



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 01:15 PM JST

PDB ID : 7Y3F / pdb_00007y3f
EMDB ID : EMD-33593
Title : Structure of the Anabaena PSI-monomer-IsiA supercomplex
Authors : Nagao, R.; Kato, K.; Hamaguchi, T.; Kawakami, K.; Yonekura, K.; Shen, J.R.
Deposited on : 2022-06-10
Resolution : 2.62 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:

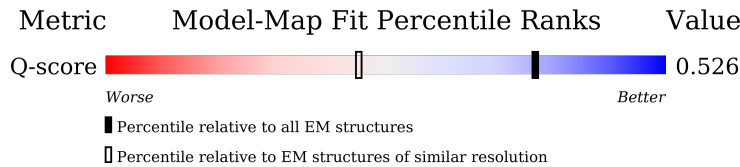
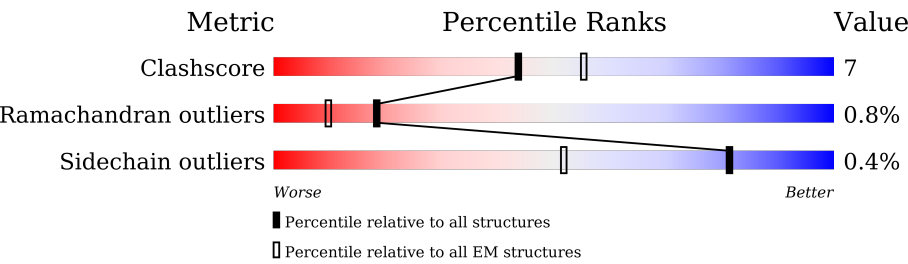
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 2.62 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.



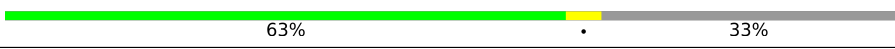
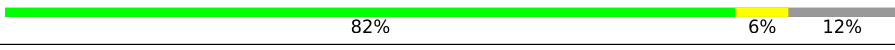
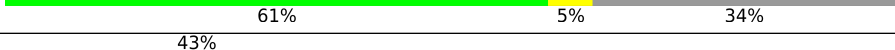
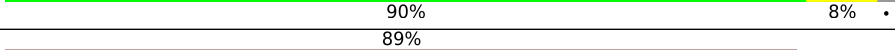
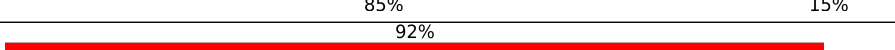
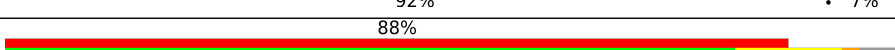
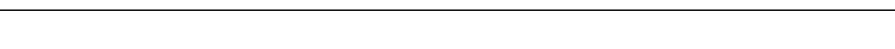
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8810 (2.12 - 3.12)

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	752	88% 10% .
2	B	741	90% 10% .
3	C	81	91% 7% .
4	D	139	92% 5% .

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Mol	Chain	Length	Quality of chain
5	E	70	
6	F	164	
7	I	46	
8	J	49	
9	K	82	
10	M	40	
11	X	44	
12	1	476	
13	2	325	
13	3	325	
13	6	325	
14	4	344	
14	5	344	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 39463 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
			5824	3821	1003	979	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

- 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
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	135	Total	C	N	O	S	0	0
			1043	668	179	195	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	31	Total	C	N	O	0	0
			253	177	35	41		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	43	Total	C	N	O	0	0
			347	236	52	59		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 10 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	30	Total	C	N	O	0	0
			235	157	36	42		

- Molecule 11 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	29	Total	C	N	O	0	0
			243	170	37	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	466	Total	C	N	O	S	0	0
			3590	2380	578	624	8		

- Molecule 13 is a protein called IsiA.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	2	302	Total	C	N	O	0	0
			1474	870	302	302		
13	3	277	Total	C	N	O	0	0
			1354	800	277	277		

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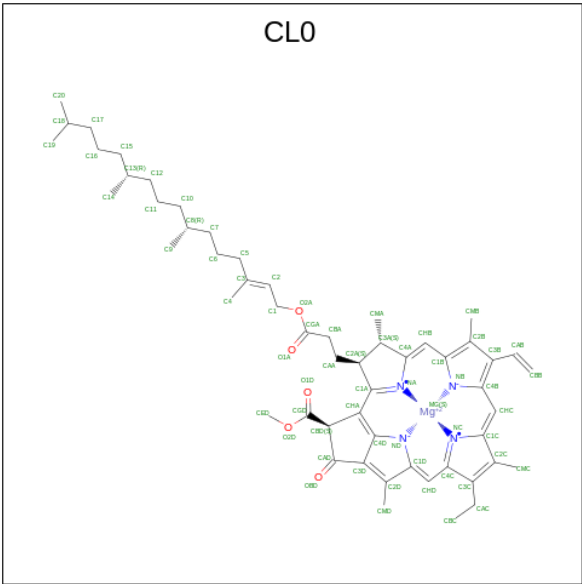
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Mol	Chain	Residues	Atoms				AltConf	Trace
13	6	303	Total	C	N	O	0	0
			1479	873	303	303		

- Molecule 14 is a protein called Iron stress-induced chlorophyll-binding protein.

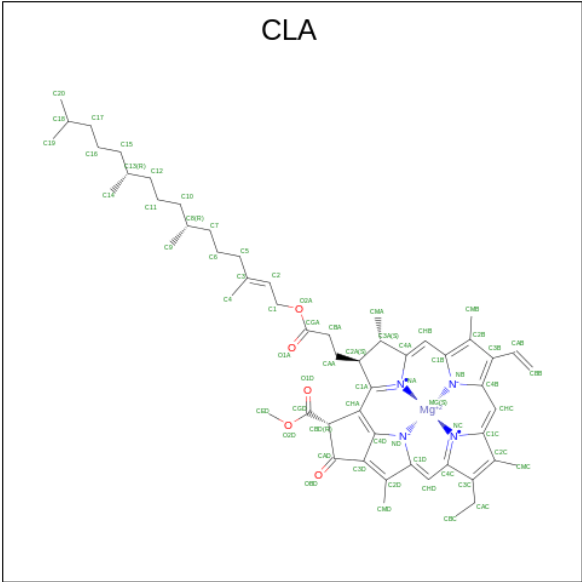
Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	329	Total	C	N	O	S	0	0
			2562	1709	424	425	4		
14	5	332	Total	C	N	O	S	0	0
			2589	1725	429	431	4		

- Molecule 15 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	F	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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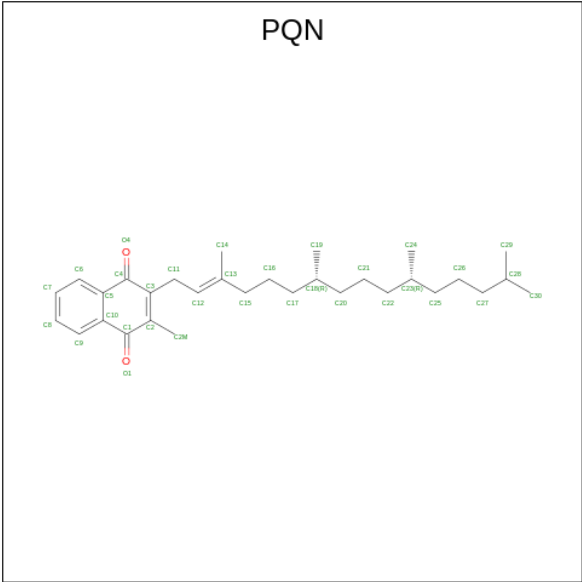
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16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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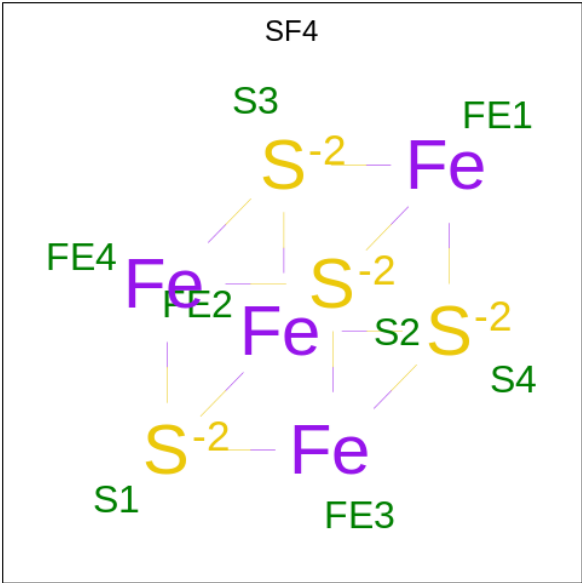
Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



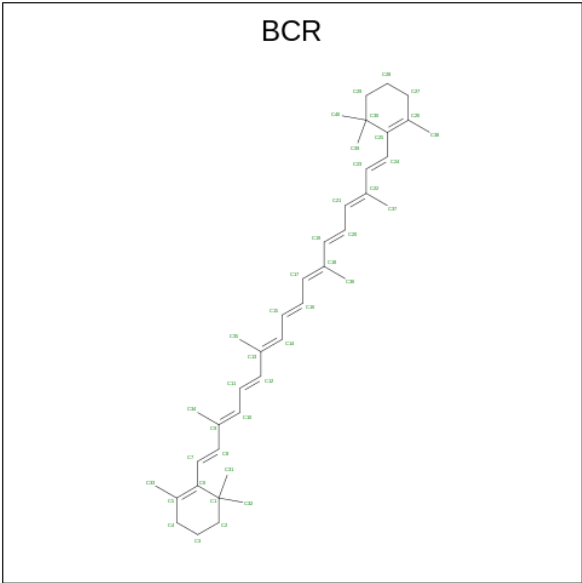
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



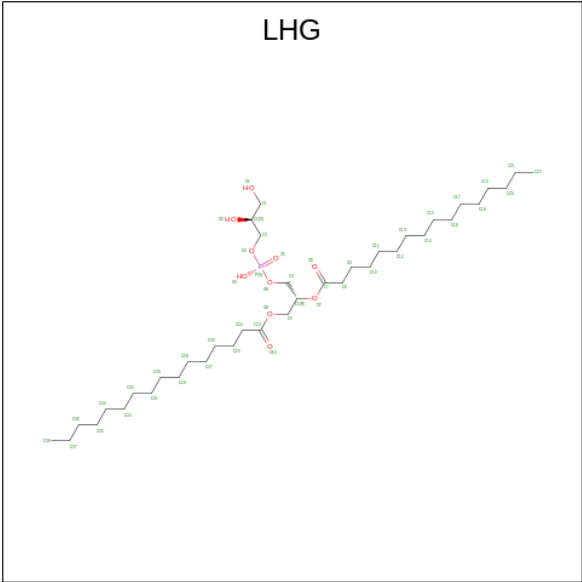
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	

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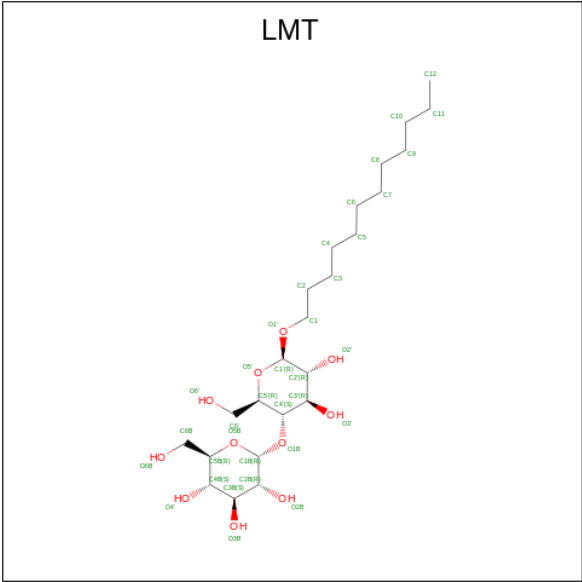
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	M	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	1	1	Total C 40 40	0
19	4	1	Total C 40 40	0
19	5	1	Total C 40 40	0
19	5	1	Total C 40 40	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



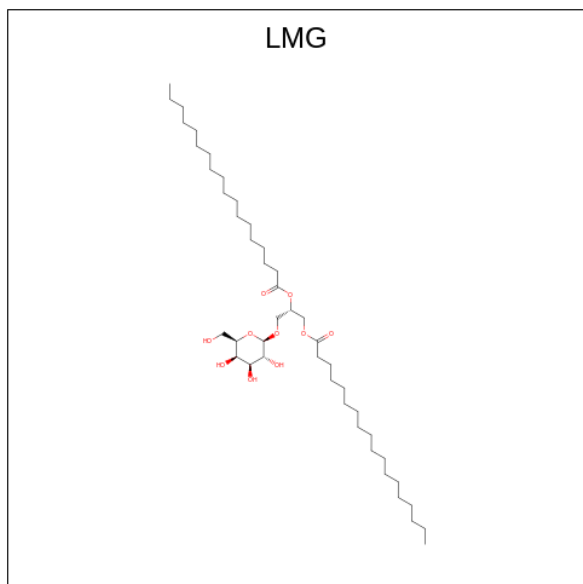
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			35	24	11	
21	B	1	Total	C	O	0
			35	24	11	
21	B	1	Total	C	O	0
			35	24	11	
21	M	1	Total	C	O	0
			35	24	11	
21	1	1	Total	C	O	0
			35	24	11	
21	5	1	Total	C	O	0
			35	24	11	

- Molecule 22 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			55	45	10	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	9	Total	O	0
			9	9	
23	B	12	Total	O	0
			12	12	

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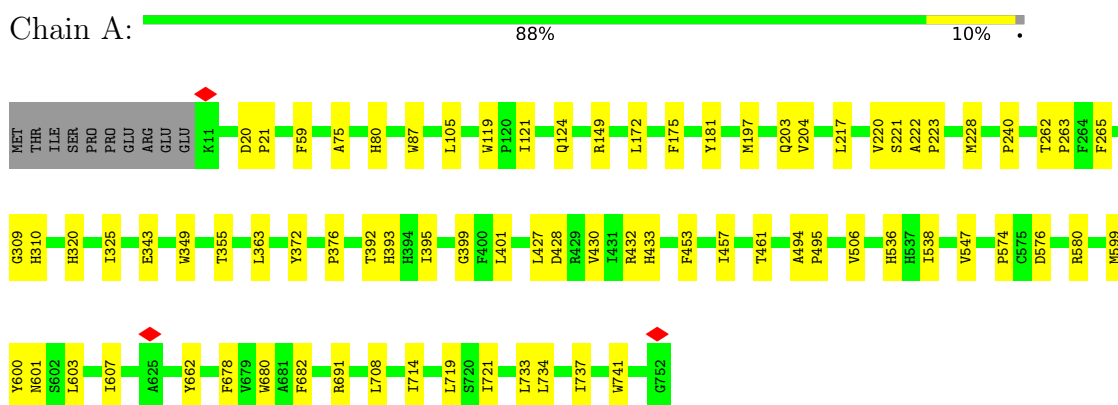
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Mol	Chain	Residues	Atoms		AltConf
23	F	2	Total 2	O 2	0
23	K	1	Total 1	O 1	0
23	1	2	Total 2	O 2	0

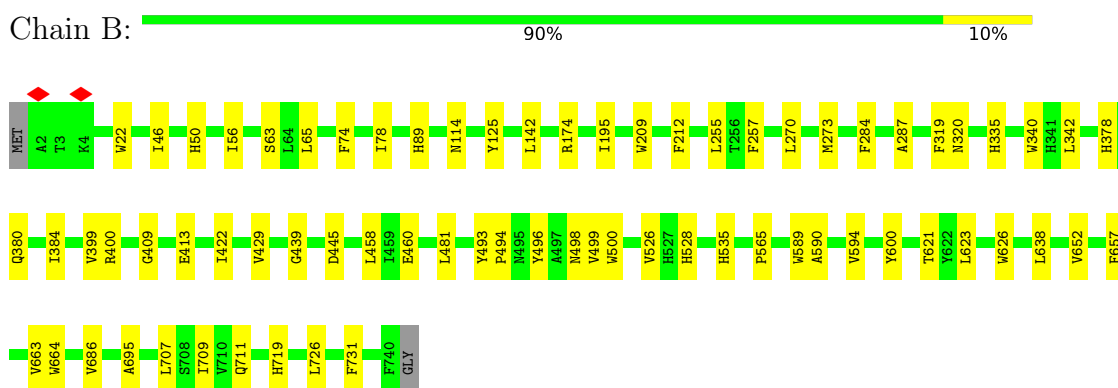
3 Residue-property plots

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.

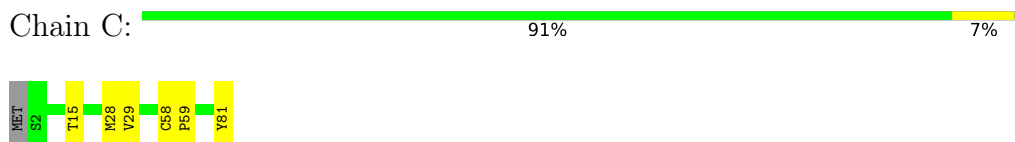
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



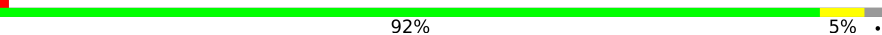
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1



- Molecule 3: Photosystem I iron-sulfur center



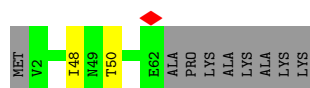
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  92% 5%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  84% 13%



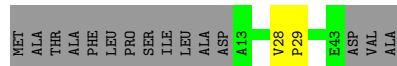
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  79% 7% 14%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  63% 33%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  82% 6% 12%



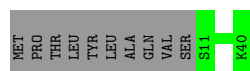
- Molecule 9: Unknown

Chain K:  80% 7% 12%

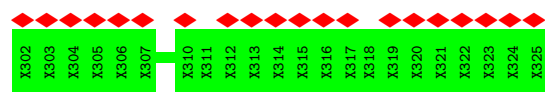


- Molecule 10: PsaM

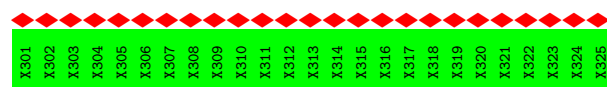
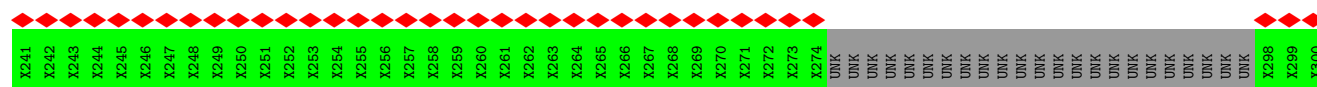
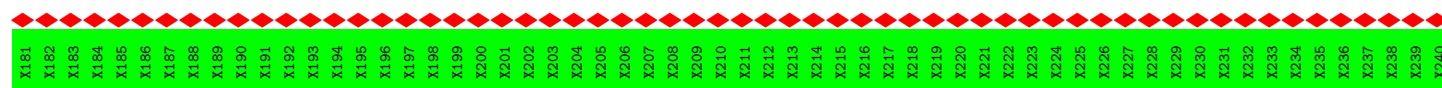
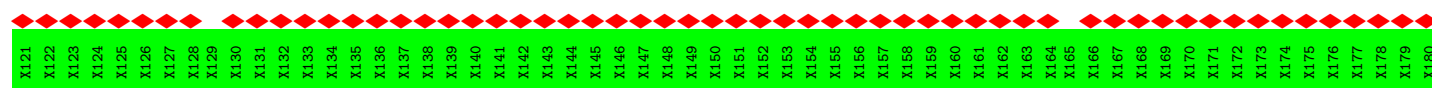
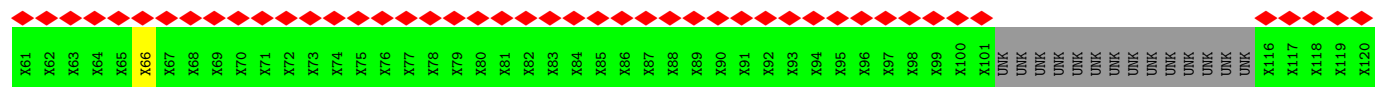
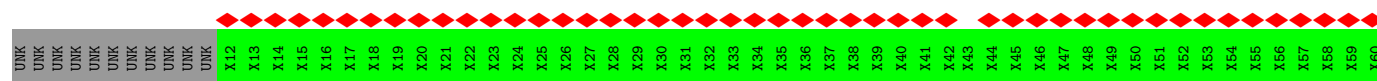
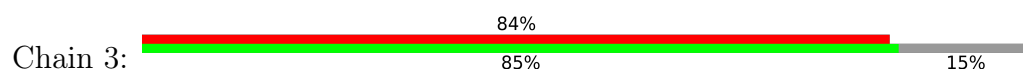
Chain M:  75% 25%



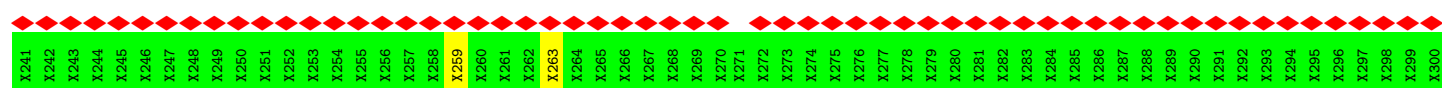
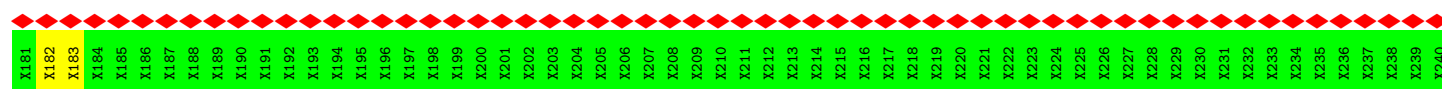
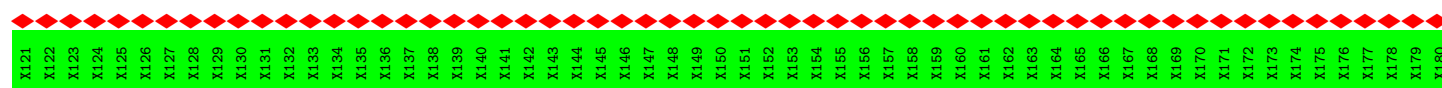
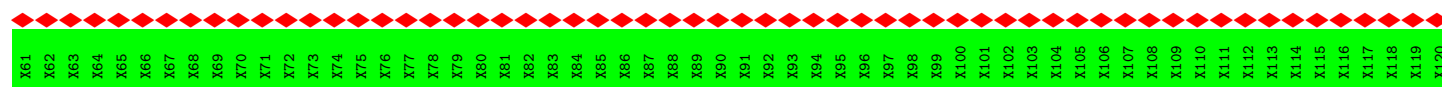
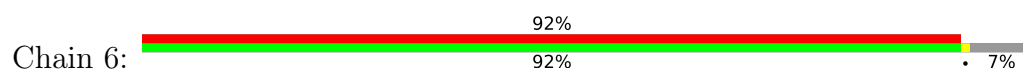
- Molecule 11: Photosystem I 4.8 kDa protein

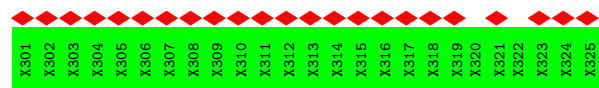


• Molecule 13: IsiA

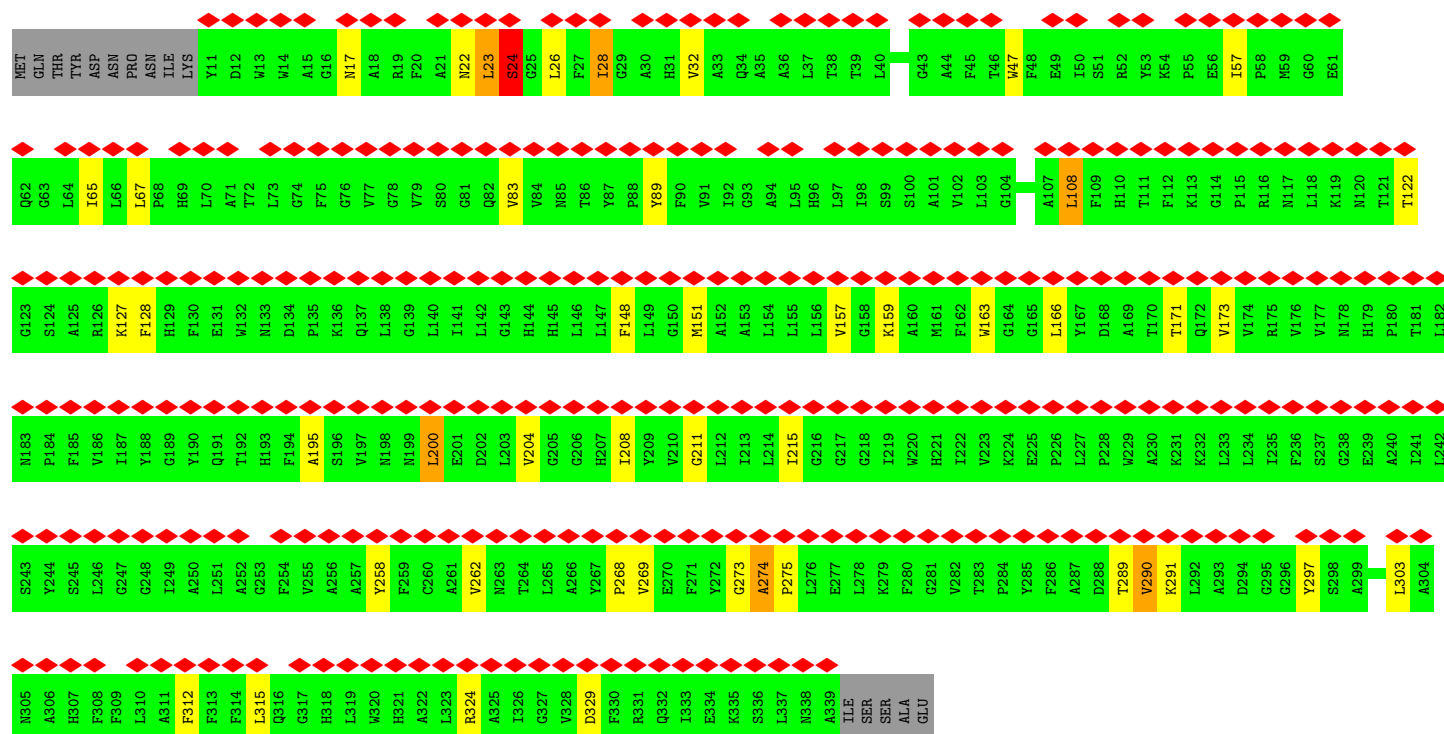
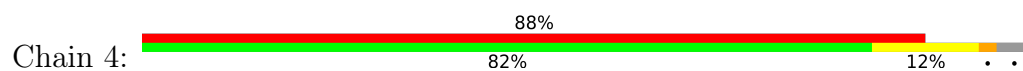


• Molecule 13: IsiA

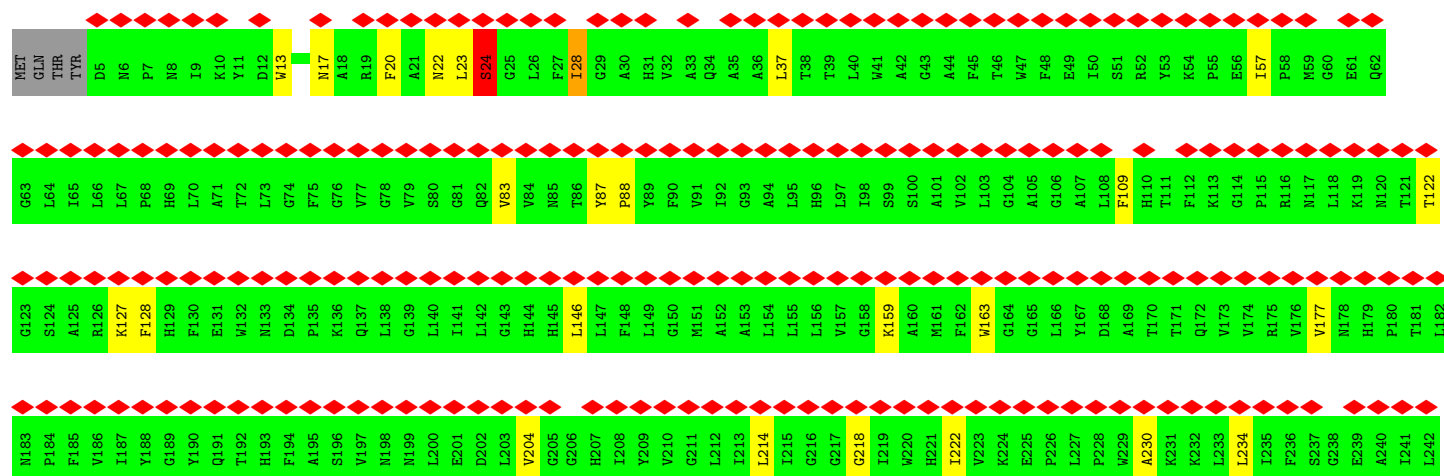
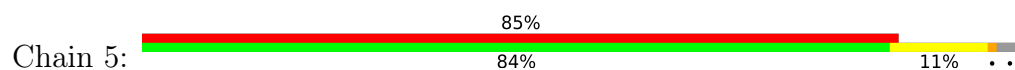


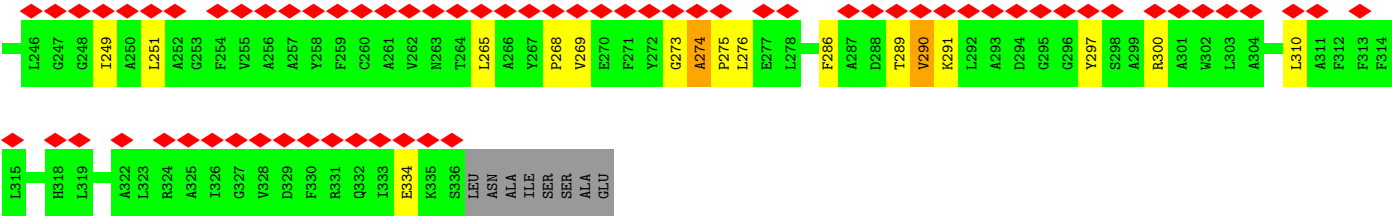


• Molecule 14: Iron stress-induced chlorophyll-binding protein



• Molecule 14: Iron stress-induced chlorophyll-binding protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	11.70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	229.68001, 229.68001, 229.68001	wwPDB
Map dimensions	232, 232, 232	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.99, 0.99, 0.99	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.94	0/6023	1.49	0/8216
2	B	0.93	0/6143	1.49	0/8398
3	C	0.96	0/609	1.39	0/826
4	D	0.96	0/1067	1.38	0/1441
5	E	0.99	0/499	1.29	0/677
6	F	0.97	0/1104	1.53	0/1500
7	I	0.93	0/262	1.50	0/358
8	J	0.91	0/358	1.50	0/490
10	M	0.95	0/239	1.63	0/326
11	X	0.88	0/253	1.55	0/347
12	1	1.02	0/3702	1.61	1/5059 (0.0%)
14	4	1.05	0/2648	1.65	2/3611 (0.1%)
14	5	1.06	0/2676	1.62	2/3649 (0.1%)
All	All	0.98	0/25583	1.53	5/34898 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	28	ILE	CA-C-N	5.57	126.17	119.98
14	4	28	ILE	C-N-CA	5.57	126.17	119.98
14	5	28	ILE	CA-C-N	5.36	125.89	119.94
14	5	28	ILE	C-N-CA	5.36	125.89	119.94
12	1	435	GLY	CA-C-O	-5.16	118.67	122.23

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	5824	0	5701	69	0
2	B	5919	0	5676	65	0
3	C	599	0	577	5	0
4	D	1043	0	1049	5	0
5	E	490	0	484	2	0
6	F	1080	0	1076	8	0
7	I	253	0	255	1	0
8	J	347	0	352	3	0
9	K	360	0	77	5	0
10	M	235	0	251	0	0
11	X	243	0	244	2	0
12	1	3590	0	3568	25	0
13	2	1474	0	277	0	0
13	3	1354	0	264	1	0
13	6	1479	0	284	2	0
14	4	2562	0	2544	32	0
14	5	2589	0	2569	28	0
15	A	65	0	72	7	0
16	1	959	0	764	26	0
16	2	270	0	198	6	0
16	3	45	0	33	2	0
16	4	450	0	330	10	0
16	5	851	0	623	30	0
16	6	401	0	293	9	0
16	A	2460	0	2456	102	0
16	B	2489	0	2585	121	0
16	F	96	0	74	6	0
16	J	90	0	66	3	0
16	K	86	0	62	9	0
16	X	45	0	33	2	0
17	A	33	0	46	4	0
17	B	33	0	46	4	0
18	A	8	0	0	0	0
18	C	16	0	0	1	0
19	1	200	0	280	7	0
19	4	40	0	56	3	0
19	5	80	0	112	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	240	0	336	11	0
19	B	280	0	392	13	0
19	F	80	0	112	4	0
19	I	80	0	112	6	0
19	J	80	0	112	4	0
19	K	40	0	56	5	0
19	M	40	0	56	2	0
20	A	76	0	98	4	0
20	B	49	0	74	3	0
20	F	49	0	74	0	0
21	1	35	0	46	0	0
21	5	35	0	46	0	0
21	A	35	0	46	0	0
21	B	70	0	92	0	0
21	M	35	0	46	2	0
22	B	55	0	86	3	0
23	1	2	0	0	0	0
23	A	9	0	0	0	0
23	B	12	0	0	0	0
23	F	2	0	0	0	0
23	K	1	0	0	0	0
All	All	39463	0	35161	488	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 7.

The worst 5 of 488 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)
14:5:28:ILE:HD11	16:5:414:CLA:HBC3	1.49	0.94
16:A:804:CLA:H201	16:B:802:CLA:H141	1.49	0.92
14:4:157:VAL:HG11	14:4:208:ILE:HD11	1.64	0.79
14:5:276:LEU:HD23	14:5:300:ARG:HD2	1.66	0.77
16:A:806:CLA:H93	16:A:814:CLA:H42	1.66	0.76

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	740/752 (98%)	714 (96%)	26 (4%)	0	100	100
2	B	737/741 (100%)	713 (97%)	22 (3%)	2 (0%)	36	56
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
5	E	59/70 (84%)	59 (100%)	0	0	100	100
6	F	139/164 (85%)	137 (99%)	1 (1%)	1 (1%)	18	35
7	I	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
8	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
10	M	28/40 (70%)	28 (100%)	0	0	100	100
11	X	27/44 (61%)	26 (96%)	1 (4%)	0	100	100
12	1	464/476 (98%)	446 (96%)	18 (4%)	0	100	100
14	4	327/344 (95%)	290 (89%)	26 (8%)	11 (3%)	3	4
14	5	330/344 (96%)	289 (88%)	31 (9%)	10 (3%)	3	5
All	All	3132/3290 (95%)	2976 (95%)	132 (4%)	24 (1%)	18	31

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	481	LEU
14	4	274	ALA
14	5	274	ALA
6	F	26	ALA
14	4	24	SER

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	595/605 (98%)	595 (100%)	0	100	100
2	B	601/602 (100%)	601 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	108/110 (98%)	108 (100%)	0	100	100
5	E	54/60 (90%)	54 (100%)	0	100	100
6	F	110/129 (85%)	110 (100%)	0	100	100
7	I	28/39 (72%)	28 (100%)	0	100	100
8	J	38/42 (90%)	38 (100%)	0	100	100
10	M	25/34 (74%)	25 (100%)	0	100	100
11	X	24/34 (71%)	24 (100%)	0	100	100
12	1	364/373 (98%)	364 (100%)	0	100	100
14	4	252/266 (95%)	247 (98%)	5 (2%)	48	73
14	5	256/266 (96%)	252 (98%)	4 (2%)	55	78
All	All	2523/2629 (96%)	2514 (100%)	9 (0%)	81	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	5	265	LEU
14	5	334	GLU
14	4	200	LEU
14	4	269	VAL
14	5	24	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	38	GLN
14	4	85	ASN
12	1	269	ASN
14	4	129	HIS
1	A	638	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

201 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	SF4	C	101	3	0,12,12	-	-	-		
16	CLA	A	818	1	58,62,73	2.17	18 (31%)	69,99,113	3.24	27 (39%)
16	CLA	K	101	-	46,49,73	2.30	18 (39%)	55,83,113	3.12	24 (43%)
16	CLA	5	413	14	49,53,73	2.50	21 (42%)	59,89,113	3.25	28 (47%)
16	CLA	B	811	2	69,73,73	1.95	19 (27%)	83,113,113	2.83	29 (34%)
16	CLA	6	408	-	45,49,73	2.55	20 (44%)	54,84,113	3.34	27 (50%)
16	CLA	B	803	-	69,73,73	1.91	18 (26%)	83,113,113	2.60	29 (34%)
16	CLA	4	402	14	49,53,73	2.47	21 (42%)	59,89,113	3.30	27 (45%)
19	BCR	1	523	-	41,41,41	1.61	10 (24%)	56,56,56	1.35	8 (14%)
19	BCR	B	844	-	41,41,41	1.67	9 (21%)	56,56,56	1.33	8 (14%)
16	CLA	B	841	2	69,73,73	1.92	20 (28%)	83,113,113	2.87	26 (31%)
16	CLA	1	519	12	69,73,73	2.07	19 (27%)	83,113,113	2.79	28 (33%)
16	CLA	B	804	2	58,62,73	2.18	19 (32%)	69,99,113	2.98	32 (46%)
16	CLA	5	411	14	49,53,73	2.46	19 (38%)	59,89,113	3.17	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	A	854	-	36,36,36	0.42	0	47,47,47	0.99	4 (8%)
16	CLA	B	815	2	49,53,73	2.38	18 (36%)	59,89,113	3.32	27 (45%)
16	CLA	A	827	23	59,63,73	2.15	18 (30%)	71,101,113	3.07	26 (36%)
16	CLA	1	501	20	49,53,73	2.35	18 (36%)	59,89,113	3.18	31 (52%)
16	CLA	A	817	23	53,57,73	2.27	20 (37%)	62,93,113	3.06	26 (41%)
16	CLA	A	839	1	69,73,73	1.93	18 (26%)	83,113,113	2.87	32 (38%)
16	CLA	B	814	2	60,64,73	2.09	19 (31%)	72,102,113	3.08	28 (38%)
16	CLA	B	825	23	69,73,73	1.98	20 (28%)	83,113,113	2.90	34 (40%)
16	CLA	1	514	12	49,53,73	2.48	21 (42%)	59,89,113	3.24	26 (44%)
16	CLA	K	103	23	49,53,73	2.38	21 (42%)	59,89,113	3.23	27 (45%)
16	CLA	B	828	2	69,73,73	1.95	18 (26%)	83,113,113	2.79	30 (36%)
16	CLA	4	410	14	49,53,73	2.52	21 (42%)	59,89,113	3.21	26 (44%)
19	BCR	A	846	-	41,41,41	1.62	9 (21%)	56,56,56	1.35	10 (17%)
16	CLA	1	508	-	49,53,73	2.39	21 (42%)	59,89,113	3.14	29 (49%)
19	BCR	M	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.35	8 (14%)
16	CLA	B	813	2	69,73,73	1.96	18 (26%)	83,113,113	2.95	27 (32%)
16	CLA	A	810	1	69,73,73	1.99	18 (26%)	83,113,113	2.79	29 (34%)
16	CLA	1	506	12	49,53,73	2.45	20 (40%)	59,89,113	3.20	27 (45%)
16	CLA	2	406	-	49,53,73	2.50	21 (42%)	59,89,113	3.17	24 (40%)
16	CLA	B	829	2	69,73,73	1.96	19 (27%)	83,113,113	2.84	32 (38%)
19	BCR	A	851	-	41,41,41	1.69	8 (19%)	56,56,56	1.40	10 (17%)
19	BCR	I	102	-	41,41,41	1.69	7 (17%)	56,56,56	1.68	12 (21%)
15	CL0	A	801	1	69,73,73	1.94	20 (28%)	83,113,113	2.94	32 (38%)
16	CLA	5	408	14	49,53,73	2.51	21 (42%)	59,89,113	3.32	25 (42%)
16	CLA	1	526	-	49,53,73	2.50	21 (42%)	59,89,113	3.23	28 (47%)
16	CLA	A	842	1	69,73,73	1.98	19 (27%)	83,113,113	2.82	27 (32%)
16	CLA	4	411	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
16	CLA	B	810	2	69,73,73	1.94	19 (27%)	83,113,113	2.91	29 (34%)
16	CLA	B	837	2	64,68,73	2.06	18 (28%)	77,107,113	2.88	29 (37%)
16	CLA	A	826	23	69,73,73	1.97	21 (30%)	83,113,113	2.67	32 (38%)
16	CLA	A	838	1	55,59,73	2.19	18 (32%)	66,96,113	3.14	27 (40%)
16	CLA	A	819	1	58,62,73	2.15	19 (32%)	69,99,113	3.07	28 (40%)
16	CLA	2	401	-	49,53,73	2.50	20 (40%)	59,89,113	3.26	25 (42%)
16	CLA	A	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.87	31 (37%)
19	BCR	B	843	-	41,41,41	1.64	8 (19%)	56,56,56	1.35	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	831	2	69,73,73	2.02	21 (30%)	83,113,113	2.82	31 (37%)
16	CLA	1	503	12	55,59,73	2.33	20 (36%)	66,96,113	2.99	30 (45%)
19	BCR	1	518	-	41,41,41	1.72	8 (19%)	56,56,56	1.49	10 (17%)
16	CLA	5	407	14	49,53,73	2.47	20 (40%)	59,89,113	3.19	28 (47%)
19	BCR	A	849	-	41,41,41	1.66	7 (17%)	56,56,56	1.58	11 (19%)
16	CLA	4	406	14	49,53,73	2.47	19 (38%)	59,89,113	3.25	26 (44%)
16	CLA	5	409	-	49,53,73	2.42	21 (42%)	59,89,113	3.29	26 (44%)
16	CLA	A	802	23	69,73,73	1.86	18 (26%)	83,113,113	2.80	30 (36%)
16	CLA	A	829	1	69,73,73	1.99	19 (27%)	83,113,113	3.00	32 (38%)
16	CLA	5	417	14	49,53,73	2.50	21 (42%)	59,89,113	3.21	28 (47%)
16	CLA	A	808	1	55,59,73	2.22	18 (32%)	66,96,113	3.14	28 (42%)
16	CLA	4	405	14	49,53,73	2.49	21 (42%)	59,89,113	3.24	26 (44%)
16	CLA	B	838	2	69,73,73	1.92	17 (24%)	83,113,113	2.82	30 (36%)
16	CLA	B	802	23	69,73,73	1.94	20 (28%)	83,113,113	2.91	32 (38%)
16	CLA	5	406	-	49,53,73	2.51	21 (42%)	59,89,113	3.21	28 (47%)
16	CLA	1	507	12	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
16	CLA	B	836	23	49,53,73	2.42	20 (40%)	59,89,113	3.21	28 (47%)
17	PQN	A	844	-	34,34,34	1.56	2 (5%)	42,45,45	1.12	4 (9%)
19	BCR	B	846	-	41,41,41	1.58	10 (24%)	56,56,56	1.32	7 (12%)
16	CLA	B	826	2	69,73,73	1.94	19 (27%)	83,113,113	2.90	28 (33%)
16	CLA	A	822	23	69,73,73	2.03	18 (26%)	83,113,113	2.77	30 (36%)
16	CLA	4	408	14	49,53,73	2.50	21 (42%)	59,89,113	3.15	27 (45%)
16	CLA	A	812	16,1	69,73,73	1.90	18 (26%)	83,113,113	2.86	32 (38%)
16	CLA	A	807	1	69,73,73	1.96	20 (28%)	83,113,113	2.88	28 (33%)
16	CLA	A	843	23	69,73,73	1.99	17 (24%)	83,113,113	2.81	31 (37%)
16	CLA	B	806	2	69,73,73	1.92	18 (26%)	83,113,113	2.79	30 (36%)
16	CLA	F	201	23	55,59,73	2.16	19 (34%)	66,96,113	2.88	26 (39%)
16	CLA	A	834	1	69,73,73	1.87	17 (24%)	83,113,113	2.78	30 (36%)
19	BCR	K	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.38	9 (16%)
19	BCR	5	402	-	41,41,41	1.67	8 (19%)	56,56,56	1.41	8 (14%)
16	CLA	1	505	-	49,53,73	2.49	21 (42%)	59,89,113	3.24	27 (45%)
16	CLA	B	827	2	69,73,73	1.95	20 (28%)	83,113,113	3.06	30 (36%)
16	CLA	2	403	-	49,53,73	2.50	21 (42%)	59,89,113	3.19	27 (45%)
16	CLA	A	809	1	69,73,73	1.99	19 (27%)	83,113,113	2.81	33 (39%)
16	CLA	A	804	1	69,73,73	1.90	18 (26%)	83,113,113	2.85	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	815	1	49,53,73	2.33	20 (40%)	59,89,113	3.24	26 (44%)
16	CLA	A	832	1	54,58,73	2.14	17 (31%)	65,95,113	3.17	29 (44%)
16	CLA	B	839	2	69,73,73	1.94	20 (28%)	83,113,113	2.93	29 (34%)
16	CLA	4	407	14	49,53,73	2.51	20 (40%)	59,89,113	3.29	29 (49%)
16	CLA	6	407	-	49,53,73	2.52	21 (42%)	59,89,113	3.21	26 (44%)
19	BCR	B	853	-	41,41,41	1.65	9 (21%)	56,56,56	1.29	7 (12%)
16	CLA	B	834	2	69,73,73	1.97	18 (26%)	83,113,113	2.76	32 (38%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
16	CLA	1	525	-	49,53,73	2.49	20 (40%)	59,89,113	3.17	28 (47%)
19	BCR	1	516	-	41,41,41	1.66	7 (17%)	56,56,56	1.53	10 (17%)
19	BCR	5	420	-	41,41,41	1.71	8 (19%)	56,56,56	1.33	9 (16%)
22	LMG	B	849	-	55,55,55	0.24	0	63,63,63	0.39	0
16	CLA	B	805	2	69,73,73	1.91	20 (28%)	83,113,113	2.93	31 (37%)
16	CLA	1	509	12	49,53,73	2.36	18 (36%)	59,89,113	3.24	27 (45%)
16	CLA	5	405	14	49,53,73	2.48	21 (42%)	59,89,113	3.31	27 (45%)
16	CLA	A	828	1	69,73,73	1.95	19 (27%)	83,113,113	2.90	29 (34%)
16	CLA	B	819	23	69,73,73	2.07	18 (26%)	83,113,113	2.81	30 (36%)
16	CLA	A	813	1	58,62,73	2.15	19 (32%)	69,99,113	2.98	30 (43%)
21	LMT	5	401	-	36,36,36	0.43	0	47,47,47	0.75	1 (2%)
19	BCR	A	848	-	41,41,41	1.65	10 (24%)	56,56,56	1.34	9 (16%)
16	CLA	5	419	-	49,53,73	2.47	21 (42%)	59,89,113	3.19	25 (42%)
19	BCR	1	517	-	41,41,41	1.74	8 (19%)	56,56,56	1.53	9 (16%)
16	CLA	B	808	2	69,73,73	1.88	19 (27%)	83,113,113	2.96	31 (37%)
16	CLA	2	404	-	49,53,73	2.49	21 (42%)	59,89,113	3.21	26 (44%)
16	CLA	A	820	1	69,73,73	1.93	19 (27%)	83,113,113	2.88	31 (37%)
16	CLA	1	511	12	55,59,73	2.31	18 (32%)	66,96,113	3.06	29 (43%)
16	CLA	A	821	1	54,58,73	2.23	18 (33%)	65,95,113	3.15	29 (44%)
17	PQN	B	842	-	34,34,34	1.66	2 (5%)	42,45,45	0.83	1 (2%)
16	CLA	5	403	14	49,53,73	2.47	20 (40%)	59,89,113	3.30	25 (42%)
16	CLA	6	406	-	49,53,73	2.51	21 (42%)	59,89,113	3.18	27 (45%)
16	CLA	B	833	2	62,66,73	2.06	19 (30%)	74,104,113	2.99	31 (41%)
19	BCR	I	101	-	41,41,41	1.64	9 (21%)	56,56,56	1.42	9 (16%)
16	CLA	A	805	16,1	58,62,73	2.12	18 (31%)	69,99,113	3.09	31 (44%)
16	CLA	1	513	12	49,53,73	2.44	20 (40%)	59,89,113	3.13	27 (45%)
16	CLA	2	402	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	5	414	14	49,53,73	2.41	21 (42%)	59,89,113	3.10	25 (42%)
16	CLA	A	840	1	69,73,73	1.92	20 (28%)	83,113,113	2.92	26 (31%)
21	LMT	B	852	-	36,36,36	0.49	0	47,47,47	0.94	3 (6%)
16	CLA	1	504	12	49,53,73	2.41	21 (42%)	59,89,113	3.45	26 (44%)
16	CLA	5	422	-	49,53,73	2.50	20 (40%)	59,89,113	3.19	27 (45%)
16	CLA	B	822	23	59,63,73	2.19	20 (33%)	71,101,113	2.89	29 (40%)
16	CLA	5	418	-	49,53,73	2.50	21 (42%)	59,89,113	3.18	29 (49%)
16	CLA	1	515	12	49,53,73	2.52	20 (40%)	59,89,113	3.26	27 (45%)
19	BCR	4	401	-	41,41,41	1.67	8 (19%)	56,56,56	1.48	9 (16%)
16	CLA	4	409	14	49,53,73	2.49	20 (40%)	59,89,113	3.30	27 (45%)
16	CLA	B	816	2	59,63,73	2.12	18 (30%)	71,101,113	3.19	28 (39%)
16	CLA	F	204	23	49,53,73	2.37	19 (38%)	59,89,113	3.16	27 (45%)
16	CLA	5	412	-	49,53,73	2.48	20 (40%)	59,89,113	3.20	27 (45%)
20	LHG	B	850	-	48,48,48	0.27	0	51,54,54	0.33	0
16	CLA	5	410	14	49,53,73	2.46	18 (36%)	59,89,113	3.17	26 (44%)
16	CLA	B	818	2	69,73,73	1.87	18 (26%)	83,113,113	2.92	32 (38%)
16	CLA	1	520	12	69,73,73	2.00	18 (26%)	83,113,113	2.97	29 (34%)
19	BCR	F	205	-	41,41,41	1.65	8 (19%)	56,56,56	1.32	8 (14%)
19	BCR	A	850	-	41,41,41	1.61	12 (29%)	56,56,56	1.30	7 (12%)
16	CLA	B	807	2	69,73,73	1.99	19 (27%)	83,113,113	2.78	28 (33%)
16	CLA	A	823	1	53,57,73	2.20	19 (35%)	62,93,113	3.36	28 (45%)
16	CLA	2	405	-	49,53,73	2.51	20 (40%)	59,89,113	3.18	27 (45%)
16	CLA	5	404	14	49,53,73	2.38	20 (40%)	59,89,113	3.08	22 (37%)
16	CLA	A	835	1	69,73,73	1.90	18 (26%)	83,113,113	2.88	29 (34%)
16	CLA	J	101	8	49,53,73	2.38	19 (38%)	59,89,113	3.15	26 (44%)
16	CLA	A	811	1	49,53,73	2.32	19 (38%)	59,89,113	3.27	28 (47%)
18	SF4	A	845	2,1	0,12,12	-	-	-	-	-
19	BCR	B	845	-	41,41,41	1.60	8 (19%)	56,56,56	1.36	8 (14%)
16	CLA	3	401	-	49,53,73	2.51	21 (42%)	59,89,113	3.20	27 (45%)
16	CLA	5	421	-	49,53,73	2.49	21 (42%)	59,89,113	3.18	30 (50%)
16	CLA	B	821	2	49,53,73	2.38	19 (38%)	59,89,113	3.19	27 (45%)
19	BCR	B	848	-	41,41,41	1.65	11 (26%)	56,56,56	1.36	9 (16%)
16	CLA	A	816	1	49,53,73	2.33	17 (34%)	59,89,113	3.24	28 (47%)
16	CLA	A	836	1	55,59,73	2.19	18 (32%)	66,96,113	3.03	29 (43%)
16	CLA	1	502	12	49,53,73	2.45	20 (40%)	59,89,113	3.30	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BCR	J	103	-	41,41,41	1.60	8 (19%)	56,56,56	1.31	7 (12%)
16	CLA	6	403	-	49,53,73	2.48	21 (42%)	59,89,113	3.18	28 (47%)
16	CLA	B	801	2	69,73,73	1.93	19 (27%)	83,113,113	2.99	32 (38%)
21	LMT	B	851	-	36,36,36	0.51	1 (2%)	47,47,47	0.69	1 (2%)
20	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.50	0
21	LMT	M	101	-	36,36,36	0.47	0	47,47,47	0.67	0
16	CLA	A	803	-	69,73,73	1.94	19 (27%)	83,113,113	2.83	31 (37%)
16	CLA	B	823	2	69,73,73	1.94	19 (27%)	83,113,113	2.89	34 (40%)
16	CLA	J	102	8	49,53,73	2.41	19 (38%)	59,89,113	3.23	27 (45%)
16	CLA	1	510	12	49,53,73	2.44	20 (40%)	59,89,113	3.18	26 (44%)
16	CLA	6	405	-	49,53,73	2.51	21 (42%)	59,89,113	3.18	29 (49%)
16	CLA	B	824	2	69,73,73	1.98	18 (26%)	83,113,113	2.90	32 (38%)
16	CLA	A	830	1	69,73,73	1.95	18 (26%)	83,113,113	2.70	25 (30%)
16	CLA	B	809	2	69,73,73	1.89	18 (26%)	83,113,113	2.73	31 (37%)
16	CLA	1	512	12	49,53,73	2.45	19 (38%)	59,89,113	3.21	30 (50%)
19	BCR	B	847	-	41,41,41	1.62	10 (24%)	56,56,56	1.35	7 (12%)
16	CLA	B	812	2	49,53,73	2.35	20 (40%)	59,89,113	3.27	30 (50%)
16	CLA	B	820	2	51,55,73	2.33	20 (39%)	61,91,113	3.24	31 (50%)
16	CLA	B	832	2	69,73,73	1.90	17 (24%)	83,113,113	2.98	27 (32%)
16	CLA	4	403	14	49,53,73	2.48	20 (40%)	59,89,113	3.28	26 (44%)
16	CLA	B	835	23	49,53,73	2.35	18 (36%)	59,89,113	3.16	24 (40%)
16	CLA	A	814	1	69,73,73	1.97	19 (27%)	83,113,113	2.80	27 (32%)
16	CLA	6	409	13	49,53,73	2.51	21 (42%)	59,89,113	3.16	27 (45%)
16	CLA	6	401	-	49,53,73	2.52	21 (42%)	59,89,113	3.19	28 (47%)
16	CLA	A	831	1	69,73,73	1.92	19 (27%)	83,113,113	2.86	25 (30%)
16	CLA	A	841	1	69,73,73	1.94	19 (27%)	83,113,113	2.89	29 (34%)
16	CLA	6	404	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
20	LHG	A	853	16	26,26,48	0.32	0	29,32,54	0.48	0
19	BCR	1	522	-	41,41,41	1.64	9 (21%)	56,56,56	1.23	9 (16%)
16	CLA	X	101	11	49,53,73	2.35	20 (40%)	59,89,113	3.16	26 (44%)
19	BCR	A	847	-	41,41,41	1.64	8 (19%)	56,56,56	1.27	7 (12%)
16	CLA	A	806	1	69,73,73	1.89	17 (24%)	83,113,113	2.88	29 (34%)
16	CLA	B	840	23	69,73,73	1.96	18 (26%)	83,113,113	2.71	26 (31%)
20	LHG	F	203	-	48,48,48	0.27	0	51,54,54	0.37	0
16	CLA	A	837	1	49,53,73	2.32	20 (40%)	59,89,113	3.19	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	1	521	23	56,60,73	2.33	18 (32%)	67,97,113	3.07	29 (43%)
16	CLA	A	824	1	55,59,73	2.20	18 (32%)	66,96,113	3.16	29 (43%)
19	BCR	F	202	-	41,41,41	1.63	10 (24%)	56,56,56	1.32	8 (14%)
16	CLA	B	817	2	63,67,73	2.04	19 (30%)	75,105,113	2.99	29 (38%)
19	BCR	J	104	-	41,41,41	1.58	9 (21%)	56,56,56	1.38	9 (16%)
16	CLA	A	825	1	51,55,73	2.31	19 (37%)	61,91,113	3.20	25 (40%)
16	CLA	5	415	14	49,53,73	2.49	21 (42%)	59,89,113	3.38	26 (44%)
16	CLA	6	402	-	49,53,73	2.50	21 (42%)	59,89,113	3.16	26 (44%)
16	CLA	5	416	14	45,49,73	2.52	21 (46%)	54,84,113	3.38	27 (50%)
16	CLA	B	830	2	69,73,73	1.98	19 (27%)	83,113,113	2.73	29 (34%)
16	CLA	4	404	-	49,53,73	2.52	21 (42%)	59,89,113	3.19	27 (45%)
21	LMT	1	524	-	36,36,36	0.53	1 (2%)	47,47,47	0.64	1 (2%)

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	SF4	C	101	3	-	-	0/6/5/5
16	CLA	A	818	1	-	1/26/102/115	-
16	CLA	K	101	-	-	3/9/81/115	-
16	CLA	5	413	14	-	4/15/91/115	-
16	CLA	B	811	2	-	5/39/115/115	-
16	CLA	6	408	-	-	2/10/86/115	-
16	CLA	B	803	-	-	8/39/115/115	-
16	CLA	4	402	14	-	6/15/91/115	-
19	BCR	1	523	-	-	5/29/63/63	0/2/2/2
19	BCR	B	844	-	-	6/29/63/63	0/2/2/2
16	CLA	B	841	2	-	8/39/115/115	-
16	CLA	1	519	12	-	11/39/115/115	-
16	CLA	B	804	2	-	6/26/102/115	-
16	CLA	5	411	14	-	5/15/91/115	-
21	LMT	A	854	-	-	6/21/61/61	0/2/2/2
16	CLA	B	815	2	-	4/15/91/115	-
16	CLA	A	827	23	-	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	501	20	-	5/15/91/115	-
16	CLA	A	817	23	-	4/20/96/115	-
16	CLA	A	839	1	-	10/39/115/115	-
16	CLA	B	814	2	-	9/29/105/115	-
16	CLA	B	825	23	-	14/39/115/115	-
16	CLA	1	514	12	-	5/15/91/115	-
16	CLA	K	103	23	-	3/15/91/115	-
16	CLA	B	828	2	-	10/39/115/115	-
16	CLA	4	410	14	-	5/15/91/115	-
19	BCR	A	846	-	-	9/29/63/63	0/2/2/2
16	CLA	1	508	-	-	6/15/91/115	-
19	BCR	M	102	-	-	10/29/63/63	0/2/2/2
16	CLA	B	813	2	-	9/39/115/115	-
16	CLA	A	810	1	-	12/39/115/115	-
16	CLA	1	506	12	-	6/15/91/115	-
16	CLA	2	406	-	-	8/15/91/115	-
16	CLA	B	829	2	-	19/39/115/115	-
19	BCR	A	851	-	-	9/29/63/63	0/2/2/2
19	BCR	I	102	-	-	7/29/63/63	0/2/2/2
15	CL0	A	801	1	-	2/39/115/115	-
16	CLA	5	408	14	-	4/15/91/115	-
16	CLA	1	526	-	-	7/15/91/115	-
16	CLA	A	842	1	-	8/39/115/115	-
16	CLA	4	411	-	-	7/15/91/115	-
16	CLA	B	810	2	-	10/39/115/115	-
16	CLA	B	837	2	-	7/33/109/115	-
16	CLA	A	826	23	-	12/39/115/115	-
16	CLA	A	838	1	-	7/23/99/115	-
16	CLA	A	819	1	-	6/26/102/115	-
16	CLA	2	401	-	-	5/15/91/115	-
16	CLA	A	833	1	-	10/39/115/115	-
19	BCR	B	843	-	-	8/29/63/63	0/2/2/2
16	CLA	B	831	2	-	7/39/115/115	-
16	CLA	1	503	12	-	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	1	518	-	-	6/29/63/63	0/2/2/2
16	CLA	5	407	14	-	3/15/91/115	-
19	BCR	A	849	-	-	16/29/63/63	0/2/2/2
16	CLA	4	406	14	-	6/15/91/115	-
16	CLA	5	409	-	-	6/15/91/115	-
16	CLA	A	802	23	-	3/39/115/115	-
16	CLA	A	829	1	-	14/39/115/115	-
16	CLA	5	417	14	-	6/15/91/115	-
16	CLA	A	808	1	-	4/23/99/115	-
16	CLA	4	405	14	-	2/15/91/115	-
16	CLA	B	838	2	-	8/39/115/115	-
16	CLA	B	802	23	-	8/39/115/115	-
16	CLA	5	406	-	-	5/15/91/115	-
16	CLA	1	507	12	-	8/15/91/115	-
16	CLA	B	836	23	-	4/15/91/115	-
17	PQN	A	844	-	-	3/23/43/43	0/2/2/2
19	BCR	B	846	-	-	6/29/63/63	0/2/2/2
16	CLA	B	826	2	-	10/39/115/115	-
16	CLA	A	822	23	-	10/39/115/115	-
16	CLA	4	408	14	-	4/15/91/115	-
16	CLA	A	812	16,1	-	7/39/115/115	-
16	CLA	A	807	1	-	9/39/115/115	-
16	CLA	A	843	23	-	10/39/115/115	-
16	CLA	B	806	2	-	11/39/115/115	-
16	CLA	F	201	23	-	8/23/99/115	-
16	CLA	A	834	1	-	7/39/115/115	-
19	BCR	K	102	-	-	12/29/63/63	0/2/2/2
19	BCR	5	402	-	-	4/29/63/63	0/2/2/2
16	CLA	1	505	-	-	3/15/91/115	-
16	CLA	B	827	2	-	11/39/115/115	-
16	CLA	2	403	-	-	2/15/91/115	-
16	CLA	A	809	1	-	11/39/115/115	-
16	CLA	A	804	1	-	11/39/115/115	-
16	CLA	A	815	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	832	1	-	3/21/97/115	-
16	CLA	B	839	2	-	9/39/115/115	-
16	CLA	4	407	14	-	5/15/91/115	-
16	CLA	6	407	-	-	5/15/91/115	-
19	BCR	B	853	-	-	6/29/63/63	0/2/2/2
16	CLA	B	834	2	-	7/39/115/115	-
18	SF4	C	102	3	-	-	0/6/5/5
16	CLA	1	525	-	-	8/15/91/115	-
19	BCR	1	516	-	-	11/29/63/63	0/2/2/2
19	BCR	5	420	-	-	9/29/63/63	0/2/2/2
22	LMG	B	849	-	-	16/50/70/70	0/1/1/1
16	CLA	B	805	2	-	11/39/115/115	-
16	CLA	1	509	12	-	5/15/91/115	-
16	CLA	5	405	14	-	2/15/91/115	-
16	CLA	A	828	1	-	6/39/115/115	-
16	CLA	B	819	23	-	10/39/115/115	-
16	CLA	A	813	1	-	11/26/102/115	-
21	LMT	5	401	-	-	3/21/61/61	0/2/2/2
19	BCR	A	848	-	-	3/29/63/63	0/2/2/2
16	CLA	5	419	-	-	5/15/91/115	-
19	BCR	1	517	-	-	12/29/63/63	0/2/2/2
16	CLA	B	808	2	-	10/39/115/115	-
16	CLA	2	404	-	-	5/15/91/115	-
16	CLA	A	820	1	-	14/39/115/115	-
16	CLA	1	511	12	-	7/23/99/115	-
16	CLA	A	821	1	-	7/21/97/115	-
17	PQN	B	842	-	-	2/23/43/43	0/2/2/2
16	CLA	5	403	14	-	6/15/91/115	-
16	CLA	6	406	-	-	2/15/91/115	-
16	CLA	B	833	2	-	10/31/107/115	-
19	BCR	I	101	-	-	1/29/63/63	0/2/2/2
16	CLA	A	805	16,1	-	8/26/102/115	-
16	CLA	1	513	12	-	2/15/91/115	-
16	CLA	2	402	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	5	414	14	-	7/15/91/115	-
16	CLA	A	840	1	-	11/39/115/115	-
21	LMT	B	852	-	-	5/21/61/61	0/2/2/2
16	CLA	1	504	12	-	5/15/91/115	-
16	CLA	5	422	-	-	7/15/91/115	-
16	CLA	B	822	23	-	11/27/103/115	-
16	CLA	5	418	-	-	6/15/91/115	-
16	CLA	1	515	12	-	5/15/91/115	-
19	BCR	4	401	-	-	19/29/63/63	0/2/2/2
16	CLA	4	409	14	-	3/15/91/115	-
16	CLA	B	816	2	-	6/27/103/115	-
16	CLA	F	204	23	-	0/15/91/115	-
16	CLA	5	412	-	-	5/15/91/115	-
20	LHG	B	850	-	-	15/53/53/53	-
16	CLA	5	410	14	-	2/15/91/115	-
16	CLA	B	818	2	-	12/39/115/115	-
16	CLA	1	520	12	-	9/39/115/115	-
19	BCR	F	205	-	-	2/29/63/63	0/2/2/2
19	BCR	A	850	-	-	6/29/63/63	0/2/2/2
16	CLA	B	807	2	-	5/39/115/115	-
16	CLA	A	823	1	-	10/20/96/115	-
16	CLA	2	405	-	-	5/15/91/115	-
16	CLA	5	404	14	-	4/15/91/115	-
16	CLA	A	835	1	-	11/39/115/115	-
16	CLA	J	101	8	-	8/15/91/115	-
16	CLA	A	811	1	-	2/15/91/115	-
19	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	SF4	A	845	2,1	-	-	0/6/5/5
16	CLA	3	401	-	-	5/15/91/115	-
16	CLA	5	421	-	-	7/15/91/115	-
16	CLA	B	821	2	-	3/15/91/115	-
19	BCR	B	848	-	-	2/29/63/63	0/2/2/2
16	CLA	A	816	1	-	3/15/91/115	-
16	CLA	A	836	1	-	5/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	502	12	-	6/15/91/115	-
19	BCR	J	103	-	-	8/29/63/63	0/2/2/2
16	CLA	6	403	-	-	4/15/91/115	-
16	CLA	B	801	2	-	11/39/115/115	-
21	LMT	B	851	-	-	6/21/61/61	0/2/2/2
20	LHG	A	852	-	-	21/53/53/53	-
21	LMT	M	101	-	-	4/21/61/61	0/2/2/2
16	CLA	A	803	-	-	11/39/115/115	-
16	CLA	B	823	2	-	8/39/115/115	-
16	CLA	J	102	8	-	5/15/91/115	-
16	CLA	1	510	12	-	5/15/91/115	-
16	CLA	6	405	-	-	5/15/91/115	-
16	CLA	B	824	2	-	10/39/115/115	-
16	CLA	A	830	1	-	9/39/115/115	-
16	CLA	B	809	2	-	10/39/115/115	-
16	CLA	1	512	12	-	5/15/91/115	-
19	BCR	B	847	-	-	7/29/63/63	0/2/2/2
16	CLA	B	812	2	-	1/15/91/115	-
16	CLA	B	820	2	-	6/18/94/115	-
16	CLA	B	832	2	-	9/39/115/115	-
16	CLA	4	403	14	-	5/15/91/115	-
16	CLA	B	835	23	-	6/15/91/115	-
16	CLA	A	814	1	-	15/39/115/115	-
16	CLA	6	409	13	-	5/15/91/115	-
16	CLA	6	401	-	-	6/15/91/115	-
16	CLA	A	831	1	-	5/39/115/115	-
16	CLA	A	841	1	-	8/39/115/115	-
16	CLA	6	404	-	-	5/15/91/115	-
20	LHG	A	853	16	-	8/31/31/53	-
19	BCR	1	522	-	-	4/29/63/63	0/2/2/2
16	CLA	X	101	11	-	7/15/91/115	-
19	BCR	A	847	-	-	5/29/63/63	0/2/2/2
16	CLA	A	806	1	-	13/39/115/115	-
16	CLA	B	840	23	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	F	203	-	-	20/53/53/53	-
16	CLA	A	837	1	-	7/15/91/115	-
16	CLA	1	521	23	-	6/24/100/115	-
16	CLA	A	824	1	-	7/23/99/115	-
19	BCR	F	202	-	-	4/29/63/63	0/2/2/2
16	CLA	B	817	2	-	5/32/108/115	-
19	BCR	J	104	-	-	11/29/63/63	0/2/2/2
16	CLA	A	825	1	-	7/18/94/115	-
16	CLA	5	415	14	-	5/15/91/115	-
16	CLA	6	402	-	-	6/15/91/115	-
16	CLA	5	416	14	-	4/10/86/115	-
16	CLA	B	830	2	-	11/39/115/115	-
16	CLA	4	404	-	-	1/15/91/115	-
21	LMT	1	524	-	-	7/21/61/61	0/2/2/2

The worst 5 of 3286 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	842	PQN	C3-C2	7.90	1.49	1.35
17	A	844	PQN	C3-C2	7.37	1.48	1.35
16	1	519	CLA	C3C-C2C	5.56	1.48	1.36
16	5	407	CLA	C3C-C2C	5.54	1.48	1.36
16	5	404	CLA	O2D-CGD	5.49	1.46	1.33

The worst 5 of 4655 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	816	CLA	C1D-ND-C4D	-11.19	98.39	106.33
16	A	823	CLA	C1D-ND-C4D	-11.09	98.46	106.33
16	1	520	CLA	C1D-ND-C4D	-11.05	98.48	106.33
16	B	841	CLA	C1D-ND-C4D	-10.97	98.54	106.33
16	B	832	CLA	C1D-ND-C4D	-10.81	98.66	106.33

There are no chirality outliers.

5 of 1388 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	806	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	806	CLA	CHA-CBD-CGD-O1D
16	A	806	CLA	CHA-CBD-CGD-O2D
16	A	806	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

174 monomers are involved in 355 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	818	CLA	1	0
16	K	101	CLA	5	0
16	5	413	CLA	2	0
16	B	811	CLA	1	0
16	6	408	CLA	1	0
16	B	803	CLA	1	0
16	4	402	CLA	1	0
19	1	523	BCR	5	0
19	B	844	BCR	3	0
16	B	841	CLA	3	0
16	1	519	CLA	2	0
16	B	804	CLA	1	0
16	B	815	CLA	3	0
16	A	827	CLA	3	0
16	1	501	CLA	2	0
16	A	817	CLA	1	0
16	A	839	CLA	4	0
16	B	814	CLA	2	0
16	B	825	CLA	5	0
16	1	514	CLA	1	0
16	K	103	CLA	4	0
16	B	828	CLA	5	0
16	4	410	CLA	1	0
19	A	846	BCR	4	0
16	1	508	CLA	2	0
19	M	102	BCR	2	0
16	B	813	CLA	5	0
16	A	810	CLA	4	0
16	1	506	CLA	1	0
16	2	406	CLA	1	0
16	B	829	CLA	5	0
19	A	851	BCR	4	0
19	I	102	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	801	CL0	7	0
16	5	408	CLA	2	0
16	1	526	CLA	1	0
16	A	842	CLA	4	0
16	4	411	CLA	2	0
16	B	810	CLA	4	0
16	A	826	CLA	3	0
16	A	838	CLA	1	0
16	A	819	CLA	5	0
16	2	401	CLA	1	0
16	A	833	CLA	7	0
19	B	843	BCR	1	0
16	B	831	CLA	3	0
16	1	503	CLA	1	0
16	5	407	CLA	5	0
19	A	849	BCR	1	0
16	5	409	CLA	1	0
16	A	802	CLA	3	0
16	A	829	CLA	7	0
16	5	417	CLA	1	0
16	A	808	CLA	2	0
16	B	838	CLA	4	0
16	B	802	CLA	11	0
16	5	406	CLA	1	0
17	A	844	PQN	4	0
16	B	826	CLA	3	0
16	A	822	CLA	3	0
16	4	408	CLA	2	0
16	A	812	CLA	1	0
16	A	807	CLA	4	0
16	A	843	CLA	3	0
16	B	806	CLA	4	0
16	F	201	CLA	4	0
16	A	834	CLA	3	0
19	K	102	BCR	5	0
19	5	402	BCR	4	0
16	B	827	CLA	6	0
16	2	403	CLA	1	0
16	A	809	CLA	3	0
16	A	804	CLA	3	0
16	A	815	CLA	1	0
16	B	839	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	4	407	CLA	1	0
16	6	407	CLA	1	0
19	B	853	BCR	3	0
16	B	834	CLA	5	0
18	C	102	SF4	1	0
16	1	525	CLA	1	0
19	5	420	BCR	1	0
22	B	849	LMG	3	0
16	B	805	CLA	1	0
16	1	509	CLA	1	0
16	5	405	CLA	1	0
16	A	828	CLA	2	0
16	B	819	CLA	2	0
16	A	813	CLA	1	0
16	5	419	CLA	1	0
19	1	517	BCR	2	0
16	B	808	CLA	5	0
16	2	404	CLA	1	0
16	A	820	CLA	4	0
16	1	511	CLA	3	0
16	A	821	CLA	4	0
17	B	842	PQN	4	0
16	5	403	CLA	1	0
16	6	406	CLA	1	0
16	B	833	CLA	3	0
19	I	101	BCR	2	0
16	A	805	CLA	1	0
16	1	513	CLA	1	0
16	2	402	CLA	1	0
16	5	414	CLA	4	0
16	A	840	CLA	4	0
16	1	504	CLA	2	0
16	5	422	CLA	1	0
16	B	822	CLA	2	0
16	5	418	CLA	1	0
16	1	515	CLA	1	0
19	4	401	BCR	3	0
16	4	409	CLA	1	0
16	F	204	CLA	2	0
16	5	412	CLA	1	0
20	B	850	LHG	3	0
16	B	818	CLA	2	0

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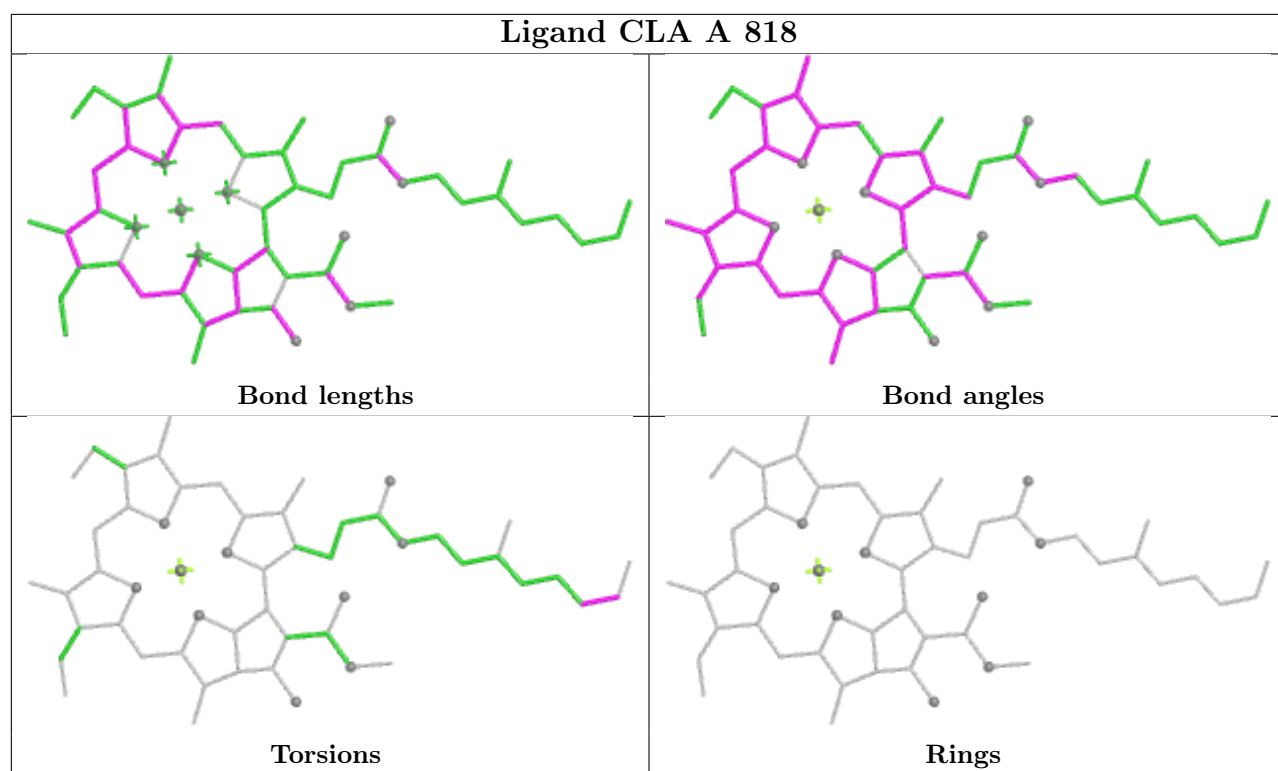
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	520	CLA	3	0
19	A	850	BCR	2	0
16	B	807	CLA	7	0
16	A	823	CLA	2	0
16	2	405	CLA	1	0
16	5	404	CLA	4	0
16	A	835	CLA	1	0
16	J	101	CLA	2	0
16	A	811	CLA	4	0
19	B	845	BCR	4	0
16	3	401	CLA	2	0
16	5	421	CLA	2	0
16	B	821	CLA	1	0
16	A	816	CLA	1	0
16	A	836	CLA	2	0
16	1	502	CLA	1	0
19	J	103	BCR	3	0
16	6	403	CLA	1	0
16	B	801	CLA	5	0
20	A	852	LHG	3	0
21	M	101	LMT	2	0
16	A	803	CLA	2	0
16	B	823	CLA	3	0
16	J	102	CLA	1	0
16	1	510	CLA	1	0
16	6	405	CLA	1	0
16	B	824	CLA	3	0
16	A	830	CLA	2	0
16	B	809	CLA	6	0
16	1	512	CLA	2	0
19	B	847	BCR	3	0
16	B	812	CLA	1	0
16	B	820	CLA	2	0
16	B	832	CLA	2	0
16	4	403	CLA	1	0
16	B	835	CLA	3	0
16	A	814	CLA	3	0
16	6	409	CLA	1	0
16	6	401	CLA	1	0
16	A	831	CLA	4	0
16	A	841	CLA	4	0
16	6	404	CLA	1	0

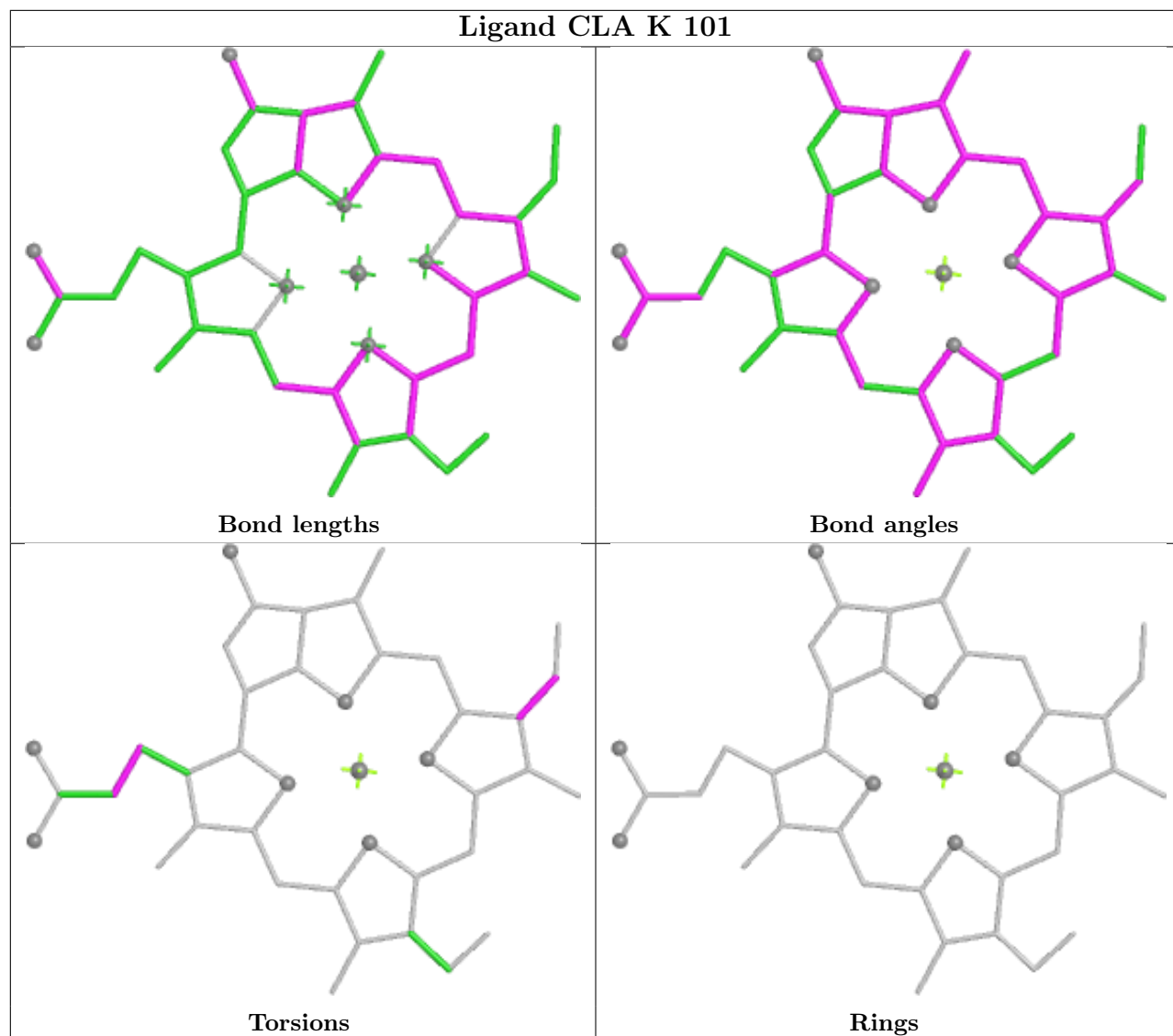
Continued on next page...

