



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 07:39 PM JST

PDB ID : 7Y3F
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

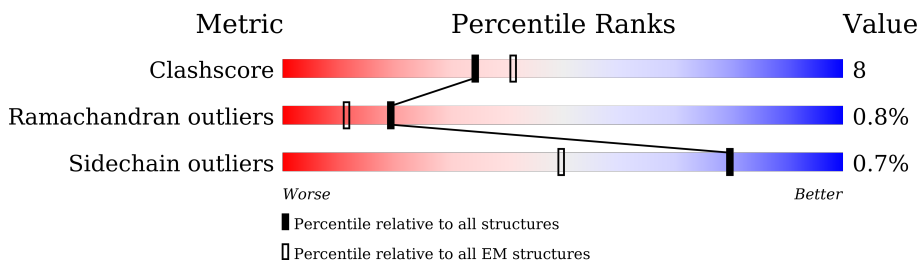
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
2	B	741	
3	C	81	
4	D	139	
5	E	70	
6	F	164	
7	I	46	
8	J	49	

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Mol	Chain	Length	Quality of chain
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CL0	A	801	X	-	-	-
16	CLA	1	501	X	-	-	-
16	CLA	1	502	X	-	-	-
16	CLA	1	503	X	-	-	-
16	CLA	1	505	X	-	-	-
16	CLA	1	506	X	-	-	-
16	CLA	1	507	X	-	-	-
16	CLA	1	508	X	-	-	-
16	CLA	1	509	X	-	-	-
16	CLA	1	510	X	-	-	-
16	CLA	1	511	X	-	-	-
16	CLA	1	512	X	-	-	-
16	CLA	1	513	X	-	-	-
16	CLA	1	514	X	-	-	-
16	CLA	1	515	X	-	-	-
16	CLA	1	521	X	-	-	-
16	CLA	1	525	X	-	-	-
16	CLA	1	526	X	-	-	-
16	CLA	2	401	X	-	-	-
16	CLA	2	402	X	-	-	-
16	CLA	2	403	X	-	-	-
16	CLA	2	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	2	405	X	-	-	-
16	CLA	2	406	X	-	-	-
16	CLA	3	401	X	-	-	-
16	CLA	4	402	X	-	-	-
16	CLA	4	403	X	-	-	-
16	CLA	4	404	X	-	-	-
16	CLA	4	405	X	-	-	-
16	CLA	4	406	X	-	-	-
16	CLA	4	407	X	-	-	-
16	CLA	4	408	X	-	-	-
16	CLA	4	409	X	-	-	-
16	CLA	4	410	X	-	-	-
16	CLA	4	411	X	-	-	-
16	CLA	5	403	X	-	-	-
16	CLA	5	404	X	-	-	-
16	CLA	5	405	X	-	-	-
16	CLA	5	406	X	-	-	-
16	CLA	5	407	X	-	-	-
16	CLA	5	408	X	-	-	-
16	CLA	5	409	X	-	-	-
16	CLA	5	410	X	-	-	-
16	CLA	5	411	X	-	-	-
16	CLA	5	412	X	-	-	-
16	CLA	5	413	X	-	-	-
16	CLA	5	414	X	-	-	-
16	CLA	5	415	X	-	-	-
16	CLA	5	416	X	-	-	-
16	CLA	5	417	X	-	-	-
16	CLA	5	418	X	-	-	-
16	CLA	5	419	X	-	-	-
16	CLA	5	421	X	-	-	-
16	CLA	5	422	X	-	-	-
16	CLA	6	401	X	-	-	-
16	CLA	6	402	X	-	-	-
16	CLA	6	403	X	-	-	-
16	CLA	6	404	X	-	-	-
16	CLA	6	405	X	-	-	-
16	CLA	6	406	X	-	-	-
16	CLA	6	407	X	-	-	-
16	CLA	6	408	X	-	-	-
16	CLA	6	409	X	-	-	-
16	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	840	X	-	-	-
16	CLA	A	841	X	-	-	-
16	CLA	A	842	X	-	-	-
16	CLA	A	843	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	-	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-
16	CLA	B	832	X	-	-	-
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	B	839	X	-	-	-
16	CLA	B	840	X	-	-	-
16	CLA	F	201	X	-	-	-
16	CLA	F	204	X	-	-	-
16	CLA	J	101	X	-	-	-
16	CLA	J	102	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	103	X	-	-	-
16	CLA	X	101	X	-	-	-

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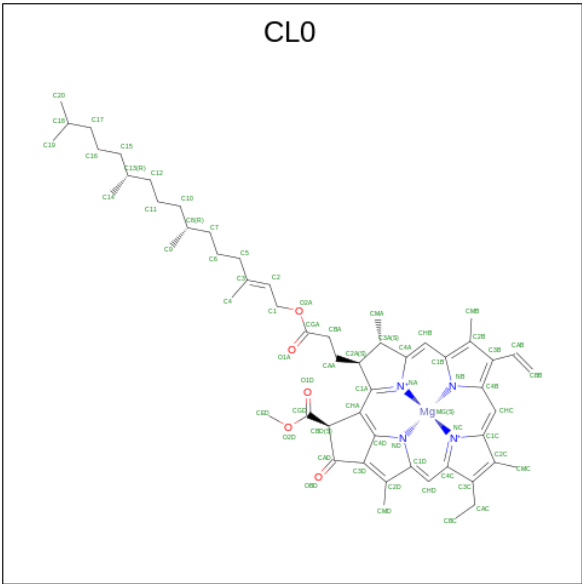
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Mol	Chain	Residues	Atoms				AltConf	Trace
13	6	303	Total	C	N	O	0	0
			1479	873	303	303		

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

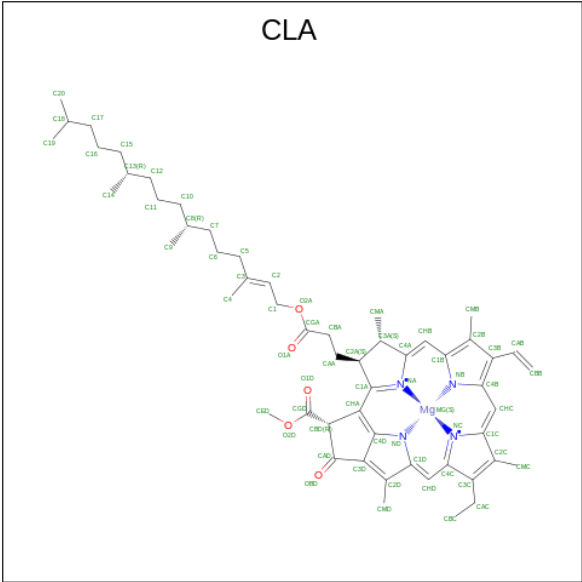
Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	329	Total	C	N	O	S	0	0
			2562	1709	424	425	4		
14	5	332	Total	C	N	O	S	0	0
			2589	1725	429	431	4		

- Molecule 15 is CHLOROPHYLL A ISOMER (three-letter code: 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 (three-letter code: 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
			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	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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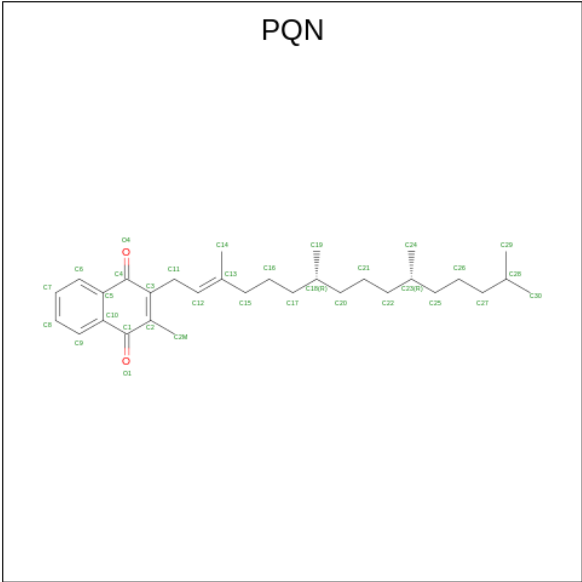
Mol	Chain	Residues	Atoms					AltConf
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	4	1	Total 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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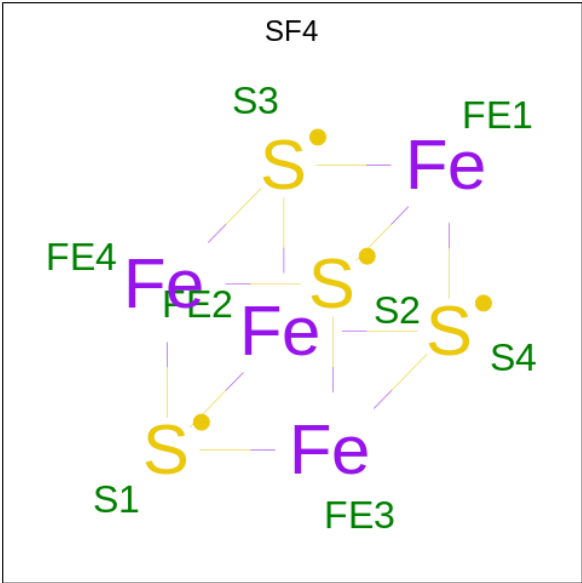
Mol	Chain	Residues	Atoms					AltConf
16	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	6	1	Total	C	Mg	N	O	0
			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
			41	33	1	4	3	
16	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 17 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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 (three-letter code: SF4) (formula: Fe₄S₄).



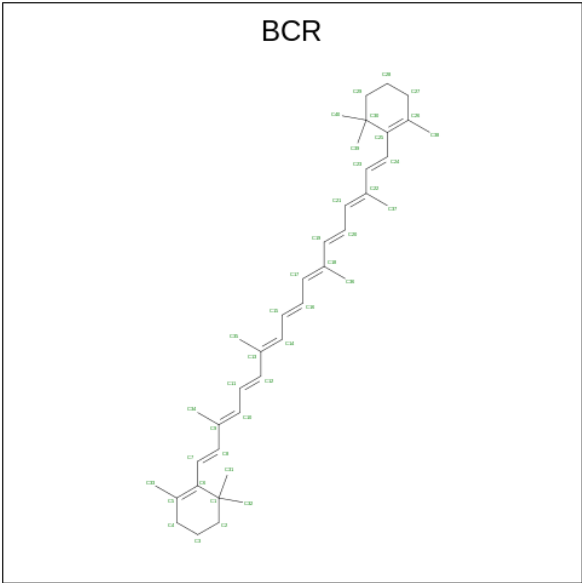
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



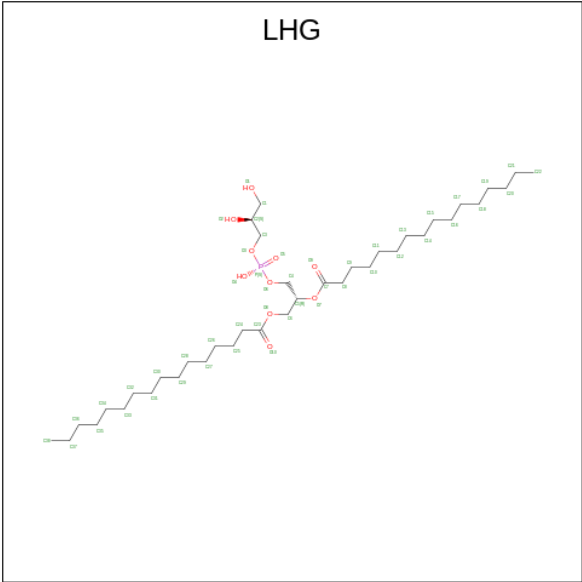
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	A	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	
19	B	1	Total	C	0
			40	40	

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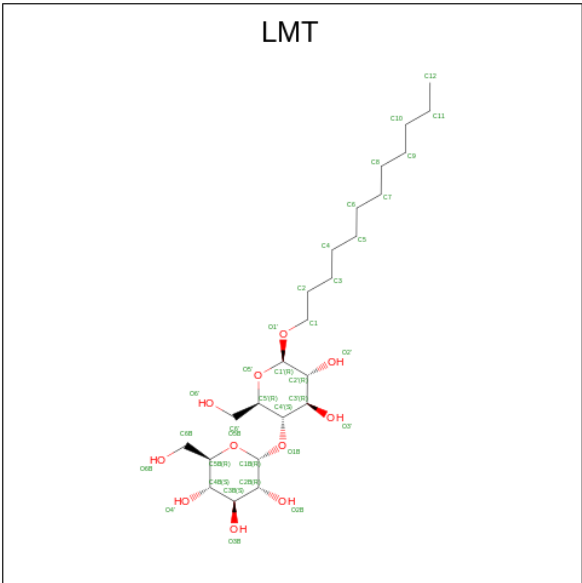
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	M	1	Total C 40 40	0
19	1	1	Total C 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 (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



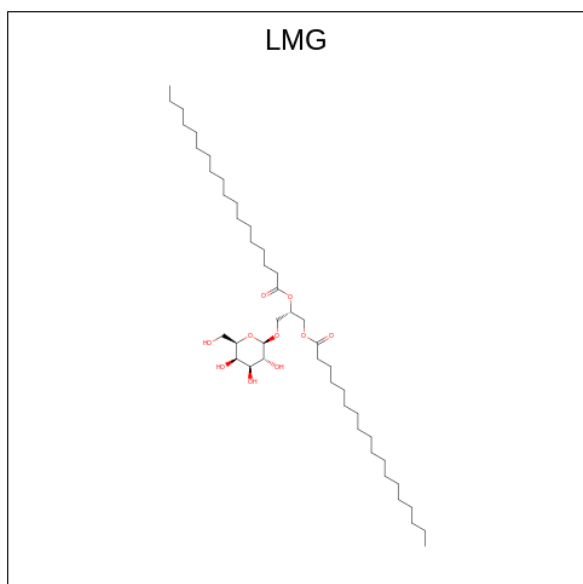
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			27	16	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	F	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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 (three-letter code: 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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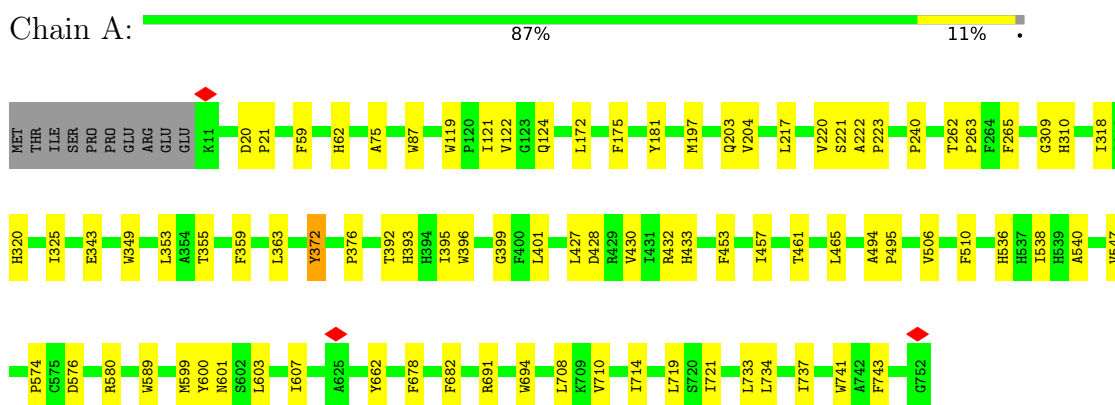
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Mol	Chain	Residues	Atoms		AltConf
23	F	2	Total 2	O 2	0
23	K	1	Total 1	O 1	0
23	1	2	Total 2	O 2	0

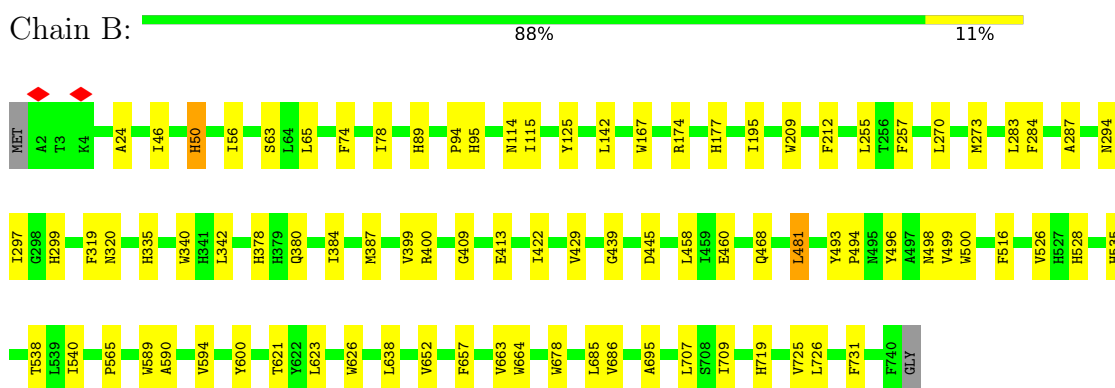
3 Residue-property plots

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.

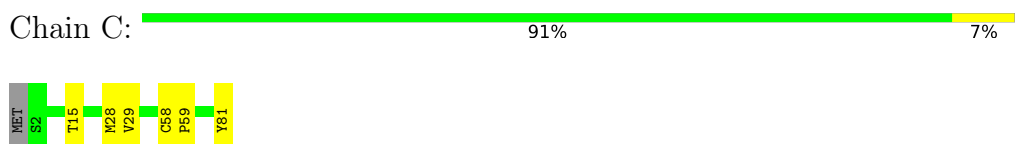
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



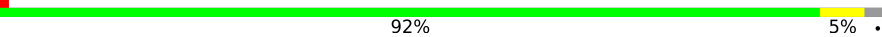
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1



- Molecule 3: Photosystem I iron-sulfur center




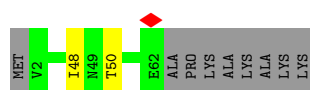
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  92% 5%




- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  84% 13%



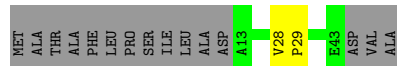
- Molecule 6: Photosystem I reaction center subunit III

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%




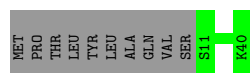
- Molecule 9: Unknown

Chain K:  80% 7% 12%

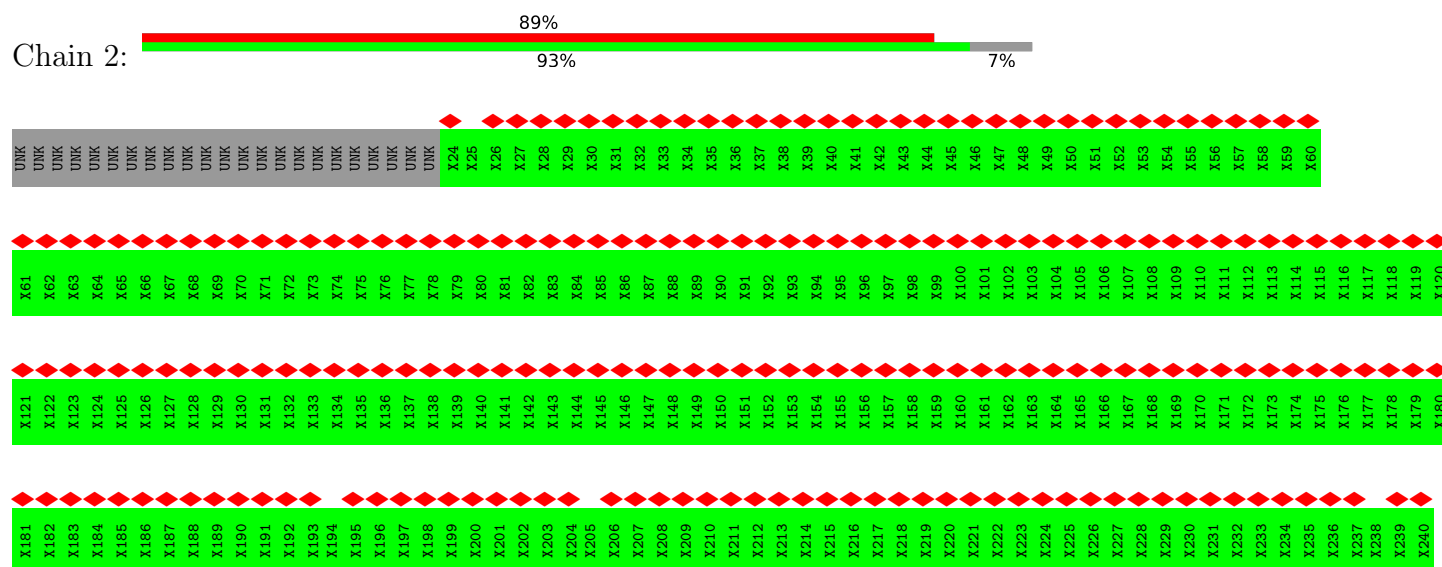


- Molecule 10: Psam

Chain M:  75% 25%

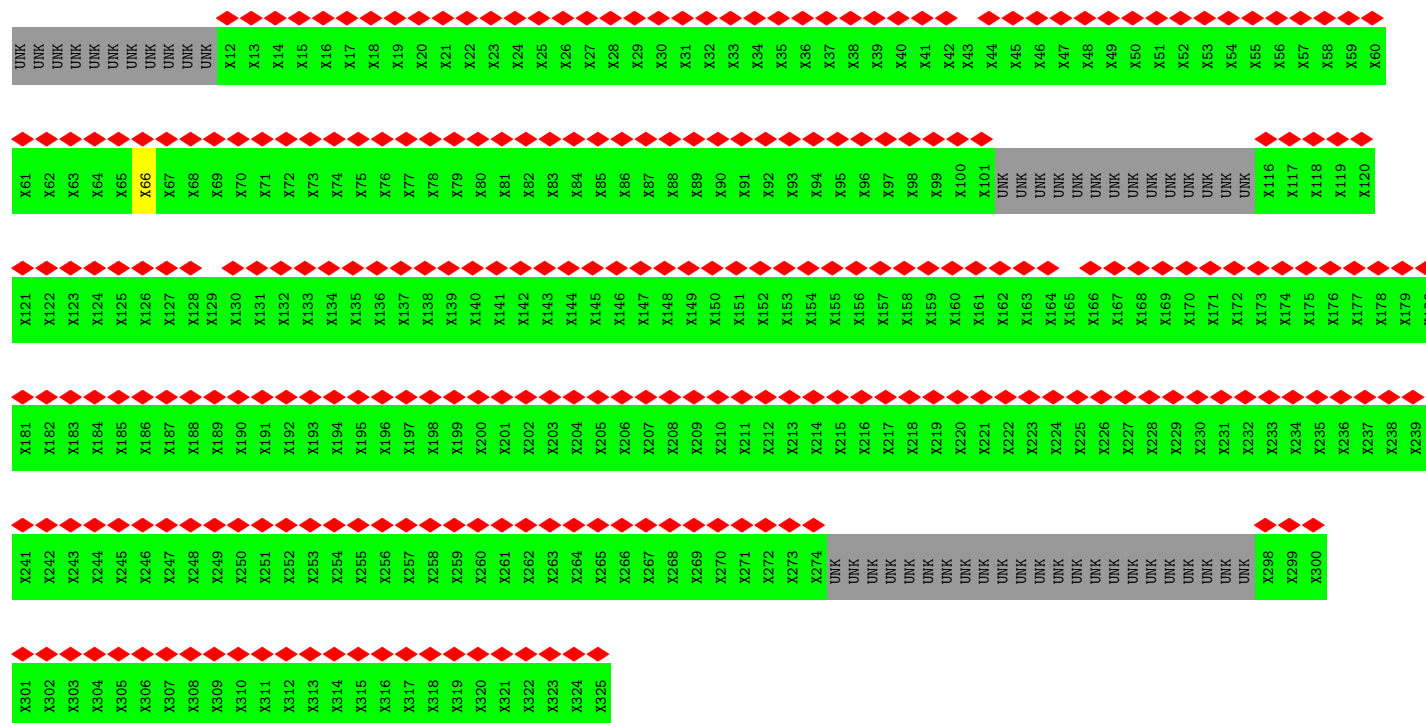
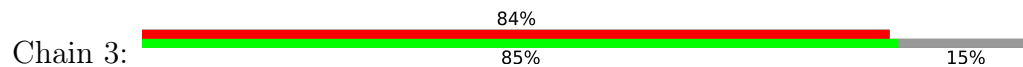


- Molecule 11: Photosystem I 4.8 kDa protein

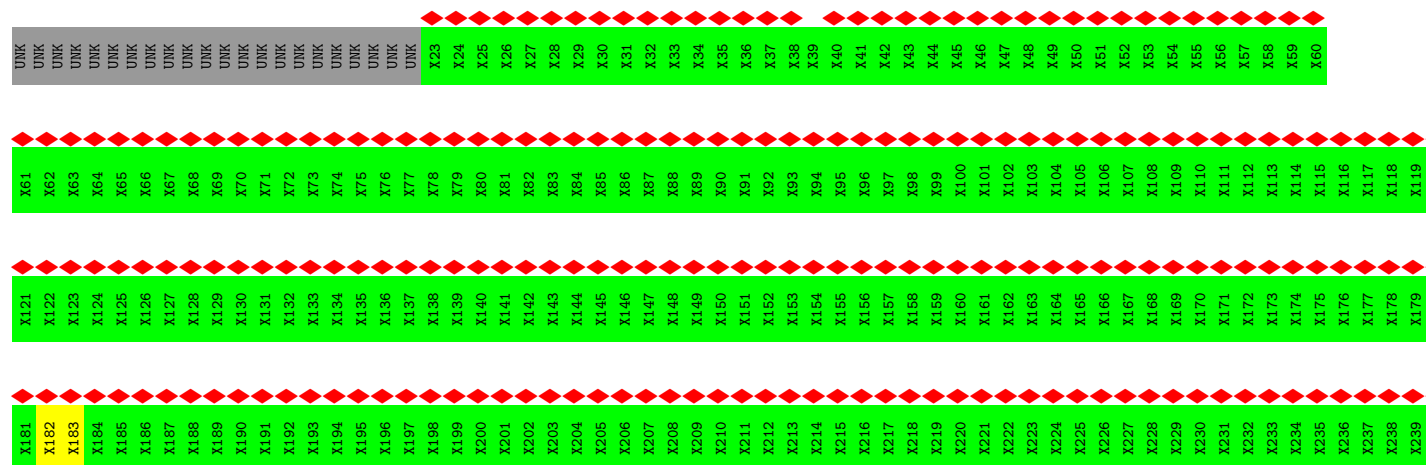
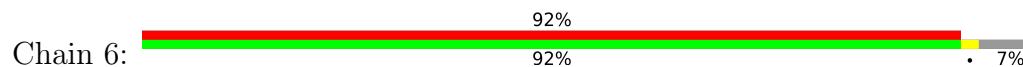


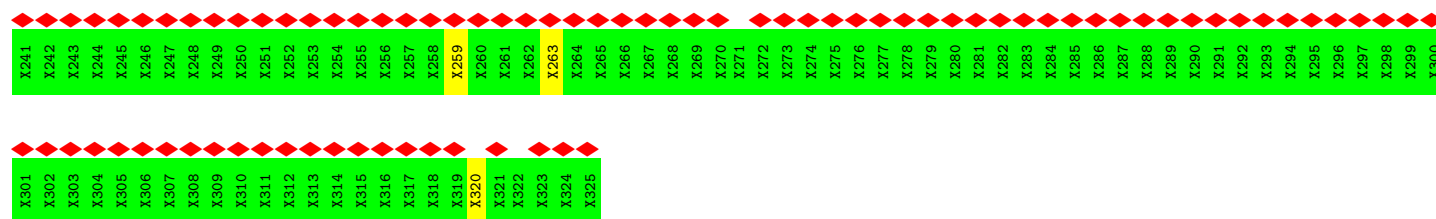


• Molecule 13: IsiA



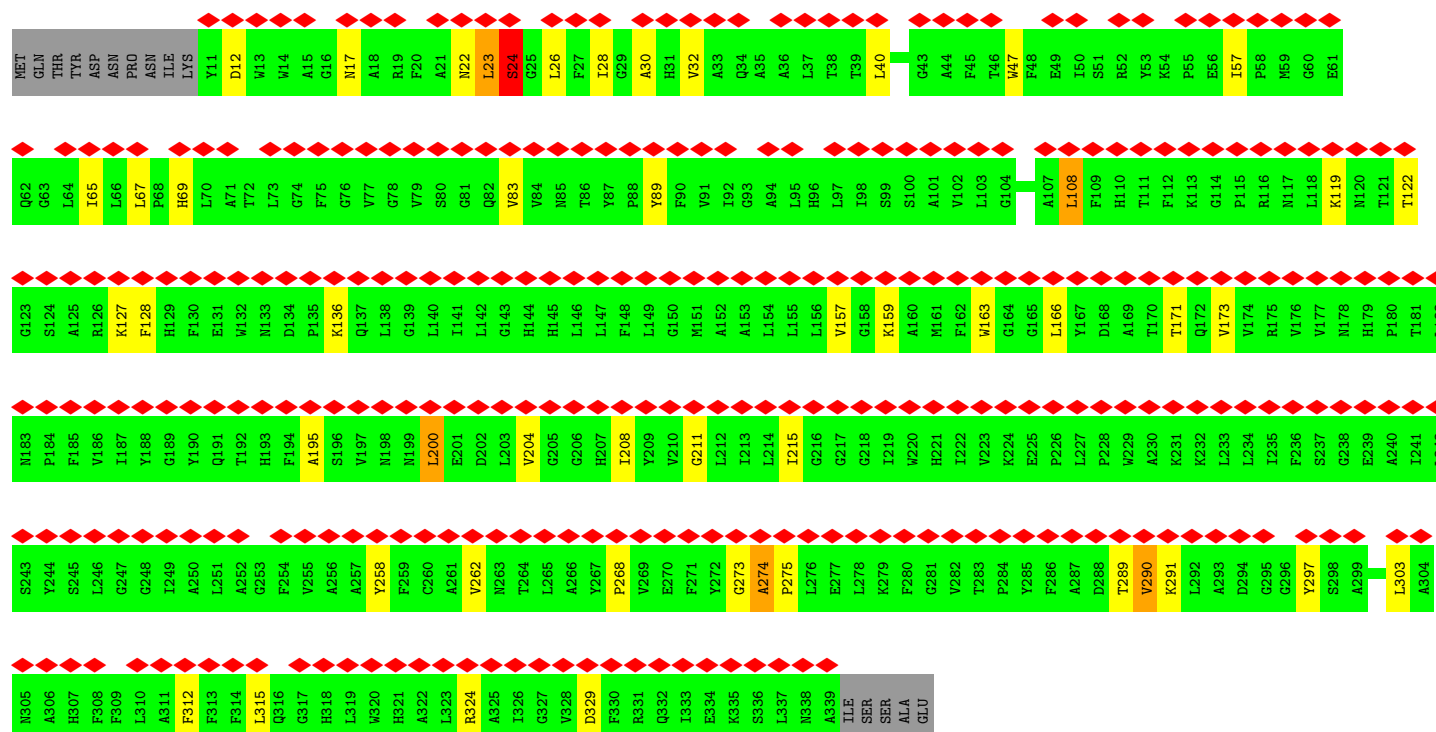
• Molecule 13: IsiA





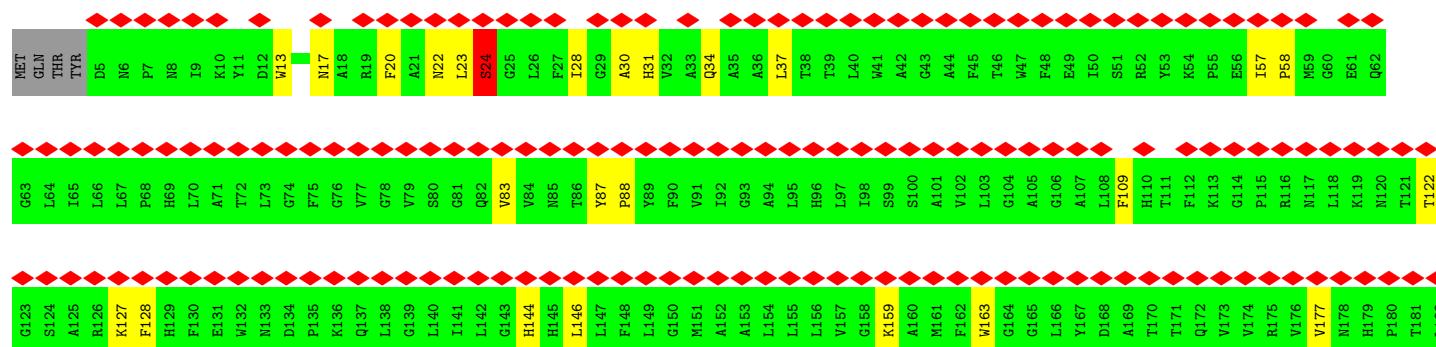
• Molecule 14: Iron stress-induced chlorophyll-binding protein

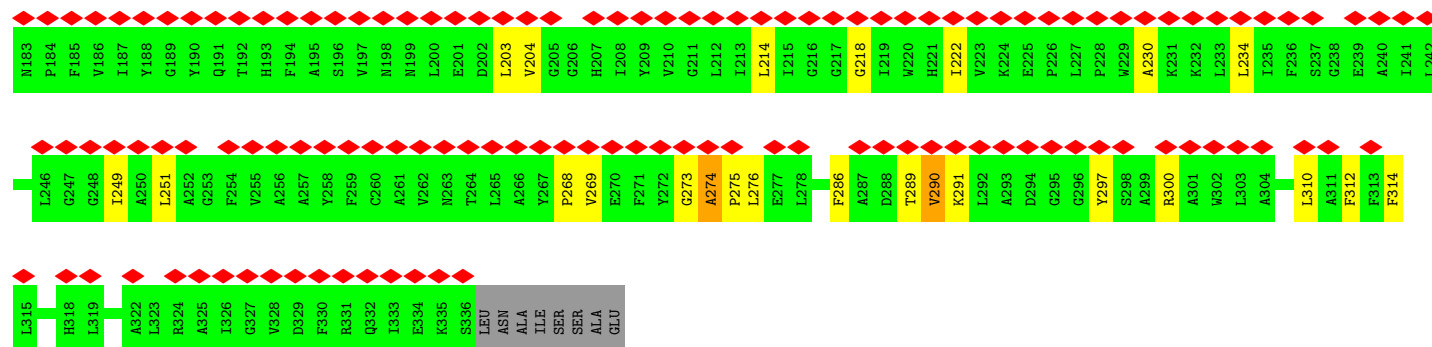
Chain 4: 88%
81% 13% . .



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

Chain 5: 85%
82% 13% . .





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 (Å)	229.68001, 229.68001, 229.68001	wwPDB
Map dimensions	232, 232, 232	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CLA, LHG, CL0, SF4, BCR, LMT, LMG, PQN

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	0.61	0/6023	0.71	0/8216
2	B	0.60	0/6143	0.72	0/8398
3	C	0.63	0/609	0.79	0/826
4	D	0.63	0/1067	0.76	0/1441
5	E	0.64	0/499	0.77	0/677
6	F	0.63	0/1104	0.76	0/1500
7	I	0.63	0/262	0.68	0/358
8	J	0.61	0/358	0.67	0/490
10	M	0.64	0/239	0.68	0/326
11	X	0.59	0/253	0.67	0/347
12	1	0.67	0/3702	0.72	0/5059
14	4	0.68	0/2648	0.79	0/3611
14	5	0.69	0/2676	0.77	0/3649
All	All	0.64	0/25583	0.74	0/34898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5701	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5919	0	5676	87	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	9	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	33	0
13	2	1474	0	277	0	0
13	3	1354	0	264	1	0
13	6	1479	0	284	3	0
14	4	2562	0	2544	35	0
14	5	2589	0	2569	38	0
15	A	65	0	72	7	0
16	1	959	0	764	39	0
16	2	270	0	198	8	0
16	3	45	0	33	2	0
16	4	450	0	330	13	0
16	5	851	0	623	46	0
16	6	401	0	293	10	0
16	A	2460	0	2456	138	0
16	B	2489	0	2585	161	0
16	F	96	0	74	8	0
16	J	90	0	66	4	0
16	K	86	0	62	10	0
16	X	45	0	33	2	0
17	A	33	0	46	5	0
17	B	33	0	46	5	0
18	A	8	0	0	0	0
18	C	16	0	0	1	0
19	1	200	0	280	8	0
19	4	40	0	56	3	0
19	5	80	0	112	5	0
19	A	240	0	336	14	0
19	B	280	0	392	15	0
19	F	80	0	112	4	0
19	I	80	0	112	7	0
19	J	80	0	112	4	0
19	K	40	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	592	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 8.

The worst 5 of 592 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
16:B:807:CLA:H92	16:B:807:CLA:HMC2	1.56	0.86
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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	714 (96%)	26 (4%)	0	100	100
2	B	737/741 (100%)	713 (97%)	22 (3%)	2 (0%)	37	57
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%)	19	36
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%)	19	32

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%)	593 (100%)	2 (0%)	91	97
2	B	601/602 (100%)	600 (100%)	1 (0%)	92	98
3	C	68/69 (99%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	23 (96%)	1 (4%)	25	48
12	1	364/373 (98%)	363 (100%)	1 (0%)	91	97
14	4	252/266 (95%)	244 (97%)	8 (3%)	34	59
14	5	256/266 (96%)	252 (98%)	4 (2%)	58	78
All	All	2523/2629 (96%)	2506 (99%)	17 (1%)	80	92

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	5	37	LEU
14	5	144	HIS
14	4	24	SER
14	4	69	HIS
14	4	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
14	5	133	ASN
12	1	269	ASN
4	D	39	GLN
2	B	619	ASN
6	F	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
21	LMT	M	101	-	36,36,36	0.47	0	47,47,47	0.67	0
16	CLA	B	822	23	55,63,73	2.22	16 (29%)	64,101,113	2.83	27 (42%)
16	CLA	1	514	-	45,53,73	2.52	17 (37%)	52,89,113	3.22	22 (42%)
19	BCR	B	847	-	41,41,41	1.62	10 (24%)	56,56,56	1.35	7 (12%)
16	CLA	1	512	12	45,53,73	2.44	16 (35%)	52,89,113	3.22	26 (50%)
16	CLA	B	816	-	55,63,73	2.08	14 (25%)	64,101,113	3.12	27 (42%)
16	CLA	5	417	14	45,53,73	2.53	17 (37%)	52,89,113	3.19	24 (46%)
16	CLA	6	404	-	45,53,73	2.55	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	5	413	14	45,53,73	2.52	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	B	836	23	45,53,73	2.44	16 (35%)	52,89,113	3.16	24 (46%)
19	BCR	1	518	-	41,41,41	1.72	8 (19%)	56,56,56	1.49	10 (17%)
16	CLA	4	402	-	45,53,73	2.51	17 (37%)	52,89,113	3.27	23 (44%)
16	CLA	B	839	-	65,73,73	1.92	18 (27%)	76,113,113	2.83	27 (35%)
16	CLA	1	513	-	45,53,73	2.48	16 (35%)	52,89,113	3.11	23 (44%)
19	BCR	I	101	-	41,41,41	1.64	9 (21%)	56,56,56	1.42	9 (16%)
16	CLA	A	840	-	65,73,73	1.88	18 (27%)	76,113,113	2.86	24 (31%)
16	CLA	6	405	-	45,53,73	2.55	17 (37%)	52,89,113	3.15	25 (48%)
16	CLA	B	818	-	65,73,73	1.86	14 (21%)	76,113,113	2.87	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	2	402	-	45,53,73	2.55	17 (37%)	52,89,113	3.15	22 (42%)
16	CLA	B	837	-	60,68,73	2.01	16 (26%)	70,107,113	2.79	26 (37%)
16	CLA	A	819	-	54,62,73	2.13	16 (29%)	62,99,113	2.94	25 (40%)
16	CLA	B	828	-	65,73,73	1.90	15 (23%)	76,113,113	2.59	25 (32%)
16	CLA	B	813	-	65,73,73	1.90	15 (23%)	76,113,113	2.83	23 (30%)
19	BCR	J	103	-	41,41,41	1.60	8 (19%)	56,56,56	1.31	7 (12%)
16	CLA	B	817	-	59,67,73	2.02	16 (27%)	68,105,113	2.91	27 (39%)
16	CLA	K	101	-	42,49,73	2.31	15 (35%)	48,83,113	3.12	21 (43%)
16	CLA	A	807	-	65,73,73	1.93	16 (24%)	76,113,113	2.77	25 (32%)
19	BCR	A	847	-	41,41,41	1.64	8 (19%)	56,56,56	1.27	7 (12%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
16	CLA	B	832	-	65,73,73	1.87	15 (23%)	76,113,113	2.93	24 (31%)
16	CLA	B	823	-	65,73,73	1.97	15 (23%)	76,113,113	2.85	33 (43%)
19	BCR	K	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.38	9 (16%)
19	BCR	F	205	-	41,41,41	1.65	8 (19%)	56,56,56	1.32	8 (14%)
16	CLA	A	817	23	49,57,73	2.33	16 (32%)	55,93,113	3.07	24 (43%)
16	CLA	A	821	-	50,58,73	2.25	17 (34%)	58,95,113	3.11	25 (43%)
19	BCR	M	102	-	41,41,41	1.65	8 (19%)	56,56,56	1.35	8 (14%)
16	CLA	6	409	13	45,53,73	2.55	17 (37%)	52,89,113	3.17	23 (44%)
20	LHG	A	853	16	26,26,48	0.32	0	29,32,54	0.48	0
16	CLA	J	102	-	45,53,73	2.43	16 (35%)	52,89,113	3.18	24 (46%)
16	CLA	K	103	23	45,53,73	2.39	17 (37%)	52,89,113	3.23	24 (46%)
16	CLA	1	515	12	45,53,73	2.56	16 (35%)	52,89,113	3.18	23 (44%)
16	CLA	J	101	8	45,53,73	2.39	16 (35%)	52,89,113	3.13	24 (46%)
16	CLA	B	802	23	65,73,73	1.93	18 (27%)	76,113,113	2.85	30 (39%)
16	CLA	1	519	12	65,73,73	2.08	14 (21%)	76,113,113	2.69	26 (34%)
19	BCR	A	849	-	41,41,41	1.66	7 (17%)	56,56,56	1.58	11 (19%)
16	CLA	B	805	-	65,73,73	1.93	15 (23%)	76,113,113	2.83	29 (38%)
16	CLA	A	830	-	65,73,73	1.93	15 (23%)	76,113,113	2.61	21 (27%)
16	CLA	A	828	-	65,73,73	1.91	17 (26%)	76,113,113	2.78	25 (32%)
16	CLA	B	827	-	65,73,73	1.94	16 (24%)	76,113,113	2.97	28 (36%)
16	CLA	2	403	-	45,53,73	2.54	17 (37%)	52,89,113	3.16	23 (44%)
16	CLA	5	407	-	45,53,73	2.51	16 (35%)	52,89,113	3.16	24 (46%)
16	CLA	A	806	-	65,73,73	1.89	16 (24%)	76,113,113	2.87	28 (36%)
16	CLA	5	411	-	45,53,73	2.45	16 (35%)	52,89,113	3.08	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMT	1	524	-	36,36,36	0.53	1 (2%)	47,47,47	0.64	1 (2%)
19	BCR	B	848	-	41,41,41	1.65	11 (26%)	56,56,56	1.36	9 (16%)
20	LHG	B	850	-	48,48,48	0.27	0	51,54,54	0.33	0
16	CLA	B	819	23	65,73,73	2.02	15 (23%)	76,113,113	2.69	29 (38%)
16	CLA	6	403	-	45,53,73	2.52	17 (37%)	52,89,113	3.14	24 (46%)
16	CLA	A	843	23	65,73,73	1.97	16 (24%)	76,113,113	2.79	27 (35%)
16	CLA	4	409	-	45,53,73	2.53	17 (37%)	52,89,113	3.25	22 (42%)
16	CLA	5	421	-	45,53,73	2.53	17 (37%)	52,89,113	3.15	25 (48%)
16	CLA	4	410	14	45,53,73	2.56	17 (37%)	52,89,113	3.19	22 (42%)
16	CLA	A	815	-	45,53,73	2.36	18 (40%)	52,89,113	3.15	24 (46%)
16	CLA	A	810	1	65,73,73	1.98	17 (26%)	76,113,113	2.71	26 (34%)
16	CLA	B	830	-	65,73,73	1.96	16 (24%)	76,113,113	2.59	27 (35%)
16	CLA	6	401	-	45,53,73	2.56	17 (37%)	52,89,113	3.16	23 (44%)
16	CLA	5	405	-	45,53,73	2.52	17 (37%)	52,89,113	3.30	23 (44%)
16	CLA	1	508	-	45,53,73	2.43	17 (37%)	52,89,113	3.12	25 (48%)
16	CLA	A	805	16	54,62,73	2.15	14 (25%)	62,99,113	3.02	29 (46%)
16	CLA	1	511	-	51,59,73	2.32	16 (31%)	59,96,113	3.03	27 (45%)
16	CLA	5	412	-	45,53,73	2.52	16 (35%)	52,89,113	3.19	24 (46%)
21	LMT	5	401	-	36,36,36	0.43	0	47,47,47	0.75	1 (2%)
16	CLA	A	836	-	51,59,73	2.17	17 (33%)	59,96,113	3.00	26 (44%)
16	CLA	B	840	23	65,73,73	1.93	16 (24%)	76,113,113	2.63	24 (31%)
16	CLA	A	834	-	65,73,73	1.87	14 (21%)	76,113,113	2.69	29 (38%)
19	BCR	A	846	-	41,41,41	1.62	9 (21%)	56,56,56	1.35	10 (17%)
19	BCR	J	104	-	41,41,41	1.58	9 (21%)	56,56,56	1.38	9 (16%)
20	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.50	0
16	CLA	4	404	-	45,53,73	2.57	17 (37%)	52,89,113	3.17	23 (44%)
16	CLA	5	409	-	45,53,73	2.45	17 (37%)	52,89,113	3.27	22 (42%)
16	CLA	1	501	20	45,53,73	2.34	16 (35%)	52,89,113	3.12	26 (50%)
16	CLA	5	414	-	45,53,73	2.44	17 (37%)	52,89,113	3.06	22 (42%)
16	CLA	A	820	-	65,73,73	1.91	16 (24%)	76,113,113	2.85	28 (36%)
16	CLA	6	408	-	41,49,73	2.59	16 (39%)	47,84,113	3.34	22 (46%)
17	PQN	B	842	-	34,34,34	1.66	2 (5%)	42,45,45	0.83	1 (2%)
16	CLA	B	807	-	65,73,73	1.94	16 (24%)	76,113,113	2.66	25 (32%)
19	BCR	A	848	-	41,41,41	1.65	10 (24%)	56,56,56	1.34	9 (16%)
17	PQN	A	844	-	34,34,34	1.56	2 (5%)	42,45,45	1.12	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	SF4	A	845	1,2	0,12,12	-	-	-		
16	CLA	A	804	-	65,73,73	1.89	15 (23%)	76,113,113	2.78	27 (35%)
16	CLA	X	101	11	45,53,73	2.37	18 (40%)	52,89,113	3.12	22 (42%)
16	CLA	A	813	-	54,62,73	2.15	17 (31%)	62,99,113	2.98	27 (43%)
16	CLA	5	406	-	45,53,73	2.54	17 (37%)	52,89,113	3.21	24 (46%)
16	CLA	5	415	-	45,53,73	2.53	17 (37%)	52,89,113	3.36	22 (42%)
16	CLA	A	809	1	65,73,73	2.02	15 (23%)	76,113,113	2.75	31 (40%)
16	CLA	1	507	-	45,53,73	2.55	16 (35%)	52,89,113	3.20	22 (42%)
16	CLA	A	814	-	65,73,73	1.95	16 (24%)	76,113,113	2.67	25 (32%)
16	CLA	A	842	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
16	CLA	3	401	-	45,53,73	2.55	17 (37%)	52,89,113	3.17	22 (42%)
16	CLA	1	505	-	45,53,73	2.52	17 (37%)	52,89,113	3.19	23 (44%)
16	CLA	A	802	23	65,73,73	1.85	16 (24%)	76,113,113	2.81	28 (36%)
16	CLA	2	405	-	45,53,73	2.55	16 (35%)	52,89,113	3.15	23 (44%)
16	CLA	B	806	-	65,73,73	1.90	16 (24%)	76,113,113	2.71	27 (35%)
16	CLA	4	408	14	45,53,73	2.52	17 (37%)	52,89,113	3.14	22 (42%)
19	BCR	B	844	-	41,41,41	1.67	9 (21%)	56,56,56	1.33	8 (14%)
16	CLA	B	812	-	45,53,73	2.36	16 (35%)	52,89,113	3.27	27 (51%)
16	CLA	A	832	-	50,58,73	2.11	15 (30%)	58,95,113	3.14	28 (48%)
16	CLA	2	404	-	45,53,73	2.53	17 (37%)	52,89,113	3.19	22 (42%)
16	CLA	A	826	23	65,73,73	2.00	18 (27%)	76,113,113	2.64	30 (39%)
16	CLA	5	408	-	45,53,73	2.56	17 (37%)	52,89,113	3.31	22 (42%)
16	CLA	A	823	-	49,57,73	2.20	16 (32%)	55,93,113	3.38	25 (45%)
16	CLA	A	808	-	51,59,73	2.22	15 (29%)	59,96,113	3.09	25 (42%)
16	CLA	4	407	14	45,53,73	2.54	16 (35%)	52,89,113	3.25	25 (48%)
19	BCR	B	843	-	41,41,41	1.64	8 (19%)	56,56,56	1.35	8 (14%)
16	CLA	5	403	-	45,53,73	2.51	16 (35%)	52,89,113	3.28	21 (40%)
19	BCR	5	402	-	41,41,41	1.67	8 (19%)	56,56,56	1.41	8 (14%)
21	LMT	B	851	-	36,36,36	0.51	1 (2%)	47,47,47	0.69	1 (2%)
19	BCR	A	850	-	41,41,41	1.61	12 (29%)	56,56,56	1.30	7 (12%)
19	BCR	F	202	-	41,41,41	1.63	10 (24%)	56,56,56	1.32	8 (14%)
16	CLA	B	810	-	65,73,73	1.92	16 (24%)	76,113,113	2.85	25 (32%)
19	BCR	4	401	-	41,41,41	1.67	8 (19%)	56,56,56	1.48	9 (16%)
16	CLA	A	811	-	45,53,73	2.29	16 (35%)	52,89,113	3.20	26 (50%)
16	CLA	A	829	-	65,73,73	1.91	15 (23%)	76,113,113	2.82	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	824	-	51,59,73	2.22	16 (31%)	59,96,113	3.14	25 (42%)
16	CLA	F	204	23	45,53,73	2.38	16 (35%)	52,89,113	3.19	23 (44%)
16	CLA	5	419	-	45,53,73	2.50	17 (37%)	52,89,113	3.21	22 (42%)
16	CLA	1	502	-	45,53,73	2.50	16 (35%)	52,89,113	3.28	22 (42%)
21	LMT	B	852	-	36,36,36	0.49	0	47,47,47	0.94	3 (6%)
16	CLA	6	406	-	45,53,73	2.55	17 (37%)	52,89,113	3.14	23 (44%)
16	CLA	6	407	-	45,53,73	2.55	17 (37%)	52,89,113	3.18	22 (42%)
16	CLA	B	808	-	65,73,73	1.86	16 (24%)	76,113,113	2.92	29 (38%)
16	CLA	5	404	-	45,53,73	2.42	17 (37%)	52,89,113	3.15	20 (38%)
16	CLA	A	833	-	65,73,73	2.05	18 (27%)	76,113,113	2.78	29 (38%)
16	CLA	B	824	2	65,73,73	1.91	16 (24%)	76,113,113	2.78	28 (36%)
16	CLA	A	827	23	55,63,73	2.12	15 (27%)	64,101,113	2.93	23 (35%)
16	CLA	1	520	-	65,73,73	1.94	14 (21%)	76,113,113	2.80	27 (35%)
16	CLA	1	521	23	52,60,73	2.31	16 (30%)	60,97,113	3.01	25 (41%)
16	CLA	1	510	-	45,53,73	2.48	16 (35%)	52,89,113	3.13	24 (46%)
16	CLA	5	410	-	45,53,73	2.49	17 (37%)	52,89,113	3.19	23 (44%)
19	BCR	B	845	-	41,41,41	1.60	8 (19%)	56,56,56	1.36	8 (14%)
16	CLA	F	201	23	51,59,73	2.15	16 (31%)	59,96,113	2.85	24 (40%)
16	CLA	A	825	-	47,55,73	2.29	18 (38%)	54,91,113	3.17	21 (38%)
16	CLA	B	815	-	45,53,73	2.37	14 (31%)	52,89,113	3.22	25 (48%)
19	BCR	B	846	-	41,41,41	1.58	10 (24%)	56,56,56	1.32	7 (12%)
16	CLA	A	831	-	65,73,73	1.93	16 (24%)	76,113,113	2.86	23 (30%)
16	CLA	1	504	-	45,53,73	2.44	17 (37%)	52,89,113	3.43	23 (44%)
16	CLA	A	822	23	65,73,73	1.97	15 (23%)	76,113,113	2.65	26 (34%)
16	CLA	5	422	-	45,53,73	2.54	16 (35%)	52,89,113	3.17	23 (44%)
16	CLA	A	835	-	65,73,73	1.88	14 (21%)	76,113,113	2.81	28 (36%)
16	CLA	A	816	-	45,53,73	2.36	14 (31%)	52,89,113	3.18	25 (48%)
16	CLA	6	402	-	45,53,73	2.54	17 (37%)	52,89,113	3.16	23 (44%)
19	BCR	A	851	-	41,41,41	1.69	8 (19%)	56,56,56	1.40	10 (17%)
16	CLA	5	418	-	45,53,73	2.54	17 (37%)	52,89,113	3.14	24 (46%)
19	BCR	5	420	-	41,41,41	1.71	8 (19%)	56,56,56	1.33	9 (16%)
16	CLA	1	506	-	45,53,73	2.47	16 (35%)	52,89,113	3.17	23 (44%)
19	BCR	1	517	-	41,41,41	1.74	8 (19%)	56,56,56	1.53	9 (16%)
16	CLA	B	804	2	54,62,73	2.18	16 (29%)	62,99,113	2.91	30 (48%)
16	CLA	A	839	-	65,73,73	1.92	16 (24%)	76,113,113	2.85	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	803	-	65,73,73	1.91	15 (23%)	76,113,113	2.55	28 (36%)
22	LMG	B	849	-	55,55,55	0.24	0	63,63,63	0.39	0
16	CLA	4	403	-	45,53,73	2.52	16 (35%)	52,89,113	3.28	22 (42%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
16	CLA	B	809	2	65,73,73	1.84	15 (23%)	76,113,113	2.69	27 (35%)
16	CLA	4	406	-	45,53,73	2.47	16 (35%)	52,89,113	3.15	21 (40%)
16	CLA	B	835	23	45,53,73	2.33	17 (37%)	52,89,113	3.16	20 (38%)
15	CL0	A	801	-	65,73,73	1.97	18 (27%)	76,113,113	2.85	30 (39%)
16	CLA	1	526	-	45,53,73	2.53	17 (37%)	52,89,113	3.20	23 (44%)
16	CLA	4	411	-	45,53,73	2.55	17 (37%)	52,89,113	3.20	23 (44%)
19	BCR	1	523	-	41,41,41	1.61	10 (24%)	56,56,56	1.35	8 (14%)
16	CLA	A	837	1	45,53,73	2.38	17 (37%)	52,89,113	3.24	24 (46%)
16	CLA	2	401	-	45,53,73	2.54	16 (35%)	52,89,113	3.24	21 (40%)
16	CLA	2	406	-	45,53,73	2.53	17 (37%)	52,89,113	3.17	21 (40%)
19	BCR	I	102	-	41,41,41	1.69	7 (17%)	56,56,56	1.68	12 (21%)
19	BCR	1	516	-	41,41,41	1.66	7 (17%)	56,56,56	1.53	10 (17%)
16	CLA	4	405	-	45,53,73	2.55	17 (37%)	52,89,113	3.24	25 (48%)
16	CLA	1	509	-	45,53,73	2.37	15 (33%)	52,89,113	3.24	24 (46%)
20	LHG	F	203	-	48,48,48	0.27	0	51,54,54	0.37	0
16	CLA	B	829	-	65,73,73	1.90	17 (26%)	76,113,113	2.81	28 (36%)
16	CLA	B	826	-	65,73,73	1.92	16 (24%)	76,113,113	2.82	23 (30%)
16	CLA	5	416	-	41,49,73	2.57	17 (41%)	47,84,113	3.37	23 (48%)
16	CLA	B	838	-	65,73,73	1.88	15 (23%)	76,113,113	2.70	27 (35%)
16	CLA	A	803	-	65,73,73	1.96	14 (21%)	76,113,113	2.72	30 (39%)
16	CLA	A	838	-	51,59,73	2.18	17 (33%)	59,96,113	3.10	25 (42%)
16	CLA	1	503	-	51,59,73	2.36	16 (31%)	59,96,113	2.97	27 (45%)
16	CLA	B	834	-	65,73,73	1.93	17 (26%)	76,113,113	2.66	28 (36%)
19	BCR	B	853	-	41,41,41	1.65	9 (21%)	56,56,56	1.29	7 (12%)
16	CLA	A	812	16	65,73,73	1.87	16 (24%)	76,113,113	2.77	29 (38%)
16	CLA	B	821	-	45,53,73	2.44	15 (33%)	52,89,113	3.17	25 (48%)
16	CLA	B	801	-	65,73,73	1.90	16 (24%)	76,113,113	2.89	30 (39%)
21	LMT	A	854	-	36,36,36	0.42	0	47,47,47	0.99	4 (8%)
16	CLA	A	818	-	54,62,73	2.14	15 (27%)	62,99,113	3.15	22 (35%)
16	CLA	B	833	-	58,66,73	2.02	17 (29%)	67,104,113	2.90	27 (40%)
16	CLA	A	841	-	65,73,73	1.95	17 (26%)	76,113,113	2.80	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	820	-	47,55,73	2.35	16 (34%)	54,91,113	3.23	27 (50%)
16	CLA	B	814	-	56,64,73	2.12	16 (28%)	65,102,113	2.99	25 (38%)
16	CLA	B	841	-	65,73,73	1.90	18 (27%)	76,113,113	2.86	23 (30%)
16	CLA	B	831	-	65,73,73	2.03	17 (26%)	76,113,113	2.77	29 (38%)
16	CLA	1	525	-	45,53,73	2.52	16 (35%)	52,89,113	3.13	24 (46%)
19	BCR	1	522	-	41,41,41	1.64	9 (21%)	56,56,56	1.23	9 (16%)
16	CLA	B	811	-	65,73,73	1.93	15 (23%)	76,113,113	2.68	25 (32%)
16	CLA	B	825	23	65,73,73	2.00	15 (23%)	76,113,113	2.81	33 (43%)

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
21	LMT	M	101	-	-	4/21/61/61	0/2/2/2
16	CLA	B	822	23	1/1/13/20	10/25/103/115	-
16	CLA	1	514	-	1/1/11/20	5/13/91/115	-
19	BCR	B	847	-	-	7/29/63/63	0/2/2/2
16	CLA	1	512	12	1/1/11/20	5/13/91/115	-
16	CLA	B	816	-	-	6/25/103/115	-
16	CLA	5	417	14	1/1/11/20	6/13/91/115	-
16	CLA	6	404	-	1/1/11/20	5/13/91/115	-
16	CLA	5	413	14	1/1/11/20	4/13/91/115	-
16	CLA	B	836	23	1/1/11/20	4/13/91/115	-
19	BCR	1	518	-	-	6/29/63/63	0/2/2/2
16	CLA	4	402	-	1/1/11/20	6/13/91/115	-
16	CLA	B	839	-	1/1/15/20	9/37/115/115	-
16	CLA	1	513	-	1/1/11/20	2/13/91/115	-
19	BCR	I	101	-	-	1/29/63/63	0/2/2/2
16	CLA	A	840	-	1/1/15/20	11/37/115/115	-
16	CLA	6	405	-	1/1/11/20	5/13/91/115	-
16	CLA	B	818	-	1/1/15/20	12/37/115/115	-
16	CLA	2	402	-	1/1/11/20	5/13/91/115	-
16	CLA	B	837	-	1/1/14/20	7/31/109/115	-
16	CLA	A	819	-	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	828	-	1/1/15/20	10/37/115/115	-
16	CLA	B	813	-	1/1/15/20	9/37/115/115	-
19	BCR	J	103	-	-	8/29/63/63	0/2/2/2
16	CLA	B	817	-	1/1/13/20	5/30/108/115	-
16	CLA	K	101	-	1/1/9/20	3/7/81/115	-
16	CLA	A	807	-	1/1/15/20	9/37/115/115	-
19	BCR	A	847	-	-	5/29/63/63	0/2/2/2
18	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	832	-	1/1/15/20	9/37/115/115	-
16	CLA	B	823	-	1/1/15/20	8/37/115/115	-
19	BCR	K	102	-	-	12/29/63/63	0/2/2/2
19	BCR	F	205	-	-	2/29/63/63	0/2/2/2
16	CLA	A	817	23	-	4/18/96/115	-
16	CLA	A	821	-	-	7/19/97/115	-
19	BCR	M	102	-	-	10/29/63/63	0/2/2/2
16	CLA	6	409	13	1/1/11/20	5/13/91/115	-
20	LHG	A	853	16	-	8/31/31/53	-
16	CLA	J	102	-	1/1/11/20	5/13/91/115	-
16	CLA	K	103	23	1/1/11/20	3/13/91/115	-
16	CLA	1	515	12	1/1/11/20	5/13/91/115	-
16	CLA	J	101	8	1/1/11/20	8/13/91/115	-
16	CLA	B	802	23	1/1/15/20	8/37/115/115	-
16	CLA	1	519	12	-	11/37/115/115	-
19	BCR	A	849	-	-	16/29/63/63	0/2/2/2
16	CLA	B	805	-	1/1/15/20	11/37/115/115	-
16	CLA	A	830	-	1/1/15/20	9/37/115/115	-
16	CLA	A	828	-	1/1/15/20	6/37/115/115	-
16	CLA	B	827	-	1/1/15/20	11/37/115/115	-
16	CLA	2	403	-	1/1/11/20	2/13/91/115	-
16	CLA	5	407	-	1/1/11/20	3/13/91/115	-
16	CLA	A	806	-	1/1/15/20	13/37/115/115	-
16	CLA	5	411	-	1/1/11/20	5/13/91/115	-
21	LMT	1	524	-	-	7/21/61/61	0/2/2/2
19	BCR	B	848	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	B	850	-	-	15/53/53/53	-
16	CLA	B	819	23	1/1/15/20	10/37/115/115	-
16	CLA	6	403	-	1/1/11/20	4/13/91/115	-
16	CLA	A	843	23	1/1/15/20	10/37/115/115	-
16	CLA	4	409	-	1/1/11/20	3/13/91/115	-
16	CLA	5	421	-	1/1/11/20	7/13/91/115	-
16	CLA	4	410	14	1/1/11/20	5/13/91/115	-
16	CLA	A	815	-	1/1/11/20	2/13/91/115	-
16	CLA	6	401	-	1/1/11/20	6/13/91/115	-
16	CLA	B	830	-	1/1/15/20	11/37/115/115	-
16	CLA	A	810	1	-	12/37/115/115	-
16	CLA	5	405	-	1/1/11/20	2/13/91/115	-
16	CLA	1	508	-	1/1/11/20	6/13/91/115	-
16	CLA	A	805	16	1/1/12/20	8/24/102/115	-
16	CLA	1	511	-	1/1/12/20	7/21/99/115	-
16	CLA	5	412	-	1/1/11/20	5/13/91/115	-
21	LMT	5	401	-	-	3/21/61/61	0/2/2/2
16	CLA	A	836	-	1/1/12/20	5/21/99/115	-
16	CLA	B	840	23	1/1/15/20	11/37/115/115	-
16	CLA	A	834	-	1/1/15/20	7/37/115/115	-
19	BCR	A	846	-	-	9/29/63/63	0/2/2/2
19	BCR	J	104	-	-	11/29/63/63	0/2/2/2
20	LHG	A	852	-	-	21/53/53/53	-
16	CLA	4	404	-	1/1/11/20	1/13/91/115	-
16	CLA	5	409	-	1/1/11/20	6/13/91/115	-
16	CLA	1	501	20	1/1/11/20	5/13/91/115	-
16	CLA	5	414	-	1/1/11/20	7/13/91/115	-
16	CLA	A	820	-	1/1/15/20	14/37/115/115	-
16	CLA	6	408	-	1/1/10/20	2/8/86/115	-
17	PQN	B	842	-	-	2/23/43/43	0/2/2/2
16	CLA	B	807	-	1/1/15/20	5/37/115/115	-
19	BCR	A	848	-	-	3/29/63/63	0/2/2/2
17	PQN	A	844	-	-	3/23/43/43	0/2/2/2
18	SF4	A	845	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	804	-	1/1/15/20	11/37/115/115	-
16	CLA	X	101	11	1/1/11/20	7/13/91/115	-
16	CLA	A	813	-	1/1/12/20	11/24/102/115	-
16	CLA	5	406	-	1/1/11/20	5/13/91/115	-
16	CLA	5	415	-	1/1/11/20	5/13/91/115	-
16	CLA	A	809	1	1/1/15/20	11/37/115/115	-
16	CLA	1	507	-	1/1/11/20	6/13/91/115	-
16	CLA	A	814	-	1/1/15/20	15/37/115/115	-
16	CLA	A	842	-	1/1/15/20	8/37/115/115	-
16	CLA	3	401	-	1/1/11/20	5/13/91/115	-
16	CLA	1	505	-	1/1/11/20	3/13/91/115	-
16	CLA	A	802	23	1/1/15/20	3/37/115/115	-
16	CLA	2	405	-	1/1/11/20	5/13/91/115	-
16	CLA	B	806	-	1/1/15/20	11/37/115/115	-
16	CLA	4	408	14	1/1/11/20	4/13/91/115	-
19	BCR	B	844	-	-	6/29/63/63	0/2/2/2
16	CLA	B	812	-	1/1/11/20	0/13/91/115	-
16	CLA	A	832	-	-	3/19/97/115	-
16	CLA	2	404	-	1/1/11/20	5/13/91/115	-
16	CLA	A	826	23	1/1/15/20	11/37/115/115	-
16	CLA	5	408	-	1/1/11/20	4/13/91/115	-
16	CLA	A	823	-	-	10/18/96/115	-
16	CLA	A	808	-	1/1/12/20	4/21/99/115	-
16	CLA	4	407	14	1/1/11/20	5/13/91/115	-
19	BCR	B	843	-	-	8/29/63/63	0/2/2/2
16	CLA	5	403	-	1/1/11/20	6/13/91/115	-
19	BCR	5	402	-	-	4/29/63/63	0/2/2/2
21	LMT	B	851	-	-	6/21/61/61	0/2/2/2
19	BCR	A	850	-	-	6/29/63/63	0/2/2/2
19	BCR	F	202	-	-	4/29/63/63	0/2/2/2
16	CLA	B	810	-	1/1/15/20	10/37/115/115	-
19	BCR	4	401	-	-	19/29/63/63	0/2/2/2
16	CLA	A	811	-	1/1/11/20	2/13/91/115	-
16	CLA	A	829	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	824	-	-	7/21/99/115	-
16	CLA	F	204	23	1/1/11/20	0/13/91/115	-
16	CLA	5	419	-	1/1/11/20	5/13/91/115	-
16	CLA	1	502	-	1/1/11/20	6/13/91/115	-
21	LMT	B	852	-	-	5/21/61/61	0/2/2/2
16	CLA	6	406	-	1/1/11/20	2/13/91/115	-
16	CLA	6	407	-	1/1/11/20	5/13/91/115	-
16	CLA	B	808	-	1/1/15/20	10/37/115/115	-
16	CLA	5	404	-	1/1/11/20	4/13/91/115	-
16	CLA	A	833	-	1/1/15/20	10/37/115/115	-
16	CLA	B	824	2	1/1/15/20	10/37/115/115	-
16	CLA	A	827	23	1/1/13/20	5/25/103/115	-
16	CLA	1	521	23	1/1/12/20	6/22/100/115	-
16	CLA	5	410	-	1/1/11/20	2/13/91/115	-
16	CLA	1	510	-	1/1/11/20	5/13/91/115	-
16	CLA	1	520	-	-	9/37/115/115	-
19	BCR	B	845	-	-	9/29/63/63	0/2/2/2
16	CLA	F	201	23	1/1/12/20	8/21/99/115	-
16	CLA	A	825	-	-	7/16/94/115	-
16	CLA	B	815	-	-	4/13/91/115	-
19	BCR	B	846	-	-	6/29/63/63	0/2/2/2
16	CLA	A	831	-	1/1/15/20	5/37/115/115	-
16	CLA	1	504	-	-	5/13/91/115	-
16	CLA	A	822	23	1/1/15/20	10/37/115/115	-
16	CLA	5	422	-	1/1/11/20	6/13/91/115	-
16	CLA	A	835	-	1/1/15/20	11/37/115/115	-
16	CLA	A	816	-	1/1/11/20	3/13/91/115	-
16	CLA	6	402	-	1/1/11/20	6/13/91/115	-
19	BCR	A	851	-	-	9/29/63/63	0/2/2/2
16	CLA	5	418	-	1/1/11/20	6/13/91/115	-
19	BCR	5	420	-	-	9/29/63/63	0/2/2/2
16	CLA	1	506	-	1/1/11/20	6/13/91/115	-
19	BCR	1	517	-	-	12/29/63/63	0/2/2/2
16	CLA	B	804	2	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	839	-	1/1/15/20	10/37/115/115	-
16	CLA	B	803	-	1/1/15/20	8/37/115/115	-
22	LMG	B	849	-	-	16/50/70/70	0/1/1/1
16	CLA	4	403	-	1/1/11/20	5/13/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
16	CLA	B	809	2	1/1/15/20	10/37/115/115	-
16	CLA	4	406	-	1/1/11/20	6/13/91/115	-
16	CLA	B	835	23	1/1/11/20	6/13/91/115	-
15	CL0	A	801	-	2/2/20/25	2/37/135/135	-
16	CLA	1	526	-	1/1/11/20	6/13/91/115	-
16	CLA	4	411	-	1/1/11/20	7/13/91/115	-
19	BCR	1	523	-	-	5/29/63/63	0/2/2/2
16	CLA	A	837	1	1/1/11/20	7/13/91/115	-
16	CLA	2	401	-	1/1/11/20	5/13/91/115	-
16	CLA	2	406	-	1/1/11/20	7/13/91/115	-
19	BCR	I	102	-	-	7/29/63/63	0/2/2/2
19	BCR	1	516	-	-	11/29/63/63	0/2/2/2
16	CLA	4	405	-	1/1/11/20	2/13/91/115	-
16	CLA	1	509	-	1/1/11/20	5/13/91/115	-
20	LHG	F	203	-	-	20/53/53/53	-
16	CLA	B	829	-	1/1/15/20	19/37/115/115	-
16	CLA	B	826	-	1/1/15/20	10/37/115/115	-
16	CLA	5	416	-	1/1/10/20	4/8/86/115	-
16	CLA	B	838	-	1/1/15/20	8/37/115/115	-
16	CLA	A	803	-	1/1/15/20	11/37/115/115	-
16	CLA	A	838	-	1/1/12/20	7/21/99/115	-
16	CLA	1	503	-	1/1/12/20	7/21/99/115	-
16	CLA	B	834	-	1/1/15/20	7/37/115/115	-
19	BCR	B	853	-	-	6/29/63/63	0/2/2/2
16	CLA	A	812	16	1/1/15/20	7/37/115/115	-
16	CLA	B	821	-	-	3/13/91/115	-
16	CLA	B	801	-	1/1/15/20	11/37/115/115	-
21	LMT	A	854	-	-	6/21/61/61	0/2/2/2
16	CLA	A	818	-	-	1/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	833	-	1/1/13/20	10/29/107/115	-
16	CLA	A	841	-	1/1/15/20	8/37/115/115	-
16	CLA	1	525	-	1/1/11/20	8/13/91/115	-
16	CLA	B	814	-	1/1/13/20	9/27/105/115	-
16	CLA	B	820	-	-	5/16/94/115	-
16	CLA	B	831	-	1/1/15/20	7/37/115/115	-
16	CLA	B	841	-	-	8/37/115/115	-
19	BCR	1	522	-	-	4/29/63/63	0/2/2/2
16	CLA	B	811	-	1/1/15/20	5/37/115/115	-
16	CLA	B	825	23	1/1/15/20	14/37/115/115	-

The worst 5 of 2785 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	B	822	CLA	C3B-C2B	6.39	1.49	1.40
16	A	837	CLA	C3B-C2B	6.33	1.49	1.40
16	A	826	CLA	C3B-C2B	6.27	1.49	1.40

The worst 5 of 4163 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

5 of 141 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	801	CL0	NC
15	A	801	CL0	ND
16	A	802	CLA	ND
16	A	803	CLA	ND
16	A	804	CLA	ND

5 of 1379 torsion outliers are listed below:

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

183 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	M	101	LMT	2	0
16	B	822	CLA	3	0
16	1	514	CLA	2	0
19	B	847	BCR	4	0
16	1	512	CLA	4	0
16	B	816	CLA	1	0
16	5	417	CLA	2	0
16	6	404	CLA	1	0
16	5	413	CLA	4	0
16	4	402	CLA	1	0
16	B	839	CLA	13	0
16	1	513	CLA	1	0
19	I	101	BCR	2	0
16	A	840	CLA	4	0
16	6	405	CLA	1	0
16	B	818	CLA	3	0
16	2	402	CLA	1	0
16	B	837	CLA	1	0
16	A	819	CLA	5	0
16	B	828	CLA	6	0
16	B	813	CLA	7	0
19	J	103	BCR	3	0
16	B	817	CLA	3	0
16	K	101	CLA	6	0
16	A	807	CLA	4	0
16	B	832	CLA	4	0
16	B	823	CLA	5	0
19	K	102	BCR	6	0
16	A	817	CLA	1	0
16	A	821	CLA	5	0
19	M	102	BCR	2	0
16	6	409	CLA	2	0
20	A	853	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	J	102	CLA	2	0
16	K	103	CLA	4	0
16	1	515	CLA	2	0
16	J	101	CLA	2	0
16	B	802	CLA	12	0
16	1	519	CLA	2	0
19	A	849	BCR	2	0
16	B	805	CLA	1	0
16	A	830	CLA	2	0
16	A	828	CLA	4	0
16	B	827	CLA	7	0
16	2	403	CLA	1	0
16	5	407	CLA	6	0
16	A	806	CLA	5	0
16	5	411	CLA	1	0
20	B	850	LHG	3	0
16	B	819	CLA	5	0
16	6	403	CLA	1	0
16	A	843	CLA	5	0
16	4	409	CLA	1	0
16	5	421	CLA	2	0
16	4	410	CLA	1	0
16	A	815	CLA	2	0
16	A	810	CLA	4	0
16	B	830	CLA	7	0
16	6	401	CLA	1	0
16	5	405	CLA	1	0
16	1	508	CLA	2	0
16	A	805	CLA	2	0
16	1	511	CLA	4	0
16	5	412	CLA	4	0
16	A	836	CLA	2	0
16	B	840	CLA	4	0
16	A	834	CLA	7	0
19	A	846	BCR	4	0
19	J	104	BCR	1	0
20	A	852	LHG	3	0
16	4	404	CLA	1	0
16	5	409	CLA	1	0
16	1	501	CLA	4	0
16	5	414	CLA	5	0
16	A	820	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	6	408	CLA	1	0
17	B	842	PQN	5	0
16	B	807	CLA	7	0
19	A	848	BCR	1	0
17	A	844	PQN	5	0
16	A	804	CLA	3	0
16	X	101	CLA	2	0
16	A	813	CLA	1	0
16	5	406	CLA	2	0
16	5	415	CLA	2	0
16	A	809	CLA	5	0
16	A	814	CLA	3	0
16	A	842	CLA	6	0
16	3	401	CLA	2	0
16	A	802	CLA	5	0
16	2	405	CLA	1	0
16	B	806	CLA	6	0
16	4	408	CLA	3	0
19	B	844	BCR	4	0
16	B	812	CLA	3	0
16	A	832	CLA	2	0
16	2	404	CLA	1	0
16	A	826	CLA	6	0
16	5	408	CLA	2	0
16	A	823	CLA	2	0
16	A	808	CLA	1	0
16	4	407	CLA	1	0
19	B	843	BCR	2	0
16	5	403	CLA	2	0
19	5	402	BCR	4	0
19	A	850	BCR	2	0
19	F	202	BCR	4	0
16	B	810	CLA	5	0
19	4	401	BCR	3	0
16	A	811	CLA	4	0
16	A	829	CLA	10	0
16	A	824	CLA	1	0
16	F	204	CLA	2	0
16	5	419	CLA	4	0
16	1	502	CLA	1	0
16	6	406	CLA	1	0
16	6	407	CLA	1	0

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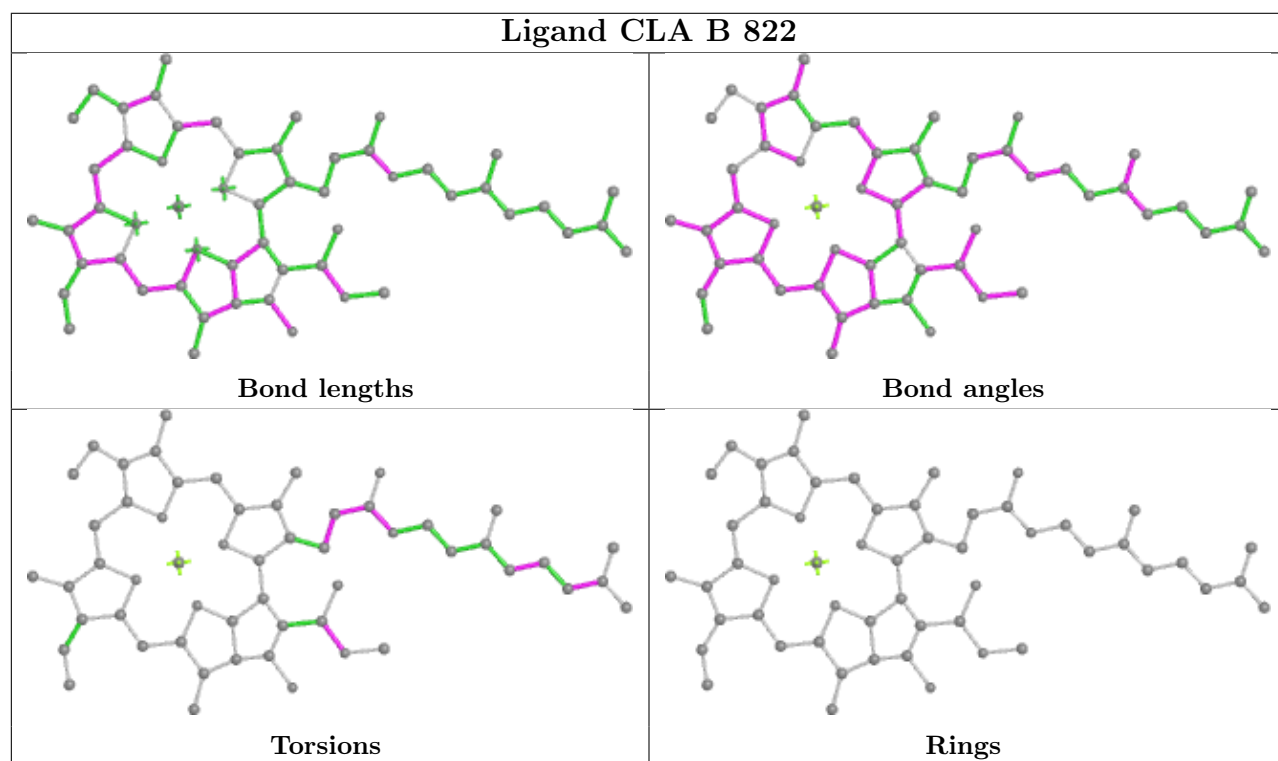
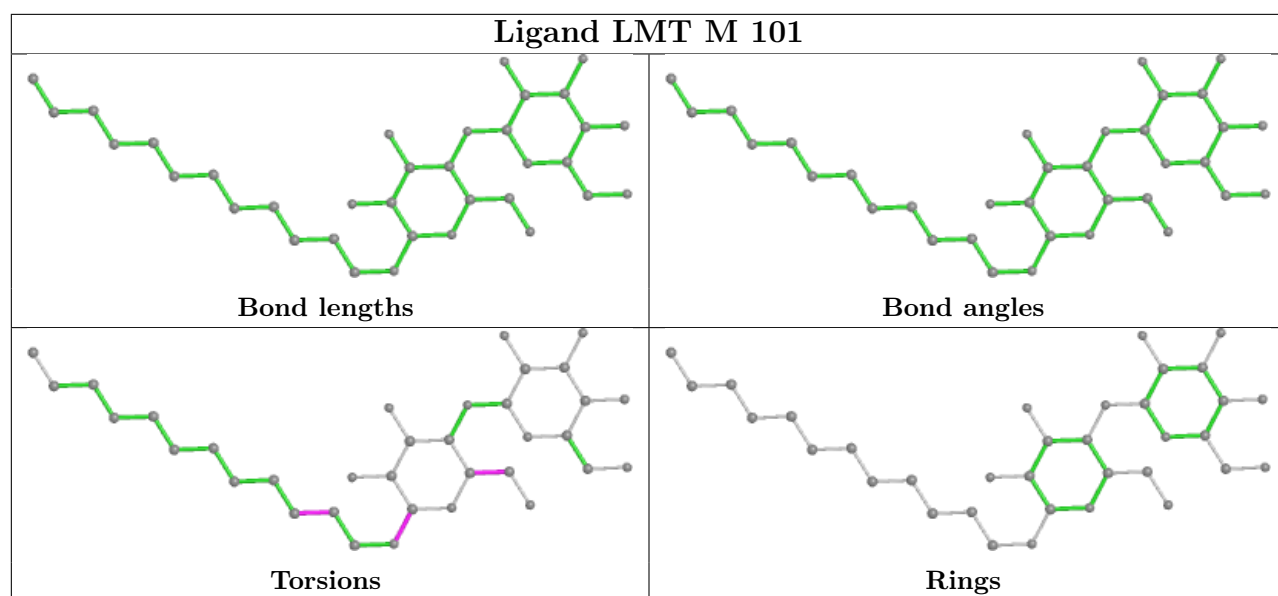
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	808	CLA	5	0
16	5	404	CLA	6	0
16	A	833	CLA	9	0
16	B	824	CLA	6	0
16	A	827	CLA	3	0
16	1	520	CLA	5	0
16	1	521	CLA	3	0
16	1	510	CLA	3	0
16	5	410	CLA	1	0
19	B	845	BCR	3	0
16	F	201	CLA	6	0
16	A	825	CLA	2	0
16	B	815	CLA	3	0
16	A	831	CLA	6	0
16	1	504	CLA	2	0
16	A	822	CLA	6	0
16	5	422	CLA	2	0
16	A	835	CLA	2	0
16	A	816	CLA	1	0
16	6	402	CLA	1	0
19	A	851	BCR	5	0
16	5	418	CLA	1	0
19	5	420	BCR	1	0
16	1	506	CLA	1	0
19	1	517	BCR	2	0
16	B	804	CLA	3	0
16	A	839	CLA	7	0
16	B	803	CLA	3	0
22	B	849	LMG	3	0
16	4	403	CLA	1	0
18	C	102	SF4	1	0
16	B	809	CLA	8	0
16	B	835	CLA	3	0
15	A	801	CL0	7	0
16	1	526	CLA	1	0
16	4	411	CLA	3	0
19	1	523	BCR	5	0
16	A	837	CLA	2	0
16	2	401	CLA	1	0
16	2	406	CLA	3	0
19	I	102	BCR	5	0
19	1	516	BCR	1	0

