



wwPDB EM Validation Summary Report ⓘ

Sep 30, 2025 – 04:22 PM JST

PDB ID : 9VFJ / pdb_00009vfj
EMDB ID : EMD-65026
Title : PSI-LHCI of Euglena gracilis strain Z
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on : 2025-06-11
Resolution : 2.83 Å(reported)
Based on initial model : .

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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

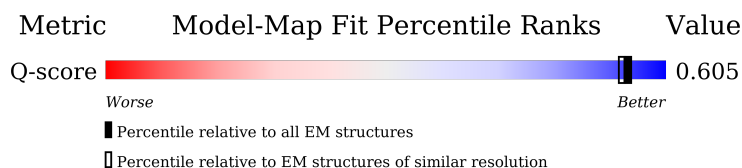
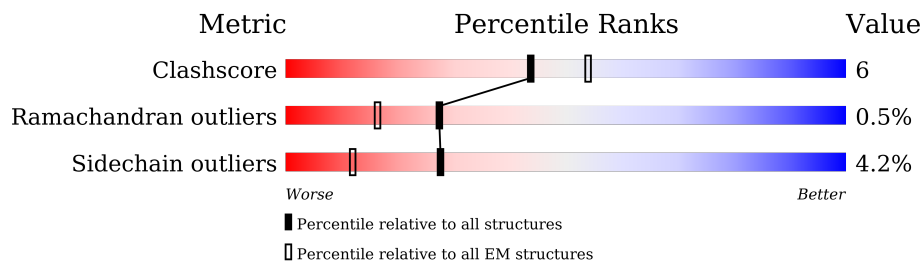
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




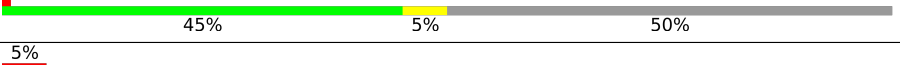
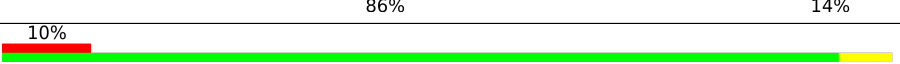
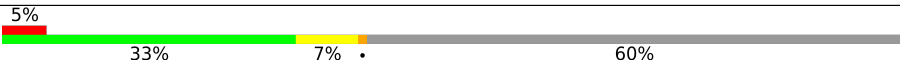

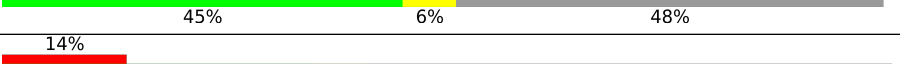
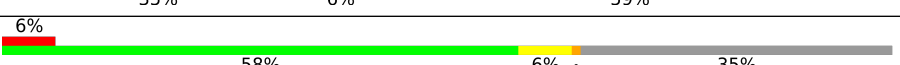



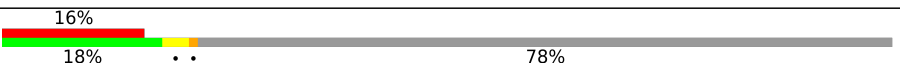
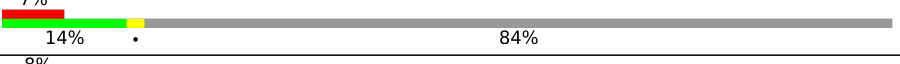

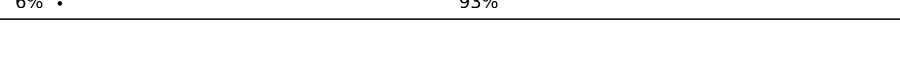
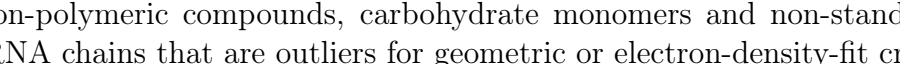
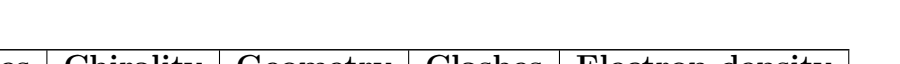
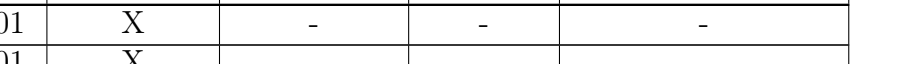
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11847 (2.33 - 3.33)

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

Mol	Chain	Length	Quality of chain
1	A	760	
2	B	734	
3	C	81	
4	D	698	

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	333	
7	J	37	
8	M	31	
9	1	492	
10	2	620	
11	3	431	
12	4	411	
13	5	252	
14	6	889	
15	7	616	
16	8	828	
17	9	873	
18	10	643	
19	11	1048	
19	12	1048	
19	13	1048	

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
20	CL0	A	801	X	-	-	-
21	CLA	1	501	X	-	-	-
21	CLA	1	504	X	-	-	-
21	CLA	1	505	X	-	-	-
21	CLA	1	506	X	-	-	-
21	CLA	1	507	X	-	-	-
21	CLA	1	509	X	-	-	-
21	CLA	1	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	511	X	-	-	-
21	CLA	1	512	X	-	-	-
21	CLA	1	514	X	-	-	-
21	CLA	1	515	X	-	-	-
21	CLA	1	516	X	-	-	-
21	CLA	10	703	X	-	-	-
21	CLA	10	704	X	-	-	-
21	CLA	10	705	X	-	-	-
21	CLA	10	706	X	-	-	-
21	CLA	10	707	X	-	-	-
21	CLA	10	708	X	-	-	-
21	CLA	10	709	X	-	-	-
21	CLA	10	710	X	-	-	-
21	CLA	10	711	X	-	-	-
21	CLA	10	712	X	-	-	-
21	CLA	11	701	X	-	-	-
21	CLA	11	702	X	-	-	-
21	CLA	11	703	X	-	-	-
21	CLA	11	704	X	-	-	-
21	CLA	11	705	X	-	-	-
21	CLA	11	706	X	-	-	-
21	CLA	11	707	X	-	-	-
21	CLA	11	708	X	-	-	-
21	CLA	11	709	X	-	-	-
21	CLA	11	711	X	-	-	-
21	CLA	12	501	X	-	-	-
21	CLA	12	502	X	-	-	-
21	CLA	12	503	X	-	-	-
21	CLA	12	504	X	-	-	-
21	CLA	12	505	X	-	-	-
21	CLA	12	506	X	-	-	-
21	CLA	12	507	X	-	-	-
21	CLA	12	508	X	-	-	-
21	CLA	13	501	X	-	-	-
21	CLA	13	502	X	-	-	-
21	CLA	13	503	X	-	-	-
21	CLA	2	503	X	-	-	-
21	CLA	2	504	X	-	-	-
21	CLA	2	505	X	-	-	-
21	CLA	2	506	X	-	-	-
21	CLA	2	508	X	-	-	-
21	CLA	2	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	510	X	-	-	-
21	CLA	2	511	X	-	-	-
21	CLA	2	513	X	-	-	-
21	CLA	2	514	X	-	-	-
21	CLA	2	515	X	-	-	-
21	CLA	2	517	X	-	-	-
21	CLA	3	701	X	-	-	-
21	CLA	3	703	X	-	-	-
21	CLA	3	704	X	-	-	-
21	CLA	3	705	X	-	-	-
21	CLA	3	706	X	-	-	-
21	CLA	3	707	X	-	-	-
21	CLA	3	708	X	-	-	-
21	CLA	3	709	X	-	-	-
21	CLA	3	711	X	-	-	-
21	CLA	3	712	X	-	-	-
21	CLA	3	713	X	-	-	-
21	CLA	3	714	X	-	-	-
21	CLA	3	715	X	-	-	-
21	CLA	4	703	X	-	-	-
21	CLA	4	704	X	-	-	-
21	CLA	4	706	X	-	-	-
21	CLA	4	707	X	-	-	-
21	CLA	4	708	X	-	-	-
21	CLA	4	709	X	-	-	-
21	CLA	4	711	X	-	-	-
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21	CLA	5	702	X	-	-	-
21	CLA	5	703	X	-	-	-
21	CLA	5	705	X	-	-	-
21	CLA	5	706	X	-	-	-
21	CLA	5	707	X	-	-	-
21	CLA	5	708	X	-	-	-
21	CLA	5	709	X	-	-	-
21	CLA	5	711	X	-	-	-
21	CLA	6	903	X	-	-	-
21	CLA	6	904	X	-	-	-
21	CLA	6	905	X	-	-	-
21	CLA	6	906	X	-	-	-
21	CLA	6	908	X	-	-	-
21	CLA	6	909	X	-	-	-
21	CLA	6	910	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	911	X	-	-	-
21	CLA	6	912	X	-	-	-
21	CLA	6	913	X	-	-	-
21	CLA	7	702	X	-	-	-
21	CLA	7	704	X	-	-	-
21	CLA	7	705	X	-	-	-
21	CLA	7	707	X	-	-	-
21	CLA	7	708	X	-	-	-
21	CLA	7	709	X	-	-	-
21	CLA	7	710	X	-	-	-
21	CLA	7	711	X	-	-	-
21	CLA	7	712	X	-	-	-
21	CLA	7	713	X	-	-	-
21	CLA	7	714	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	605	X	-	-	-
21	CLA	8	606	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	9	902	X	-	-	-
21	CLA	9	903	X	-	-	-
21	CLA	9	904	X	-	-	-
21	CLA	9	905	X	-	-	-
21	CLA	9	907	X	-	-	-
21	CLA	9	908	X	-	-	-
21	CLA	9	909	X	-	-	-
21	CLA	9	910	X	-	-	-
21	CLA	9	911	X	-	-	-
21	CLA	9	912	X	-	-	-
21	CLA	9	914	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	844	X	-	-	-
21	CLA	A	862	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	F	401	X	-	-	-
21	CLA	F	403	X	-	-	-
21	CLA	F	404	X	-	-	-
21	CLA	J	101	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 48242 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	741	Total	C	N	O	S	0	0
			5881	3861	994	1005	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5863	3857	984	1007	15		

- 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
			596	363	104	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	189	Total	C	N	O	S	0	0
			1471	941	250	278	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			500	318	84	98		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	166	Total	C	N	O	S	0	0
			1266	813	213	238	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			304	209	43	51	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 9 is a protein called LHCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	199	Total	C	N	O	S	0	0
			1513	976	258	273	6		

- Molecule 10 is a protein called LHCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2	217	Total	C	N	O	S	0	0
			1654	1080	272	298	4		

- Molecule 11 is a protein called LHCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	222	Total	C	N	O	S	0	0
			1689	1095	284	305	5		

- Molecule 12 is a protein called LHCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	169	Total	C	N	O	S	0	0
			1308	848	214	242	4		

- Molecule 13 is a protein called Chloroplast light-harvesting complex I protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	165	Total	C	N	O	S	0	0
			1269	816	219	227	7		

- Molecule 14 is a protein called LHCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6	171	Total	C	N	O	S	0	0
			1327	854	228	240	5		

- Molecule 15 is a protein called LHCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	180	Total	C	N	O	S	0	0
			1427	929	243	249	6		

- Molecule 16 is a protein called LHCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	177	Total	C	N	O	S	0	0
			1350	864	239	243	4		

- Molecule 17 is a protein called LHCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	174	Total	C	N	O	S	0	0
			1350	865	233	247	5		

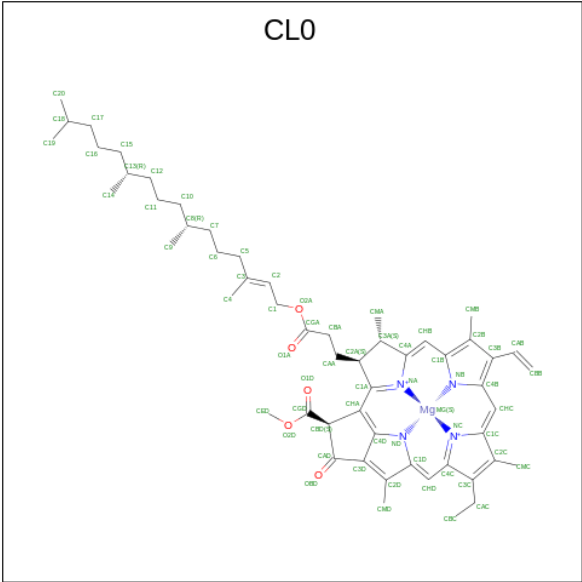
- Molecule 18 is a protein called LHCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	10	142	Total	C	N	O	S	0	0
			1102	714	190	192	6		

- Molecule 19 is a protein called LHCI-11.

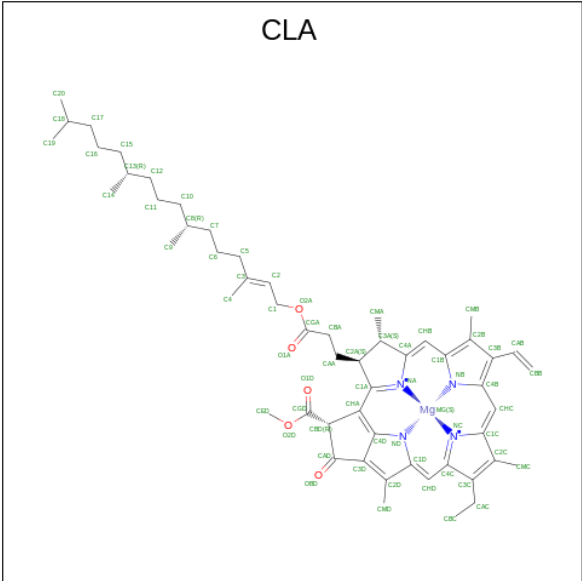
Mol	Chain	Residues	Atoms					AltConf	Trace
19	11	171	Total	C	N	O	S	0	0
			1277	822	219	232	4		
19	12	150	Total	C	N	O	S	0	0
			1127	726	190	207	4		
19	13	78	Total	C	N	O	S	0	0
			594	386	103	101	4		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	1	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	2	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	4	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	5	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	7	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	8	1	Total 62	C 52	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	10	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	10	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	10	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	10	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
21	10	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	10	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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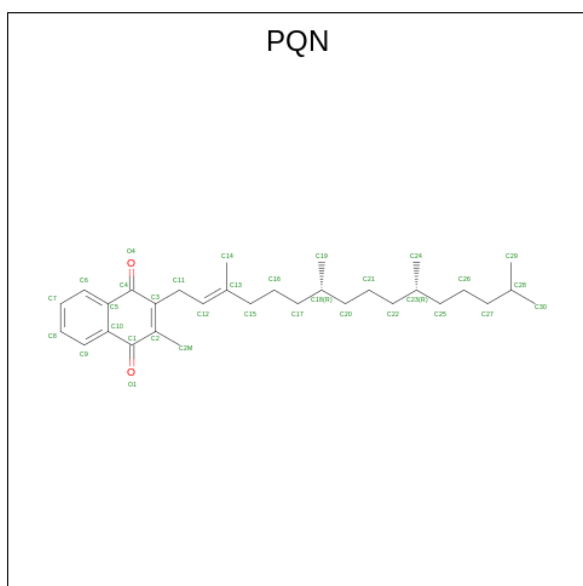
Mol	Chain	Residues	Atoms					AltConf
21	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	10	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	11	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	11	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	11	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	12	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	12	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	12	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	12	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	12	1	Total 45	C 35	Mg 1	N 4	O 5	0

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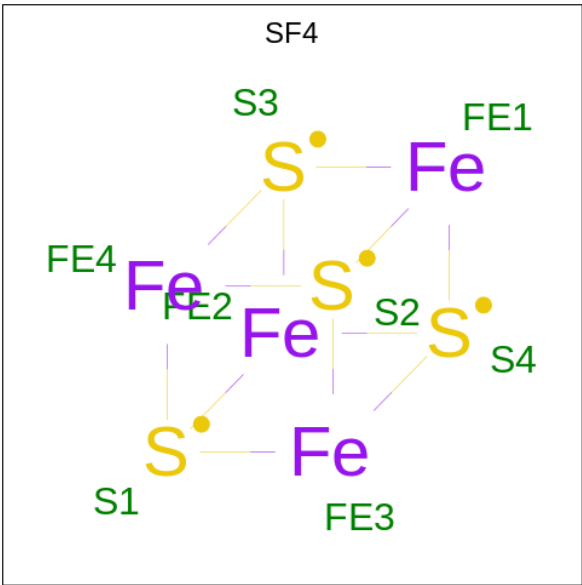
Mol	Chain	Residues	Atoms					AltConf
21	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	13	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	13	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



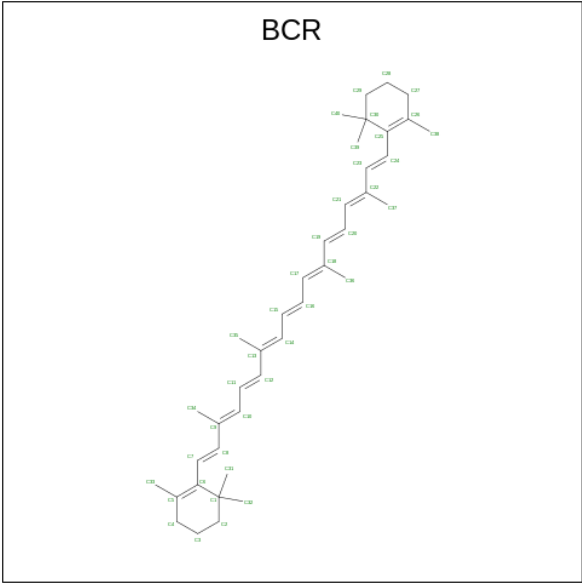
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O		0
			33	31	2		
22	B	1	Total	C	O		0
			31	29	2		

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



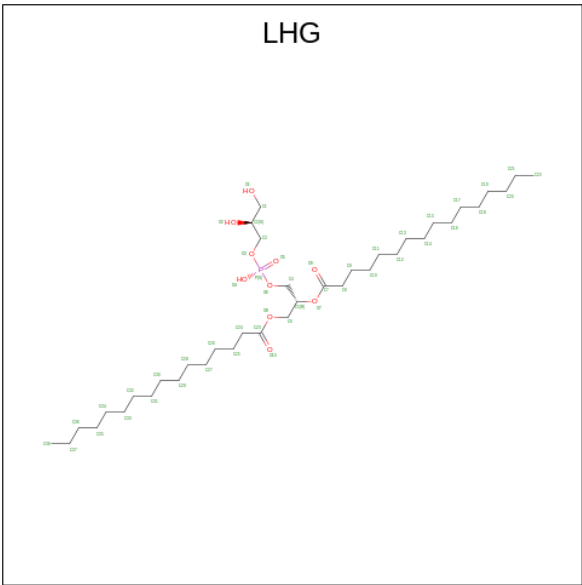
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	M	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

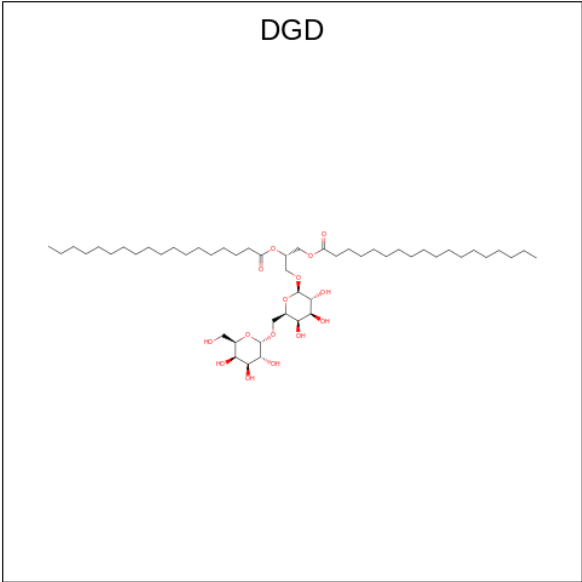


Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			27	16	10	1	
25	B	1	Total	C	O	P	0
			23	12	10	1	
25	1	1	Total	C	O	P	0
			36	25	10	1	
25	2	1	Total	C	O	P	0
			30	19	10	1	
25	3	1	Total	C	O	P	0
			25	14	10	1	
25	4	1	Total	C	O	P	0
			19	10	8	1	
25	5	1	Total	C	O	P	0
			32	21	10	1	
25	6	1	Total	C	O	P	0
			28	17	10	1	
25	7	1	Total	C	O	P	0
			48	37	10	1	
25	8	1	Total	C	O	P	0
			33	22	10	1	
25	9	1	Total	C	O	P	0
			34	23	10	1	
25	10	1	Total	C	O	P	0
			32	21	10	1	
25	11	1	Total	C	O	P	0
			30	19	10	1	

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

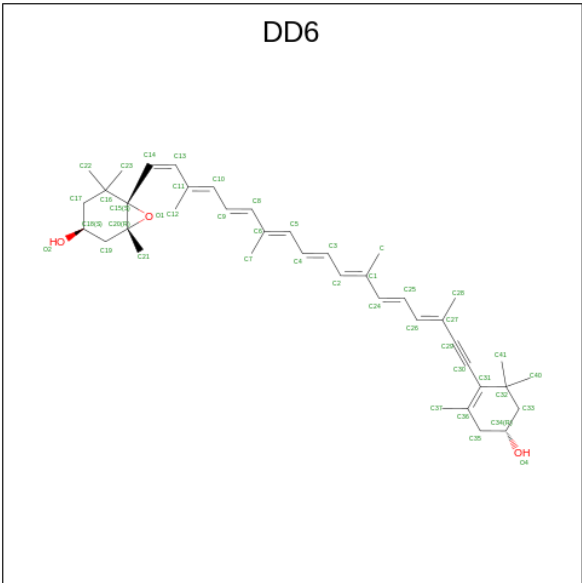
Mol	Chain	Residues	Atoms	AltConf
26	A	7	Total C 97 97	0
26	B	5	Total C 62 62	0
26	D	1	Total C 6 6	0
26	F	1	Total C 9 9	0
26	M	2	Total C 20 20	0
26	1	4	Total C 42 42	0
26	2	5	Total C 42 42	0
26	6	4	Total C 47 47	0
26	7	6	Total C 67 67	0
26	8	4	Total C 46 46	0
26	9	1	Total C 15 15	0
26	10	2	Total C 26 26	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			57	42	15	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total 43	C 40	O 3	0
28	1	1	Total 43	C 40	O 3	0
28	2	1	Total 43	C 40	O 3	0
28	2	1	Total 43	C 40	O 3	0
28	2	1	Total 43	C 40	O 3	0
28	3	1	Total 43	C 40	O 3	0
28	3	1	Total 43	C 40	O 3	0
28	3	1	Total 43	C 40	O 3	0
28	4	1	Total 43	C 40	O 3	0
28	4	1	Total 43	C 40	O 3	0
28	5	1	Total 43	C 40	O 3	0
28	5	1	Total 43	C 40	O 3	0
28	6	1	Total 43	C 40	O 3	0
28	6	1	Total 43	C 40	O 3	0
28	7	1	Total 43	C 40	O 3	0
28	7	1	Total 43	C 40	O 3	0
28	8	1	Total 43	C 40	O 3	0
28	8	1	Total 43	C 40	O 3	0
28	9	1	Total 43	C 40	O 3	0
28	9	1	Total 43	C 40	O 3	0
28	11	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
28	11	1	Total	C	O	0
			43	40	3	
28	12	1	Total	C	O	0
			43	40	3	
28	12	1	Total	C	O	0
			43	40	3	

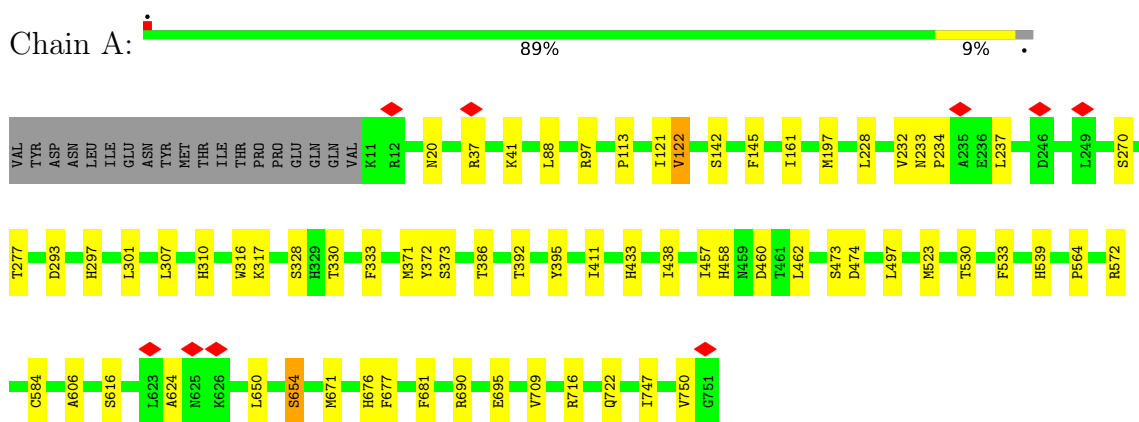
- Molecule 29 is water.

Mol	Chain	Residues	Atoms		AltConf
29	A	7	Total	O	0
			7	7	
29	B	9	Total	O	0
			9	9	
29	D	1	Total	O	0
			1	1	
29	F	1	Total	O	0
			1	1	
29	J	1	Total	O	0
			1	1	
29	1	4	Total	O	0
			4	4	
29	2	4	Total	O	0
			4	4	
29	3	4	Total	O	0
			4	4	
29	4	3	Total	O	0
			3	3	
29	5	2	Total	O	0
			2	2	
29	6	1	Total	O	0
			1	1	
29	7	2	Total	O	0
			2	2	
29	8	2	Total	O	0
			2	2	
29	9	2	Total	O	0
			2	2	
29	11	1	Total	O	0
			1	1	

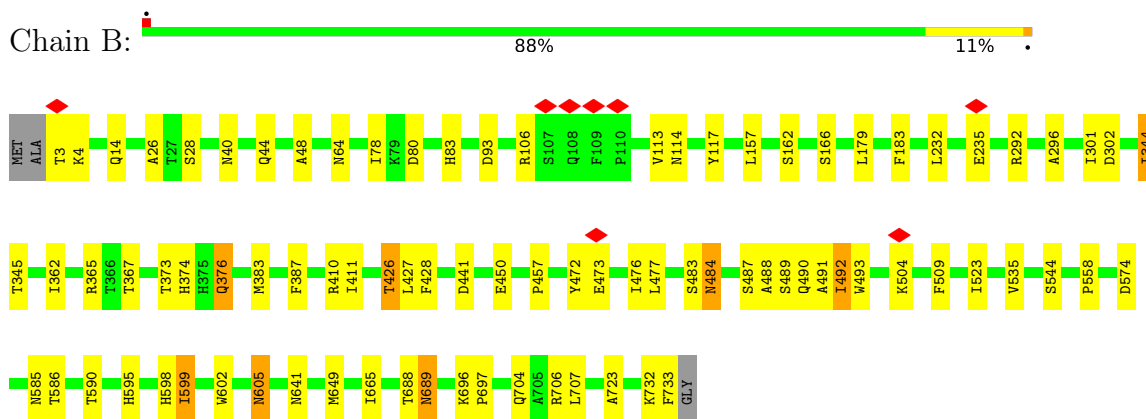
3 Residue-property plots

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

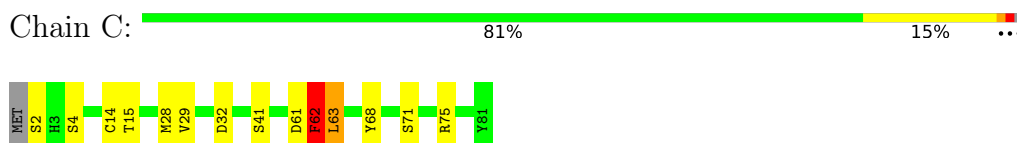
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

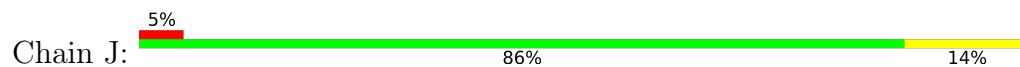


- Molecule 3: Photosystem I iron-sulfur center

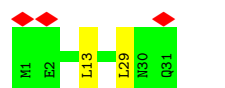


- Molecule 4: Photosystem I reaction center subunit II

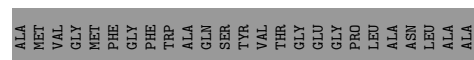
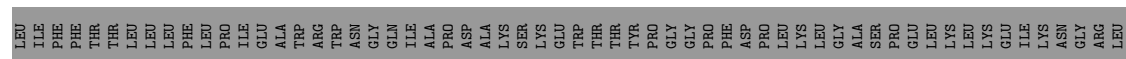
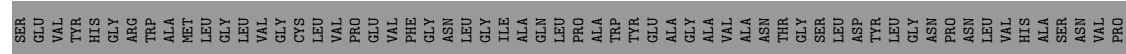
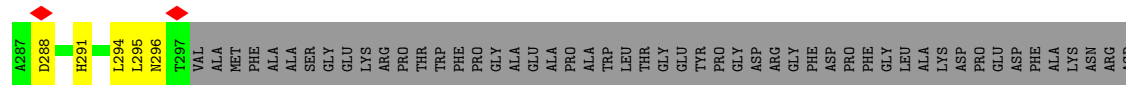
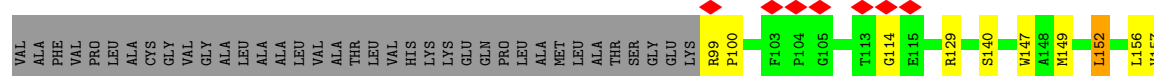
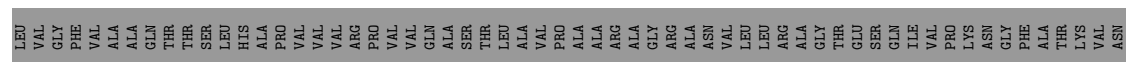
- Molecule 7: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit XII

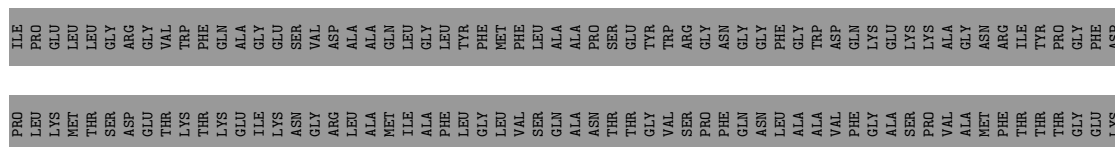
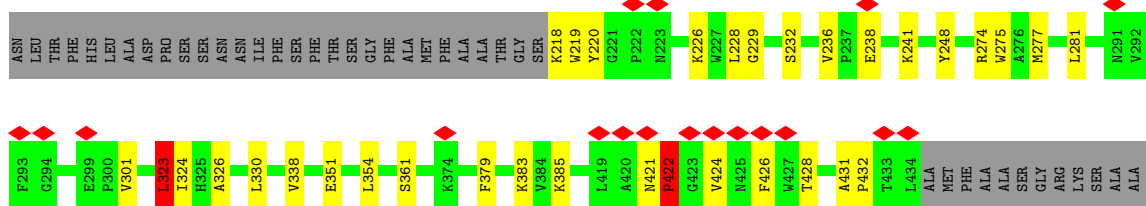


- Molecule 9: LHCI-1



- Molecule 10: LHCI-2







[illegible]

- Molecule 15: LHCI-7



MET	TYR	ASP	VAL	ALA	TYR	ARG	PRO	ASP	ARG	GLU
	SER	LEU	GLY	ALA	THR	ARG	ILE	ASP	ARG	ILE
	THR	LYS	ILE	VAL	GLY	THR	GLN	GLN	PRO	THR
	SER	LEU	VAL	HIS	ALA	THR	ALA	GLY	TRP	GLY
	GLY	THR	PRO	LYS	LYS	GLU	LYS	GLY	PHE	ARG
	GLU	THR	GLU	ASP	ASP	ILE	GLY	GLY	PRO	LEU
	K428	ASP	VAL	VAL	VAL	ASN	ALA	ALA	GLY	LEU
	Y429	THR	GLY	TRP	TRP	GLY	TYR	TYR	GLY	THR
	R430	LYS	GLY	PHE	PHE	ARG	GLU	GLU	ALA	ALA
	F434	ALA	GLY	PRO	GLY	LEU	ALA	ALA	PRO	MET
MET	P435	ALA	ALA	GLY	GLY	SER	LEU	SER	PRO	MET
	T444	ILE	PHE	THR	THR	THR	GLN	GLN	TRP	GLY
	L445	LYS	GLU	PRO	PRO	ALA	ALA	ALA	THR	LEU
	D450	ASN	ALA	PRO	PRO	MET	GLY	GLY	THR	VAL
	D461	ARG	ASN	GLY	ALA	LEU	ILE	ILE	GLN	GLN
	P462	LEU	SER	SER	HIS	GLY	VAL	VAL	HIS	SER
	E466	ALA	VAL	THR	THR	GLU	ASN	ASN	PHE	GLY
	R467	MET	ASP	GLY	GLY	VAL	GLU	ASP	ASP	ILE
	L470	GLY	ILE	THR	TYR	ARG	ALA	ALA	GLY	GLY
	G476	LEU	LEU	LEU	PRO	HIS	VAL	VAL	PHE	SER
MET	D505	THR	PHE	ALA	PHE	SER	VAL	ALA	GLY	ASN
	R508	GLN	TYR	MET	ASP	PRO	PRO	GLY	ALA	SER
	Q515	LEU	ILE	LEU	LEU	VAL	ILE	ILE	ALA	HIS
	V516	ALA	ALA	ALA	SER	ASN	GLU	VAL	PRO	LEU
	V517	THR	ALA	ALA	LEU	LEU	VAL	VAL	LYS	SER
	Y522	GLY	PRO	PRO	ALA	VAL	ARG	ALA	VAL	HIS
	W531	GLU	THR	THR	ALA	GLU	GLU	ARG	PHE	PRO
	D532	LEU	LEU	ARG	VAL	HIS	ALA	ALA	ARG	ASN
	G533	ASN	ASN	GLY	TYR	PRO	ASN	ASN	VAL	LEU
	E534	LEU	ALA	ASN	ALA	LEU	SER	SER	GLU	THR
MET	E535	ALA	ALA	GLY	MET	HIS	PRO	ASP	VAL	GLY
	S540	HIS	PHE	ASN	VAL	ILE	ASN	SER	HIS	GLY
	K560	LEU	TRP	SER	SER	ALA	ARG	ARG	GLY	SER
	M566	ASN	ASP	GLU	GLU	GLU	TYR	TYR	LEU	LEU
	L572	PRO	LYS	PHE	VAL	VAL	GLY	GLY	ALA	ALA
	P583	GLY	ALA	ALA	HIS	MET	PHE	ASP	MET	PHE
	L595	ALA	ASP	ARG	ARG	GLN	PRO	PRO	ALA	THR
	H605	ILE	ARG	SER	LEU	THR	ILE	ILE	ALA	ALA
	L605	THR	THR	TYR	MET	VAL	VAL	GLY	GLY	LYS
	H605	THR	LEU	THR	ALA	MET	THR	ASP	VAL	THR

PRO	VAL	ALA	MET	PHE	ALA	THR	THR
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- Molecule 16: LHCI-8

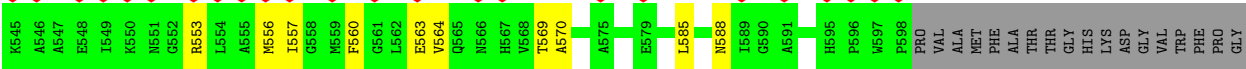
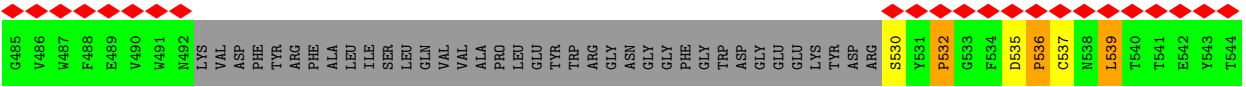


PHE PHE SER SER ILE GLU LYS LYS MET TYR GLY ALA ALA HIS ASN SER SER ASN LYS ASN ALA THR ALA SER ILE VAL PHE PHE PHE GLY CYS ALA ALA ALA VAL PHE PHE VAL VAL ALA ALA GLN PRO PRO GLY GLY ALA ALA LEU TYR ALA ALA PRO PRO ALA ALA VAL VAL ARG PRO VAL VAL SER MET

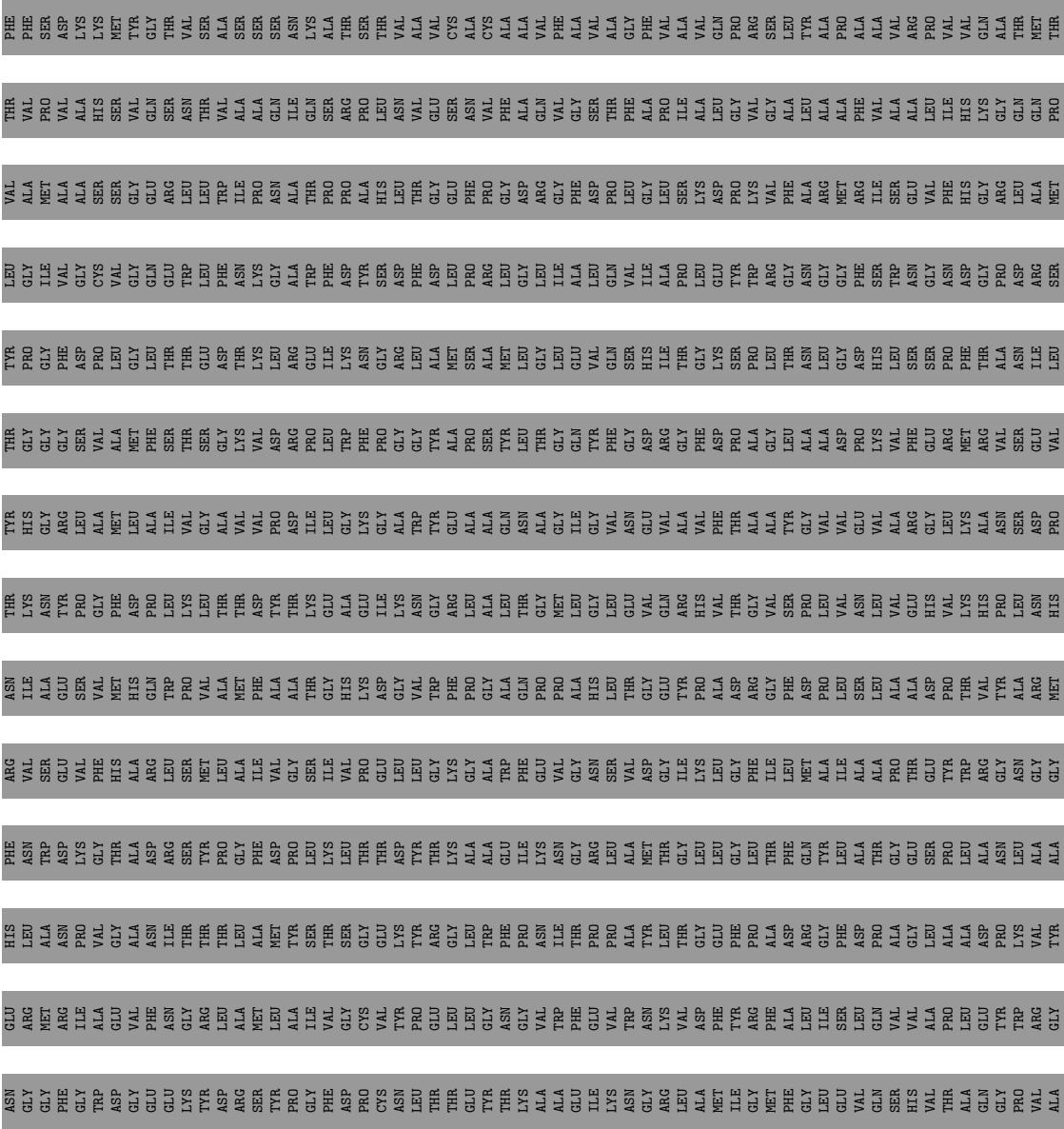
[illegible]

- Molecule 18: LHCI-10

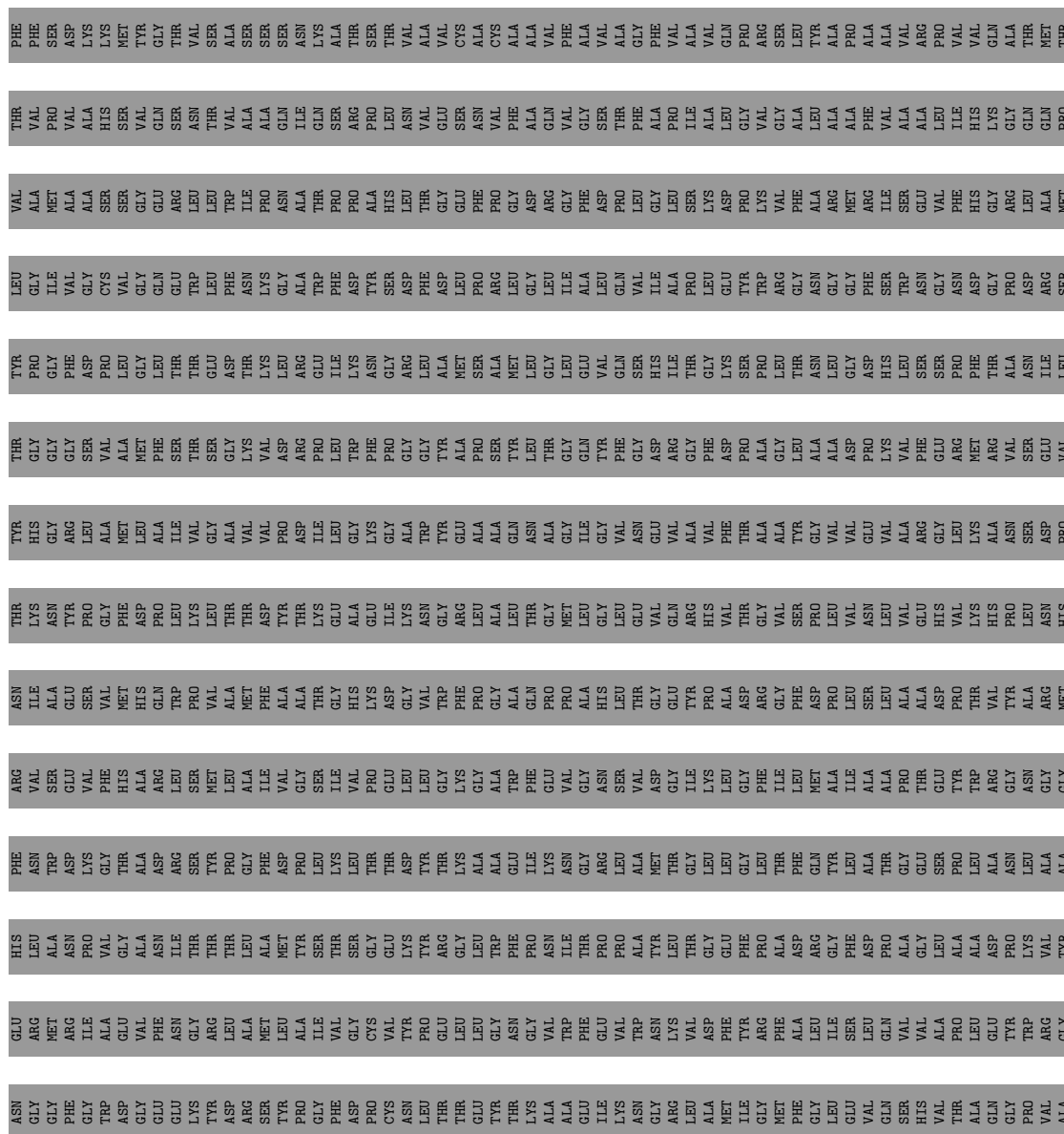
[illegible]



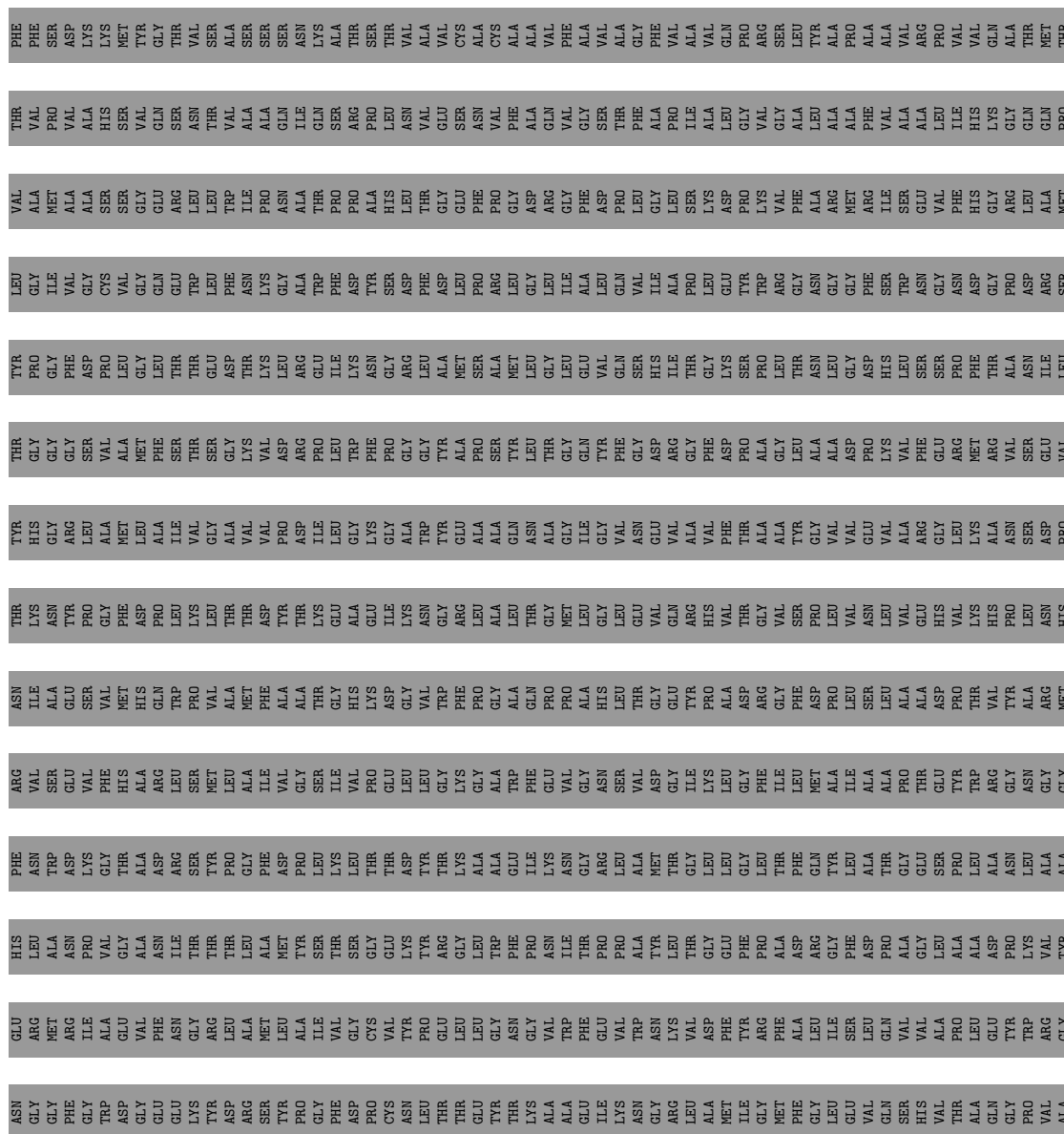
● Molecule 19: LHCI-11



- Molecule 19: LHCI-11



- Molecule 19: LHCI-11



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56060	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	216.57599, 216.57599, 216.57599	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, BCR, PQN, UNL, LHG, DD6, CL0, CLA, SF4

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	0.78	0/6082	1.06	6/8290 (0.1%)
2	B	0.77	1/6073 (0.0%)	1.07	8/8282 (0.1%)
3	C	0.80	0/606	1.16	2/819 (0.2%)
4	D	0.56	0/1507	0.98	1/2042 (0.0%)
5	E	0.51	0/512	0.89	0/696
6	F	0.58	0/1292	0.96	0/1751
7	J	0.66	0/313	0.97	0/429
8	M	0.59	0/246	0.91	0/332
9	1	0.52	0/1561	0.91	2/2134 (0.1%)
10	2	0.57	0/1704	1.11	7/2323 (0.3%)
11	3	0.54	0/1732	0.96	3/2352 (0.1%)
12	4	0.51	0/1350	0.96	1/1836 (0.1%)
13	5	0.56	0/1306	0.95	0/1765
14	6	0.51	0/1366	0.93	0/1857
15	7	0.61	0/1474	1.02	3/2009 (0.1%)
16	8	0.49	0/1388	0.95	0/1893
17	9	0.49	0/1388	0.93	2/1886 (0.1%)
18	10	0.51	0/1137	1.04	3/1554 (0.2%)
19	11	0.54	0/1314	0.96	0/1791
19	12	0.52	0/1157	1.01	1/1575 (0.1%)
19	13	0.51	0/604	0.94	1/813 (0.1%)
All	All	0.64	1/34112 (0.0%)	1.01	40/46429 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
10	2	0	1
12	4	0	1
16	8	0	1
19	12	0	2
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	598	HIS	CG-CD2	-5.10	1.30	1.35

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2	422	PRO	N-CA-CB	-18.37	83.96	103.25
10	2	422	PRO	N-CD-CG	-11.53	85.91	103.20
18	10	536	PRO	CB-CG-CD	-10.82	71.49	106.10
18	10	536	PRO	CA-N-CD	-10.76	96.93	112.00
3	C	62	PHE	CA-CB-CG	-9.64	104.16	113.80

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	ARG	Sidechain
1	A	690	ARG	Sidechain
1	A	716	ARG	Sidechain
2	B	410	ARG	Sidechain
3	C	61	ASP	Peptide

5.2 Too-close contacts [i](#)

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	5881	0	5748	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5863	0	5664	50	0
3	C	596	0	571	8	0
4	D	1471	0	1460	15	0
5	E	500	0	476	3	0
6	F	1266	0	1299	10	0
7	J	304	0	317	2	0
8	M	242	0	258	2	0
9	1	1513	0	1464	22	0
10	2	1654	0	1635	22	0
11	3	1689	0	1700	13	0
12	4	1308	0	1256	10	0
13	5	1269	0	1228	12	0
14	6	1327	0	1300	13	0
15	7	1427	0	1379	13	0
16	8	1350	0	1326	12	0
17	9	1350	0	1322	8	0
18	10	1102	0	1071	16	0
19	11	1277	0	1248	15	0
19	12	1127	0	1111	20	0
19	13	594	0	608	7	0
20	A	65	0	72	2	0
21	1	727	0	586	21	0
21	10	470	0	369	11	0
21	11	555	0	480	13	0
21	12	383	0	304	12	0
21	13	139	0	103	3	0
21	2	724	0	577	30	0
21	3	712	0	565	22	0
21	4	525	0	415	14	0
21	5	530	0	418	14	0
21	6	581	0	464	13	0
21	7	650	0	540	16	0
21	8	598	0	499	11	0
21	9	635	0	513	11	0
21	A	2561	0	2534	92	0
21	B	2179	0	2080	64	0
21	F	141	0	107	5	0
21	J	45	0	33	1	0
22	A	33	0	46	2	0
22	B	31	0	39	0	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	240	0	336	21	0
24	B	240	0	336	13	0
24	F	80	0	112	5	0
24	J	80	0	112	8	0
24	M	40	0	56	2	0
25	1	36	0	42	0	0
25	10	32	0	34	0	0
25	11	30	0	30	0	0
25	2	30	0	30	1	0
25	3	25	0	20	1	0
25	4	19	0	11	3	0
25	5	32	0	34	0	0
25	6	28	0	26	0	0
25	7	48	0	69	0	0
25	8	33	0	36	0	0
25	9	34	0	38	0	0
25	A	76	0	98	1	0
25	B	23	0	16	0	0
26	1	42	0	0	0	0
26	10	26	0	0	0	0
26	2	42	0	0	0	0
26	6	47	0	0	0	0
26	7	67	0	0	0	0
26	8	46	0	0	0	0
26	9	15	0	0	0	0
26	A	97	0	0	0	0
26	B	62	0	0	0	0
26	D	6	0	0	0	0
26	F	9	0	0	0	0
26	M	20	0	0	0	0
27	B	57	0	75	3	0
28	1	129	0	0	1	0
28	11	86	0	0	1	0
28	12	86	0	0	0	0
28	2	129	0	0	0	0
28	3	129	0	0	1	0
28	4	86	0	0	2	0
28	5	86	0	0	0	0
28	6	86	0	0	1	0
28	7	86	0	0	0	0
28	8	86	0	0	0	0
28	9	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	43	0	0	0	0
29	1	4	0	0	1	0
29	11	1	0	0	0	0
29	2	4	0	0	0	0
29	3	4	0	0	0	0
29	4	3	0	0	0	0
29	5	2	0	0	0	0
29	6	1	0	0	0	0
29	7	2	0	0	0	0
29	8	2	0	0	0	0
29	9	2	0	0	0	0
29	A	7	0	0	0	0
29	B	9	0	0	0	0
29	D	1	0	0	1	0
29	F	1	0	0	0	0
29	J	1	0	0	0	0
All	All	48242	0	44696	585	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 6.

The worst 5 of 585 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)
16:8:83:ARG:HD2	21:8:603:CLA:O1D	1.69	0.93
10:2:218:LYS:O	10:2:218:LYS:NZ	2.08	0.85
1:A:197:MET:HE1	21:A:826:CLA:H142	1.60	0.81
21:2:505:CLA:HBB1	21:2:505:CLA:HHC	1.64	0.79
21:B:831:CLA:HBC2	21:B:831:CLA:HHD	1.62	0.79

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	739/760 (97%)	706 (96%)	30 (4%)	3 (0%)	30	49
2	B	729/734 (99%)	700 (96%)	26 (4%)	3 (0%)	30	49
3	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	10	20
4	D	187/698 (27%)	177 (95%)	10 (5%)	0	100	100
5	E	60/161 (37%)	60 (100%)	0	0	100	100
6	F	164/333 (49%)	159 (97%)	5 (3%)	0	100	100
7	J	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
8	M	29/31 (94%)	29 (100%)	0	0	100	100
9	1	197/492 (40%)	188 (95%)	9 (5%)	0	100	100
10	2	215/620 (35%)	201 (94%)	13 (6%)	1 (0%)	25	44
11	3	220/431 (51%)	204 (93%)	14 (6%)	2 (1%)	14	28
12	4	167/411 (41%)	152 (91%)	12 (7%)	3 (2%)	7	15
13	5	163/252 (65%)	151 (93%)	12 (7%)	0	100	100
14	6	169/889 (19%)	158 (94%)	11 (6%)	0	100	100
15	7	178/616 (29%)	173 (97%)	3 (2%)	2 (1%)	12	24
16	8	175/828 (21%)	166 (95%)	8 (5%)	1 (1%)	22	40
17	9	172/873 (20%)	164 (95%)	8 (5%)	0	100	100
18	10	138/643 (22%)	125 (91%)	11 (8%)	2 (1%)	9	19
19	11	169/1048 (16%)	157 (93%)	12 (7%)	0	100	100
19	12	148/1048 (14%)	135 (91%)	10 (7%)	3 (2%)	6	13
19	13	72/1048 (7%)	67 (93%)	5 (7%)	0	100	100
All	All	4204/12034 (35%)	3978 (95%)	205 (5%)	21 (0%)	27	44

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	PHE
10	2	422	PRO
12	4	132	ALA
12	4	198	PRO
16	8	138	ILE

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	622/641 (97%)	609 (98%)	13 (2%)	48	72
2	B	608/609 (100%)	590 (97%)	18 (3%)	36	61
3	C	69/70 (99%)	65 (94%)	4 (6%)	17	34
4	D	154/557 (28%)	146 (95%)	8 (5%)	19	39
5	E	53/127 (42%)	52 (98%)	1 (2%)	52	75
6	F	132/259 (51%)	129 (98%)	3 (2%)	45	70
7	J	34/34 (100%)	32 (94%)	2 (6%)	16	33
8	M	26/26 (100%)	26 (100%)	0	100	100
9	1	152/372 (41%)	140 (92%)	12 (8%)	10	21
10	2	166/465 (36%)	160 (96%)	6 (4%)	30	55
11	3	174/343 (51%)	168 (97%)	6 (3%)	32	57
12	4	131/310 (42%)	122 (93%)	9 (7%)	13	26
13	5	125/186 (67%)	118 (94%)	7 (6%)	17	35
14	6	140/688 (20%)	131 (94%)	9 (6%)	14	30
15	7	142/471 (30%)	139 (98%)	3 (2%)	48	72
16	8	136/633 (22%)	130 (96%)	6 (4%)	24	47
17	9	142/672 (21%)	133 (94%)	9 (6%)	15	30
18	10	111/497 (22%)	101 (91%)	10 (9%)	8	16
19	11	123/803 (15%)	117 (95%)	6 (5%)	21	42
19	12	110/803 (14%)	107 (97%)	3 (3%)	40	65
19	13	57/803 (7%)	50 (88%)	7 (12%)	4	7
All	All	3407/9369 (36%)	3265 (96%)	142 (4%)	27	49

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	9	263	LEU
18	10	459	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	11	370	THR
7	J	17	LEU
7	J	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
17	9	215	ASN
17	9	262	ASN
5	E	153	ASN
3	C	16	GLN
19	11	402	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 342 ligands modelled in this entry, 42 are unknown - leaving 300 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	CLA	2	512	10	55,63,73	2.19	17 (30%)	64,101,113	3.02	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	802	-	65,73,73	1.82	15 (23%)	76,113,113	2.84	32 (42%)
21	CLA	F	404	6	45,53,73	2.28	17 (37%)	52,89,113	3.31	27 (51%)
21	CLA	2	515	10	45,53,73	2.41	17 (37%)	52,89,113	3.21	28 (53%)
21	CLA	2	514	29	45,53,73	2.50	17 (37%)	52,89,113	3.06	26 (50%)
21	CLA	1	513	9	60,68,73	1.98	17 (28%)	69,106,113	2.77	25 (36%)
21	CLA	A	815	1	60,68,73	1.85	17 (28%)	70,107,113	3.27	35 (50%)
21	CLA	3	705	29	47,55,73	2.27	17 (36%)	54,91,113	3.28	25 (46%)
21	CLA	A	841	1	65,73,73	1.75	16 (24%)	76,113,113	2.87	27 (35%)
21	CLA	3	714	29	45,53,73	2.33	18 (40%)	52,89,113	3.05	25 (48%)
21	CLA	6	906	14	50,58,73	2.33	16 (32%)	58,95,113	3.12	28 (48%)
21	CLA	1	507	29	50,58,73	2.37	16 (32%)	58,95,113	2.84	27 (46%)
21	CLA	12	508	19	45,53,73	2.52	17 (37%)	52,89,113	3.20	26 (50%)
21	CLA	B	806	2	65,73,73	1.87	15 (23%)	76,113,113	2.70	33 (43%)
21	CLA	4	708	25	43,51,73	2.40	17 (39%)	49,86,113	3.12	24 (48%)
21	CLA	4	709	12	45,53,73	2.55	17 (37%)	52,89,113	3.31	29 (55%)
21	CLA	12	503	-	45,53,73	2.50	18 (40%)	52,89,113	3.25	26 (50%)
21	CLA	B	832	2	58,66,73	2.07	16 (27%)	67,104,113	3.10	31 (46%)
21	CLA	A	839	1	65,73,73	1.84	20 (30%)	76,113,113	2.90	34 (44%)
21	CLA	2	503	10	45,53,73	2.32	15 (33%)	52,89,113	3.17	25 (48%)
21	CLA	B	812	2	65,73,73	1.81	15 (23%)	76,113,113	2.70	28 (36%)
21	CLA	8	611	16	45,53,73	2.42	16 (35%)	52,89,113	3.17	28 (53%)
21	CLA	12	502	19	45,53,73	2.40	16 (35%)	52,89,113	3.07	28 (53%)
25	LHG	3	719	21	24,24,48	0.38	0	27,30,54	0.58	0
21	CLA	A	823	1	45,53,73	2.23	13 (28%)	52,89,113	3.37	26 (50%)
21	CLA	9	904	17	45,53,73	2.51	17 (37%)	52,89,113	3.11	25 (48%)
24	BCR	J	102	-	41,41,41	1.67	10 (24%)	56,56,56	1.51	7 (12%)
21	CLA	B	808	2	45,53,73	2.33	20 (44%)	52,89,113	3.08	28 (53%)
21	CLA	8	609	16	62,70,73	2.19	15 (24%)	72,109,113	2.61	25 (34%)
21	CLA	A	809	1	65,73,73	1.98	17 (26%)	76,113,113	2.64	34 (44%)
21	CLA	1	508	29	47,55,73	2.30	17 (36%)	54,91,113	3.41	31 (57%)
21	CLA	B	813	2	65,73,73	2.01	21 (32%)	76,113,113	2.54	28 (36%)
21	CLA	A	803	-	65,73,73	1.93	16 (24%)	76,113,113	2.88	30 (39%)
21	CLA	B	838	2	45,53,73	1.95	15 (33%)	52,89,113	3.66	32 (61%)
21	CLA	B	807	2	65,73,73	1.78	20 (30%)	76,113,113	2.65	29 (38%)
21	CLA	7	705	29	50,58,73	2.22	15 (30%)	58,95,113	3.17	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	705	29	47,55,73	2.24	16 (34%)	54,91,113	3.27	28 (51%)
21	CLA	B	804	2	65,73,73	1.85	19 (29%)	76,113,113	2.90	36 (47%)
21	CLA	7	709	25	43,51,73	2.24	17 (39%)	49,86,113	3.11	31 (63%)
21	CLA	7	713	15	47,55,73	2.32	16 (34%)	54,91,113	3.20	26 (48%)
21	CLA	A	808	1	51,59,73	2.11	19 (37%)	59,96,113	3.01	25 (42%)
21	CLA	11	707	19	54,62,73	2.31	16 (29%)	62,99,113	2.74	26 (41%)
25	LHG	B	848	21	22,22,48	0.37	0	25,28,54	1.07	2 (8%)
21	CLA	9	908	17	62,70,73	2.17	15 (24%)	72,109,113	2.67	27 (37%)
25	LHG	4	714	21	18,18,48	0.56	0	22,23,54	0.84	1 (4%)
21	CLA	8	607	29	47,55,73	2.27	17 (36%)	54,91,113	3.20	28 (51%)
25	LHG	9	917	21	33,33,48	0.38	0	36,39,54	0.83	1 (2%)
21	CLA	A	862	29	65,73,73	1.74	16 (24%)	76,113,113	3.26	37 (48%)
25	LHG	7	717	21	47,47,48	0.50	0	50,53,54	1.02	3 (6%)
21	CLA	A	825	1	59,67,73	1.84	15 (25%)	68,105,113	2.86	27 (39%)
28	DD6	11	712	-	39,45,45	1.64	8 (20%)	52,67,67	1.40	9 (17%)
25	LHG	A	853	-	48,48,48	0.66	1 (2%)	51,54,54	0.67	1 (1%)
28	DD6	4	712	-	39,45,45	1.48	8 (20%)	52,67,67	1.61	11 (21%)
21	CLA	3	702	11	60,68,73	1.91	16 (26%)	70,107,113	3.00	31 (44%)
28	DD6	7	715	-	39,45,45	1.53	8 (20%)	52,67,67	1.52	7 (13%)
21	CLA	5	711	13	45,53,73	2.53	16 (35%)	52,89,113	3.12	24 (46%)
21	CLA	7	702	15	47,55,73	2.28	16 (34%)	54,91,113	3.35	29 (53%)
21	CLA	13	503	19	47,55,73	2.37	16 (34%)	54,91,113	3.14	26 (48%)
21	CLA	B	822	2	45,53,73	2.31	18 (40%)	52,89,113	3.06	30 (57%)
21	CLA	4	702	12	55,63,73	2.19	17 (30%)	64,101,113	3.02	26 (40%)
28	DD6	2	520	-	39,45,45	1.54	8 (20%)	52,67,67	1.54	8 (15%)
21	CLA	7	712	15	45,53,73	2.30	15 (33%)	52,89,113	3.36	31 (59%)
21	CLA	9	912	17	45,53,73	2.46	18 (40%)	52,89,113	3.24	25 (48%)
24	BCR	A	848	-	41,41,41	1.61	8 (19%)	56,56,56	1.69	12 (21%)
21	CLA	5	705	29	47,55,73	2.37	16 (34%)	54,91,113	3.01	29 (53%)
24	BCR	A	852	-	41,41,41	2.03	7 (17%)	56,56,56	1.40	7 (12%)
21	CLA	12	507	19	45,53,73	2.50	15 (33%)	52,89,113	3.24	27 (51%)
21	CLA	6	903	14	47,55,73	2.43	16 (34%)	54,91,113	3.28	29 (53%)
21	CLA	A	822	29	65,73,73	1.95	19 (29%)	76,113,113	2.57	32 (42%)
21	CLA	2	505	10	45,53,73	2.28	15 (33%)	52,89,113	2.96	25 (48%)
21	CLA	9	902	17	42,50,73	2.38	17 (40%)	48,85,113	3.15	25 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	806	1	65,73,73	1.94	16 (24%)	76,113,113	2.63	34 (44%)
28	DD6	1	520	-	39,45,45	1.57	8 (20%)	52,67,67	1.59	10 (19%)
21	CLA	A	836	1	54,62,73	1.91	15 (27%)	62,99,113	2.98	28 (45%)
21	CLA	12	506	19	55,63,73	2.23	14 (25%)	64,101,113	2.87	28 (43%)
21	CLA	11	709	19	45,53,73	2.46	17 (37%)	52,89,113	3.04	26 (50%)
21	CLA	1	512	9	45,53,73	2.43	14 (31%)	52,89,113	3.19	29 (55%)
24	BCR	B	842	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
21	CLA	9	906	29	47,55,73	2.36	17 (36%)	54,91,113	3.19	26 (48%)
21	CLA	7	707	15	47,55,73	2.25	16 (34%)	54,91,113	3.04	25 (46%)
21	CLA	J	101	7	45,53,73	2.45	18 (40%)	52,89,113	3.28	30 (57%)
21	CLA	2	506	29	50,58,73	2.29	16 (32%)	58,95,113	2.95	30 (51%)
21	CLA	4	701	-	41,49,73	2.44	15 (36%)	47,84,113	3.69	25 (53%)
21	CLA	7	708	15	62,70,73	1.97	17 (27%)	72,109,113	2.70	31 (43%)
21	CLA	10	703	18	41,49,73	2.54	15 (36%)	47,84,113	3.10	26 (55%)
21	CLA	11	702	19	60,68,73	2.03	16 (26%)	70,107,113	2.63	29 (41%)
28	DD6	2	518	-	39,45,45	1.58	6 (15%)	52,67,67	1.69	10 (19%)
21	CLA	1	510	9	62,70,73	2.06	16 (25%)	72,109,113	2.65	28 (38%)
21	CLA	9	913	17	47,55,73	2.42	18 (38%)	54,91,113	3.21	26 (48%)
21	CLA	B	827	2	65,73,73	1.85	16 (24%)	76,113,113	2.75	32 (42%)
21	CLA	8	605	16	45,53,73	2.48	16 (35%)	52,89,113	3.09	25 (48%)
21	CLA	B	828	2	65,73,73	1.75	18 (27%)	76,113,113	3.05	31 (40%)
24	BCR	A	847	-	41,41,41	1.51	10 (24%)	56,56,56	1.62	9 (16%)
21	CLA	B	821	2	55,63,73	2.13	15 (27%)	64,101,113	3.23	33 (51%)
21	CLA	A	817	29	49,57,73	2.07	16 (32%)	55,93,113	3.17	26 (47%)
21	CLA	5	704	29	50,58,73	2.37	15 (30%)	58,95,113	3.07	27 (46%)
25	LHG	1	521	21	35,35,48	0.38	0	38,41,54	0.90	2 (5%)
28	DD6	12	510	-	39,45,45	1.52	8 (20%)	52,67,67	2.08	14 (26%)
21	CLA	7	714	15	47,55,73	2.26	16 (34%)	54,91,113	3.21	26 (48%)
21	CLA	A	804	1	65,73,73	1.77	14 (21%)	76,113,113	2.84	32 (42%)
21	CLA	2	511	10	45,53,73	2.50	15 (33%)	52,89,113	3.17	27 (51%)
21	CLA	8	603	16	47,55,73	2.24	12 (25%)	54,91,113	3.29	26 (48%)
28	DD6	7	716	-	39,45,45	1.52	8 (20%)	52,67,67	1.52	8 (15%)
21	CLA	B	836	2	47,55,73	2.11	16 (34%)	54,91,113	3.69	35 (64%)
21	CLA	2	508	10	47,55,73	2.27	14 (29%)	54,91,113	3.17	28 (51%)
21	CLA	11	708	25	43,51,73	2.41	17 (39%)	49,86,113	3.28	26 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	819	1	54,62,73	2.07	16 (29%)	62,99,113	2.87	30 (48%)
21	CLA	F	401	29	51,59,73	2.05	14 (27%)	59,96,113	3.15	25 (42%)
21	CLA	4	706	12	47,55,73	2.41	15 (31%)	54,91,113	3.03	27 (50%)
21	CLA	1	509	9	47,55,73	2.48	15 (31%)	54,91,113	3.18	26 (48%)
21	CLA	5	702	13	60,68,73	2.00	18 (30%)	70,107,113	2.60	30 (42%)
21	CLA	6	905	14	45,53,73	2.36	16 (35%)	52,89,113	3.05	26 (50%)
21	CLA	11	701	19	41,49,73	2.49	17 (41%)	47,84,113	3.25	26 (55%)
21	CLA	5	701	13	45,53,73	2.34	17 (37%)	52,89,113	2.99	29 (55%)
21	CLA	A	816	1	45,53,73	2.32	15 (33%)	52,89,113	3.31	27 (51%)
21	CLA	7	710	15	45,53,73	2.37	15 (33%)	52,89,113	3.24	26 (50%)
23	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	2	510	25	43,51,73	2.24	14 (32%)	49,86,113	3.49	24 (48%)
28	DD6	1	519	-	39,45,45	1.61	7 (17%)	52,67,67	1.56	11 (21%)
21	CLA	4	710	12	45,53,73	2.44	16 (35%)	52,89,113	3.23	22 (42%)
27	DGD	B	847	-	58,58,67	1.01	4 (6%)	72,72,81	1.34	8 (11%)
21	CLA	B	811	2	45,53,73	2.29	14 (31%)	52,89,113	3.24	25 (48%)
21	CLA	4	703	12	45,53,73	2.35	16 (35%)	52,89,113	3.31	27 (51%)
21	CLA	B	830	2	49,57,73	2.37	17 (34%)	55,93,113	3.25	32 (58%)
21	CLA	B	805	2	65,73,73	1.97	12 (18%)	76,113,113	2.39	27 (35%)
21	CLA	F	403	29	45,53,73	2.25	14 (31%)	52,89,113	3.10	28 (53%)
28	DD6	12	509	-	39,45,45	1.52	8 (20%)	52,67,67	1.52	8 (15%)
21	CLA	3	703	11	45,53,73	2.46	16 (35%)	52,89,113	3.08	29 (55%)
21	CLA	B	823	29	54,62,73	2.10	16 (29%)	62,99,113	2.99	28 (45%)
21	CLA	2	516	29	45,53,73	2.37	17 (37%)	52,89,113	2.91	23 (44%)
21	CLA	A	805	1	59,67,73	1.95	18 (30%)	68,105,113	3.10	30 (44%)
21	CLA	8	612	16	65,73,73	1.94	15 (23%)	76,113,113	2.63	27 (35%)
23	SF4	A	846	2,1	0,12,12	-	-	-	-	-
25	LHG	11	714	21	29,29,48	0.36	0	32,35,54	0.72	1 (3%)
28	DD6	11	713	-	39,45,45	1.60	8 (20%)	52,67,67	1.64	9 (17%)
21	CLA	A	842	1	65,73,73	1.86	15 (23%)	76,113,113	2.73	27 (35%)
21	CLA	3	712	29	45,53,73	2.45	16 (35%)	52,89,113	3.04	27 (51%)
21	CLA	6	907	29	47,55,73	2.32	18 (38%)	54,91,113	3.10	30 (55%)
25	LHG	6	917	21	27,27,48	0.36	0	30,33,54	1.21	4 (13%)
28	DD6	2	519	-	39,45,45	1.78	7 (17%)	52,67,67	1.69	14 (26%)
24	BCR	F	405	-	41,41,41	1.65	9 (21%)	56,56,56	1.97	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	3	707	11	62,70,73	2.01	14 (22%)	72,109,113	2.77	29 (40%)
21	CLA	4	711	29	45,53,73	2.34	15 (33%)	52,89,113	3.13	28 (53%)
21	CLA	5	708	25	43,51,73	2.43	15 (34%)	49,86,113	3.21	24 (48%)
24	BCR	M	102	-	41,41,41	1.58	11 (26%)	56,56,56	1.49	7 (12%)
28	DD6	3	718	-	39,45,45	1.55	9 (23%)	52,67,67	1.58	10 (19%)
21	CLA	A	807	1	65,73,73	2.02	16 (24%)	76,113,113	2.68	35 (46%)
21	CLA	B	820	2	45,53,73	2.34	16 (35%)	52,89,113	3.34	23 (44%)
21	CLA	B	831	2	65,73,73	1.87	14 (21%)	76,113,113	2.88	27 (35%)
21	CLA	11	710	19	45,53,73	2.35	19 (42%)	52,89,113	3.35	25 (48%)
28	DD6	8	616	-	39,45,45	1.54	8 (20%)	52,67,67	1.56	8 (15%)
28	DD6	3	717	-	39,45,45	1.83	7 (17%)	52,67,67	1.96	11 (21%)
24	BCR	B	843	-	41,41,41	1.68	7 (17%)	56,56,56	1.49	10 (17%)
21	CLA	A	840	1	47,55,73	2.24	16 (34%)	54,91,113	4.00	32 (59%)
21	CLA	9	905	29	50,58,73	2.31	15 (30%)	58,95,113	3.03	28 (48%)
21	CLA	6	904	14	60,68,73	2.10	16 (26%)	70,107,113	2.74	32 (45%)
21	CLA	11	703	19	65,73,73	1.94	16 (24%)	76,113,113	2.69	27 (35%)
21	CLA	9	909	25	43,51,73	2.34	16 (37%)	49,86,113	3.18	23 (46%)
21	CLA	1	505	9	60,68,73	2.09	15 (25%)	70,107,113	2.52	25 (35%)
21	CLA	2	507	29	47,55,73	2.16	17 (36%)	54,91,113	3.21	27 (50%)
21	CLA	8	613	16	45,53,73	2.49	16 (35%)	52,89,113	3.32	30 (57%)
21	CLA	3	701	11	41,49,73	2.46	15 (36%)	47,84,113	3.35	23 (48%)
21	CLA	B	809	2	45,53,73	2.30	16 (35%)	52,89,113	3.09	27 (51%)
21	CLA	B	837	29	45,53,73	2.41	14 (31%)	52,89,113	2.88	23 (44%)
28	DD6	5	713	-	39,45,45	1.85	9 (23%)	52,67,67	1.89	13 (25%)
28	DD6	9	916	-	39,45,45	1.61	7 (17%)	52,67,67	1.67	10 (19%)
21	CLA	B	815	2	55,63,73	2.05	18 (32%)	64,101,113	2.67	25 (39%)
21	CLA	2	504	10	60,68,73	2.00	15 (25%)	70,107,113	2.78	32 (45%)
24	BCR	B	846	-	41,41,41	1.75	12 (29%)	56,56,56	1.39	10 (17%)
21	CLA	6	913	14	45,53,73	2.49	15 (33%)	52,89,113	3.13	27 (51%)
21	CLA	9	911	17	55,63,73	2.18	16 (29%)	64,101,113	2.91	26 (40%)
28	DD6	1	518	-	39,45,45	1.53	8 (20%)	52,67,67	1.49	8 (15%)
21	CLA	8	604	16	60,68,73	1.96	16 (26%)	70,107,113	2.88	28 (40%)
21	CLA	A	837	1	45,53,73	2.42	15 (33%)	52,89,113	3.26	26 (50%)
22	PQN	A	845	-	34,34,34	1.68	4 (11%)	42,45,45	1.42	6 (14%)
21	CLA	13	501	19	45,53,73	2.49	18 (40%)	52,89,113	3.12	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	9	907	17	47,55,73	2.44	16 (34%)	54,91,113	3.61	31 (57%)
21	CLA	7	706	29	47,55,73	2.21	17 (36%)	54,91,113	3.10	27 (50%)
21	CLA	B	839	25	65,73,73	1.96	20 (30%)	76,113,113	2.88	33 (43%)
21	CLA	6	911	14	45,53,73	2.45	14 (31%)	52,89,113	3.17	27 (51%)
21	CLA	A	810	1	65,73,73	1.91	17 (26%)	76,113,113	2.86	26 (34%)
21	CLA	2	517	-	45,53,73	2.58	16 (35%)	52,89,113	3.15	24 (46%)
21	CLA	3	706	11	47,55,73	2.34	16 (34%)	54,91,113	3.22	30 (55%)
21	CLA	A	811	1	45,53,73	2.28	13 (28%)	52,89,113	3.37	27 (51%)
21	CLA	A	824	1	51,59,73	2.01	14 (27%)	59,96,113	3.36	30 (50%)
21	CLA	8	608	16	47,55,73	2.39	16 (34%)	54,91,113	3.14	30 (55%)
21	CLA	B	814	2	45,53,73	2.32	18 (40%)	52,89,113	3.23	28 (53%)
24	BCR	A	851	-	41,41,41	1.74	12 (29%)	56,56,56	1.31	7 (12%)
21	CLA	12	505	19	47,55,73	2.32	14 (29%)	54,91,113	3.06	27 (50%)
21	CLA	13	502	-	47,55,73	2.43	17 (36%)	54,91,113	3.06	26 (48%)
24	BCR	J	103	-	41,41,41	1.67	10 (24%)	56,56,56	1.55	7 (12%)
21	CLA	10	709	18	45,53,73	2.36	16 (35%)	52,89,113	3.28	26 (50%)
21	CLA	11	704	29	45,53,73	2.43	17 (37%)	52,89,113	3.21	26 (50%)
21	CLA	8	614	16	47,55,73	2.31	18 (38%)	54,91,113	3.09	24 (44%)
21	CLA	A	829	1	65,73,73	1.69	16 (24%)	76,113,113	2.87	35 (46%)
21	CLA	B	817	2	60,68,73	1.88	16 (26%)	70,107,113	3.06	34 (48%)
21	CLA	9	914	17	47,55,73	2.48	16 (34%)	54,91,113	3.11	26 (48%)
28	DD6	J	104	-	39,45,45	1.60	8 (20%)	52,67,67	1.63	9 (17%)
21	CLA	4	707	12	62,70,73	2.12	16 (25%)	72,109,113	2.80	33 (45%)
21	CLA	1	504	9	42,50,73	2.48	16 (38%)	48,85,113	3.15	25 (52%)
25	LHG	5	714	21	31,31,48	0.35	0	34,37,54	0.62	0
21	CLA	B	819	2	47,55,73	2.38	17 (36%)	54,91,113	3.19	30 (55%)
21	CLA	6	909	14	62,70,73	2.02	15 (24%)	72,109,113	2.80	28 (38%)
21	CLA	1	506	9	45,53,73	2.34	15 (33%)	52,89,113	2.98	26 (50%)
21	CLA	A	813	1	54,62,73	2.16	19 (35%)	62,99,113	2.76	25 (40%)
21	CLA	6	914	14	47,55,73	2.33	15 (31%)	54,91,113	3.16	27 (50%)
25	LHG	8	617	21	32,32,48	0.40	0	35,38,54	0.98	1 (2%)
23	SF4	C	102	3	0,12,12	-	-	-	-	-
21	CLA	9	910	17	45,53,73	2.37	17 (37%)	52,89,113	3.49	30 (57%)
25	LHG	A	854	21	26,26,48	0.46	0	29,32,54	1.25	5 (17%)
21	CLA	6	908	14	45,53,73	2.23	16 (35%)	52,89,113	3.33	28 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	812	1	65,73,73	1.76	15 (23%)	76,113,113	2.80	33 (43%)
21	CLA	7	703	15	60,68,73	2.07	17 (28%)	70,107,113	2.92	26 (37%)
21	CLA	A	821	1	61,69,73	1.74	13 (21%)	71,108,113	3.10	26 (36%)
21	CLA	A	802	29	65,73,73	1.85	20 (30%)	76,113,113	2.79	33 (43%)
21	CLA	11	711	19	45,53,73	2.52	17 (37%)	52,89,113	3.22	26 (50%)
21	CLA	10	712	18	47,55,73	2.41	17 (36%)	54,91,113	3.15	24 (44%)
21	CLA	B	829	2	45,53,73	2.40	16 (35%)	52,89,113	3.55	30 (57%)
21	CLA	B	825	2	65,73,73	1.82	16 (24%)	76,113,113	2.63	34 (44%)
21	CLA	A	827	29	60,68,73	2.01	19 (31%)	70,107,113	2.86	30 (42%)
21	CLA	B	833	2	45,53,73	2.28	15 (33%)	52,89,113	3.42	32 (61%)
21	CLA	A	828	1	65,73,73	1.80	15 (23%)	76,113,113	2.88	29 (38%)
21	CLA	A	838	1	51,59,73	2.14	18 (35%)	59,96,113	2.92	24 (40%)
21	CLA	1	501	29	45,53,73	2.34	18 (40%)	52,89,113	3.24	27 (51%)
21	CLA	1	517	29	45,53,73	2.43	18 (40%)	52,89,113	3.07	24 (46%)
21	CLA	3	715	11	45,53,73	2.46	15 (33%)	52,89,113	3.26	29 (55%)
21	CLA	9	903	17	60,68,73	2.22	14 (23%)	70,107,113	2.95	30 (42%)
21	CLA	2	513	10	45,53,73	2.46	16 (35%)	52,89,113	3.19	25 (48%)
21	CLA	10	704	18	60,68,73	2.19	16 (26%)	70,107,113	2.84	27 (38%)
24	BCR	B	841	-	41,41,41	1.50	8 (19%)	56,56,56	1.53	9 (16%)
24	BCR	F	402	-	41,41,41	1.58	8 (19%)	56,56,56	1.66	10 (17%)
21	CLA	11	705	-	47,55,73	2.33	17 (36%)	54,91,113	2.97	28 (51%)
21	CLA	A	814	1	60,68,73	2.12	18 (30%)	70,107,113	2.61	28 (40%)
21	CLA	B	824	29	46,54,73	2.22	16 (34%)	53,90,113	3.31	31 (58%)
20	CL0	A	801	1	65,73,73	2.11	21 (32%)	76,113,113	2.78	32 (42%)
21	CLA	A	843	29	52,60,73	2.06	15 (28%)	60,97,113	3.10	31 (51%)
21	CLA	8	606	29	45,53,73	2.42	18 (40%)	52,89,113	3.18	23 (44%)
21	CLA	A	833	1	65,73,73	1.86	17 (26%)	76,113,113	2.92	30 (39%)
21	CLA	3	709	11	45,53,73	2.23	16 (35%)	52,89,113	3.14	28 (53%)
21	CLA	B	826	2	65,73,73	1.85	20 (30%)	76,113,113	2.92	30 (39%)
21	CLA	5	706	13	45,53,73	2.43	14 (31%)	52,89,113	3.20	29 (55%)
21	CLA	11	706	19	65,73,73	1.96	16 (24%)	76,113,113	2.74	32 (42%)
28	DD6	9	915	-	39,45,45	1.62	8 (20%)	52,67,67	1.65	9 (17%)
21	CLA	B	818	29	65,73,73	1.92	15 (23%)	76,113,113	2.76	25 (32%)
28	DD6	4	713	-	39,45,45	1.58	7 (17%)	52,67,67	1.61	8 (15%)
21	CLA	B	803	2	54,62,73	2.05	17 (31%)	62,99,113	3.21	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	830	1	65,73,73	2.03	17 (26%)	76,113,113	2.67	34 (44%)
21	CLA	A	835	1	45,53,73	2.28	18 (40%)	52,89,113	3.23	25 (48%)
21	CLA	B	810	2	45,53,73	2.29	16 (35%)	52,89,113	3.29	29 (55%)
21	CLA	5	710	13	50,58,73	2.36	16 (32%)	58,95,113	3.38	29 (50%)
24	BCR	A	849	-	41,41,41	1.83	10 (24%)	56,56,56	1.61	14 (25%)
24	BCR	A	850	-	41,41,41	1.61	10 (24%)	56,56,56	1.50	13 (23%)
21	CLA	A	818	1	54,62,73	2.10	15 (27%)	62,99,113	2.89	28 (45%)
21	CLA	5	703	13	45,53,73	2.25	13 (28%)	52,89,113	2.97	25 (48%)
21	CLA	8	610	25	43,51,73	2.15	14 (32%)	49,86,113	3.21	28 (57%)
21	CLA	10	711	18	45,53,73	2.44	18 (40%)	52,89,113	3.10	25 (48%)
28	DD6	6	915	-	39,45,45	1.55	8 (20%)	52,67,67	1.58	13 (25%)
21	CLA	A	820	1	65,73,73	1.76	17 (26%)	76,113,113	3.05	32 (42%)
21	CLA	1	511	25	43,51,73	2.35	16 (37%)	49,86,113	3.21	24 (48%)
21	CLA	6	910	25	43,51,73	2.38	15 (34%)	49,86,113	3.37	27 (55%)
21	CLA	12	504	-	41,49,73	2.53	16 (39%)	47,84,113	2.96	24 (51%)
22	PQN	B	840	-	32,32,34	1.75	5 (15%)	39,42,45	1.76	8 (20%)
21	CLA	10	705	18	45,53,73	2.50	15 (33%)	52,89,113	3.42	25 (48%)
24	BCR	B	845	-	41,41,41	1.63	10 (24%)	56,56,56	1.49	9 (16%)
25	LHG	10	713	21	31,31,48	0.32	0	34,37,54	0.94	2 (5%)
28	DD6	5	712	-	39,45,45	1.57	9 (23%)	52,67,67	1.47	8 (15%)
21	CLA	6	912	14	45,53,73	2.46	16 (35%)	52,89,113	3.09	26 (50%)
24	BCR	B	844	-	41,41,41	1.72	9 (21%)	56,56,56	1.49	10 (17%)
21	CLA	10	707	18	48,56,73	2.43	17 (35%)	55,92,113	3.07	29 (52%)
21	CLA	3	704	29	42,50,73	2.22	16 (38%)	48,85,113	3.35	26 (54%)
21	CLA	10	710	18	55,63,73	2.19	16 (29%)	64,101,113	2.80	25 (39%)
21	CLA	A	831	1	65,73,73	1.73	16 (24%)	76,113,113	3.01	30 (39%)
28	DD6	3	716	-	39,45,45	1.40	7 (17%)	52,67,67	1.58	9 (17%)
21	CLA	1	515	29	45,53,73	2.43	14 (31%)	52,89,113	3.07	27 (51%)
21	CLA	3	708	25	43,51,73	2.31	15 (34%)	49,86,113	3.07	26 (53%)
21	CLA	B	835	2	65,73,73	1.93	17 (26%)	76,113,113	2.58	33 (43%)
21	CLA	A	834	1	45,53,73	2.21	13 (28%)	52,89,113	3.59	27 (51%)
21	CLA	12	501	19	60,68,73	2.10	16 (26%)	70,107,113	2.85	30 (42%)
21	CLA	A	826	29	65,73,73	1.97	17 (26%)	76,113,113	2.66	32 (42%)
28	DD6	6	916	-	39,45,45	1.41	7 (17%)	52,67,67	1.55	8 (15%)
21	CLA	B	801	2	65,73,73	2.02	20 (30%)	76,113,113	2.49	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	5	707	13	55,63,73	2.25	16 (29%)	64,101,113	2.95	28 (43%)
21	CLA	B	834	2	60,68,73	2.22	19 (31%)	70,107,113	2.93	32 (45%)
21	CLA	2	509	10	62,70,73	2.00	17 (27%)	72,109,113	2.78	25 (34%)
21	CLA	1	516	9	45,53,73	2.41	16 (35%)	52,89,113	3.06	27 (51%)
21	CLA	1	514	9	45,53,73	2.48	15 (33%)	52,89,113	3.08	27 (51%)
21	CLA	3	713	11	45,53,73	2.44	16 (35%)	52,89,113	3.24	24 (46%)
21	CLA	A	832	1	50,58,73	2.03	11 (22%)	58,95,113	3.29	35 (60%)
21	CLA	5	709	13	45,53,73	2.50	17 (37%)	52,89,113	3.25	27 (51%)
21	CLA	7	704	15	45,53,73	2.34	16 (35%)	52,89,113	3.00	25 (48%)
21	CLA	3	711	11	45,53,73	2.40	15 (33%)	52,89,113	3.15	24 (46%)
21	CLA	10	706	-	41,49,73	2.52	15 (36%)	47,84,113	3.33	25 (53%)
25	LHG	2	521	21	29,29,48	0.39	0	32,35,54	1.24	4 (12%)
21	CLA	10	708	25	43,51,73	2.43	15 (34%)	49,86,113	3.25	24 (48%)
21	CLA	4	704	29	50,58,73	2.32	16 (32%)	58,95,113	3.00	28 (48%)
21	CLA	7	711	15	65,73,73	1.89	15 (23%)	76,113,113	2.47	24 (31%)
21	CLA	A	844	25	65,73,73	1.95	17 (26%)	76,113,113	2.97	34 (44%)
28	DD6	8	615	-	39,45,45	1.52	8 (20%)	52,67,67	1.46	8 (15%)
21	CLA	3	710	11	55,63,73	2.10	13 (23%)	64,101,113	2.95	26 (40%)
21	CLA	B	816	2	59,67,73	2.04	17 (28%)	68,105,113	3.00	32 (47%)