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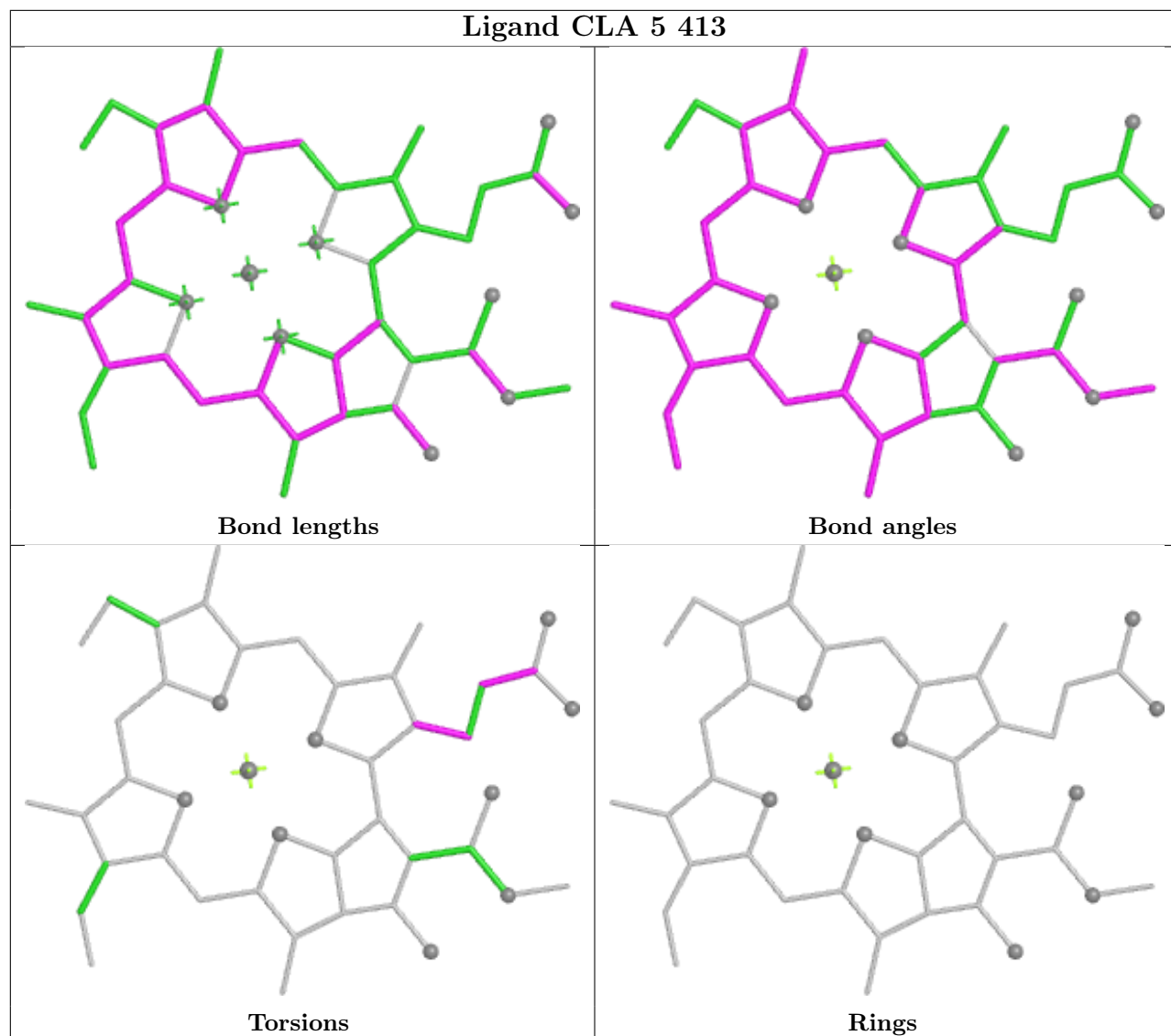
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	853	LHG	1	0
16	X	101	CLA	2	0
16	A	806	CLA	4	0
16	B	840	CLA	3	0
16	A	837	CLA	1	0
16	A	824	CLA	1	0
19	F	202	BCR	4	0
16	B	817	CLA	3	0
19	J	104	BCR	1	0
16	A	825	CLA	1	0
16	5	415	CLA	2	0
16	6	402	CLA	1	0
16	5	416	CLA	1	0
16	B	830	CLA	6	0
16	4	404	CLA	1	0

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

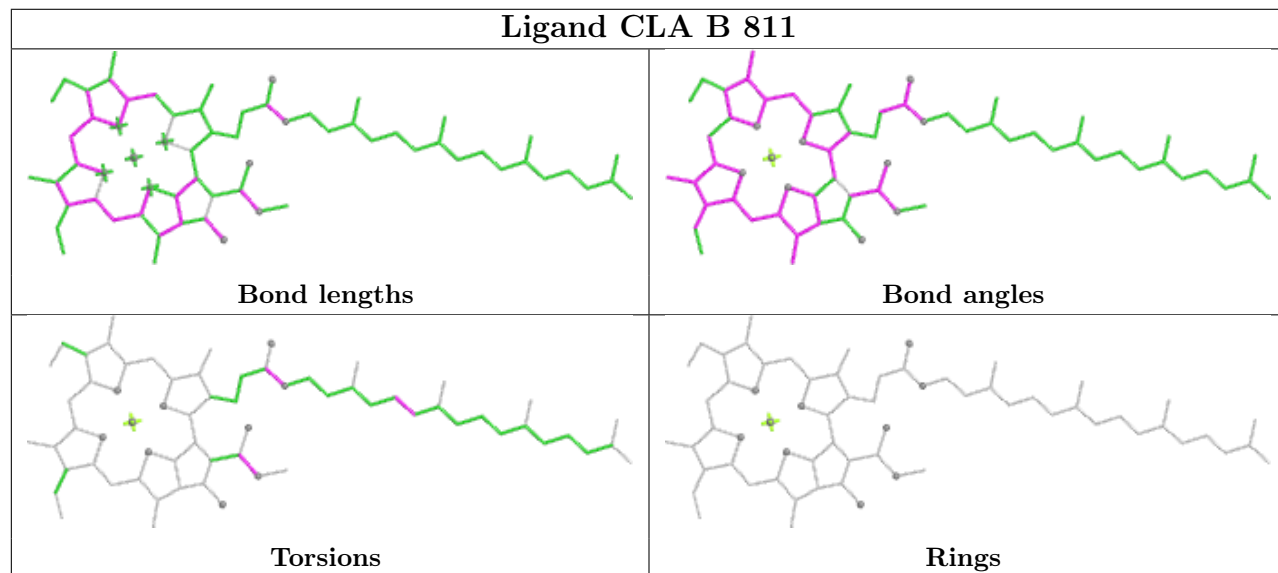




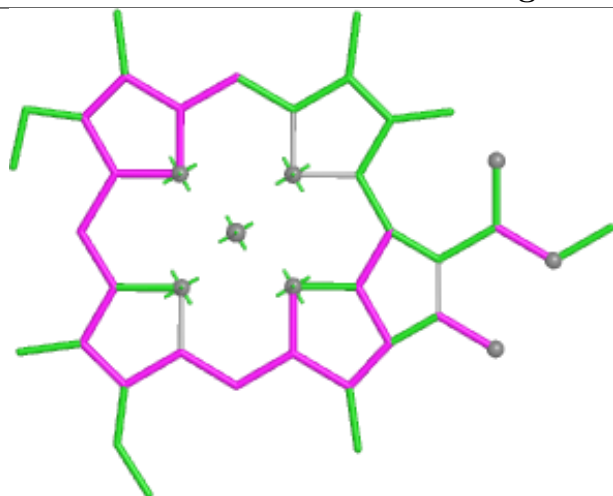
Ligand CLA 5 413



Ligand CLA B 811



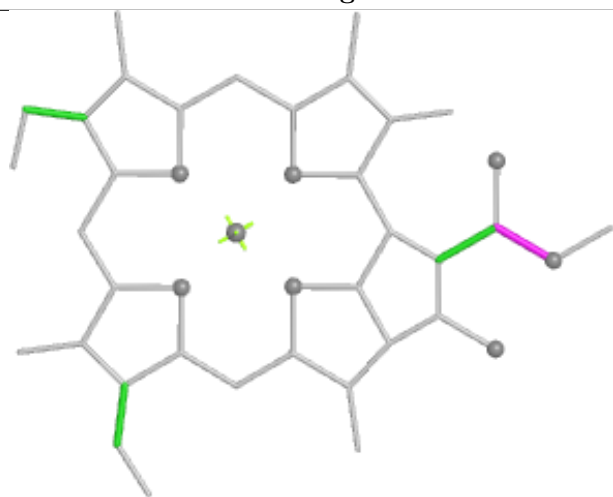
Ligand CLA 6 408



Bond lengths



Bond angles

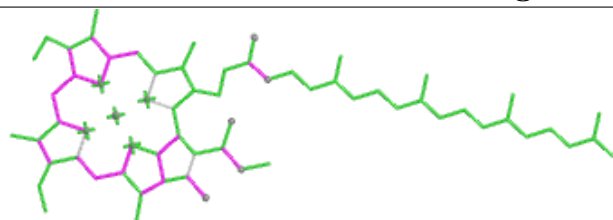


Torsions

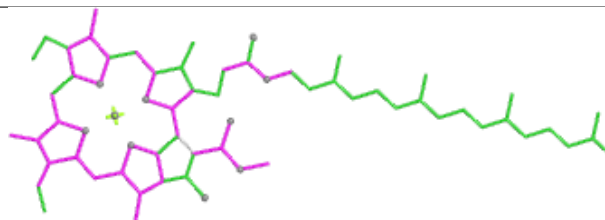


Rings

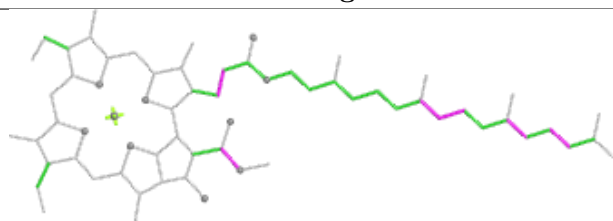
Ligand CLA B 803



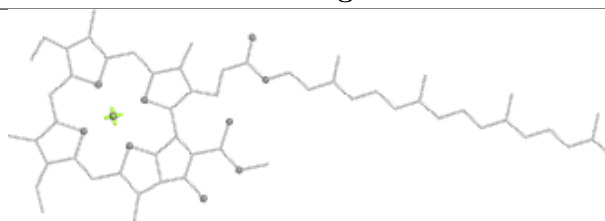
Bond lengths



Bond angles

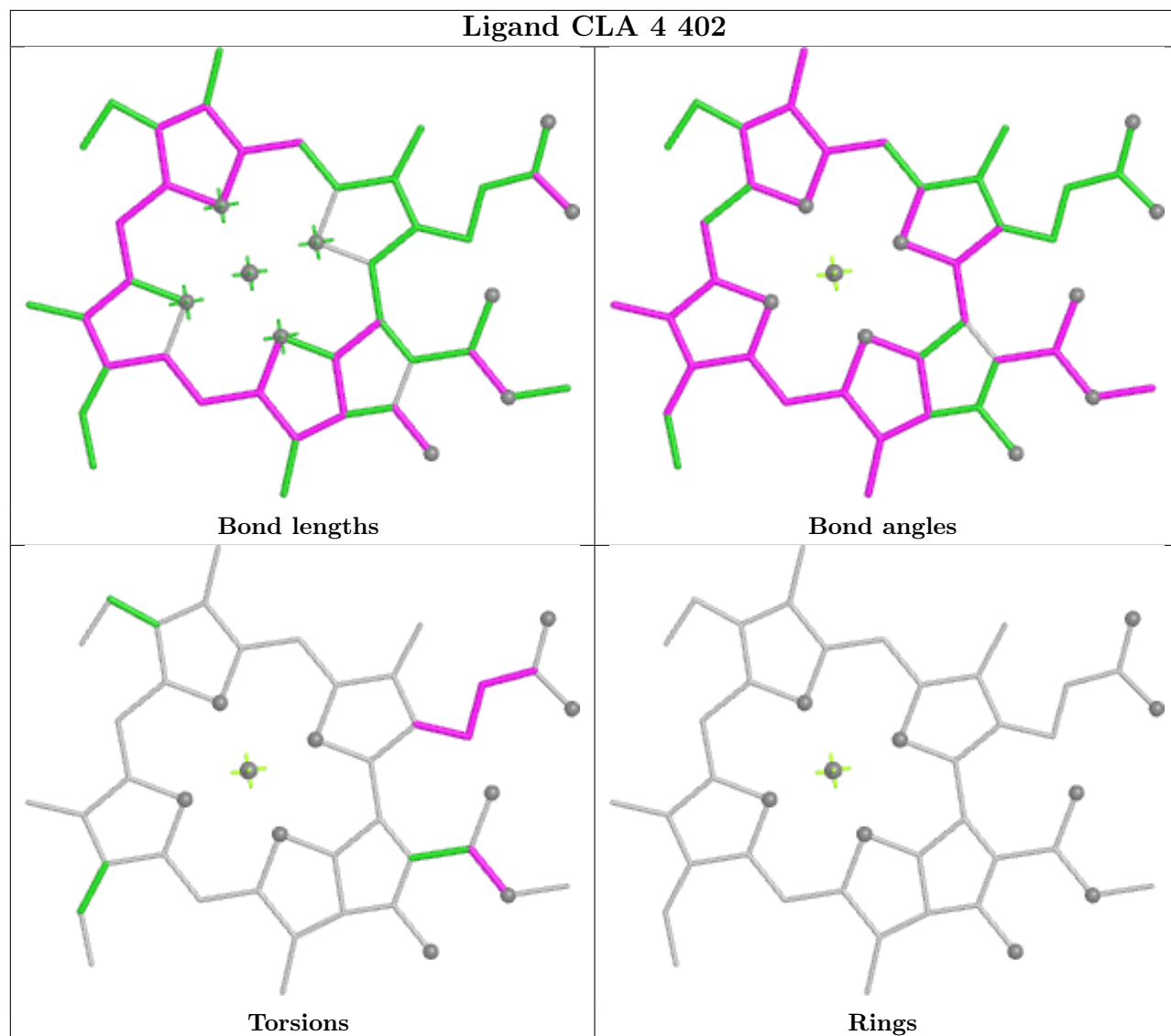


Torsions

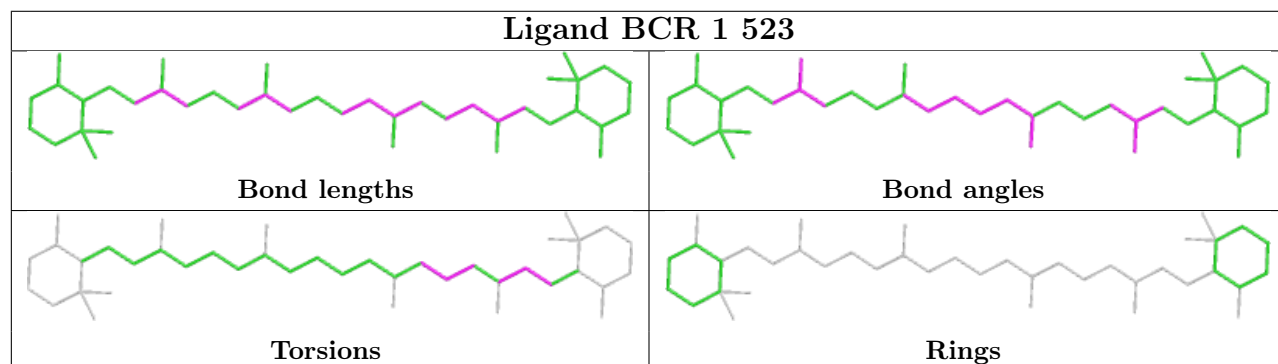


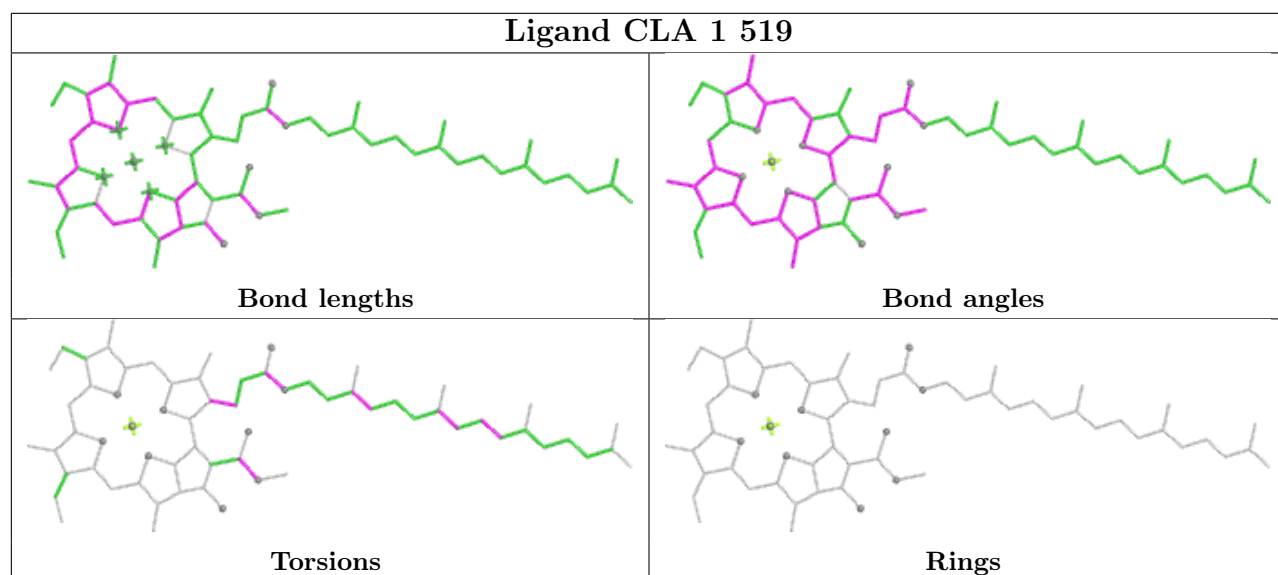
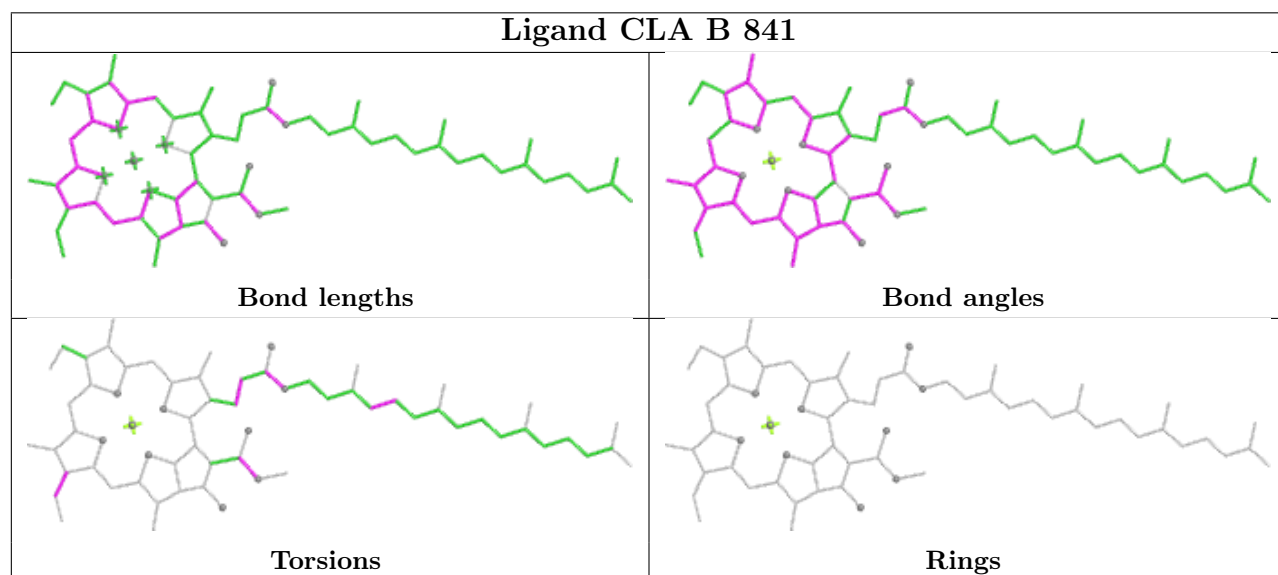
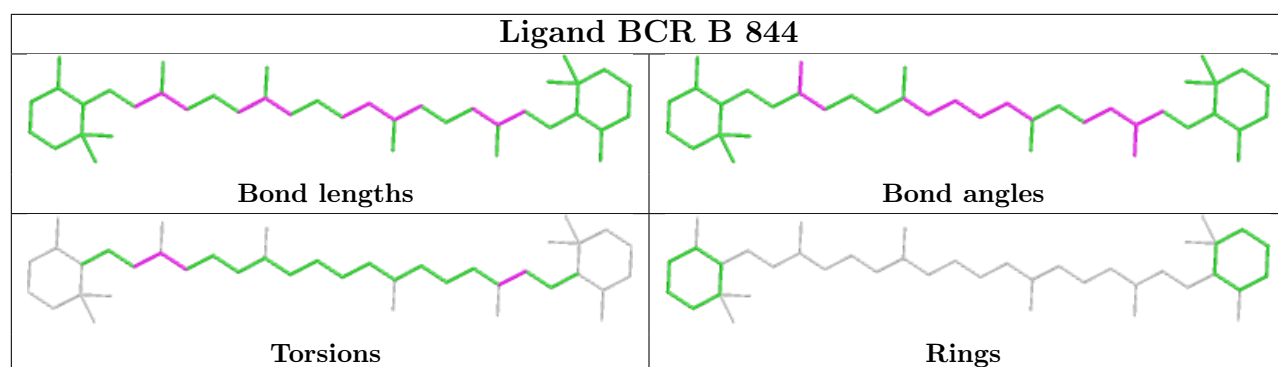
Rings

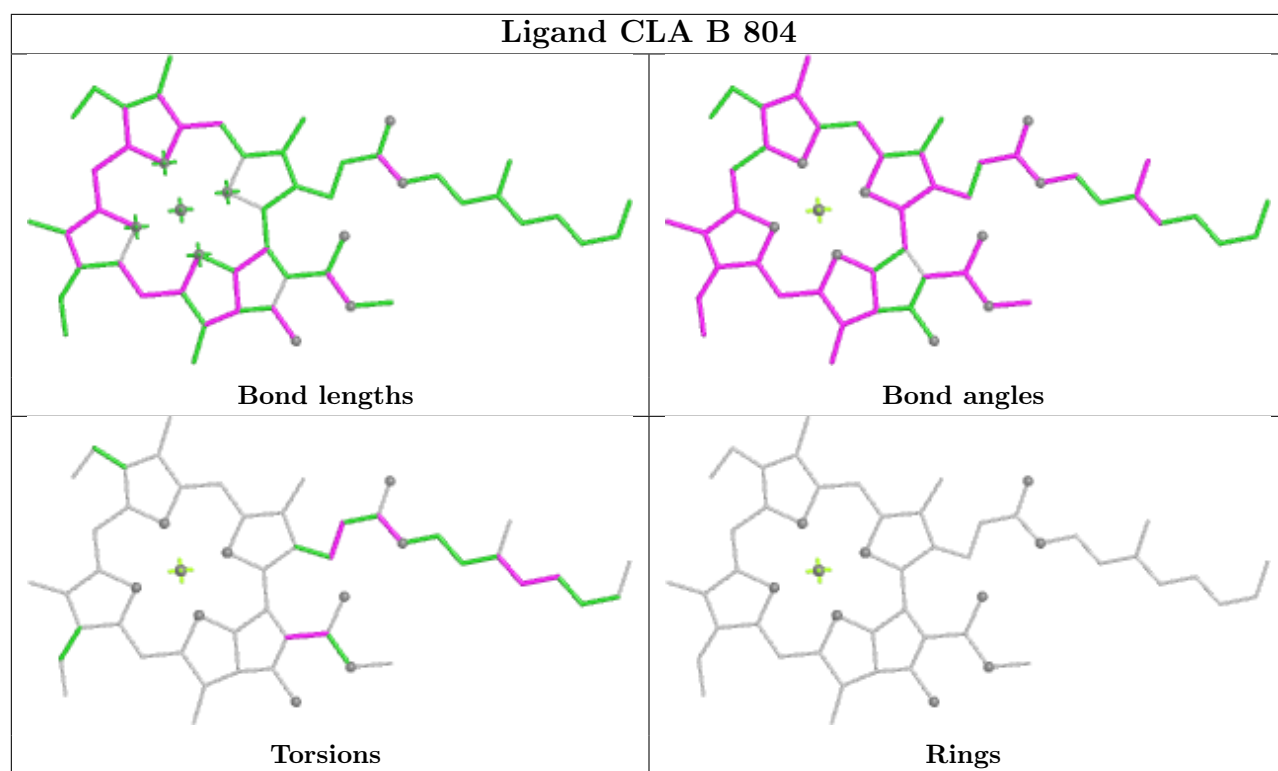
Ligand CLA 4 402



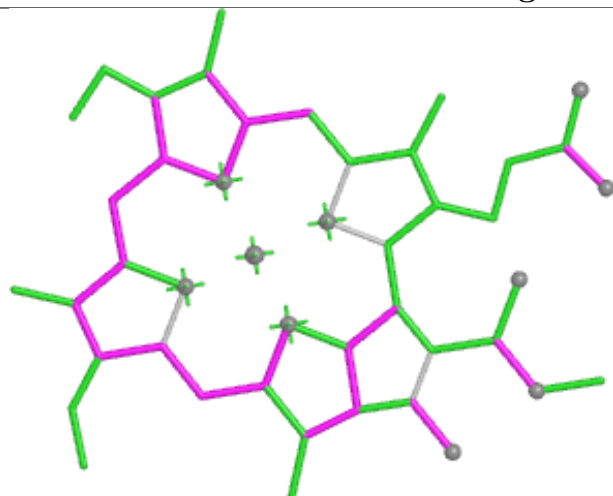
Ligand BCR 1 523



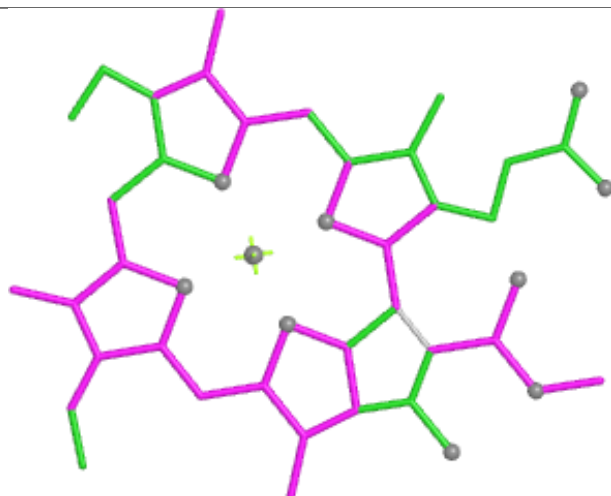




Ligand CLA 5 411



Bond lengths



Bond angles

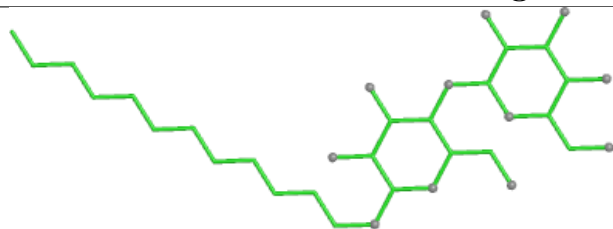


Torsions

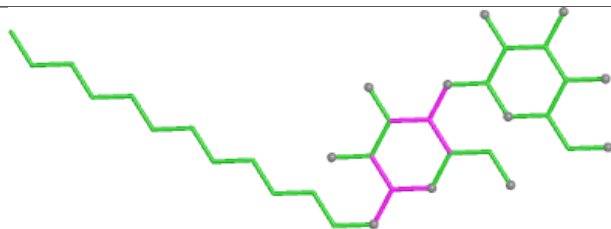


Rings

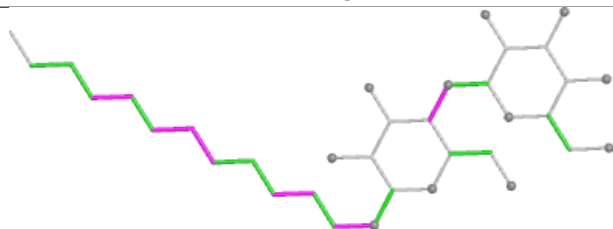
Ligand LMT A 854



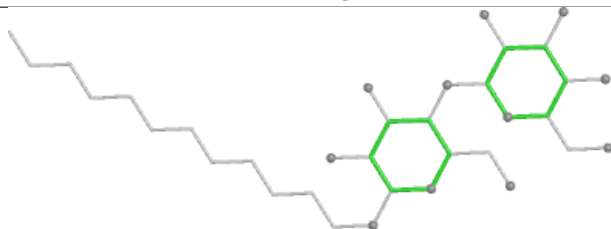
Bond lengths



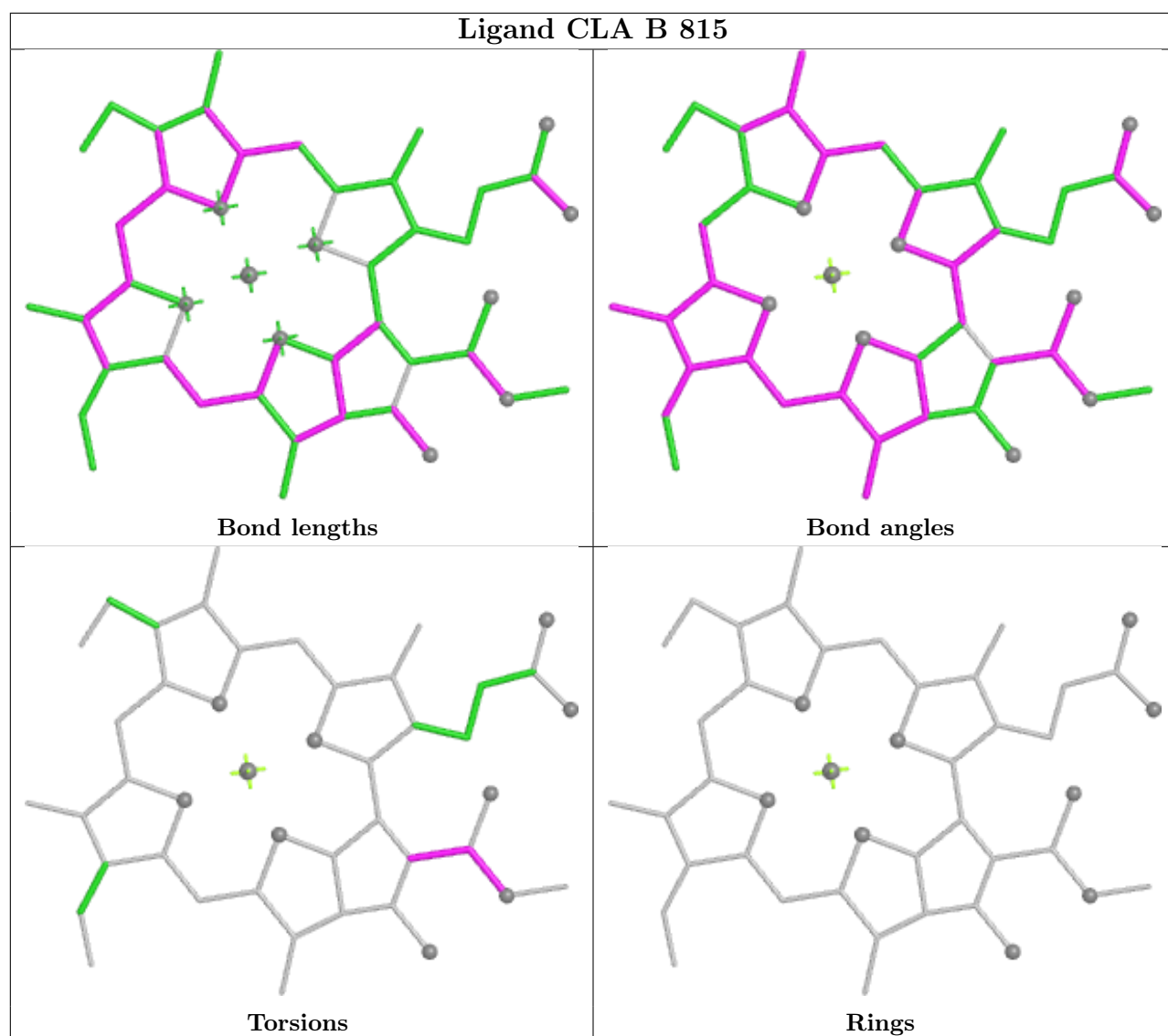
Bond angles

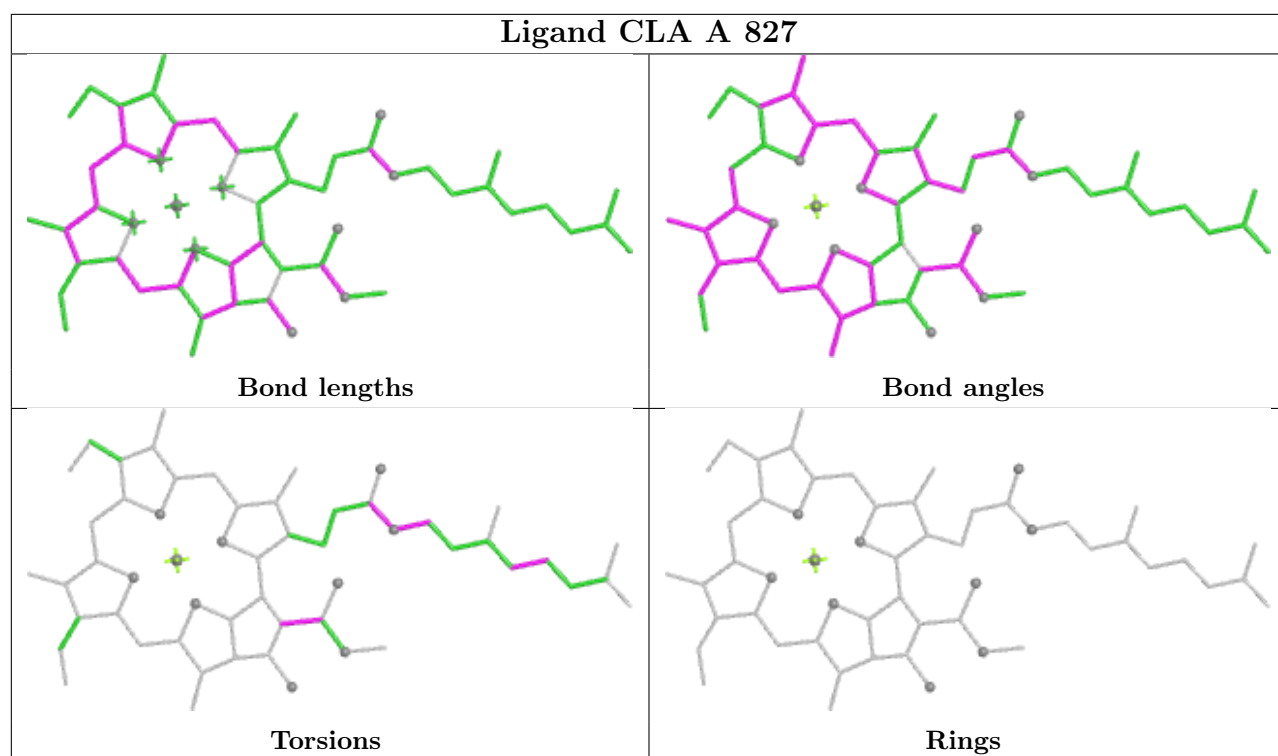


Torsions

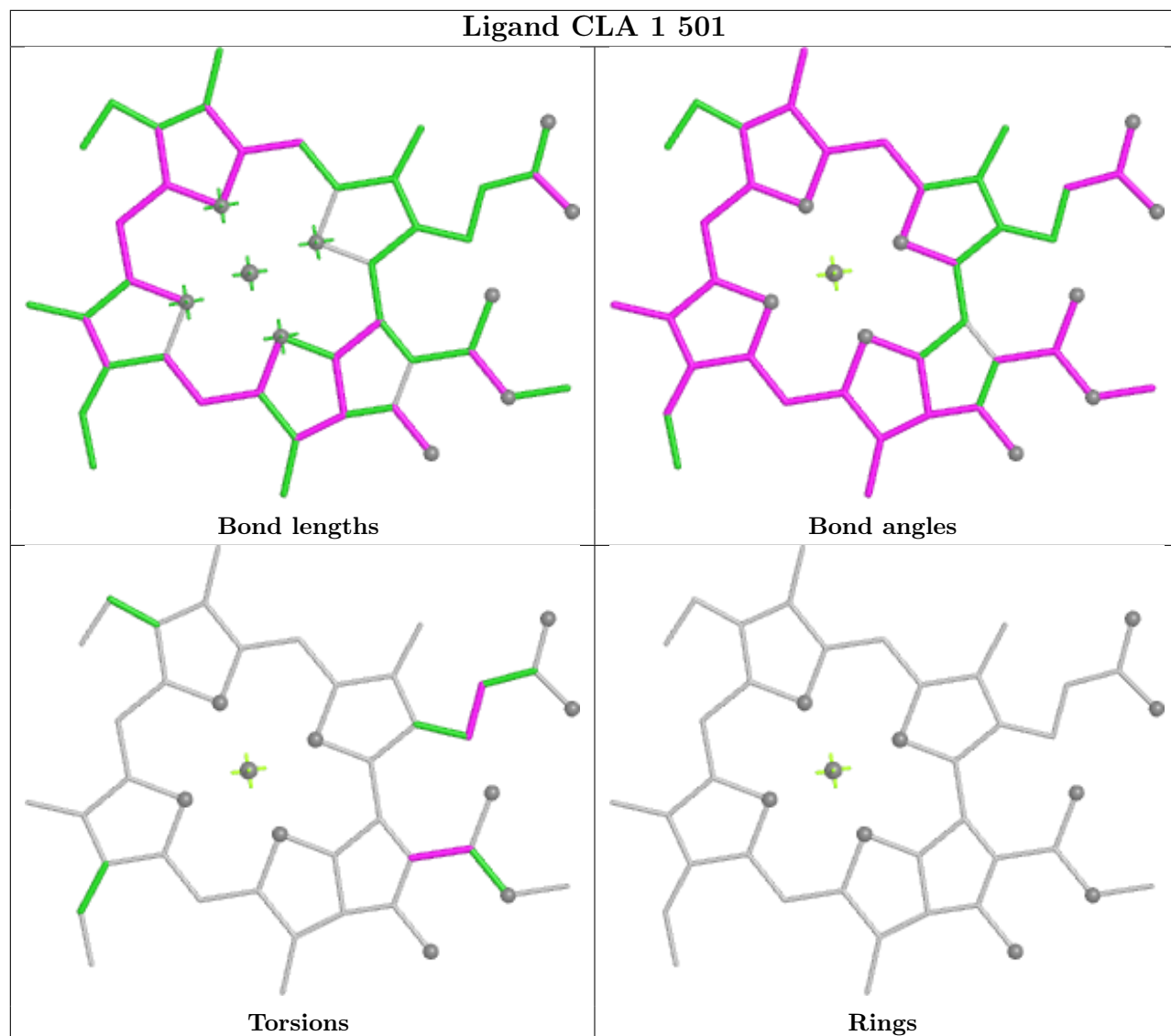


Rings

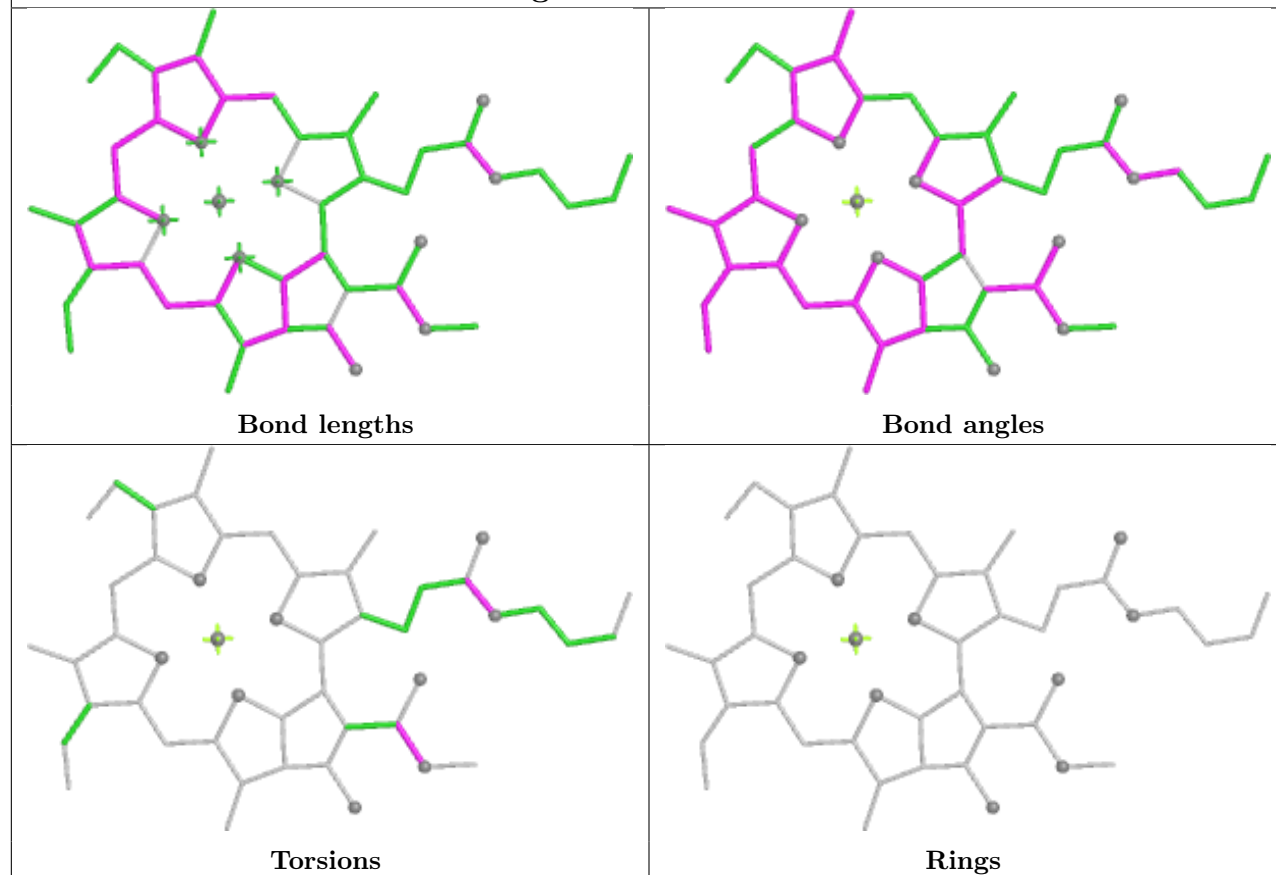




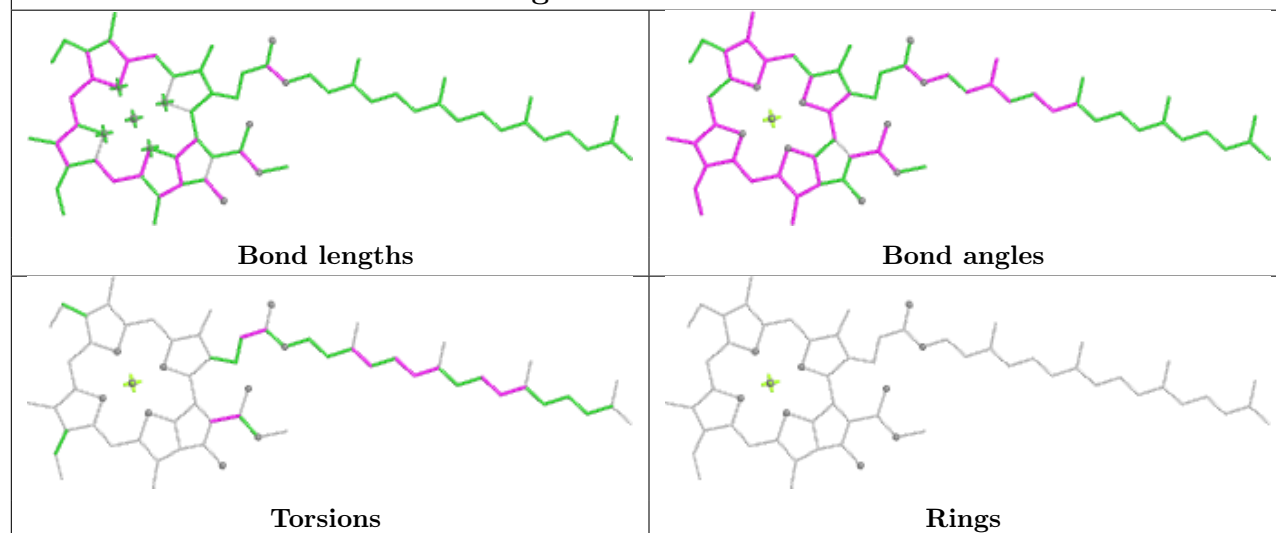
Ligand CLA 1 501

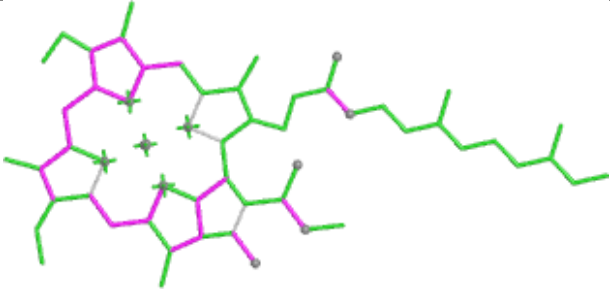
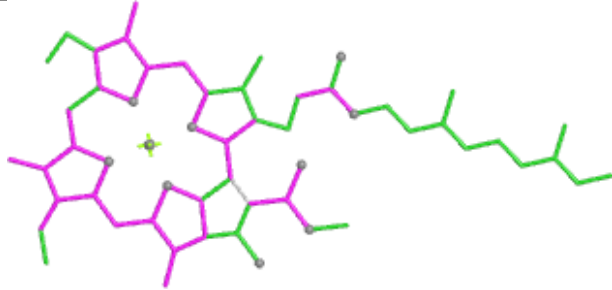
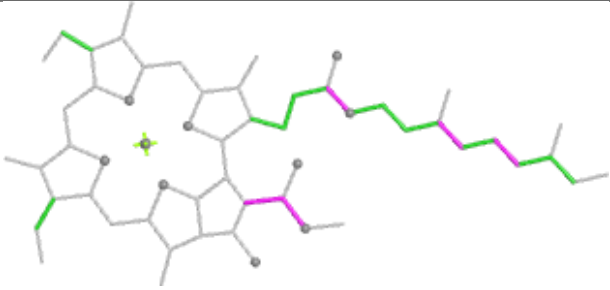
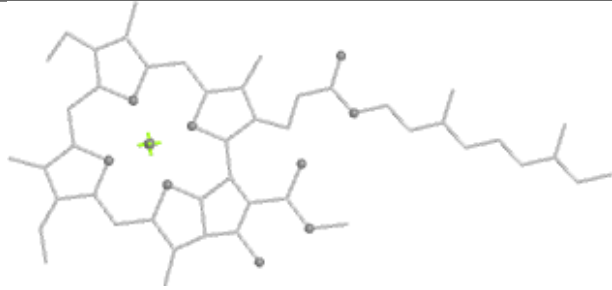
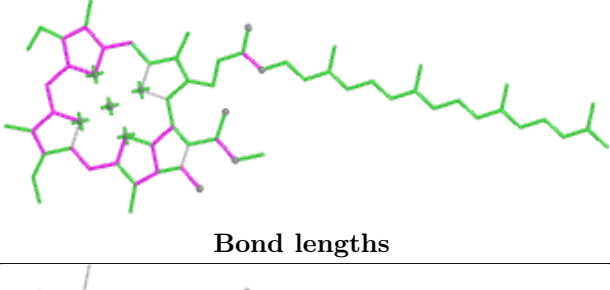
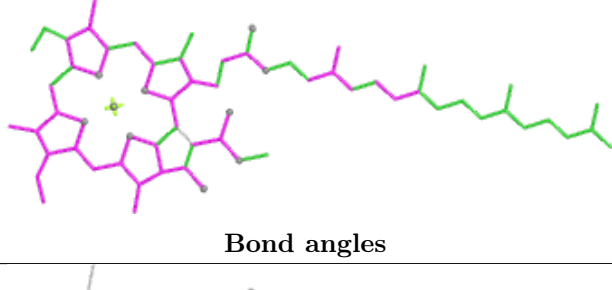
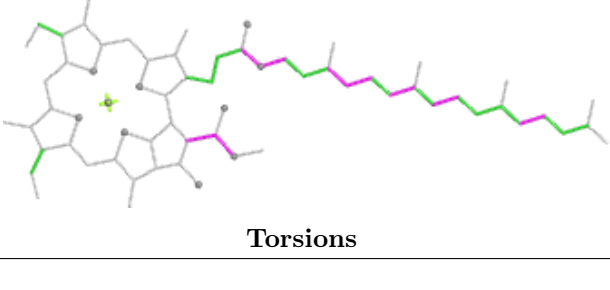
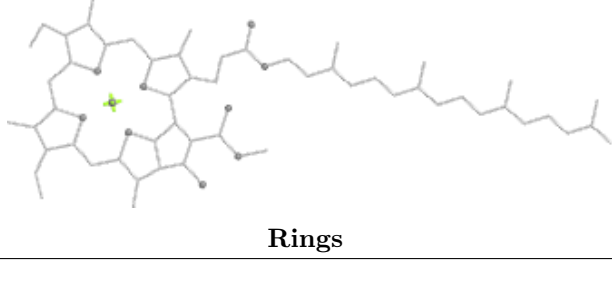


Ligand CLA A 817

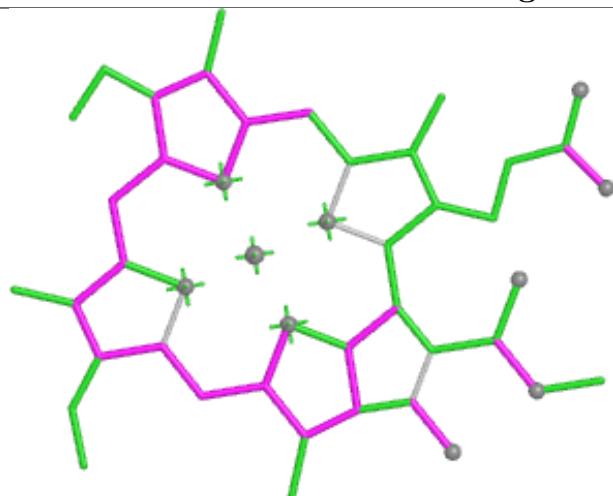


Ligand CLA A 839

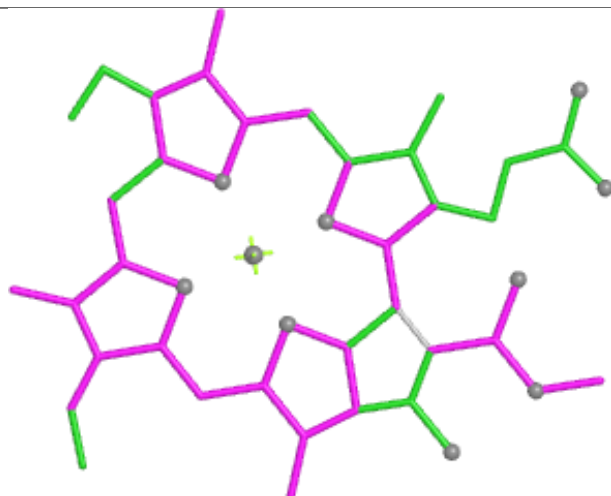


Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

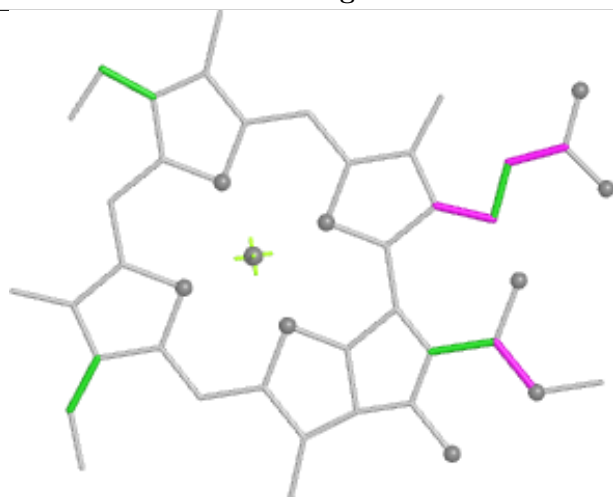
Ligand CLA 1 514



Bond lengths



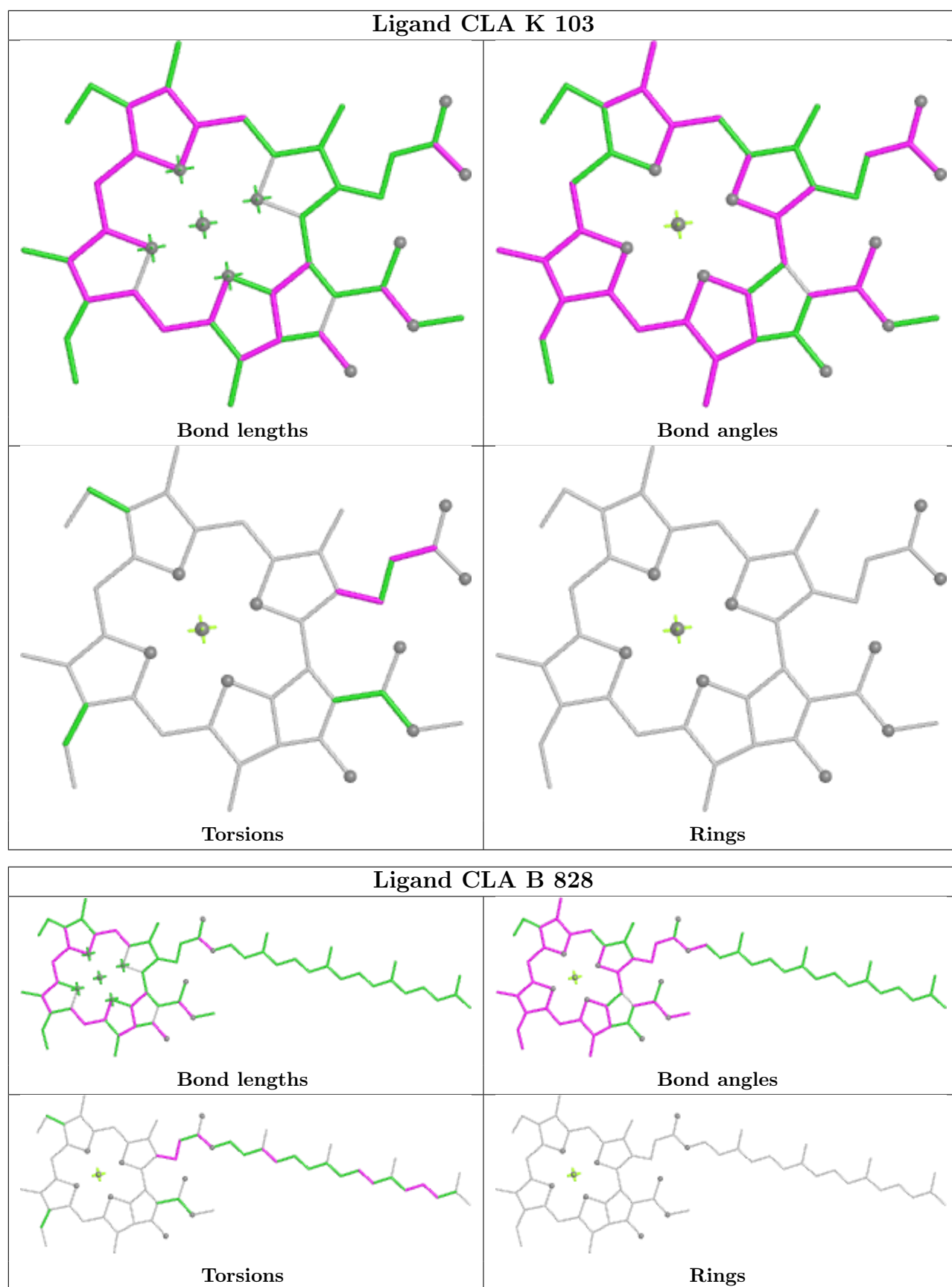
Bond angles



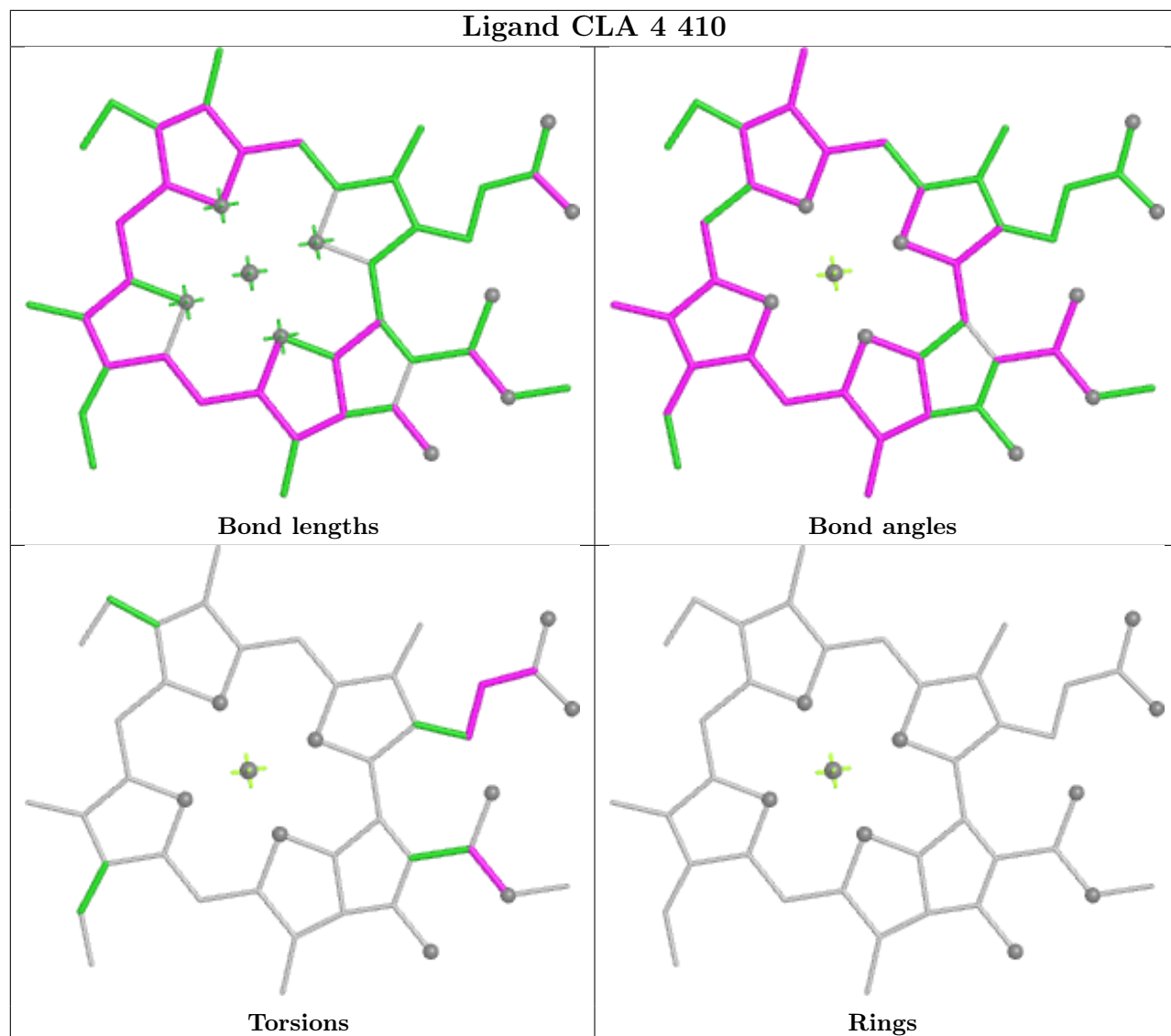
Torsions



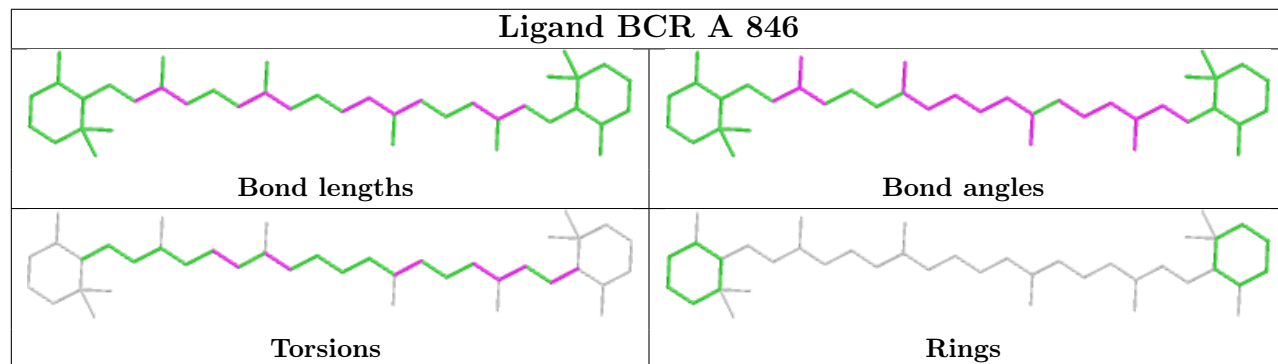
Rings



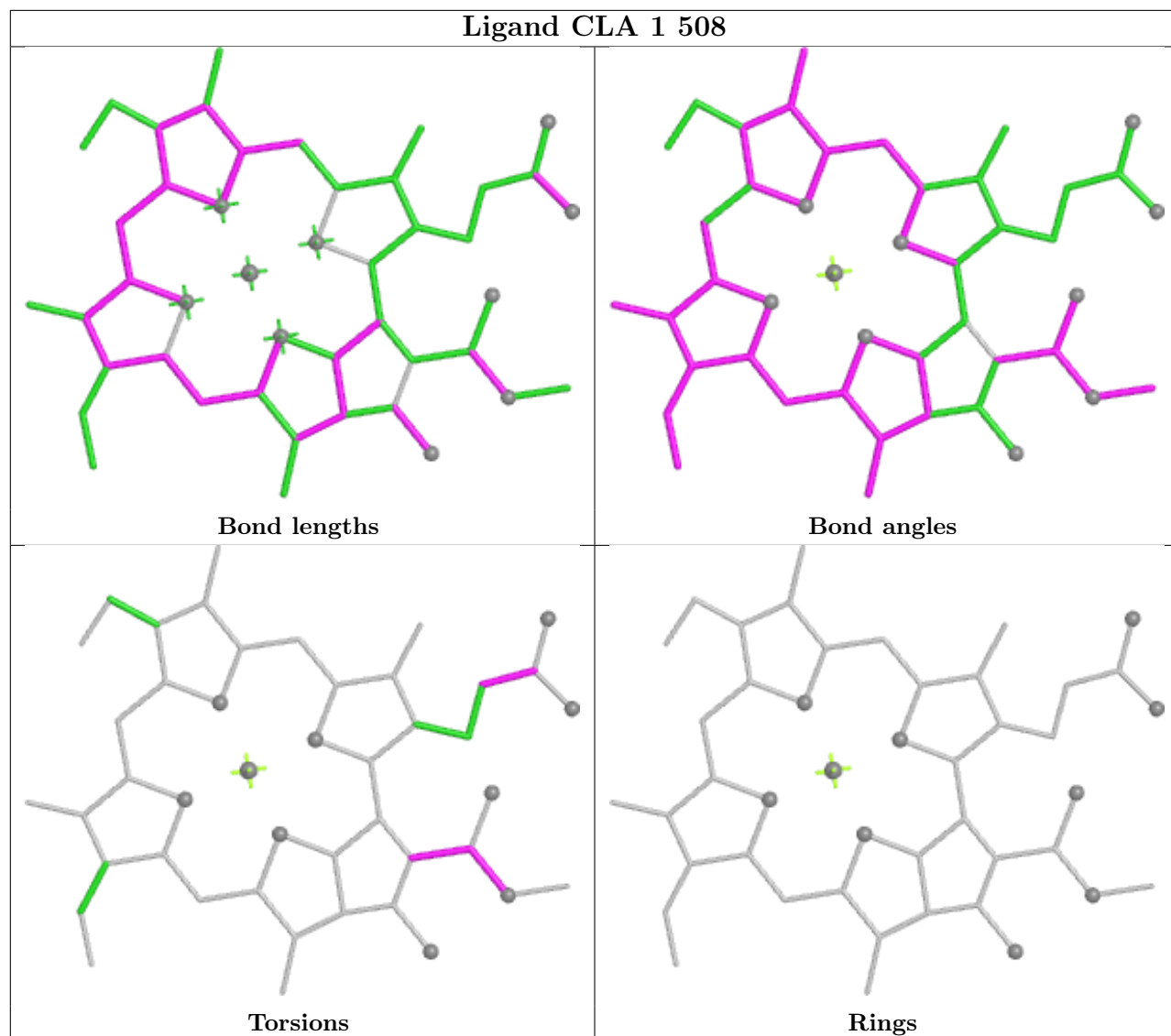
Ligand CLA 4 410



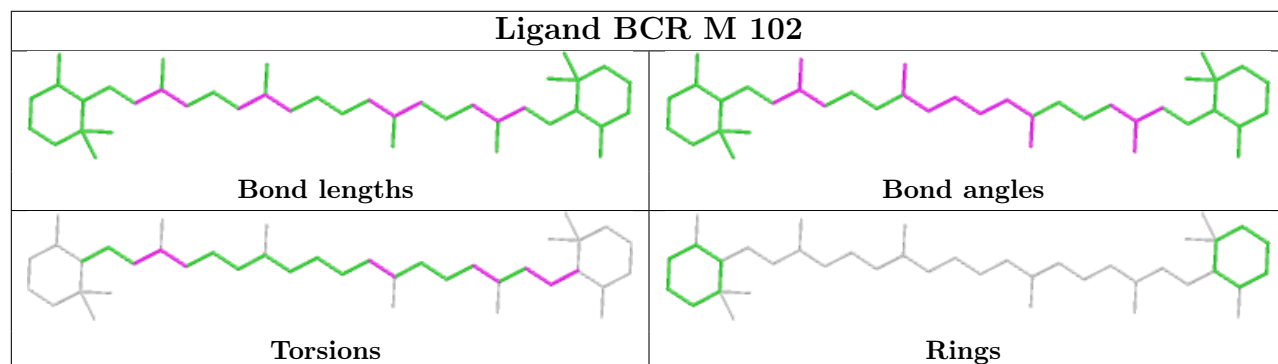
Ligand BCR A 846

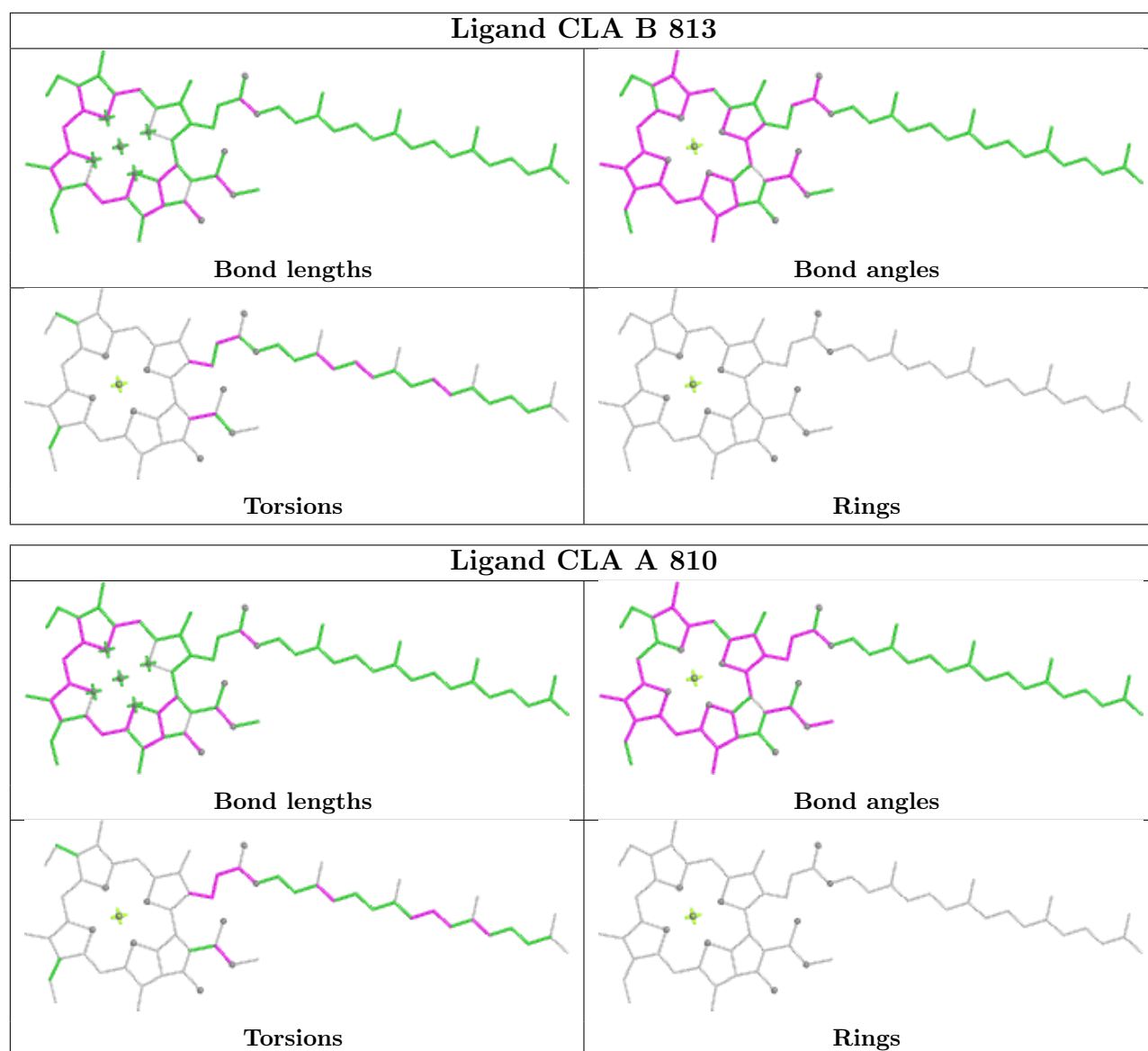


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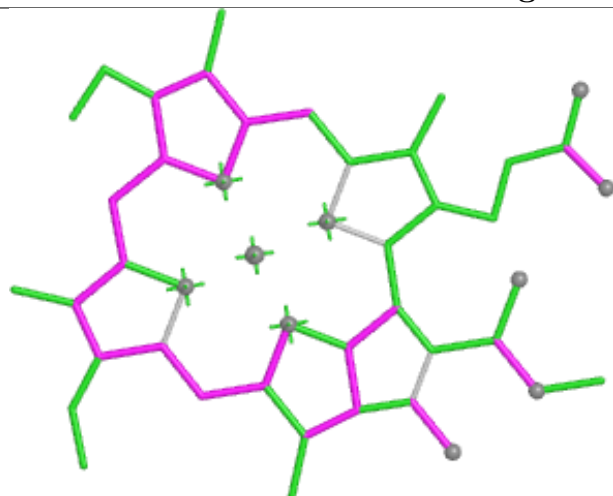


Ligand BCR M 102

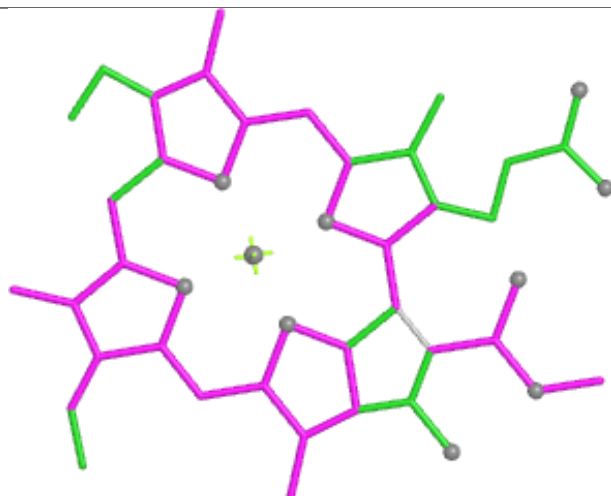




Ligand CLA 1 506



Bond lengths



Bond angles

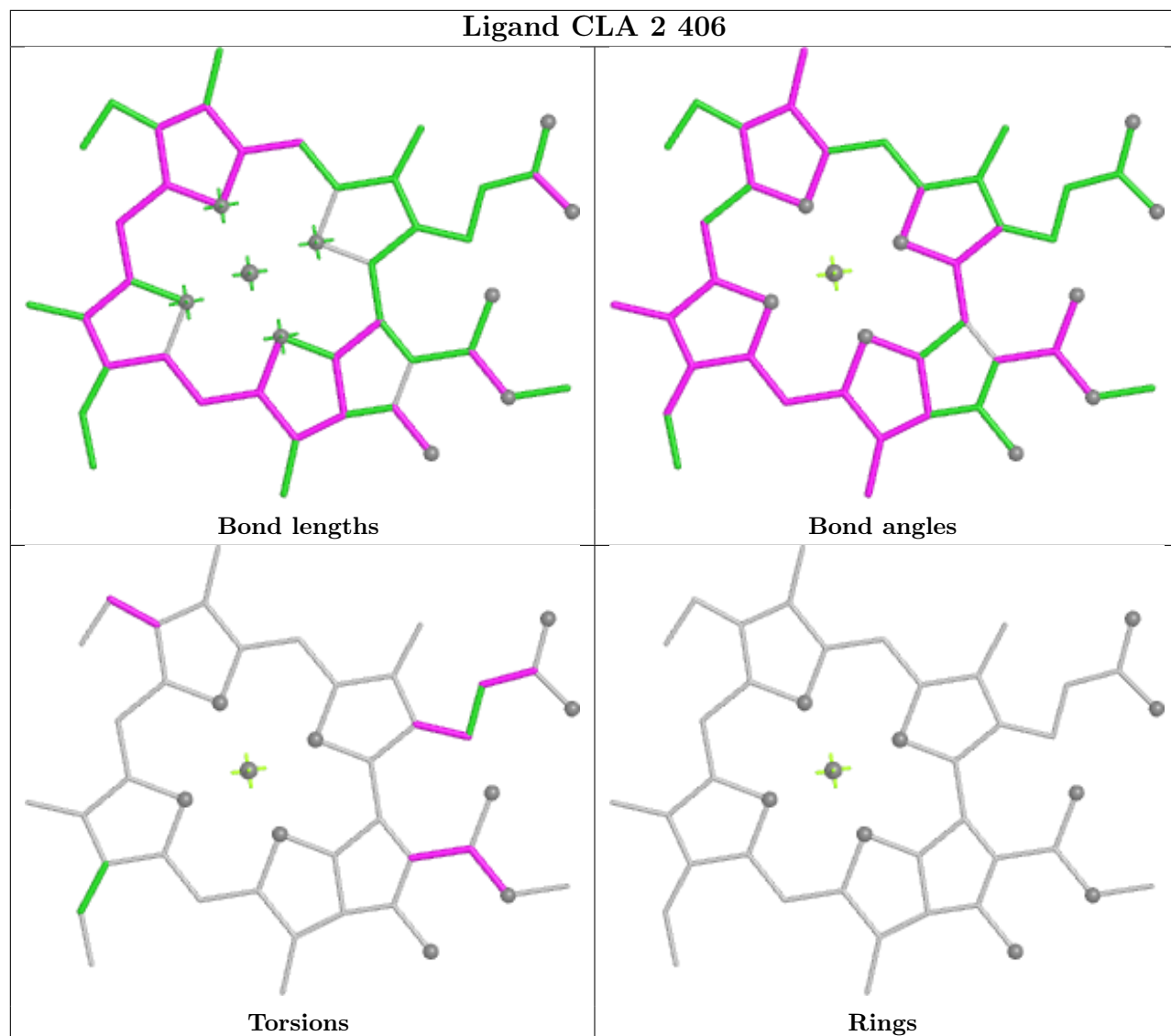


Torsions

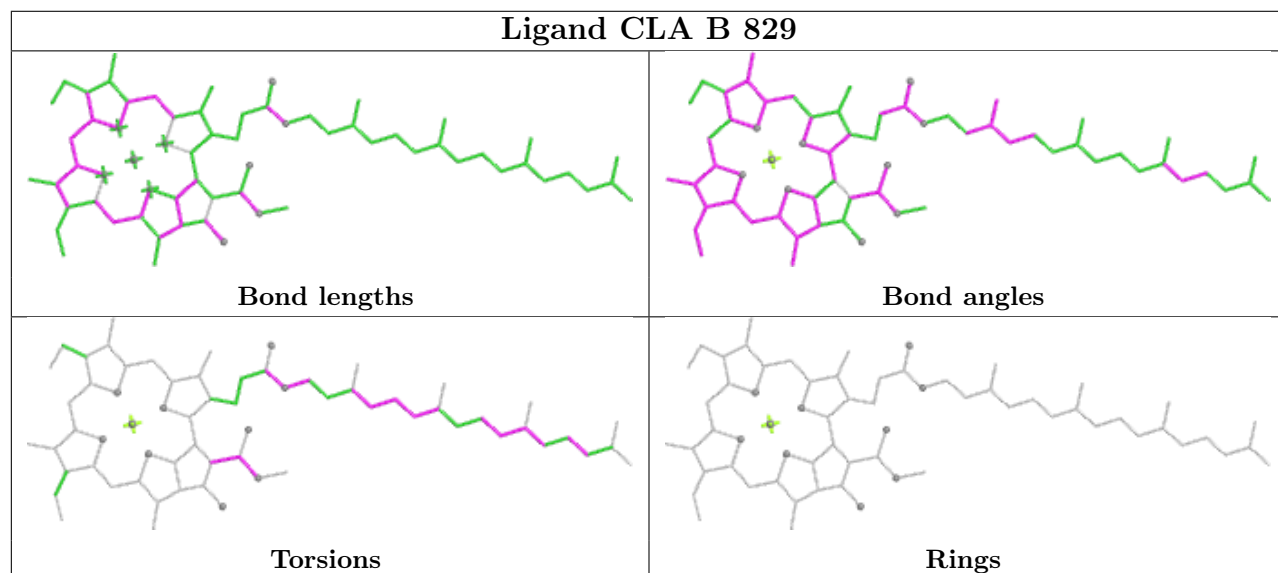


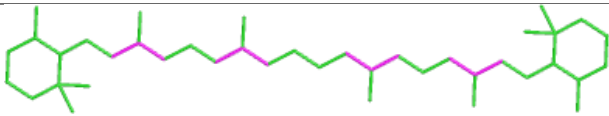
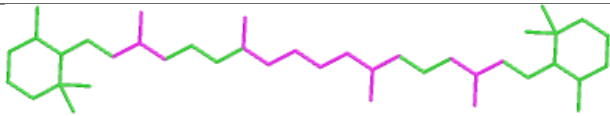
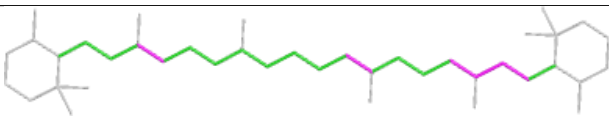
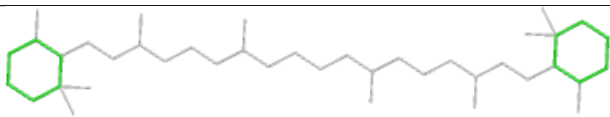
Rings

