (98%)	1 (2%)	55	75
16	L	126/126 (100%)	125 (99%)	1 (1%)	73	85
17	N	73/73 (100%)	73 (100%)	0	100	100
18	O	77/77 (100%)	77 (100%)	0	100	100
19	X	16/165 (10%)	15 (94%)	1 (6%)	16	38
19	Z	16/165 (10%)	16 (100%)	0	100	100
20	Y	16/171 (9%)	16 (100%)	0	100	100
All	All	2856/3311 (86%)	2830 (99%)	26 (1%)	68	83

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	678	LEU
10	F	224	TYR
16	L	91	SER
10	F	86	GLN
12	H	61	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	114	ASN
12	H	83	GLN
6	B	276	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	G	114	ASN
6	B	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

286 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	2	306	2	47,52,73	2.55	18 (38%)	56,88,113	3.49	26 (46%)
22	CLA	4	310	4	46,50,73	2.39	17 (36%)	55,85,113	3.26	27 (49%)
28	PQN	A	811	-	34,34,34	0.32	0	42,45,45	0.46	0
21	CHL	Z	302	-	51,55,74	2.21	18 (35%)	57,91,114	3.14	25 (43%)
22	CLA	O	210	-	45,49,73	2.62	18 (40%)	54,84,113	3.48	28 (51%)
21	CHL	1	301	1	47,51,74	2.21	17 (36%)	52,86,114	3.24	23 (44%)
22	CLA	A	830	5	54,58,73	2.46	18 (33%)	65,95,113	3.36	31 (47%)
22	CLA	B	820	6	49,53,73	2.34	18 (36%)	59,89,113	3.34	27 (45%)
26	LHG	X	314	22	21,21,48	0.35	0	22,26,54	0.50	0
22	CLA	B	807	6	65,71,73	1.94	13 (20%)	73,108,113	3.96	30 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	2	318	2	65,69,73	2.18	19 (29%)	78,108,113	2.93	29 (37%)
26	LHG	2	316	-	35,35,48	0.41	0	39,40,54	0.52	1 (2%)
26	LHG	2	315	22	31,31,48	0.32	0	34,37,54	0.44	0
22	CLA	A	834	5	50,54,73	2.41	18 (36%)	60,90,113	3.24	28 (46%)
22	CLA	Z	306	-	50,54,73	2.50	19 (38%)	60,90,113	3.41	29 (48%)
22	CLA	B	816	6	69,73,73	2.22	20 (28%)	83,113,113	3.49	32 (38%)
22	CLA	K	203	-	64,68,73	2.21	19 (29%)	77,107,113	3.00	31 (40%)
21	CHL	Z	304	-	51,55,74	2.20	17 (33%)	57,91,114	3.12	22 (38%)
25	BCR	G	202	-	41,41,41	1.86	9 (21%)	56,56,56	2.57	21 (37%)
22	CLA	B	827	6	69,73,73	2.07	18 (26%)	83,113,113	2.82	33 (39%)
22	CLA	4	315	4	44,49,73	2.58	18 (40%)	52,84,113	3.51	25 (48%)
26	LHG	3	306	-	37,37,48	0.32	0	40,43,54	0.44	0
22	CLA	Y	309	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	27 (45%)
22	CLA	B	846	6,22	50,54,73	2.45	19 (38%)	60,90,113	3.35	28 (46%)
21	CHL	Y	306	-	50,54,74	2.25	17 (34%)	56,90,114	3.17	20 (35%)
22	CLA	Z	313	-	50,54,73	2.52	20 (40%)	60,90,113	3.27	27 (45%)
22	CLA	B	847	-	69,73,73	2.12	19 (27%)	83,113,113	2.88	30 (36%)
25	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.80	14 (25%)
26	LHG	2	313	-	25,25,48	0.47	0	29,30,54	1.11	3 (10%)
22	CLA	A	833	5	69,73,73	2.13	20 (28%)	83,113,113	2.93	31 (37%)
26	LHG	A	820	-	48,48,48	0.27	0	51,54,54	0.38	0
22	CLA	Y	301	-	50,54,73	2.50	20 (40%)	60,90,113	3.29	28 (46%)
25	BCR	K	201	-	41,41,41	1.70	8 (19%)	56,56,56	1.76	13 (23%)
26	LHG	B	843	-	40,40,48	1.02	2 (5%)	43,45,54	1.08	2 (4%)
22	CLA	A	809	5	65,69,73	2.14	18 (27%)	78,108,113	2.95	30 (38%)
22	CLA	1	320	-	49,53,73	2.53	19 (38%)	59,89,113	3.31	27 (45%)
22	CLA	G	206	26	57,61,73	2.39	20 (35%)	68,98,113	3.20	28 (41%)
24	XAT	2	311	-	39,47,47	0.93	0	54,74,74	3.72	31 (57%)
22	CLA	B	818	6	69,73,73	2.07	19 (27%)	83,113,113	2.72	31 (37%)
29	SF4	C	102	7	0,12,12	-	-	-	-	-
22	CLA	A	837	5	46,50,73	2.53	18 (39%)	55,85,113	3.50	26 (47%)
22	CLA	B	829	-	69,73,73	2.12	19 (27%)	83,113,113	2.80	31 (37%)
25	BCR	L	302	-	41,41,41	1.72	9 (21%)	56,56,56	2.22	18 (32%)
22	CLA	4	314	4	43,48,73	2.58	20 (46%)	51,83,113	3.47	29 (56%)
22	CLA	B	853	6	56,60,73	2.36	20 (35%)	67,97,113	3.14	32 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	Y	303	-	50,54,74	2.24	16 (32%)	56,90,114	3.20	21 (37%)
22	CLA	1	305	26	45,49,73	2.60	19 (42%)	54,84,113	3.44	28 (51%)
22	CLA	3	308	-	53,57,73	2.41	18 (33%)	62,93,113	3.38	28 (45%)
22	CLA	X	312	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	27 (45%)
28	PQN	B	832	-	31,31,34	0.32	0	38,41,45	0.62	1 (2%)
22	CLA	1	319	-	52,56,73	2.42	19 (36%)	62,92,113	3.21	30 (48%)
22	CLA	A	802	5	69,73,73	2.13	18 (26%)	83,113,113	2.88	32 (38%)
22	CLA	1	309	-	46,50,73	2.52	19 (41%)	55,85,113	3.52	29 (52%)
25	BCR	B	840	-	30,30,41	2.15	8 (26%)	39,39,56	2.73	14 (35%)
25	BCR	A	818	-	40,40,41	1.57	7 (17%)	54,54,56	1.67	12 (22%)
22	CLA	Z	309	-	50,54,73	2.52	20 (40%)	60,90,113	3.32	26 (43%)
22	CLA	N	202	-	47,52,73	2.55	20 (42%)	56,88,113	3.34	25 (44%)
27	MGE	3	304	-	32,32,48	0.53	0	40,40,56	0.92	3 (7%)
25	BCR	O	203	-	41,41,41	1.79	8 (19%)	56,56,56	2.31	15 (26%)
21	CHL	Y	313	20	50,54,74	2.24	18 (36%)	56,90,114	3.20	20 (35%)
22	CLA	A	851	-	54,58,73	2.37	20 (37%)	65,95,113	3.23	30 (46%)
21	CHL	2	302	-	51,55,74	2.16	17 (33%)	57,91,114	3.03	21 (36%)
22	CLA	4	312	-	49,53,73	2.50	19 (38%)	59,89,113	3.31	28 (47%)
22	CLA	A	803	5	60,64,73	2.21	18 (30%)	72,102,113	3.00	29 (40%)
25	BCR	A	816	-	41,41,41	1.69	9 (21%)	56,56,56	2.27	15 (26%)
22	CLA	X	311	26	50,54,73	2.51	20 (40%)	60,90,113	3.28	28 (46%)
31	DGD	J	104	-	59,59,67	0.94	3 (5%)	73,73,81	1.09	4 (5%)
22	CLA	Z	314	-	50,54,73	2.49	20 (40%)	60,90,113	3.28	27 (45%)
21	CHL	4	317	4	44,49,74	2.34	18 (40%)	48,84,114	3.35	21 (43%)
22	CLA	A	859	-	62,66,73	2.21	18 (29%)	74,104,113	3.06	30 (40%)
27	MGE	3	305	-	26,26,48	0.59	0	32,33,56	0.80	1 (3%)
31	DGD	B	841	-	60,60,67	0.89	2 (3%)	74,74,81	0.90	3 (4%)
25	BCR	B	844	-	41,41,41	1.69	9 (21%)	56,56,56	1.81	16 (28%)
22	CLA	A	831	5	69,73,73	2.10	18 (26%)	83,113,113	2.96	30 (36%)
22	CLA	H	201	12	45,49,73	2.61	20 (44%)	54,84,113	3.50	29 (53%)
21	CHL	4	307	-	48,53,74	2.22	16 (33%)	53,89,114	3.10	21 (39%)
21	CHL	X	306	-	51,55,74	2.22	17 (33%)	57,91,114	3.12	23 (40%)
25	BCR	2	312	-	41,41,41	1.64	8 (19%)	56,56,56	2.32	19 (33%)
22	CLA	2	308	2	56,60,73	2.38	20 (35%)	67,97,113	3.37	32 (47%)
22	CLA	Z	307	-	50,54,73	2.51	20 (40%)	60,90,113	3.30	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	313	3	49,53,73	2.54	19 (38%)	59,89,113	3.35	26 (44%)
22	CLA	Y	310	-	50,54,73	2.52	20 (40%)	60,90,113	3.32	28 (46%)
21	CHL	Z	301	19	51,55,74	2.19	17 (33%)	57,91,114	3.17	21 (36%)
22	CLA	A	845	5	49,53,73	2.46	18 (36%)	59,89,113	3.44	30 (50%)
22	CLA	X	303	-	50,54,73	2.51	20 (40%)	60,90,113	3.29	27 (45%)
22	CLA	Y	314	-	50,54,73	2.51	20 (40%)	60,90,113	3.36	27 (45%)
25	BCR	B	835	-	41,41,41	1.71	8 (19%)	56,56,56	1.88	17 (30%)
31	DGD	G	201	-	39,39,67	1.04	2 (5%)	47,47,81	1.22	6 (12%)
22	CLA	B	803	6	69,73,73	2.18	20 (28%)	83,113,113	3.06	30 (36%)
22	CLA	4	311	4	49,53,73	2.50	19 (38%)	59,89,113	3.26	29 (49%)
22	CLA	Z	308	-	50,54,73	2.52	20 (40%)	60,90,113	3.30	28 (46%)
22	CLA	B	809	-	64,68,73	2.13	17 (26%)	77,107,113	2.86	31 (40%)
21	CHL	2	309	2	50,54,74	2.24	18 (36%)	56,90,114	3.19	21 (37%)
25	BCR	B	837	-	41,41,41	1.74	8 (19%)	56,56,56	2.11	19 (33%)
22	CLA	B	806	6	61,65,73	2.22	19 (31%)	73,103,113	3.02	29 (39%)
22	CLA	B	849	6	56,60,73	2.36	19 (33%)	67,97,113	3.22	32 (47%)
24	XAT	3	302	-	39,47,47	0.92	1 (2%)	54,74,74	4.13	25 (46%)
21	CHL	Z	305	-	51,55,74	2.22	17 (33%)	57,91,114	3.08	21 (36%)
22	CLA	A	847	5	46,50,73	2.49	17 (36%)	55,85,113	3.42	24 (43%)
26	LHG	4	303	-	35,35,48	0.34	0	38,40,54	0.45	0
22	CLA	A	838	5	69,73,73	2.19	18 (26%)	83,113,113	3.02	28 (33%)
21	CHL	2	301	-	54,58,74	2.13	16 (29%)	59,94,114	3.12	24 (40%)
22	CLA	3	311	-	49,53,73	2.50	19 (38%)	59,89,113	3.38	30 (50%)
22	CLA	3	317	-	47,52,73	2.57	19 (40%)	56,88,113	3.46	26 (46%)
22	CLA	3	319	3	49,53,73	2.53	20 (40%)	59,89,113	3.34	26 (44%)
22	CLA	L	307	-	49,53,73	2.50	20 (40%)	59,89,113	3.37	28 (47%)
22	CLA	1	304	1	57,61,73	2.33	19 (33%)	68,98,113	3.17	33 (48%)
22	CLA	B	845	-	69,73,73	2.06	16 (23%)	83,113,113	2.67	30 (36%)
22	CLA	Y	308	-	50,54,73	2.49	20 (40%)	60,90,113	3.34	30 (50%)
22	CLA	3	312	3	69,73,73	2.15	19 (27%)	83,113,113	2.94	32 (38%)
26	LHG	G	203	-	35,35,48	0.33	0	38,41,54	0.72	1 (2%)
21	CHL	Y	307	-	50,54,74	2.25	17 (34%)	56,90,114	3.15	22 (39%)
22	CLA	2	304	2	59,63,73	2.27	19 (32%)	71,101,113	2.96	32 (45%)
22	CLA	A	839	5	49,53,73	2.49	19 (38%)	59,89,113	3.32	26 (44%)
22	CLA	1	306	-	47,52,73	2.55	19 (40%)	56,88,113	3.37	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	844	5	69,73,73	2.09	19 (27%)	83,113,113	2.87	29 (34%)
22	CLA	Y	312	-	50,54,73	2.53	20 (40%)	60,90,113	3.36	26 (43%)
25	BCR	B	838	-	41,41,41	1.67	13 (31%)	56,56,56	1.98	19 (33%)
22	CLA	3	316	3	49,53,73	2.50	20 (40%)	59,89,113	3.38	26 (44%)
21	CHL	X	307	-	50,54,74	2.25	17 (34%)	56,90,114	3.21	21 (37%)
25	BCR	F	302	-	41,41,41	1.70	9 (21%)	56,56,56	1.70	13 (23%)
22	CLA	A	808	5	69,73,73	2.10	19 (27%)	83,113,113	2.84	30 (36%)
21	CHL	Y	304	-	50,54,74	2.26	15 (30%)	56,90,114	3.16	21 (37%)
21	CHL	3	307	2	55,59,74	2.08	20 (36%)	60,95,114	3.18	24 (40%)
22	CLA	F	306	10	50,54,73	2.45	19 (38%)	60,90,113	3.28	28 (46%)
22	CLA	K	204	15	50,54,73	2.52	18 (36%)	60,90,113	3.21	26 (43%)
21	CHL	Z	303	-	50,54,74	2.26	19 (38%)	56,90,114	3.17	23 (41%)
22	CLA	B	828	6	51,55,73	2.39	19 (37%)	61,91,113	3.33	27 (44%)
22	CLA	B	848	-	61,65,73	2.23	19 (31%)	73,103,113	3.06	29 (39%)
22	CLA	B	851	6	69,73,73	2.03	17 (24%)	83,113,113	2.71	29 (34%)
23	LUT	1	310	-	42,43,43	1.63	8 (19%)	51,60,60	1.80	13 (25%)
29	SF4	C	101	7	0,12,12	-	-	-	-	-
22	CLA	O	207	-	68,72,73	2.11	19 (27%)	81,111,113	2.94	31 (38%)
25	BCR	O	202	-	41,41,41	1.59	8 (19%)	56,56,56	2.71	21 (37%)
22	CLA	3	320	-	45,50,73	2.54	19 (42%)	53,85,113	3.37	25 (47%)
22	CLA	A	841	-	50,54,73	2.45	19 (38%)	60,90,113	3.34	27 (45%)
22	CLA	A	827	-	69,73,73	2.00	19 (27%)	83,113,113	2.60	25 (30%)
22	CLA	G	207	11	49,53,73	2.50	20 (40%)	59,89,113	3.26	28 (47%)
26	LHG	1	322	-	32,32,48	0.29	0	34,34,54	0.56	0
22	CLA	2	303	2	49,53,73	2.45	19 (38%)	59,89,113	3.18	25 (42%)
22	CLA	A	854	5	69,73,73	2.03	18 (26%)	83,113,113	2.71	31 (37%)
22	CLA	B	831	26	69,73,73	2.10	18 (26%)	83,113,113	2.82	29 (34%)
22	CLA	A	801	5	64,68,73	2.17	19 (29%)	79,106,113	3.03	32 (40%)
22	CLA	L	305	16	49,53,73	2.49	19 (38%)	59,89,113	3.32	29 (49%)
22	CLA	1	317	1	61,65,73	2.24	19 (31%)	73,103,113	3.18	31 (42%)
22	CLA	Y	311	-	69,73,73	2.15	19 (27%)	83,113,113	2.91	31 (37%)
22	CLA	2	305	26	49,53,73	2.46	19 (38%)	59,89,113	3.35	28 (47%)
26	LHG	1	314	-	28,28,48	0.27	0	29,29,54	0.22	0
22	CLA	1	318	-	59,63,73	2.30	19 (32%)	71,101,113	3.05	28 (39%)
22	CLA	O	206	-	50,54,73	2.51	19 (38%)	60,90,113	3.25	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	802	6	49,53,73	2.45	20 (40%)	59,89,113	3.50	28 (47%)
22	CLA	2	322	4	47,52,73	2.53	20 (42%)	56,88,113	3.32	26 (46%)
22	CLA	2	317	-	45,49,73	2.65	20 (44%)	54,84,113	3.45	28 (51%)
22	CLA	O	208	-	64,68,73	2.17	19 (29%)	77,107,113	3.07	29 (37%)
21	CHL	X	305	19	52,56,74	2.20	16 (30%)	58,92,114	3.13	22 (37%)
25	BCR	1	312	-	41,41,41	1.88	8 (19%)	56,56,56	2.50	14 (25%)
24	XAT	4	320	-	39,47,47	0.89	1 (2%)	54,74,74	2.63	19 (35%)
26	LHG	F	301	-	30,30,48	0.44	0	34,35,54	1.19	3 (8%)
22	CLA	A	812	26	59,63,73	2.30	19 (32%)	71,101,113	3.08	30 (42%)
22	CLA	B	817	-	62,66,73	2.16	19 (30%)	74,104,113	3.00	30 (40%)
22	CLA	A	856	5	55,59,73	2.32	19 (34%)	66,96,113	3.15	31 (46%)
22	CLA	A	853	5	69,73,73	2.09	20 (28%)	83,113,113	2.90	31 (37%)
26	LHG	A	821	-	23,23,48	0.49	0	27,28,54	0.71	1 (3%)
21	CHL	X	308	-	51,55,74	2.21	16 (31%)	57,91,114	3.16	21 (36%)
22	CLA	B	819	6	64,68,73	2.17	19 (29%)	77,107,113	2.81	31 (40%)
22	CLA	Z	310	-	50,54,73	2.51	20 (40%)	60,90,113	3.32	28 (46%)
22	CLA	A	857	5	60,64,73	2.26	19 (31%)	72,102,113	3.00	29 (40%)
21	CHL	X	309	-	50,54,74	2.25	17 (34%)	56,90,114	3.14	20 (35%)
22	CLA	A	840	5	49,53,73	2.51	19 (38%)	59,89,113	3.31	26 (44%)
22	CLA	A	846	-	69,73,73	2.13	19 (27%)	83,113,113	2.72	29 (34%)
22	CLA	B	804	6	69,73,73	2.06	19 (27%)	83,113,113	2.85	30 (36%)
22	CLA	B	824	6	64,68,73	2.23	20 (31%)	77,107,113	3.01	30 (38%)
22	CLA	G	205	-	49,53,73	2.53	19 (38%)	59,89,113	3.34	27 (45%)
25	BCR	L	303	-	41,41,41	1.68	9 (21%)	56,56,56	1.79	16 (28%)
22	CLA	A	832	5	51,55,73	2.46	19 (37%)	61,91,113	3.31	28 (45%)
26	LHG	4	301	-	28,28,48	0.36	0	31,33,54	0.60	1 (3%)
25	BCR	B	836	-	41,41,41	1.72	8 (19%)	56,56,56	1.82	15 (26%)
25	BCR	J	101	-	41,41,41	1.74	10 (24%)	56,56,56	1.88	19 (33%)
22	CLA	A	855	5	69,73,73	2.07	19 (27%)	83,113,113	2.72	31 (37%)
22	CLA	A	858	-	69,73,73	2.07	19 (27%)	83,113,113	3.00	29 (34%)
26	LHG	G	204	22	24,24,48	0.49	0	28,29,54	0.63	1 (3%)
31	DGD	O	201	-	54,54,67	0.95	2 (3%)	68,68,81	1.26	7 (10%)
22	CLA	A	805	-	54,58,73	2.33	19 (35%)	65,95,113	3.23	29 (44%)
22	CLA	B	825	-	50,54,73	2.46	20 (40%)	60,90,113	3.17	27 (45%)
25	BCR	A	817	-	41,41,41	1.67	8 (19%)	56,56,56	1.86	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	MGE	N	201	-	32,32,48	0.59	0	40,40,56	0.77	1 (2%)
21	CHL	1	316	1	50,54,74	2.17	17 (34%)	56,90,114	3.11	20 (35%)
22	CLA	B	850	6	69,73,73	2.08	18 (26%)	83,113,113	2.85	31 (37%)
24	XAT	1	311	-	39,47,47	0.95	0	54,74,74	3.65	29 (53%)
26	LHG	A	823	22	32,32,48	0.29	0	35,38,54	0.39	0
25	BCR	A	814	-	41,41,41	1.64	9 (21%)	56,56,56	1.75	14 (25%)
22	CLA	B	808	6	69,73,73	2.15	19 (27%)	83,113,113	2.89	31 (37%)
22	CLA	4	316	4	45,49,73	2.55	18 (40%)	54,84,113	3.46	27 (50%)
22	CLA	3	309	3	63,67,73	2.23	19 (30%)	75,105,113	3.02	32 (42%)
25	BCR	J	103	-	41,41,41	1.69	9 (21%)	56,56,56	1.87	17 (30%)
21	CHL	4	309	-	50,54,74	2.18	18 (36%)	56,90,114	3.01	22 (39%)
22	CLA	3	318	3	49,53,73	2.47	20 (40%)	59,89,113	3.29	28 (47%)
22	CLA	A	810	-	69,73,73	2.07	19 (27%)	83,113,113	2.75	31 (37%)
22	CLA	A	829	5,22	54,58,73	2.36	20 (37%)	65,95,113	3.24	31 (47%)
22	CLA	X	313	-	50,54,73	2.51	20 (40%)	60,90,113	3.36	28 (46%)
22	CLA	X	304	-	50,54,73	2.75	22 (44%)	60,90,113	4.23	29 (48%)
22	CLA	A	836	5,22	64,68,73	2.21	19 (29%)	77,107,113	2.91	29 (37%)
22	CLA	A	806	5	57,61,73	2.35	20 (35%)	68,98,113	3.11	30 (44%)
22	CLA	K	202	15	47,52,73	2.54	20 (42%)	56,88,113	3.29	25 (44%)
22	CLA	A	850	-	69,73,73	2.04	19 (27%)	83,113,113	2.82	31 (37%)
22	CLA	B	815	-	62,66,73	2.18	20 (32%)	74,104,113	2.93	29 (39%)
22	CLA	B	833	22	60,64,73	2.29	19 (31%)	72,102,113	3.12	32 (44%)
22	CLA	3	310	-	62,66,73	2.23	19 (30%)	74,104,113	2.99	28 (37%)
22	CLA	1	308	1	45,49,73	2.58	18 (40%)	54,84,113	3.53	29 (53%)
22	CLA	L	306	16	69,73,73	2.04	19 (27%)	83,113,113	2.92	31 (37%)
25	BCR	L	301	-	41,41,41	1.65	8 (19%)	56,56,56	1.83	17 (30%)
22	CLA	X	301	-	50,54,73	2.49	20 (40%)	60,90,113	3.29	27 (45%)
22	CLA	3	315	3	45,49,73	2.53	20 (44%)	54,84,113	3.26	27 (50%)
22	CLA	B	814	-	69,73,73	2.02	16 (23%)	83,113,113	3.00	34 (40%)
22	CLA	O	209	18	51,55,73	2.51	20 (39%)	61,91,113	3.32	27 (44%)
23	LUT	4	322	-	42,43,43	1.60	8 (19%)	51,60,60	3.12	17 (33%)
25	BCR	A	819	-	41,41,41	1.67	9 (21%)	56,56,56	1.91	16 (28%)
23	LUT	4	319	-	42,43,43	1.57	8 (19%)	51,60,60	1.61	12 (23%)
25	BCR	A	815	-	41,41,41	1.68	9 (21%)	56,56,56	1.86	16 (28%)
27	MGE	F	303	-	37,37,48	0.51	0	45,45,56	1.04	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	3	314	-	50,54,74	2.15	18 (36%)	56,90,114	3.15	20 (35%)
25	BCR	L	304	-	41,41,41	1.68	8 (19%)	56,56,56	1.70	13 (23%)
26	LHG	A	824	-	39,39,48	0.39	0	43,44,54	0.74	1 (2%)
22	CLA	4	304	4	59,63,73	2.27	19 (32%)	71,101,113	3.05	29 (40%)
22	CLA	1	321	1	47,52,73	2.56	20 (42%)	56,88,113	3.29	26 (46%)
22	CLA	4	313	-	47,52,73	2.55	19 (40%)	56,88,113	3.43	26 (46%)
22	CLA	A	804	-	46,50,73	2.51	17 (36%)	55,85,113	3.50	29 (52%)
22	CLA	Y	302	-	50,54,73	2.52	20 (40%)	60,90,113	3.29	28 (46%)
22	CLA	B	811	6	60,64,73	2.24	19 (31%)	72,102,113	3.18	31 (43%)
22	CLA	2	307	2	64,68,73	2.18	19 (29%)	77,107,113	2.98	31 (40%)
22	CLA	B	852	6	59,63,73	2.29	20 (33%)	71,101,113	3.07	30 (42%)
22	CLA	B	812	6	63,67,73	2.18	19 (30%)	75,105,113	2.98	31 (41%)
21	CHL	4	308	-	48,53,74	2.25	18 (37%)	53,89,114	3.24	24 (45%)
21	CHL	Z	312	19	50,54,74	2.27	16 (32%)	56,90,114	3.15	23 (41%)
22	CLA	B	813	6	57,61,73	2.32	20 (35%)	68,98,113	3.02	31 (45%)
22	CLA	B	826	6	54,58,73	2.23	17 (31%)	65,95,113	3.35	30 (46%)
23	LUT	2	310	-	42,43,43	1.74	8 (19%)	51,60,60	2.01	14 (27%)
27	MGE	1	315	-	37,37,48	0.57	0	45,45,56	1.06	3 (6%)
26	LHG	O	204	-	28,28,48	0.45	0	32,33,54	0.63	1 (3%)
22	CLA	1	307	1	59,63,73	2.26	19 (32%)	71,101,113	3.11	30 (42%)
22	CLA	A	807	5	65,69,73	2.15	20 (30%)	78,108,113	3.12	32 (41%)
22	CLA	B	801	-	59,63,73	2.15	15 (25%)	71,101,113	3.10	26 (36%)
21	CHL	Y	305	-	50,54,74	2.25	19 (38%)	56,90,114	3.16	22 (39%)
22	CLA	A	842	5	61,65,73	2.18	18 (29%)	72,102,113	3.01	28 (38%)
25	BCR	4	321	-	41,41,41	1.69	8 (19%)	56,56,56	1.81	14 (25%)
30	CL0	A	825	5	69,73,73	2.00	19 (27%)	83,113,113	2.68	28 (33%)
23	LUT	3	301	-	42,43,43	1.62	8 (19%)	51,60,60	1.46	11 (21%)
21	CHL	2	321	-	48,53,74	2.19	17 (35%)	53,89,114	3.23	23 (43%)
22	CLA	4	306	-	47,52,73	2.57	20 (42%)	56,88,113	3.28	26 (46%)
22	CLA	A	826	-	69,73,73	2.08	19 (27%)	83,113,113	2.94	28 (33%)
22	CLA	B	805	6	50,54,73	2.47	19 (38%)	60,90,113	3.29	26 (43%)
25	BCR	3	303	-	41,41,41	1.66	8 (19%)	56,56,56	1.73	13 (23%)
22	CLA	B	821	6	49,53,73	2.48	20 (40%)	59,89,113	3.33	28 (47%)
22	CLA	4	305	-	47,52,73	2.51	19 (40%)	56,88,113	3.42	28 (50%)
22	CLA	A	835	5	46,50,73	2.42	16 (34%)	55,85,113	3.30	25 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	839	-	41,41,41	1.71	9 (21%)	56,56,56	1.90	15 (26%)
22	CLA	J	102	14	44,49,73	2.56	19 (43%)	52,84,113	3.45	26 (50%)
26	LHG	1	313	22	41,41,48	0.30	0	44,47,54	0.37	0
22	CLA	A	843	5	60,64,73	2.25	19 (31%)	72,102,113	3.10	29 (40%)
22	CLA	B	810	6	54,58,73	2.33	18 (33%)	65,95,113	3.26	29 (44%)
22	CLA	A	849	5	69,73,73	2.08	18 (26%)	83,113,113	2.84	30 (36%)
22	CLA	3	321	3	49,53,73	2.50	19 (38%)	59,89,113	3.27	27 (45%)
22	CLA	2	320	-	54,58,73	2.41	19 (35%)	65,95,113	3.12	33 (50%)
27	MGE	F	304	-	28,28,48	0.61	0	36,36,56	0.88	2 (5%)
22	CLA	A	828	5	43,48,73	2.71	21 (48%)	51,83,113	3.58	28 (54%)
22	CLA	A	848	5	49,53,73	2.47	19 (38%)	59,89,113	3.35	27 (45%)
26	LHG	2	314	-	28,28,48	0.45	0	32,33,54	0.83	2 (6%)
22	CLA	F	305	-	50,54,73	2.45	19 (38%)	60,90,113	3.27	26 (43%)
22	CLA	1	302	-	47,52,73	2.55	20 (42%)	56,88,113	3.32	25 (44%)
22	CLA	X	310	-	50,54,73	2.50	20 (40%)	60,90,113	3.34	28 (46%)
26	LHG	A	822	-	29,29,48	0.36	0	32,34,54	0.58	0
22	CLA	Z	311	-	50,54,73	2.51	20 (40%)	60,90,113	3.32	26 (43%)
26	LHG	4	302	-	26,26,48	0.36	0	29,32,54	0.62	0
26	LHG	B	842	22	29,29,48	0.32	0	32,35,54	0.49	0
29	SF4	A	813	5,6	0,12,12	-	-	-	-	-
22	CLA	4	318	4	50,54,73	2.53	20 (40%)	60,90,113	3.32	28 (46%)
22	CLA	A	852	-	65,69,73	2.17	19 (29%)	78,108,113	3.17	29 (37%)
21	CHL	X	302	-	51,55,74	2.22	19 (37%)	57,91,114	3.14	21 (36%)
22	CLA	B	823	6	65,69,73	2.15	19 (29%)	78,108,113	2.97	32 (41%)
22	CLA	B	822	6	69,73,73	2.07	19 (27%)	83,113,113	2.85	30 (36%)
26	LHG	O	205	-	27,27,48	0.46	0	31,32,54	0.60	1 (3%)
22	CLA	2	319	2	51,55,73	2.57	20 (39%)	61,91,113	3.50	29 (47%)
22	CLA	B	830	6	69,73,73	2.12	19 (27%)	83,113,113	2.92	33 (39%)
22	CLA	K	205	15	45,49,73	2.60	20 (44%)	54,84,113	3.48	30 (55%)
25	BCR	B	834	-	41,41,41	1.74	8 (19%)	56,56,56	2.03	17 (30%)
22	CLA	1	303	1	49,53,73	2.52	19 (38%)	59,89,113	3.38	31 (52%)

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
22	CLA	2	306	2	-	2/13/89/115	-
22	CLA	4	310	4	-	5/12/88/115	-
28	PQN	A	811	-	-	4/23/43/43	0/2/2/2
21	CHL	Z	302	-	-	1/19/95/117	-
22	CLA	O	210	-	-	2/10/86/115	-
21	CHL	1	301	1	-	11/14/90/117	-
22	CLA	A	830	5	-	3/21/97/115	-
22	CLA	B	820	6	-	3/15/91/115	-
26	LHG	X	314	22	-	3/25/25/53	-
22	CLA	B	807	6	1/1/15/20	12/39/111/115	-
22	CLA	2	318	2	1/1/14/20	13/35/111/115	-
26	LHG	2	316	-	-	2/37/37/53	-
26	LHG	2	315	22	-	10/36/36/53	-
22	CLA	A	834	5	-	8/17/93/115	-
22	CLA	Z	306	-	-	4/17/93/115	-
22	CLA	B	816	6	1/1/15/20	10/39/115/115	-
22	CLA	K	203	-	1/1/14/20	5/33/109/115	-
21	CHL	Z	304	-	-	7/19/95/117	-
25	BCR	G	202	-	-	8/29/63/63	0/2/2/2
22	CLA	B	827	6	1/1/15/20	11/39/115/115	-
22	CLA	4	315	4	-	3/10/86/115	-
26	LHG	3	306	-	-	12/42/42/53	-
22	CLA	Y	309	-	-	4/17/93/115	-
22	CLA	B	846	6,22	-	5/17/93/115	-
21	CHL	Y	306	-	-	7/17/93/117	-
22	CLA	Z	313	-	-	5/17/93/115	-
22	CLA	B	847	-	1/1/15/20	18/39/115/115	-
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
26	LHG	2	313	-	-	6/27/27/53	-
22	CLA	A	833	5	1/1/15/20	10/39/115/115	-
26	LHG	A	820	-	-	10/53/53/53	-
22	CLA	Y	301	-	-	1/17/93/115	-
25	BCR	K	201	-	-	2/29/63/63	0/2/2/2
26	LHG	B	843	-	-	21/44/44/53	-
22	CLA	A	809	5	1/1/14/20	13/35/111/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	320	-	-	2/15/91/115	-
22	CLA	G	206	26	-	10/25/101/115	-
24	XAT	2	311	-	-	5/31/93/93	0/4/4/4
22	CLA	B	818	6	1/1/15/20	12/39/115/115	-
29	SF4	C	102	7	-	-	0/6/5/5
22	CLA	A	837	5	-	4/12/88/115	-
22	CLA	B	829	-	1/1/15/20	10/39/115/115	-
25	BCR	L	302	-	-	4/29/63/63	0/2/2/2
22	CLA	4	314	4	-	0/8/84/115	-
22	CLA	B	853	6	-	10/24/100/115	-
21	CHL	Y	303	-	-	7/17/93/117	-
22	CLA	1	305	26	-	3/10/86/115	-
22	CLA	3	308	-	-	7/20/96/115	-
22	CLA	X	312	-	-	2/17/93/115	-
28	PQN	B	832	-	-	4/20/40/43	0/2/2/2
22	CLA	1	319	-	-	4/19/95/115	-
22	CLA	A	802	5	1/1/15/20	18/39/115/115	-
22	CLA	1	309	-	-	3/12/88/115	-
25	BCR	B	840	-	-	5/24/41/63	0/1/1/2
25	BCR	A	818	-	-	6/27/61/63	0/2/2/2
22	CLA	Z	309	-	-	4/17/93/115	-
22	CLA	N	202	-	-	2/13/89/115	-
27	MGE	3	304	-	-	5/27/47/63	0/1/1/1
25	BCR	O	203	-	-	4/29/63/63	0/2/2/2
21	CHL	Y	313	20	-	9/17/93/117	-
22	CLA	A	851	-	-	3/21/97/115	-
21	CHL	2	302	-	-	9/19/95/117	-
22	CLA	A	803	5	1/1/13/20	8/29/105/115	-
22	CLA	4	312	-	-	2/15/91/115	-
25	BCR	A	816	-	-	3/29/63/63	0/2/2/2
22	CLA	X	311	26	-	1/17/93/115	-
31	DGD	J	104	-	-	13/47/87/95	0/2/2/2
22	CLA	Z	314	-	-	5/17/93/115	-
21	CHL	4	317	4	-	6/10/86/117	-
22	CLA	A	859	-	1/1/13/20	13/31/107/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	MGE	3	305	-	-	11/20/40/63	0/1/1/1
31	DGD	B	841	-	-	11/48/88/95	0/2/2/2
25	BCR	B	844	-	-	3/29/63/63	0/2/2/2
22	CLA	A	831	5	1/1/15/20	12/39/115/115	-
22	CLA	H	201	12	-	2/10/86/115	-
21	CHL	4	307	-	-	11/15/91/117	-
21	CHL	X	306	-	-	8/19/95/117	-
25	BCR	2	312	-	-	8/29/63/63	0/2/2/2
22	CLA	2	308	2	-	7/24/100/115	-
22	CLA	Z	307	-	-	0/17/93/115	-
22	CLA	3	313	3	-	0/15/91/115	-
22	CLA	Y	310	-	-	5/17/93/115	-
21	CHL	Z	301	19	-	7/19/95/117	-
22	CLA	A	845	5	-	6/15/91/115	-
22	CLA	X	303	-	-	6/17/93/115	-
22	CLA	Y	314	-	-	2/17/93/115	-
25	BCR	B	835	-	-	4/29/63/63	0/2/2/2
22	CLA	B	803	6	1/1/15/20	19/39/115/115	-
22	CLA	4	311	4	-	7/15/91/115	-
22	CLA	Z	308	-	-	0/17/93/115	-
22	CLA	B	809	-	1/1/14/20	11/33/109/115	-
21	CHL	2	309	2	-	5/17/93/117	-
25	BCR	B	837	-	-	5/29/63/63	0/2/2/2
22	CLA	B	806	6	1/1/13/20	12/30/106/115	-
22	CLA	B	849	6	-	10/24/100/115	-
24	XAT	3	302	-	-	7/31/93/93	0/4/4/4
21	CHL	Z	305	-	-	9/19/95/117	-
22	CLA	A	847	5	-	2/12/88/115	-
26	LHG	4	303	-	-	1/39/39/53	-
22	CLA	A	838	5	1/1/15/20	21/39/115/115	-
21	CHL	2	301	-	-	9/22/98/117	-
22	CLA	3	311	-	-	6/15/91/115	-
22	CLA	3	317	-	-	3/13/89/115	-
22	CLA	3	319	3	-	4/15/91/115	-
22	CLA	L	307	-	-	5/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	304	1	-	8/25/101/115	-
22	CLA	B	845	-	1/1/15/20	17/39/115/115	-
22	CLA	Y	308	-	-	8/17/93/115	-
22	CLA	3	312	3	1/1/15/20	15/39/115/115	-
26	LHG	G	203	-	-	8/40/40/53	-
21	CHL	Y	307	-	-	7/17/93/117	-
22	CLA	2	304	2	1/1/13/20	7/27/103/115	-
22	CLA	A	839	5	-	6/15/91/115	-
22	CLA	1	306	-	-	4/13/89/115	-
22	CLA	A	844	5	1/1/15/20	9/39/115/115	-
22	CLA	Y	312	-	-	6/17/93/115	-
25	BCR	B	838	-	-	1/29/63/63	0/2/2/2
22	CLA	3	316	3	-	7/15/91/115	-
21	CHL	X	307	-	-	7/17/93/117	-
25	BCR	F	302	-	-	5/29/63/63	0/2/2/2
22	CLA	A	808	5	1/1/15/20	13/39/115/115	-
21	CHL	Y	304	-	-	11/17/93/117	-
21	CHL	3	307	2	-	9/23/99/117	-
22	CLA	F	306	10	-	7/17/93/115	-
22	CLA	K	204	15	-	5/17/93/115	-
22	CLA	B	848	-	1/1/13/20	6/30/106/115	-
22	CLA	B	851	6	1/1/15/20	18/39/115/115	-
21	CHL	Z	303	-	-	9/17/93/117	-
22	CLA	B	828	6	-	5/18/94/115	-
23	LUT	1	310	-	-	2/29/67/67	0/2/2/2
31	DGD	G	201	-	-	5/33/53/95	0/1/1/2
22	CLA	O	207	-	1/1/14/20	10/38/114/115	-
25	BCR	O	202	-	-	3/29/63/63	0/2/2/2
29	SF4	C	101	7	-	-	0/6/5/5
22	CLA	3	320	-	-	2/11/87/115	-
22	CLA	A	841	-	-	1/17/93/115	-
22	CLA	A	827	-	1/1/15/20	13/39/115/115	-
22	CLA	G	207	11	-	6/15/91/115	-
26	LHG	1	322	-	-	5/34/34/53	-
22	CLA	2	303	2	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	831	26	1/1/15/20	19/39/115/115	-
22	CLA	A	854	5	1/1/15/20	11/39/115/115	-
22	CLA	A	801	5	1/1/13/20	10/32/108/115	-
22	CLA	L	305	16	-	4/15/91/115	-
22	CLA	1	317	1	1/1/13/20	14/30/106/115	-
22	CLA	Y	311	-	1/1/15/20	15/39/115/115	-
22	CLA	2	305	26	-	1/15/91/115	-
26	LHG	1	314	-	-	2/28/28/53	-
22	CLA	1	318	-	1/1/13/20	9/27/103/115	-
22	CLA	O	206	-	-	0/17/93/115	-
22	CLA	B	802	6	-	0/15/91/115	-
22	CLA	2	322	4	-	2/13/89/115	-
22	CLA	O	208	-	1/1/14/20	14/33/109/115	-
22	CLA	2	317	-	-	3/10/86/115	-
21	CHL	X	305	19	-	8/20/96/117	-
25	BCR	1	312	-	-	6/29/63/63	0/2/2/2
24	XAT	4	320	-	-	3/31/93/93	0/4/4/4
26	LHG	F	301	-	-	8/32/32/53	-
22	CLA	A	812	26	1/1/13/20	13/27/103/115	-
22	CLA	B	817	-	1/1/13/20	10/31/107/115	-
22	CLA	A	856	5	-	4/23/99/115	-
22	CLA	A	853	5	1/1/15/20	16/39/115/115	-
26	LHG	A	821	-	-	3/25/25/53	-
21	CHL	X	308	-	-	11/19/95/117	-
22	CLA	B	819	6	1/1/14/20	13/33/109/115	-
22	CLA	Z	310	-	-	0/17/93/115	-
22	CLA	A	857	5	1/1/13/20	4/29/105/115	-
21	CHL	X	309	-	-	10/17/93/117	-
22	CLA	A	846	-	1/1/15/20	12/39/115/115	-
22	CLA	B	804	6	1/1/15/20	13/39/115/115	-
22	CLA	B	824	6	1/1/14/20	7/33/109/115	-
22	CLA	A	840	5	-	5/15/91/115	-
22	CLA	G	205	-	-	8/15/91/115	-
25	BCR	L	303	-	-	2/29/63/63	0/2/2/2
22	CLA	A	832	5	-	1/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	4	301	-	-	8/32/32/53	-
25	BCR	B	836	-	-	4/29/63/63	0/2/2/2
25	BCR	J	101	-	-	4/29/63/63	0/2/2/2
22	CLA	A	855	5	1/1/15/20	7/39/115/115	-
22	CLA	A	858	-	1/1/15/20	13/39/115/115	-
26	LHG	G	204	22	-	1/26/26/53	-
31	DGD	O	201	-	-	11/42/82/95	0/2/2/2
22	CLA	A	805	-	-	6/21/97/115	-
22	CLA	B	825	-	-	5/17/93/115	-
25	BCR	A	817	-	-	4/29/63/63	0/2/2/2
27	MGE	N	201	-	-	7/26/46/63	0/1/1/1
21	CHL	1	316	1	-	8/17/93/117	-
22	CLA	B	850	6	1/1/15/20	18/39/115/115	-
24	XAT	1	311	-	-	11/31/93/93	0/4/4/4
26	LHG	A	823	22	-	1/36/36/53	-
25	BCR	A	814	-	-	2/29/63/63	0/2/2/2
22	CLA	B	808	6	1/1/15/20	13/39/115/115	-
22	CLA	4	316	4	-	3/10/86/115	-
22	CLA	3	309	3	1/1/13/20	14/32/108/115	-
25	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	CHL	4	309	-	-	11/17/93/117	-
22	CLA	A	810	-	1/1/15/20	18/39/115/115	-
22	CLA	3	318	3	-	4/15/91/115	-
22	CLA	A	829	5,22	-	10/21/97/115	-
22	CLA	X	313	-	-	9/17/93/115	-
22	CLA	X	304	-	-	7/17/93/115	-
22	CLA	A	836	5,22	1/1/14/20	6/33/109/115	-
22	CLA	A	806	5	-	10/25/101/115	-
22	CLA	K	202	15	-	7/13/89/115	-
22	CLA	A	850	-	1/1/15/20	11/39/115/115	-
22	CLA	B	815	-	1/1/13/20	15/31/107/115	-
22	CLA	B	833	22	1/1/13/20	13/29/105/115	-
22	CLA	3	310	-	1/1/13/20	19/31/107/115	-
22	CLA	1	308	1	-	3/10/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	306	16	1/1/15/20	21/39/115/115	-
25	BCR	L	301	-	-	7/29/63/63	0/2/2/2
22	CLA	X	301	-	-	0/17/93/115	-
22	CLA	3	315	3	-	6/10/86/115	-
22	CLA	B	814	-	1/1/15/20	10/39/115/115	-
22	CLA	O	209	18	-	4/18/94/115	-
23	LUT	4	322	-	-	3/29/67/67	0/2/2/2
25	BCR	A	819	-	-	4/29/63/63	0/2/2/2
23	LUT	4	319	-	-	0/29/67/67	0/2/2/2
25	BCR	A	815	-	-	3/29/63/63	0/2/2/2
27	MGE	F	303	-	-	14/32/52/63	0/1/1/1
21	CHL	3	314	-	-	6/17/93/117	-
25	BCR	L	304	-	-	0/29/63/63	0/2/2/2
26	LHG	A	824	-	-	8/41/41/53	-
22	CLA	4	304	4	1/1/13/20	7/27/103/115	-
22	CLA	1	321	1	-	2/13/89/115	-
22	CLA	4	313	-	-	4/13/89/115	-
22	CLA	A	804	-	-	4/12/88/115	-
22	CLA	Y	302	-	-	6/17/93/115	-
22	CLA	B	811	6	1/1/13/20	9/29/105/115	-
22	CLA	2	307	2	1/1/14/20	17/33/109/115	-
22	CLA	B	852	6	1/1/13/20	8/27/103/115	-
22	CLA	B	812	6	1/1/13/20	12/32/108/115	-
21	CHL	4	308	-	-	8/15/91/117	-
21	CHL	Z	312	19	-	7/17/93/117	-
22	CLA	B	813	6	-	11/25/101/115	-
22	CLA	B	826	6	-	8/21/97/115	-
23	LUT	2	310	-	-	4/29/67/67	0/2/2/2
27	MGE	1	315	-	-	15/32/52/63	0/1/1/1
26	LHG	O	204	-	-	4/30/30/53	-
22	CLA	1	307	1	1/1/13/20	9/27/103/115	-
22	CLA	A	807	5	1/1/14/20	17/35/111/115	-
22	CLA	B	801	-	1/1/13/20	10/27/103/115	-
30	CL0	A	825	5	1/1/15/20	10/39/115/115	-
22	CLA	A	842	5	1/1/12/20	7/29/105/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	Y	305	-	-	8/17/93/117	-
25	BCR	4	321	-	-	6/29/63/63	0/2/2/2
23	LUT	3	301	-	-	0/29/67/67	0/2/2/2
21	CHL	2	321	-	-	9/15/91/117	-
22	CLA	A	826	-	1/1/15/20	13/39/115/115	-
22	CLA	4	306	-	-	7/13/89/115	-
22	CLA	B	805	6	-	6/17/93/115	-
25	BCR	3	303	-	-	5/29/63/63	0/2/2/2
22	CLA	B	821	6	-	8/15/91/115	-
22	CLA	4	305	-	-	4/13/89/115	-
22	CLA	A	835	5	-	5/12/88/115	-
25	BCR	B	839	-	-	2/29/63/63	0/2/2/2
22	CLA	J	102	14	-	1/10/86/115	-
26	LHG	1	313	22	-	8/46/46/53	-
22	CLA	A	843	5	1/1/13/20	9/29/105/115	-
22	CLA	B	810	6	-	5/21/97/115	-
22	CLA	A	849	5	1/1/15/20	10/39/115/115	-
22	CLA	3	321	3	-	2/15/91/115	-
22	CLA	2	320	-	-	4/21/97/115	-
27	MGE	F	304	-	-	12/23/43/63	0/1/1/1
22	CLA	A	828	5	-	0/8/84/115	-
22	CLA	A	848	5	-	1/15/91/115	-
26	LHG	2	314	-	-	4/30/30/53	-
22	CLA	F	305	-	-	2/17/93/115	-
22	CLA	1	302	-	-	3/13/89/115	-
22	CLA	X	310	-	-	7/17/93/115	-
26	LHG	A	822	-	-	9/33/33/53	-
22	CLA	Z	311	-	-	4/17/93/115	-
26	LHG	4	302	-	-	14/31/31/53	-
26	LHG	B	842	22	-	6/34/34/53	-
29	SF4	A	813	5,6	-	-	0/6/5/5
22	CLA	A	852	-	1/1/14/20	16/35/111/115	-
22	CLA	4	318	4	-	8/17/93/115	-
21	CHL	X	302	-	-	7/19/95/117	-
22	CLA	B	823	6	1/1/14/20	12/35/111/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	822	6	1/1/15/20	9/39/115/115	-
26	LHG	O	205	-	-	3/29/29/53	-
22	CLA	2	319	2	-	5/17/93/115	-
22	CLA	B	830	6	1/1/15/20	17/39/115/115	-
22	CLA	K	205	15	-	2/10/86/115	-
25	BCR	B	834	-	-	5/29/63/63	0/2/2/2
22	CLA	1	303	1	-	6/15/91/115	-

The worst 5 of 4216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	304	CLA	C1D-ND	10.04	1.50	1.37
22	3	317	CLA	C1D-ND	8.97	1.48	1.37
22	4	318	CLA	C1D-ND	8.90	1.48	1.37
22	Y	312	CLA	C1D-ND	8.87	1.48	1.37
22	A	830	CLA	C1D-ND	8.85	1.48	1.37

The worst 5 of 6469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	304	CLA	C4D-CHA-C1A	-18.66	98.54	121.25
22	B	807	CLA	C1D-C2D-C3D	-17.44	102.03	110.84
22	B	807	CLA	C2B-C1B-NB	15.81	120.83	110.23
22	B	816	CLA	C1D-ND-C4D	-12.50	97.45	106.33
22	B	814	CLA	C1D-ND-C4D	-11.29	98.32	106.33

5 of 72 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	1	307	CLA	C8
22	1	317	CLA	C8
22	1	318	CLA	C8
22	2	304	CLA	C8
22	2	307	CLA	C8

5 of 2014 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	301	CHL	C1A-C2A-CAA-CBA
21	1	301	CHL	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	301	CHL	C1C-C2C-CMC-OMC
21	1	301	CHL	C3C-C2C-CMC-OMC
21	1	301	CHL	CBD-CGD-O2D-CED

There are no ring outliers.

227 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	310	CLA	3	0
28	A	811	PQN	4	0
21	Z	302	CHL	2	0
22	A	830	CLA	6	0
22	B	820	CLA	2	0
22	B	807	CLA	8	0
22	2	318	CLA	7	0
26	2	316	LHG	2	0
26	2	315	LHG	1	0
22	A	834	CLA	4	0
22	B	816	CLA	10	0
22	K	203	CLA	2	0
25	G	202	BCR	4	0
22	B	827	CLA	7	0
26	3	306	LHG	3	0
22	B	846	CLA	2	0
22	B	847	CLA	5	0
25	I	101	BCR	5	0
26	2	313	LHG	2	0
22	A	833	CLA	3	0
26	A	820	LHG	5	0
25	K	201	BCR	5	0
26	B	843	LHG	9	0
22	A	809	CLA	5	0
22	1	320	CLA	2	0
22	G	206	CLA	4	0
24	2	311	XAT	9	0
22	B	818	CLA	6	0
29	C	102	SF4	1	0
22	A	837	CLA	3	0
22	B	829	CLA	5	0
25	L	302	BCR	3	0
22	3	308	CLA	1	0
28	B	832	PQN	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	319	CLA	1	0
22	A	802	CLA	1	0
25	B	840	BCR	6	0
25	A	818	BCR	6	0
27	3	304	MGE	1	0
25	O	203	BCR	4	0
21	Y	313	CHL	1	0
21	2	302	CHL	4	0
22	4	312	CLA	1	0
22	A	803	CLA	3	0
25	A	816	BCR	6	0
21	4	317	CHL	1	0
22	A	859	CLA	3	0
27	3	305	MGE	2	0
31	B	841	DGD	4	0
25	B	844	BCR	6	0
22	A	831	CLA	5	0
25	2	312	BCR	12	0
22	2	308	CLA	3	0
22	3	313	CLA	1	0
22	A	845	CLA	2	0
22	X	303	CLA	2	0
22	Y	314	CLA	1	0
25	B	835	BCR	6	0
31	G	201	DGD	9	0
22	B	803	CLA	11	0
22	4	311	CLA	5	0
22	B	809	CLA	6	0
21	2	309	CHL	3	0
25	B	837	BCR	5	0
22	B	806	CLA	3	0
22	B	849	CLA	7	0
24	3	302	XAT	7	0
21	Z	305	CHL	1	0
22	A	847	CLA	2	0
22	A	838	CLA	10	0
21	2	301	CHL	1	0
22	3	311	CLA	1	0
22	3	317	CLA	2	0
22	L	307	CLA	4	0
22	1	304	CLA	5	0
22	B	845	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	312	CLA	6	0
26	G	203	LHG	1	0
21	Y	307	CHL	2	0
22	A	839	CLA	3	0
22	1	306	CLA	1	0
22	A	844	CLA	10	0
25	B	838	BCR	4	0
22	3	316	CLA	4	0
25	F	302	BCR	6	0
22	A	808	CLA	2	0
21	Y	304	CHL	1	0
21	3	307	CHL	2	0
22	F	306	CLA	2	0
22	K	204	CLA	6	0
21	Z	303	CHL	2	0
22	B	828	CLA	5	0
22	B	848	CLA	3	0
22	B	851	CLA	5	0
23	1	310	LUT	4	0
29	C	101	SF4	1	0
22	O	207	CLA	1	0
25	O	202	BCR	5	0
22	3	320	CLA	2	0
22	A	841	CLA	1	0
22	A	827	CLA	8	0
22	G	207	CLA	1	0
26	1	322	LHG	2	0
22	2	303	CLA	3	0
22	A	854	CLA	8	0
22	B	831	CLA	5	0
22	A	801	CLA	1	0
22	1	317	CLA	9	0
22	Y	311	CLA	2	0
26	1	314	LHG	2	0
22	1	318	CLA	3	0
22	B	802	CLA	4	0
22	2	322	CLA	3	0
22	2	317	CLA	1	0
22	O	208	CLA	4	0
25	1	312	BCR	6	0
24	4	320	XAT	5	0
26	F	301	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	812	CLA	3	0
22	B	817	CLA	4	0
22	A	856	CLA	2	0
22	A	853	CLA	13	0
26	A	821	LHG	1	0
22	B	819	CLA	6	0
22	A	857	CLA	7	0
22	A	840	CLA	3	0
22	A	846	CLA	9	0
22	B	804	CLA	6	0
22	B	824	CLA	2	0
22	G	205	CLA	7	0
25	L	303	BCR	3	0
22	A	832	CLA	3	0
26	4	301	LHG	3	0
25	B	836	BCR	4	0
25	J	101	BCR	6	0
22	A	855	CLA	8	0
22	A	858	CLA	8	0
26	G	204	LHG	1	0
31	O	201	DGD	4	0
22	A	805	CLA	1	0
22	B	825	CLA	4	0
25	A	817	BCR	10	0
27	N	201	MGE	2	0
21	1	316	CHL	2	0
22	B	850	CLA	5	0
24	1	311	XAT	4	0
26	A	823	LHG	3	0
25	A	814	BCR	4	0
22	B	808	CLA	7	0
22	4	316	CLA	3	0
22	3	309	CLA	4	0
25	J	103	BCR	5	0
21	4	309	CHL	4	0
22	3	318	CLA	1	0
22	A	810	CLA	7	0
22	A	829	CLA	2	0
22	X	304	CLA	1	0
22	A	836	CLA	3	0
22	A	806	CLA	2	0
22	A	850	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	815	CLA	5	0
22	B	833	CLA	3	0
22	3	310	CLA	2	0
22	1	308	CLA	1	0
22	L	306	CLA	12	0
25	L	301	BCR	6	0
22	X	301	CLA	1	0
22	B	814	CLA	7	0
22	O	209	CLA	1	0
23	4	322	LUT	6	0
25	A	819	BCR	5	0
23	4	319	LUT	3	0
25	A	815	BCR	3	0
27	F	303	MGE	2	0
21	3	314	CHL	1	0
25	L	304	BCR	1	0
26	A	824	LHG	2	0
22	4	304	CLA	2	0
22	1	321	CLA	2	0
22	4	313	CLA	2	0
22	A	804	CLA	2	0
22	B	811	CLA	5	0
22	2	307	CLA	1	0
22	B	852	CLA	6	0
22	B	812	CLA	5	0
21	4	308	CHL	1	0
21	Z	312	CHL	1	0
22	B	813	CLA	2	0
23	2	310	LUT	4	0
27	1	315	MGE	3	0
22	1	307	CLA	1	0
22	A	807	CLA	2	0
22	B	801	CLA	4	0
22	A	842	CLA	3	0
25	4	321	BCR	1	0
30	A	825	CL0	4	0
23	3	301	LUT	5	0
21	2	321	CHL	3	0
22	A	826	CLA	4	0
22	B	805	CLA	1	0
25	3	303	BCR	2	0
22	A	835	CLA	4	0

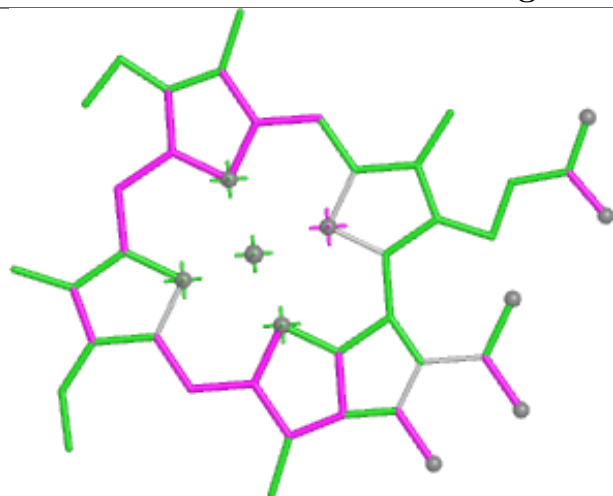
Continued on next page...

Continued from previous page...

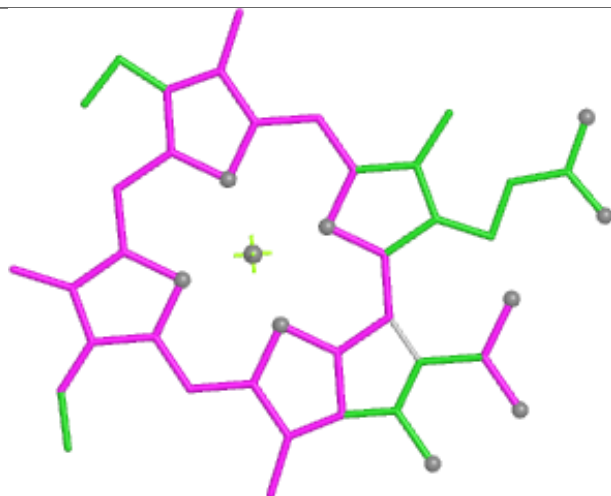
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	839	BCR	6	0
22	J	102	CLA	1	0
26	1	313	LHG	2	0
22	A	843	CLA	2	0
22	B	810	CLA	1	0
22	A	849	CLA	9	0
22	2	320	CLA	2	0
27	F	304	MGE	1	0
22	A	828	CLA	4	0
22	A	848	CLA	2	0
26	2	314	LHG	5	0
22	F	305	CLA	2	0
26	A	822	LHG	18	0
26	4	302	LHG	2	0
26	B	842	LHG	1	0
22	4	318	CLA	1	0
22	A	852	CLA	5	0
22	B	823	CLA	6	0
22	B	822	CLA	7	0
26	O	205	LHG	2	0
22	2	319	CLA	1	0
22	B	830	CLA	4	0
22	K	205	CLA	1	0
25	B	834	BCR	8	0
22	1	303	CLA	6	0

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

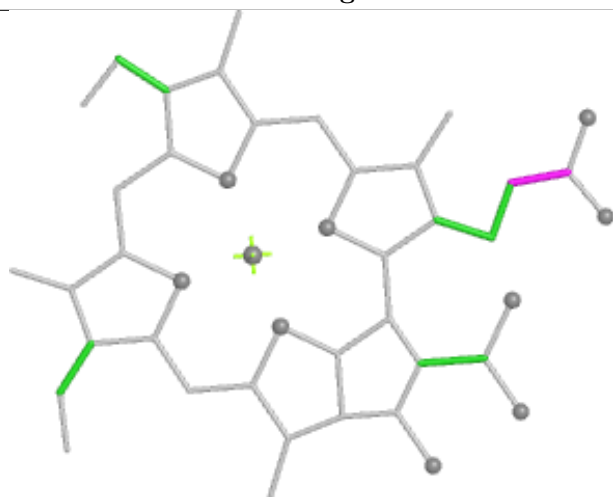
Ligand CLA 2 306



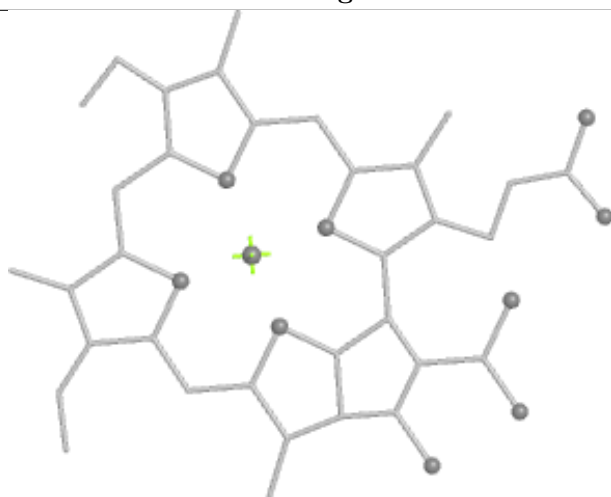
Bond lengths



Bond angles

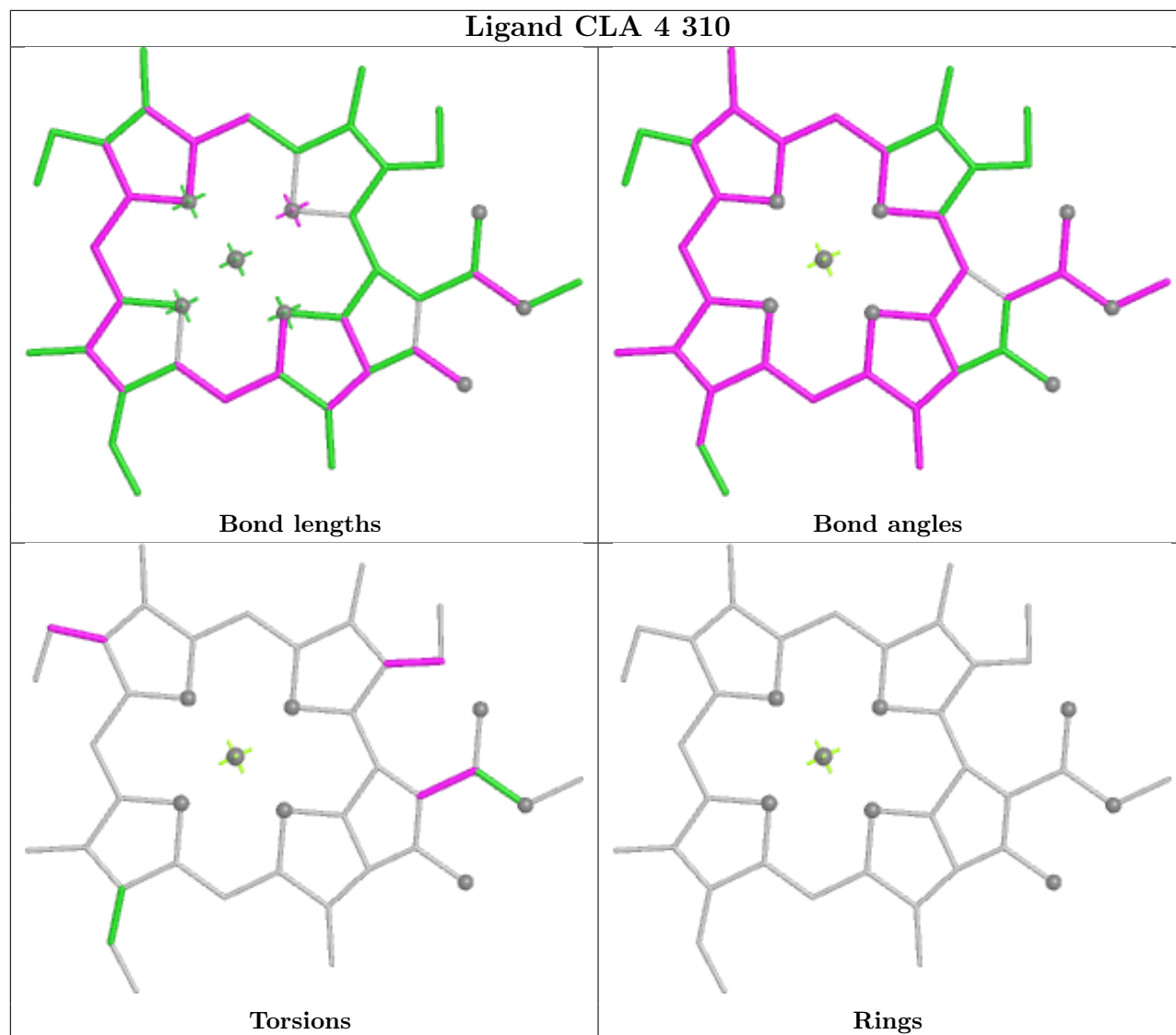


Torsions

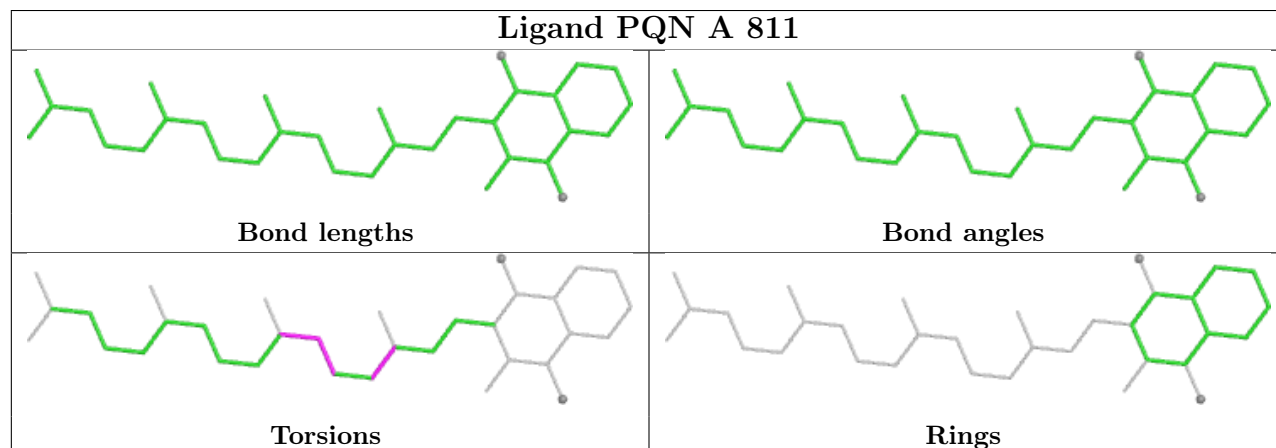


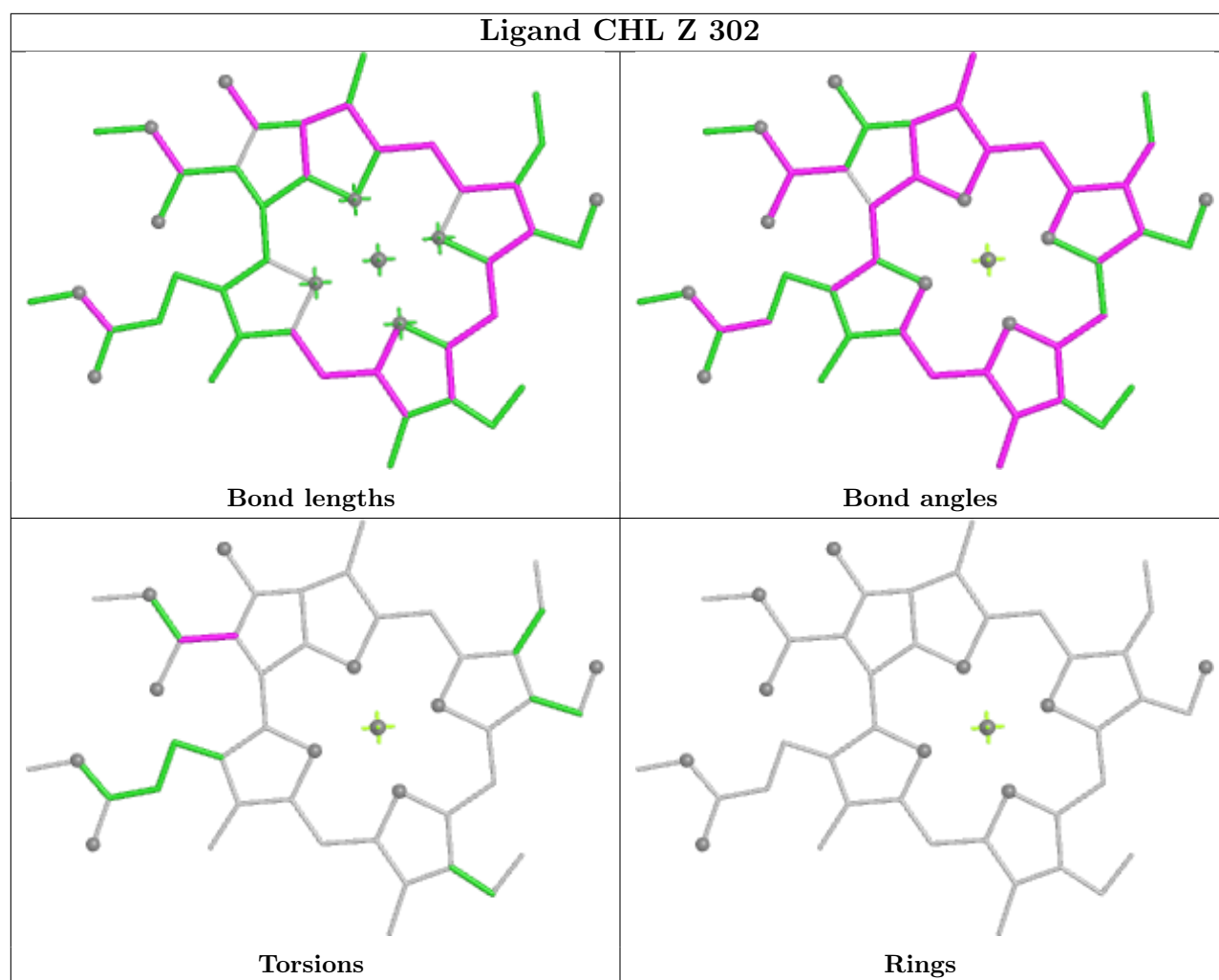
Rings

Ligand CLA 4 310

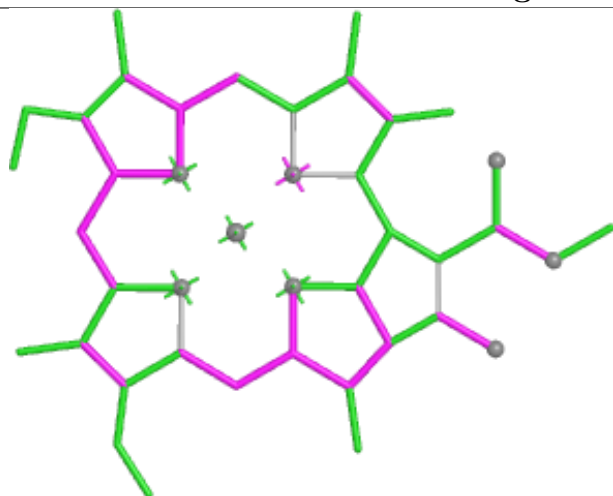


Ligand PQN A 811





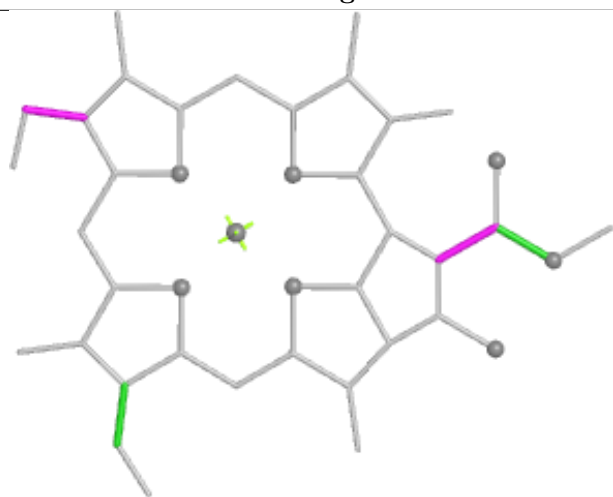
Ligand CLA O 210



Bond lengths



Bond angles

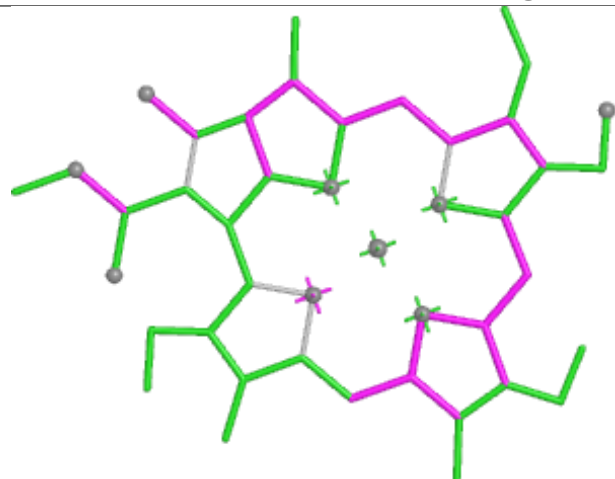


Torsions

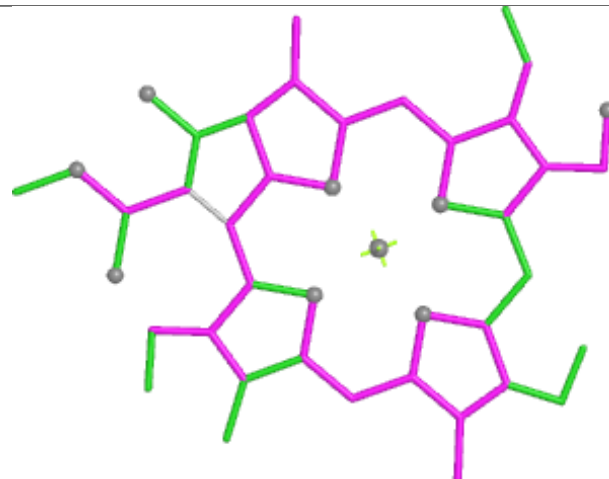


Rings

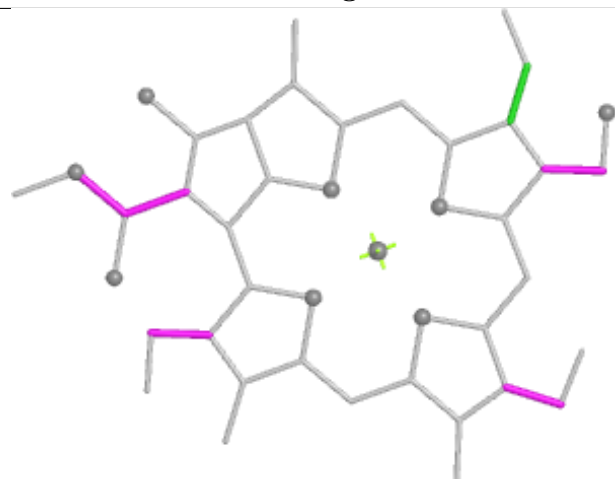
Ligand CHL 1 301



Bond lengths



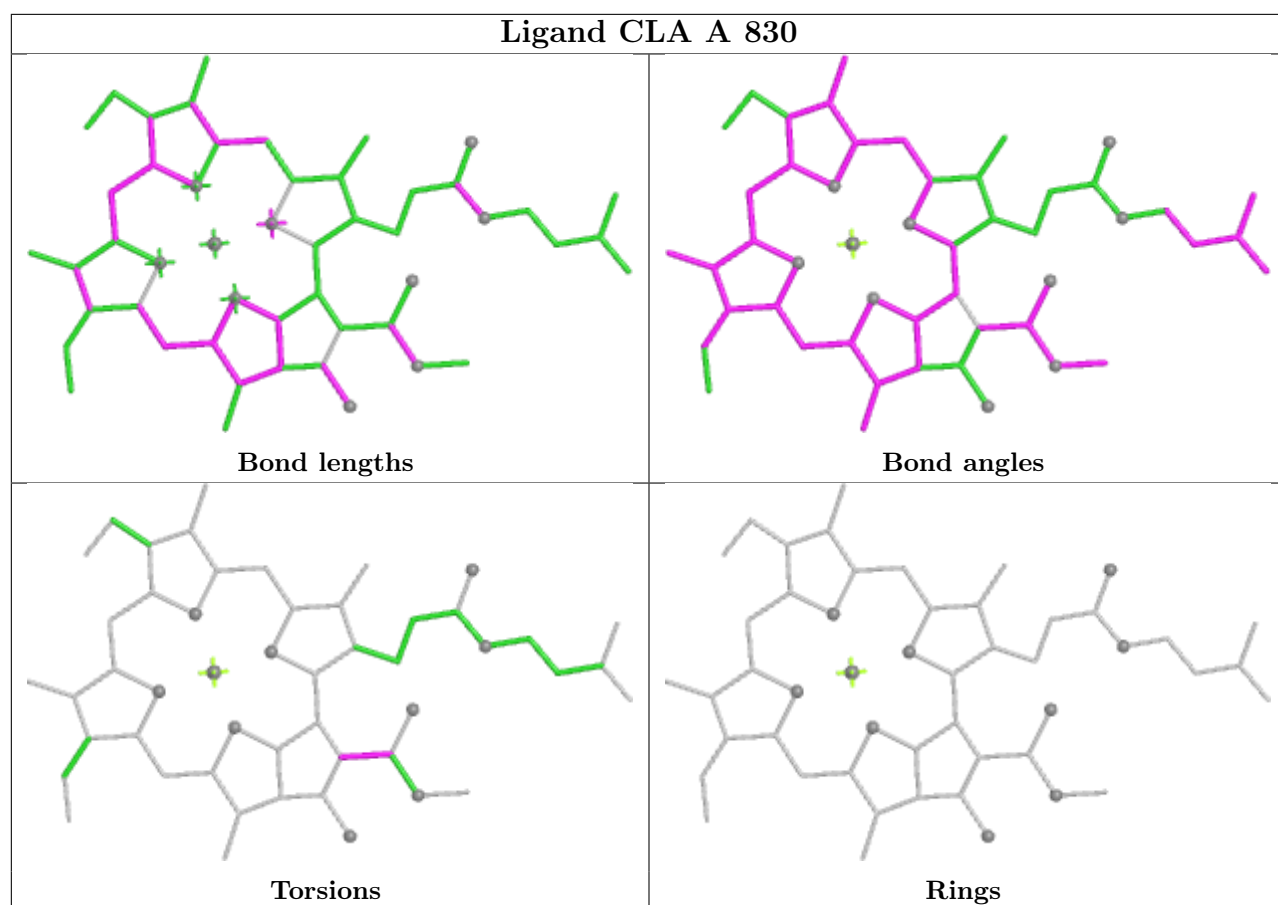
Bond angles

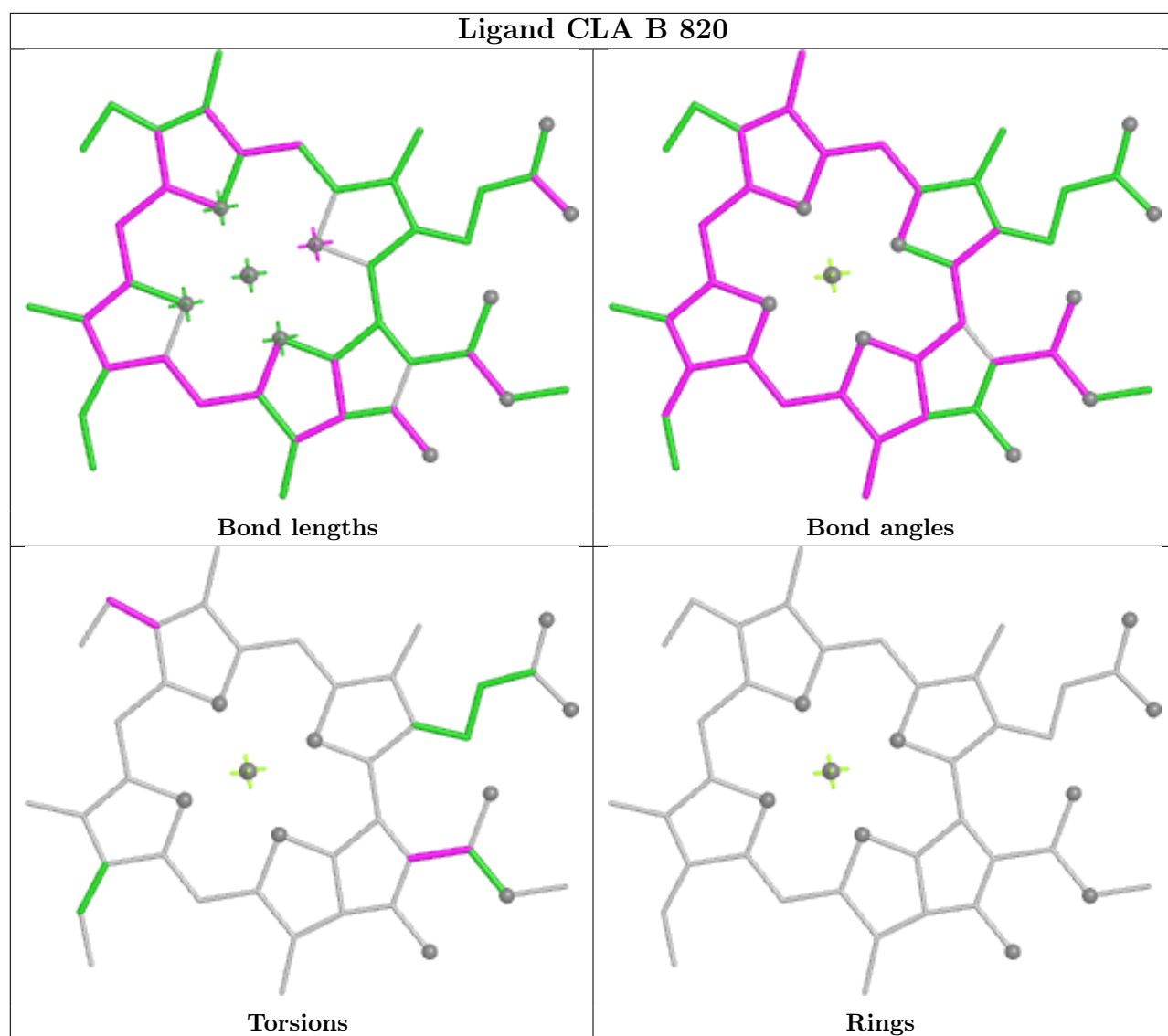


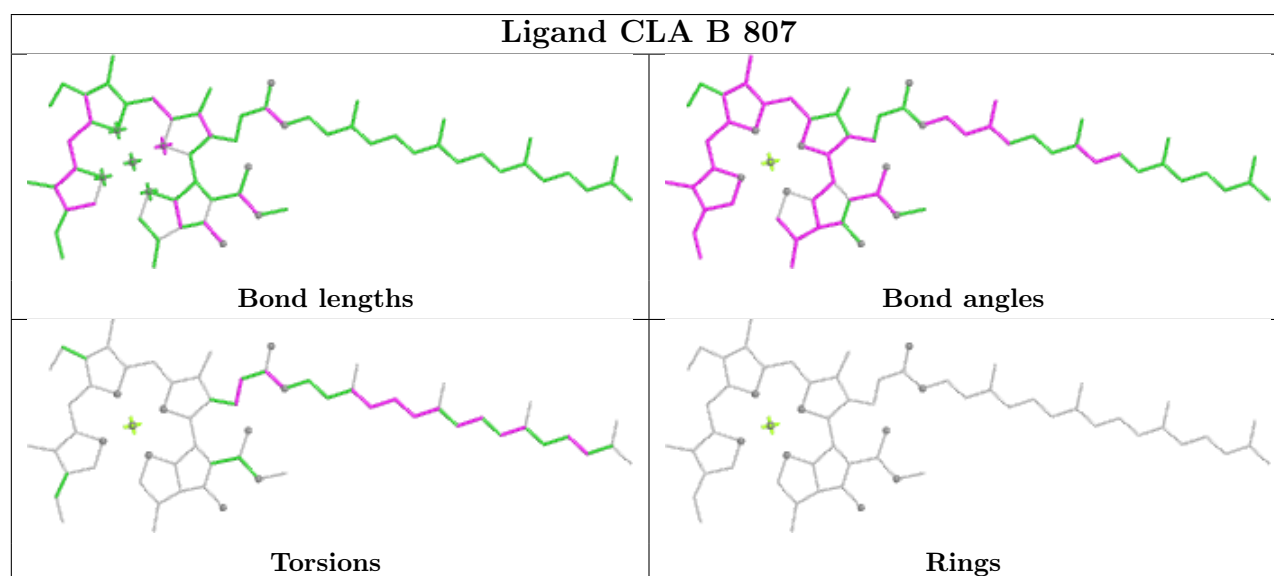
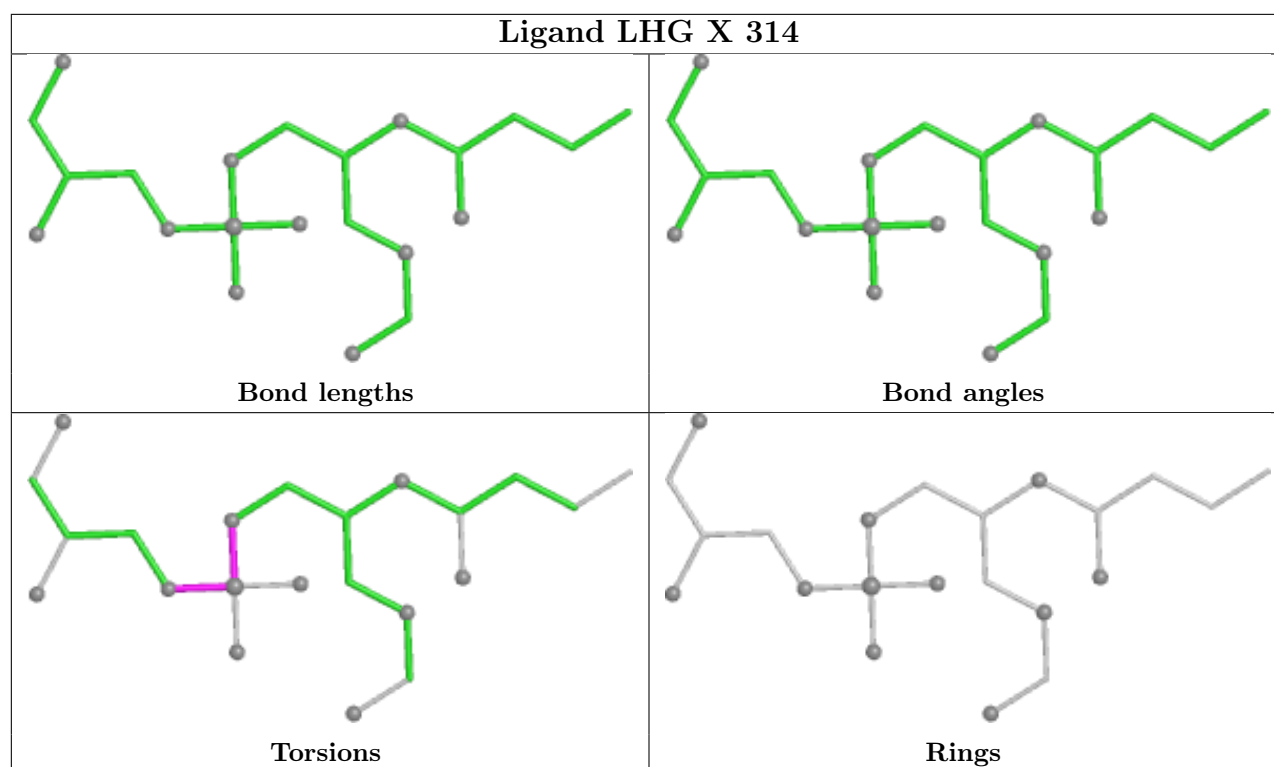
Torsions

