



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 01:43 AM JST

PDB ID : 6L35 / pdb_00006l35
EMDB ID : EMD-0821
Title : PSI-LHCI Supercomplex from *Physcometrella patens*
Authors : Zhao, L.; Yan, Q.J.; Qin, X.C.
Deposited on : 2019-10-09
Resolution : 3.23 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:

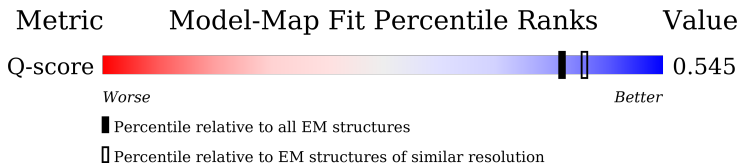
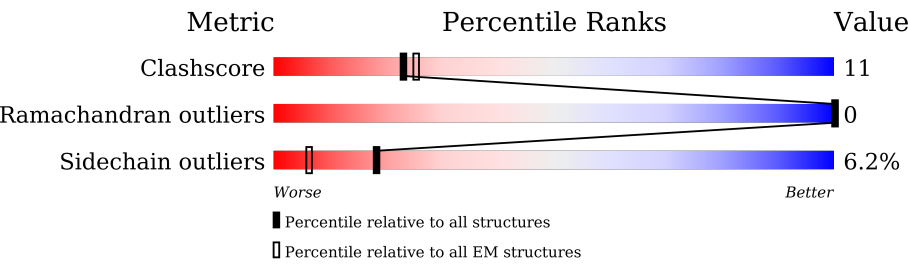
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 3.23 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	14612 (2.73 - 3.73)

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

Mol	Chain	Length	Quality of chain
1	A	742	78% 21%
2	B	733	76% 23%
3	C	80	6% 61% 32% 6%
4	D	141	6% 82% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	62	
6	F	159	
7	G	98	
8	H	90	
9	I	34	
10	J	41	
11	K	79	
12	L	159	
13	M	29	
14	2	210	
15	6	192	
16	3	213	
17	5	205	

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	SF4	C	101	-	-	X	-
22	SF4	C	102	-	-	X	-
27	XAT	2	620	-	-	X	-
27	XAT	5	620	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34822 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5837	3827	993	998	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			595	365	103	116	11		

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1226	793	209	221	3		

- Molecule 7 is a protein called Predicted protein PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			693	445	117	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			550	346	96	105	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1189	781	192	214	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			214	141	34	39		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	206	Total	C	N	O	S	0	0
			1595	1039	267	285	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

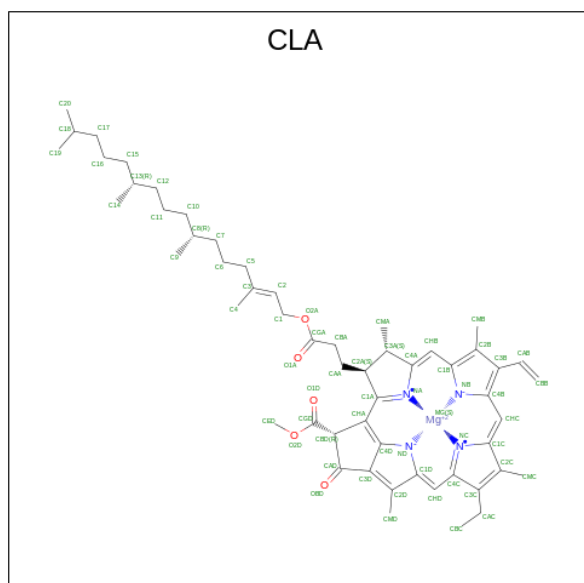
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	202	Total	C	N	O	S	0	0
			1566	1020	258	282	6		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 43	C 33	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	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
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	G	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 42	C 34	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

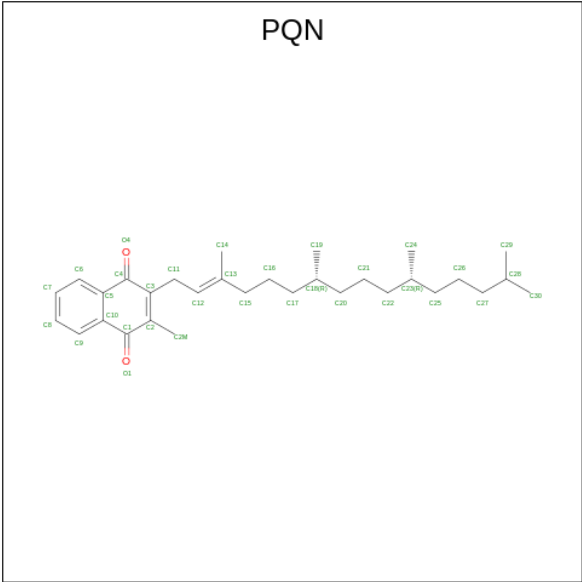
Mol	Chain	Residues	Atoms					AltConf
18	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	6	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	6	1	Total 43	C 33	Mg 1	N 4	O 5	0
18	6	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	6	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	6	1	Total 43	C 33	Mg 1	N 4	O 5	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

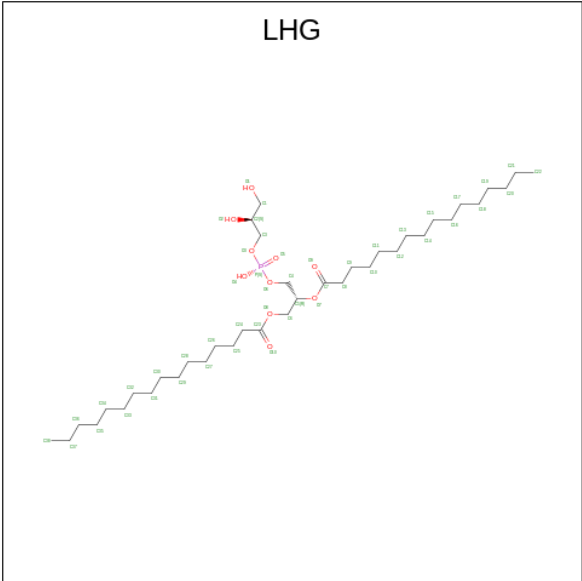
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



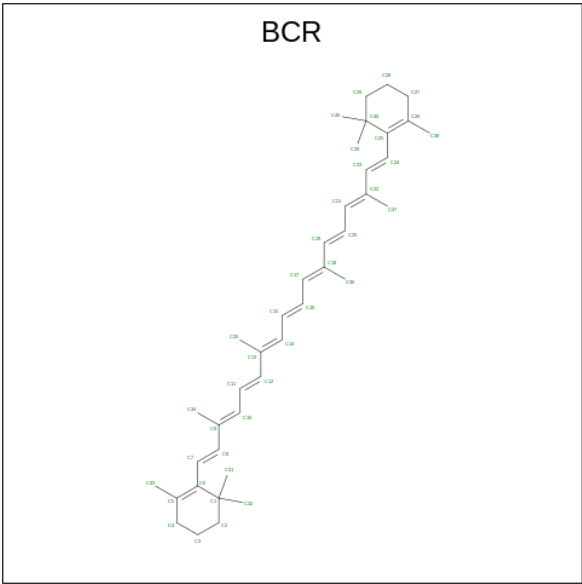
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			23	12	10	1	
20	2	1	Total	C	O	P	0
			35	24	10	1	
20	6	1	Total	C	O	P	0
			28	17	10	1	
20	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



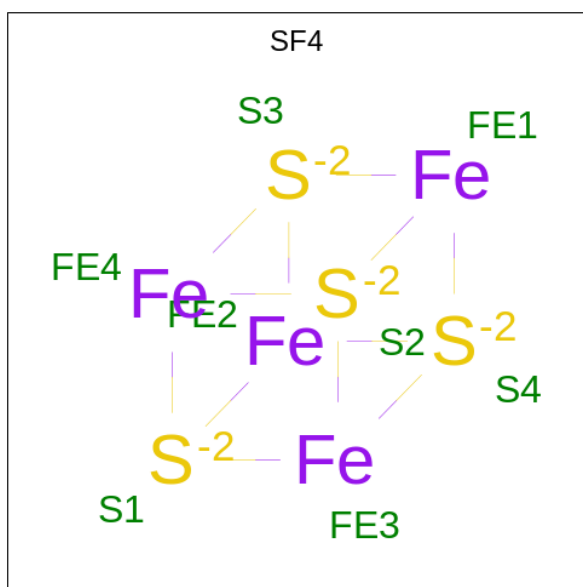
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

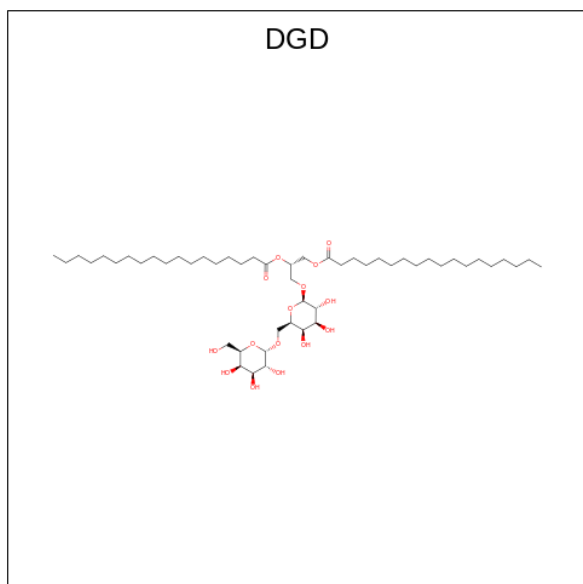
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	5	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



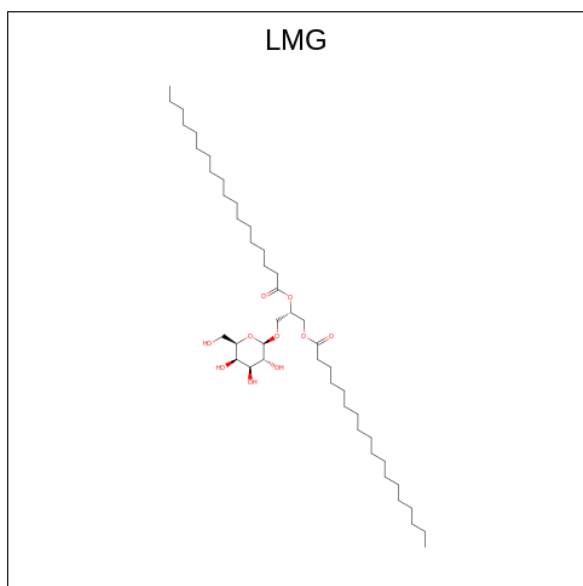
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



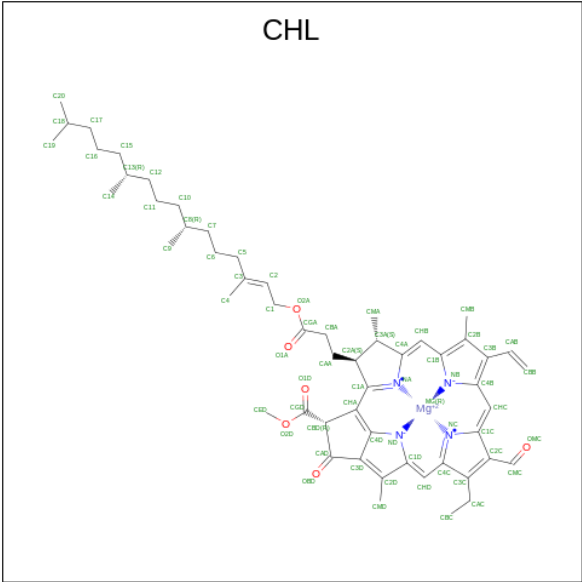
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			66	51	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



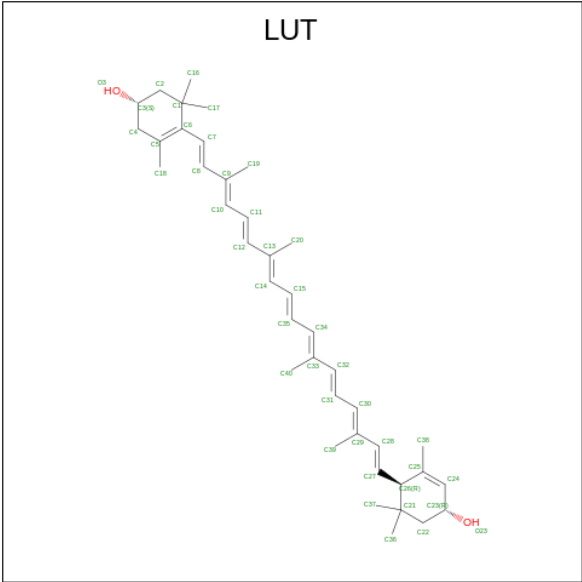
Mol	Chain	Residues	Atoms			AltConf
24	J	1	Total	C	O	0
			30	20	10	
24	2	1	Total	C	O	0
			13	7	6	
24	2	1	Total	C	O	0
			13	7	6	

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



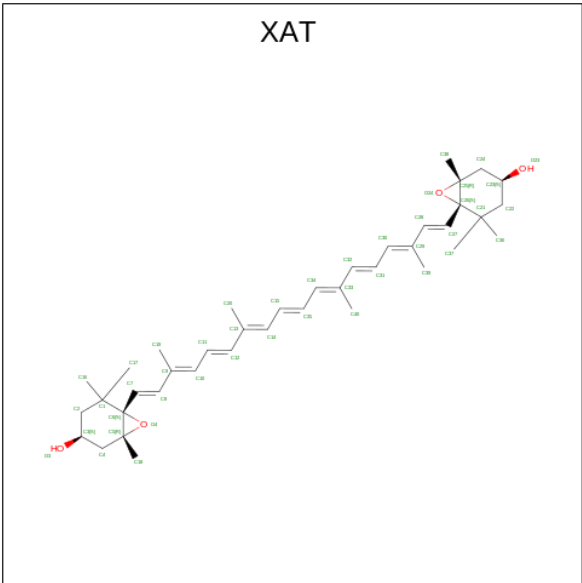
Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
25	5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
25	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
26	2	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).

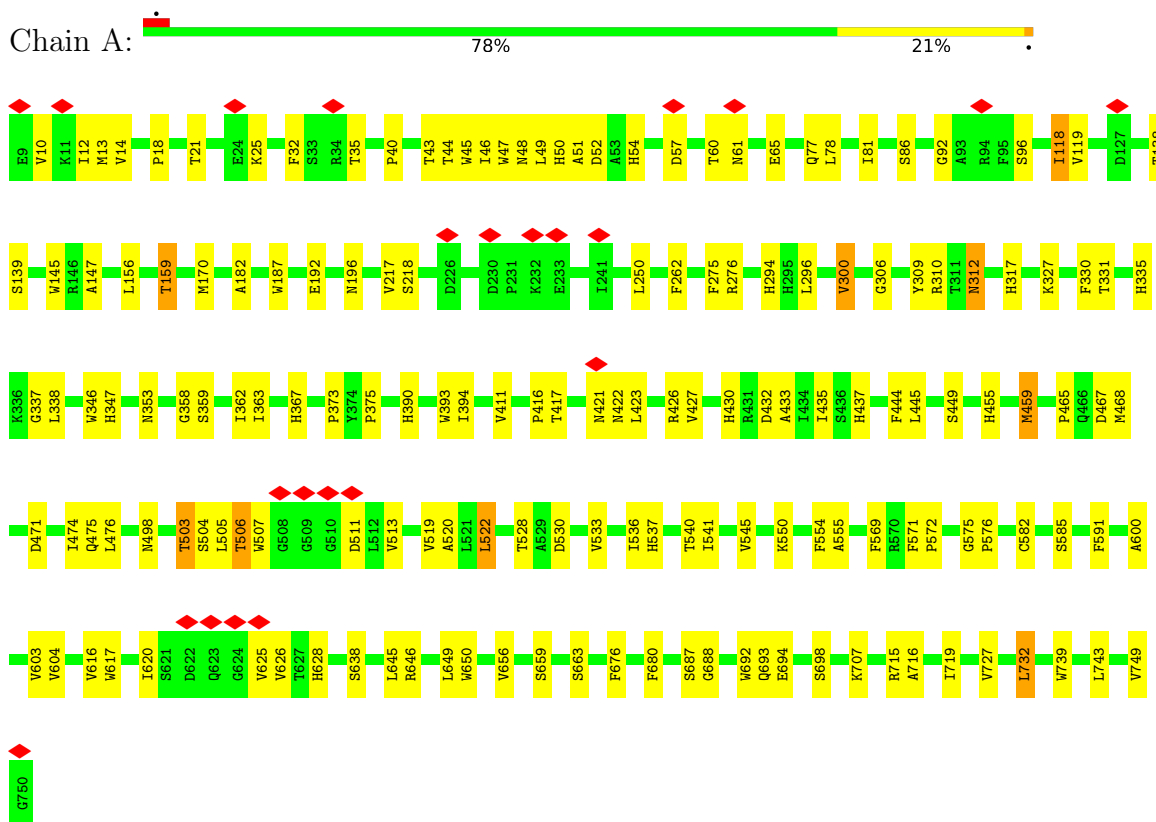


Mol	Chain	Residues	Atoms			AltConf
27	2	1	Total 44	C 40	O 4	0
27	6	1	Total 44	C 40	O 4	0
27	3	1	Total 44	C 40	O 4	0
27	5	1	Total 44	C 40	O 4	0

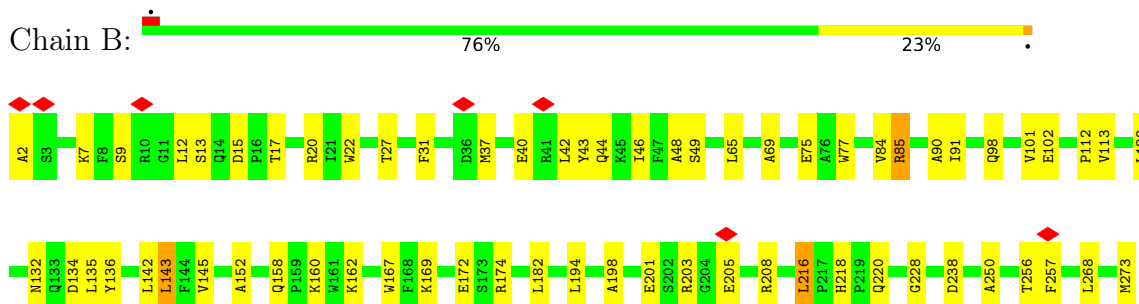
3 Residue-property plots

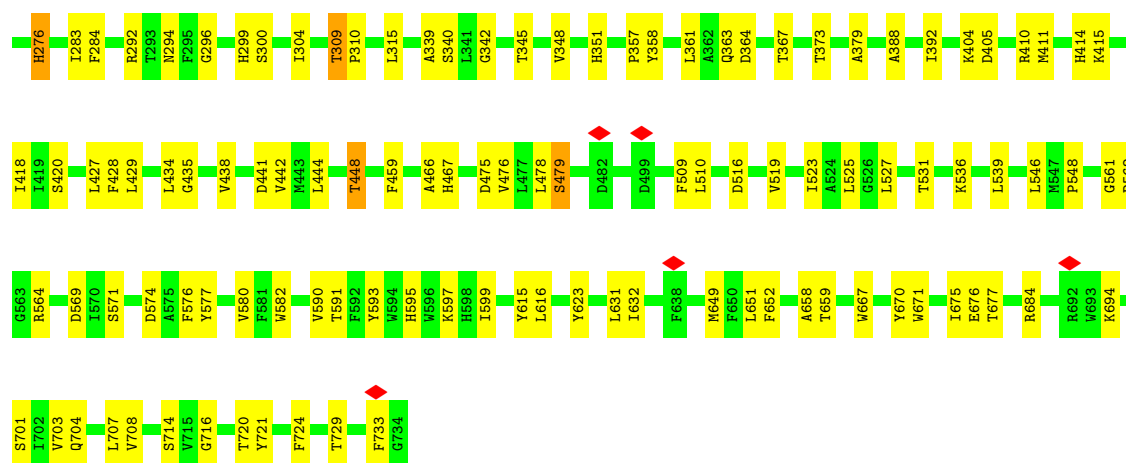
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

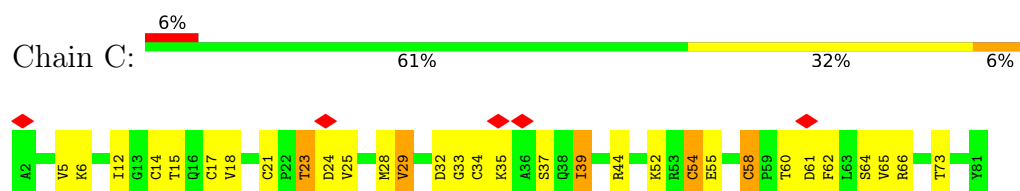


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

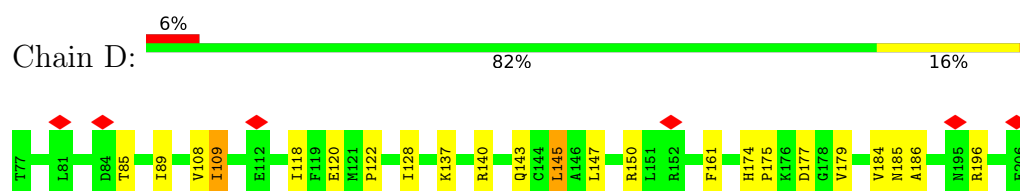




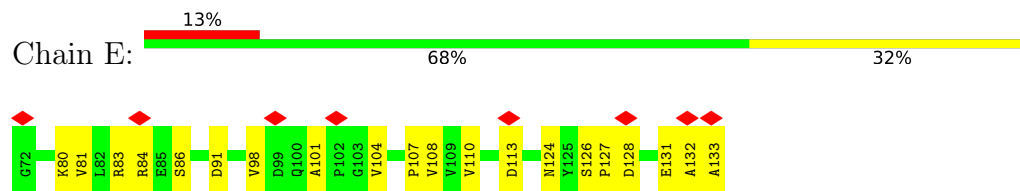
- Molecule 3: Photosystem I iron-sulfur center



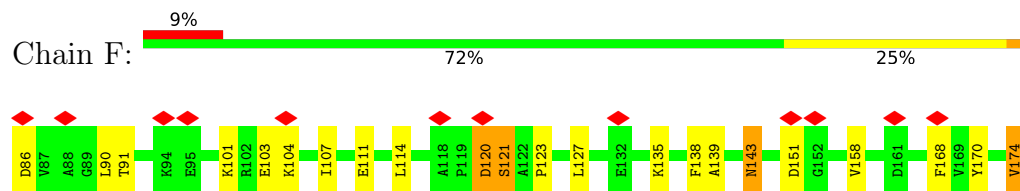
- Molecule 4: Predicted protein Psad



- Molecule 5: Psae

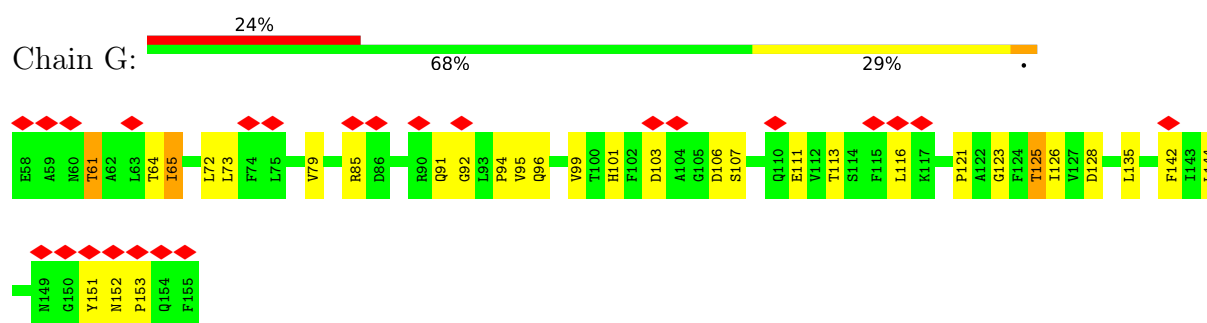


- Molecule 6: PSI-F

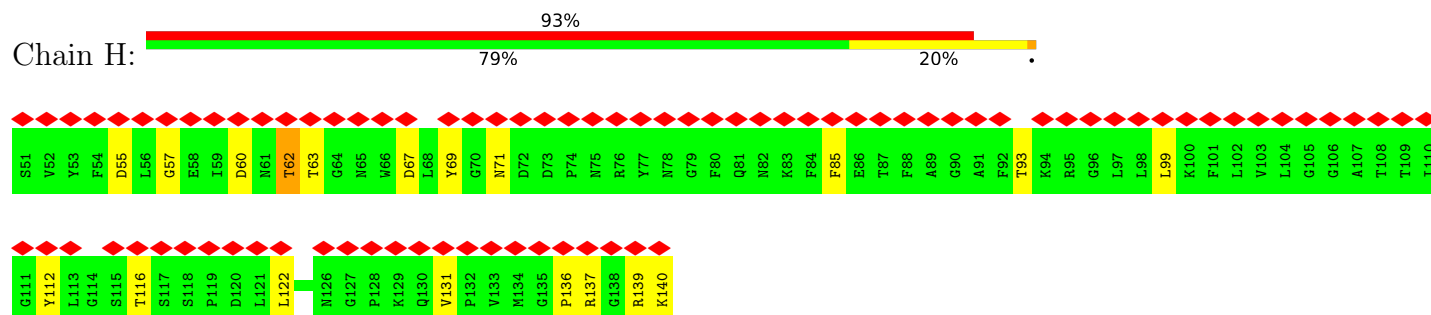


- Molecule 7: Predicted protein Psag

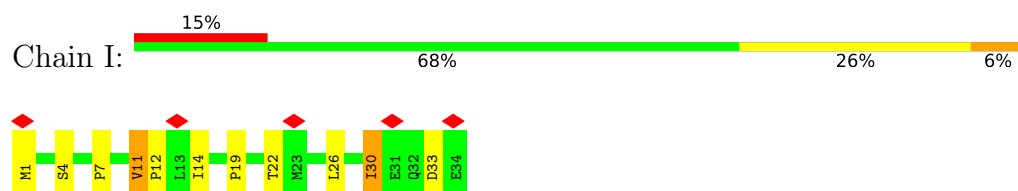




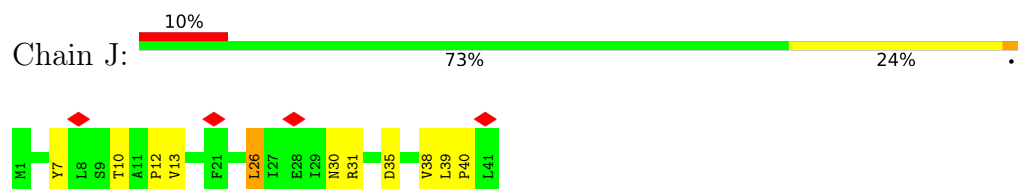
- Molecule 8: PsaH photosystem I reaction center subunit



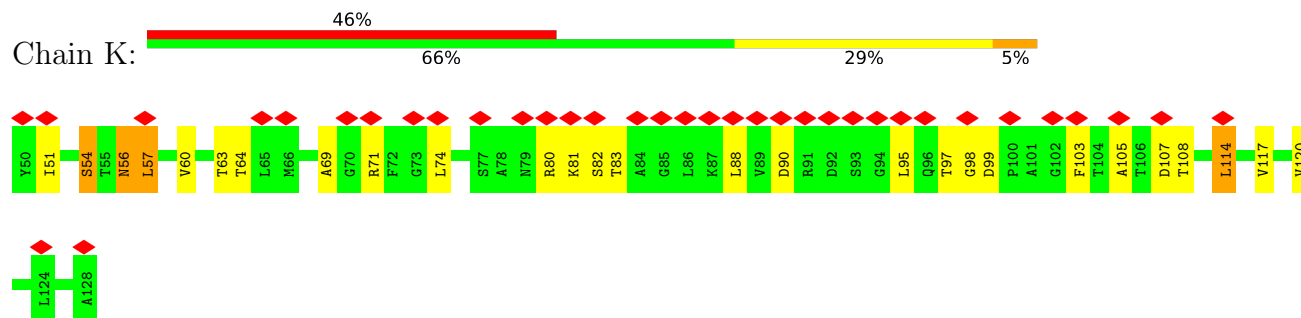
- Molecule 9: Photosystem I reaction center subunit VIII



- Molecule 10: Photosystem I reaction center subunit IX

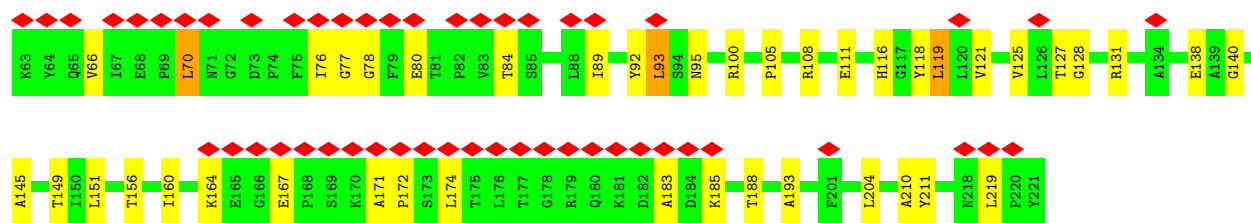


- Molecule 11: PsaK

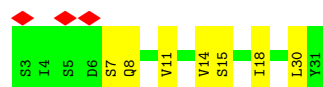
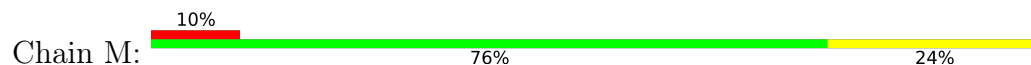


- Molecule 12: PSI subunit V

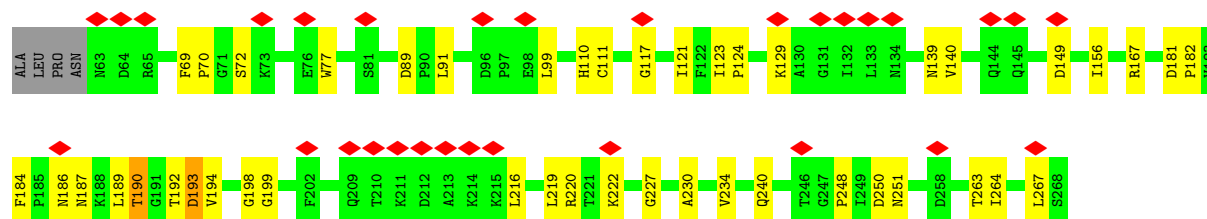
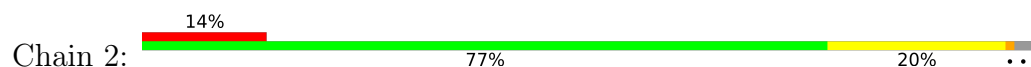




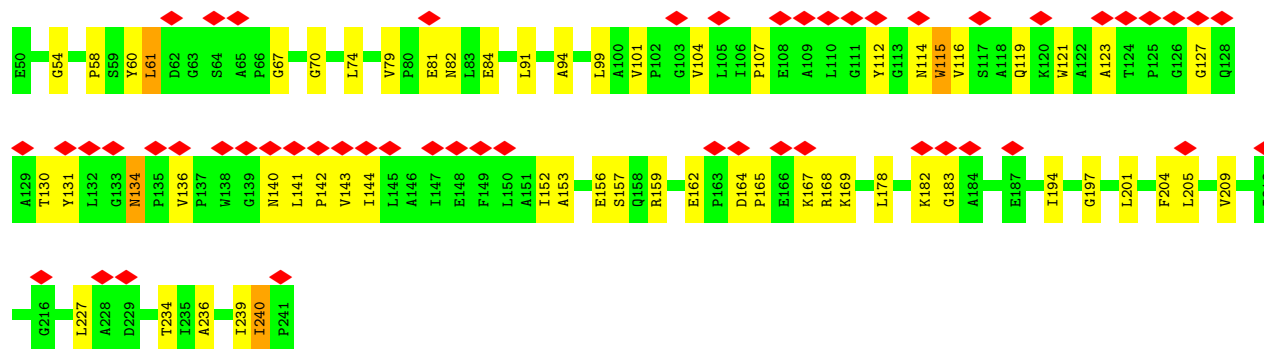
• Molecule 13: Photosystem I reaction center subunit XII



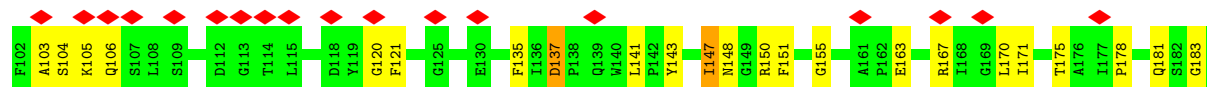
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

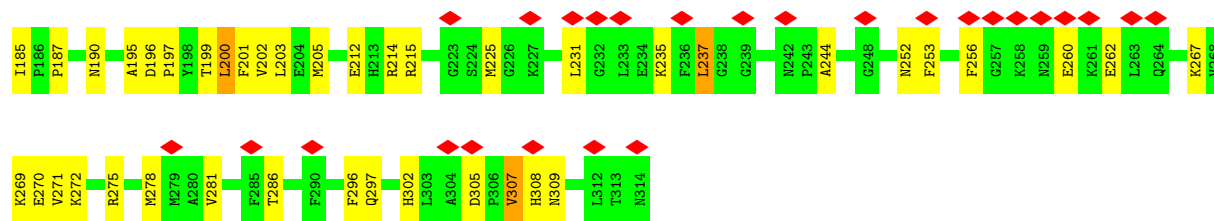


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

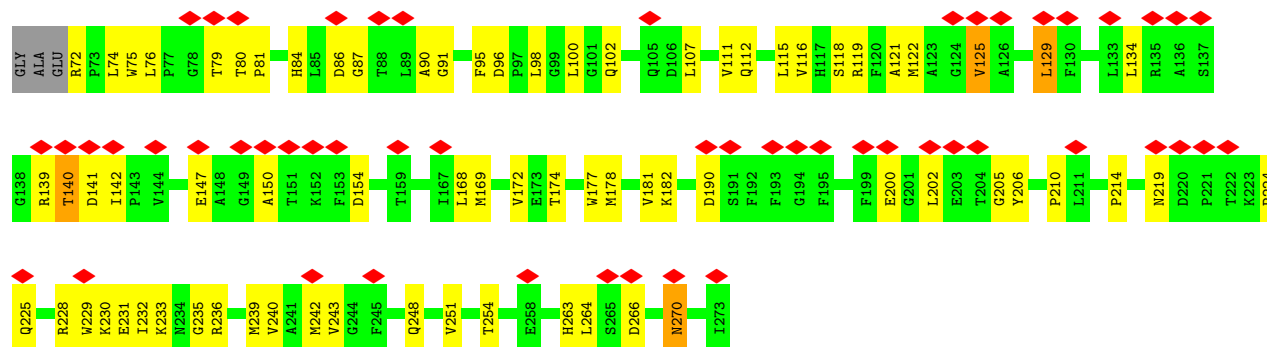


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic





- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	407.424, 407.424, 407.424	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/6032	0.30	0/8227
2	B	0.14	0/6063	0.30	0/8274
3	C	0.18	0/605	0.41	0/821
4	D	0.13	0/1132	0.36	0/1532
5	E	0.12	0/498	0.31	0/677
6	F	0.14	0/1251	0.41	2/1692 (0.1%)
7	G	0.13	0/767	0.36	0/1046
8	H	0.09	0/710	0.26	0/961
9	I	0.15	0/273	0.45	0/373
10	J	0.12	0/334	0.26	0/457
11	K	0.14	0/556	0.37	0/752
12	L	0.12	0/1222	0.31	0/1671
13	M	0.11	0/215	0.22	0/290
14	2	0.13	0/1646	0.30	0/2252
15	6	0.13	0/1522	0.32	0/2081
16	3	0.13	0/1695	0.35	0/2302
17	5	0.14	0/1614	0.37	0/2201
All	All	0.14	0/26135	0.32	2/35609 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	207	ASP	CA-C-N	6.26	124.19	120.24
6	F	207	ASP	C-N-CA	6.26	124.19	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	111	0
2	B	5849	0	5623	123	0
3	C	595	0	576	26	0
4	D	1104	0	1112	15	0
5	E	487	0	480	11	0
6	F	1226	0	1269	28	0
7	G	749	0	729	19	0
8	H	693	0	672	16	0
9	I	266	0	274	7	0
10	J	325	0	341	8	0
11	K	550	0	566	15	0
12	L	1189	0	1200	28	0
13	M	214	0	236	5	0
14	2	1595	0	1561	36	0
15	6	1473	0	1446	44	0
16	3	1644	0	1598	58	0
17	5	1566	0	1531	64	0
18	2	410	0	310	10	0
18	3	577	0	422	11	0
18	5	445	0	318	17	0
18	6	525	0	355	1	0
18	A	2421	0	2229	76	0
18	B	2093	0	1861	58	0
18	F	176	0	128	4	0
18	G	139	0	102	4	0
18	J	42	0	31	0	0
18	K	180	0	126	3	0
18	L	132	0	97	4	0
19	A	33	0	46	1	0
19	B	33	0	46	6	0
20	2	35	0	40	3	0
20	5	37	0	44	5	0
20	6	28	0	26	1	0
20	A	76	0	98	3	0
20	B	23	0	16	1	0
21	2	40	0	56	4	0
21	3	80	0	112	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	5	40	0	56	2	0
21	A	240	0	336	14	0
21	B	280	0	392	19	0
21	F	40	0	56	4	0
21	G	40	0	56	3	0
21	I	40	0	56	2	0
21	J	80	0	110	6	0
21	K	80	0	112	3	0
21	L	80	0	112	2	0
22	A	8	0	0	0	0
22	C	16	0	0	11	0
23	B	66	0	96	4	0
24	2	26	0	22	0	0
24	J	30	0	30	1	0
25	2	221	0	143	16	0
25	3	40	0	23	1	0
25	5	178	0	116	16	0
25	6	86	0	52	8	0
26	2	42	0	56	3	0
26	3	42	0	55	1	0
26	5	42	0	56	3	0
26	6	42	0	56	3	0
27	2	44	0	56	25	0
27	3	44	0	56	15	0
27	5	44	0	56	30	0
27	6	44	0	56	13	0
All	All	34822	0	33617	760	0

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

The worst 5 of 760 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:121:ILE:HD11	27:2:620:XAT:C17	1.25	1.61
3:C:21:CYS:SG	22:C:101:SF4:FE2	1.20	1.34
3:C:14:CYS:SG	22:C:102:SF4:S4	2.29	1.29
14:2:121:ILE:CD1	27:2:620:XAT:H173	1.68	1.22
3:C:21:CYS:SG	22:C:101:SF4:S1	2.38	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	700 (95%)	40 (5%)	0	100	100
2	B	731/733 (100%)	696 (95%)	35 (5%)	0	100	100
3	C	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
6	F	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
7	G	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
8	H	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
12	L	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	2	204/210 (97%)	192 (94%)	12 (6%)	0	100	100
15	6	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
16	3	211/213 (99%)	195 (92%)	16 (8%)	0	100	100
17	5	200/205 (98%)	173 (86%)	27 (14%)	0	100	100
All	All	3226/3267 (99%)	3013 (93%)	213 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	575 (95%)	28 (5%)	24	55
2	B	595/595 (100%)	569 (96%)	26 (4%)	25	55
3	C	67/67 (100%)	57 (85%)	10 (15%)	3	14
4	D	115/115 (100%)	109 (95%)	6 (5%)	21	51
5	E	52/52 (100%)	48 (92%)	4 (8%)	12	39
6	F	128/129 (99%)	118 (92%)	10 (8%)	11	38
7	G	78/78 (100%)	69 (88%)	9 (12%)	5	23
8	H	72/73 (99%)	67 (93%)	5 (7%)	14	43
9	I	30/30 (100%)	27 (90%)	3 (10%)	7	28
10	J	35/35 (100%)	31 (89%)	4 (11%)	5	23
11	K	56/57 (98%)	47 (84%)	9 (16%)	2	11
12	L	121/122 (99%)	112 (93%)	9 (7%)	13	40
13	M	24/24 (100%)	24 (100%)	0	100	100
14	2	164/167 (98%)	154 (94%)	10 (6%)	17	47
15	6	148/148 (100%)	141 (95%)	7 (5%)	23	54
16	3	166/166 (100%)	156 (94%)	10 (6%)	17	47
17	5	162/164 (99%)	151 (93%)	11 (7%)	14	43
All	All	2616/2625 (100%)	2455 (94%)	161 (6%)	18	46

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	70	LEU
16	3	175	THR
12	L	127	THR
14	2	194	VAL
17	5	125	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	90	ASN
8	H	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	3	148	ASN
5	E	124	ASN
7	G	137	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

205 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	CLA	A	823	1	48,52,73	1.50	8 (16%)	58,88,113	1.50	6 (10%)
19	PQN	A	844	-	34,34,34	0.39	0	42,45,45	0.47	0
18	CLA	5	612	-	48,52,73	1.51	9 (18%)	58,88,113	1.46	6 (10%)
18	CLA	3	603	-	59,63,73	1.36	9 (15%)	71,101,113	1.32	5 (7%)
25	CHL	5	607	-	47,51,74	2.41	18 (38%)	52,86,114	3.03	23 (44%)
25	CHL	5	608	-	55,59,74	2.15	18 (32%)	62,96,114	2.91	23 (37%)
18	CLA	A	836	1	54,58,73	1.41	9 (16%)	65,95,113	1.41	6 (9%)
18	CLA	A	811	1	49,53,73	1.48	9 (18%)	59,89,113	1.46	7 (11%)
18	CLA	3	611	-	43,48,73	1.57	8 (18%)	51,83,113	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	5 (8%)
18	CLA	A	801	-	69,73,73	1.25	9 (13%)	83,113,113	1.24	5 (6%)
18	CLA	B	836	-	64,68,73	1.30	9 (14%)	77,107,113	1.32	7 (9%)
18	CLA	B	811	2	58,62,73	1.43	10 (17%)	73,100,113	1.39	7 (9%)
20	LHG	B	851	18	22,22,48	0.83	0	25,28,54	1.20	1 (4%)
25	CHL	6	607	15	44,49,74	2.49	19 (43%)	48,84,114	3.04	22 (45%)
18	CLA	A	837	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	8 (13%)
18	CLA	B	828	-	69,73,73	1.25	9 (13%)	83,113,113	1.22	6 (7%)
18	CLA	B	834	-	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
18	CLA	L	302	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
18	CLA	A	814	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	9 (10%)
18	CLA	A	813	-	58,62,73	1.36	8 (13%)	69,99,113	1.37	5 (7%)
18	CLA	A	803	-	69,73,73	1.25	8 (11%)	83,113,113	1.21	5 (6%)
18	CLA	B	806	2	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
18	CLA	A	827	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	8 (9%)
22	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	B	819	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	7 (11%)
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	B	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
18	CLA	3	610	-	45,49,73	1.51	9 (20%)	54,84,113	1.50	6 (11%)
18	CLA	J	101	-	46,50,73	1.51	8 (17%)	55,85,113	1.45	5 (9%)
18	CLA	2	614	-	46,50,73	1.51	9 (19%)	55,85,113	1.45	5 (9%)
18	CLA	B	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
18	CLA	A	805	1	59,63,73	1.33	9 (15%)	71,101,113	1.41	8 (11%)
18	CLA	B	820	2	47,51,73	1.47	8 (17%)	56,86,113	1.48	5 (8%)
25	CHL	2	607	-	47,51,74	2.34	18 (38%)	52,86,114	3.06	23 (44%)
18	CLA	K	201	11	50,54,73	1.51	5 (10%)	60,90,113	1.45	5 (8%)
18	CLA	A	804	1	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
18	CLA	2	613	14	49,53,73	1.49	8 (16%)	59,89,113	1.43	6 (10%)
27	XAT	2	620	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	22 (40%)
18	CLA	2	602	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
18	CLA	A	821	1	48,52,73	1.51	9 (18%)	58,88,113	1.47	6 (10%)
18	CLA	B	826	2	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
18	CLA	5	609	17	47,51,73	1.49	8 (17%)	55,86,113	1.44	7 (12%)
18	CLA	B	827	-	49,53,73	1.47	9 (18%)	59,89,113	1.41	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	611	20	45,50,73	1.53	8 (17%)	56,85,113	1.46	5 (8%)
18	CLA	6	603	-	59,63,73	1.35	8 (13%)	71,101,113	1.38	7 (9%)
18	CLA	B	823	2	49,53,73	1.48	9 (18%)	59,89,113	1.45	4 (6%)
25	CHL	5	606	-	45,49,74	2.29	17 (37%)	54,84,114	3.22	23 (42%)
24	LMG	J	104	-	30,30,55	0.94	0	38,38,63	1.27	5 (13%)
18	CLA	6	608	-	47,52,73	1.52	9 (19%)	56,88,113	1.44	5 (8%)
18	CLA	6	610	15	46,51,73	1.53	9 (19%)	55,87,113	1.43	5 (9%)
18	CLA	B	832	2	49,53,73	1.47	8 (16%)	59,89,113	1.48	9 (15%)
18	CLA	2	610	14	49,53,73	1.43	8 (16%)	59,89,113	1.45	6 (10%)
20	LHG	6	620	15,18	27,27,48	0.80	1 (3%)	30,33,54	1.25	2 (6%)
18	CLA	A	817	-	43,48,73	1.54	8 (18%)	51,83,113	1.50	6 (11%)
18	CLA	3	615	-	41,44,73	1.60	9 (21%)	49,77,113	1.43	4 (8%)
18	CLA	B	816	2	57,62,73	1.38	9 (15%)	68,100,113	1.33	5 (7%)
18	CLA	G	204	7	47,52,73	1.52	9 (19%)	56,88,113	1.43	6 (10%)
18	CLA	A	832	1	45,49,73	1.50	9 (20%)	54,84,113	1.55	8 (14%)
18	CLA	B	841	20	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
18	CLA	F	303	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)
21	BCR	A	850	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	6 (10%)
21	BCR	B	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
20	LHG	5	622	-	36,36,48	0.72	1 (2%)	39,42,54	1.25	4 (10%)
21	BCR	5	621	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
18	CLA	B	822	-	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
27	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.74	20 (37%)
18	CLA	A	807	1	47,52,73	1.51	9 (19%)	56,88,113	1.43	5 (8%)
21	BCR	L	301	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	A	834	1	69,73,73	1.26	9 (13%)	83,113,113	1.26	5 (6%)
18	CLA	A	845	20	56,60,73	1.39	8 (14%)	67,97,113	1.41	6 (8%)
18	CLA	A	841	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
25	CHL	2	608	-	44,49,74	2.40	19 (43%)	48,84,114	3.09	21 (43%)
21	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.26	9 (16%)
18	CLA	B	807	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
18	CLA	3	604	-	45,50,73	1.62	10 (22%)	57,86,113	1.51	7 (12%)
21	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
24	LMG	2	617	-	13,13,55	1.01	0	18,18,63	1.55	4 (22%)
18	CLA	A	825	1	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	604	-	54,58,73	1.39	8 (14%)	65,95,113	1.47	7 (10%)
18	CLA	B	818	2	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
18	CLA	5	603	-	47,52,73	1.52	9 (19%)	56,88,113	1.43	5 (8%)
21	BCR	J	103	2	41,41,41	1.15	3 (7%)	56,56,56	1.30	7 (12%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.45	0
21	BCR	J	102	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	6 (10%)
27	XAT	6	619	-	39,47,47	0.98	2 (5%)	54,74,74	3.10	21 (38%)
18	CLA	3	613	-	57,62,73	1.39	8 (14%)	68,100,113	1.36	7 (10%)
18	CLA	L	303	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
27	XAT	5	620	-	39,47,47	1.03	3 (7%)	54,74,74	2.76	21 (38%)
18	CLA	A	818	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
18	CLA	B	817	2	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
18	CLA	B	837	2	50,54,73	1.45	10 (20%)	60,90,113	1.45	7 (11%)
18	CLA	L	304	-	46,50,73	1.50	8 (17%)	55,85,113	1.49	6 (10%)
21	BCR	B	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	6	602	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
18	CLA	A	809	1	49,53,73	1.47	9 (18%)	59,89,113	1.48	8 (13%)
18	CLA	B	835	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
18	CLA	6	609	-	44,48,73	1.60	10 (22%)	56,83,113	1.57	8 (14%)
21	BCR	K	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	6 (10%)
21	BCR	A	856	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)
22	SF4	A	853	1,2	0,12,12	-	-	-	-	-
18	CLA	A	842	1	47,52,73	1.50	9 (19%)	56,88,113	1.43	6 (10%)
21	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
18	CLA	A	829	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
18	CLA	A	810	1	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
18	CLA	6	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
18	CLA	3	609	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	4 (6%)
18	CLA	2	612	-	45,49,73	1.54	9 (20%)	54,84,113	1.49	6 (11%)
24	LMG	2	618	-	13,13,55	1.07	0	18,18,63	1.54	4 (22%)
25	CHL	5	615	17	47,51,74	2.28	17 (36%)	52,86,114	3.13	23 (44%)
18	CLA	6	606	-	43,48,73	1.54	9 (20%)	52,82,113	1.59	7 (13%)
18	CLA	B	812	2	49,53,73	1.48	8 (16%)	59,89,113	1.47	5 (8%)
18	CLA	6	613	15	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
26	LUT	5	619	-	42,43,43	7.28	26 (61%)	51,60,60	3.85	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	820	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)
18	CLA	5	614	-	47,51,73	1.50	8 (17%)	56,86,113	1.44	5 (8%)
21	BCR	3	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	6 (10%)
18	CLA	3	607	16	43,48,73	1.61	10 (23%)	54,83,113	1.52	7 (12%)
21	BCR	L	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	9 (16%)
21	BCR	K	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
21	BCR	G	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	A	839	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
21	BCR	3	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
21	BCR	I	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	4 (7%)
21	BCR	F	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
25	CHL	2	616	-	50,54,74	2.31	17 (34%)	56,90,114	3.02	21 (37%)
18	CLA	5	604	-	47,51,73	1.49	7 (14%)	55,86,113	1.47	6 (10%)
18	CLA	A	838	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	7 (10%)
18	CLA	A	828	1	50,54,73	1.45	10 (20%)	60,90,113	1.39	4 (6%)
18	CLA	B	821	2	50,54,73	1.46	8 (16%)	60,90,113	1.41	6 (10%)
18	CLA	B	830	2	49,53,73	1.49	9 (18%)	59,89,113	1.47	7 (11%)
21	BCR	2	621	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
18	CLA	5	601	17	49,53,73	1.49	8 (16%)	59,89,113	1.44	6 (10%)
21	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	4 (7%)
18	CLA	A	831	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
18	CLA	3	602	16	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
21	BCR	A	852	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	6 (10%)
18	CLA	A	854	-	69,73,73	1.24	8 (11%)	83,113,113	1.25	7 (8%)
18	CLA	B	809	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
18	CLA	B	808	-	54,58,73	1.39	10 (18%)	65,95,113	1.44	8 (12%)
18	CLA	B	833	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	9 (15%)
18	CLA	A	806	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
18	CLA	5	610	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	7 (9%)
18	CLA	A	824	1	55,59,73	1.40	9 (16%)	66,96,113	1.41	4 (6%)
23	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	1.44	11 (13%)
25	CHL	2	601	14	49,53,74	2.38	19 (38%)	58,89,114	3.01	25 (43%)
18	CLA	3	606	-	44,49,73	1.55	9 (20%)	52,84,113	1.45	5 (9%)
18	CLA	6	616	15	47,51,73	1.60	8 (17%)	60,87,113	1.55	6 (10%)
18	CLA	A	802	-	49,53,73	1.46	9 (18%)	59,89,113	1.47	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	614	-	43,48,73	1.56	9 (20%)	51,83,113	1.49	5 (9%)
18	CLA	5	613	17	49,53,73	1.49	9 (18%)	59,89,113	1.49	6 (10%)
18	CLA	G	201	-	49,53,73	1.49	6 (12%)	59,89,113	1.42	5 (8%)
18	CLA	6	611	20	41,46,73	1.67	10 (24%)	52,81,113	1.57	7 (13%)
18	CLA	B	802	-	57,61,73	1.37	10 (17%)	68,98,113	1.30	6 (8%)
18	CLA	K	203	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
18	CLA	F	305	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
18	CLA	A	843	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	8 (9%)
18	CLA	F	304	-	45,49,73	1.52	8 (17%)	54,84,113	1.53	5 (9%)
18	CLA	5	602	-	49,53,73	1.50	9 (18%)	59,89,113	1.39	6 (10%)
26	LUT	3	618	16	42,43,43	7.26	24 (57%)	51,60,60	3.85	22 (43%)
20	LHG	A	846	-	48,48,48	0.64	1 (2%)	51,54,54	1.27	6 (11%)
20	LHG	A	847	18	26,26,48	0.83	1 (3%)	29,32,54	1.35	3 (10%)
18	CLA	6	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.43	7 (11%)
18	CLA	B	813	2	69,73,73	1.24	9 (13%)	83,113,113	1.35	10 (12%)
18	CLA	A	826	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
18	CLA	K	204	-	48,52,73	1.56	9 (18%)	61,88,113	1.53	6 (9%)
18	CLA	6	614	-	41,46,73	1.66	8 (19%)	52,81,113	1.51	9 (17%)
18	CLA	3	612	-	47,51,73	1.51	6 (12%)	56,86,113	1.43	5 (8%)
25	CHL	2	606	14	50,54,74	2.25	16 (32%)	56,90,114	3.15	21 (37%)
18	CLA	A	835	1	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
18	CLA	F	301	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	5 (8%)
18	CLA	A	819	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
18	CLA	A	840	-	49,53,73	1.48	9 (18%)	59,89,113	1.41	5 (8%)
21	BCR	B	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
18	CLA	A	812	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
26	LUT	6	617	-	42,43,43	7.20	25 (59%)	51,60,60	3.87	19 (37%)
18	CLA	2	603	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
18	CLA	B	839	-	44,49,73	1.53	9 (20%)	52,84,113	1.47	5 (9%)
18	CLA	B	815	2	64,68,73	1.30	10 (15%)	77,107,113	1.32	5 (6%)
18	CLA	A	816	-	46,50,73	1.49	8 (17%)	55,85,113	1.49	7 (12%)
18	CLA	B	824	-	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
18	CLA	B	829	2	49,53,73	1.50	9 (18%)	59,89,113	1.50	7 (11%)
18	CLA	B	814	2	47,52,73	1.51	9 (19%)	56,88,113	1.46	5 (8%)
18	CLA	A	815	1	49,53,73	1.48	9 (18%)	59,89,113	1.44	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	810	2	50,54,73	1.46	8 (16%)	60,90,113	1.41	4 (6%)
18	CLA	B	838	-	51,55,73	1.43	8 (15%)	61,91,113	1.42	6 (9%)
18	CLA	A	822	-	47,51,73	1.58	10 (21%)	60,87,113	1.53	7 (11%)
26	LUT	2	619	-	42,43,43	7.18	25 (59%)	51,60,60	4.12	21 (41%)
21	BCR	B	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	4 (7%)
25	CHL	3	608	-	43,48,74	2.38	18 (41%)	51,83,114	2.99	22 (43%)
18	CLA	A	833	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	7 (11%)
18	CLA	A	808	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	7 (11%)
18	CLA	A	830	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	4 (4%)
18	CLA	B	804	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	5 (8%)
18	CLA	3	617	-	43,48,73	1.55	8 (18%)	51,83,113	1.50	7 (13%)
18	CLA	B	840	2	69,73,73	1.24	9 (13%)	83,113,113	1.32	4 (4%)
18	CLA	G	203	7	54,58,73	1.42	9 (16%)	65,95,113	1.39	7 (10%)
20	LHG	2	622	14,18	34,34,48	0.72	0	37,40,54	1.27	4 (10%)
21	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
18	CLA	B	805	2	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
18	CLA	B	831	2	53,57,73	1.42	9 (16%)	62,93,113	1.40	4 (6%)
18	CLA	2	609	14	59,63,73	1.35	9 (15%)	71,101,113	1.34	6 (8%)
25	CHL	6	601	15	48,53,74	2.35	19 (39%)	53,89,114	3.00	20 (37%)
18	CLA	K	206	11	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
18	CLA	5	611	-	41,45,73	2.55	11 (26%)	47,76,113	1.33	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	823	1	-	5/13/89/115	-
19	PQN	A	844	-	-	8/23/43/43	0/2/2/2
18	CLA	5	612	-	-	7/13/89/115	-
18	CLA	3	603	-	-	8/27/103/115	-
25	CHL	5	607	-	-	4/14/90/117	-
25	CHL	5	608	-	-	8/23/99/117	-
18	CLA	A	836	1	-	0/21/97/115	-
18	CLA	A	811	1	-	2/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	611	-	-	4/8/84/115	-
21	BCR	B	845	-	-	19/29/63/63	0/2/2/2
18	CLA	A	801	-	-	8/39/115/115	-
18	CLA	B	836	-	-	7/33/109/115	-
18	CLA	B	811	2	-	9/25/101/115	-
20	LHG	B	851	18	-	10/26/26/53	-
25	CHL	6	607	15	-	2/10/86/117	-
18	CLA	A	837	1	-	4/15/91/115	-
18	CLA	B	828	-	-	12/39/115/115	-
18	CLA	B	834	-	-	6/15/91/115	-
18	CLA	L	302	-	-	2/15/91/115	-
18	CLA	A	814	-	-	16/39/115/115	-
18	CLA	A	813	-	-	3/26/102/115	-
18	CLA	A	803	-	-	7/39/115/115	-
18	CLA	B	806	2	-	19/39/115/115	-
18	CLA	A	827	-	-	12/39/115/115	-
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	B	819	-	-	3/15/91/115	-
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	B	803	-	-	10/39/115/115	-
18	CLA	3	610	-	-	3/10/86/115	-
18	CLA	J	101	-	-	7/12/88/115	-
18	CLA	2	614	-	-	4/12/88/115	-
18	CLA	B	825	-	-	11/39/115/115	-
18	CLA	A	805	1	-	10/27/103/115	-
18	CLA	B	820	2	-	1/13/89/115	-
25	CHL	2	607	-	-	3/14/90/117	-
18	CLA	K	201	11	-	9/17/93/115	-
18	CLA	A	804	1	-	9/39/115/115	-
18	CLA	2	613	14	-	8/15/91/115	-
27	XAT	2	620	-	-	3/31/93/93	0/4/4/4
18	CLA	2	602	-	-	6/15/91/115	-
18	CLA	A	821	1	-	8/13/89/115	-
18	CLA	B	826	2	-	12/39/115/115	-
18	CLA	5	609	17	-	6/11/87/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	827	-	-	5/15/91/115	-
18	CLA	2	611	20	-	0/9/85/115	-
18	CLA	6	603	-	-	14/27/103/115	-
18	CLA	B	823	2	-	5/15/91/115	-
25	CHL	5	606	-	-	2/10/86/117	-
24	LMG	J	104	-	-	12/25/45/70	0/1/1/1
18	CLA	6	608	-	-	5/13/89/115	-
18	CLA	6	610	15	-	1/11/87/115	-
18	CLA	B	832	2	-	6/15/91/115	-
18	CLA	2	610	14	-	4/15/91/115	-
20	LHG	6	620	15,18	-	17/32/32/53	-
18	CLA	A	817	-	-	0/8/84/115	-
18	CLA	3	615	-	-	2/2/74/115	-
18	CLA	B	816	2	-	5/25/101/115	-
18	CLA	G	204	7	-	6/13/89/115	-
18	CLA	A	832	1	-	6/10/86/115	-
18	CLA	B	841	20	-	16/39/115/115	-
18	CLA	F	303	-	-	6/15/91/115	-
21	BCR	A	850	-	-	3/29/63/63	0/2/2/2
21	BCR	B	844	-	-	6/29/63/63	0/2/2/2
20	LHG	5	622	-	-	19/41/41/53	-
21	BCR	5	621	-	-	9/29/63/63	0/2/2/2
18	CLA	B	822	-	-	8/27/103/115	-
27	XAT	3	619	-	-	0/31/93/93	0/4/4/4
18	CLA	A	807	1	-	4/13/89/115	-
21	BCR	L	301	-	-	10/29/63/63	0/2/2/2
18	CLA	A	834	1	-	14/39/115/115	-
18	CLA	A	845	20	-	12/24/100/115	-
18	CLA	A	841	-	-	15/39/115/115	-
25	CHL	2	608	-	-	3/10/86/117	-
21	BCR	A	851	-	-	9/29/63/63	0/2/2/2
18	CLA	B	807	2	-	12/39/115/115	-
18	CLA	3	604	-	-	0/9/85/115	-
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
24	LMG	2	617	-	-	4/4/24/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	825	1	-	11/27/103/115	-
18	CLA	2	604	-	-	7/21/97/115	-
18	CLA	B	818	2	-	4/15/91/115	-
18	CLA	5	603	-	-	6/13/89/115	-
21	BCR	J	103	2	-	23/29/63/63	0/2/2/2
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
21	BCR	J	102	-	-	9/29/63/63	0/2/2/2
27	XAT	6	619	-	-	1/31/93/93	0/4/4/4
18	CLA	3	613	-	-	9/25/101/115	-
18	CLA	L	303	-	-	2/15/91/115	-
27	XAT	5	620	-	-	3/31/93/93	0/4/4/4
18	CLA	A	818	1	-	18/39/115/115	-
18	CLA	B	817	2	-	4/15/91/115	-
18	CLA	B	837	2	-	6/17/93/115	-
18	CLA	L	304	-	-	2/12/88/115	-
21	BCR	B	846	-	-	17/29/63/63	0/2/2/2
18	CLA	6	602	-	-	7/15/91/115	-
18	CLA	A	809	1	-	5/15/91/115	-
18	CLA	B	835	-	-	8/15/91/115	-
18	CLA	6	609	-	-	3/8/84/115	-
21	BCR	K	207	-	-	11/29/63/63	0/2/2/2
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
22	SF4	A	853	1,2	-	-	0/6/5/5
18	CLA	A	842	1	-	5/13/89/115	-
21	BCR	A	849	-	-	8/29/63/63	0/2/2/2
18	CLA	A	829	-	-	20/39/115/115	-
18	CLA	A	810	1	-	6/15/91/115	-
18	CLA	6	612	-	-	4/15/91/115	-
18	CLA	3	609	-	-	1/15/91/115	-
18	CLA	2	612	-	-	2/10/86/115	-
24	LMG	2	618	-	-	2/4/24/70	0/1/1/1
25	CHL	5	615	17	-	3/14/90/117	-
18	CLA	6	606	-	-	5/10/82/115	-
18	CLA	B	812	2	-	3/15/91/115	-
18	CLA	6	613	15	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	5	619	-	-	8/29/67/67	0/2/2/2
18	CLA	A	820	-	-	4/15/91/115	-
18	CLA	5	614	-	-	7/13/89/115	-
21	BCR	3	620	-	-	9/29/63/63	0/2/2/2
18	CLA	3	607	16	-	1/8/84/115	-
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
21	BCR	K	202	-	-	8/29/63/63	0/2/2/2
21	BCR	G	205	-	-	5/29/63/63	0/2/2/2
18	CLA	A	839	-	-	15/39/115/115	-
21	BCR	3	622	-	-	10/29/63/63	0/2/2/2
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
21	BCR	F	302	-	-	14/29/63/63	0/2/2/2
25	CHL	2	616	-	-	6/17/93/117	-
18	CLA	5	604	-	-	5/11/88/115	-
18	CLA	A	838	-	-	5/23/99/115	-
18	CLA	A	828	1	-	7/17/93/115	-
18	CLA	B	821	2	-	9/17/93/115	-
18	CLA	B	830	2	-	1/15/91/115	-
21	BCR	2	621	-	-	8/29/63/63	0/2/2/2
18	CLA	5	601	17	-	4/15/91/115	-
21	BCR	A	848	-	-	6/29/63/63	0/2/2/2
18	CLA	A	831	-	-	14/39/115/115	-
18	CLA	3	602	16	-	9/33/109/115	-
21	BCR	A	852	-	-	11/29/63/63	0/2/2/2
18	CLA	A	854	-	-	15/39/115/115	-
18	CLA	B	809	-	-	9/39/115/115	-
18	CLA	B	808	-	-	4/21/97/115	-
18	CLA	B	833	-	-	8/15/91/115	-
18	CLA	A	806	1	-	14/39/115/115	-
18	CLA	5	610	-	-	5/27/103/115	-
18	CLA	A	824	1	-	11/23/99/115	-
23	DGD	B	850	-	-	29/55/95/95	0/2/2/2
25	CHL	2	601	14	-	8/15/91/117	-
18	CLA	3	606	-	-	0/10/86/115	-
18	CLA	6	616	15	-	4/11/87/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	802	-	-	7/15/91/115	-
18	CLA	3	614	-	-	3/8/84/115	-
18	CLA	5	613	17	-	7/15/91/115	-
18	CLA	G	201	-	-	5/15/91/115	-
18	CLA	6	611	20	-	1/4/80/115	-
18	CLA	B	802	-	-	4/25/101/115	-
18	CLA	K	203	-	-	6/15/91/115	-
18	CLA	F	305	-	-	7/15/91/115	-
18	CLA	A	843	-	-	12/39/115/115	-
18	CLA	F	304	-	-	2/10/86/115	-
18	CLA	5	602	-	-	5/15/91/115	-
26	LUT	3	618	16	-	7/29/67/67	0/2/2/2
20	LHG	A	846	-	-	24/53/53/53	-
20	LHG	A	847	18	-	19/31/31/53	-
18	CLA	6	604	-	-	10/20/96/115	-
18	CLA	B	813	2	-	16/39/115/115	-
18	CLA	A	826	-	-	12/39/115/115	-
18	CLA	K	204	-	-	5/13/89/115	-
18	CLA	6	614	-	-	2/4/80/115	-
18	CLA	3	612	-	-	3/13/89/115	-
25	CHL	2	606	14	-	5/17/93/117	-
18	CLA	A	835	1	-	9/39/115/115	-
18	CLA	F	301	-	-	5/15/91/115	-
18	CLA	A	819	-	-	6/15/91/115	-
18	CLA	A	840	-	-	6/15/91/115	-
21	BCR	B	848	-	-	13/29/63/63	0/2/2/2
18	CLA	A	812	-	-	13/39/115/115	-
26	LUT	6	617	-	-	12/29/67/67	0/2/2/2
18	CLA	2	603	-	-	7/15/91/115	-
18	CLA	B	839	-	-	2/10/86/115	-
18	CLA	B	815	2	-	13/33/109/115	-
18	CLA	A	816	-	-	4/12/88/115	-
18	CLA	B	824	-	-	4/15/91/115	-
18	CLA	B	829	2	-	0/15/91/115	-
18	CLA	B	814	2	-	1/13/89/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	815	1	-	7/15/91/115	-
18	CLA	B	810	2	-	11/17/93/115	-
18	CLA	B	838	-	-	2/18/94/115	-
18	CLA	A	822	-	-	2/11/87/115	-
26	LUT	2	619	-	-	7/29/67/67	0/2/2/2
21	BCR	B	801	-	-	7/29/63/63	0/2/2/2
25	CHL	3	608	-	-	2/8/84/117	-
18	CLA	A	833	-	-	7/15/91/115	-
18	CLA	A	808	-	-	3/15/91/115	-
18	CLA	A	830	-	-	5/39/115/115	-
18	CLA	B	804	2	-	5/15/91/115	-
18	CLA	3	617	-	-	2/8/84/115	-
18	CLA	B	840	2	-	14/39/115/115	-
18	CLA	G	203	7	-	9/21/97/115	-
20	LHG	2	622	14,18	-	23/39/39/53	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	B	805	2	-	11/39/115/115	-
18	CLA	B	831	2	-	7/20/96/115	-
18	CLA	2	609	14	-	11/27/103/115	-
25	CHL	6	601	15	-	3/15/91/117	-
18	CLA	K	206	11	-	7/15/91/115	-
18	CLA	5	611	-	-	5/10/70/115	-

The worst 5 of 1645 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	619	LUT	C34-C33	20.14	1.62	1.35
26	3	618	LUT	C34-C33	19.98	1.62	1.35
26	2	619	LUT	C34-C33	19.80	1.62	1.35
26	6	617	LUT	C34-C33	19.76	1.62	1.35
26	5	619	LUT	C14-C13	16.75	1.58	1.35

The worst 5 of 1520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	619	LUT	C18-C5-C6	-14.02	108.78	124.53
26	5	619	LUT	C18-C5-C6	-12.36	110.65	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	617	LUT	C18-C5-C6	-12.10	110.94	124.53
26	2	619	LUT	C15-C14-C13	-11.96	110.24	127.31
26	3	618	LUT	C18-C5-C6	-11.81	111.26	124.53

There are no chirality outliers.

5 of 1481 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

151 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	844	PQN	1	0
18	5	612	CLA	1	0
25	5	607	CHL	13	0
25	5	608	CHL	3	0
18	A	811	CLA	3	0
18	3	611	CLA	2	0
21	B	845	BCR	3	0
18	A	801	CLA	1	0
18	B	811	CLA	1	0
20	B	851	LHG	1	0
25	6	607	CHL	6	0
18	A	837	CLA	2	0
18	B	828	CLA	3	0
18	L	302	CLA	2	0
18	A	814	CLA	6	0
18	A	813	CLA	1	0
18	B	806	CLA	2	0
18	A	827	CLA	4	0
22	C	102	SF4	4	0
18	B	819	CLA	2	0
22	C	101	SF4	7	0
18	B	803	CLA	2	0
18	2	614	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	825	CLA	1	0
18	A	805	CLA	1	0
25	2	607	CHL	6	0
18	K	201	CLA	1	0
18	2	613	CLA	1	0
27	2	620	XAT	25	0
18	2	602	CLA	3	0
18	A	821	CLA	1	0
18	B	826	CLA	3	0
18	B	827	CLA	2	0
18	B	823	CLA	2	0
24	J	104	LMG	1	0
18	2	610	CLA	3	0
20	6	620	LHG	1	0
18	B	816	CLA	2	0
18	G	204	CLA	2	0
18	A	832	CLA	1	0
21	A	850	BCR	1	0
21	B	844	BCR	2	0
20	5	622	LHG	5	0
21	5	621	BCR	2	0
18	B	822	CLA	1	0
27	3	619	XAT	15	0
21	L	301	BCR	1	0
18	A	834	CLA	1	0
18	A	845	CLA	1	0
18	A	841	CLA	2	0
21	A	851	BCR	1	0
18	B	807	CLA	1	0
21	B	843	BCR	5	0
18	2	604	CLA	2	0
18	B	818	CLA	3	0
21	J	103	BCR	5	0
19	B	842	PQN	6	0
21	J	102	BCR	1	0
27	6	619	XAT	13	0
18	3	613	CLA	3	0
18	L	303	CLA	1	0
27	5	620	XAT	30	0
18	A	818	CLA	1	0
18	B	817	CLA	3	0
18	B	837	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	304	CLA	1	0
21	B	846	BCR	2	0
18	A	809	CLA	4	0
18	B	835	CLA	1	0
18	6	609	CLA	1	0
21	K	207	BCR	1	0
21	A	856	BCR	4	0
18	A	842	CLA	2	0
21	A	849	BCR	2	0
18	A	829	CLA	6	0
18	A	810	CLA	1	0
18	3	609	CLA	3	0
18	B	812	CLA	1	0
26	5	619	LUT	3	0
18	A	820	CLA	4	0
18	5	614	CLA	2	0
21	3	620	BCR	5	0
21	L	305	BCR	1	0
21	K	202	BCR	2	0
21	G	205	BCR	3	0
18	A	839	CLA	2	0
21	3	622	BCR	3	0
21	I	101	BCR	2	0
21	F	302	BCR	4	0
25	2	616	CHL	1	0
18	A	838	CLA	2	0
18	A	828	CLA	1	0
18	B	821	CLA	3	0
18	B	830	CLA	1	0
21	2	621	BCR	4	0
18	5	601	CLA	2	0
21	A	848	BCR	3	0
18	A	831	CLA	2	0
18	3	602	CLA	1	0
21	A	852	BCR	4	0
18	A	854	CLA	6	0
18	B	809	CLA	3	0
18	B	808	CLA	1	0
18	B	833	CLA	3	0
18	A	806	CLA	4	0
18	5	610	CLA	2	0
18	A	824	CLA	2	0

Continued on next page...

Continued from previous page...

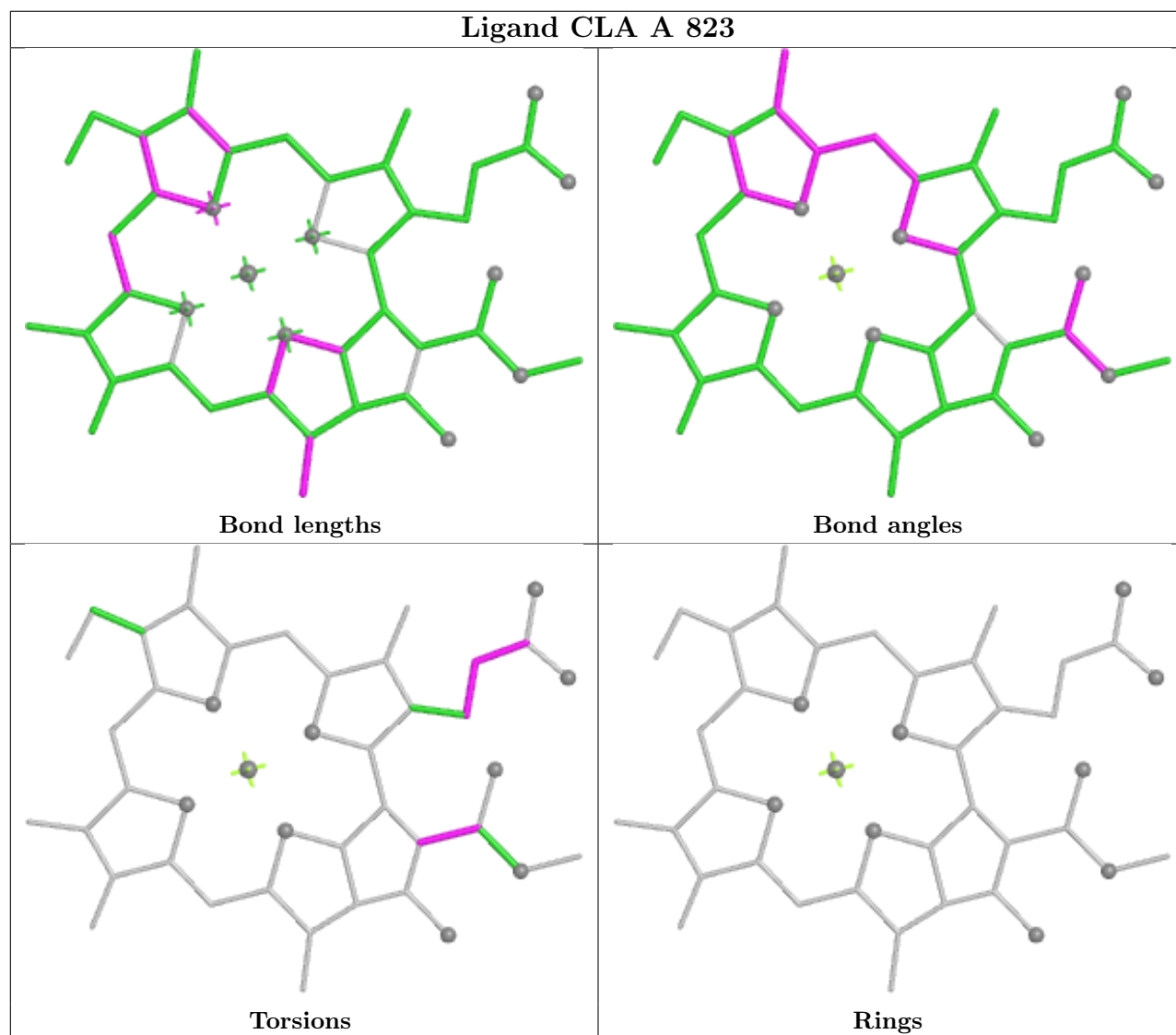
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	850	DGD	4	0
18	3	606	CLA	1	0
18	A	802	CLA	2	0
18	5	613	CLA	3	0
18	G	201	CLA	2	0
18	B	802	CLA	2	0
18	K	203	CLA	1	0
18	F	305	CLA	1	0
18	A	843	CLA	4	0
18	F	304	CLA	1	0
18	5	602	CLA	5	0
26	3	618	LUT	1	0
20	A	846	LHG	1	0
20	A	847	LHG	2	0
18	B	813	CLA	7	0
18	A	826	CLA	4	0
18	K	204	CLA	1	0
18	3	612	CLA	1	0
25	2	606	CHL	9	0
18	A	835	CLA	3	0
18	F	301	CLA	2	0
18	A	819	CLA	3	0
18	A	840	CLA	1	0
21	B	848	BCR	4	0
18	A	812	CLA	4	0
26	6	617	LUT	3	0
18	B	839	CLA	2	0
18	B	815	CLA	3	0
18	B	824	CLA	1	0
18	B	829	CLA	1	0
18	B	814	CLA	2	0
18	B	838	CLA	1	0
26	2	619	LUT	3	0
21	B	801	BCR	2	0
25	3	608	CHL	1	0
18	A	833	CLA	2	0
18	A	830	CLA	1	0
18	B	840	CLA	3	0
20	2	622	LHG	3	0
21	B	847	BCR	1	0
18	B	805	CLA	2	0
18	B	831	CLA	3	0

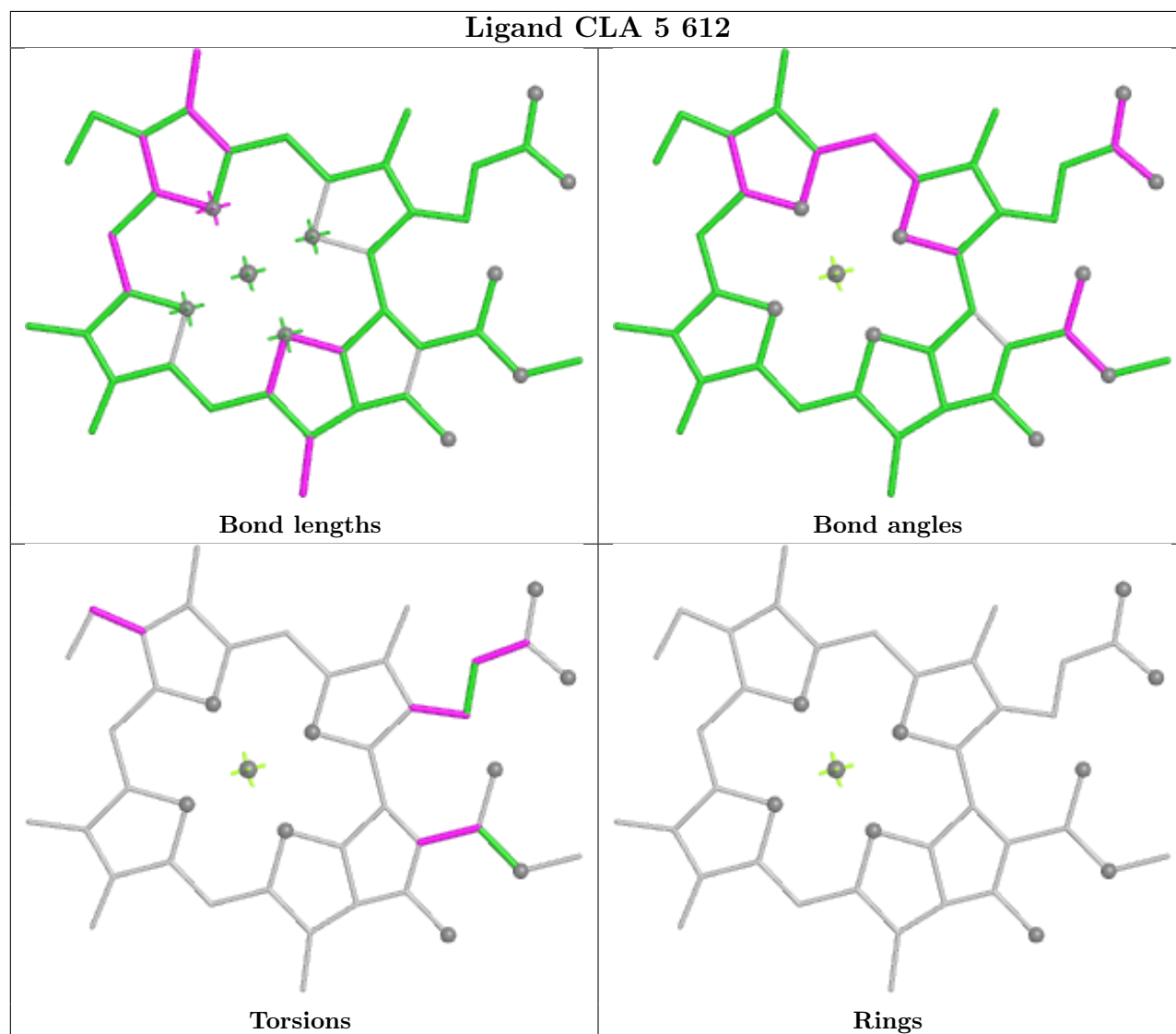
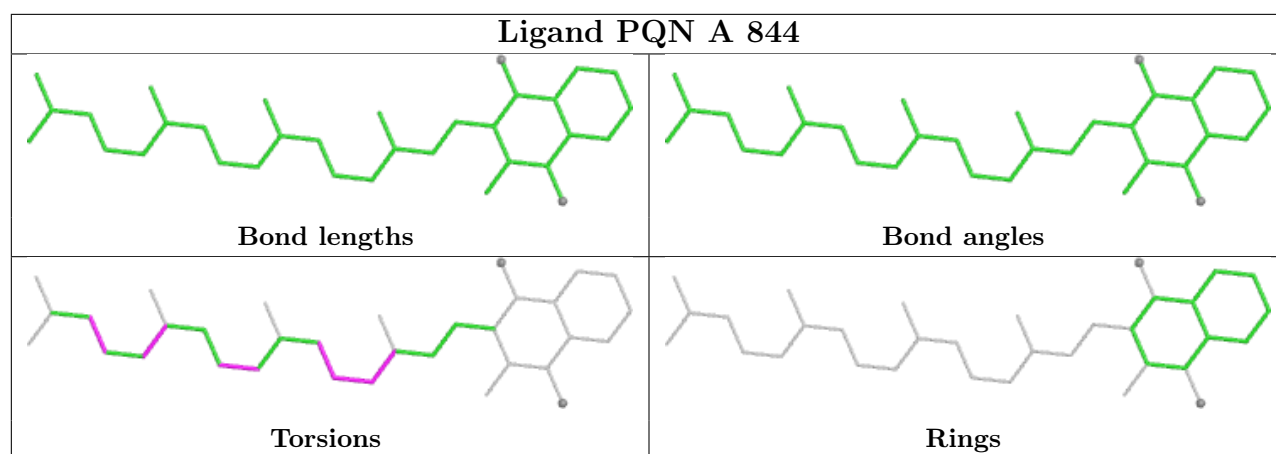
Continued on next page...