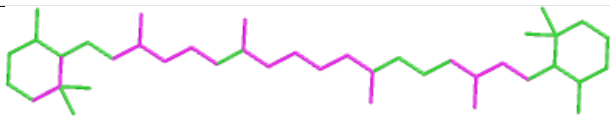
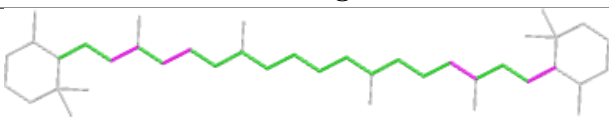
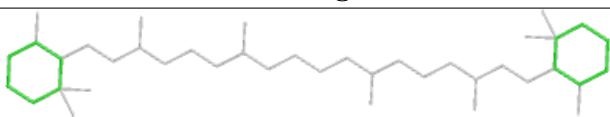
Ligand CLA 2 406

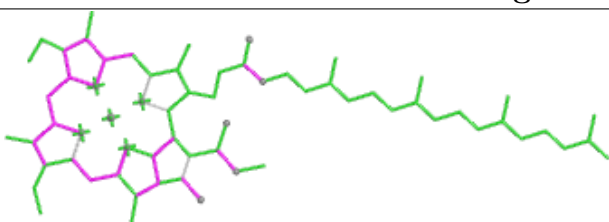
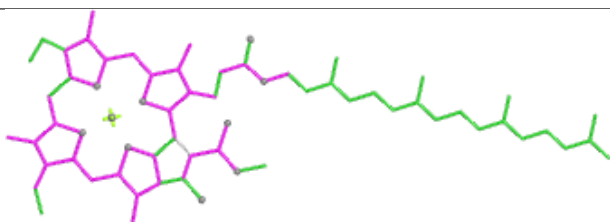
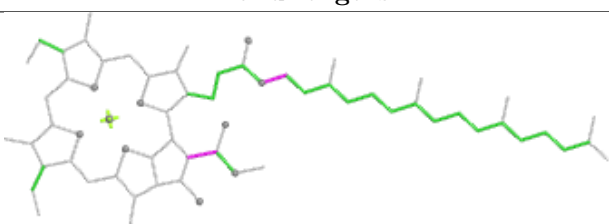
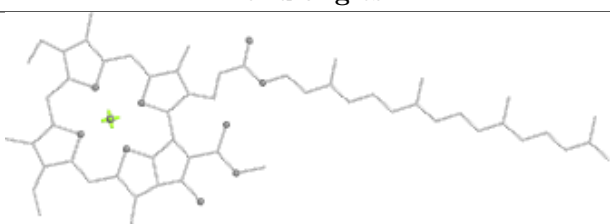


Ligand CLA B 829

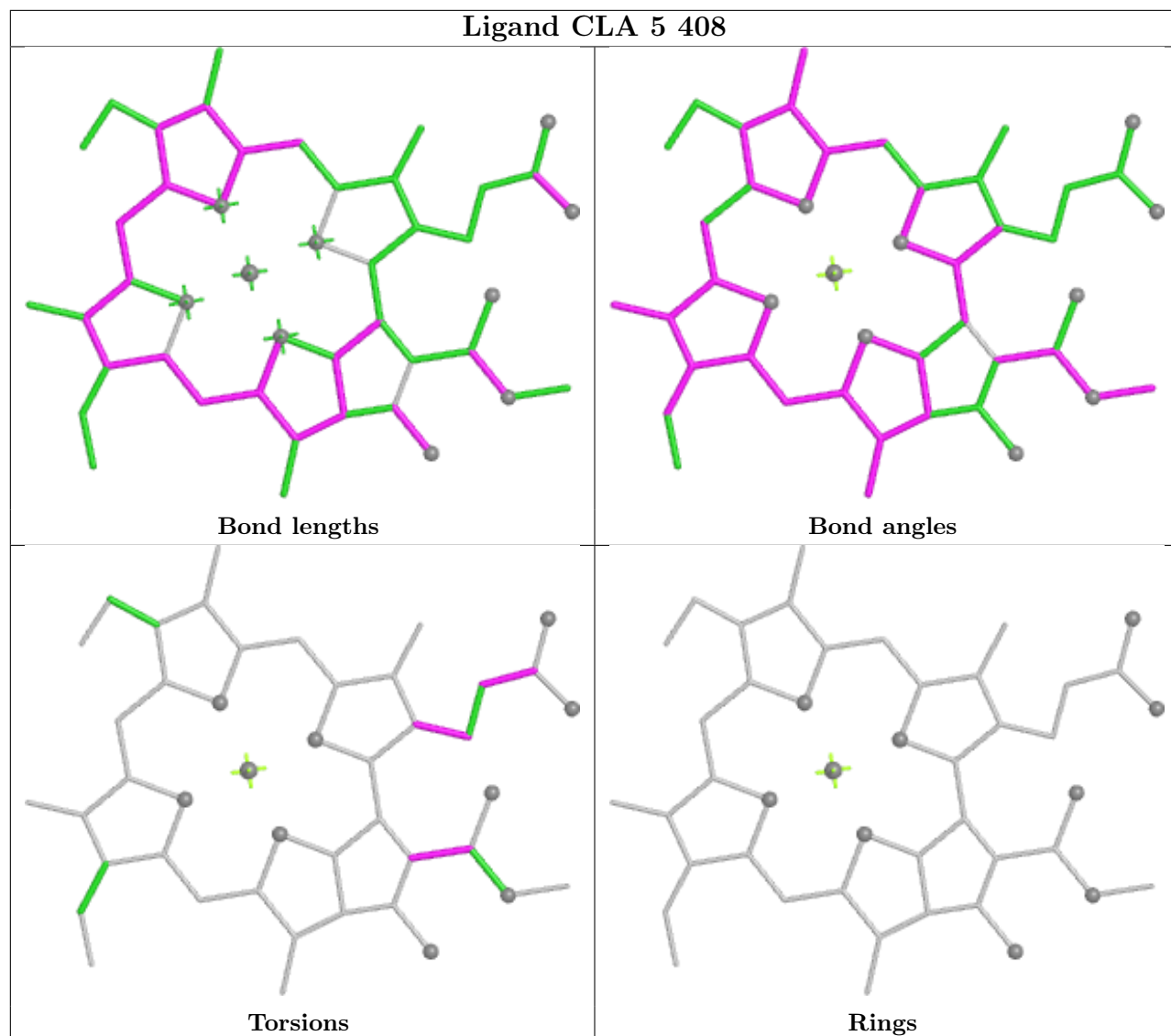


Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

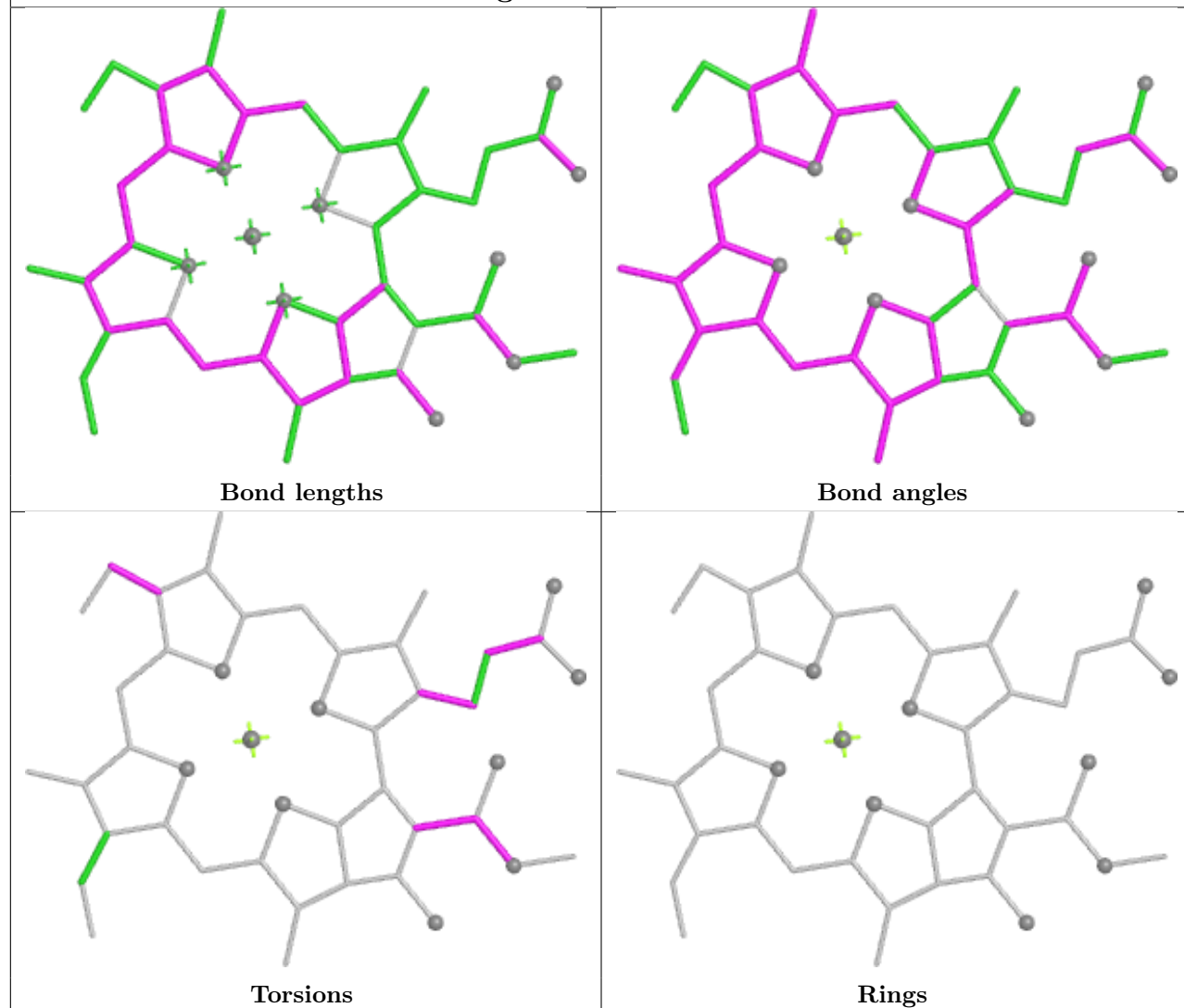
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

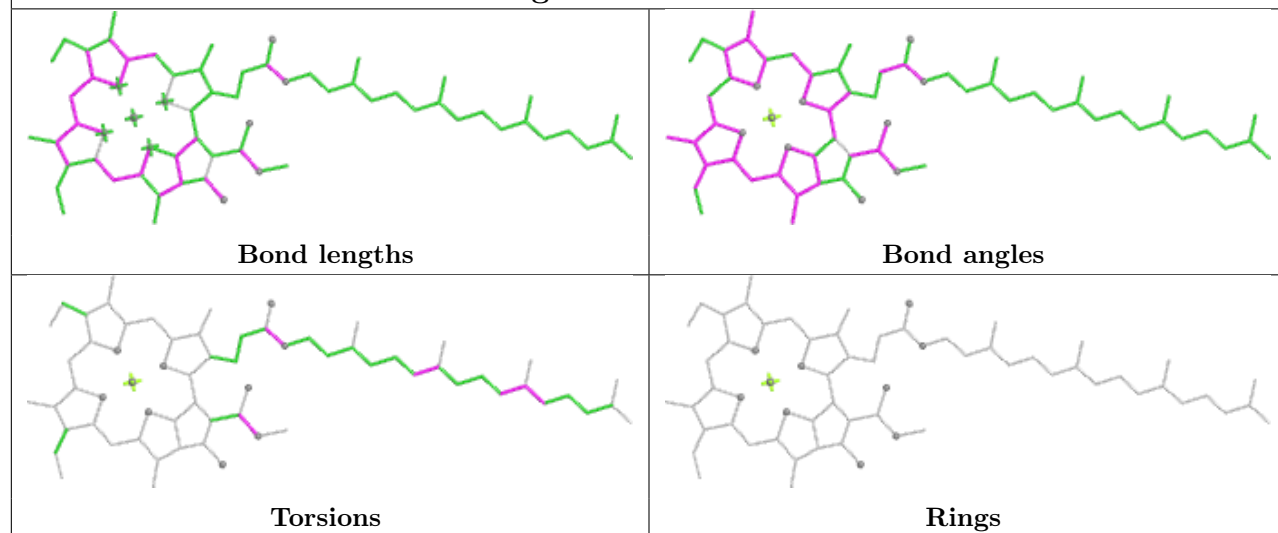
Ligand CLA 5 408



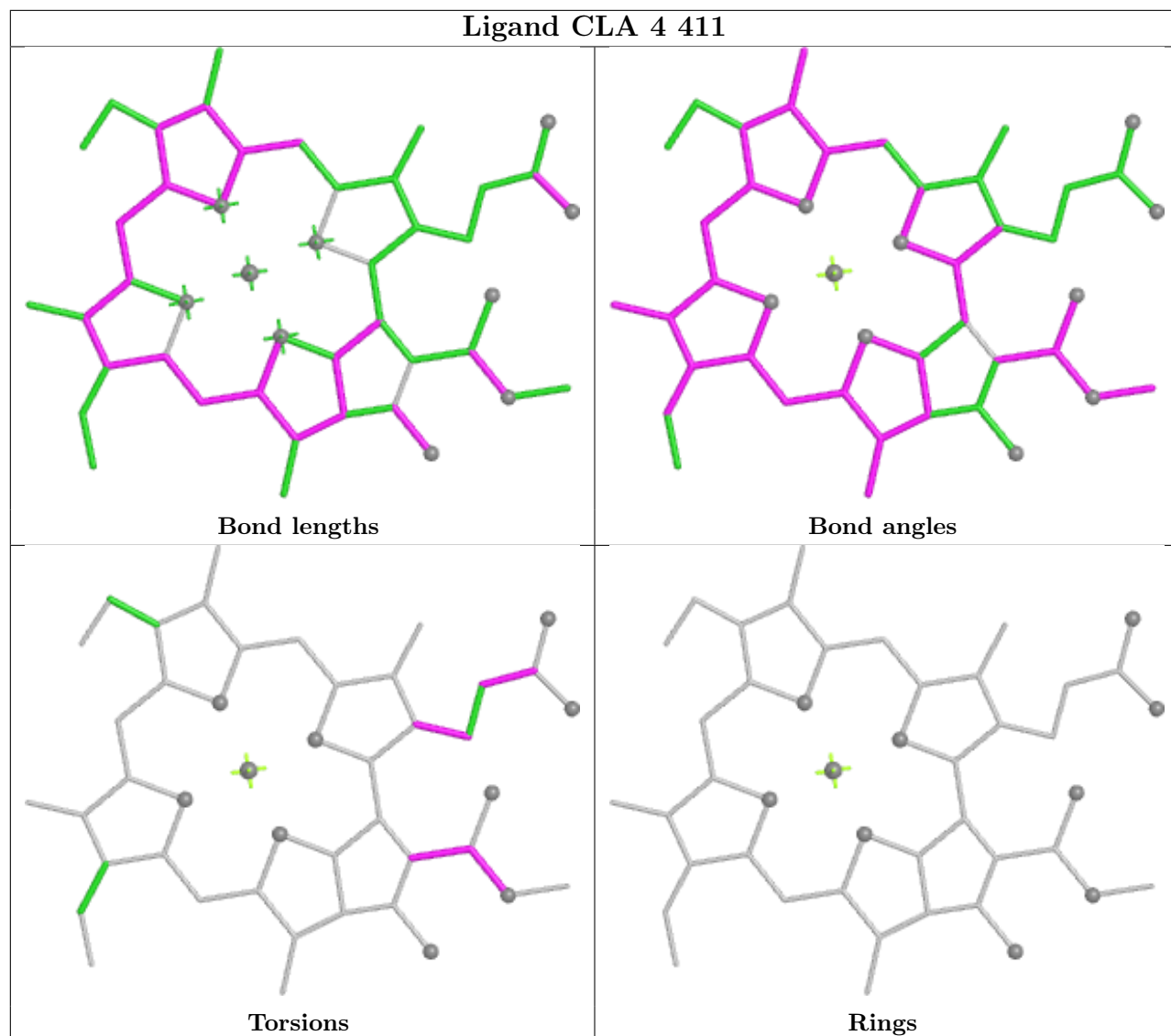
Ligand CLA 1 526



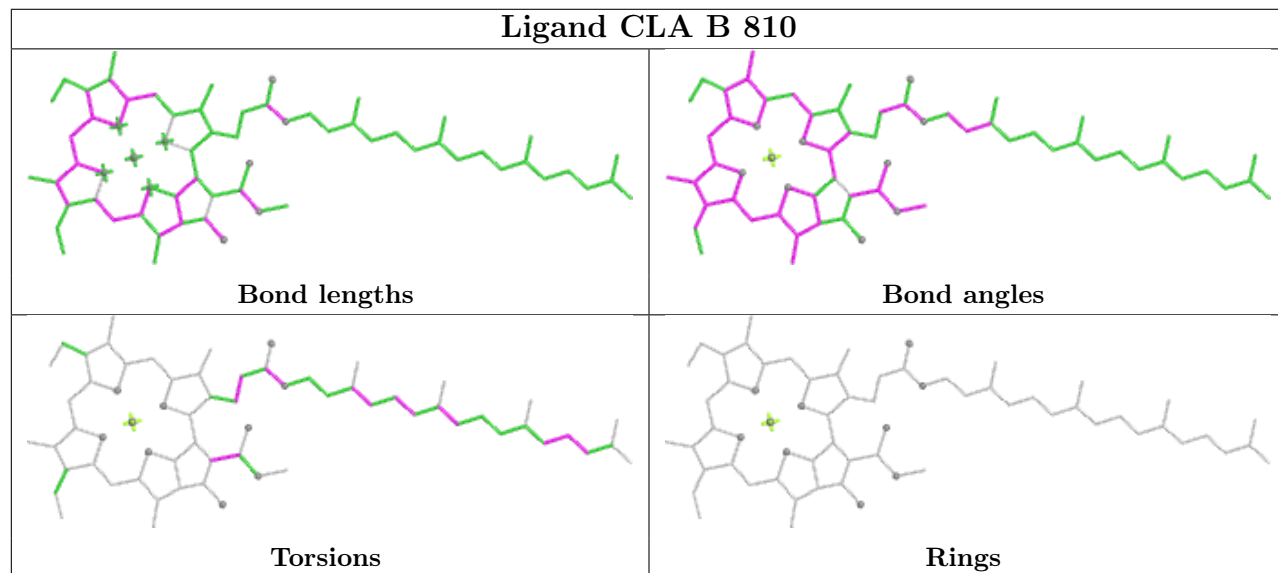
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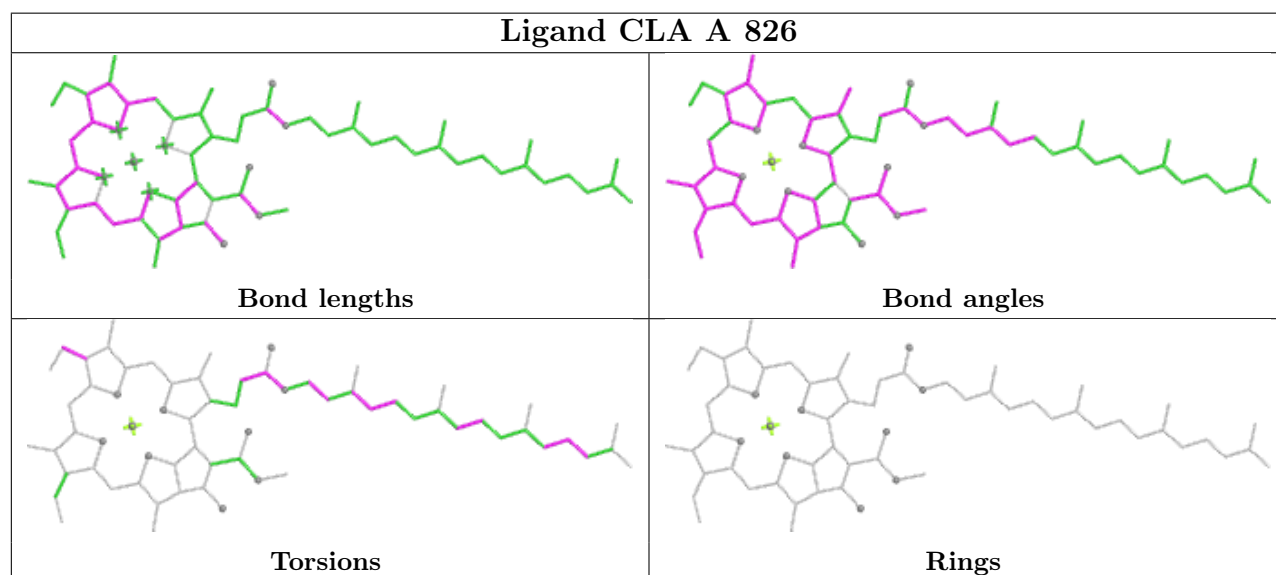
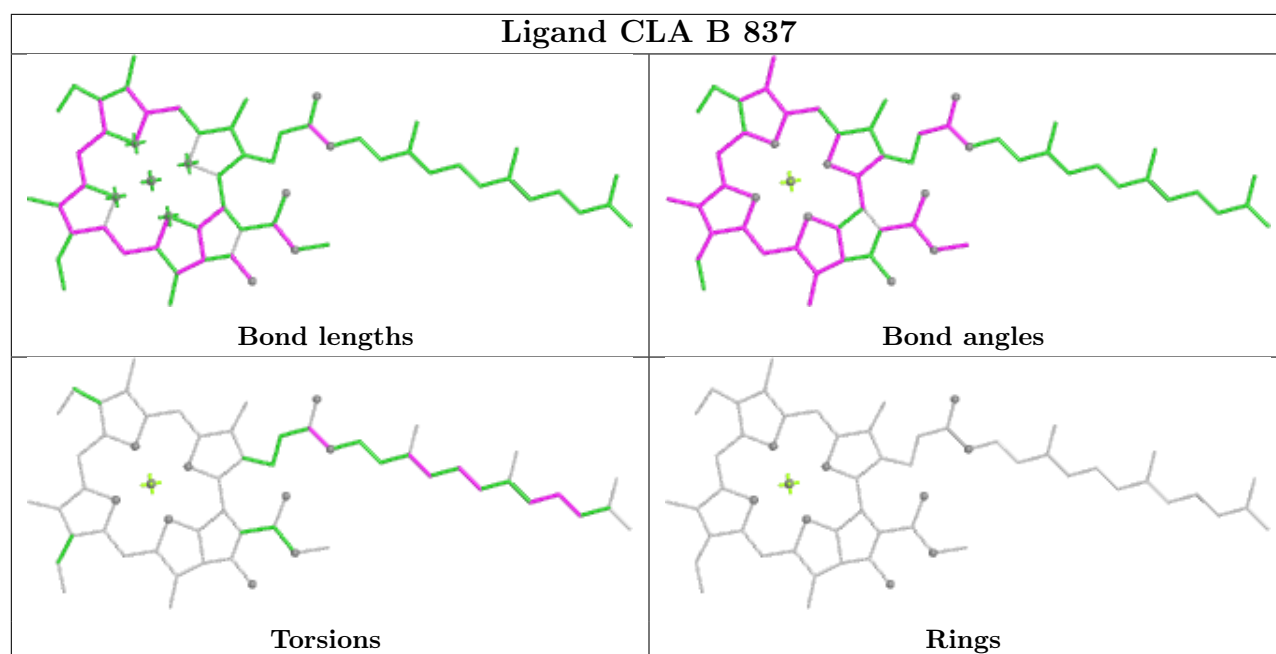


Ligand CLA 4 411

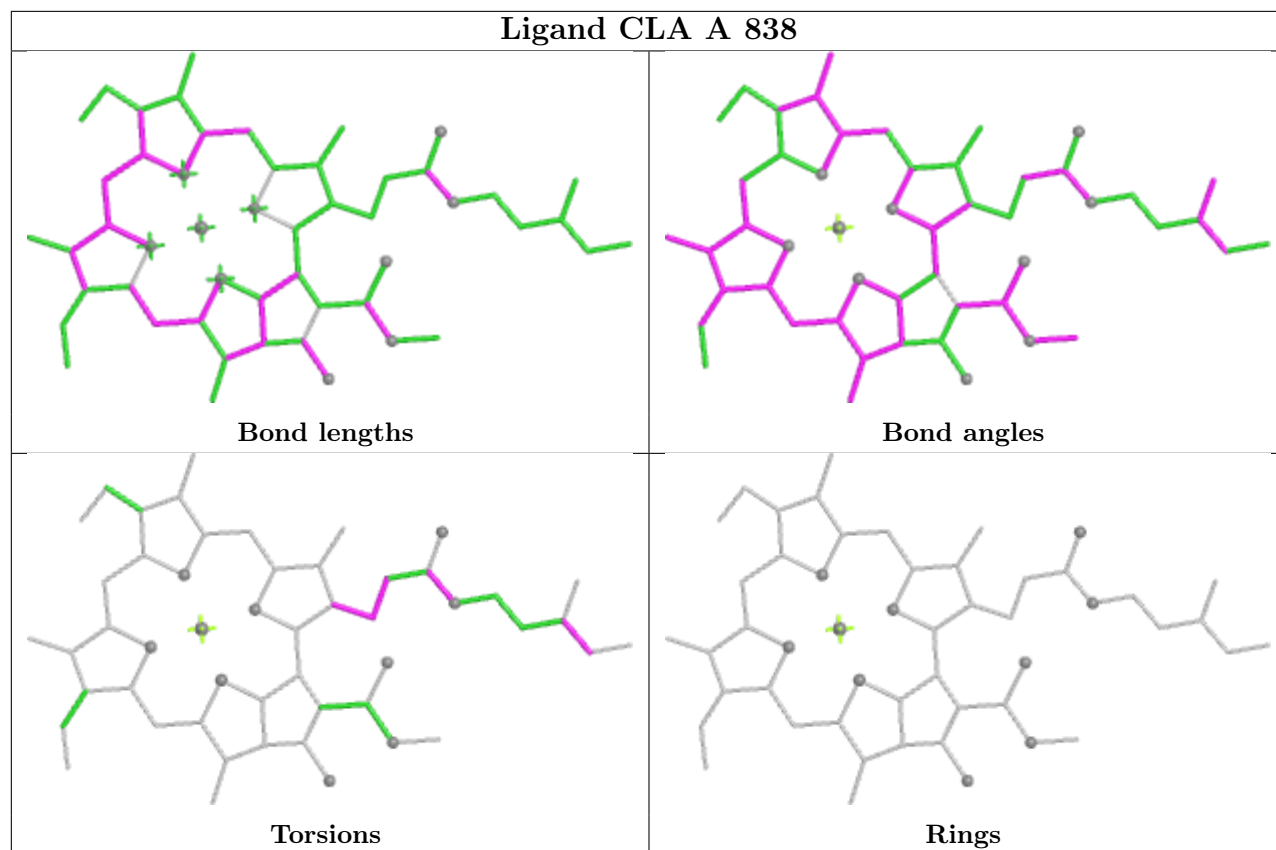


Ligand CLA B 810

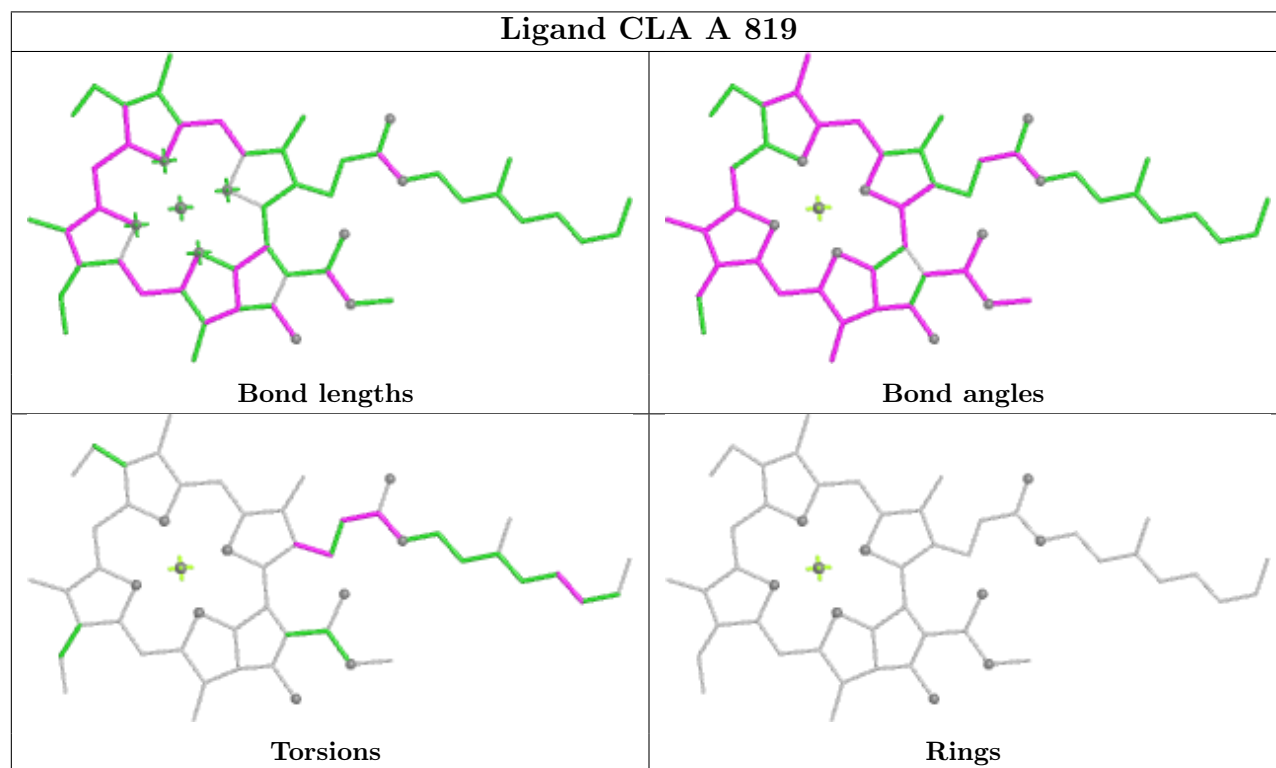




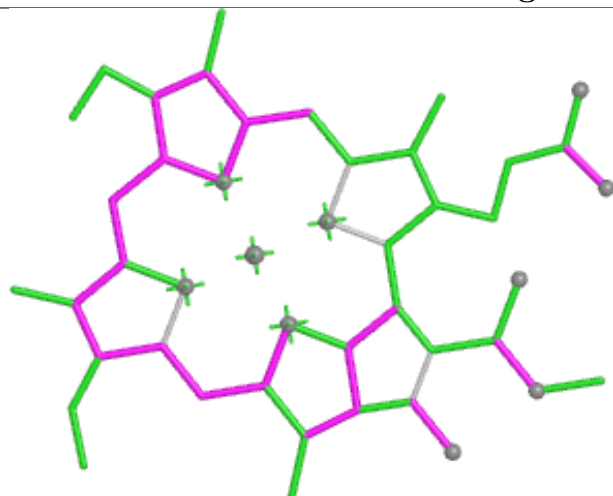
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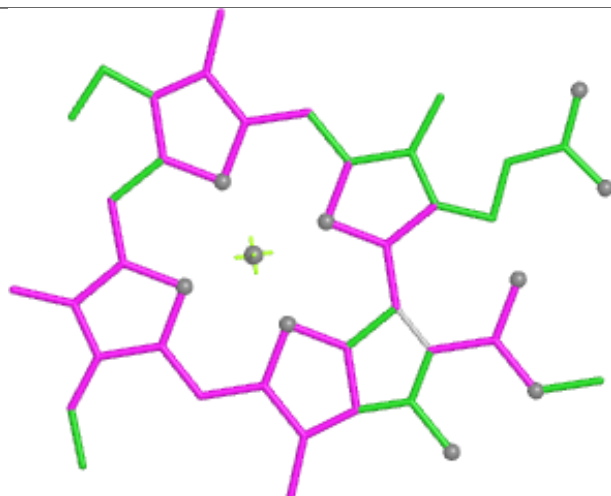
Ligand CLA A 819



Ligand CLA 2 401



Bond lengths



Bond angles

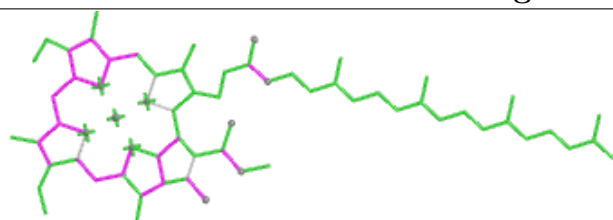


Torsions

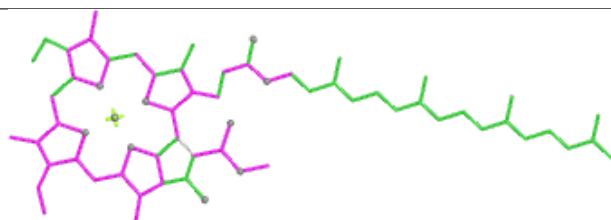


Rings

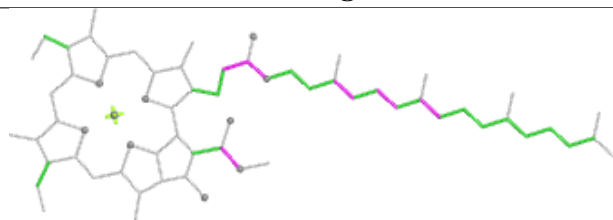
Ligand CLA A 833



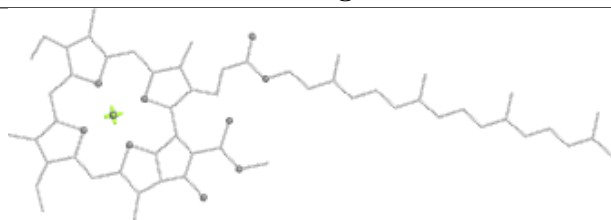
Bond lengths



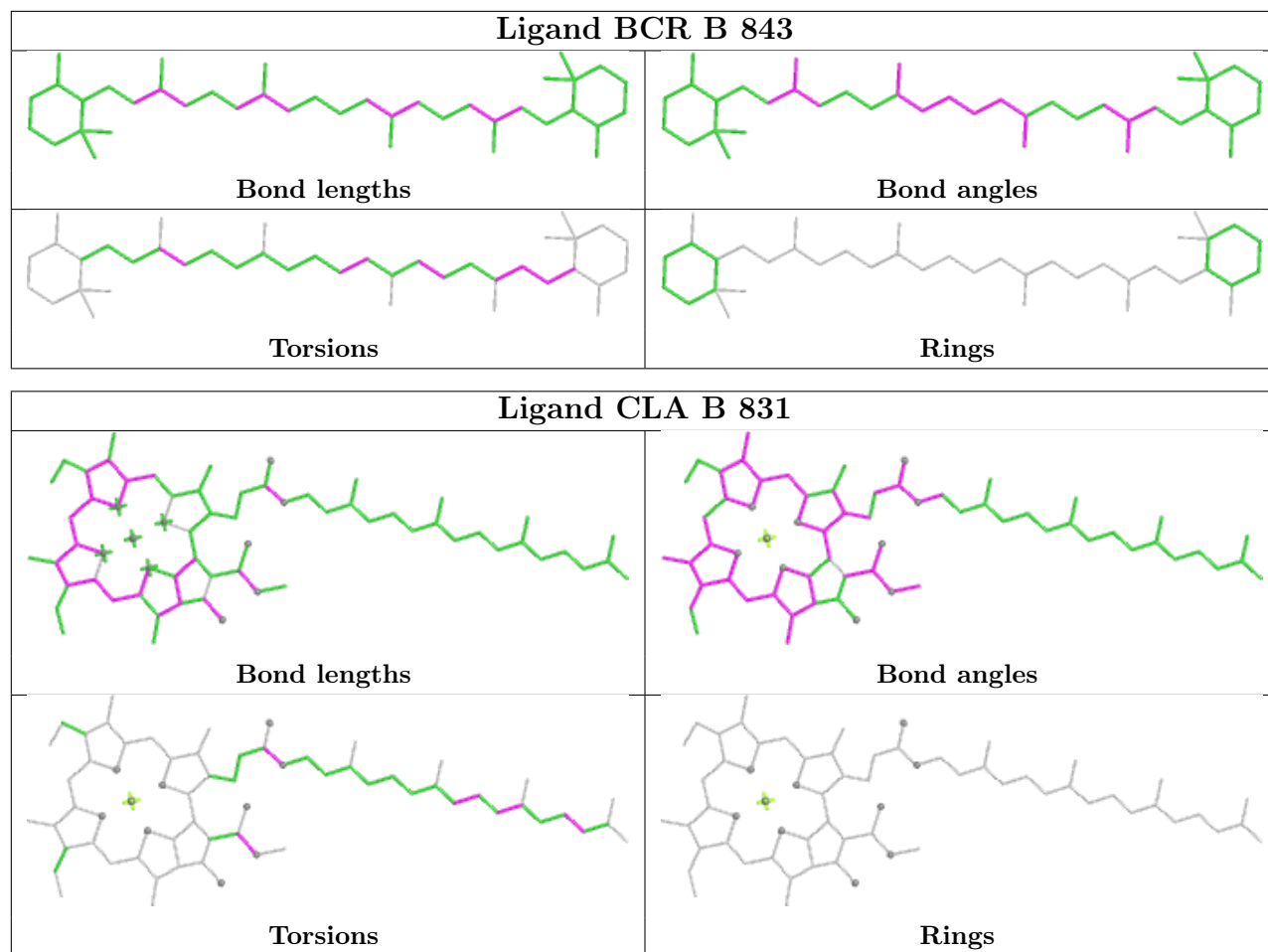
Bond angles



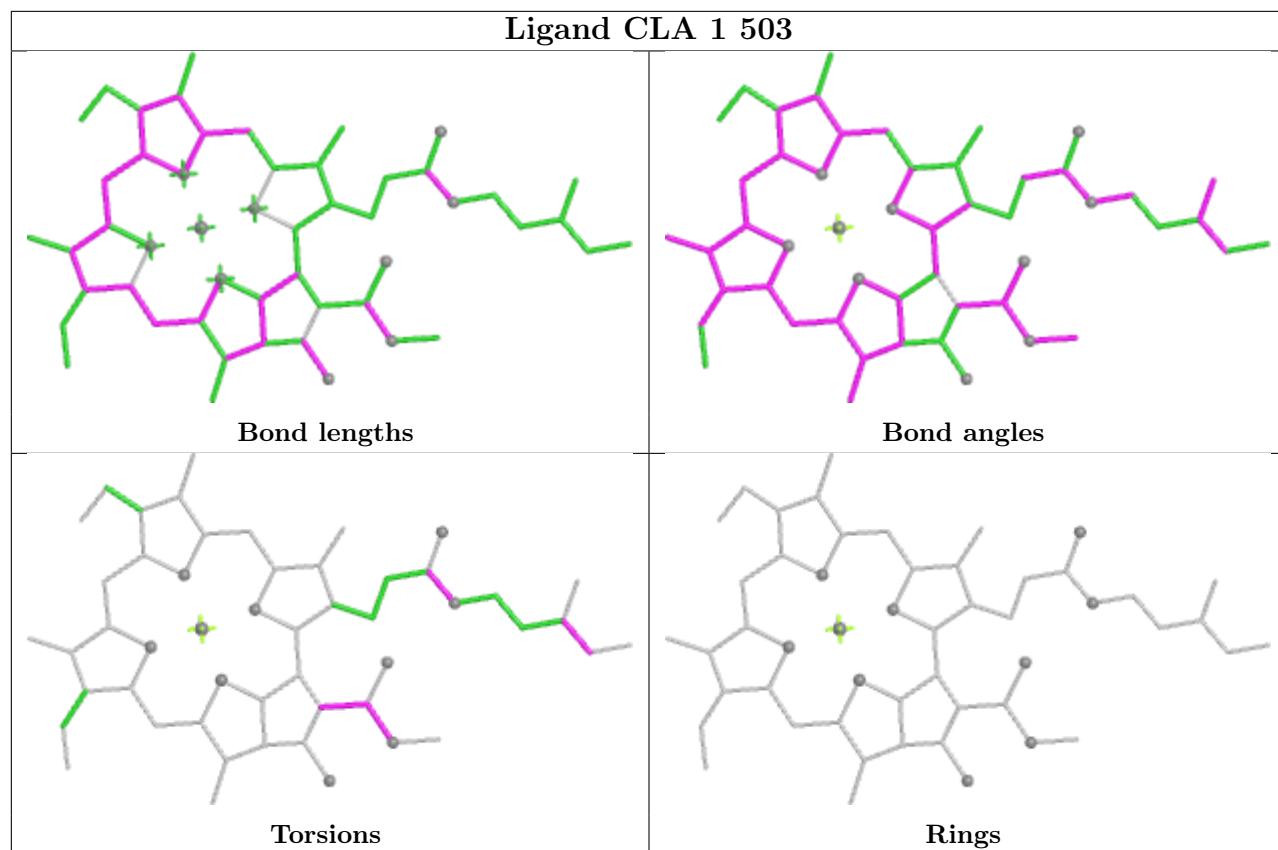
Torsions



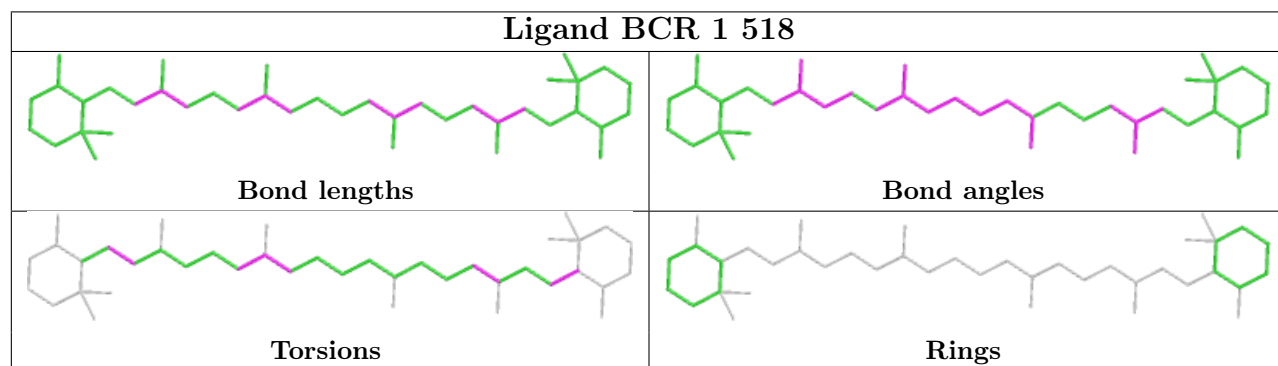
Rings



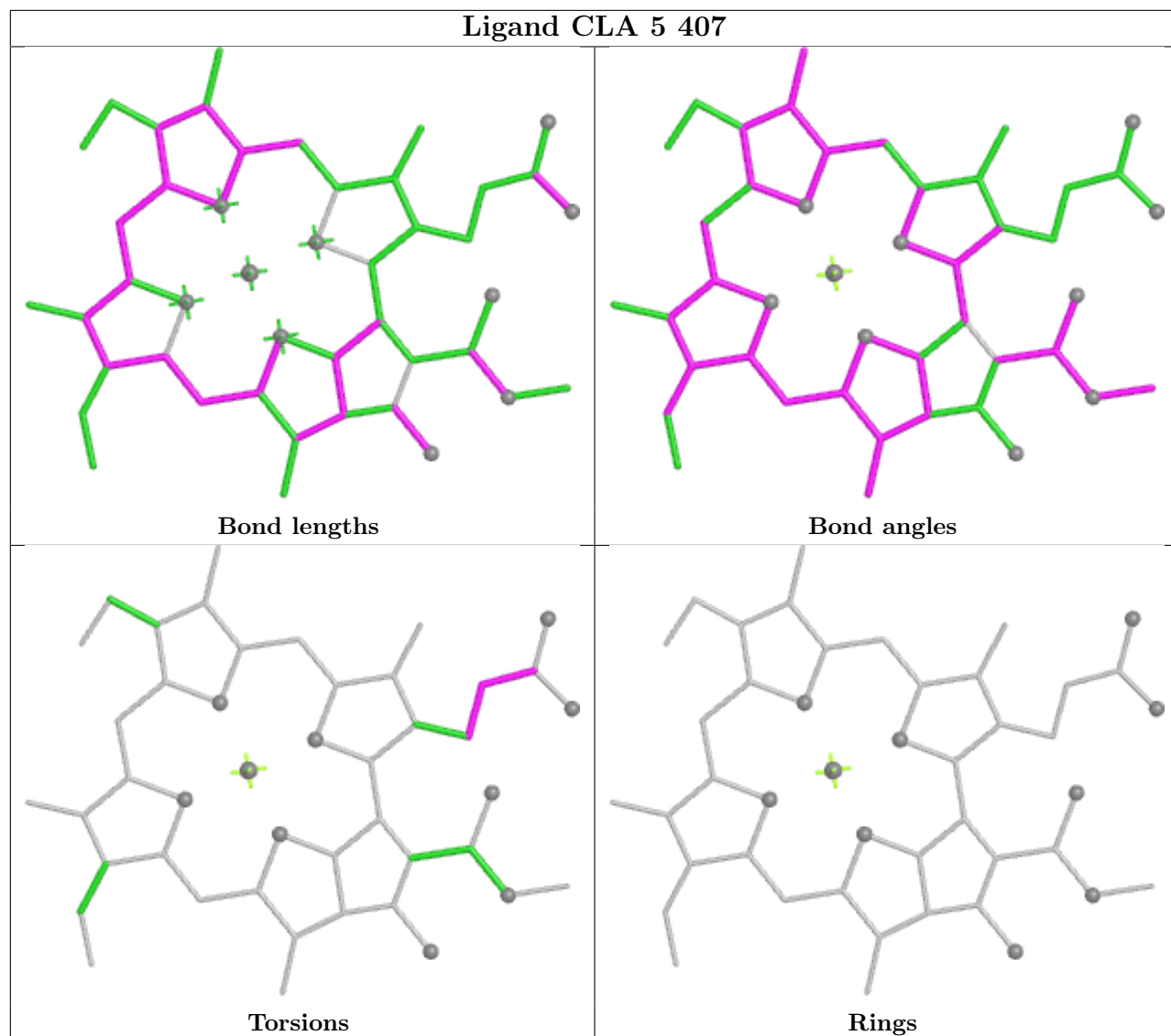
Ligand CLA 1 503



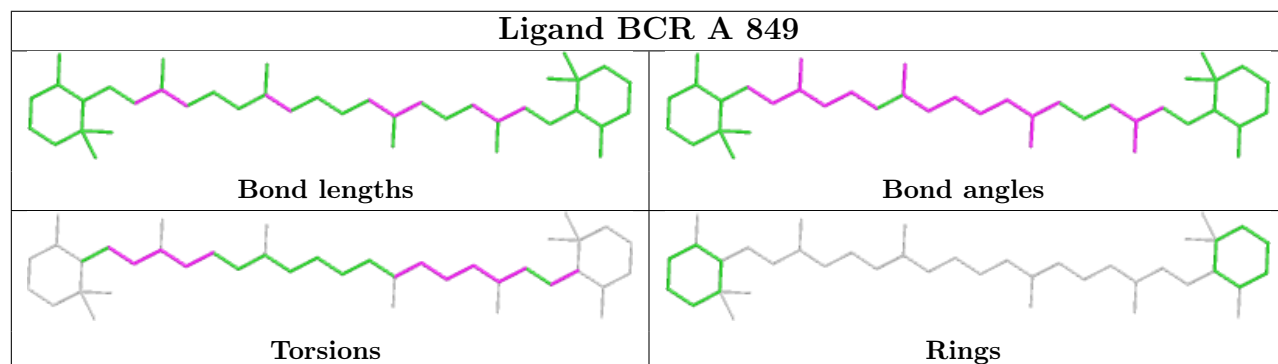
Ligand BCR 1 518



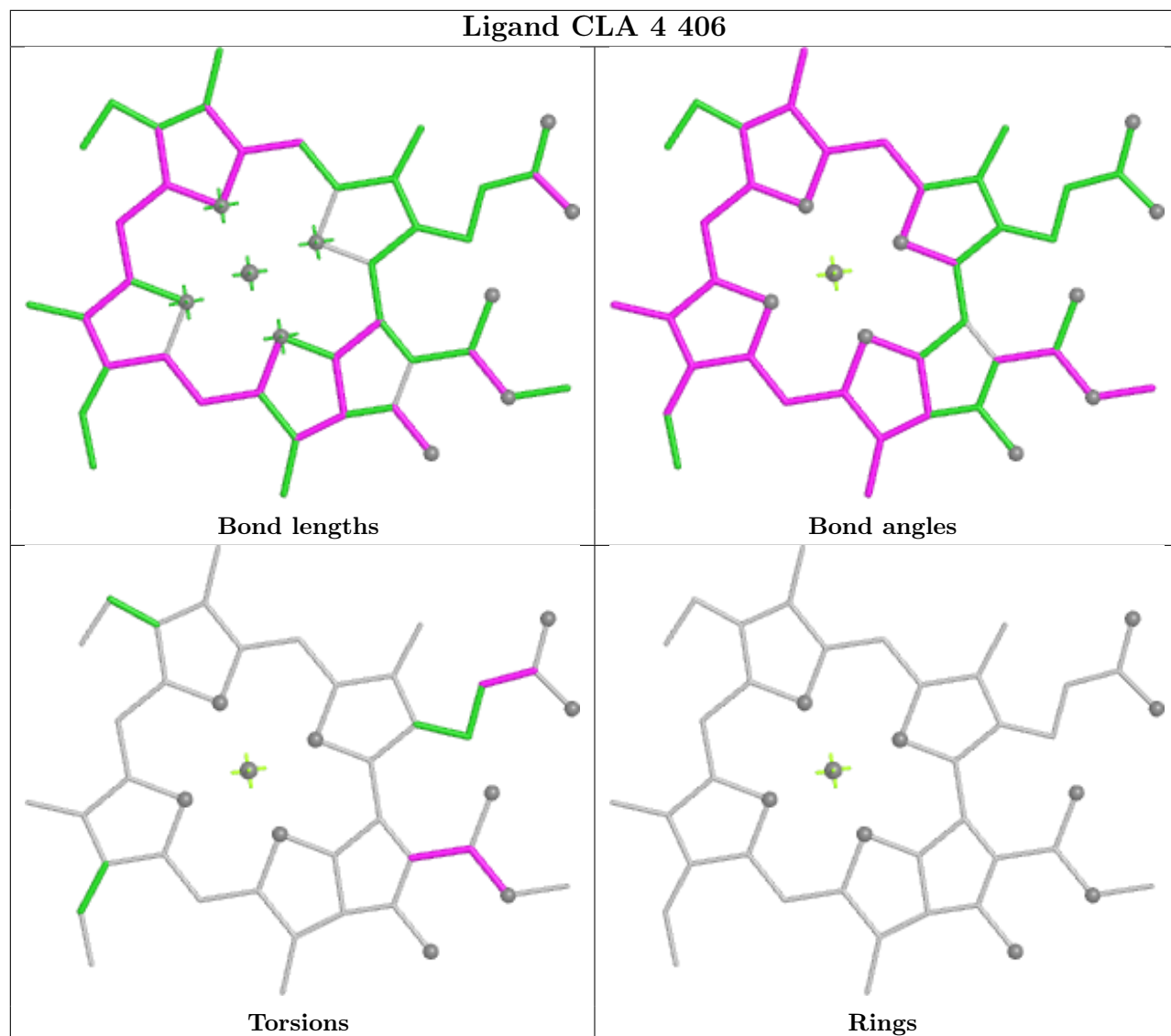
Ligand CLA 5 407



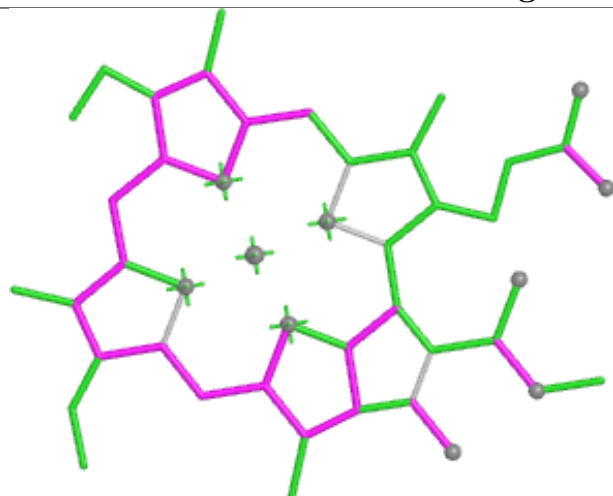
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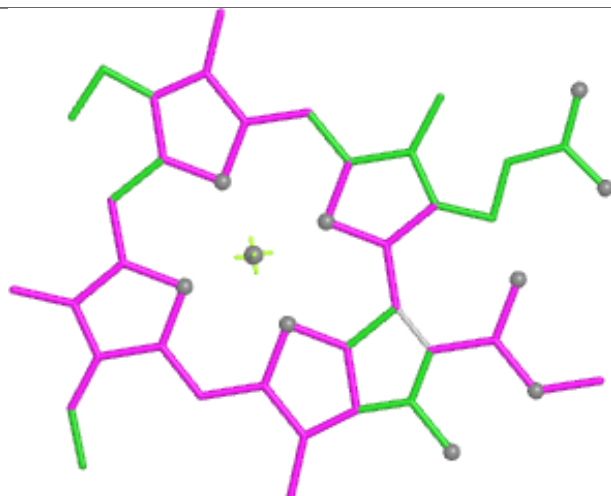
Ligand CLA 4 406



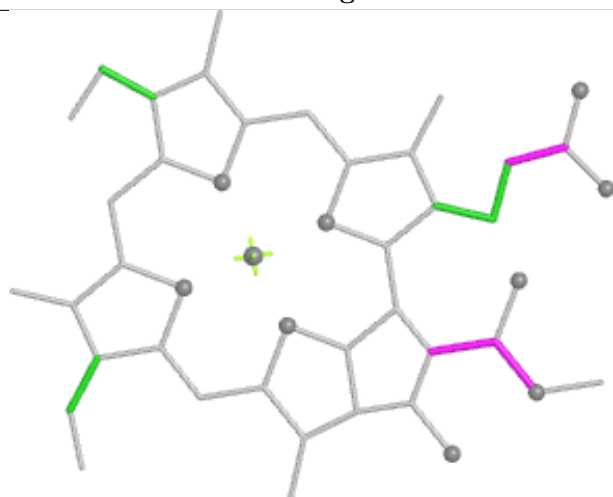
Ligand CLA 5 409



Bond lengths



Bond angles

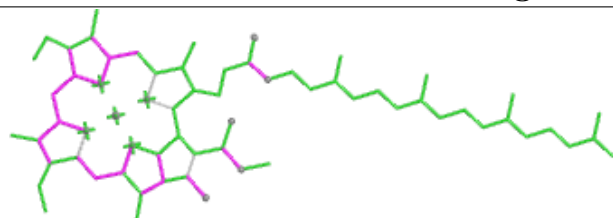


Torsions

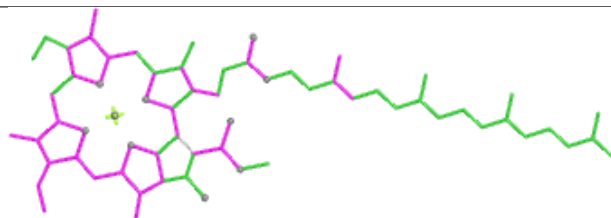


Rings

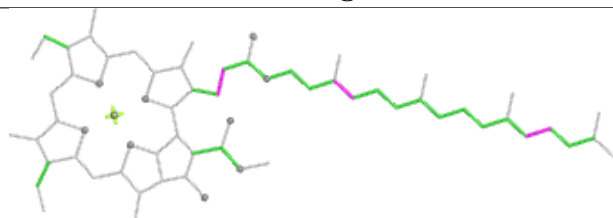
Ligand CLA A 802



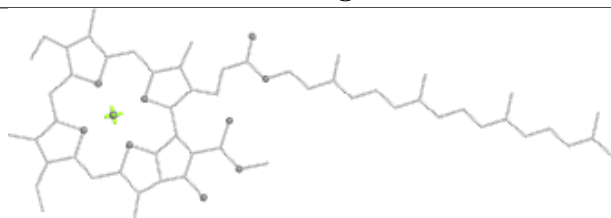
Bond lengths



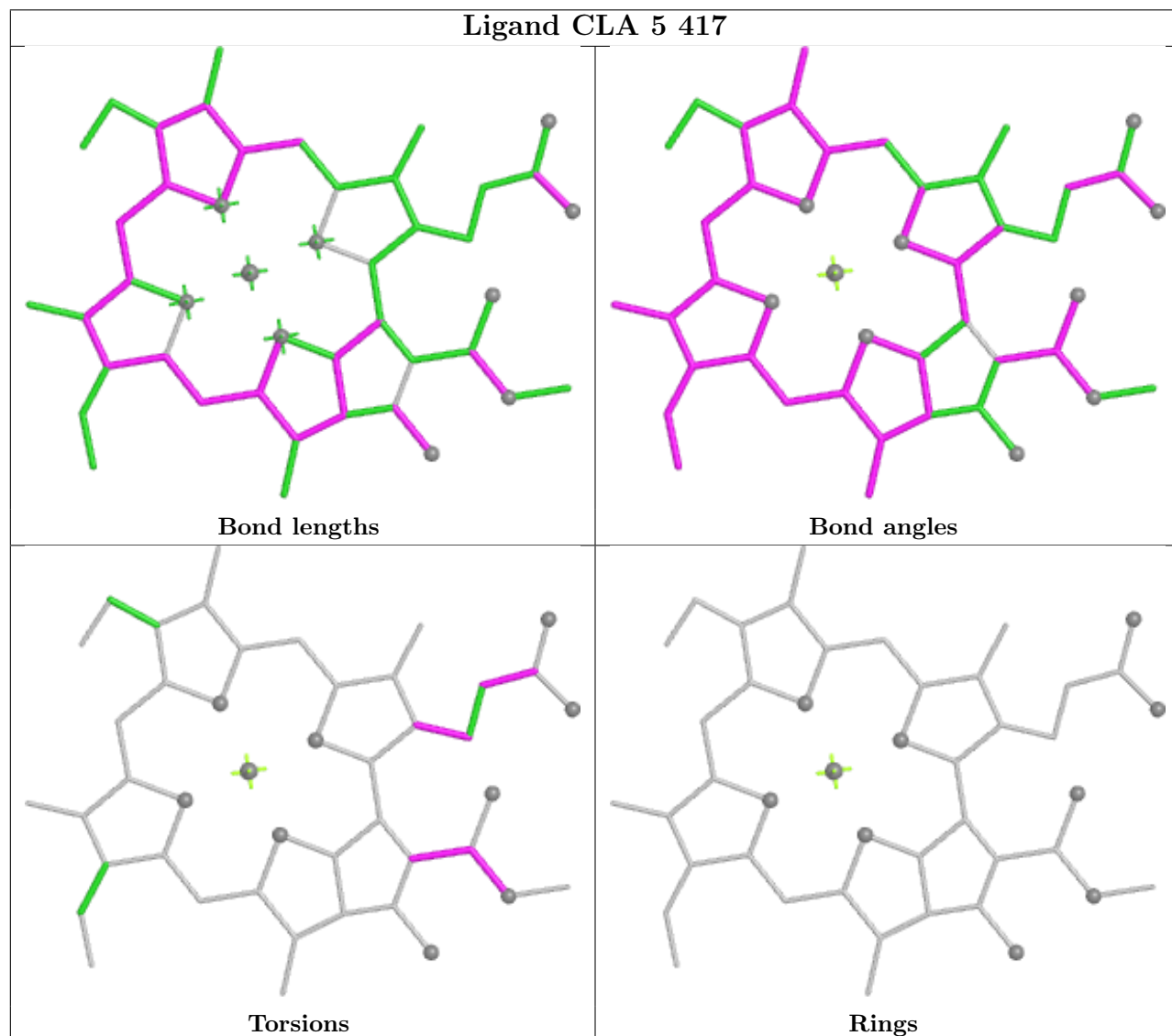
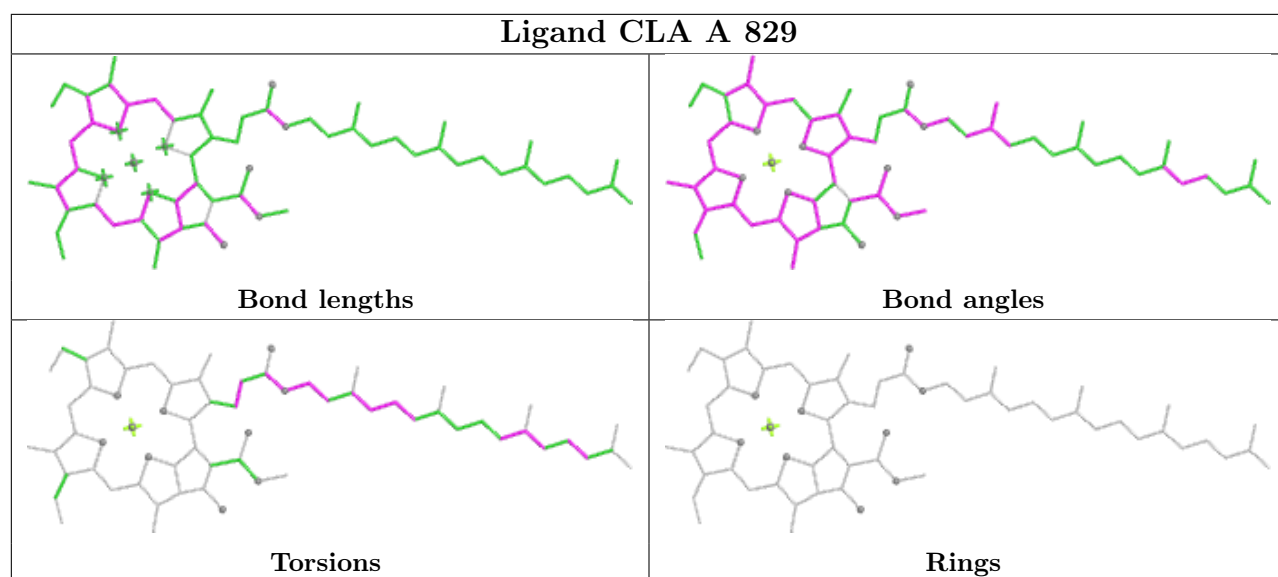
Bond angles

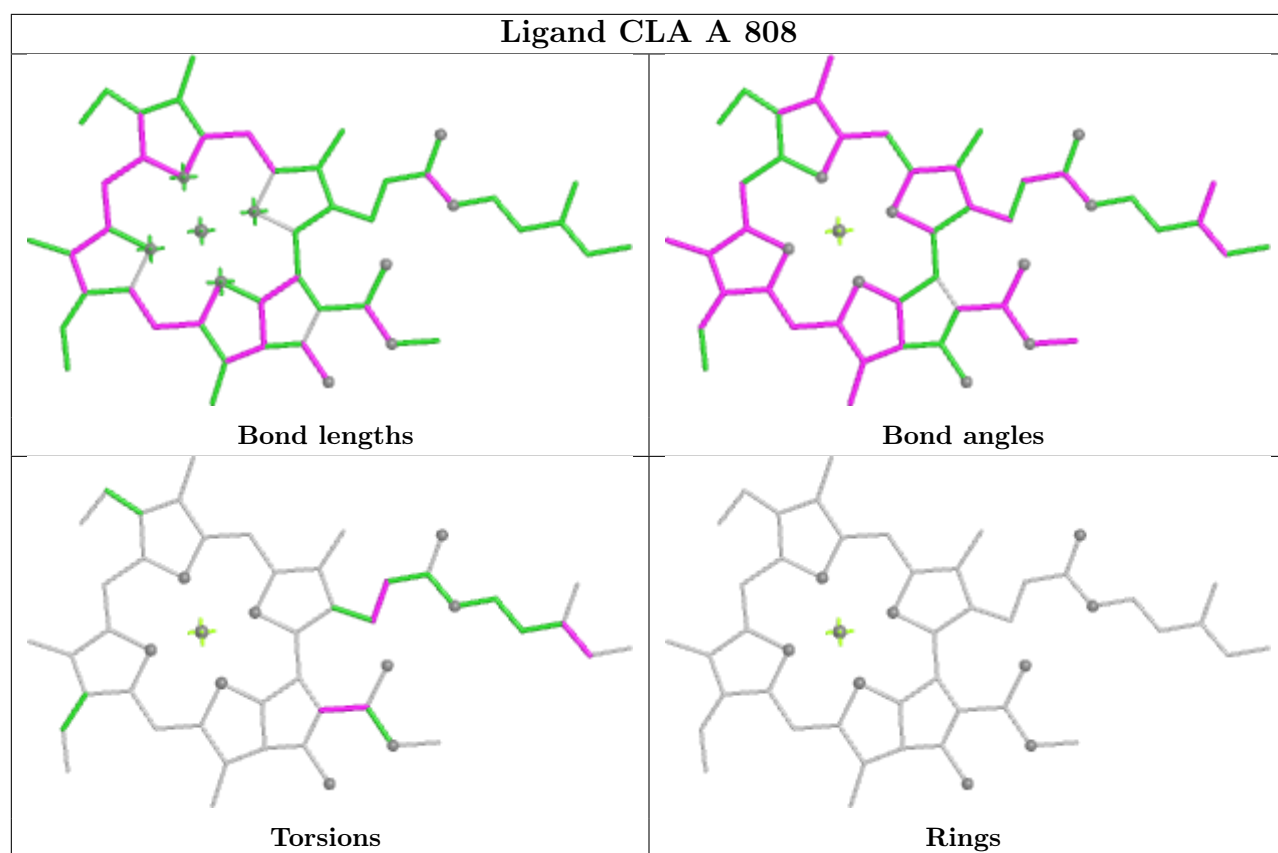


Torsions

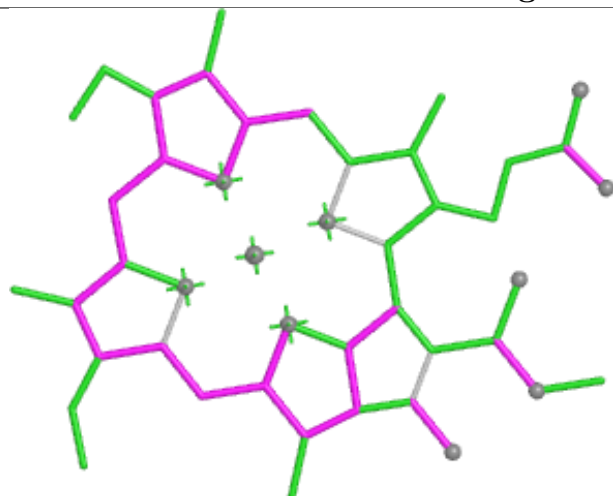


Rings

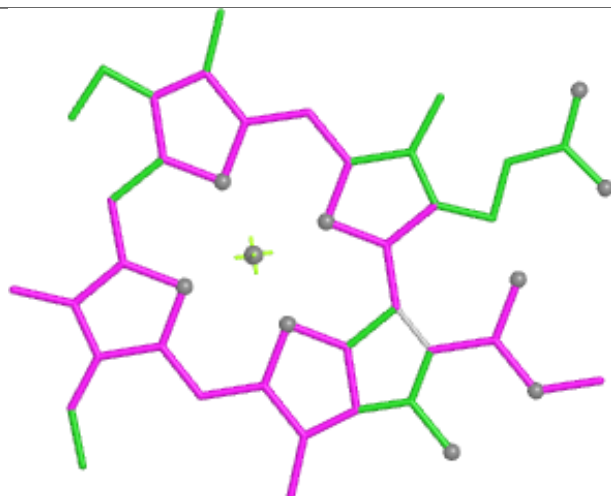




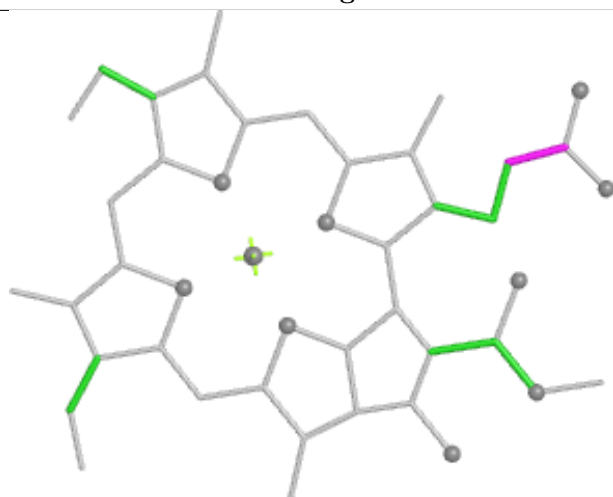
Ligand CLA 4 405



Bond lengths



Bond angles

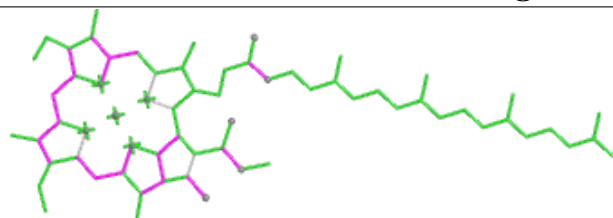


Torsions

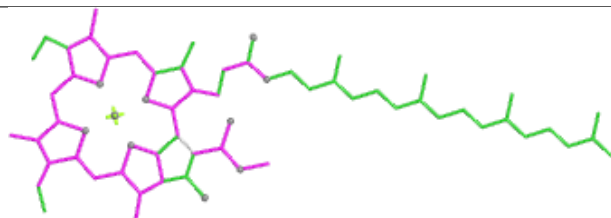


Rings

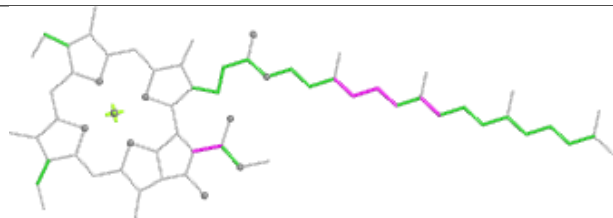
Ligand CLA B 838



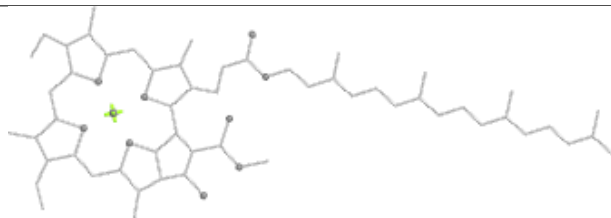
Bond lengths



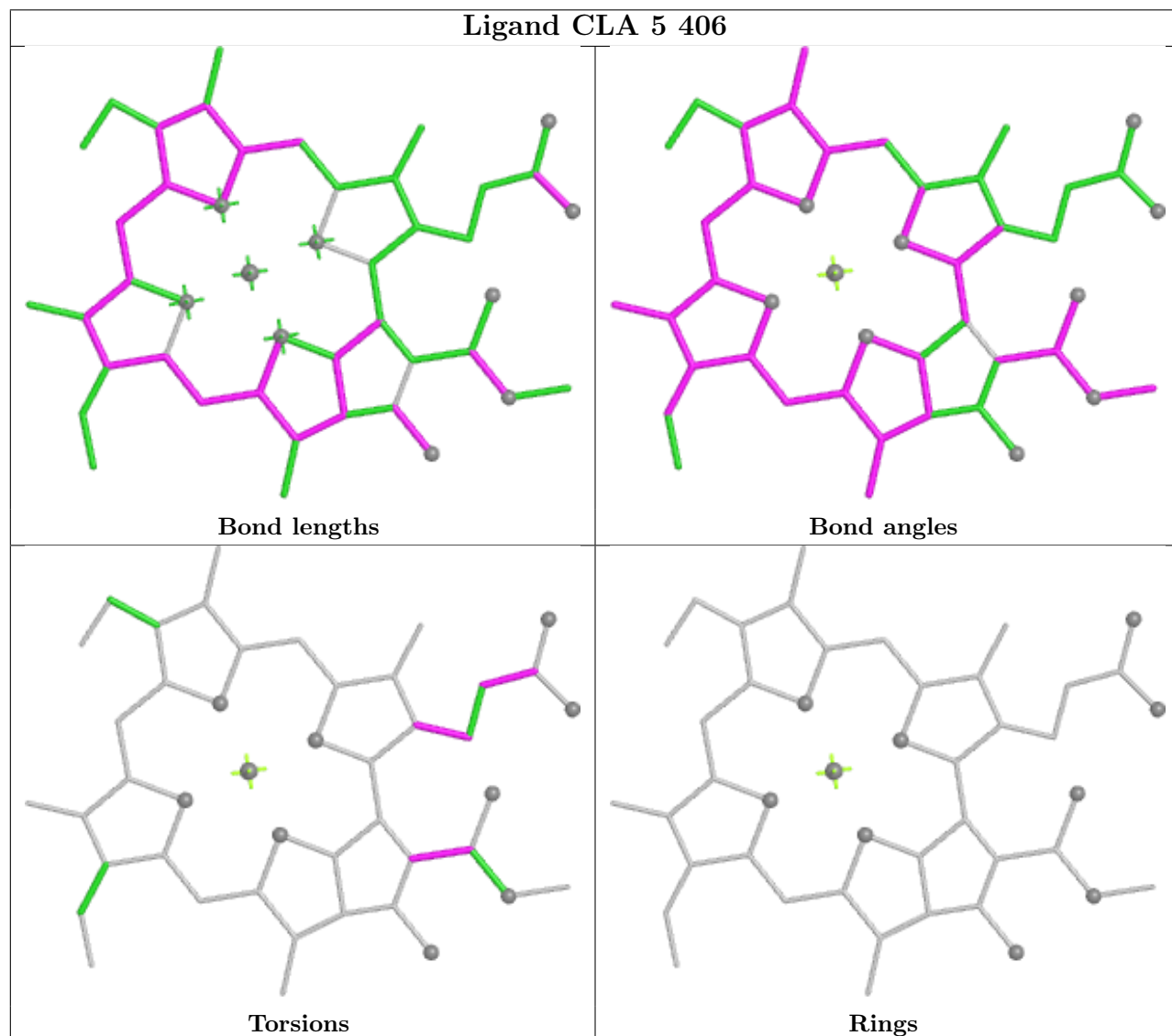
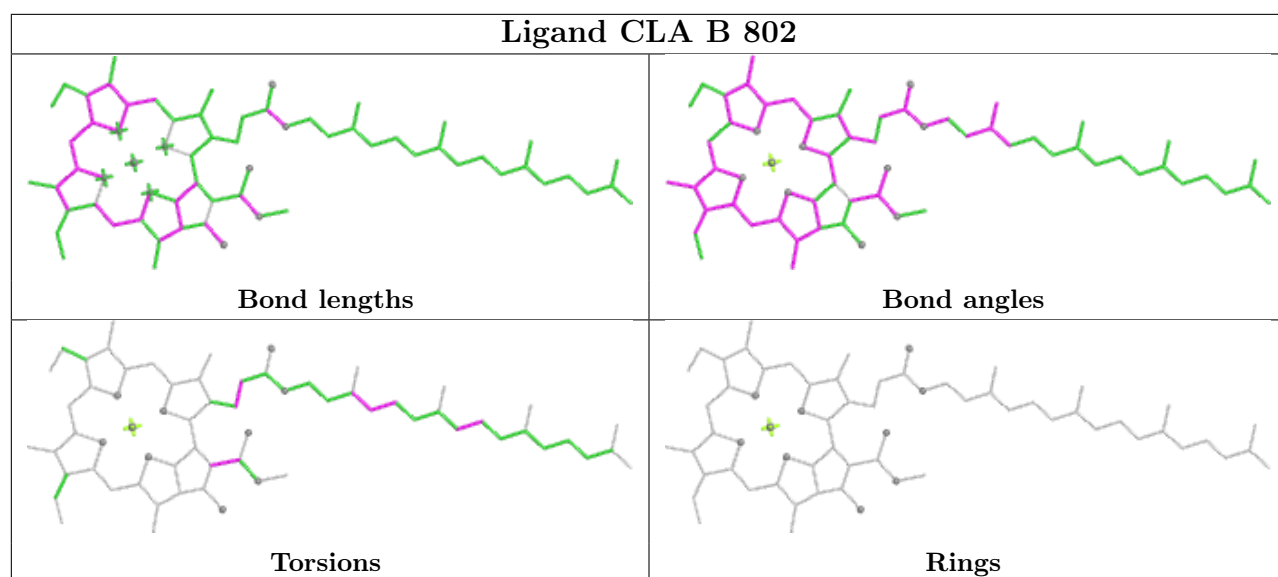
Bond angles