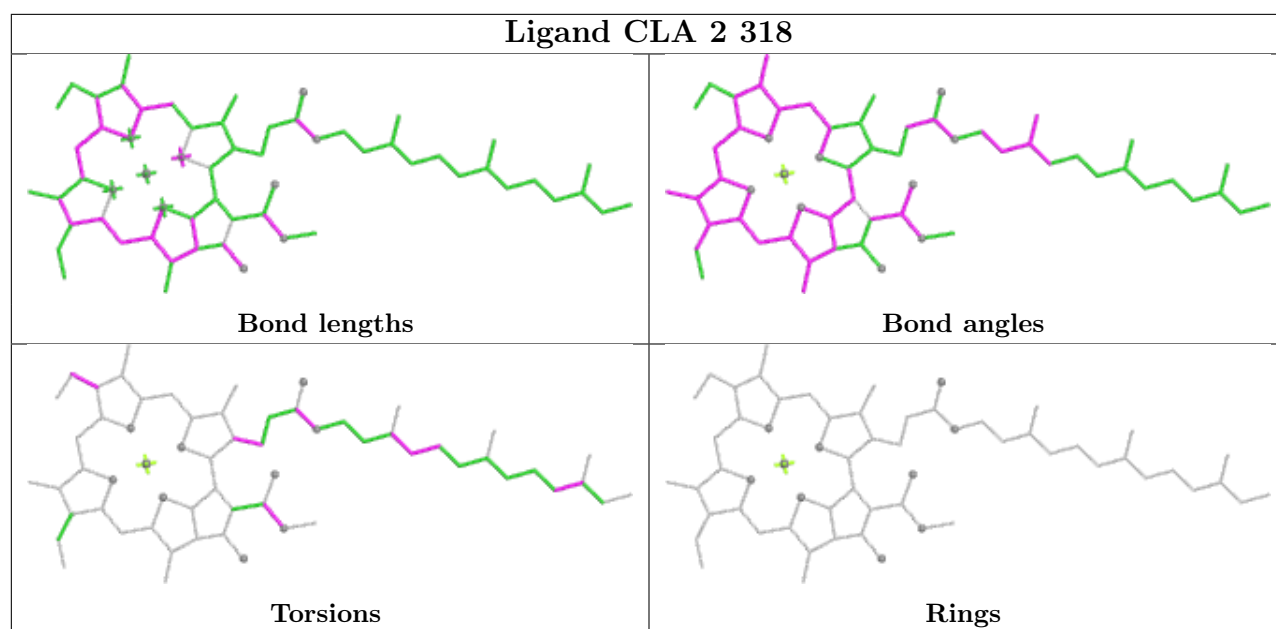


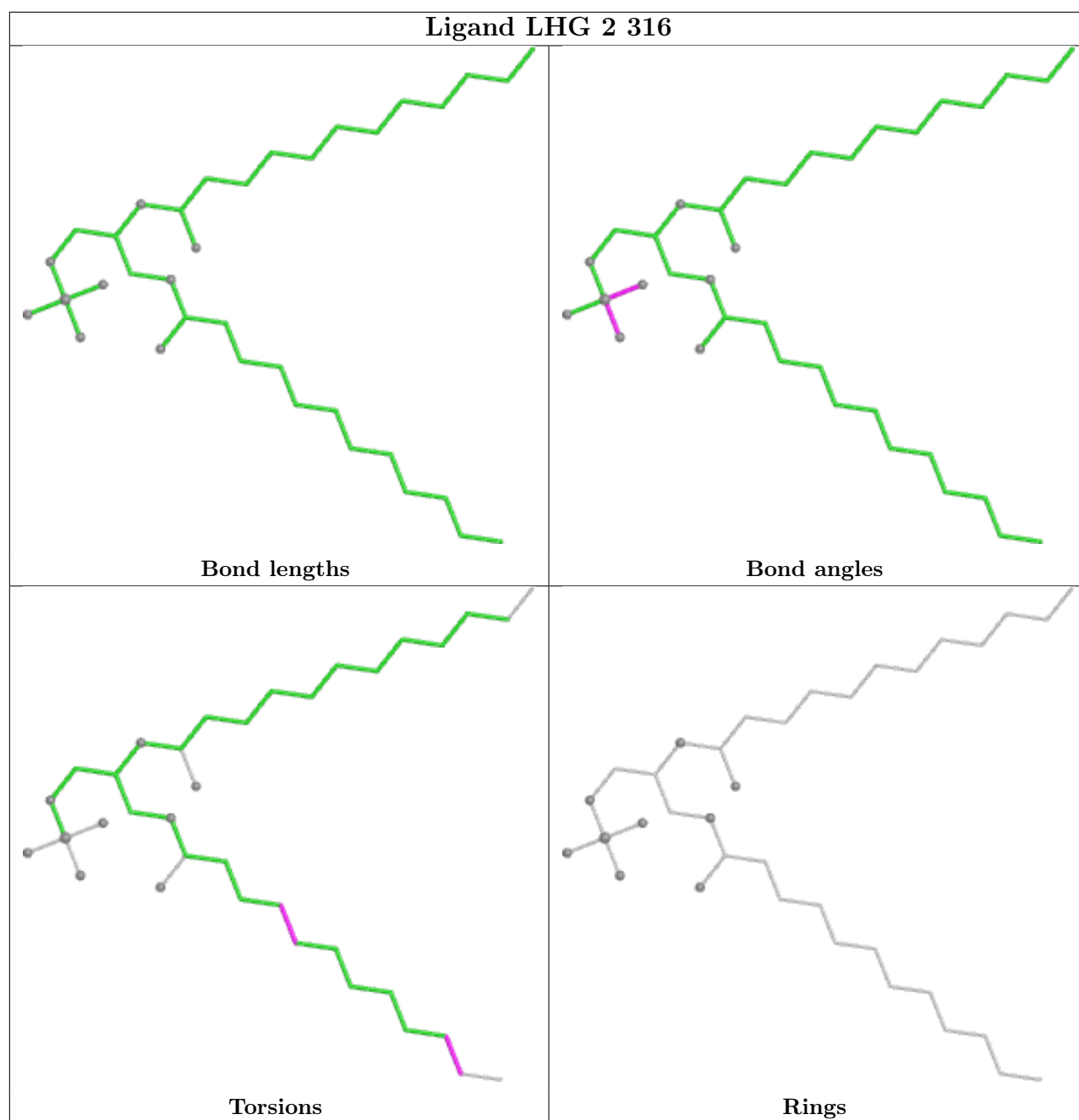
Rings

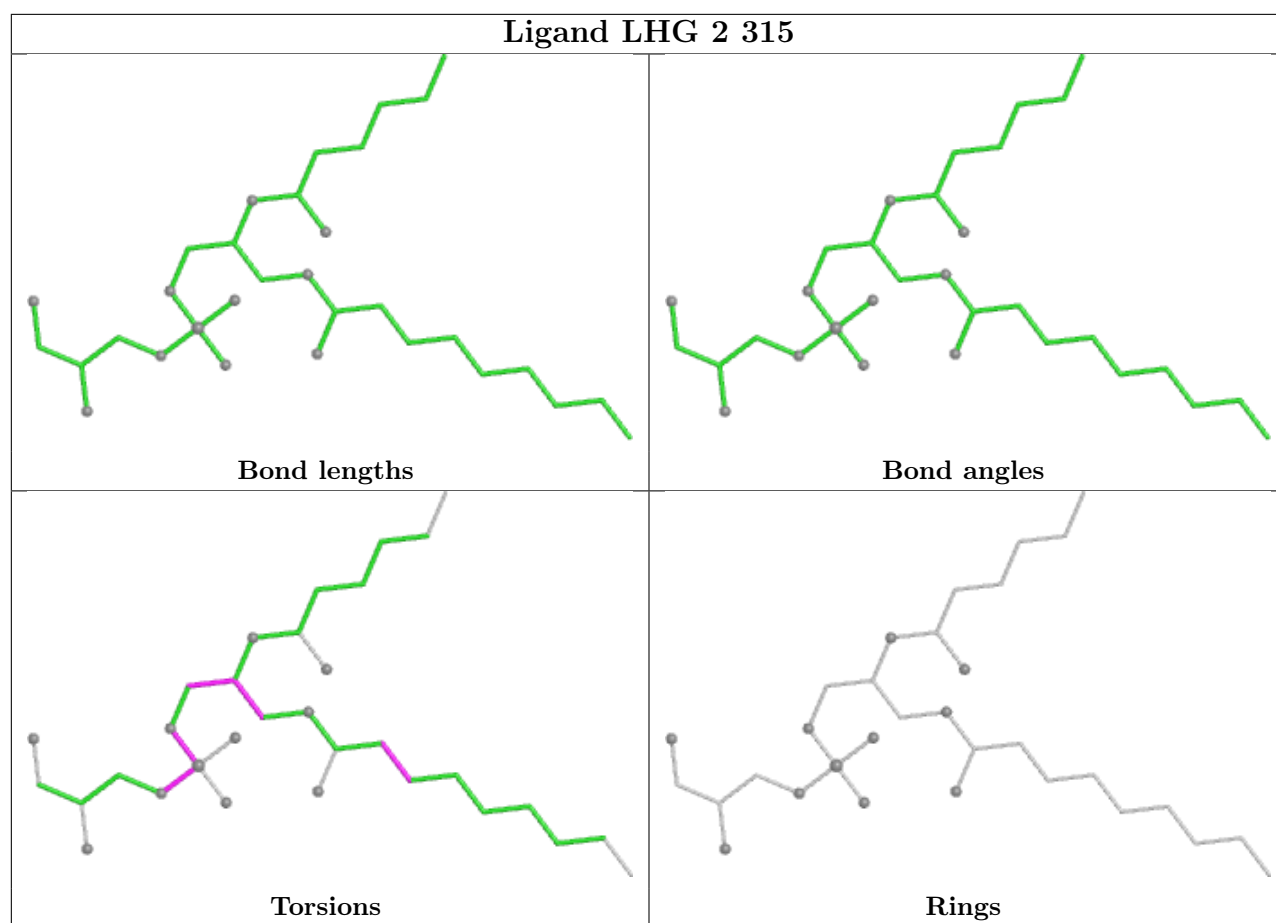




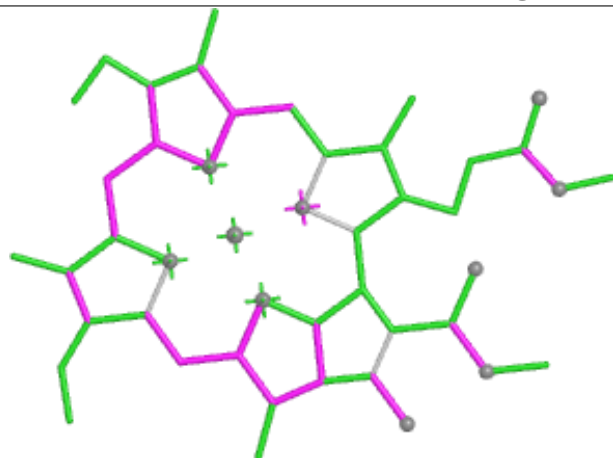




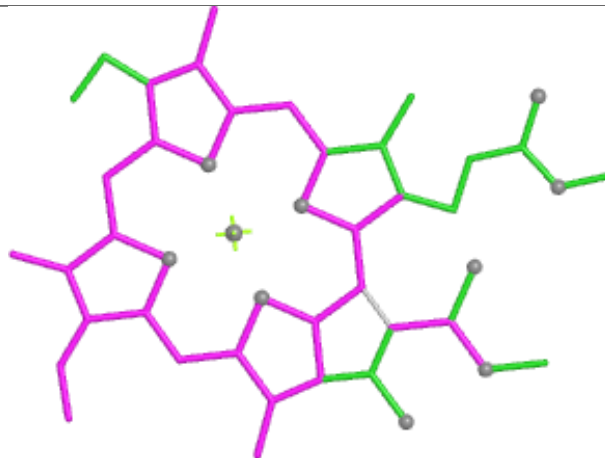




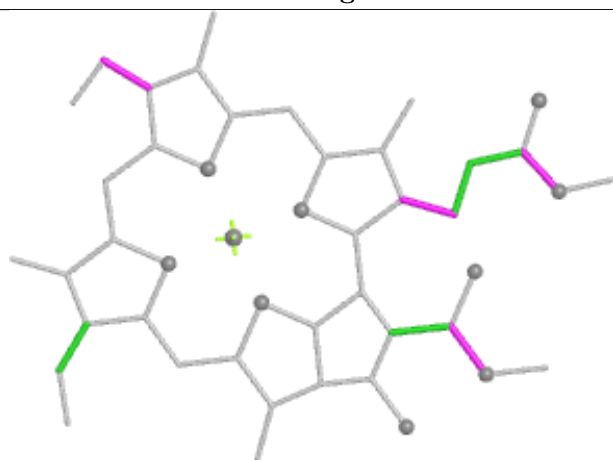
Ligand CLA A 834



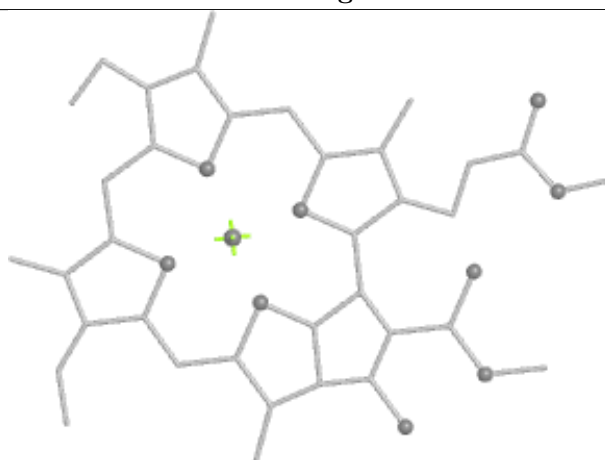
Bond lengths



Bond angles

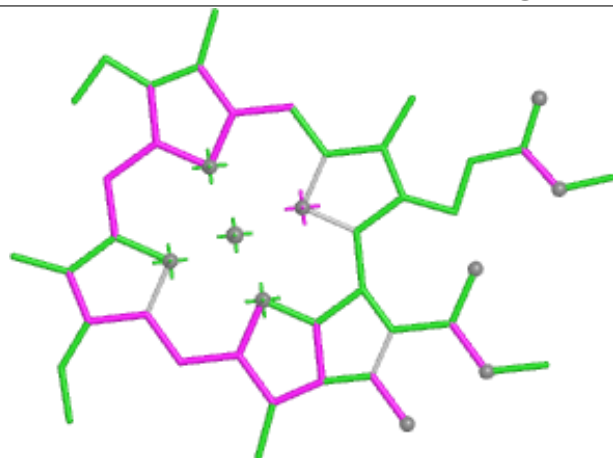


Torsions

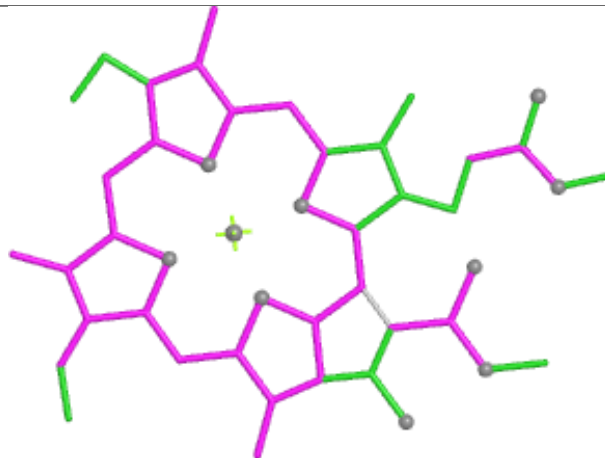


Rings

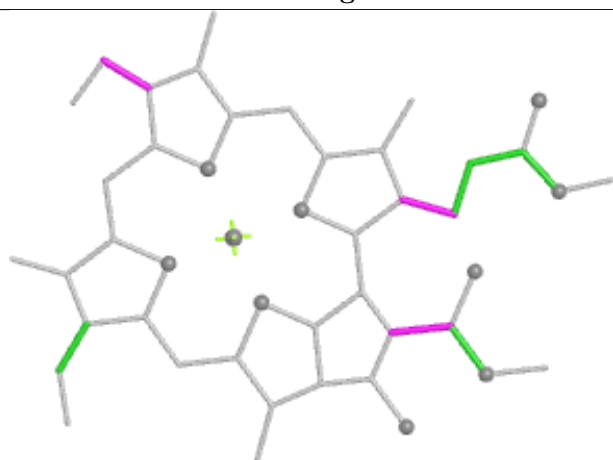
Ligand CLA Z 306



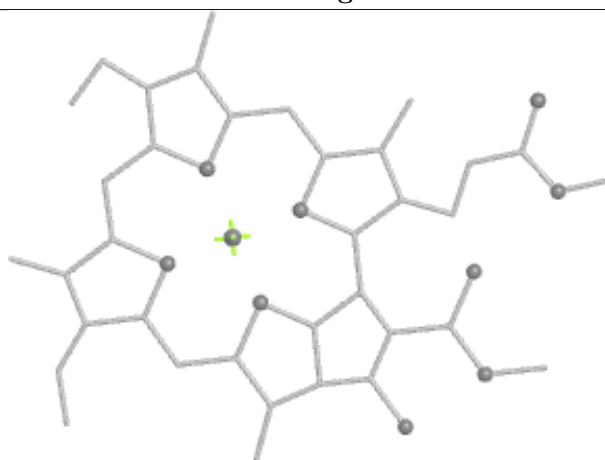
Bond lengths



Bond angles

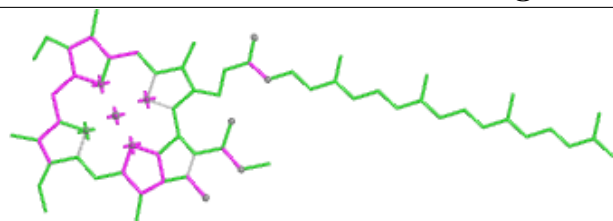


Torsions

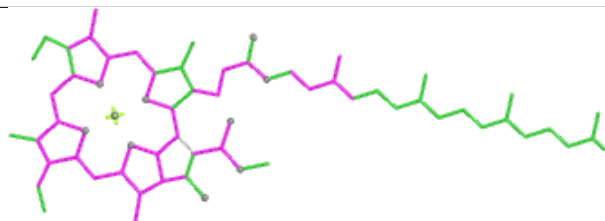


Rings

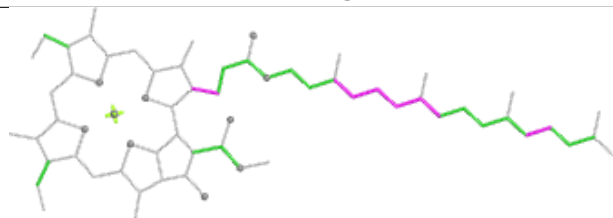
Ligand CLA B 816



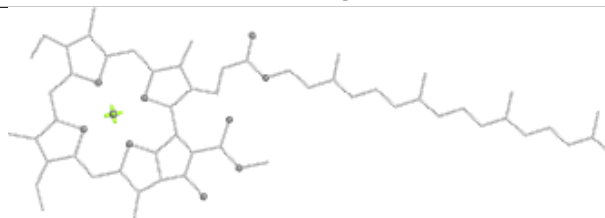
Bond lengths



Bond angles

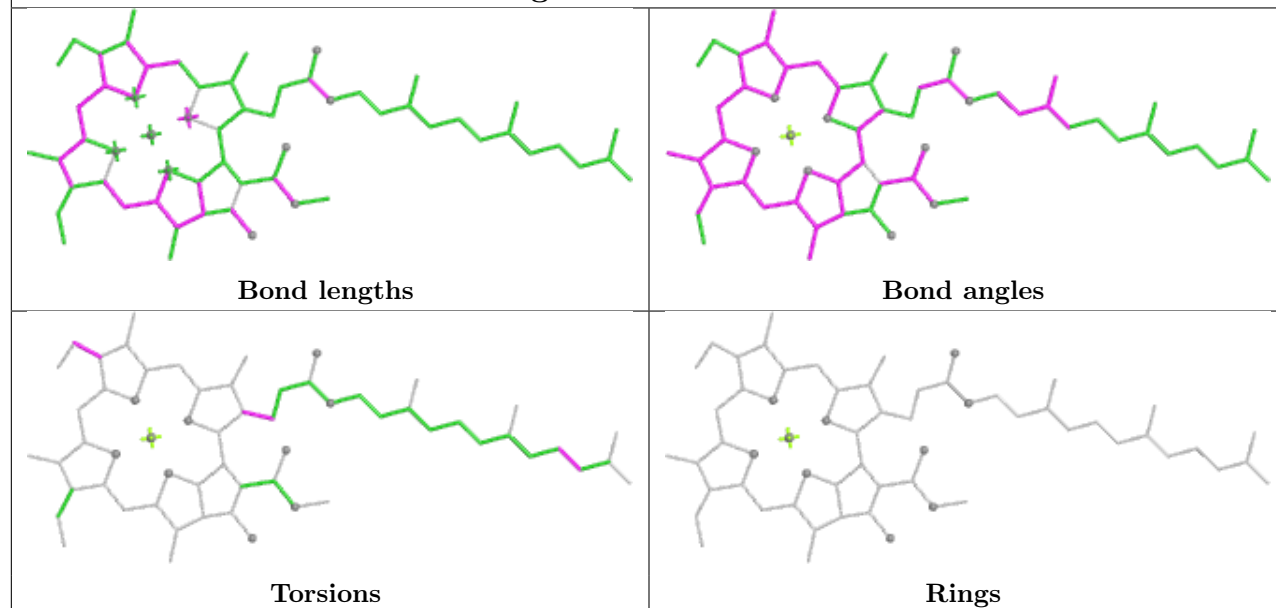


Torsions

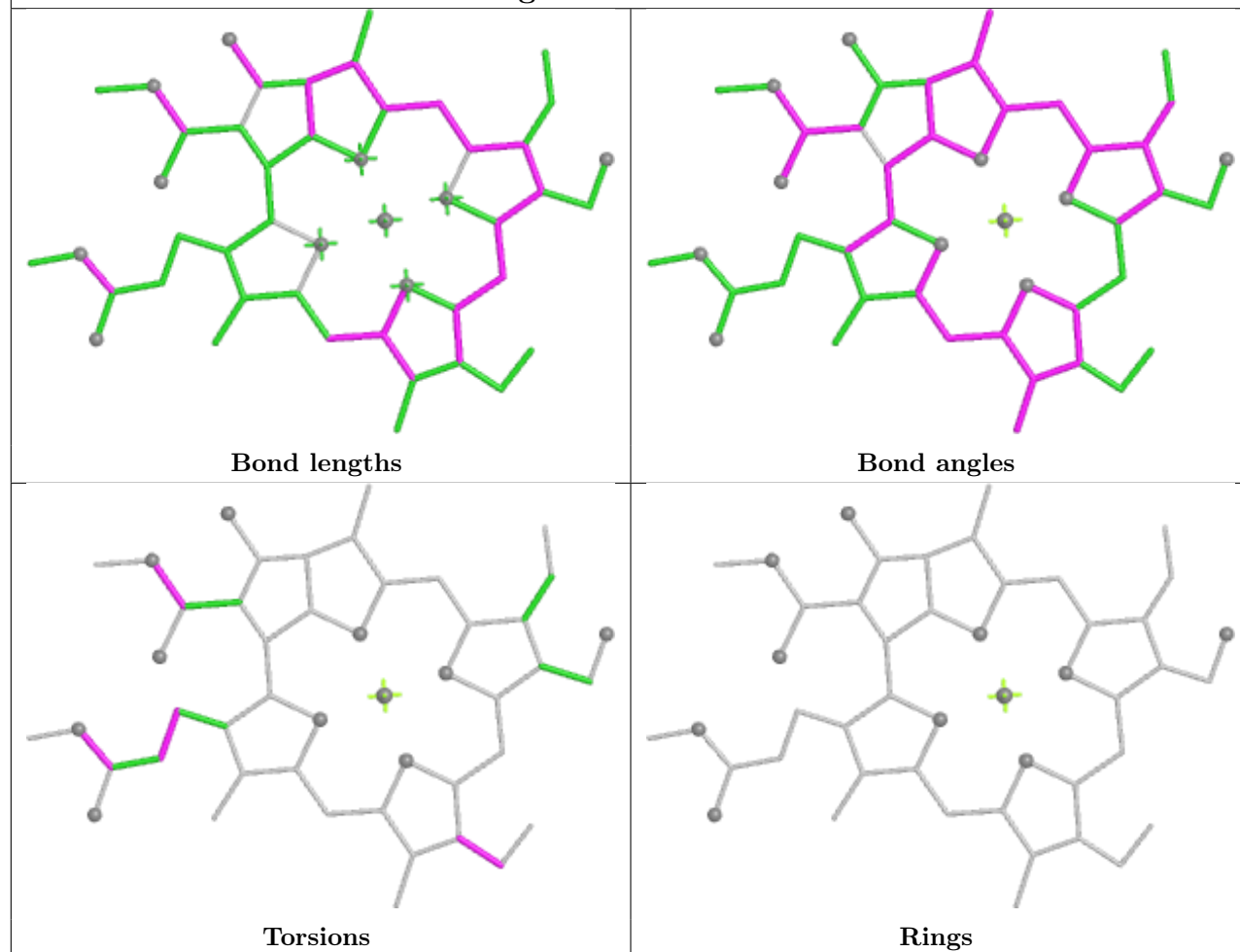


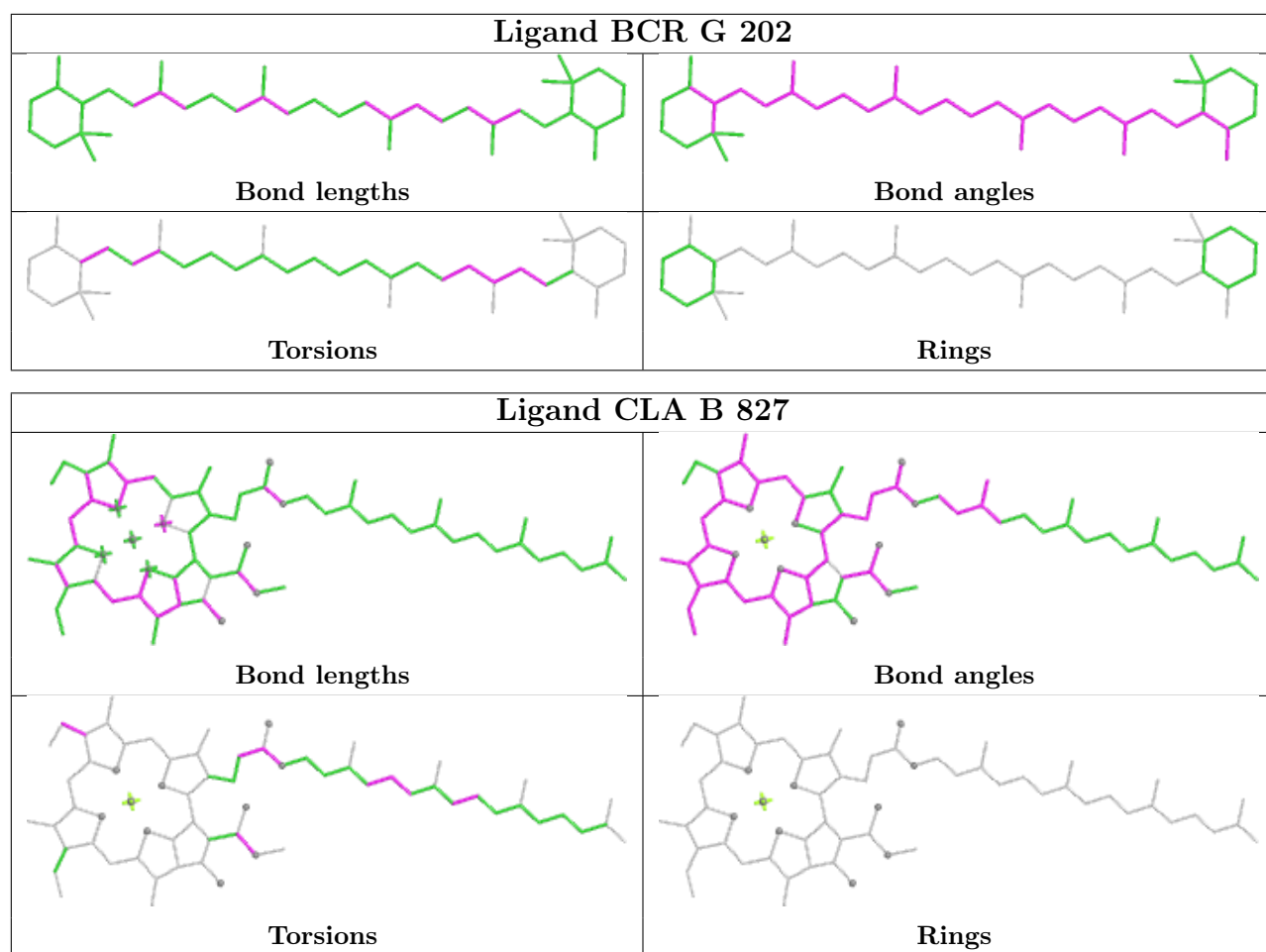
Rings

Ligand CLA K 203

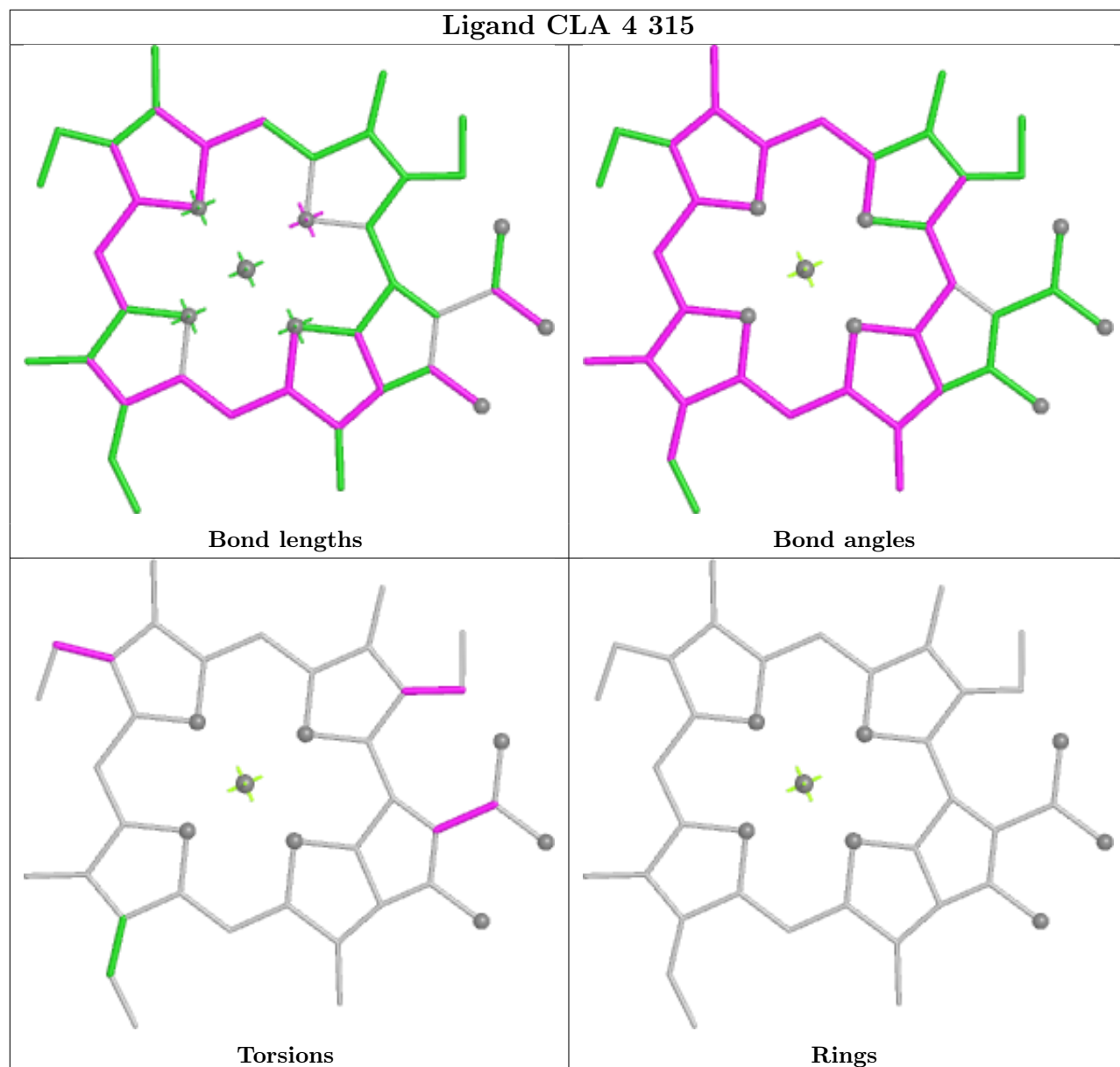


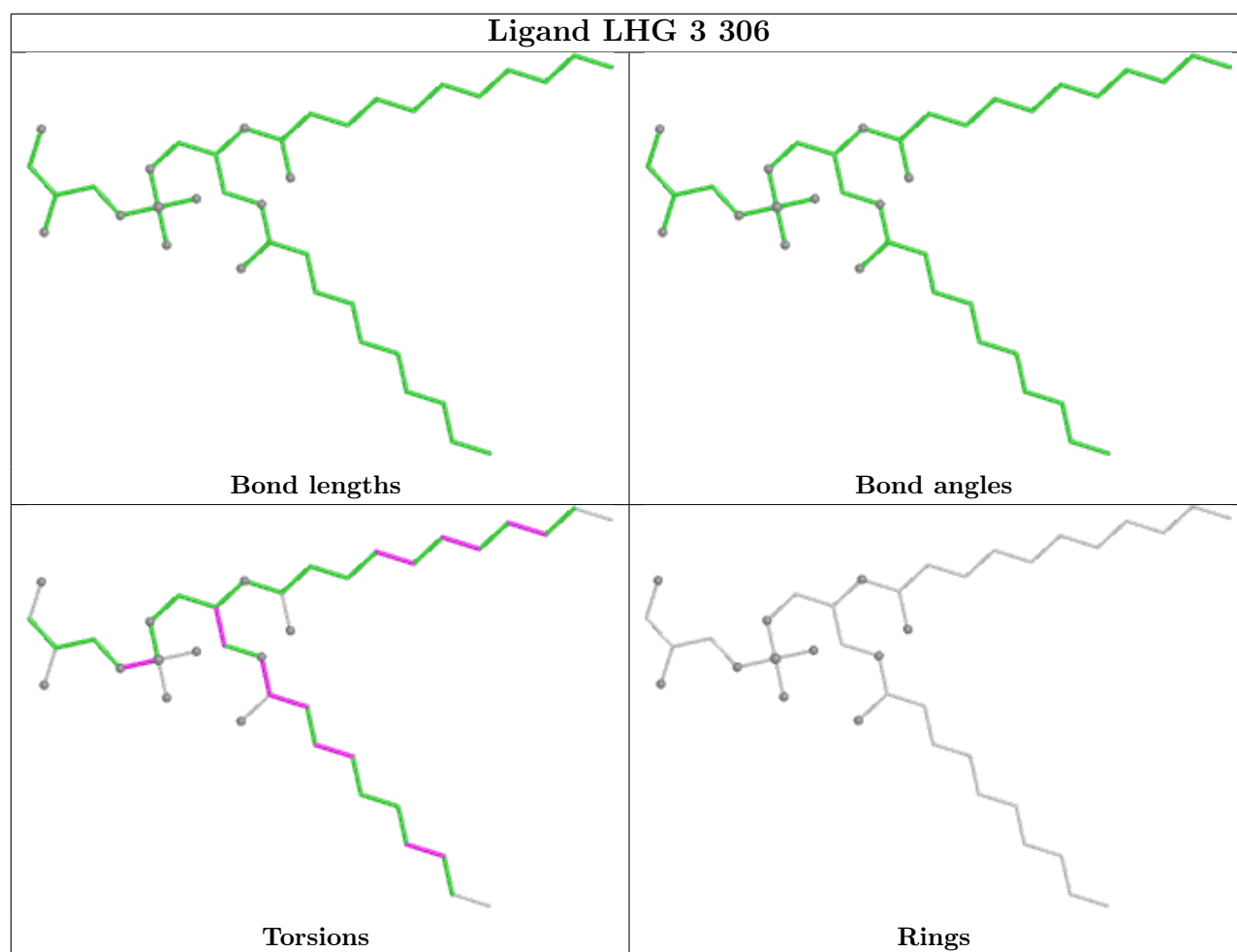
Ligand CHL Z 304



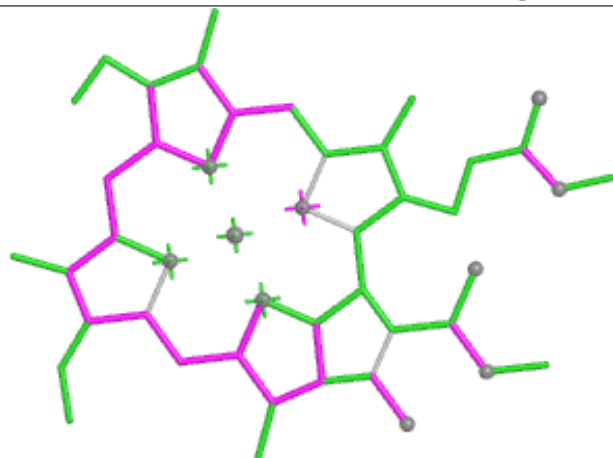


Ligand CLA 4 315

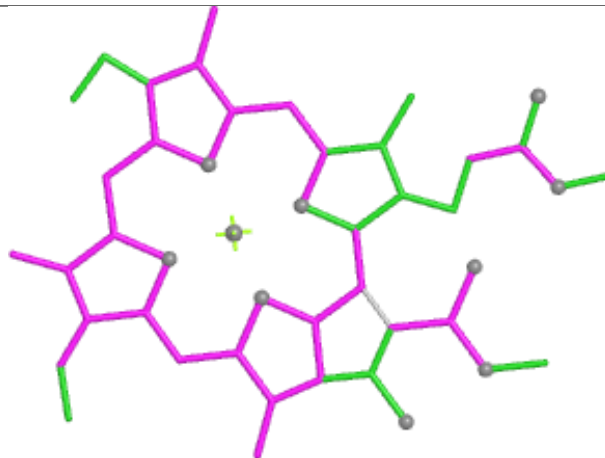




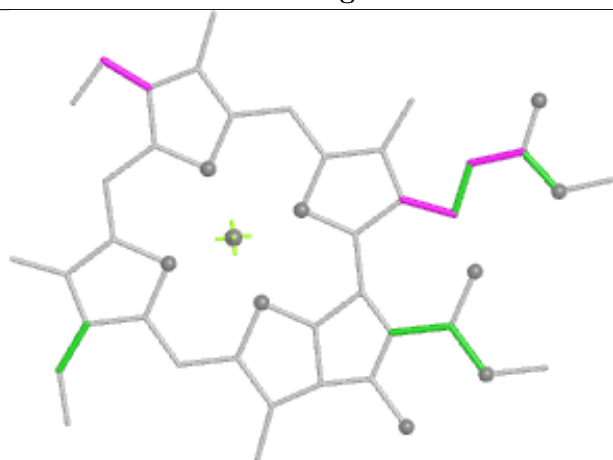
Ligand CLA Y 309



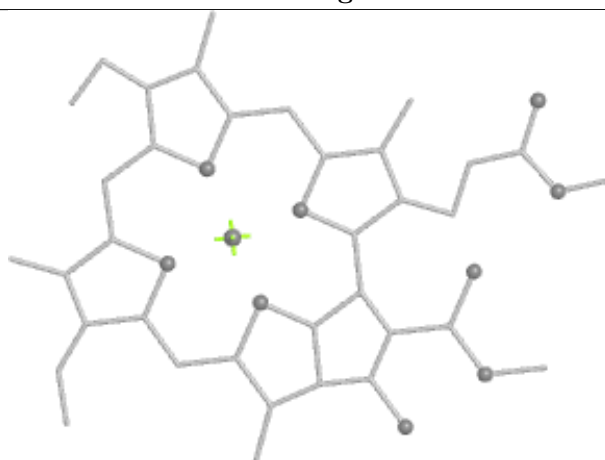
Bond lengths



Bond angles

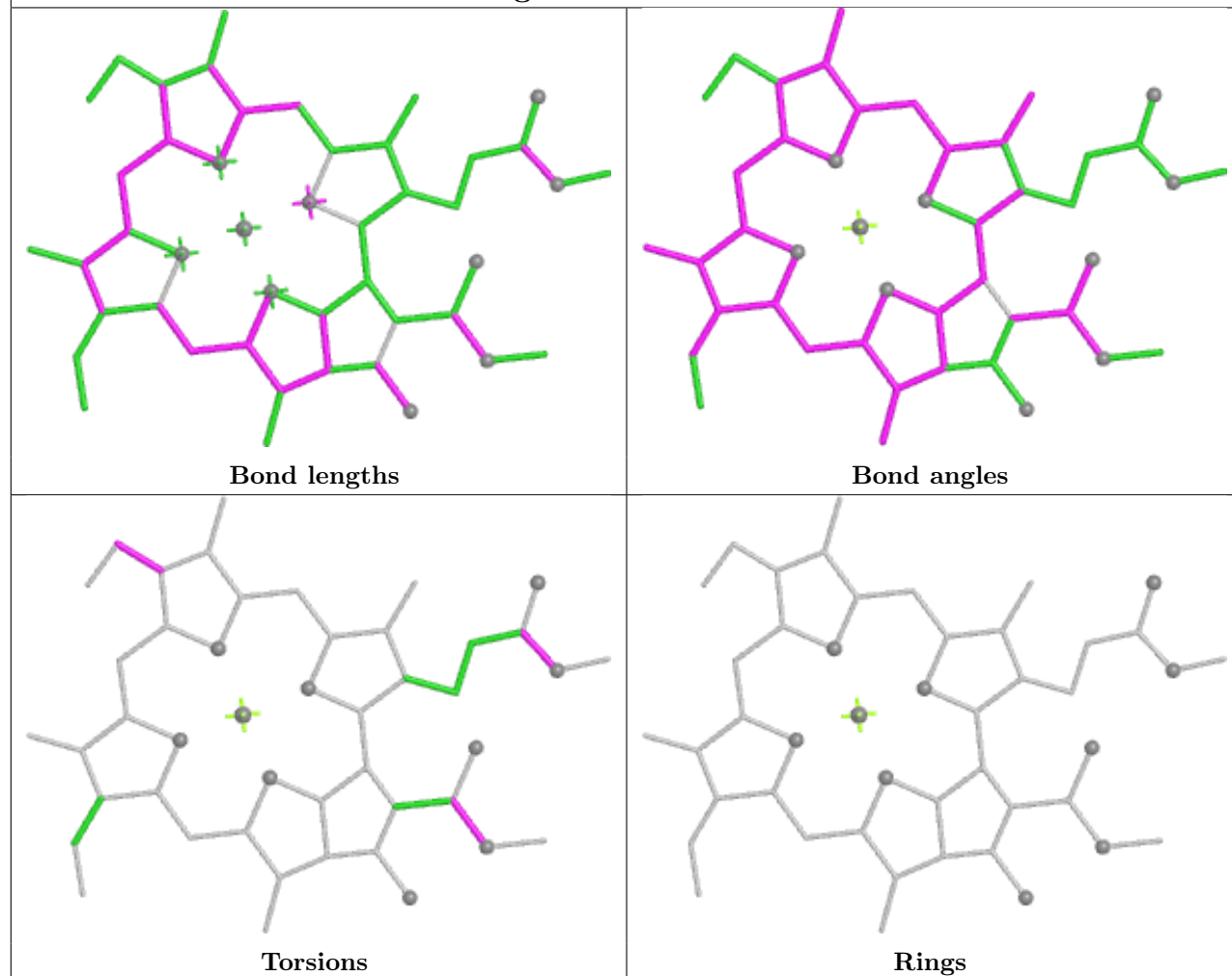


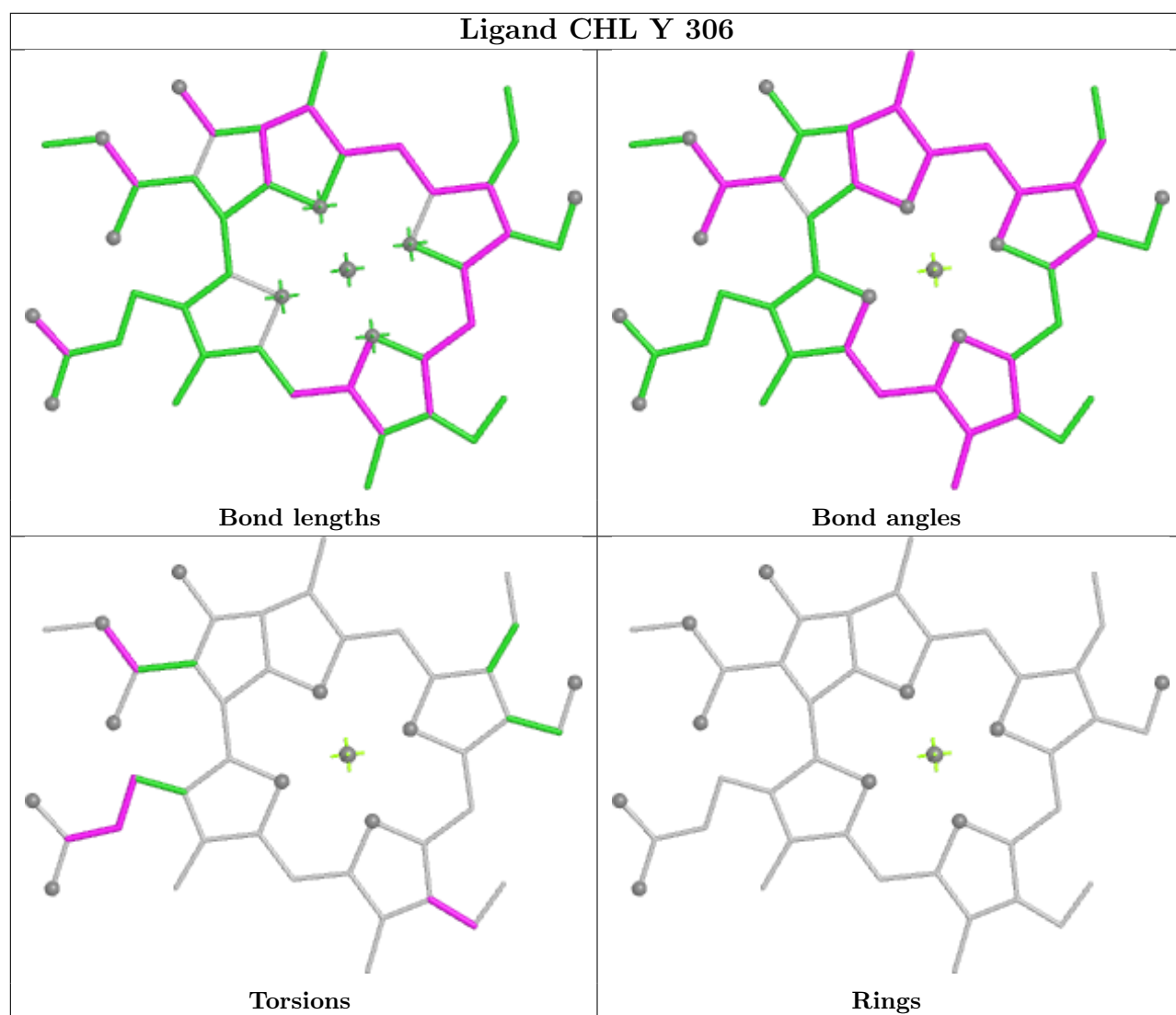
Torsions



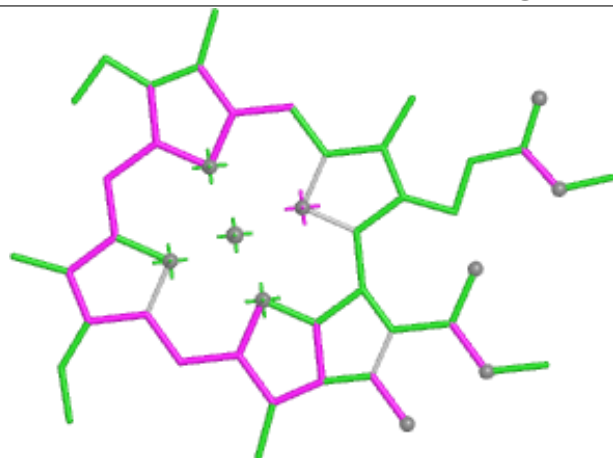
Rings

Ligand CLA B 846

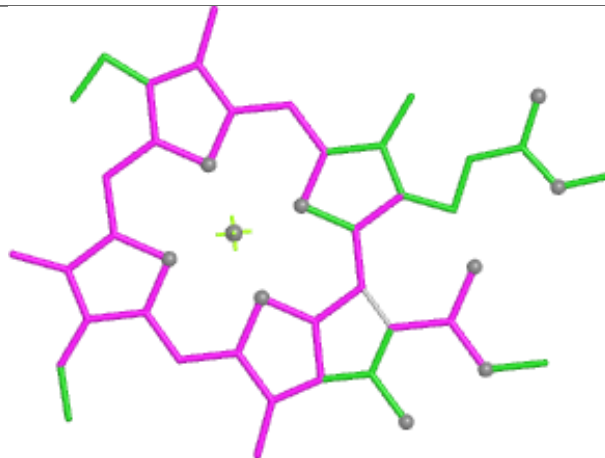




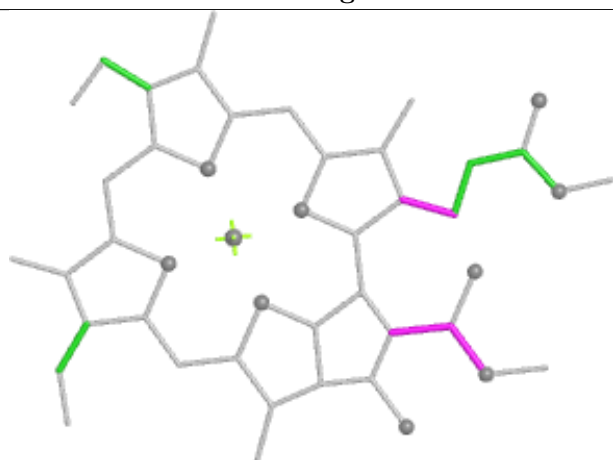
Ligand CLA Z 313



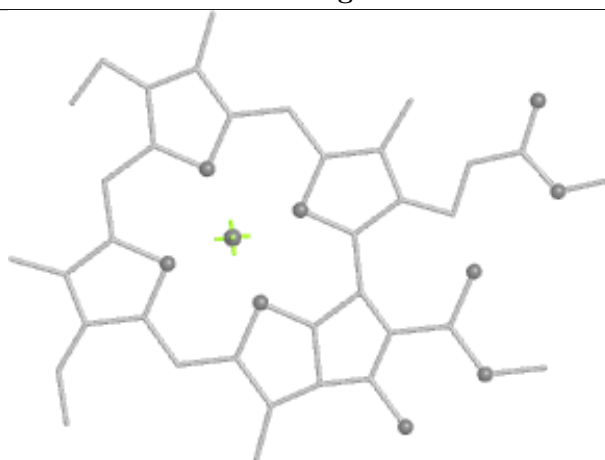
Bond lengths



Bond angles

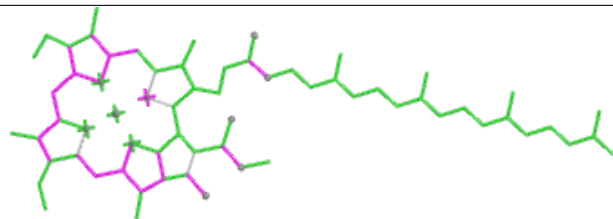


Torsions

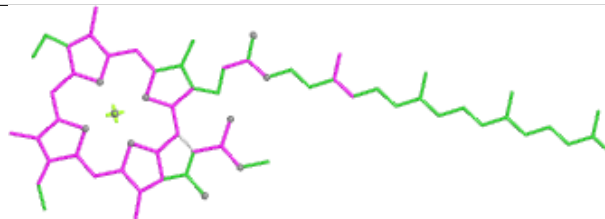


Rings

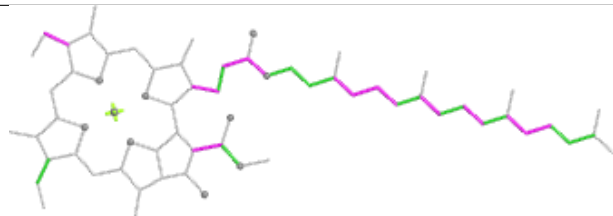
Ligand CLA B 847



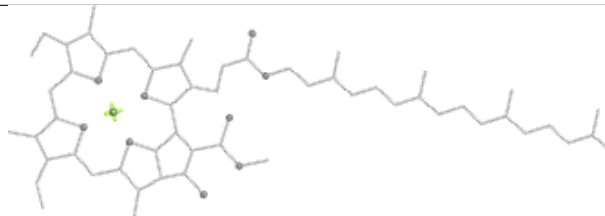
Bond lengths



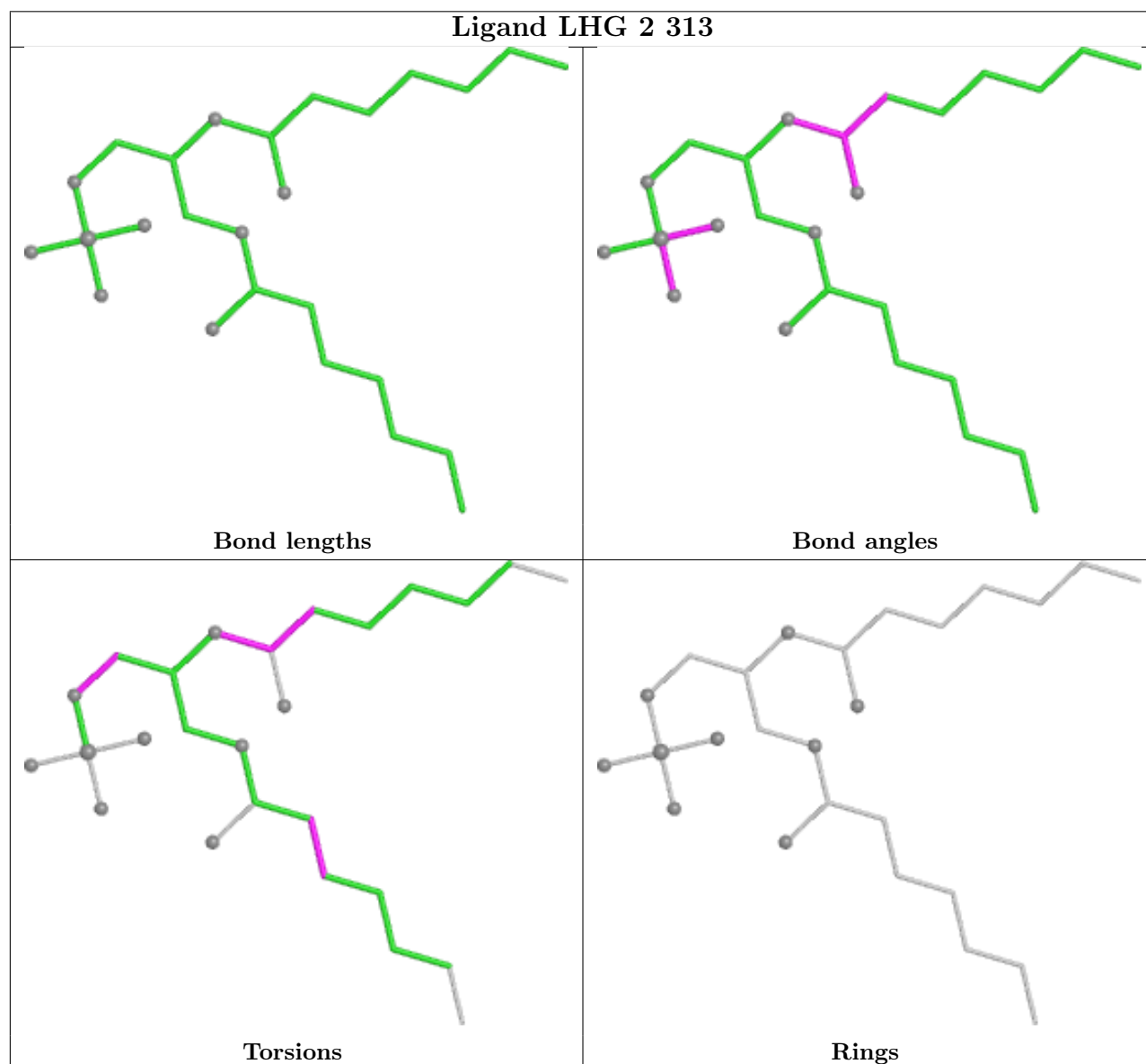
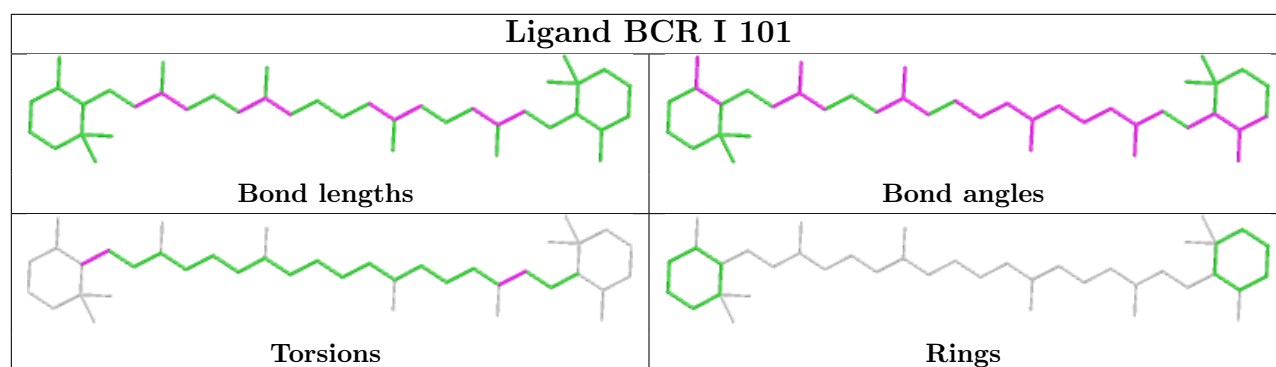
Bond angles

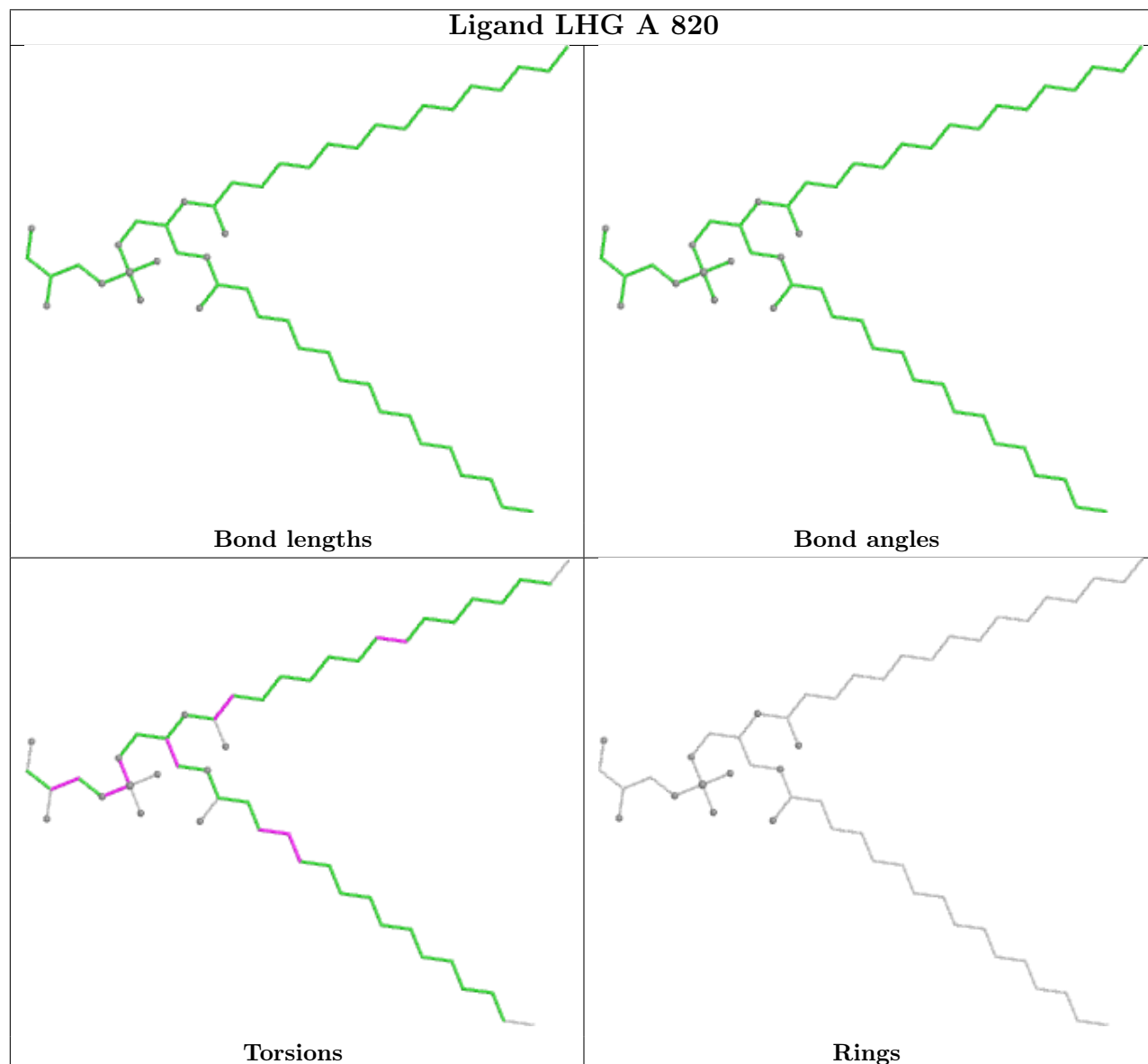
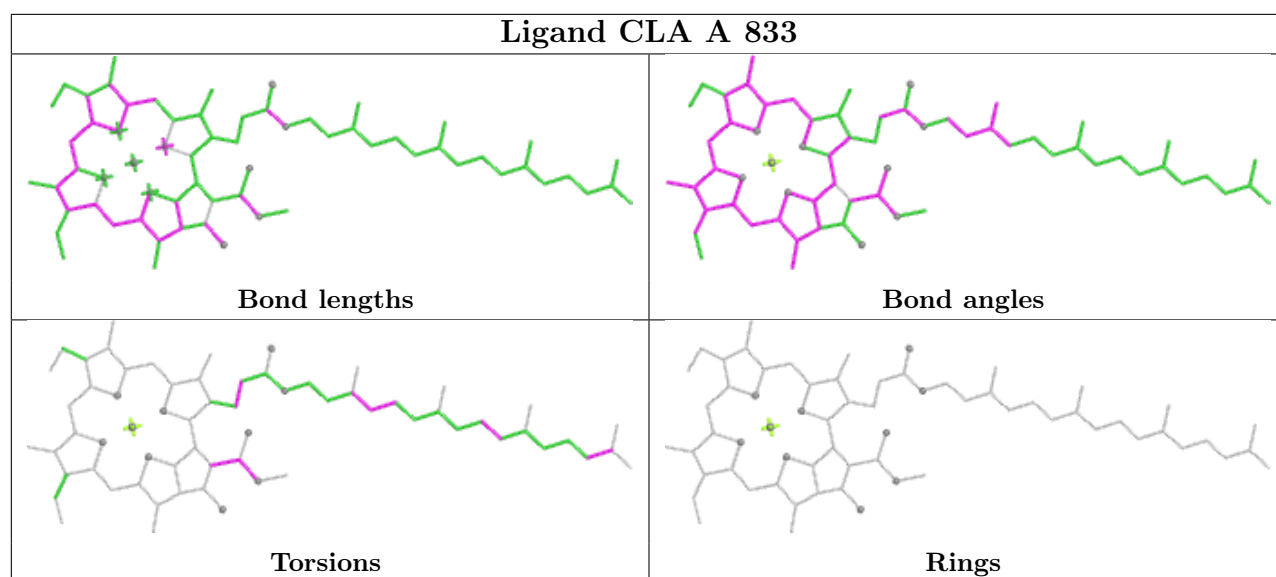


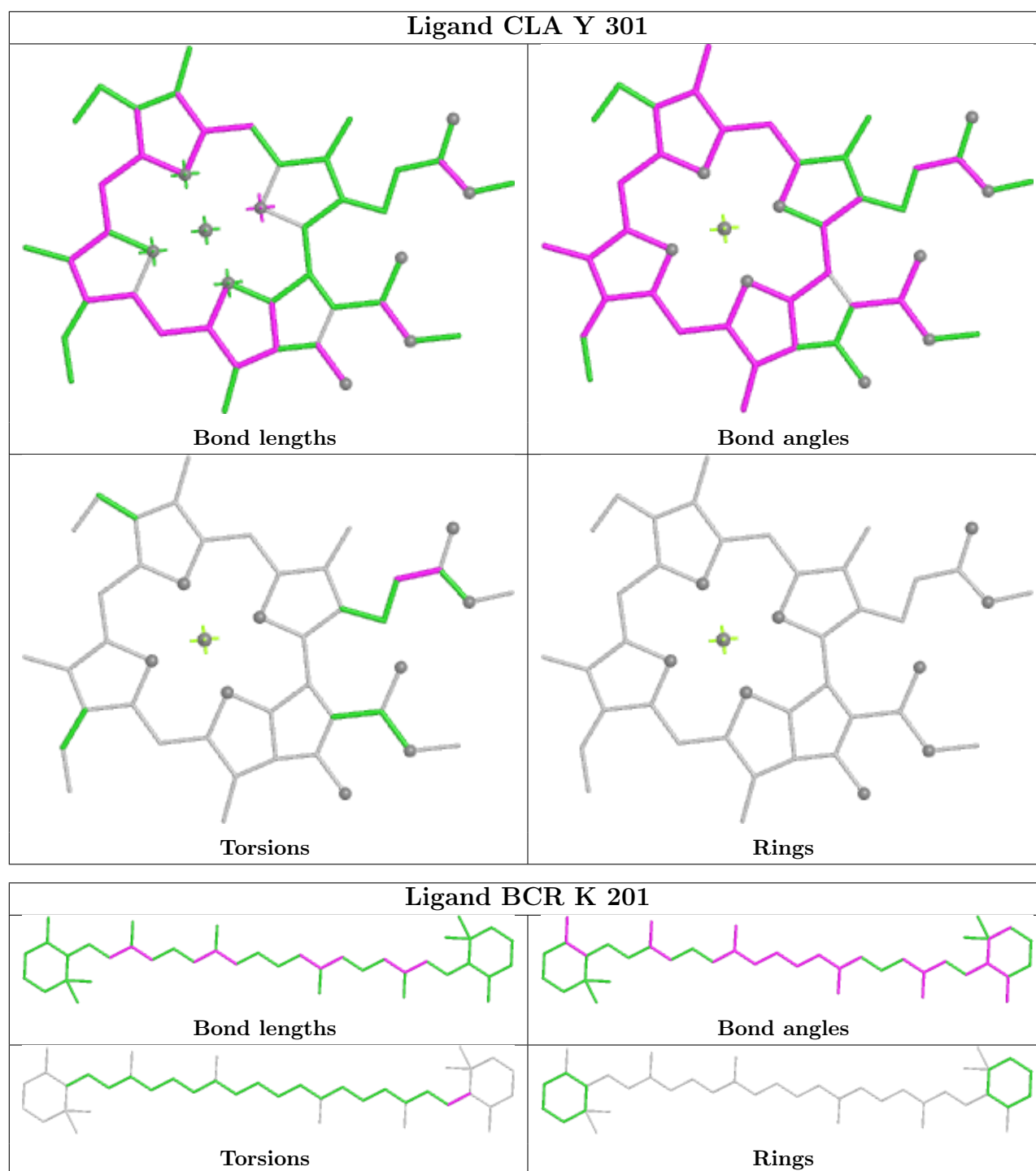
Torsions

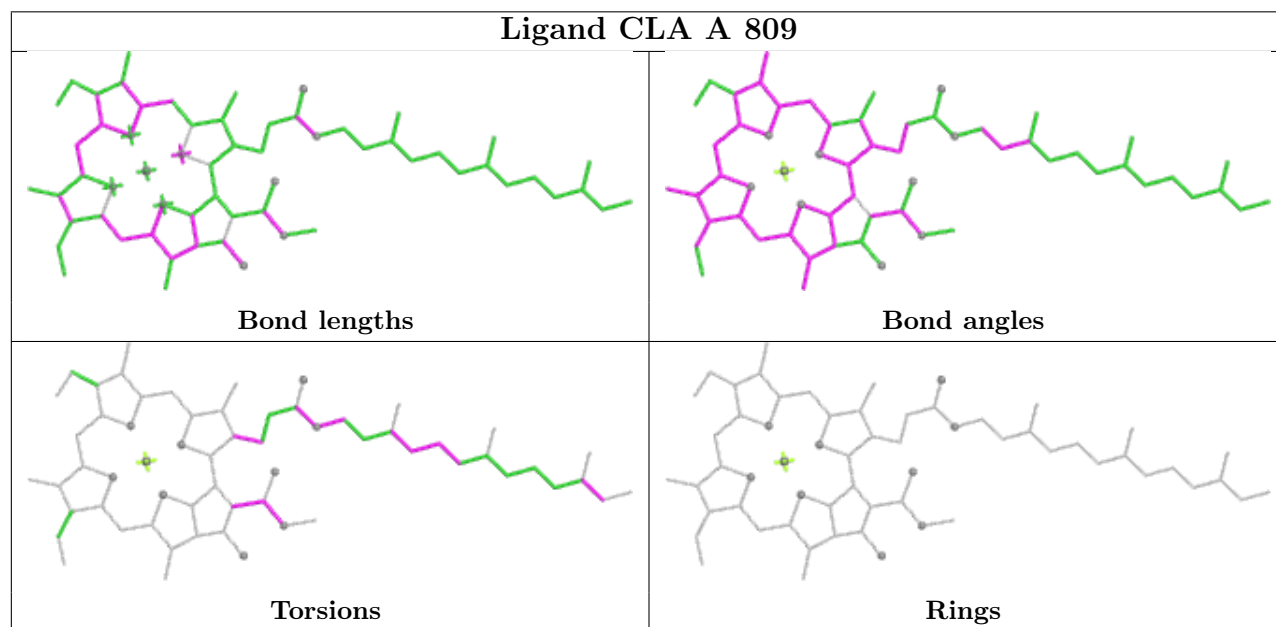
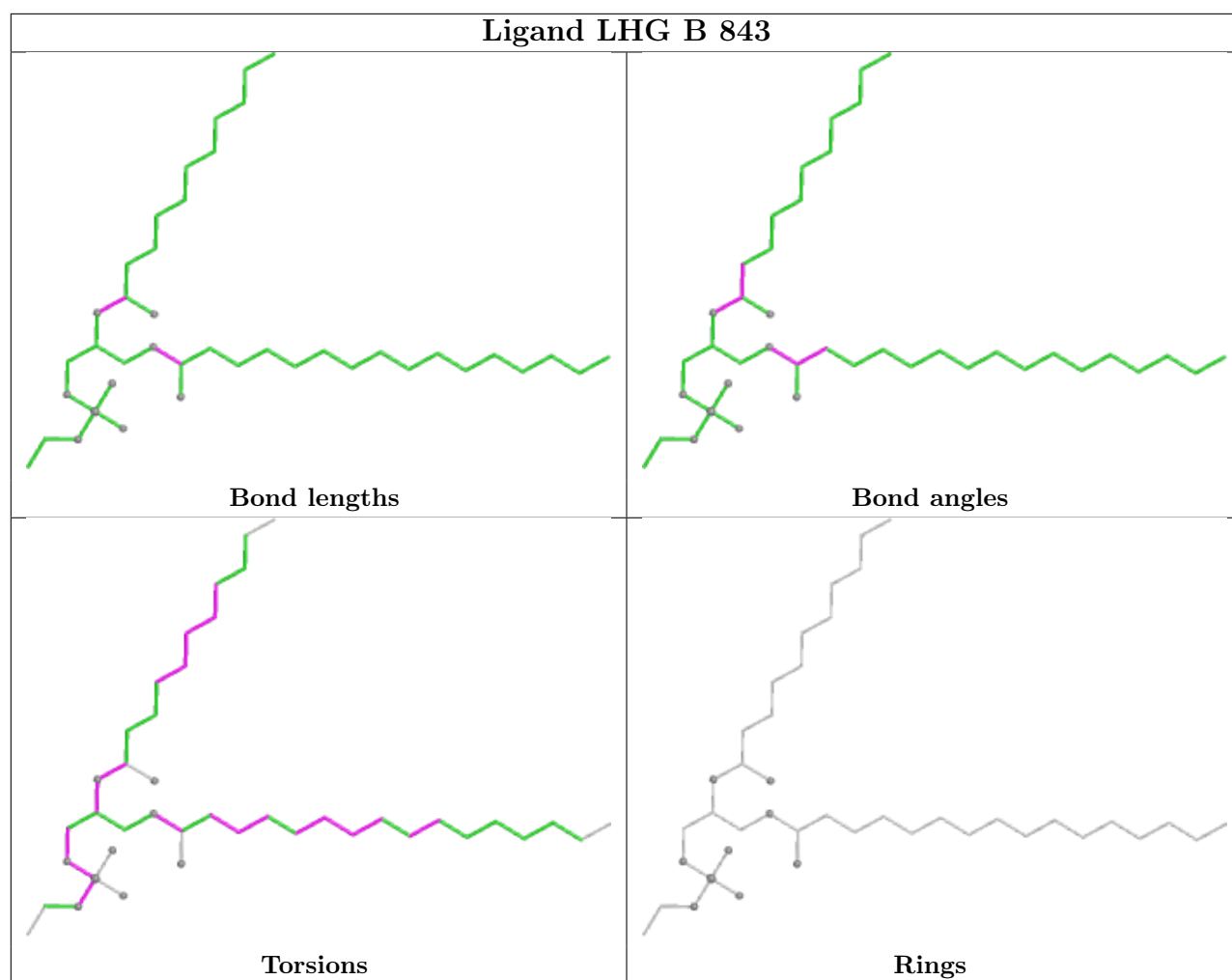


Rings

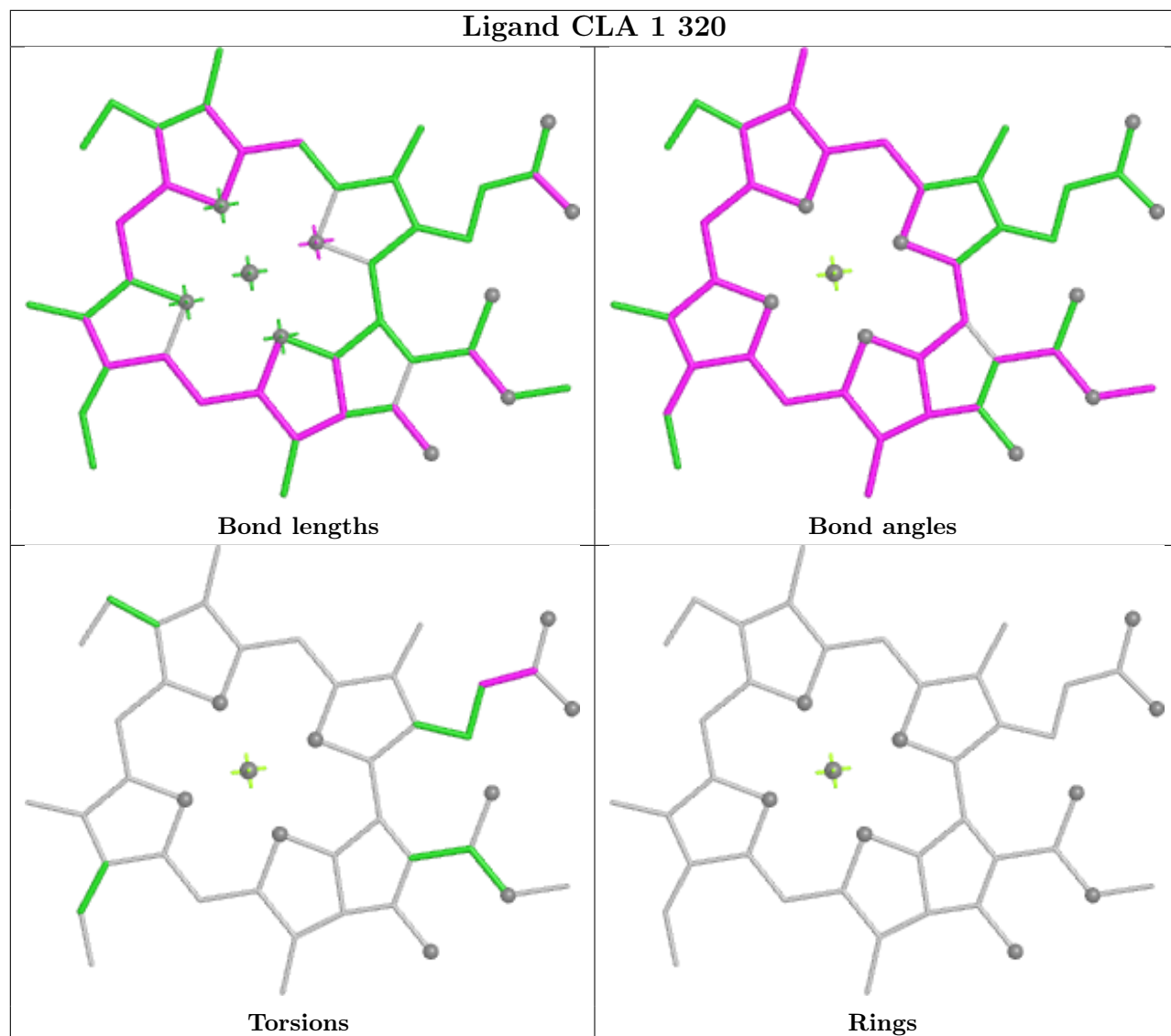


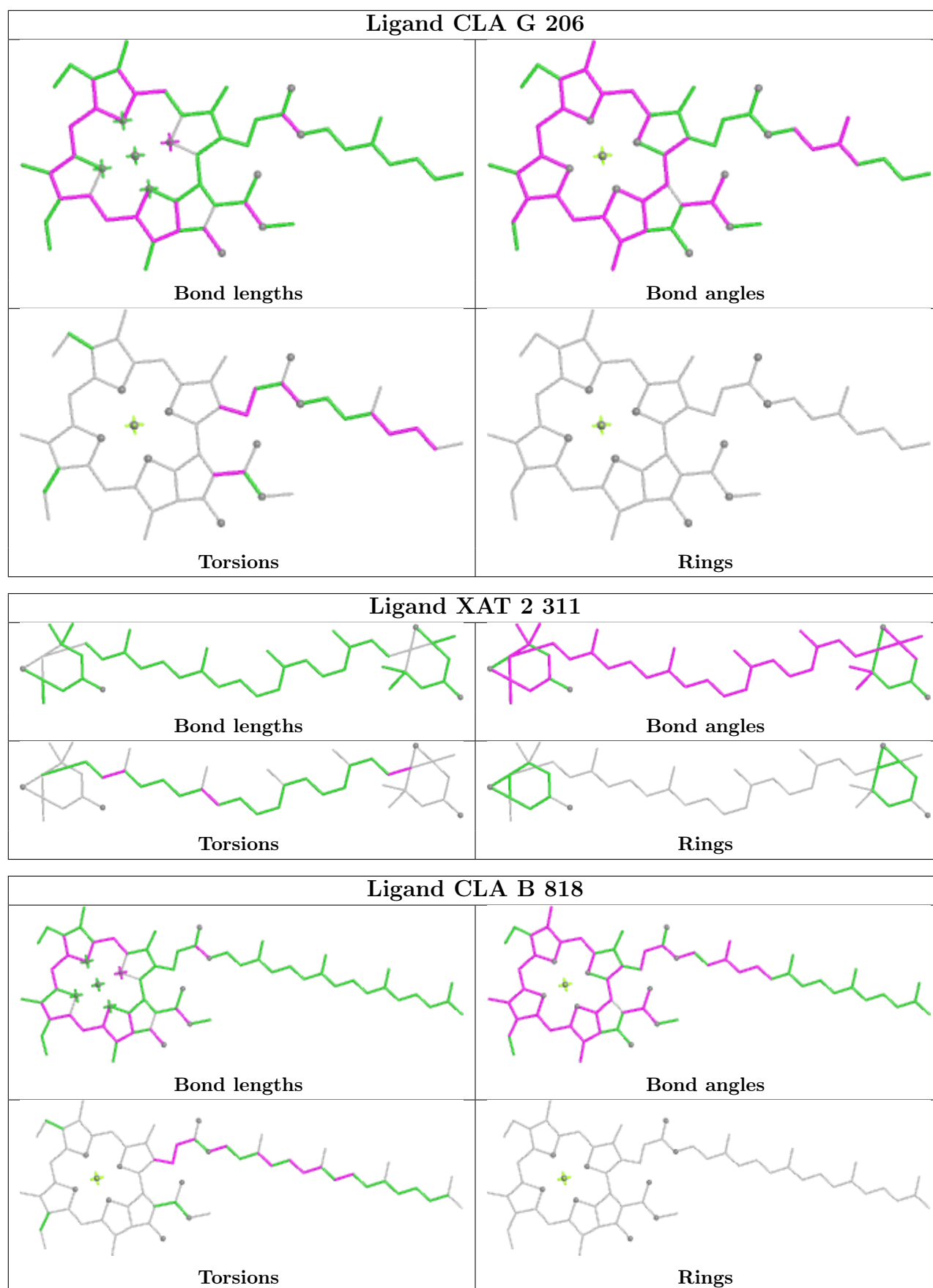


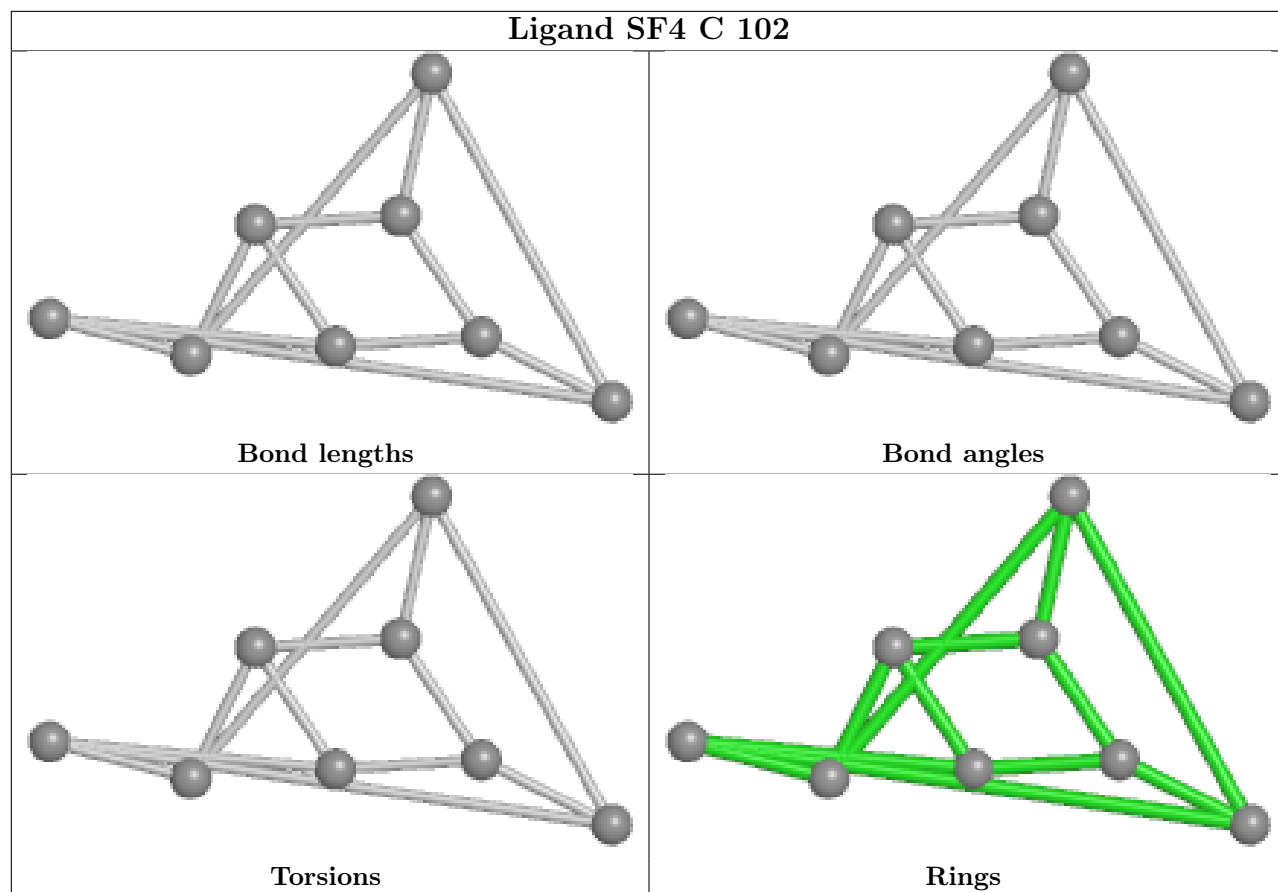


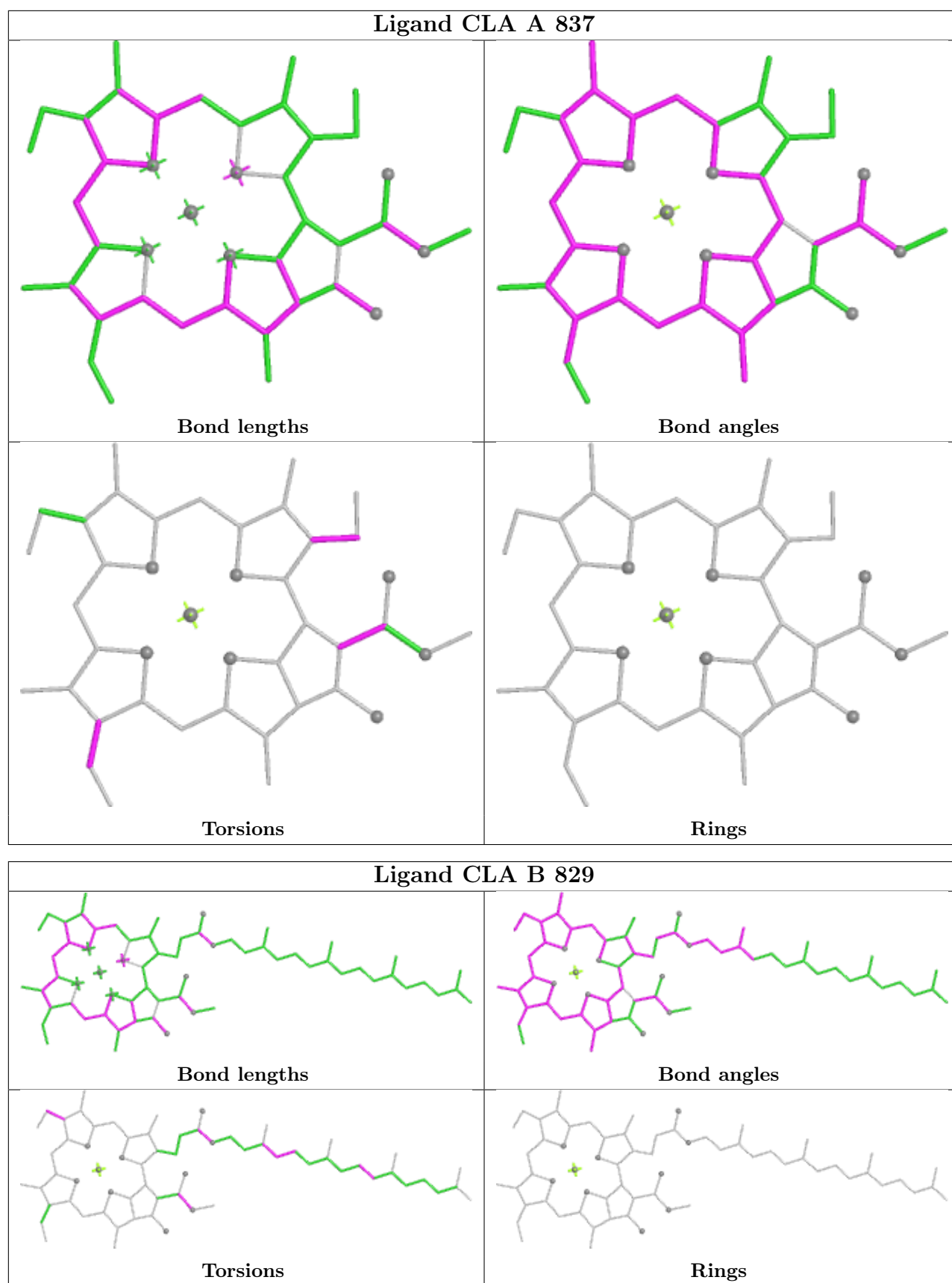


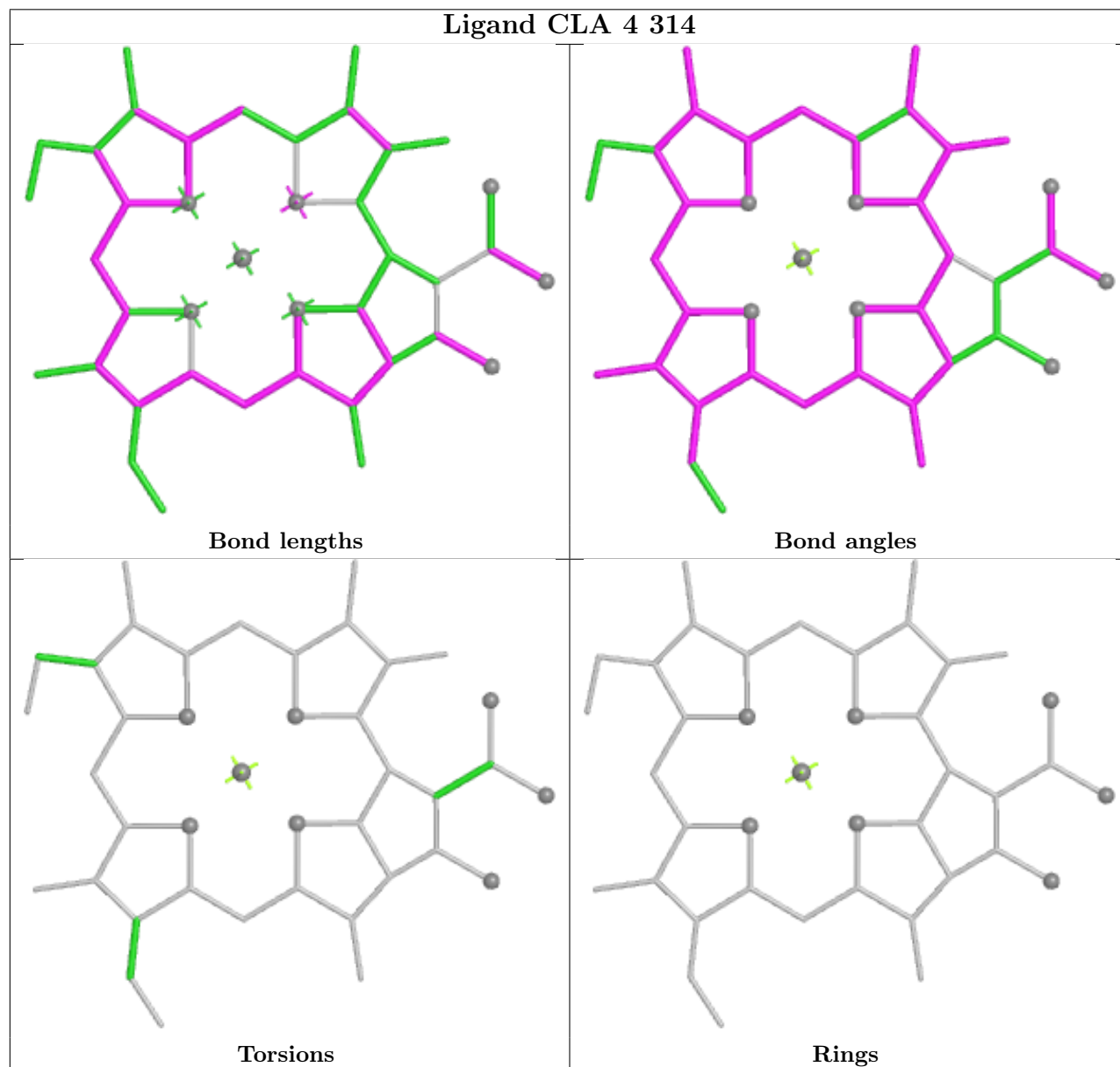
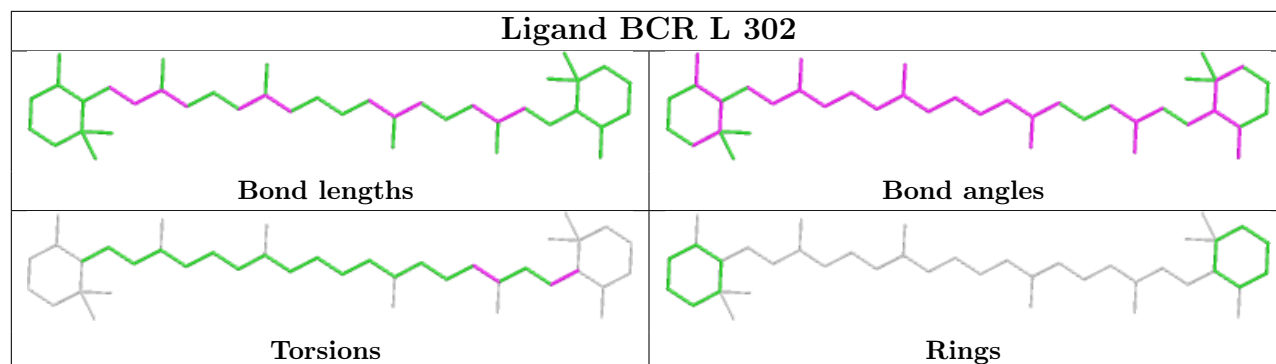
Ligand CLA 1 320

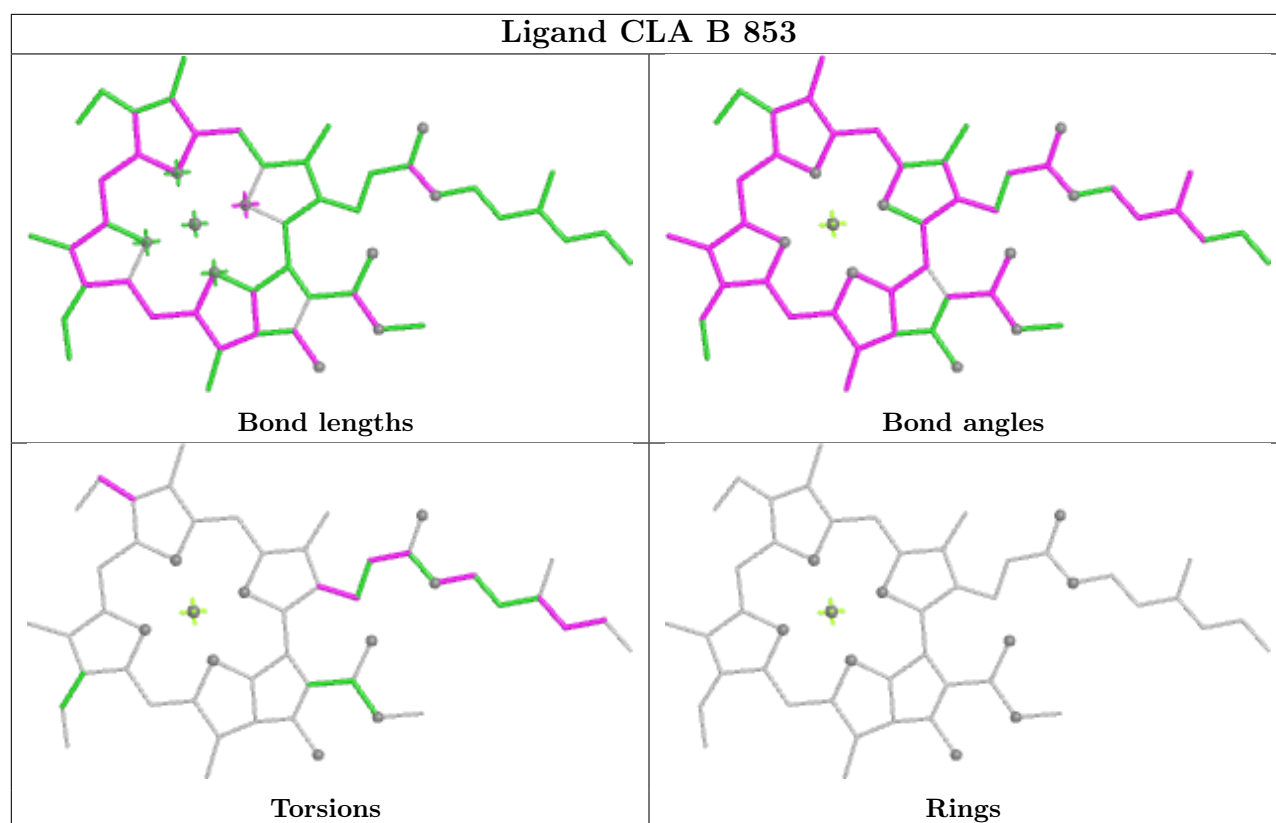


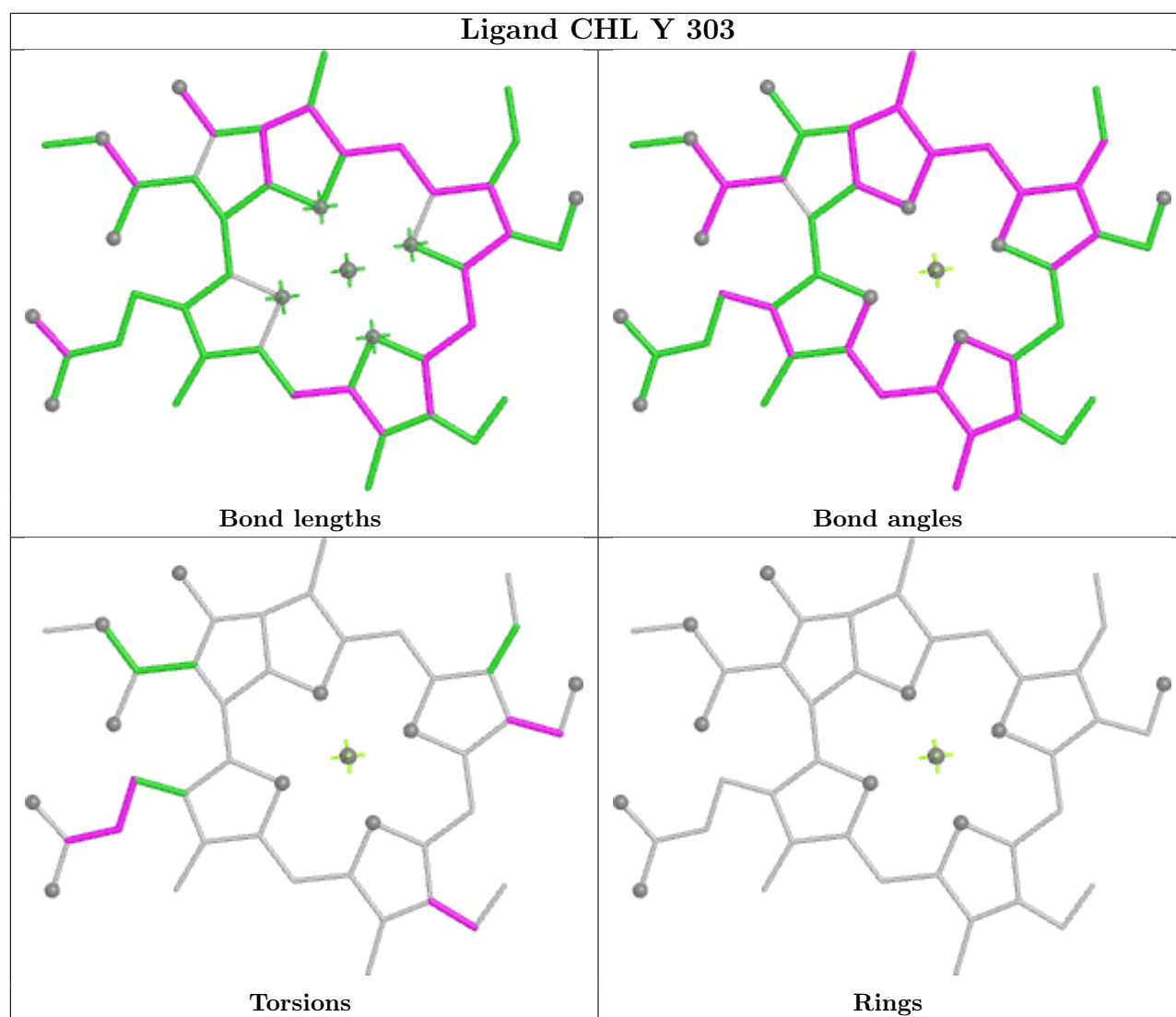




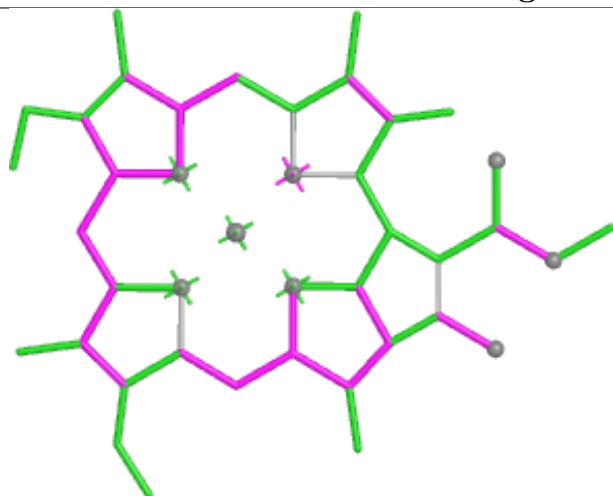








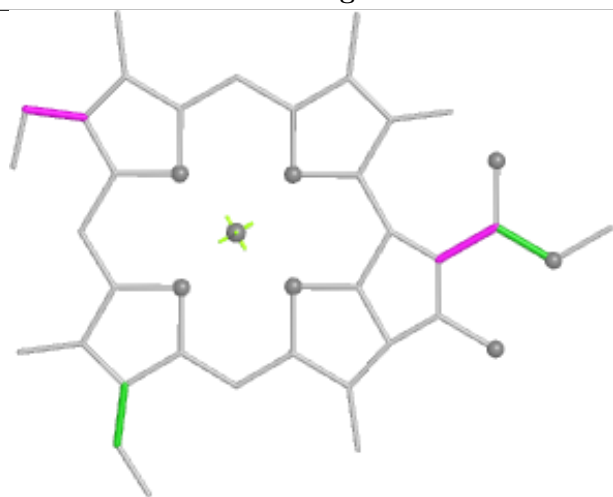
Ligand CLA 1 305



Bond lengths



Bond angles

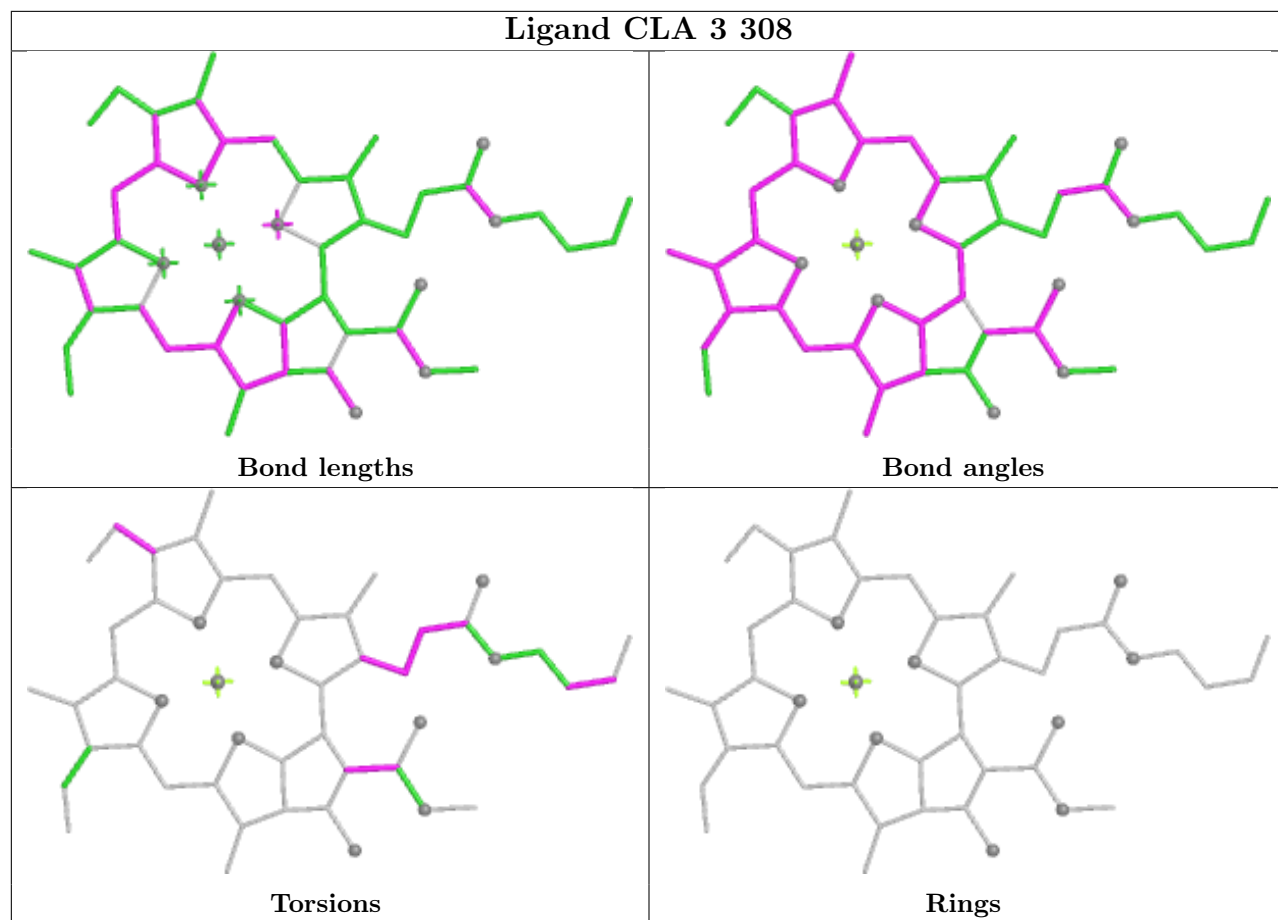


Torsions

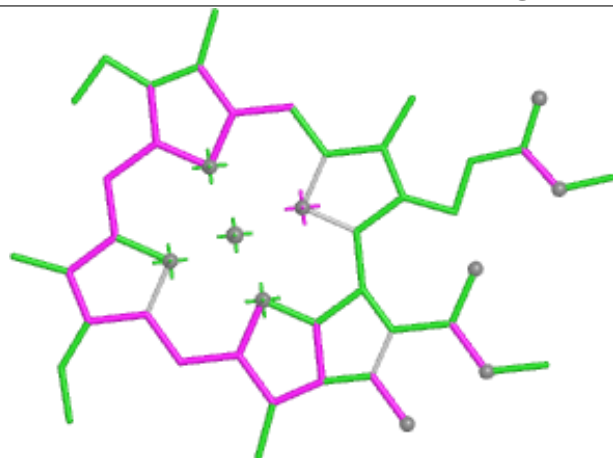


Rings

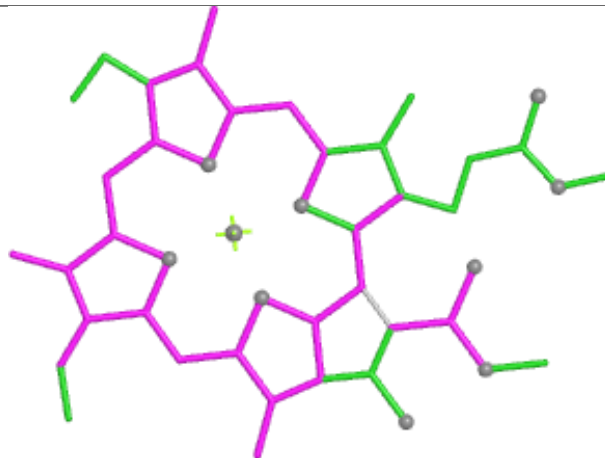
Ligand CLA 3 308



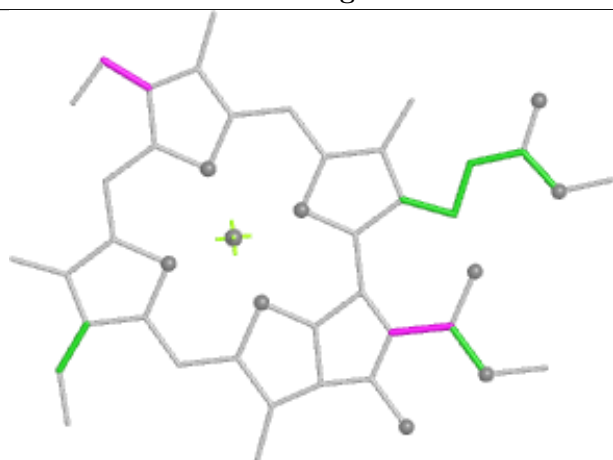
Ligand CLA X 312



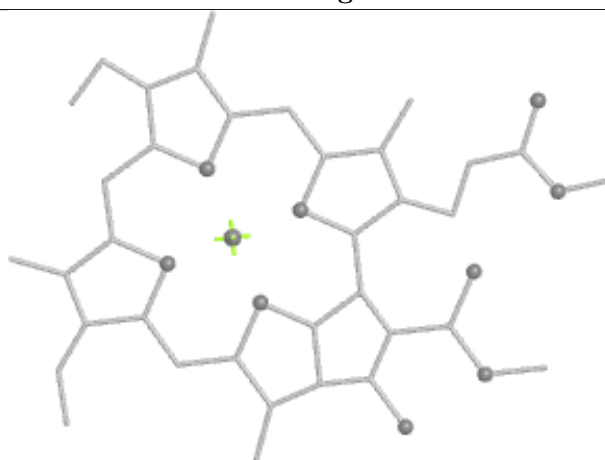
Bond lengths



Bond angles

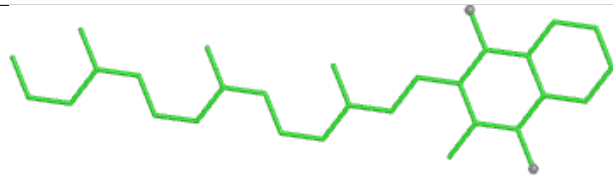


Torsions

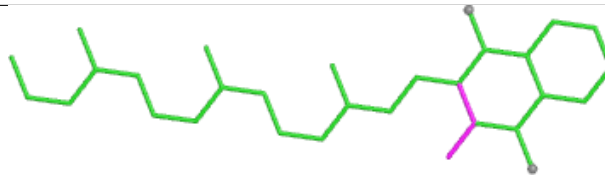


Rings

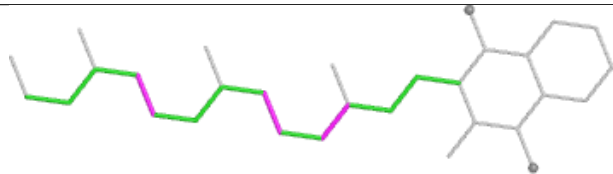
Ligand PQN B 832



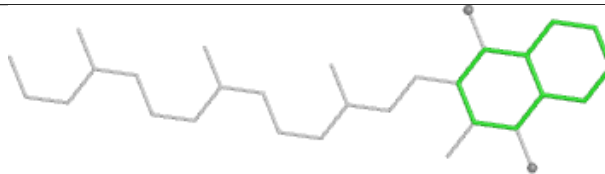
Bond lengths



Bond angles

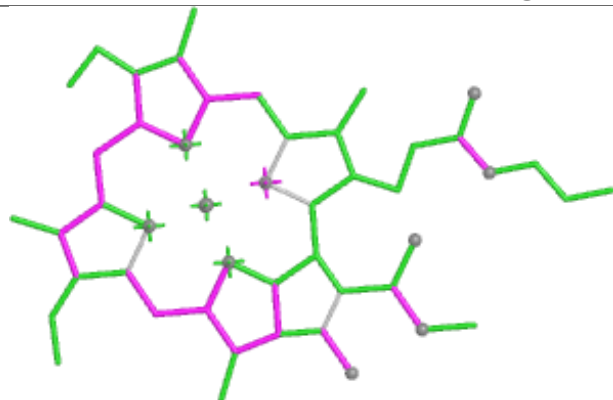


Torsions

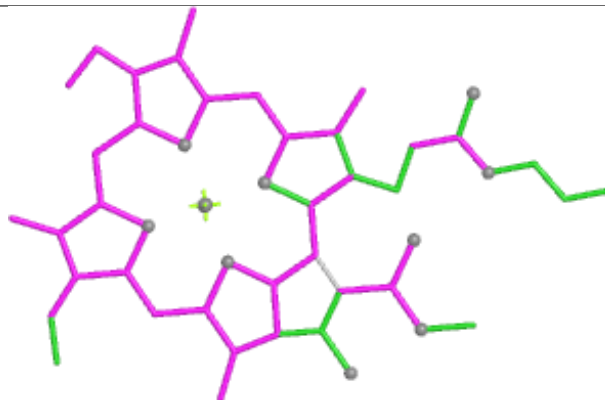


Rings

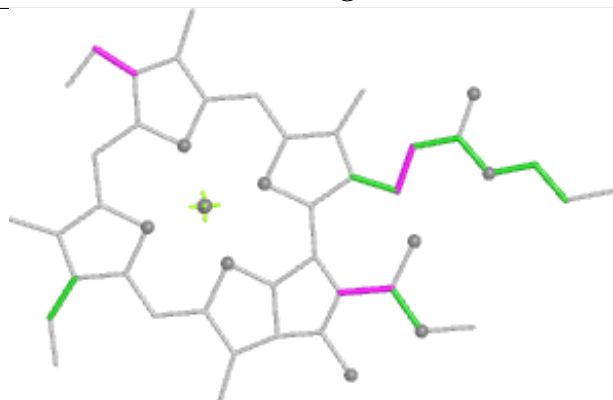
Ligand CLA 1 319



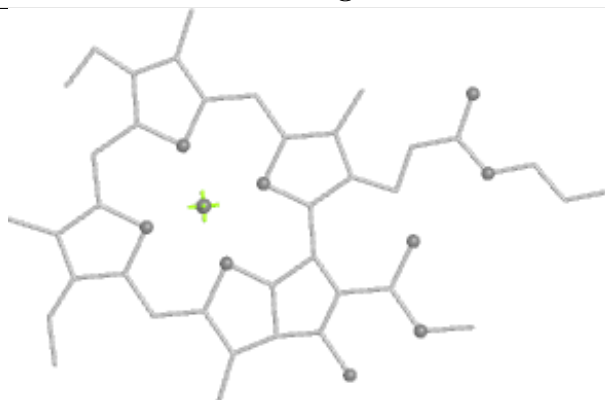
Bond lengths



Bond angles

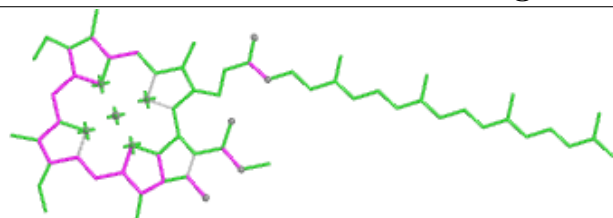


Torsions

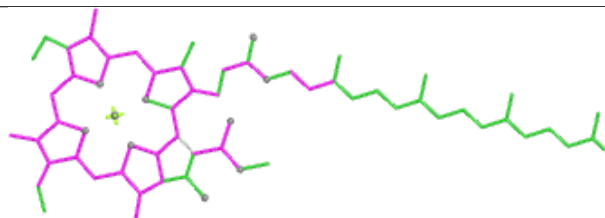


Rings

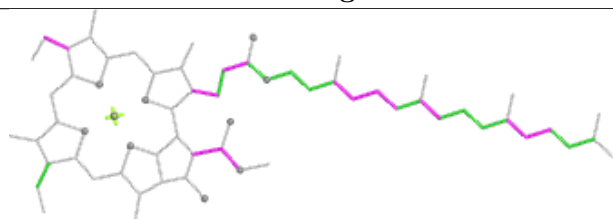
Ligand CLA A 802



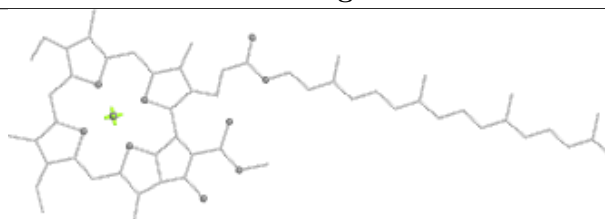
Bond lengths



Bond angles

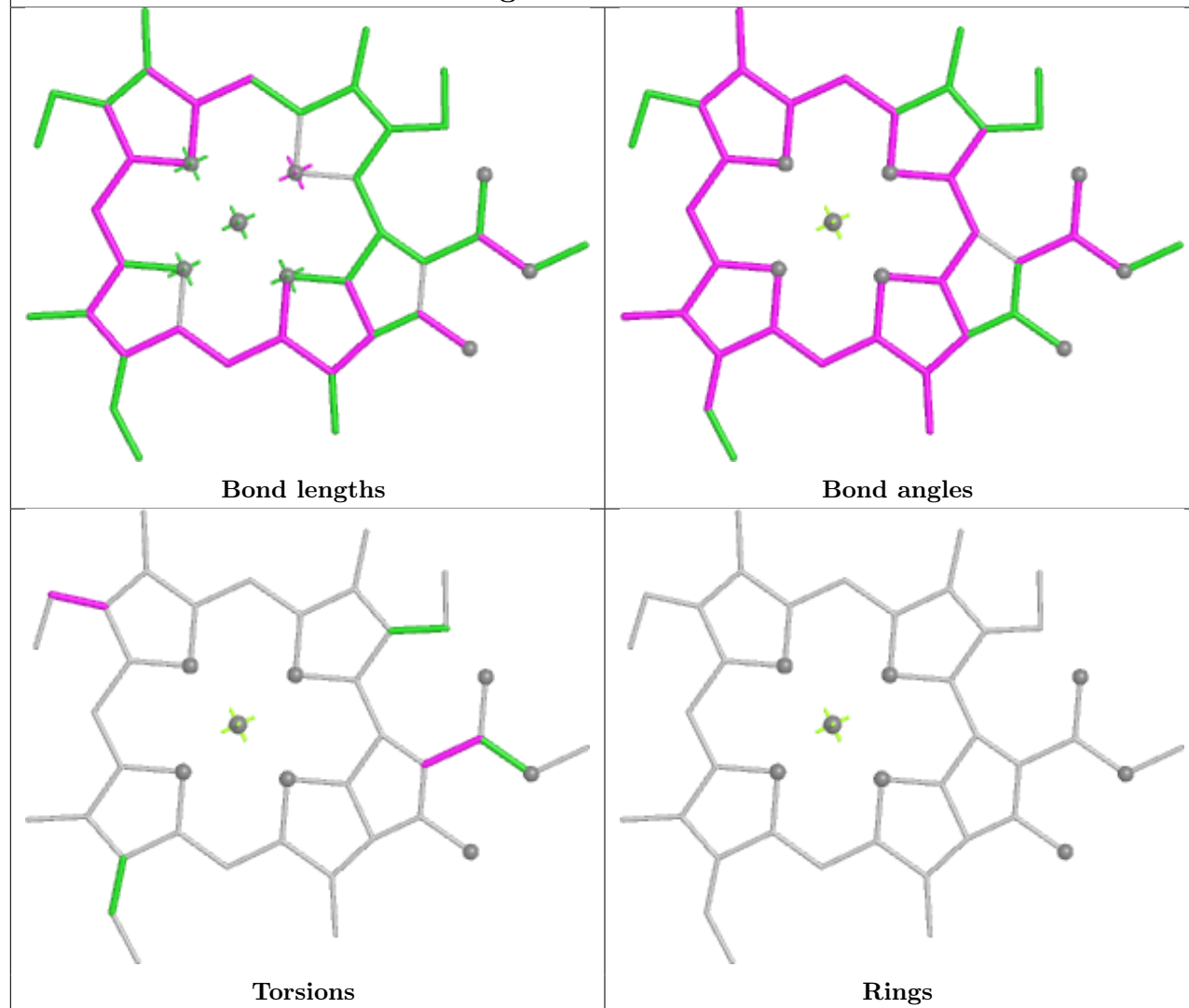


Torsions

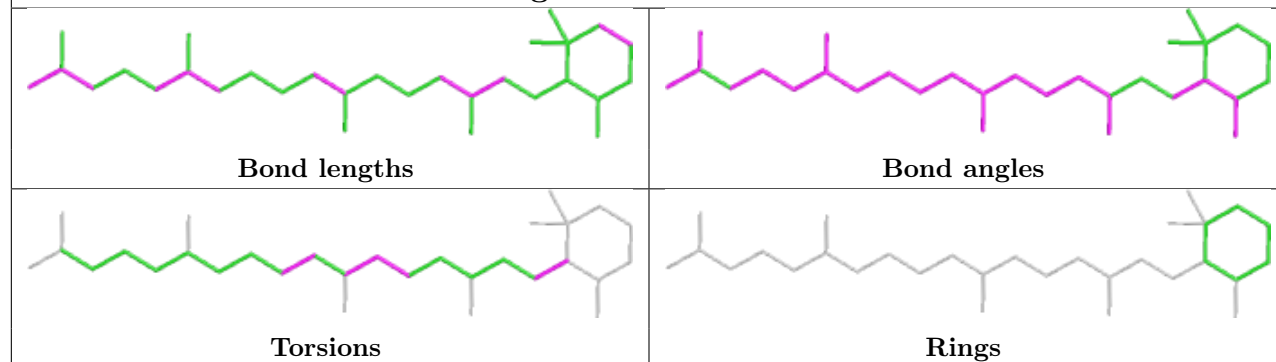


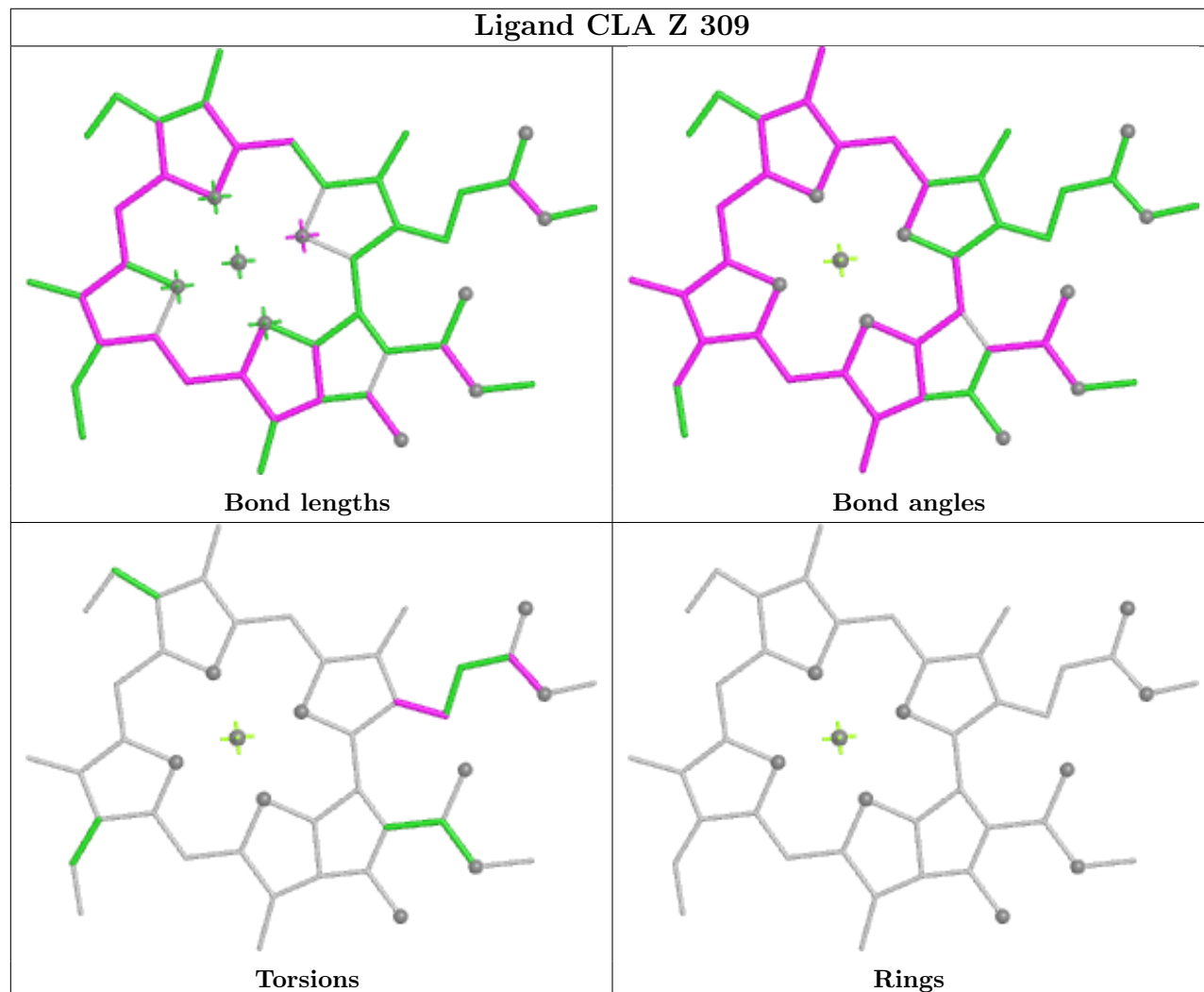
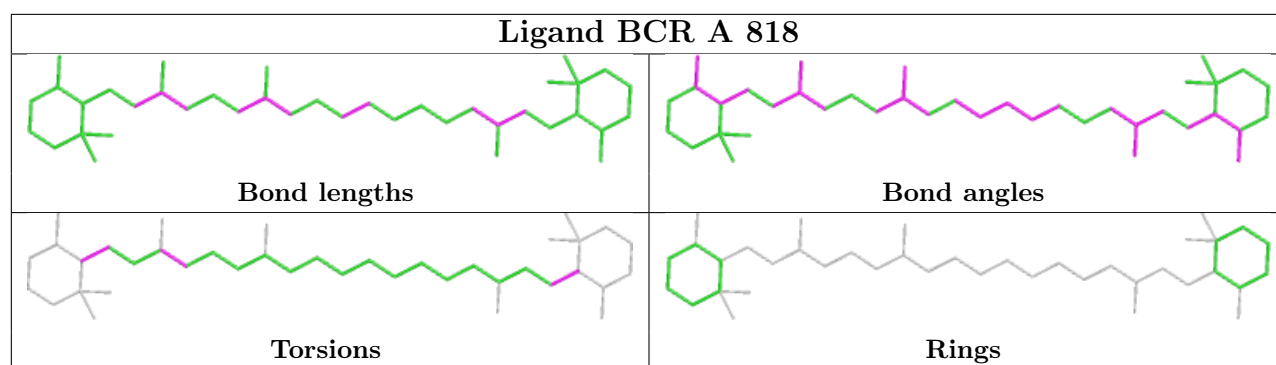
Rings

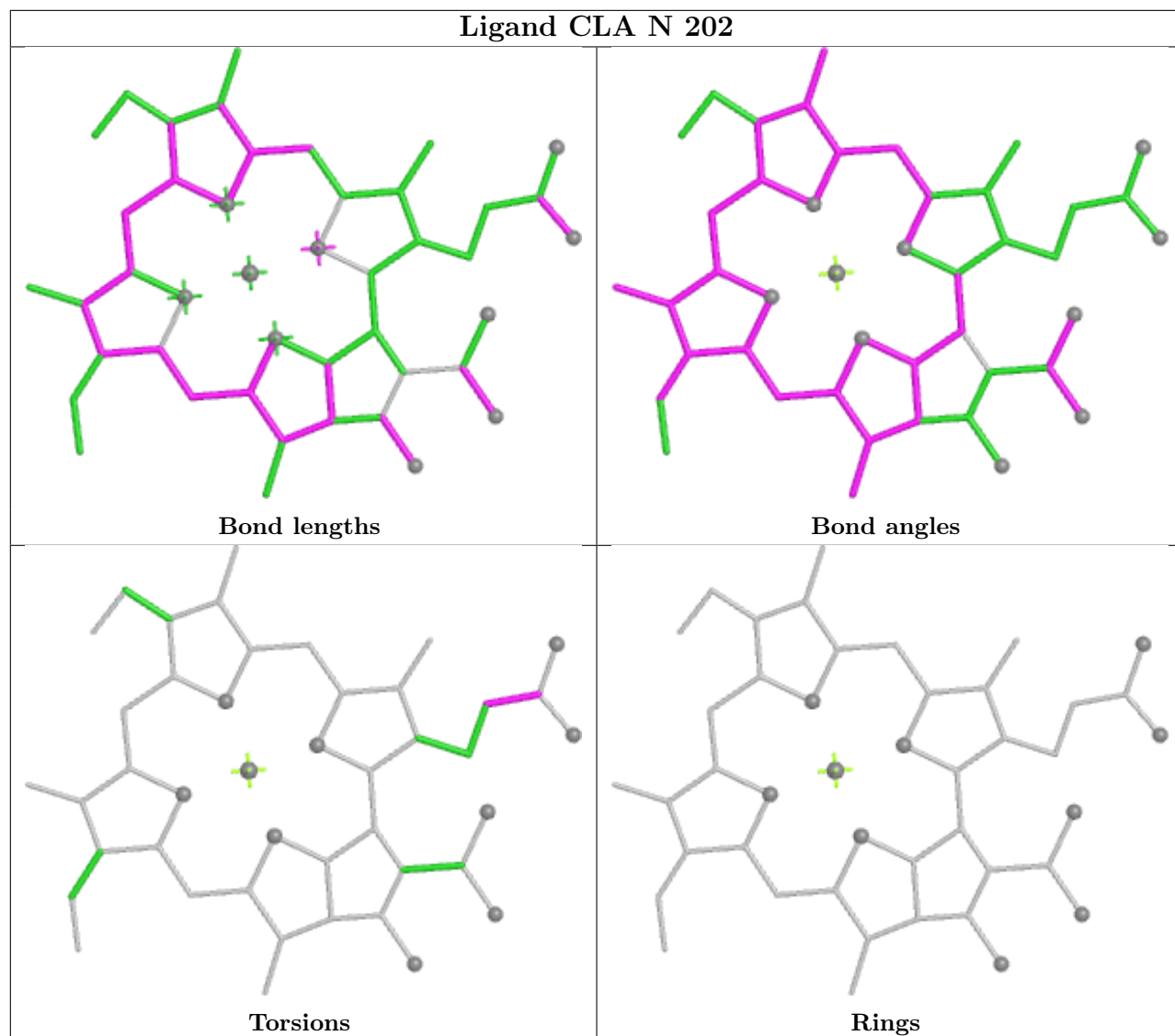
Ligand CLA 1 309

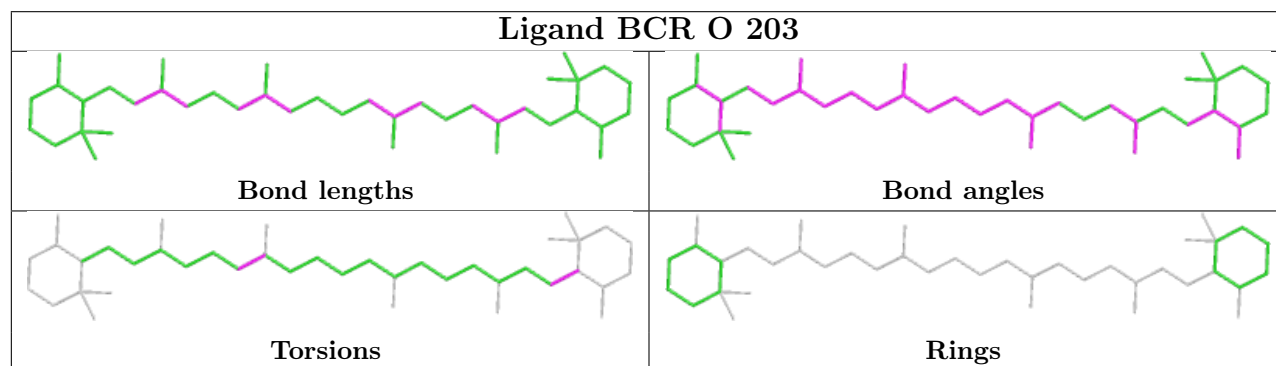
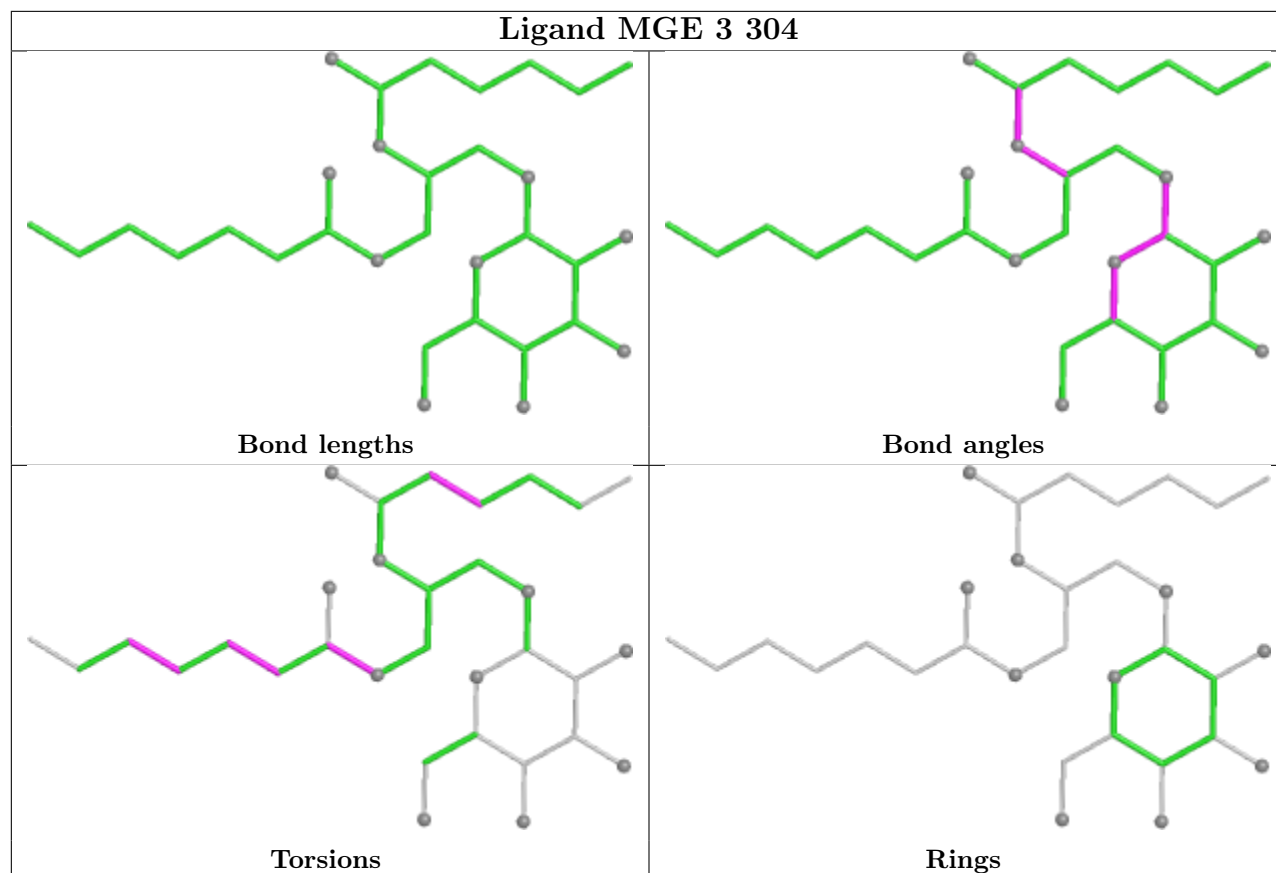