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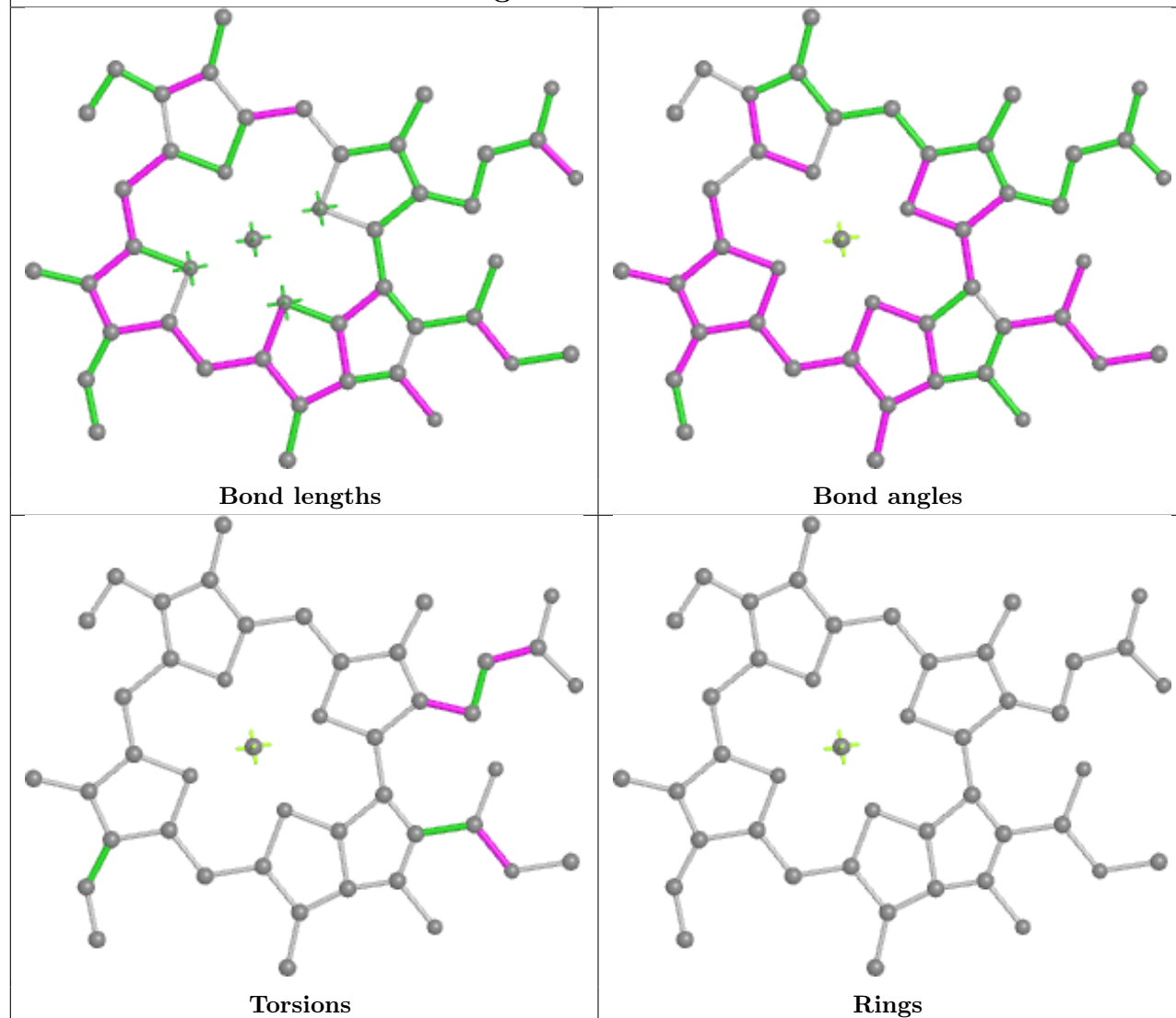
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	4	405	CLA	1	0
16	1	509	CLA	2	0
16	B	829	CLA	6	0
16	B	826	CLA	4	0
16	5	416	CLA	1	0
16	B	838	CLA	5	0
16	A	803	CLA	5	0
16	A	838	CLA	1	0
16	1	503	CLA	1	0
16	B	834	CLA	6	0
19	B	853	BCR	3	0
16	A	812	CLA	3	0
16	B	821	CLA	3	0
16	B	801	CLA	5	0
16	A	818	CLA	2	0
16	B	833	CLA	5	0
16	A	841	CLA	6	0
16	B	820	CLA	2	0
16	B	814	CLA	2	0
16	B	841	CLA	6	0
16	B	831	CLA	4	0
16	1	525	CLA	1	0
16	B	811	CLA	2	0
16	B	825	CLA	6	0

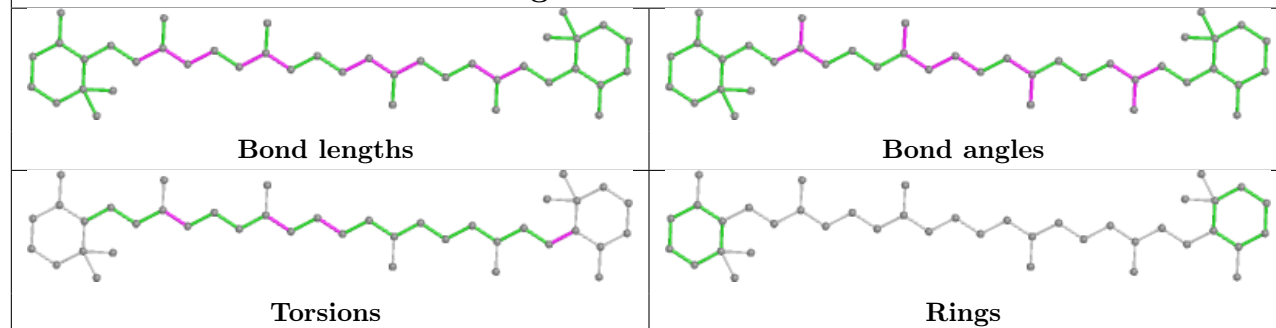
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



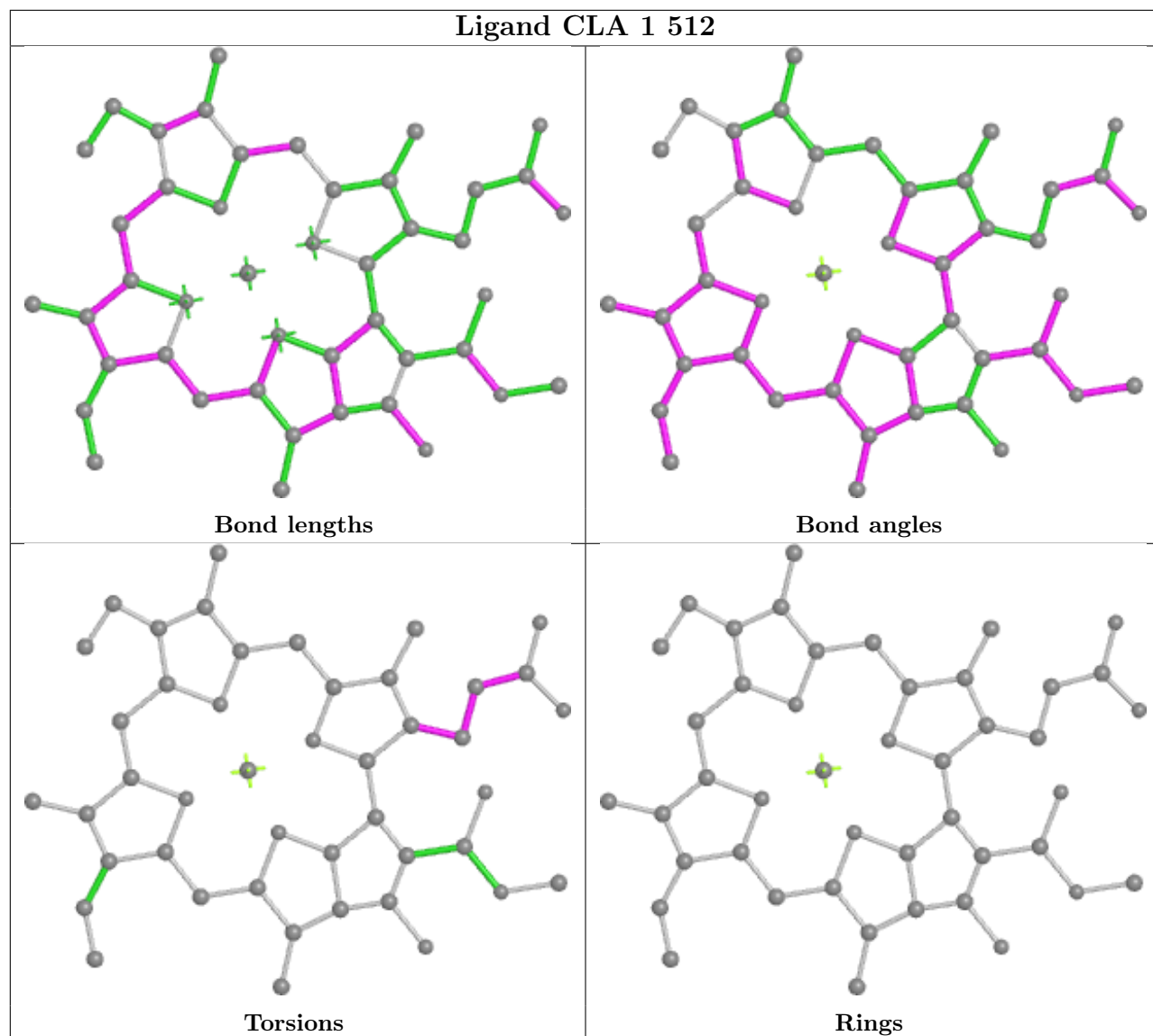
Ligand CLA 1 514

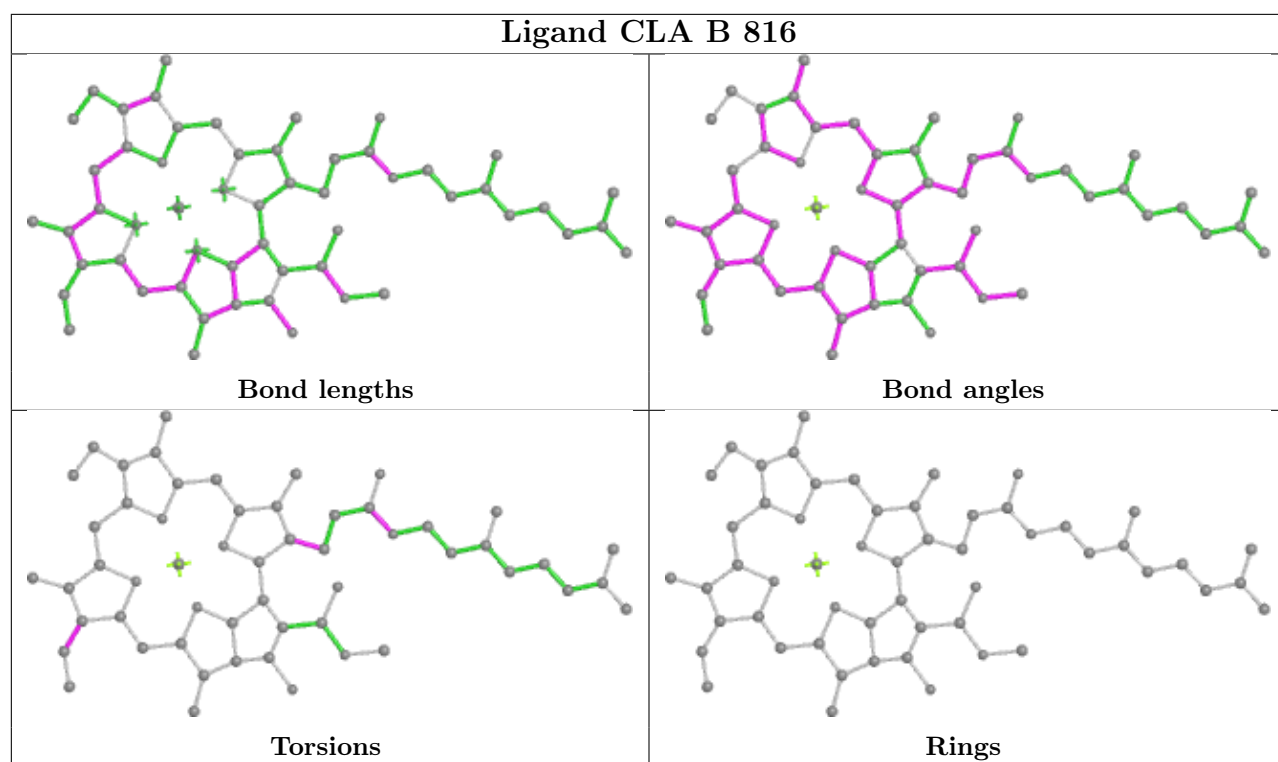


Ligand BCR B 847

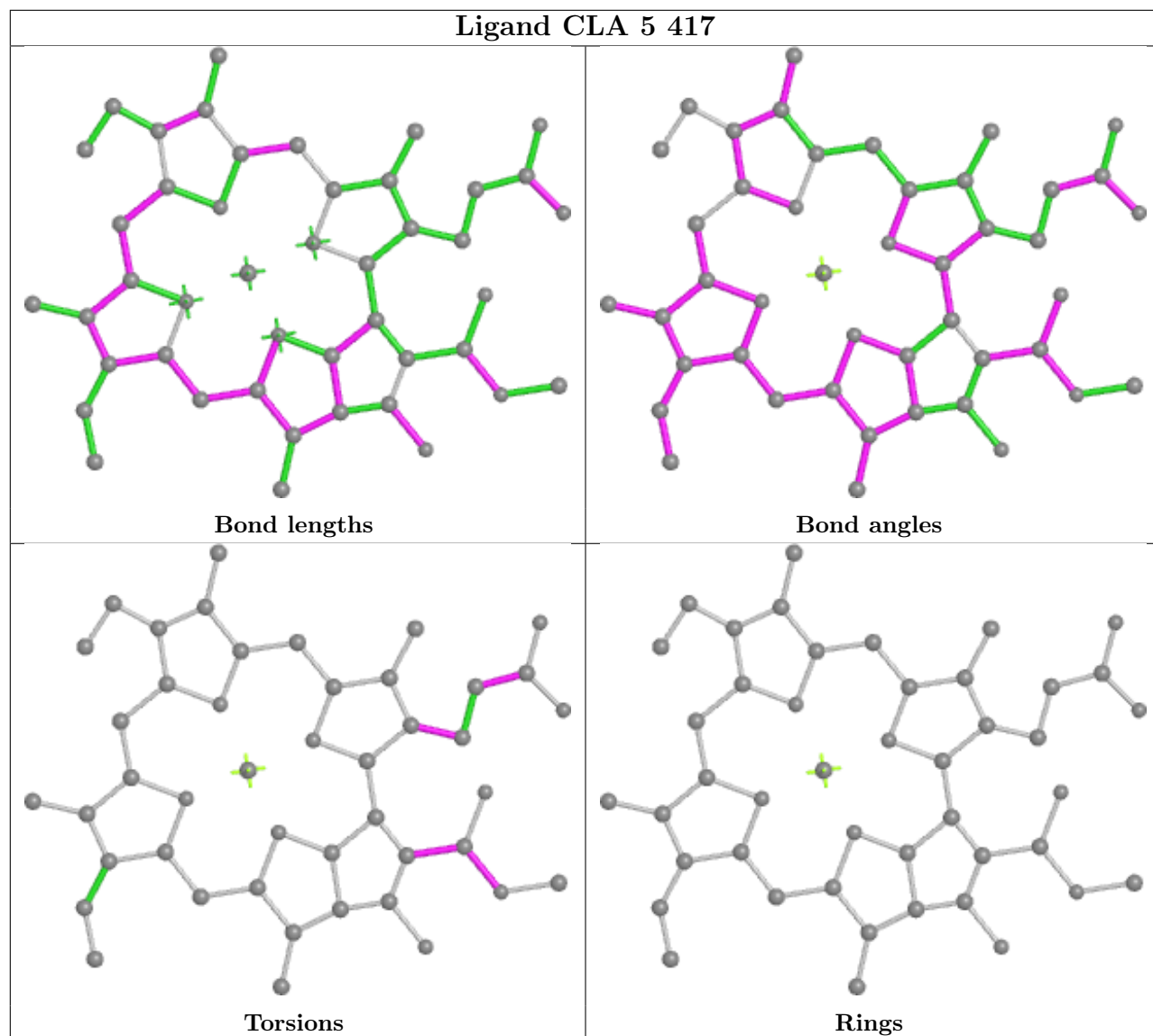


Ligand CLA 1 512

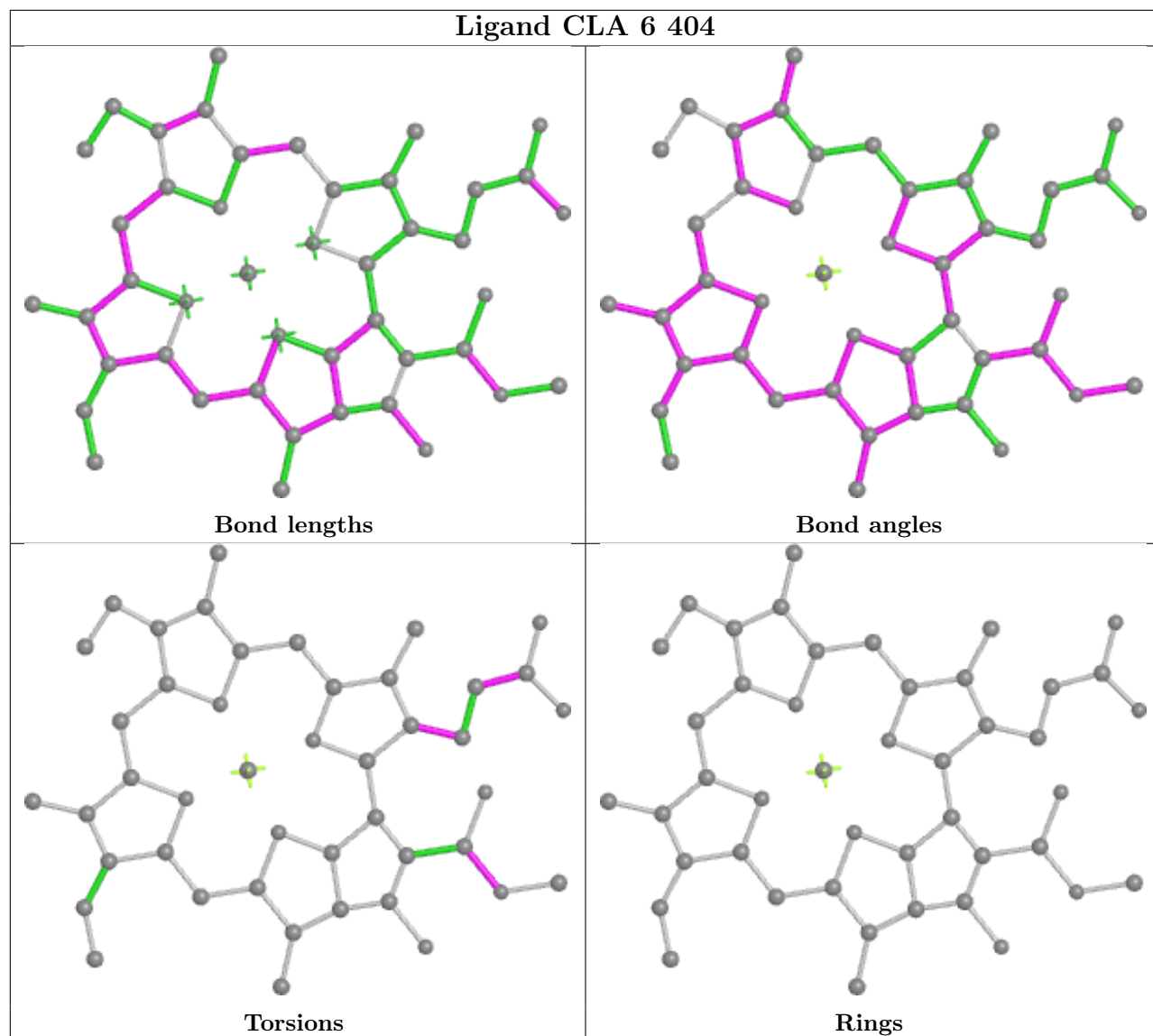




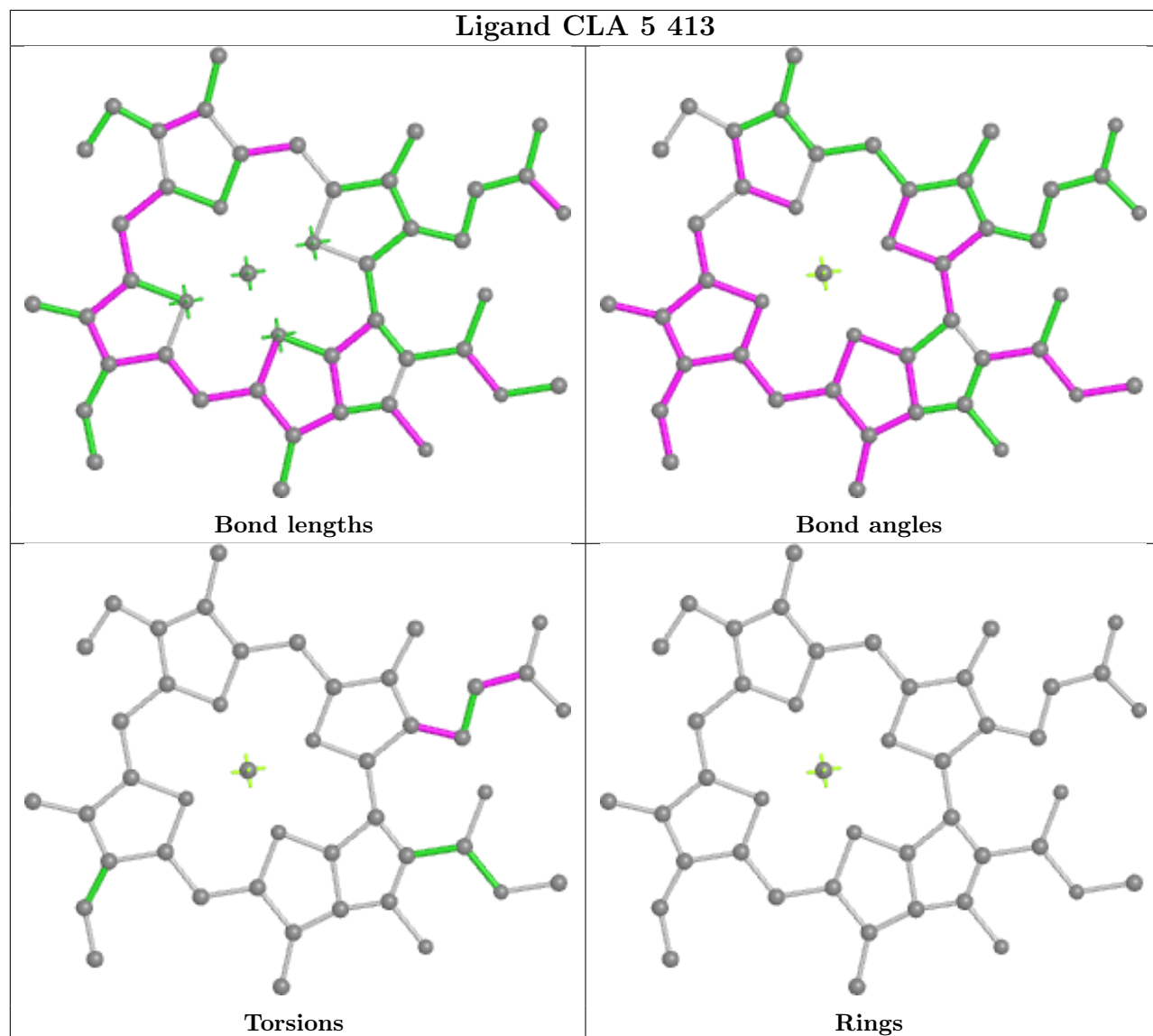
Ligand CLA 5 417



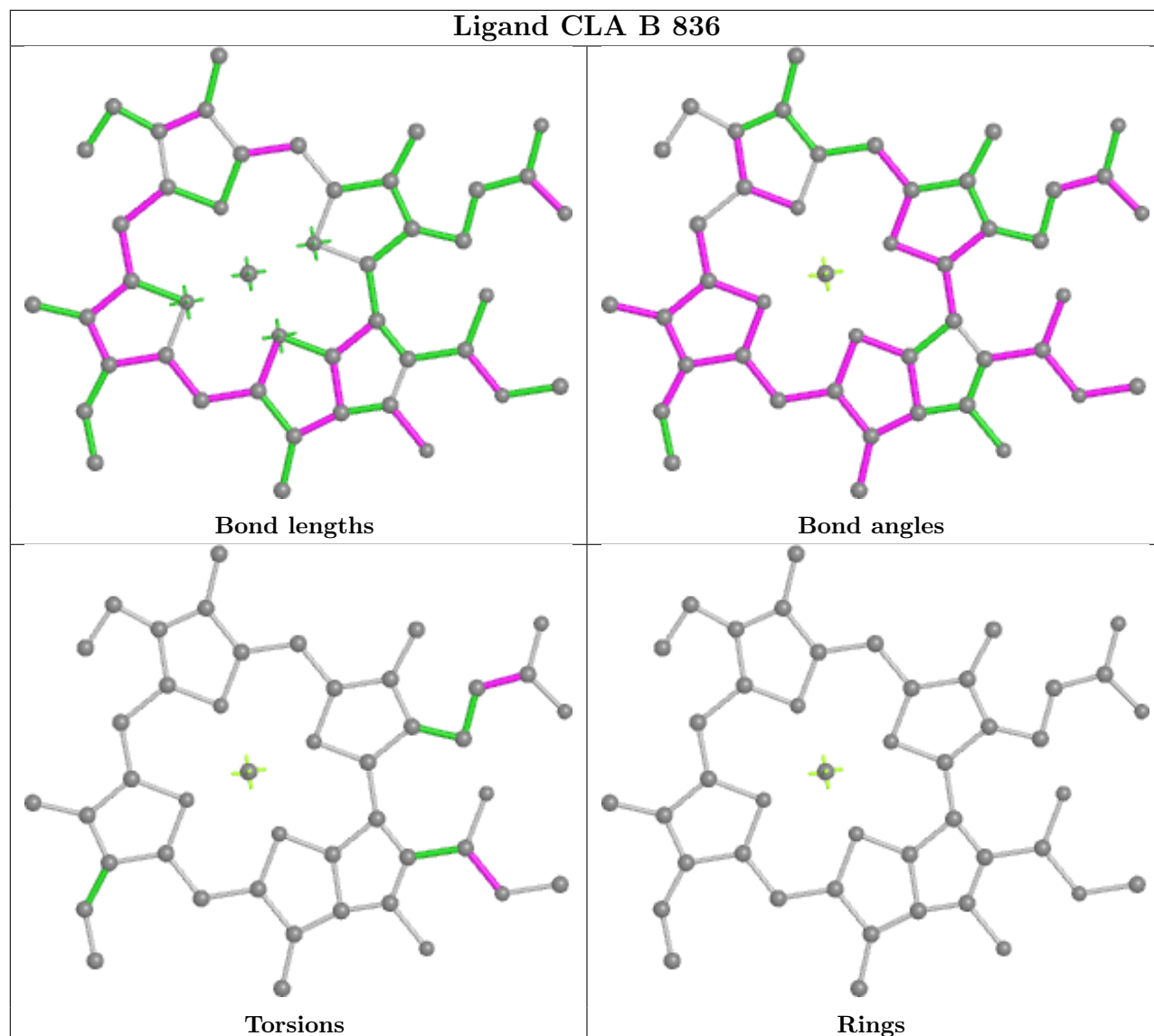
Ligand CLA 6 404



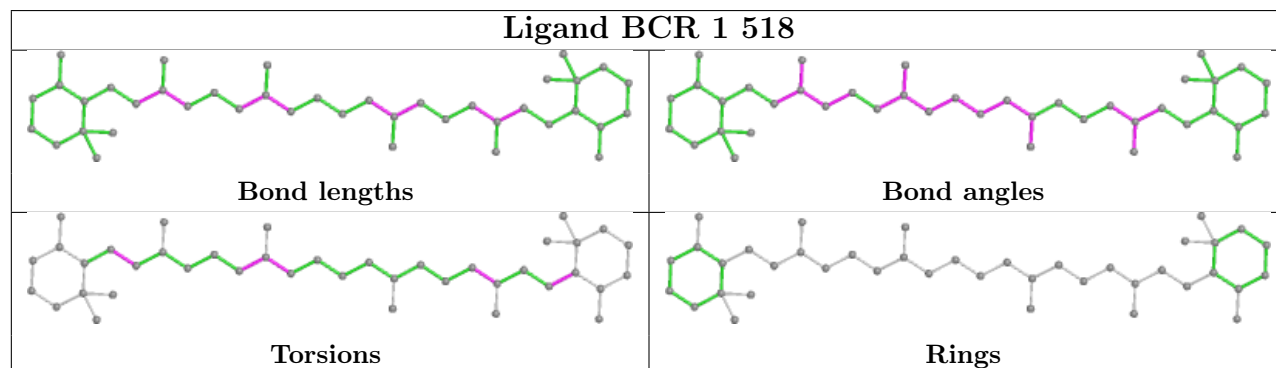
Ligand CLA 5 413



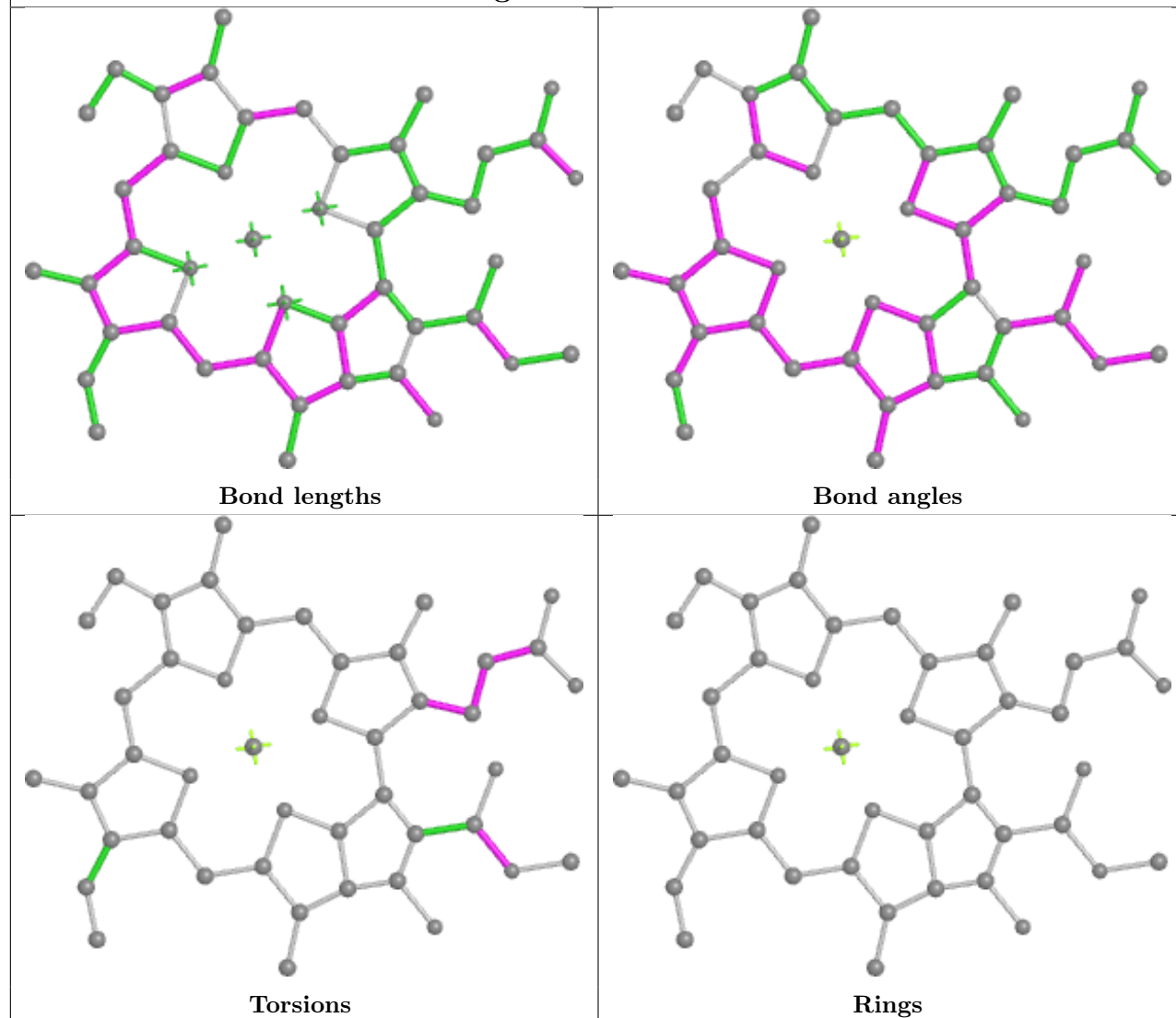
Ligand CLA B 836



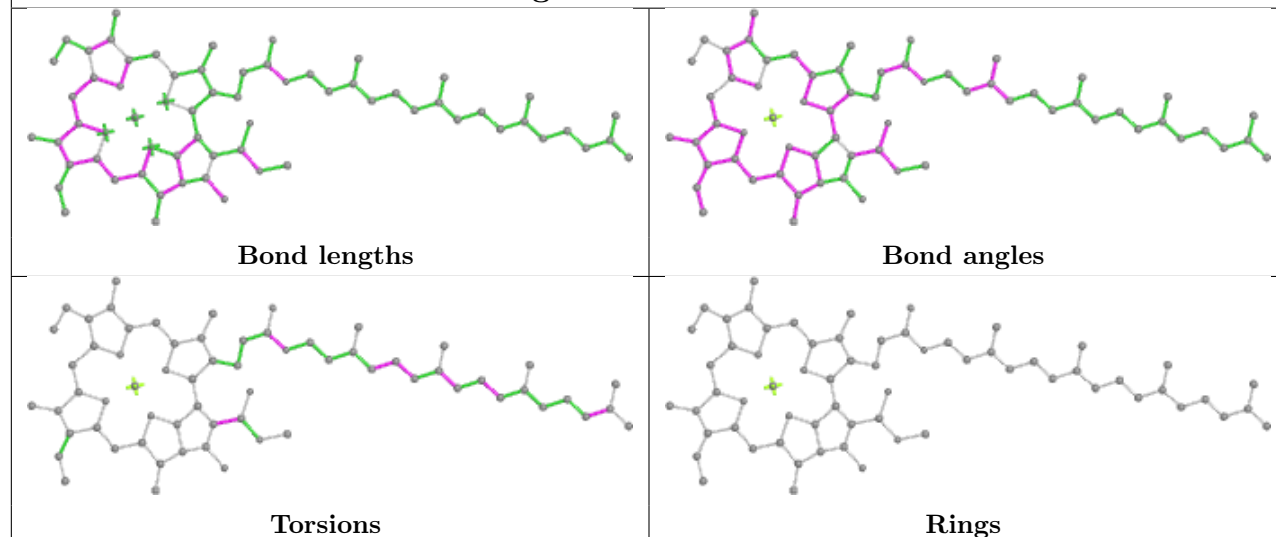
Ligand BCR 1 518



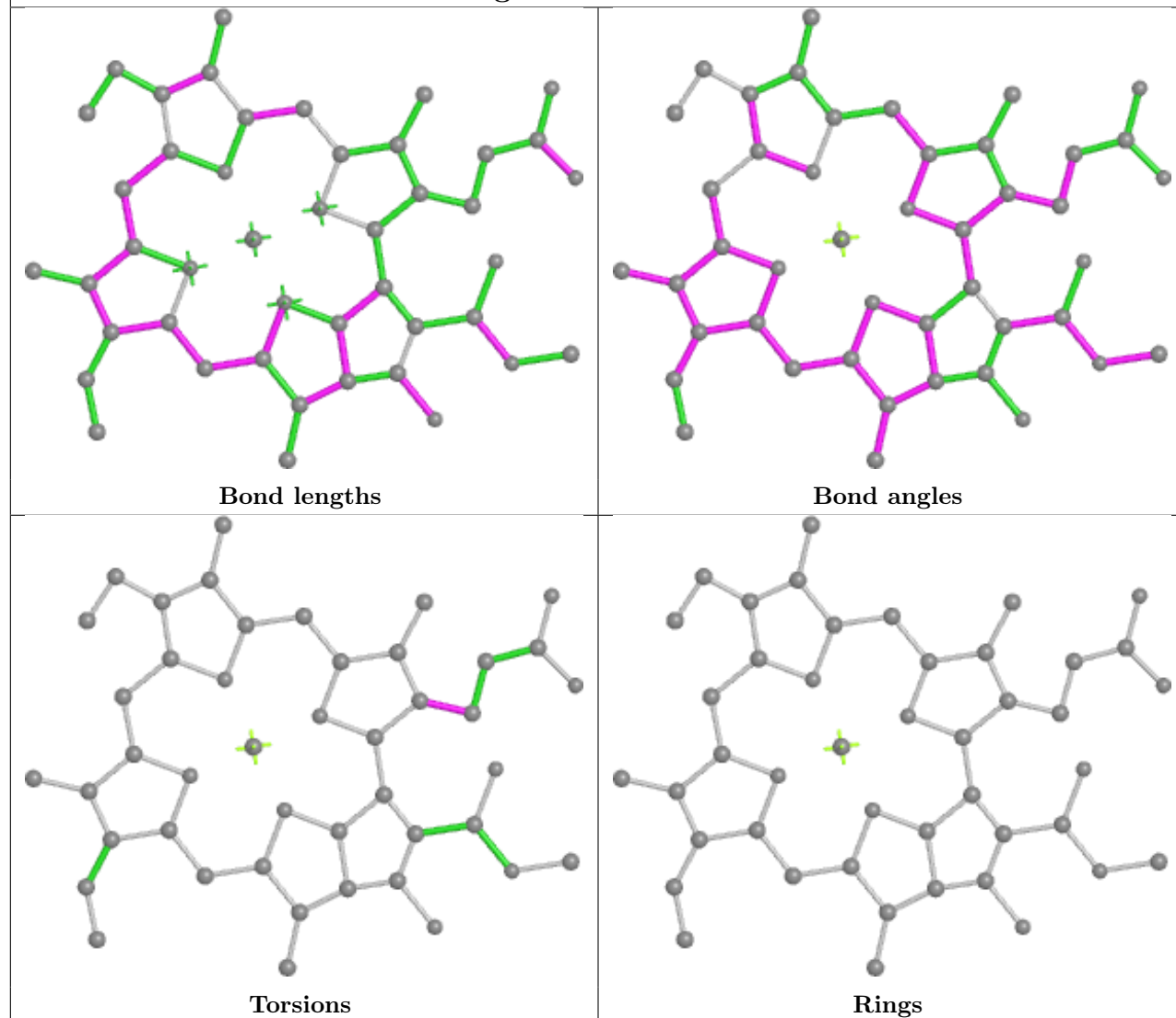
Ligand CLA 4 402



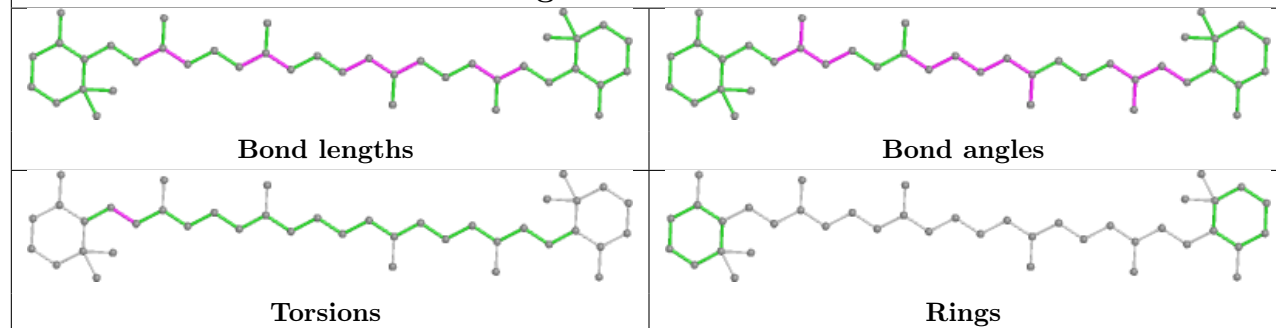
Ligand CLA B 839

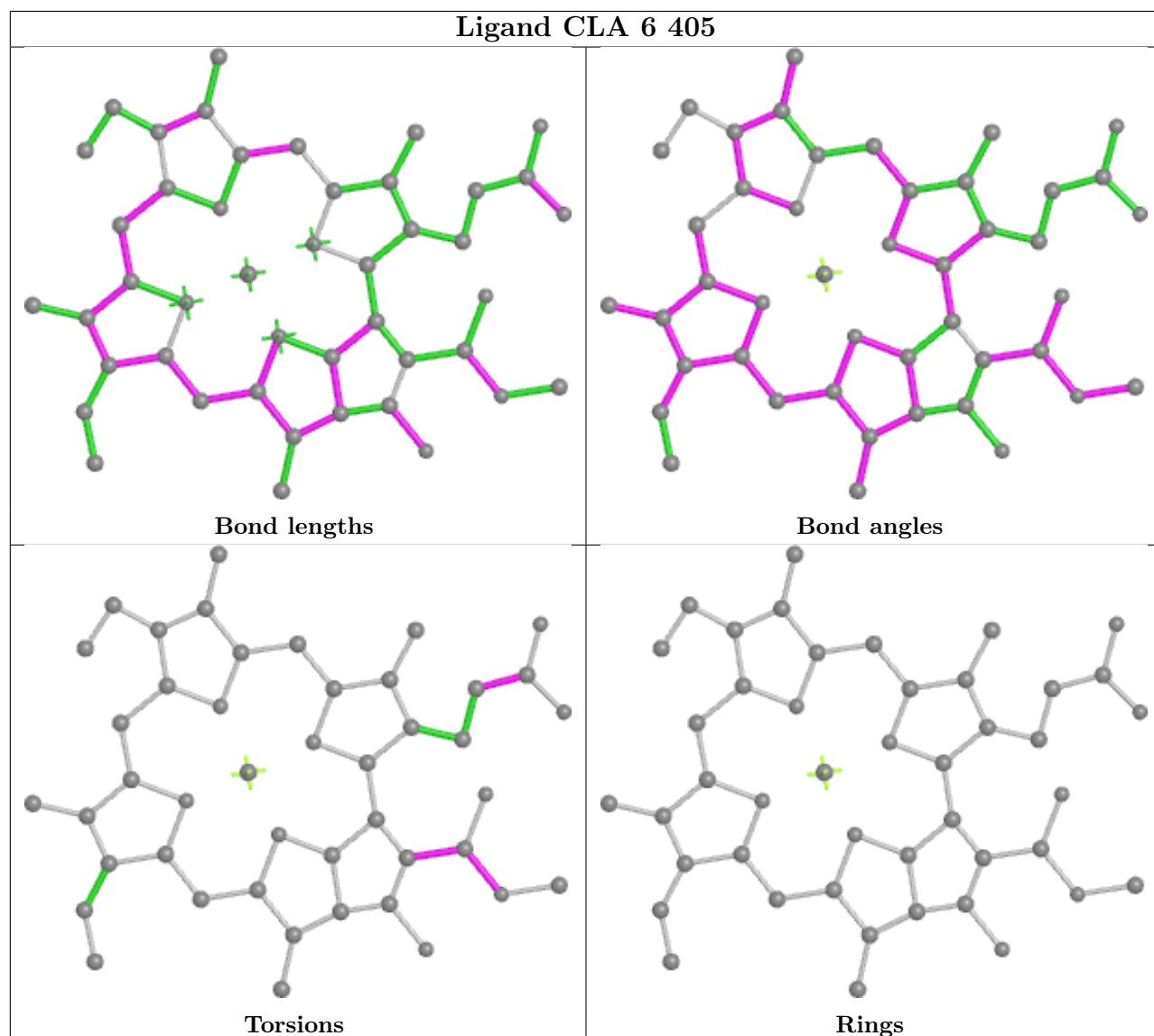
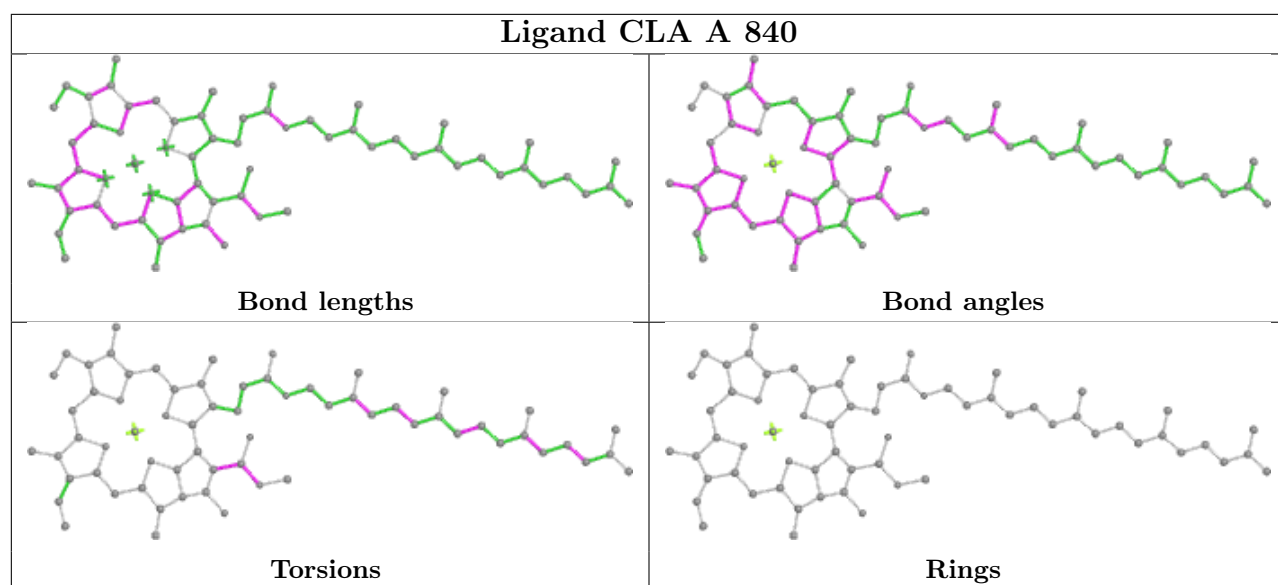


Ligand CLA 1 513

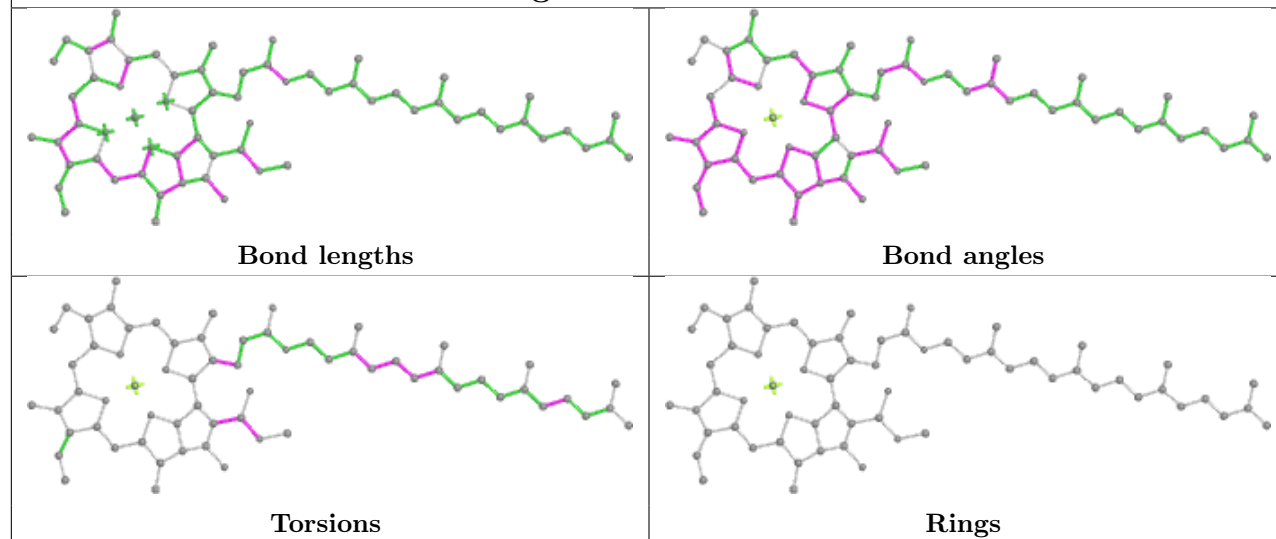


Ligand BCR I 101

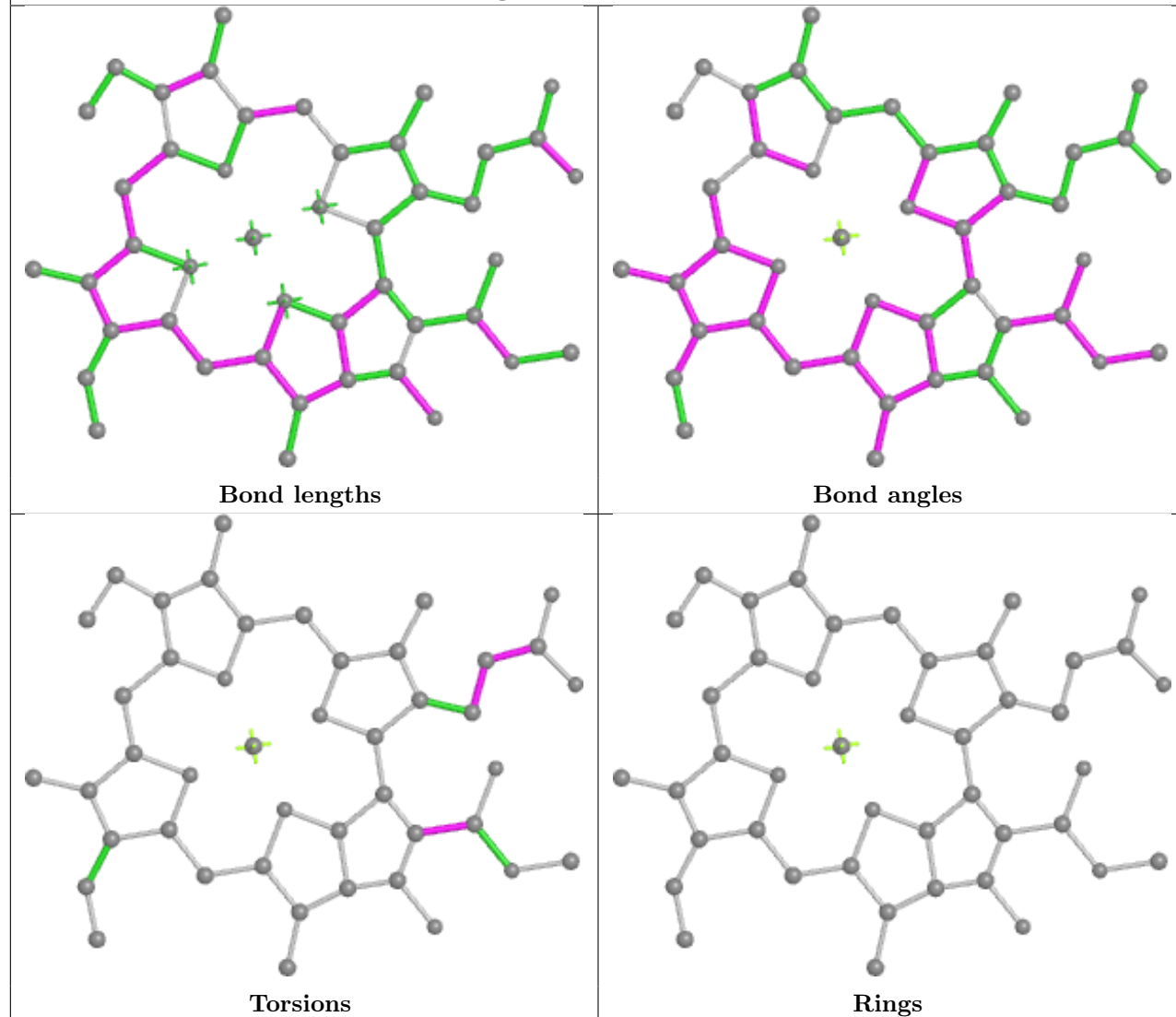




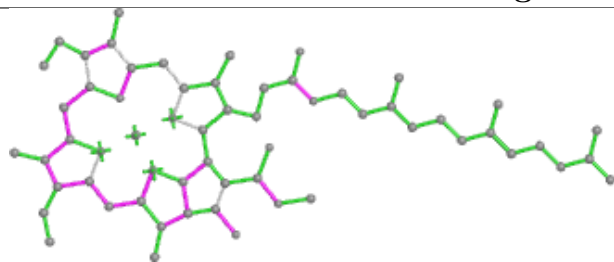
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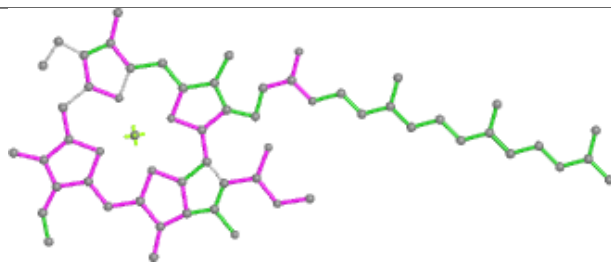
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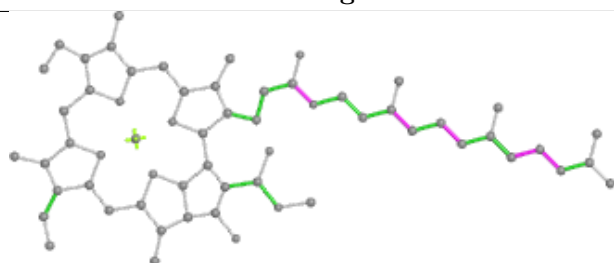
Ligand CLA B 837



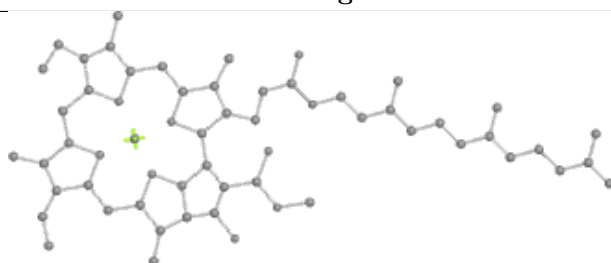
Bond lengths



Bond angles

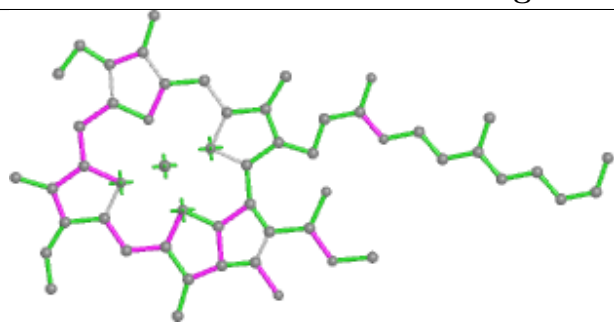


Torsions

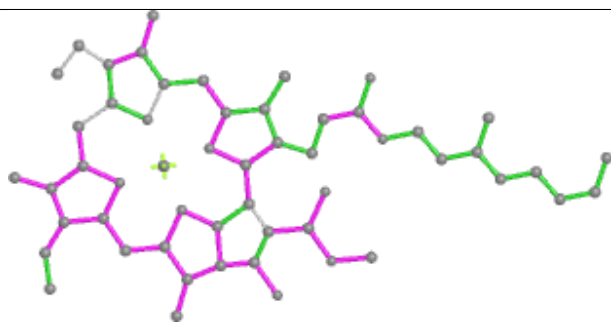


Rings

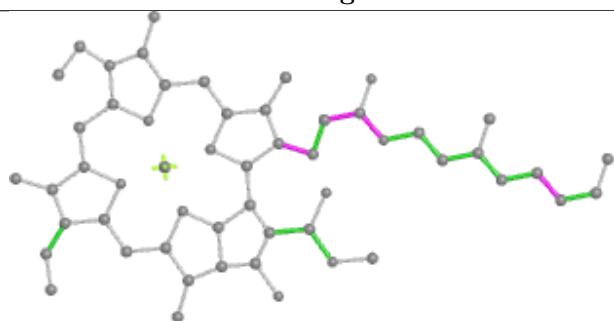
Ligand CLA A 819



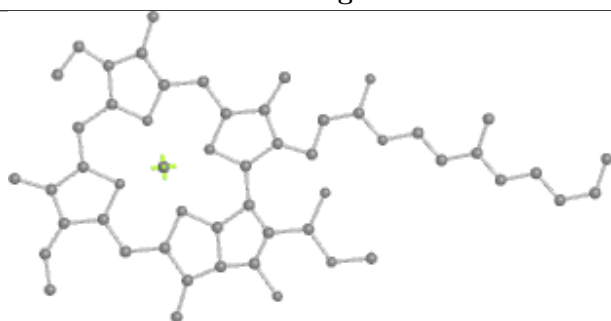
Bond lengths



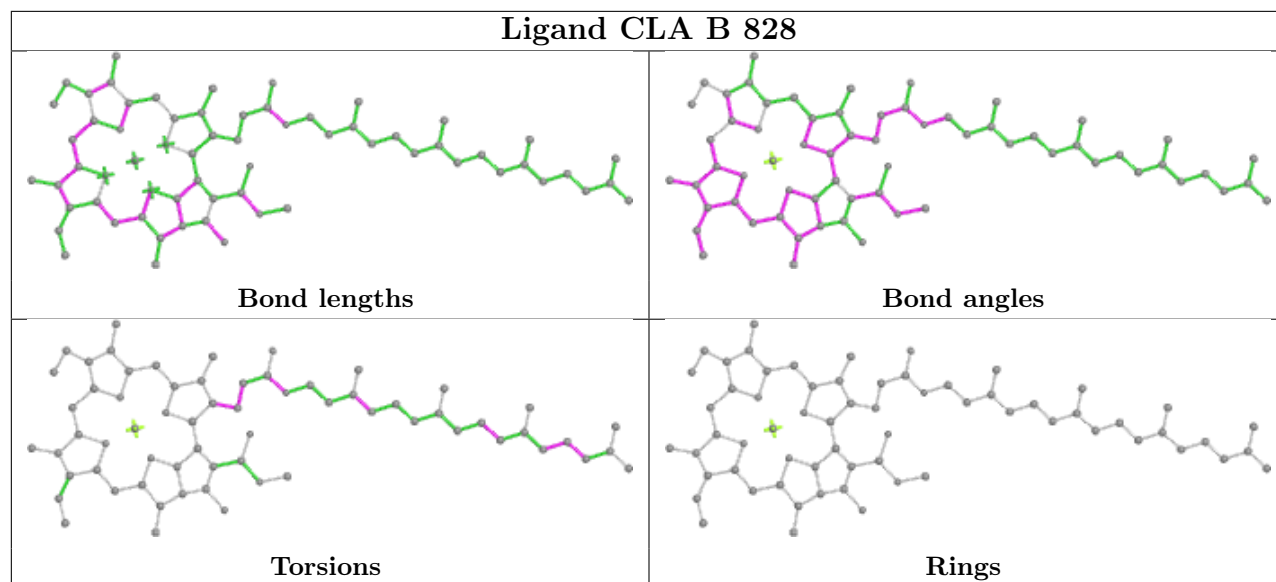
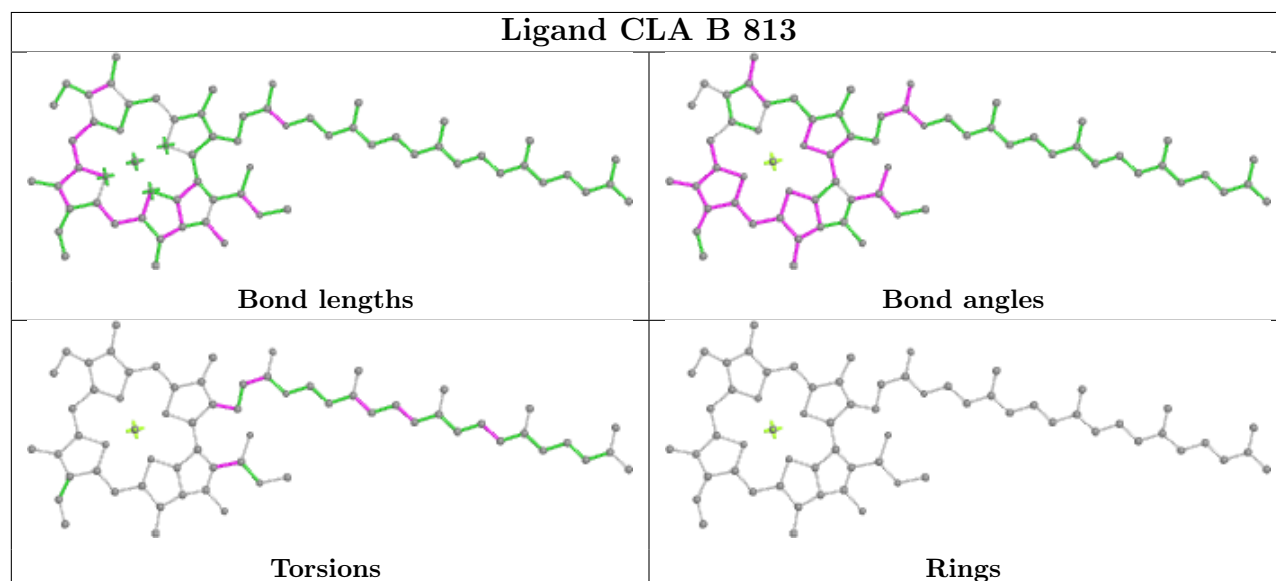
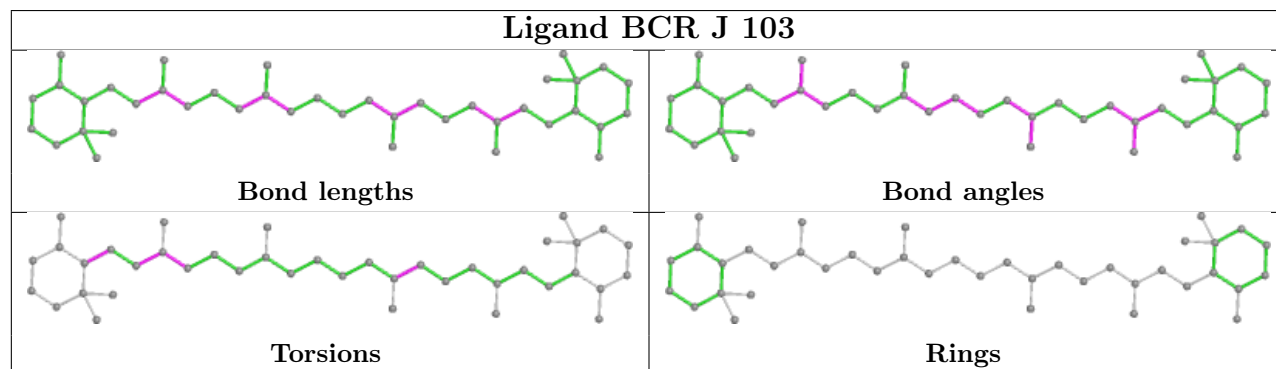
Bond angles

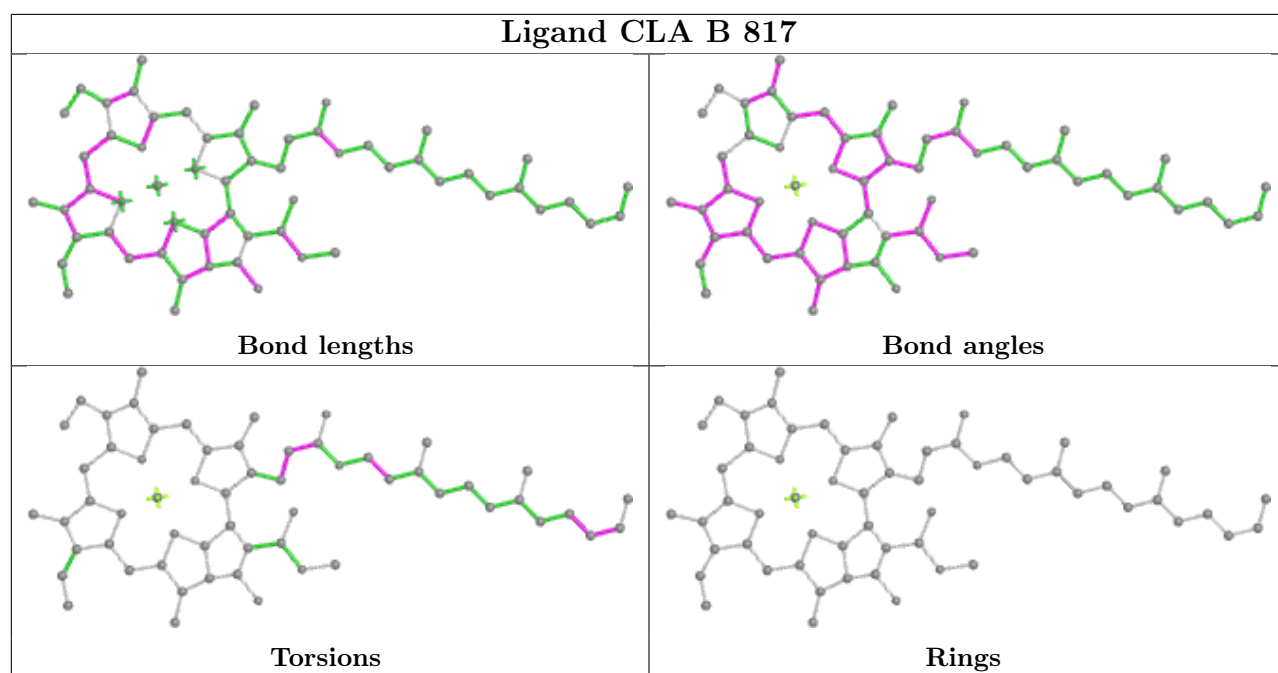


Torsions

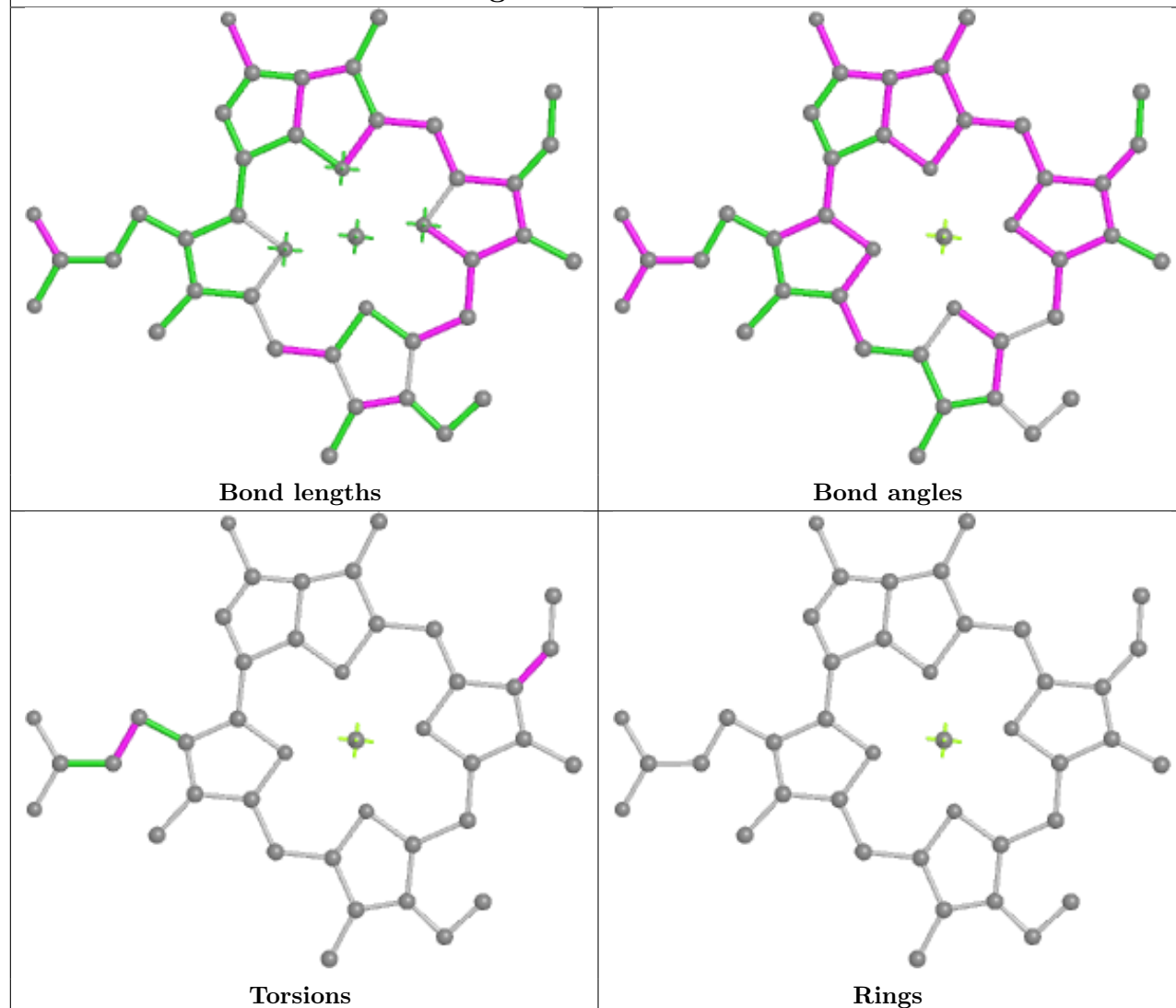


Rings

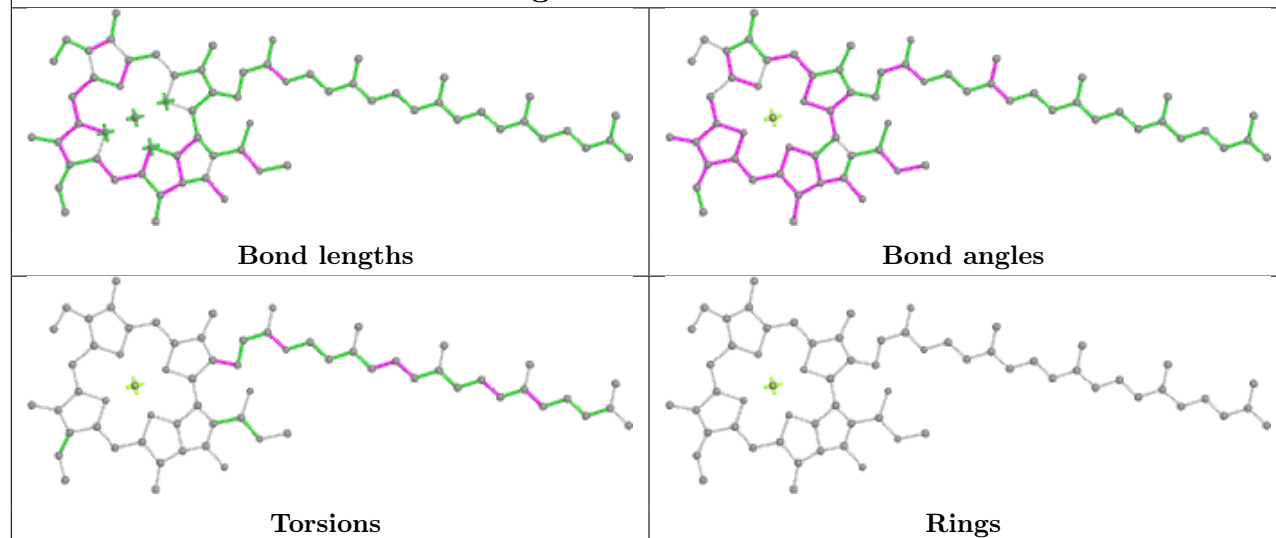
Ligand CLA B 828**Ligand CLA B 813****Ligand BCR J 103**

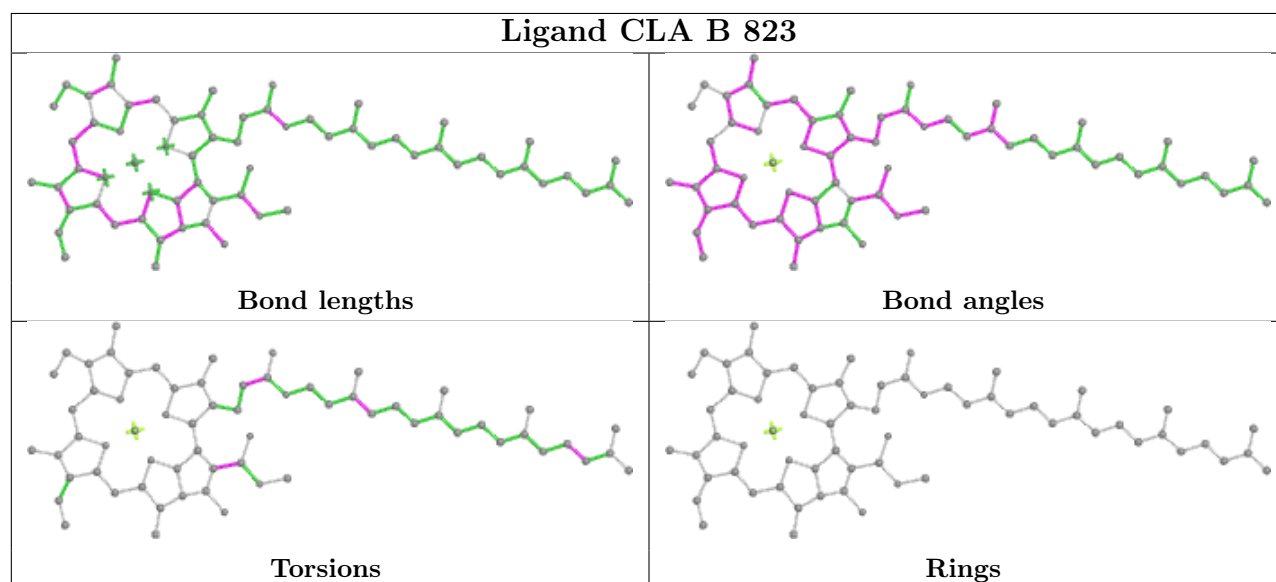
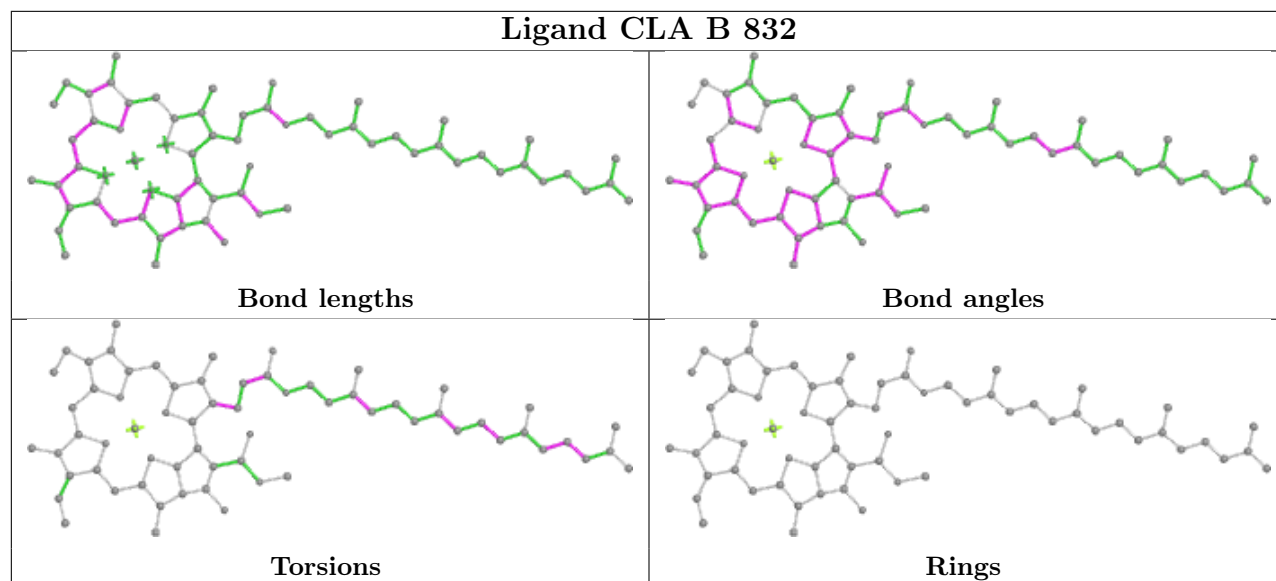
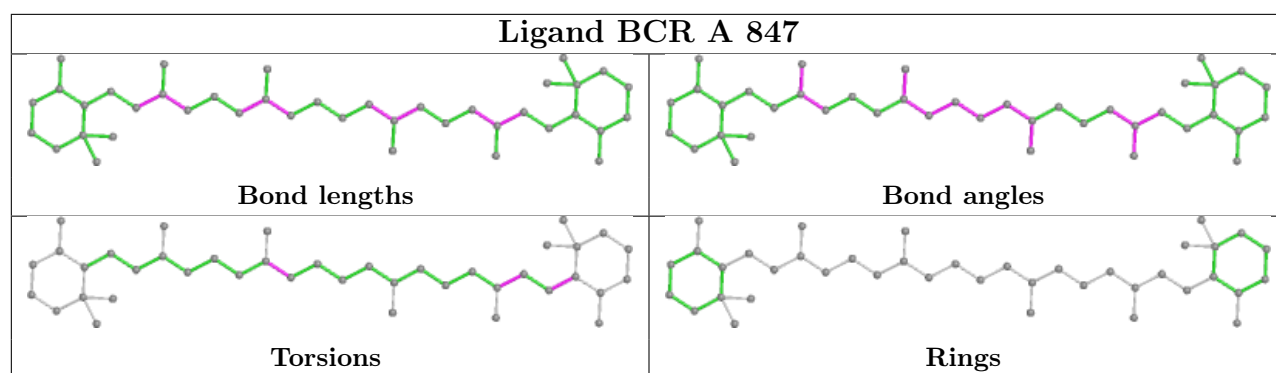