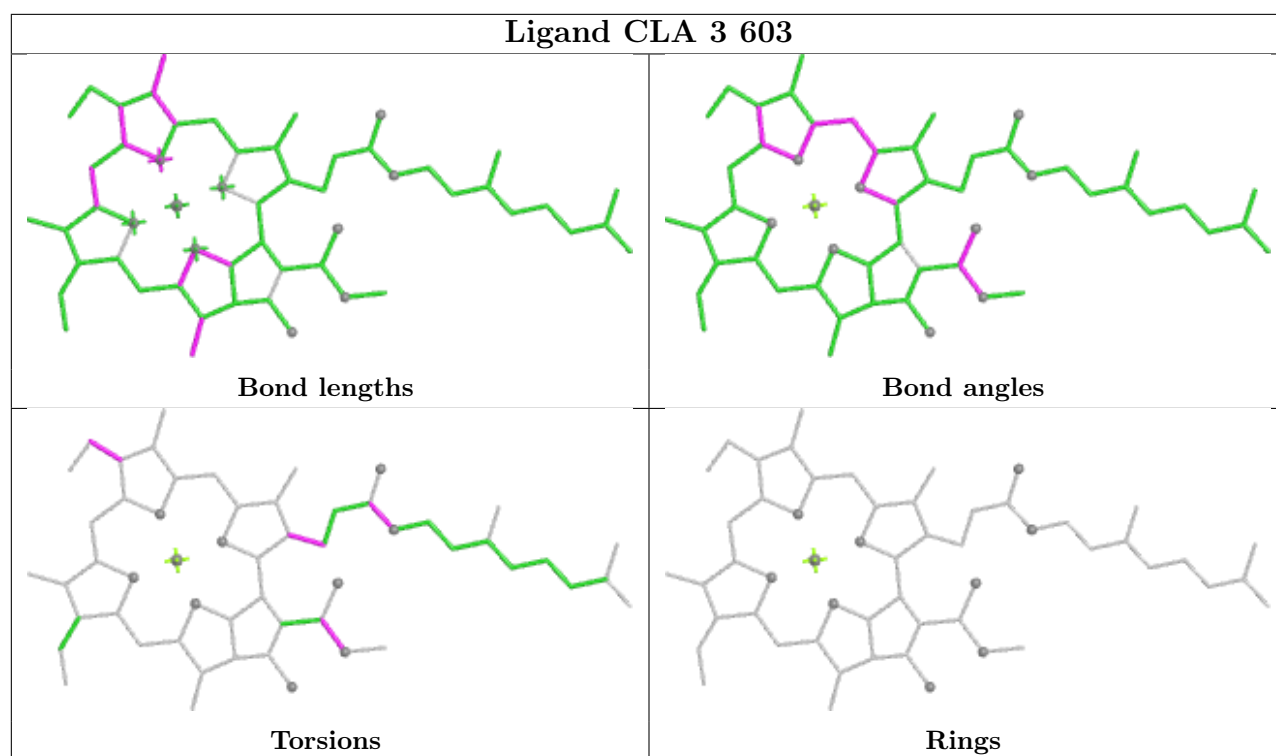
Continued from previous page...

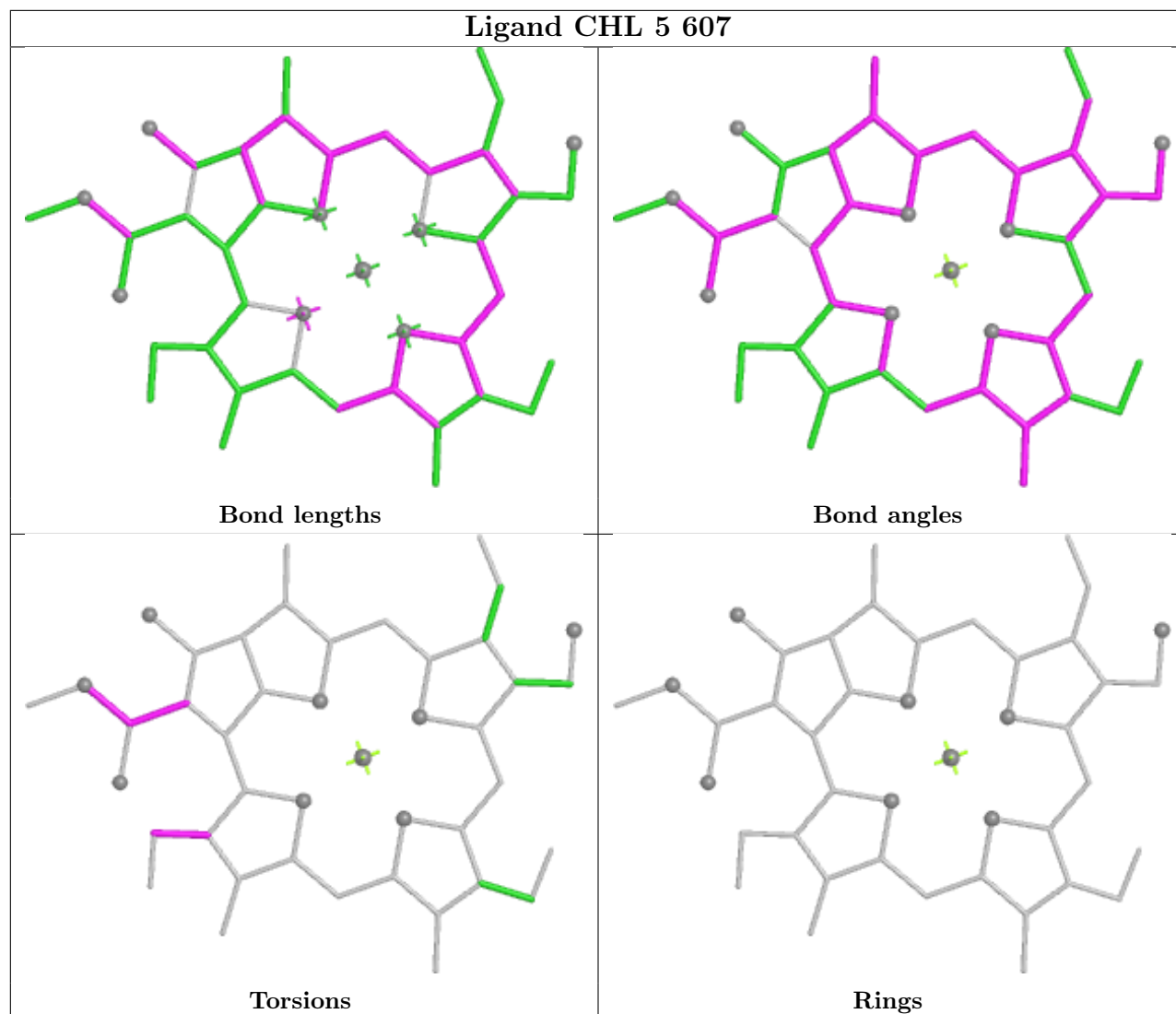
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	601	CHL	2	0
18	5	611	CLA	2	0

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.

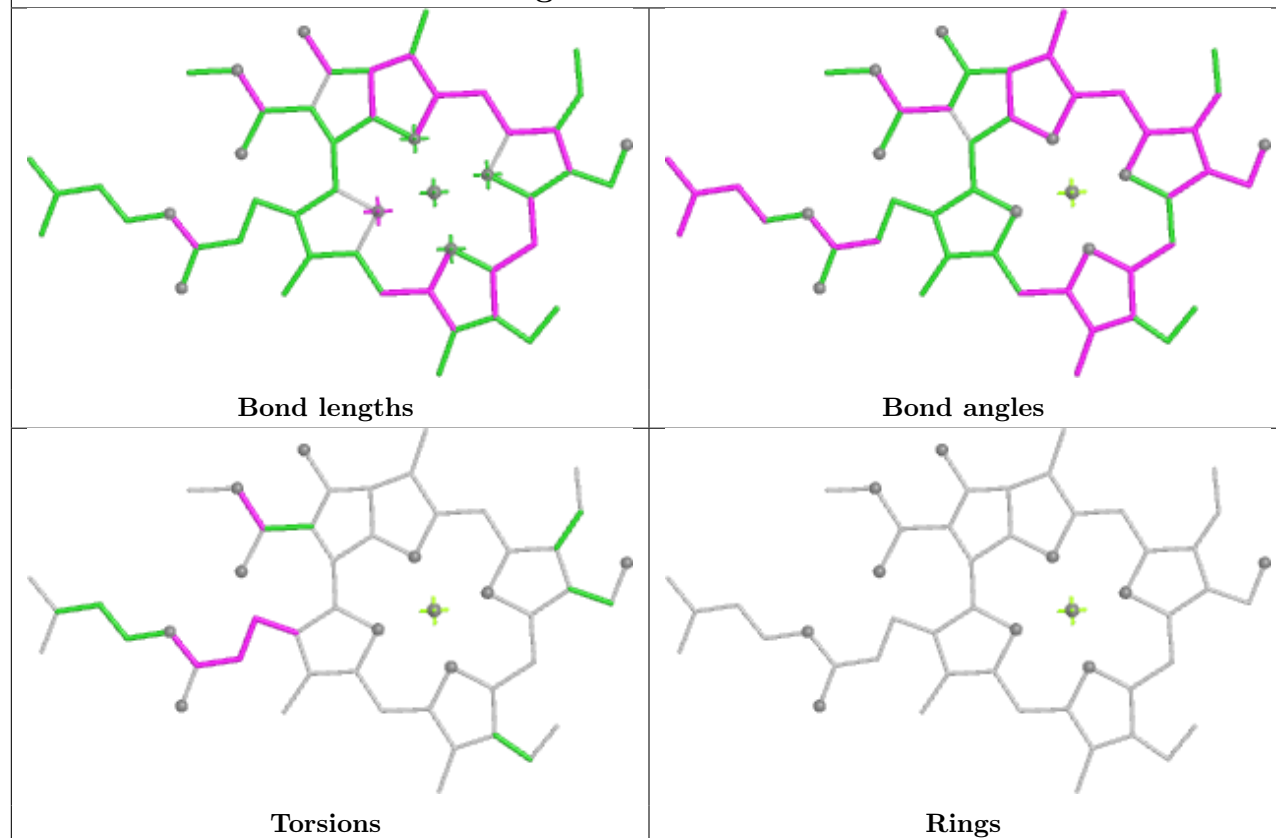




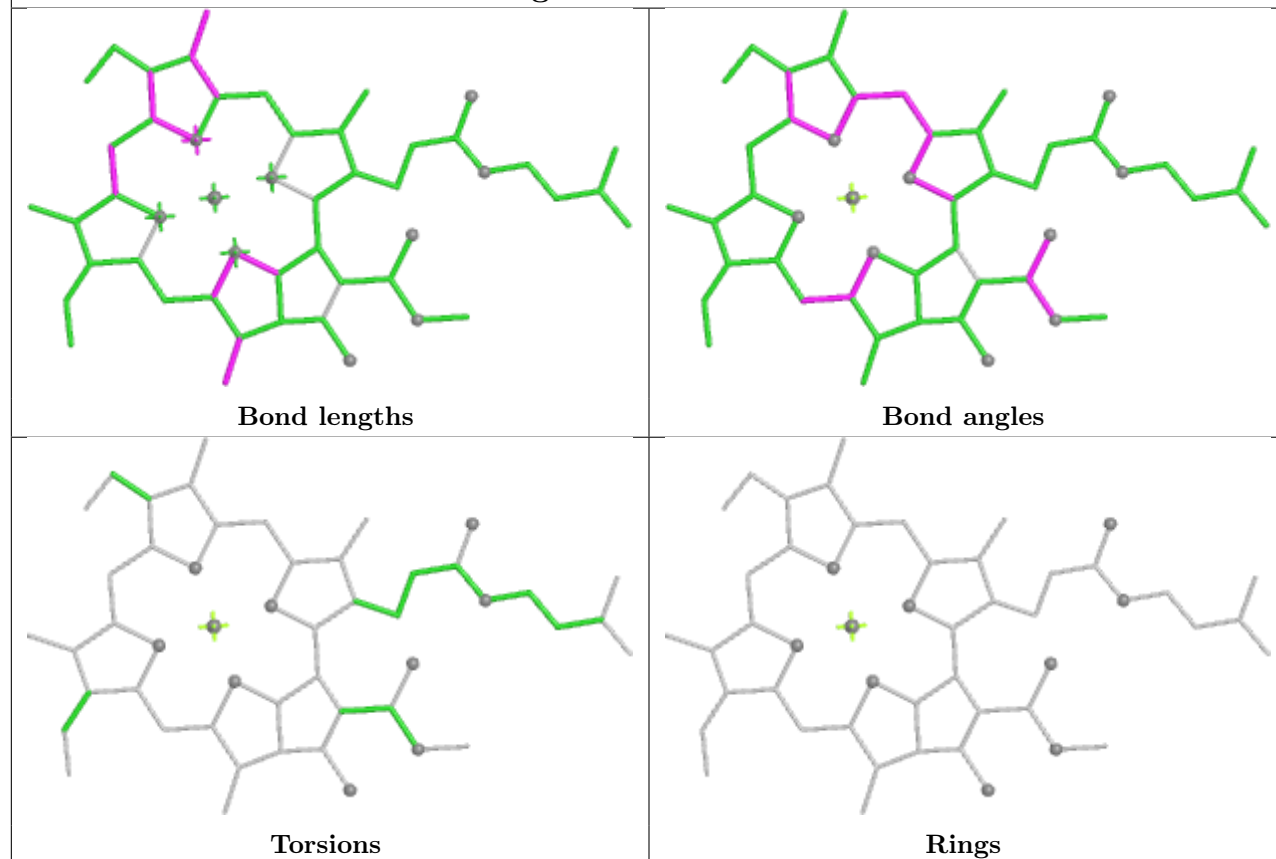




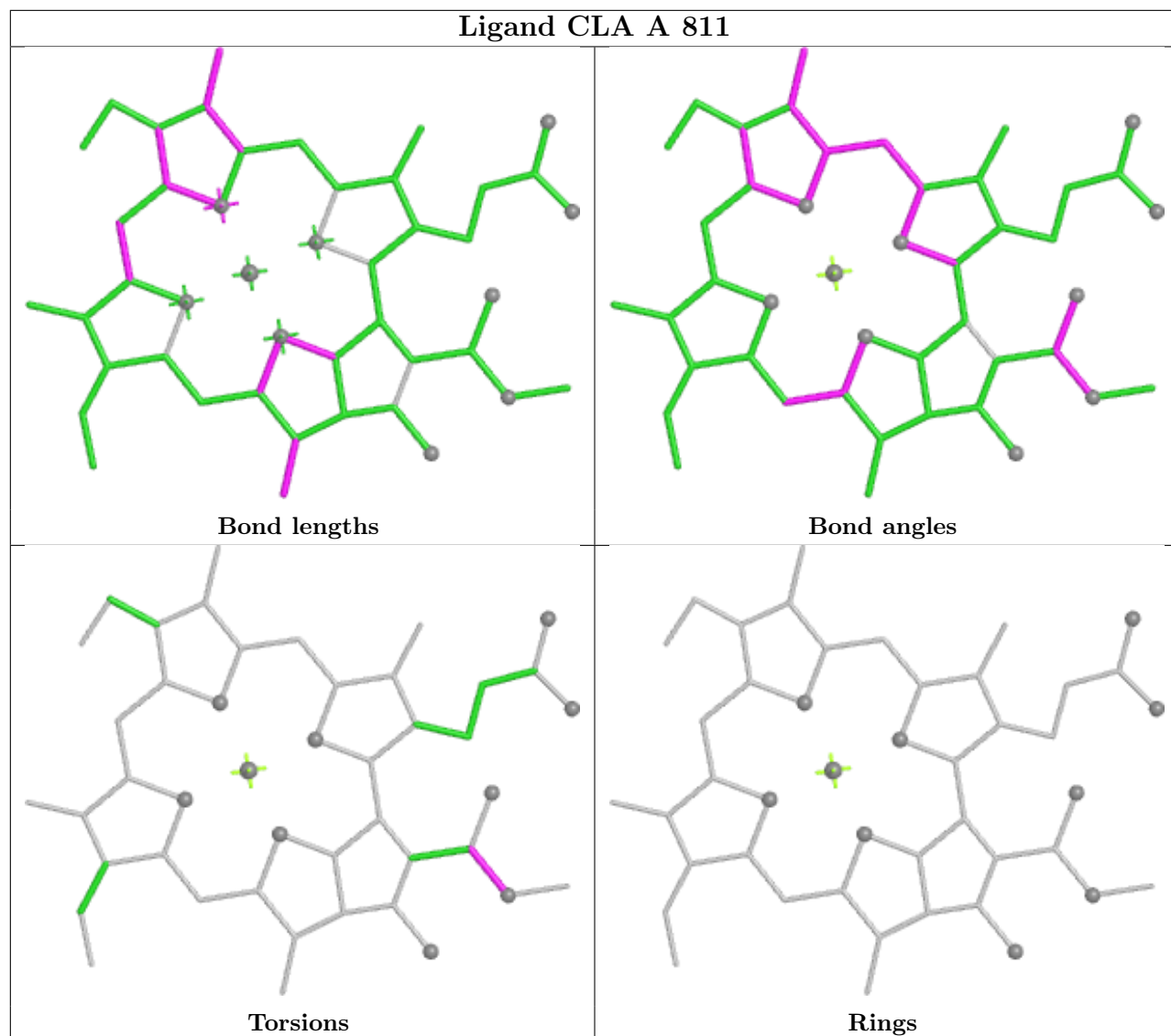
Ligand CHL 5 608



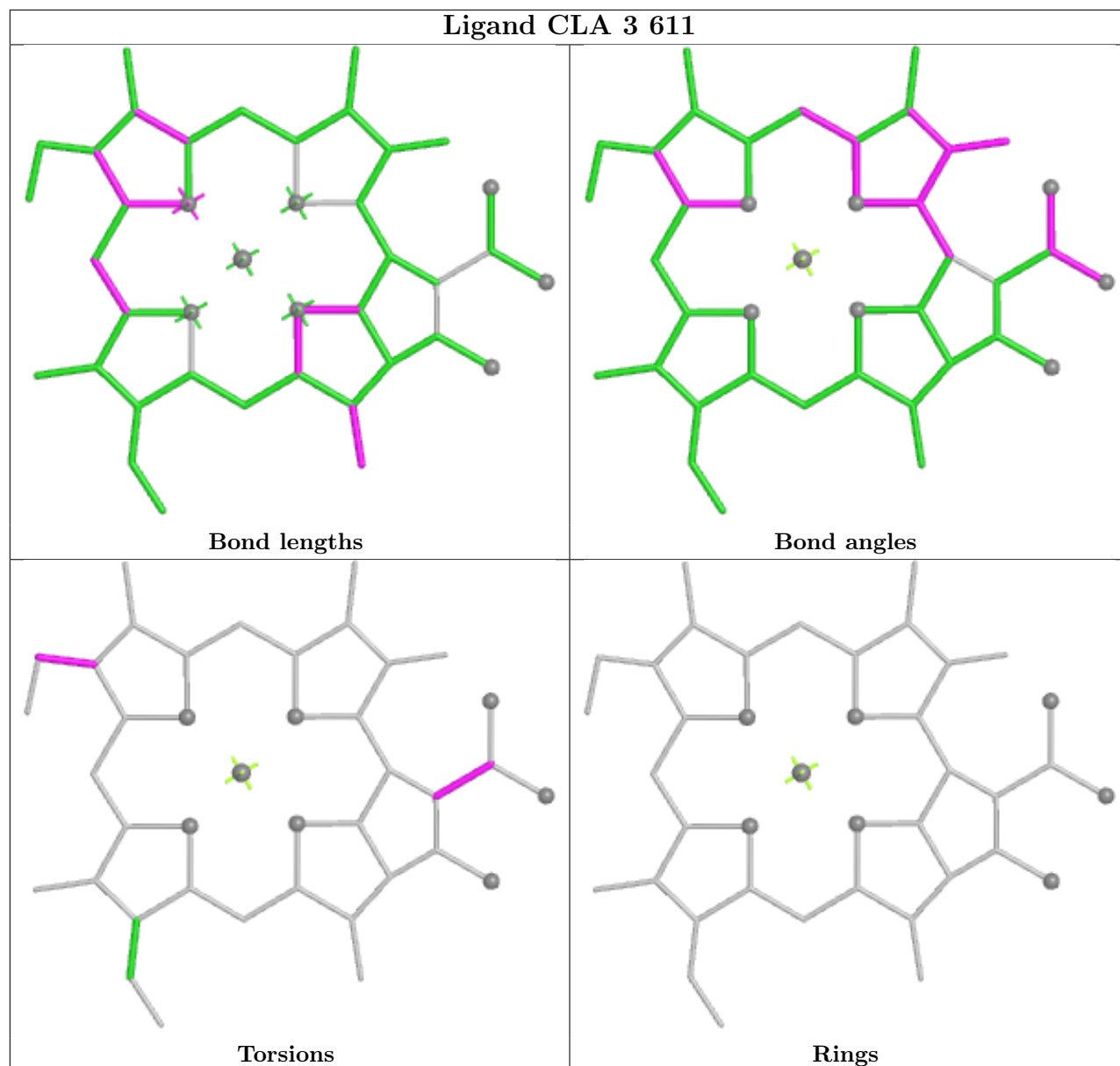
Ligand CLA A 836



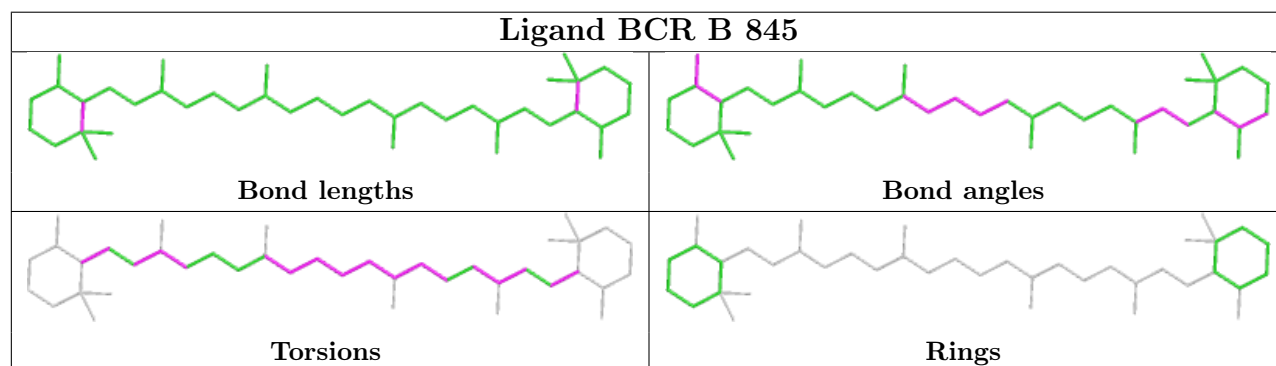
Ligand CLA A 811

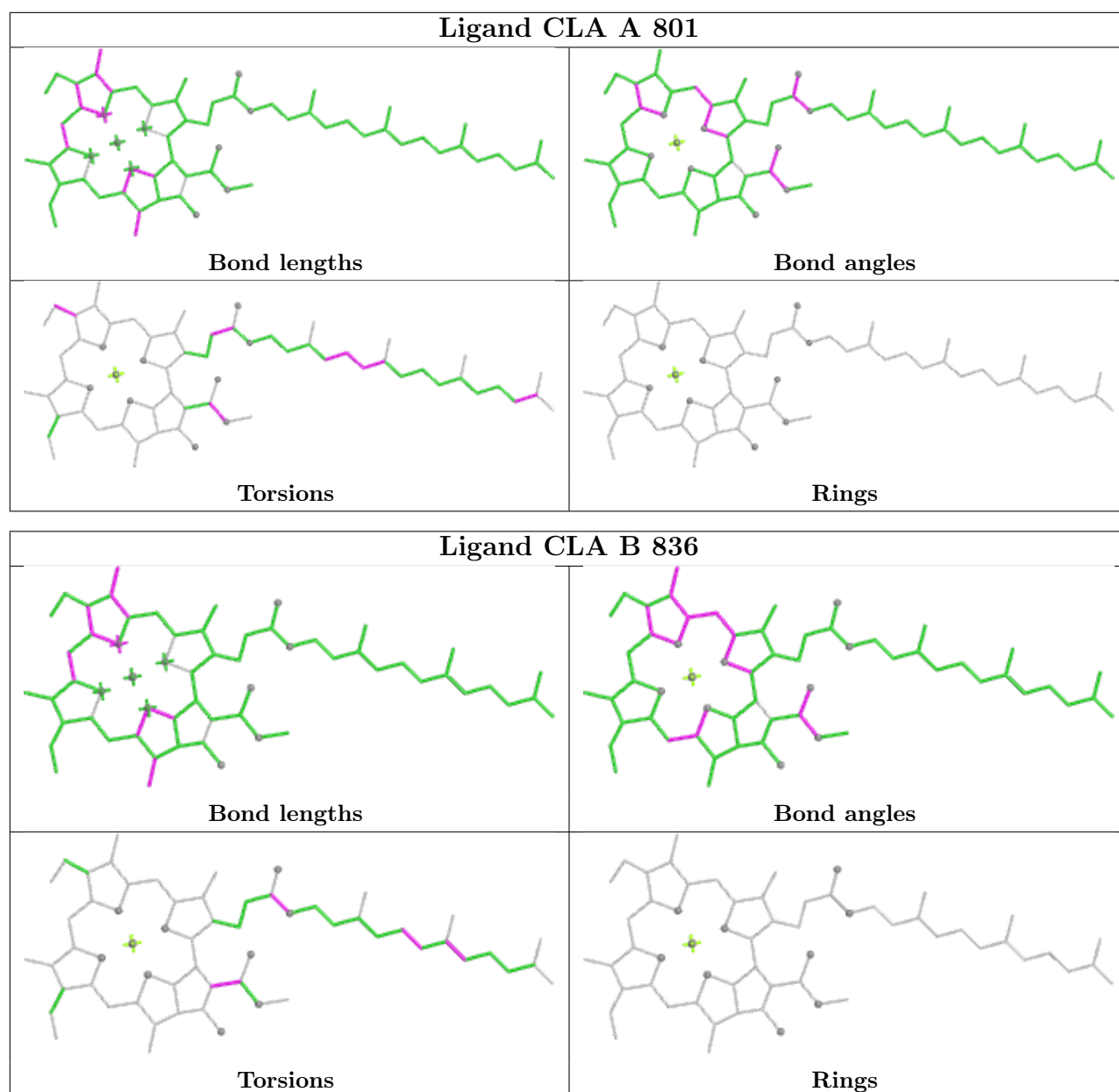


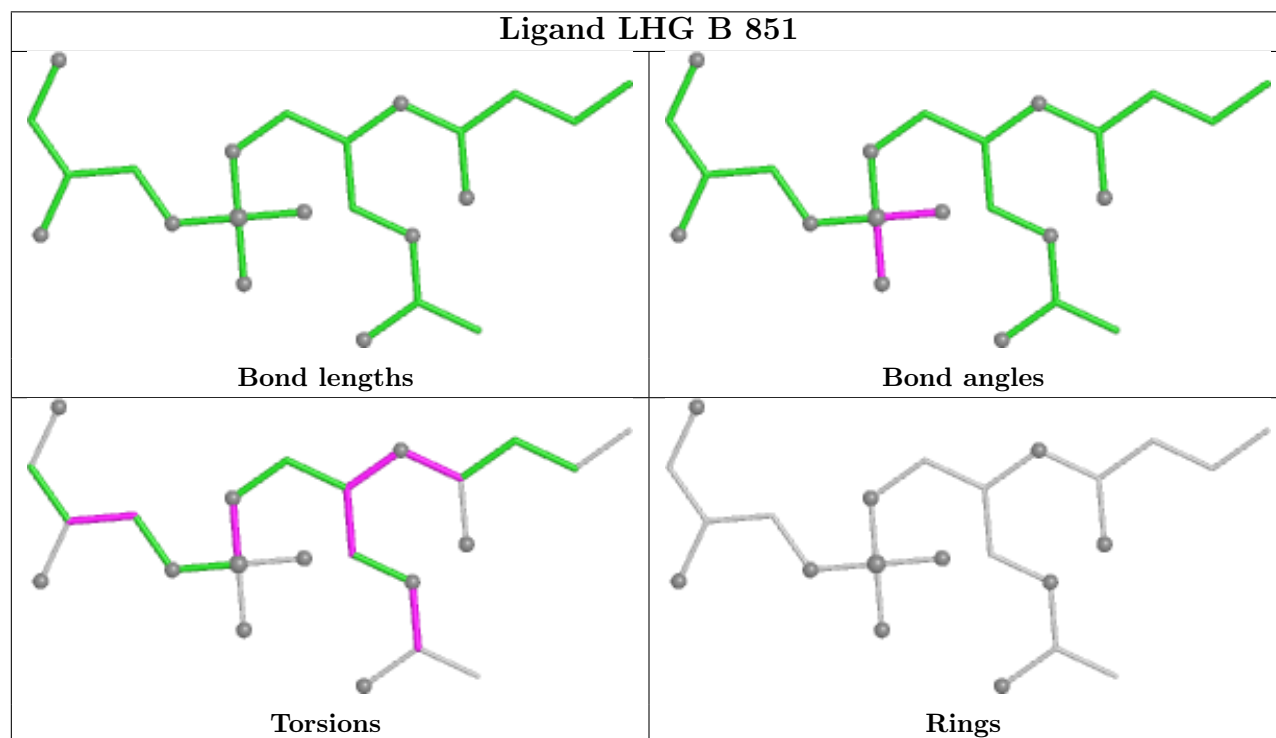
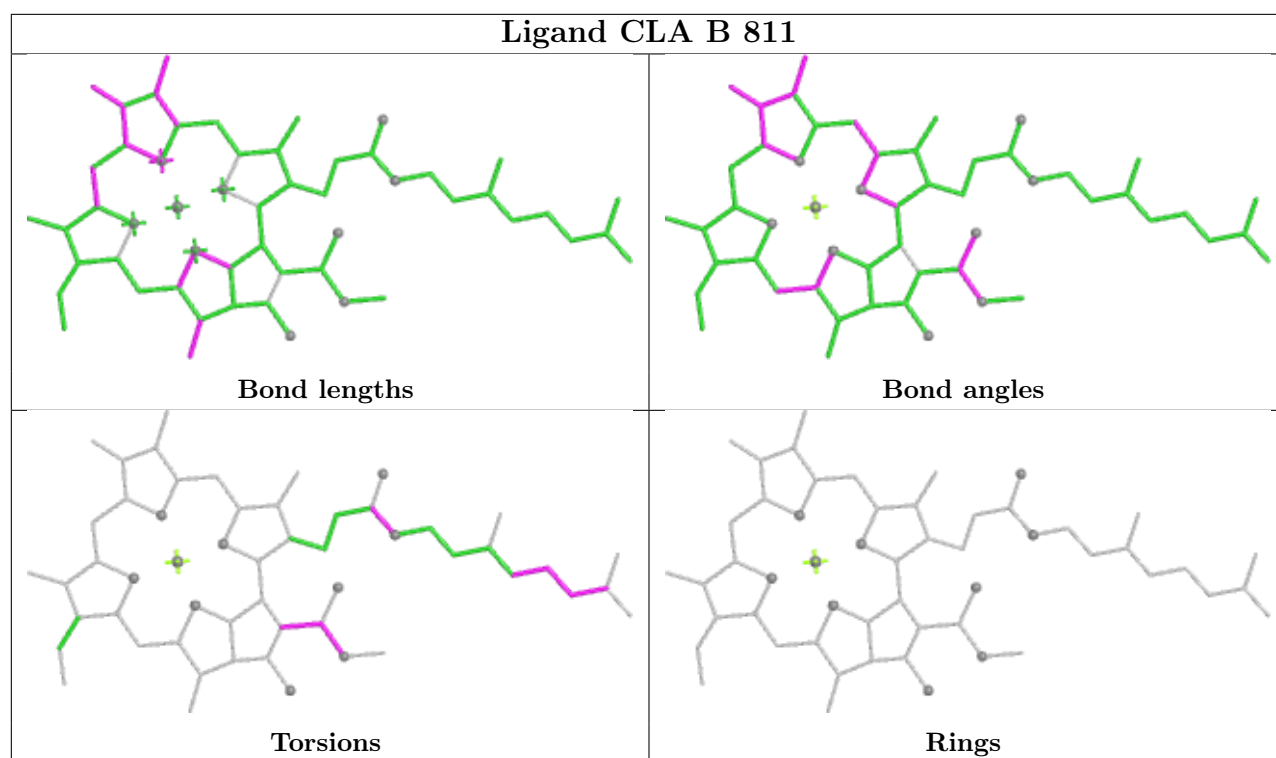
Ligand CLA 3 611