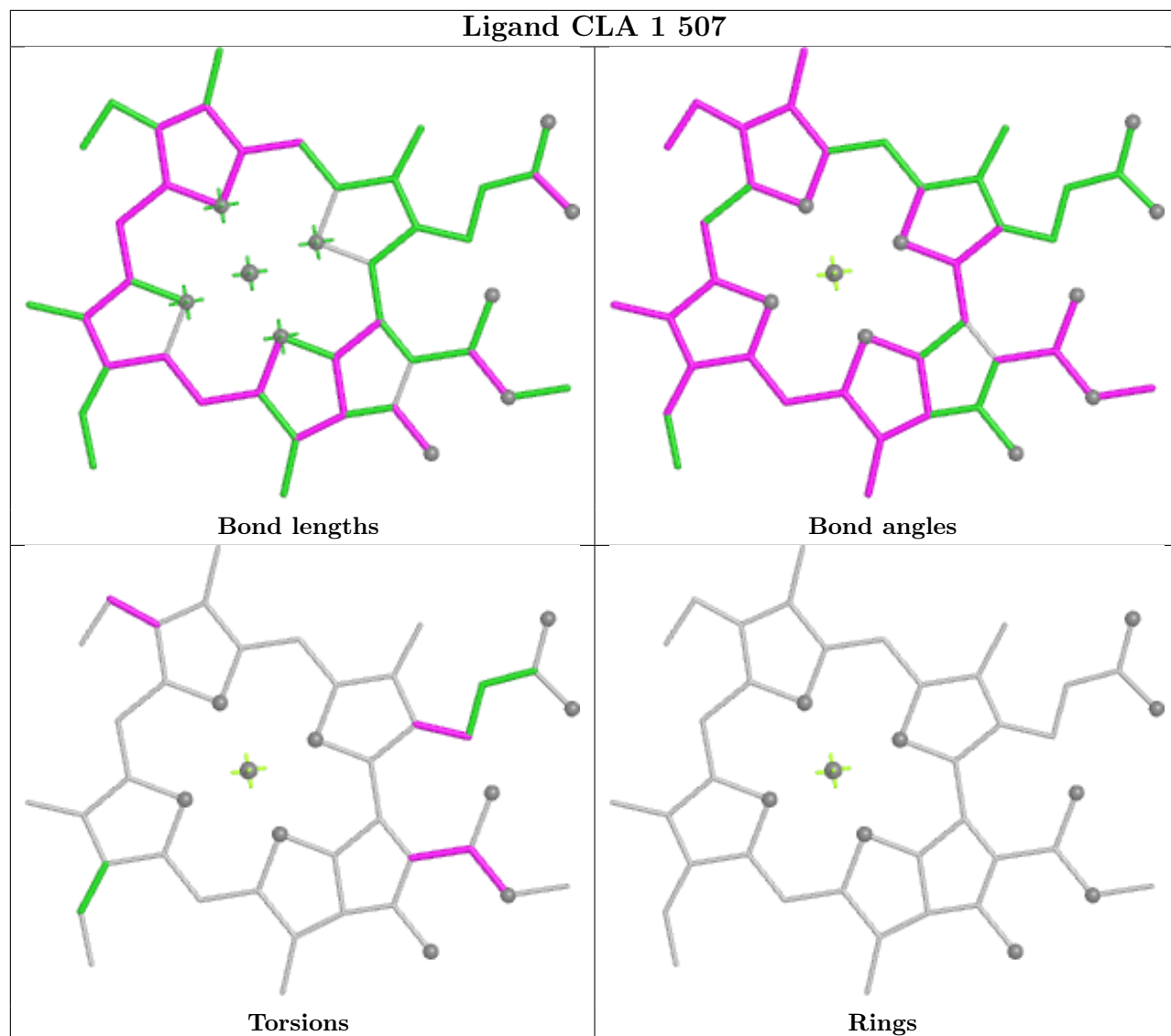
Torsions

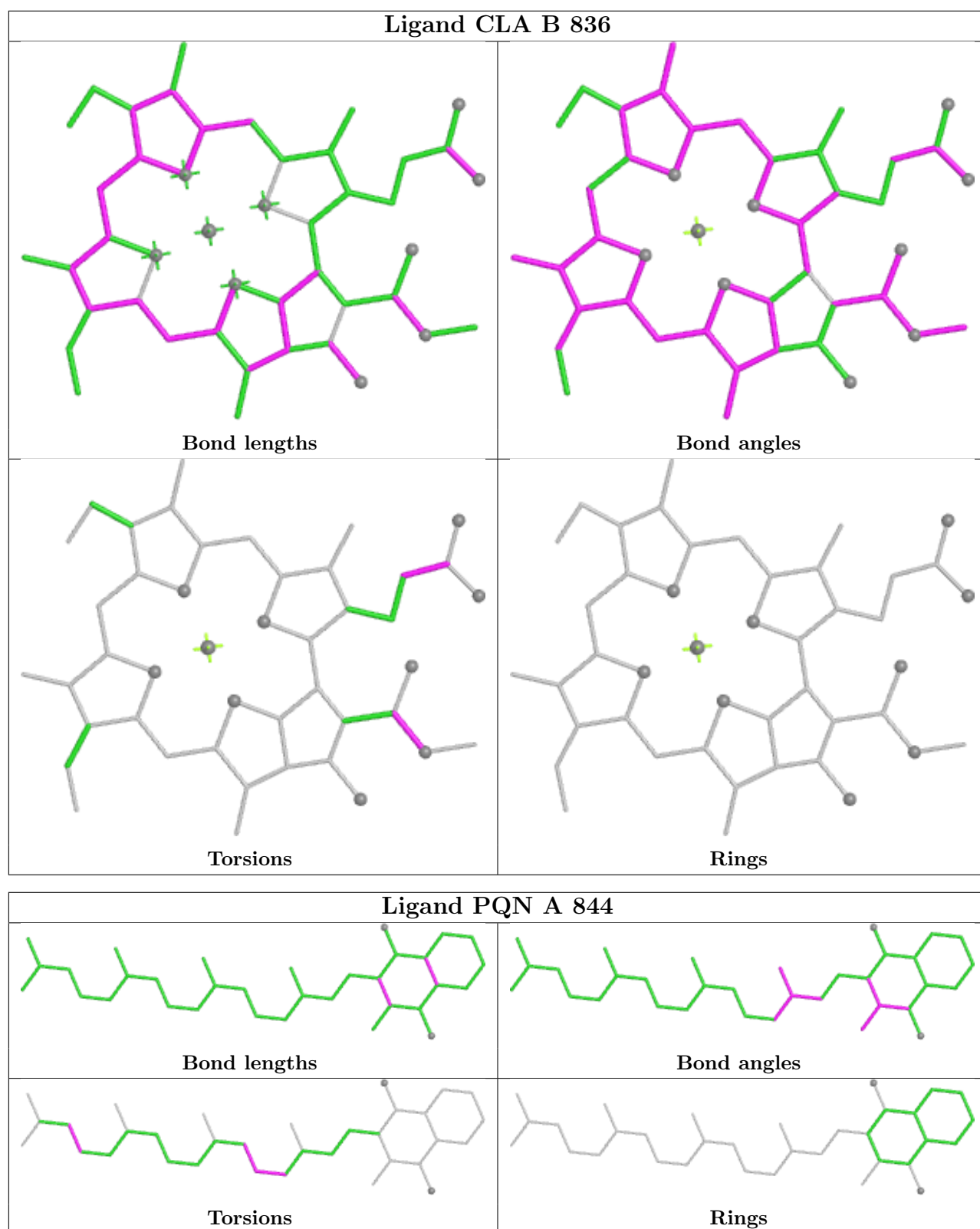


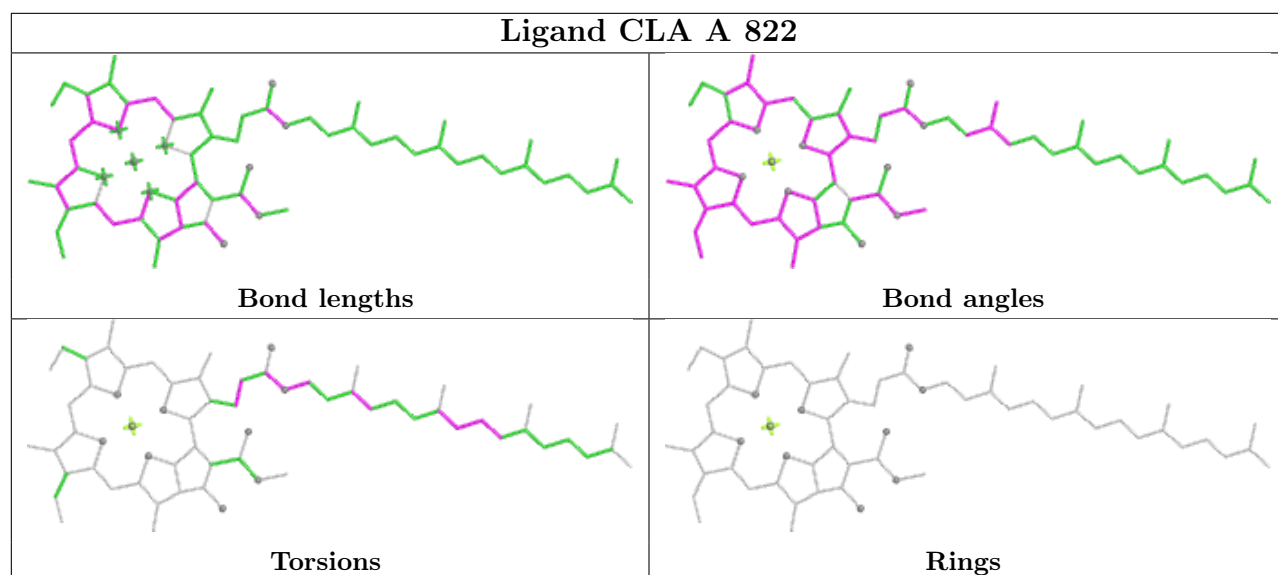
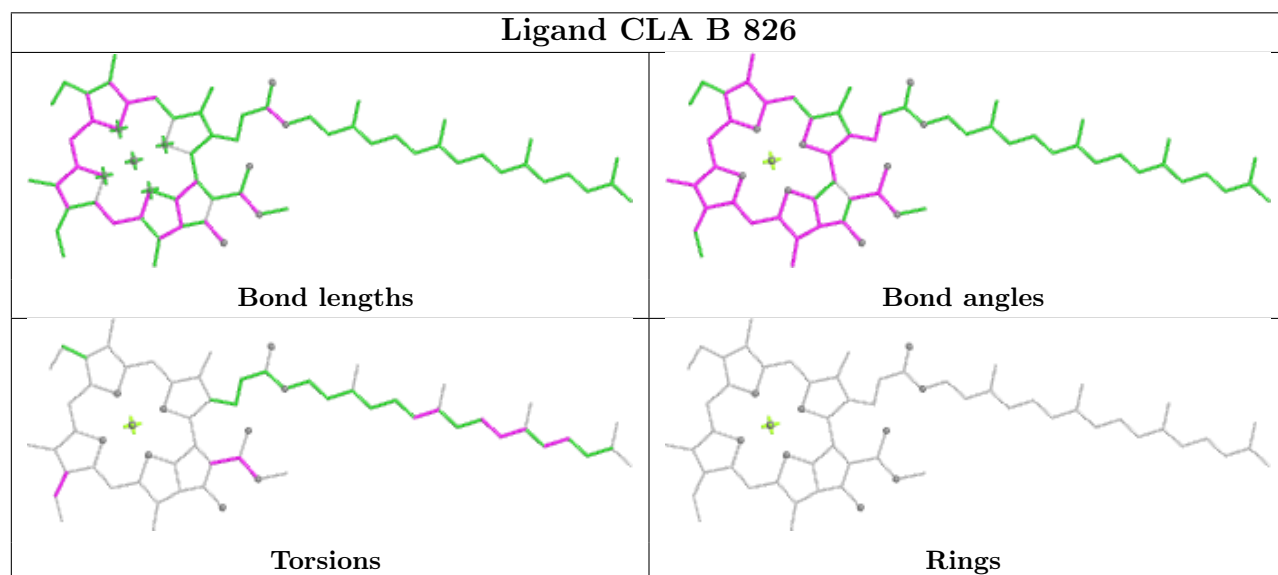
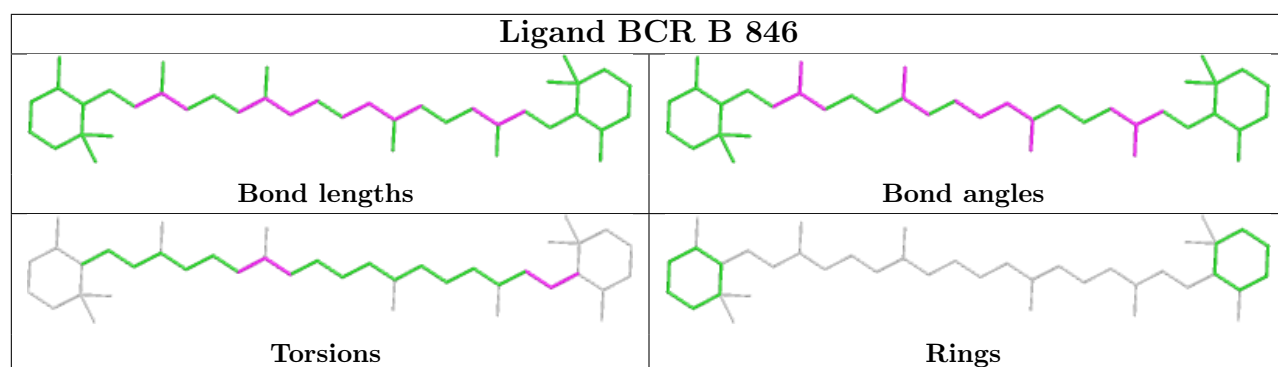
Rings



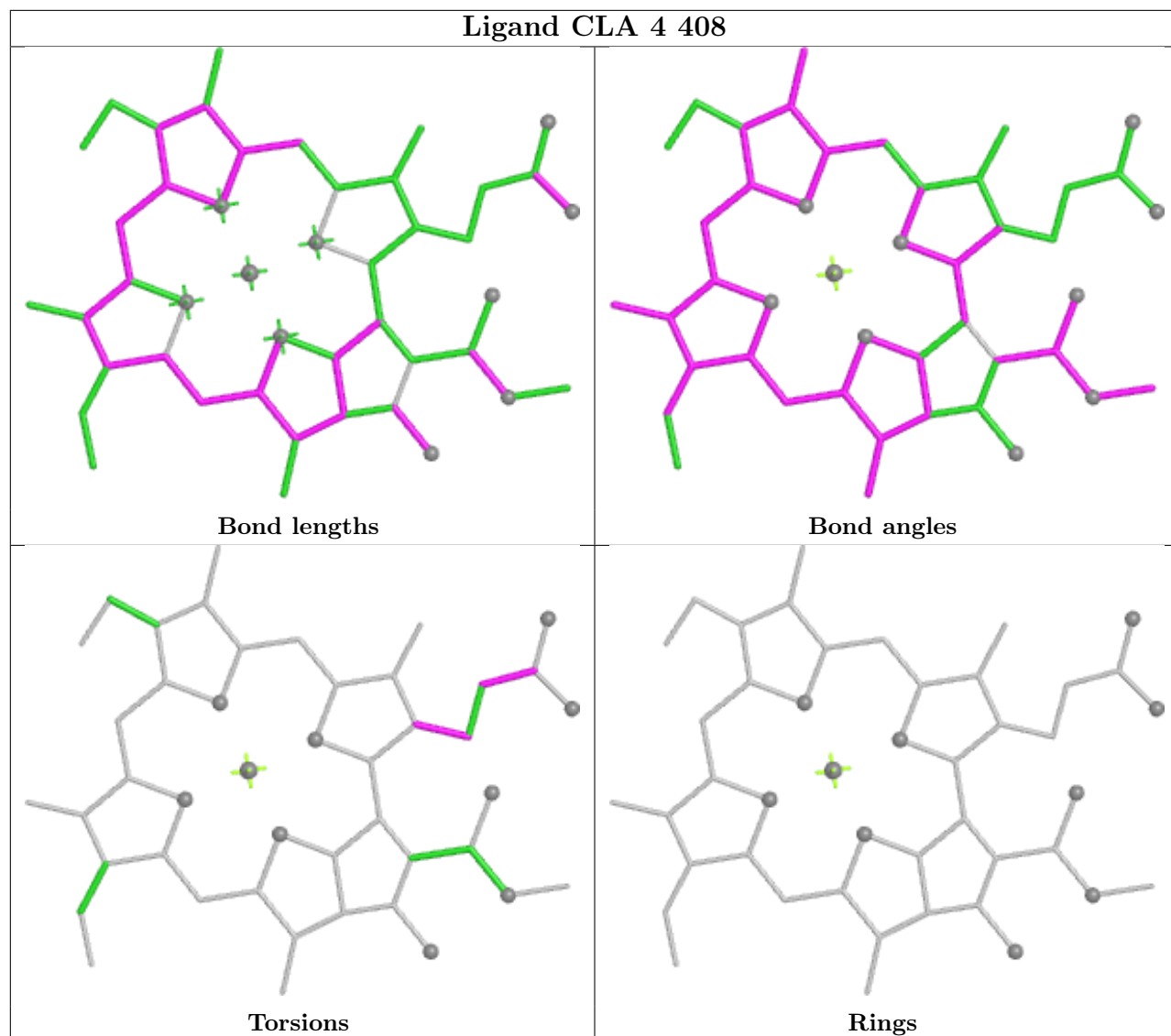
Ligand CLA 1 507



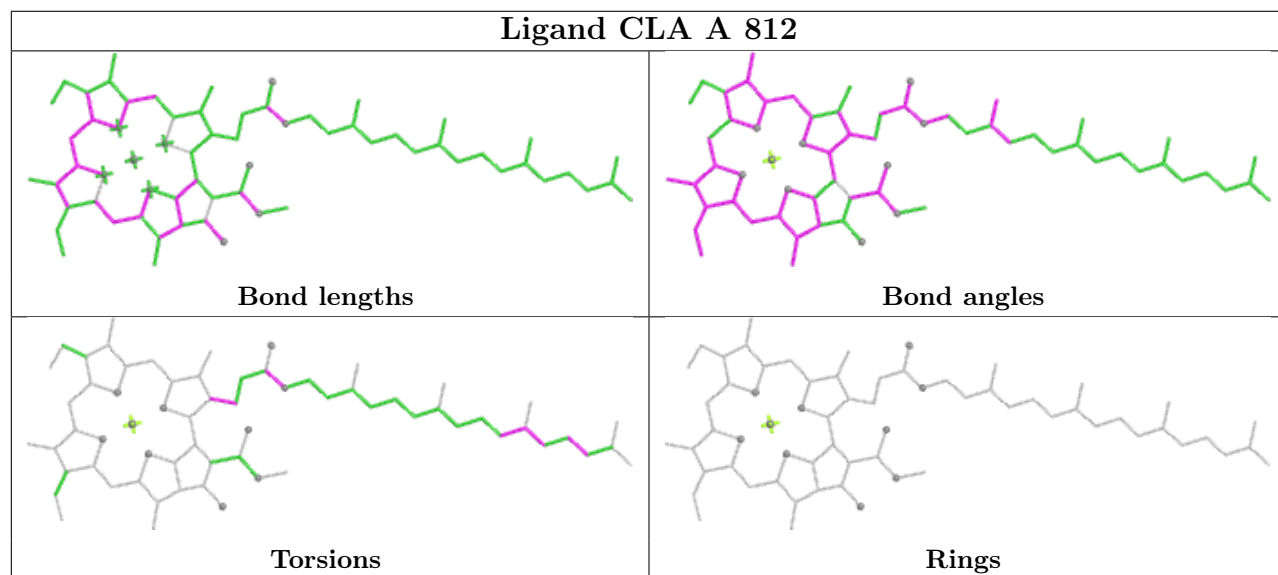


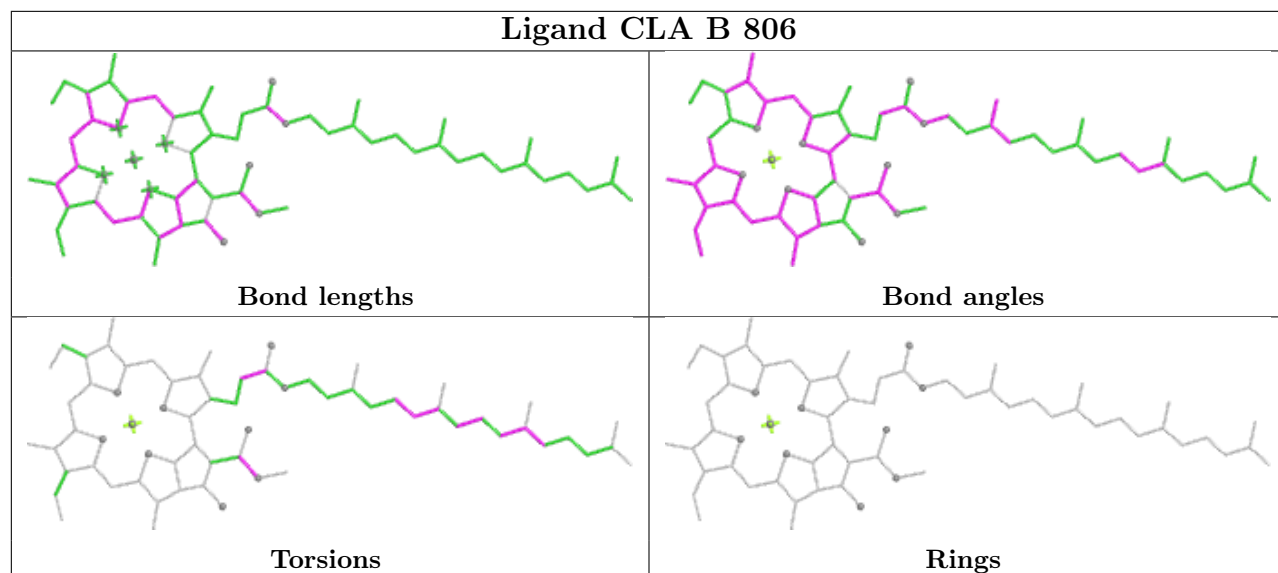
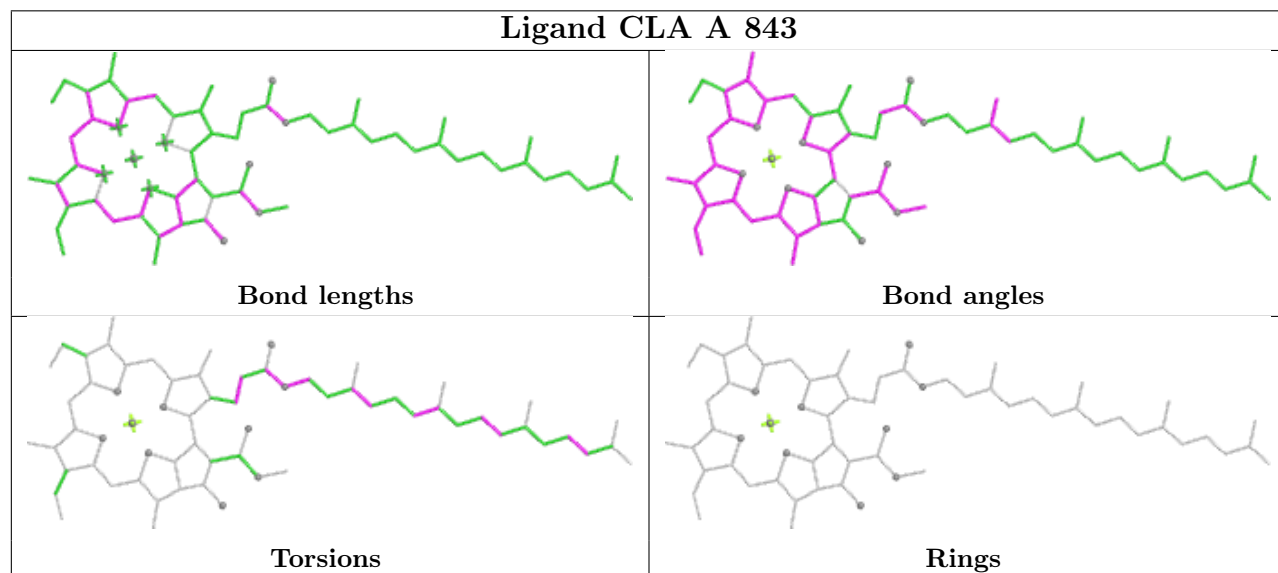
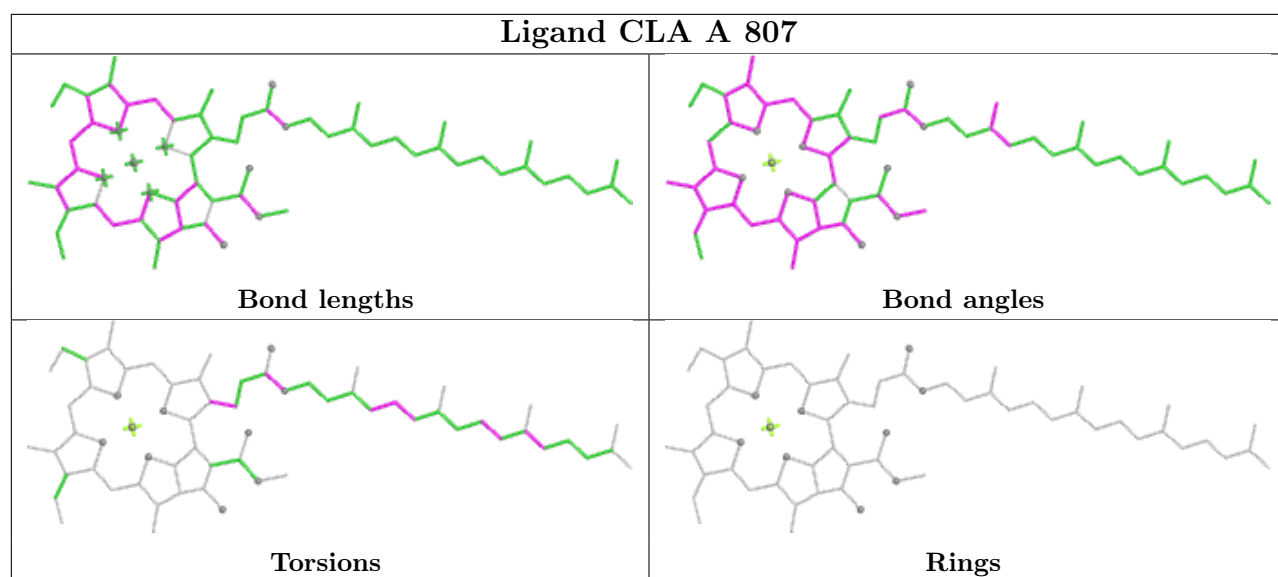


Ligand CLA 4 408

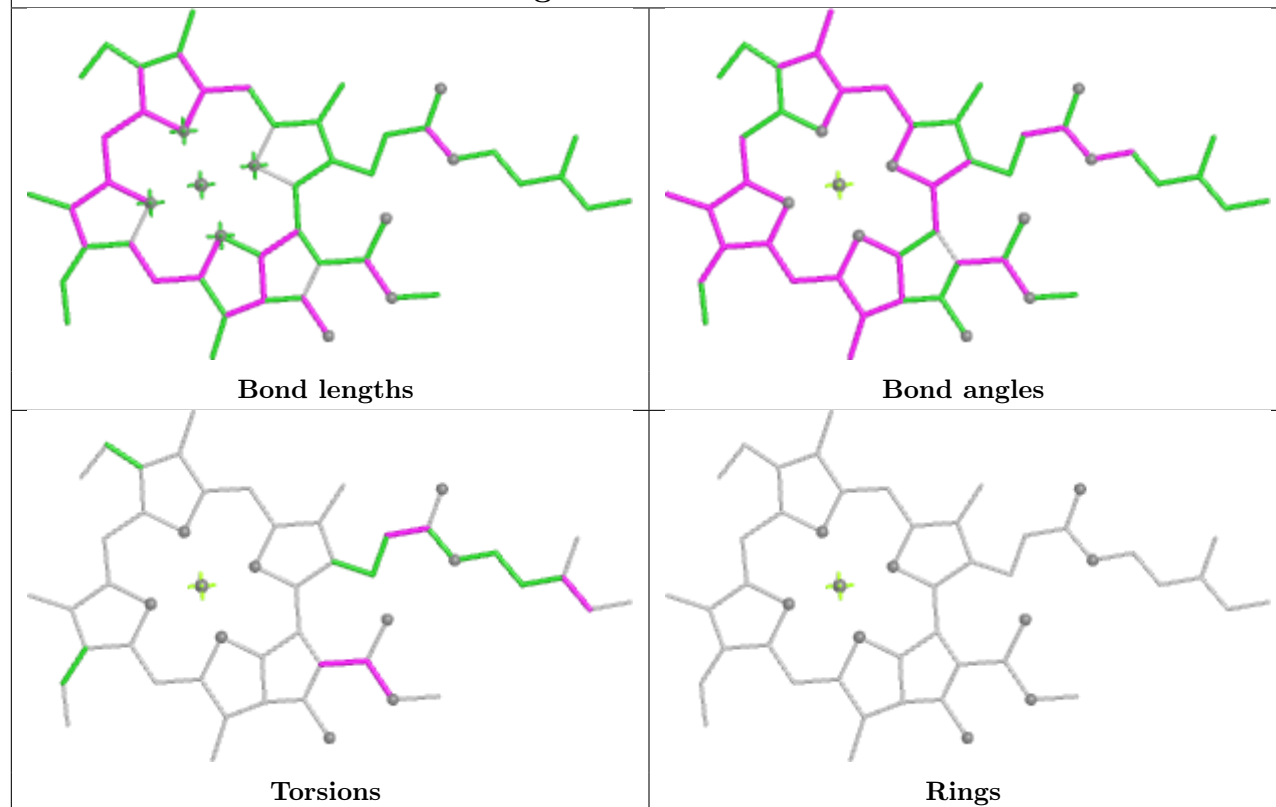


Ligand CLA A 812

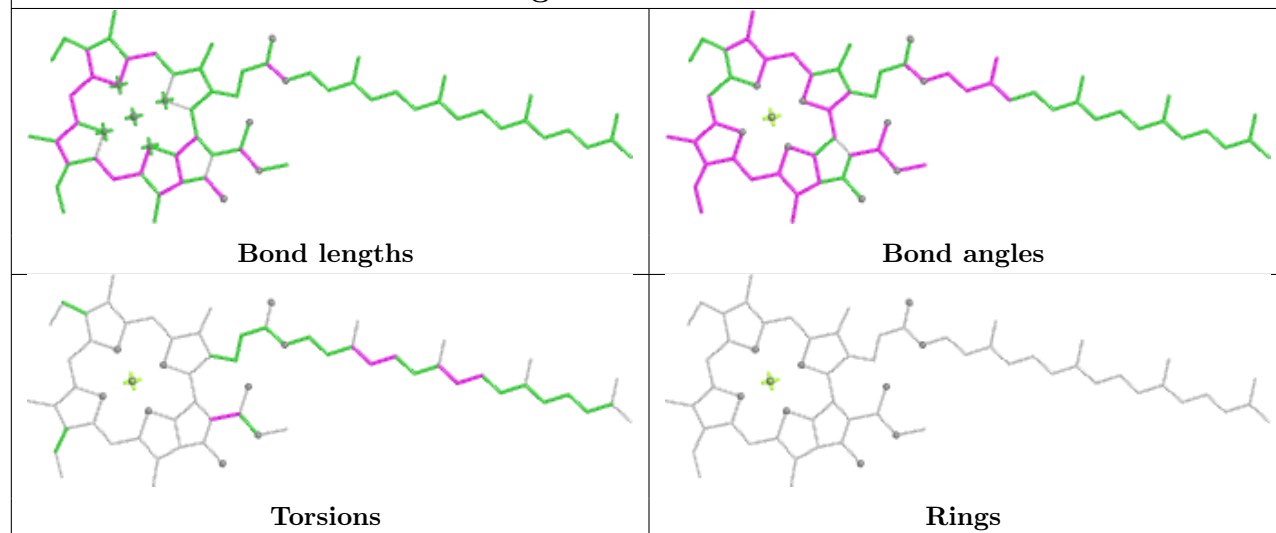


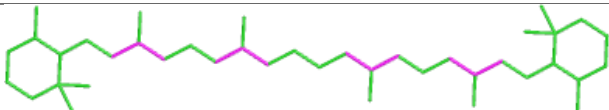
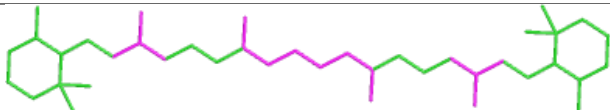
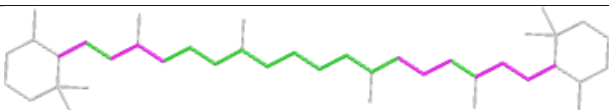
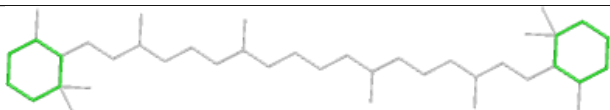


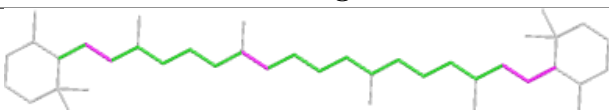
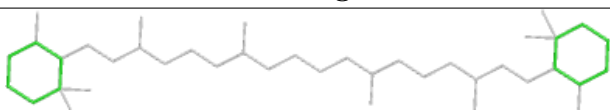
Ligand CLA F 201



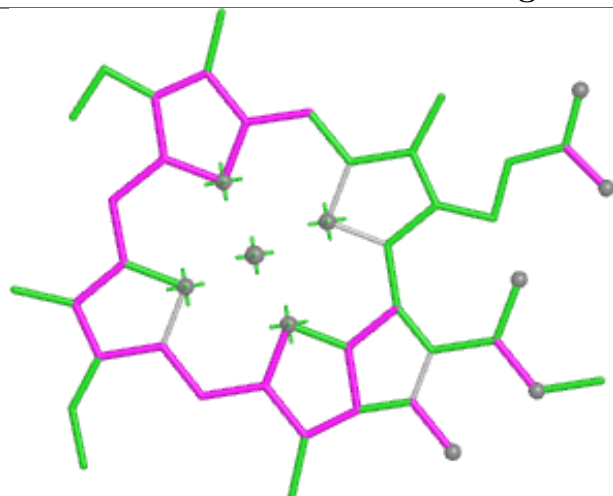
Ligand CLA A 834



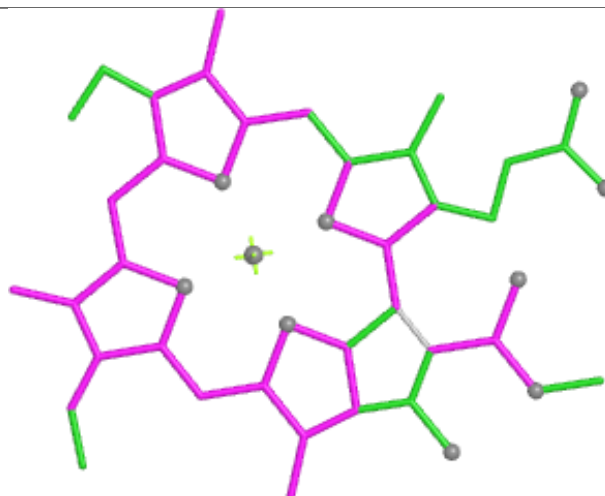
Ligand BCR K 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 5 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

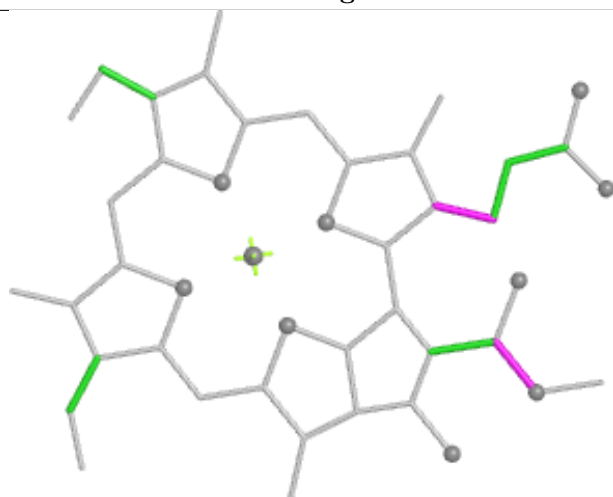
Ligand CLA 1 505



Bond lengths



Bond angles

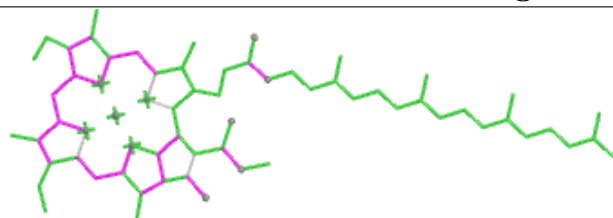


Torsions

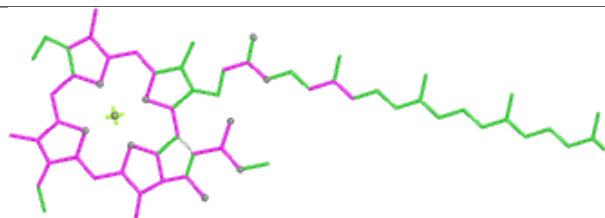


Rings

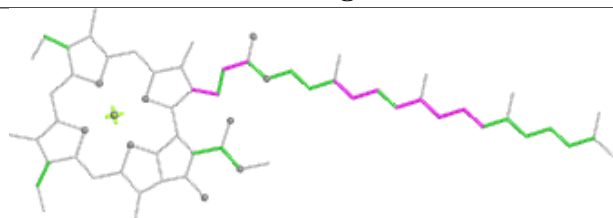
Ligand CLA B 827



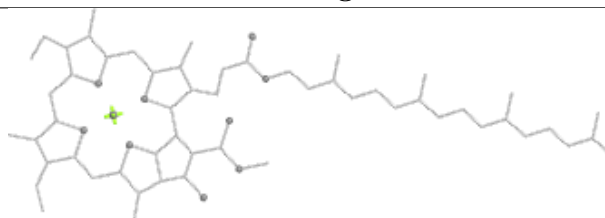
Bond lengths



Bond angles

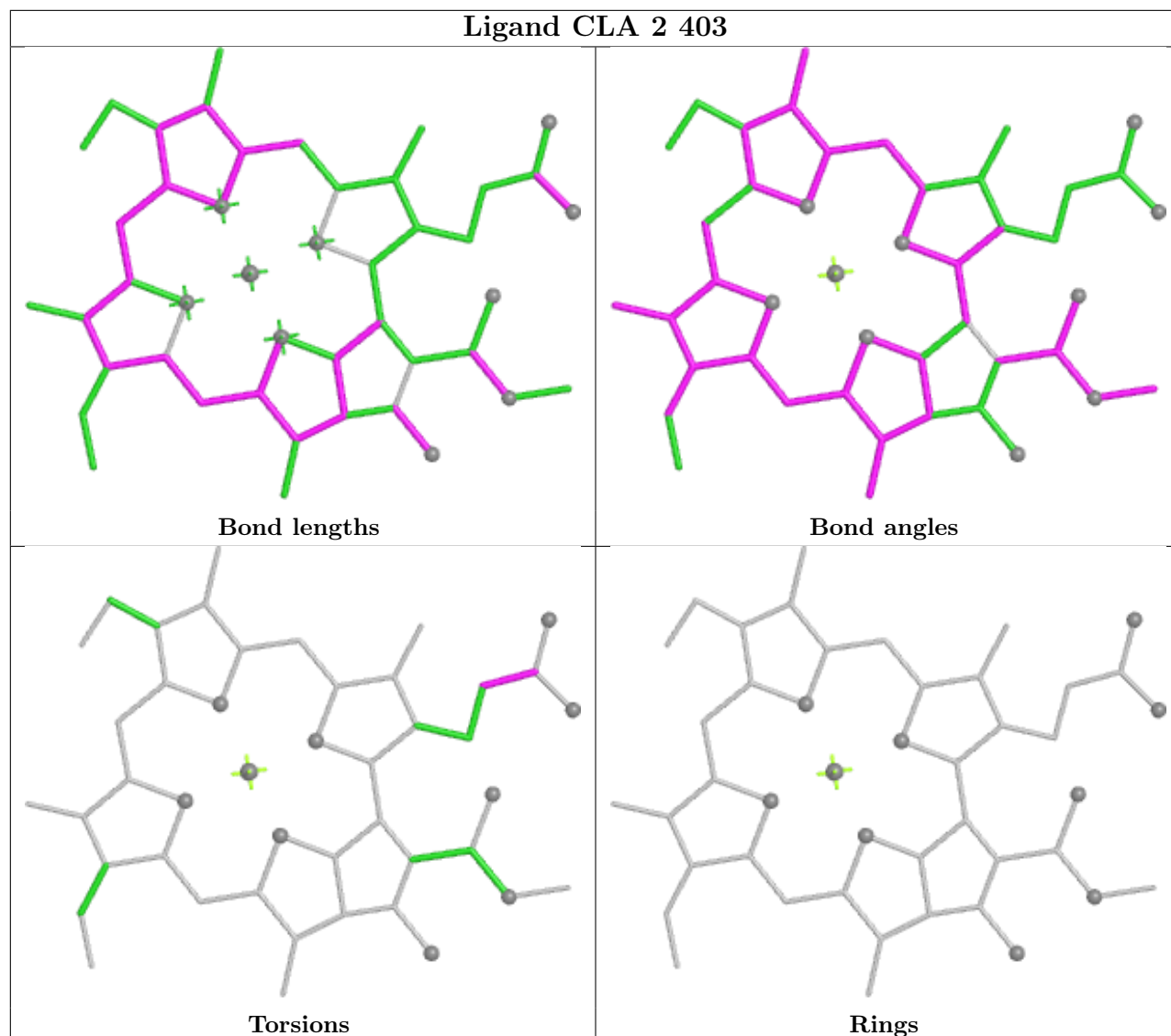


Torsions

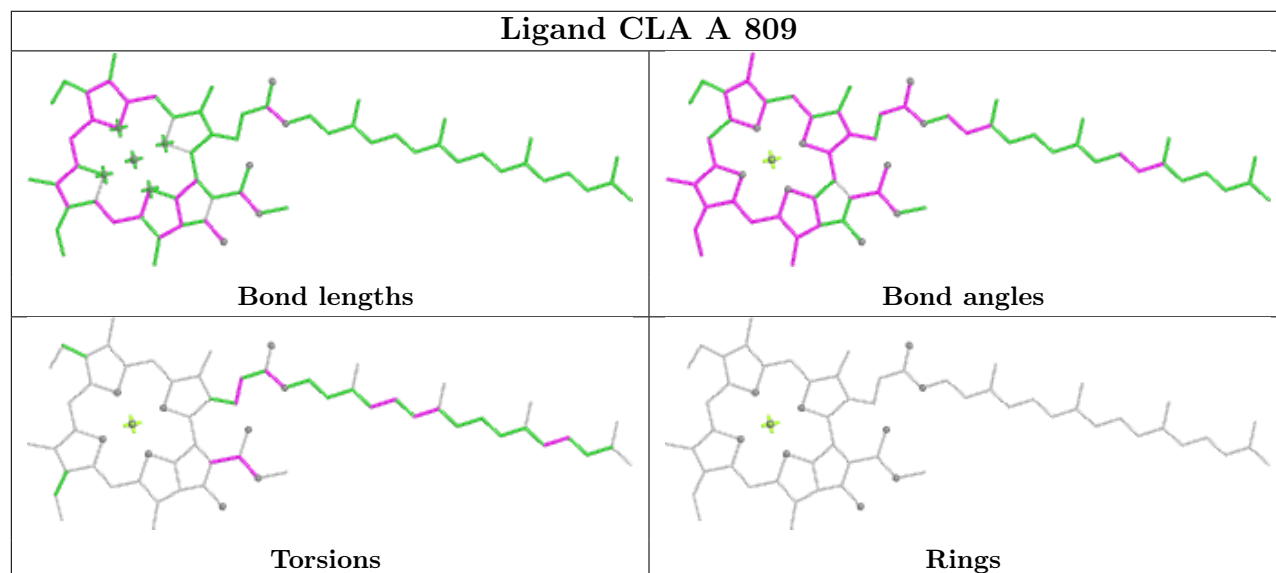


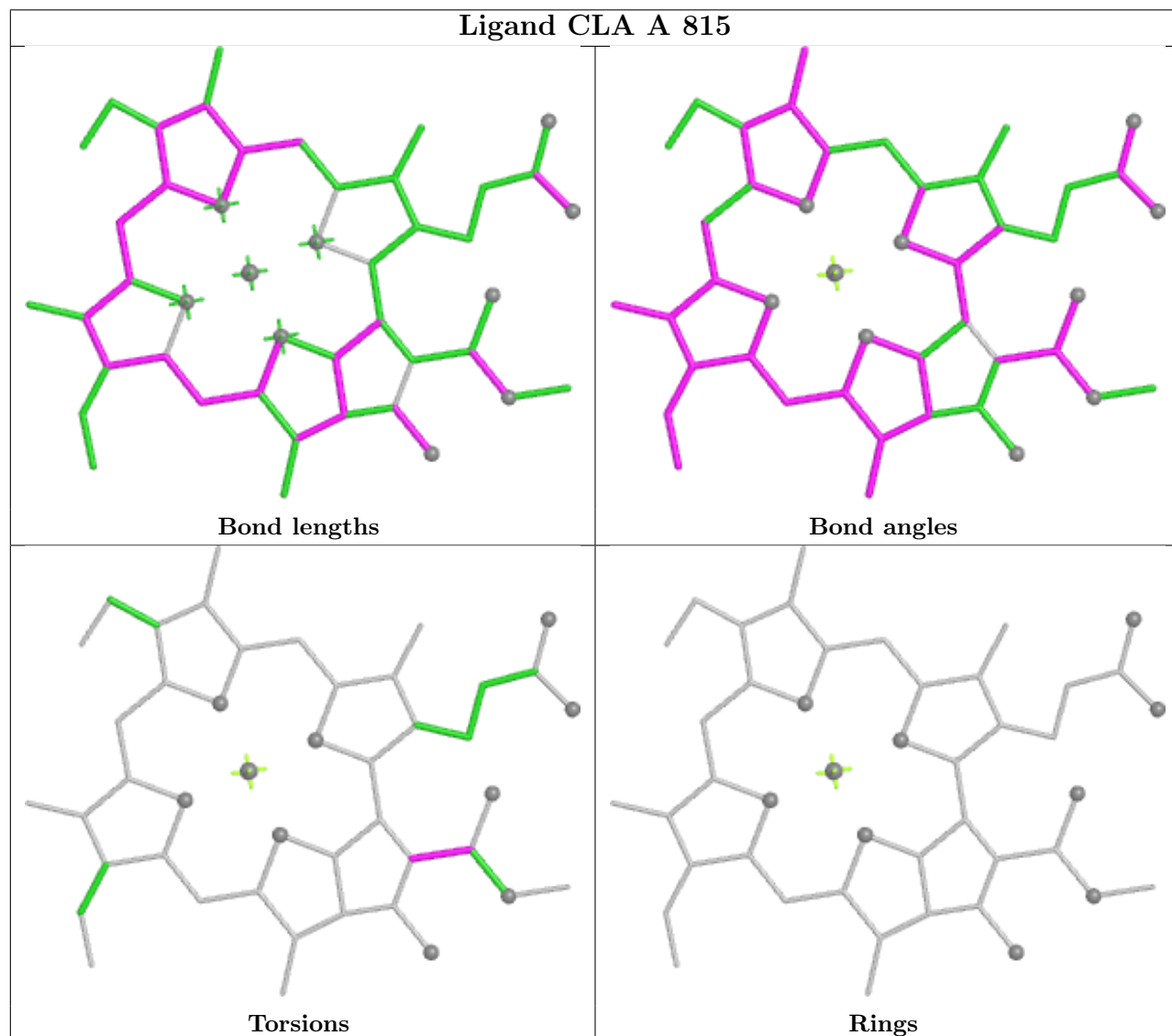
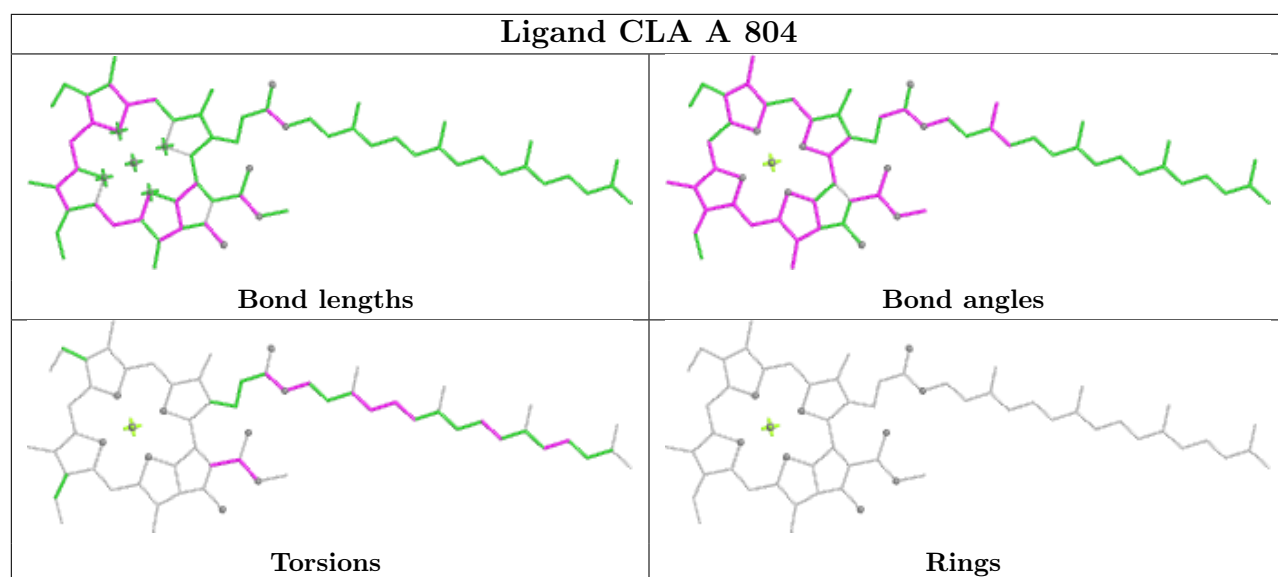
Rings

Ligand CLA 2 403

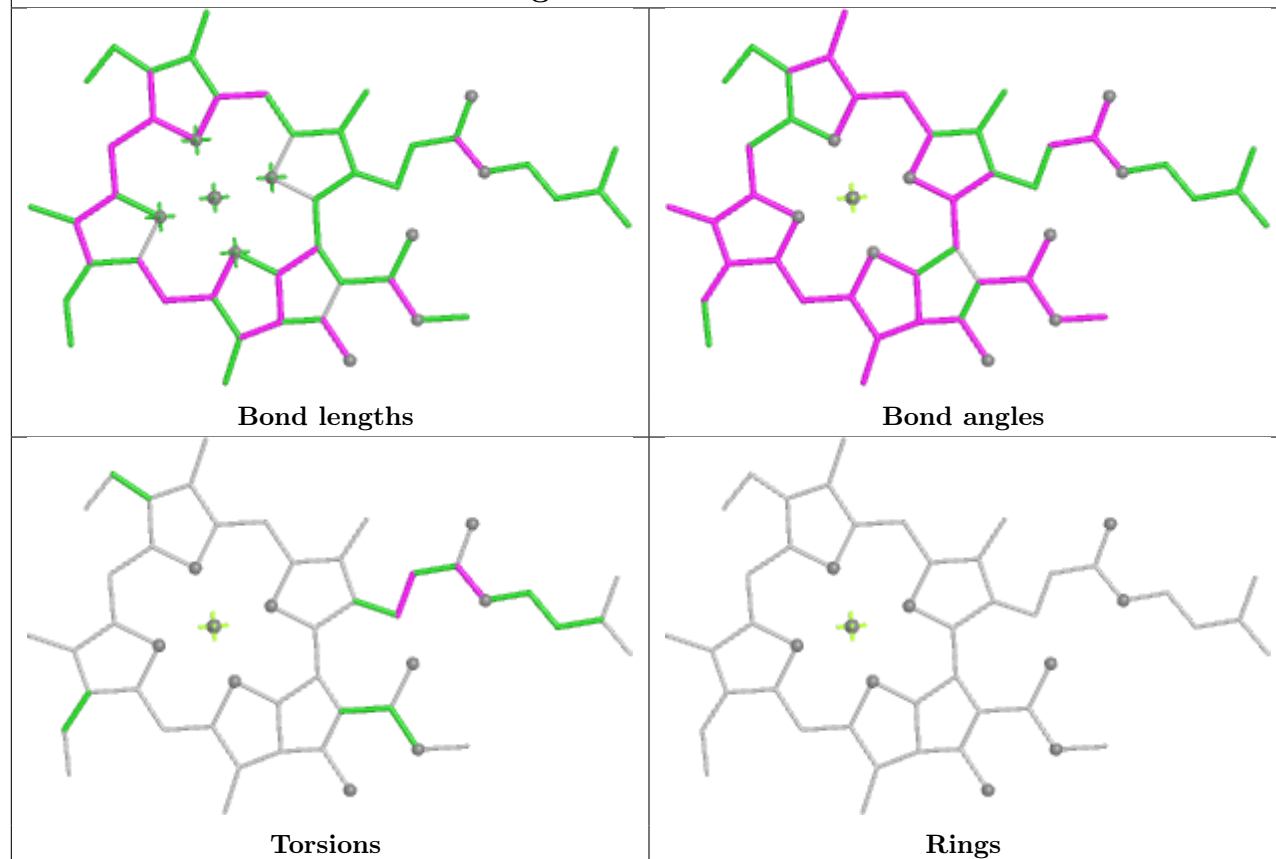


Ligand CLA A 809

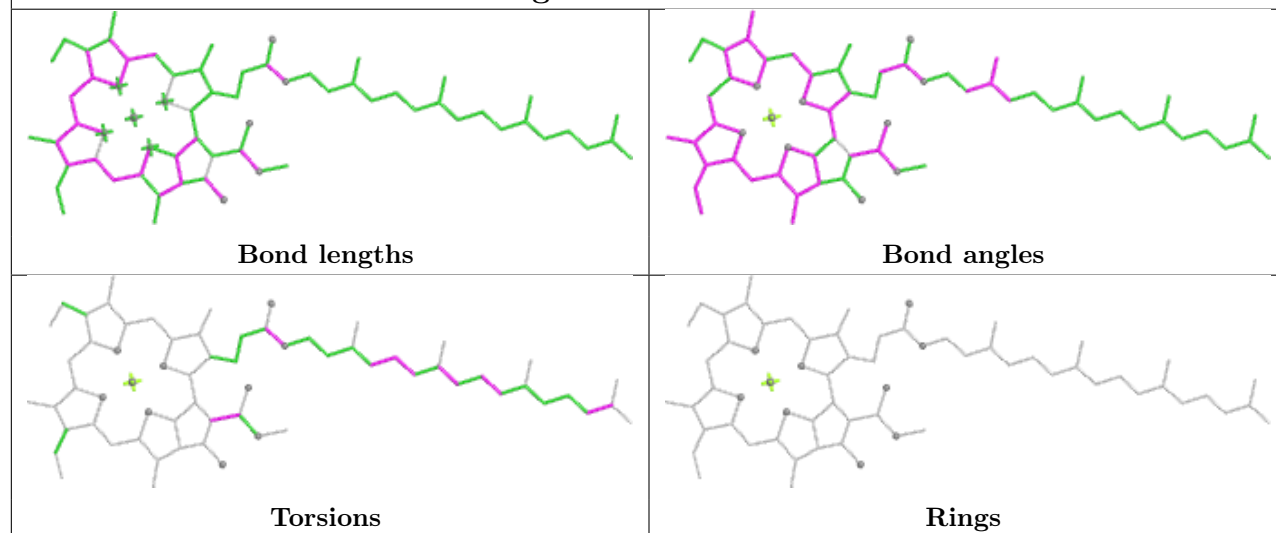




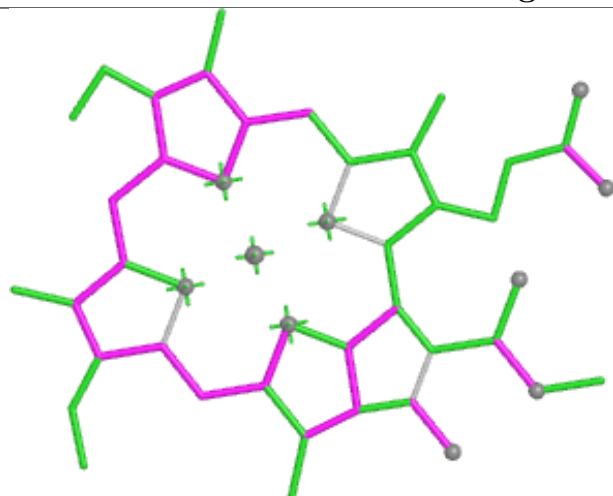
Ligand CLA A 832



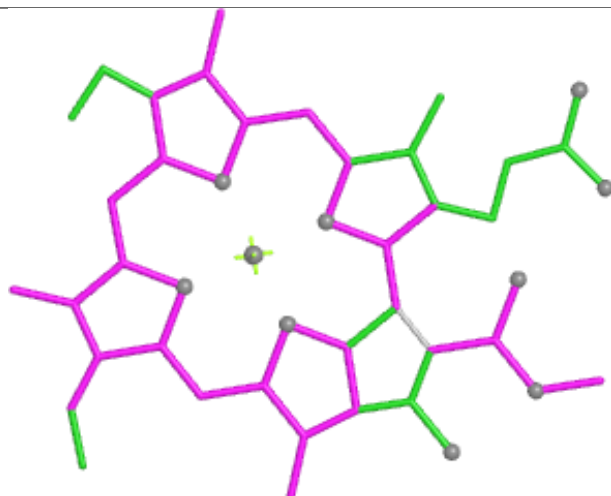
Ligand CLA B 839



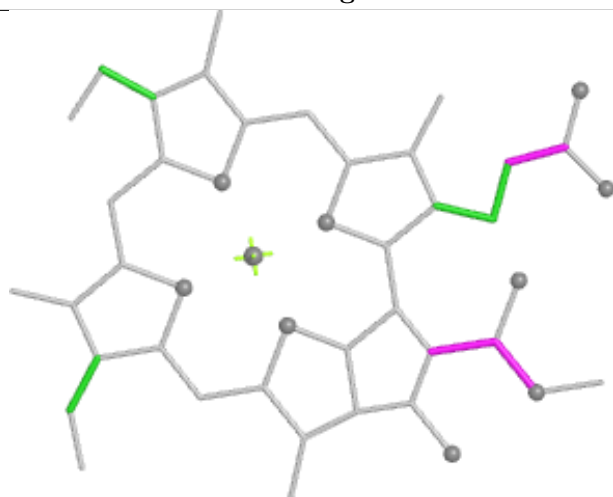
Ligand CLA 4 407



Bond lengths



Bond angles

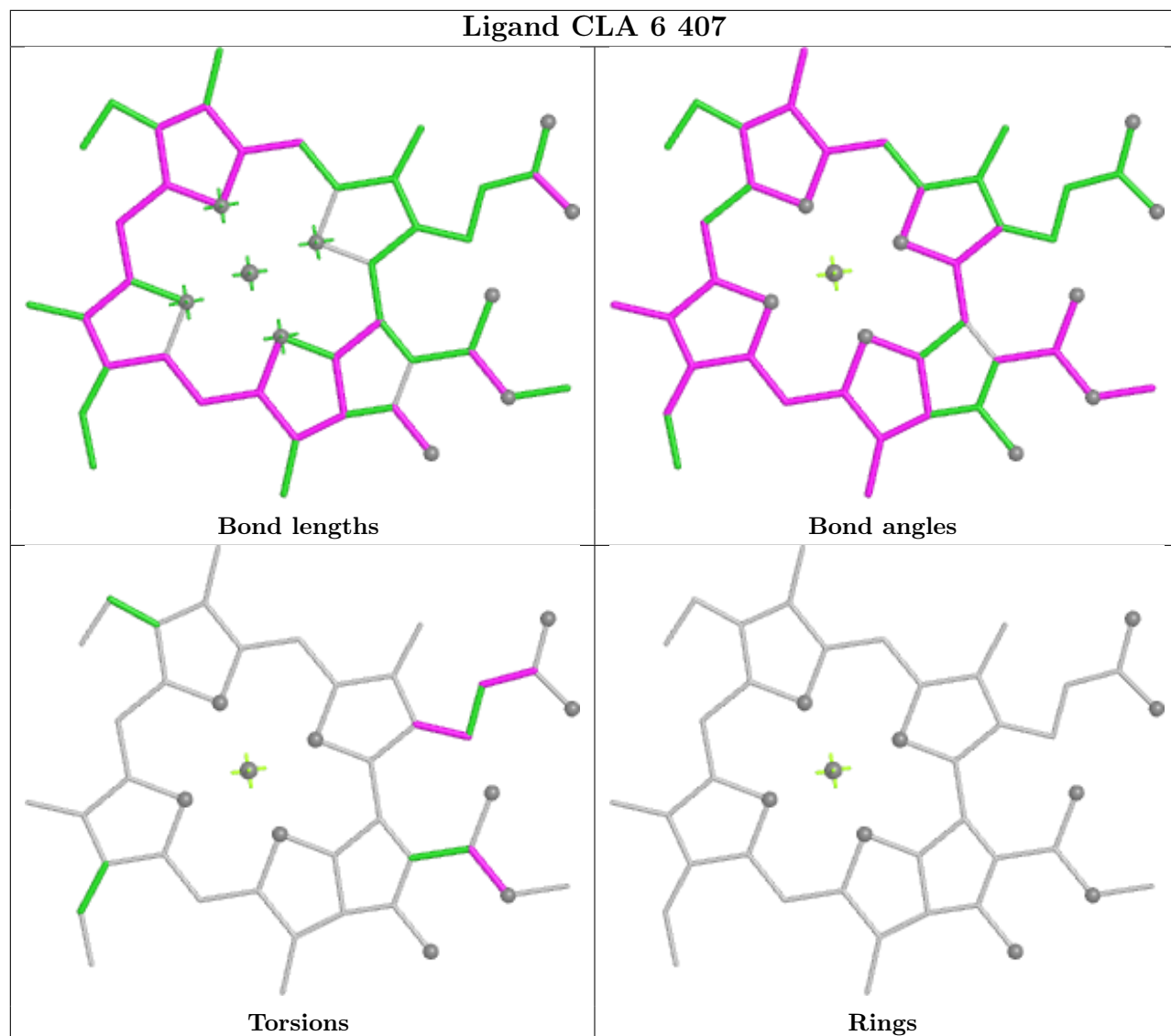


Torsions

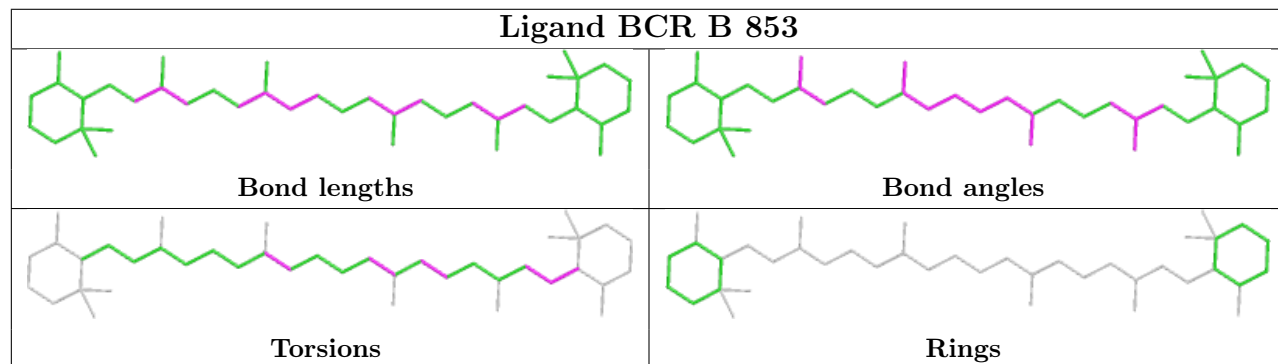


Rings

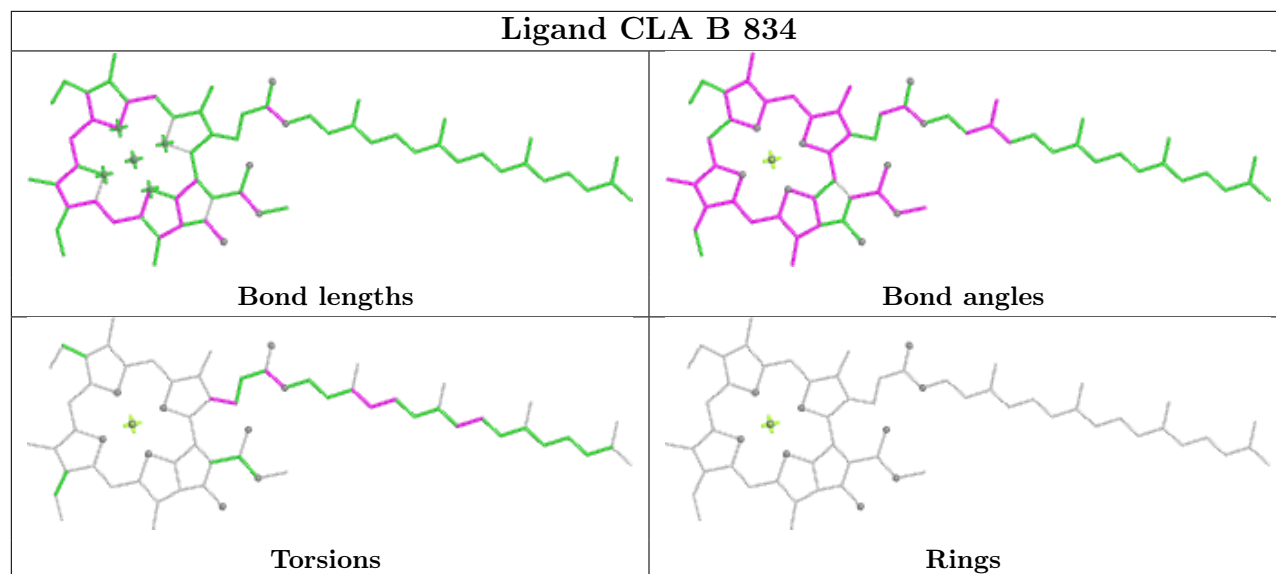
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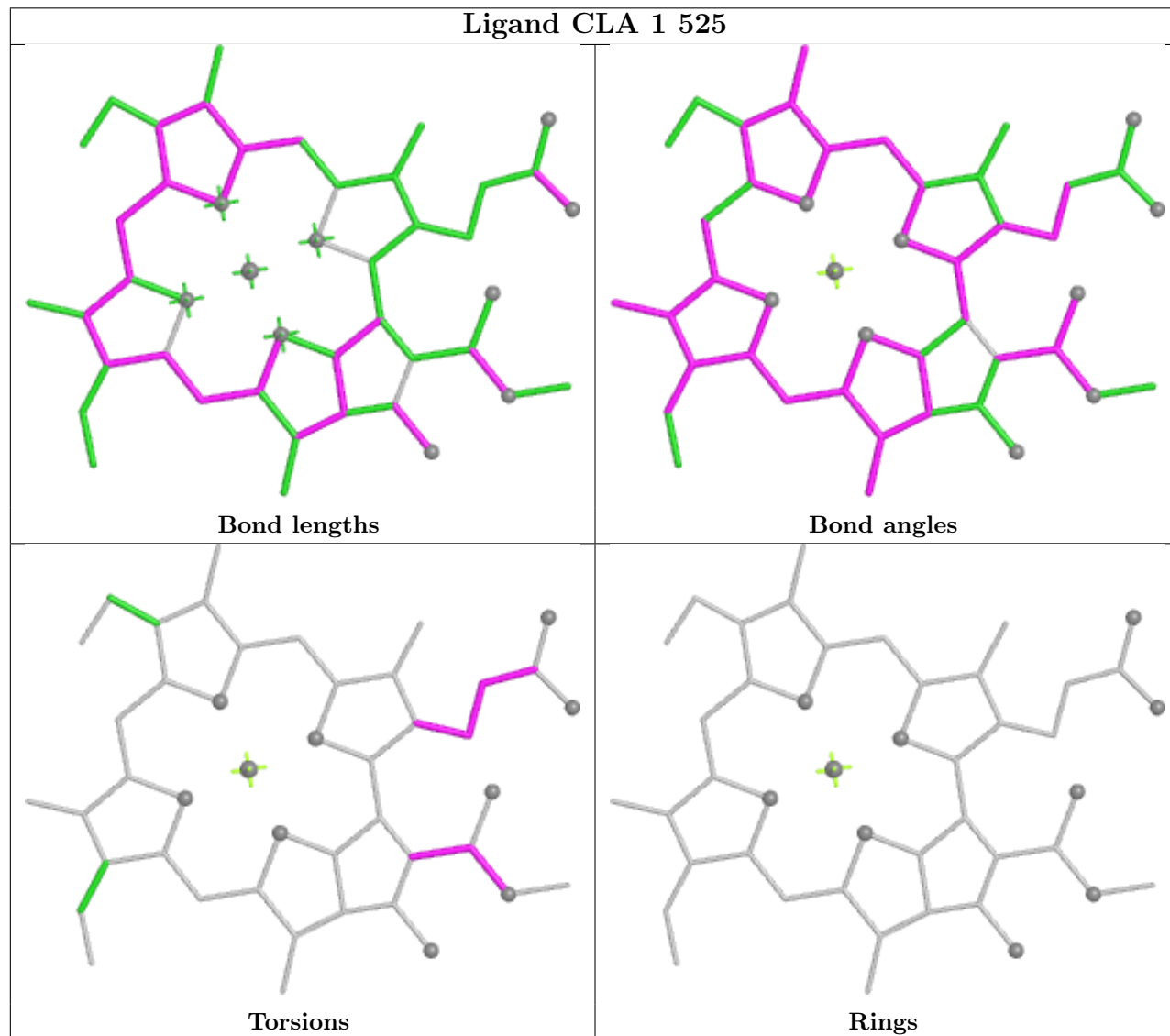
Ligand BCR B 853

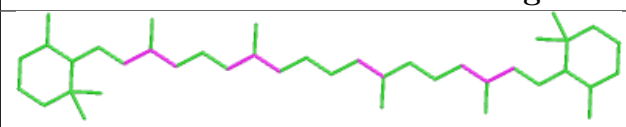
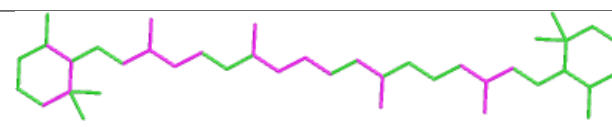
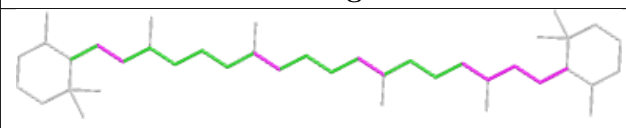
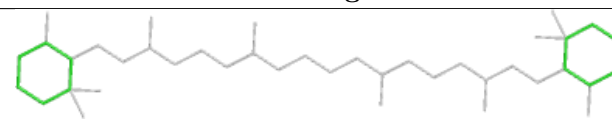
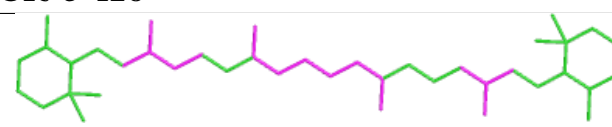
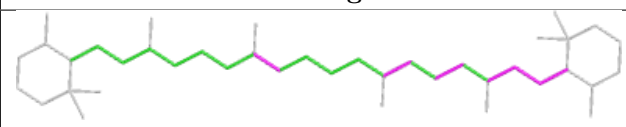
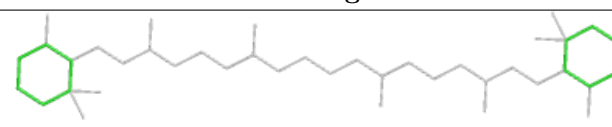
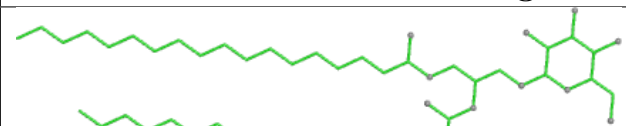
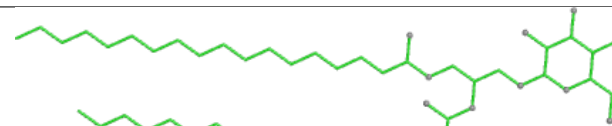
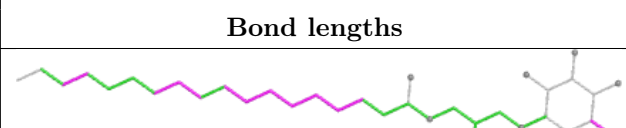
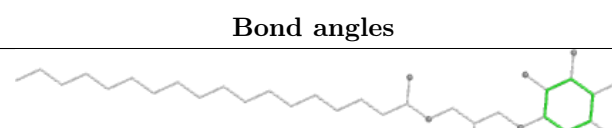
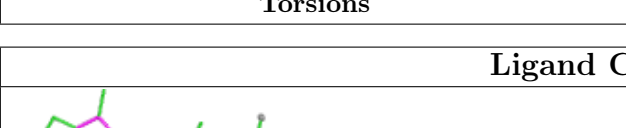


Ligand CLA B 834

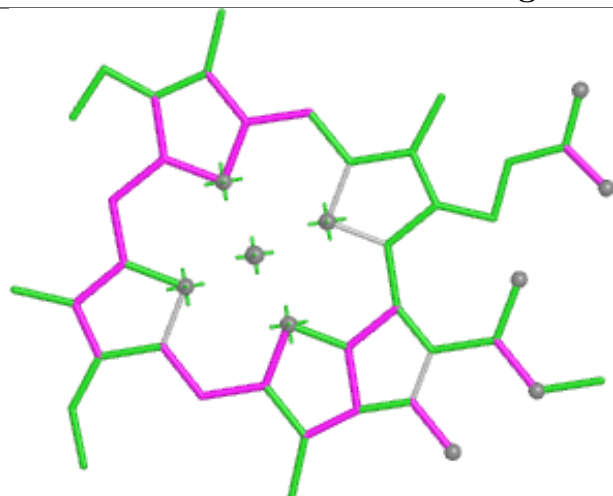


Ligand CLA 1 525

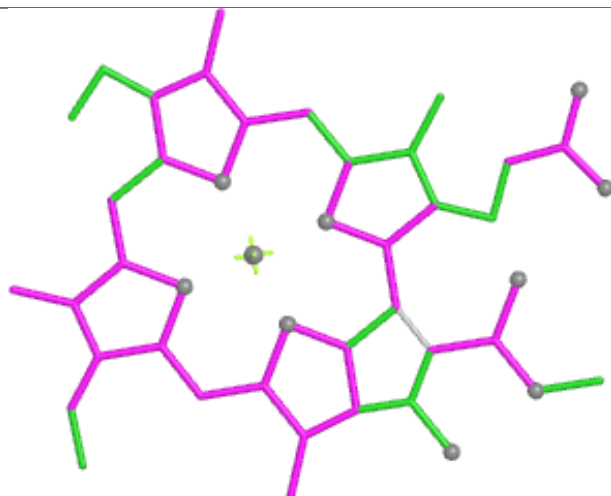


Ligand BCR 1 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 5 420	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 849	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