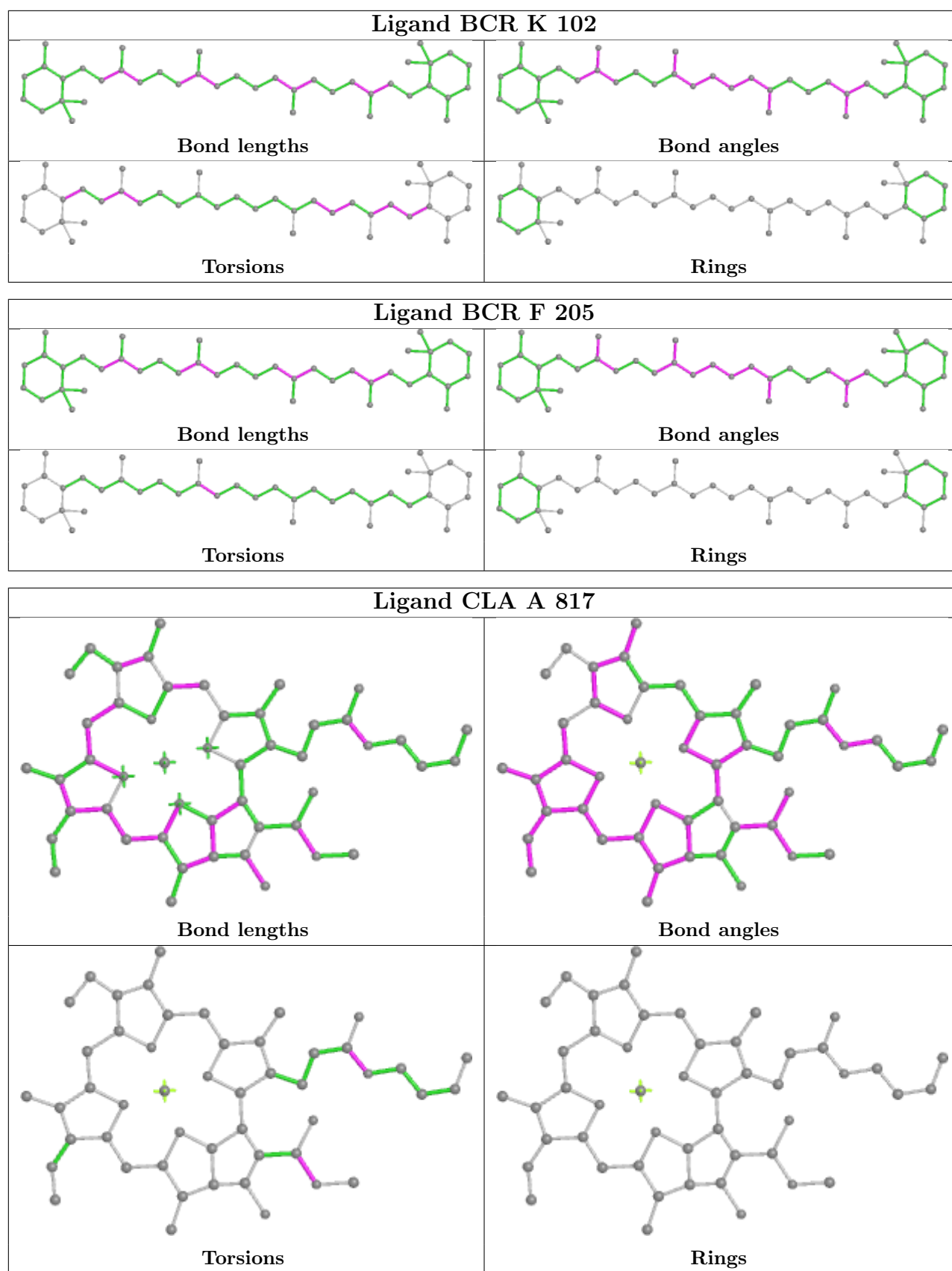
Ligand CLA K 101

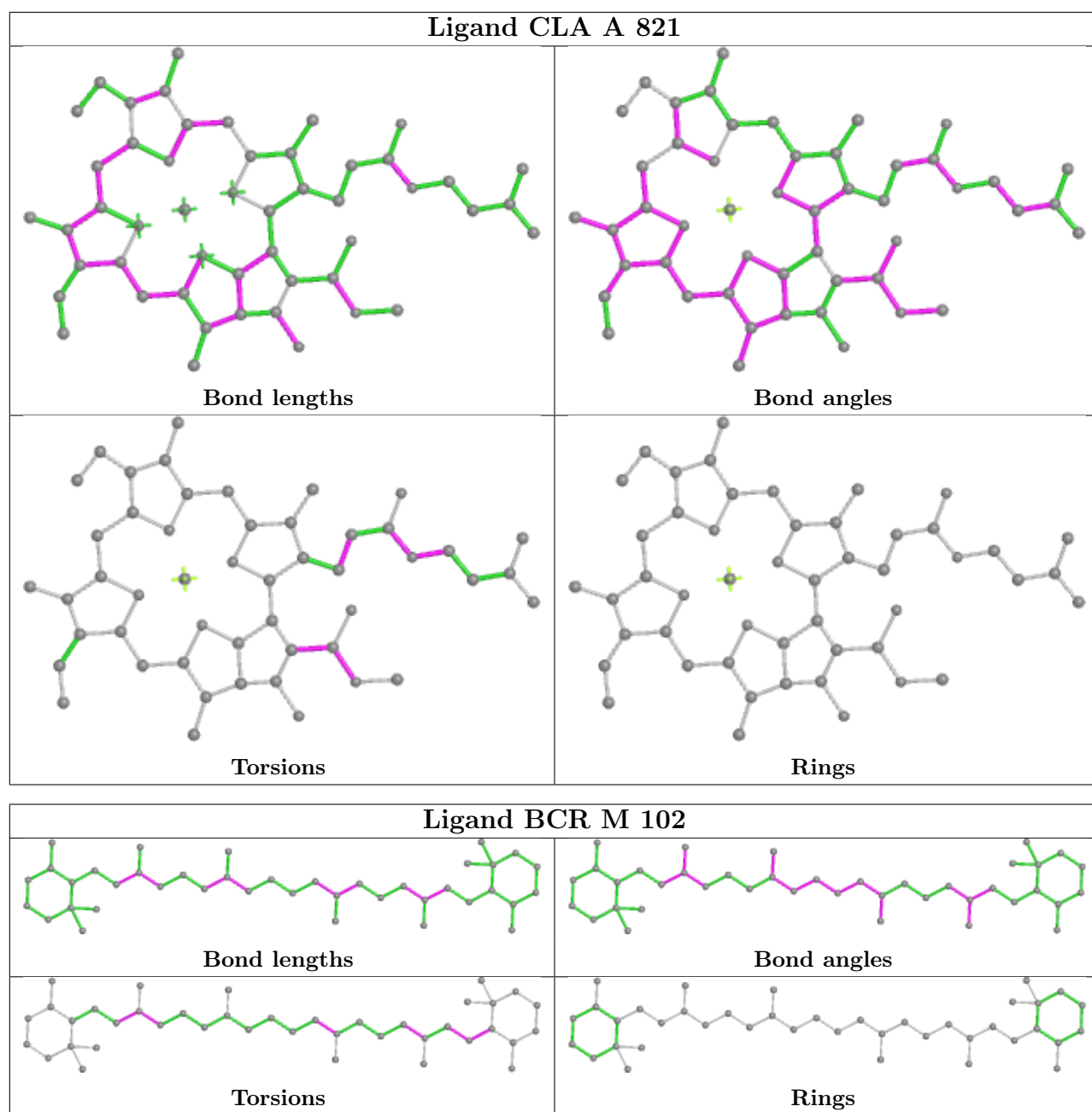


Ligand CLA A 807

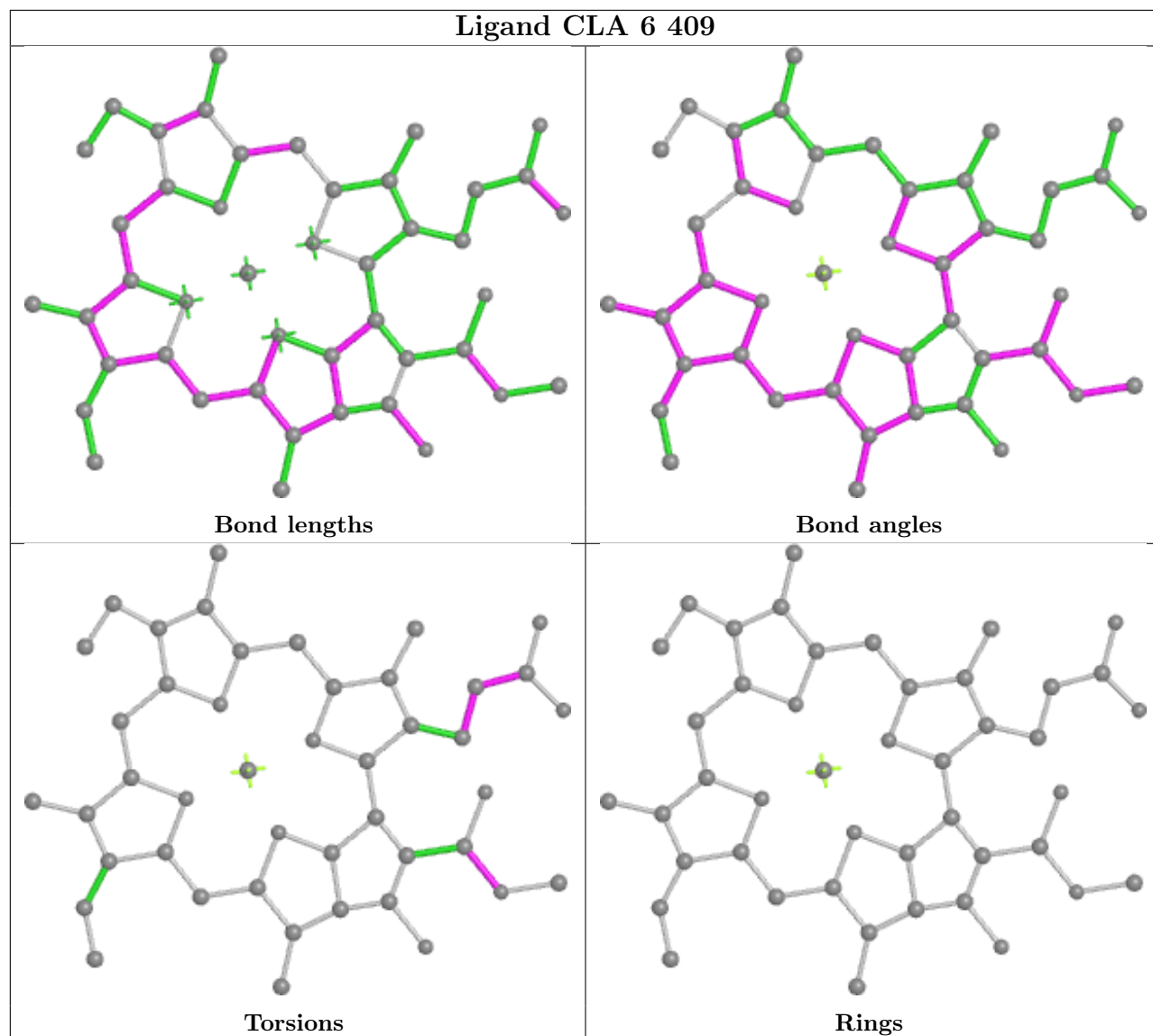


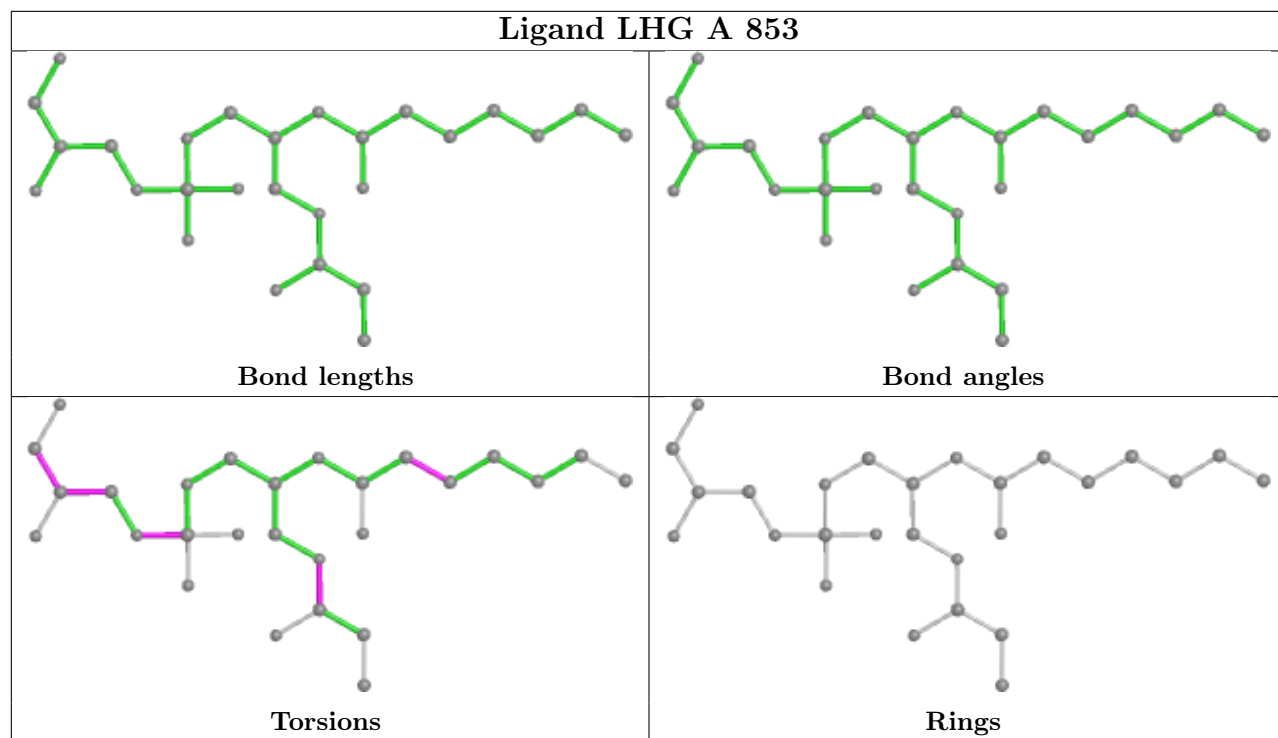




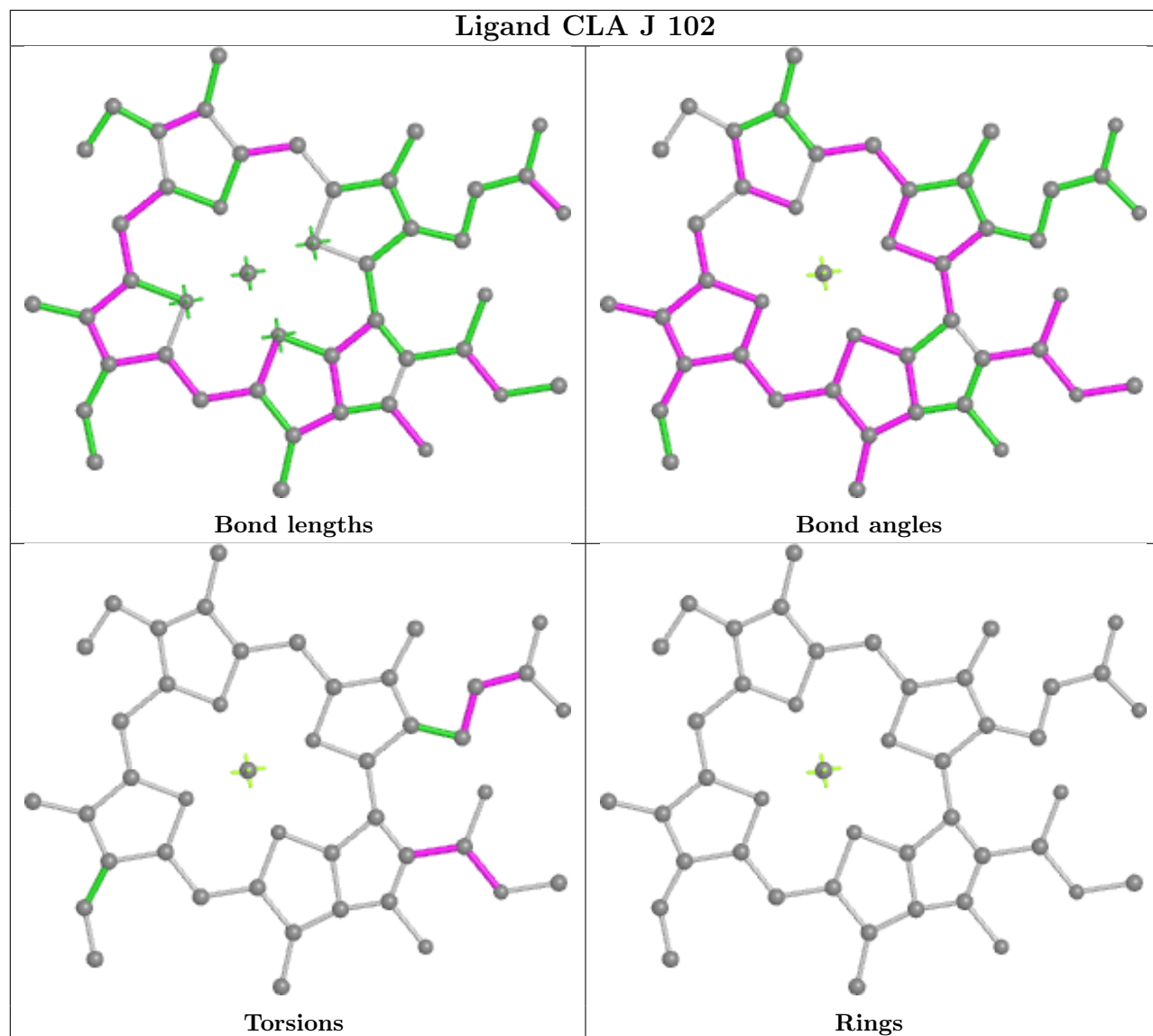


Ligand CLA 6 409

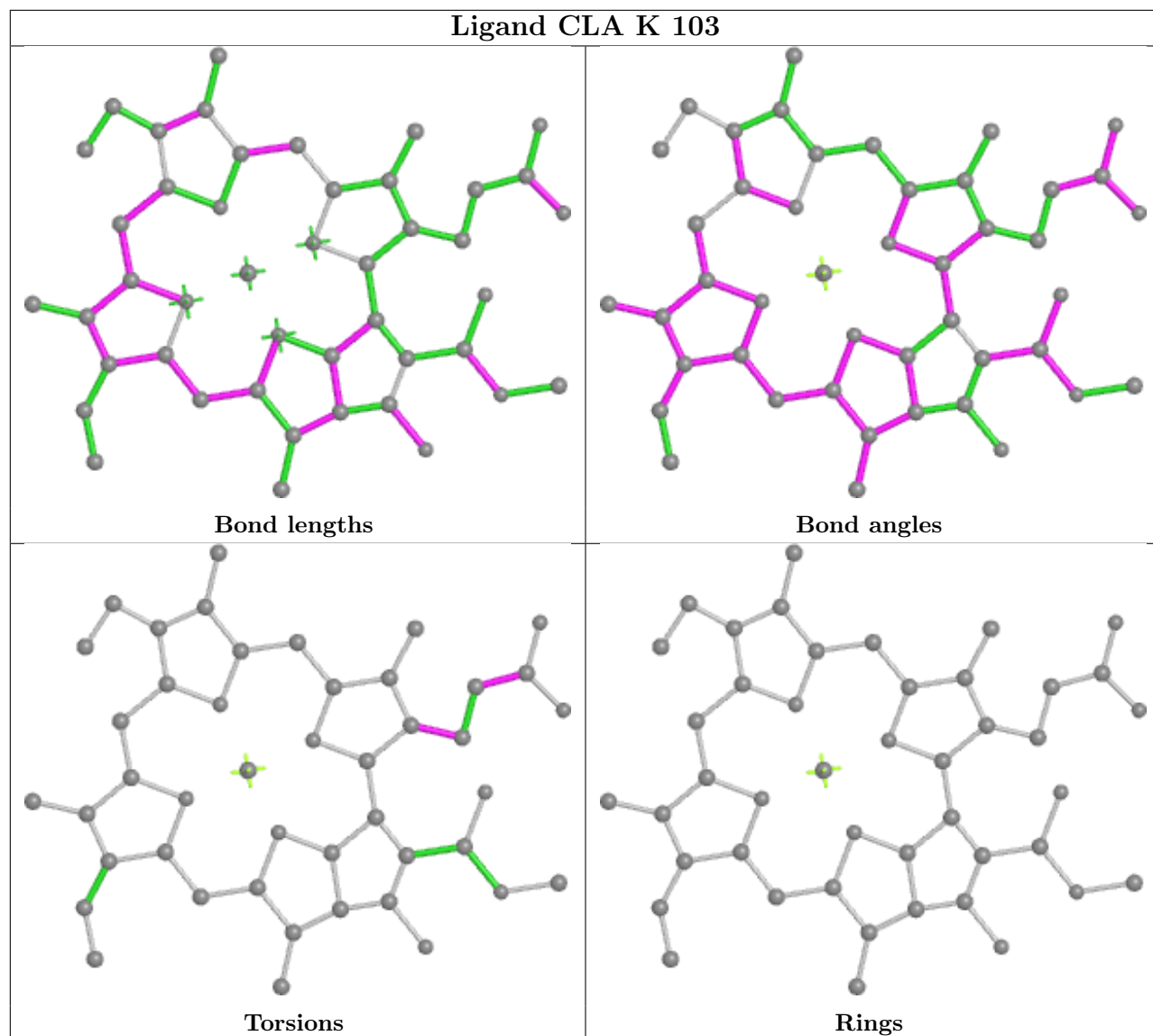




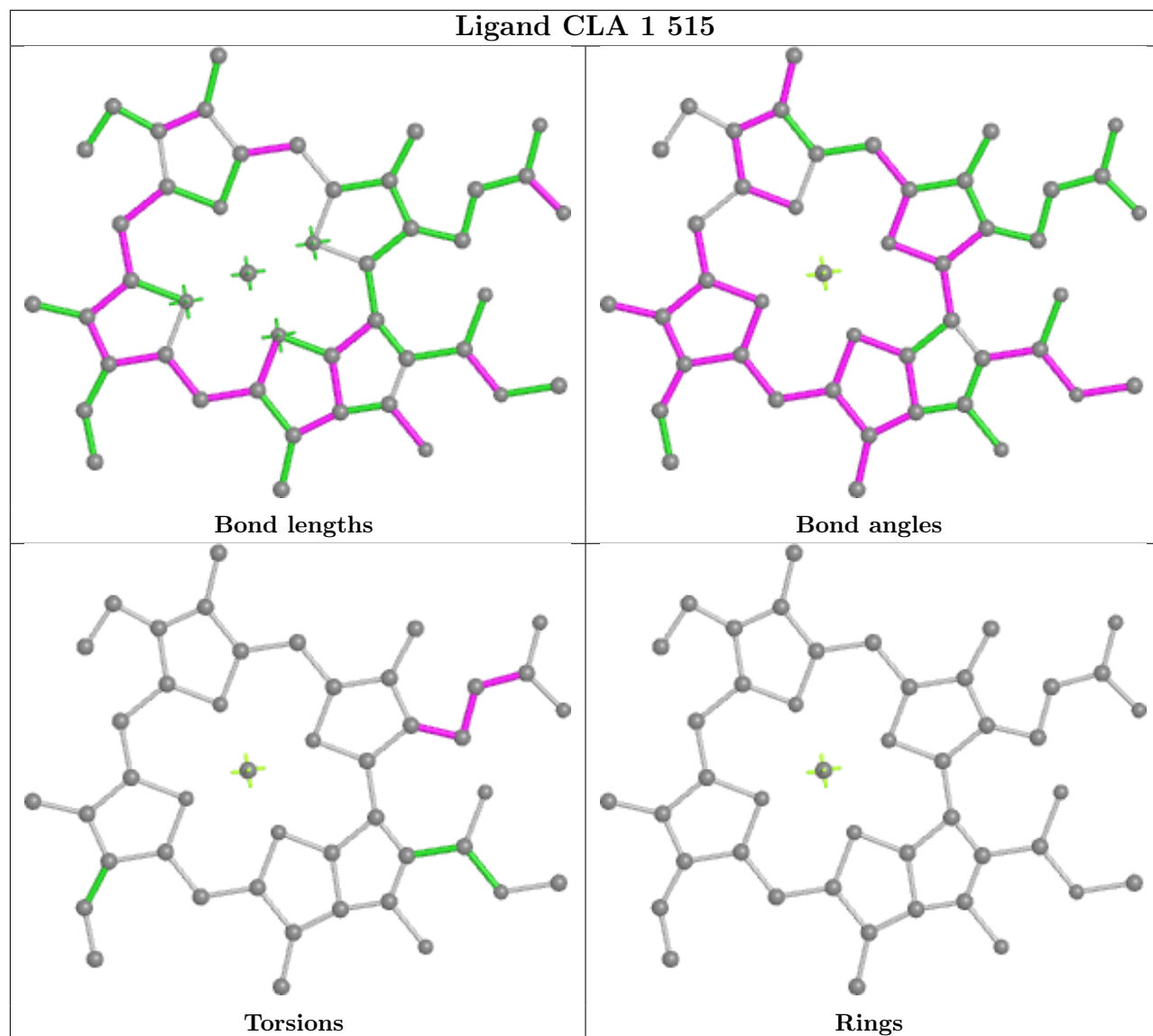
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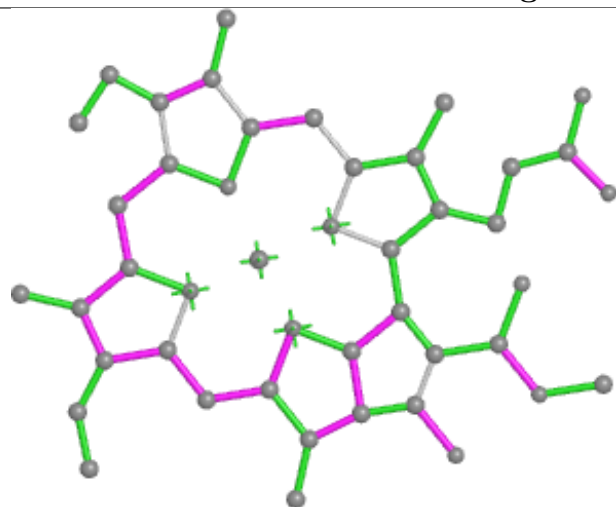
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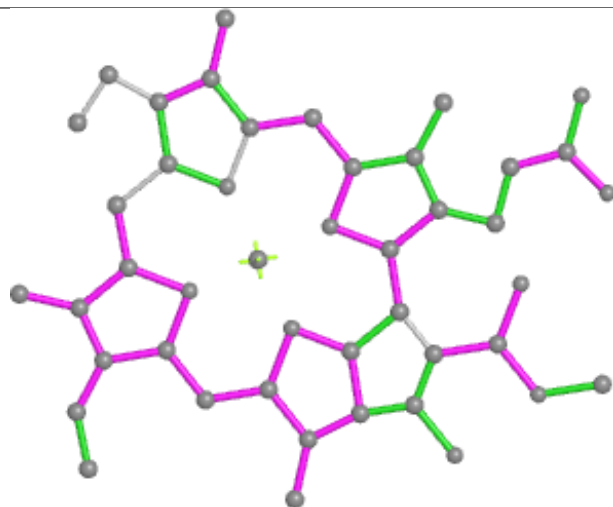
Ligand CLA 1 515



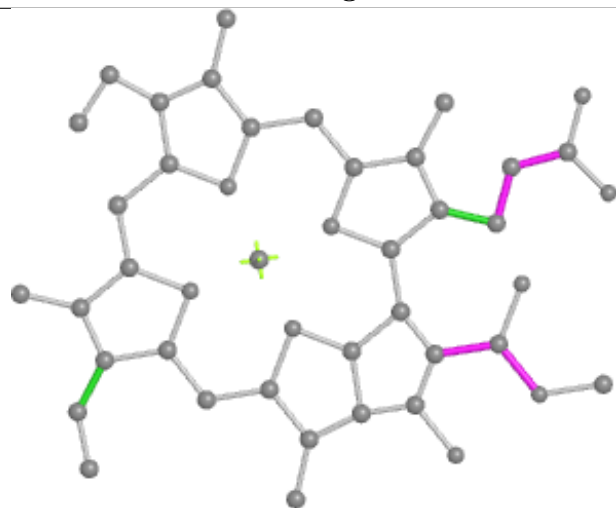
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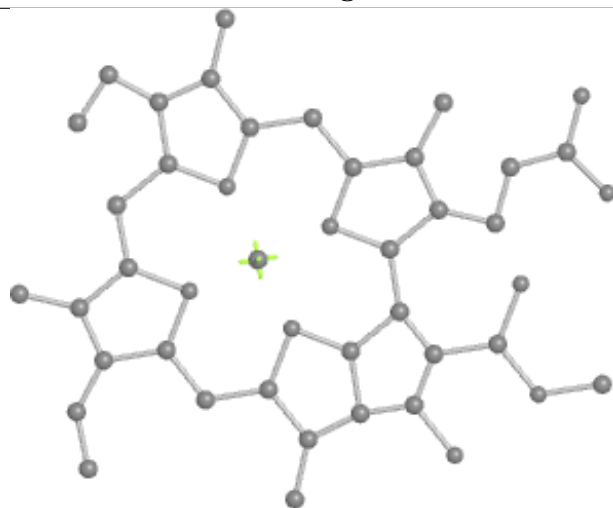
Bond lengths



Bond angles

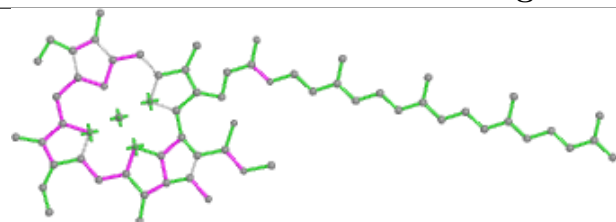


Torsions

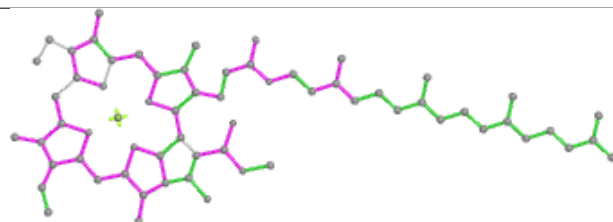


Rings

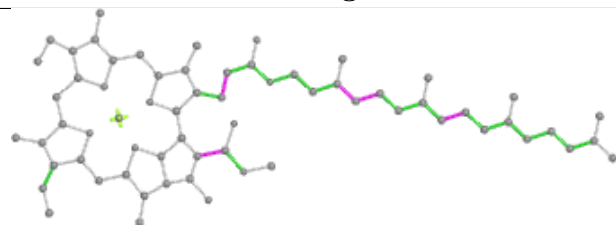
Ligand CLA B 802



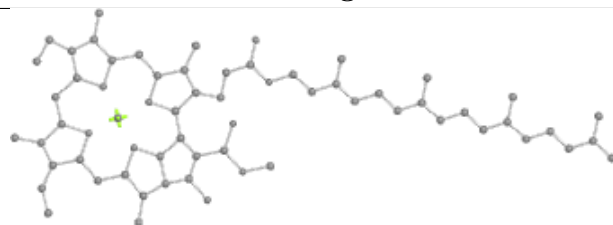
Bond lengths



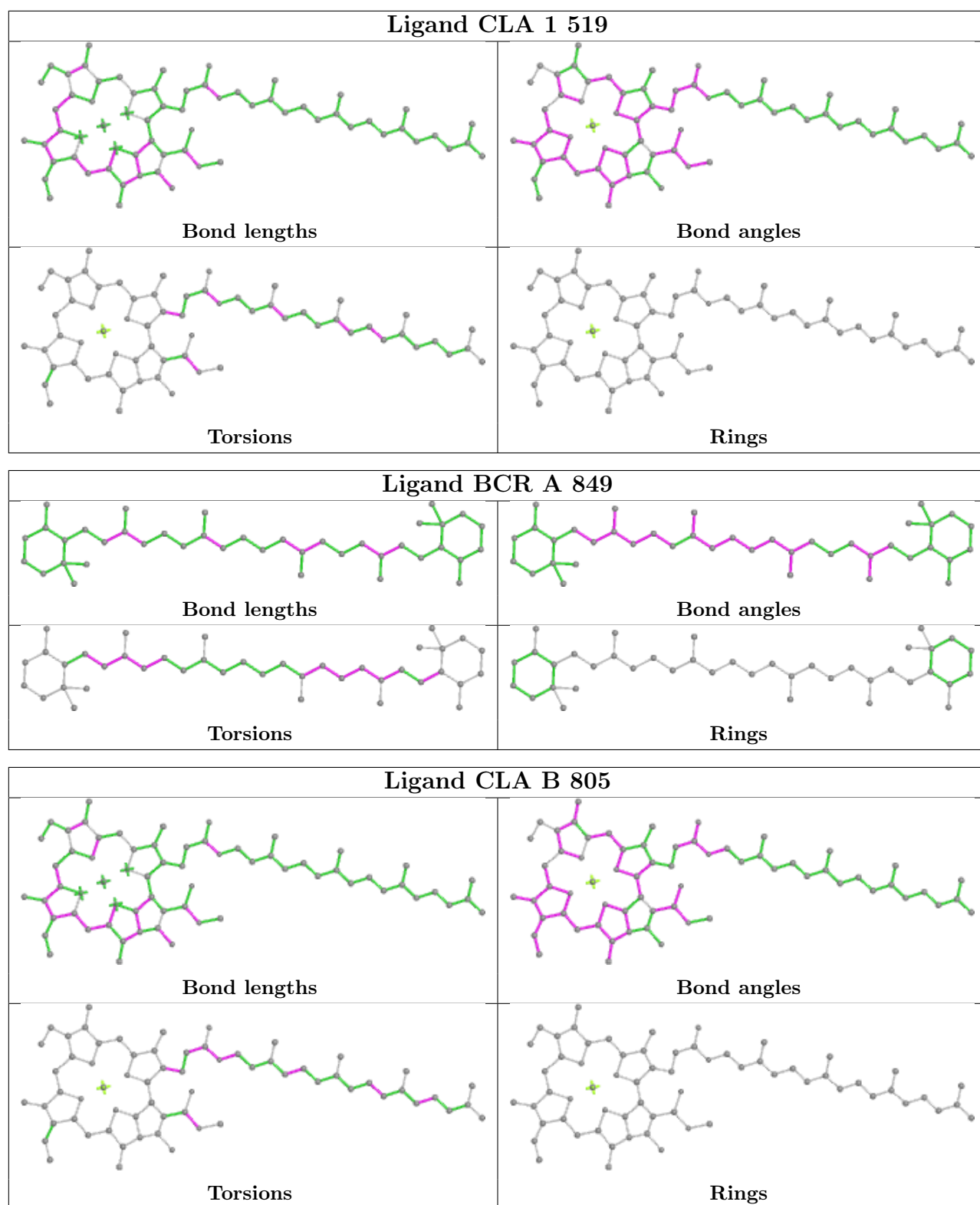
Bond angles

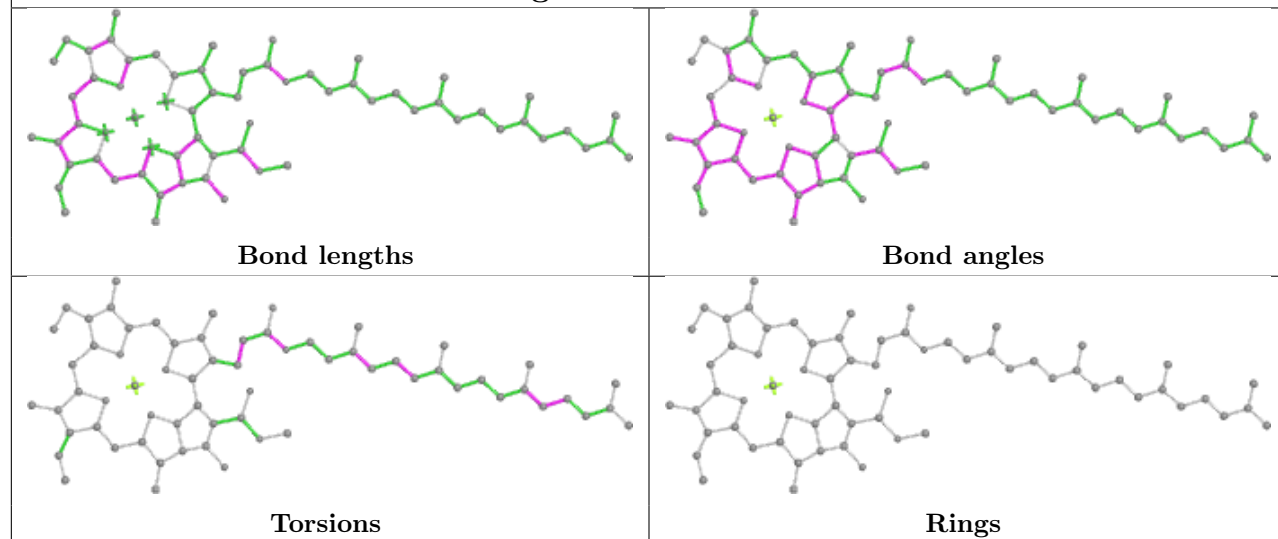
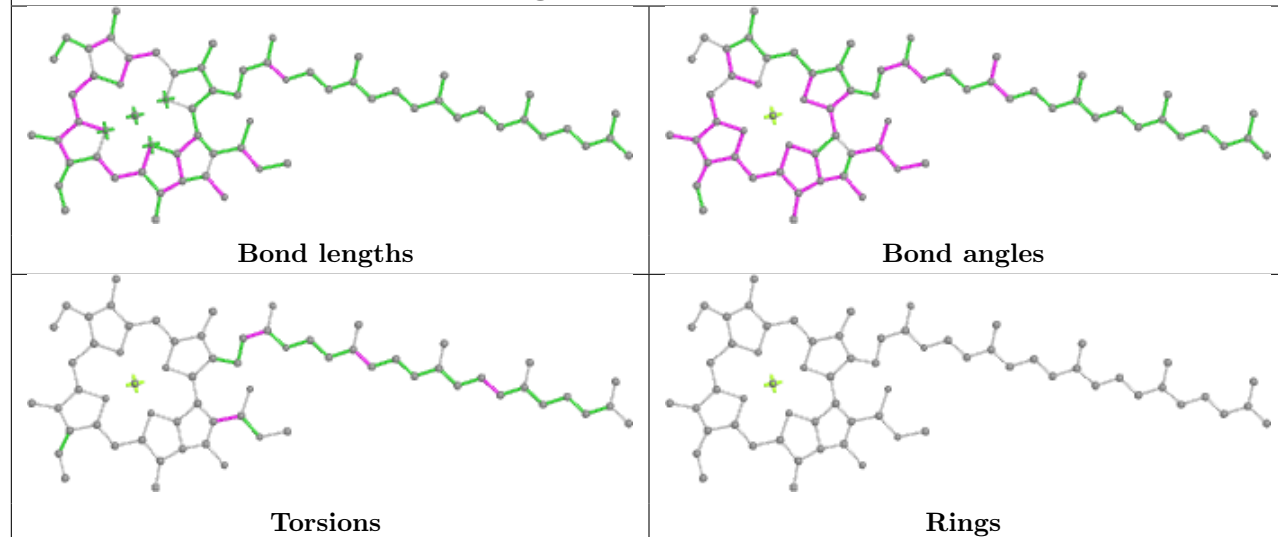
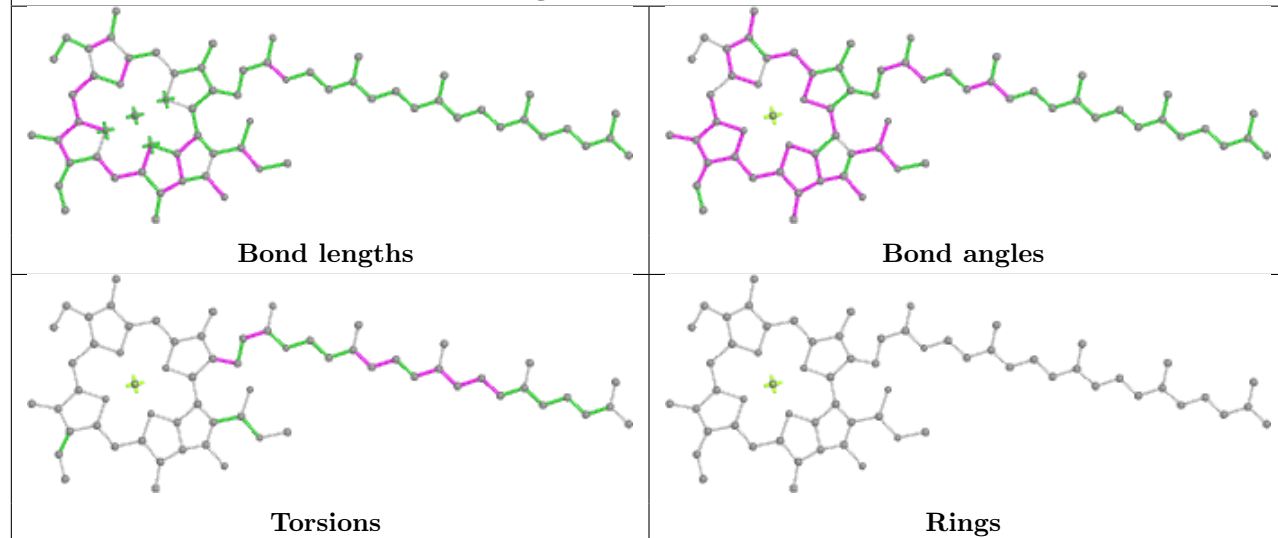


Torsions

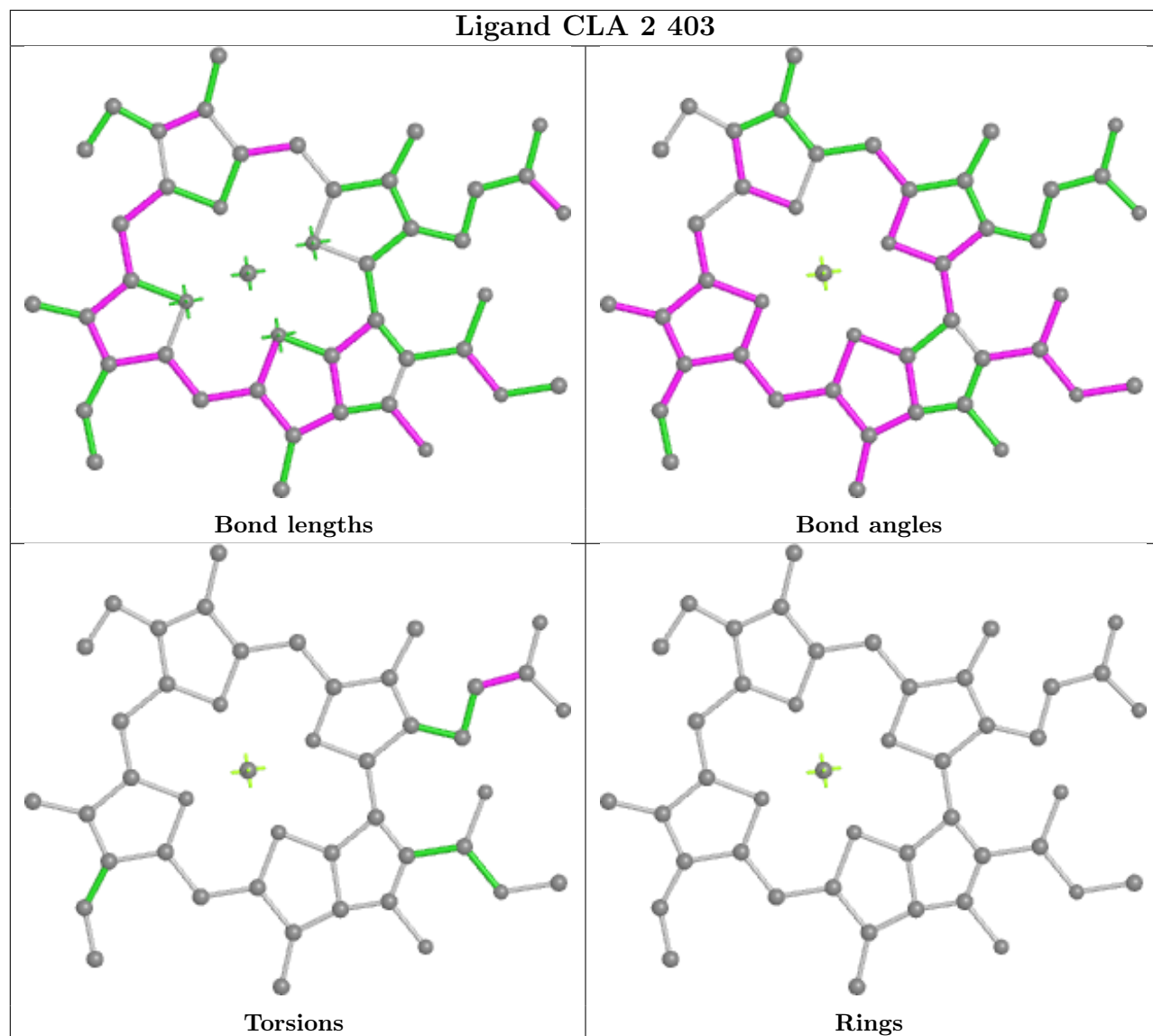


Rings

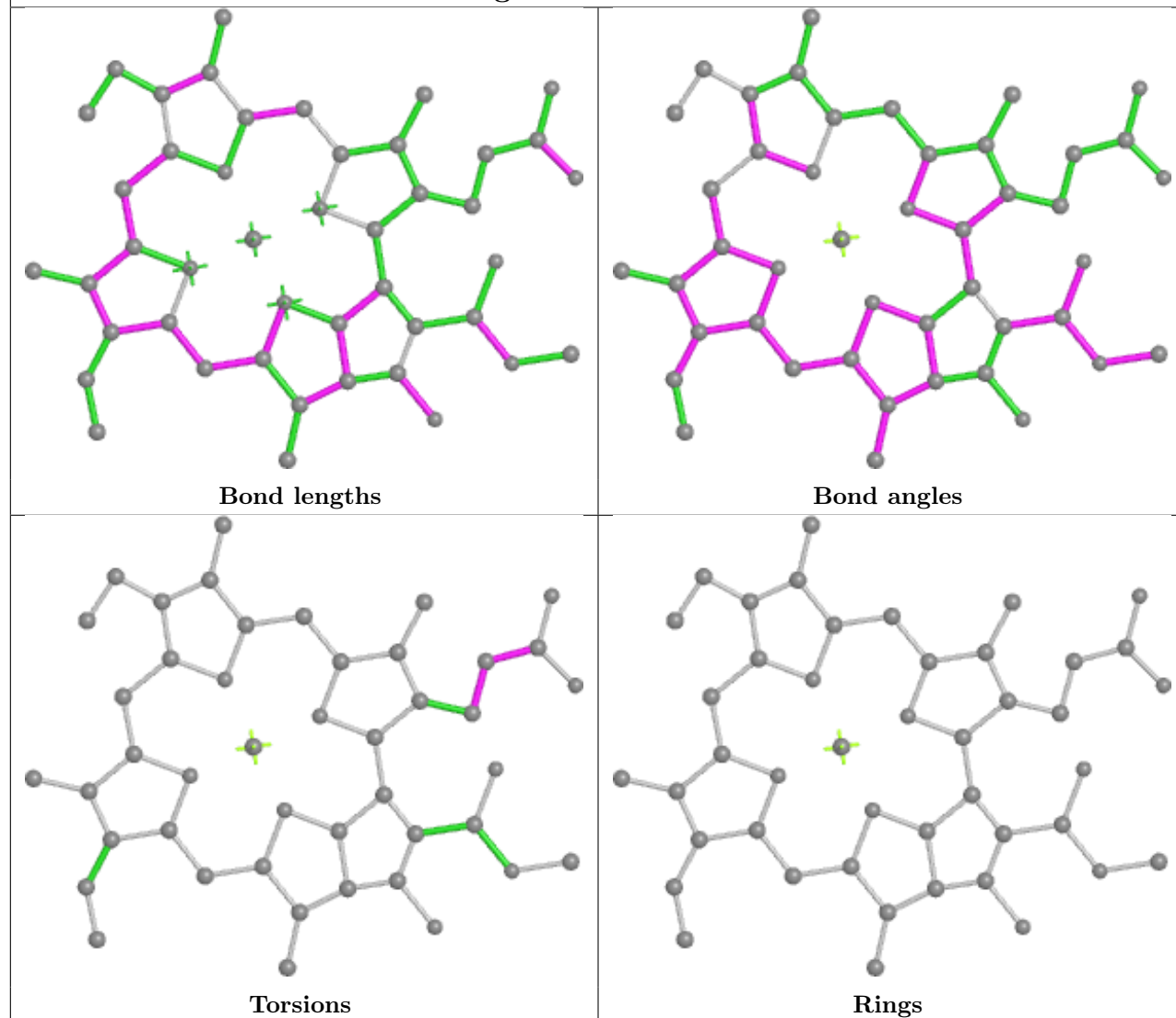


Ligand CLA A 830**Ligand CLA A 828****Ligand CLA B 827**

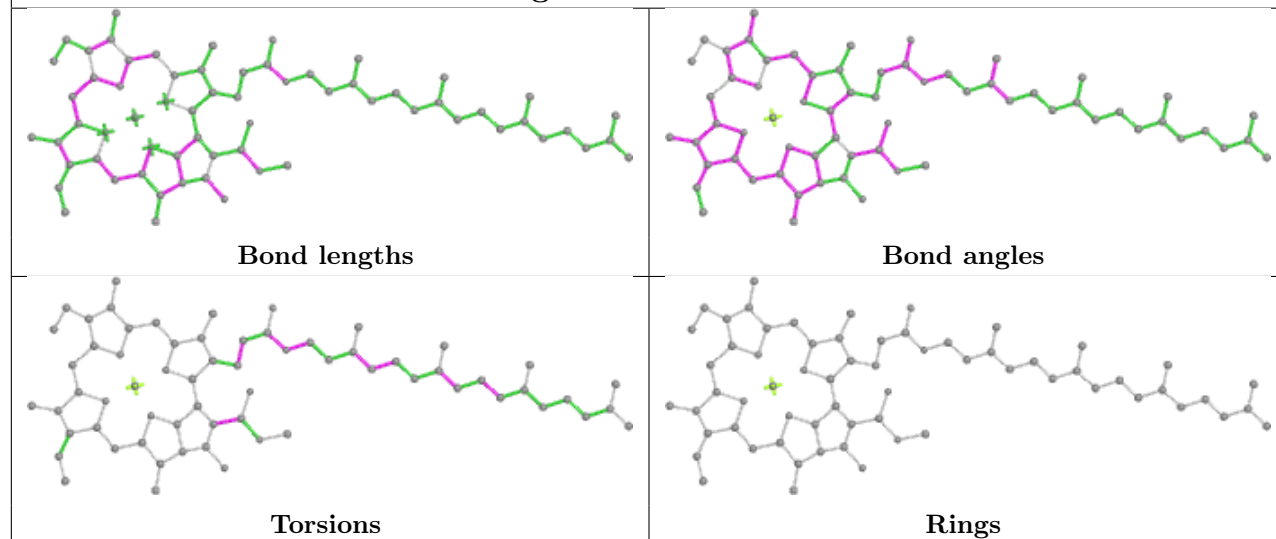
Ligand CLA 2 403



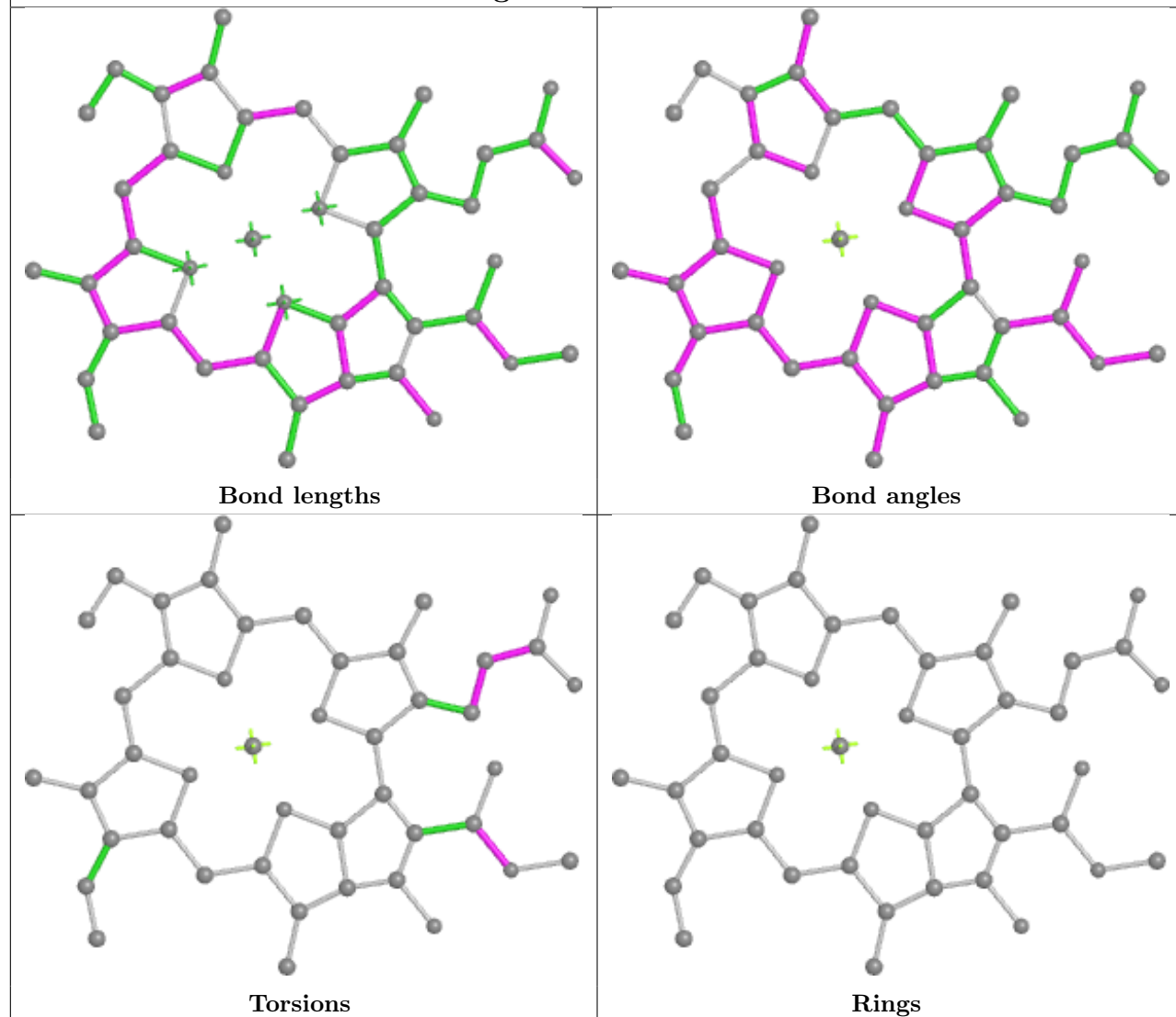
Ligand CLA 5 407



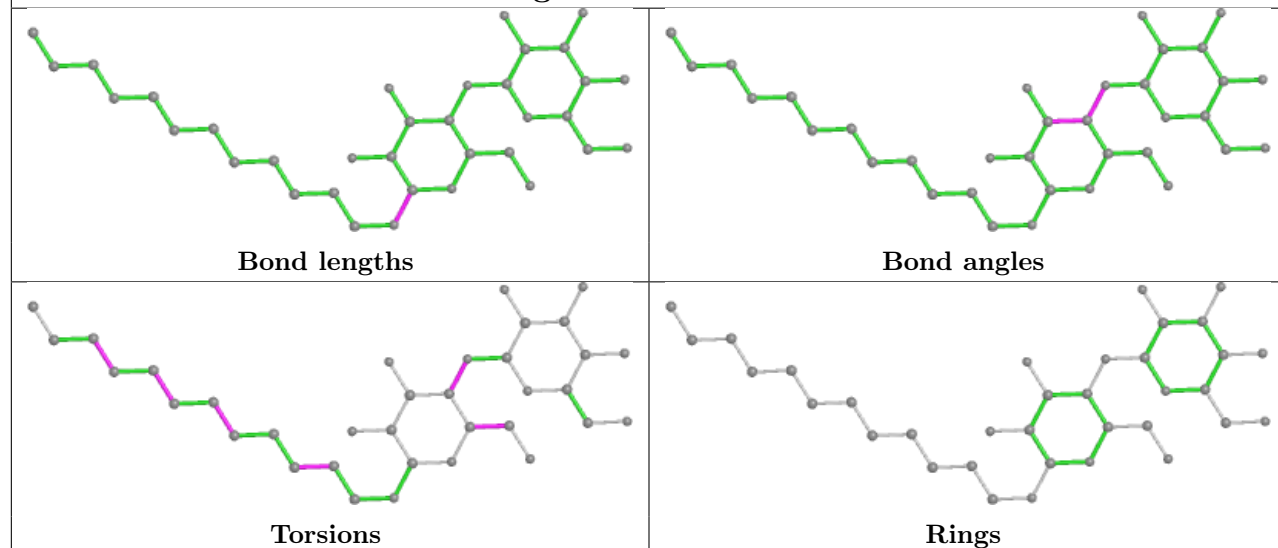
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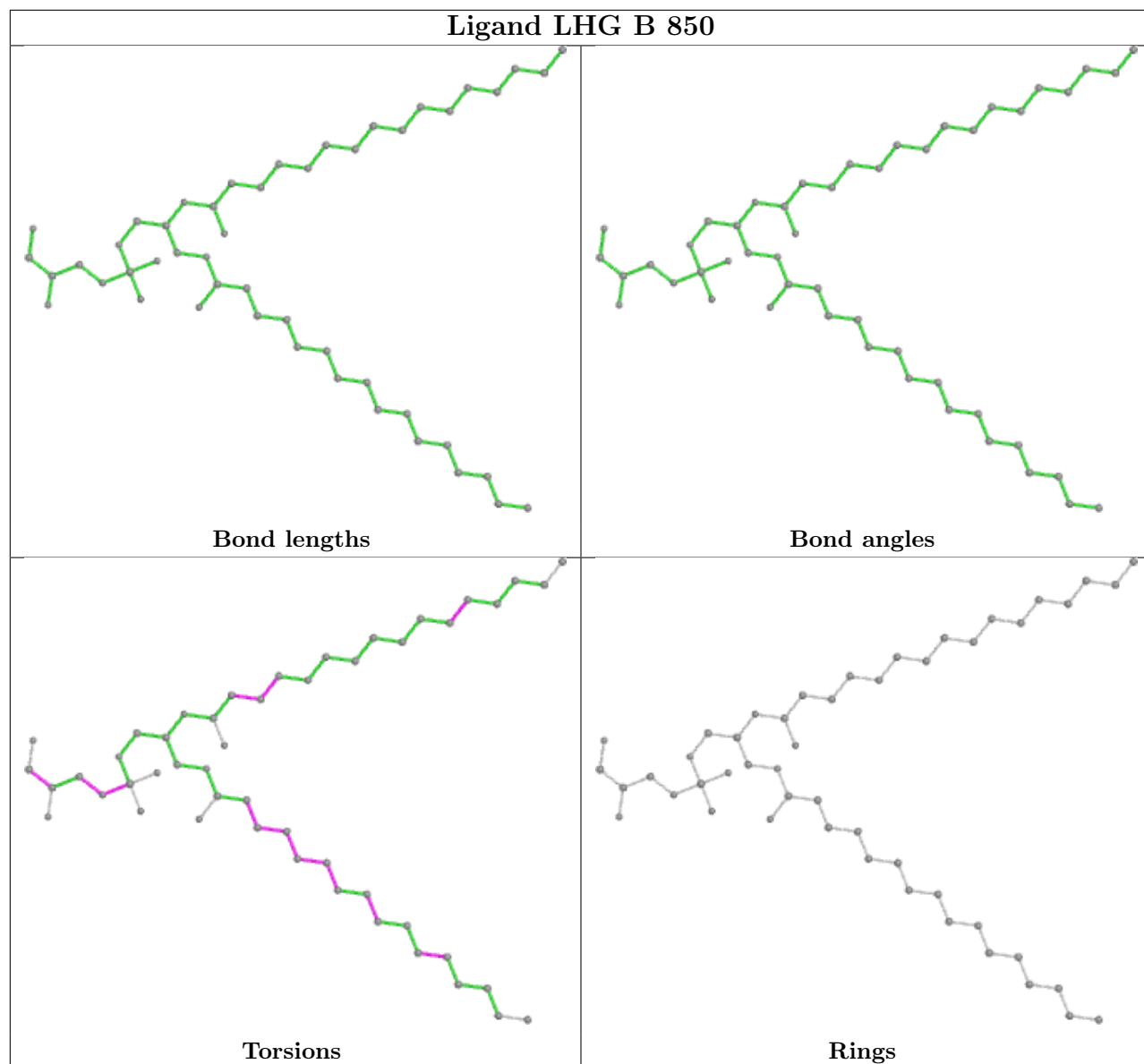
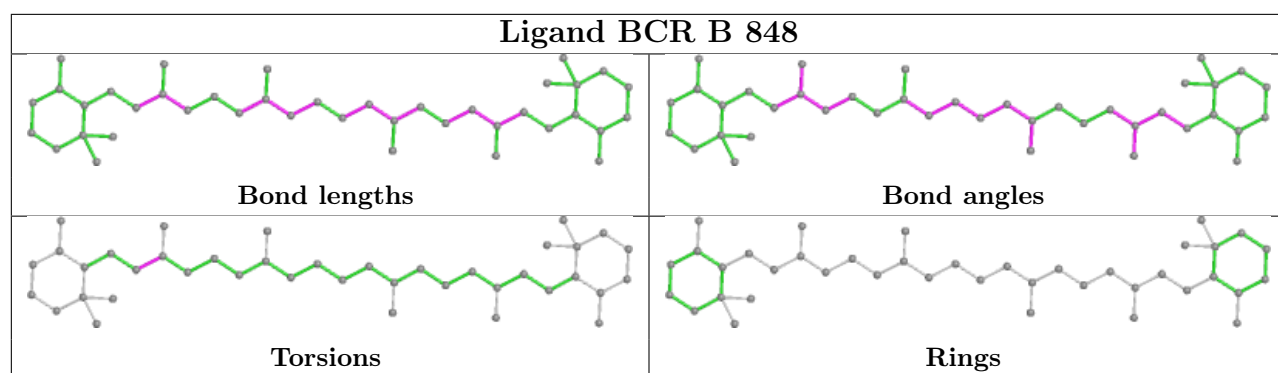


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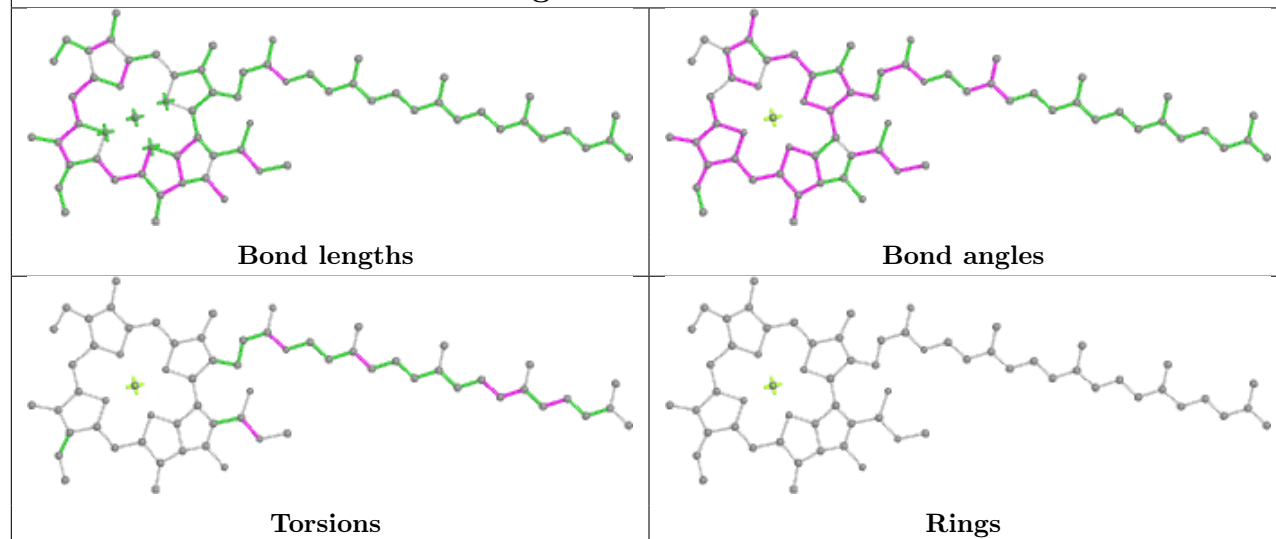


Ligand LMT 1 524

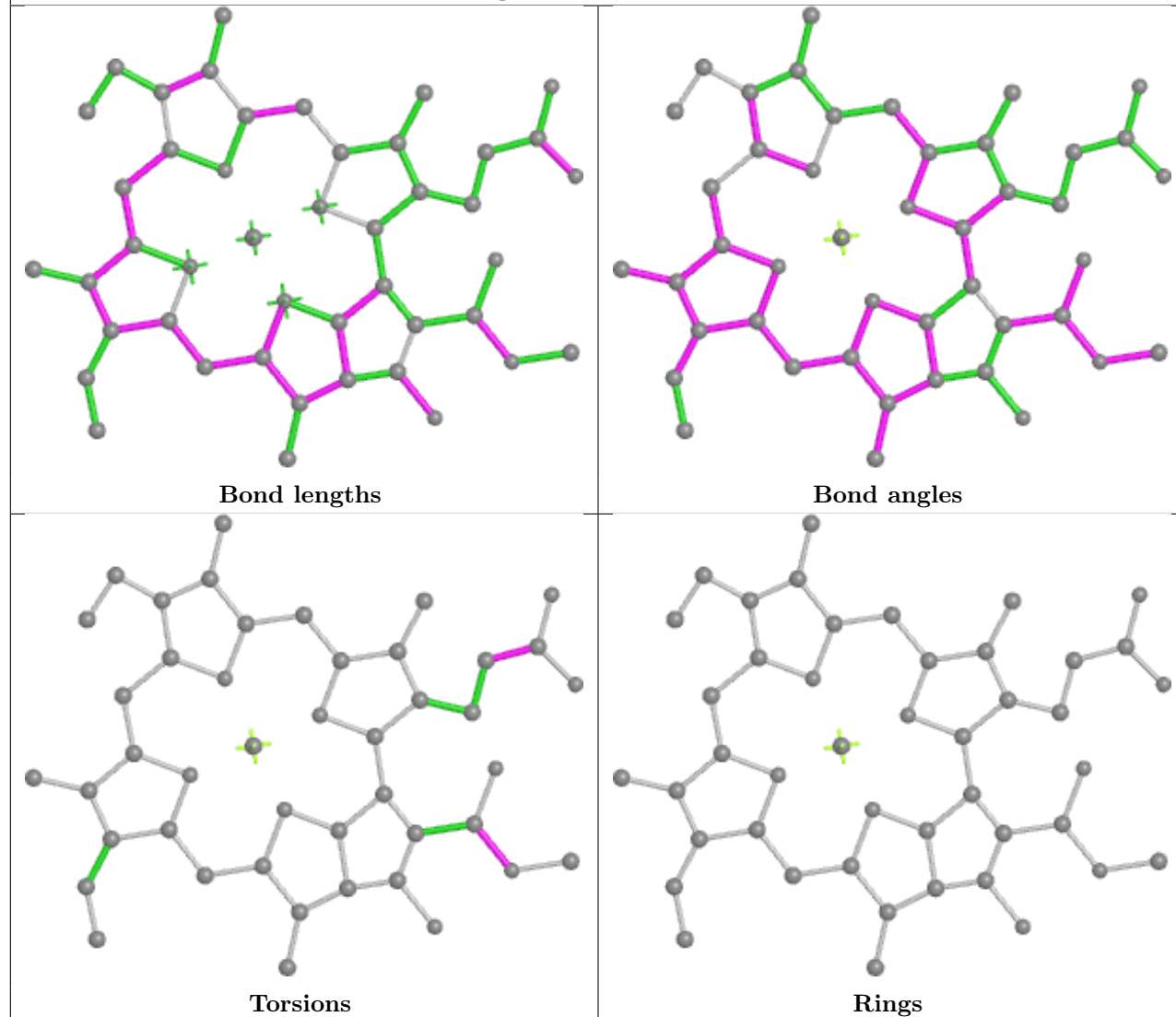




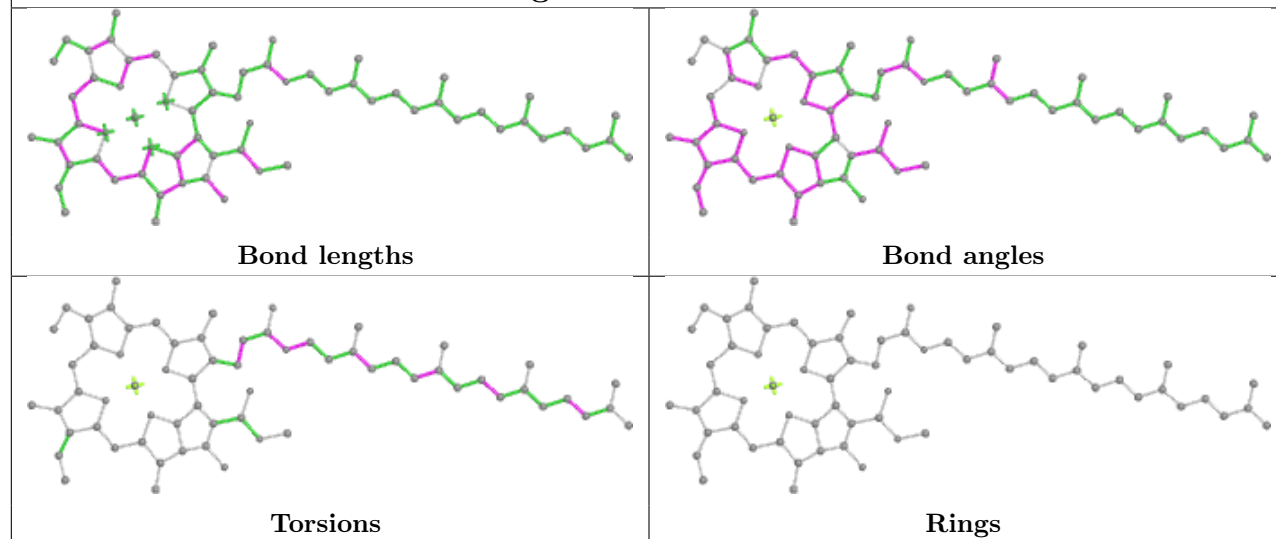
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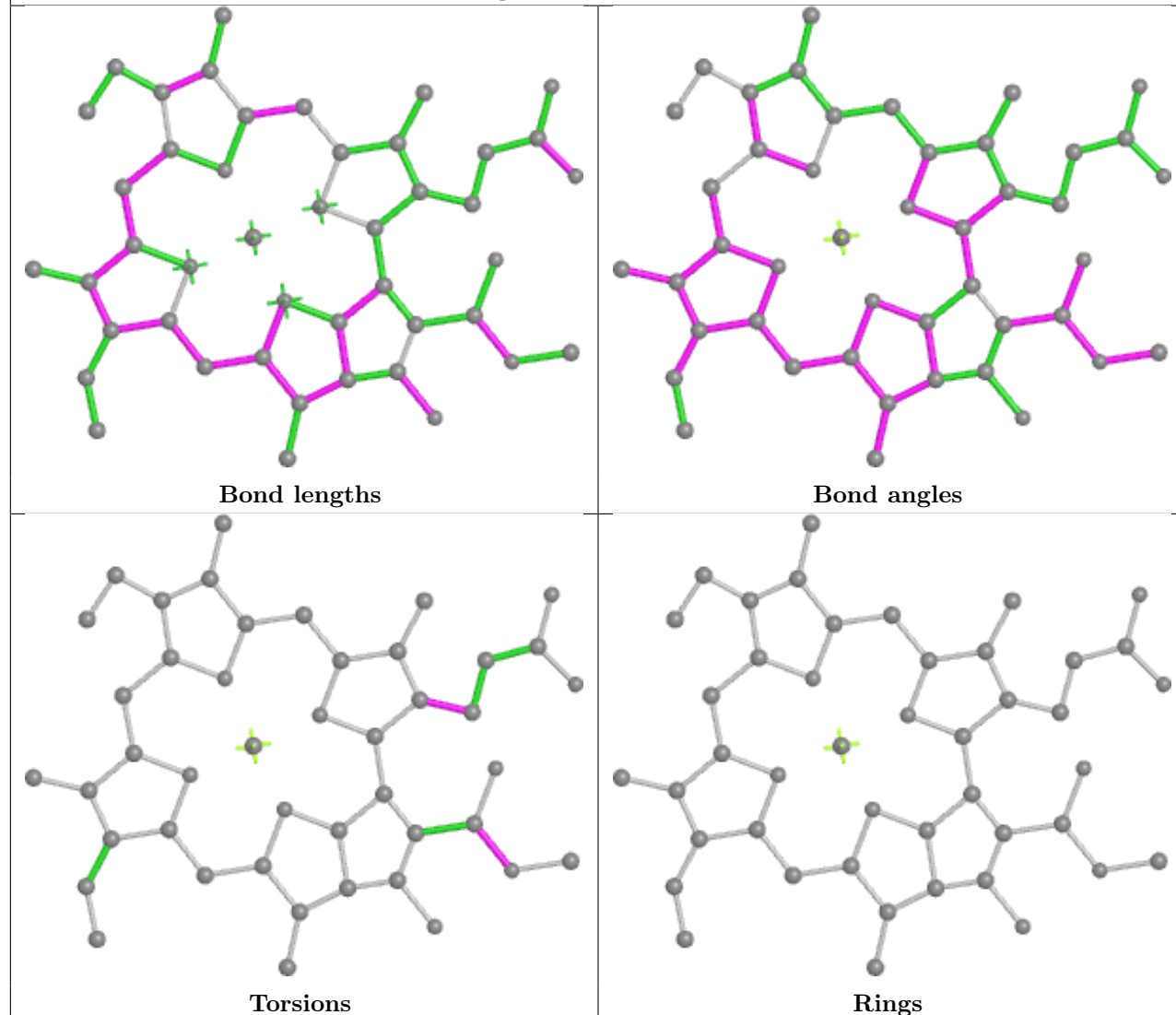
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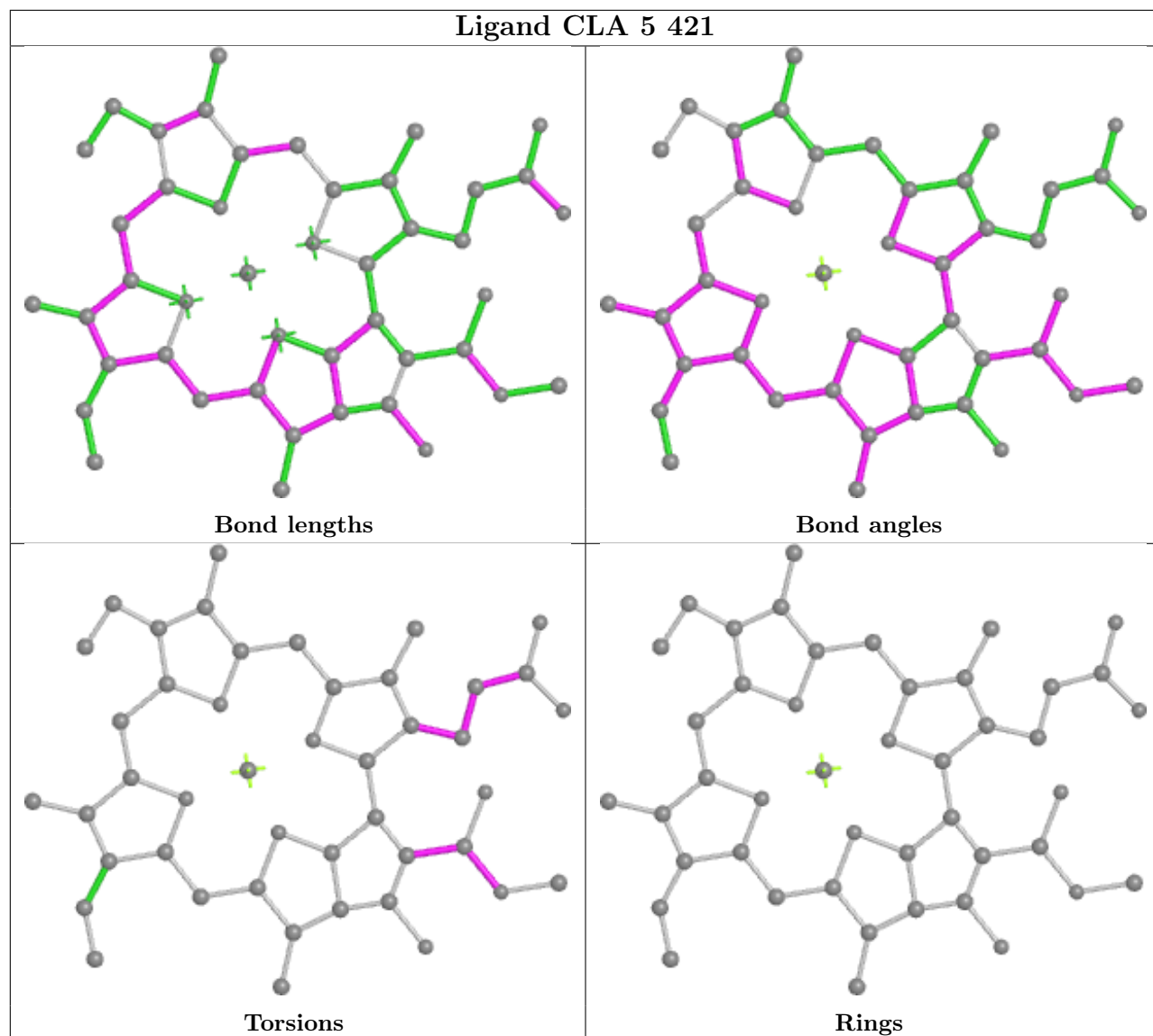
Ligand CLA A 843