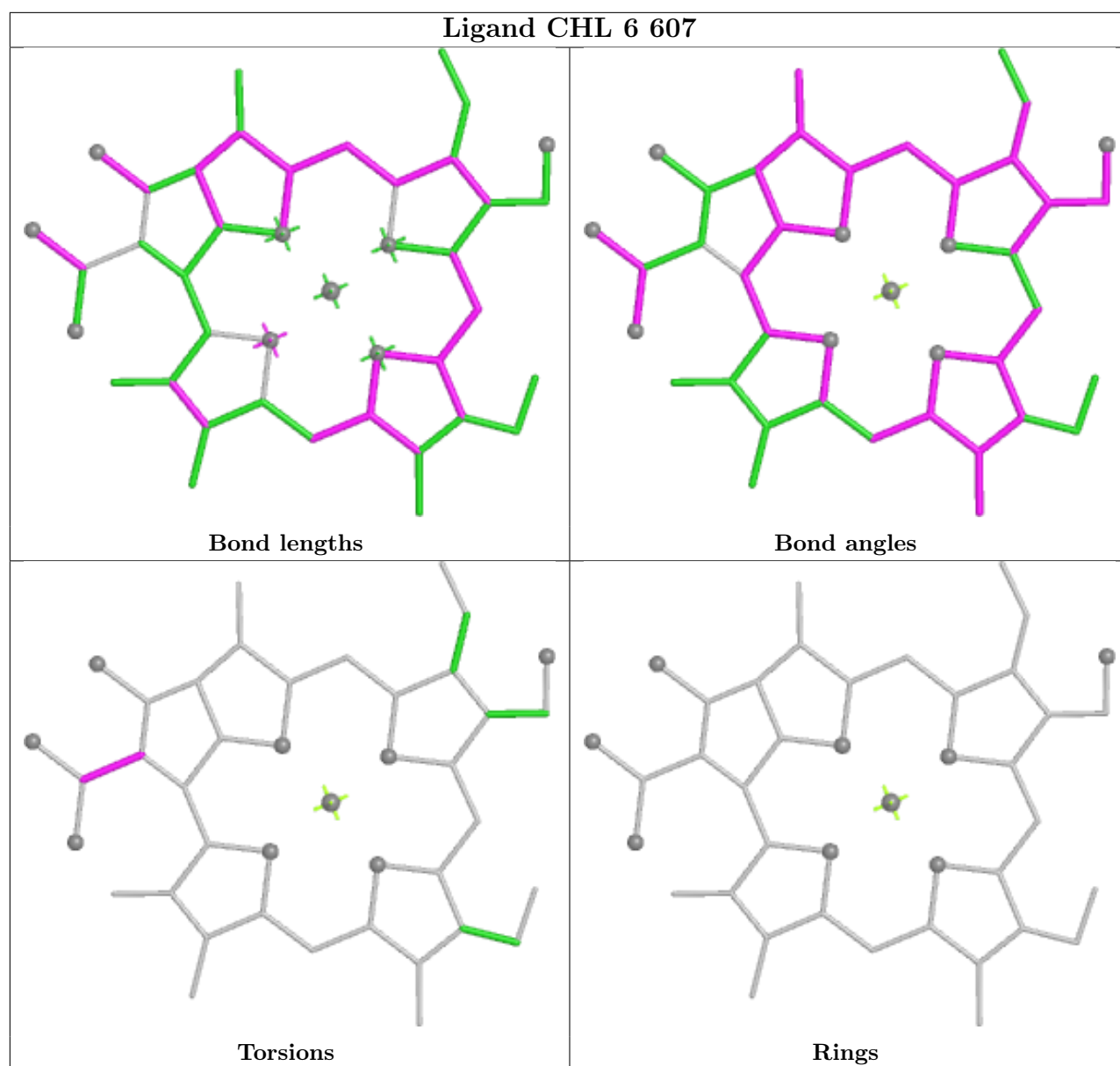


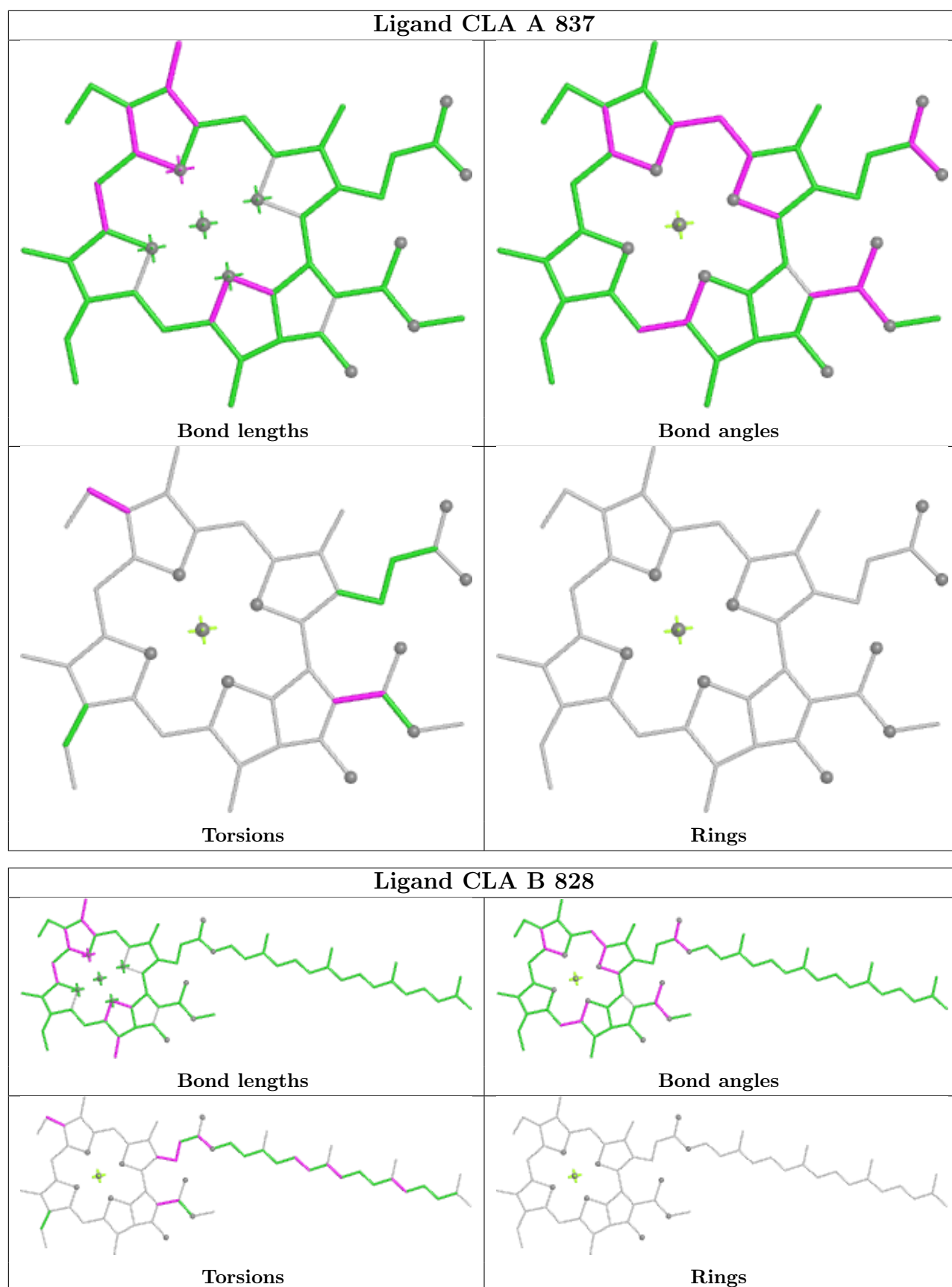
Ligand BCR B 845

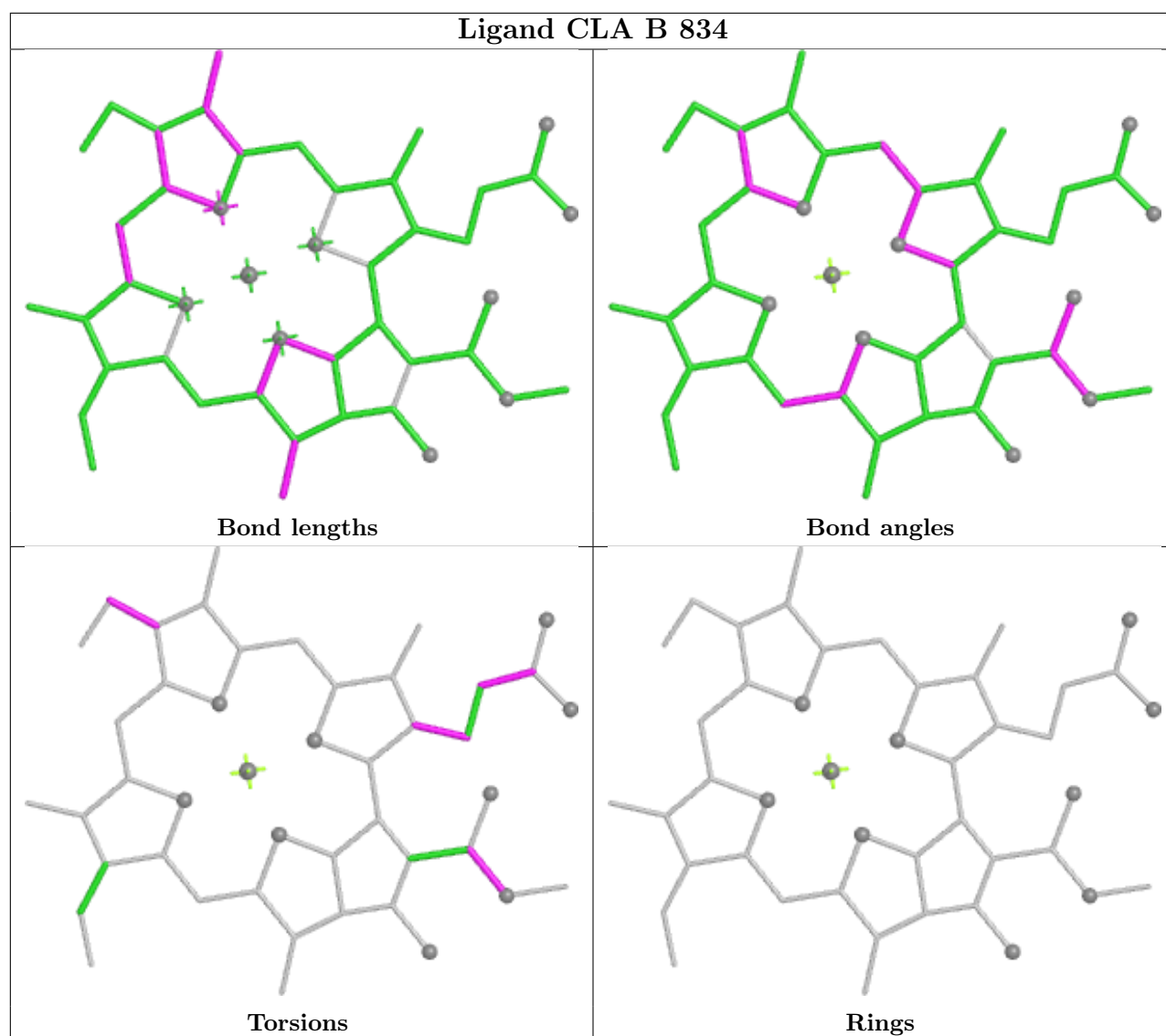


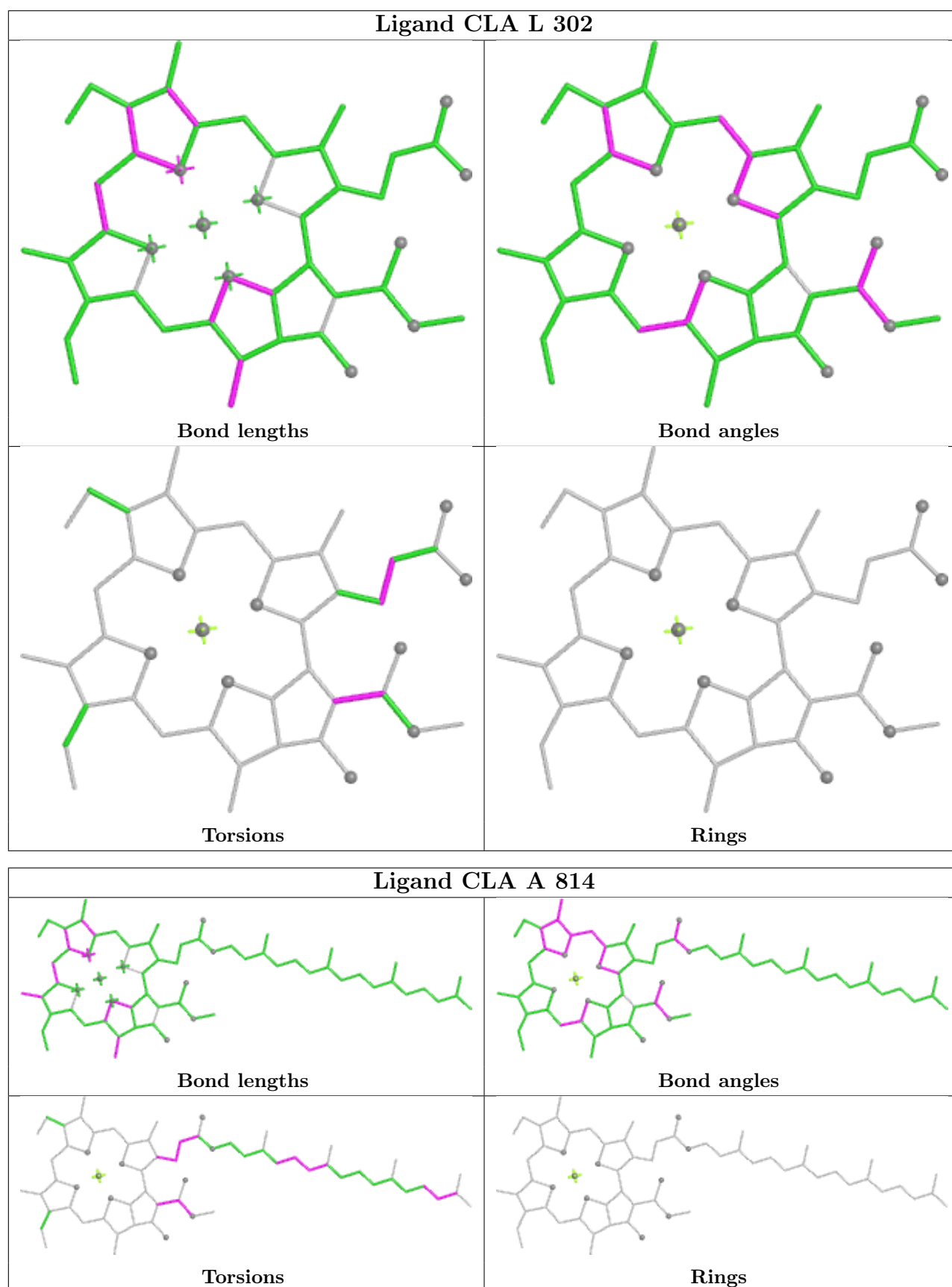


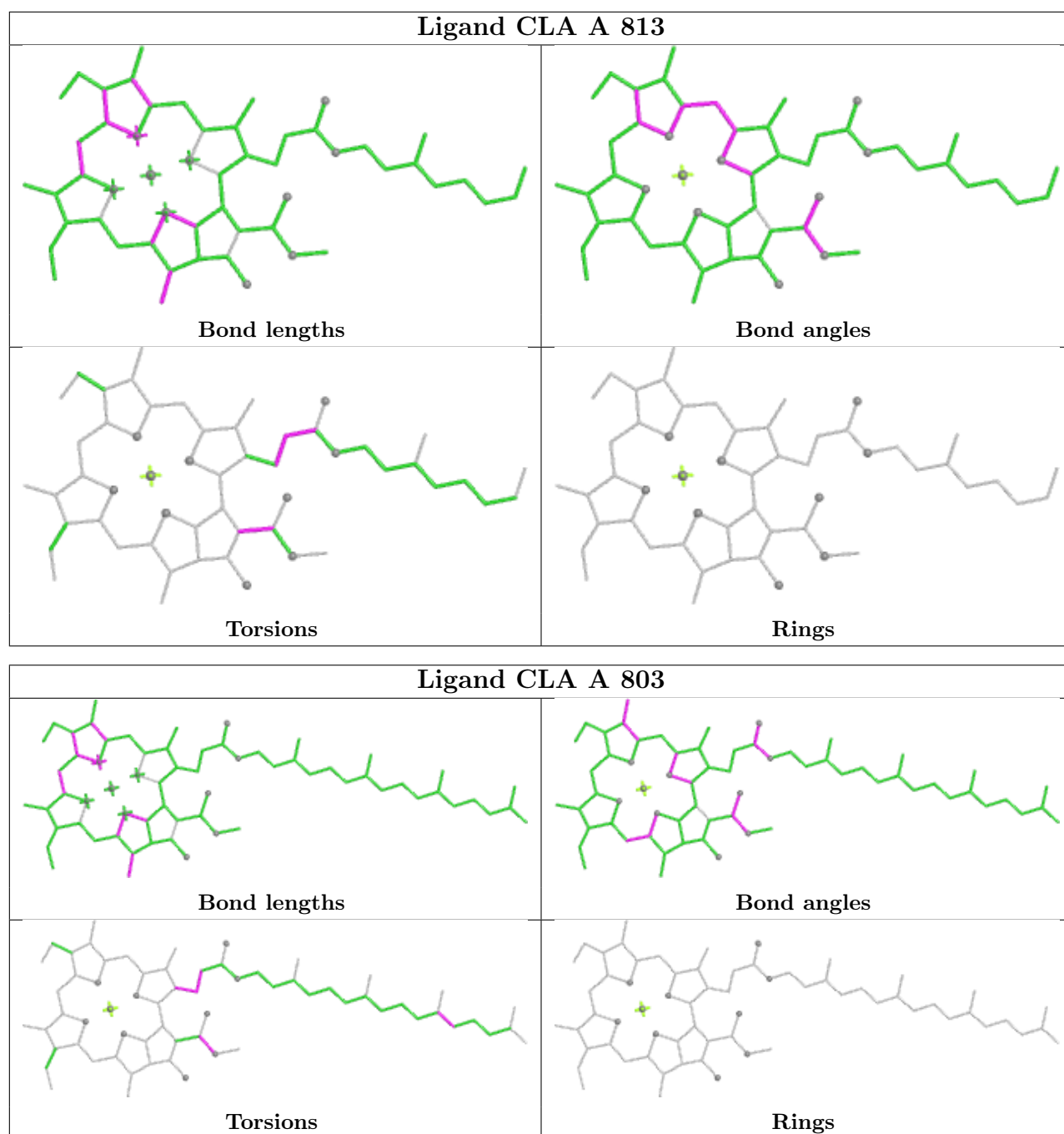


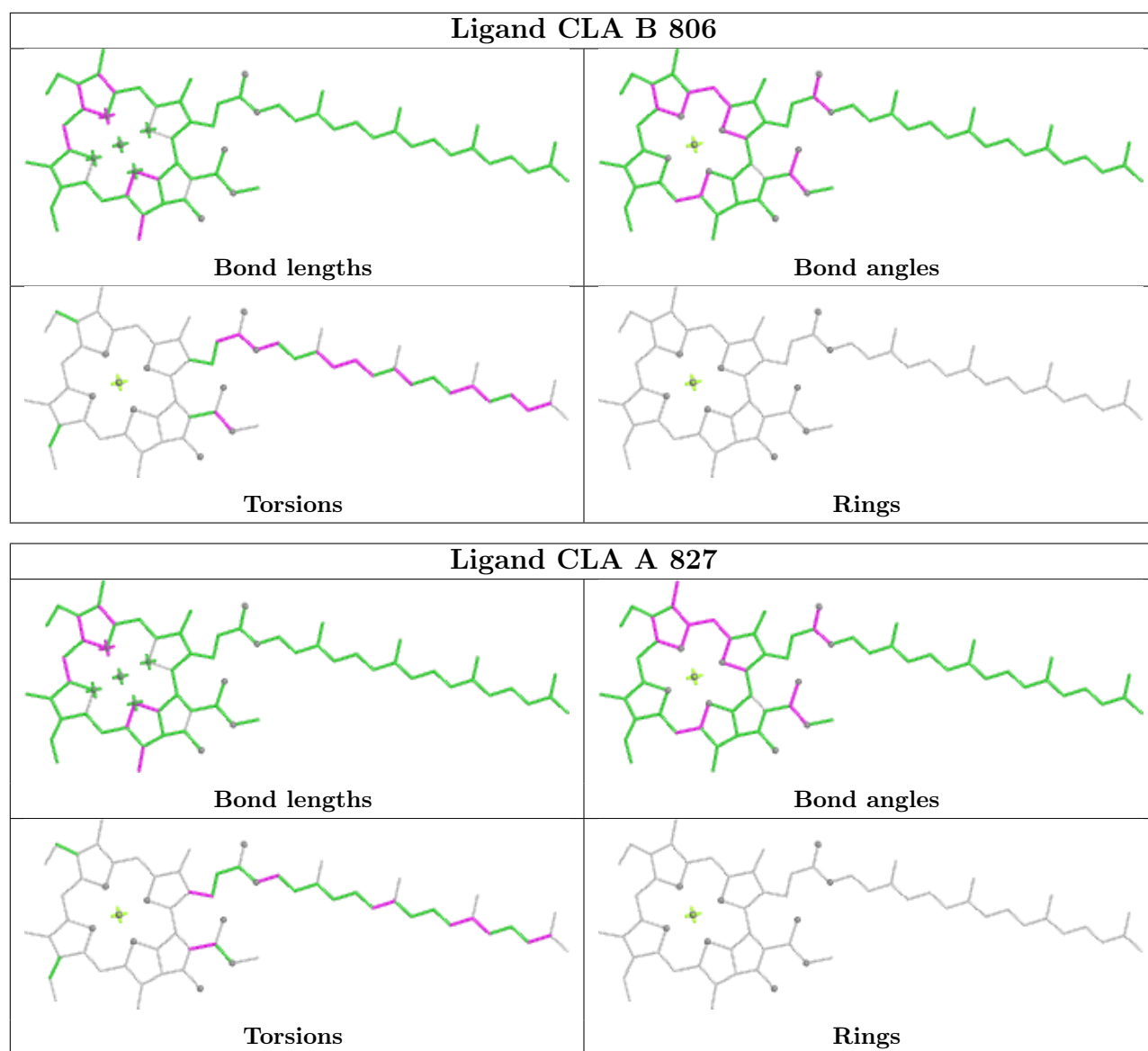


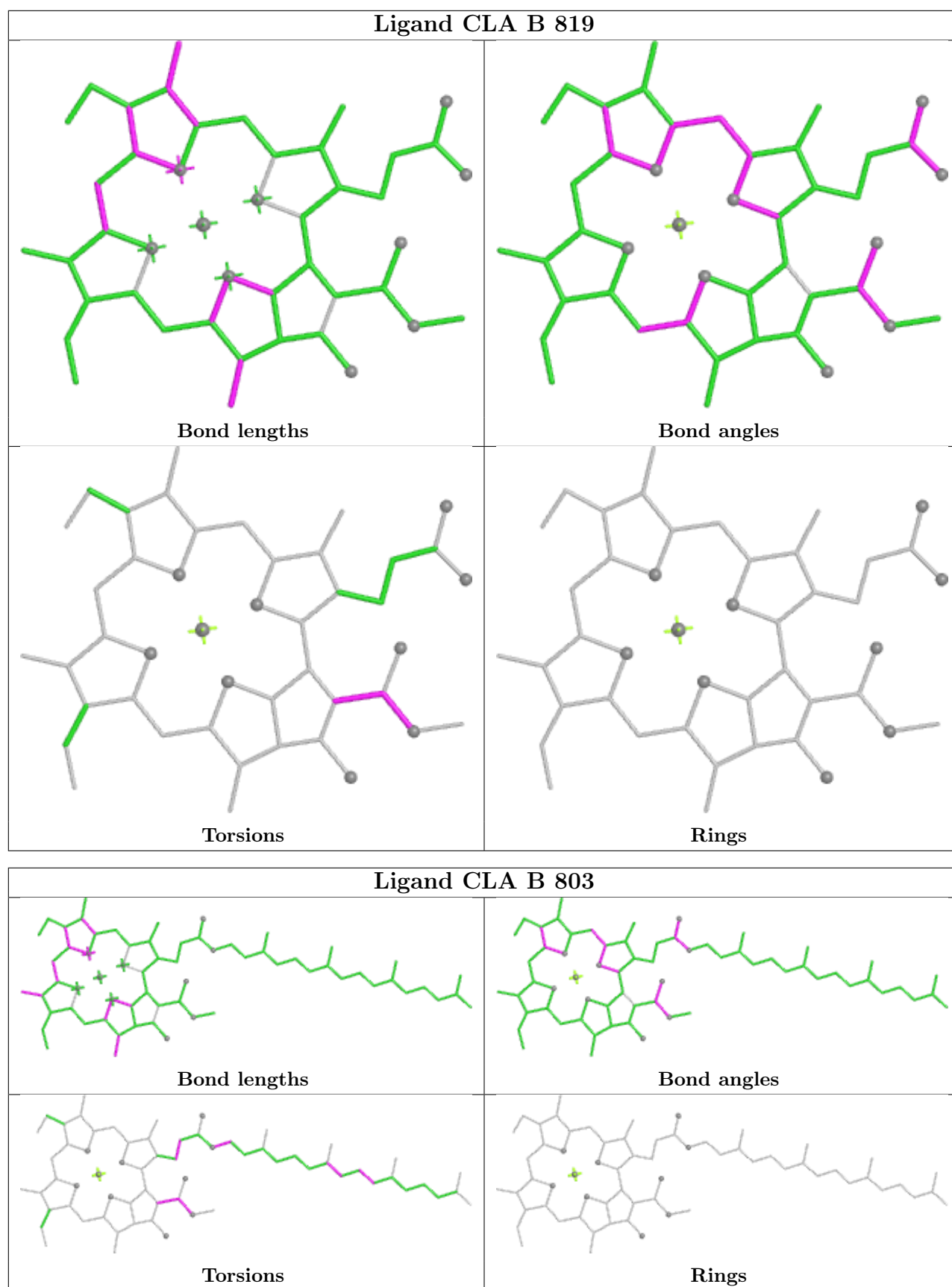




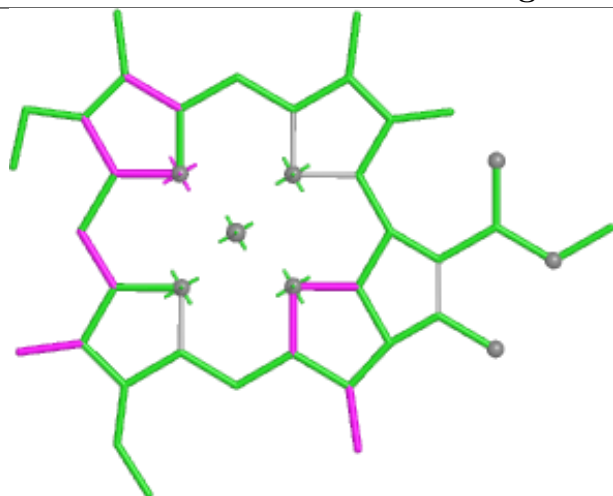




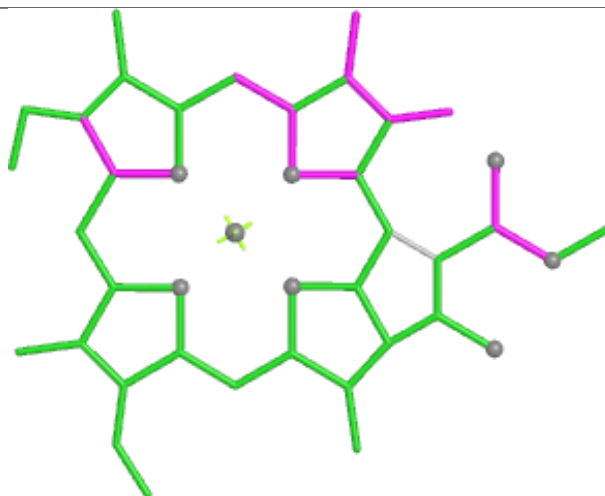




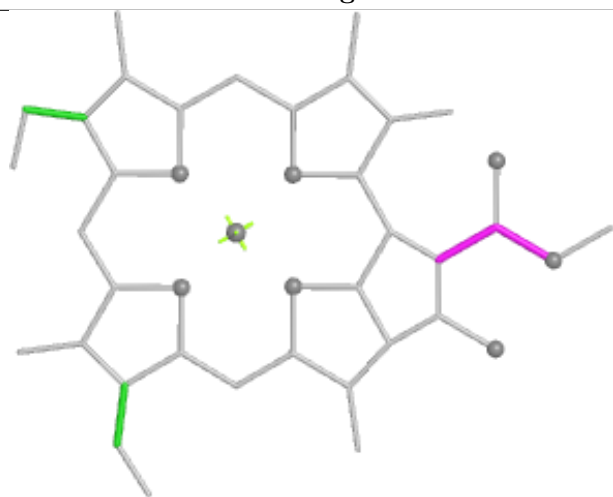
Ligand CLA 3 610



Bond lengths



Bond angles

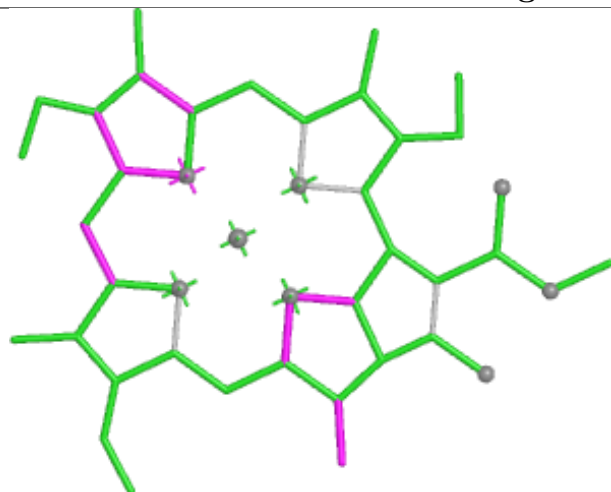


Torsions

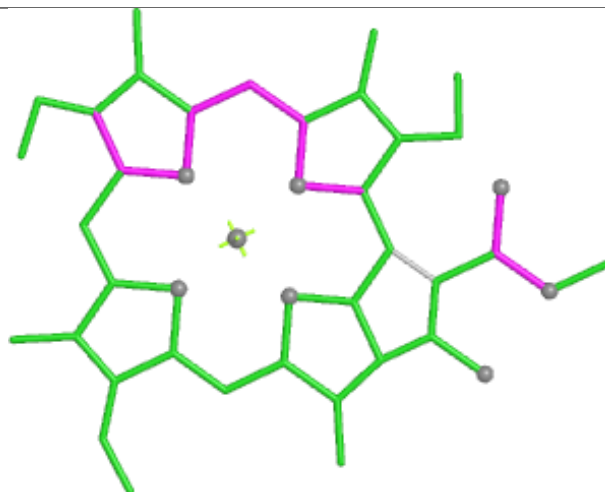


Rings

Ligand CLA J 101



Bond lengths



Bond angles

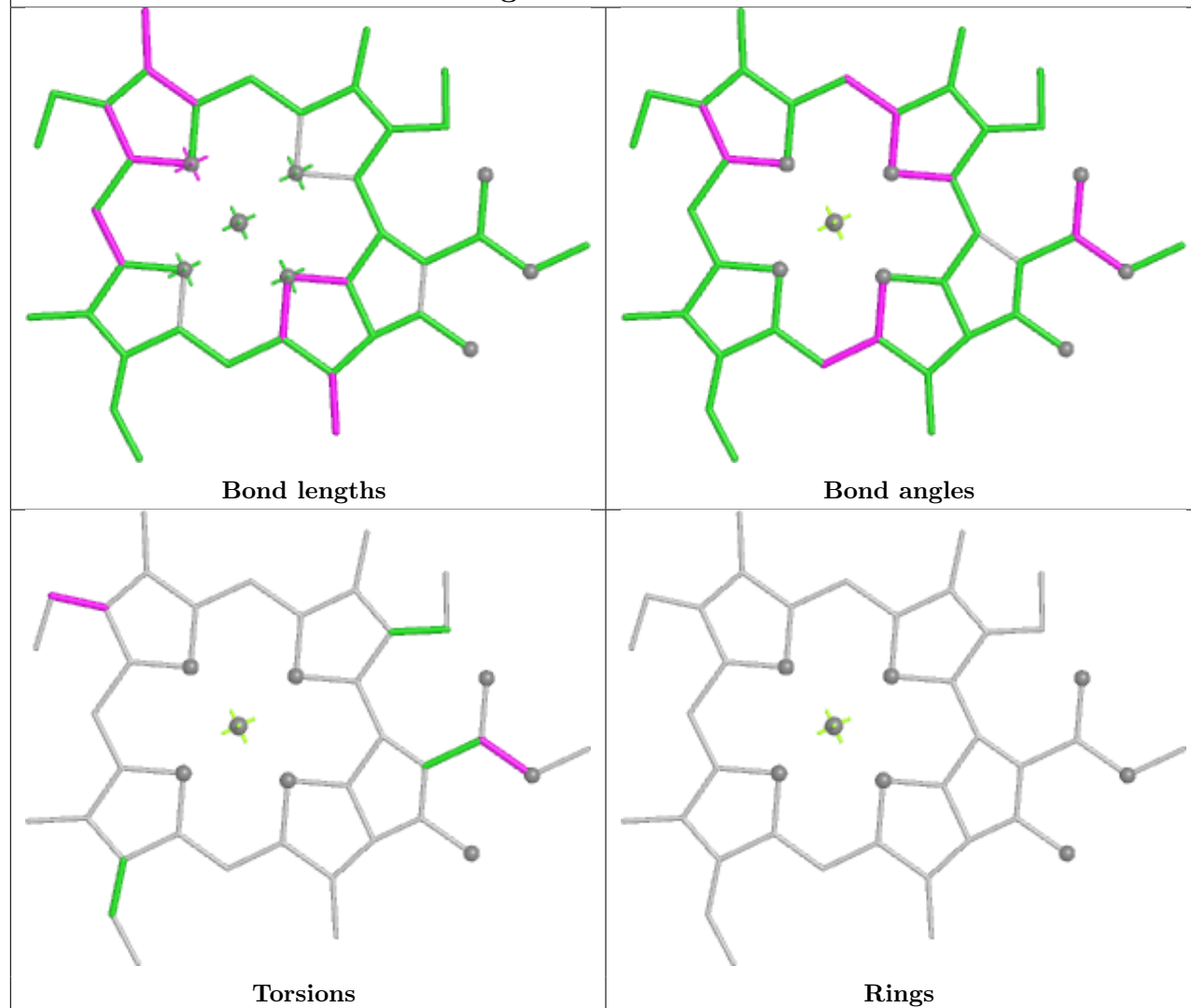


Torsions

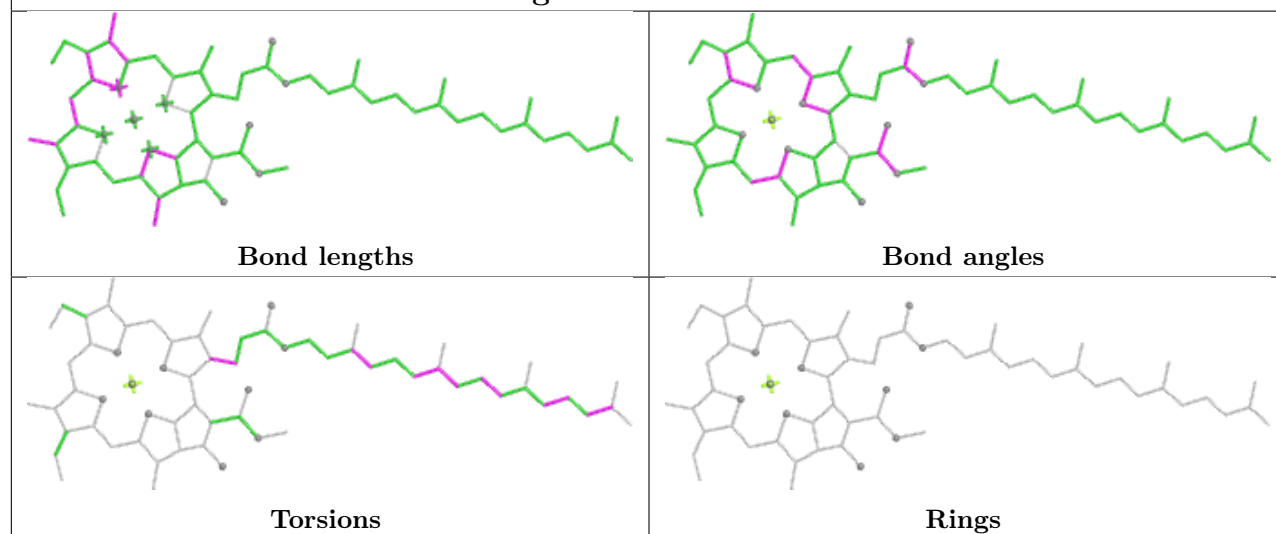


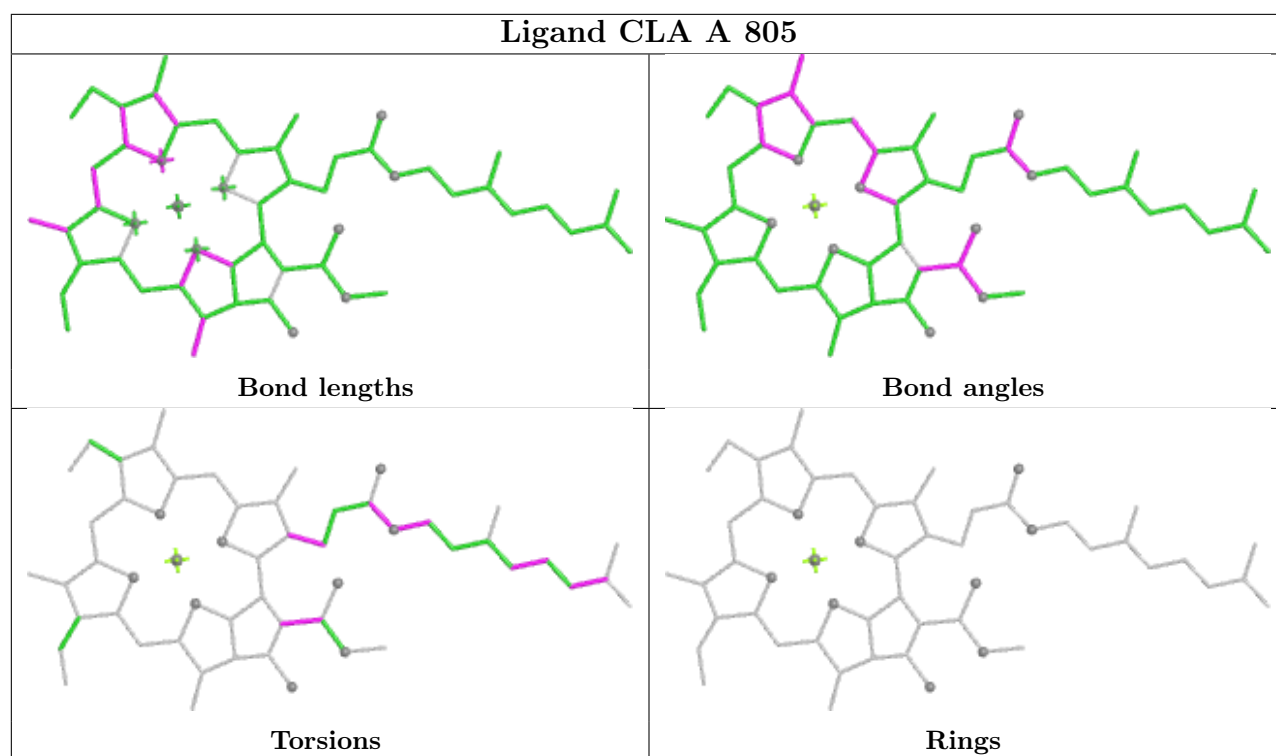
Rings

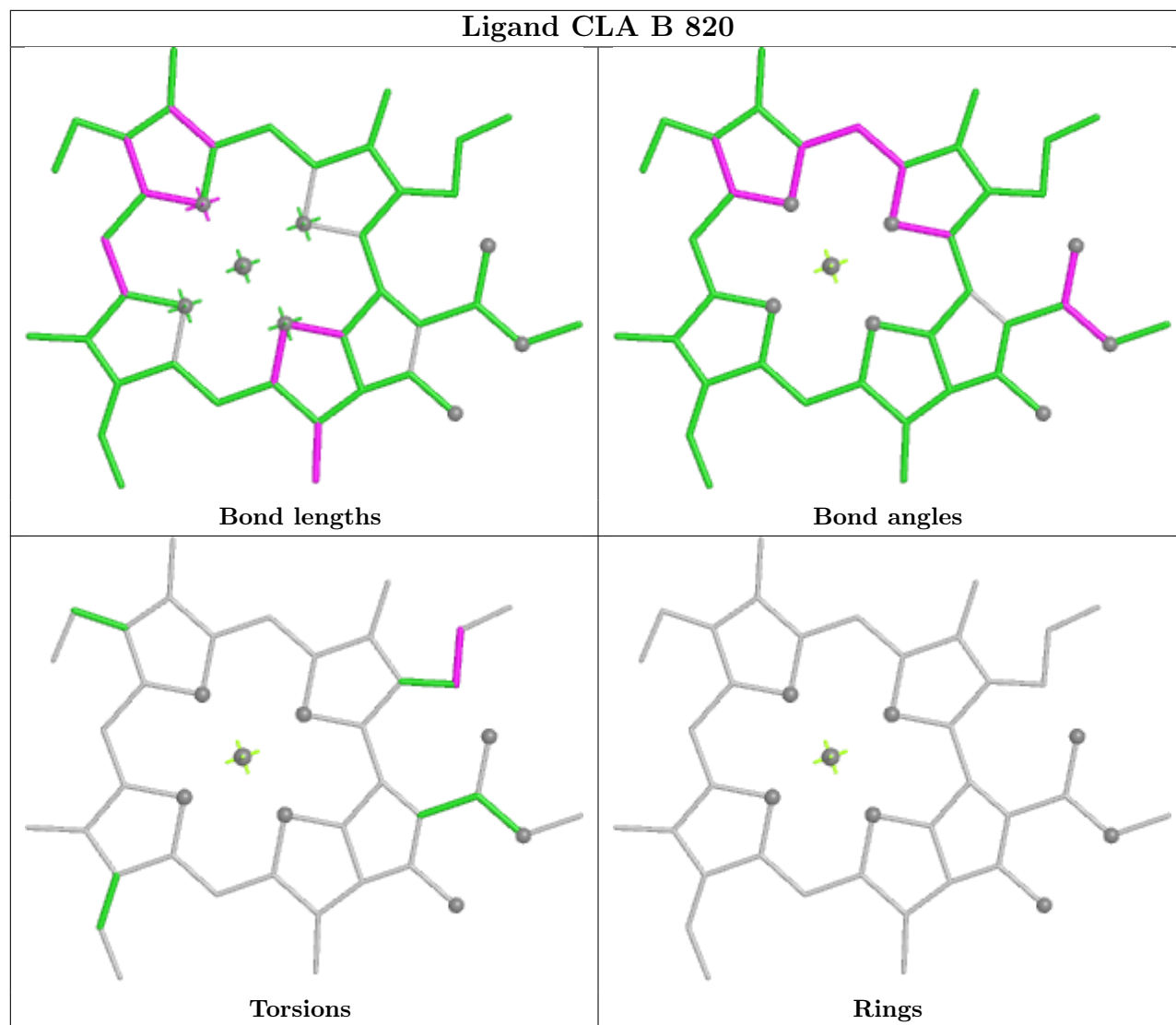
Ligand CLA 2 614

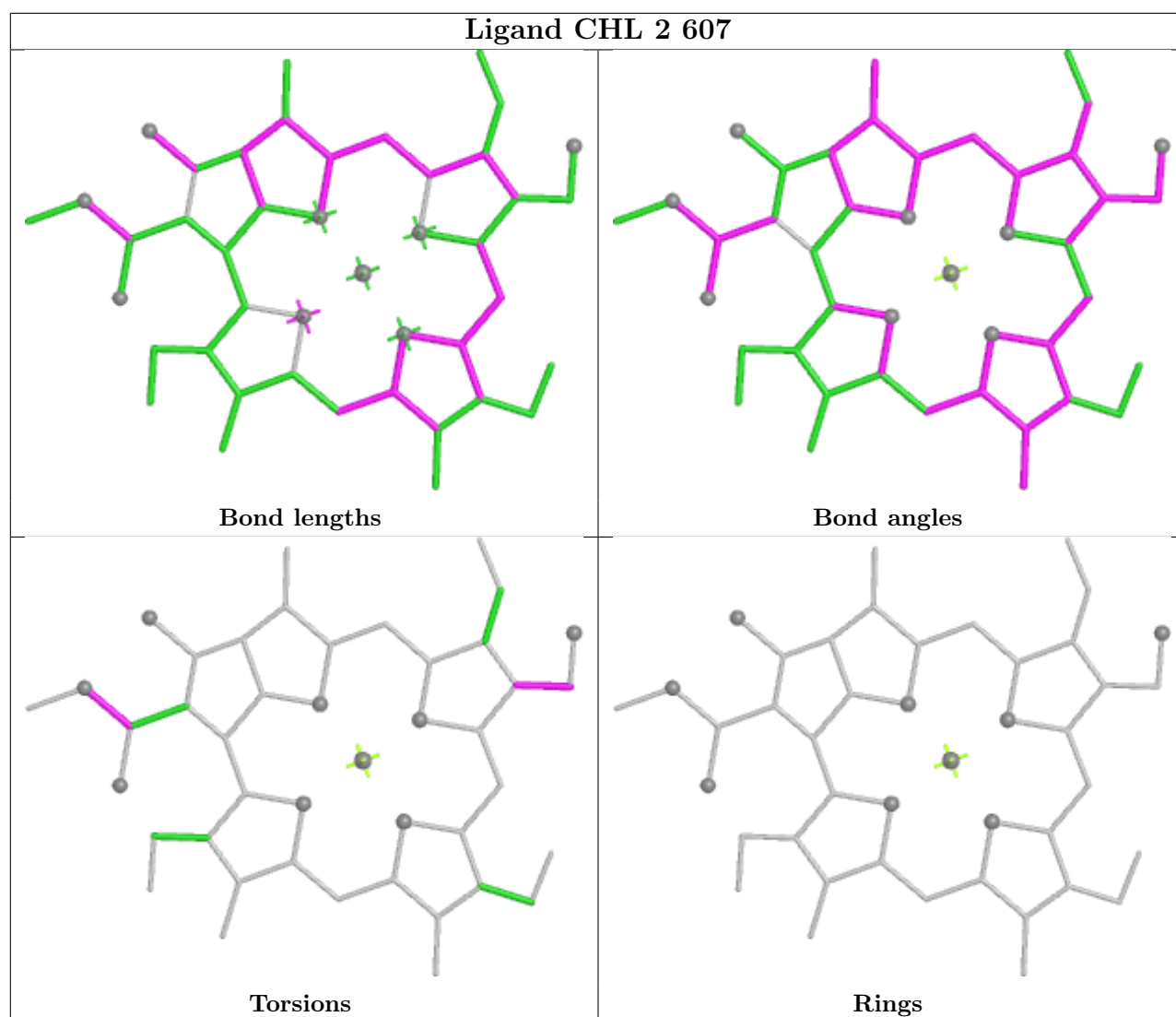


Ligand CLA B 825

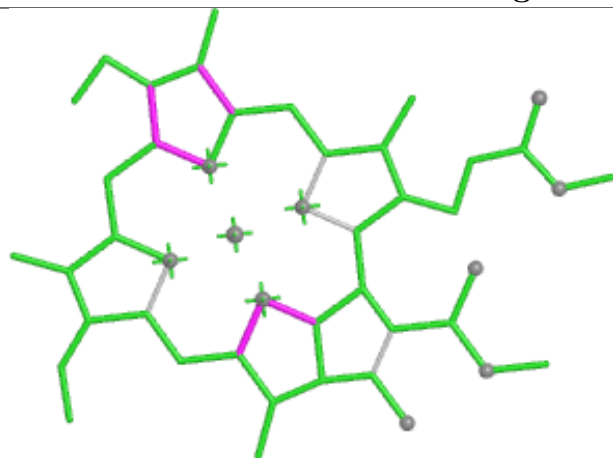




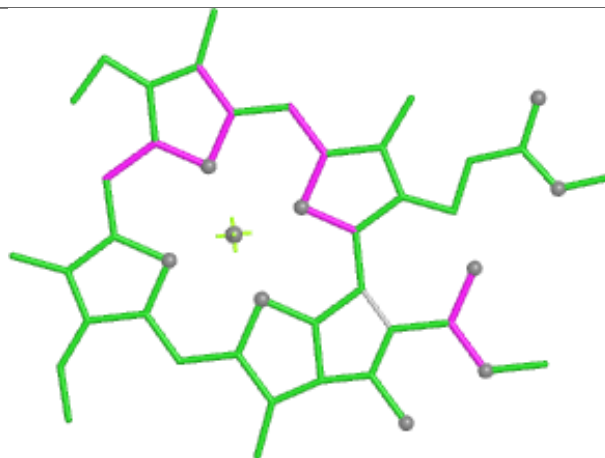




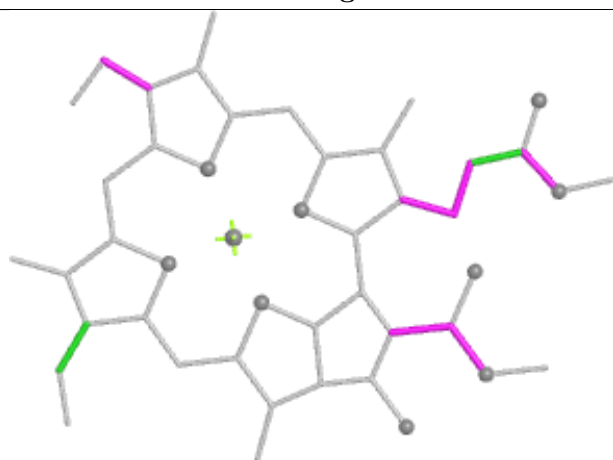
Ligand CLA K 201



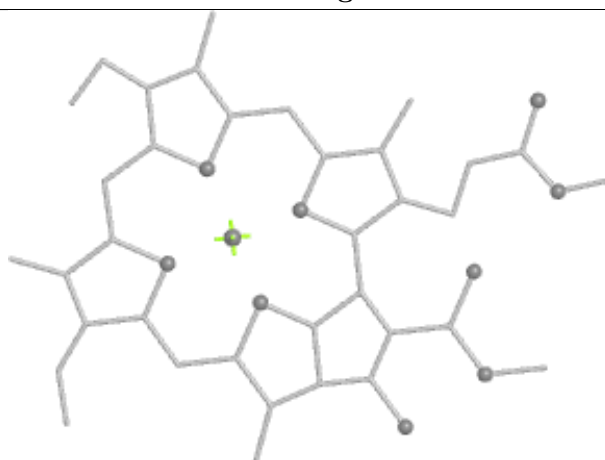
Bond lengths



Bond angles

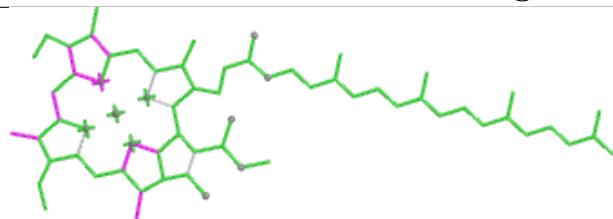


Torsions

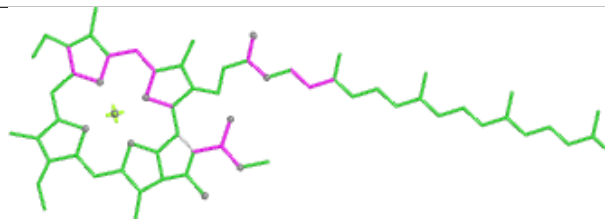


Rings

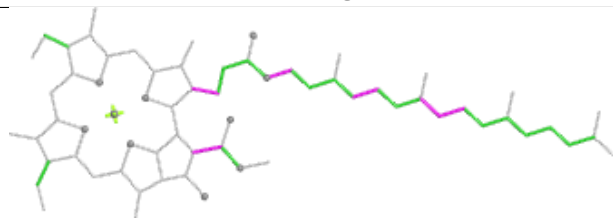
Ligand CLA A 804



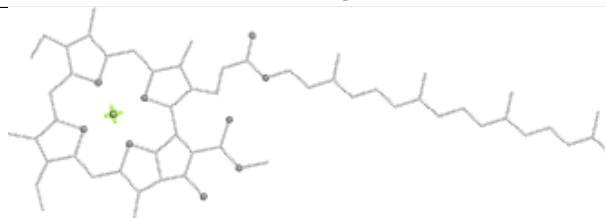
Bond lengths



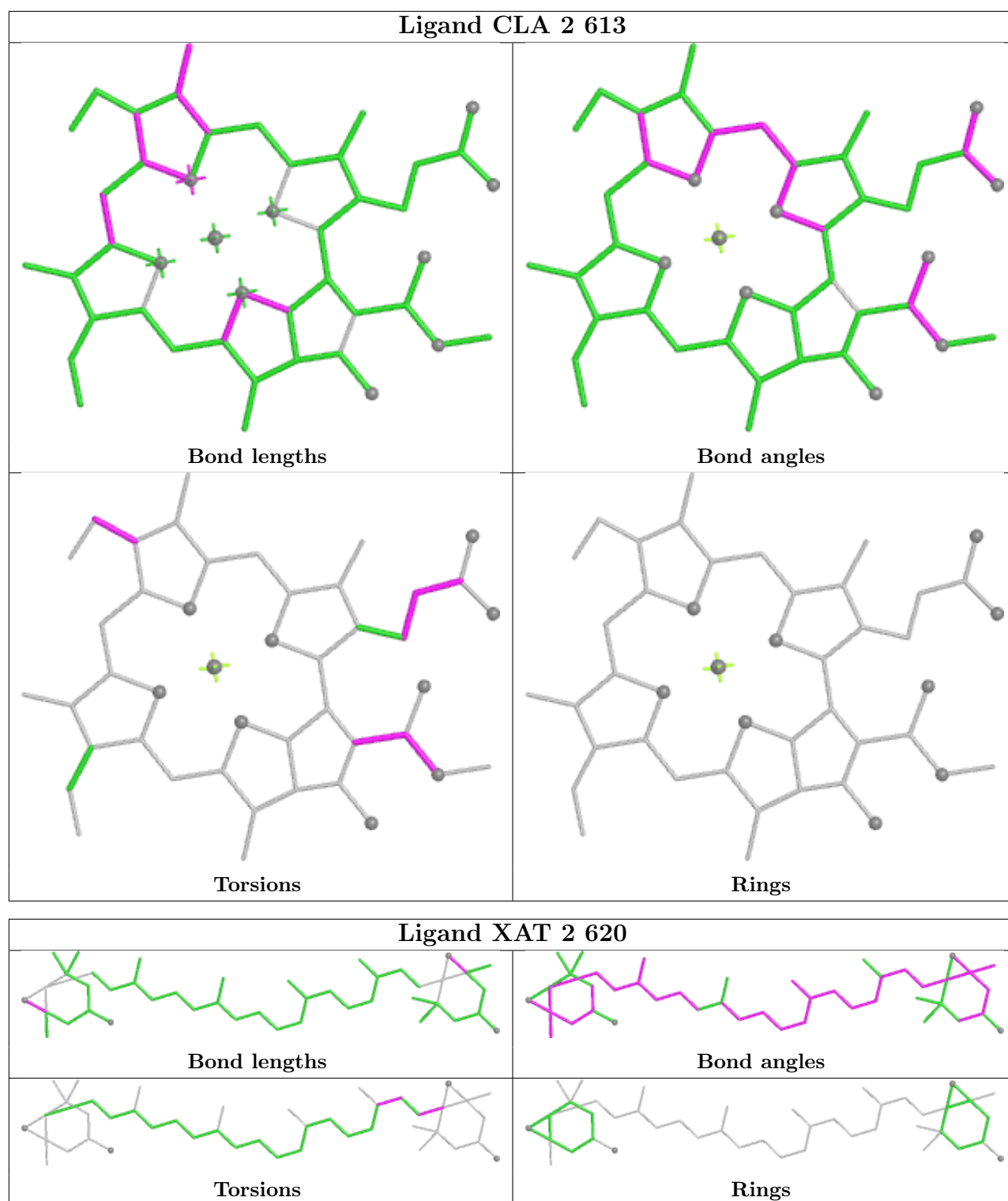
Bond angles



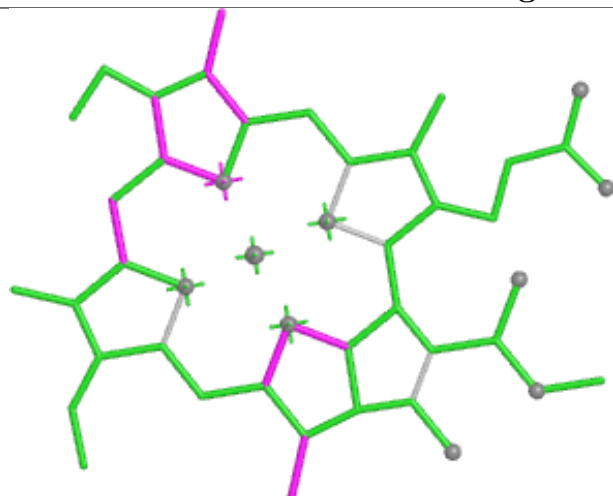
Torsions



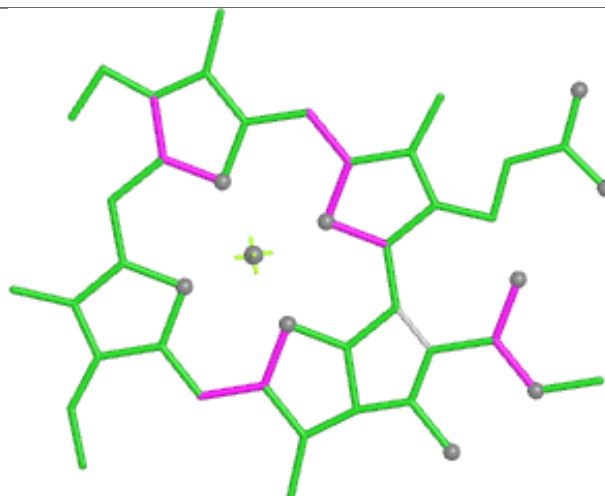
Rings



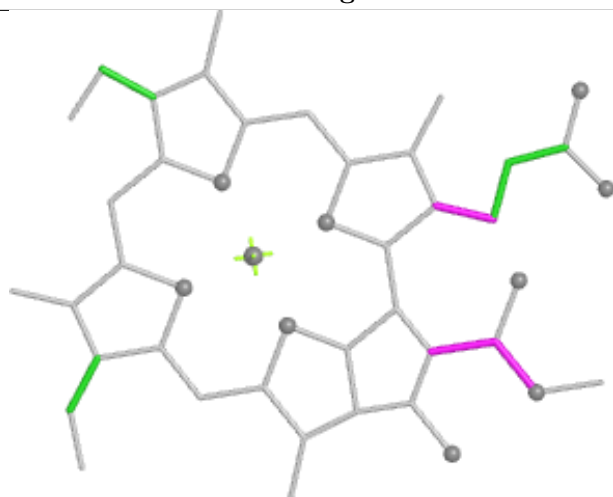
Ligand CLA 2 602



Bond lengths



Bond angles

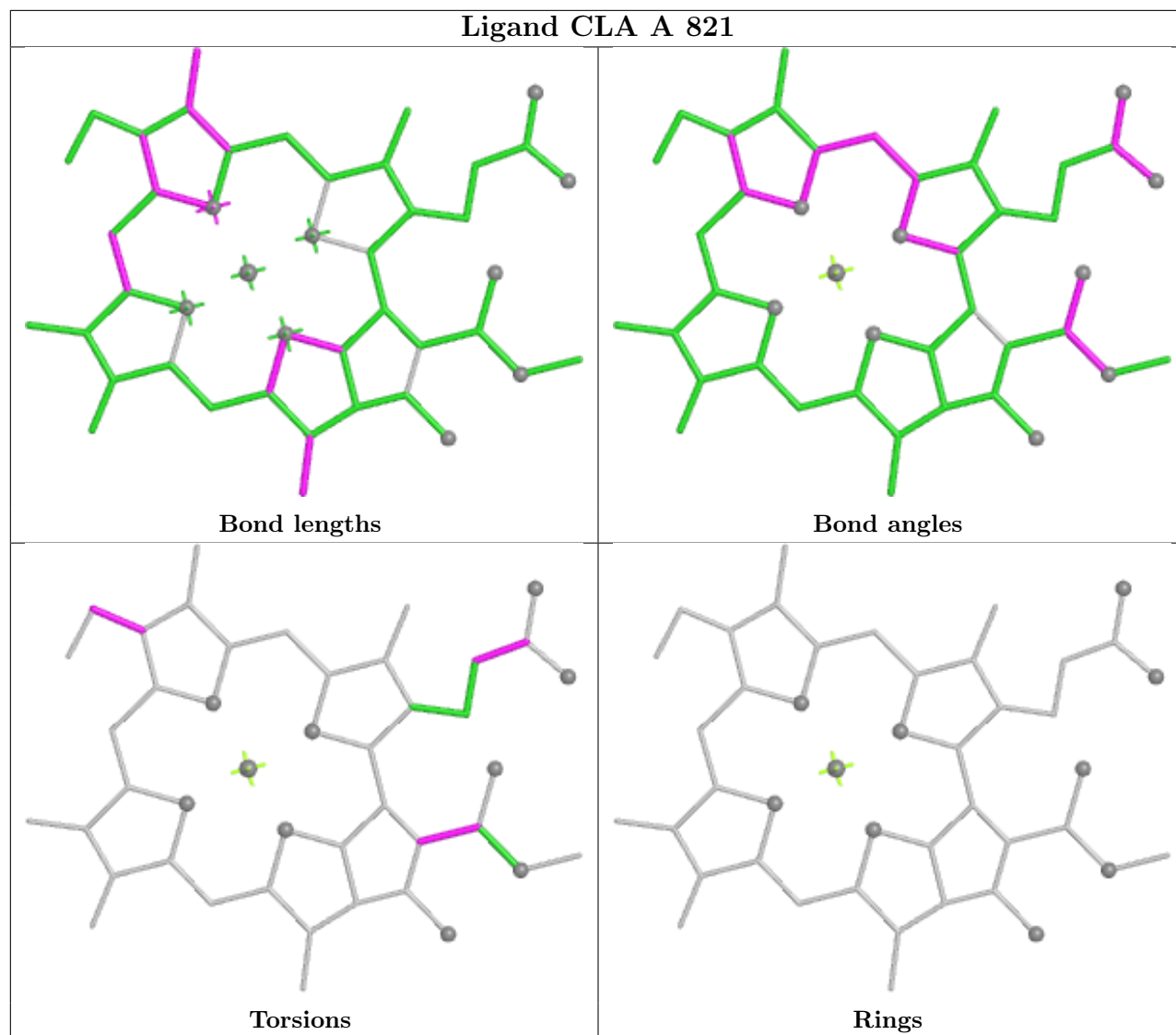


Torsions

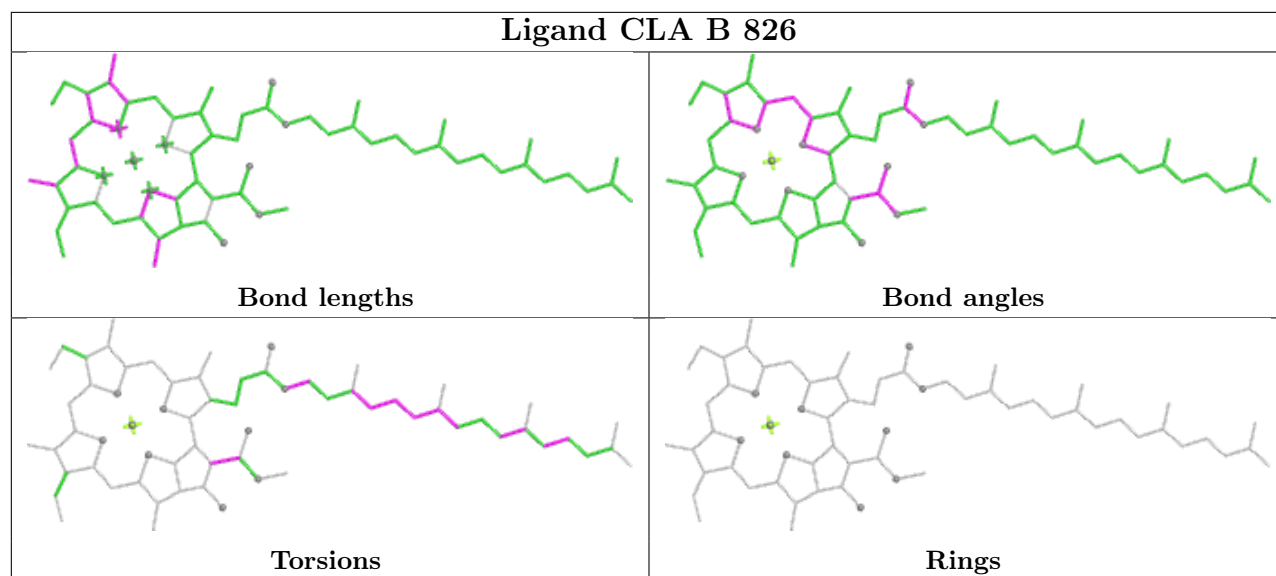


Rings

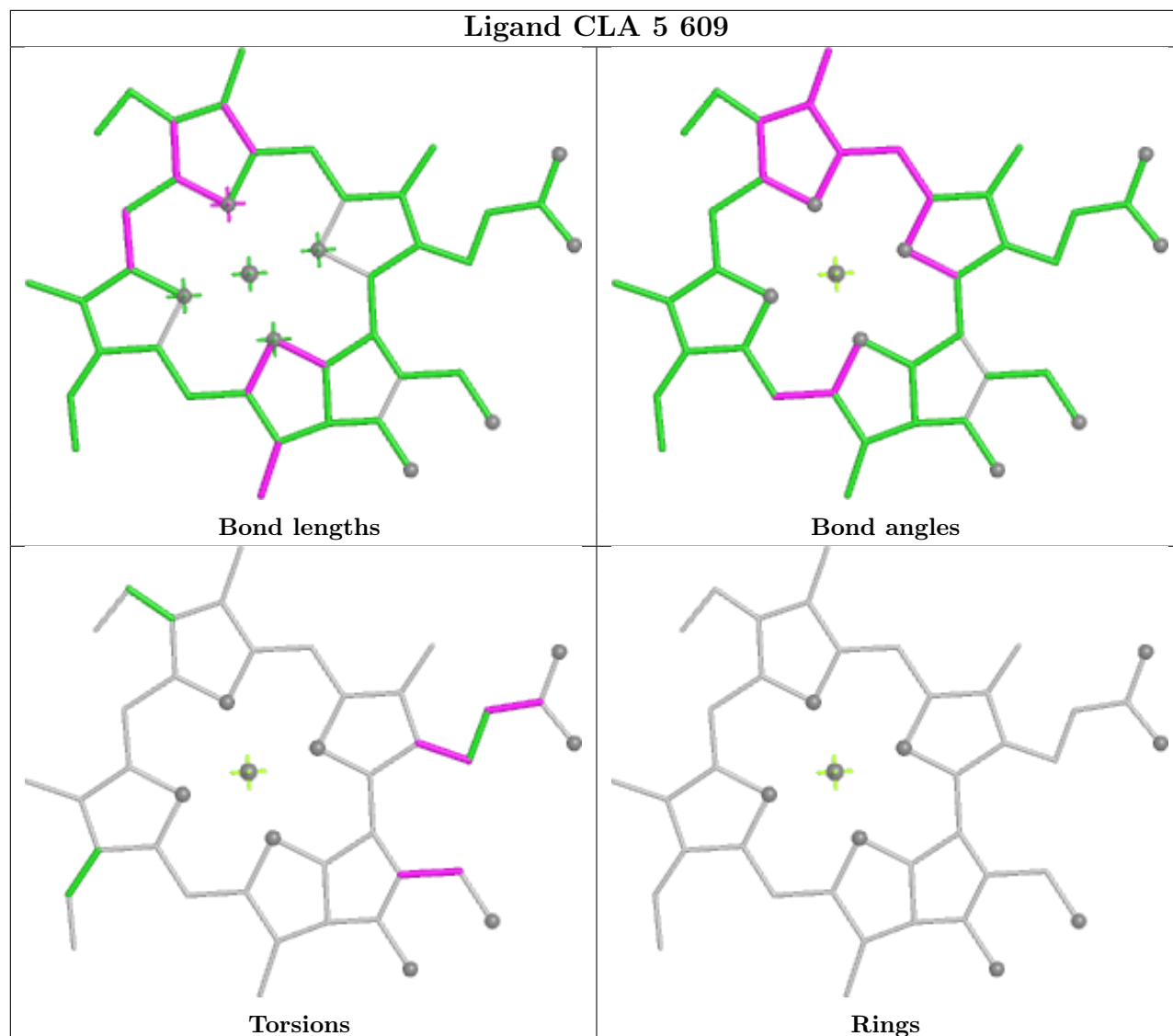
Ligand CLA A 821

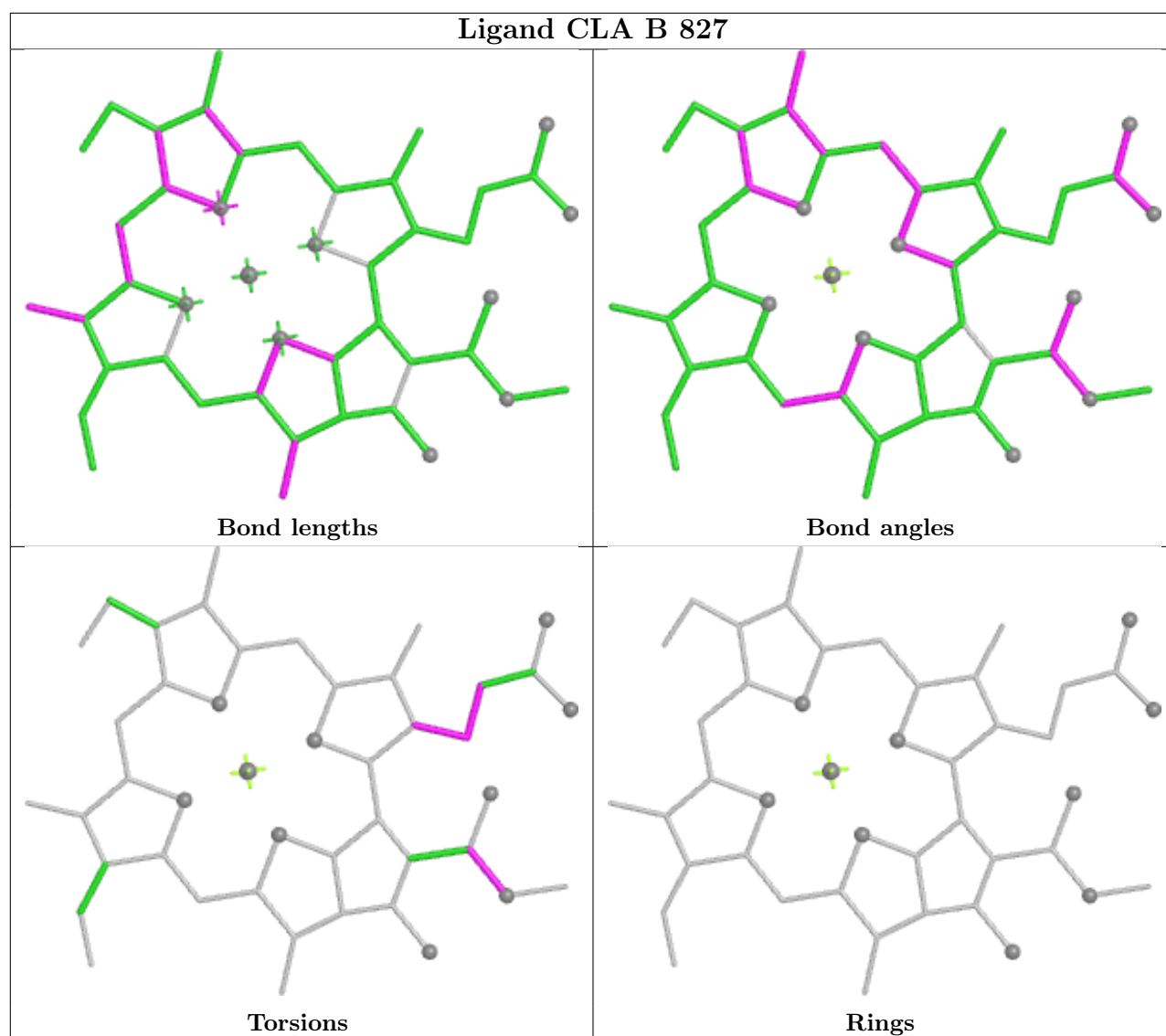


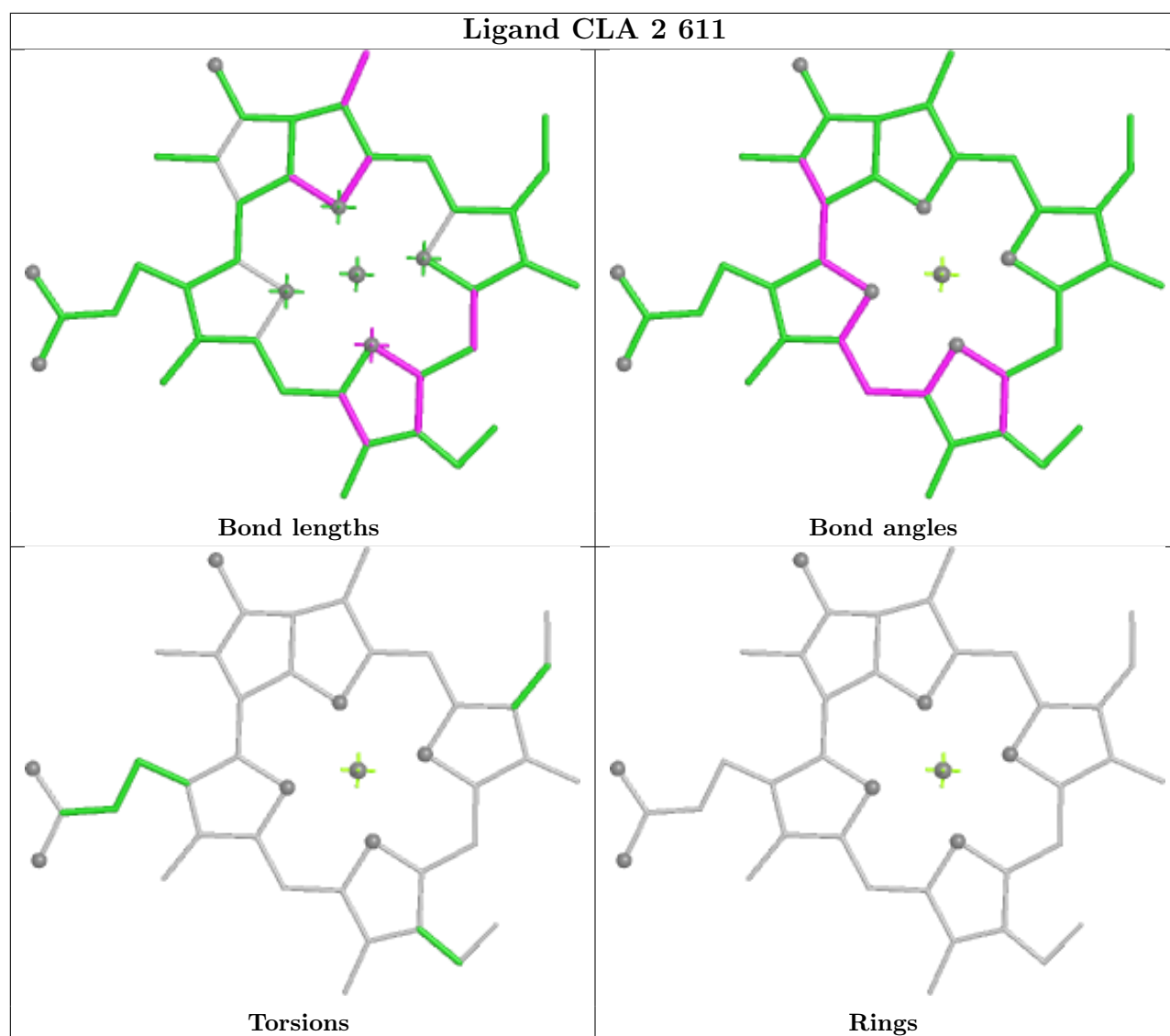
Ligand CLA B 826

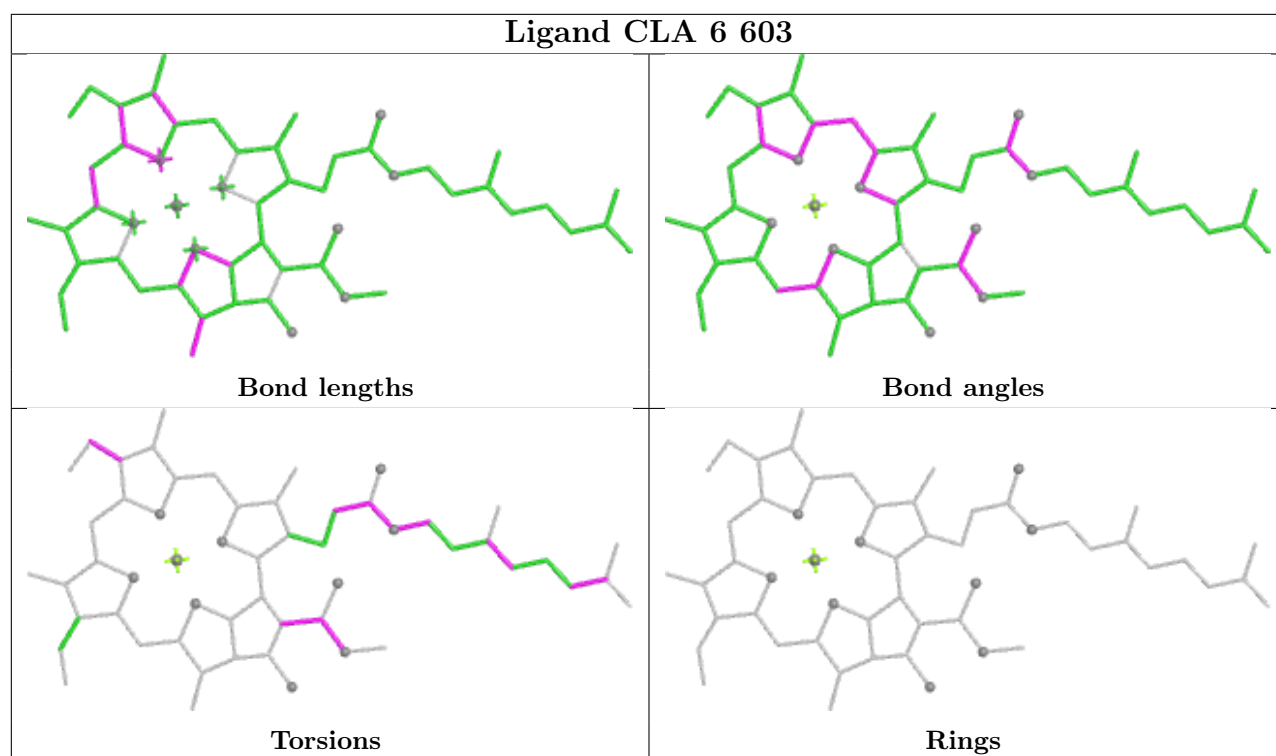


Ligand CLA 5 609

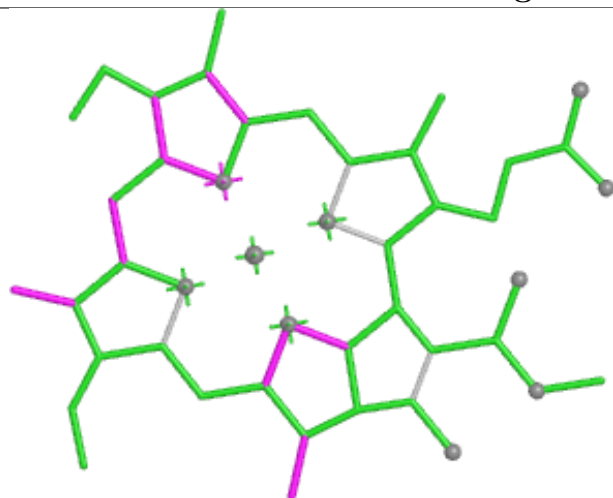




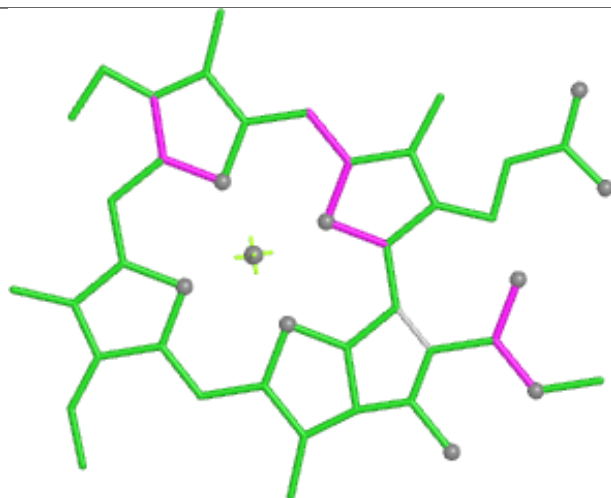




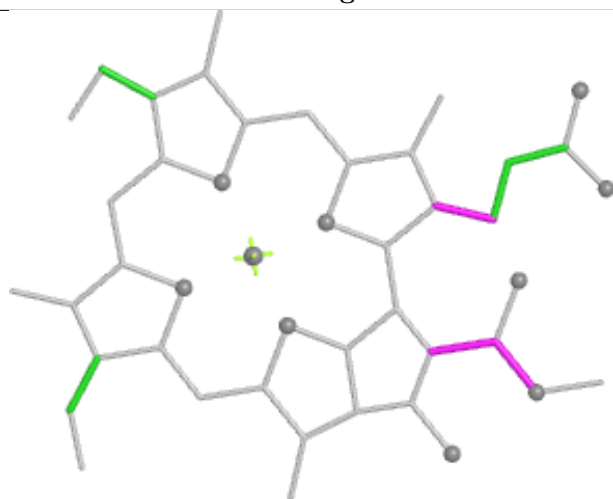
Ligand CLA B 823



Bond lengths



Bond angles

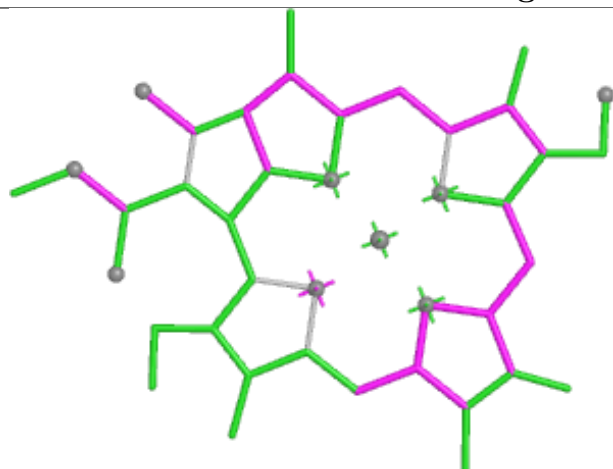


Torsions

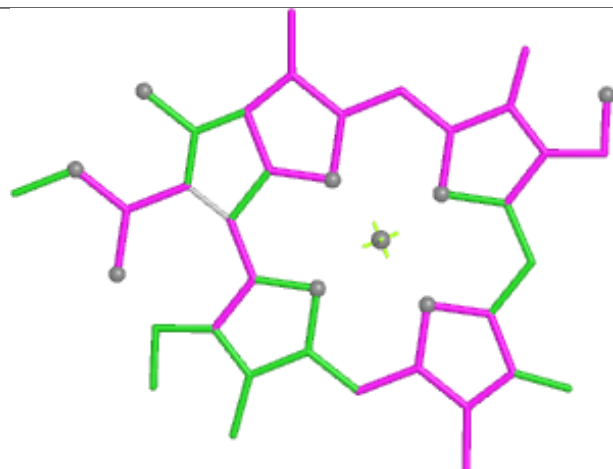


Rings

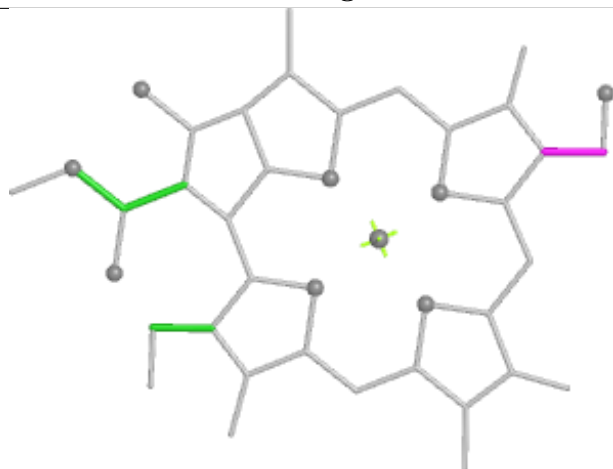
Ligand CHL 5 606



Bond lengths



Bond angles

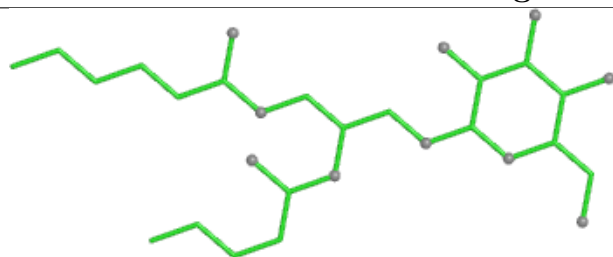


Torsions

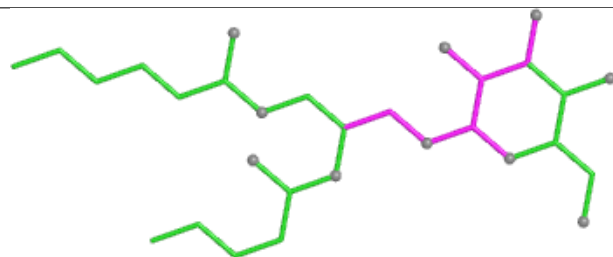


Rings

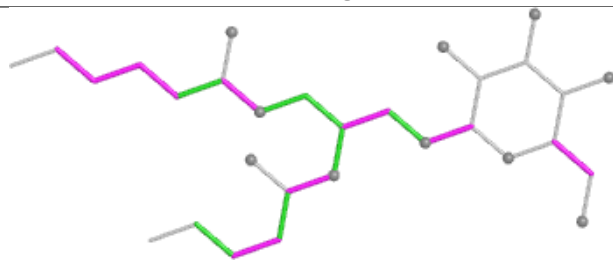
Ligand LMG J 104



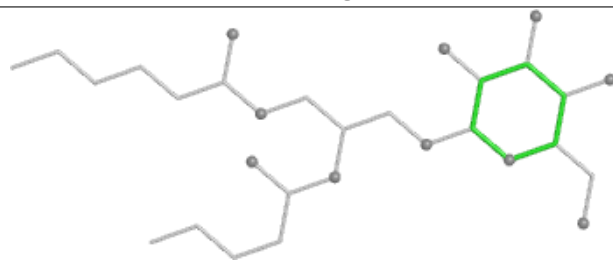
Bond lengths



Bond angles

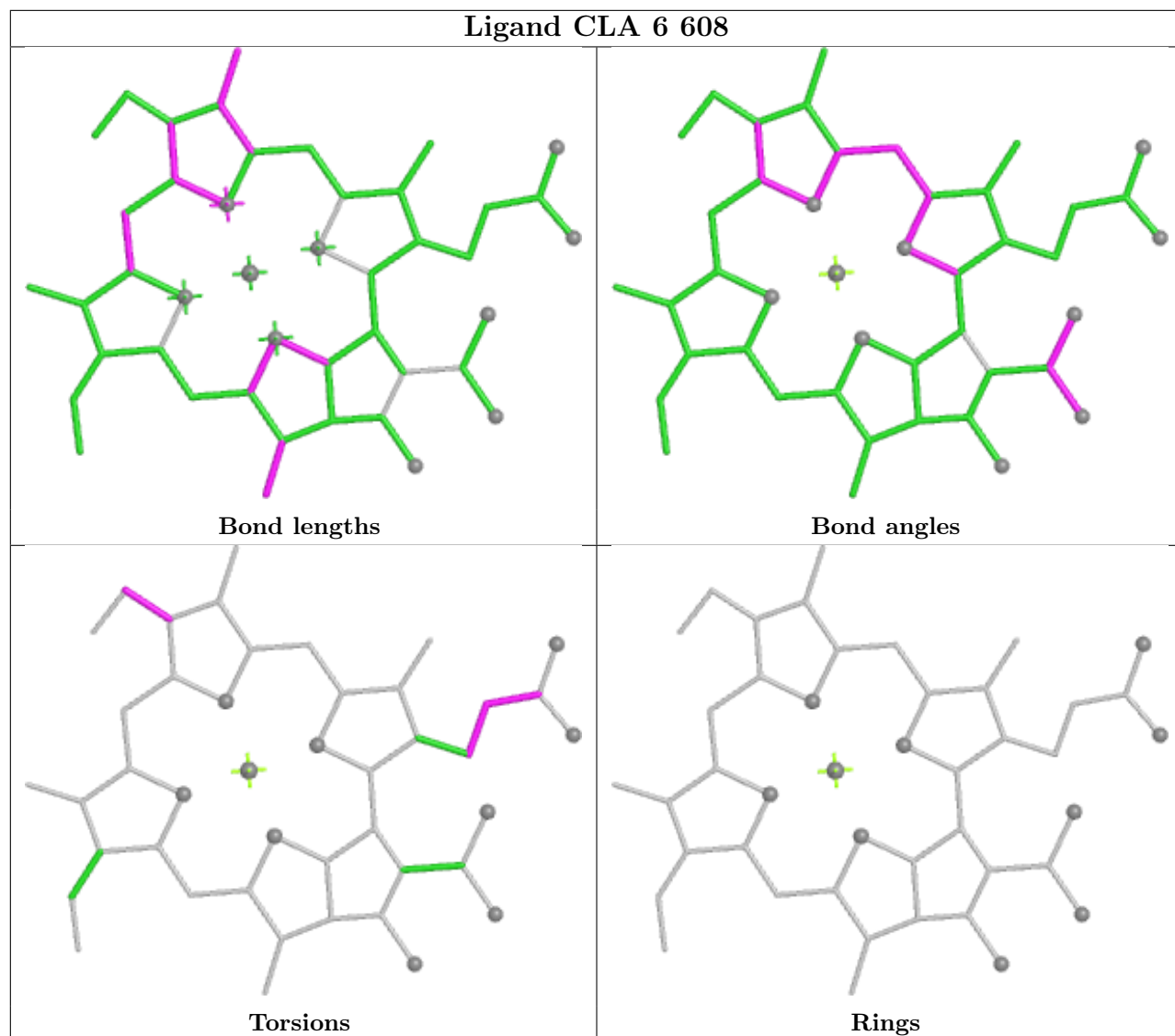


Torsions

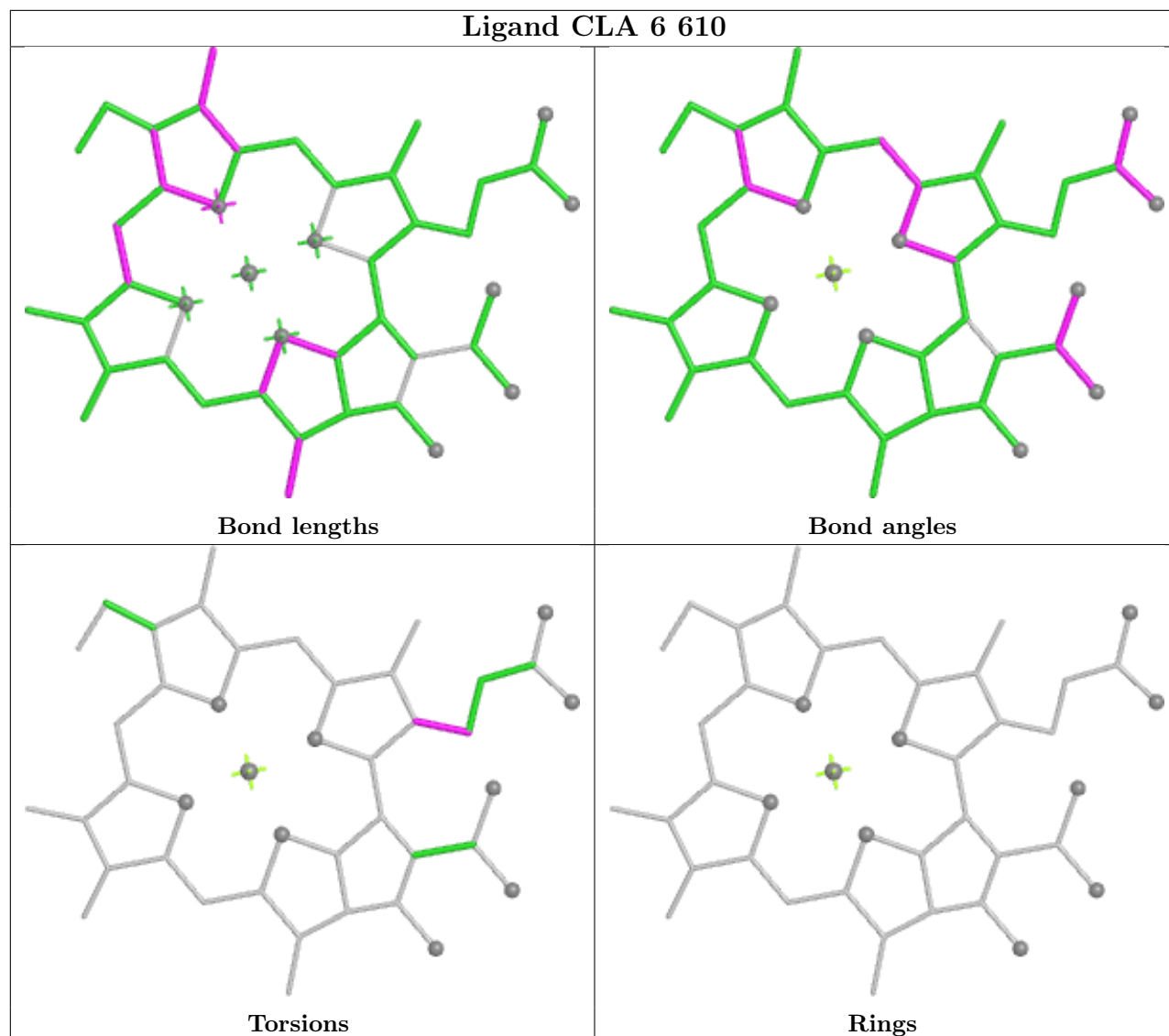


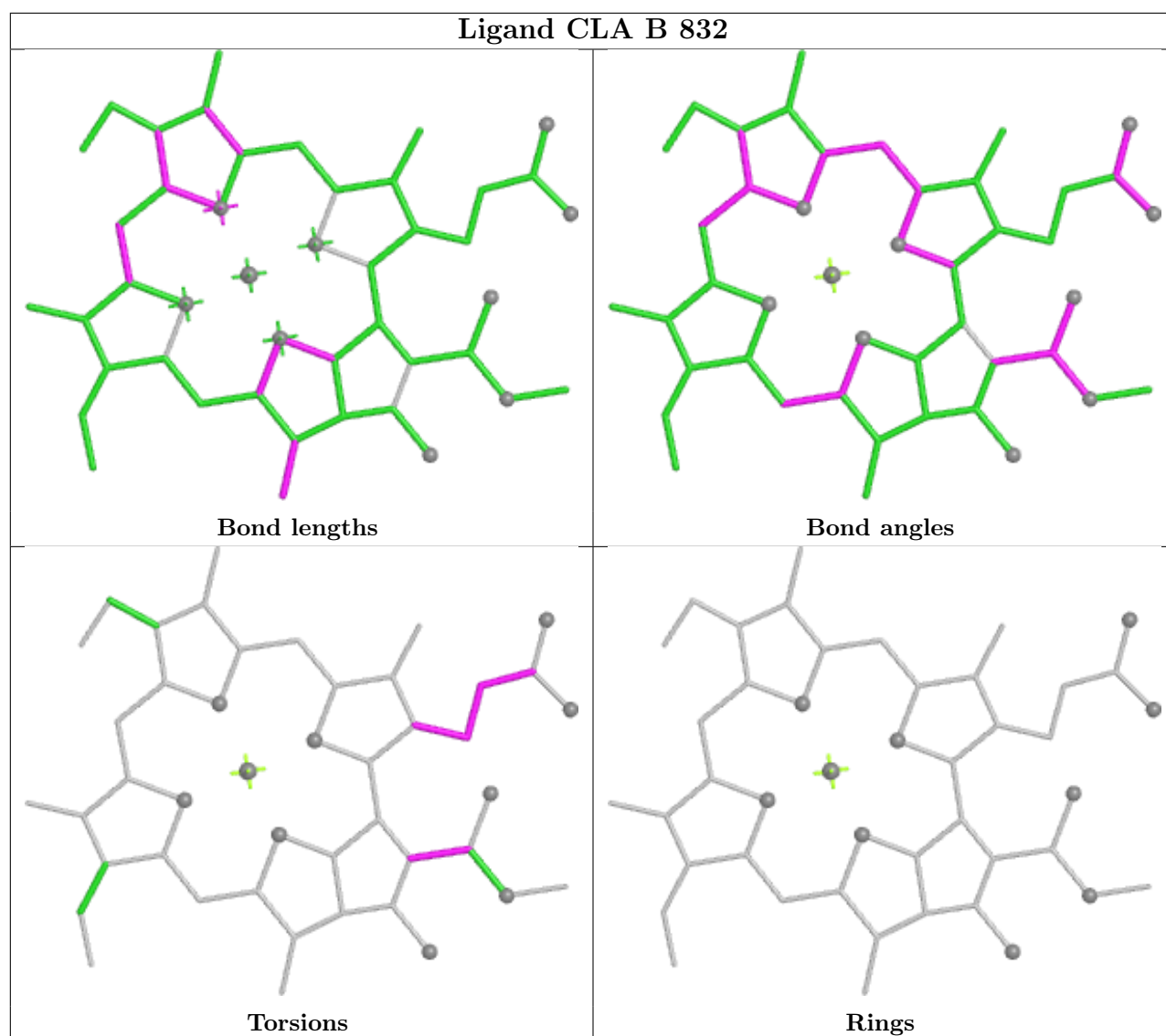
Rings

Ligand CLA 6 608

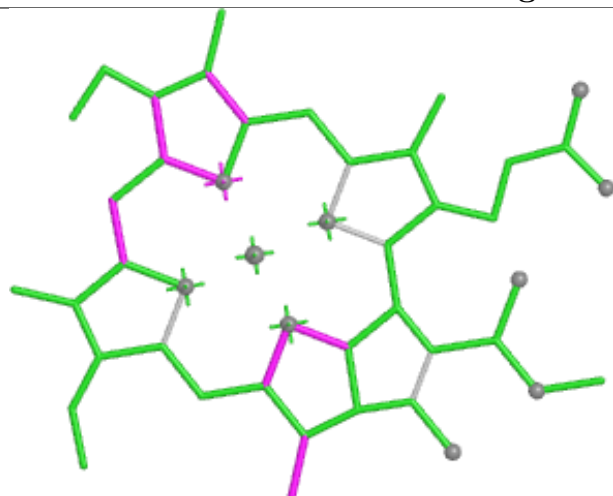


Ligand CLA 6 610

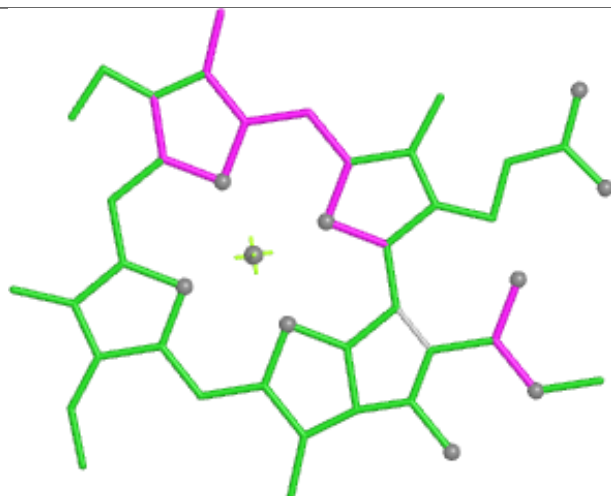




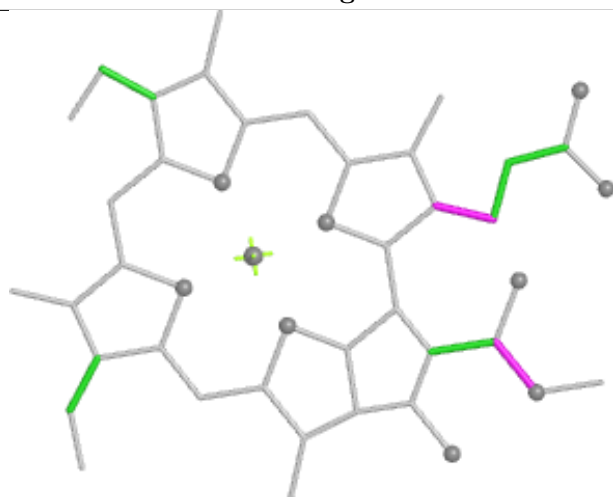
Ligand CLA 2 610



Bond lengths



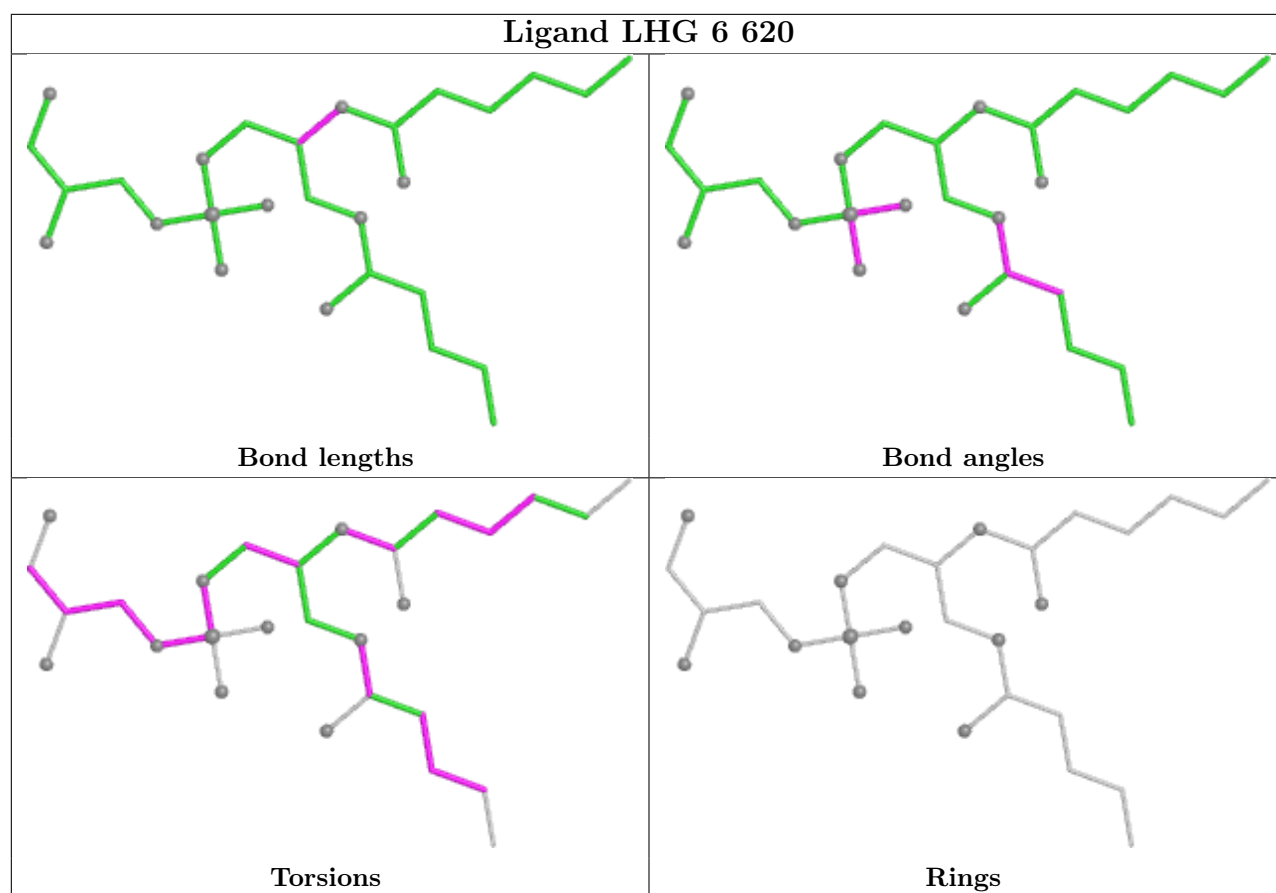
Bond angles



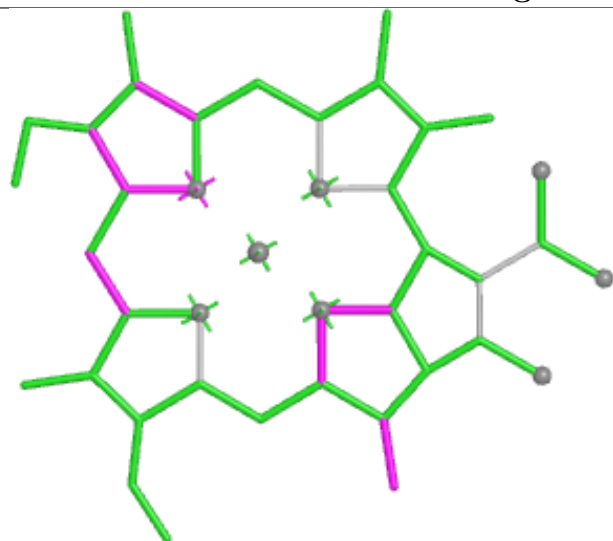
Torsions



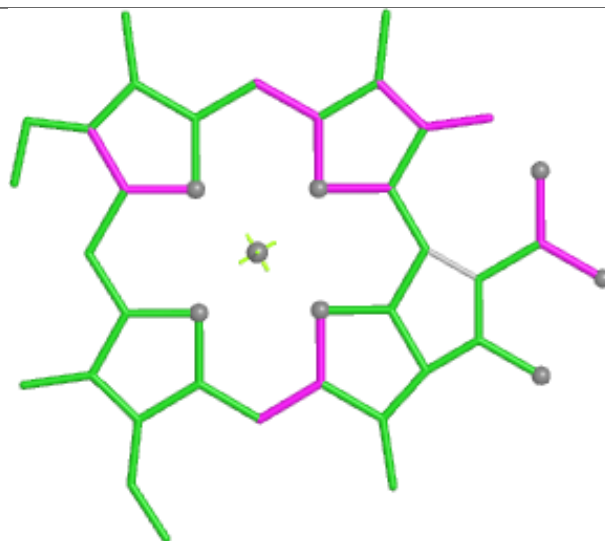
Rings



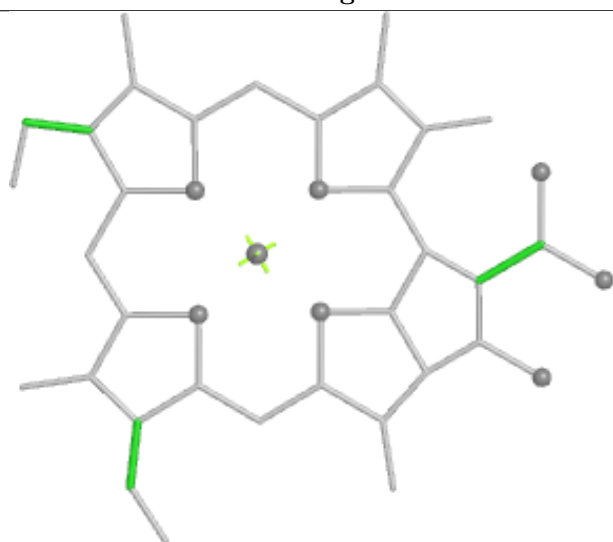
Ligand CLA A 817



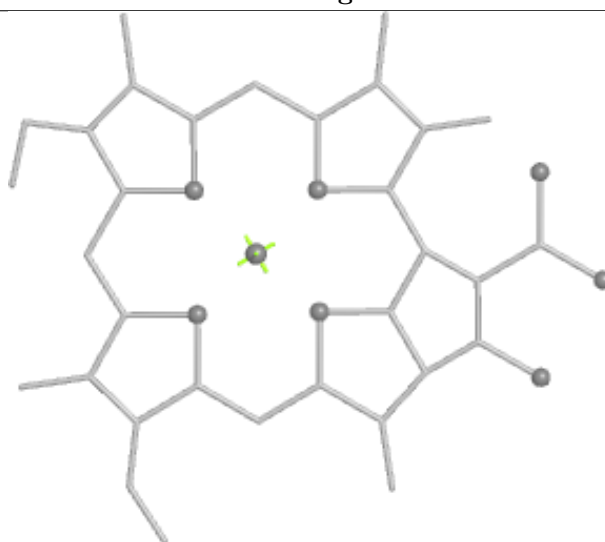
Bond lengths



Bond angles



Torsions



Rings

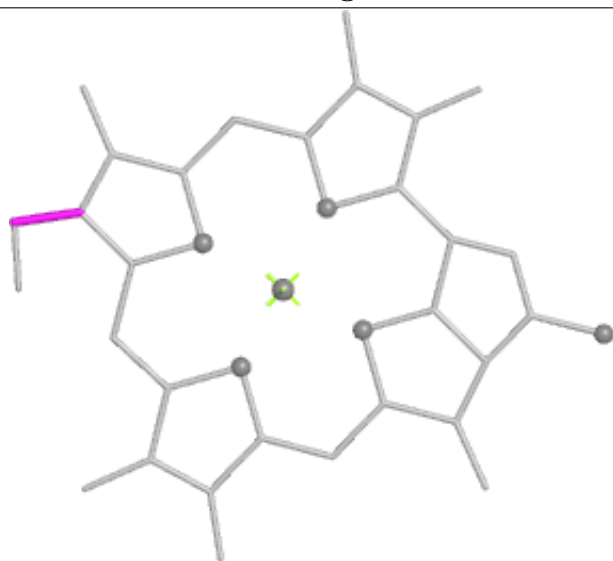
Ligand CLA 3 615



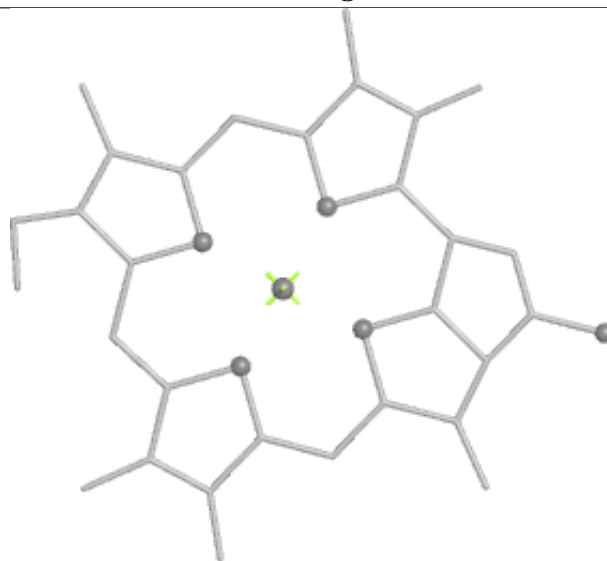
Bond lengths



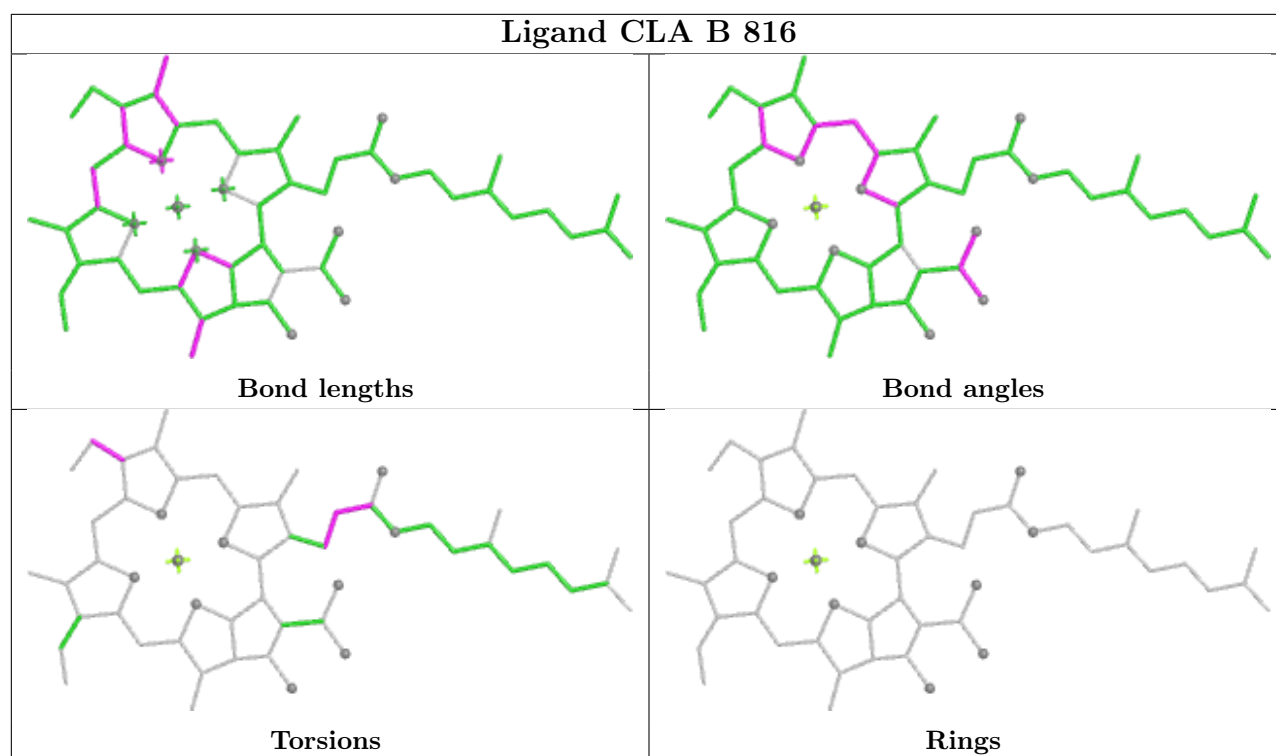
Bond angles



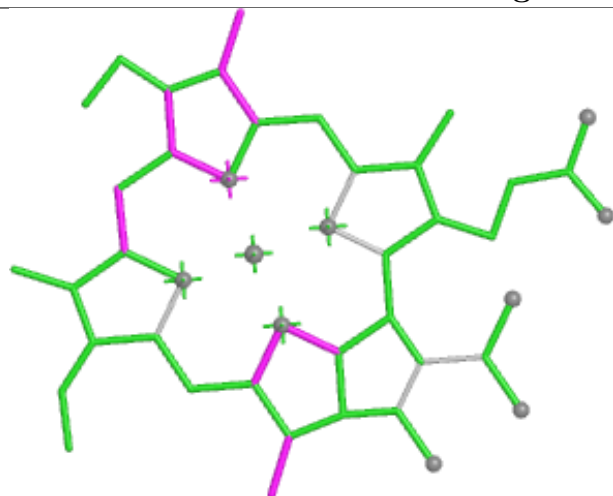
Torsions



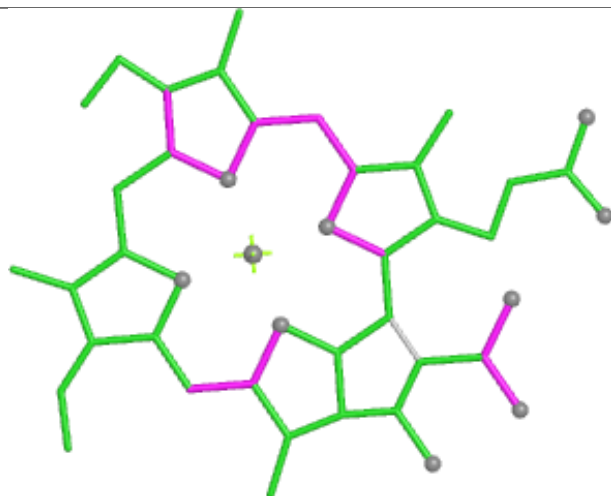
Rings



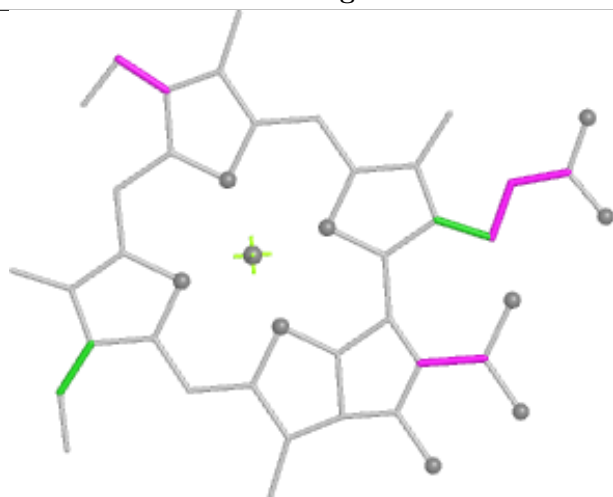
Ligand CLA G 204



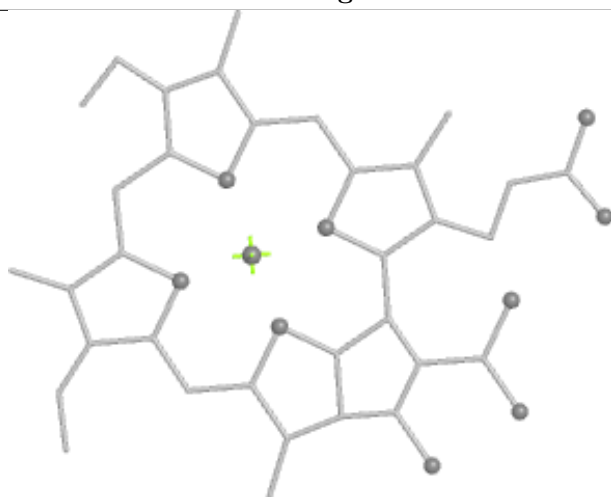
Bond lengths



Bond angles

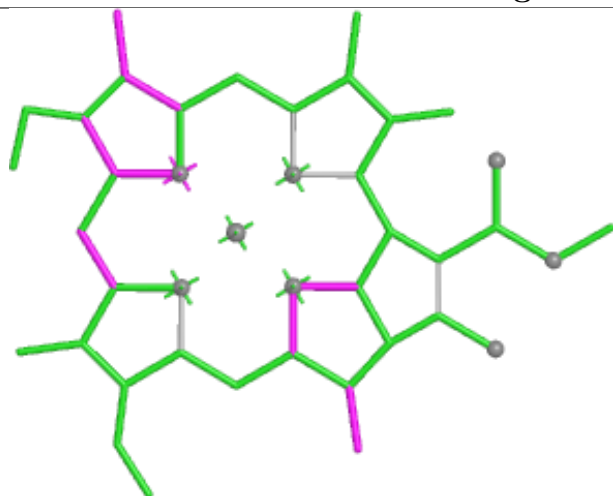


Torsions

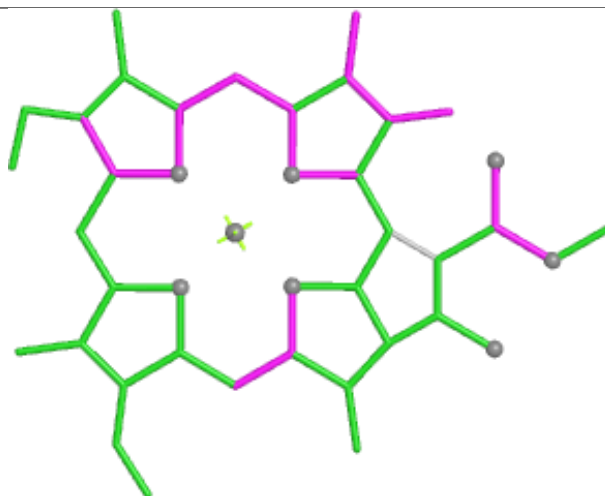


Rings

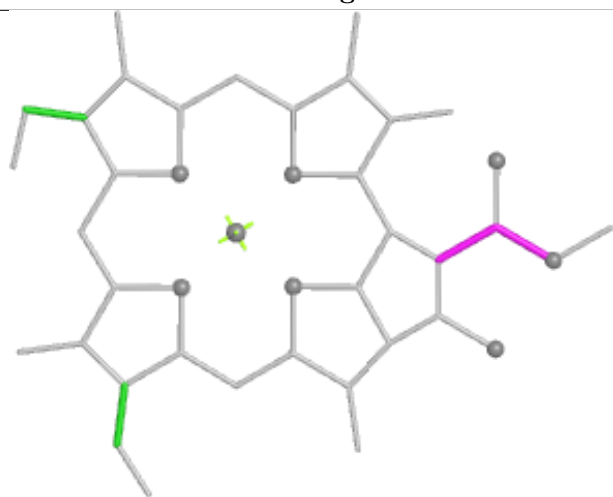
Ligand CLA A 832



Bond lengths



Bond angles

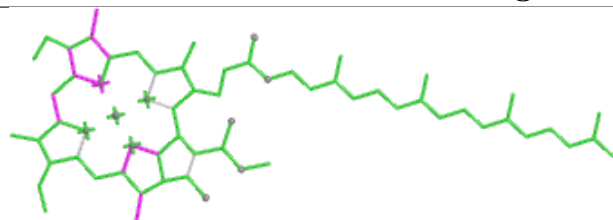


Torsions

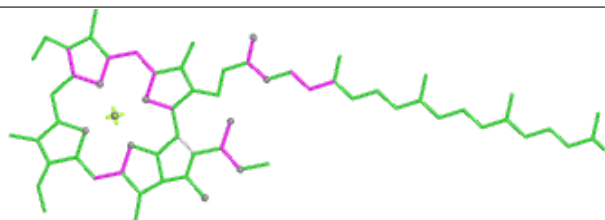


Rings

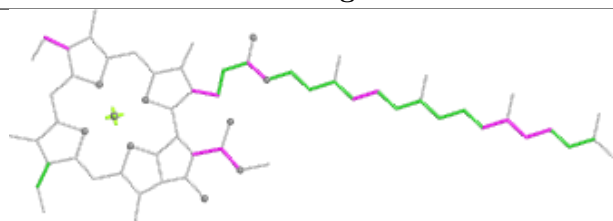
Ligand CLA B 841



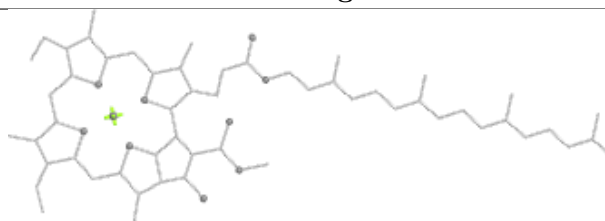
Bond lengths



Bond angles

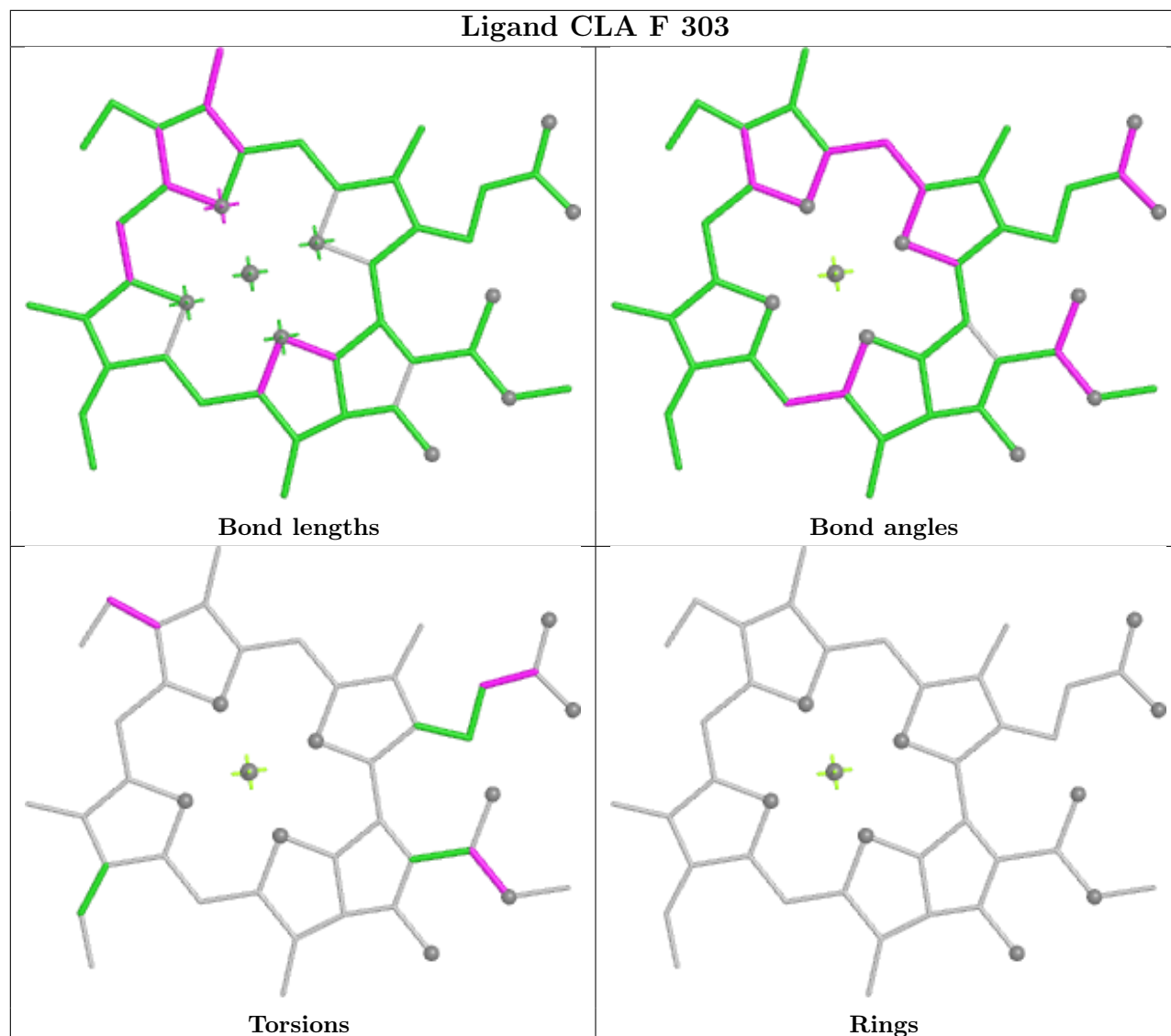


Torsions

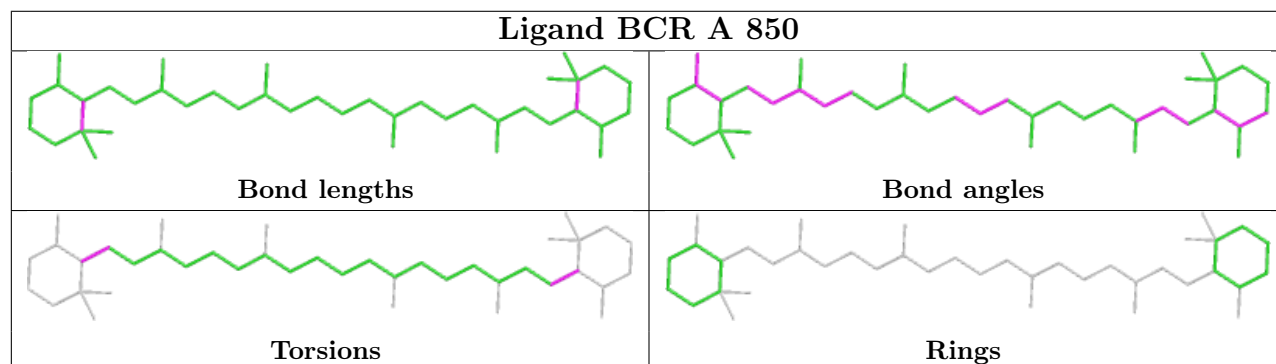


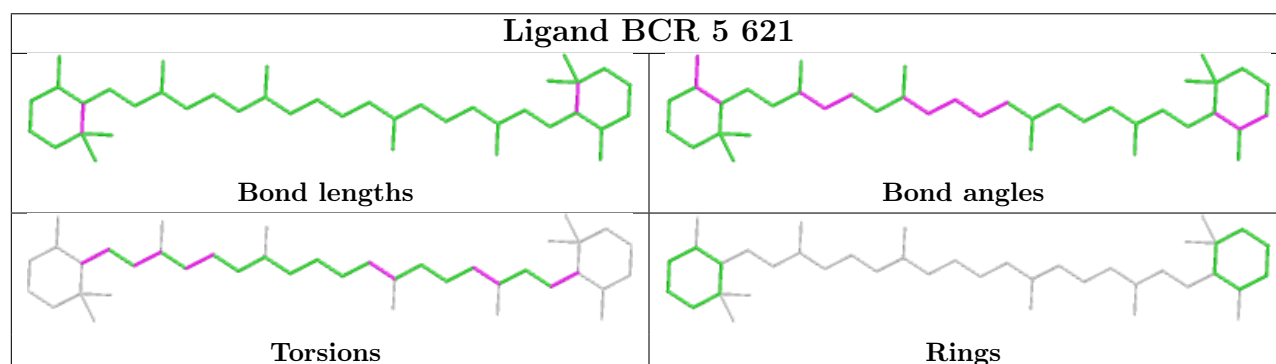
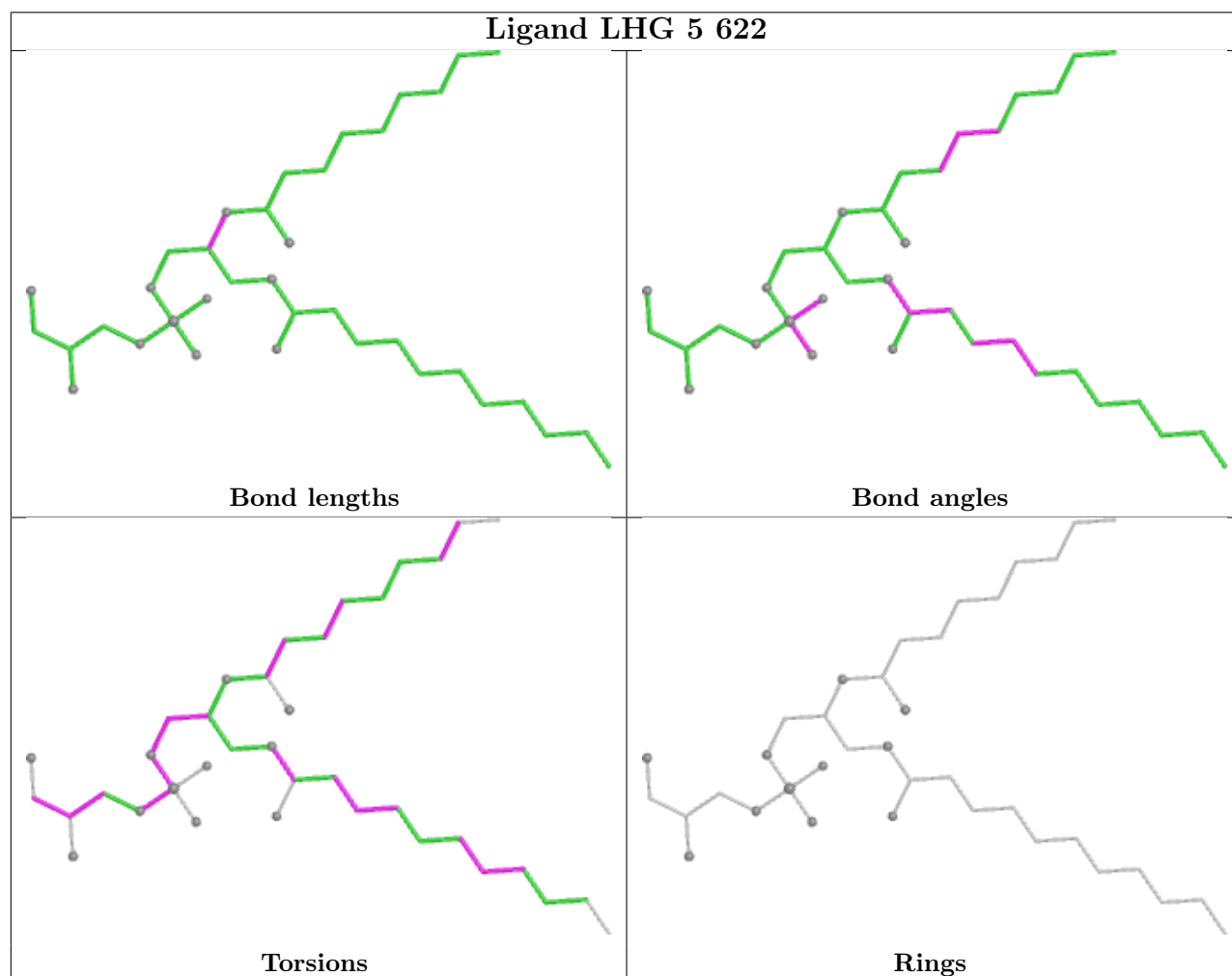
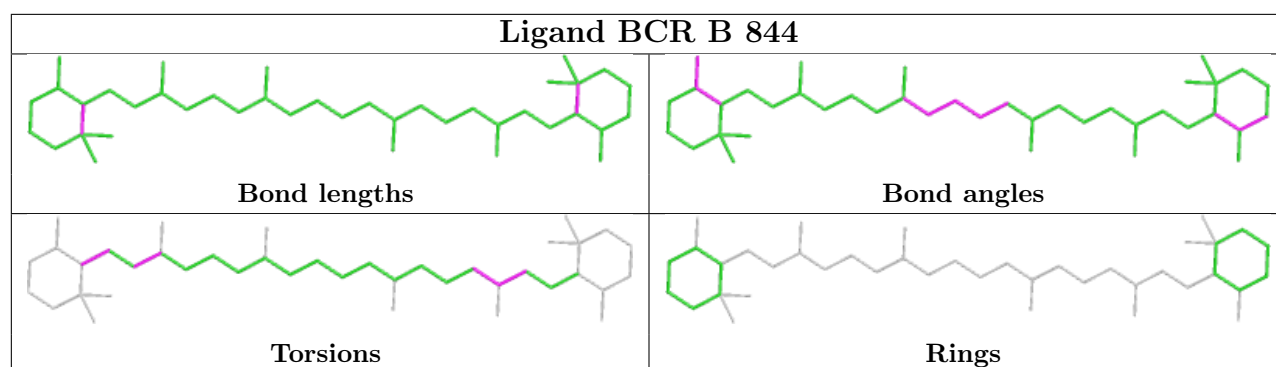
Rings