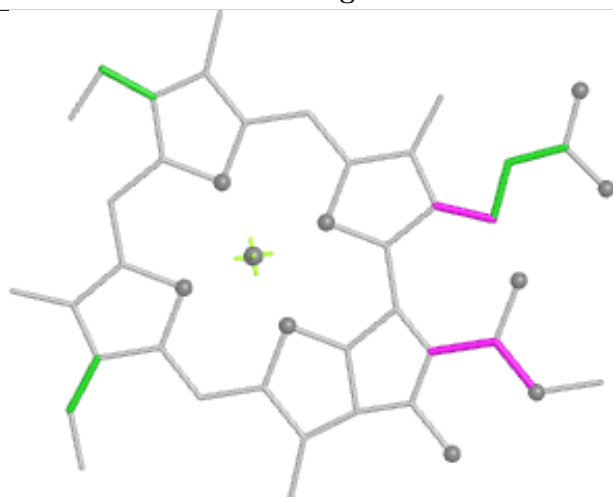
Ligand CLA 1 509



Bond lengths



Bond angles

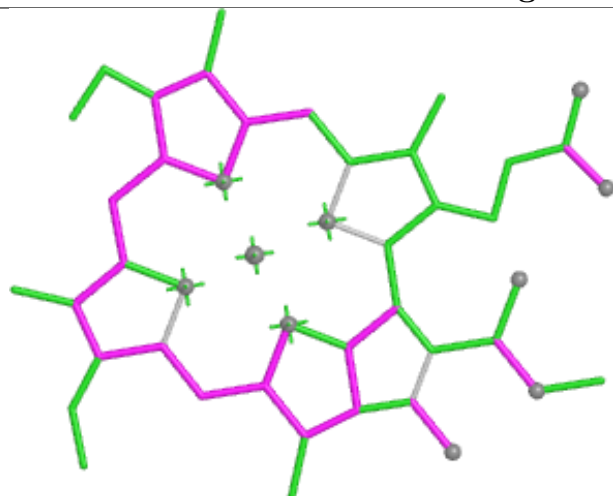


Torsions

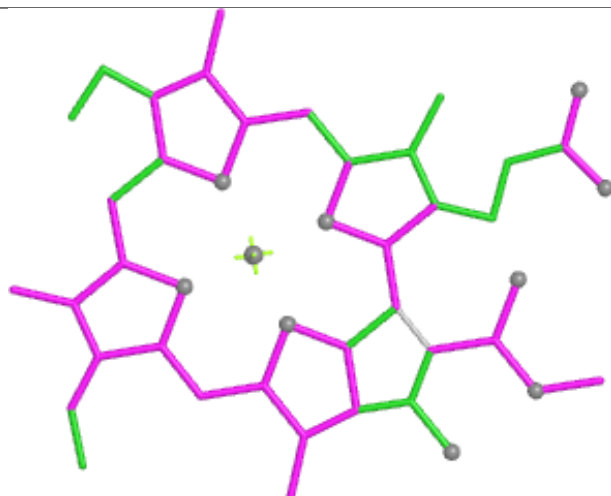


Rings

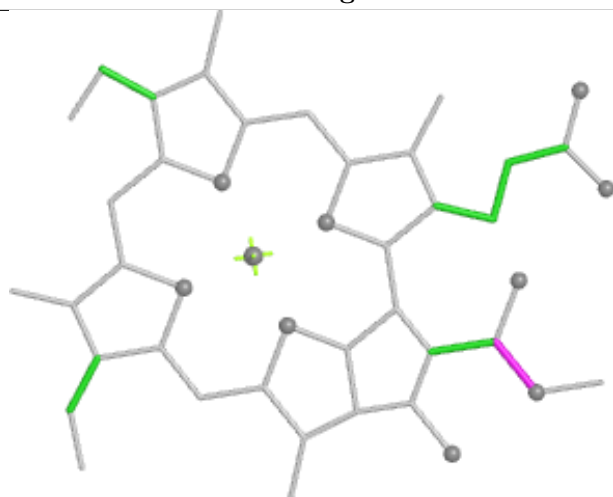
Ligand CLA 5 405



Bond lengths



Bond angles

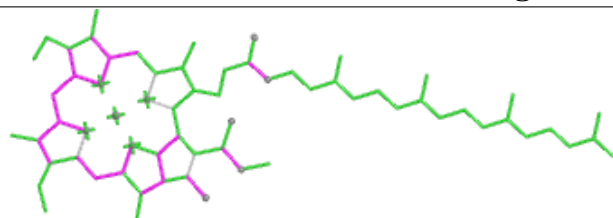


Torsions

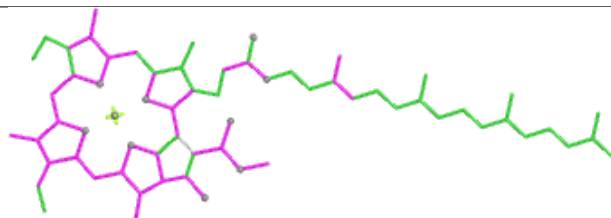


Rings

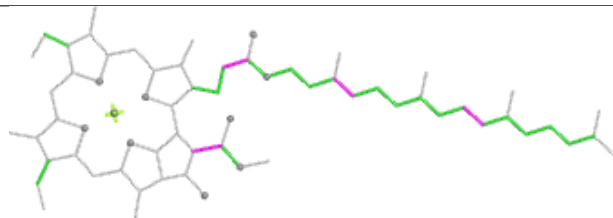
Ligand CLA A 828



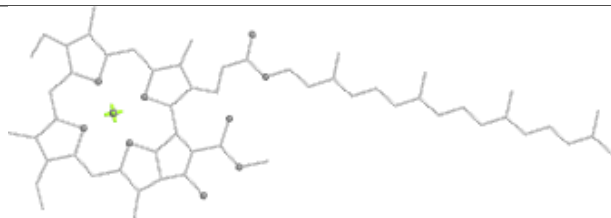
Bond lengths



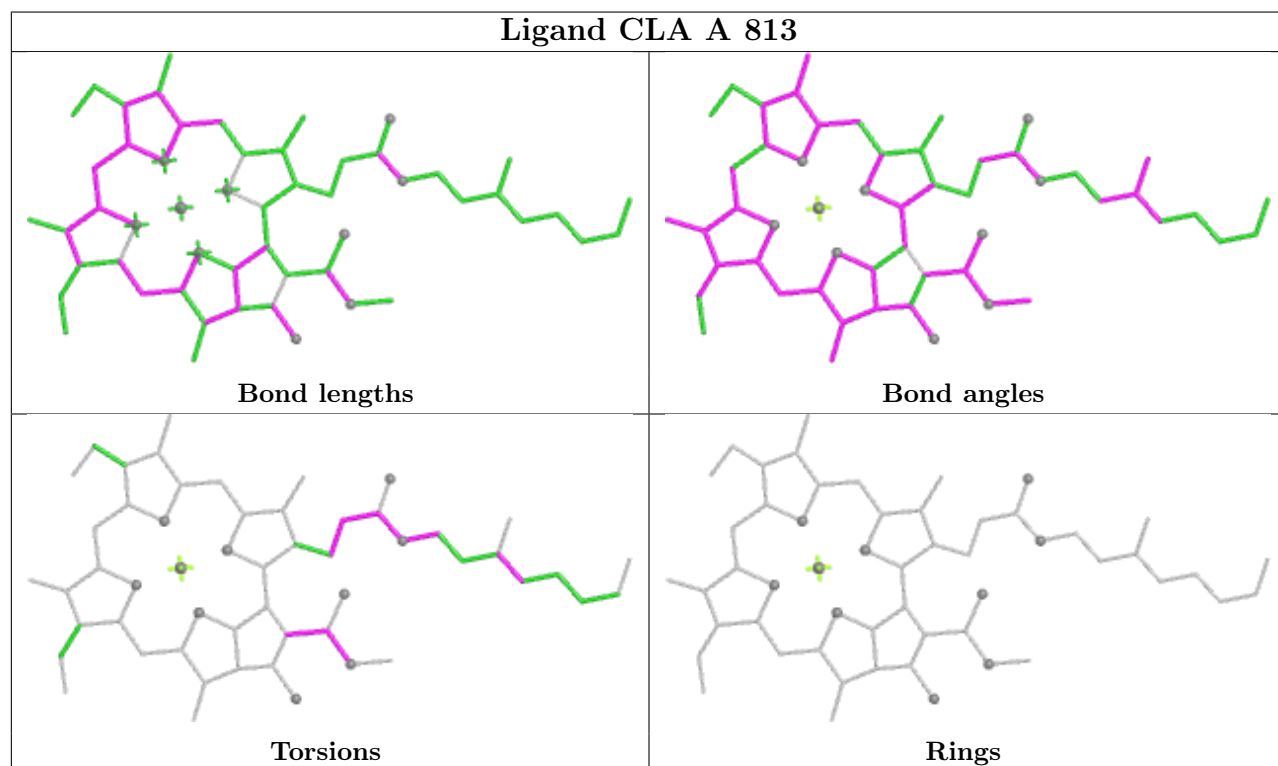
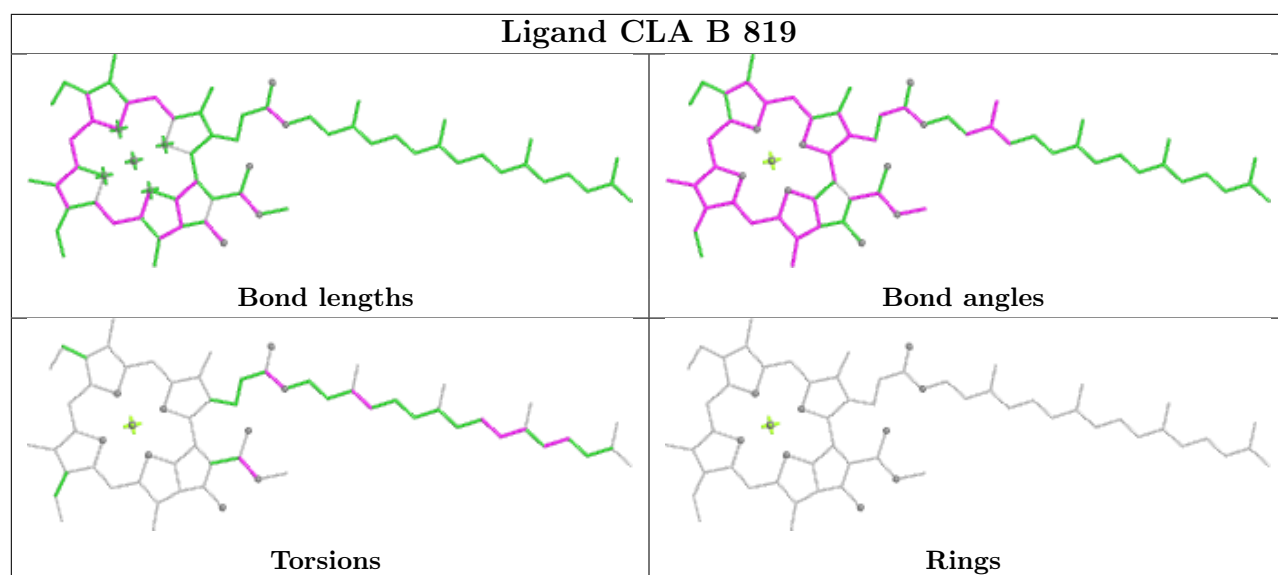
Bond angles

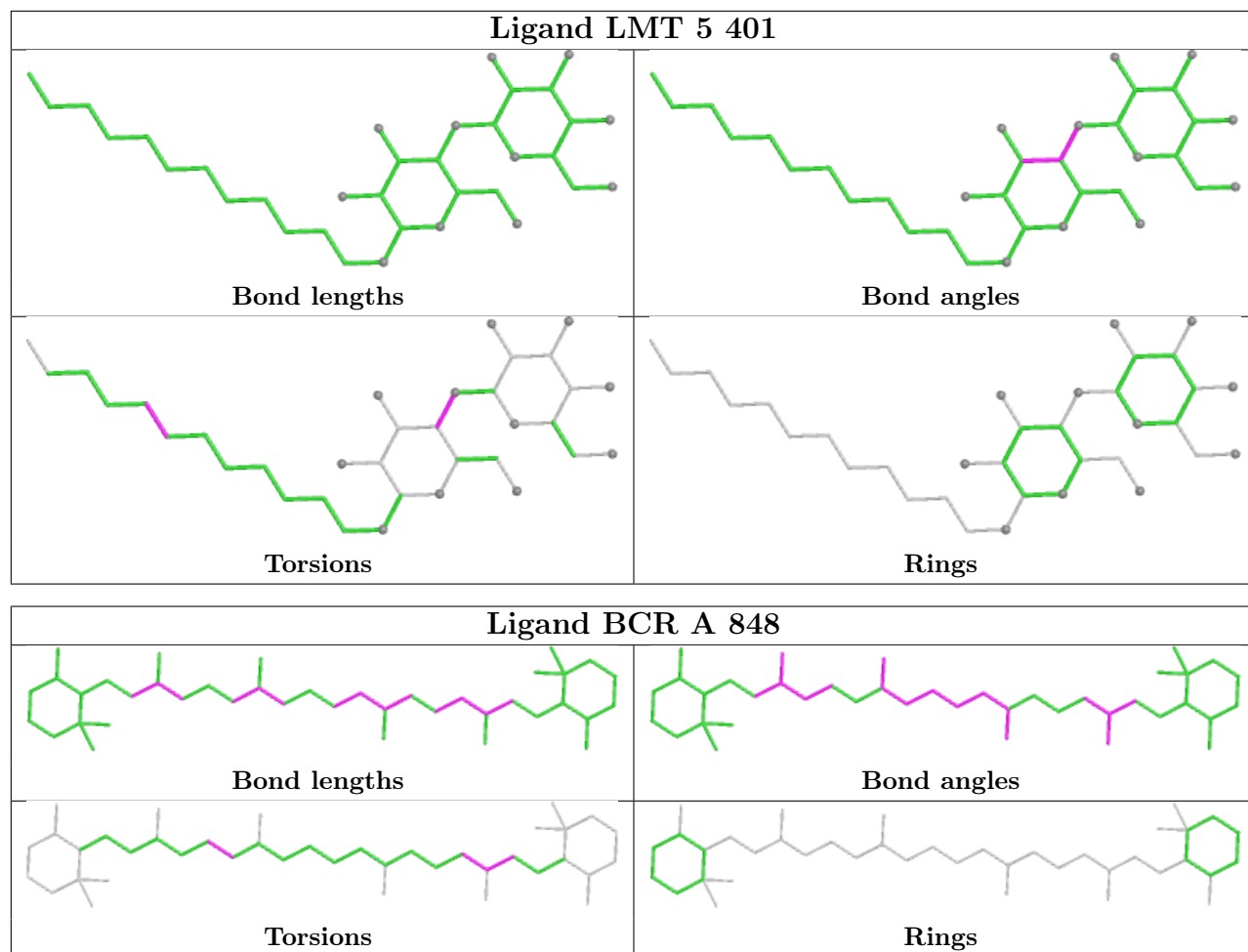


Torsions

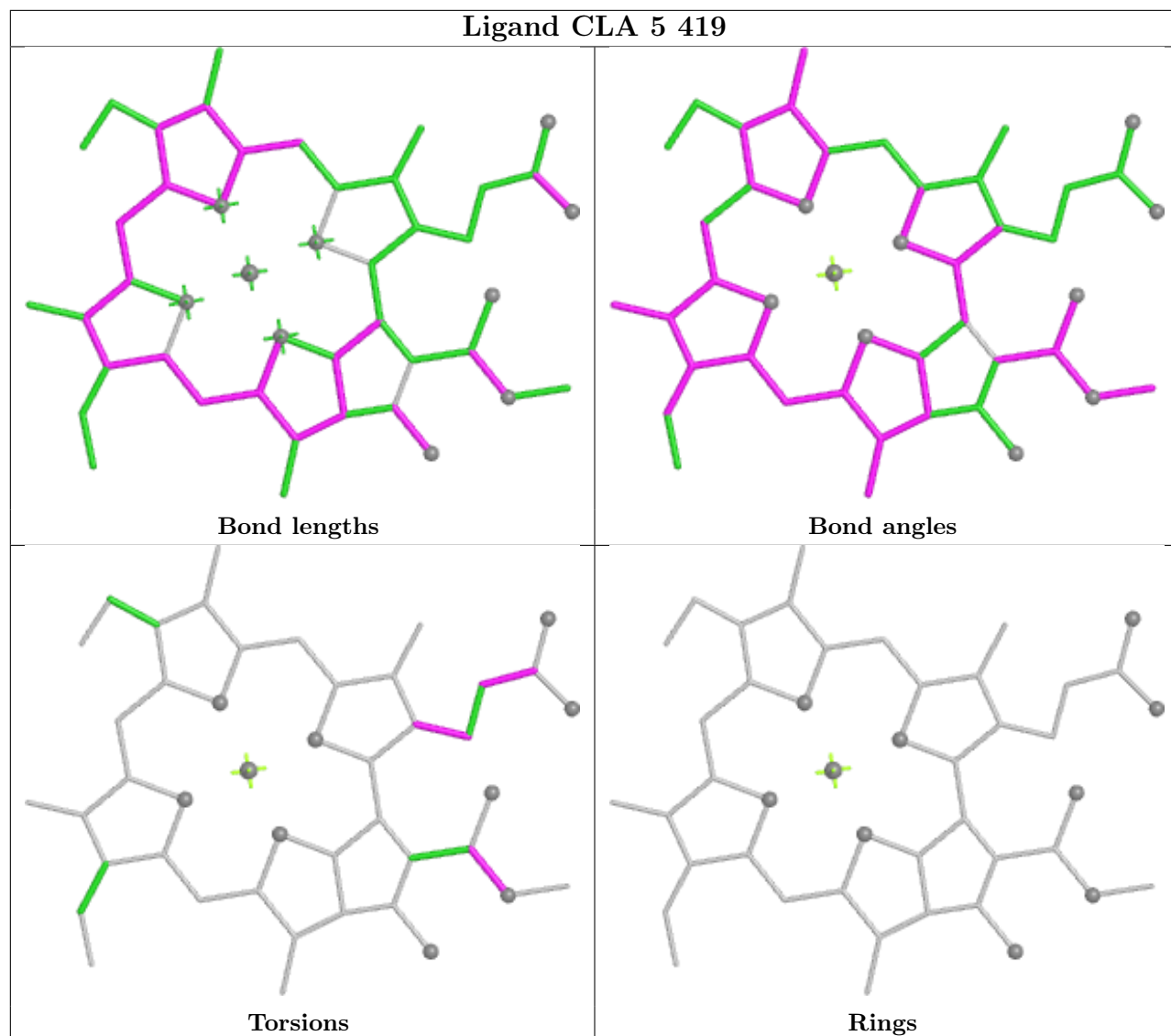


Rings

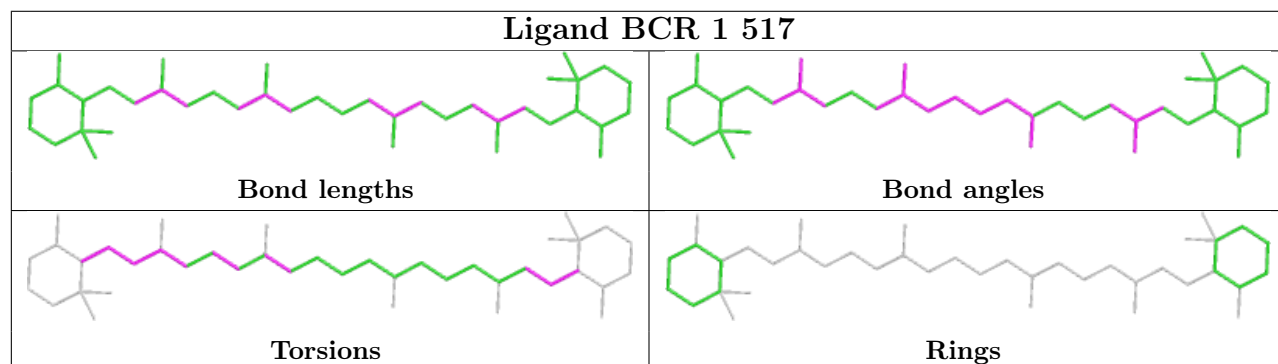


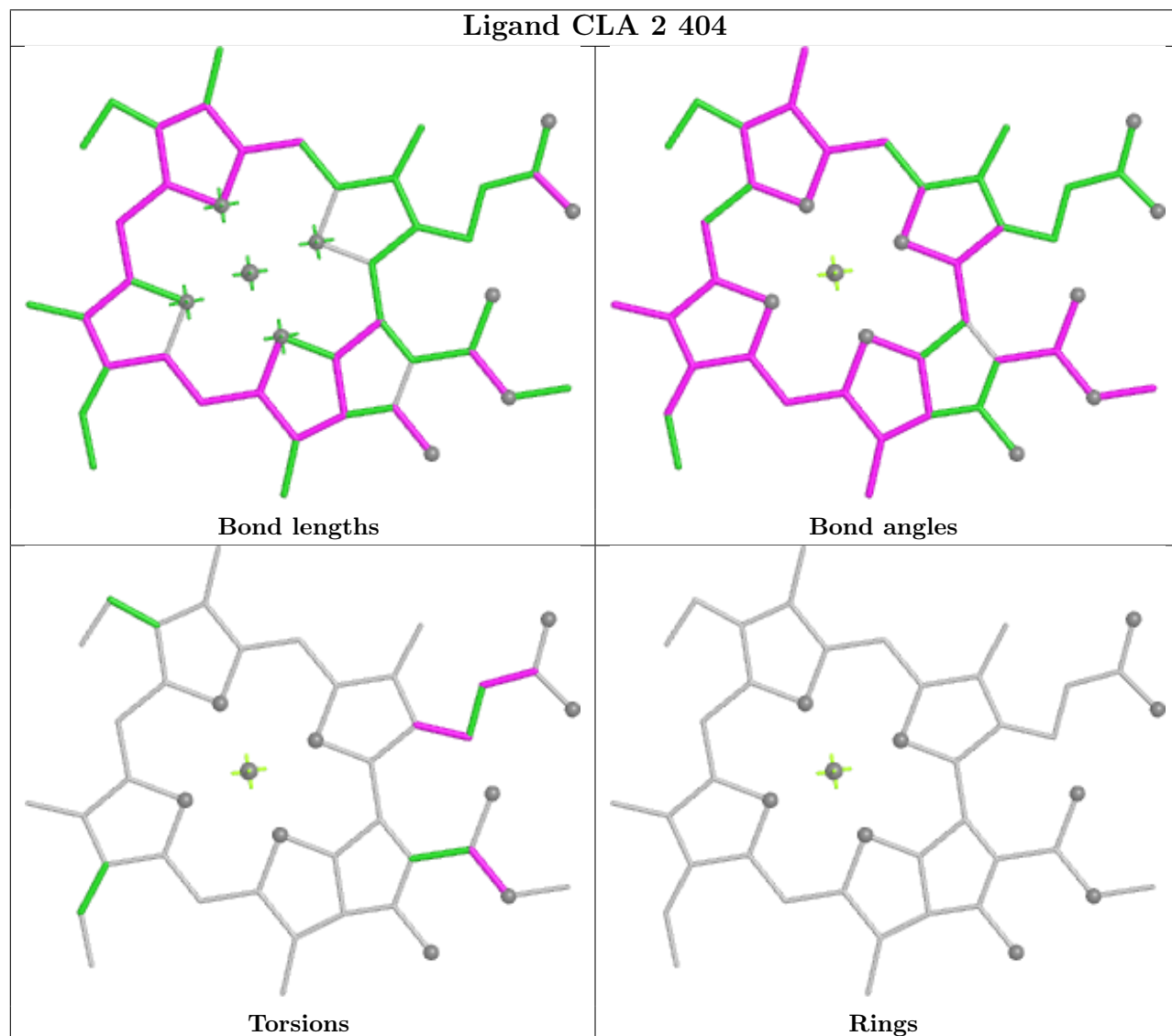
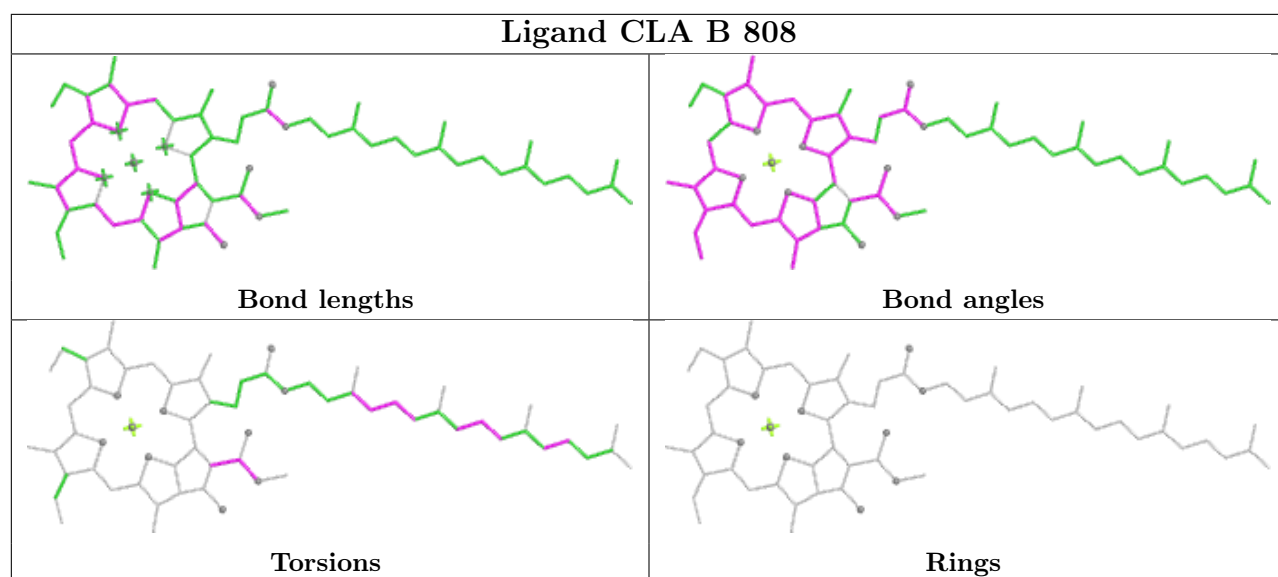


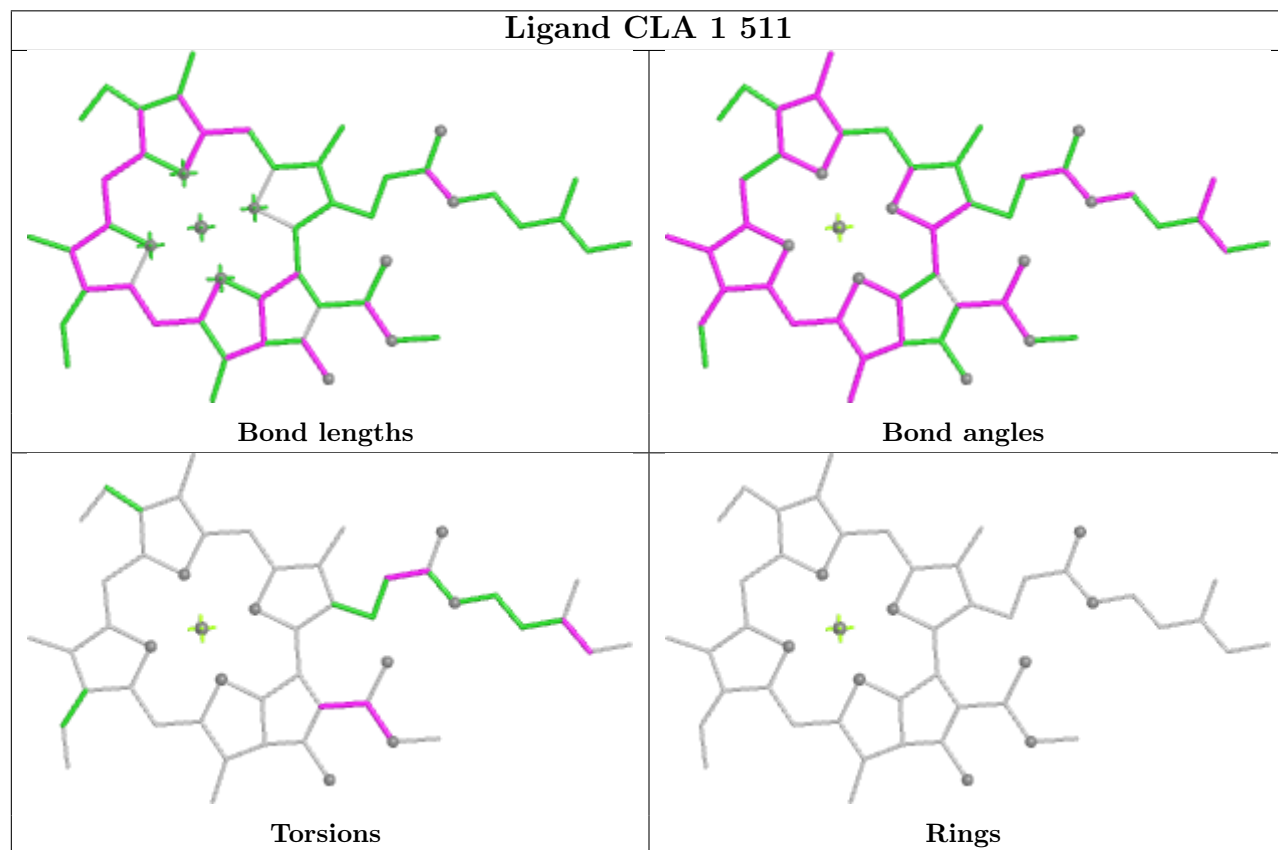
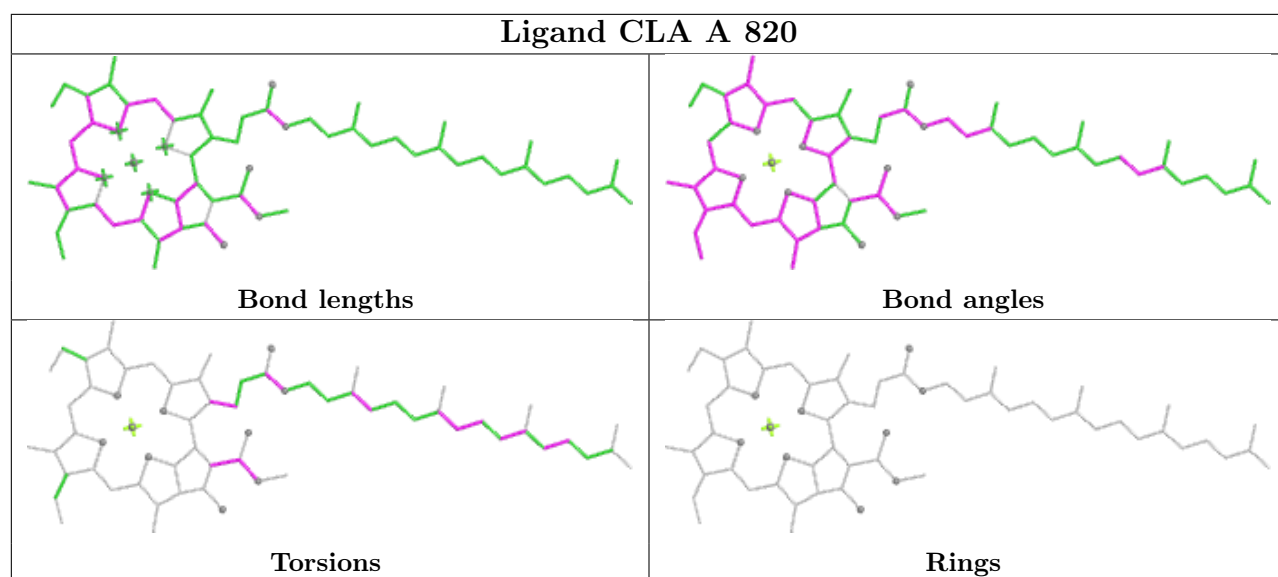
Ligand CLA 5 419

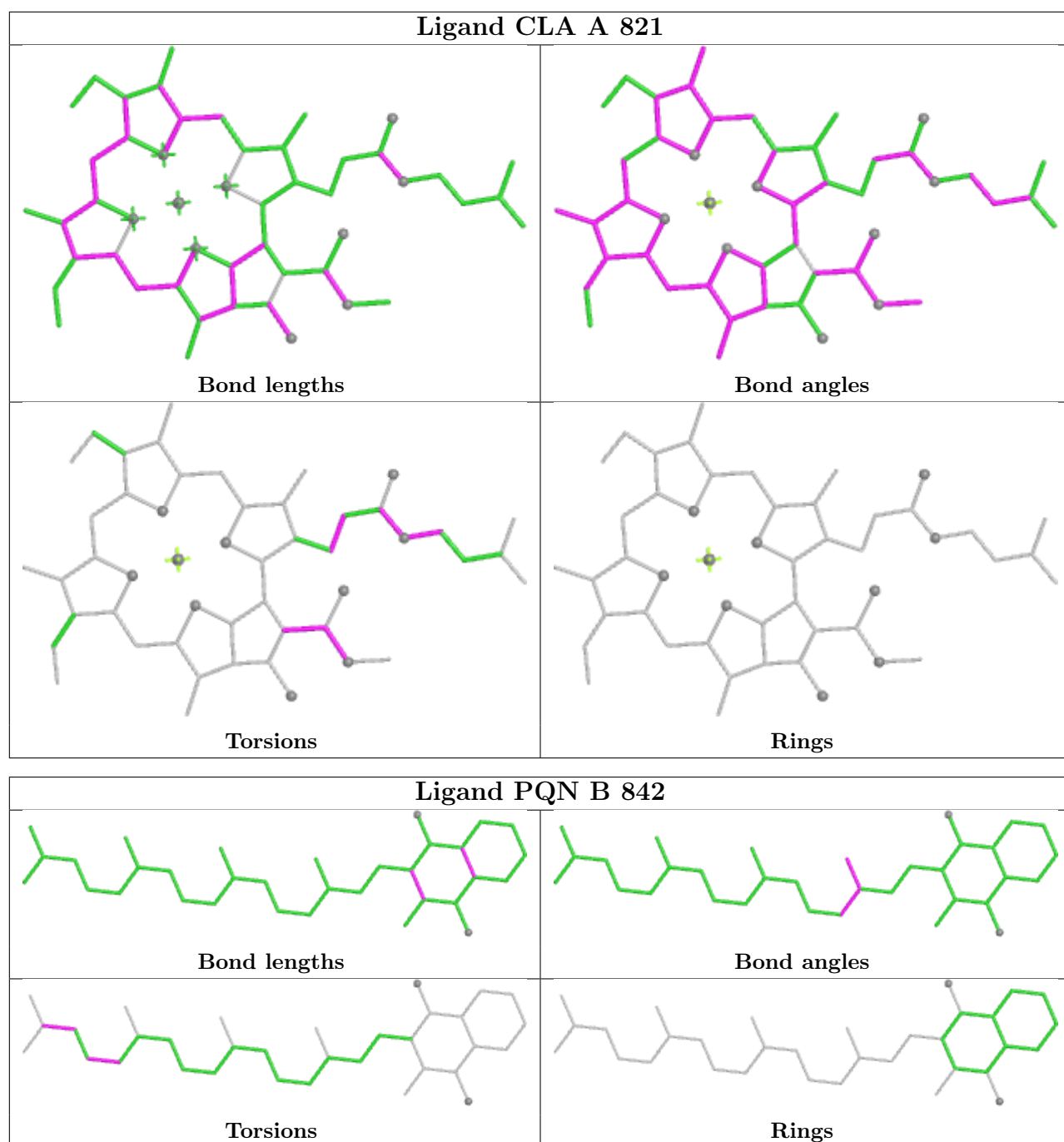


Ligand BCR 1 517

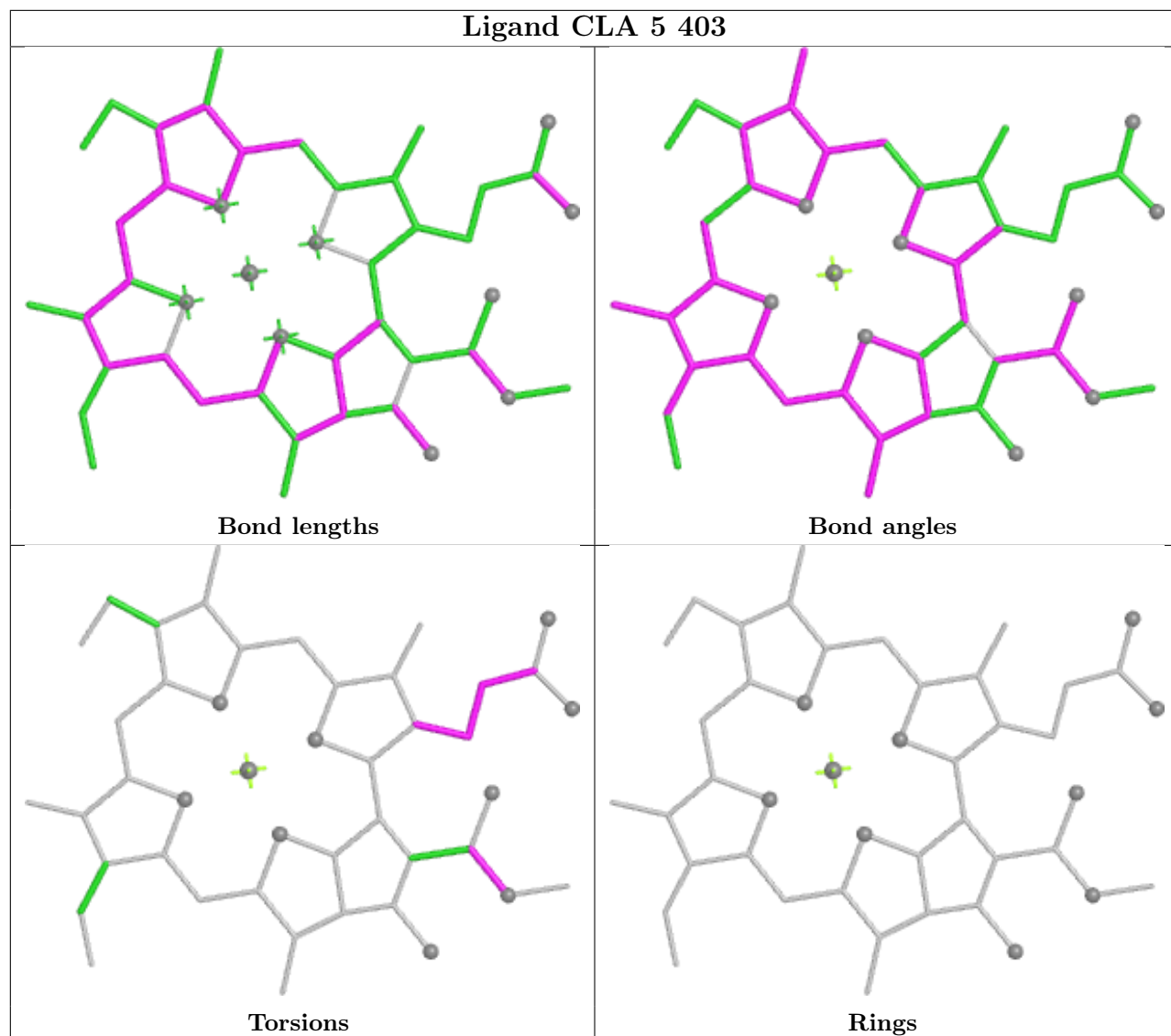




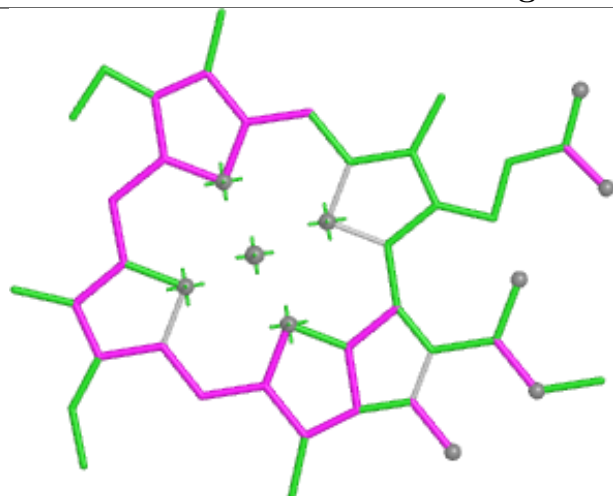




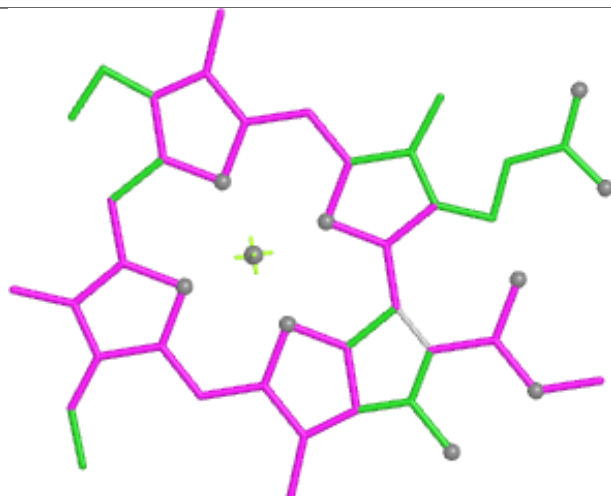
Ligand CLA 5 403



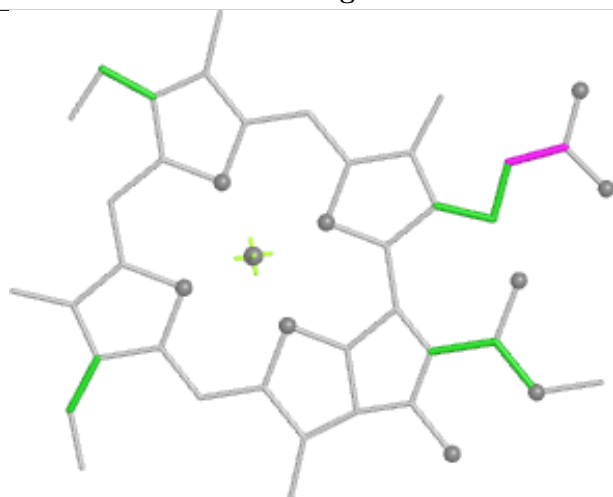
Ligand CLA 6 406



Bond lengths



Bond angles

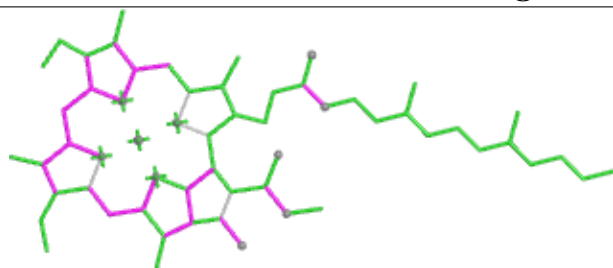


Torsions

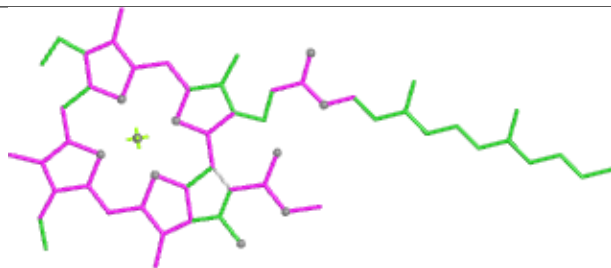


Rings

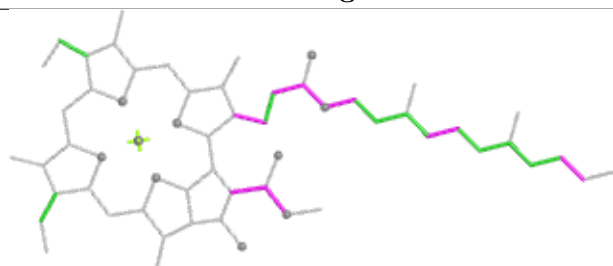
Ligand CLA B 833



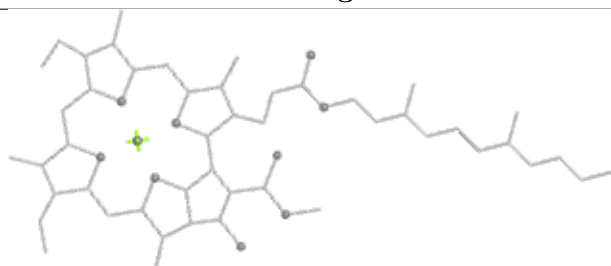
Bond lengths



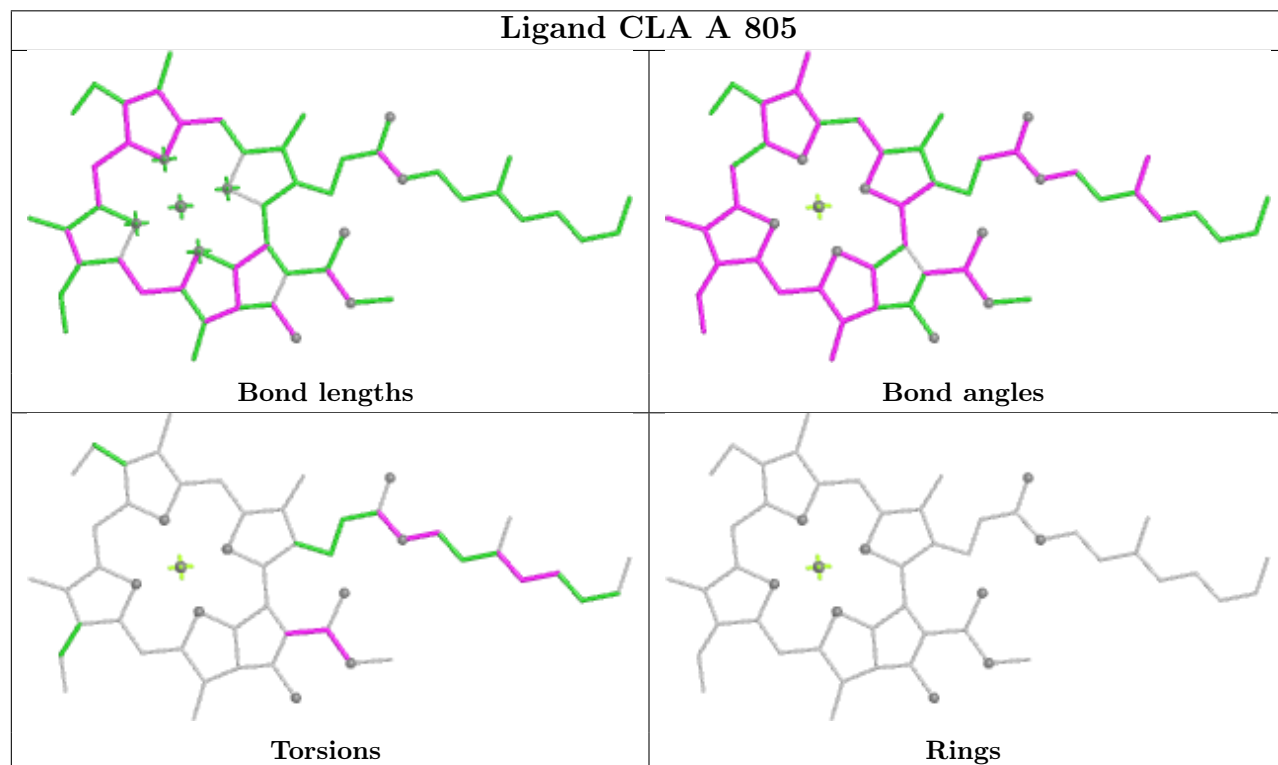
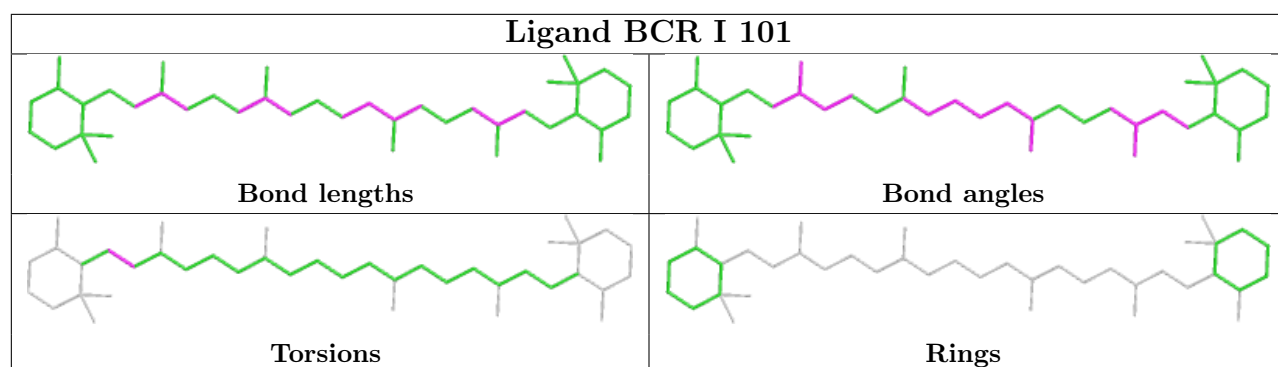
Bond angles



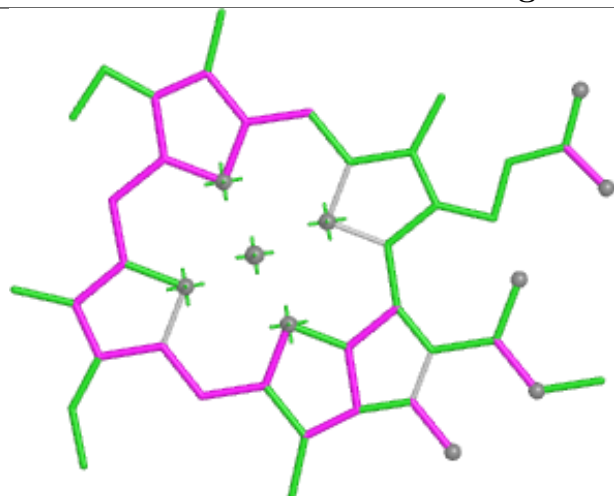
Torsions



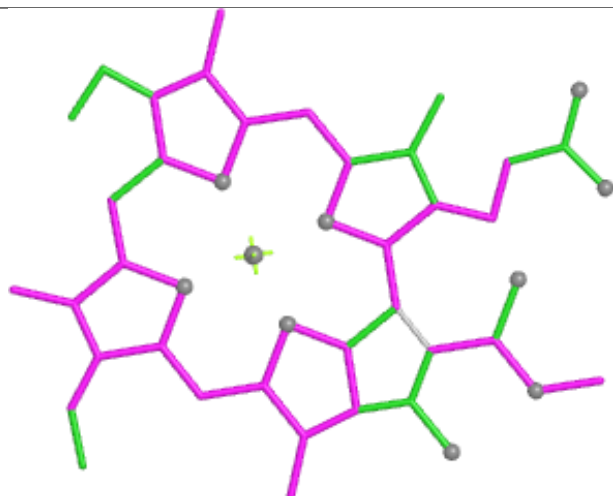
Rings



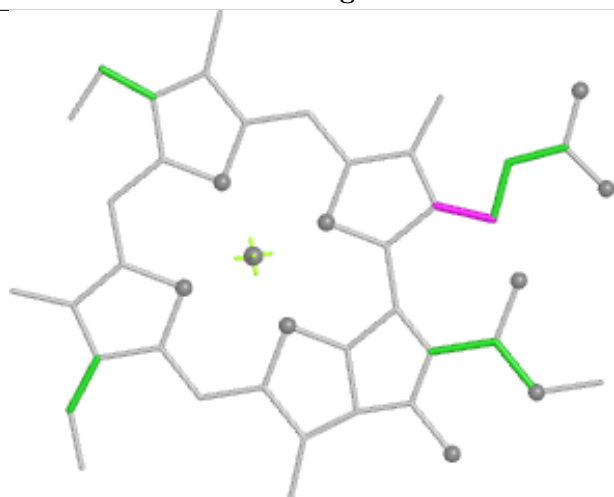
Ligand CLA 1 513



Bond lengths



Bond angles

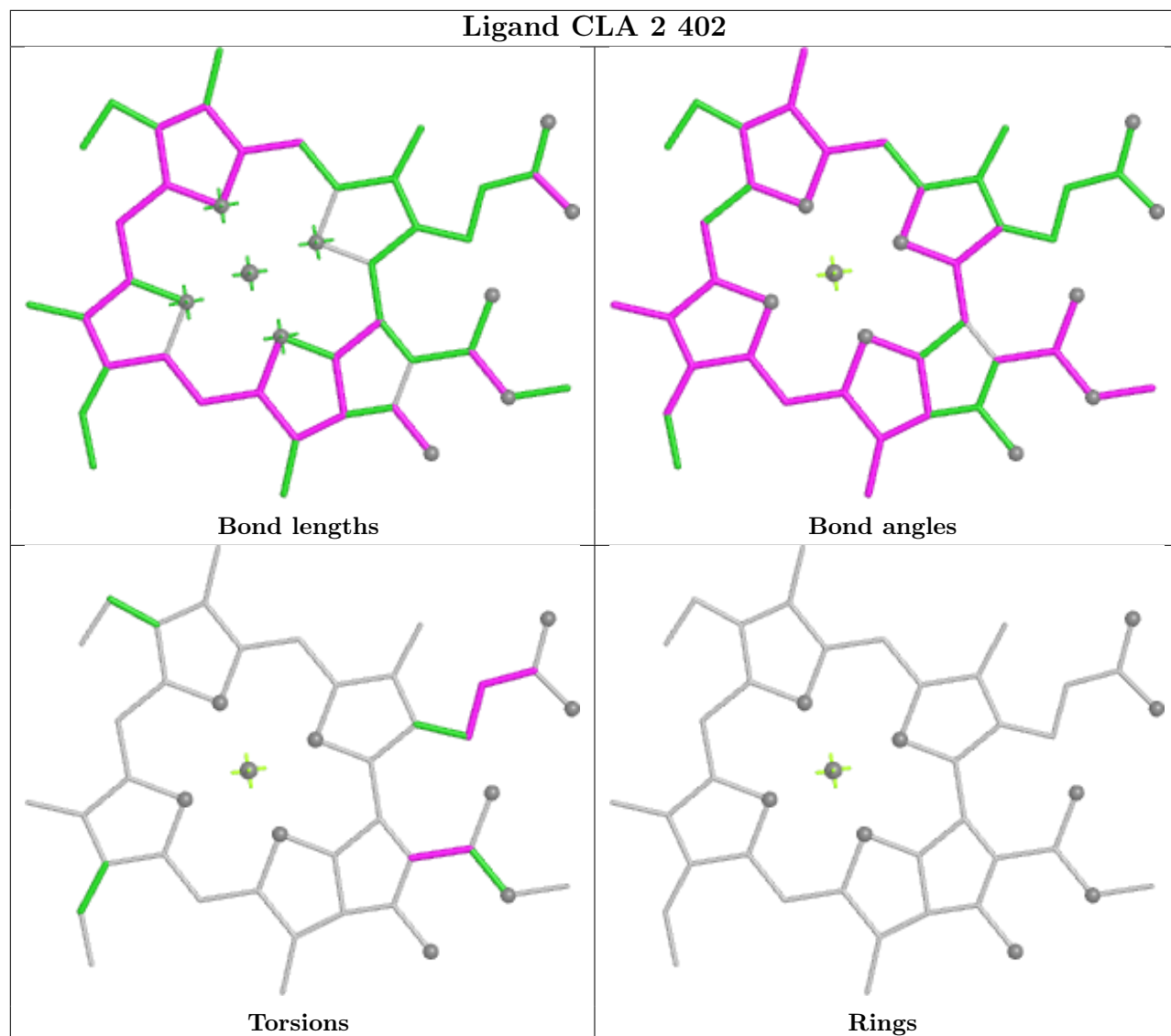


Torsions

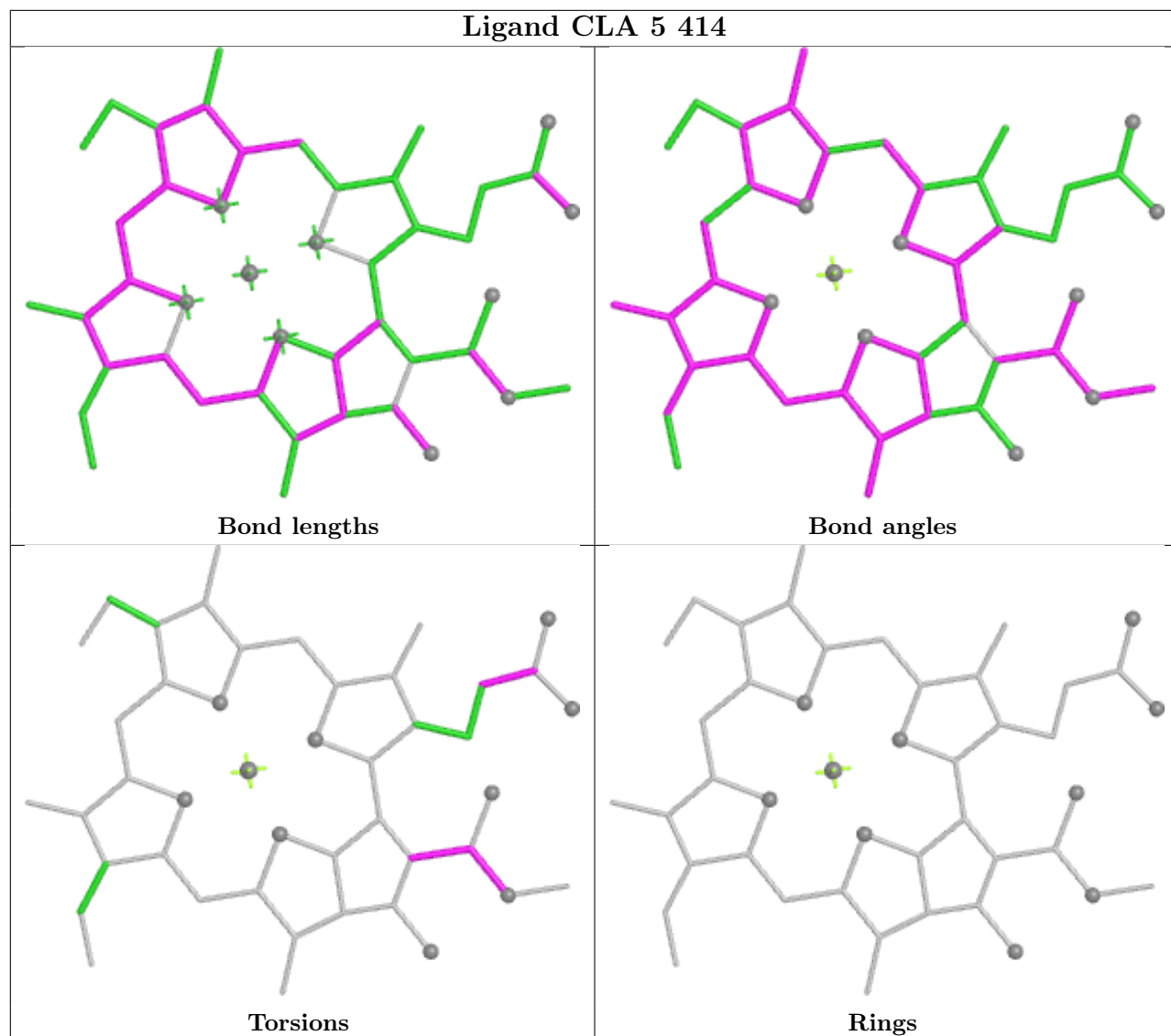


Rings

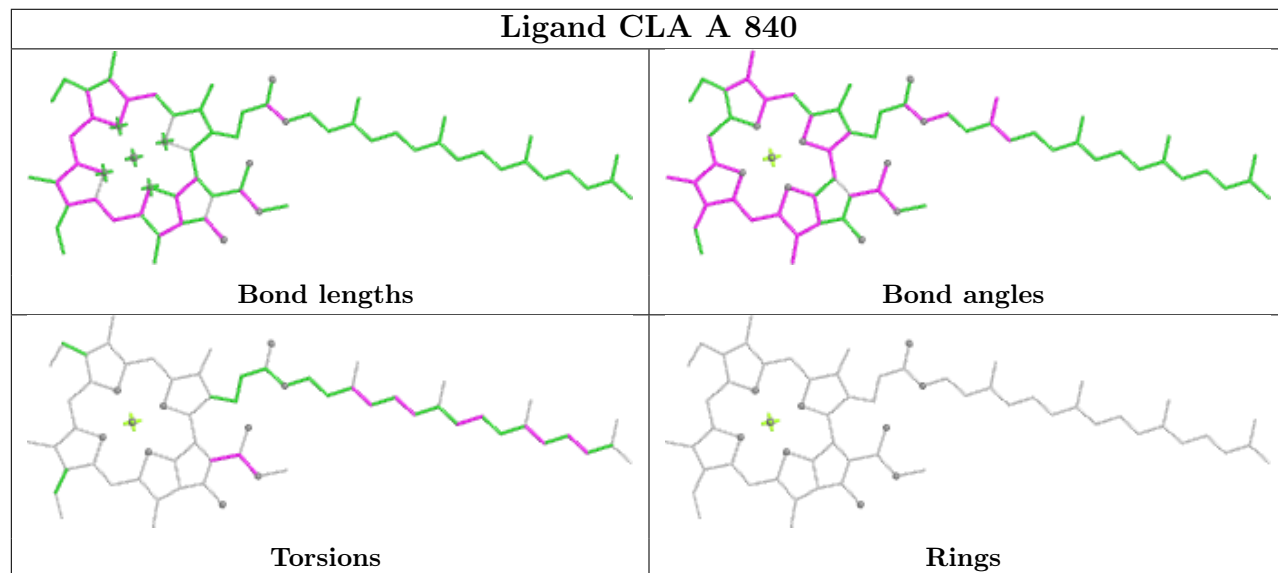
Ligand CLA 2 402

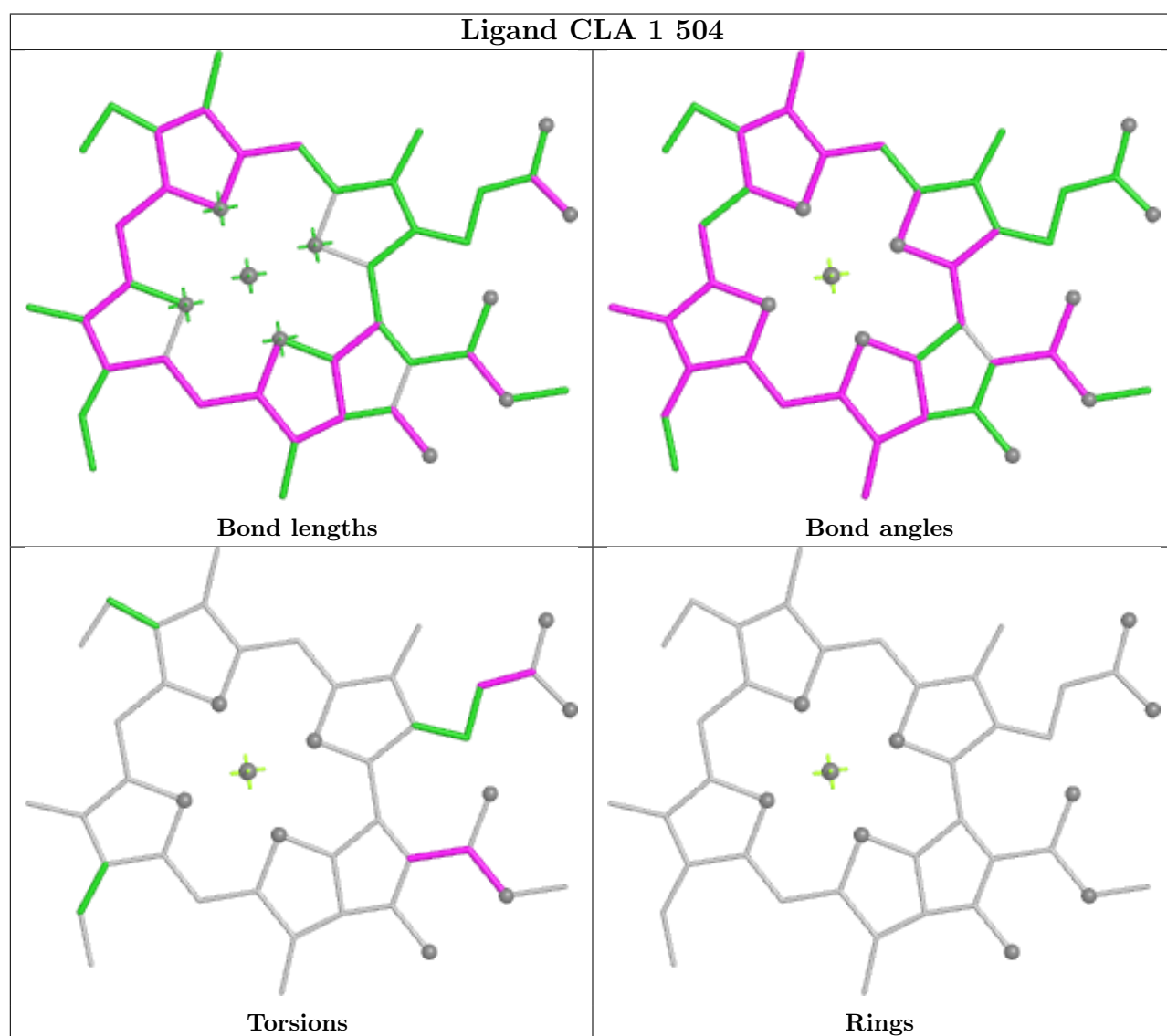
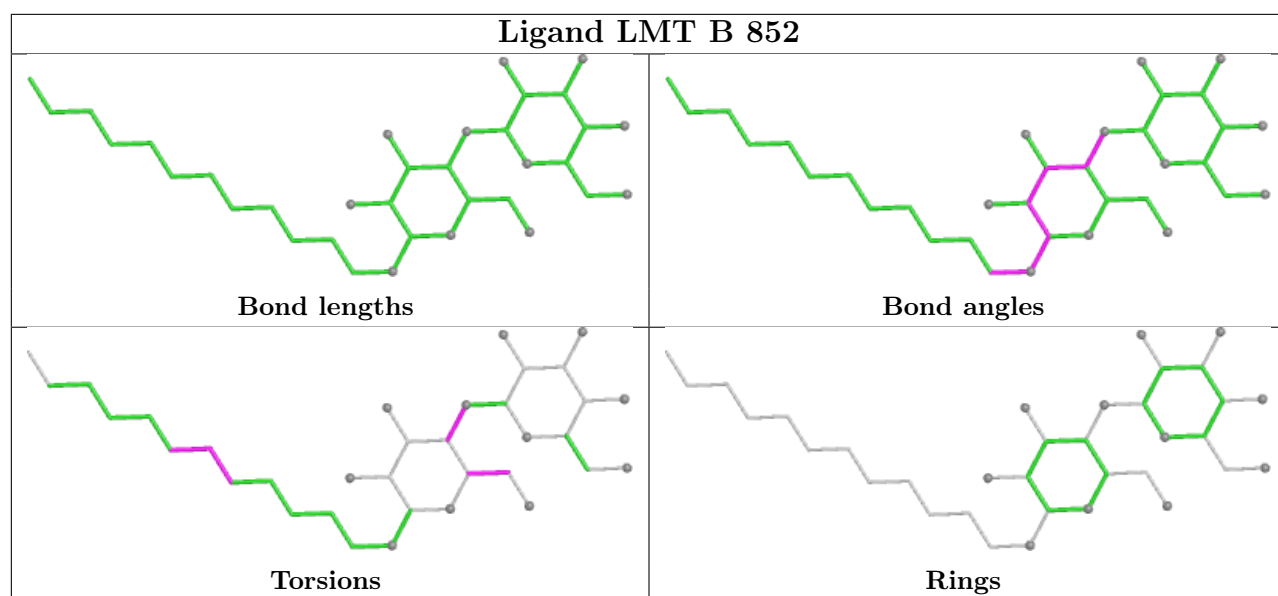