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	CLA	2	512	10	-	15/25/103/115	-
21	CLA	B	802	-	1/1/15/20	10/37/115/115	-
21	CLA	F	404	6	1/1/11/20	5/13/91/115	-
21	CLA	2	515	10	1/1/11/20	3/13/91/115	-
21	CLA	2	514	29	1/1/11/20	4/13/91/115	-
21	CLA	3	705	29	1/1/11/20	3/16/94/115	-
21	CLA	A	815	1	1/1/14/20	16/31/109/115	-
21	CLA	3	714	29	1/1/11/20	2/13/91/115	-
21	CLA	A	841	1	1/1/15/20	10/37/115/115	-
21	CLA	6	906	14	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	513	9	-	9/29/107/115	-
21	CLA	1	507	29	1/1/12/20	3/19/97/115	-
21	CLA	12	508	19	1/1/11/20	6/13/91/115	-
21	CLA	B	806	2	1/1/15/20	10/37/115/115	-
21	CLA	4	708	25	1/1/10/20	0/11/89/115	-
21	CLA	4	709	12	1/1/11/20	5/13/91/115	-
21	CLA	12	503	-	1/1/11/20	2/13/91/115	-
21	CLA	B	832	2	1/1/13/20	11/29/107/115	-
21	CLA	A	839	1	1/1/15/20	13/37/115/115	-
21	CLA	2	503	10	1/1/11/20	4/13/91/115	-
21	CLA	B	812	2	1/1/15/20	18/37/115/115	-
21	CLA	8	611	16	1/1/11/20	3/13/91/115	-
21	CLA	12	502	19	1/1/11/20	5/13/91/115	-
25	LHG	3	719	21	-	9/28/28/53	-
21	CLA	A	823	1	-	4/13/91/115	-
21	CLA	9	904	17	1/1/11/20	4/13/91/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	B	808	2	1/1/11/20	2/13/91/115	-
21	CLA	8	609	16	1/1/14/20	4/34/112/115	-
21	CLA	A	809	1	1/1/15/20	14/37/115/115	-
21	CLA	7	705	29	1/1/12/20	4/19/97/115	-
21	CLA	B	813	2	1/1/15/20	11/37/115/115	-
21	CLA	A	803	-	-	12/37/115/115	-
21	CLA	B	838	2	-	3/13/91/115	-
21	CLA	B	807	2	1/1/15/20	11/37/115/115	-
21	CLA	7	709	25	1/1/10/20	2/11/89/115	-
21	CLA	7	713	15	1/1/11/20	0/16/94/115	-
21	CLA	B	804	2	1/1/15/20	11/37/115/115	-
21	CLA	11	707	19	1/1/12/20	3/24/102/115	-
21	CLA	1	508	29	-	3/16/94/115	-
21	CLA	A	808	1	1/1/12/20	3/21/99/115	-
21	CLA	4	705	29	-	3/16/94/115	-
25	LHG	B	848	21	-	11/26/26/53	-
21	CLA	9	908	17	1/1/14/20	5/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	4	714	21	-	7/19/19/53	-
21	CLA	8	607	29	-	0/16/94/115	-
25	LHG	9	917	21	-	21/38/38/53	-
21	CLA	A	862	29	1/1/15/20	13/37/115/115	-
25	LHG	7	717	21	-	21/52/52/53	-
21	CLA	A	825	1	-	12/30/108/115	-
28	DD6	11	712	-	-	4/26/80/80	0/3/3/3
25	LHG	A	853	-	-	19/53/53/53	-
28	DD6	4	712	-	-	3/26/80/80	0/3/3/3
21	CLA	3	702	11	-	7/31/109/115	-
28	DD6	7	715	-	-	13/26/80/80	0/3/3/3
21	CLA	5	711	13	1/1/11/20	2/13/91/115	-
21	CLA	7	702	15	1/1/11/20	8/16/94/115	-
21	CLA	13	503	19	1/1/11/20	2/16/94/115	-
21	CLA	B	822	2	1/1/11/20	3/13/91/115	-
21	CLA	4	702	12	-	3/25/103/115	-
28	DD6	2	520	-	-	10/26/80/80	0/3/3/3
21	CLA	7	712	15	1/1/11/20	1/13/91/115	-
21	CLA	9	912	17	1/1/11/20	4/13/91/115	-
24	BCR	A	848	-	-	6/29/63/63	0/2/2/2
21	CLA	5	705	29	1/1/11/20	4/16/94/115	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	12	507	19	1/1/11/20	3/13/91/115	-
21	CLA	6	903	14	1/1/11/20	8/16/94/115	-
21	CLA	A	822	29	-	11/37/115/115	-
21	CLA	2	505	10	1/1/11/20	6/13/91/115	-
21	CLA	9	902	17	1/1/10/20	2/10/88/115	-
21	CLA	A	806	1	1/1/15/20	13/37/115/115	-
28	DD6	1	520	-	-	14/26/80/80	0/3/3/3
21	CLA	A	836	1	-	5/24/102/115	-
21	CLA	12	506	19	1/1/13/20	6/25/103/115	-
21	CLA	11	709	19	1/1/11/20	4/13/91/115	-
21	CLA	1	512	9	1/1/11/20	3/13/91/115	-
24	BCR	B	842	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	906	29	-	2/16/94/115	-
21	CLA	7	707	15	1/1/11/20	2/16/94/115	-
21	CLA	J	101	7	1/1/11/20	6/13/91/115	-
21	CLA	2	506	29	1/1/12/20	4/19/97/115	-
21	CLA	7	708	15	1/1/14/20	8/34/112/115	-
21	CLA	10	703	18	1/1/10/20	2/8/86/115	-
21	CLA	4	701	-	-	4/8/86/115	-
21	CLA	11	702	19	1/1/14/20	8/31/109/115	-
28	DD6	2	518	-	-	2/26/80/80	0/3/3/3
21	CLA	1	510	9	1/1/14/20	8/34/112/115	-
21	CLA	9	913	17	-	4/16/94/115	-
21	CLA	B	827	2	1/1/15/20	14/37/115/115	-
21	CLA	8	605	16	1/1/11/20	3/13/91/115	-
21	CLA	B	828	2	1/1/15/20	8/37/115/115	-
24	BCR	A	847	-	-	4/29/63/63	0/2/2/2
21	CLA	B	821	2	1/1/13/20	7/25/103/115	-
21	CLA	A	817	29	-	2/18/96/115	-
21	CLA	5	704	29	-	4/19/97/115	-
25	LHG	1	521	21	-	15/40/40/53	-
28	DD6	12	510	-	-	11/26/80/80	0/3/3/3
21	CLA	7	714	15	1/1/11/20	2/16/94/115	-
21	CLA	A	804	1	1/1/15/20	13/37/115/115	-
21	CLA	2	511	10	1/1/11/20	4/13/91/115	-
21	CLA	8	603	16	1/1/11/20	6/16/94/115	-
28	DD6	7	716	-	-	1/26/80/80	0/3/3/3
21	CLA	B	836	2	1/1/11/20	1/16/94/115	-
21	CLA	2	508	10	1/1/11/20	2/16/94/115	-
21	CLA	11	708	25	1/1/10/20	5/11/89/115	-
21	CLA	A	819	1	1/1/12/20	8/24/102/115	-
21	CLA	F	401	29	1/1/12/20	9/21/99/115	-
21	CLA	4	706	12	1/1/11/20	3/16/94/115	-
21	CLA	1	509	9	1/1/11/20	2/16/94/115	-
21	CLA	5	702	13	1/1/14/20	6/31/109/115	-
21	CLA	6	905	14	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	11	701	19	1/1/10/20	2/8/86/115	-
21	CLA	5	701	13	1/1/11/20	8/13/91/115	-
21	CLA	A	816	1	-	2/13/91/115	-
21	CLA	7	710	15	1/1/11/20	6/13/91/115	-
23	SF4	C	101	3	-	-	0/6/5/5
21	CLA	2	510	25	1/1/10/20	3/11/89/115	-
28	DD6	1	519	-	-	2/26/80/80	0/3/3/3
21	CLA	4	710	12	-	7/13/91/115	-
27	DGD	B	847	-	-	23/46/86/95	0/2/2/2
21	CLA	B	811	2	-	4/13/91/115	-
21	CLA	4	703	12	1/1/11/20	6/13/91/115	-
21	CLA	B	830	2	1/1/11/20	8/18/96/115	-
21	CLA	B	805	2	1/1/15/20	16/37/115/115	-
21	CLA	F	403	29	1/1/11/20	5/13/91/115	-
28	DD6	12	509	-	-	3/26/80/80	0/3/3/3
21	CLA	3	703	11	1/1/11/20	4/13/91/115	-
21	CLA	B	823	29	1/1/12/20	8/24/102/115	-
21	CLA	2	516	29	-	1/13/91/115	-
21	CLA	A	805	1	1/1/13/20	12/30/108/115	-
21	CLA	8	612	16	-	11/37/115/115	-
25	LHG	11	714	21	-	11/34/34/53	-
28	DD6	11	713	-	-	9/26/80/80	0/3/3/3
23	SF4	A	846	2,1	-	-	0/6/5/5
21	CLA	A	842	1	1/1/15/20	14/37/115/115	-
21	CLA	3	712	29	1/1/11/20	7/13/91/115	-
21	CLA	6	907	29	-	1/16/94/115	-
25	LHG	6	917	21	-	14/32/32/53	-
28	DD6	2	519	-	-	4/26/80/80	0/3/3/3
24	BCR	F	405	-	-	5/29/63/63	0/2/2/2
21	CLA	3	707	11	1/1/14/20	4/34/112/115	-
21	CLA	4	711	29	1/1/11/20	4/13/91/115	-
21	CLA	5	708	25	1/1/10/20	5/11/89/115	-
24	BCR	M	102	-	-	3/29/63/63	0/2/2/2
28	DD6	3	718	-	-	7/26/80/80	0/3/3/3
21	CLA	A	807	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	831	2	1/1/15/20	17/37/115/115	-
21	CLA	B	820	2	-	6/13/91/115	-
21	CLA	11	710	19	-	7/13/91/115	-
28	DD6	8	616	-	-	7/26/80/80	0/3/3/3
28	DD6	3	717	-	-	9/26/80/80	0/3/3/3
24	BCR	B	843	-	-	6/29/63/63	0/2/2/2
21	CLA	A	840	1	1/1/11/20	8/16/94/115	-
21	CLA	9	905	29	1/1/12/20	5/19/97/115	-
21	CLA	6	904	14	1/1/14/20	5/31/109/115	-
21	CLA	11	703	19	1/1/15/20	16/37/115/115	-
21	CLA	9	909	25	1/1/10/20	3/11/89/115	-
21	CLA	1	505	9	1/1/14/20	9/31/109/115	-
21	CLA	8	613	16	1/1/11/20	5/13/91/115	-
21	CLA	2	507	29	-	6/16/94/115	-
21	CLA	3	701	11	1/1/10/20	4/8/86/115	-
21	CLA	B	809	2	1/1/11/20	4/13/91/115	-
21	CLA	B	837	29	1/1/11/20	5/13/91/115	-
28	DD6	5	713	-	-	5/26/80/80	0/3/3/3
28	DD6	9	916	-	-	10/26/80/80	0/3/3/3
21	CLA	B	815	2	1/1/13/20	9/25/103/115	-
21	CLA	2	504	10	1/1/14/20	12/31/109/115	-
24	BCR	B	846	-	-	0/29/63/63	0/2/2/2
21	CLA	6	913	14	1/1/11/20	5/13/91/115	-
21	CLA	9	911	17	1/1/13/20	8/25/103/115	-
28	DD6	1	518	-	-	14/26/80/80	0/3/3/3
21	CLA	8	604	16	1/1/14/20	6/31/109/115	-
21	CLA	A	837	1	-	6/13/91/115	-
22	PQN	A	845	-	-	8/23/43/43	0/2/2/2
21	CLA	13	501	19	1/1/11/20	5/13/91/115	-
21	CLA	9	907	17	1/1/11/20	2/16/94/115	-
21	CLA	7	706	29	-	5/16/94/115	-
21	CLA	B	839	25	1/1/15/20	15/37/115/115	-
21	CLA	6	911	14	1/1/11/20	3/13/91/115	-
21	CLA	A	810	1	-	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	517	-	1/1/11/20	2/13/91/115	-
21	CLA	3	706	11	1/1/11/20	7/16/94/115	-
21	CLA	A	811	1	1/1/11/20	5/13/91/115	-
21	CLA	A	824	1	-	11/21/99/115	-
21	CLA	8	608	16	1/1/11/20	2/16/94/115	-
21	CLA	B	814	2	1/1/11/20	2/13/91/115	-
24	BCR	A	851	-	-	0/29/63/63	0/2/2/2
21	CLA	12	505	19	1/1/11/20	2/16/94/115	-
21	CLA	13	502	-	1/1/11/20	4/16/94/115	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	CLA	10	709	18	1/1/11/20	3/13/91/115	-
21	CLA	11	704	29	1/1/11/20	0/13/91/115	-
21	CLA	8	614	16	-	2/16/94/115	-
21	CLA	A	829	1	1/1/15/20	18/37/115/115	-
21	CLA	B	817	2	1/1/14/20	12/31/109/115	-
21	CLA	9	914	17	1/1/11/20	5/16/94/115	-
28	DD6	J	104	-	-	16/26/80/80	0/3/3/3
21	CLA	4	707	12	1/1/14/20	4/34/112/115	-
21	CLA	1	504	9	1/1/10/20	1/10/88/115	-
25	LHG	5	714	21	-	15/36/36/53	-
21	CLA	6	909	14	1/1/14/20	4/34/112/115	-
21	CLA	B	819	2	-	6/16/94/115	-
21	CLA	1	506	9	1/1/11/20	5/13/91/115	-
21	CLA	A	813	1	1/1/12/20	10/24/102/115	-
21	CLA	6	914	14	-	7/16/94/115	-
25	LHG	8	617	21	-	15/37/37/53	-
23	SF4	C	102	3	-	-	0/6/5/5
21	CLA	9	910	17	1/1/11/20	5/13/91/115	-
25	LHG	A	854	21	-	13/31/31/53	-
21	CLA	6	908	14	1/1/11/20	1/13/91/115	-
21	CLA	A	812	1	1/1/15/20	5/37/115/115	-
21	CLA	7	703	15	-	8/31/109/115	-
21	CLA	A	821	1	1/1/14/20	12/33/111/115	-
21	CLA	A	802	29	1/1/15/20	3/37/115/115	-
21	CLA	11	711	19	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	10	712	18	1/1/11/20	4/16/94/115	-
21	CLA	B	829	2	-	4/13/91/115	-
21	CLA	B	825	2	1/1/15/20	4/37/115/115	-
21	CLA	A	827	29	1/1/14/20	9/31/109/115	-
21	CLA	B	833	2	1/1/11/20	9/13/91/115	-
21	CLA	A	828	1	1/1/15/20	13/37/115/115	-
21	CLA	A	838	1	1/1/12/20	4/21/99/115	-
21	CLA	1	501	29	1/1/11/20	2/13/91/115	-
21	CLA	3	715	11	1/1/11/20	5/13/91/115	-
21	CLA	9	903	17	1/1/14/20	6/31/109/115	-
21	CLA	10	704	18	1/1/14/20	6/31/109/115	-
21	CLA	2	513	10	1/1/11/20	7/13/91/115	-
21	CLA	1	517	29	-	2/13/91/115	-
24	BCR	B	841	-	-	2/29/63/63	0/2/2/2
24	BCR	F	402	-	-	1/29/63/63	0/2/2/2
21	CLA	11	705	-	1/1/11/20	6/16/94/115	-
21	CLA	A	814	1	1/1/14/20	7/31/109/115	-
21	CLA	B	824	29	1/1/11/20	4/15/93/115	-
20	CL0	A	801	1	3/3/20/25	5/37/135/135	-
21	CLA	A	843	29	1/1/12/20	4/22/100/115	-
21	CLA	8	606	29	1/1/11/20	0/13/91/115	-
21	CLA	A	833	1	1/1/15/20	5/37/115/115	-
21	CLA	3	709	11	1/1/11/20	5/13/91/115	-
21	CLA	B	826	2	1/1/15/20	14/37/115/115	-
21	CLA	5	706	13	1/1/11/20	3/13/91/115	-
21	CLA	11	706	19	1/1/15/20	12/37/115/115	-
28	DD6	9	915	-	-	12/26/80/80	0/3/3/3
21	CLA	B	818	29	1/1/15/20	4/37/115/115	-
28	DD6	4	713	-	-	14/26/80/80	0/3/3/3
21	CLA	B	803	2	1/1/12/20	13/24/102/115	-
21	CLA	A	830	1	1/1/15/20	13/37/115/115	-
21	CLA	A	835	1	-	5/13/91/115	-
21	CLA	B	810	2	1/1/11/20	4/13/91/115	-
21	CLA	5	710	13	-	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	A	849	-	-	4/29/63/63	0/2/2/2
24	BCR	A	850	-	-	6/29/63/63	0/2/2/2
21	CLA	A	818	1	1/1/12/20	12/24/102/115	-
21	CLA	5	703	13	1/1/11/20	5/13/91/115	-
21	CLA	8	610	25	1/1/10/20	2/11/89/115	-
21	CLA	10	711	18	1/1/11/20	1/13/91/115	-
28	DD6	6	915	-	-	3/26/80/80	0/3/3/3
21	CLA	A	820	1	1/1/15/20	15/37/115/115	-
21	CLA	1	511	25	1/1/10/20	2/11/89/115	-
21	CLA	6	910	25	1/1/10/20	3/11/89/115	-
21	CLA	12	504	-	1/1/10/20	1/8/86/115	-
22	PQN	B	840	-	-	4/21/41/43	0/2/2/2
21	CLA	10	705	18	1/1/11/20	3/13/91/115	-
24	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	LHG	10	713	21	-	17/36/36/53	-
28	DD6	5	712	-	-	3/26/80/80	0/3/3/3
21	CLA	6	912	14	1/1/11/20	6/13/91/115	-
24	BCR	B	844	-	-	2/29/63/63	0/2/2/2
21	CLA	10	707	18	1/1/11/20	7/17/95/115	-
21	CLA	3	704	29	1/1/10/20	2/10/88/115	-
21	CLA	10	710	18	1/1/13/20	3/25/103/115	-
21	CLA	A	831	1	1/1/15/20	8/37/115/115	-
28	DD6	3	716	-	-	4/26/80/80	0/3/3/3
21	CLA	1	515	29	1/1/11/20	1/13/91/115	-
21	CLA	3	708	25	1/1/10/20	6/11/89/115	-
21	CLA	B	835	2	1/1/15/20	15/37/115/115	-
21	CLA	A	834	1	1/1/11/20	4/13/91/115	-
21	CLA	12	501	19	1/1/14/20	7/31/109/115	-
21	CLA	A	826	29	1/1/15/20	14/37/115/115	-
28	DD6	6	916	-	-	6/26/80/80	0/3/3/3
21	CLA	B	801	2	1/1/15/20	3/37/115/115	-
21	CLA	5	707	13	1/1/13/20	6/25/103/115	-
21	CLA	B	834	2	1/1/14/20	9/31/109/115	-
21	CLA	2	509	10	1/1/14/20	5/34/112/115	-
21	CLA	1	516	9	1/1/11/20	1/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	514	9	1/1/11/20	1/13/91/115	-
21	CLA	3	713	11	1/1/11/20	5/13/91/115	-
21	CLA	5	709	13	1/1/11/20	3/13/91/115	-
21	CLA	A	832	1	-	4/19/97/115	-
21	CLA	7	704	15	1/1/11/20	3/13/91/115	-
21	CLA	3	711	11	1/1/11/20	4/13/91/115	-
21	CLA	10	706	-	1/1/10/20	2/8/86/115	-
25	LHG	2	521	21	-	16/34/34/53	-
21	CLA	10	708	25	1/1/10/20	2/11/89/115	-
21	CLA	4	704	29	1/1/12/20	0/19/97/115	-
21	CLA	7	711	15	1/1/15/20	7/37/115/115	-
21	CLA	A	844	25	1/1/15/20	13/37/115/115	-
28	DD6	8	615	-	-	12/26/80/80	0/3/3/3
21	CLA	3	710	11	-	11/25/103/115	-
21	CLA	B	816	2	1/1/13/20	5/30/108/115	-

The worst 5 of 4198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	807	CLA	C1B-NB	-8.18	1.27	1.35
21	B	801	CLA	C1B-NB	-8.10	1.28	1.35
21	A	838	CLA	C1B-NB	-6.91	1.29	1.35
21	9	908	CLA	C3B-C2B	6.89	1.49	1.40
21	A	826	CLA	C1B-NB	-6.87	1.29	1.35

The worst 5 of 7093 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	829	CLA	C2D-C1D-ND	12.22	119.11	110.10
21	A	834	CLA	C1D-ND-C4D	-11.90	97.88	106.33
21	A	827	CLA	C1D-ND-C4D	-11.77	97.98	106.33
21	9	907	CLA	C1D-ND-C4D	-11.63	98.07	106.33
21	A	823	CLA	C1D-ND-C4D	-11.38	98.25	106.33

5 of 198 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CL0	NA
20	A	801	CL0	NC

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Mol	Chain	Res	Type	Atom
20	A	801	CL0	ND
21	A	802	CLA	ND
21	A	804	CLA	ND

5 of 1907 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	803	CLA	CBA-CGA-O2A-C1
21	A	803	CLA	O1A-CGA-O2A-C1
21	A	803	CLA	O2A-C1-C2-C3
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

214 monomers are involved in 397 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	802	CLA	2	0
21	F	404	CLA	1	0
21	2	515	CLA	1	0
21	2	514	CLA	1	0
21	1	513	CLA	2	0
21	3	705	CLA	2	0
21	A	841	CLA	1	0
21	3	714	CLA	1	0
21	1	507	CLA	2	0
21	12	508	CLA	1	0
21	B	806	CLA	1	0
21	4	708	CLA	2	0
21	4	709	CLA	1	0
21	A	839	CLA	4	0
21	2	503	CLA	2	0
21	B	812	CLA	2	0
21	8	611	CLA	1	0
21	12	502	CLA	1	0
25	3	719	LHG	1	0
21	A	823	CLA	3	0
24	J	102	BCR	7	0
21	8	609	CLA	2	0
21	A	809	CLA	2	0
21	1	508	CLA	2	0
21	A	803	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	838	CLA	2	0
21	B	807	CLA	2	0
21	7	705	CLA	1	0
21	B	804	CLA	3	0
21	7	709	CLA	2	0
21	7	713	CLA	3	0
21	A	808	CLA	1	0
21	11	707	CLA	3	0
25	4	714	LHG	3	0
21	8	607	CLA	1	0
21	A	862	CLA	7	0
21	A	825	CLA	1	0
25	A	853	LHG	1	0
28	4	712	DD6	2	0
21	3	702	CLA	1	0
21	5	711	CLA	1	0
21	13	503	CLA	1	0
21	4	702	CLA	2	0
24	A	848	BCR	3	0
24	A	852	BCR	9	0
21	12	507	CLA	1	0
21	6	903	CLA	1	0
21	A	822	CLA	1	0
21	2	505	CLA	3	0
21	9	902	CLA	2	0
21	A	806	CLA	2	0
21	A	836	CLA	1	0
21	12	506	CLA	4	0
21	11	709	CLA	1	0
21	1	512	CLA	1	0
24	B	842	BCR	2	0
21	7	707	CLA	1	0
21	J	101	CLA	1	0
21	2	506	CLA	1	0
21	4	701	CLA	3	0
21	7	708	CLA	4	0
21	1	510	CLA	1	0
21	9	913	CLA	3	0
21	B	827	CLA	4	0
21	B	828	CLA	2	0
24	A	847	BCR	3	0
21	B	821	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	817	CLA	3	0
21	7	714	CLA	1	0
21	A	804	CLA	3	0
21	2	511	CLA	6	0
21	8	603	CLA	1	0
21	2	508	CLA	2	0
21	11	708	CLA	1	0
21	A	819	CLA	2	0
21	F	401	CLA	2	0
21	4	706	CLA	1	0
21	1	509	CLA	1	0
21	5	702	CLA	2	0
21	11	701	CLA	1	0
21	5	701	CLA	1	0
21	7	710	CLA	1	0
21	2	510	CLA	4	0
21	4	710	CLA	2	0
27	B	847	DGD	3	0
21	B	811	CLA	1	0
21	B	830	CLA	3	0
21	B	805	CLA	1	0
21	F	403	CLA	2	0
21	3	703	CLA	1	0
21	B	823	CLA	3	0
21	A	805	CLA	1	0
21	8	612	CLA	3	0
28	11	713	DD6	1	0
21	A	842	CLA	5	0
21	3	712	CLA	1	0
21	6	907	CLA	1	0
24	F	405	BCR	4	0
21	3	707	CLA	3	0
21	4	711	CLA	2	0
21	5	708	CLA	2	0
24	M	102	BCR	2	0
21	A	807	CLA	2	0
21	B	831	CLA	6	0
21	11	710	CLA	1	0
21	A	840	CLA	1	0
21	6	904	CLA	2	0
21	11	703	CLA	3	0
21	9	909	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	505	CLA	2	0
21	2	507	CLA	4	0
21	8	613	CLA	1	0
21	3	701	CLA	2	0
21	B	815	CLA	2	0
21	2	504	CLA	1	0
21	6	913	CLA	1	0
21	9	911	CLA	1	0
28	1	518	DD6	1	0
21	8	604	CLA	2	0
21	A	837	CLA	1	0
22	A	845	PQN	2	0
21	13	501	CLA	1	0
21	9	907	CLA	1	0
21	B	839	CLA	2	0
21	6	911	CLA	2	0
21	A	810	CLA	4	0
21	2	517	CLA	1	0
21	3	706	CLA	2	0
21	A	811	CLA	1	0
21	A	824	CLA	1	0
24	A	851	BCR	3	0
21	12	505	CLA	1	0
21	13	502	CLA	1	0
24	J	103	BCR	1	0
21	10	709	CLA	1	0
21	A	829	CLA	6	0
21	B	817	CLA	1	0
21	9	914	CLA	1	0
21	1	504	CLA	2	0
21	B	819	CLA	1	0
21	6	909	CLA	2	0
21	1	506	CLA	1	0
21	A	813	CLA	2	0
21	6	914	CLA	1	0
21	9	910	CLA	2	0
21	6	908	CLA	1	0
21	A	812	CLA	2	0
21	7	703	CLA	3	0
21	A	821	CLA	4	0
21	A	802	CLA	2	0
21	11	711	CLA	1	0

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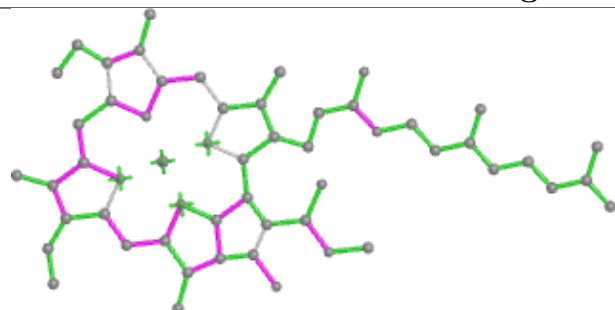
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	10	712	CLA	2	0
21	B	829	CLA	5	0
21	B	825	CLA	2	0
21	A	827	CLA	1	0
21	B	833	CLA	1	0
21	A	828	CLA	2	0
21	A	838	CLA	1	0
21	1	517	CLA	3	0
21	3	715	CLA	1	0
21	2	513	CLA	2	0
21	10	704	CLA	2	0
24	B	841	BCR	3	0
24	F	402	BCR	1	0
21	11	705	CLA	2	0
21	B	824	CLA	1	0
20	A	801	CL0	2	0
21	A	843	CLA	1	0
21	A	833	CLA	3	0
21	3	709	CLA	1	0
21	B	826	CLA	2	0
21	5	706	CLA	2	0
21	B	818	CLA	1	0
21	B	803	CLA	2	0
21	A	830	CLA	2	0
21	A	835	CLA	1	0
24	A	849	BCR	3	0
24	A	850	BCR	1	0
21	A	818	CLA	2	0
21	10	711	CLA	1	0
28	6	915	DD6	1	0
21	A	820	CLA	3	0
21	1	511	CLA	1	0
21	6	910	CLA	2	0
21	12	504	CLA	4	0
24	B	845	BCR	6	0
21	6	912	CLA	1	0
24	B	844	BCR	2	0
21	10	707	CLA	2	0
21	3	704	CLA	1	0
21	A	831	CLA	3	0
28	3	716	DD6	1	0
21	1	515	CLA	2	0

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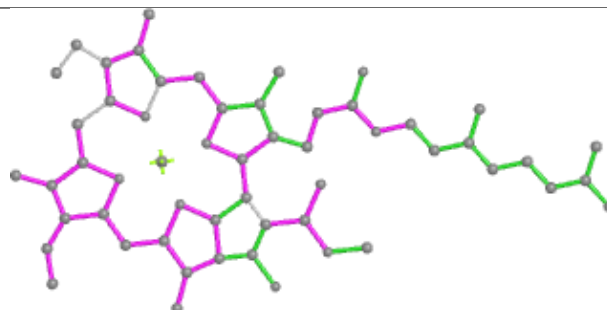
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	708	CLA	2	0
21	B	835	CLA	8	0
21	A	834	CLA	1	0
21	A	826	CLA	3	0
21	B	801	CLA	2	0
21	5	707	CLA	5	0
21	B	834	CLA	2	0
21	2	509	CLA	4	0
21	1	516	CLA	2	0
21	1	514	CLA	2	0
21	3	713	CLA	1	0
21	A	832	CLA	1	0
21	5	709	CLA	1	0
21	3	711	CLA	1	0
21	10	706	CLA	2	0
25	2	521	LHG	1	0
21	10	708	CLA	1	0
21	4	704	CLA	1	0
21	A	844	CLA	5	0
21	3	710	CLA	2	0
21	B	816	CLA	3	0

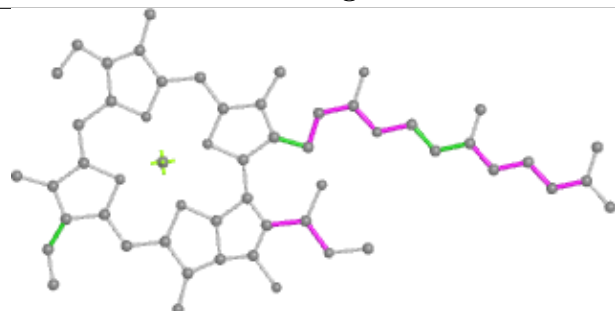
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA 2 512

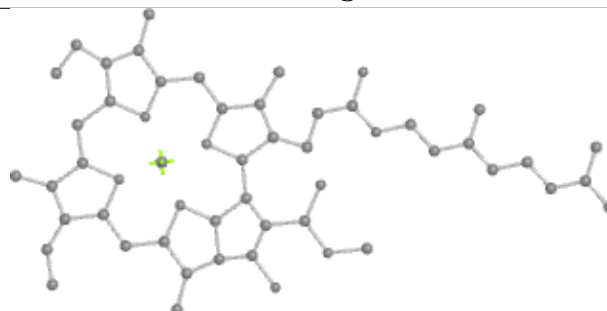
Bond lengths



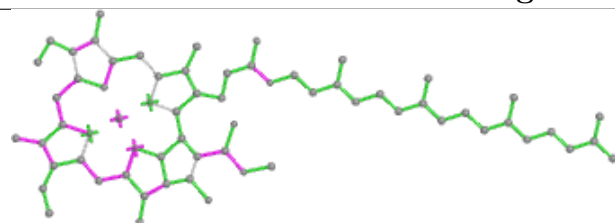
Bond angles



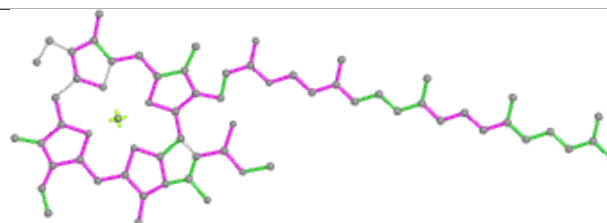
Torsions



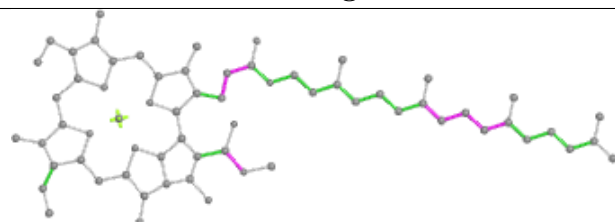
Rings

Ligand CLA B 802

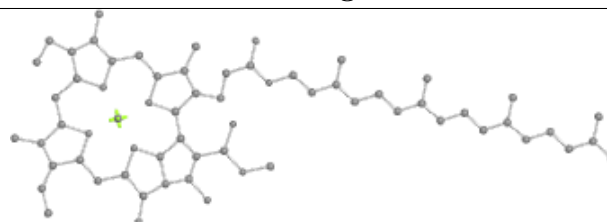
Bond lengths



Bond angles

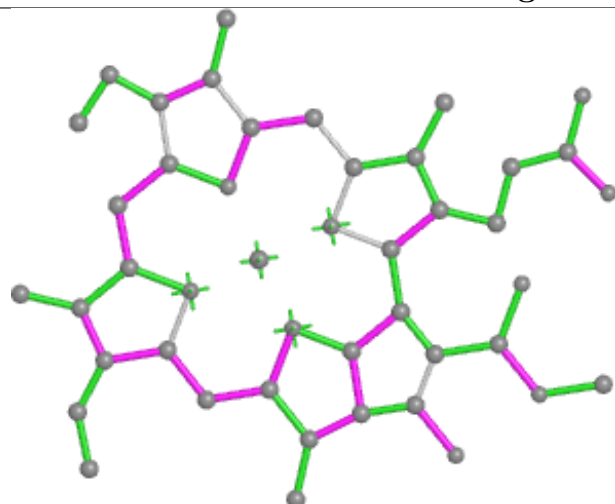


Torsions

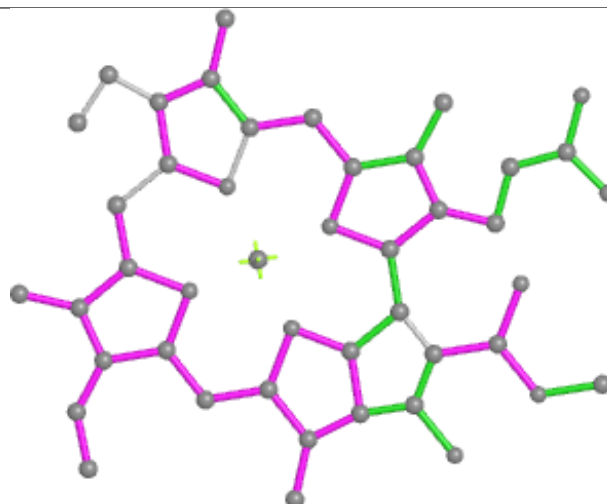


Rings

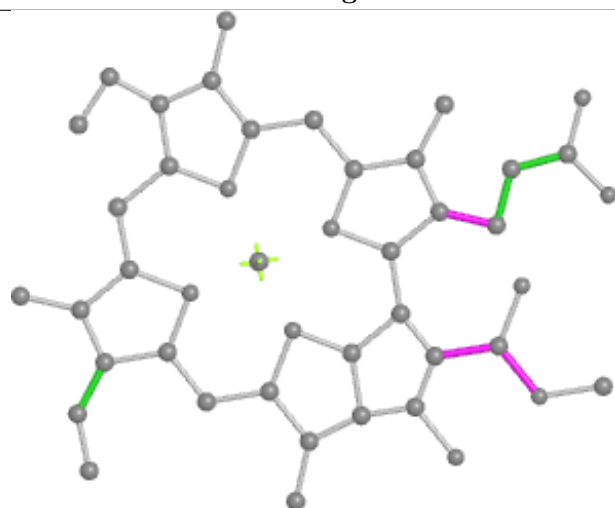
Ligand CLA F 404



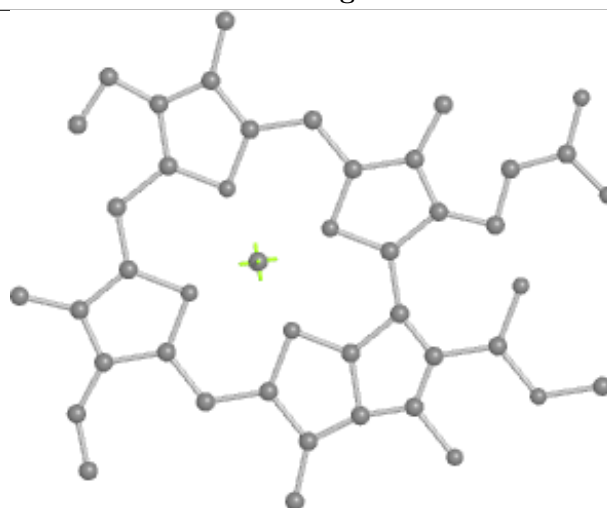
Bond lengths



Bond angles

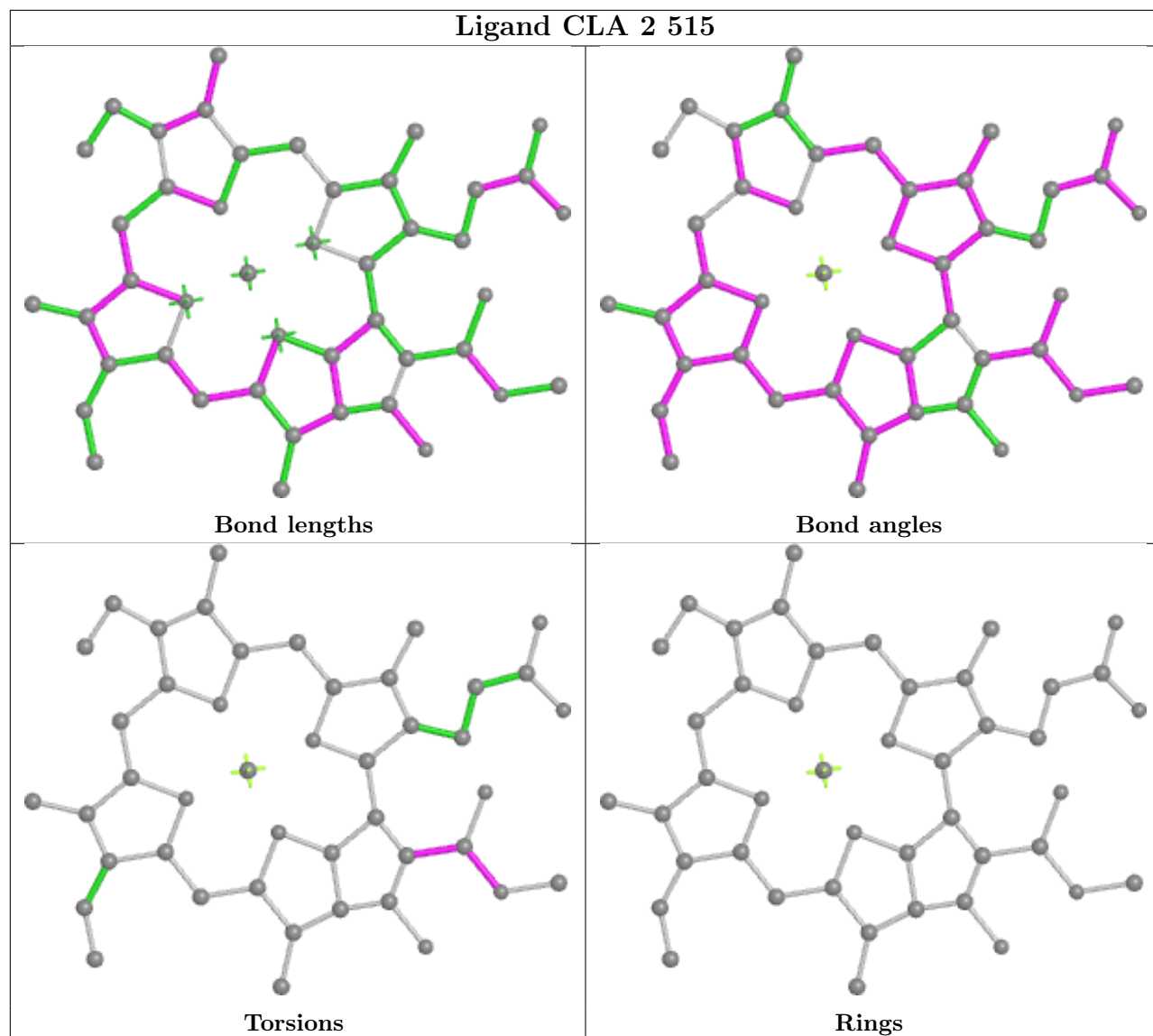


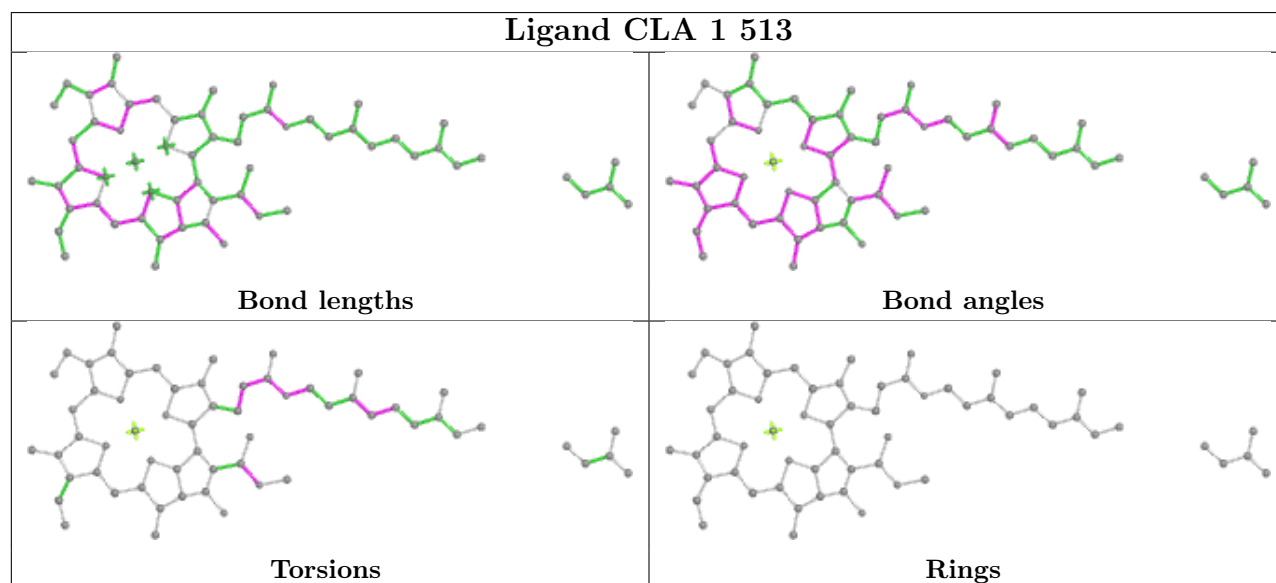
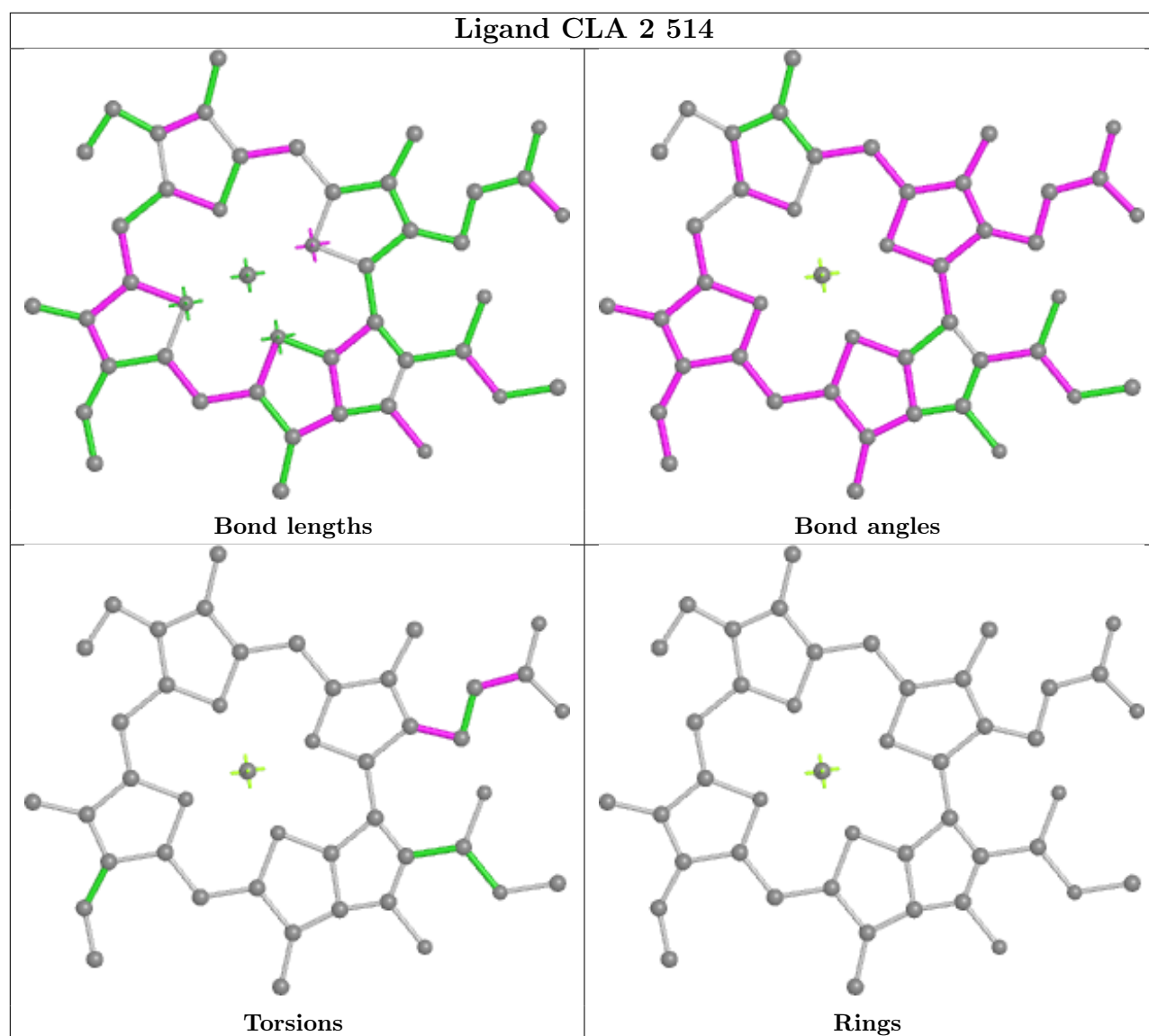
Torsions



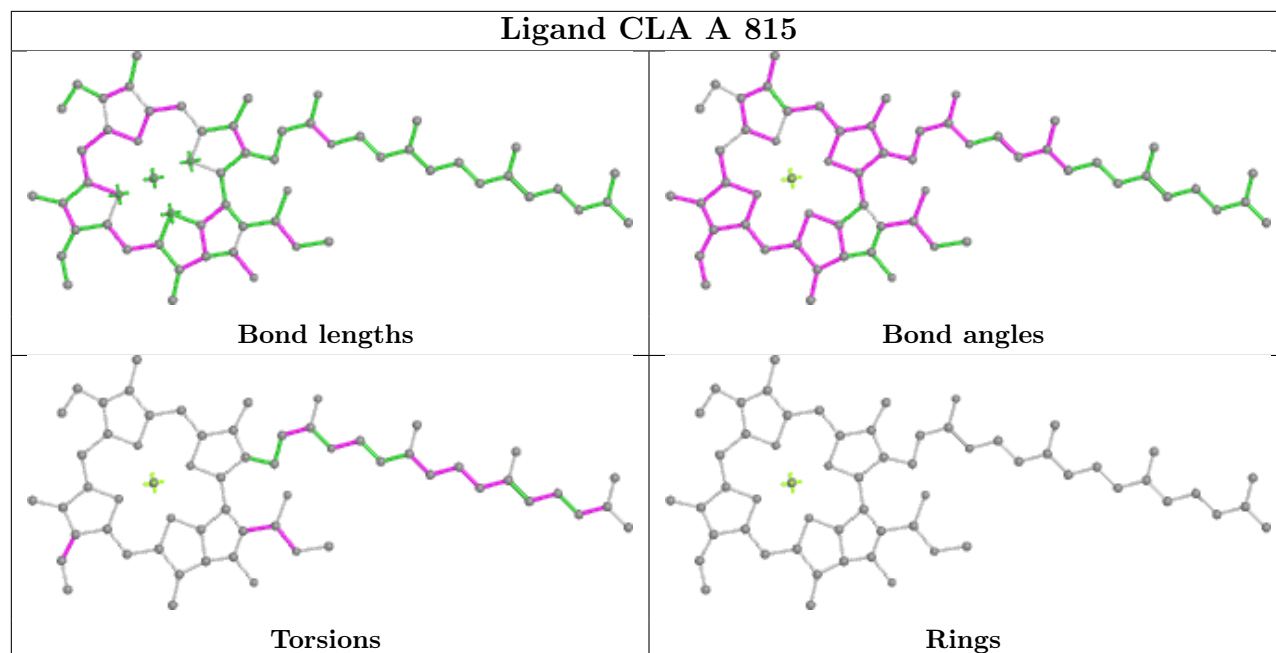
Rings

Ligand CLA 2 515

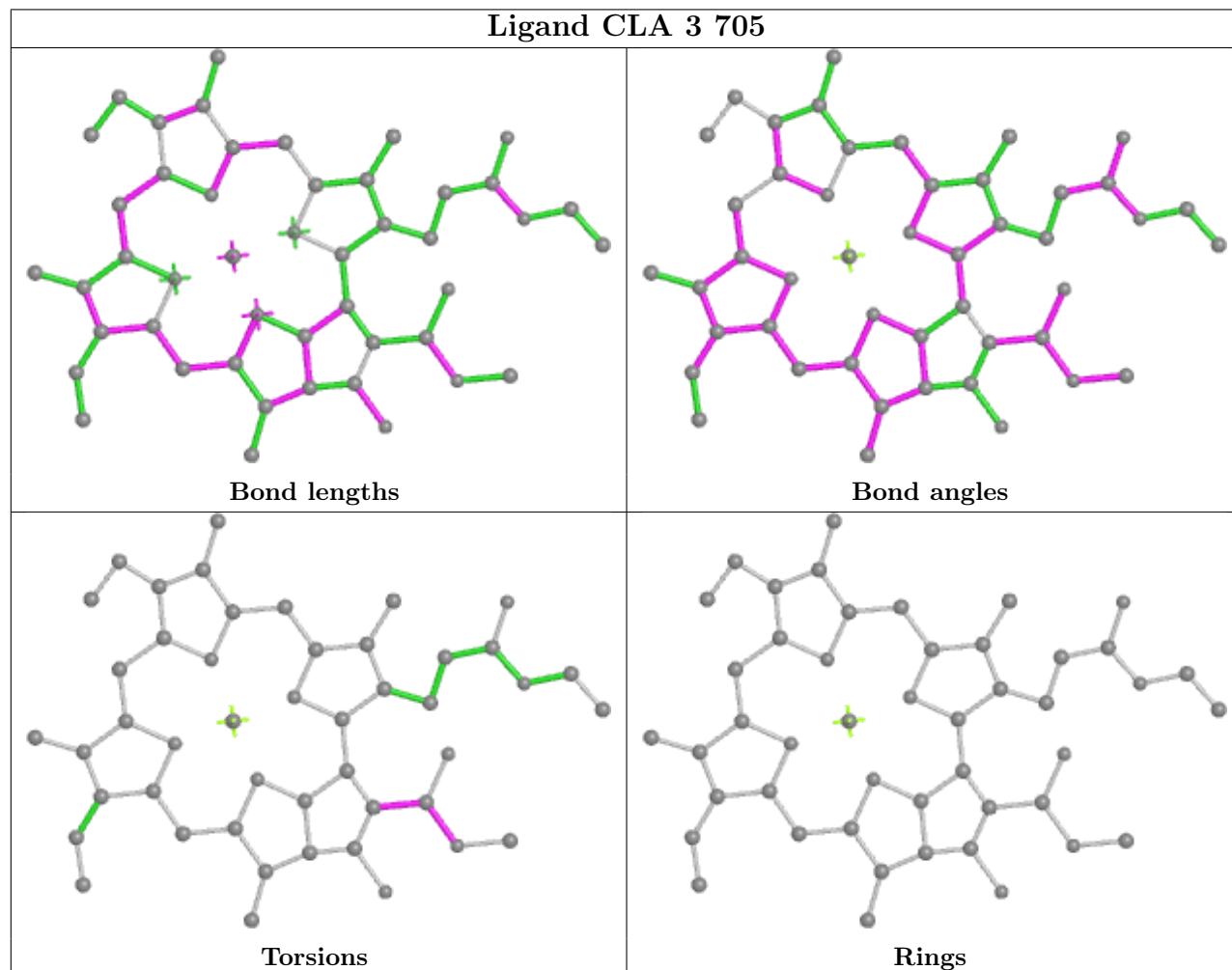




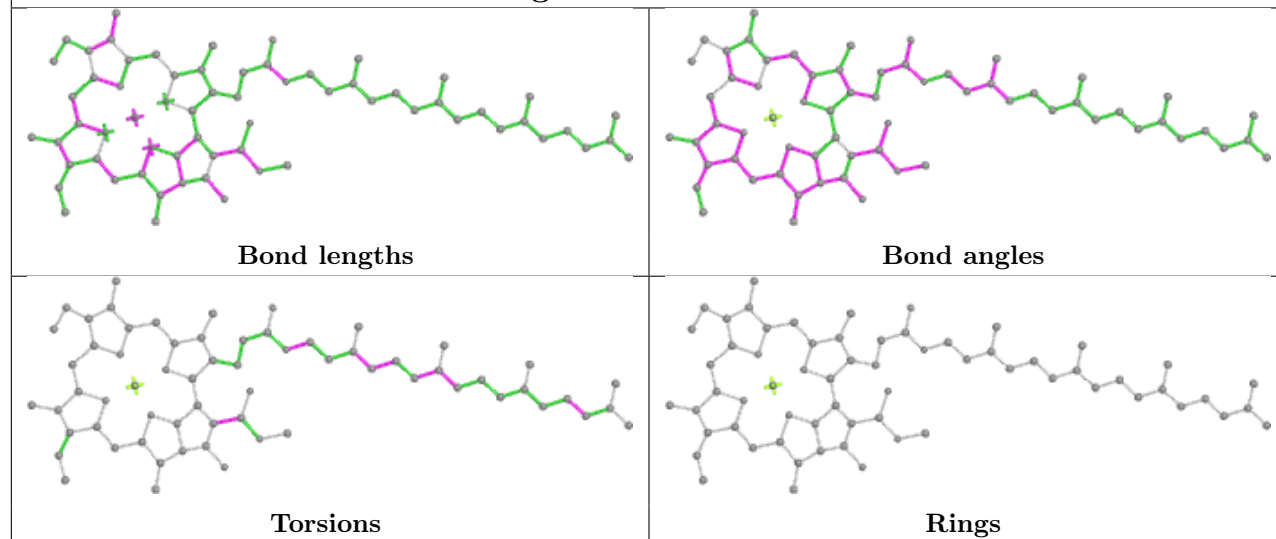
Ligand CLA A 815



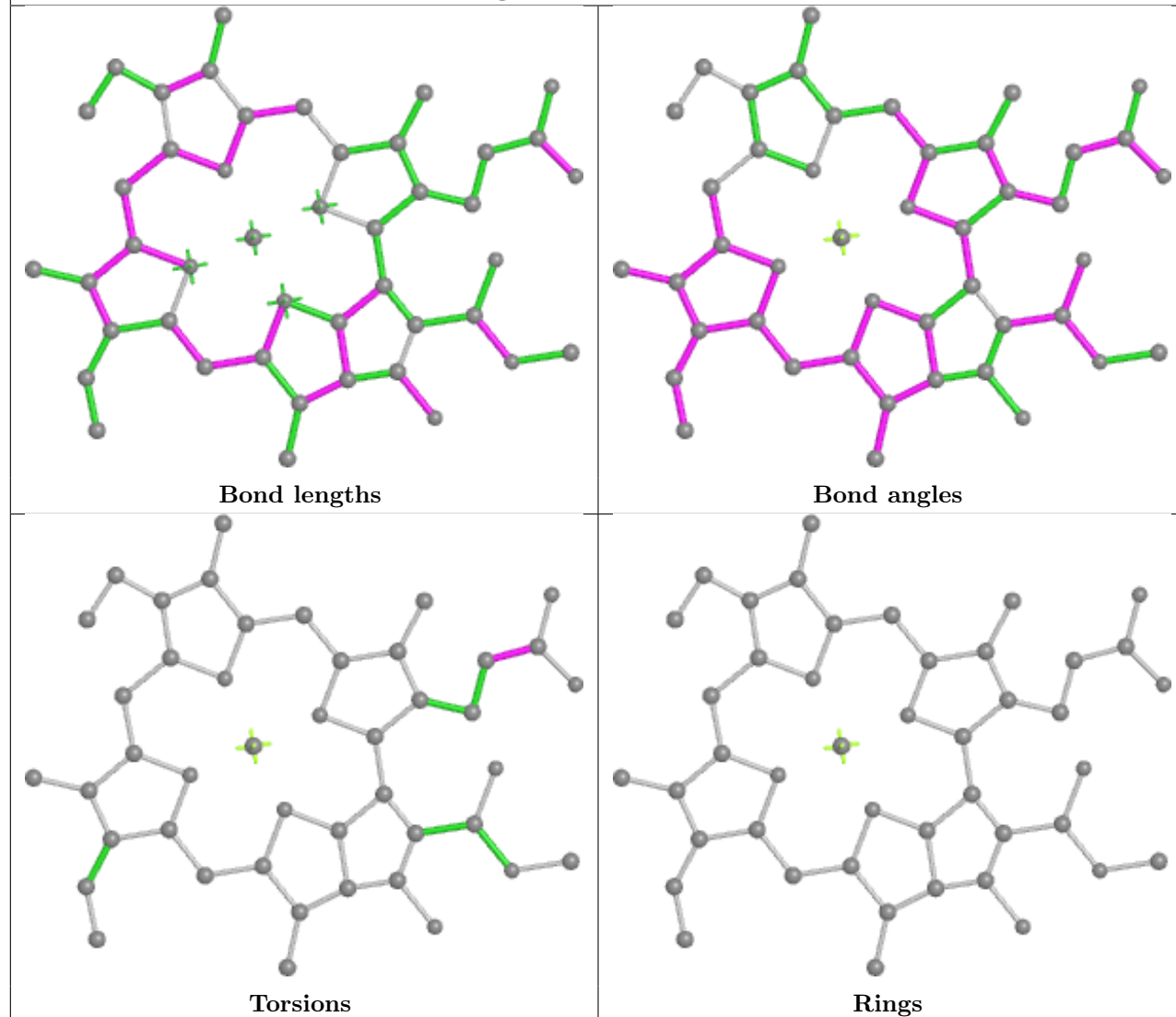
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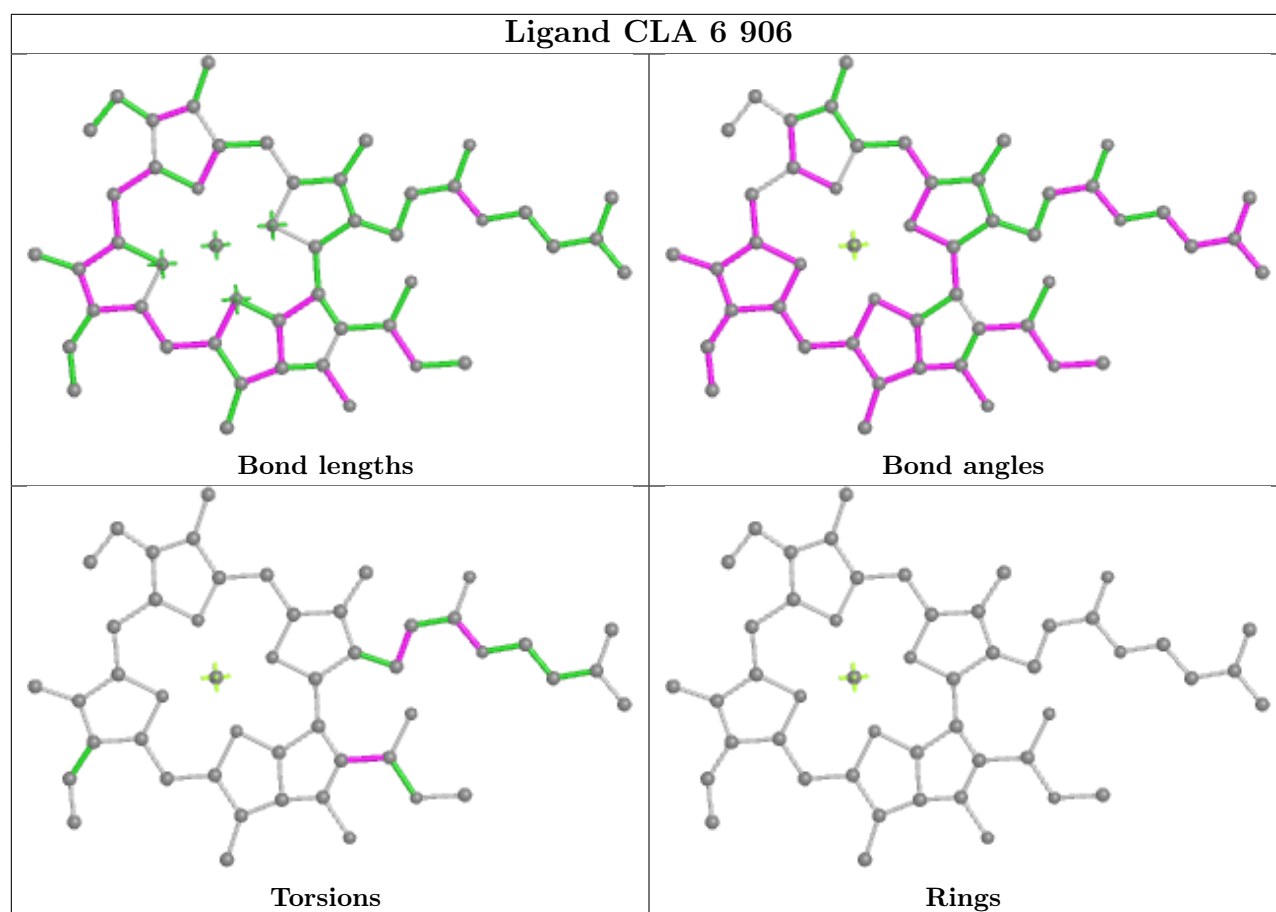


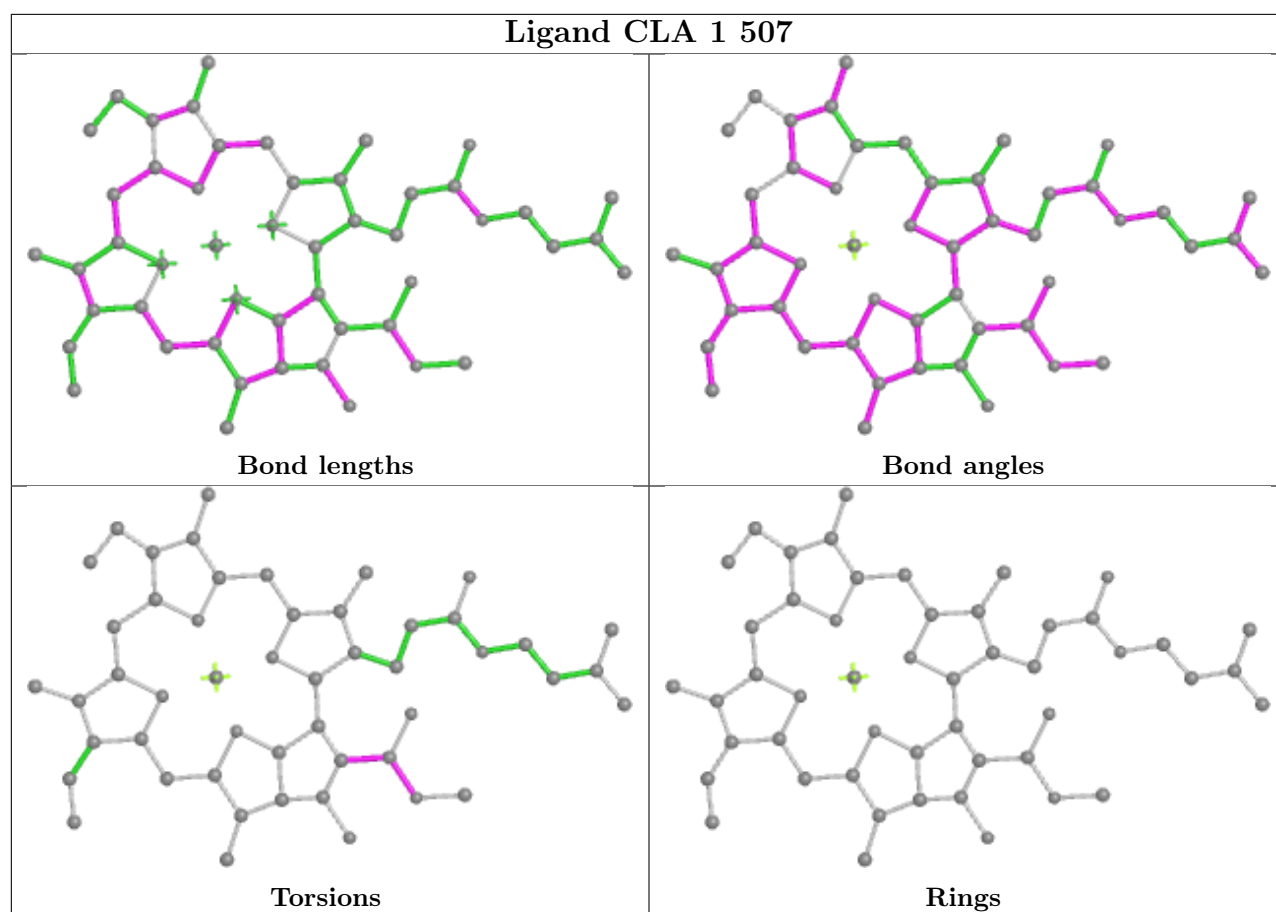
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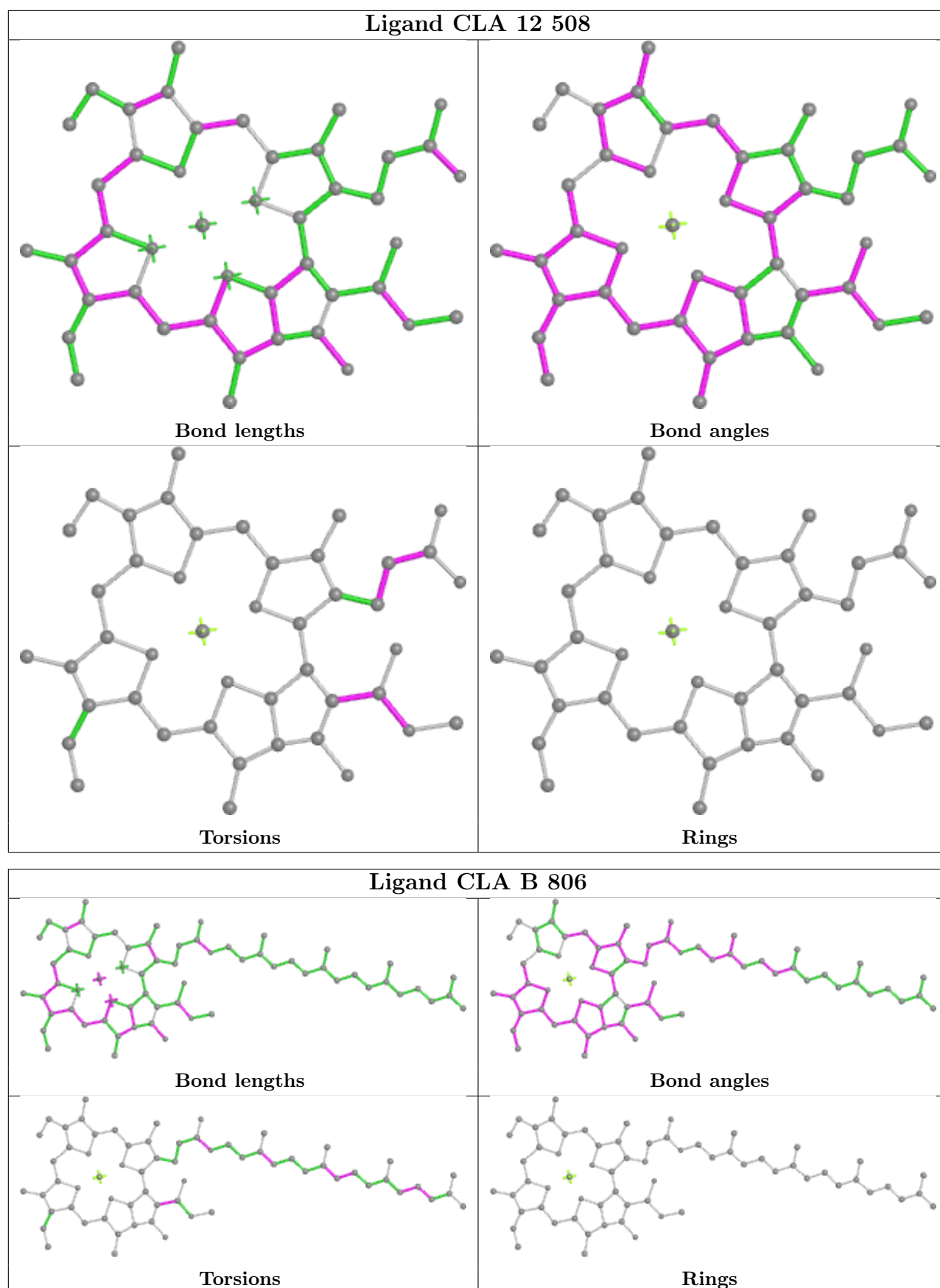