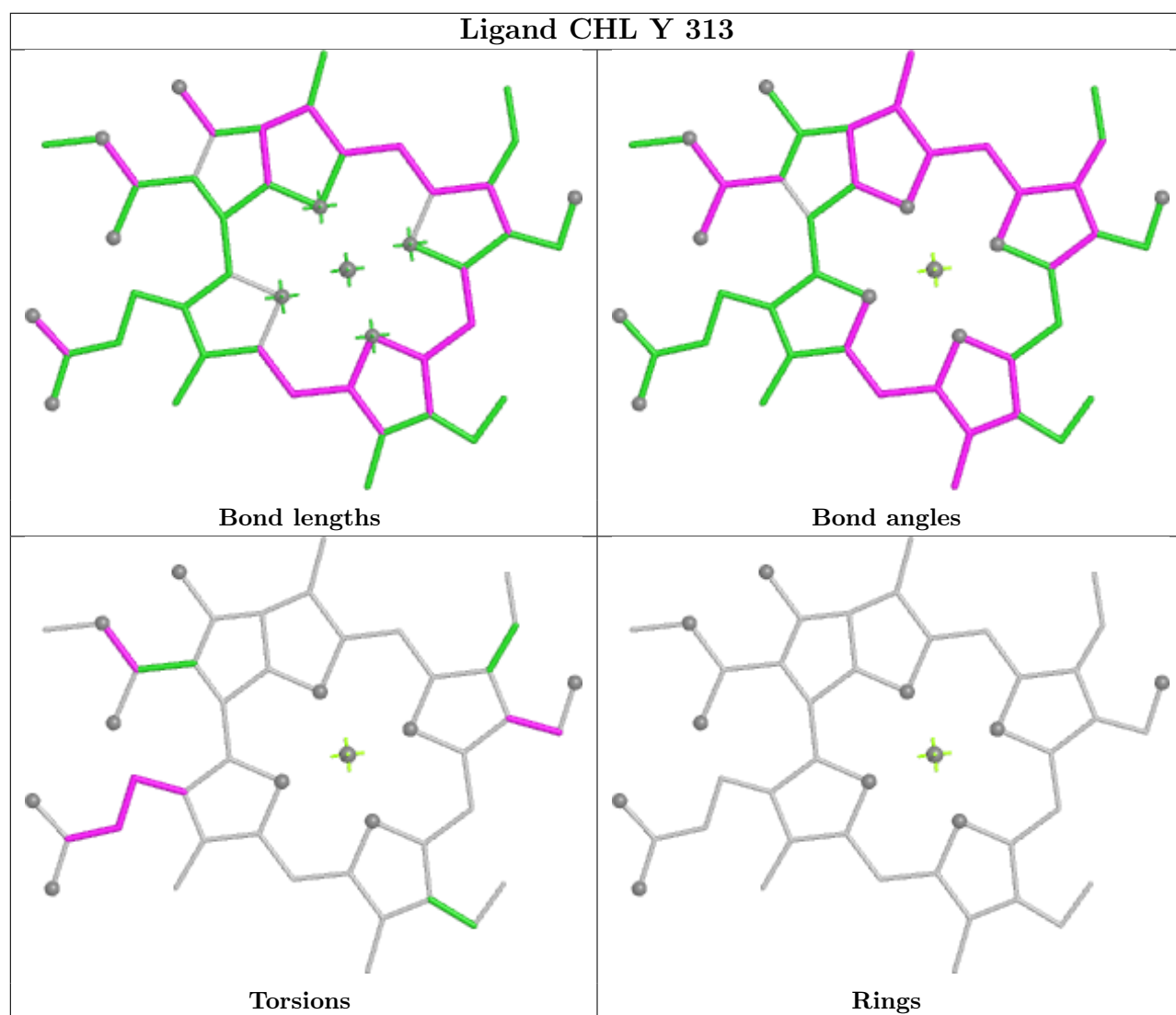
Ligand BCR B 840

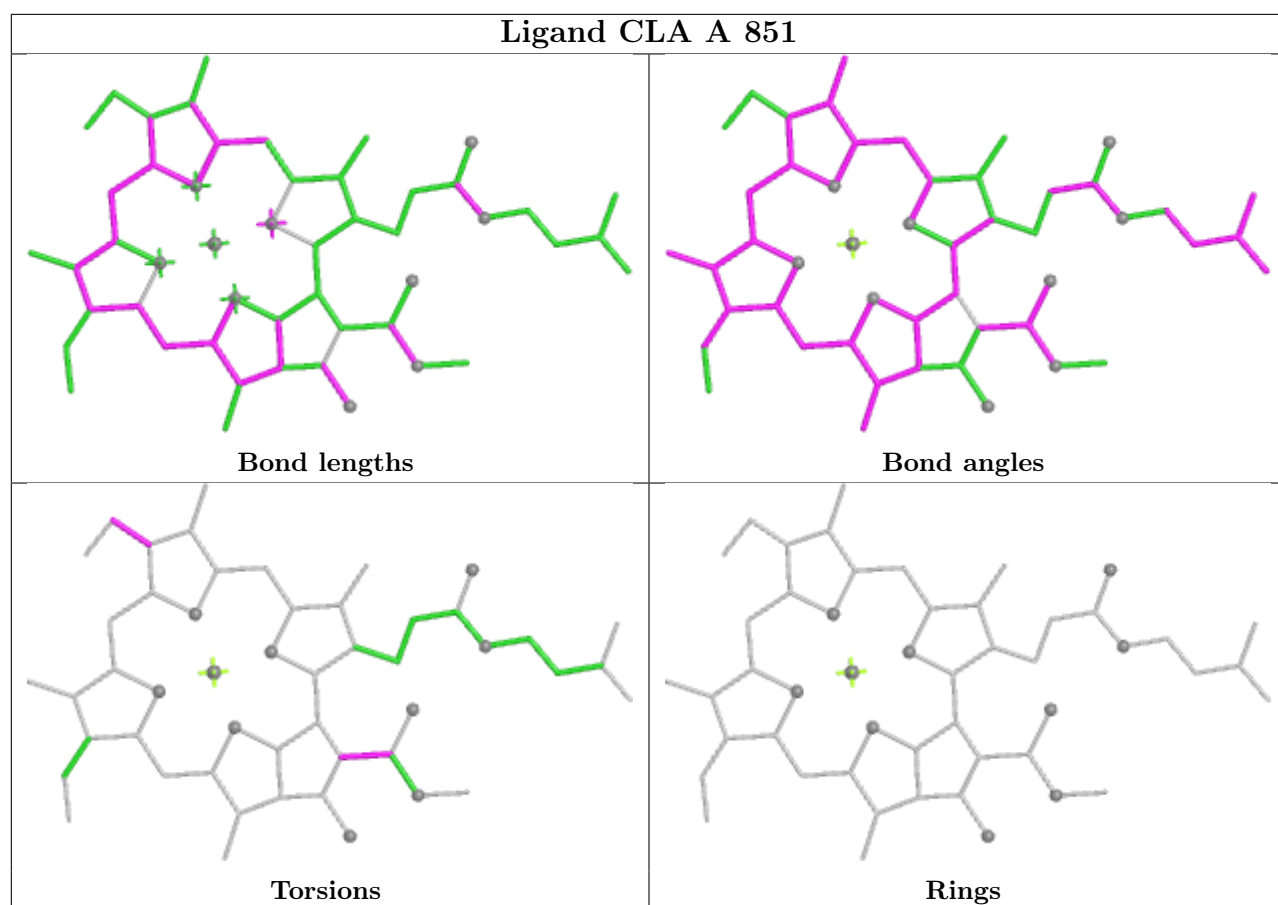


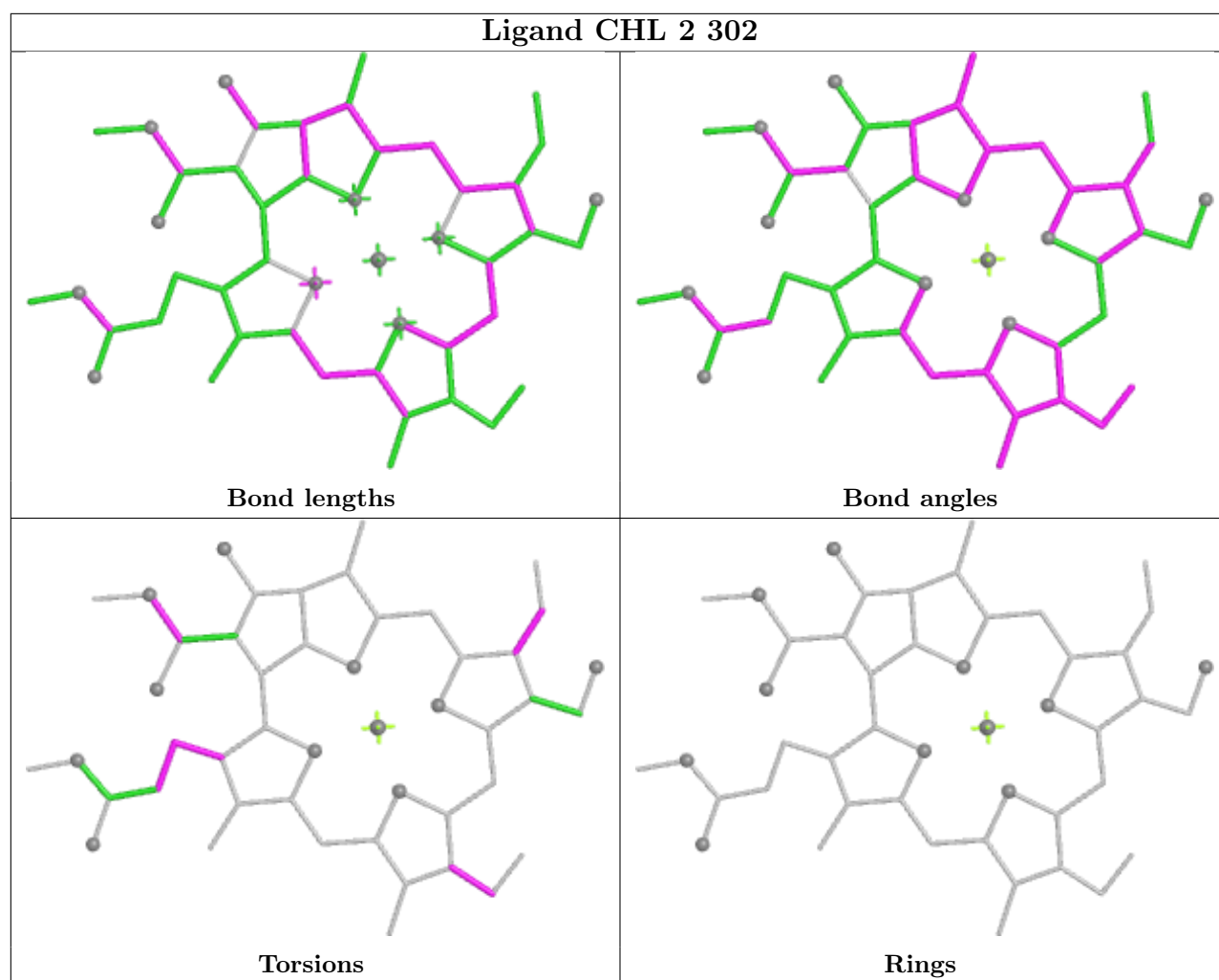




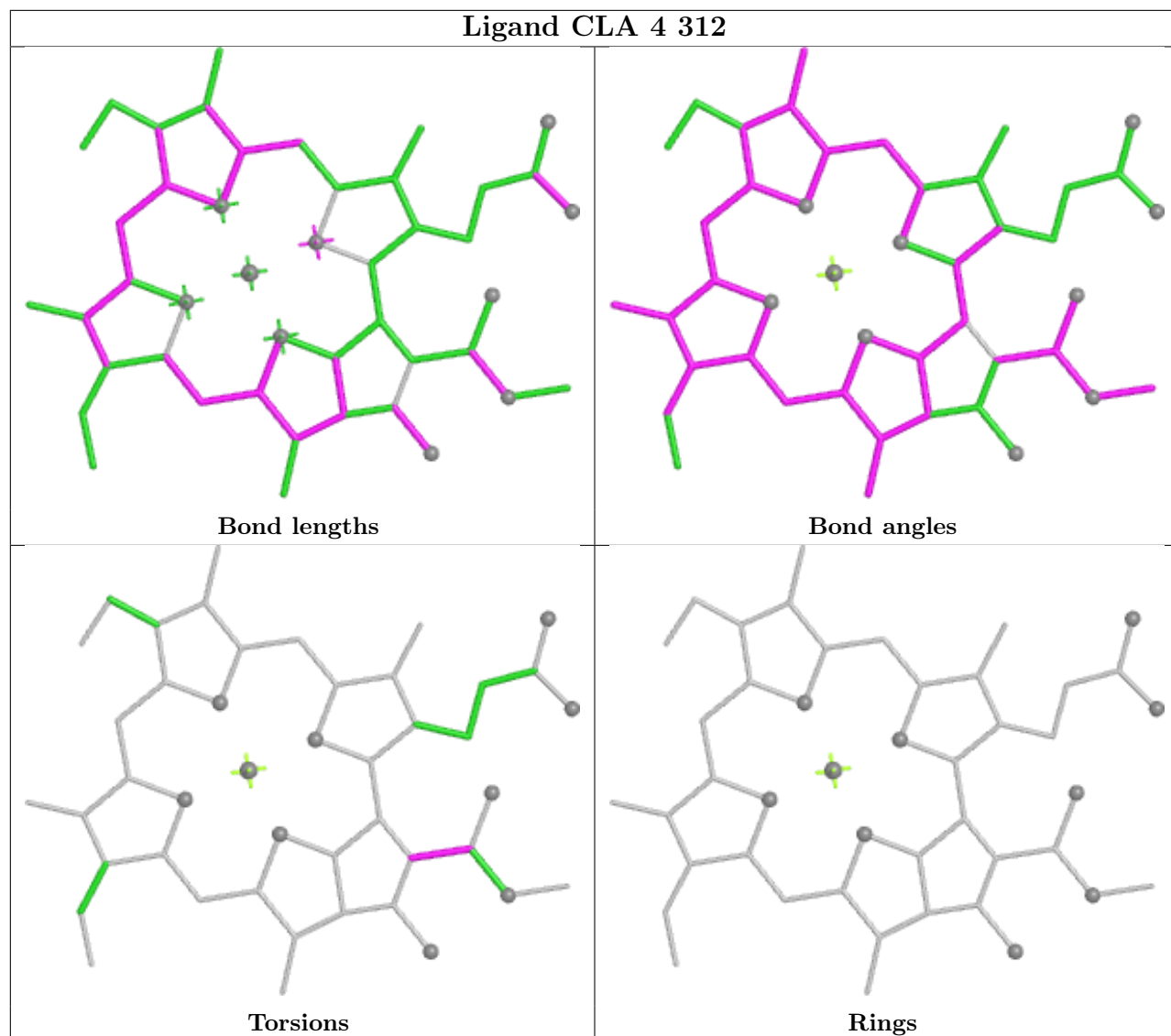


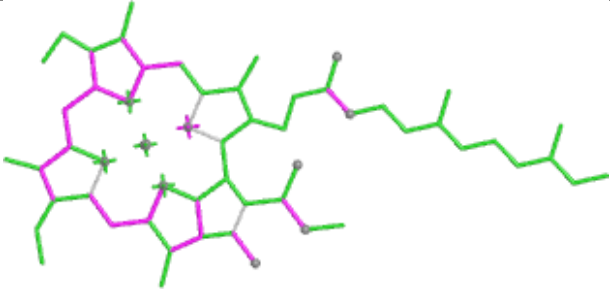
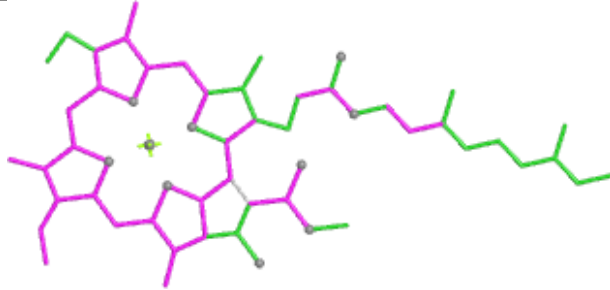
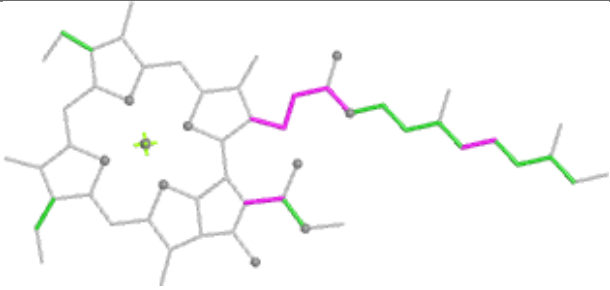
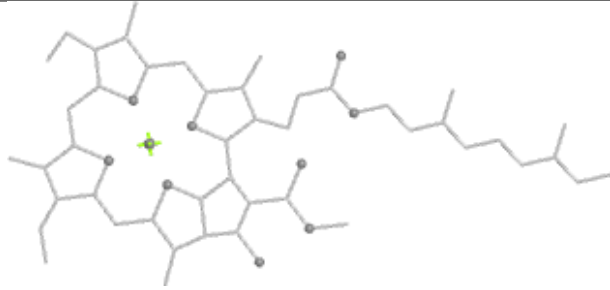
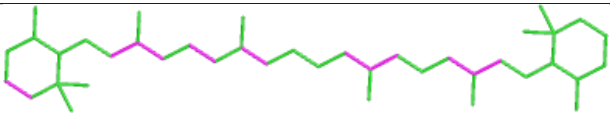
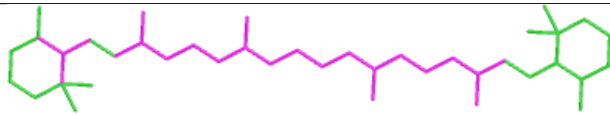
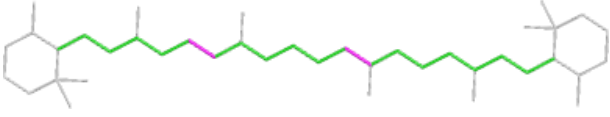
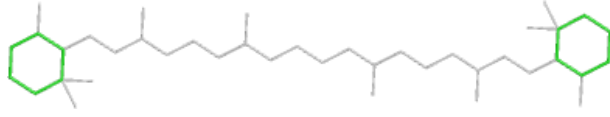




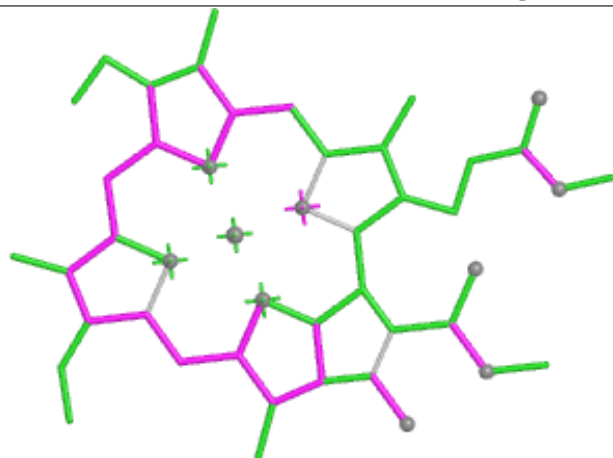


Ligand CLA 4 312

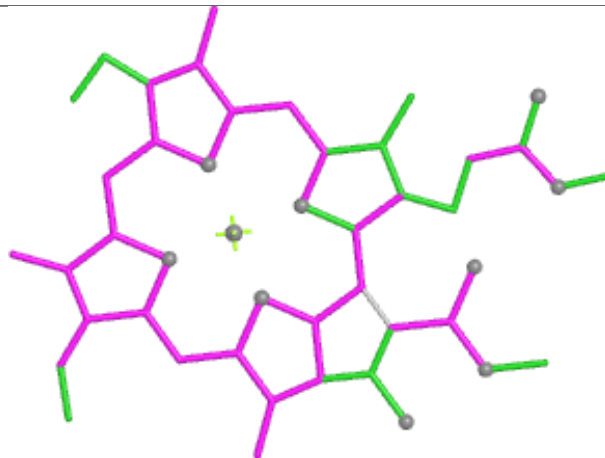


Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

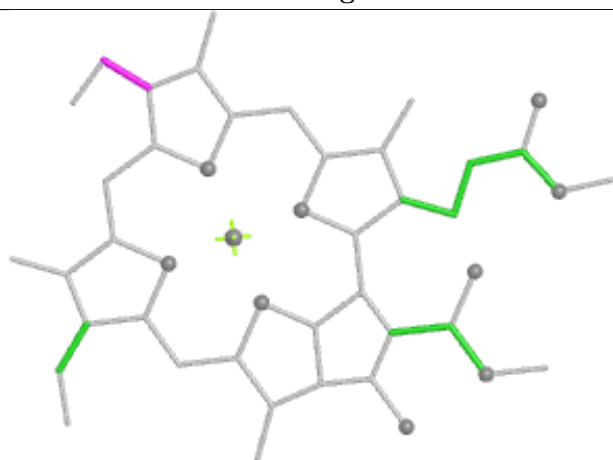
Ligand CLA X 311



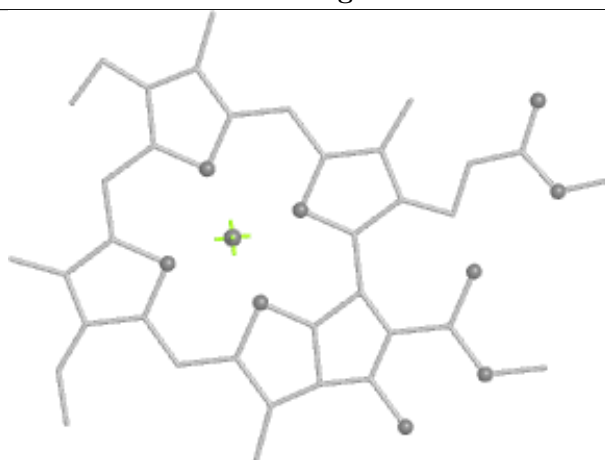
Bond lengths



Bond angles

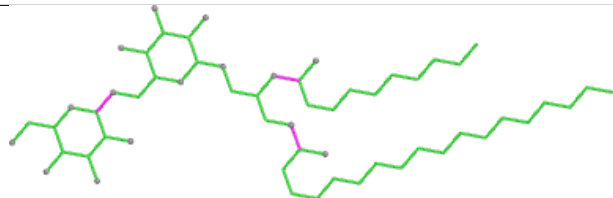


Torsions

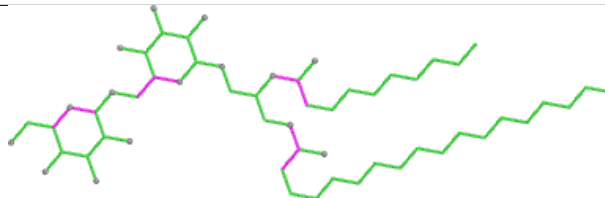


Rings

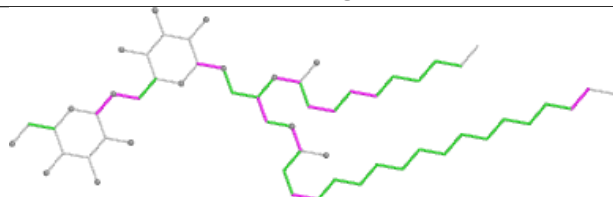
Ligand DGD J 104



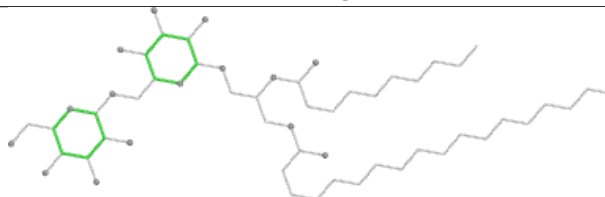
Bond lengths



Bond angles

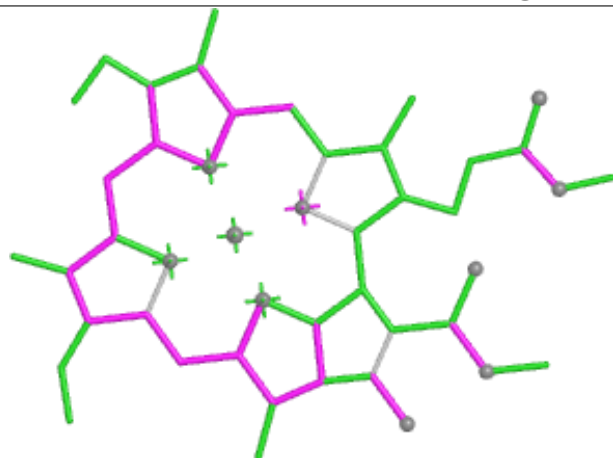


Torsions

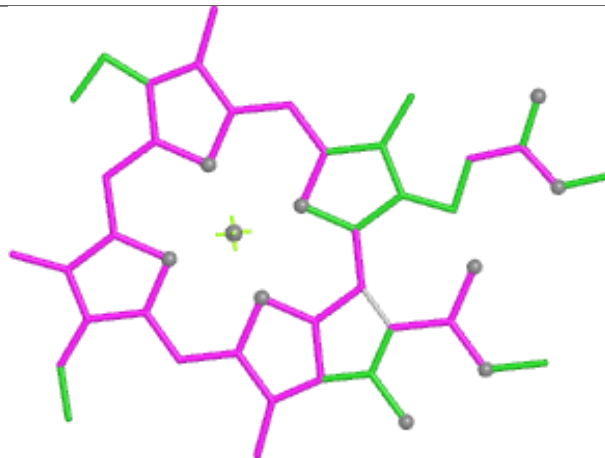


Rings

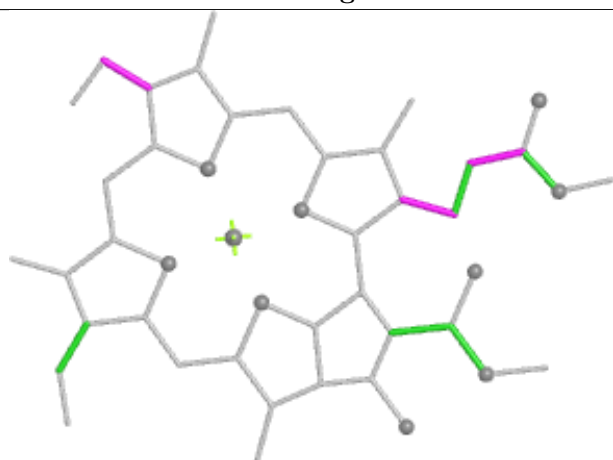
Ligand CLA Z 314



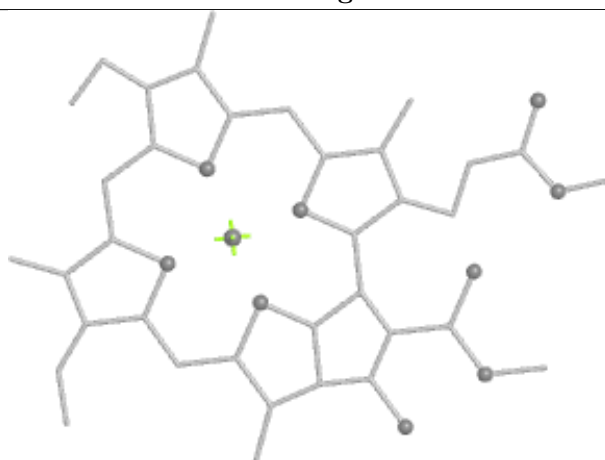
Bond lengths



Bond angles

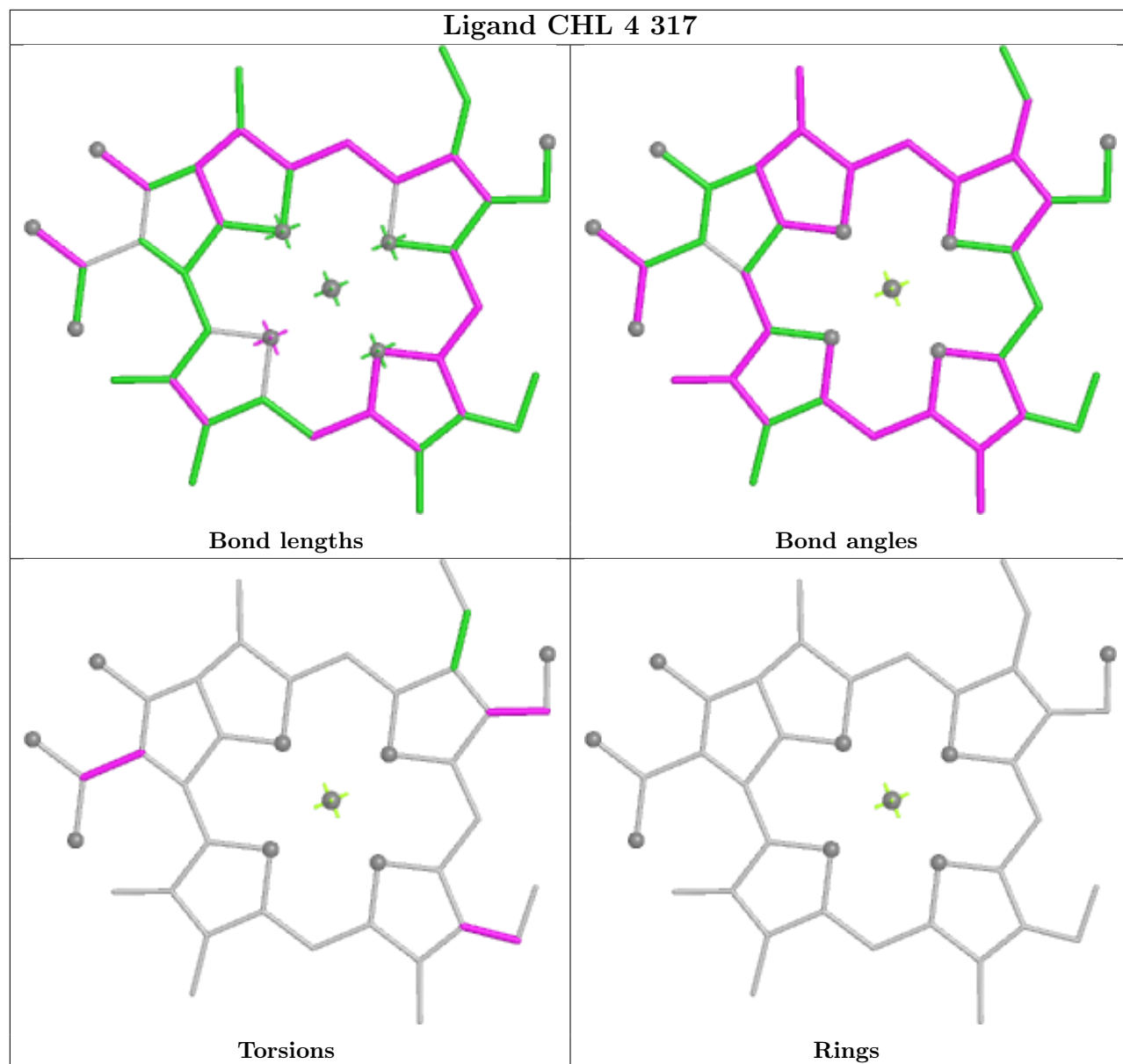


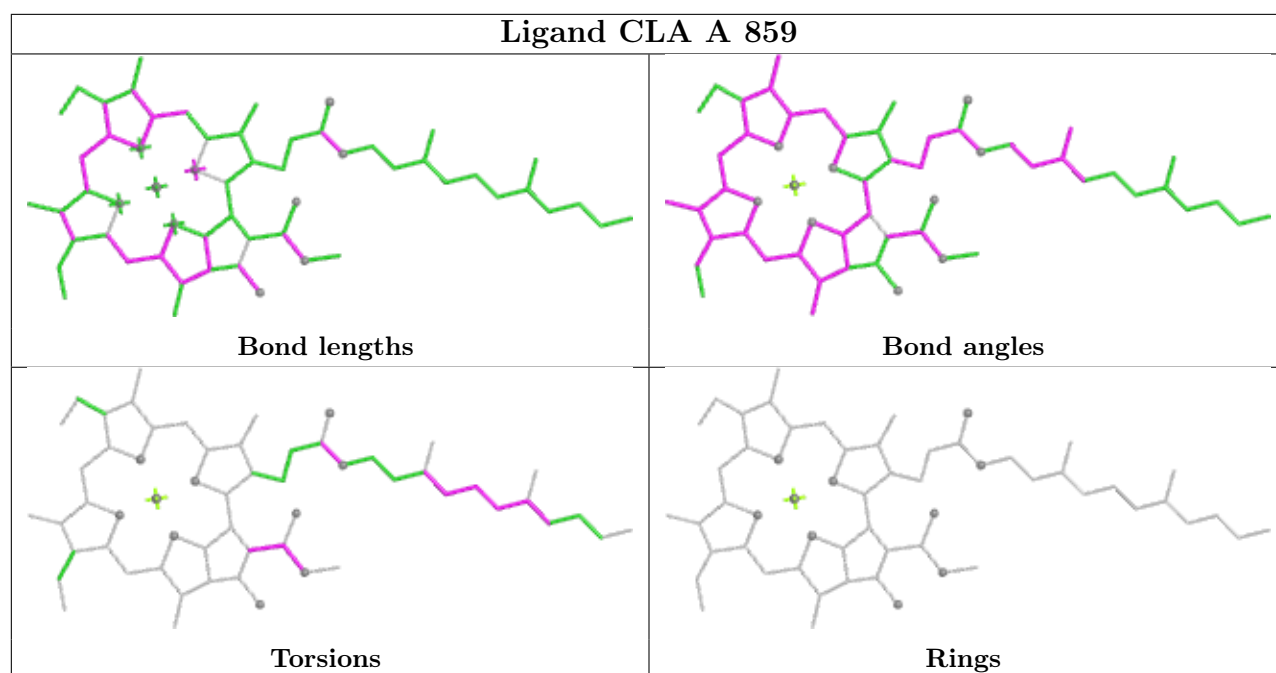
Torsions

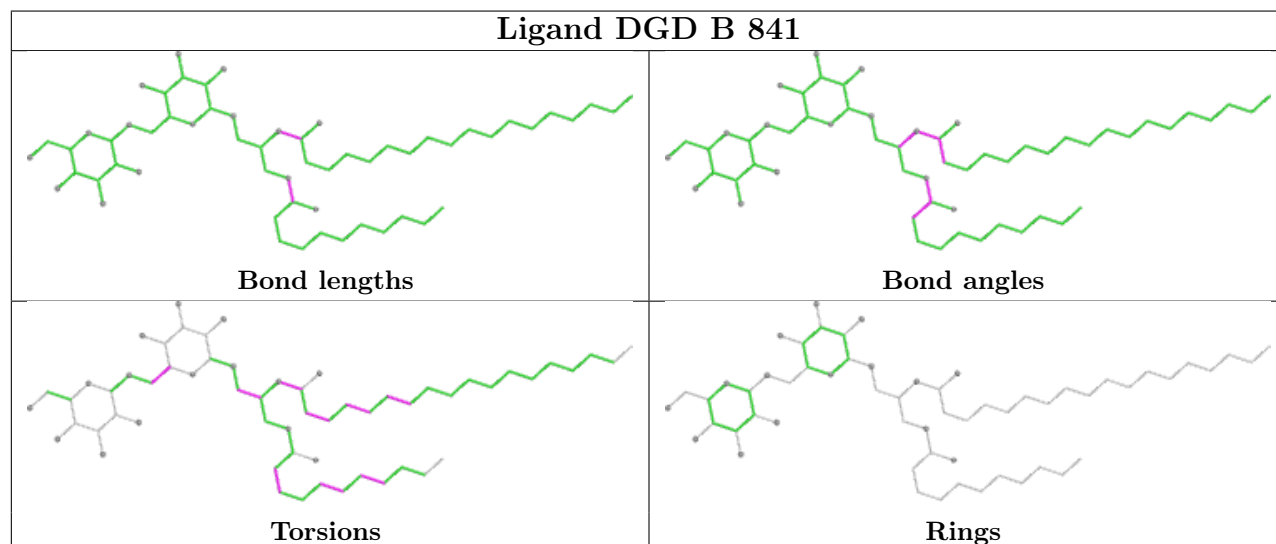
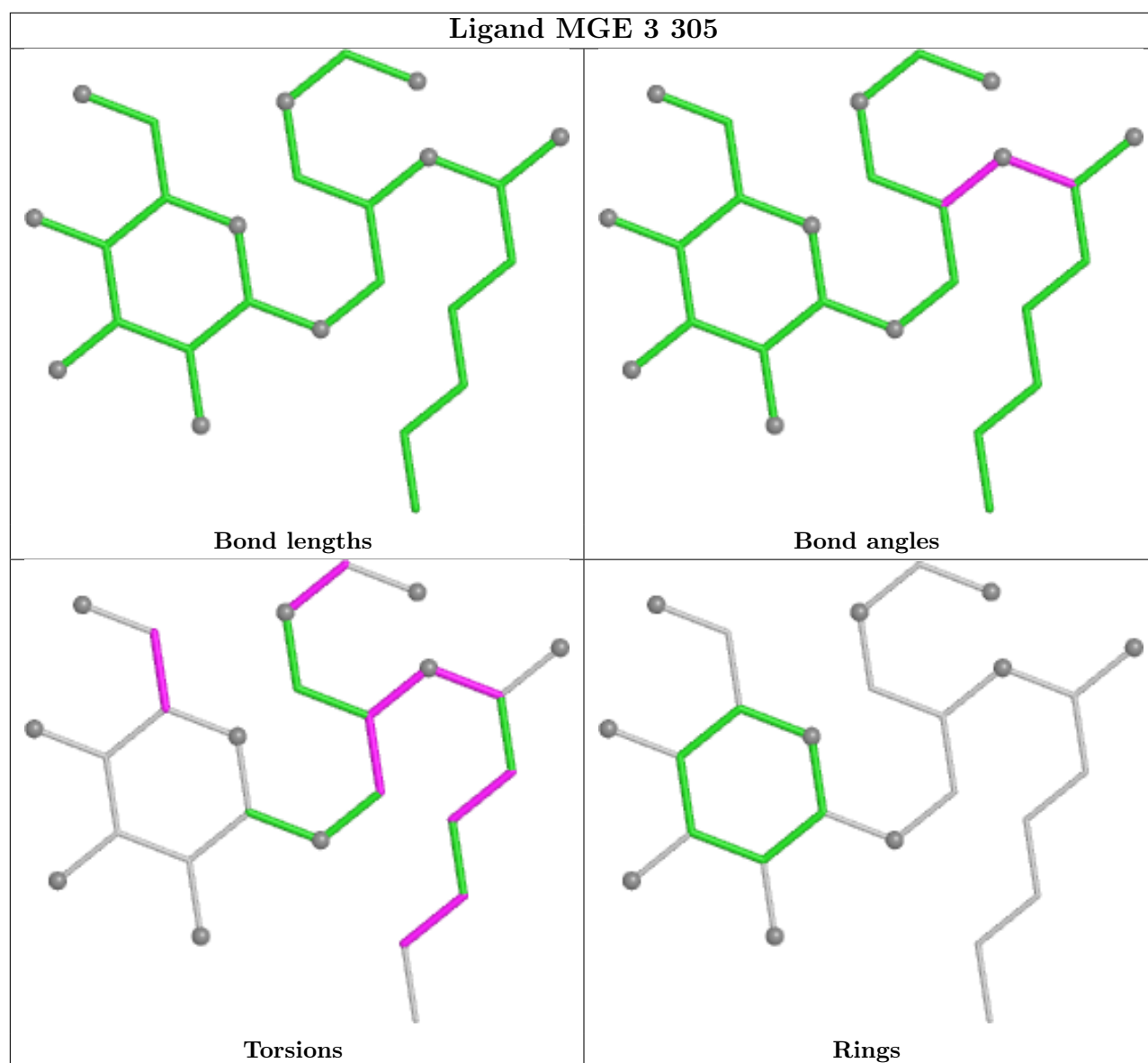


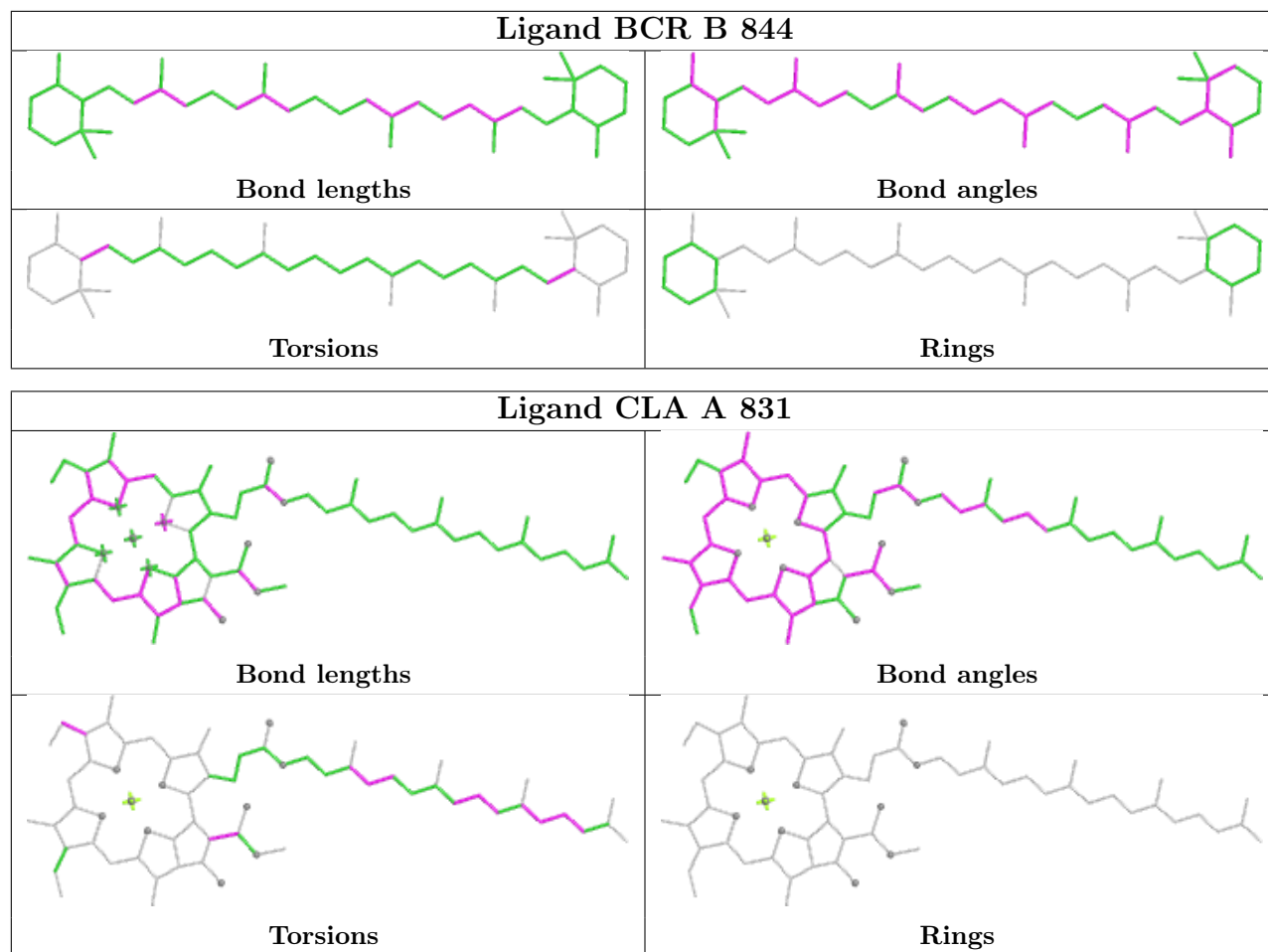
Rings

Ligand CHL 4 317

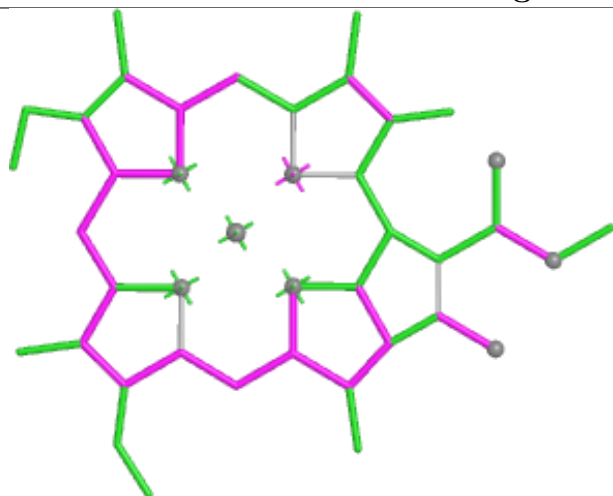




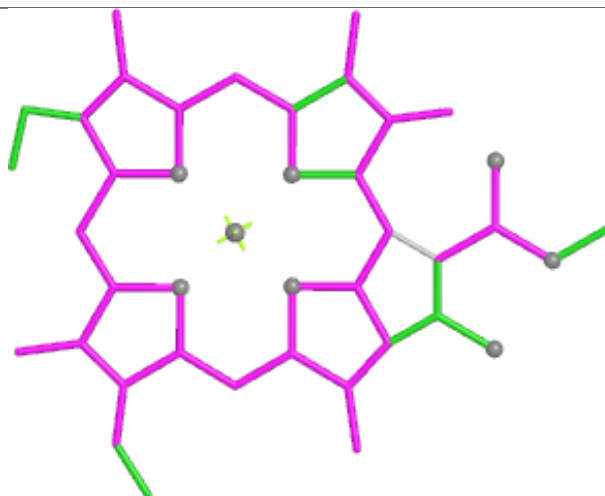




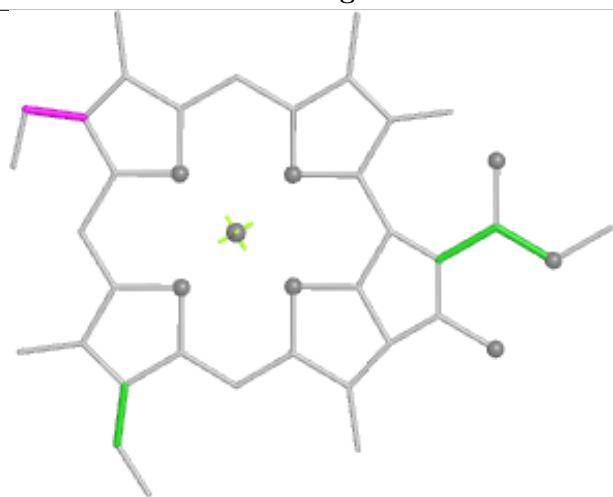
Ligand CLA H 201



Bond lengths



Bond angles

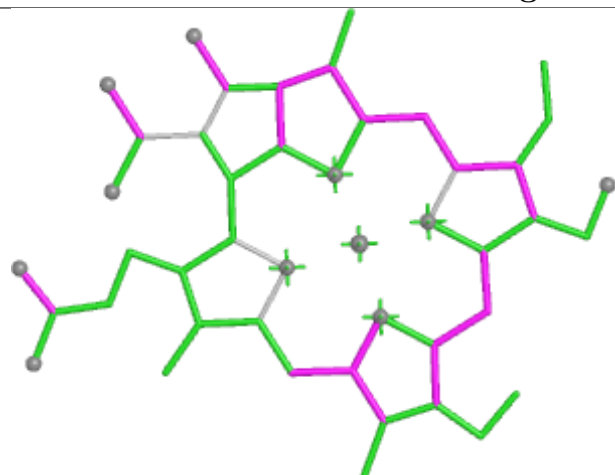


Torsions

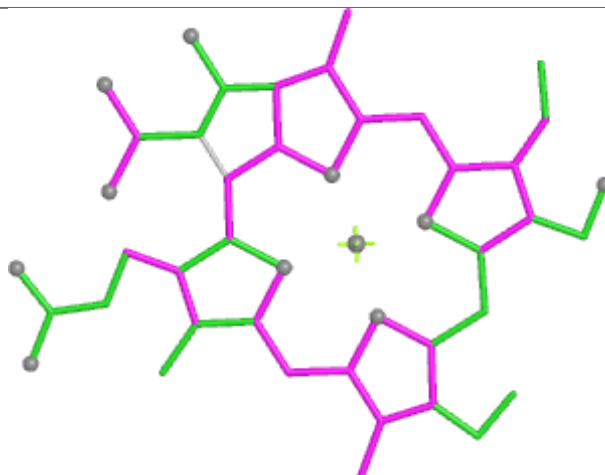


Rings

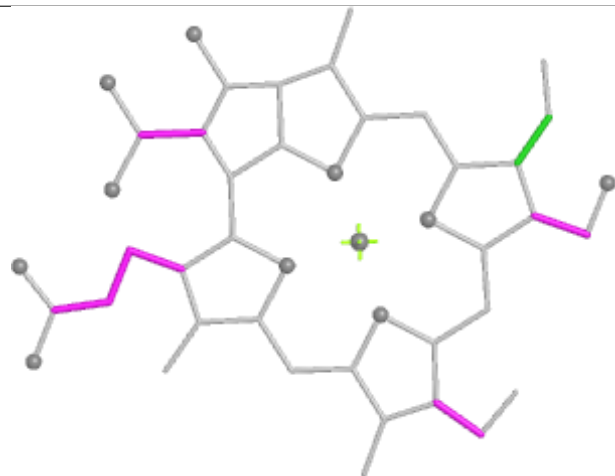
Ligand CHL 4 307



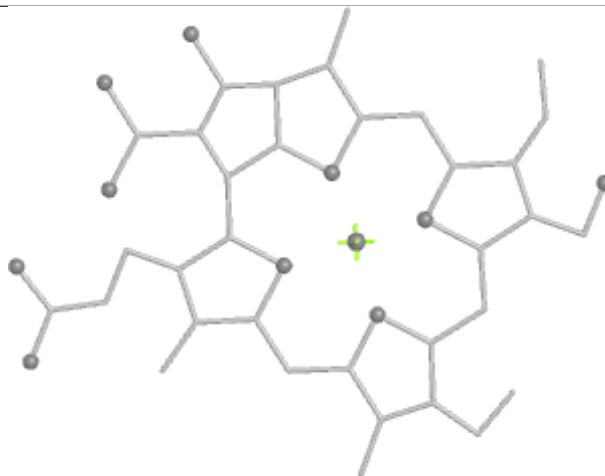
Bond lengths



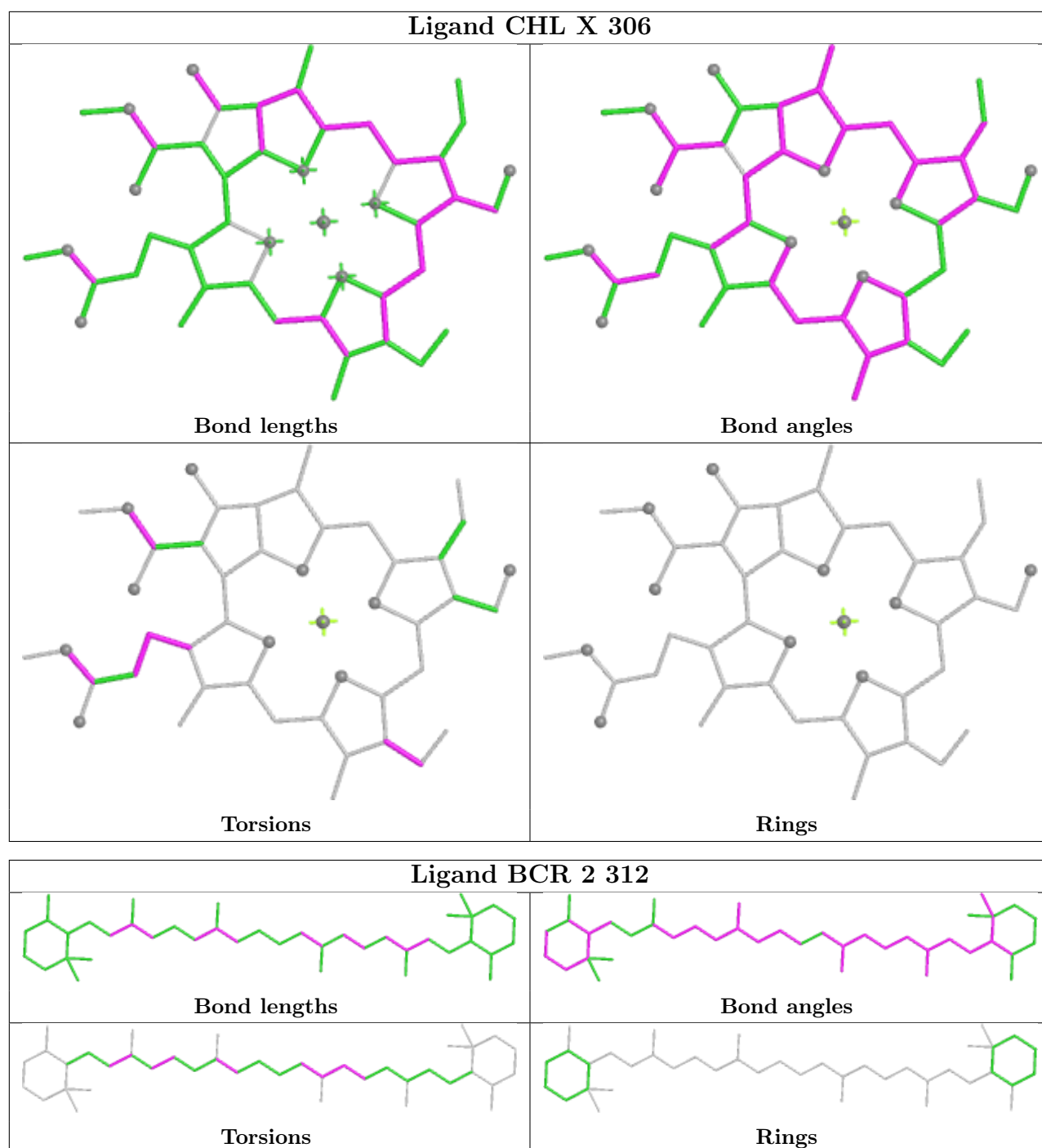
Bond angles

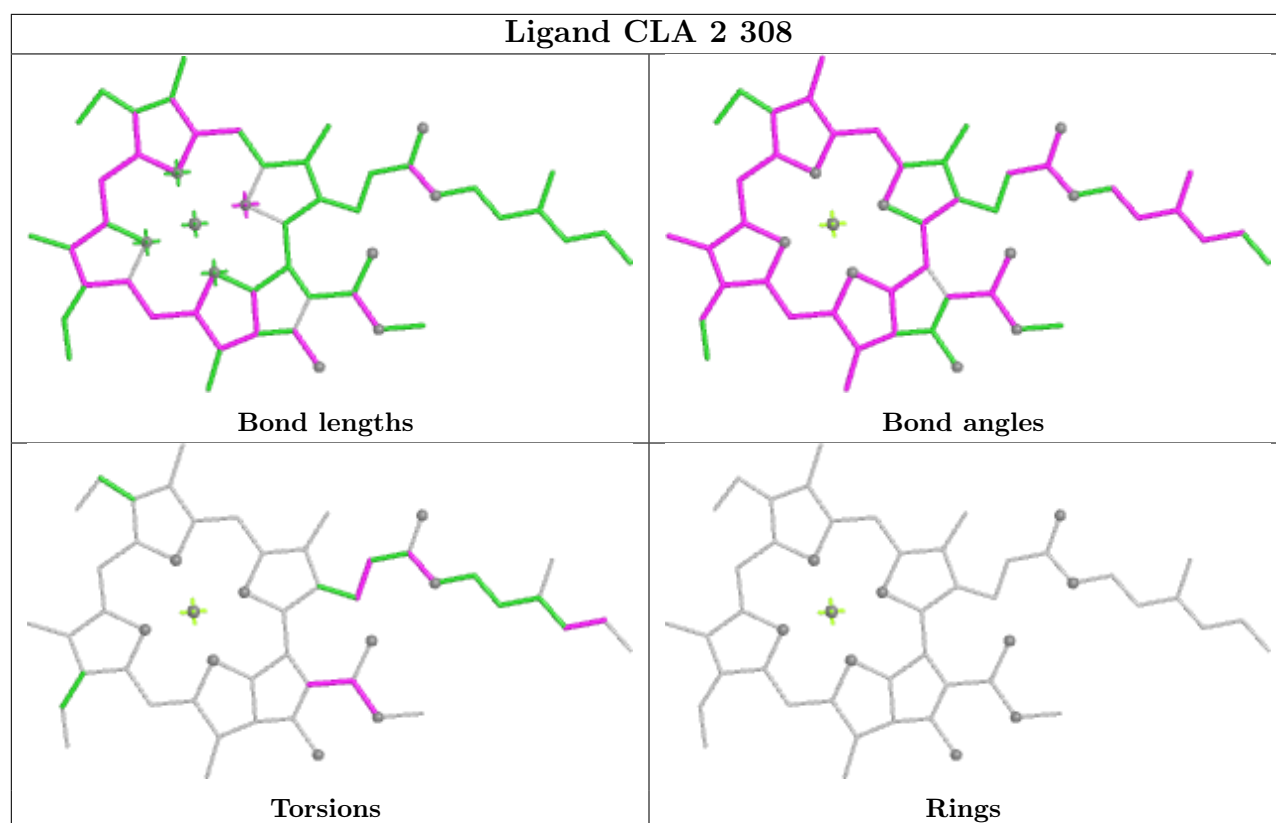


Torsions

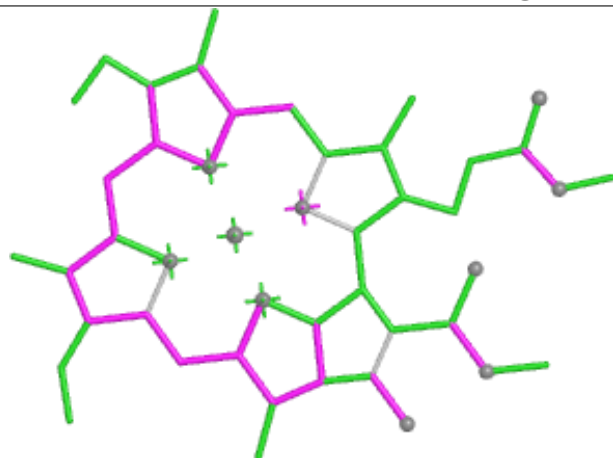


Rings

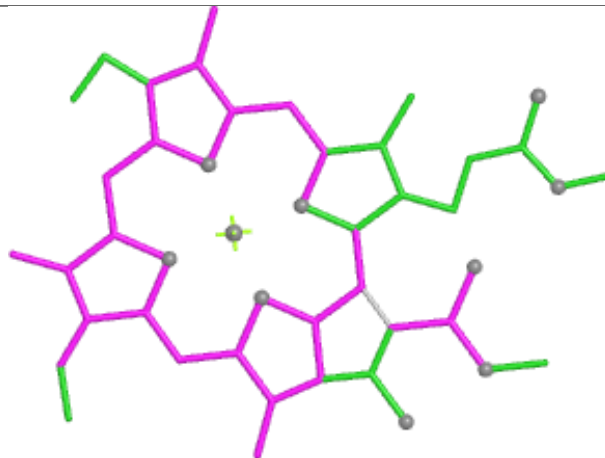




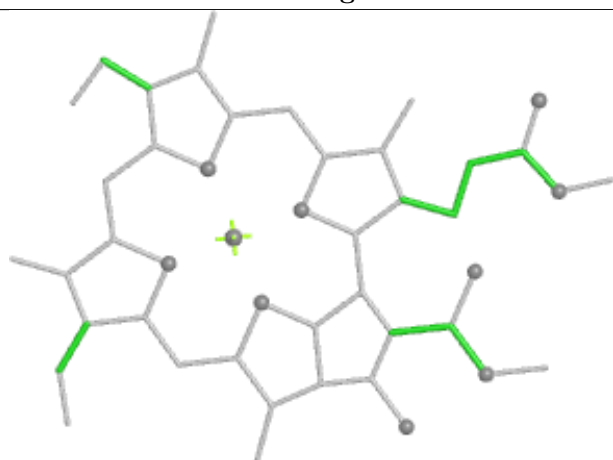
Ligand CLA Z 307



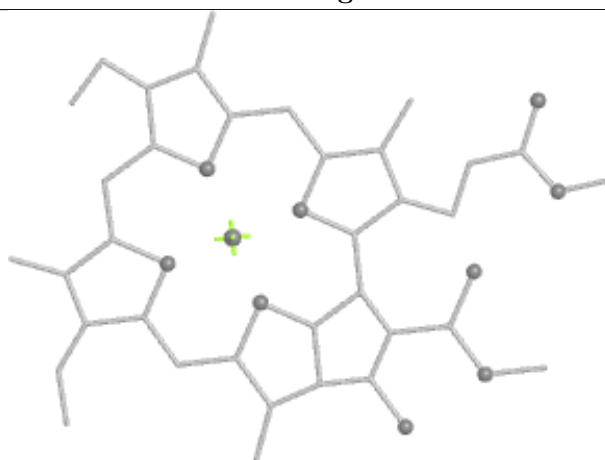
Bond lengths



Bond angles

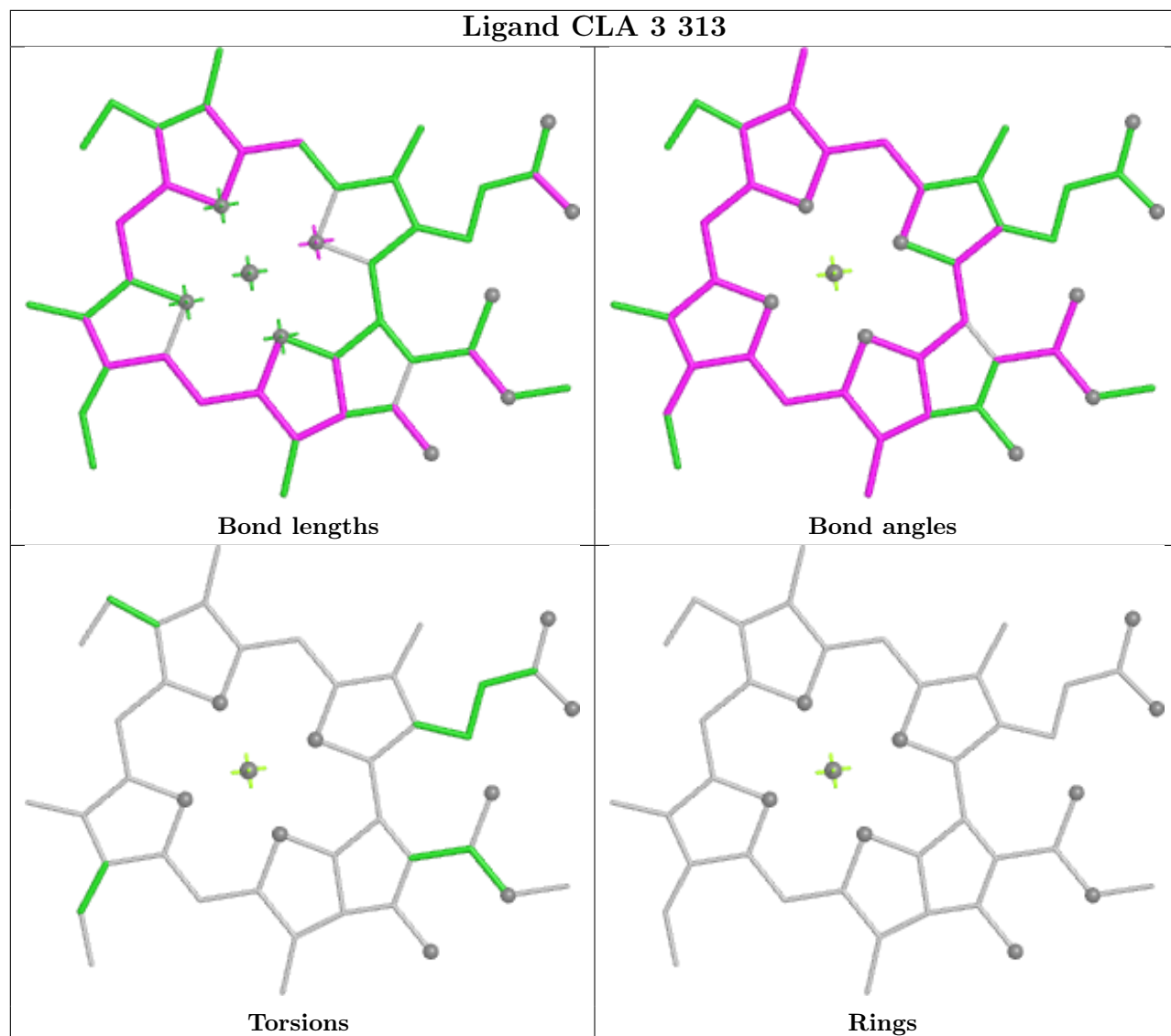


Torsions

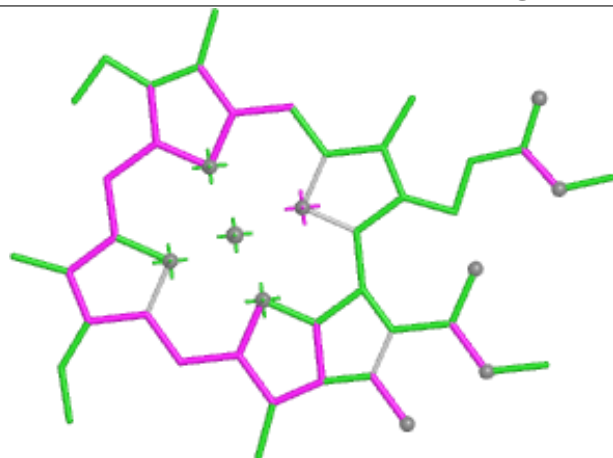


Rings

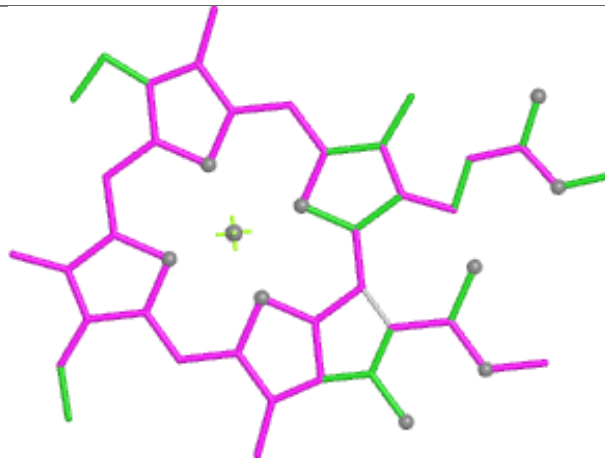
Ligand CLA 3 313



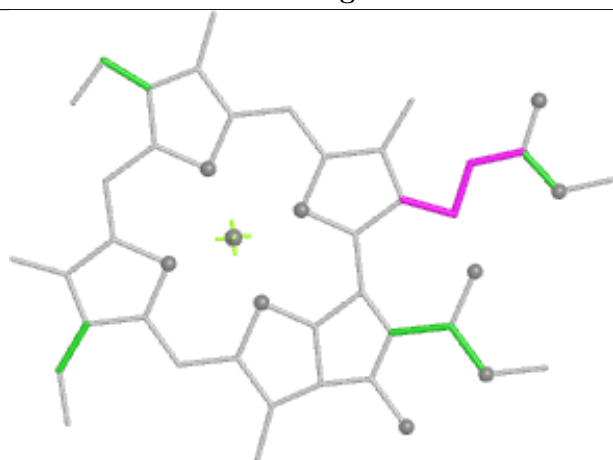
Ligand CLA Y 310



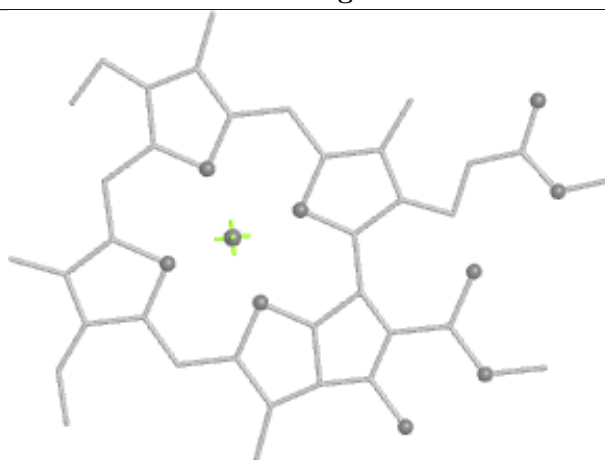
Bond lengths



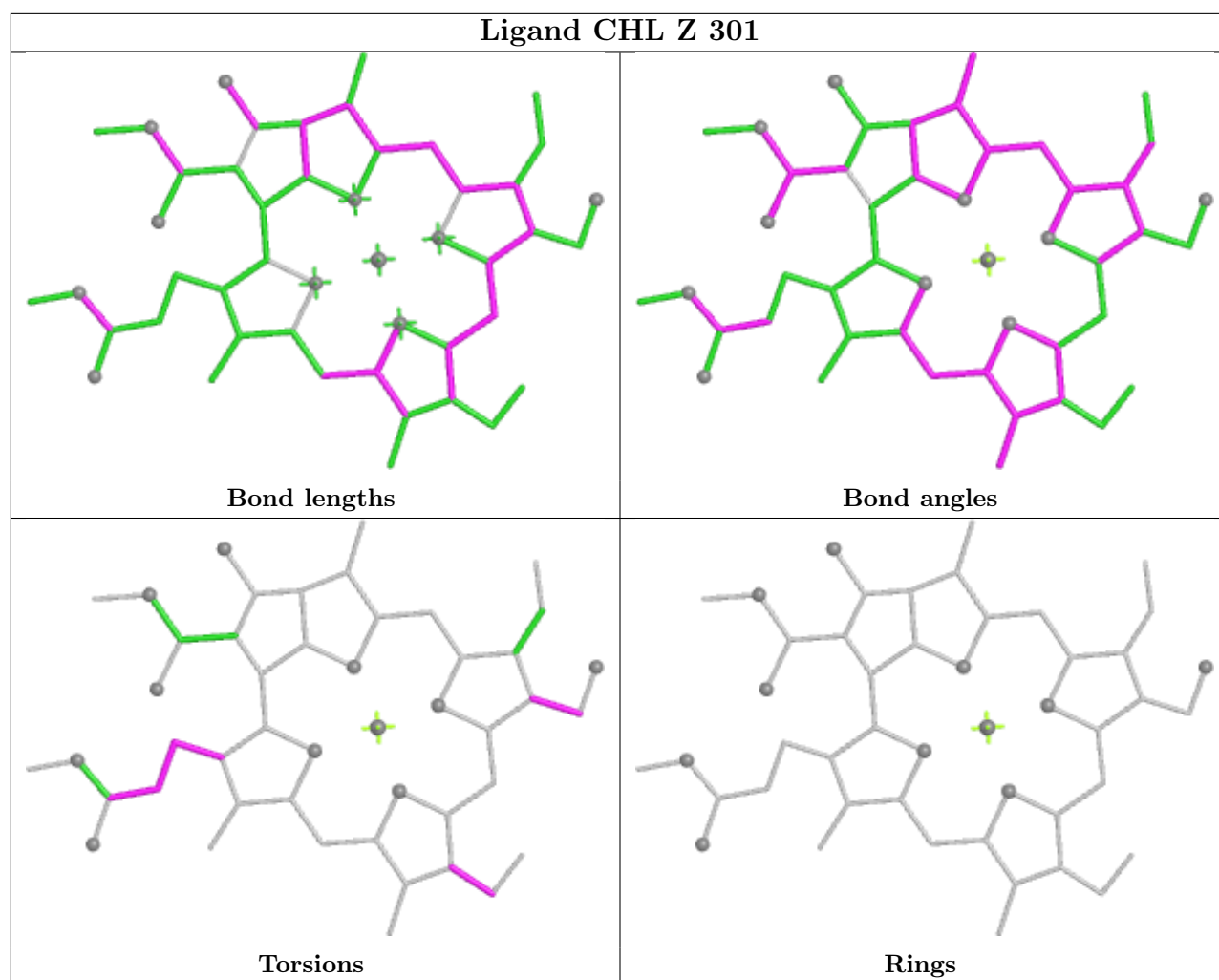
Bond angles



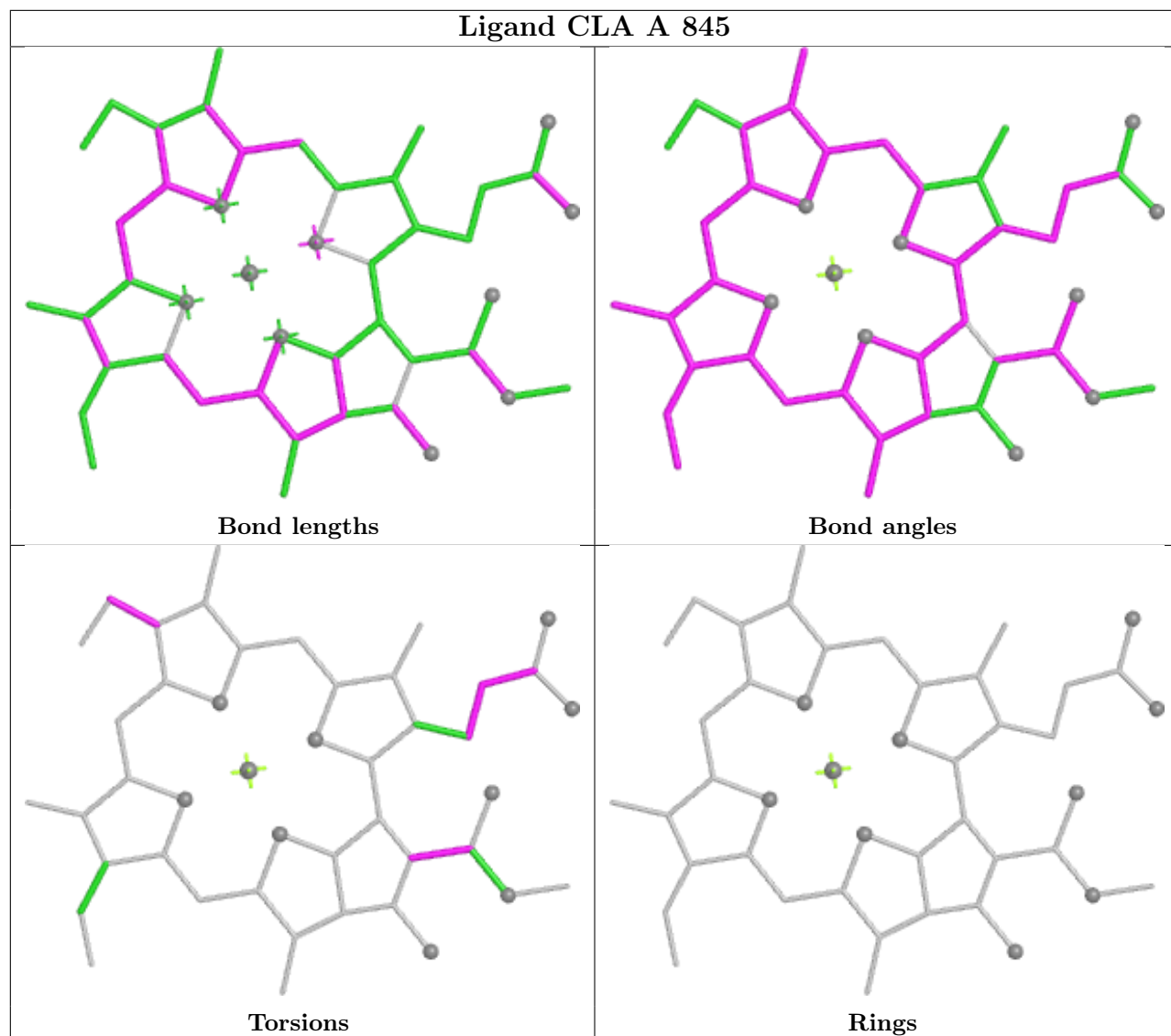
Torsions



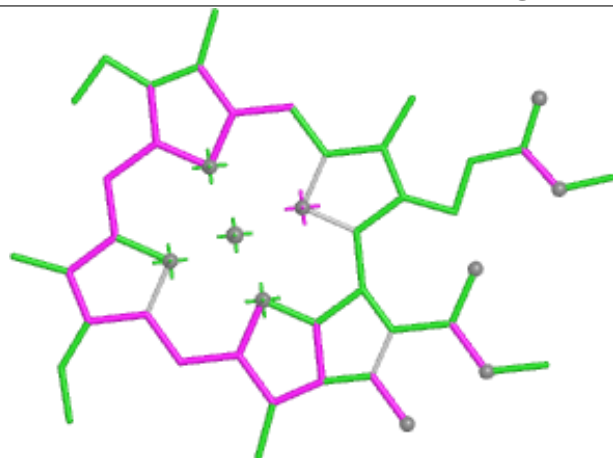
Rings



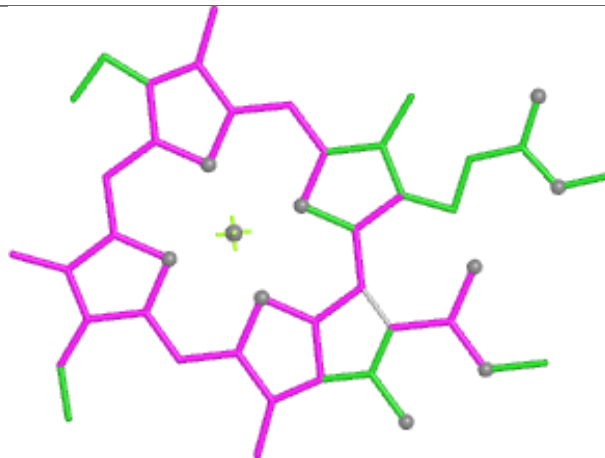
Ligand CLA A 845



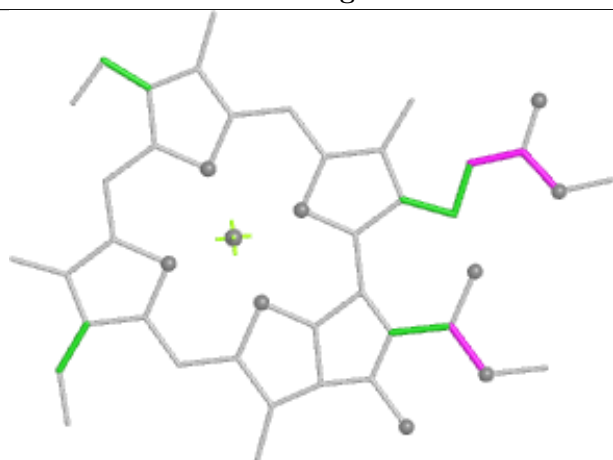
Ligand CLA X 303



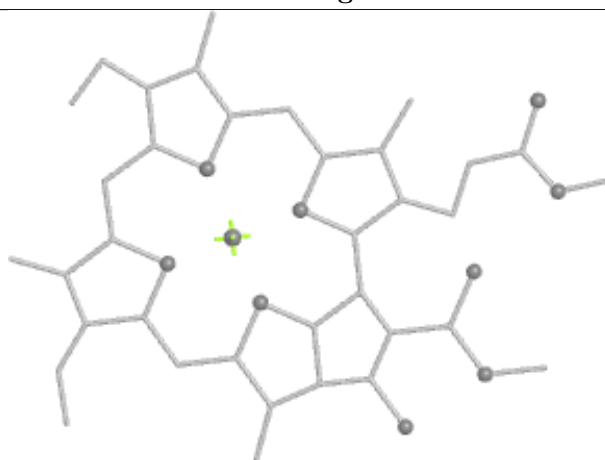
Bond lengths



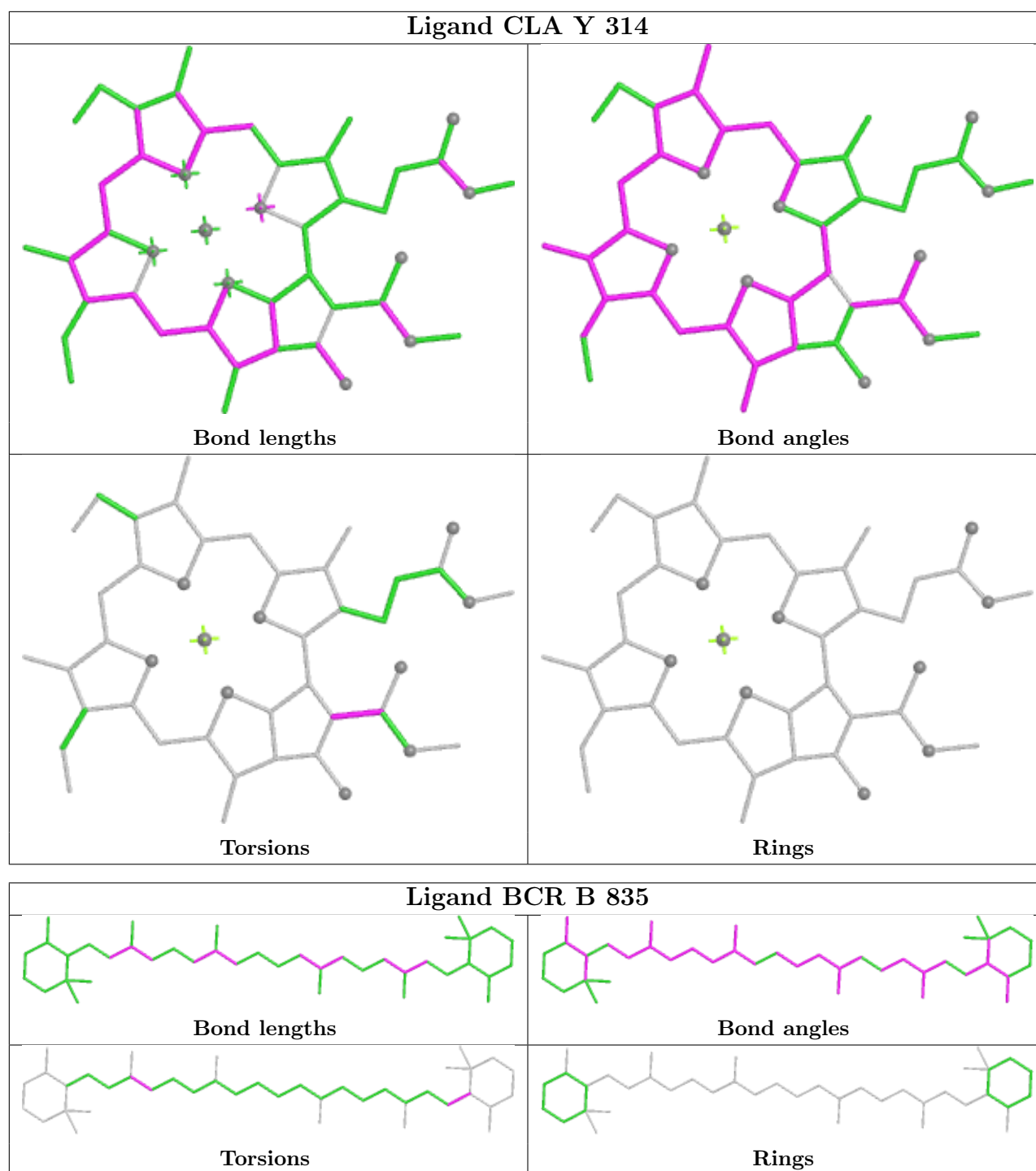
Bond angles

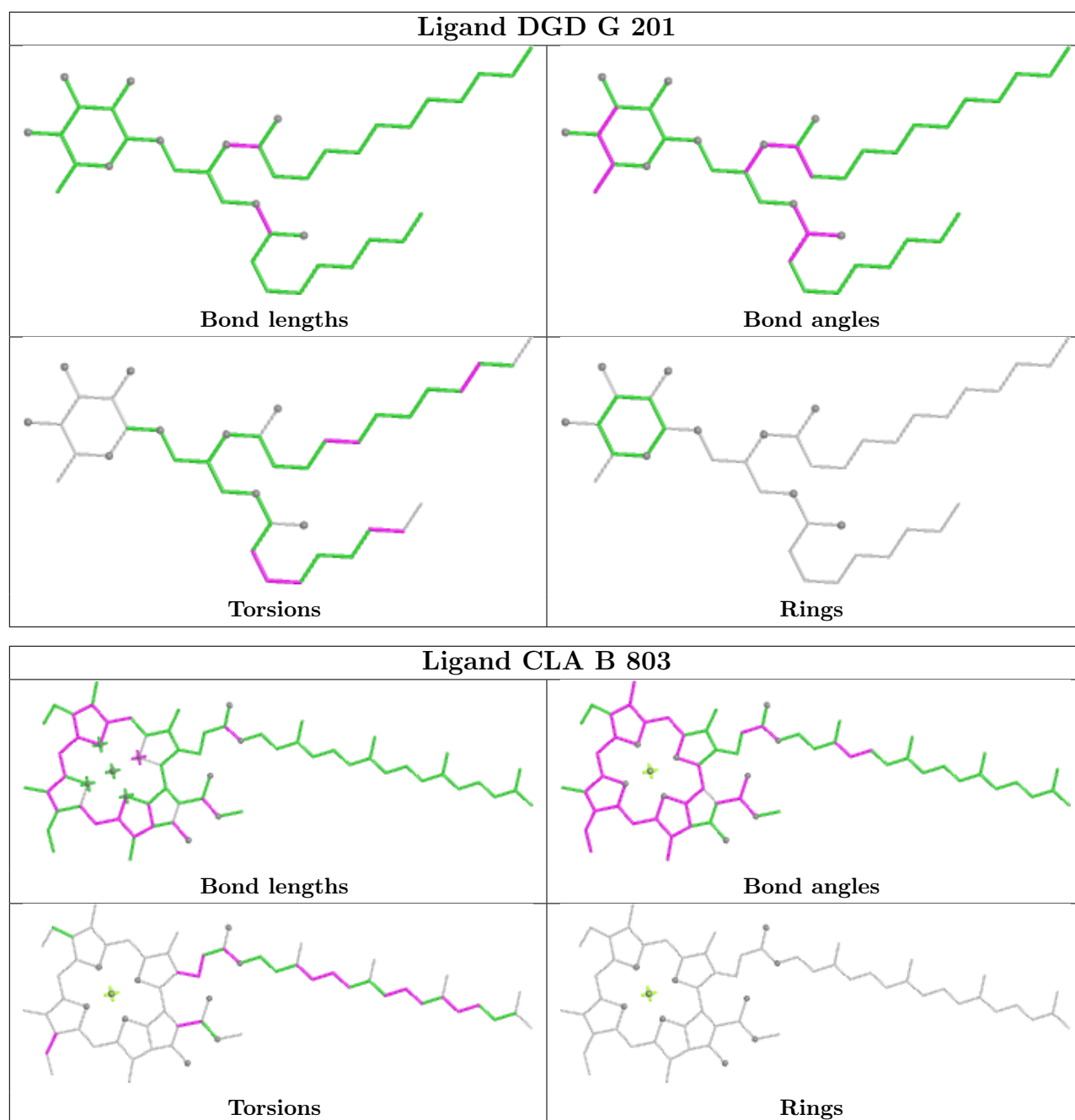


Torsions

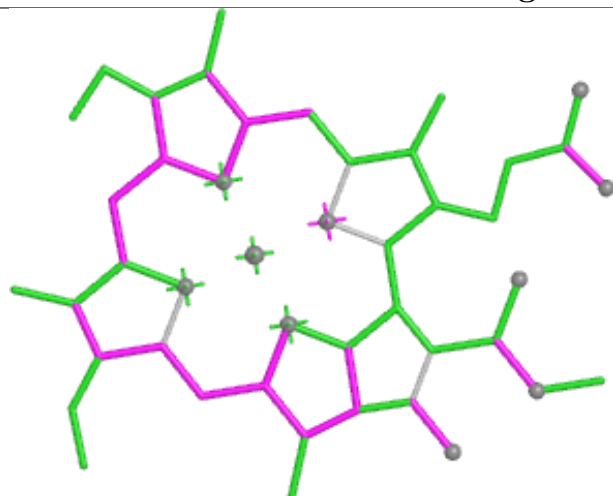


Rings

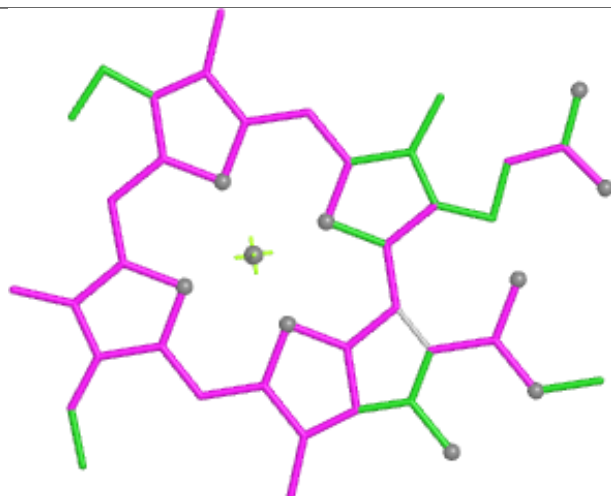




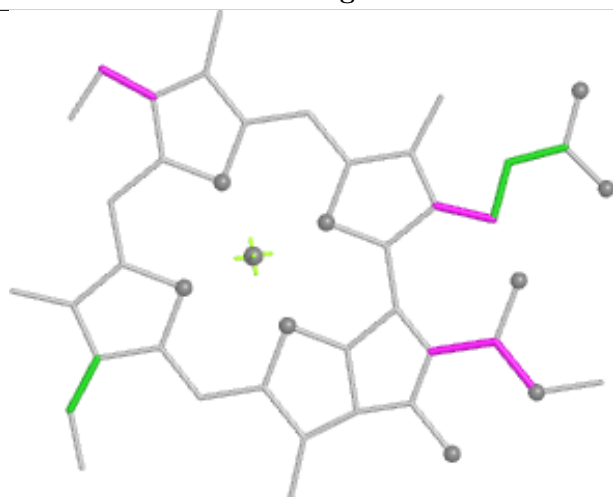
Ligand CLA 4 311



Bond lengths



Bond angles

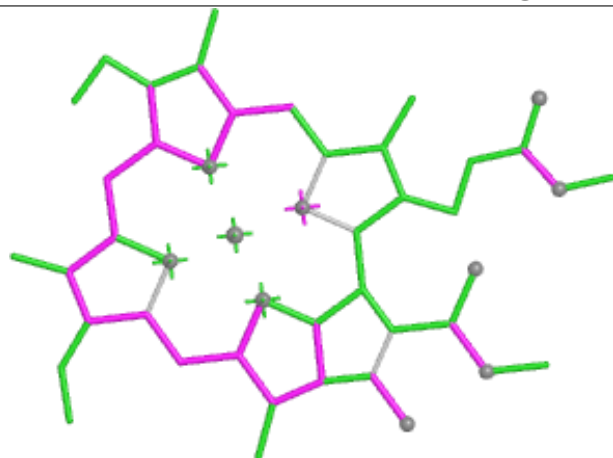


Torsions

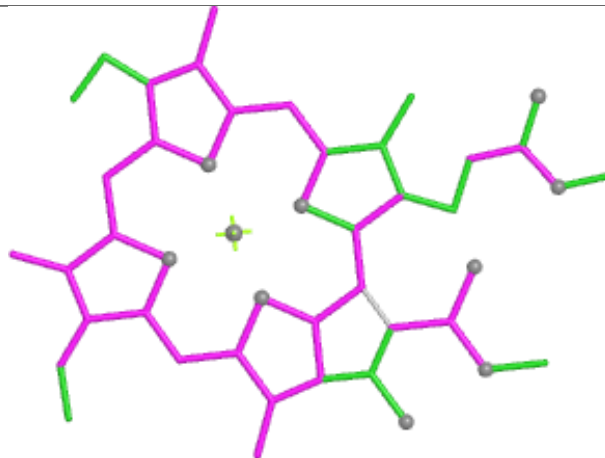


Rings

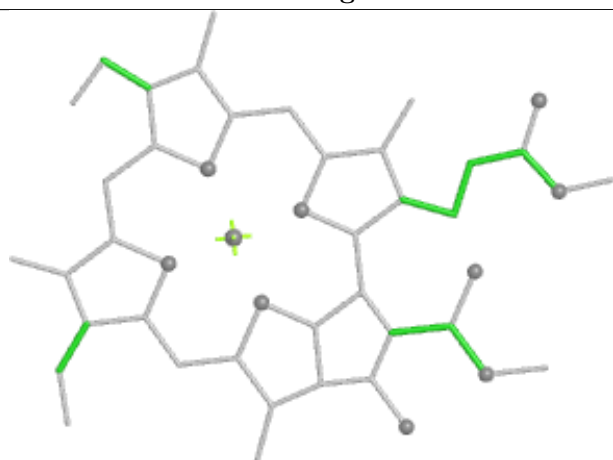
Ligand CLA Z 308



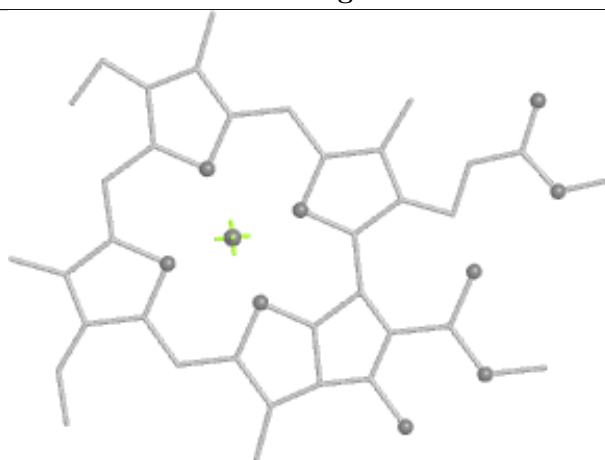
Bond lengths



Bond angles

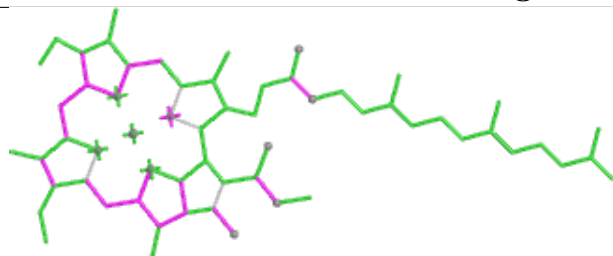


Torsions

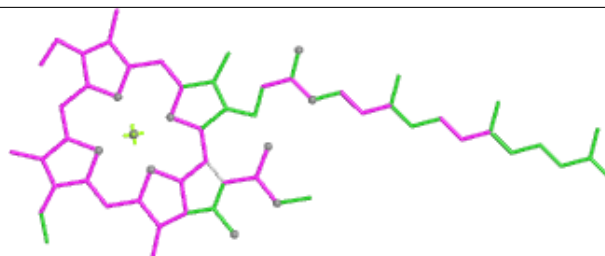


Rings

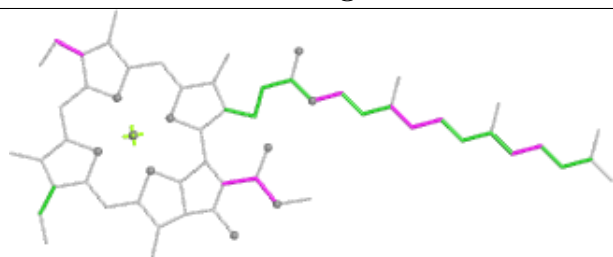
Ligand CLA B 809



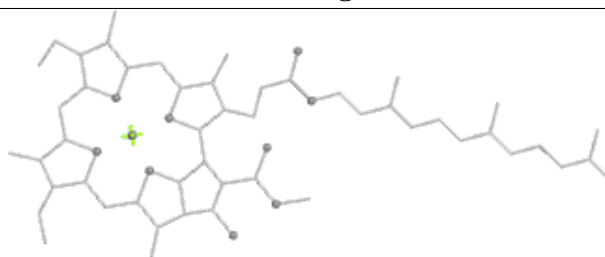
Bond lengths



Bond angles

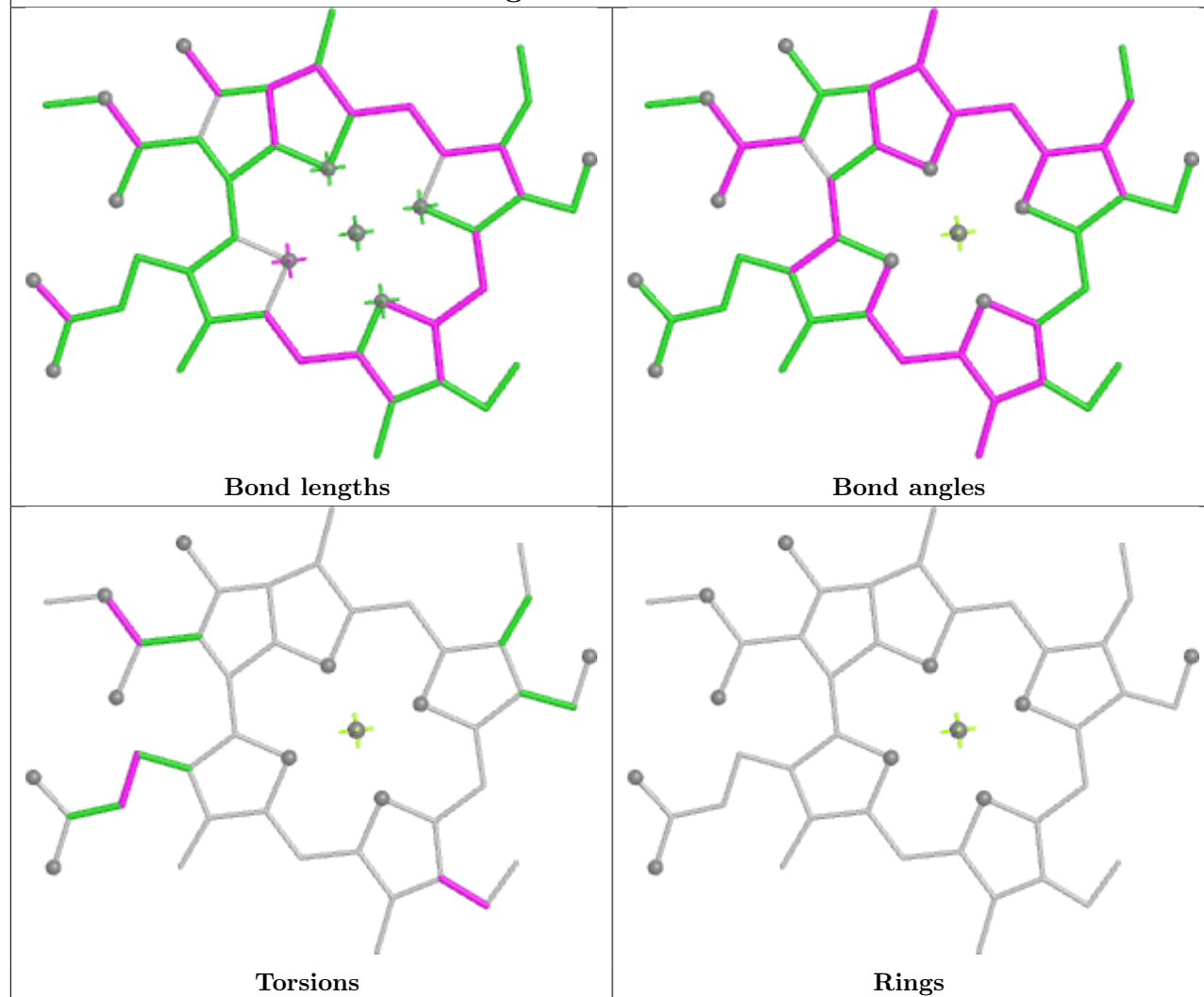


Torsions

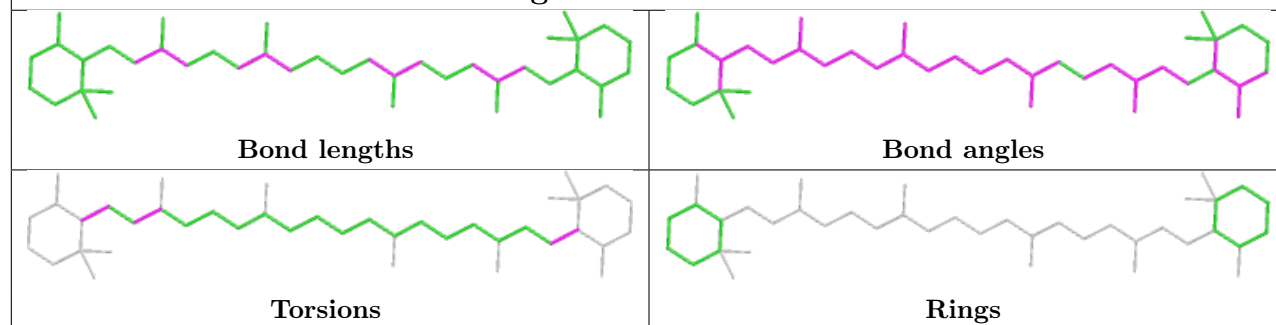


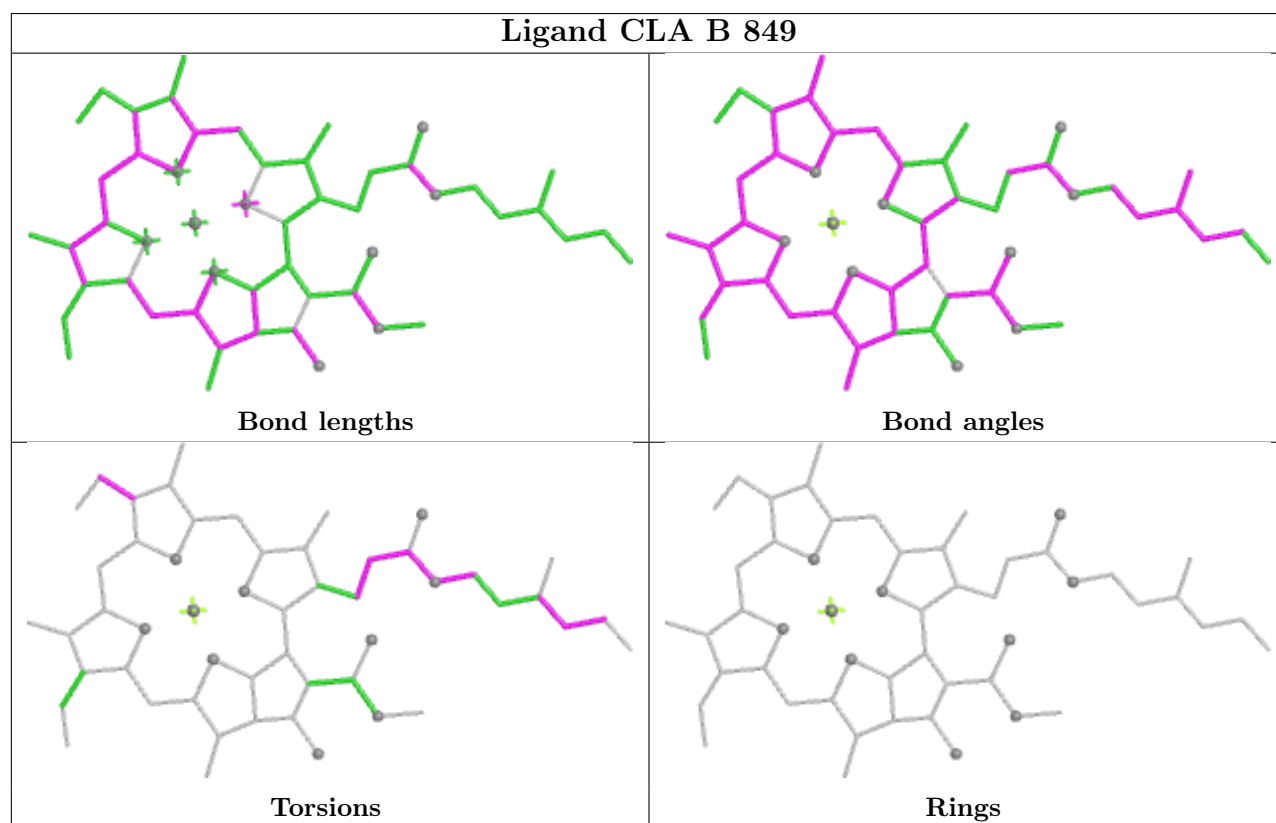
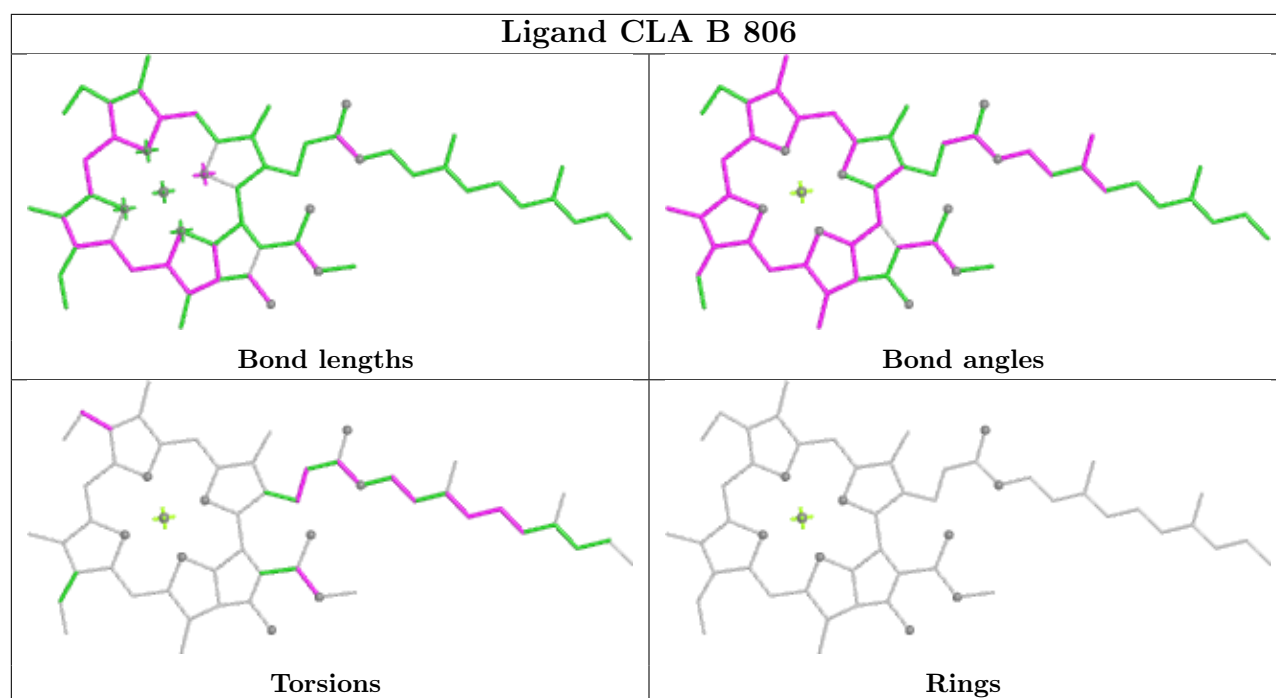
Rings

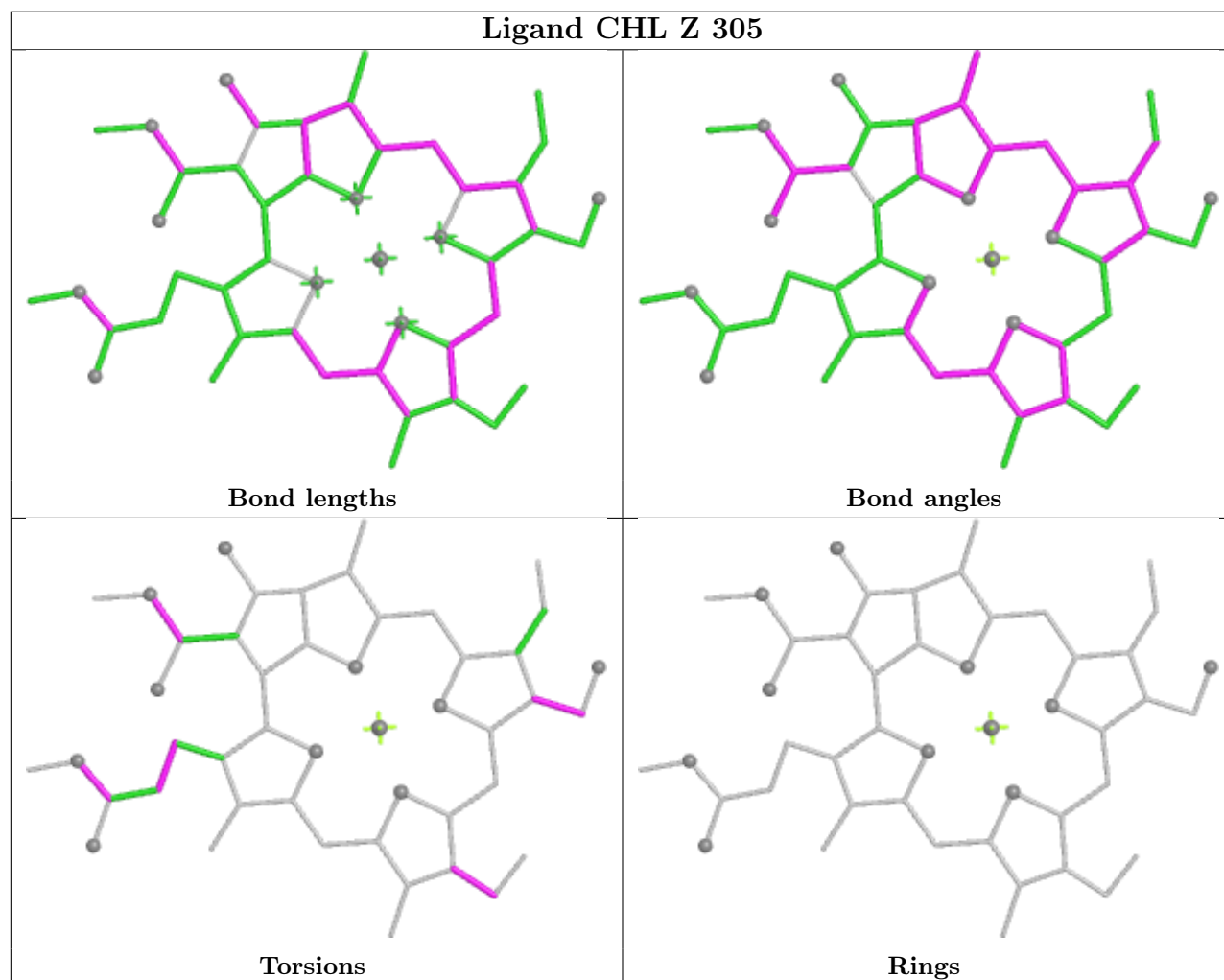
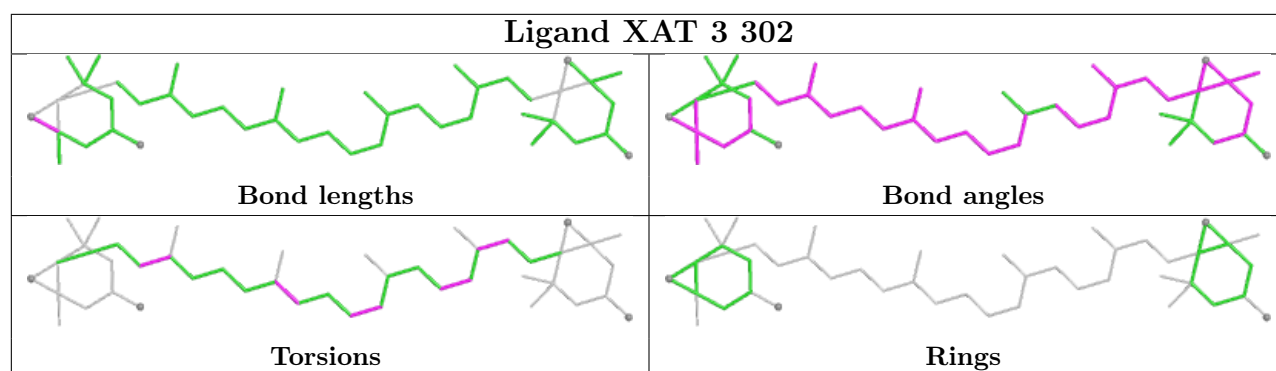
Ligand CHL 2 309