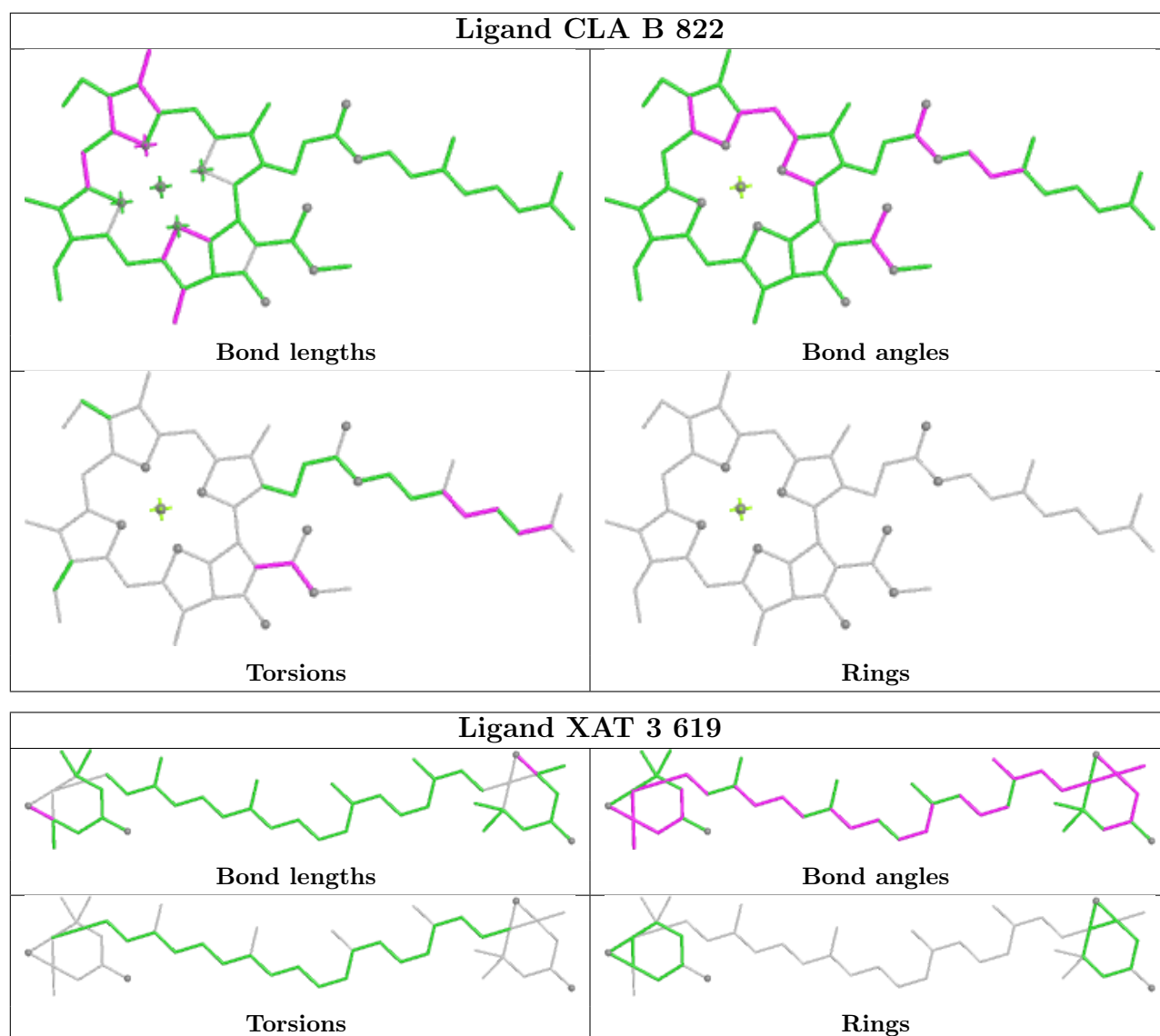
Ligand CLA F 303



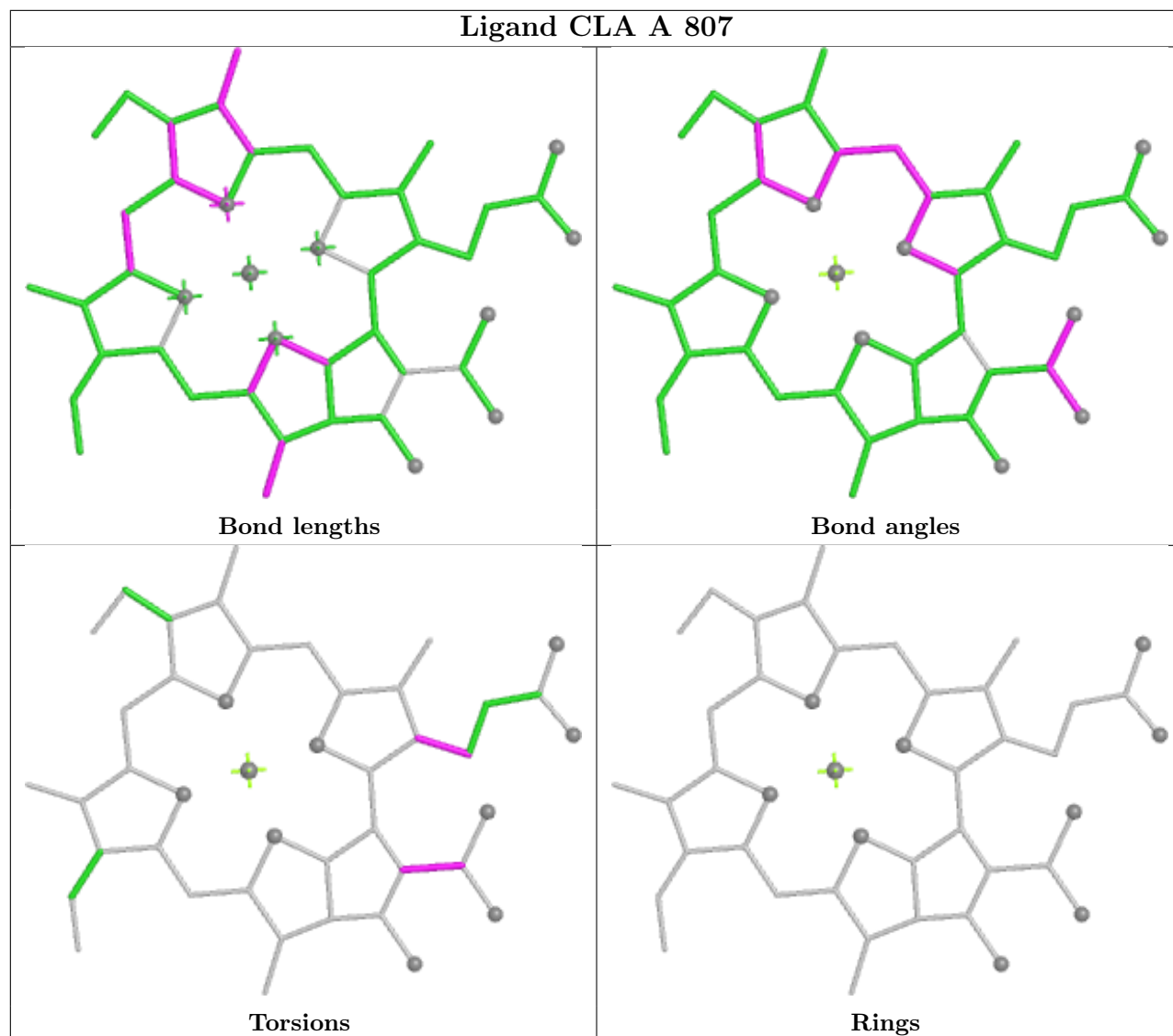
Ligand BCR A 850



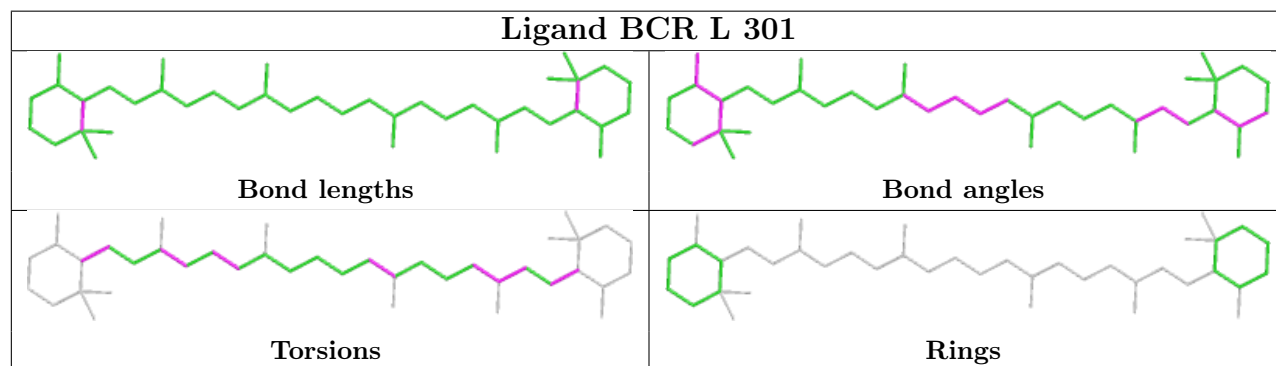


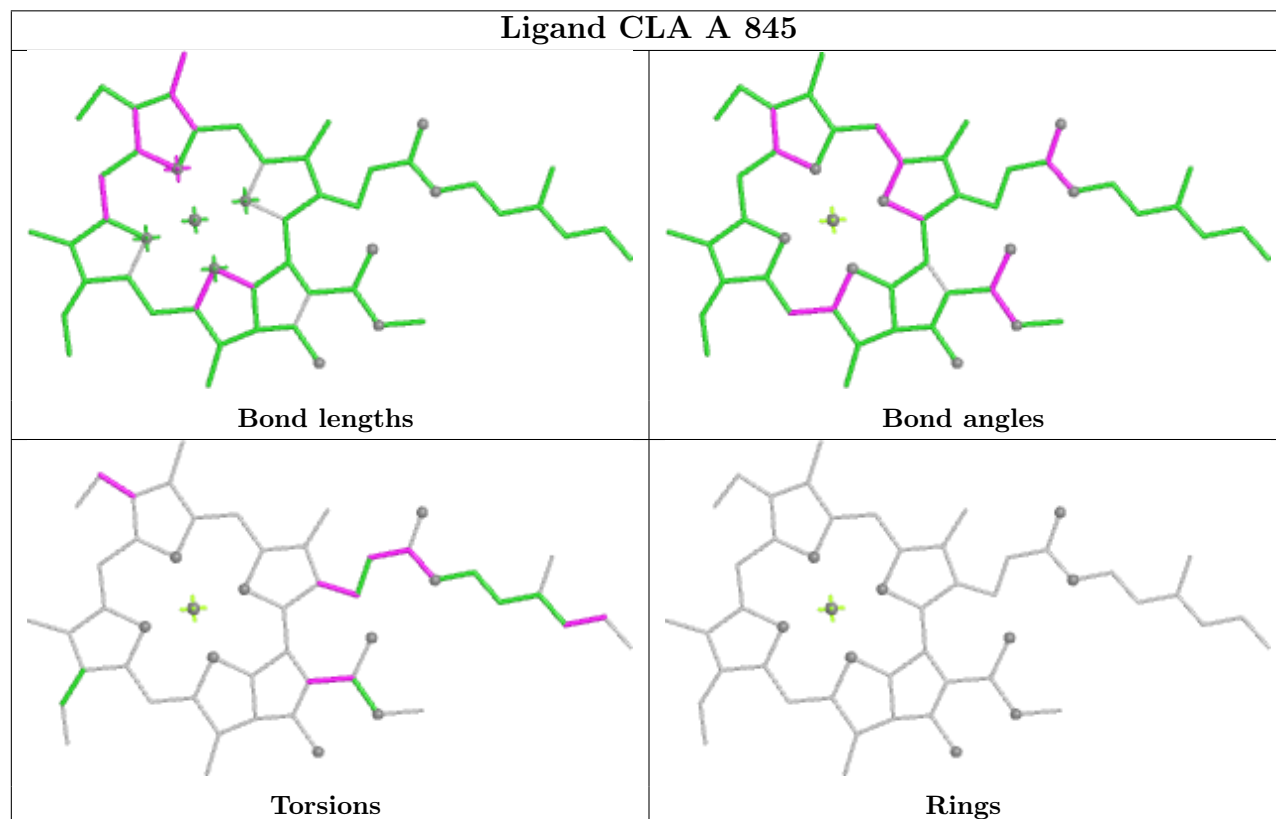
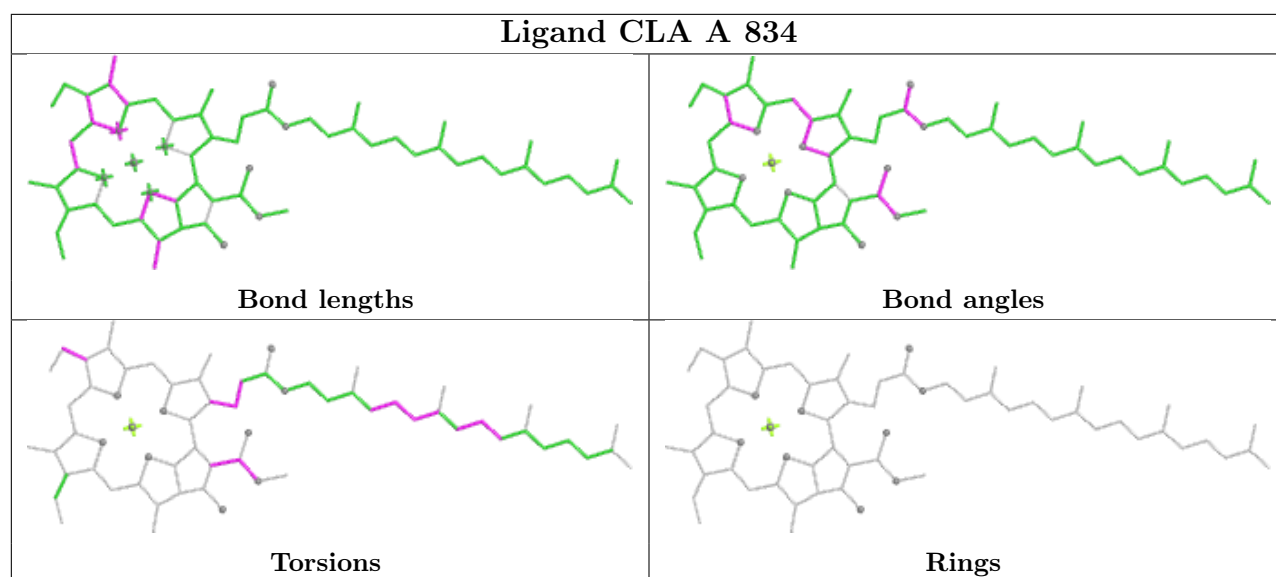


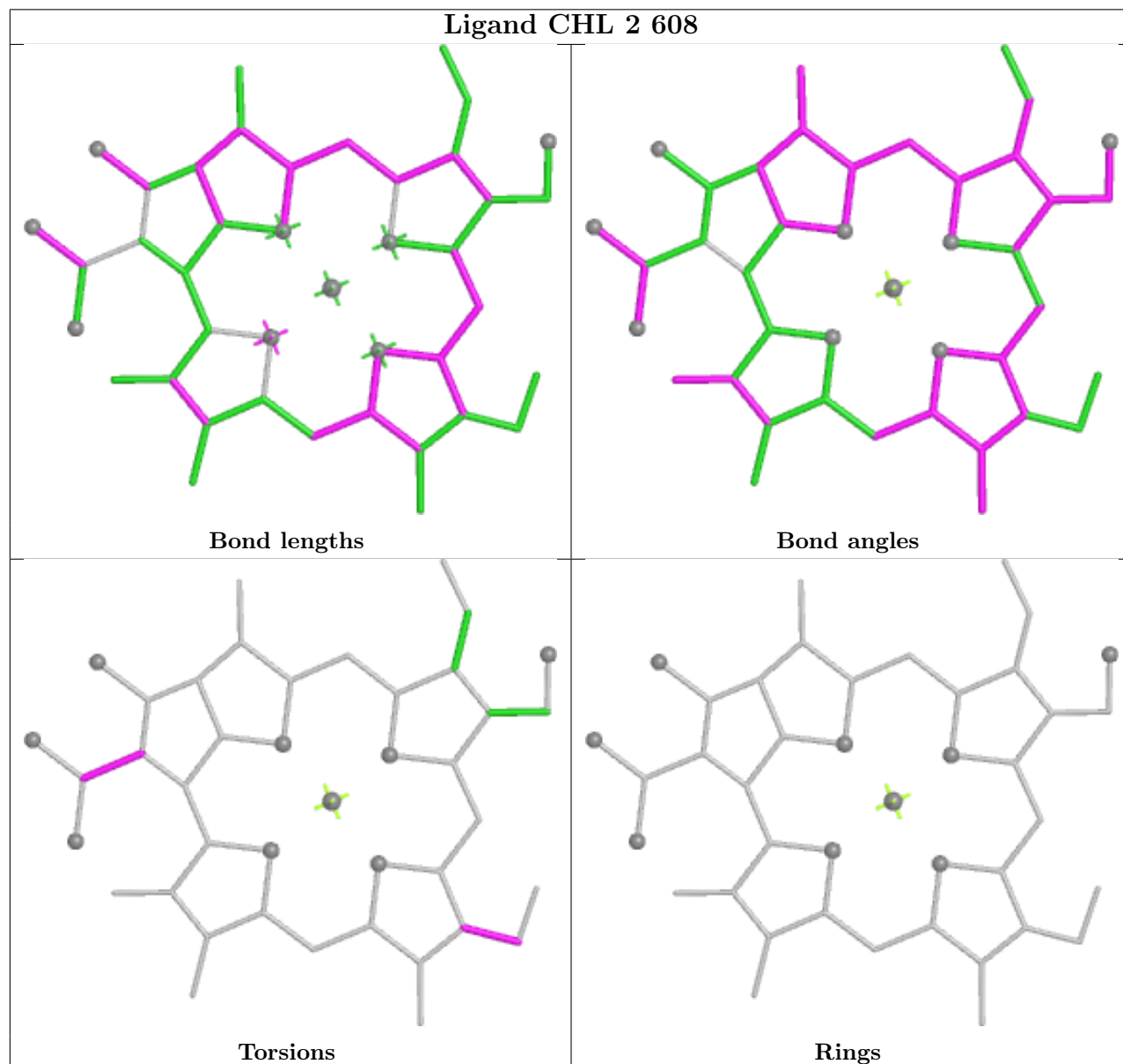
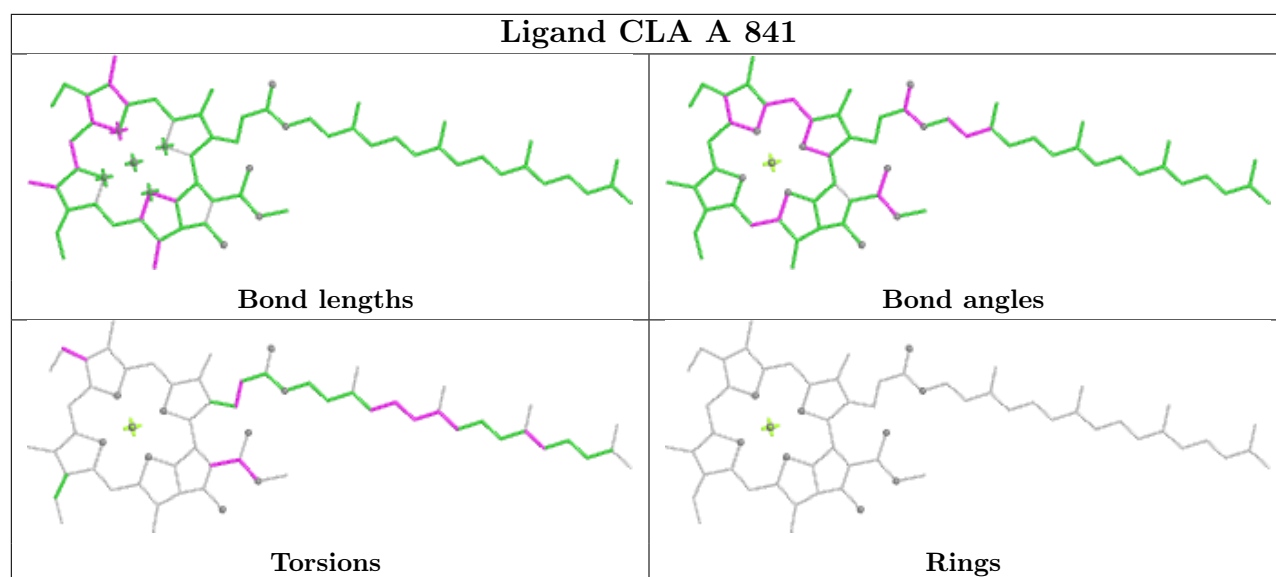
Ligand CLA A 807

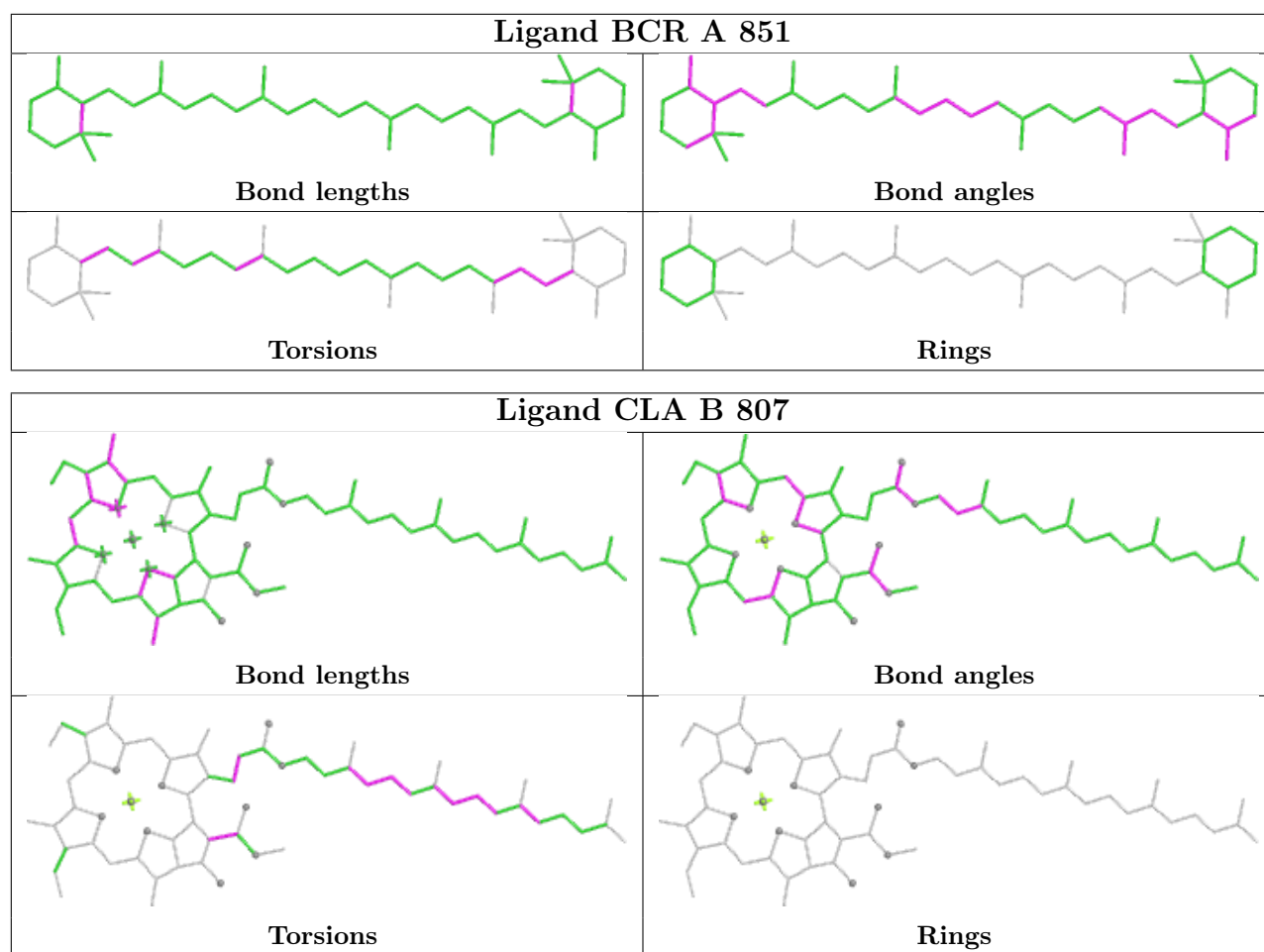


Ligand BCR L 301

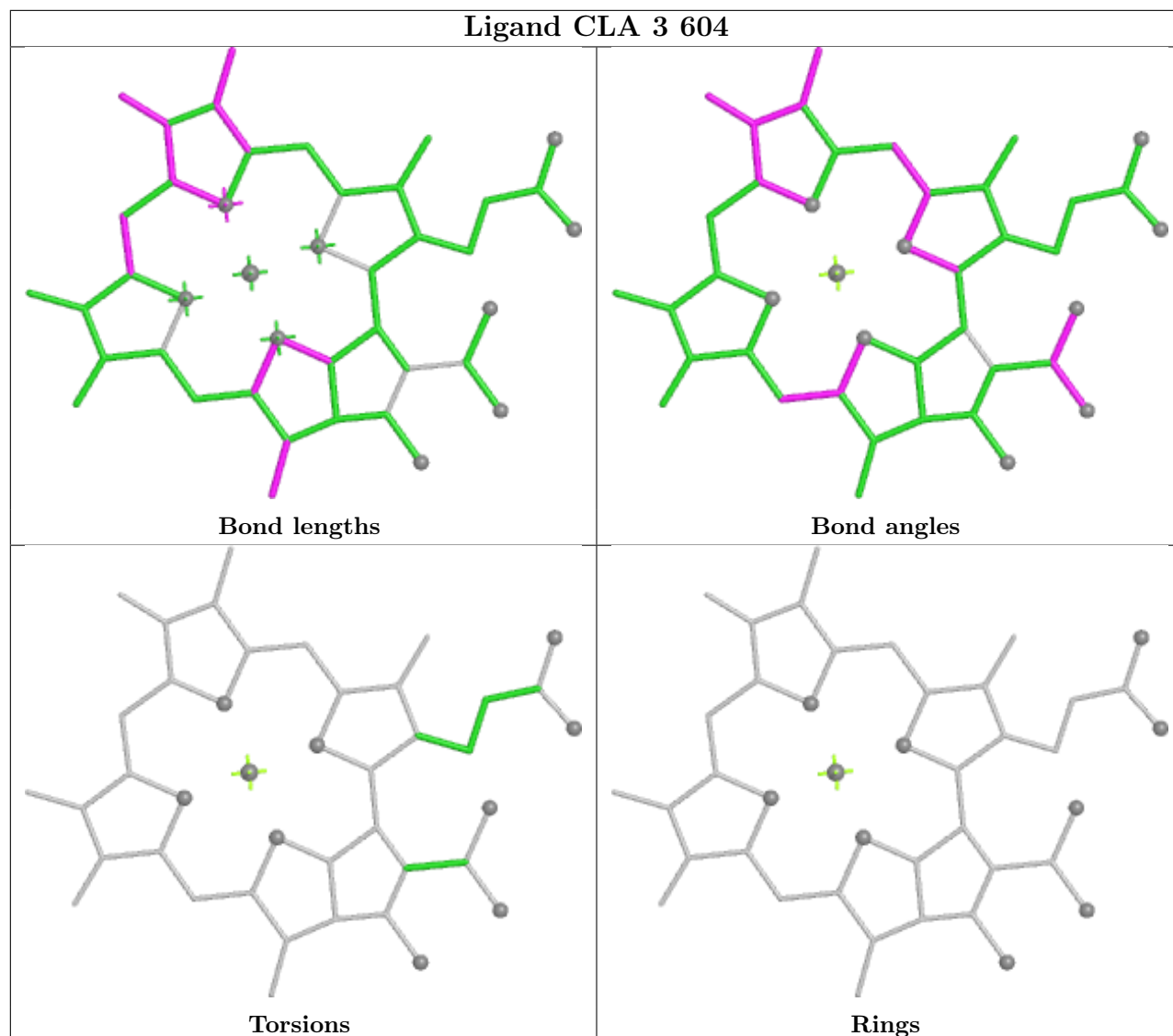




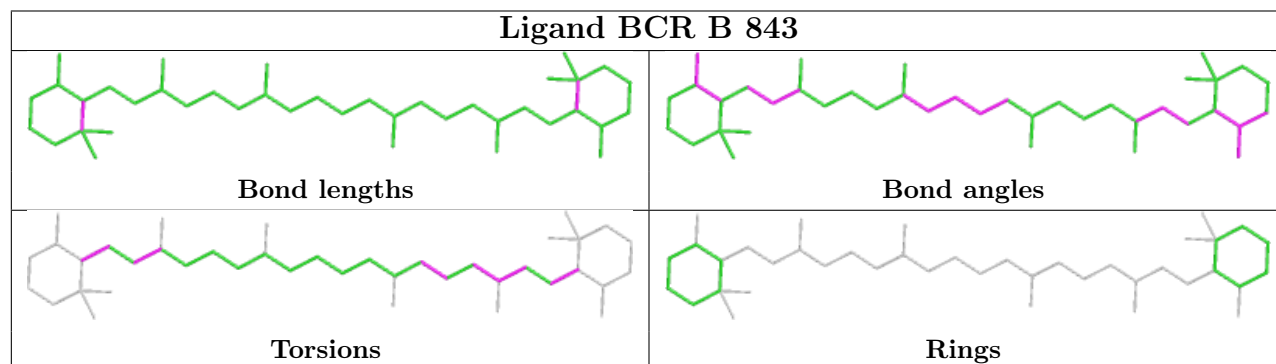


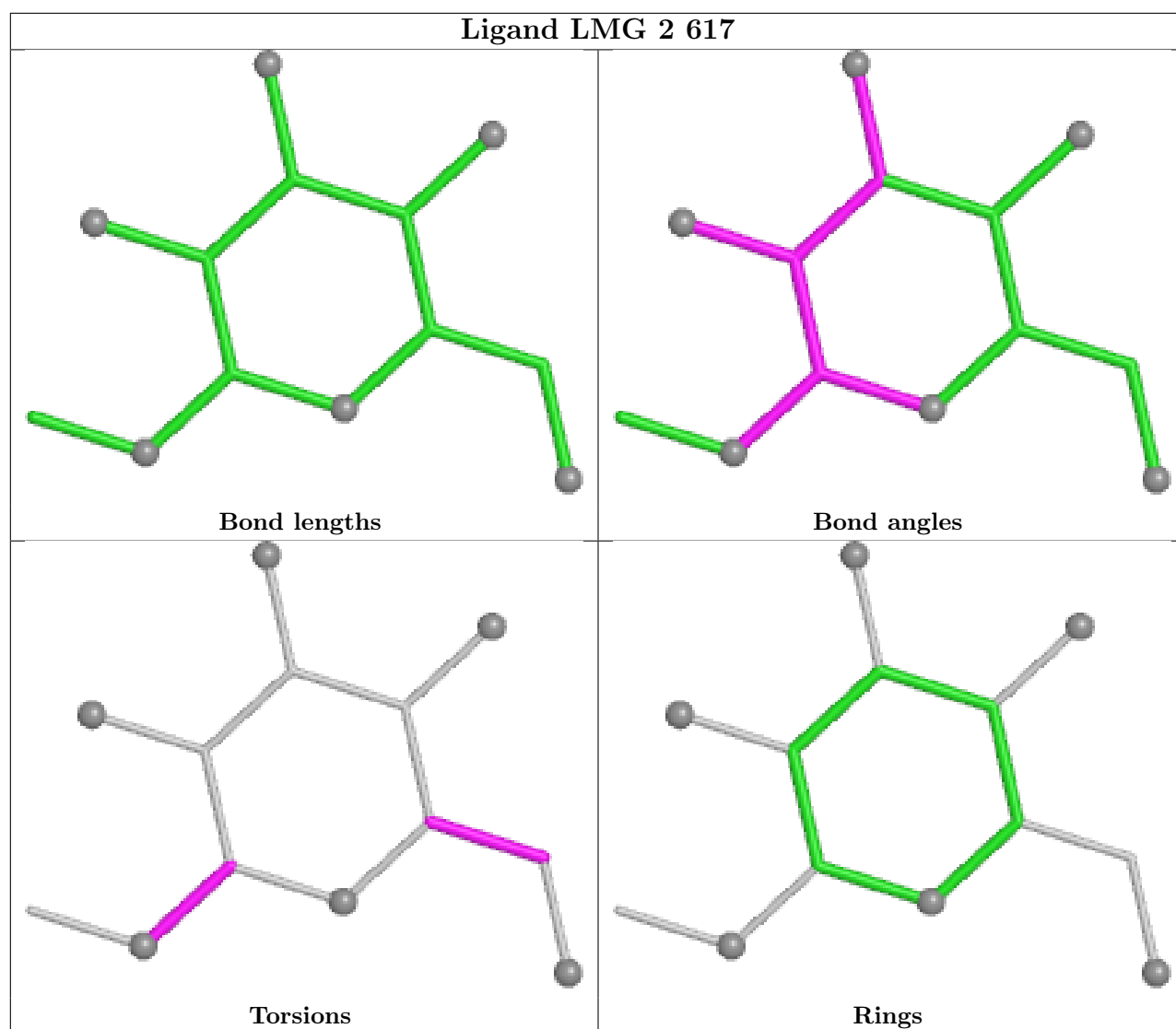


Ligand CLA 3 604

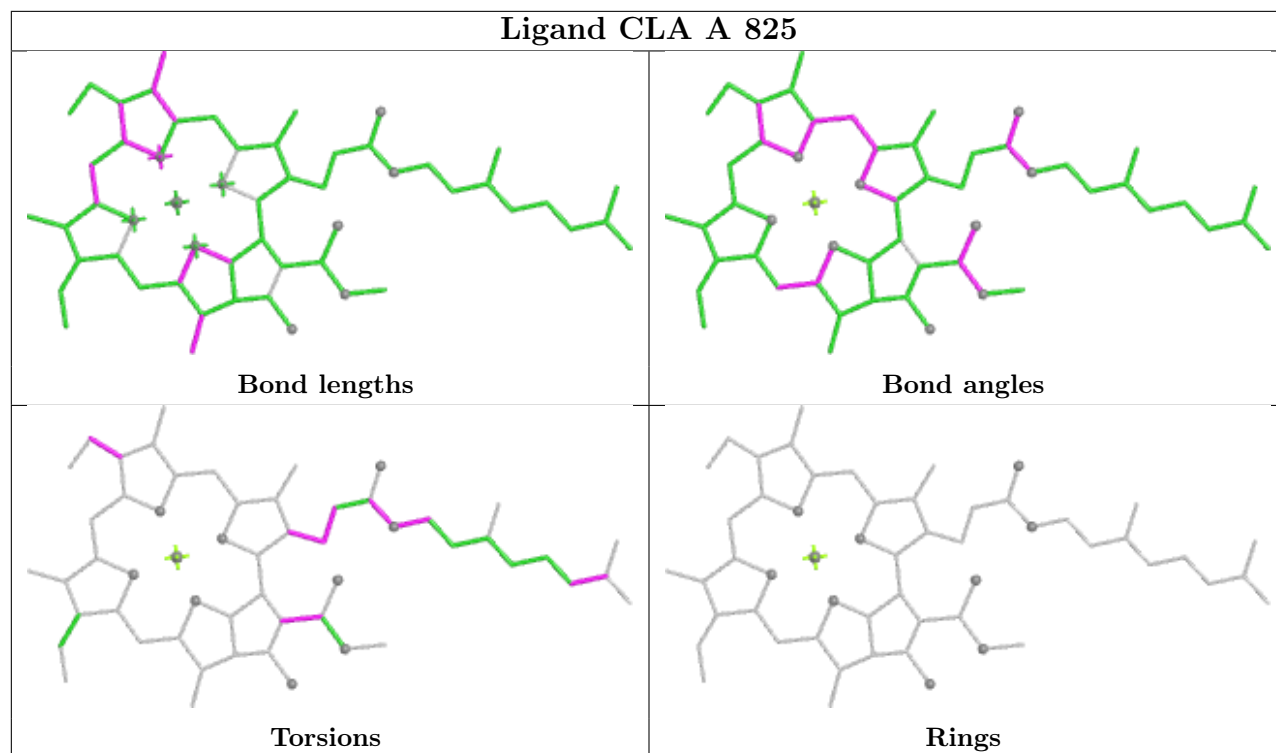


Ligand BCR B 843

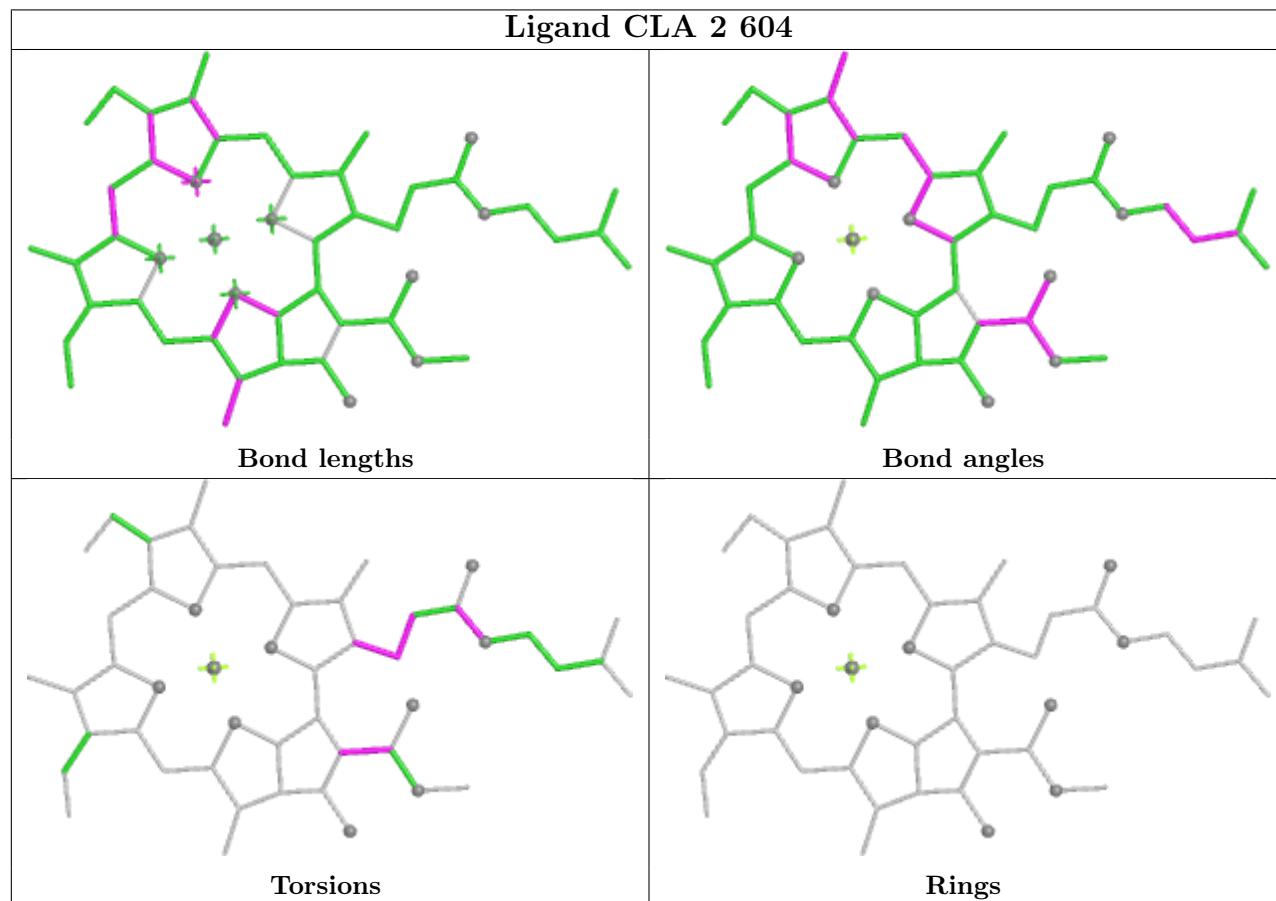


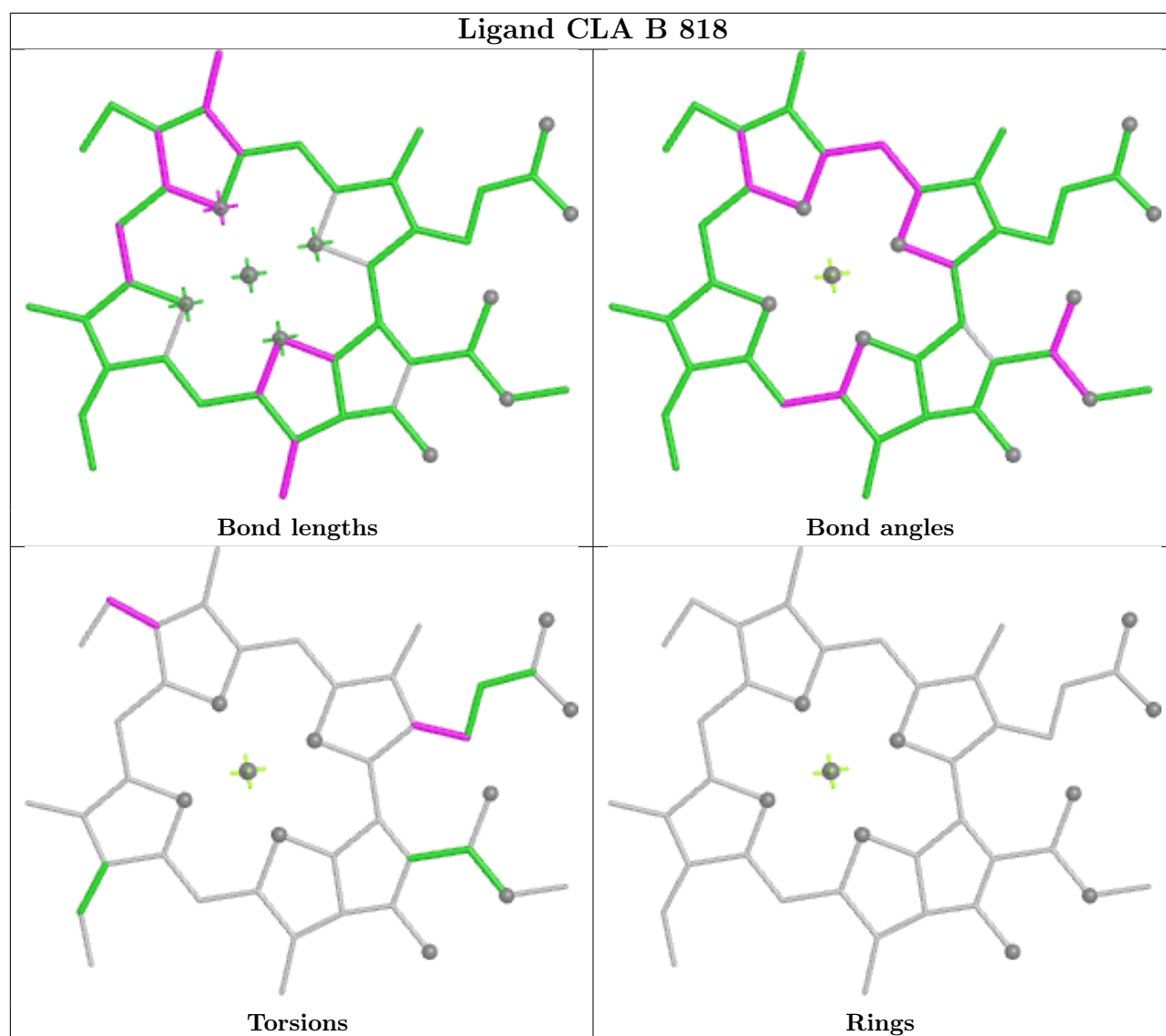


Ligand CLA A 825

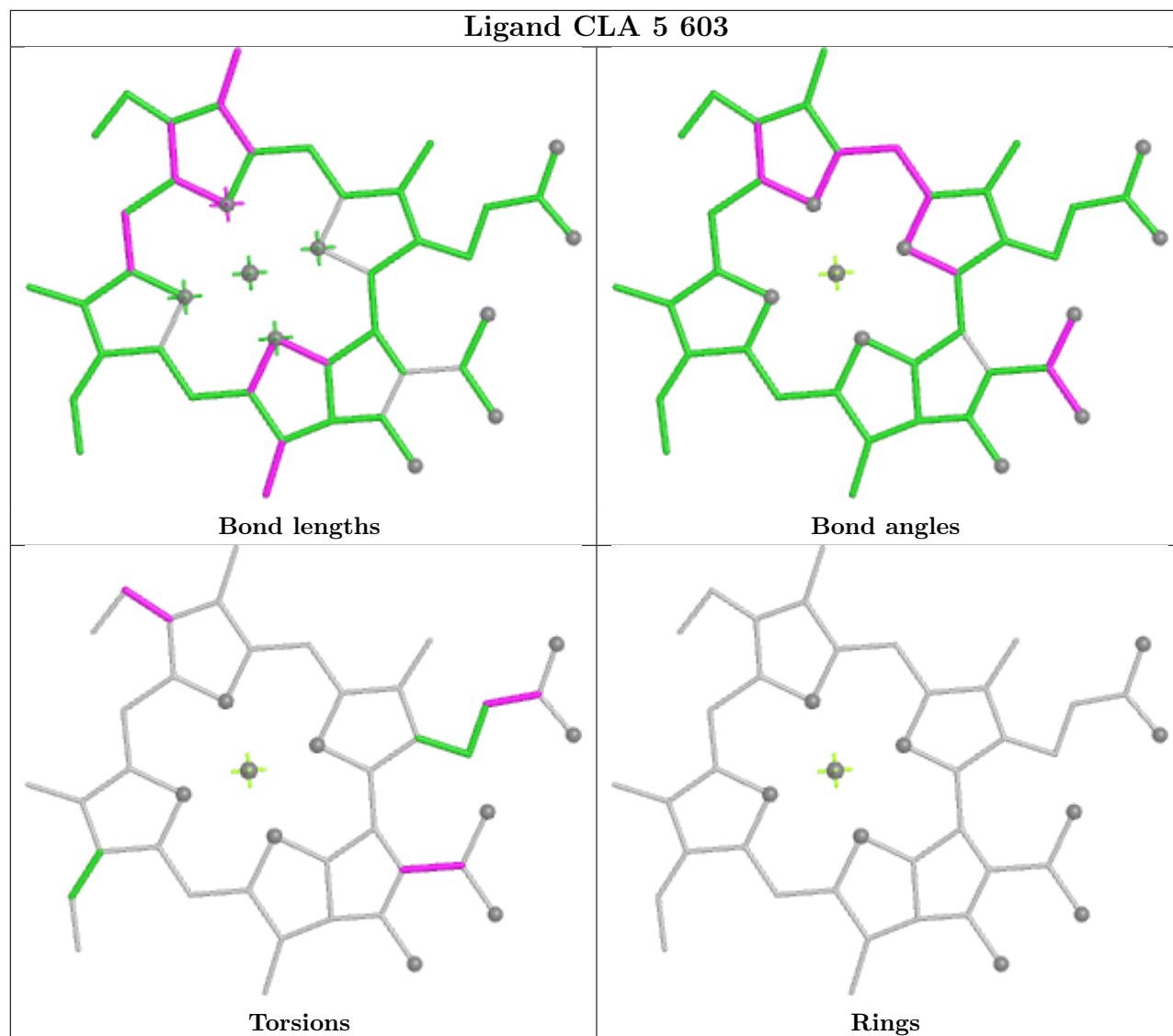


Ligand CLA 2 604

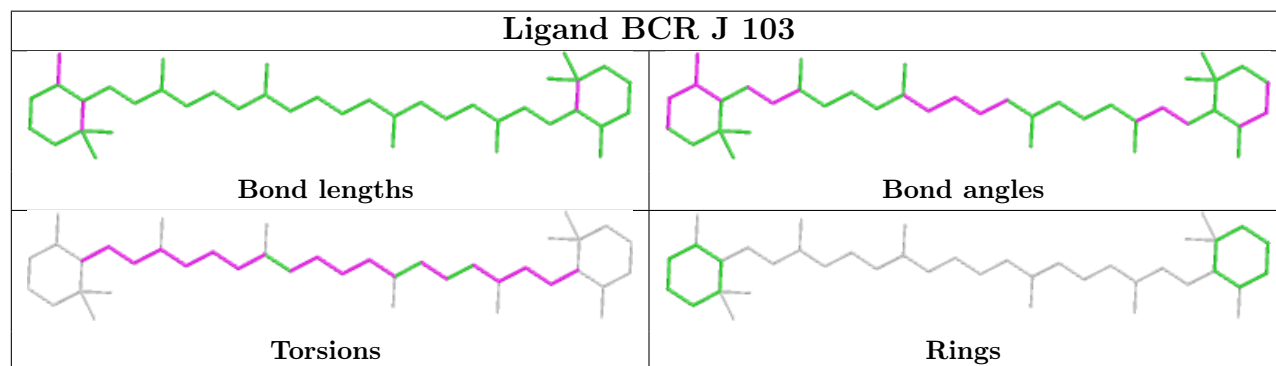


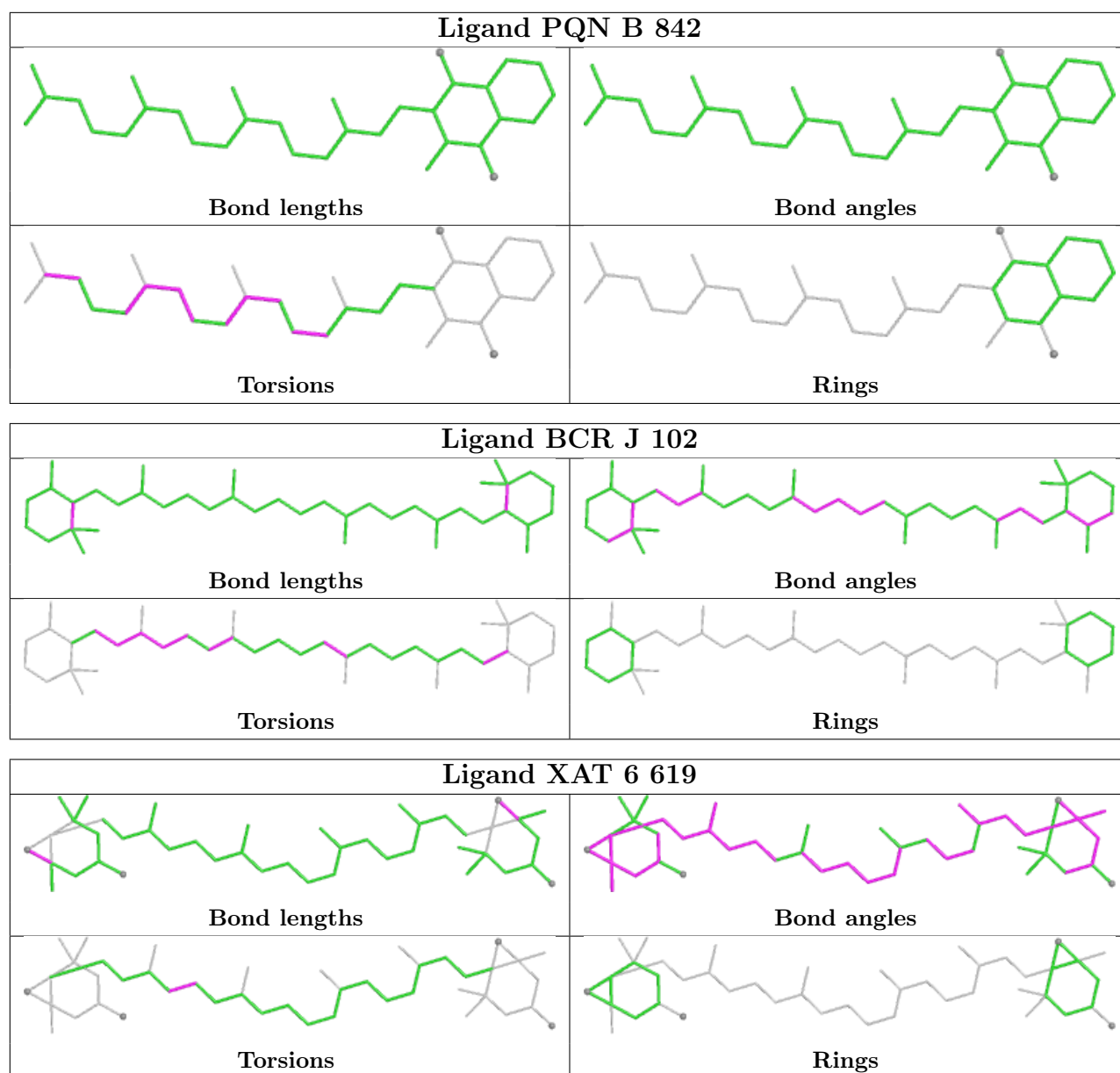


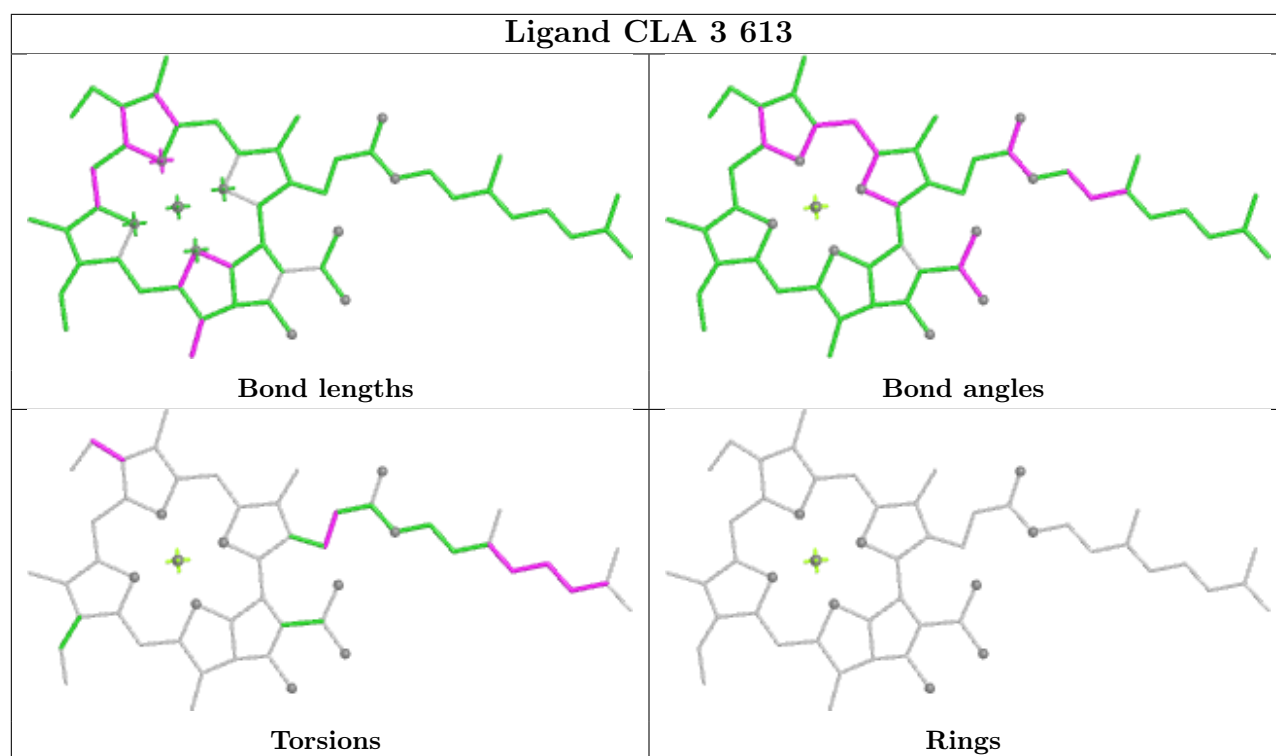
Ligand CLA 5 603



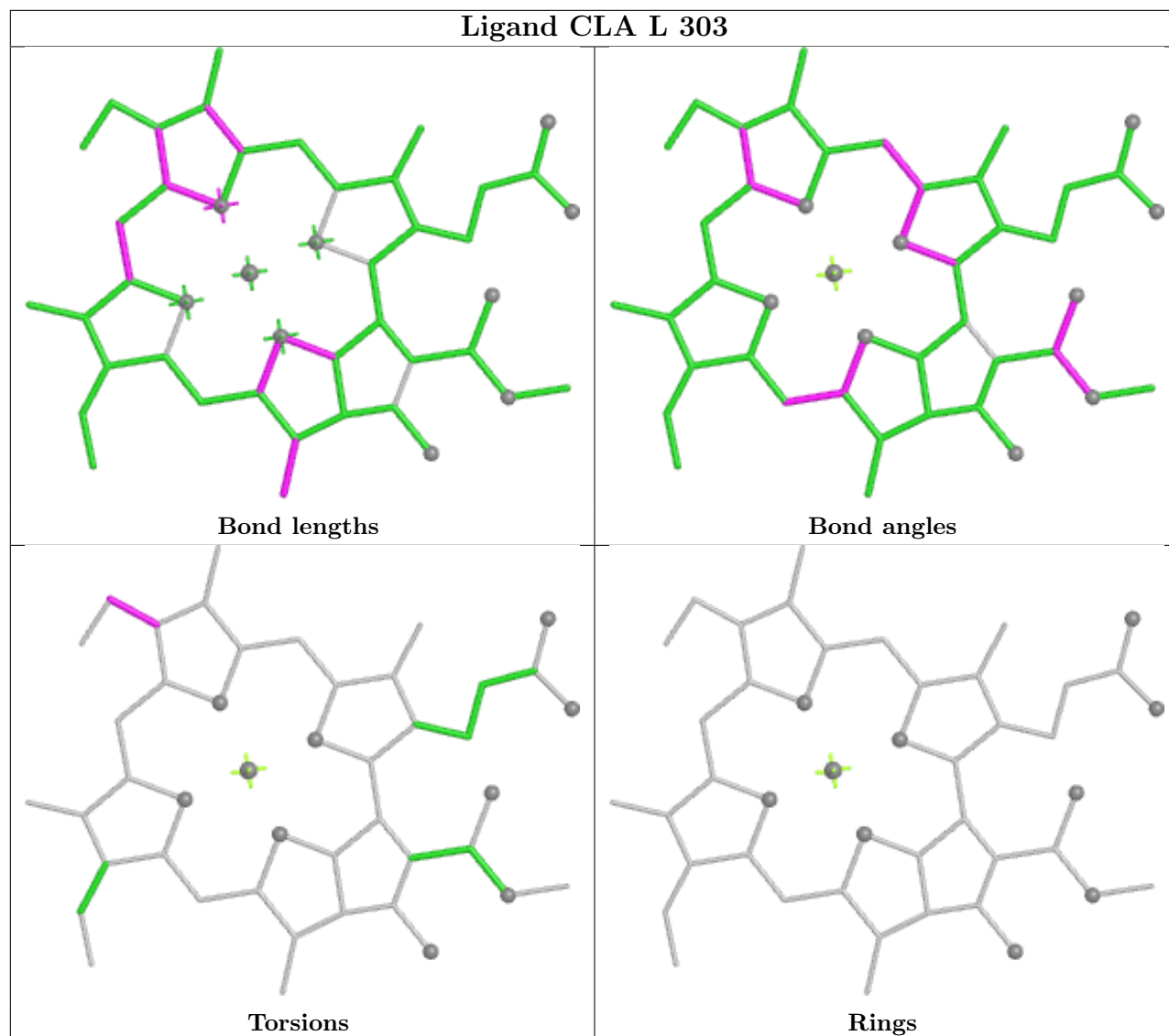
Ligand BCR J 103



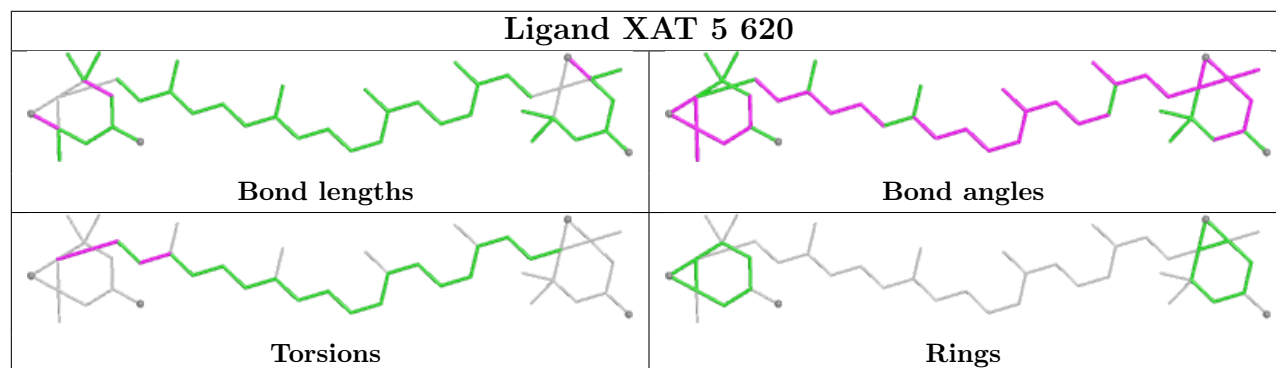


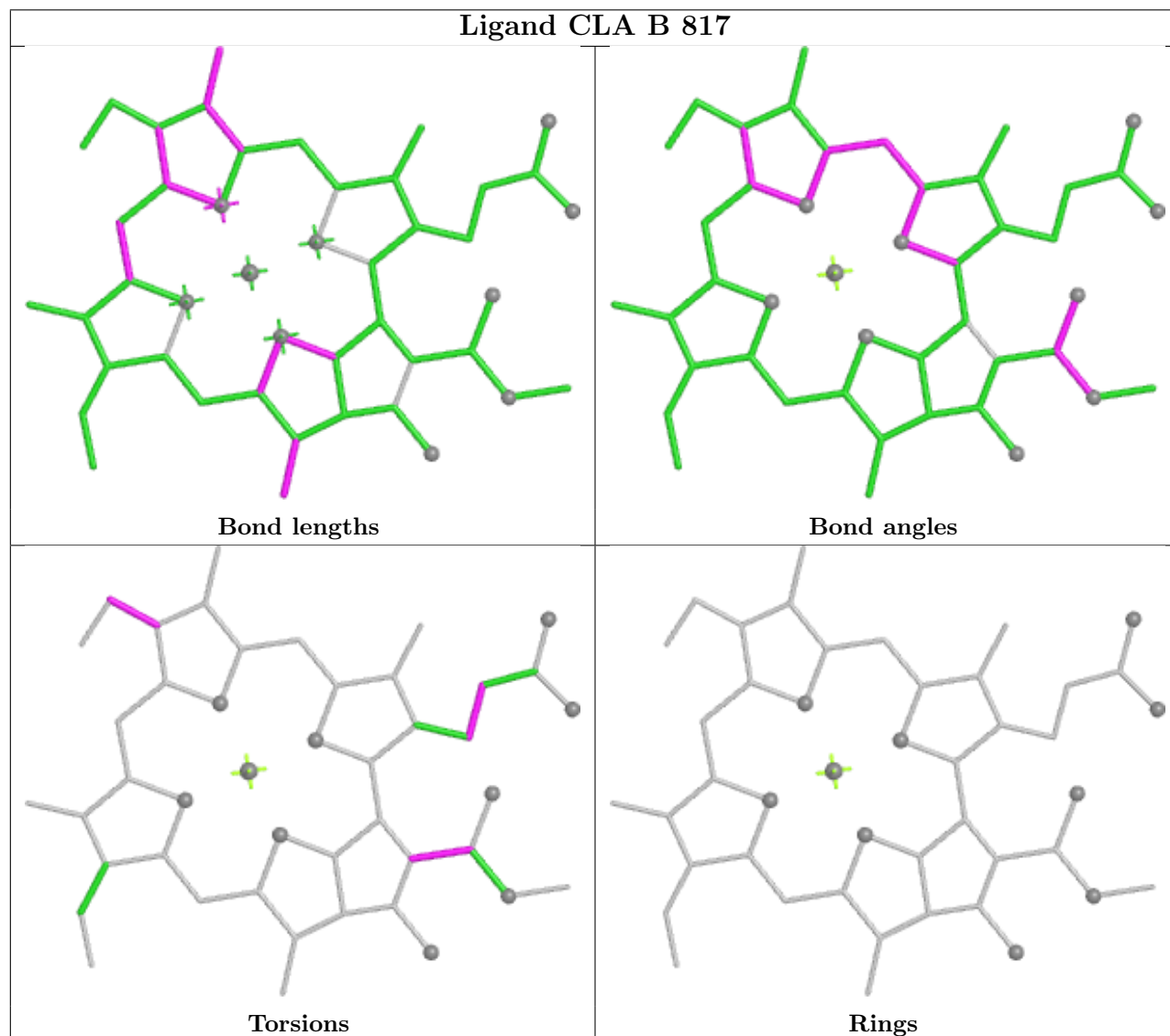
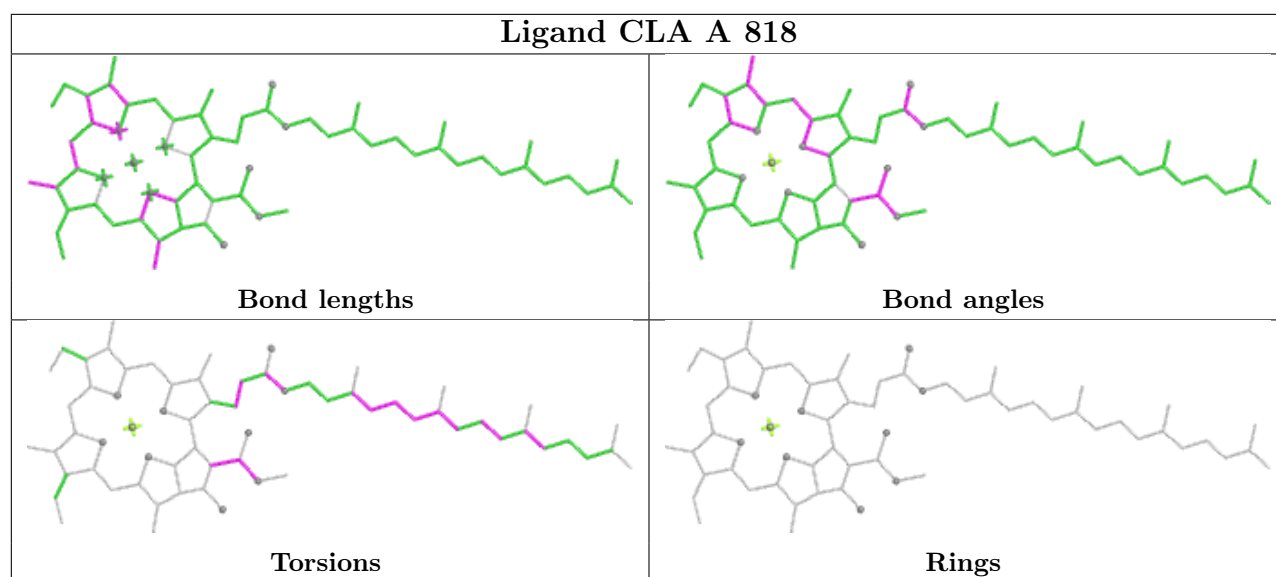


Ligand CLA L 303

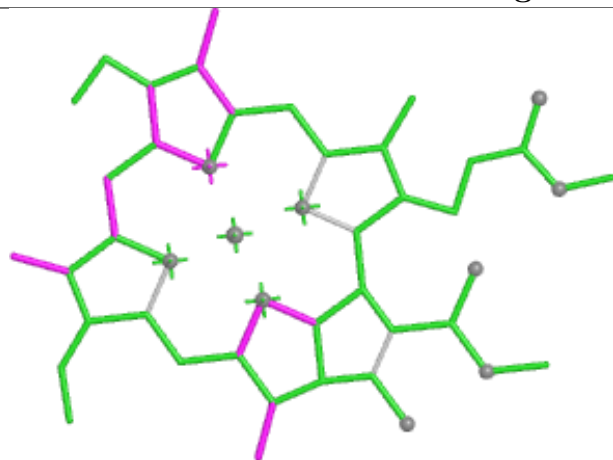


Ligand XAT 5 620

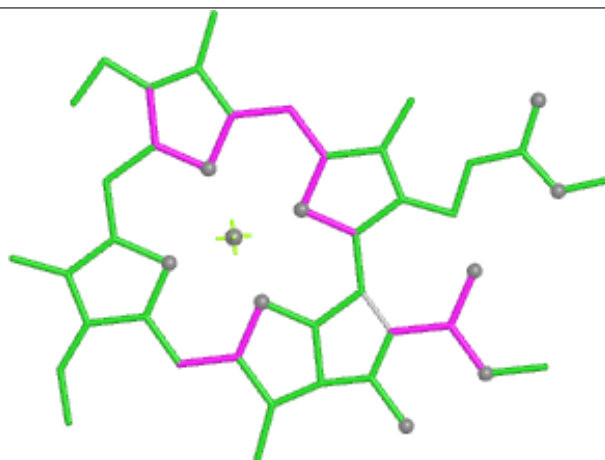




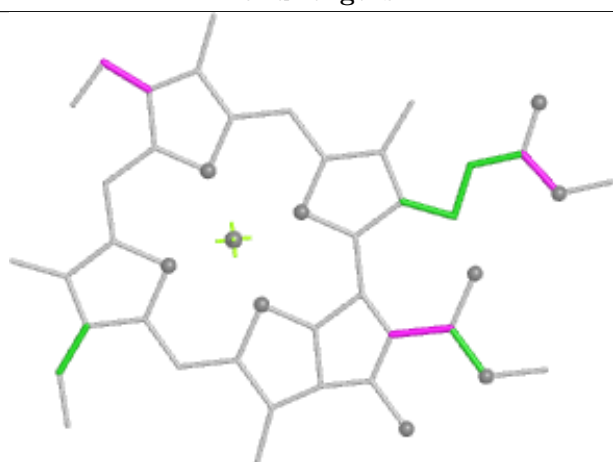
Ligand CLA B 837



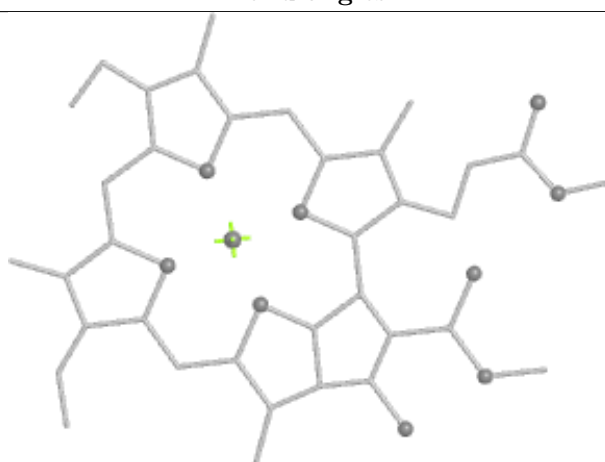
Bond lengths



Bond angles

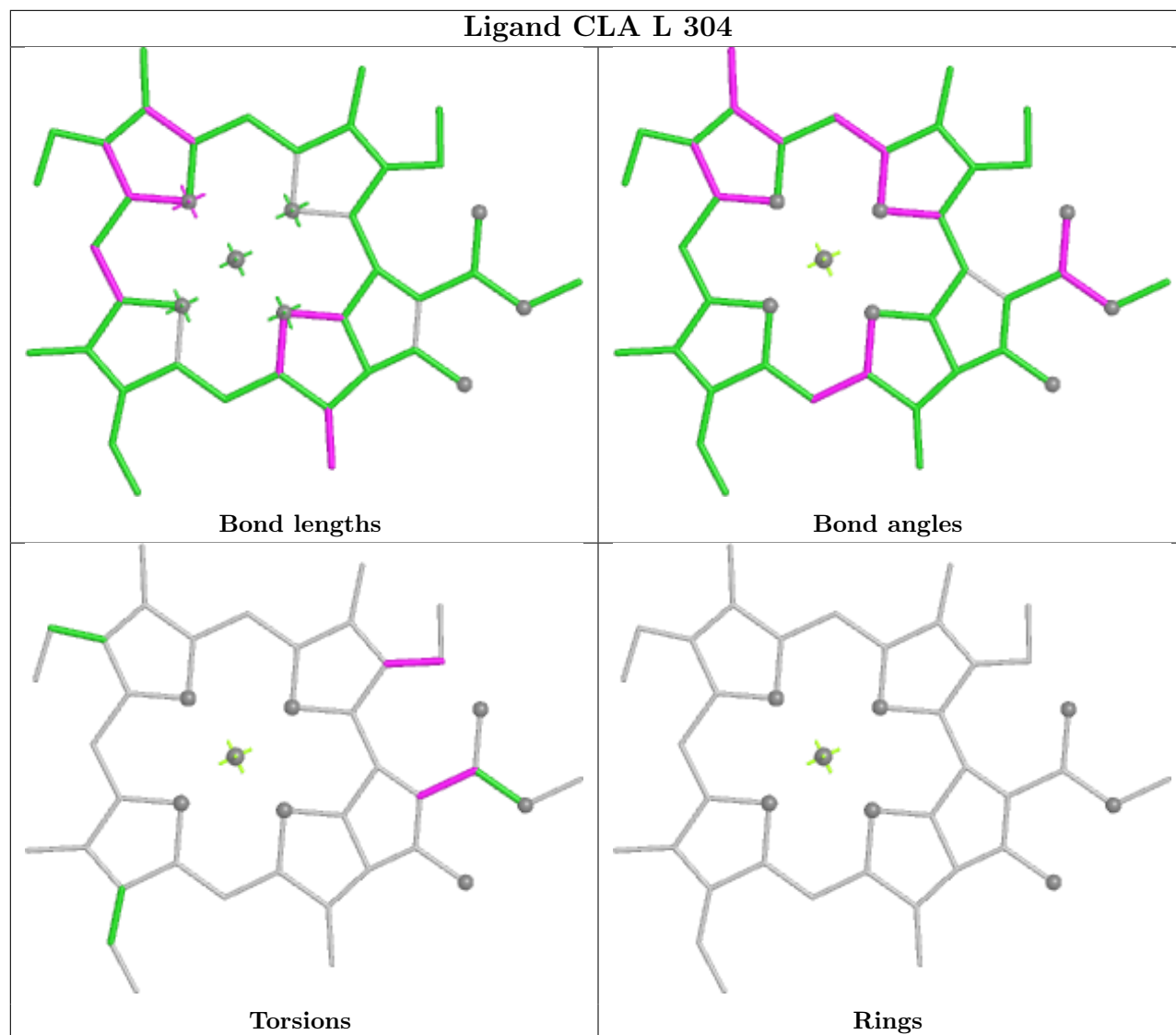


Torsions

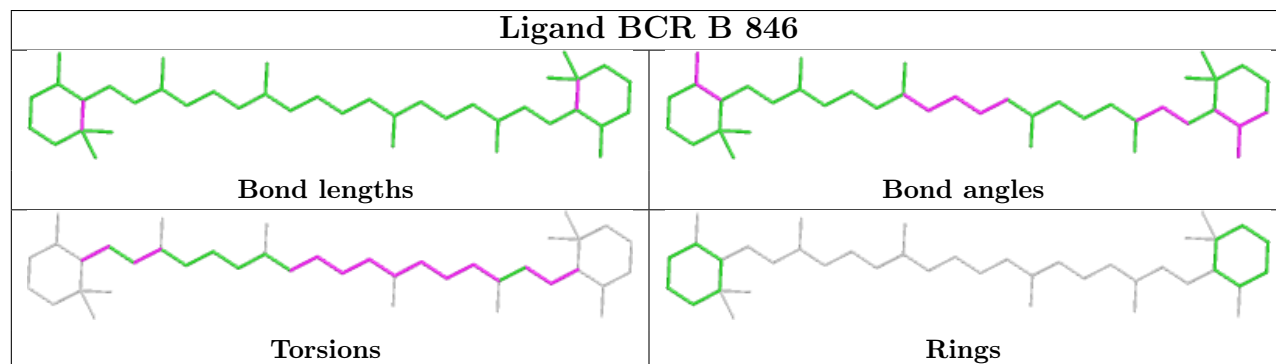


Rings

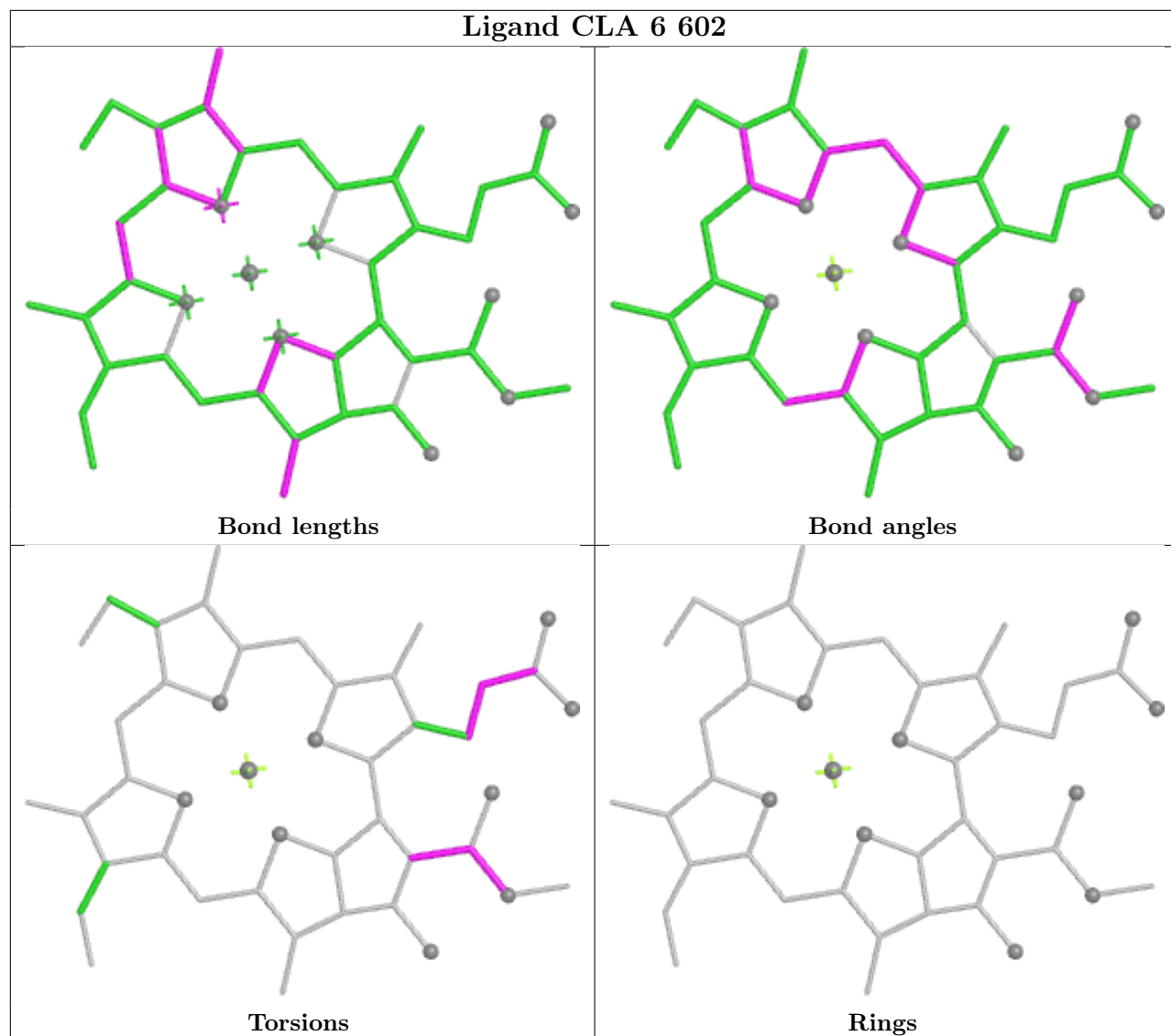
Ligand CLA L 304



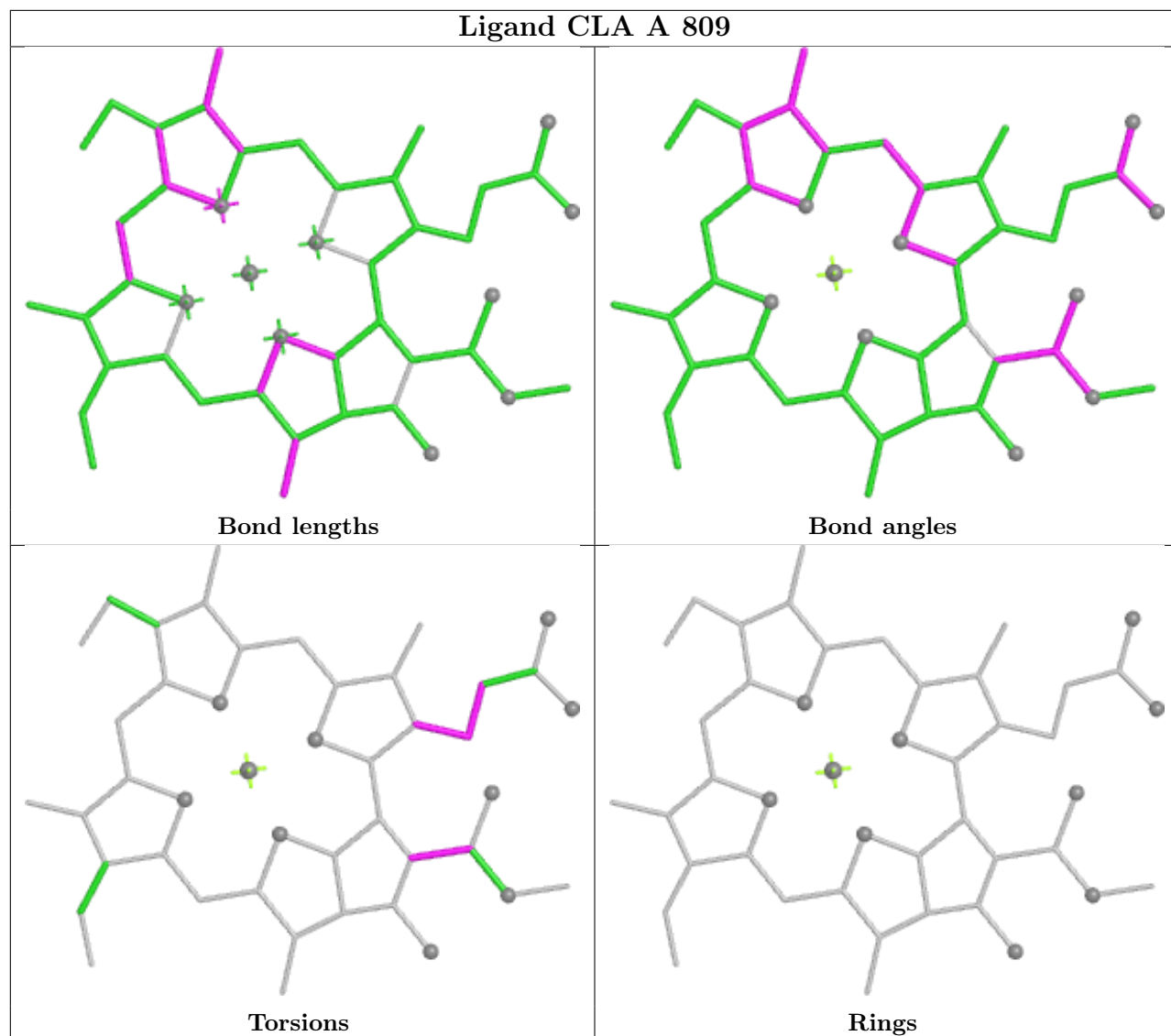
Ligand BCR B 846



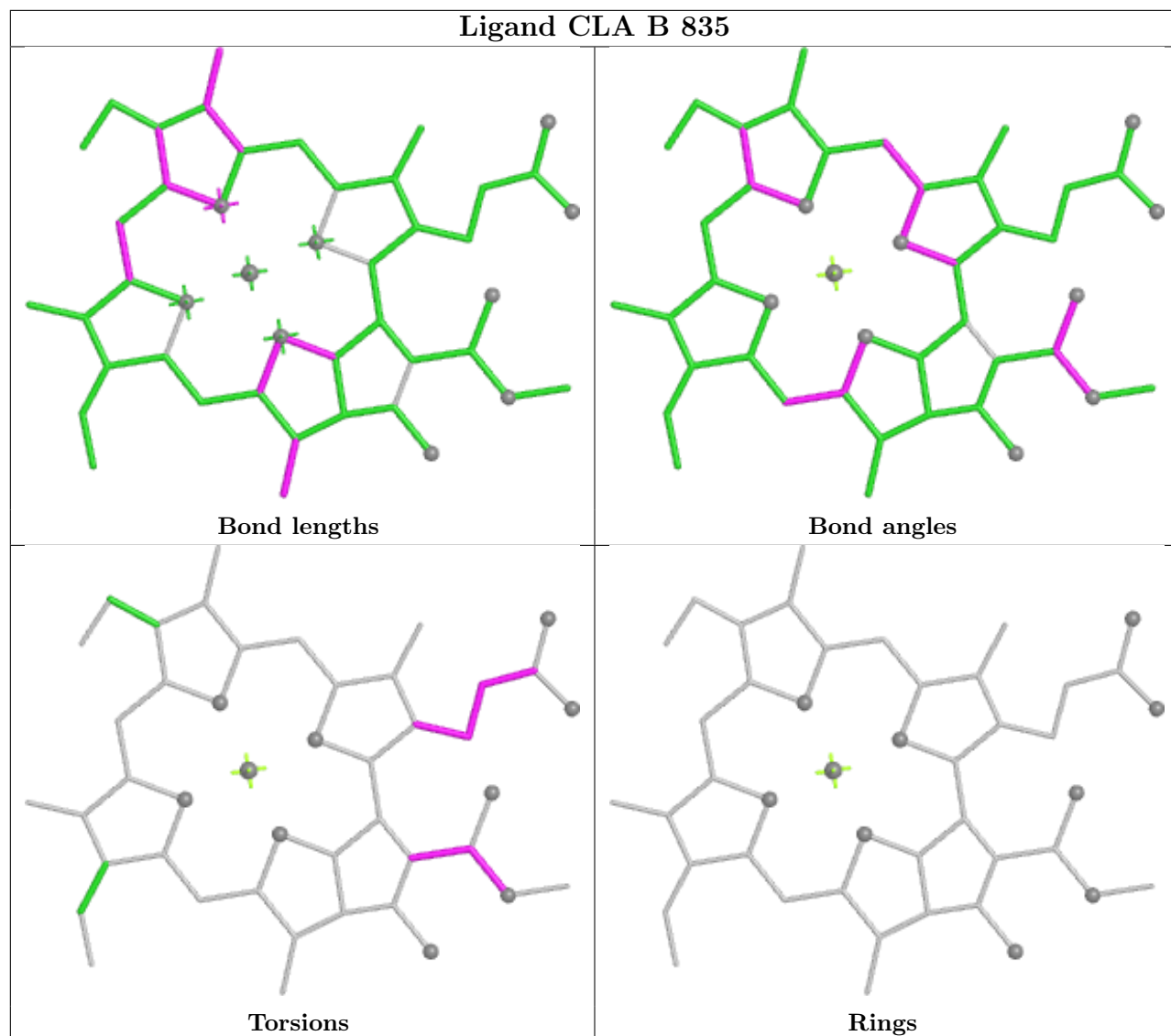
Ligand CLA 6 602



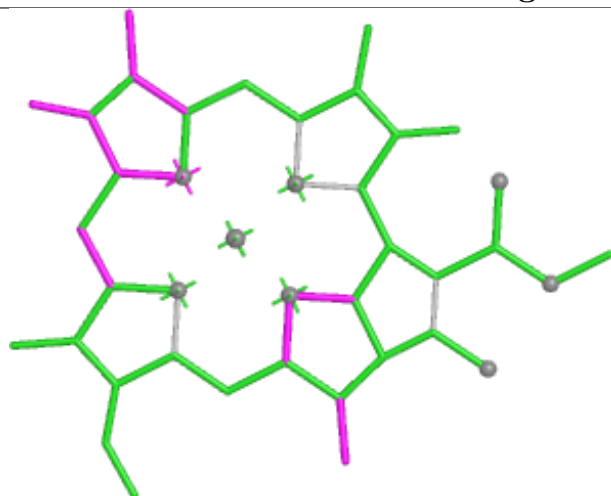
Ligand CLA A 809



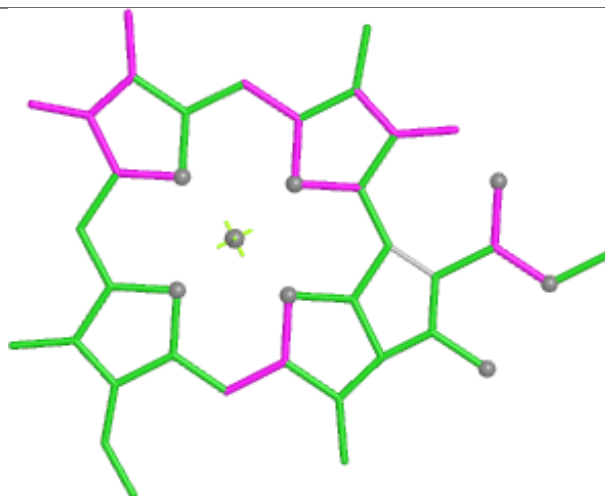
Ligand CLA B 835



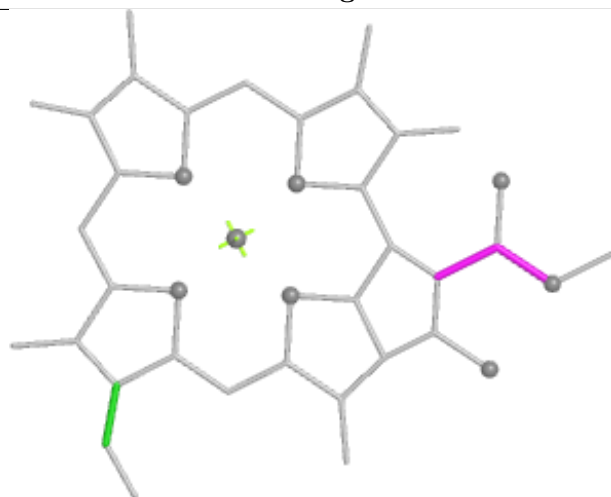
Ligand CLA 6 609



Bond lengths



Bond angles

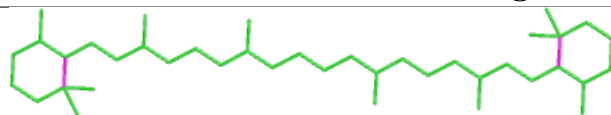


Torsions

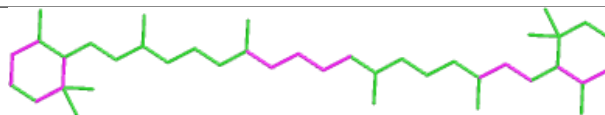


Rings

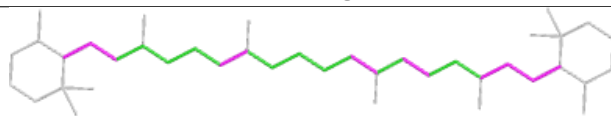
Ligand BCR K 207



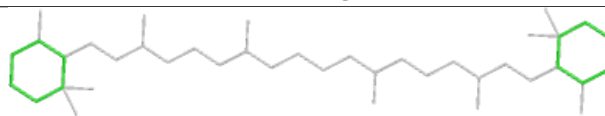
Bond lengths



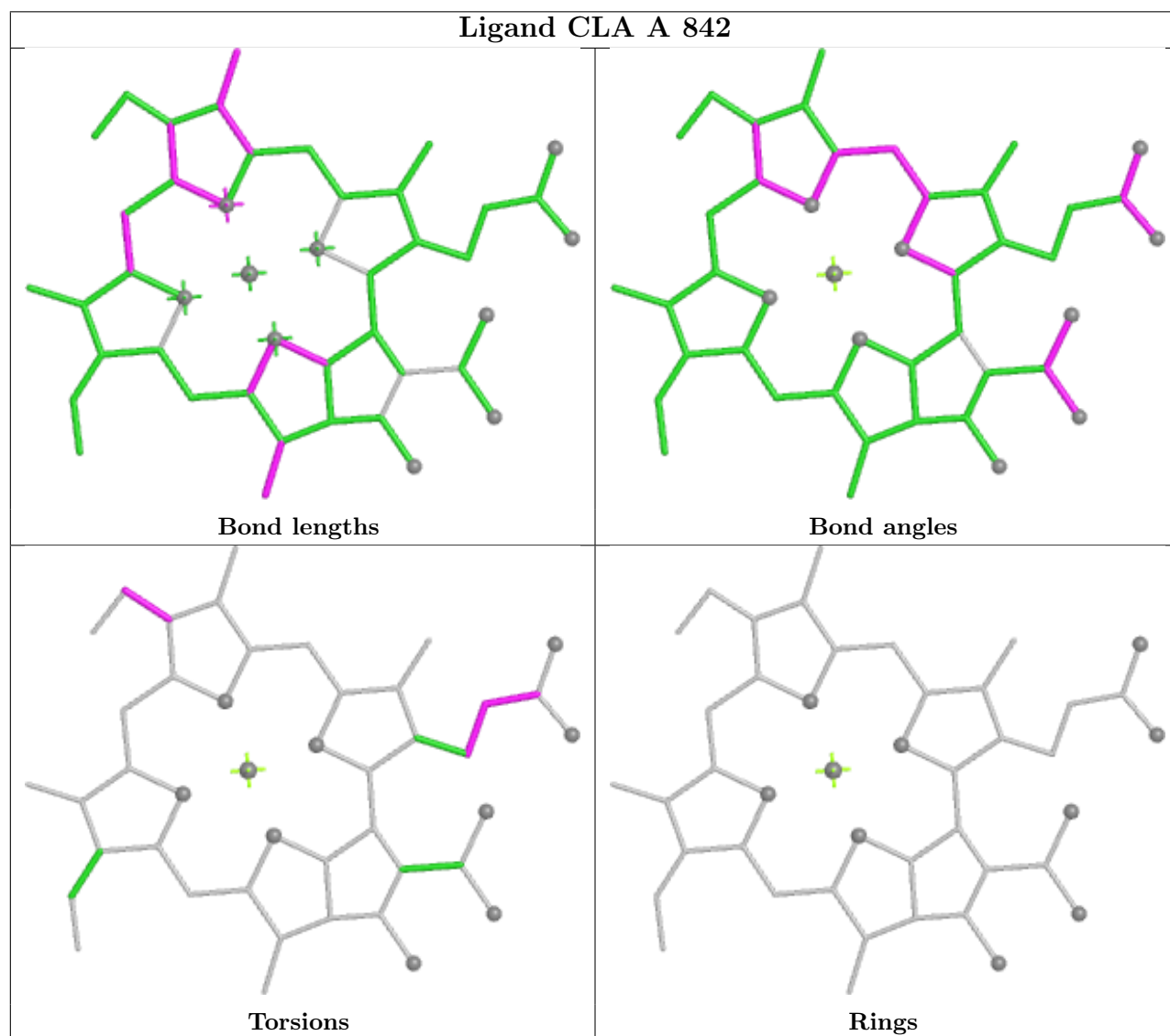
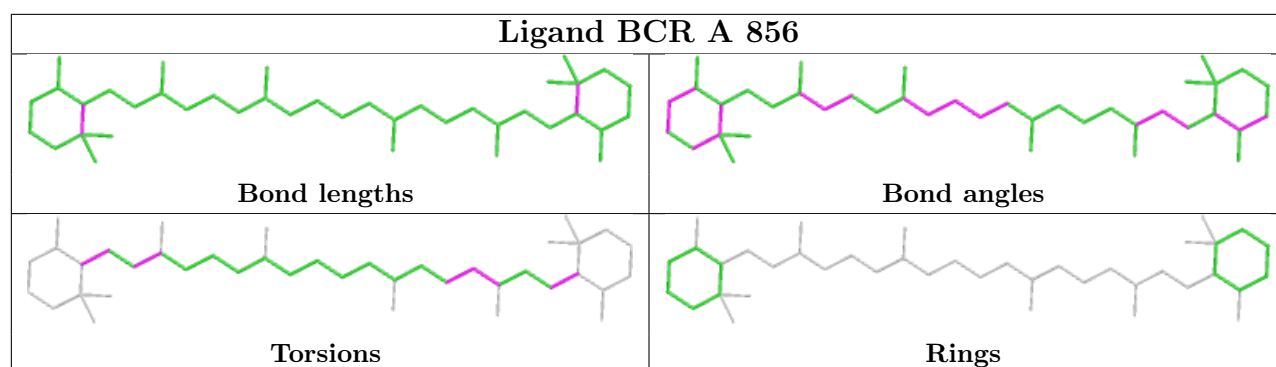
Bond angles