Ligand CLA 3 714

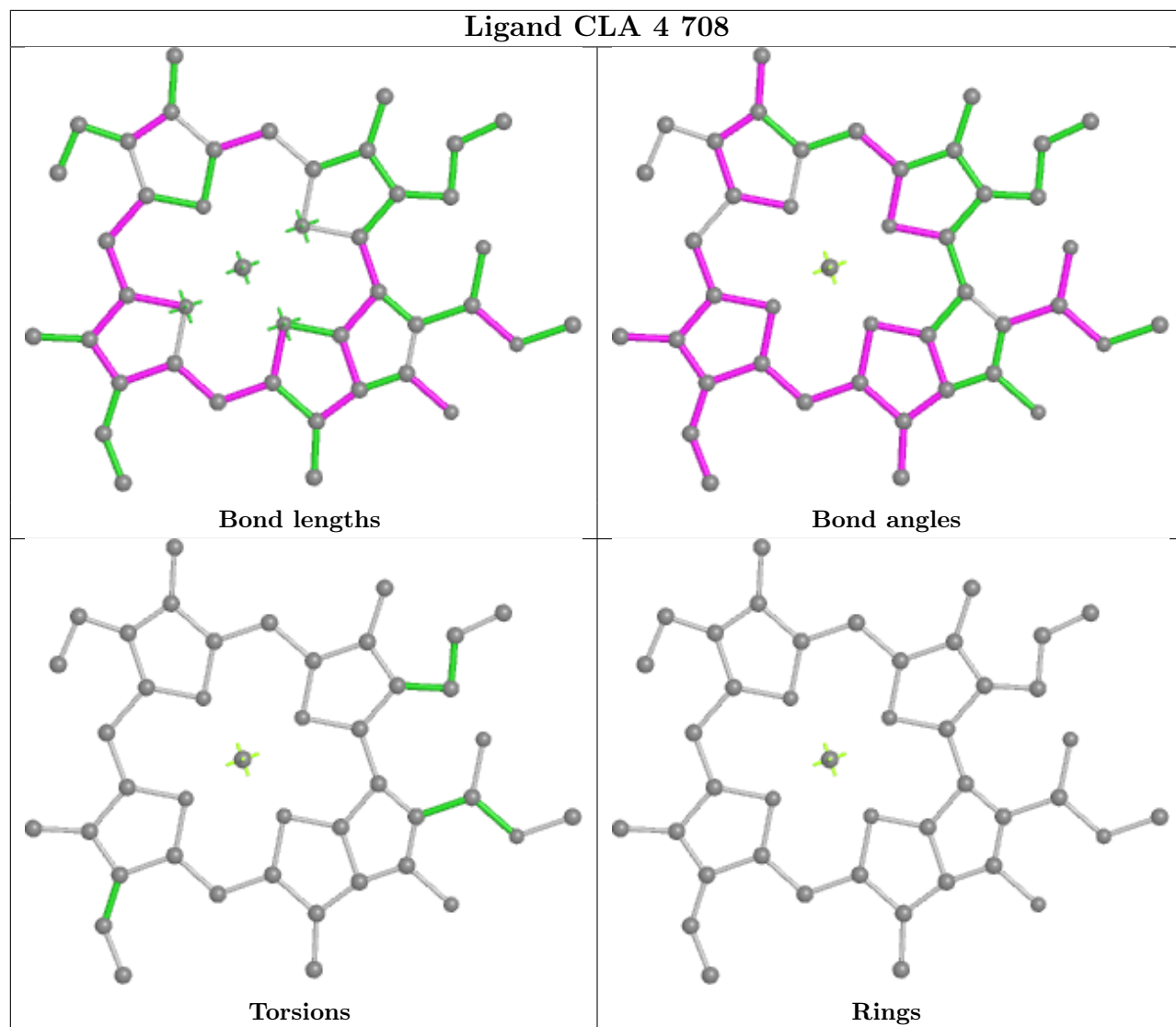




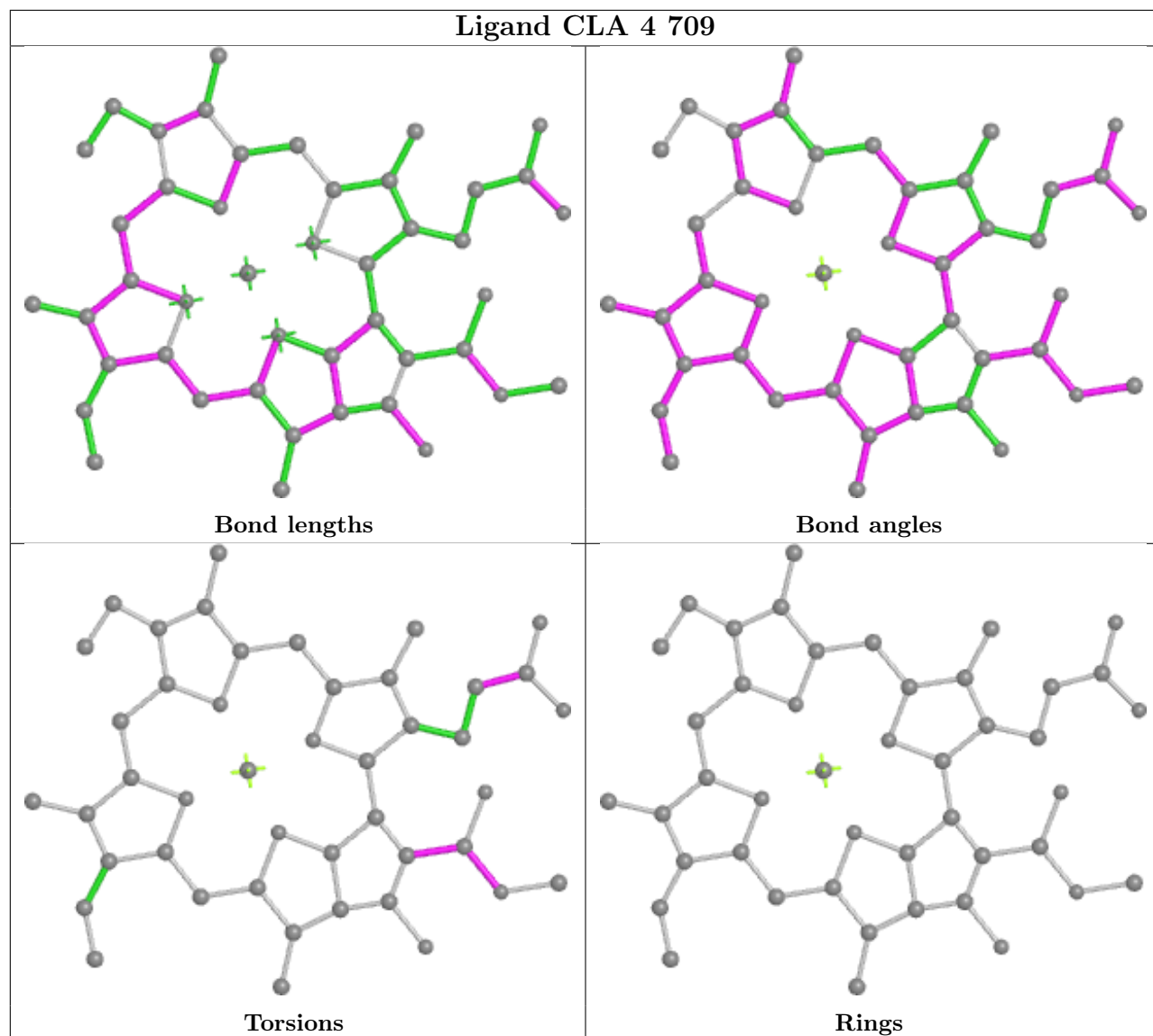


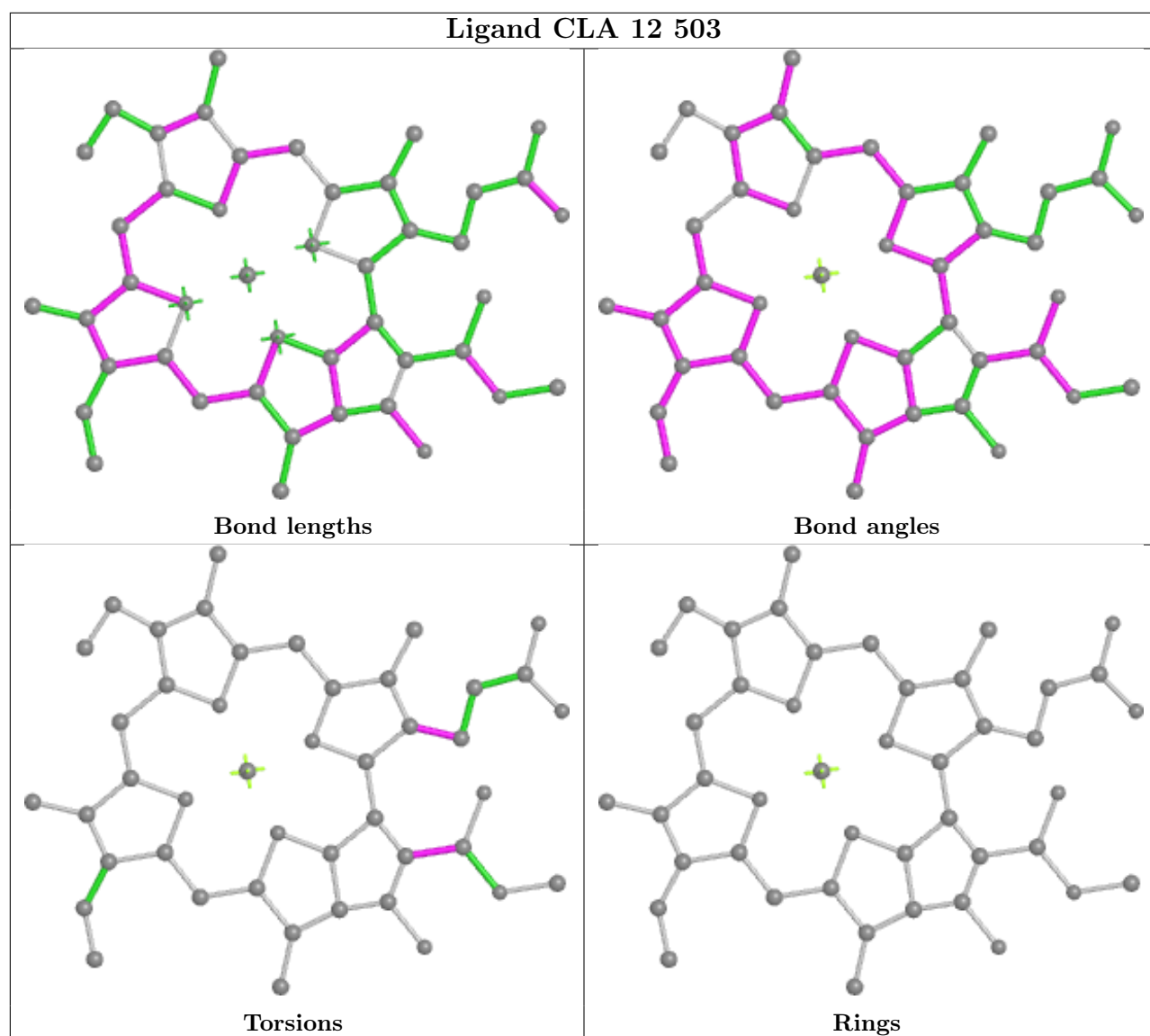


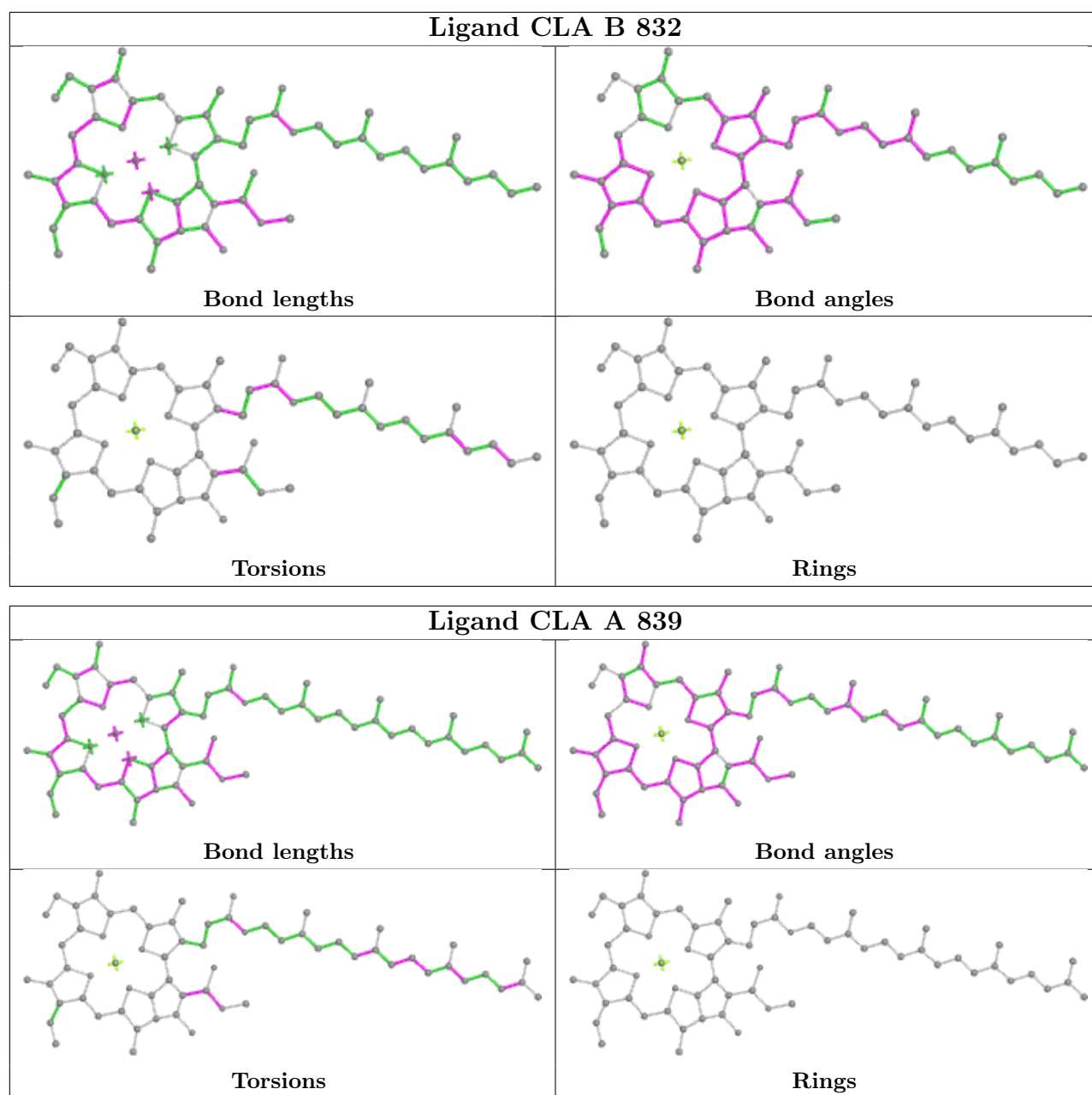
Ligand CLA 4 708



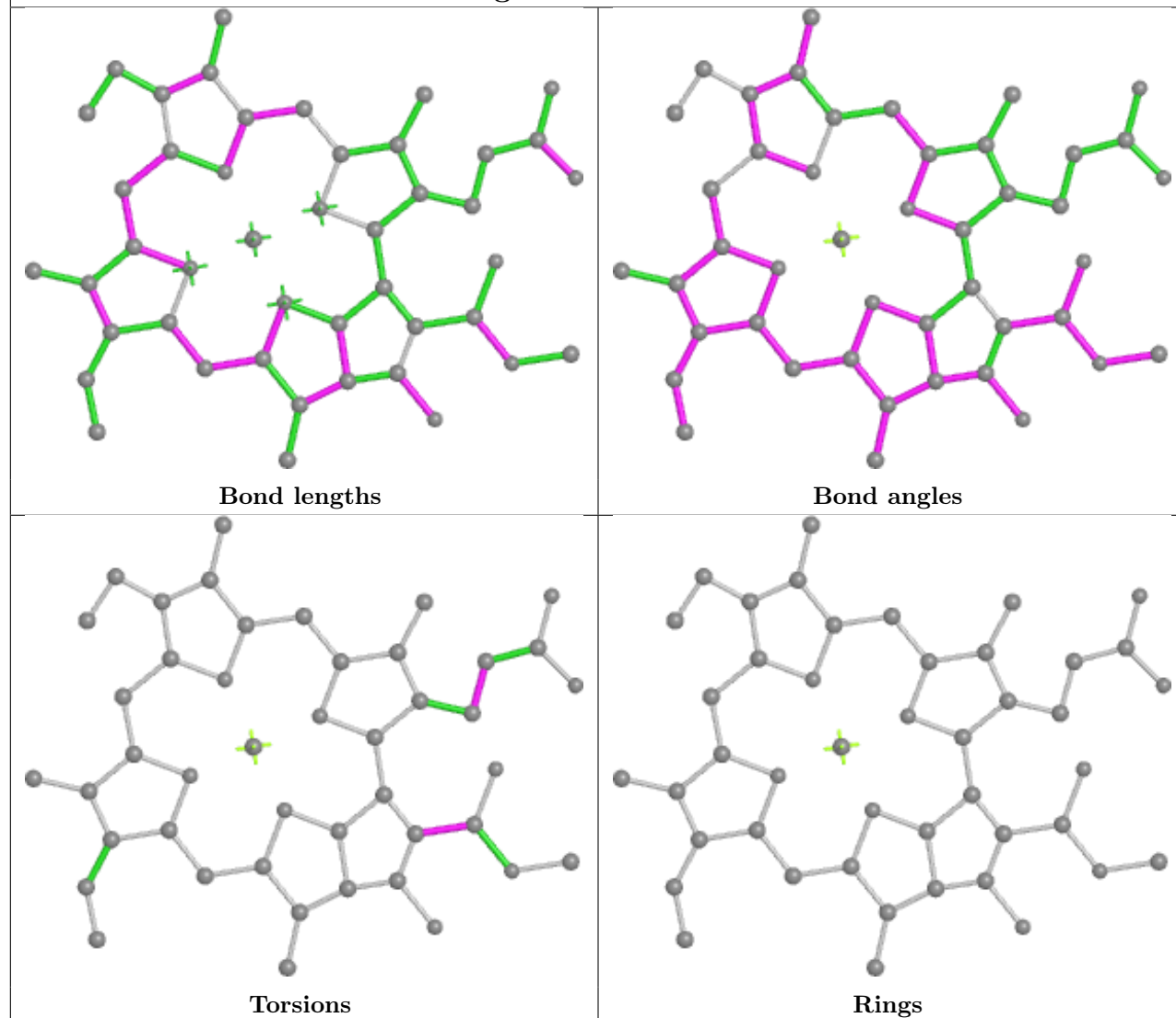
Ligand CLA 4 709



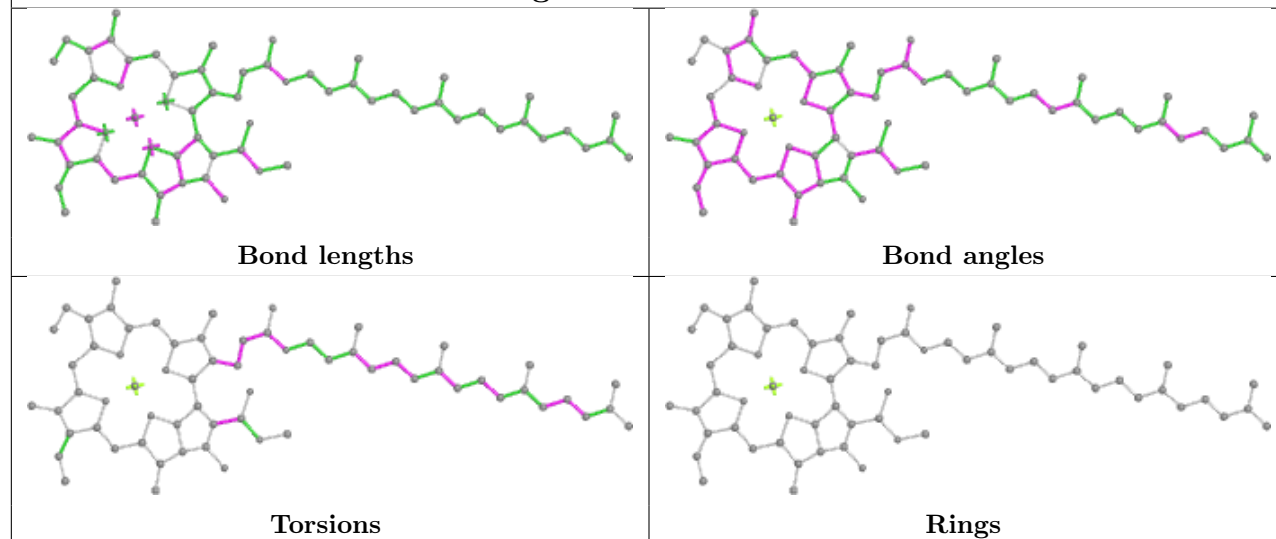




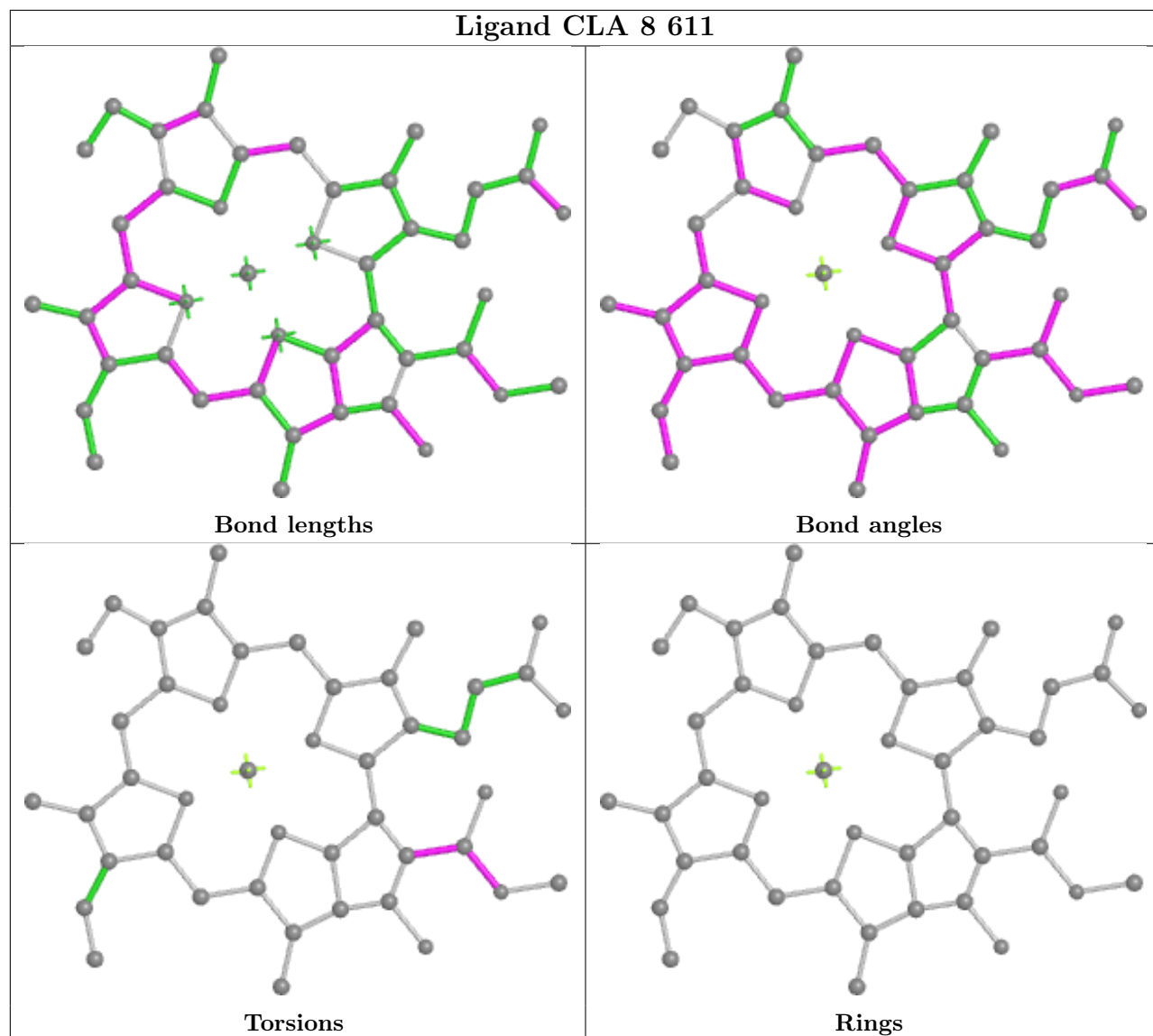
Ligand CLA 2 503

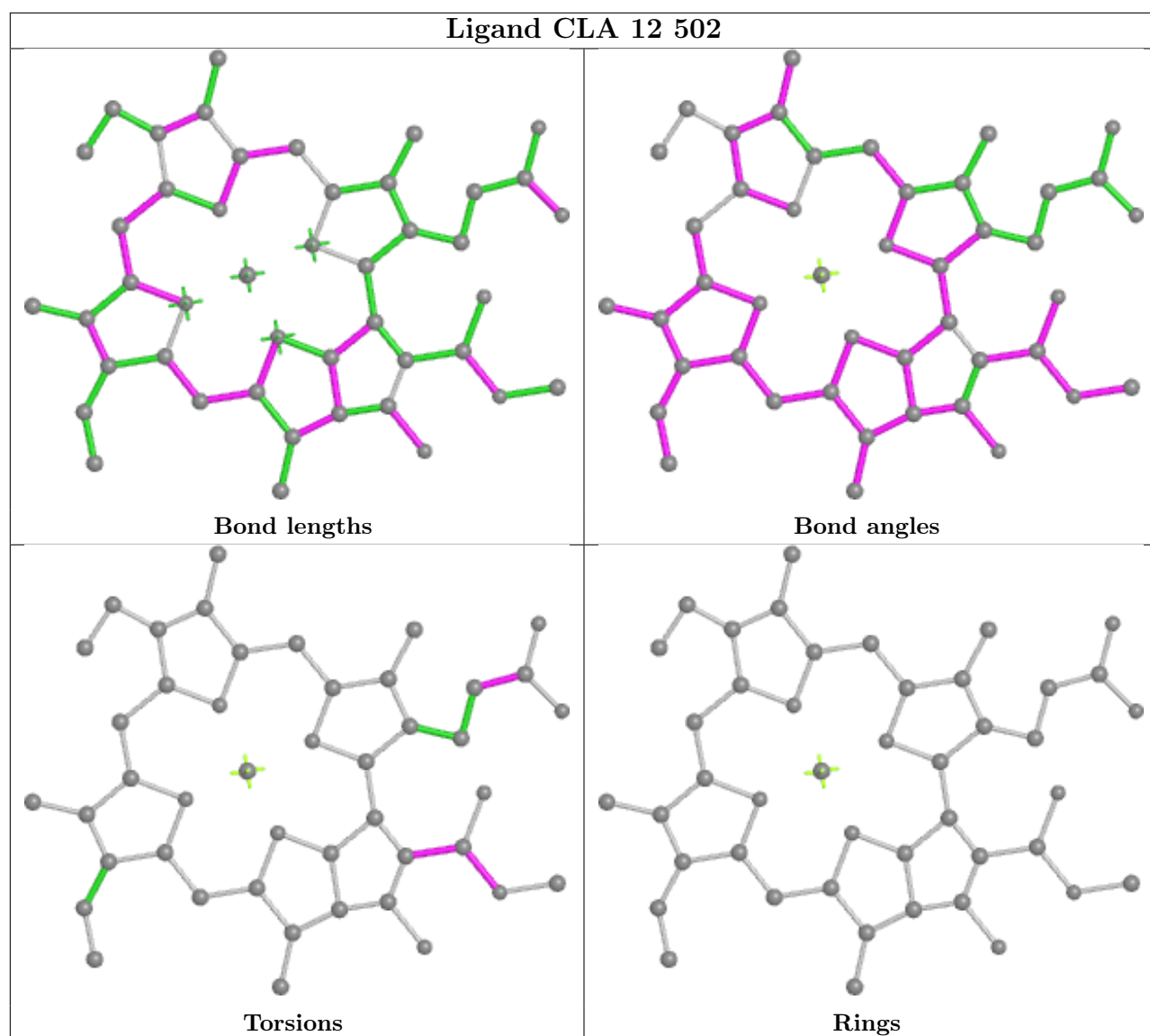


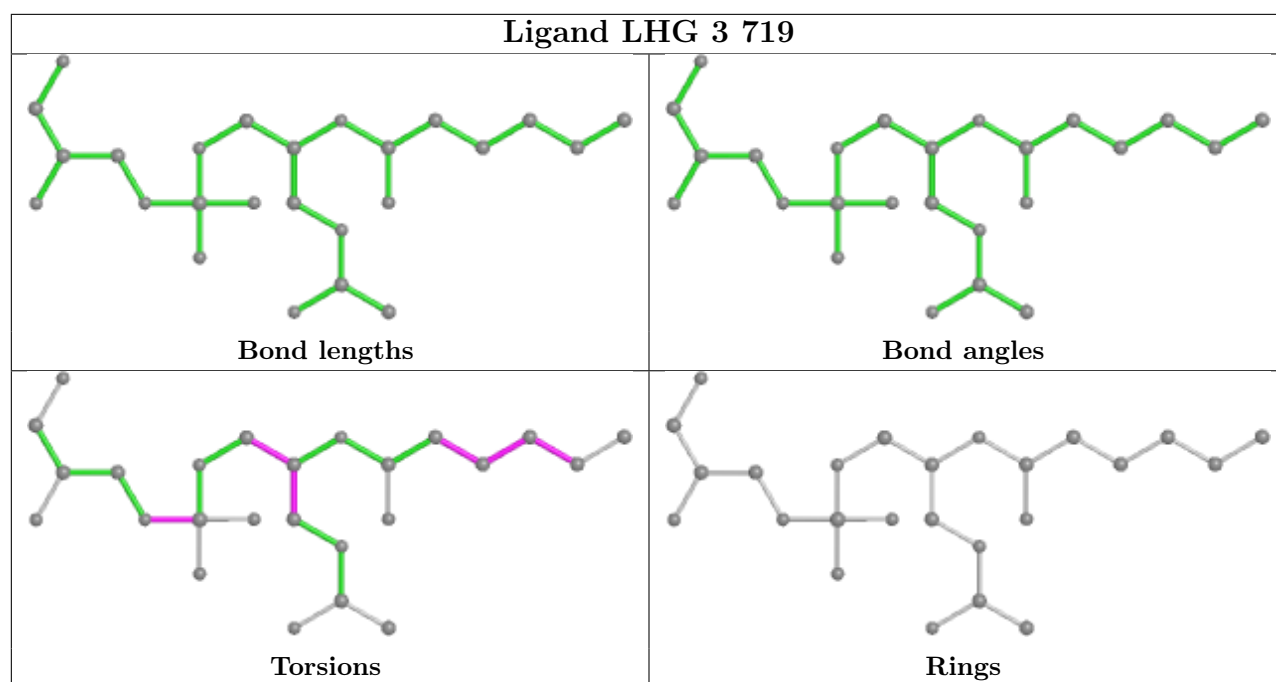
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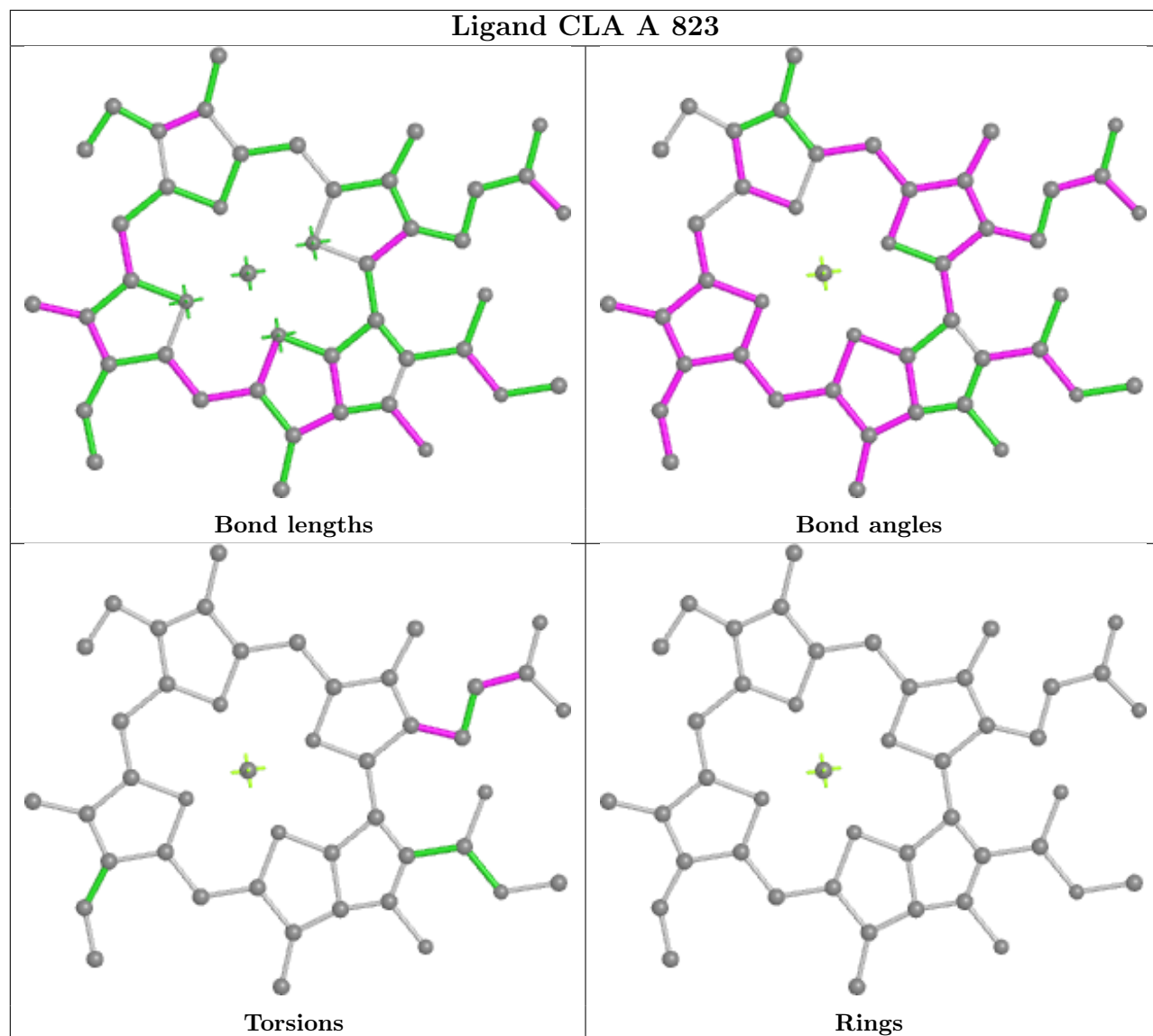
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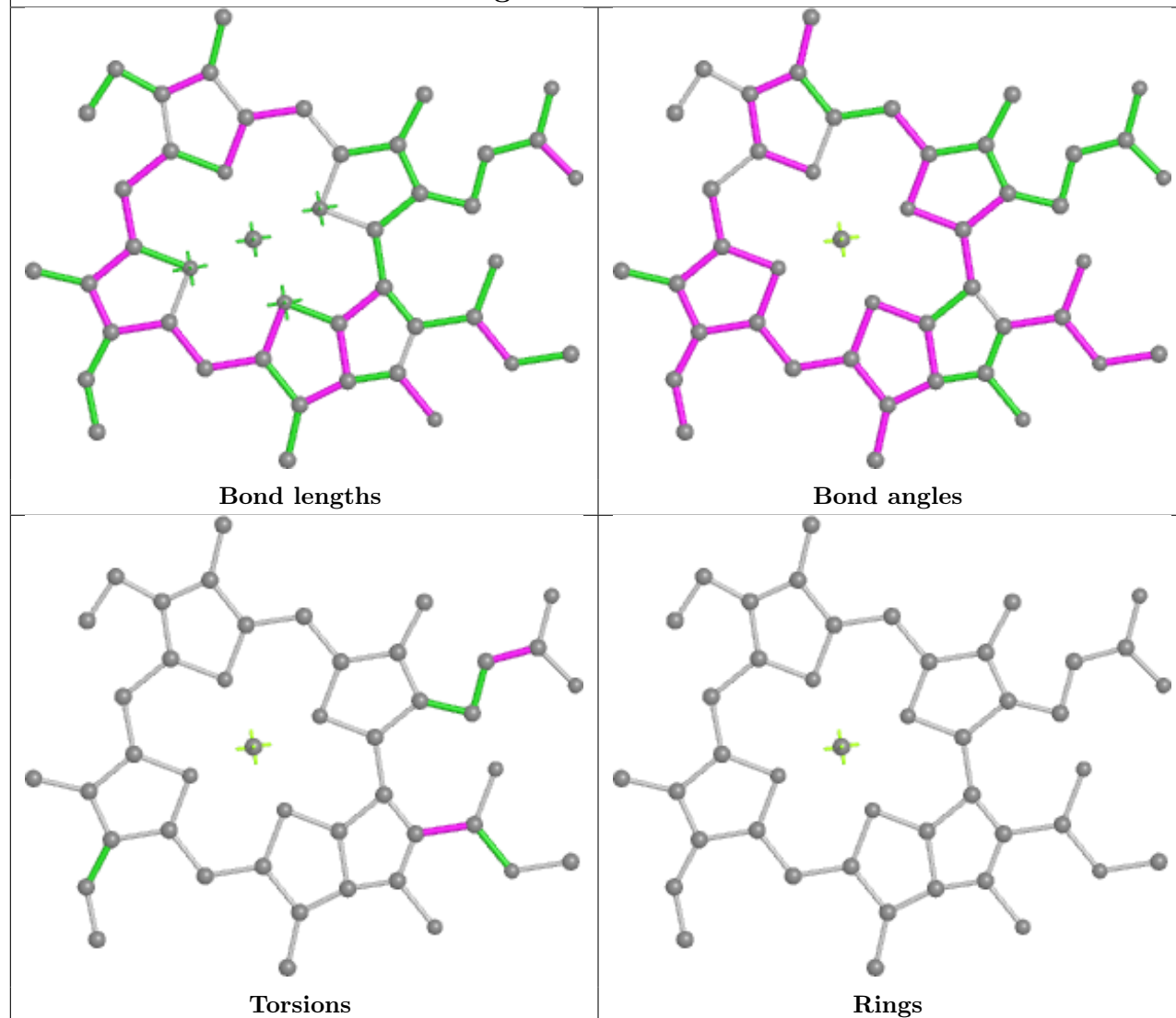




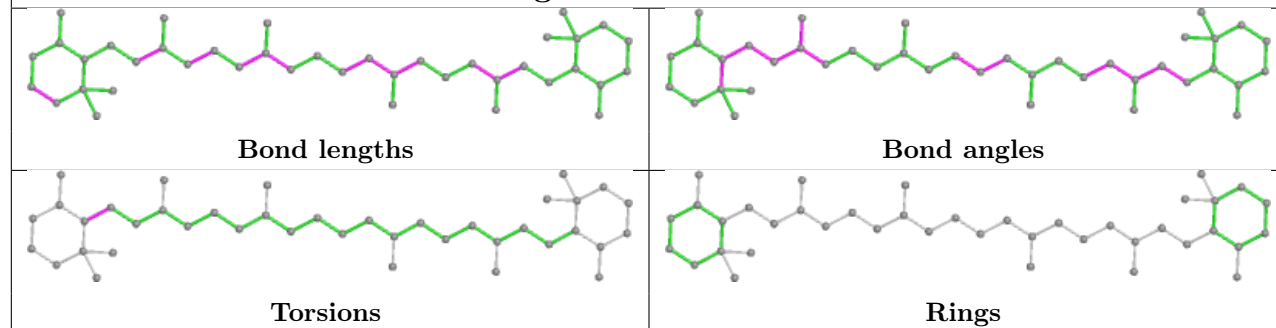
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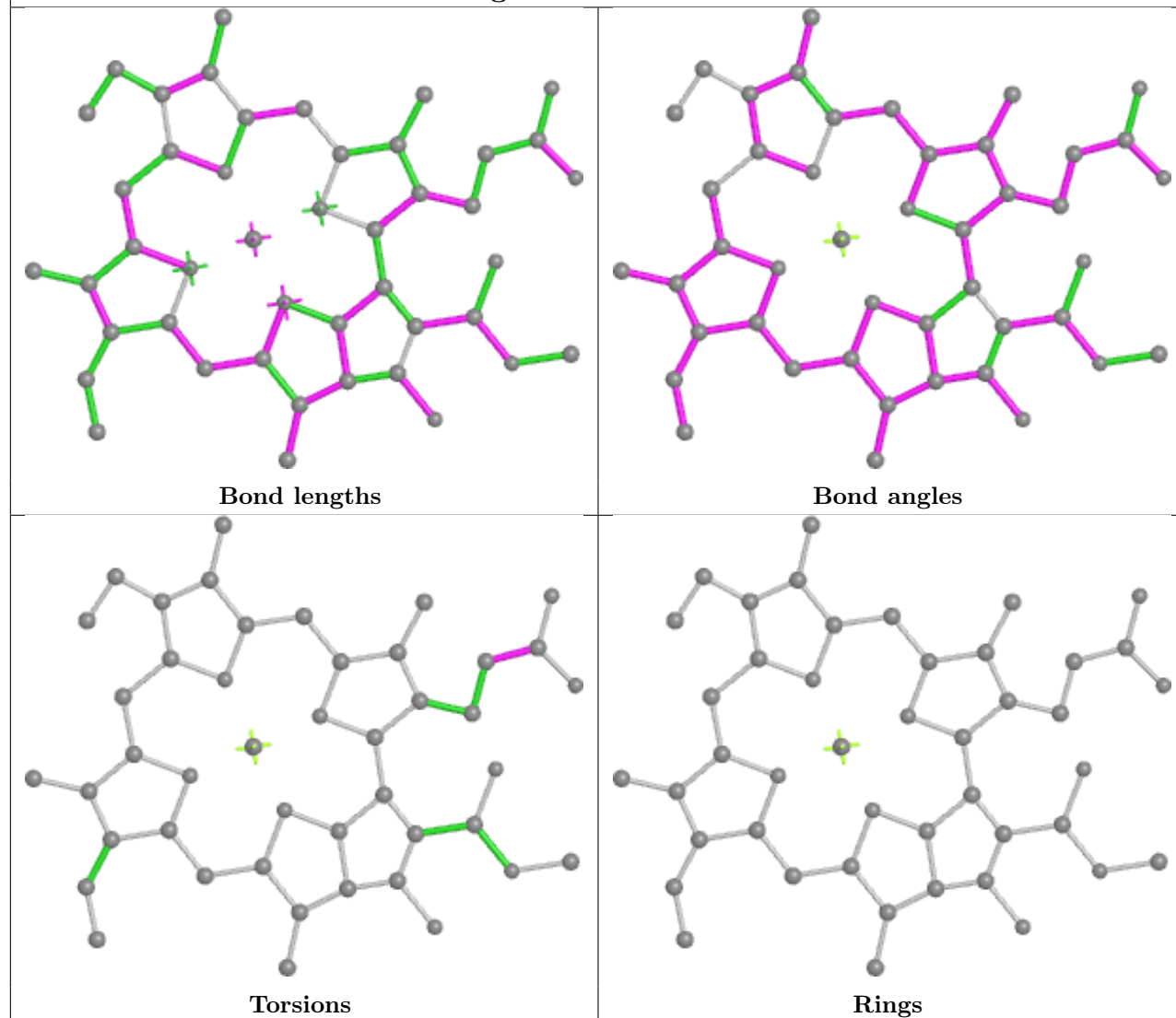
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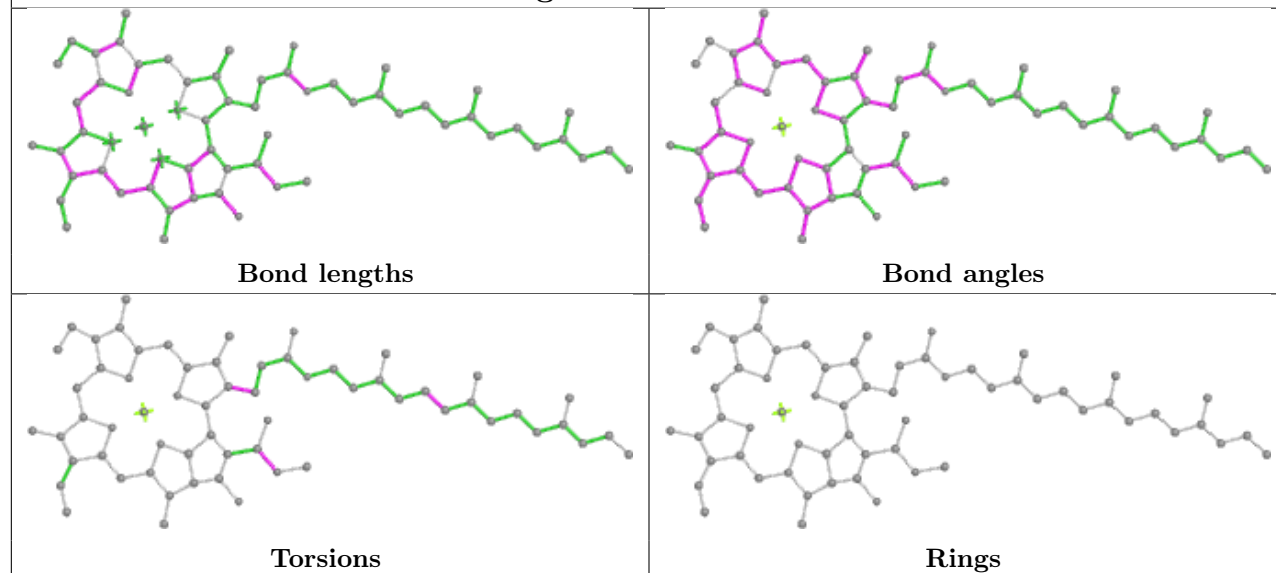
Ligand BCR J 102



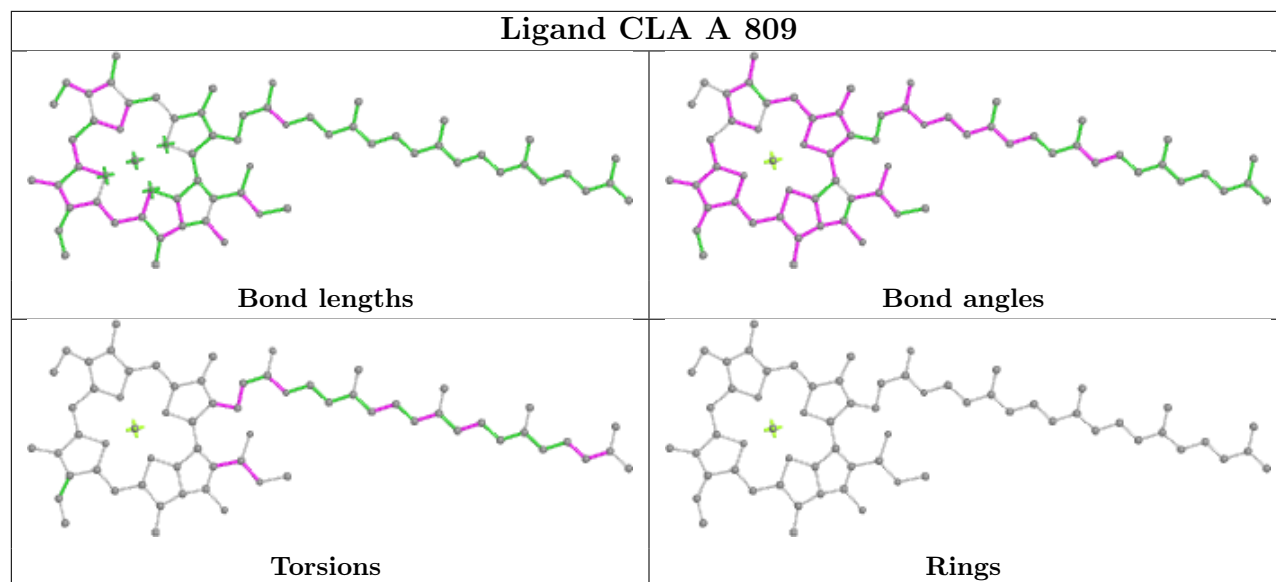
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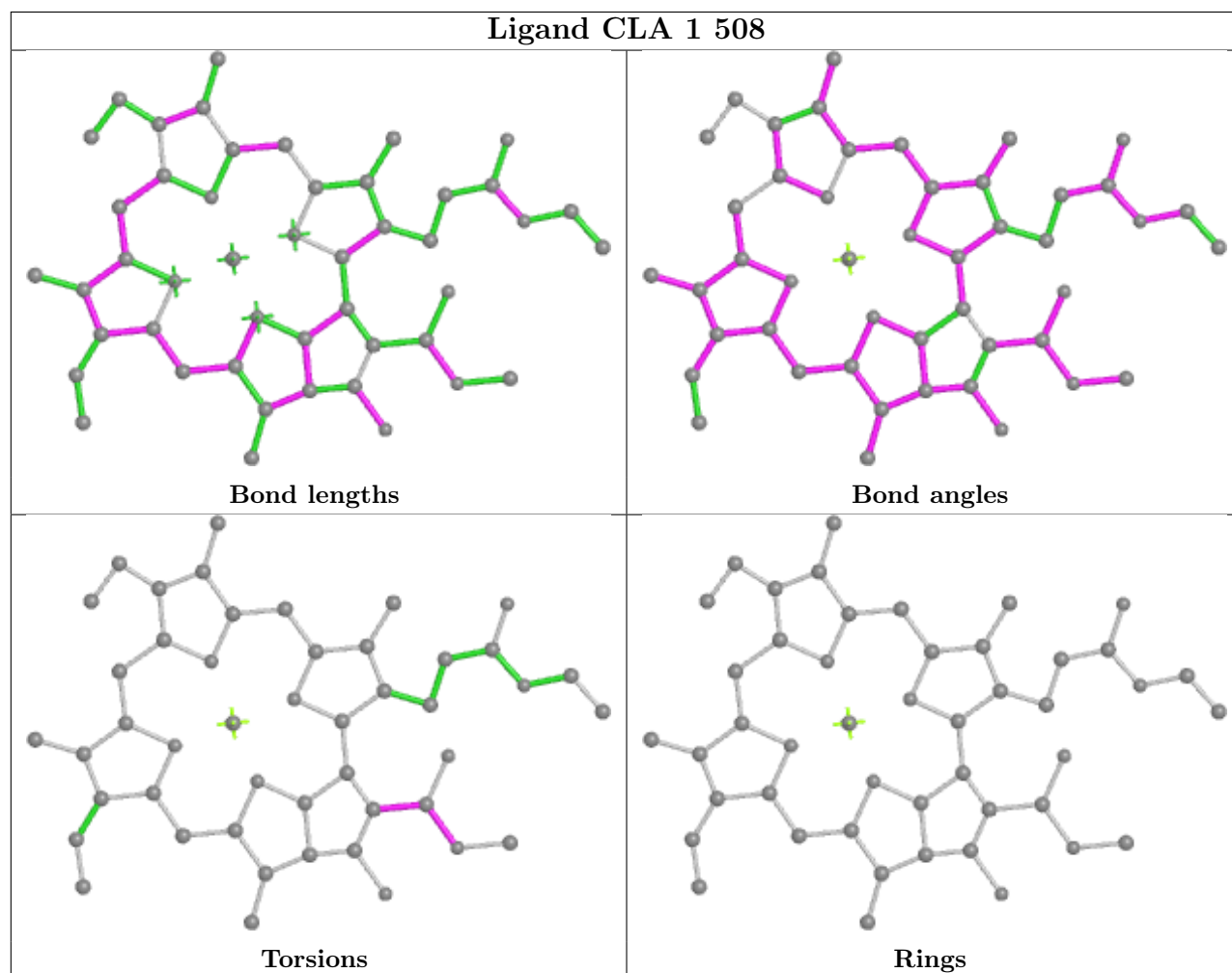
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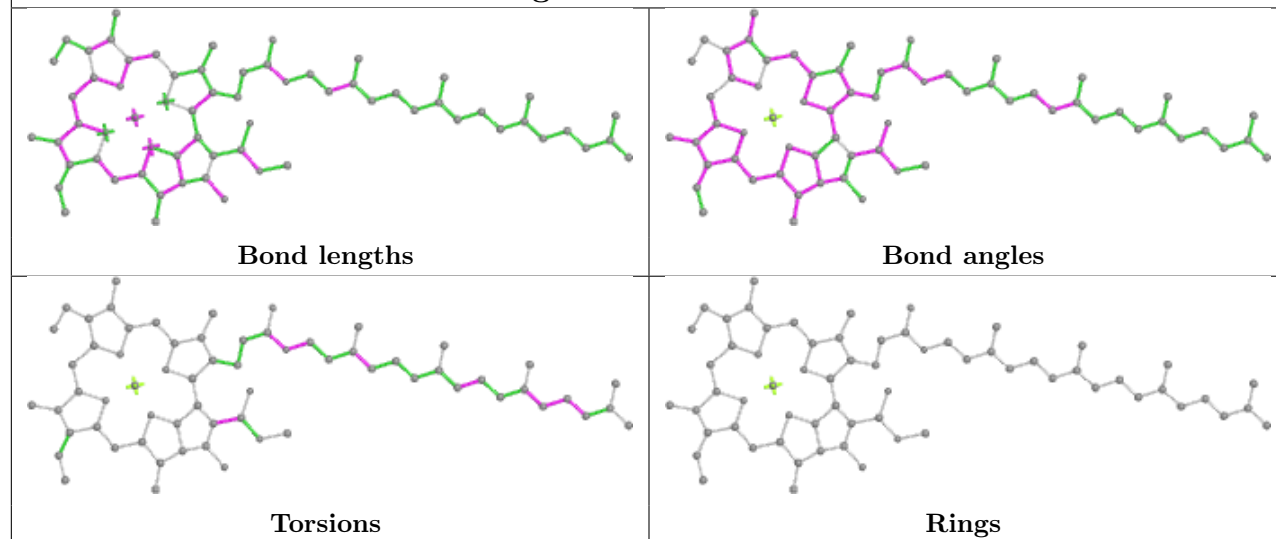
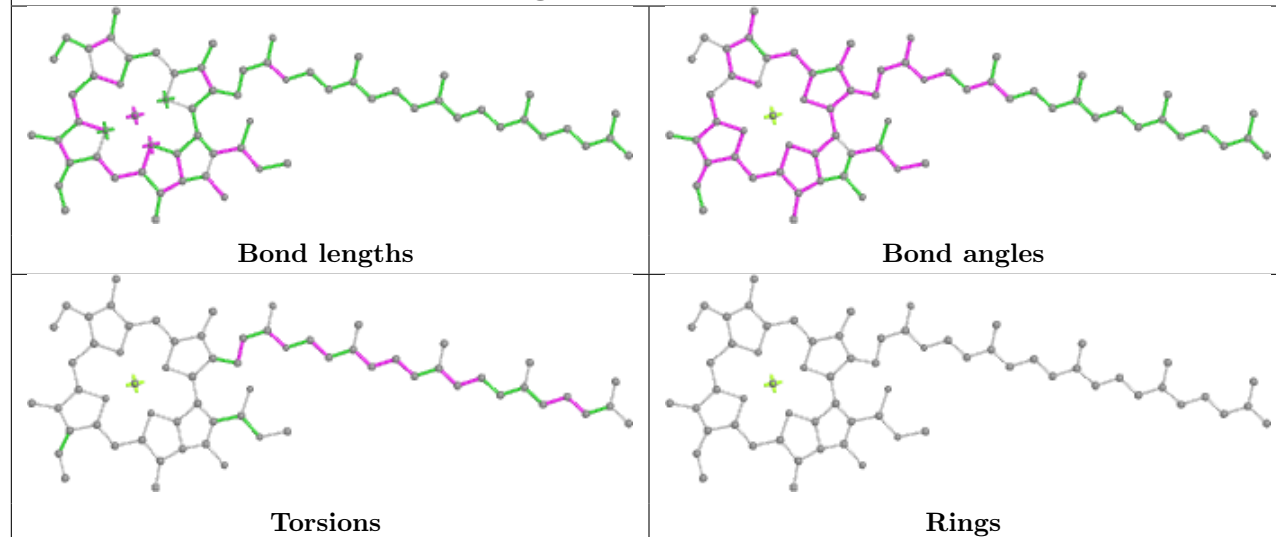


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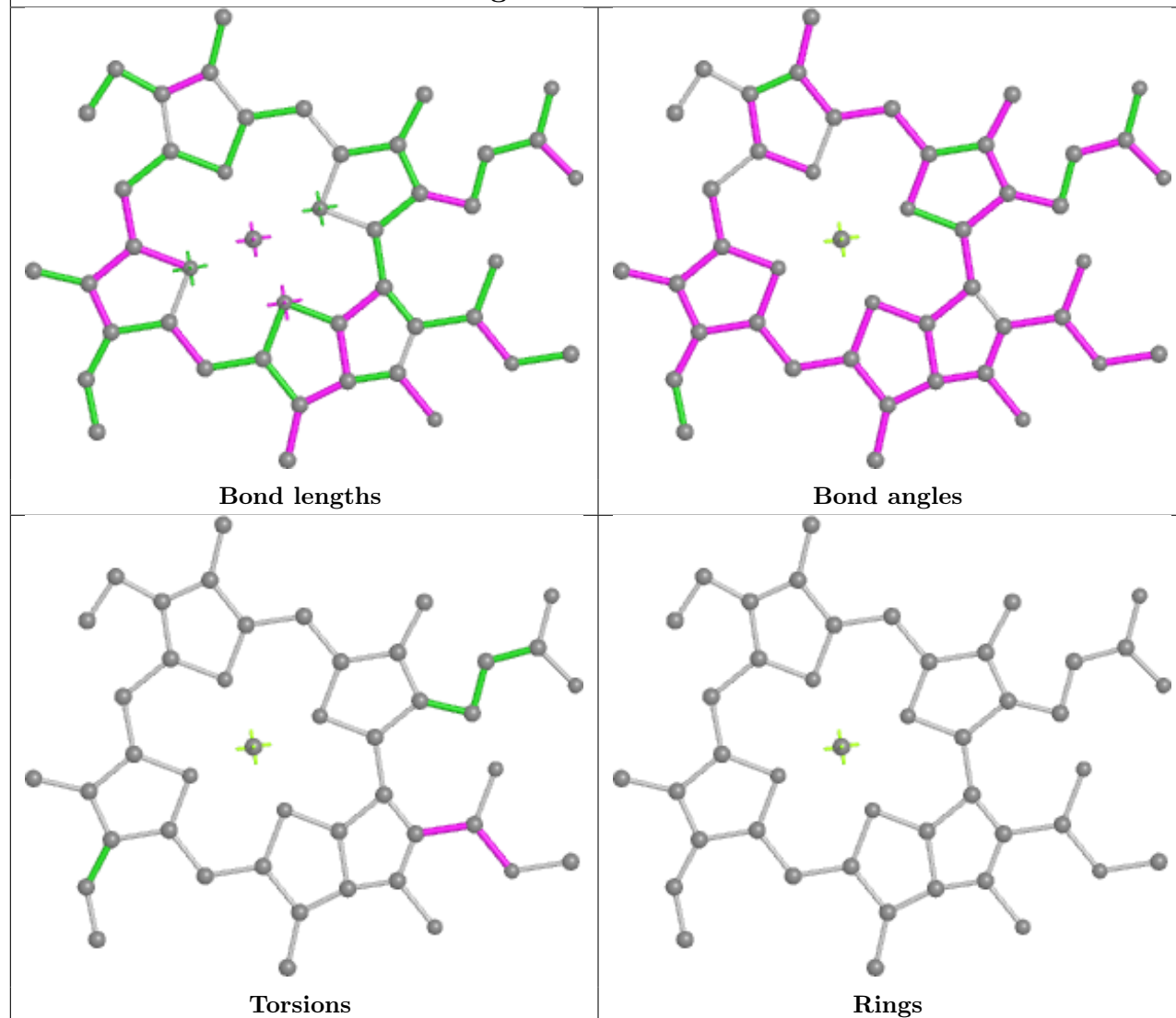


Ligand CLA 1 508

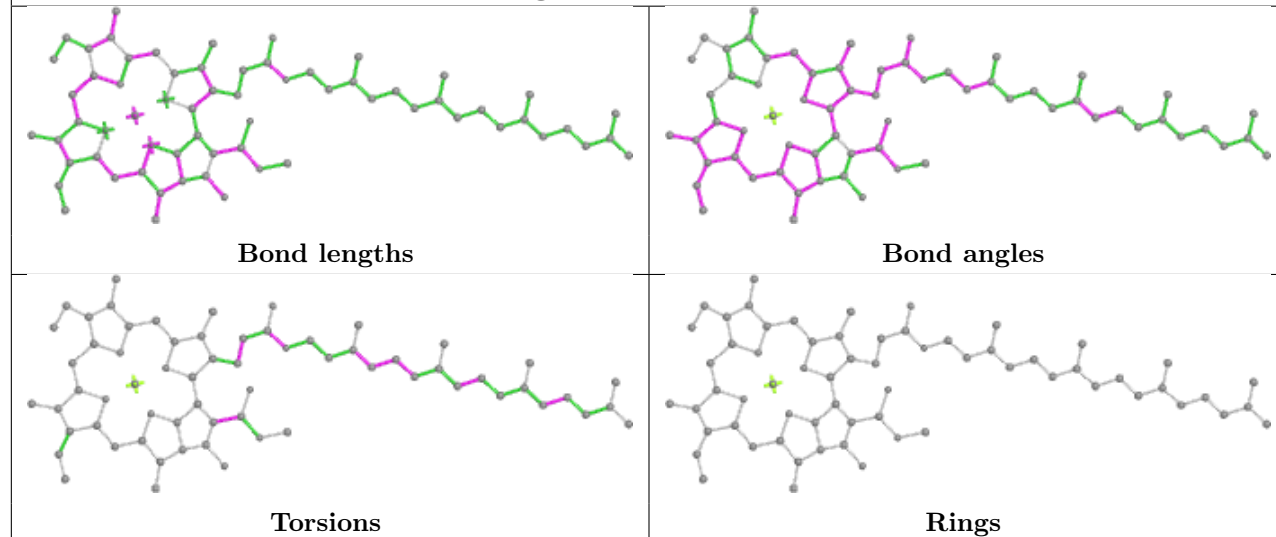


Ligand CLA B 813**Ligand CLA A 803**

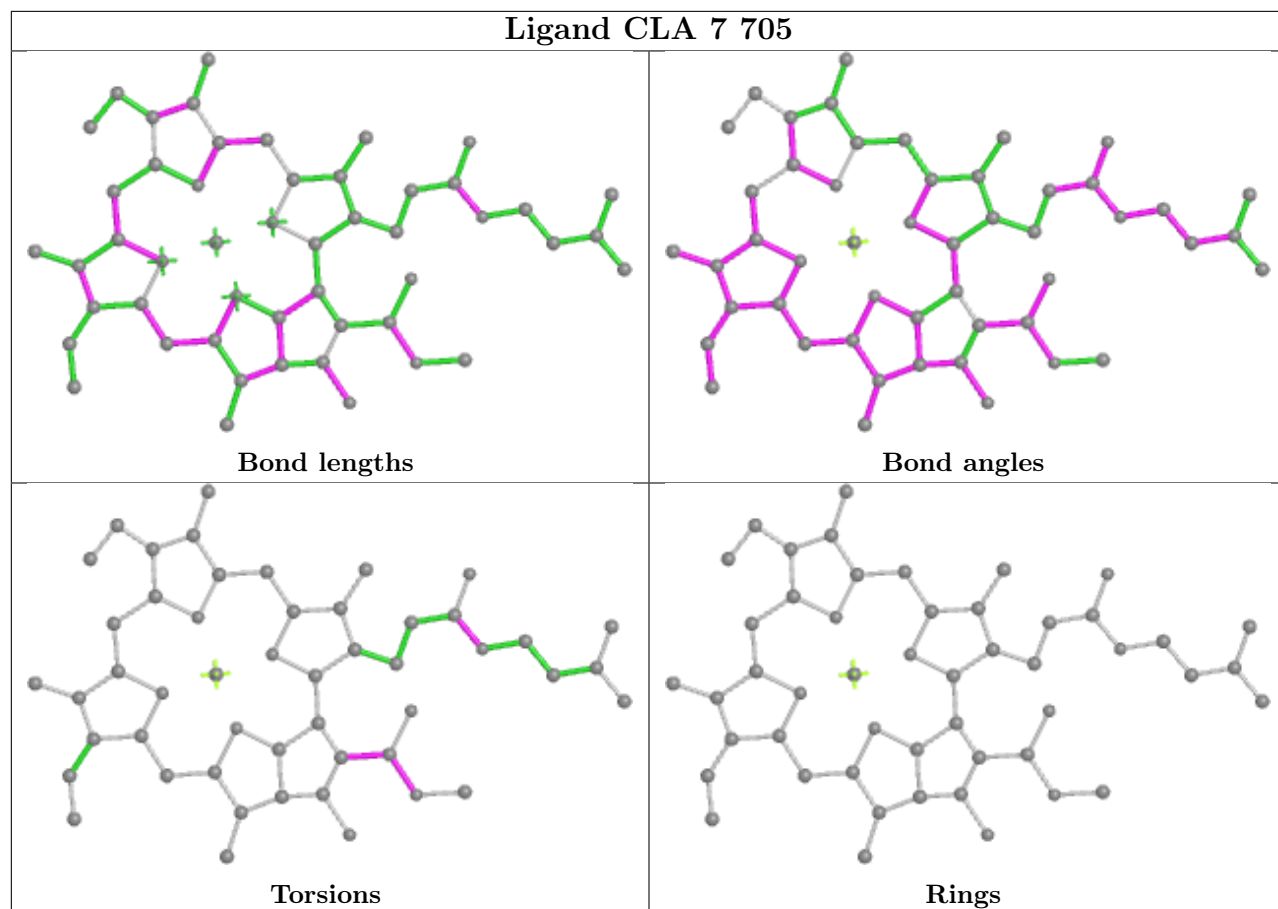
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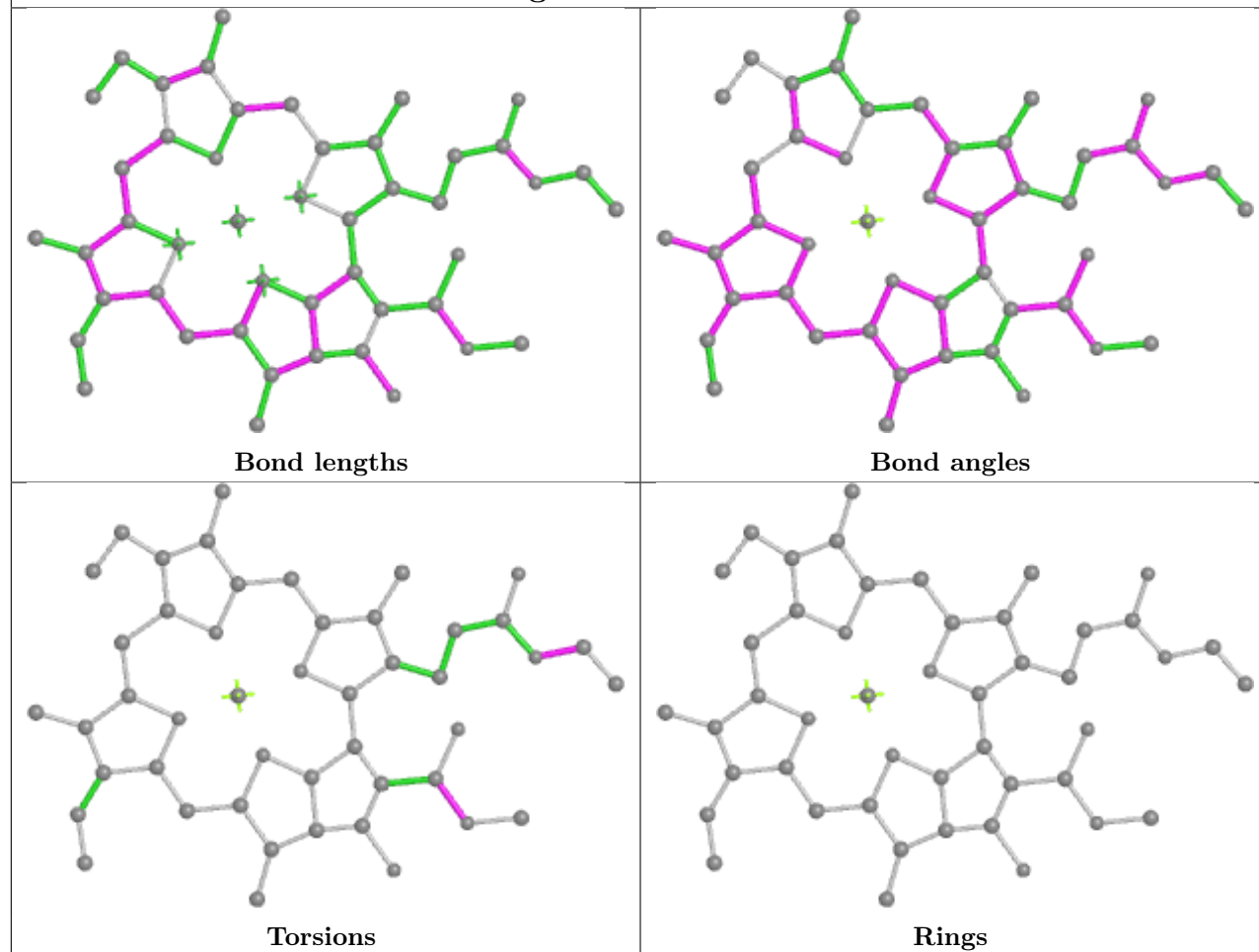
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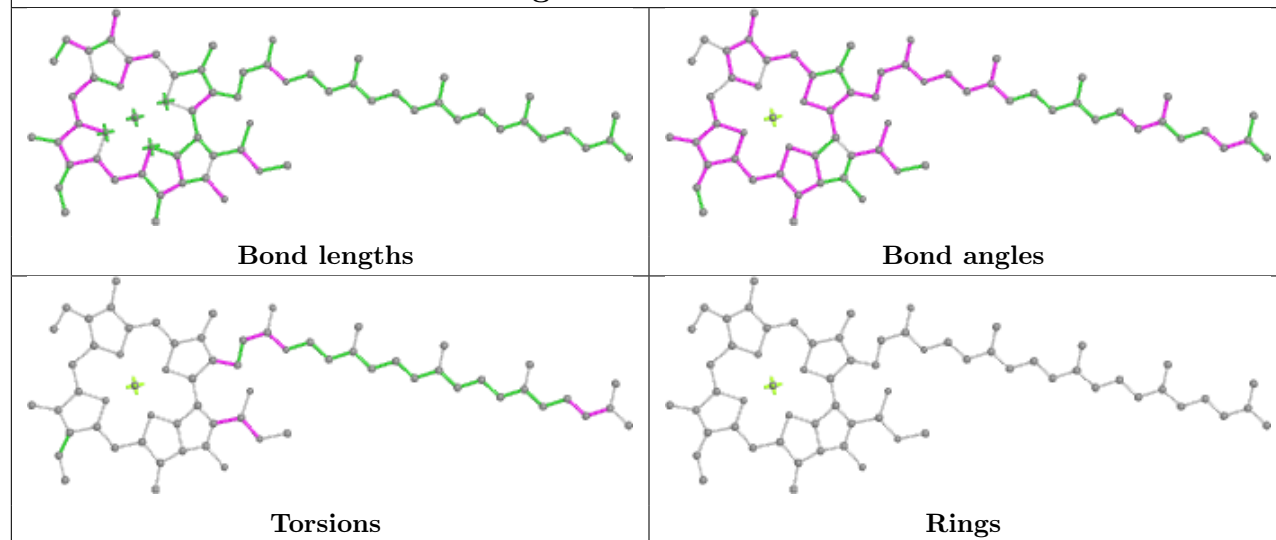
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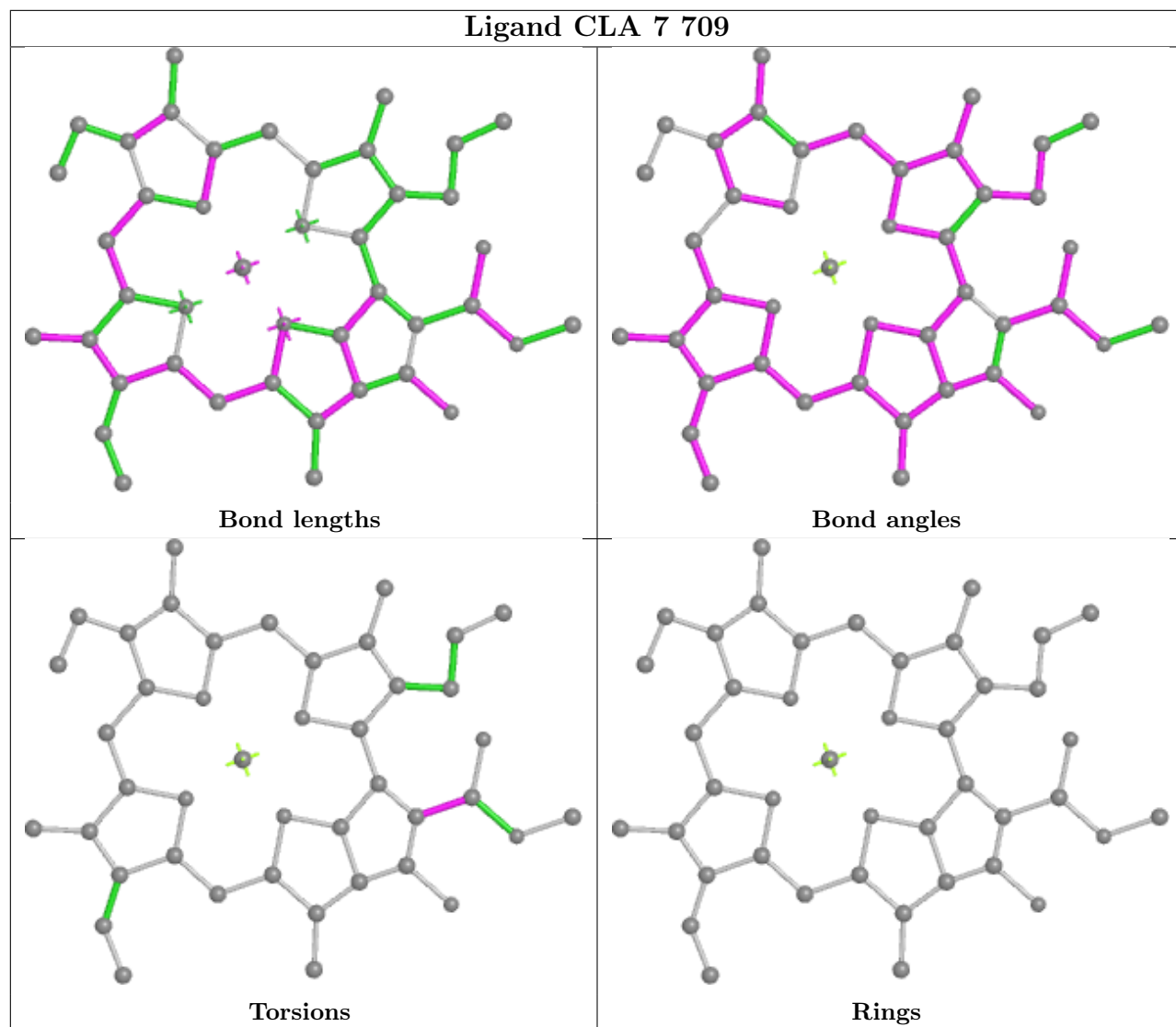
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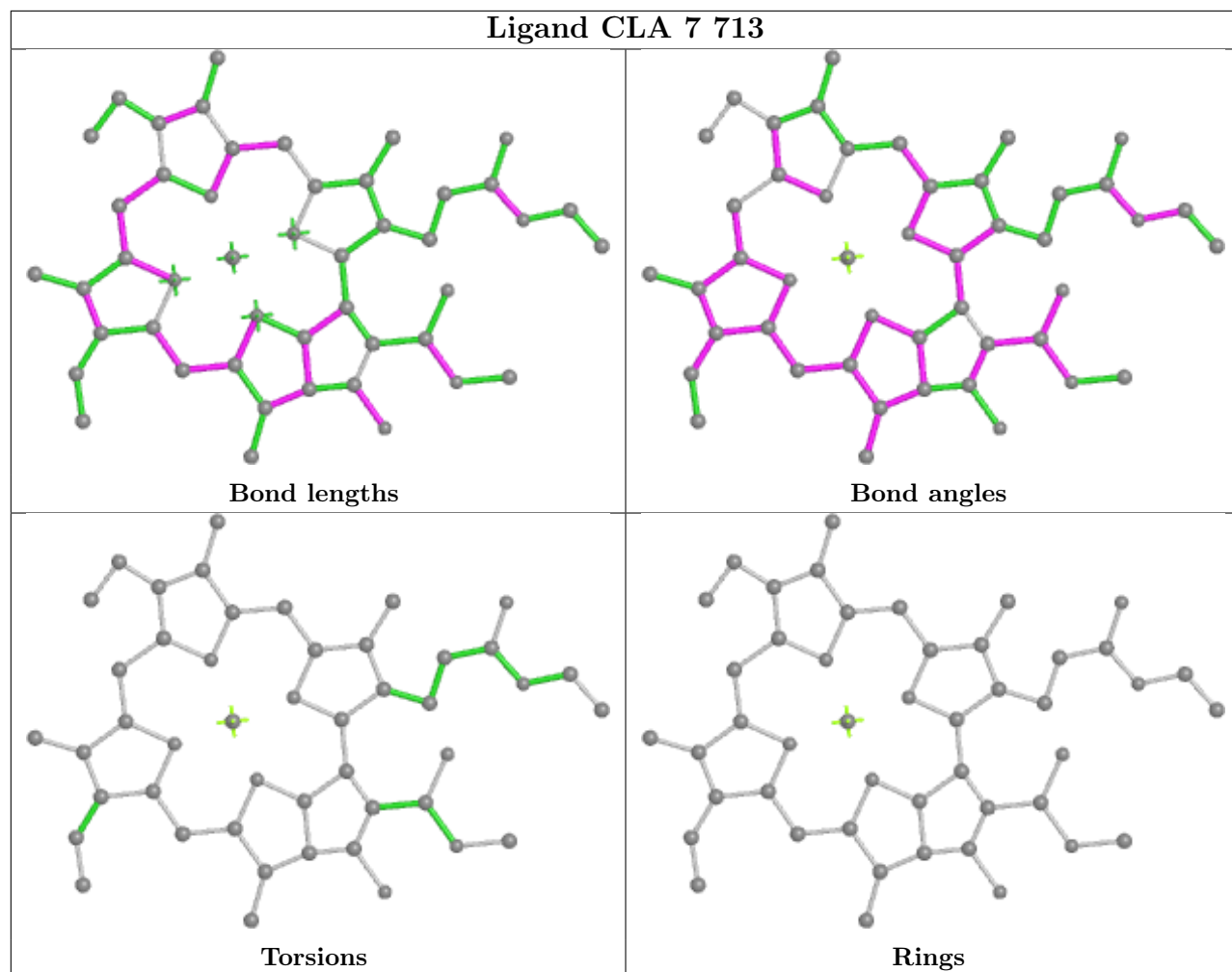
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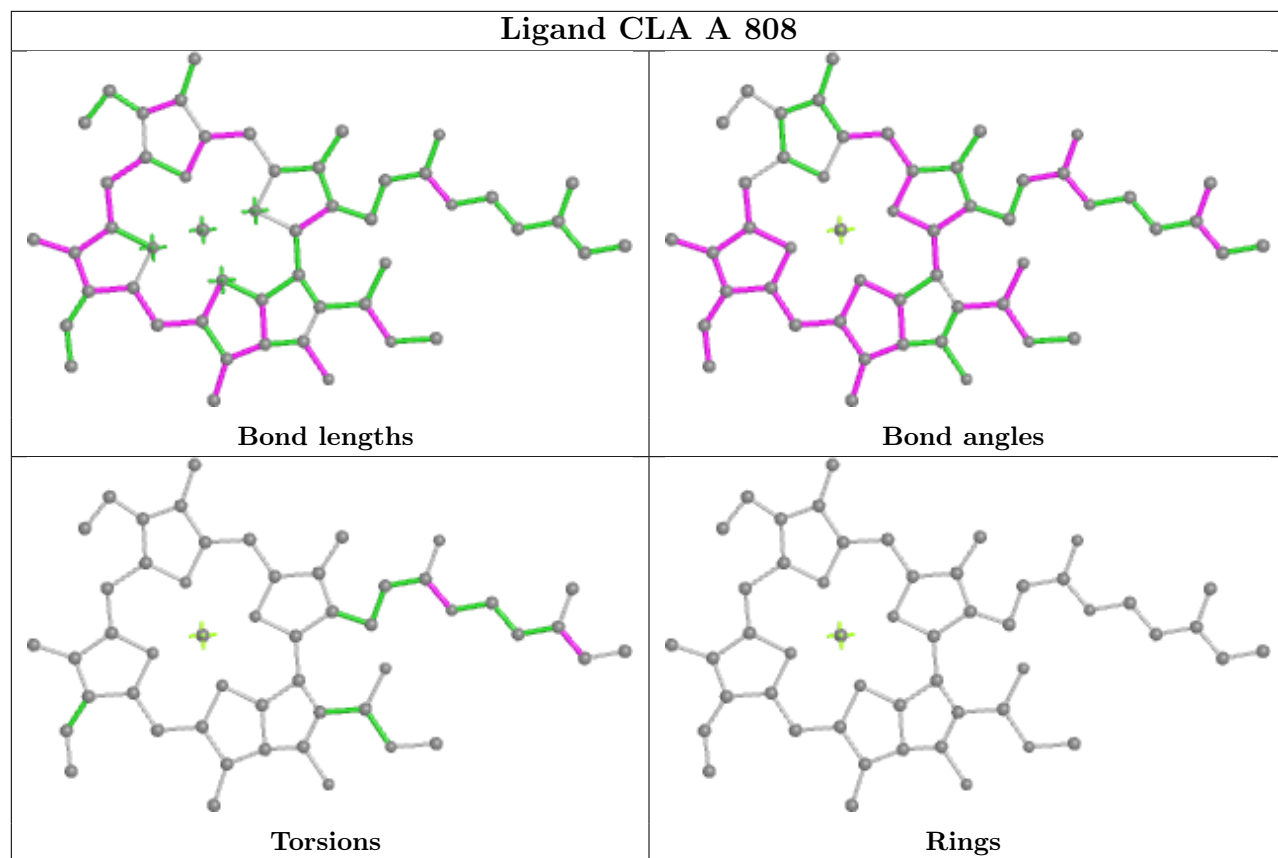
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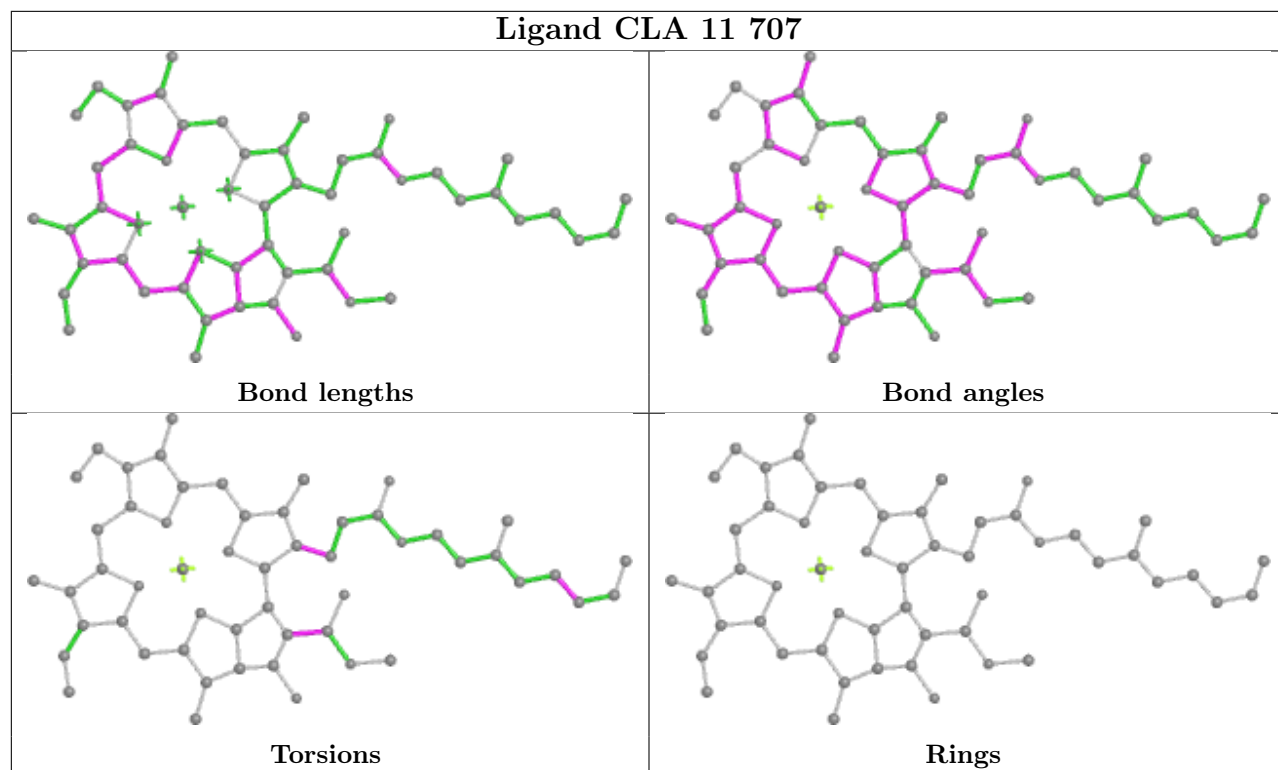
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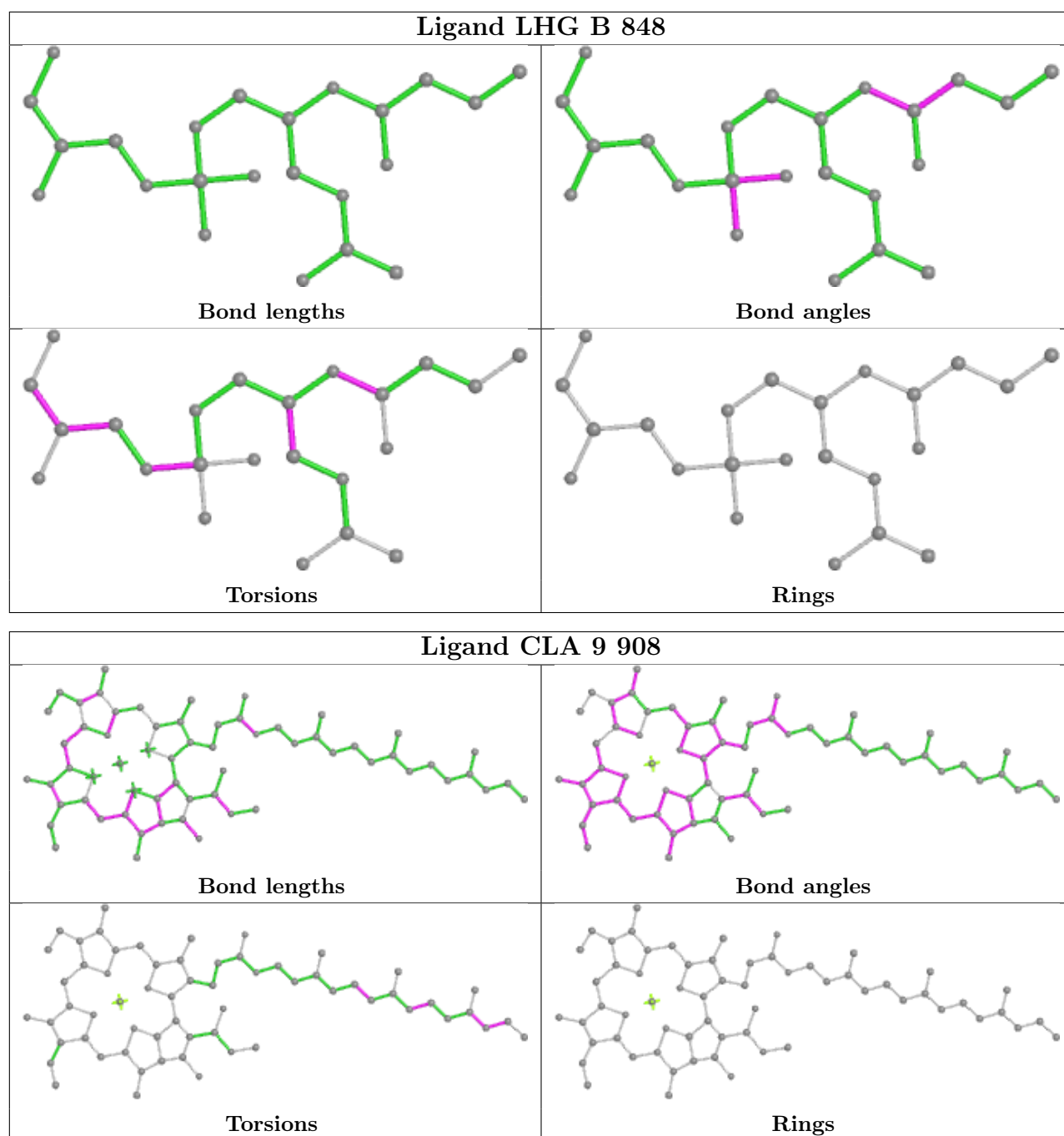


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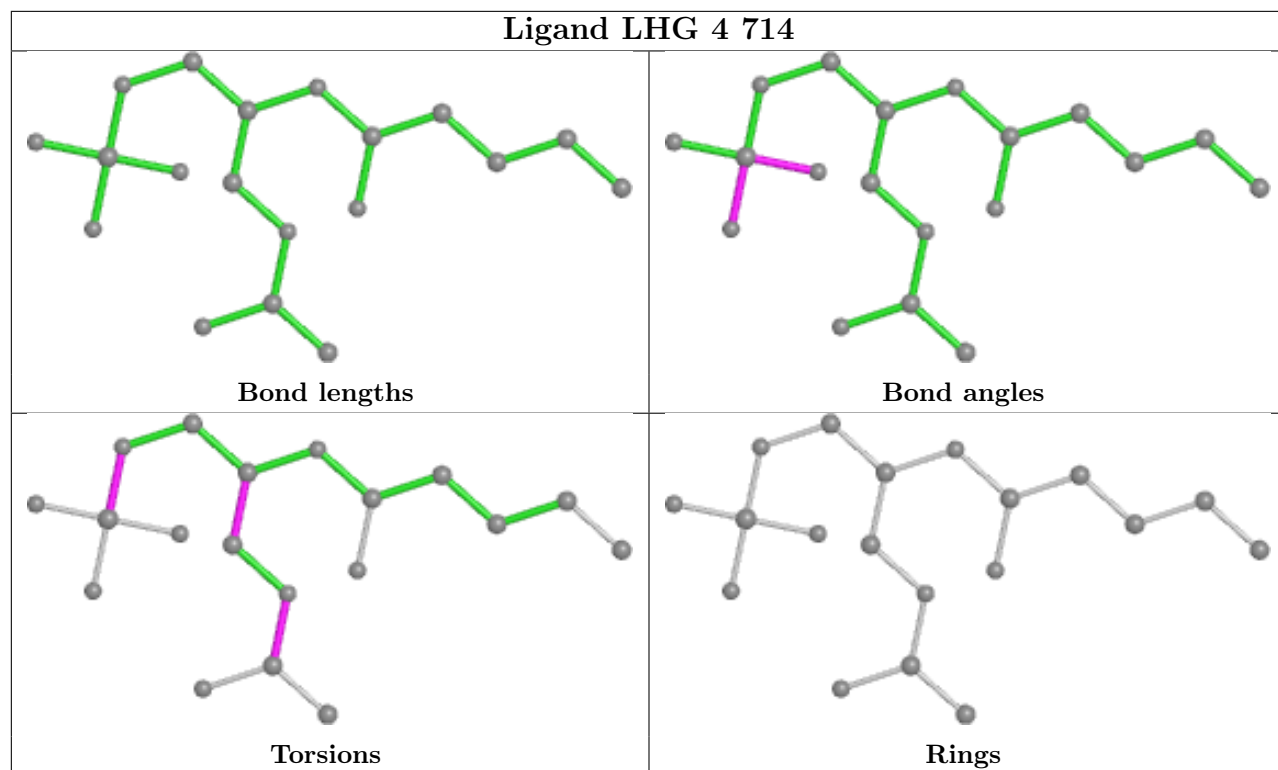


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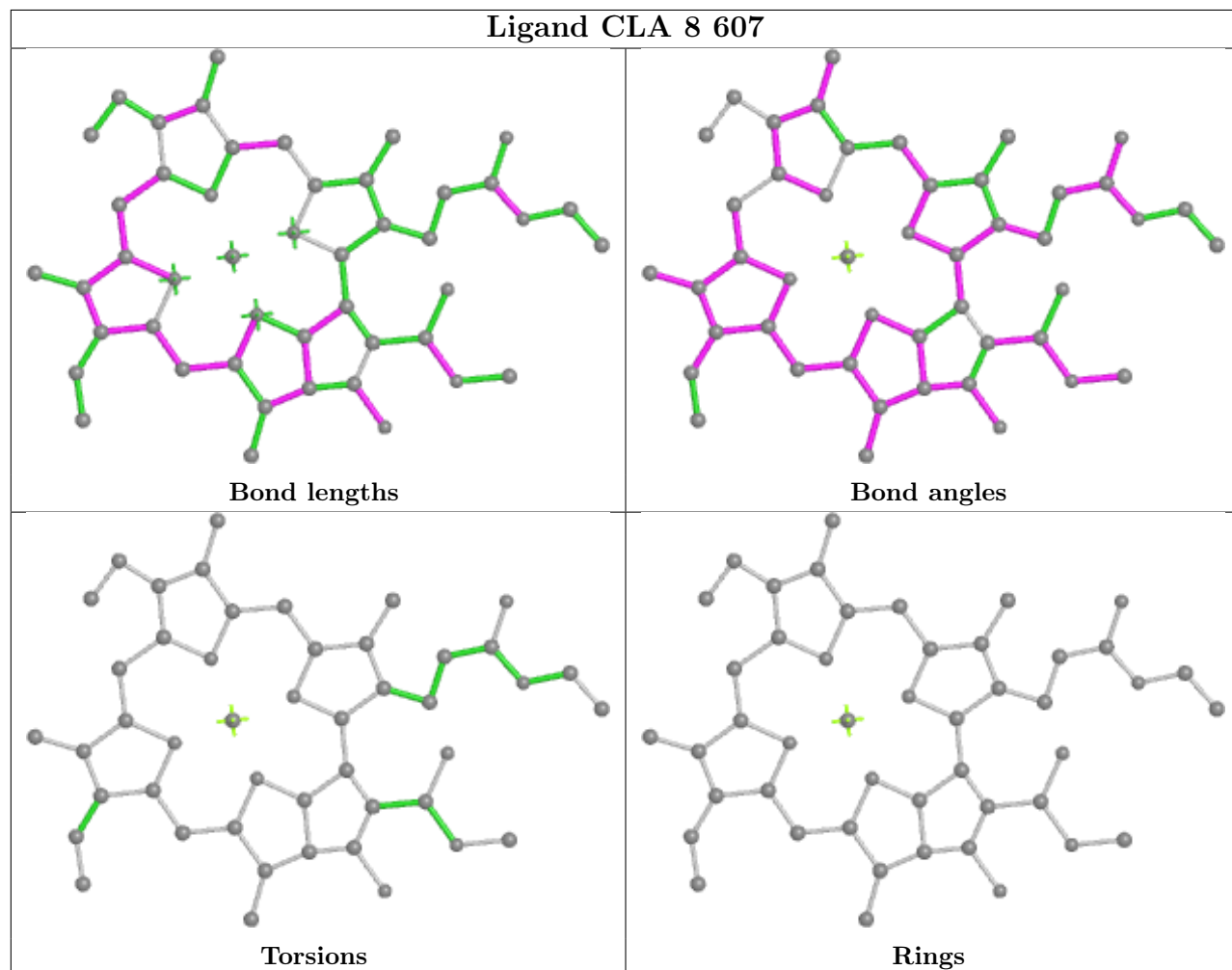


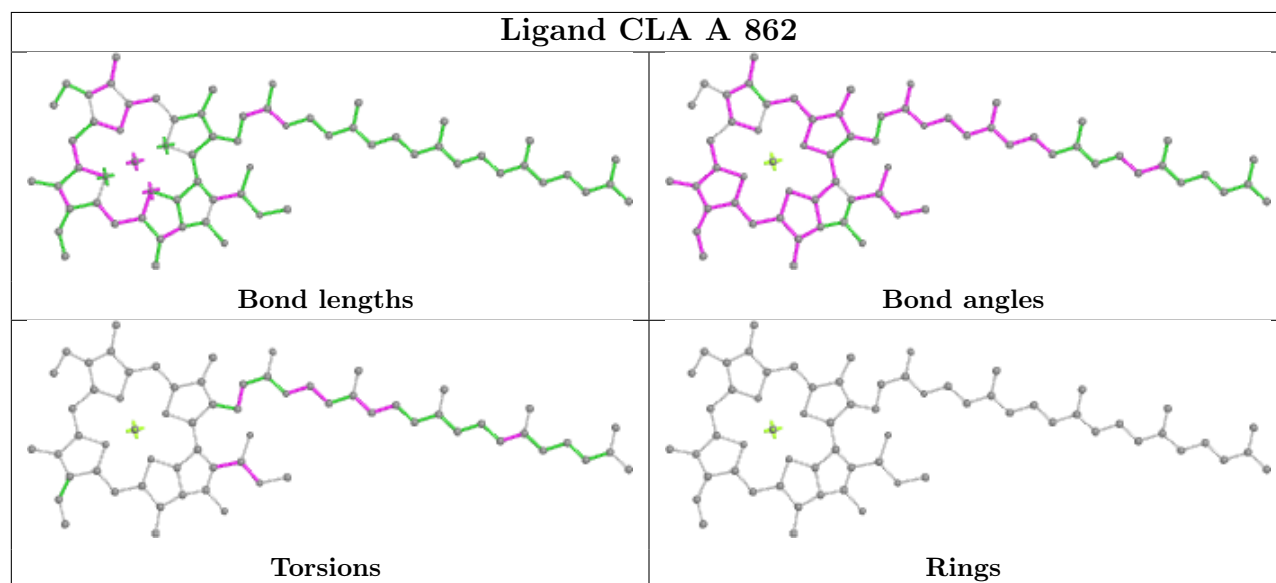
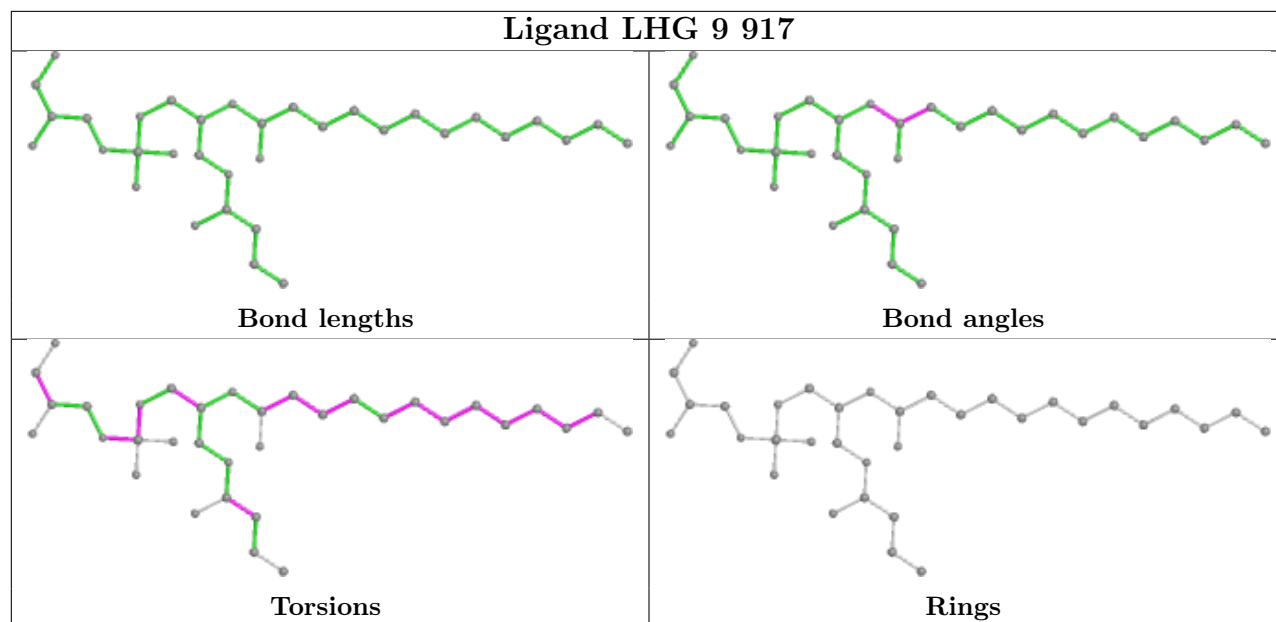