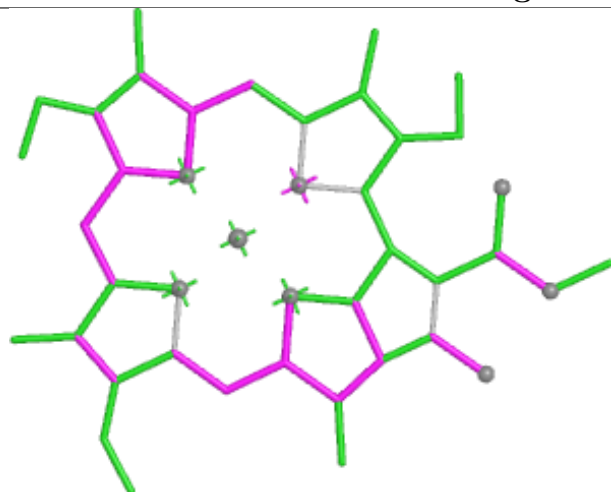
Ligand BCR B 837



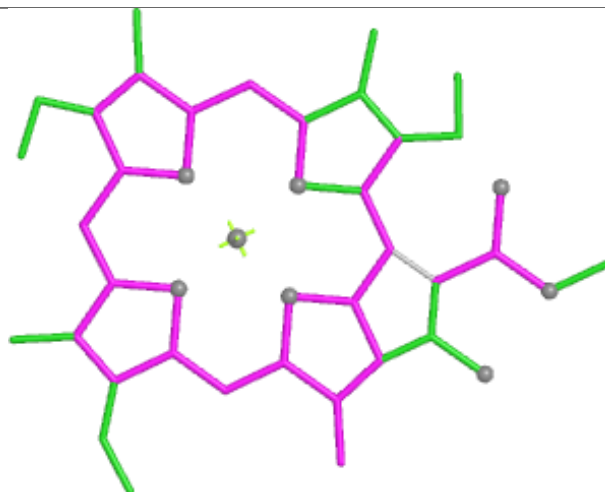




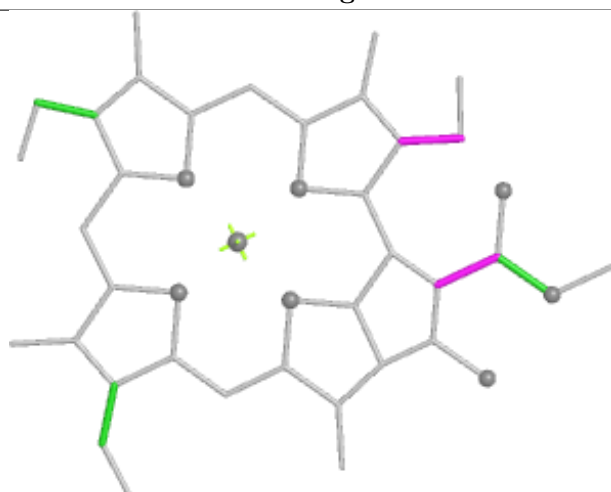
Ligand CLA A 847



Bond lengths



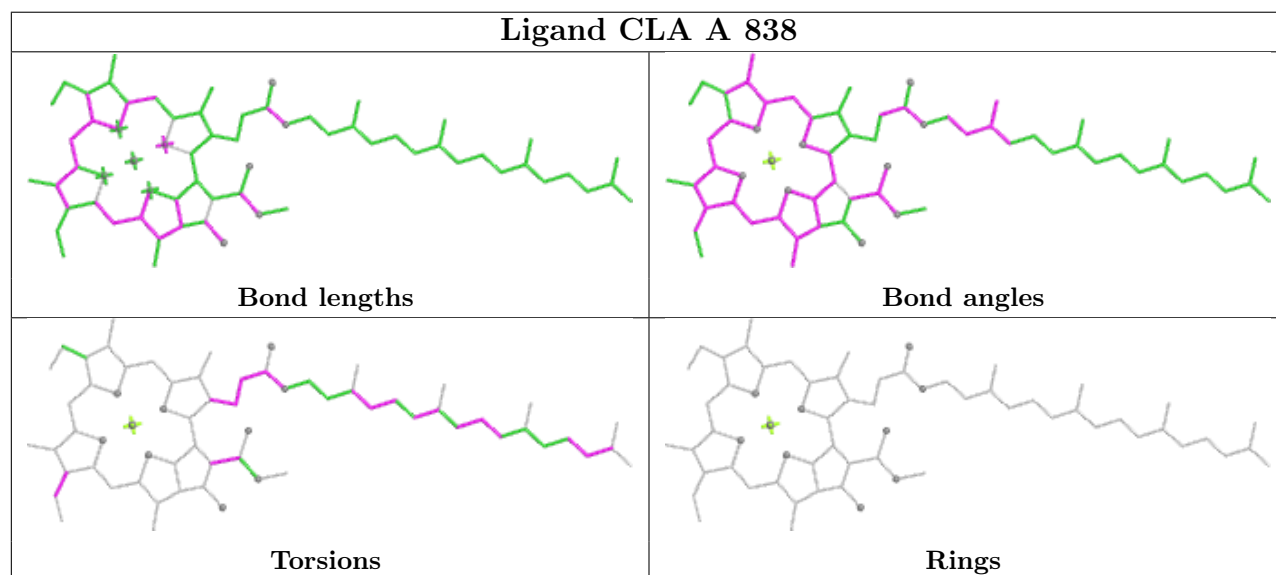
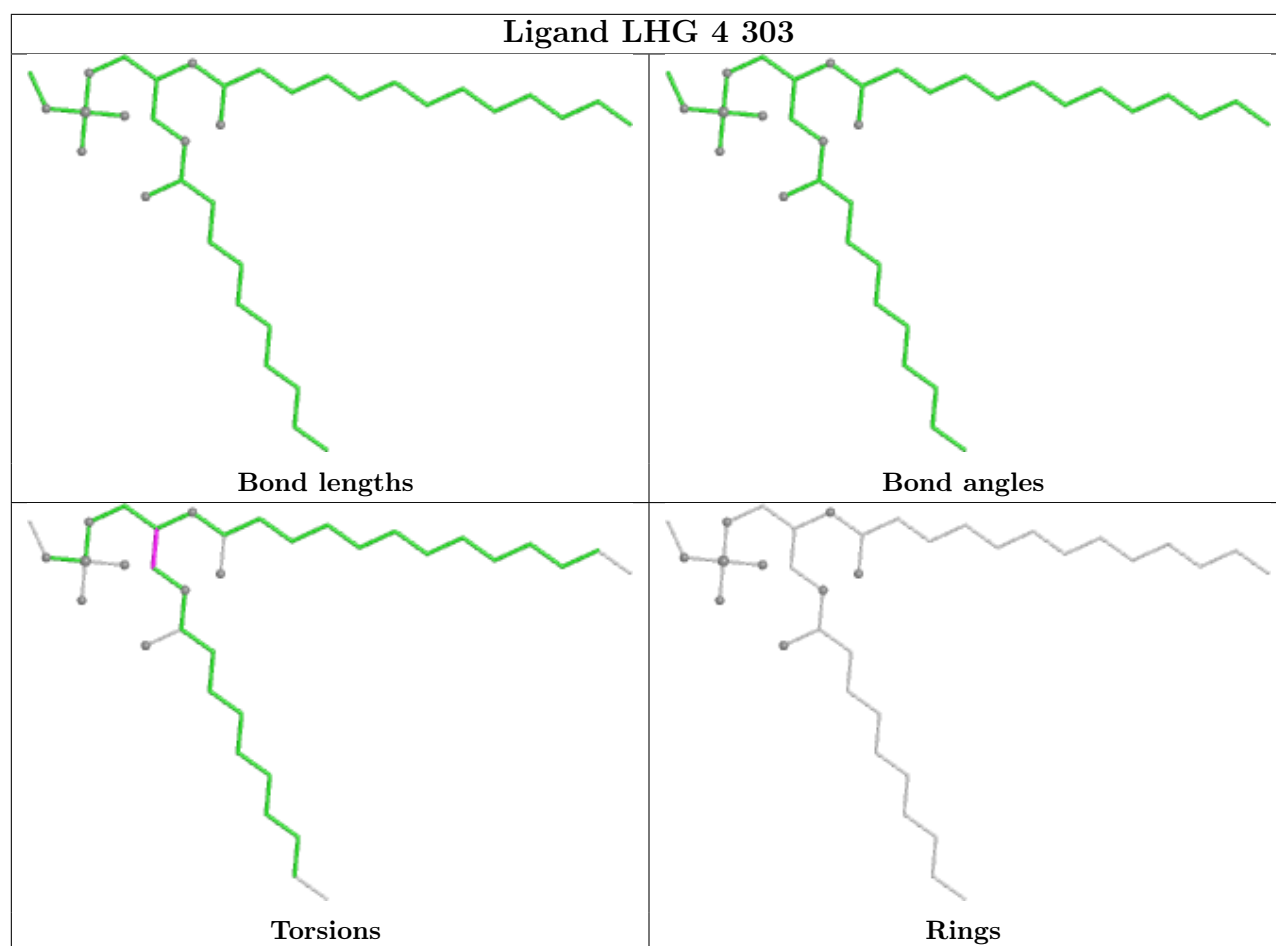
Bond angles

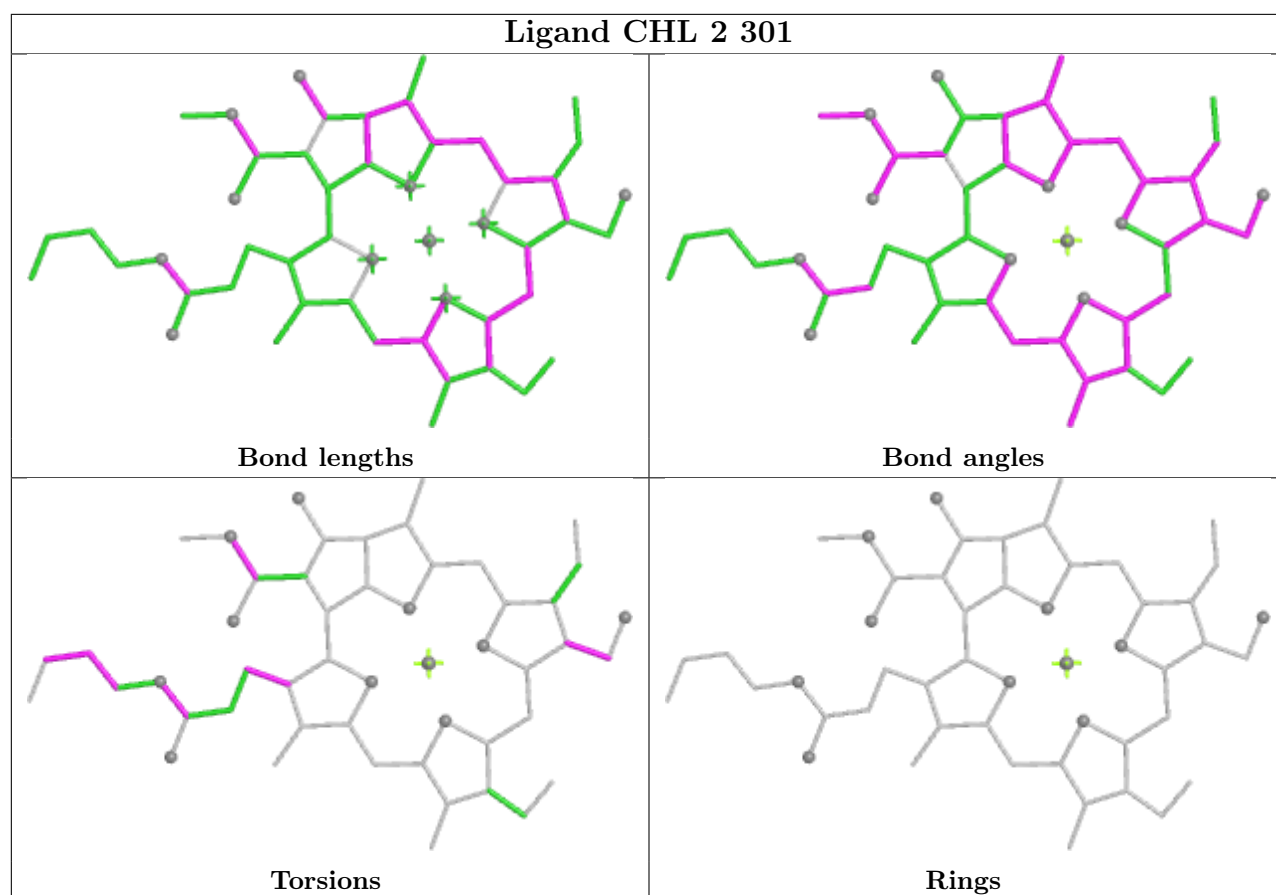


Torsions

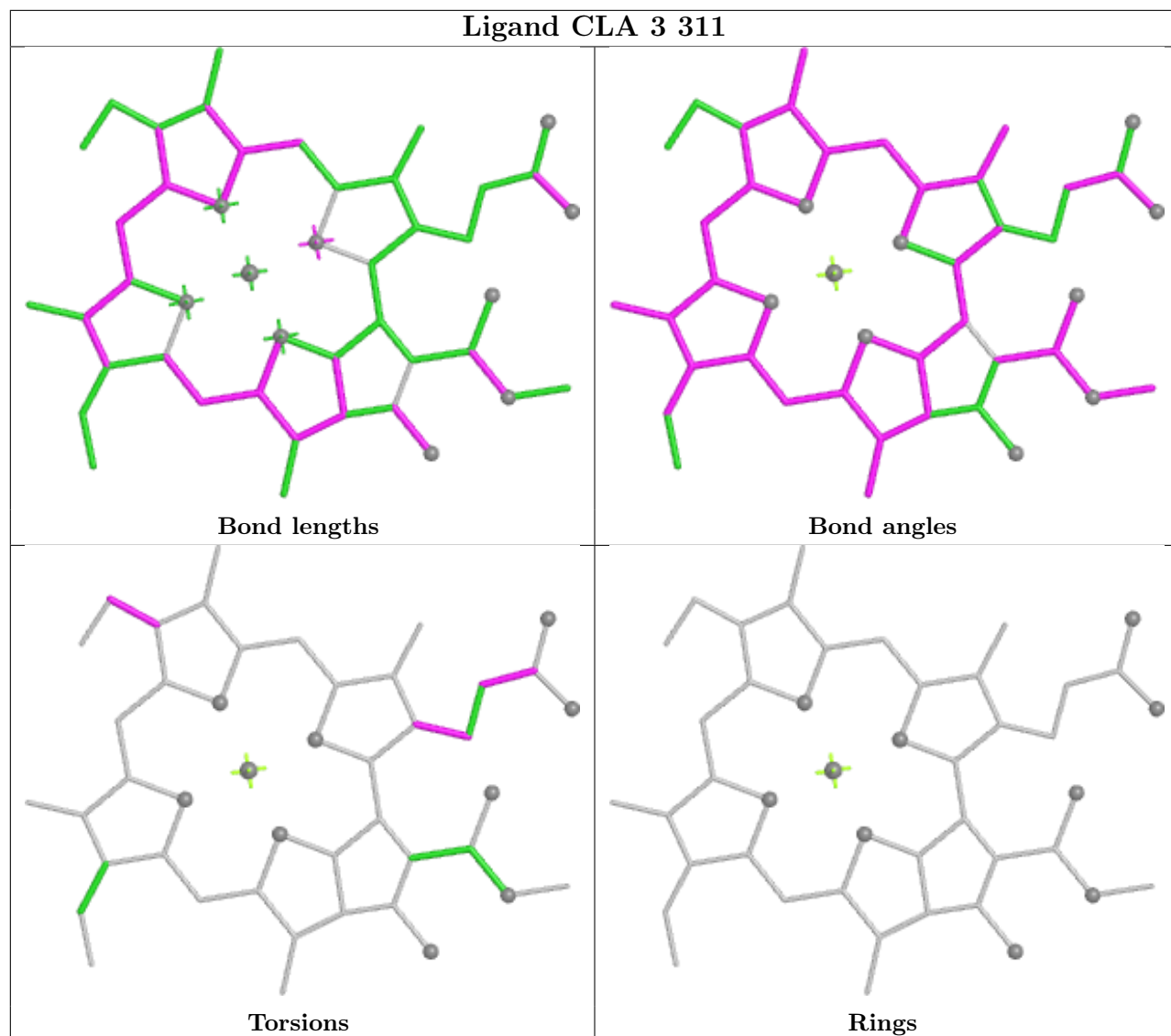


Rings

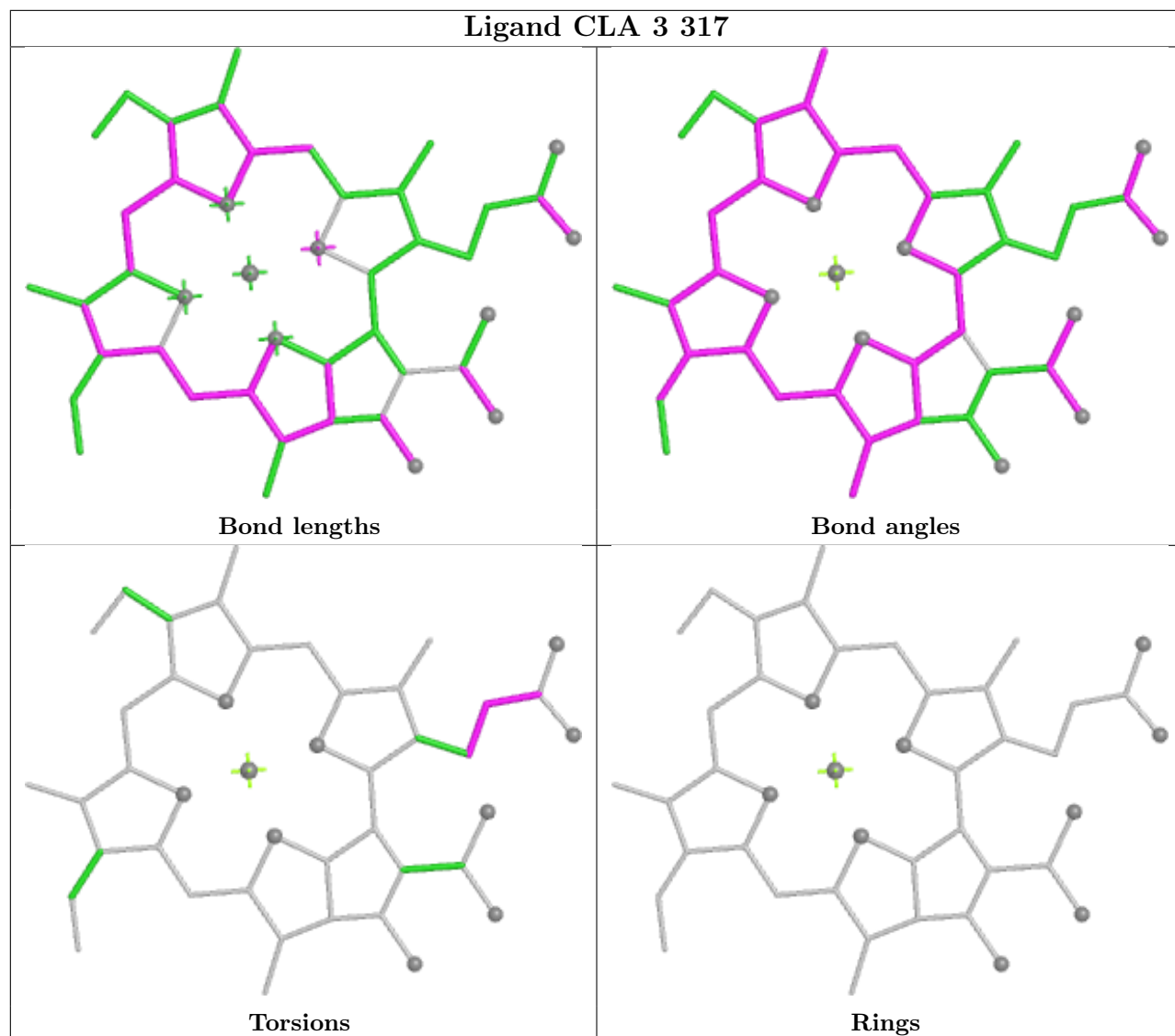




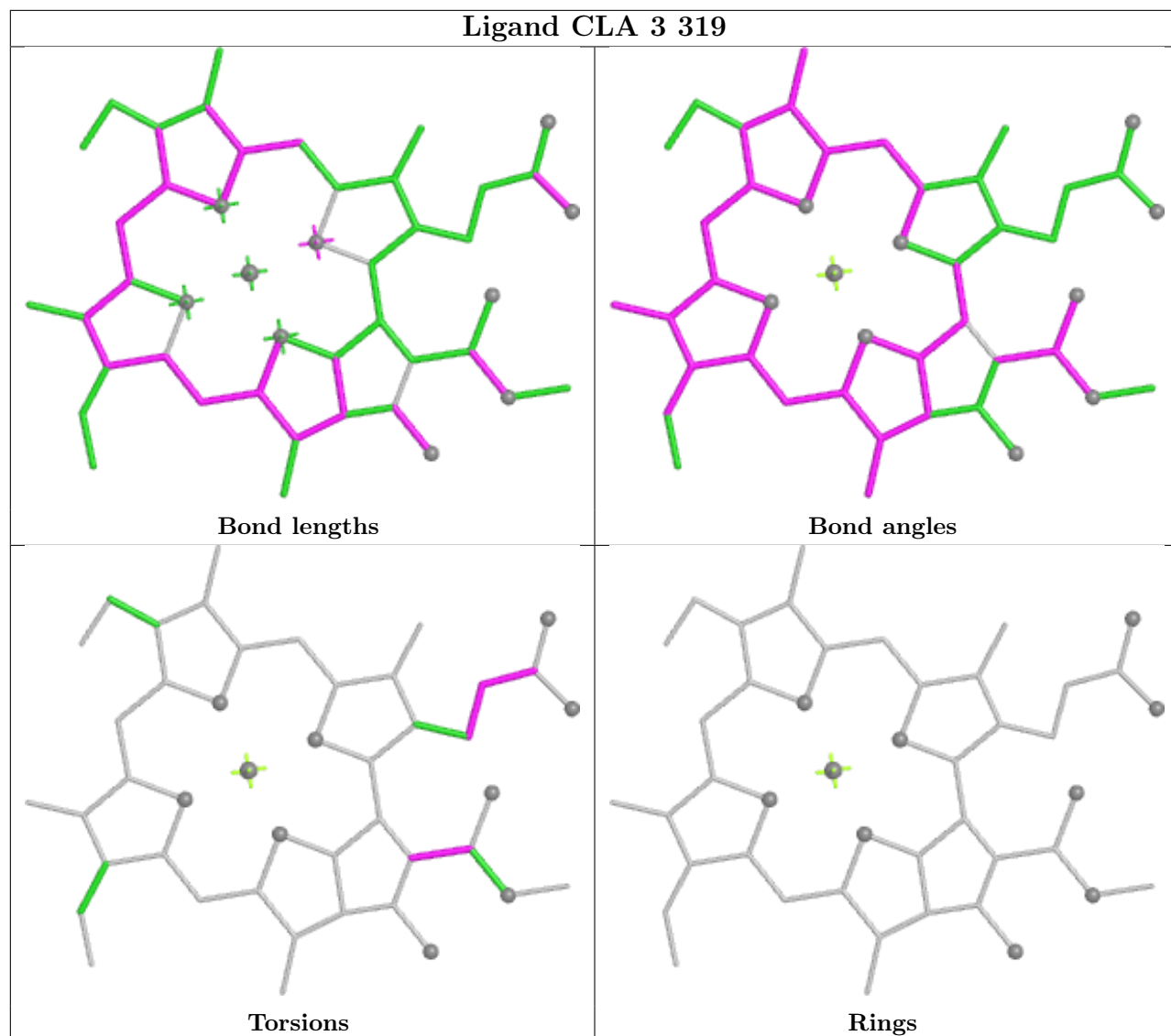
Ligand CLA 3 311



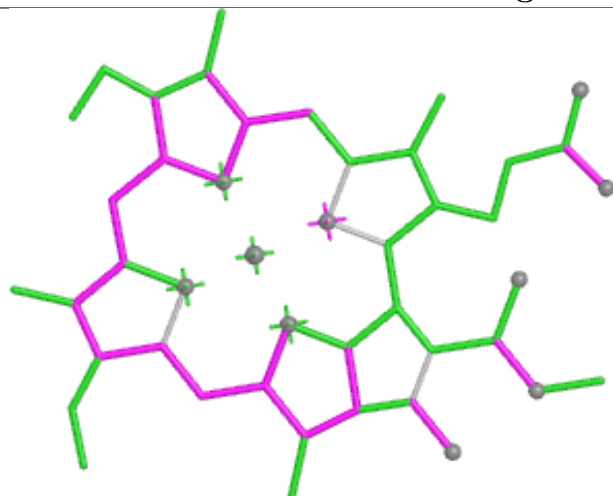
Ligand CLA 3 317



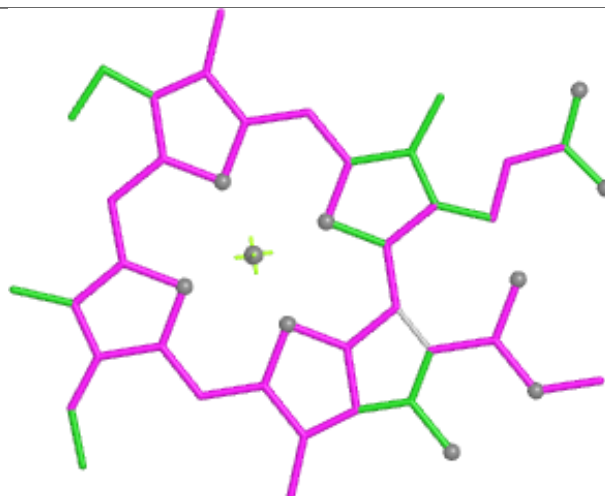
Ligand CLA 3 319



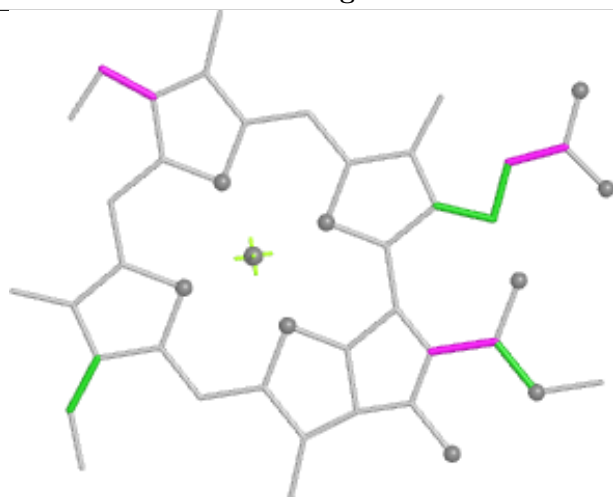
Ligand CLA L 307



Bond lengths



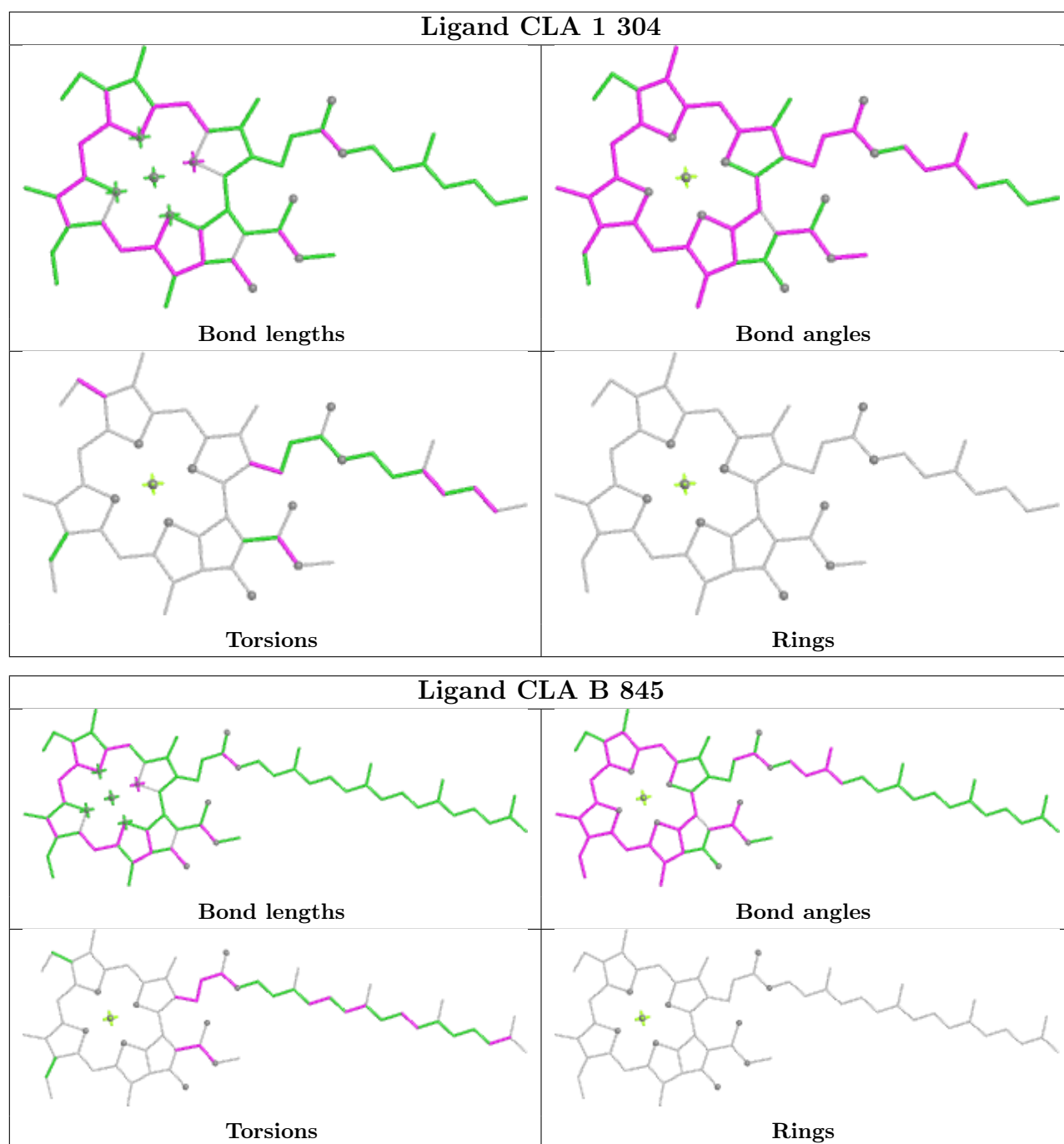
Bond angles



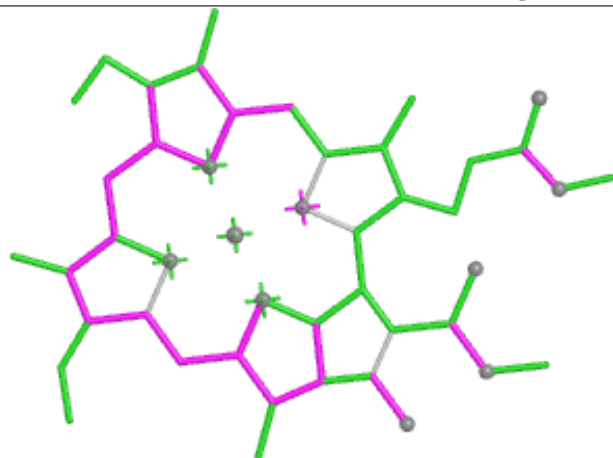
Torsions



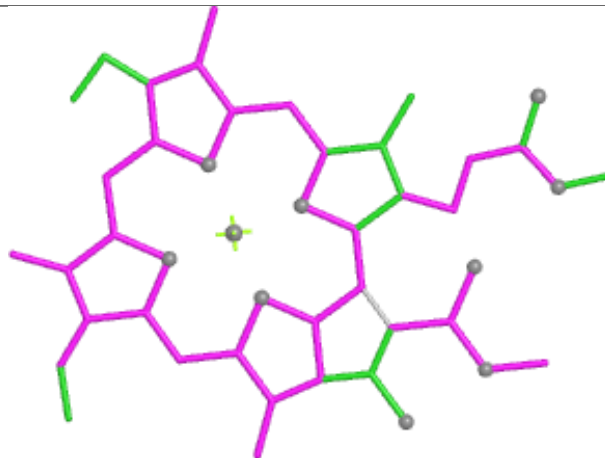
Rings



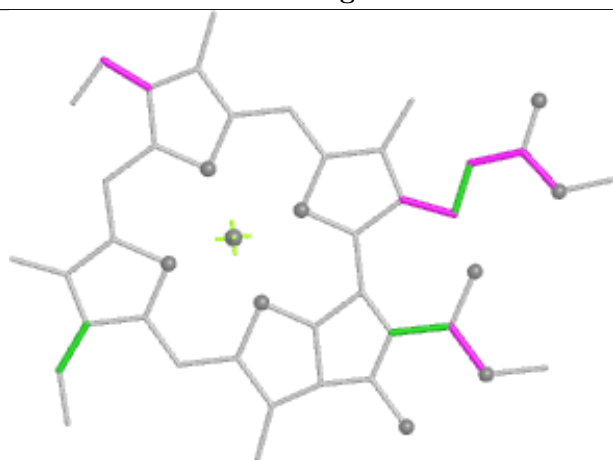
Ligand CLA Y 308



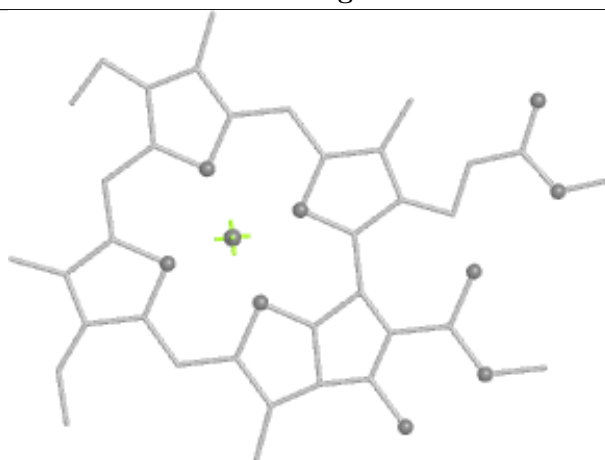
Bond lengths



Bond angles

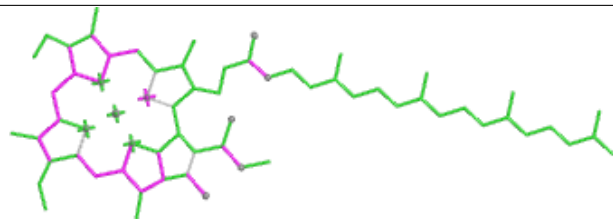


Torsions

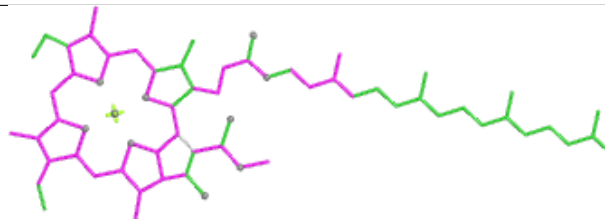


Rings

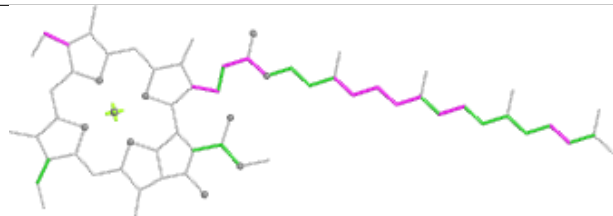
Ligand CLA 3 312



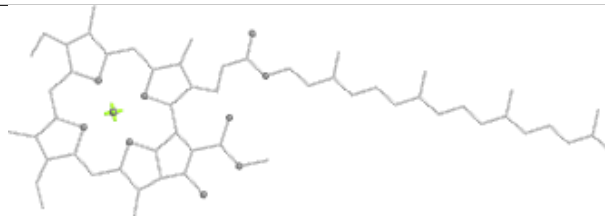
Bond lengths



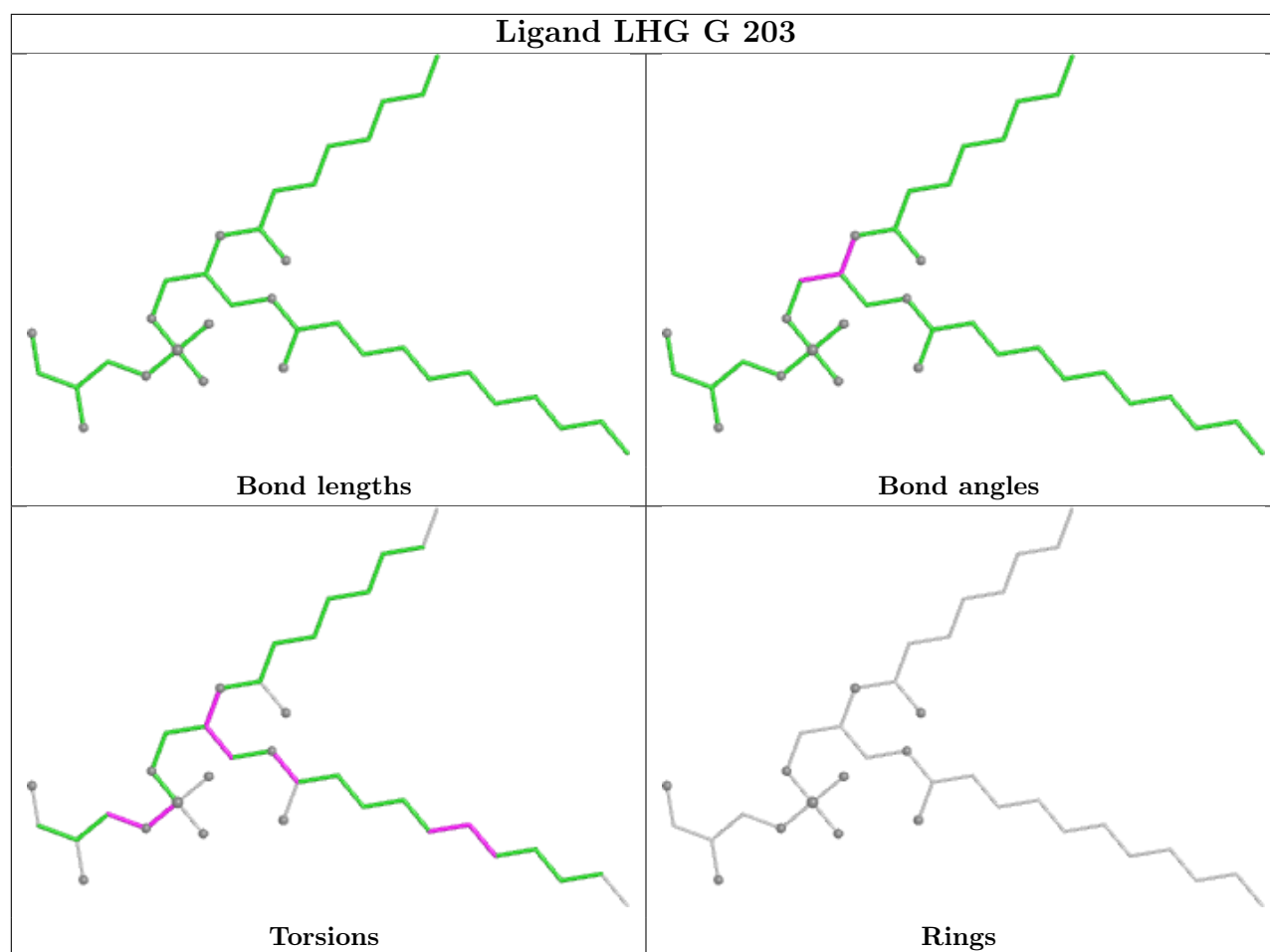
Bond angles



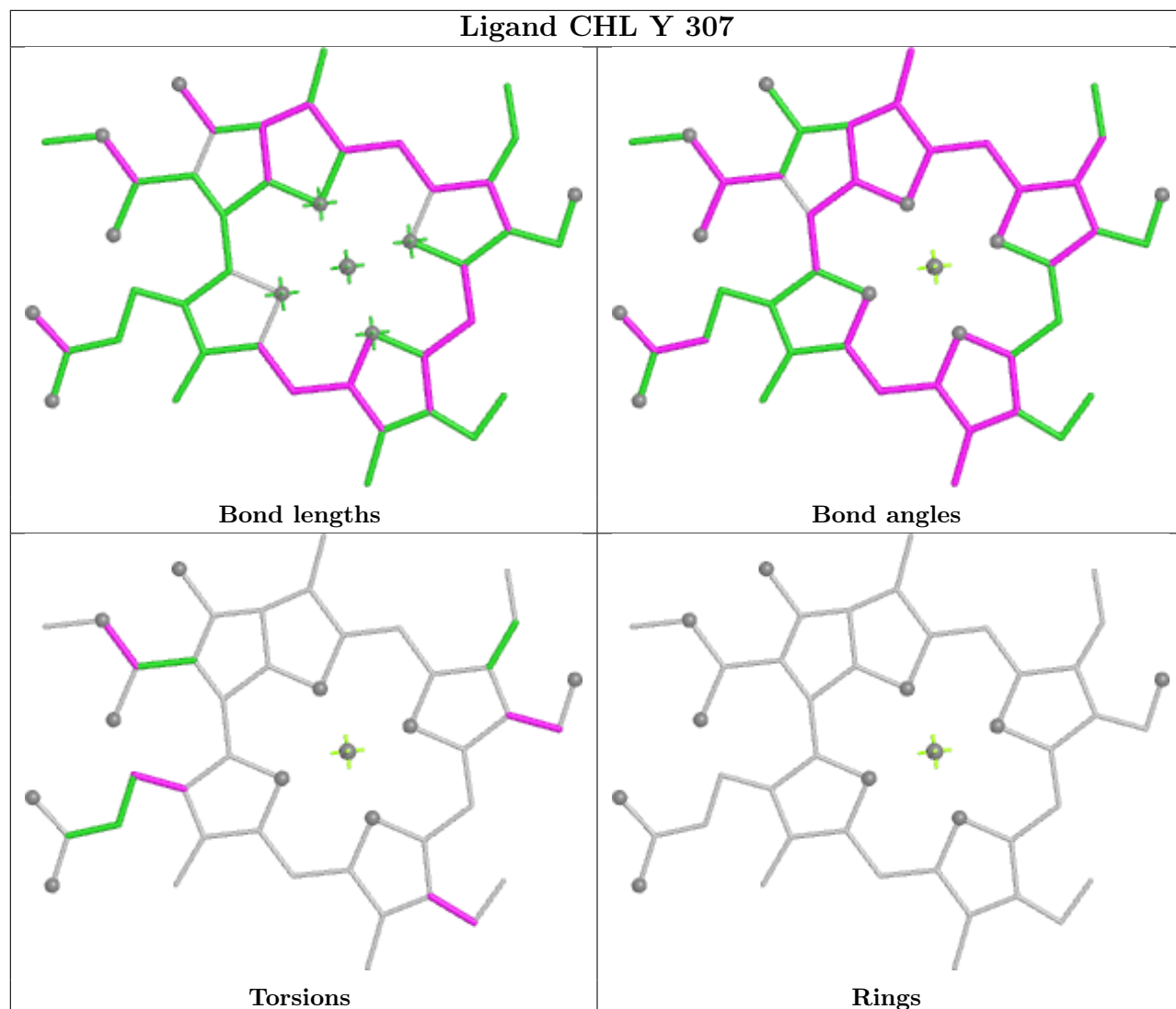
Torsions

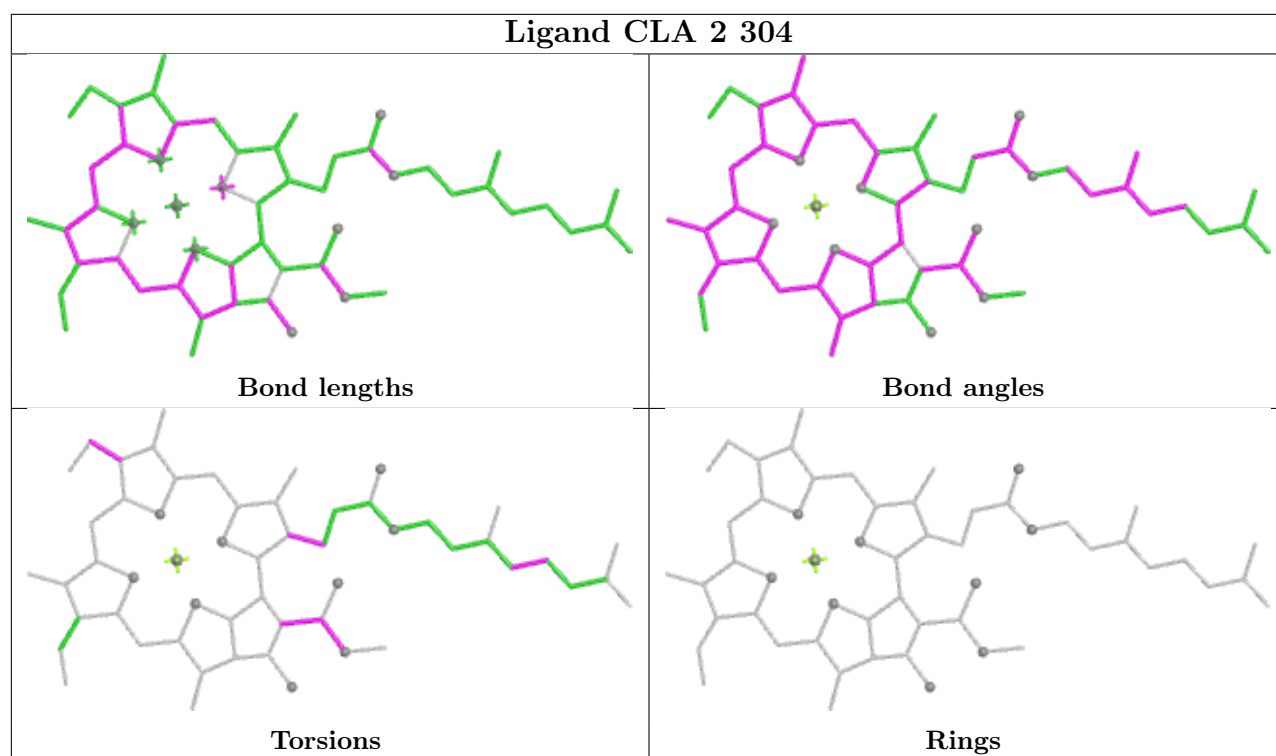


Rings

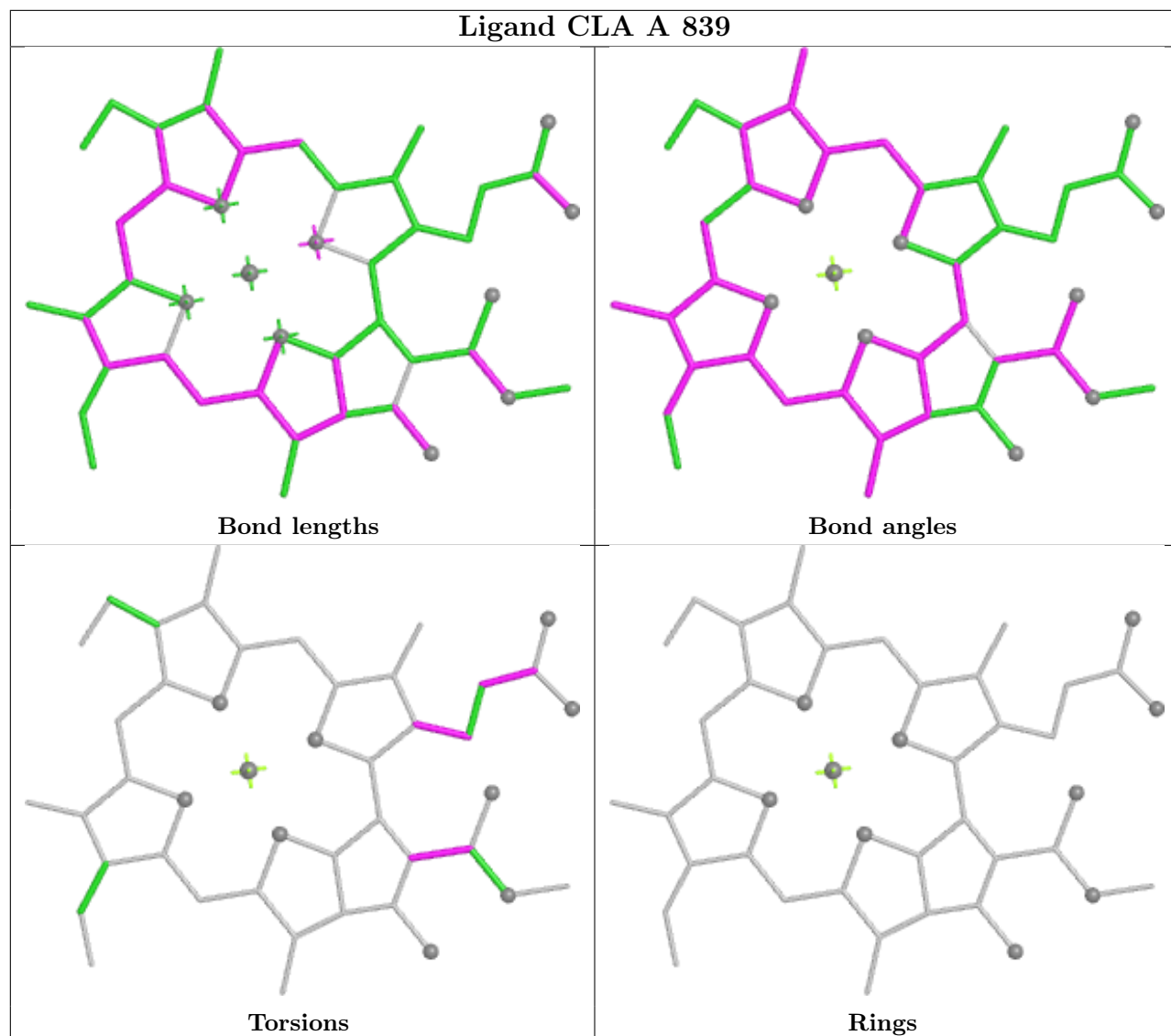


Ligand CHL Y 307

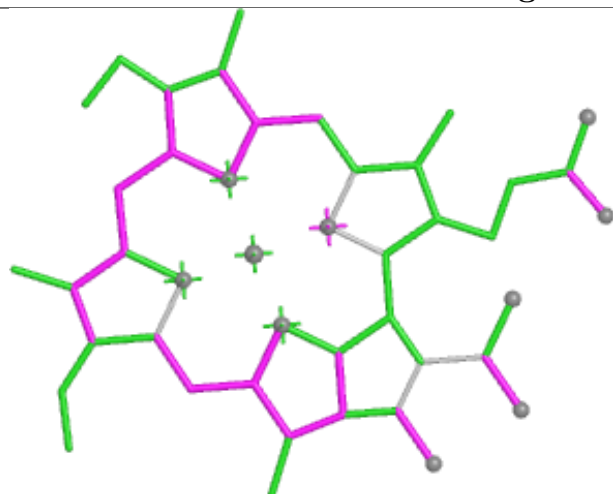




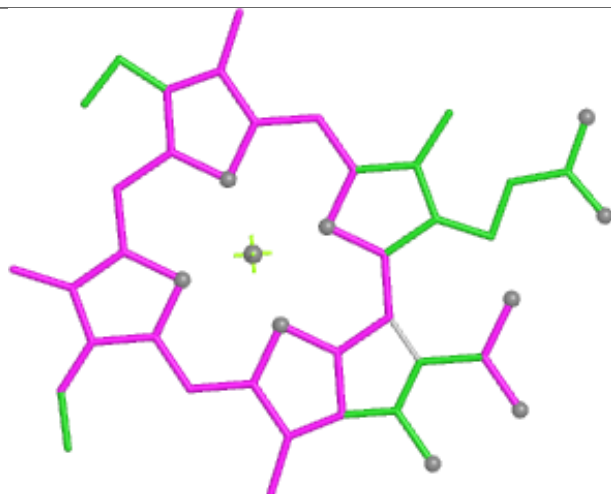
Ligand CLA A 839



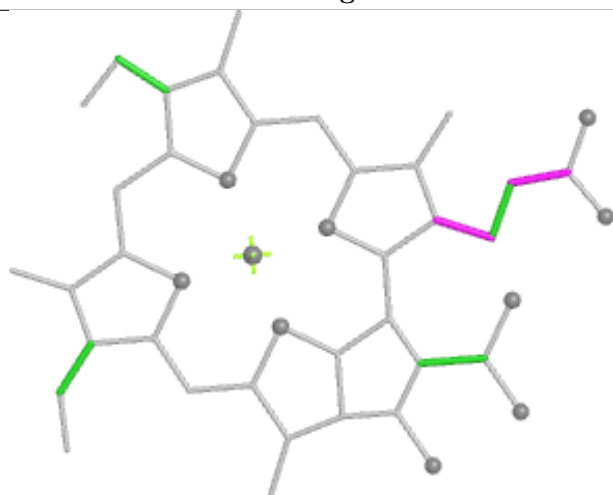
Ligand CLA 1 306



Bond lengths



Bond angles

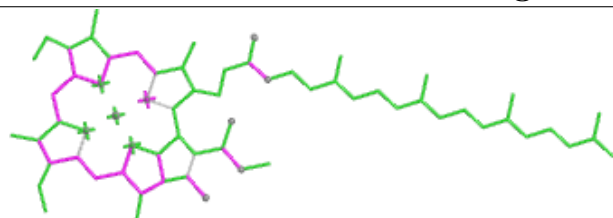


Torsions

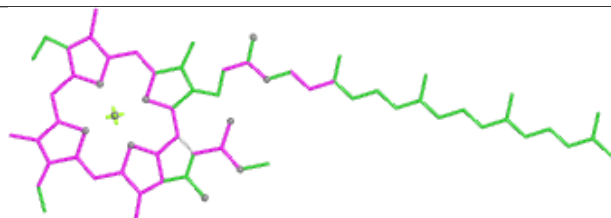


Rings

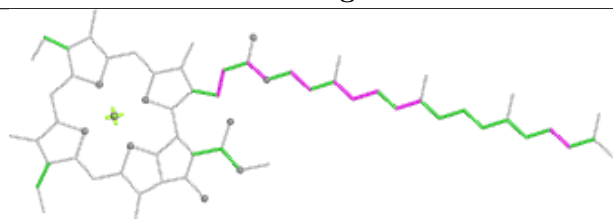
Ligand CLA A 844



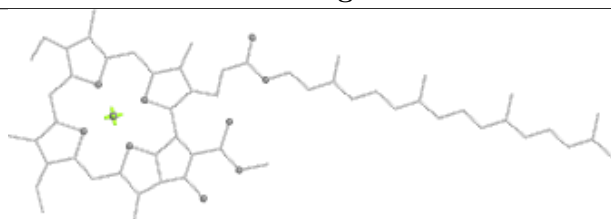
Bond lengths



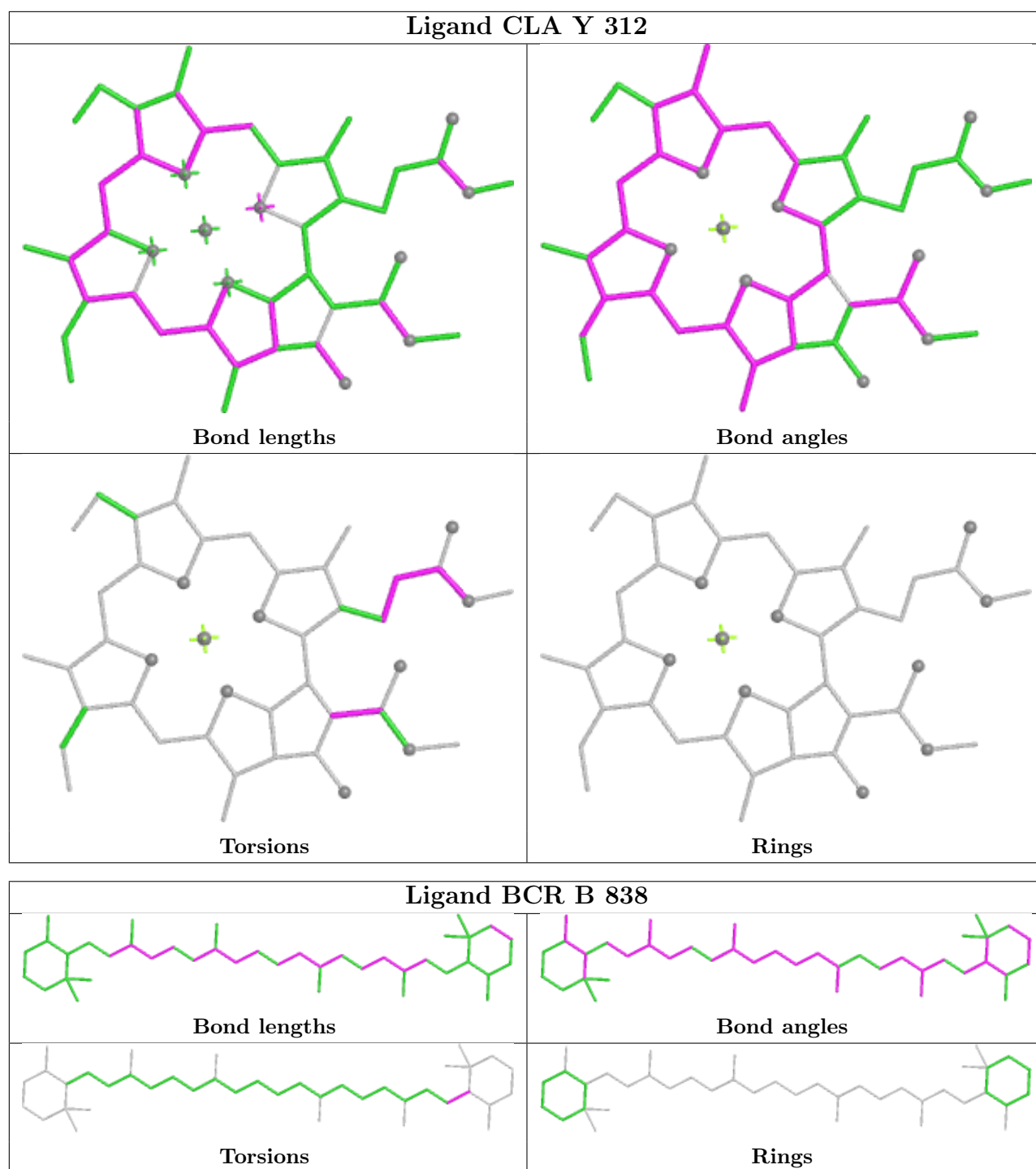
Bond angles



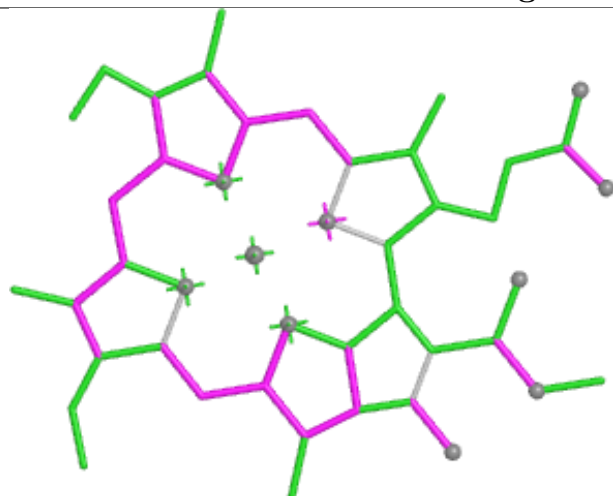
Torsions



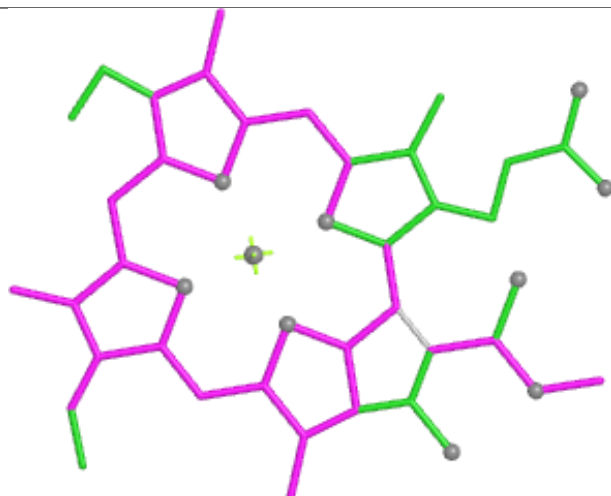
Rings



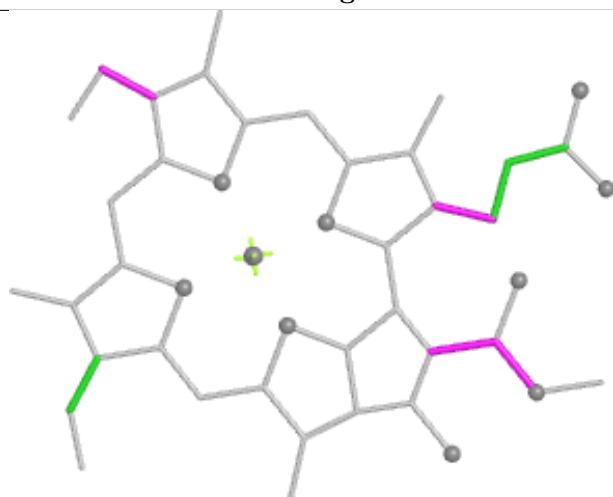
Ligand CLA 3 316



Bond lengths



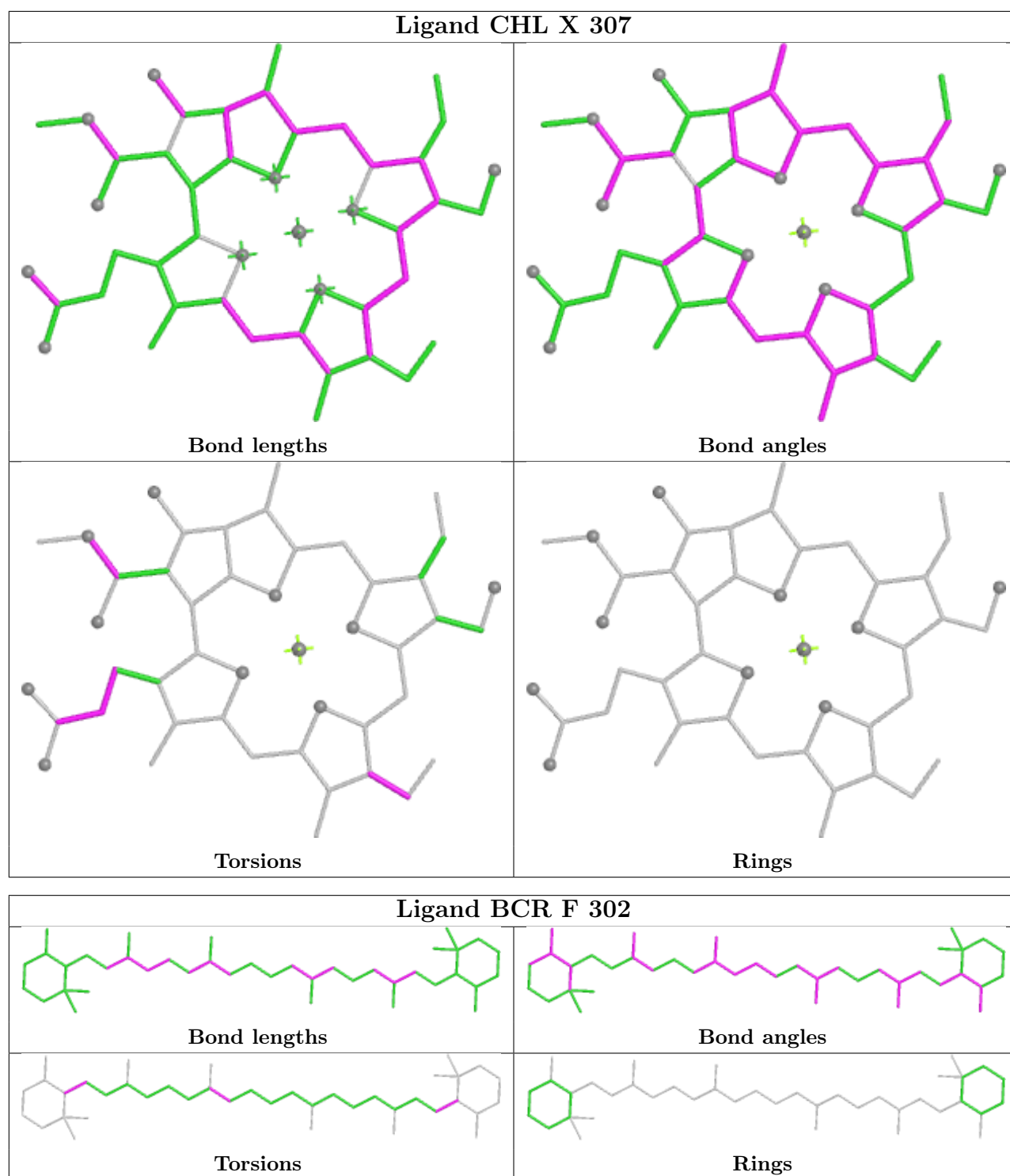
Bond angles

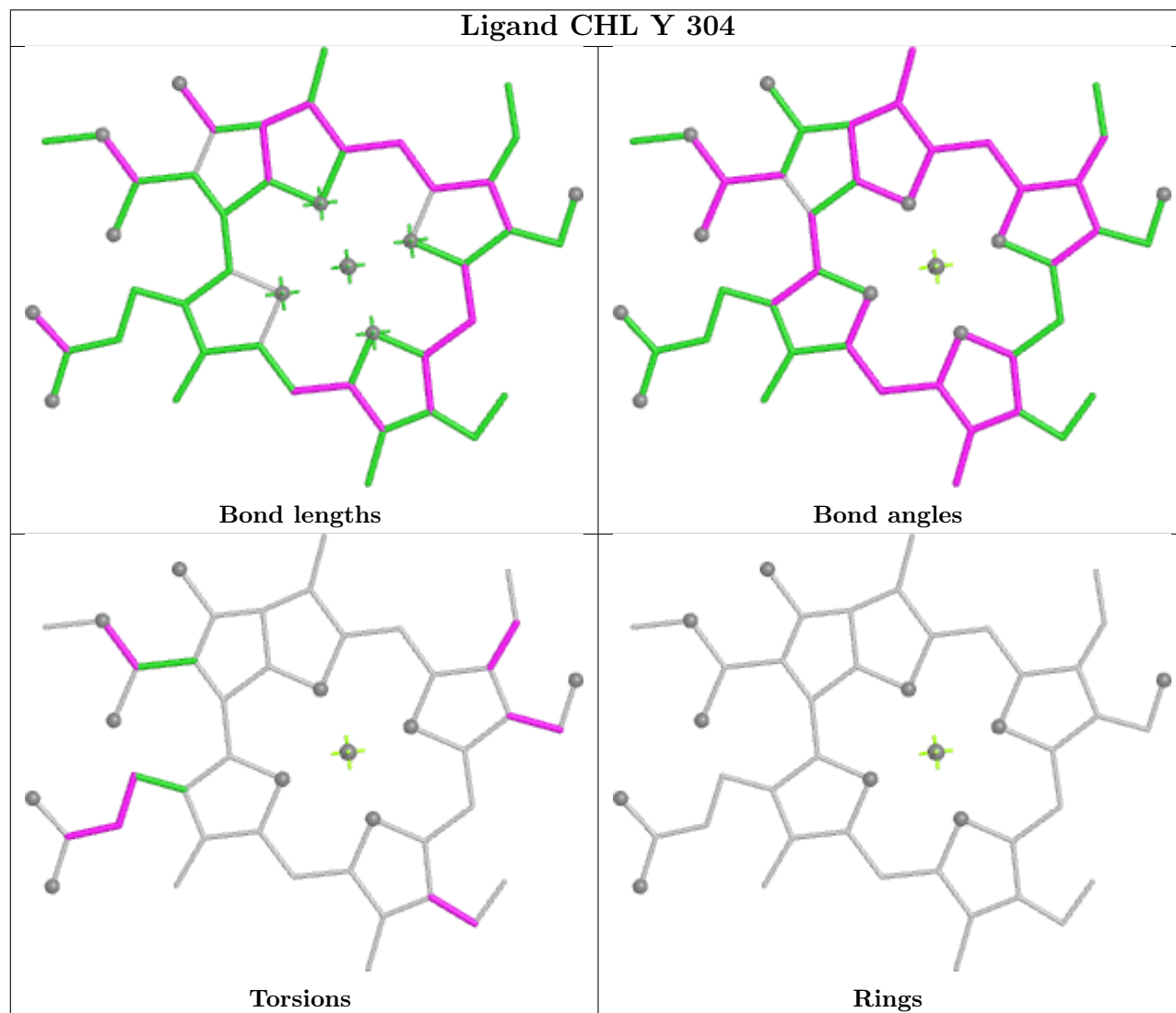
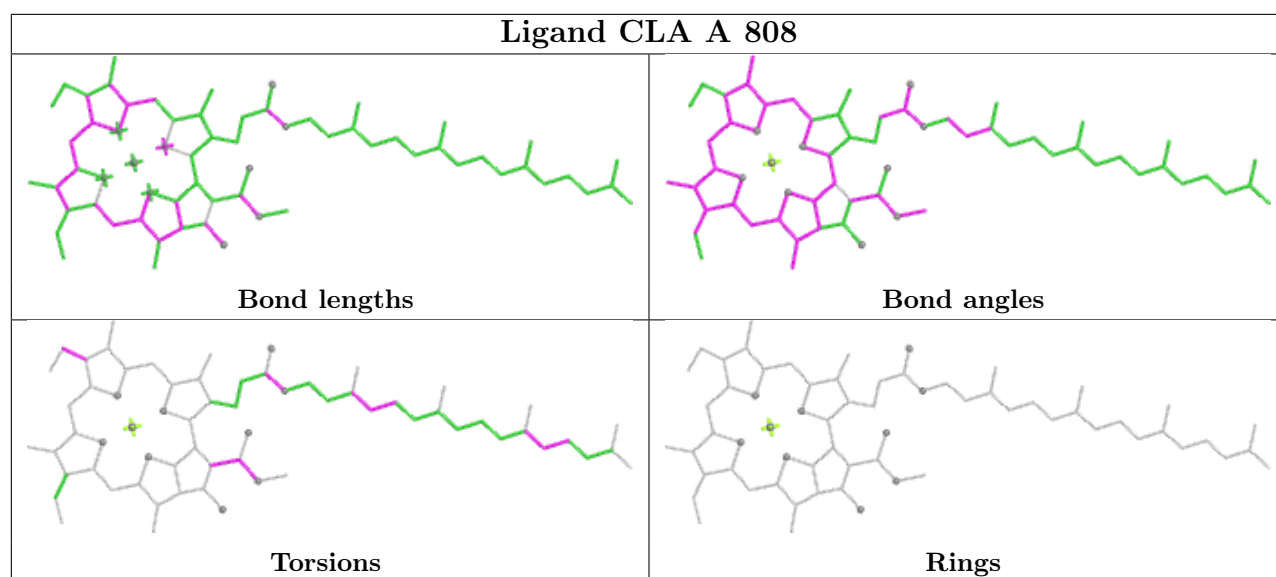


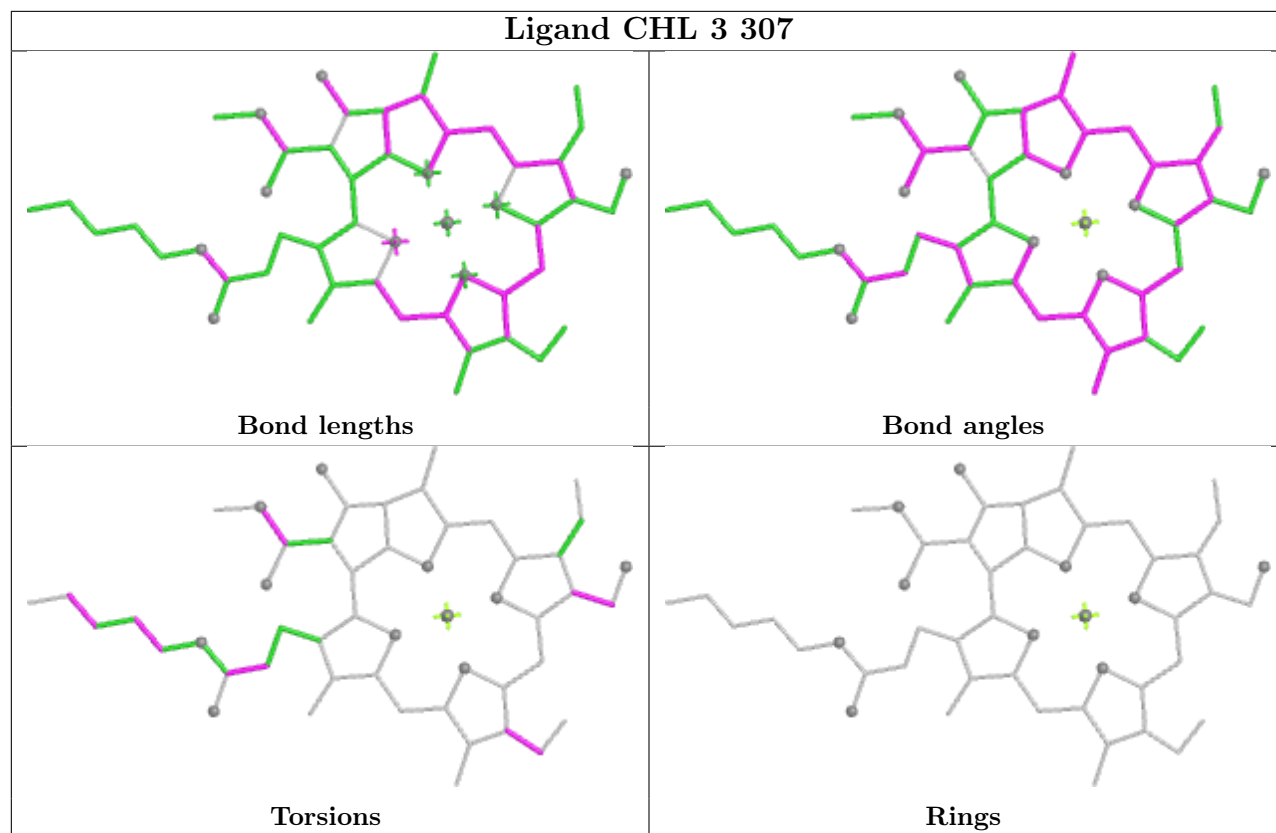
Torsions



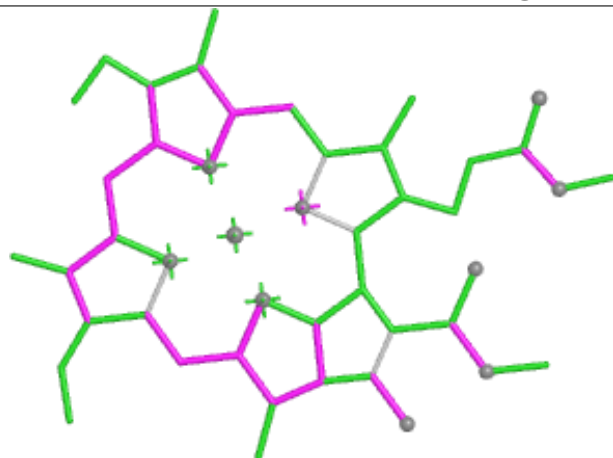
Rings



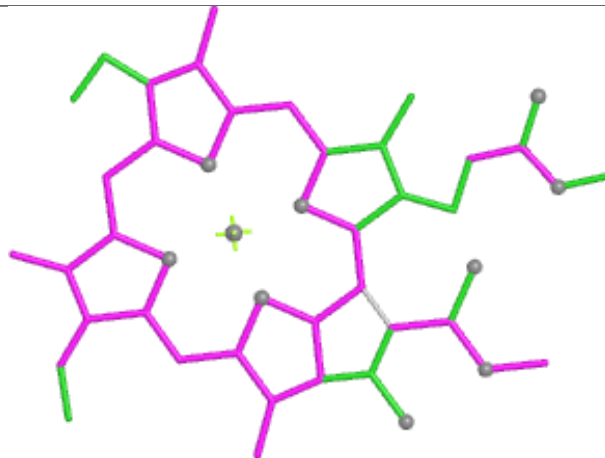




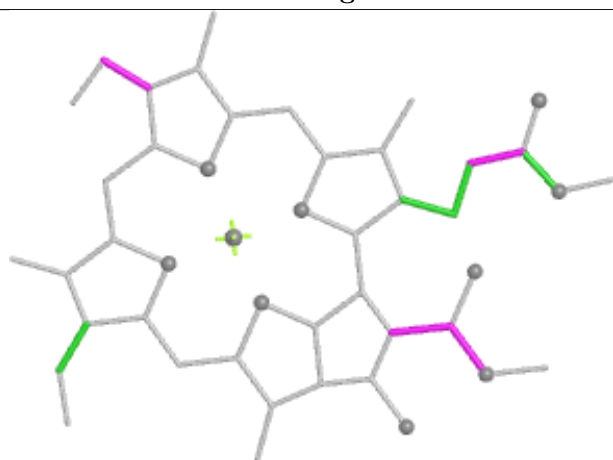
Ligand CLA F 306



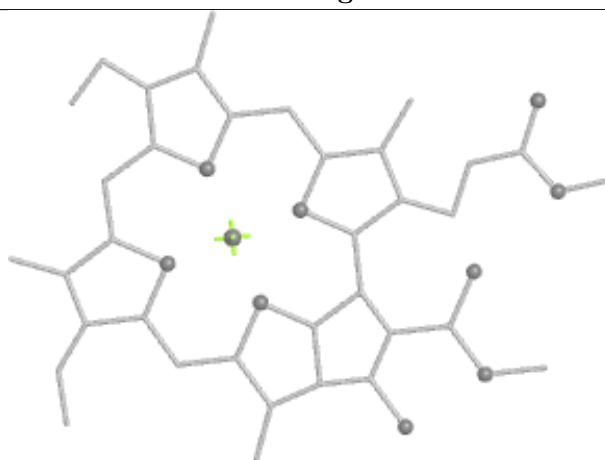
Bond lengths



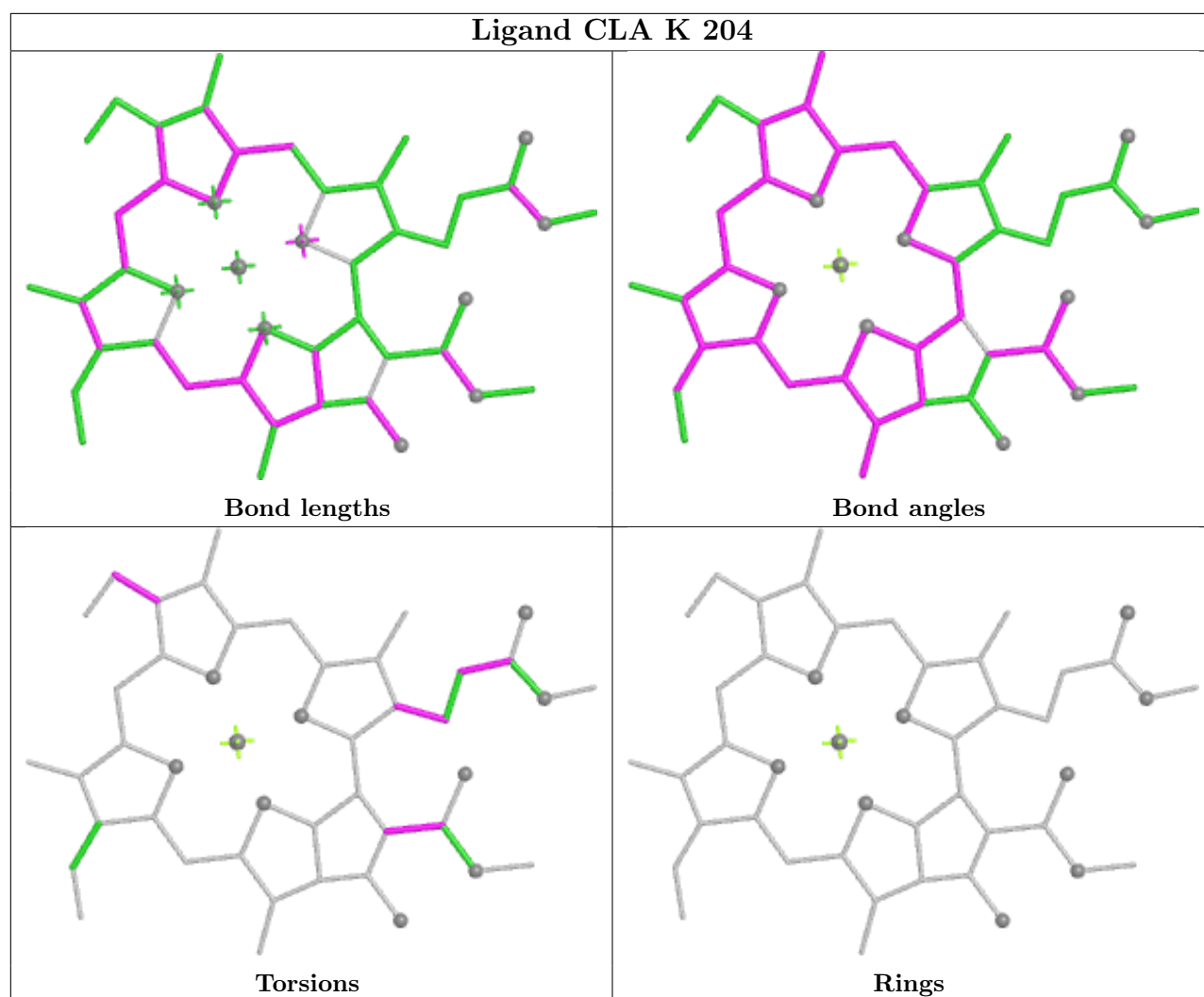
Bond angles



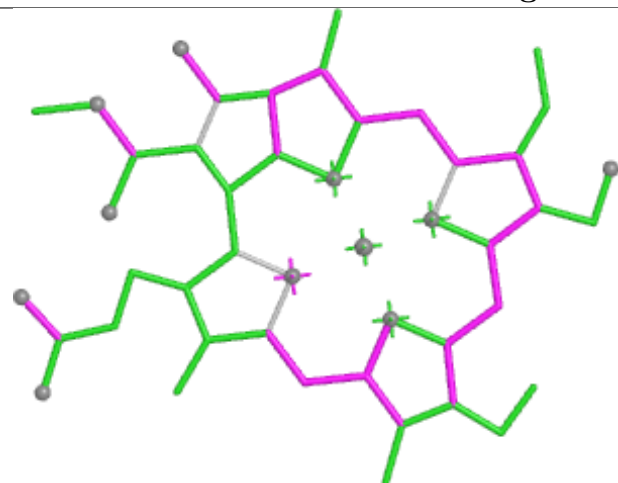
Torsions



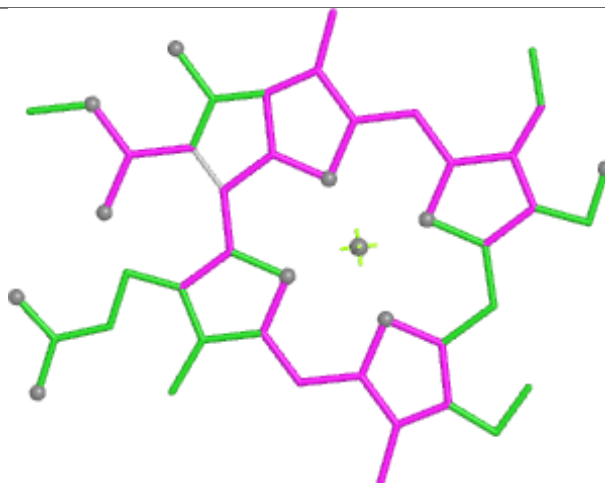
Rings



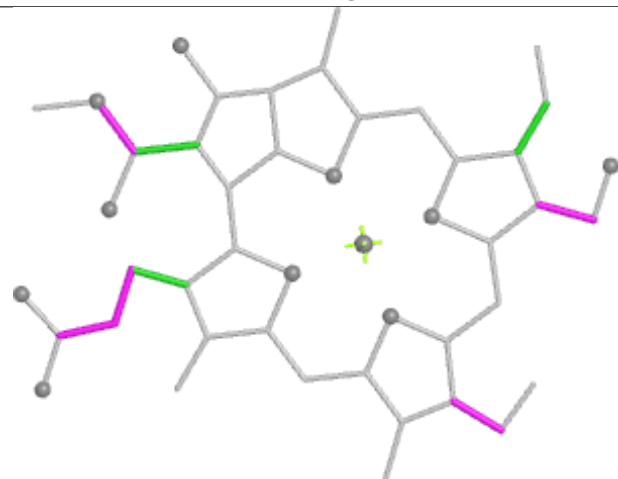
Ligand CHL Z 303



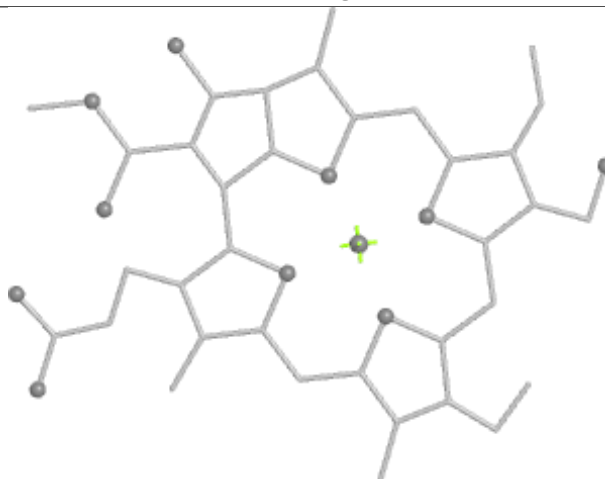
Bond lengths



Bond angles

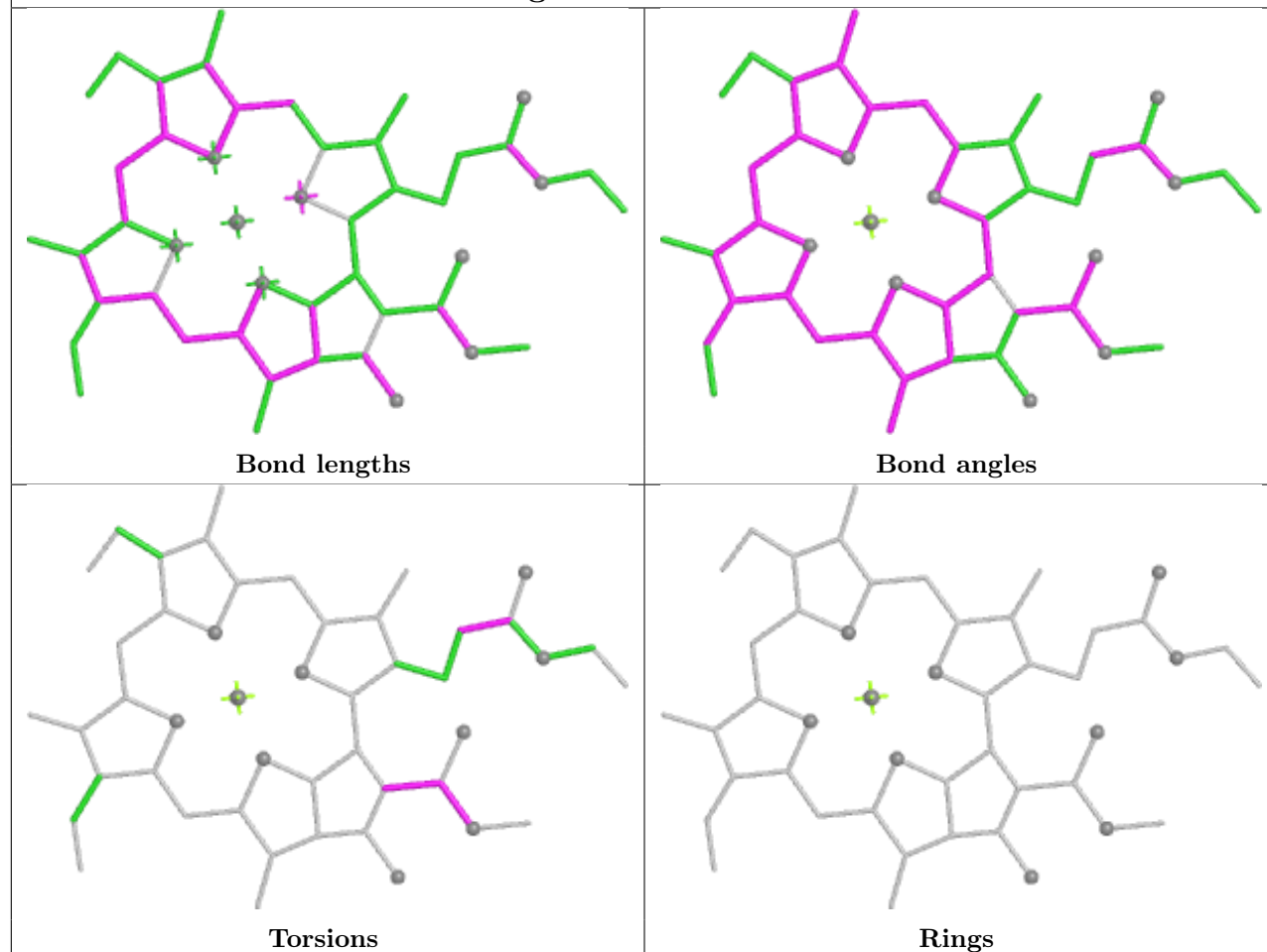


Torsions

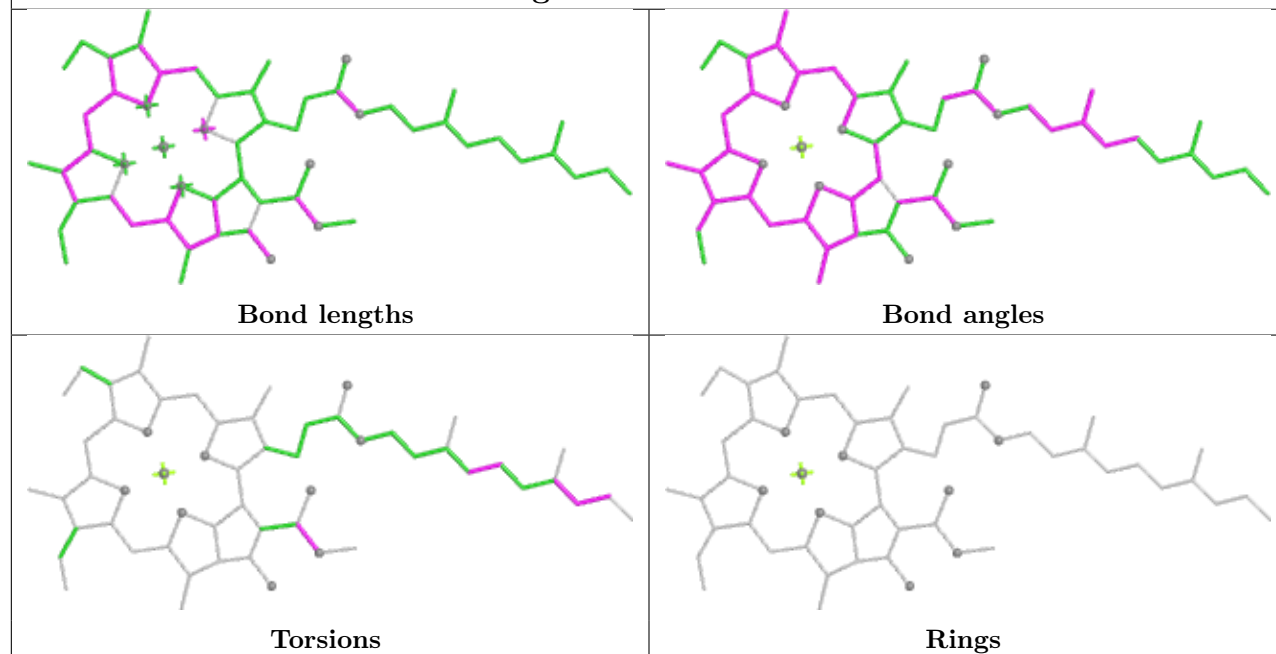


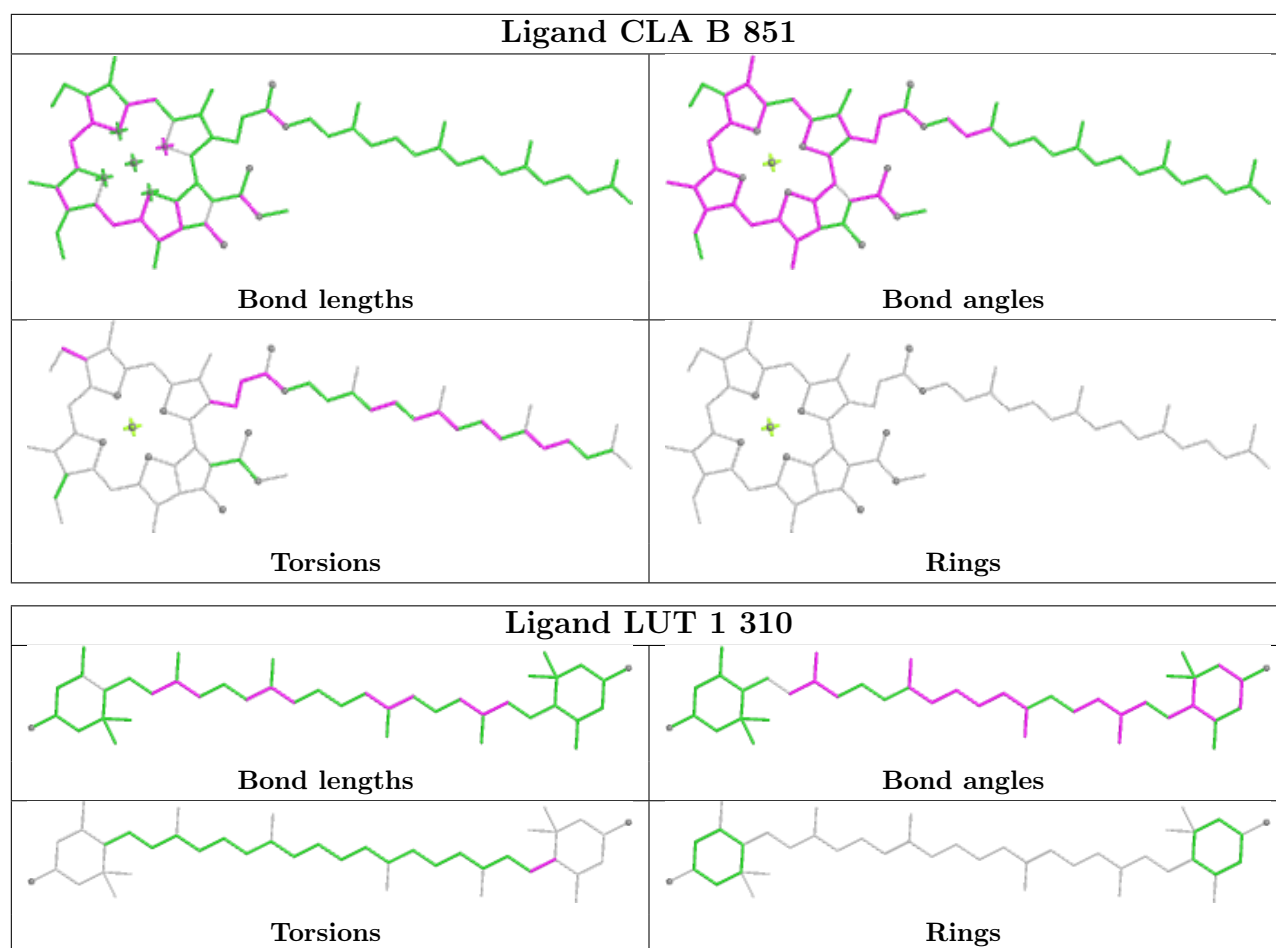
Rings

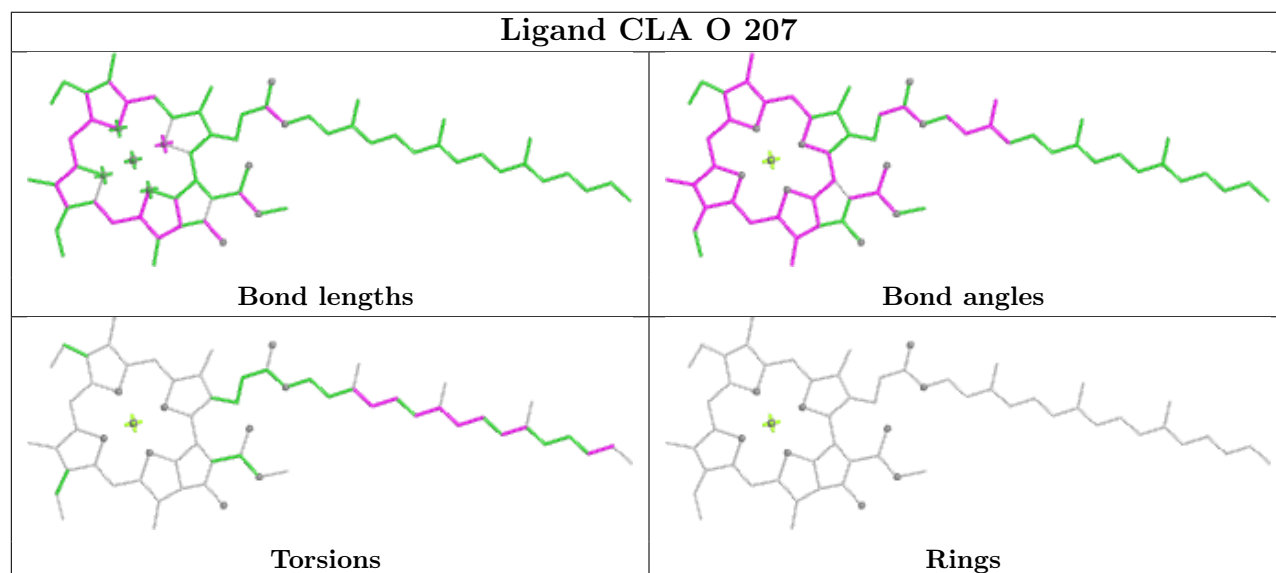
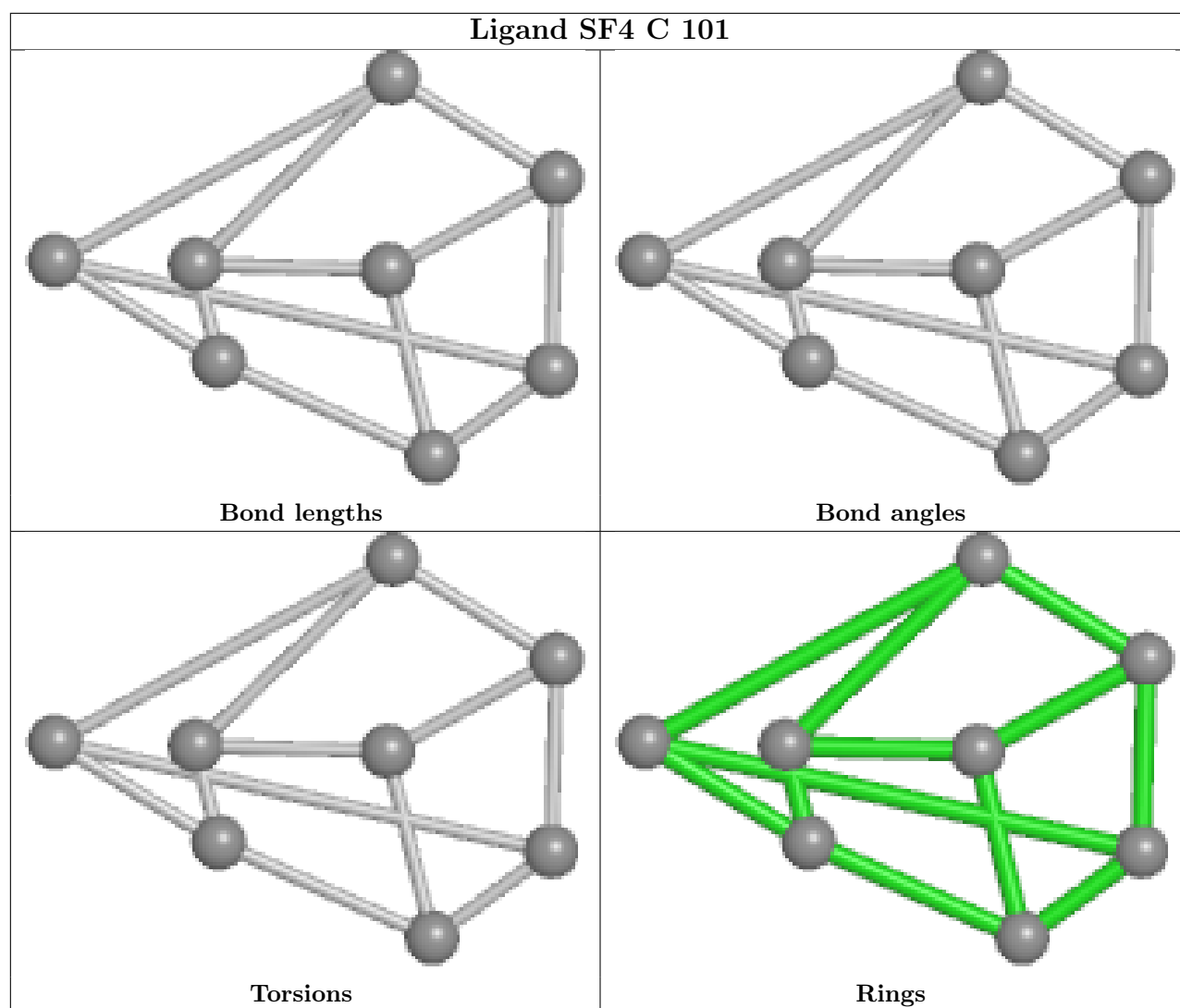
Ligand CLA B 828

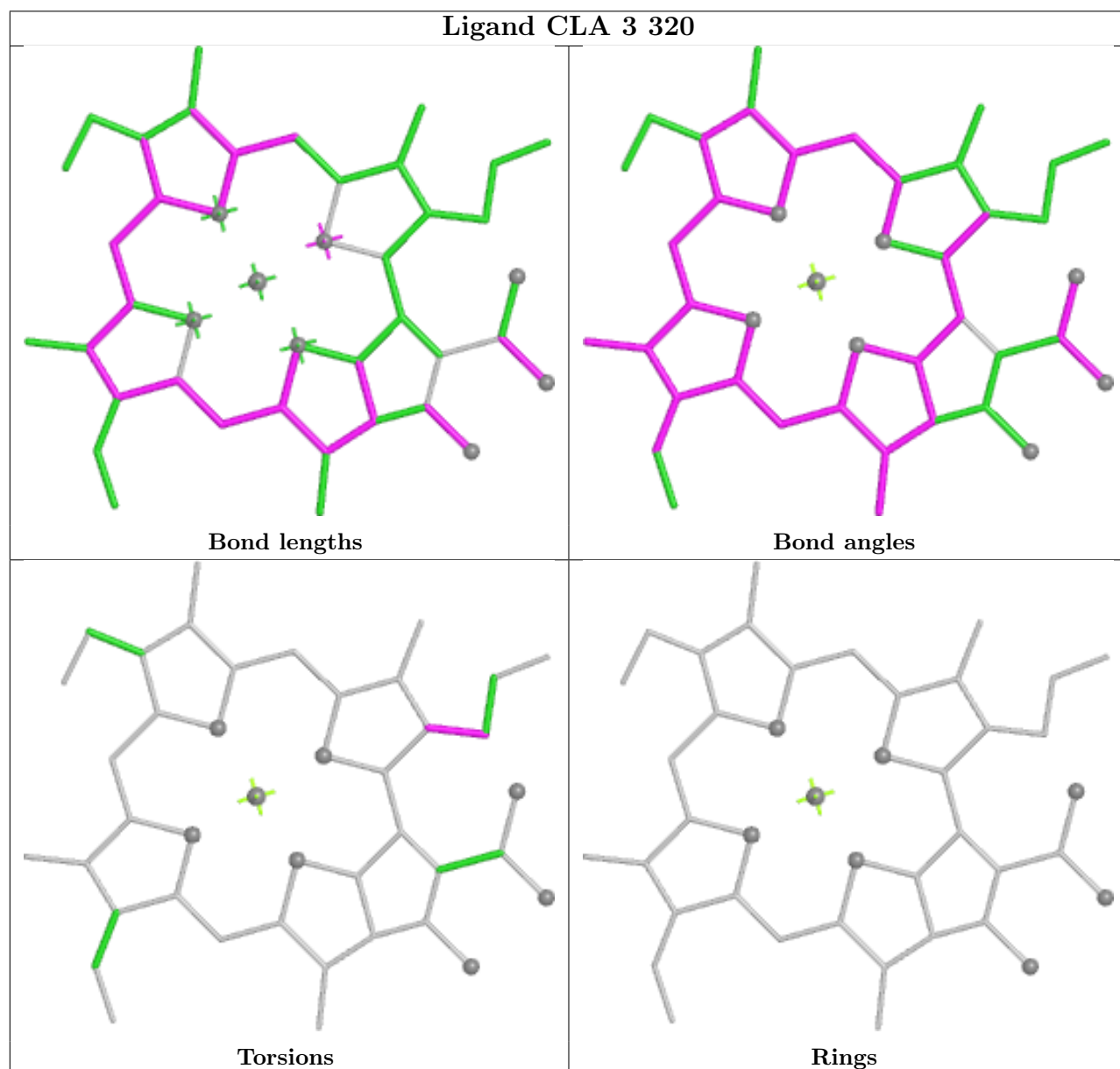
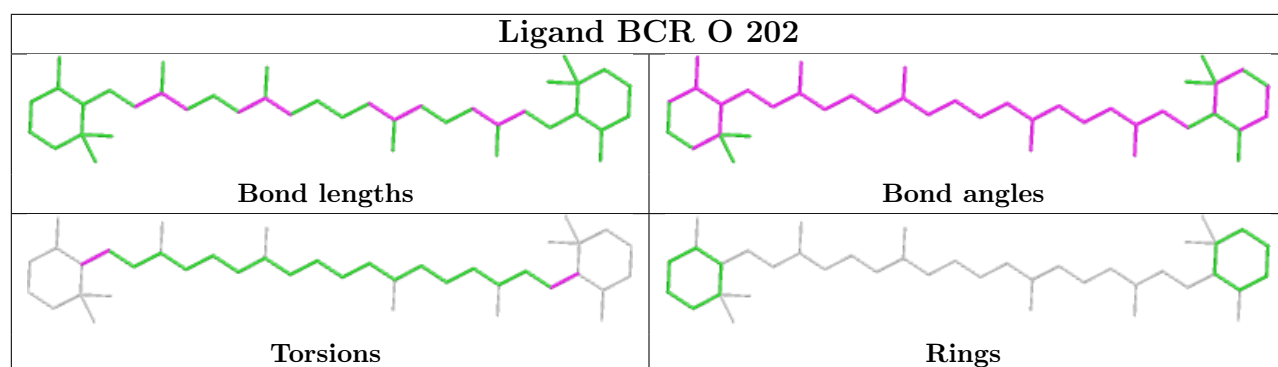