Ligand CLA 5 414

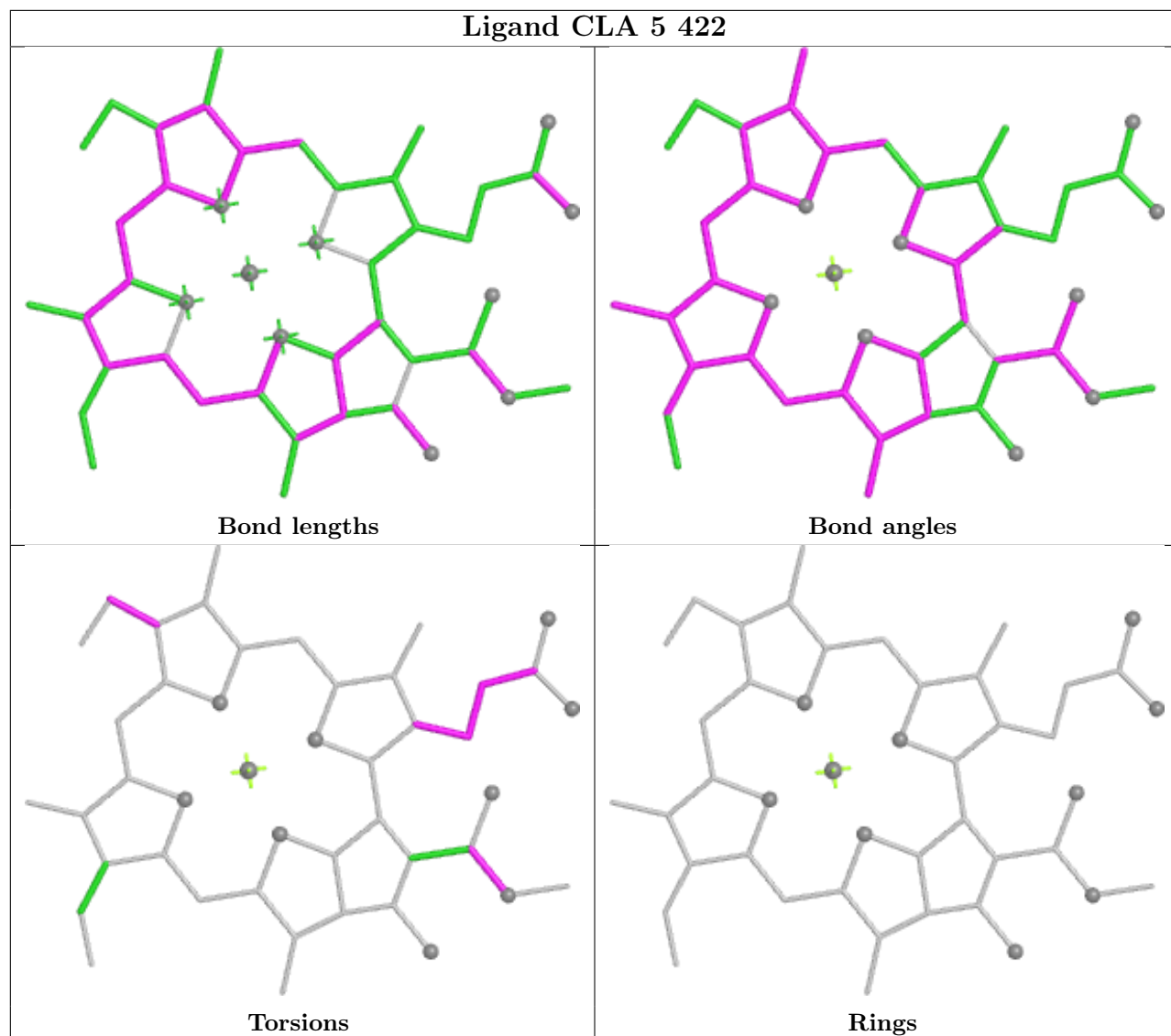


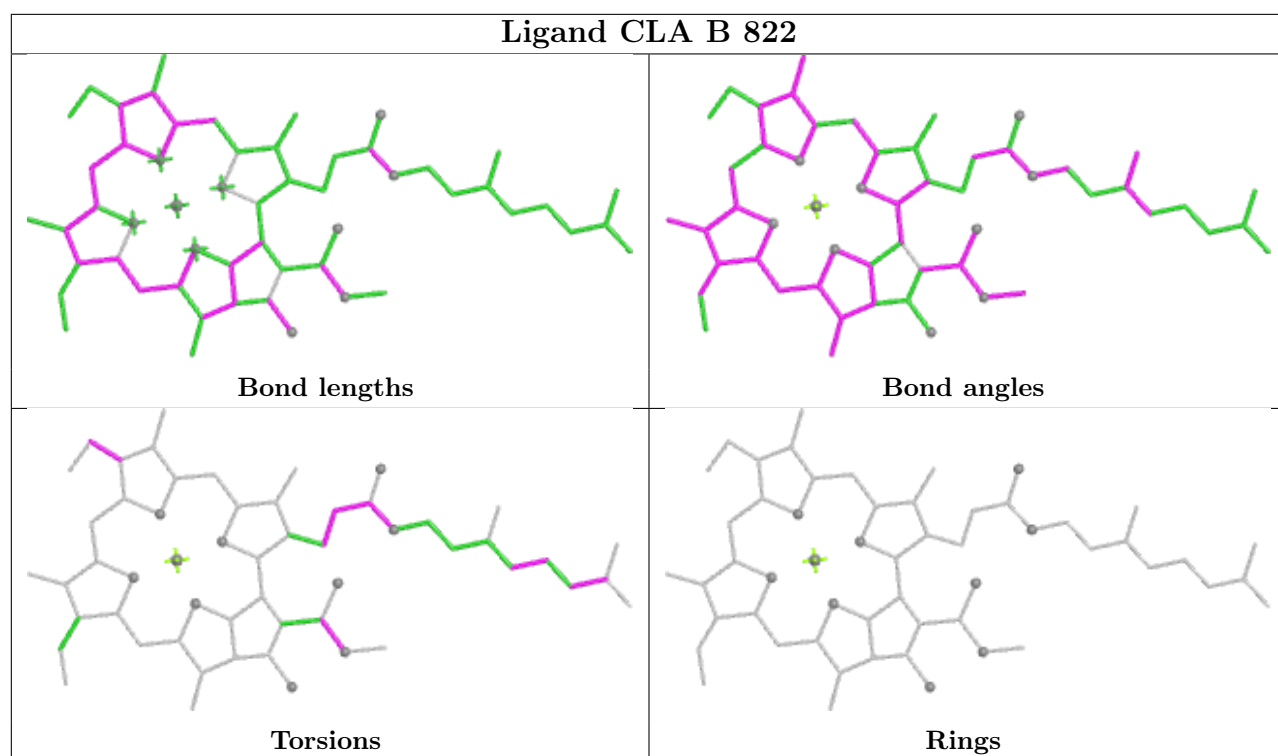
Ligand CLA A 840



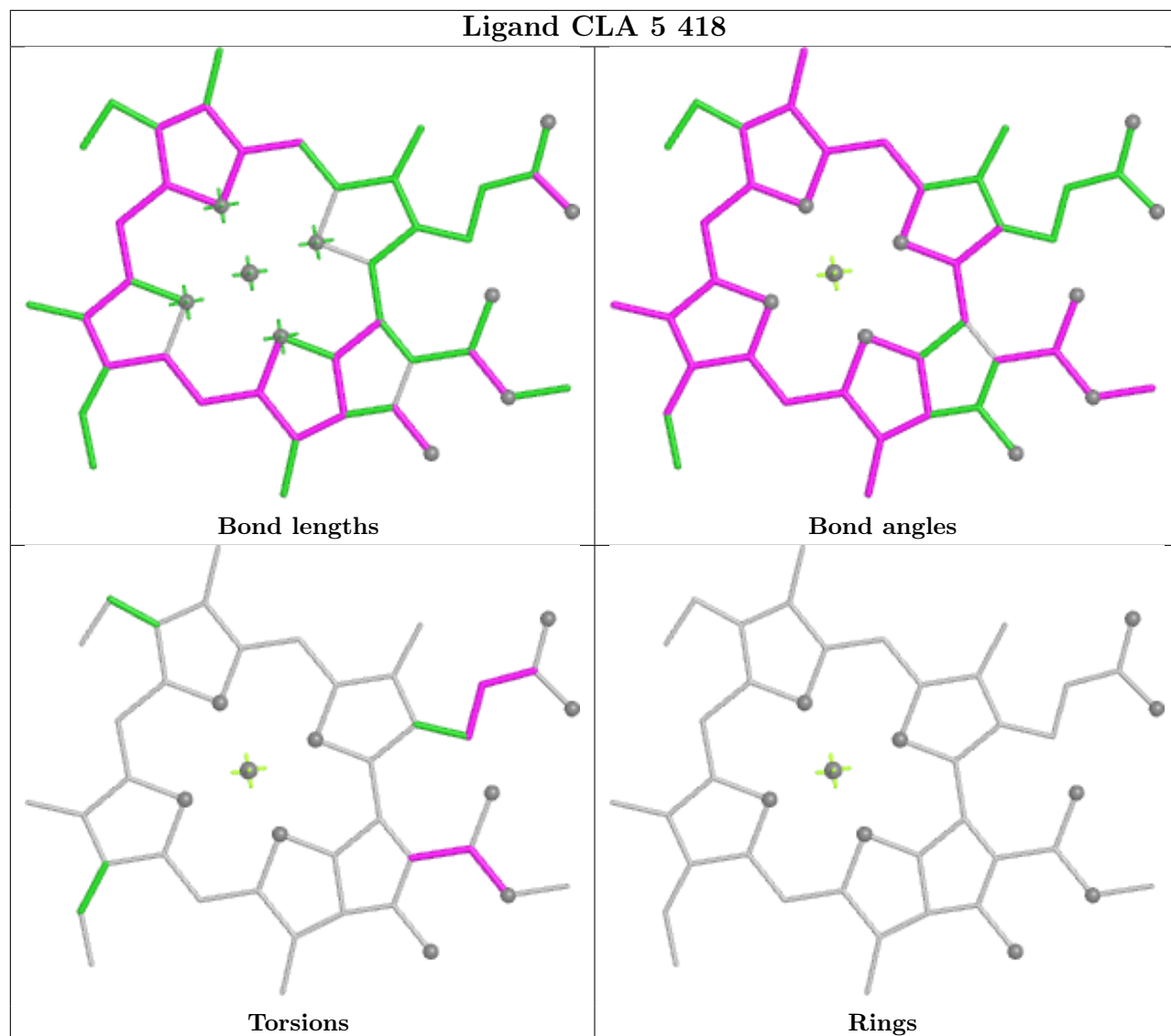


Ligand CLA 5 422

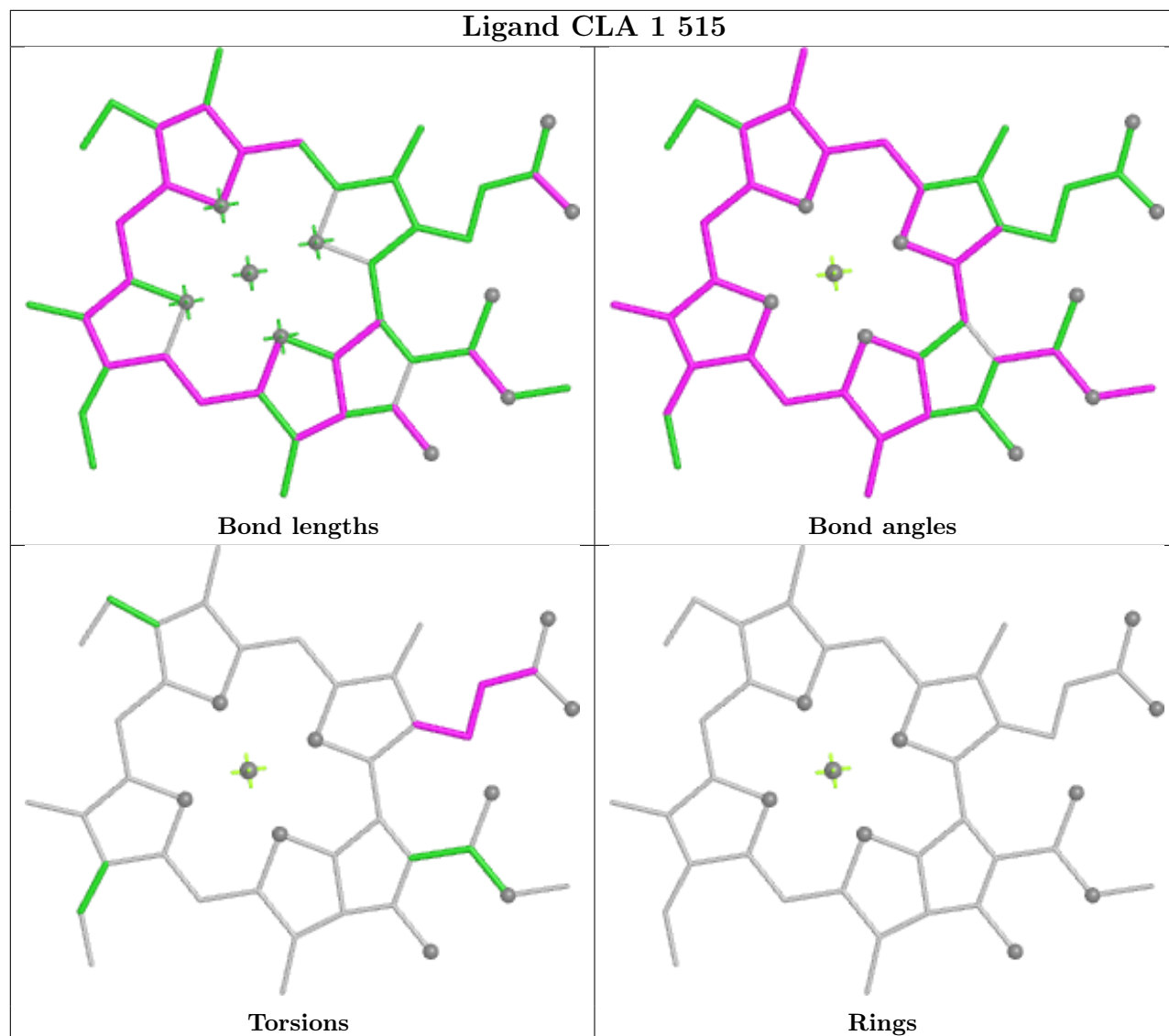




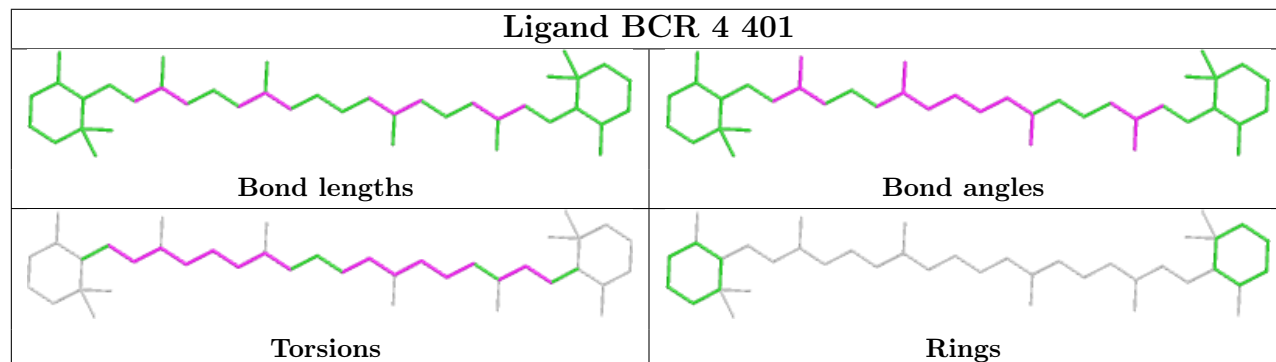
Ligand CLA 5 418



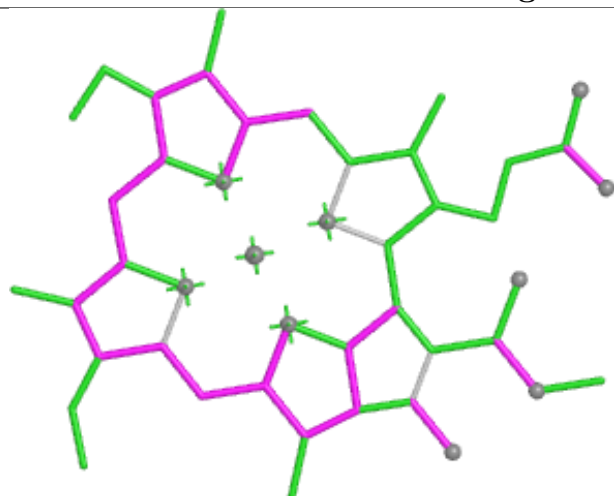
Ligand CLA 1 515



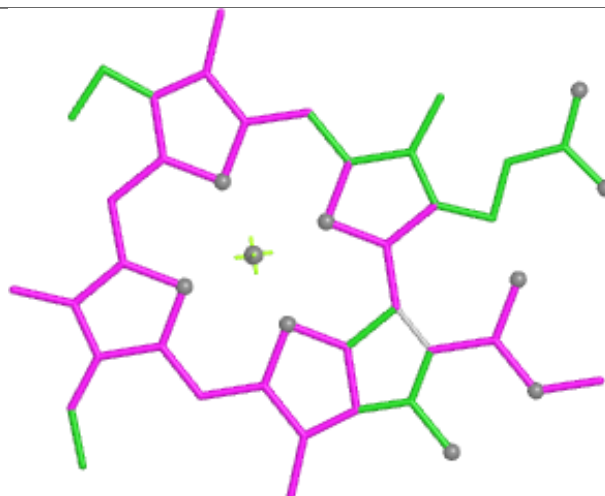
Ligand BCR 4 401



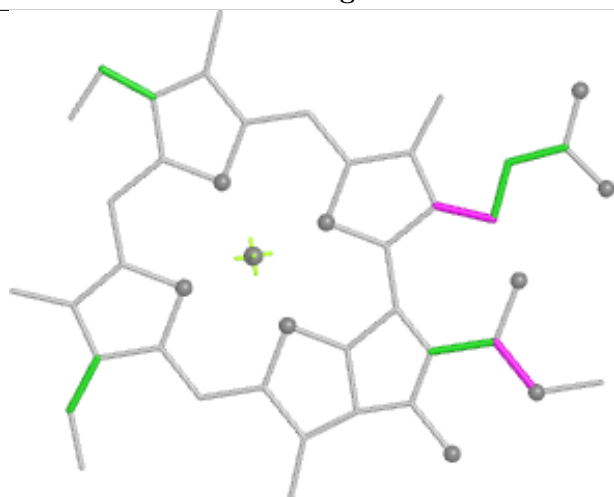
Ligand CLA 4 409



Bond lengths



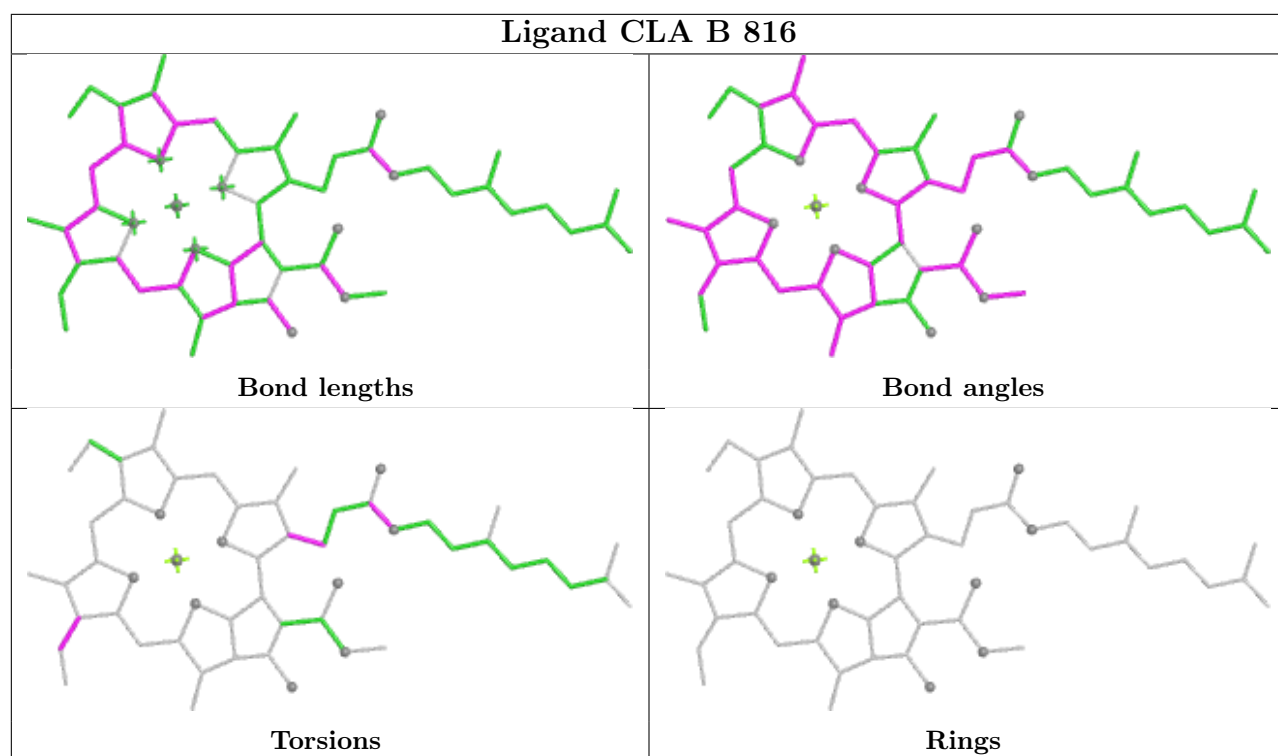
Bond angles



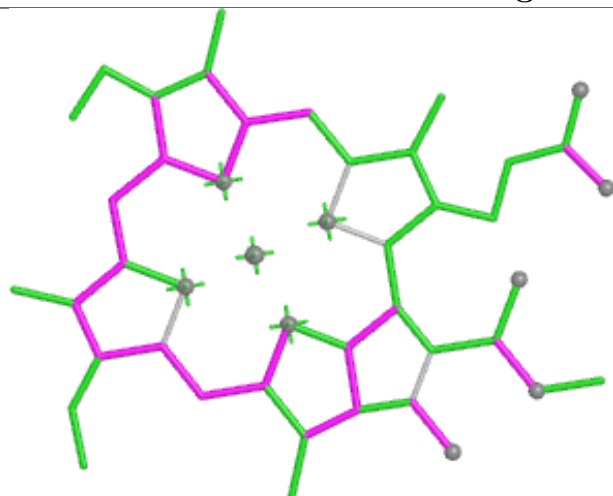
Torsions



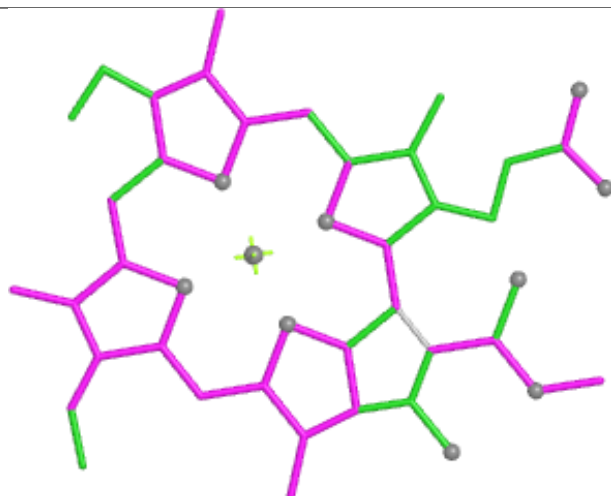
Rings



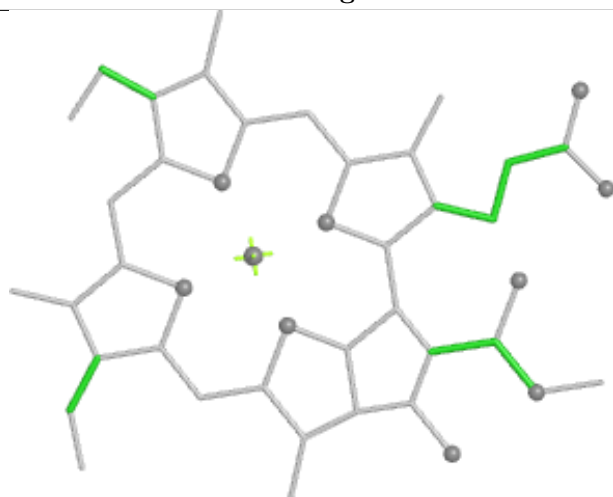
Ligand CLA F 204



Bond lengths



Bond angles

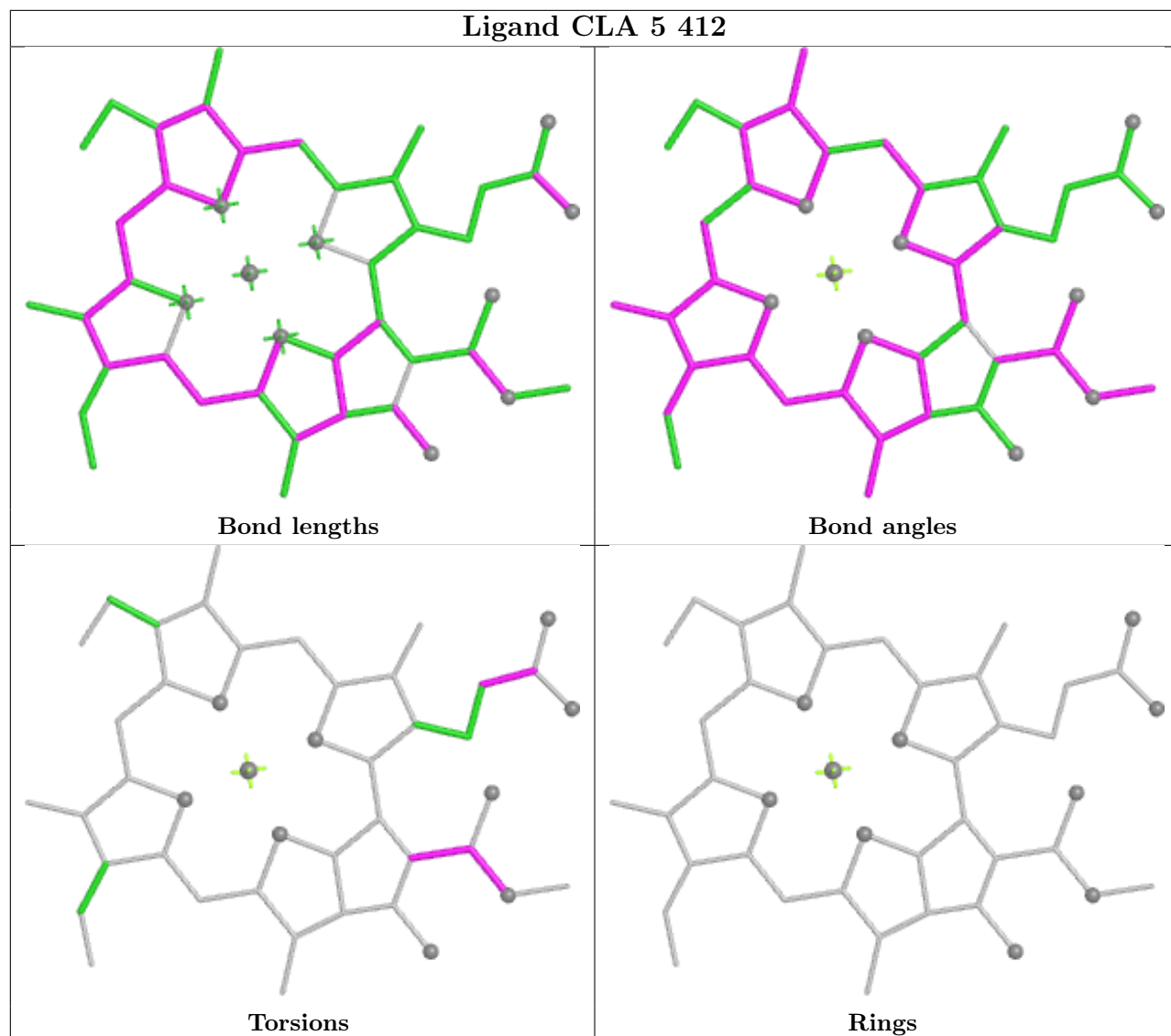


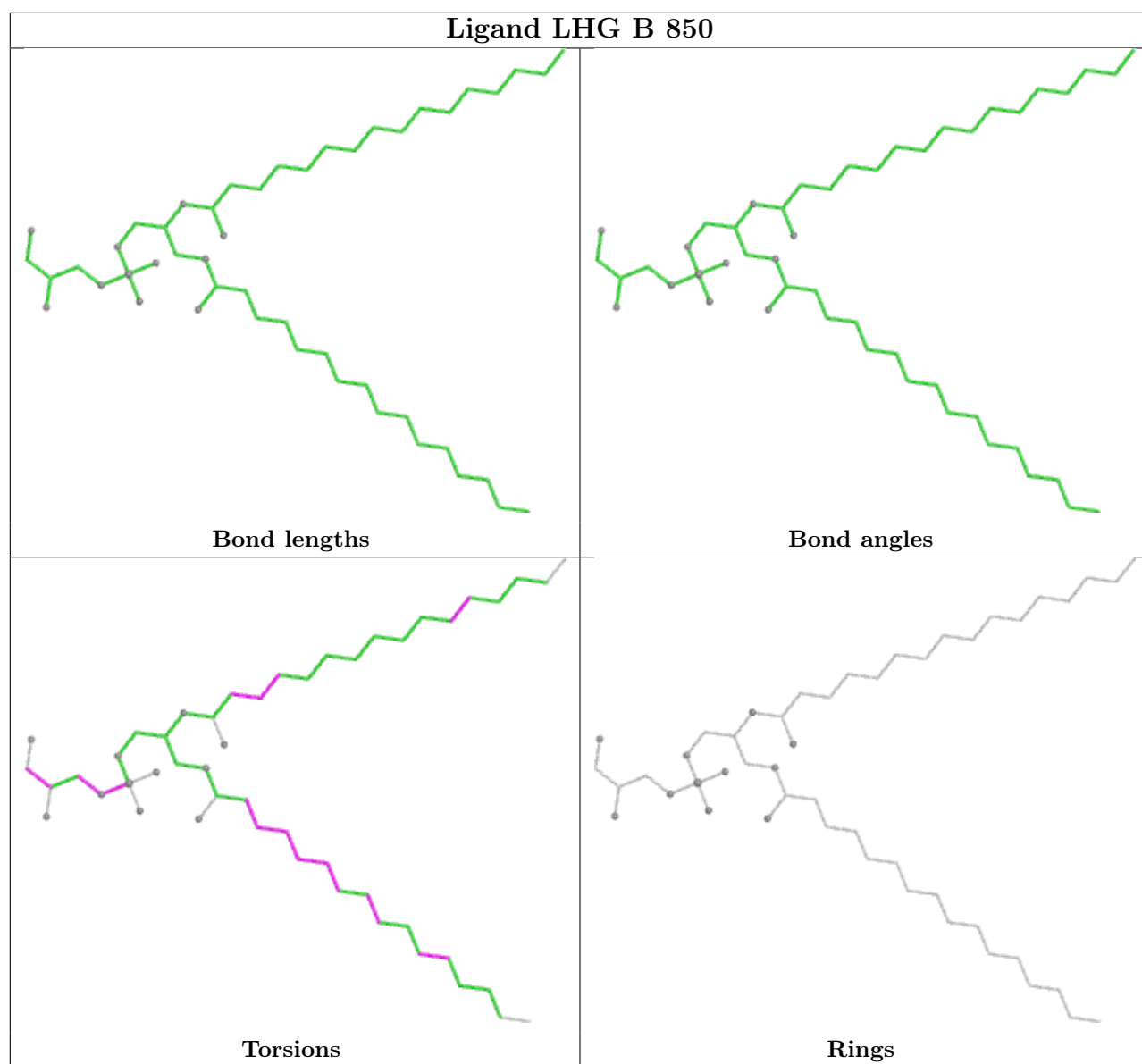
Torsions



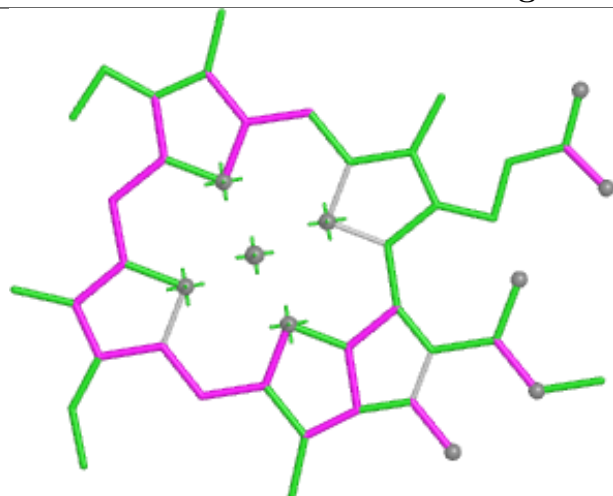
Rings

Ligand CLA 5 412

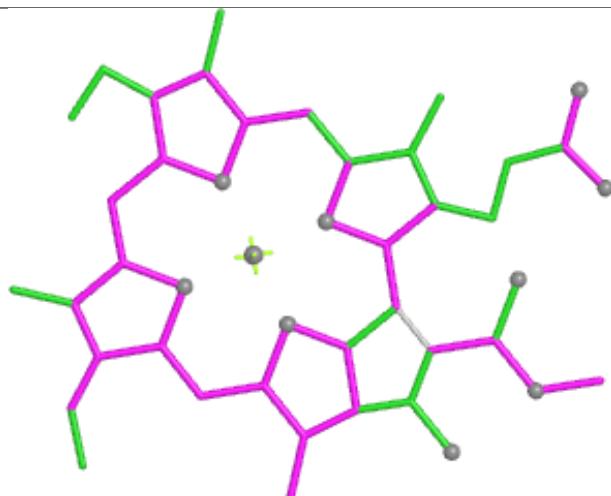




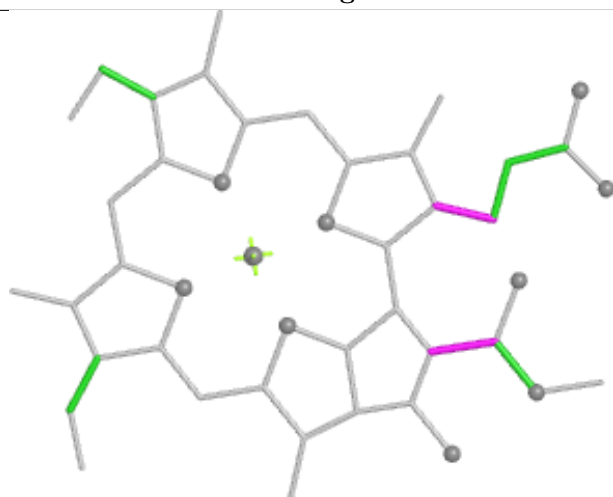
Ligand CLA 5 410



Bond lengths



Bond angles

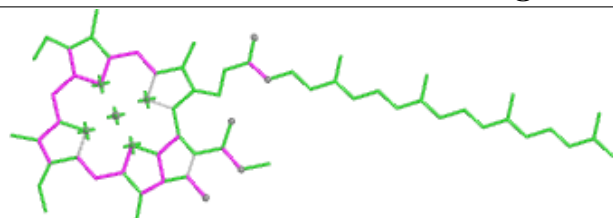


Torsions

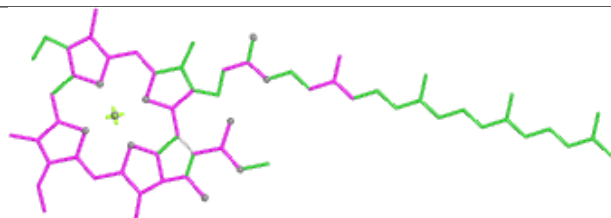


Rings

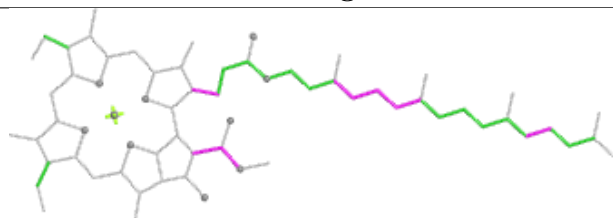
Ligand CLA B 818



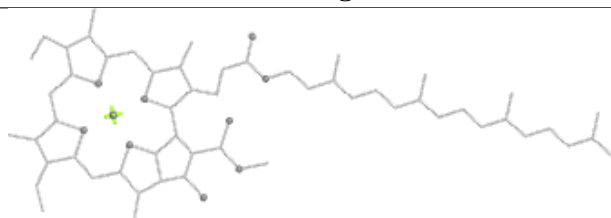
Bond lengths



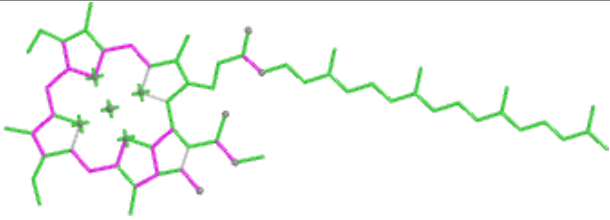
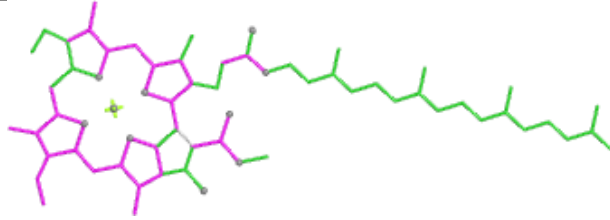
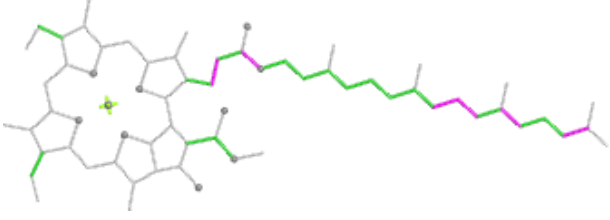
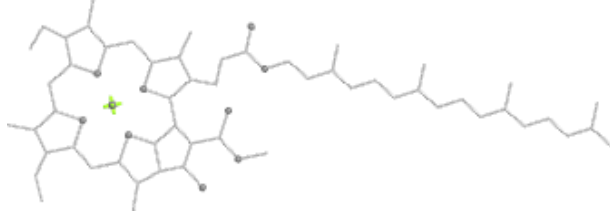
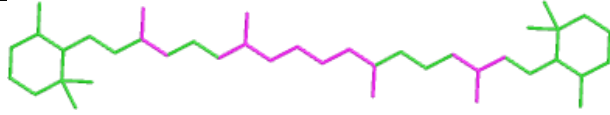
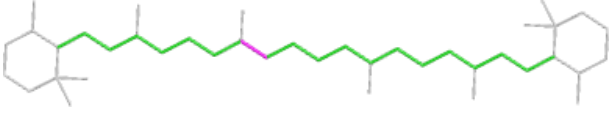
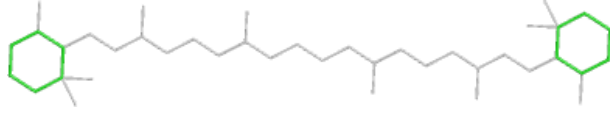
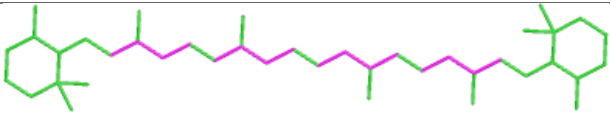
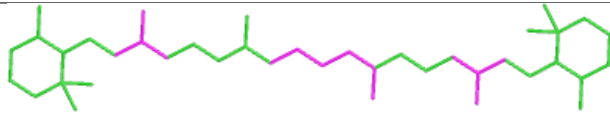
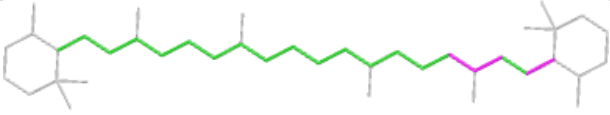
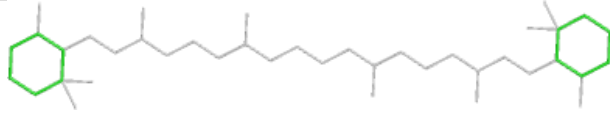
Bond angles

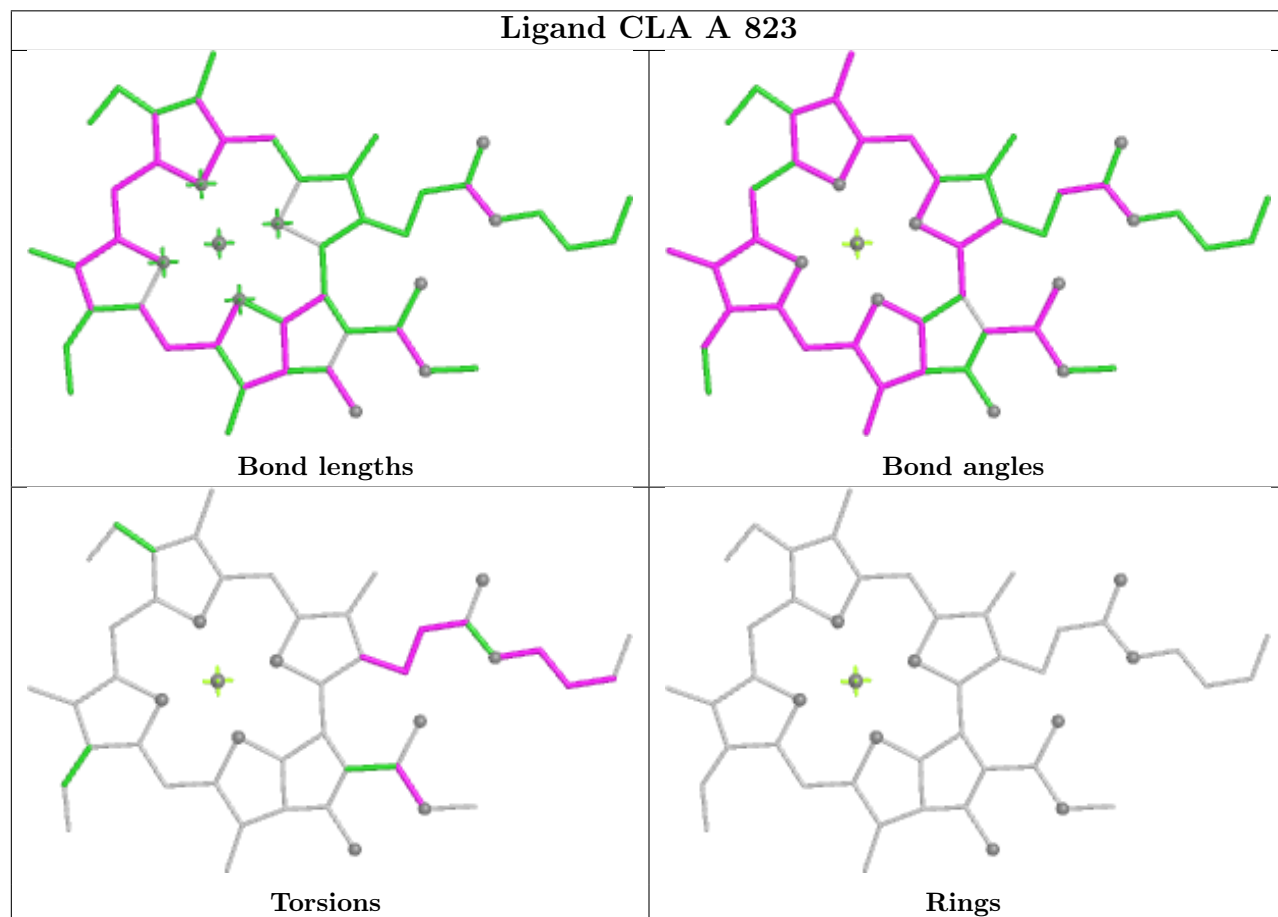
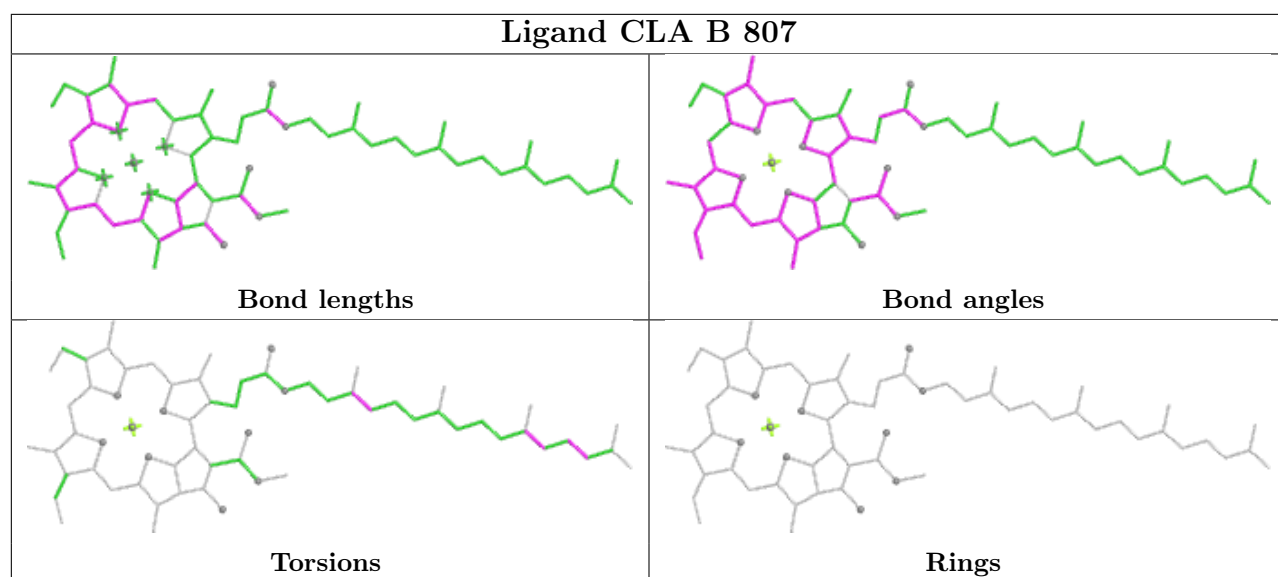


Torsions

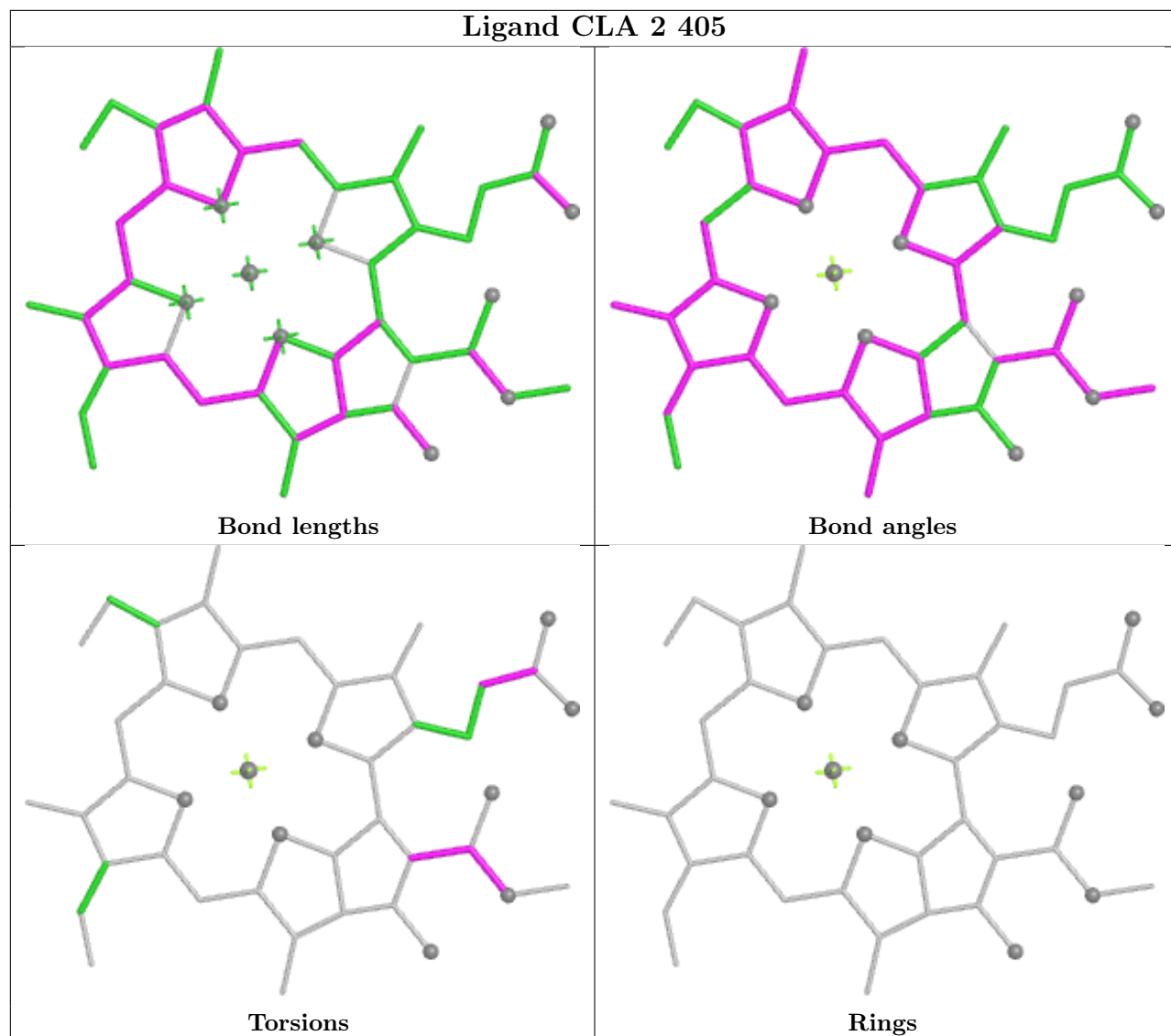


Rings

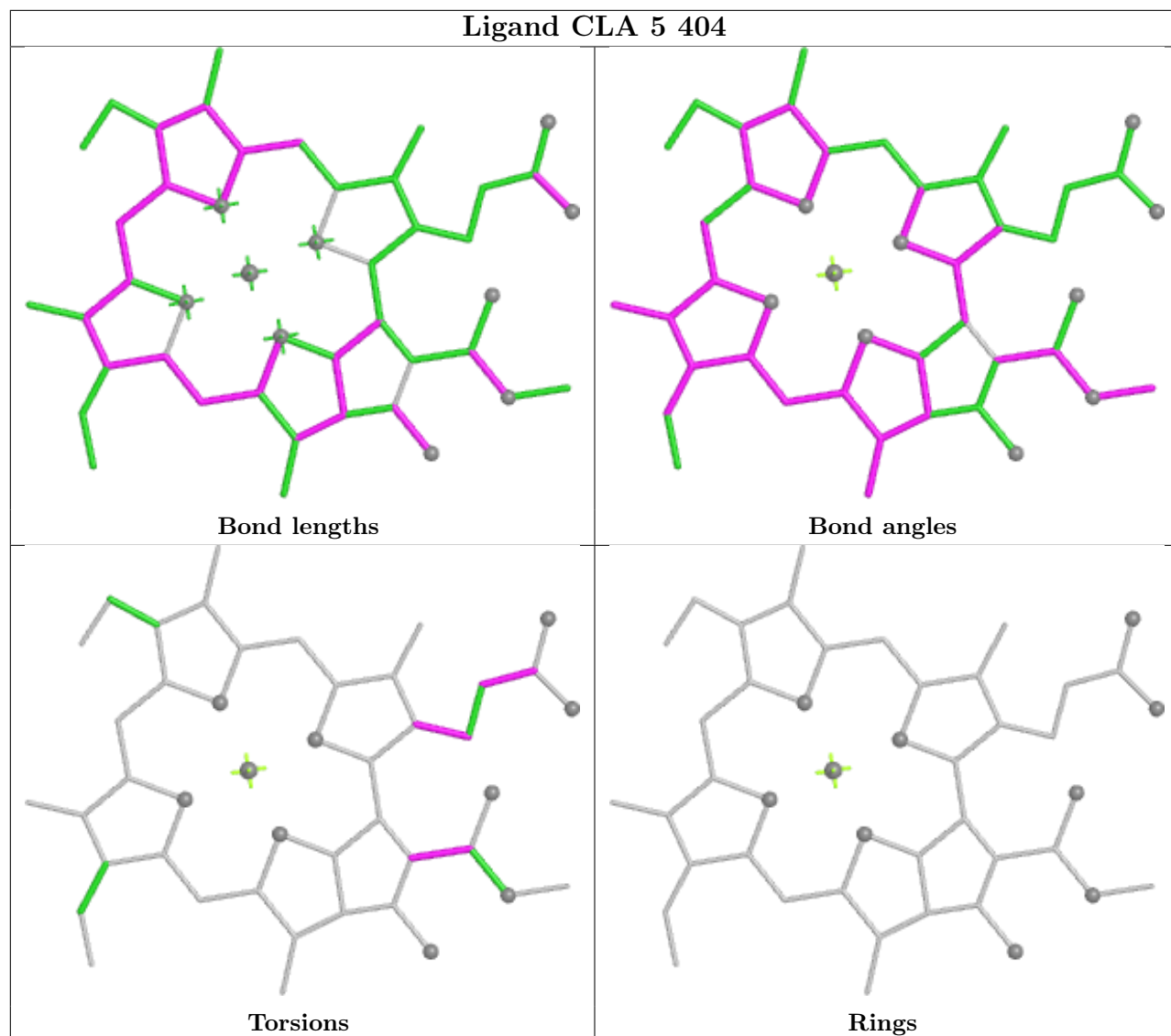
Ligand CLA 1 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings



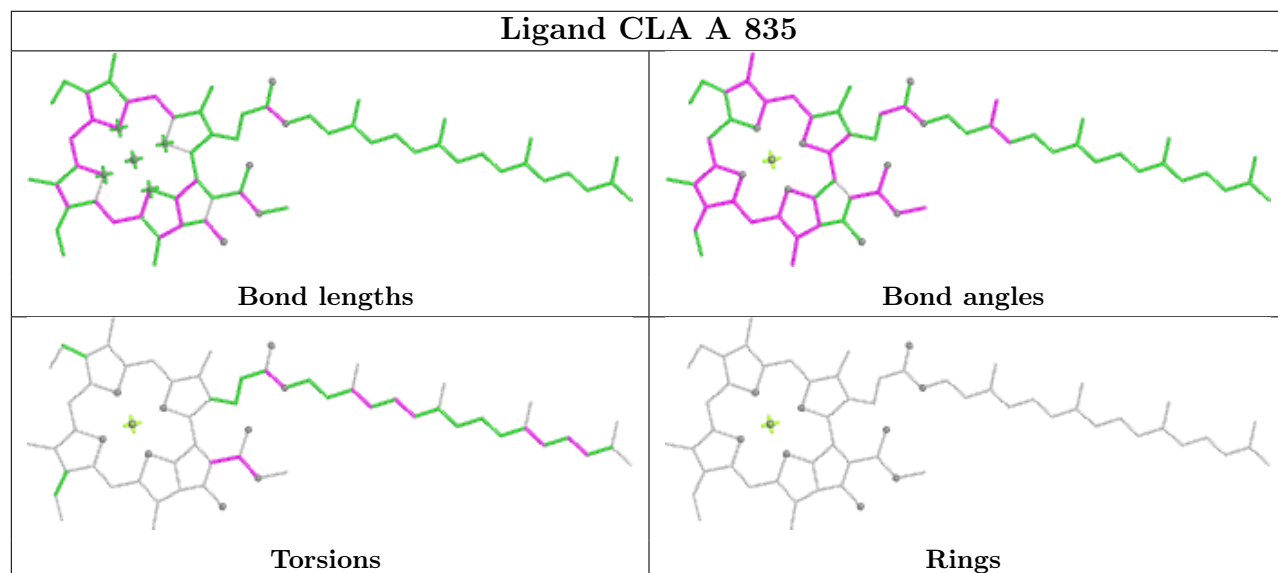
Ligand CLA 2 405



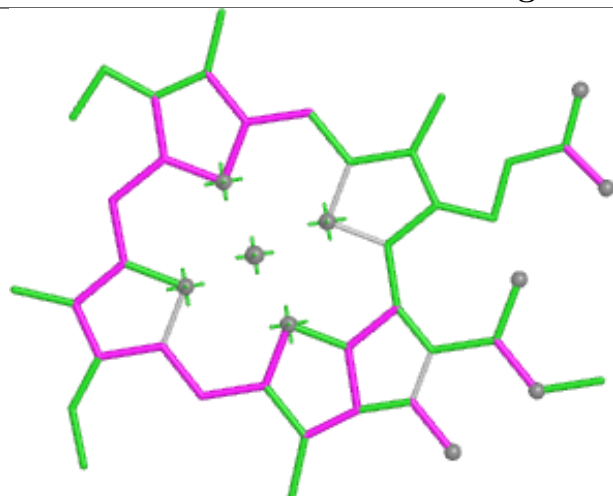
Ligand CLA 5 404



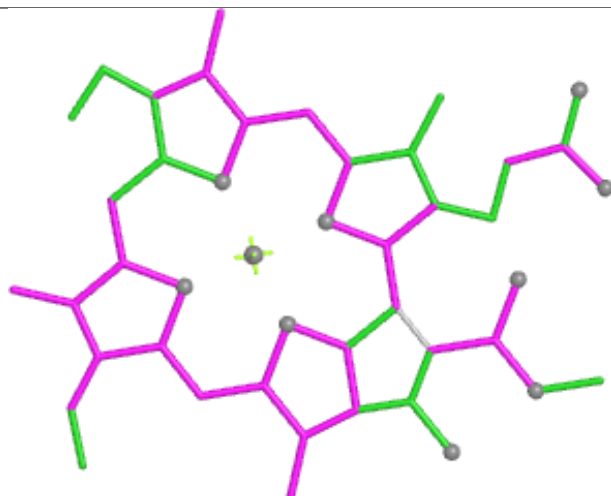
Ligand CLA A 835



Ligand CLA J 101



Bond lengths



Bond angles

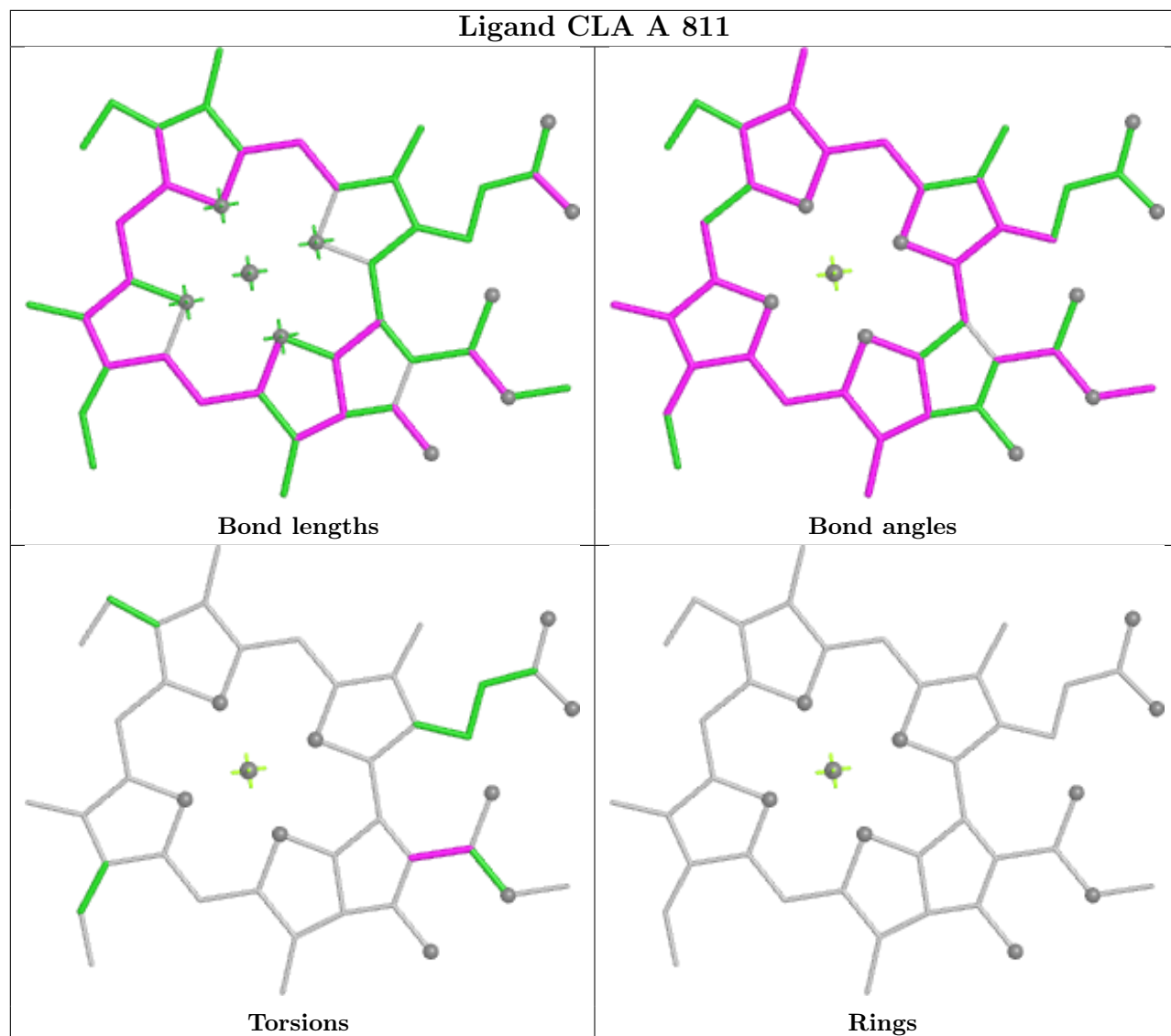


Torsions

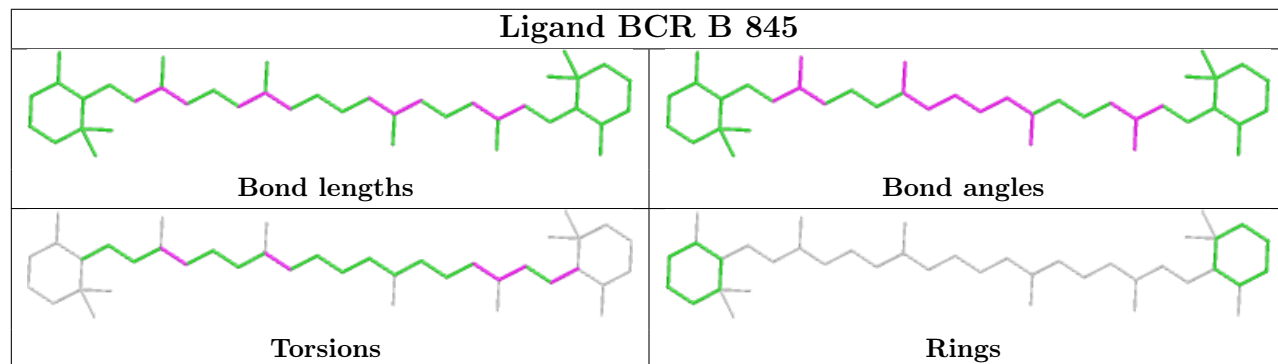


Rings

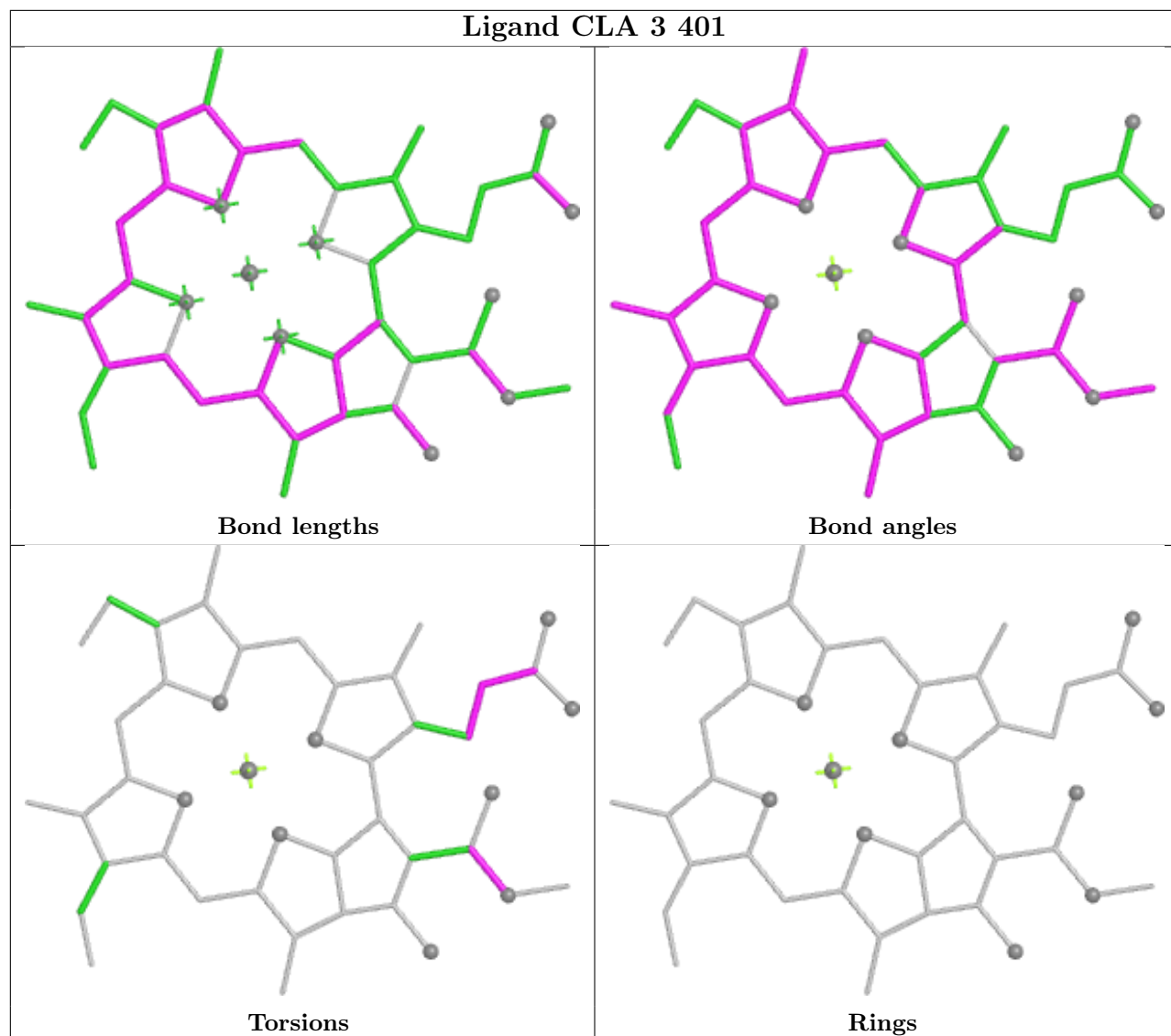
Ligand CLA A 811



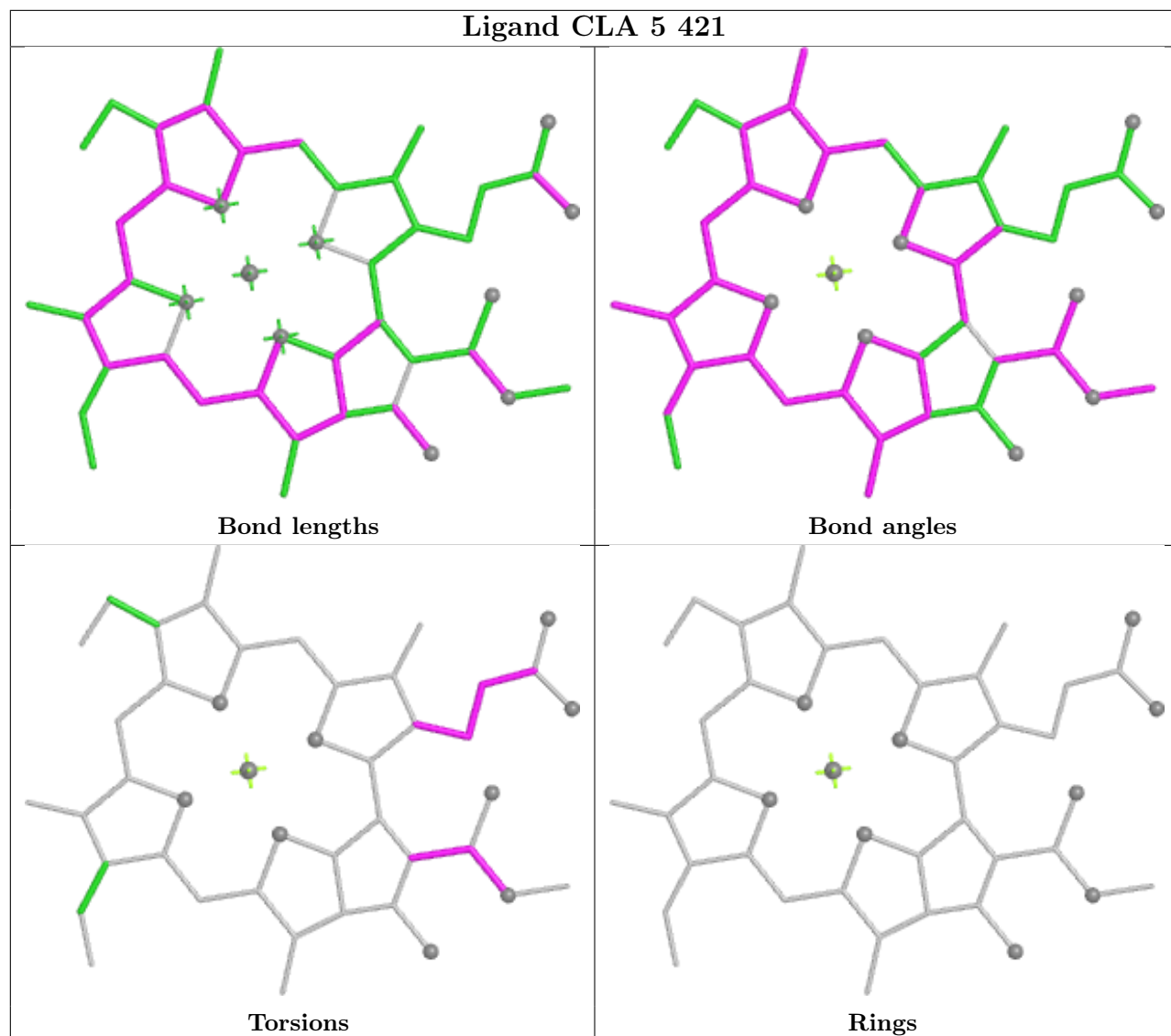
Ligand BCR B 845



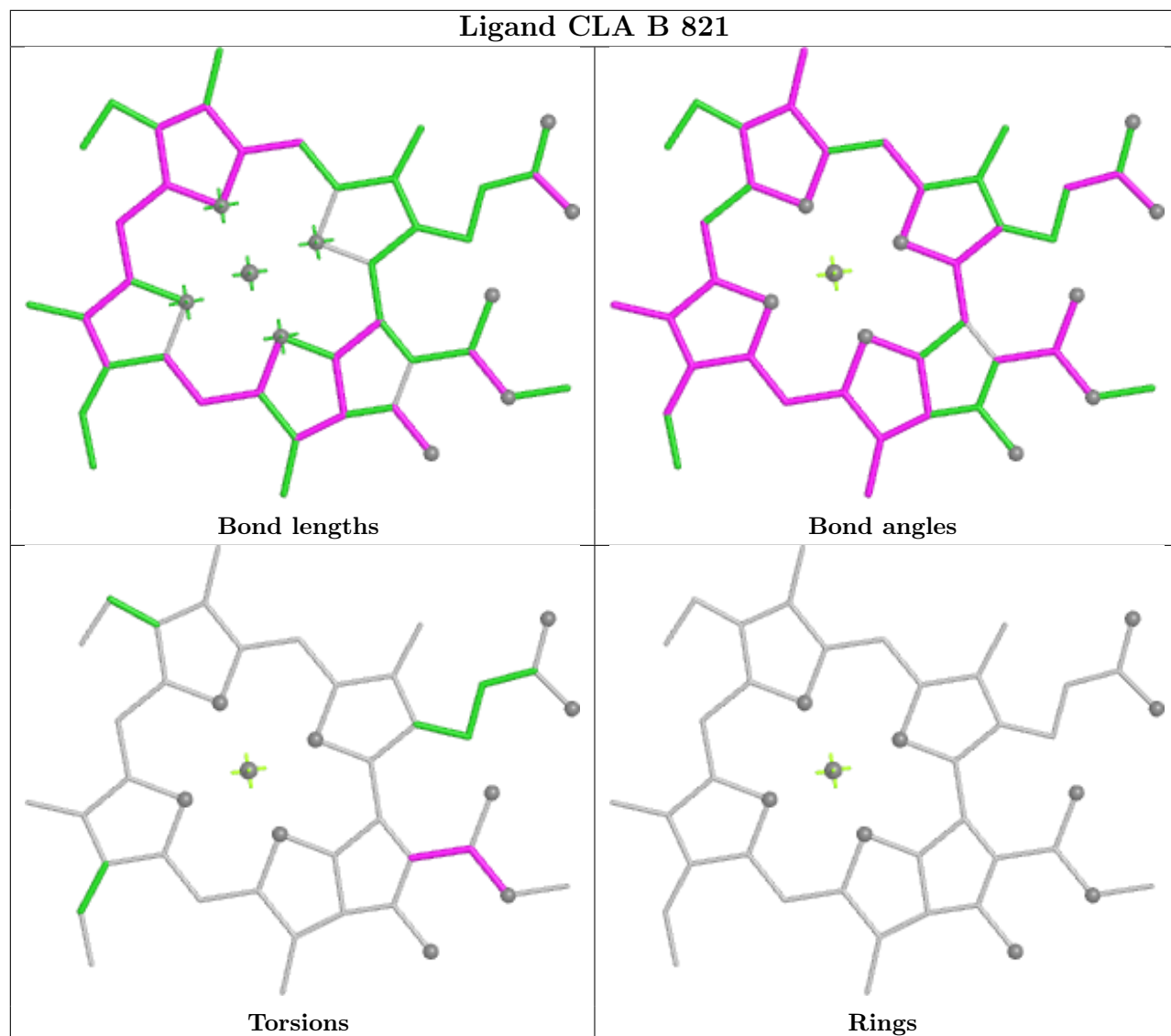
Ligand CLA 3 401



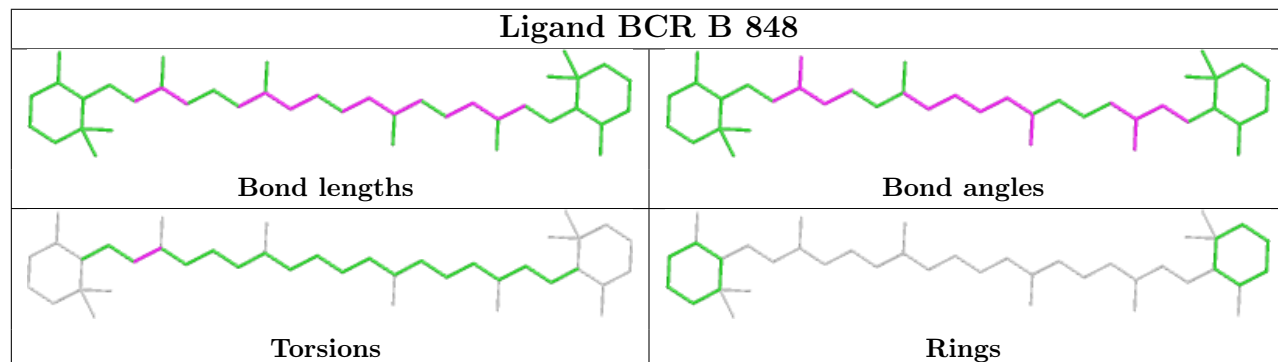
Ligand CLA 5 421



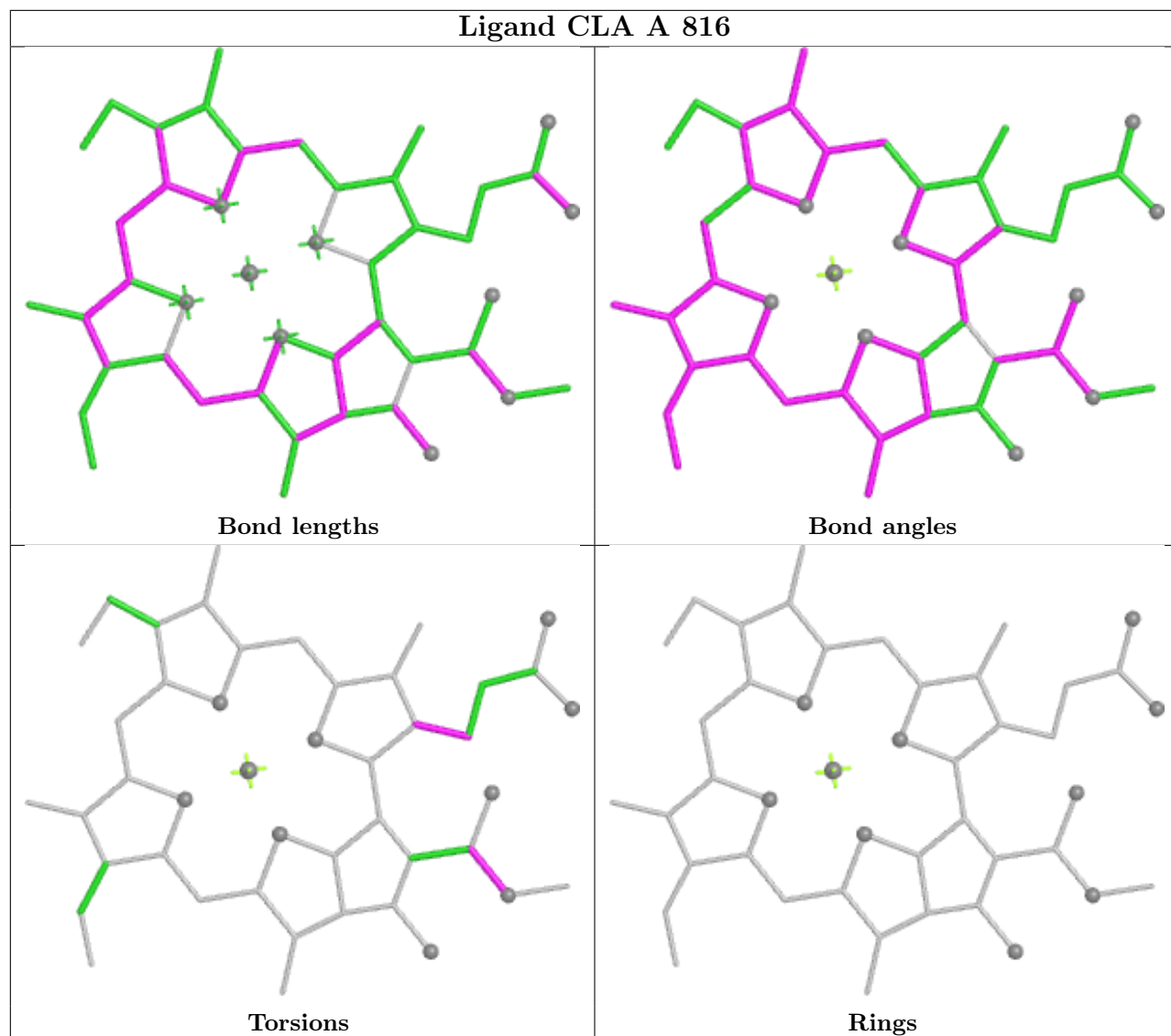
Ligand CLA B 821

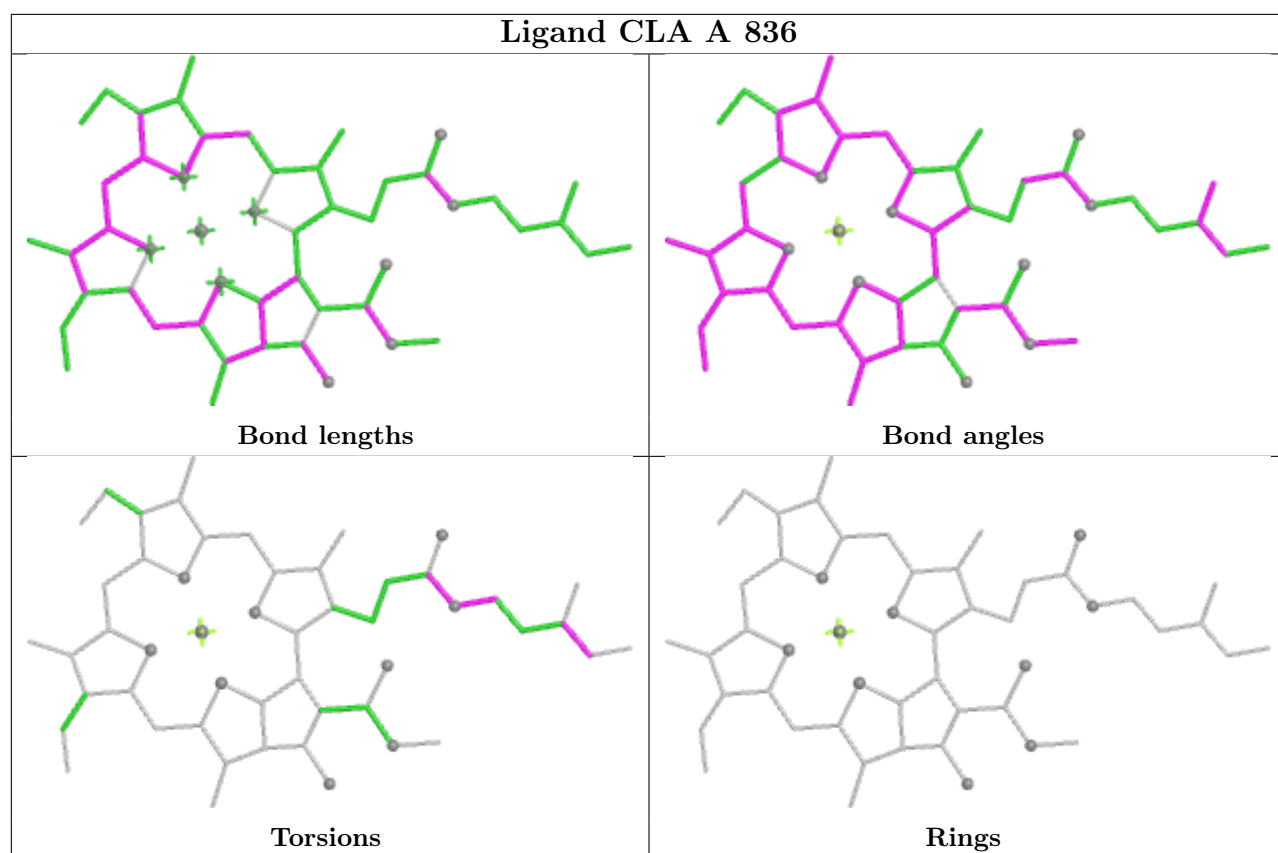


Ligand BCR B 848

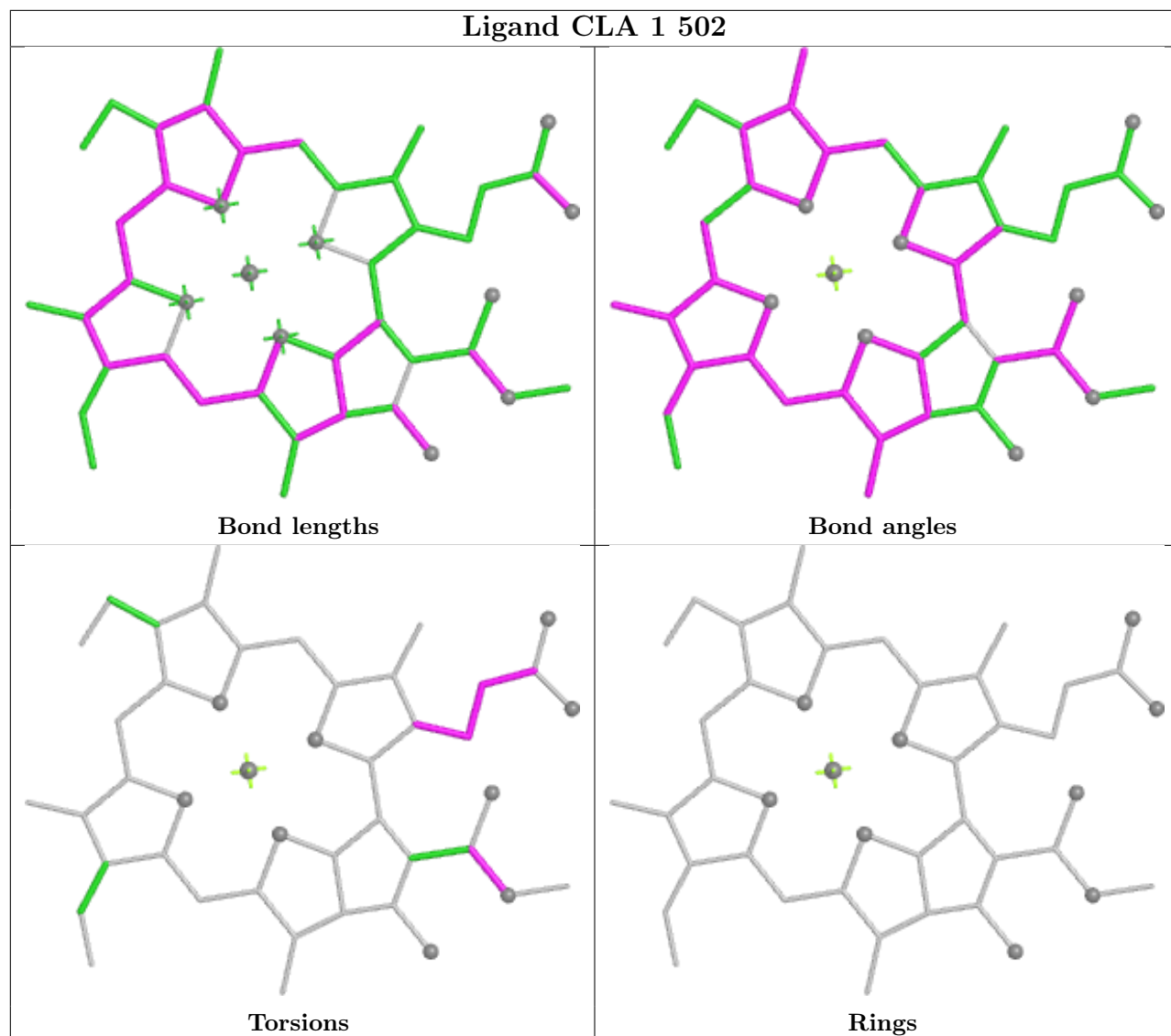


Ligand CLA A 816

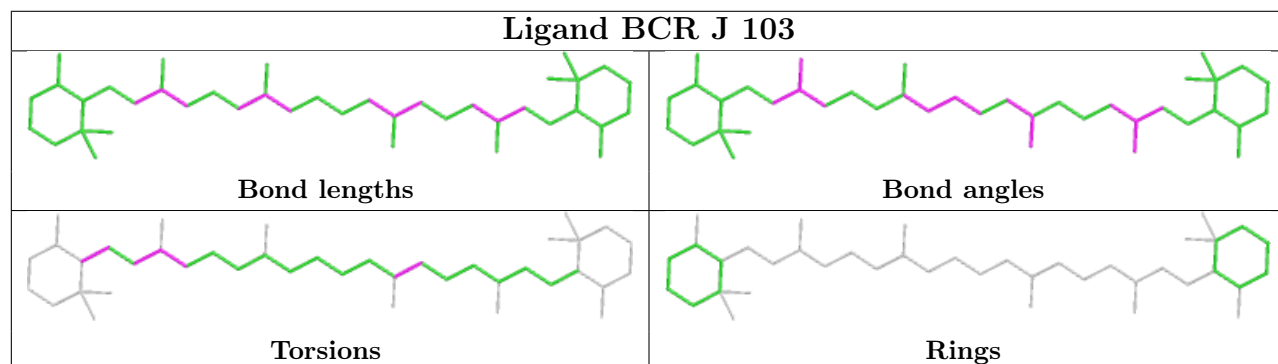




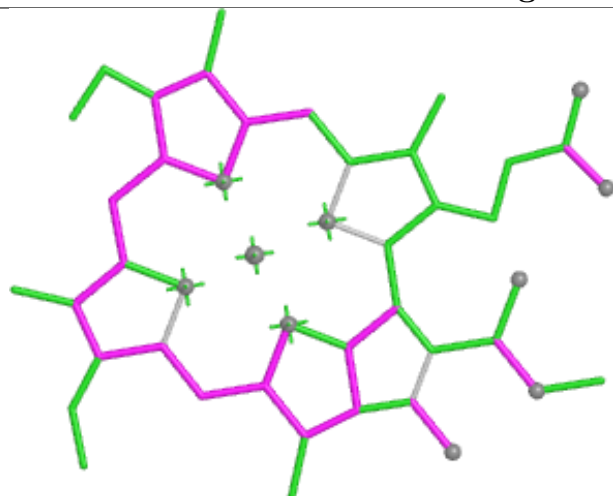
Ligand CLA 1 502



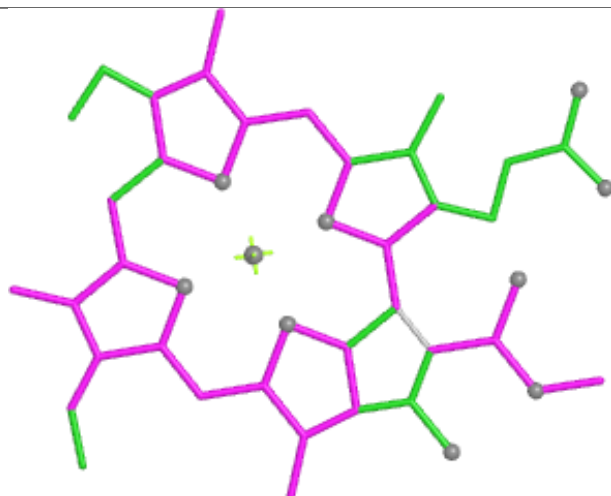
Ligand BCR J 103



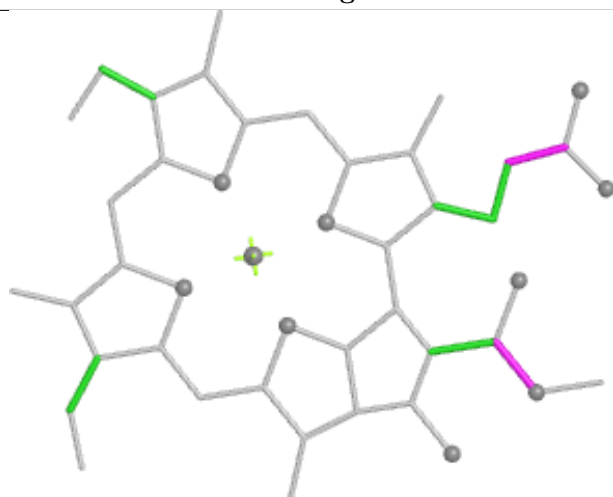
Ligand CLA 6 403



Bond lengths



Bond angles

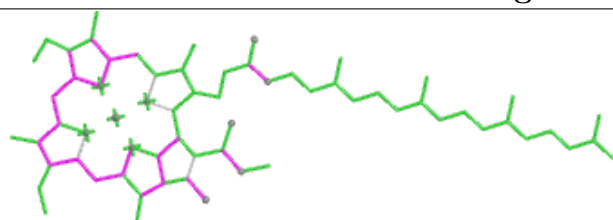


Torsions

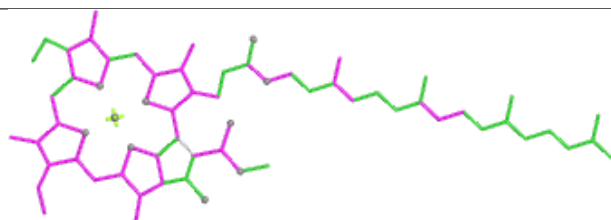


Rings

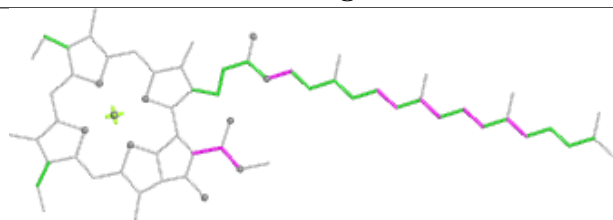
Ligand CLA B 801



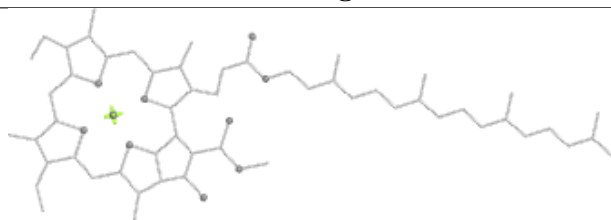
Bond lengths



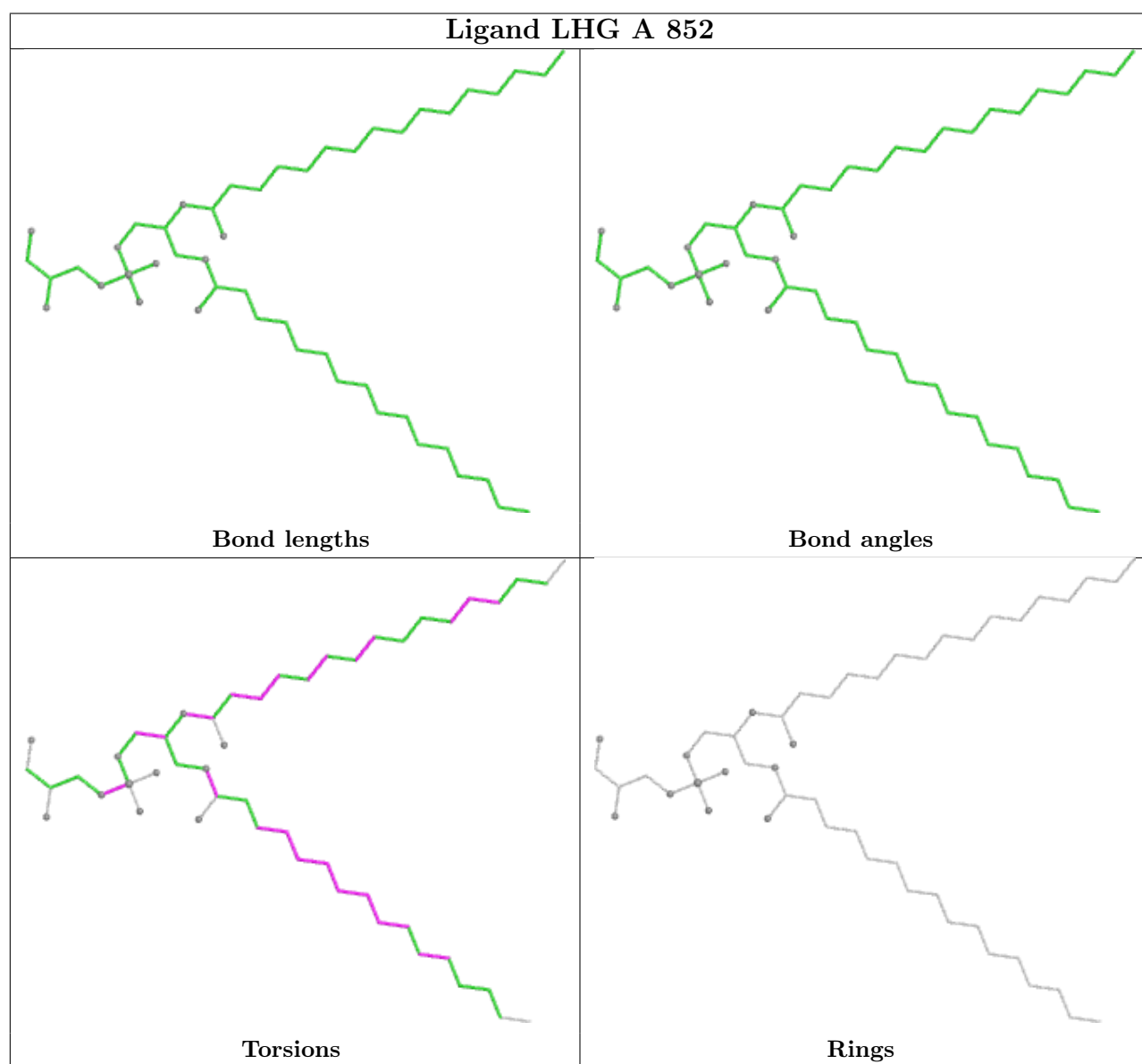
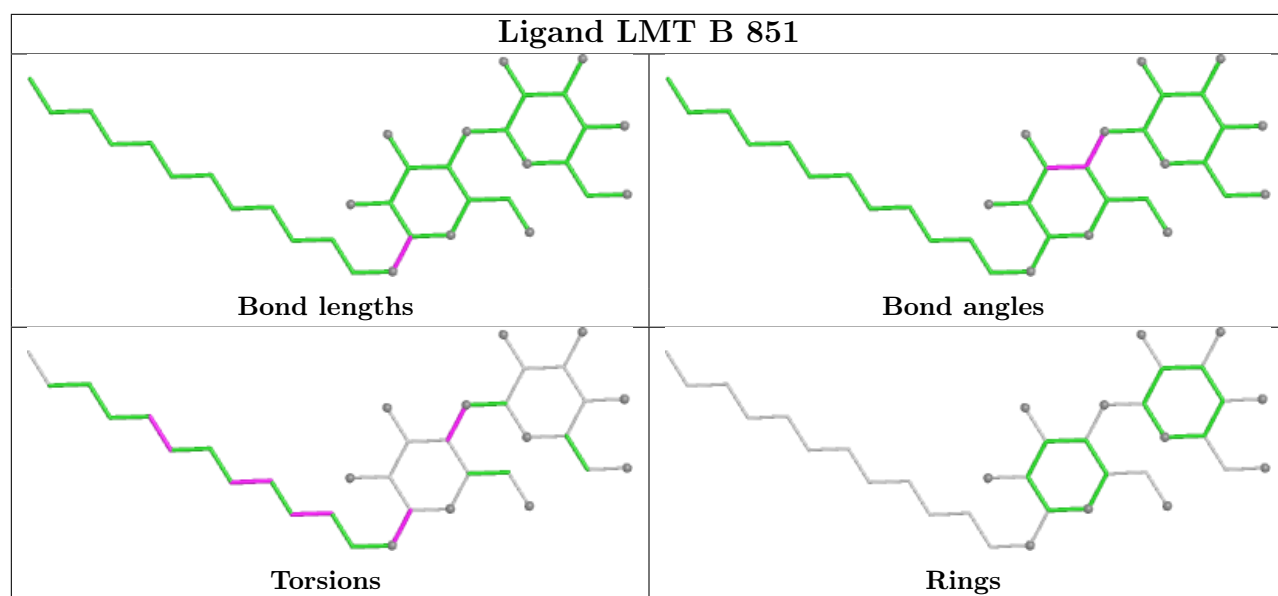
Bond angles