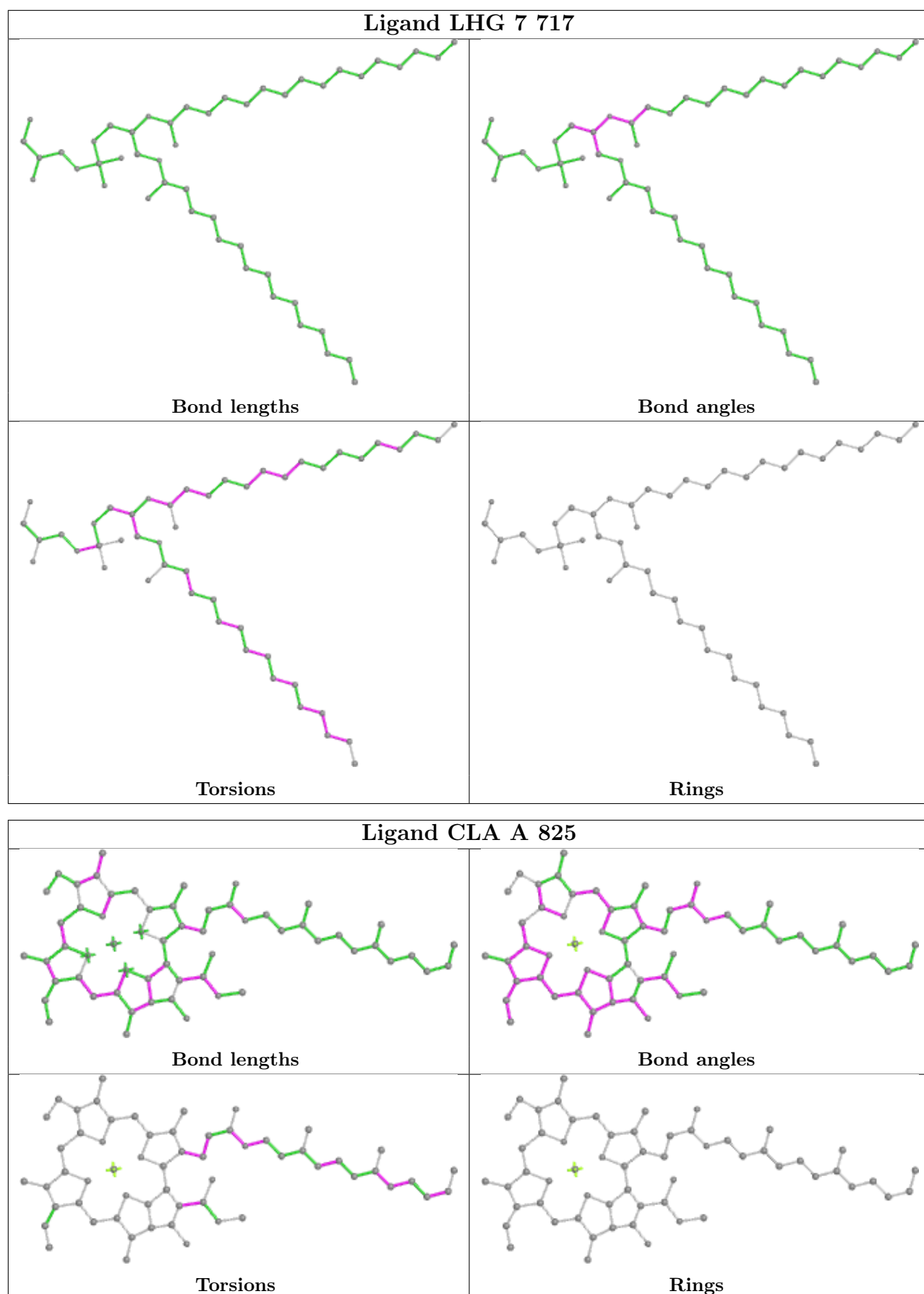
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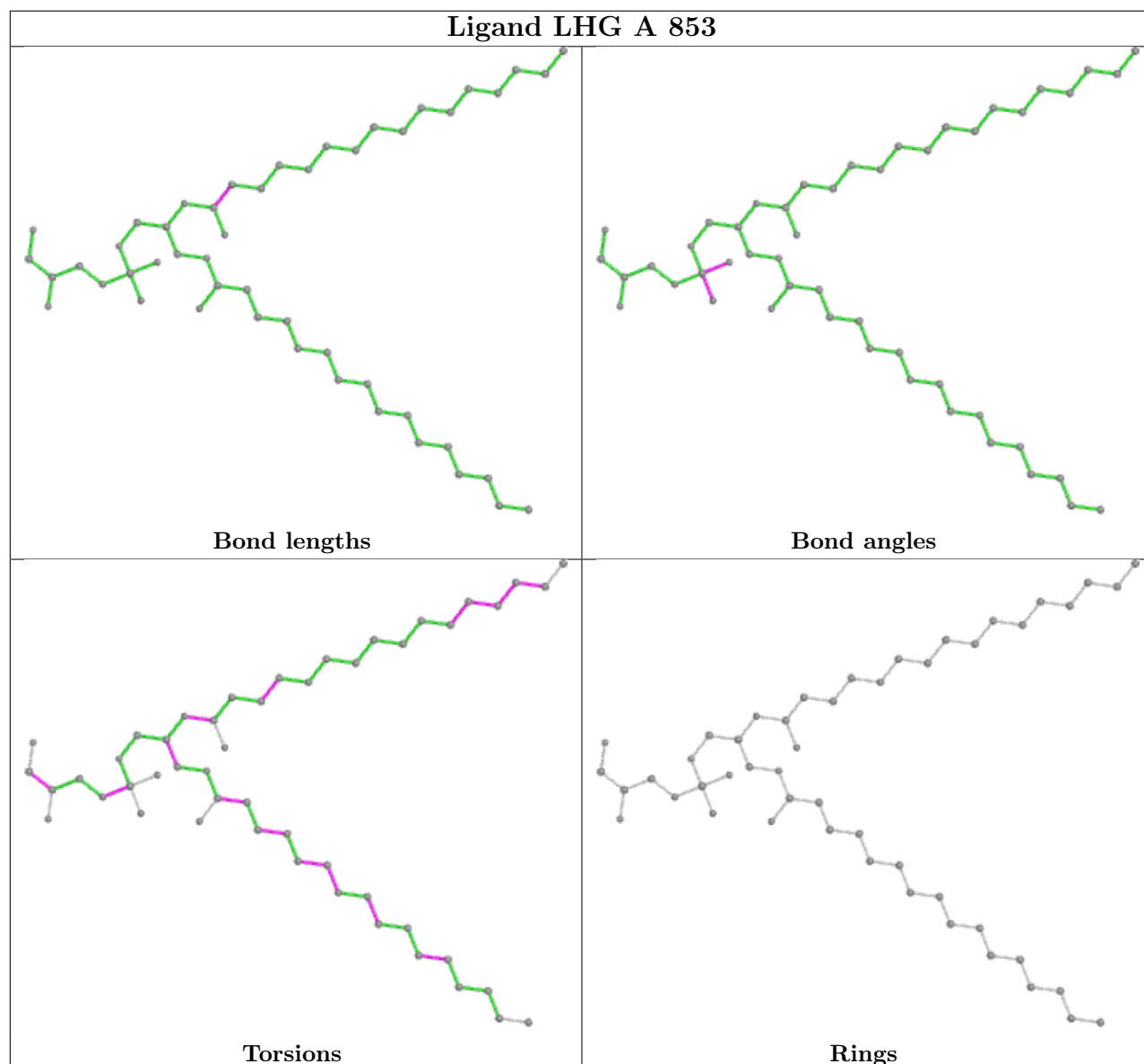
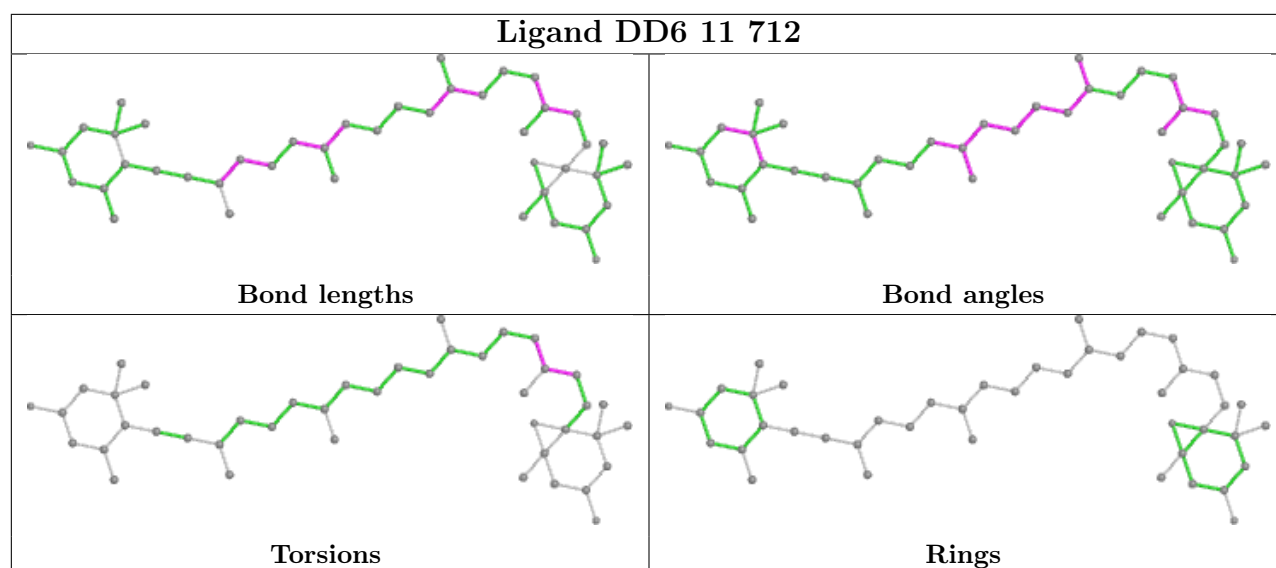


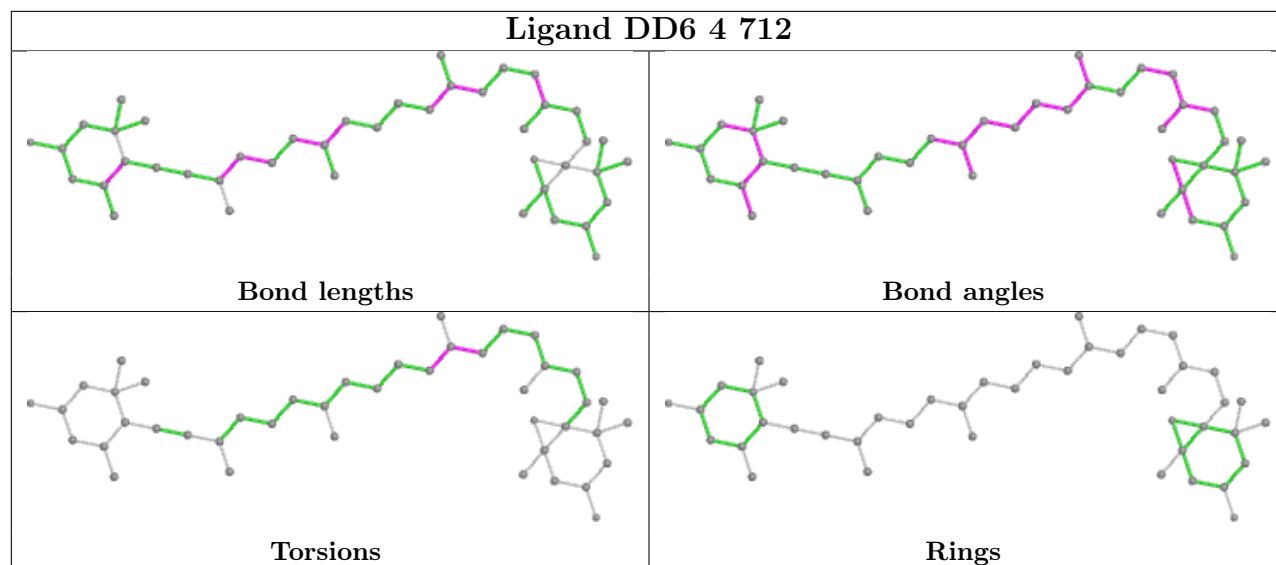
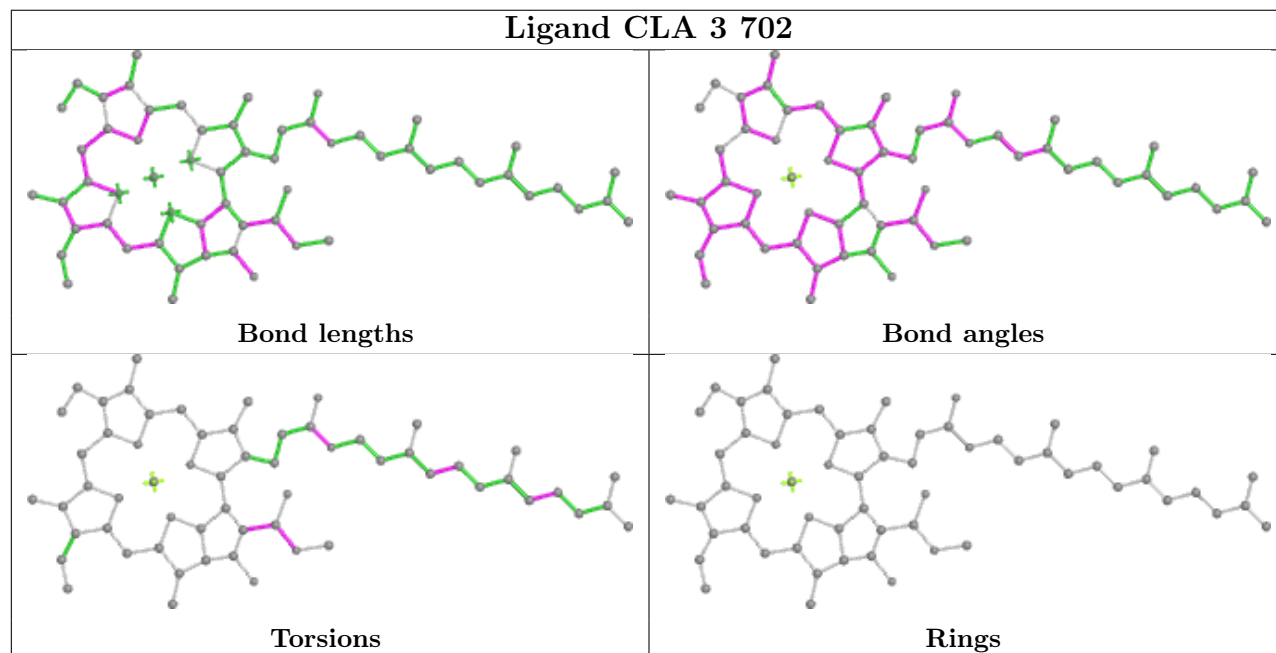
Ligand CLA 8 607



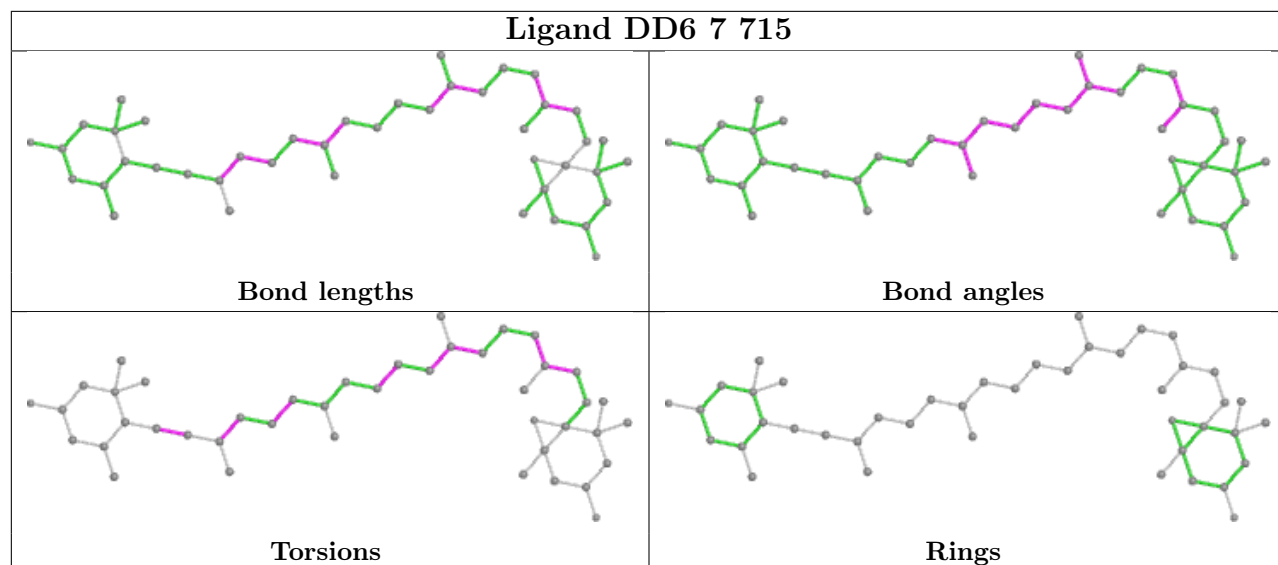




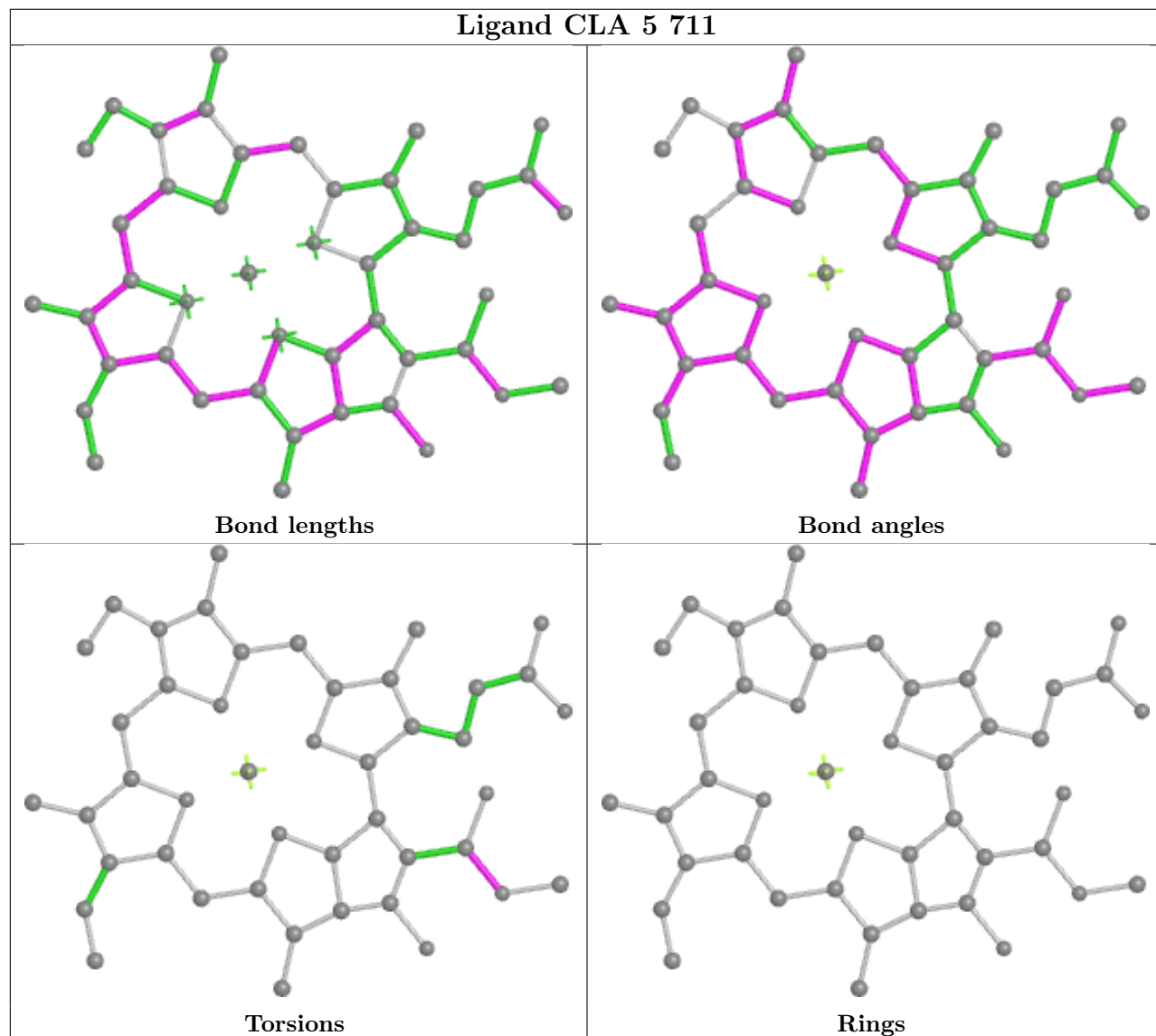


Ligand DD6 4 712**Ligand CLA 3 702**

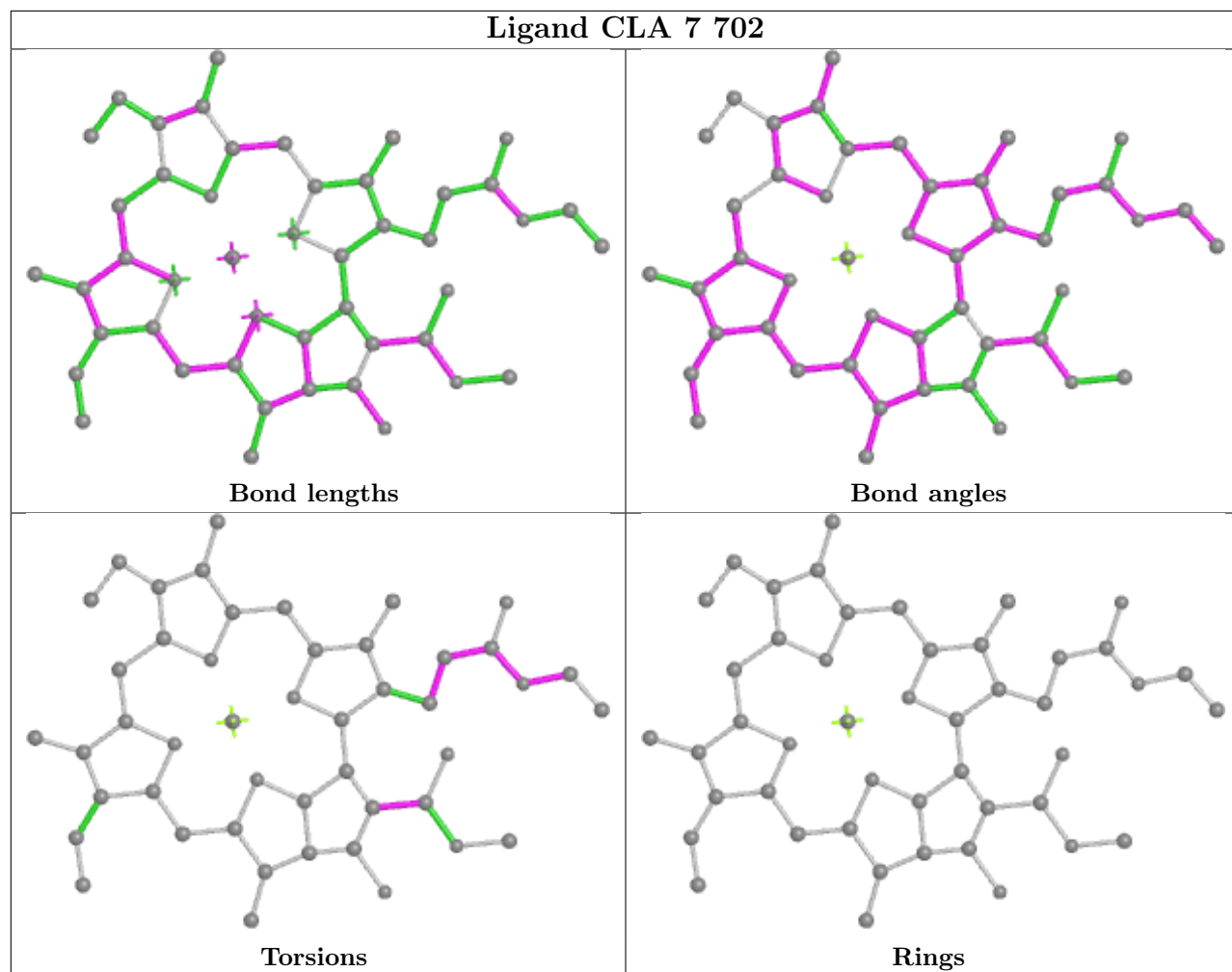
Ligand DD6 7 715

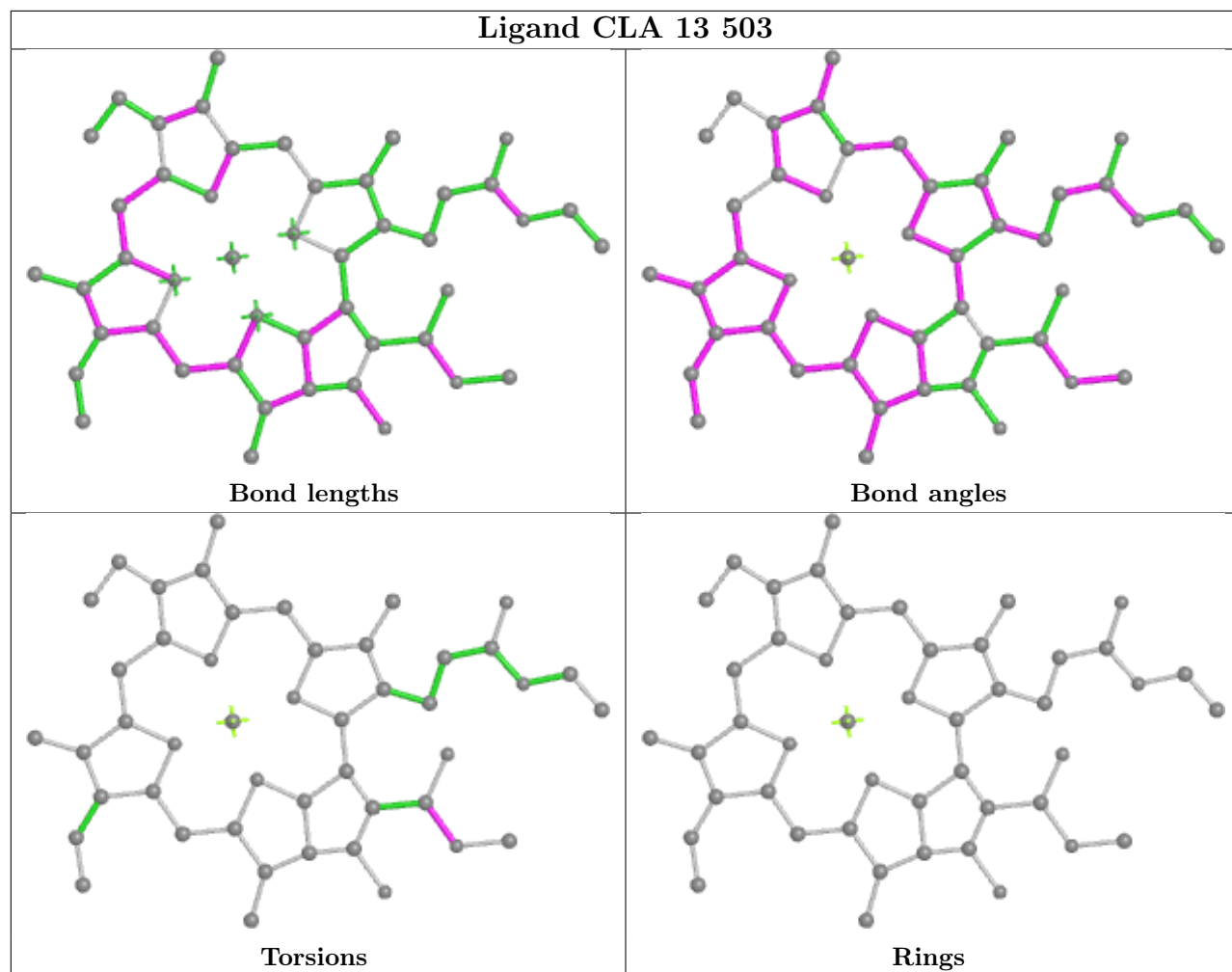


Ligand CLA 5 711

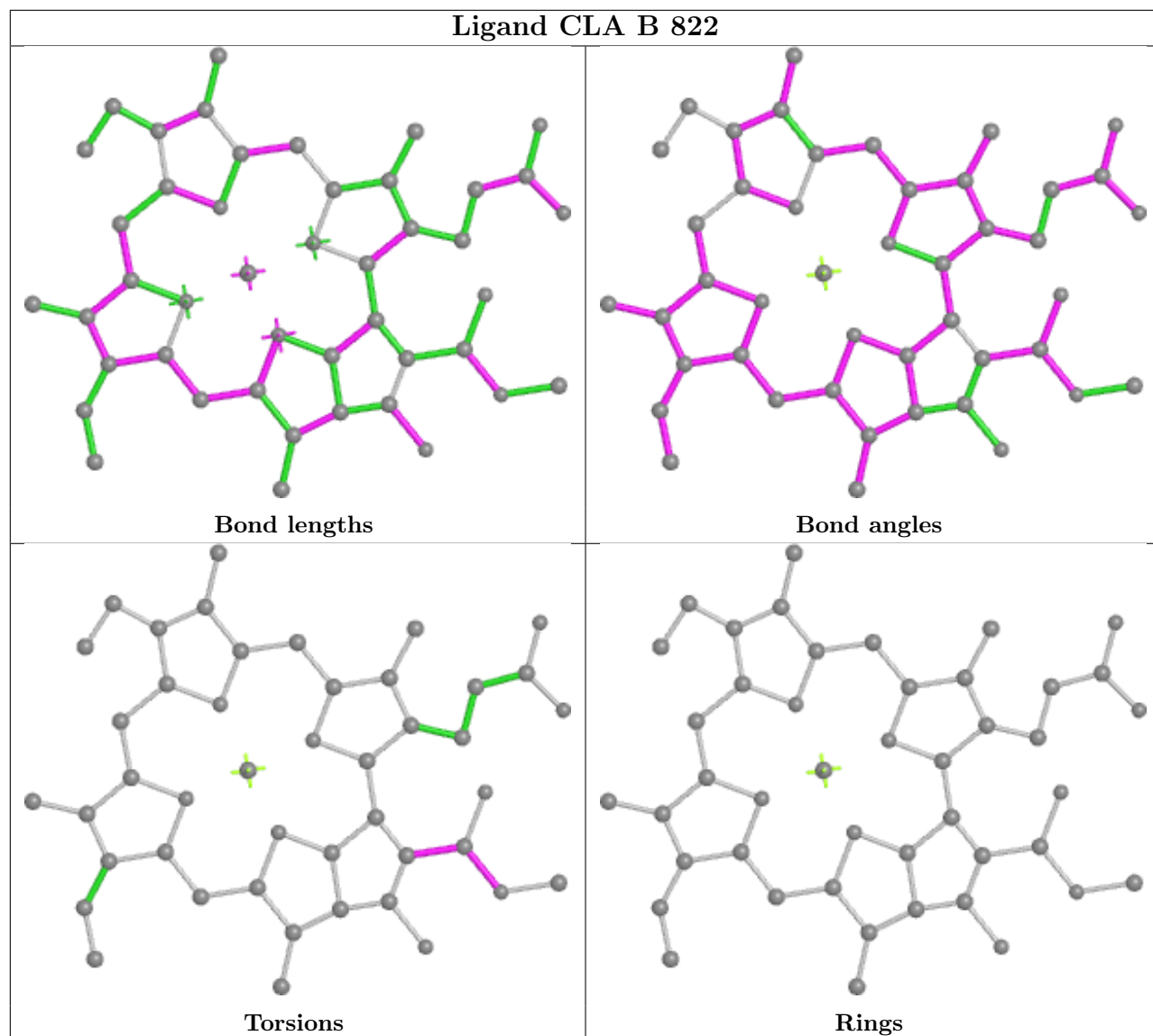


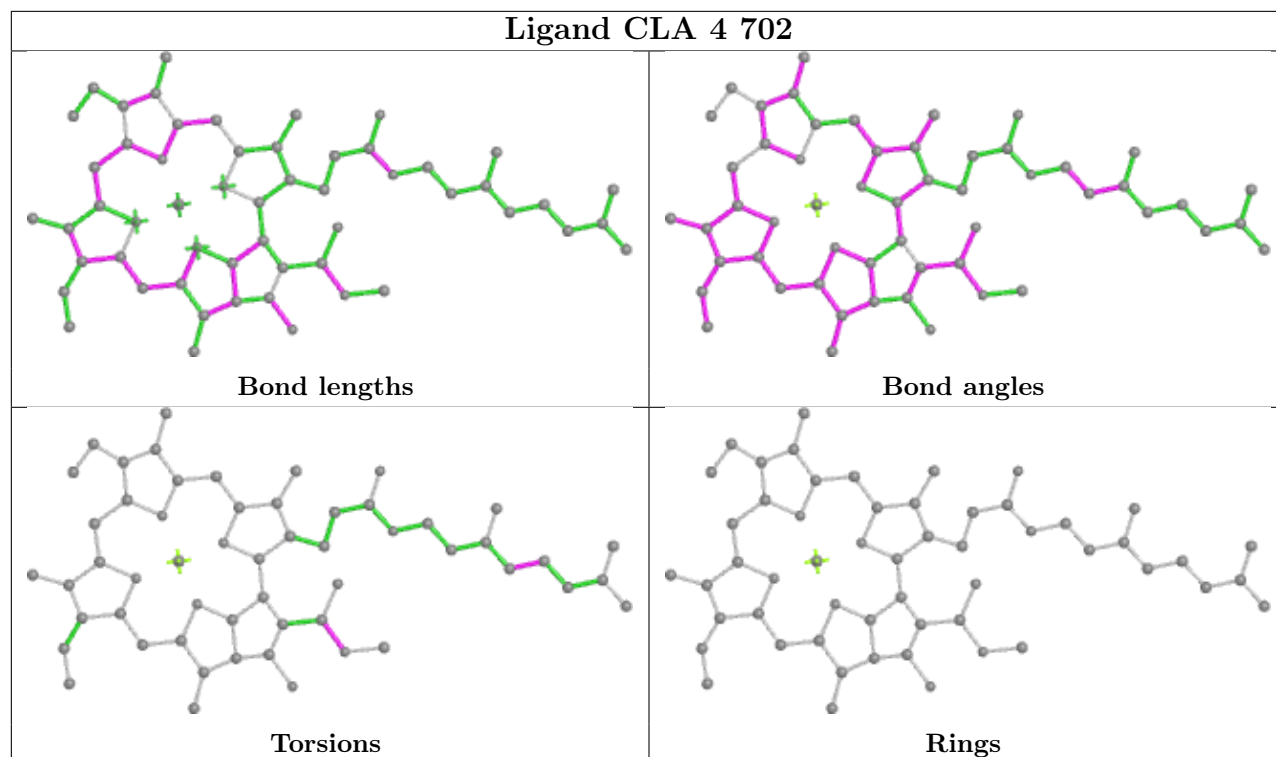
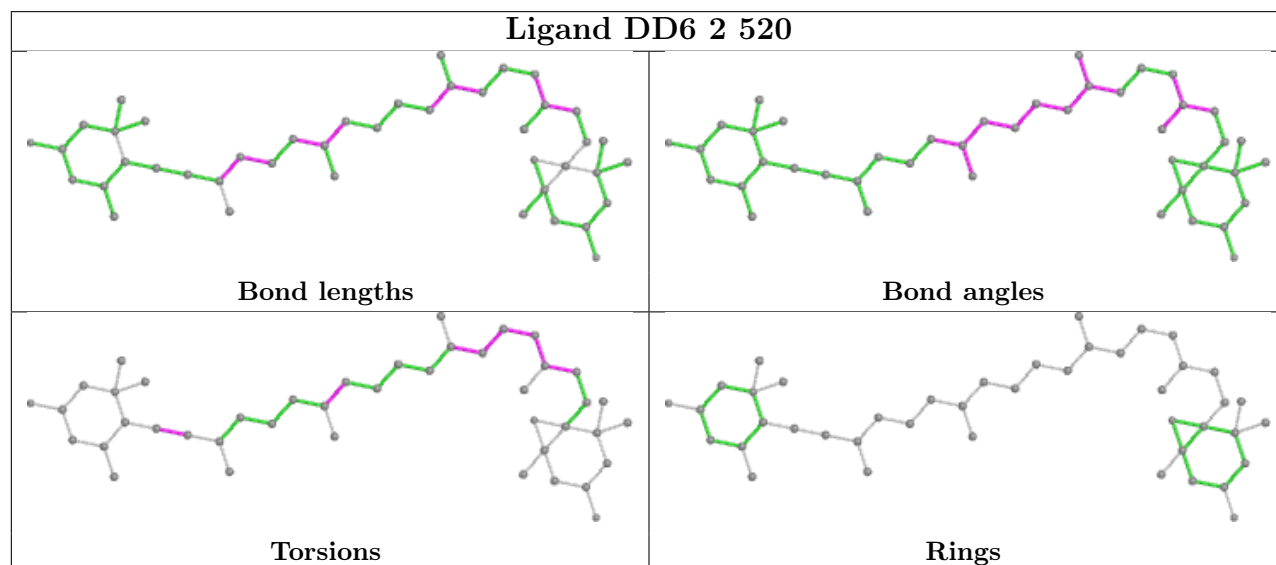
Ligand CLA 7 702



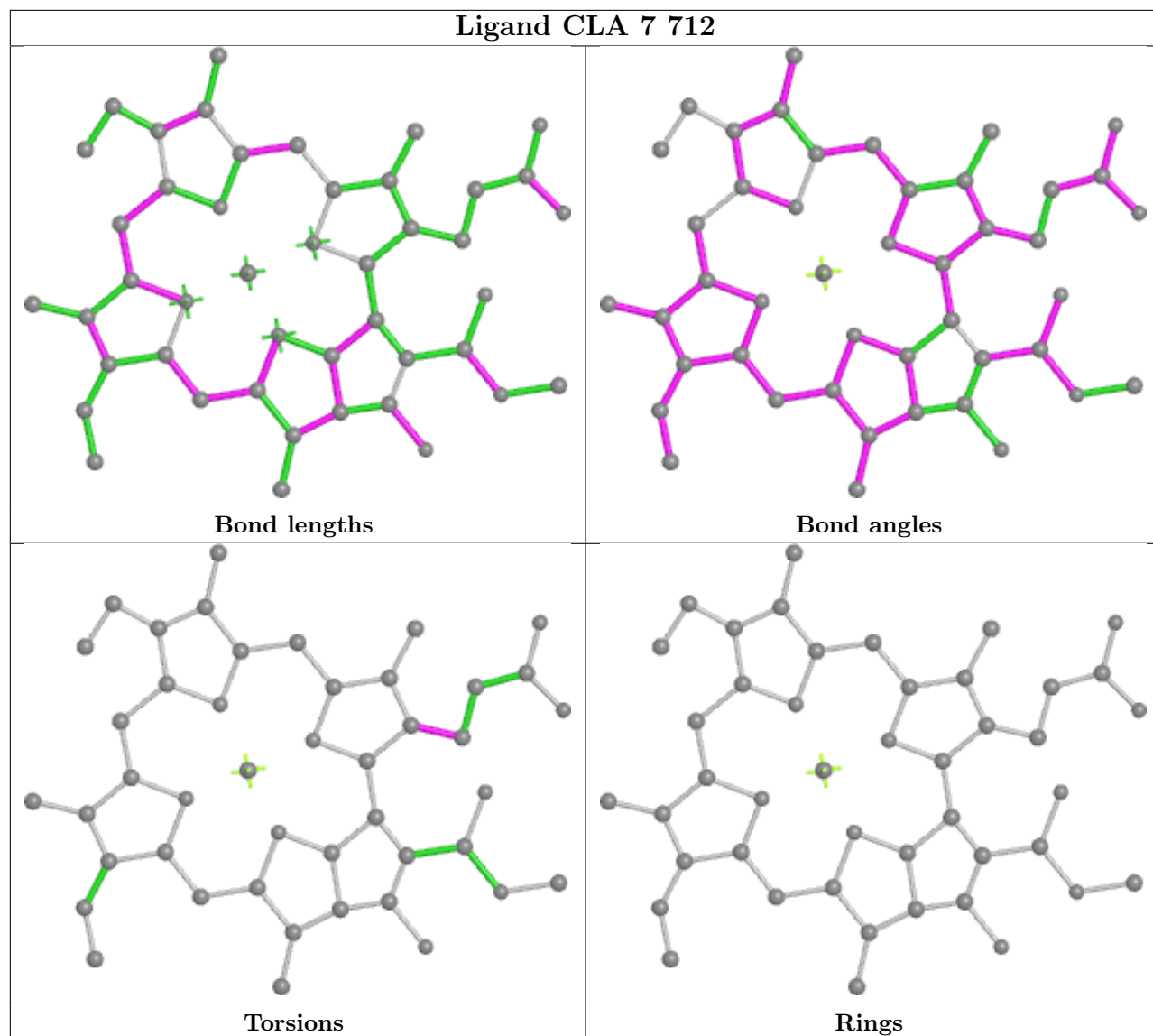


Ligand CLA B 822

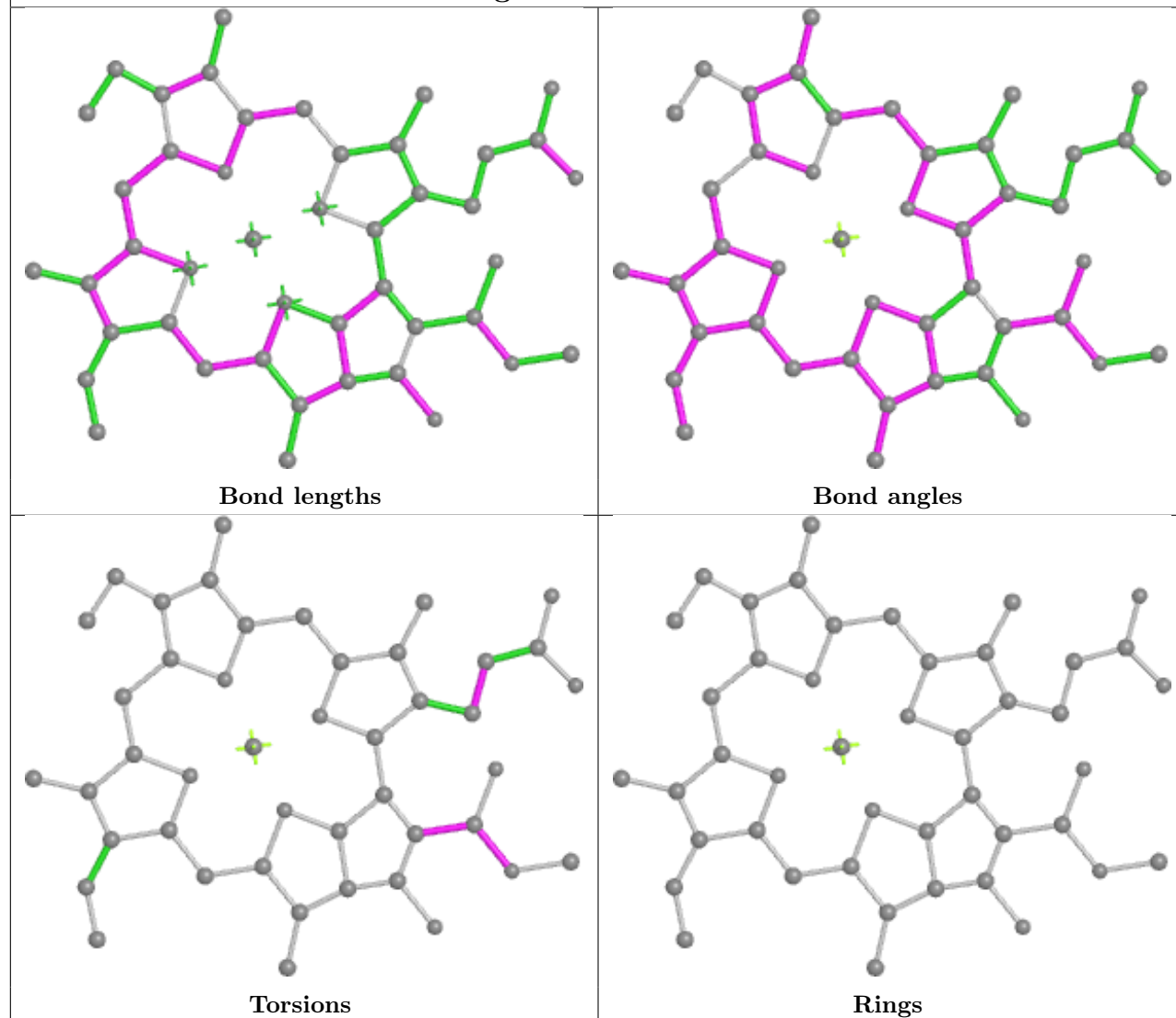


Ligand CLA 4 702**Ligand DD6 2 520**

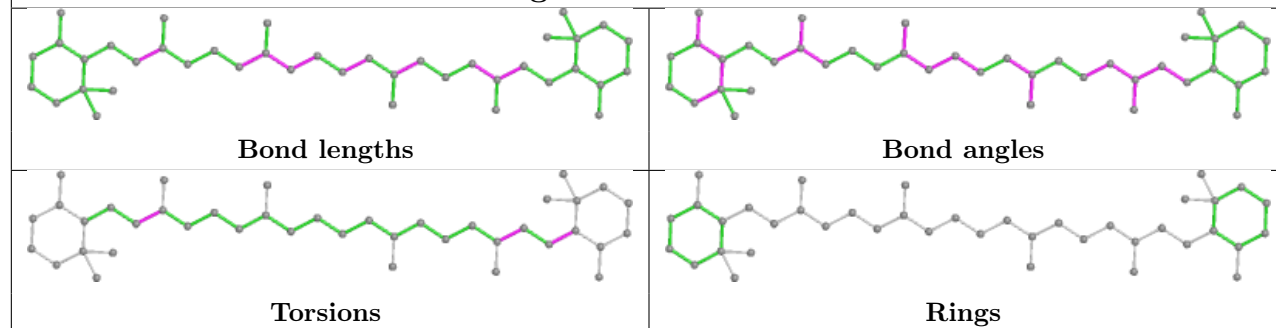
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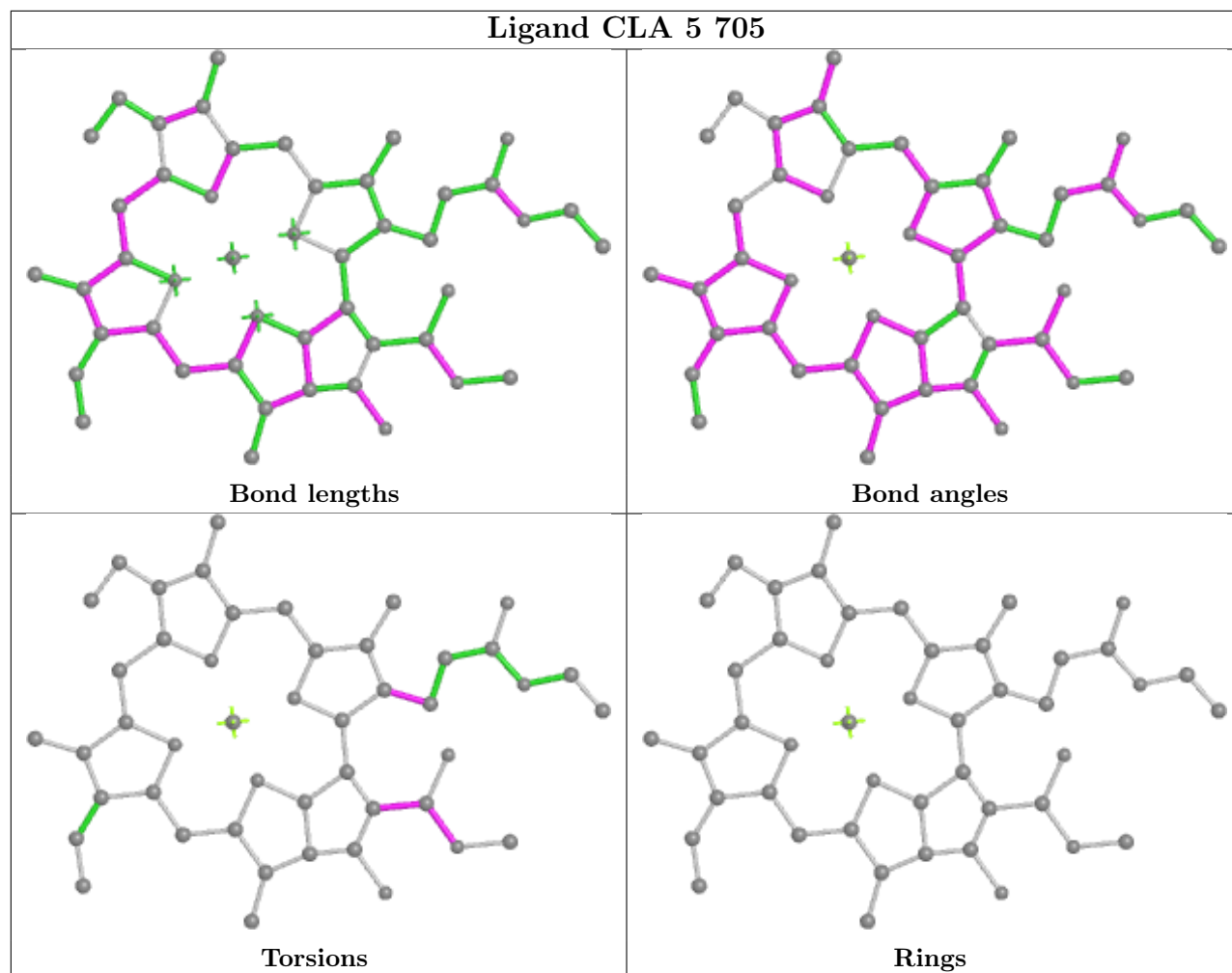
Ligand CLA 9 912



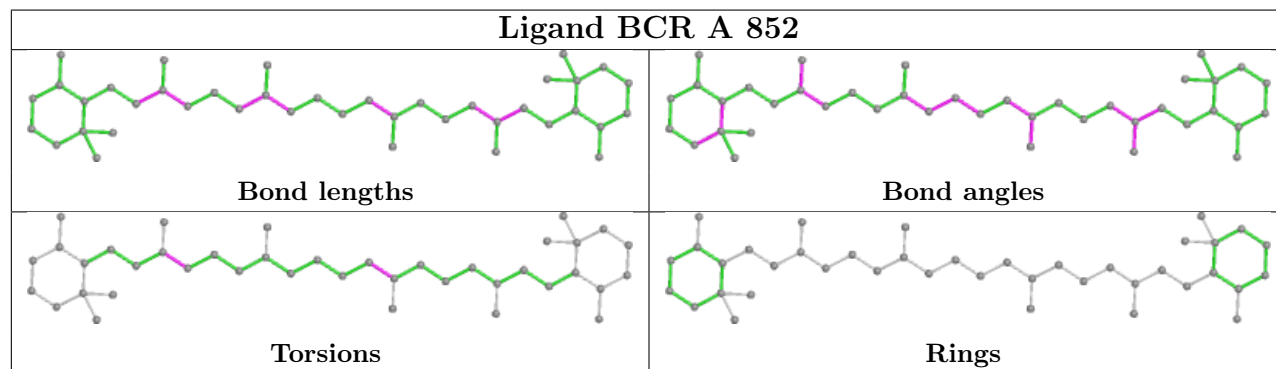
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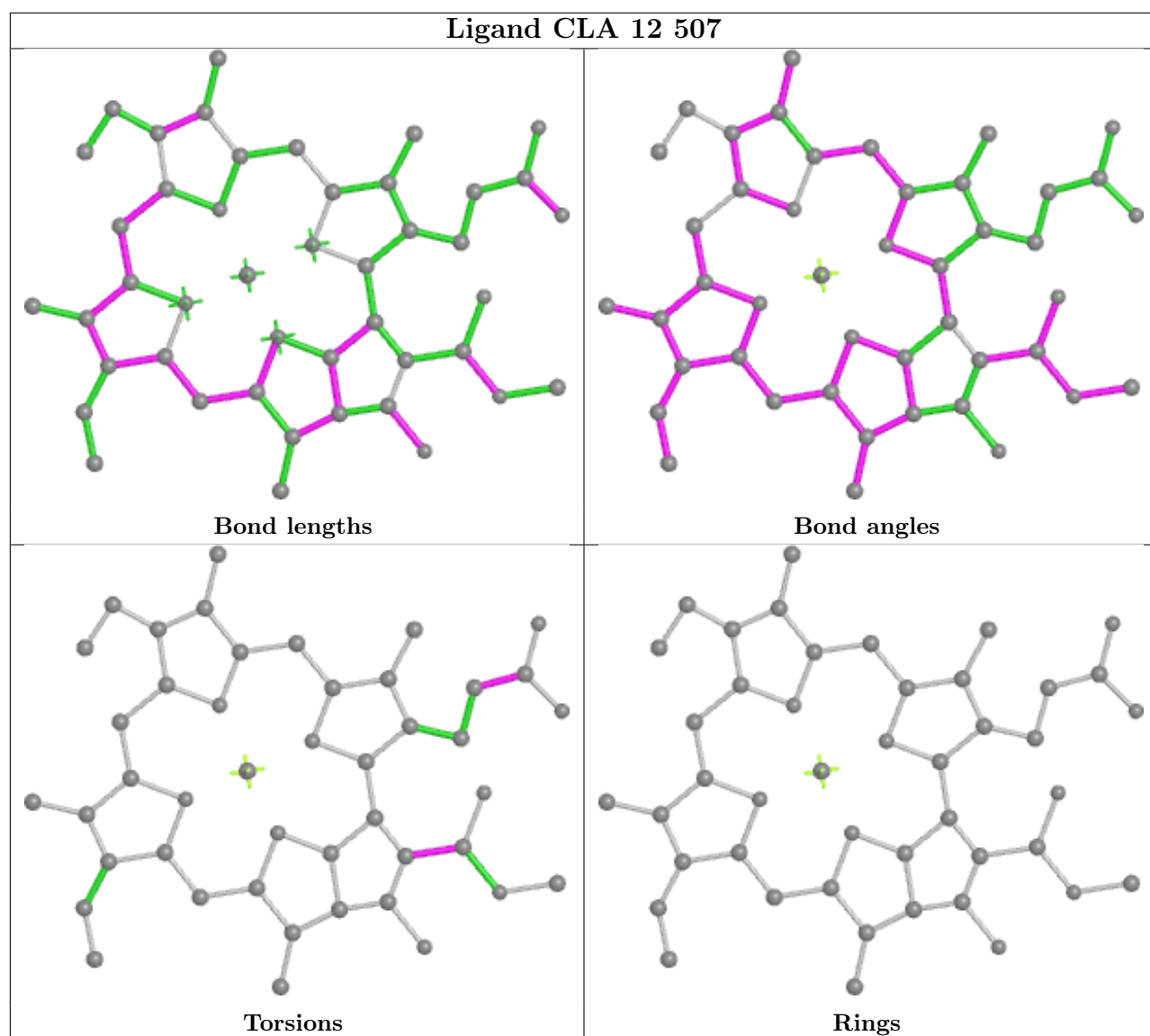


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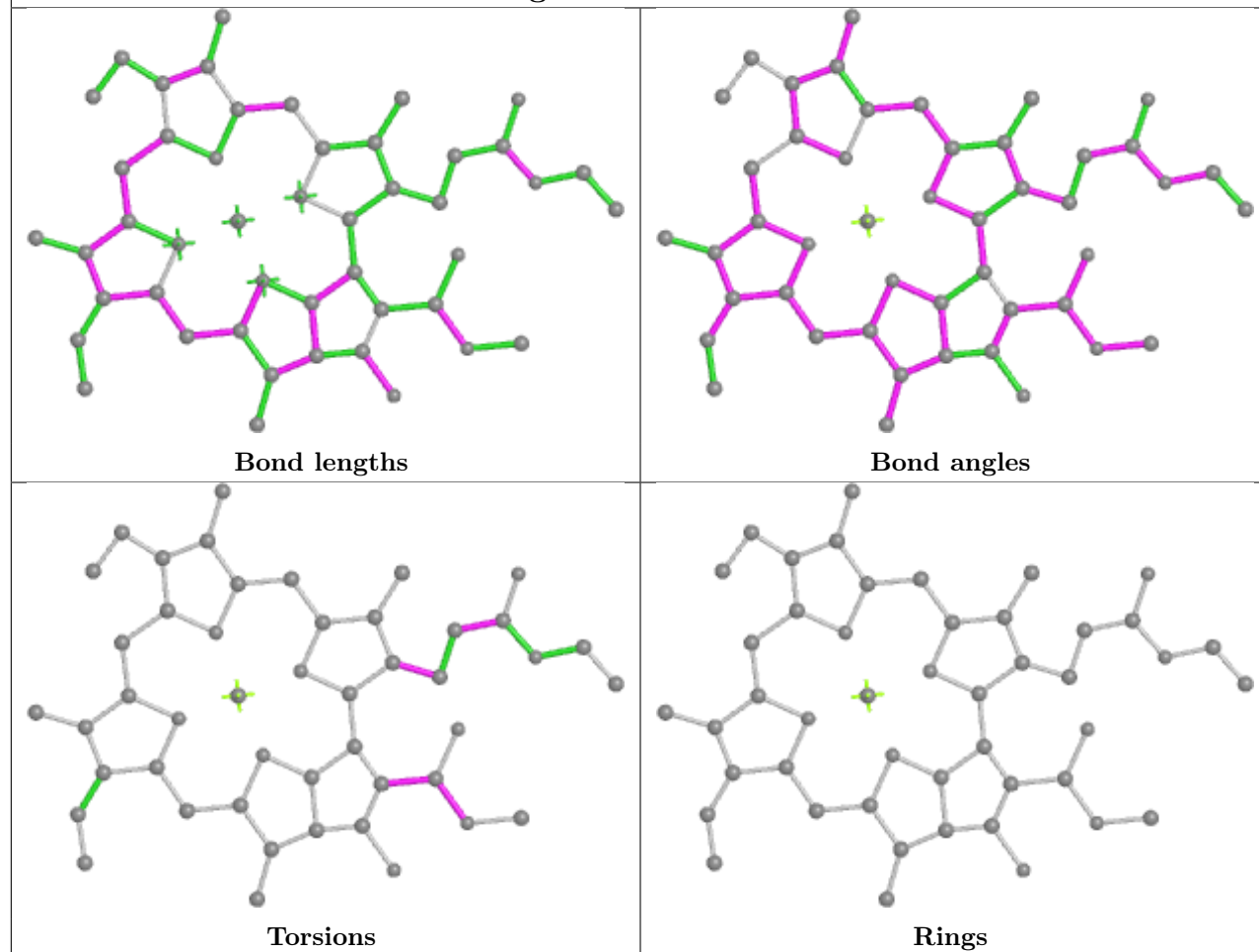


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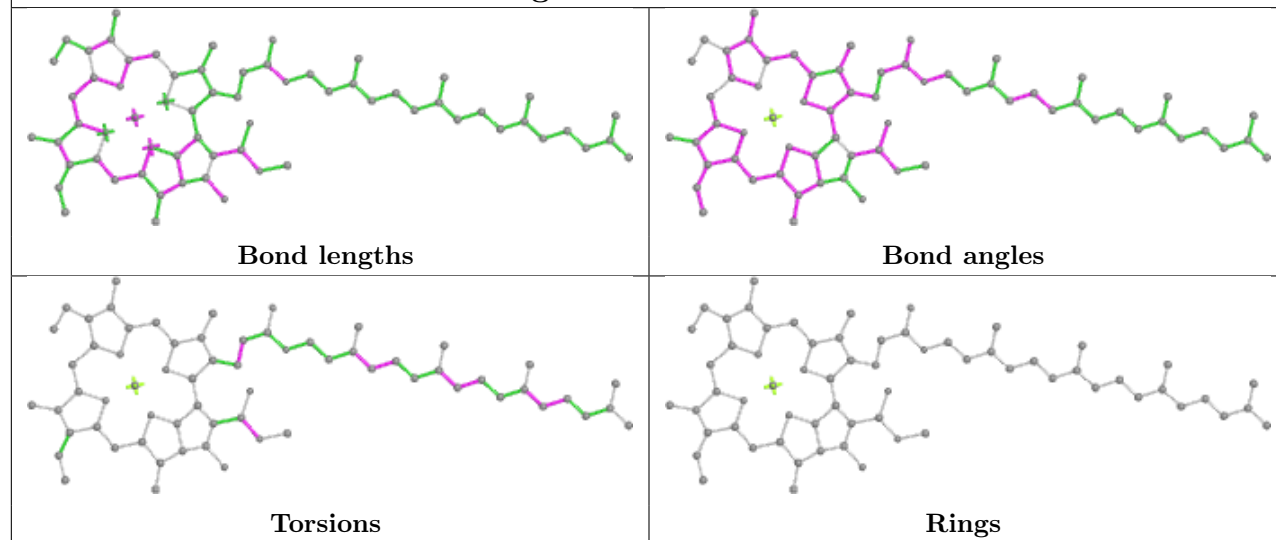




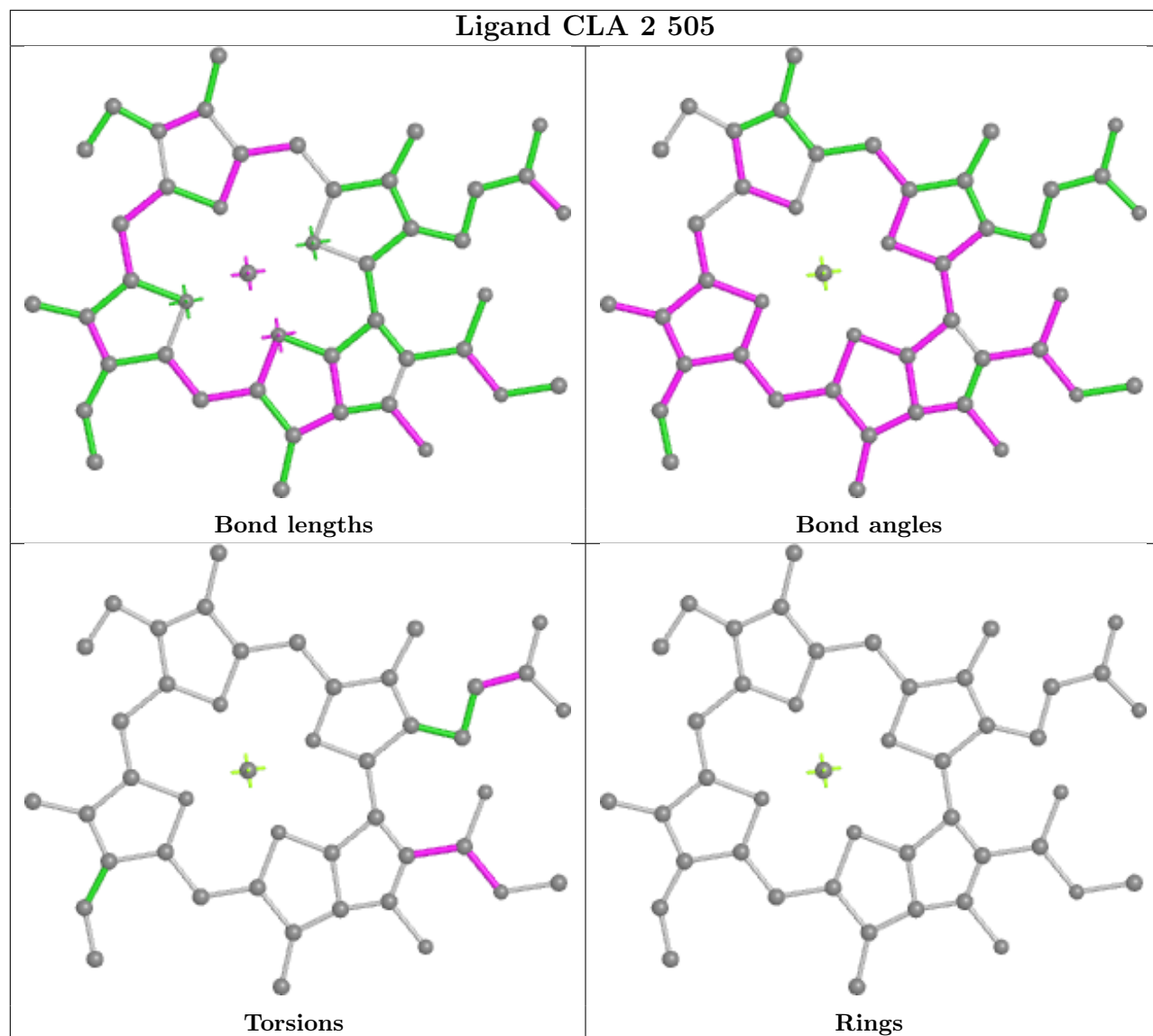
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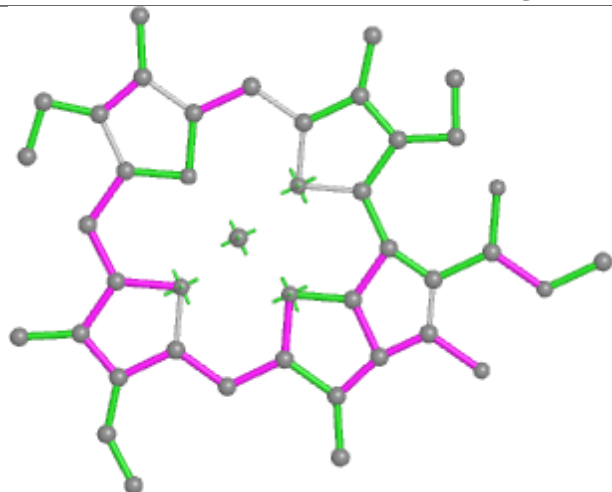
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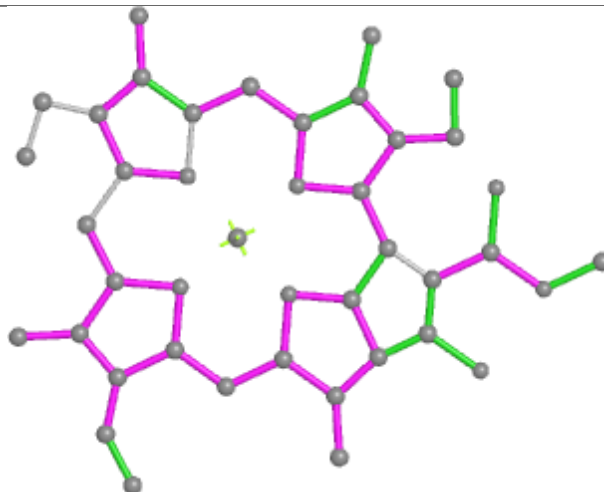
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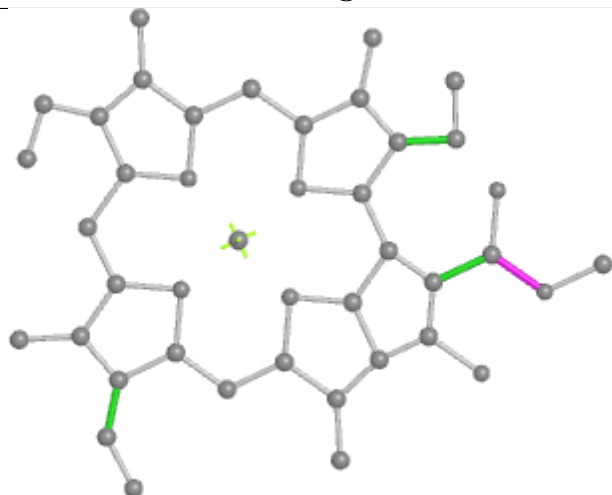
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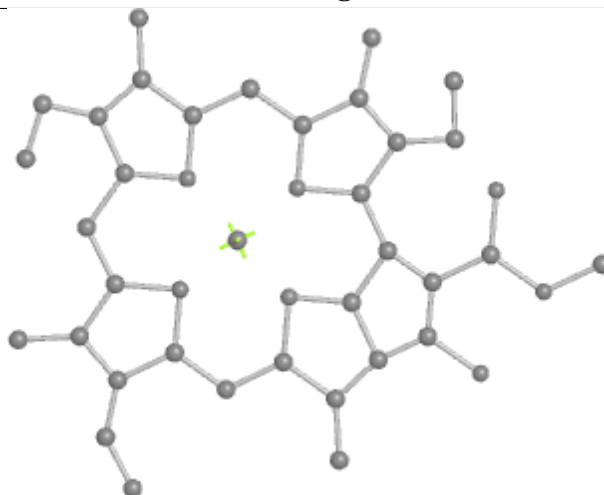
Bond lengths



Bond angles

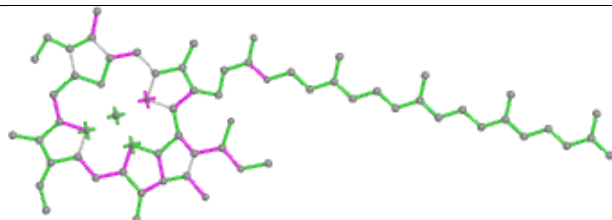


Torsions

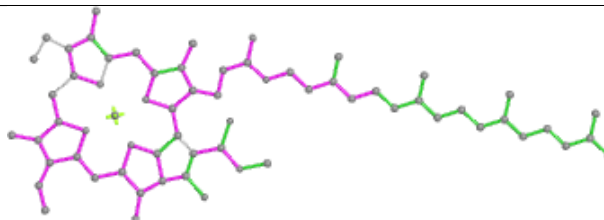


Rings

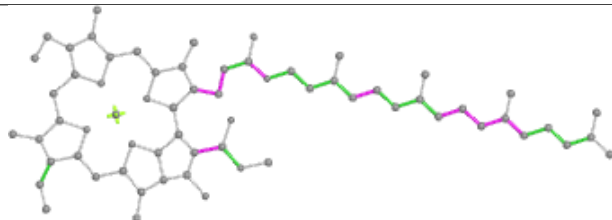
Ligand CLA A 806



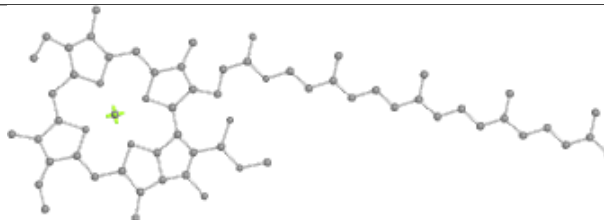
Bond lengths



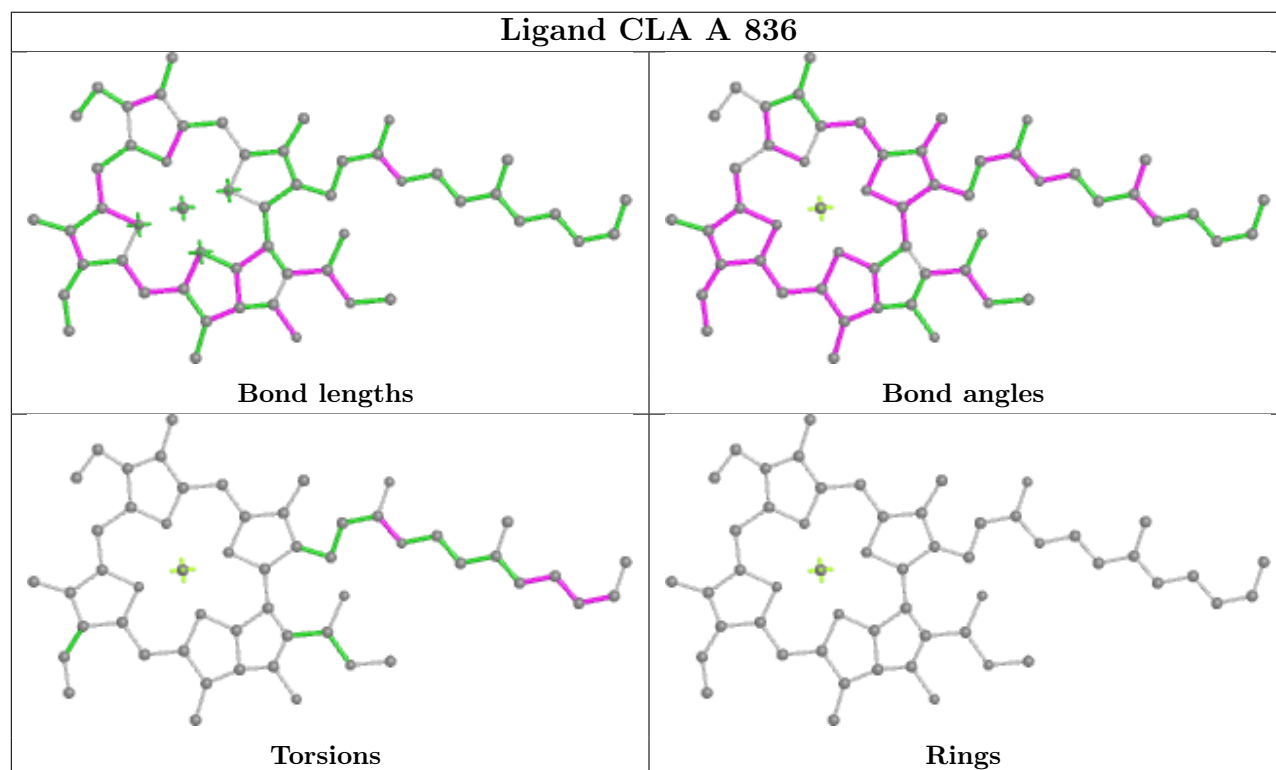
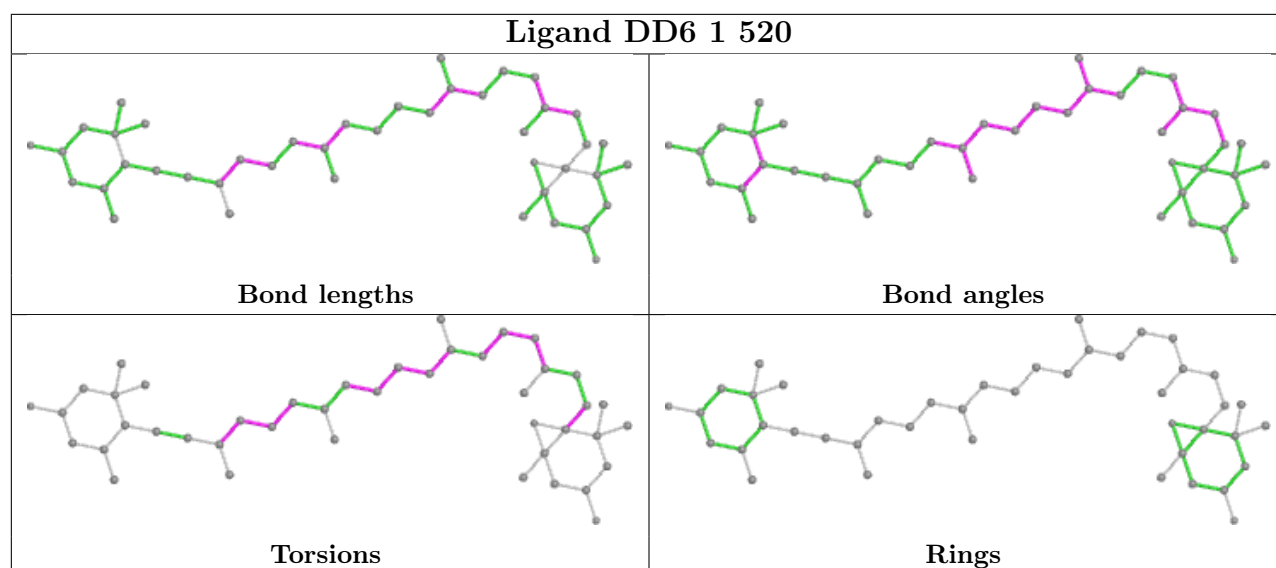
Bond angles