Ligand CLA B 848

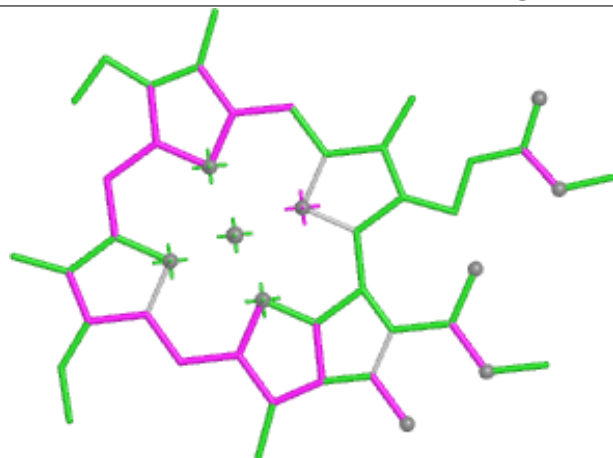




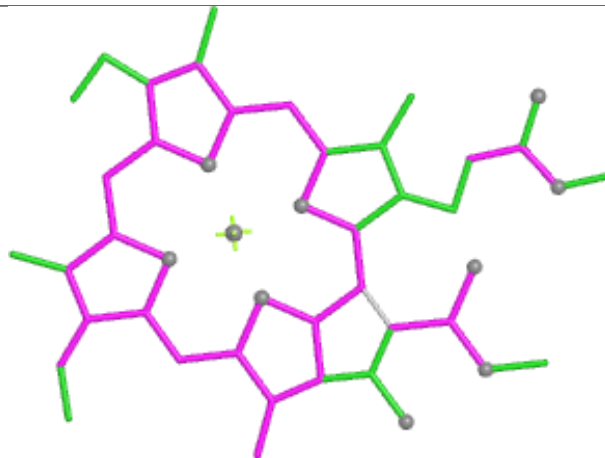




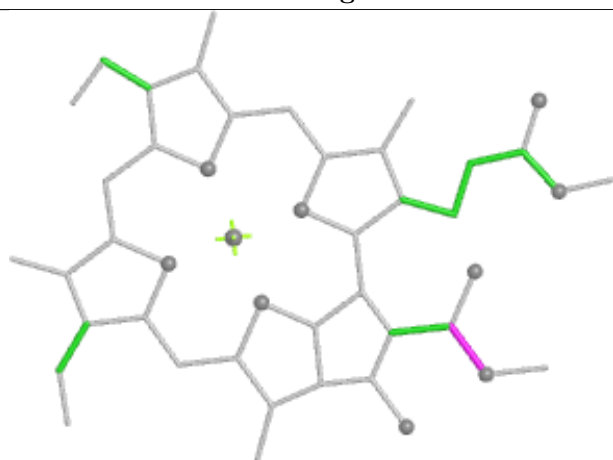
Ligand CLA A 841



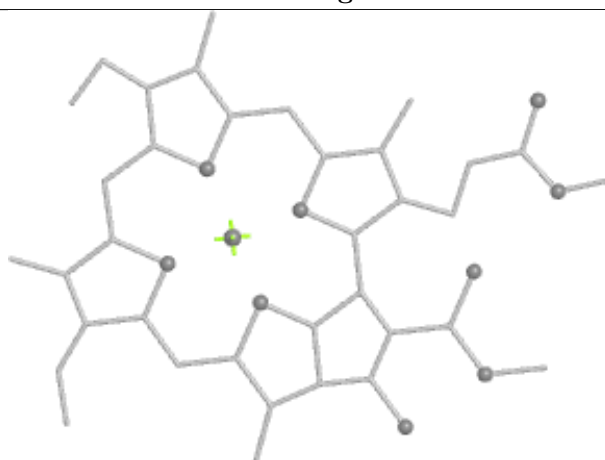
Bond lengths



Bond angles

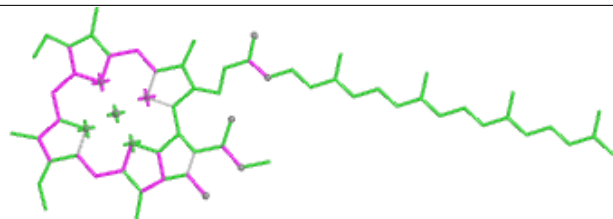


Torsions

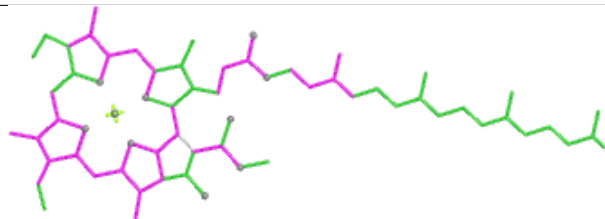


Rings

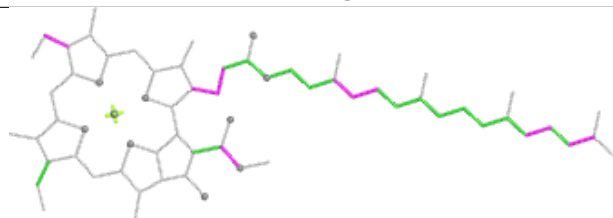
Ligand CLA A 827



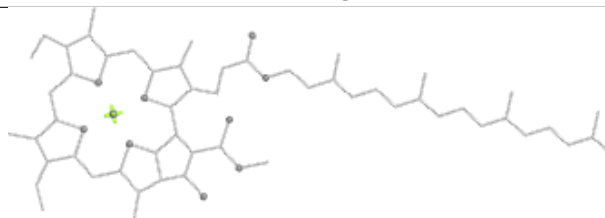
Bond lengths



Bond angles

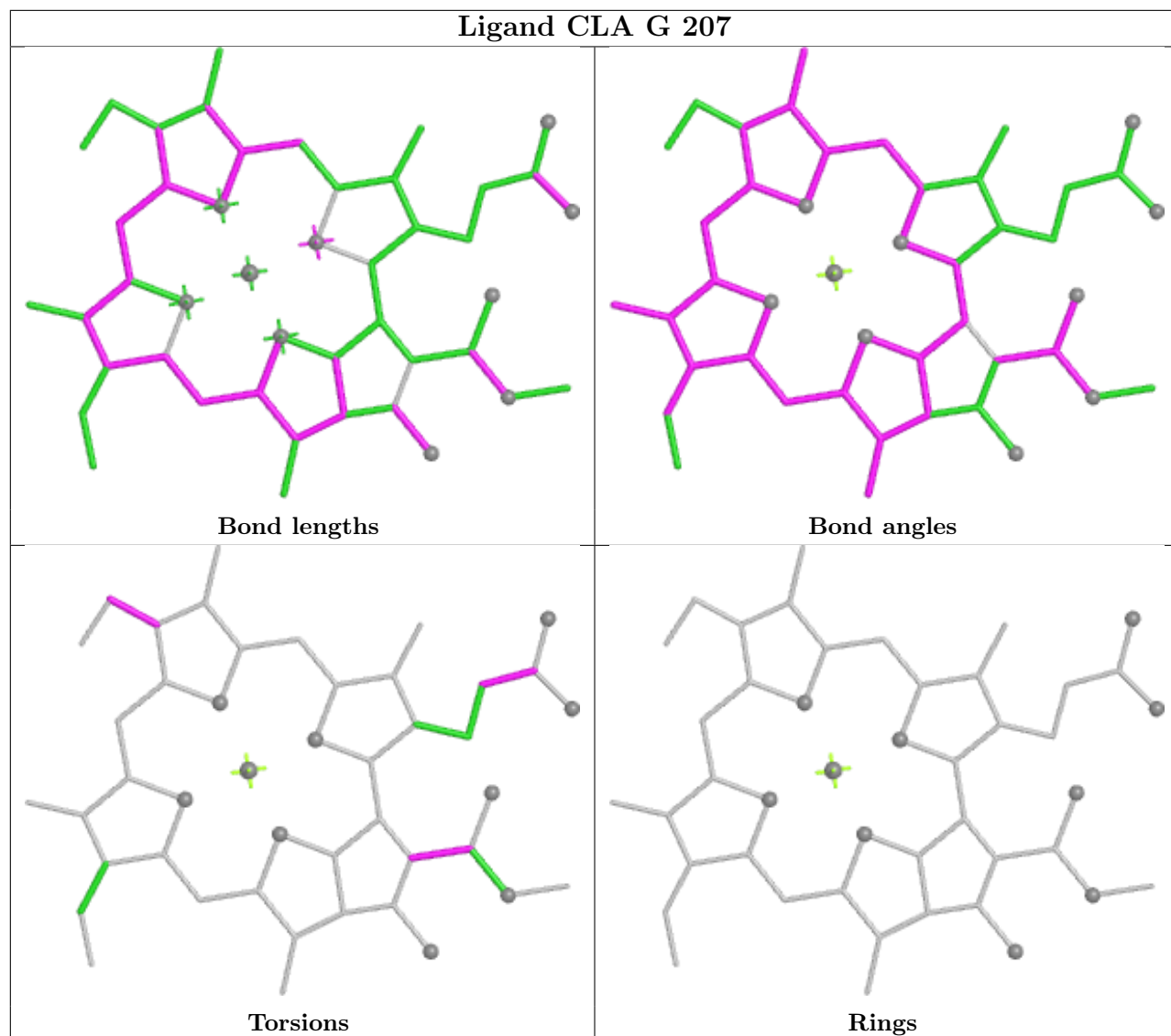


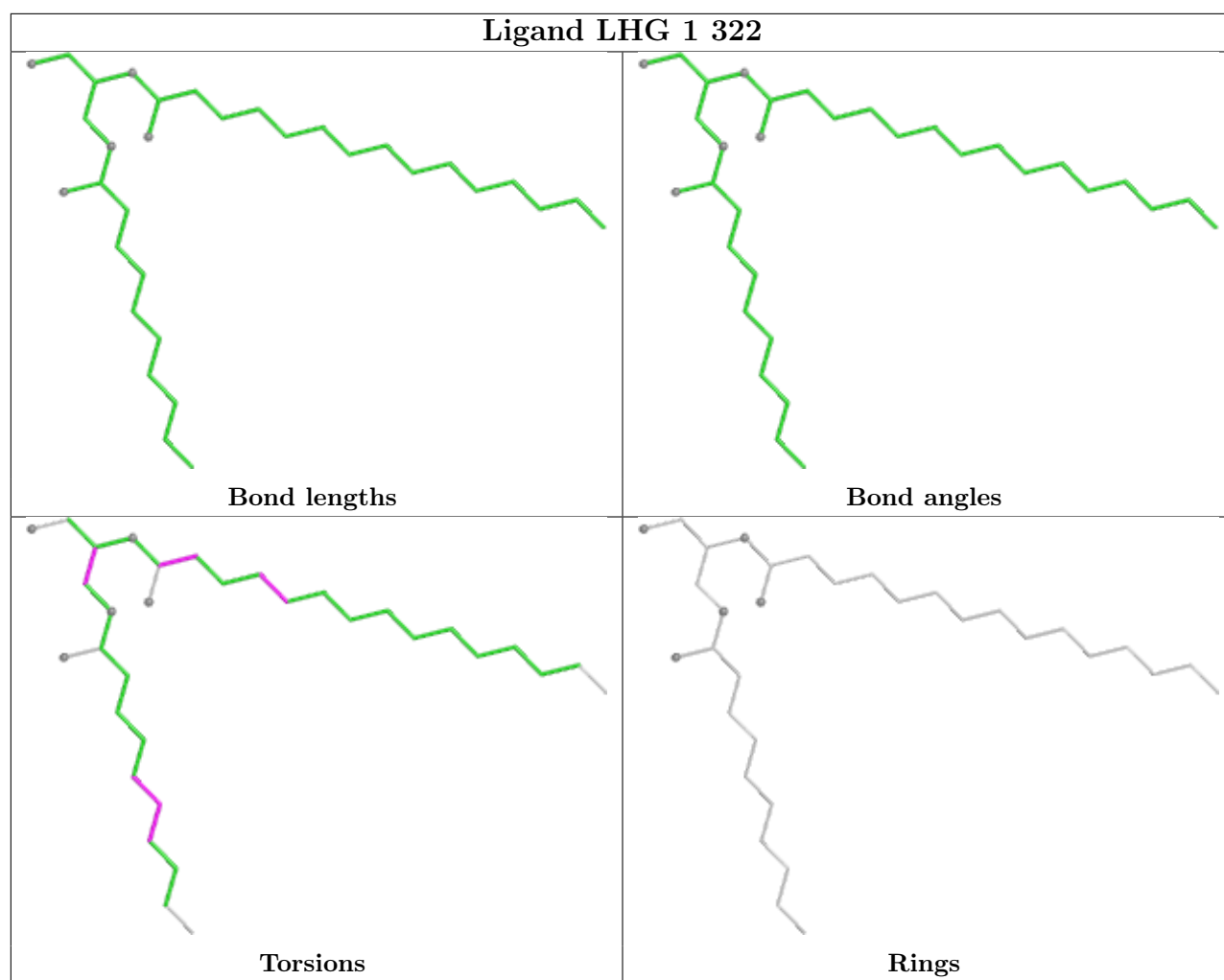
Torsions



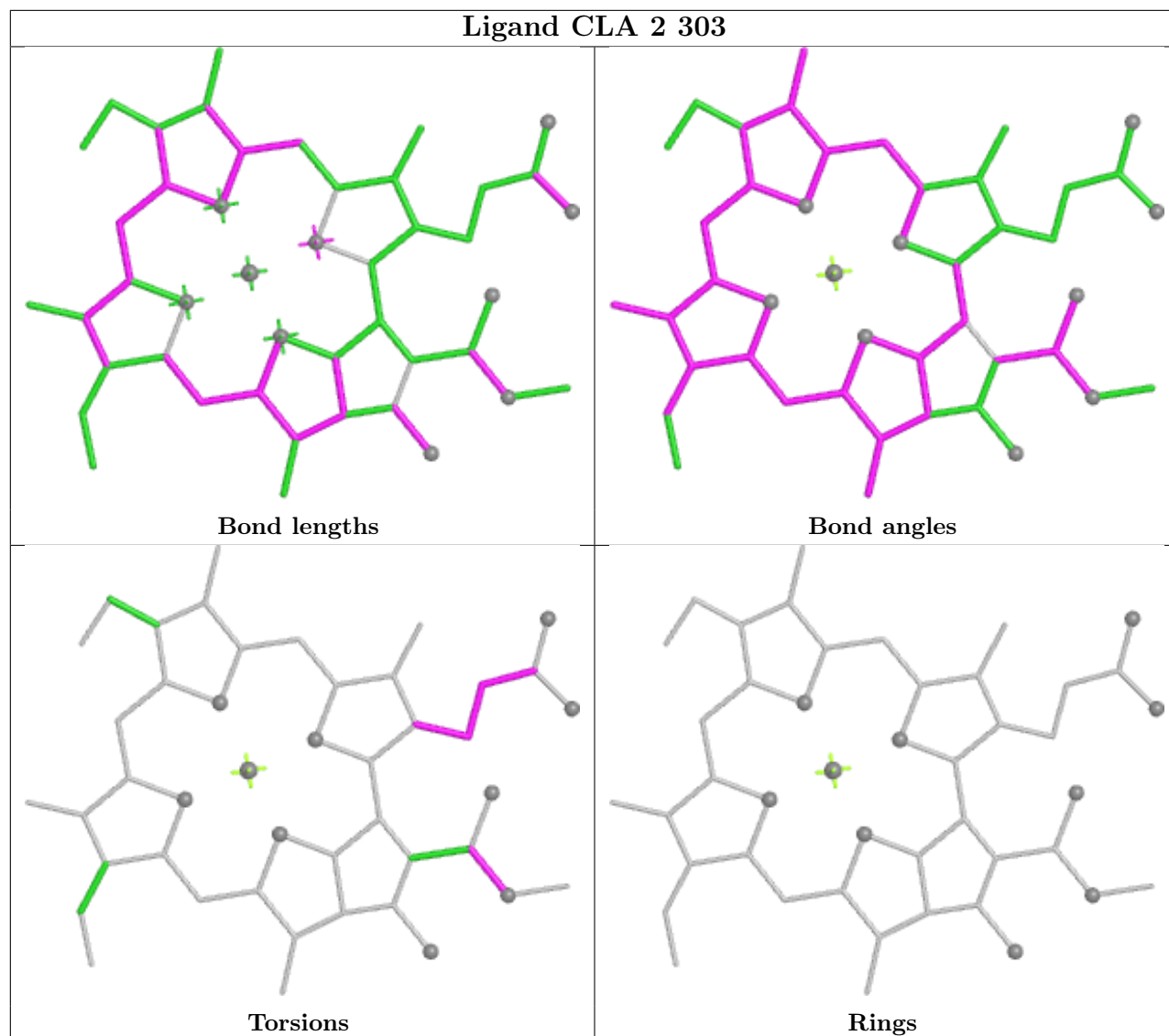
Rings

Ligand CLA G 207

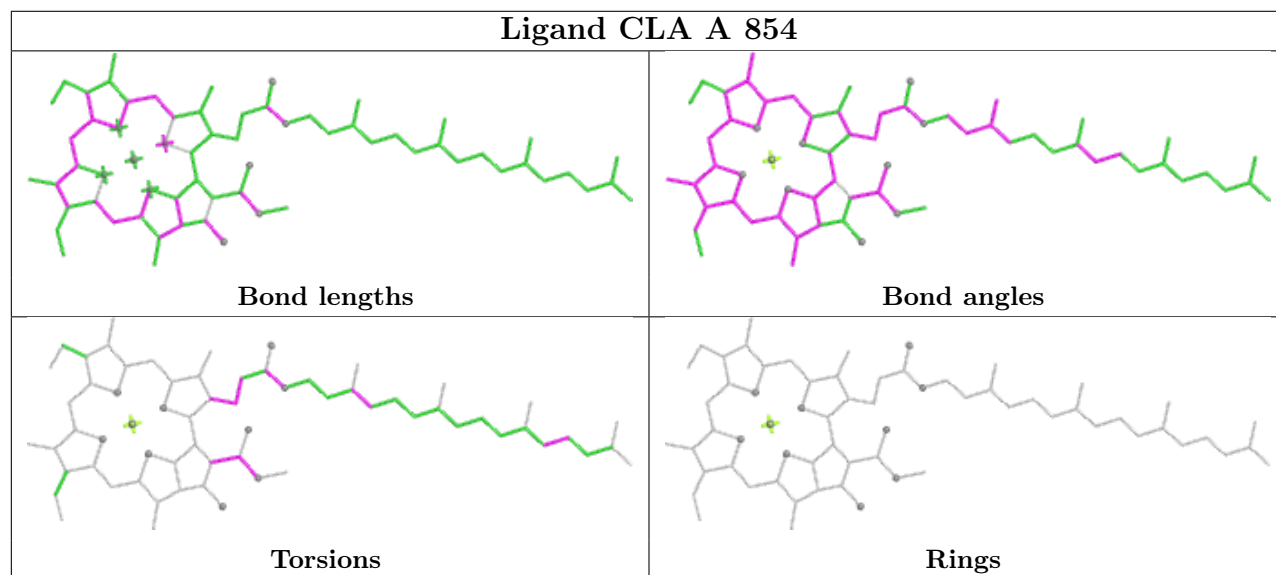


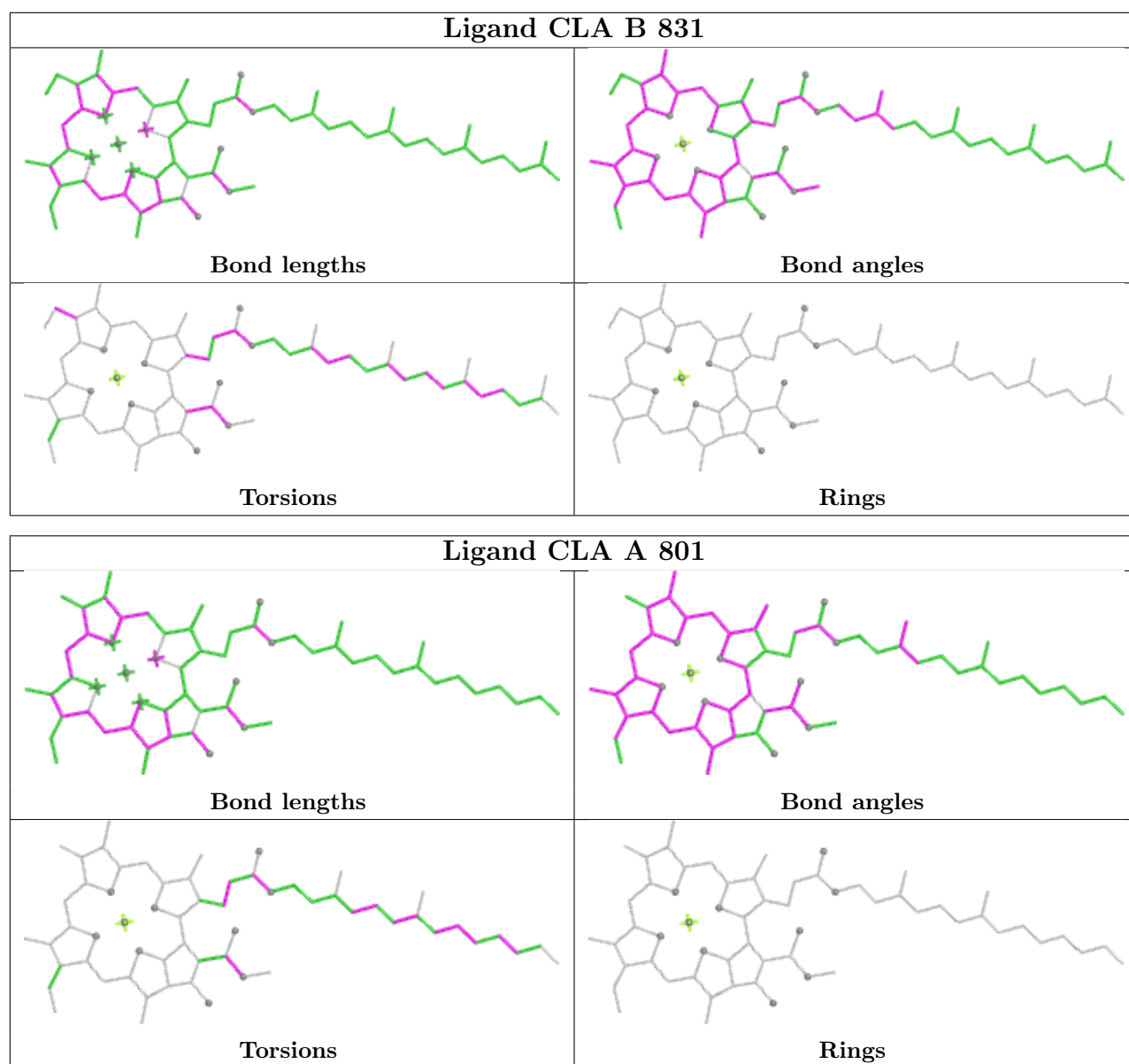


Ligand CLA 2 303

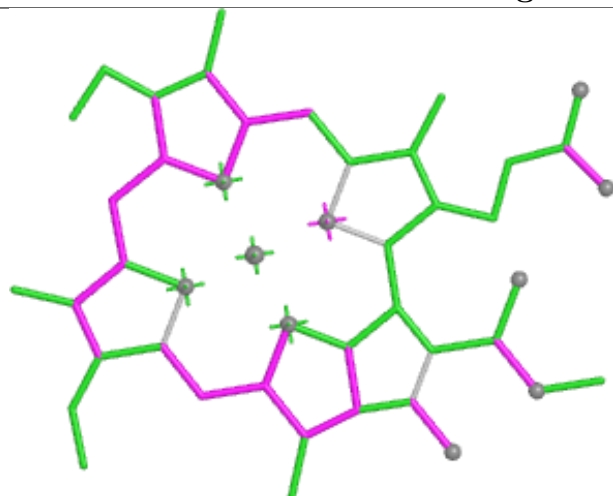


Ligand CLA A 854

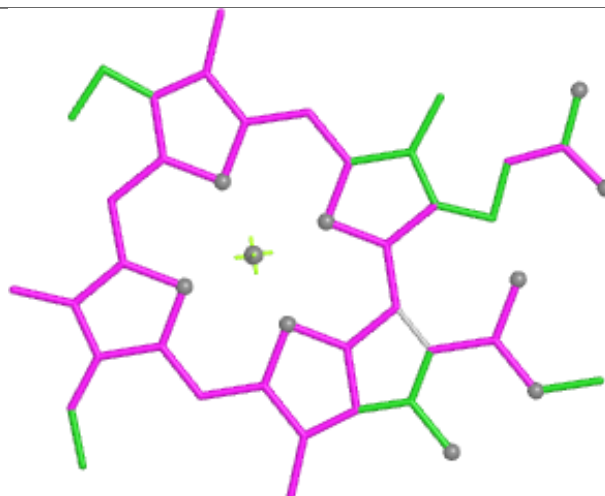




Ligand CLA L 305



Bond lengths



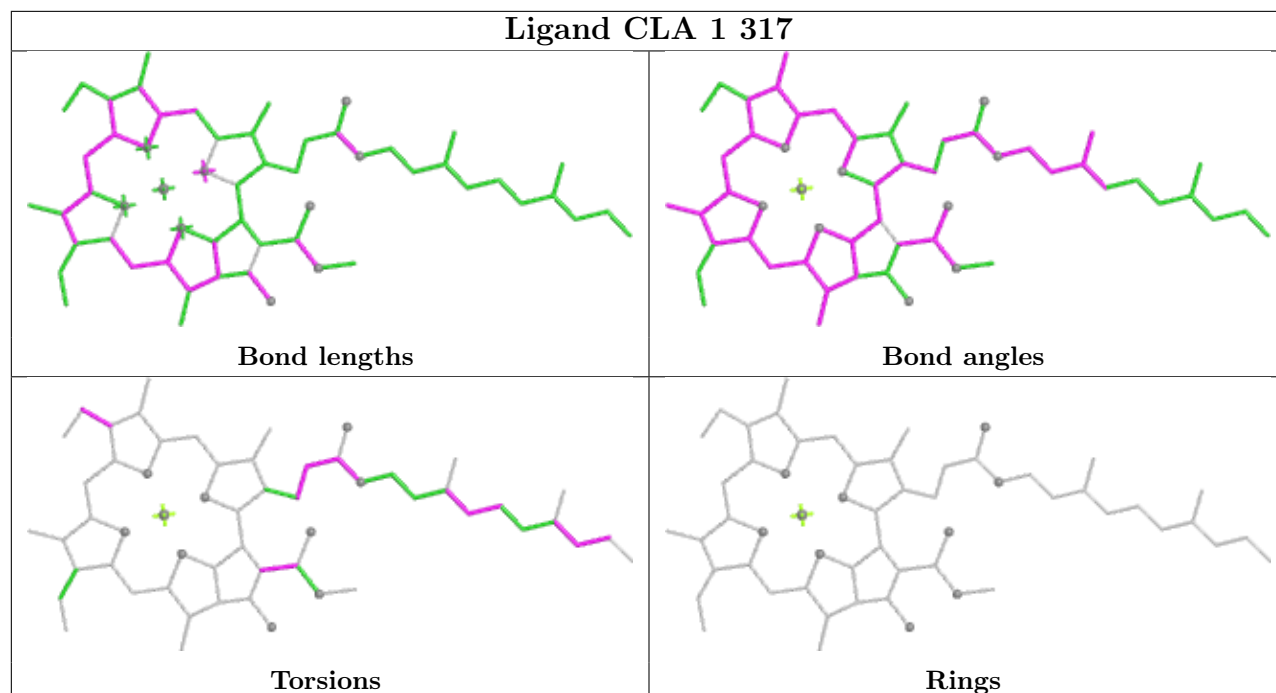
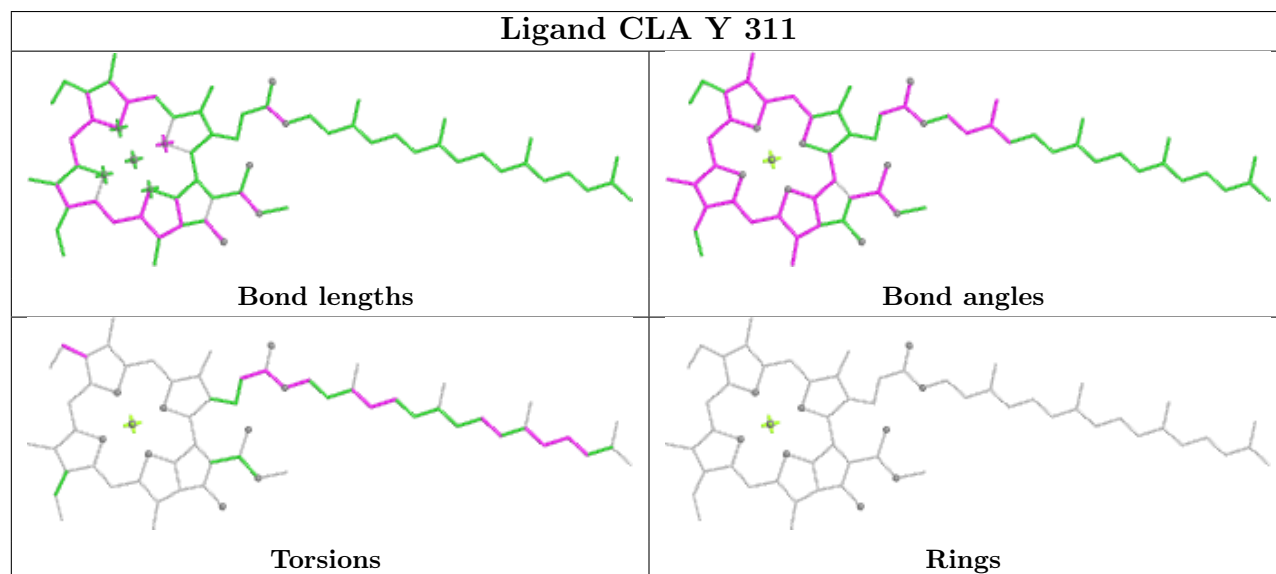
Bond angles



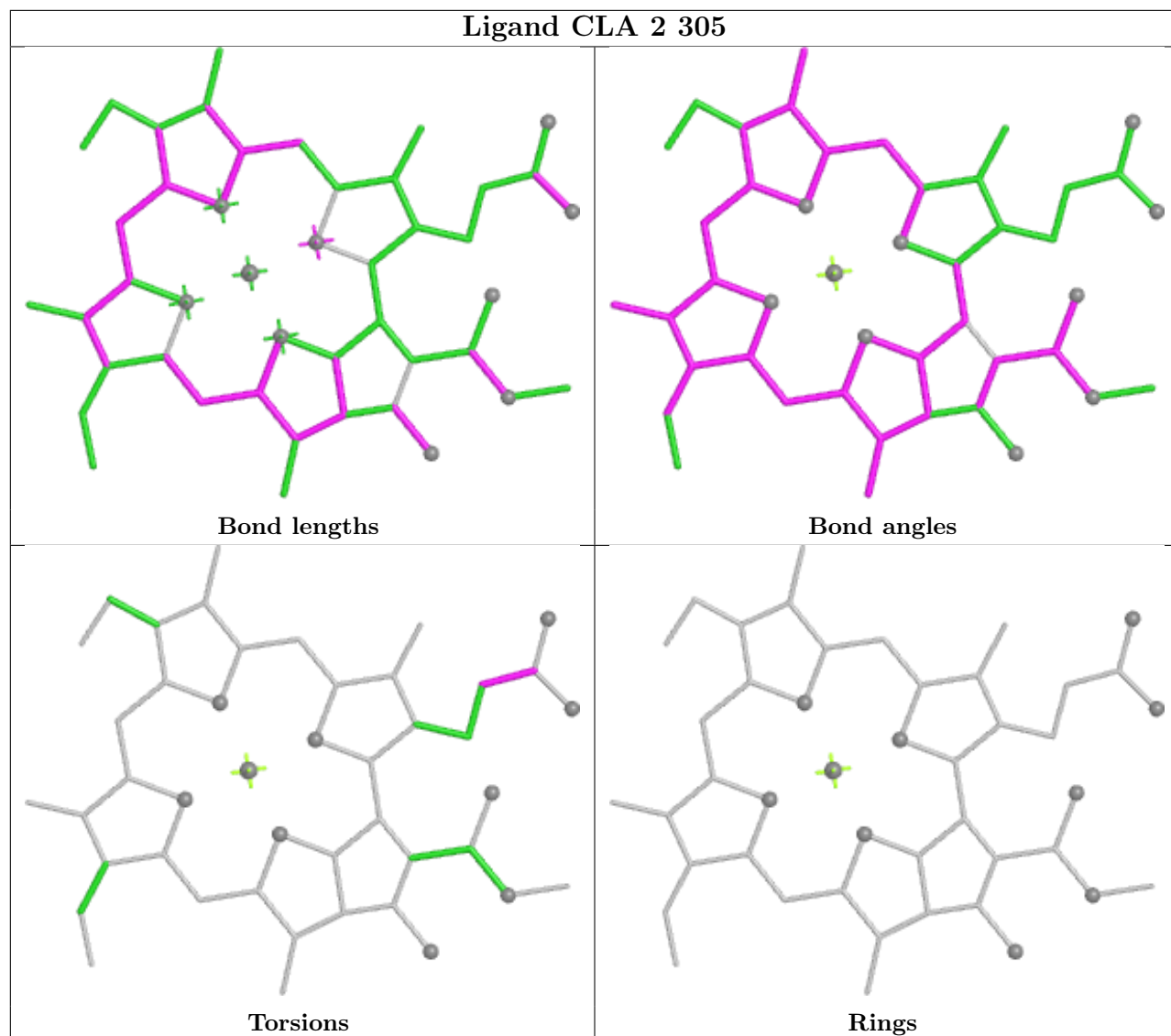
Torsions

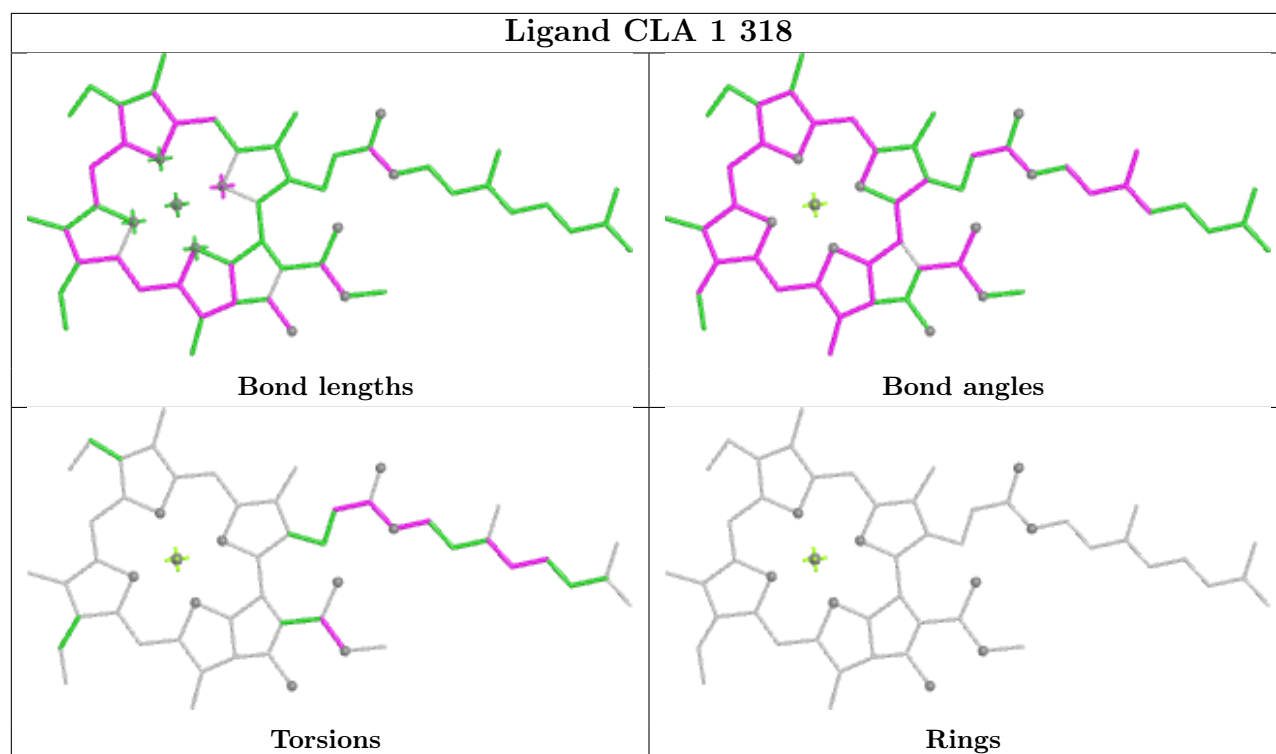
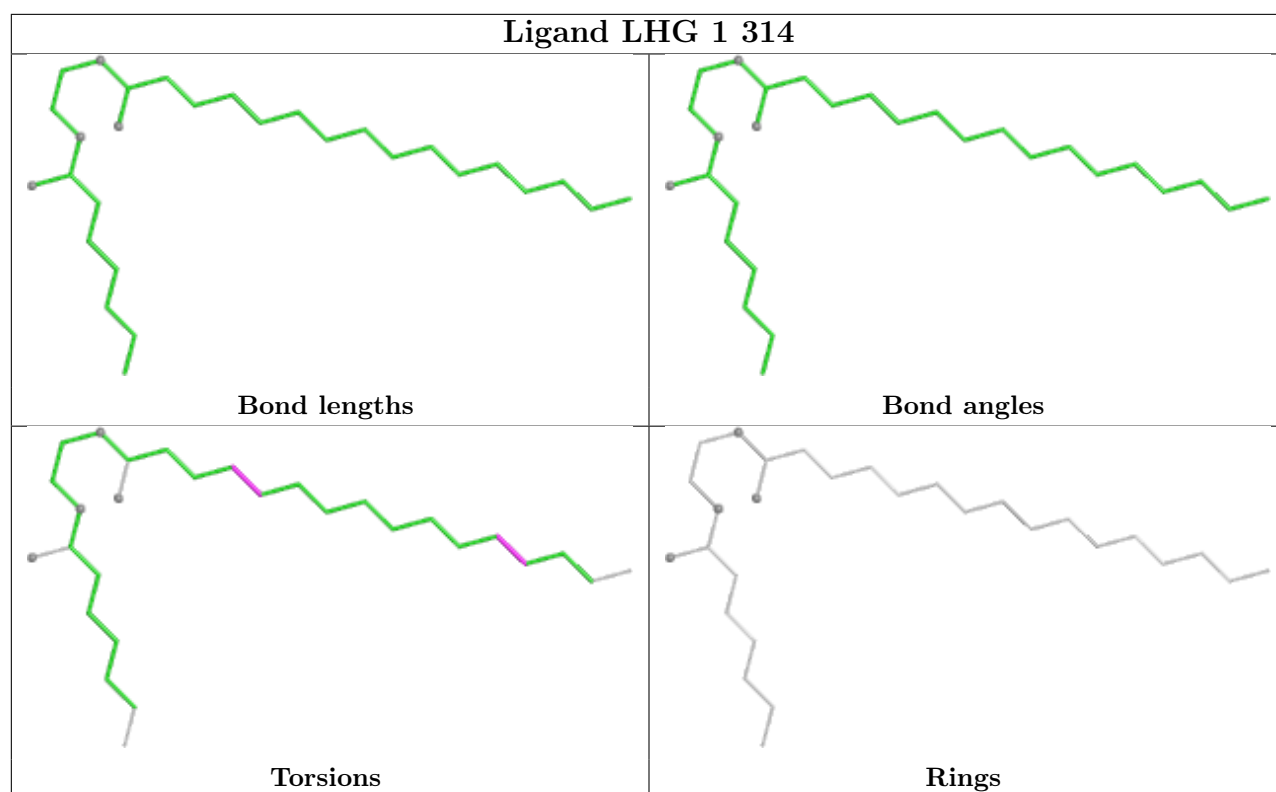


Rings

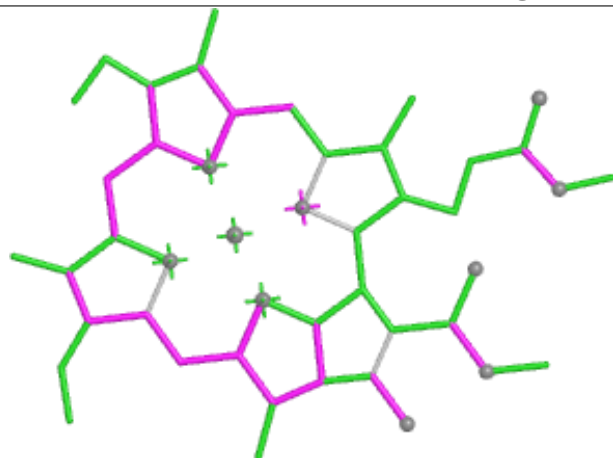
Ligand CLA 1 317**Ligand CLA Y 311**

Ligand CLA 2 305

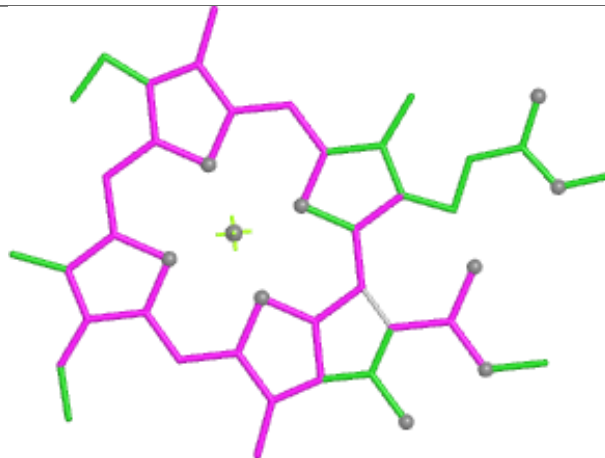




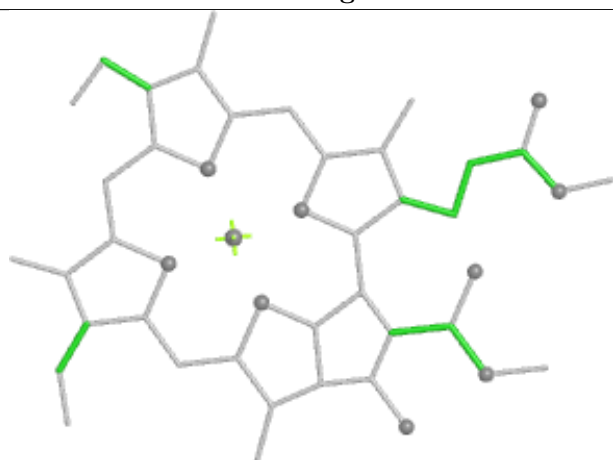
Ligand CLA O 206



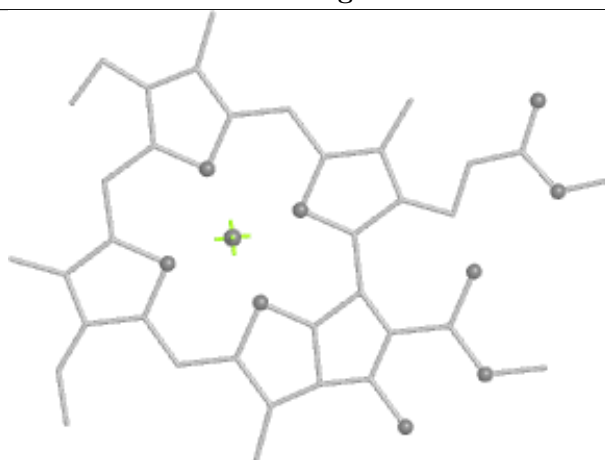
Bond lengths



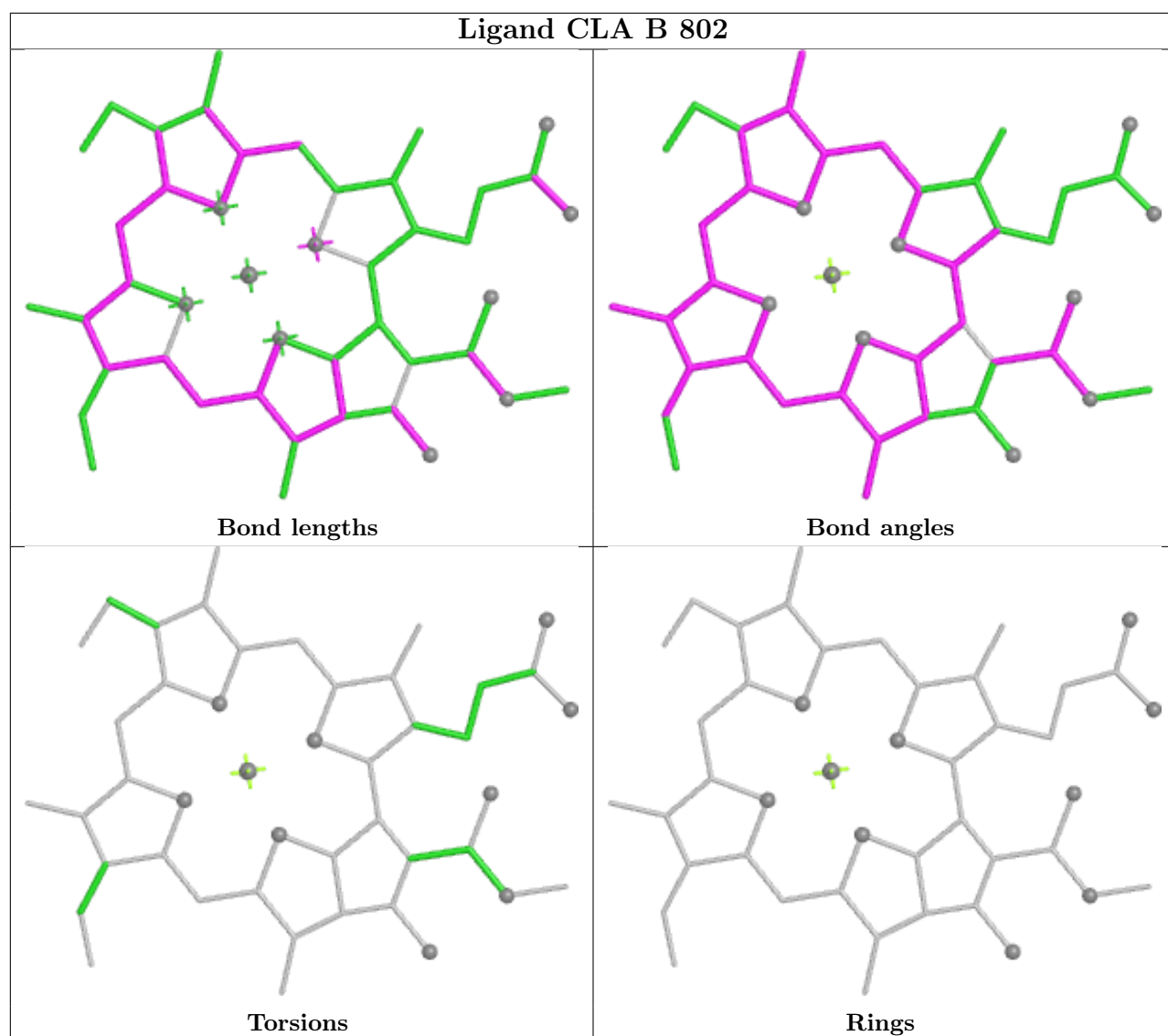
Bond angles



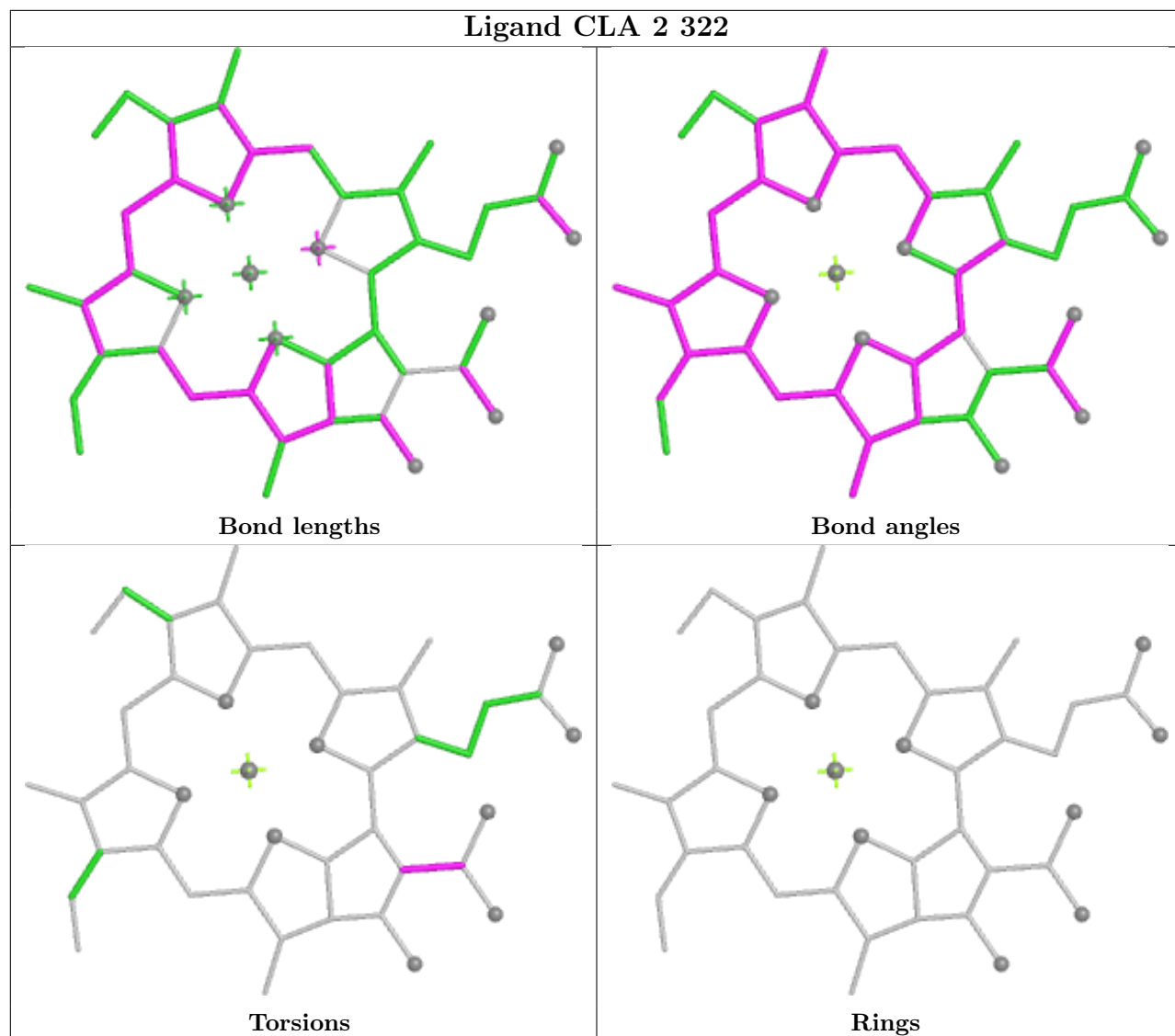
Torsions



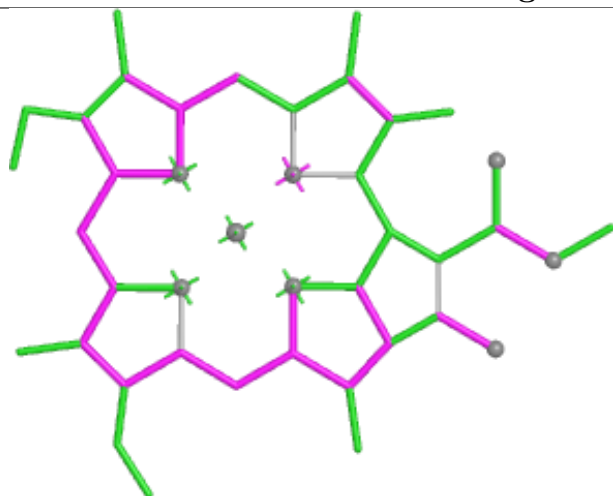
Rings



Ligand CLA 2 322



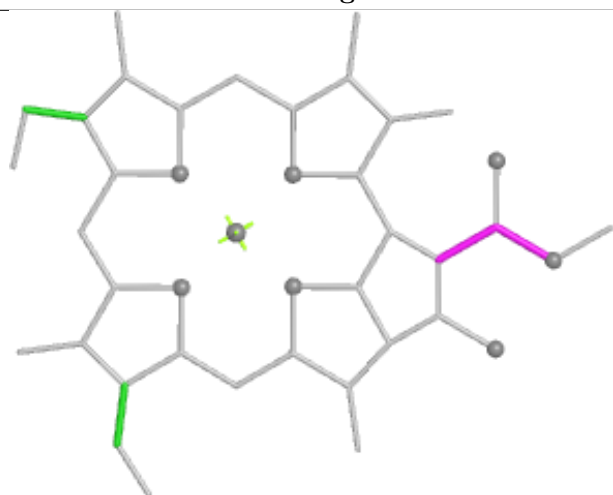
Ligand CLA 2 317



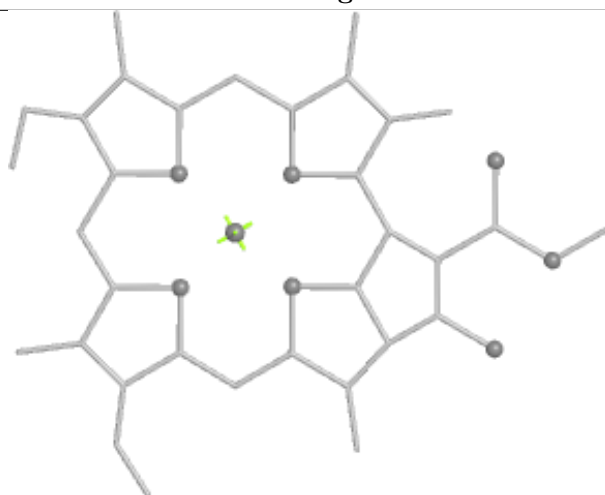
Bond lengths



Bond angles

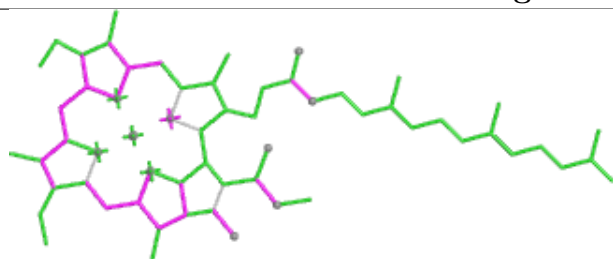


Torsions

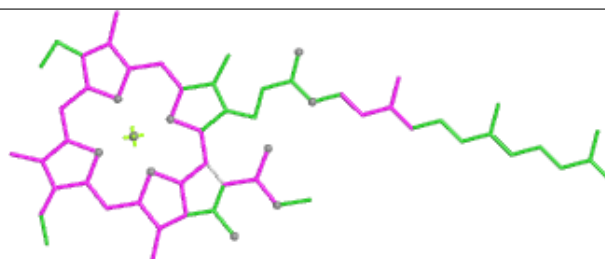


Rings

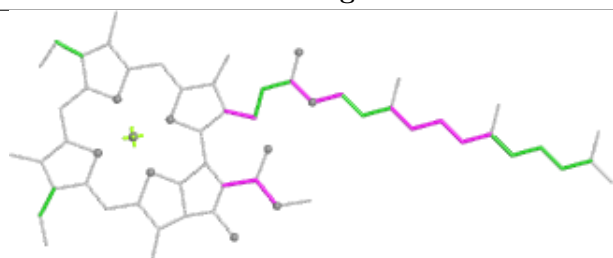
Ligand CLA O 208



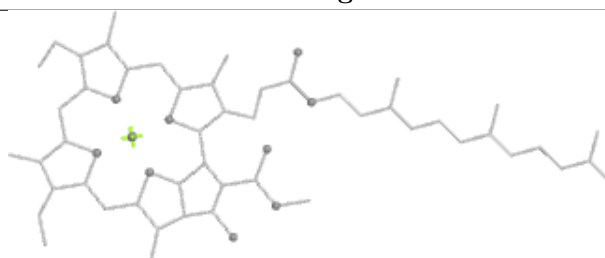
Bond lengths



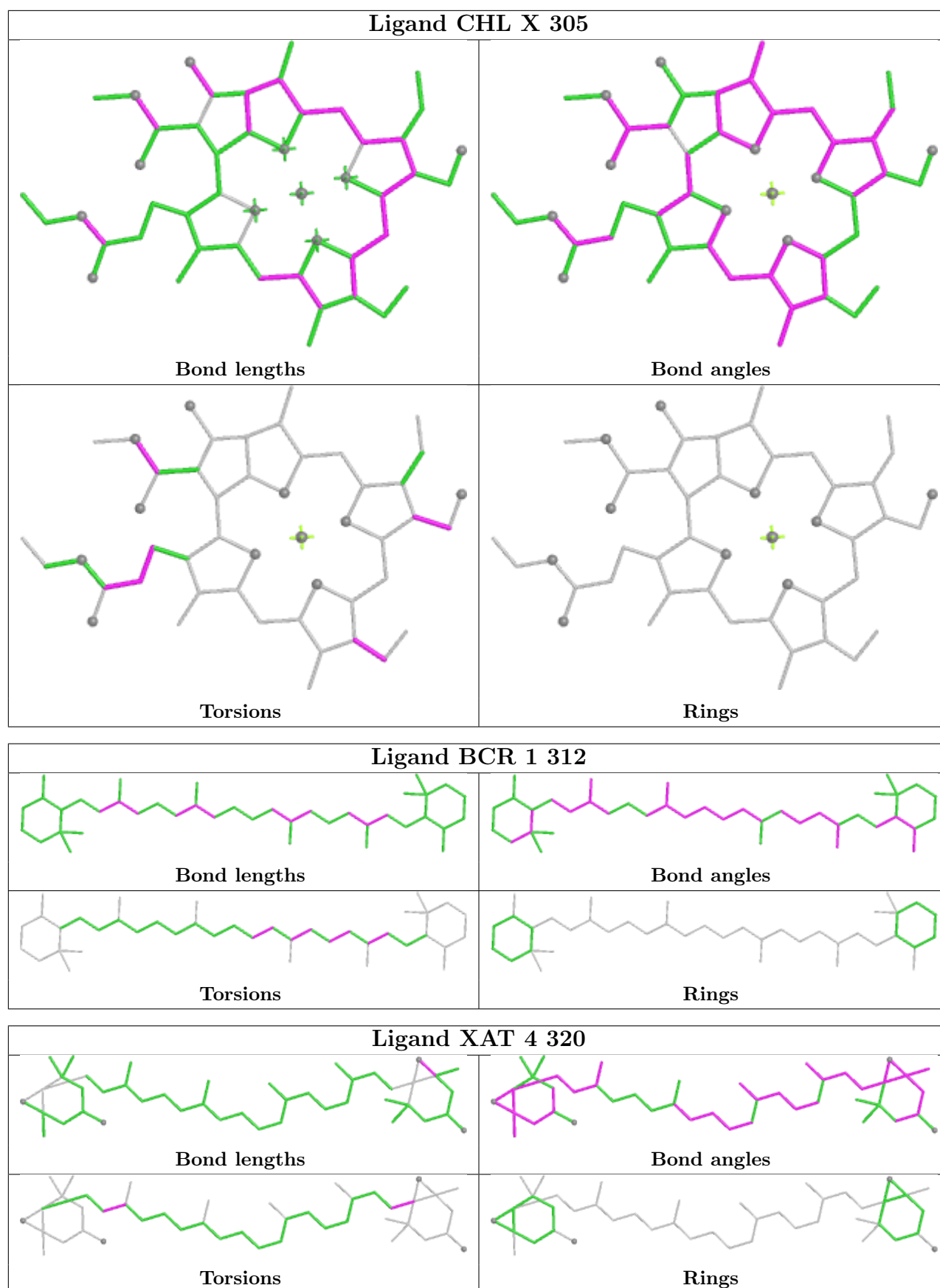
Bond angles

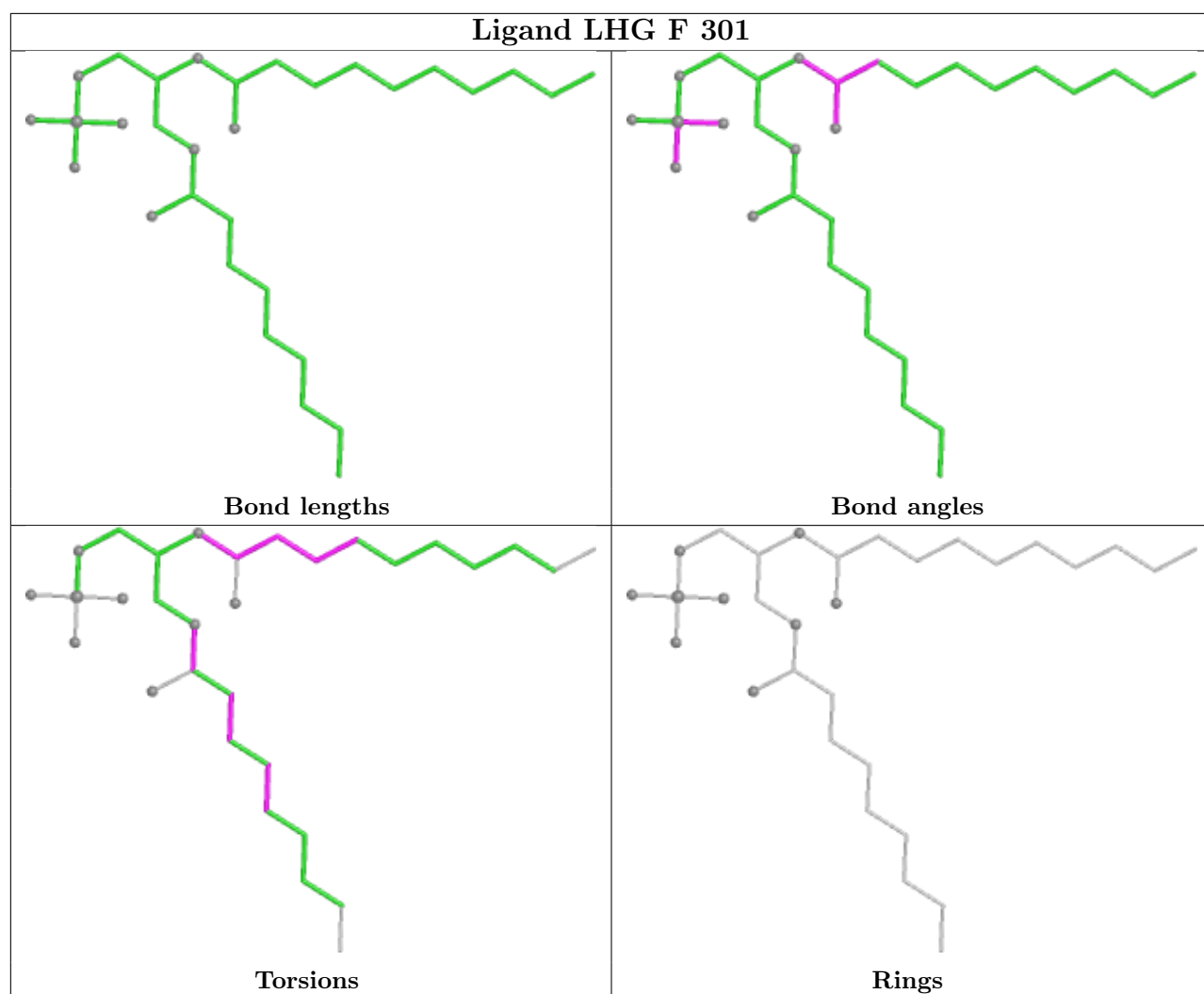


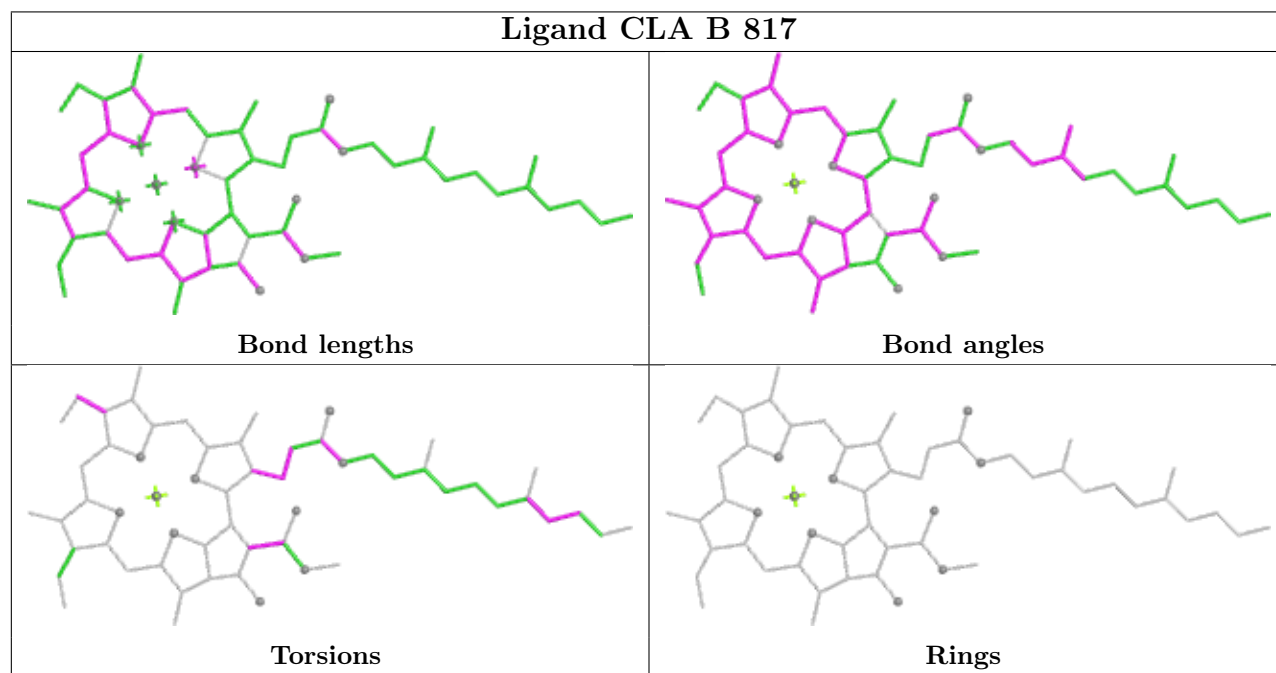
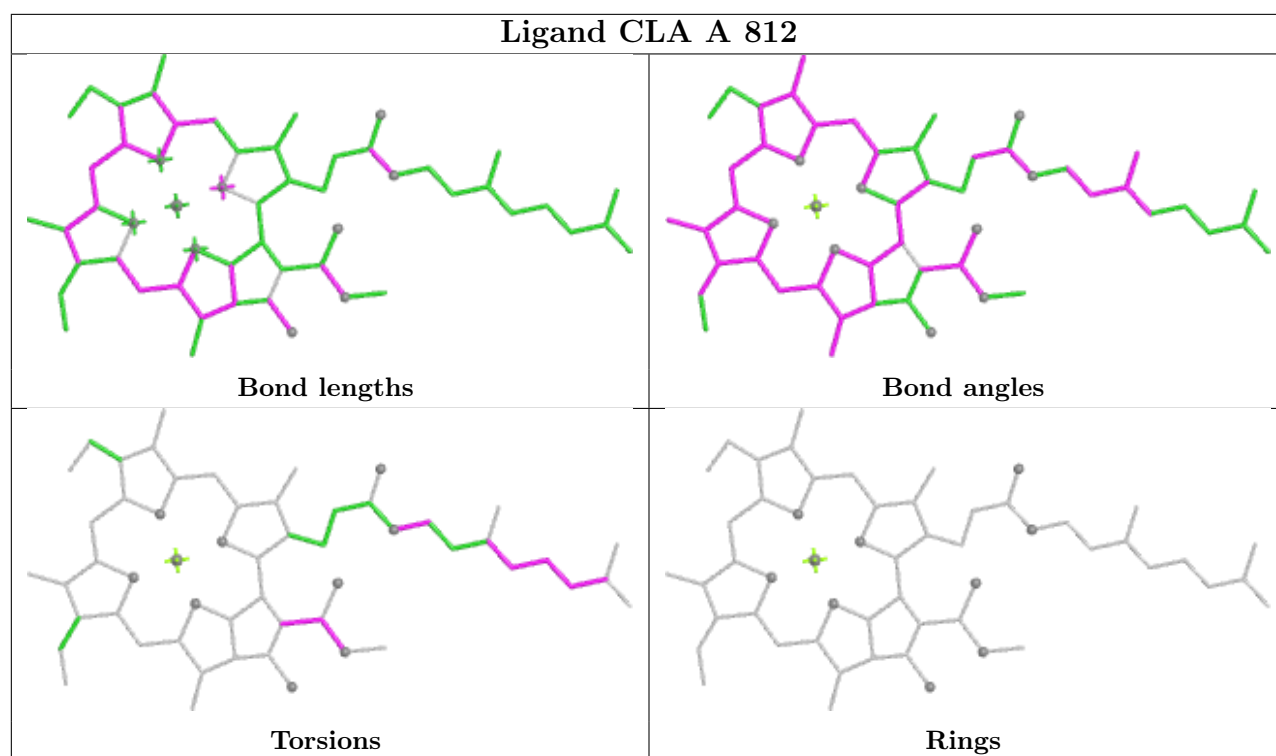
Torsions

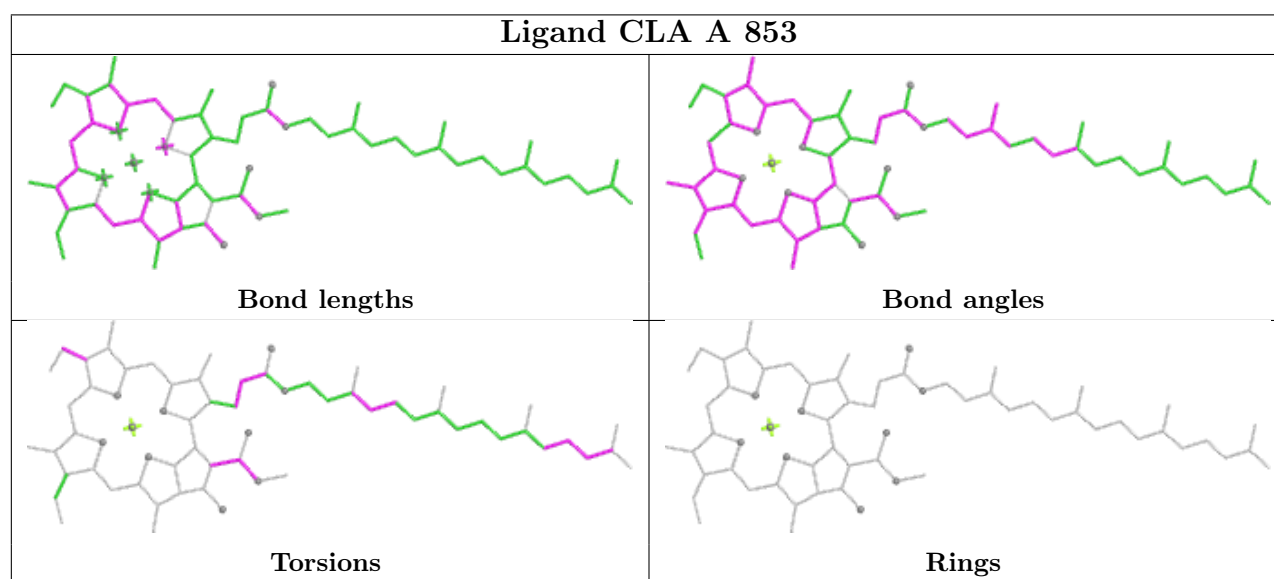
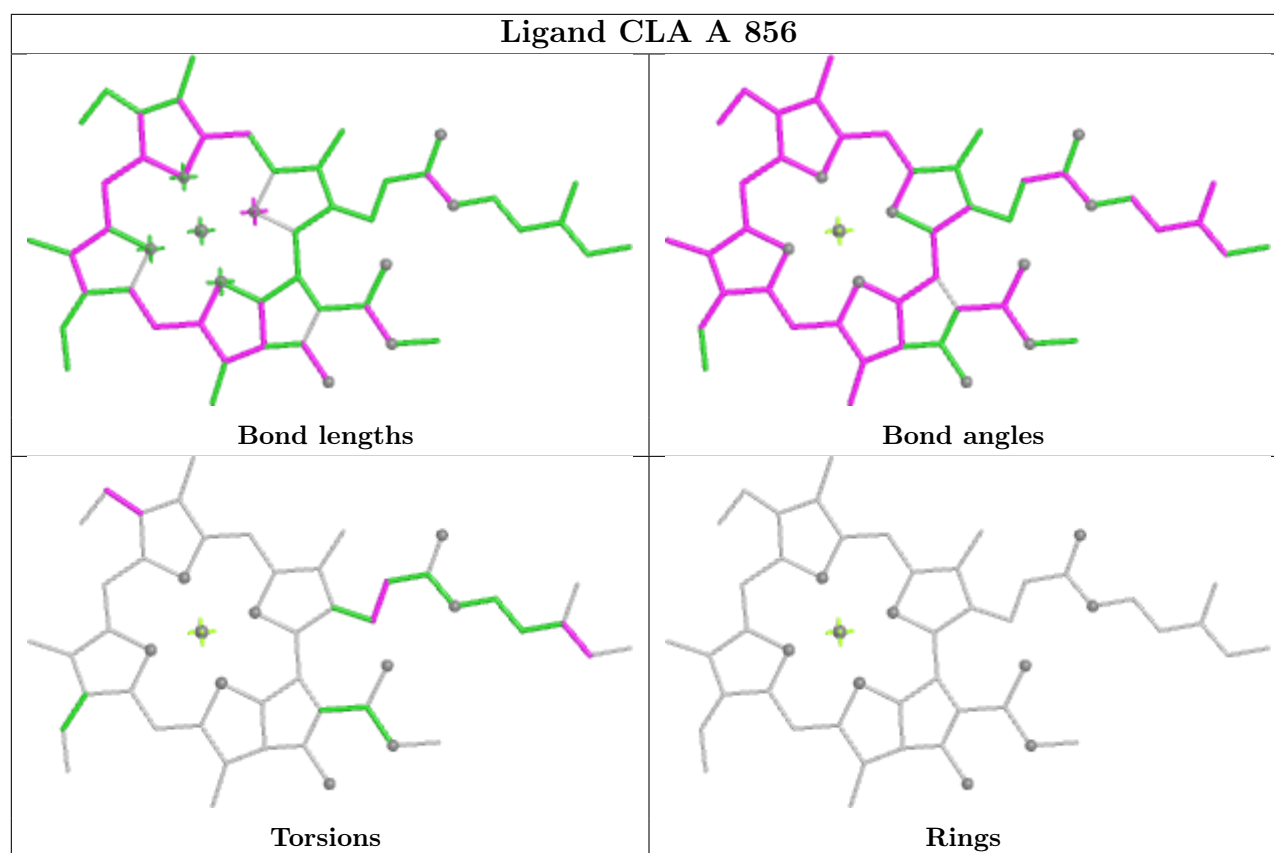


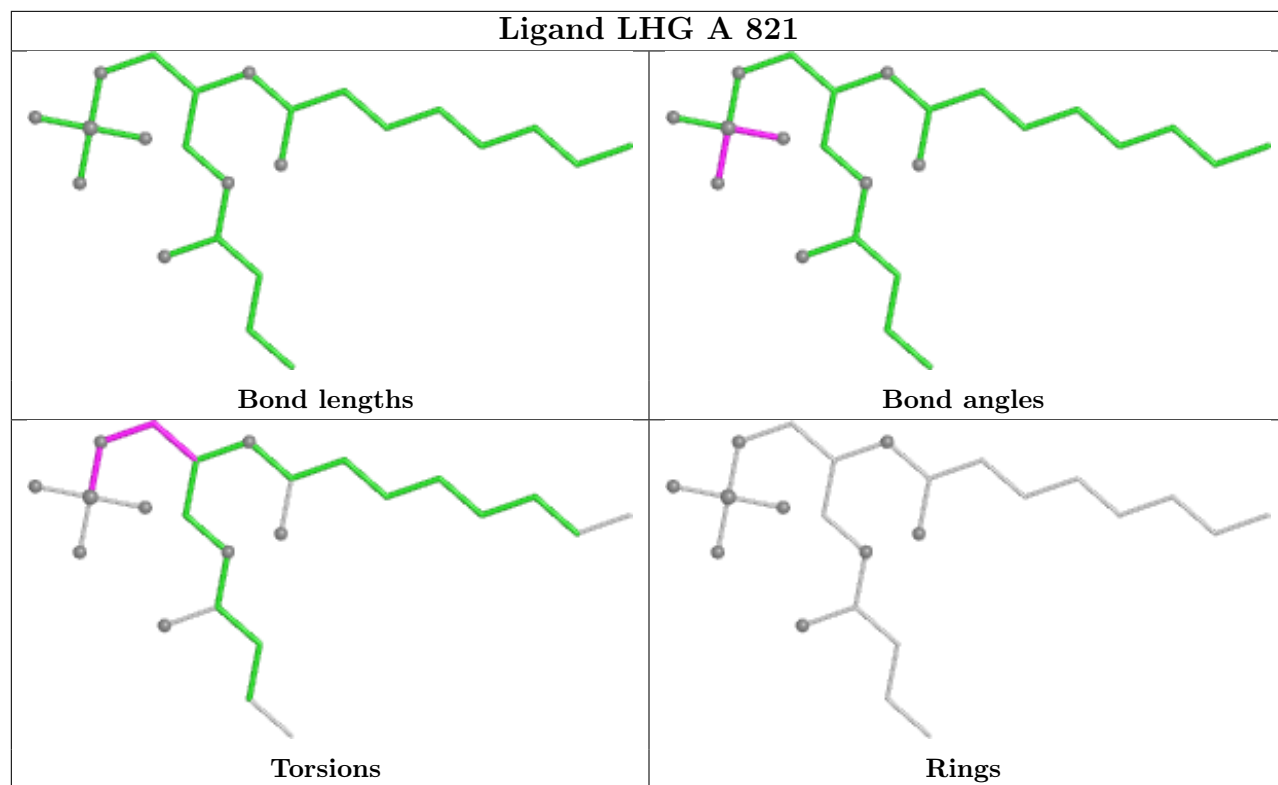
Rings



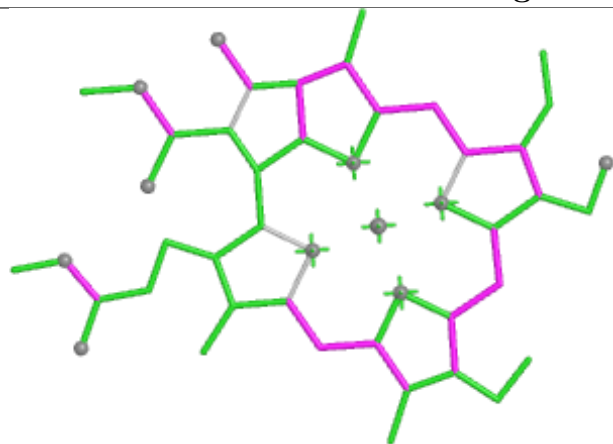




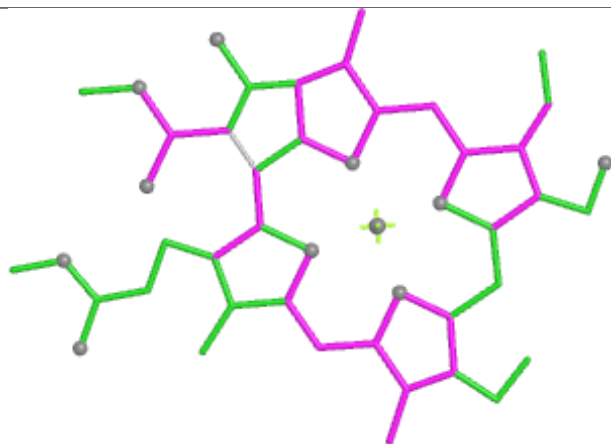




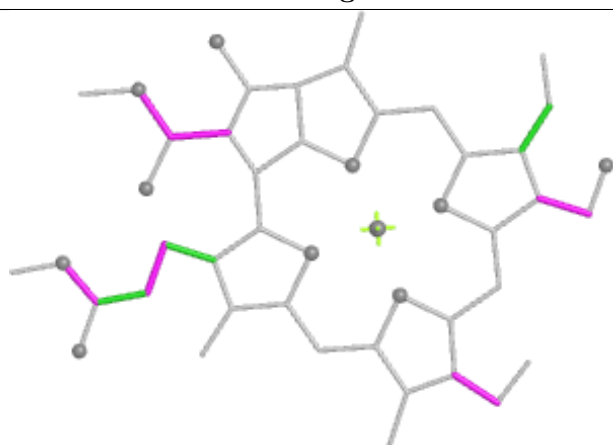
Ligand CHL X 308



Bond lengths



Bond angles

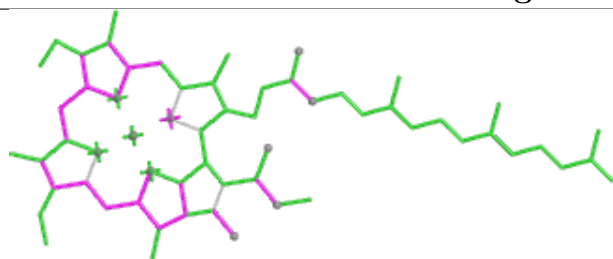


Torsions

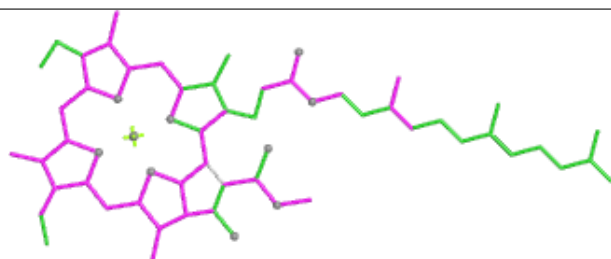


Rings

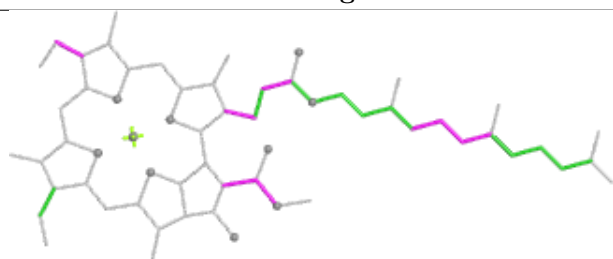
Ligand CLA B 819



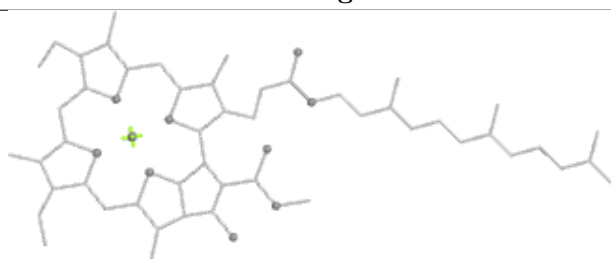
Bond lengths



Bond angles

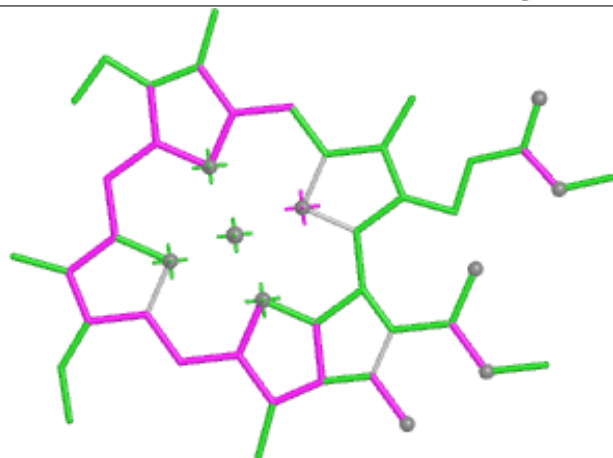


Torsions

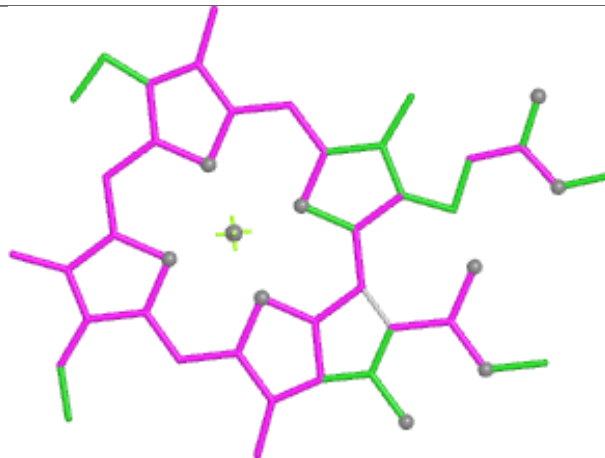


Rings

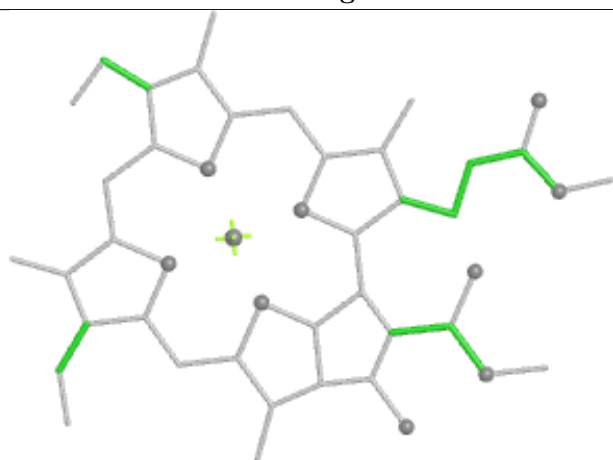
Ligand CLA Z 310



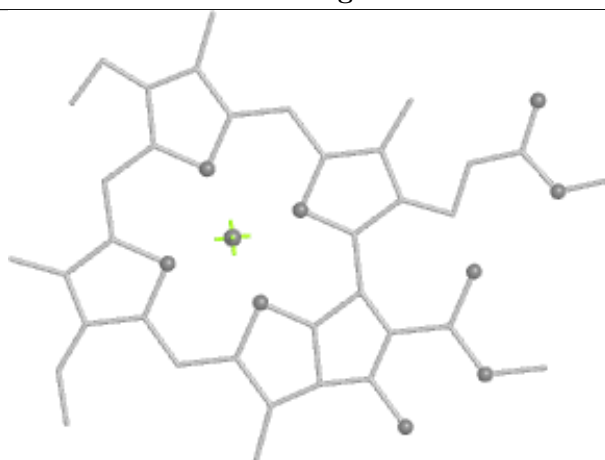
Bond lengths



Bond angles

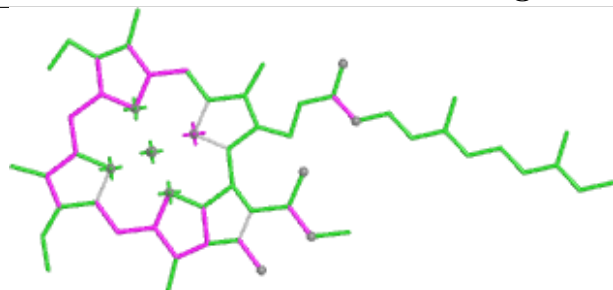


Torsions

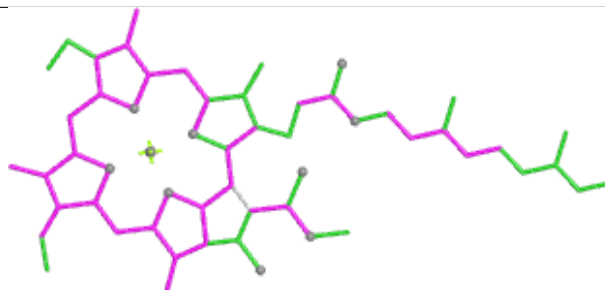


Rings

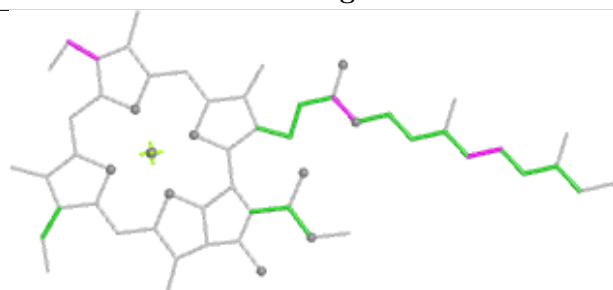
Ligand CLA A 857



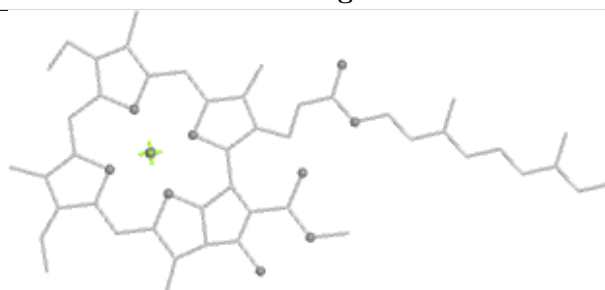
Bond lengths



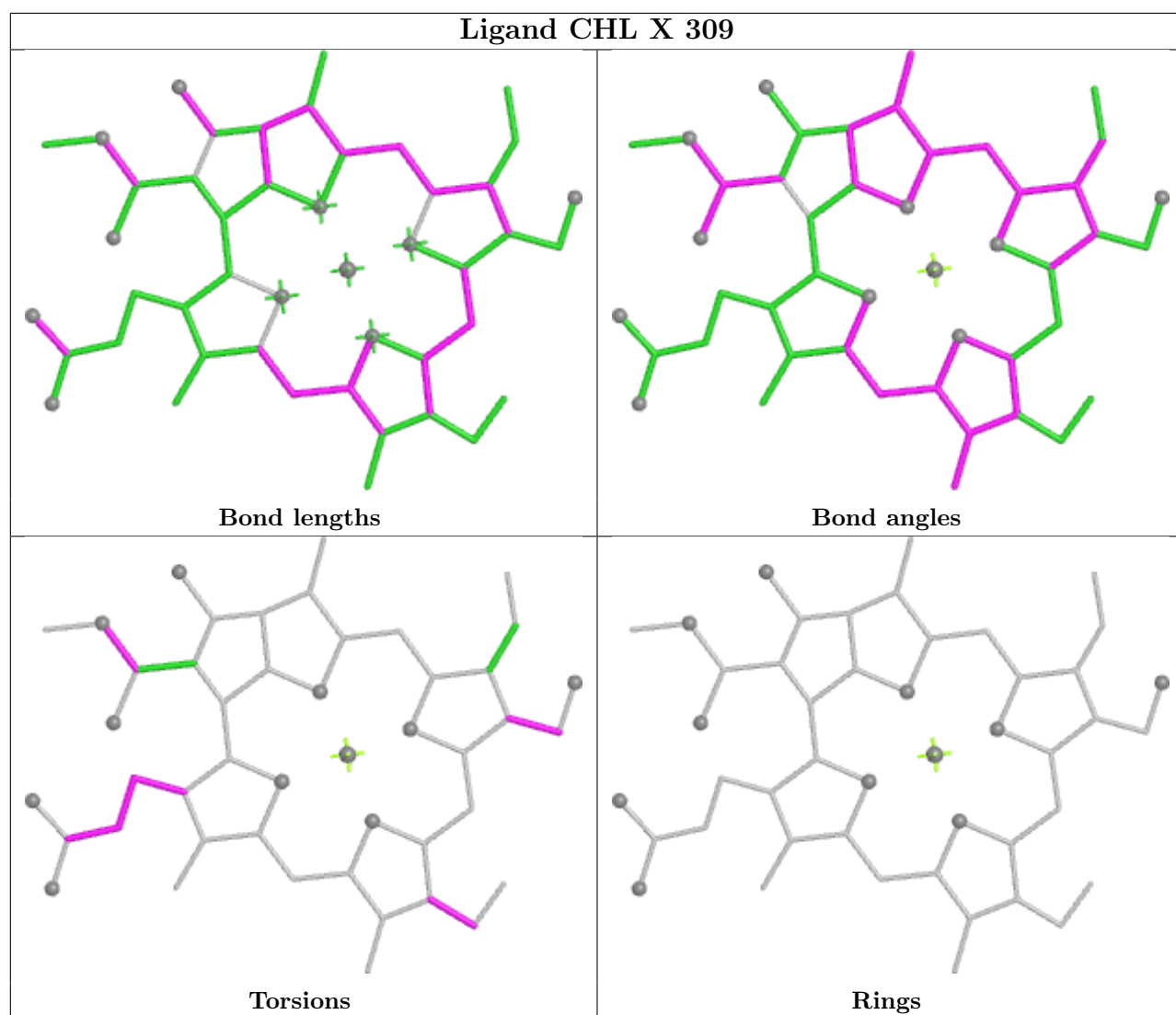
Bond angles

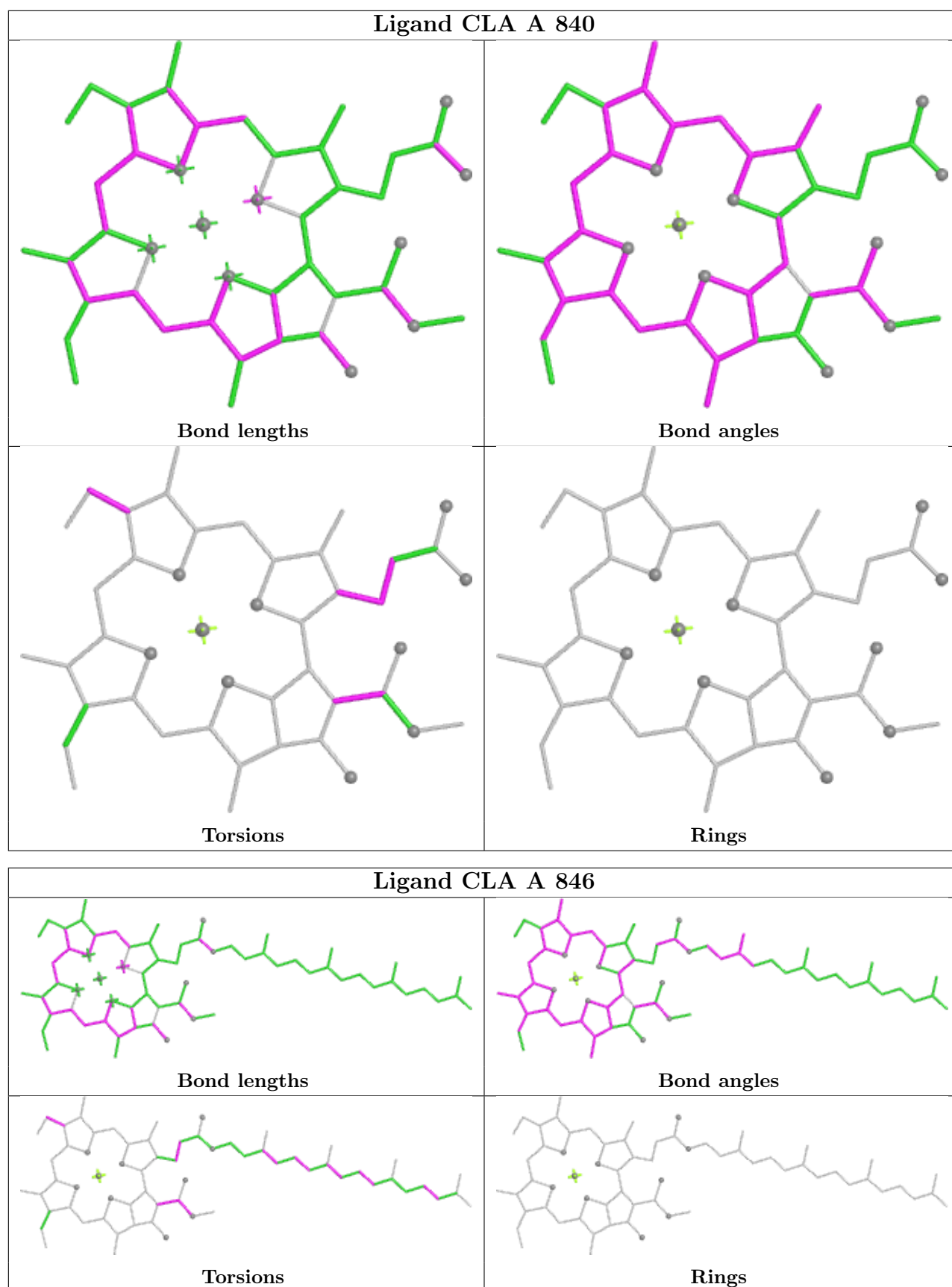


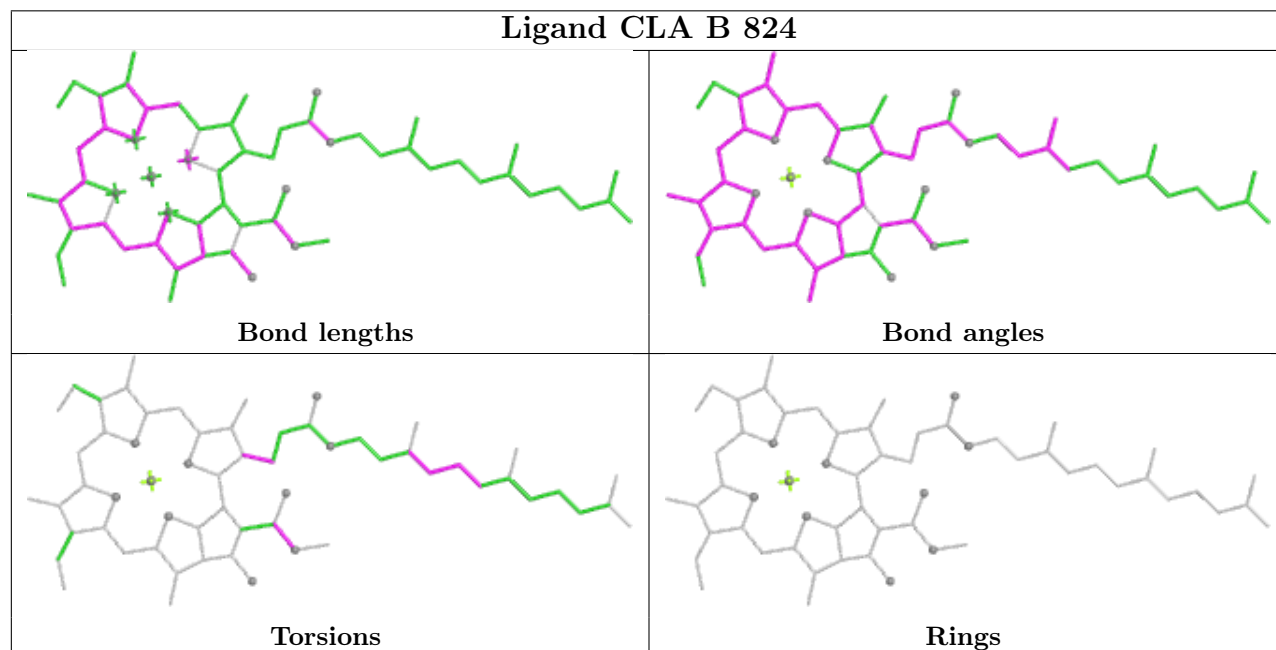
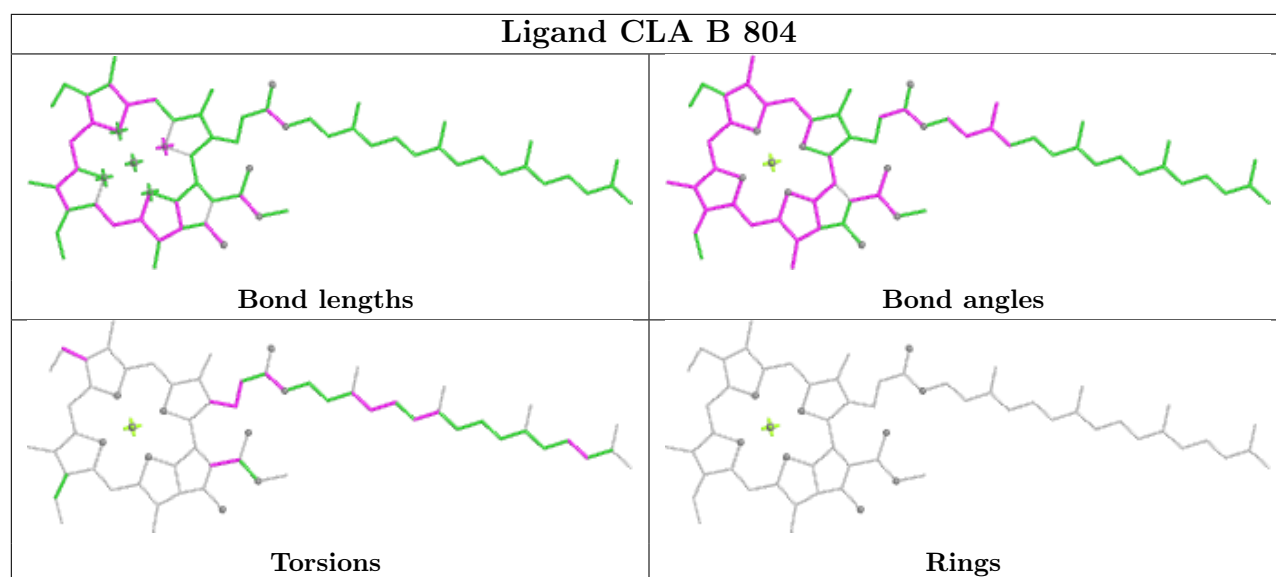
Torsions

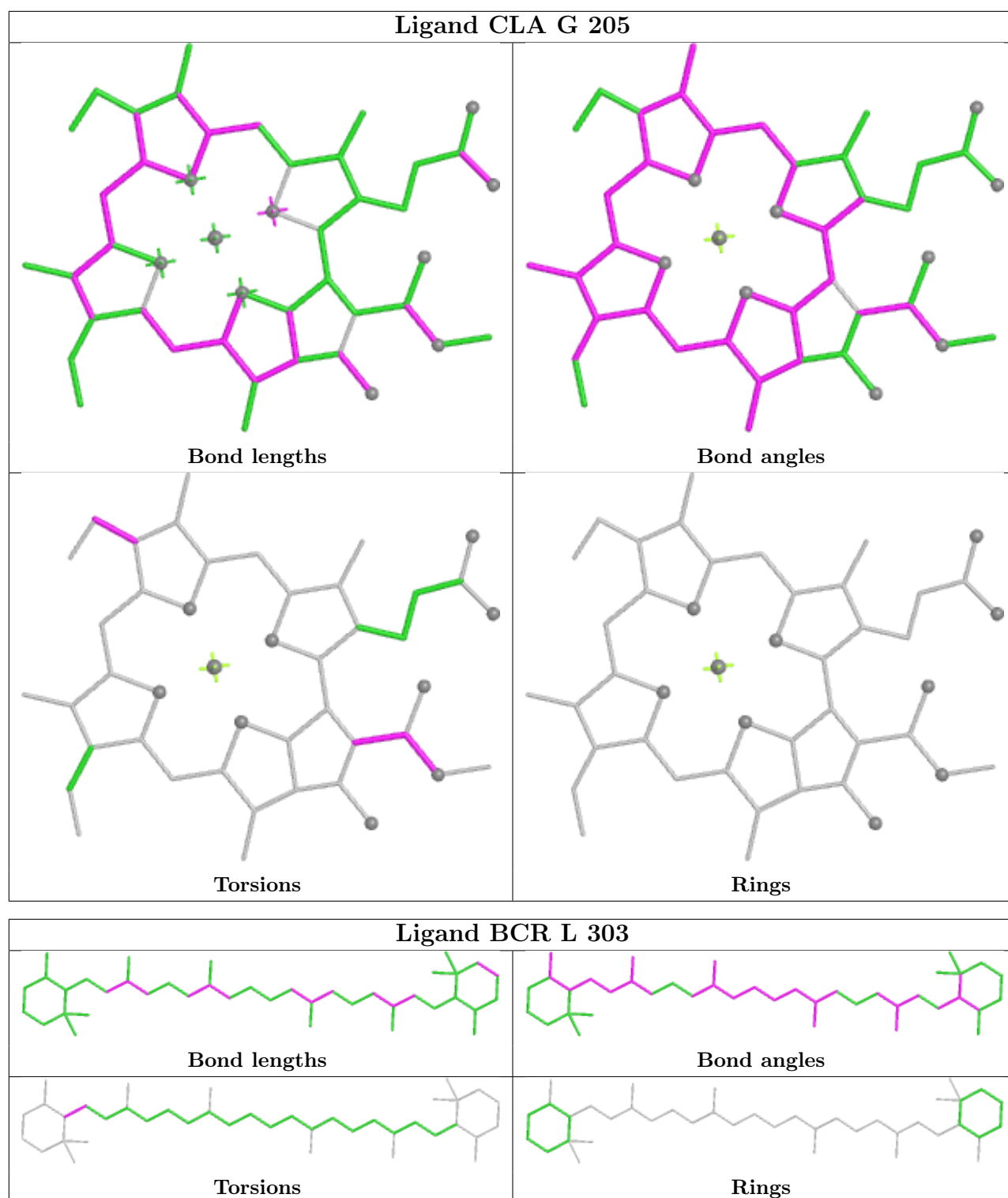


Rings

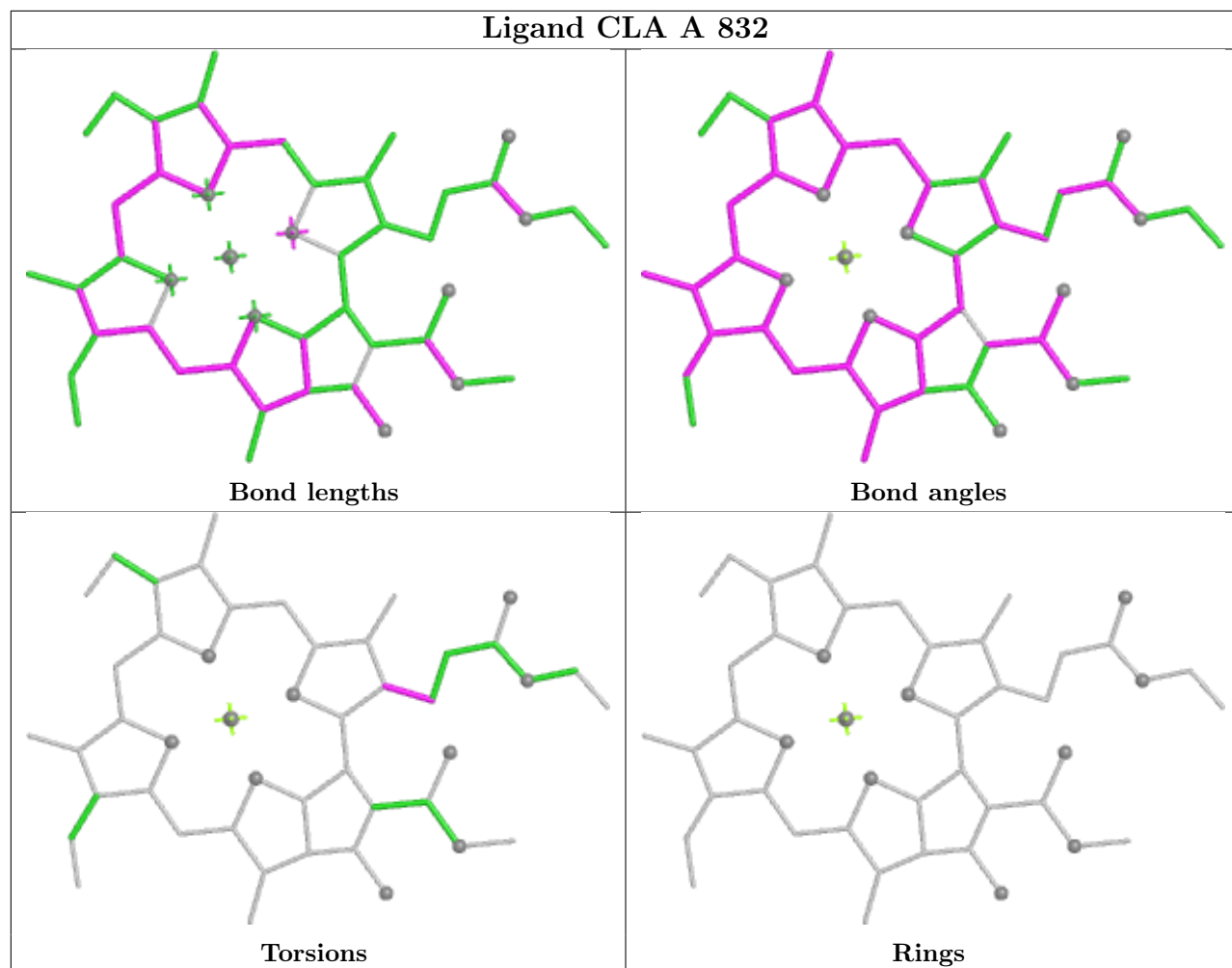


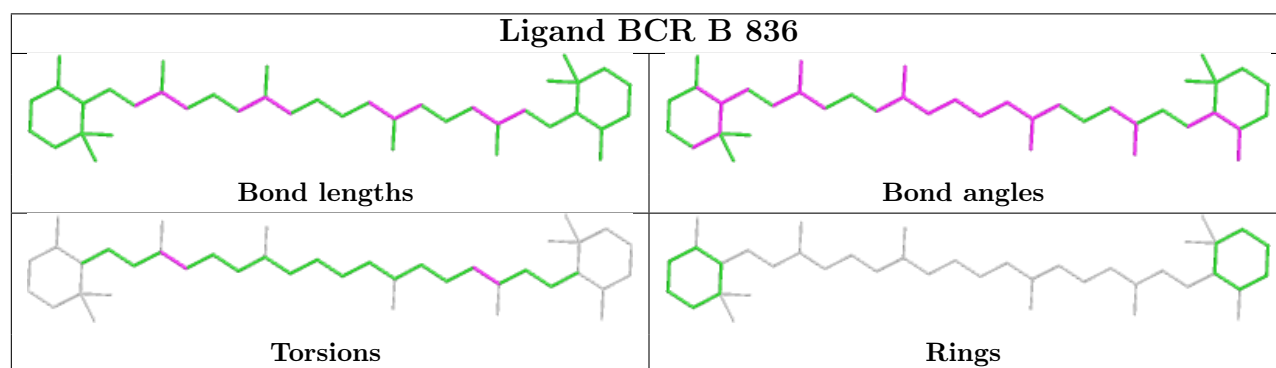
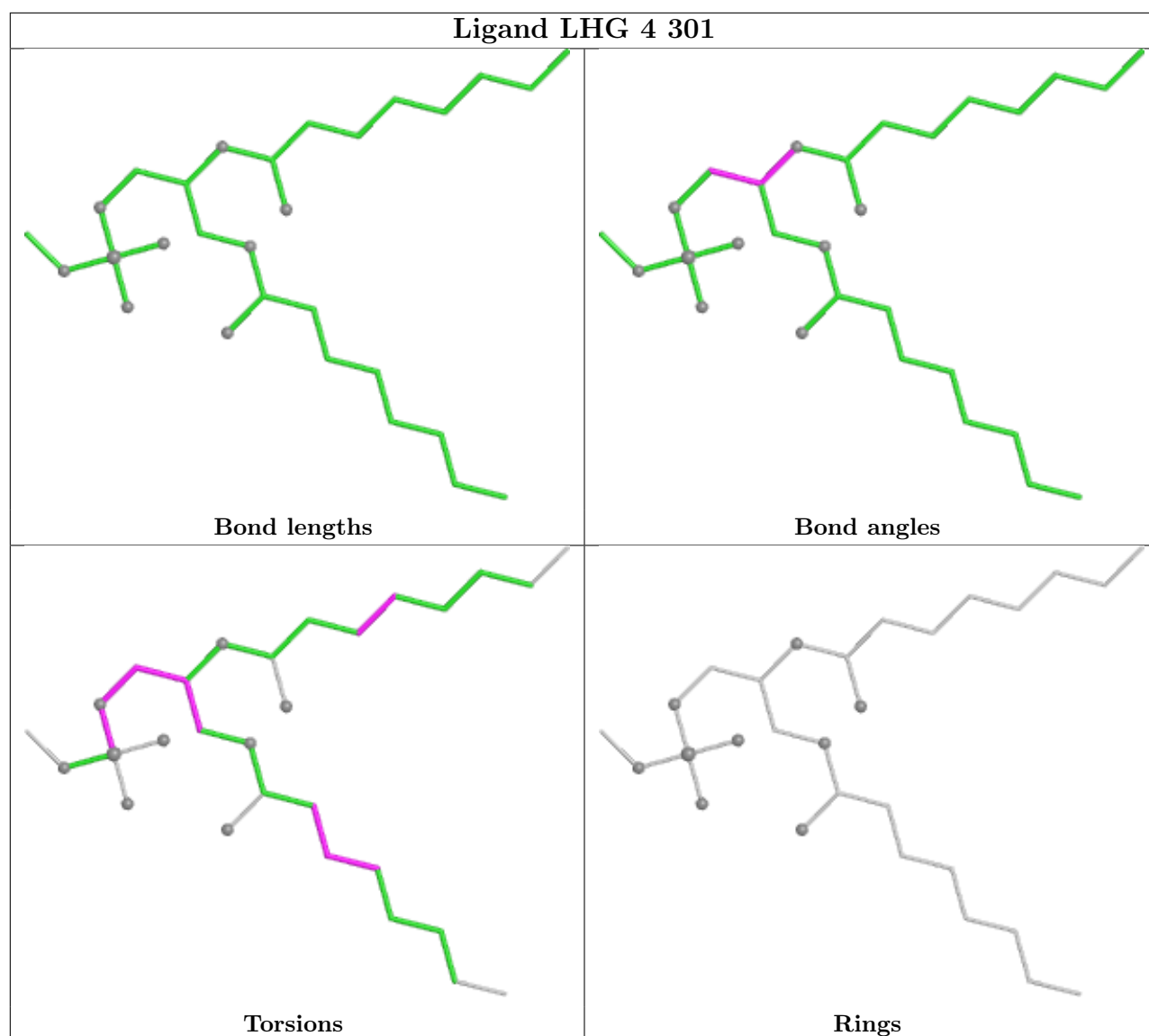


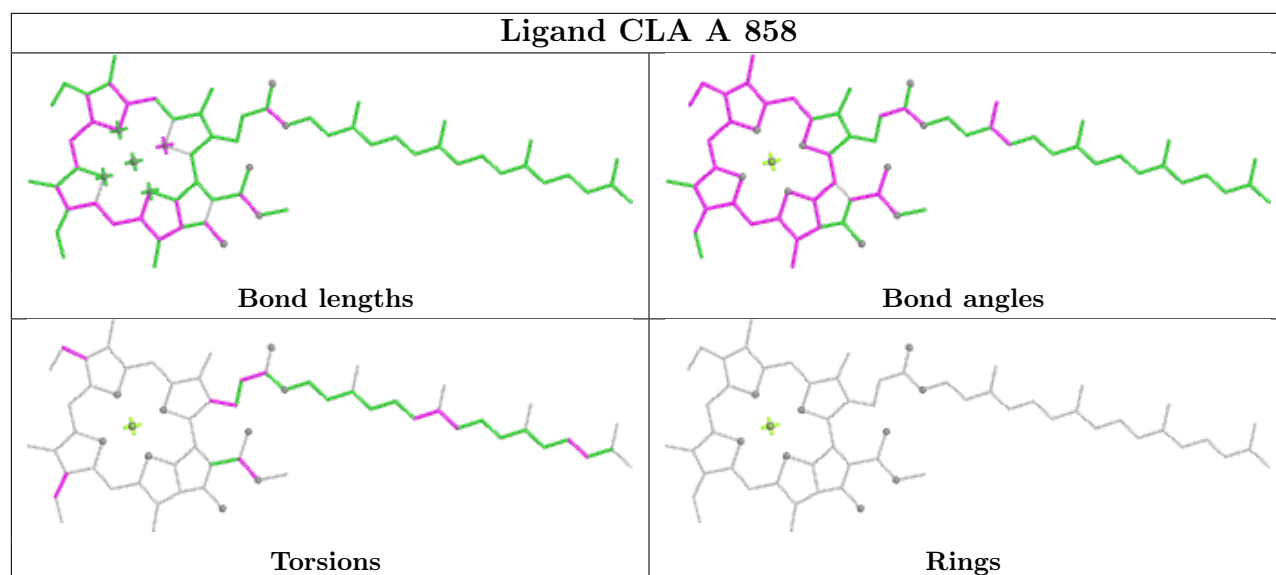
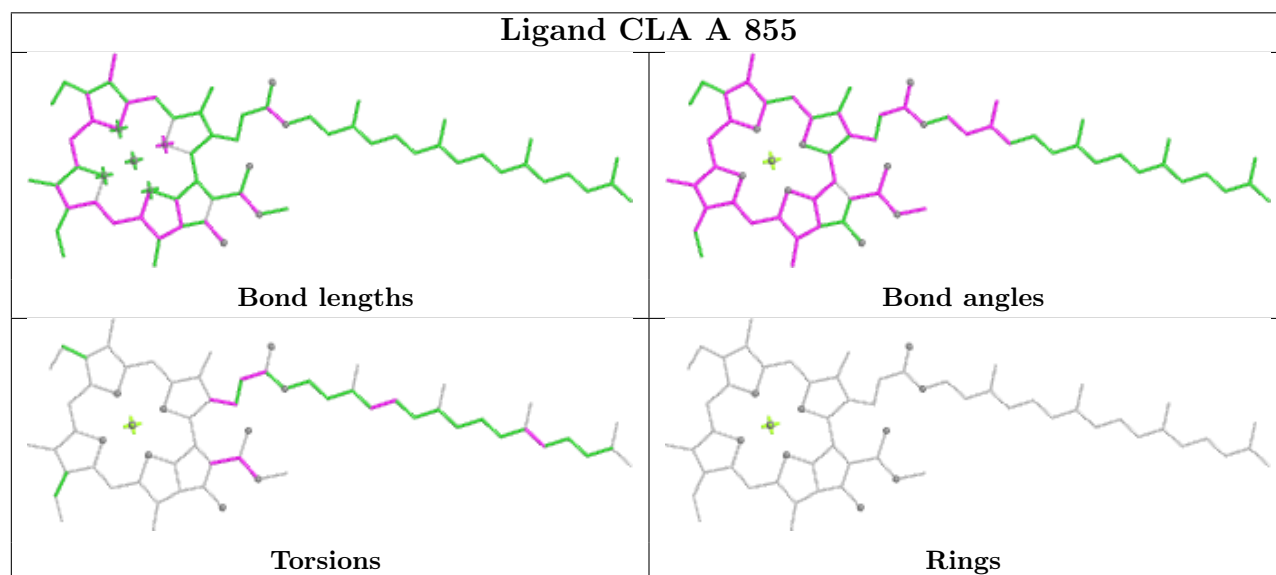
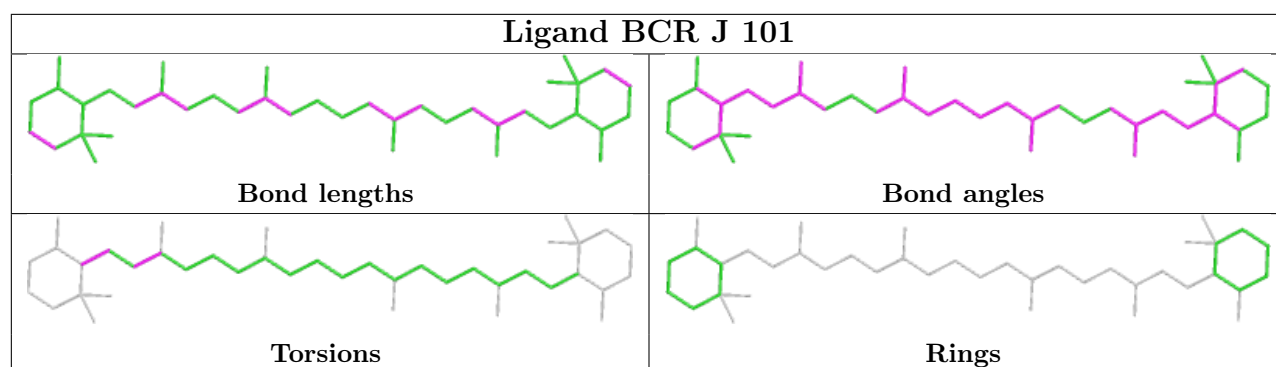