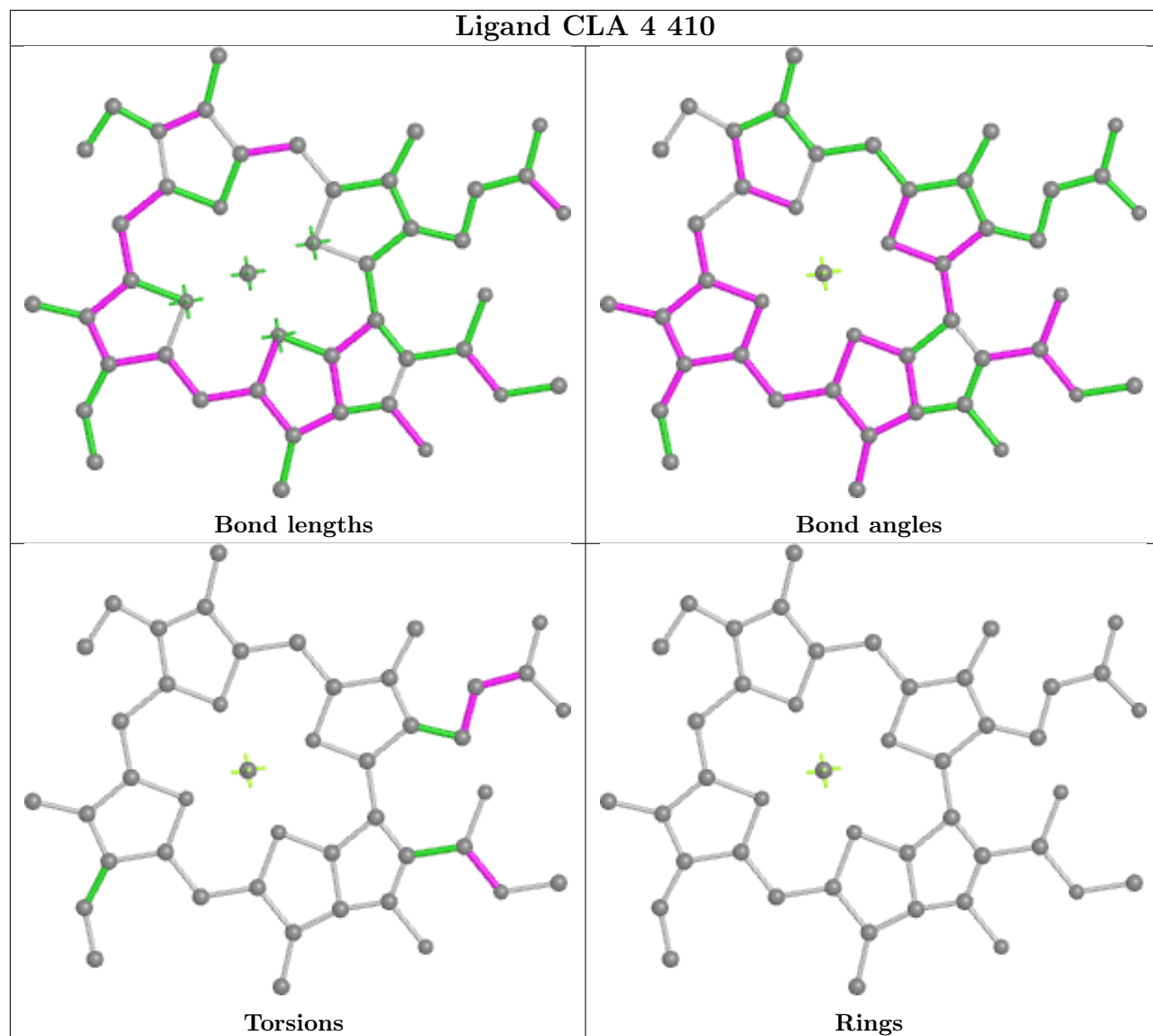
Ligand CLA 4 409



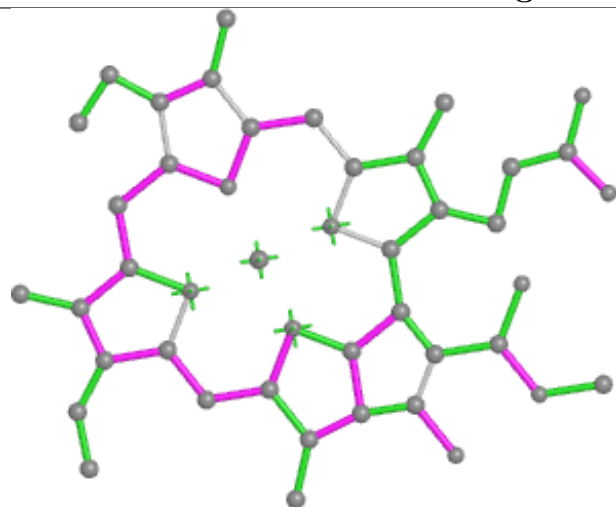
Ligand CLA 5 421



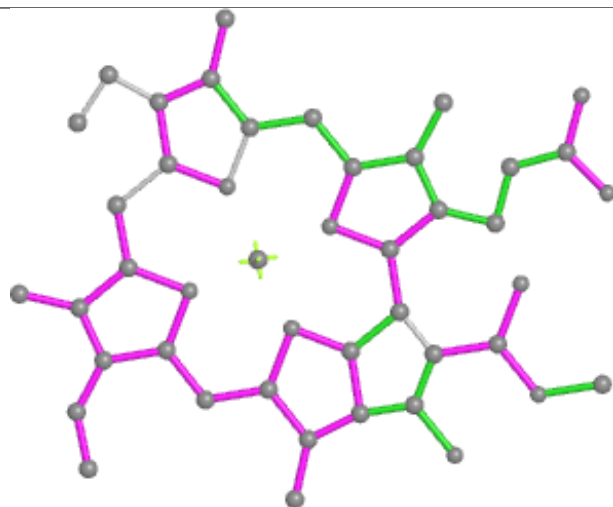
Ligand CLA 4 410



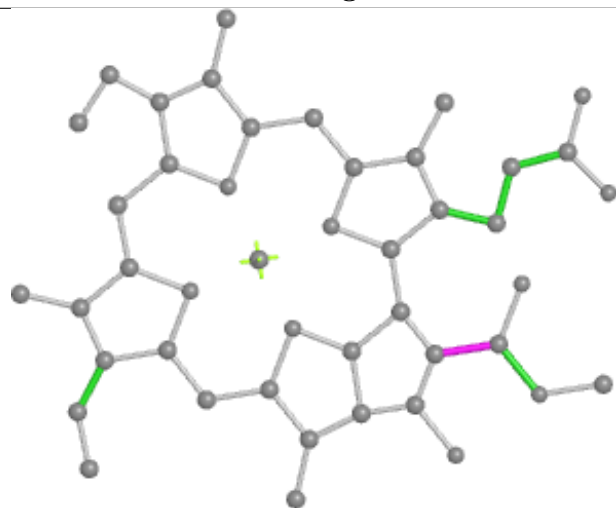
Ligand CLA A 815



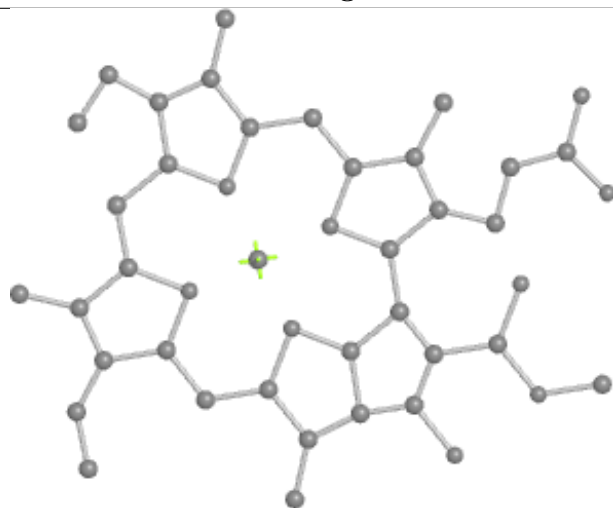
Bond lengths



Bond angles

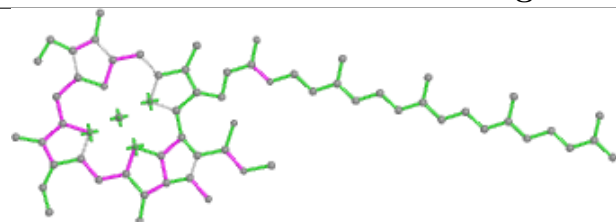


Torsions

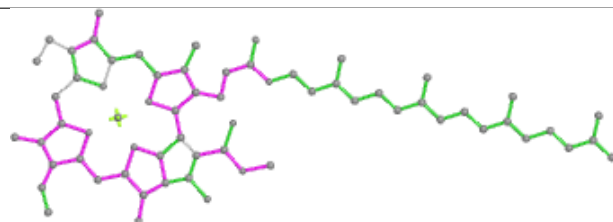


Rings

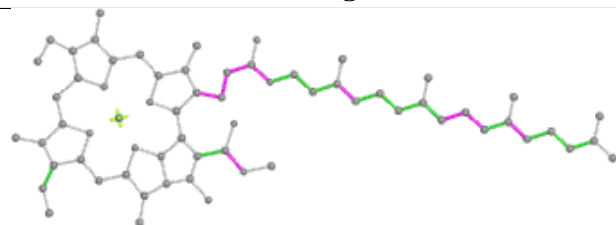
Ligand CLA A 810



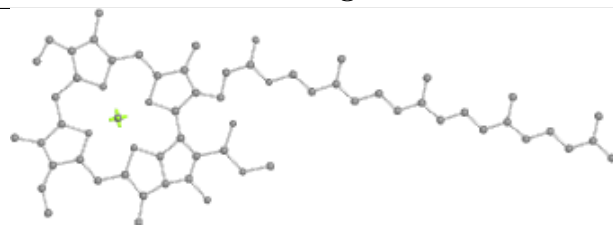
Bond lengths



Bond angles

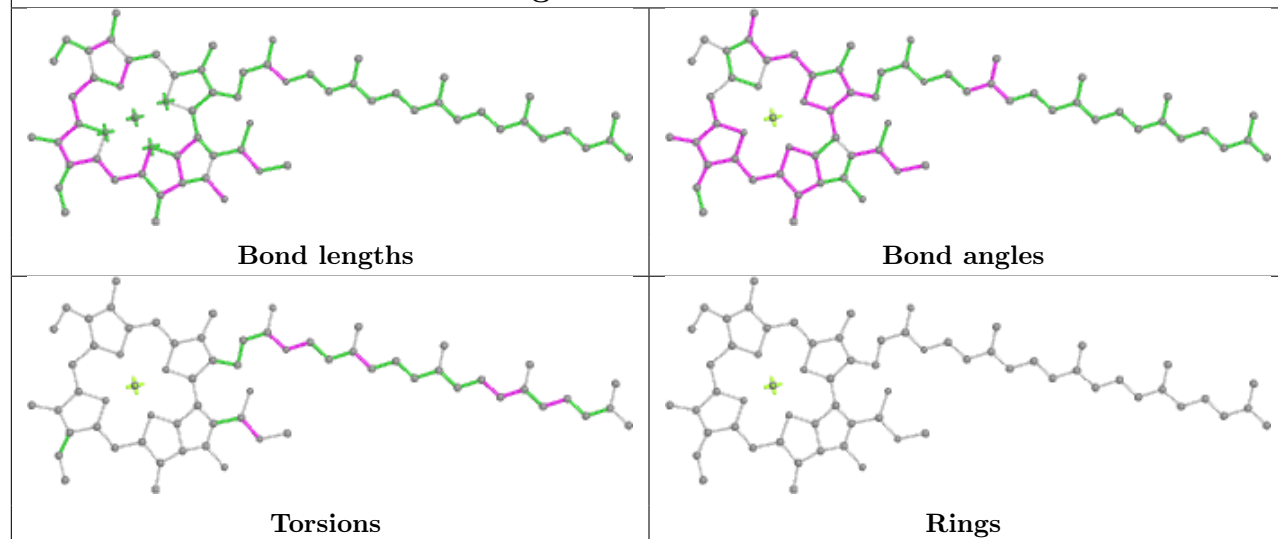


Torsions

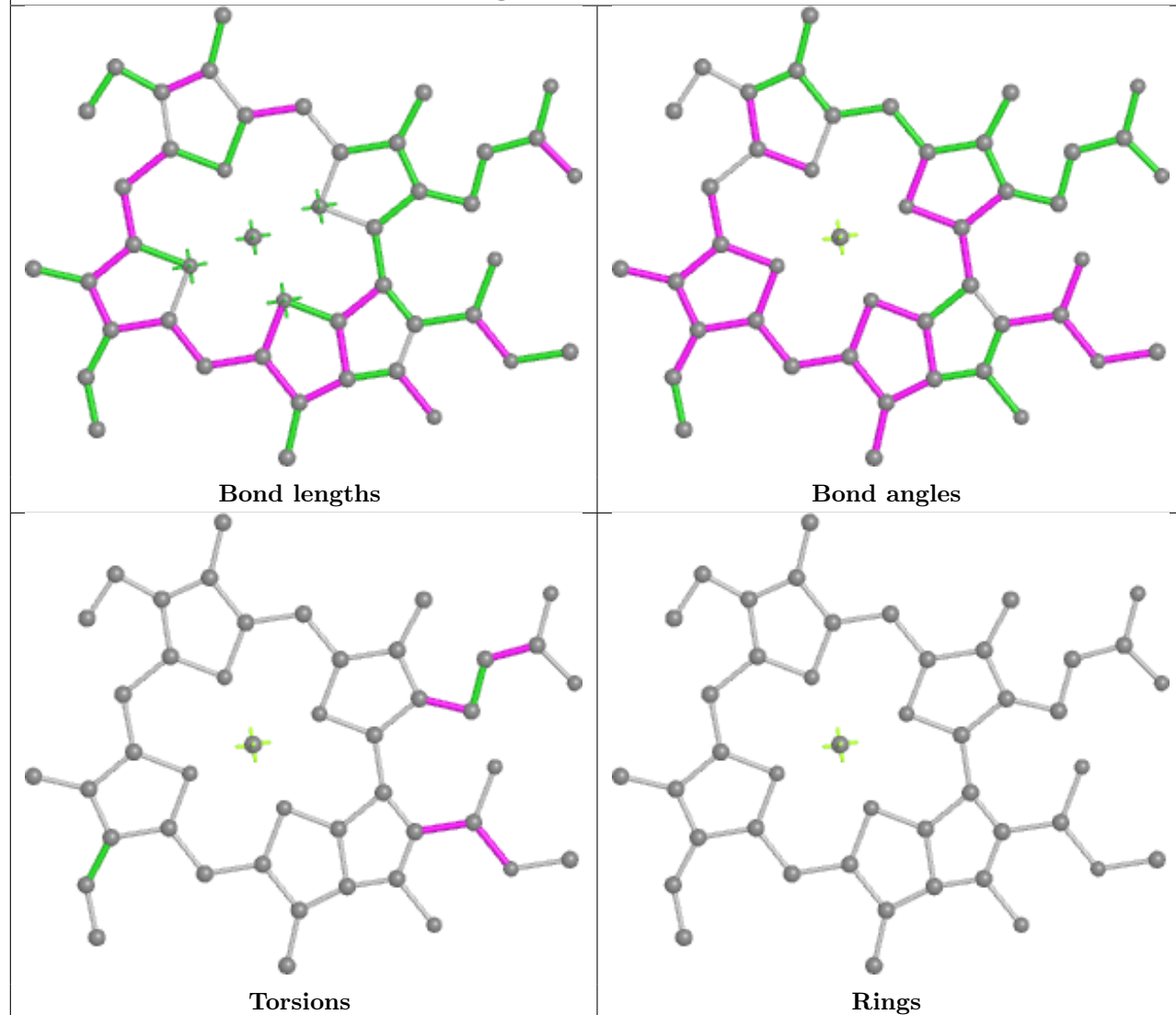


Rings

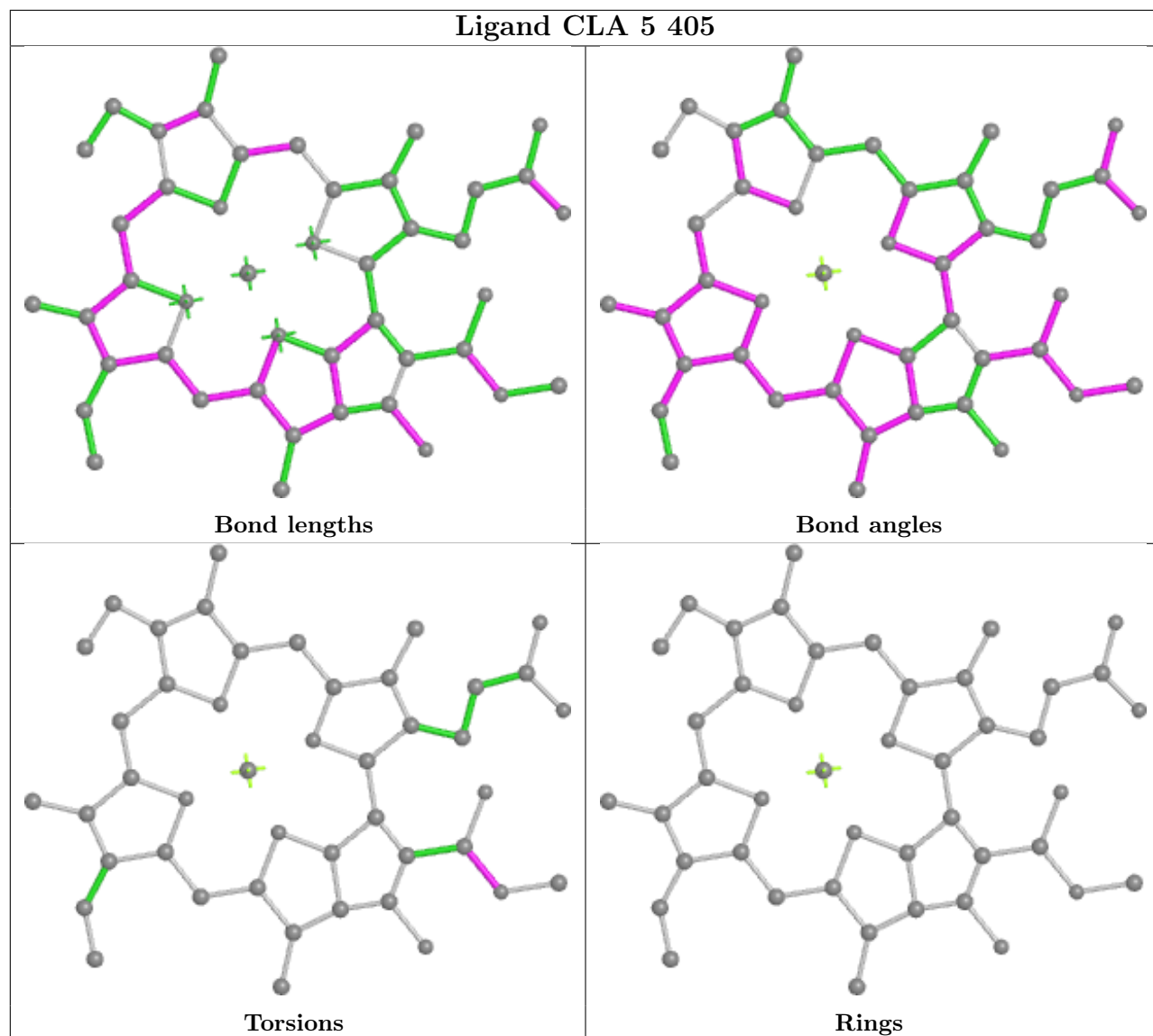
Ligand CLA B 830



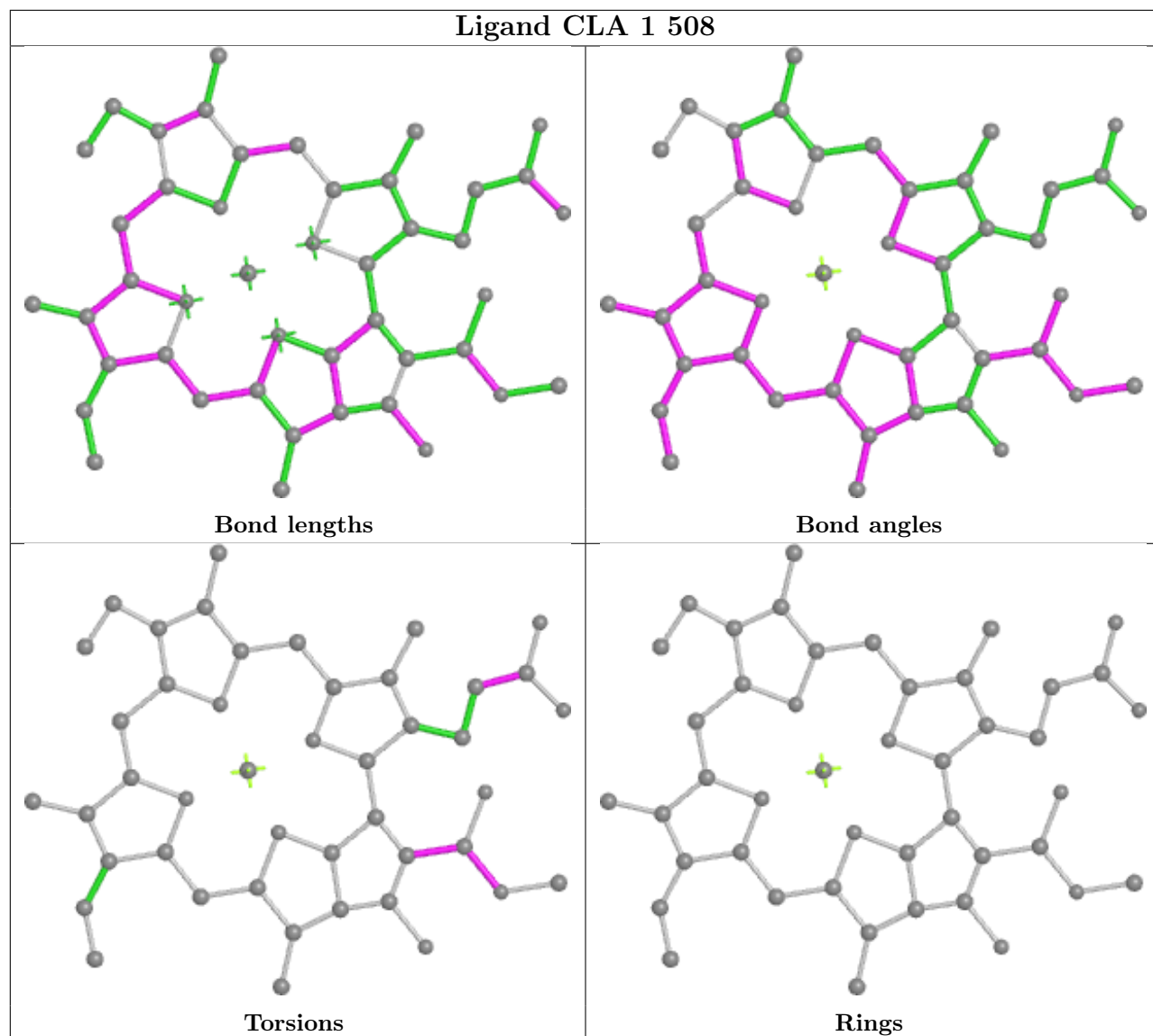
Ligand CLA 6 401



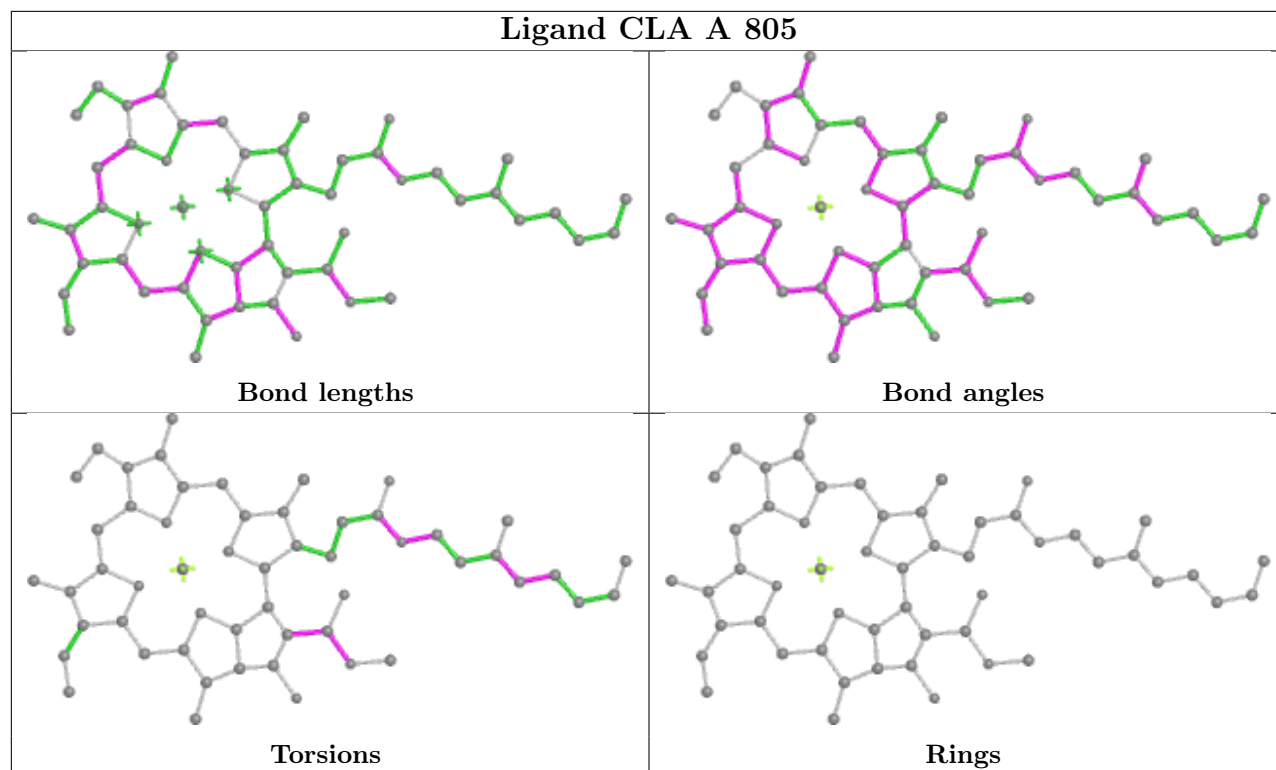
Ligand CLA 5 405



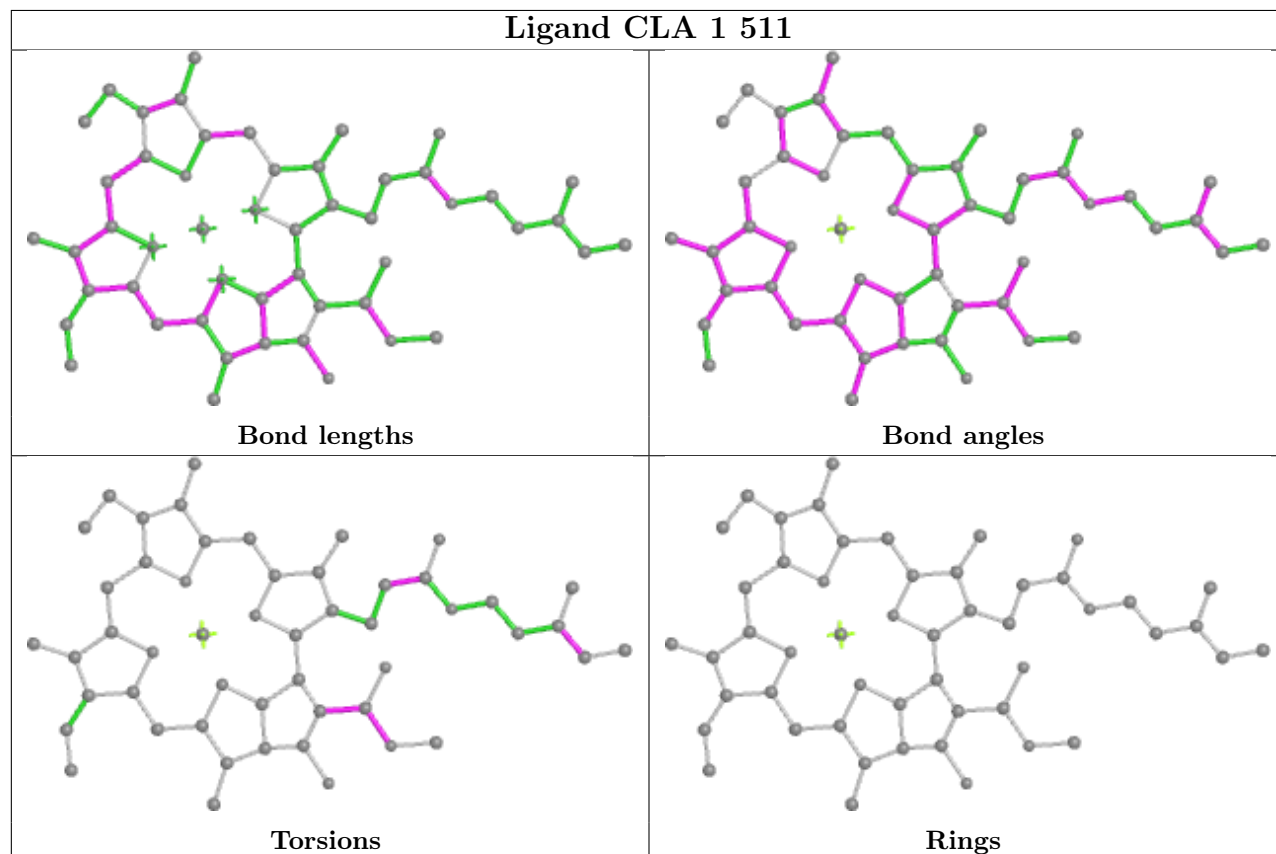
Ligand CLA 1 508



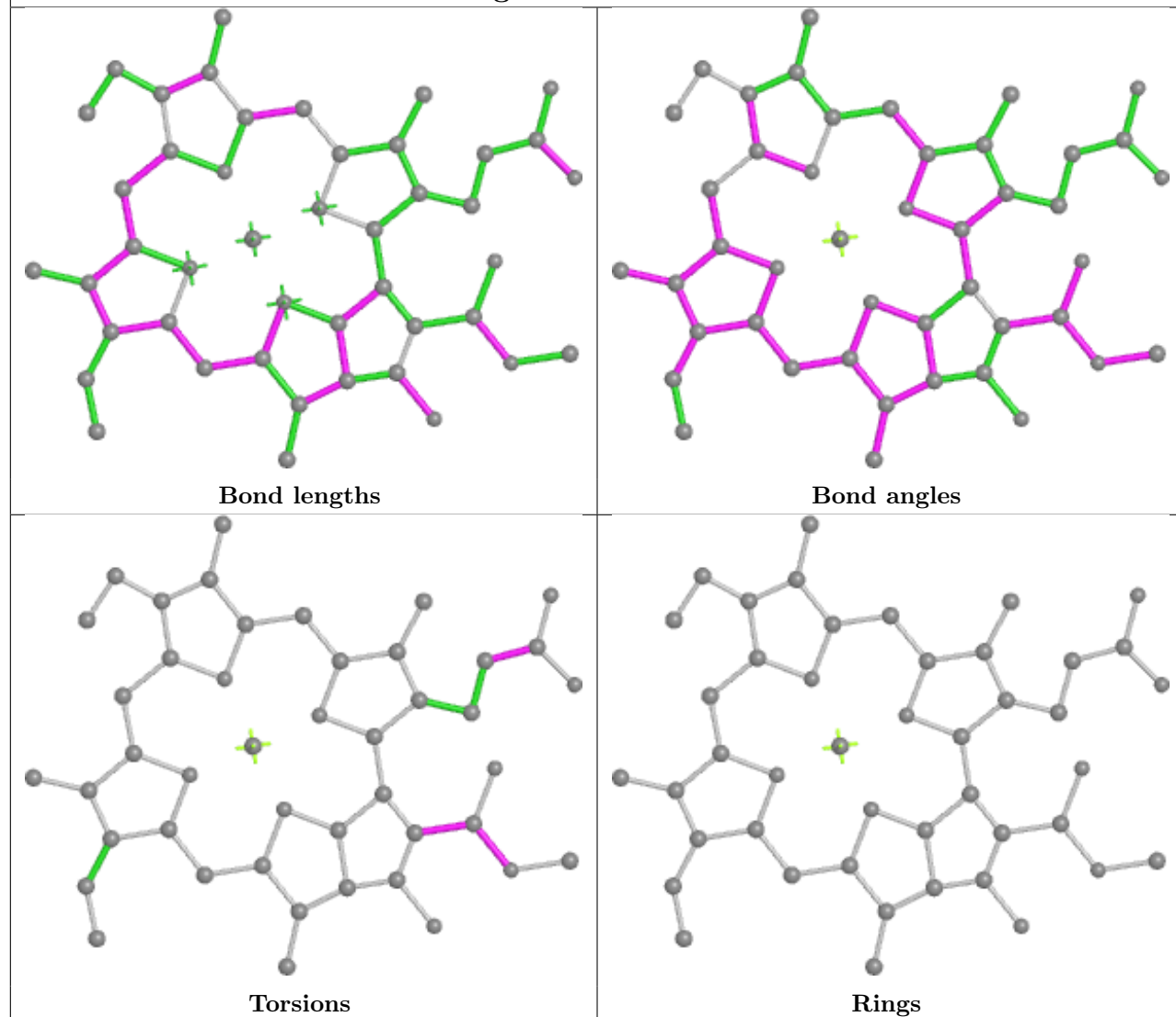
Ligand CLA A 805



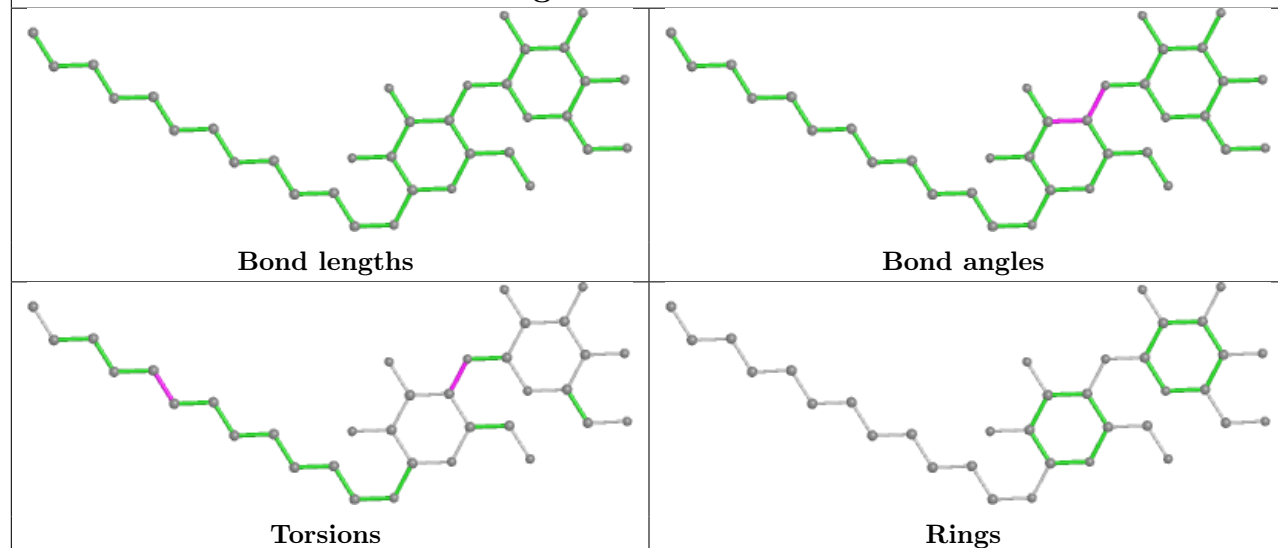
Ligand CLA 1 511

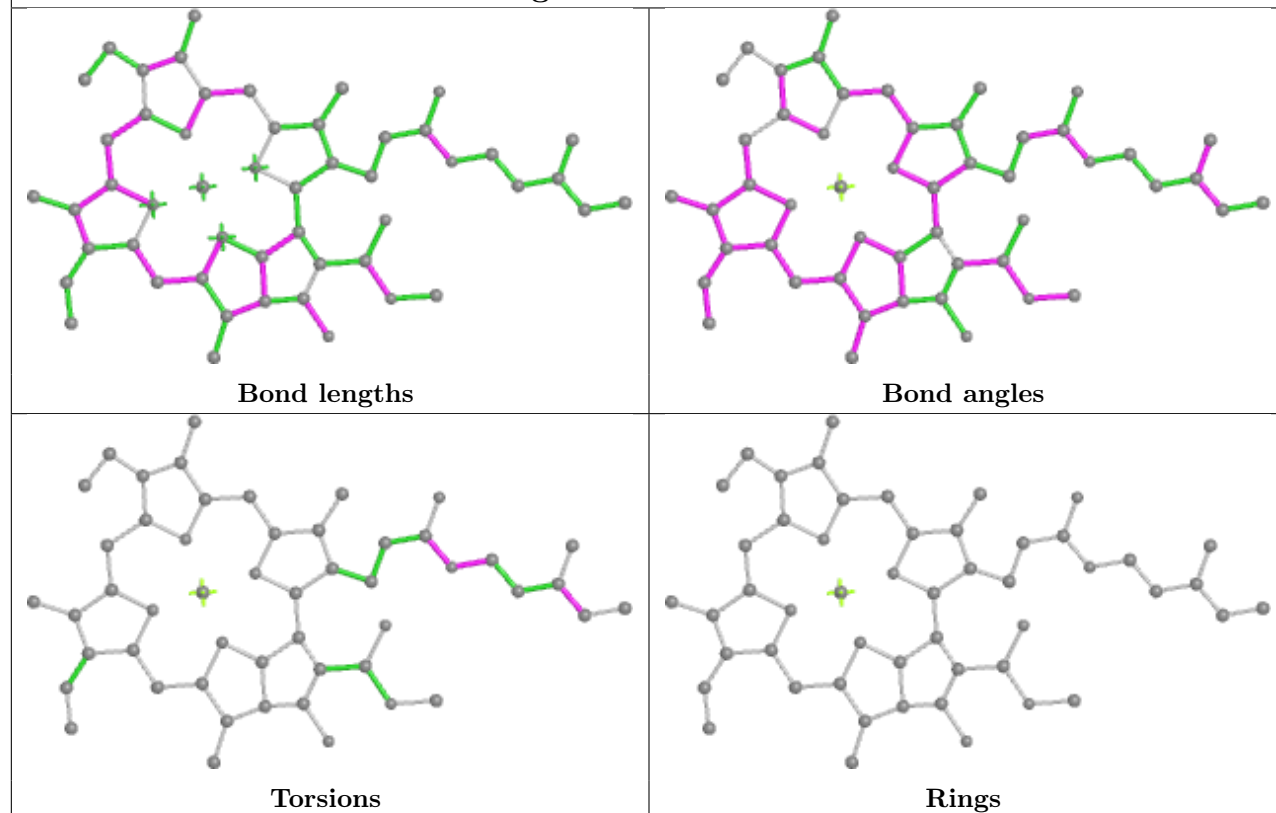
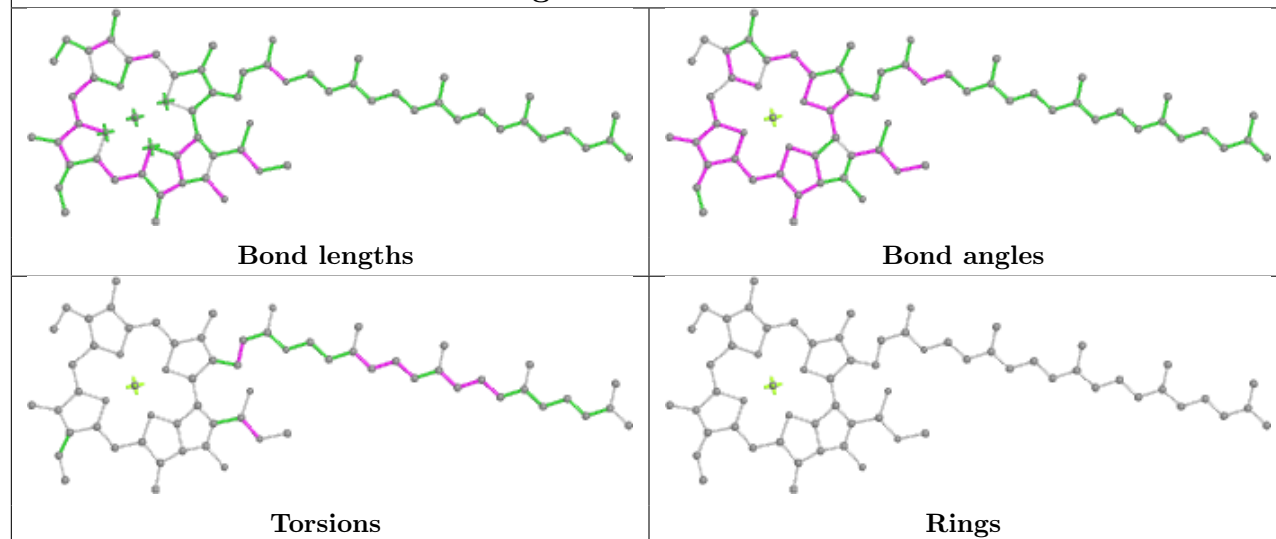


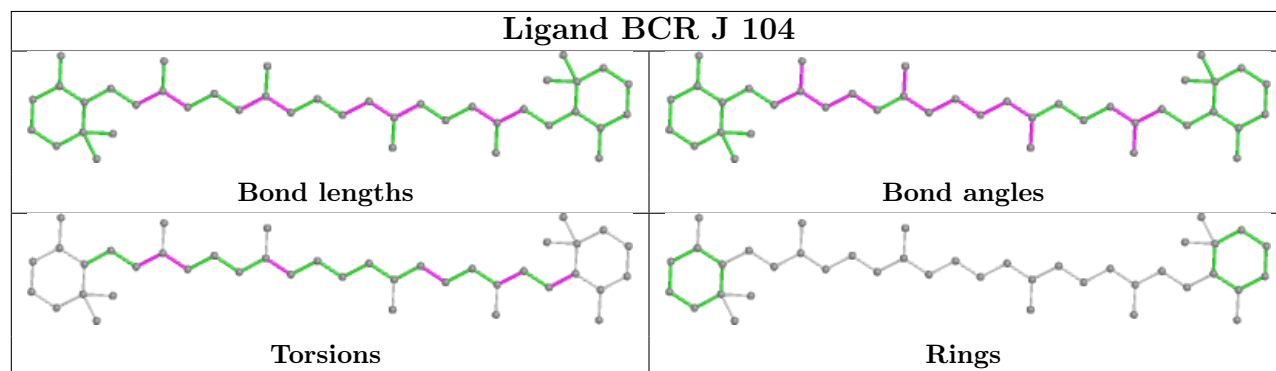
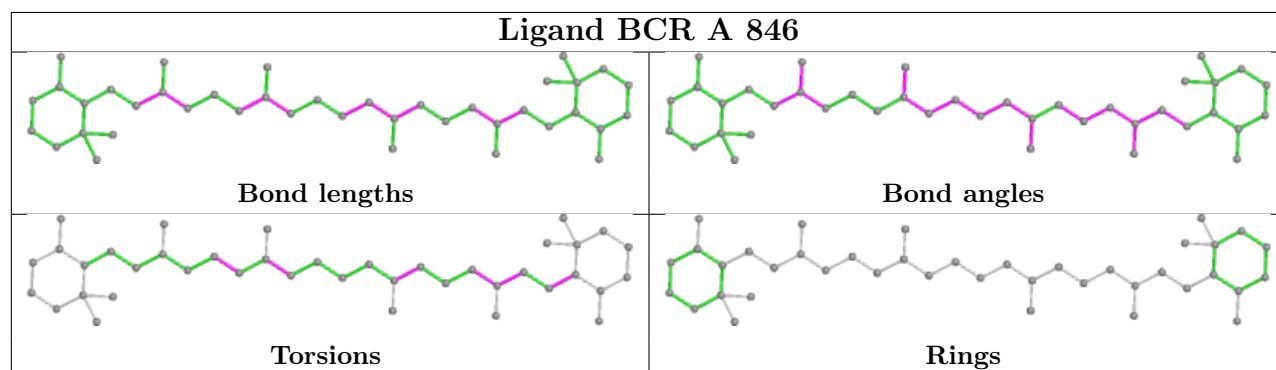
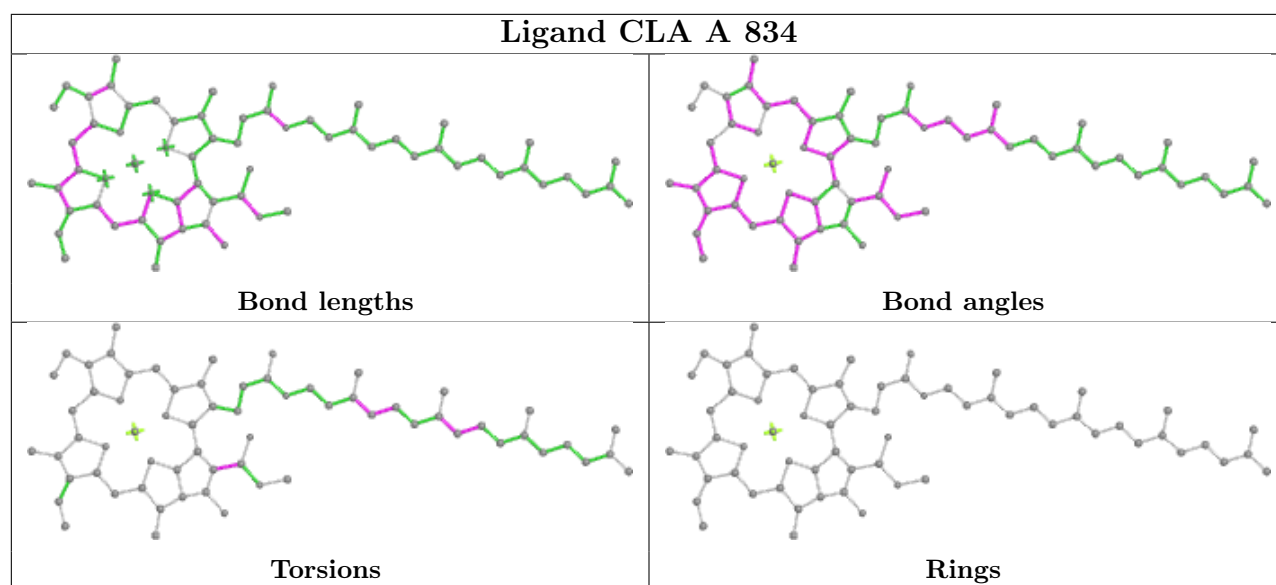
Ligand CLA 5 412

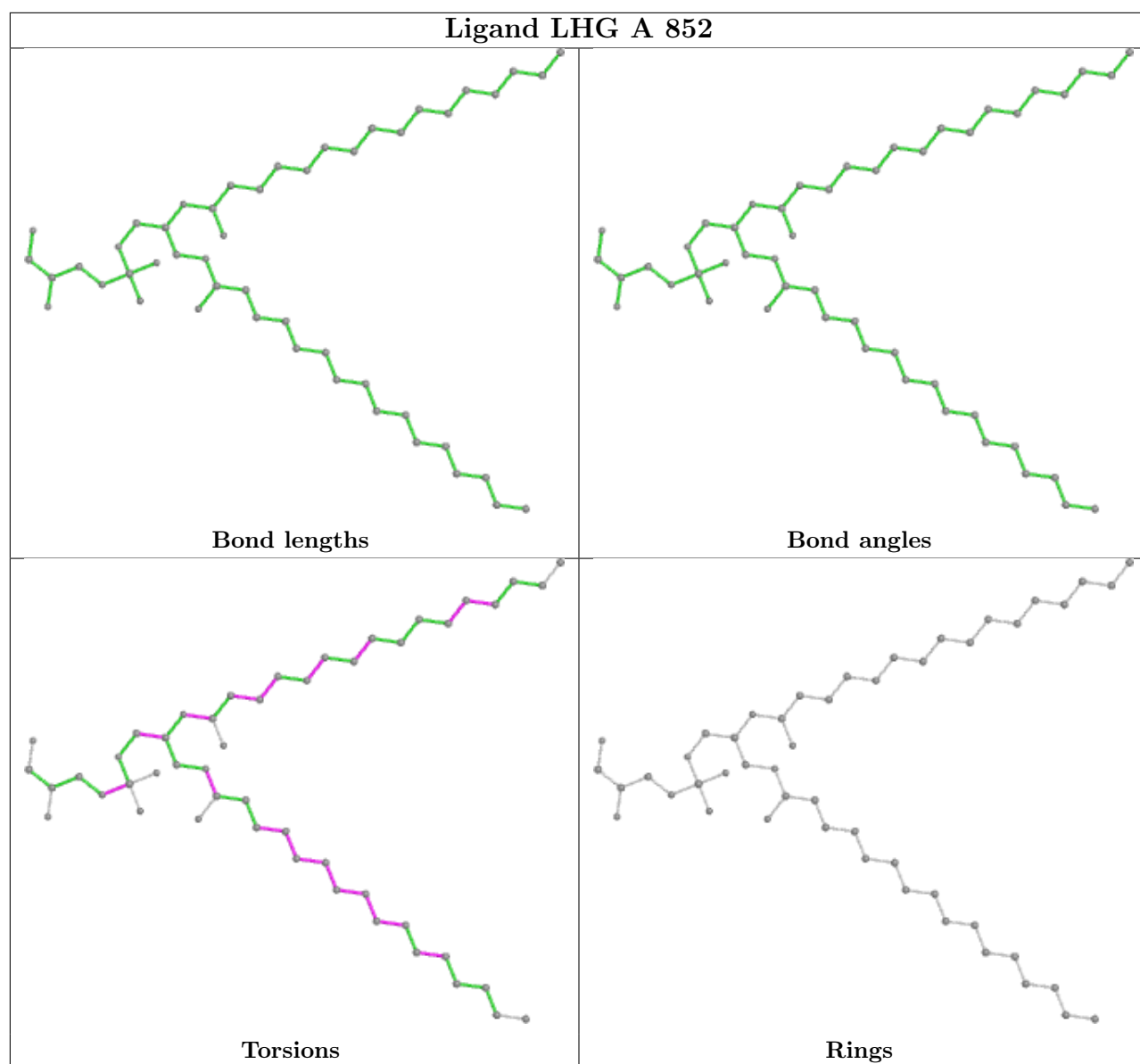


Ligand LMT 5 401

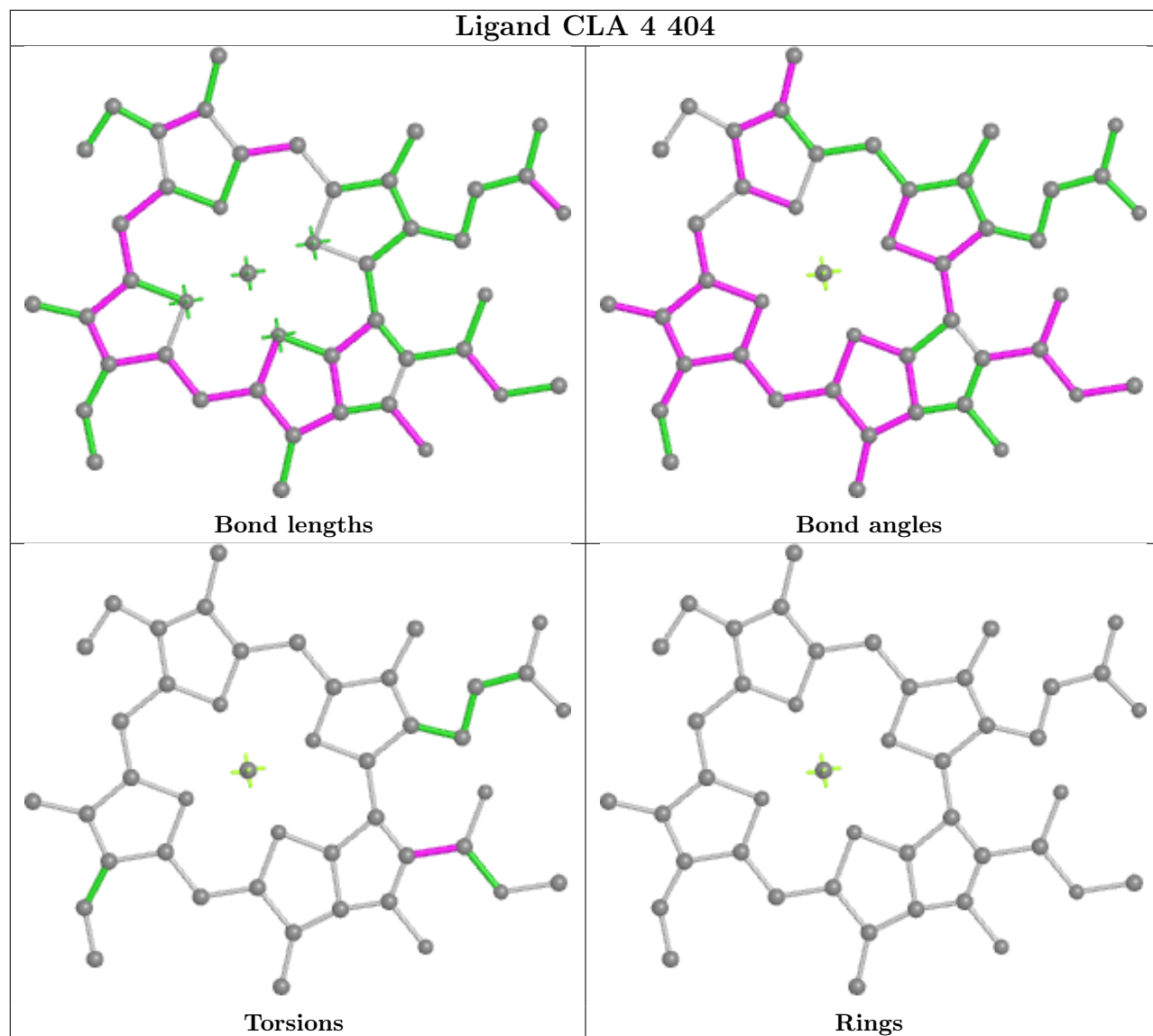


Ligand CLA A 836**Ligand CLA B 840**

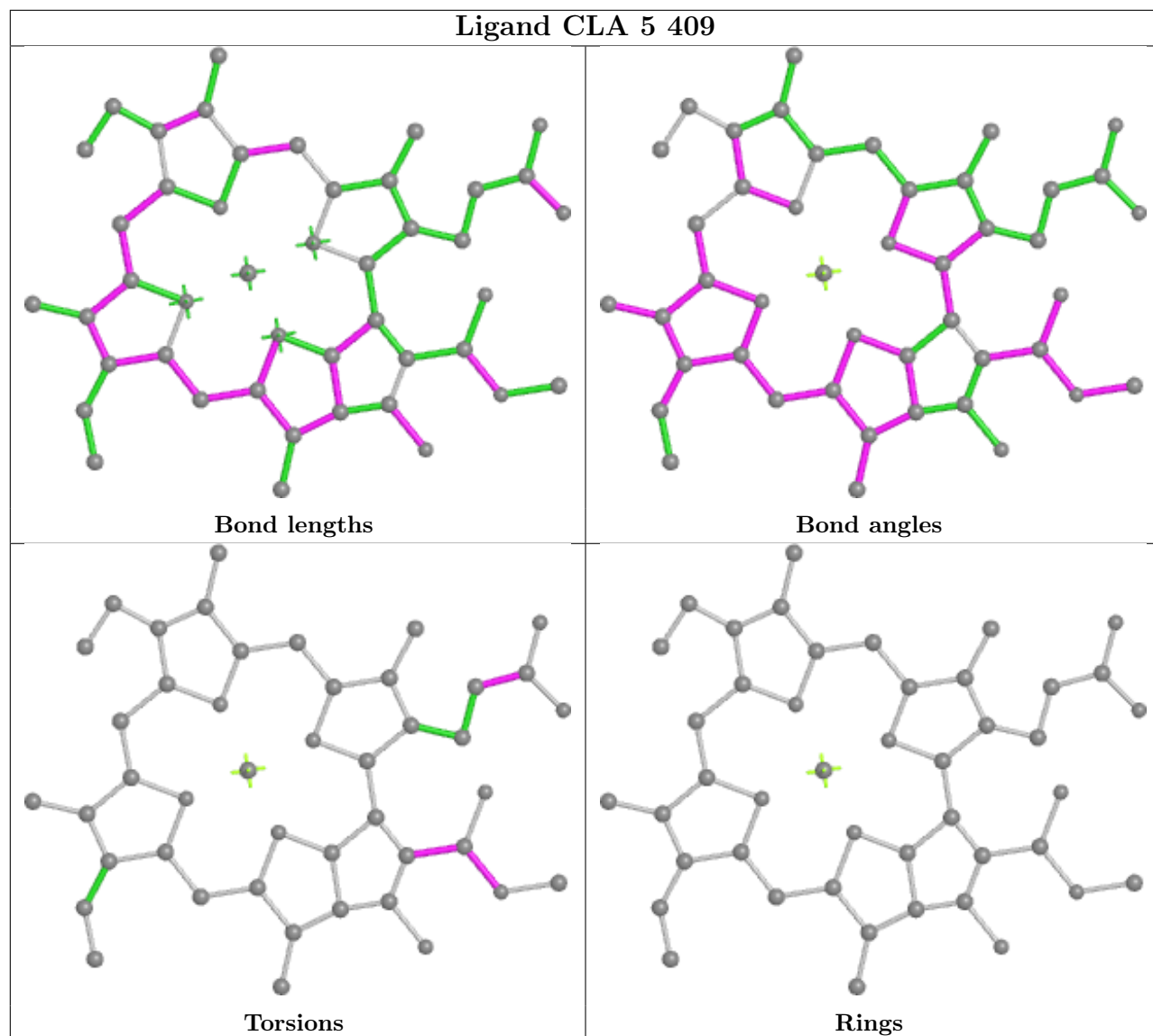




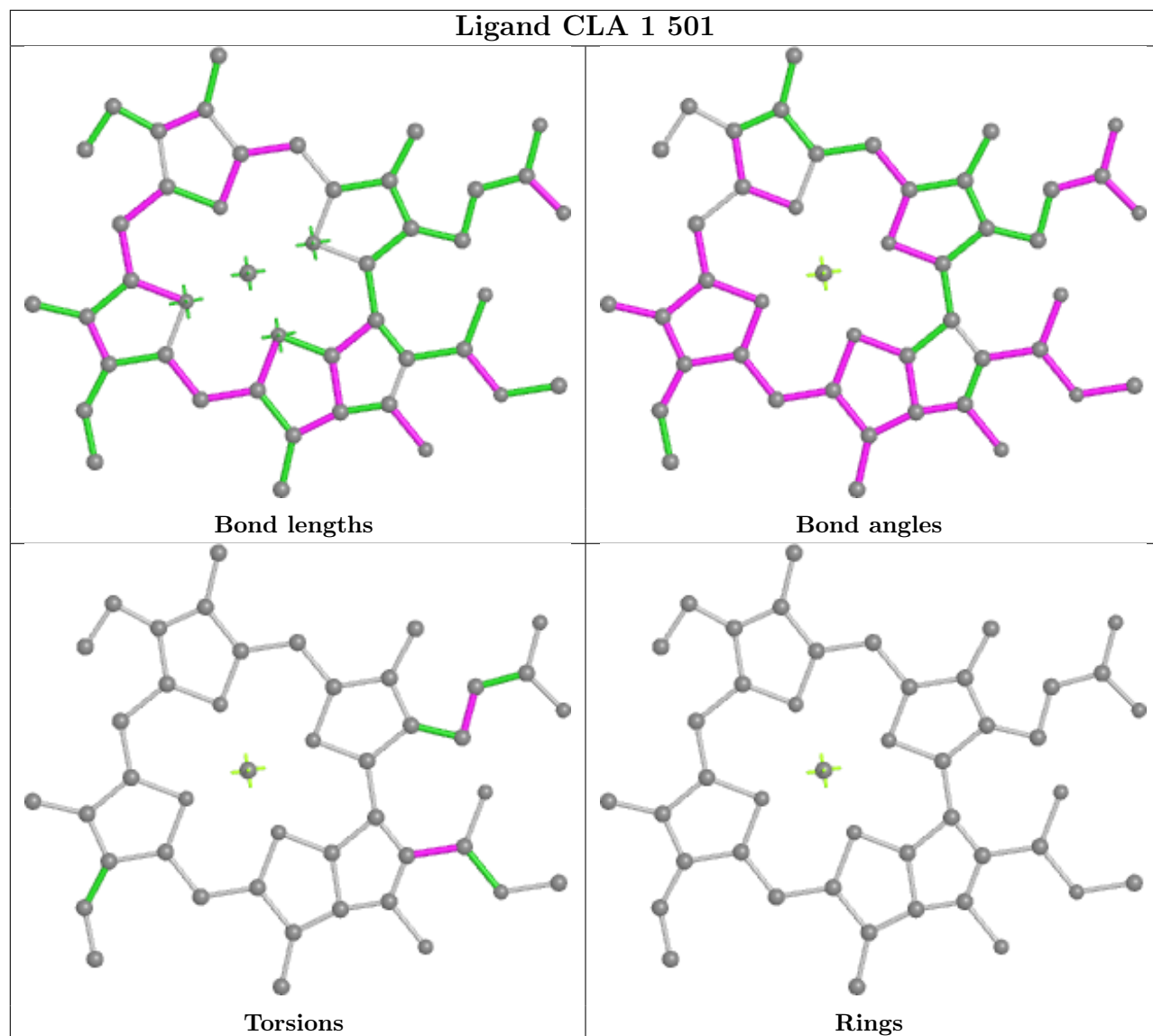
Ligand CLA 4 404



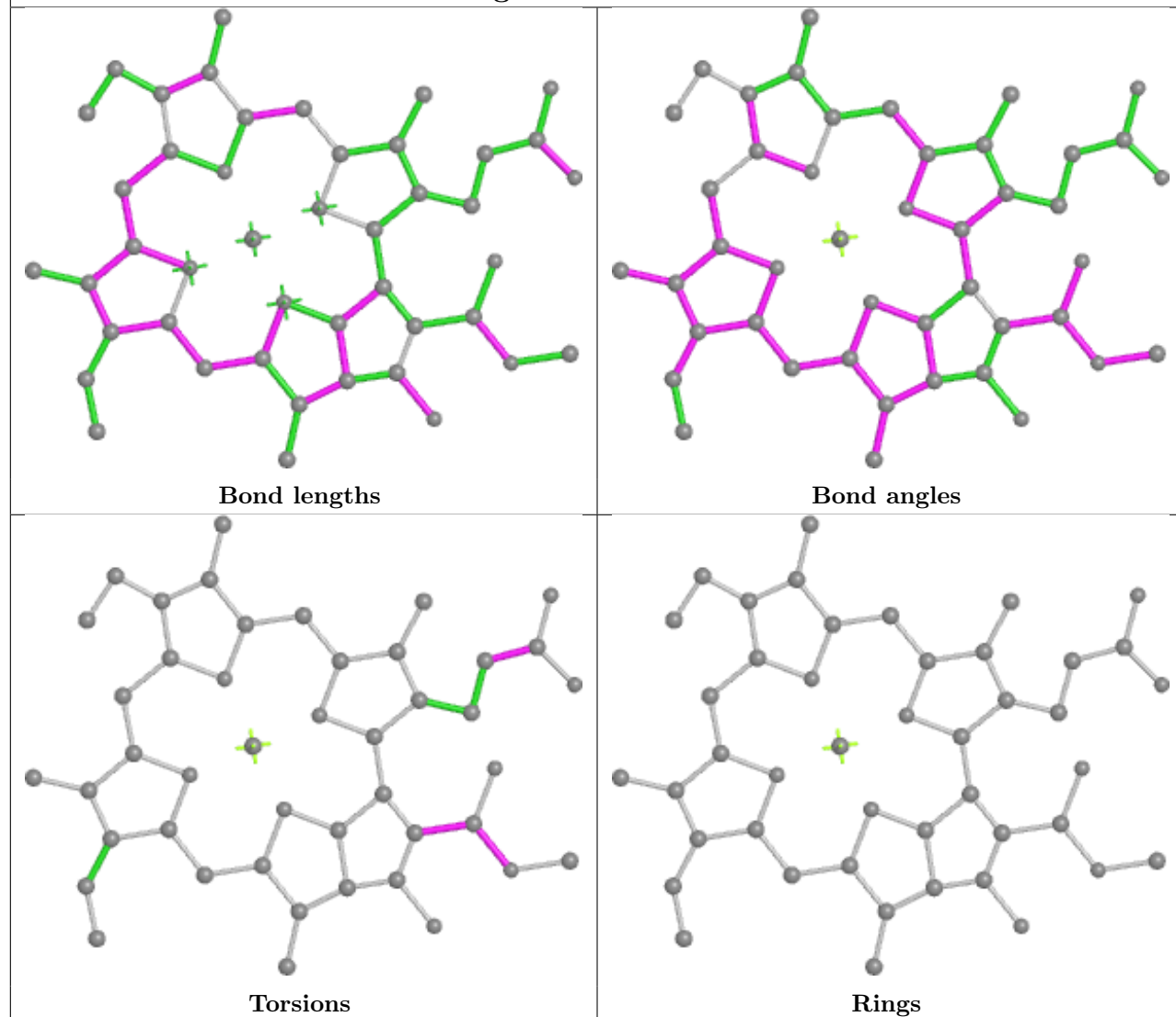
Ligand CLA 5 409



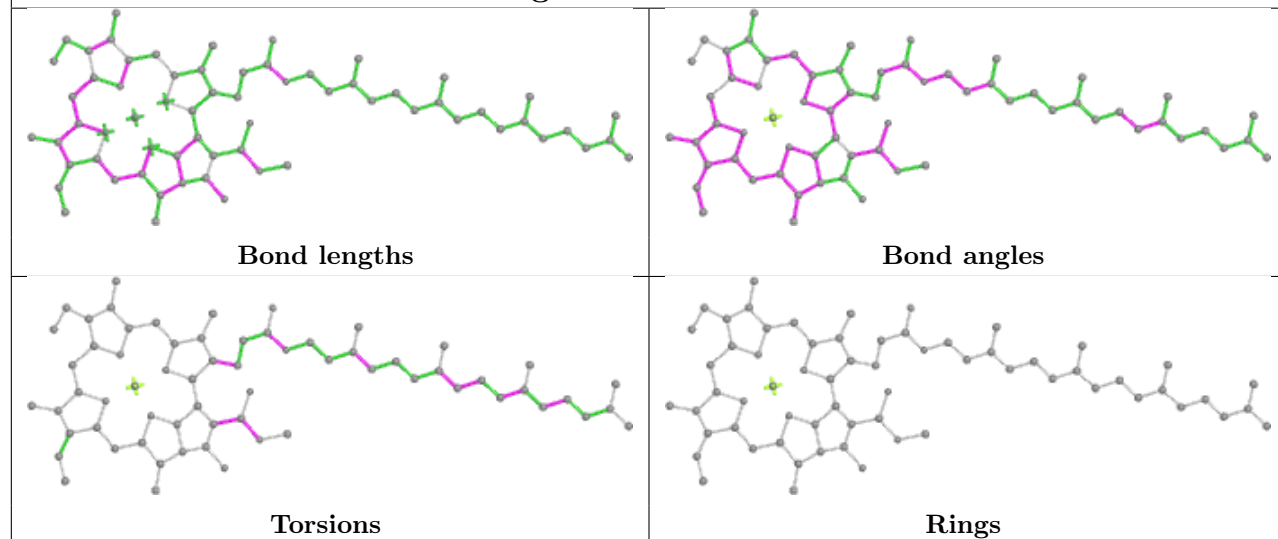
Ligand CLA 1 501



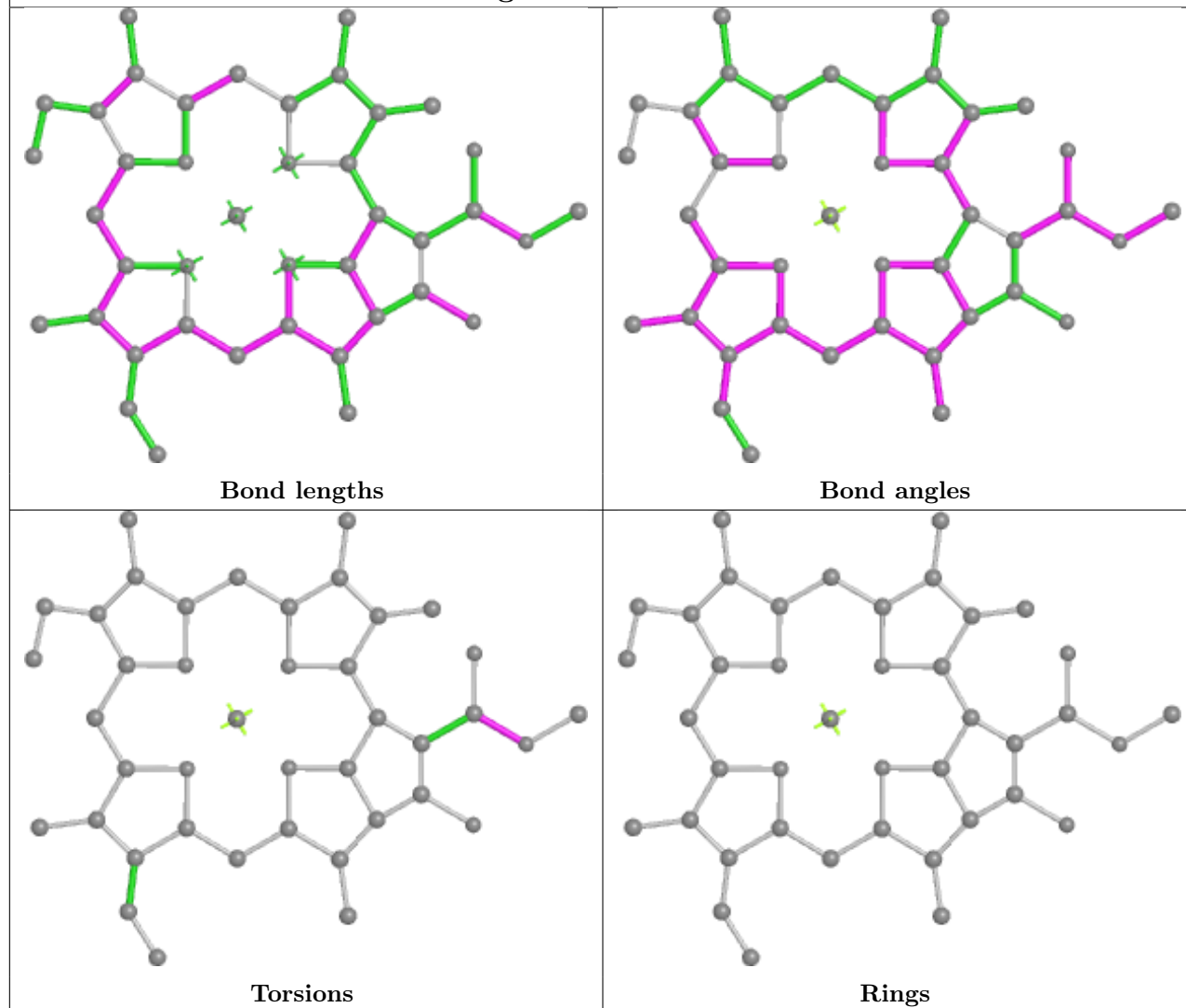
Ligand CLA 5 414



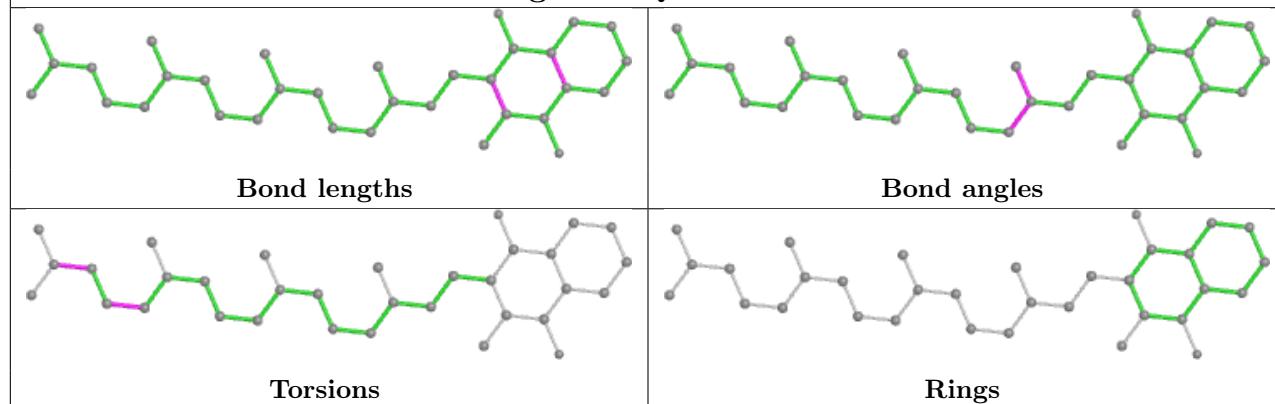
Ligand CLA A 820

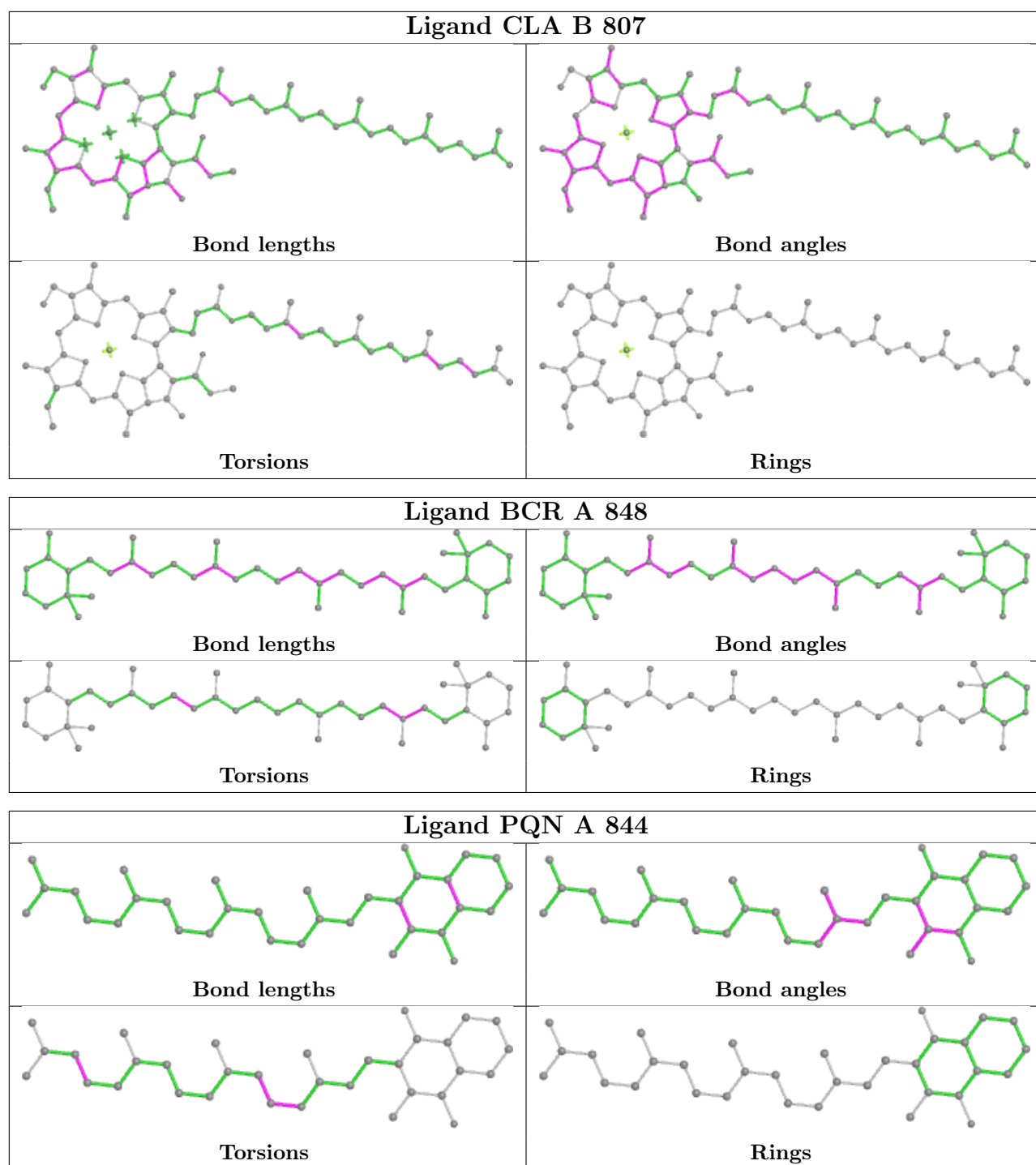


Ligand CLA 6 408

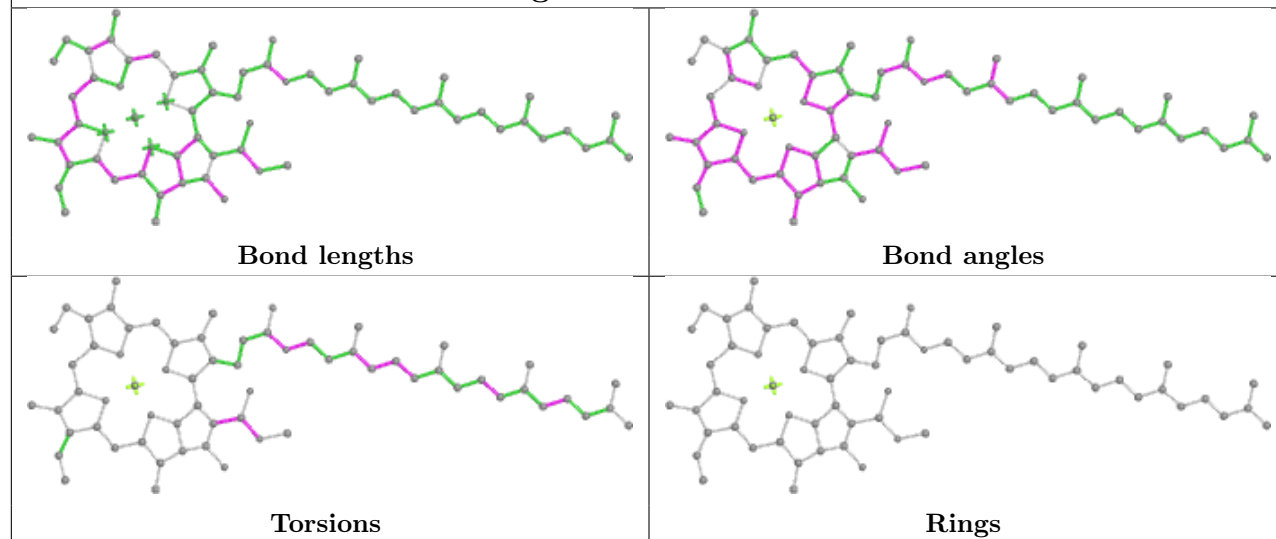


Ligand PQN B 842

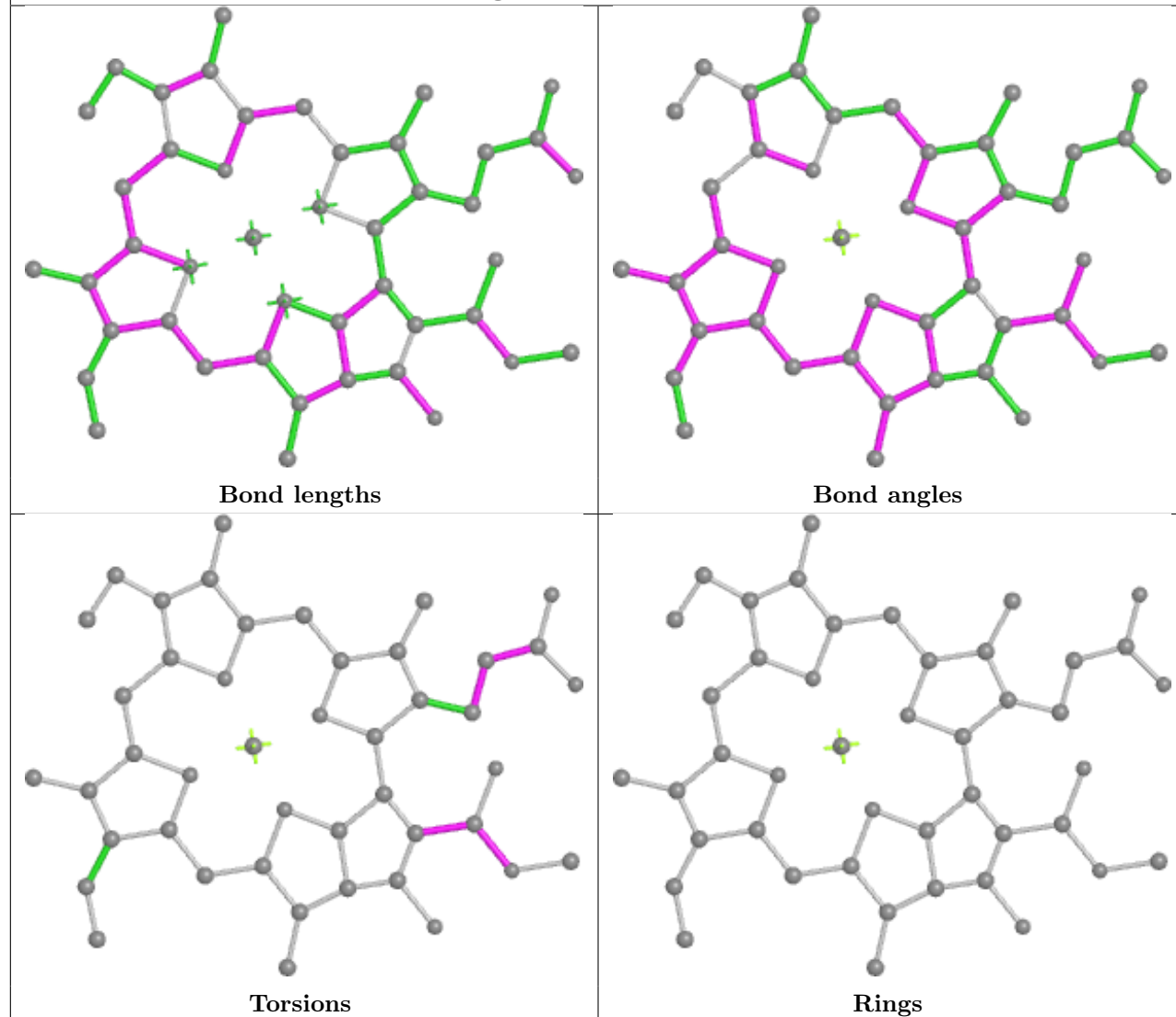


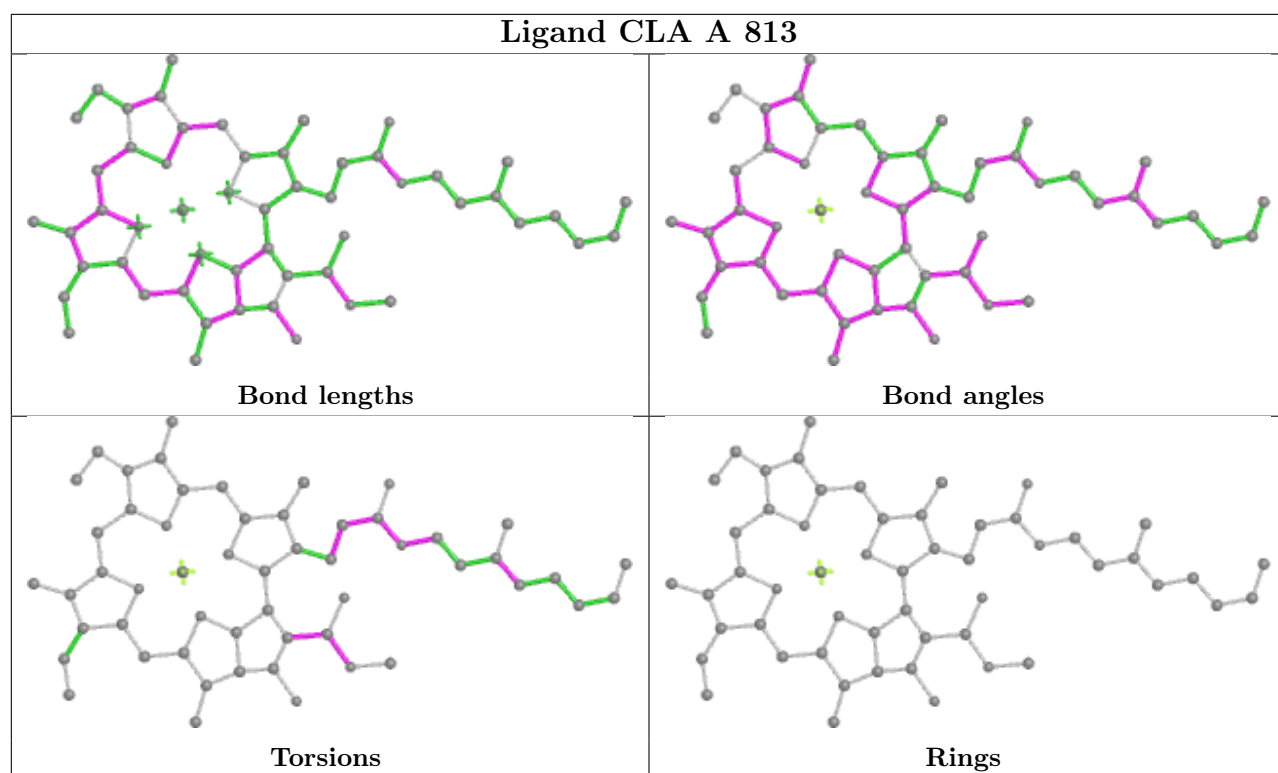


Ligand CLA A 804

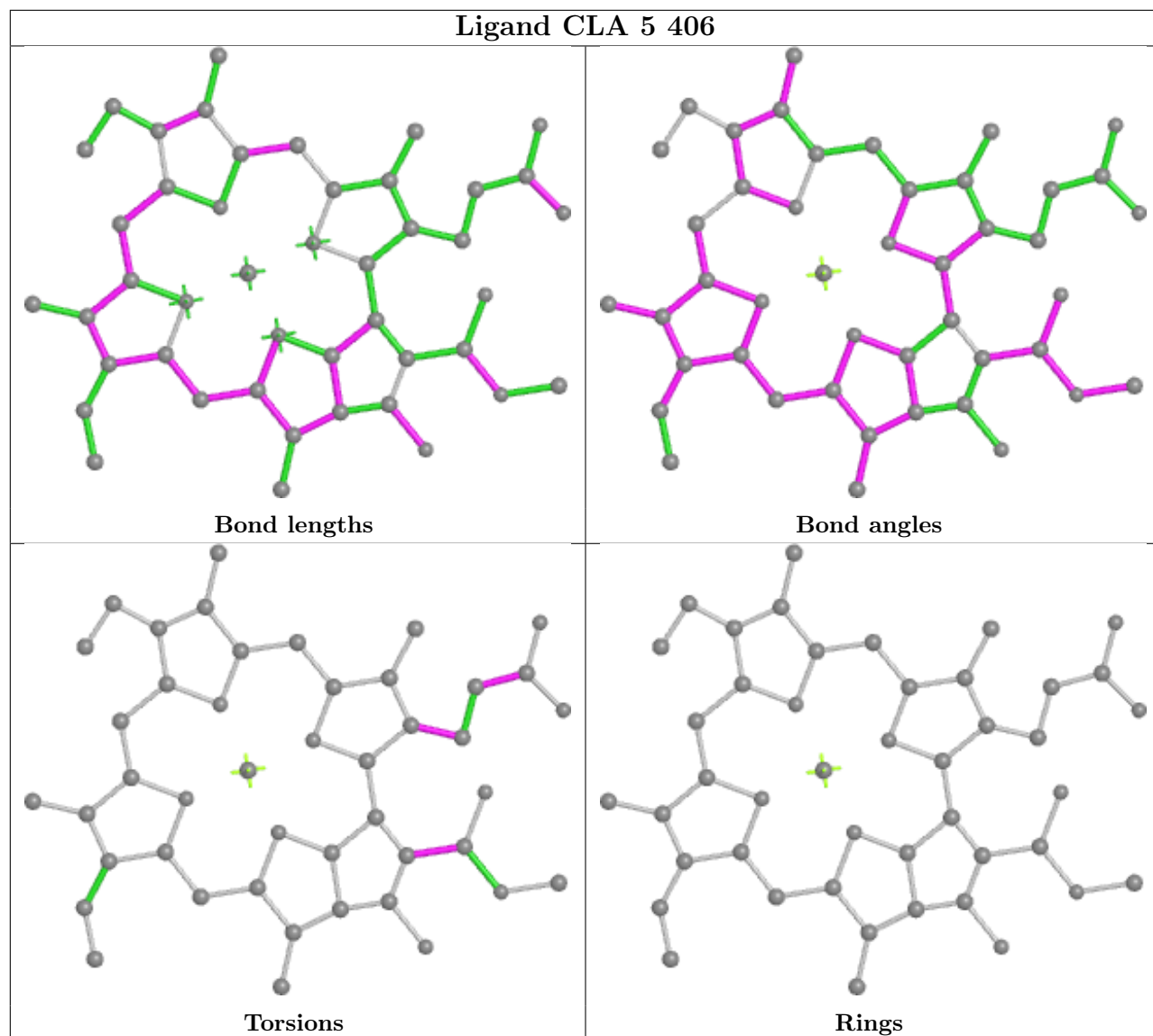


Ligand CLA X 101

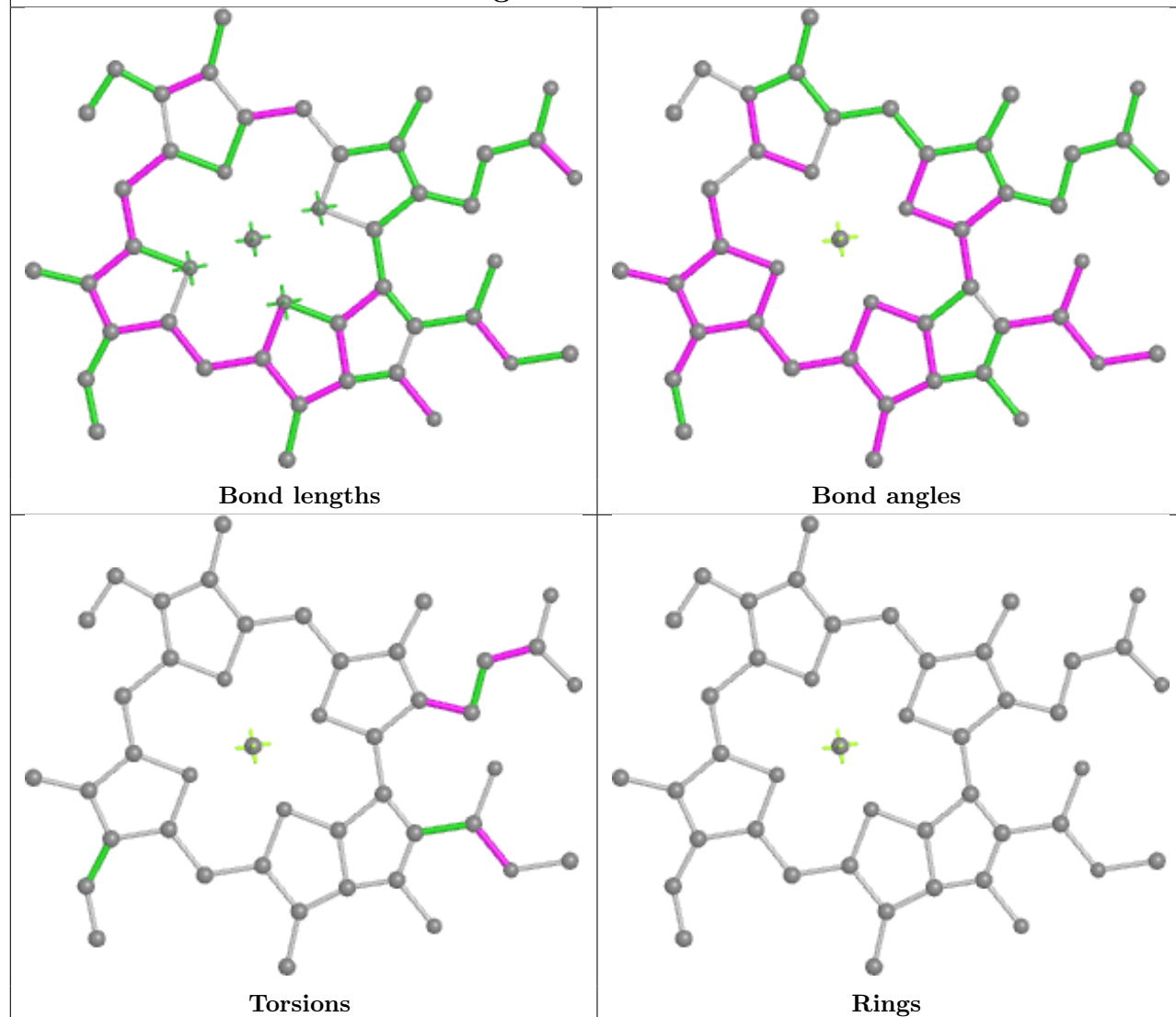




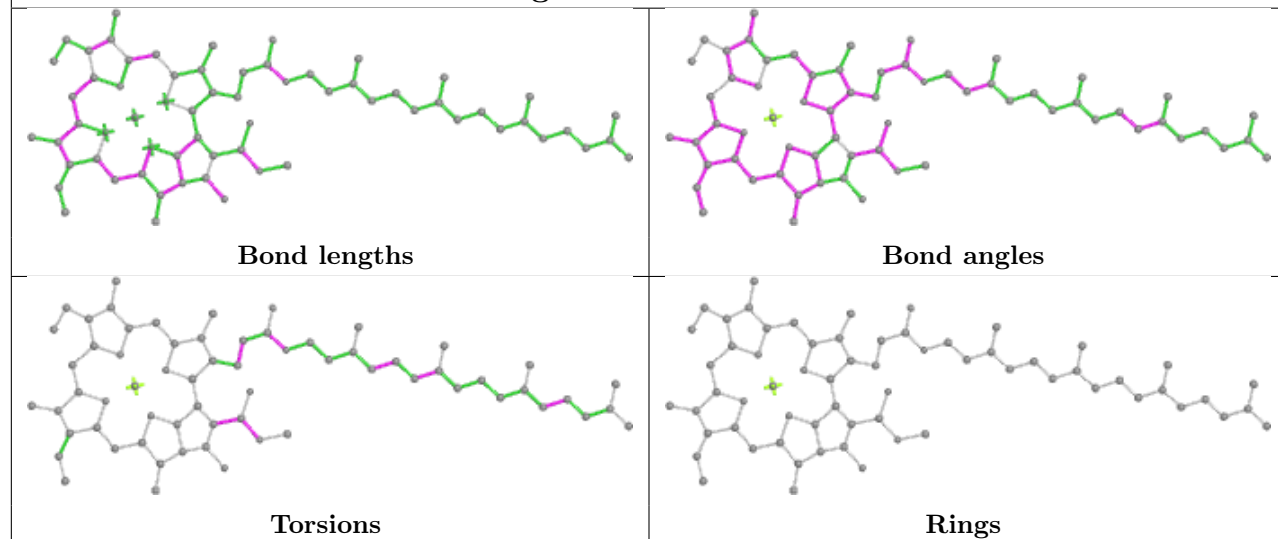
Ligand CLA 5 406



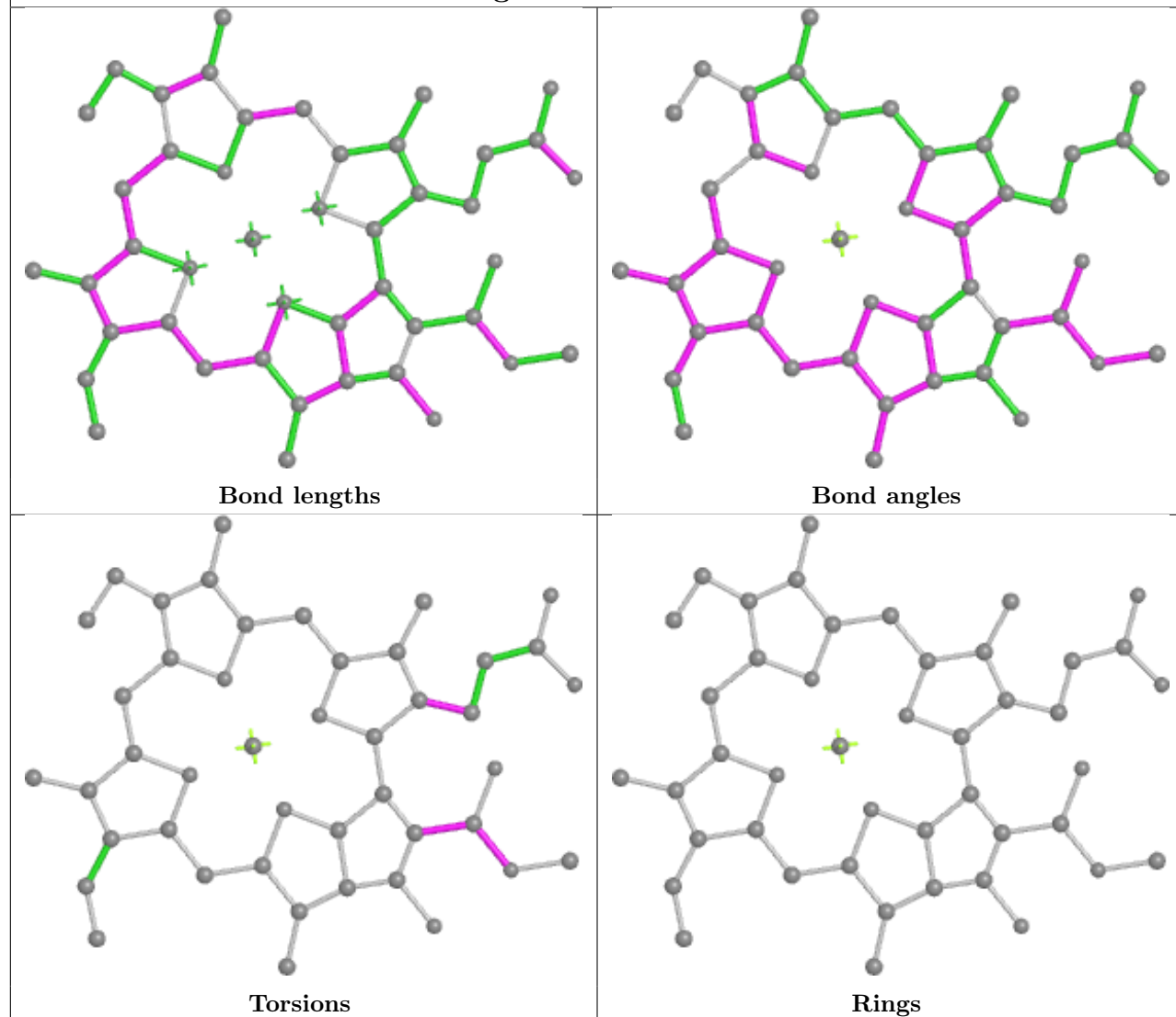
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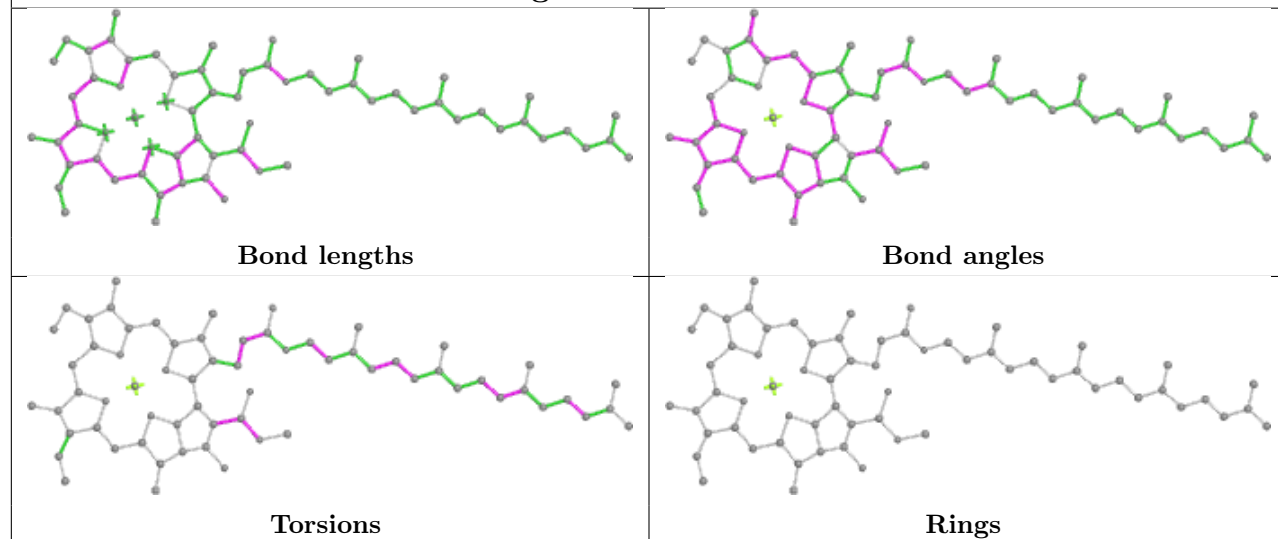
Ligand CLA A 809