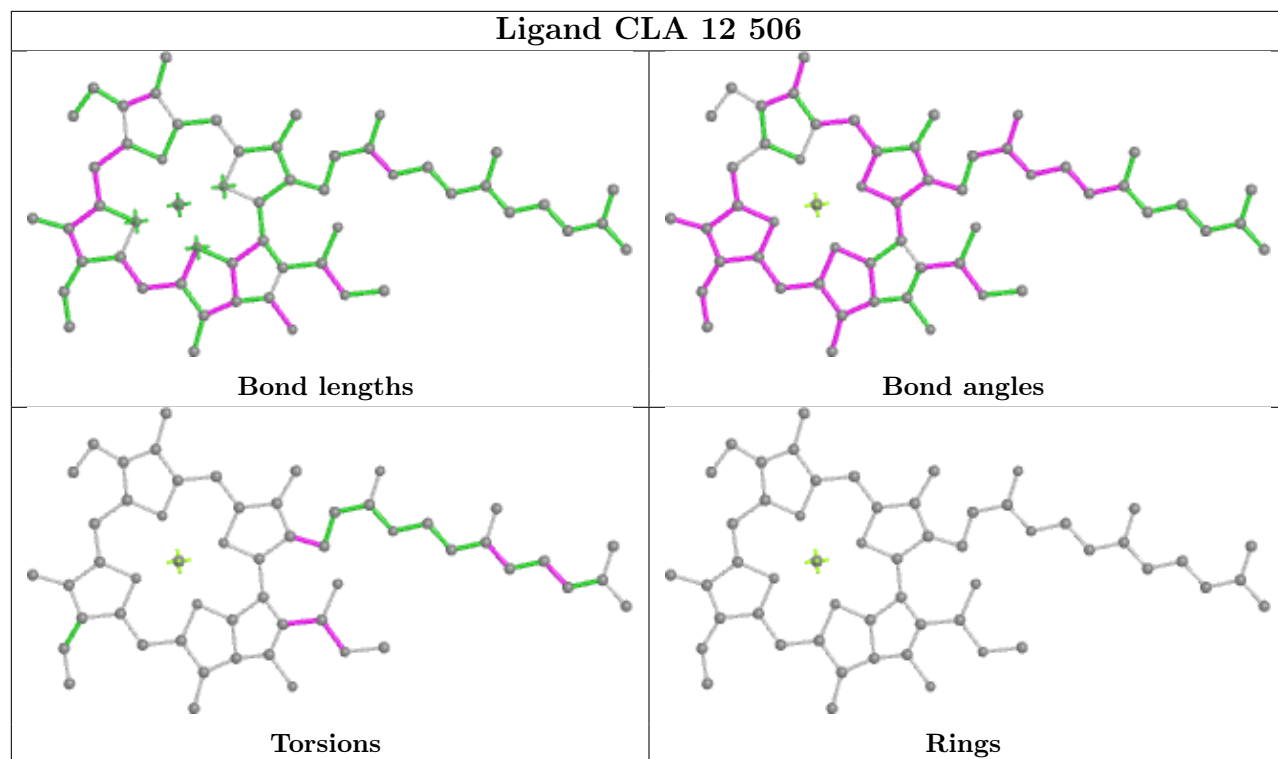


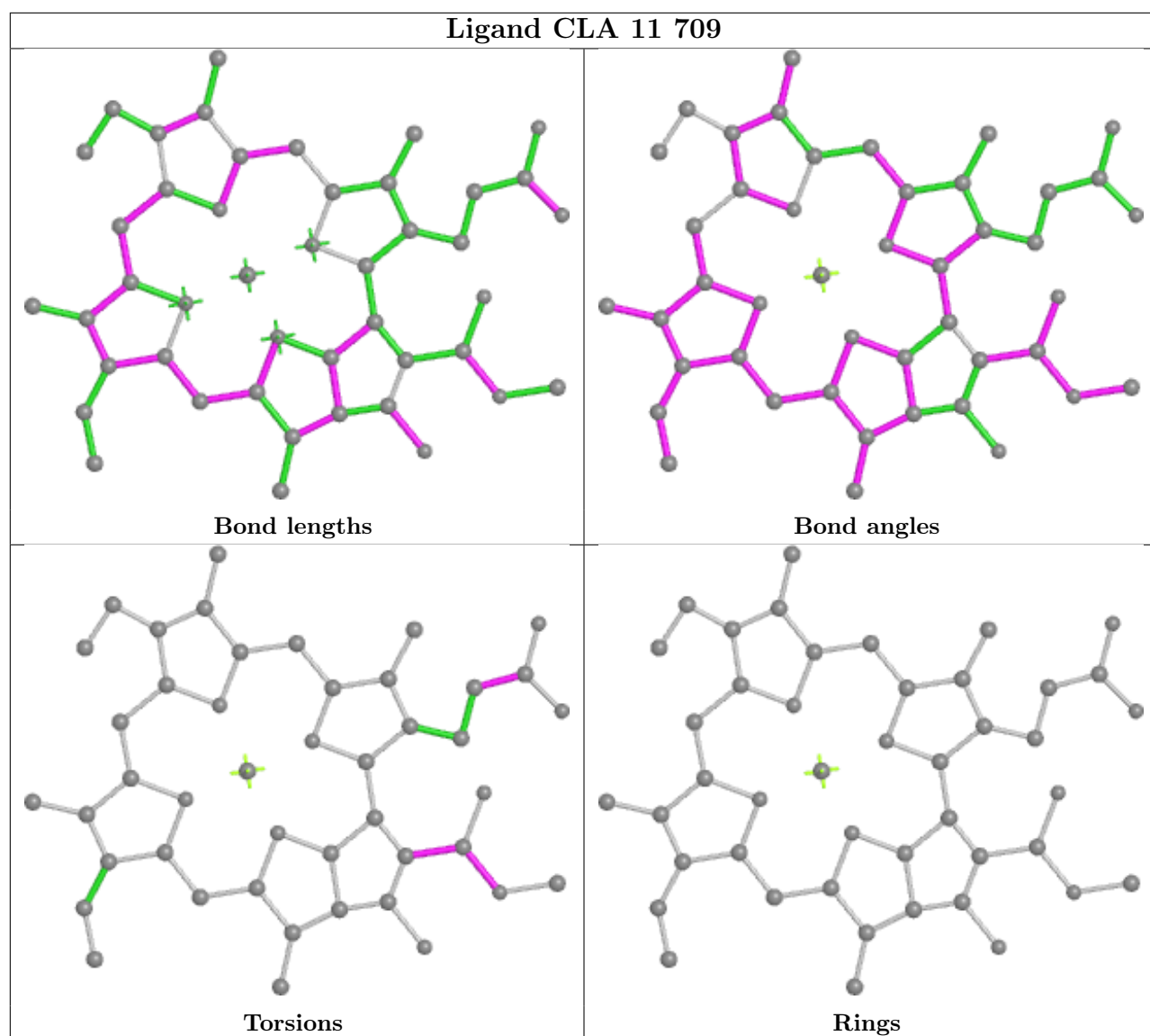
Torsions



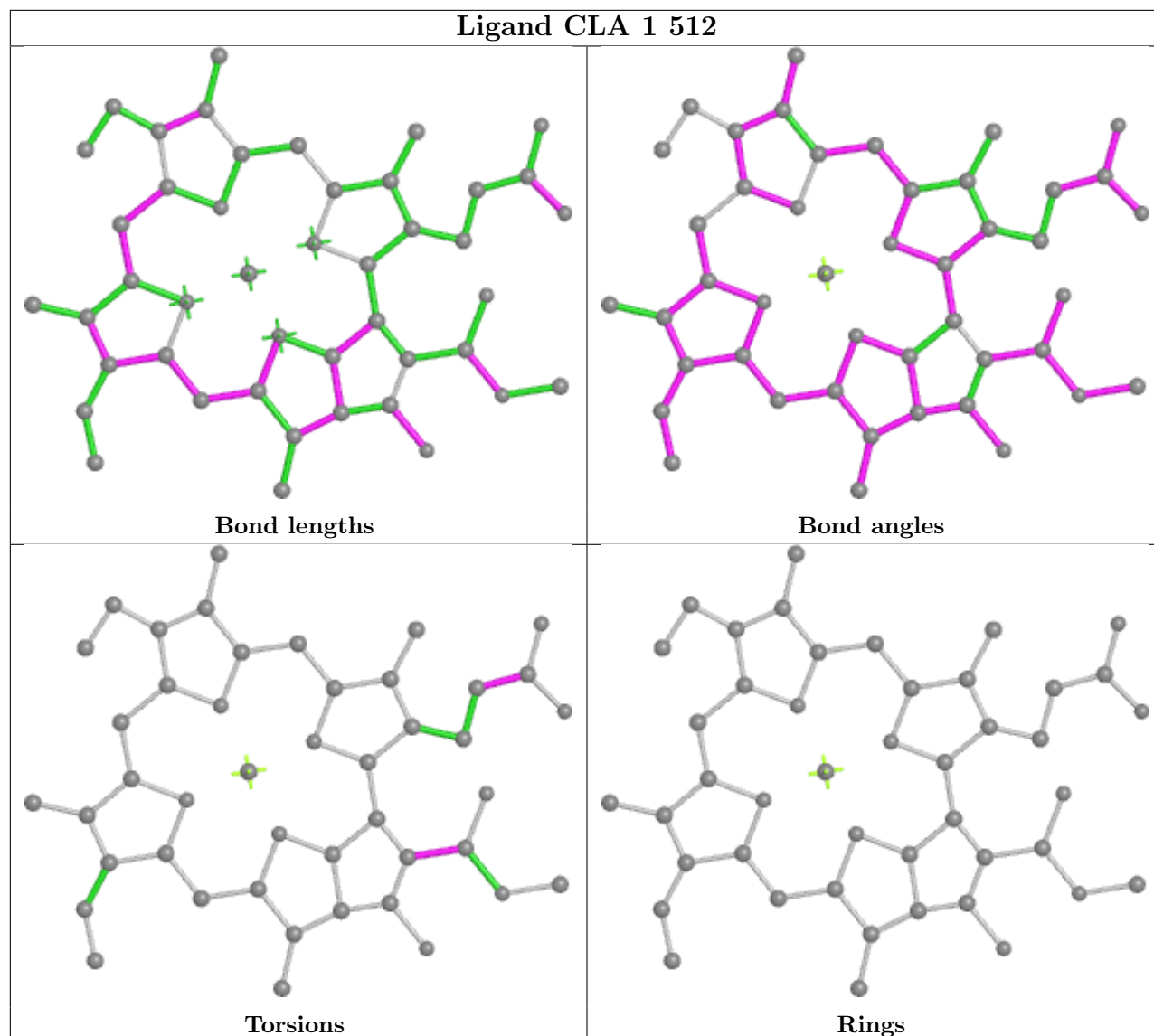
Rings



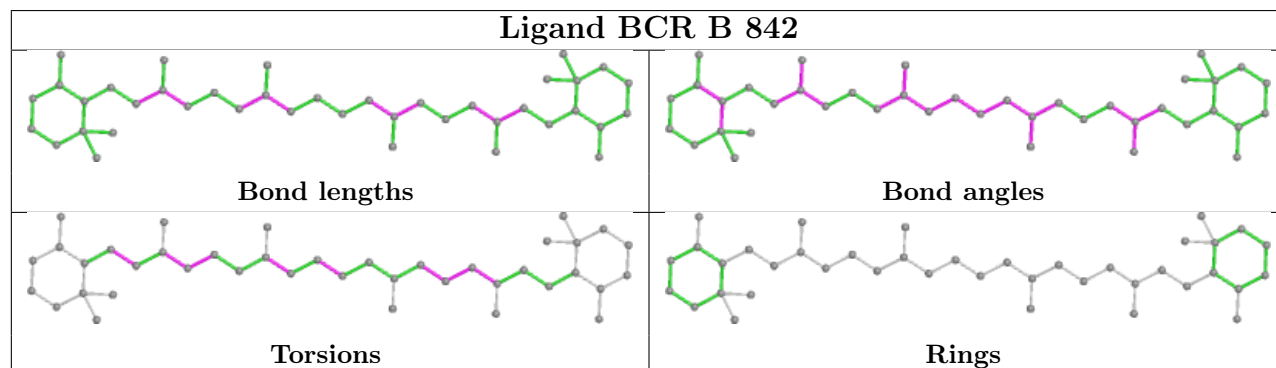




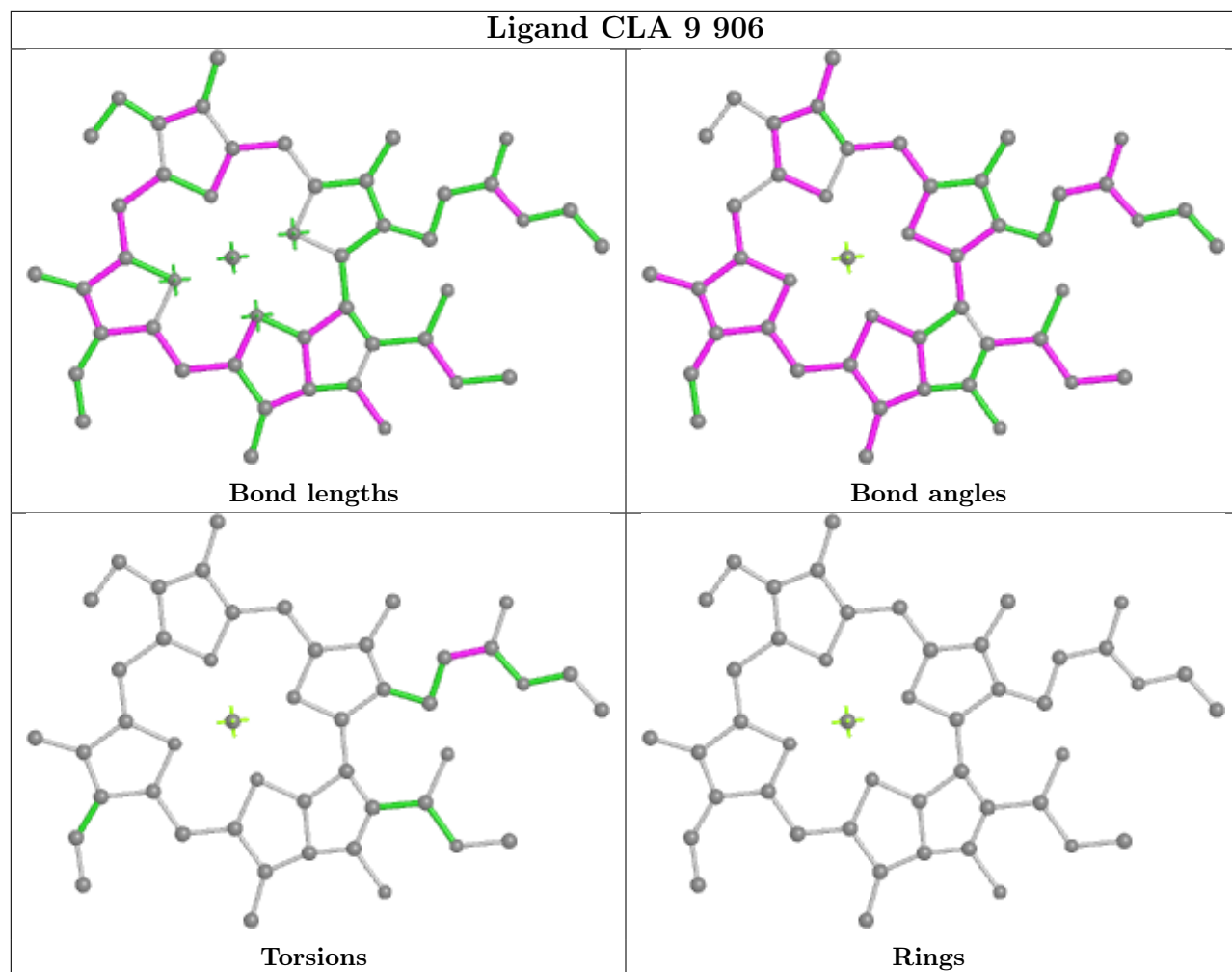
Ligand CLA 1 512



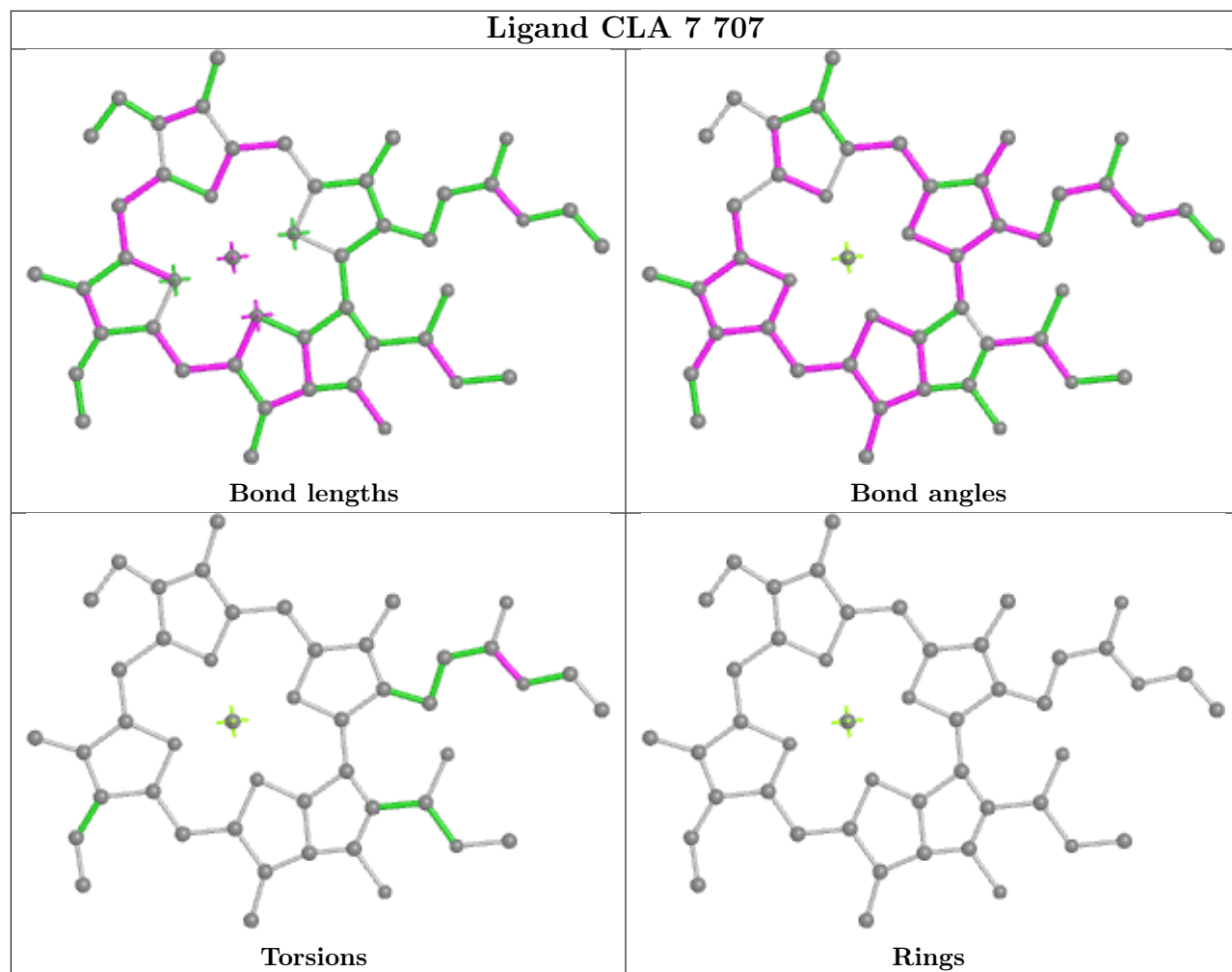
Ligand BCR B 842



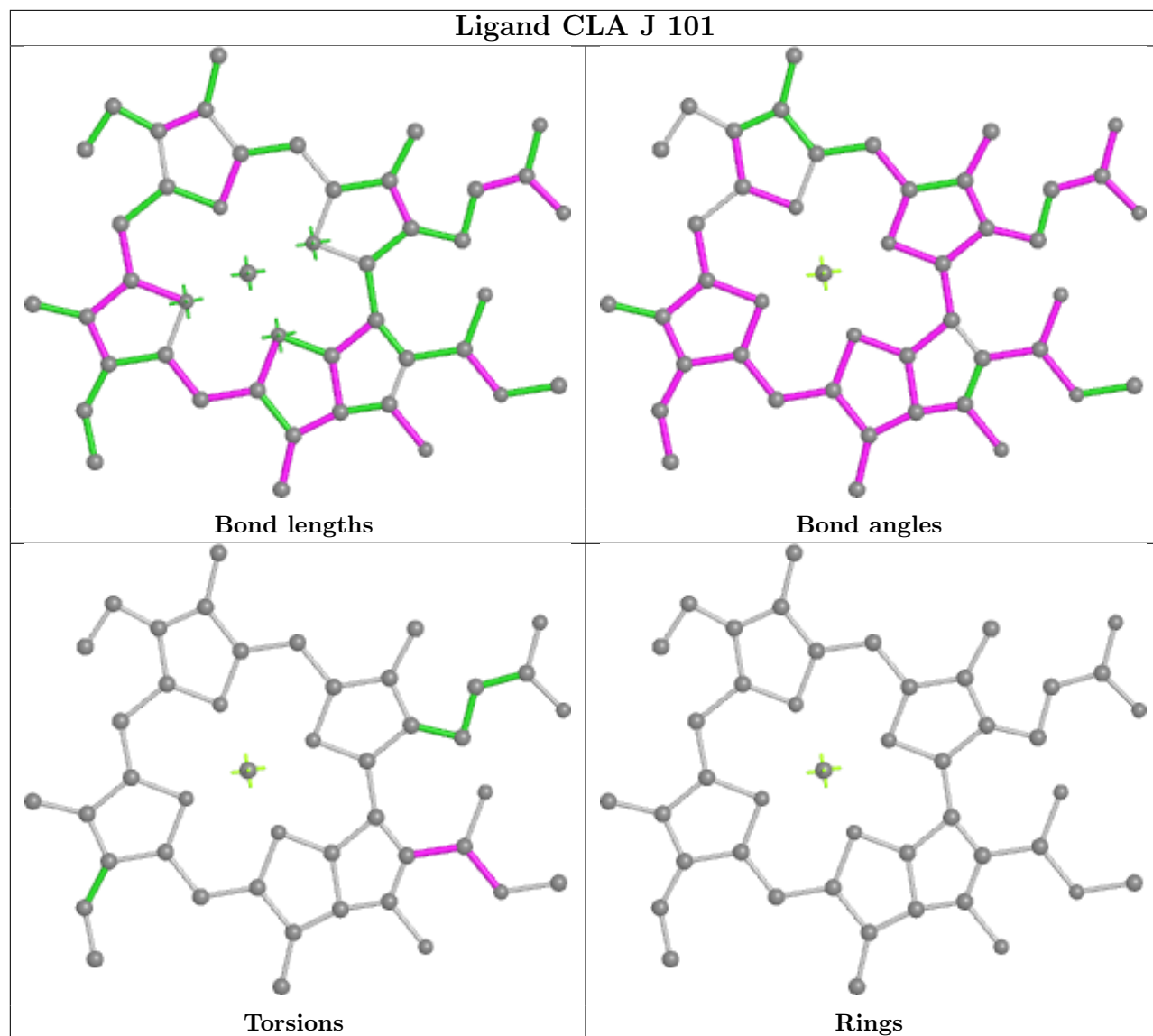
Ligand CLA 9 906



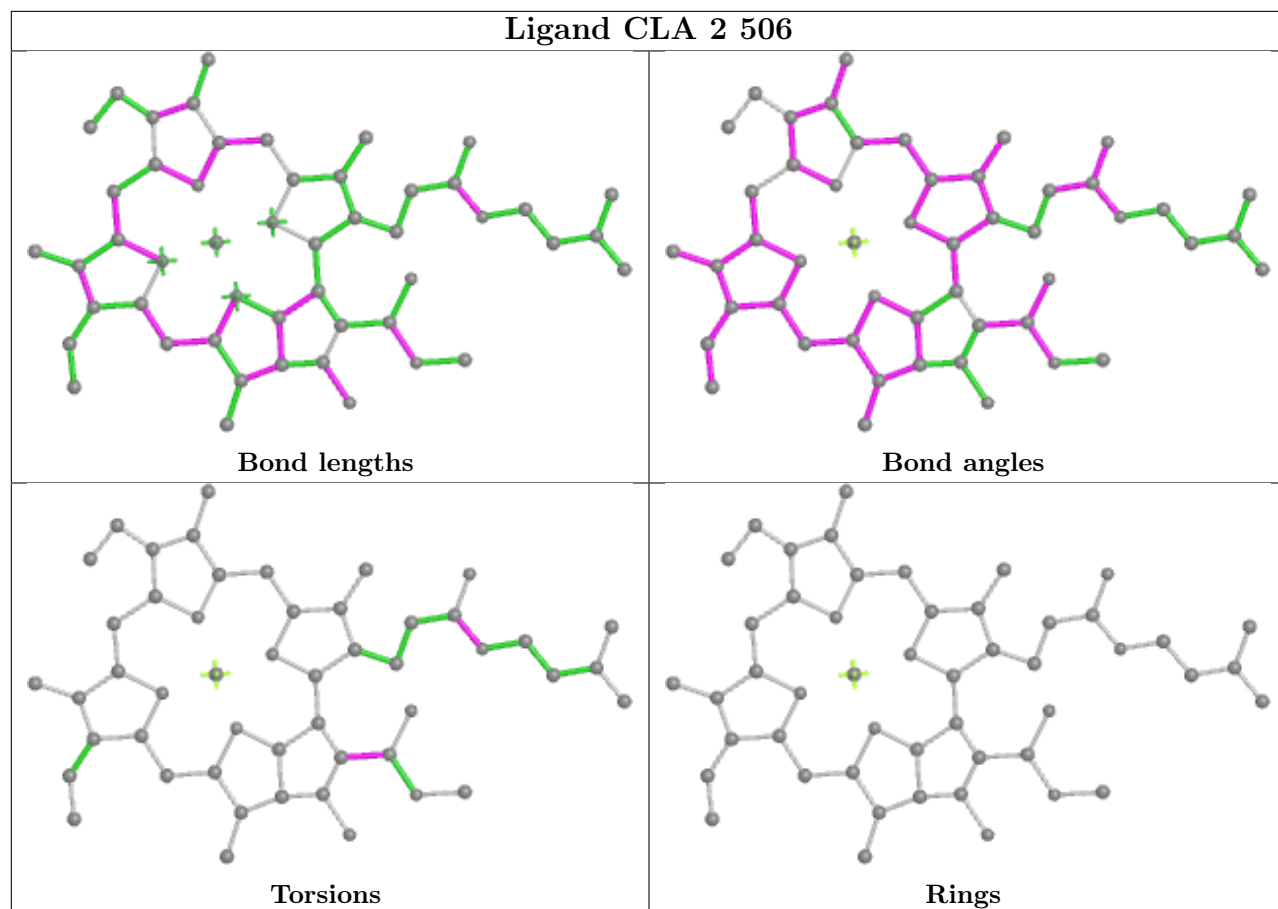
Ligand CLA 7 707



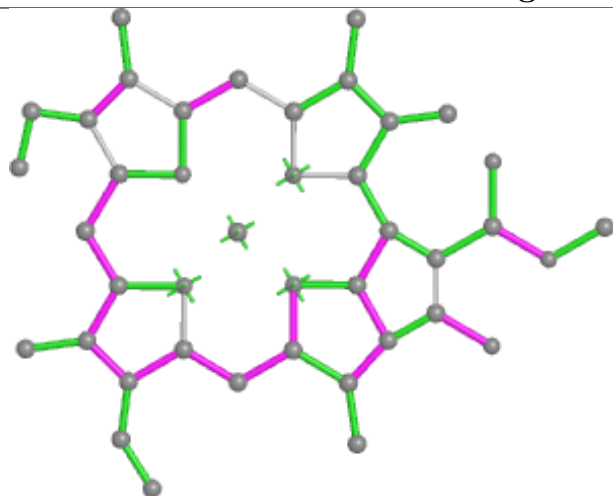
Ligand CLA J 101



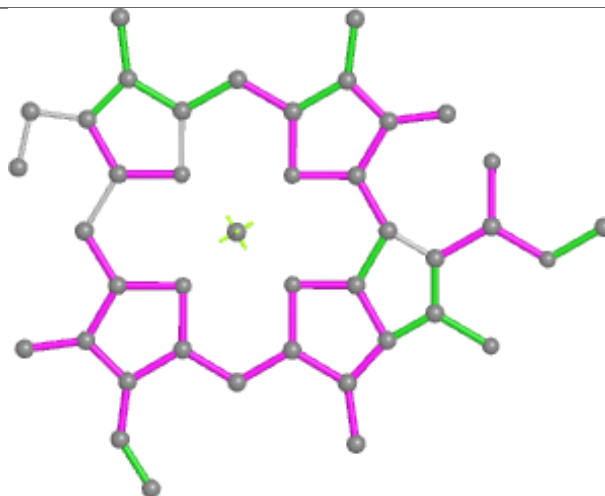
Ligand CLA 2 506



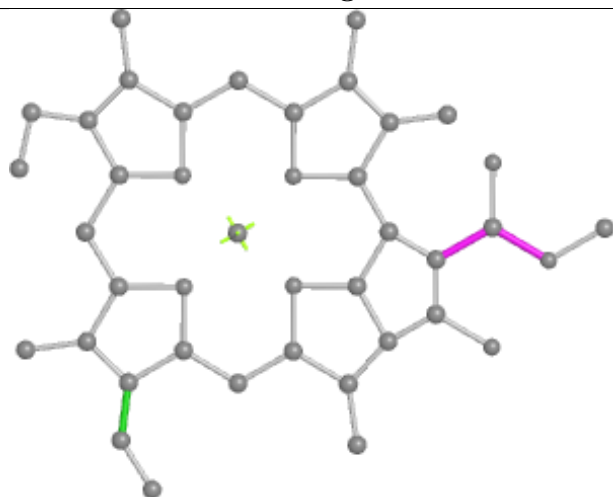
Ligand CLA 4 701



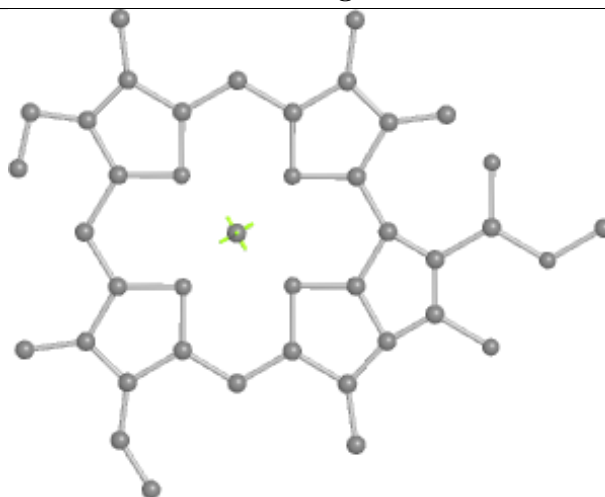
Bond lengths



Bond angles

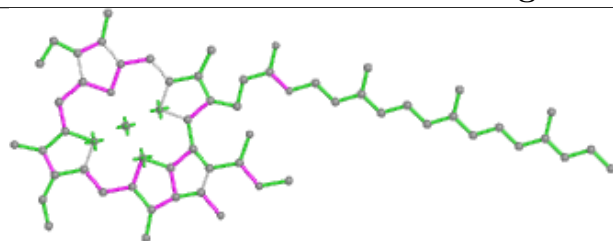


Torsions

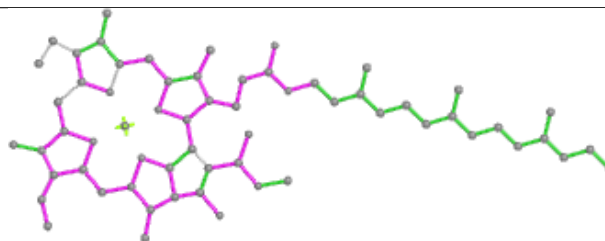


Rings

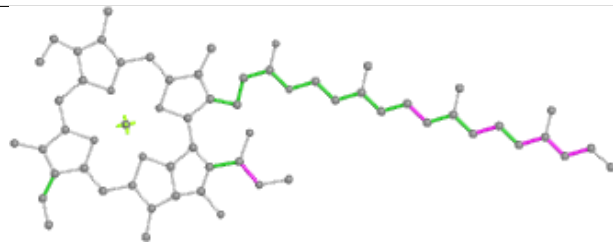
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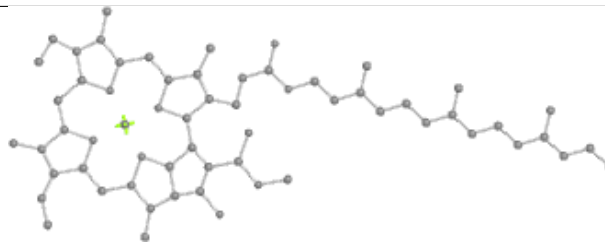
Bond lengths



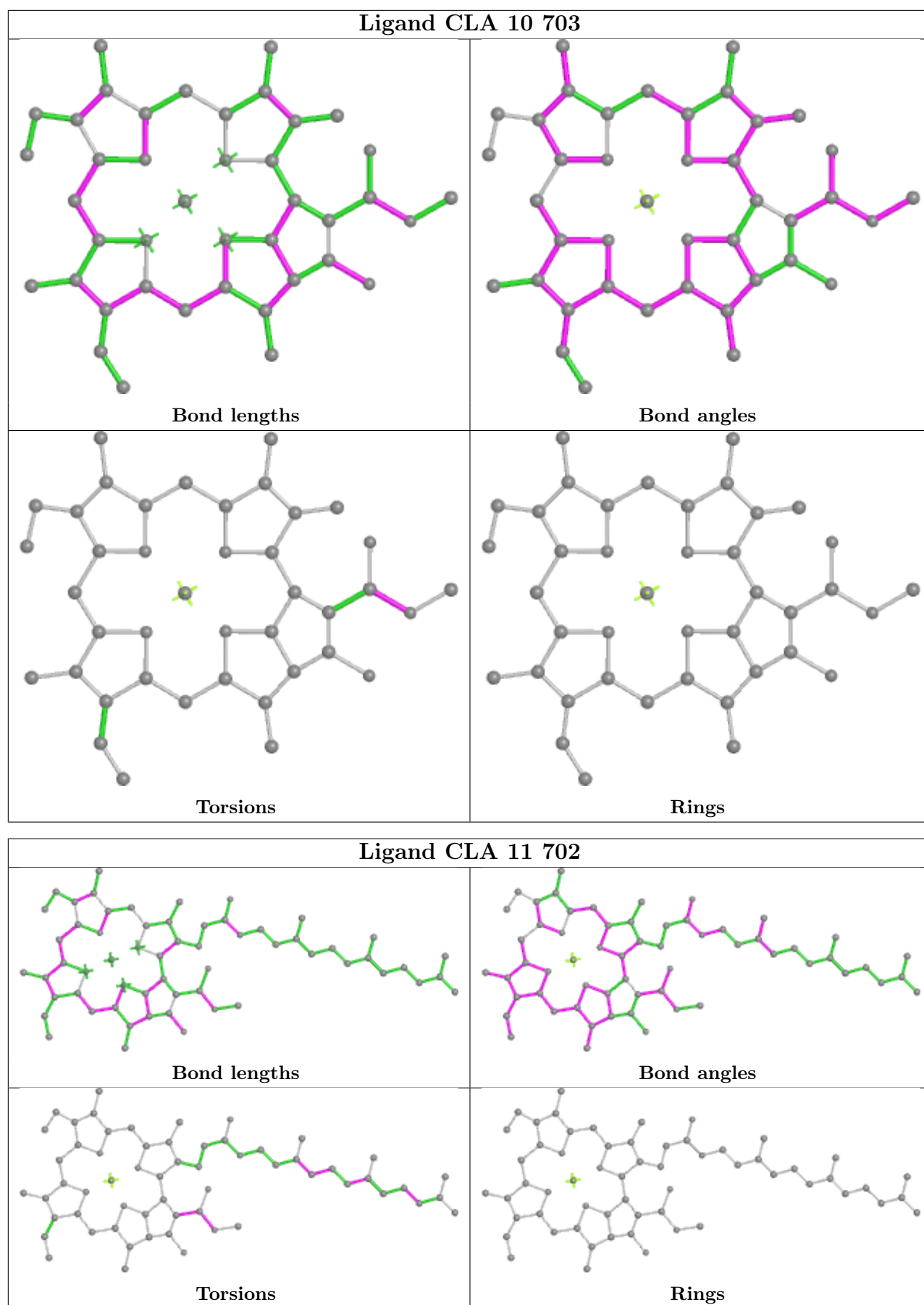
Bond angles

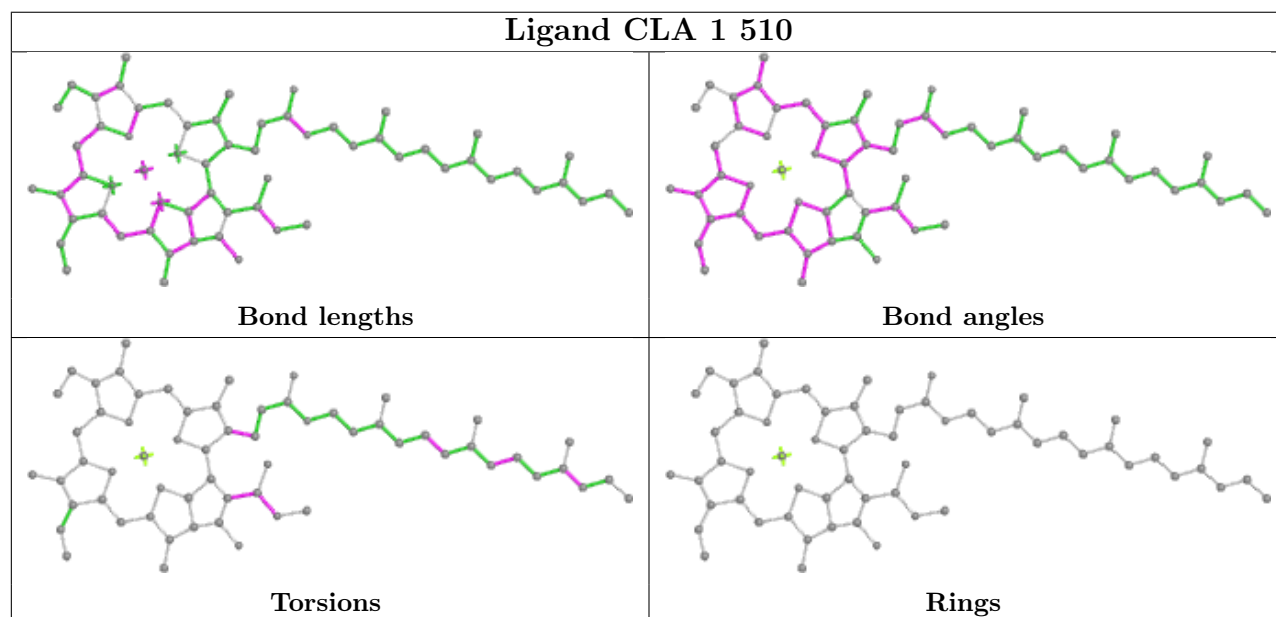
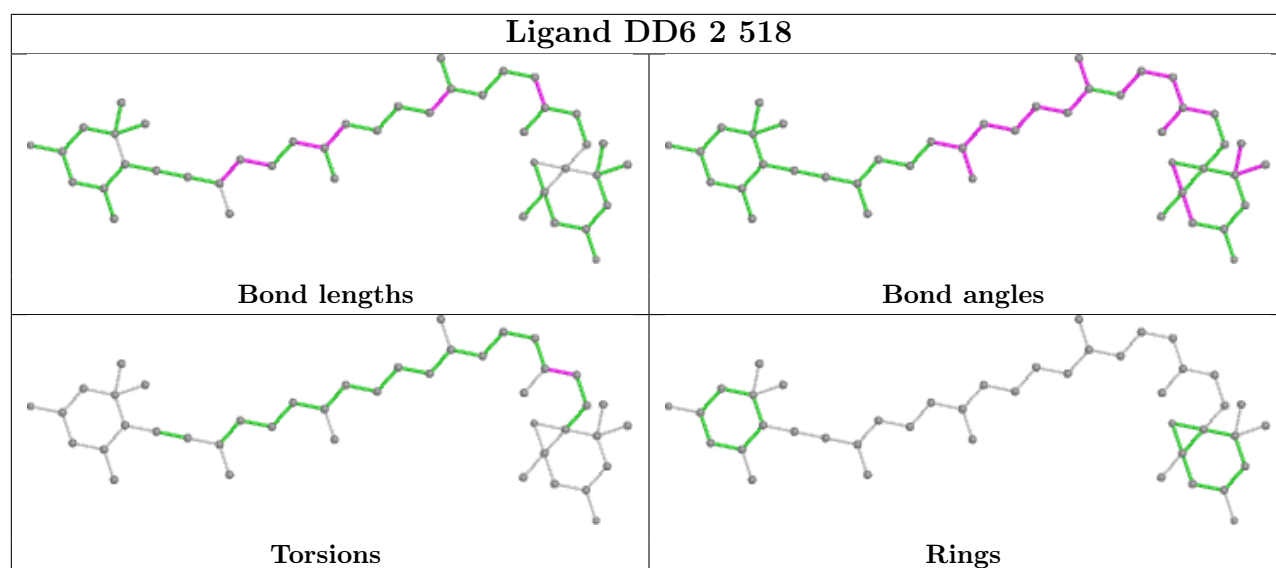


Torsions

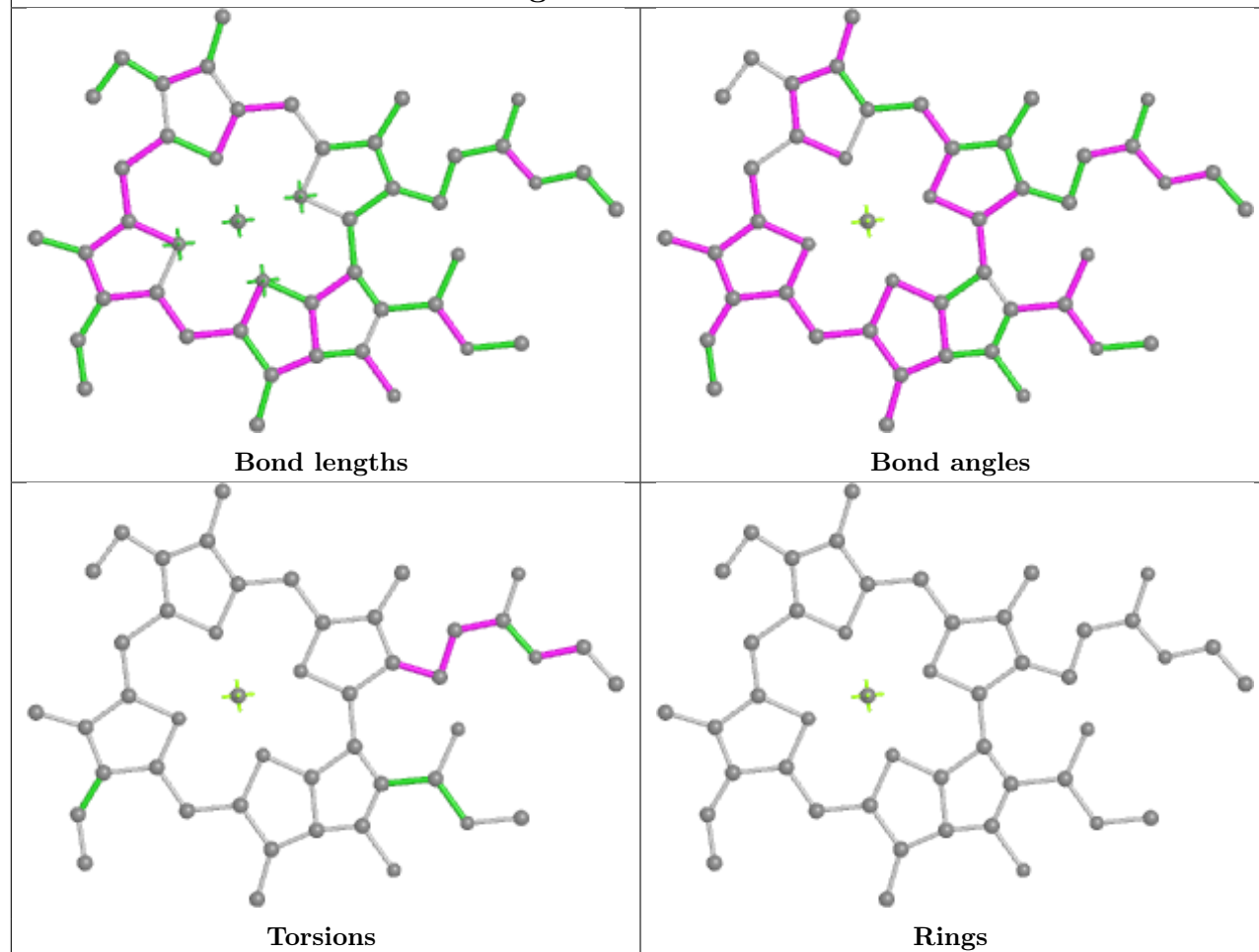


Rings

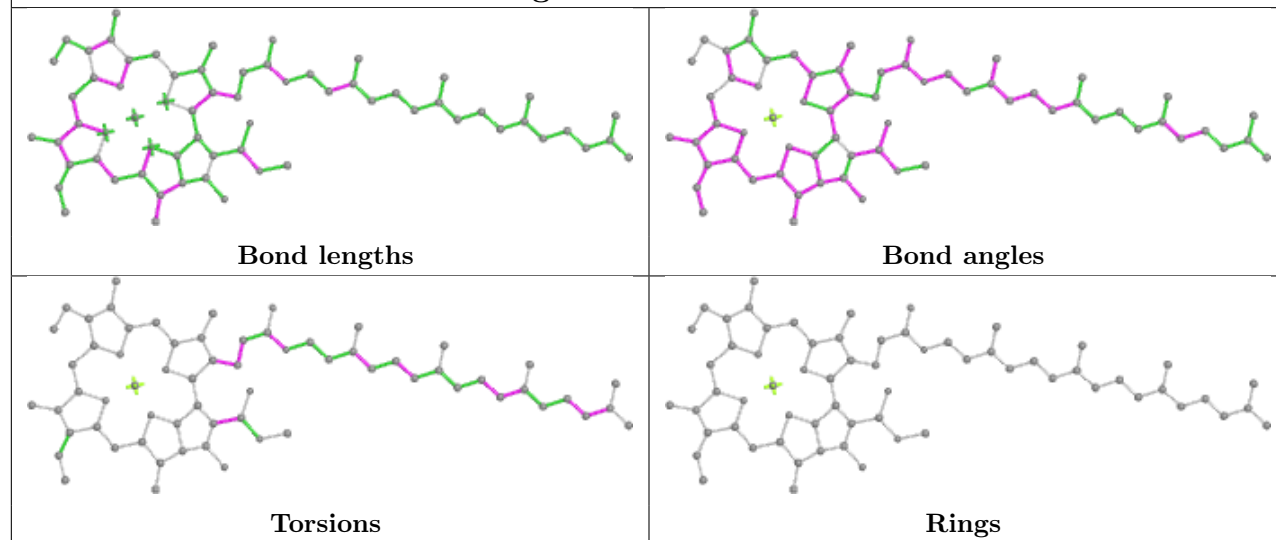




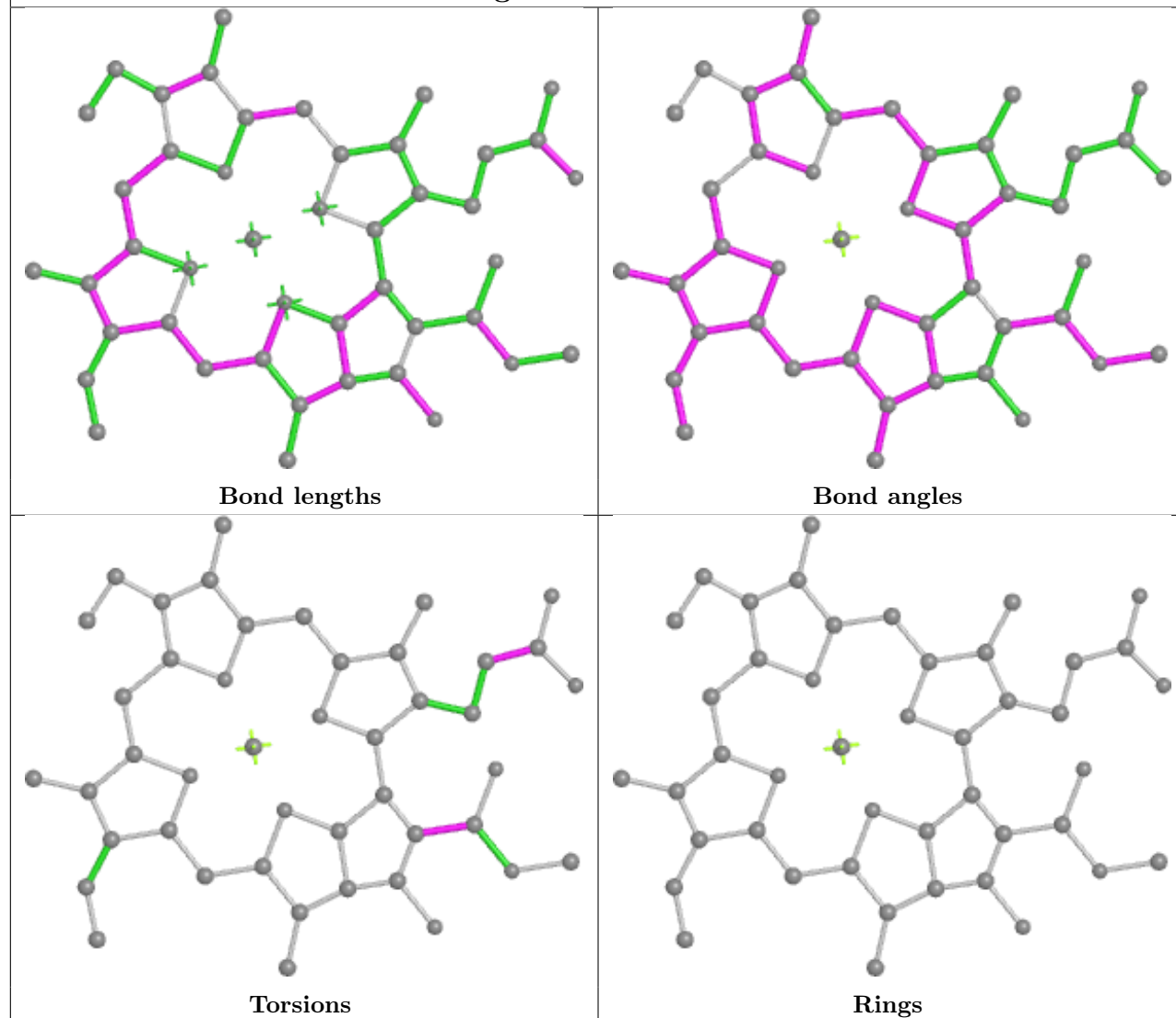
Ligand CLA 9 913



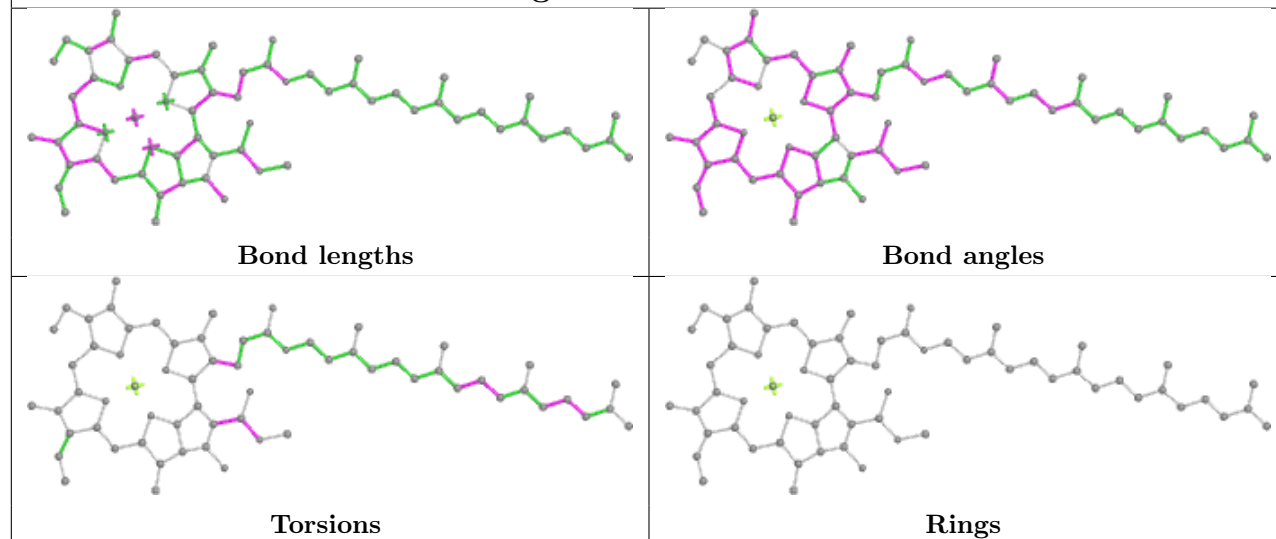
Ligand CLA B 827

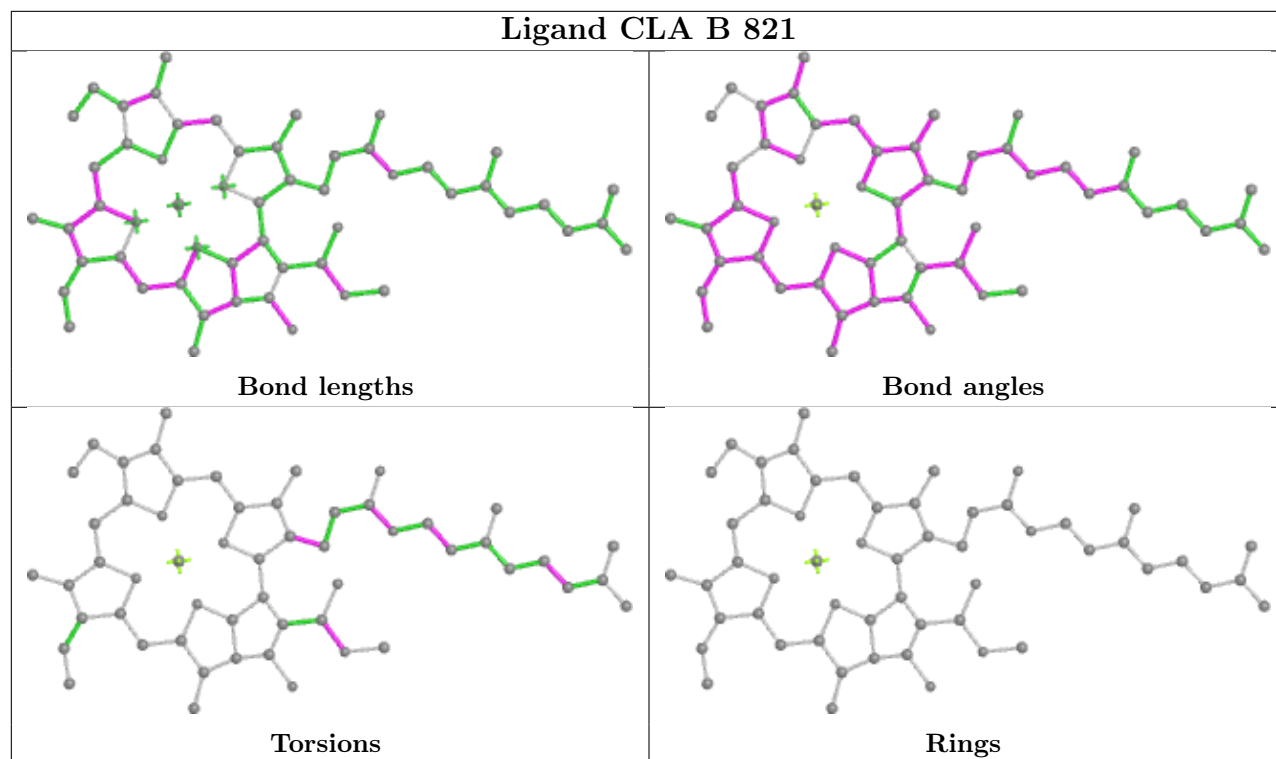
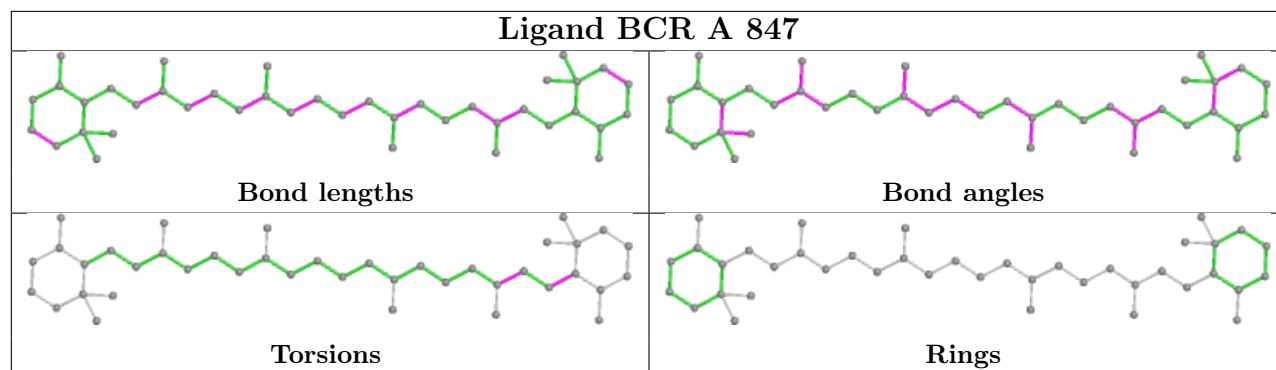


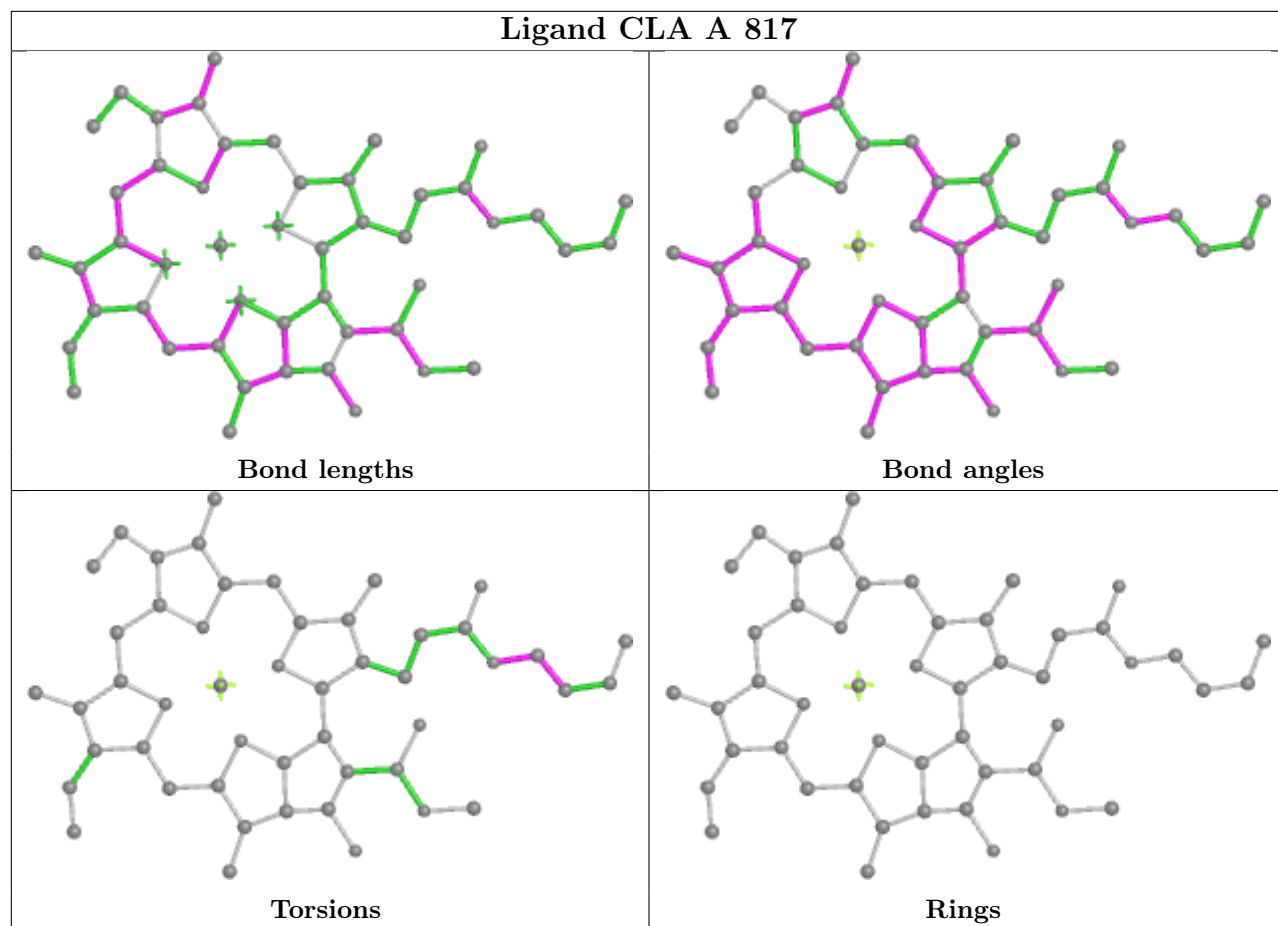
Ligand CLA 8 605



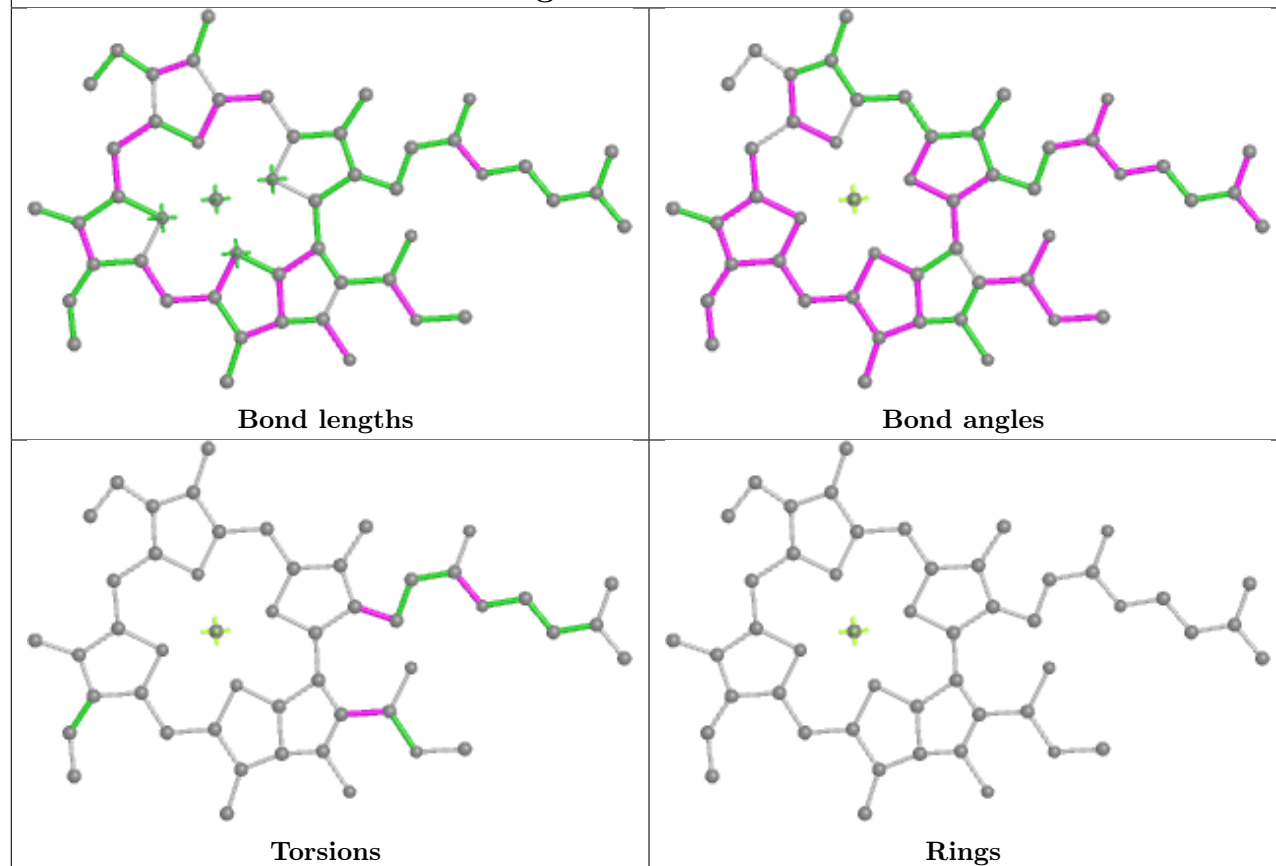
Ligand CLA B 828



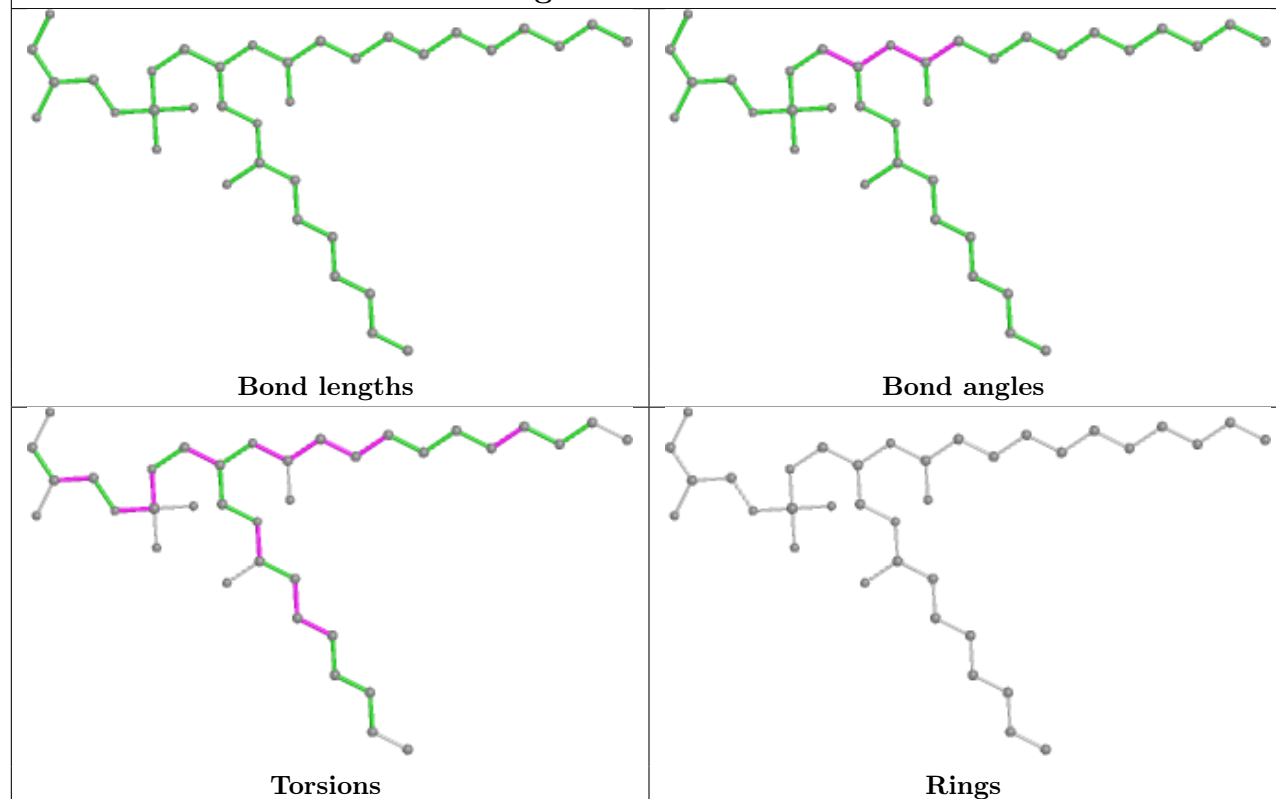


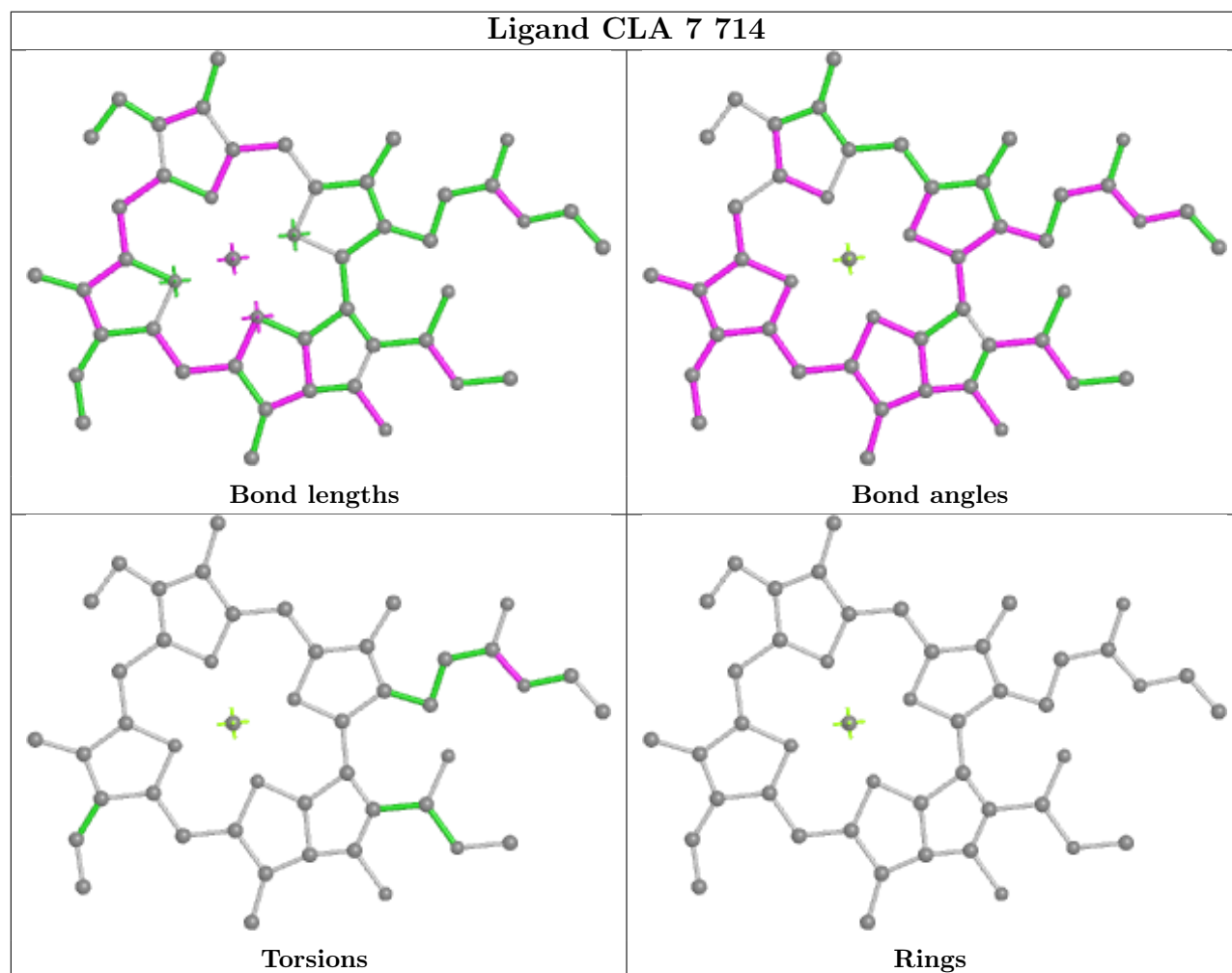
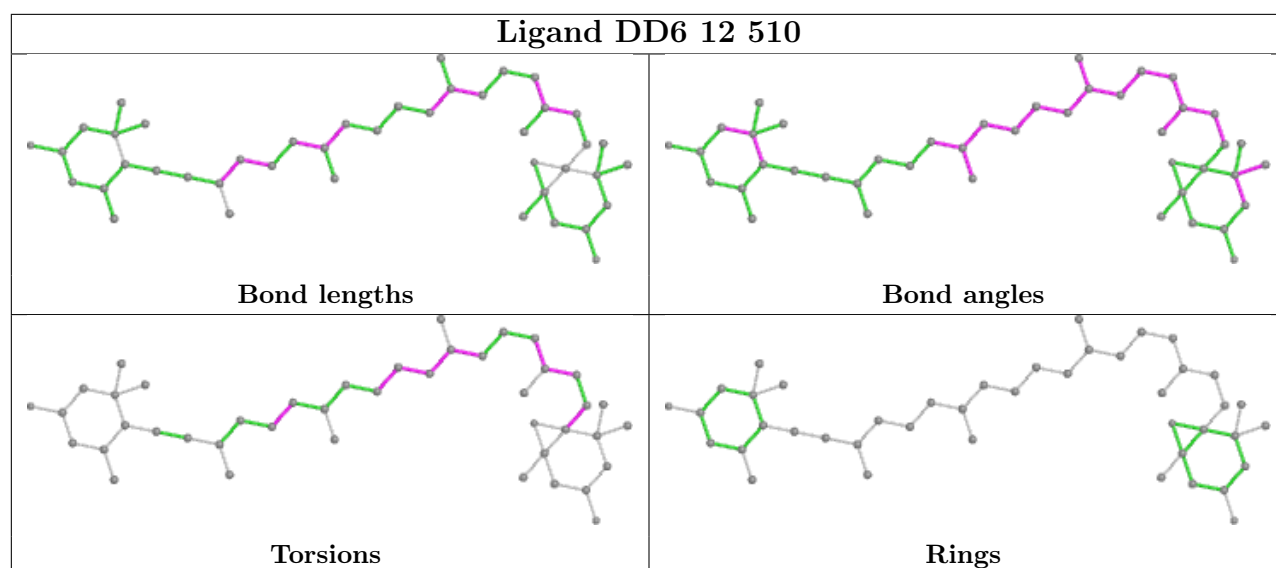


Ligand CLA 5 704

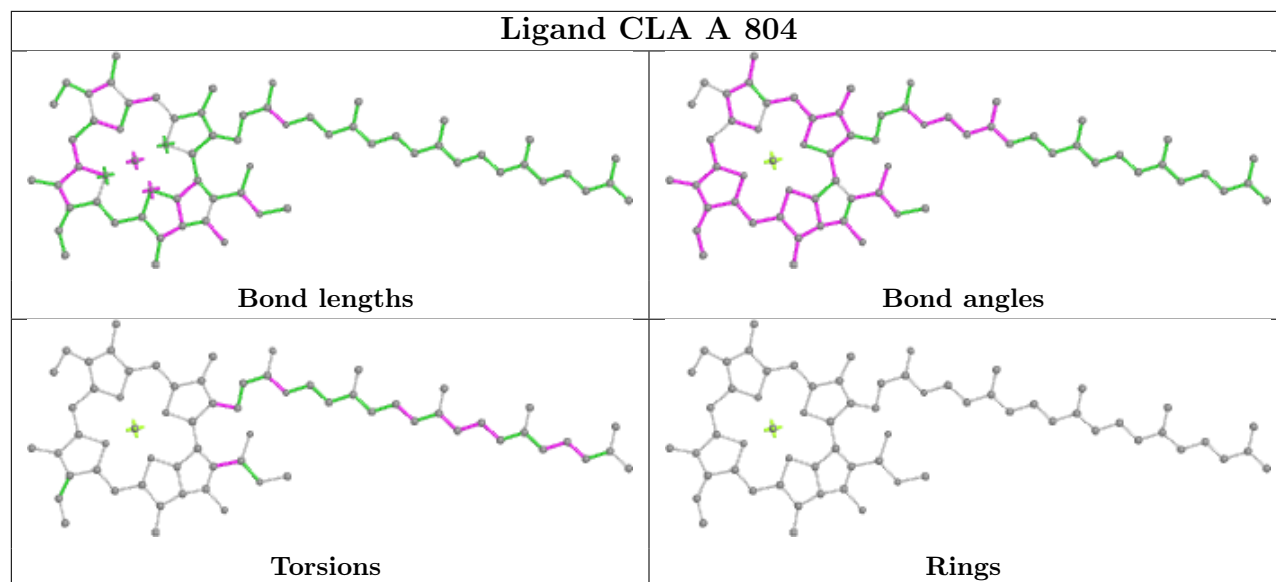


Ligand LHG 1 521

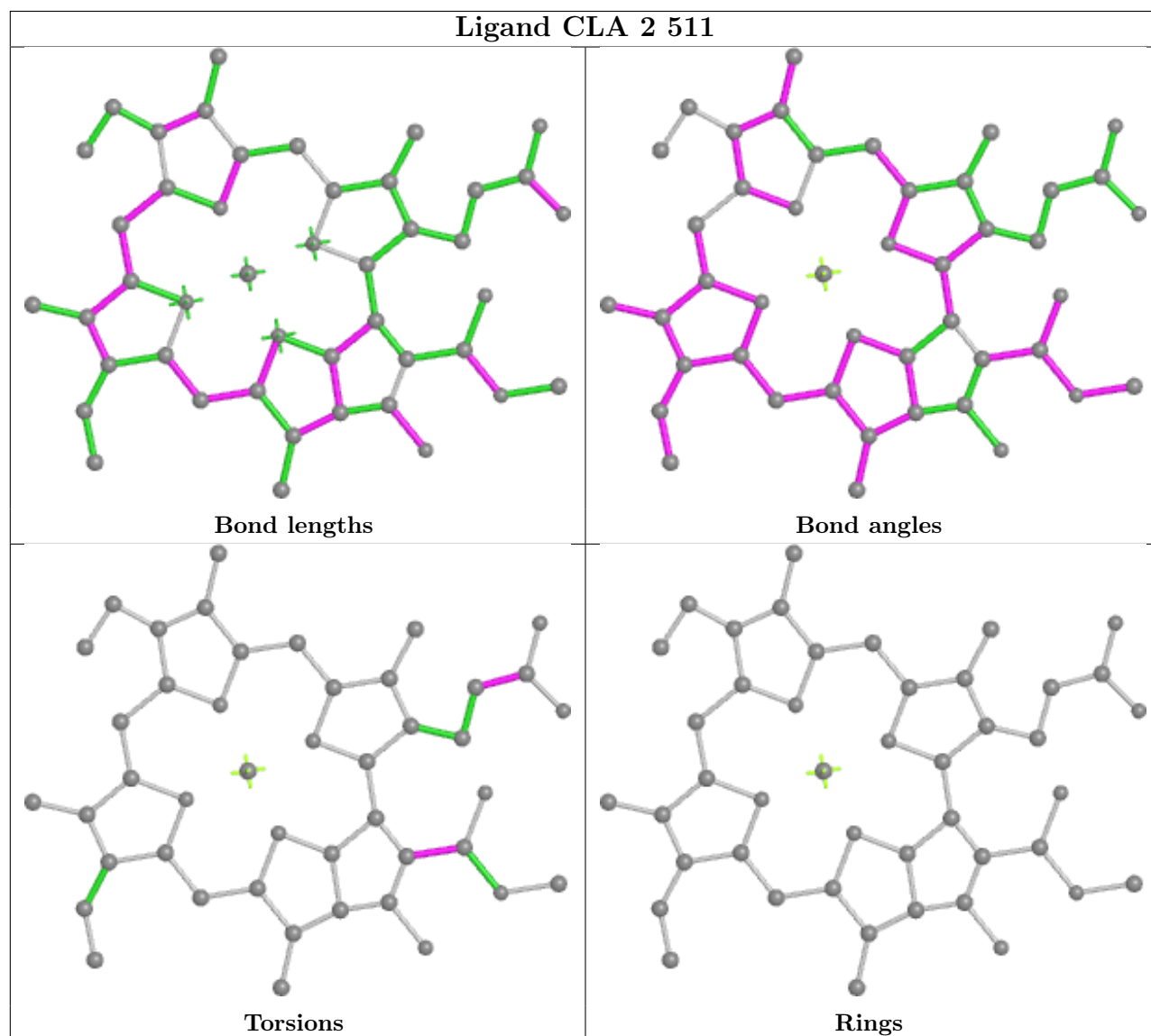




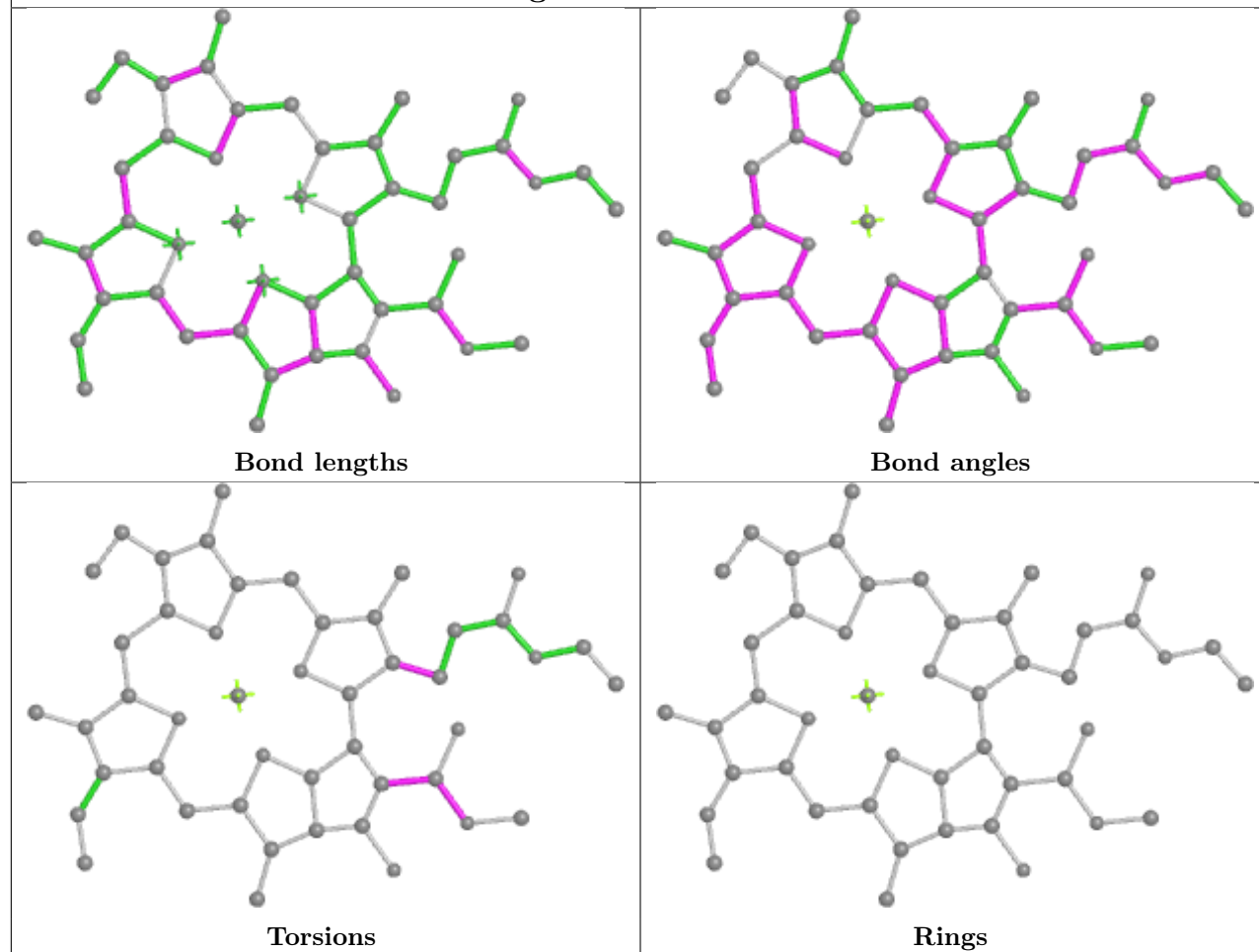
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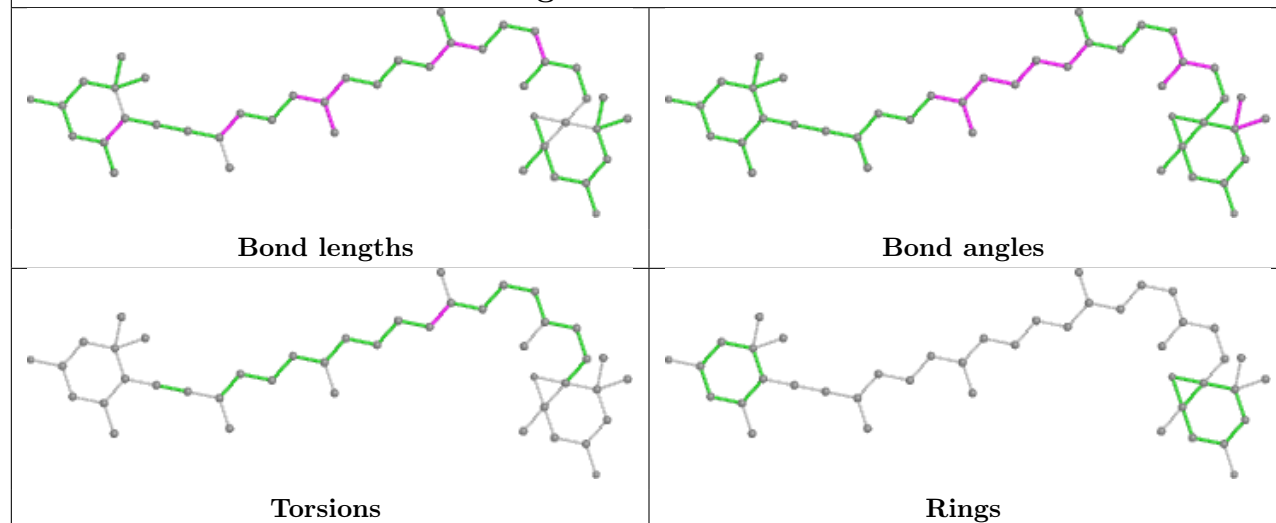
Ligand CLA 2 511