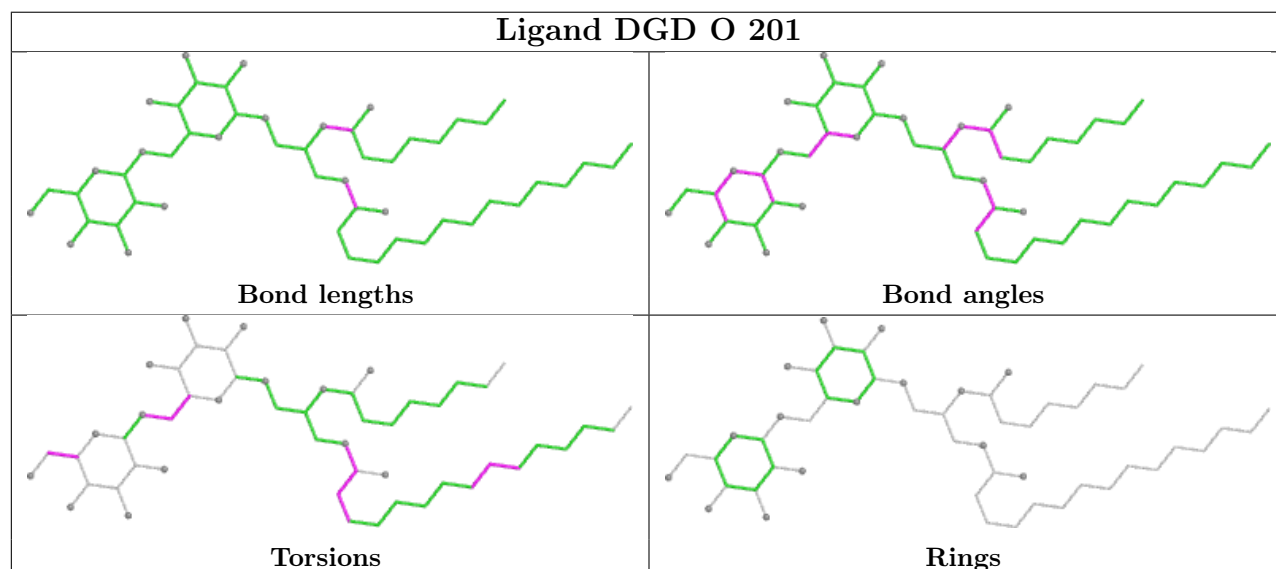
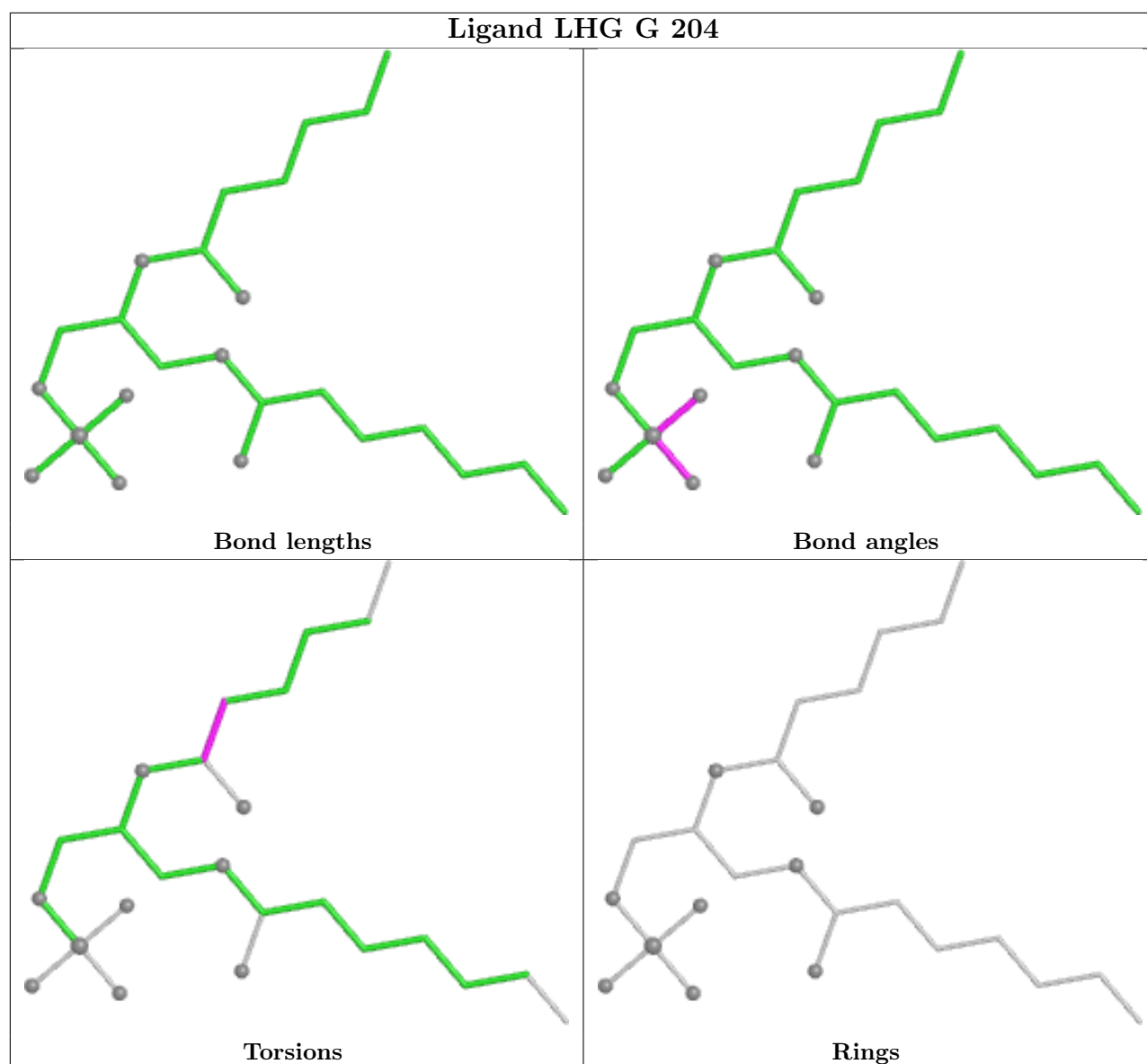


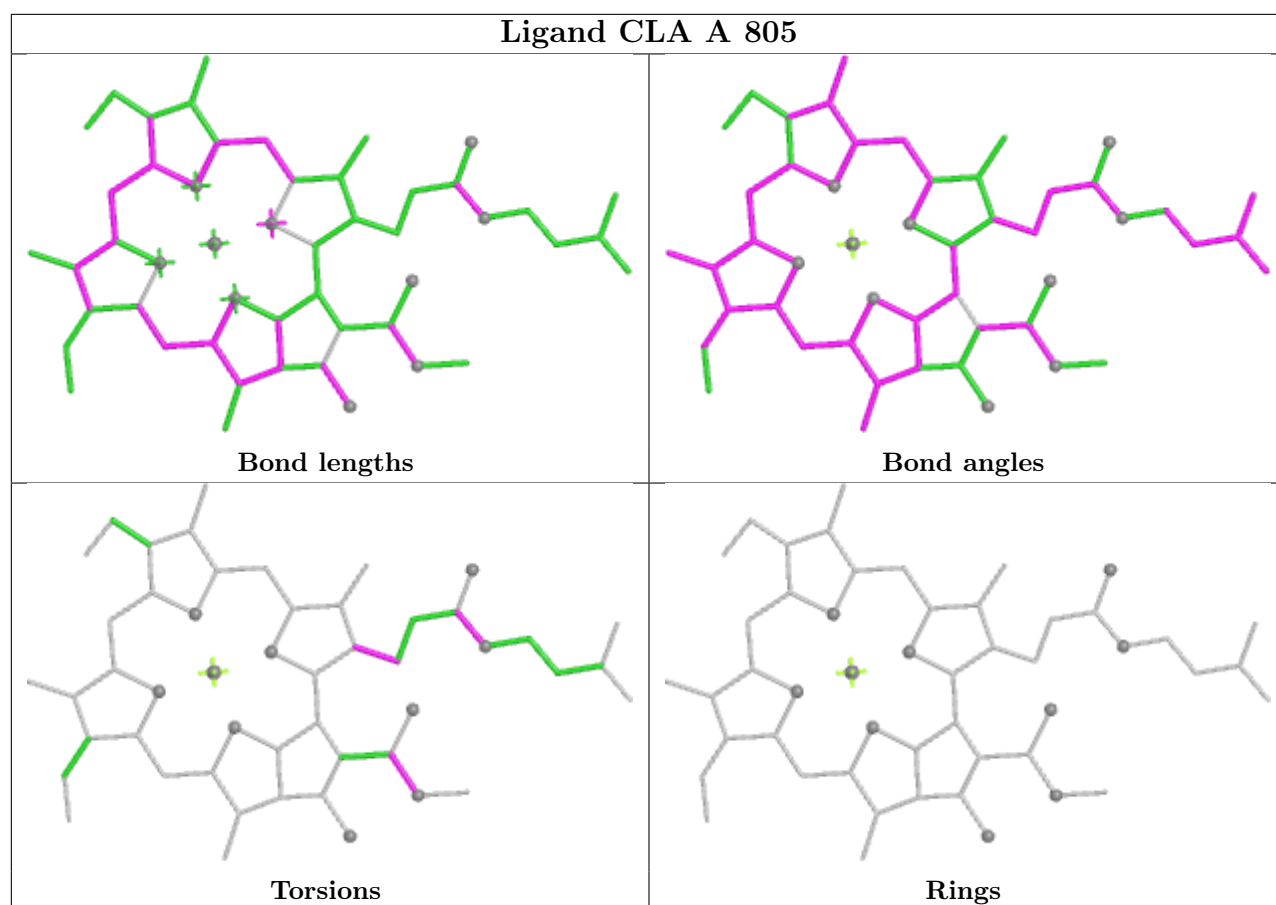
Ligand CLA A 832

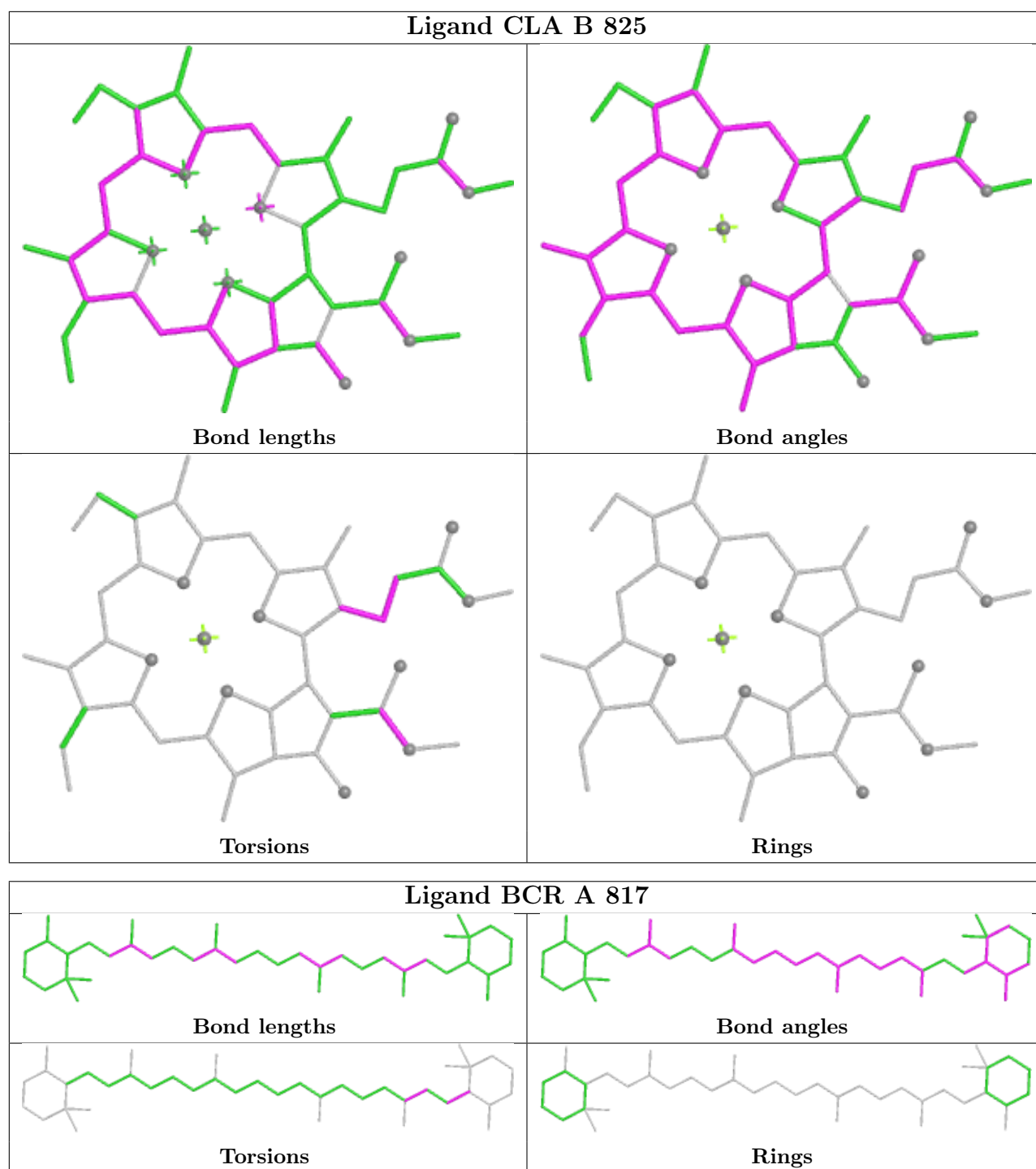


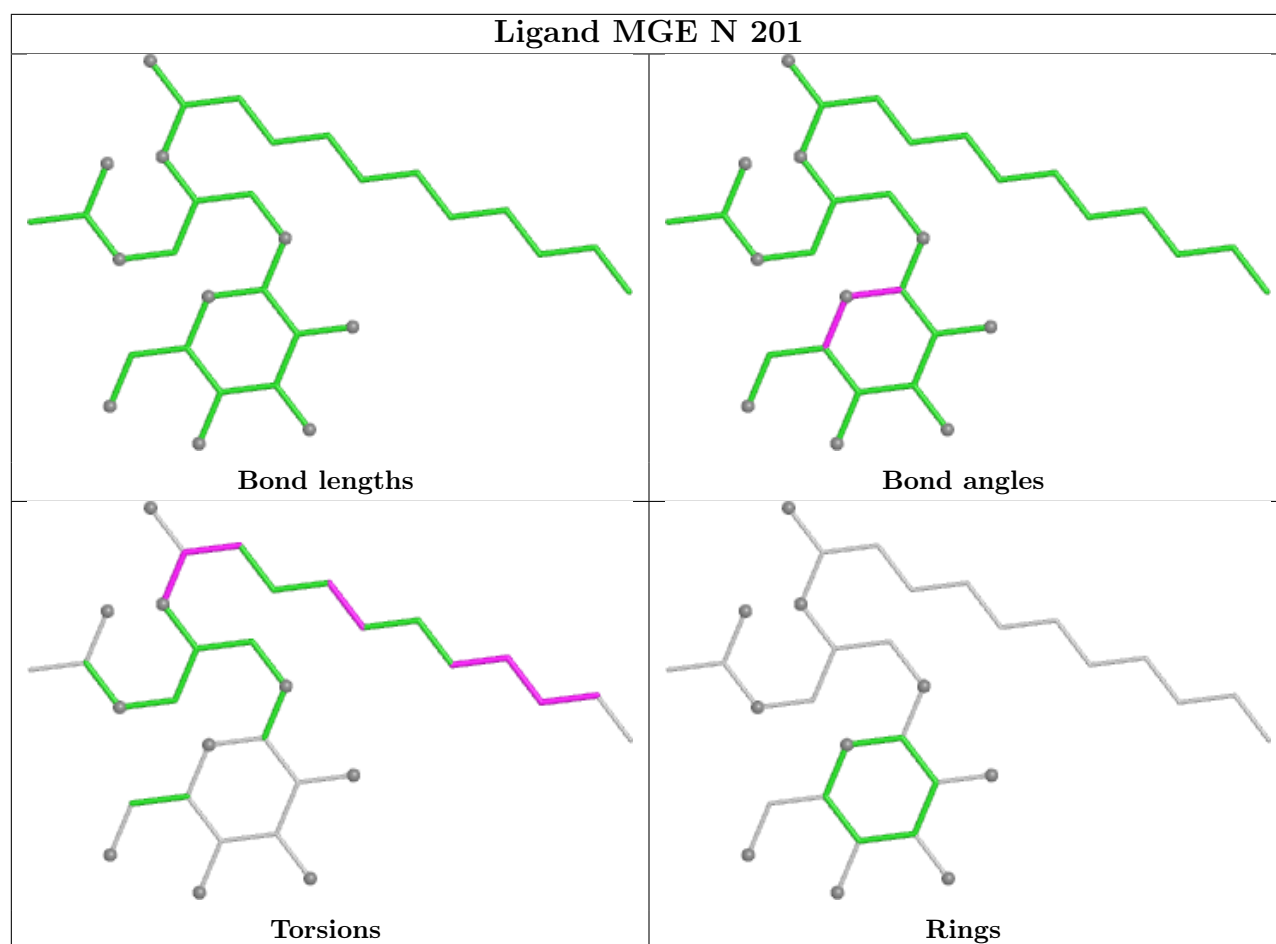




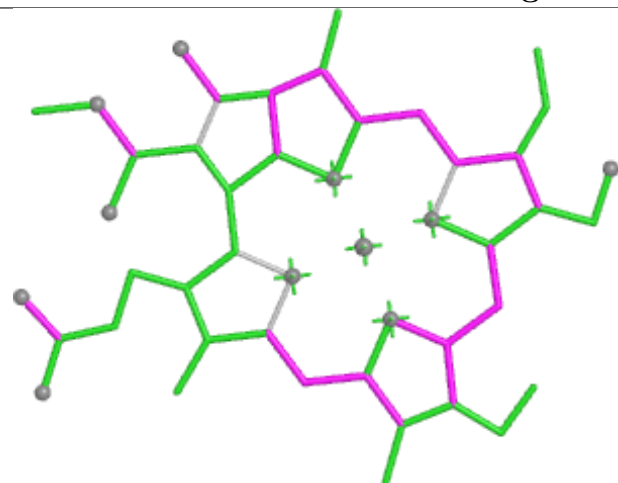




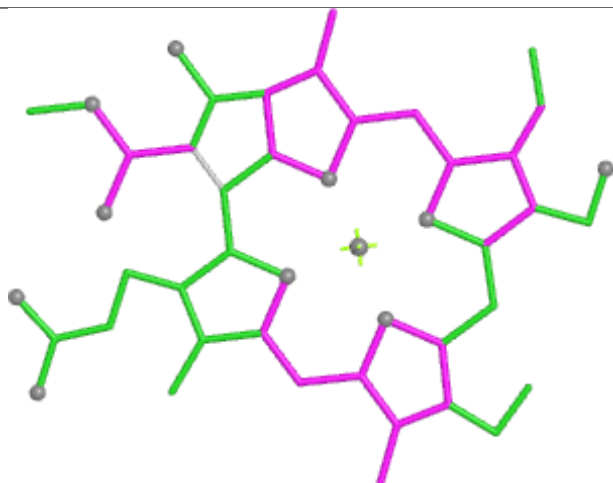




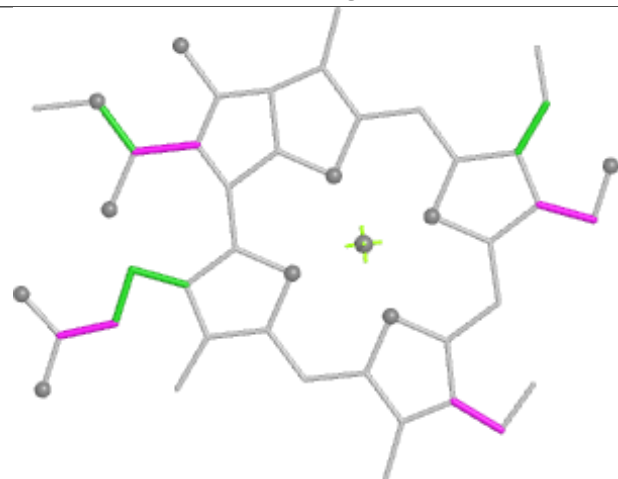
Ligand CHL 1 316



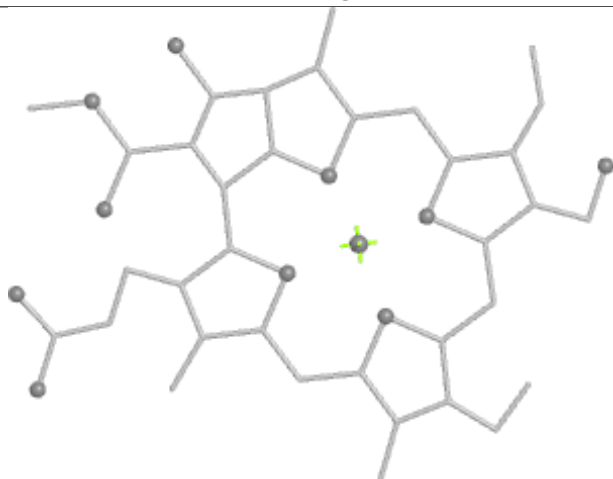
Bond lengths



Bond angles

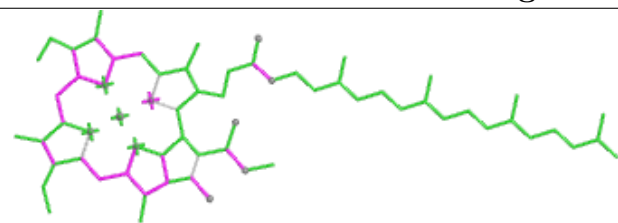


Torsions

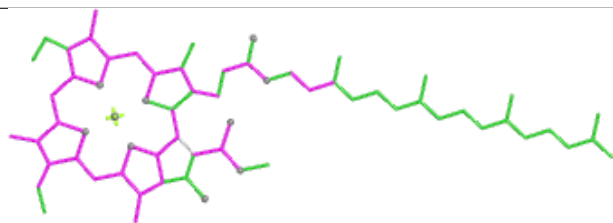


Rings

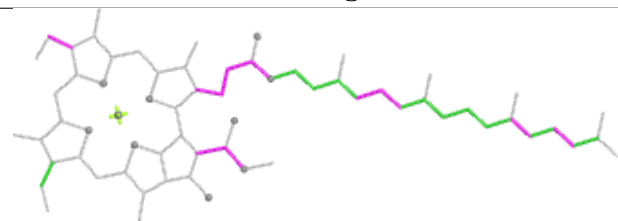
Ligand CLA B 850



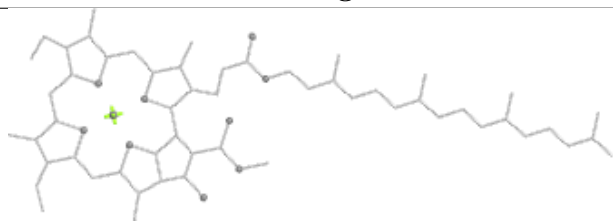
Bond lengths



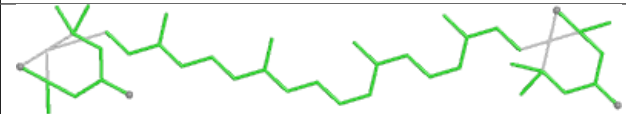
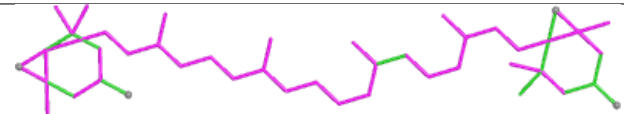
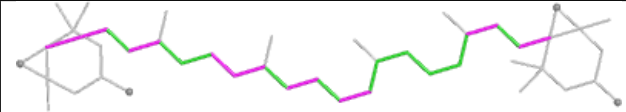
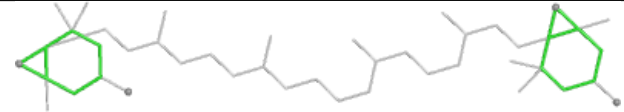
Bond angles

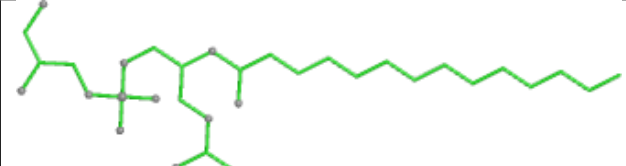
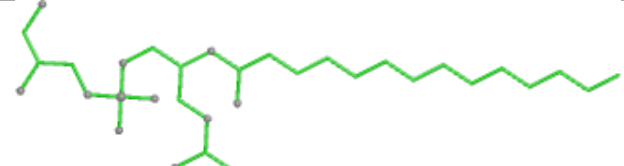
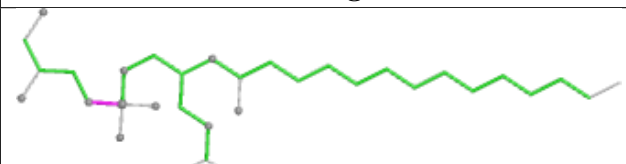
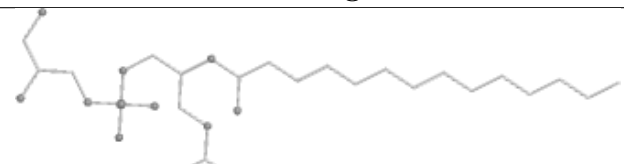


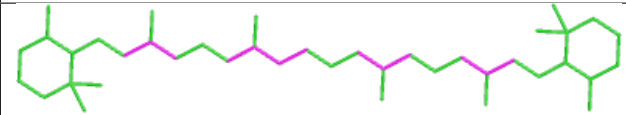
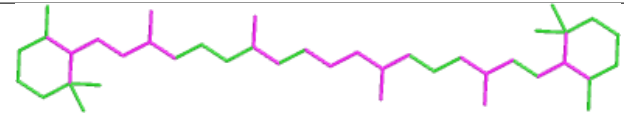
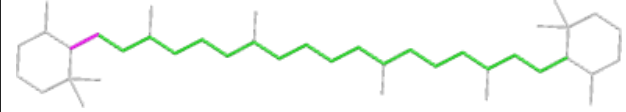
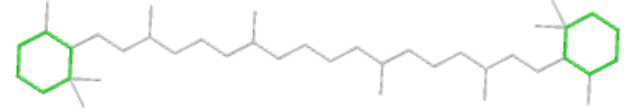
Torsions

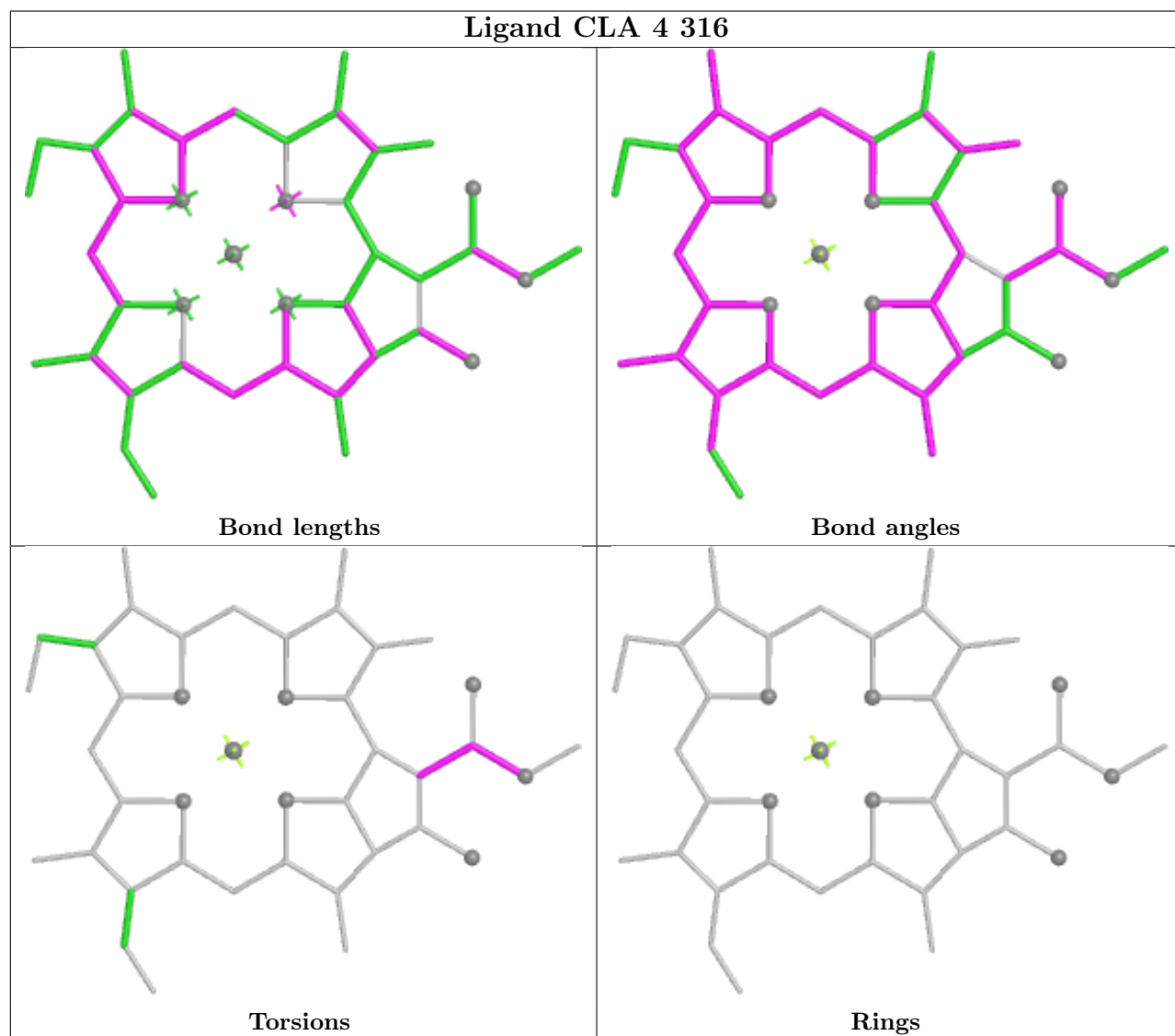
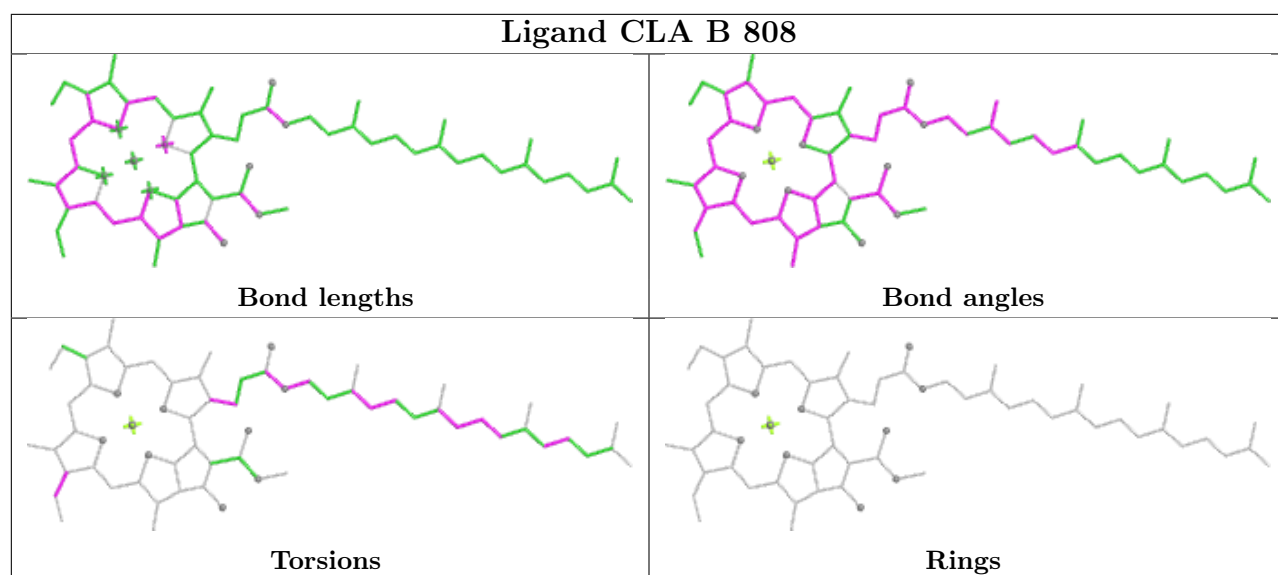


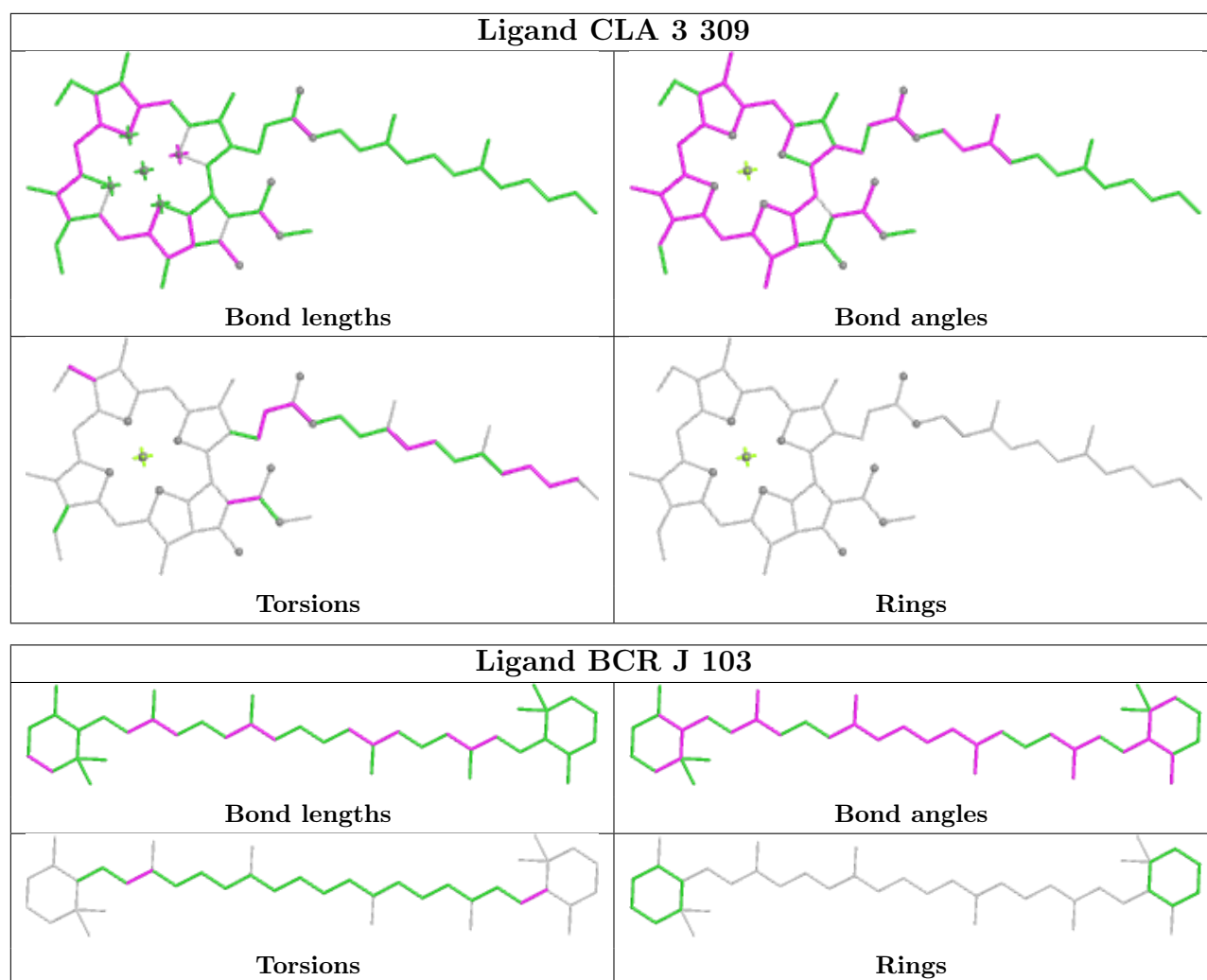
Rings

Ligand XAT 1 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

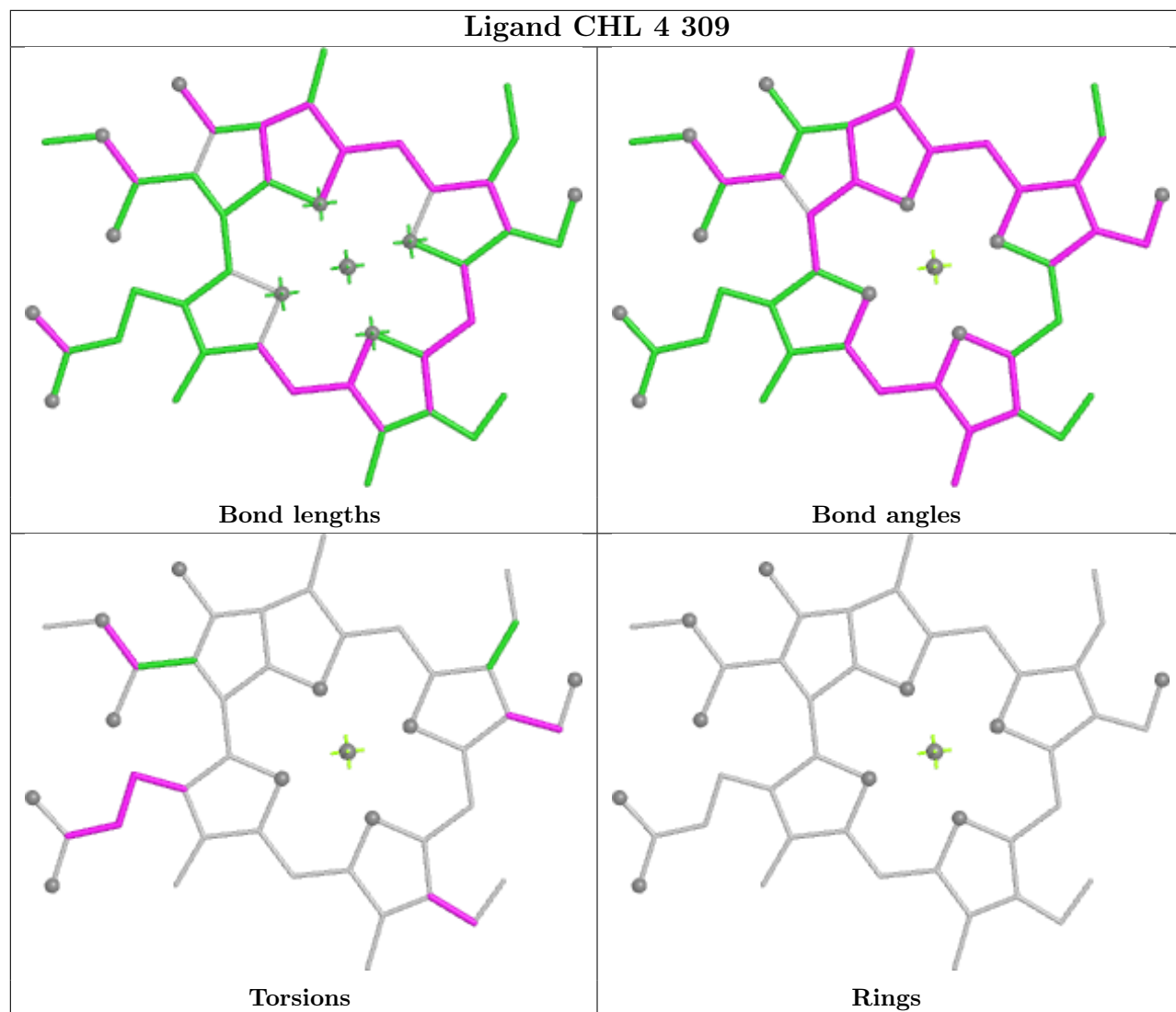
Ligand LHG A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

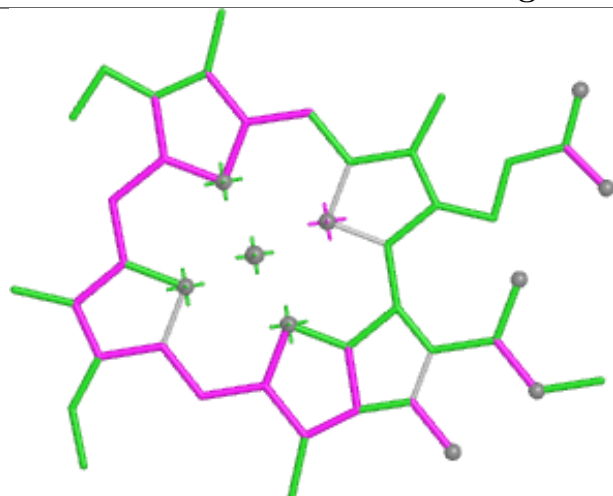




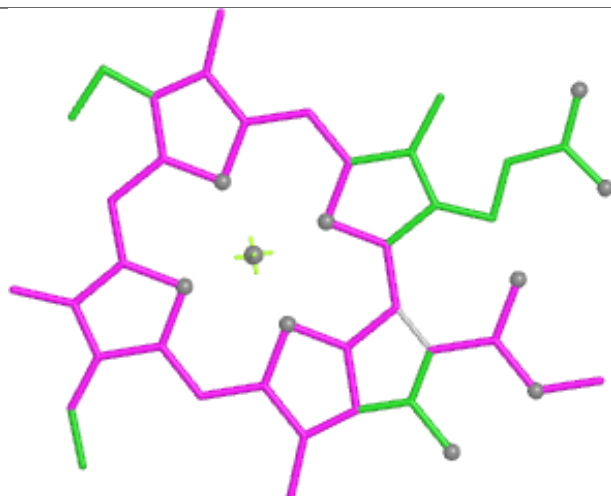
Ligand CHL 4 309



Ligand CLA 3 318



Bond lengths



Bond angles

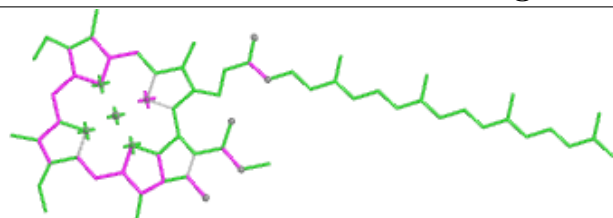


Torsions

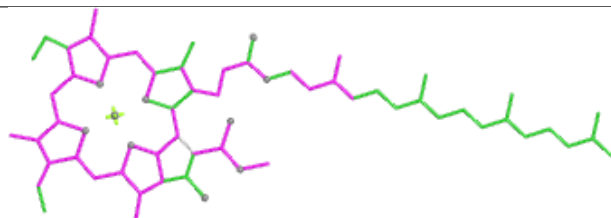


Rings

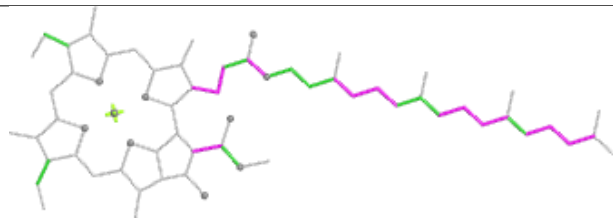
Ligand CLA A 810



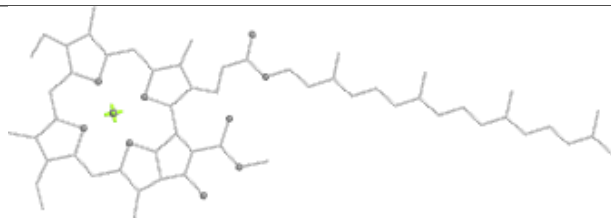
Bond lengths



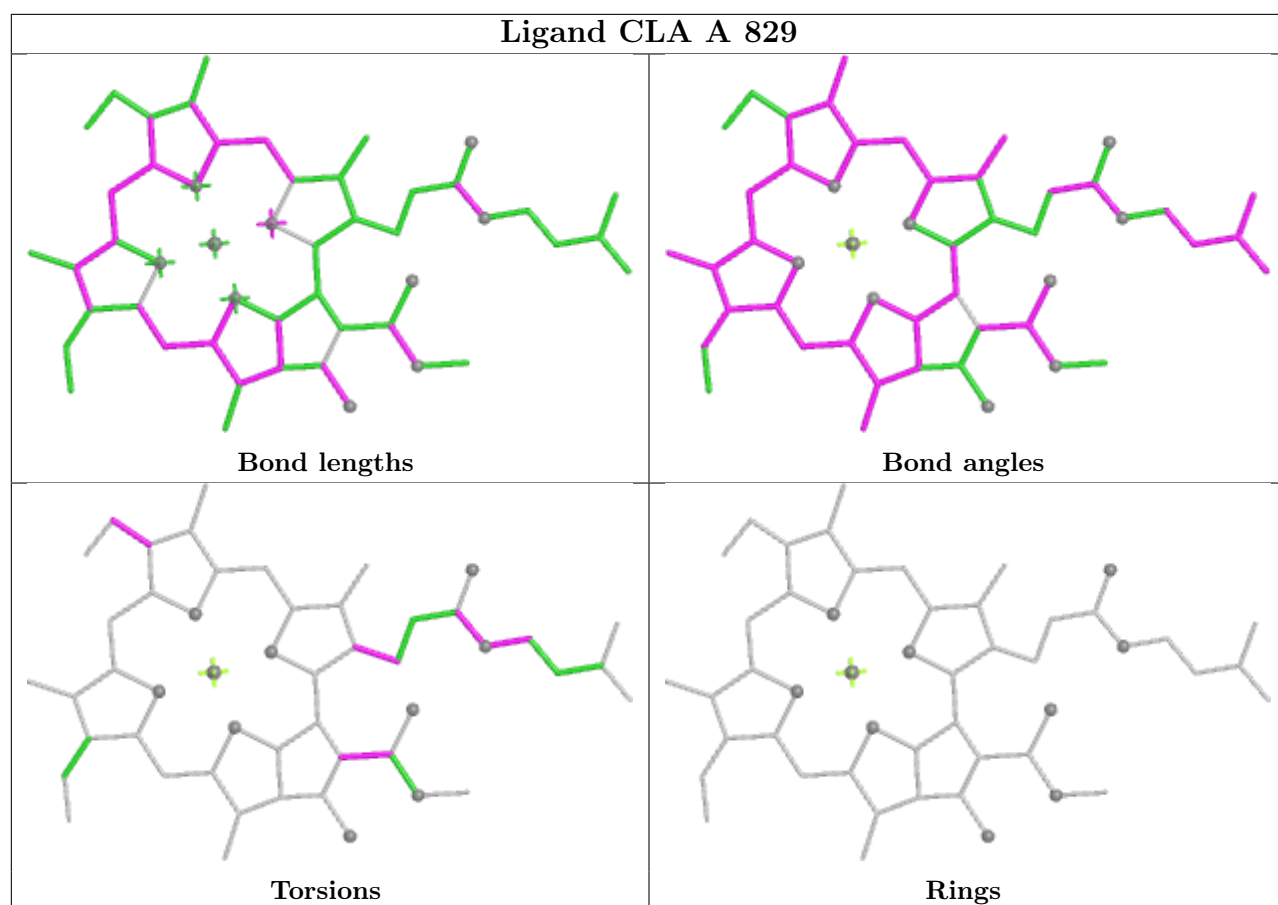
Bond angles



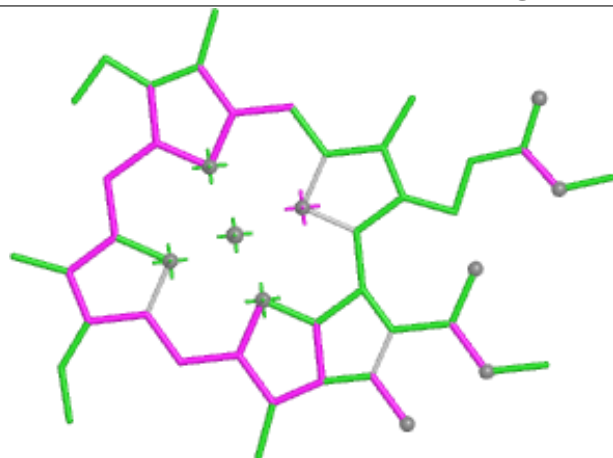
Torsions



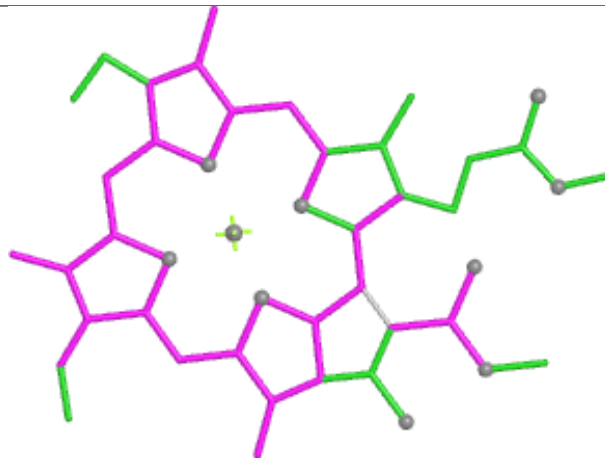
Rings



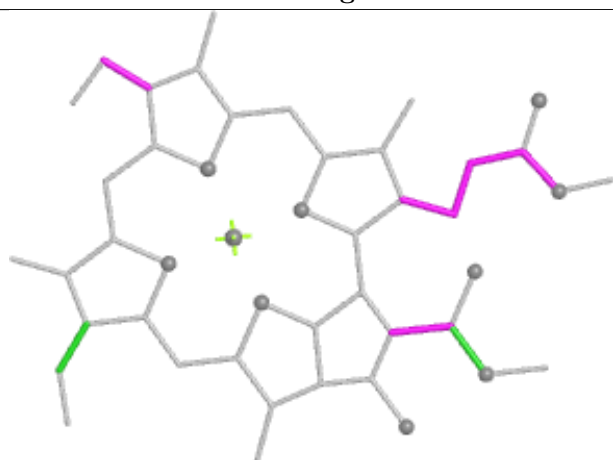
Ligand CLA X 313



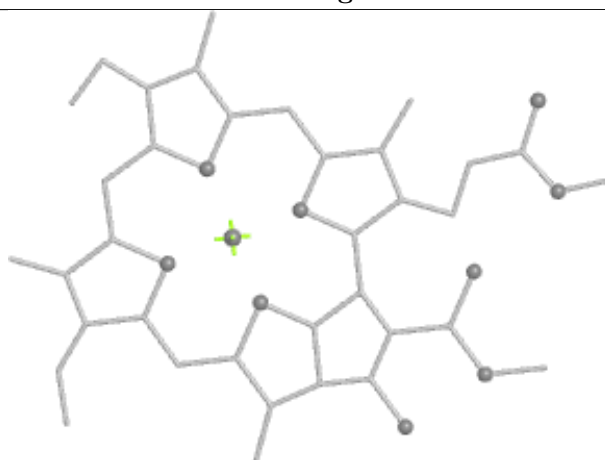
Bond lengths



Bond angles

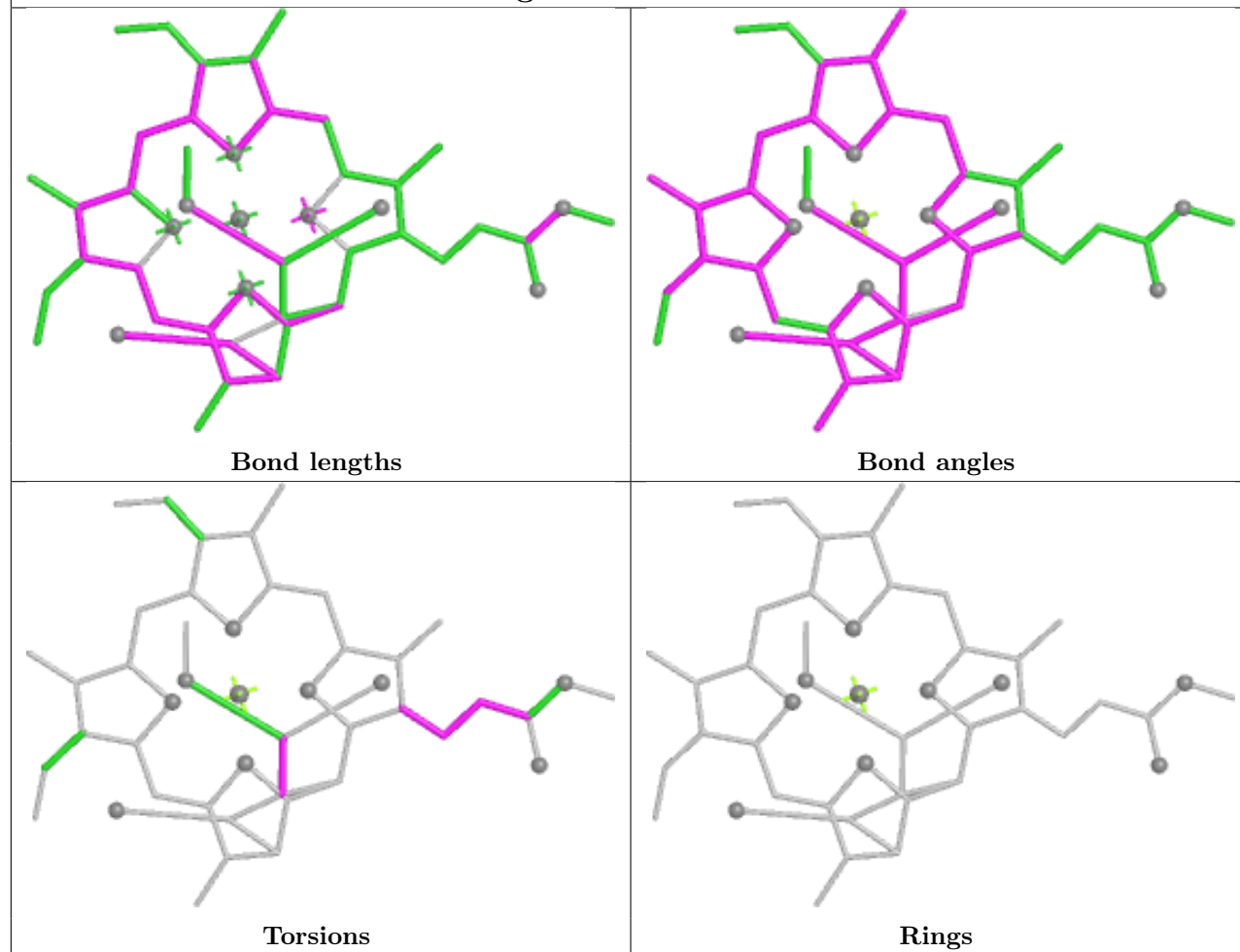


Torsions

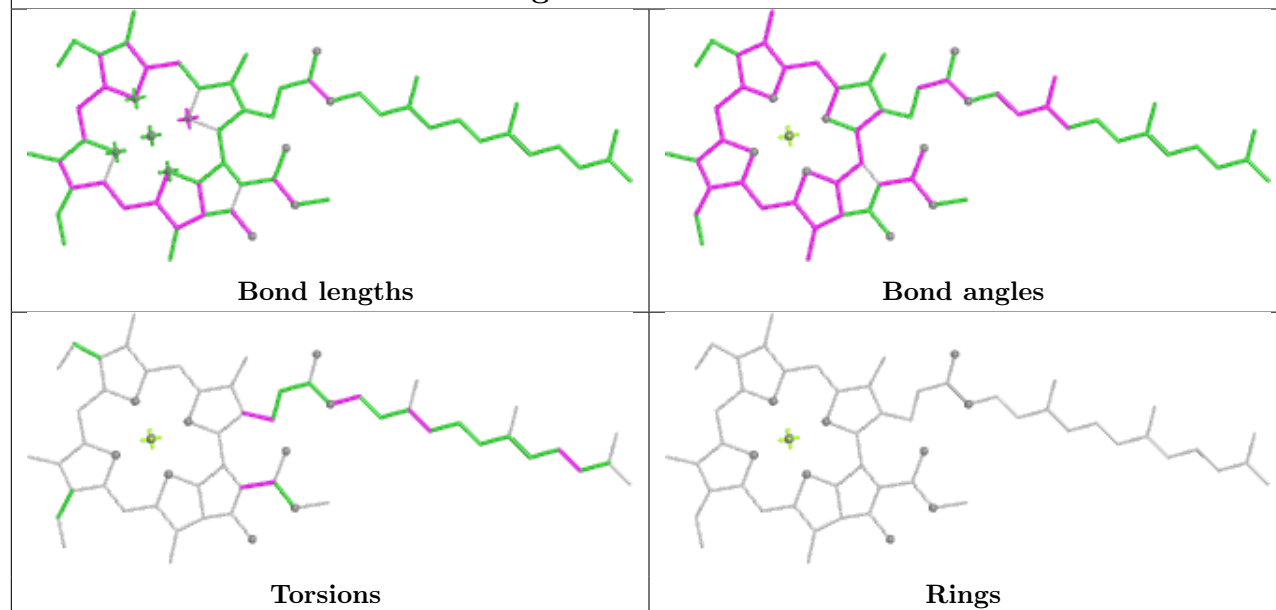


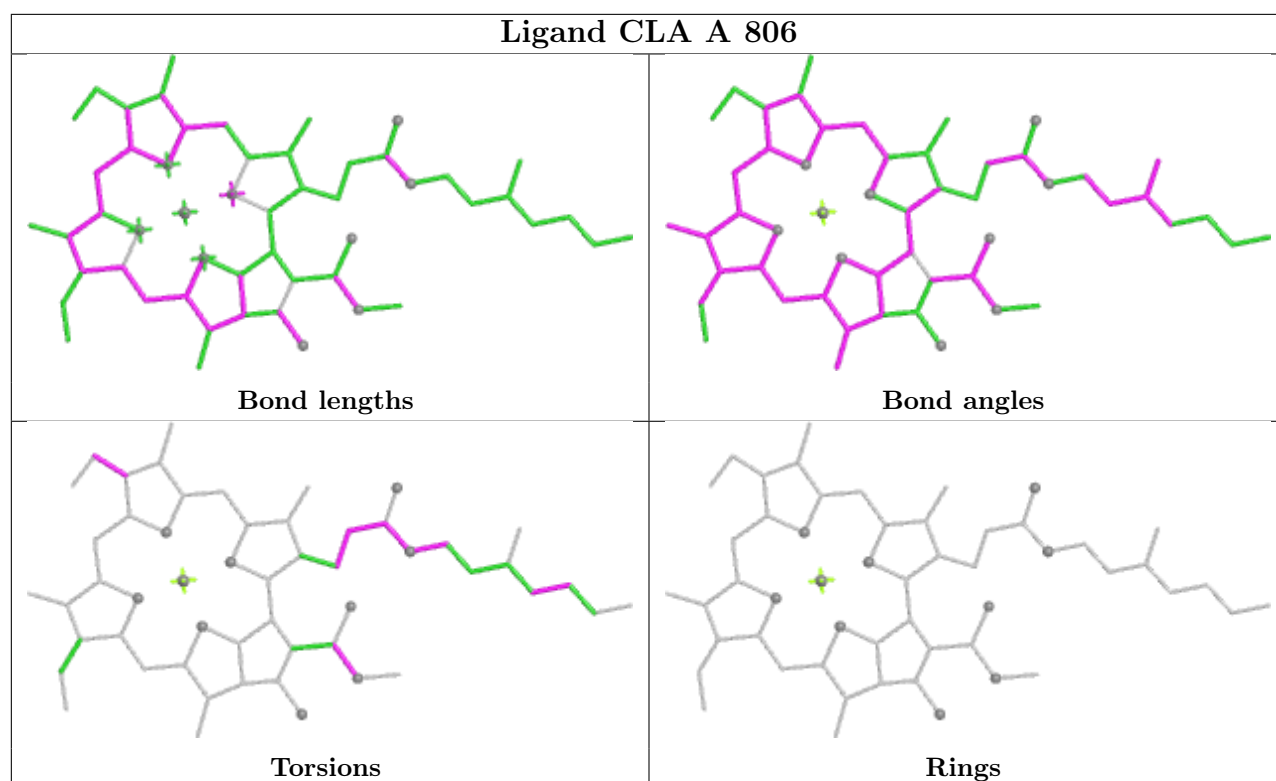
Rings

Ligand CLA X 304

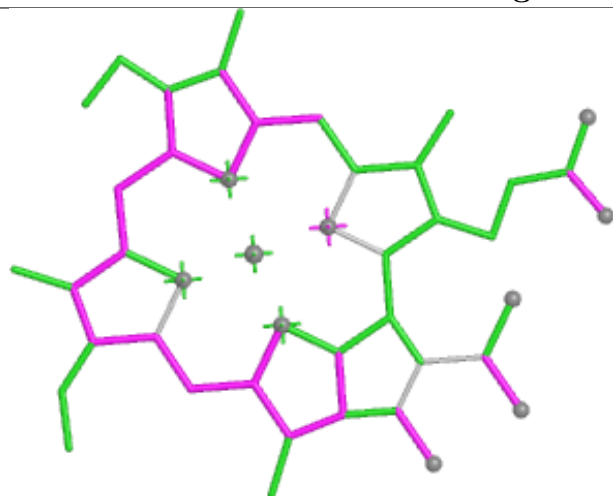


Ligand CLA A 836

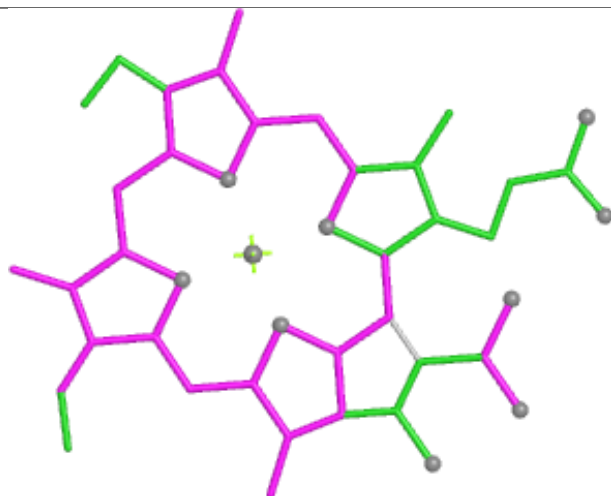




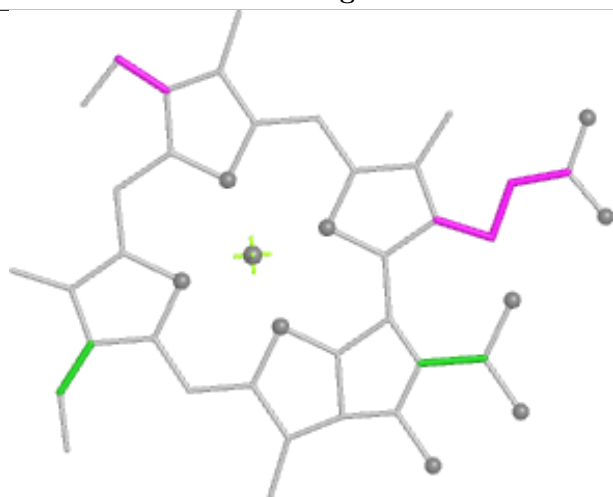
Ligand CLA K 202



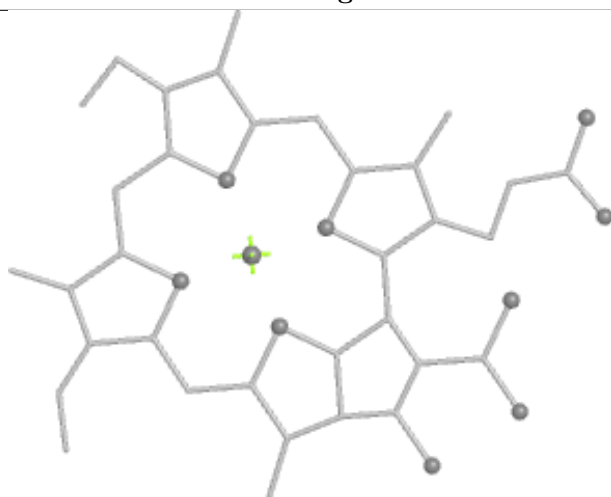
Bond lengths



Bond angles

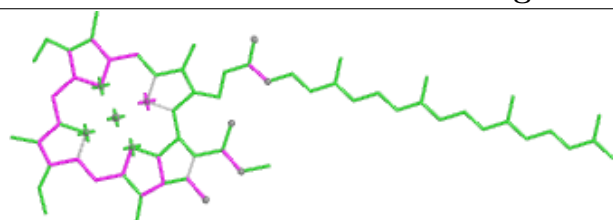


Torsions

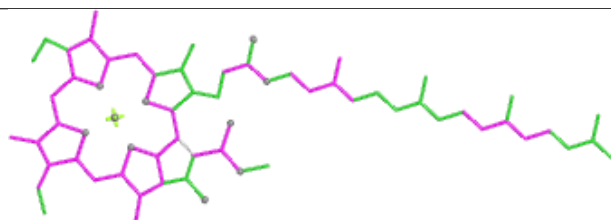


Rings

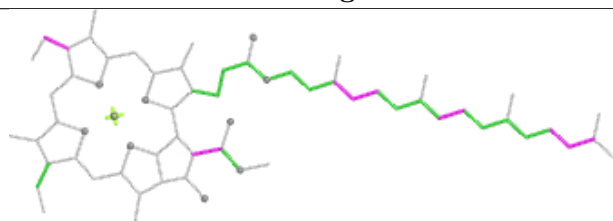
Ligand CLA A 850



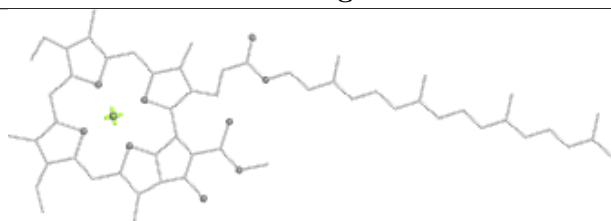
Bond lengths



Bond angles

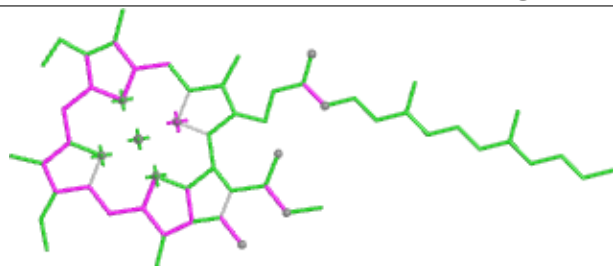


Torsions

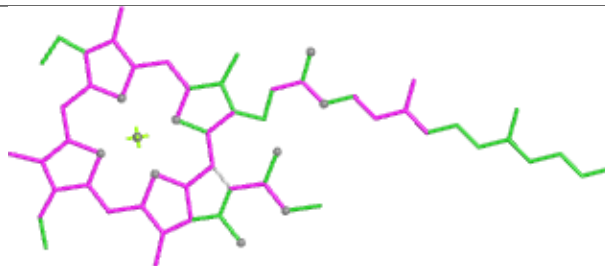


Rings

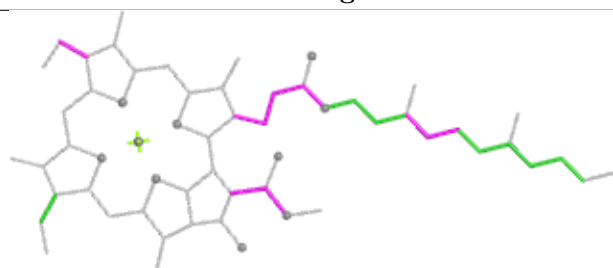
Ligand CLA B 815



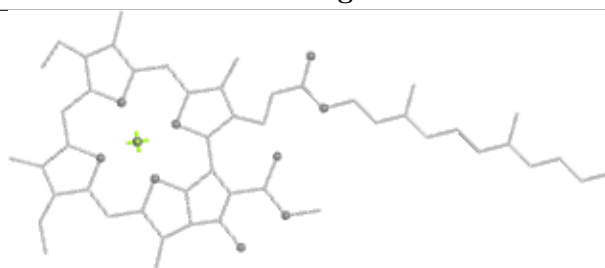
Bond lengths



Bond angles

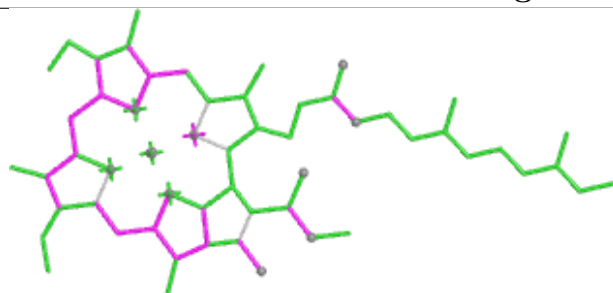


Torsions

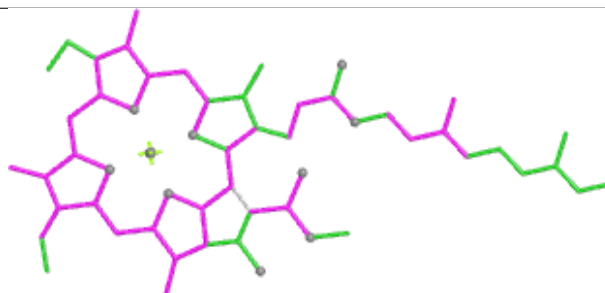


Rings

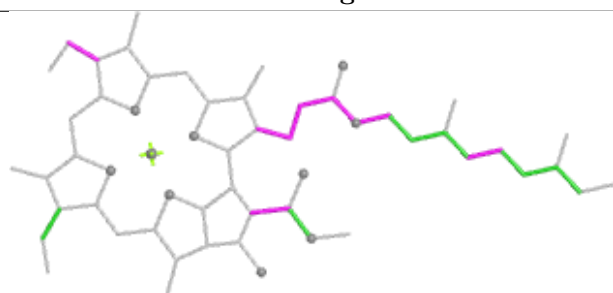
Ligand CLA B 833



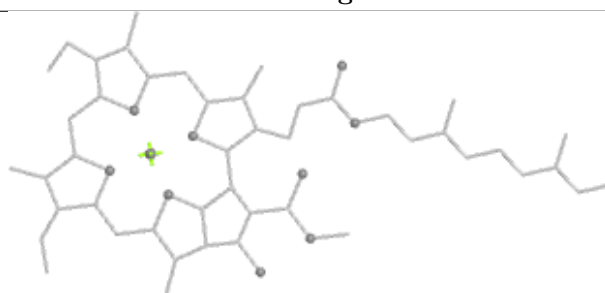
Bond lengths



Bond angles

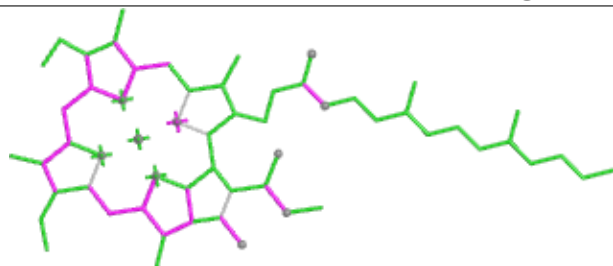


Torsions

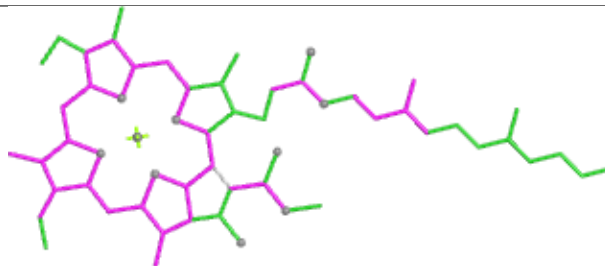


Rings

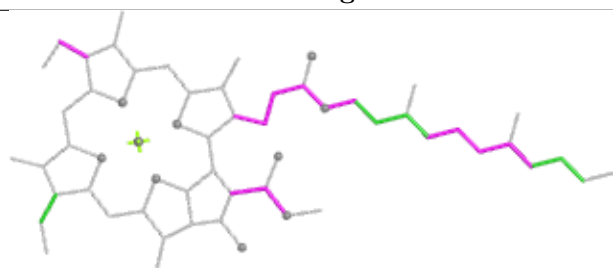
Ligand CLA 3 310



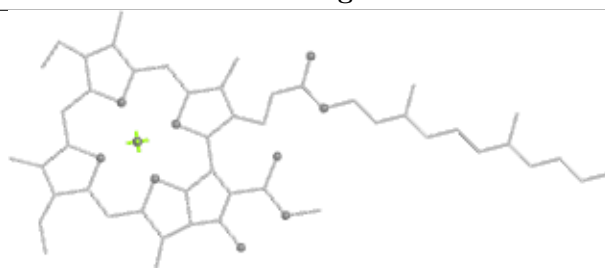
Bond lengths



Bond angles

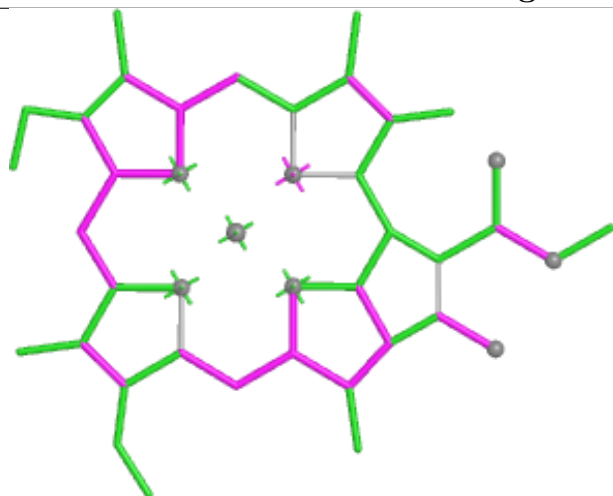


Torsions



Rings

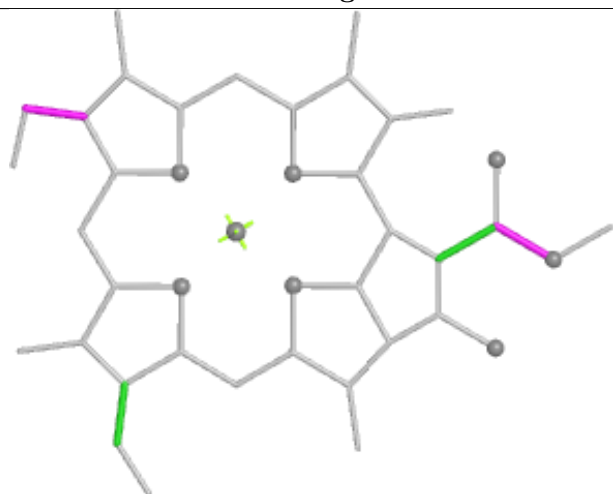
Ligand CLA 1 308



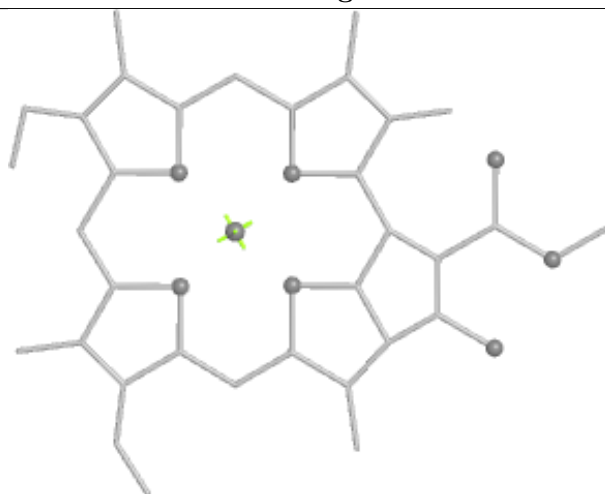
Bond lengths



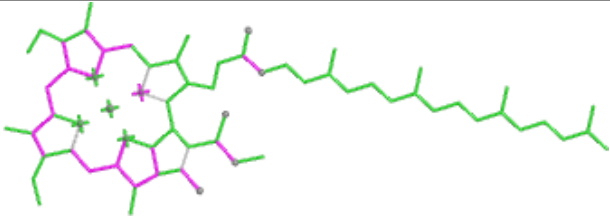
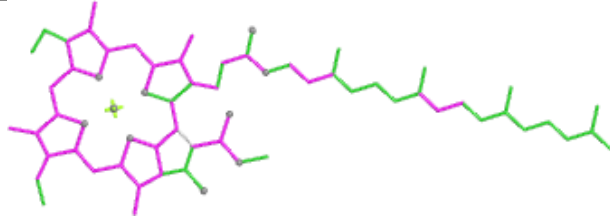
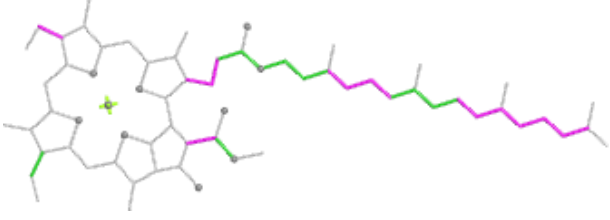
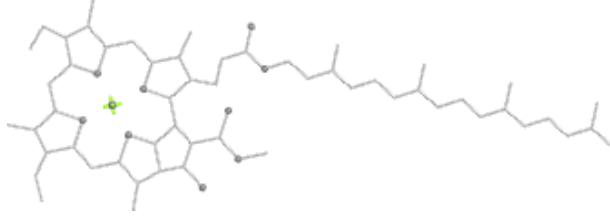
Bond angles

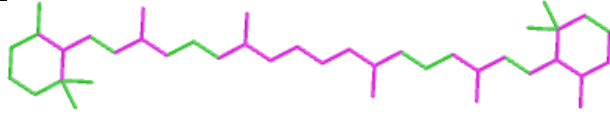
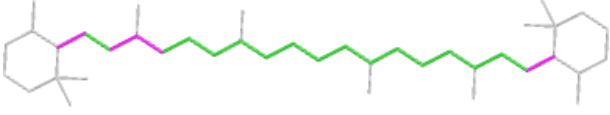
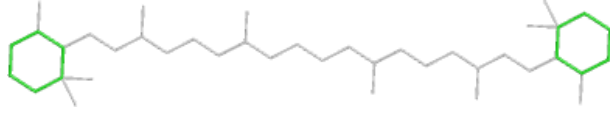


Torsions

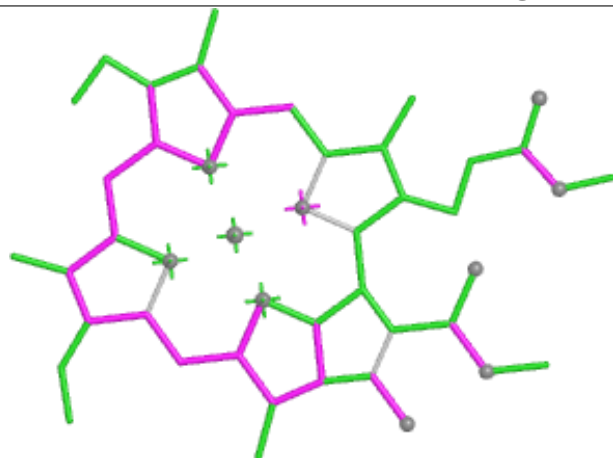


Rings

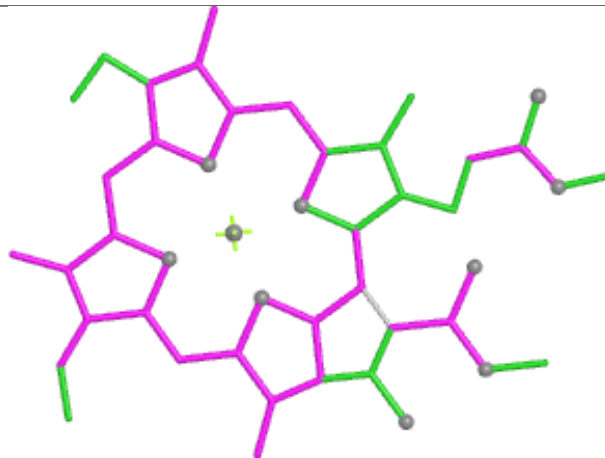
Ligand CLA L 306			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR L 301			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

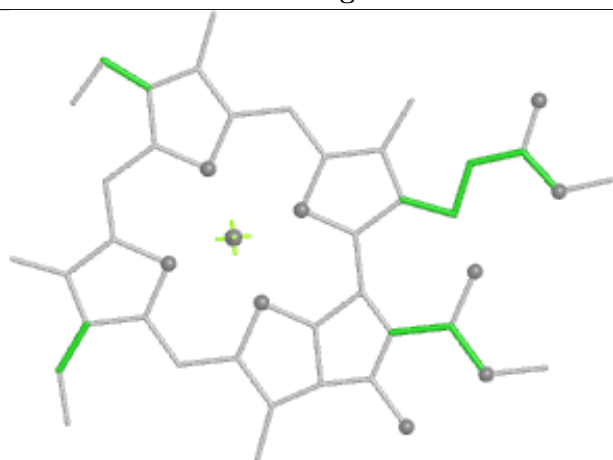
Ligand CLA X 301



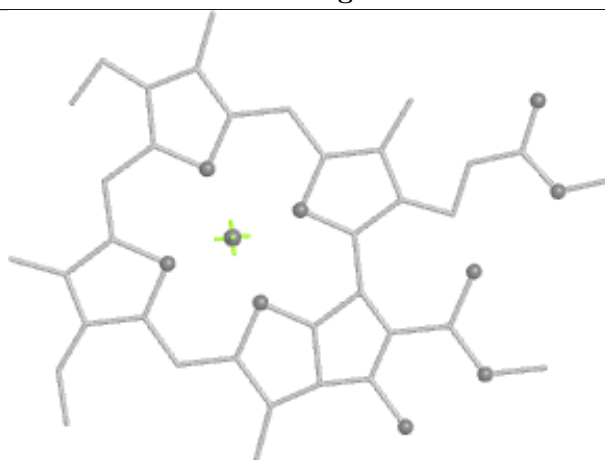
Bond lengths



Bond angles

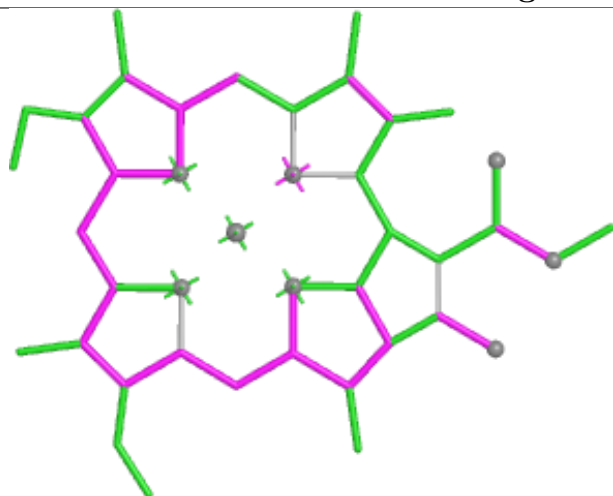


Torsions

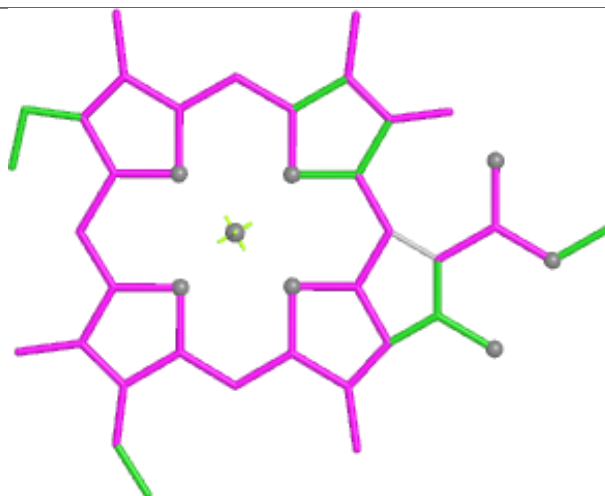


Rings

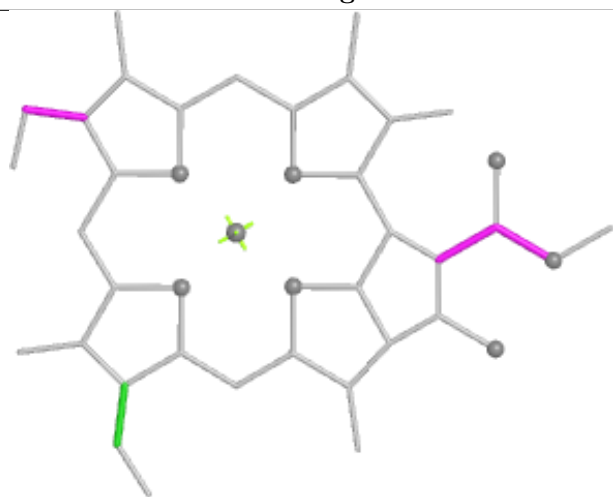
Ligand CLA 3 315



Bond lengths



Bond angles

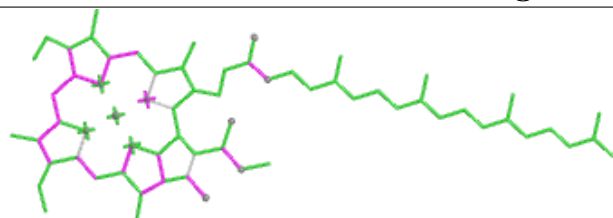


Torsions

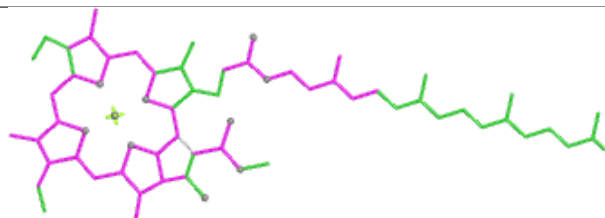


Rings

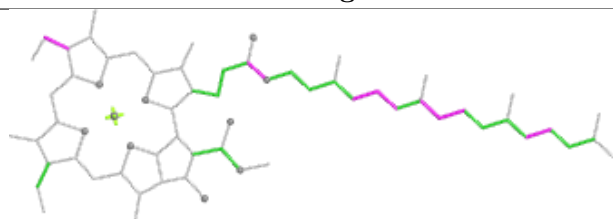
Ligand CLA B 814



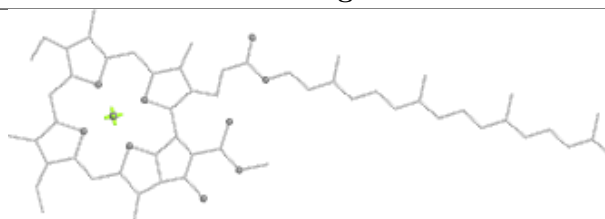
Bond lengths



Bond angles

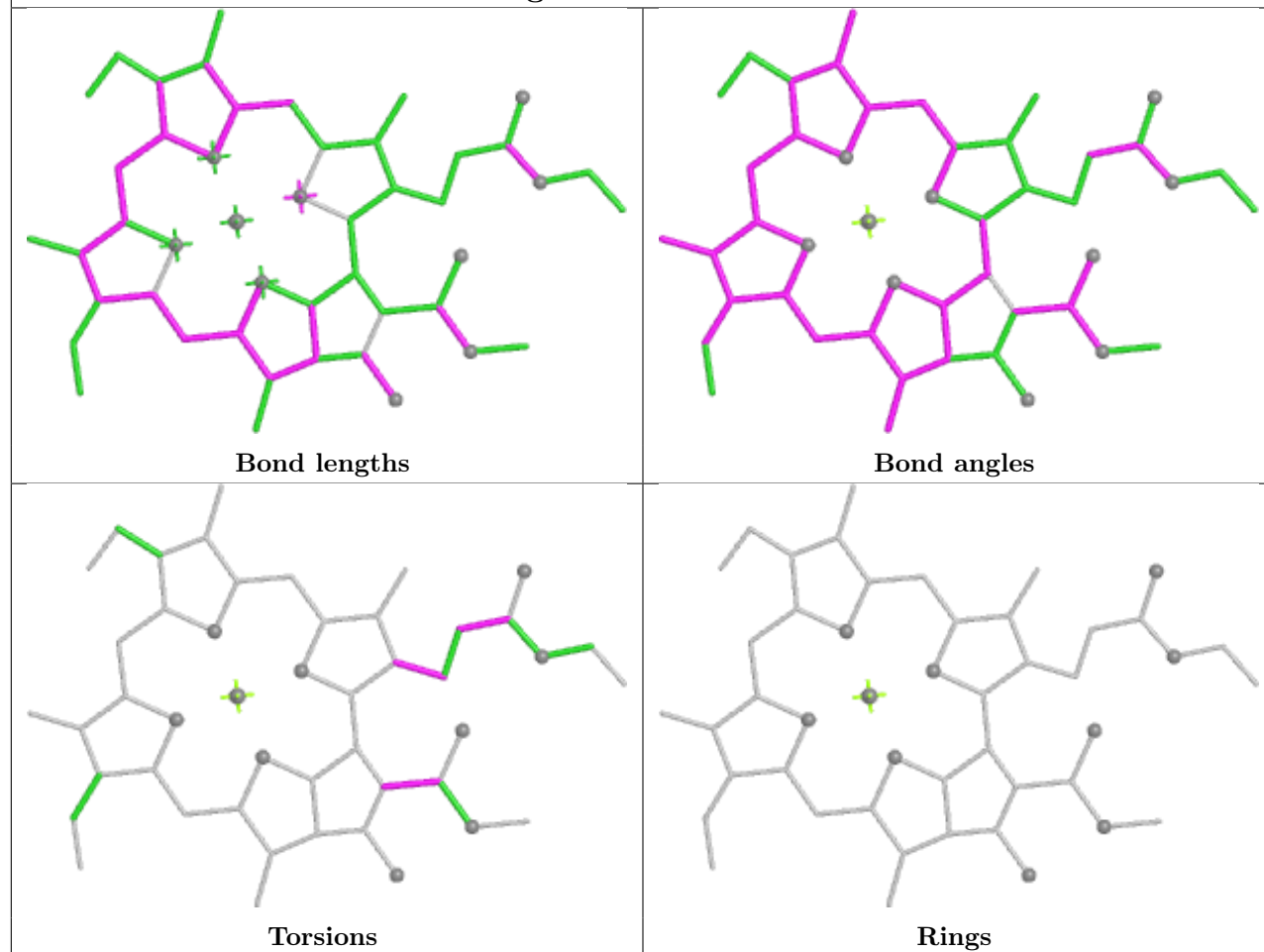


Torsions

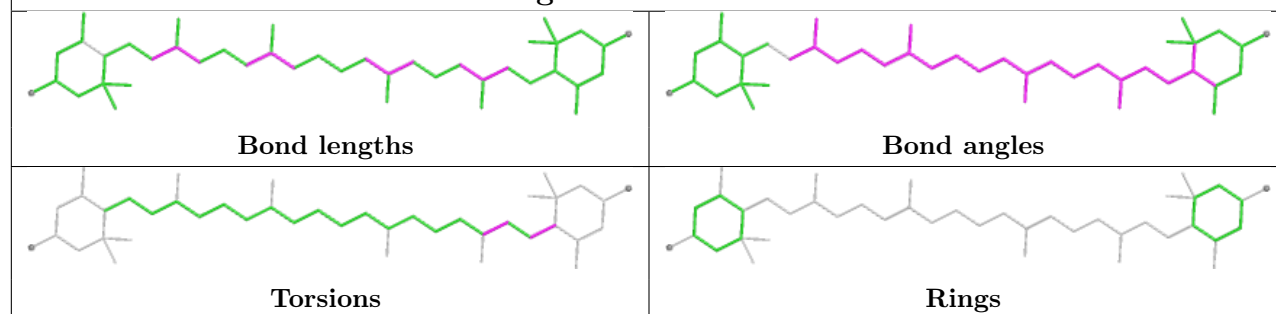


Rings

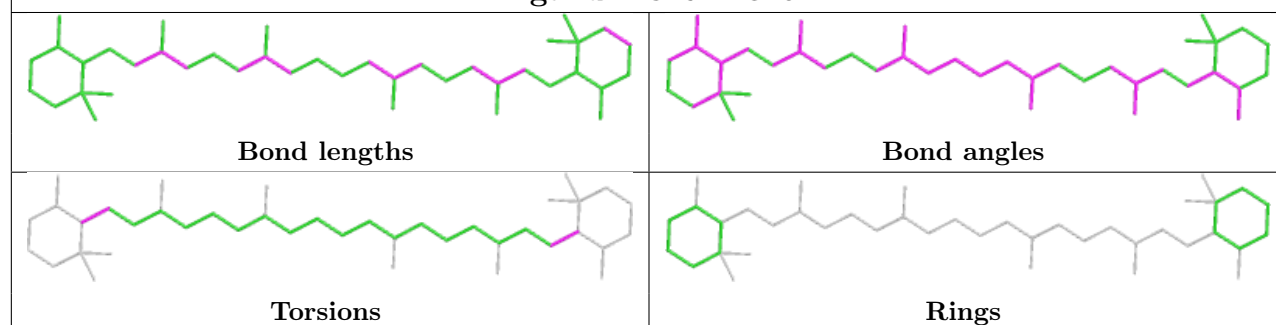
Ligand CLA O 209

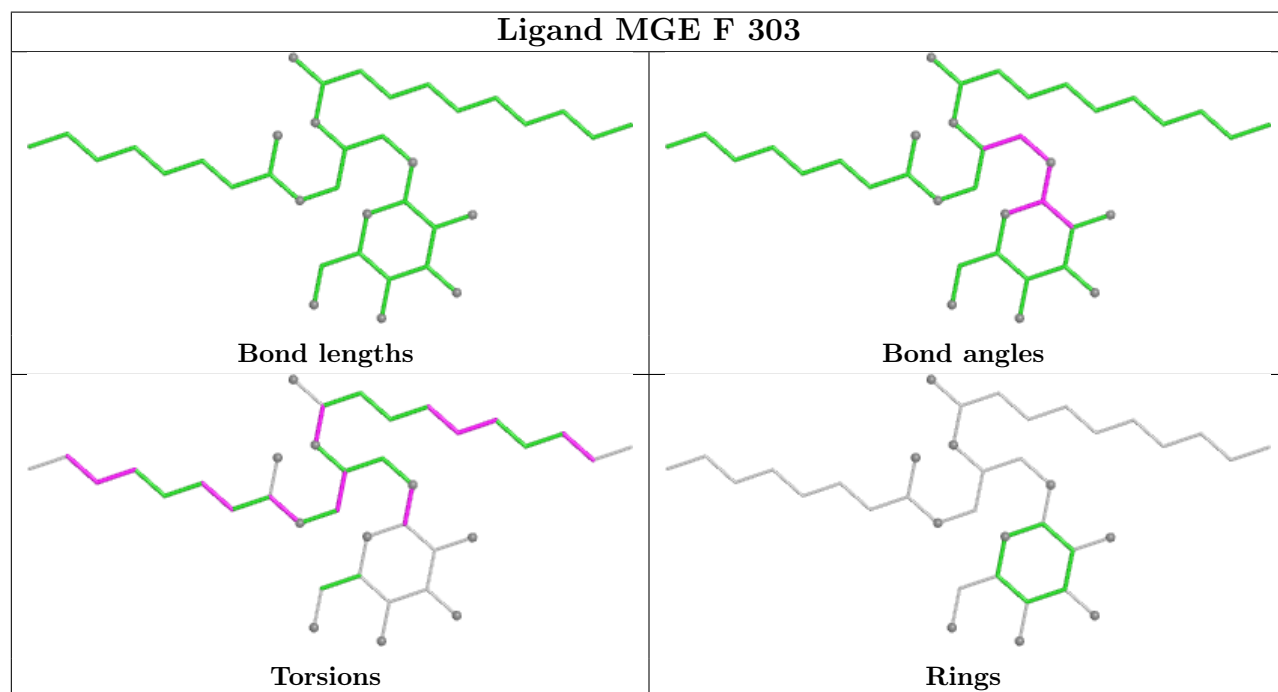
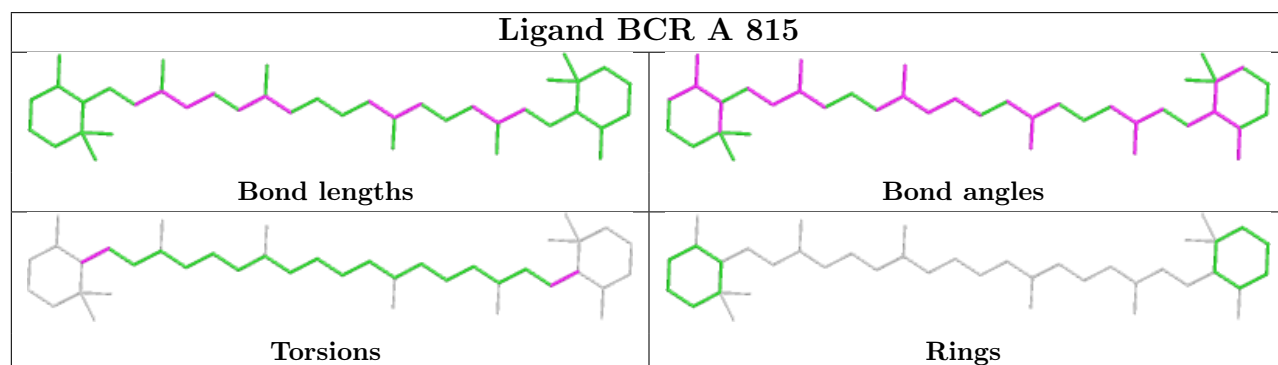
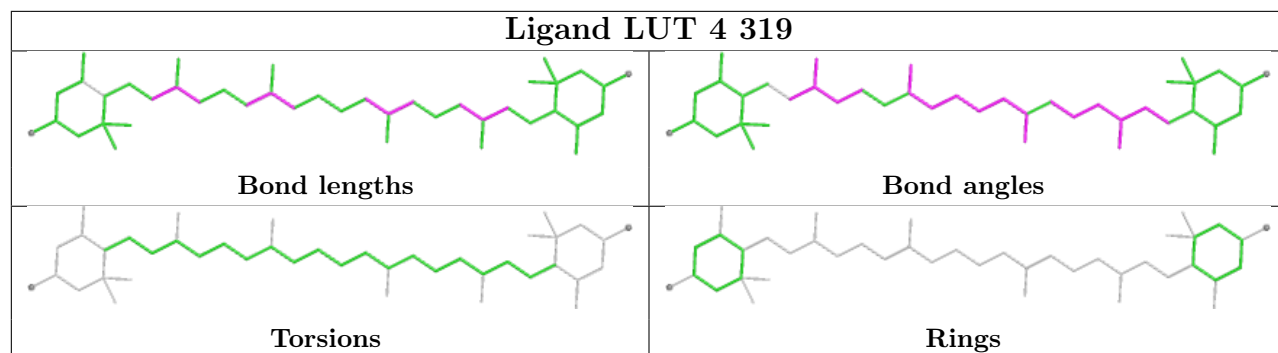