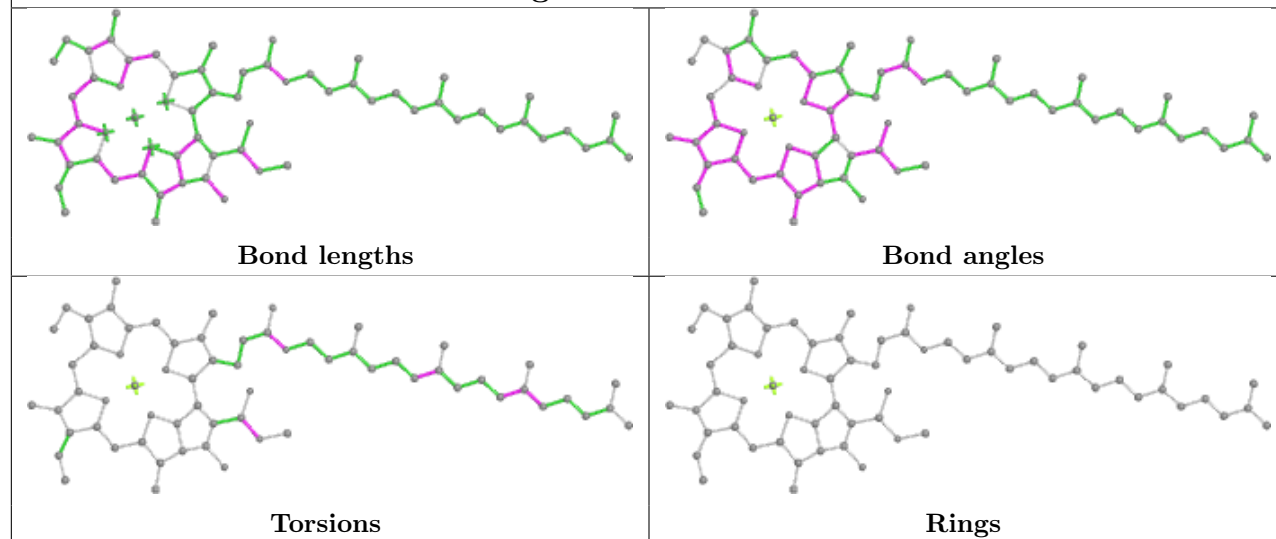
Ligand CLA 1 507



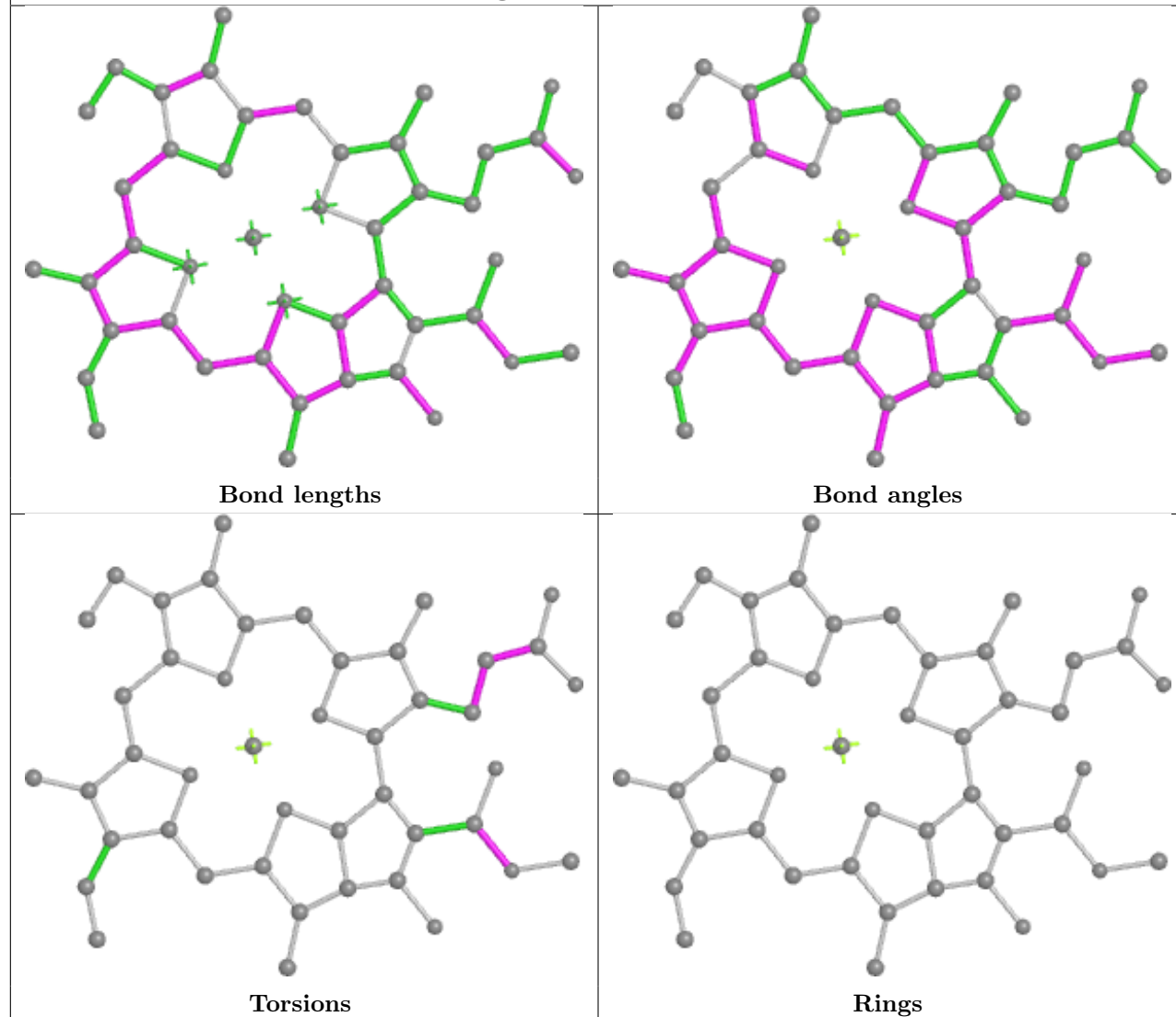
Ligand CLA A 814



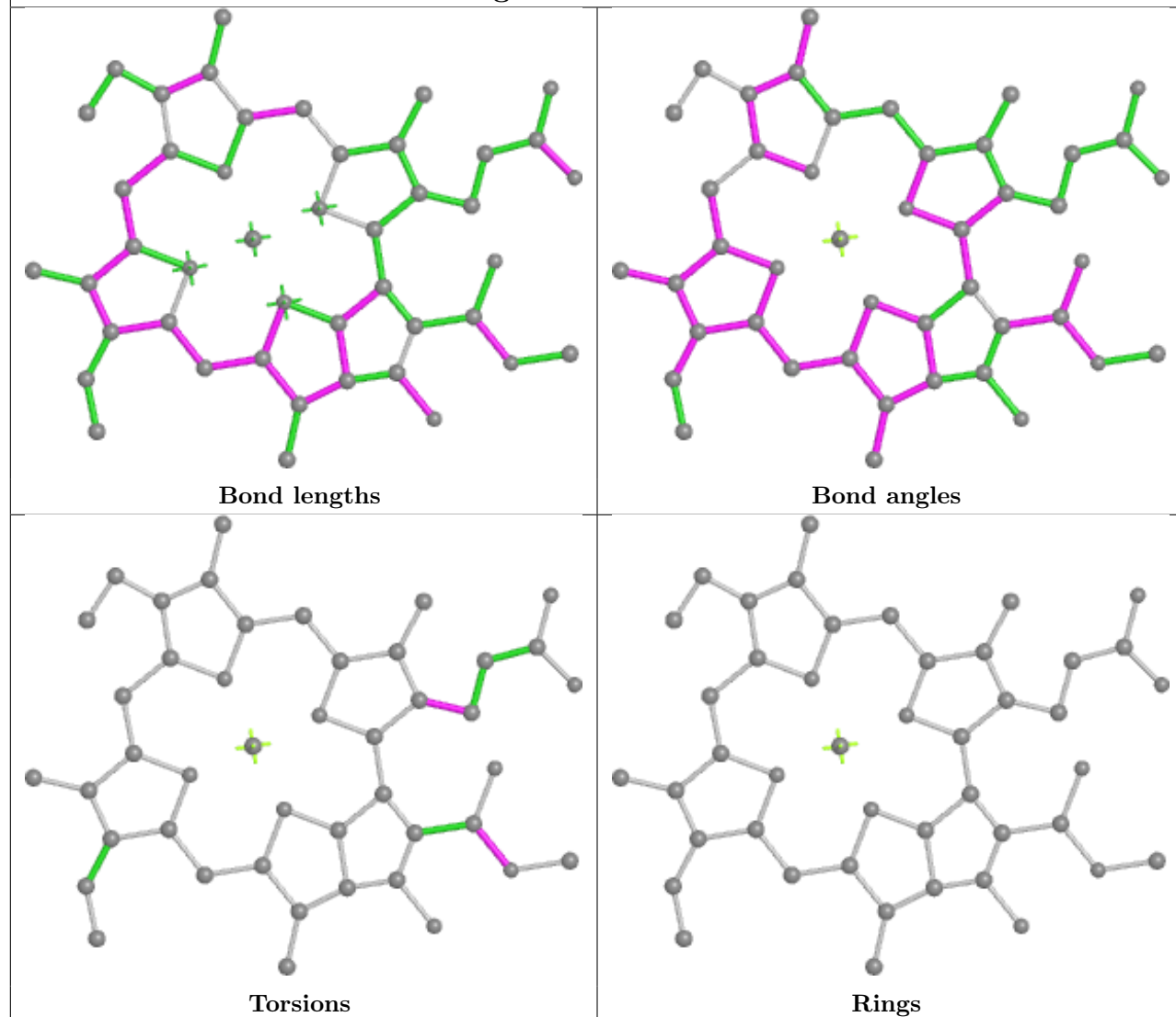
Ligand CLA A 842



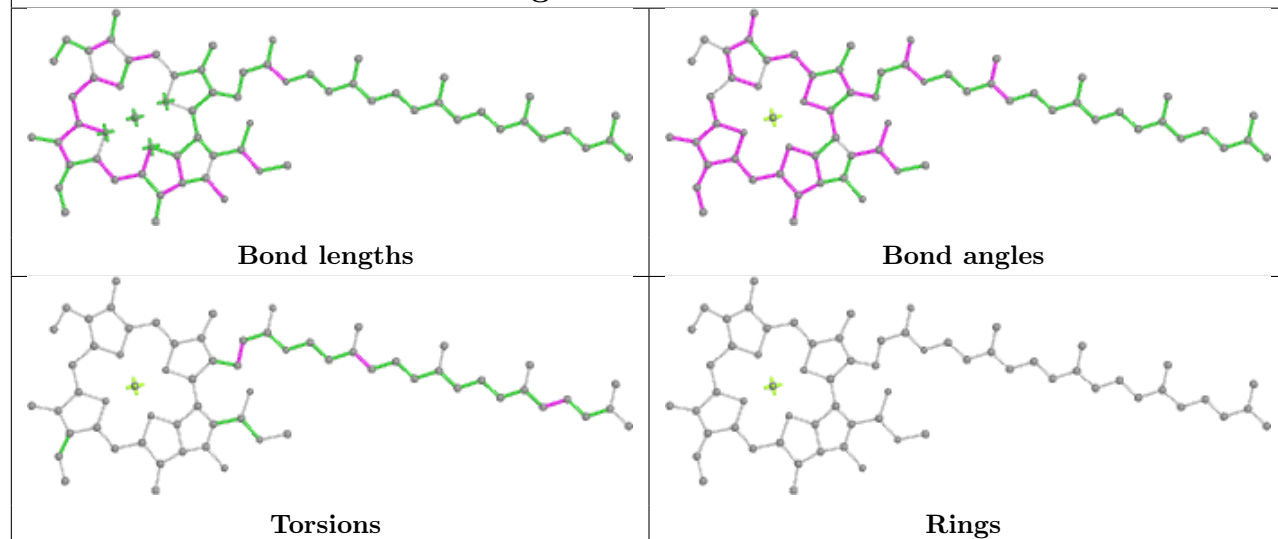
Ligand CLA 3 401



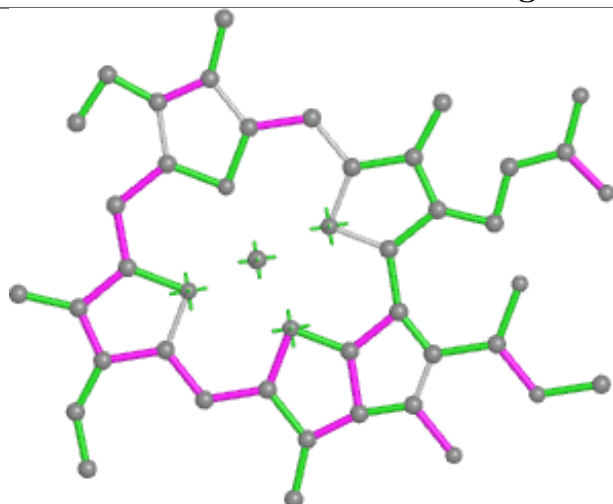
Ligand CLA 1 505



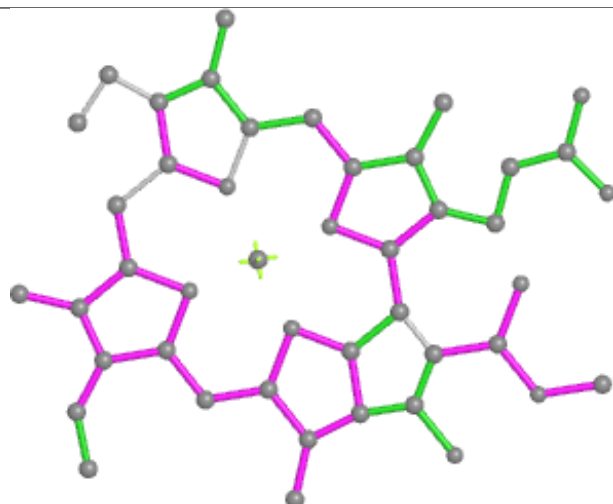
Ligand CLA A 802



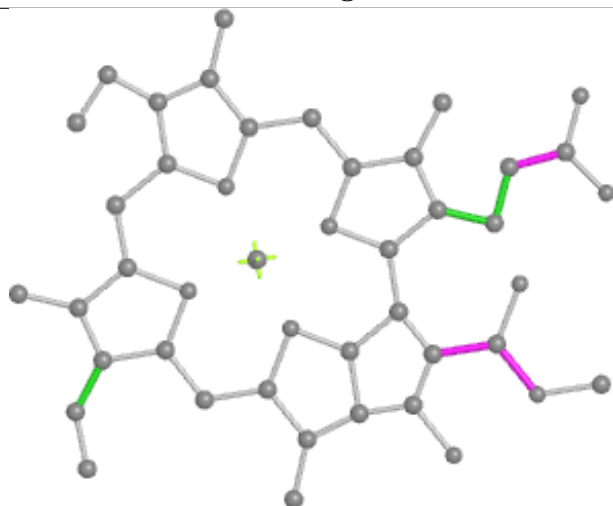
Ligand CLA 2 405



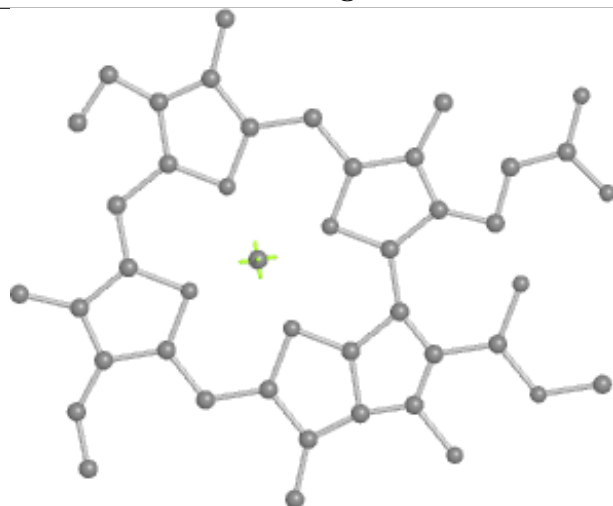
Bond lengths



Bond angles

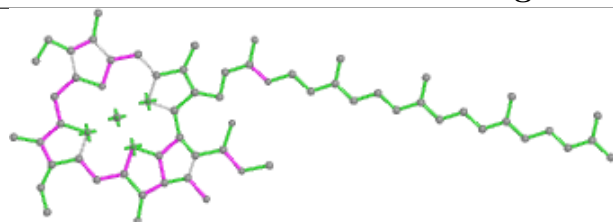


Torsions

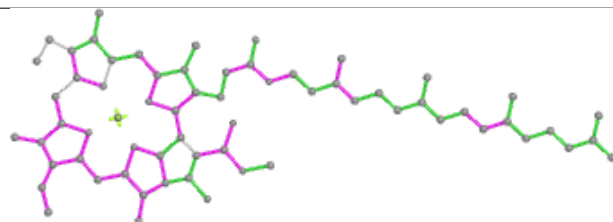


Rings

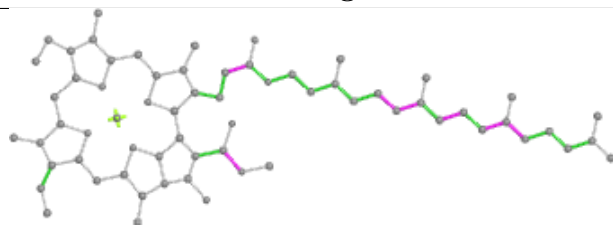
Ligand CLA B 806



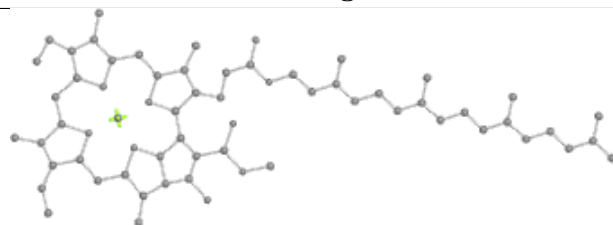
Bond lengths



Bond angles

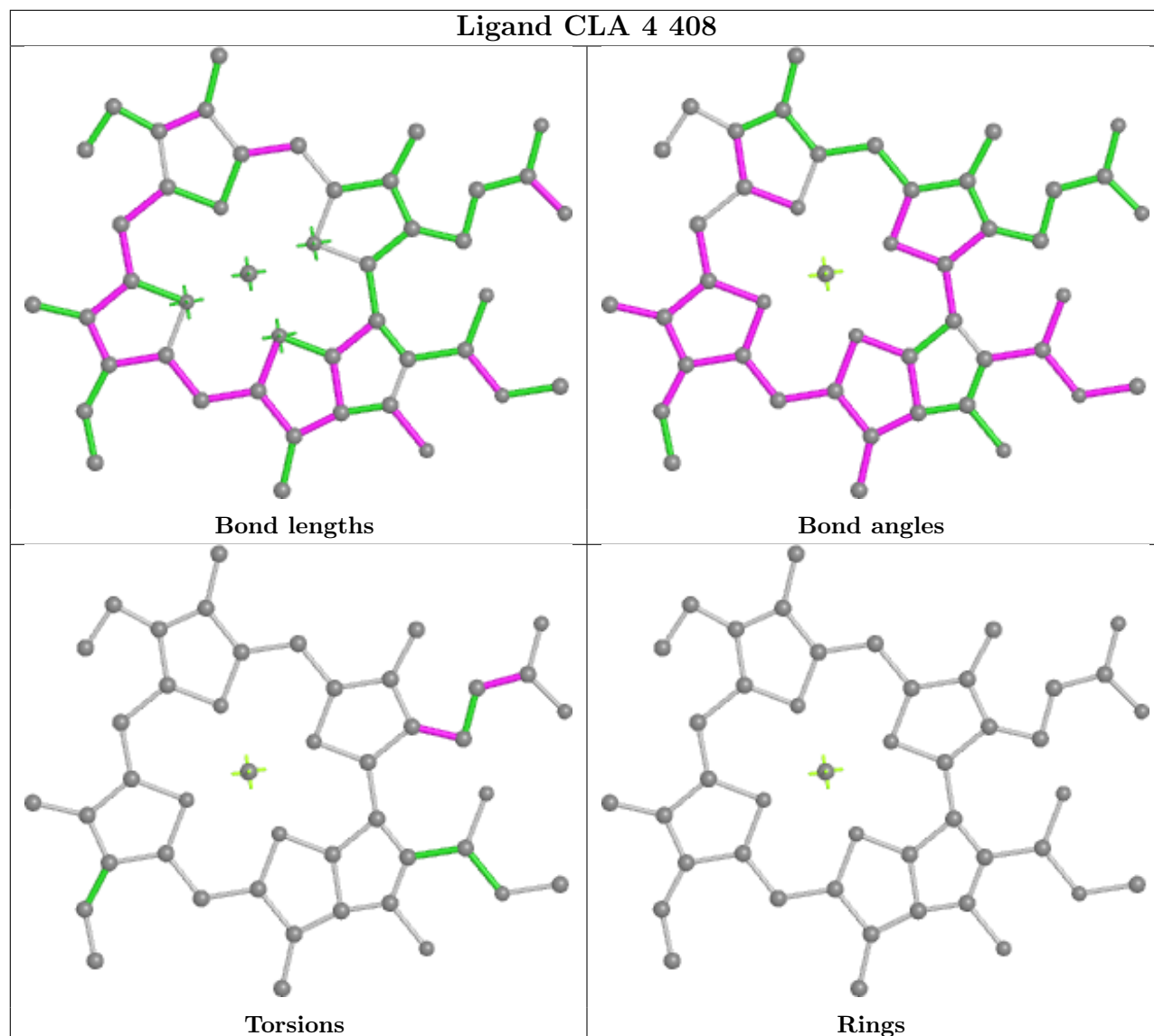


Torsions

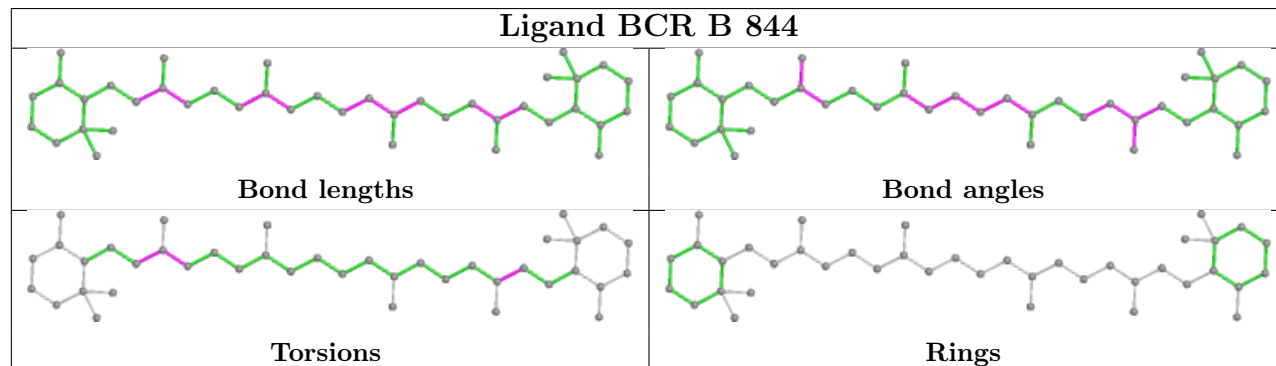


Rings

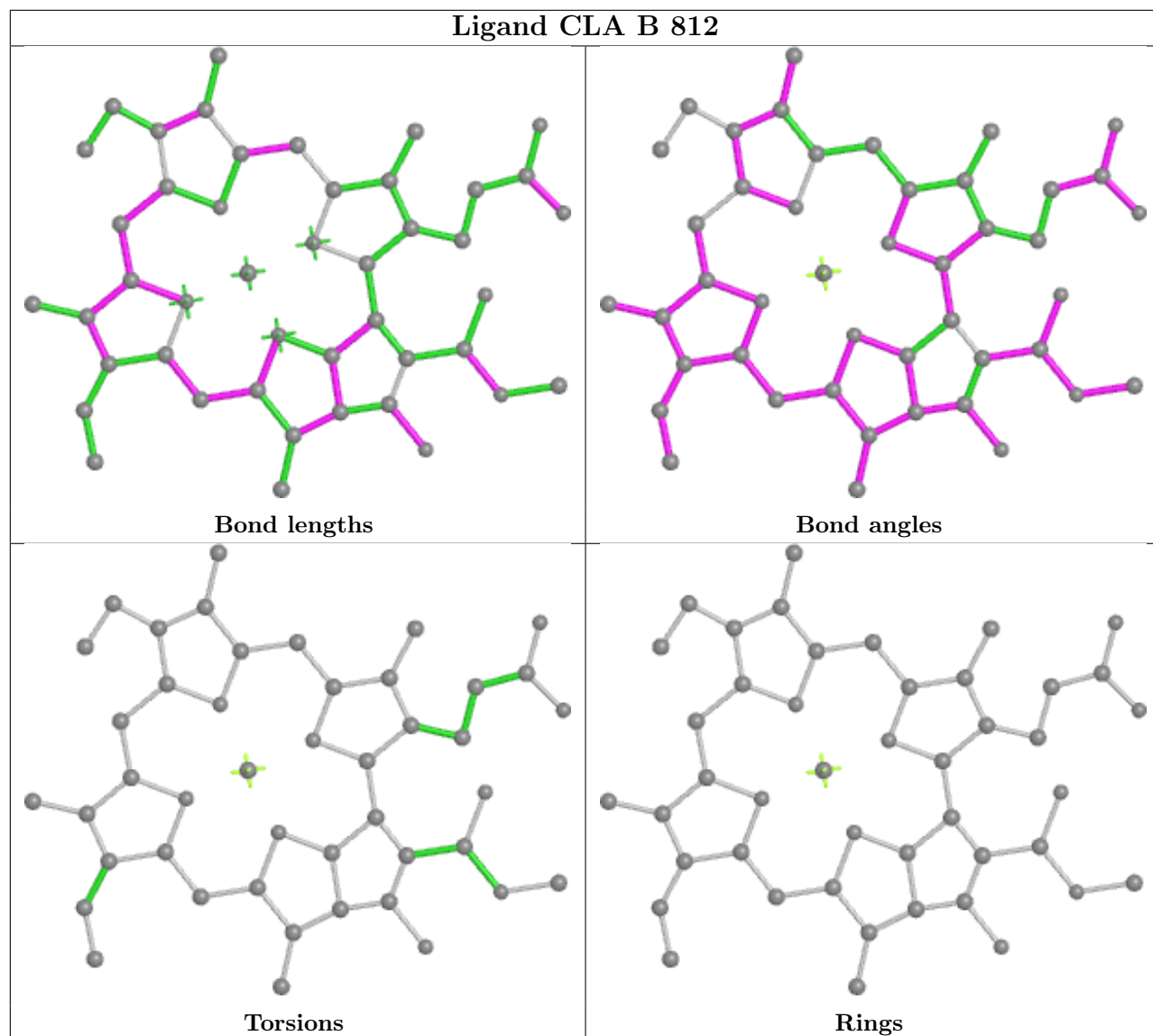
Ligand CLA 4 408

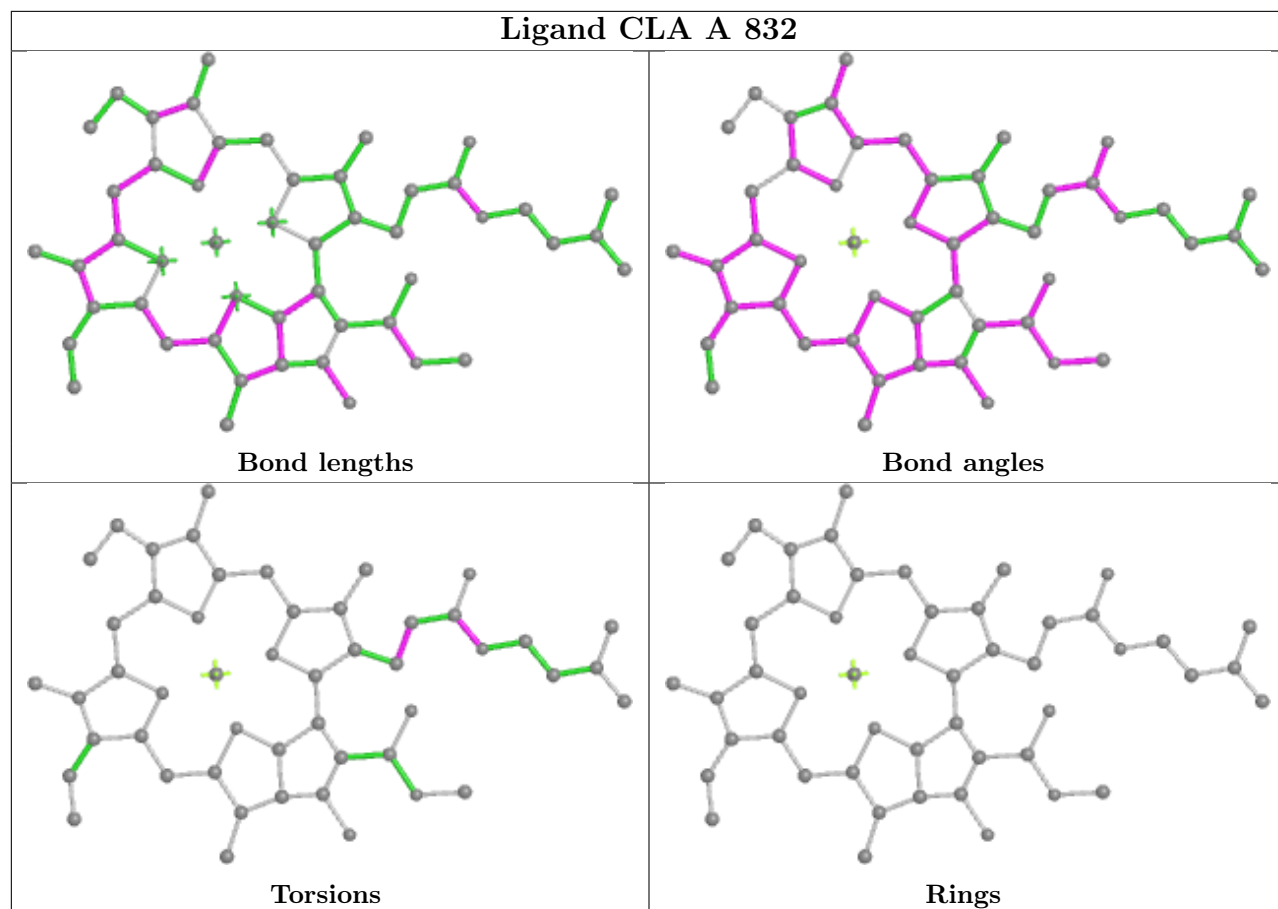


Ligand BCR B 844

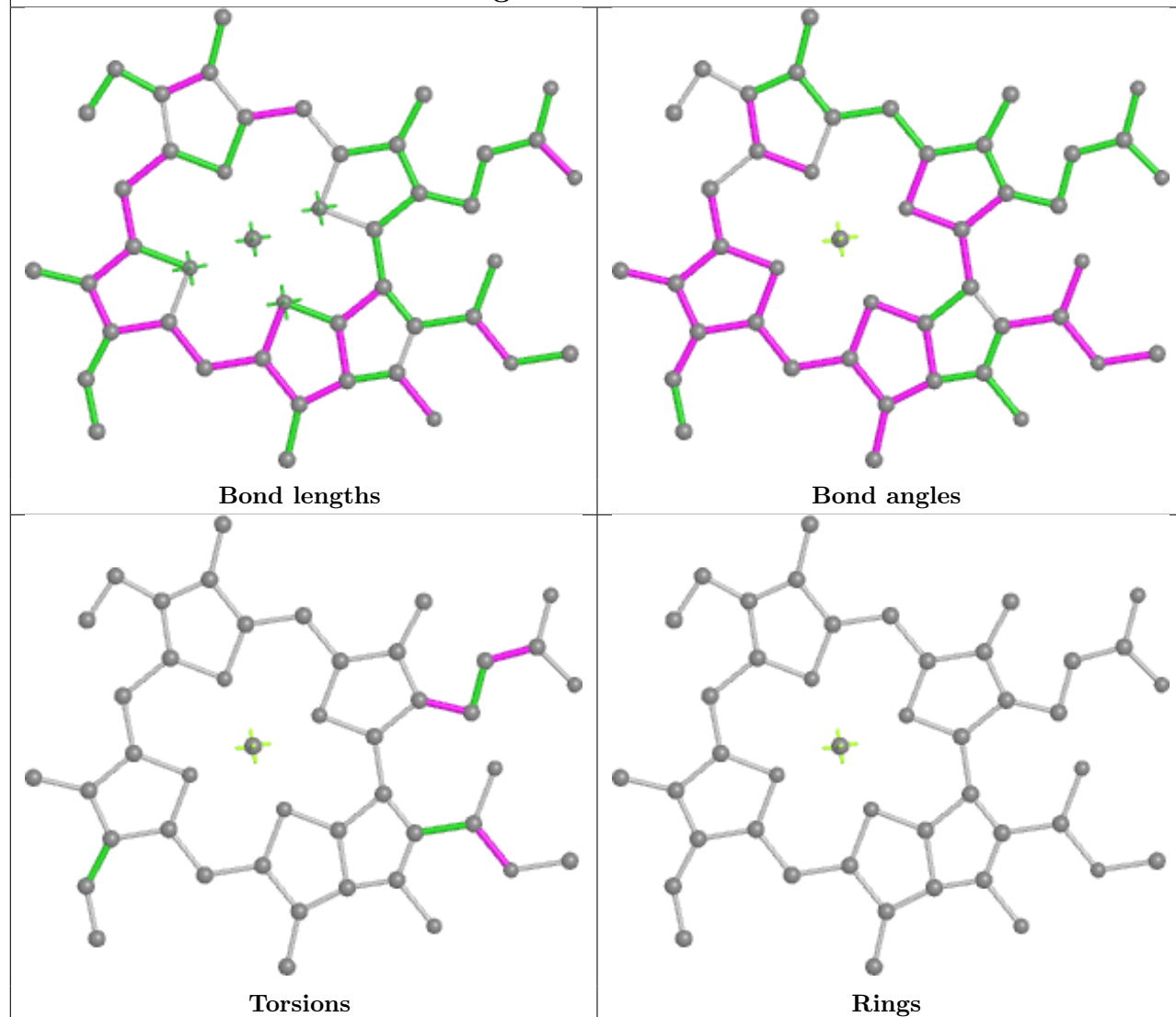


Ligand CLA B 812

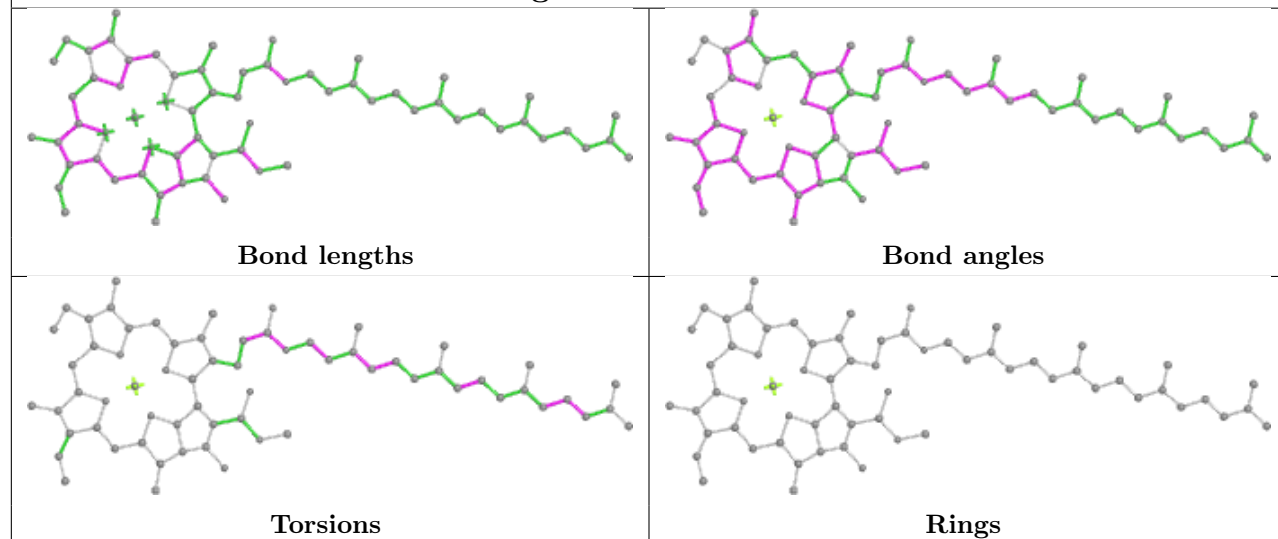




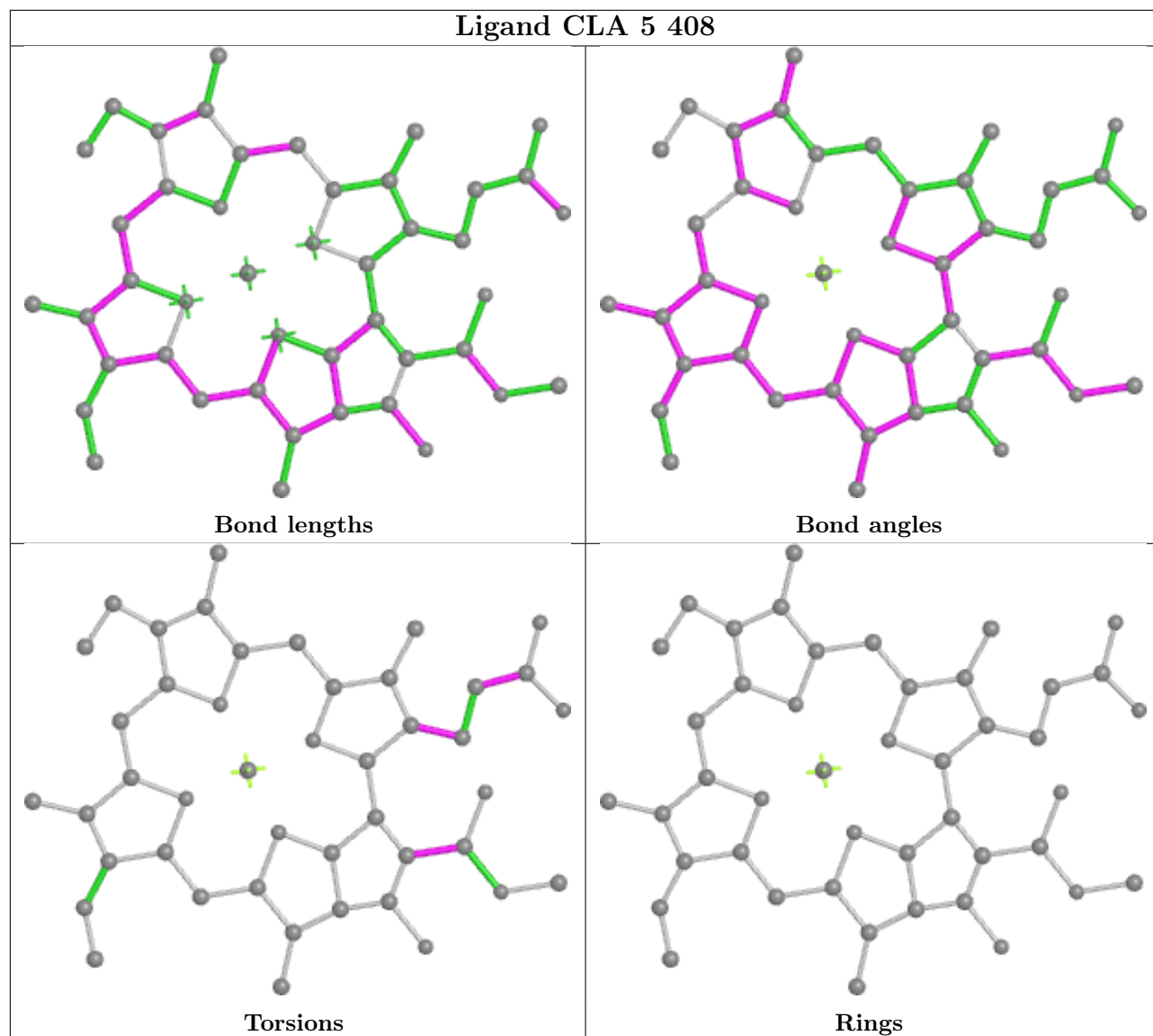
Ligand CLA 2 404



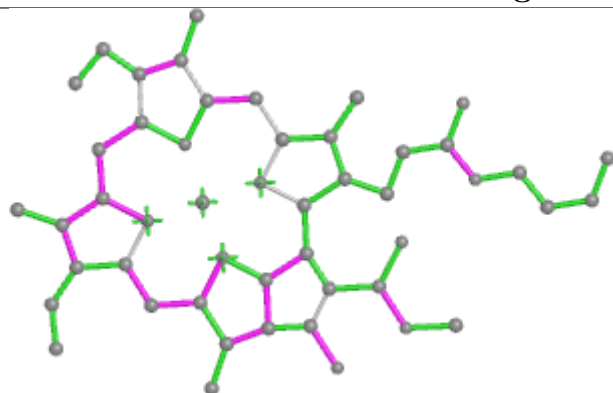
Ligand CLA A 826



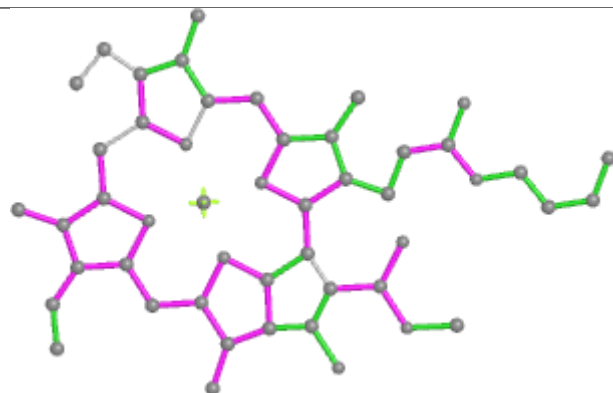
Ligand CLA 5 408



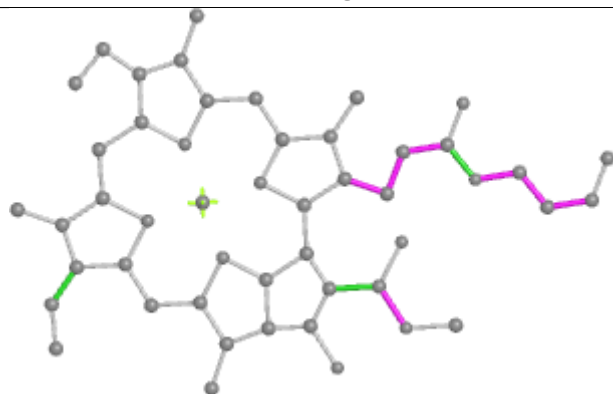
Ligand CLA A 823



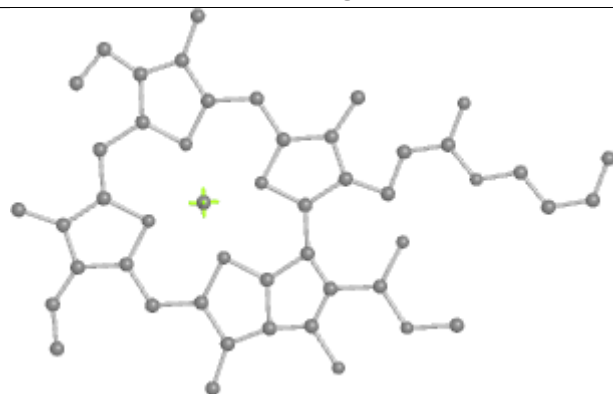
Bond lengths



Bond angles

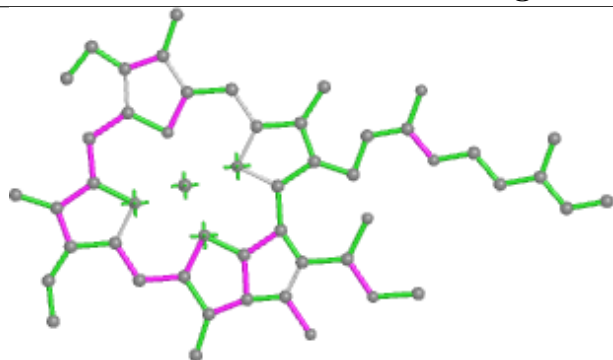


Torsions

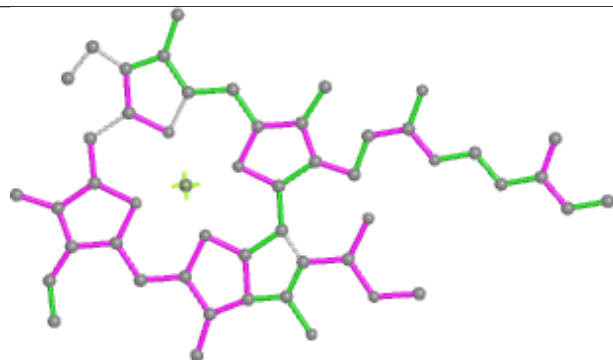


Rings

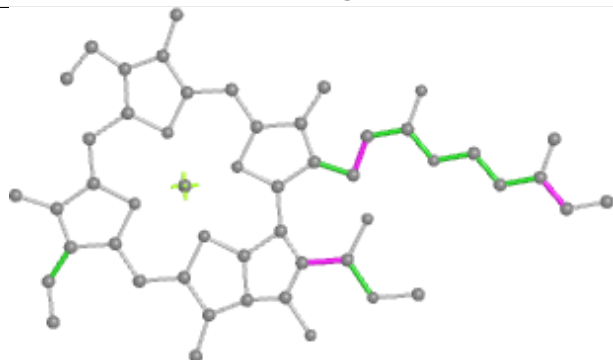
Ligand CLA A 808



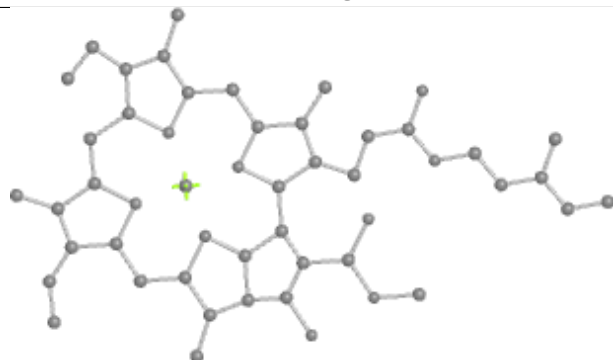
Bond lengths



Bond angles

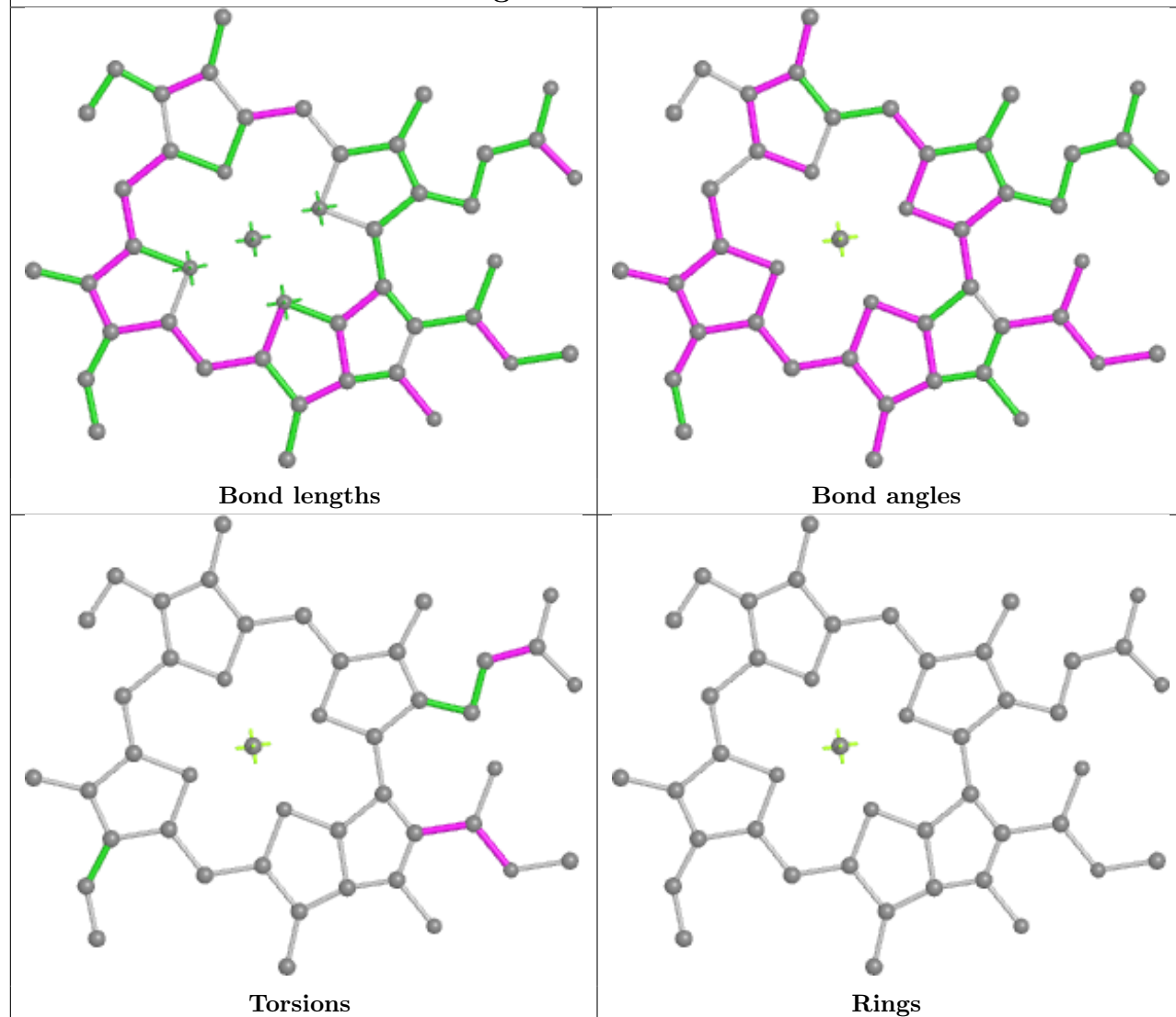


Torsions

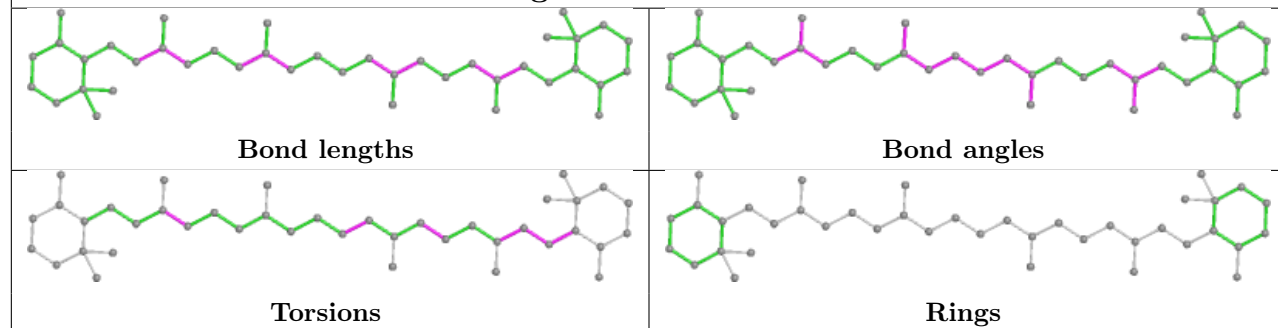


Rings

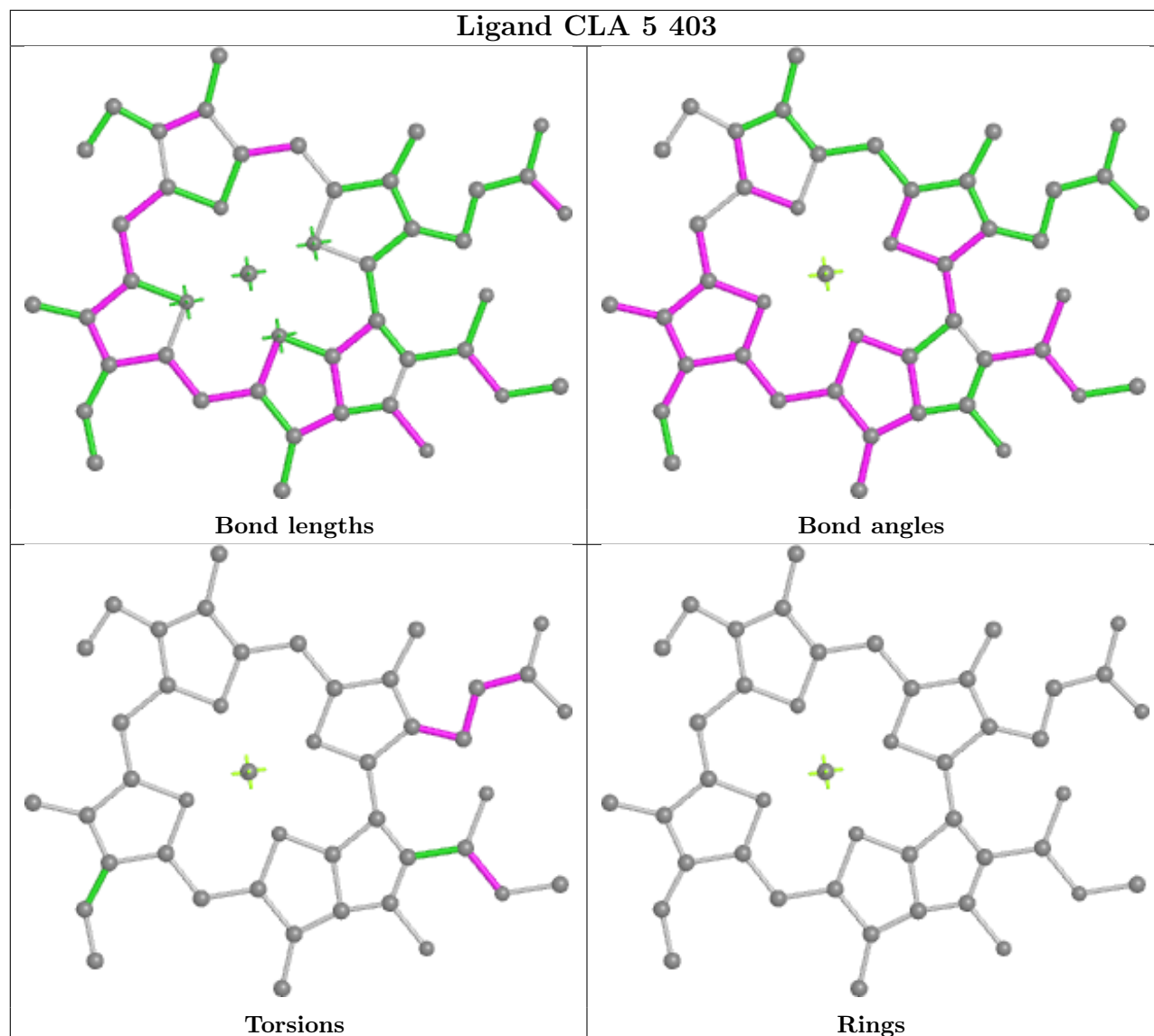
Ligand CLA 4 407



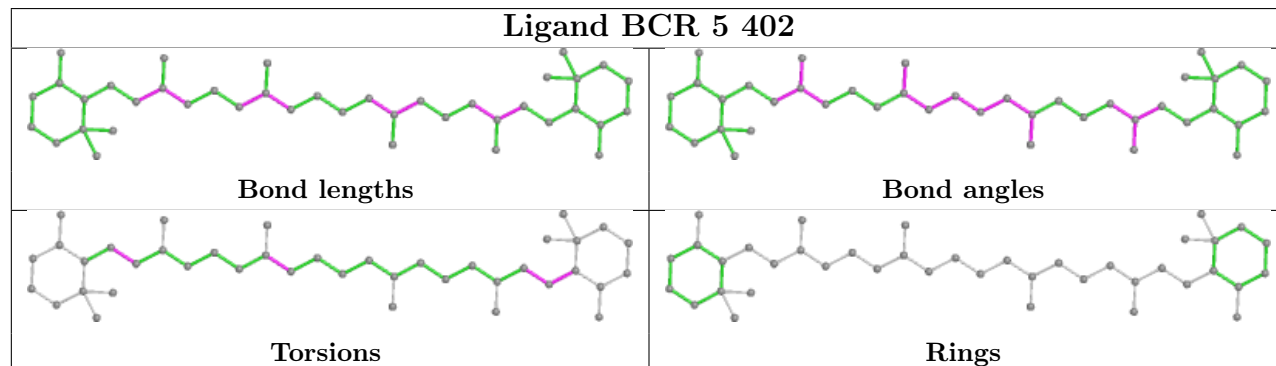
Ligand BCR B 843

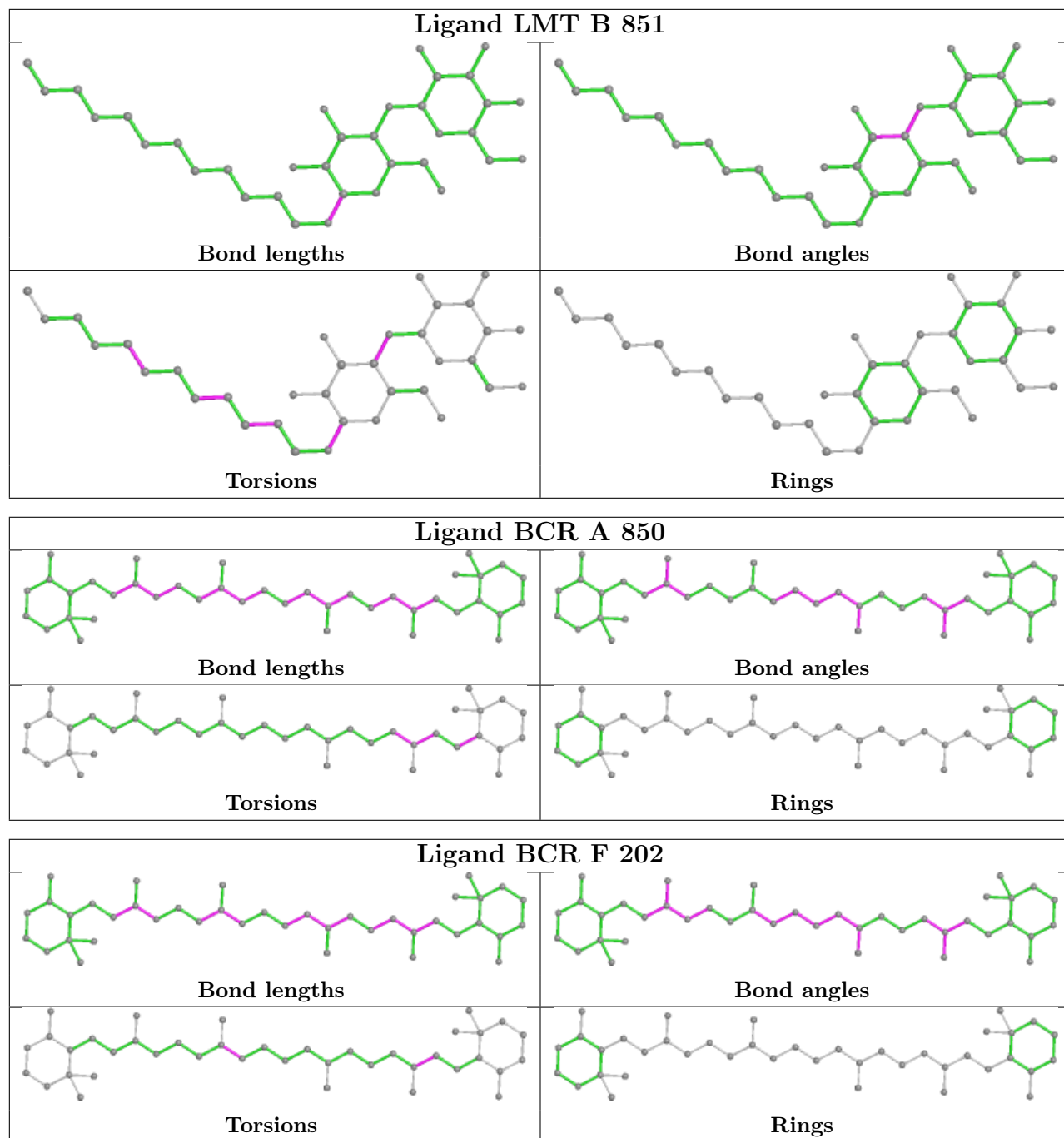


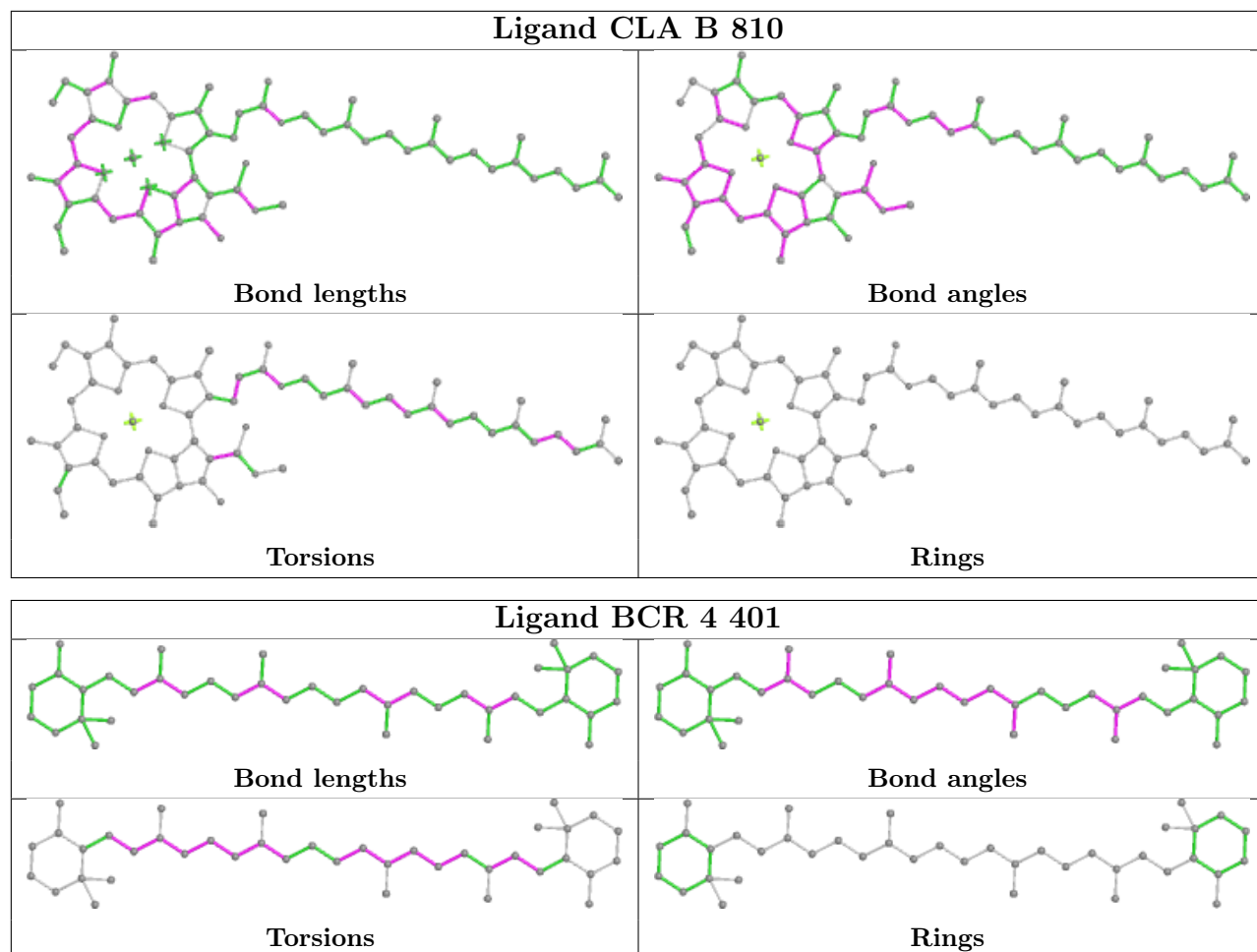