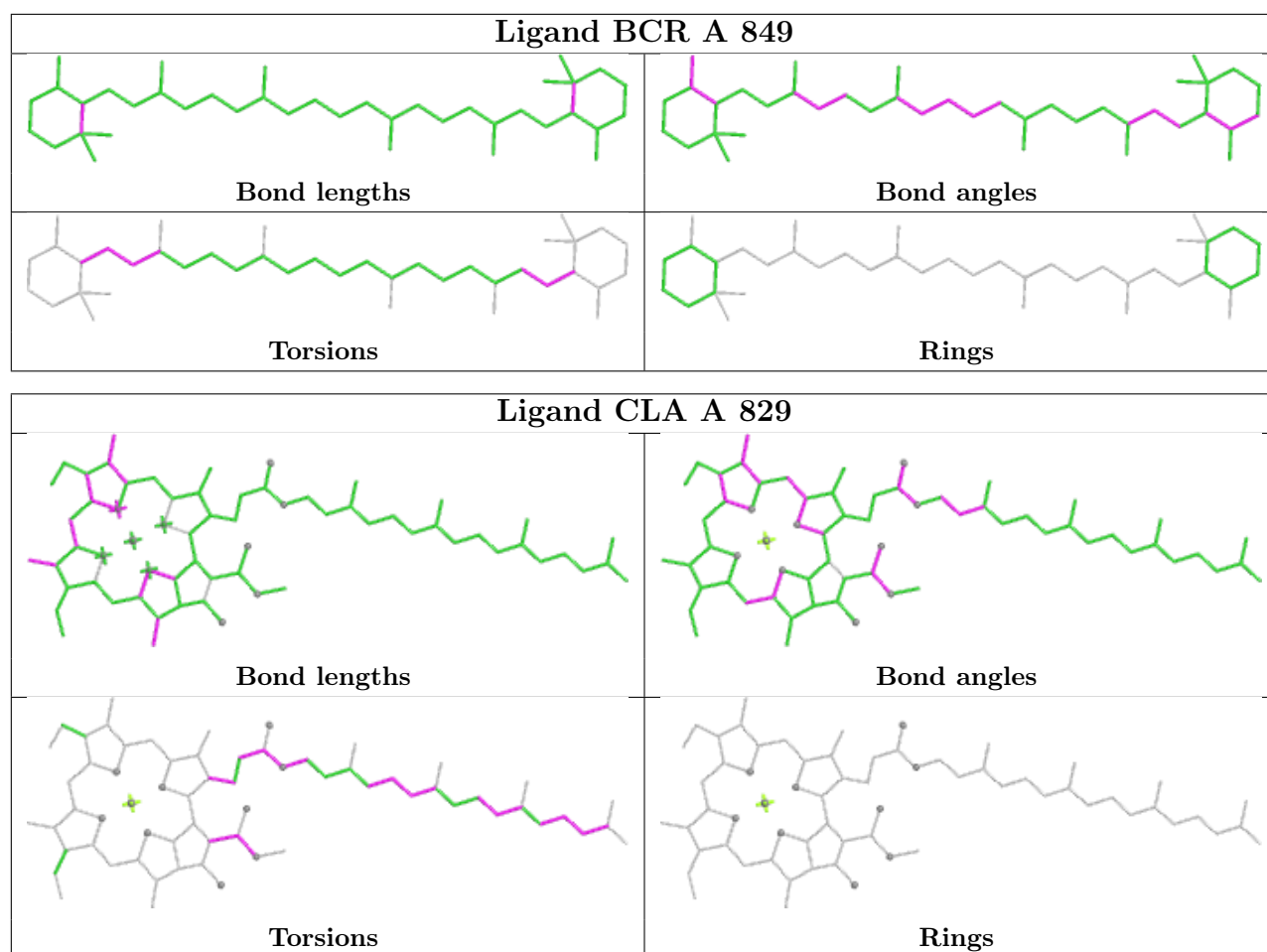


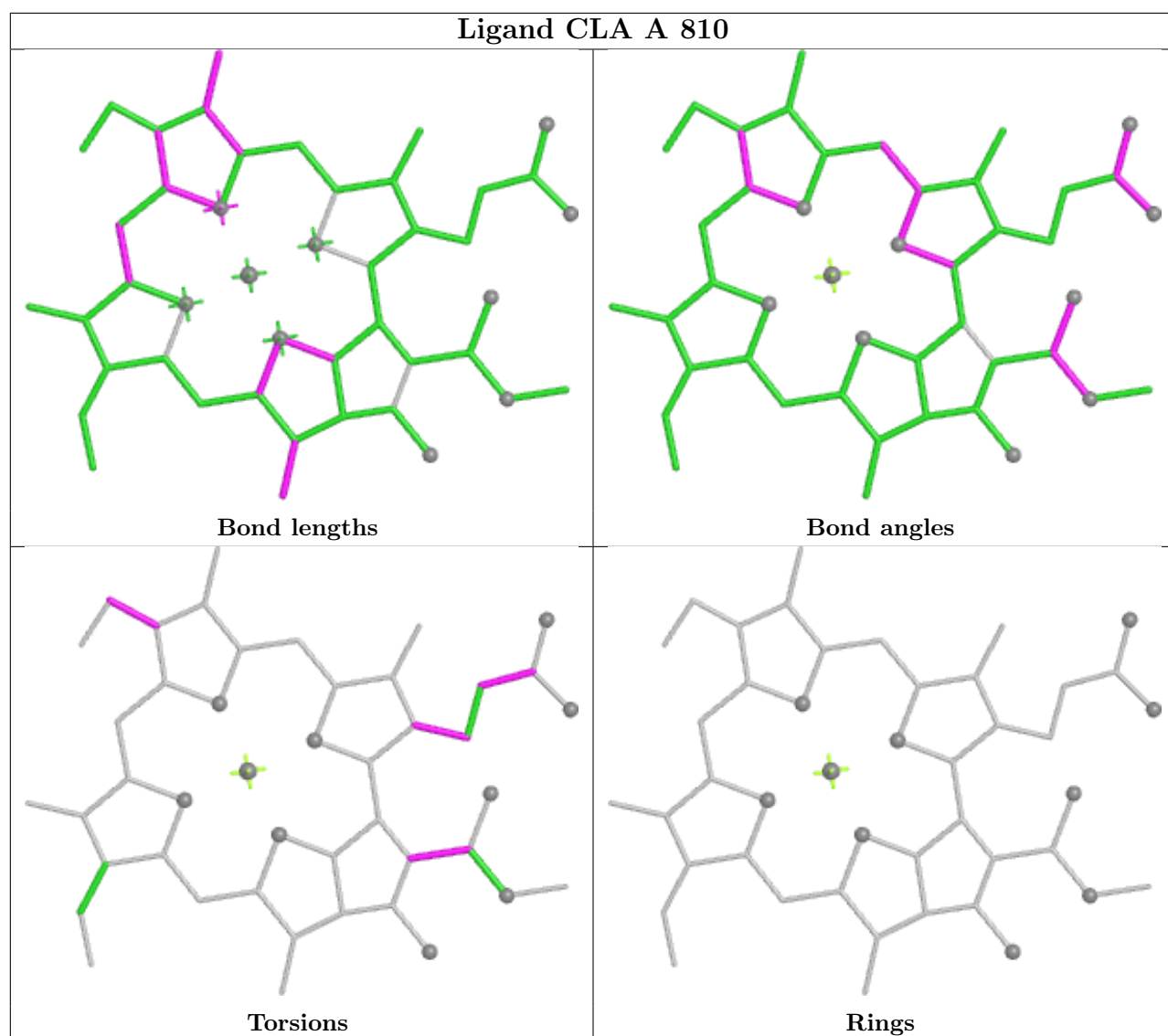
Torsions



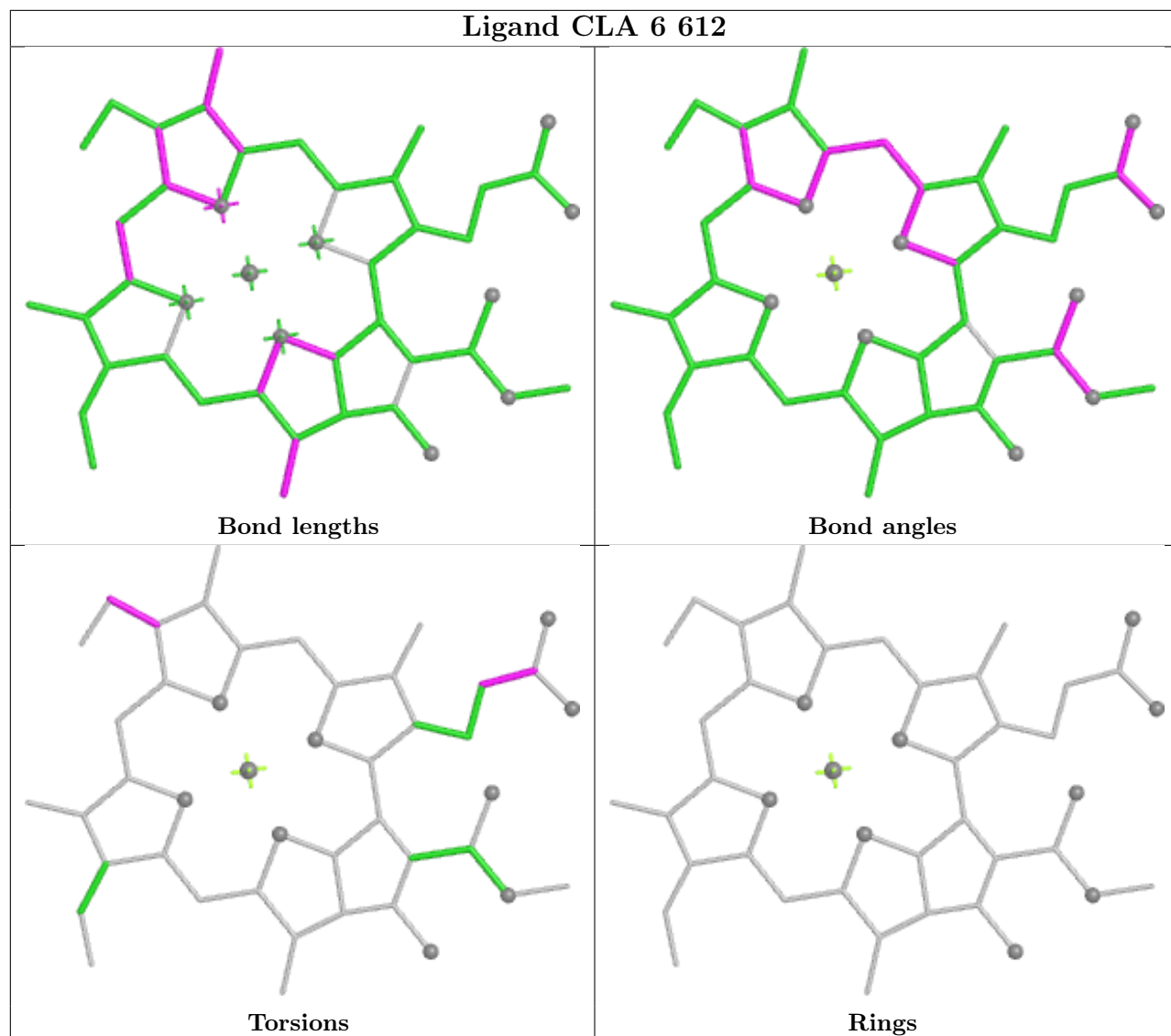
Rings



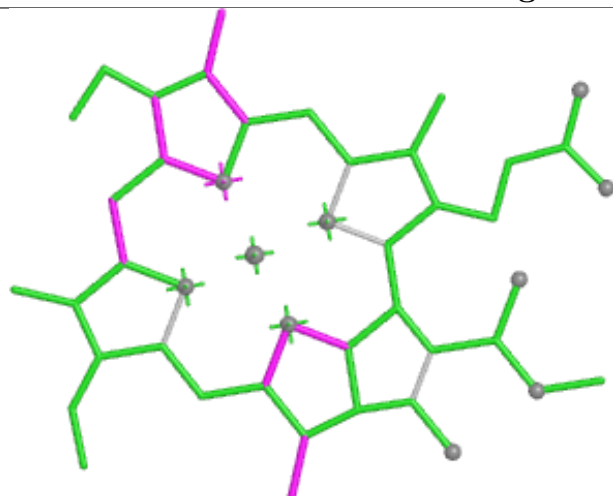




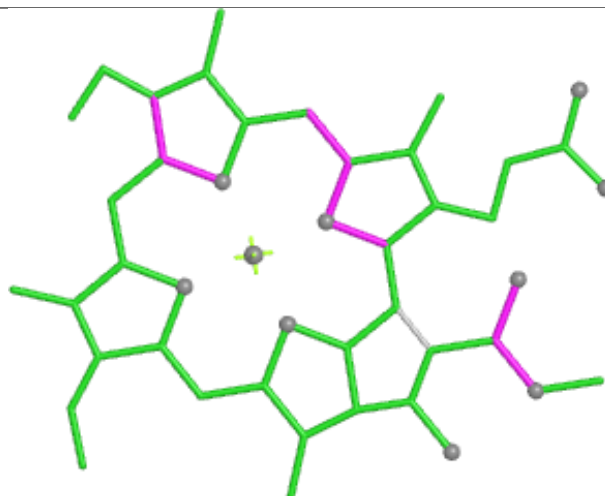
Ligand CLA 6 612



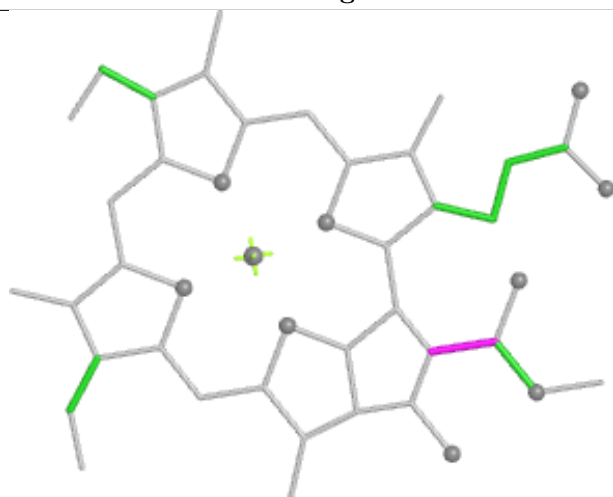
Ligand CLA 3 609



Bond lengths



Bond angles

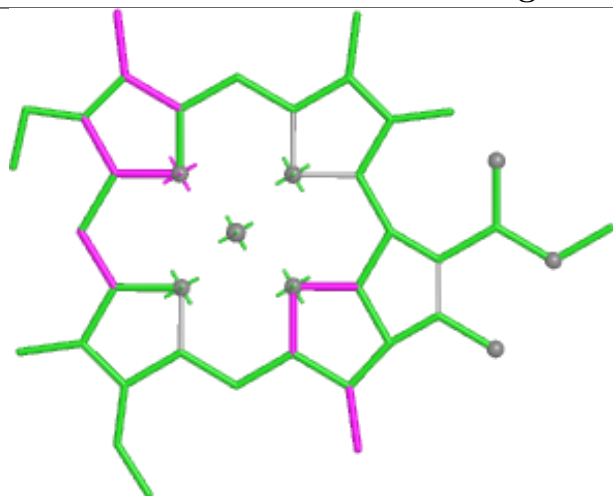


Torsions

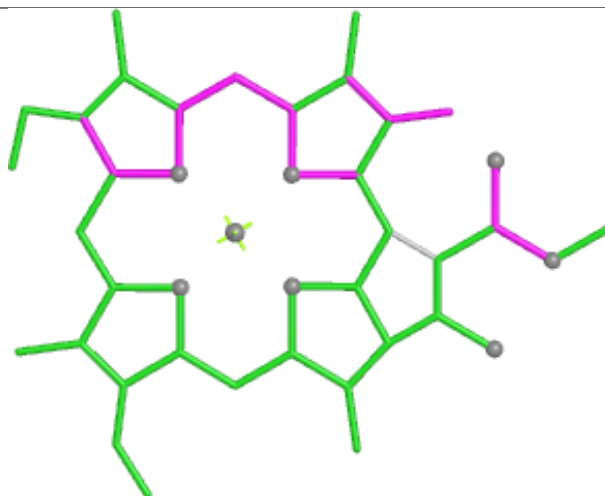


Rings

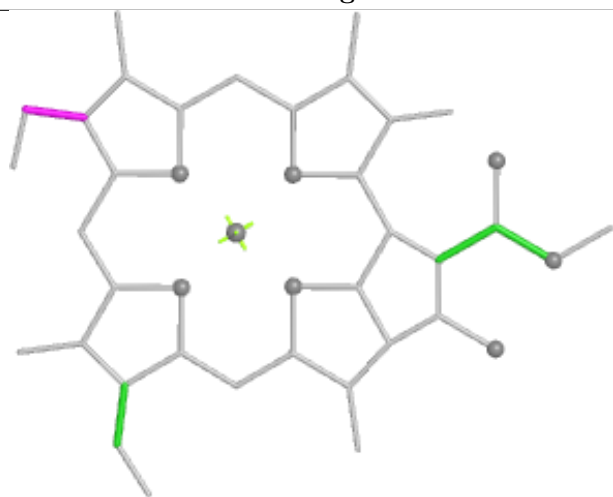
Ligand CLA 2 612



Bond lengths



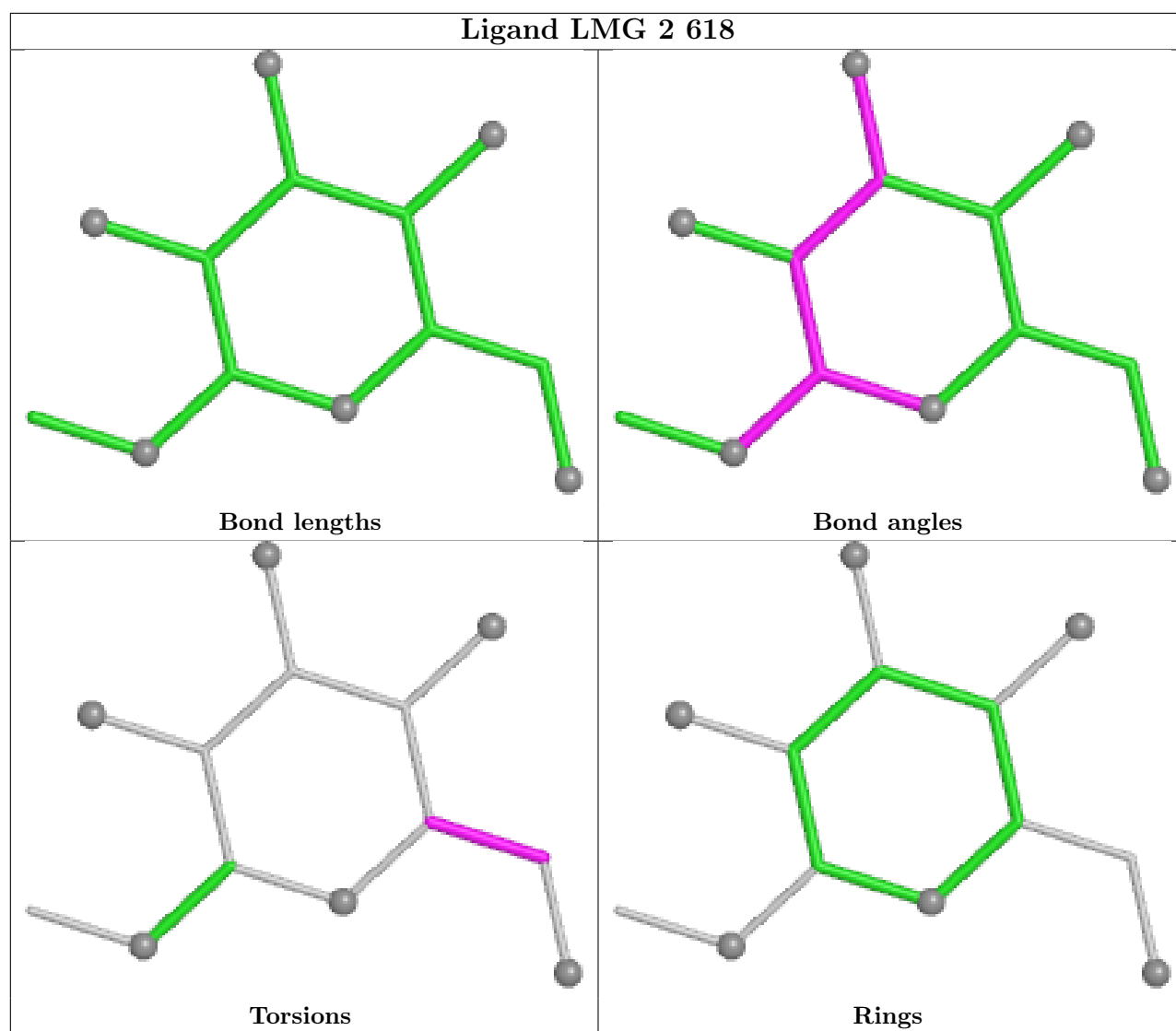
Bond angles



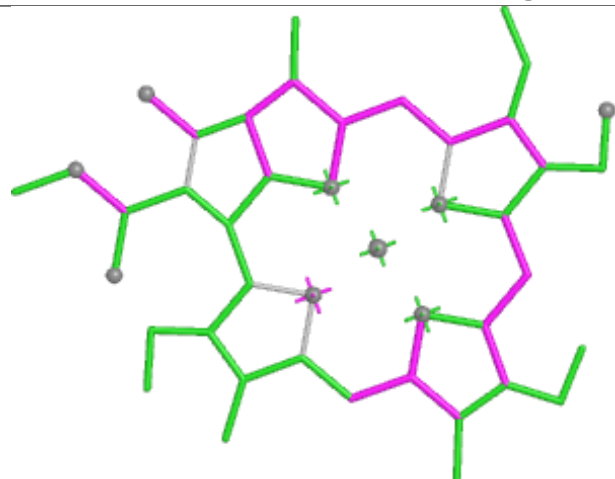
Torsions



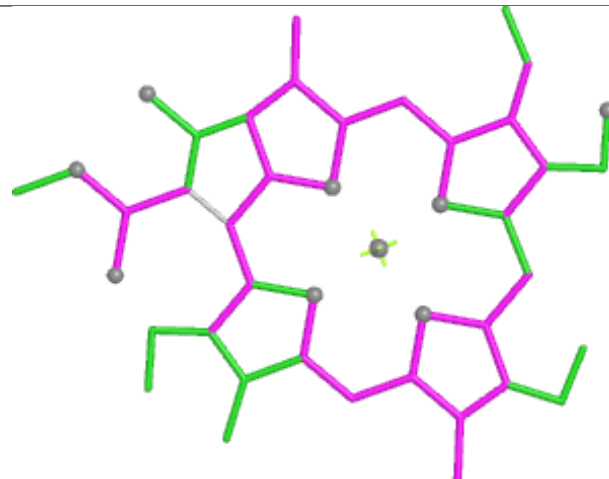
Rings



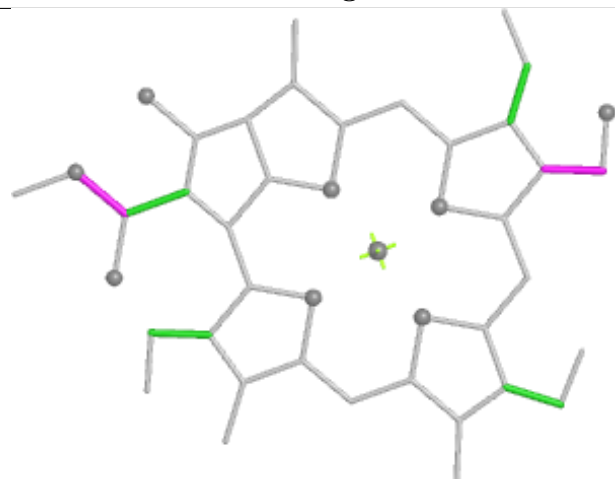
Ligand CHL 5 615



Bond lengths



Bond angles

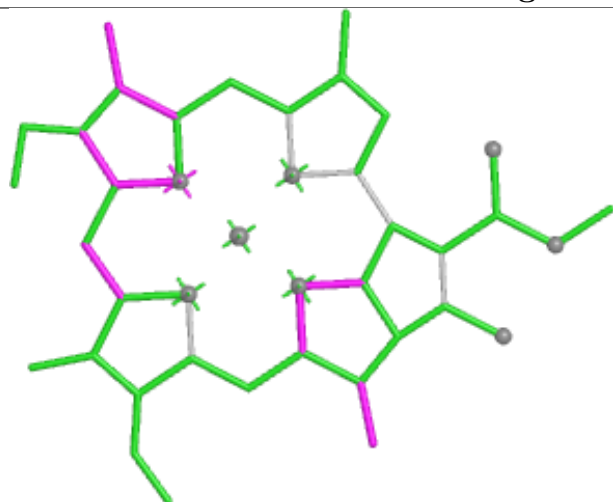


Torsions

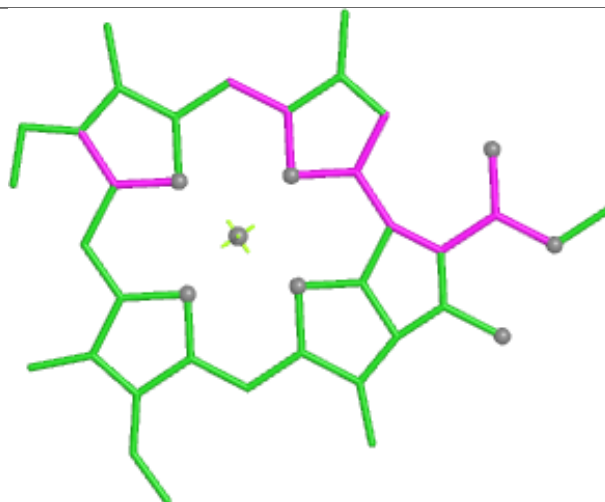


Rings

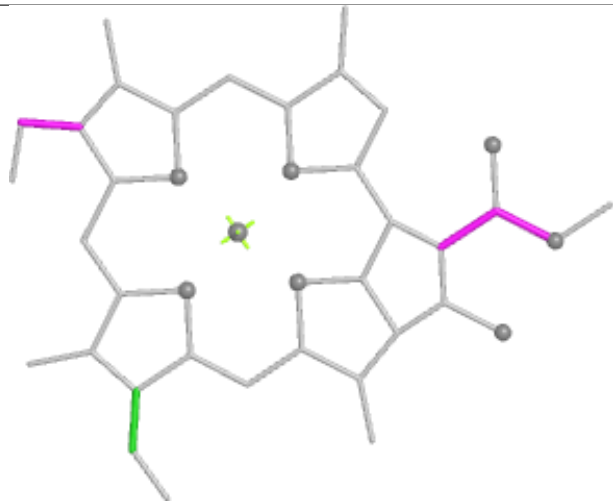
Ligand CLA 6 606



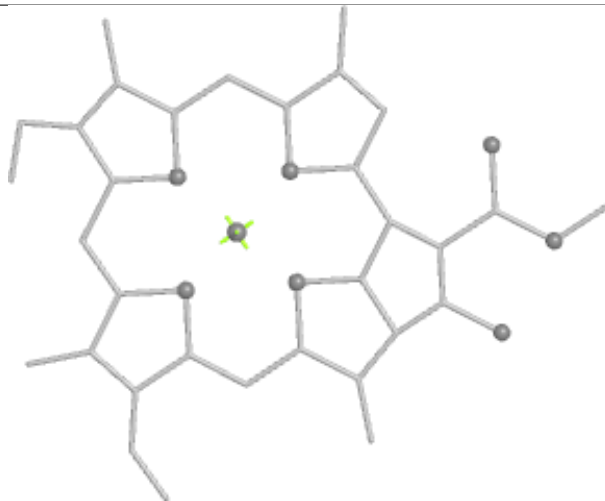
Bond lengths



Bond angles

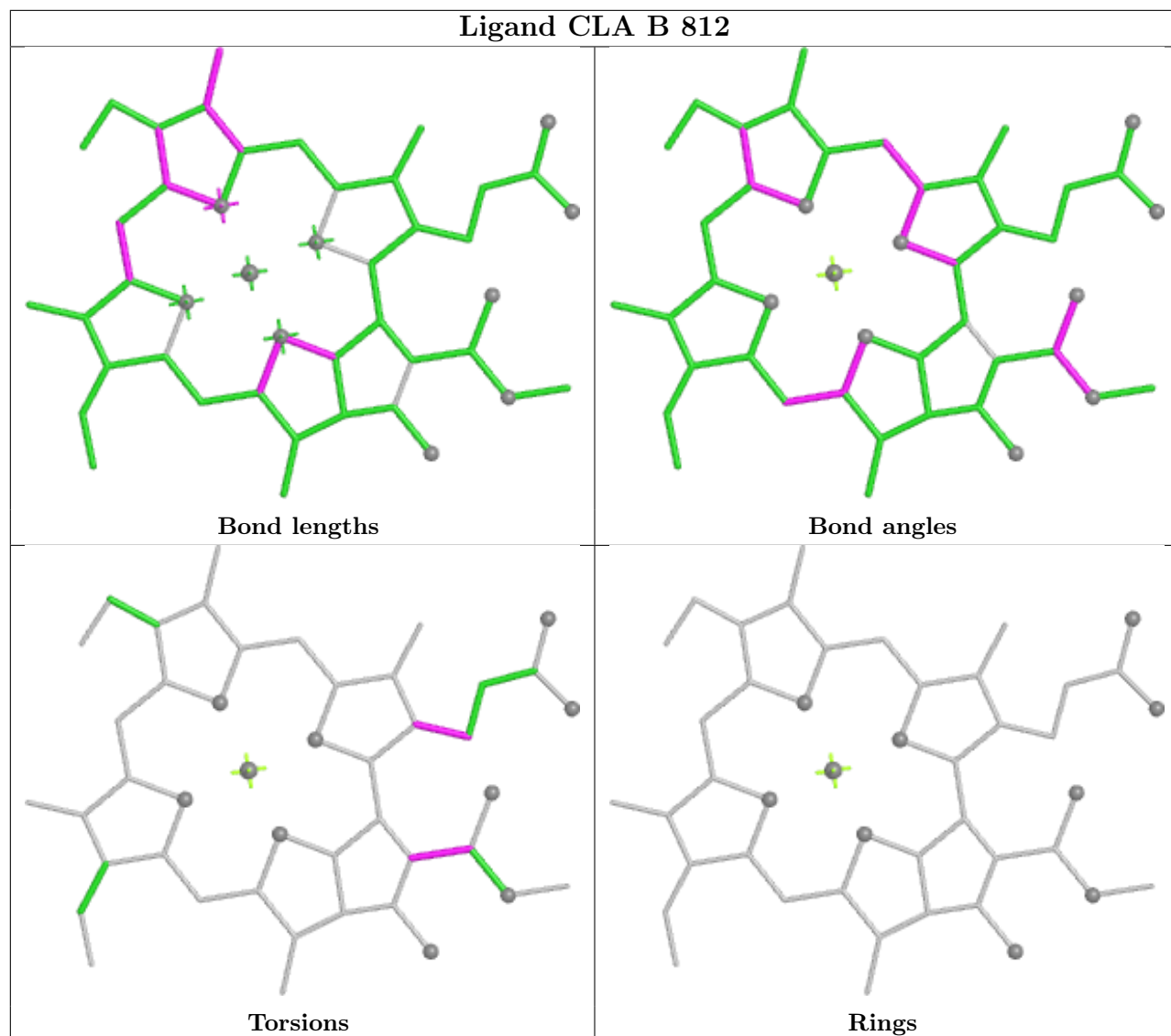


Torsions

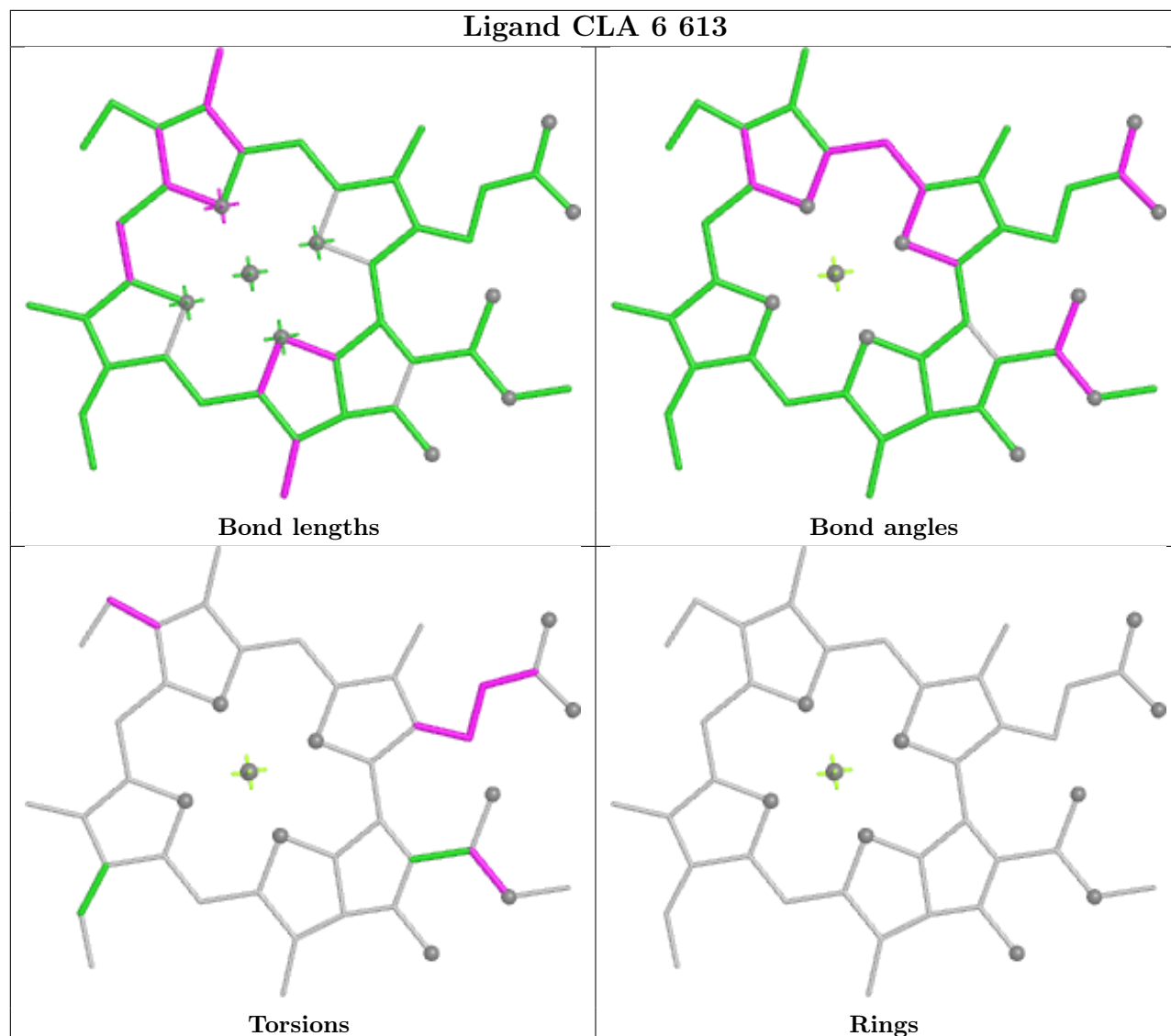


Rings

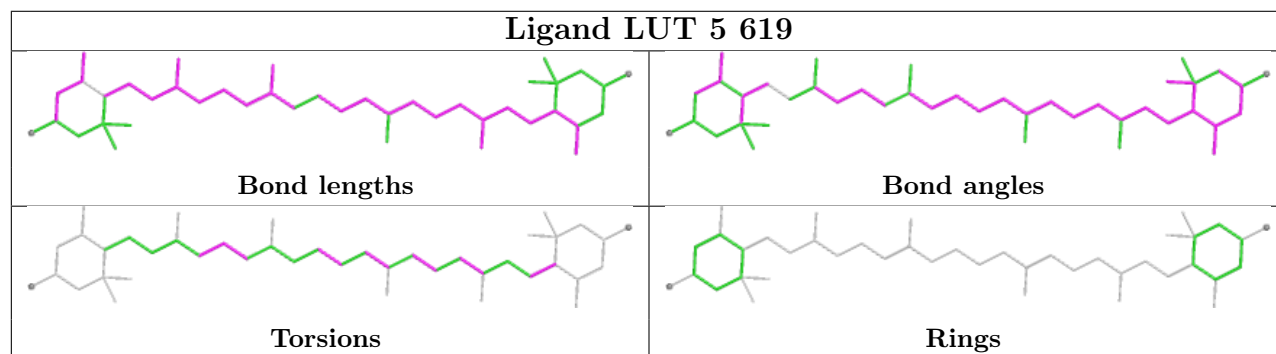
Ligand CLA B 812



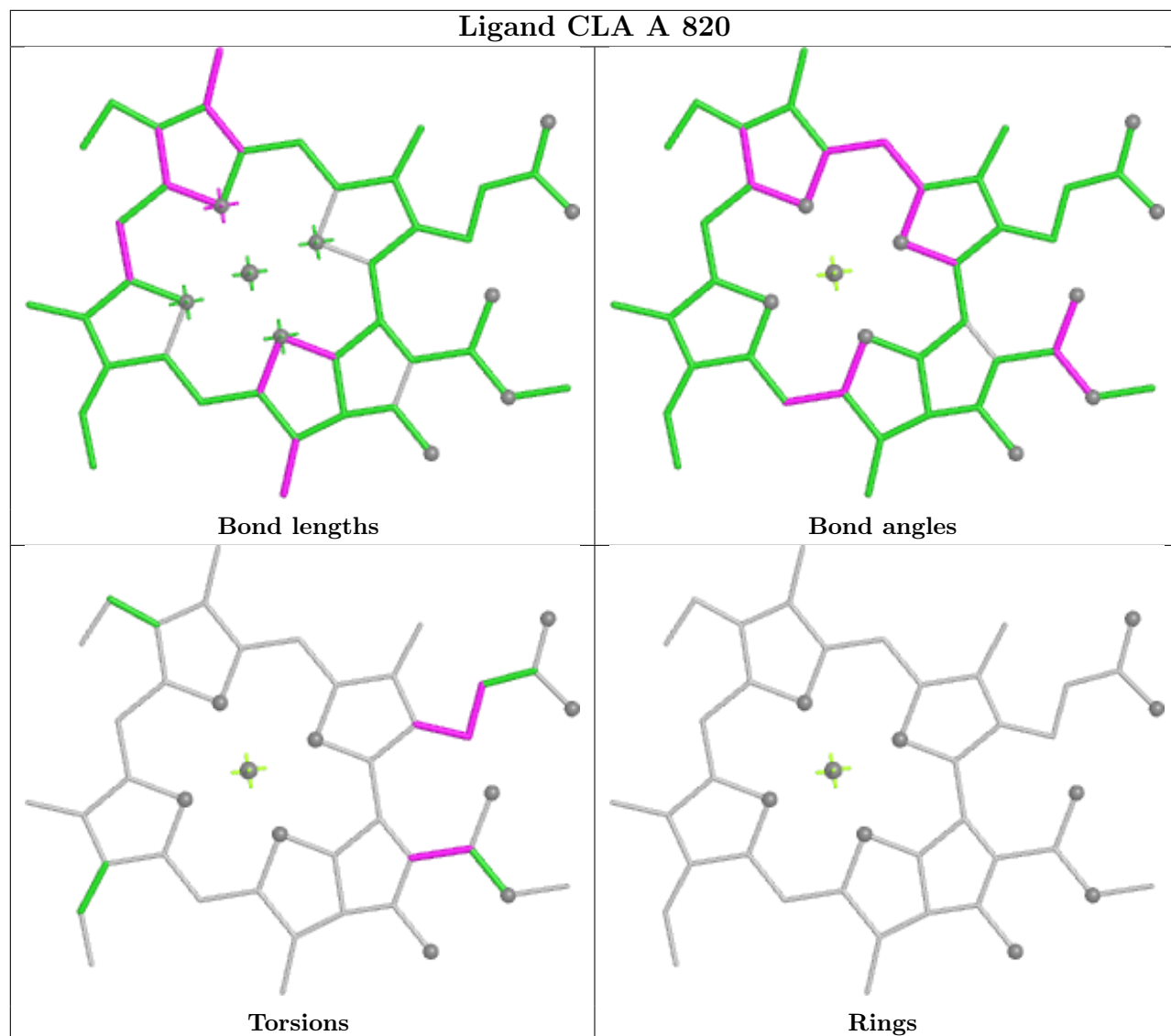
Ligand CLA 6 613



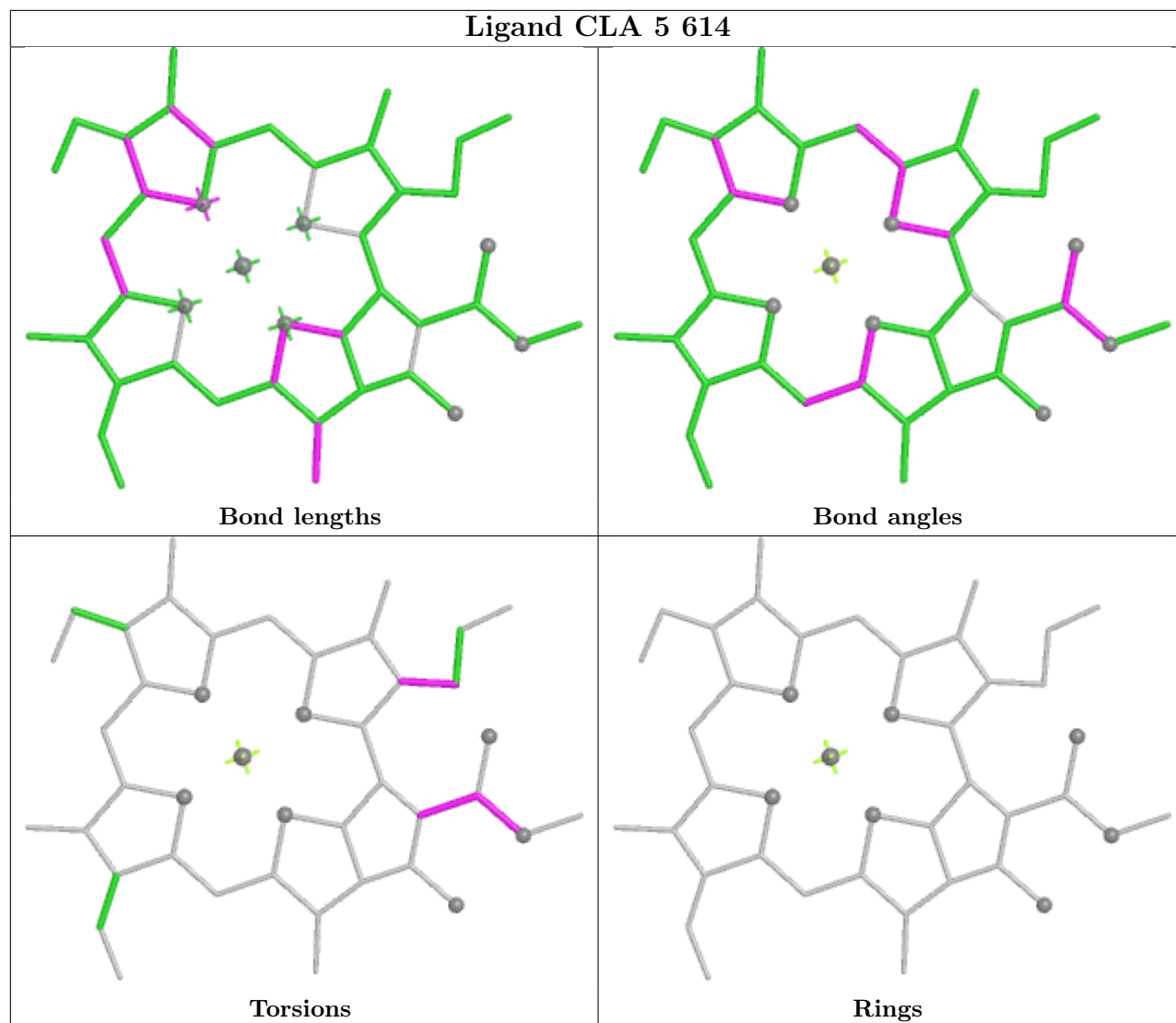
Ligand LUT 5 619



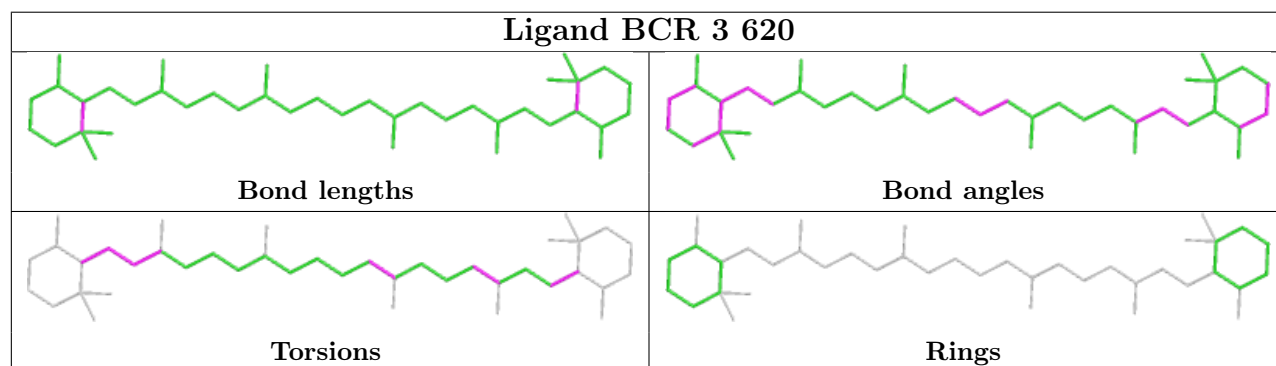
Ligand CLA A 820



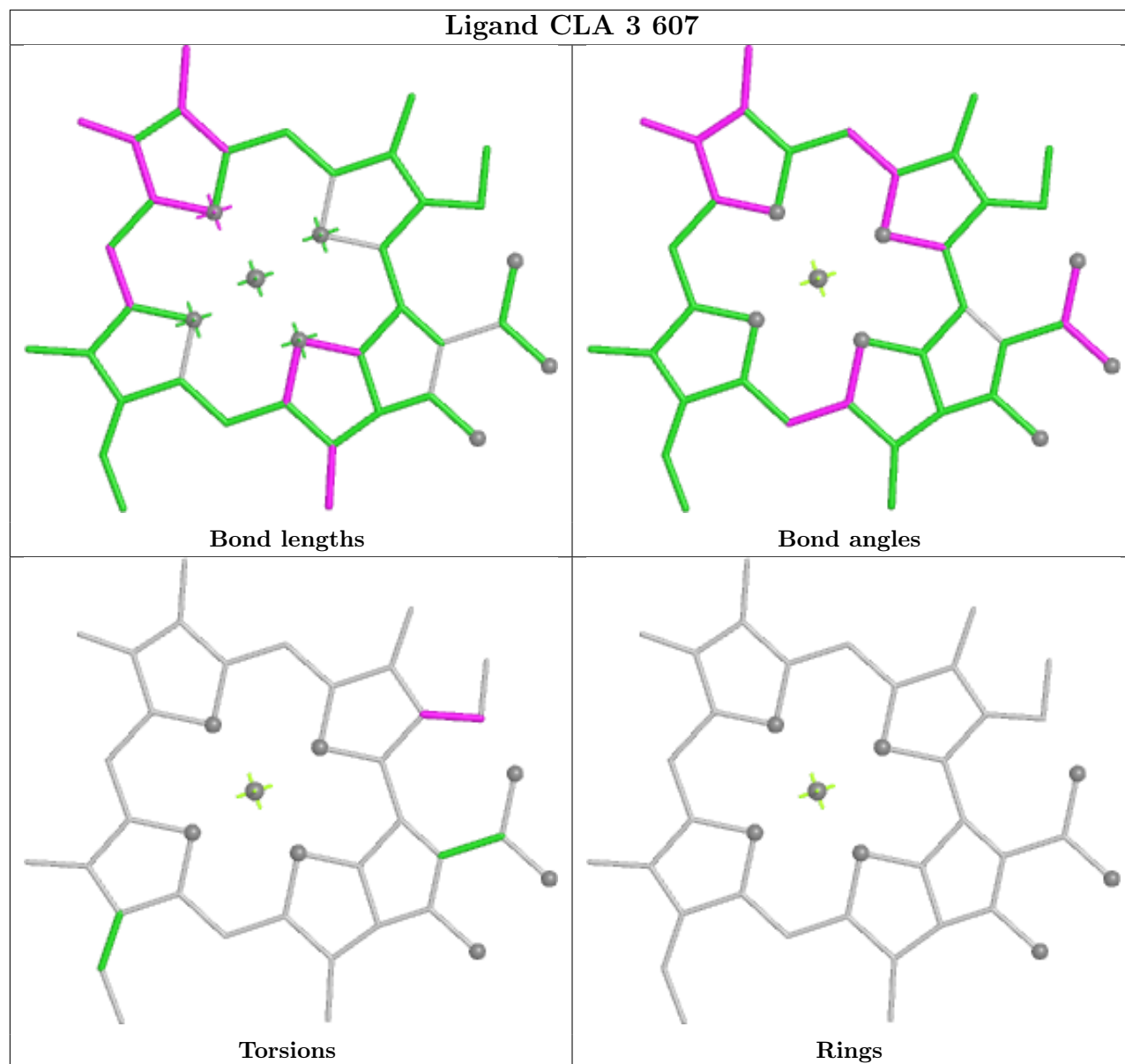
Ligand CLA 5 614



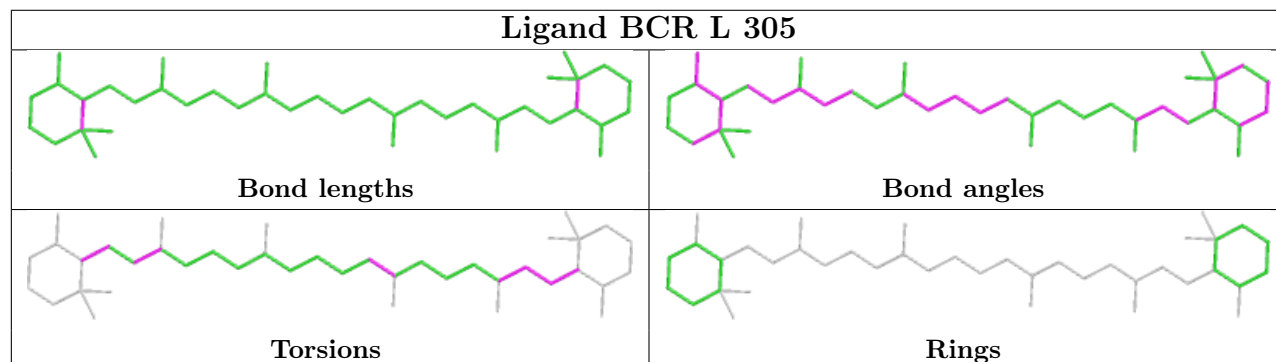
Ligand BCR 3 620

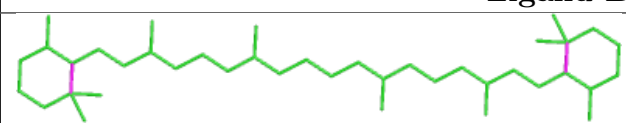
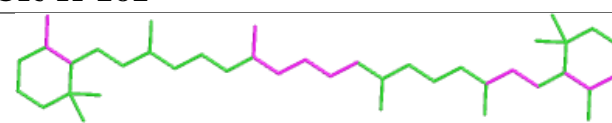
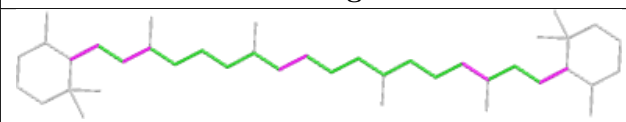
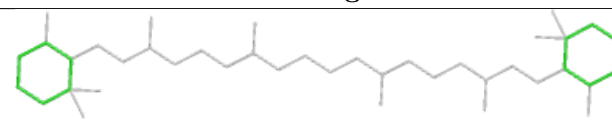


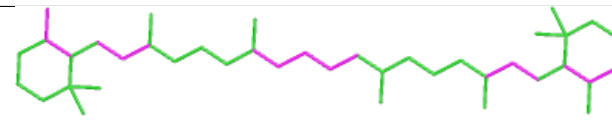
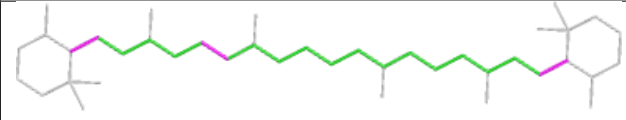
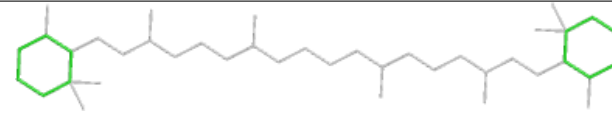
Ligand CLA 3 607

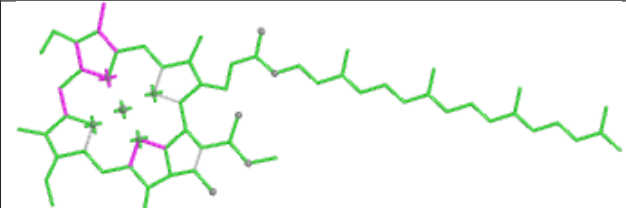
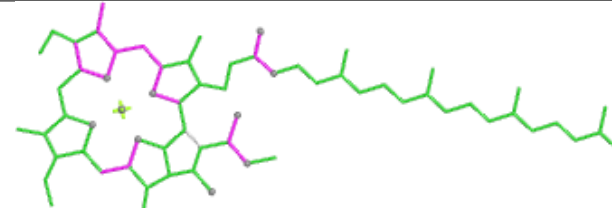
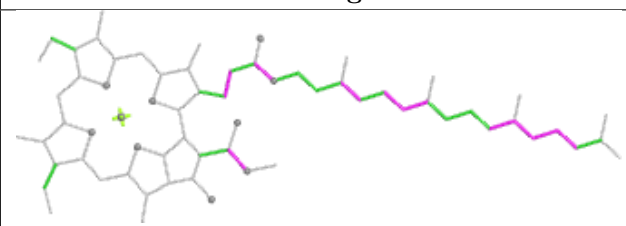
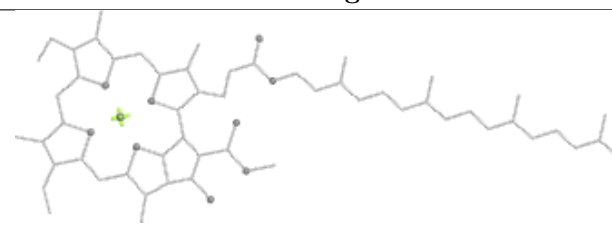


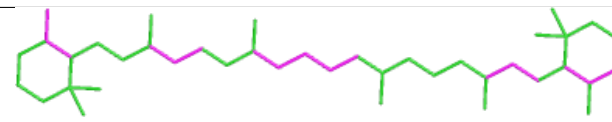
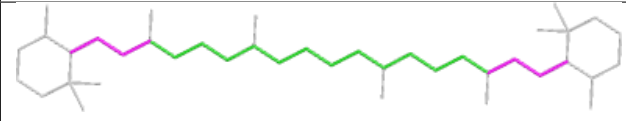
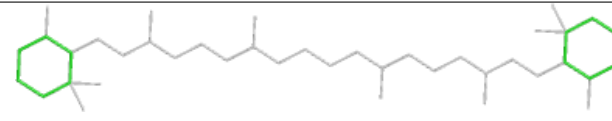
Ligand BCR L 305

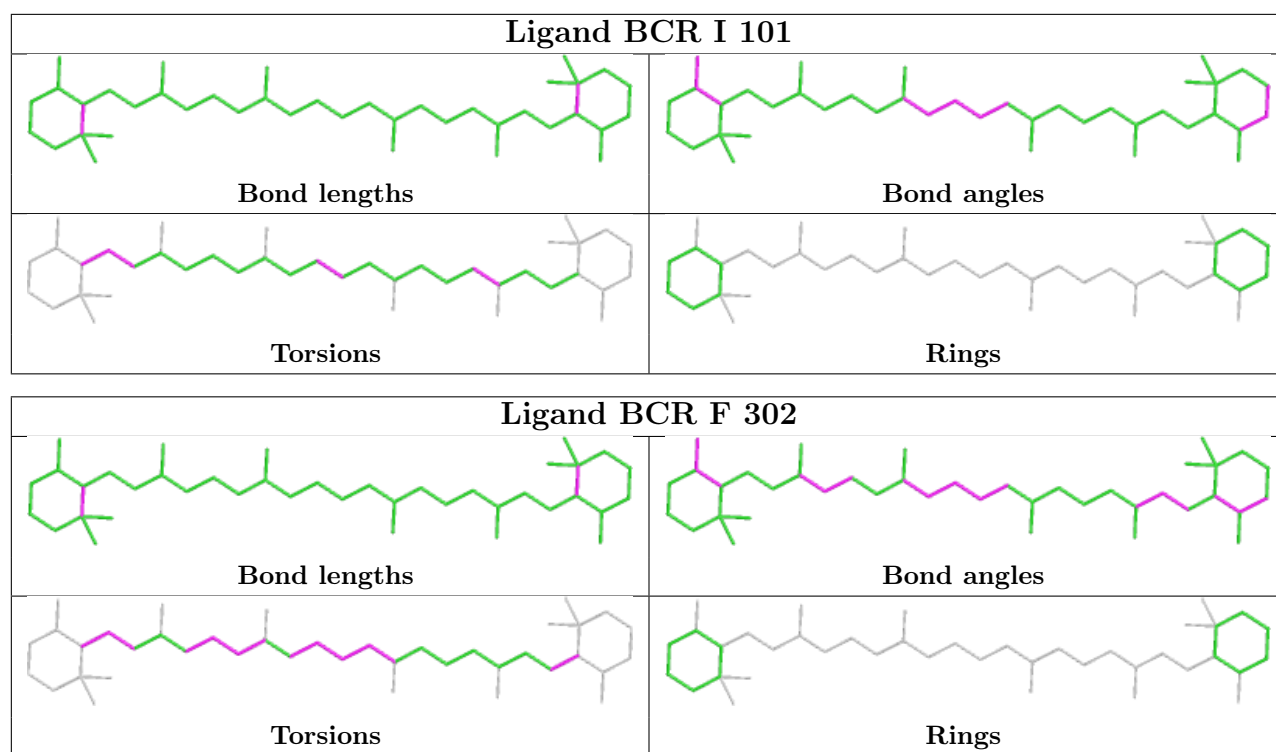


Ligand BCR K 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

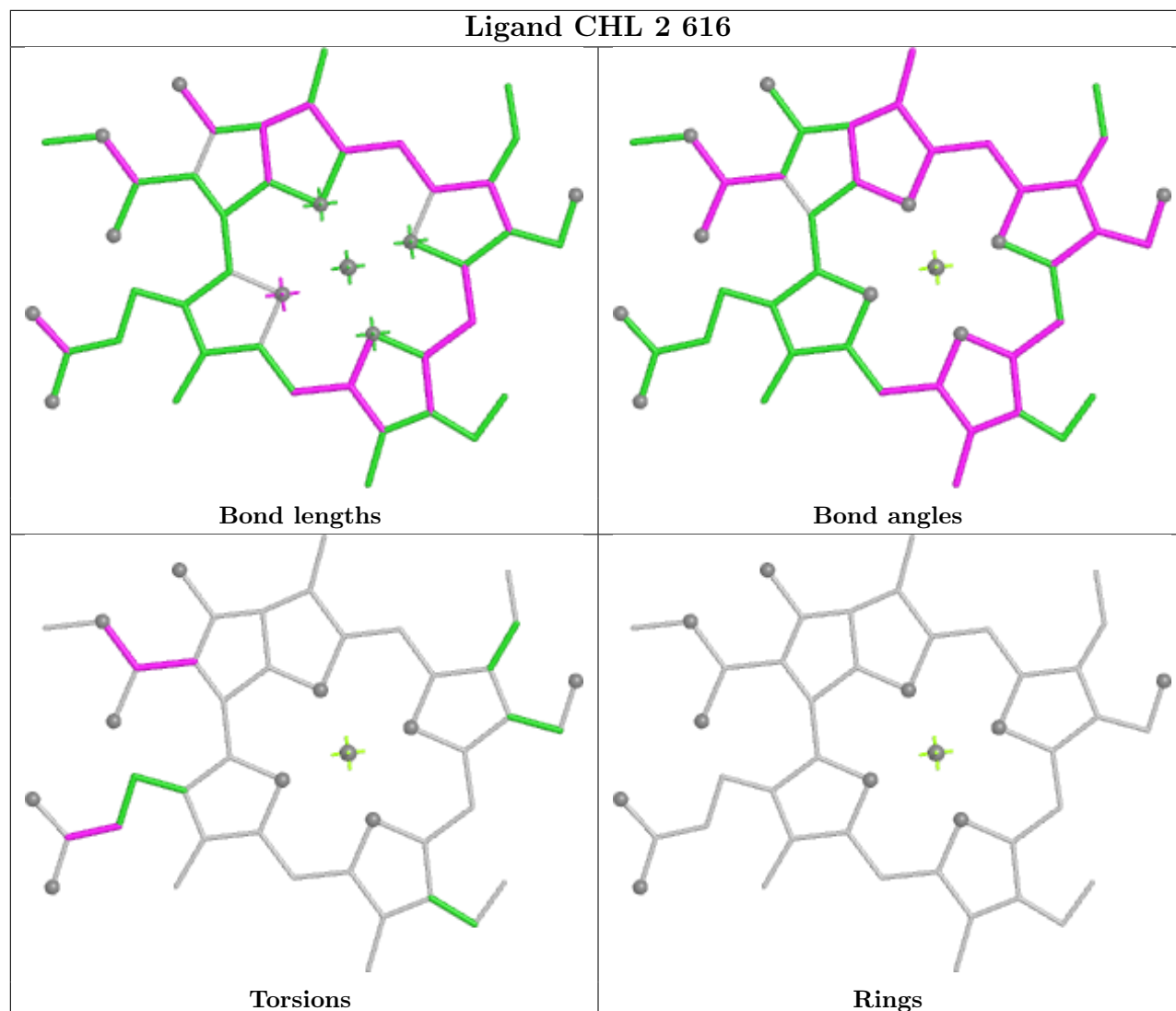
Ligand BCR G 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