Ligand LUT 4 322

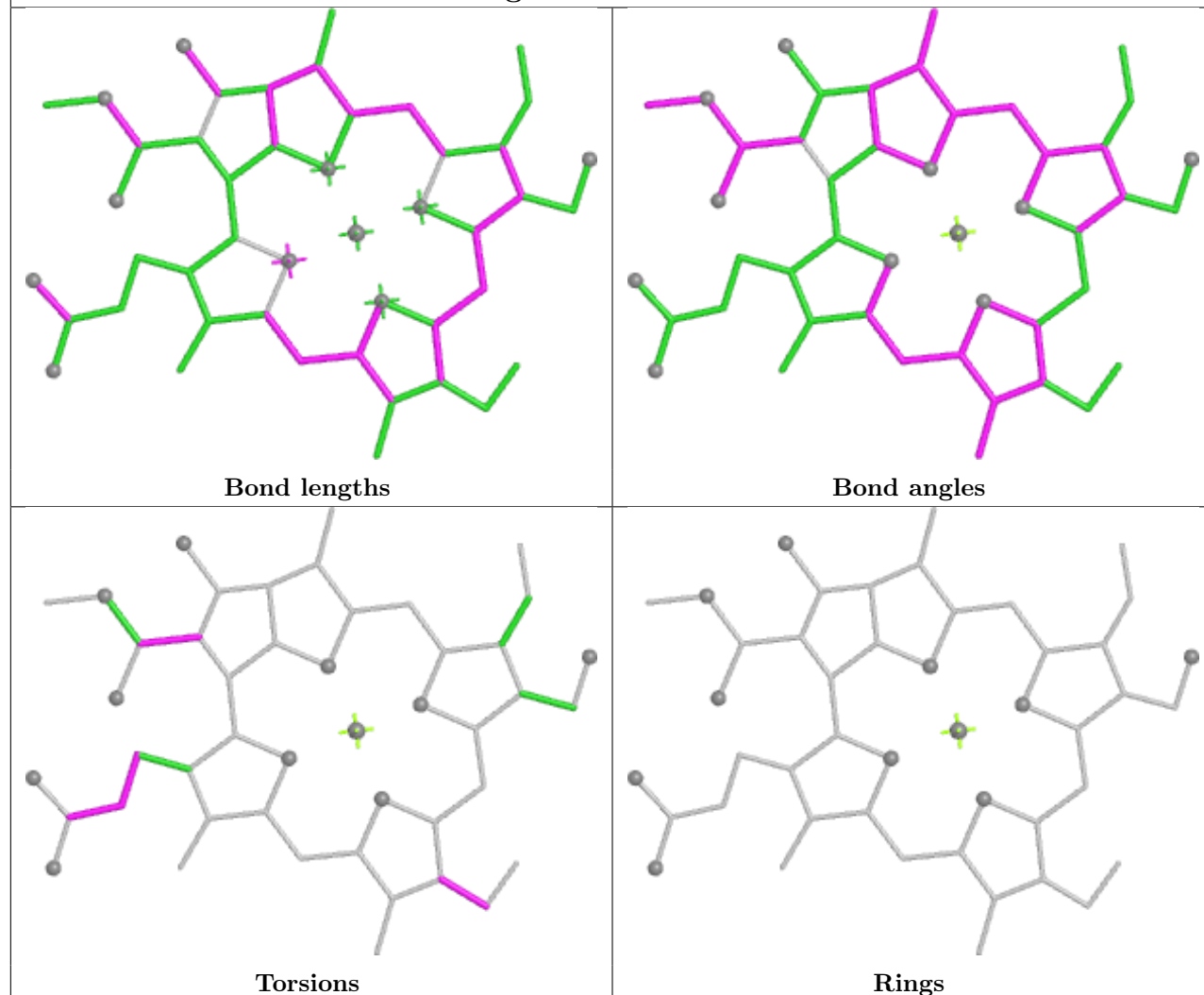


Ligand BCR A 819

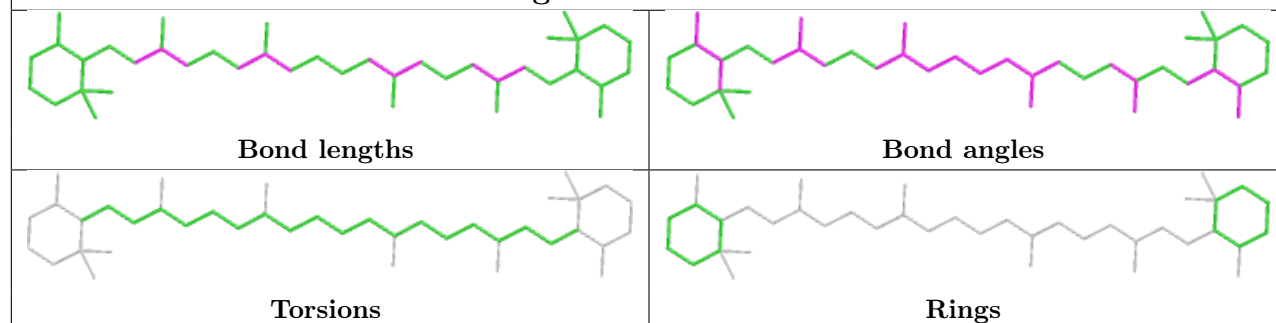


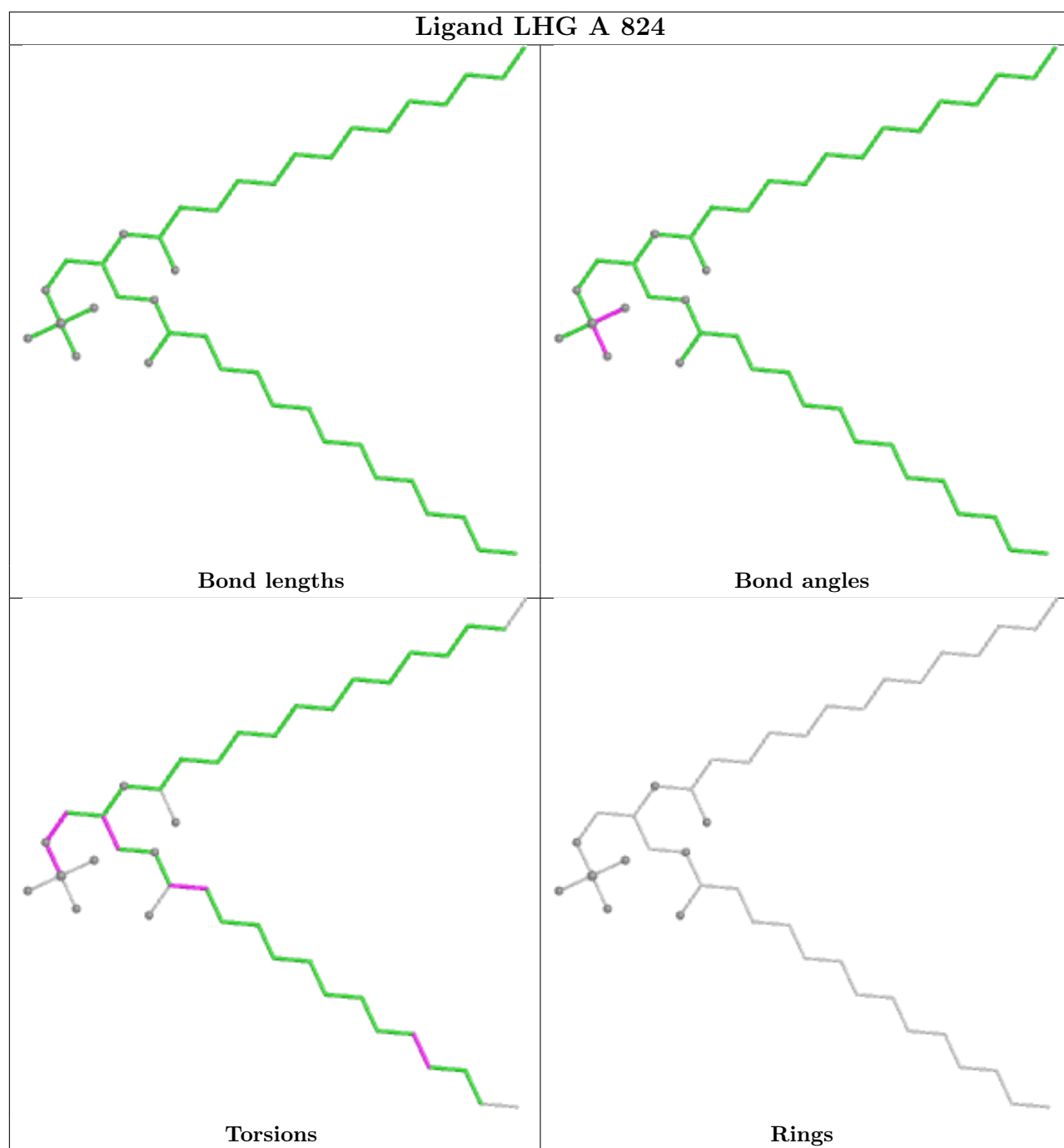


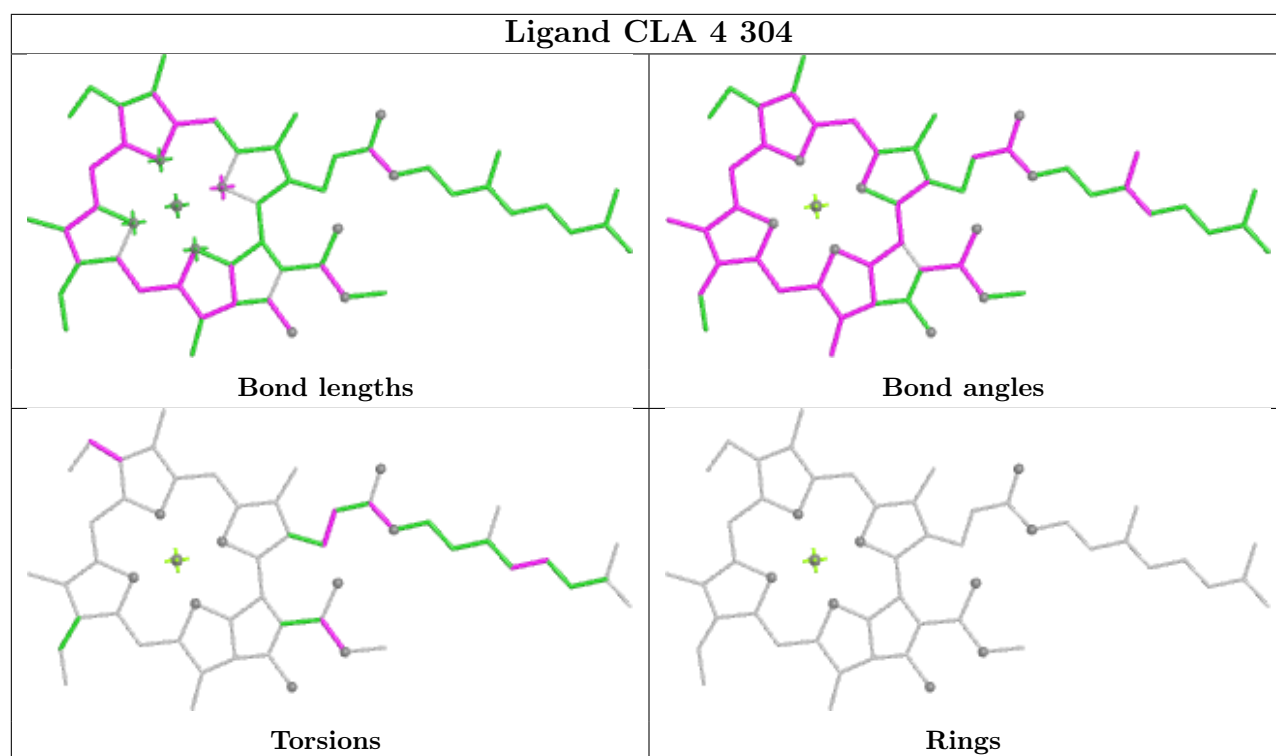
Ligand CHL 3 314



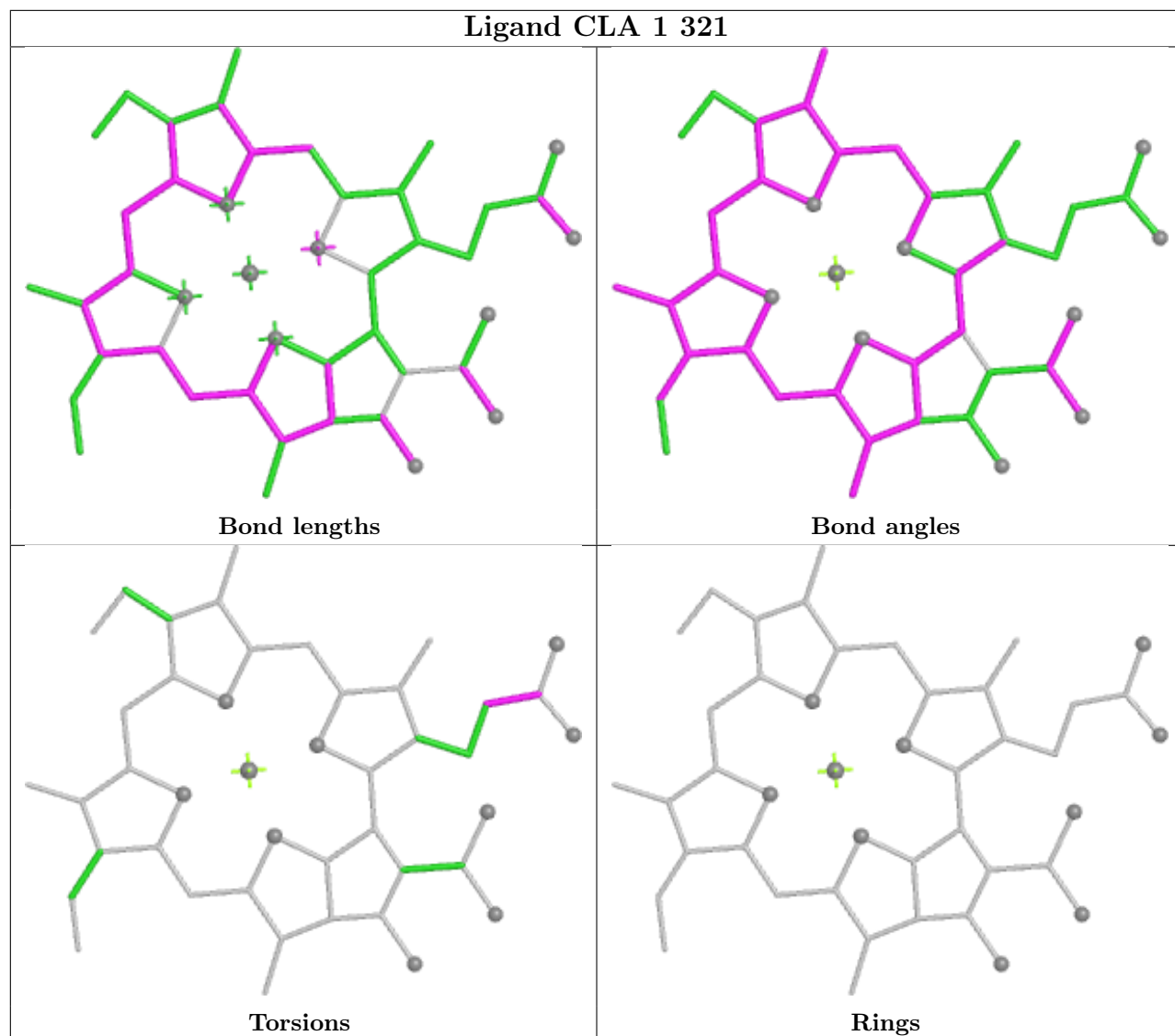
Ligand BCR L 304



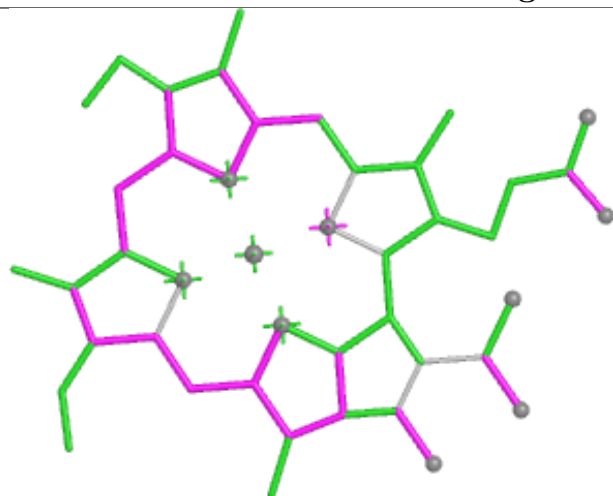




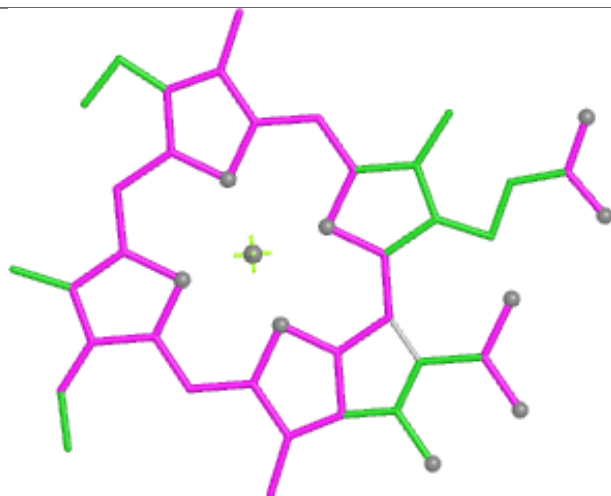
Ligand CLA 1 321



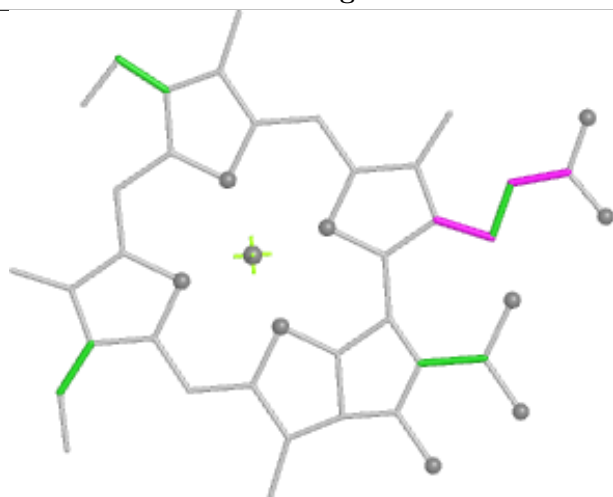
Ligand CLA 4 313



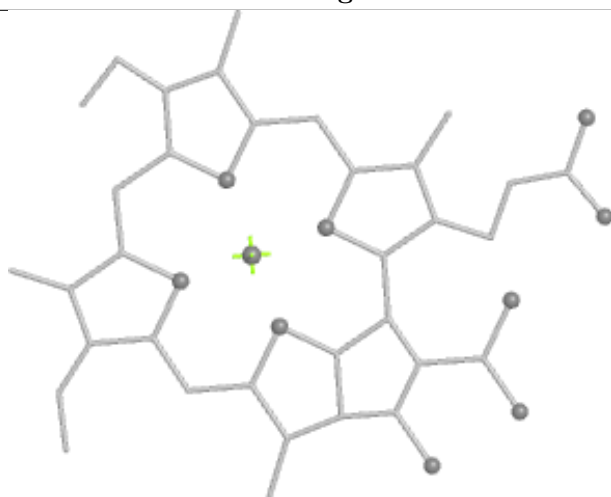
Bond lengths



Bond angles

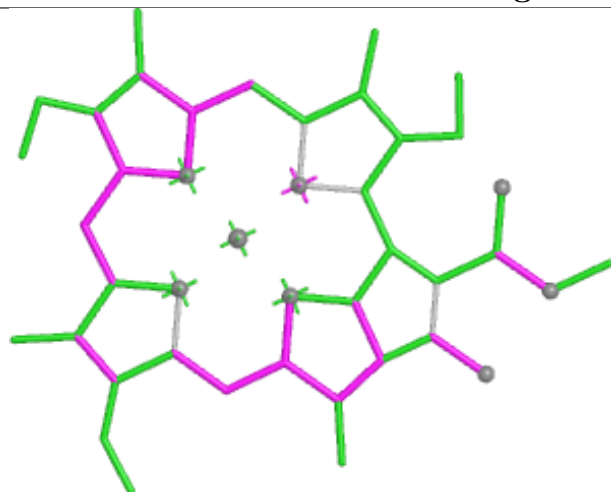


Torsions

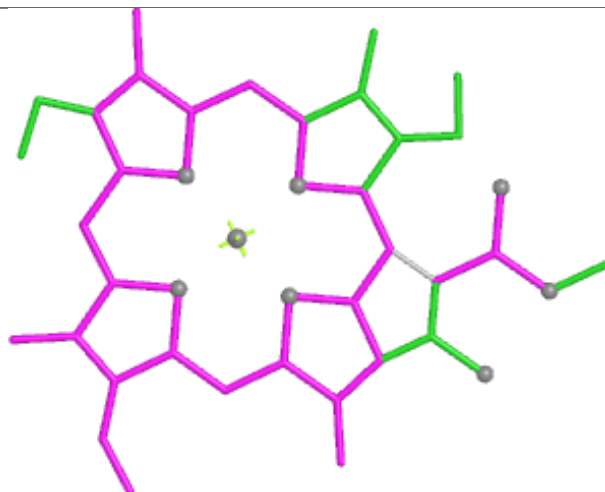


Rings

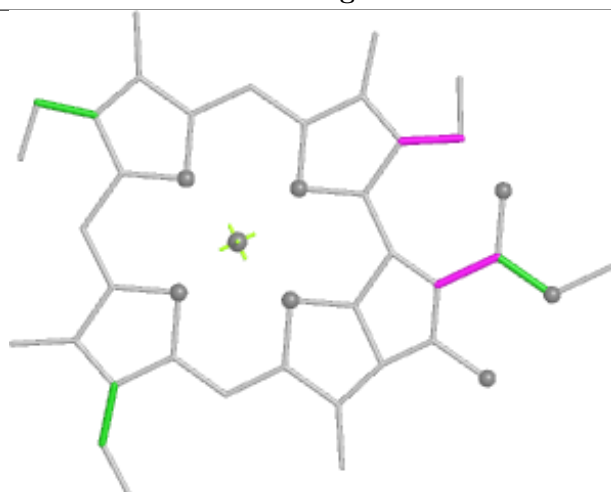
Ligand CLA A 804



Bond lengths



Bond angles

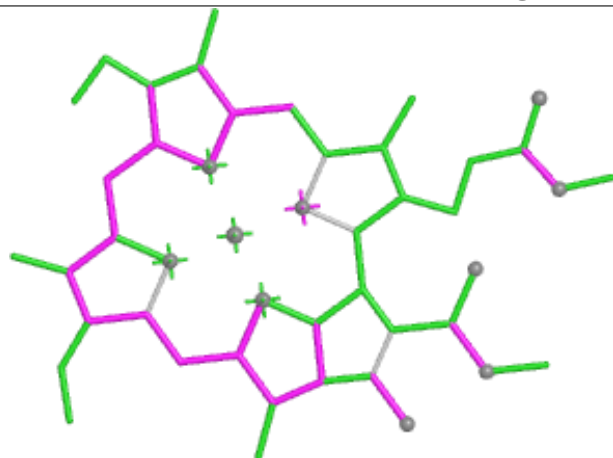


Torsions

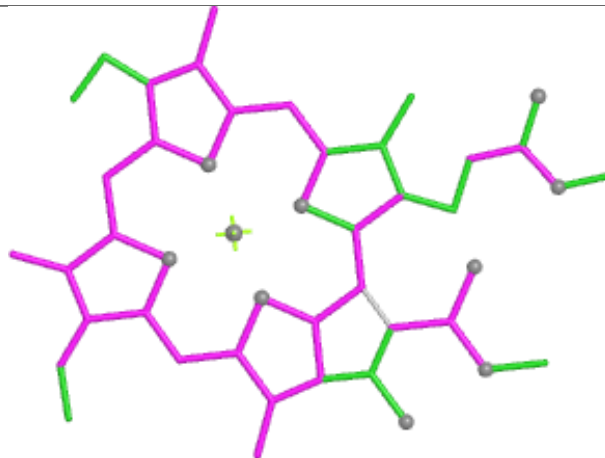


Rings

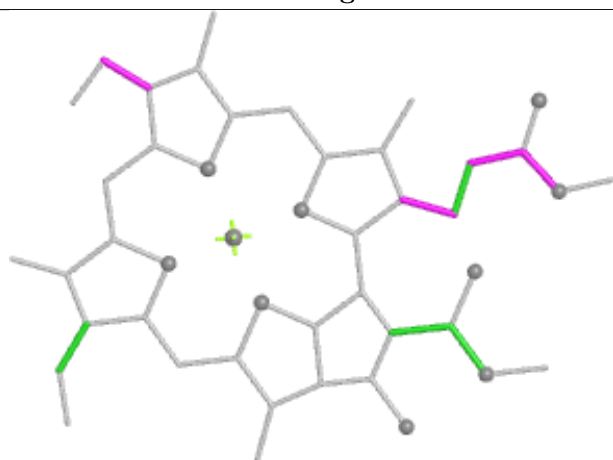
Ligand CLA Y 302



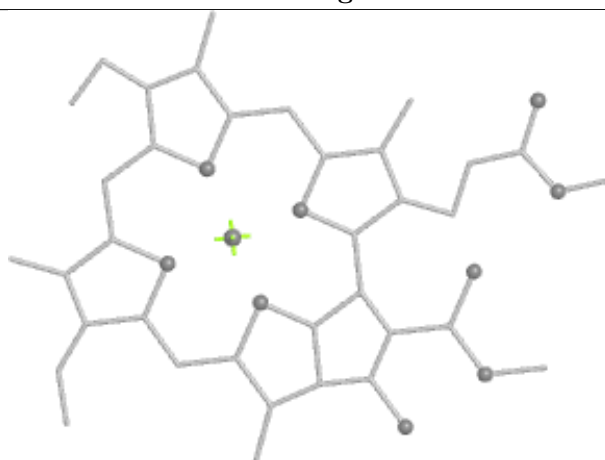
Bond lengths



Bond angles

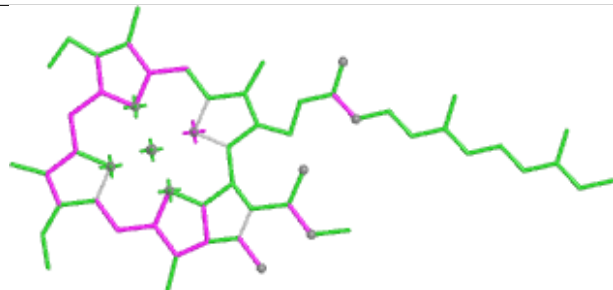


Torsions

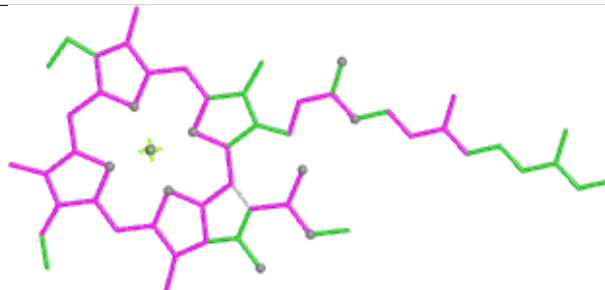


Rings

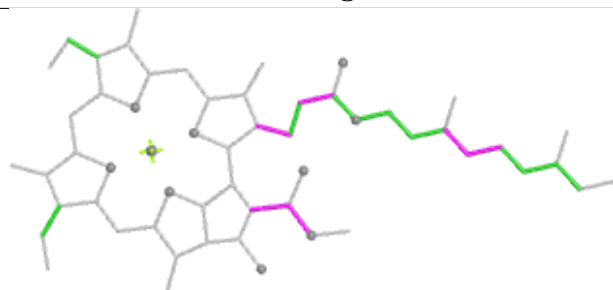
Ligand CLA B 811



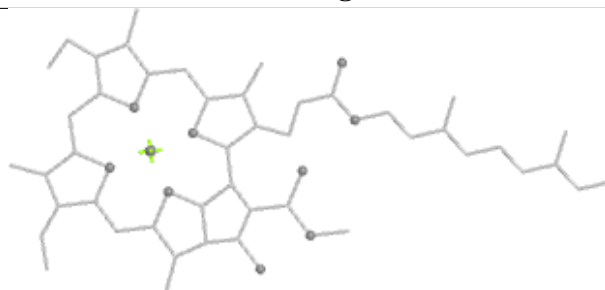
Bond lengths



Bond angles

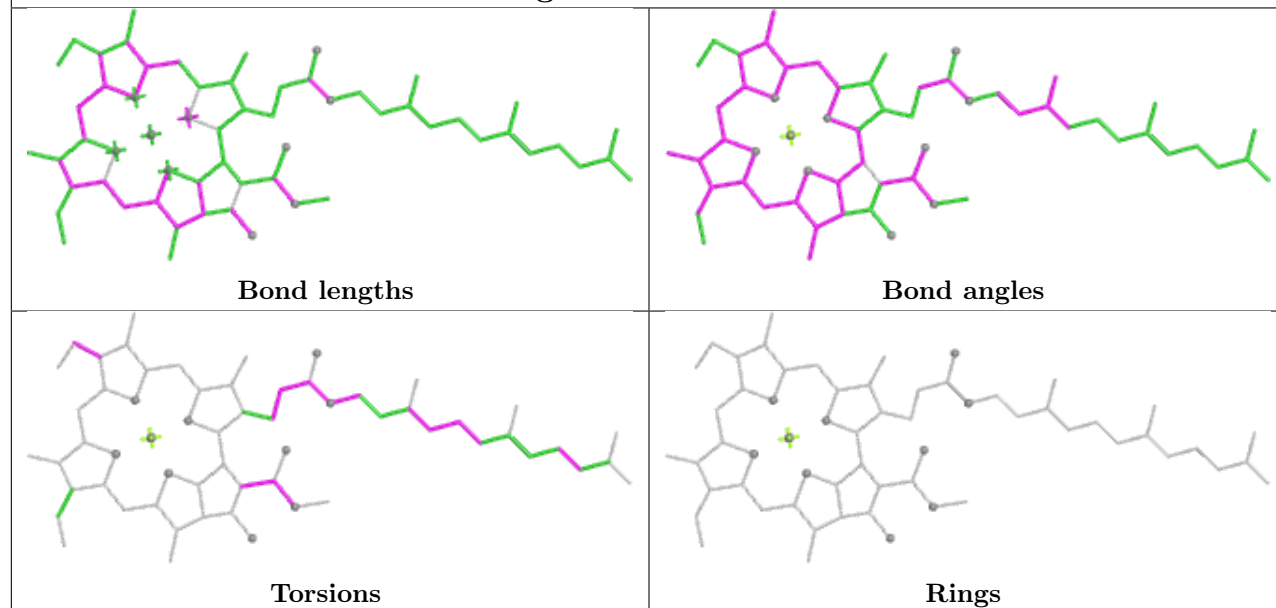


Torsions

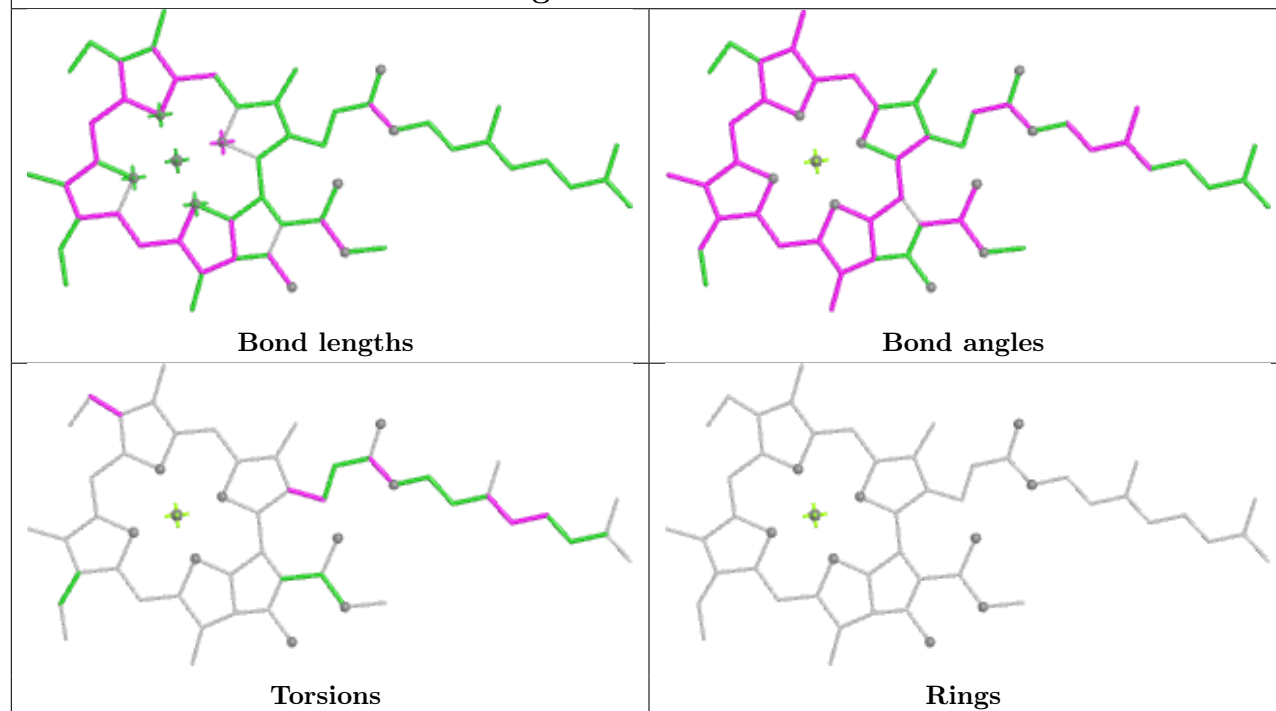


Rings

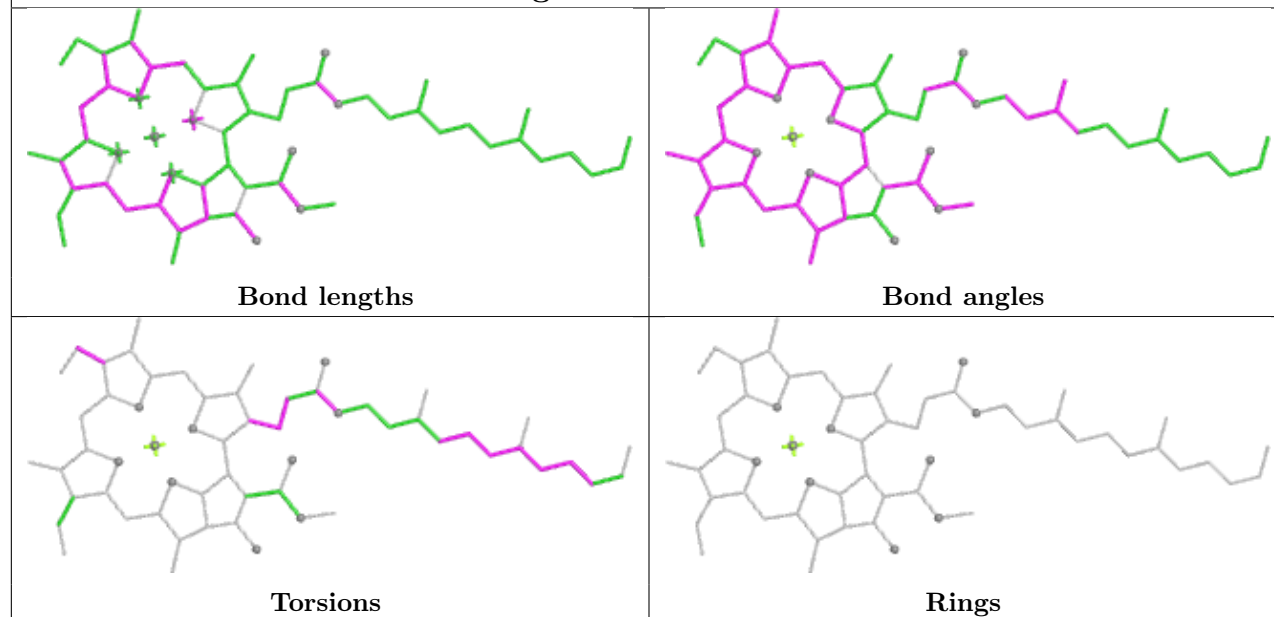
Ligand CLA 2 307



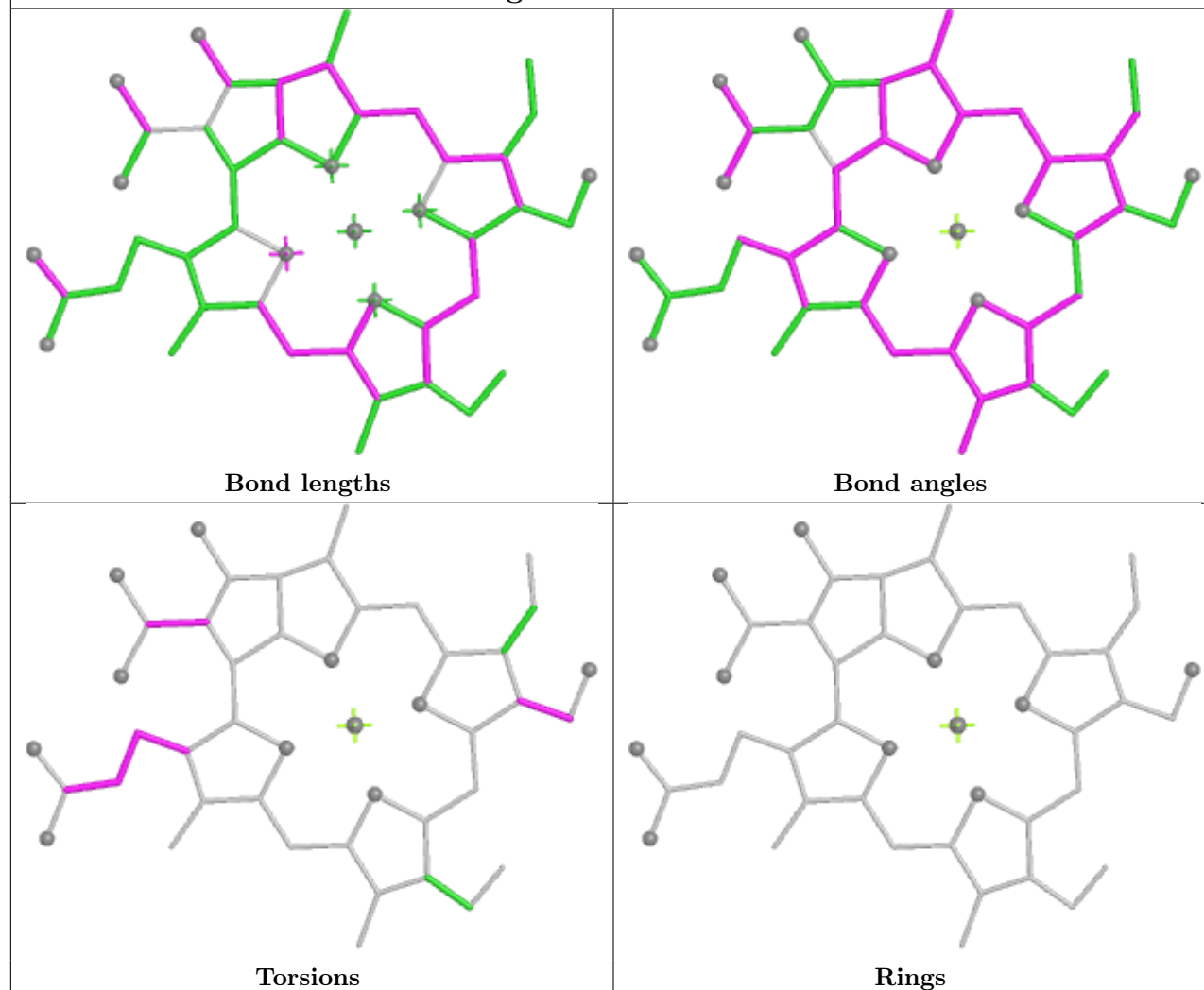
Ligand CLA B 852



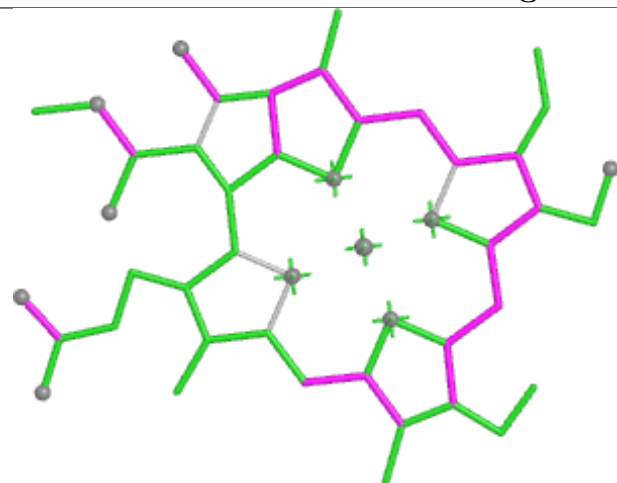
Ligand CLA B 812



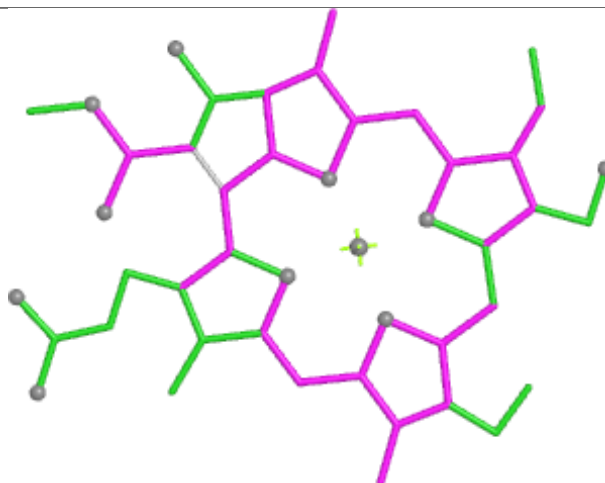
Ligand CHL 4 308



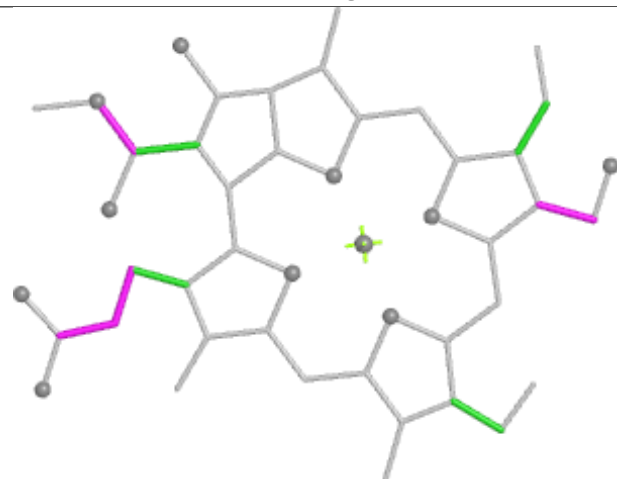
Ligand CHL Z 312



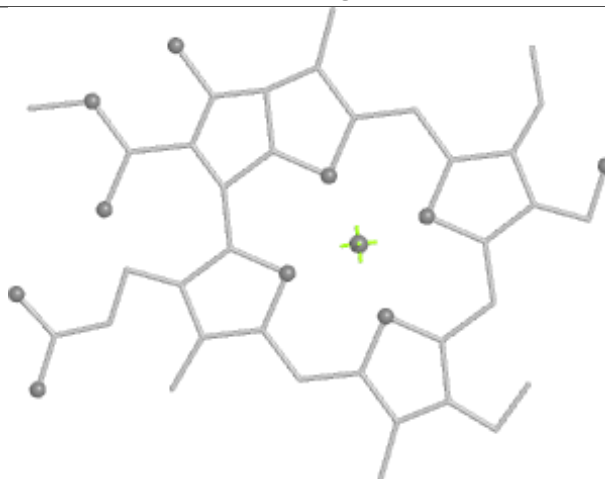
Bond lengths



Bond angles

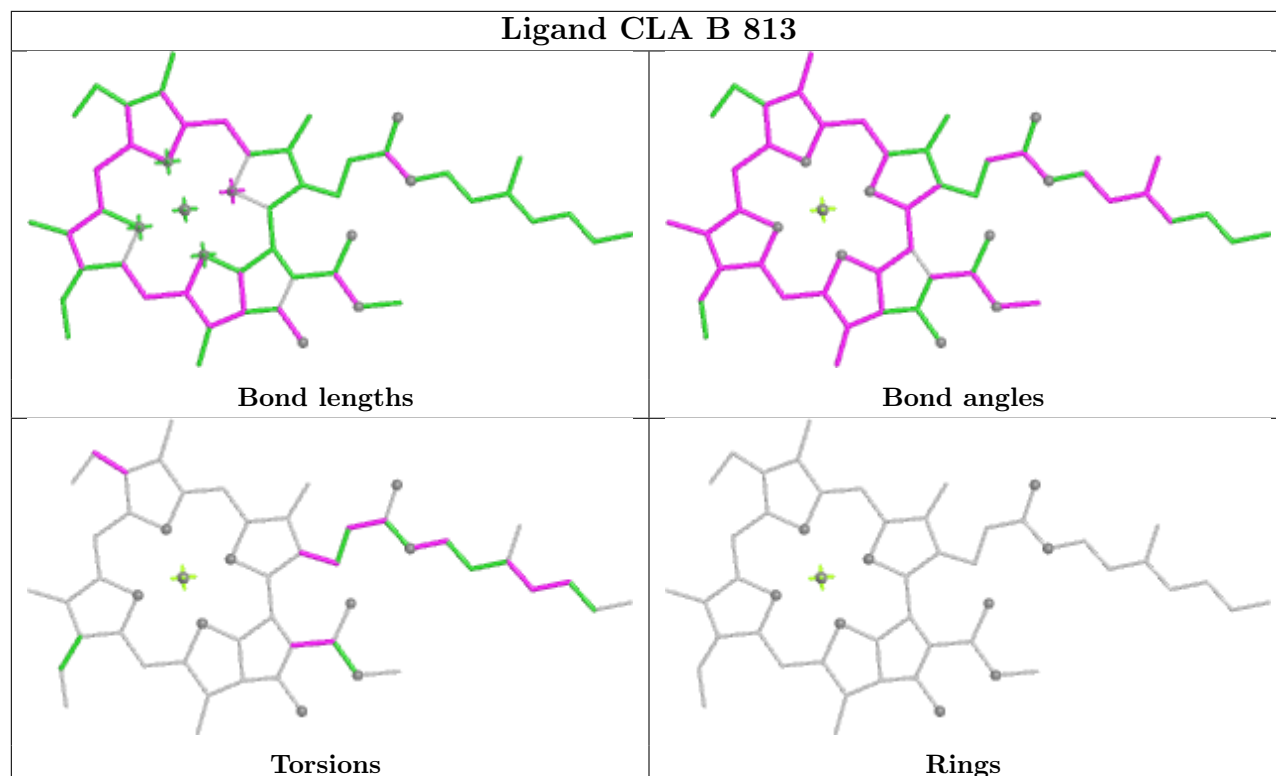


Torsions

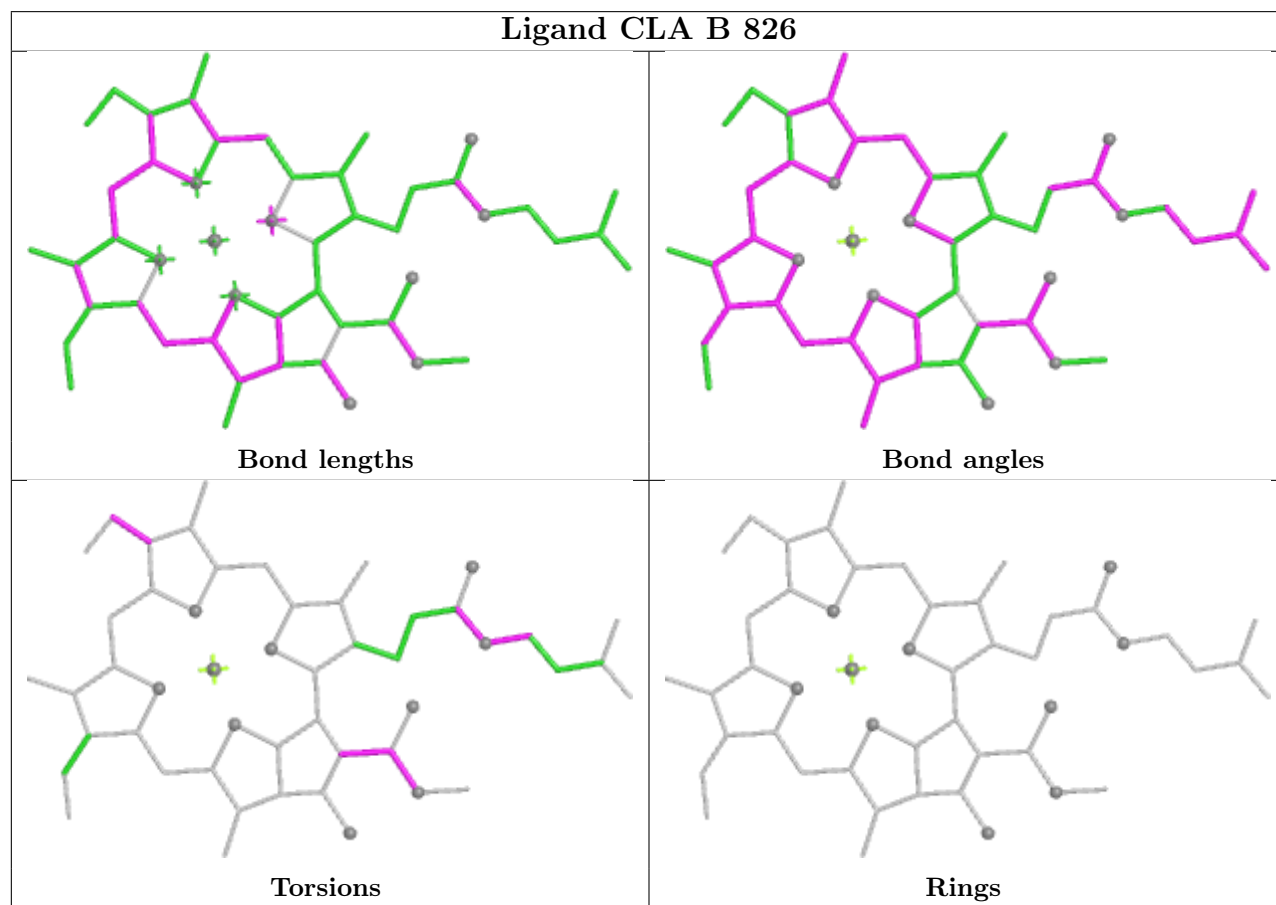


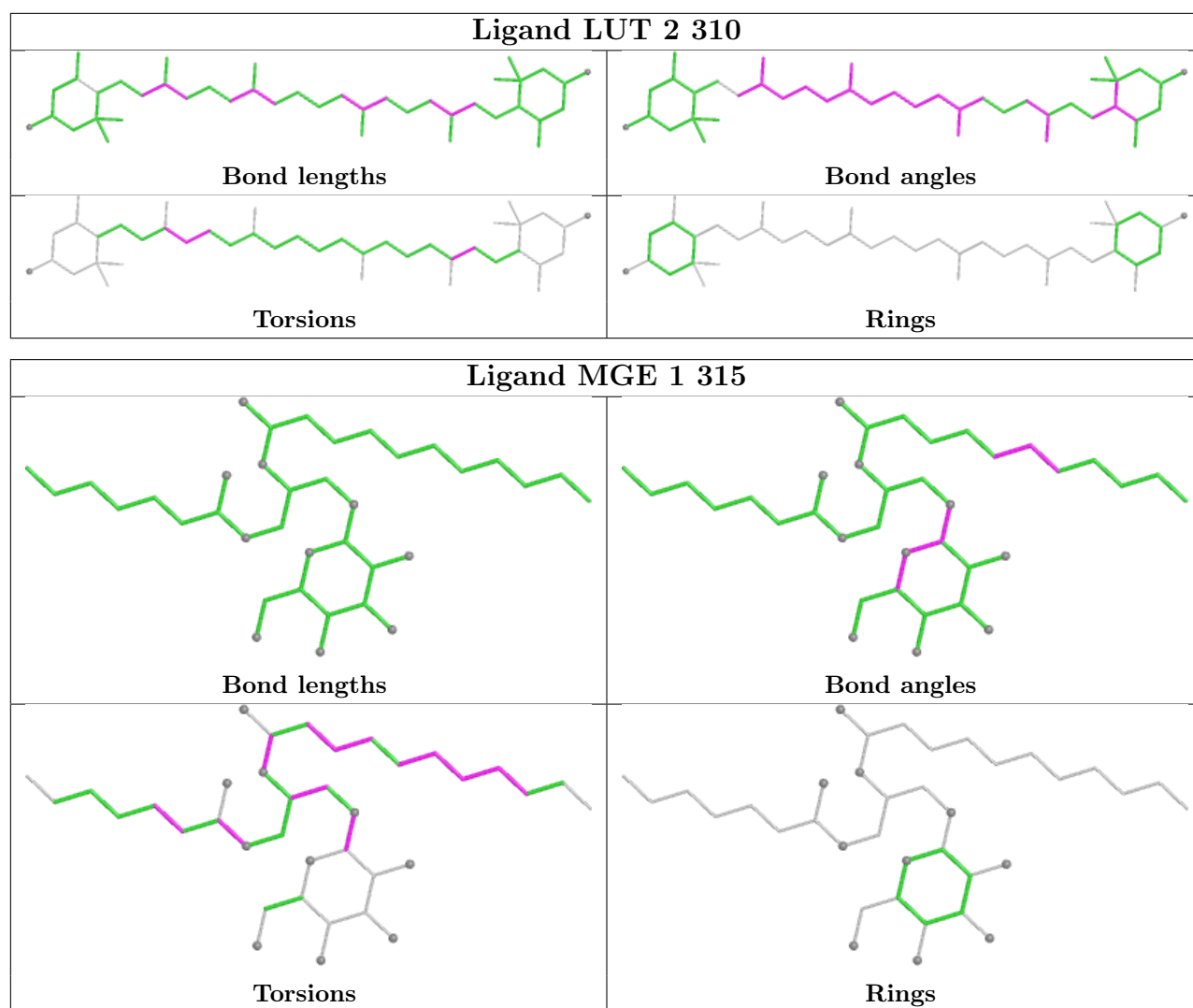
Rings

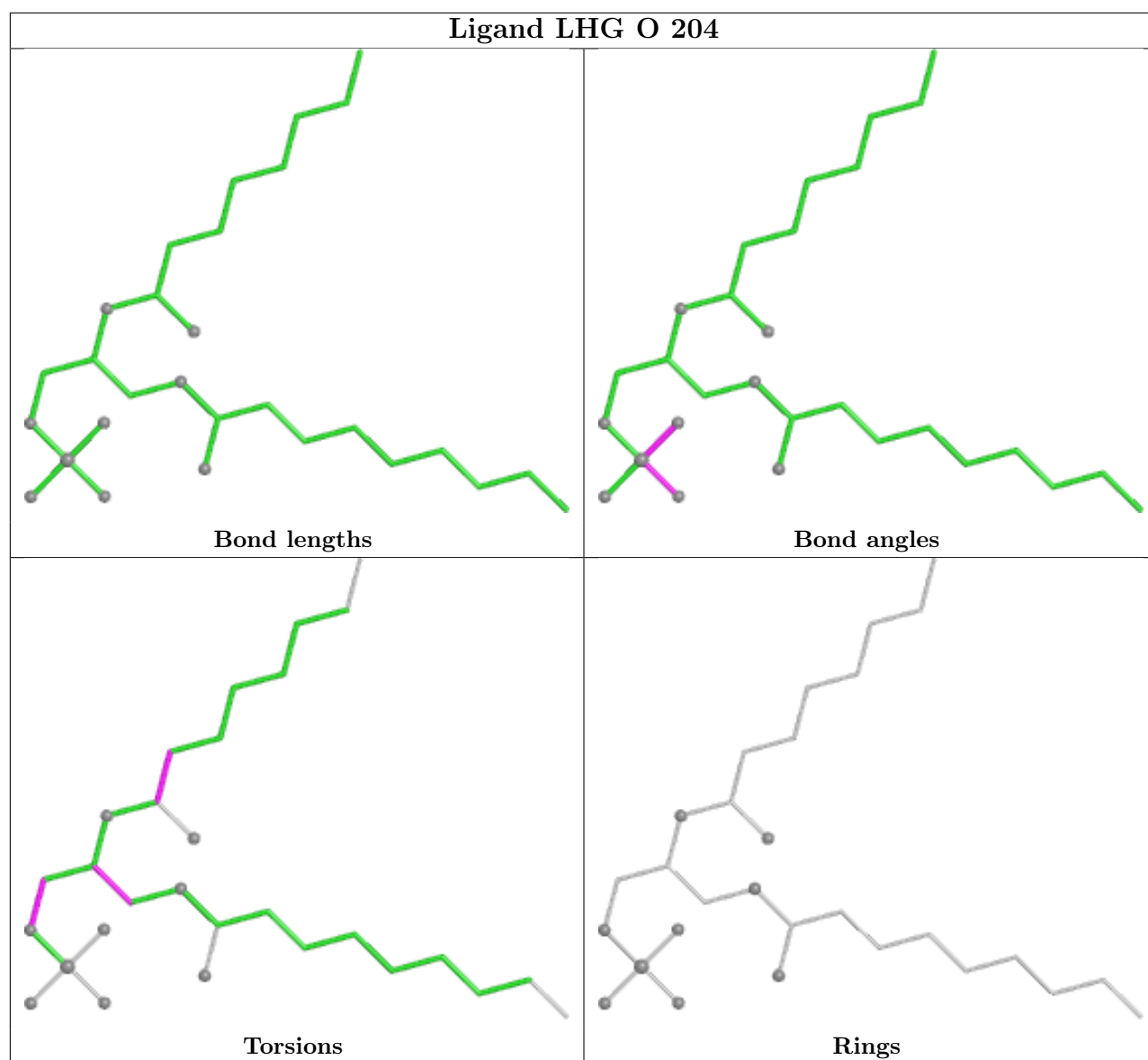
Ligand CLA B 813



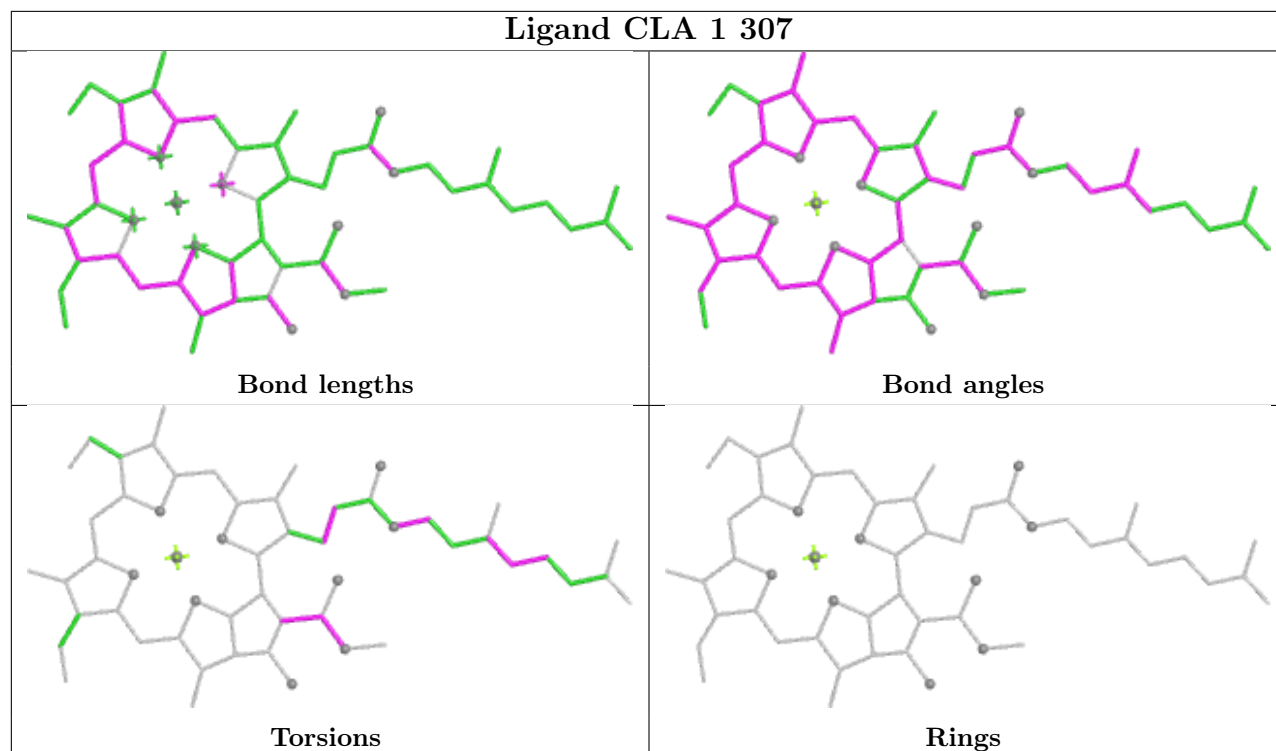
Ligand CLA B 826



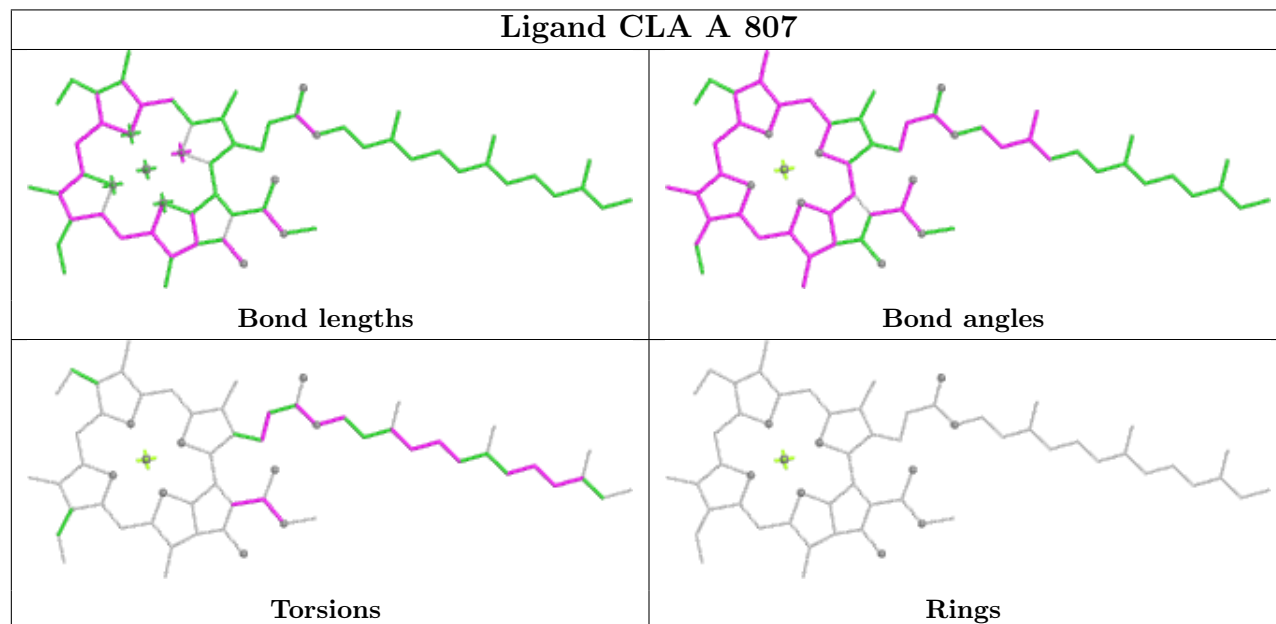


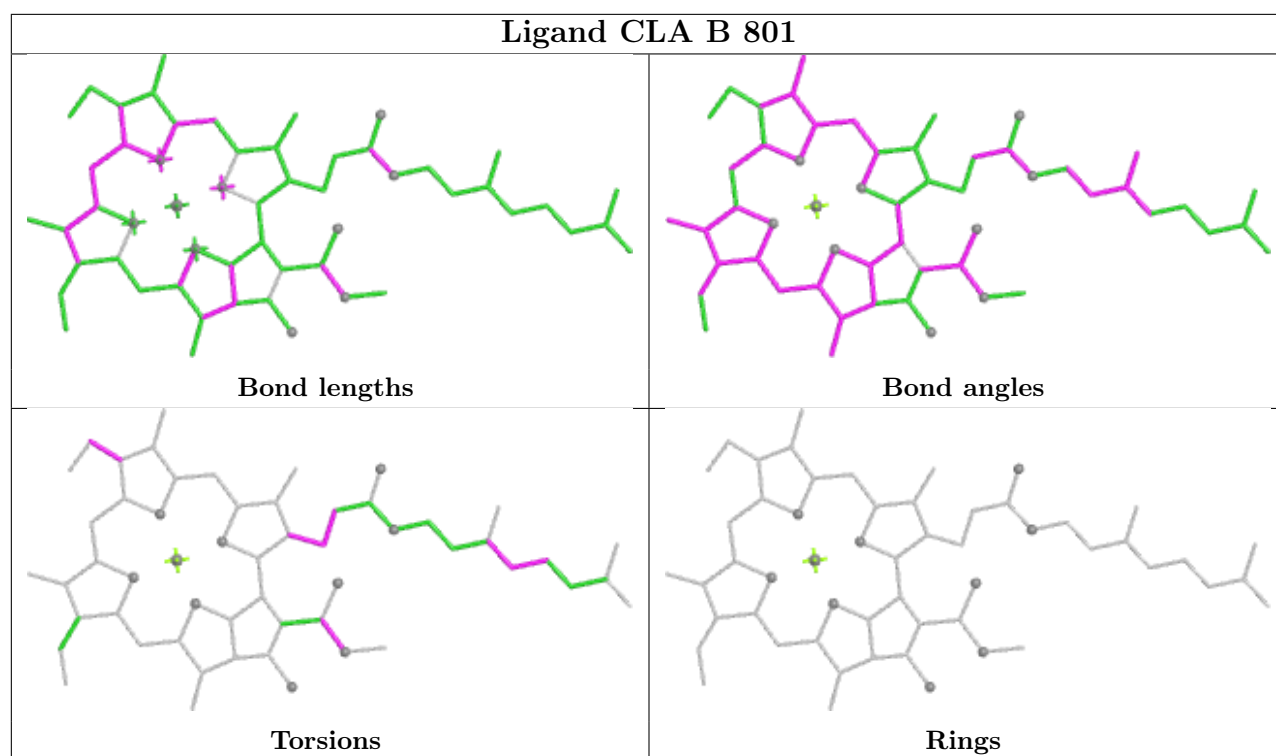


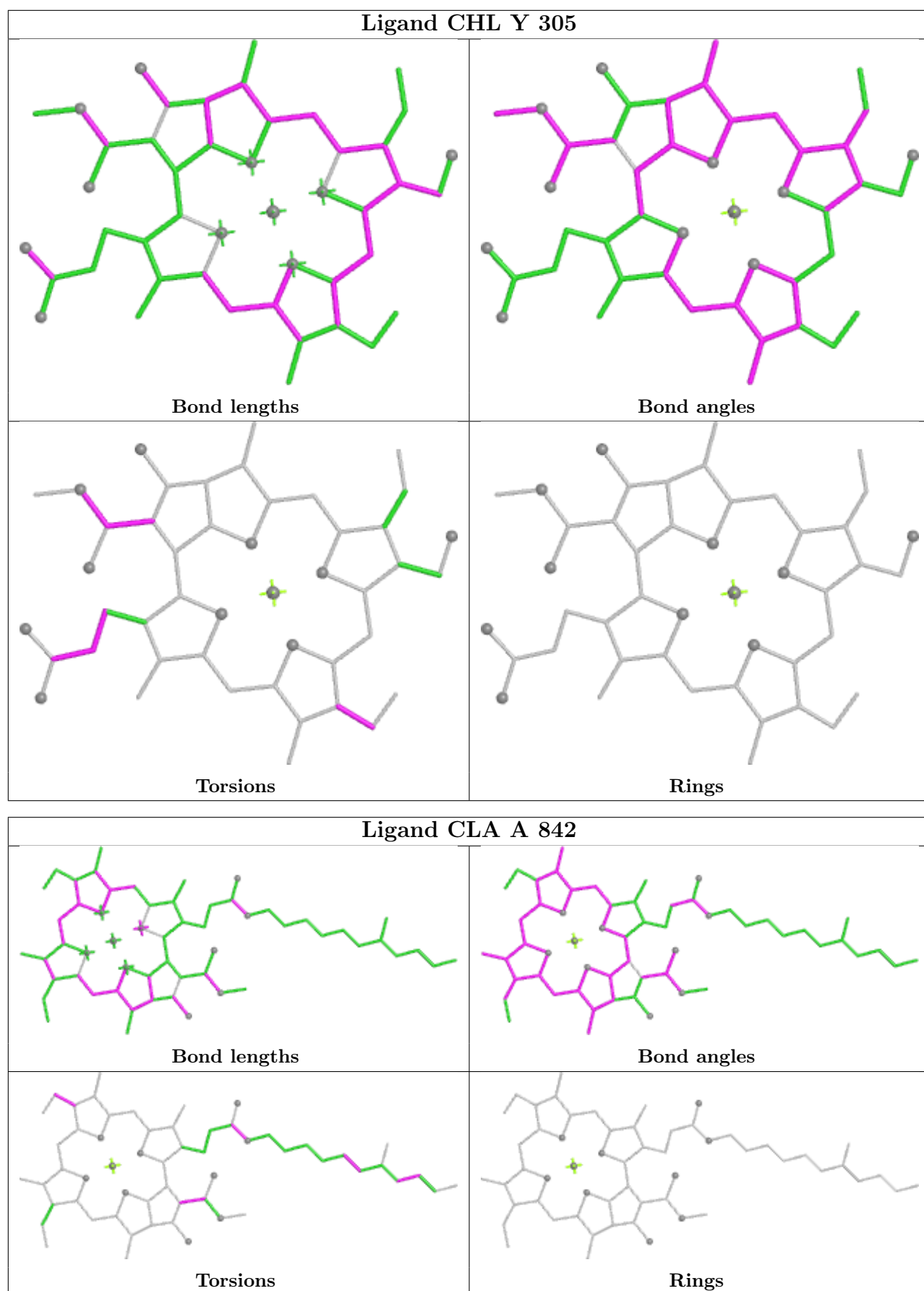
Ligand CLA 1 307

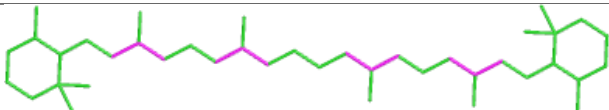
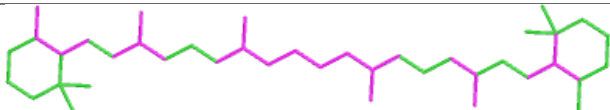
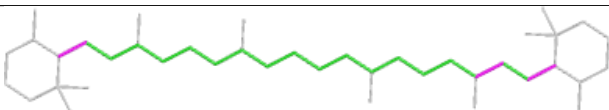
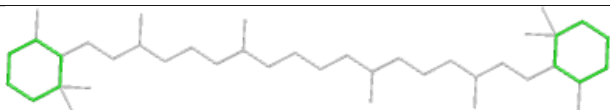


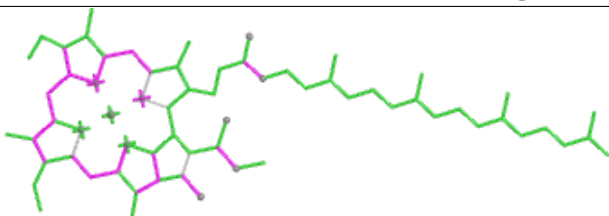
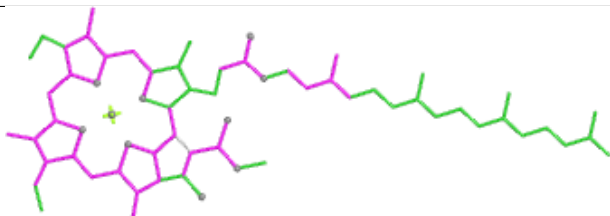
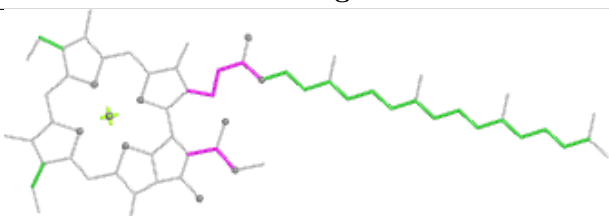
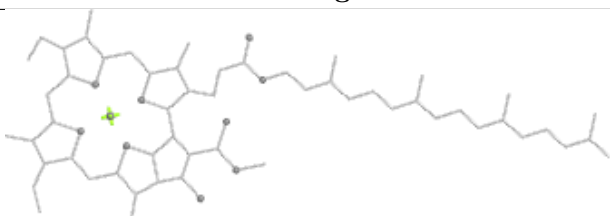
Ligand CLA A 807

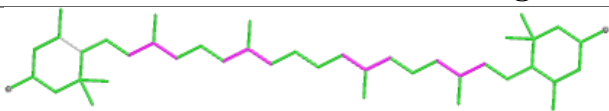
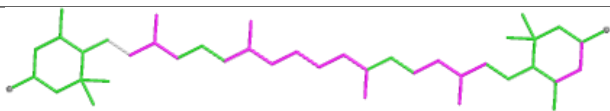
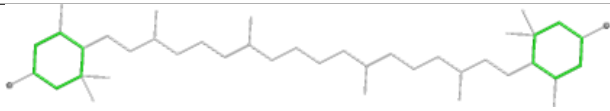




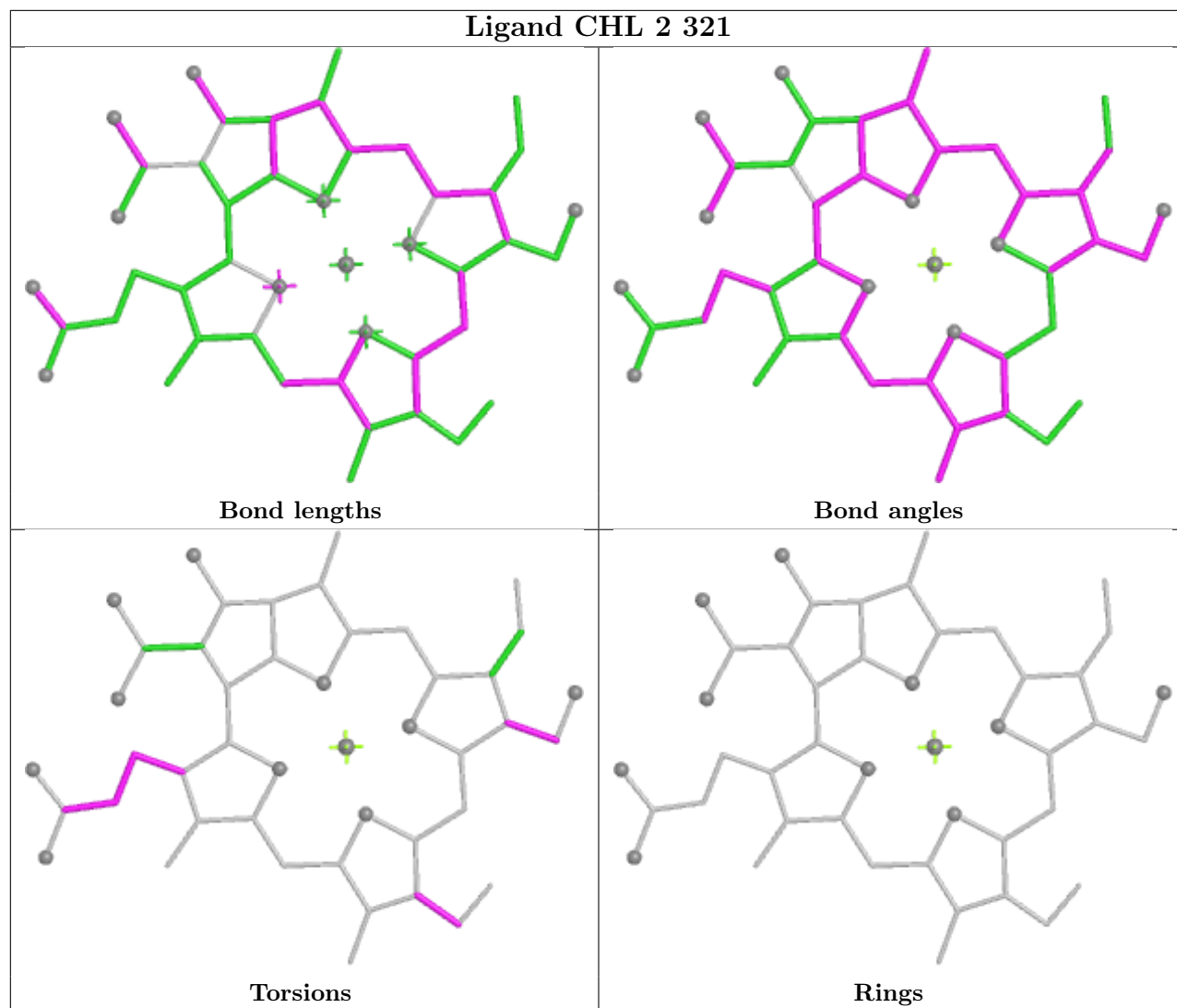


Ligand BCR 4 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

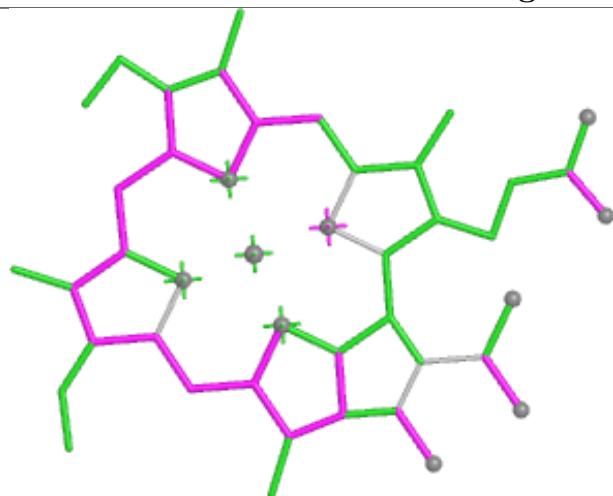
Ligand CL0 A 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

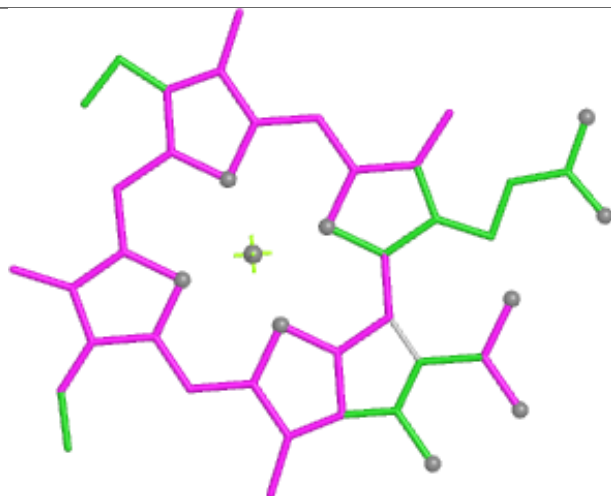
Ligand CHL 2 321



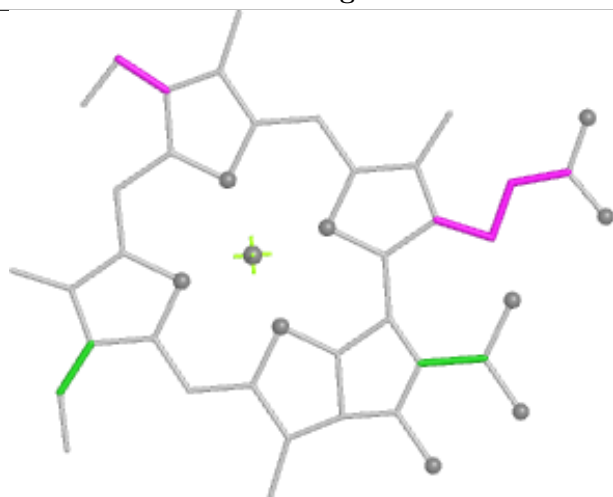
Ligand CLA 4 306



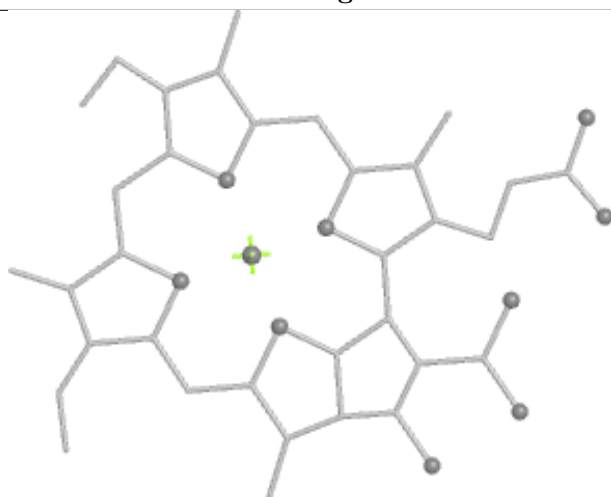
Bond lengths



Bond angles

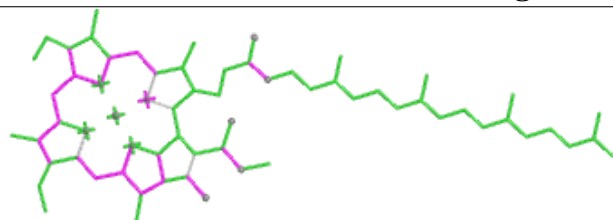


Torsions

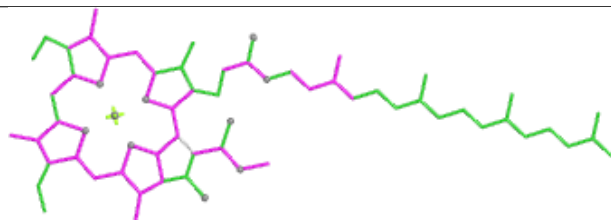


Rings

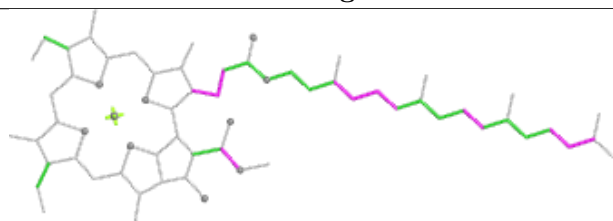
Ligand CLA A 826



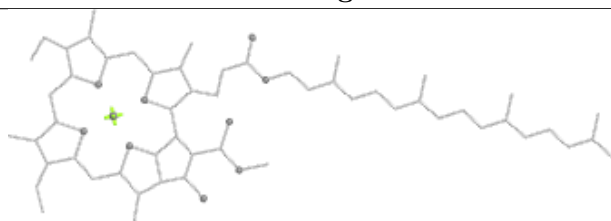
Bond lengths



Bond angles

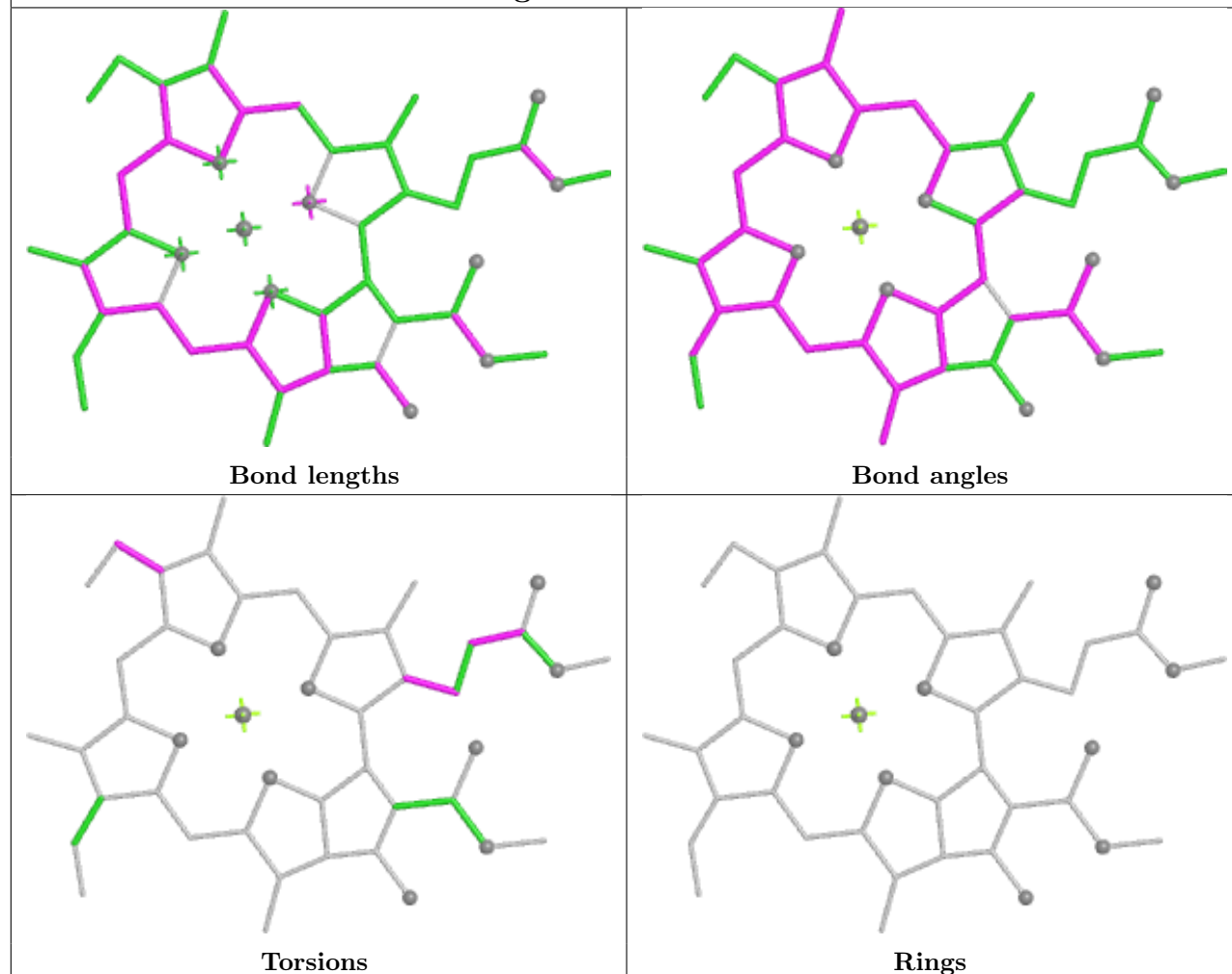


Torsions

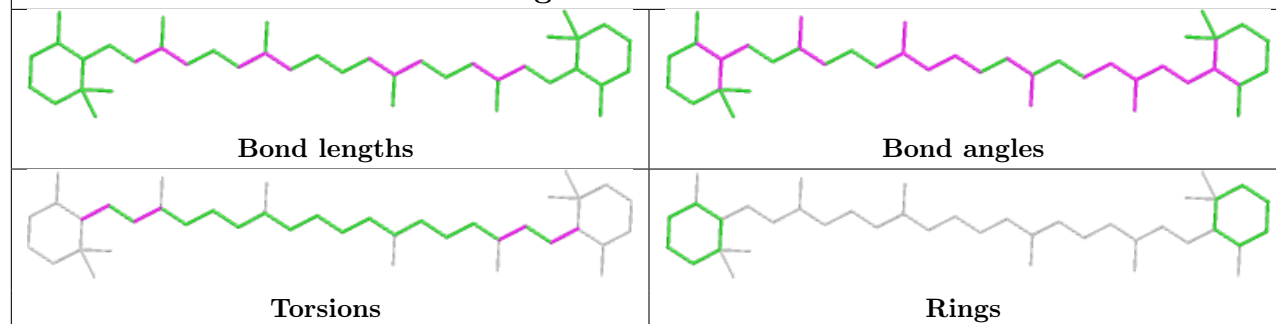


Rings

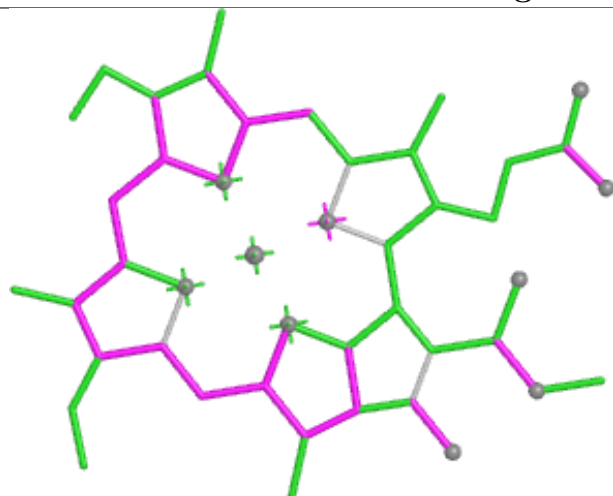
Ligand CLA B 805



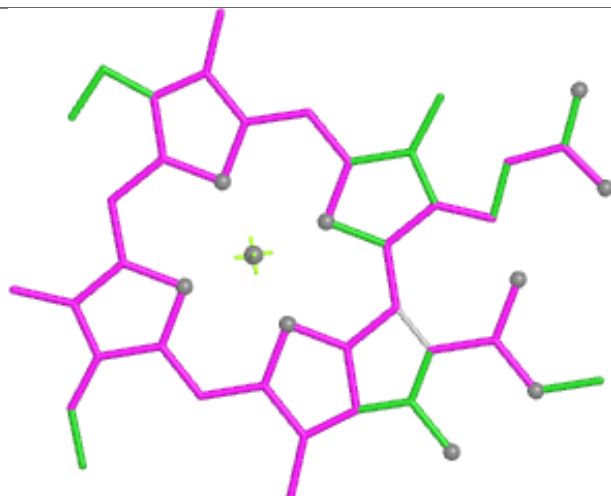
Ligand BCR 3 303



Ligand CLA B 821



Bond lengths



Bond angles

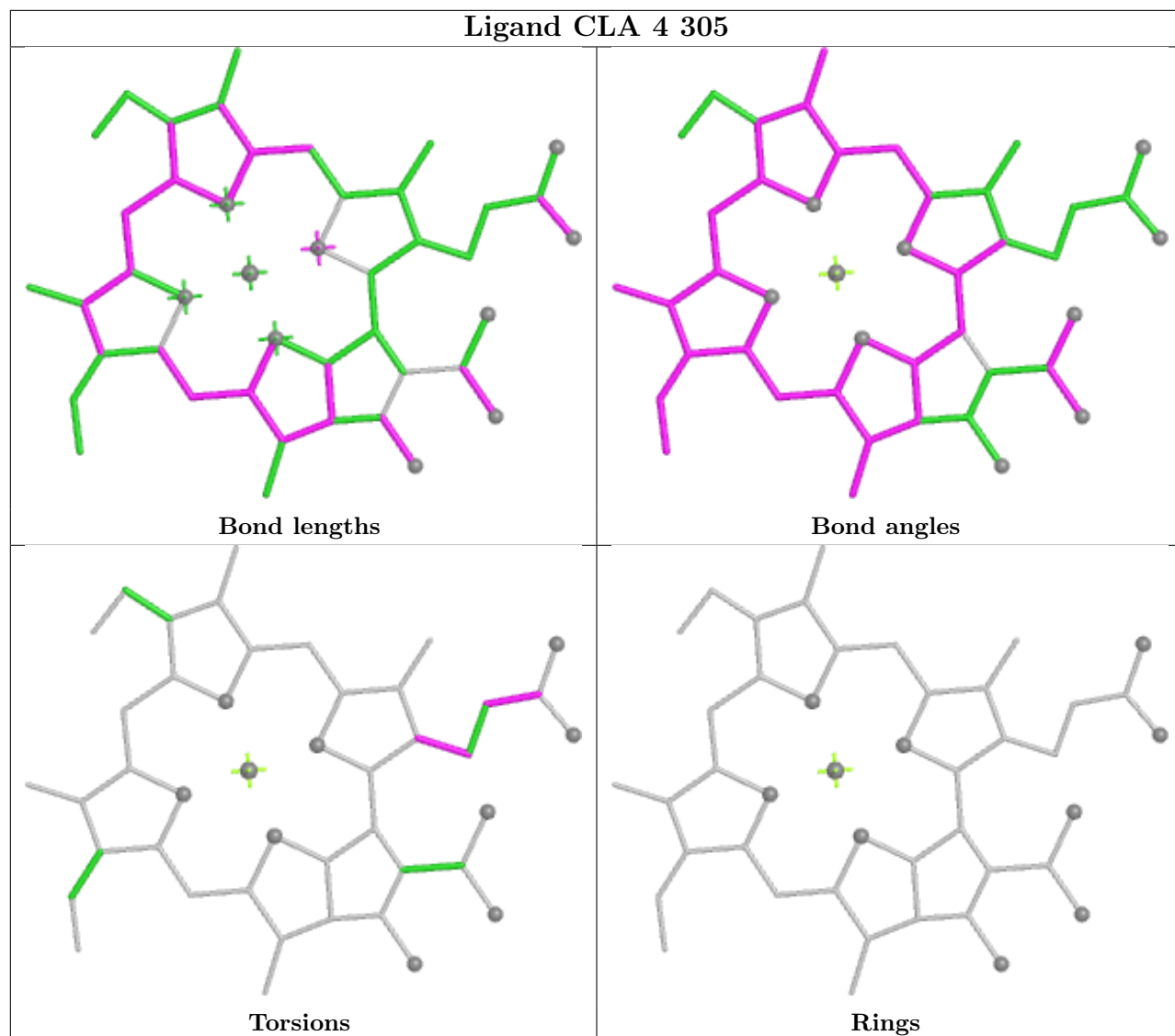


Torsions

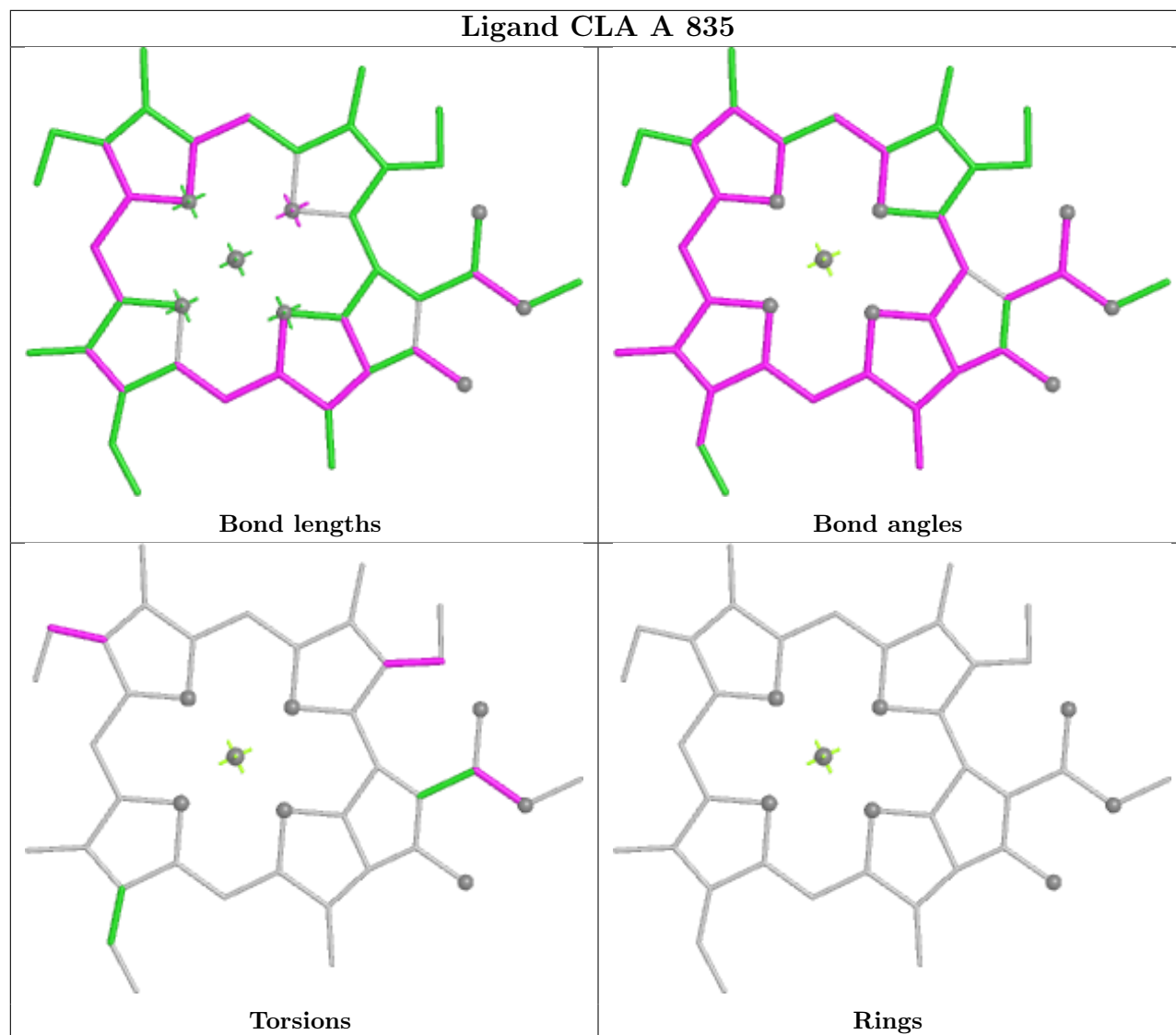


Rings

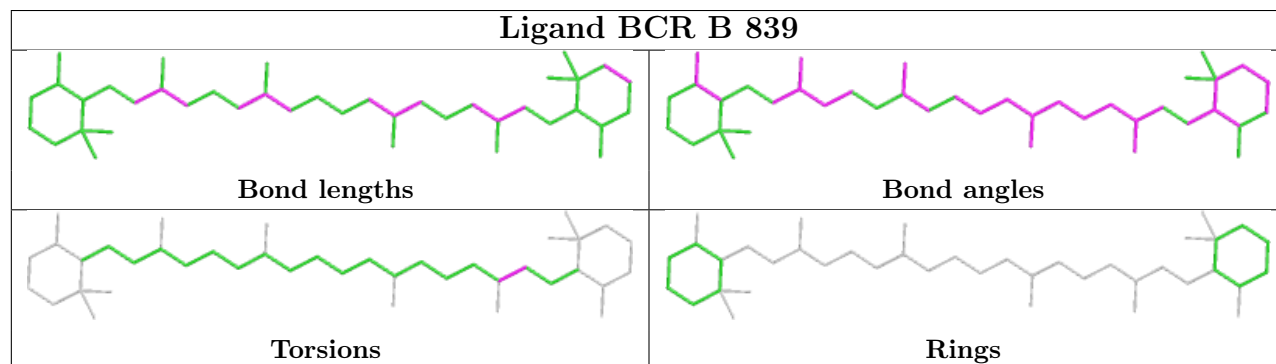
Ligand CLA 4 305



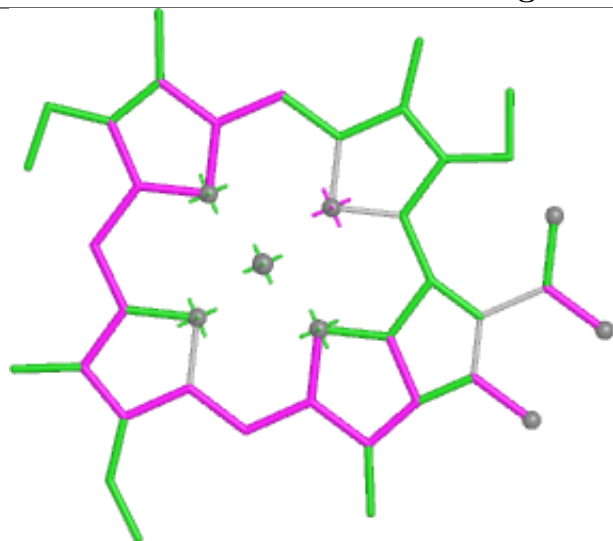
Ligand CLA A 835



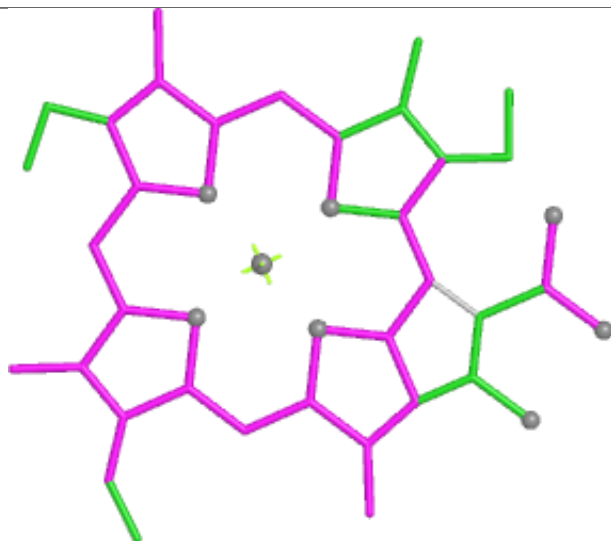
Ligand BCR B 839



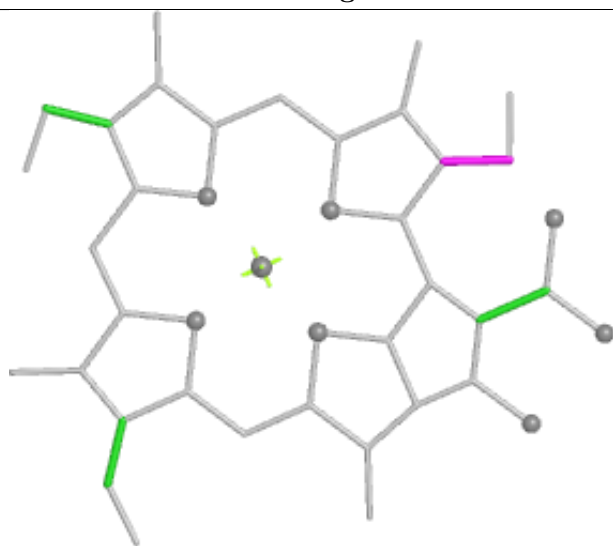
Ligand CLA J 102



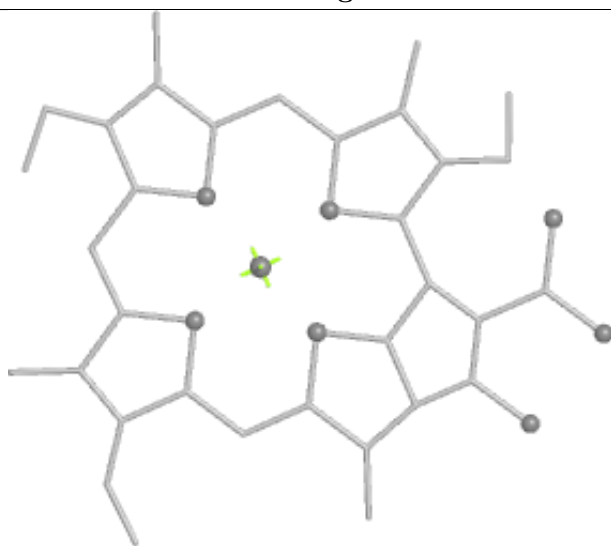
Bond lengths



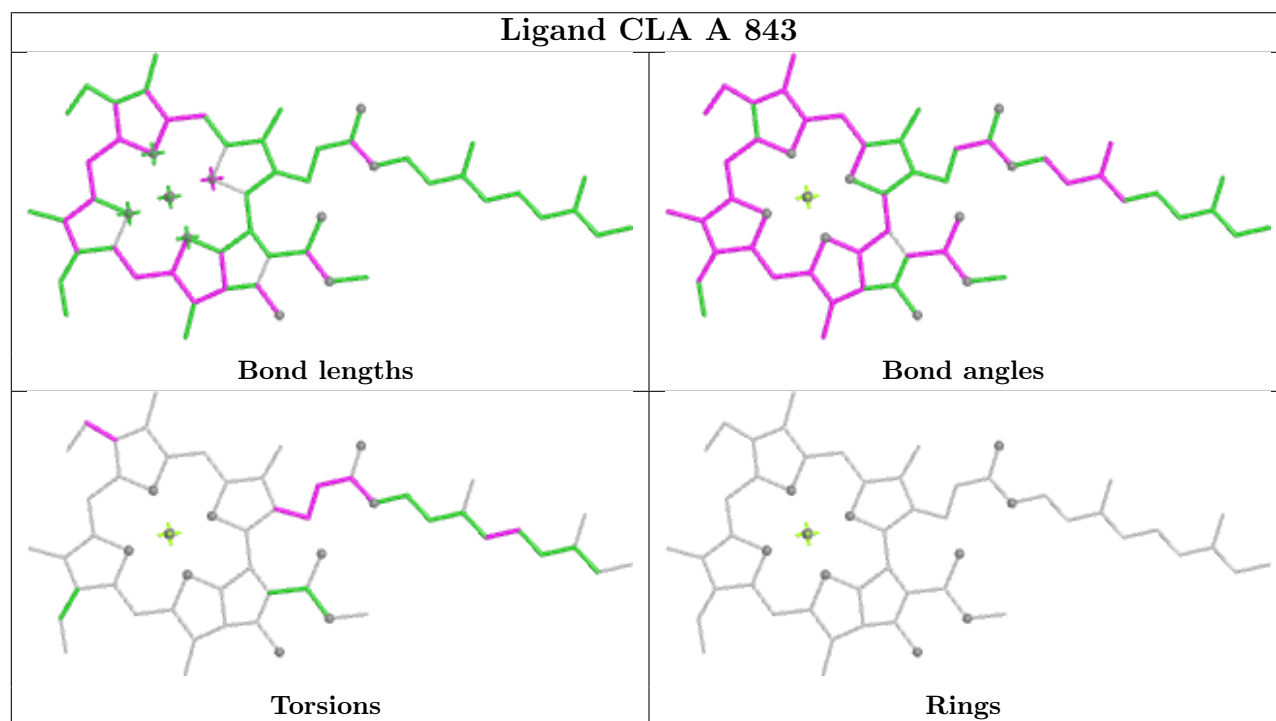
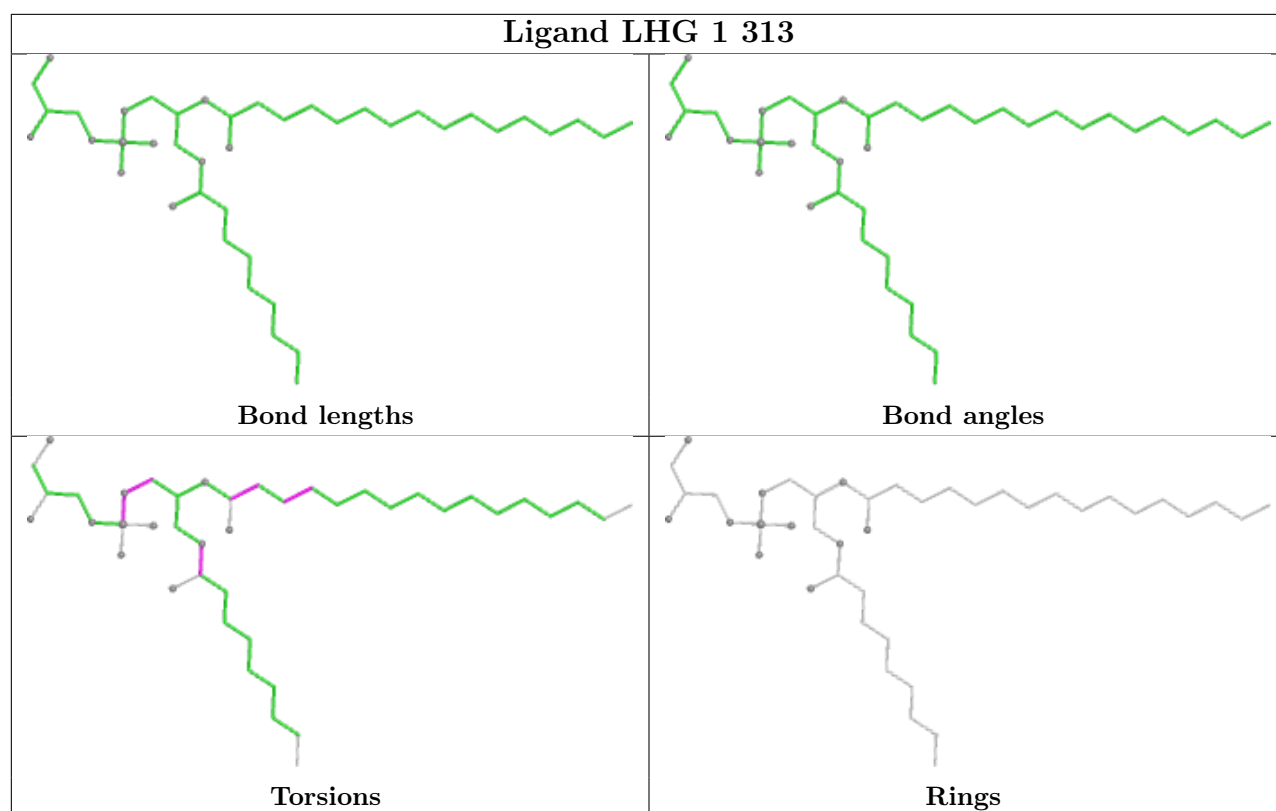
Bond angles