Ligand CLA 5 403



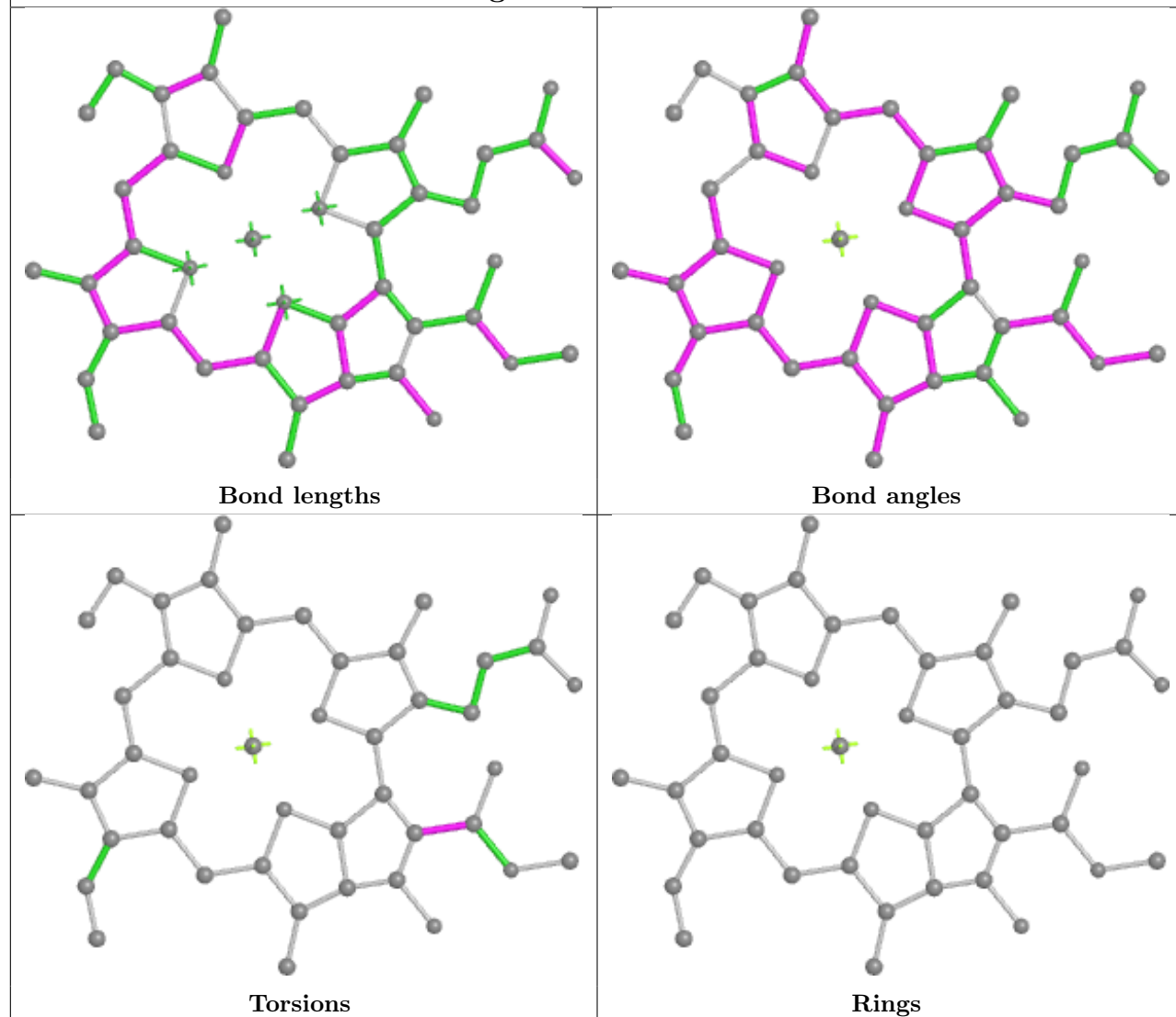
Ligand BCR 5 402



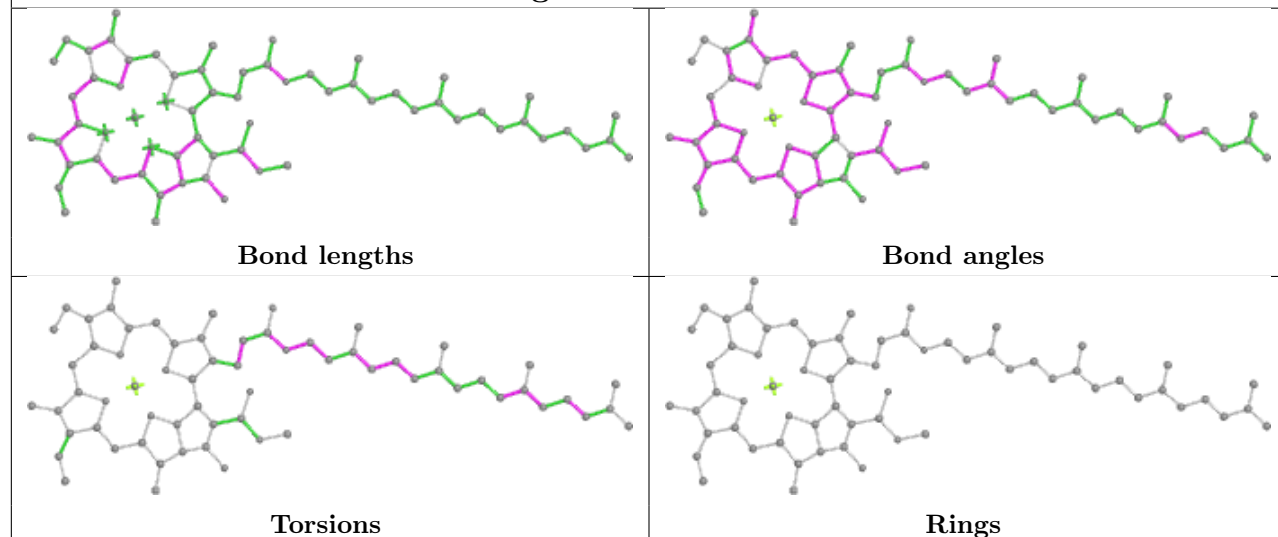


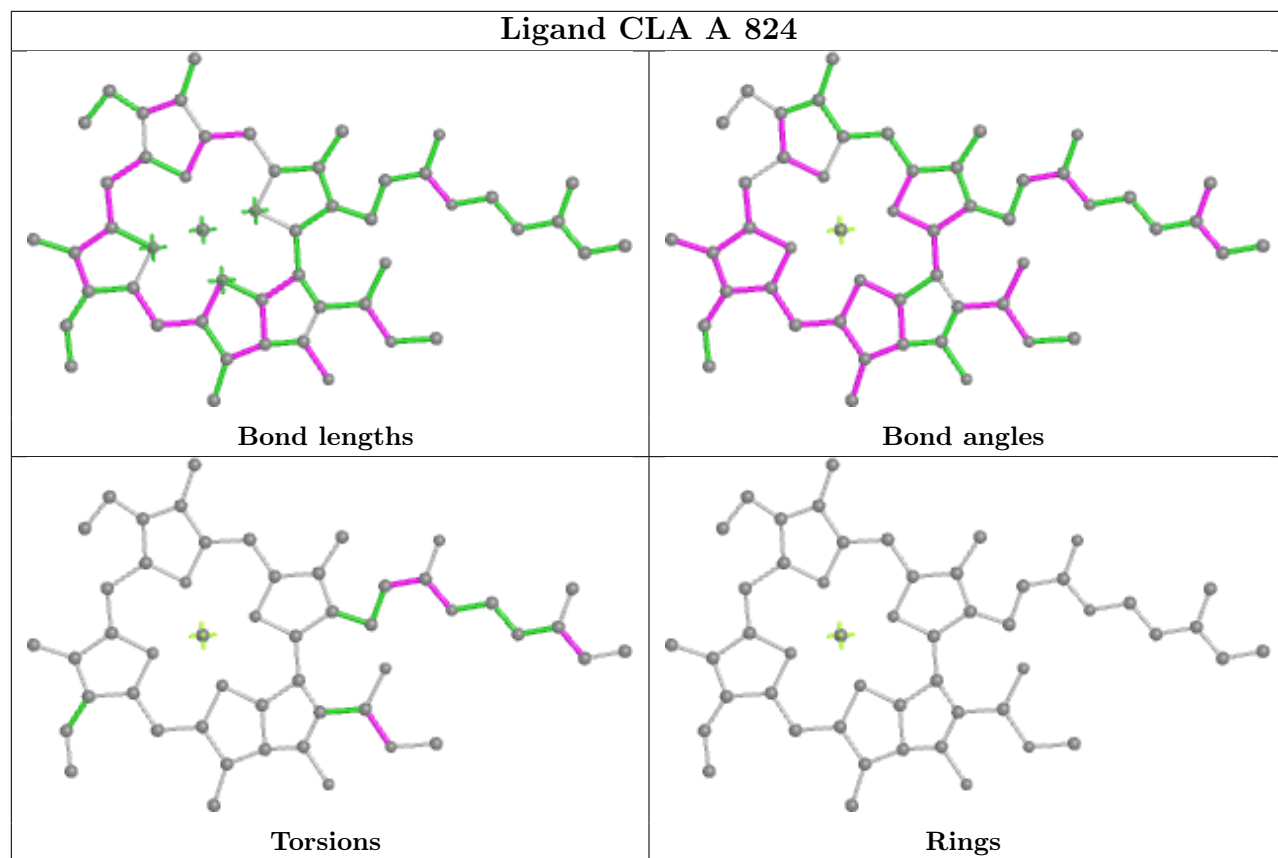


Ligand CLA A 811

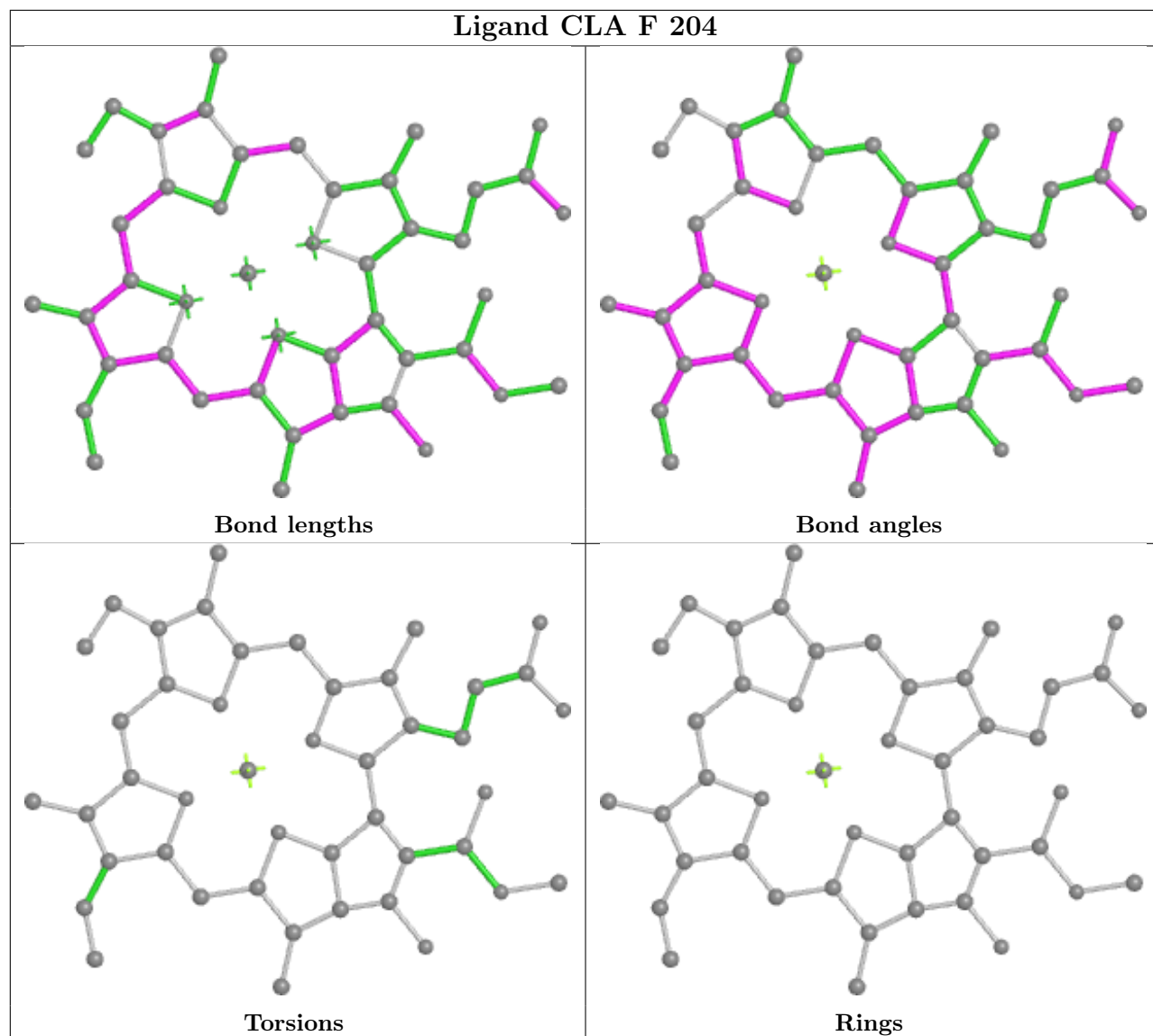


Ligand CLA A 829

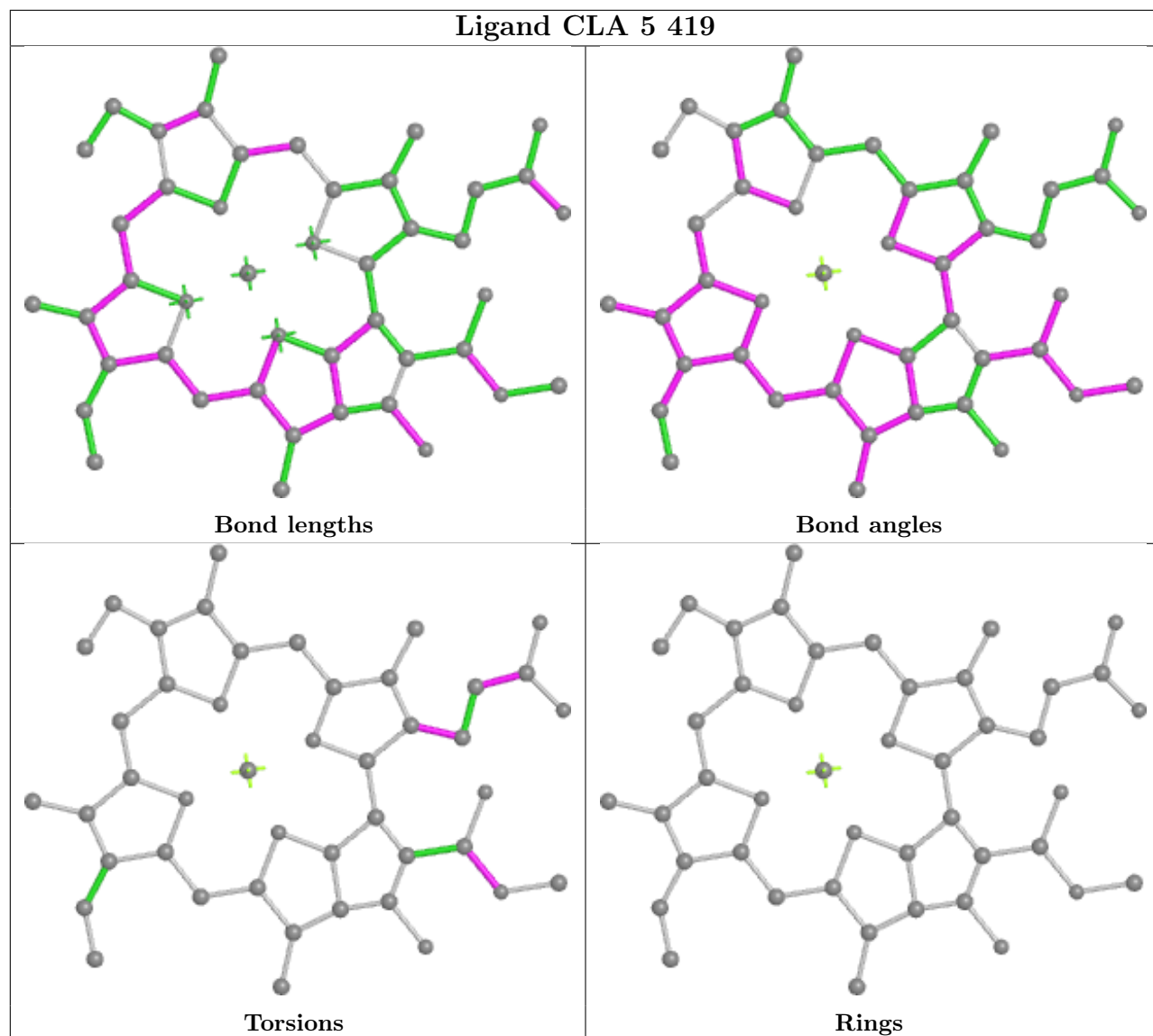




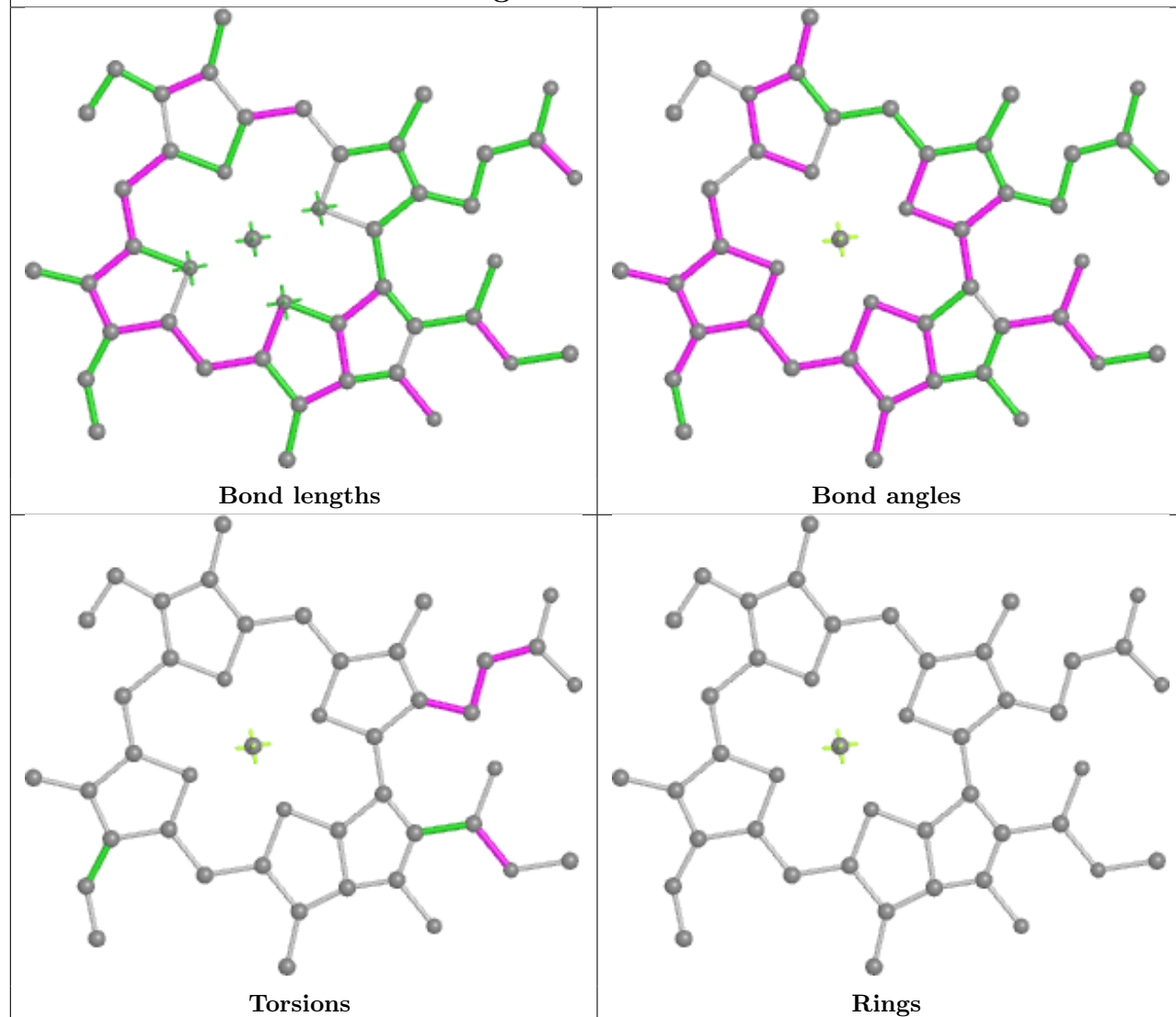
Ligand CLA F 204



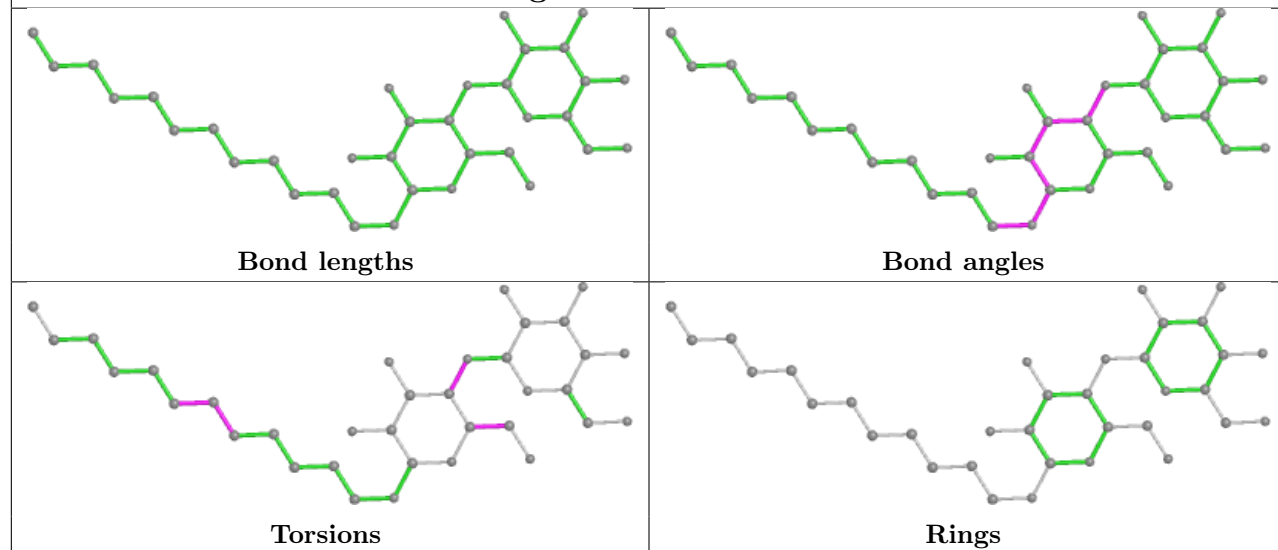
Ligand CLA 5 419



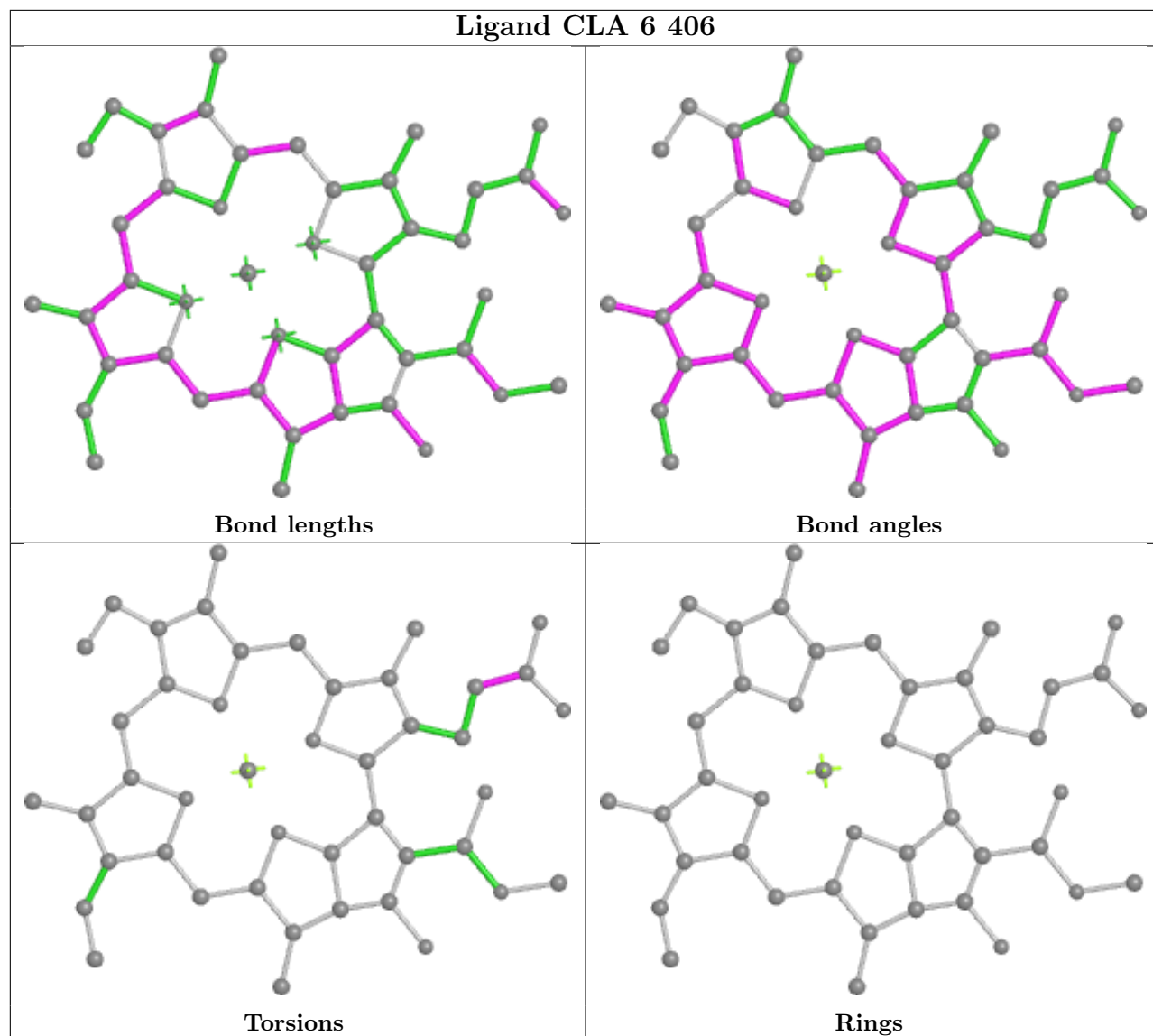
Ligand CLA 1 502



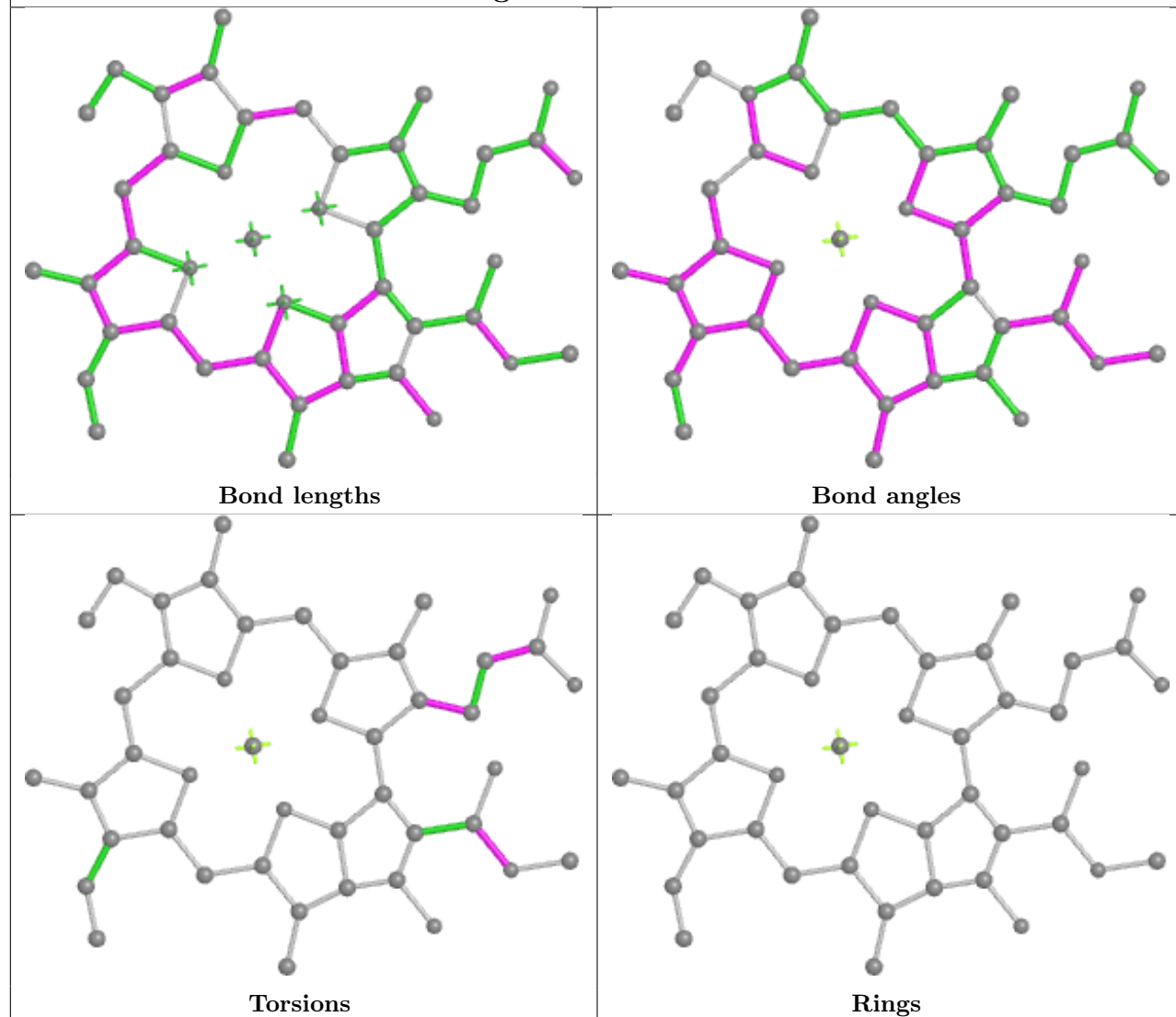
Ligand LMT B 852



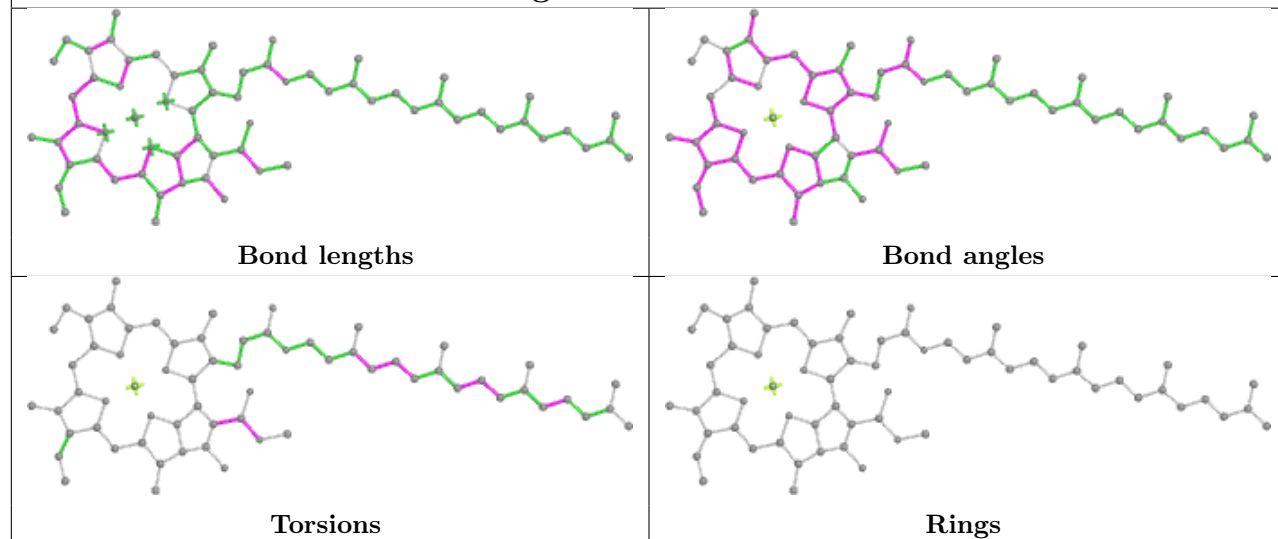
Ligand CLA 6 406



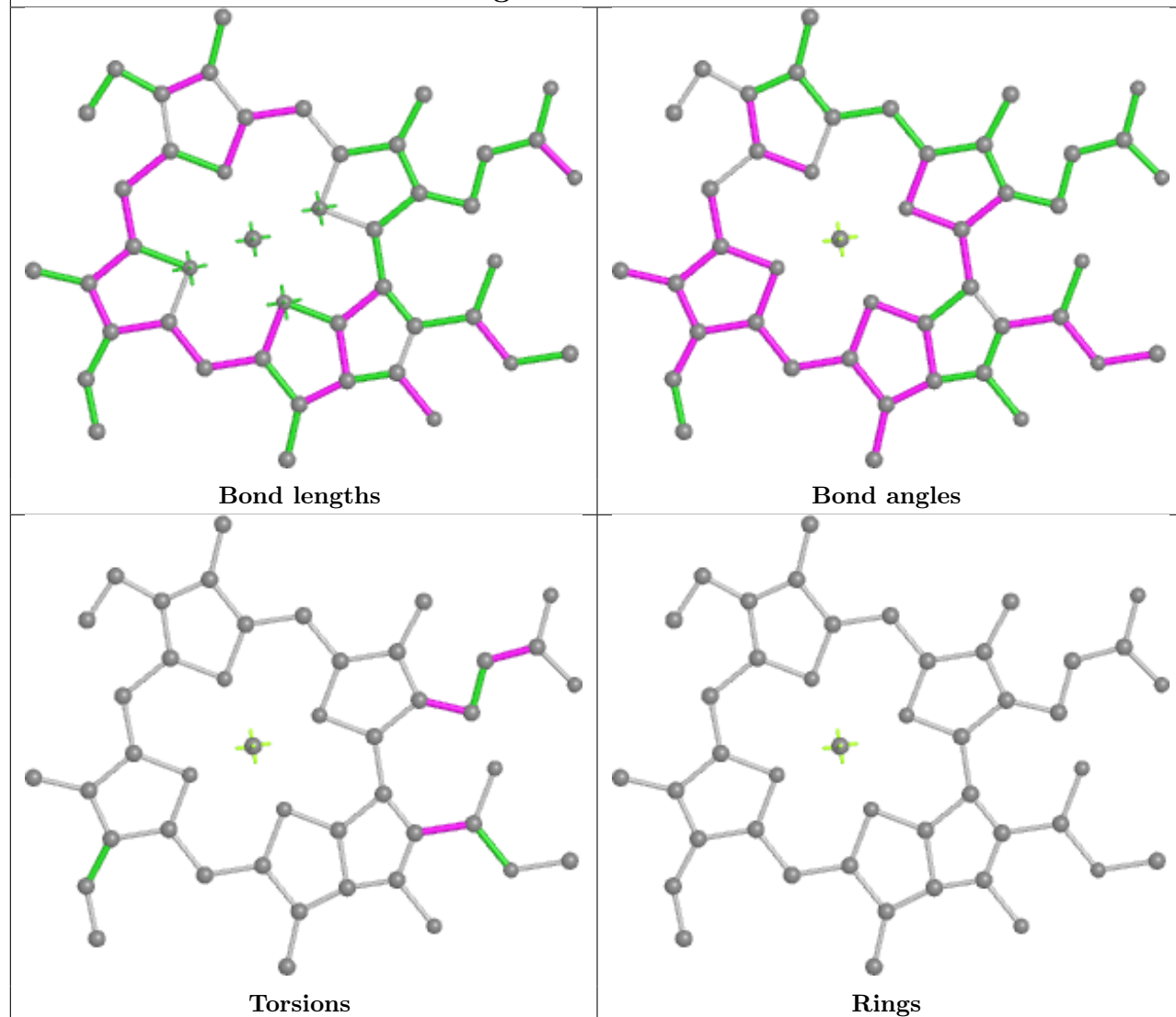
Ligand CLA 6 407



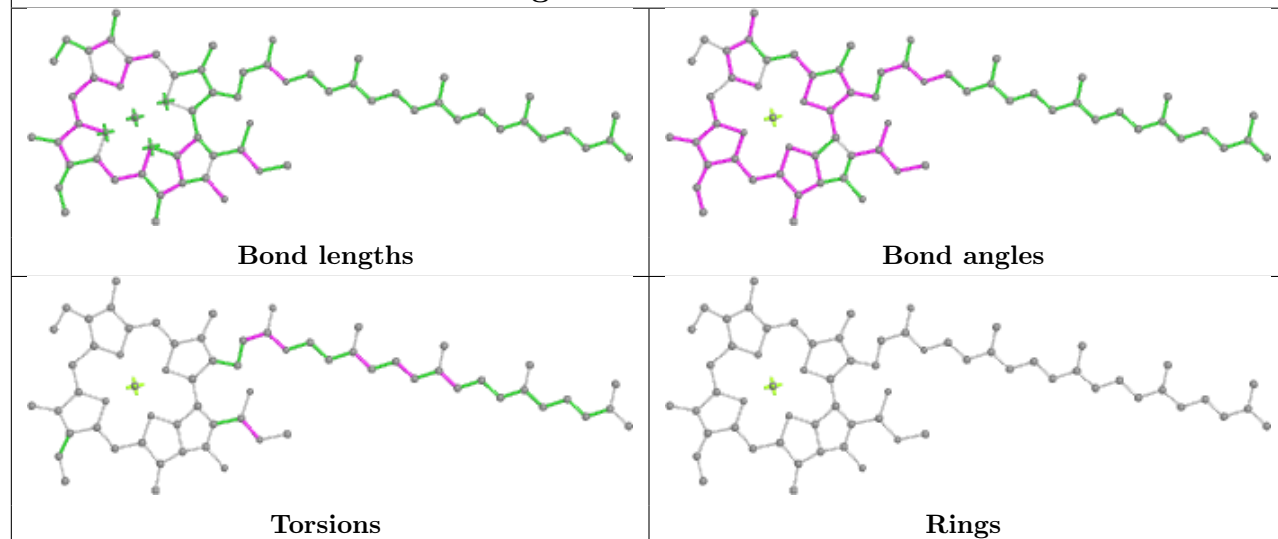
Ligand CLA B 808



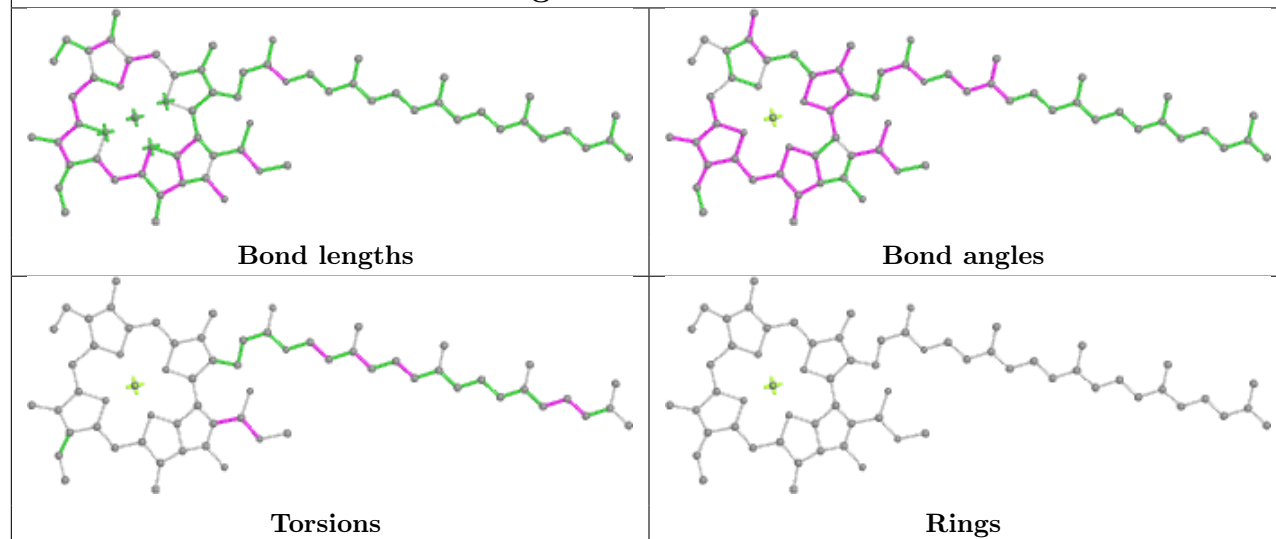
Ligand CLA 5 404



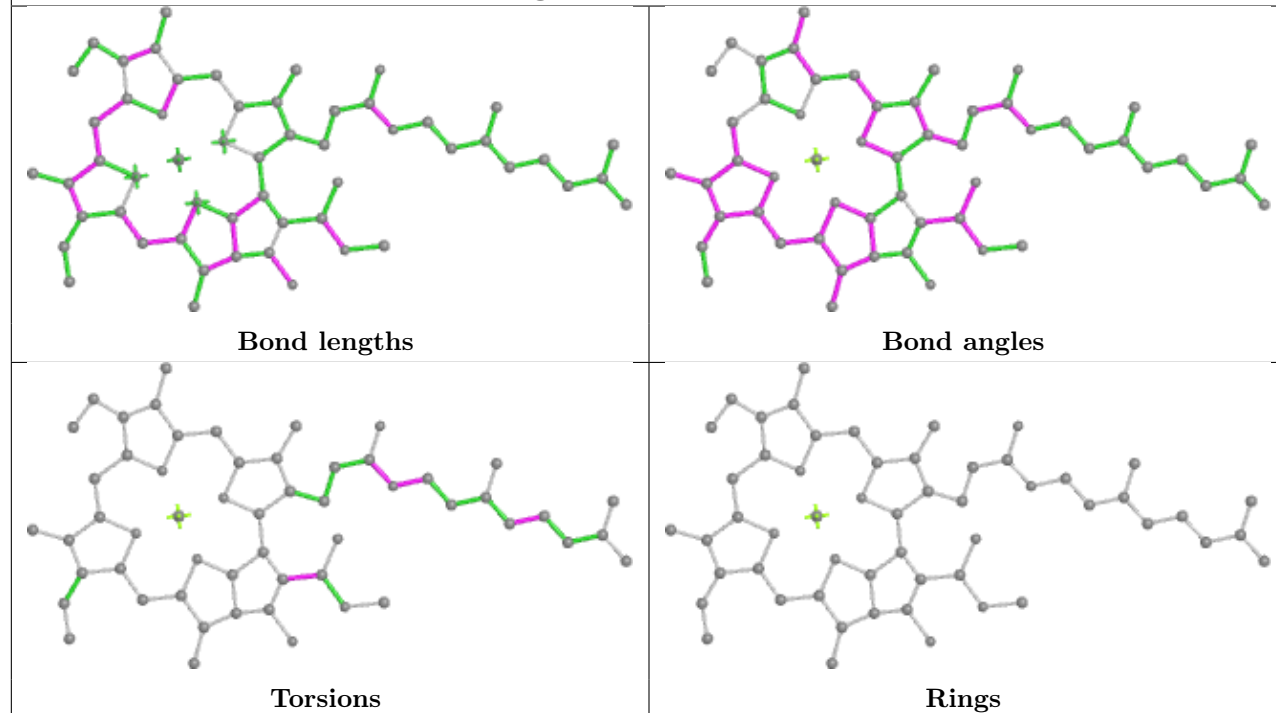
Ligand CLA A 833



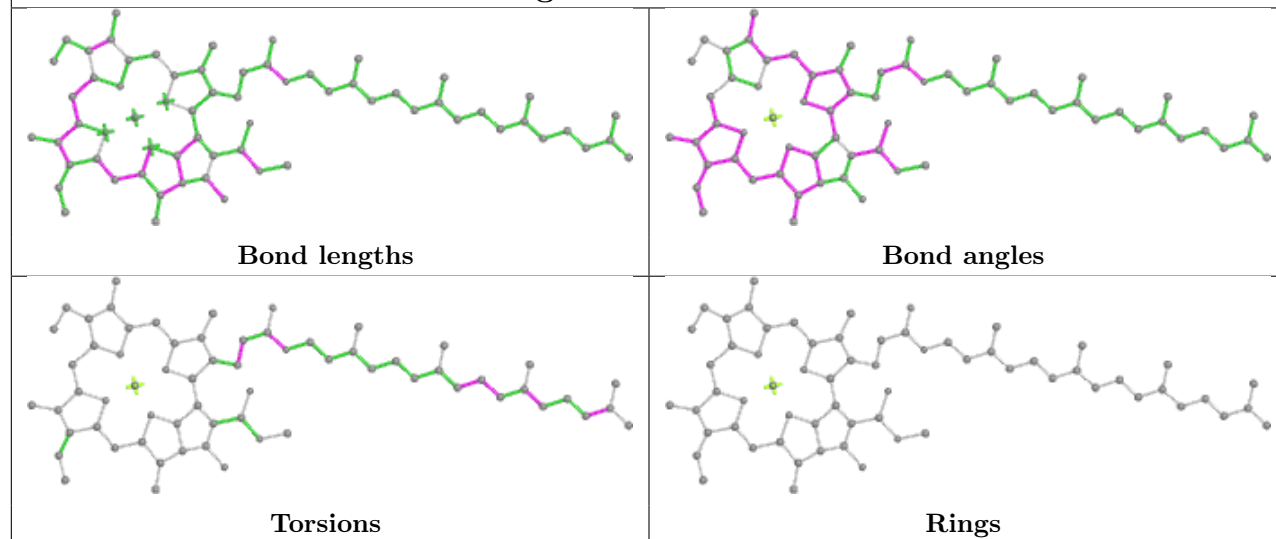
Ligand CLA B 824



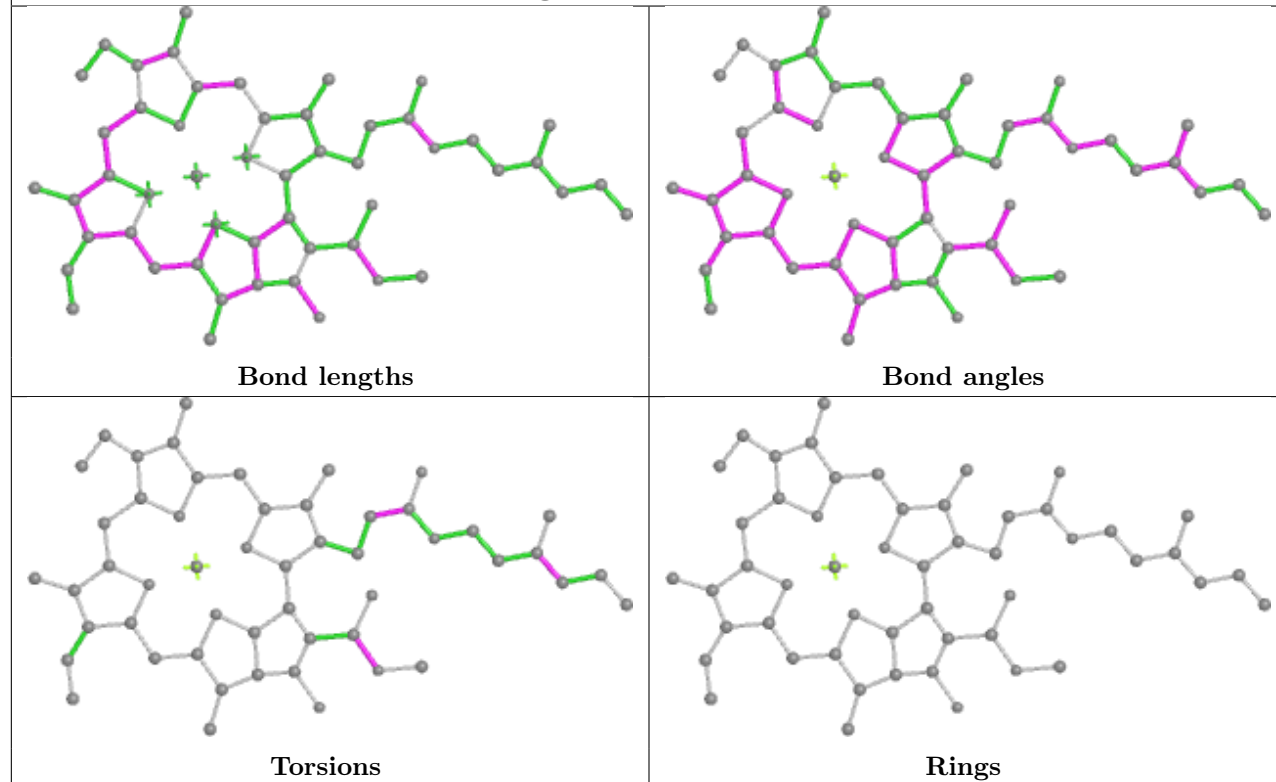
Ligand CLA A 827



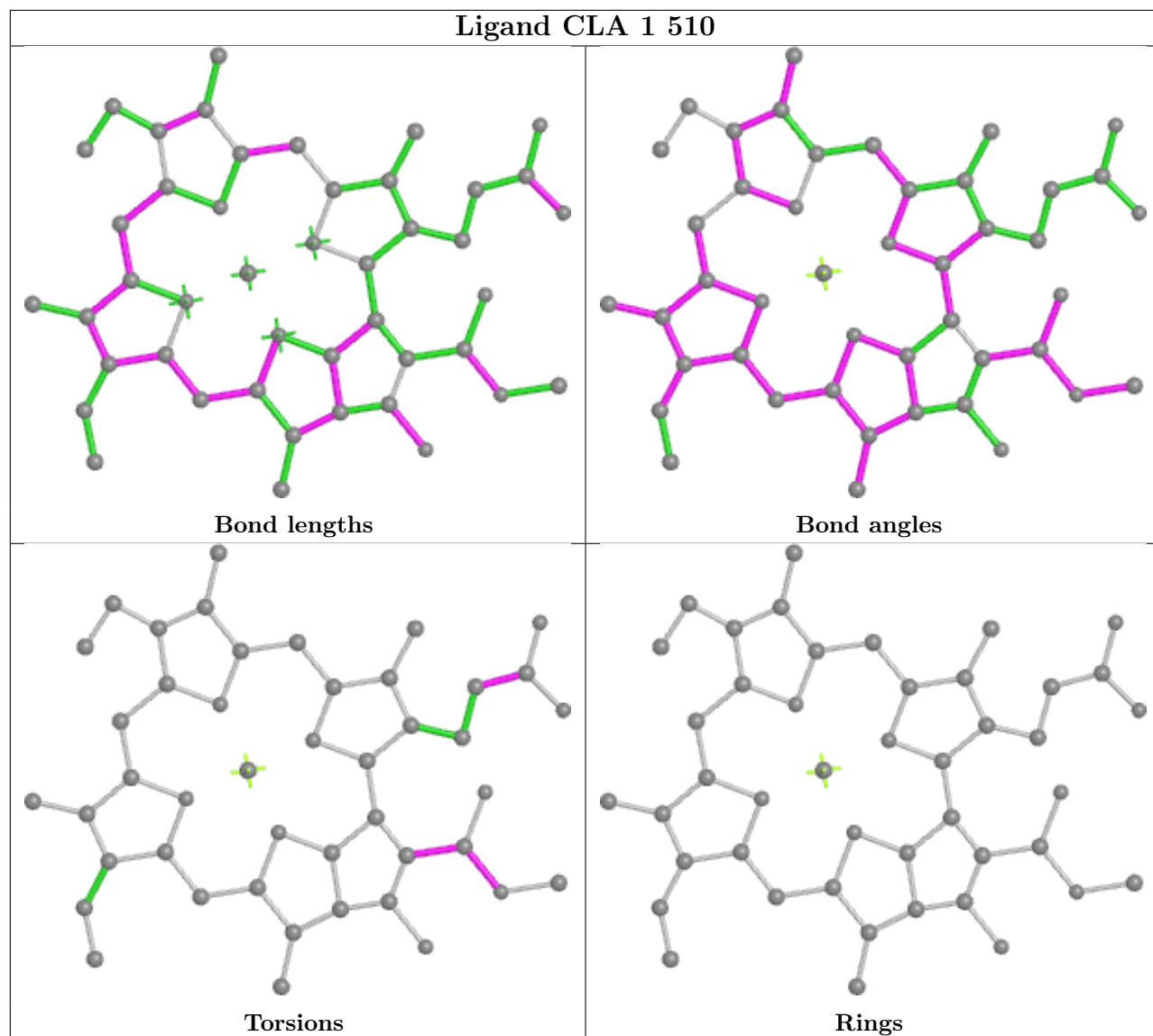
Ligand CLA 1 520



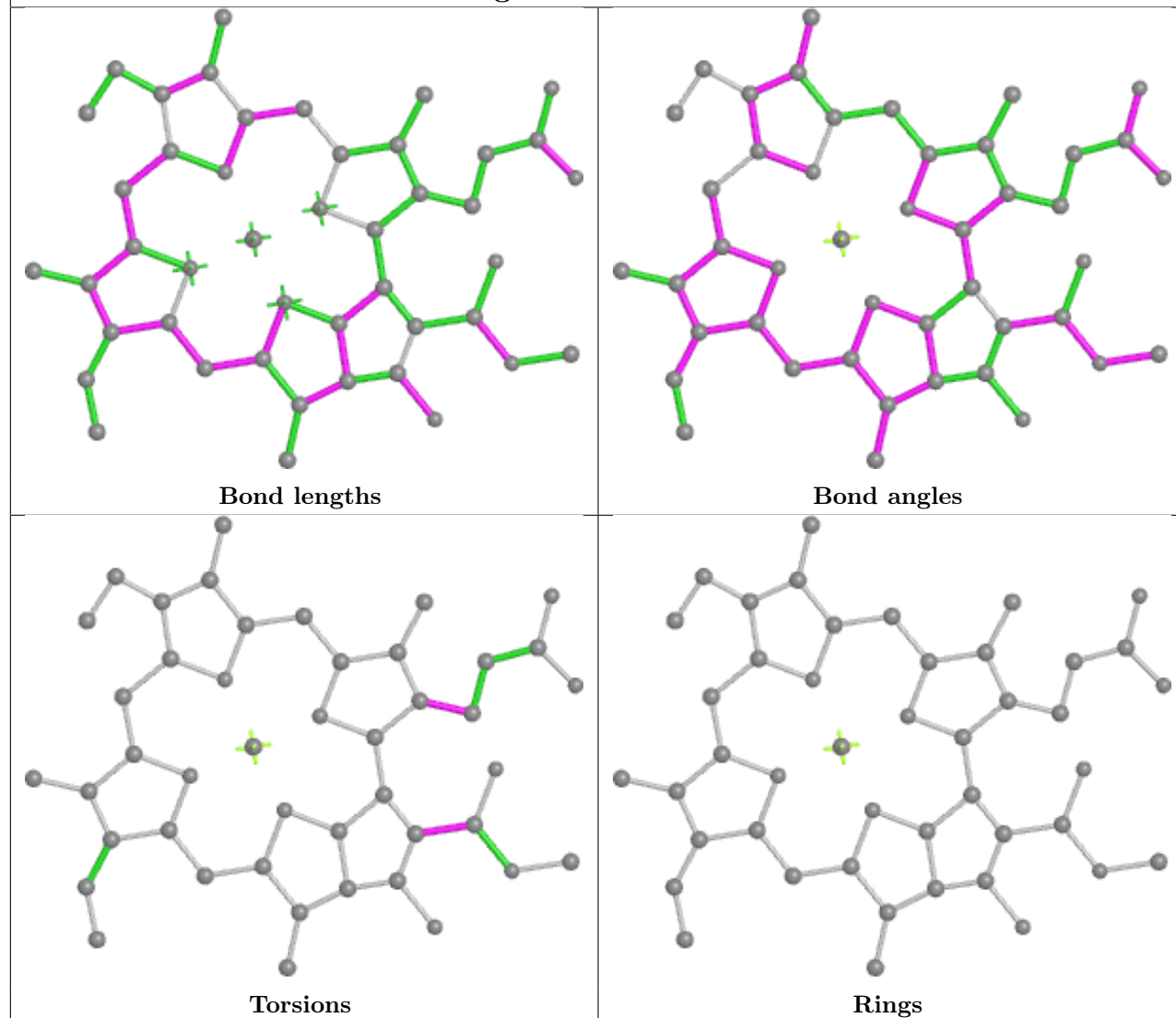
Ligand CLA 1 521



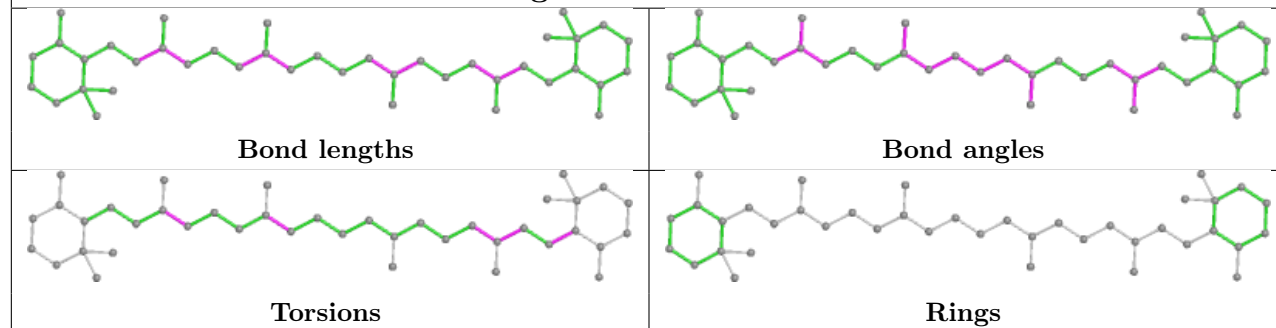
Ligand CLA 1 510

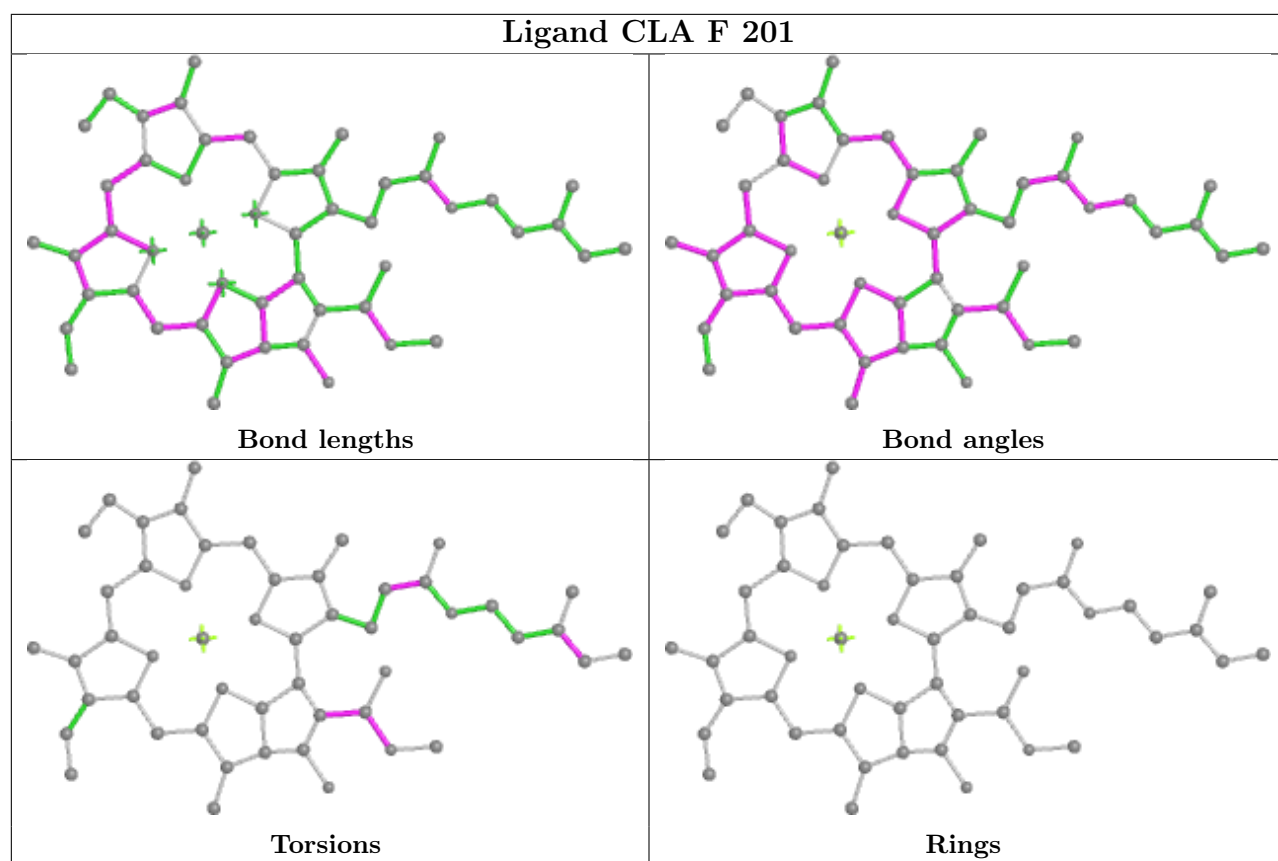


Ligand CLA 5 410

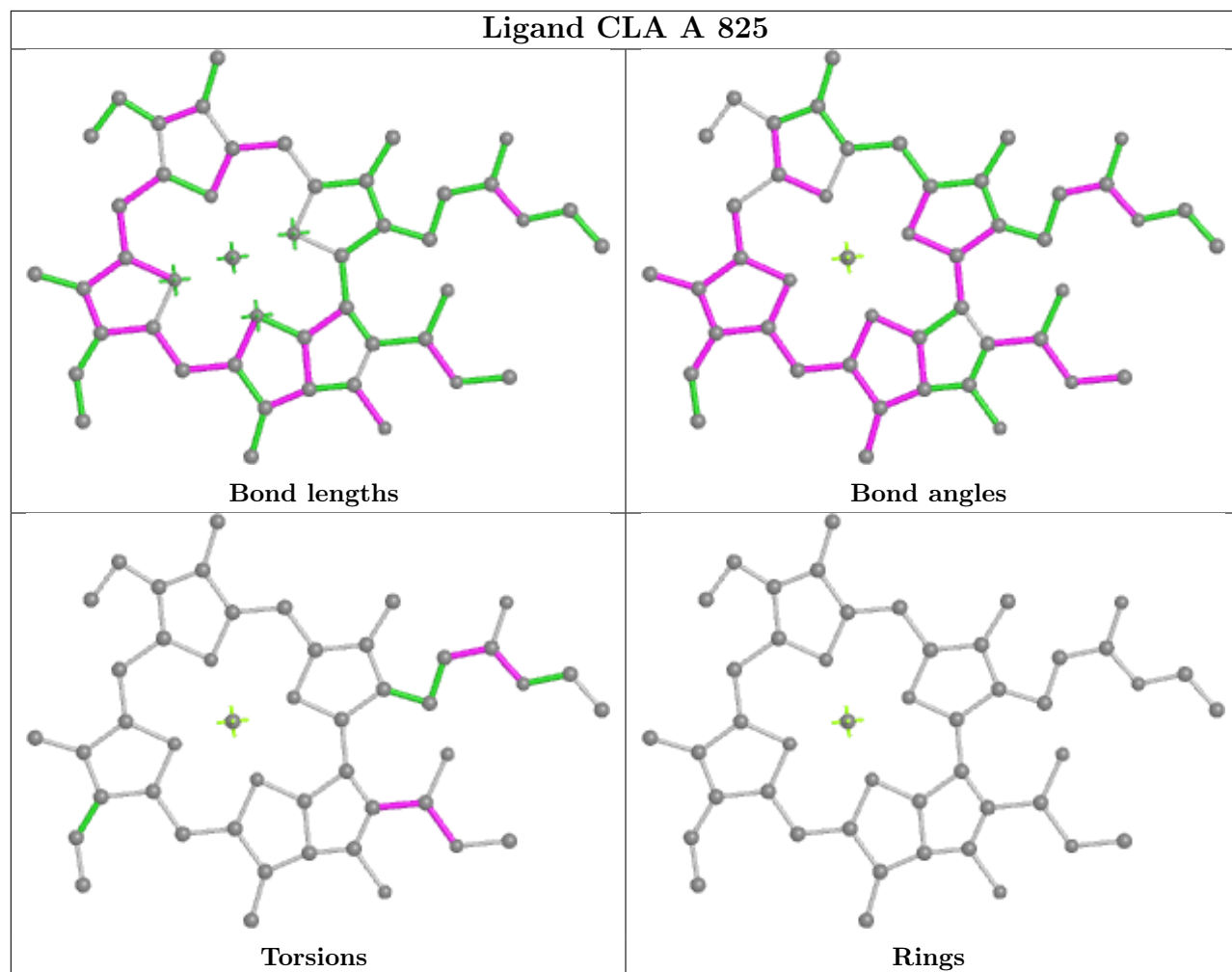


Ligand BCR B 845

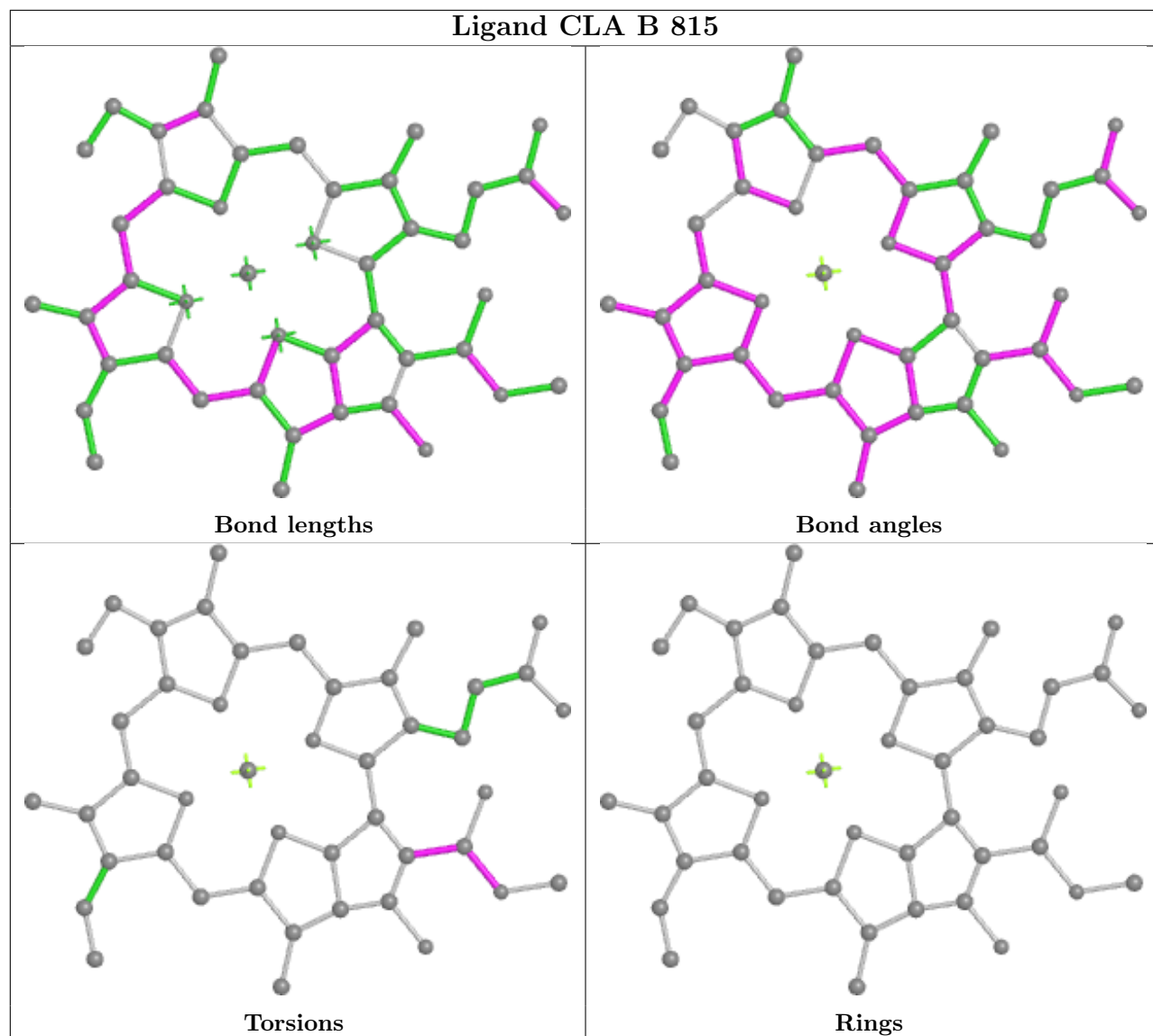




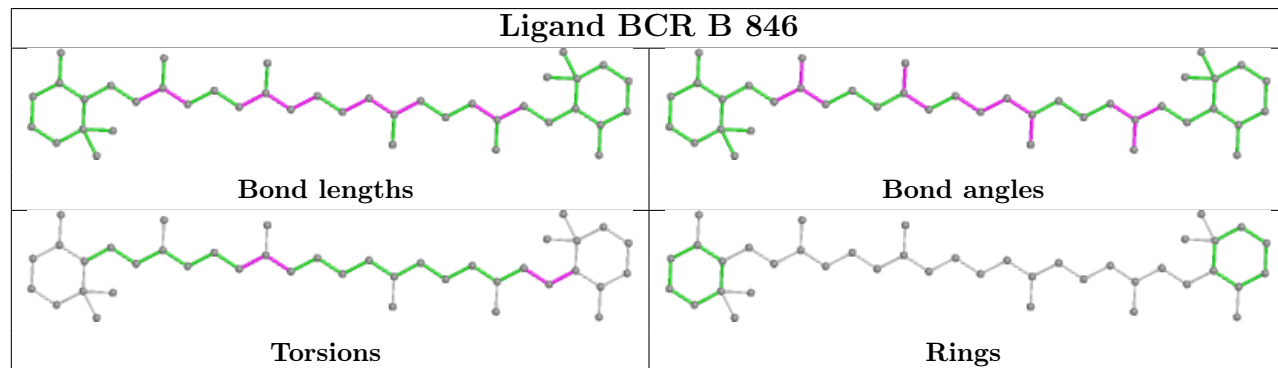
Ligand CLA A 825



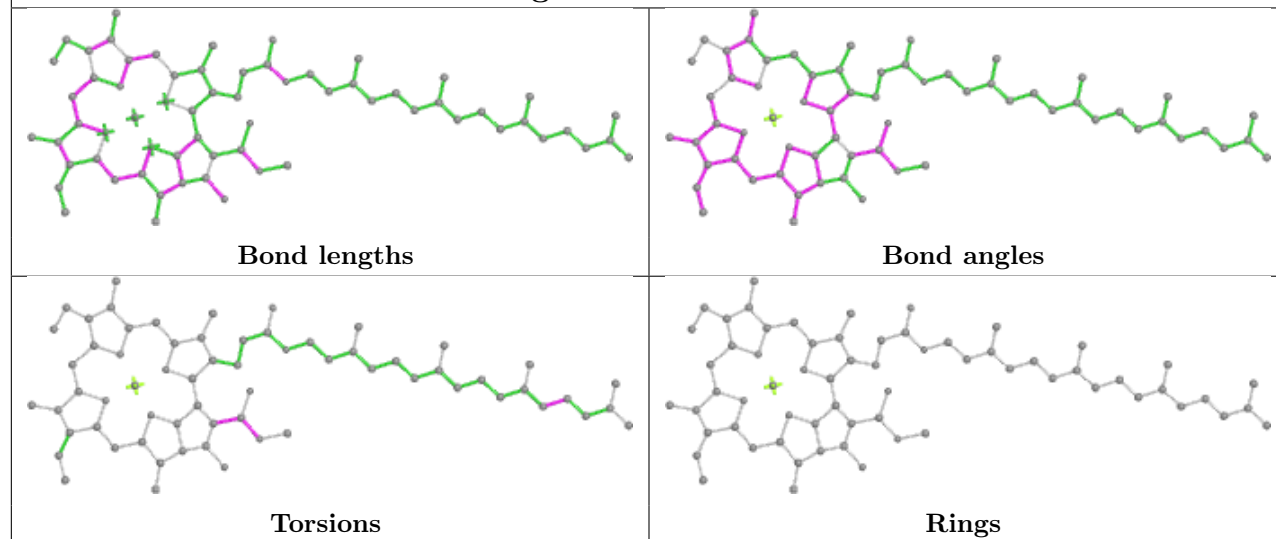
Ligand CLA B 815



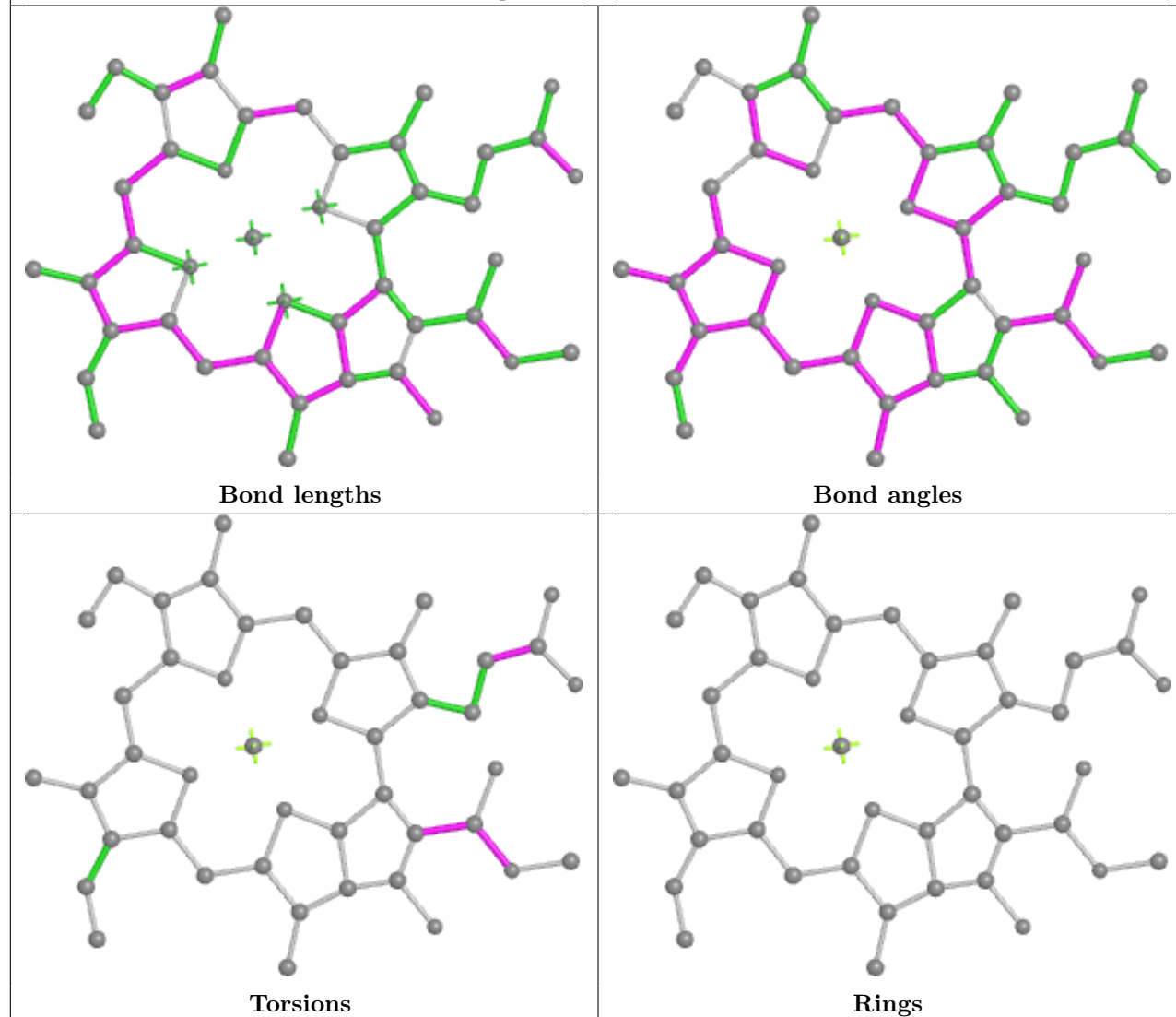
Ligand BCR B 846



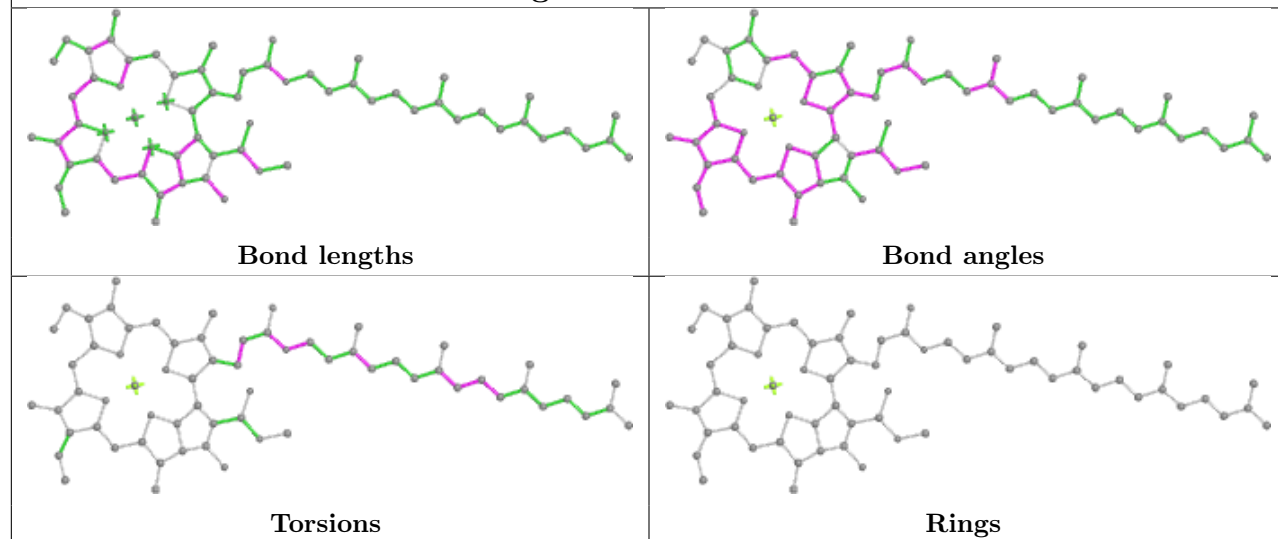
Ligand CLA A 831



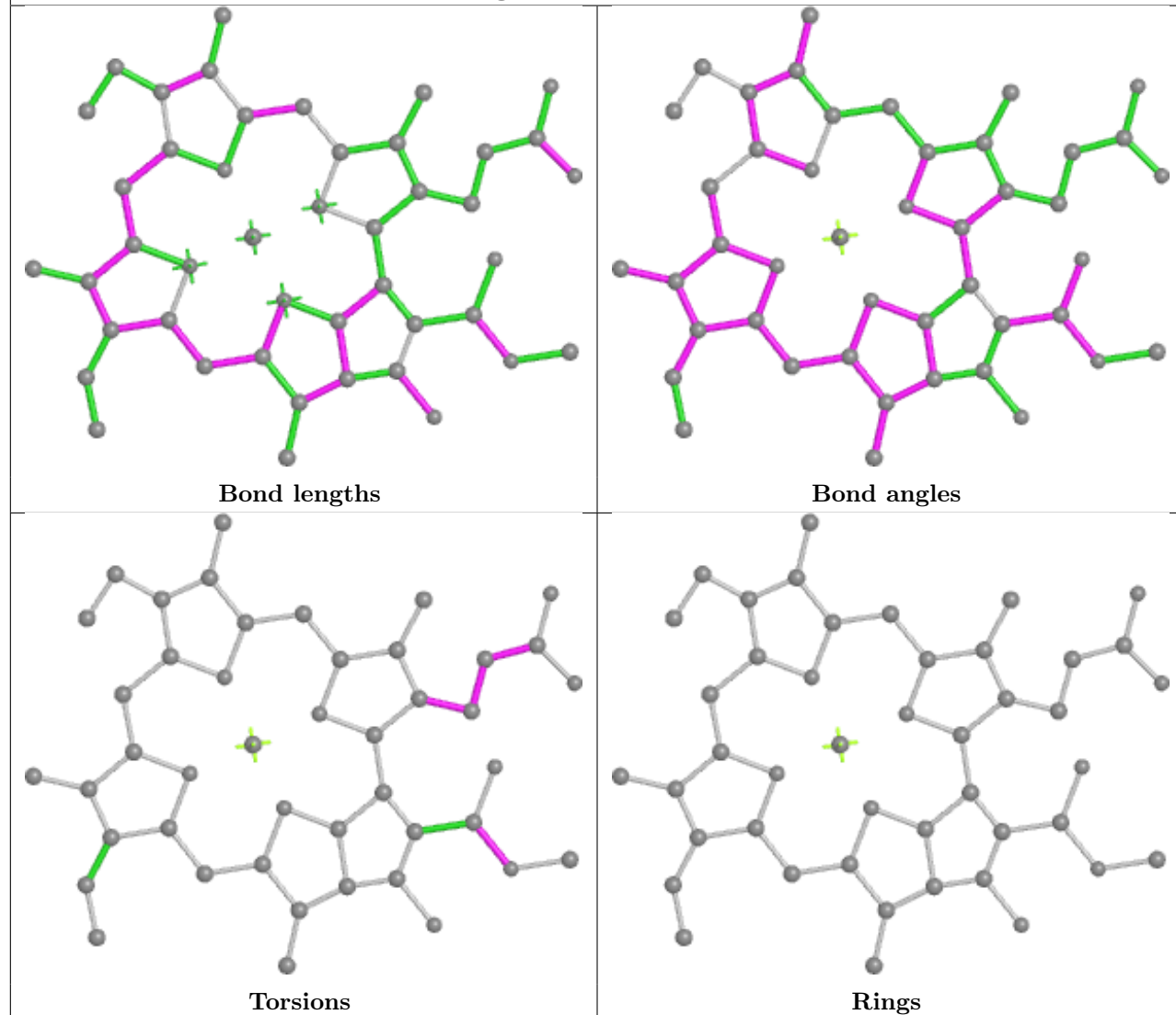
Ligand CLA 1 504



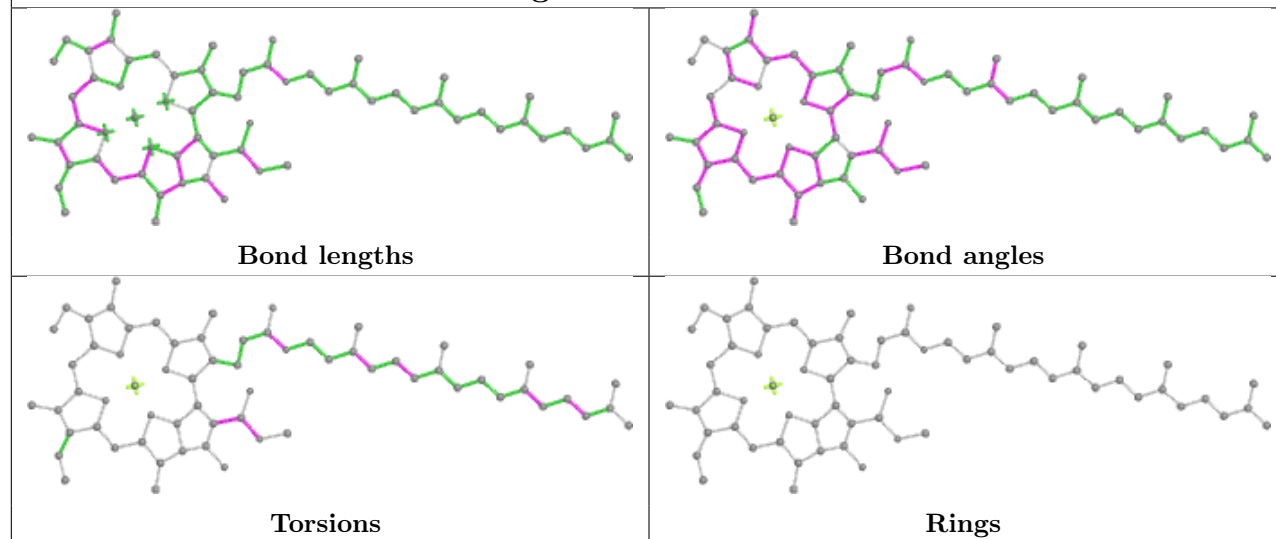
Ligand CLA A 822



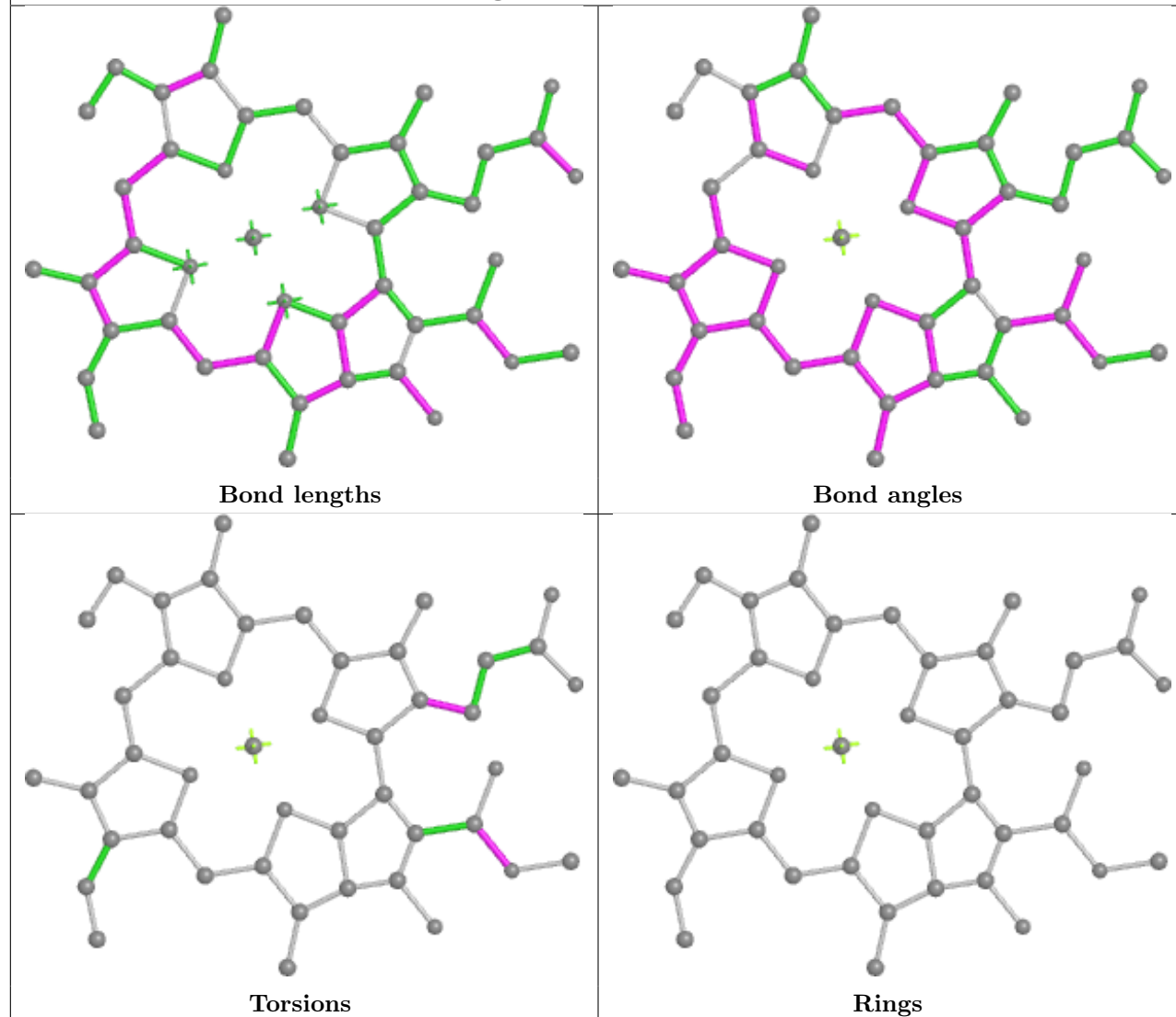
Ligand CLA 5 422



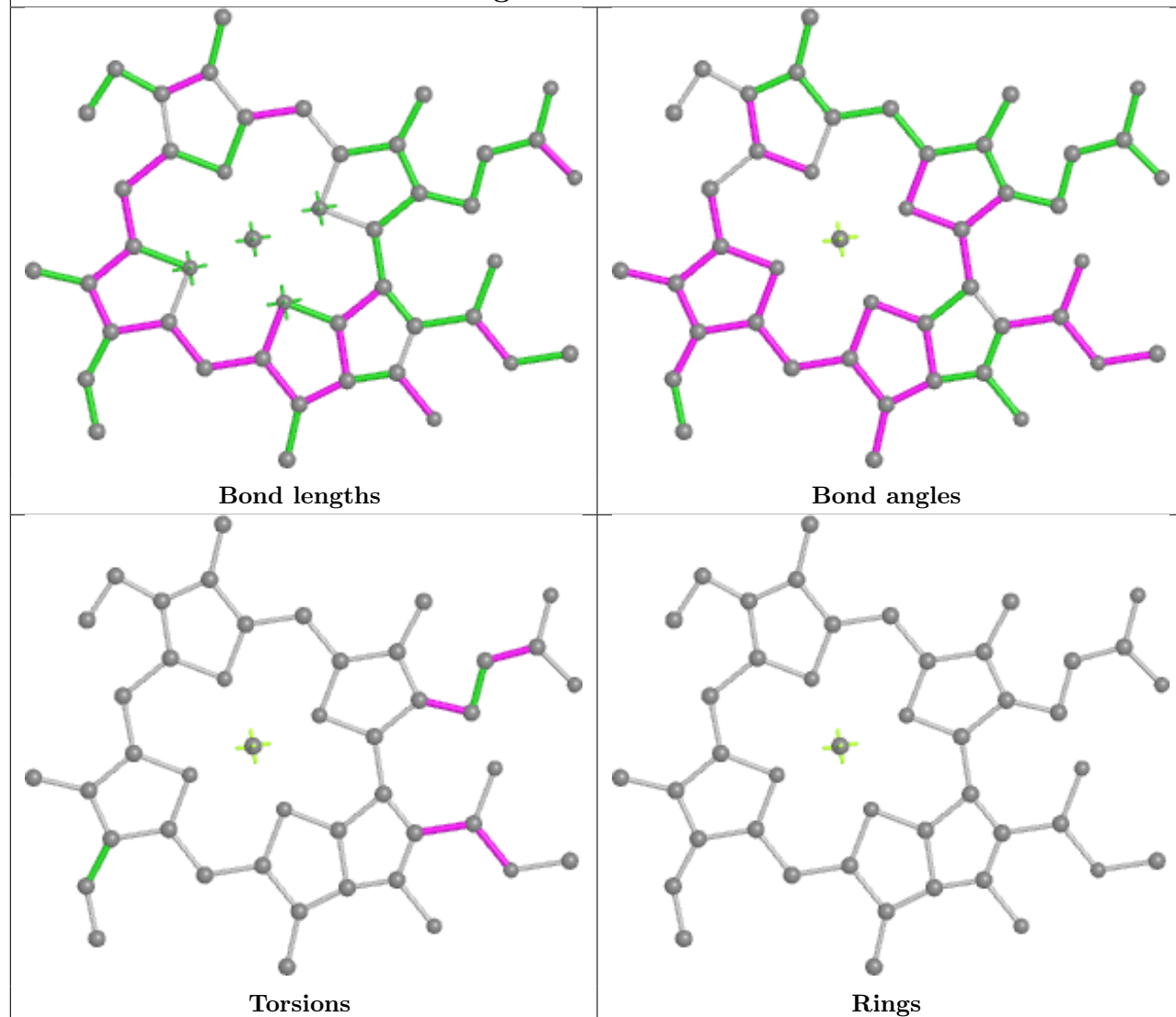
Ligand CLA A 835



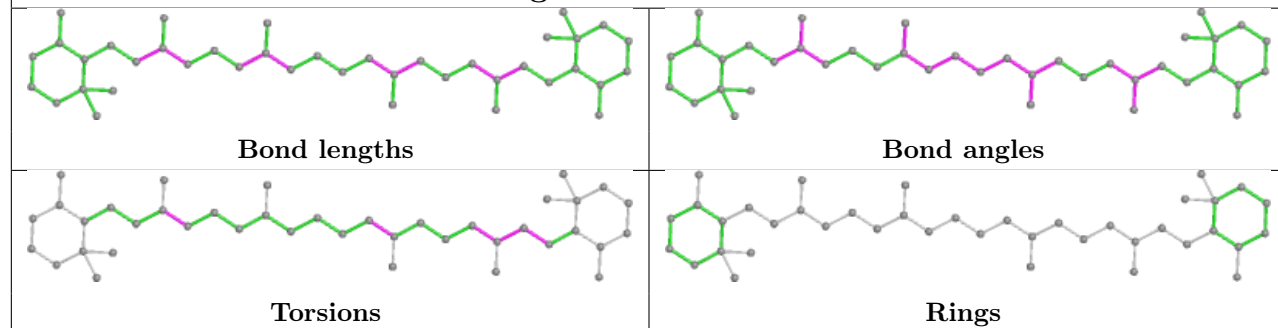
Ligand CLA A 816



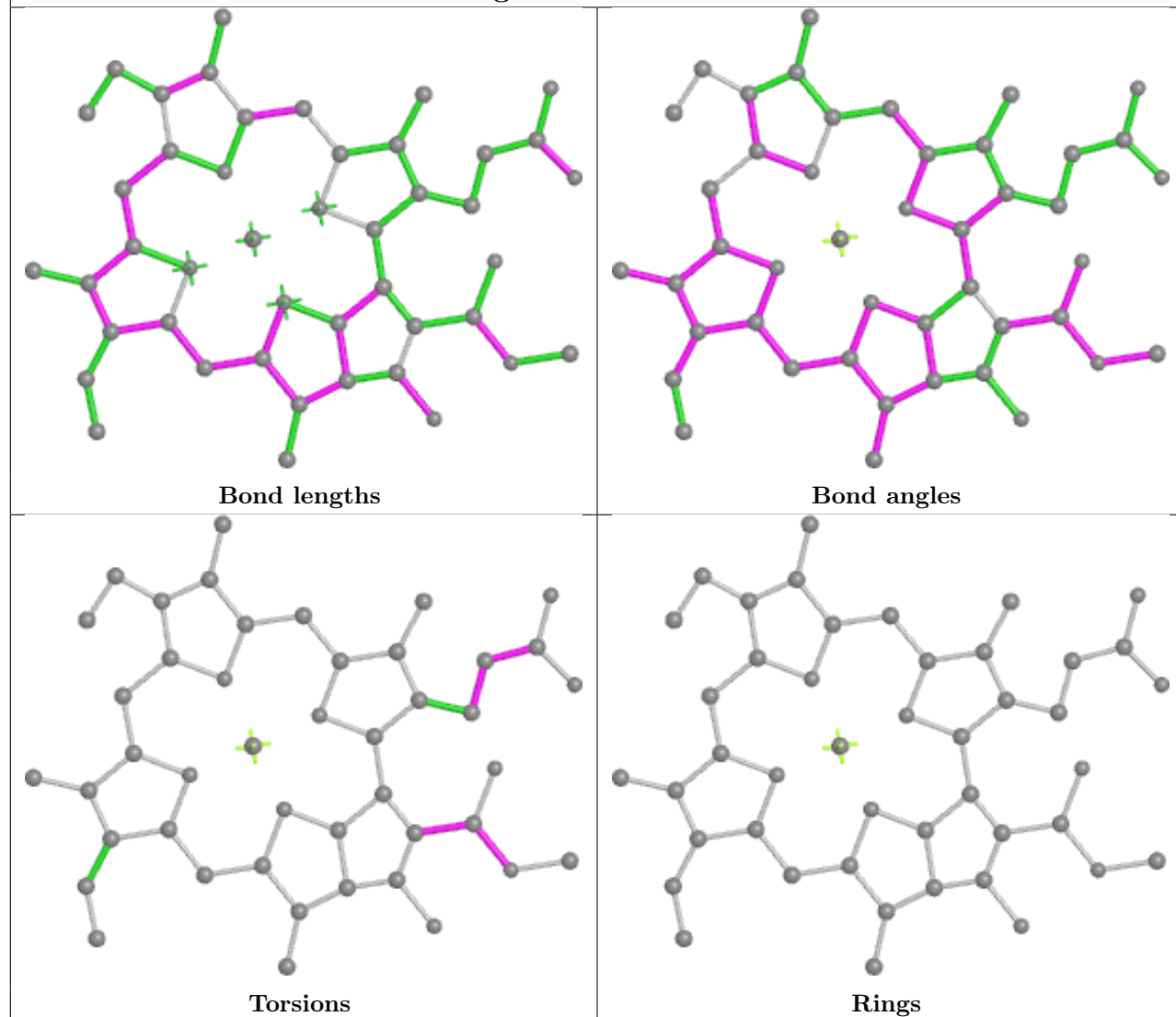