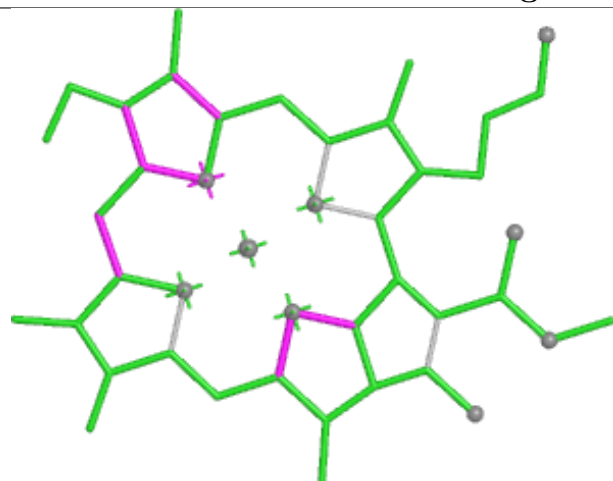
Ligand BCR 3 622	
	
Bond lengths	Bond angles
	
Torsions	Rings



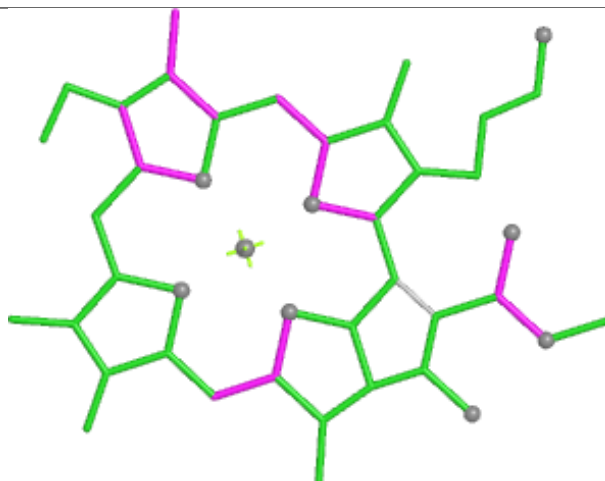
Ligand CHL 2 616



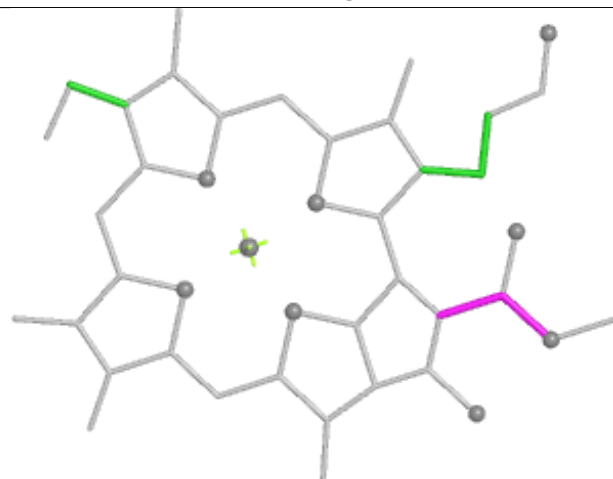
Ligand CLA 5 604



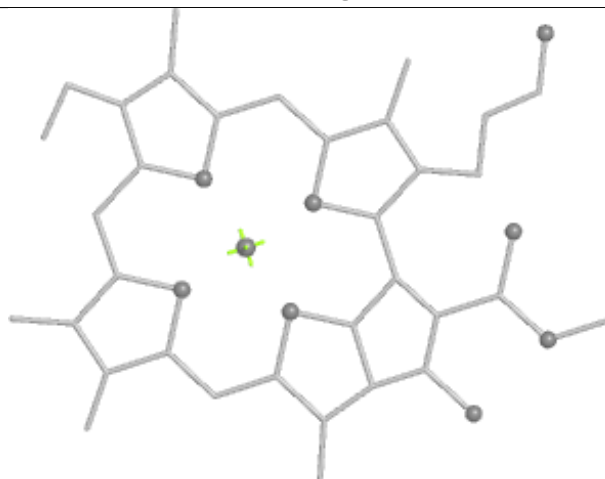
Bond lengths



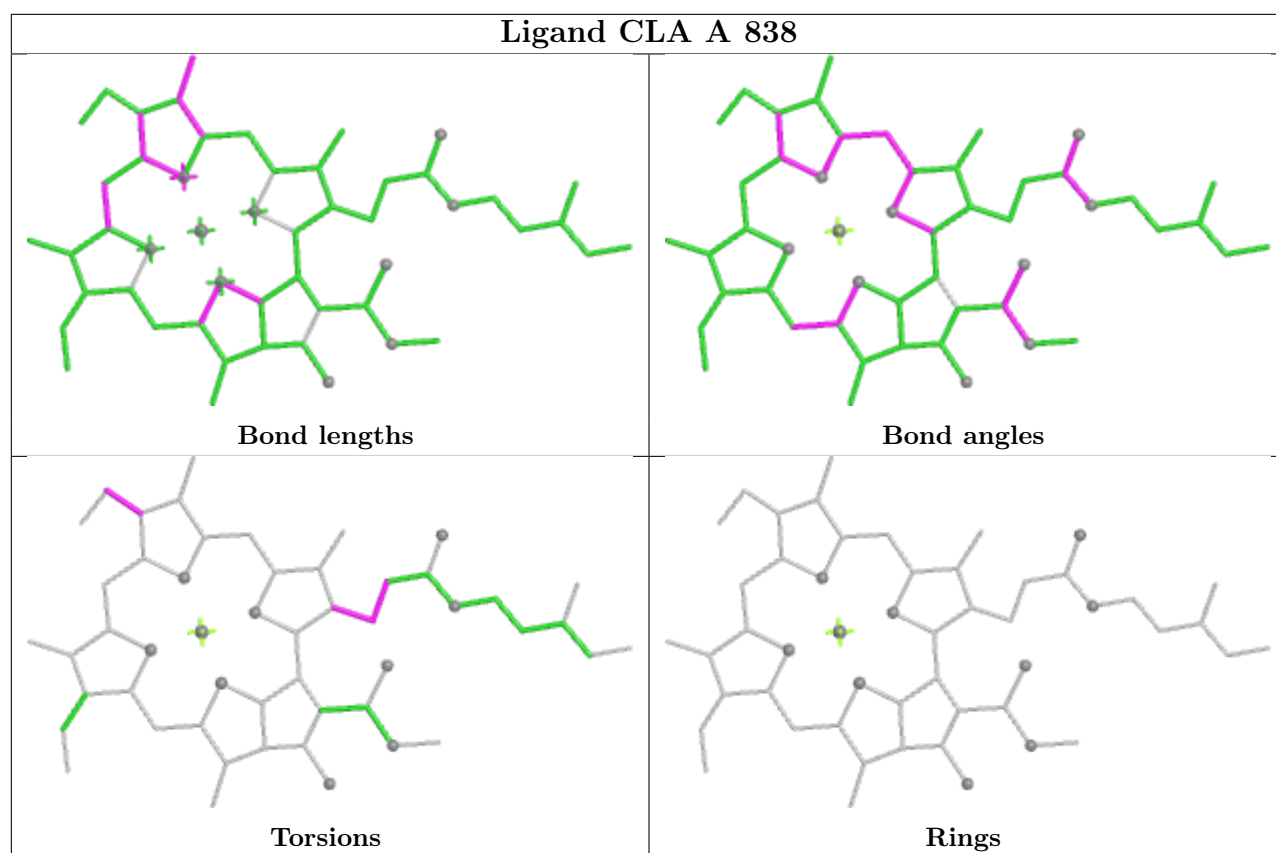
Bond angles



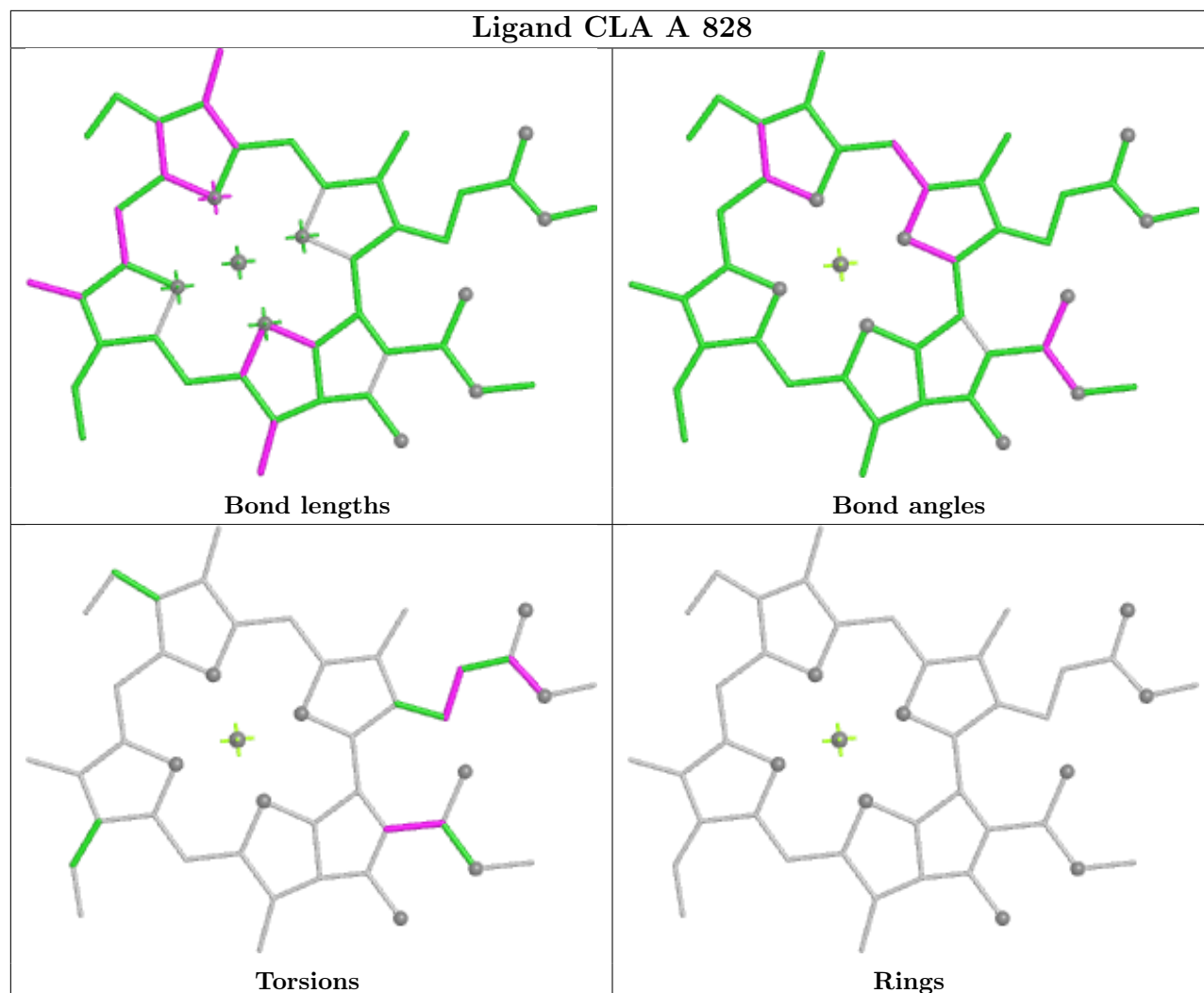
Torsions

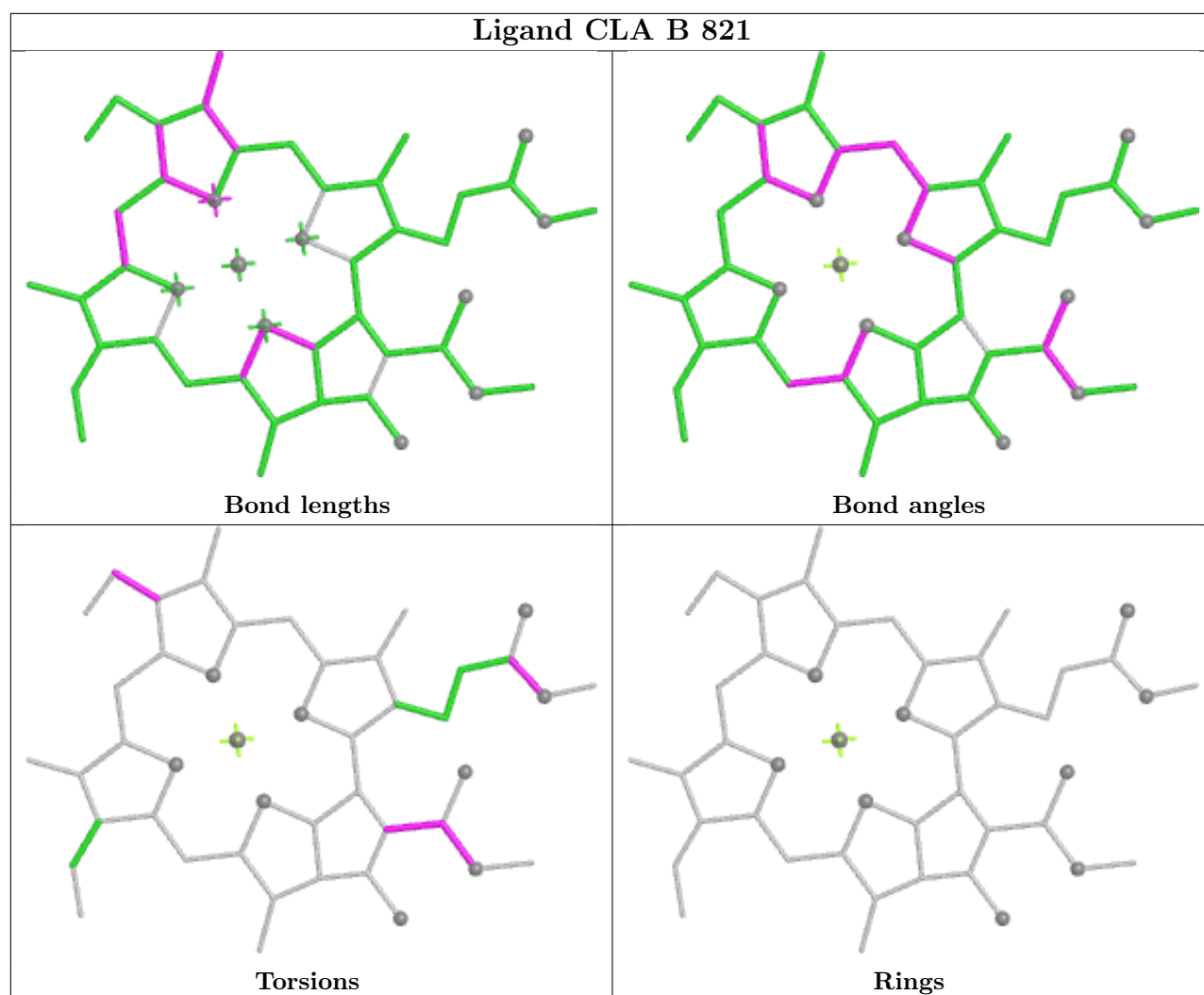


Rings

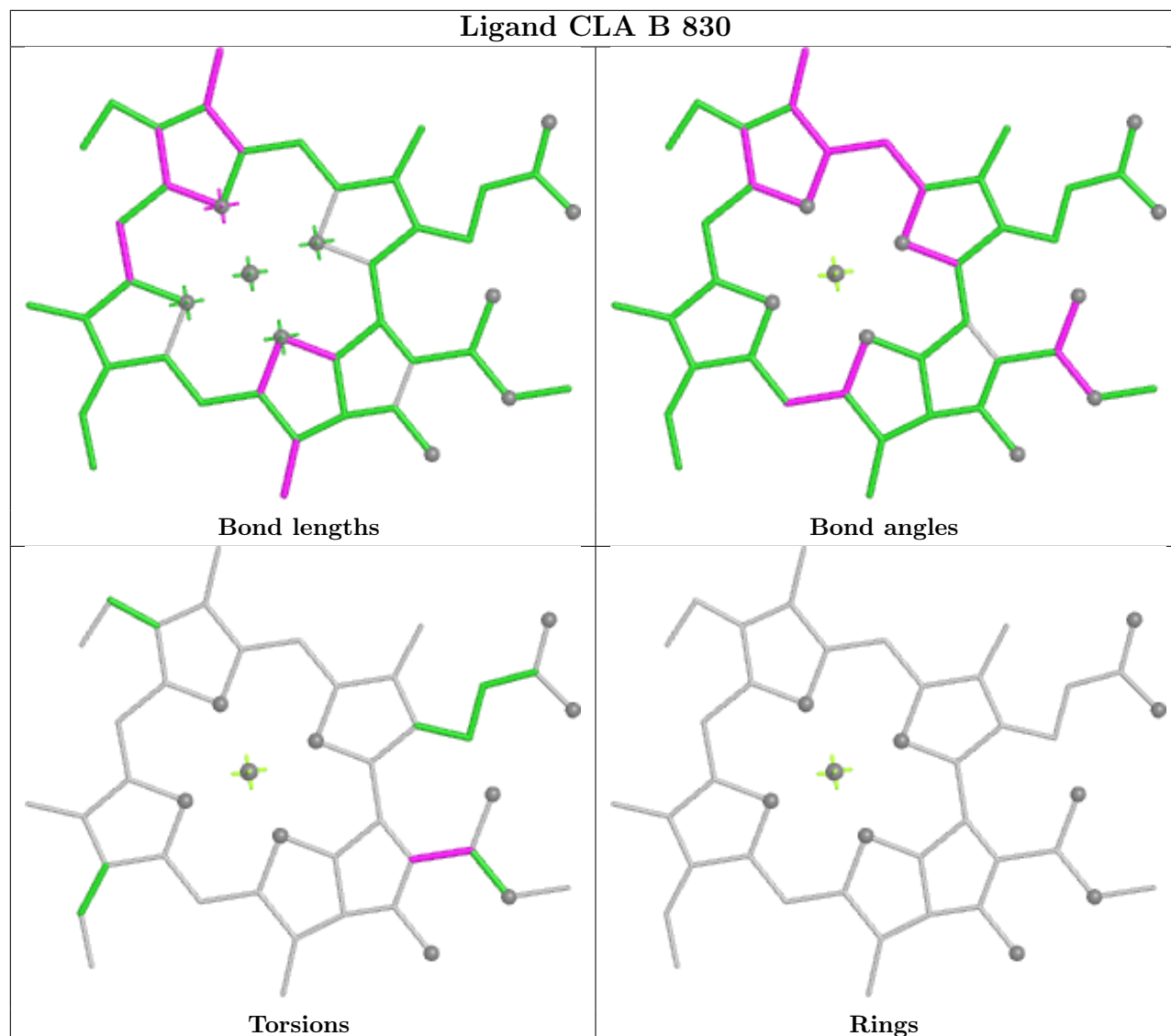


Ligand CLA A 828

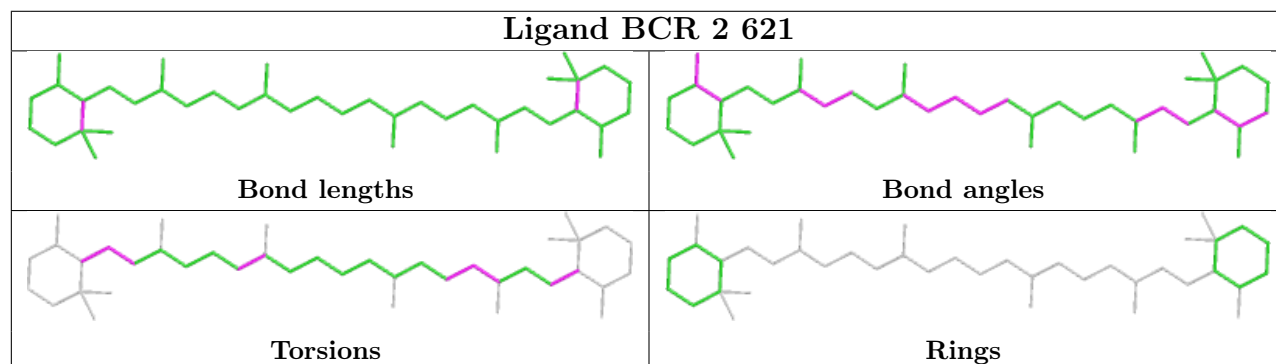




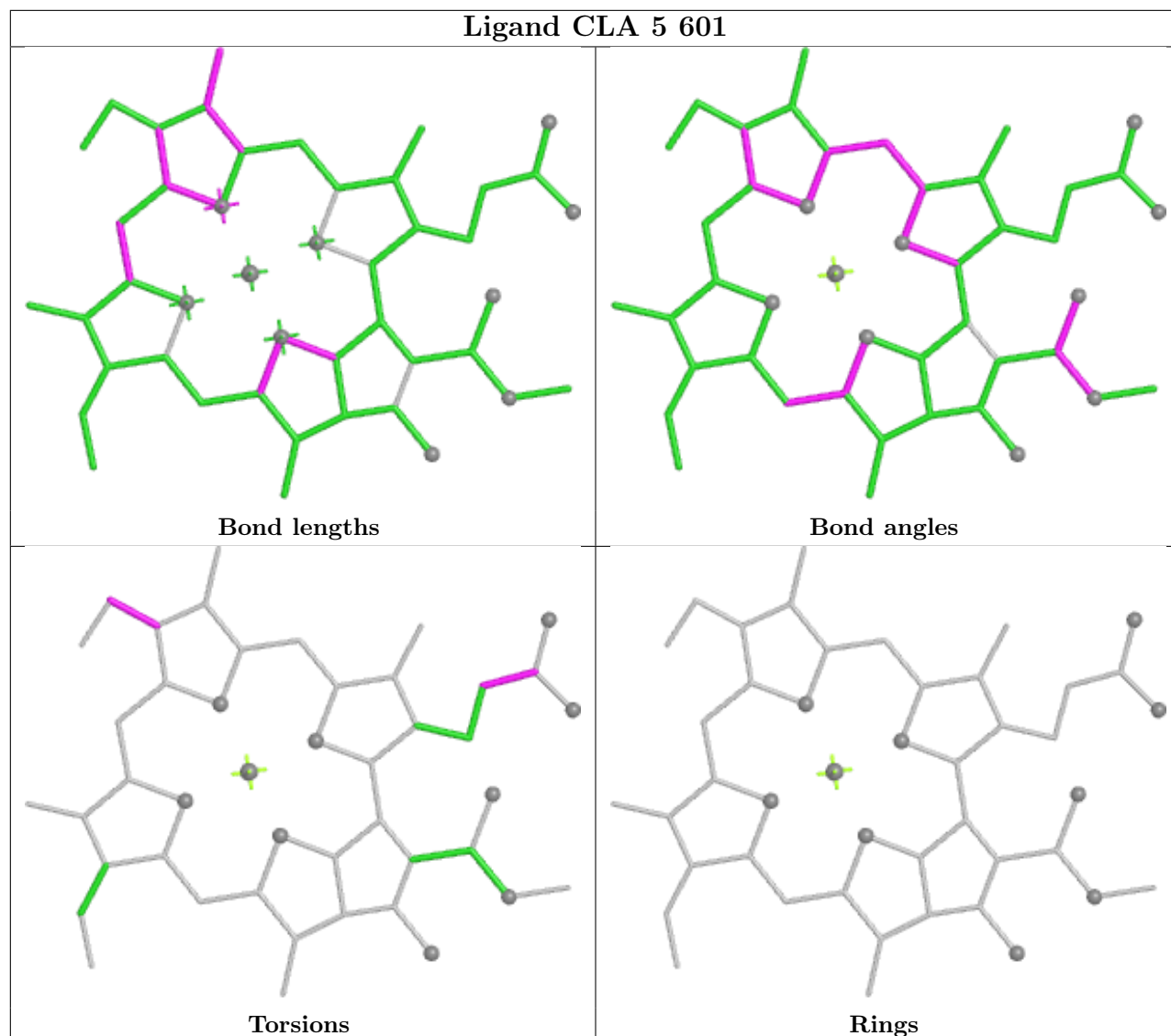
Ligand CLA B 830



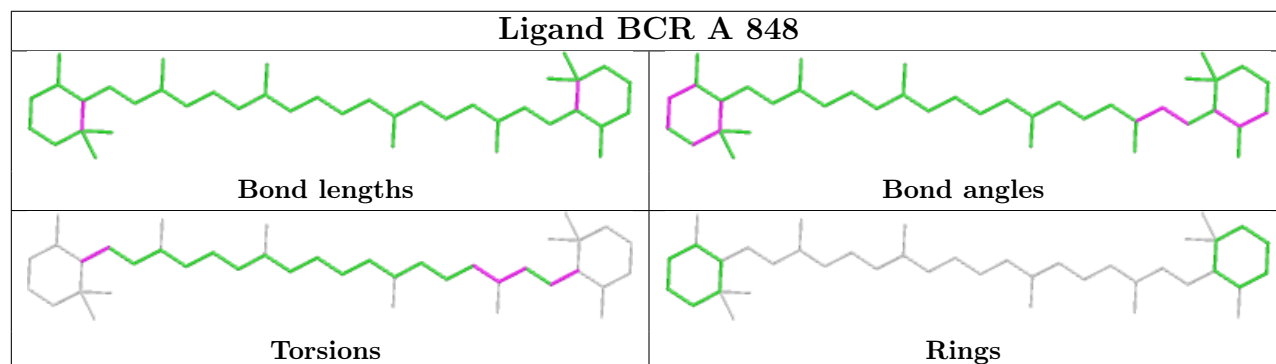
Ligand BCR 2 621

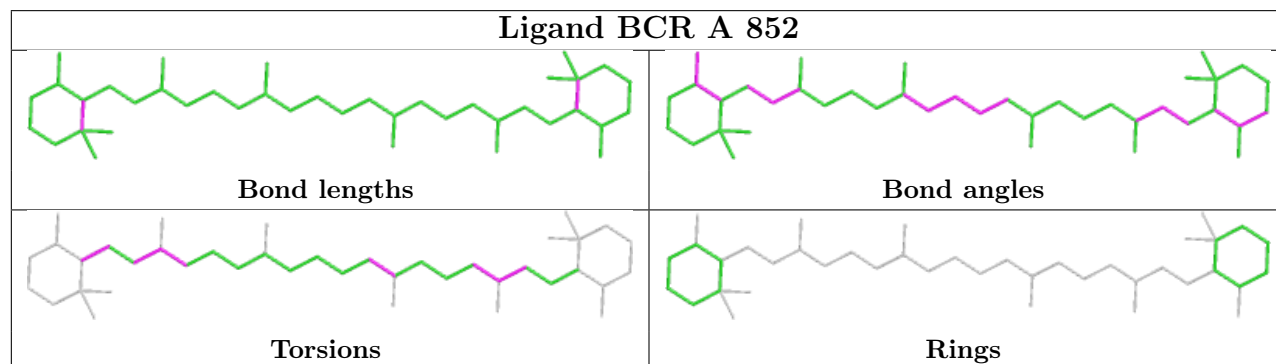
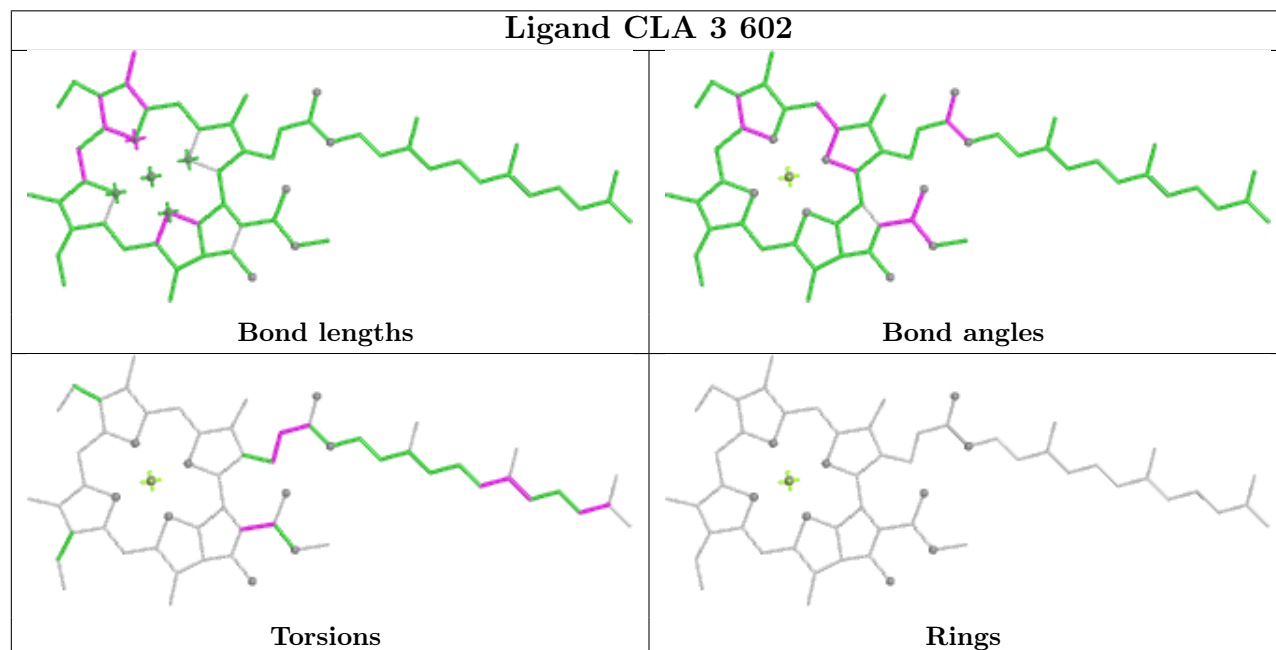
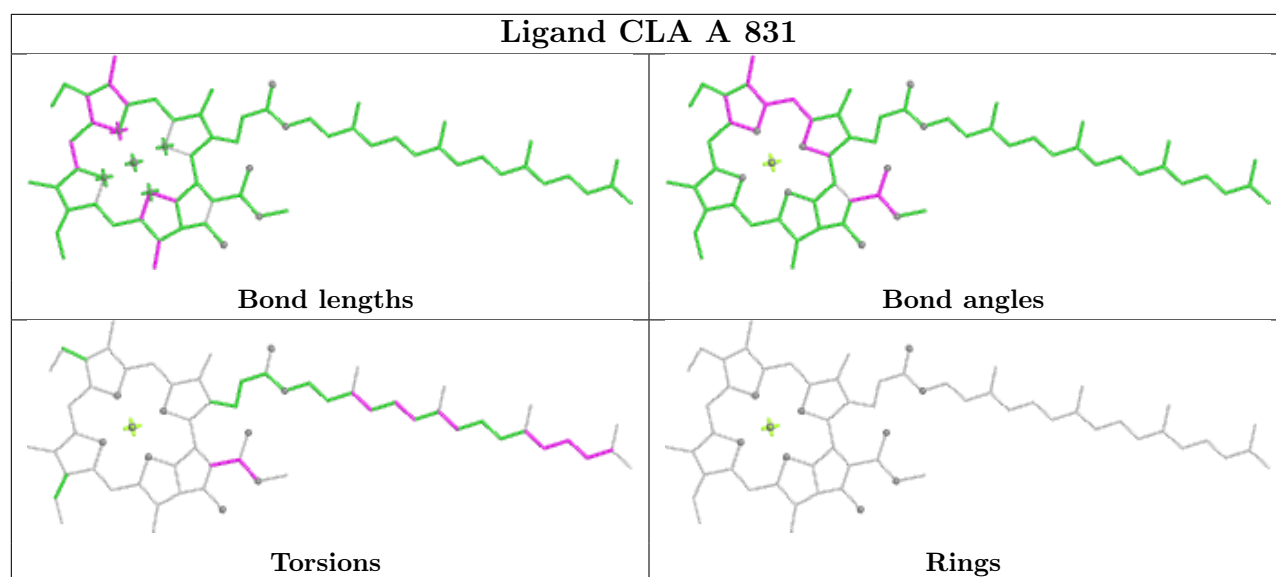


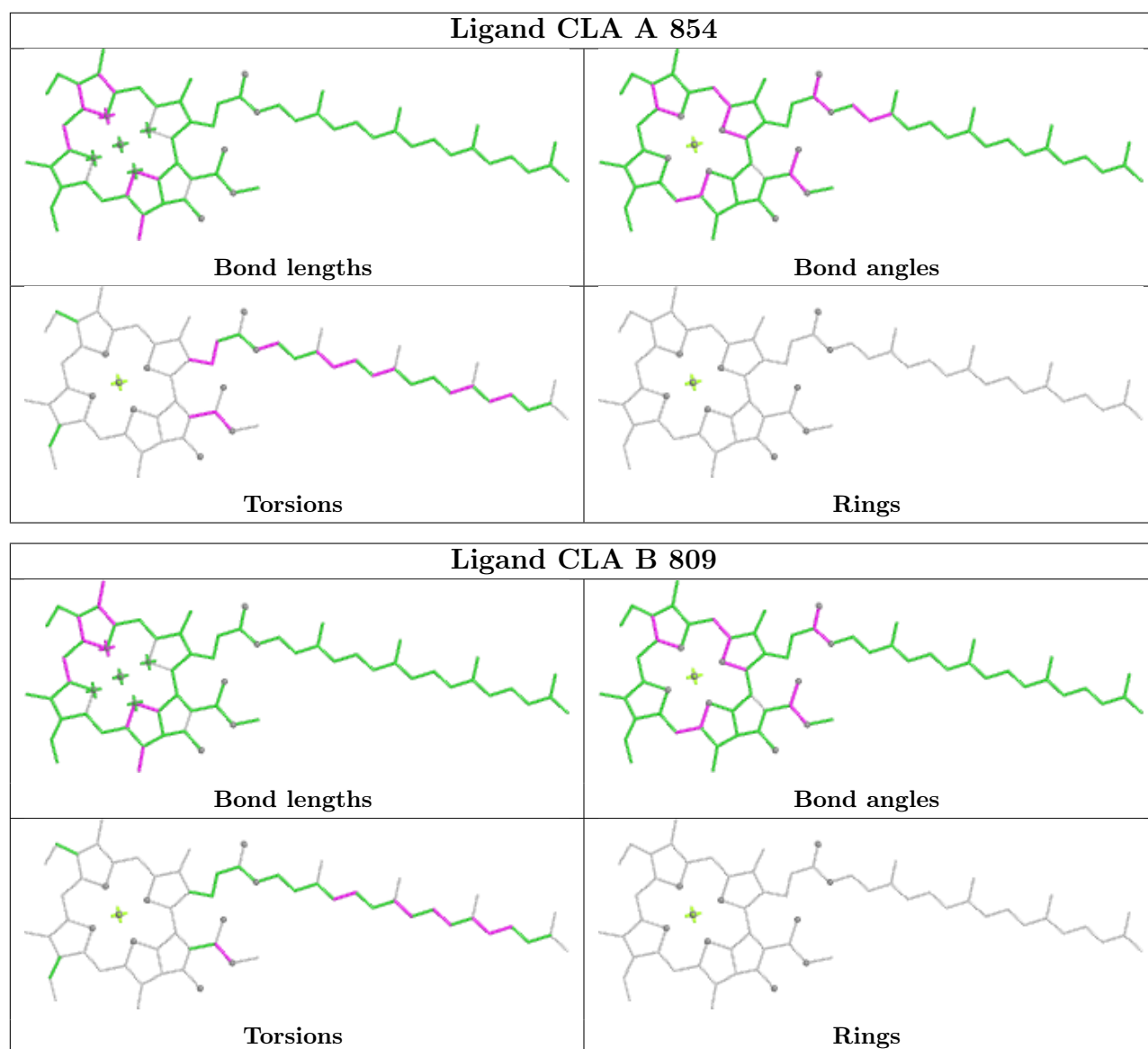
Ligand CLA 5 601

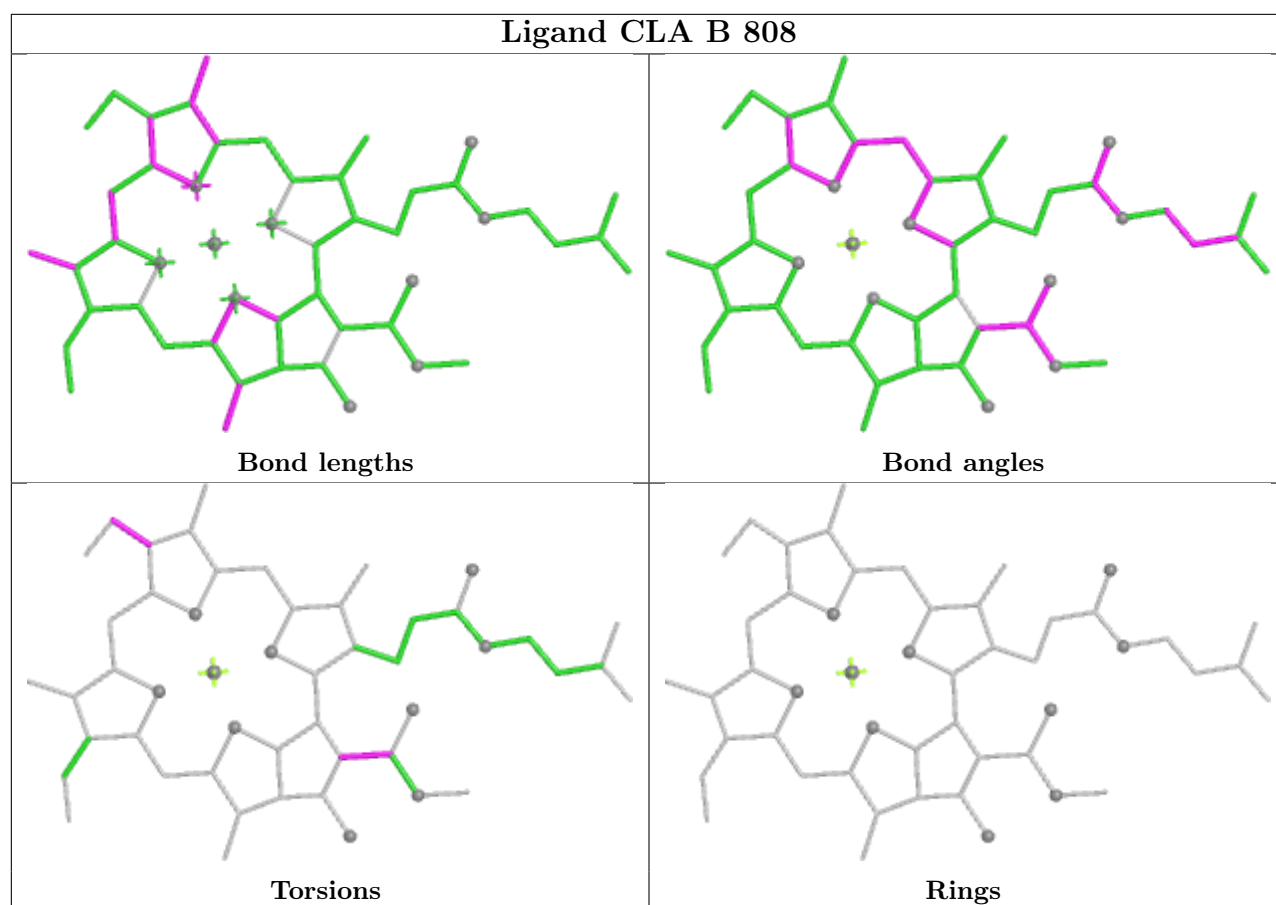


Ligand BCR A 848

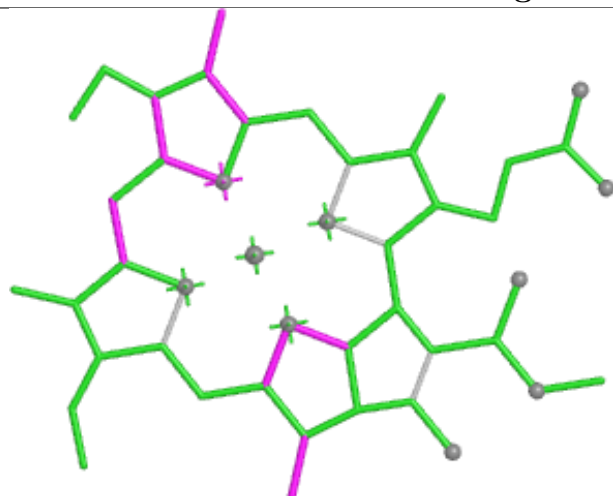




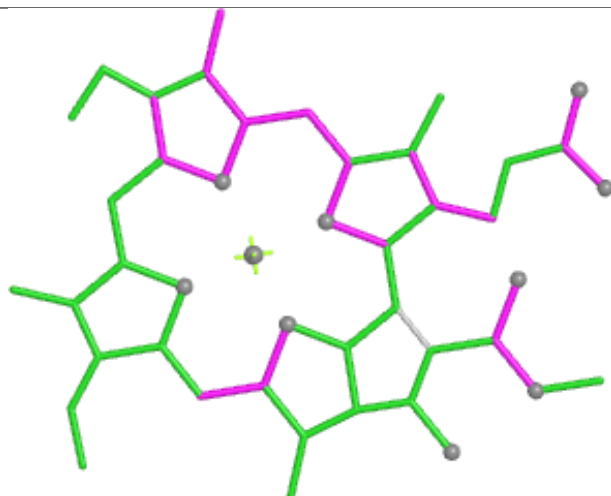




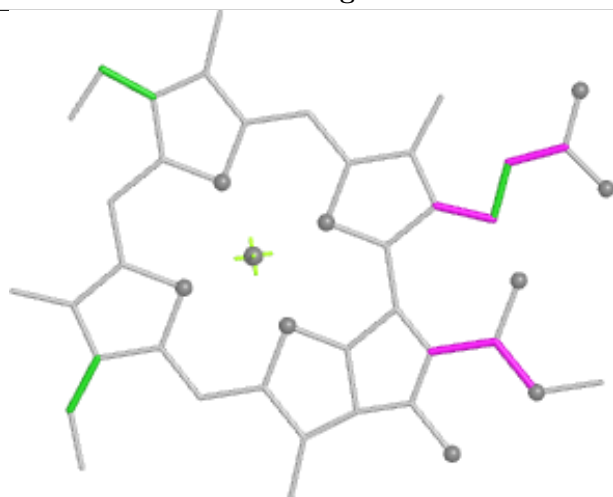
Ligand CLA B 833



Bond lengths



Bond angles

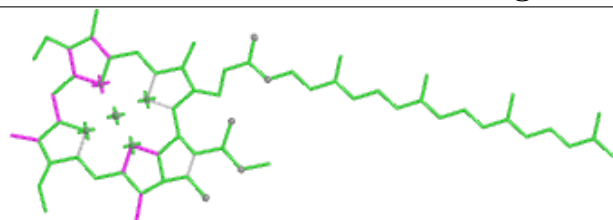


Torsions

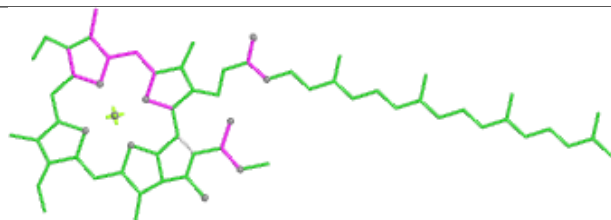


Rings

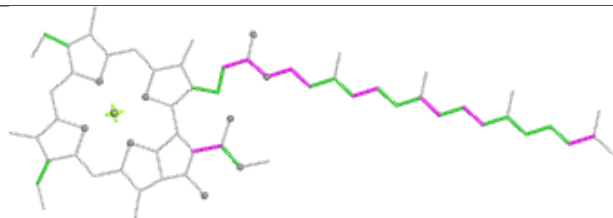
Ligand CLA A 806



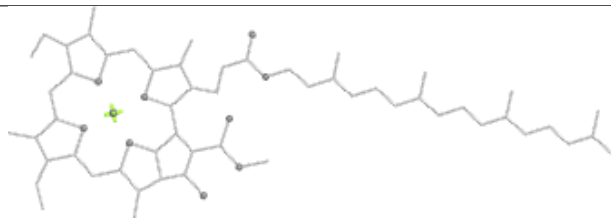
Bond lengths



Bond angles

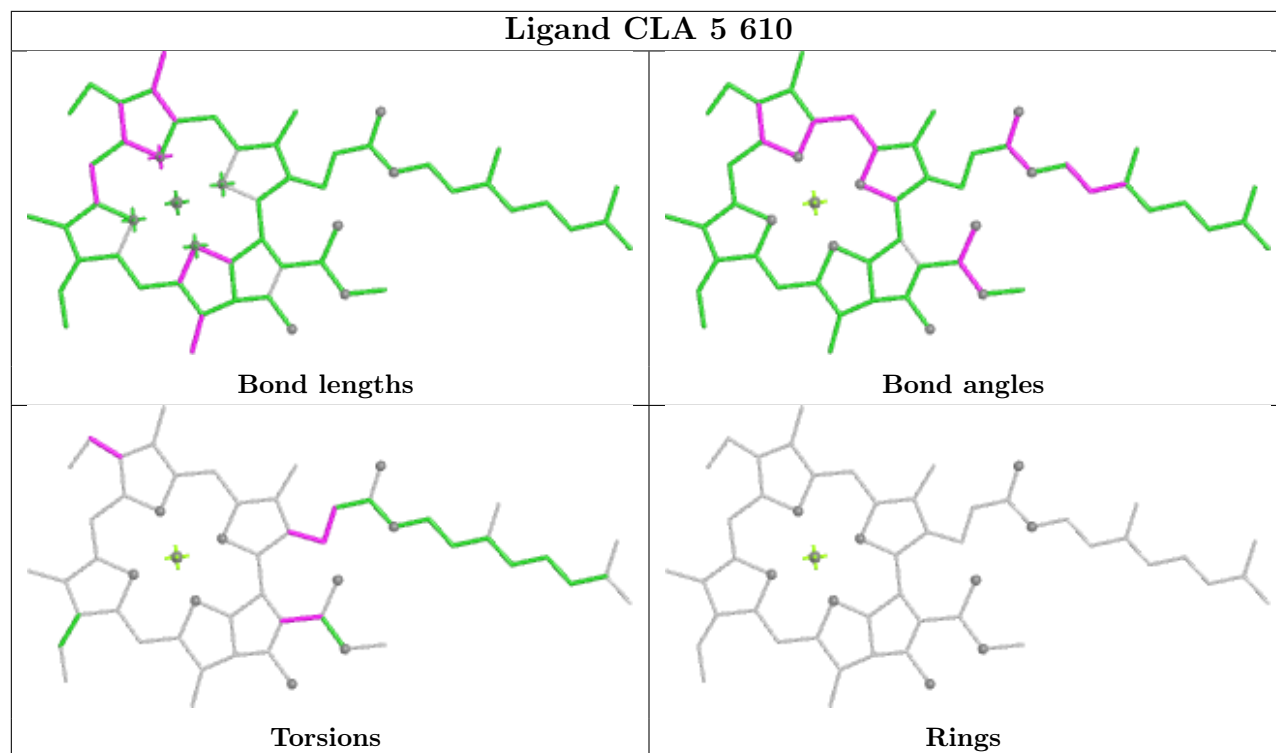


Torsions

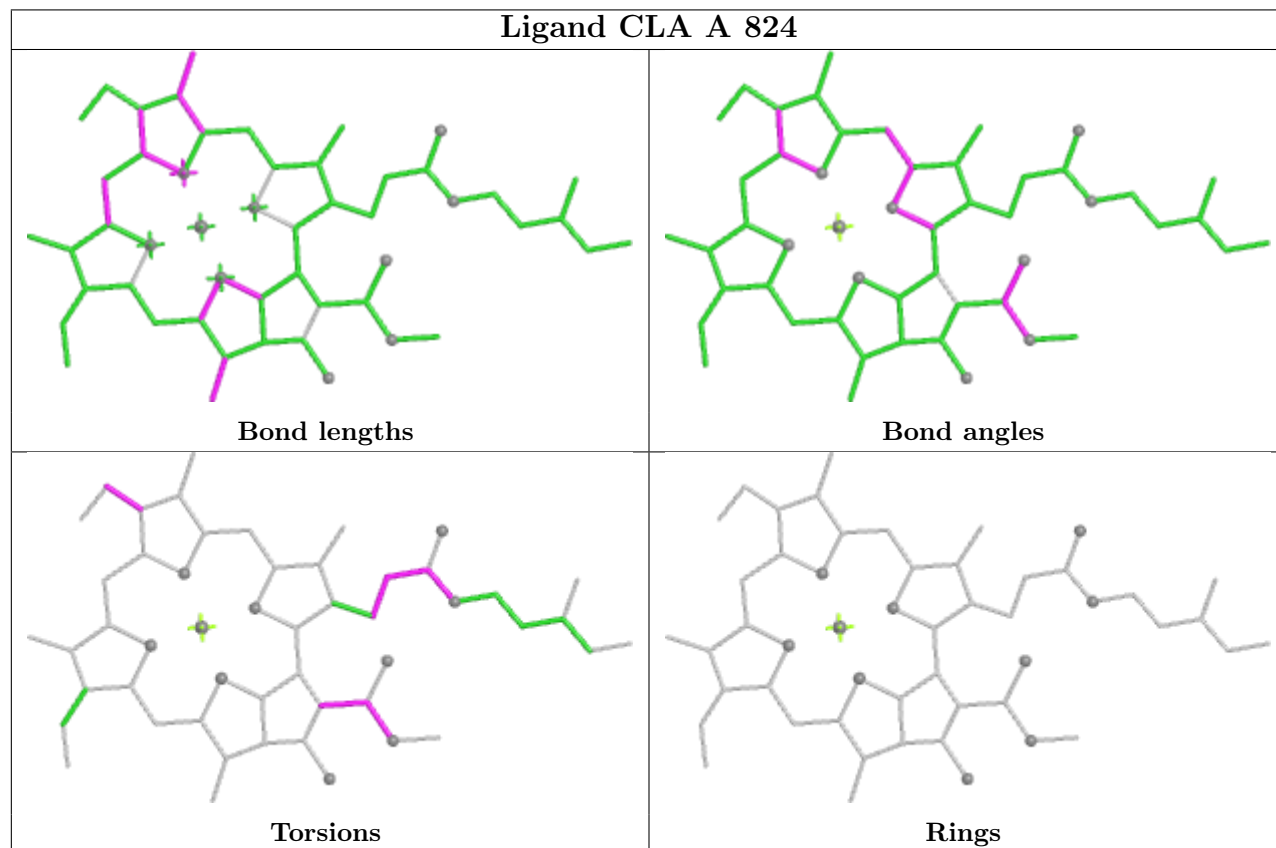


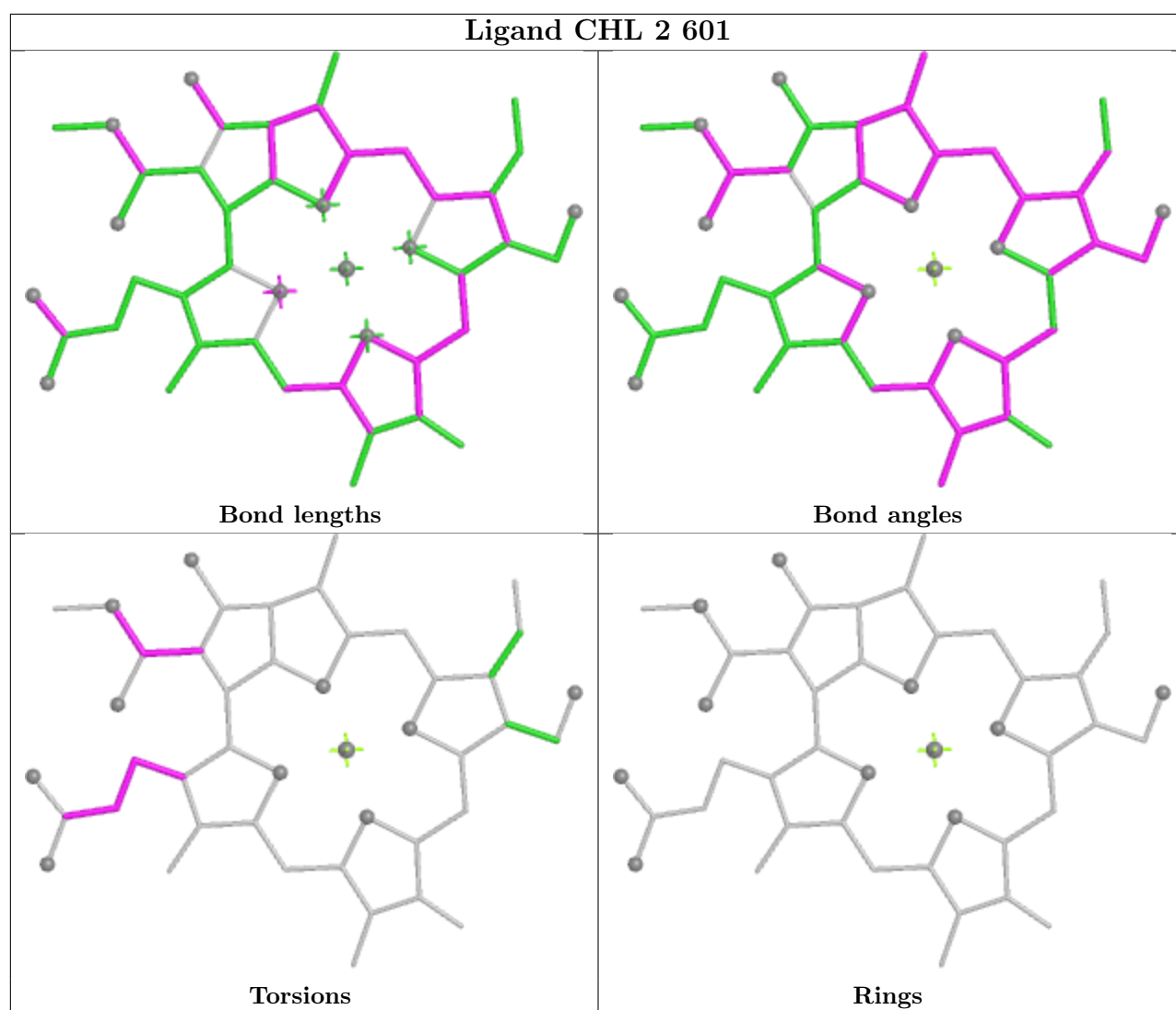
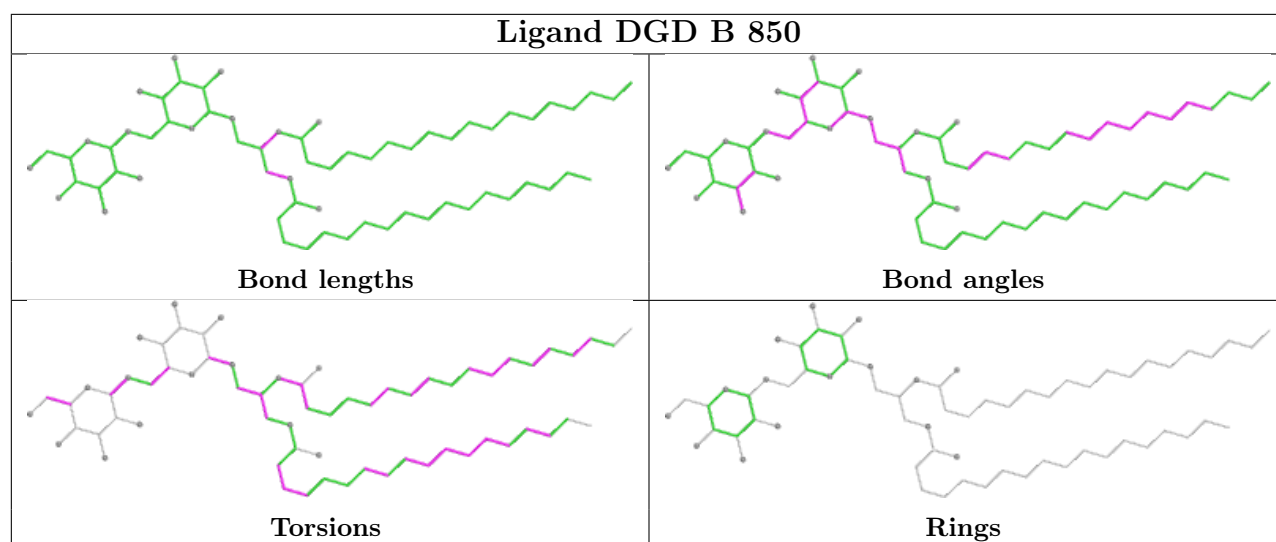
Rings