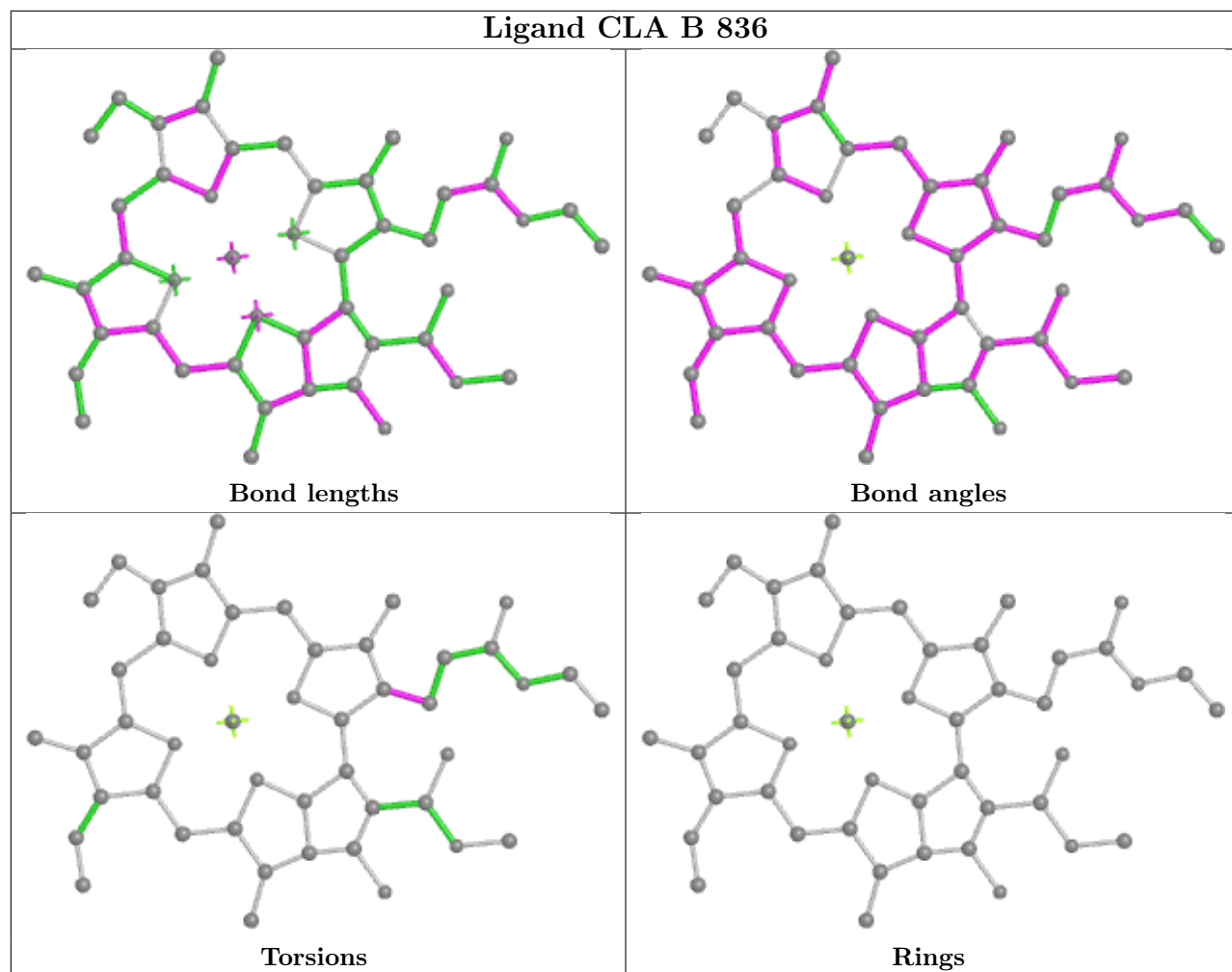
Ligand CLA 8 603



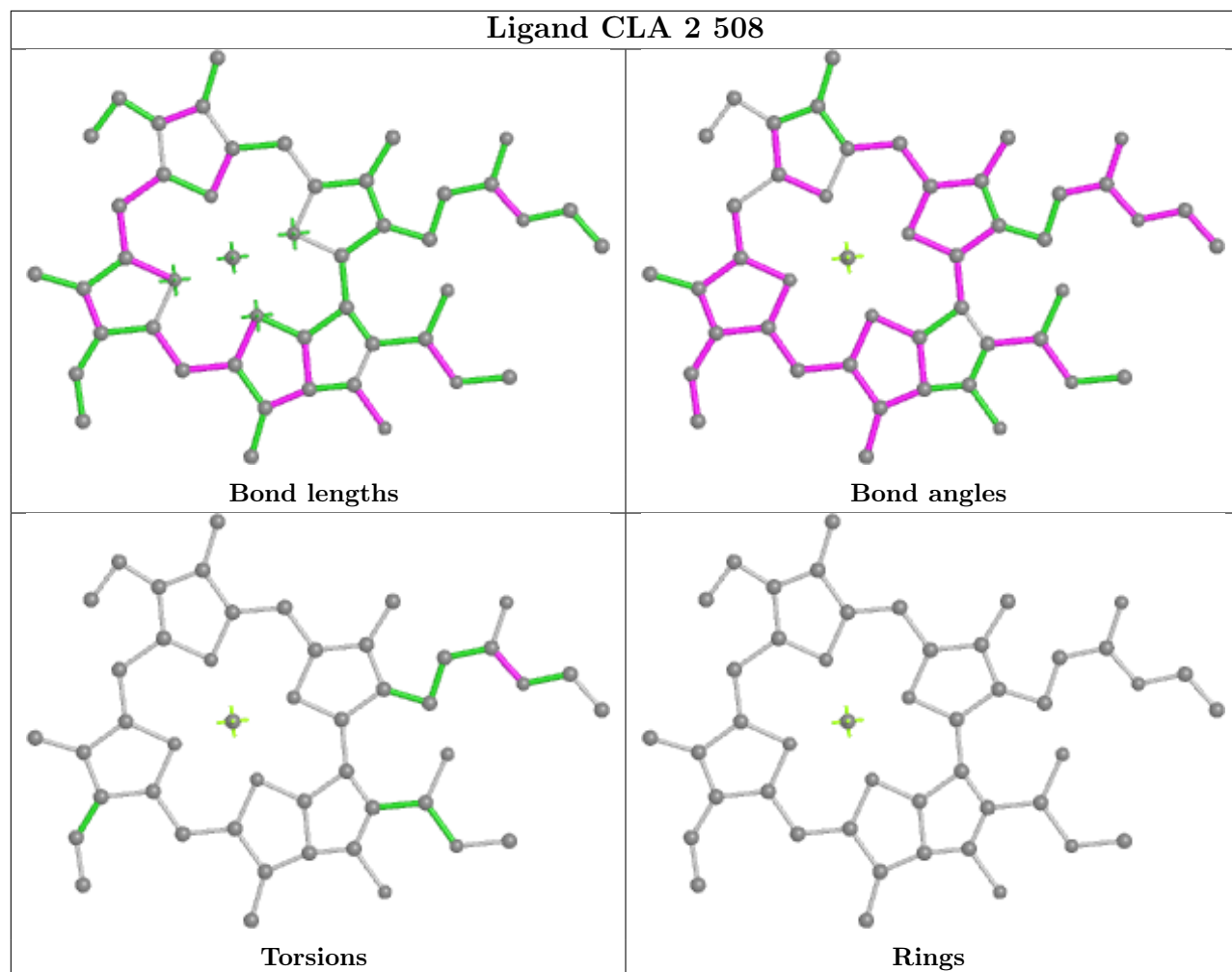
Ligand DD6 7 716

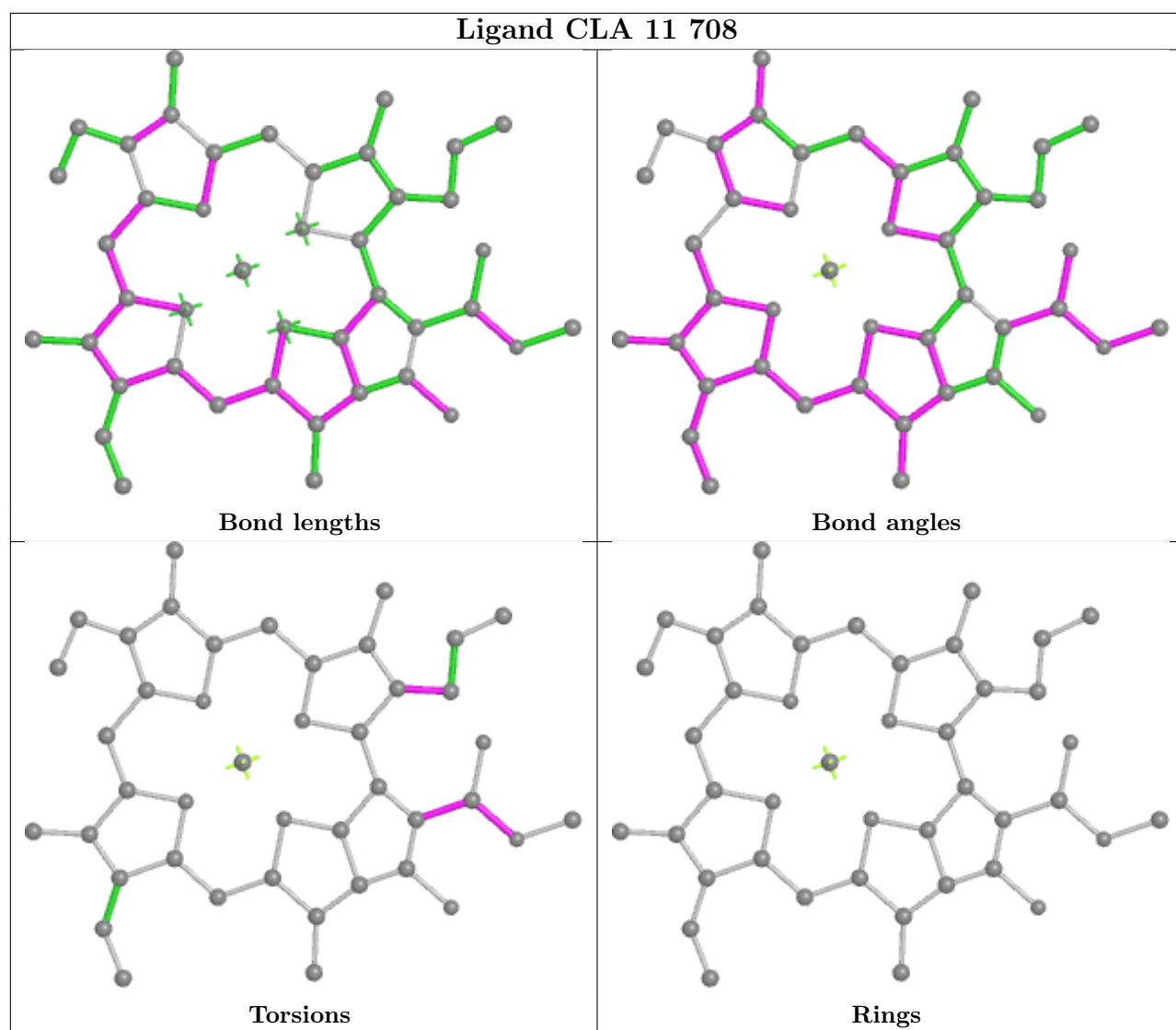


Ligand CLA B 836

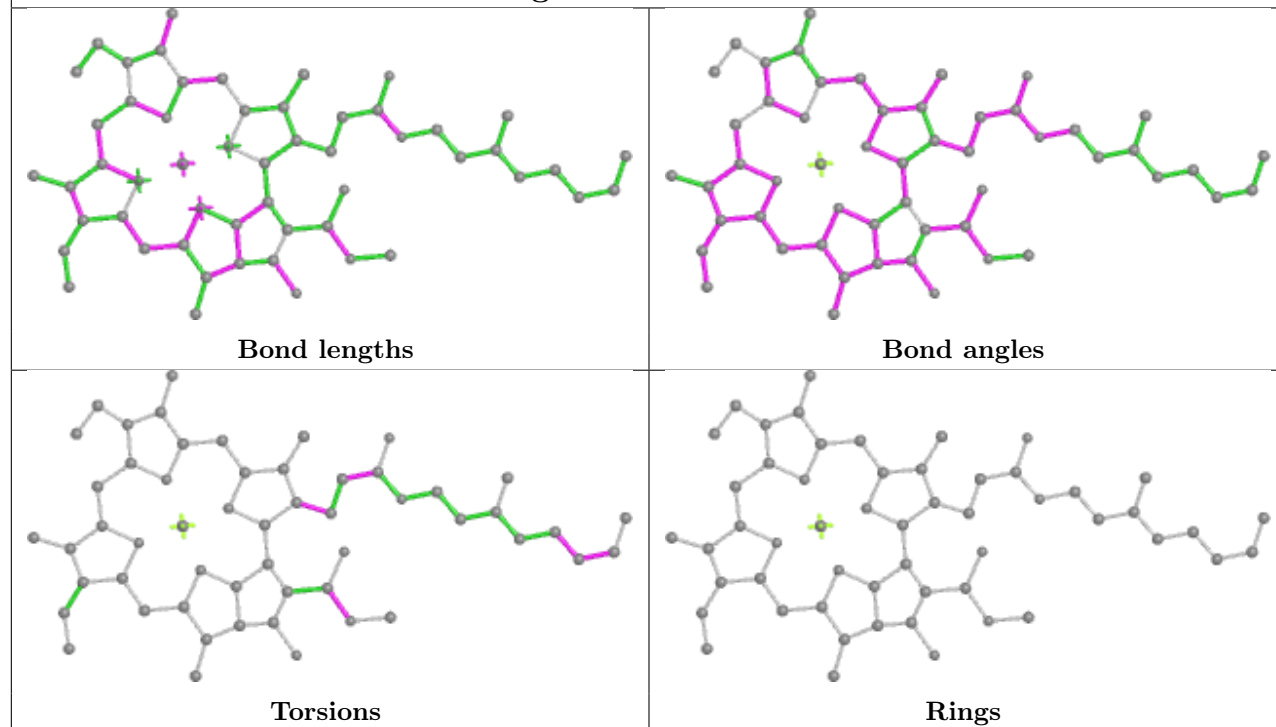


Ligand CLA 2 508

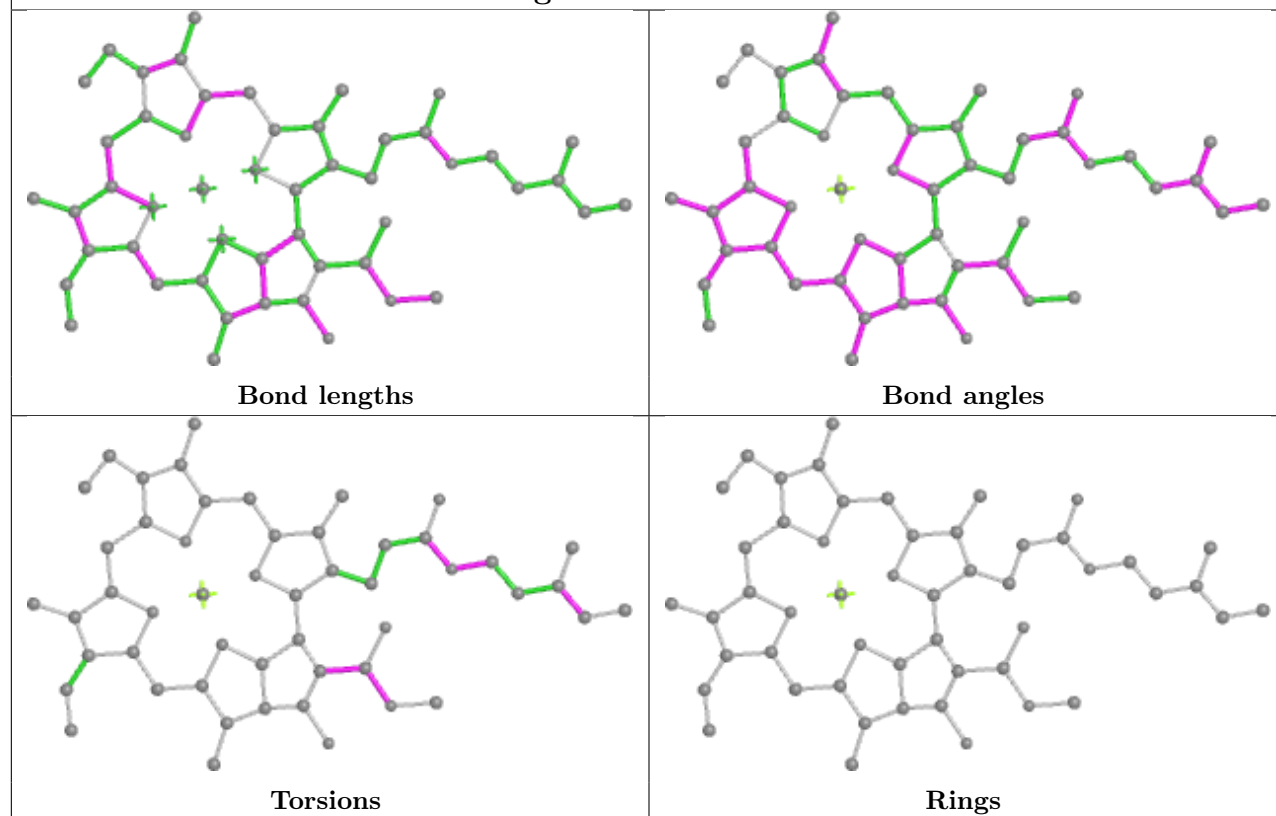




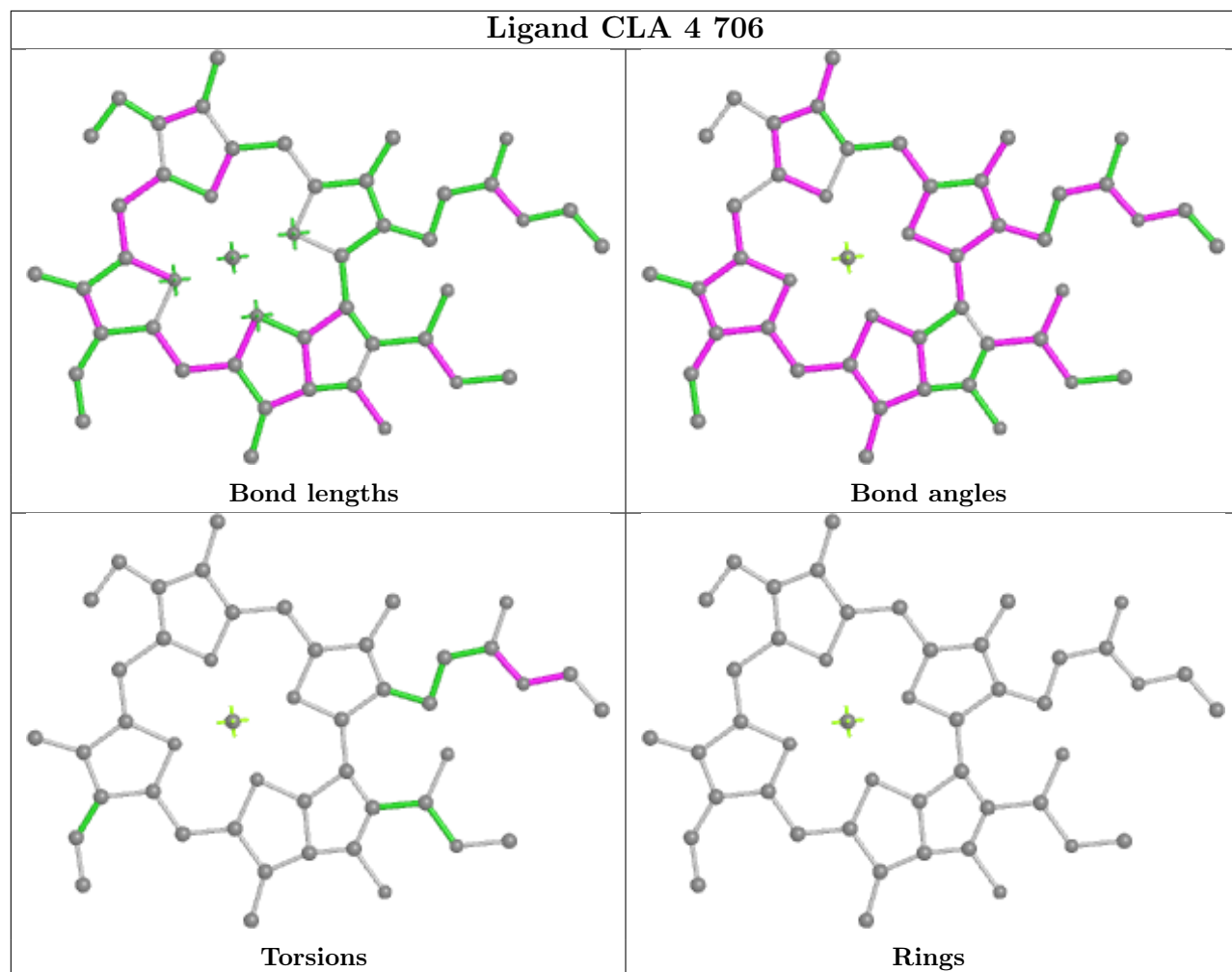
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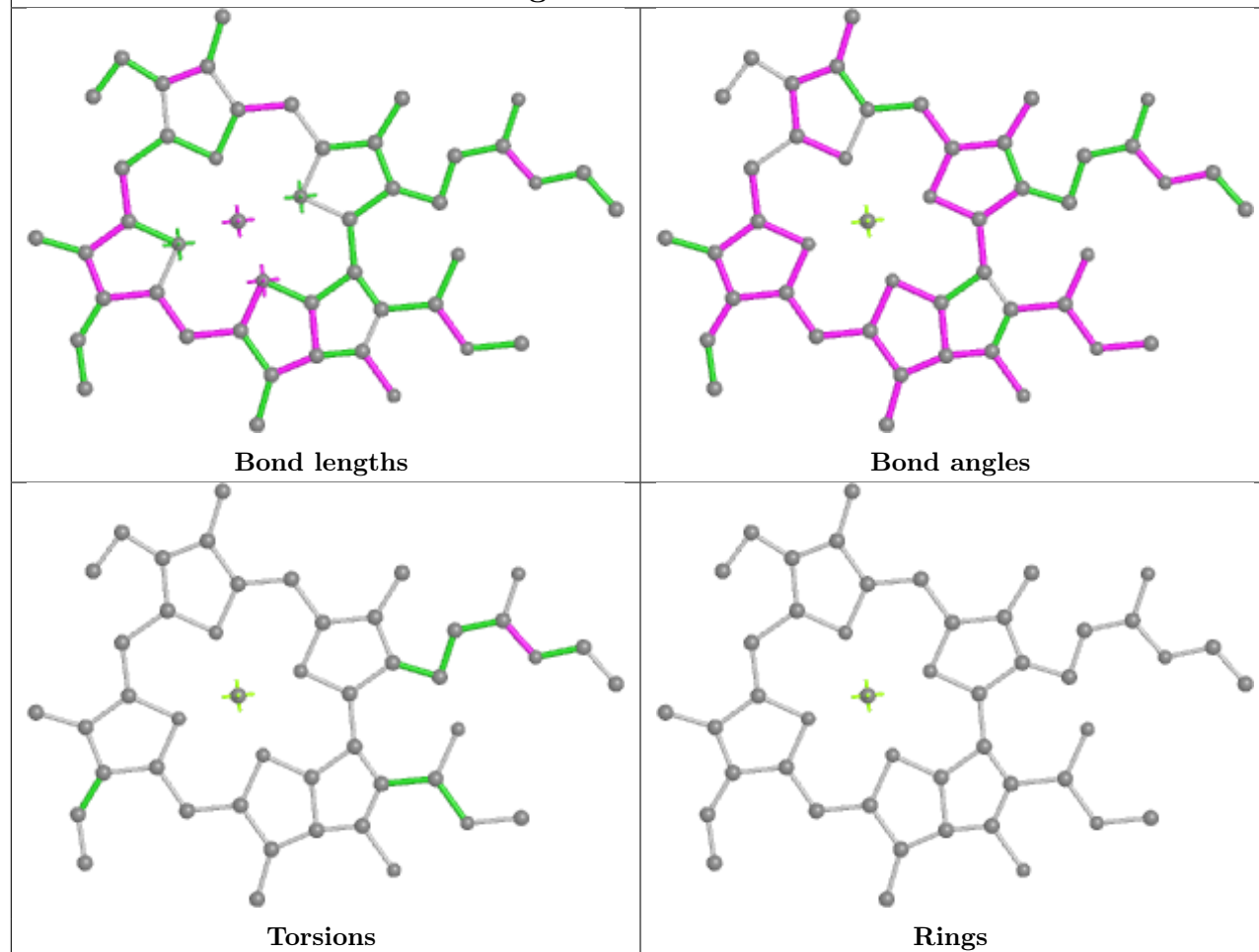
Ligand CLA F 401



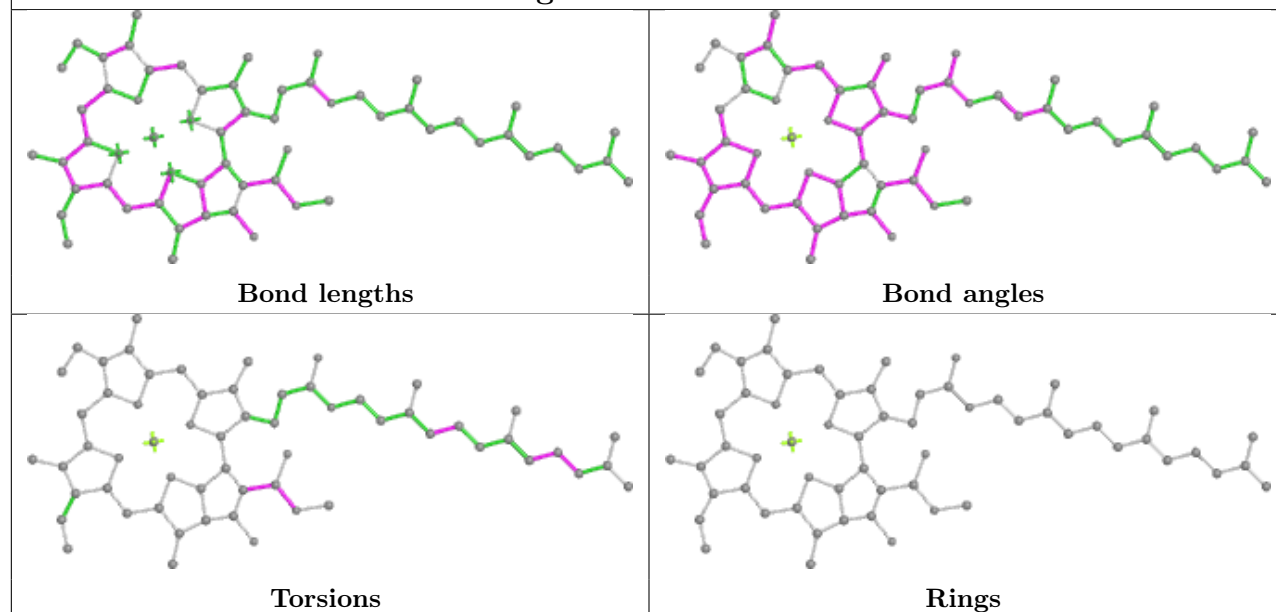
Ligand CLA 4 706



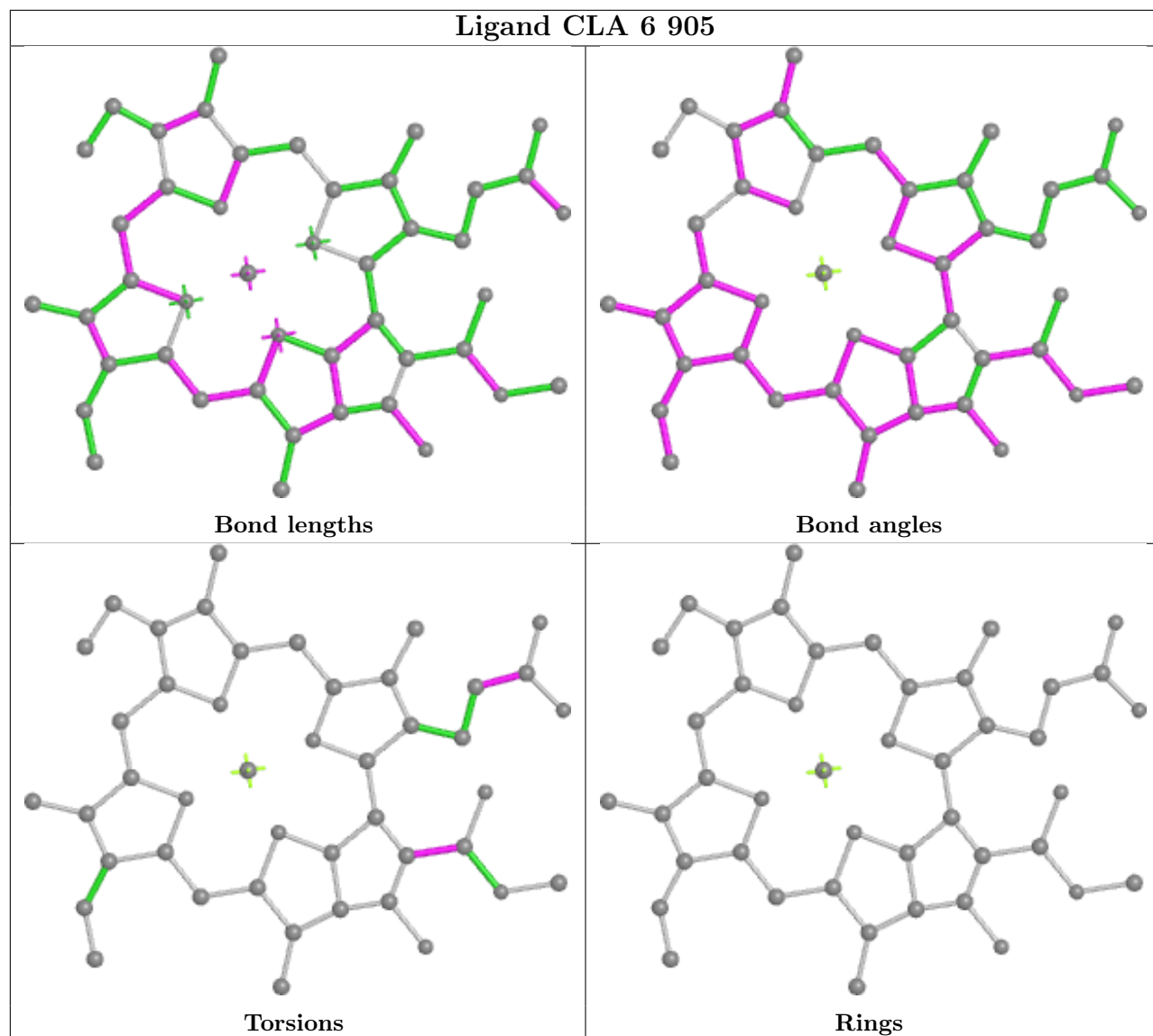
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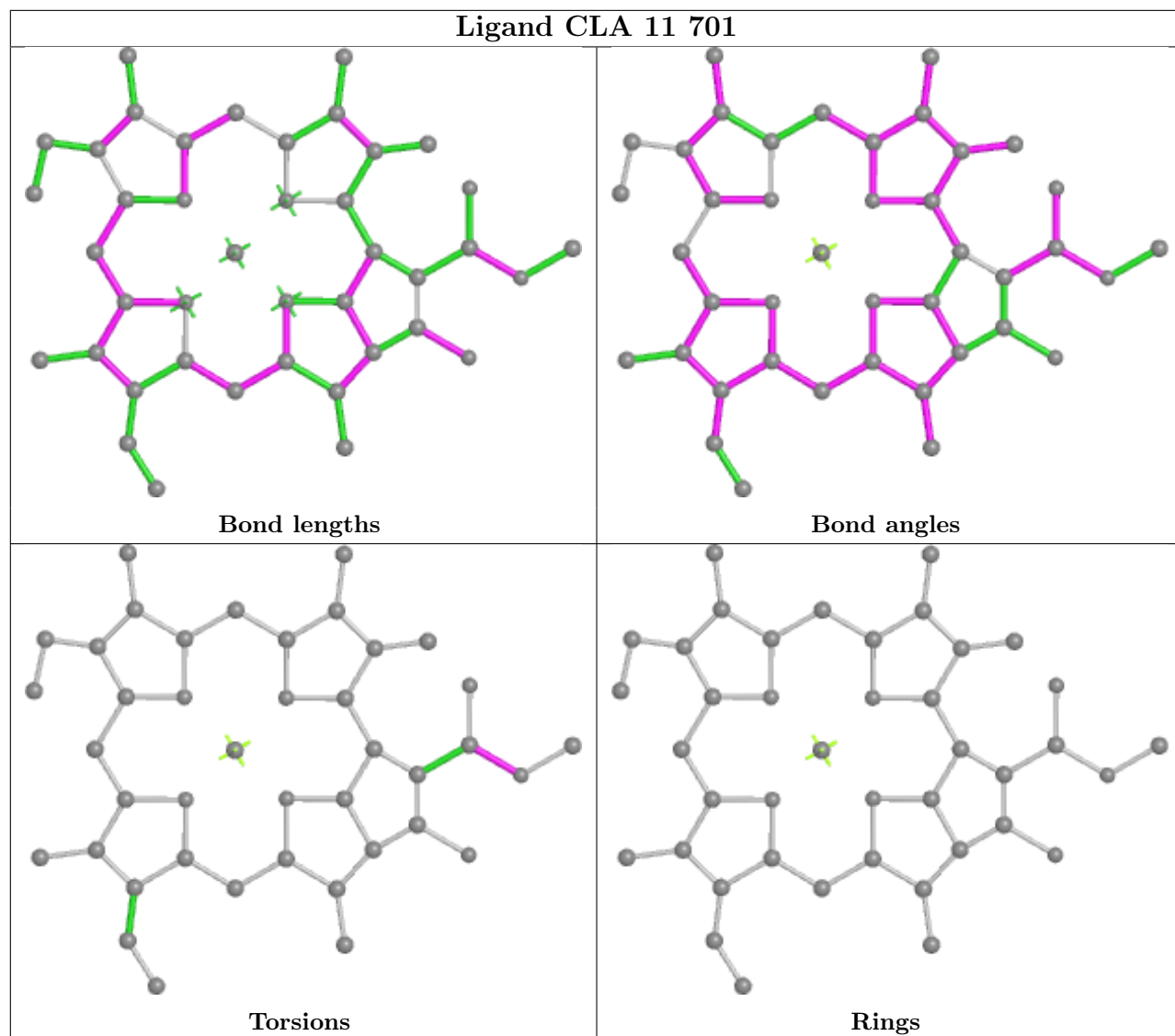


Ligand CLA 5 702

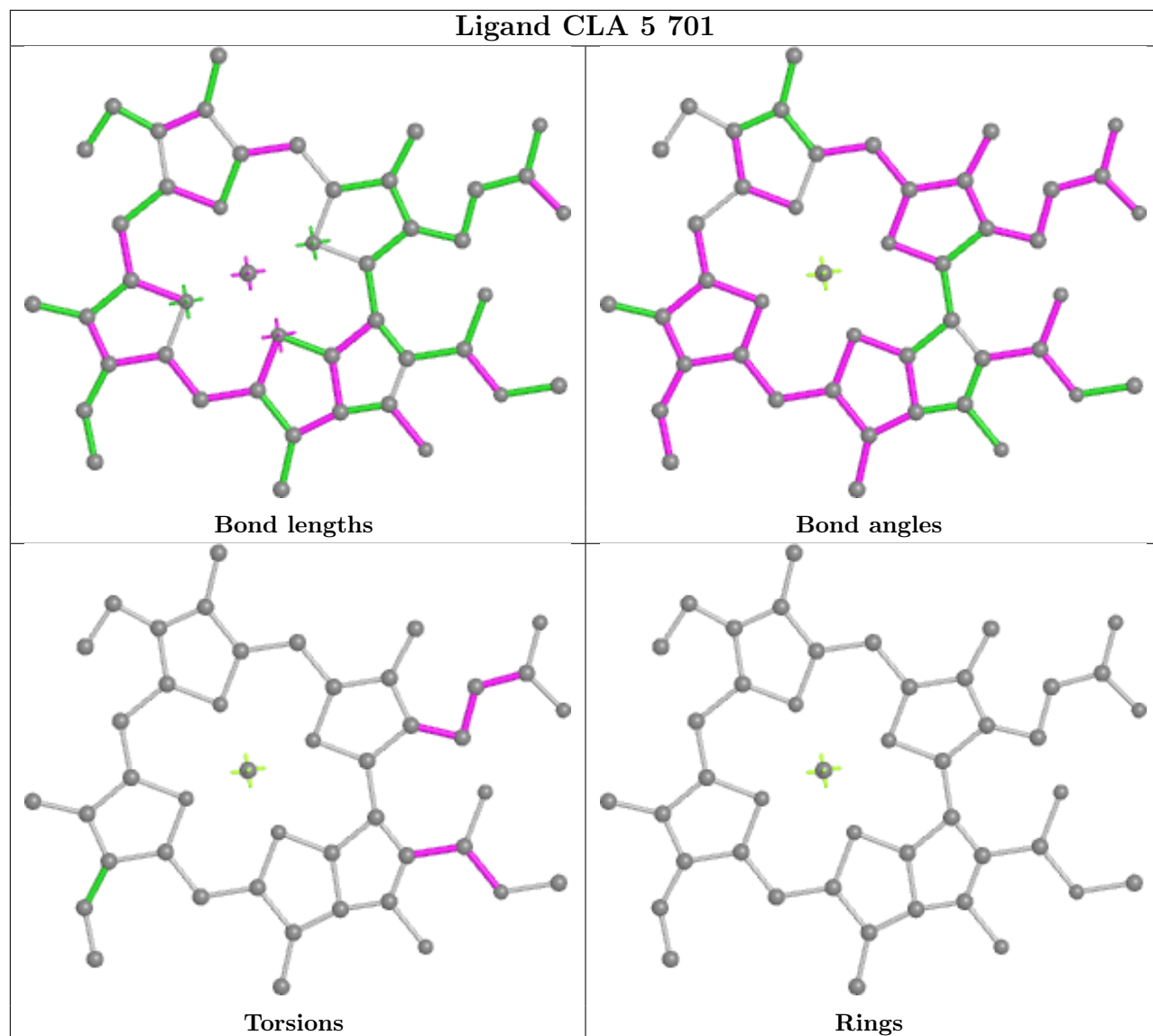


Ligand CLA 6 905

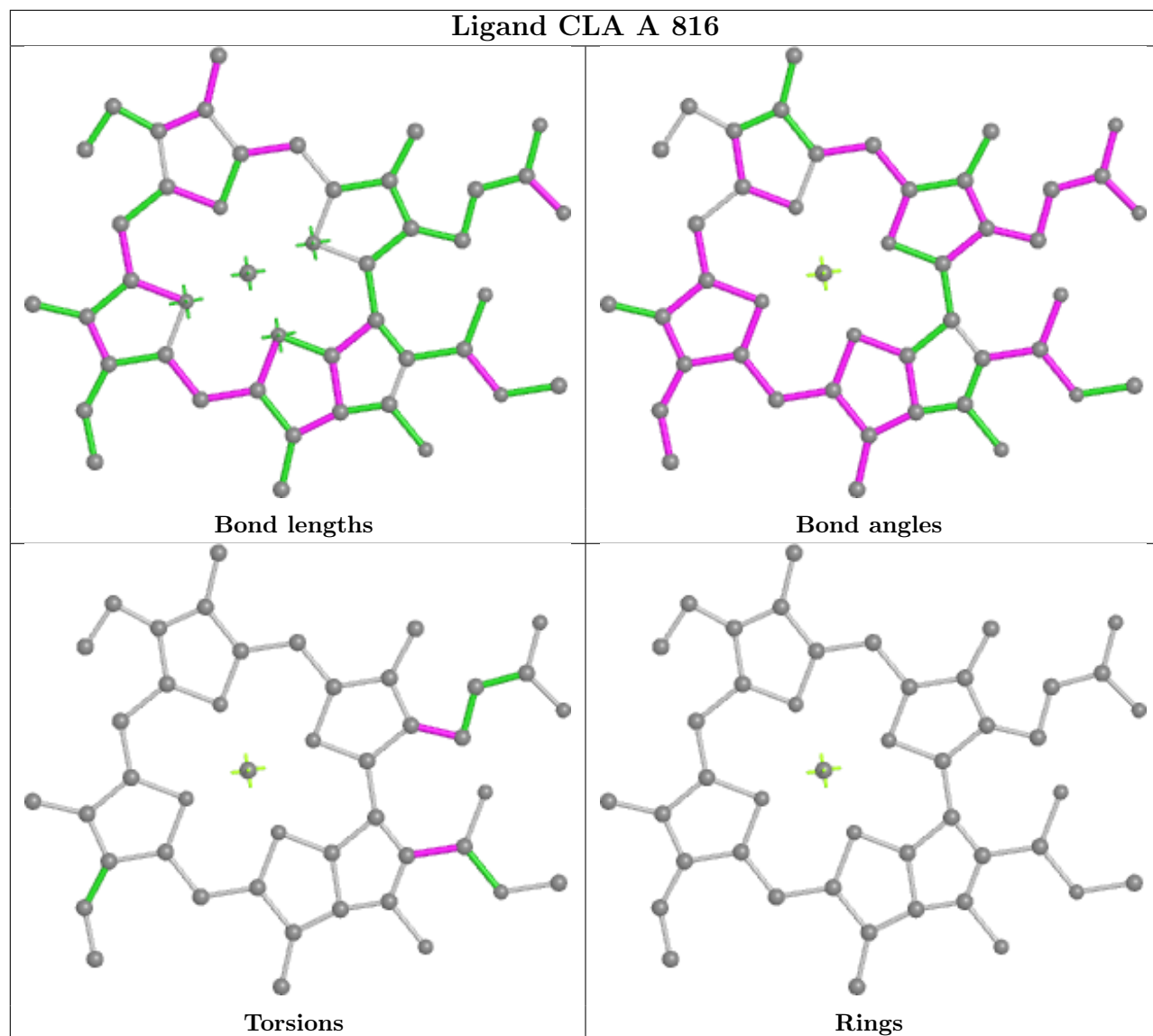




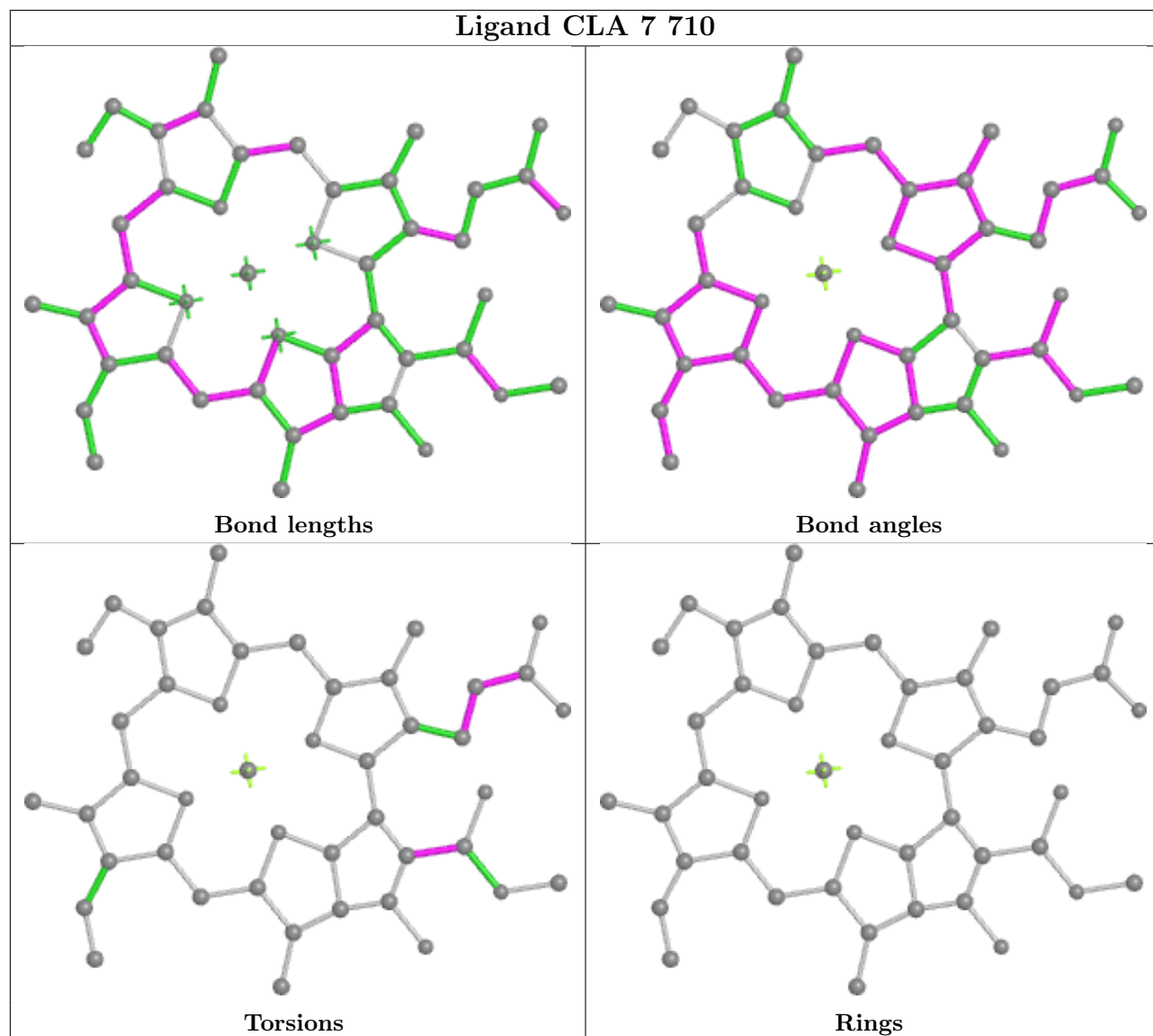
Ligand CLA 5 701

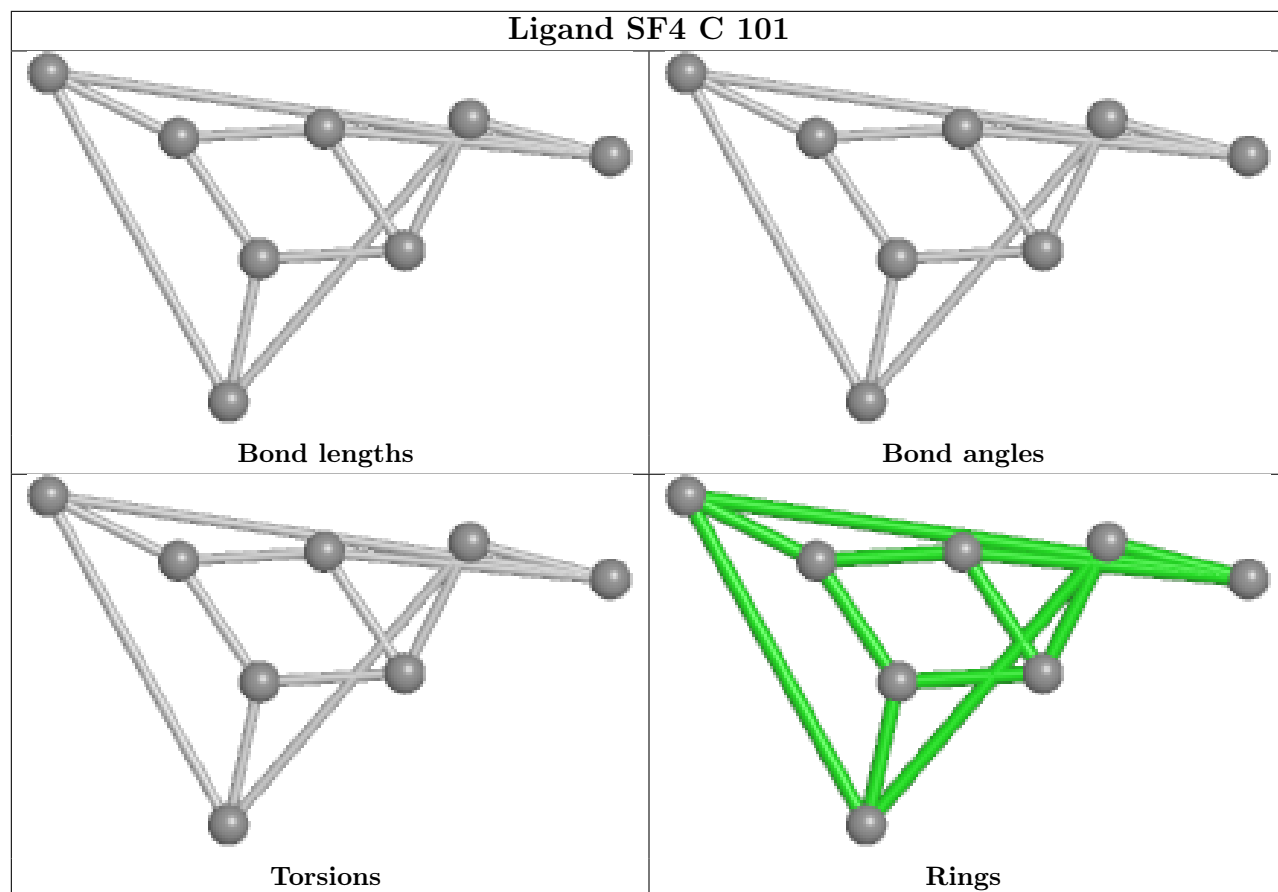


Ligand CLA A 816

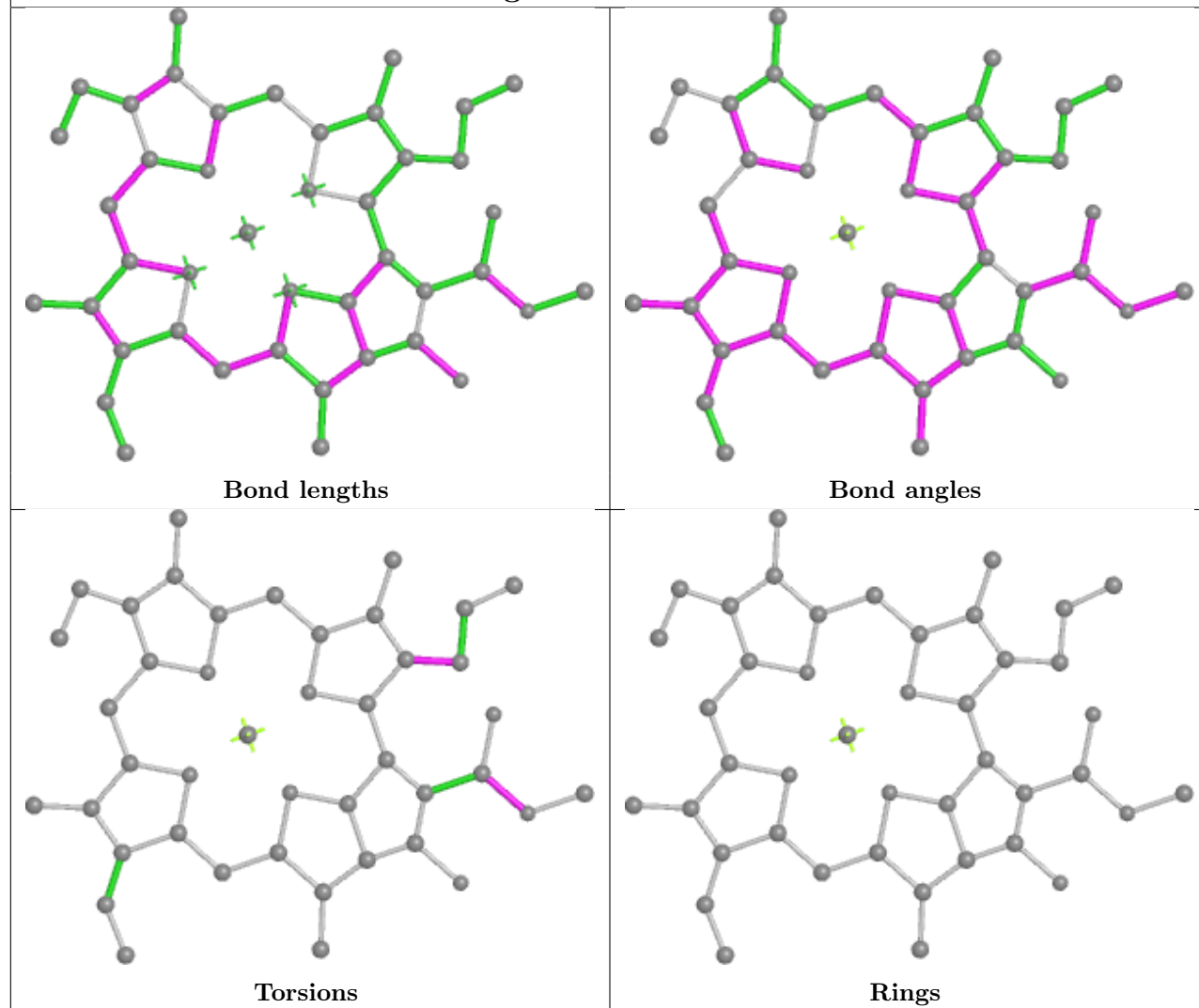


Ligand CLA 7 710

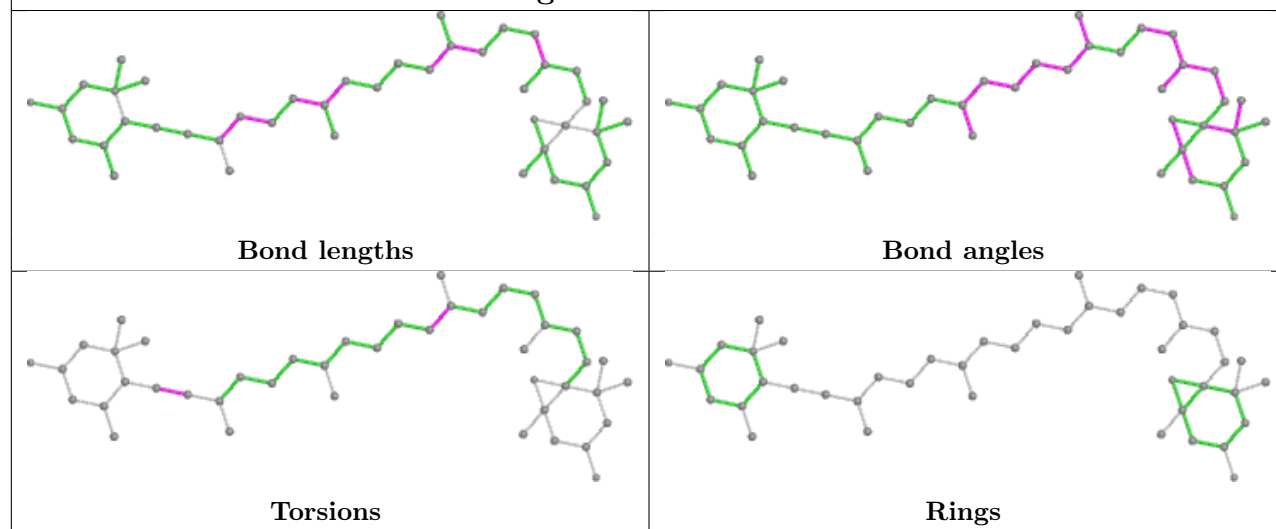




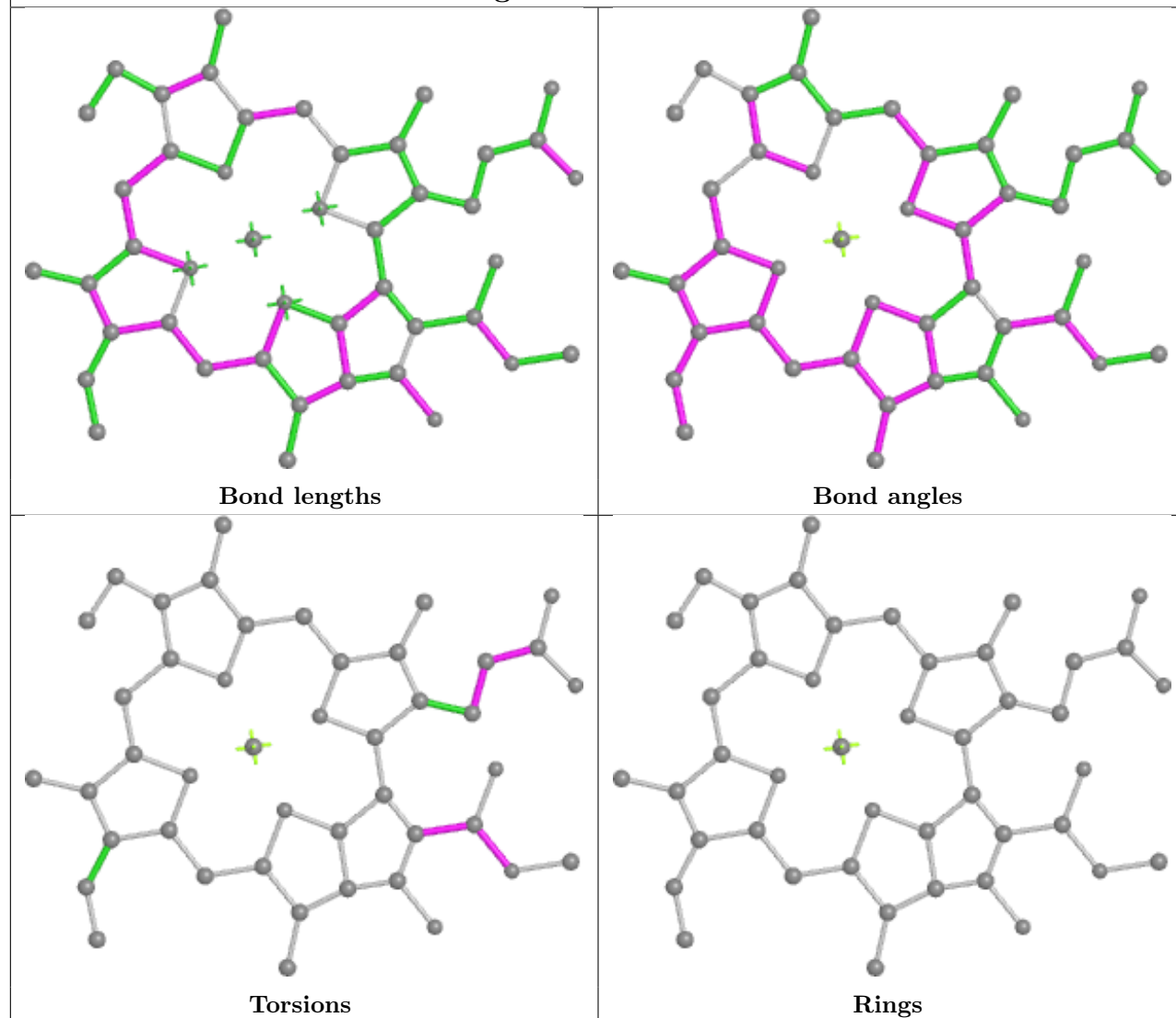
Ligand CLA 2 510



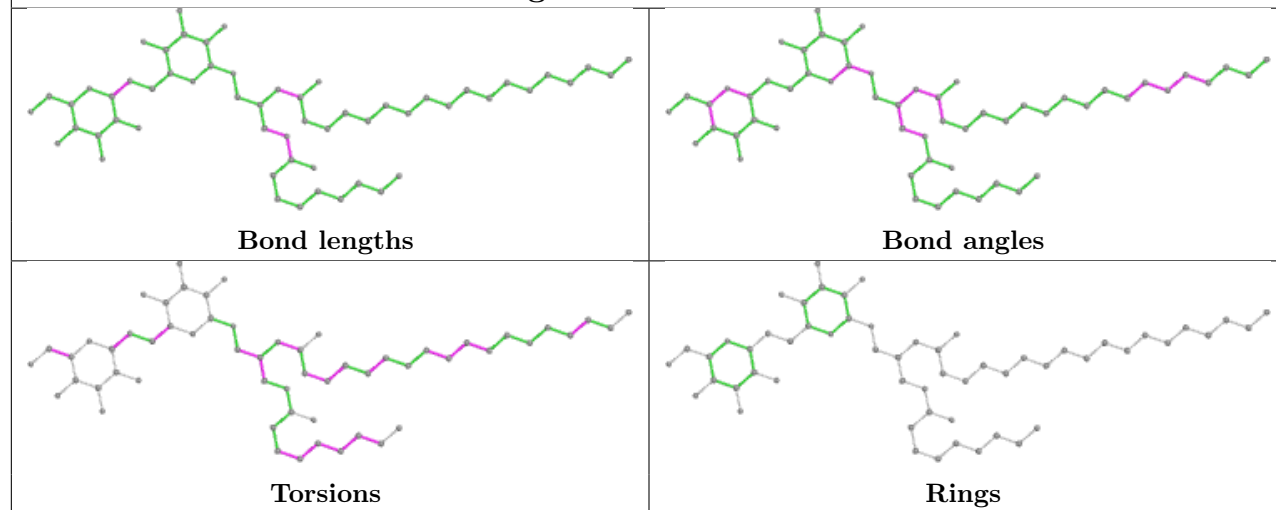
Ligand DD6 1 519



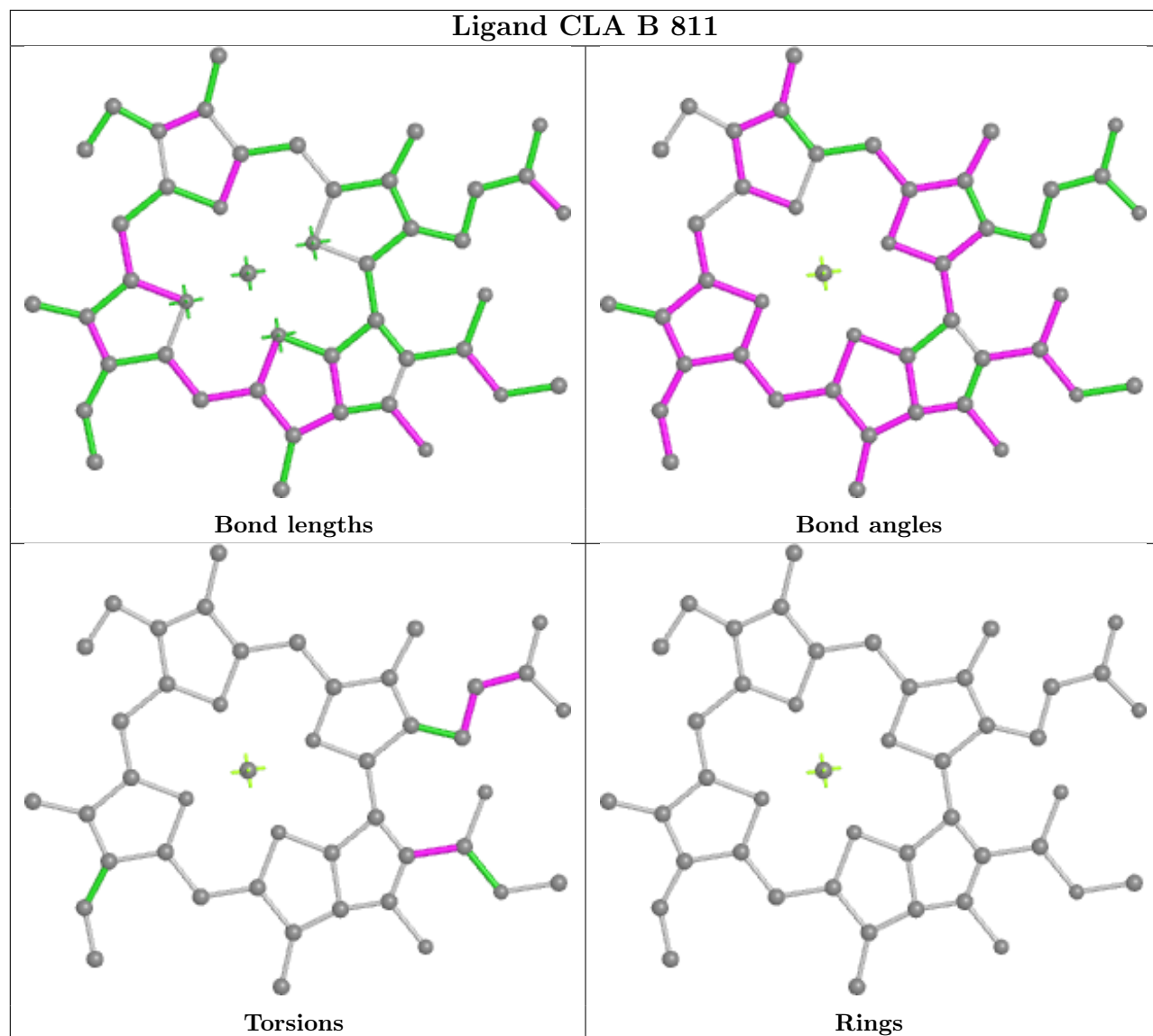
Ligand CLA 4 710



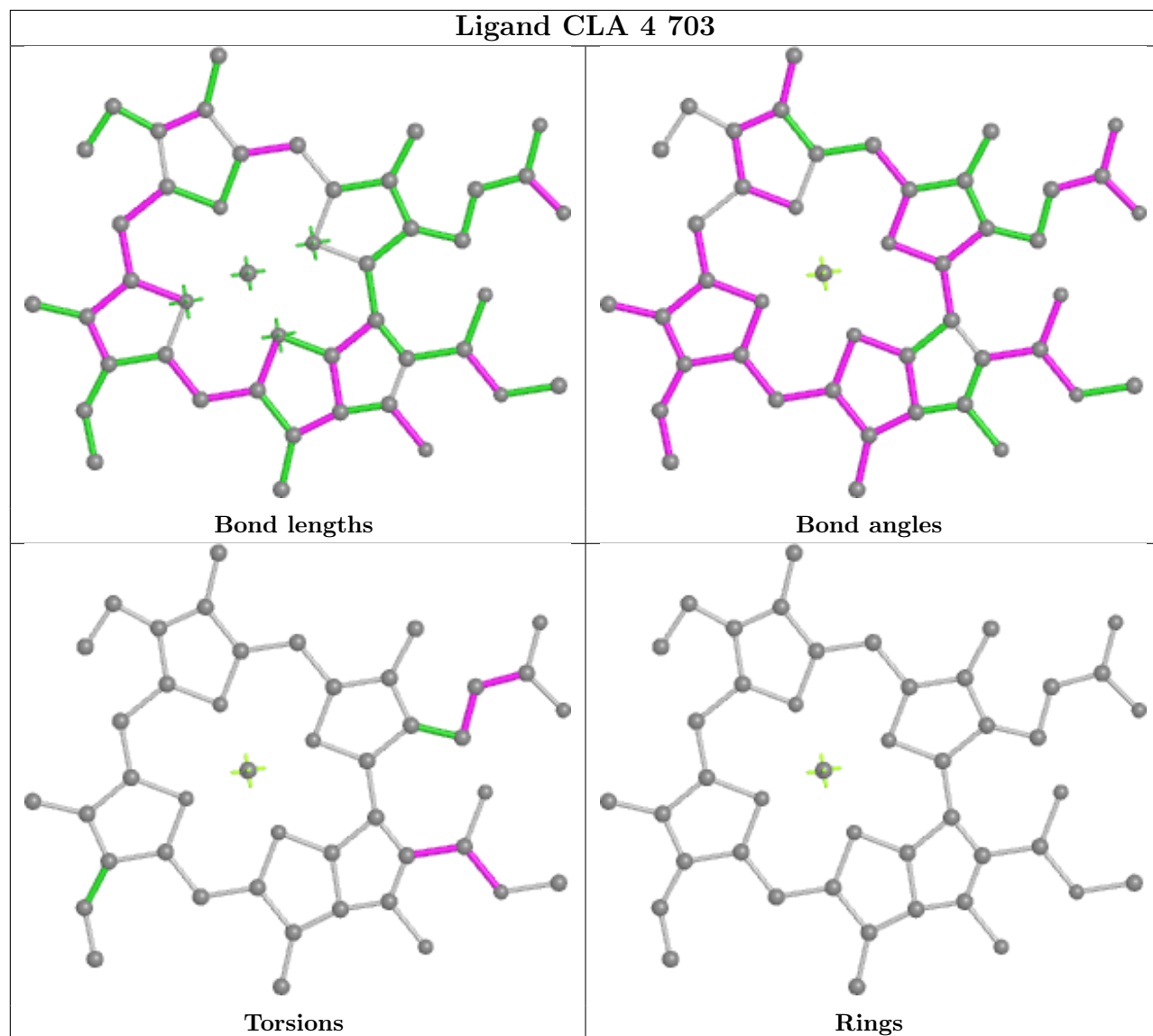
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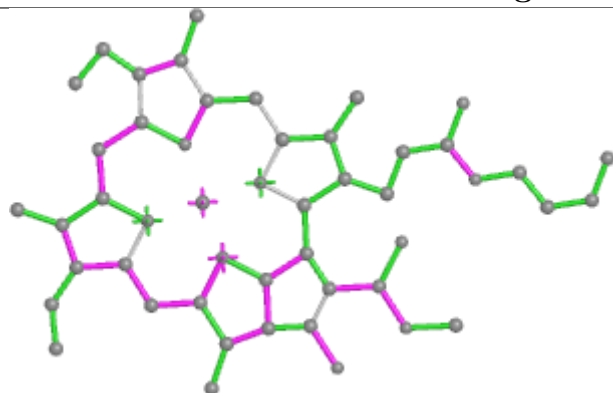
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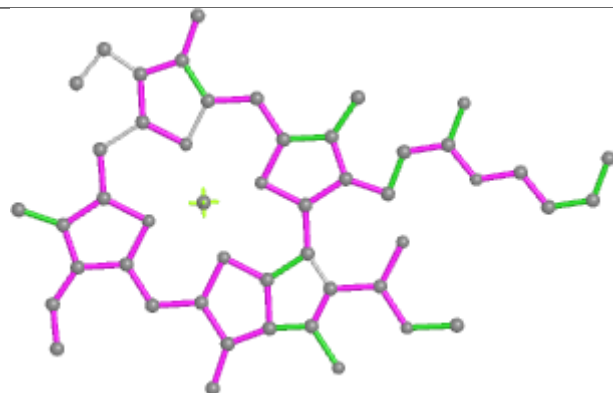
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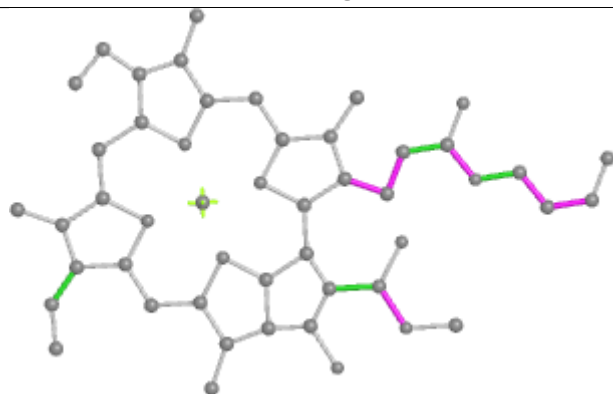
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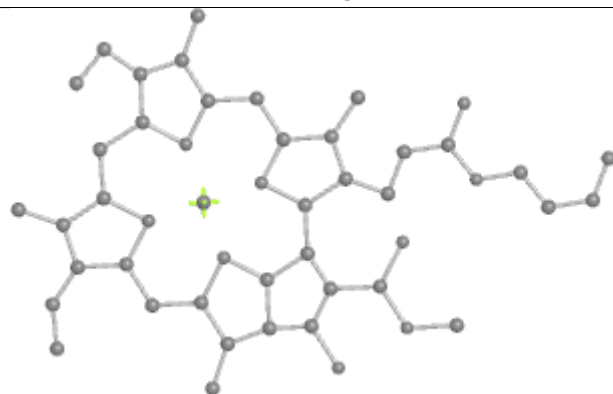
Bond lengths



Bond angles

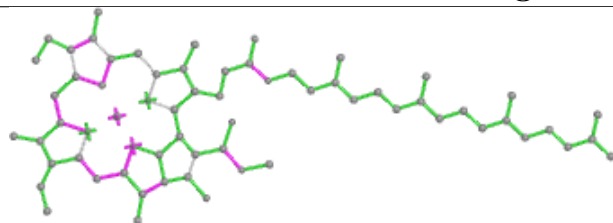


Torsions

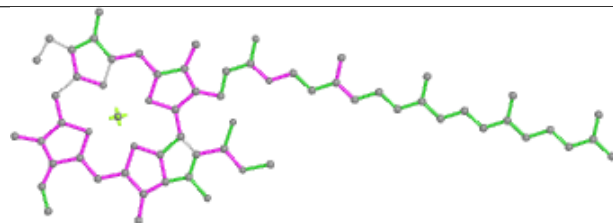


Rings

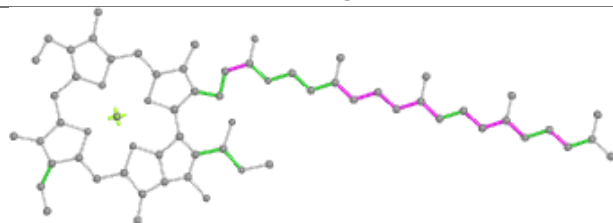
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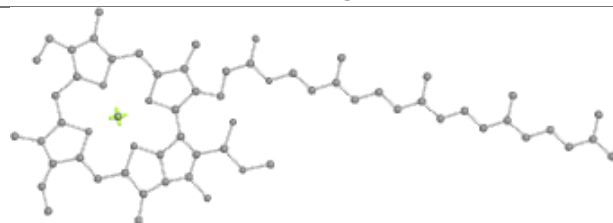
Bond lengths



Bond angles

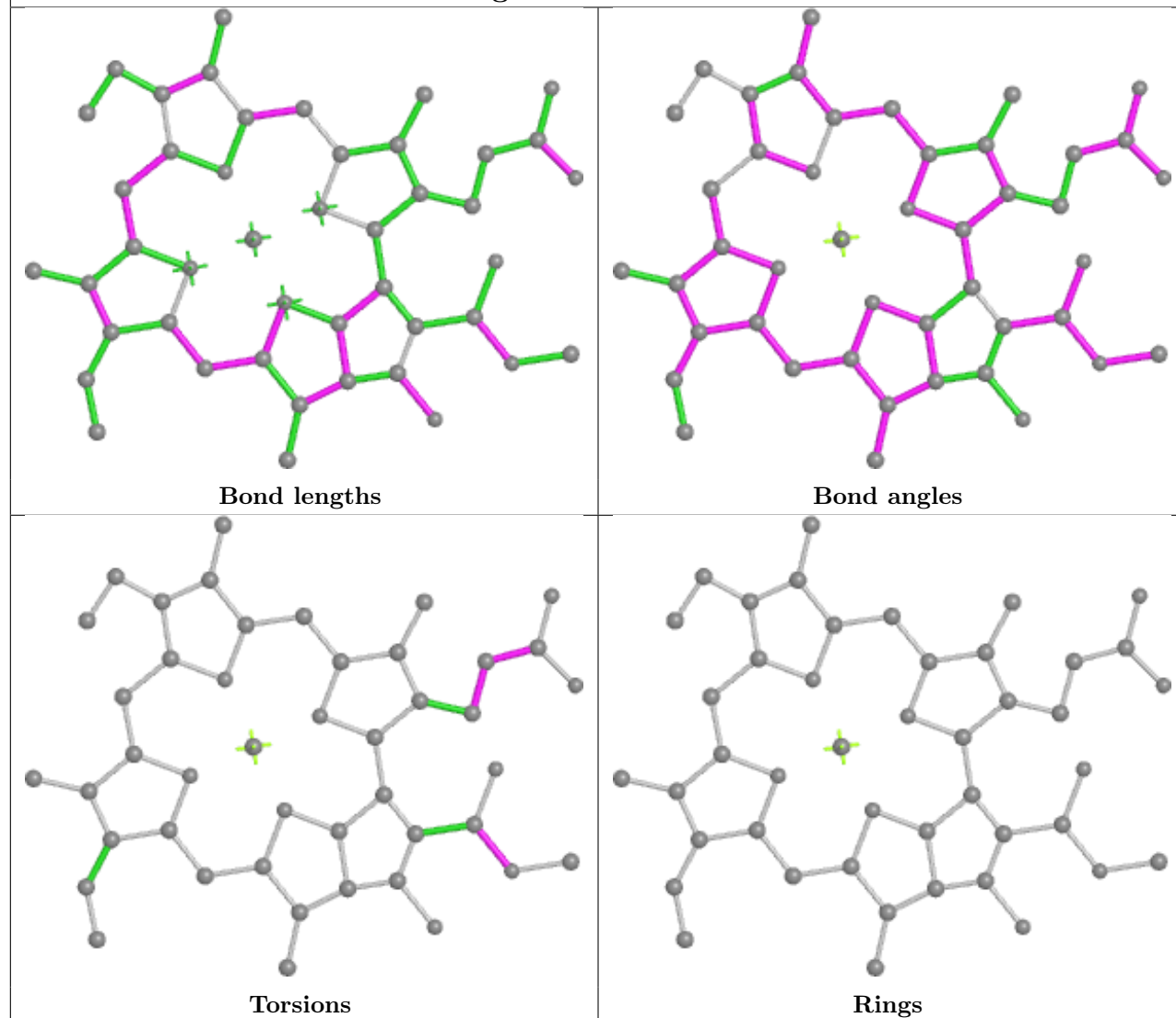


Torsions

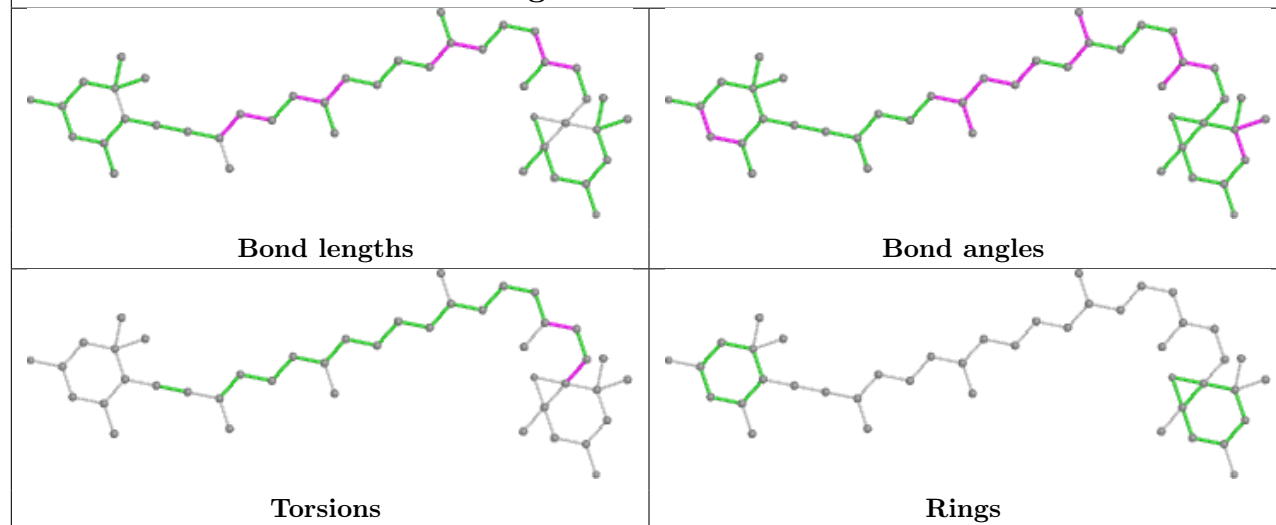


Rings

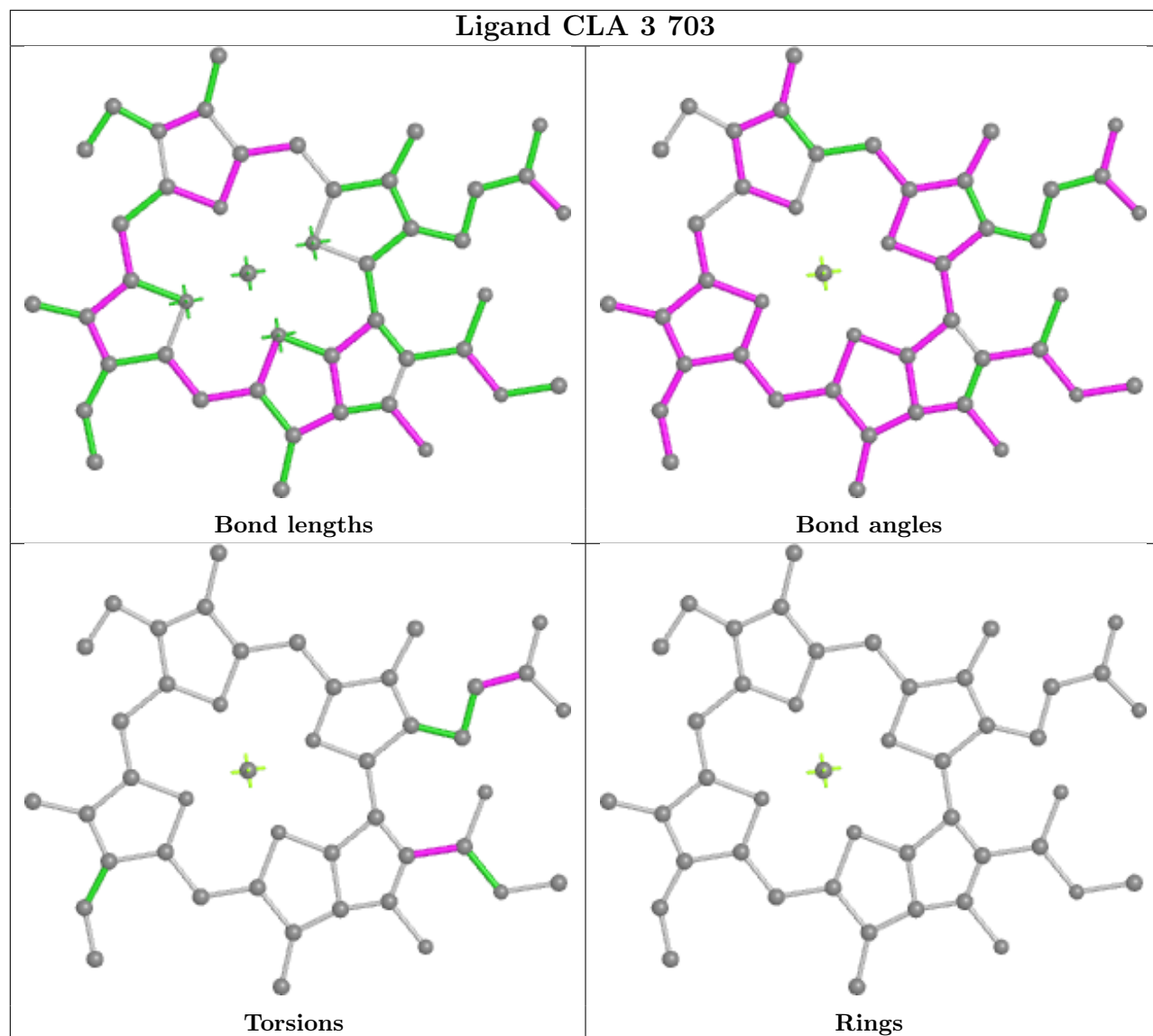
Ligand CLA F 403

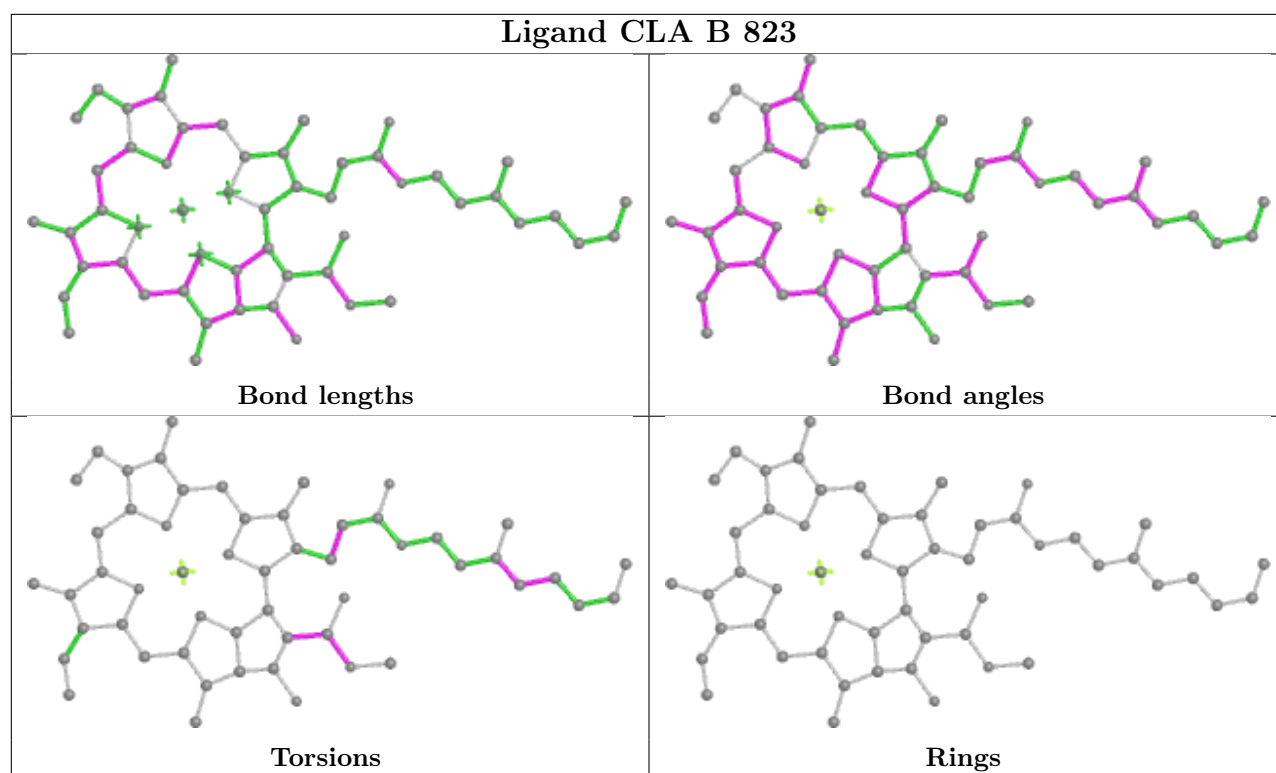


Ligand DD6 12 509

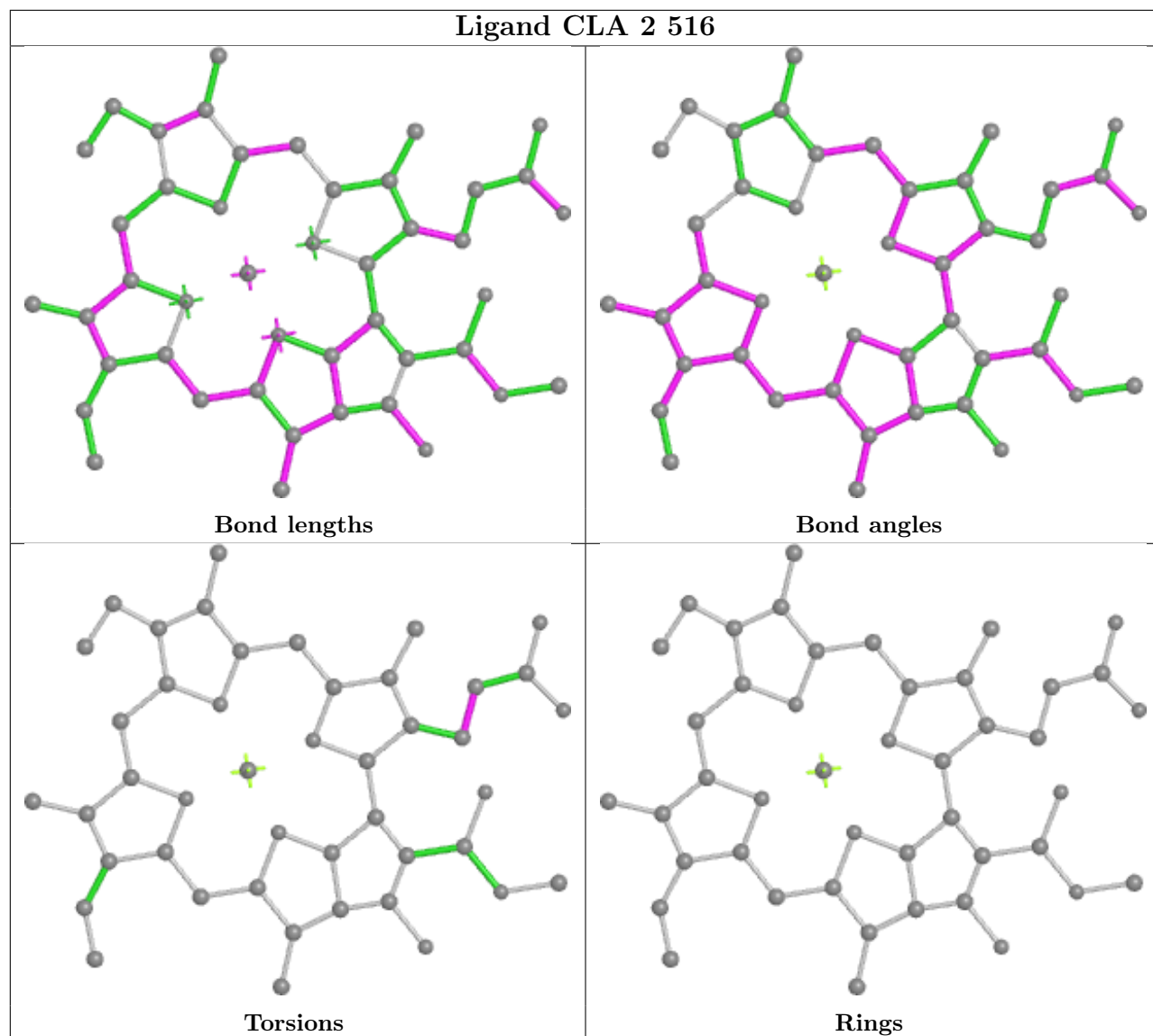


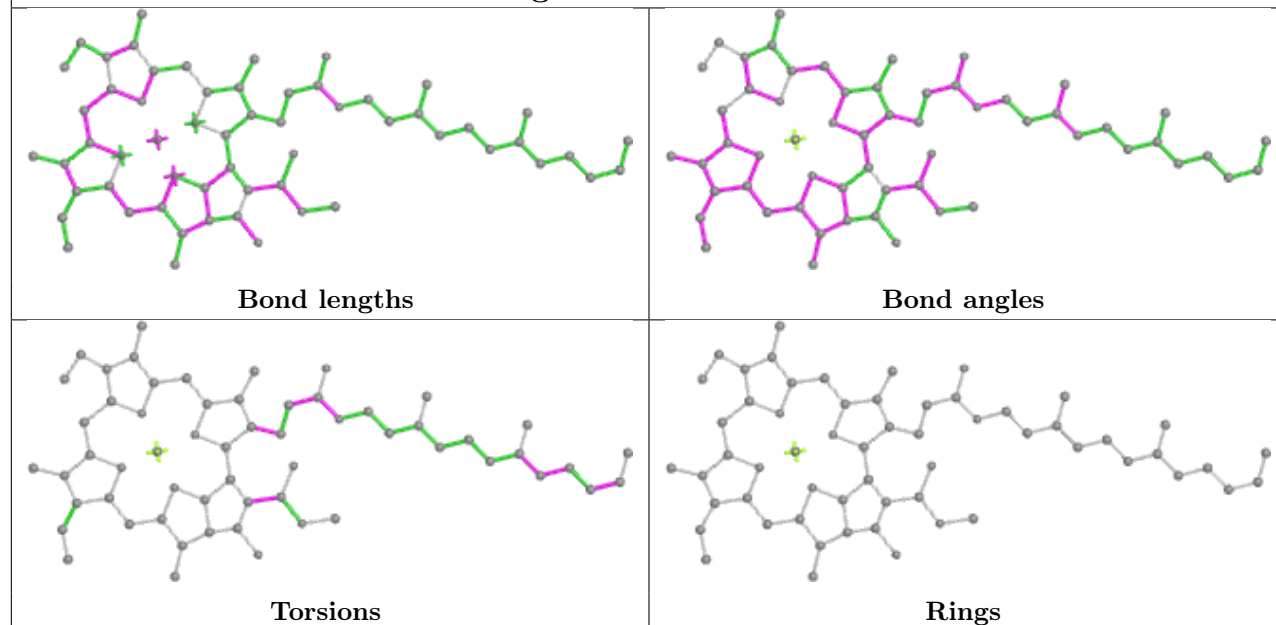
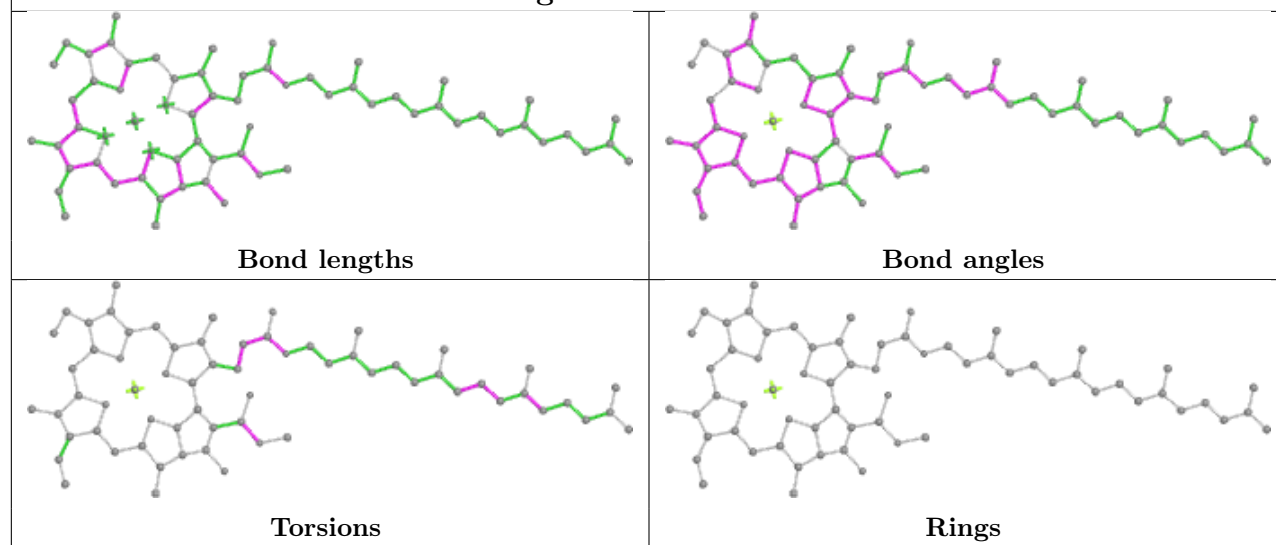
Ligand CLA 3 703