Ligand CLA 6 402



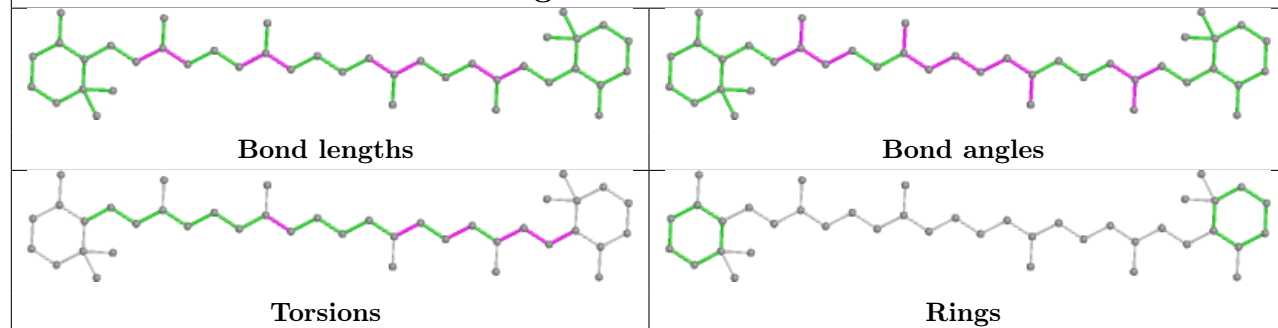
Ligand BCR A 851



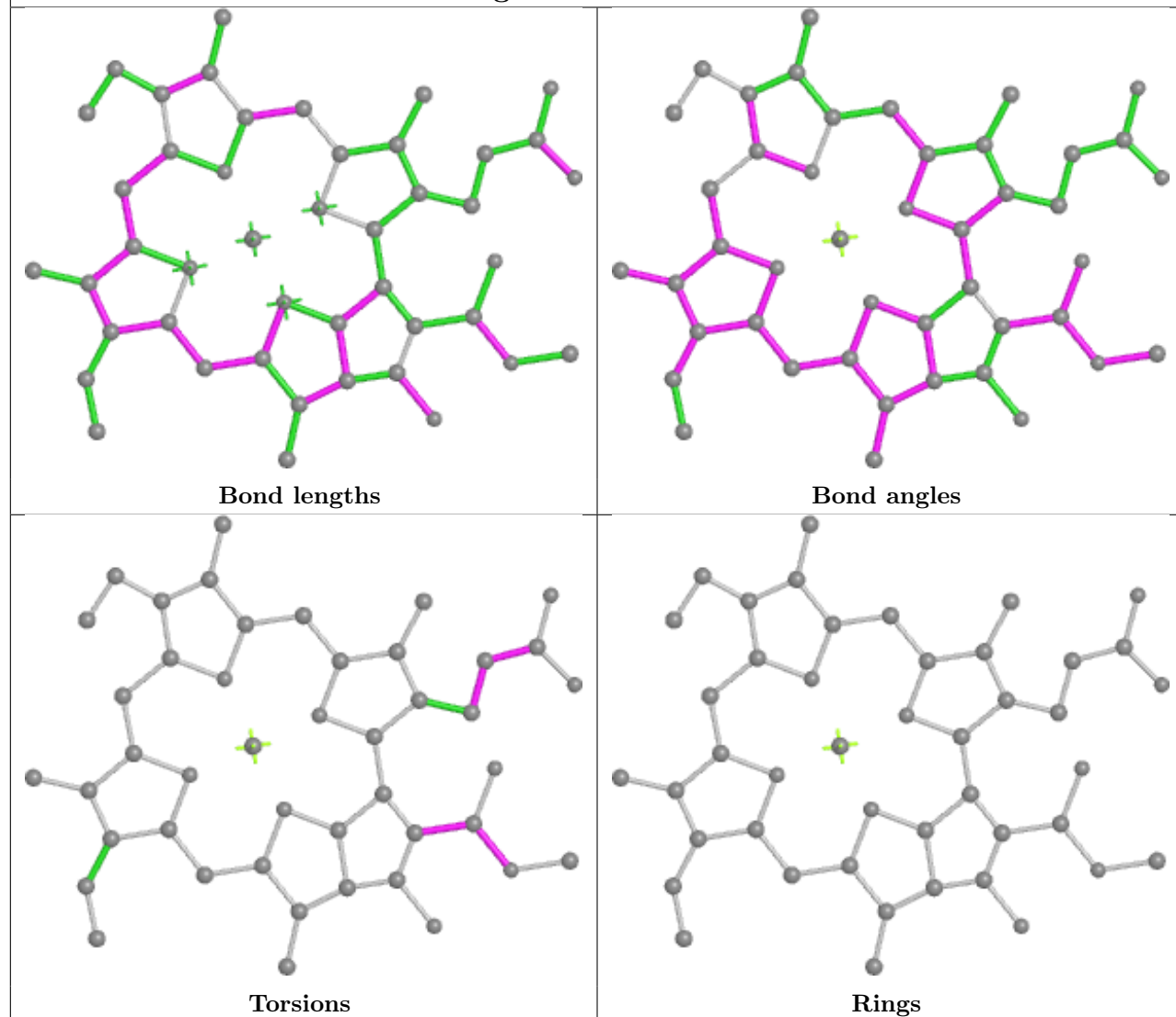
Ligand CLA 5 418



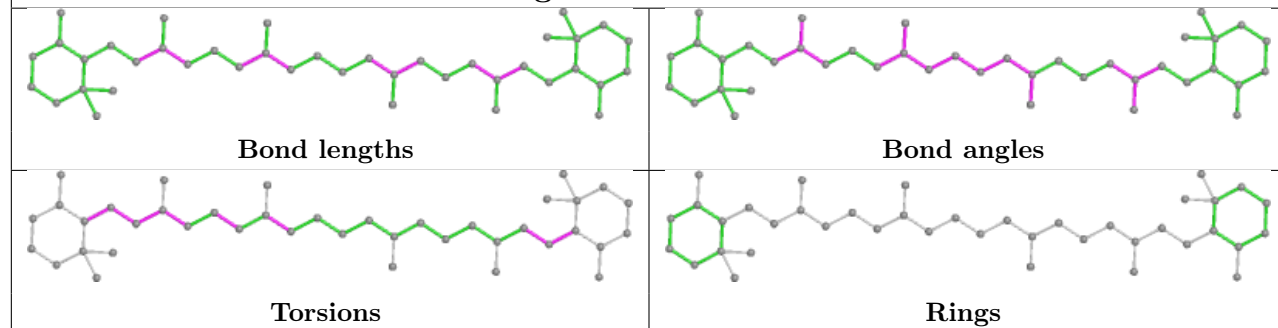
Ligand BCR 5 420



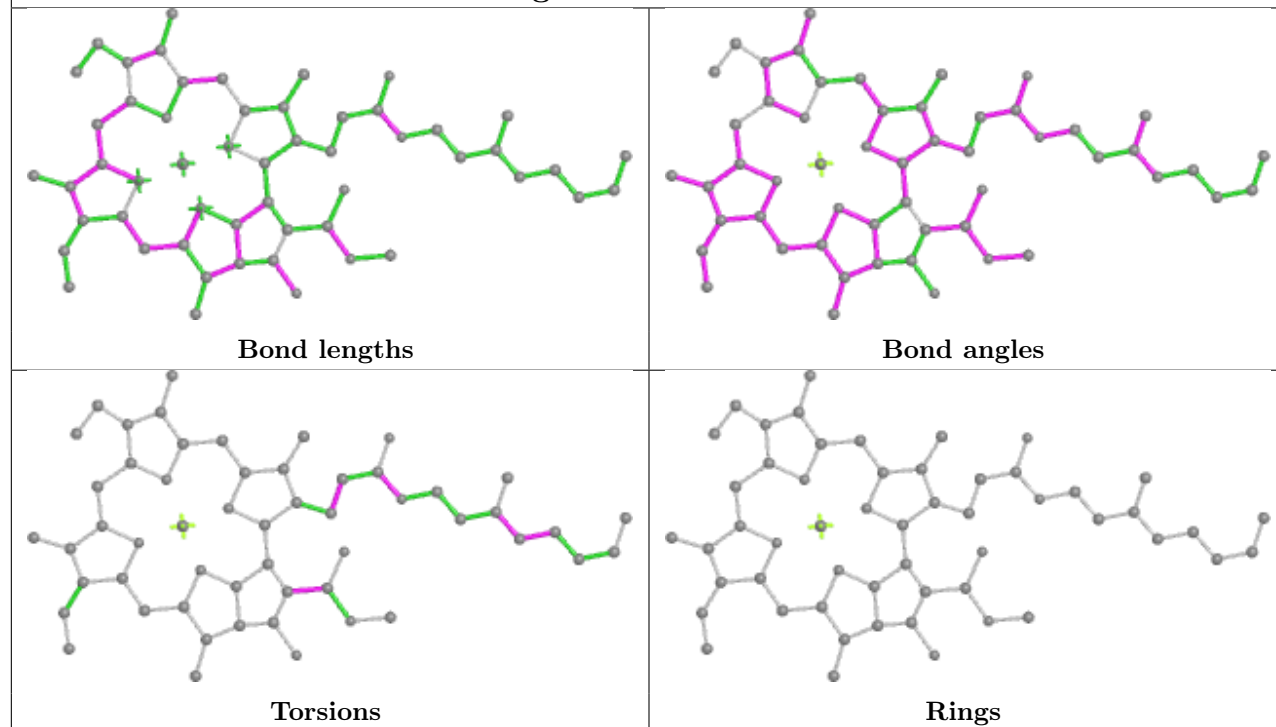
Ligand CLA 1 506



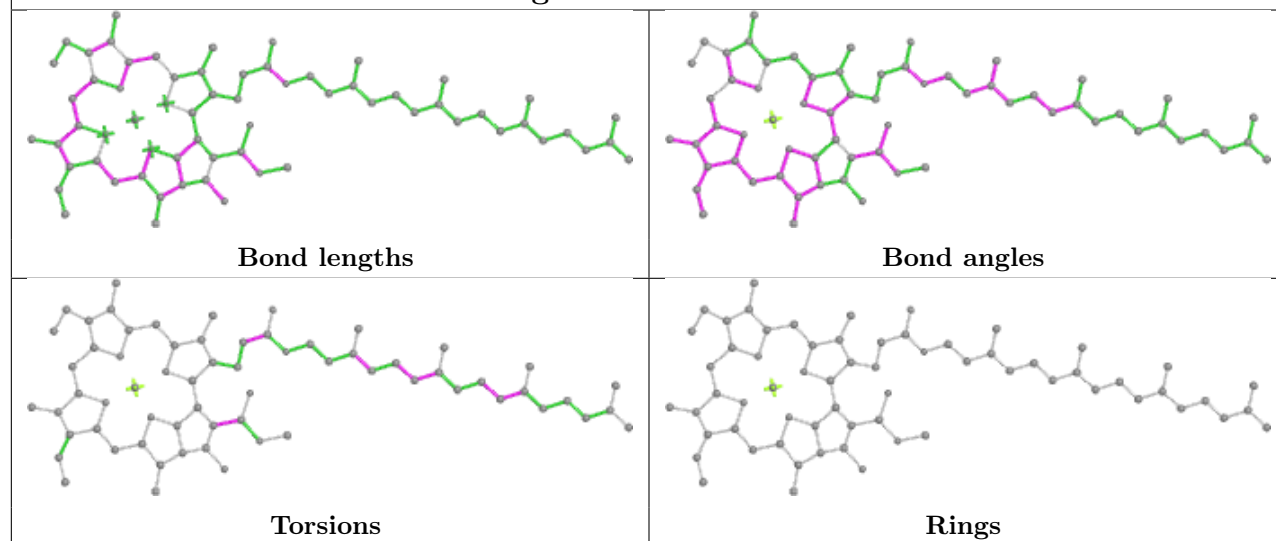
Ligand BCR 1 517

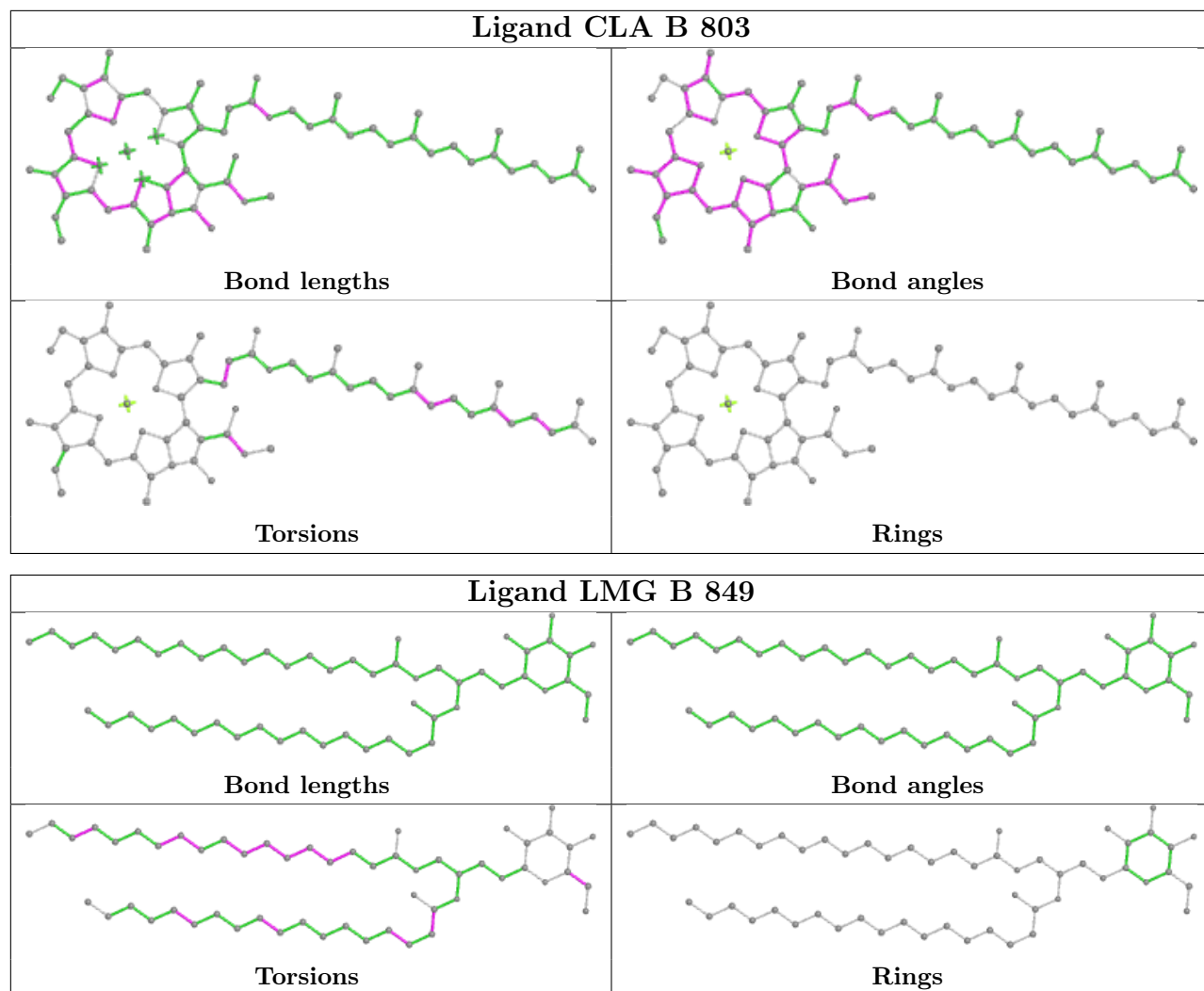


Ligand CLA B 804

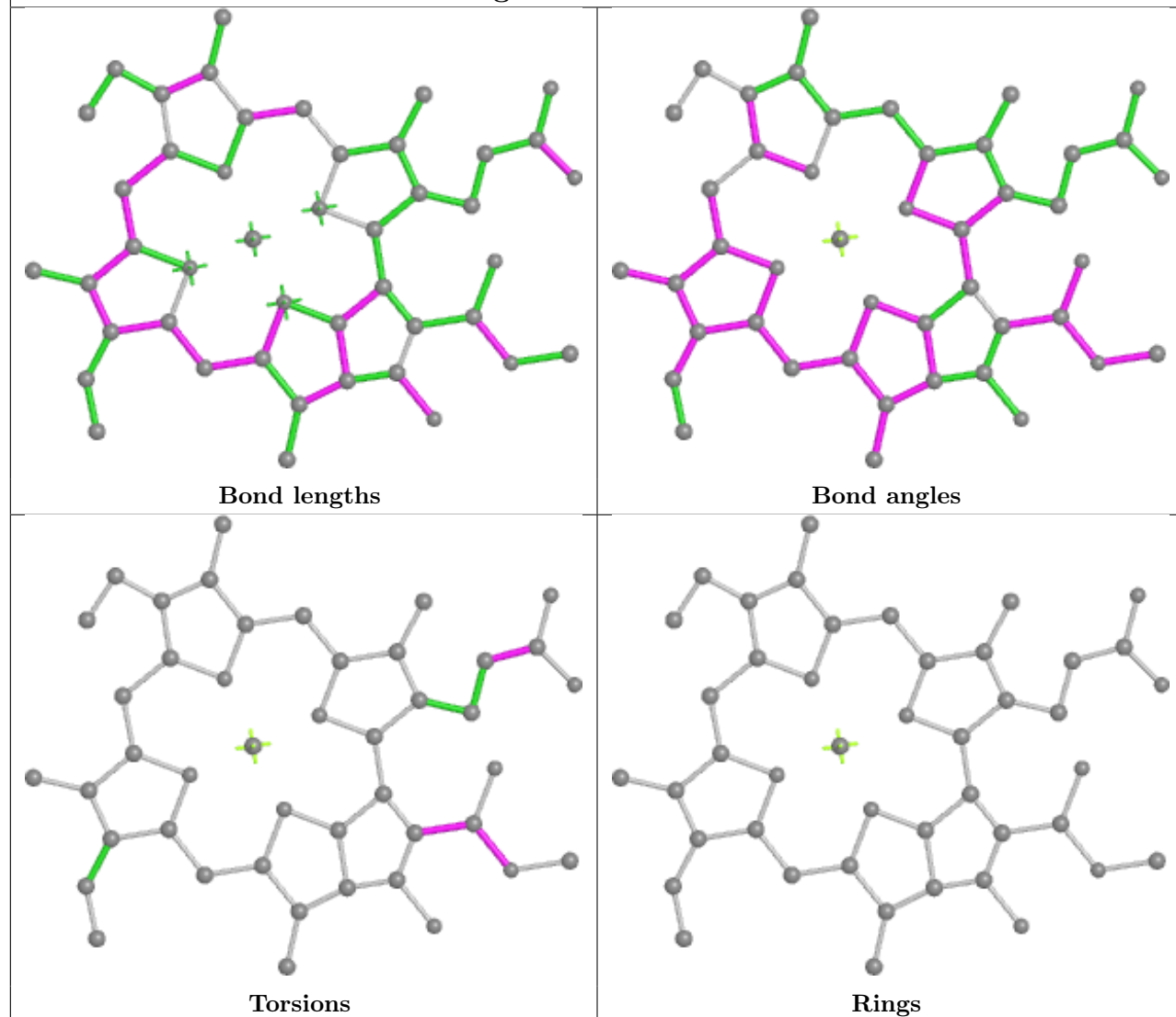


Ligand CLA A 839

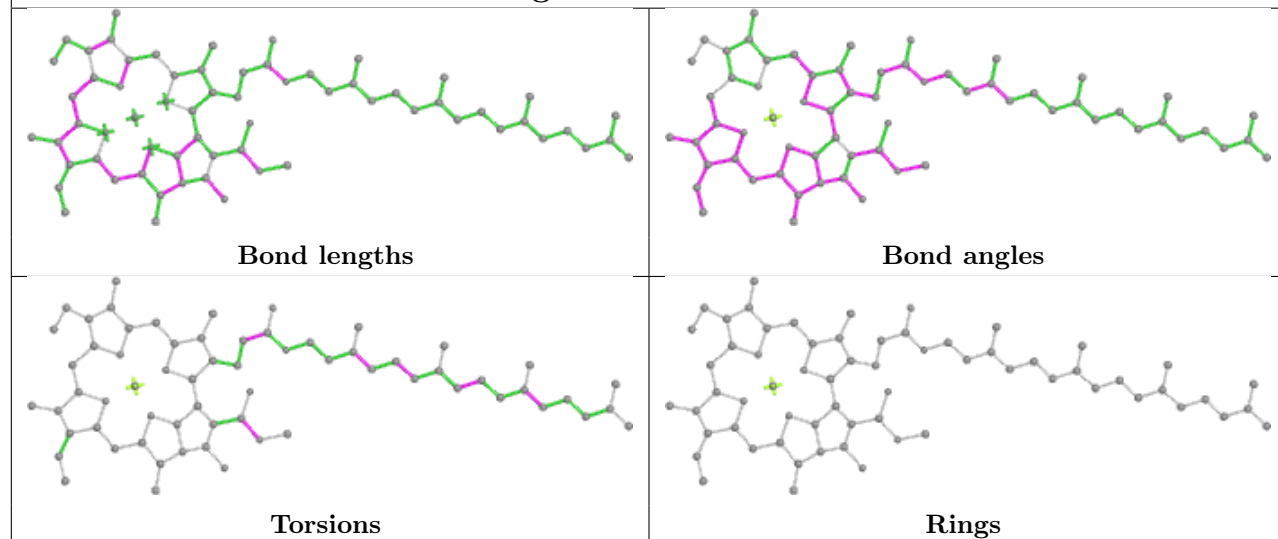




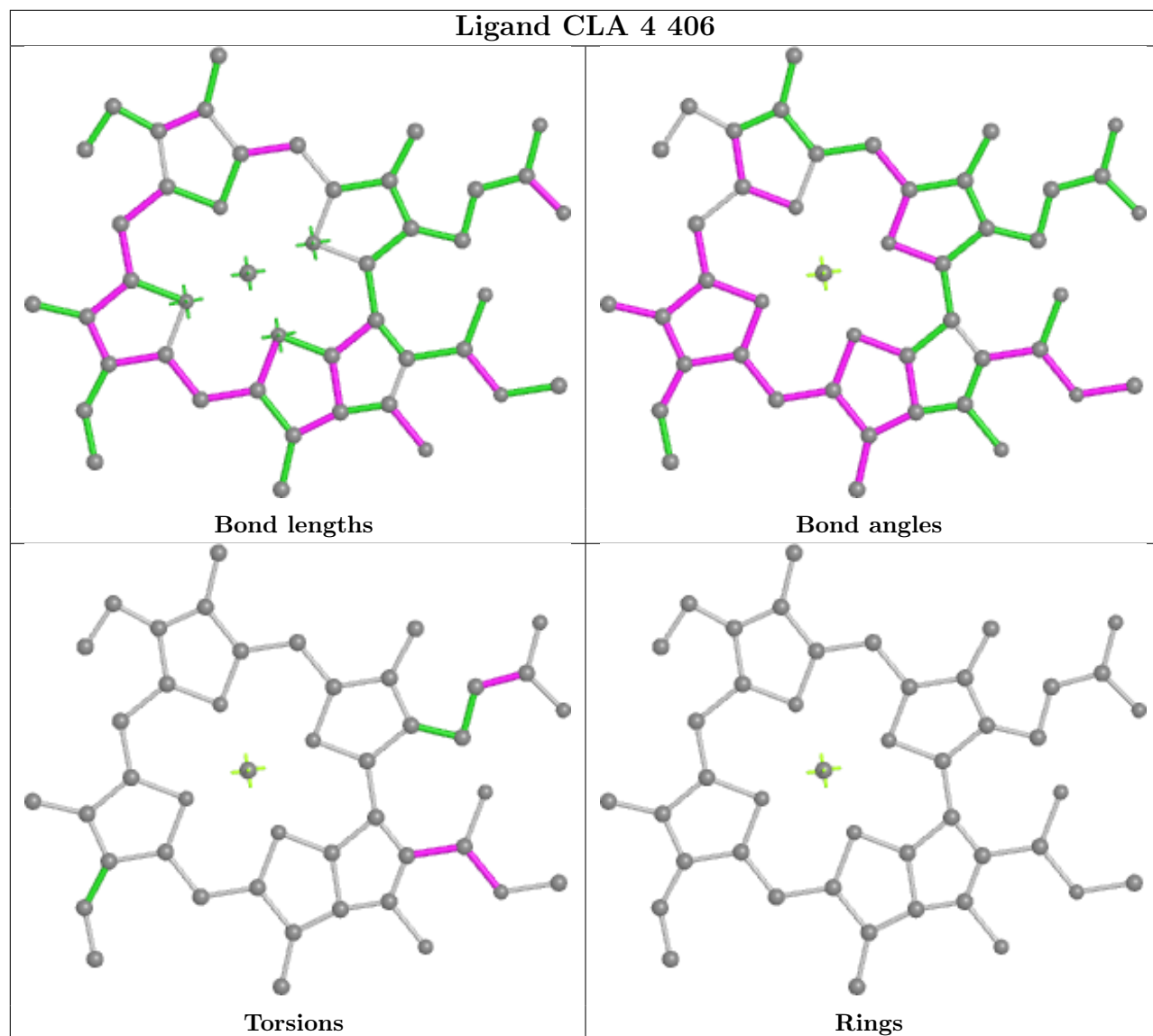
Ligand CLA 4 403



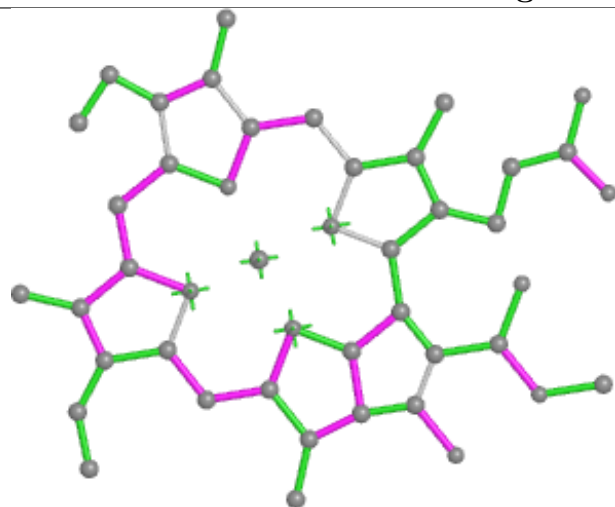
Ligand CLA B 809



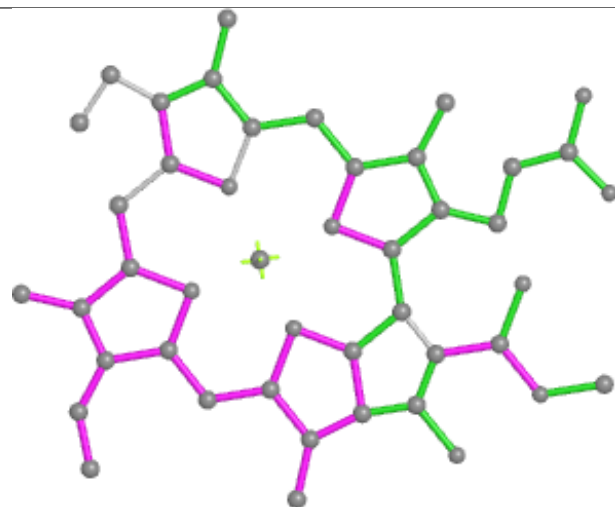
Ligand CLA 4 406



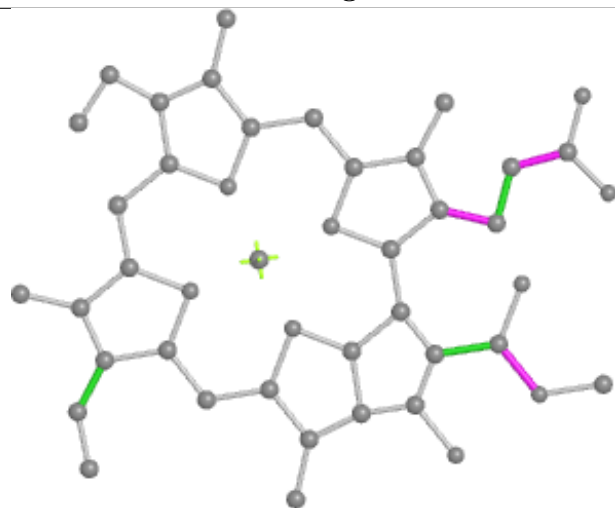
Ligand CLA B 835



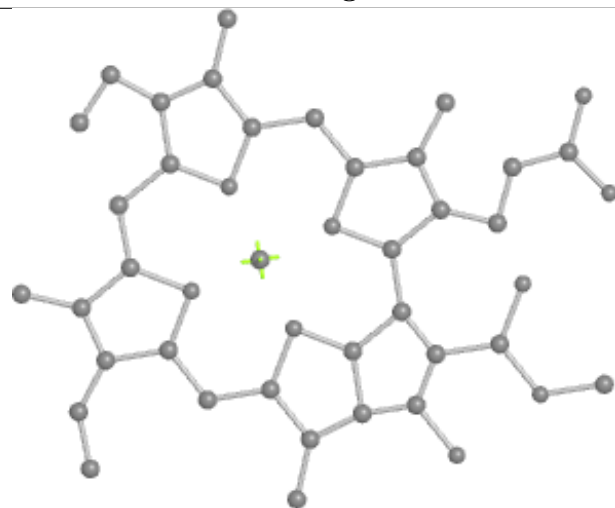
Bond lengths



Bond angles

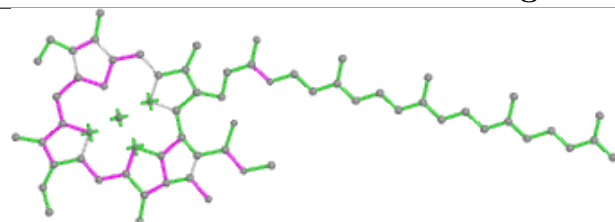


Torsions

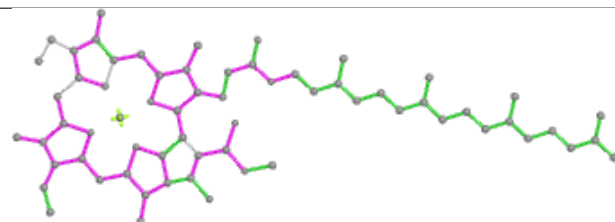


Rings

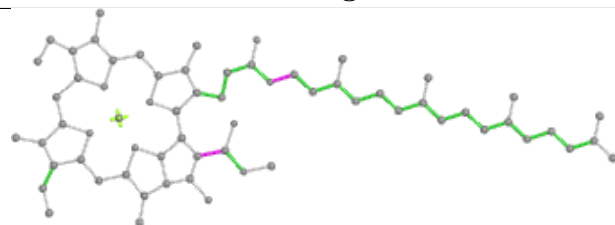
Ligand CL0 A 801



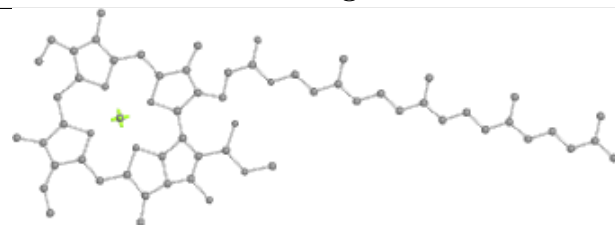
Bond lengths



Bond angles

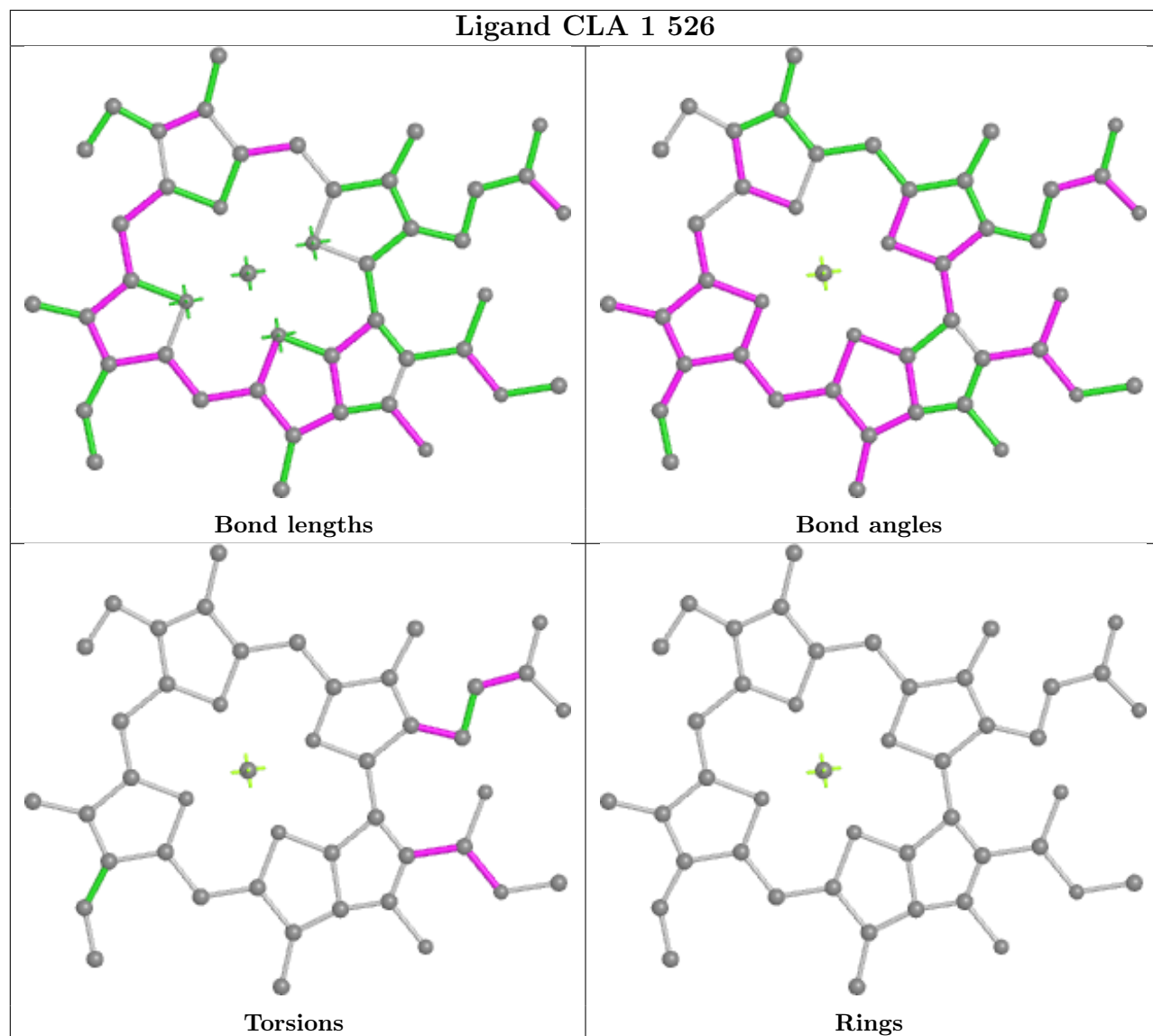


Torsions

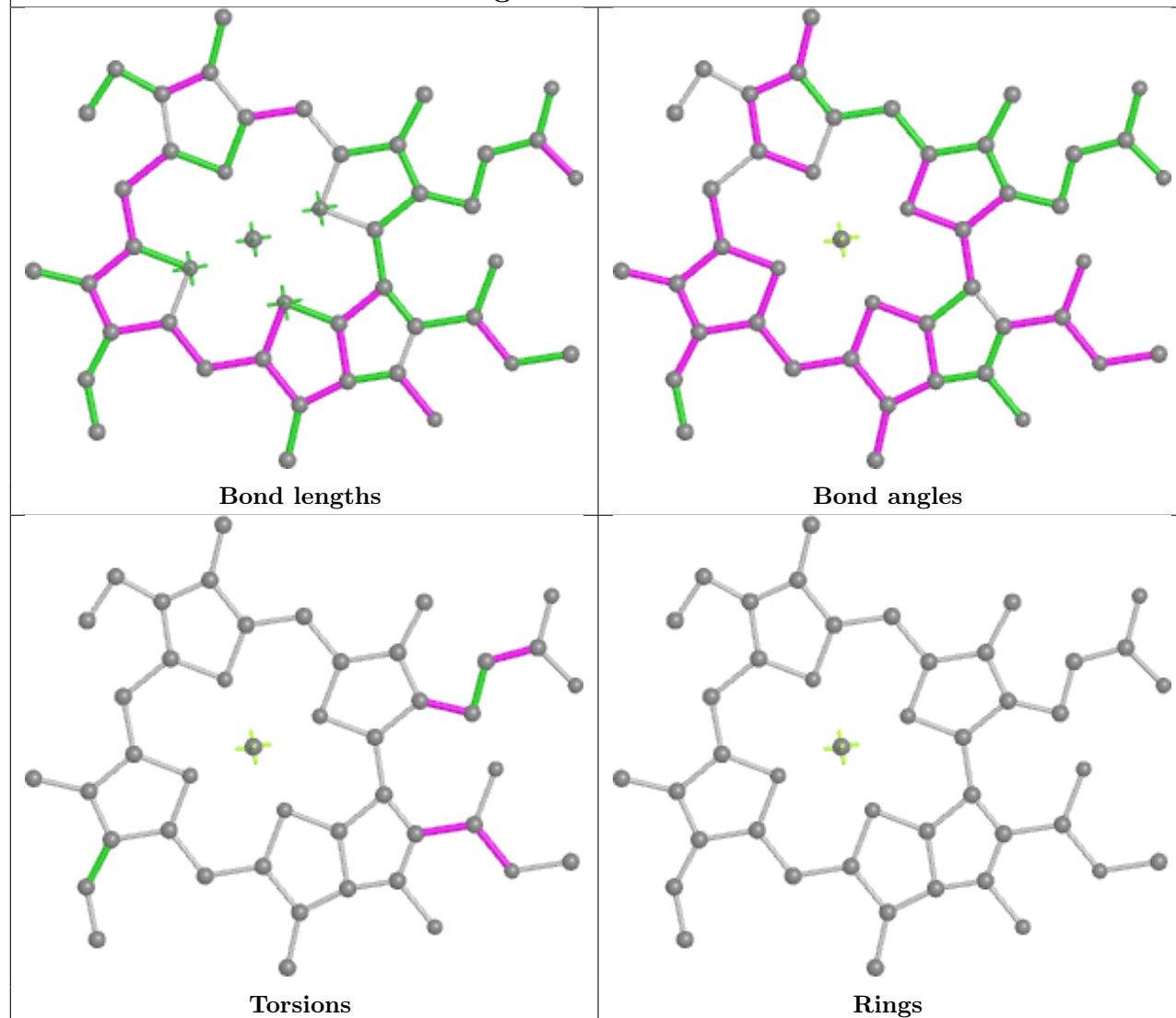


Rings

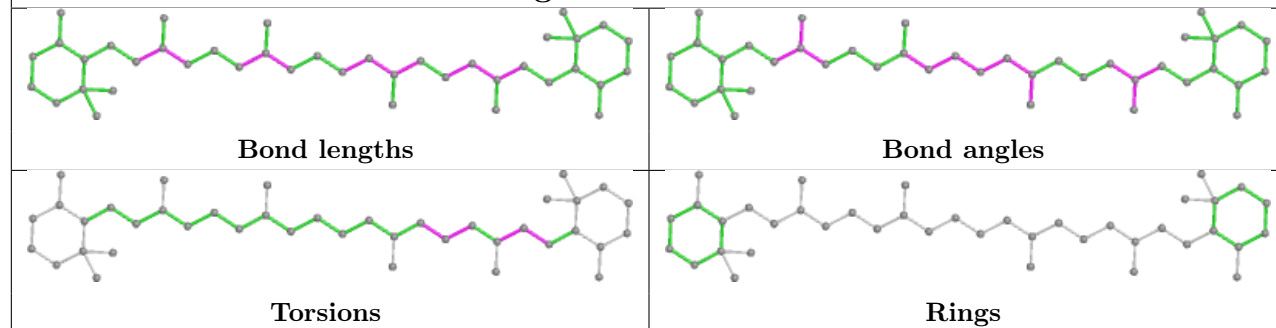
Ligand CLA 1 526



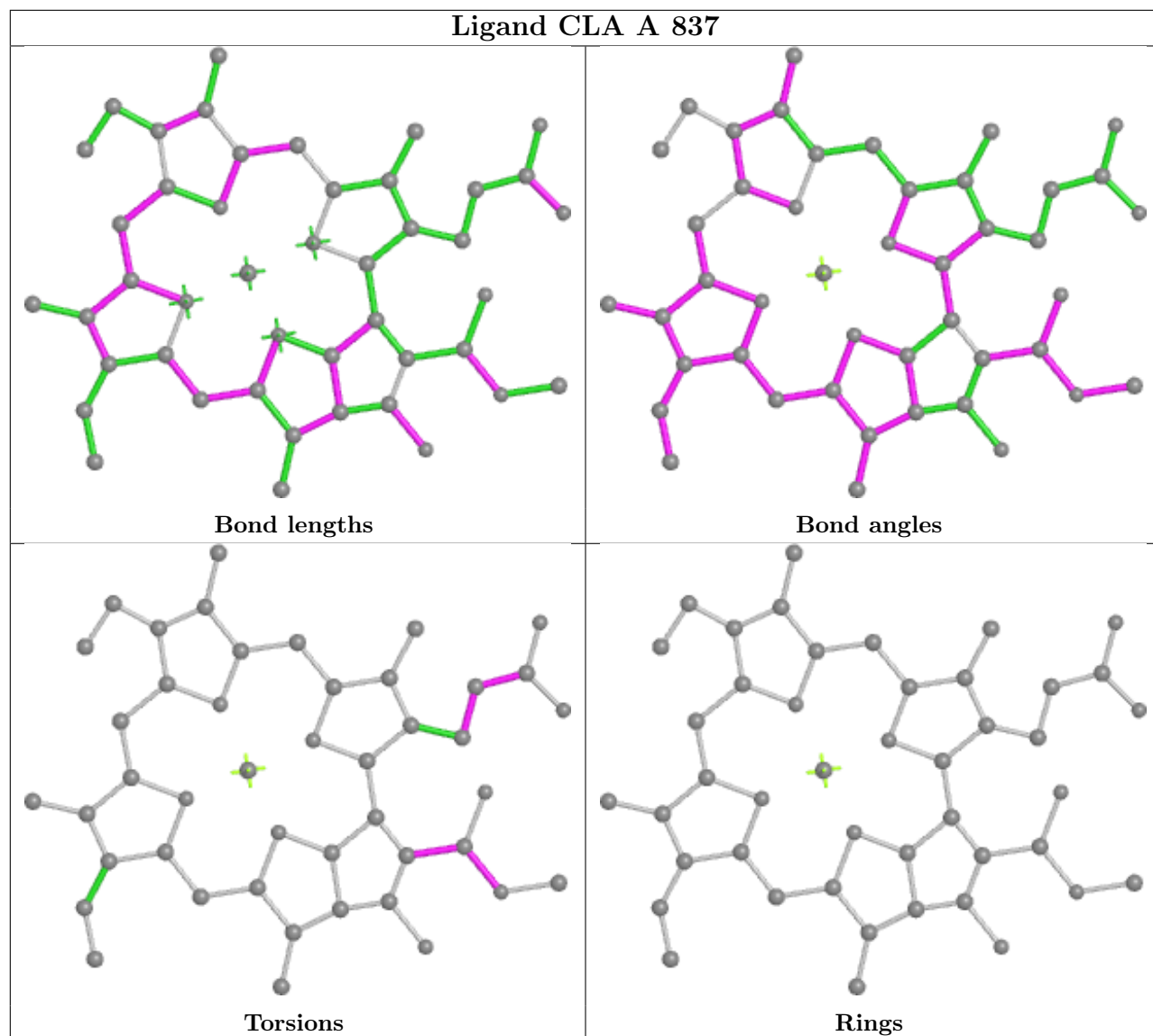
Ligand CLA 4 411



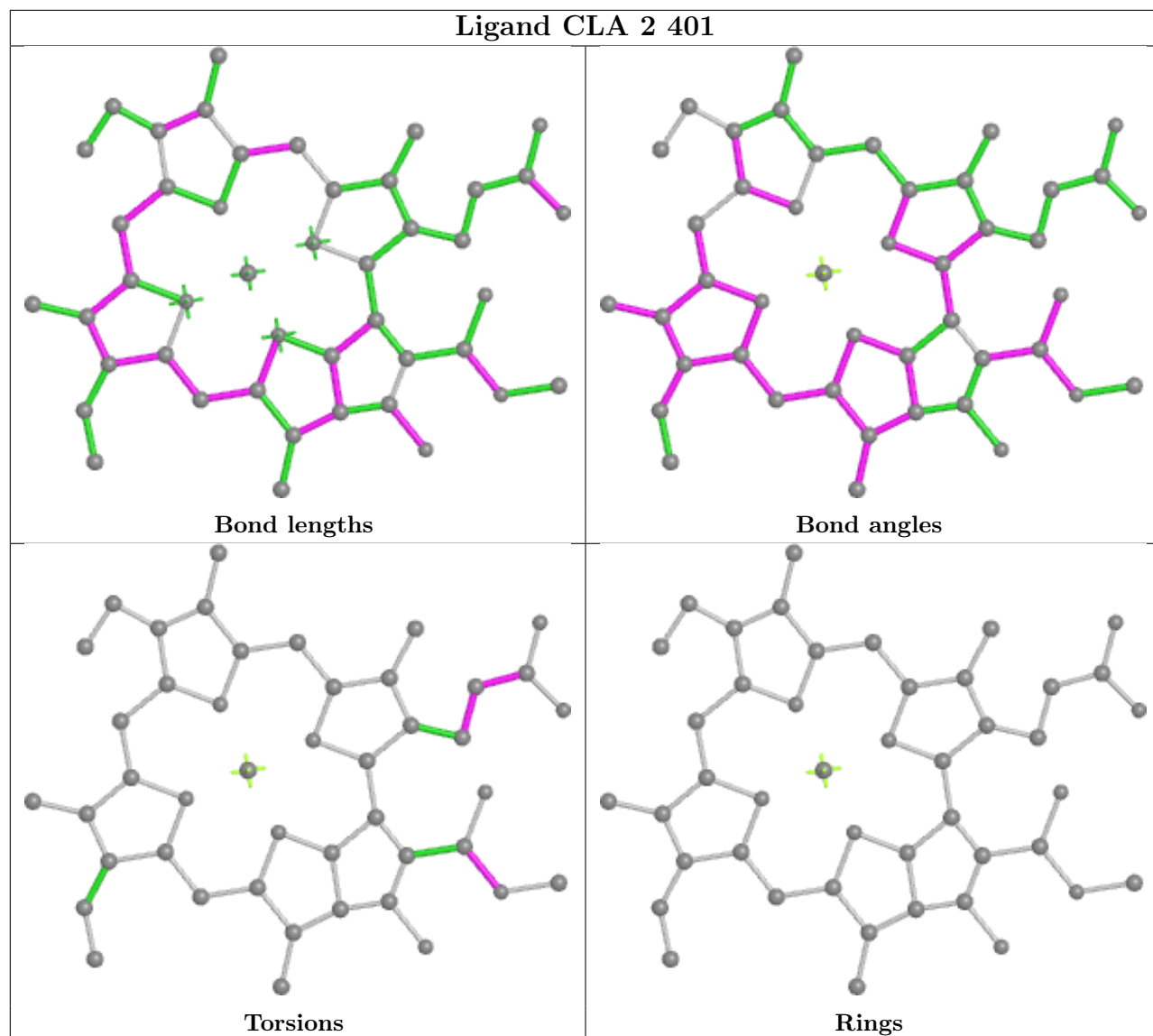
Ligand BCR 1 523



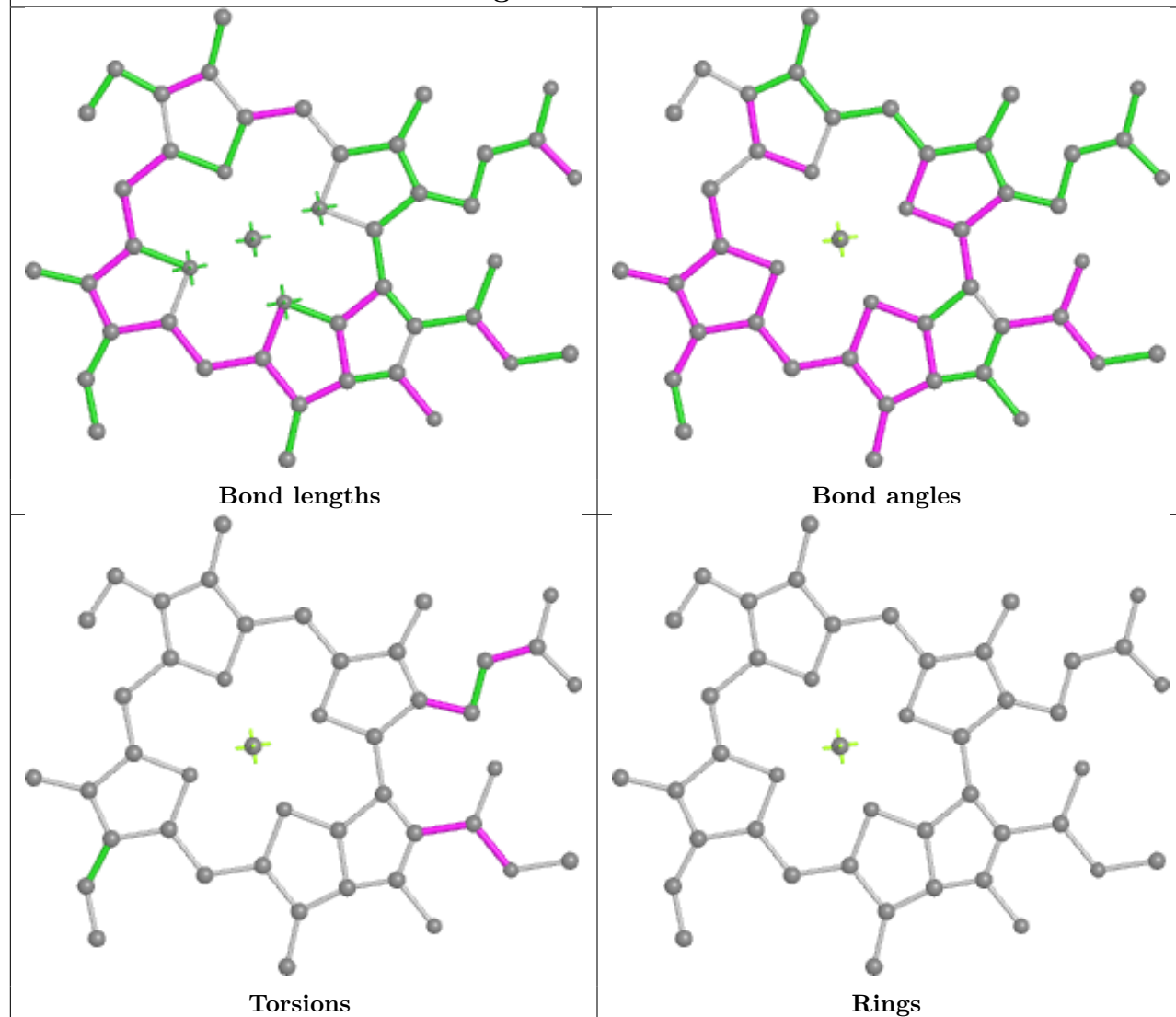
Ligand CLA A 837



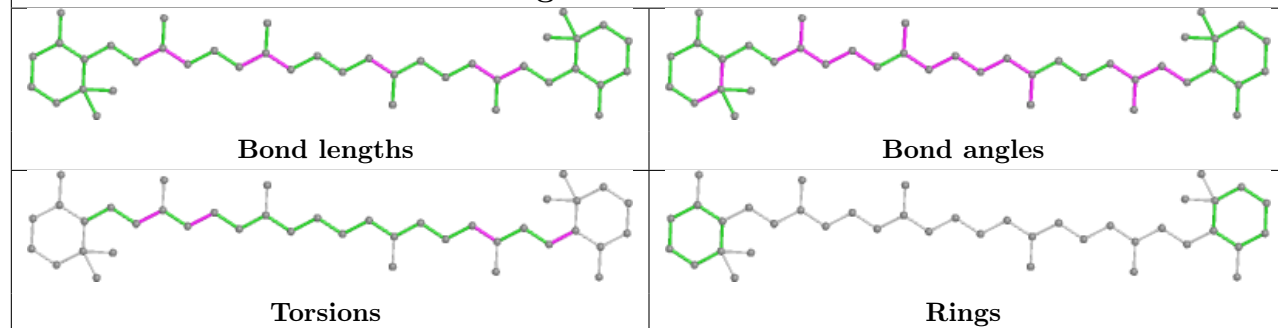
Ligand CLA 2 401

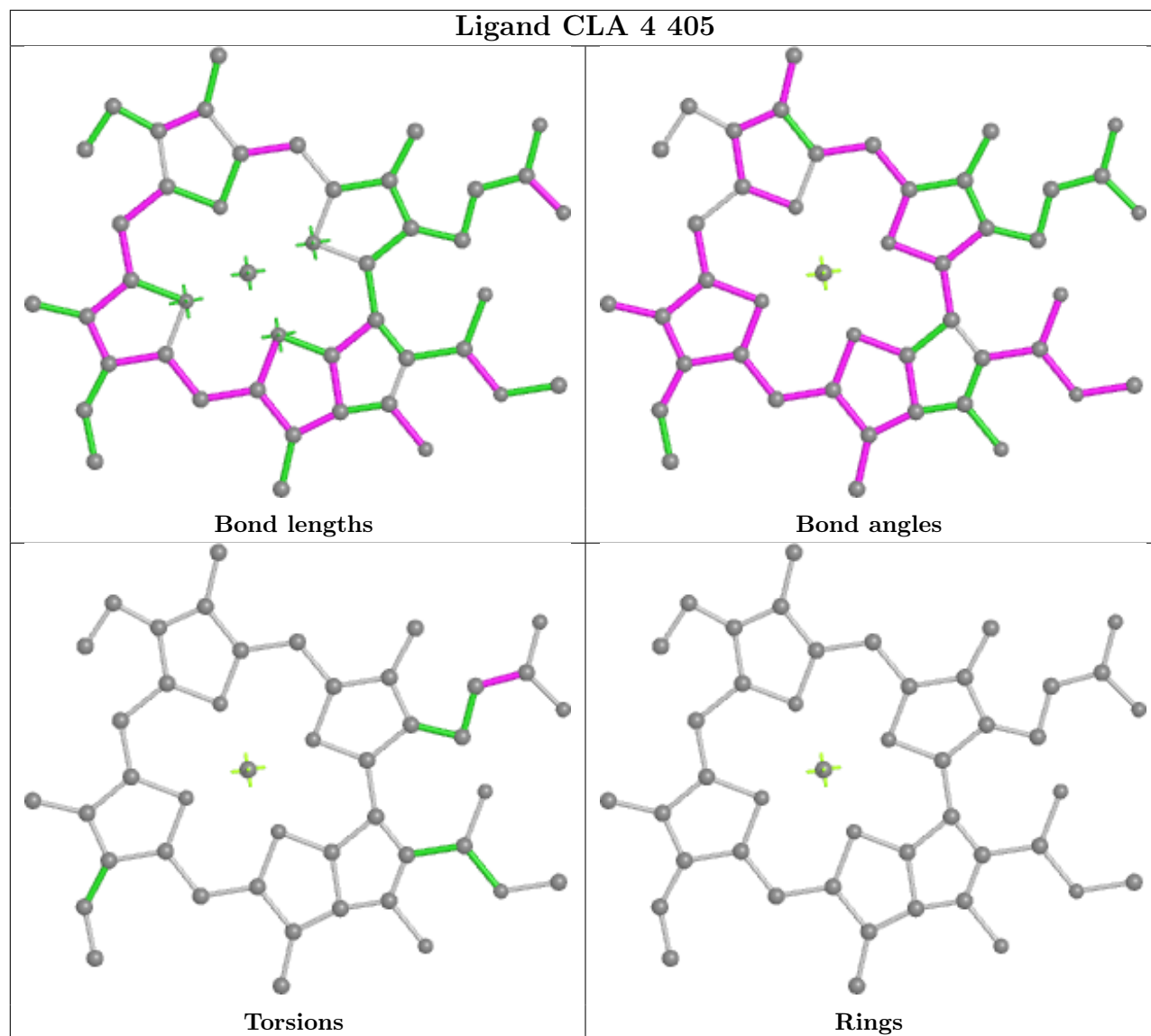
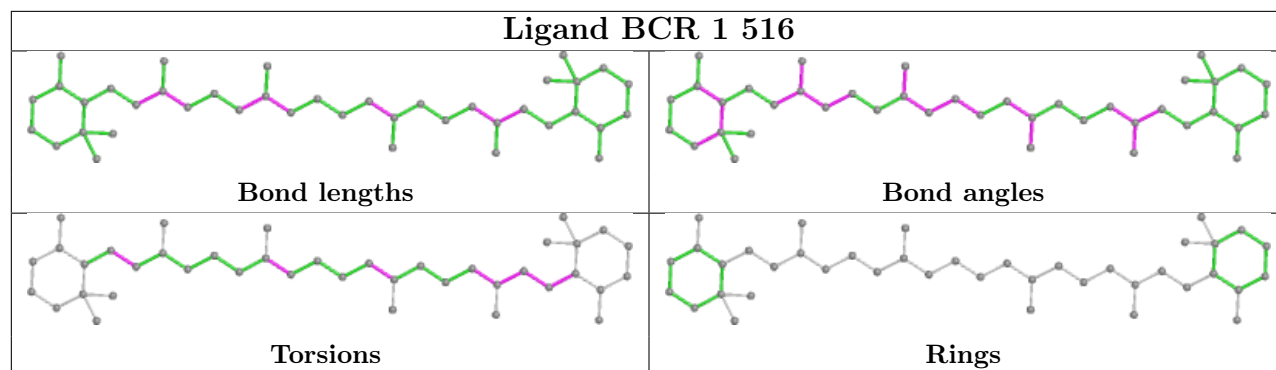


Ligand CLA 2 406

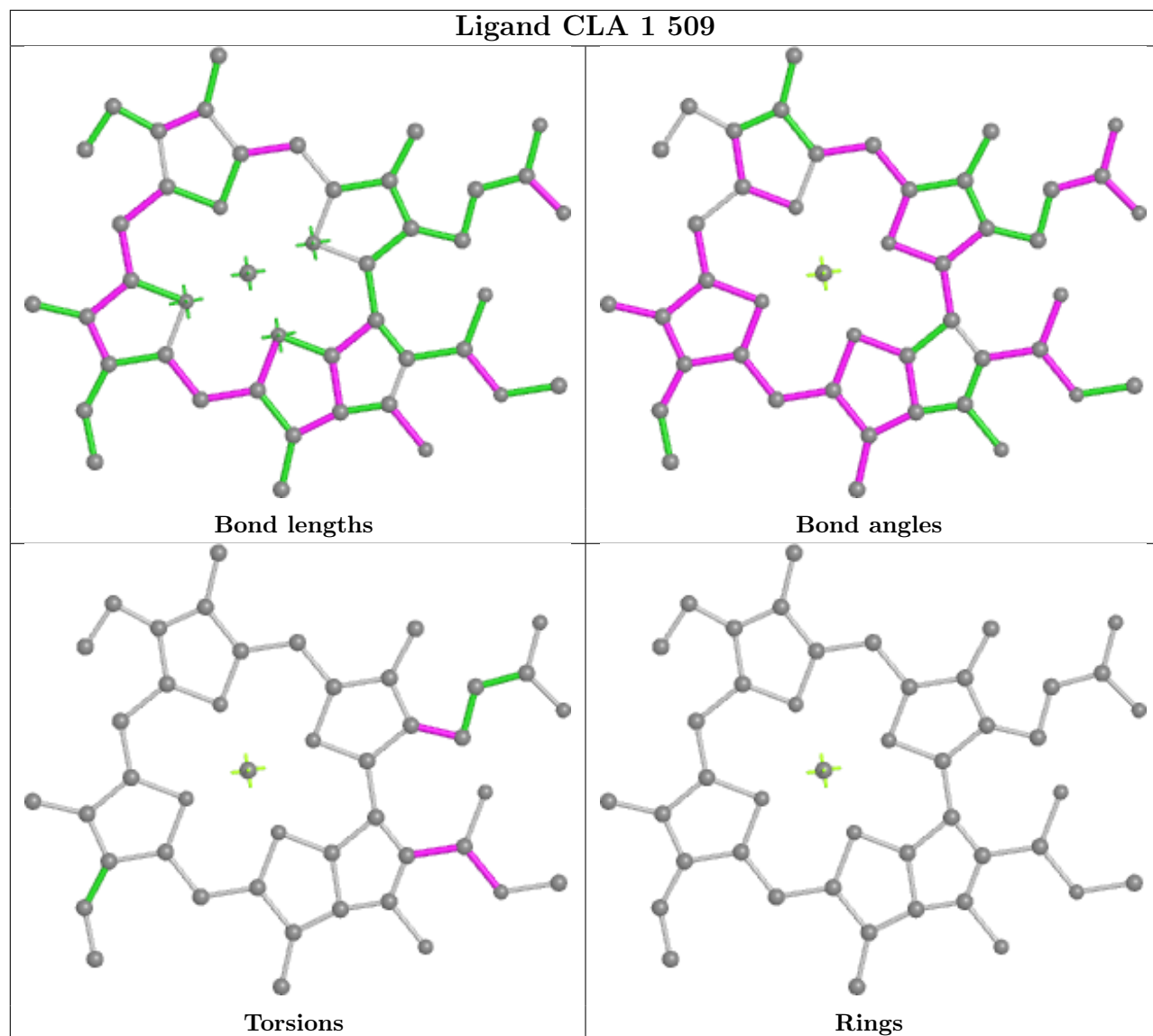


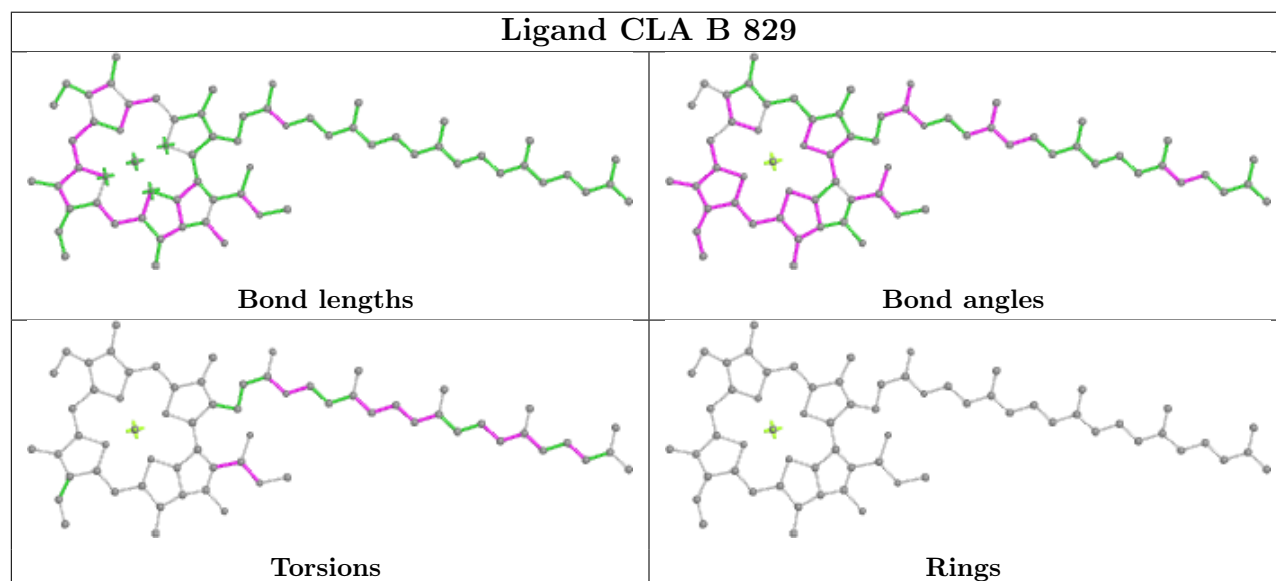
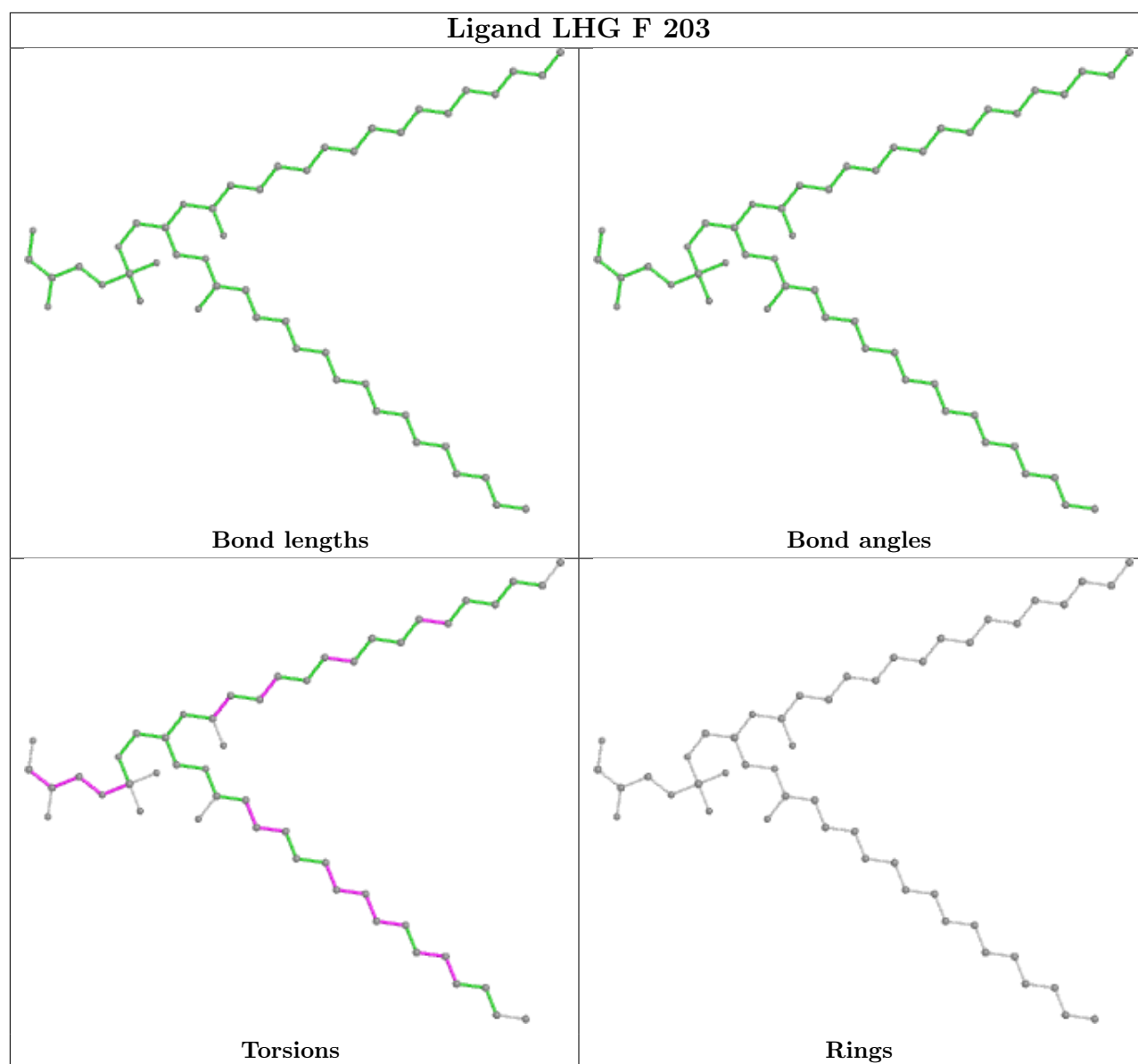
Ligand BCR I 102



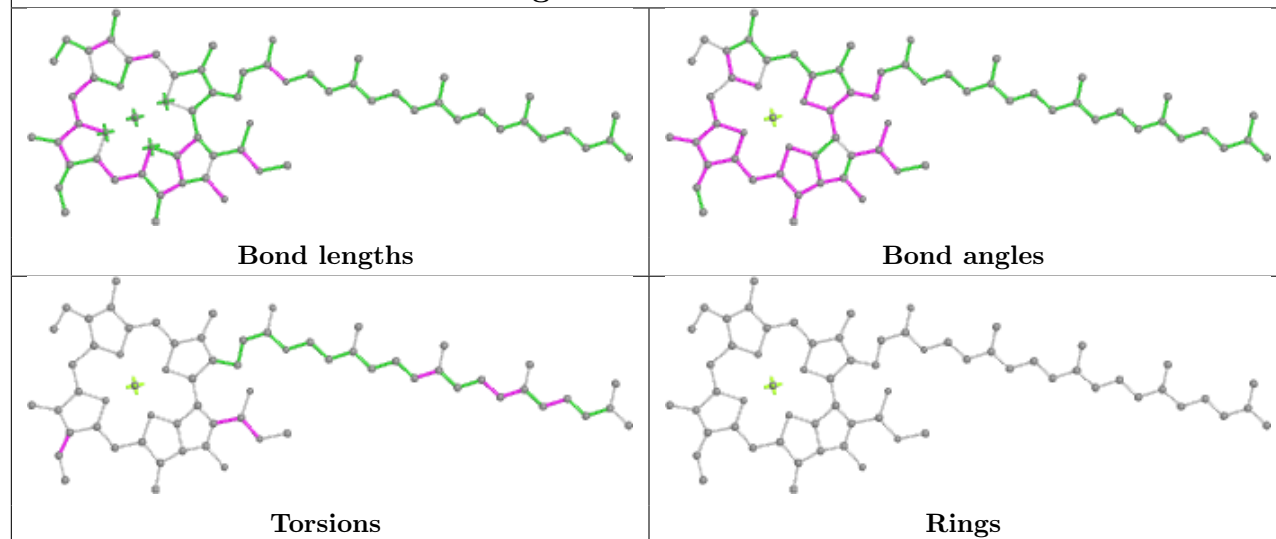


Ligand CLA 1 509

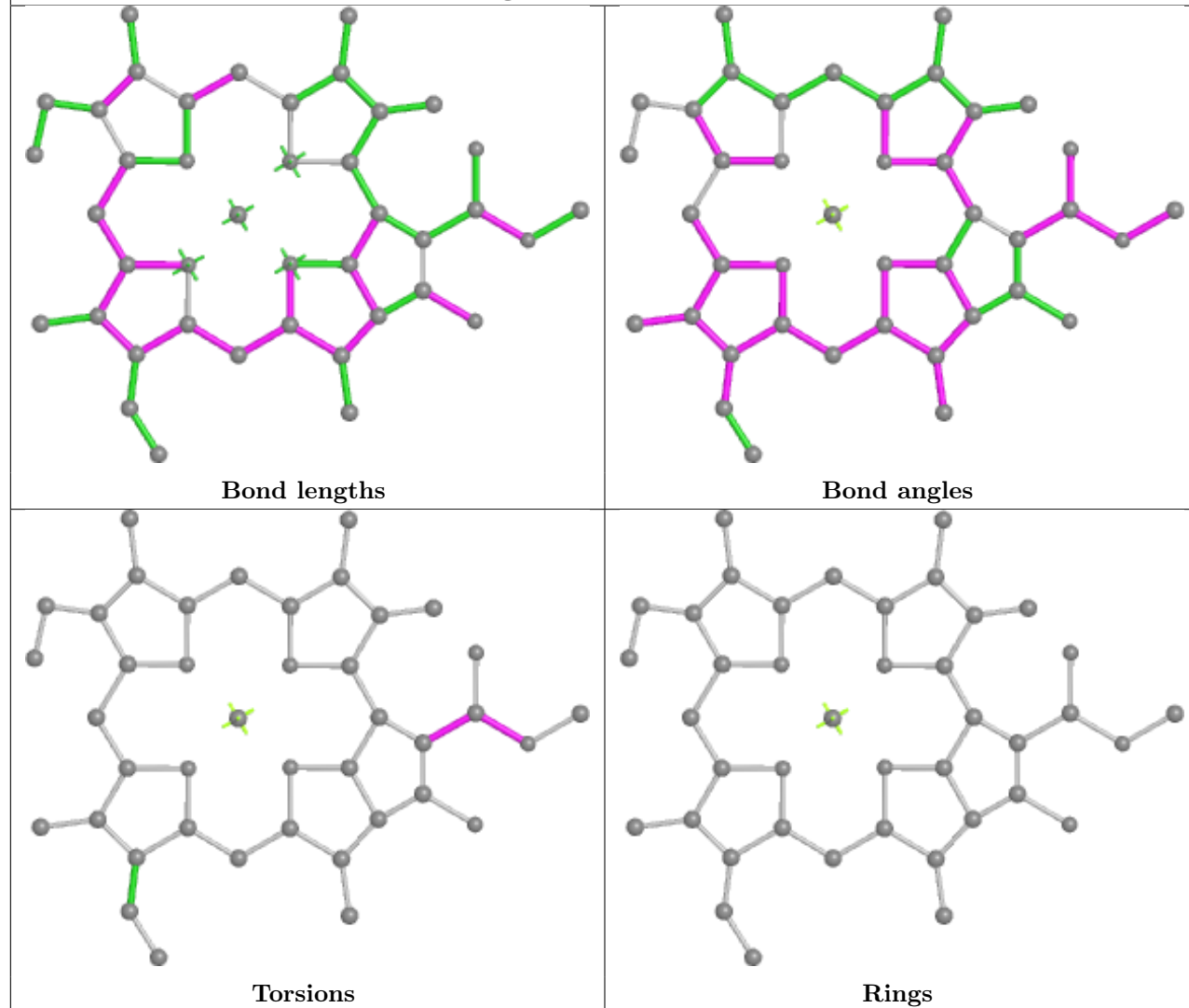


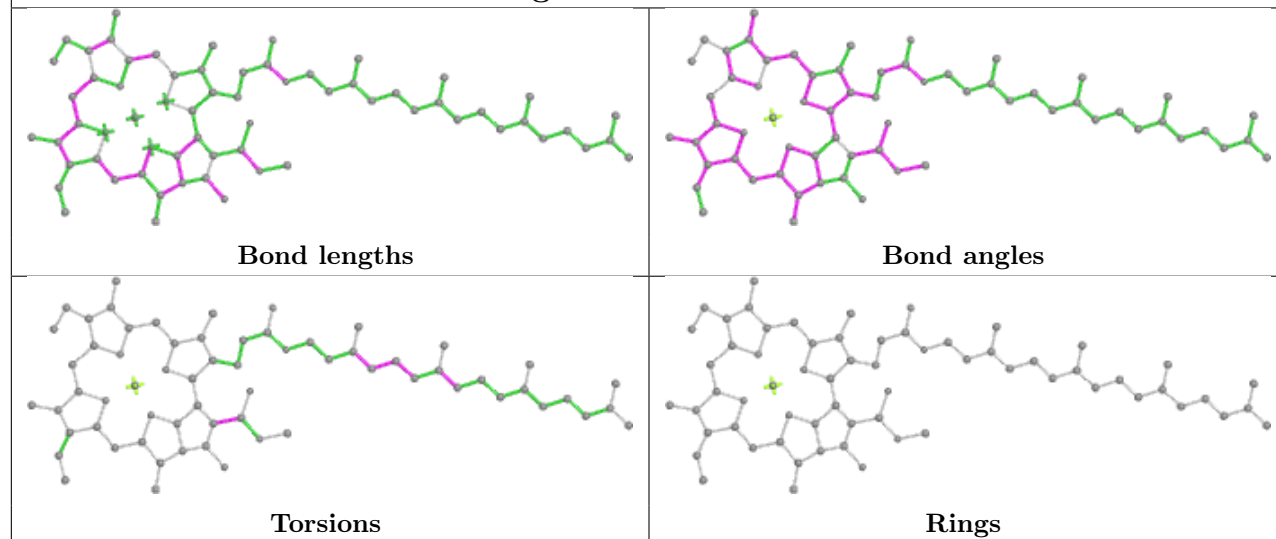
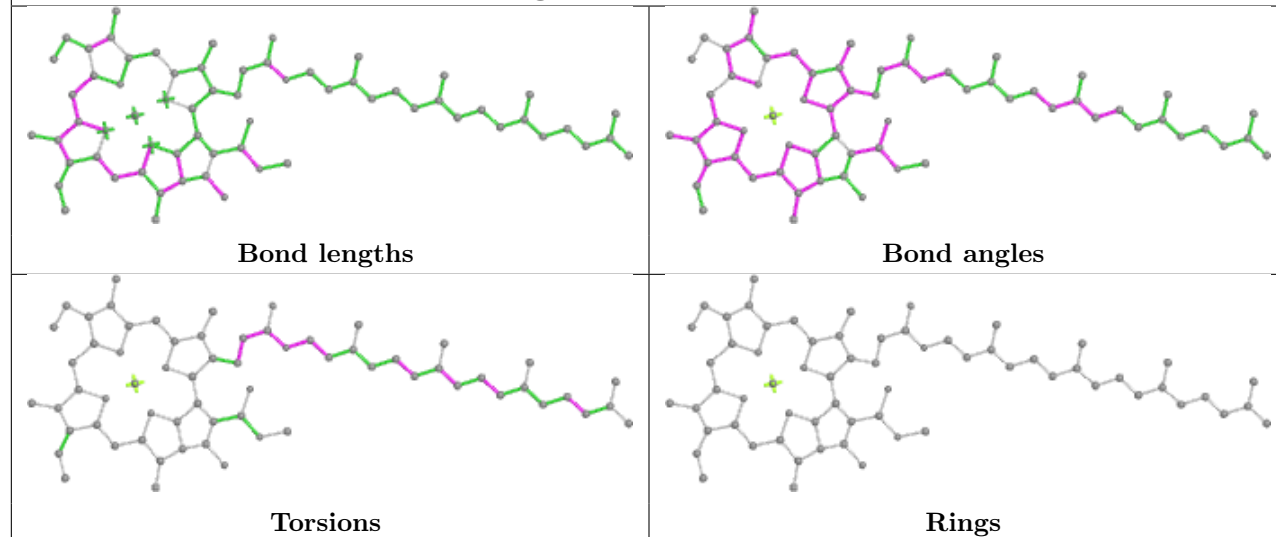