Ligand CLA 5 610

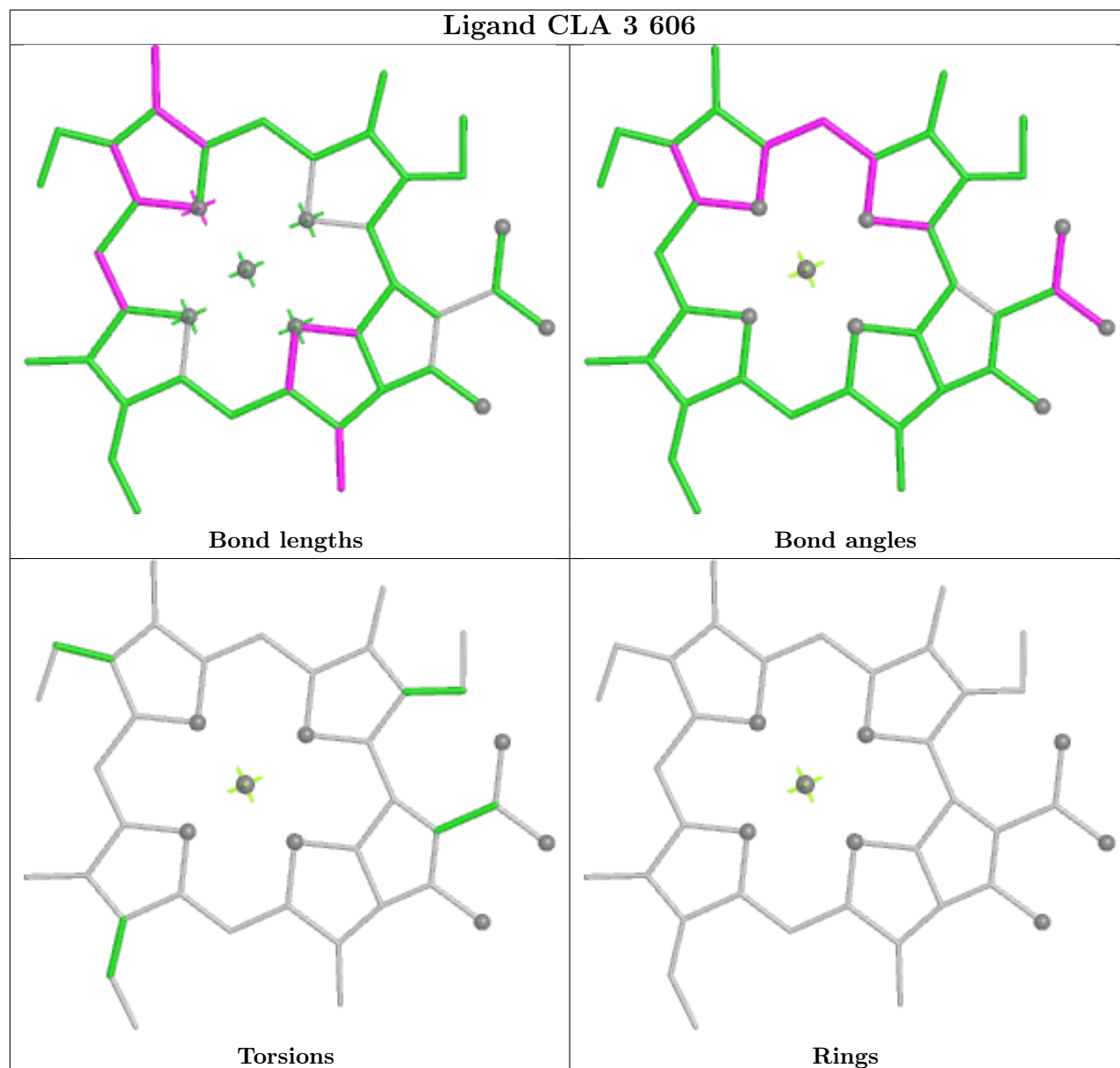


Ligand CLA A 824

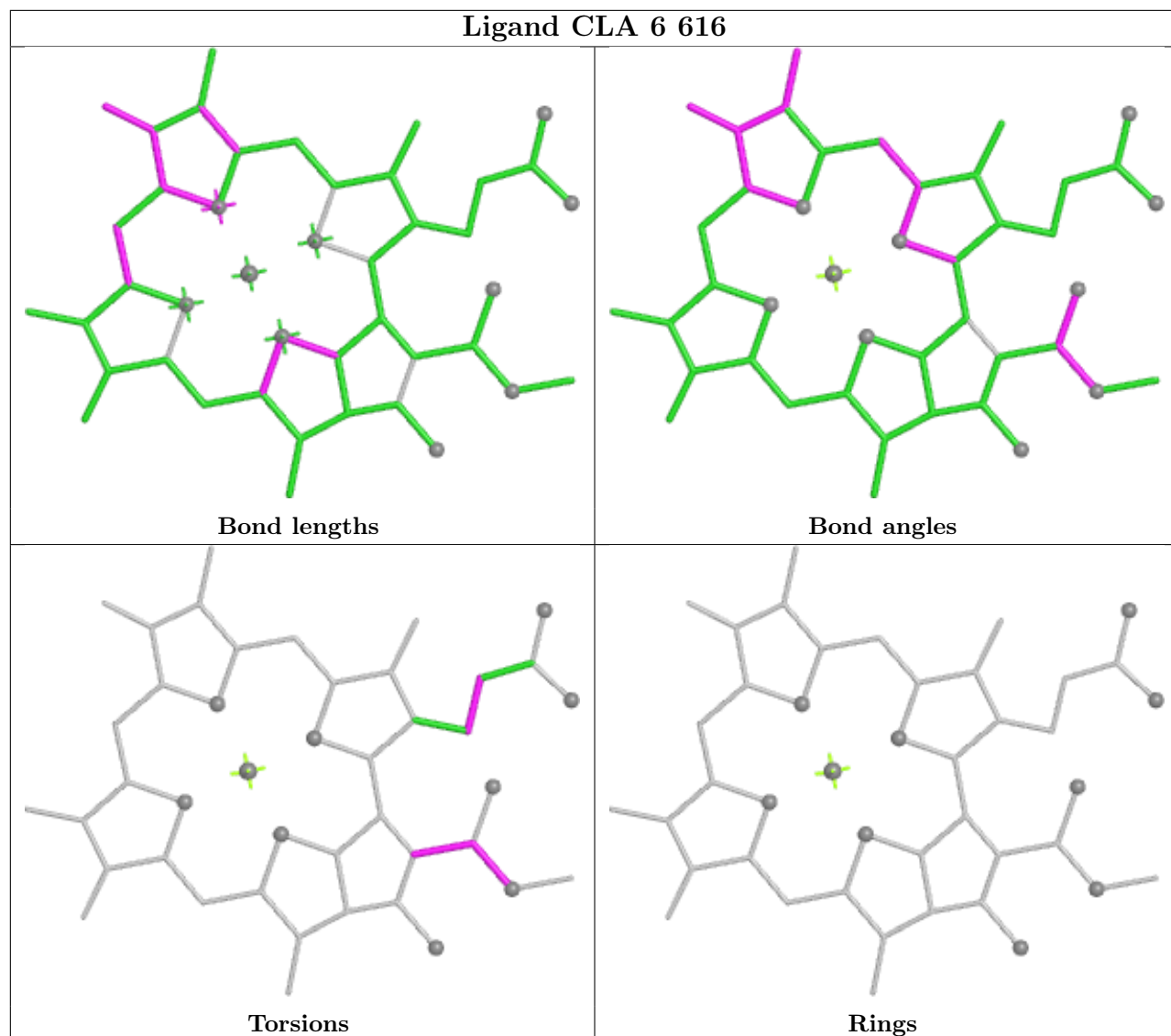




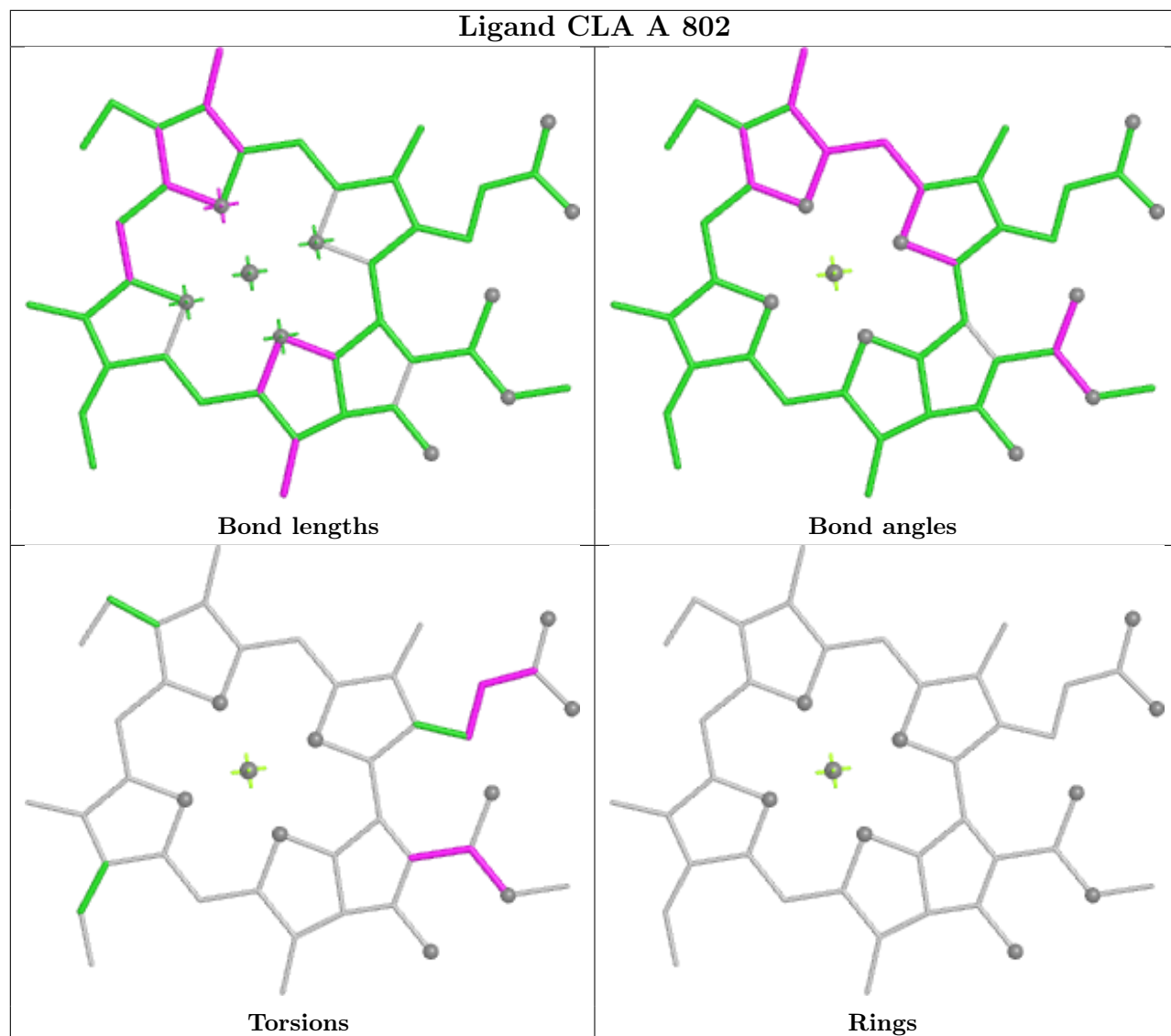
Ligand CLA 3 606



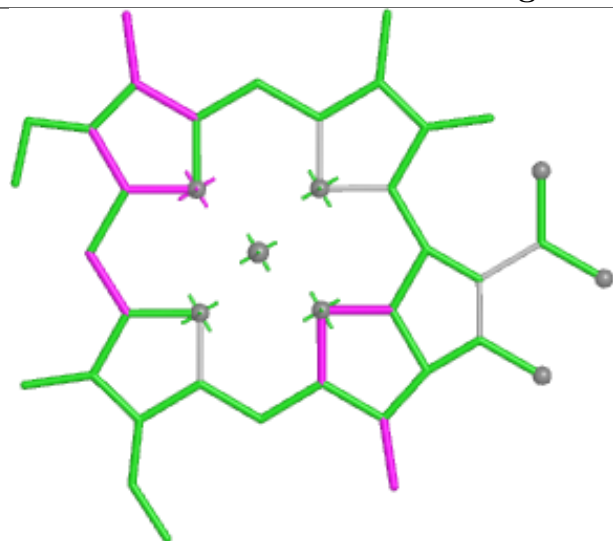
Ligand CLA 6 616



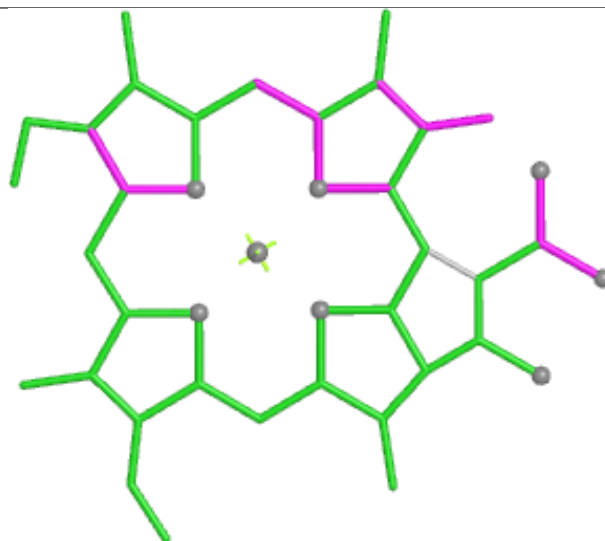
Ligand CLA A 802



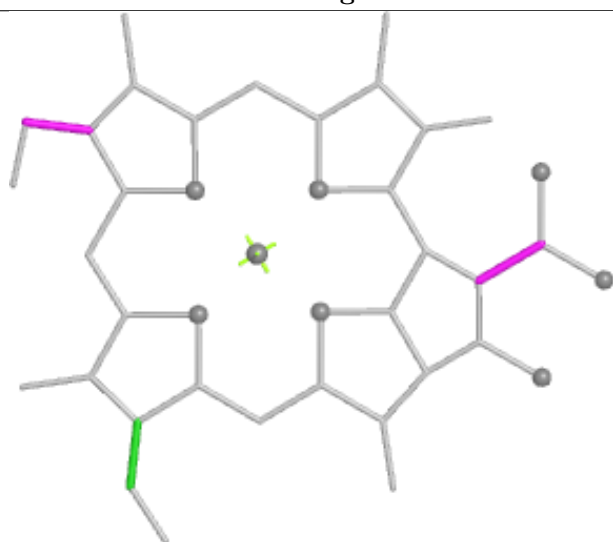
Ligand CLA 3 614



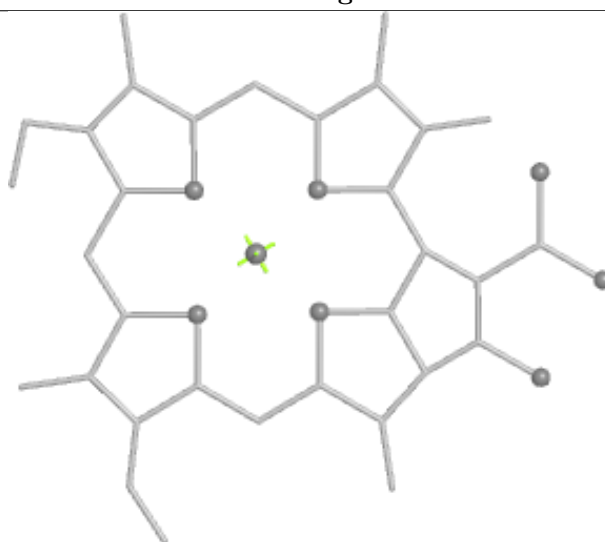
Bond lengths



Bond angles

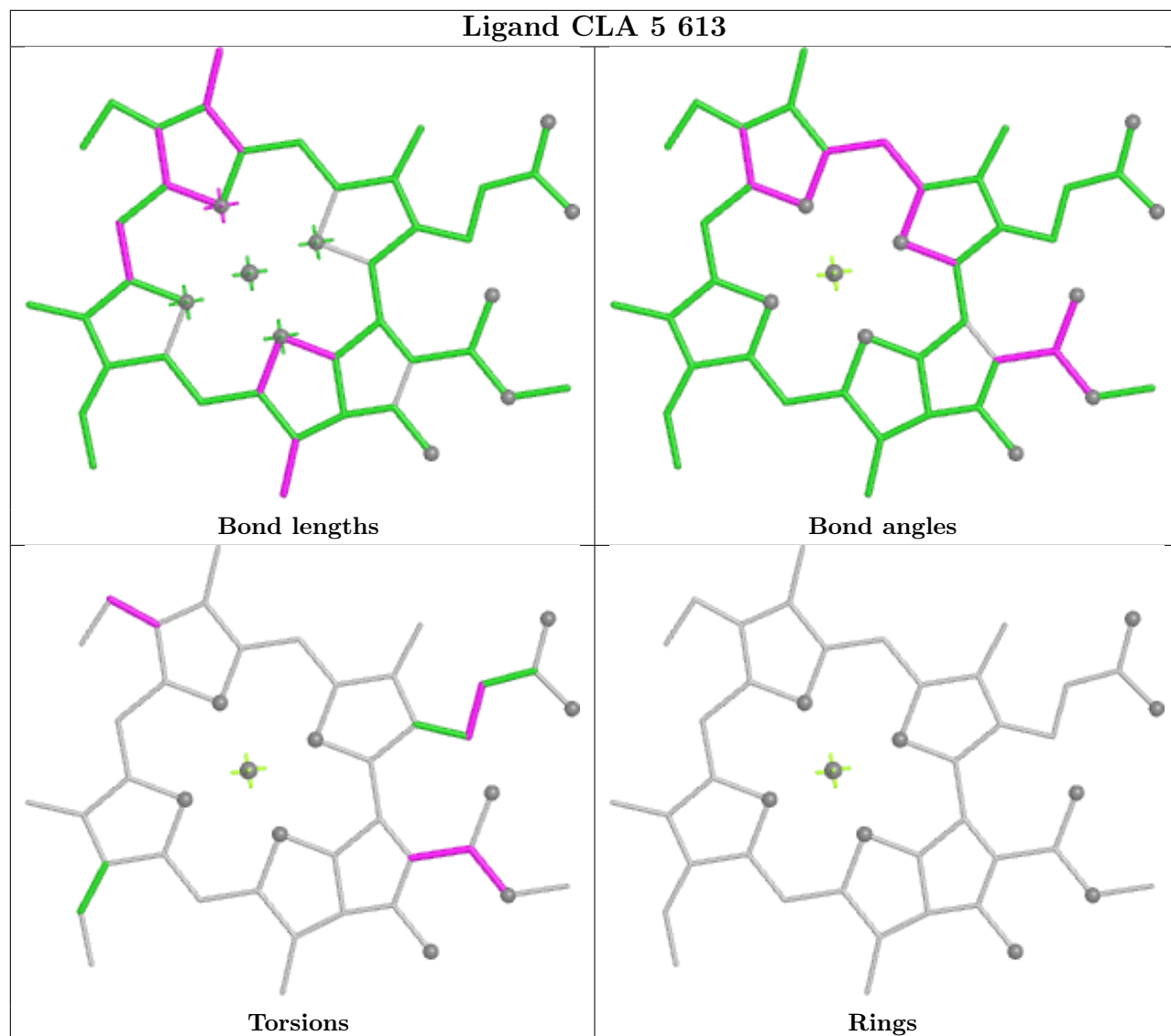


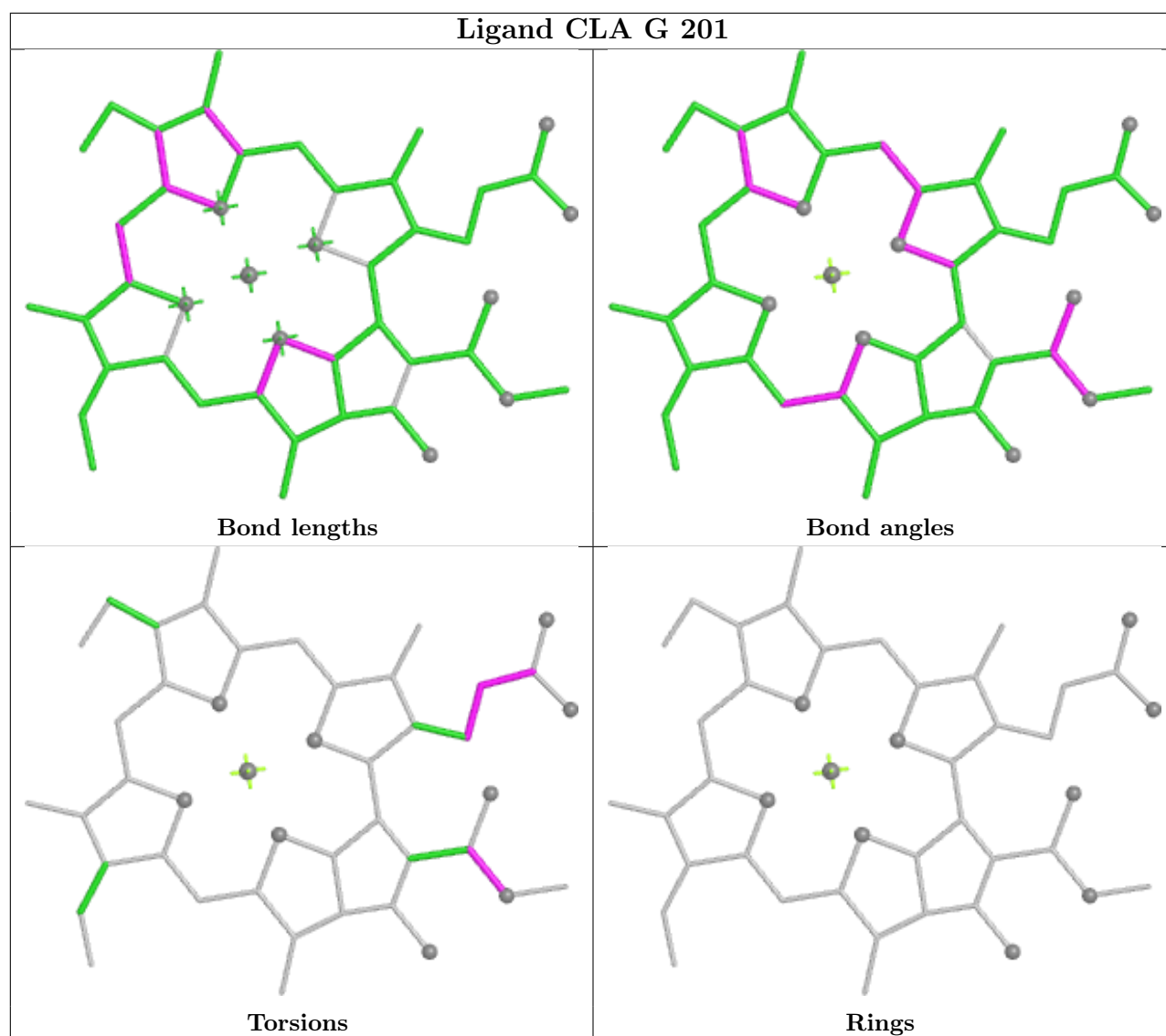
Torsions



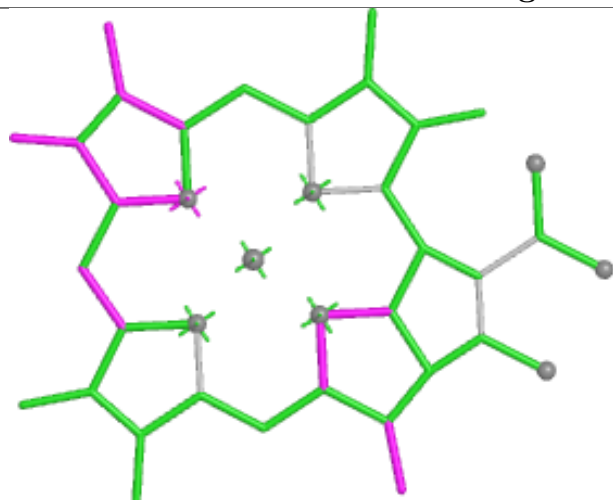
Rings

Ligand CLA 5 613

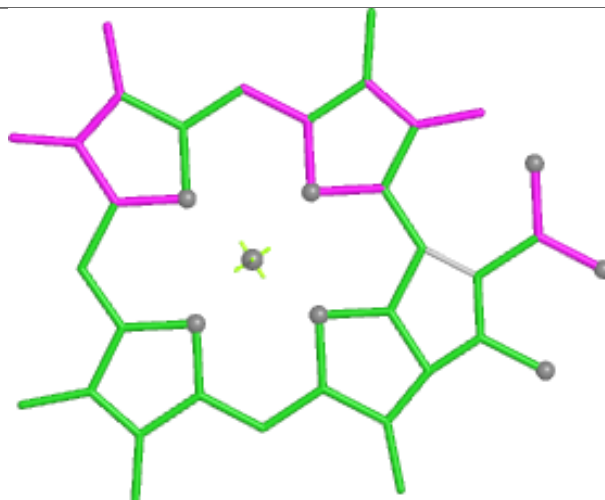




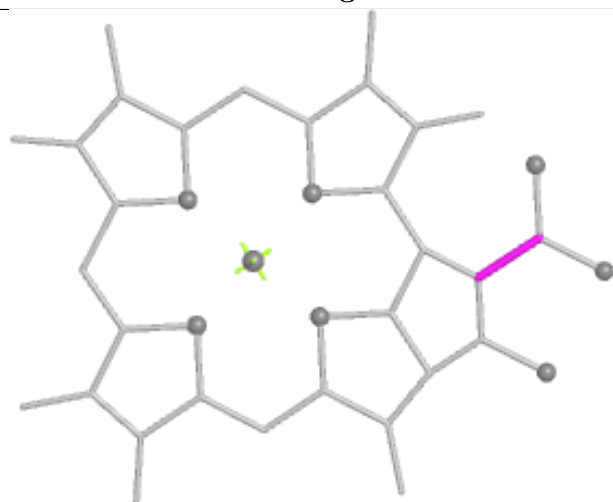
Ligand CLA 6 611



Bond lengths



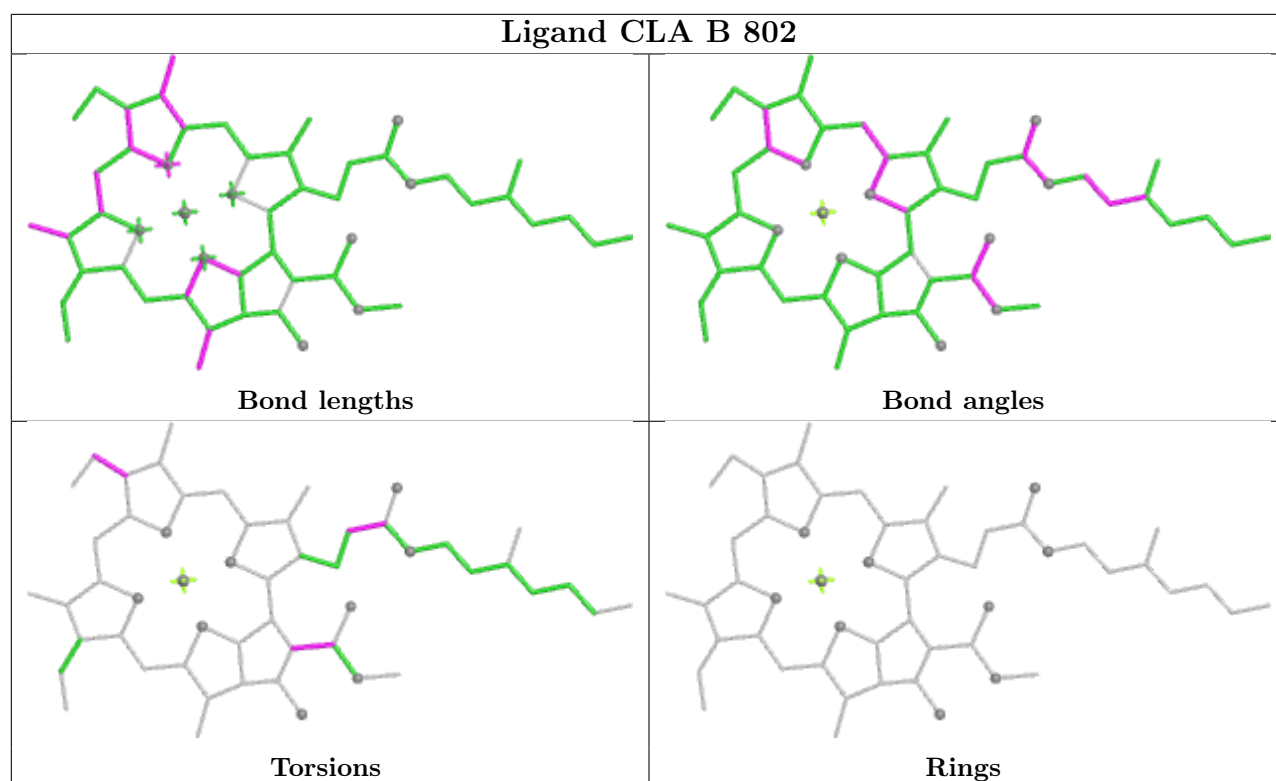
Bond angles

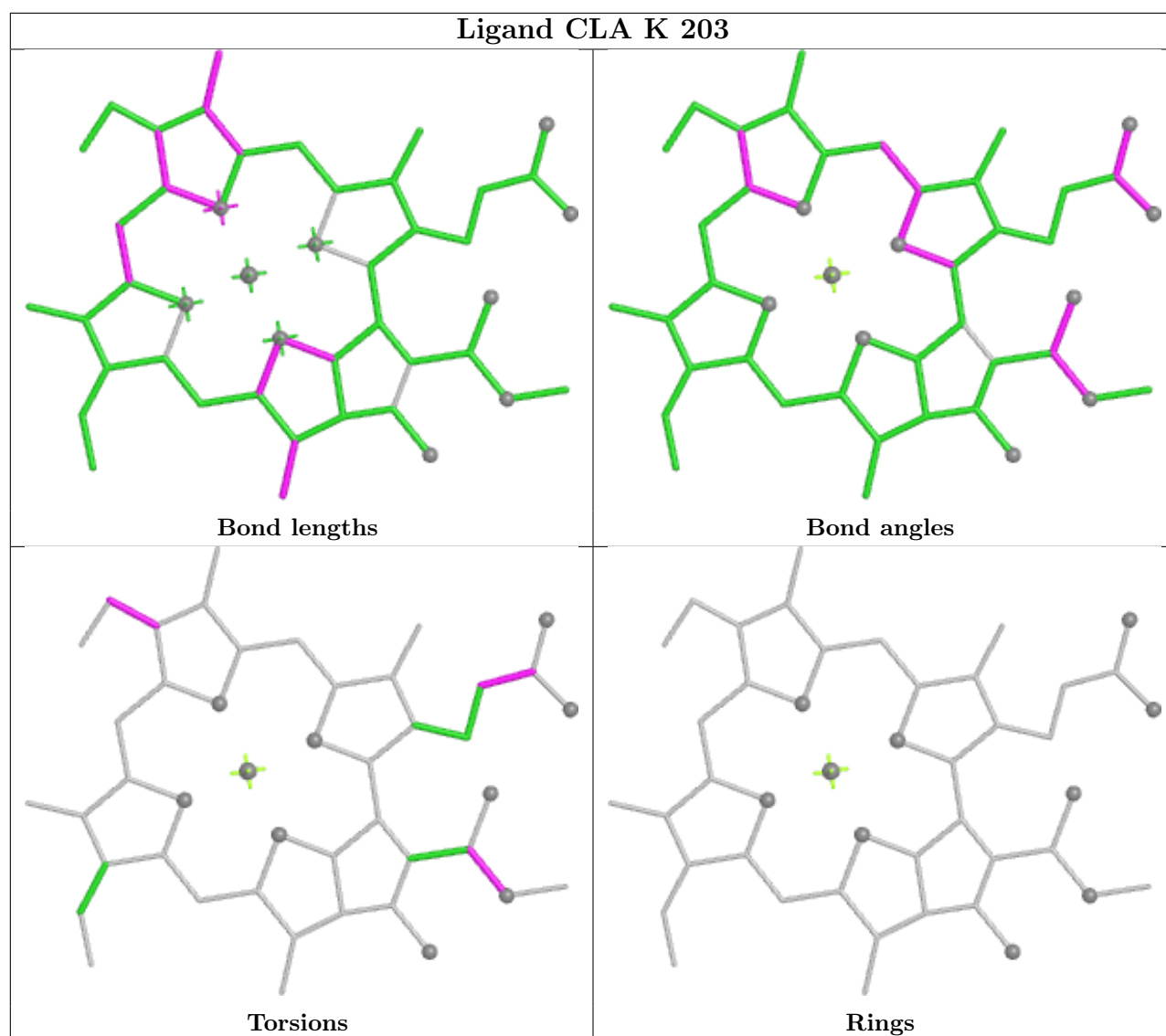


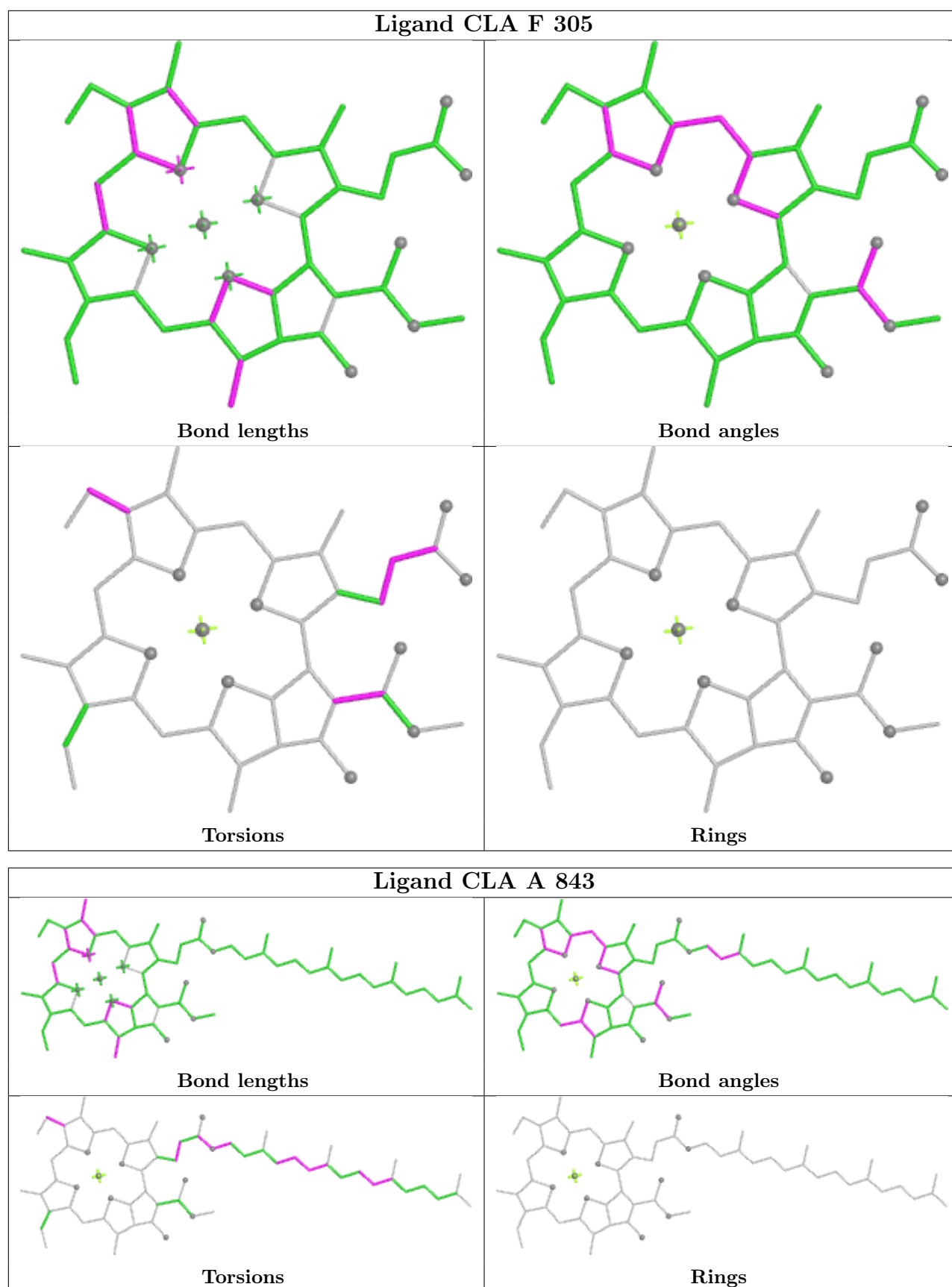
Torsions



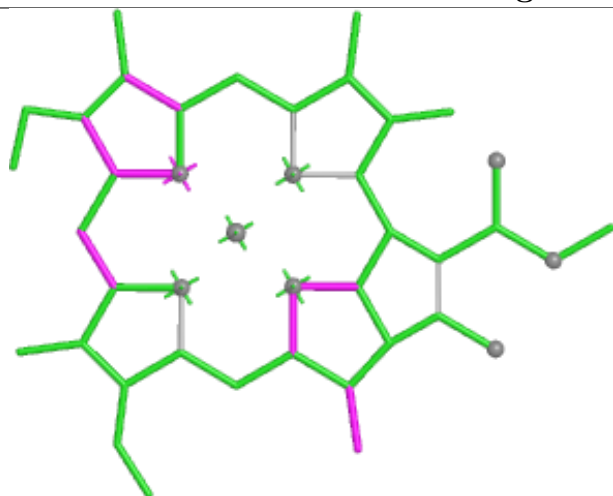
Rings



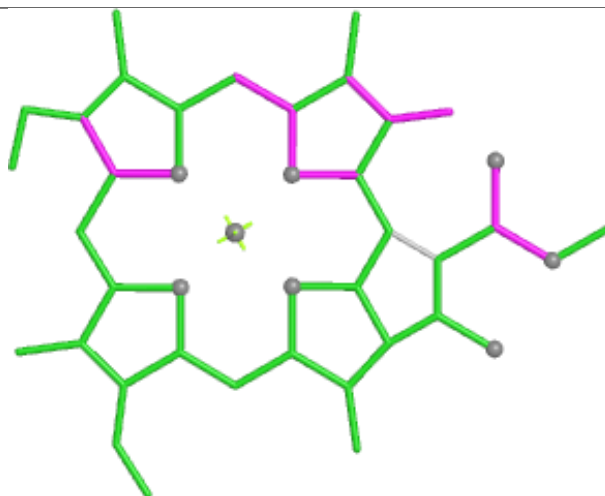




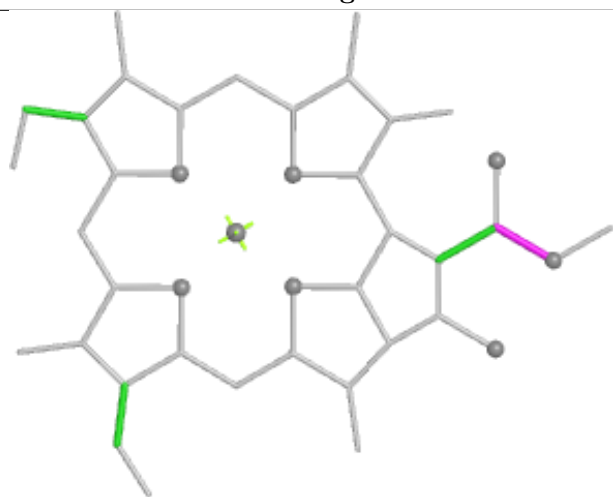
Ligand CLA F 304



Bond lengths



Bond angles

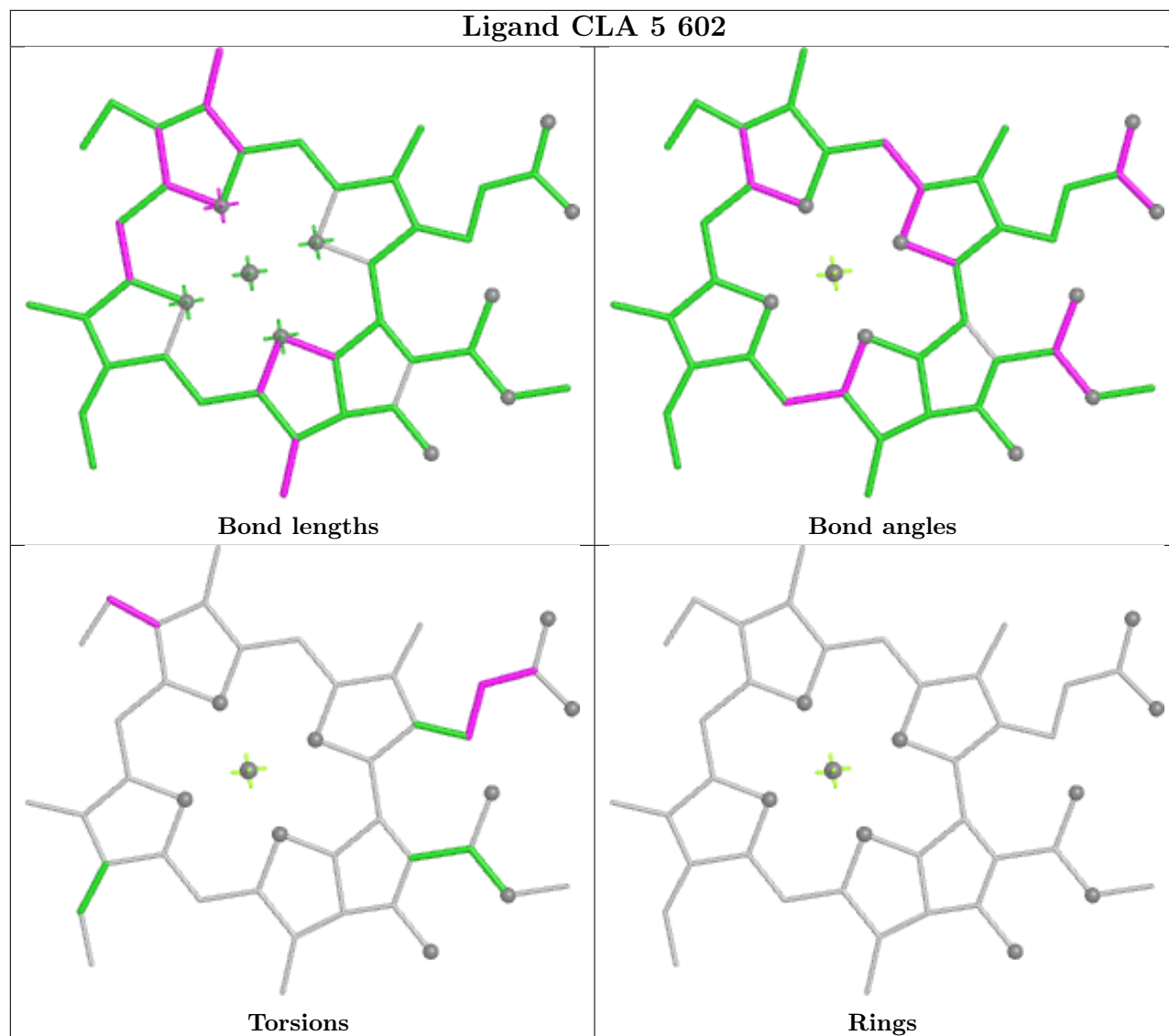


Torsions

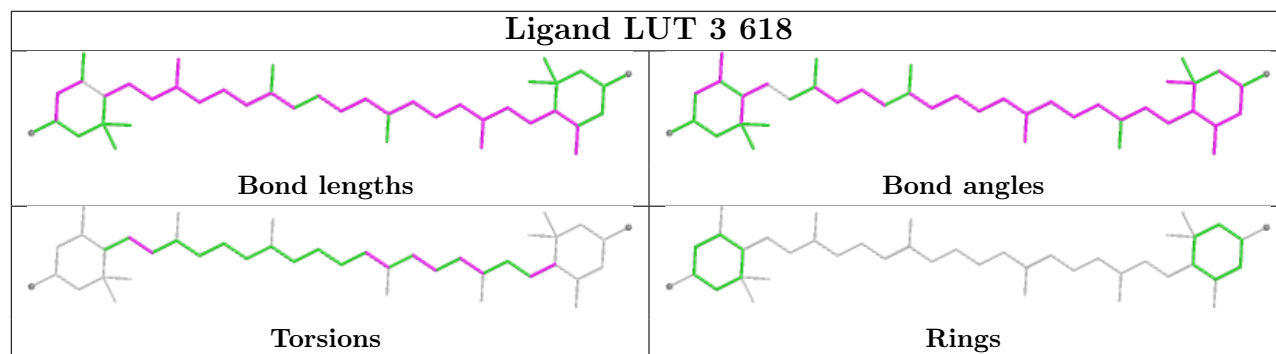


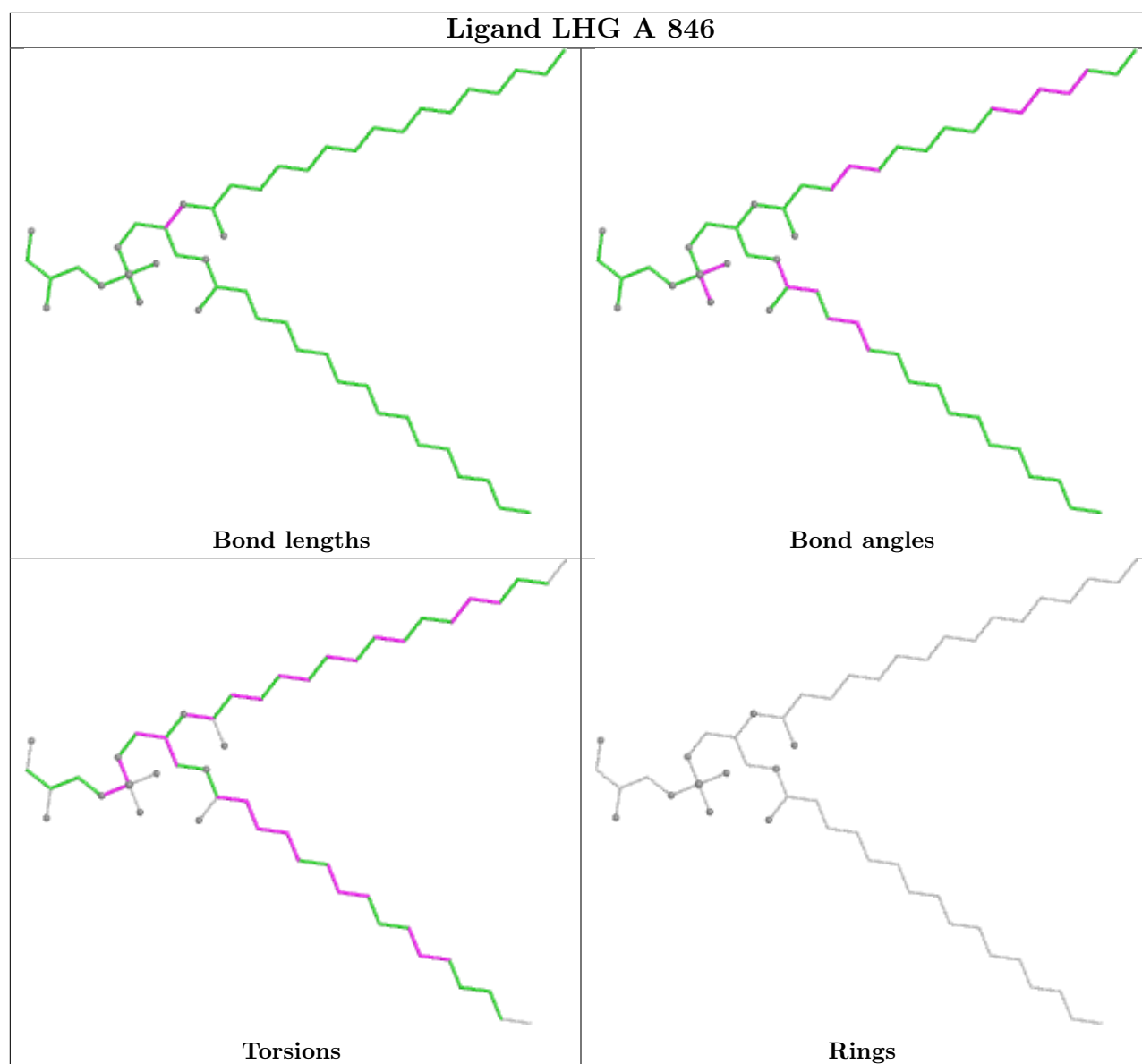
Rings

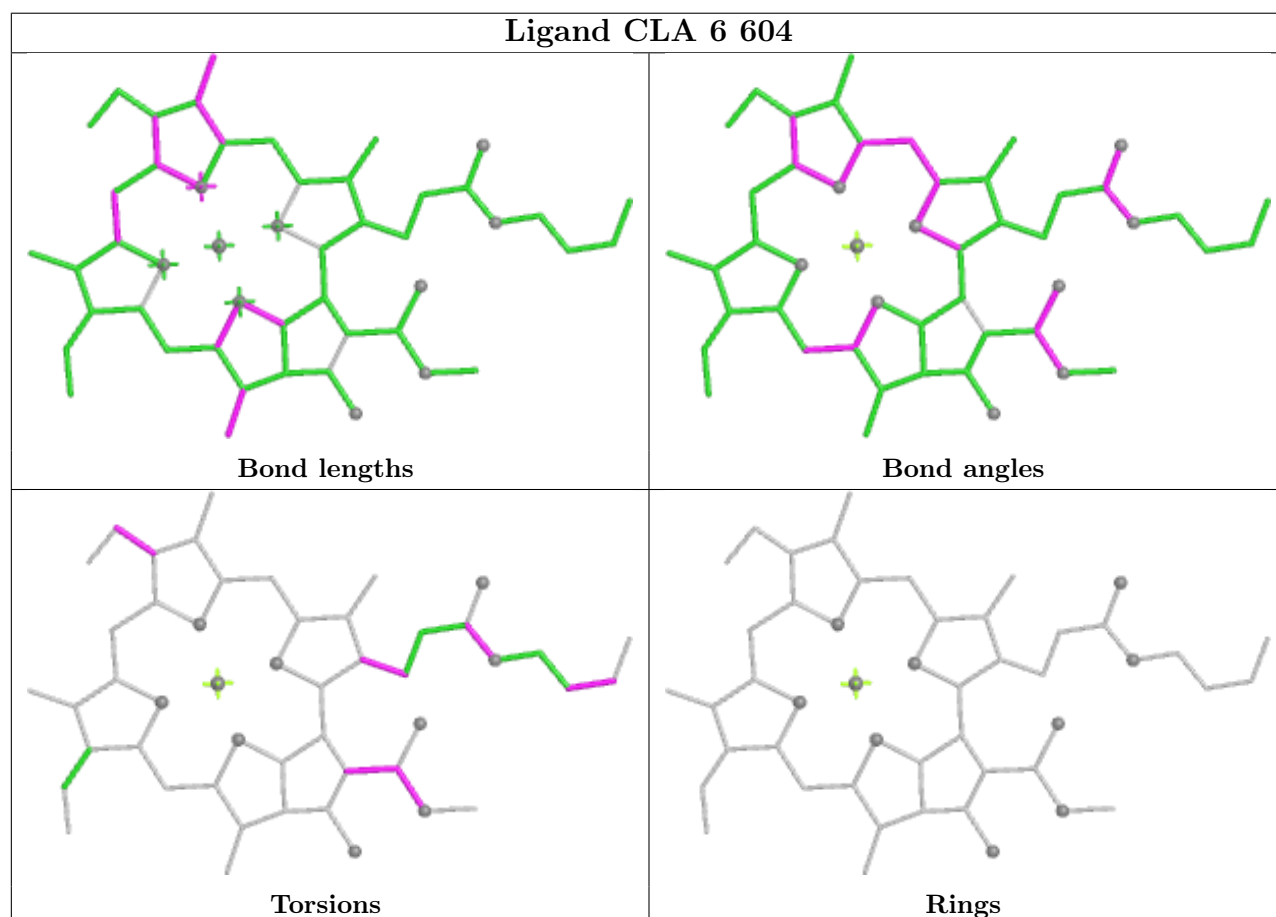
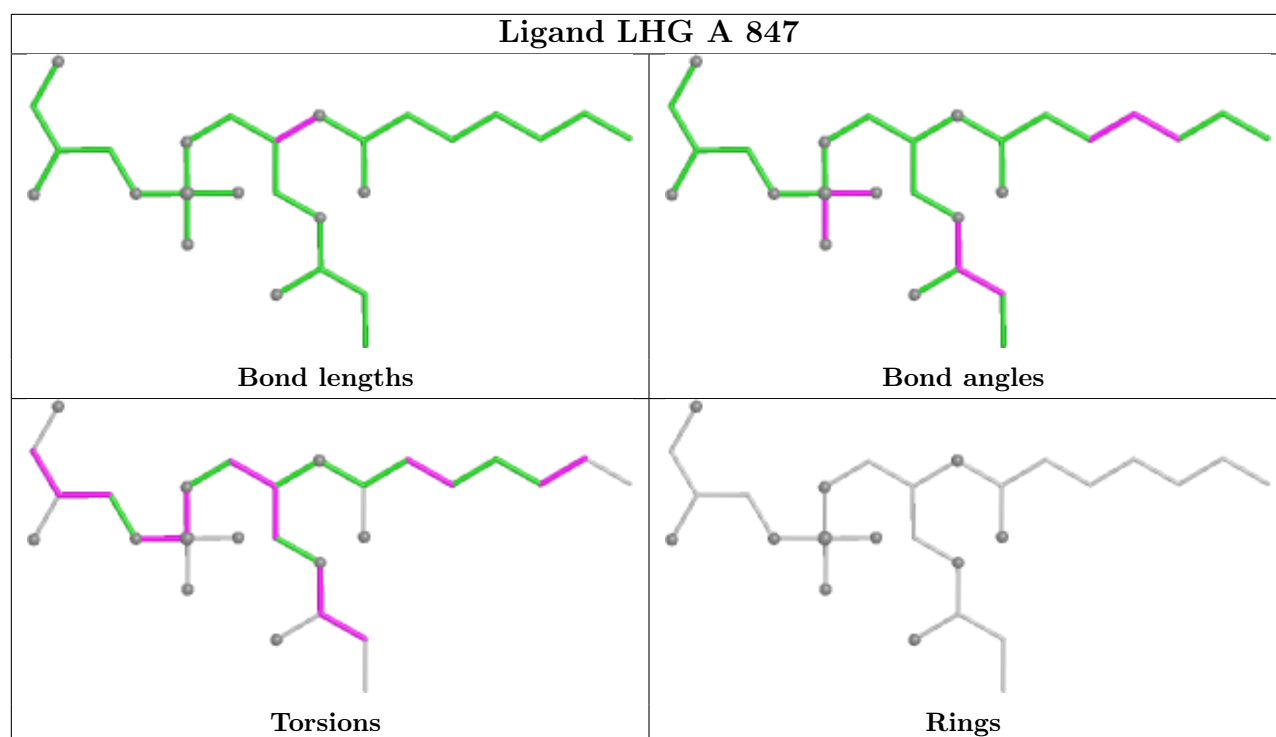
Ligand CLA 5 602

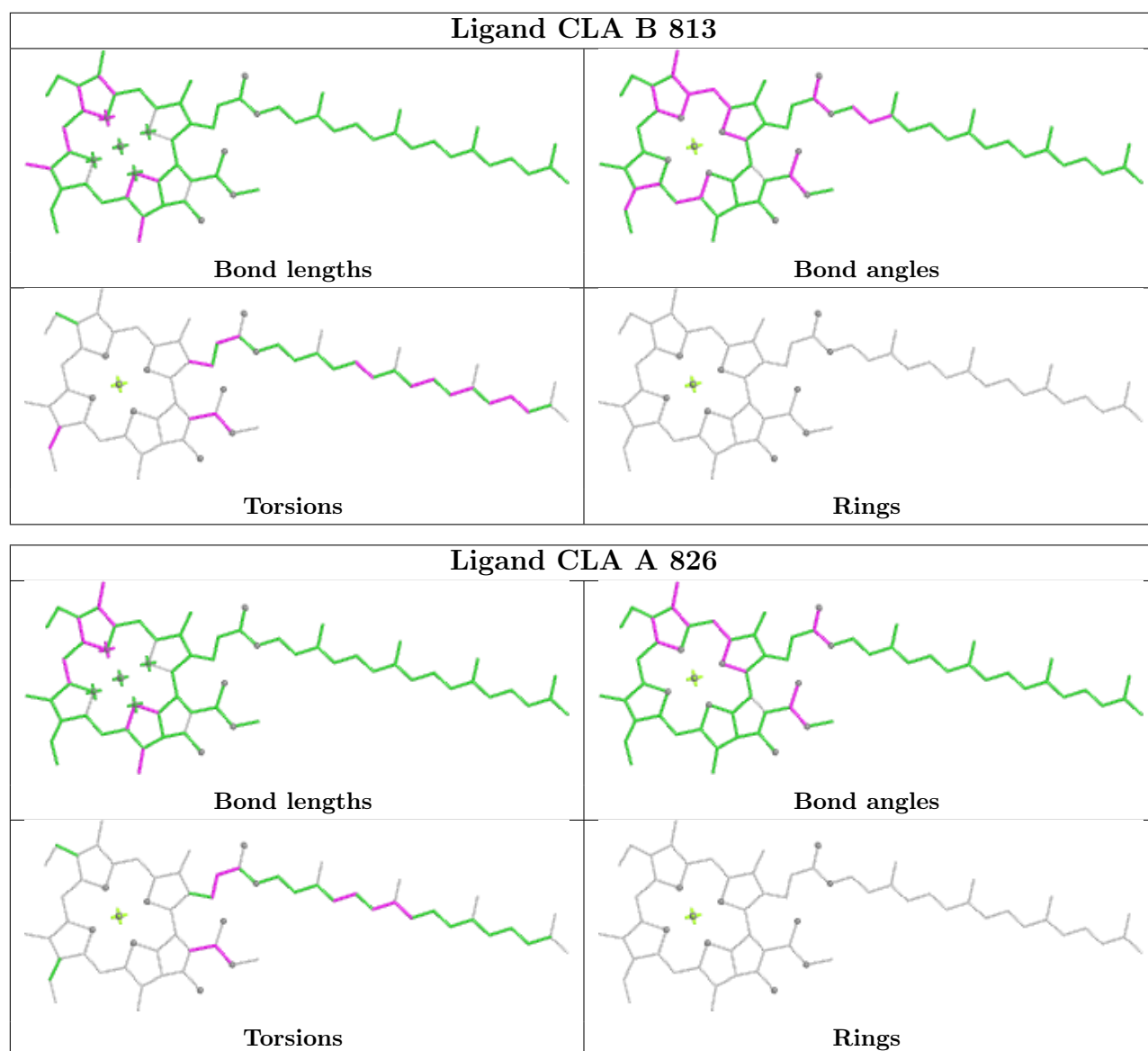


Ligand LUT 3 618

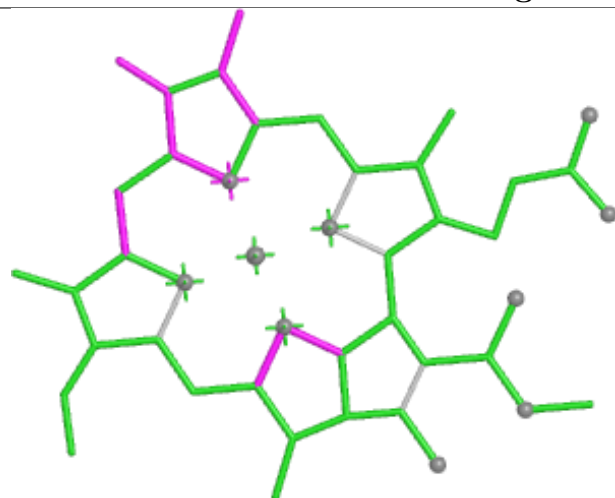




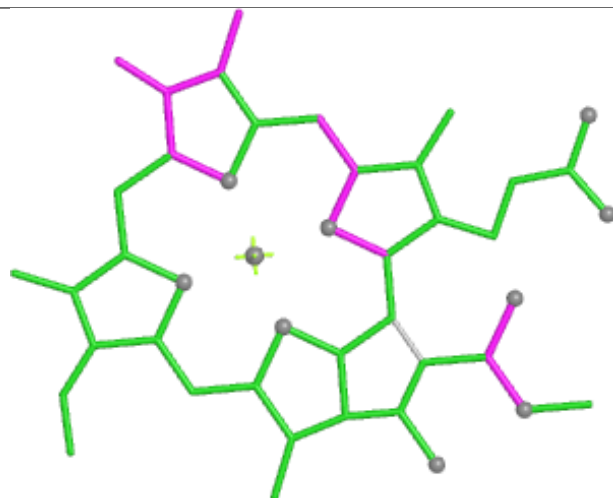




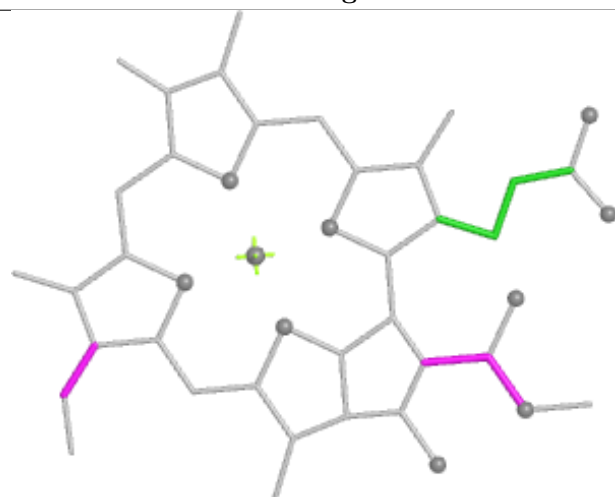
Ligand CLA K 204



Bond lengths



Bond angles

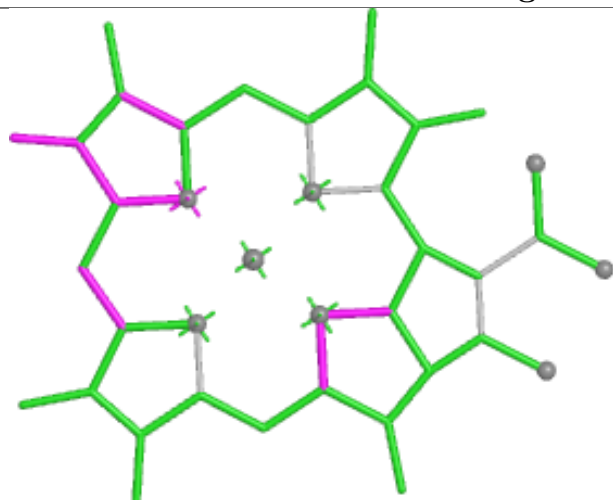


Torsions

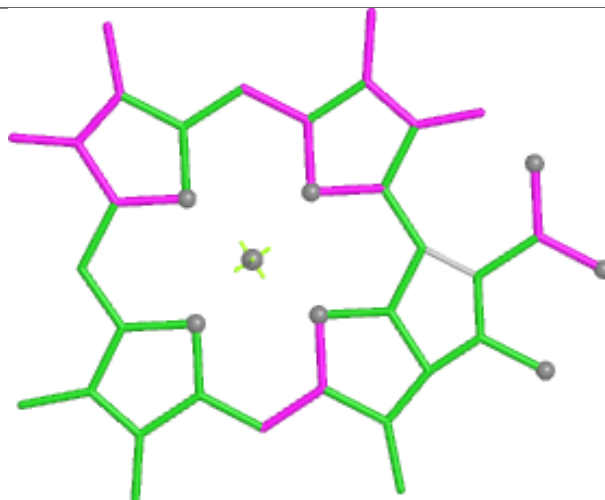


Rings

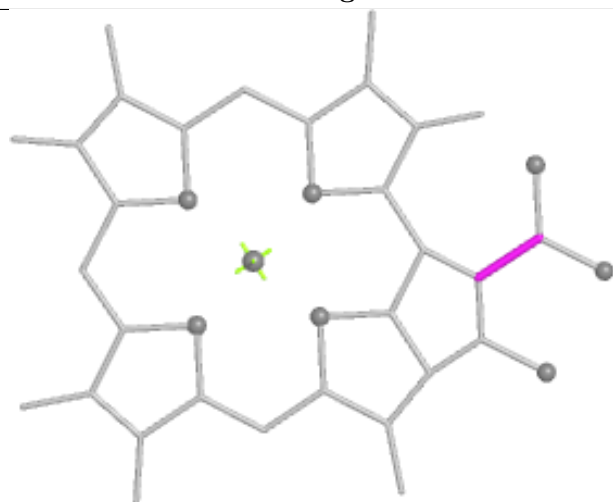
Ligand CLA 6 614



Bond lengths



Bond angles

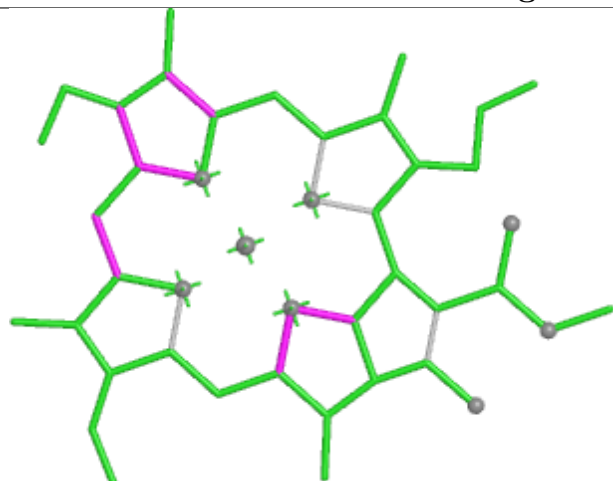


Torsions

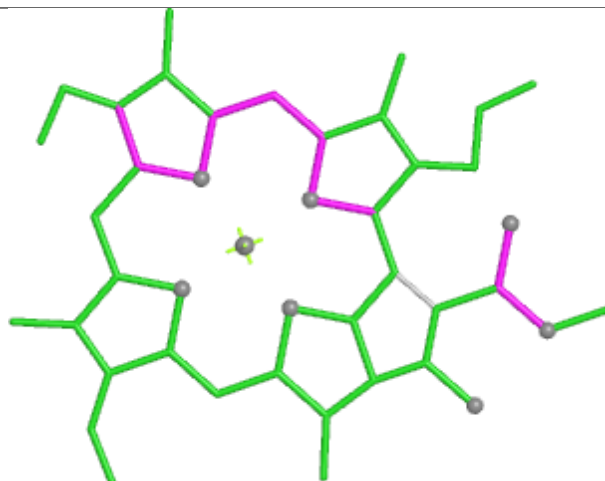


Rings

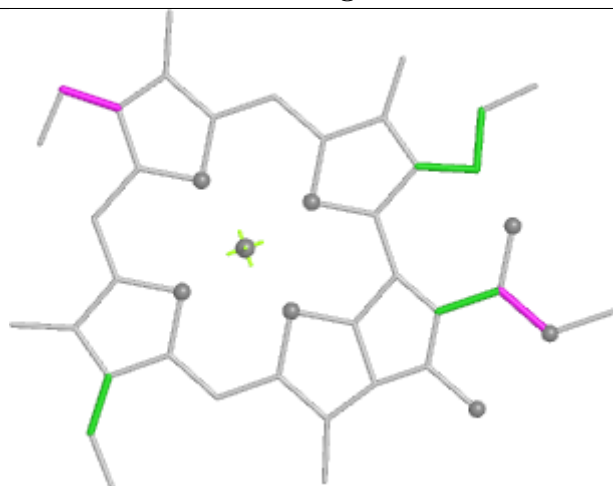
Ligand CLA 3 612



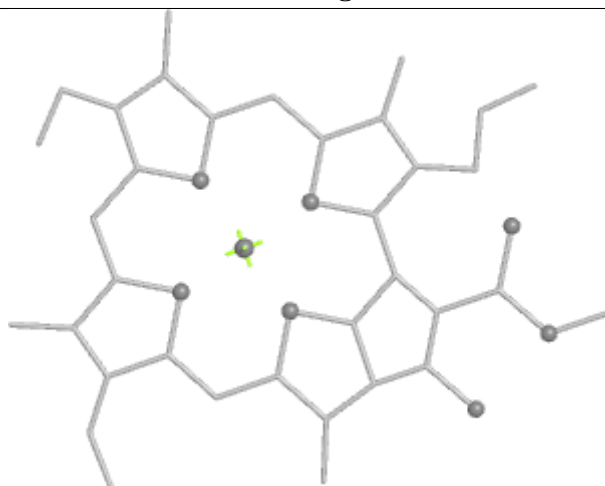
Bond lengths



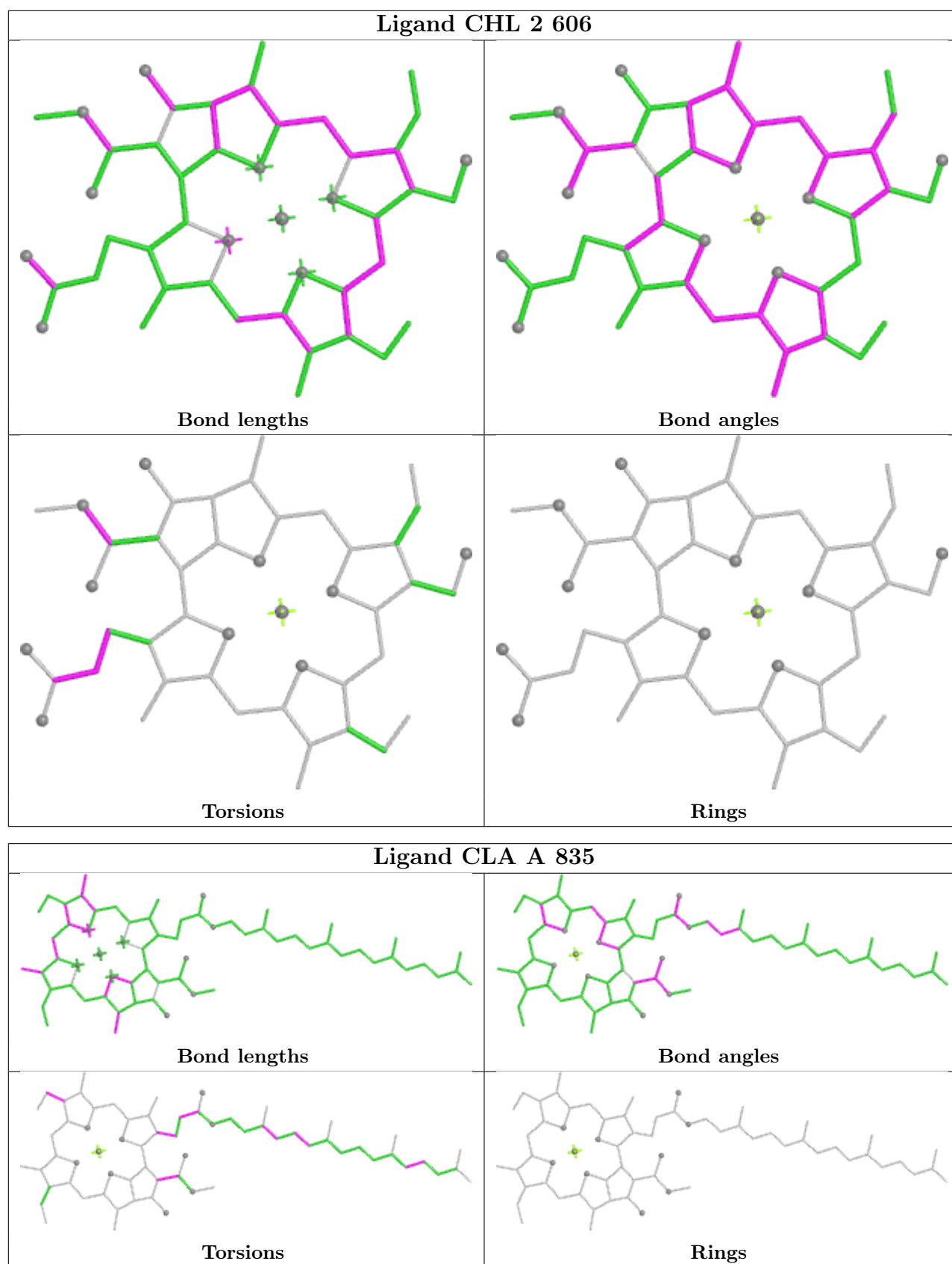
Bond angles



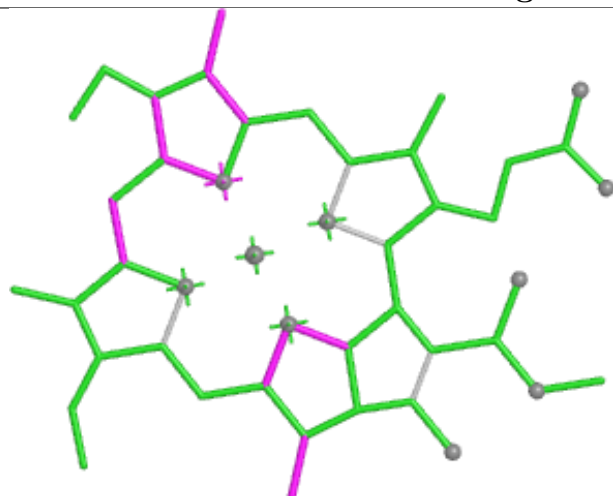
Torsions



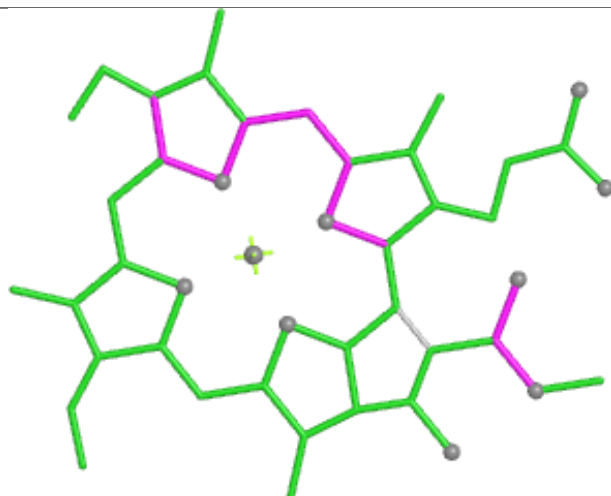
Rings



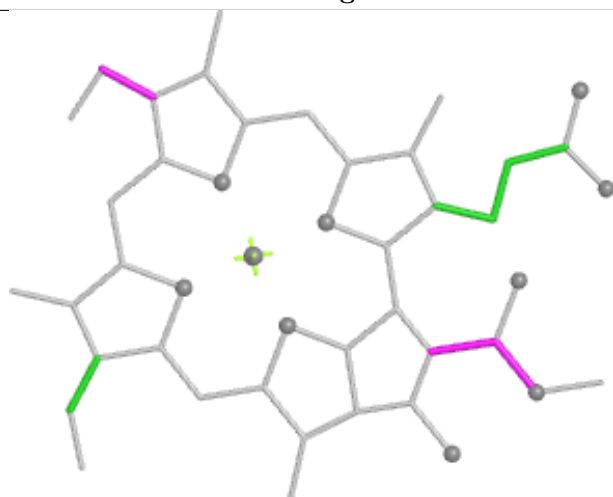
Ligand CLA F 301



Bond lengths



Bond angles

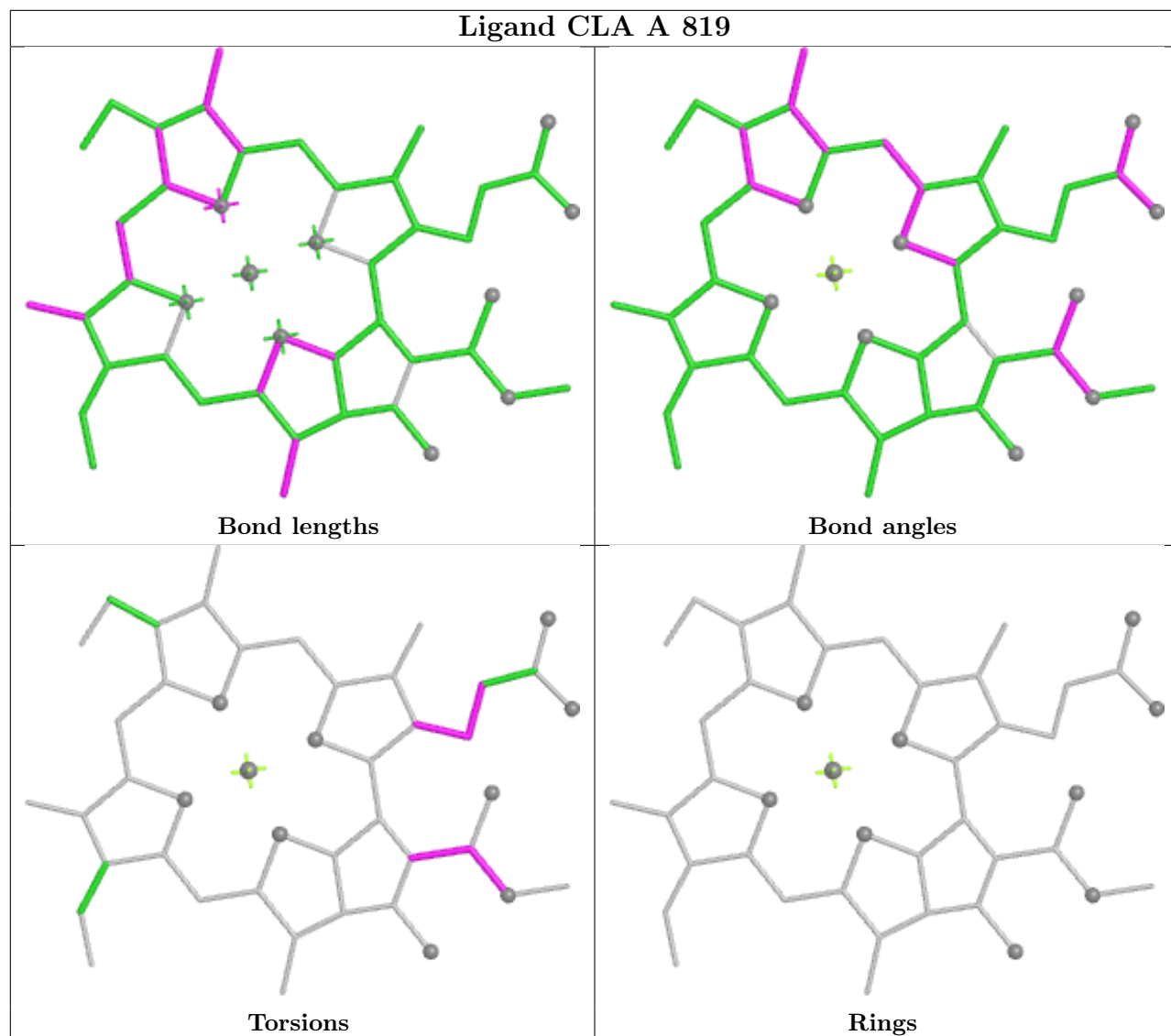


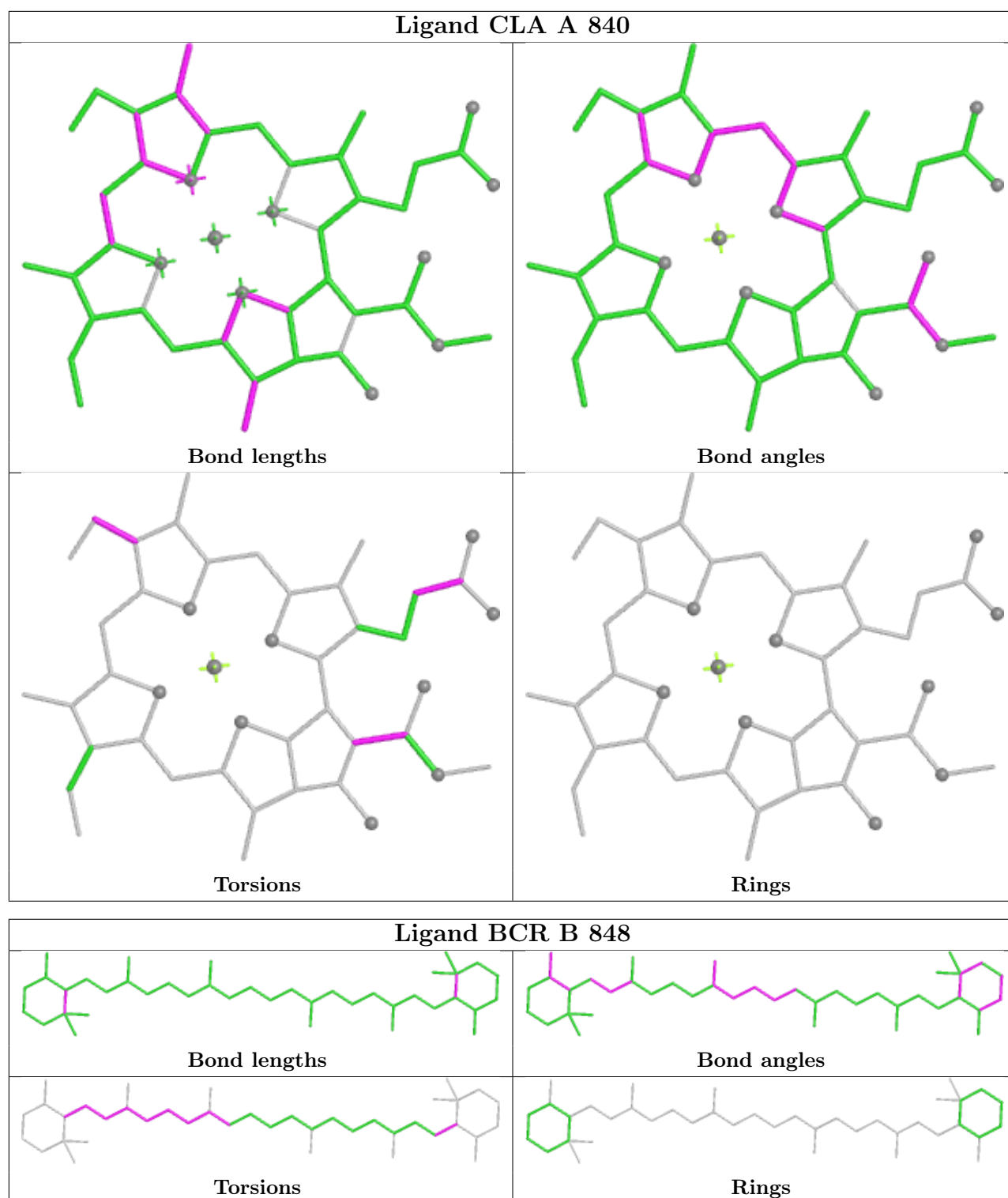
Torsions

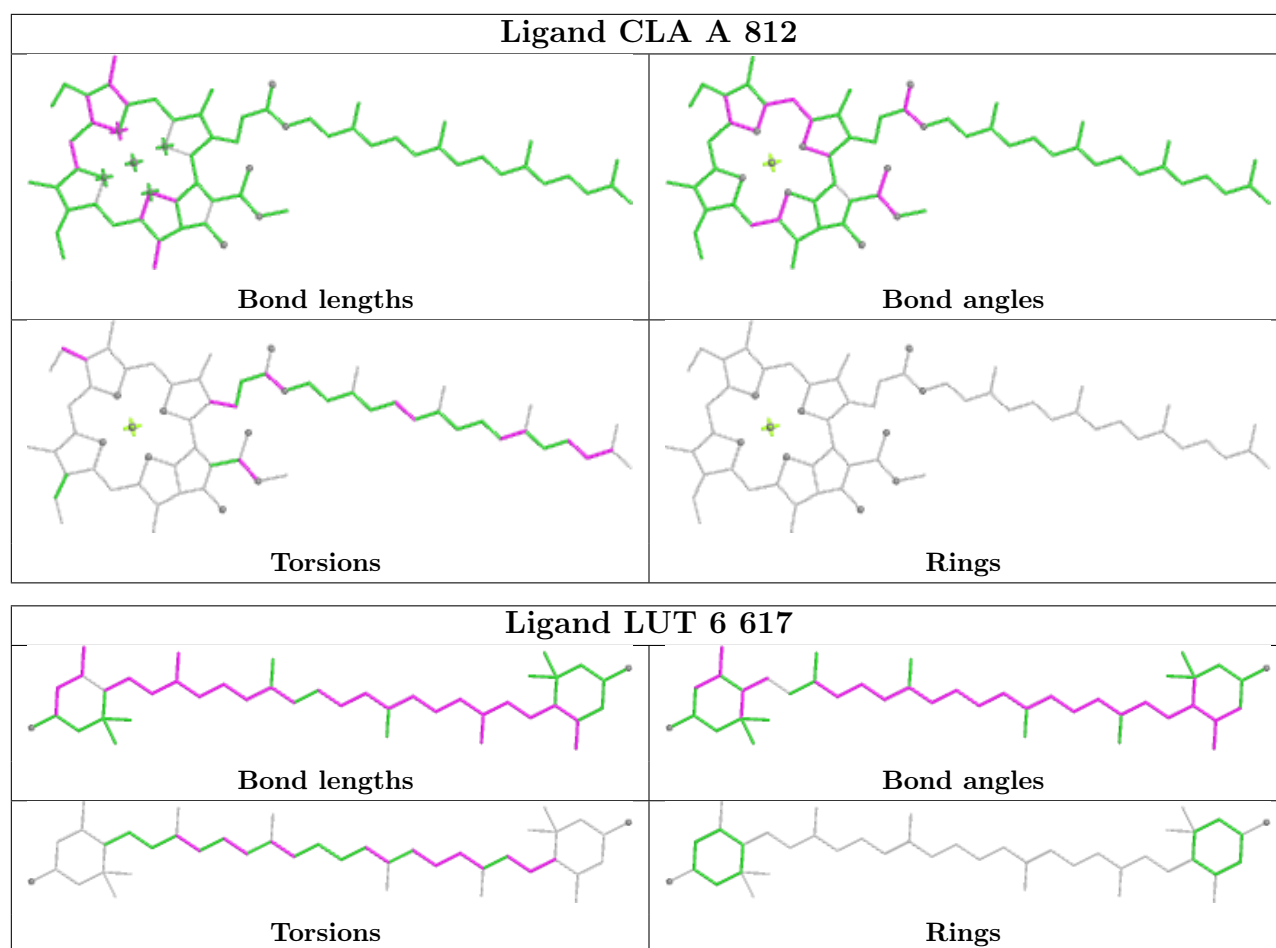


Rings

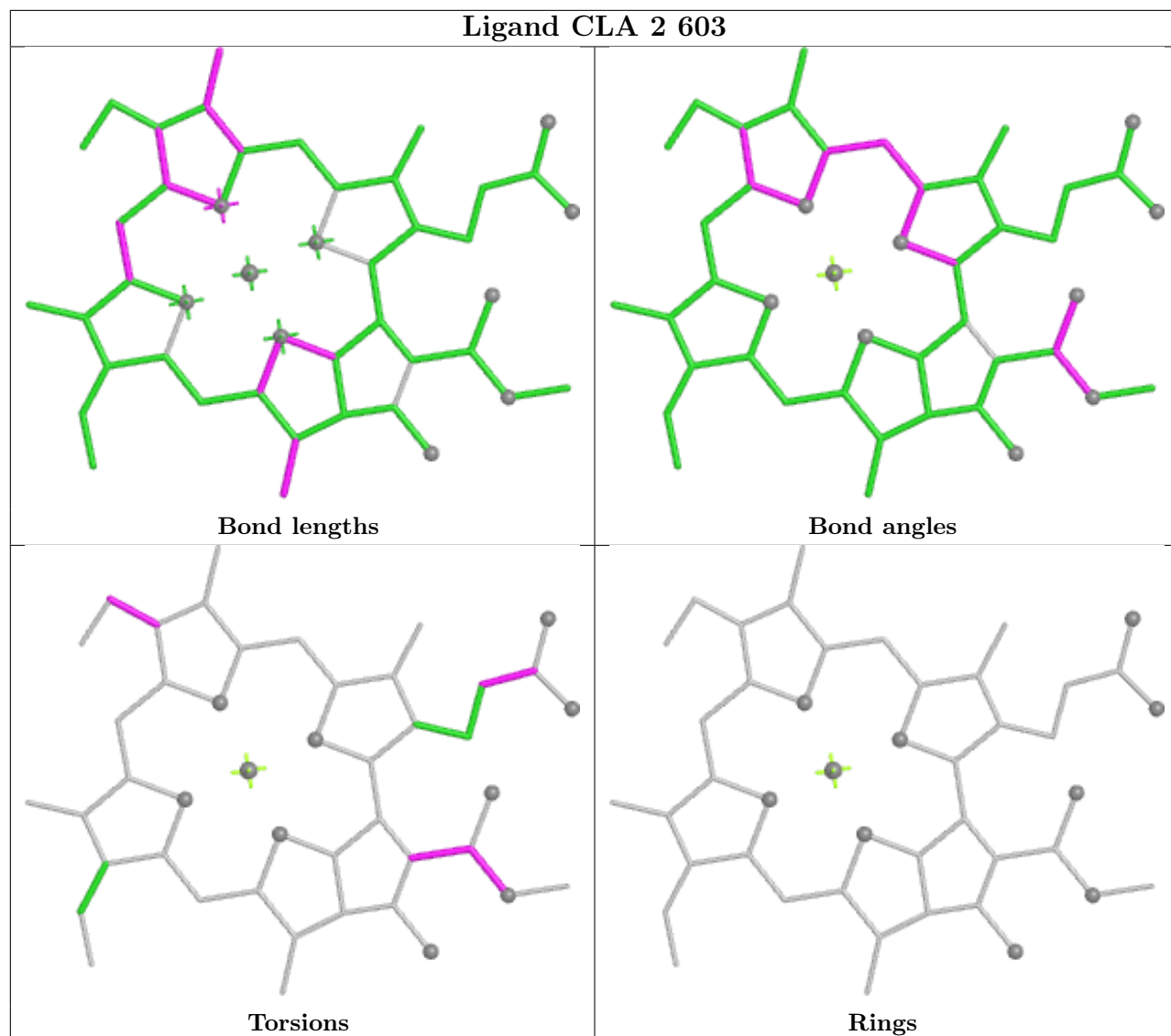
Ligand CLA A 819

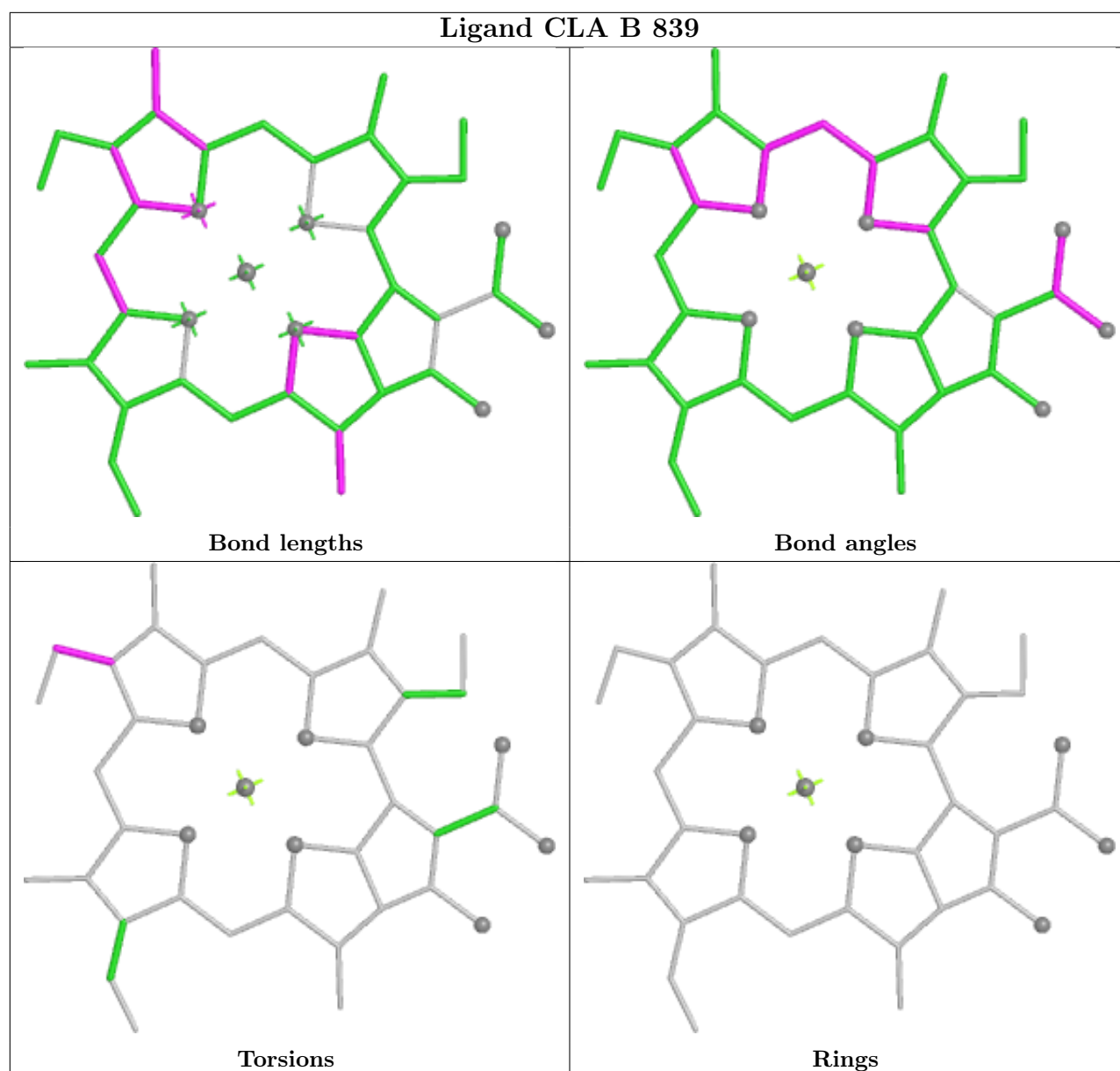




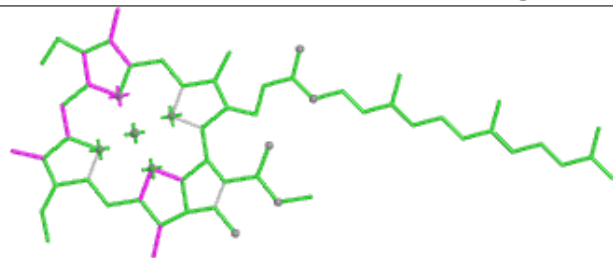


Ligand CLA 2 603

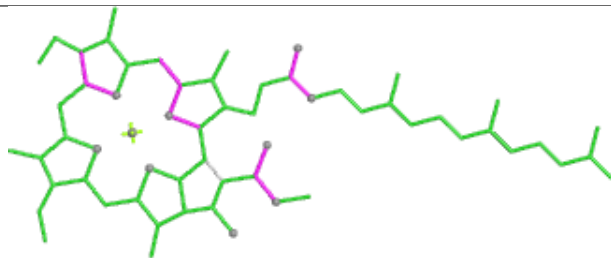




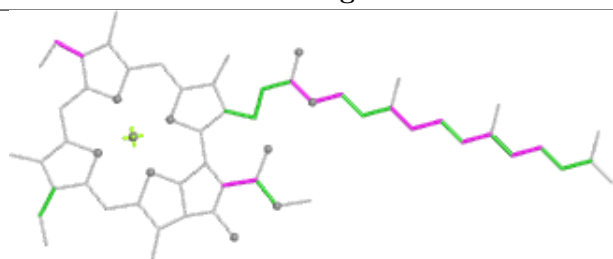
Ligand CLA B 815



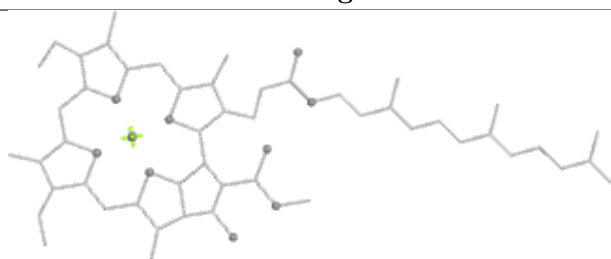
Bond lengths



Bond angles

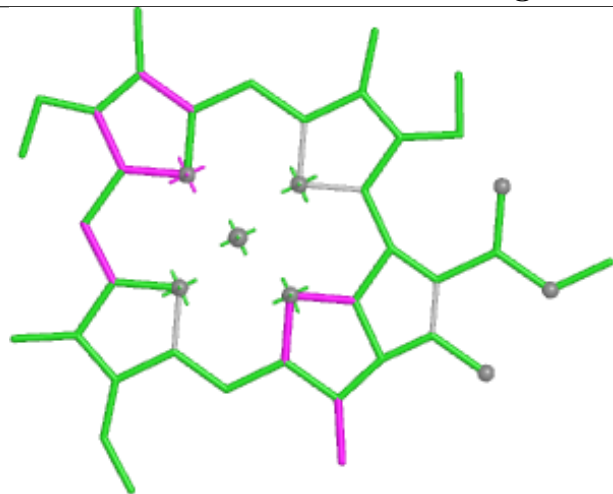


Torsions



Rings

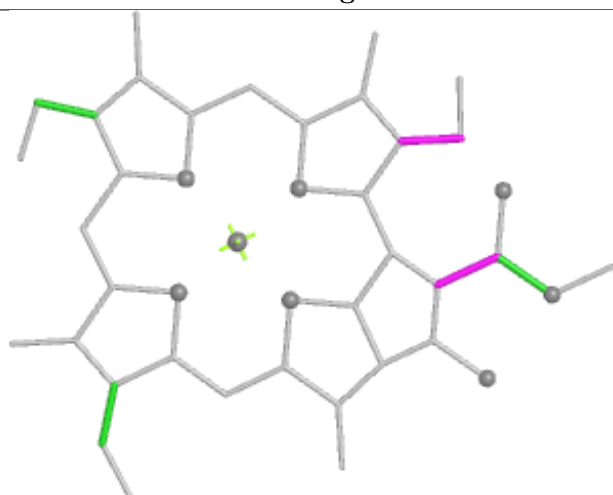
Ligand CLA A 816



Bond lengths



Bond angles

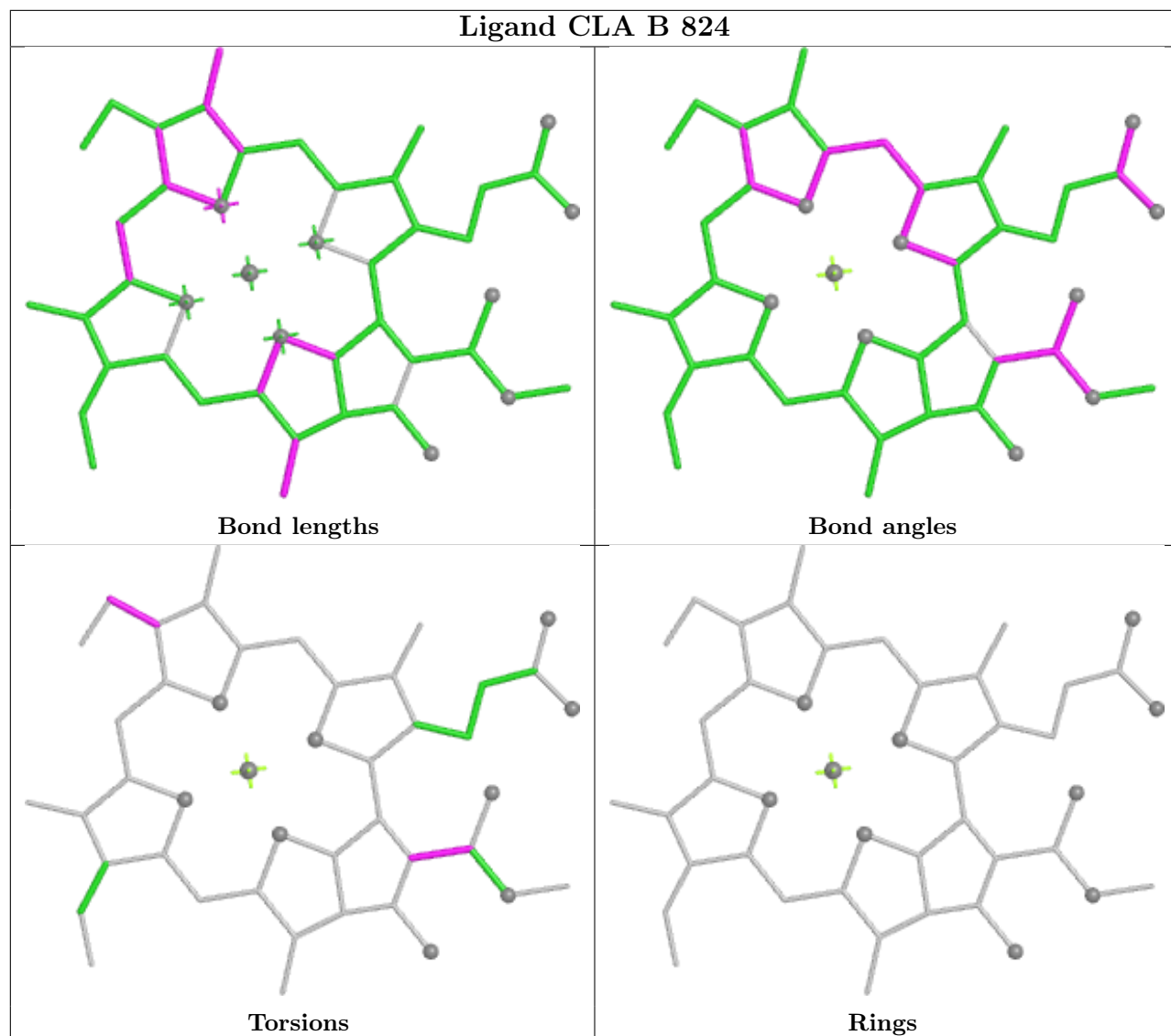


Torsions

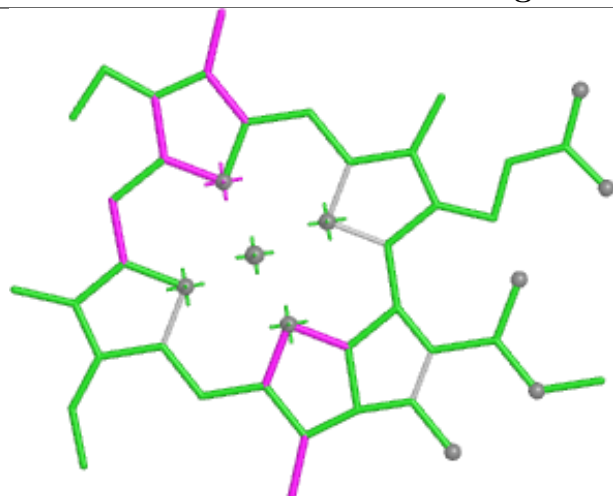


Rings

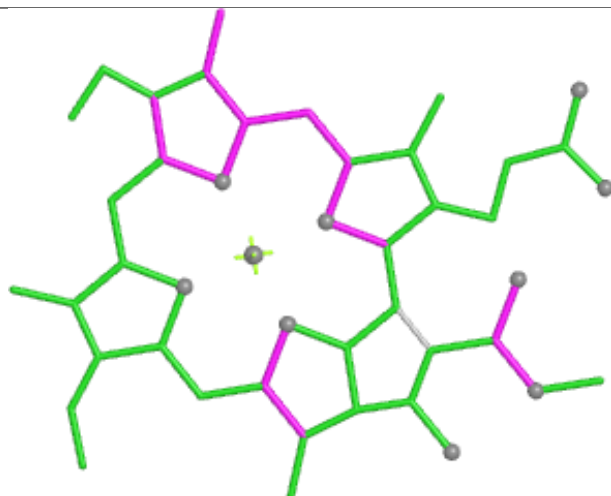
Ligand CLA B 824



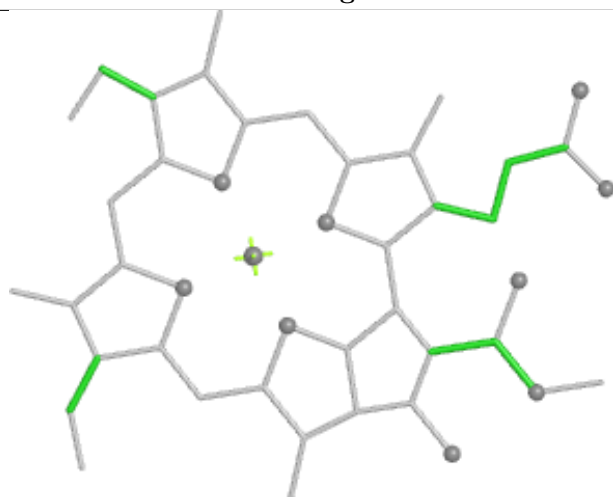
Ligand CLA B 829



Bond lengths



Bond angles

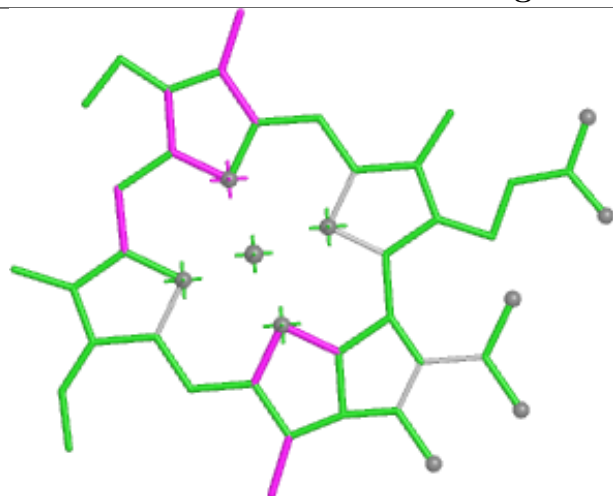


Torsions

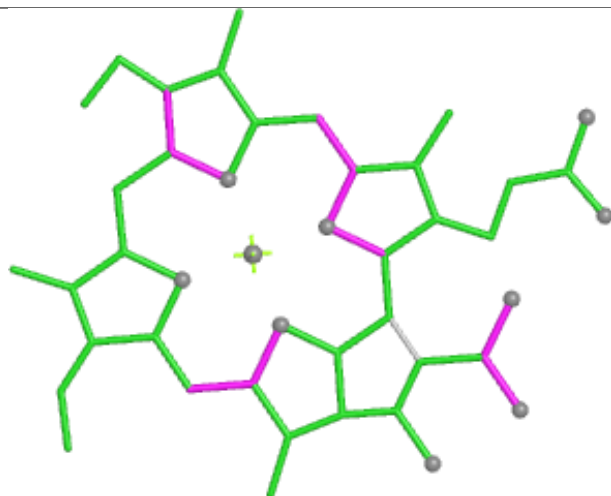


Rings

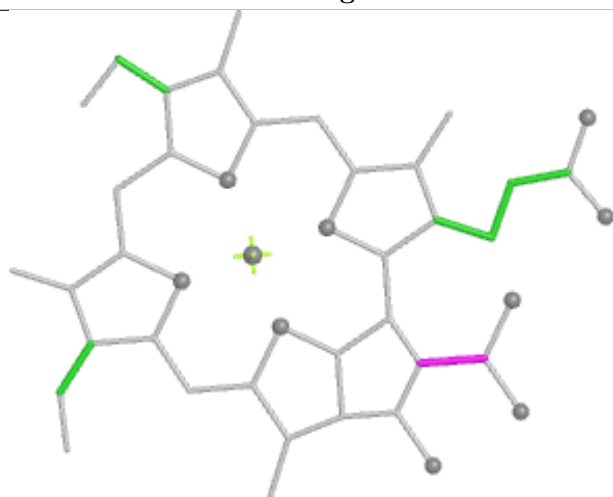
Ligand CLA B 814



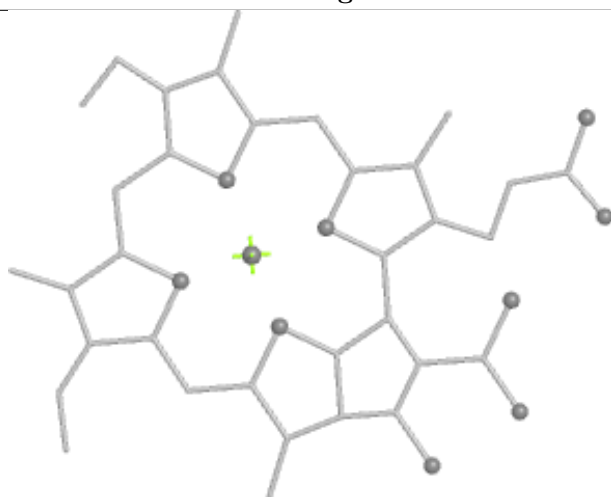
Bond lengths



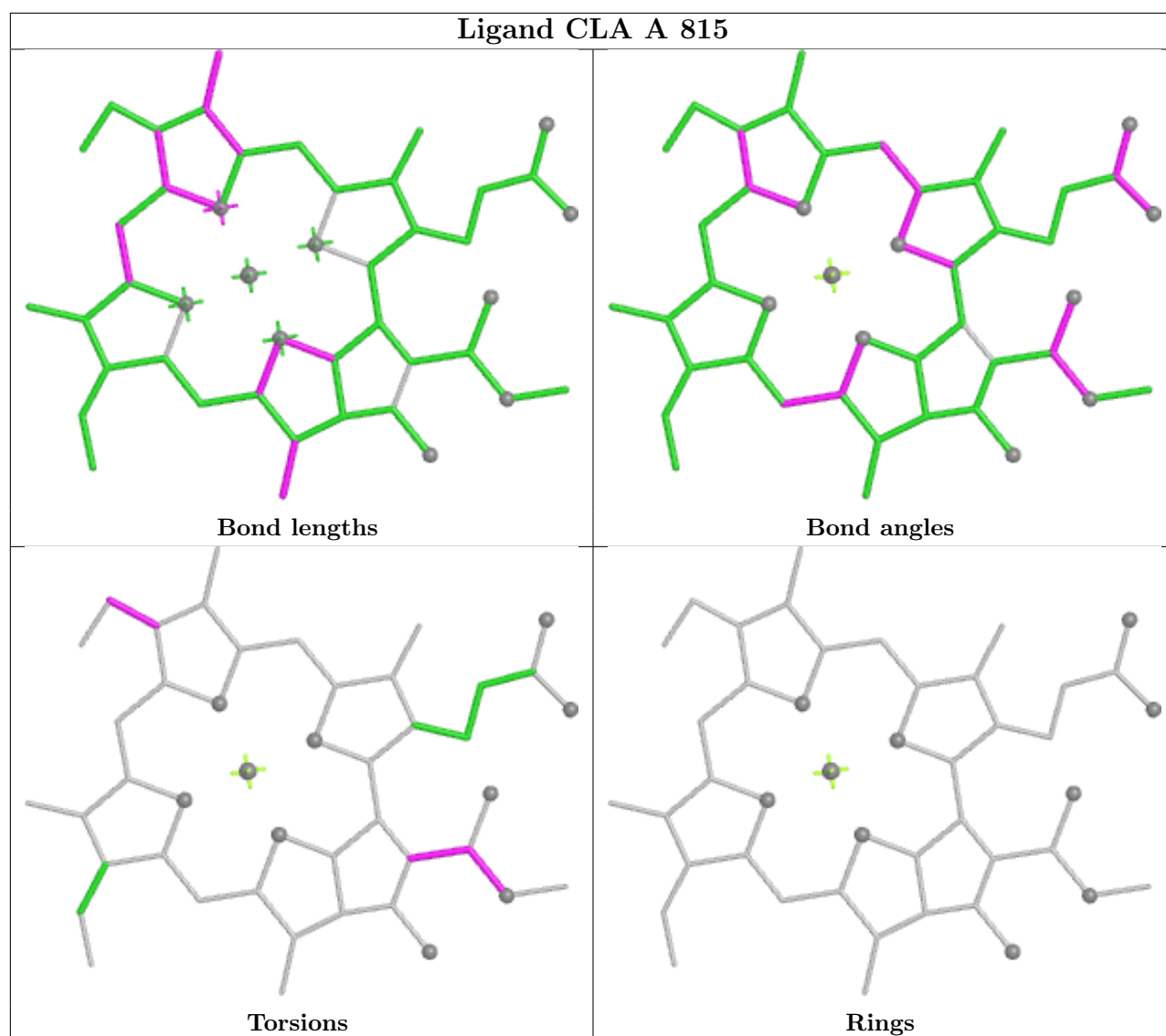
Bond angles

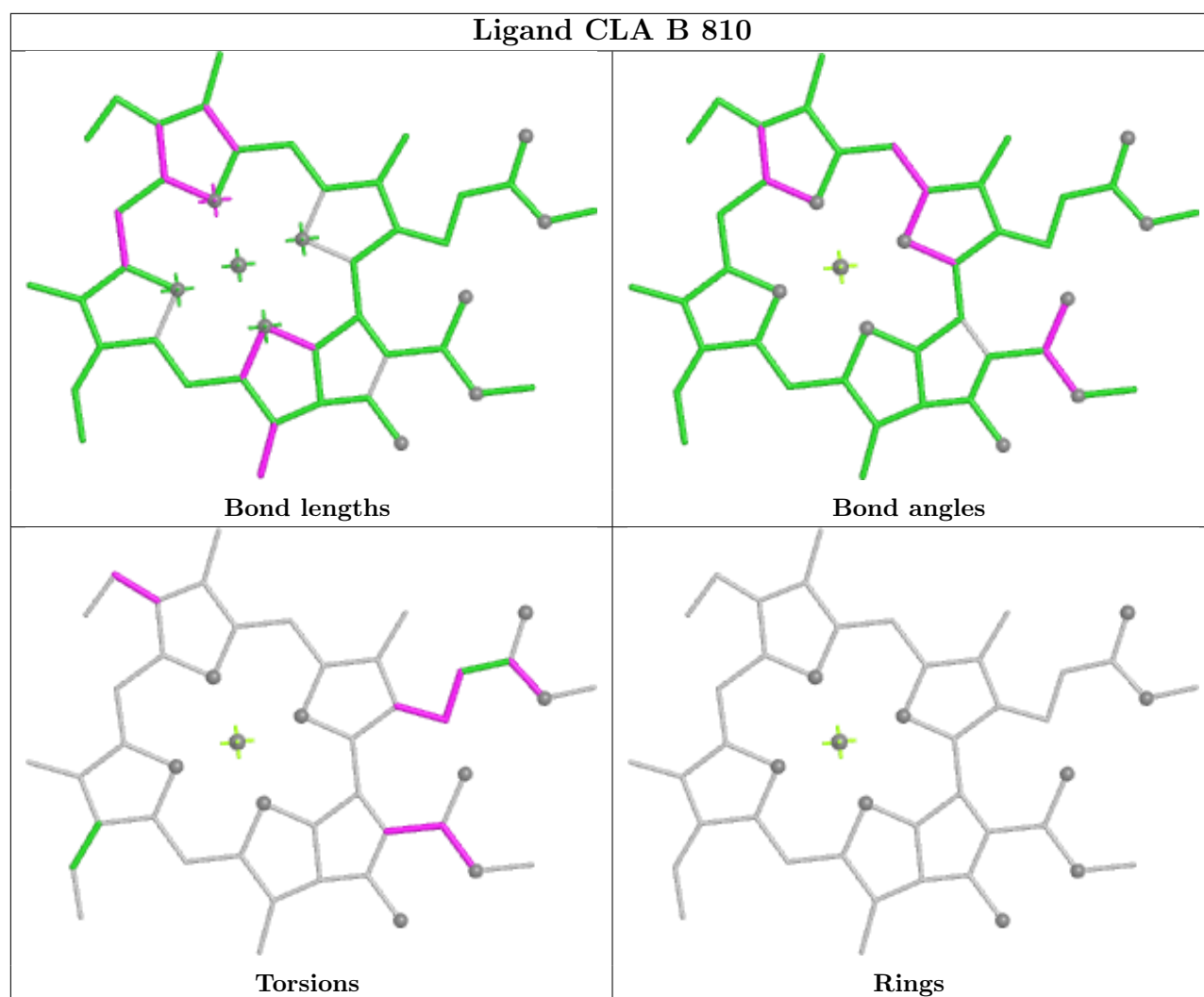


Torsions

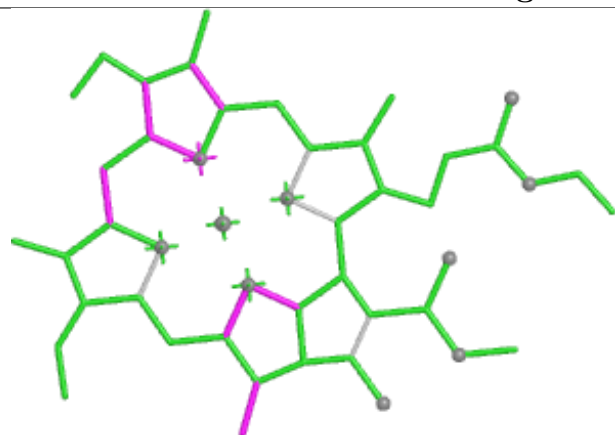


Rings





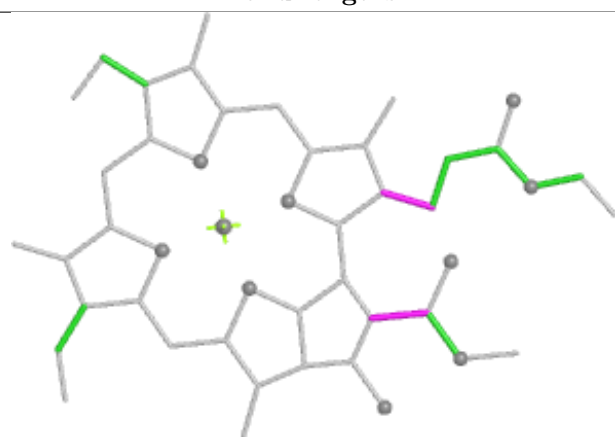
Ligand CLA B 838



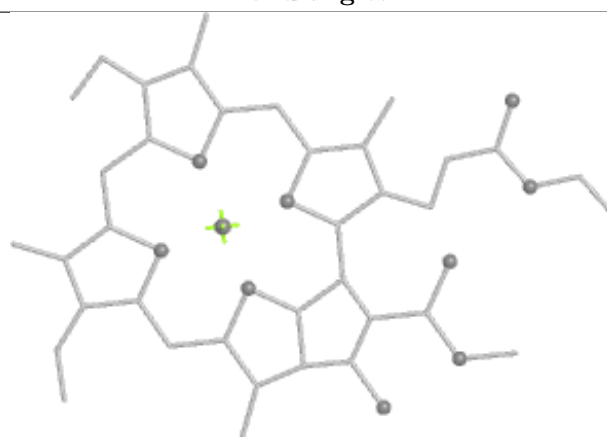
Bond lengths



Bond angles

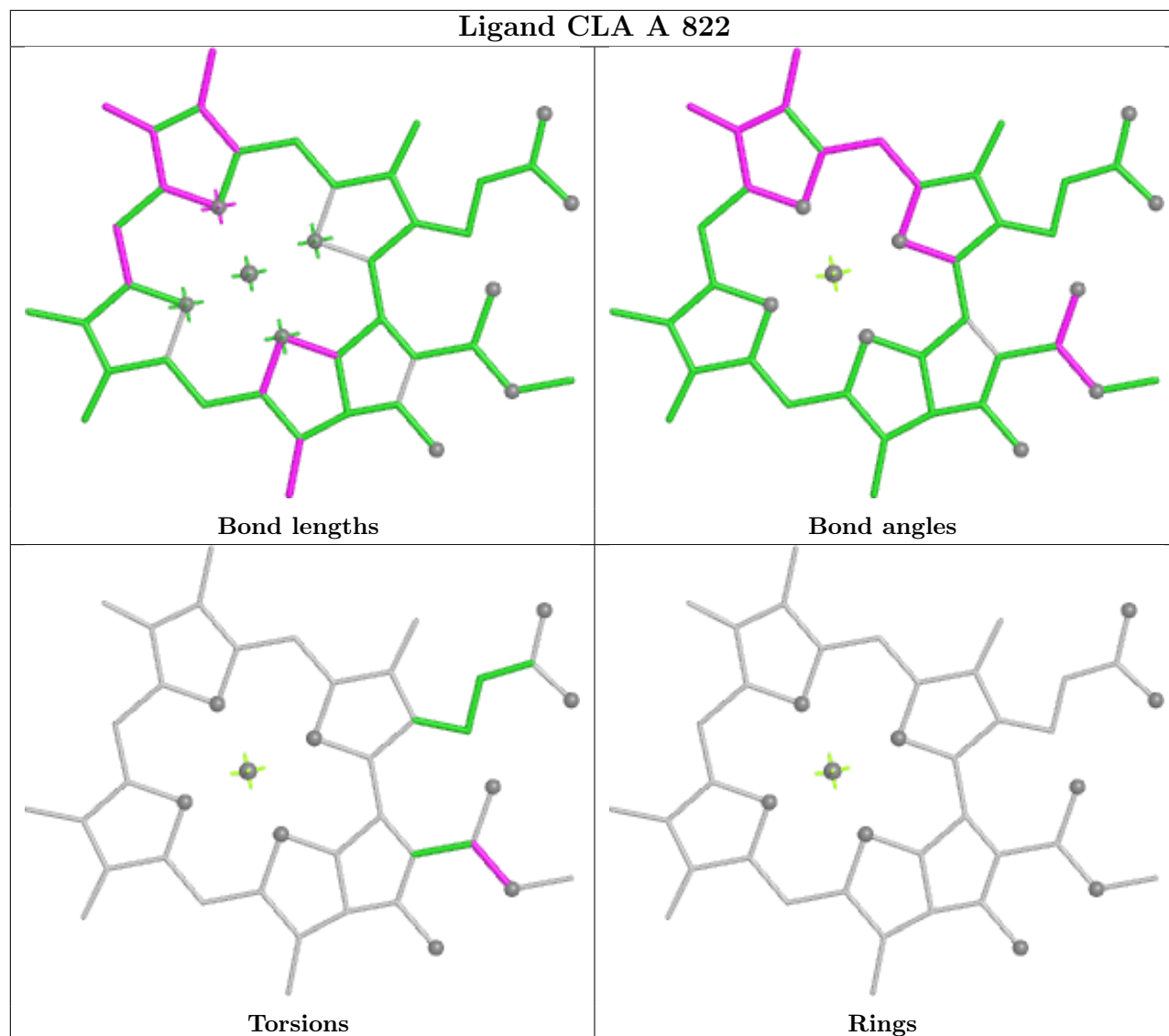


Torsions

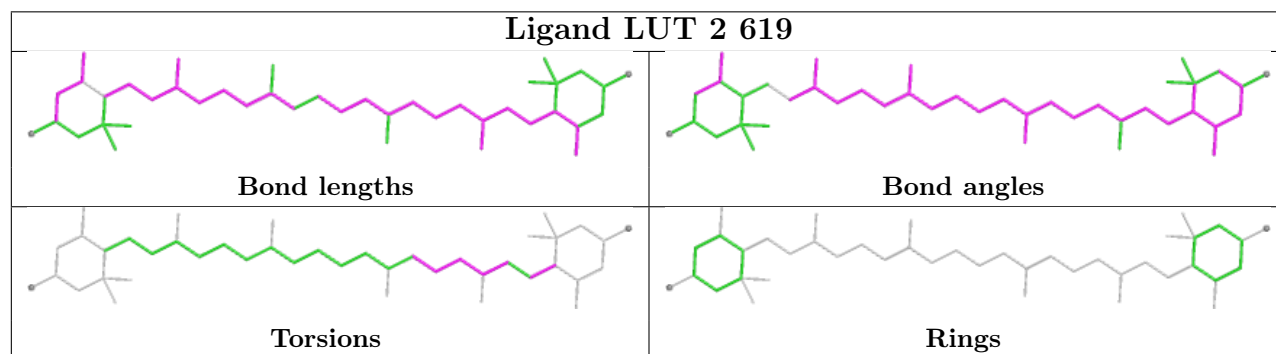


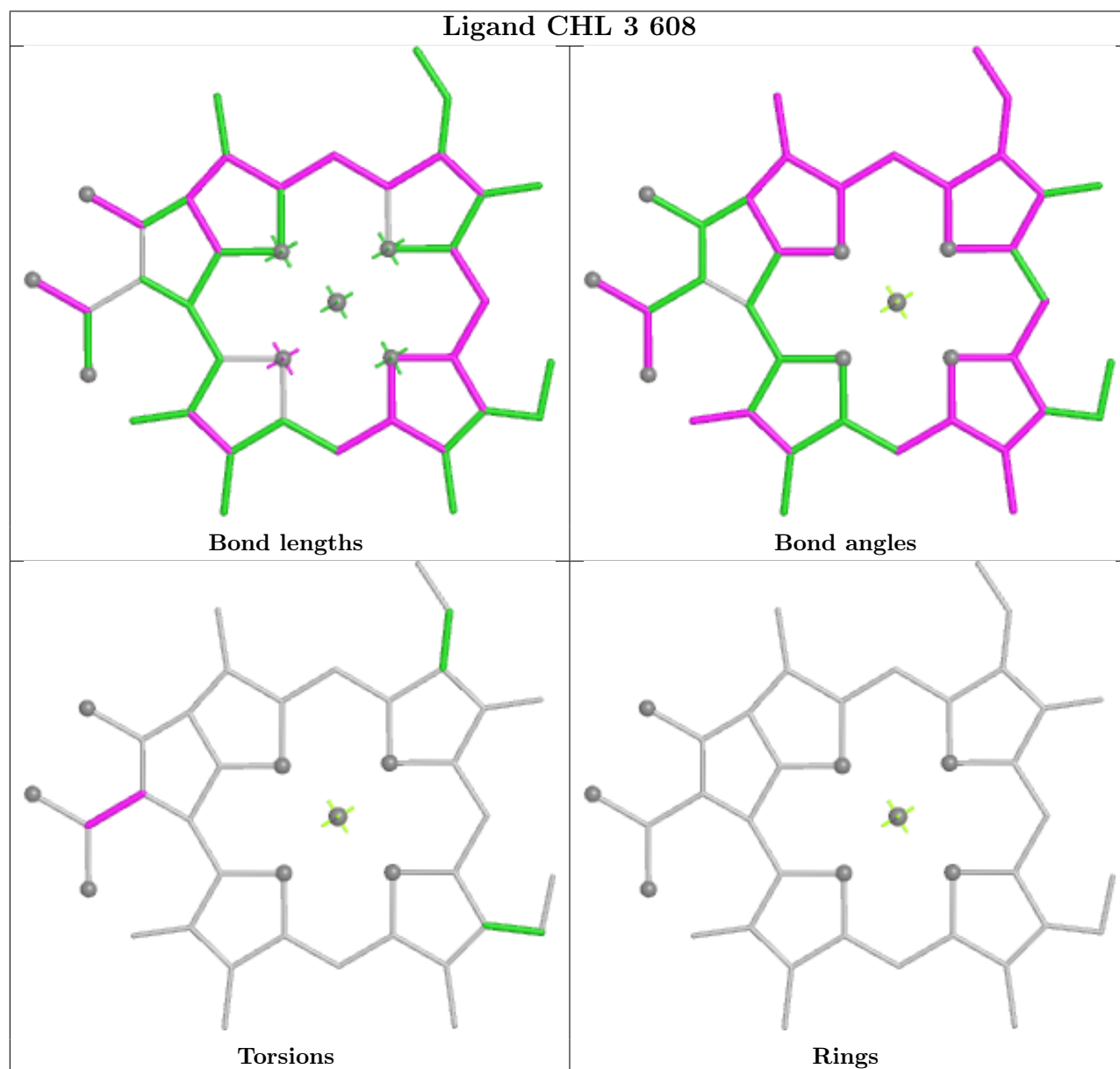
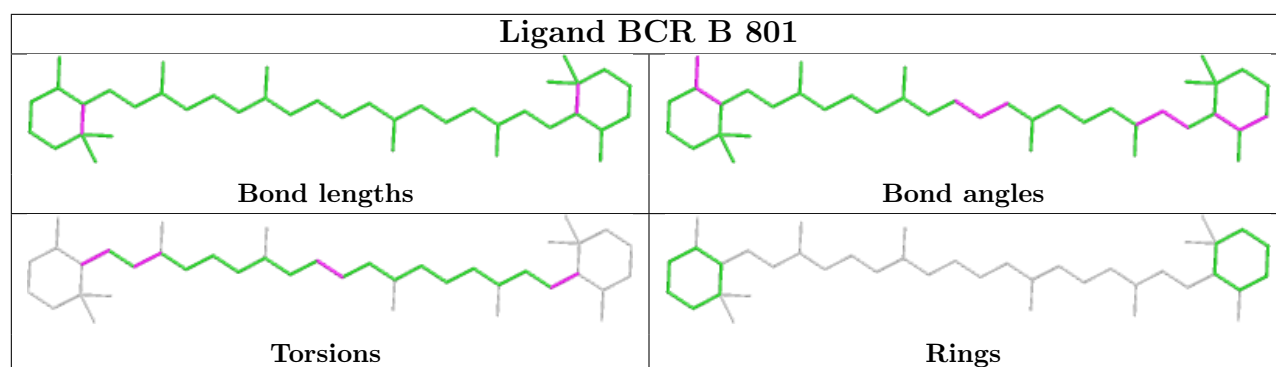
Rings