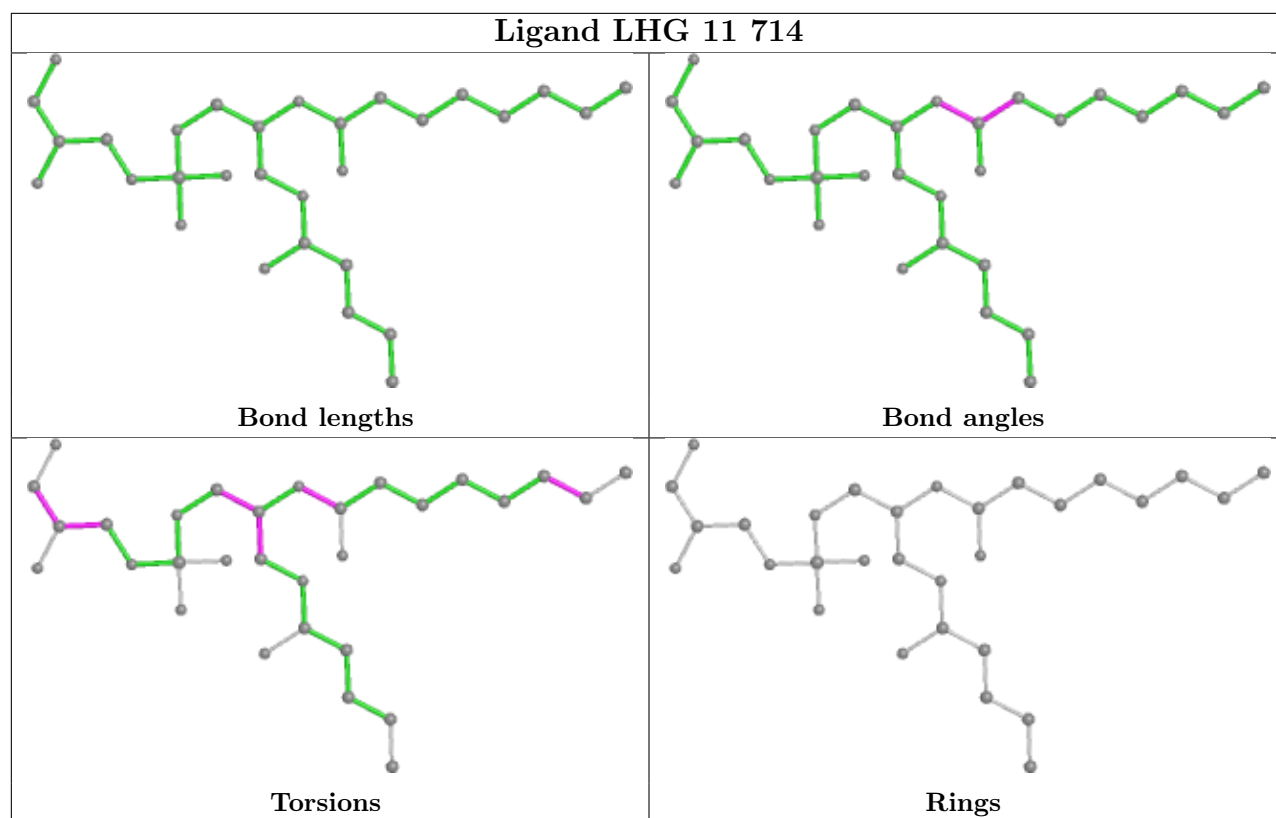
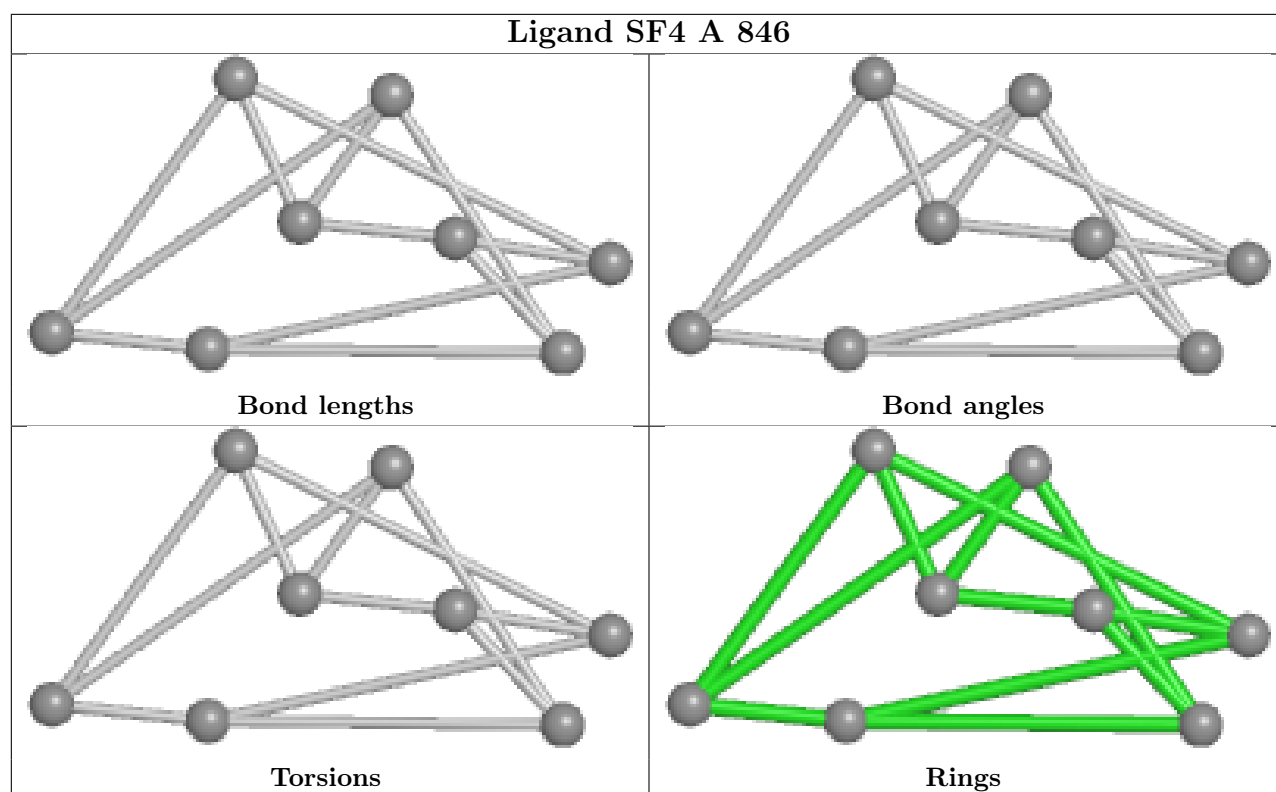


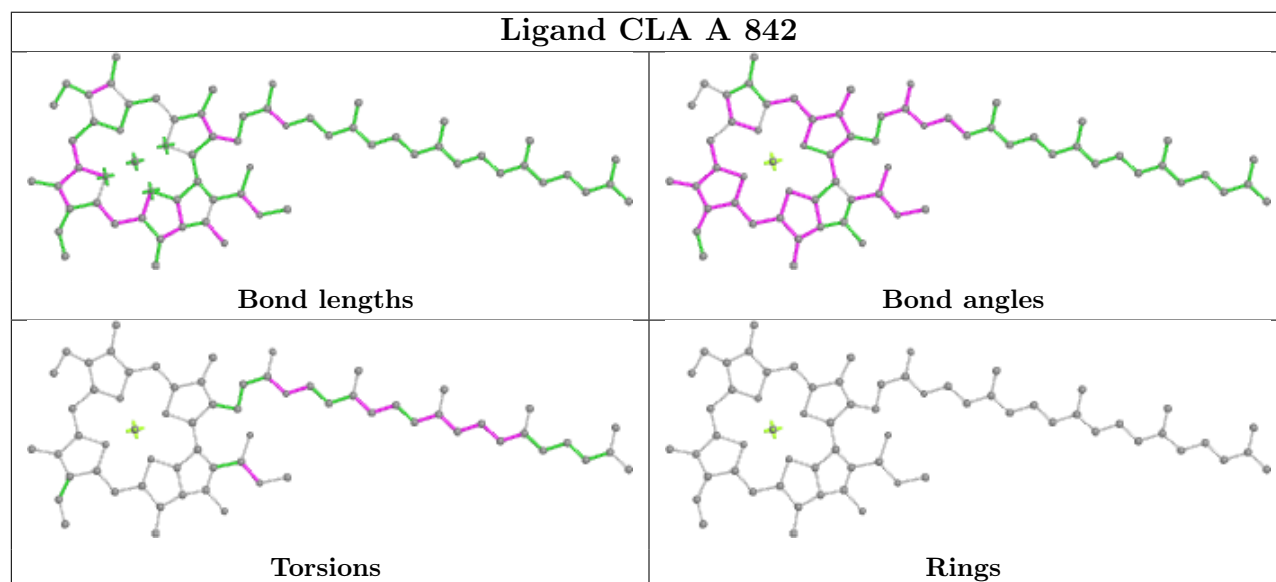
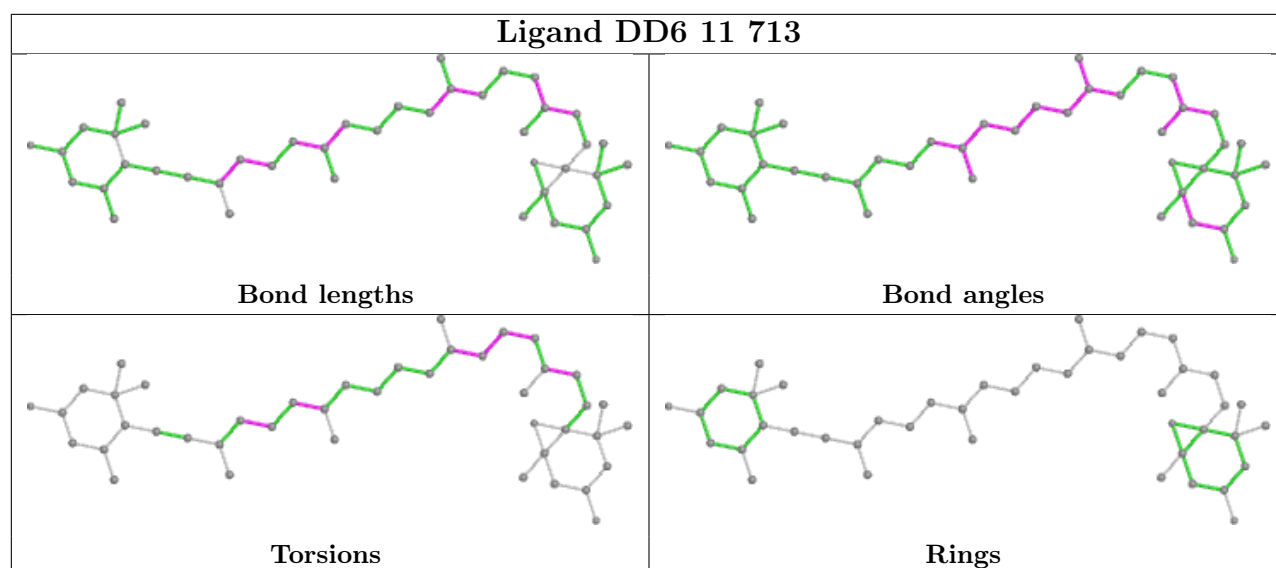


Ligand CLA 2 516

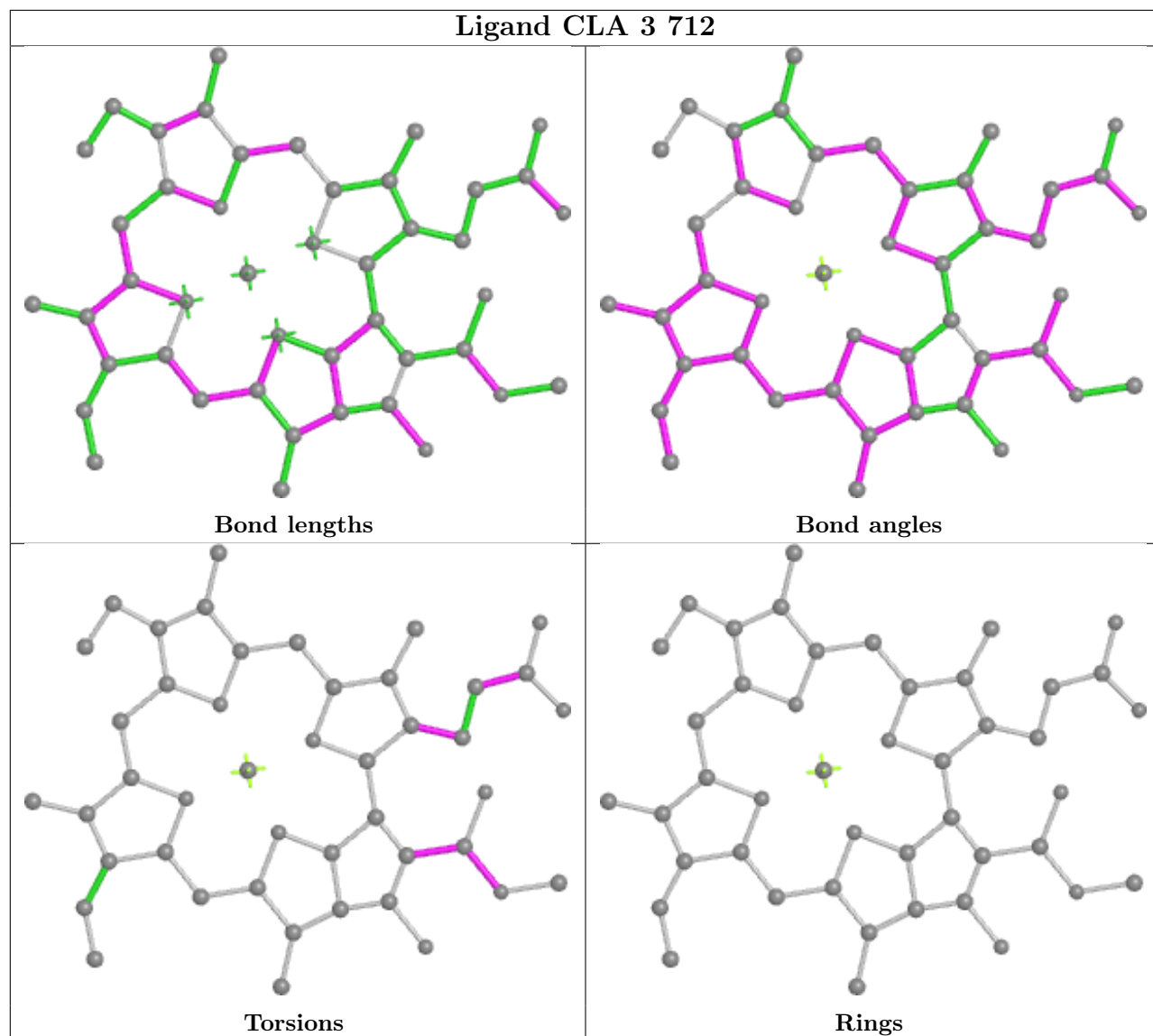


Ligand CLA A 805**Ligand CLA 8 612**

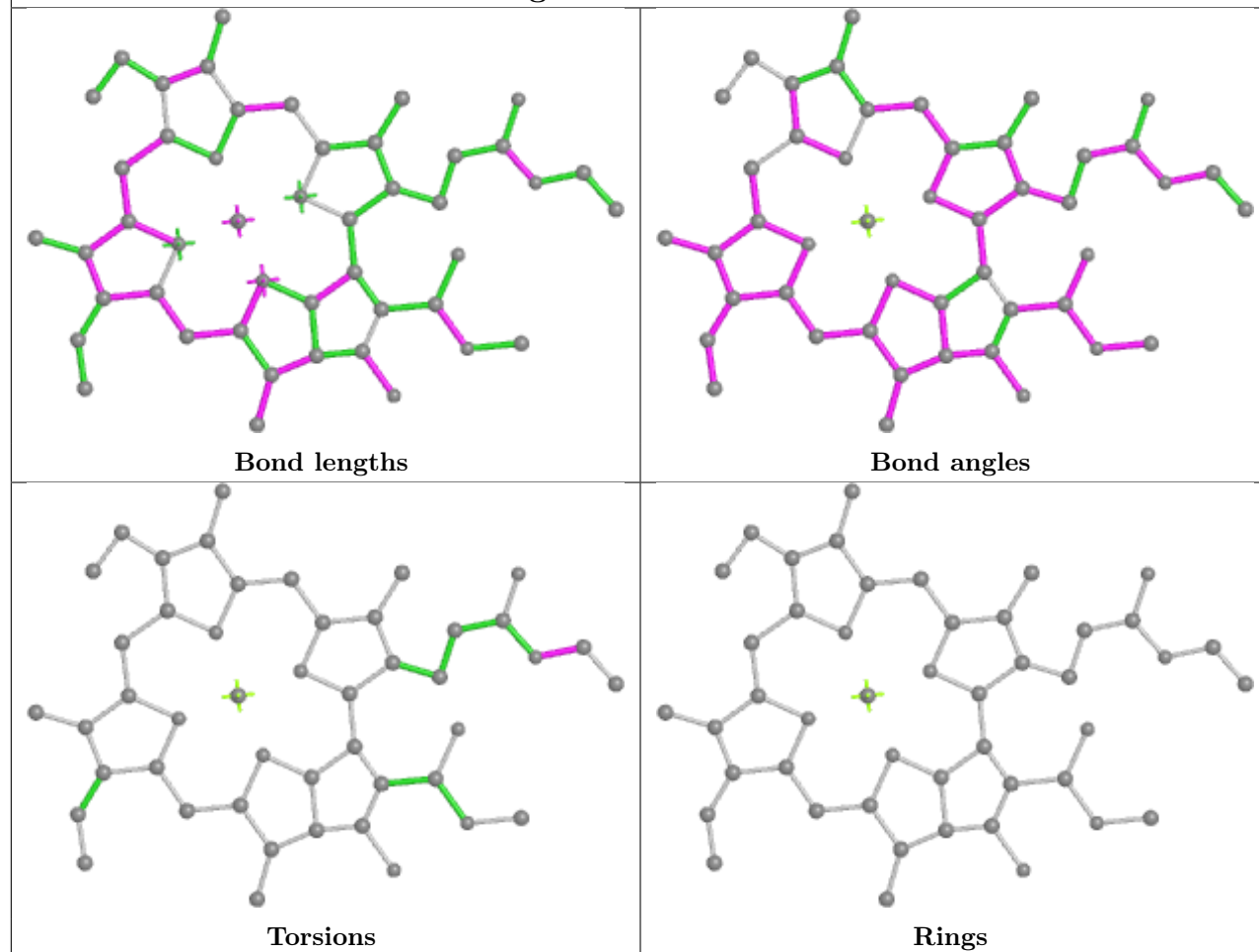




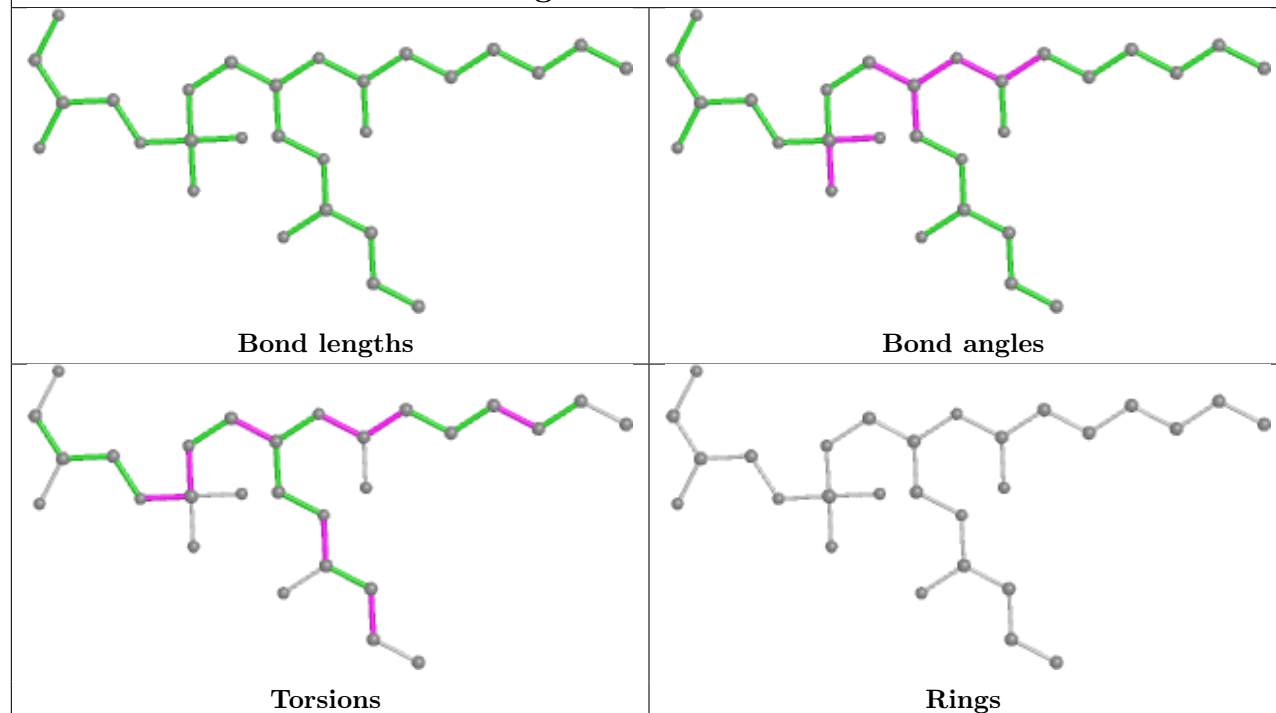
Ligand CLA 3 712

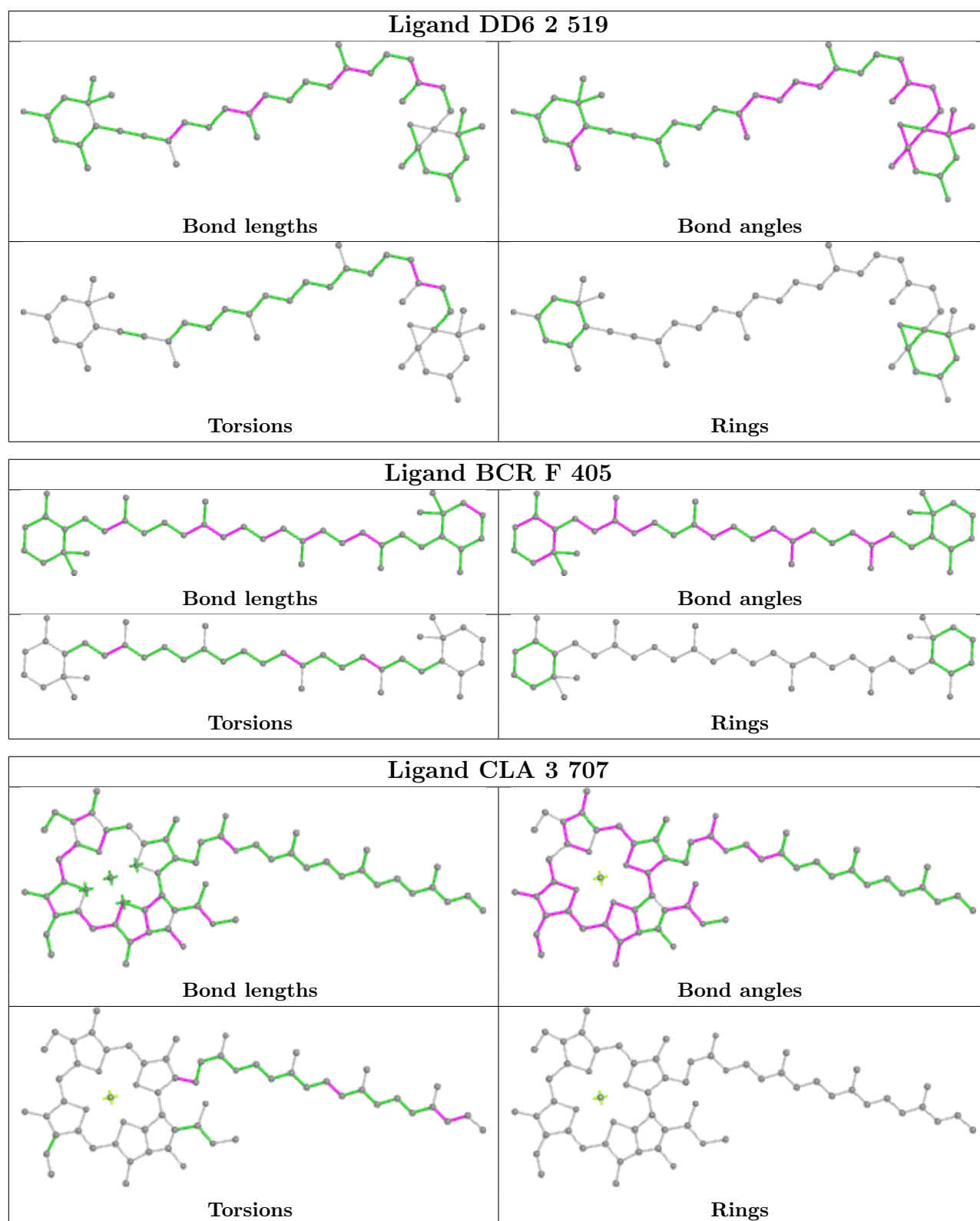


Ligand CLA 6 907

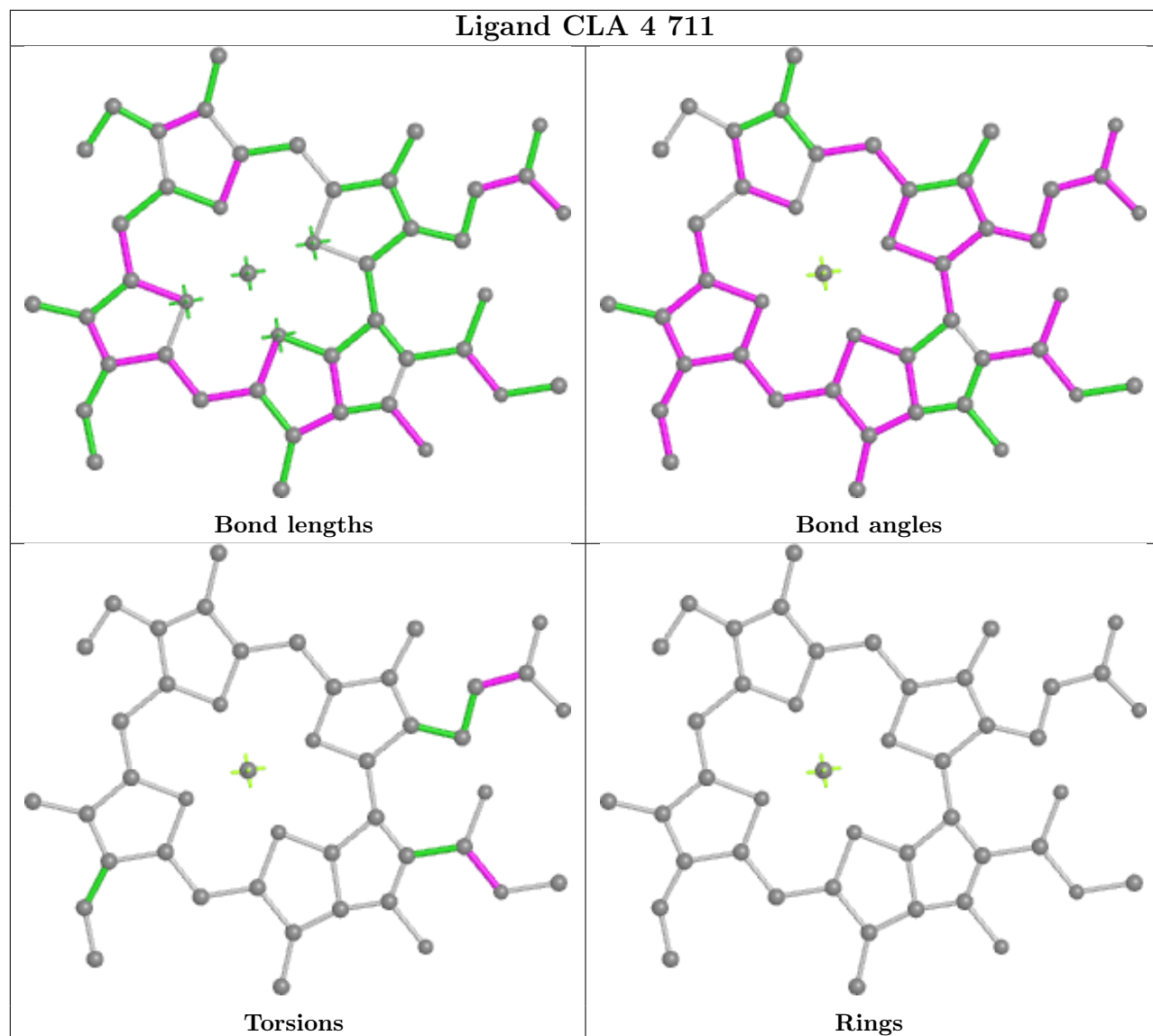


Ligand LHG 6 917

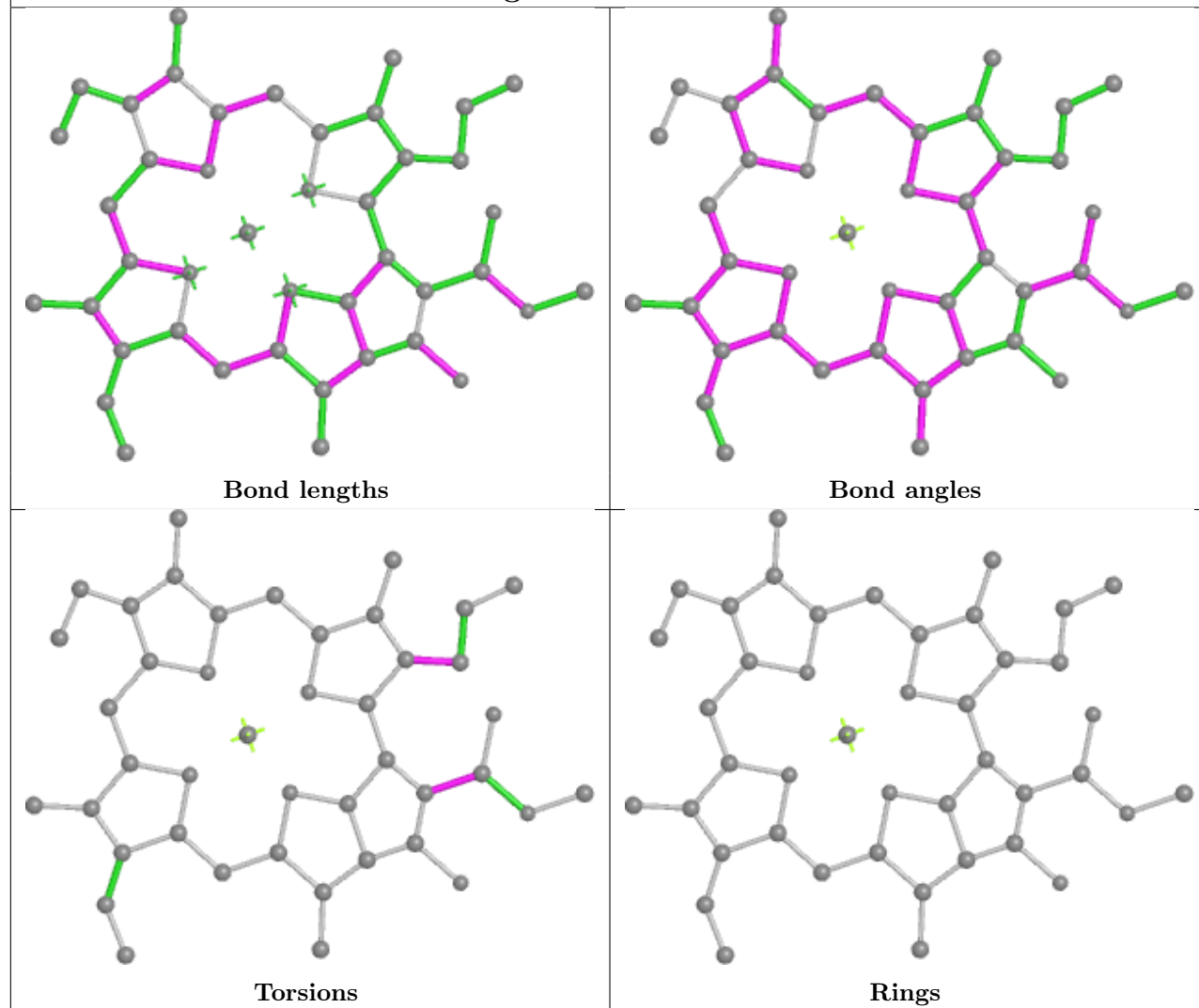




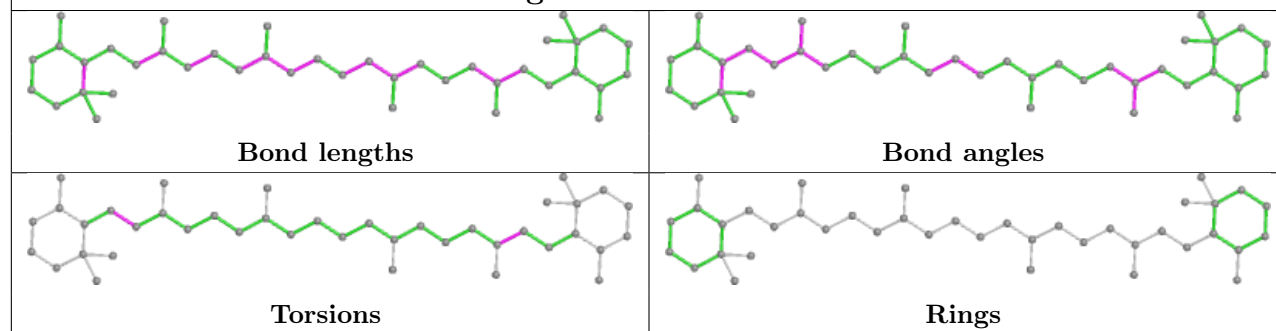
Ligand CLA 4 711

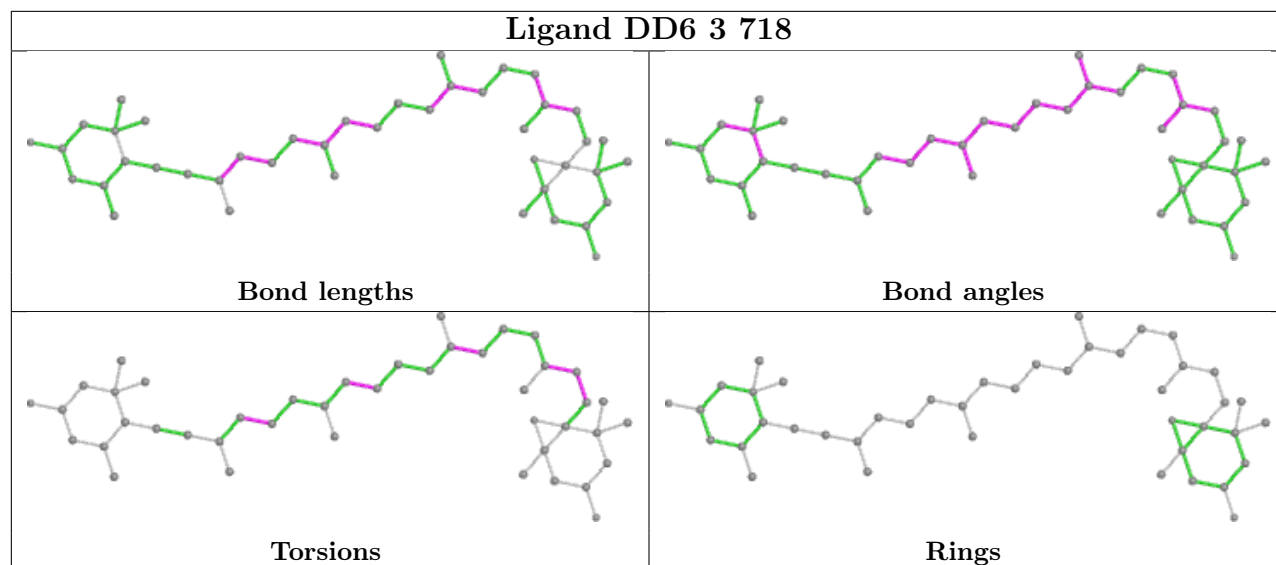
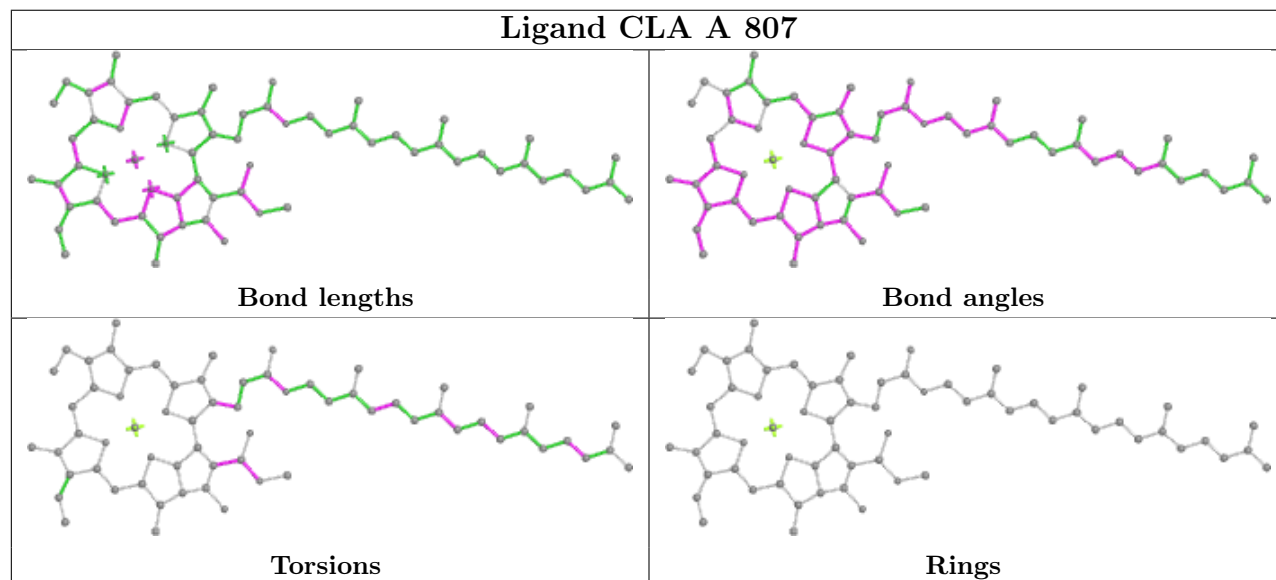


Ligand CLA 5 708

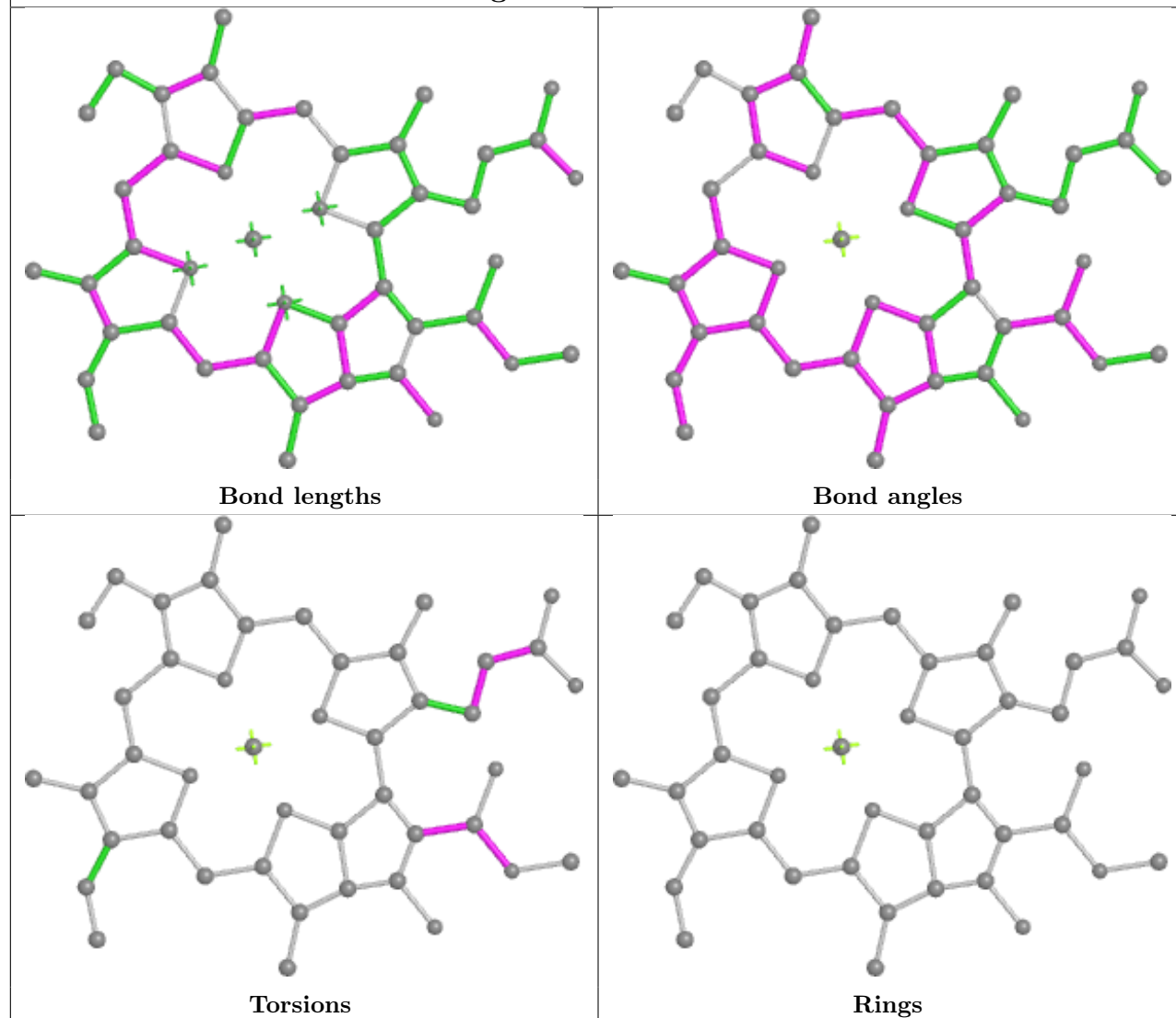


Ligand BCR M 102

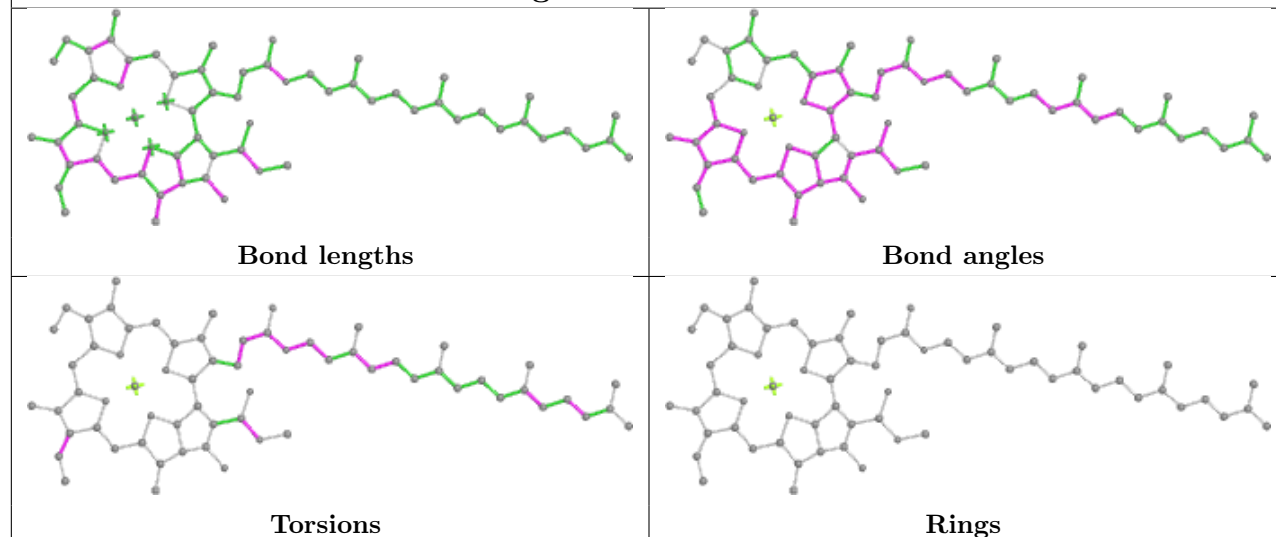


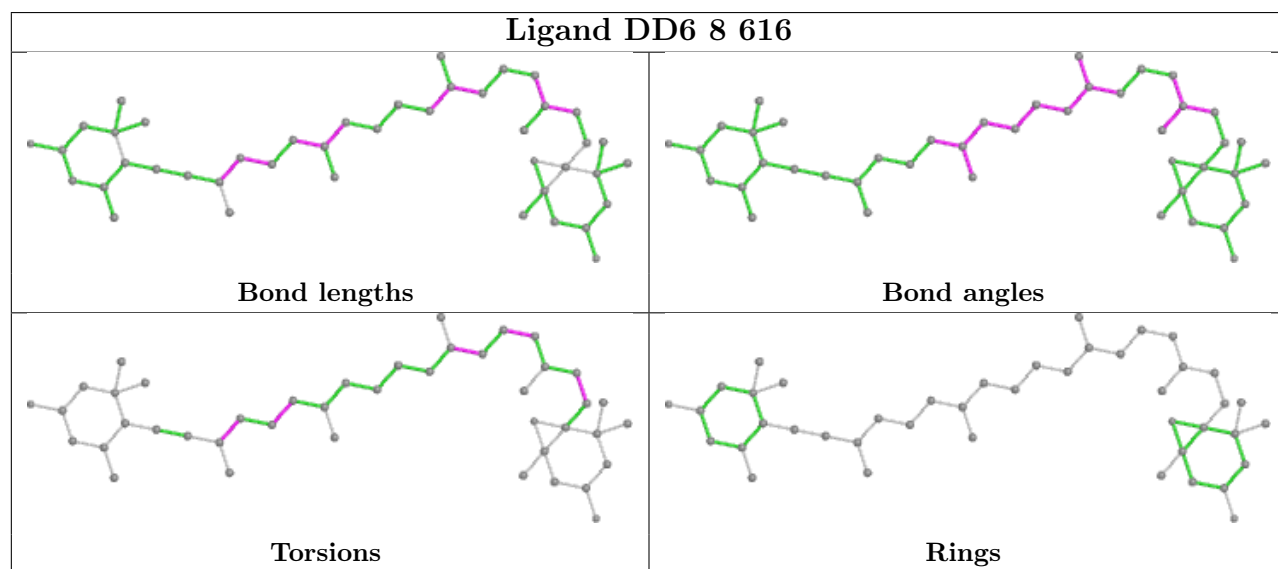
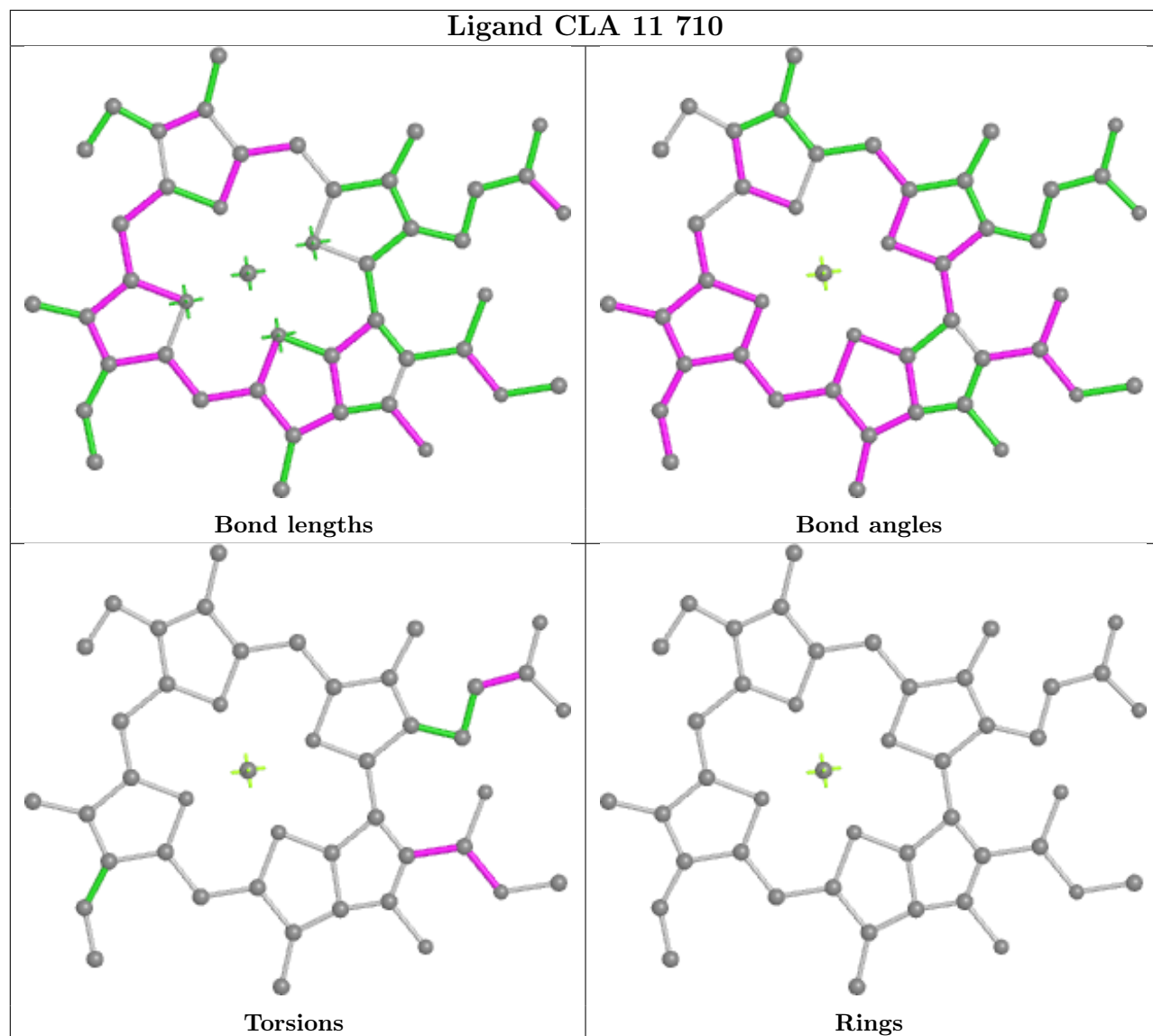
Ligand DD6 3 718**Ligand CLA A 807**

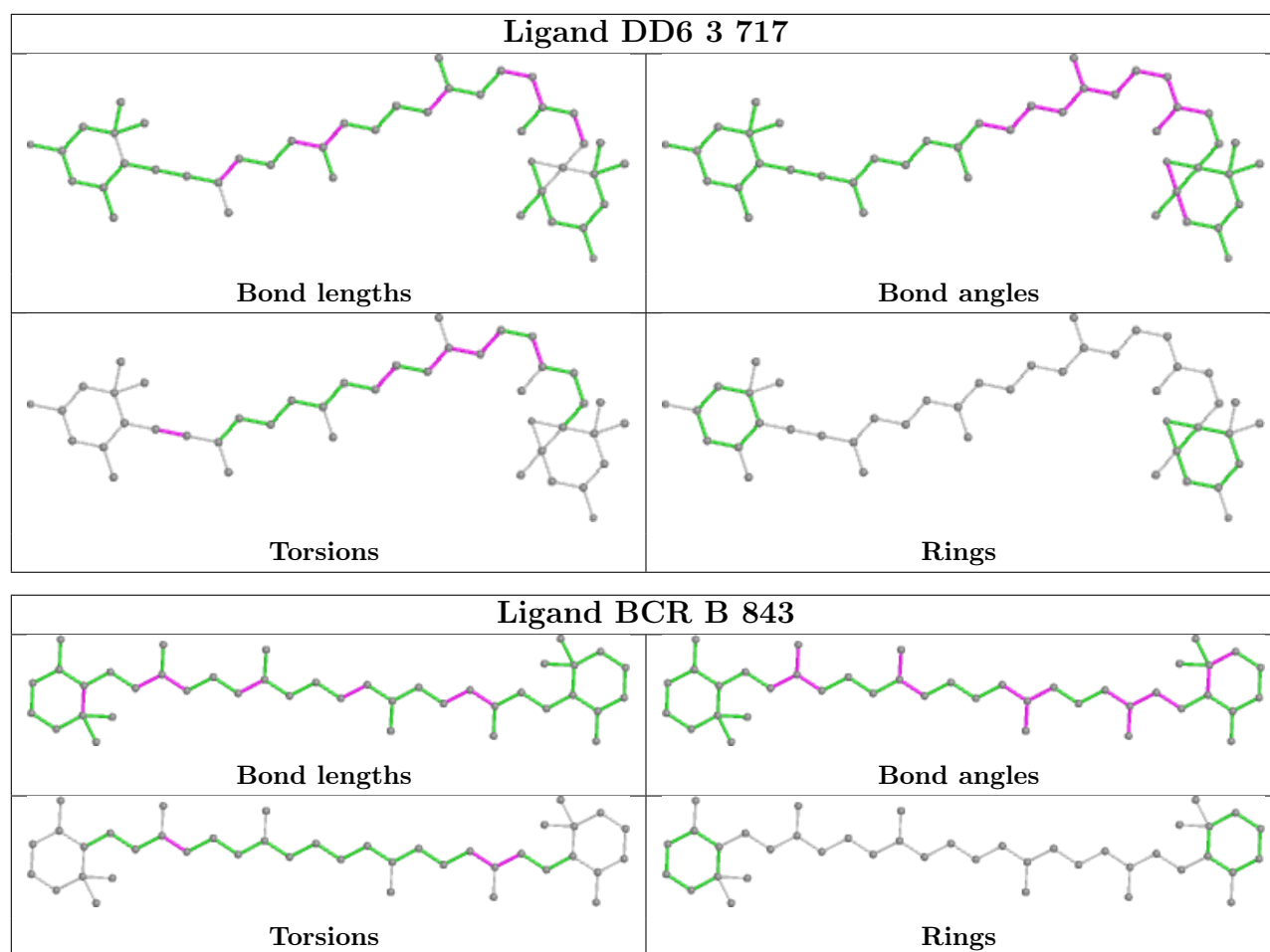
Ligand CLA B 820



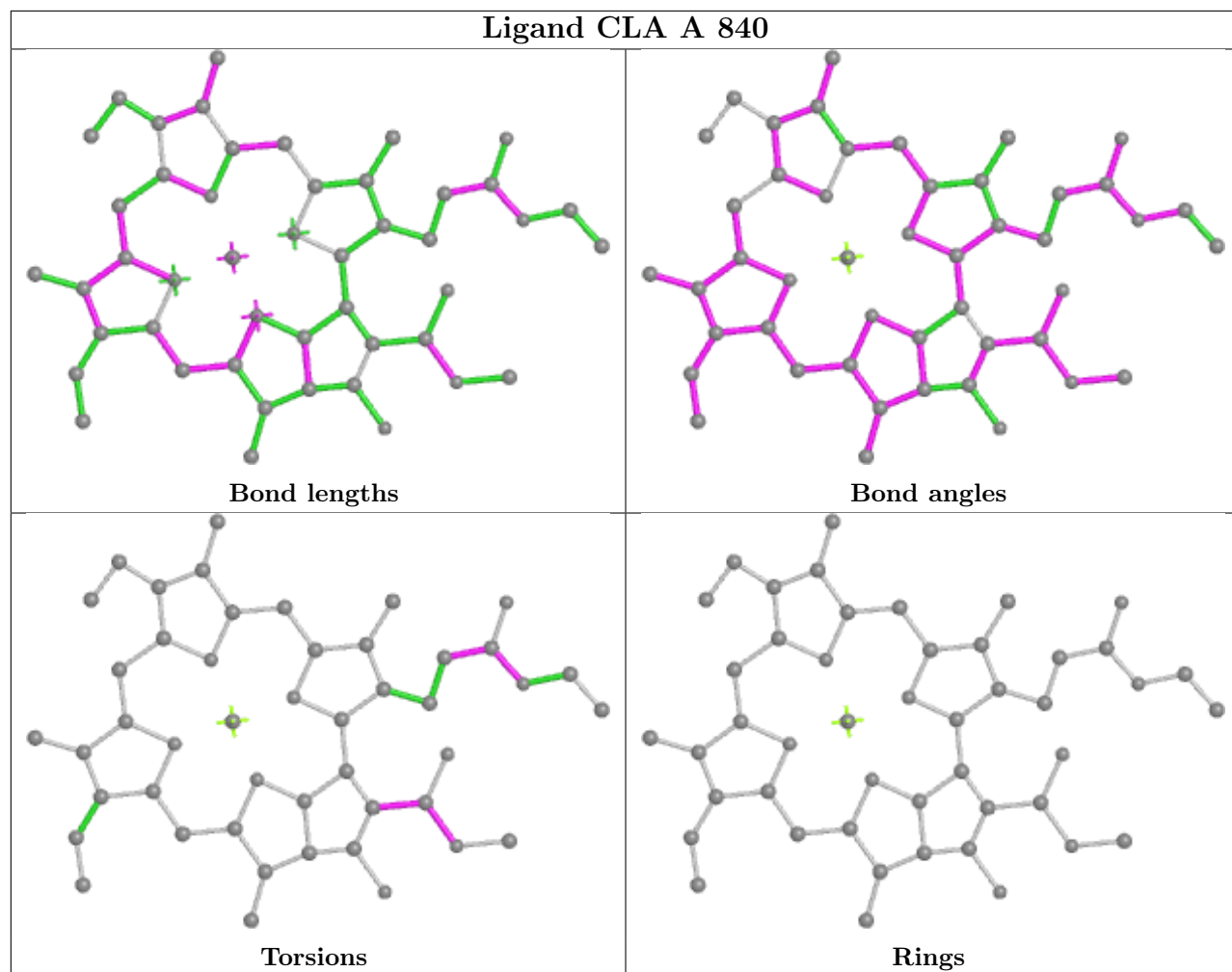
Ligand CLA B 831



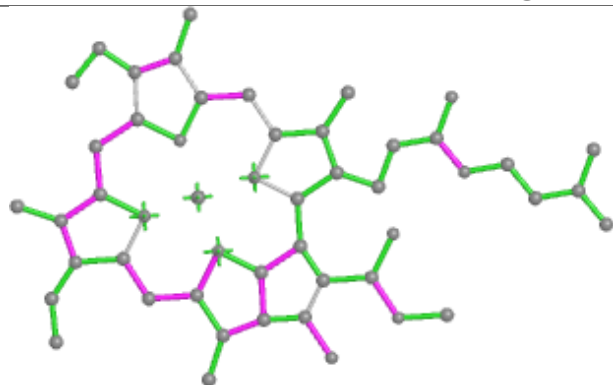




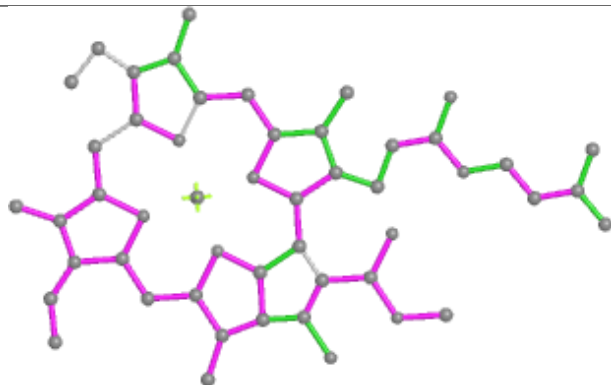
Ligand CLA A 840



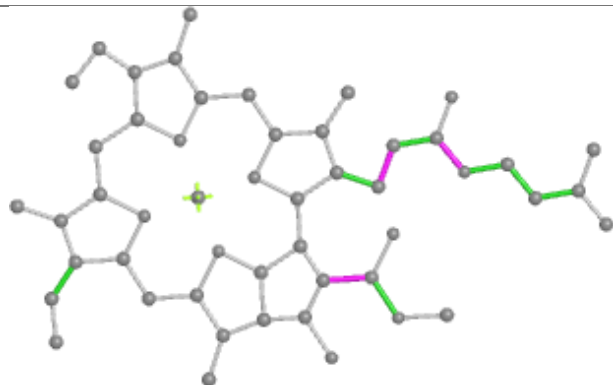
Ligand CLA 9 905



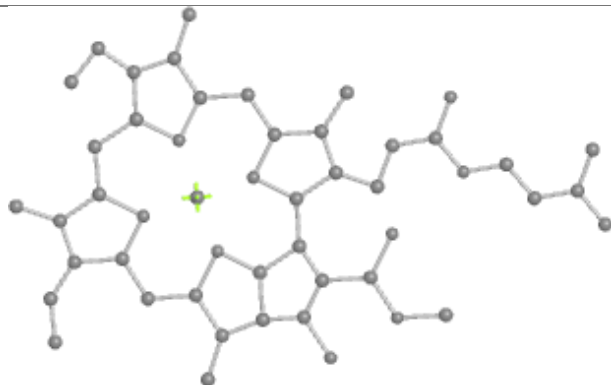
Bond lengths



Bond angles

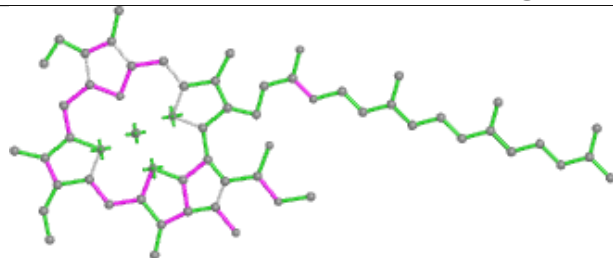


Torsions

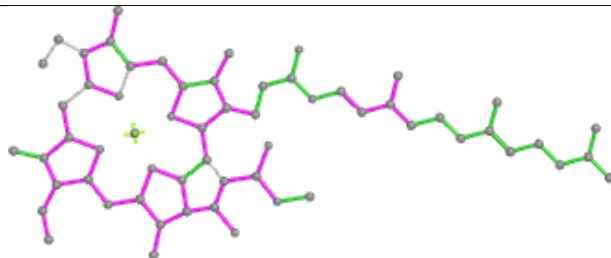


Rings

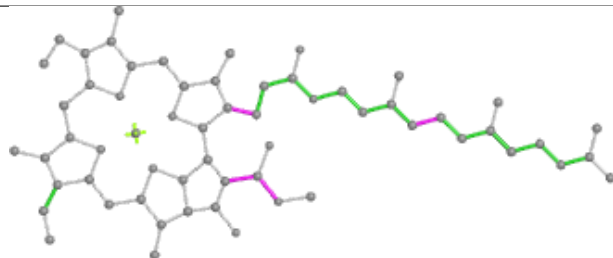
Ligand CLA 6 904



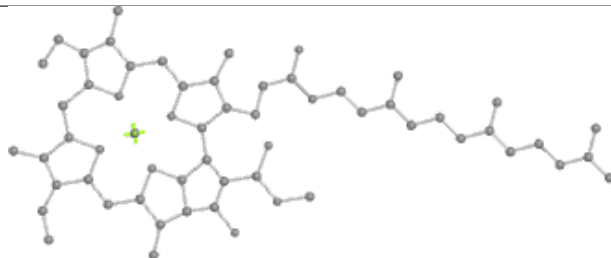
Bond lengths



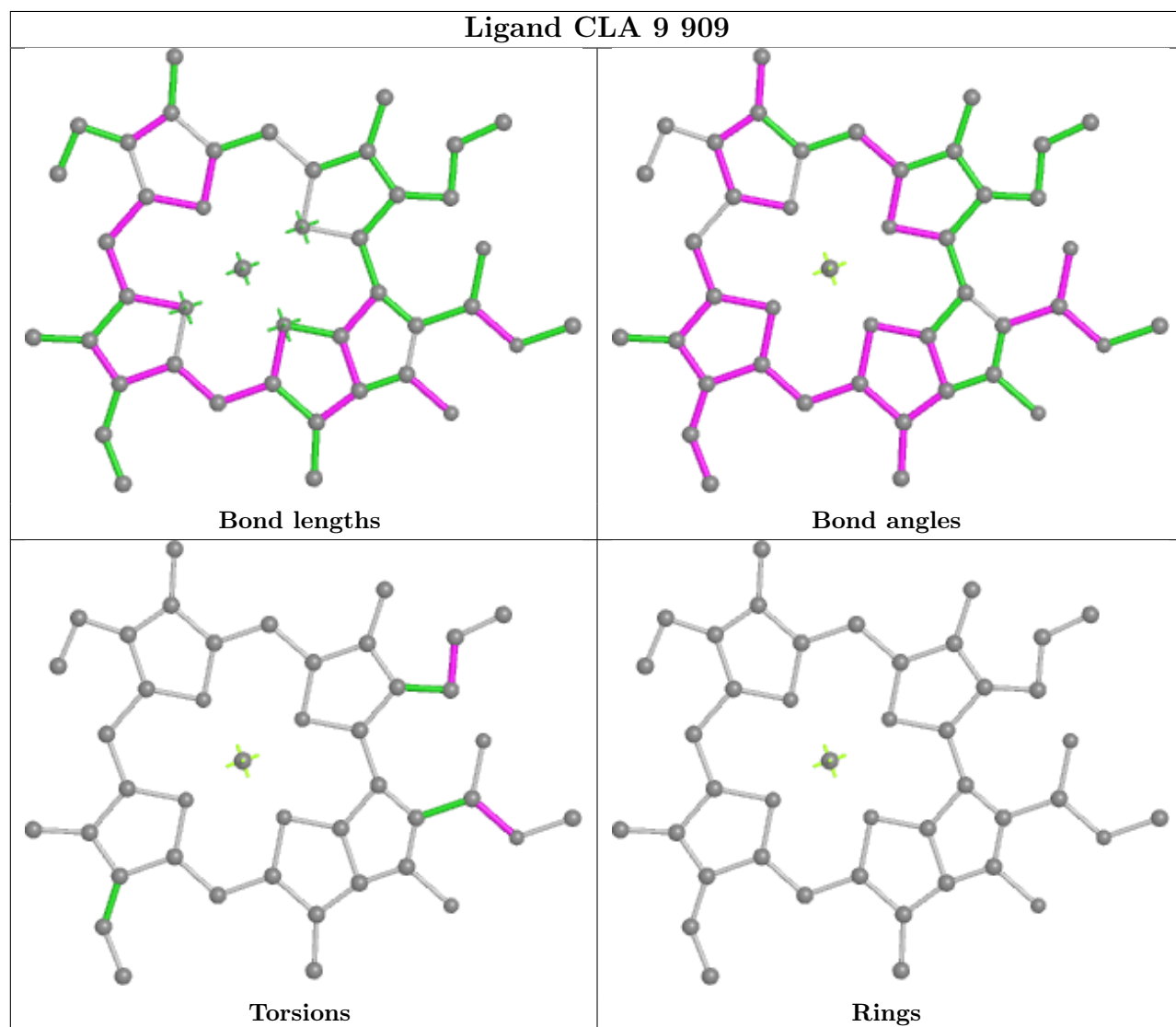
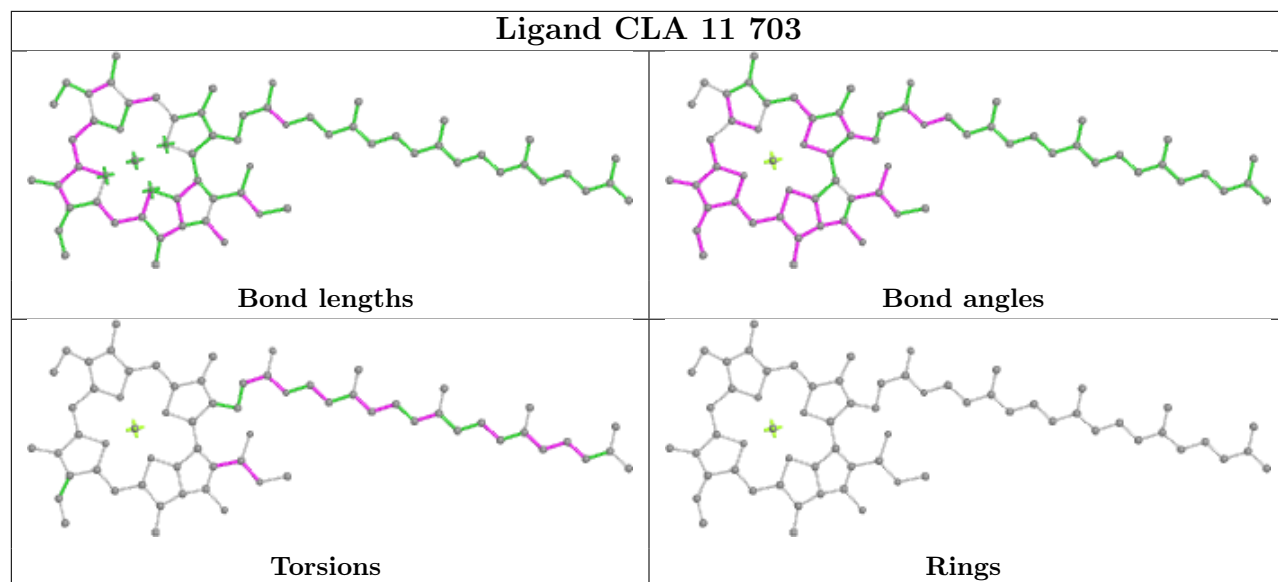
Bond angles



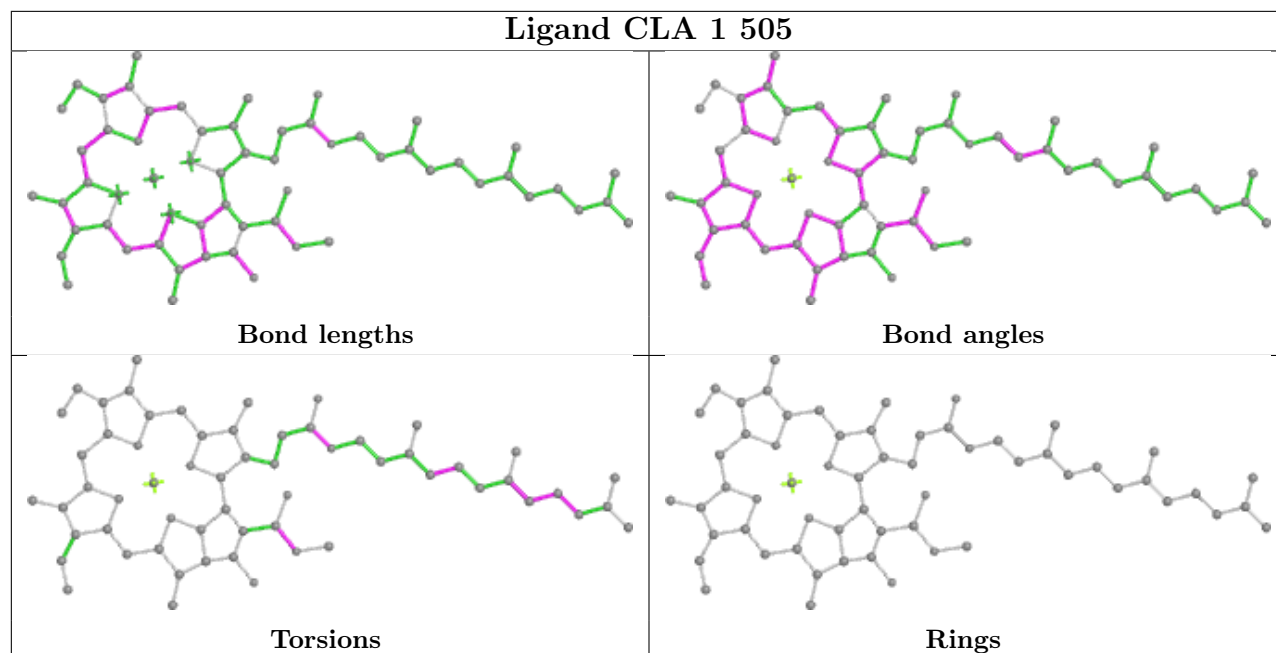
Torsions



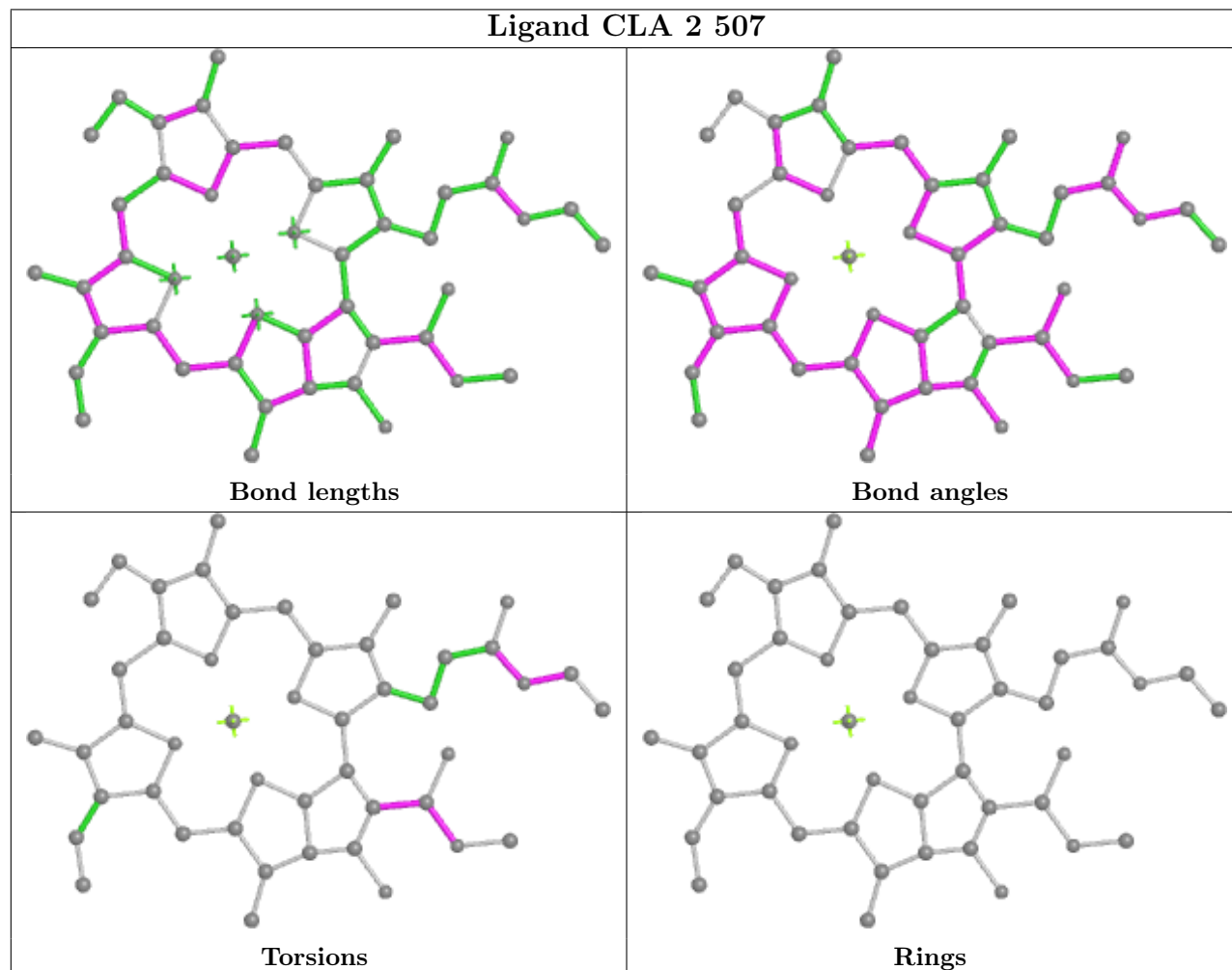
Rings



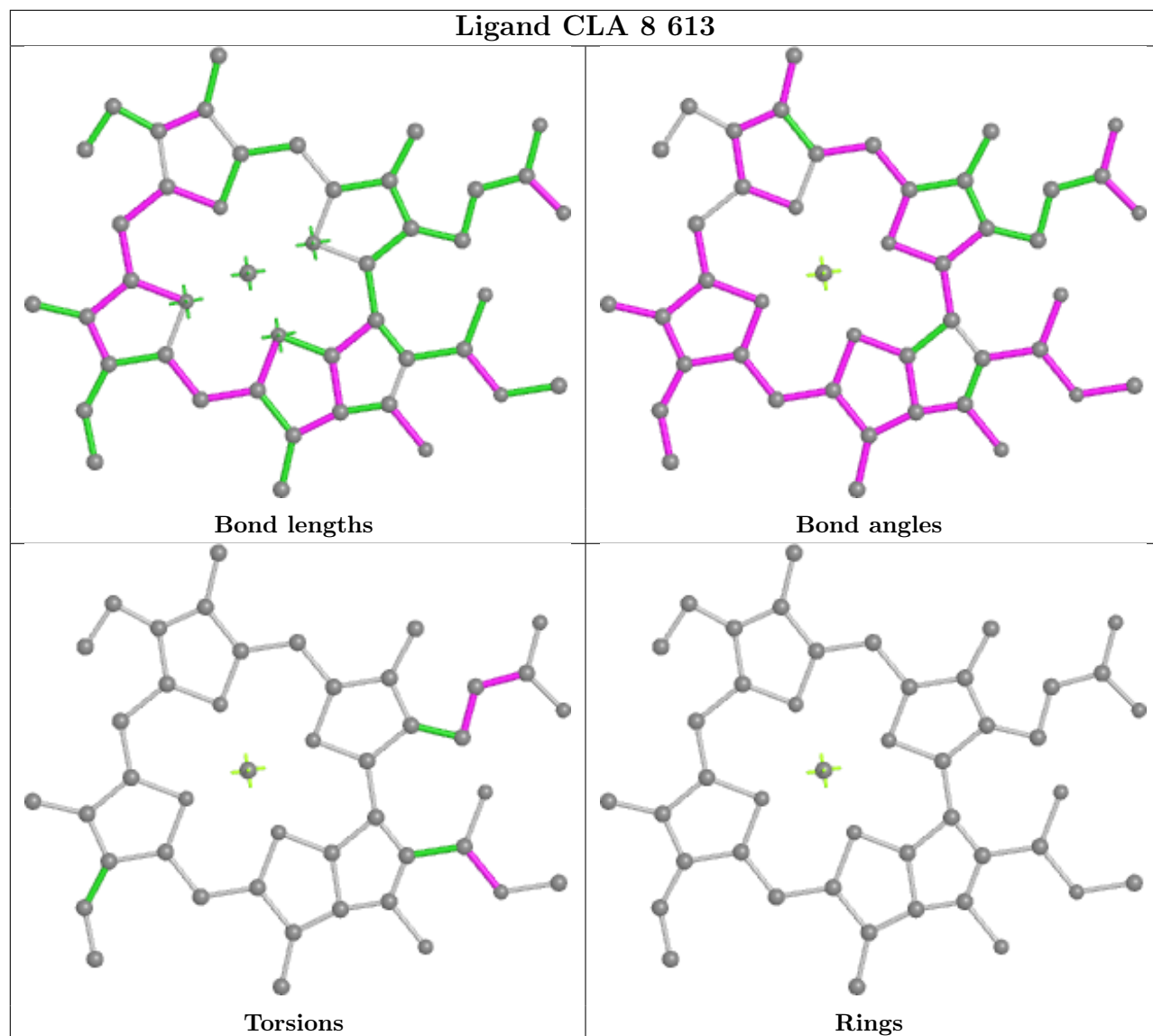
Ligand CLA 1 505



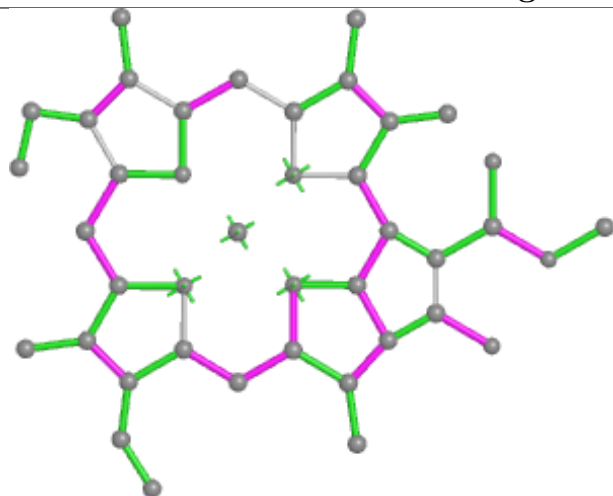
Ligand CLA 2 507



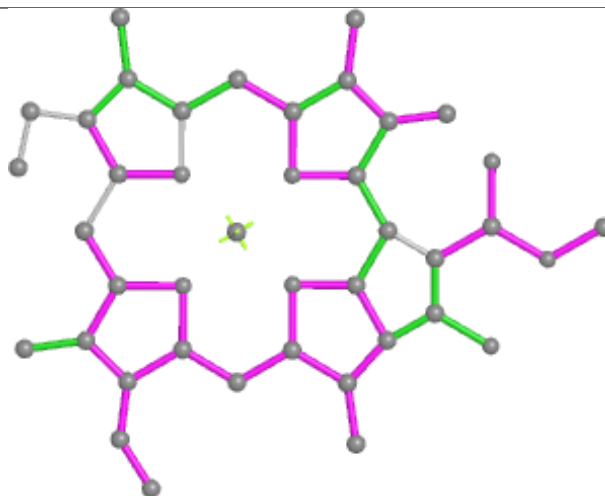
Ligand CLA 8 613



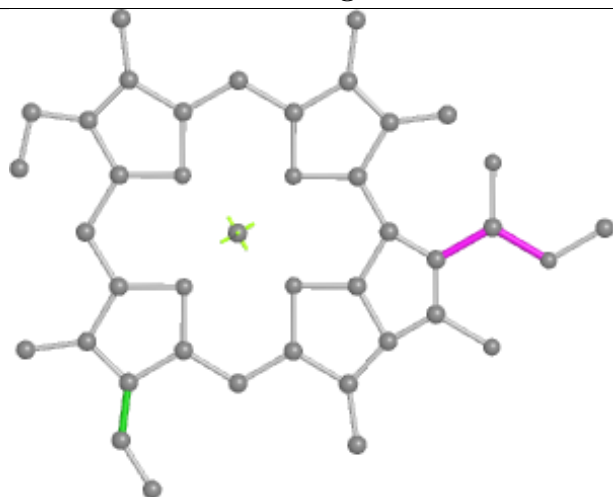
Ligand CLA 3 701



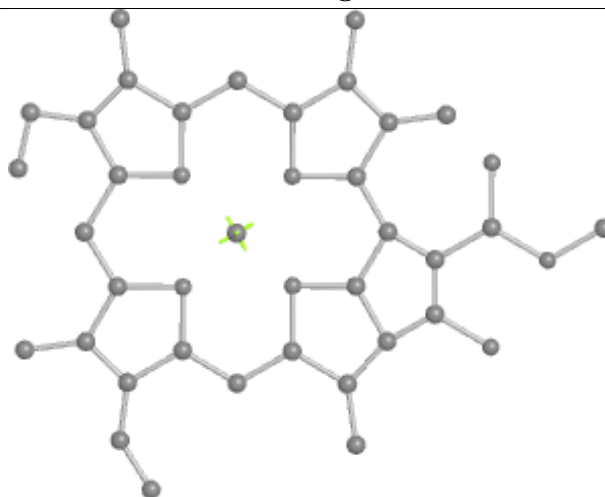
Bond lengths



Bond angles

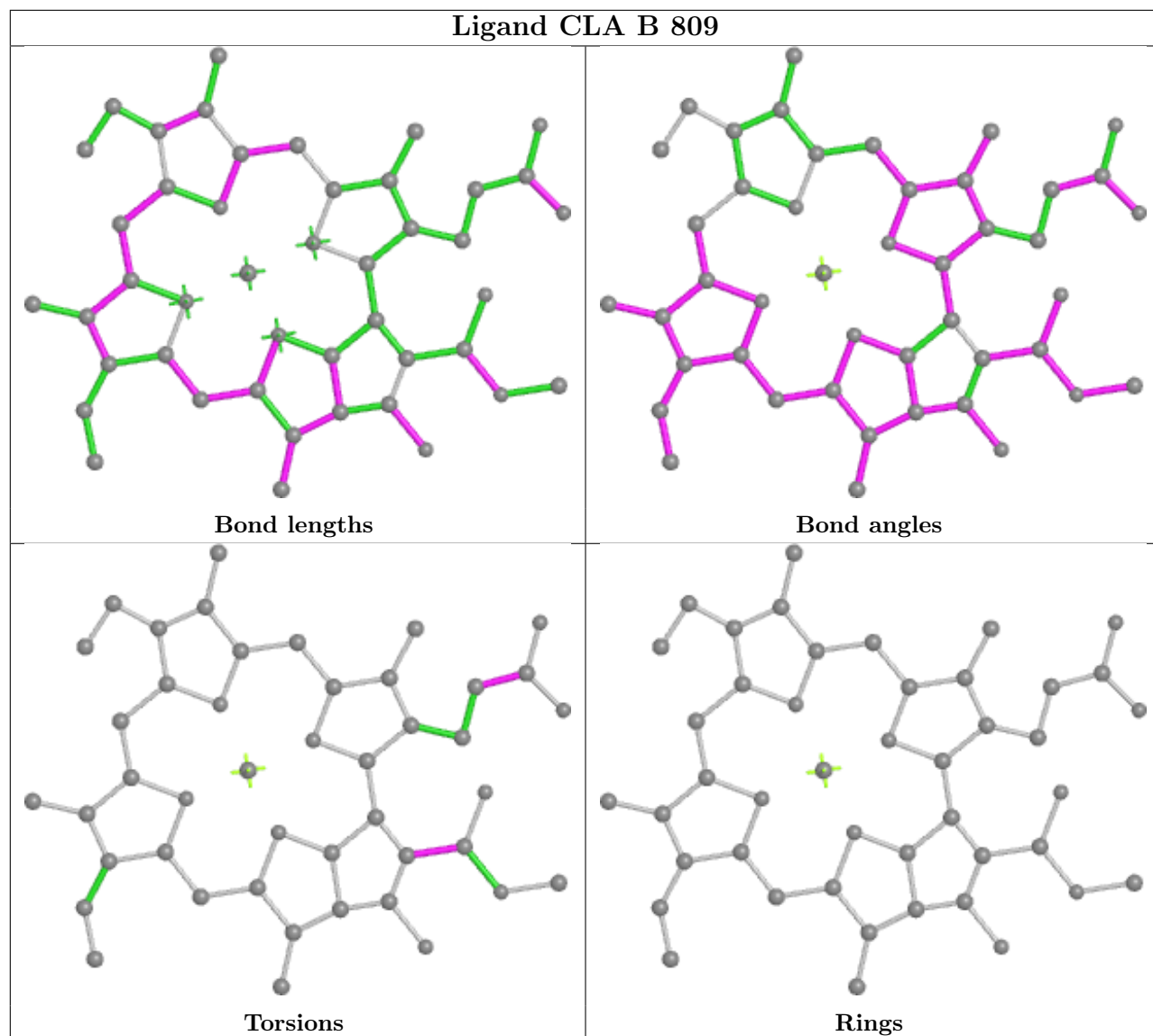


Torsions

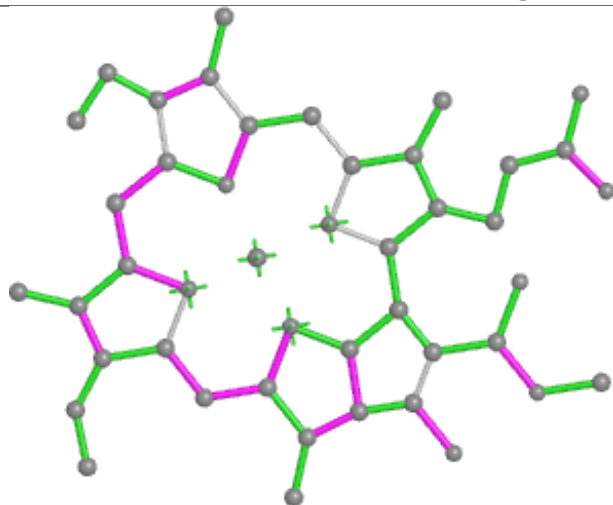


Rings

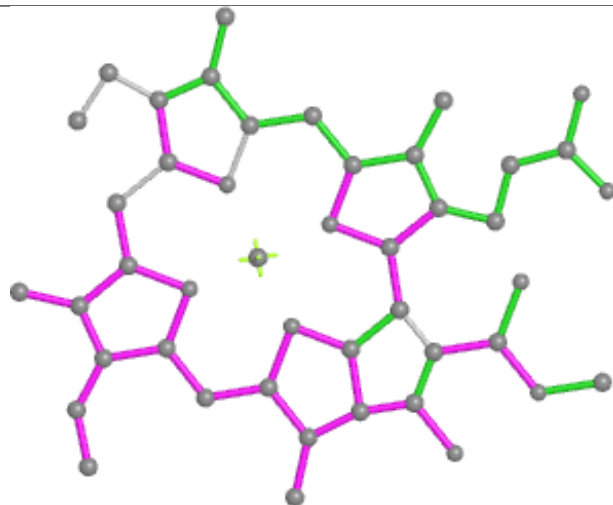
Ligand CLA B 809



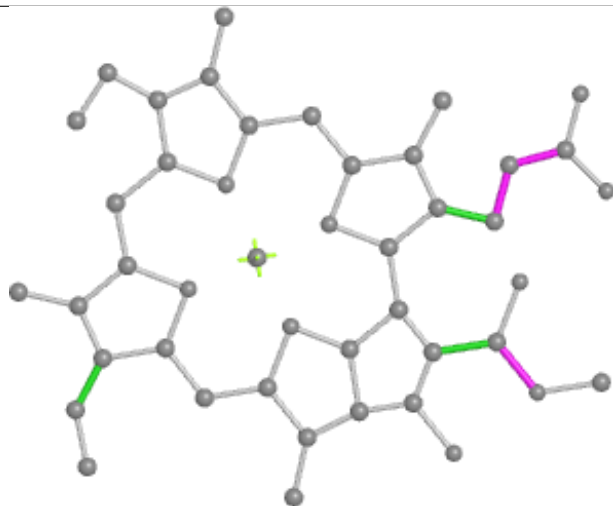
Ligand CLA B 837



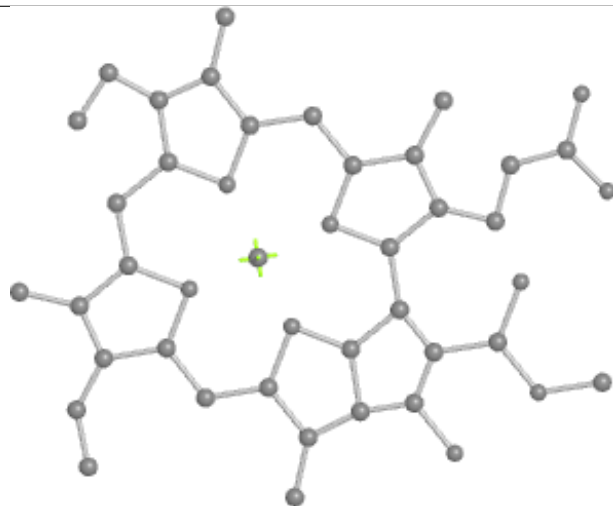
Bond lengths



Bond angles

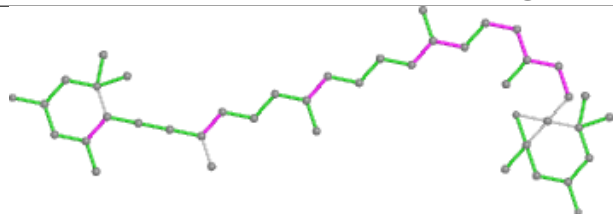


Torsions

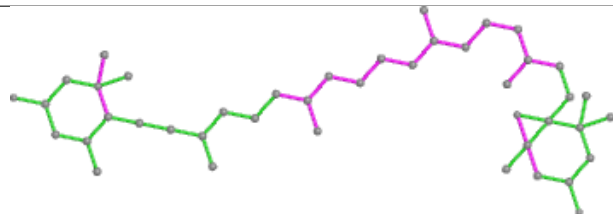


Rings

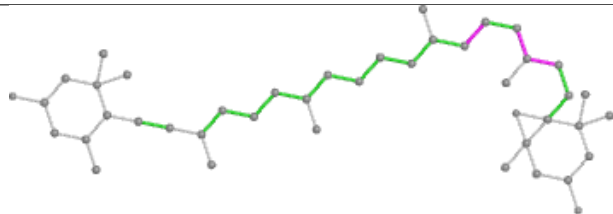
Ligand DD6 5 713



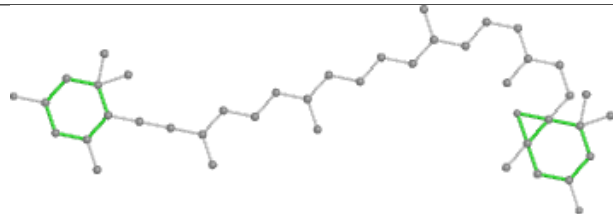
Bond lengths



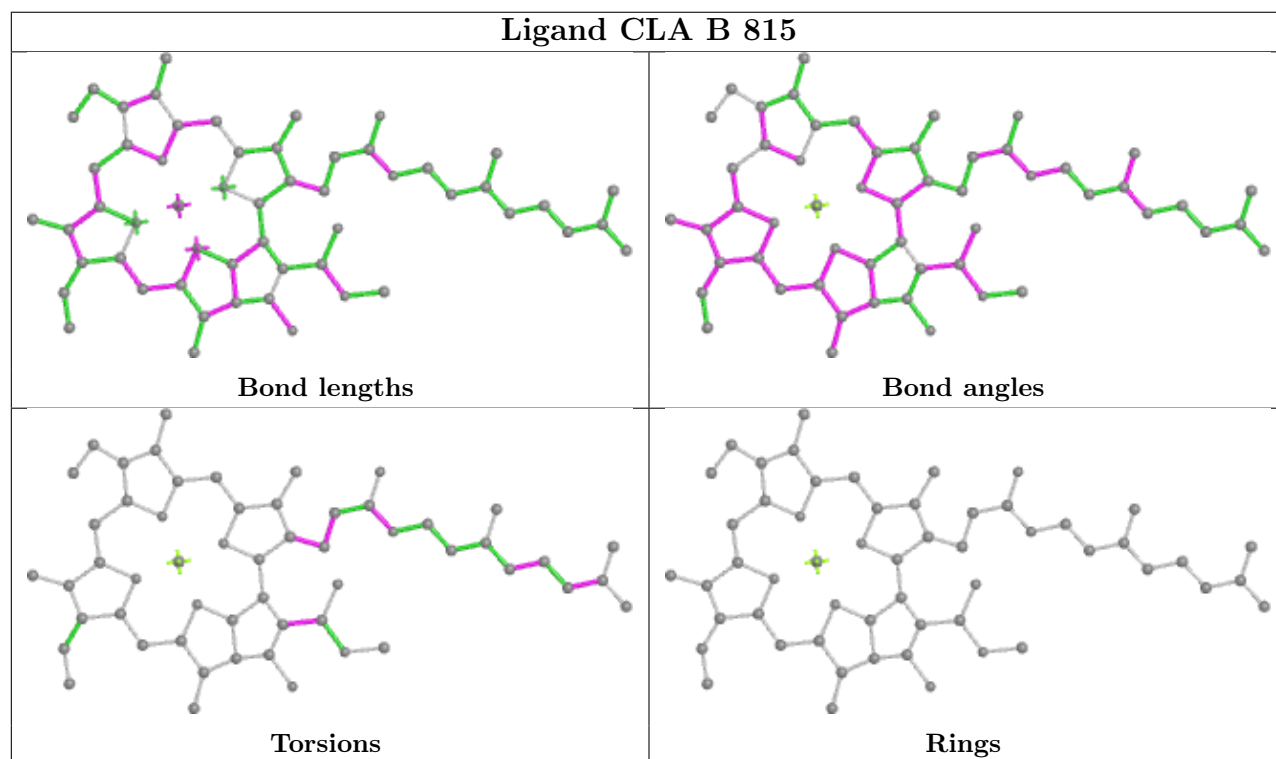
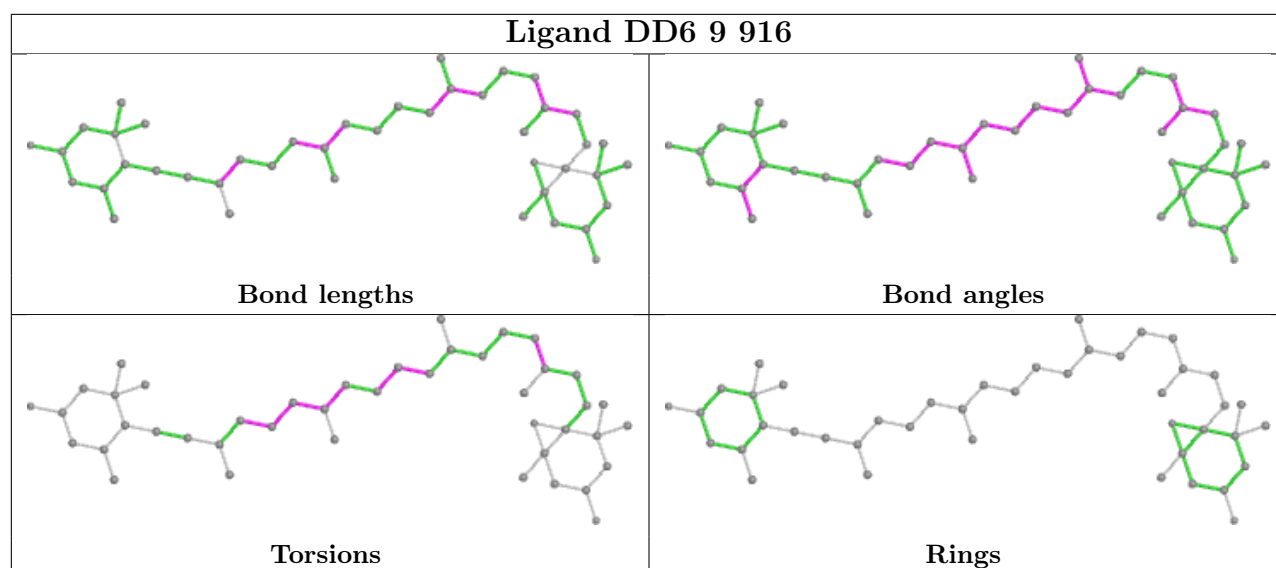
Bond angles