Ligand CLA B 826

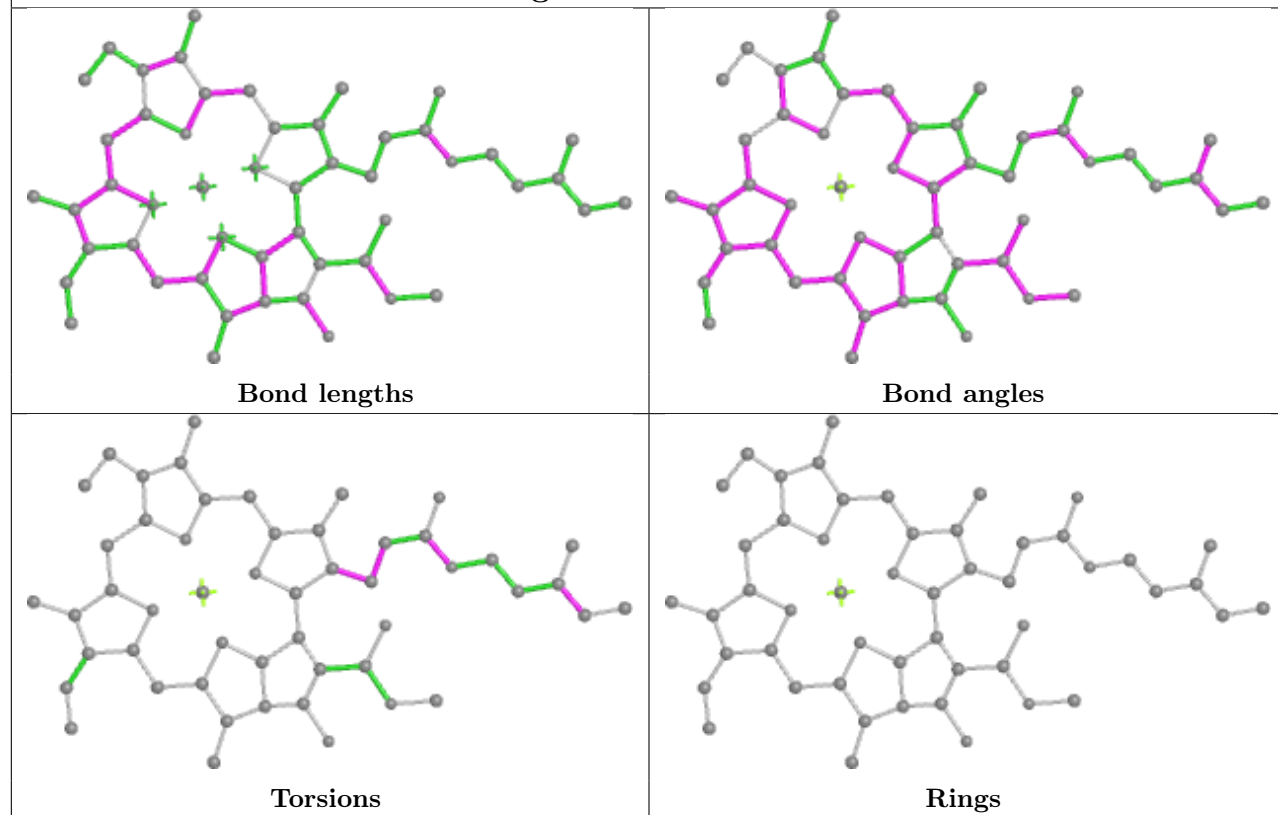


Ligand CLA 5 416

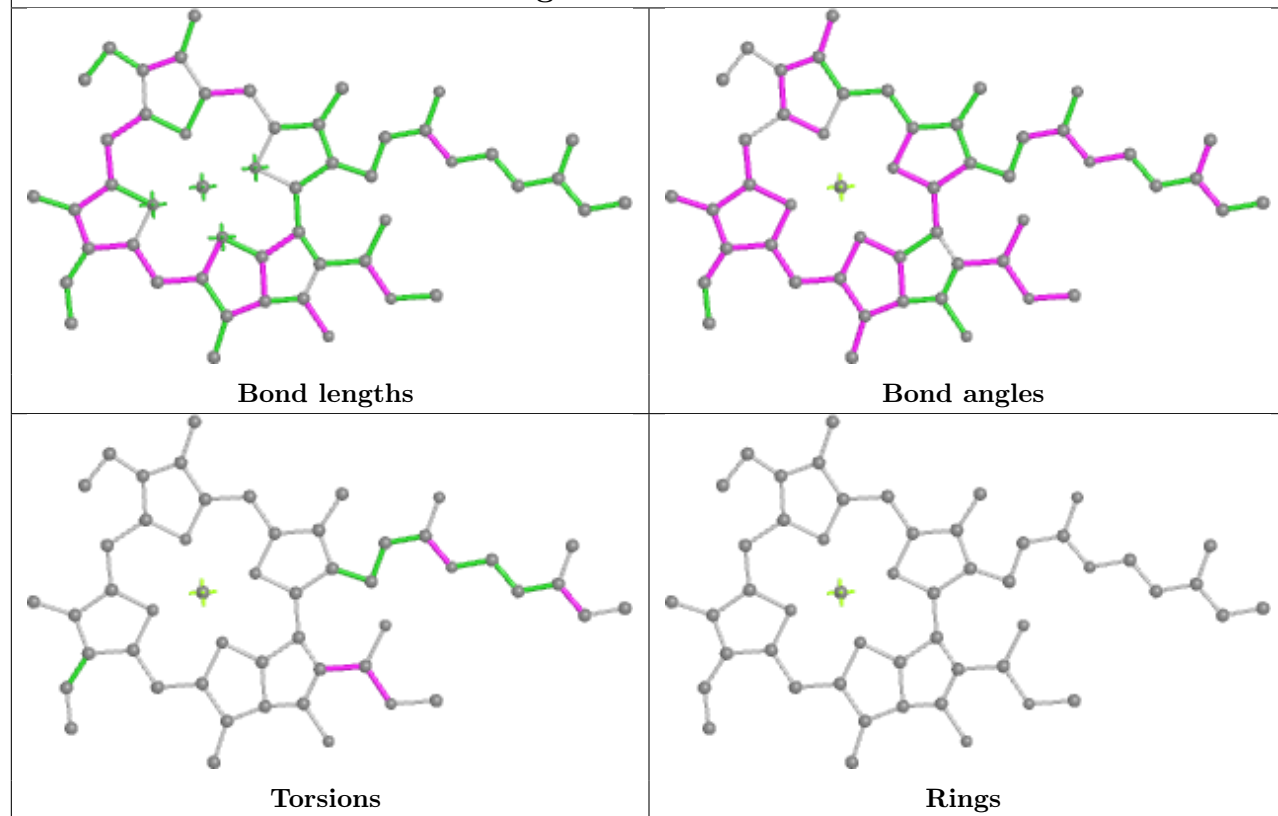


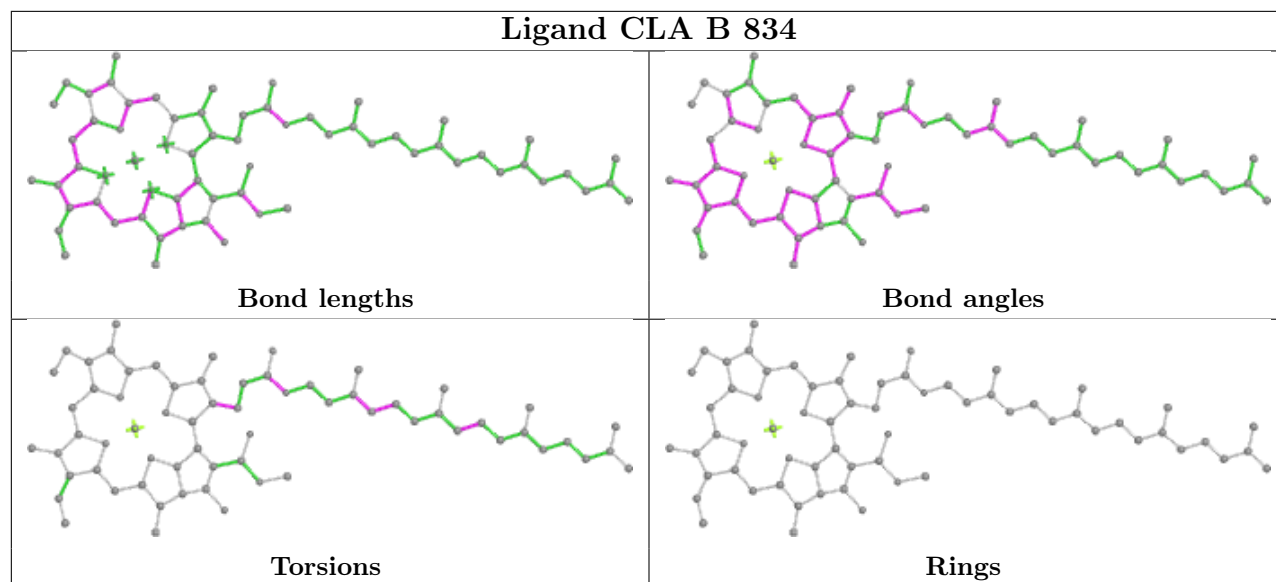
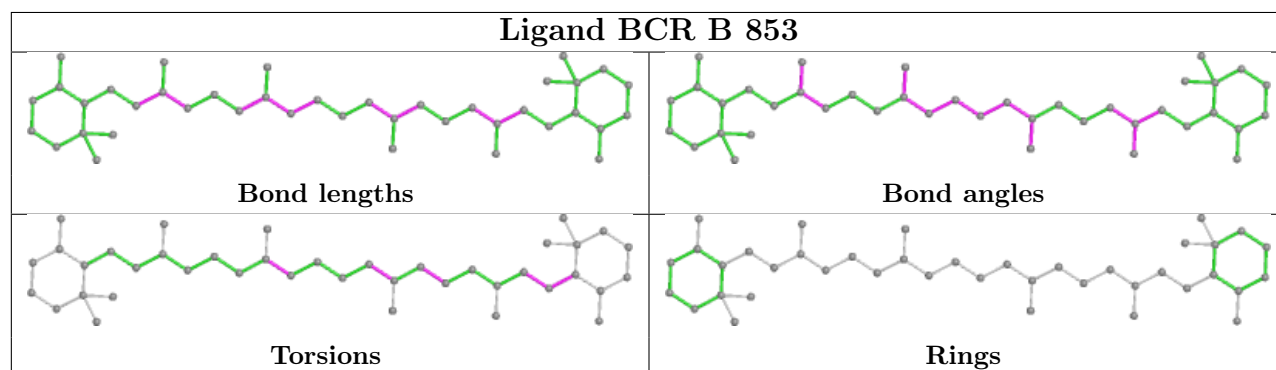
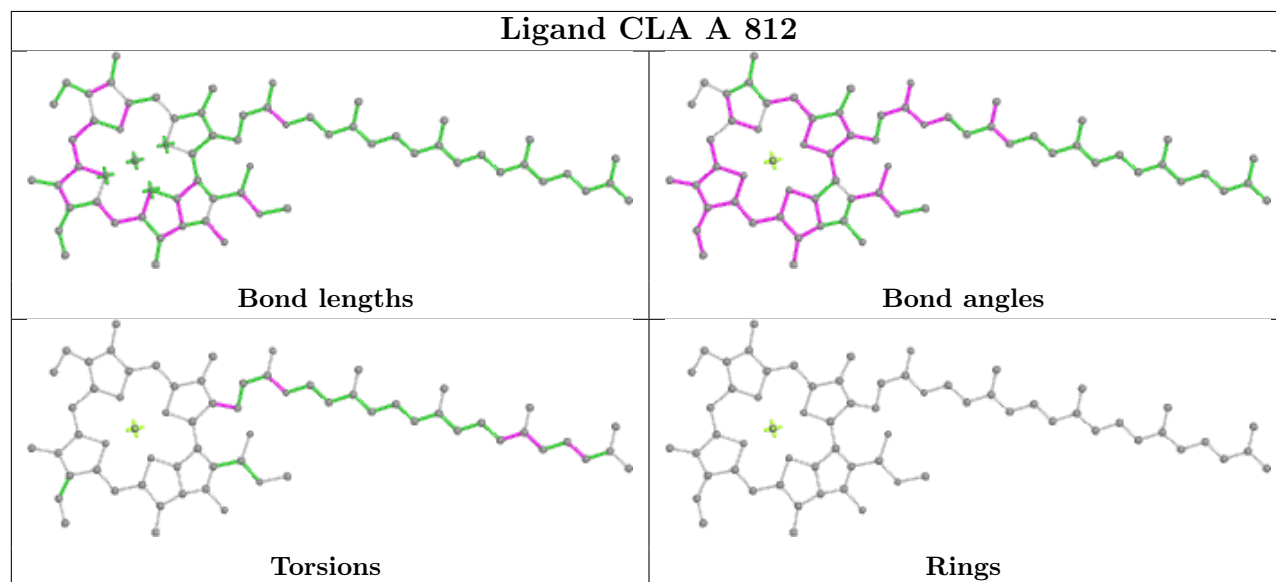
Ligand CLA B 838**Ligand CLA A 803**

Ligand CLA A 838

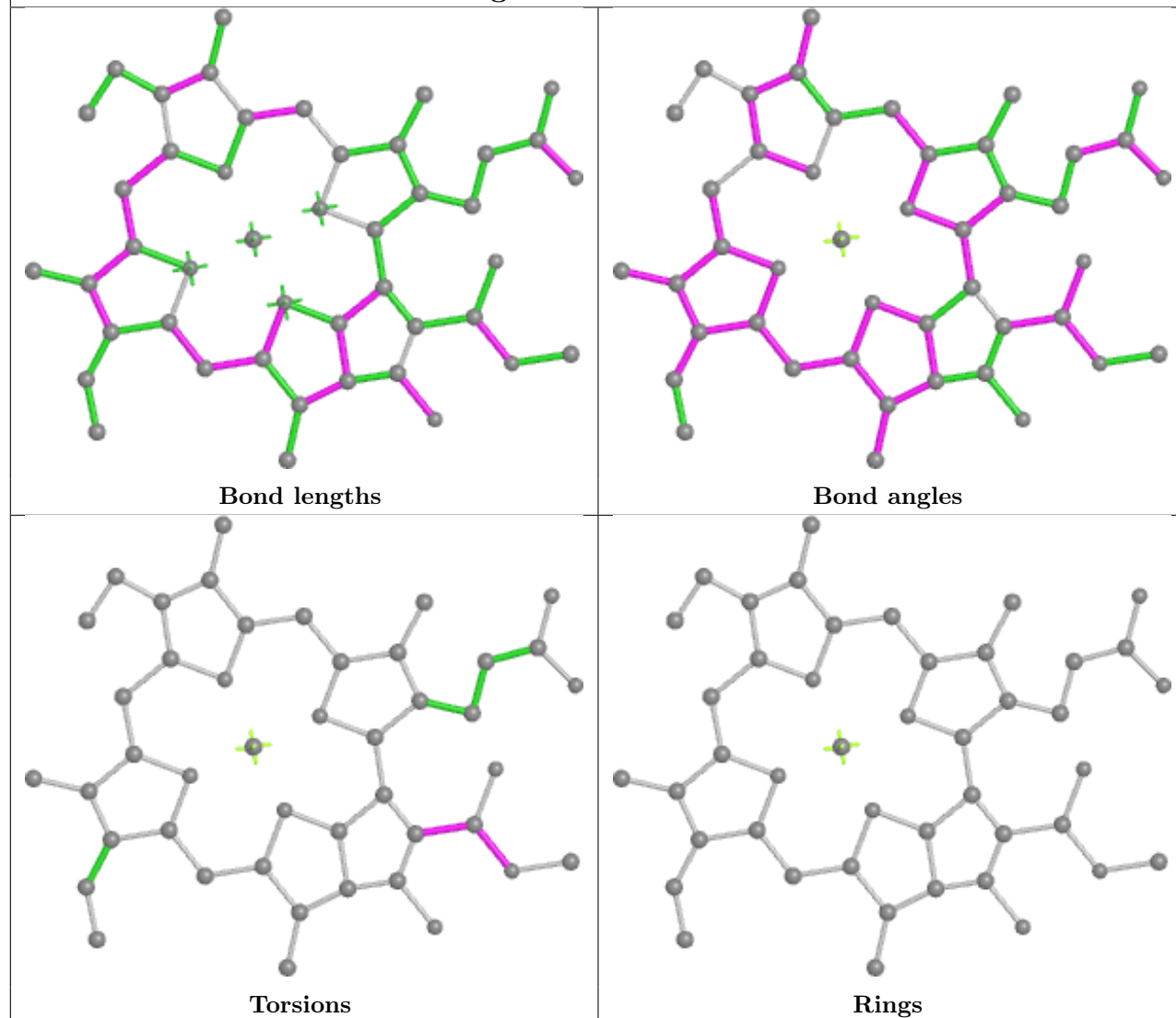


Ligand CLA 1 503

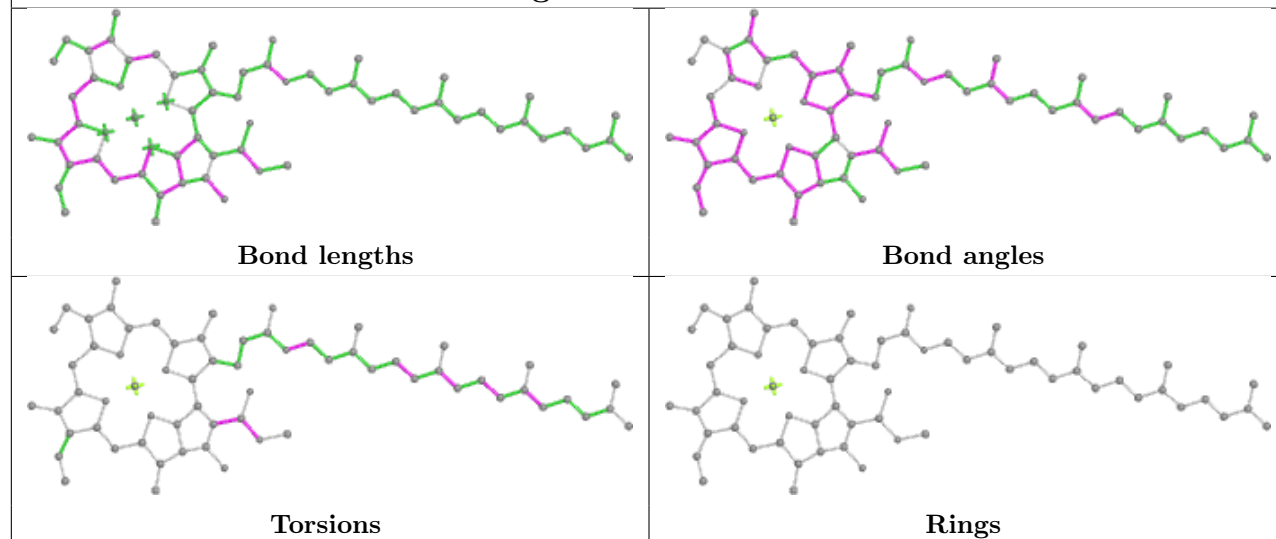


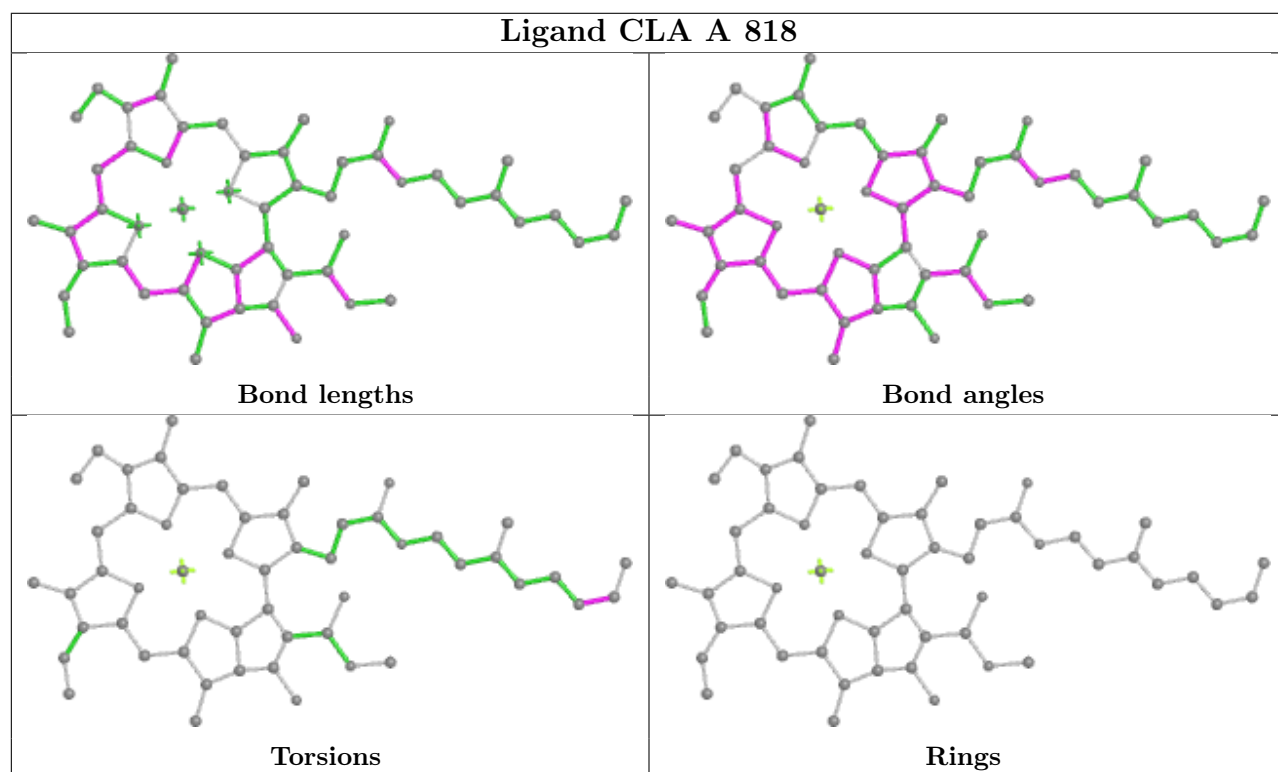
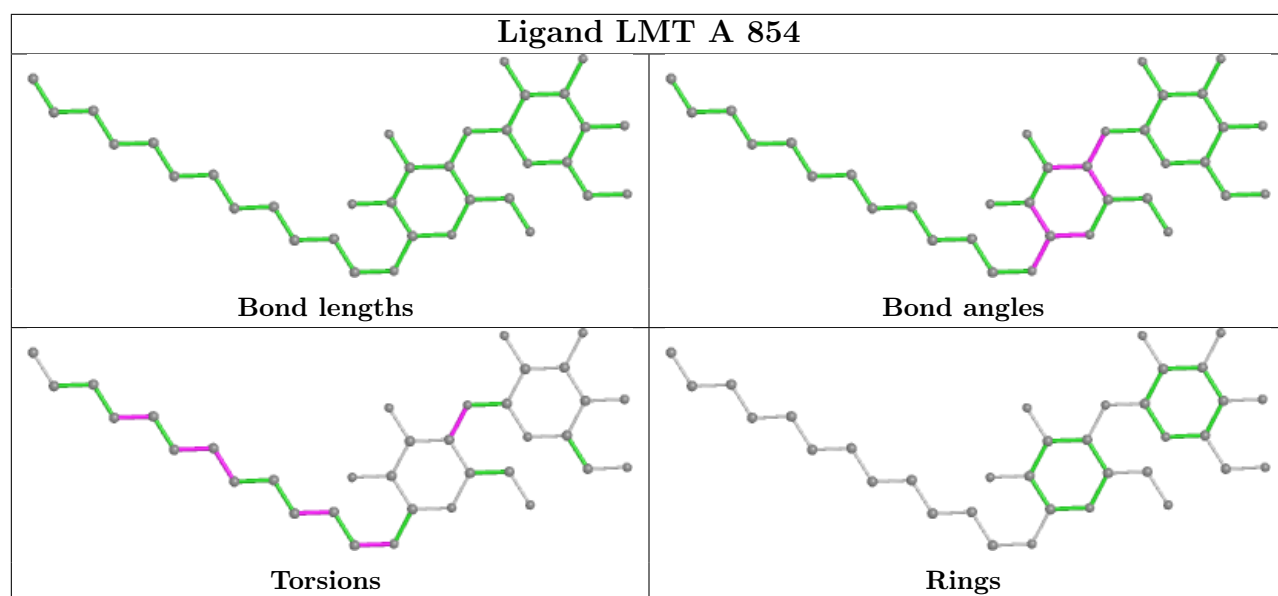
Ligand CLA B 834**Ligand BCR B 853****Ligand CLA A 812**

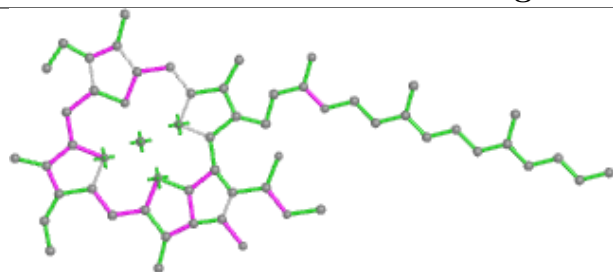
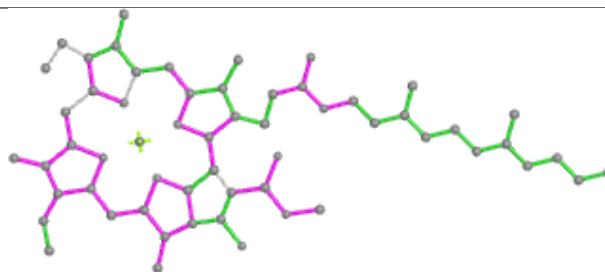
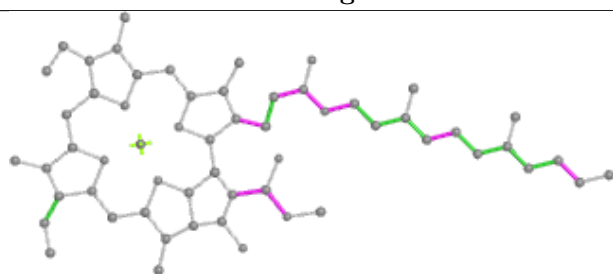
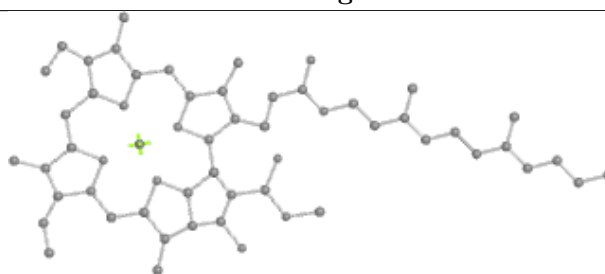
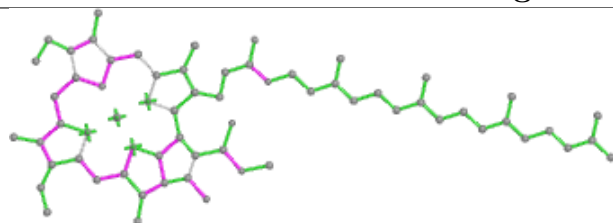
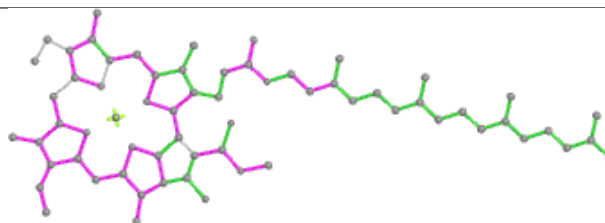
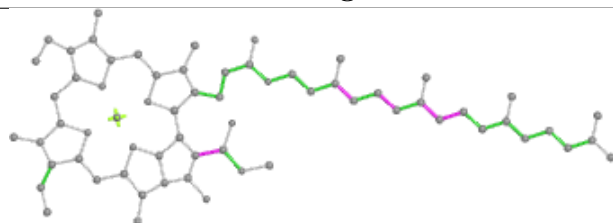
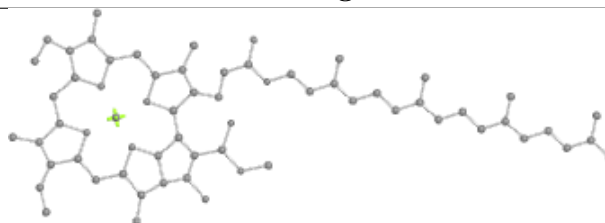
Ligand CLA B 821



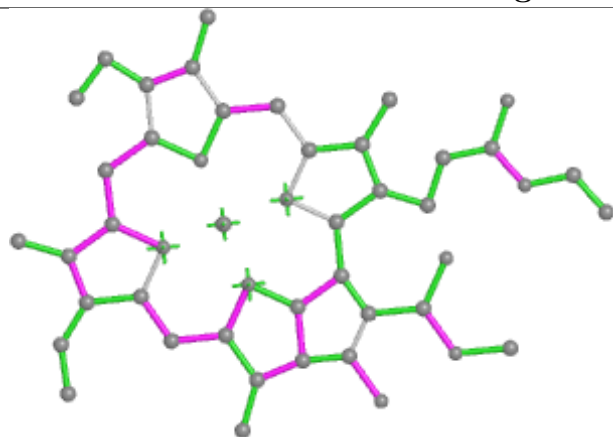
Ligand CLA B 801



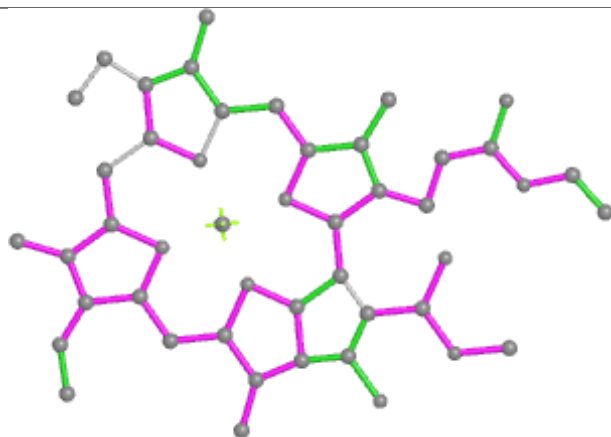


Ligand CLA B 833**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 841****Bond lengths****Bond angles****Torsions****Rings**

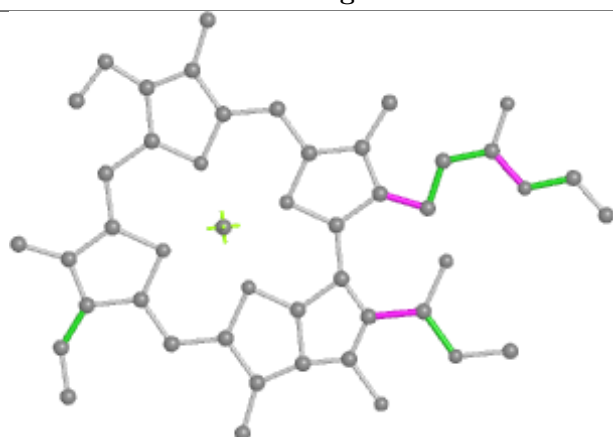
Ligand CLA B 820



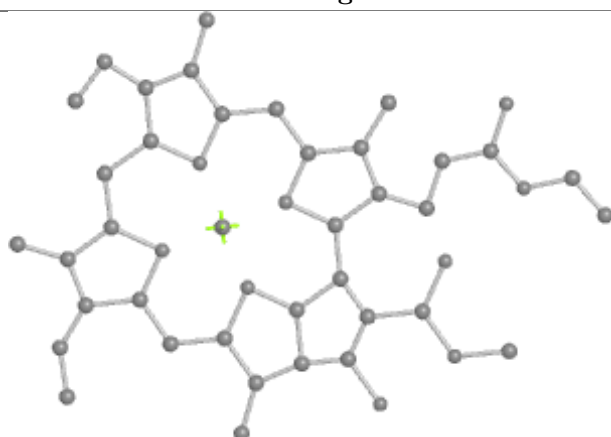
Bond lengths



Bond angles

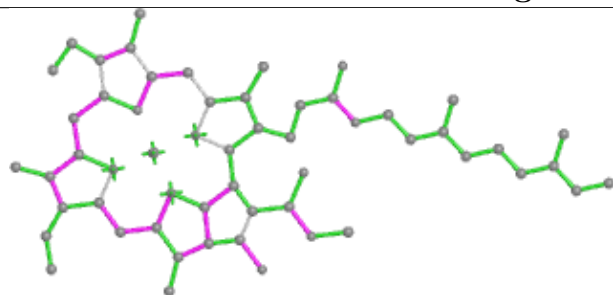


Torsions

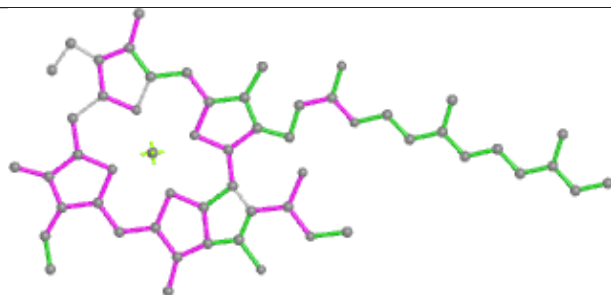


Rings

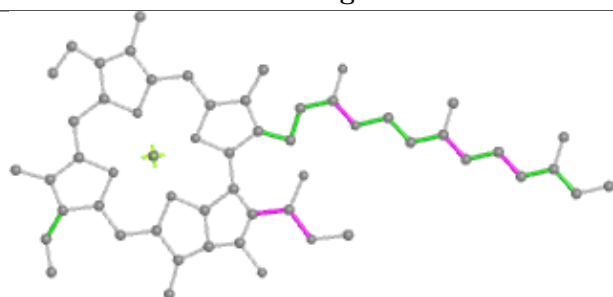
Ligand CLA B 814



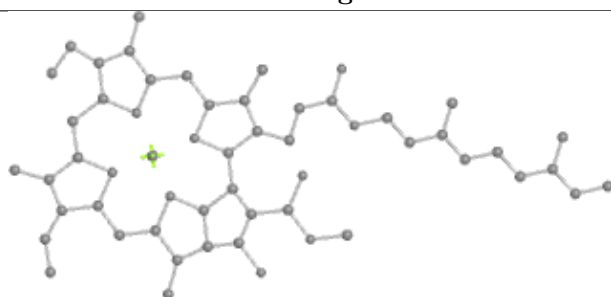
Bond lengths



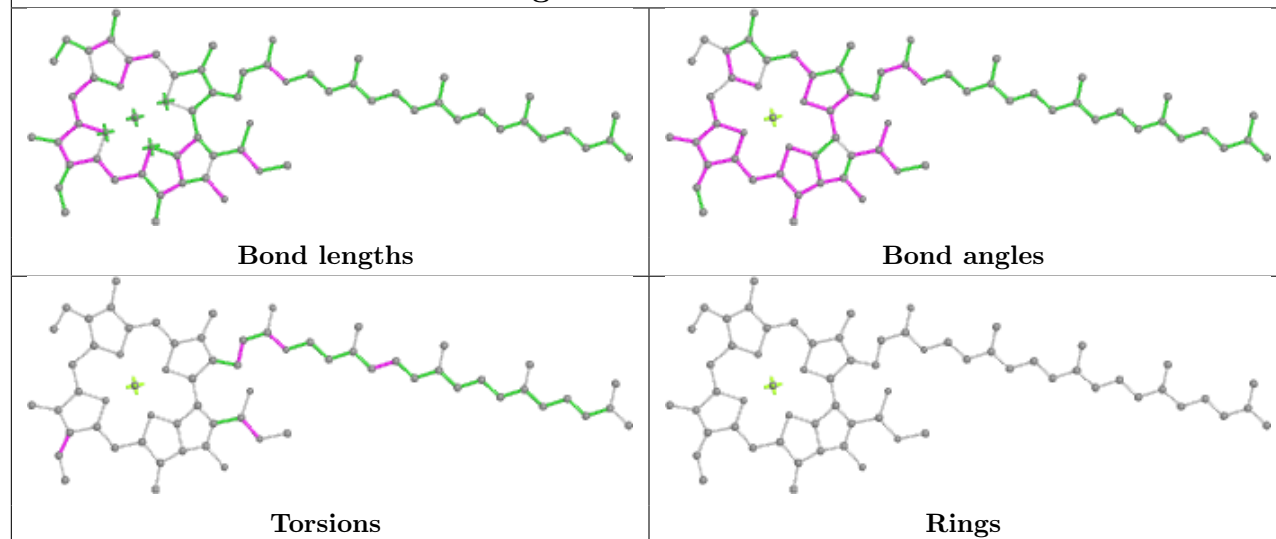
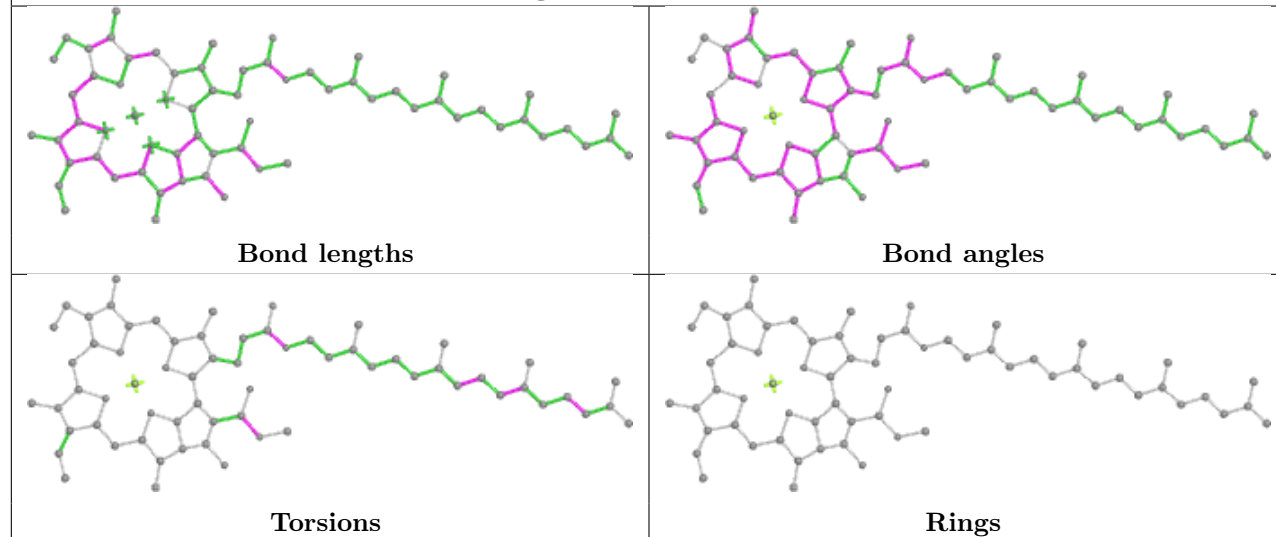
Bond angles



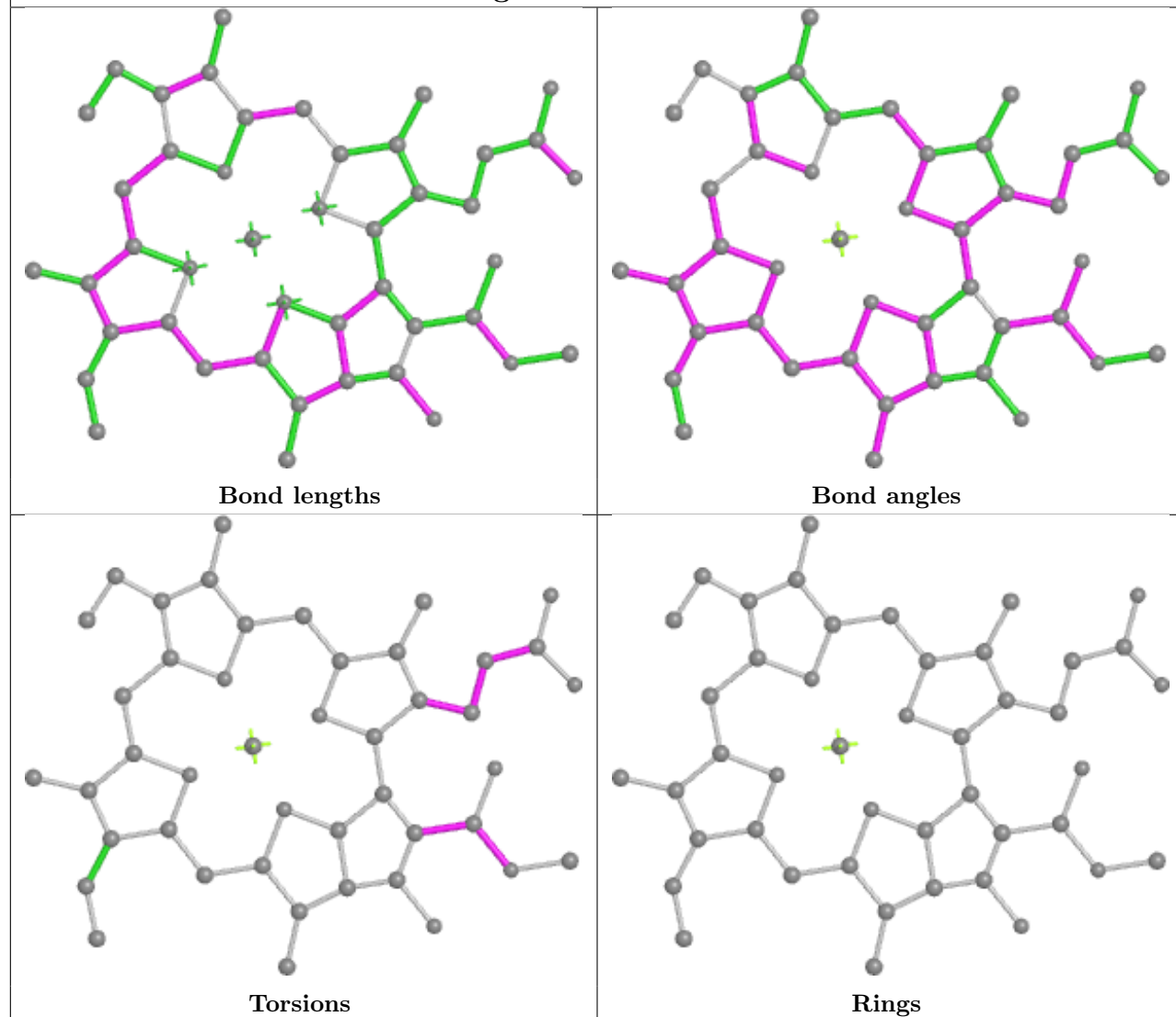
Torsions



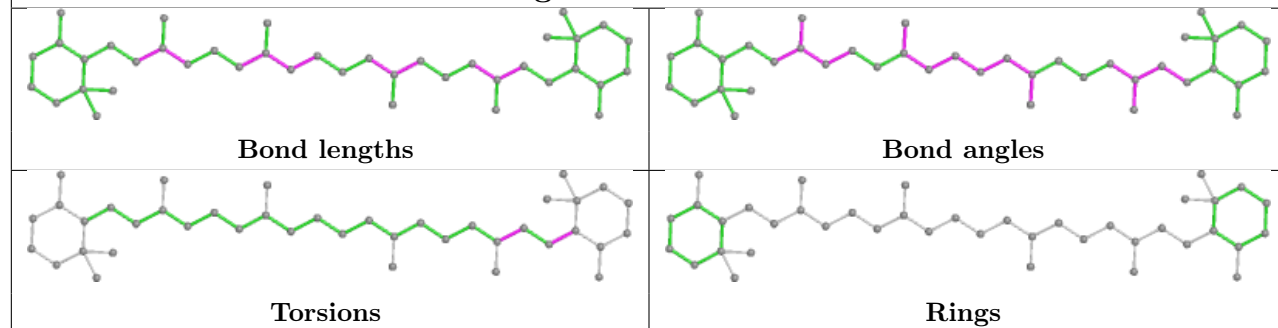
Rings

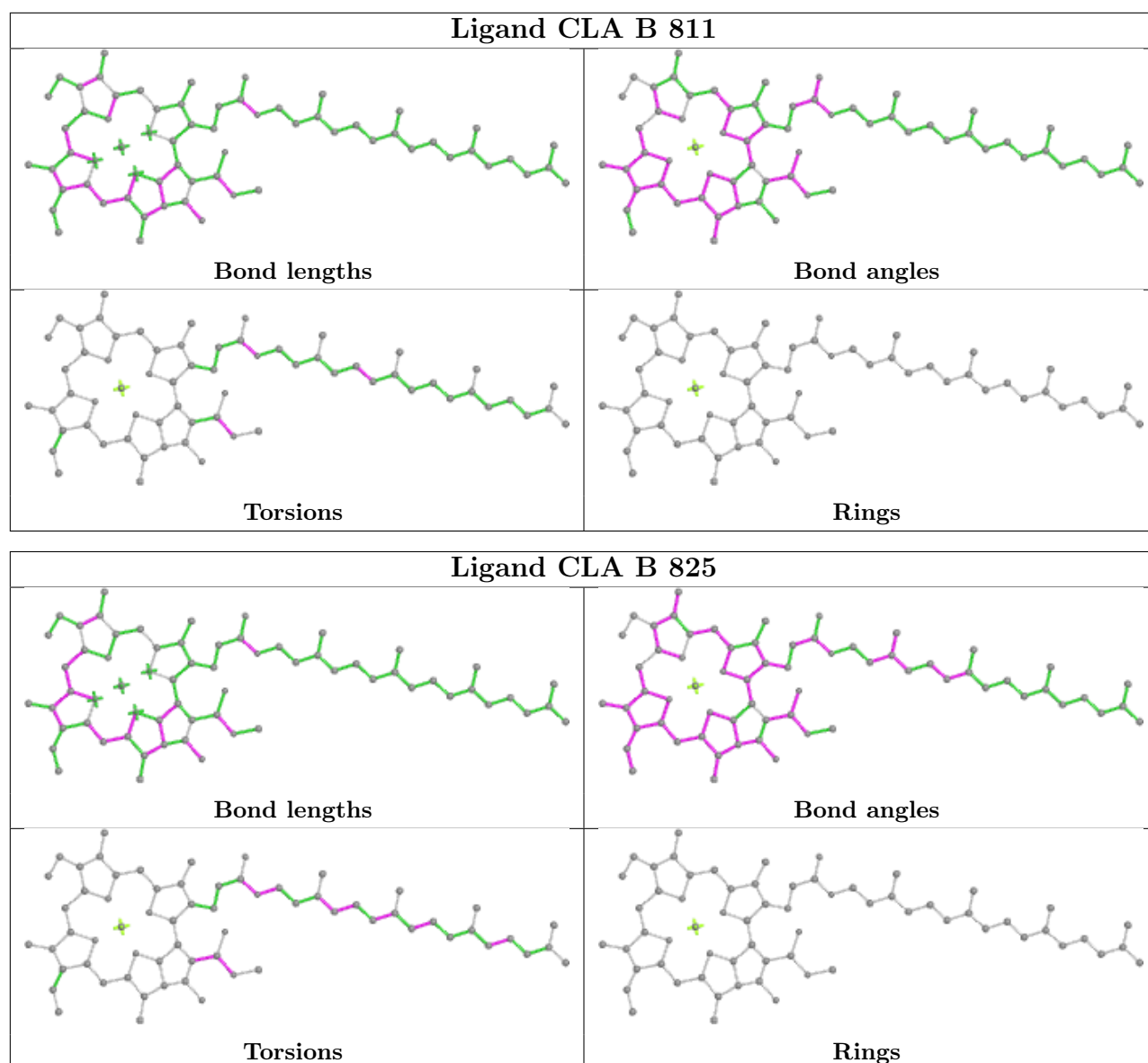
Ligand CLA B 841**Ligand CLA B 831**

Ligand CLA 1 525



Ligand BCR 1 522





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.

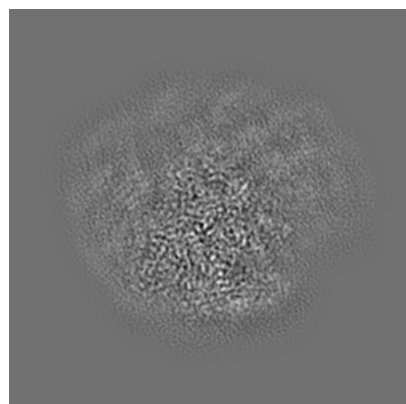
6 Map visualisation [i](#)

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.

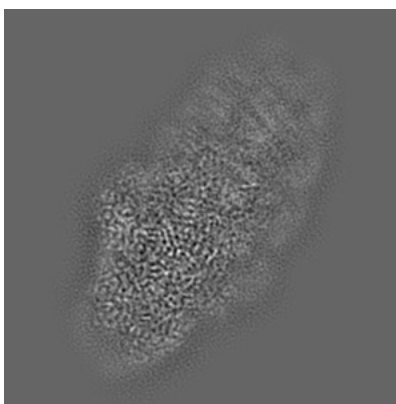
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

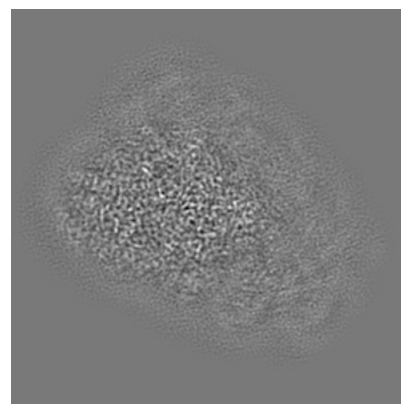
6.1.1 Primary map



X

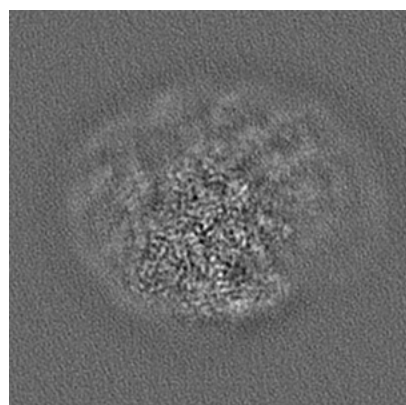


Y

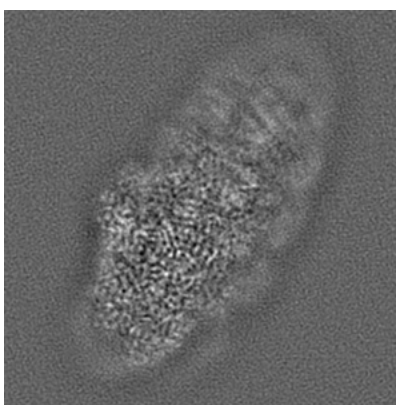


Z

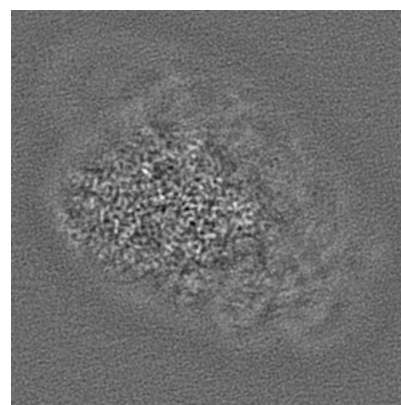
6.1.2 Raw map



X



Y

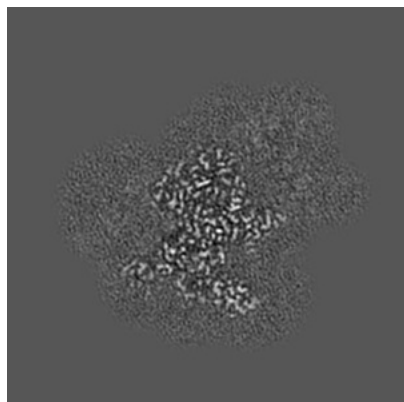


Z

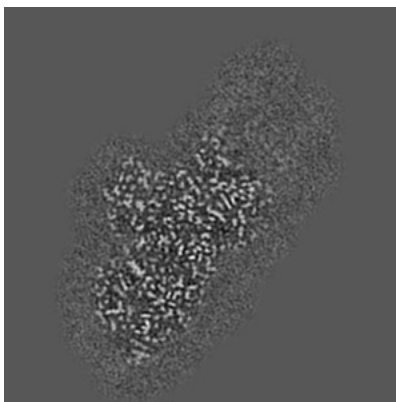
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

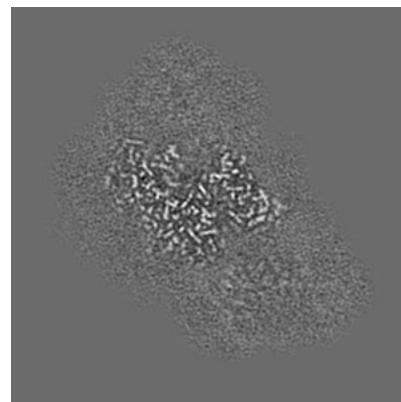
6.2.1 Primary map



X Index: 116

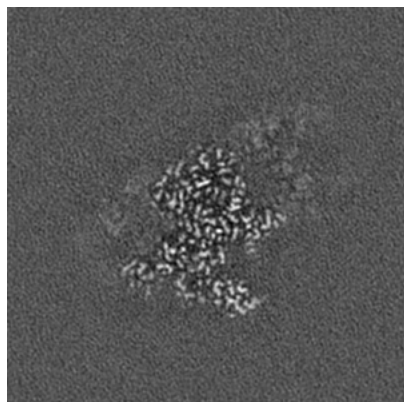


Y Index: 116

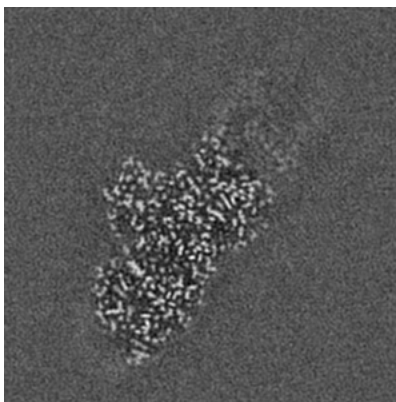


Z Index: 116

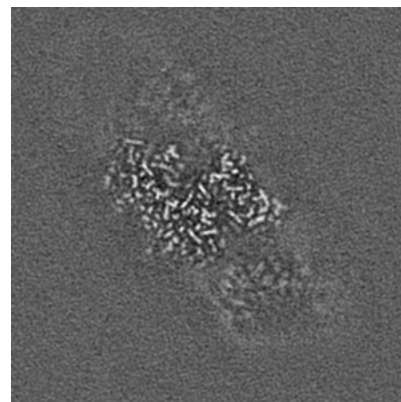
6.2.2 Raw map



X Index: 116



Y Index: 116

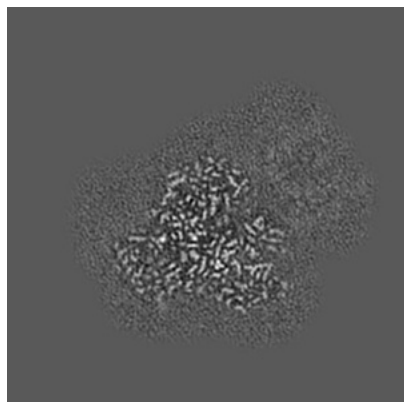


Z Index: 116

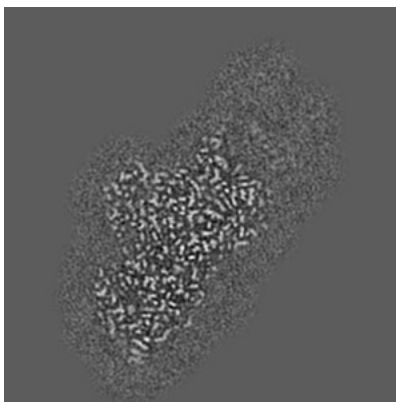
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

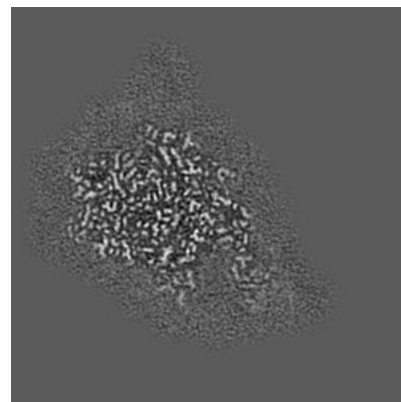
6.3.1 Primary map



X Index: 102

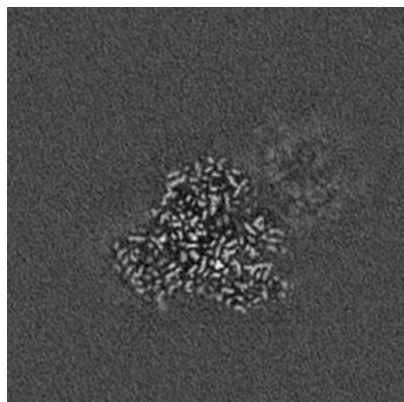


Y Index: 117

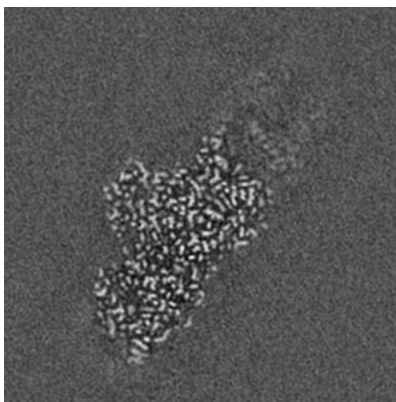


Z Index: 96

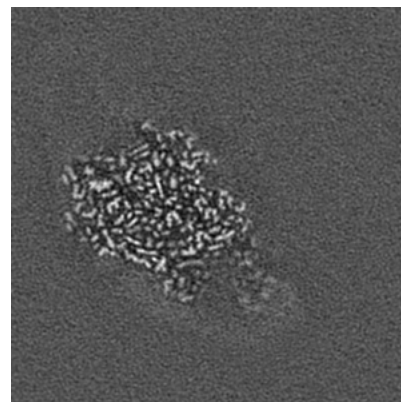
6.3.2 Raw map



X Index: 102



Y Index: 117

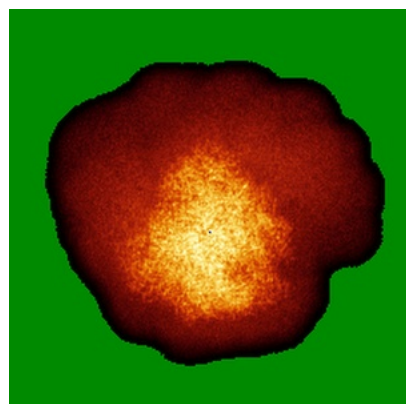


Z Index: 92

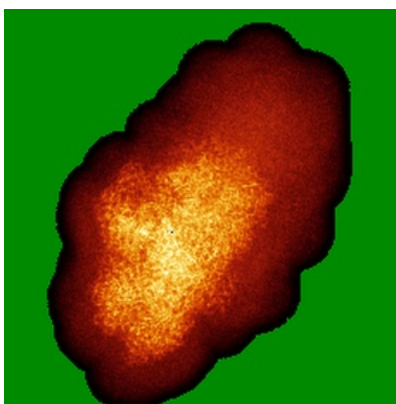
The images above show the largest variance slices of the map in three orthogonal directions.

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

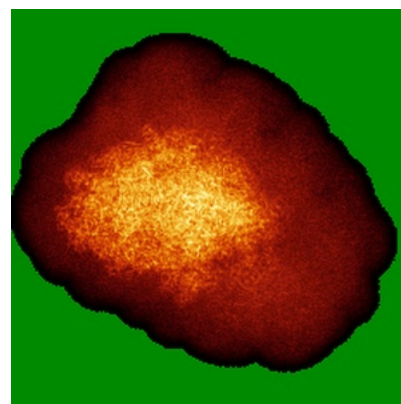
6.4.1 Primary map



X

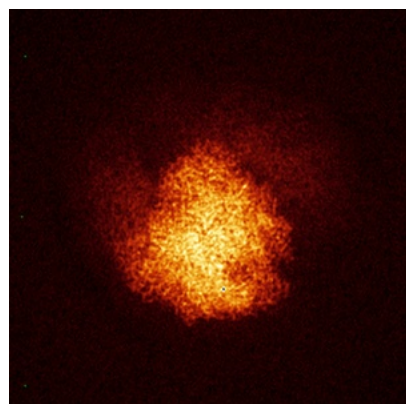


Y

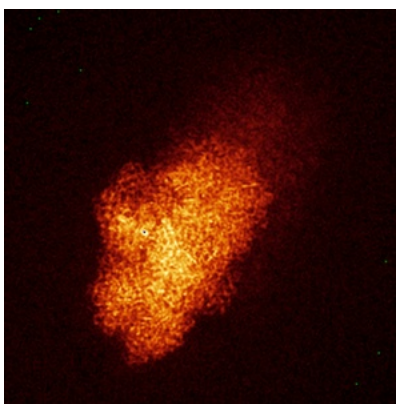


Z

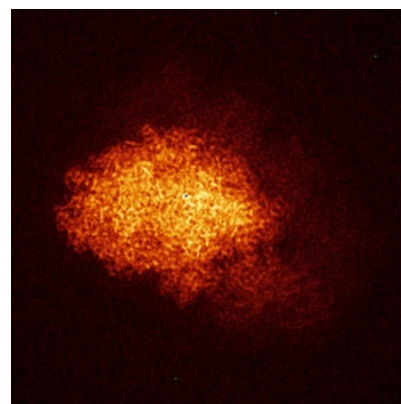
6.4.2 Raw map



X



Y

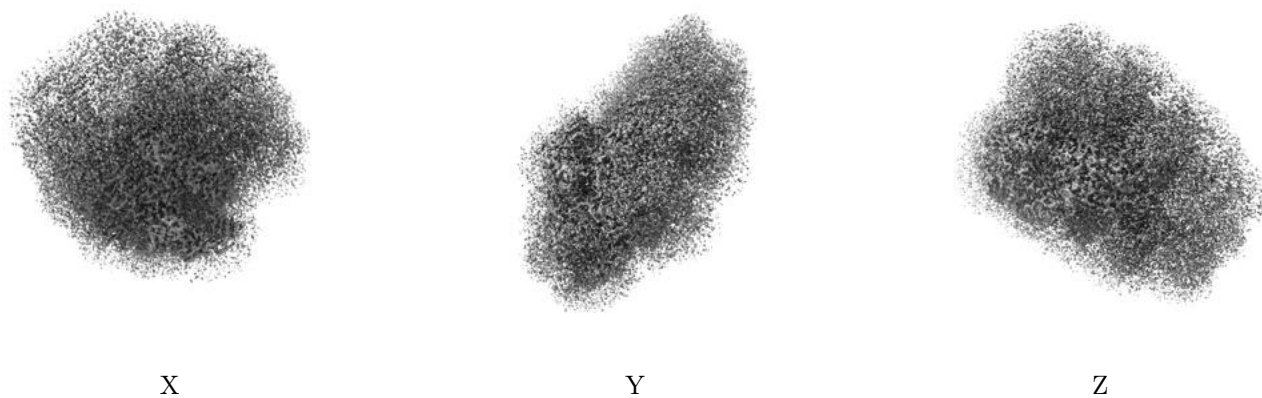


Z

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.

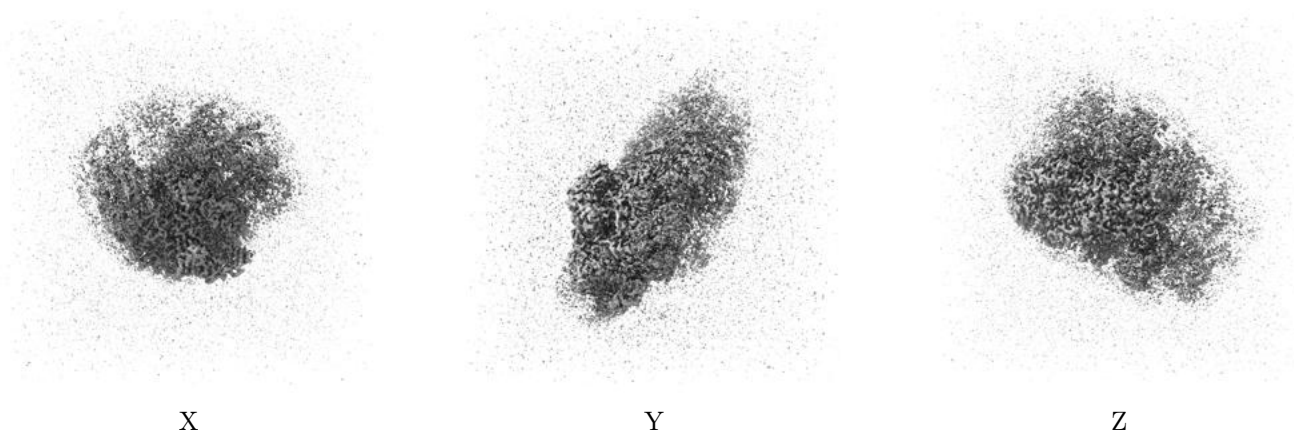
6.5 Orthogonal surface views [i](#)

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.

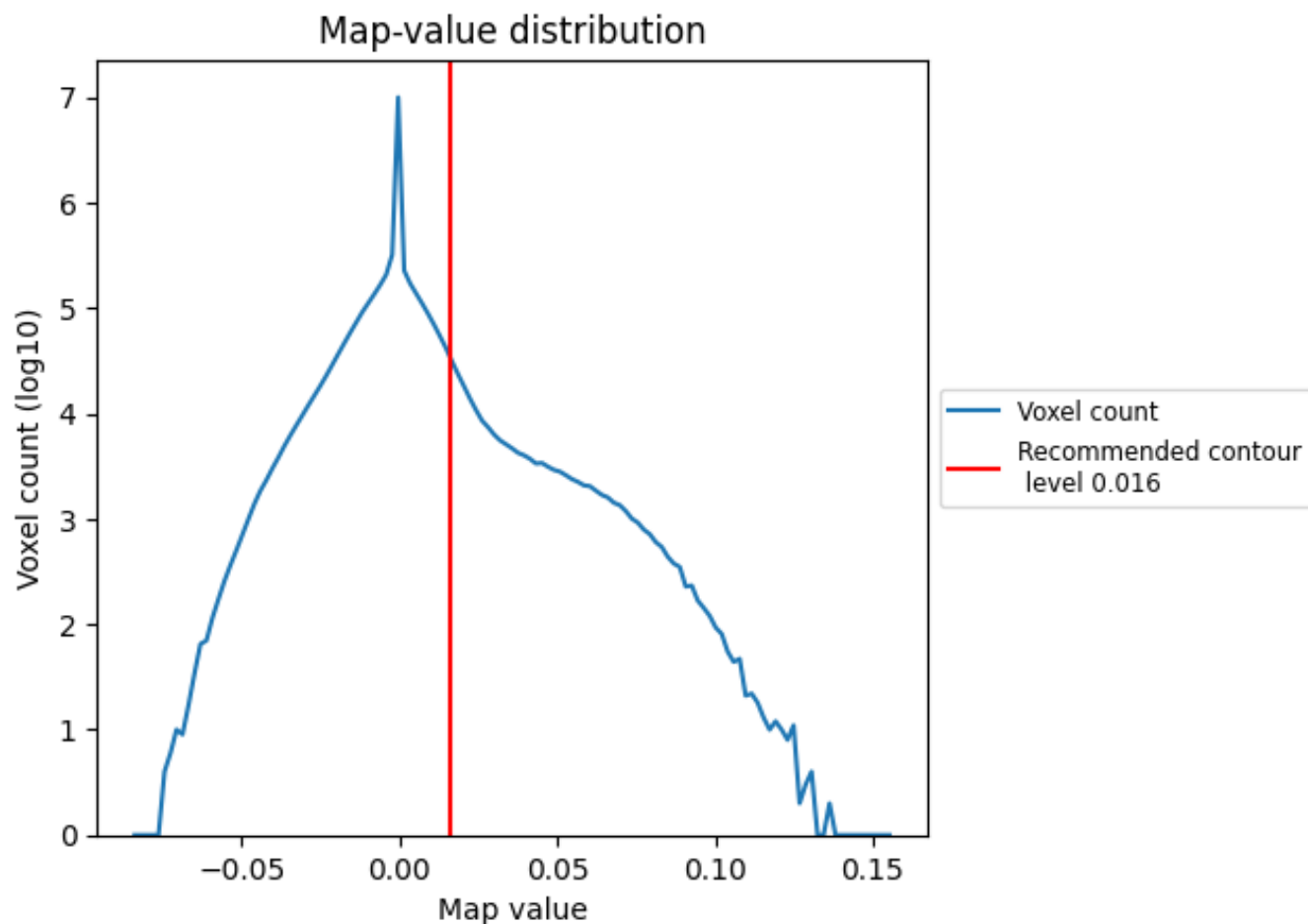
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

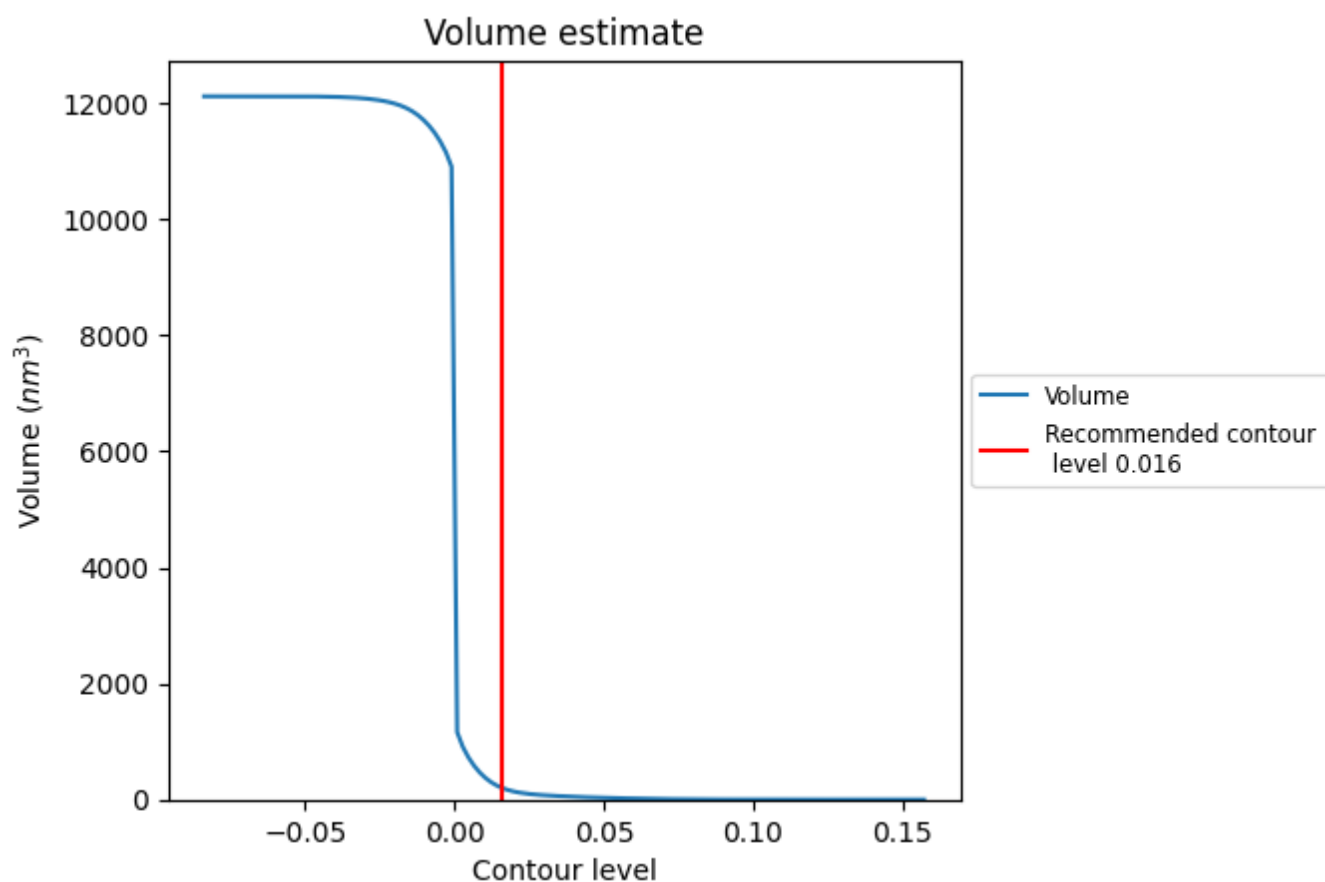
This section contains the results of statistical analysis of the map.

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.

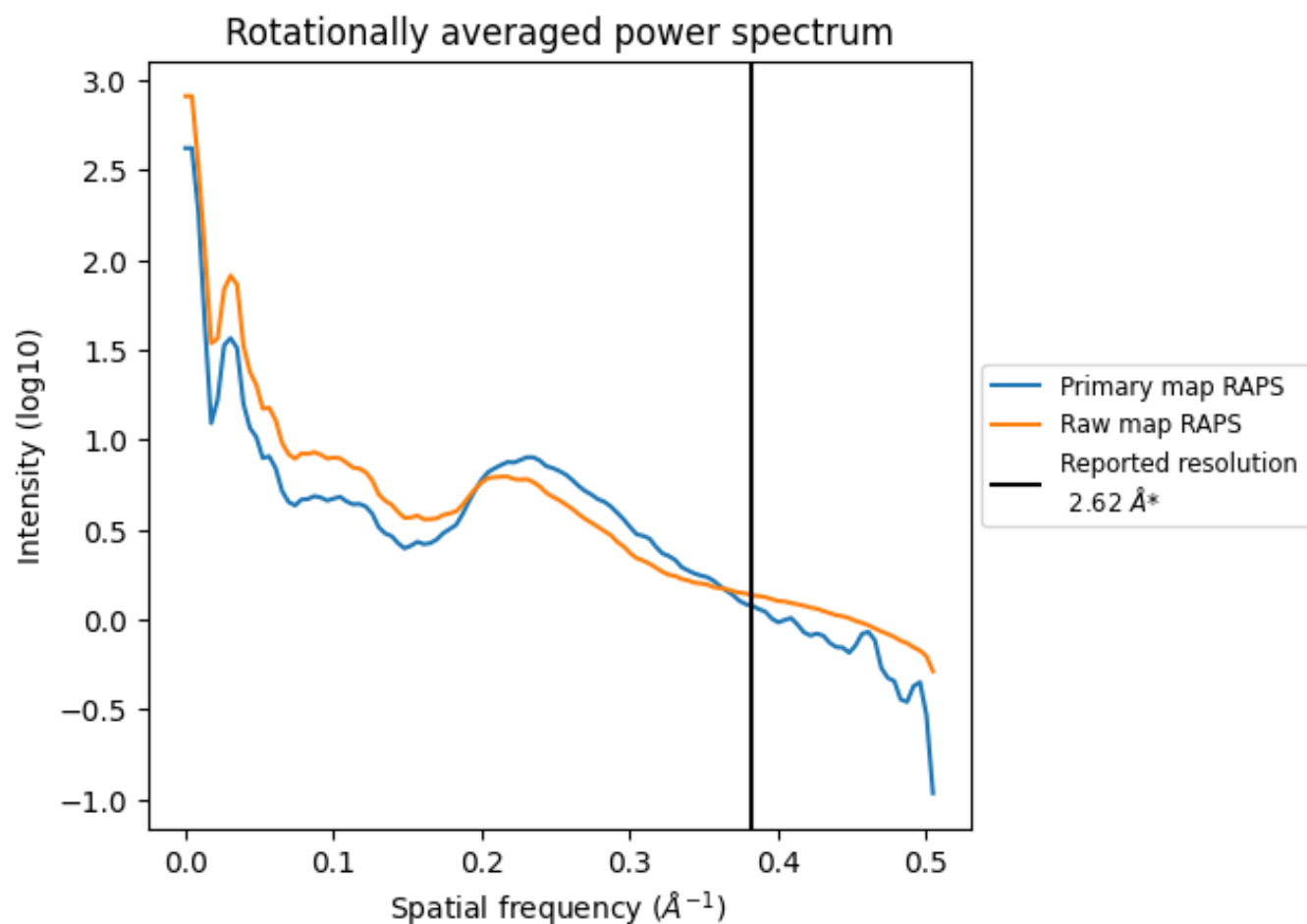
7.2 Volume estimate [i](#)



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 ⓘ

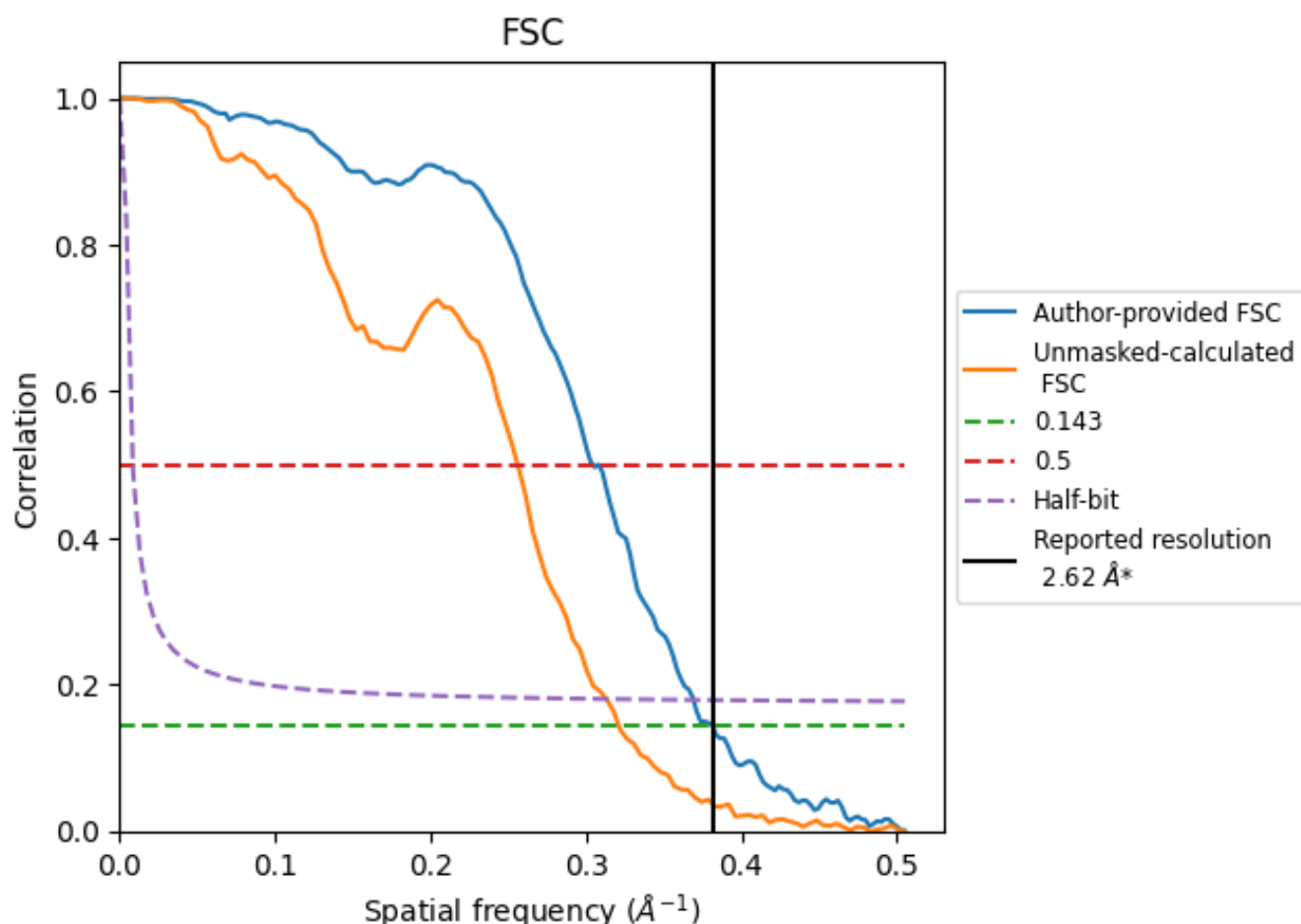


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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](#)

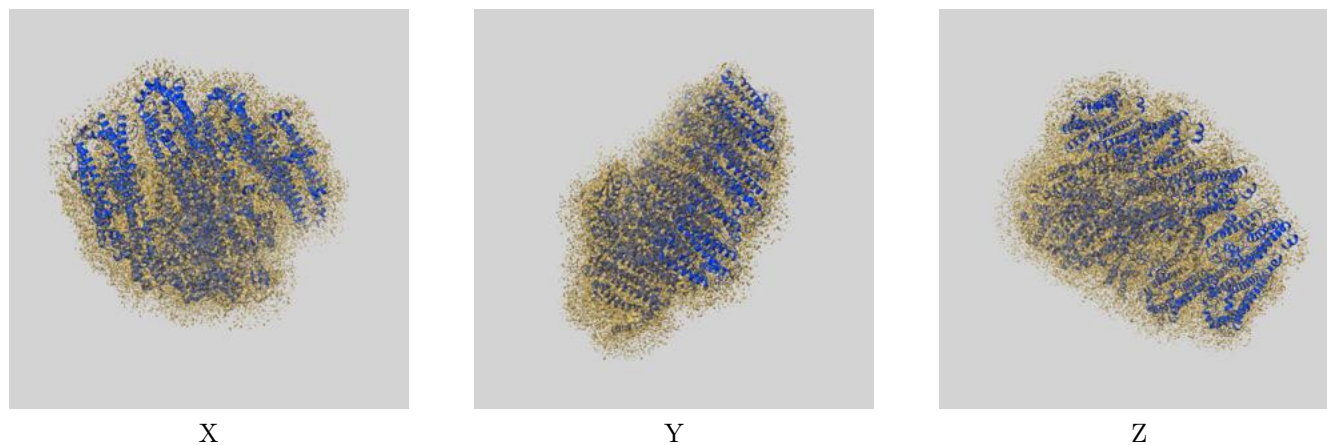
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.29	2.71
Unmasked-calculated*	3.11	3.91	3.19

*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](#)

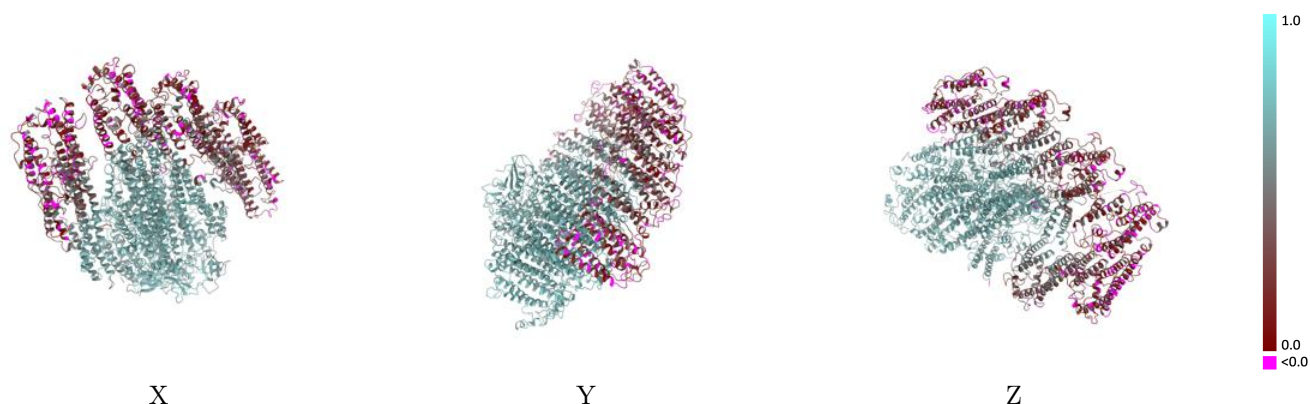
This section contains information regarding the fit between EMDB map EMD-33593 and PDB model 7Y3F. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



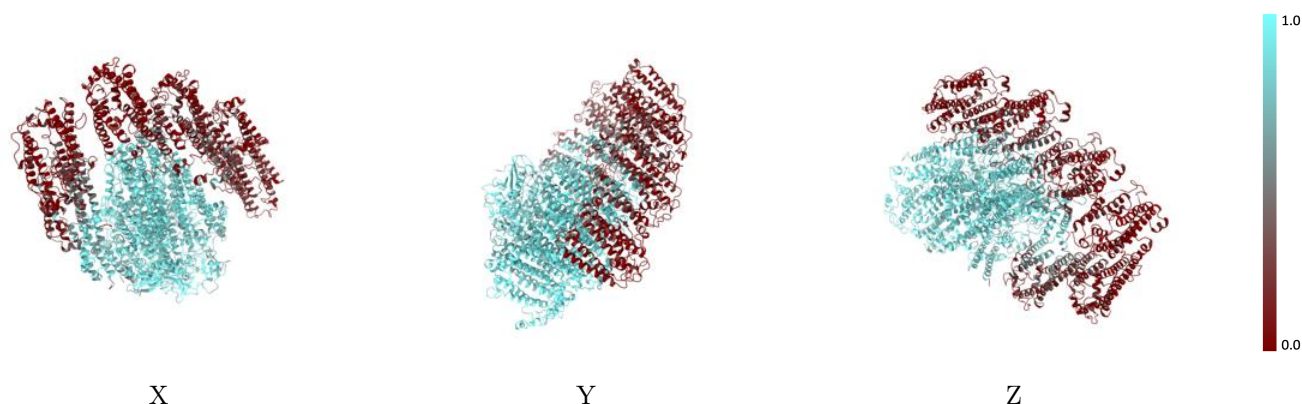
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



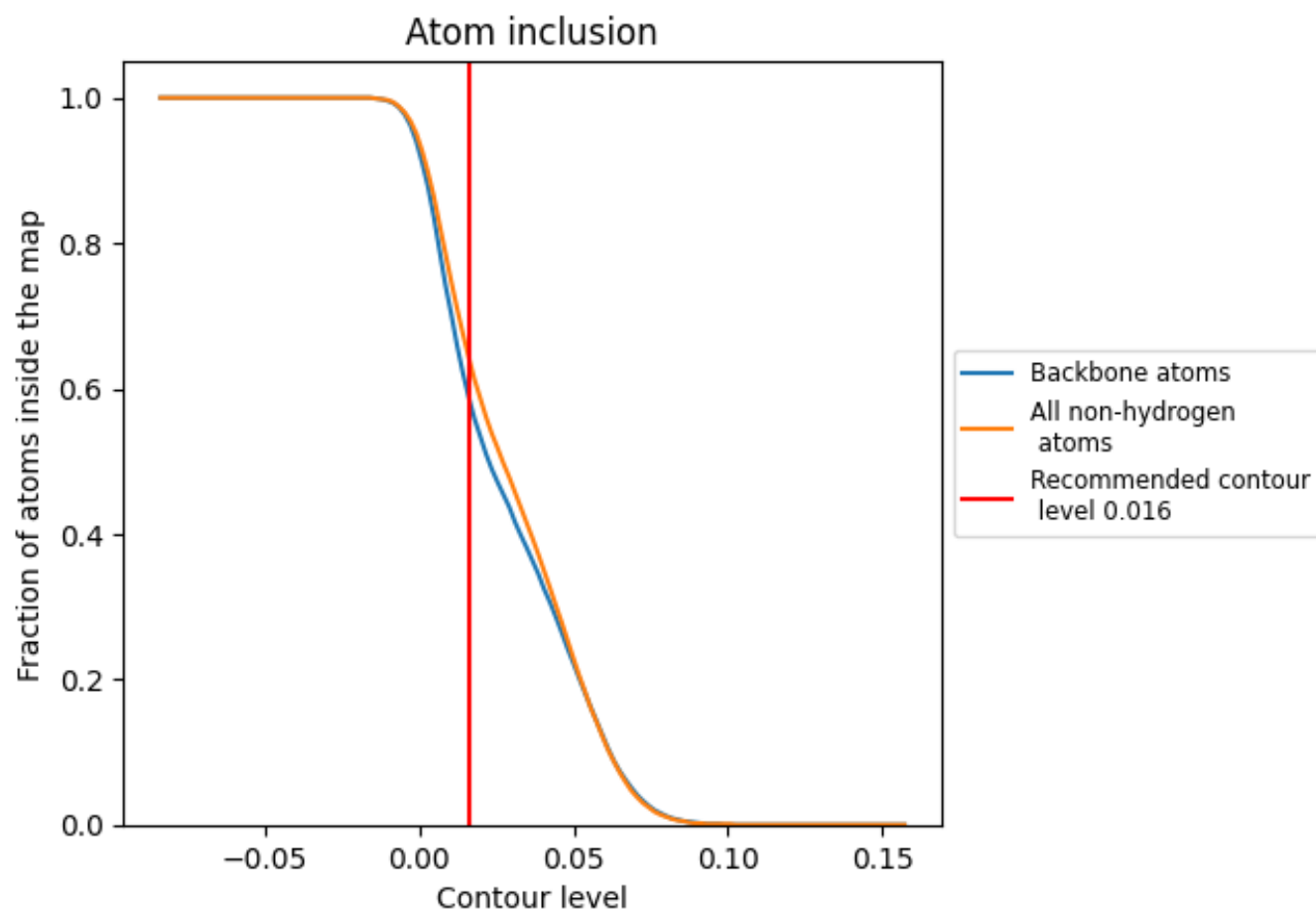
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

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

1.0

0.0

<0.0