Ligand CLA A 822

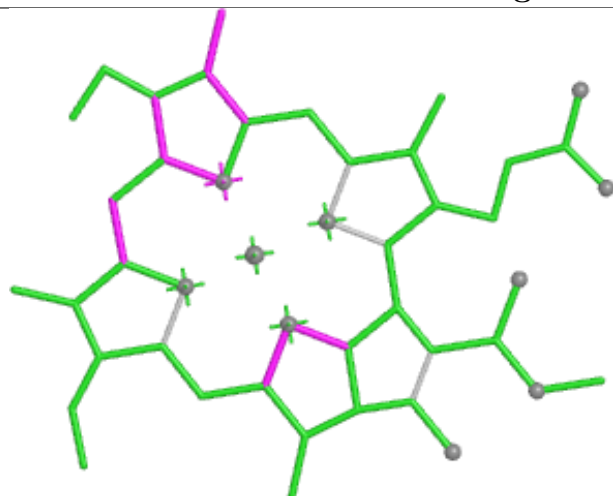


Ligand LUT 2 619

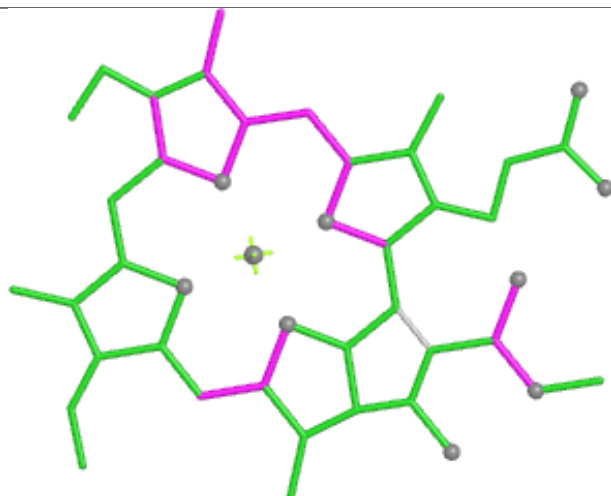




Ligand CLA A 833



Bond lengths



Bond angles

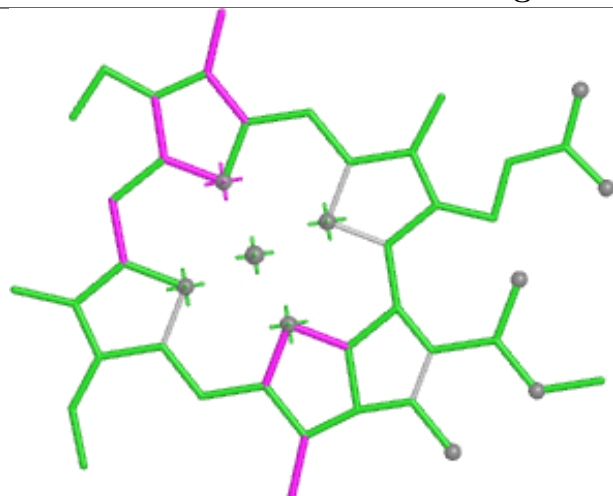


Torsions

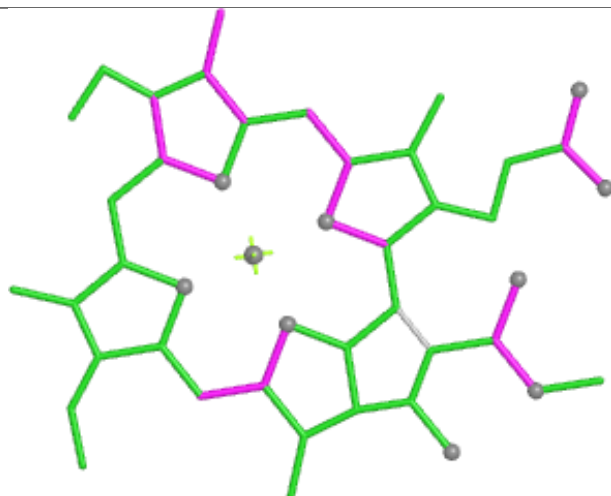


Rings

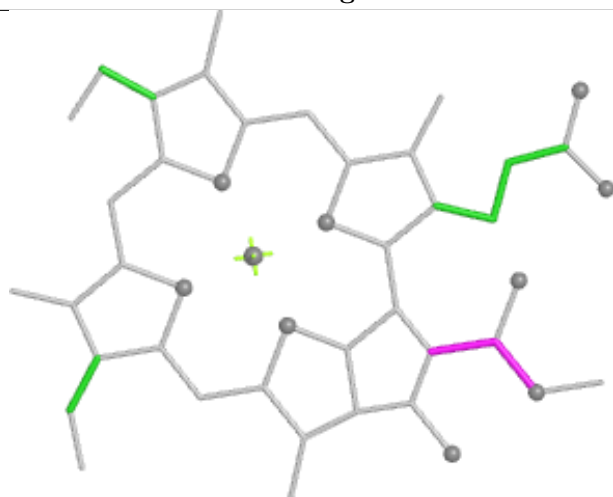
Ligand CLA A 808



Bond lengths



Bond angles

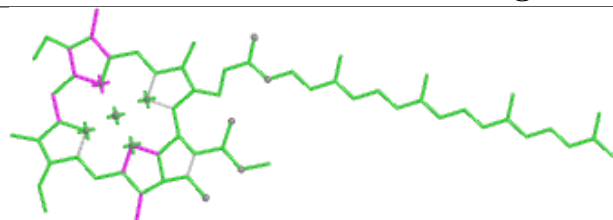


Torsions

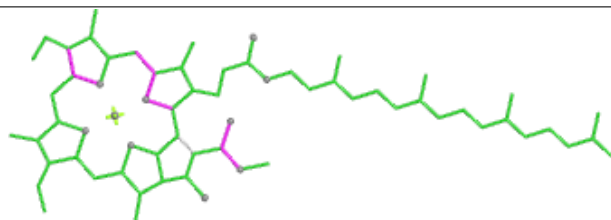


Rings

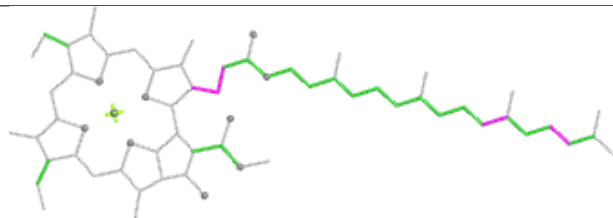
Ligand CLA A 830



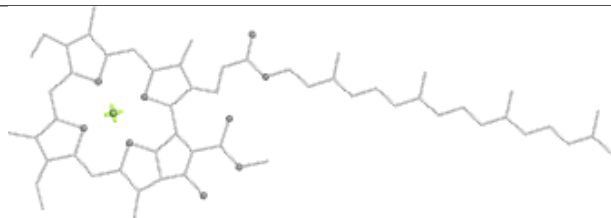
Bond lengths



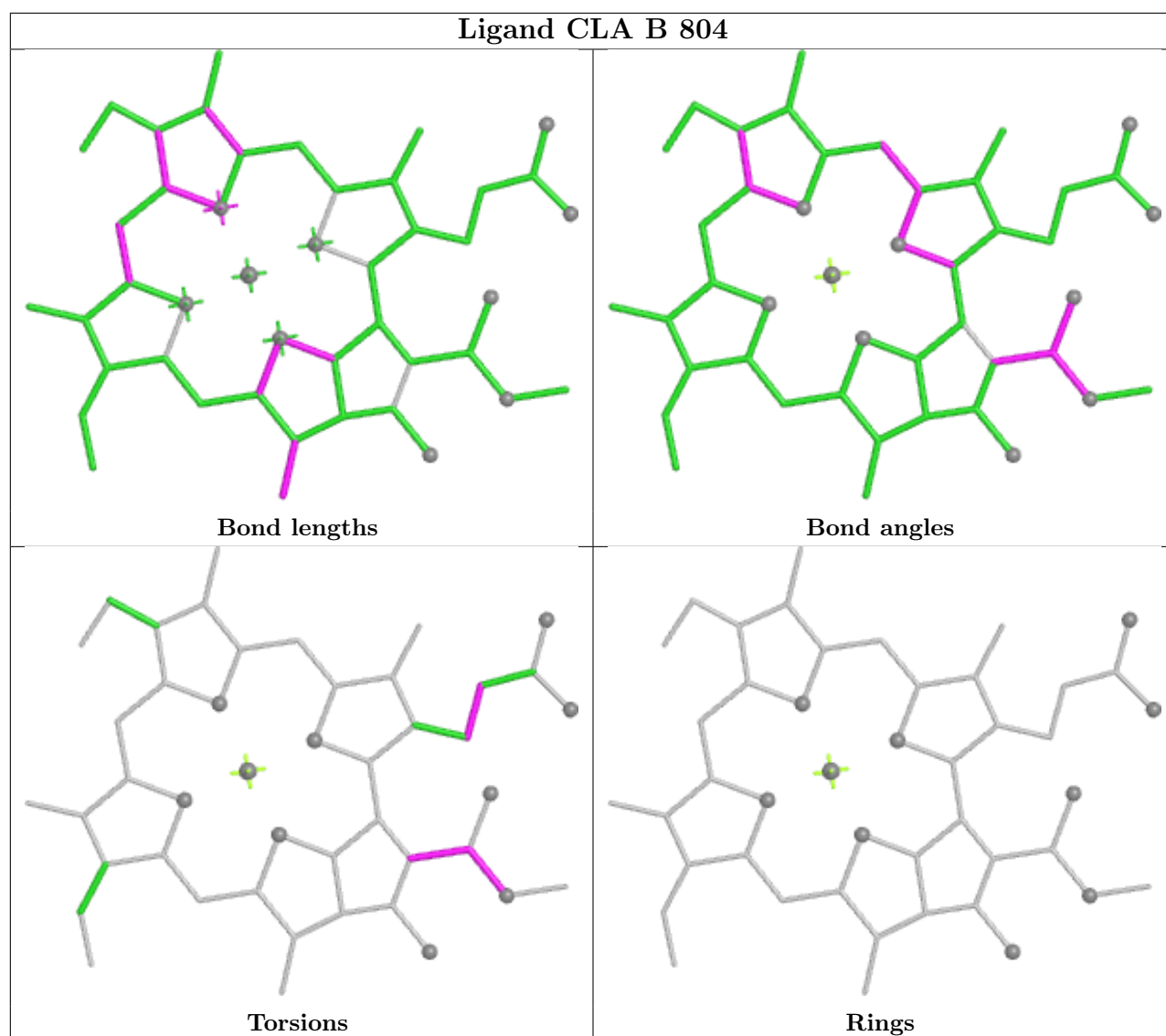
Bond angles



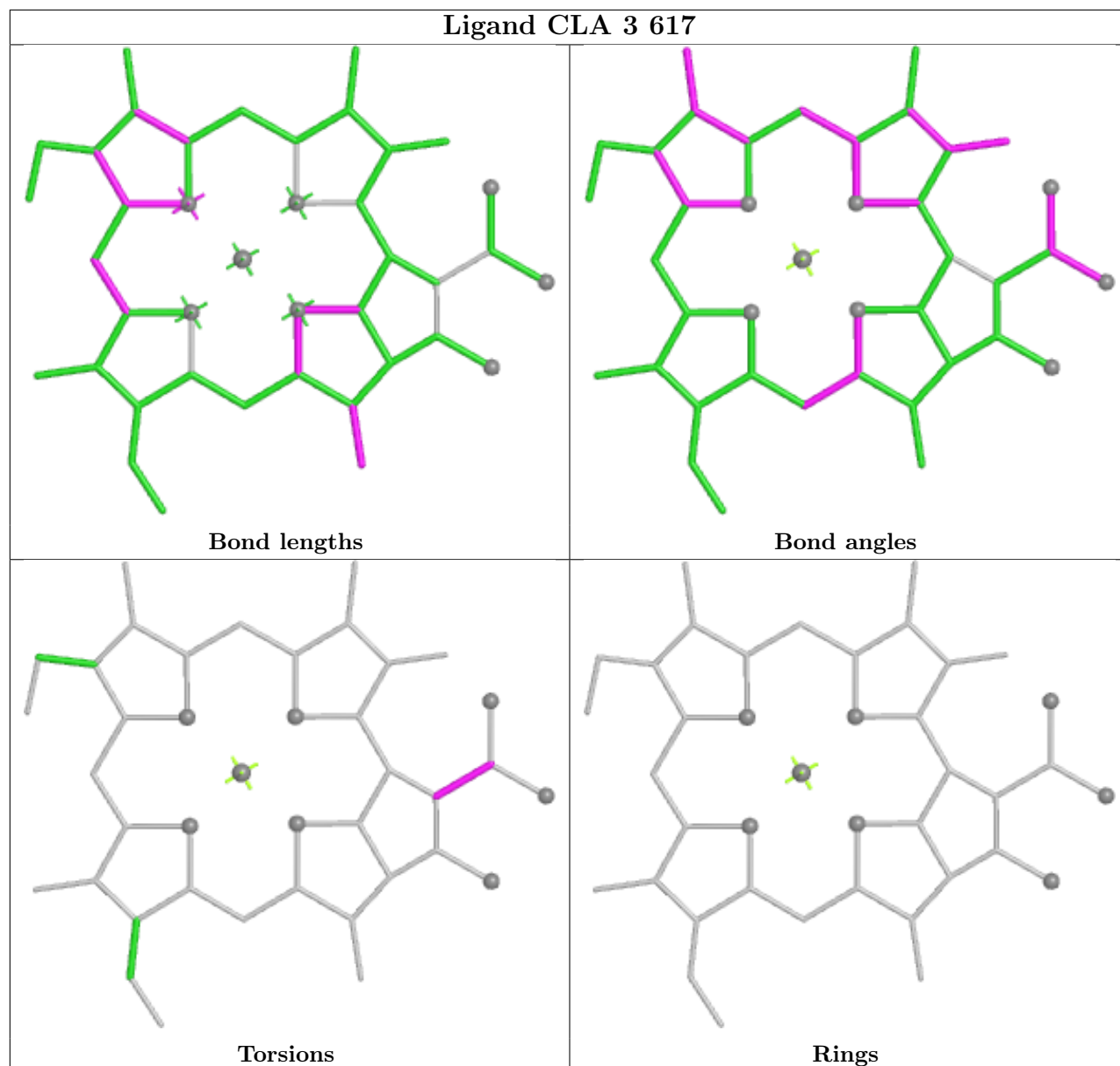
Torsions



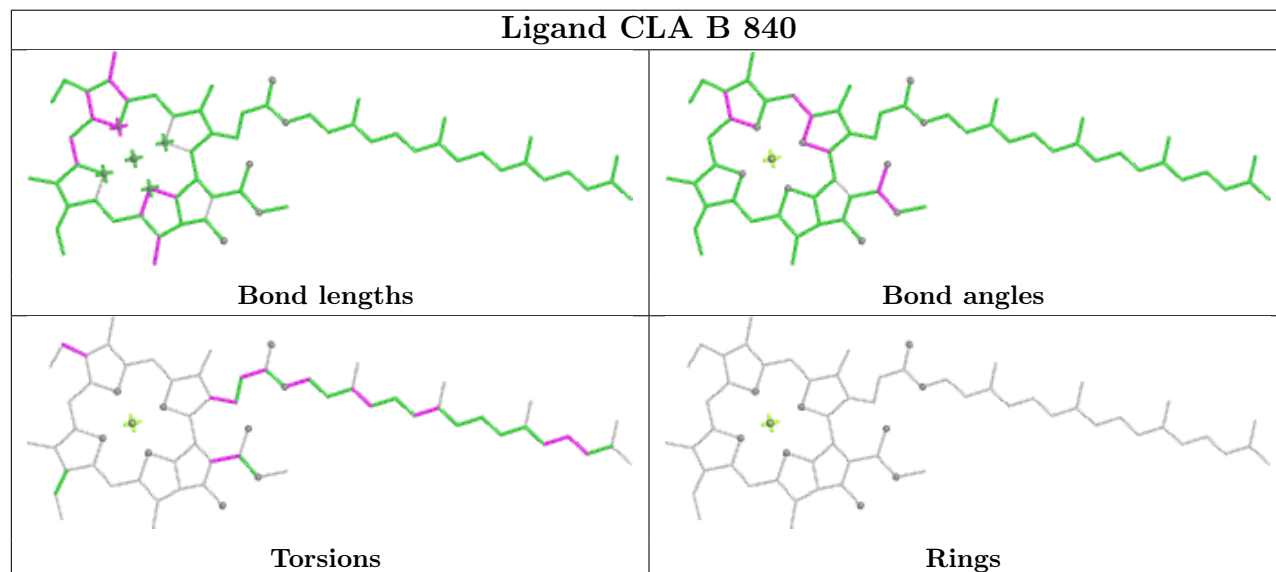
Rings

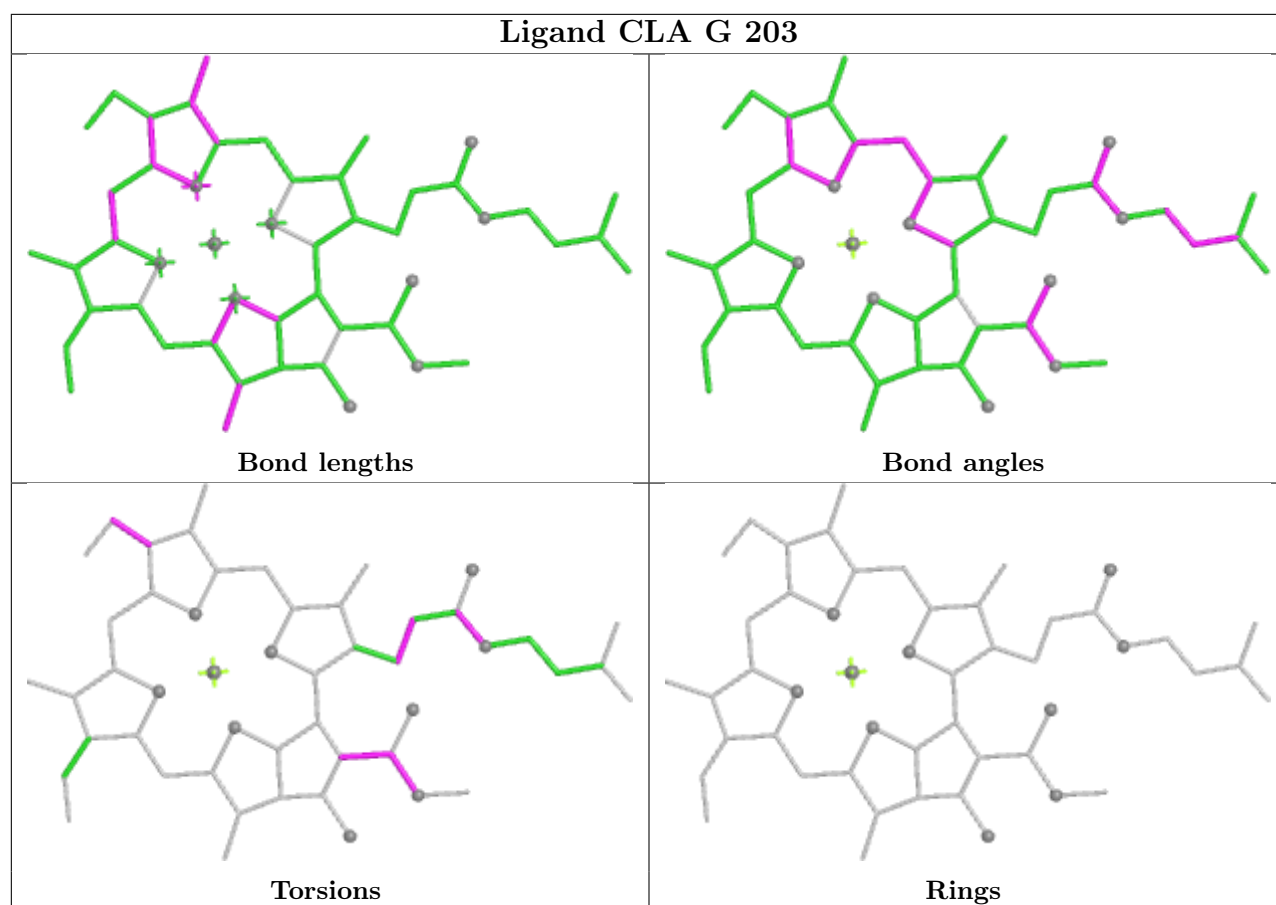


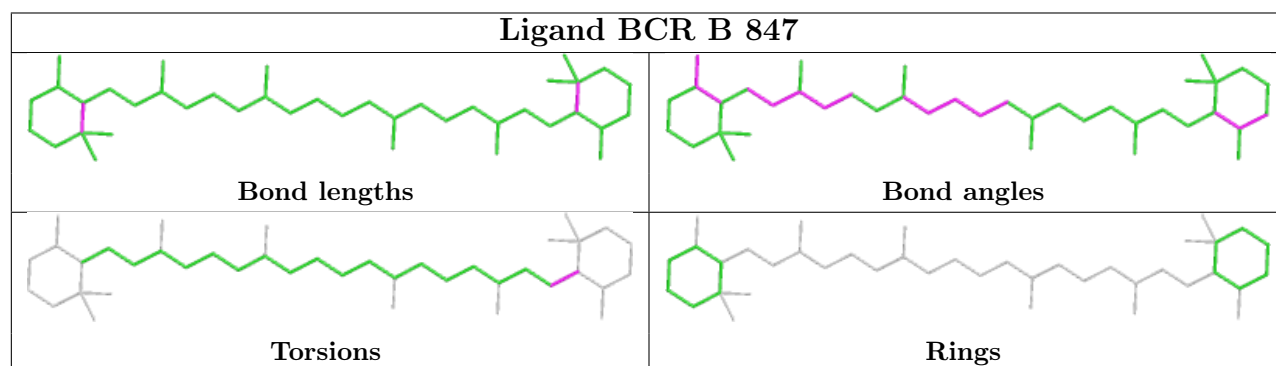
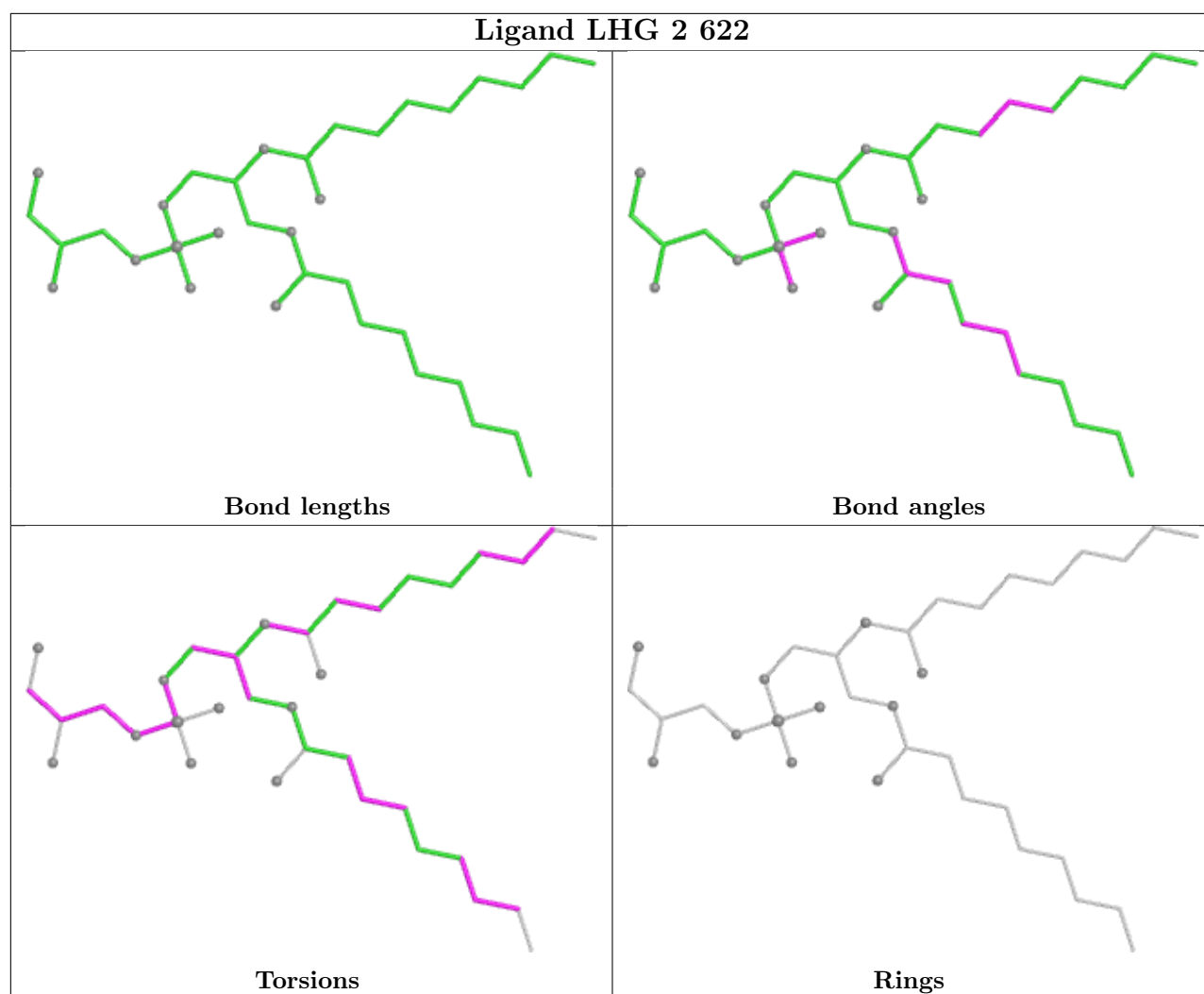
Ligand CLA 3 617

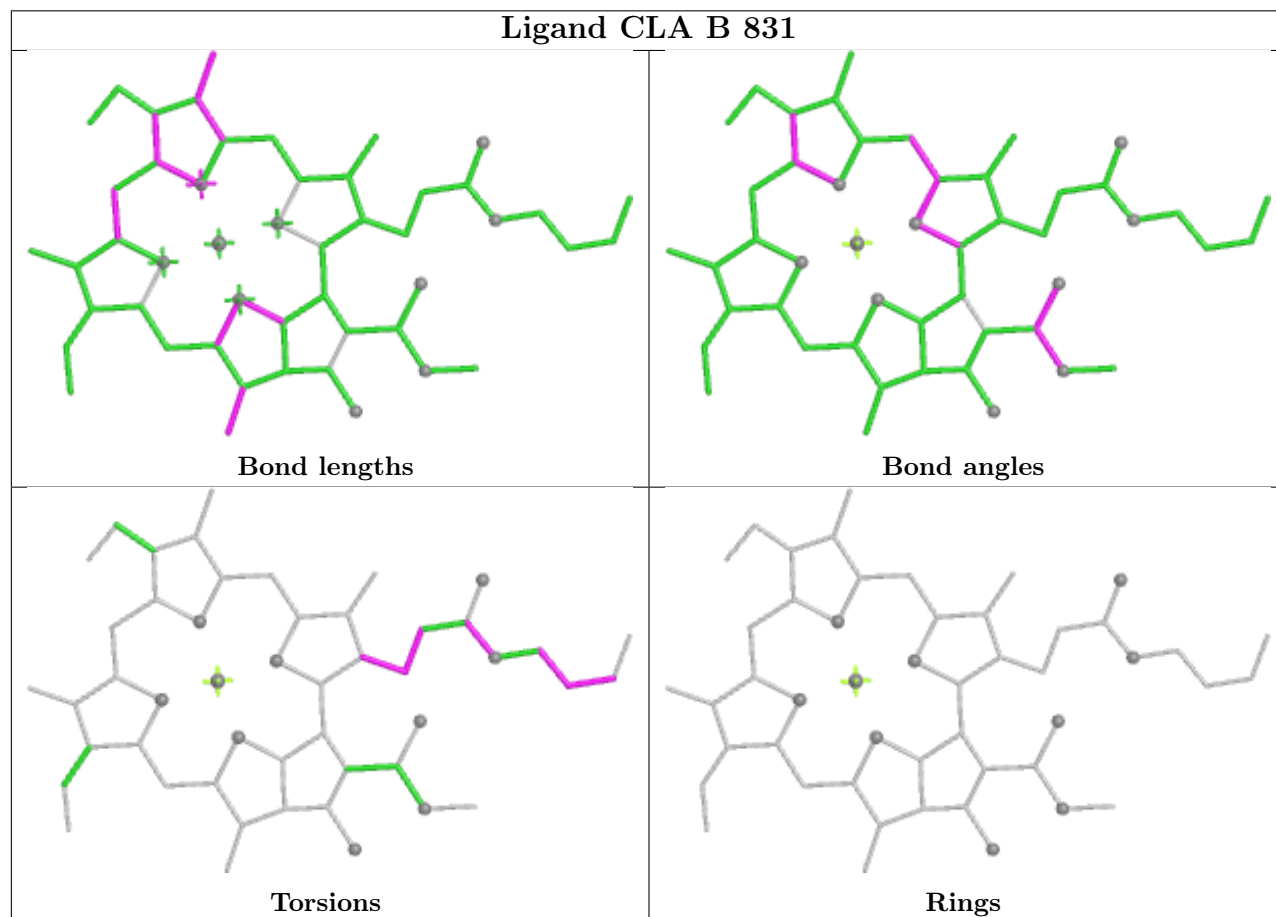
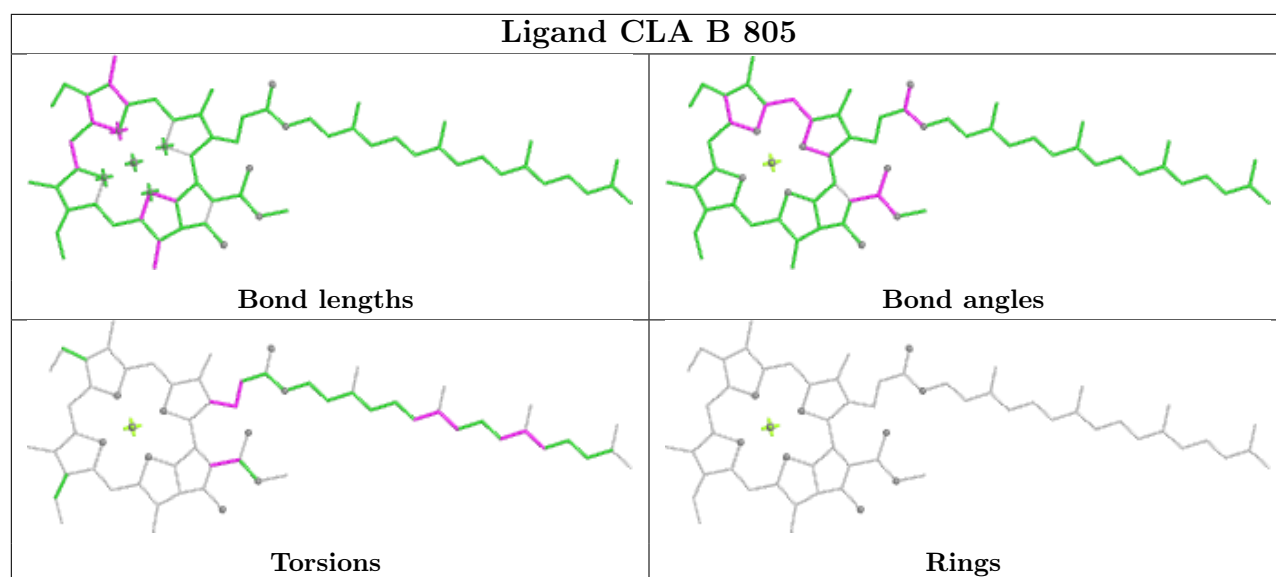


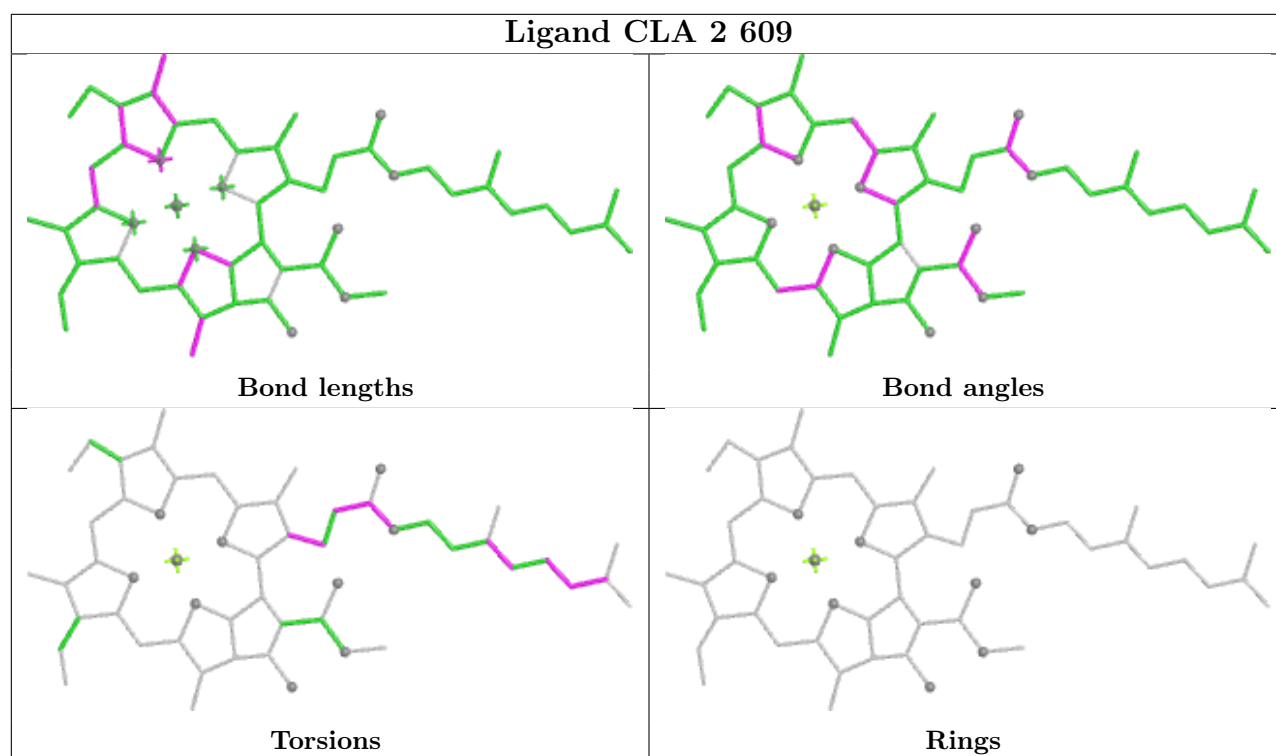
Ligand CLA B 840



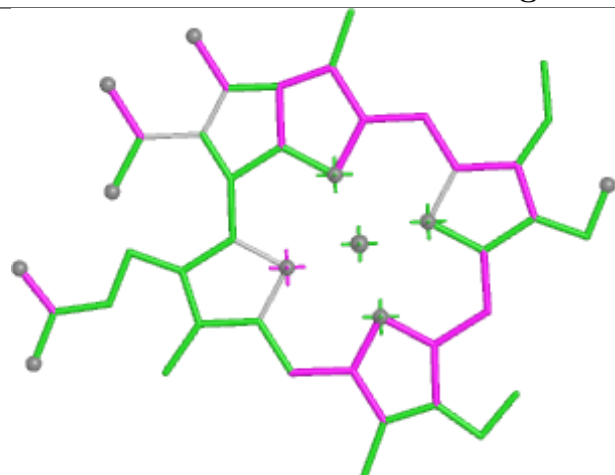




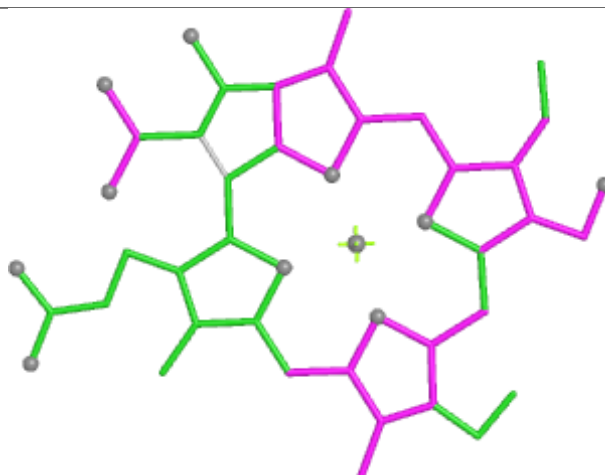




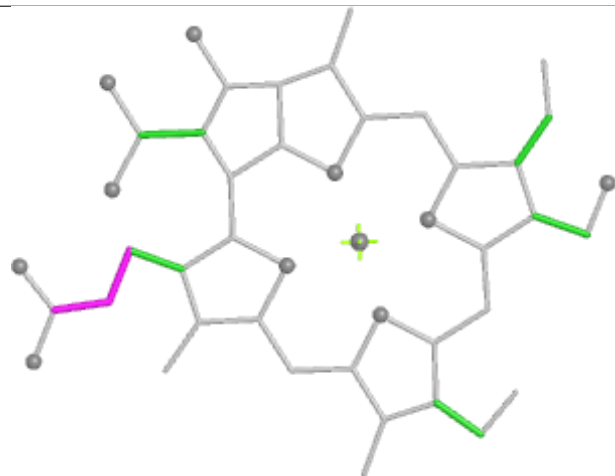
Ligand CHL 6 601



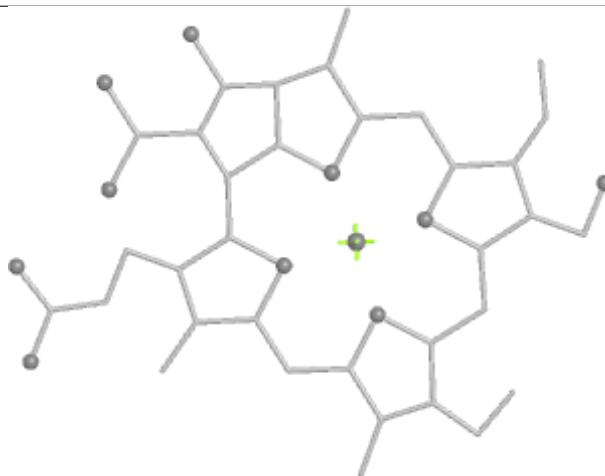
Bond lengths



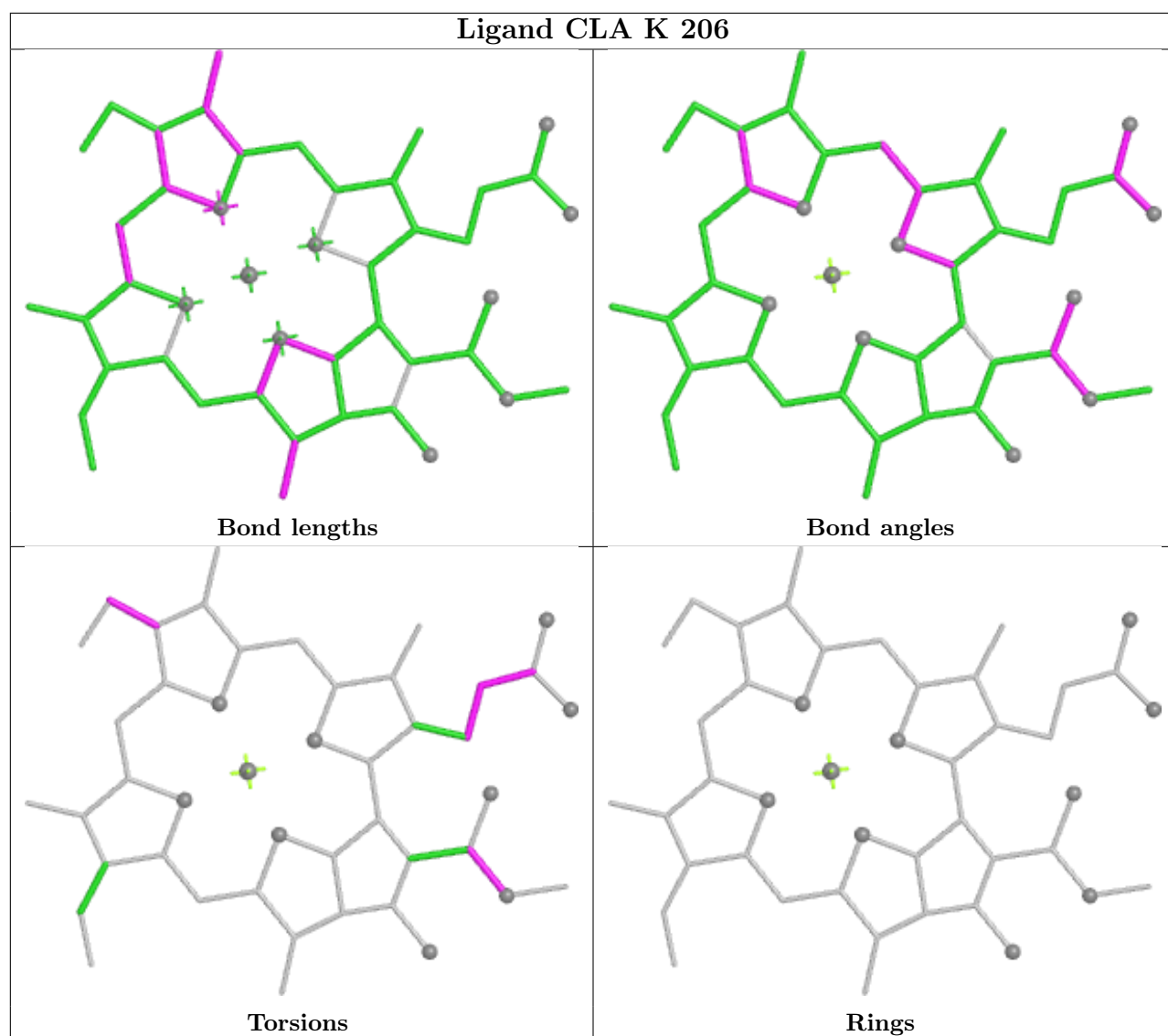
Bond angles

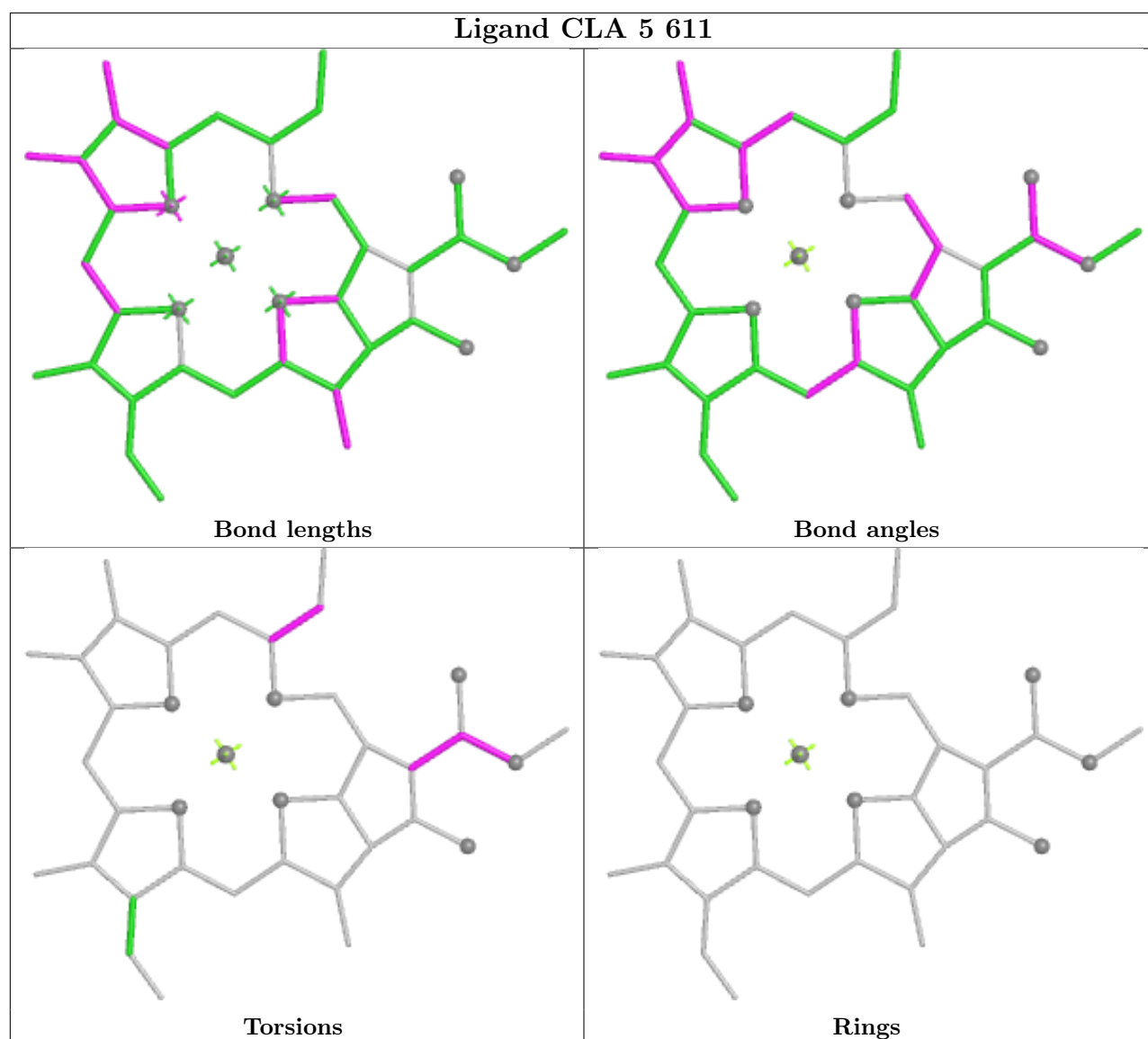


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

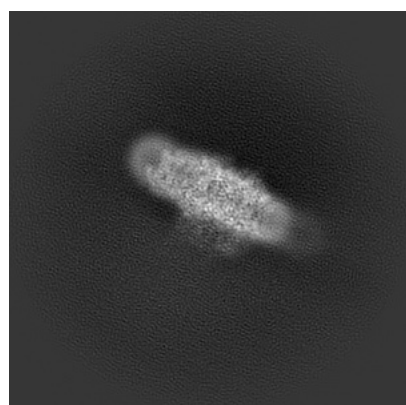
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0821. These allow visual inspection of the internal detail of the map and identification of artifacts.

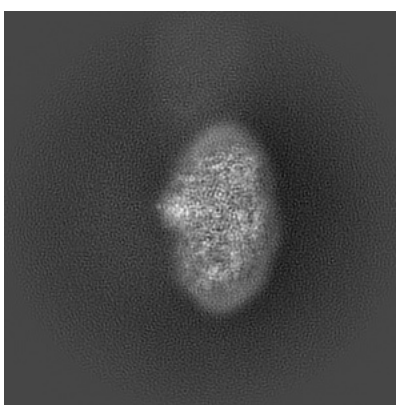
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

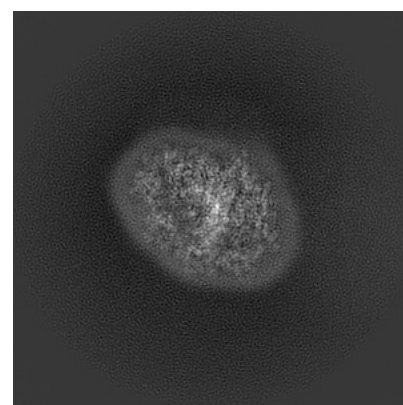
6.1.1 Primary map



X



Y

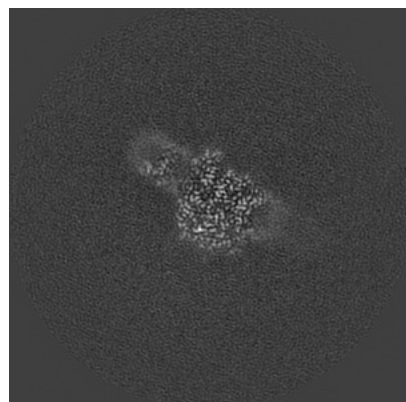


Z

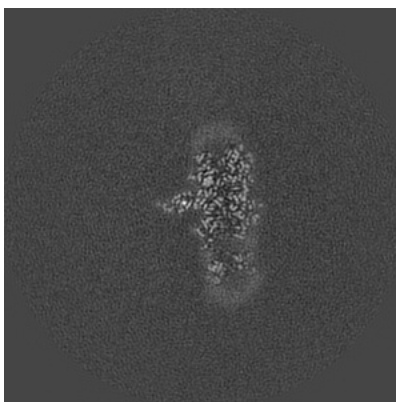
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

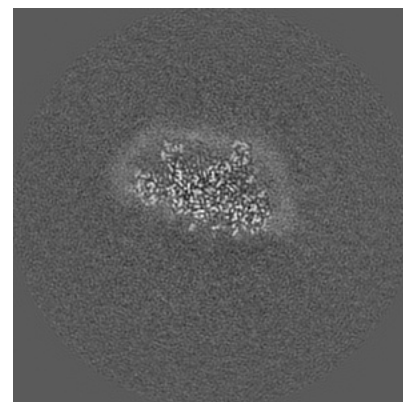
6.2.1 Primary map



X Index: 192



Y Index: 192

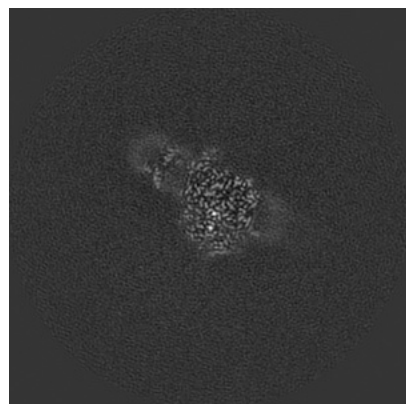


Z Index: 192

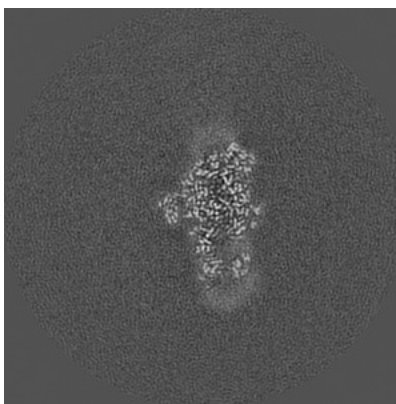
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

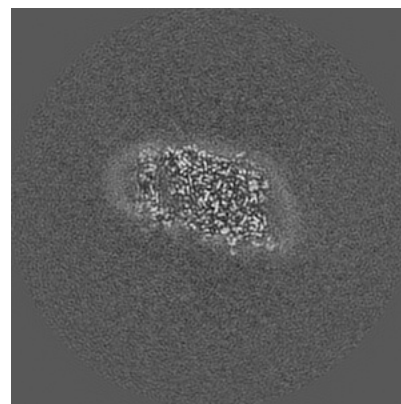
6.3.1 Primary map



X Index: 196



Y Index: 200

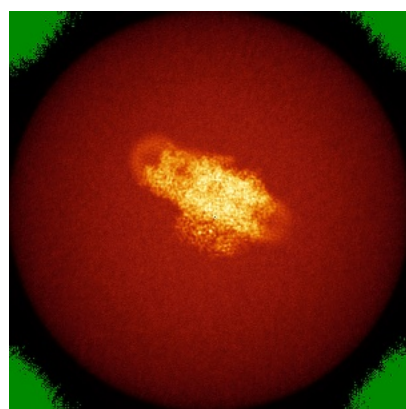


Z Index: 204

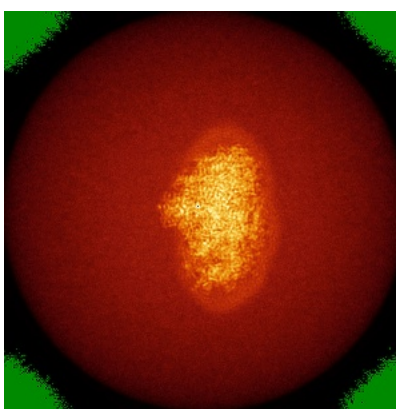
The images above show the largest variance slices of the map in three orthogonal directions.

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

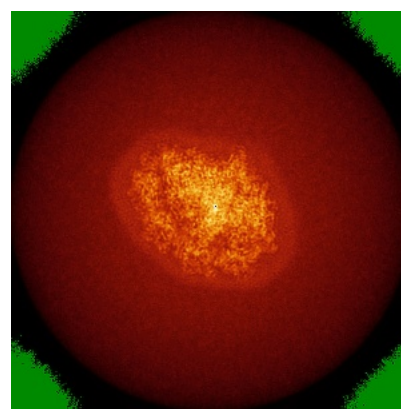
6.4.1 Primary map



X



Y

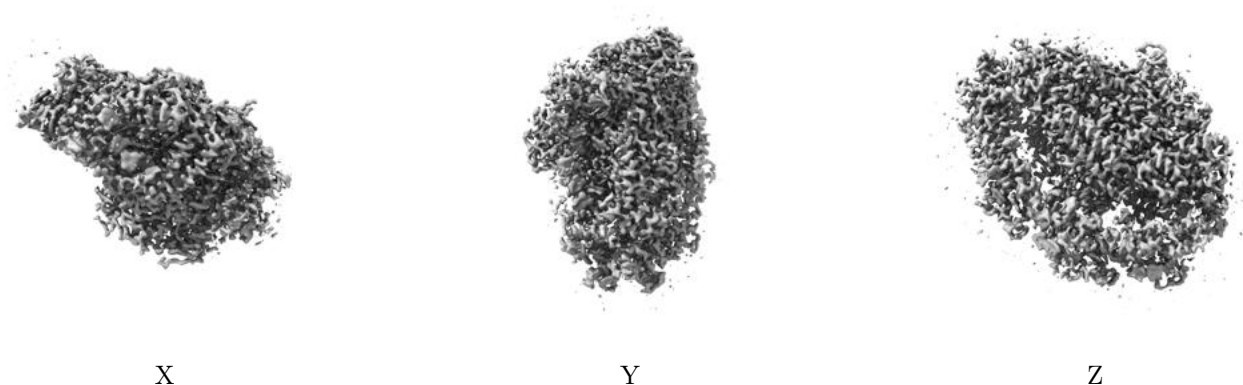


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

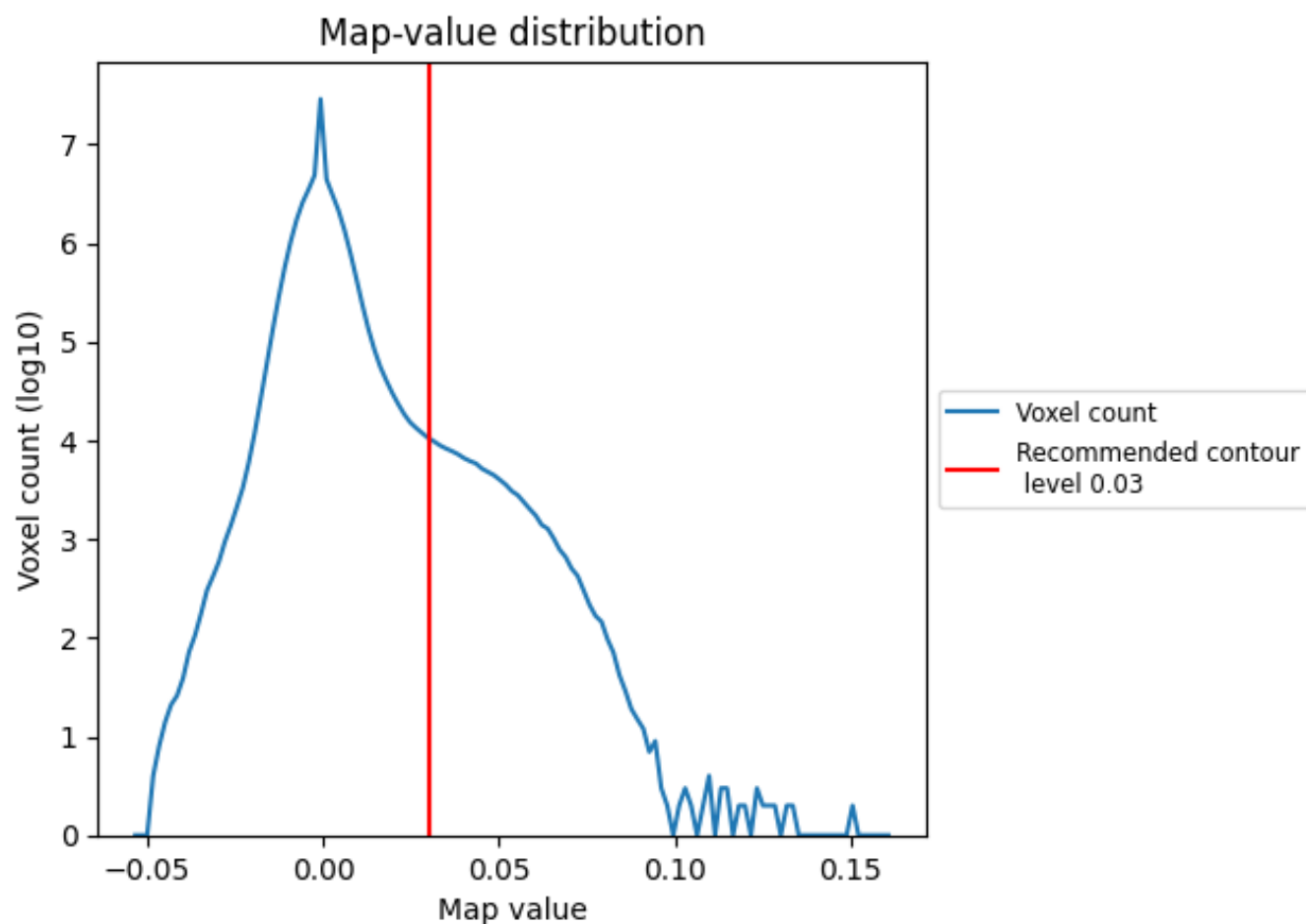
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

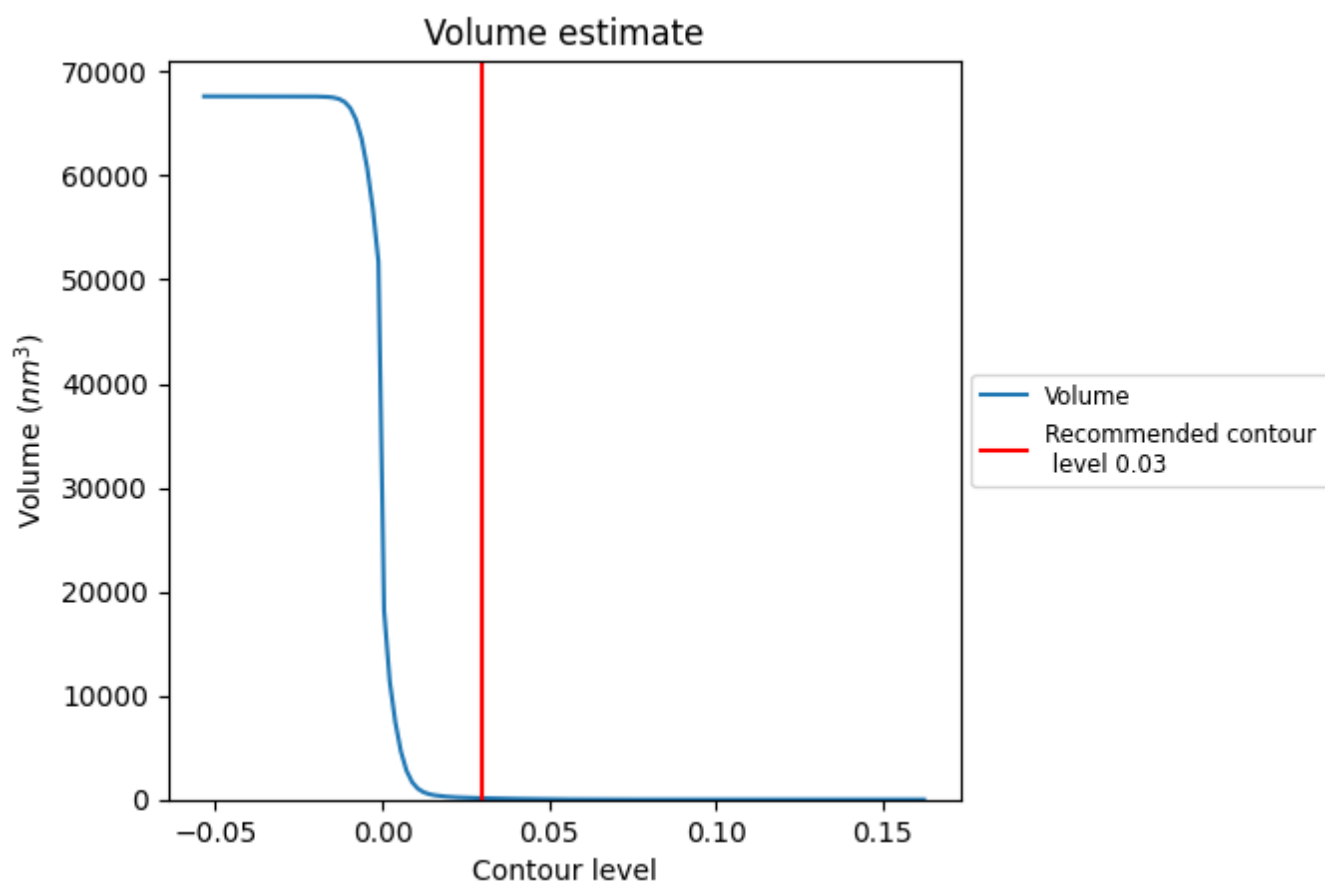
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

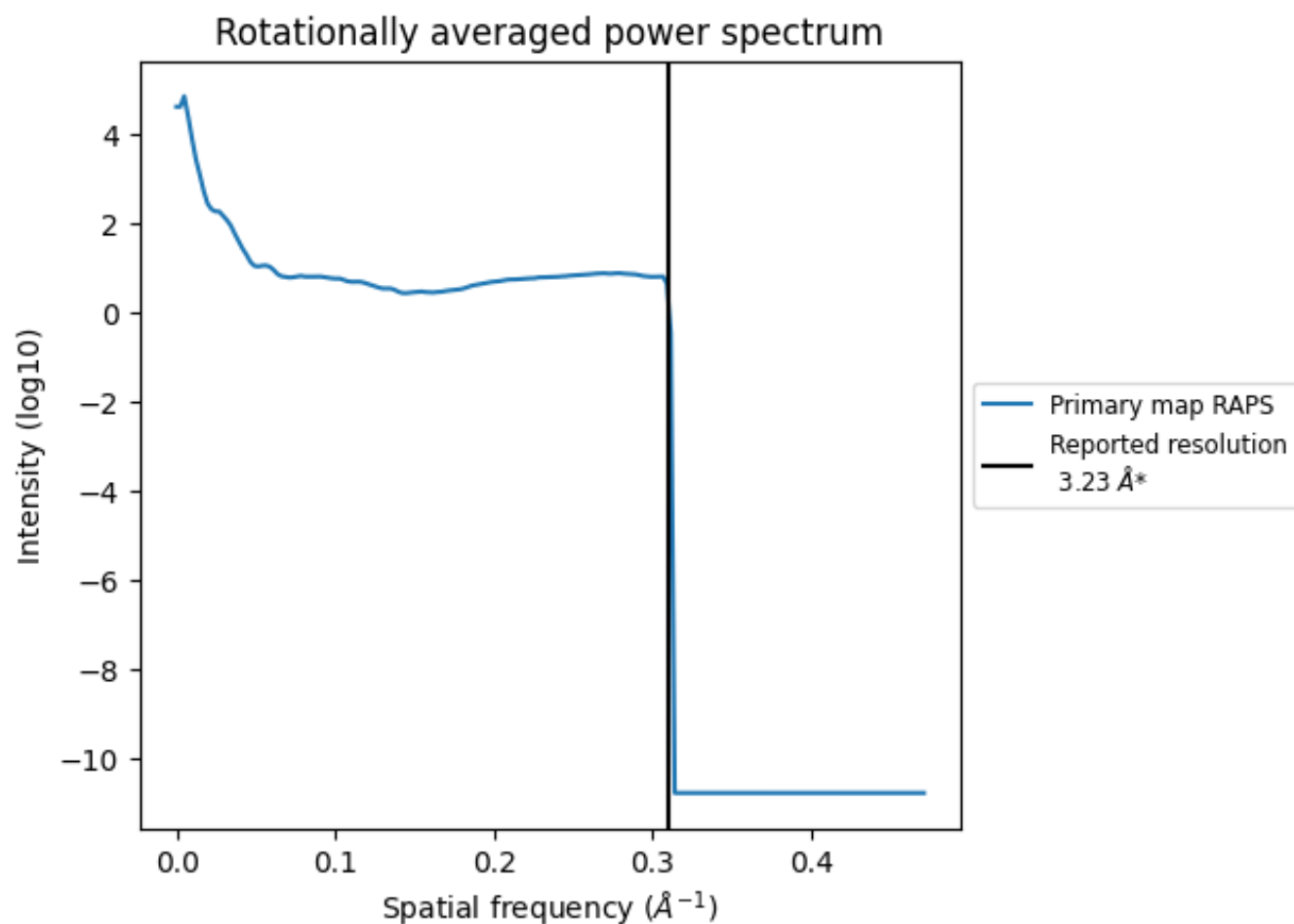
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

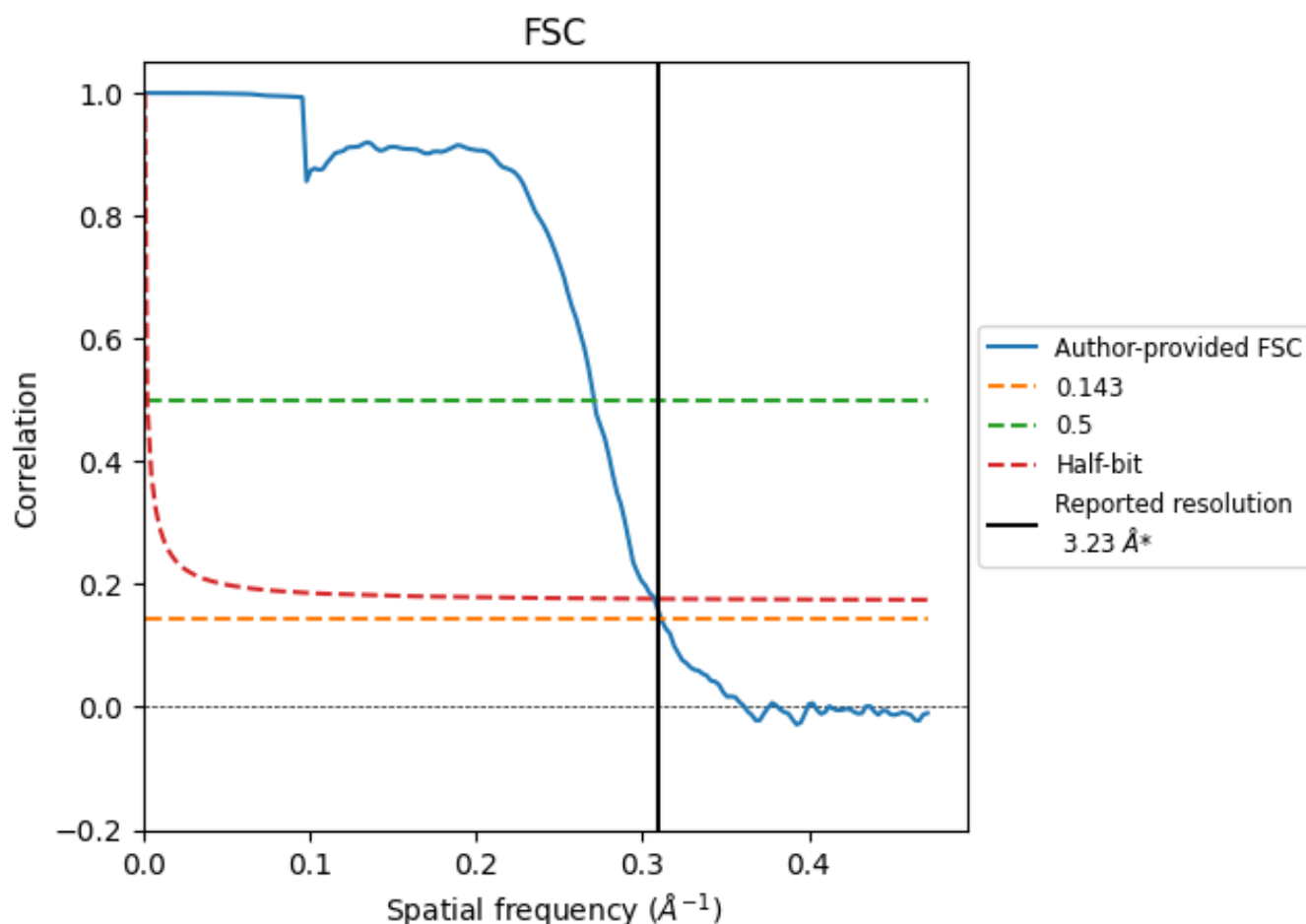


*Reported resolution corresponds to spatial frequency of 0.310 Å⁻¹

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 0.310 Å⁻¹

8.2 Resolution estimates [i](#)

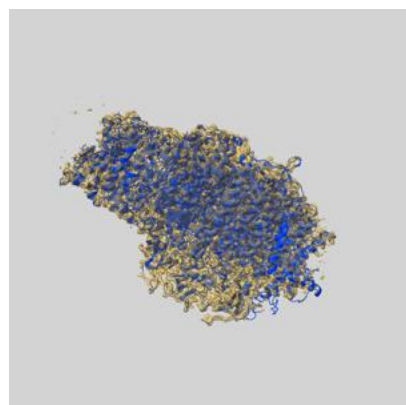
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.21	3.69	3.26
Unmasked-calculated*	-	-	-

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

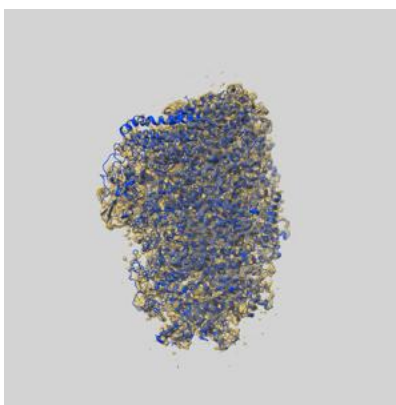
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0821 and PDB model 6L35. Per-residue inclusion information can be found in section 3 on page 22.

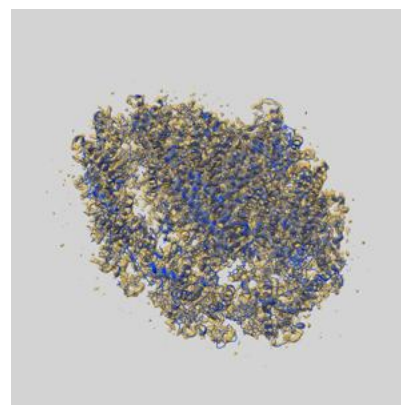
9.1 Map-model overlay [i](#)



X



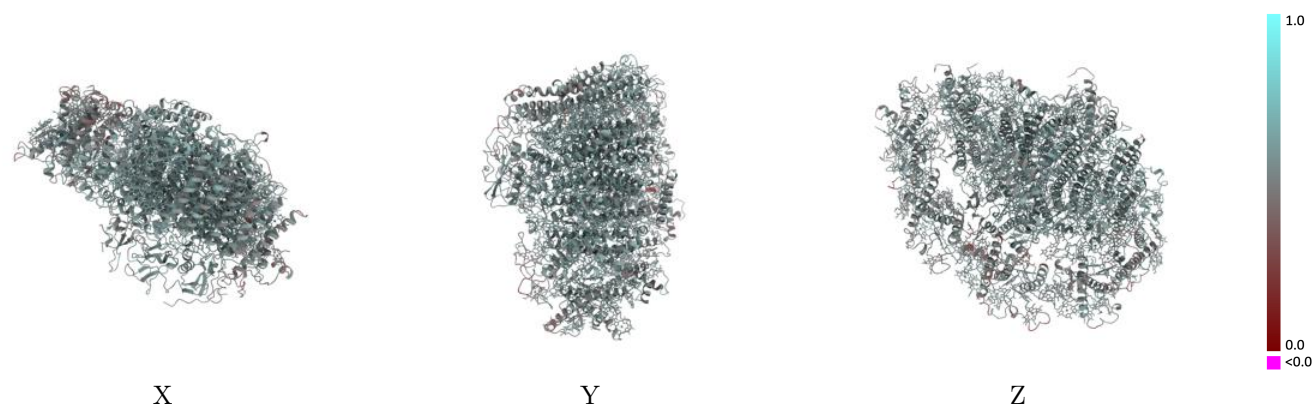
Y



Z

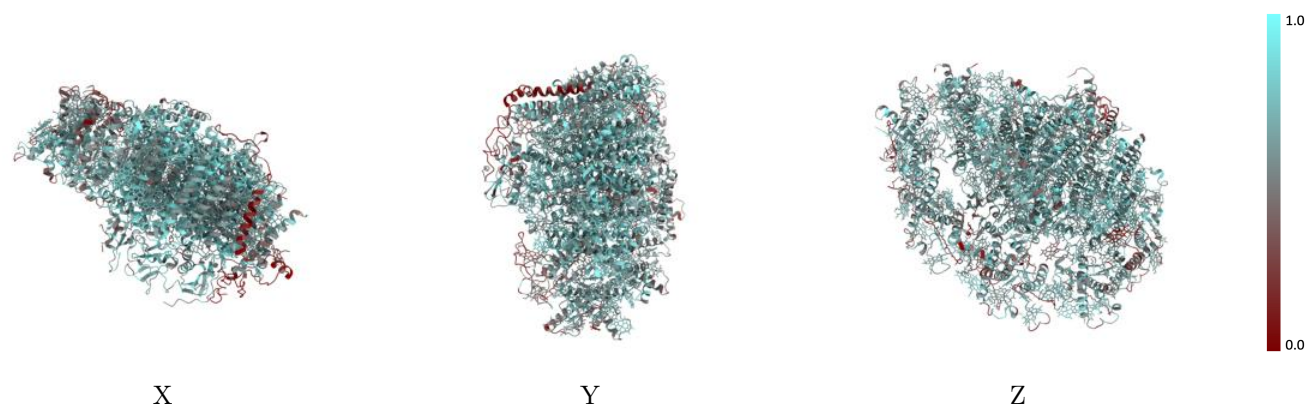
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



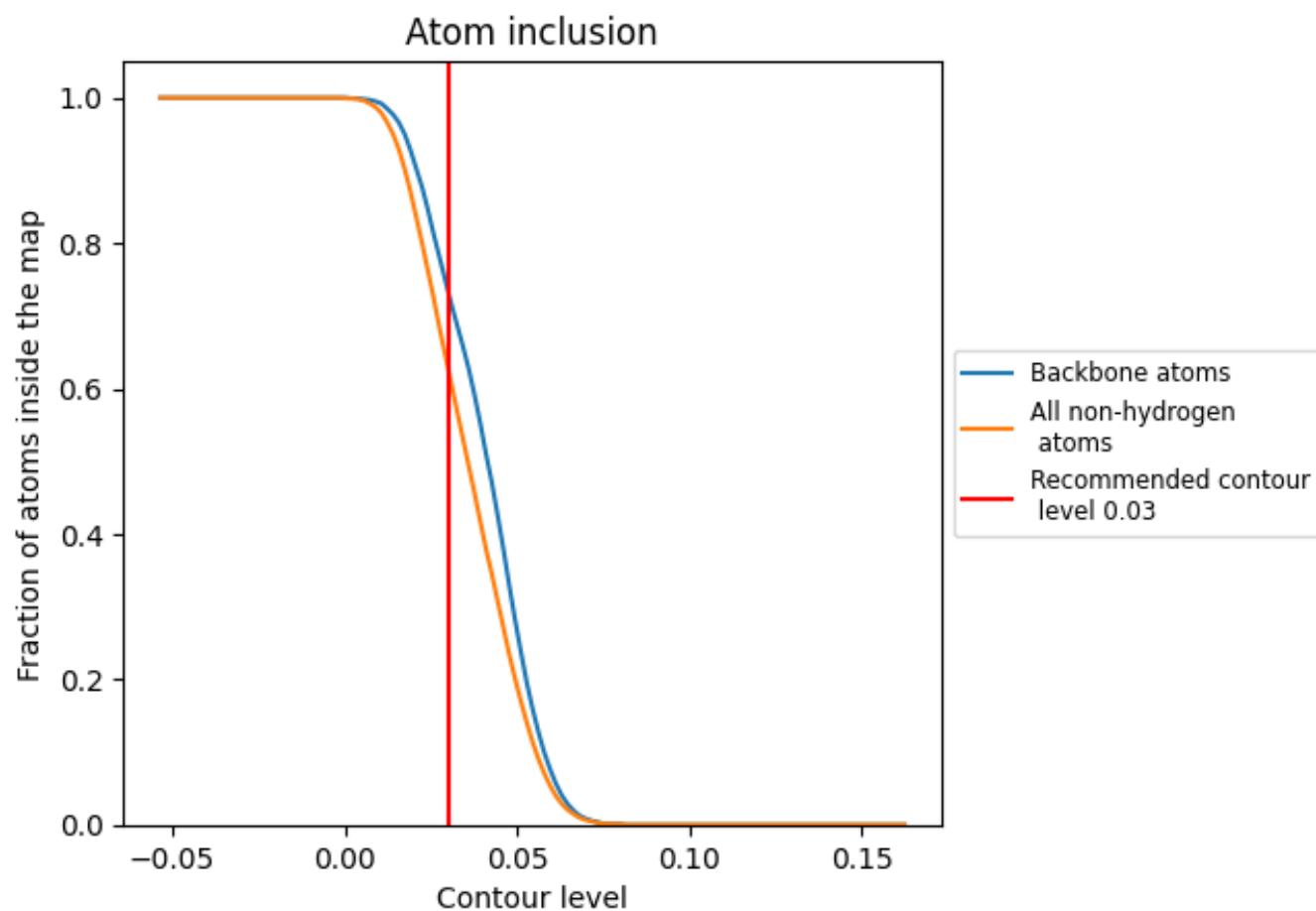
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.5450
2	0.5840	0.5210
3	0.5710	0.5210
5	0.5620	0.4890
6	0.5770	0.5130
A	0.7030	0.5700
B	0.7100	0.5730
C	0.7400	0.5450
D	0.6350	0.5460
E	0.6670	0.5550
F	0.6180	0.5420
G	0.5080	0.5190
H	0.1310	0.4850
I	0.5560	0.5500
J	0.5630	0.5490
K	0.4190	0.5040
L	0.4850	0.5170
M	0.6070	0.5250