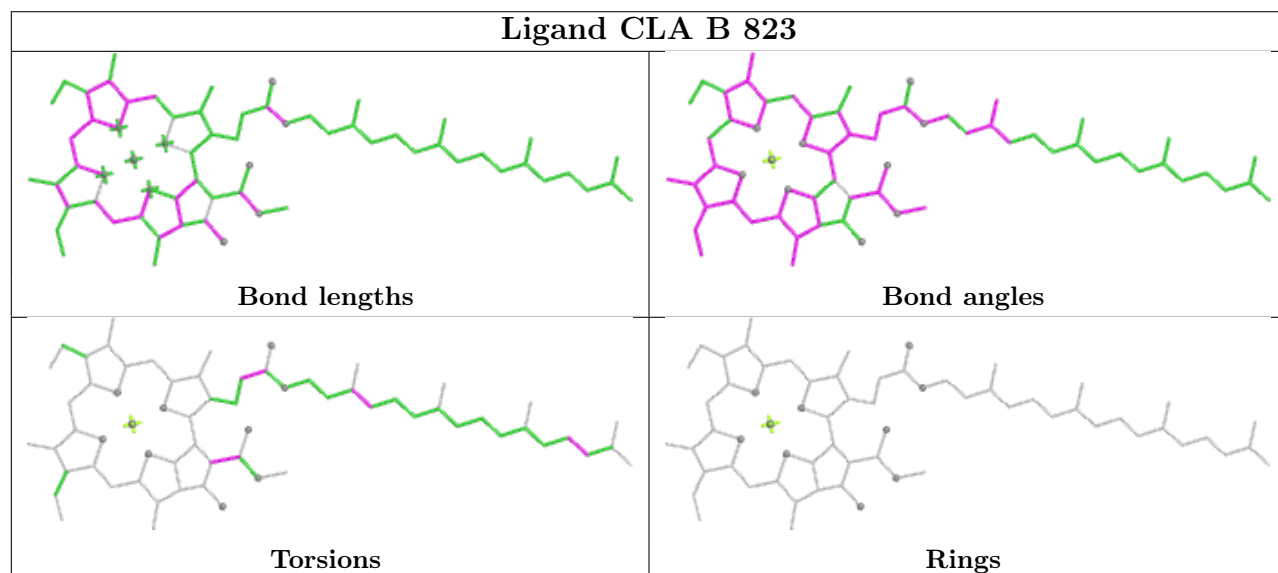
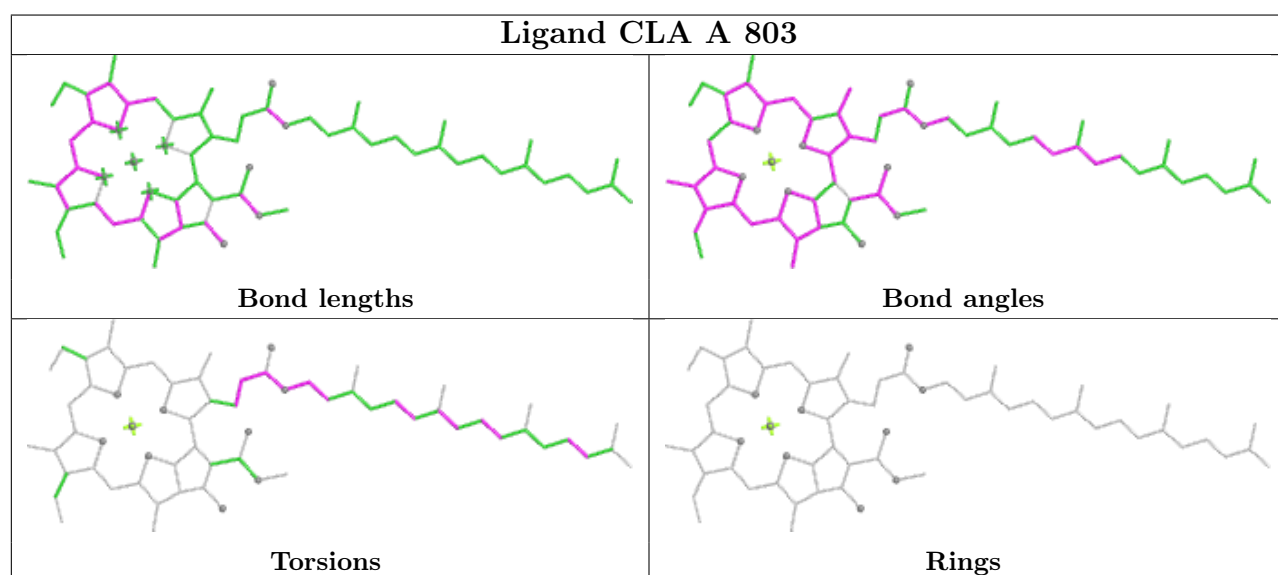
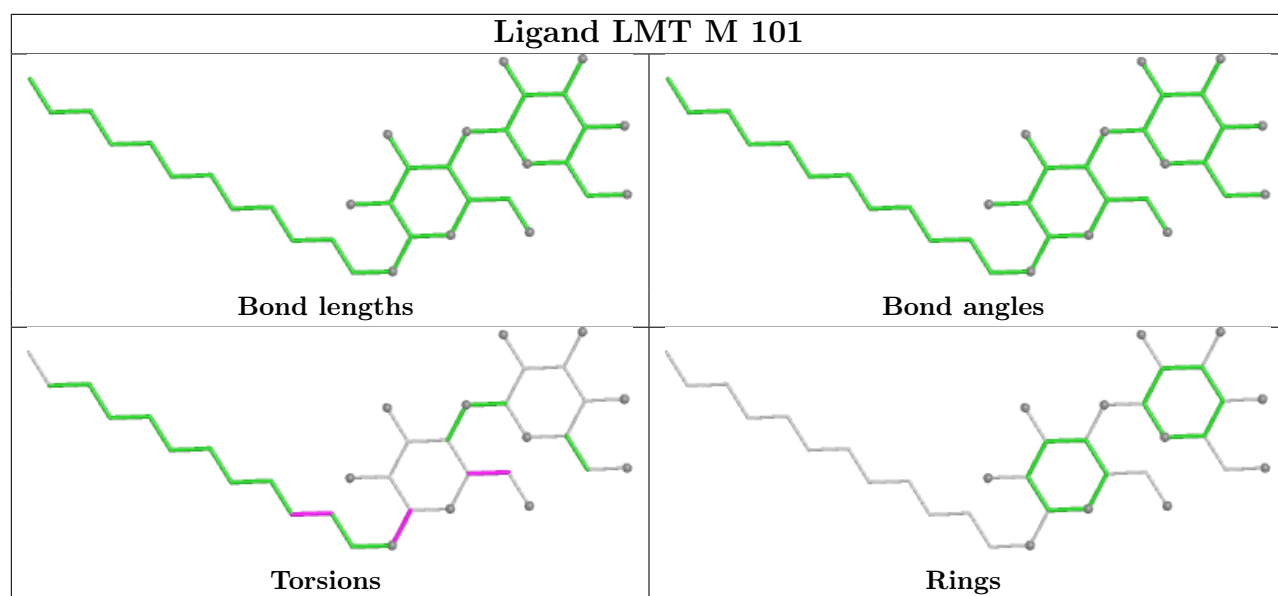


Torsions

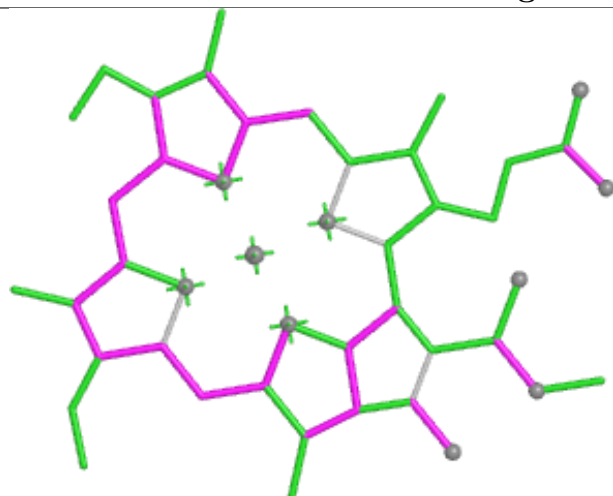


Rings

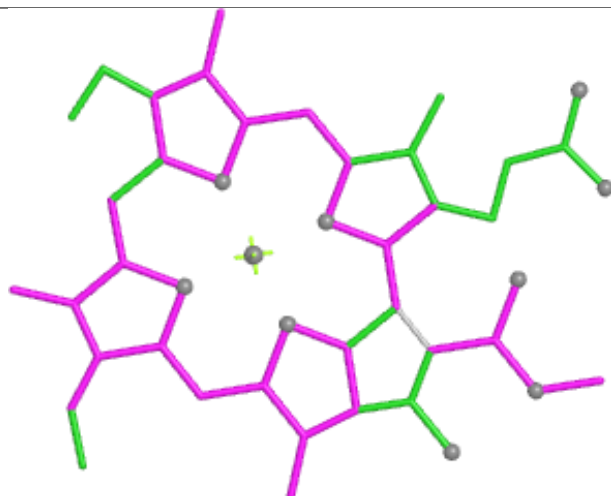




Ligand CLA J 102



Bond lengths



Bond angles

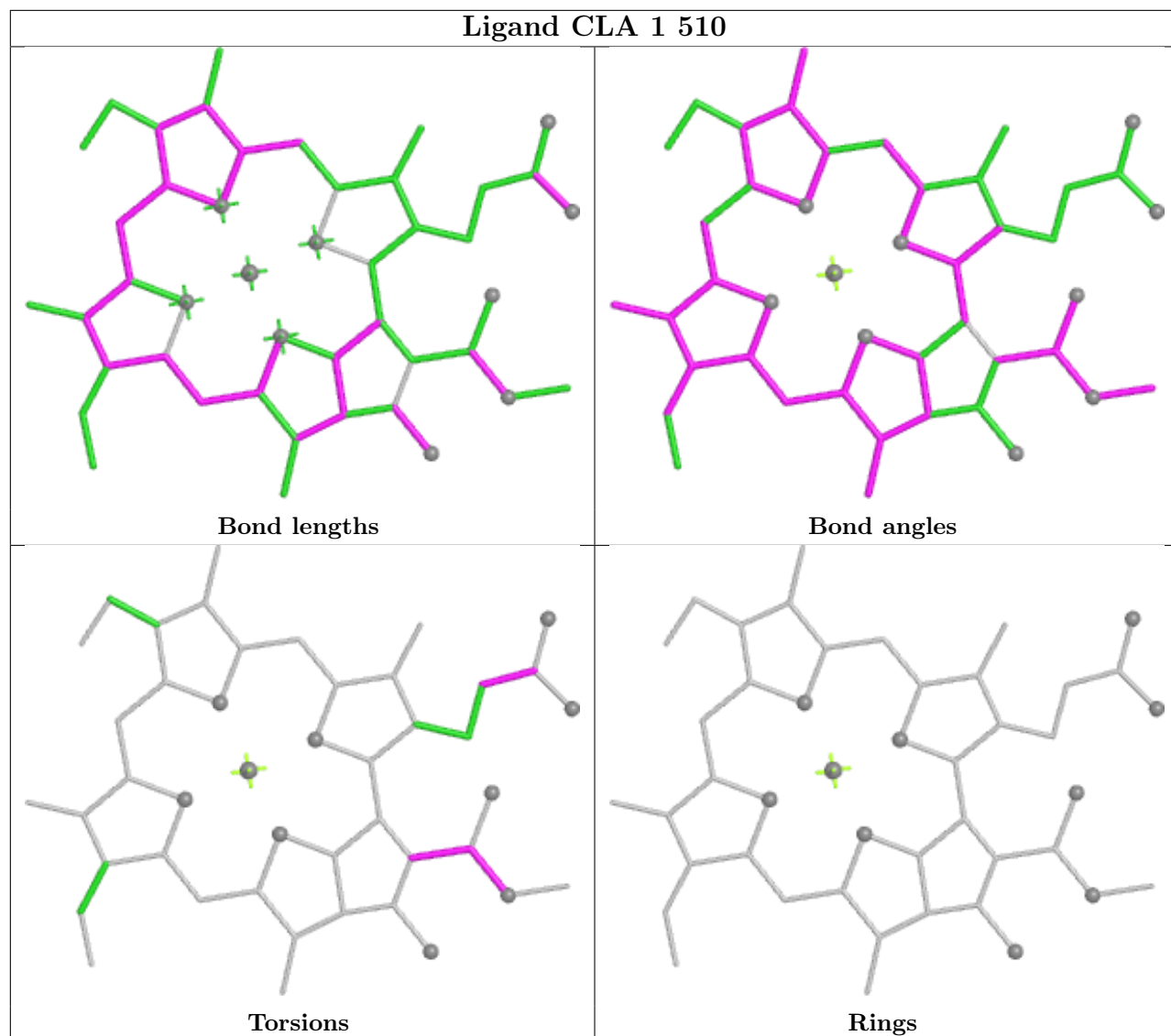


Torsions

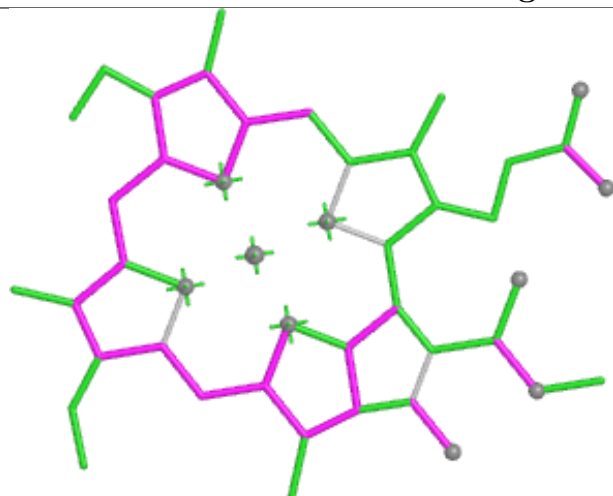


Rings

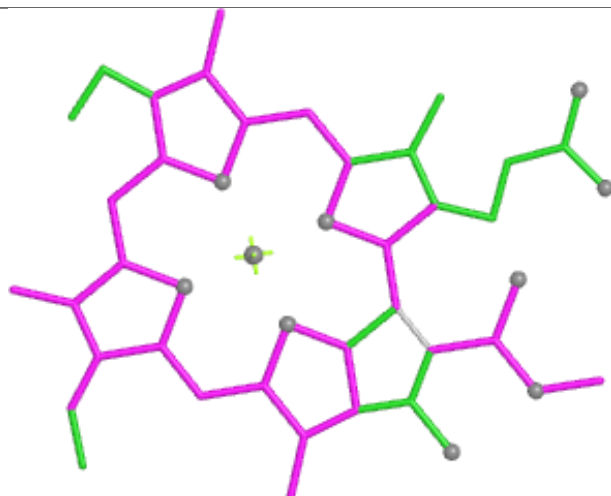
Ligand CLA 1 510



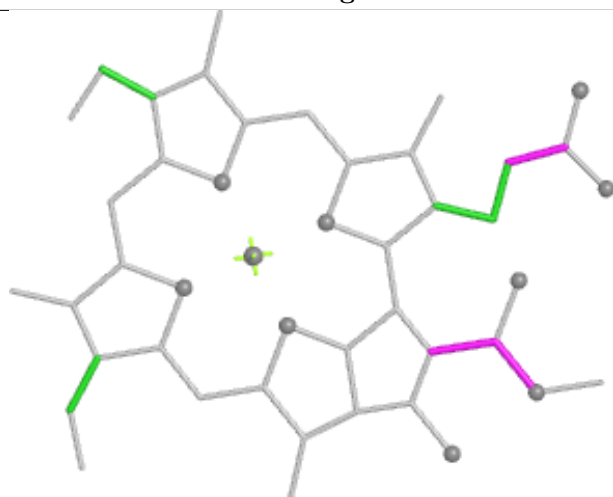
Ligand CLA 6 405



Bond lengths



Bond angles

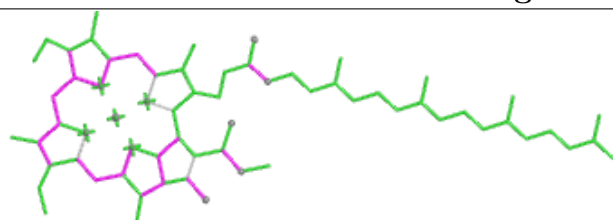


Torsions

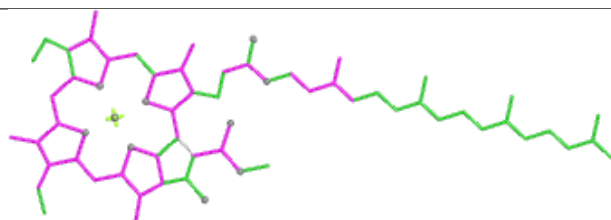


Rings

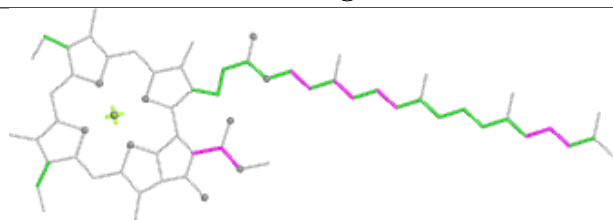
Ligand CLA B 824



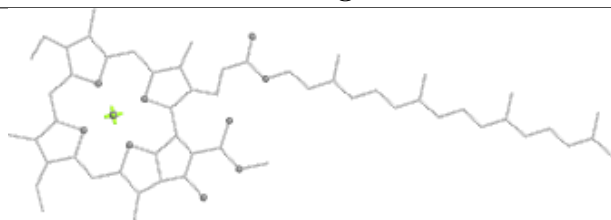
Bond lengths



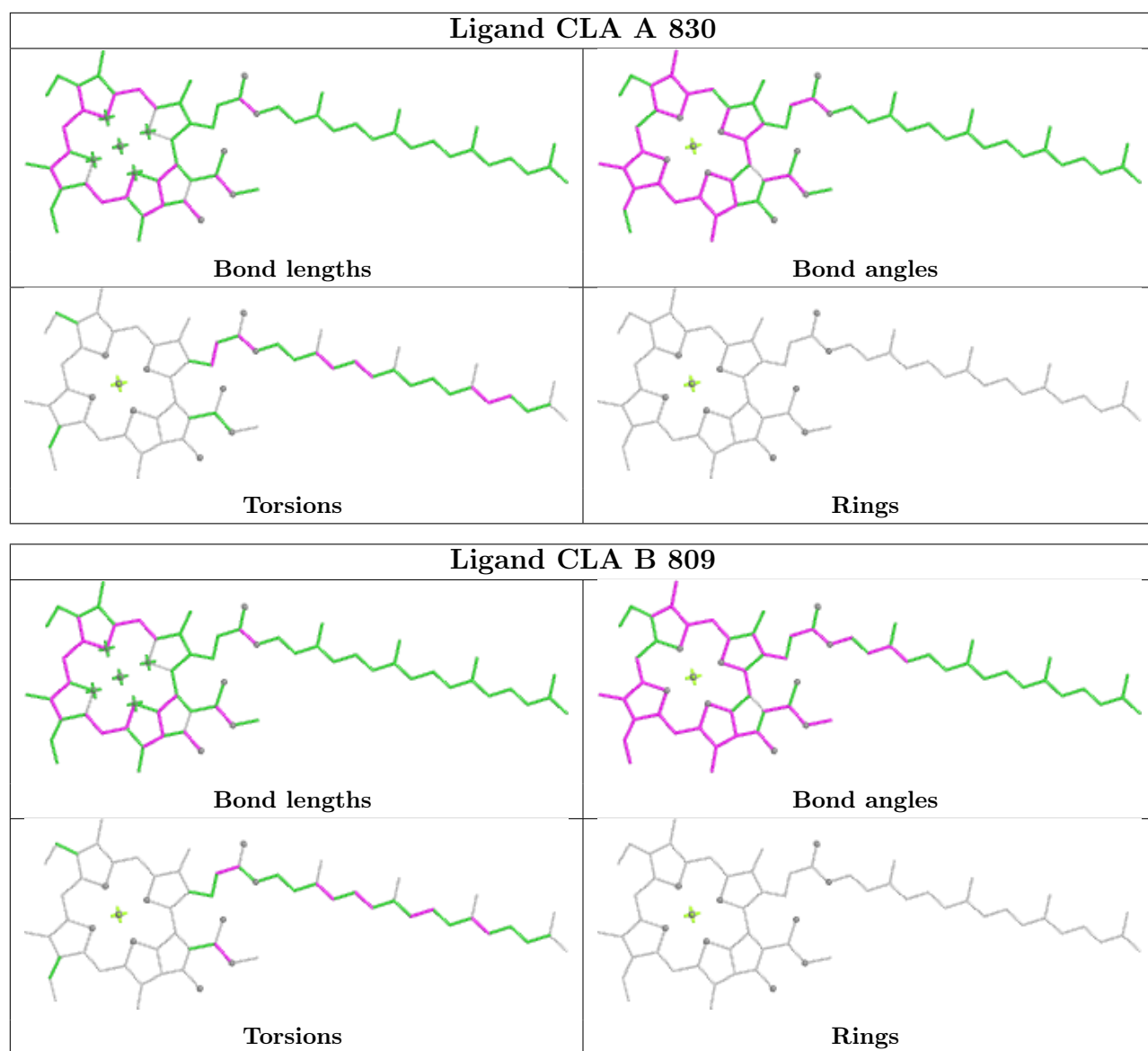
Bond angles



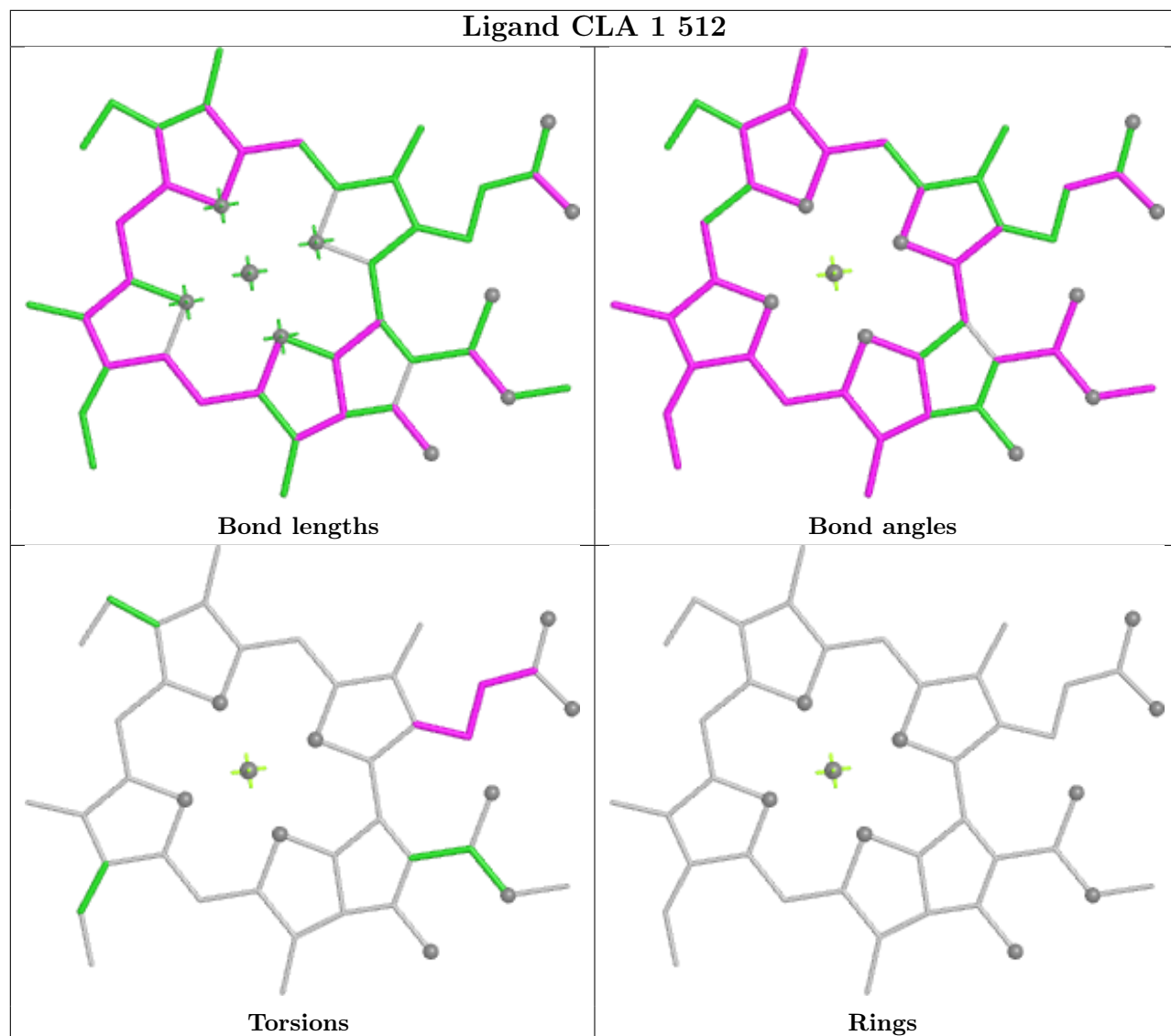
Torsions



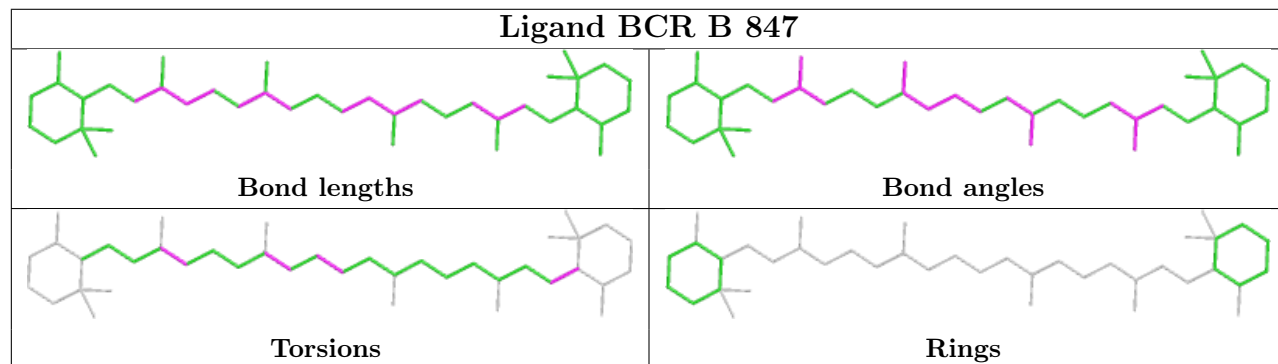
Rings



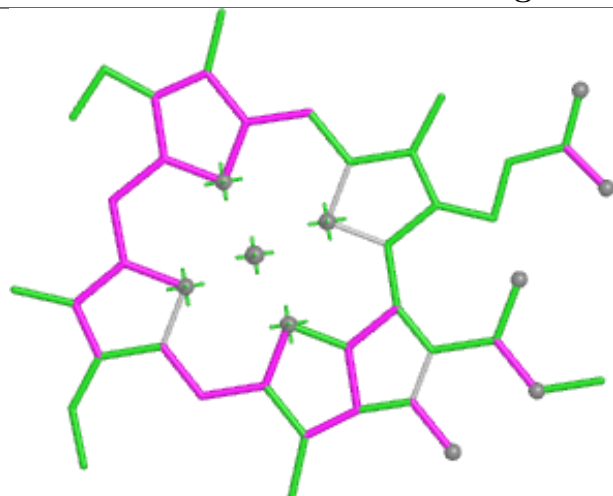
Ligand CLA 1 512



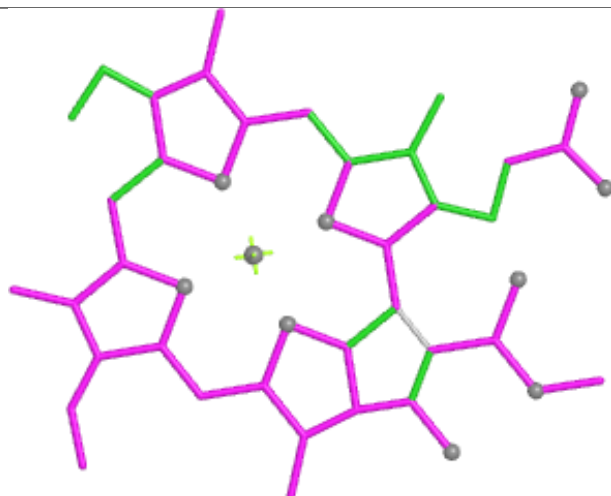
Ligand BCR B 847



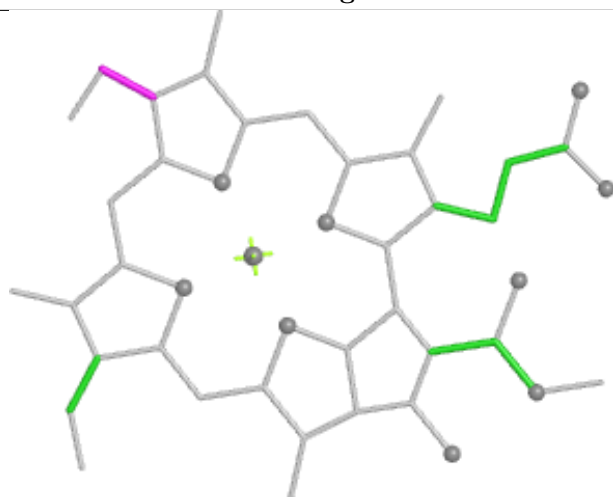
Ligand CLA B 812



Bond lengths



Bond angles

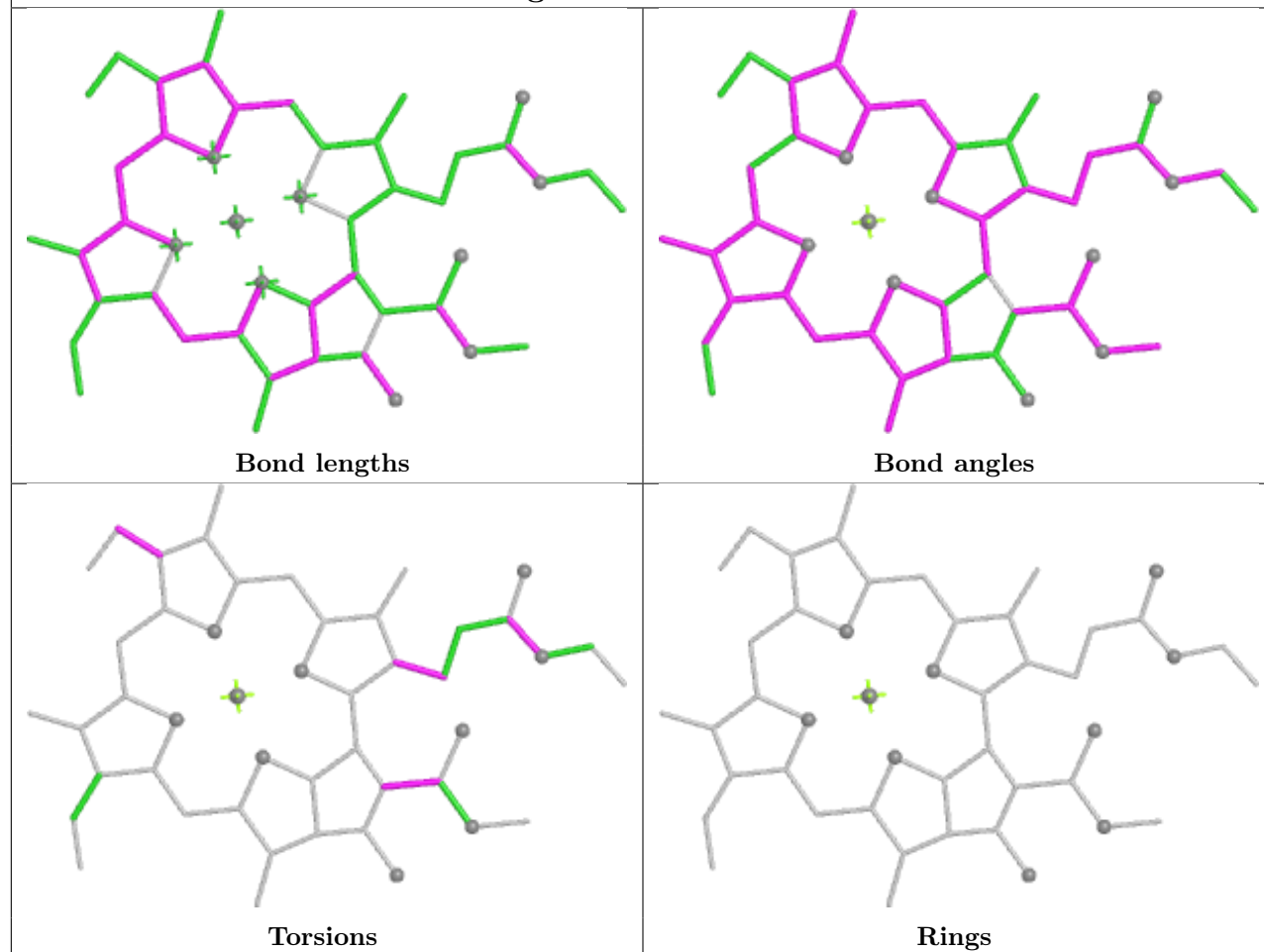


Torsions

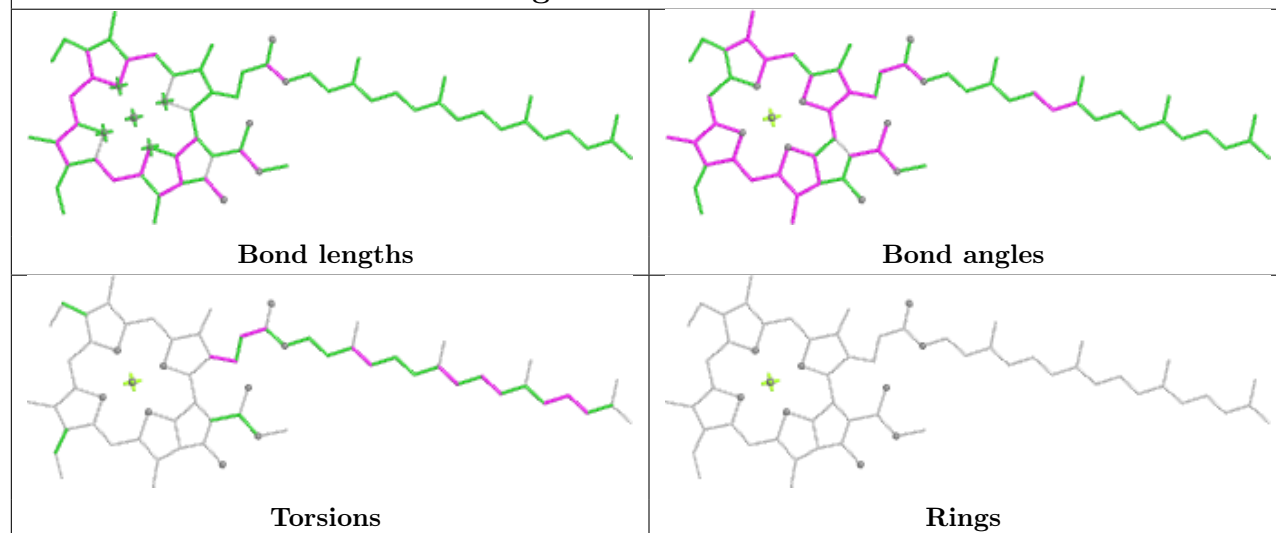


Rings

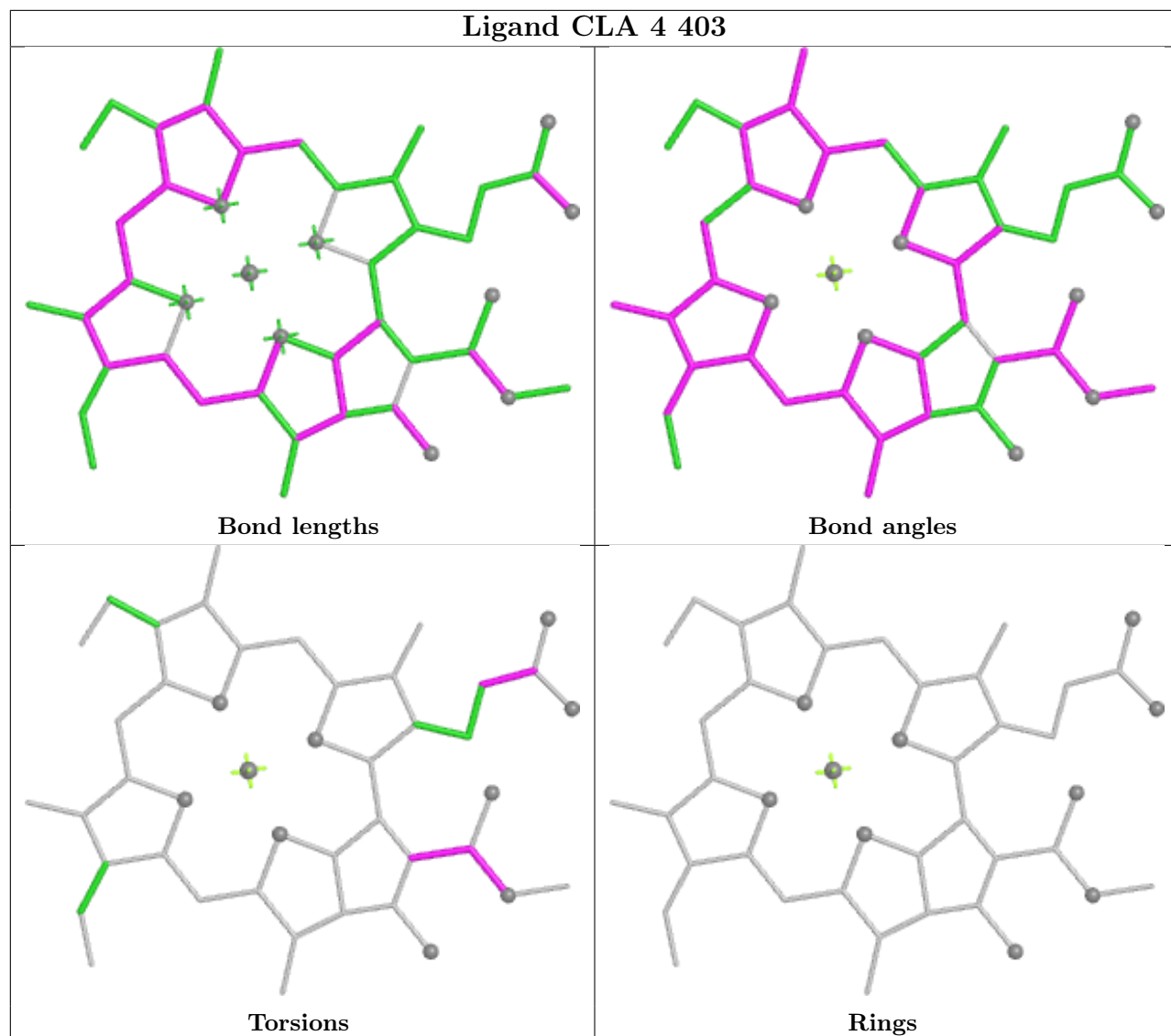
Ligand CLA B 820



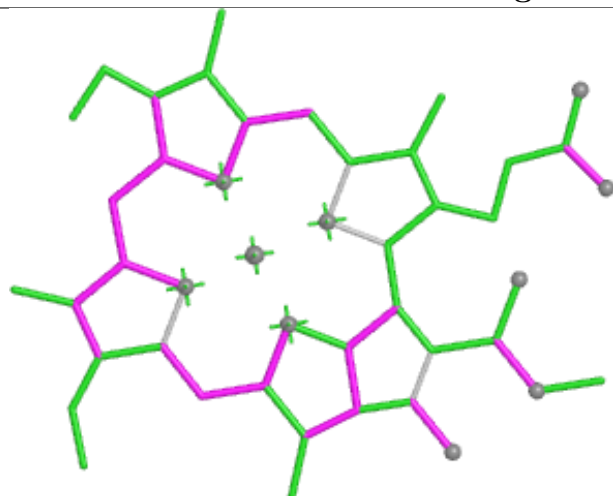
Ligand CLA B 832



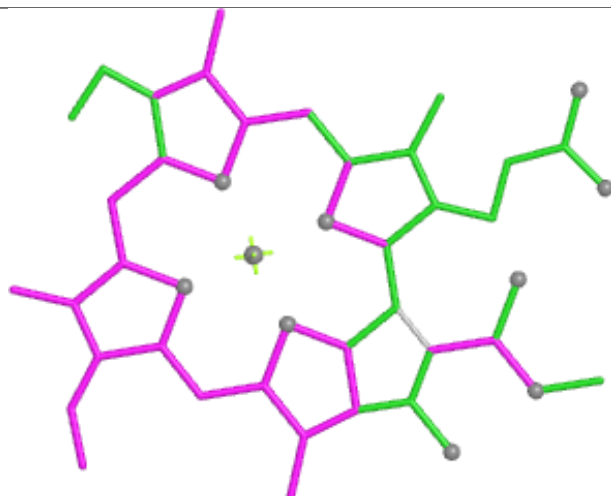
Ligand CLA 4 403



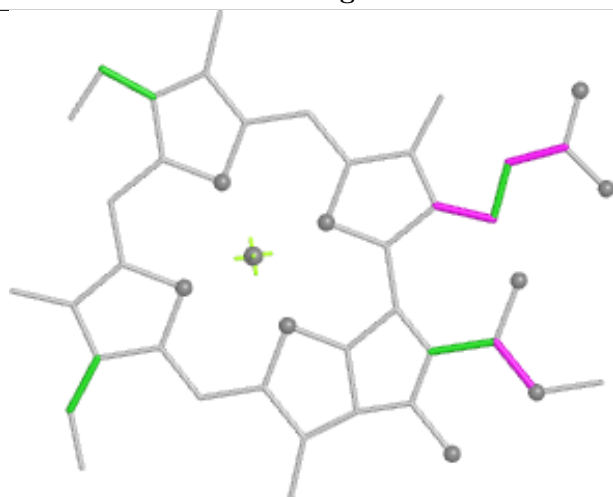
Ligand CLA B 835



Bond lengths



Bond angles

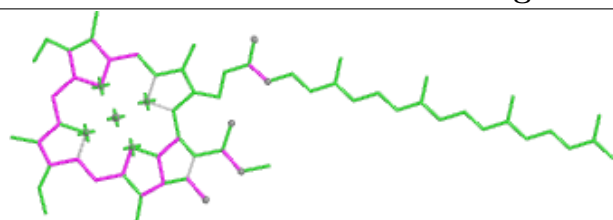


Torsions

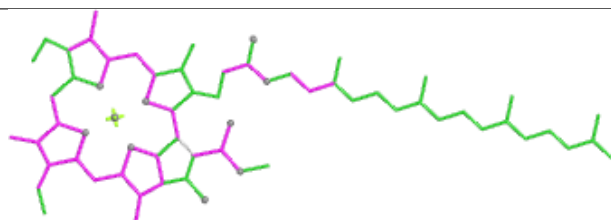


Rings

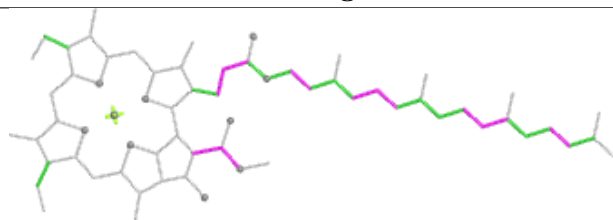
Ligand CLA A 814



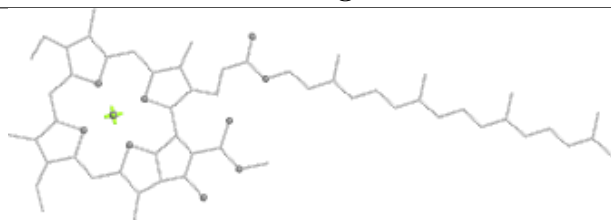
Bond lengths



Bond angles

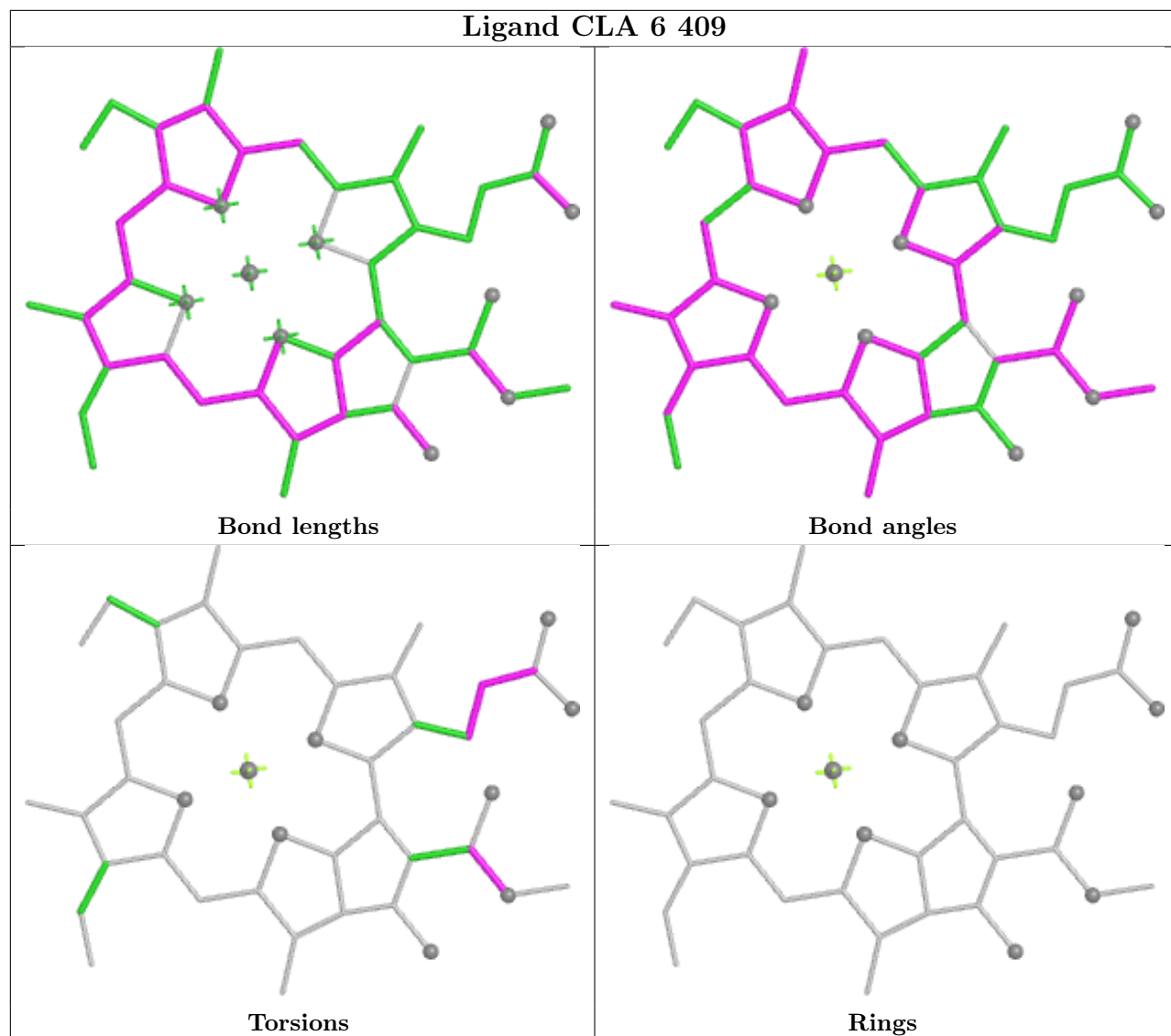


Torsions

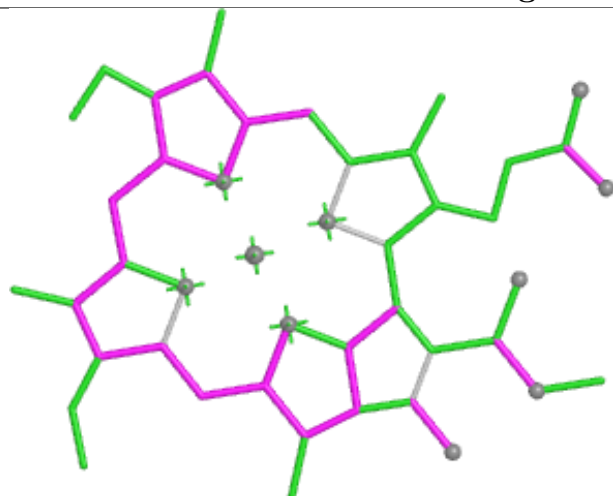


Rings

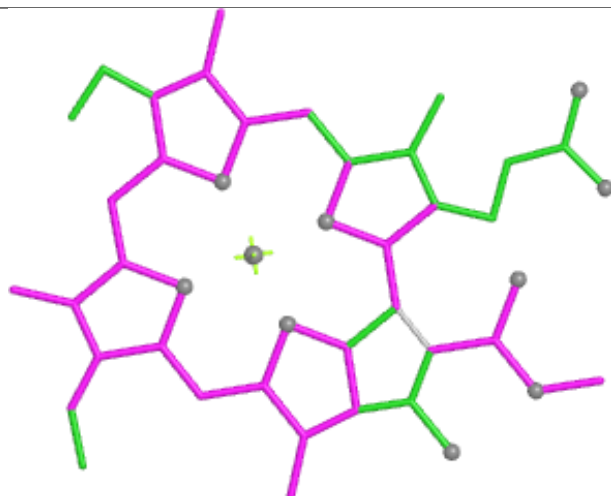
Ligand CLA 6 409



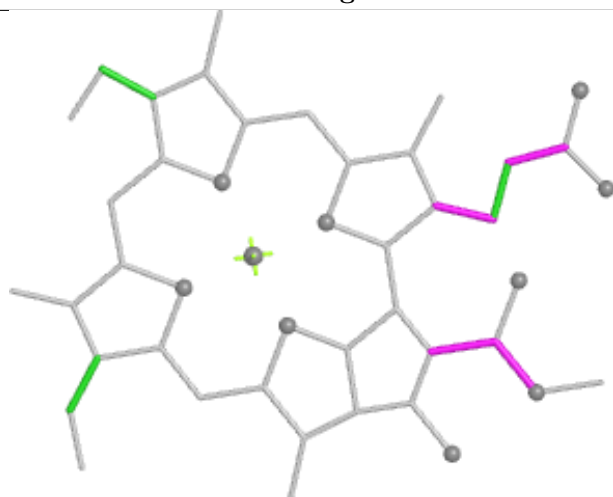
Ligand CLA 6 401



Bond lengths



Bond angles

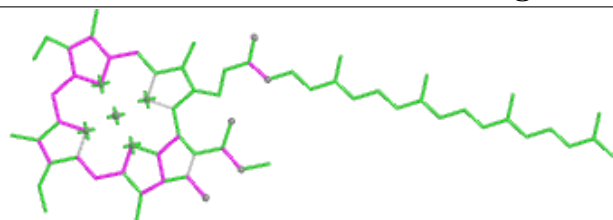


Torsions

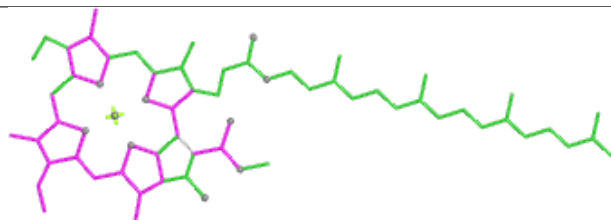


Rings

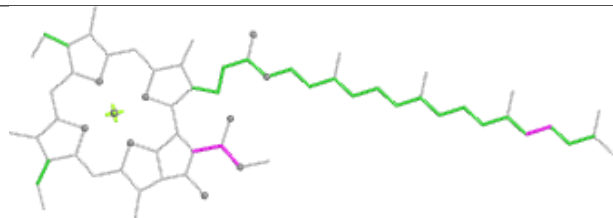
Ligand CLA A 831



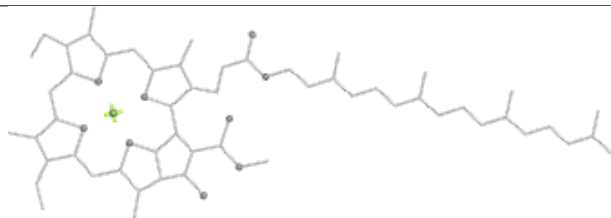
Bond lengths



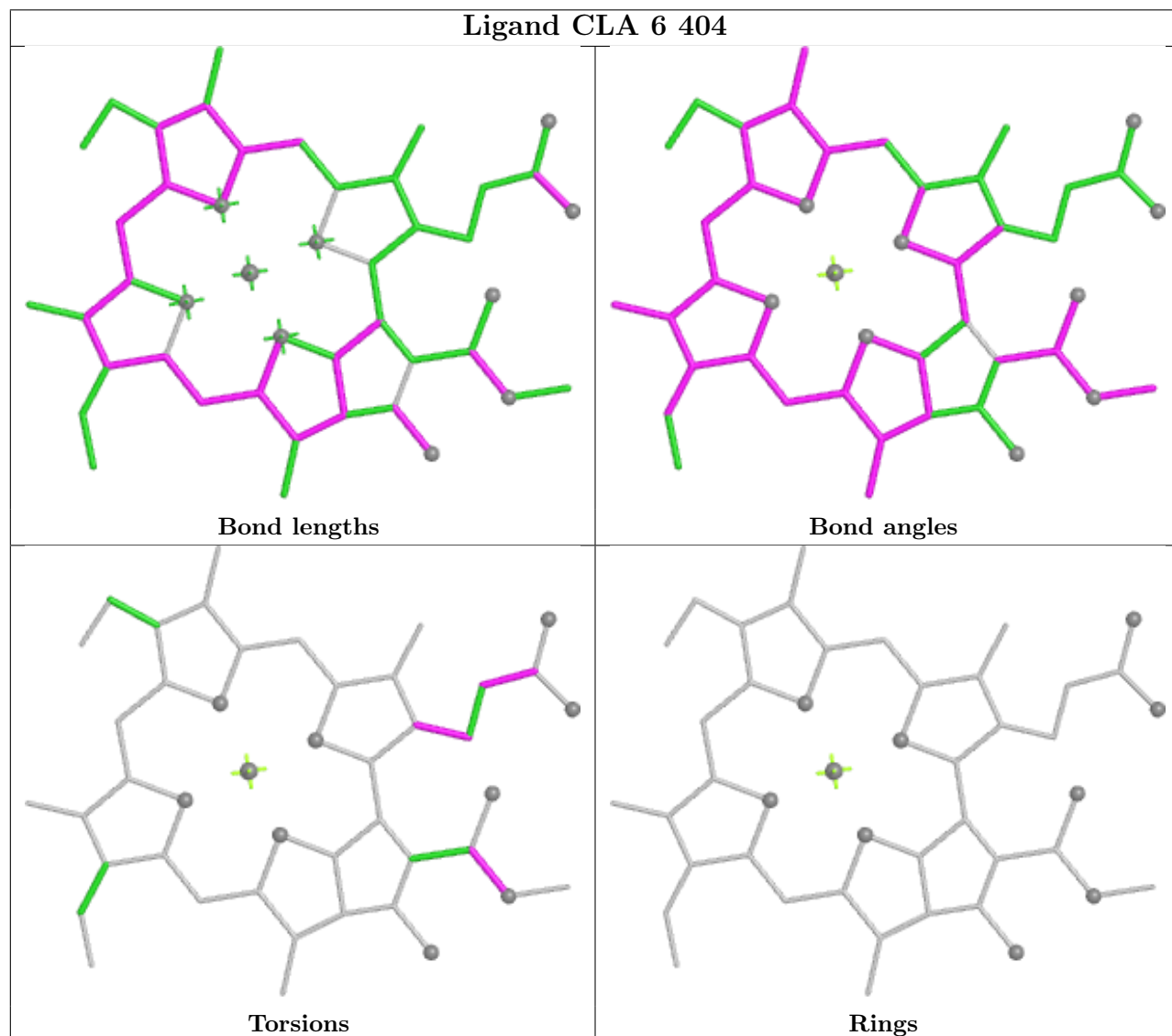
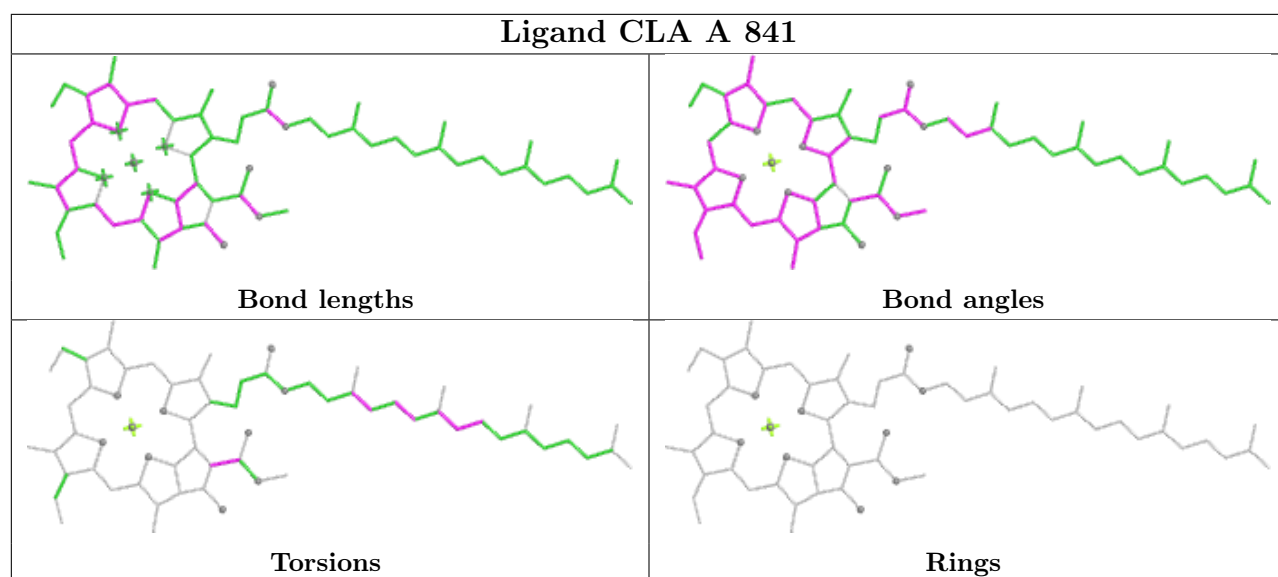
Bond angles

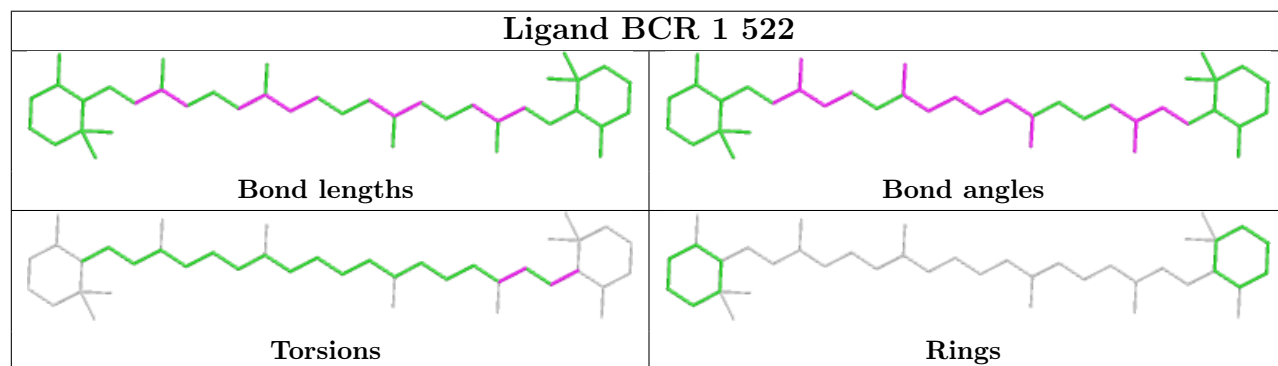
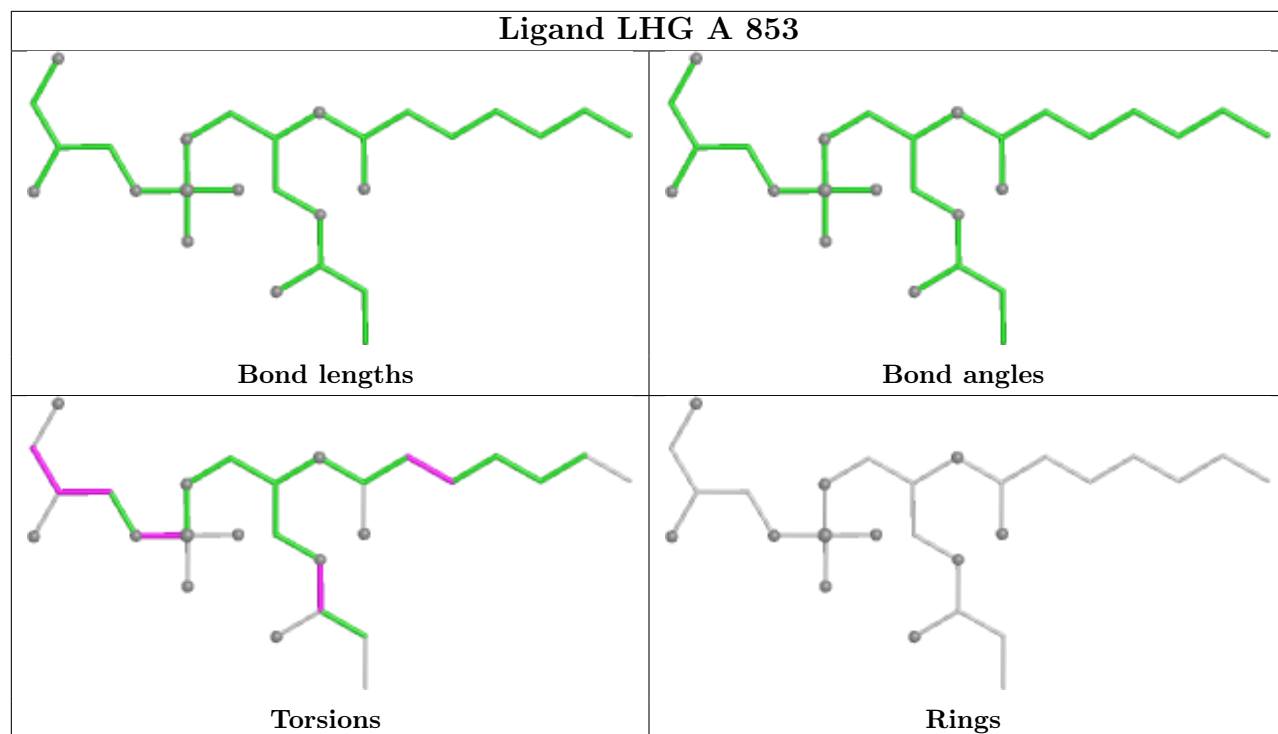