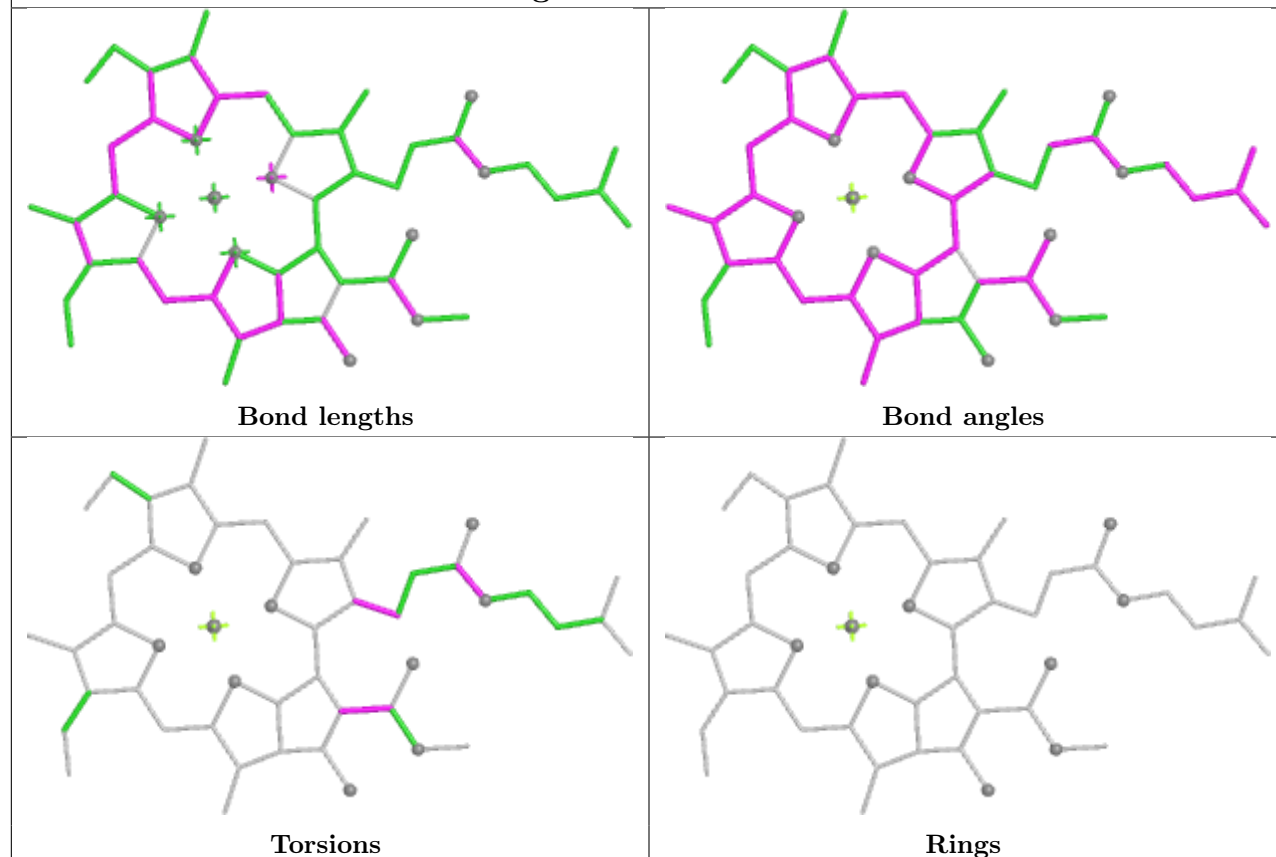
Torsions



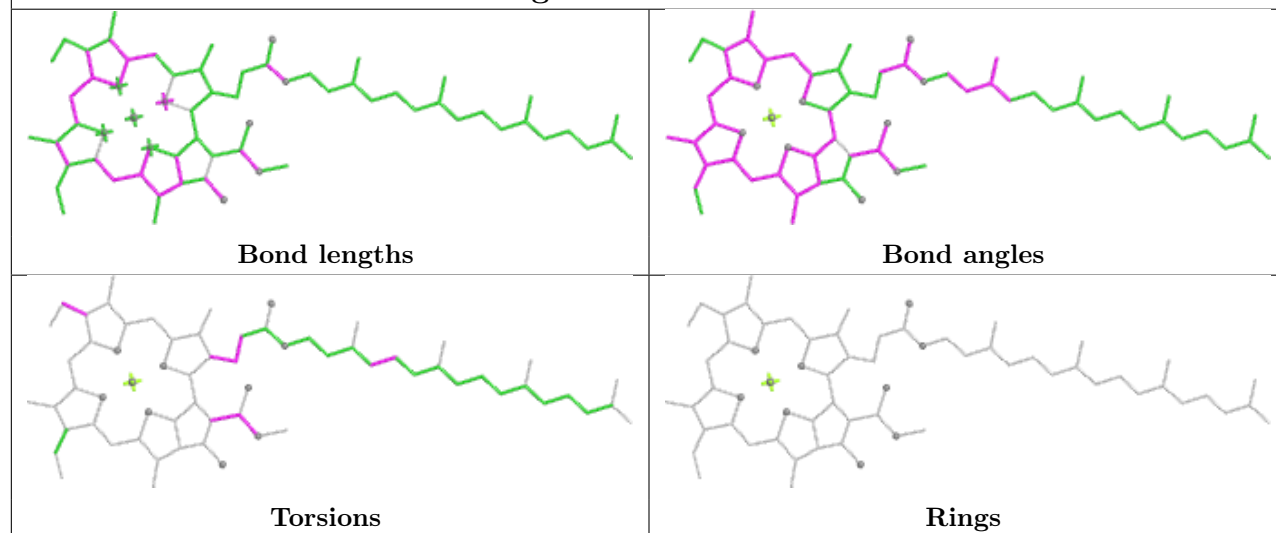
Rings



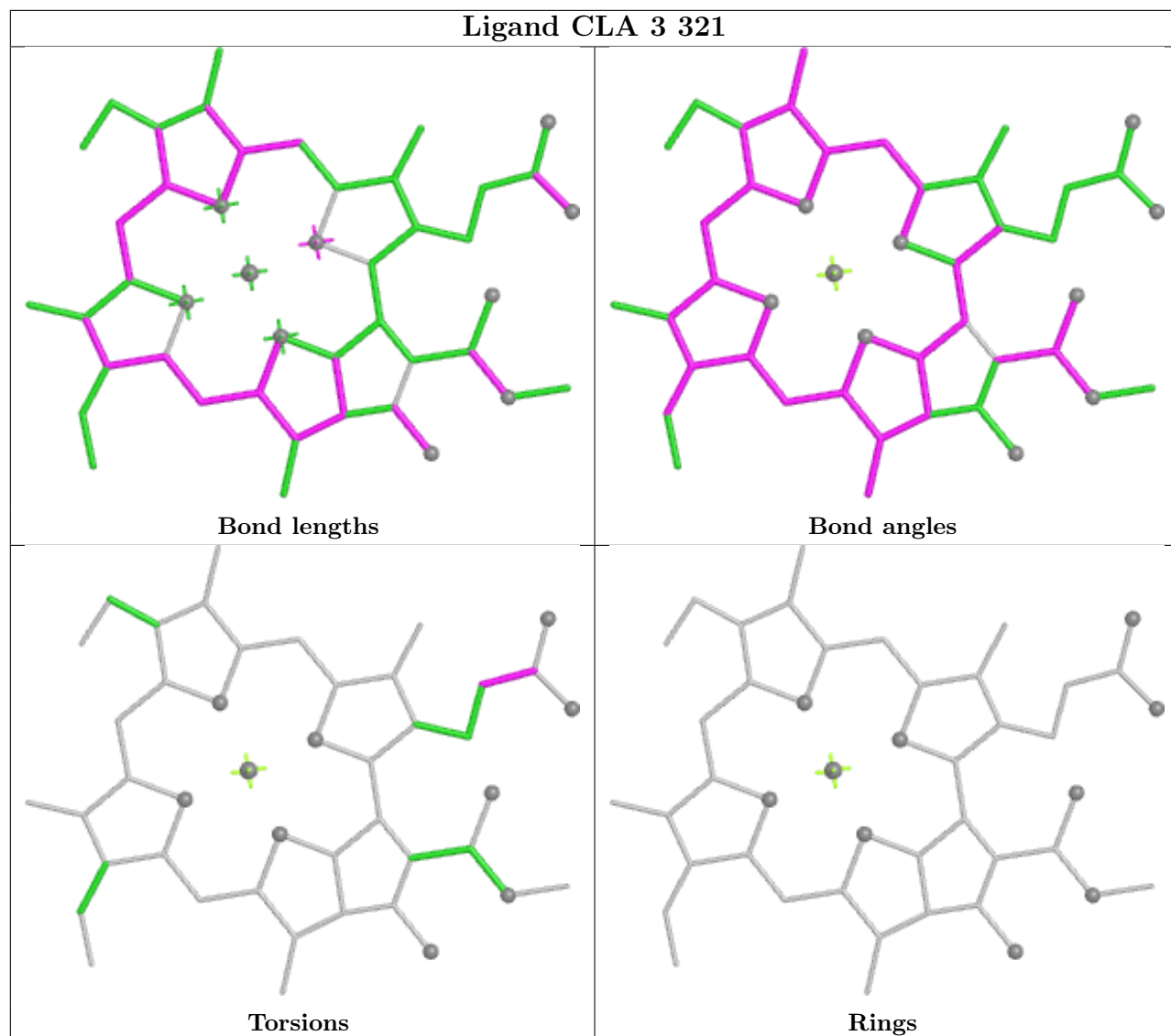
Ligand CLA B 810

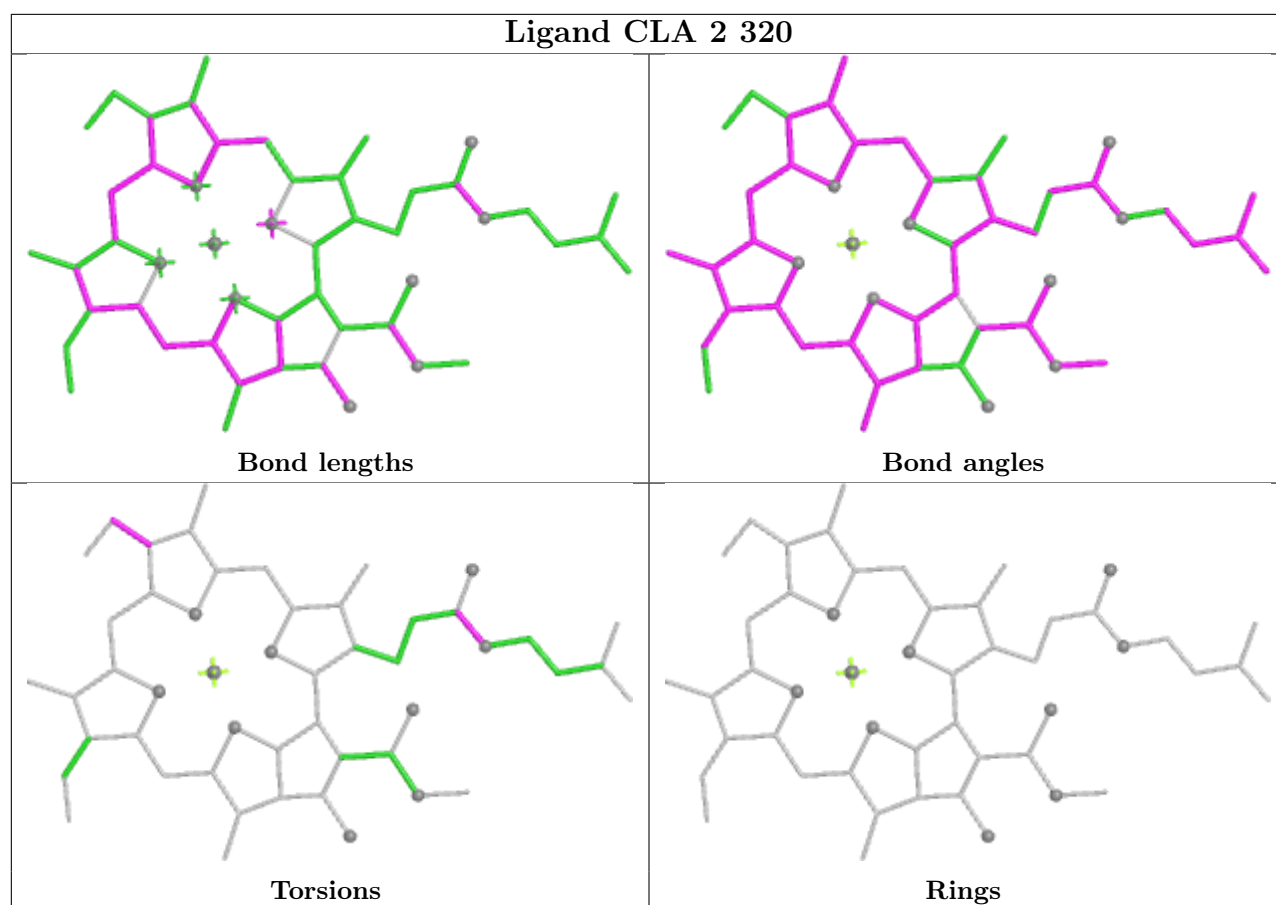


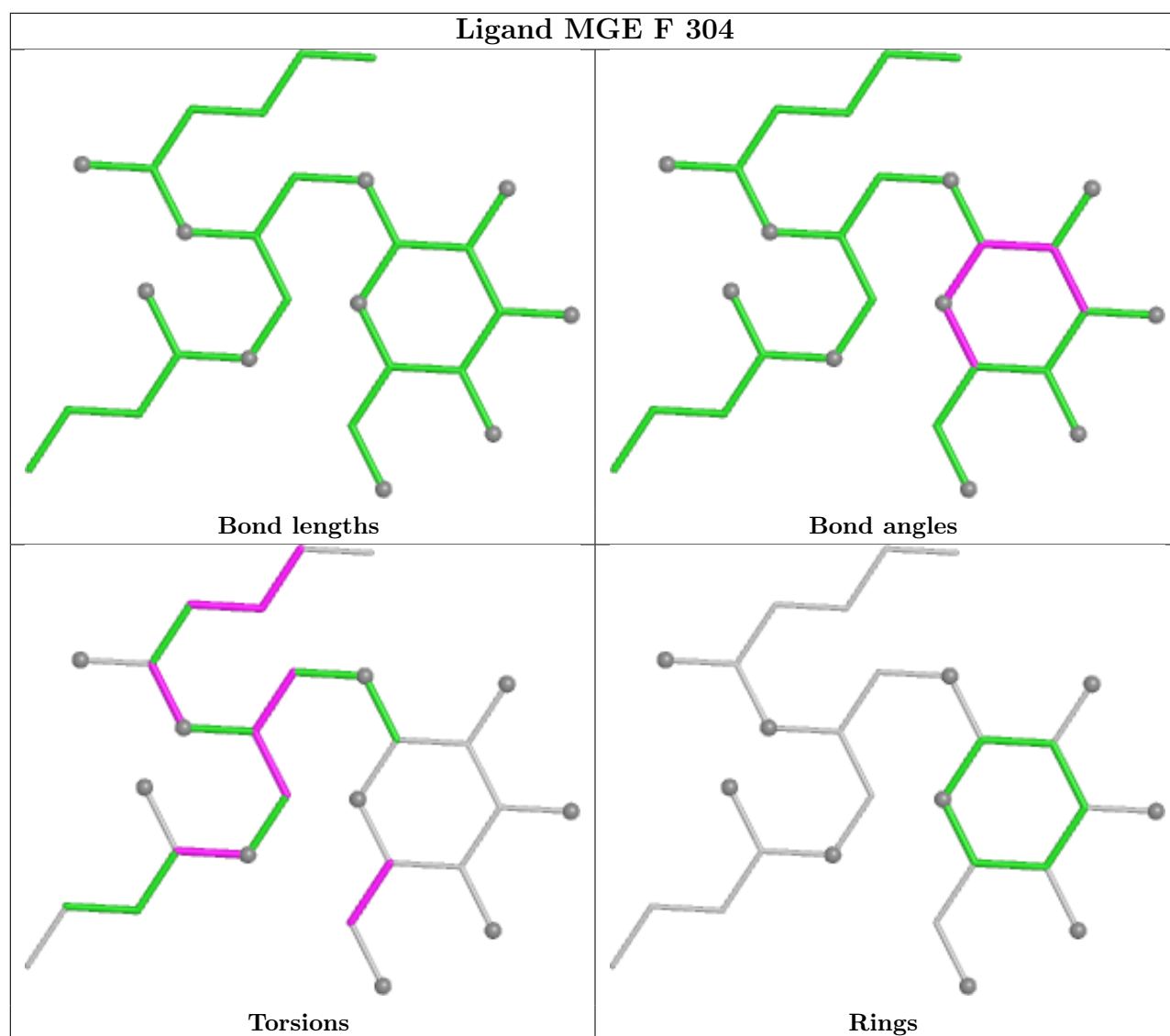
Ligand CLA A 849



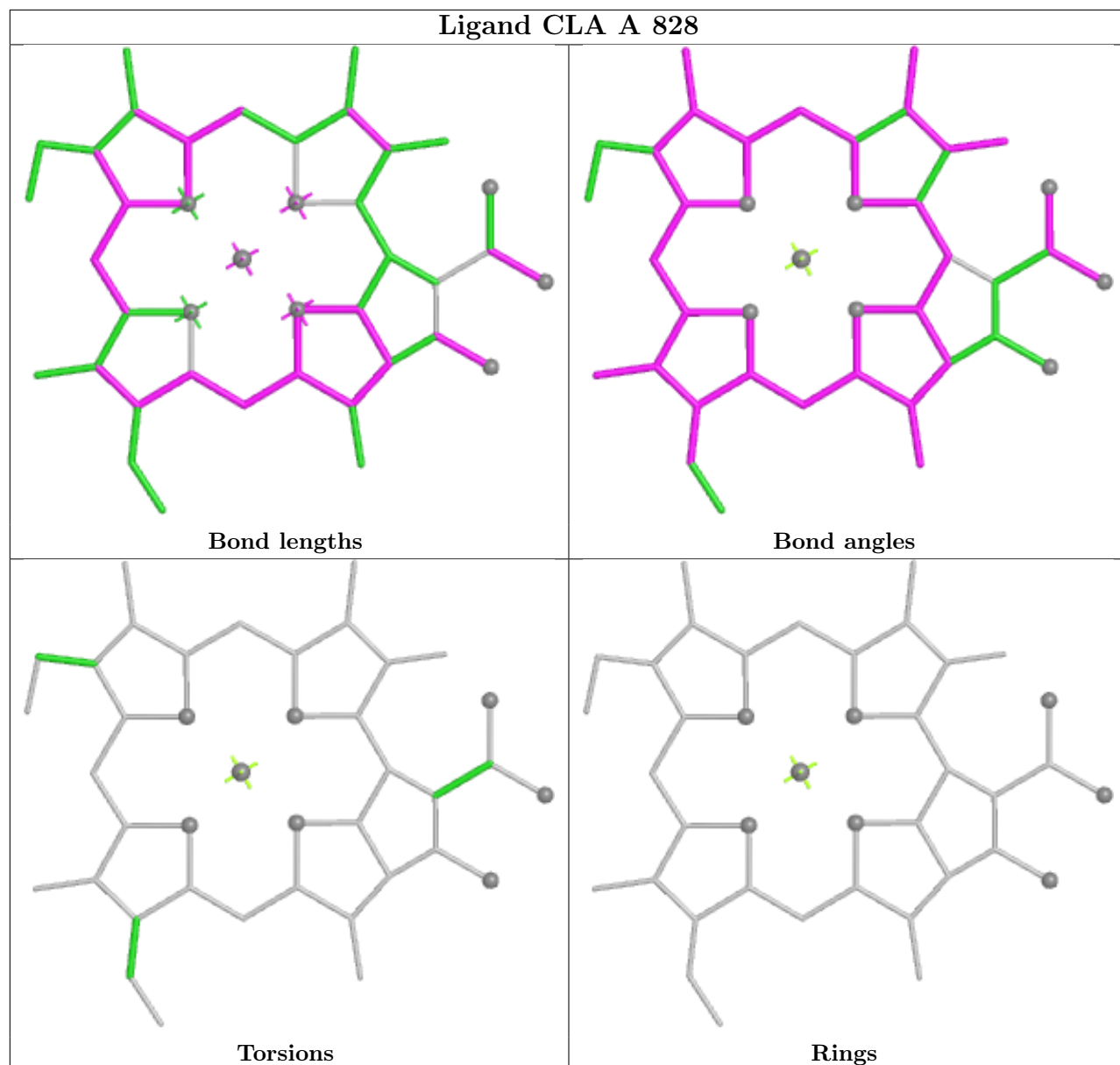
Ligand CLA 3 321



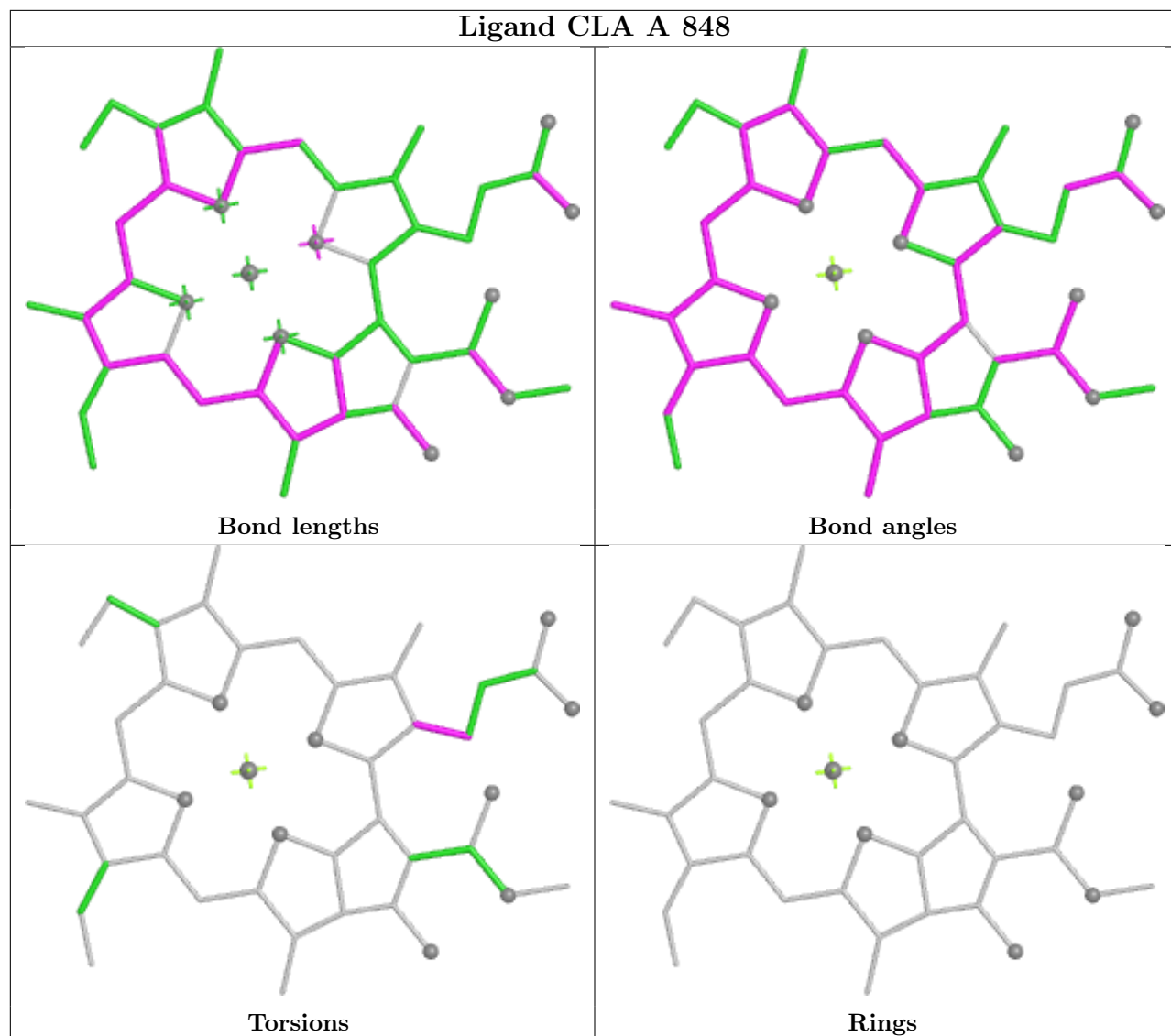


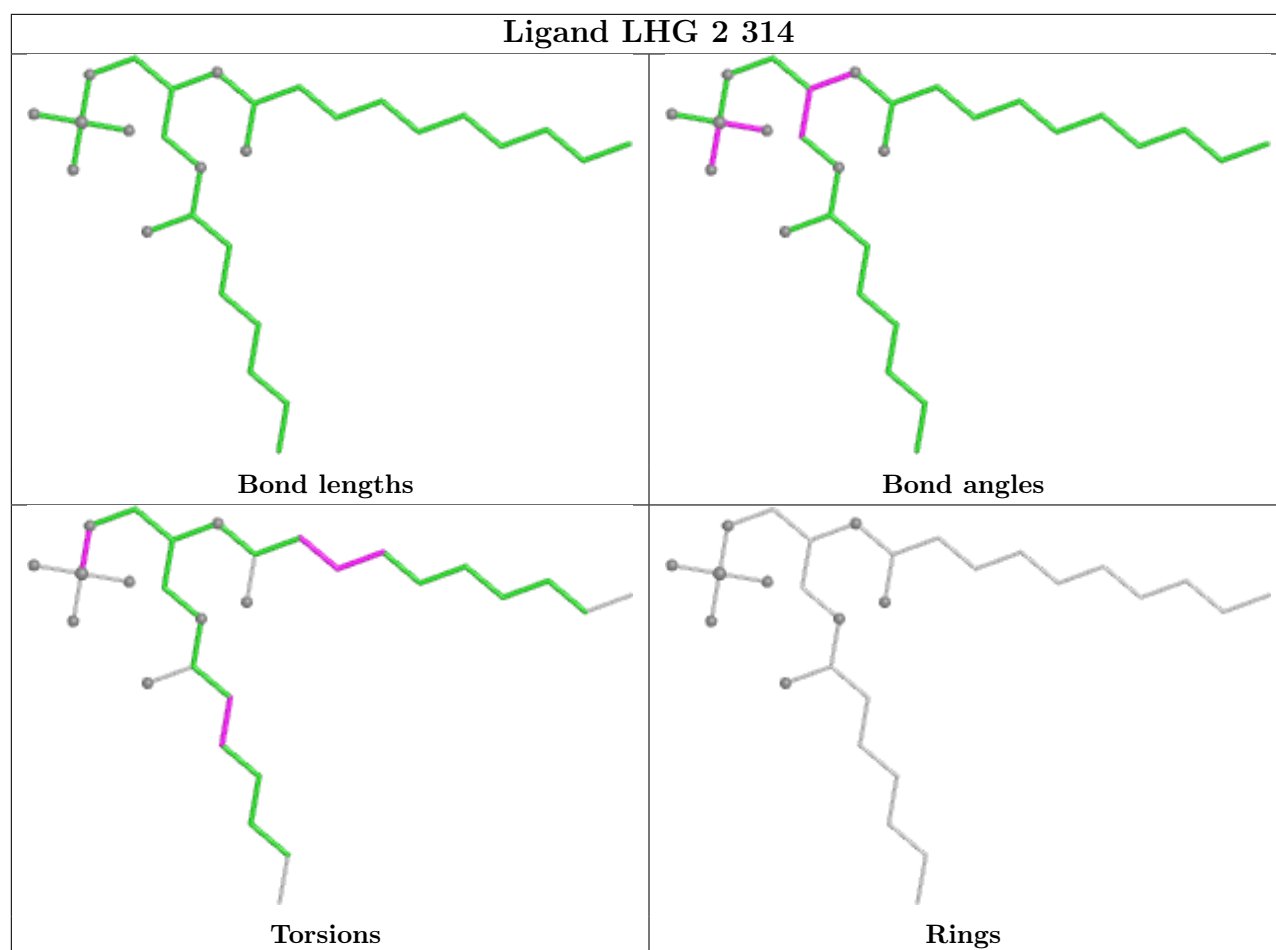


Ligand CLA A 828

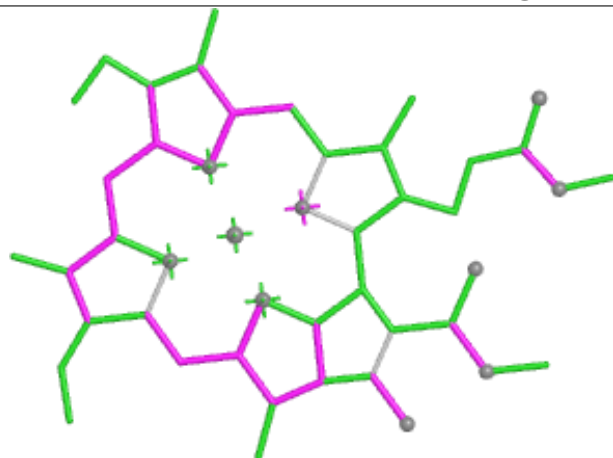


Ligand CLA A 848

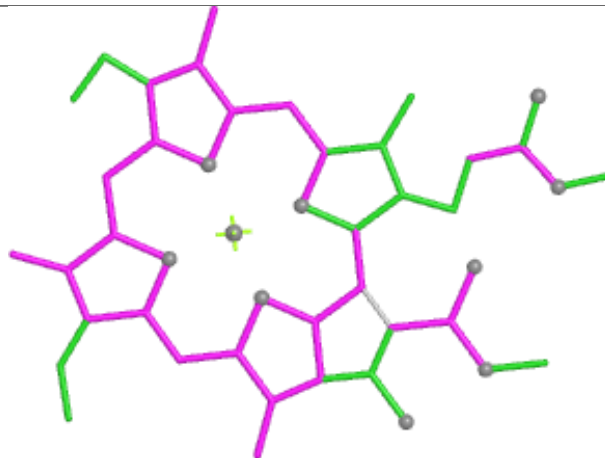




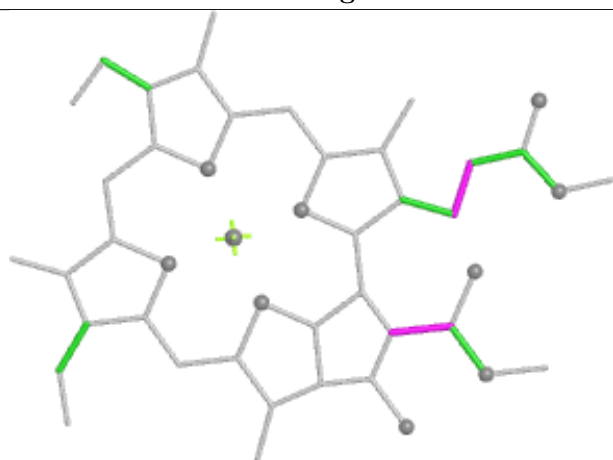
Ligand CLA F 305



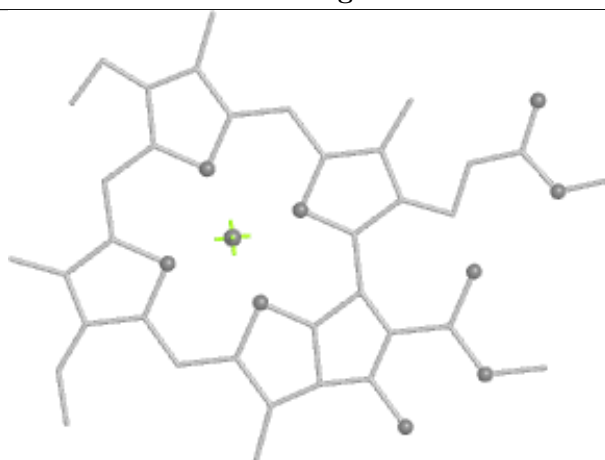
Bond lengths



Bond angles

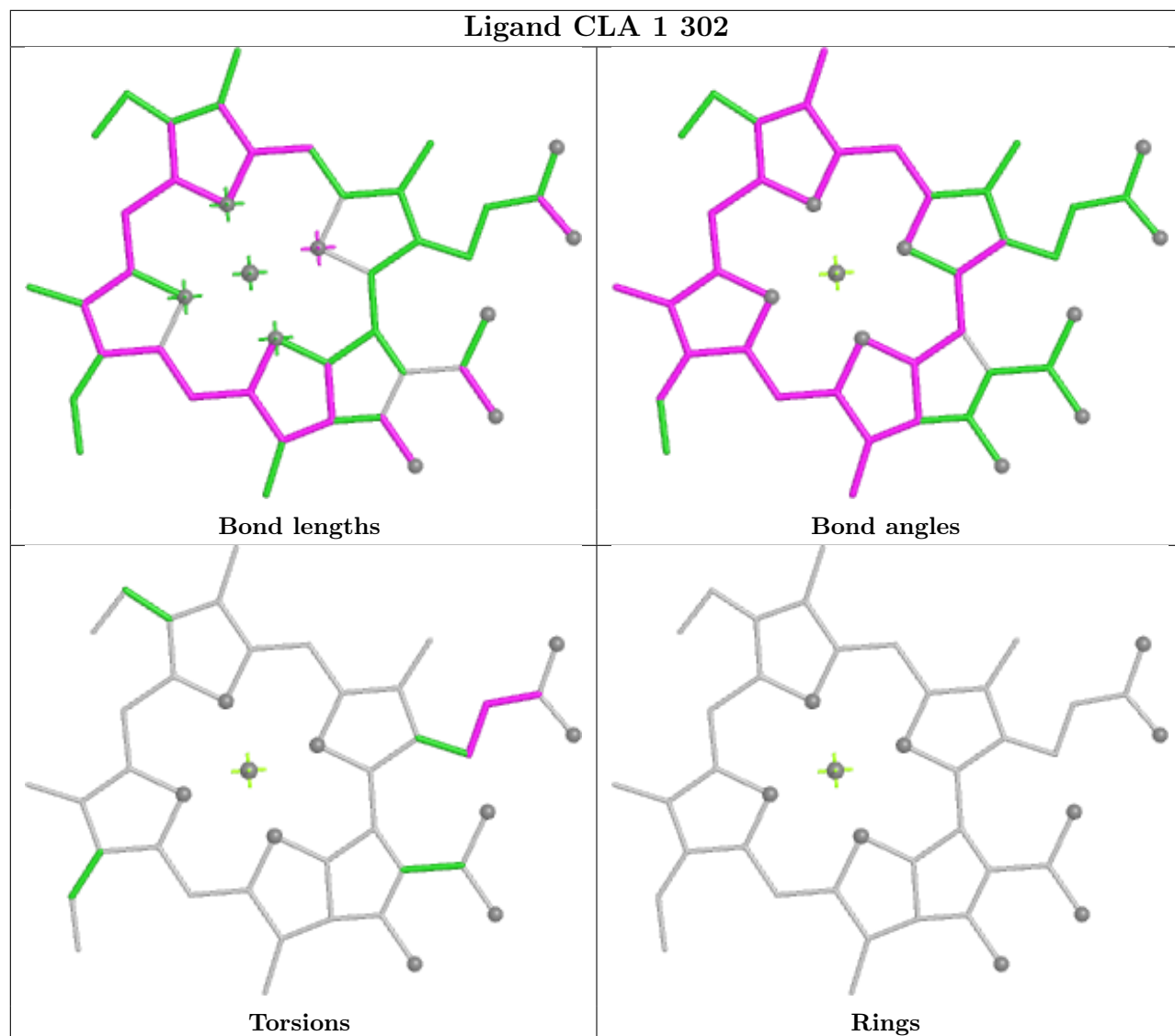


Torsions

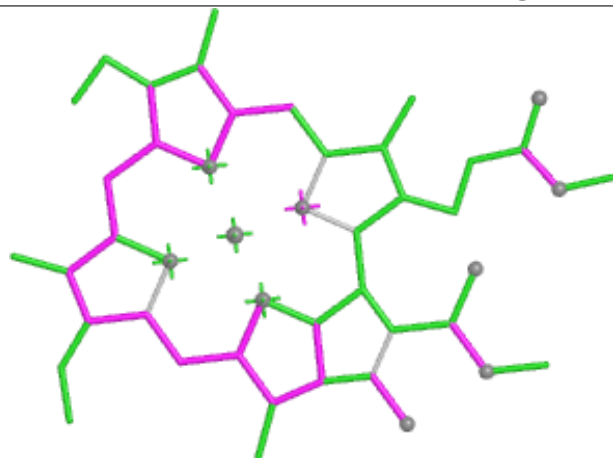


Rings

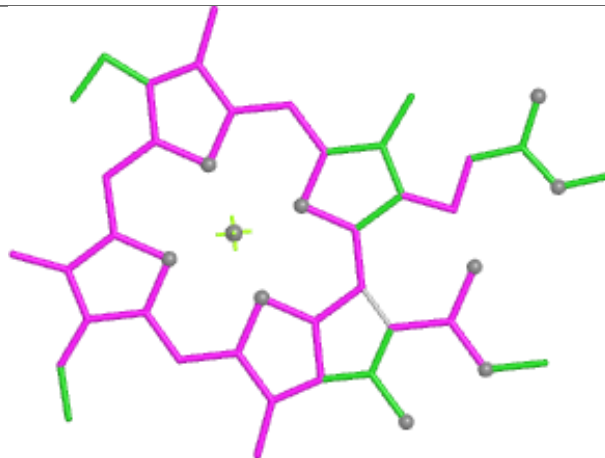
Ligand CLA 1 302



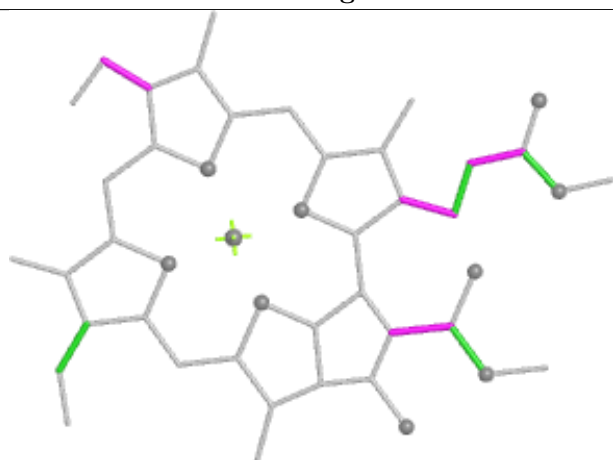
Ligand CLA X 310



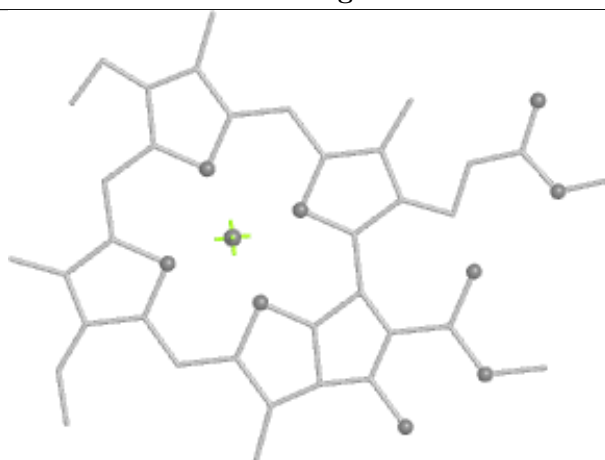
Bond lengths



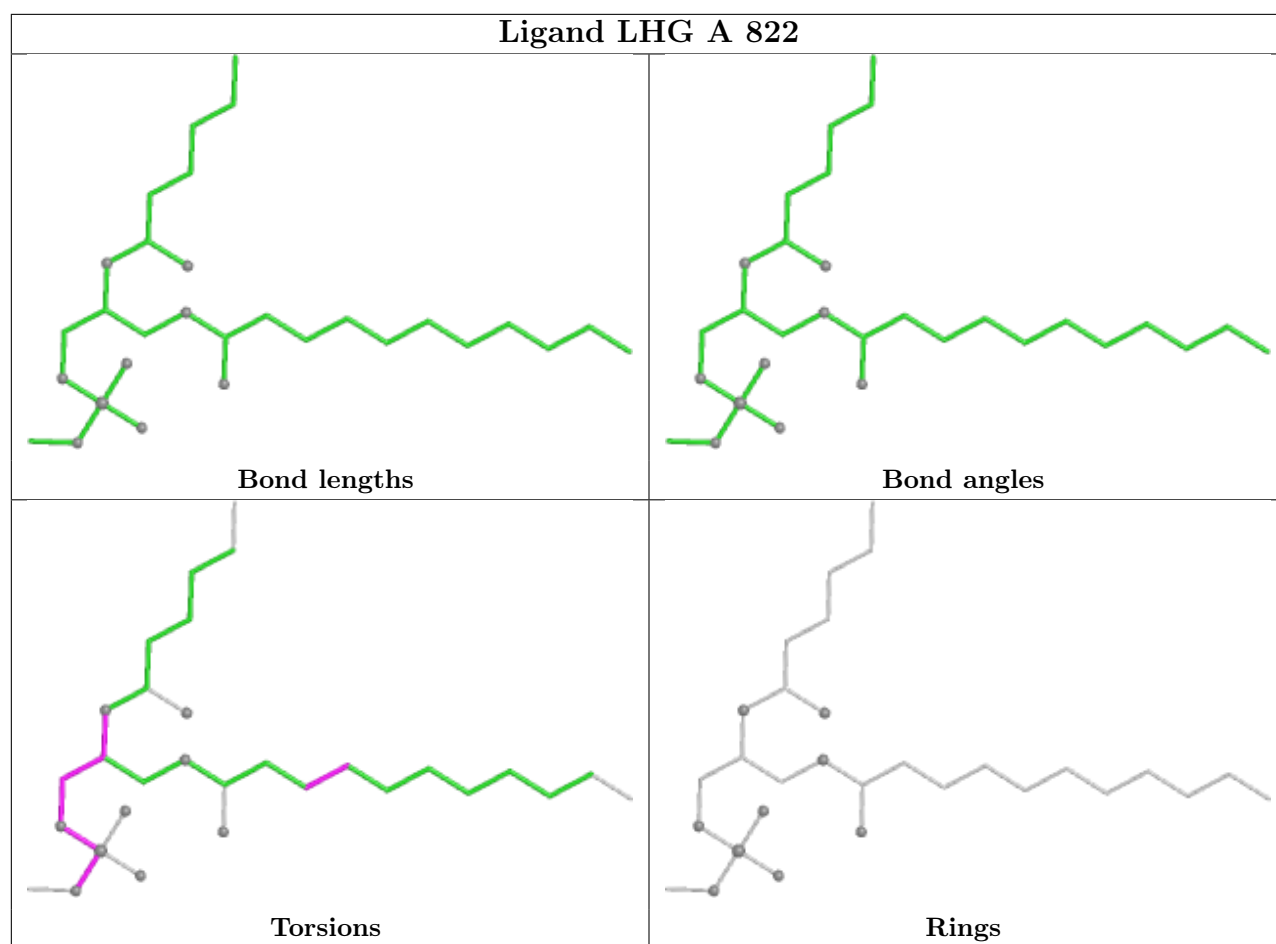
Bond angles



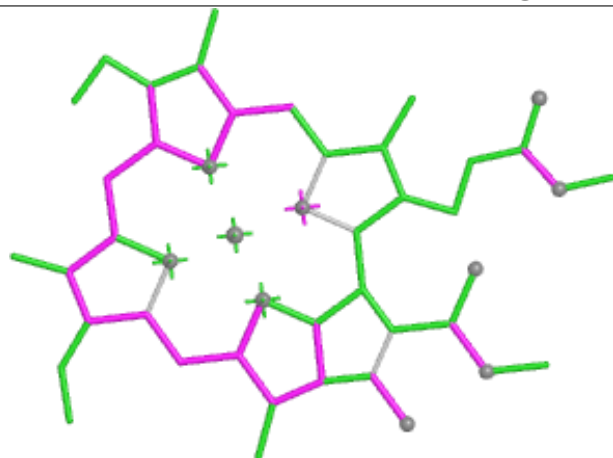
Torsions



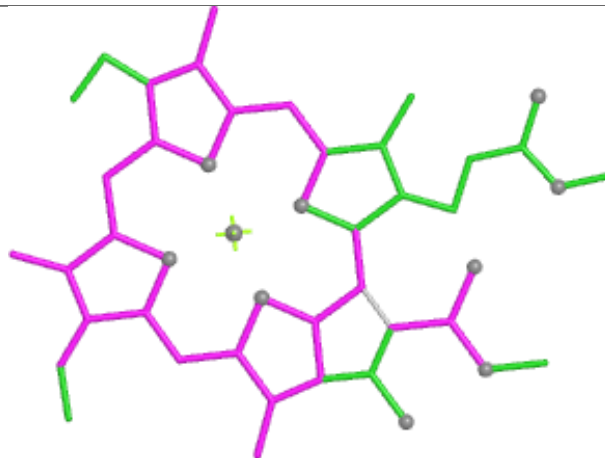
Rings



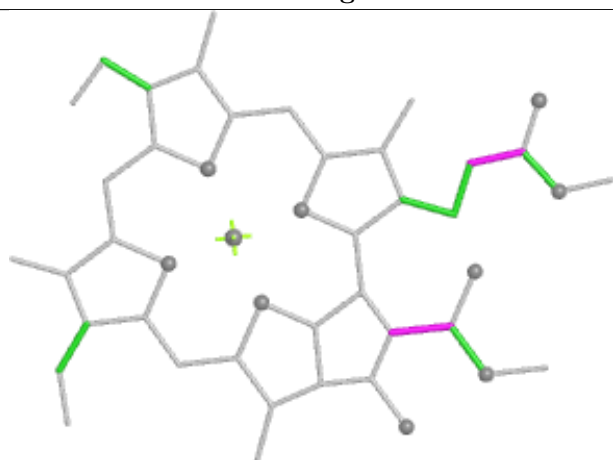
Ligand CLA Z 311



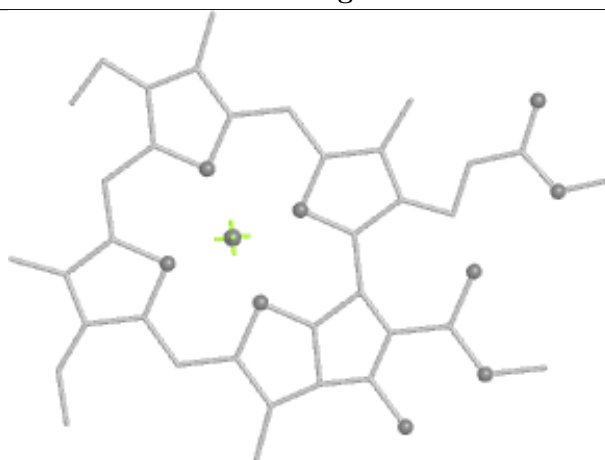
Bond lengths



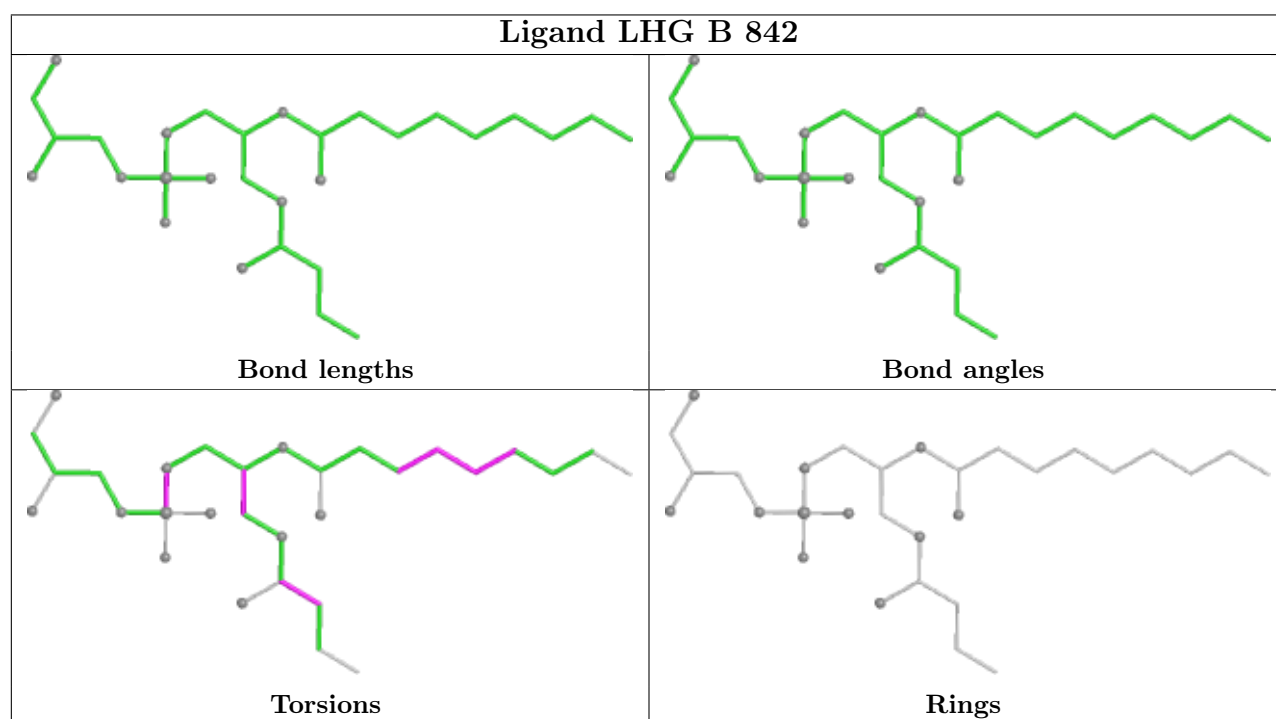
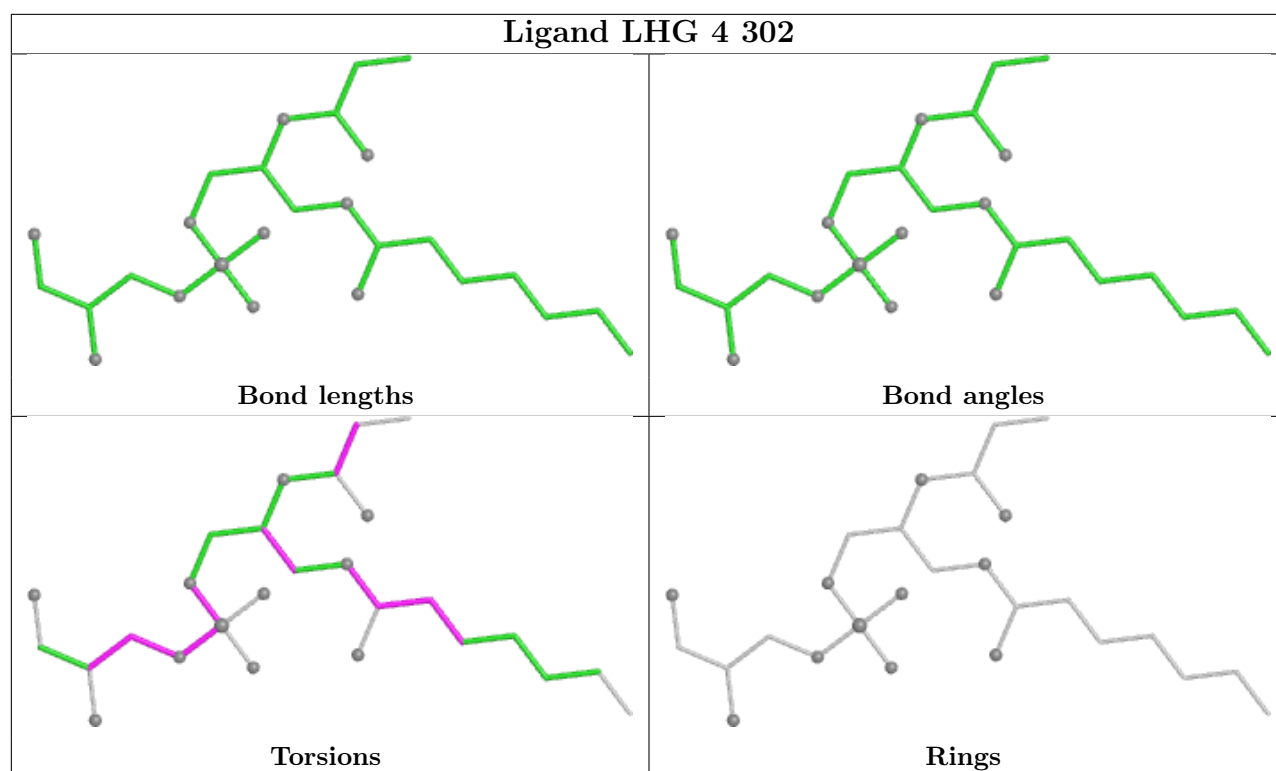
Bond angles



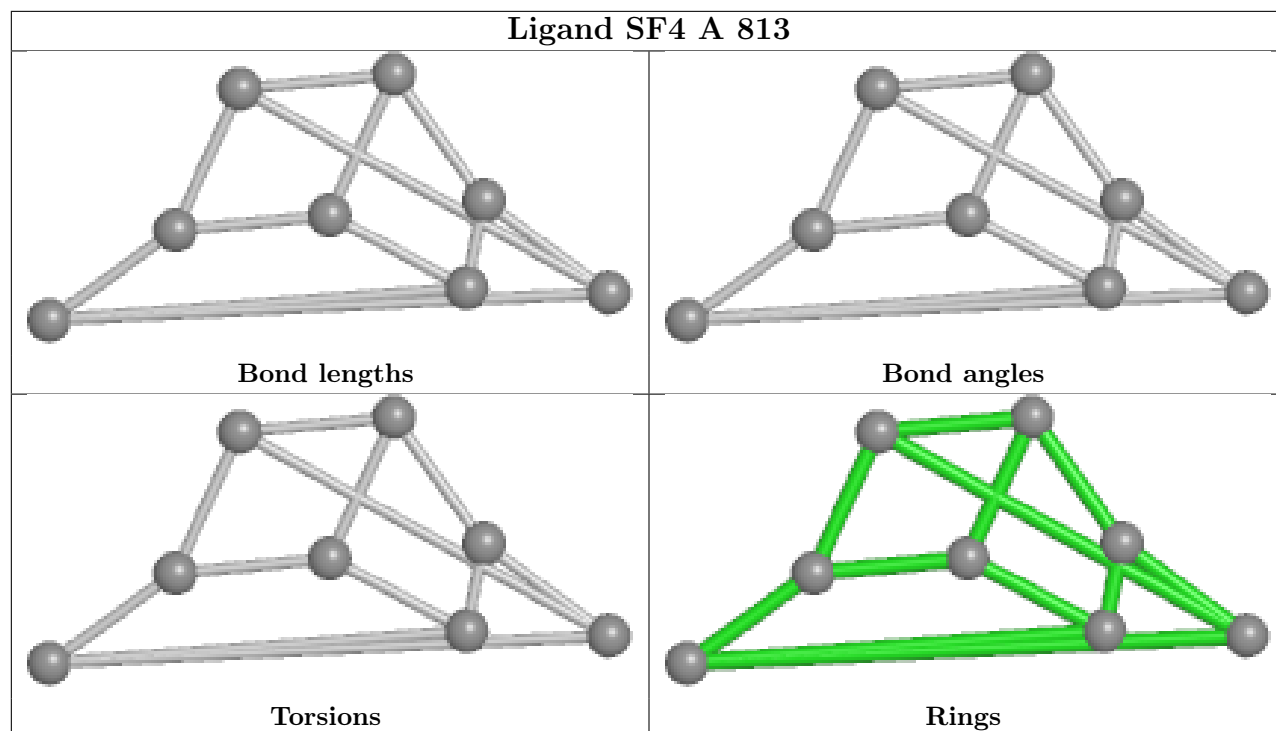
Torsions



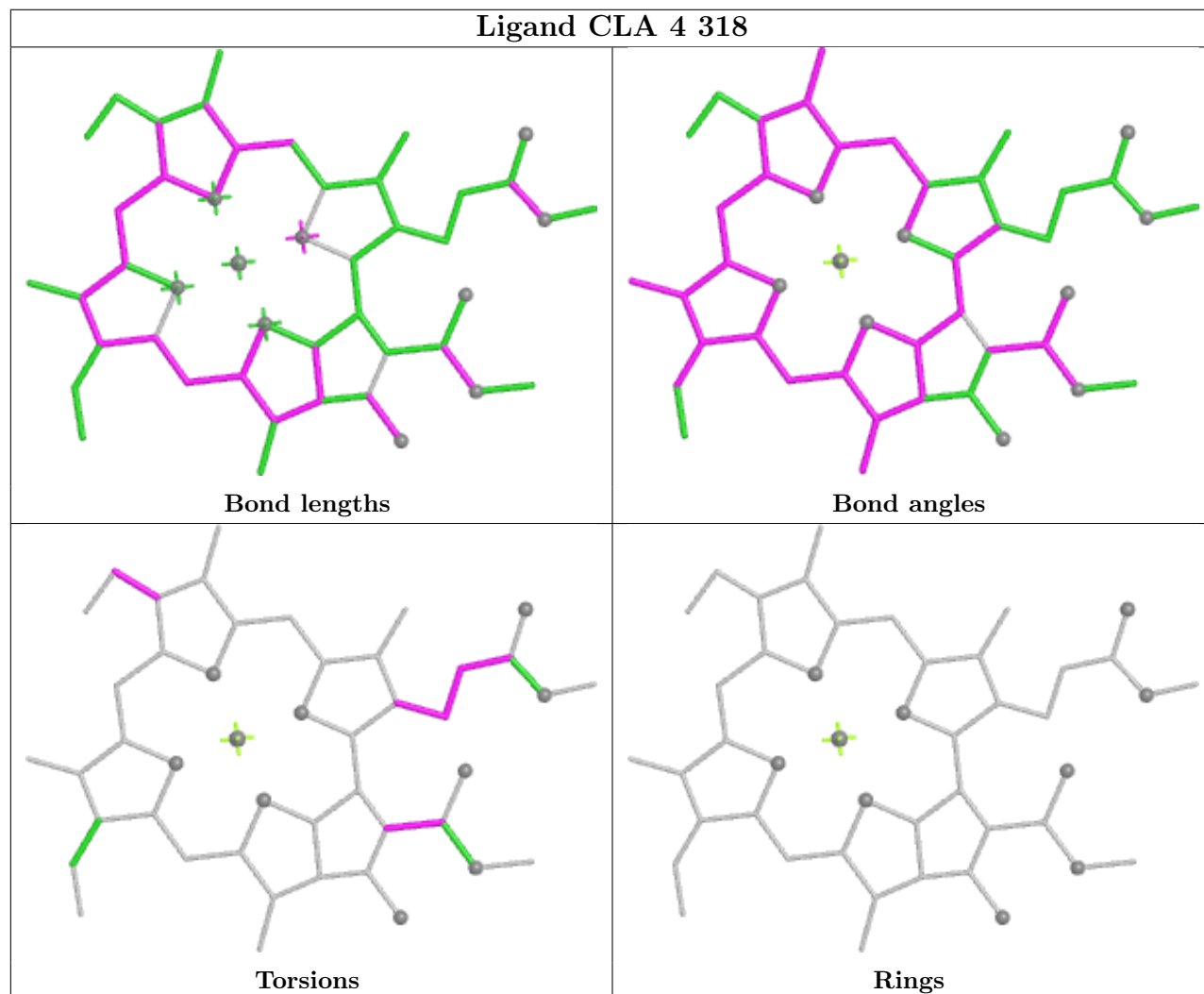
Rings



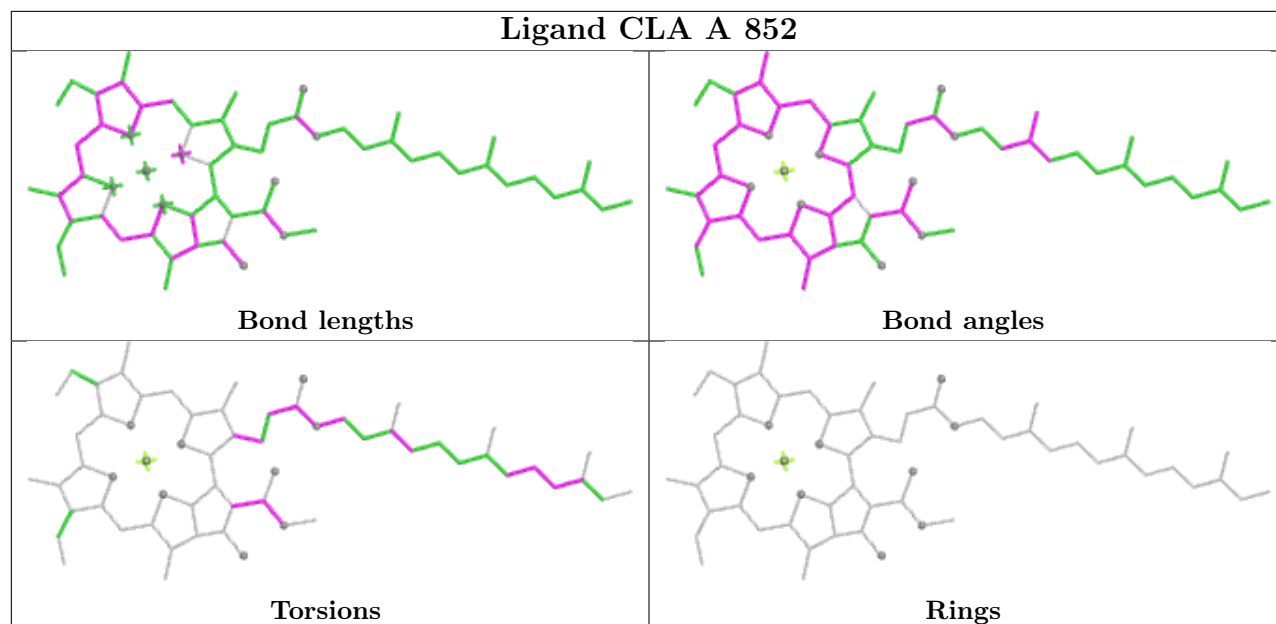
Ligand SF4 A 813



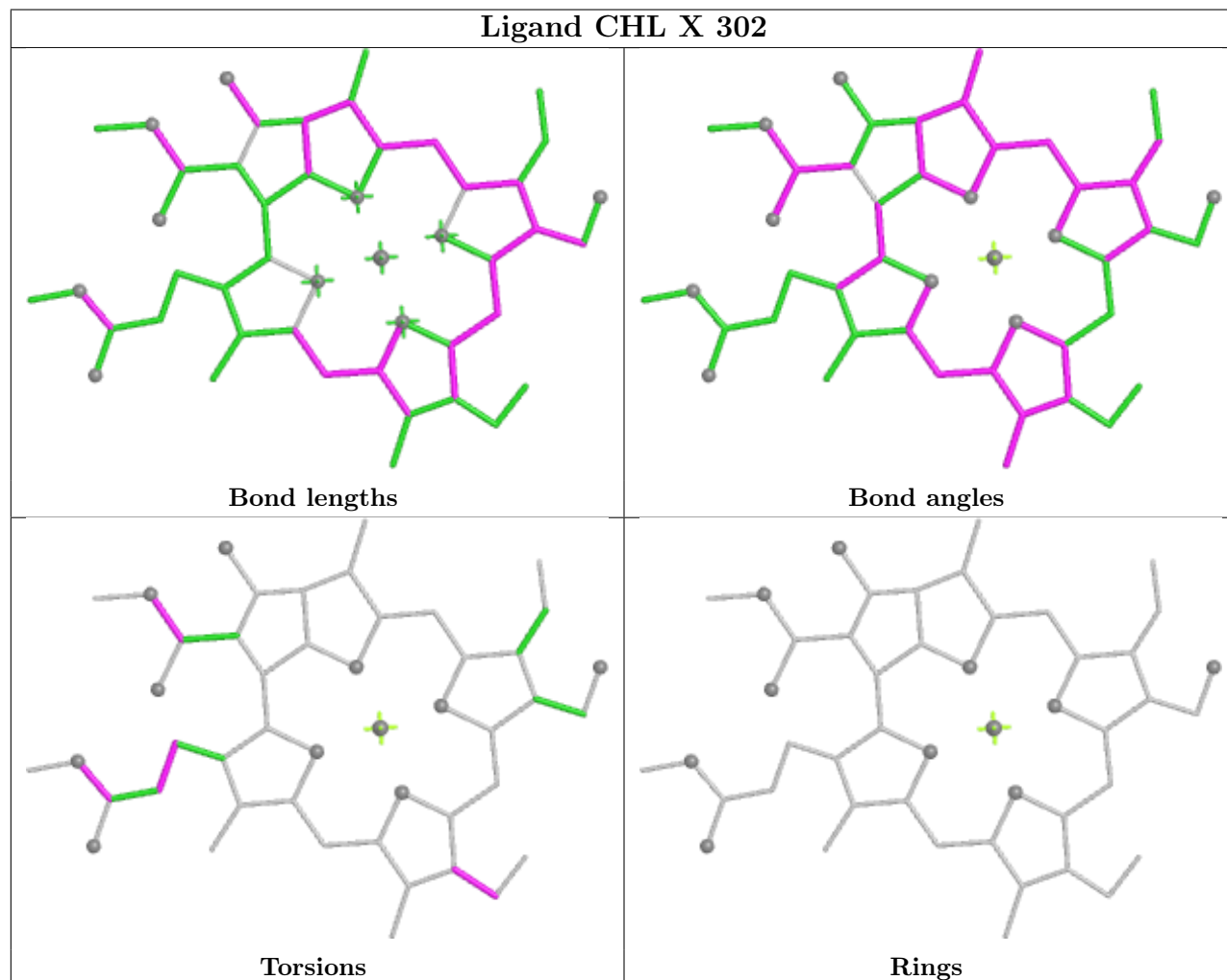
Ligand CLA 4 318

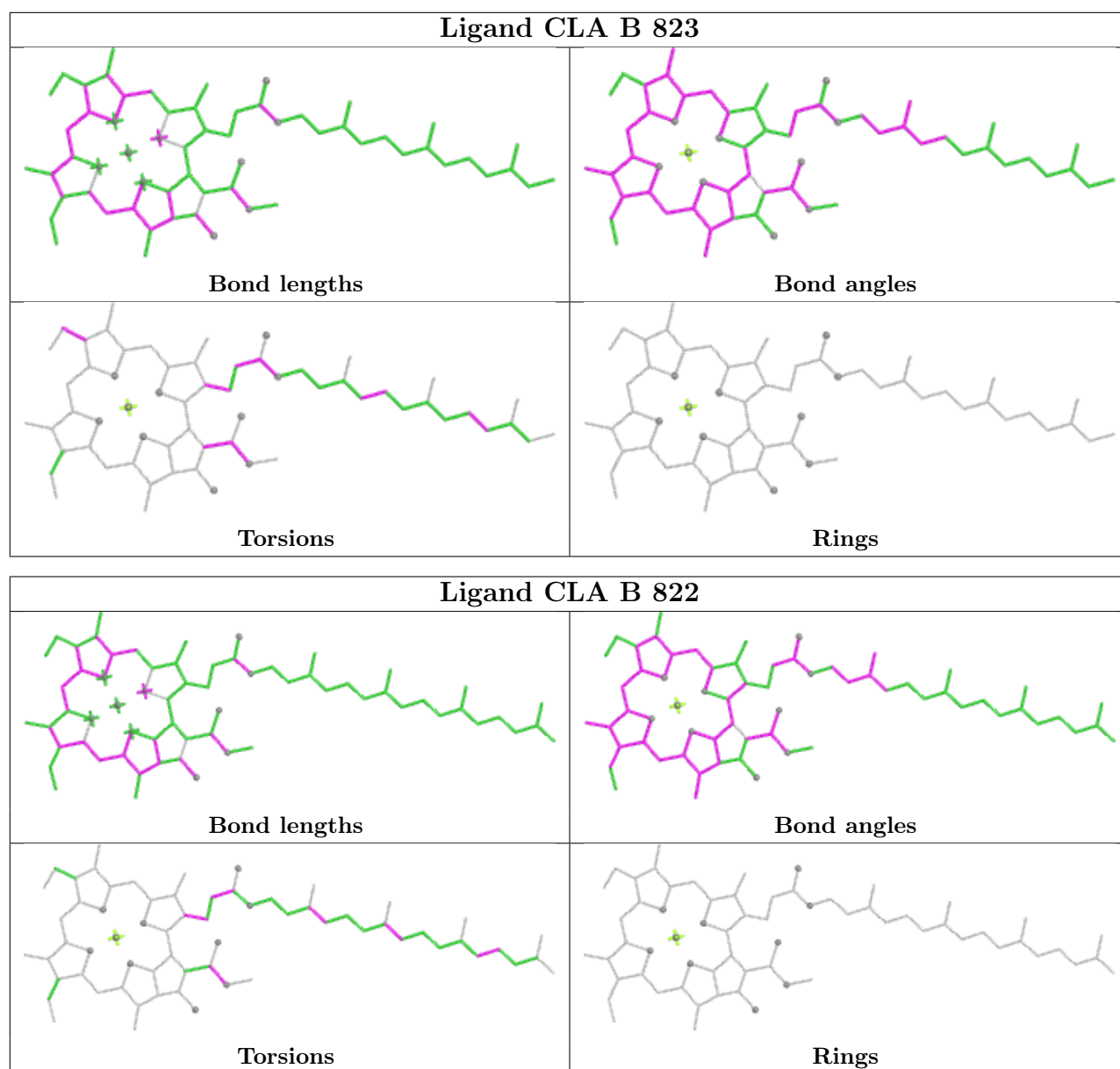


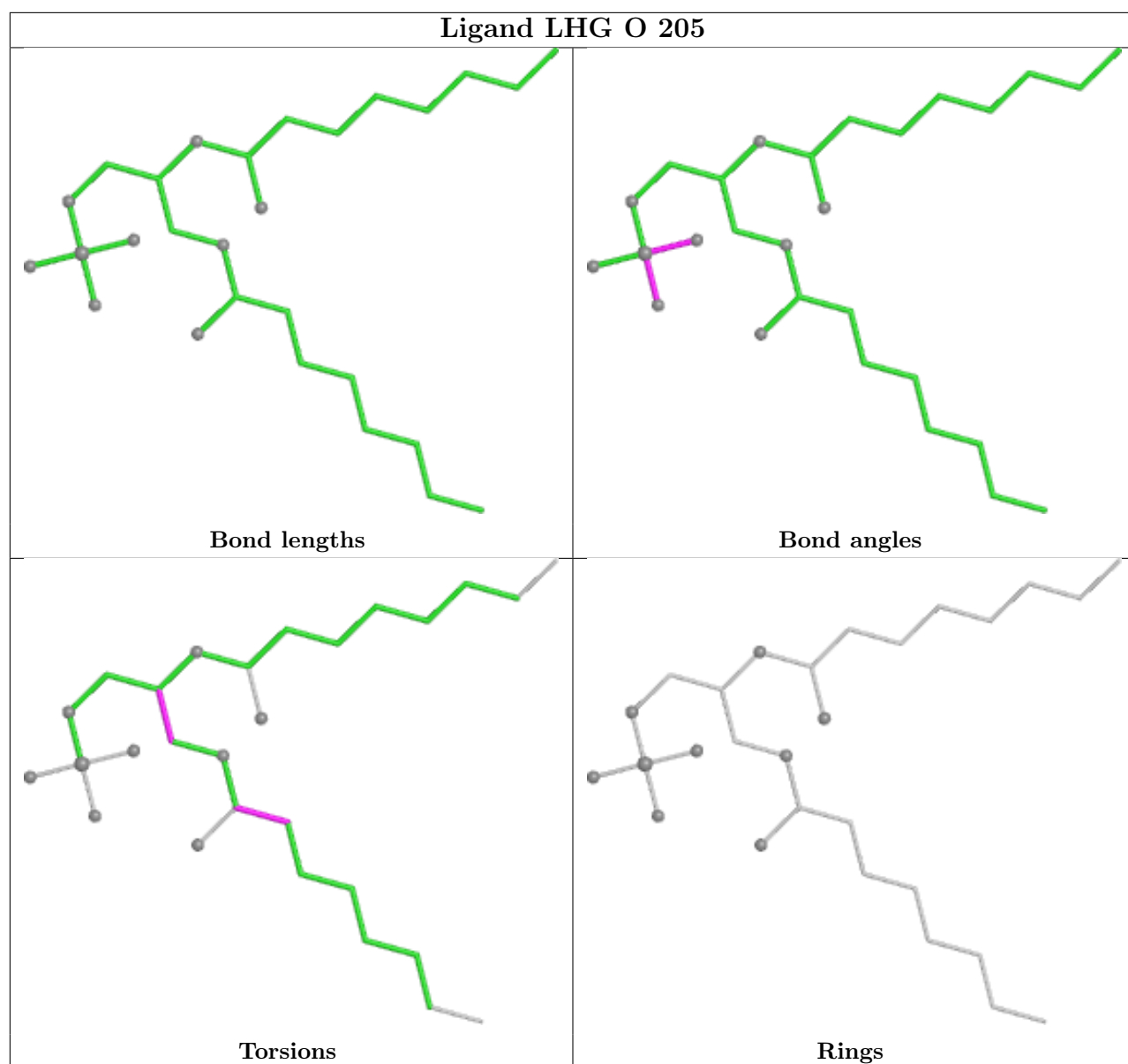
Ligand CLA A 852



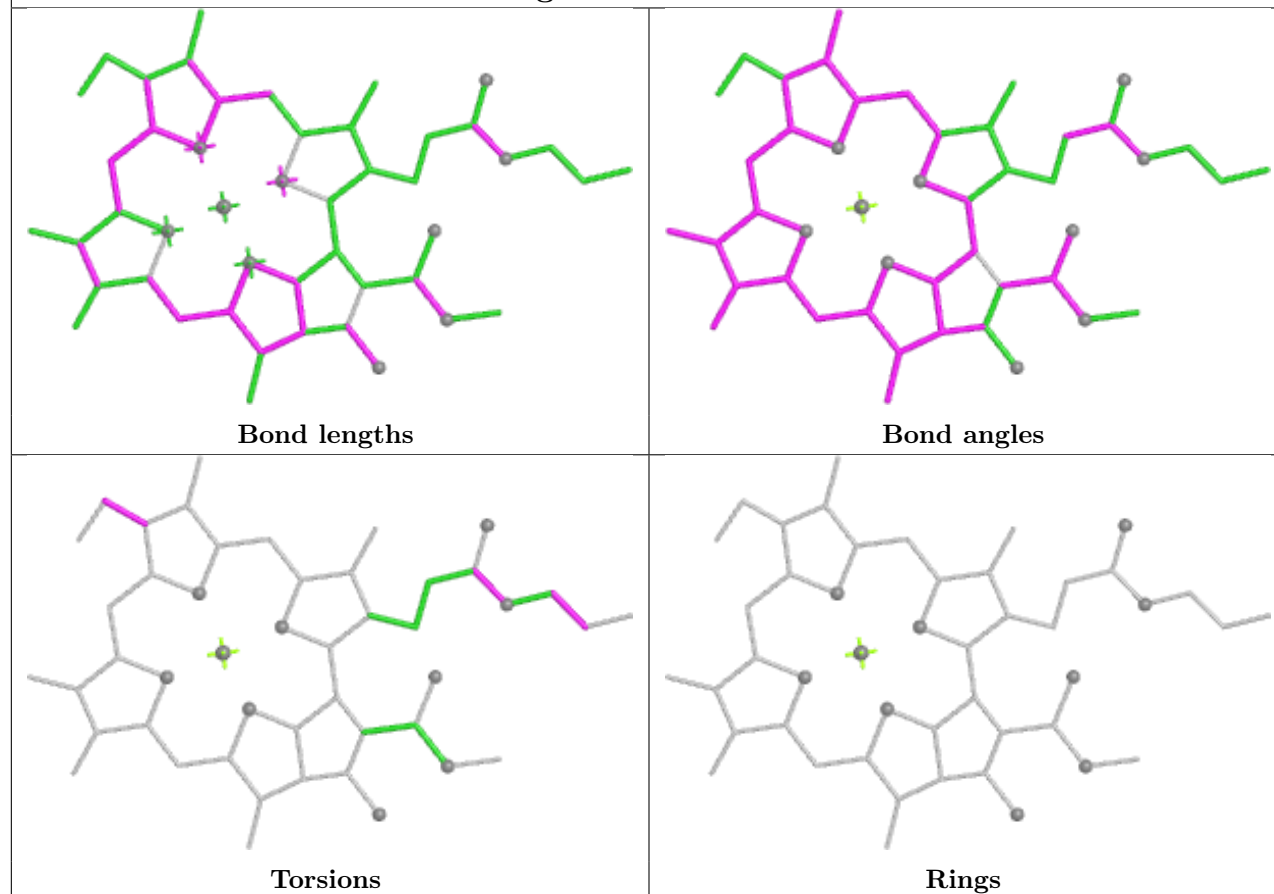
Ligand CHL X 302



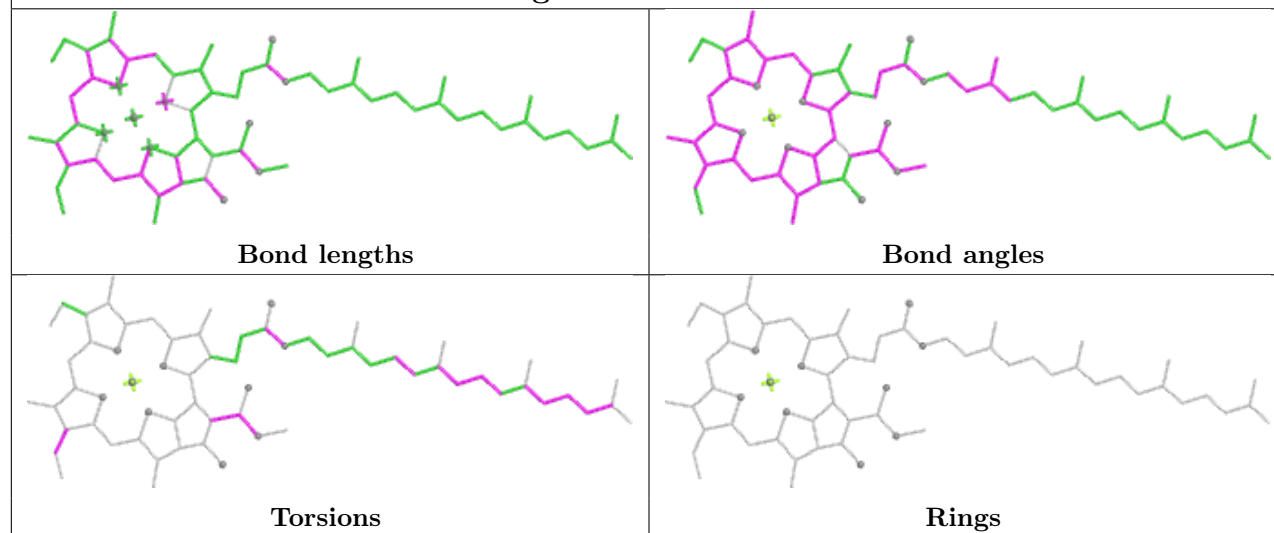




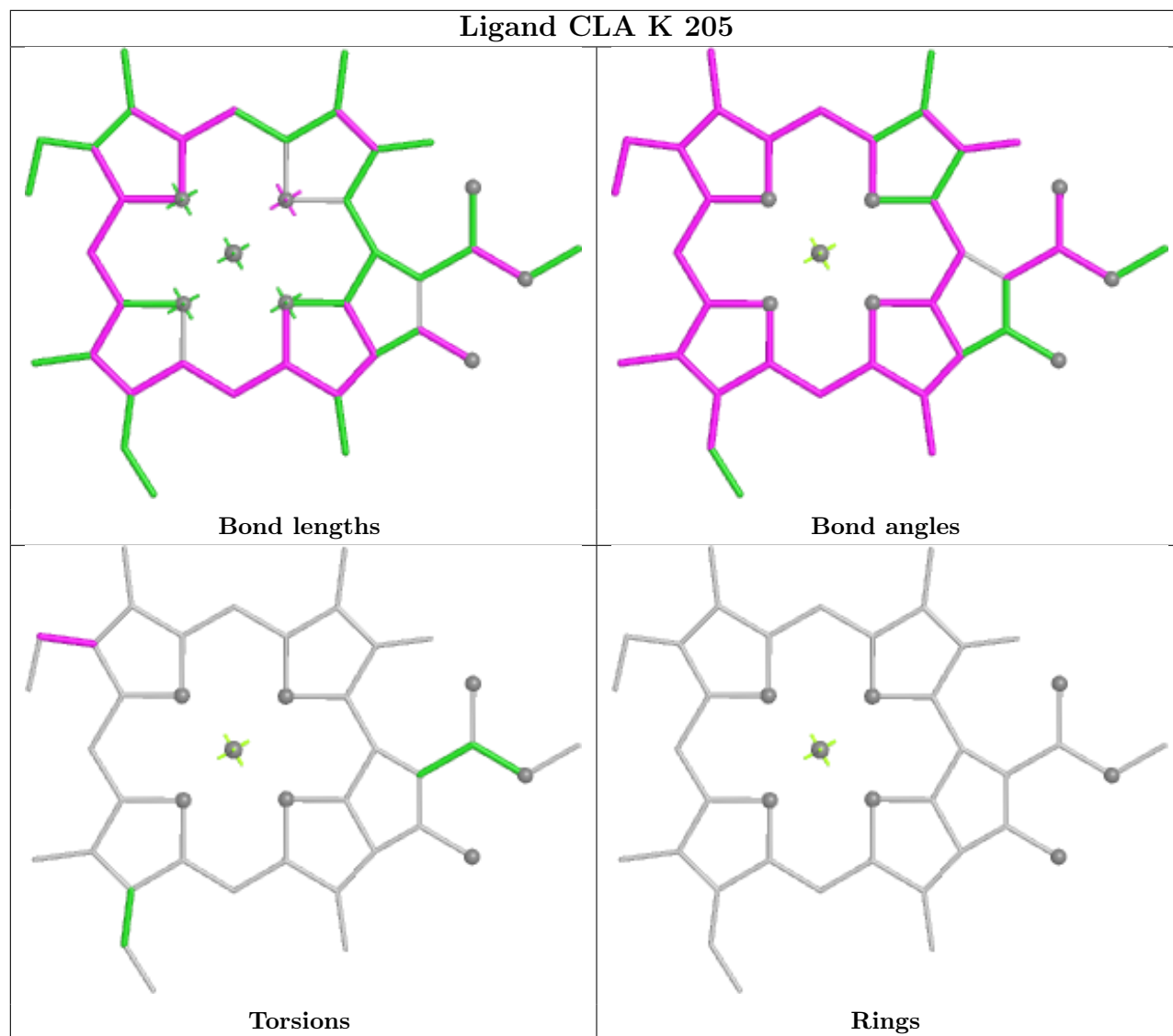
Ligand CLA 2 319



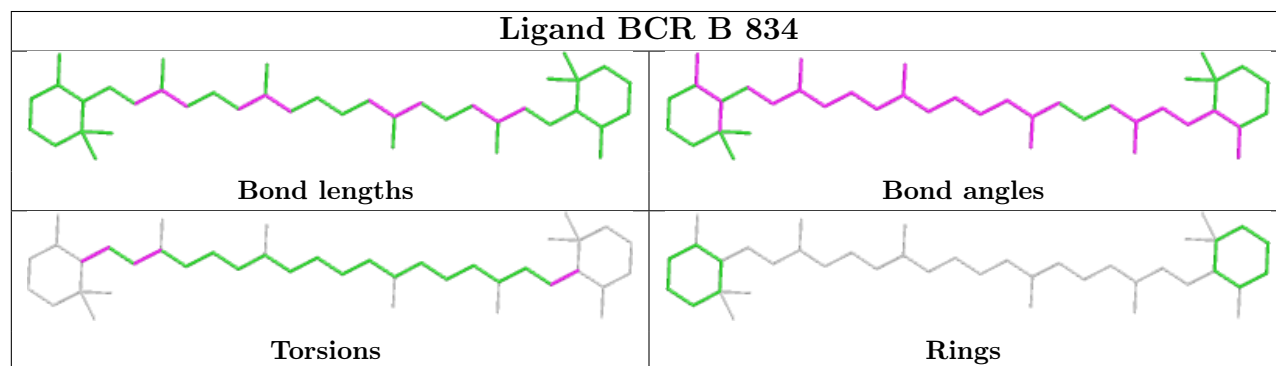
Ligand CLA B 830

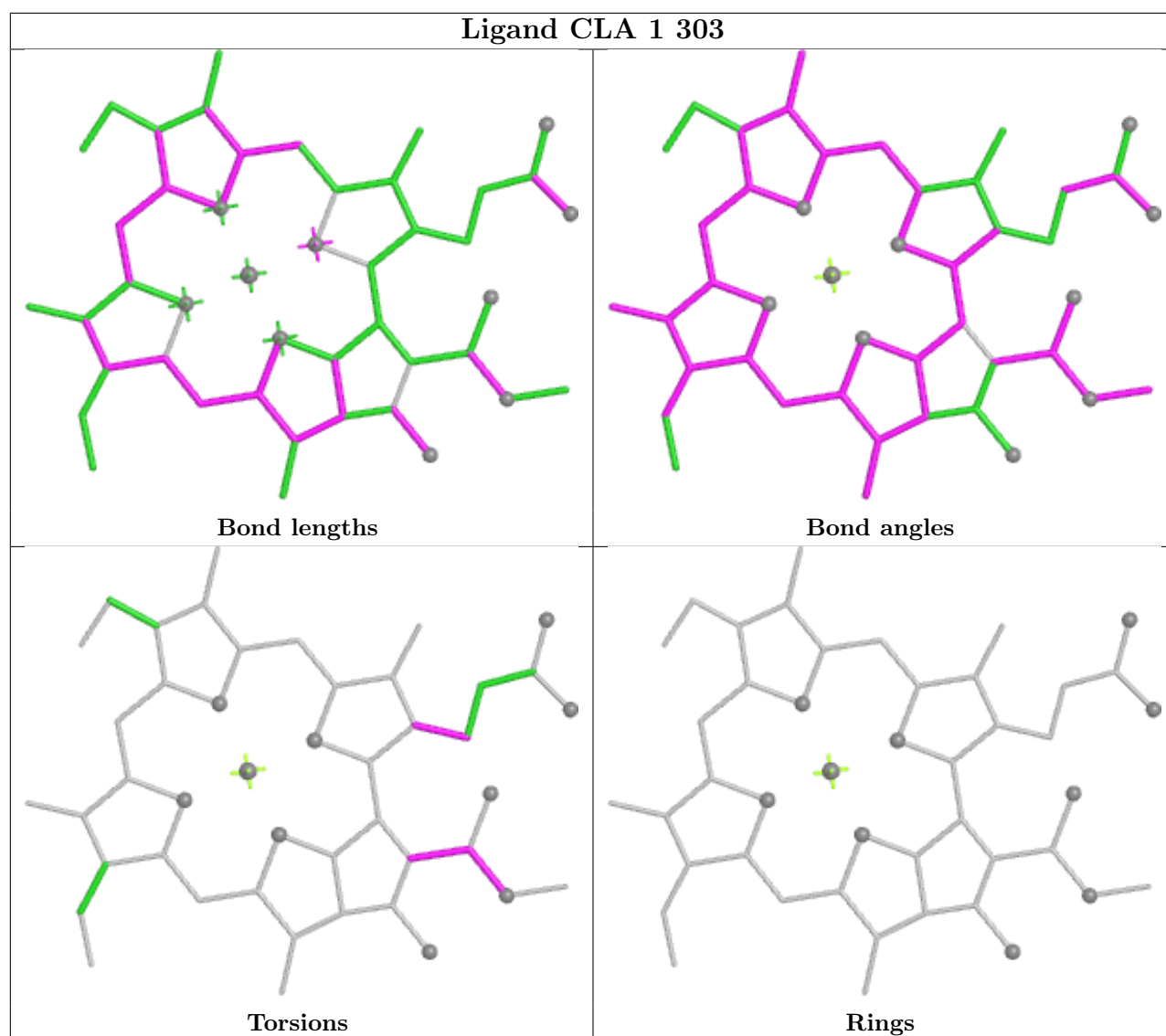


Ligand CLA K 205



Ligand BCR B 834





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.

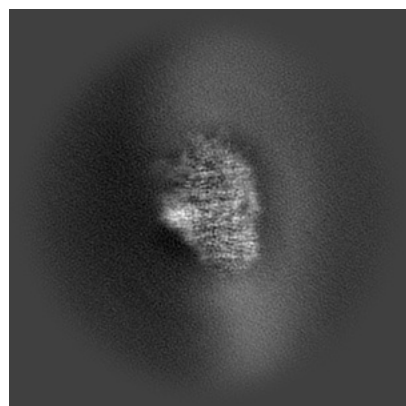
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66932. These allow visual inspection of the internal detail of the map and identification of artifacts.

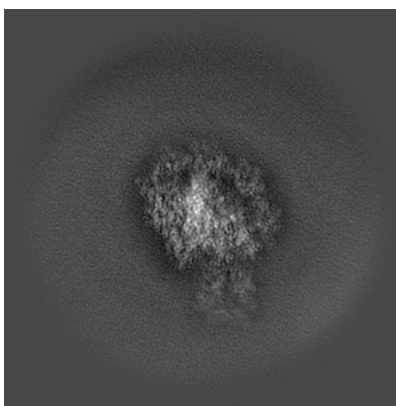
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

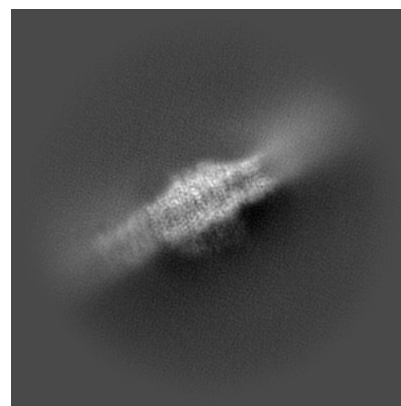
6.1.1 Primary map



X

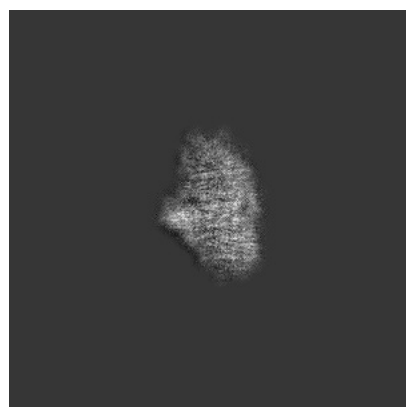


Y

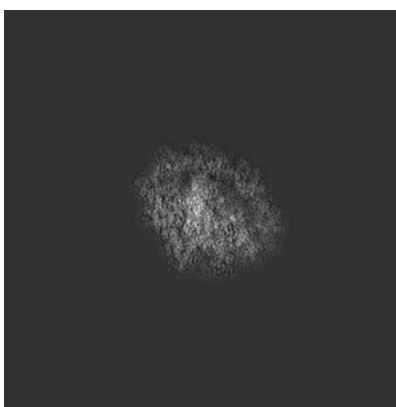


Z

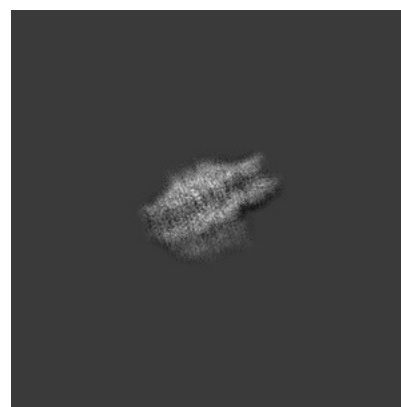
6.1.2 Raw map



X



Y

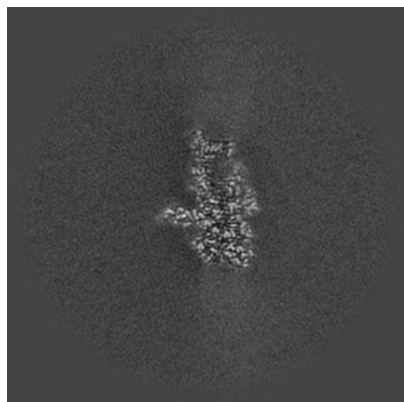


Z

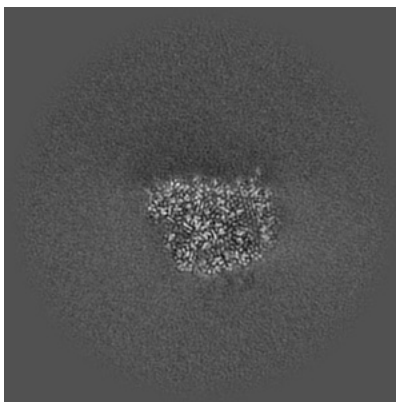
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

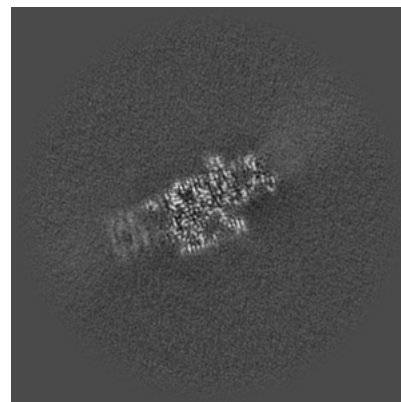
6.2.1 Primary map



X Index: 256

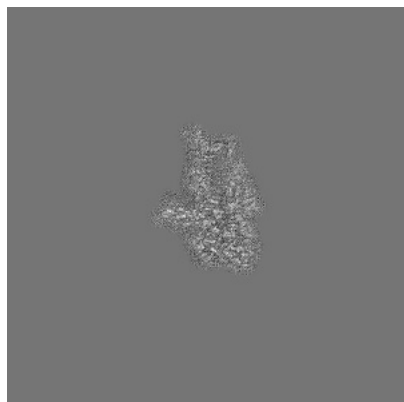


Y Index: 256

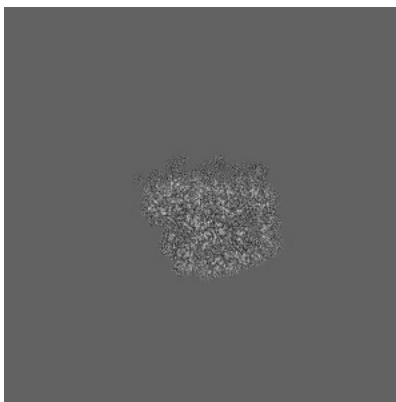


Z Index: 256

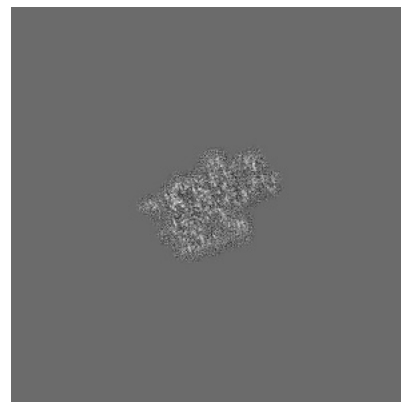
6.2.2 Raw map



X Index: 256



Y Index: 256

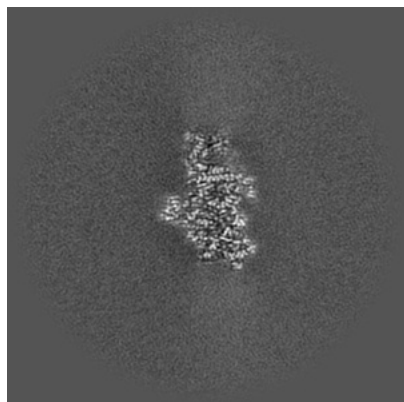


Z Index: 256

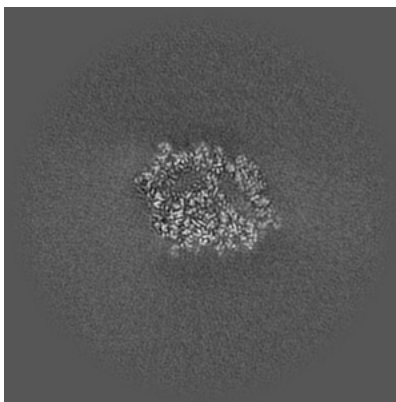
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

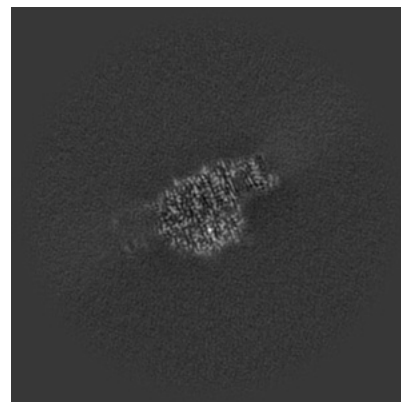
6.3.1 Primary map



X Index: 244

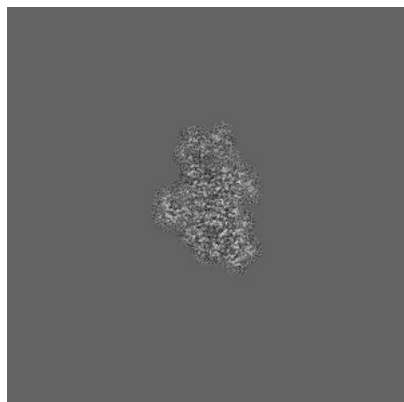


Y Index: 280

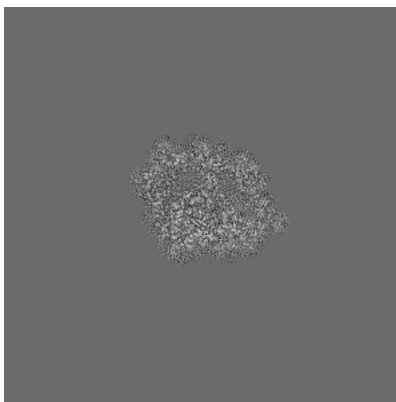


Z Index: 244

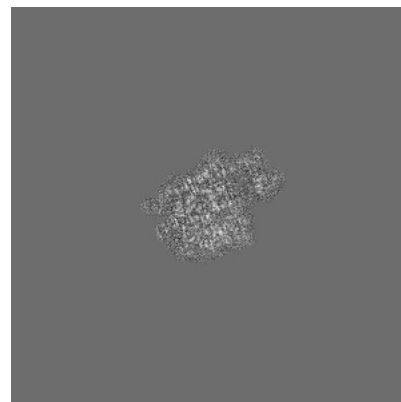
6.3.2 Raw map



X Index: 239



Y Index: 279

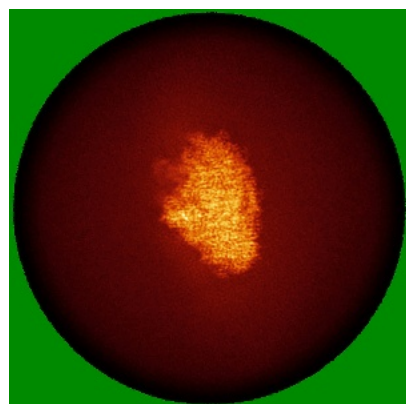


Z Index: 249

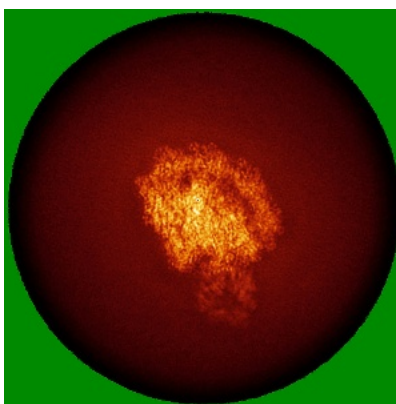
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

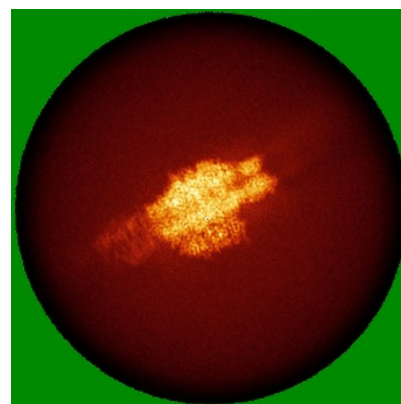
6.4.1 Primary map



X

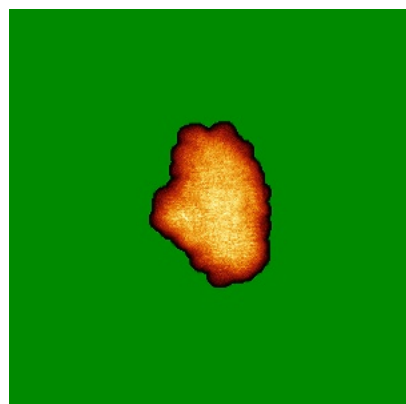


Y

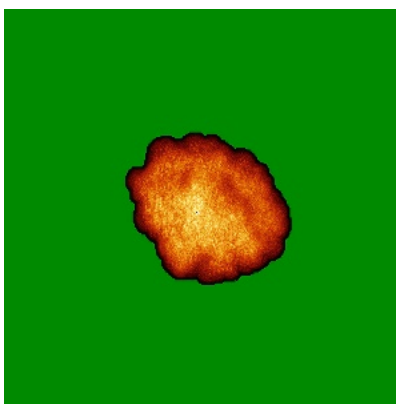


Z

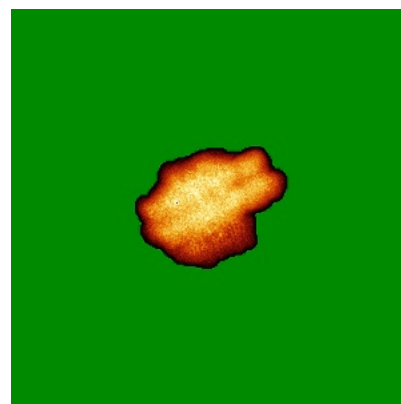
6.4.2 Raw map



X



Y

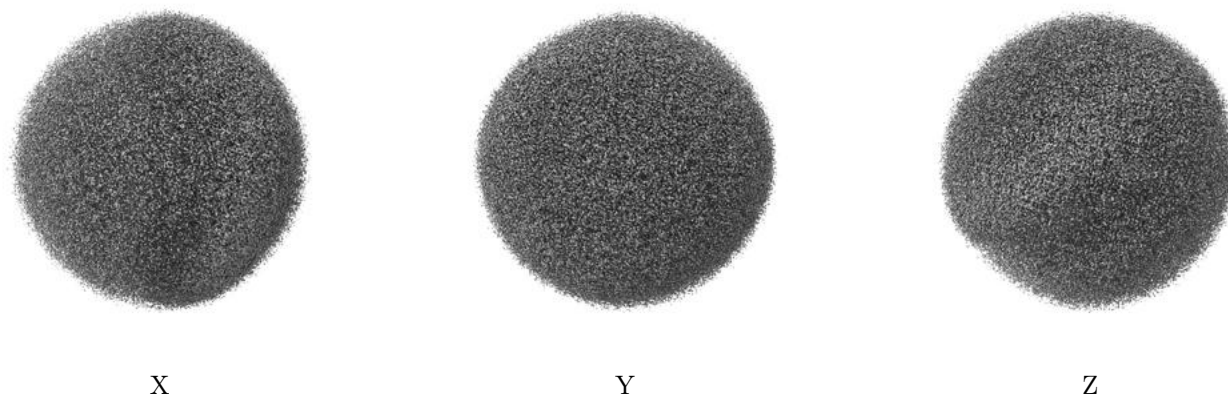


Z

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.

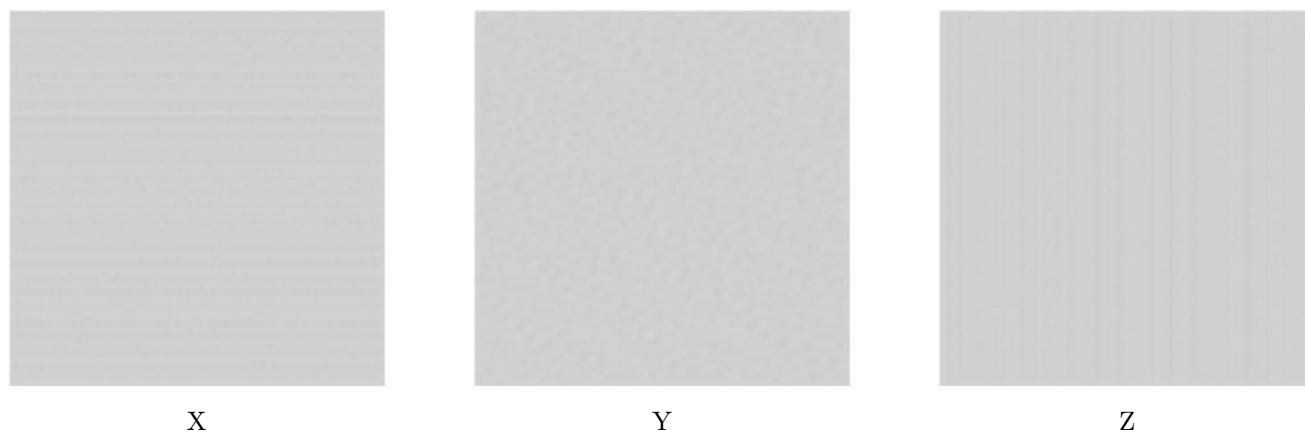
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

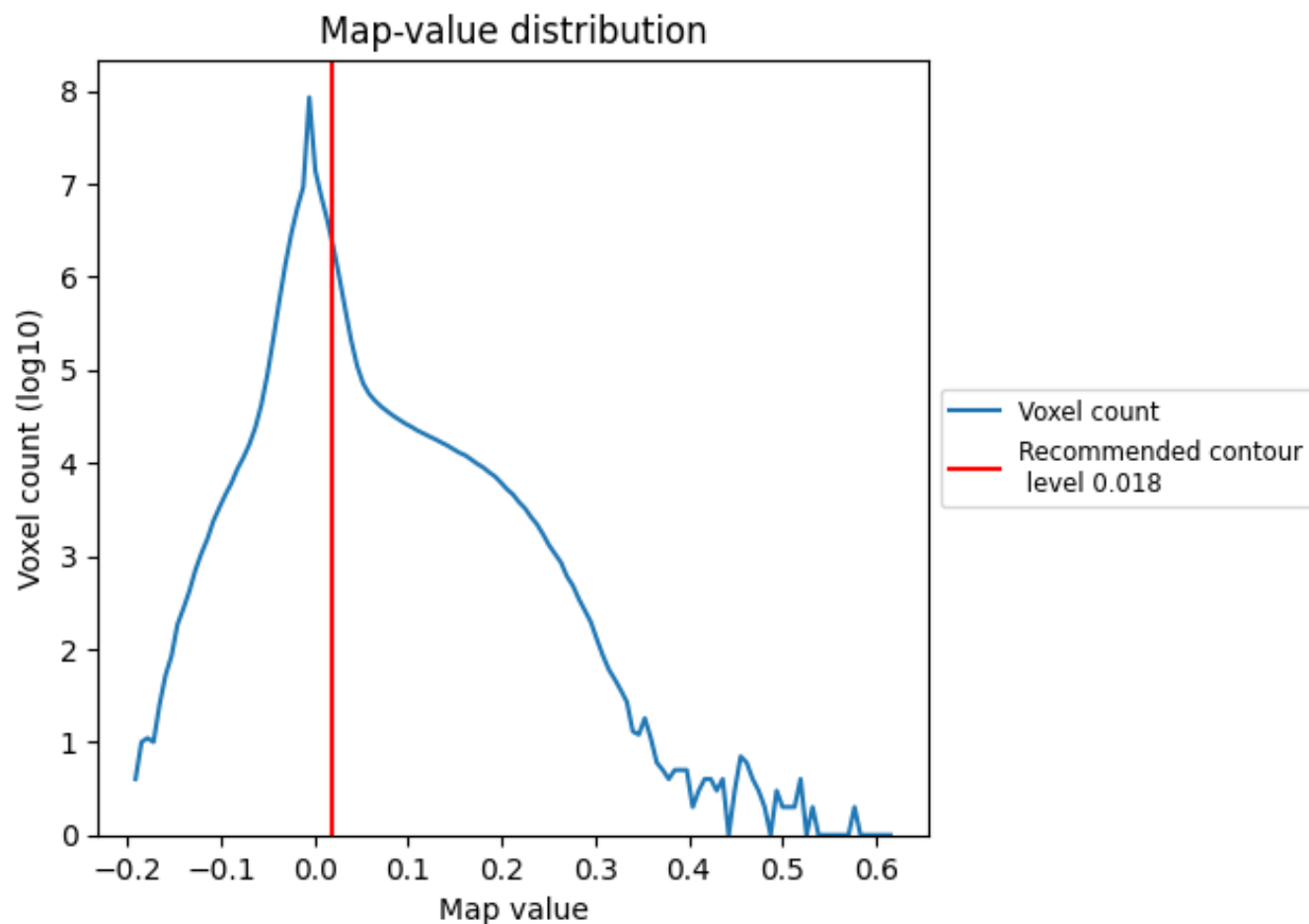
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

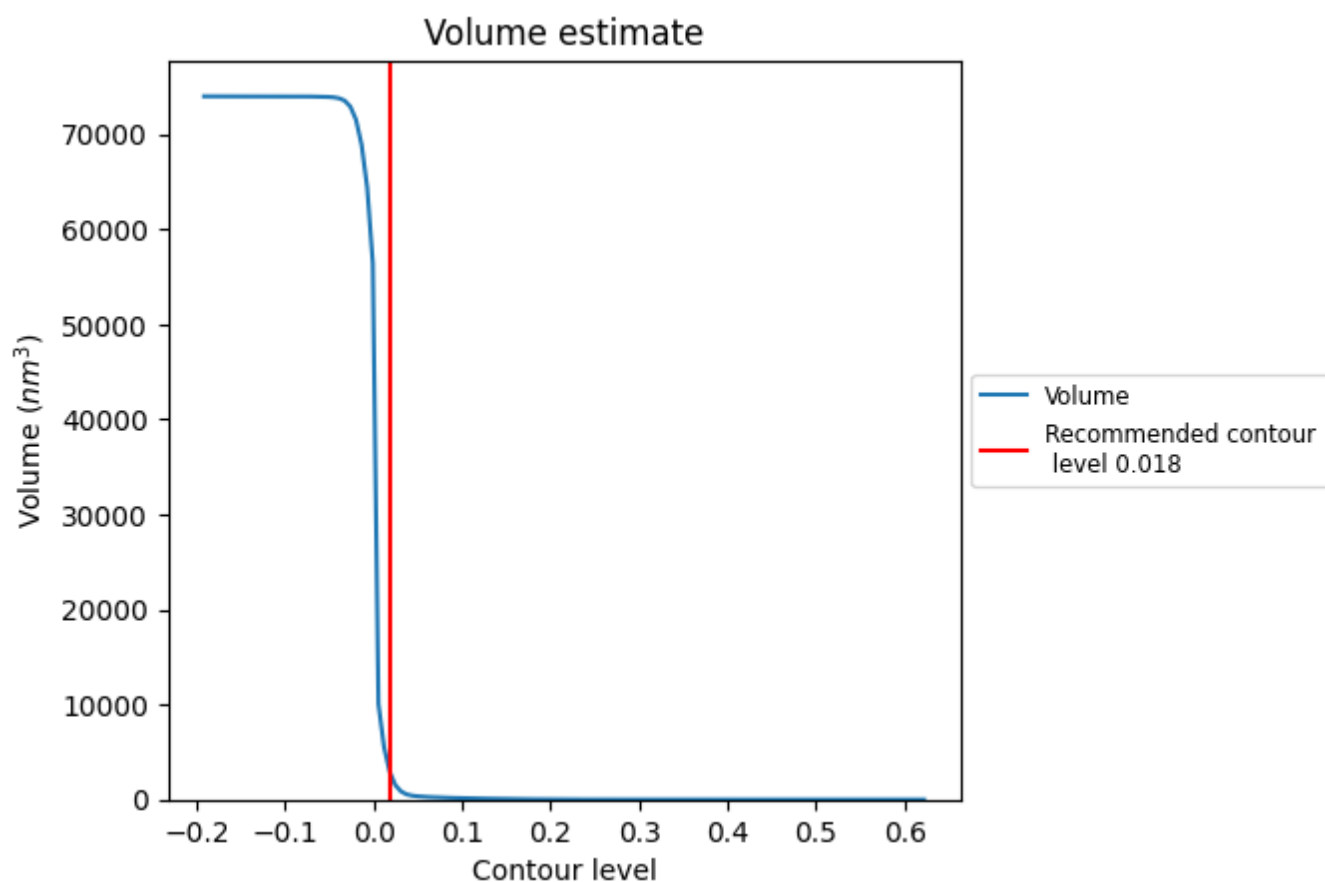
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

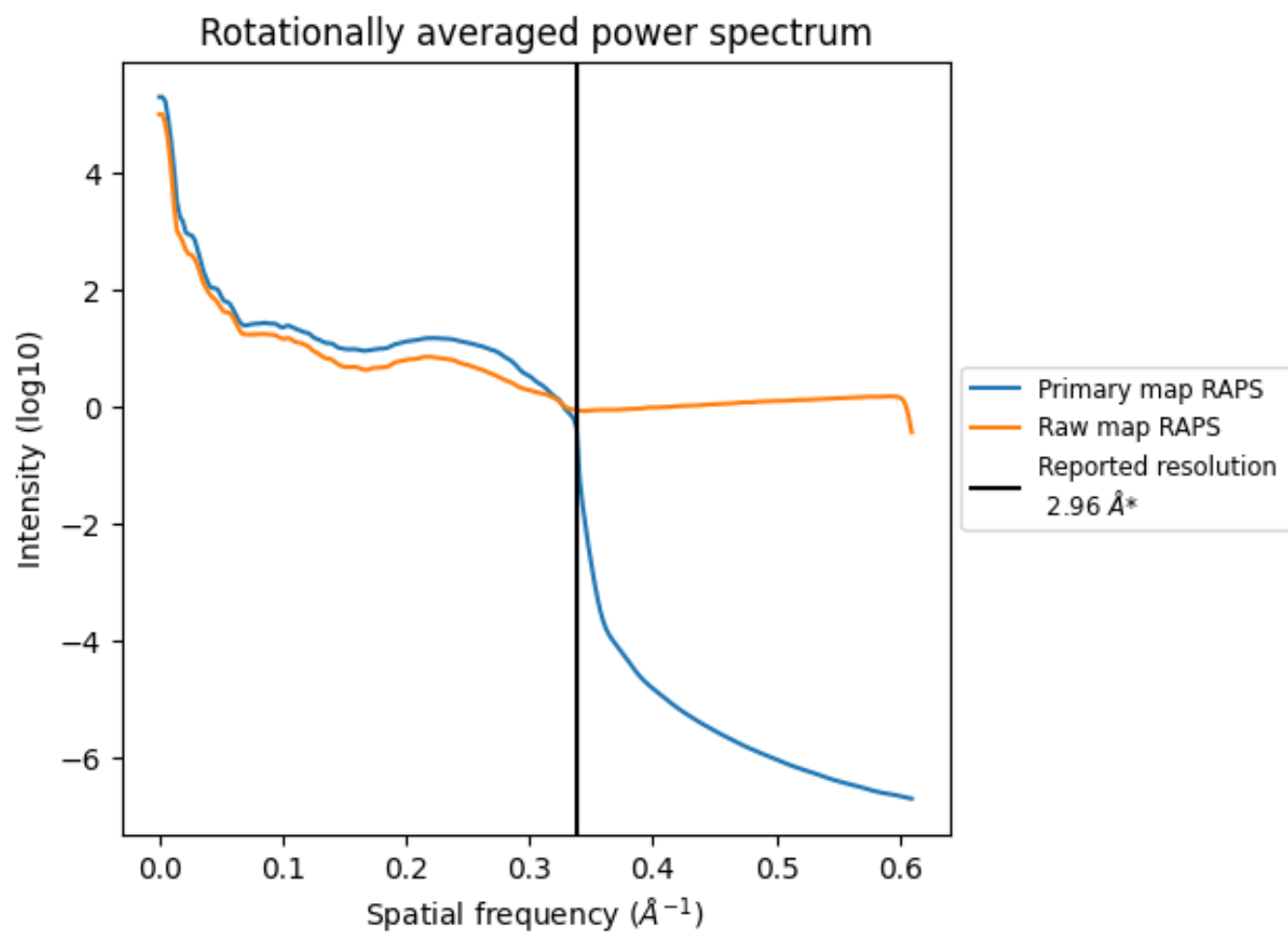
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3044 nm³; this corresponds to an approximate mass of 2750 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

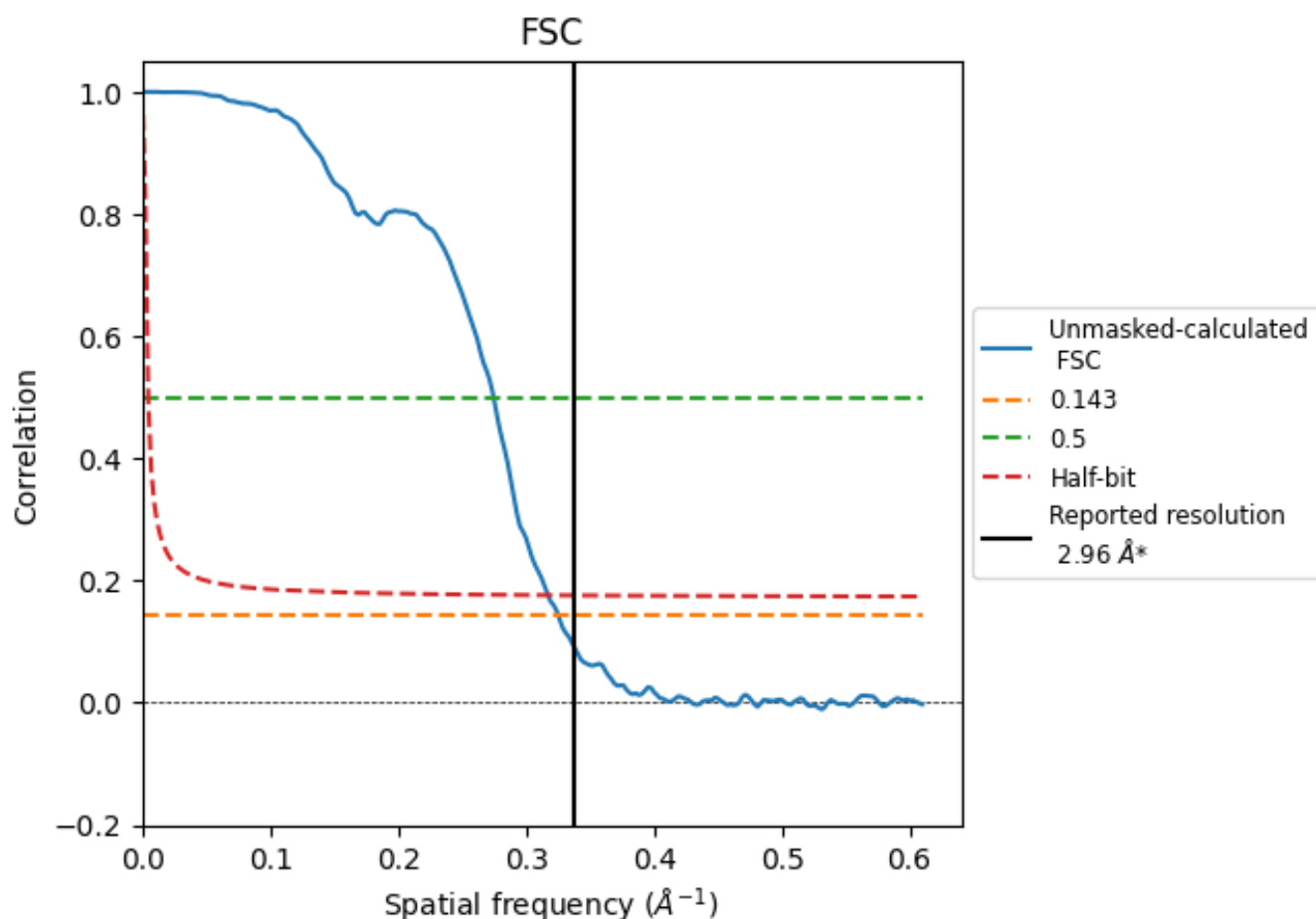


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

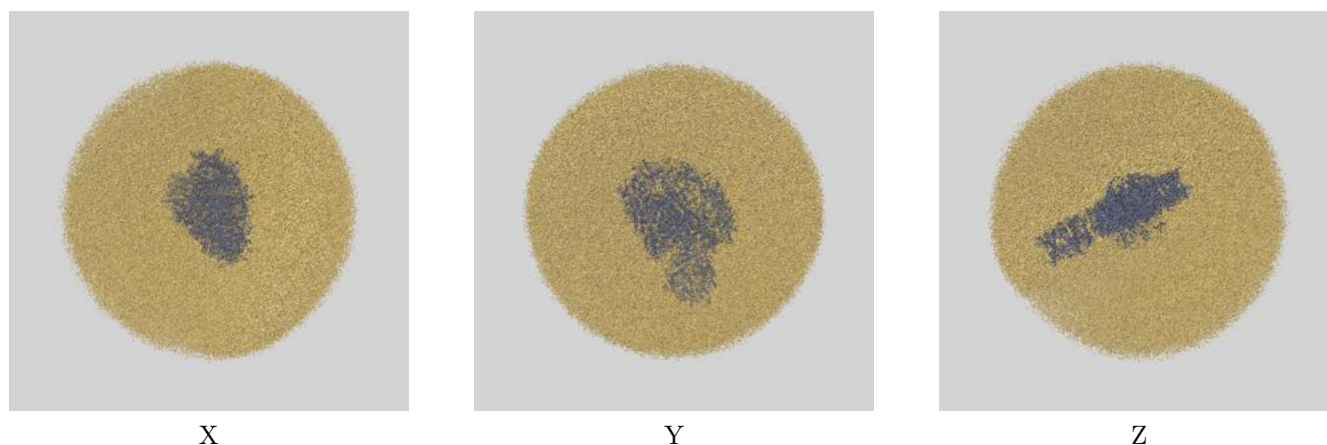
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.08	3.64	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

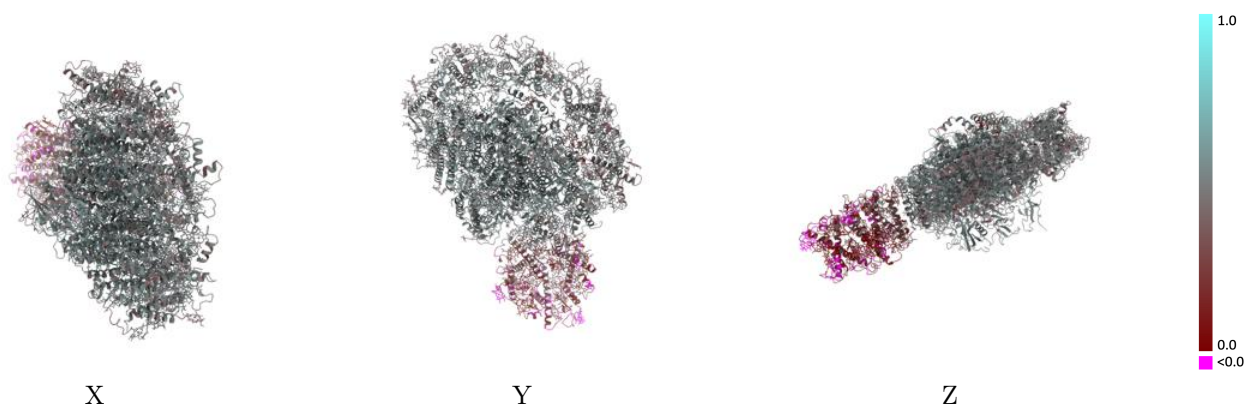
This section contains information regarding the fit between EMDB map EMD-66932 and PDB model 9XJ9. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



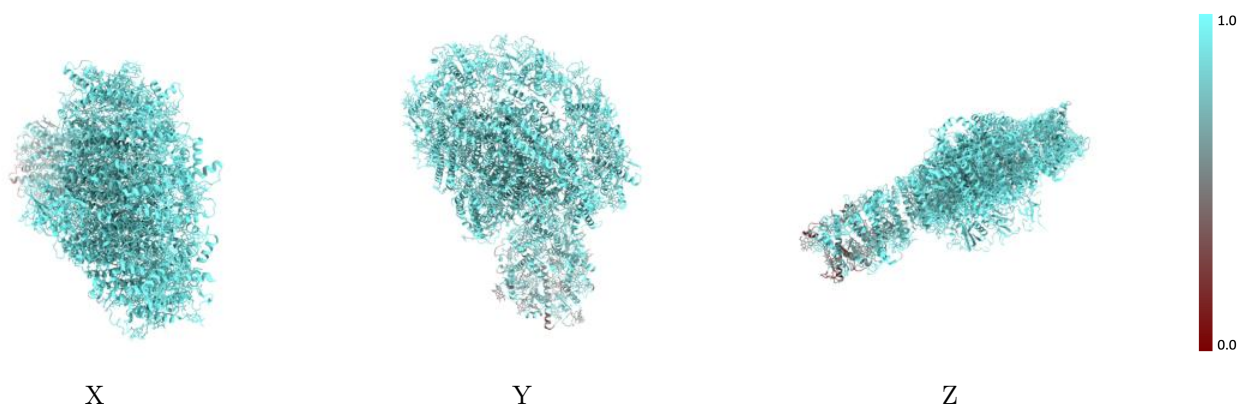
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



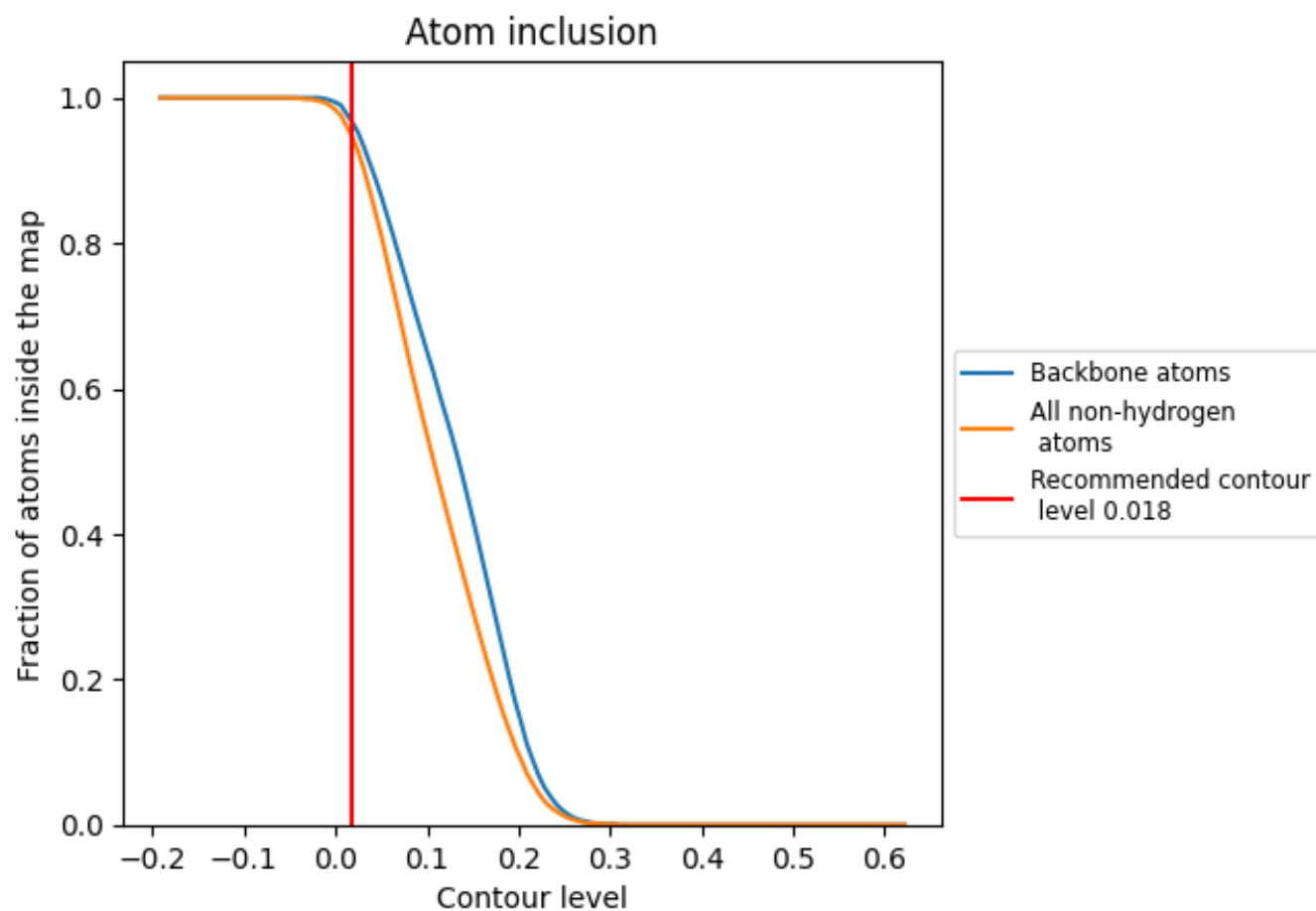
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.4640
1	 0.9600	 0.4820
2	 0.9570	 0.4710
3	 0.9520	 0.4550
4	 0.9530	 0.4780
A	 0.9790	 0.5290
B	 0.9770	 0.5240
C	 0.9970	 0.5080
D	 0.9950	 0.5100
E	 1.0000	 0.5160
F	 0.9810	 0.5000
G	 0.9570	 0.4830
H	 0.9690	 0.4990
I	 0.9930	 0.5160
J	 0.9830	 0.4930
K	 0.9610	 0.4840
L	 0.9590	 0.5110
N	 0.9790	 0.4340
O	 0.9420	 0.4780
X	 0.6450	 0.1150
Y	 0.8280	 0.2120
Z	 0.8480	 0.2110