Torsions

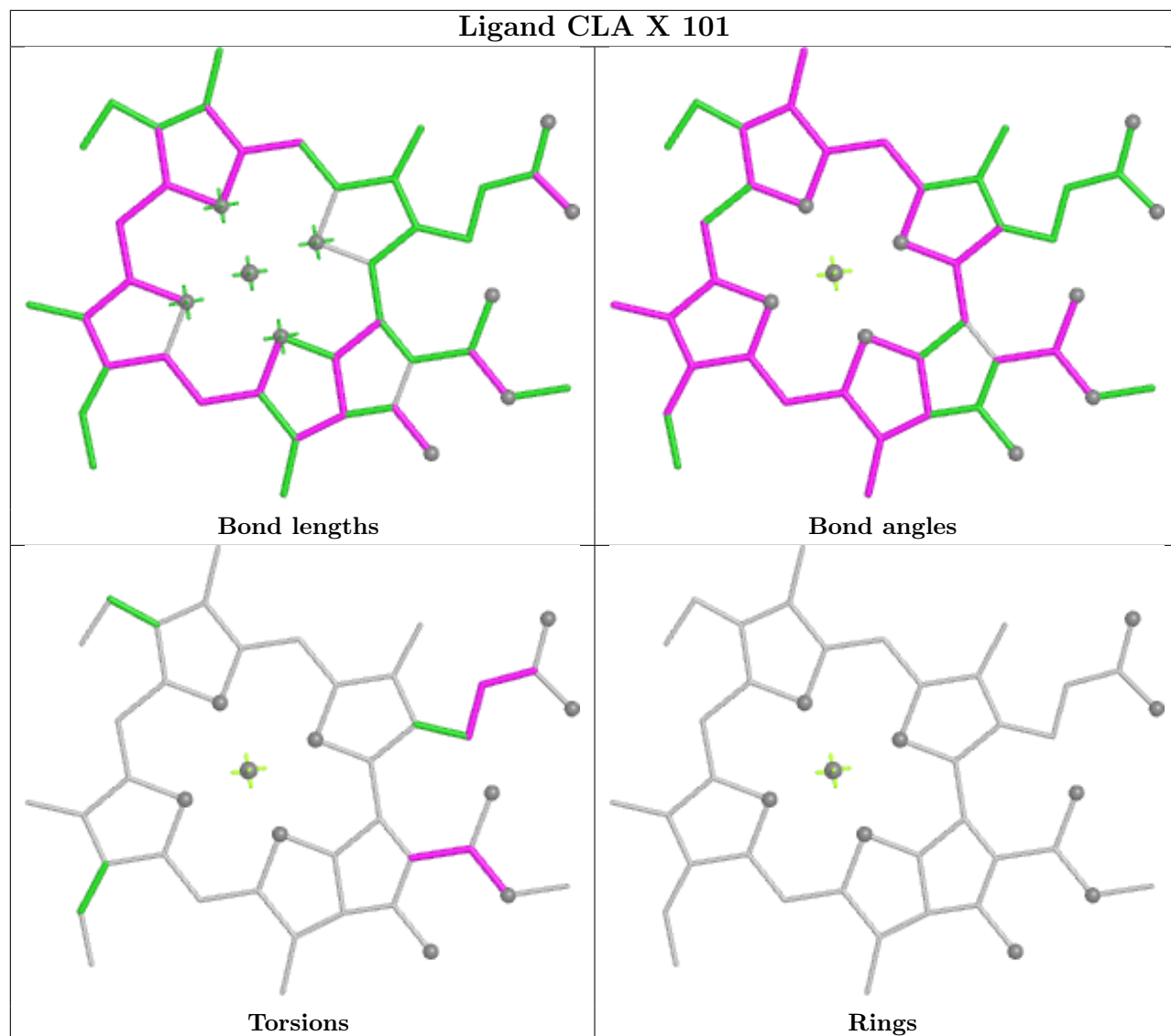


Rings

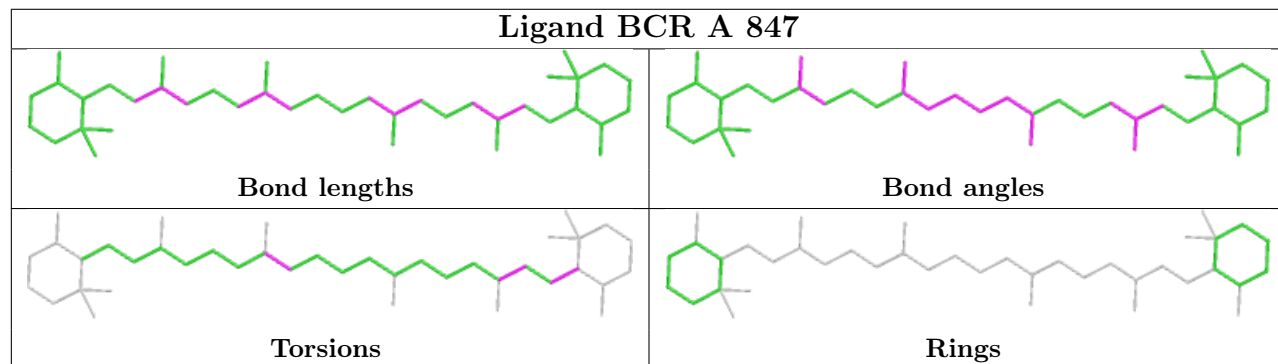


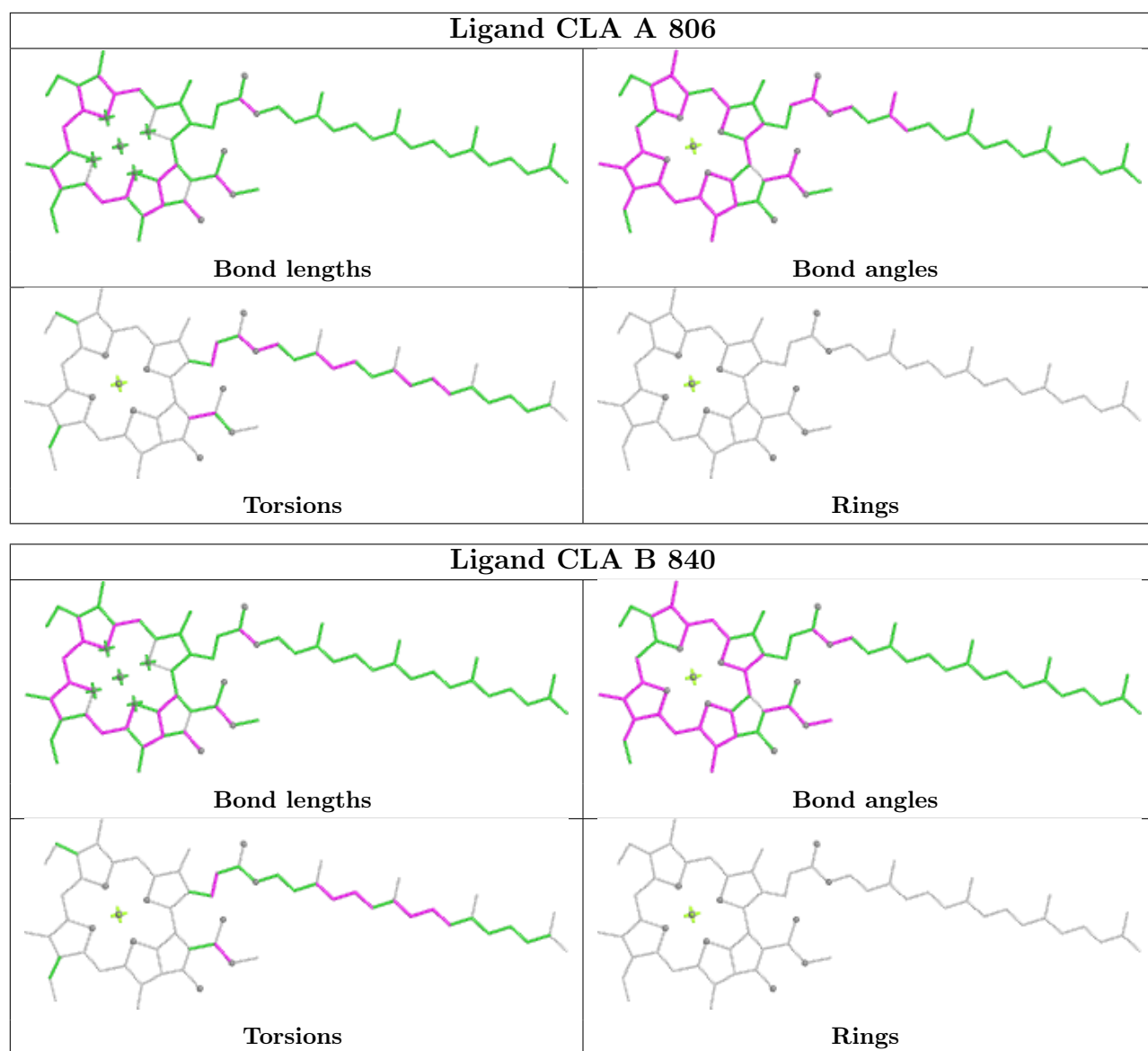


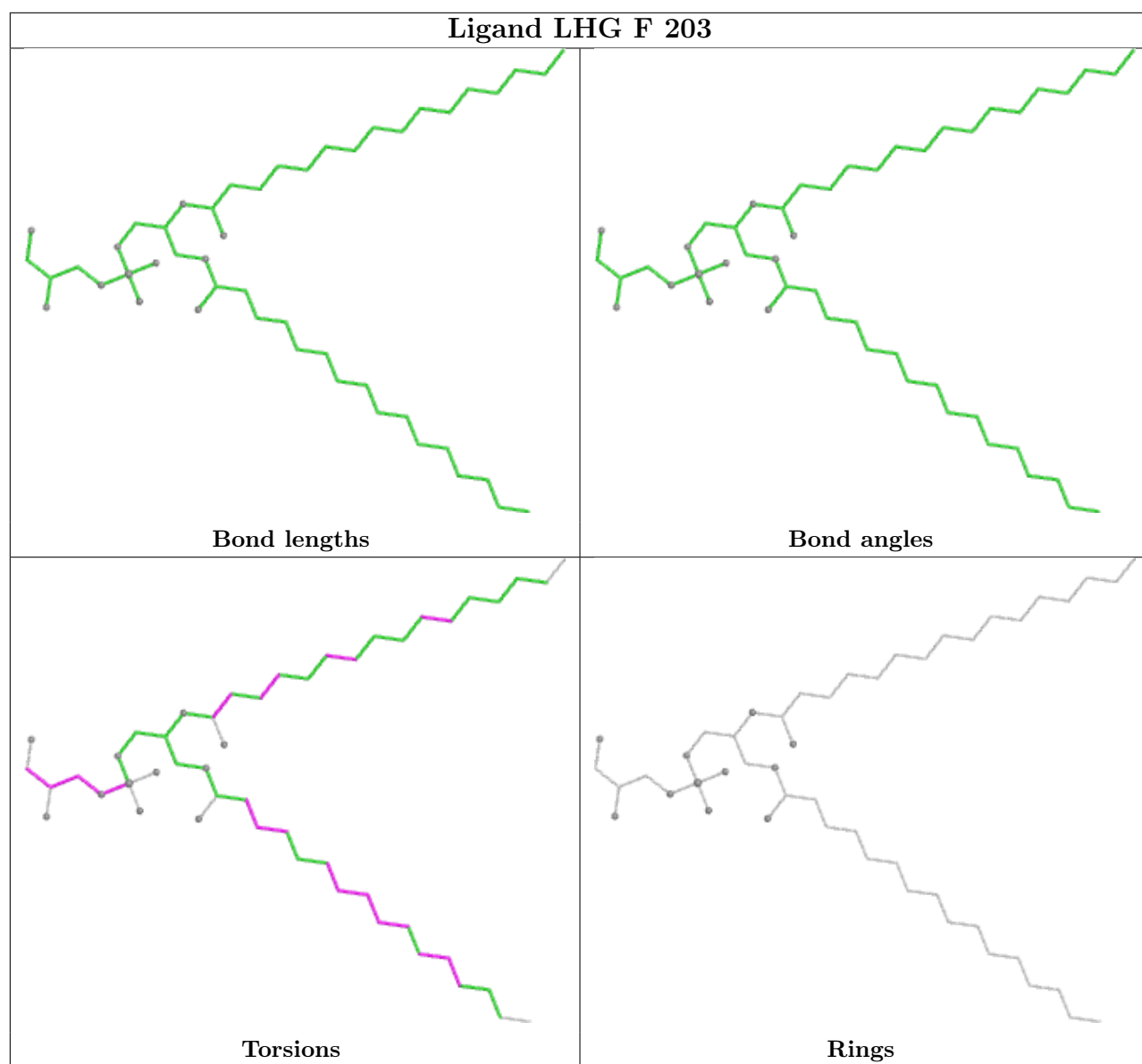
Ligand CLA X 101



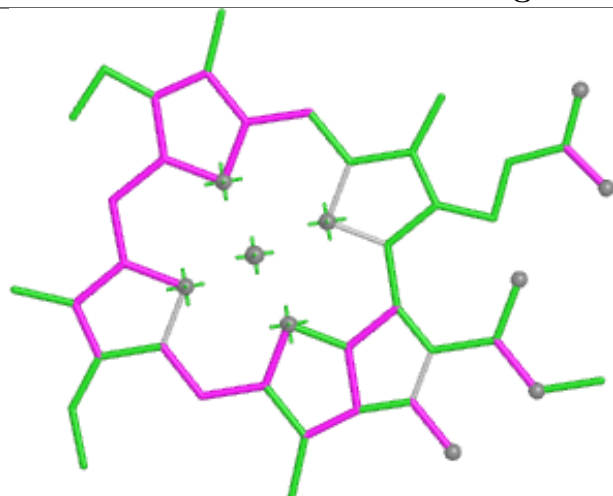
Ligand BCR A 847



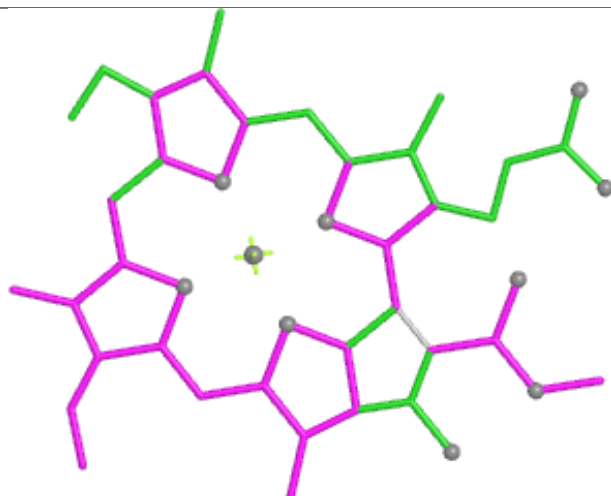




Ligand CLA A 837



Bond lengths



Bond angles

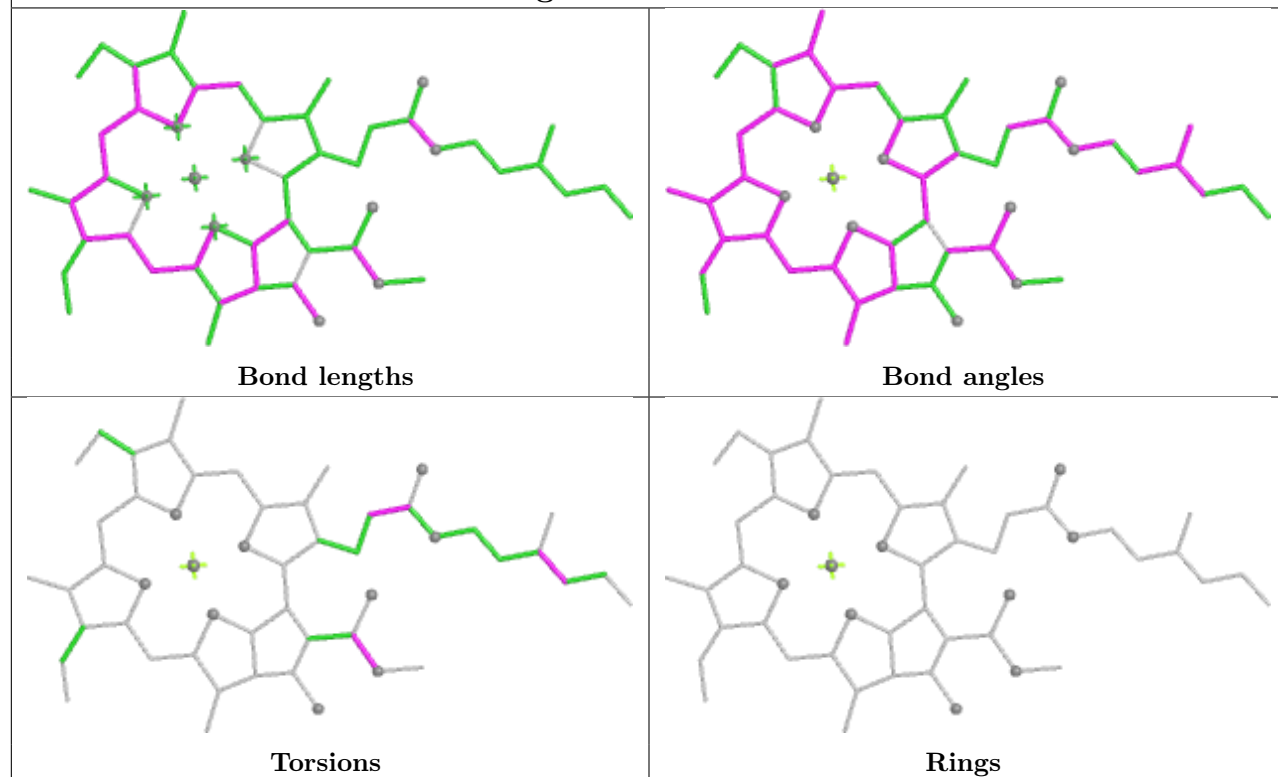


Torsions

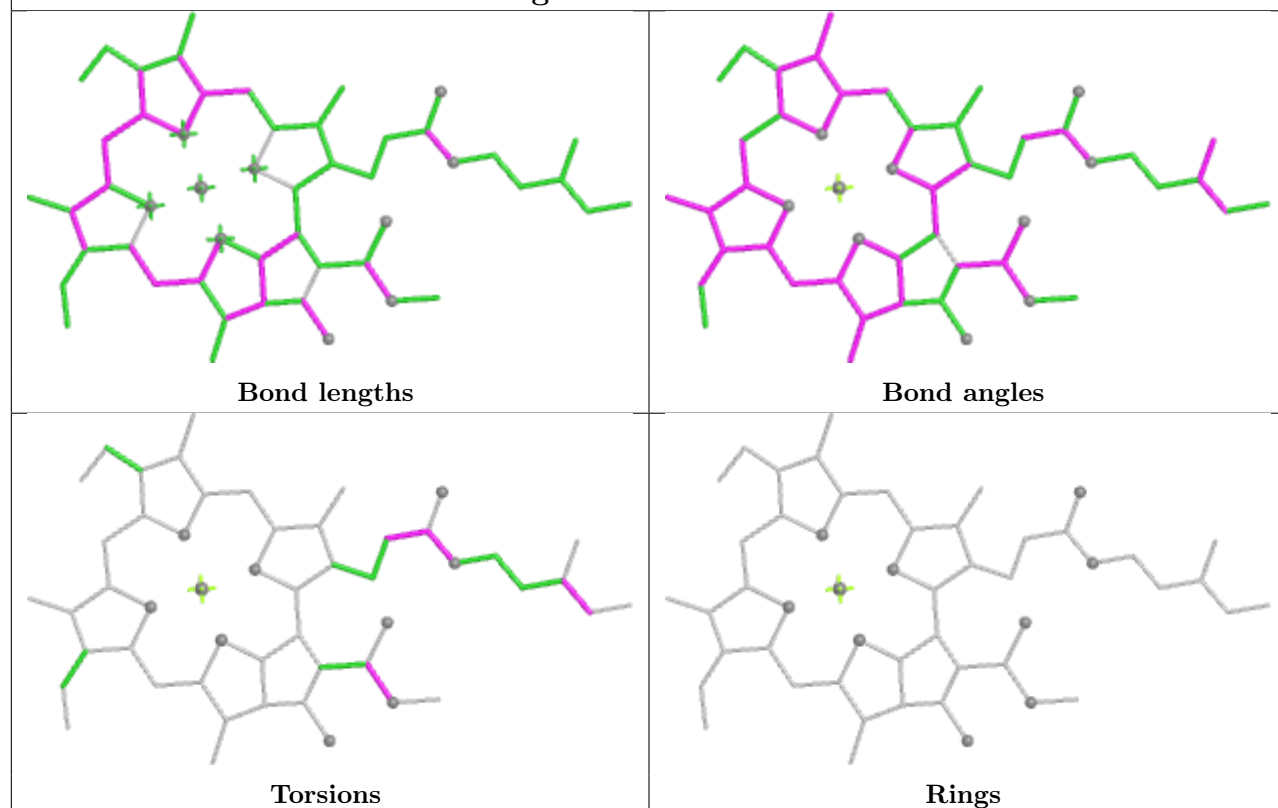


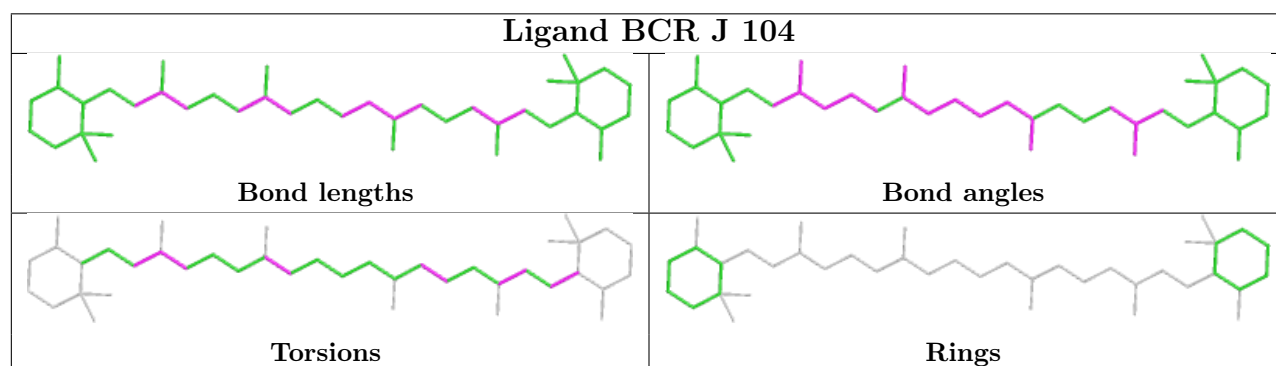
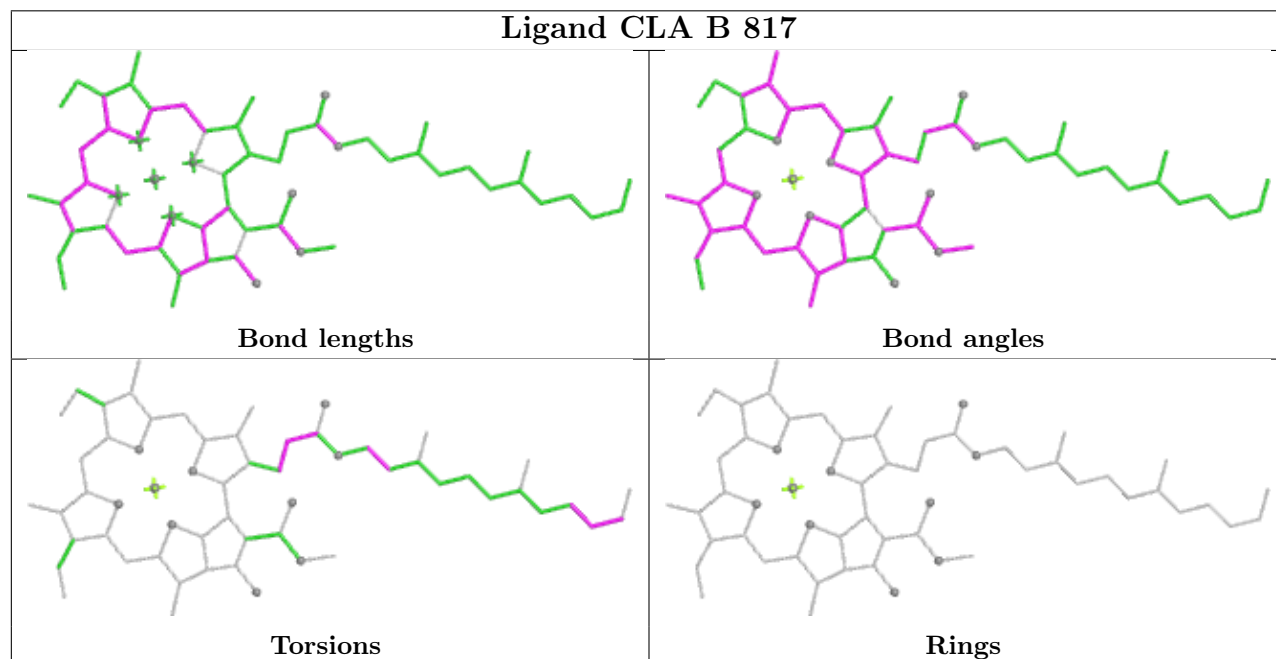
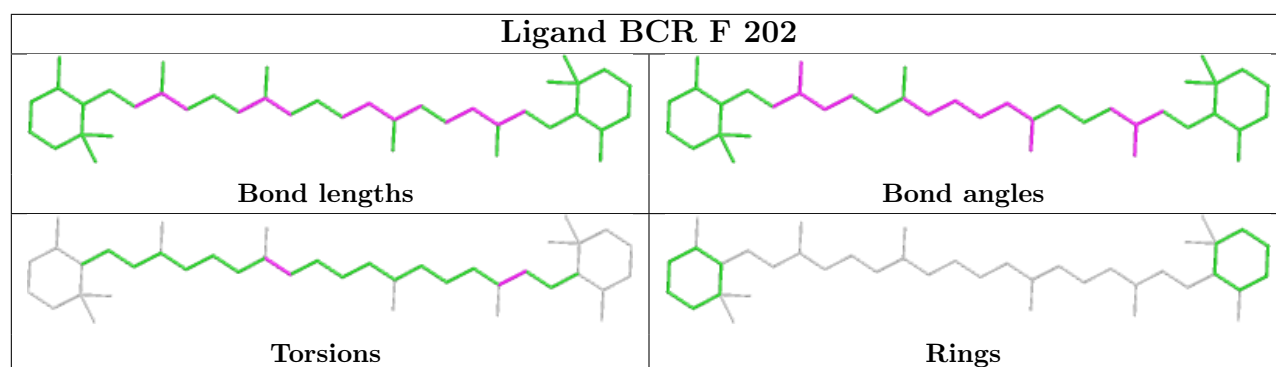
Rings

Ligand CLA 1 521

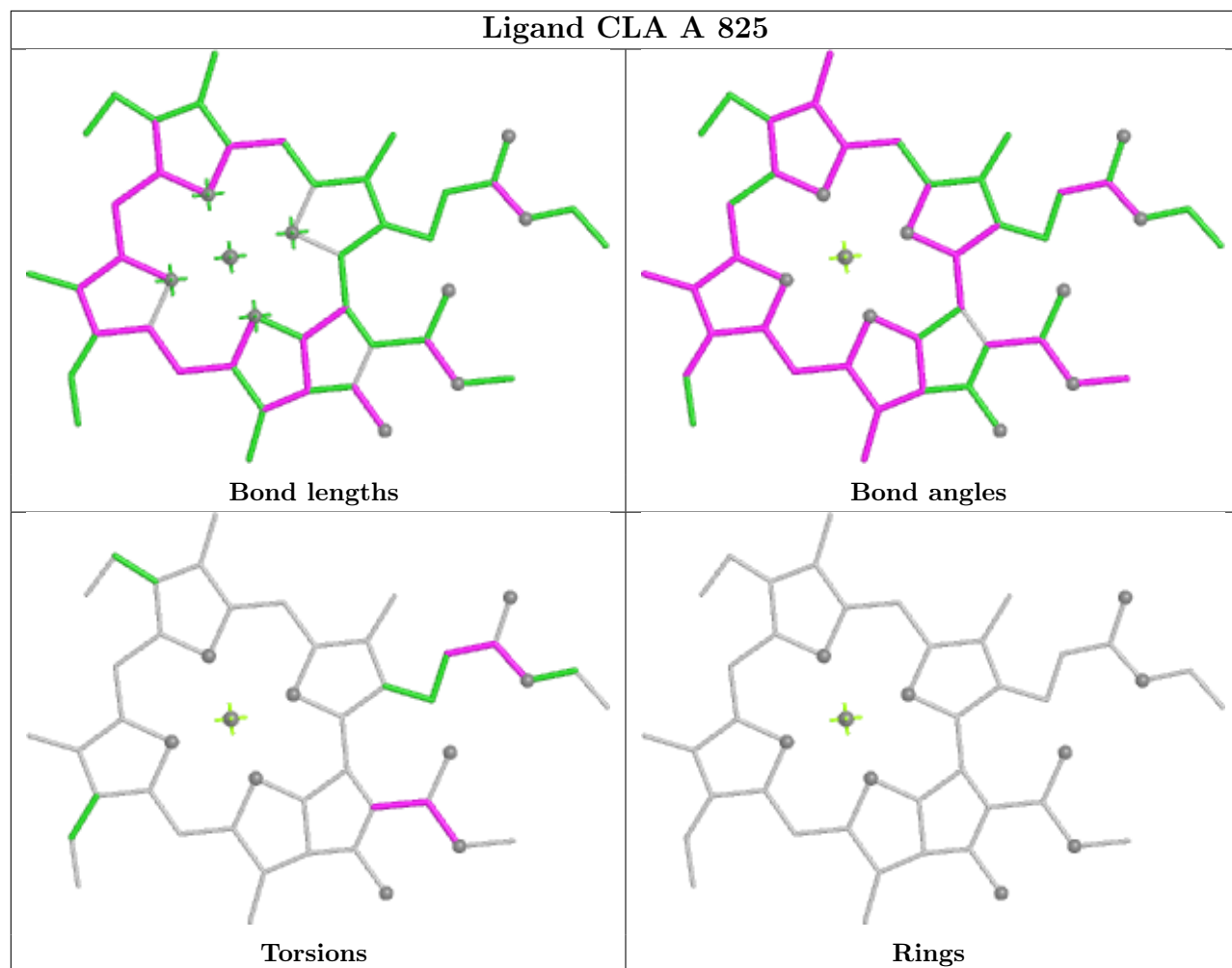


Ligand CLA A 824

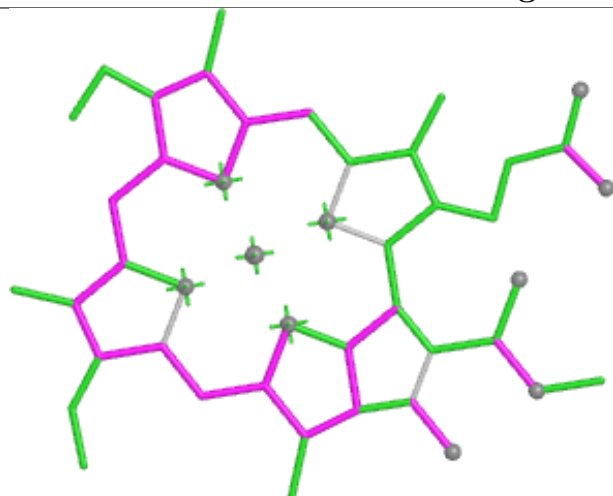




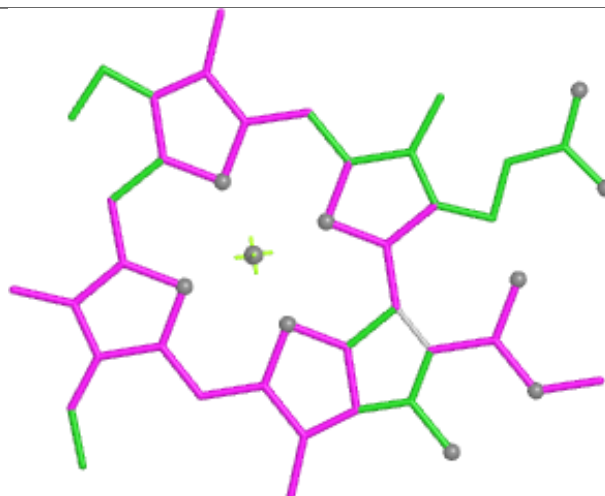
Ligand CLA A 825



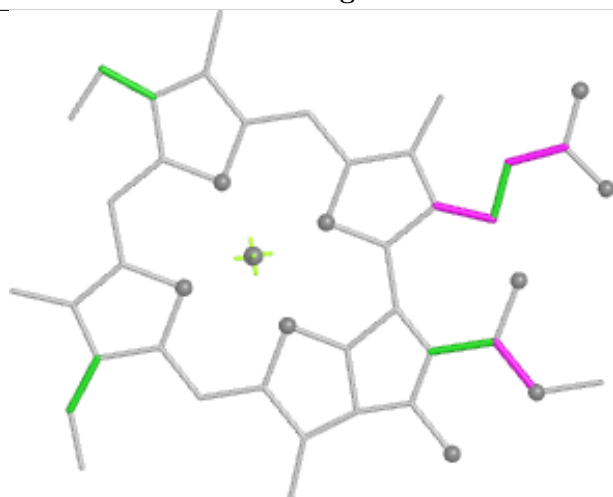
Ligand CLA 5 415



Bond lengths



Bond angles

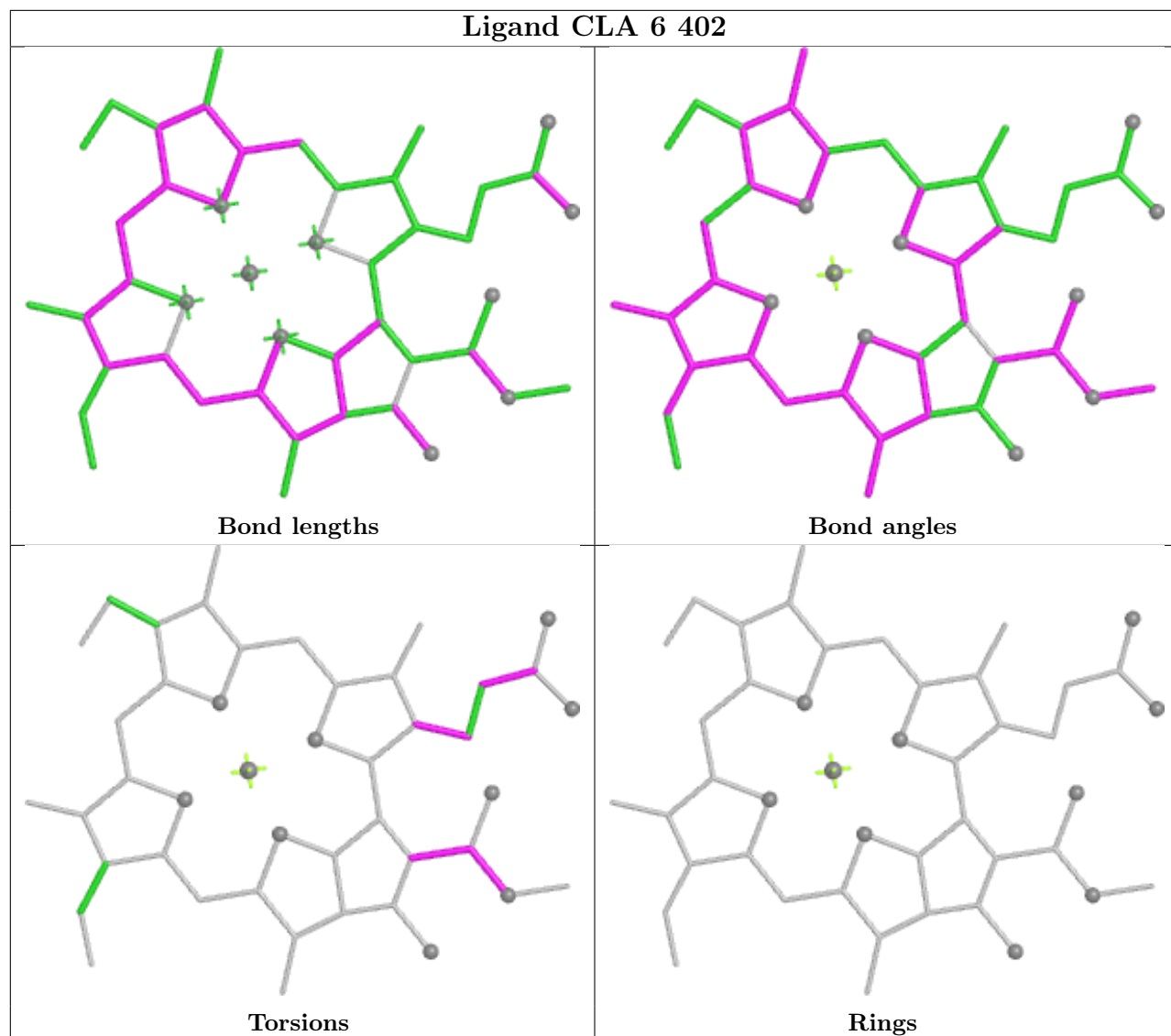


Torsions

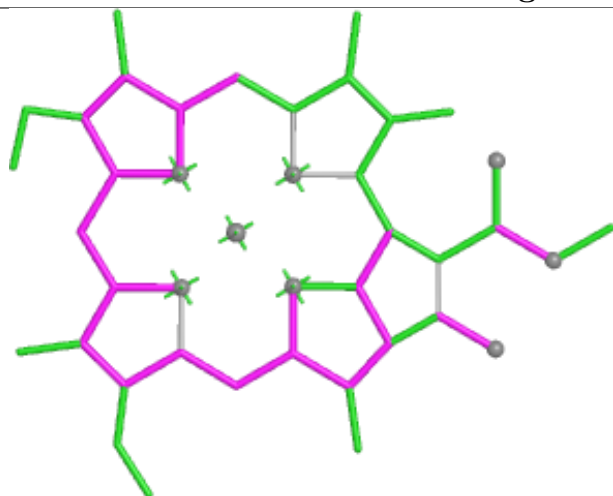


Rings

Ligand CLA 6 402



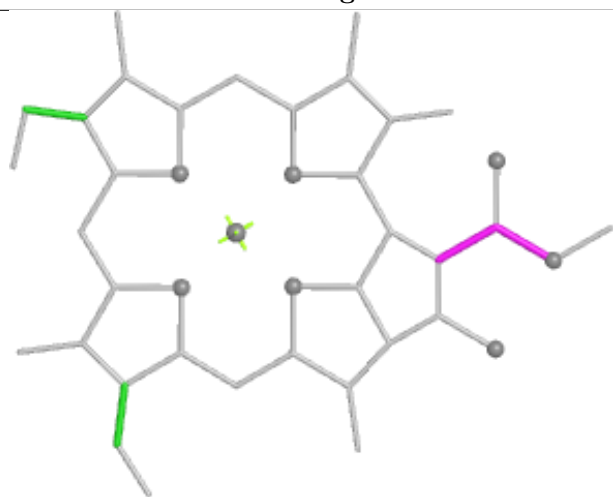
Ligand CLA 5 416



Bond lengths



Bond angles

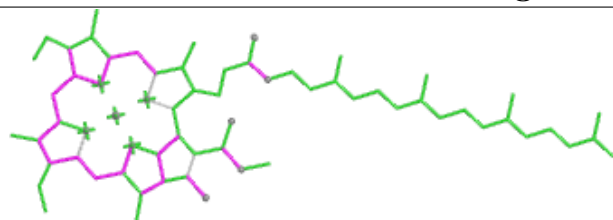


Torsions

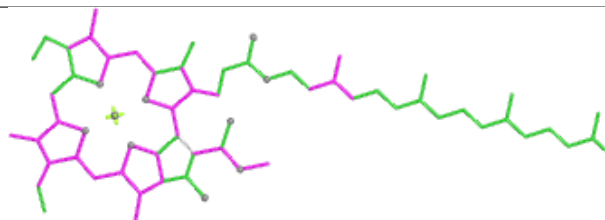


Rings

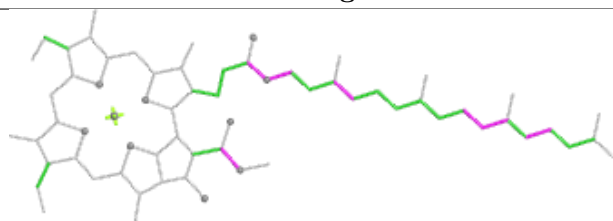
Ligand CLA B 830



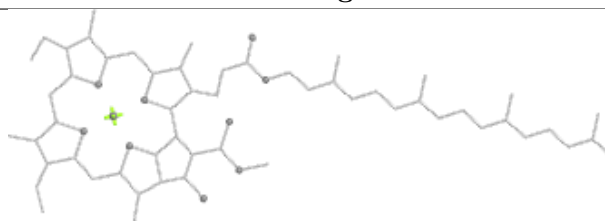
Bond lengths



Bond angles

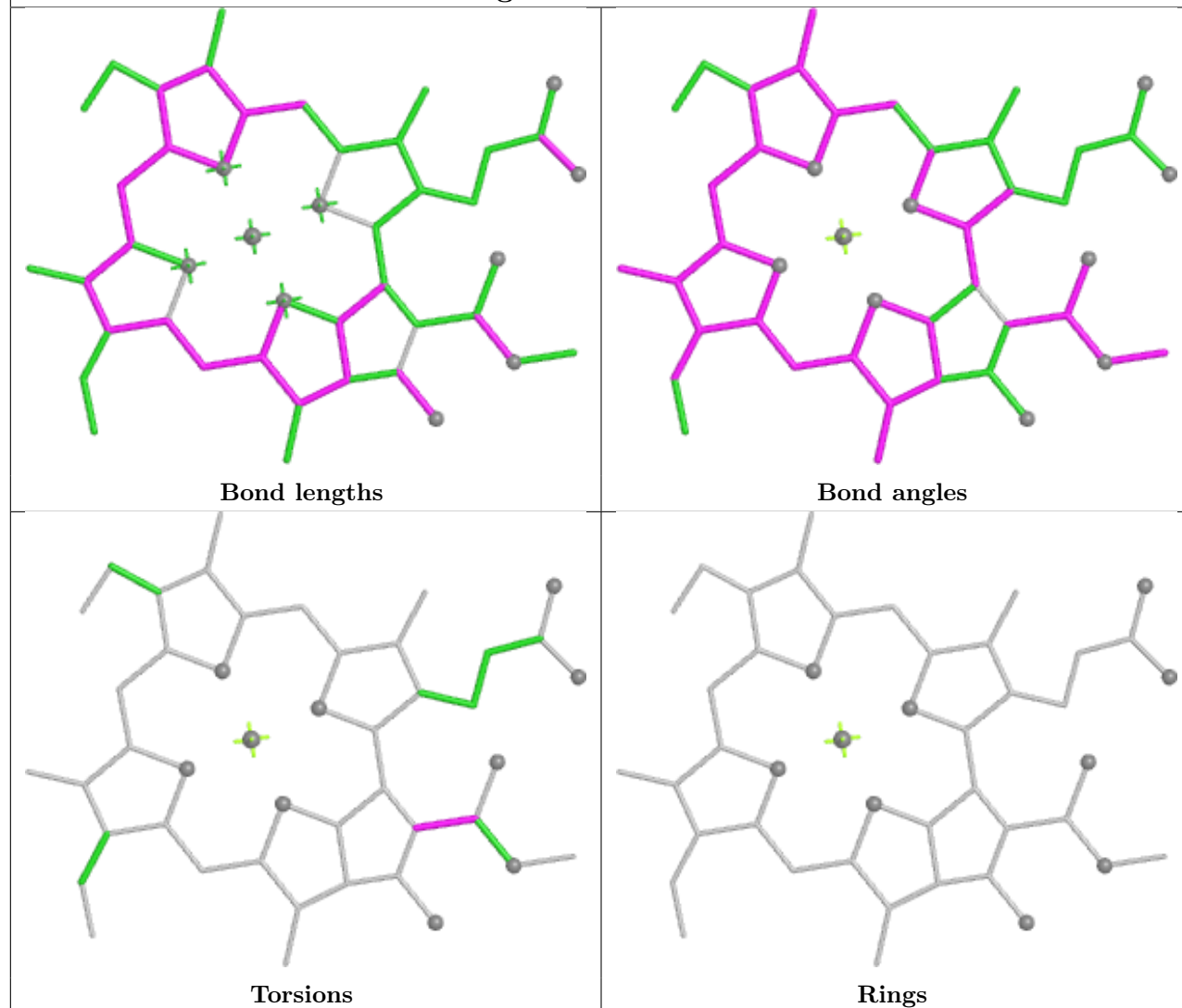


Torsions

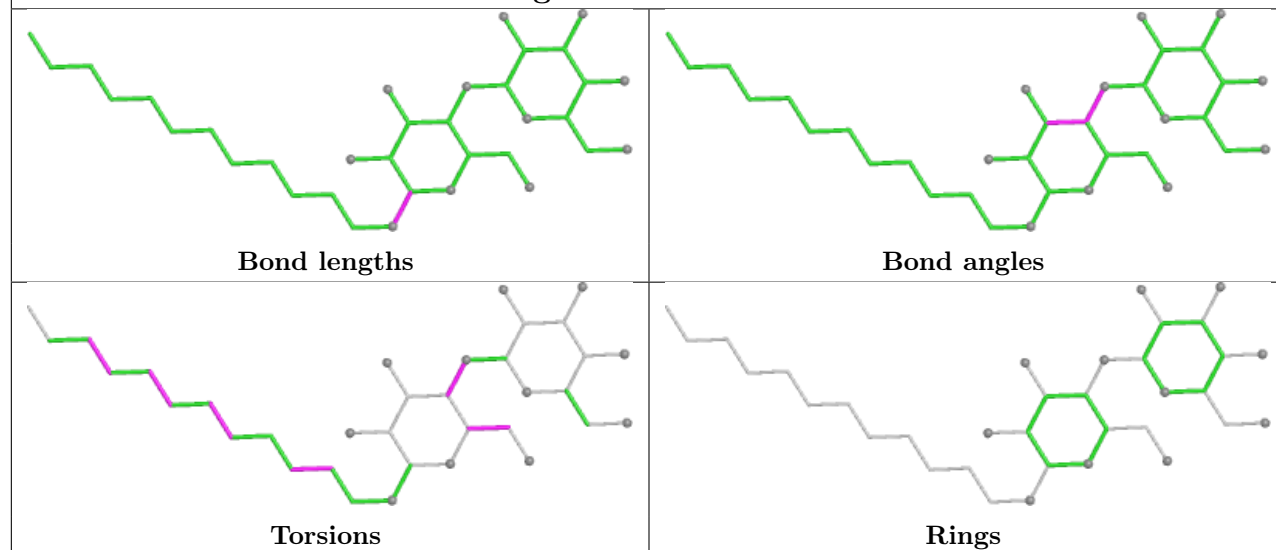


Rings

Ligand CLA 4 404



Ligand LMT 1 524



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.

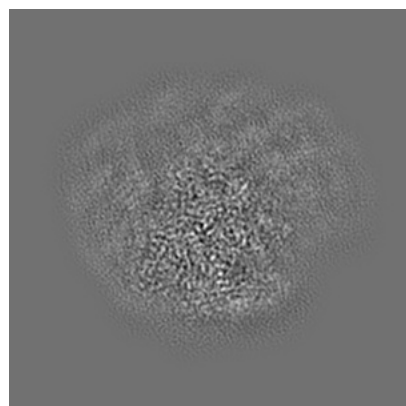
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33593. These allow visual inspection of the internal detail of the map and identification of artifacts.

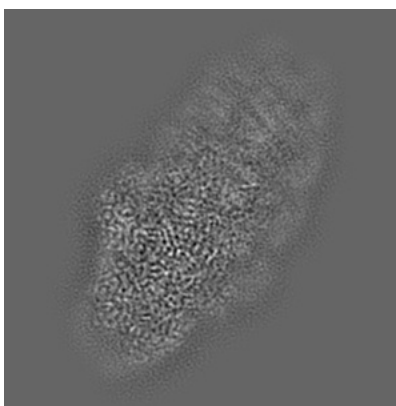
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

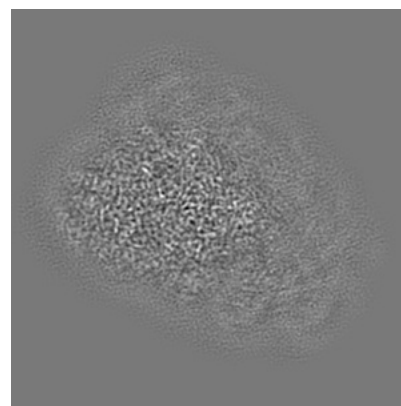
6.1.1 Primary map



X

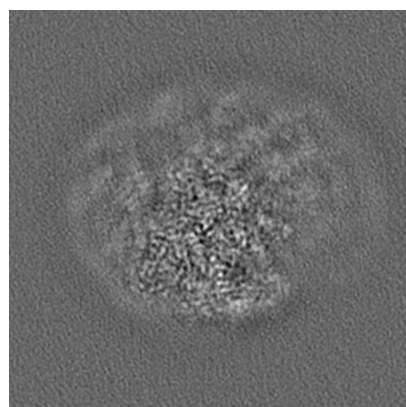


Y

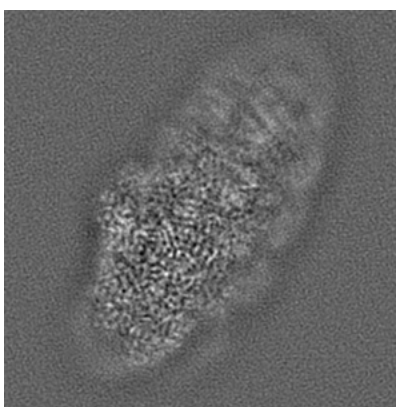


Z

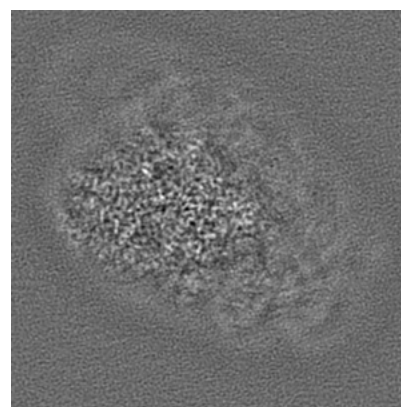
6.1.2 Raw map



X



Y

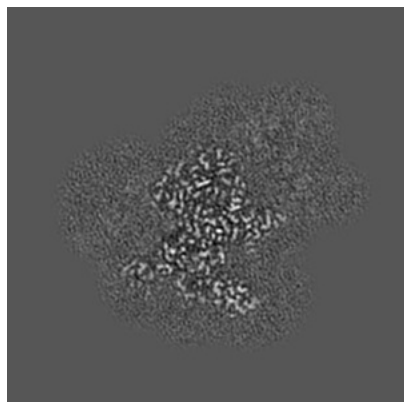


Z

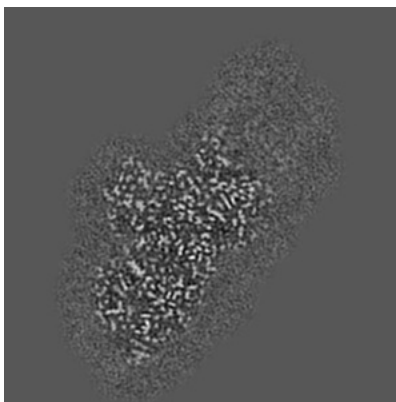
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

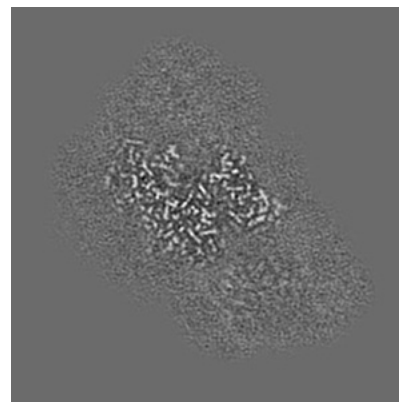
6.2.1 Primary map



X Index: 116

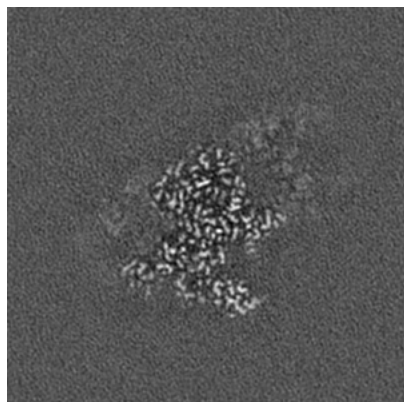


Y Index: 116

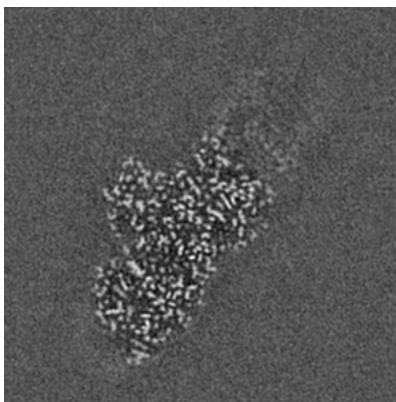


Z Index: 116

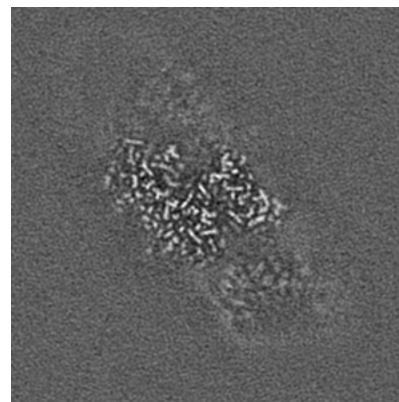
6.2.2 Raw map



X Index: 116



Y Index: 116

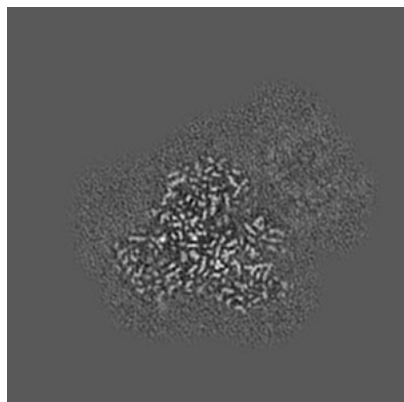


Z Index: 116

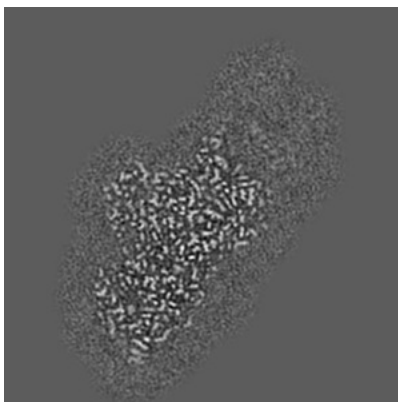
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

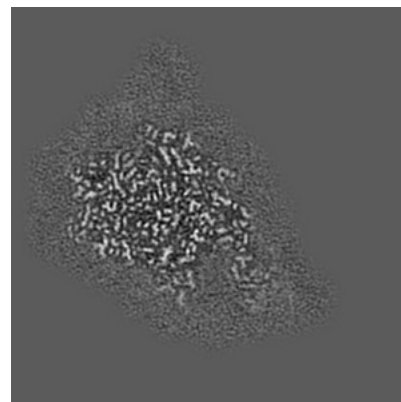
6.3.1 Primary map



X Index: 102

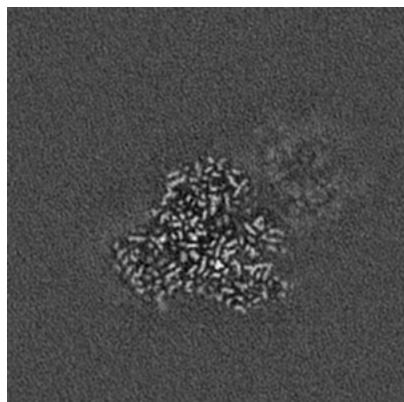


Y Index: 117

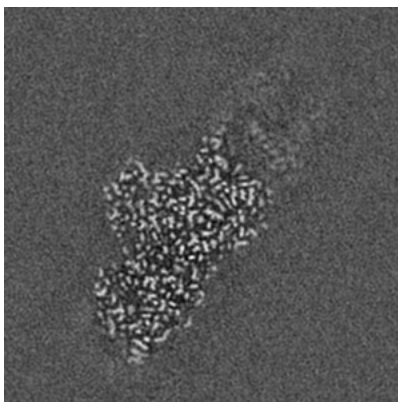


Z Index: 96

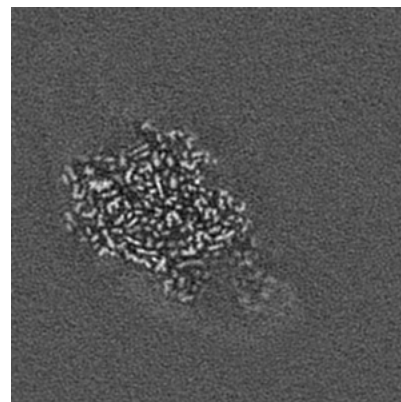
6.3.2 Raw map



X Index: 102



Y Index: 117

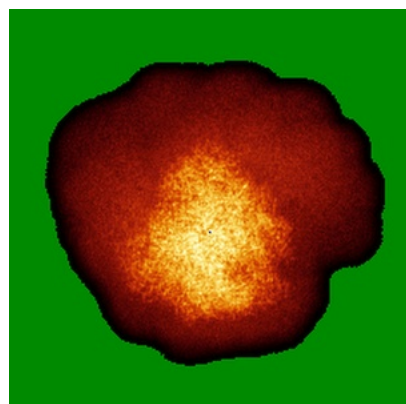


Z Index: 92

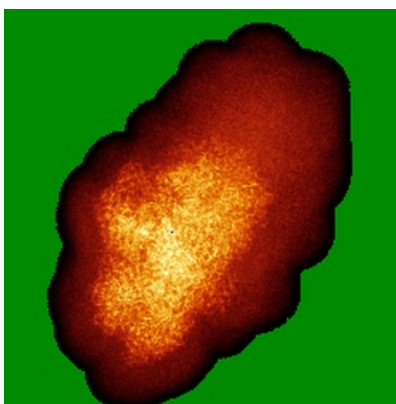
The images above show the largest variance slices of the map in three orthogonal directions.

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

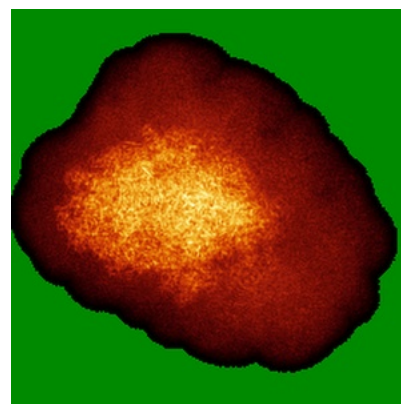
6.4.1 Primary map



X

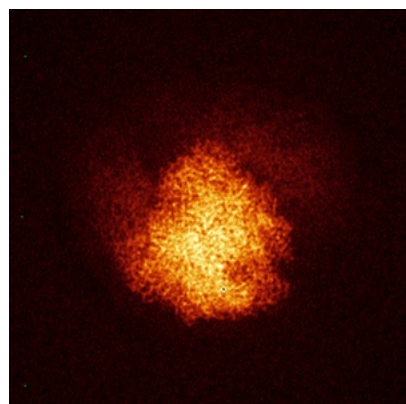


Y

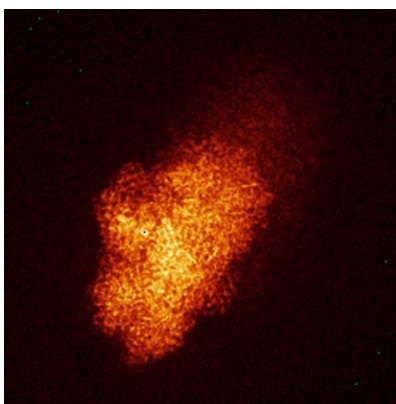


Z

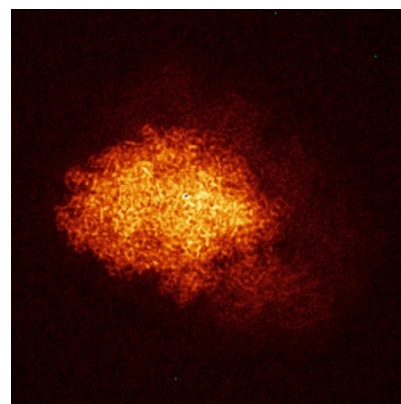
6.4.2 Raw map



X



Y

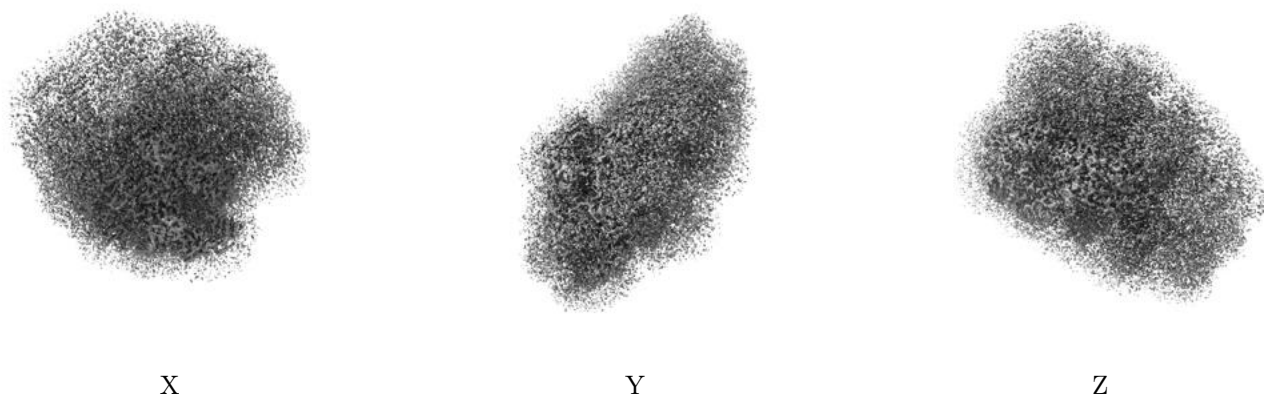


Z

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

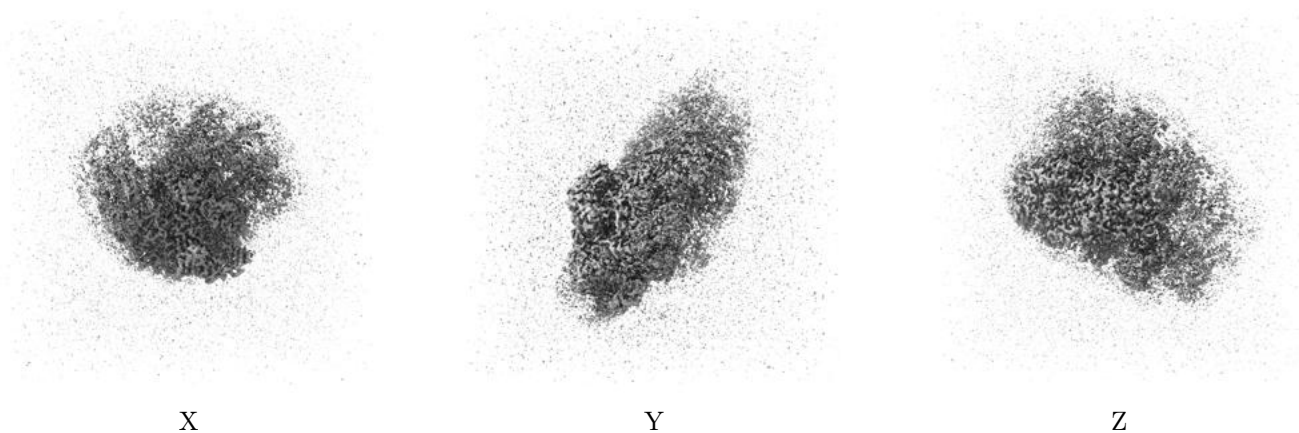
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

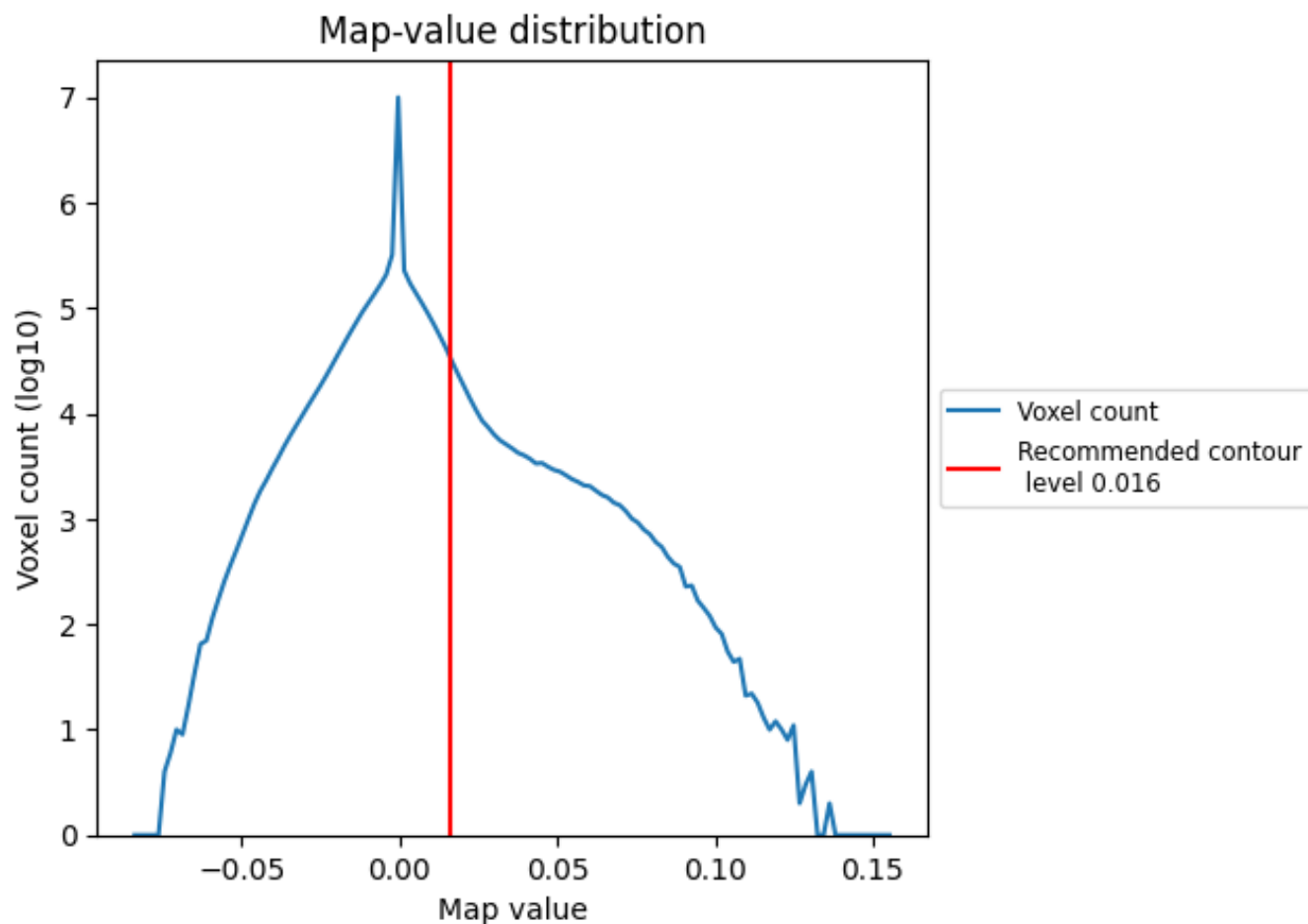
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

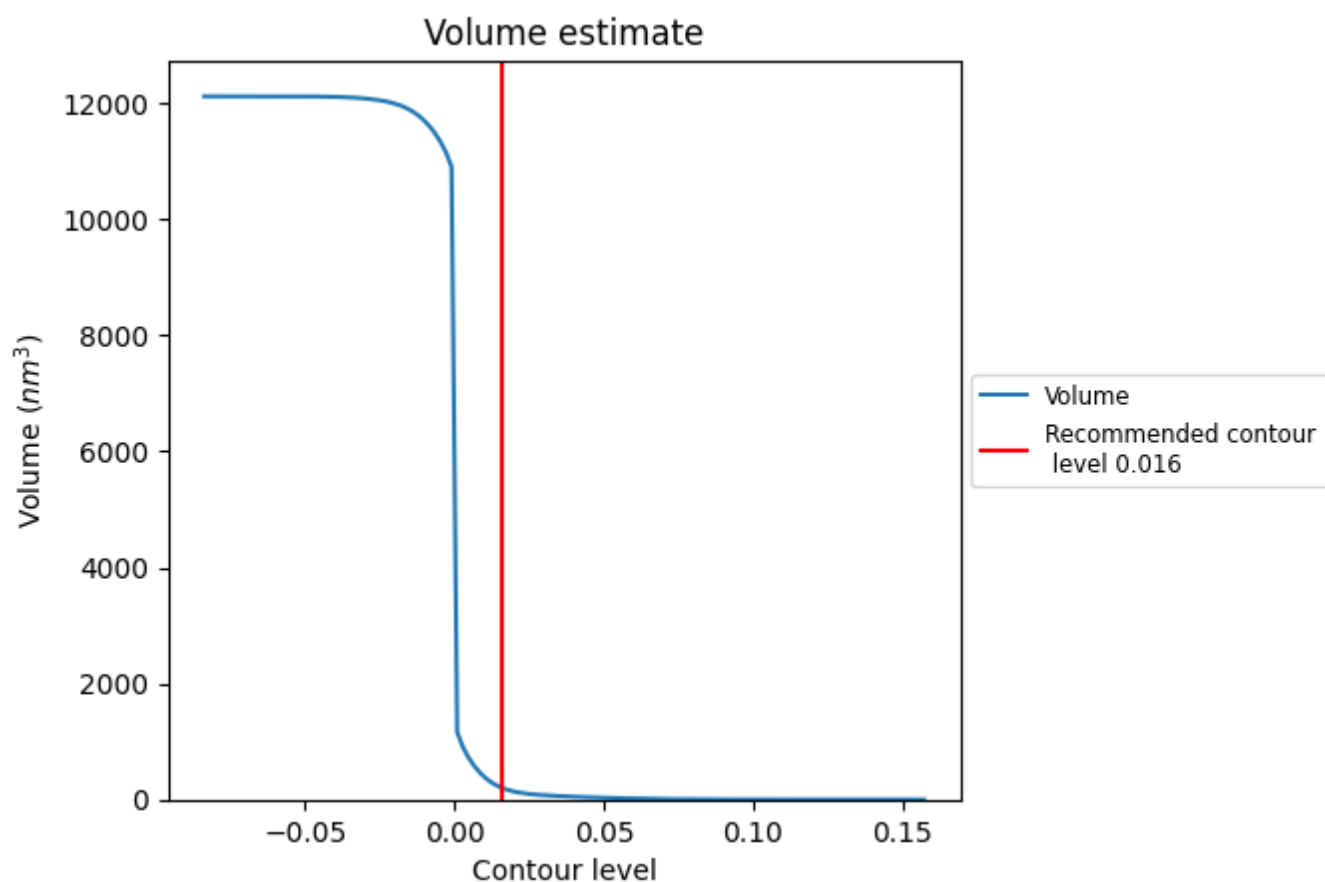
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

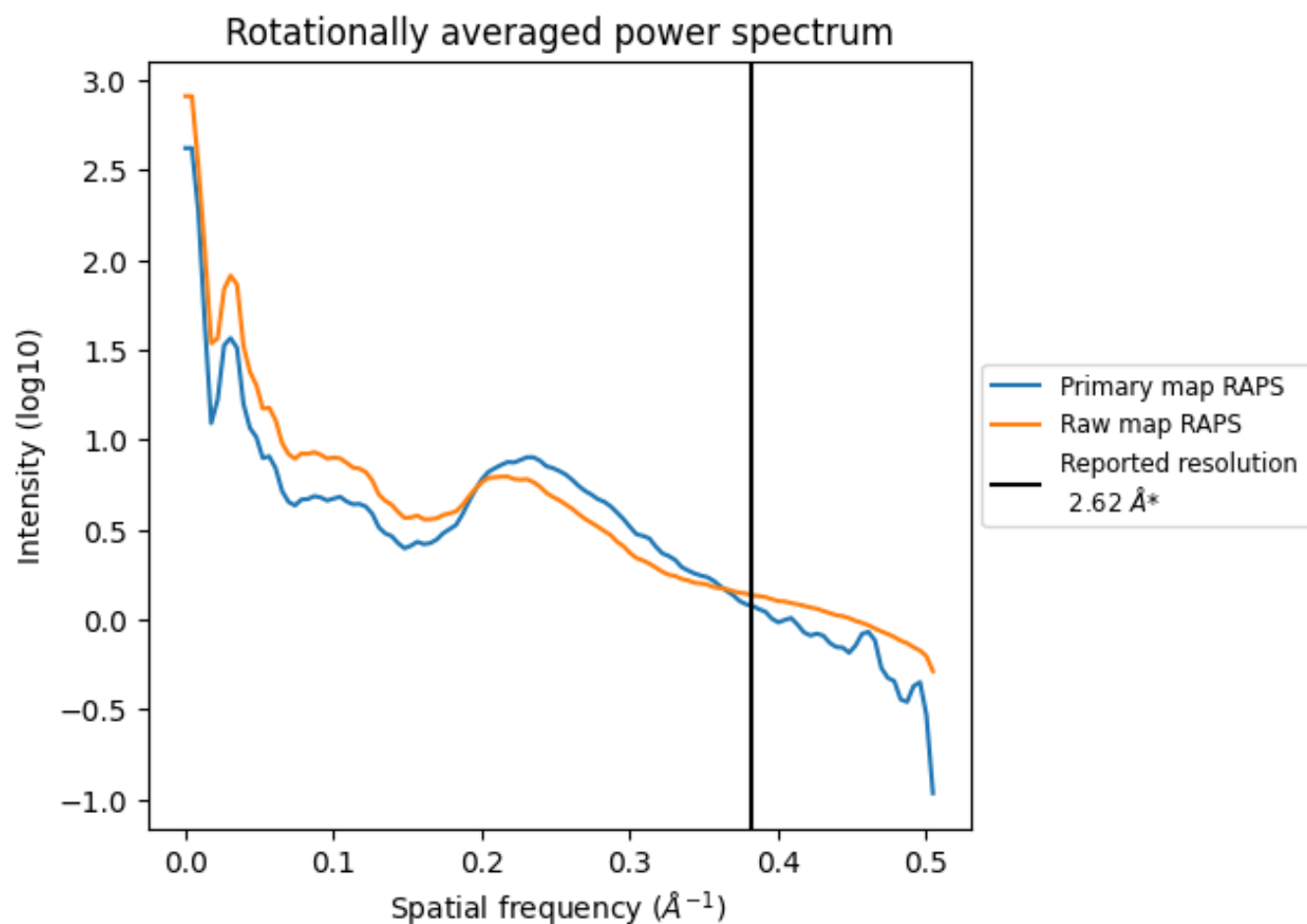
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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 ⓘ

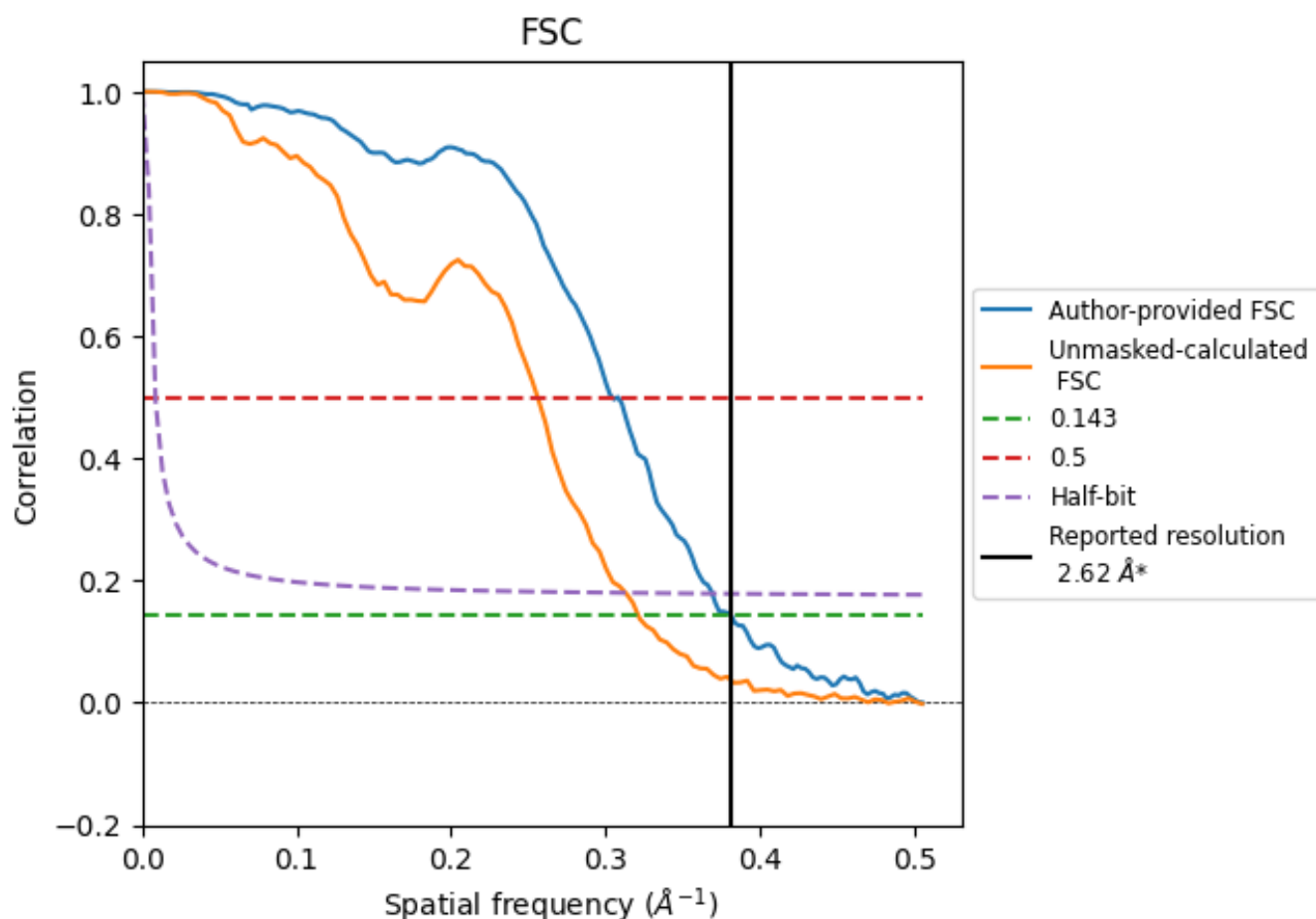


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 Å⁻¹

8.2 Resolution estimates [i](#)

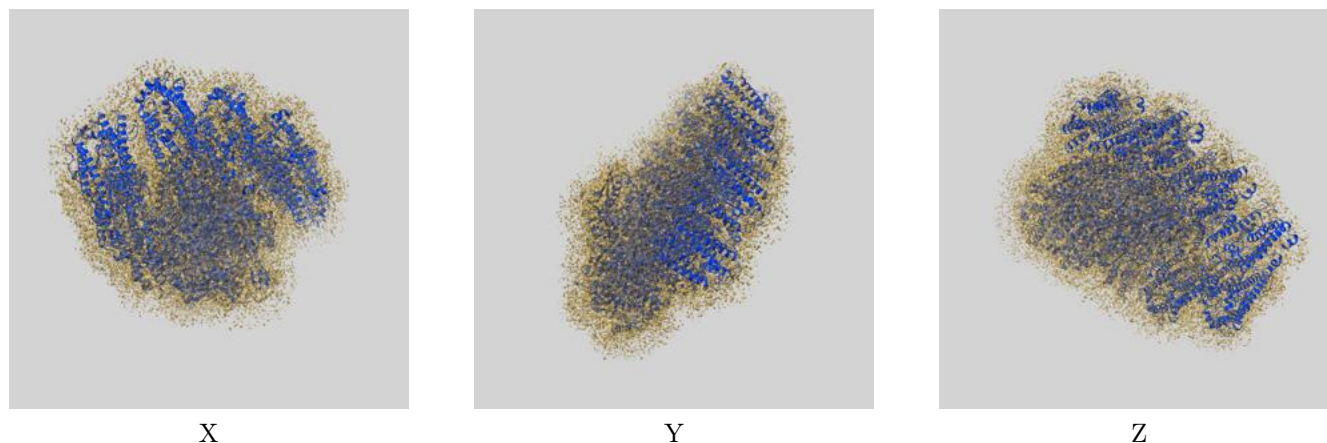
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.29	2.71
Unmasked-calculated*	3.11	3.91	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

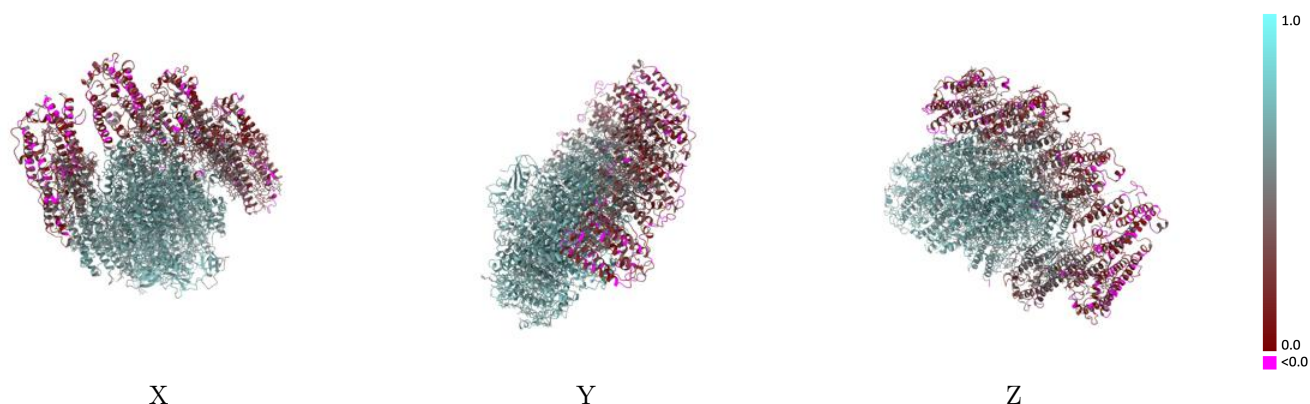
This section contains information regarding the fit between EMDB map EMD-33593 and PDB model 7Y3F. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



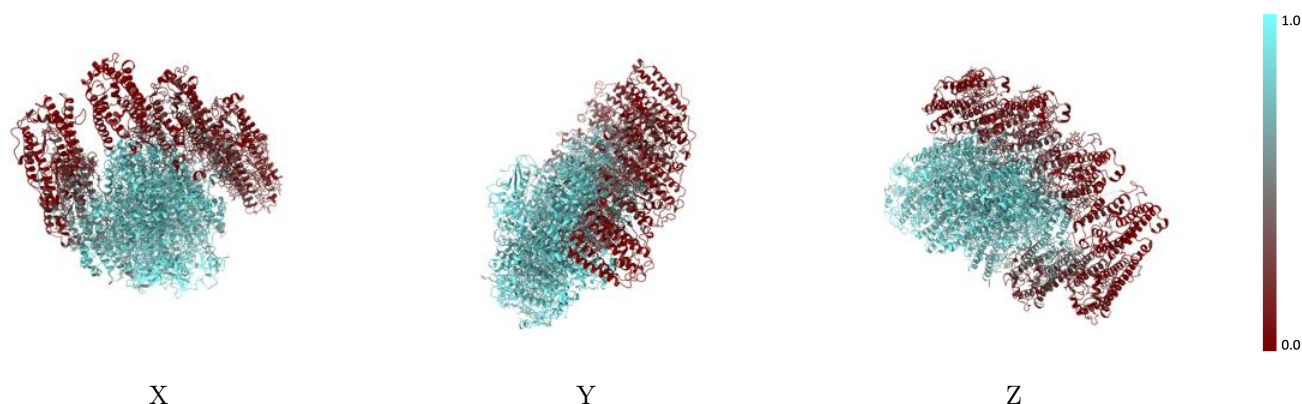
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



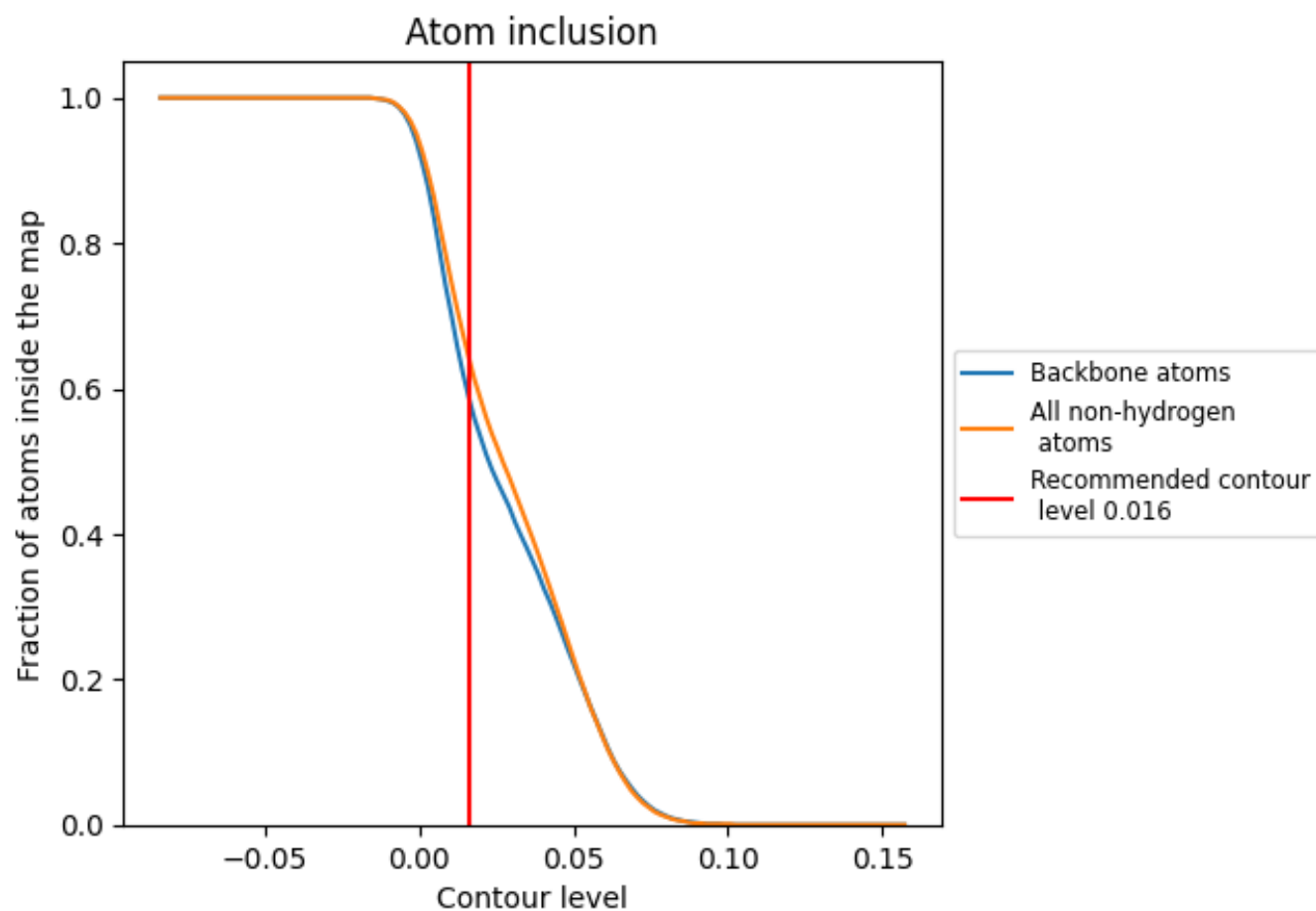
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 64% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.5260
1	0.5240	0.4830
2	0.1170	0.1960
3	0.0680	0.1850
4	0.1620	0.2490
5	0.2040	0.2940
6	0.0990	0.2000
A	0.9420	0.6910
B	0.9270	0.6830
C	0.9480	0.6910
D	0.8790	0.6540
E	0.8490	0.6230
F	0.8710	0.6580
I	0.8940	0.6640
J	0.9130	0.6690
K	0.8770	0.6230
M	0.8300	0.6290
X	0.8270	0.6290

1.0

0.0

<0.0