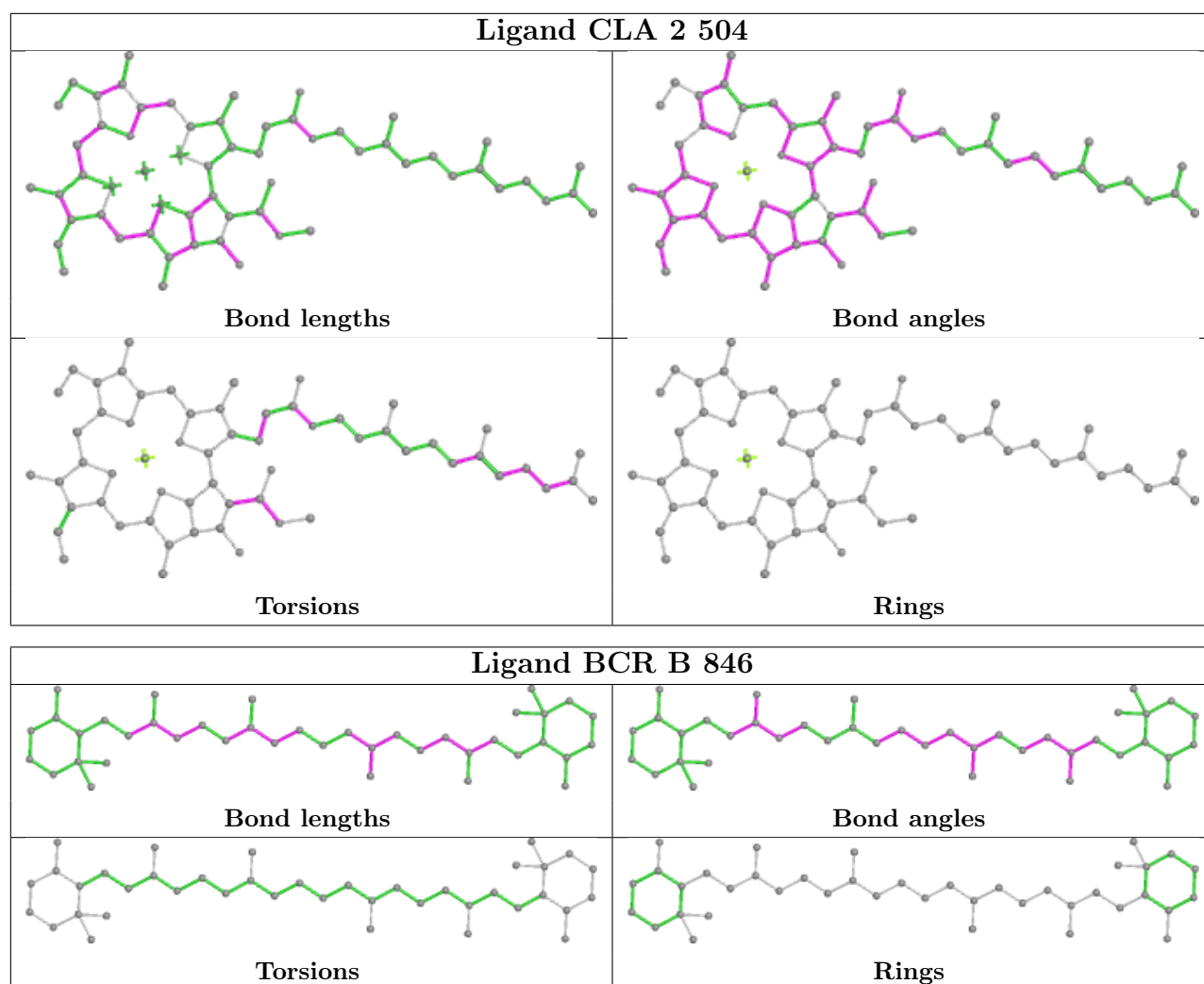


Torsions

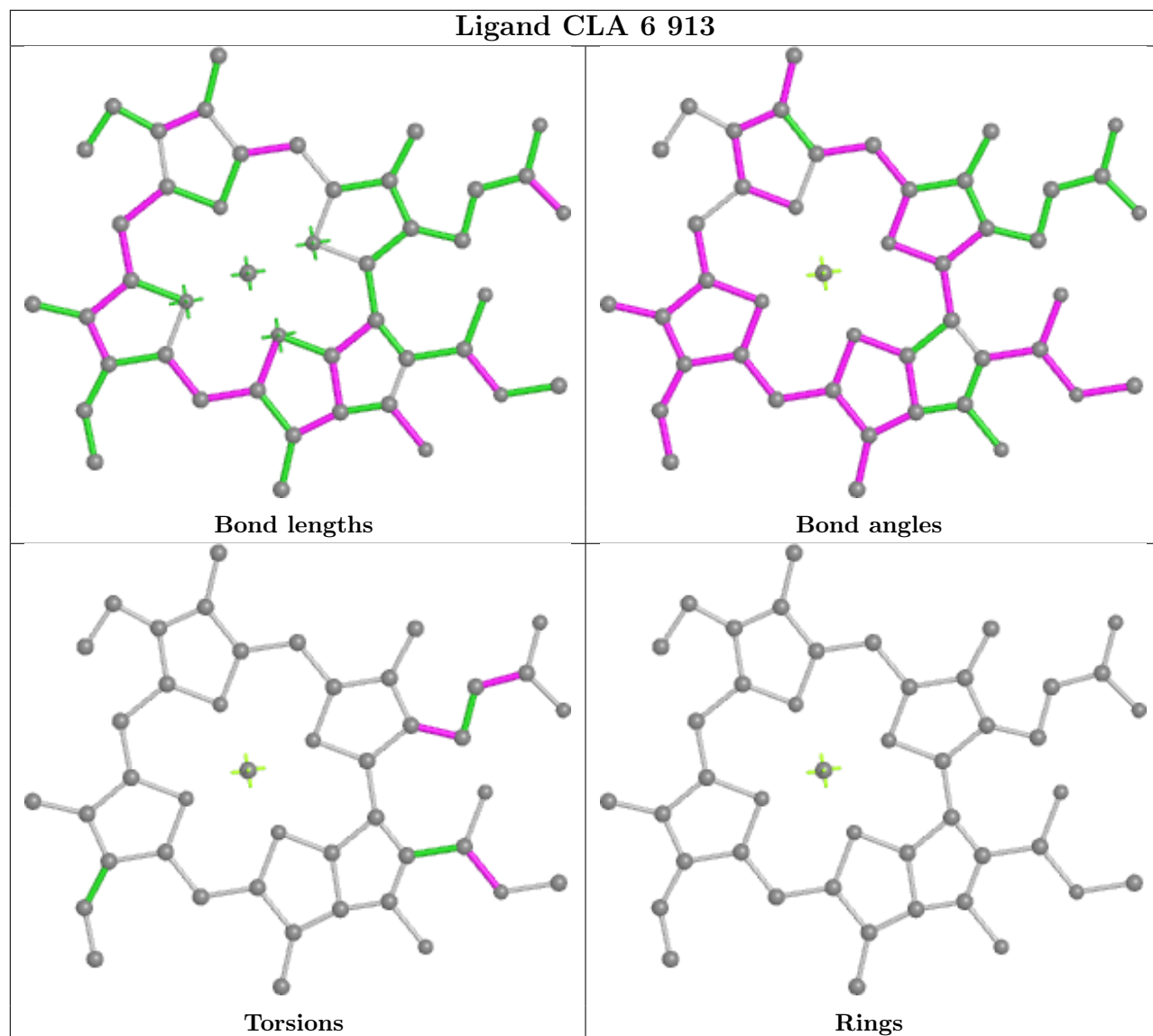


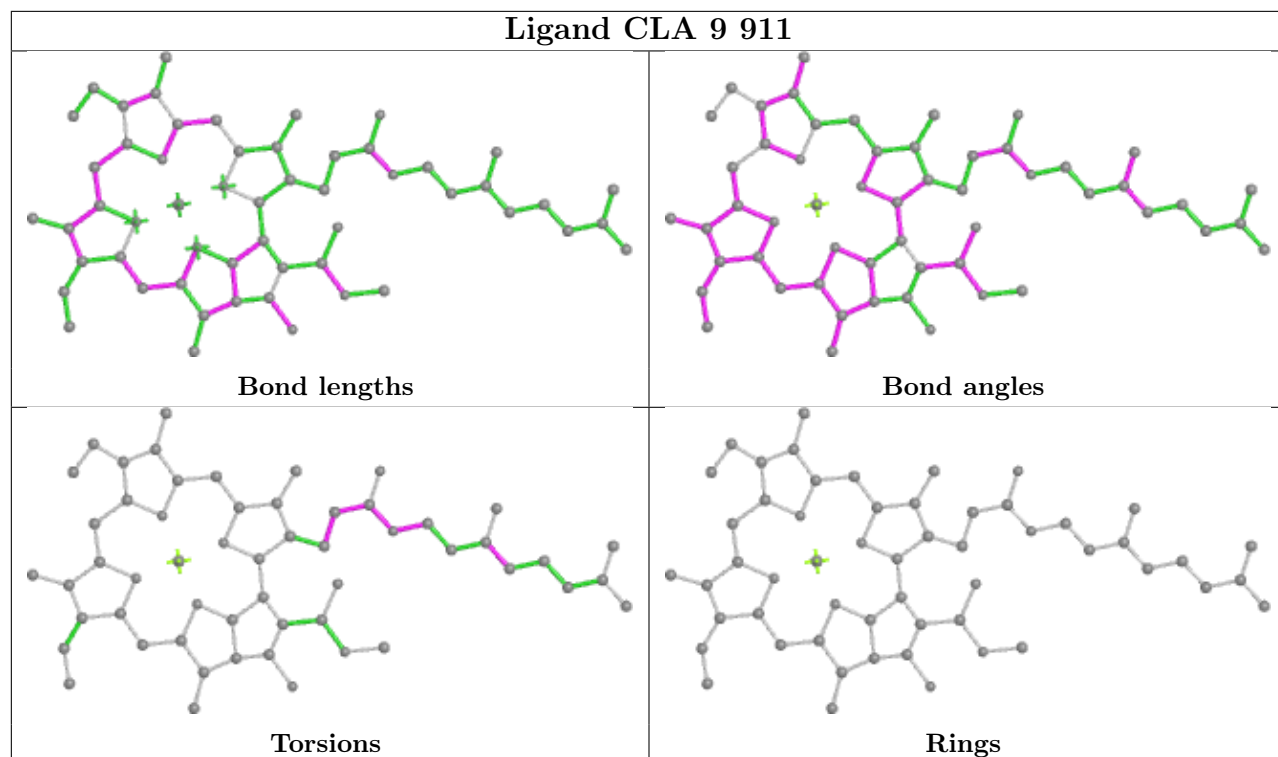
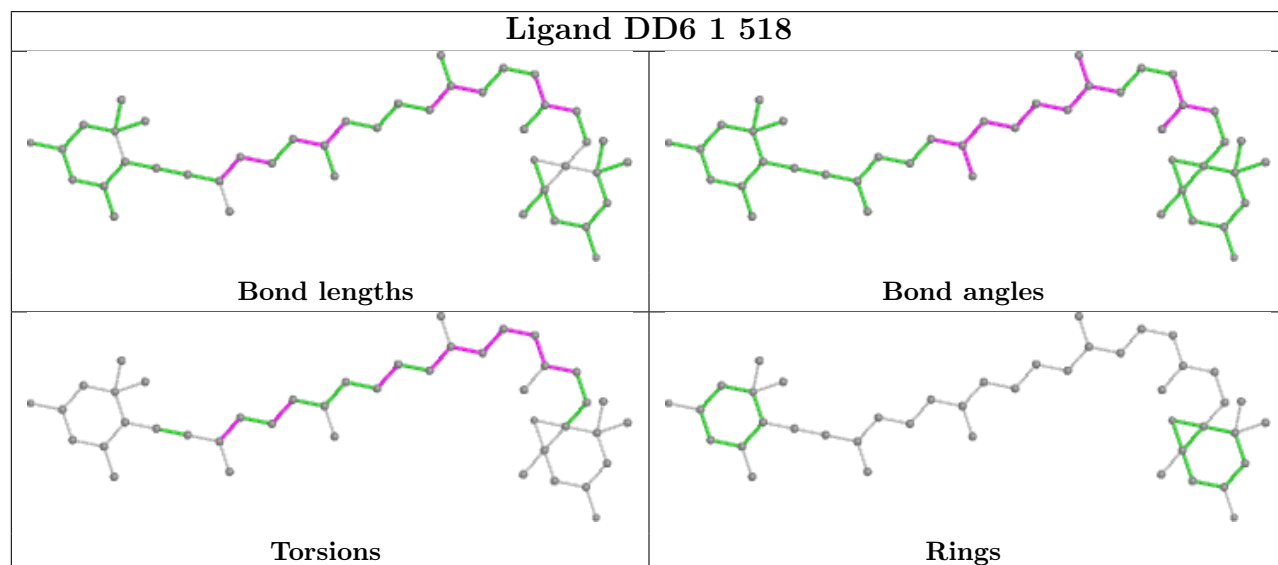
Rings



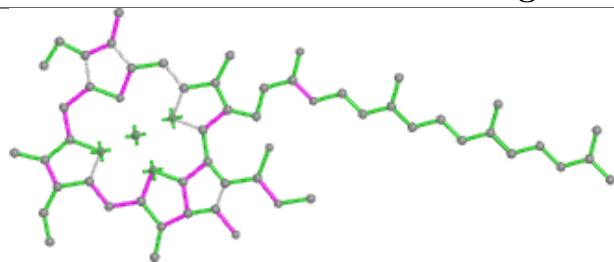


Ligand CLA 6 913

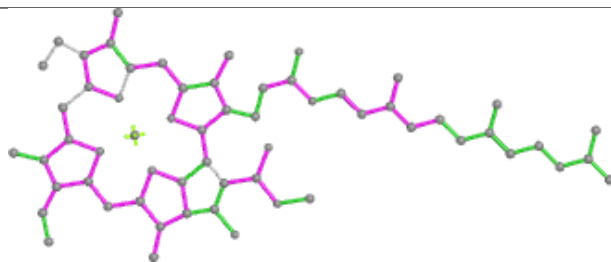


Ligand CLA 9 911**Ligand DD6 1 518**

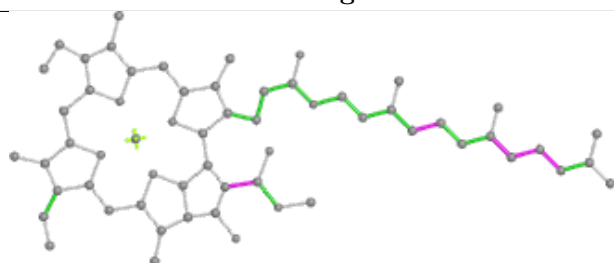
Ligand CLA 8 604



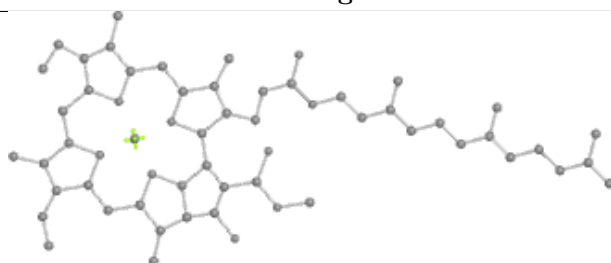
Bond lengths



Bond angles

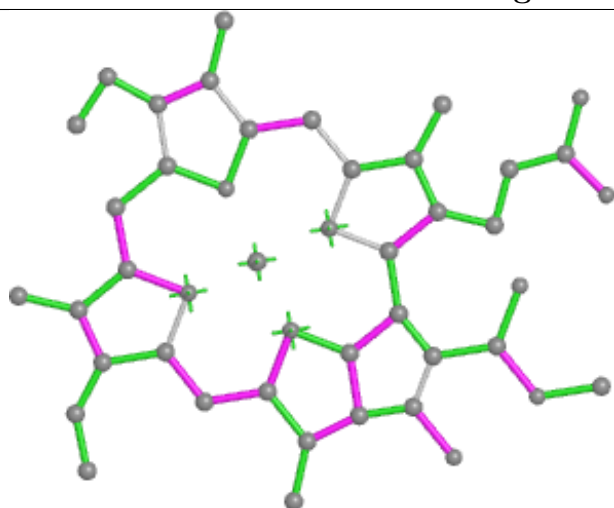


Torsions

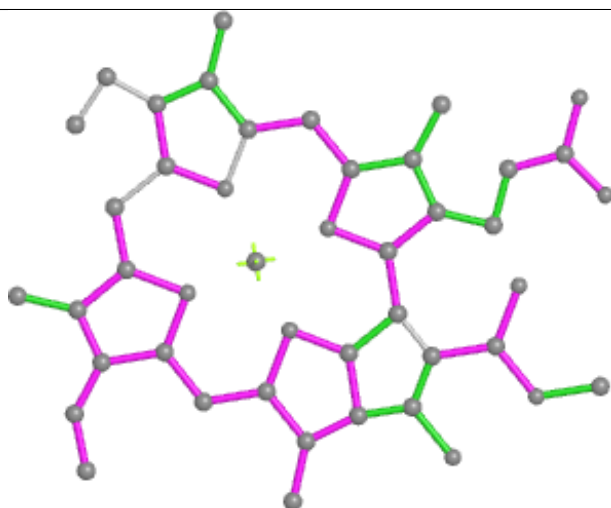


Rings

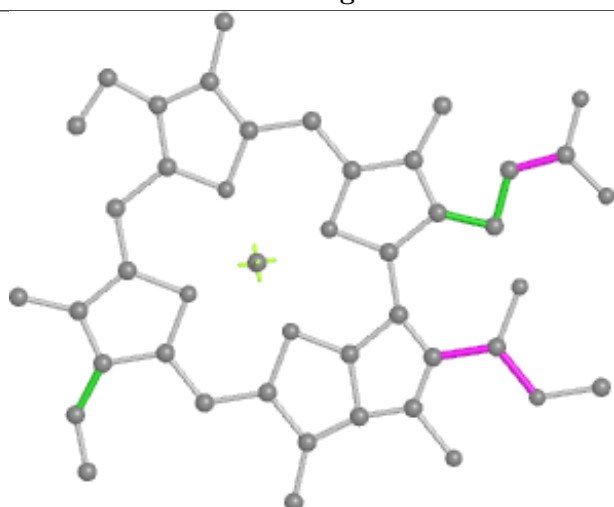
Ligand CLA A 837



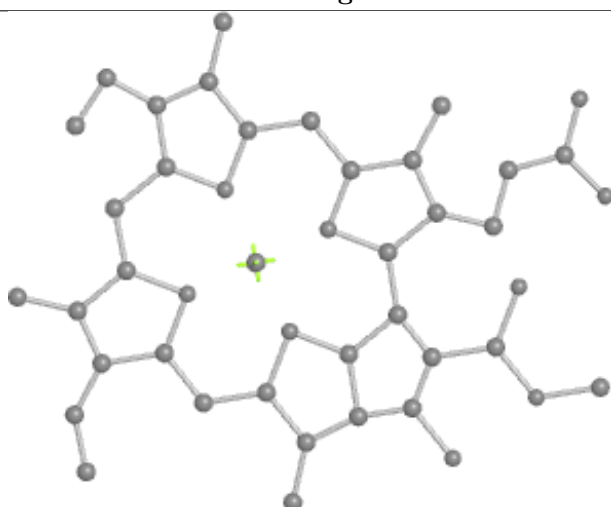
Bond lengths



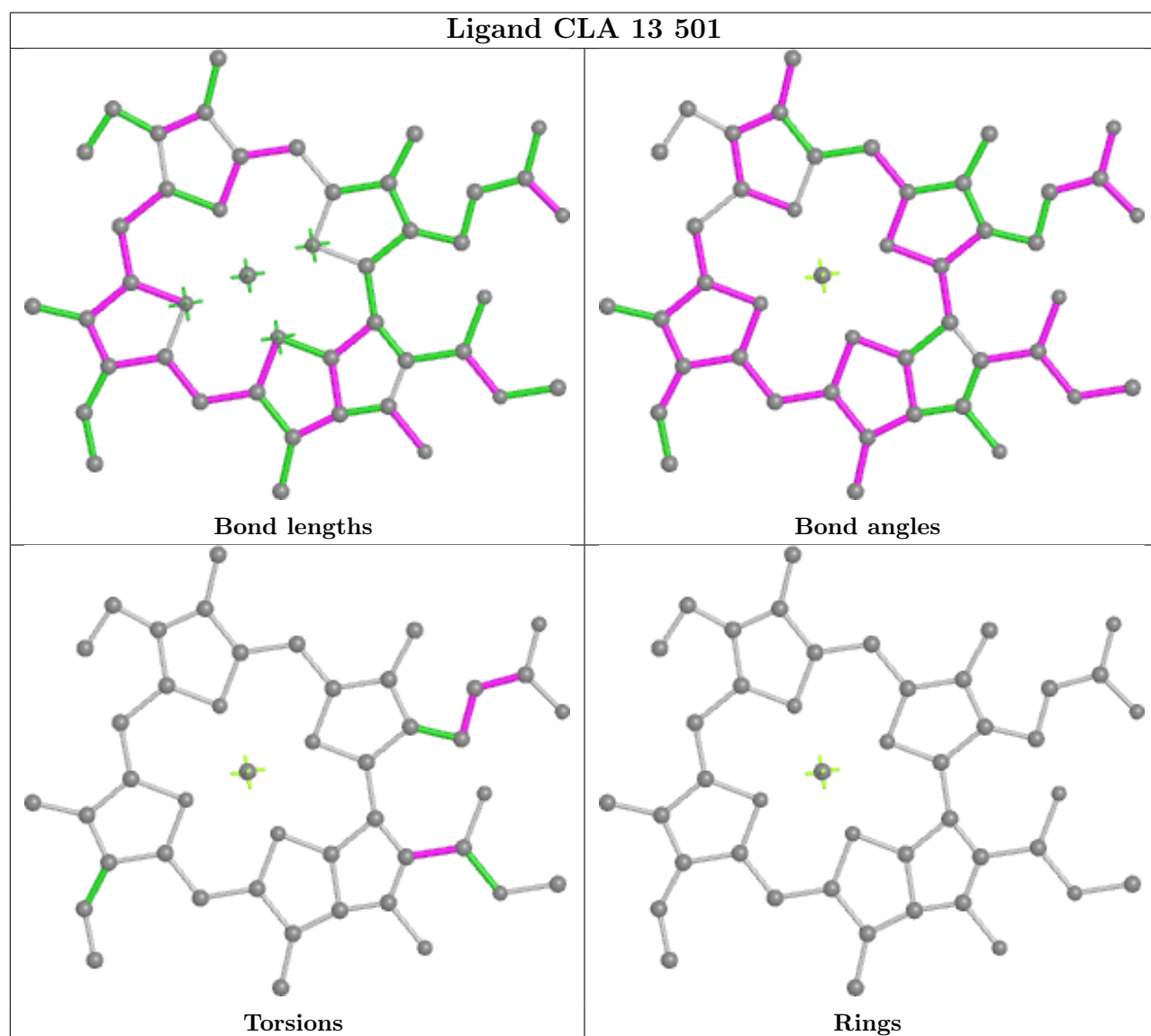
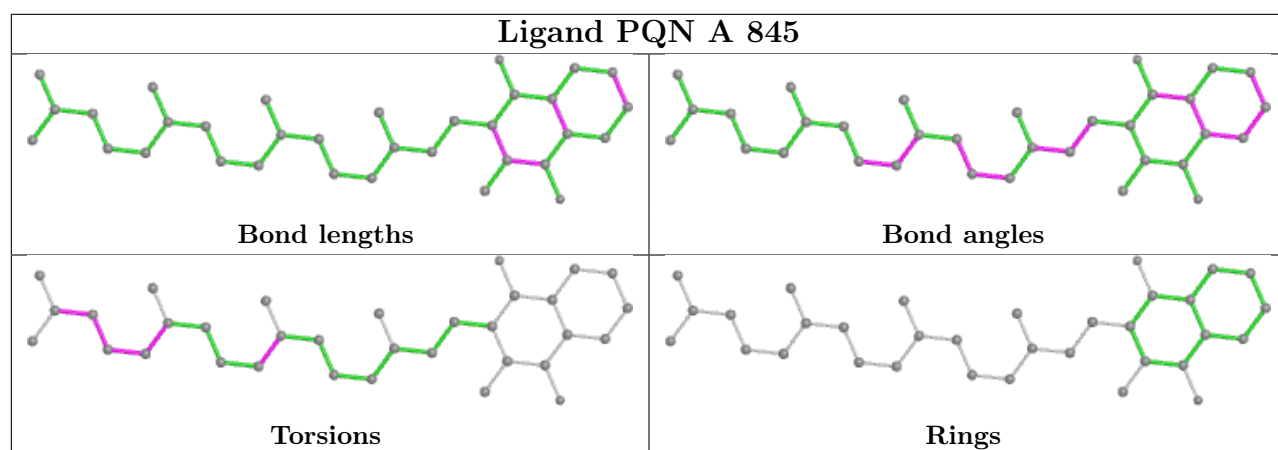
Bond angles



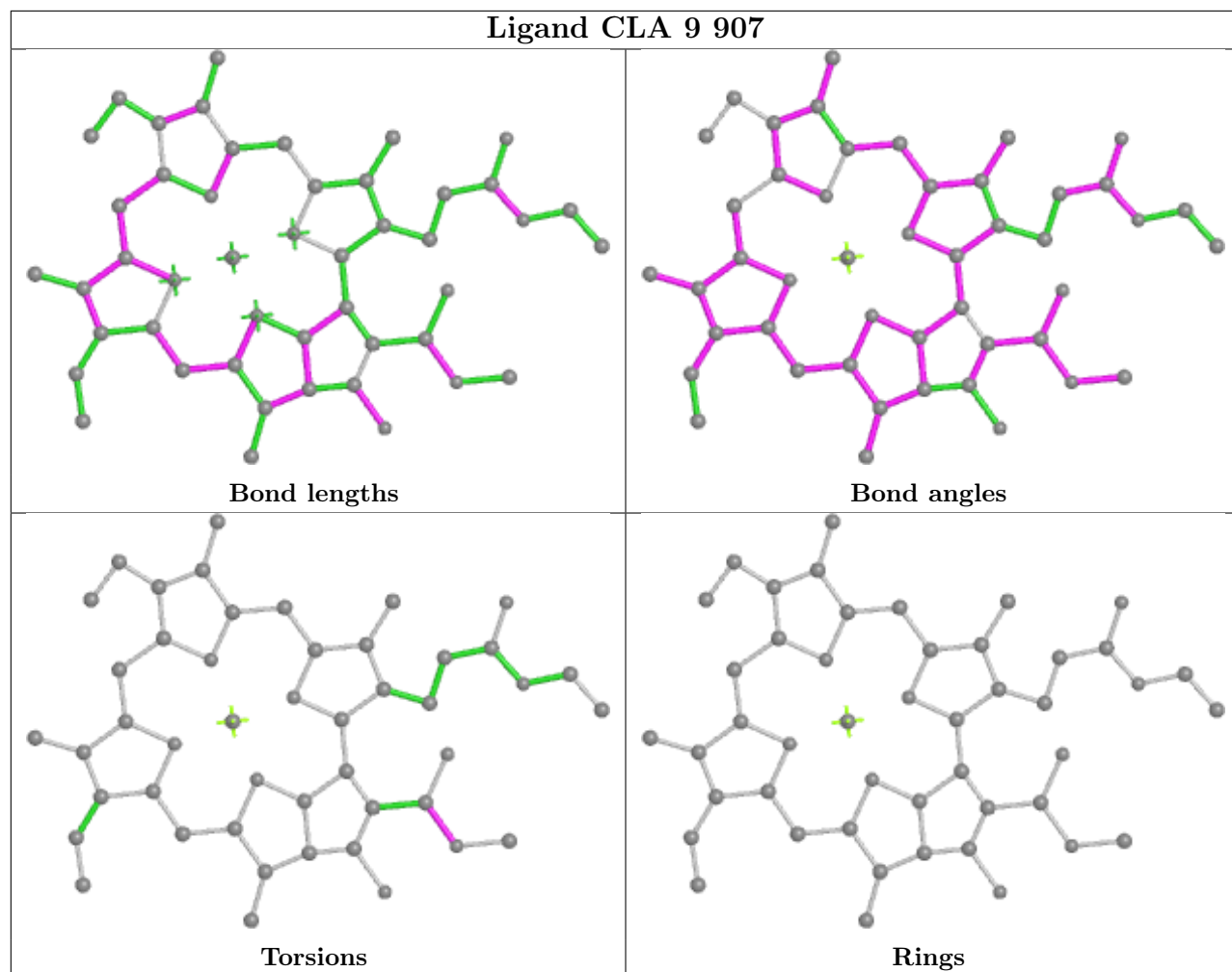
Torsions



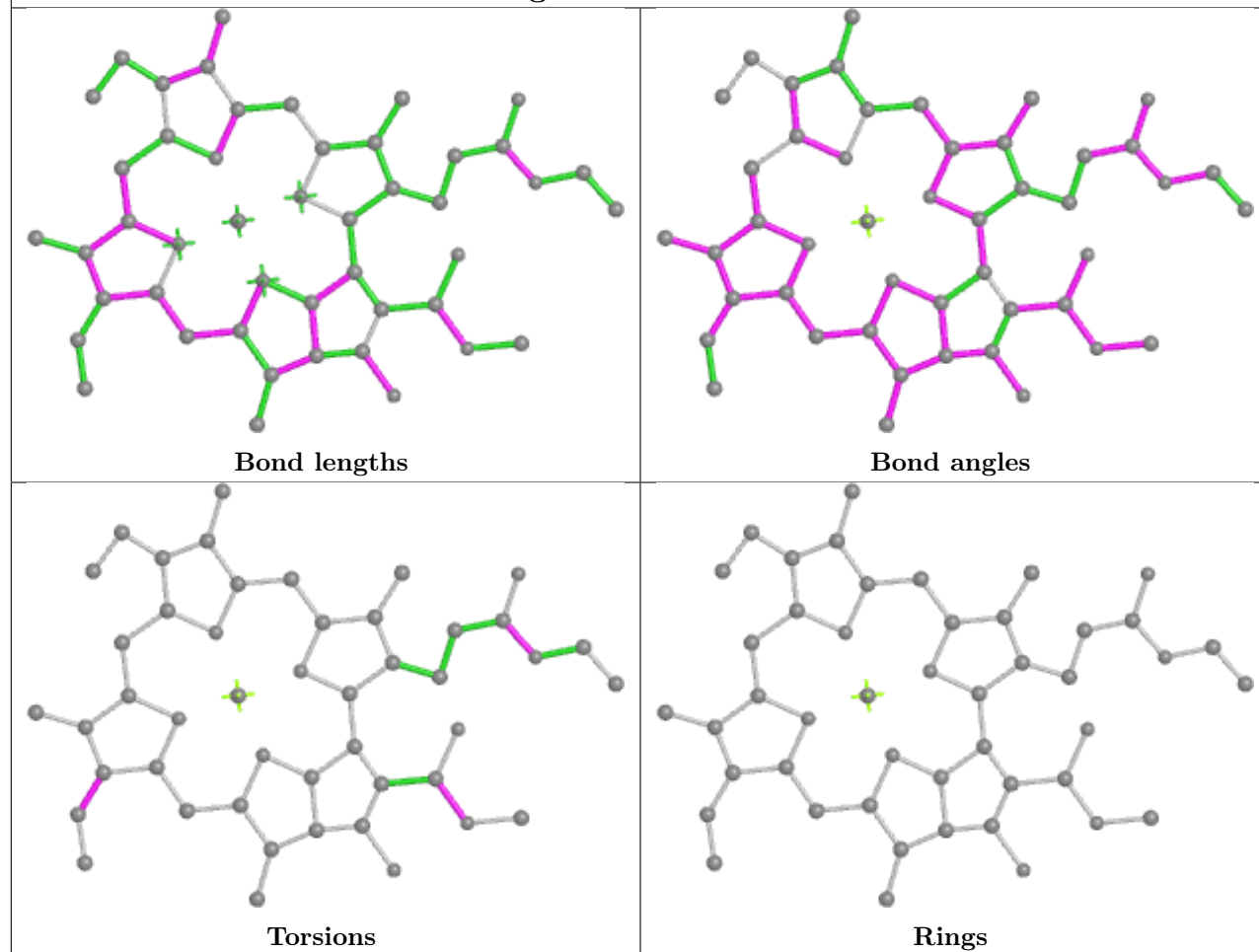
Rings



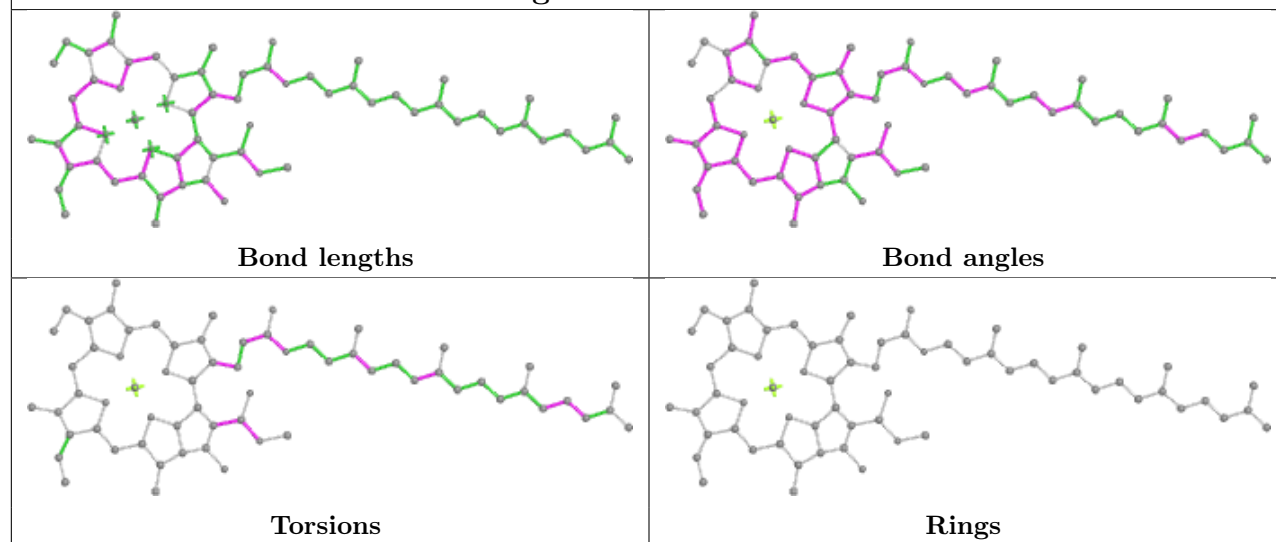
Ligand CLA 9 907



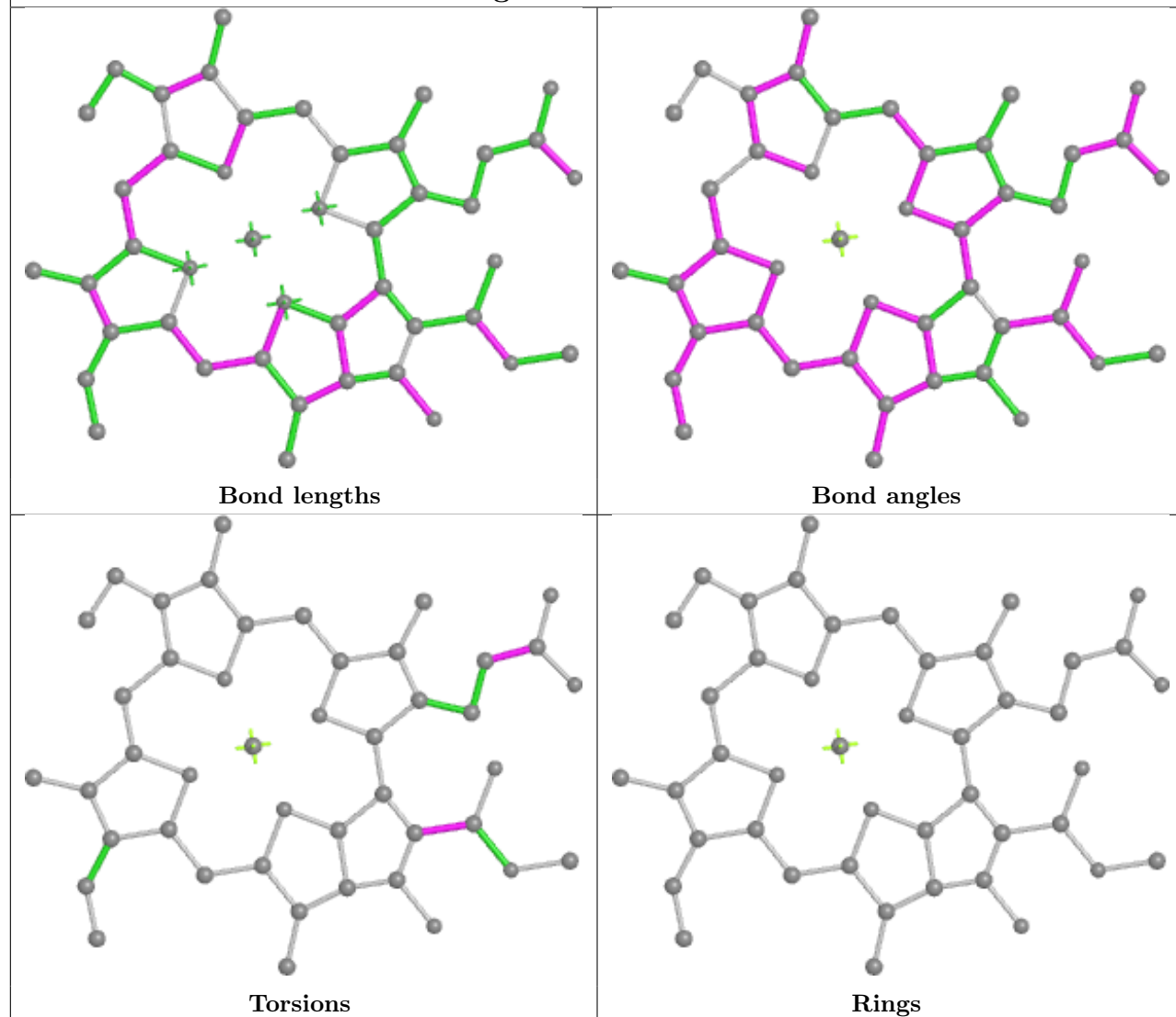
Ligand CLA 7 706



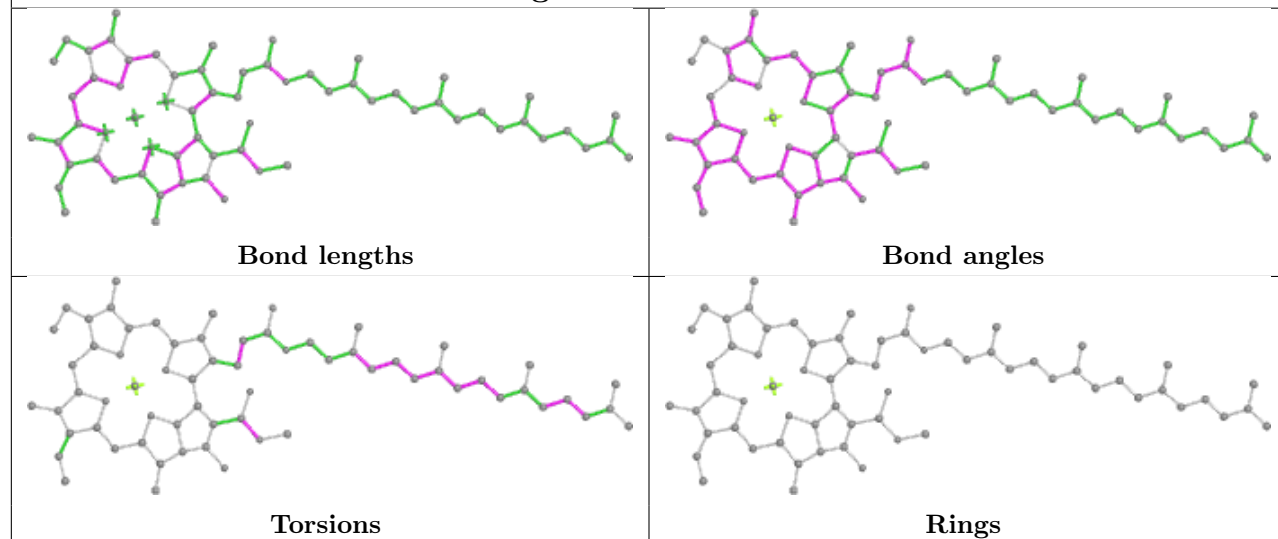
Ligand CLA B 839



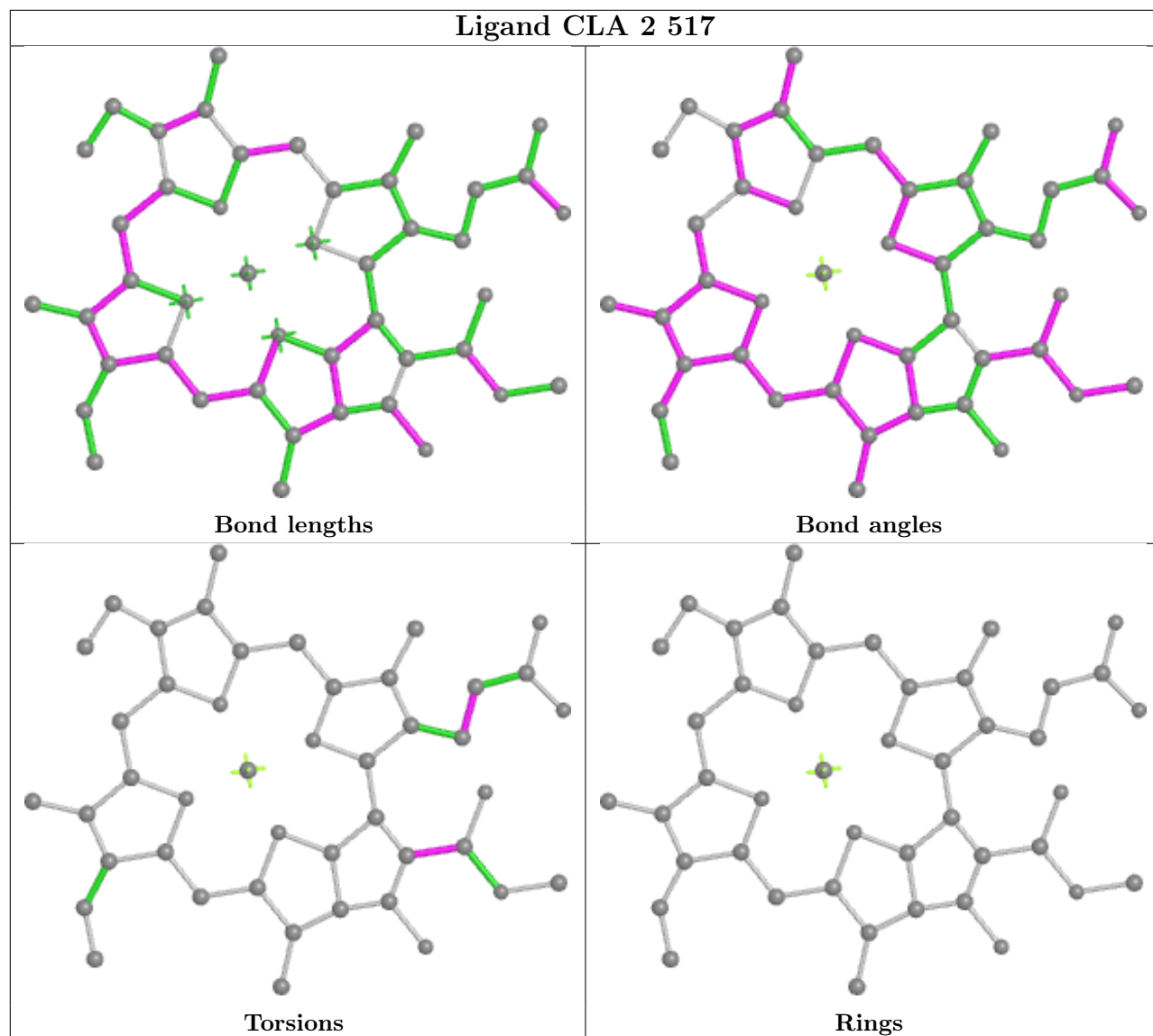
Ligand CLA 6 911



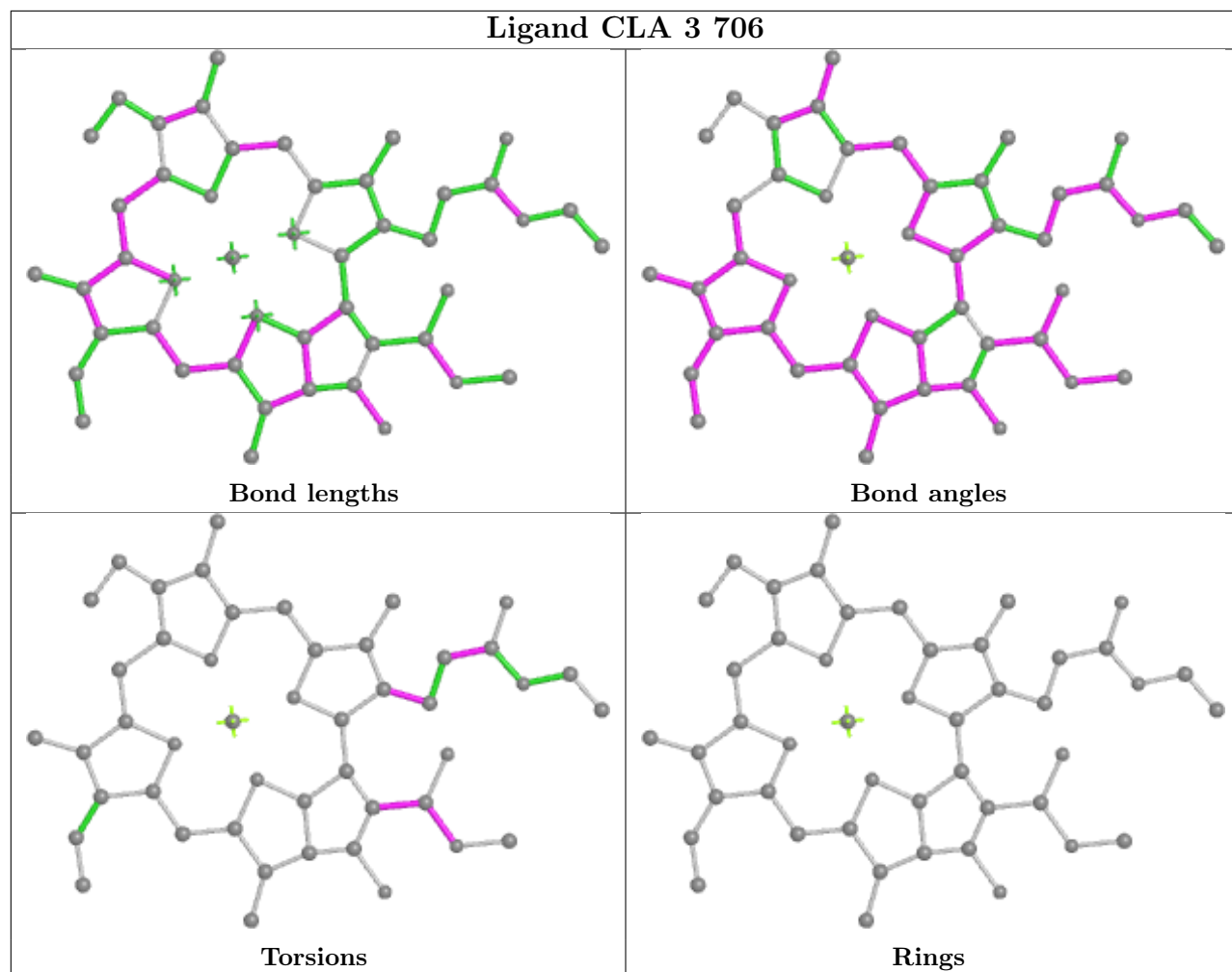
Ligand CLA A 810



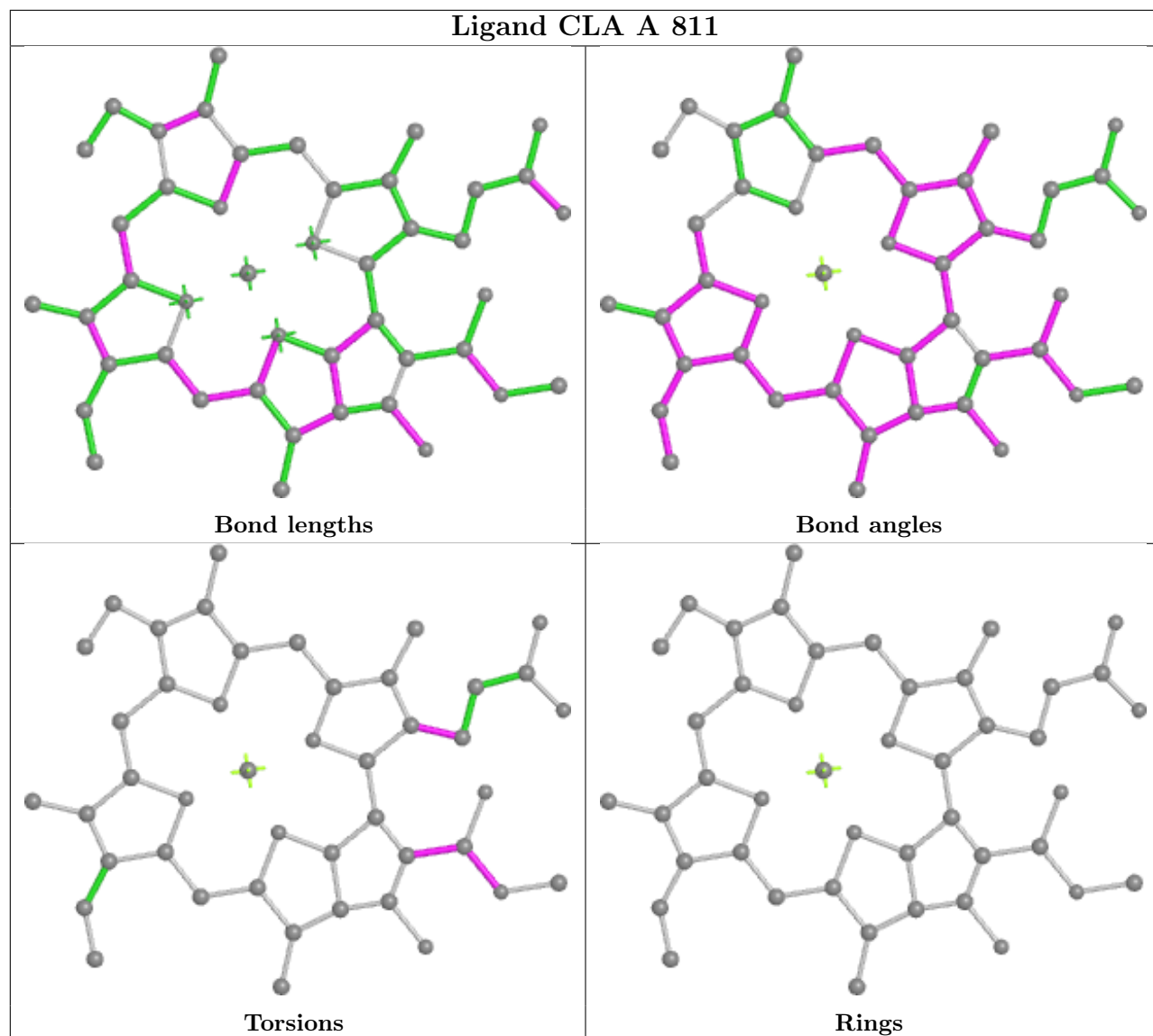
Ligand CLA 2 517

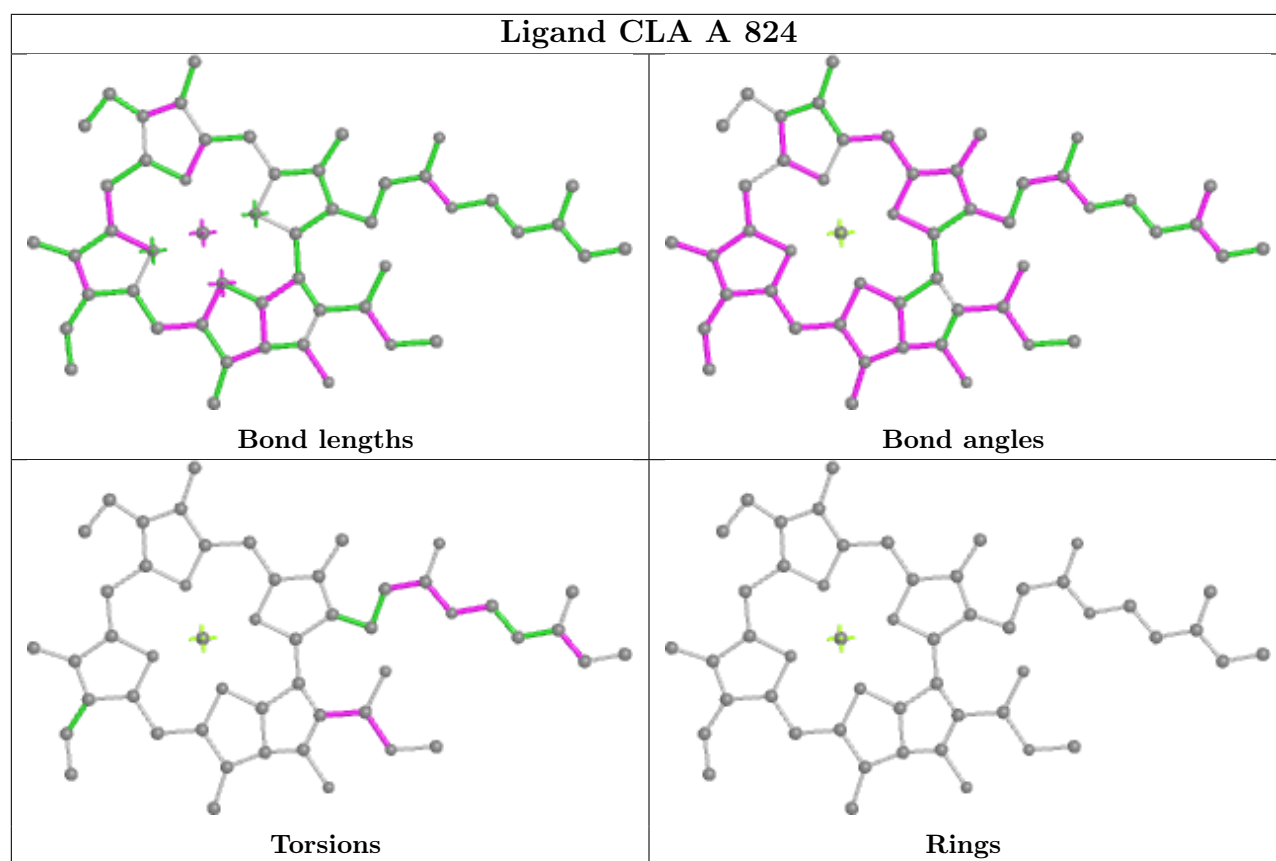


Ligand CLA 3 706

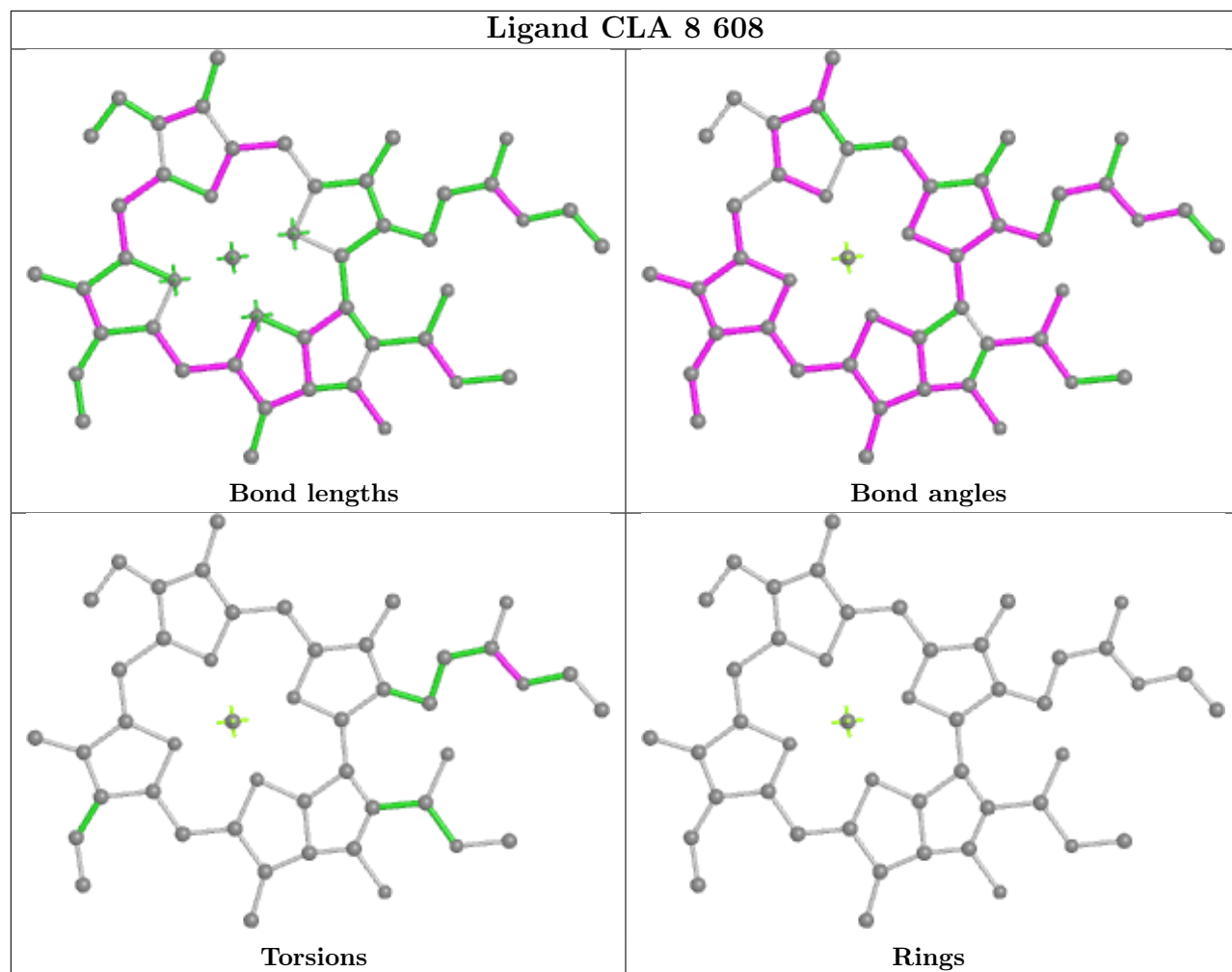


Ligand CLA A 811

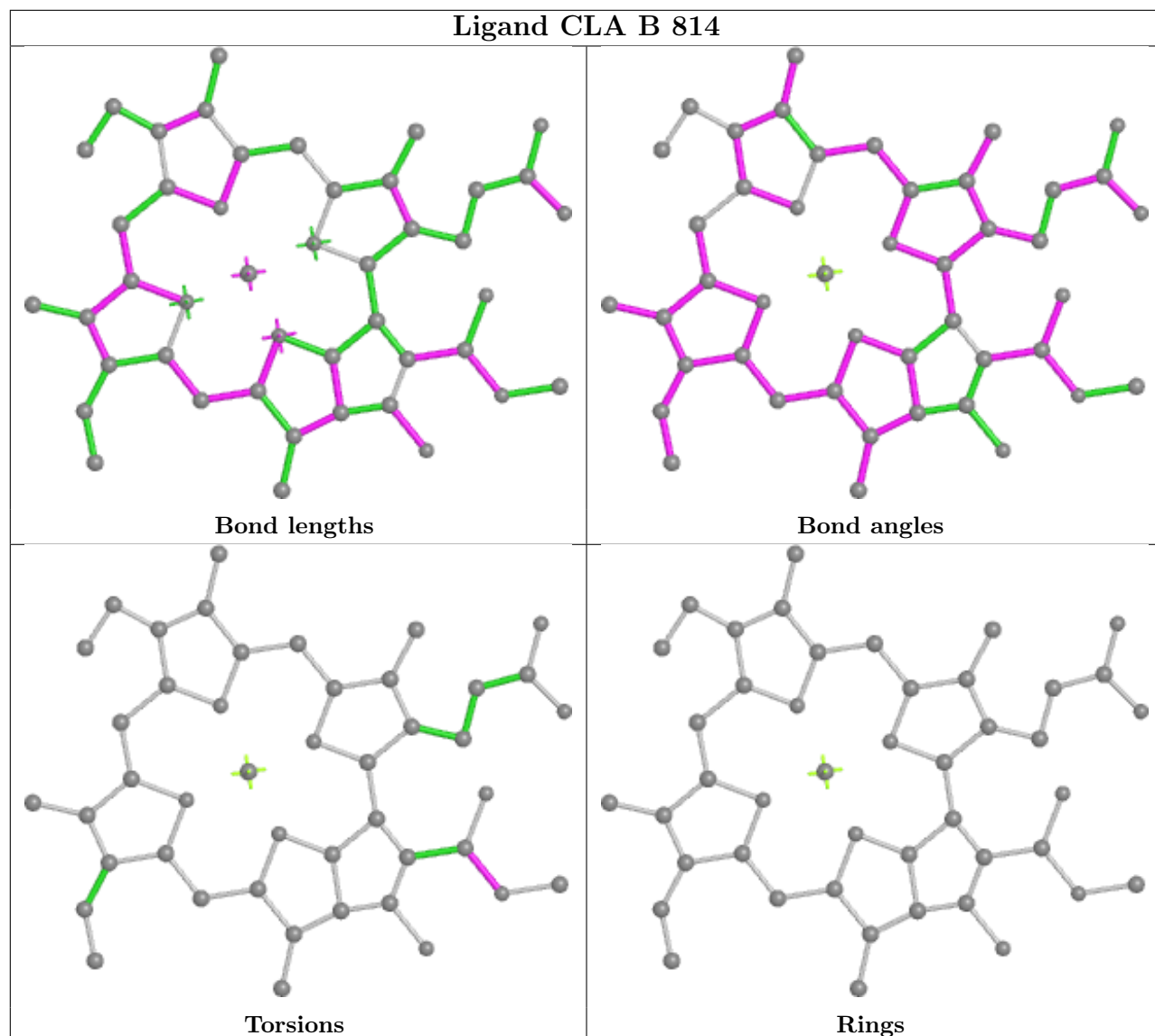




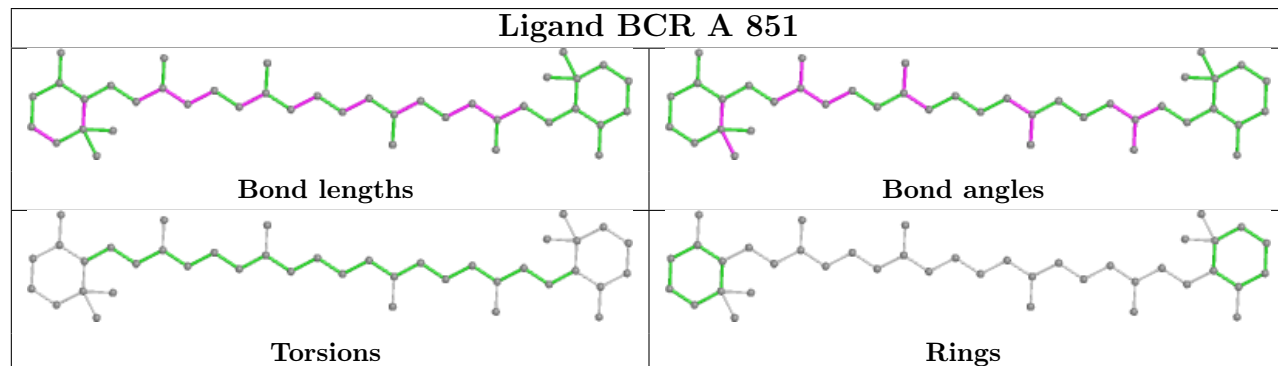
Ligand CLA 8 608

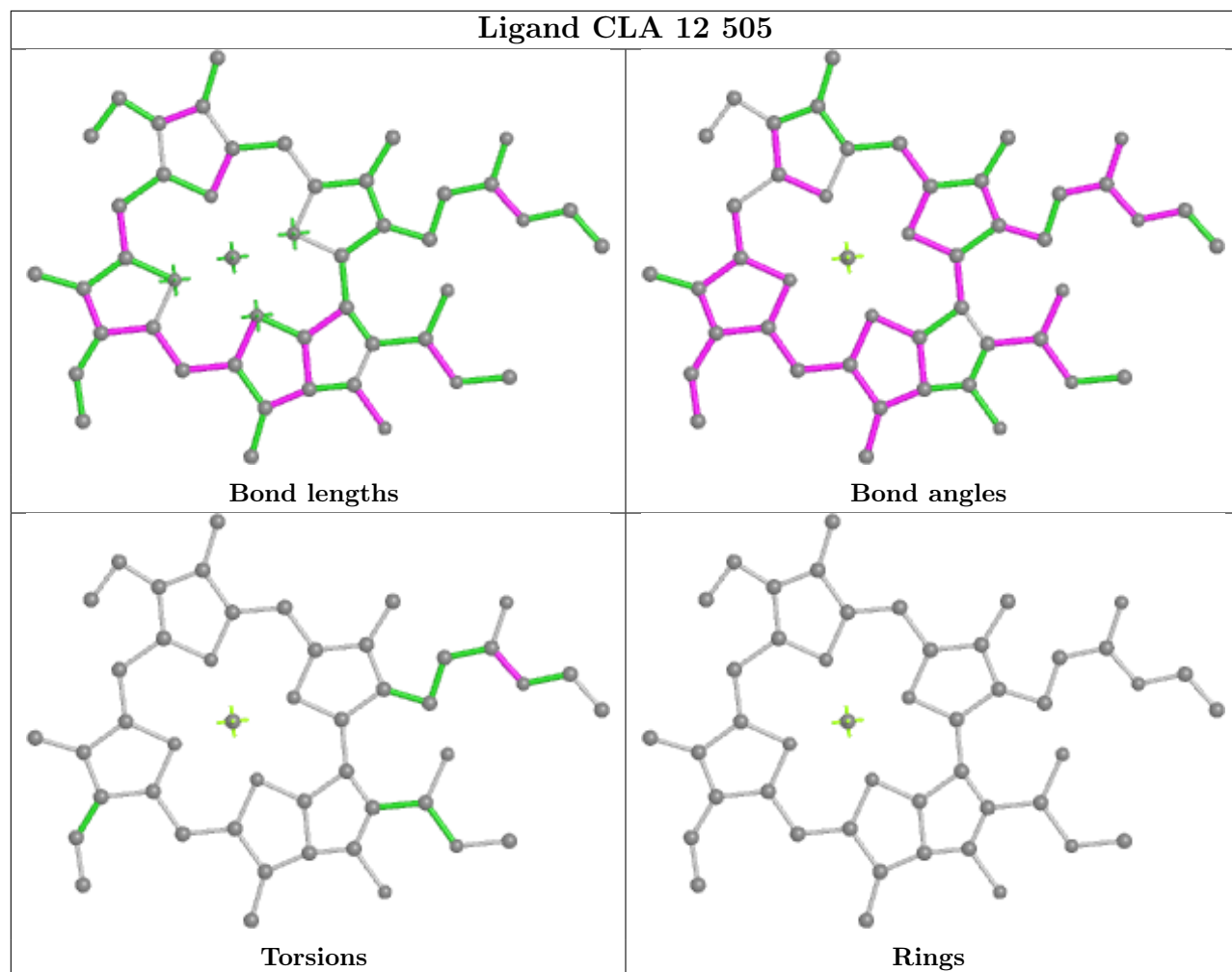


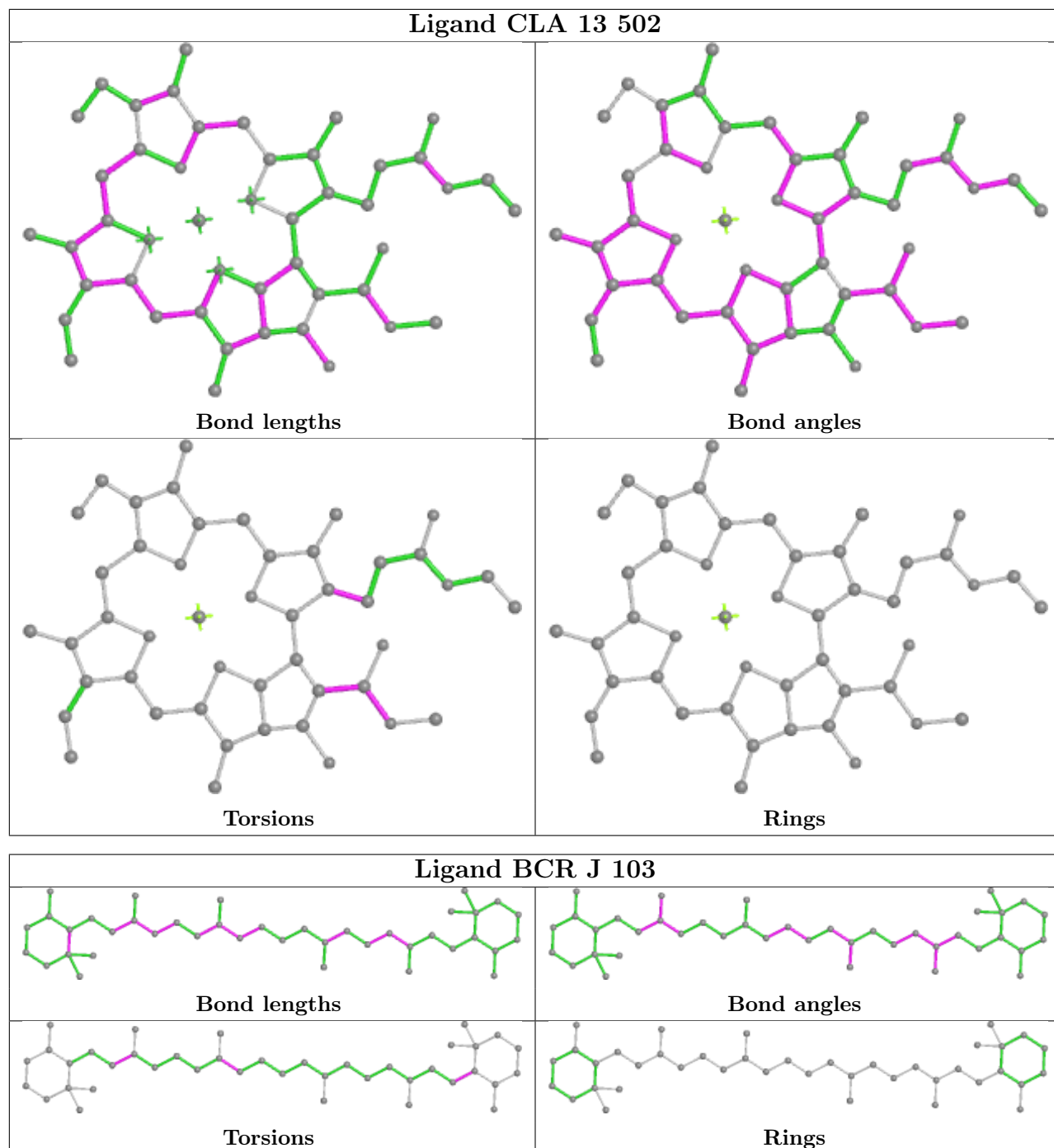
Ligand CLA B 814

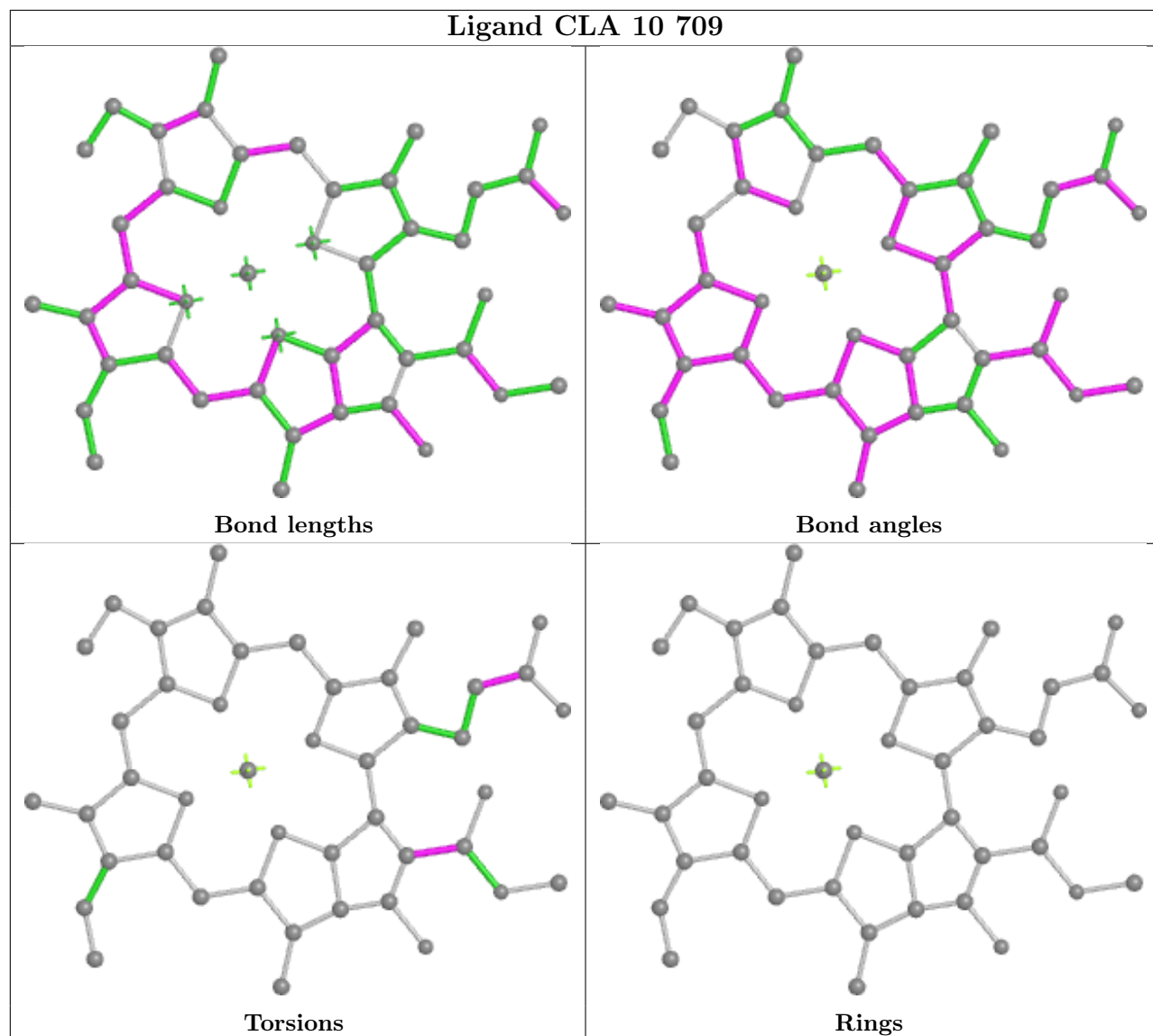


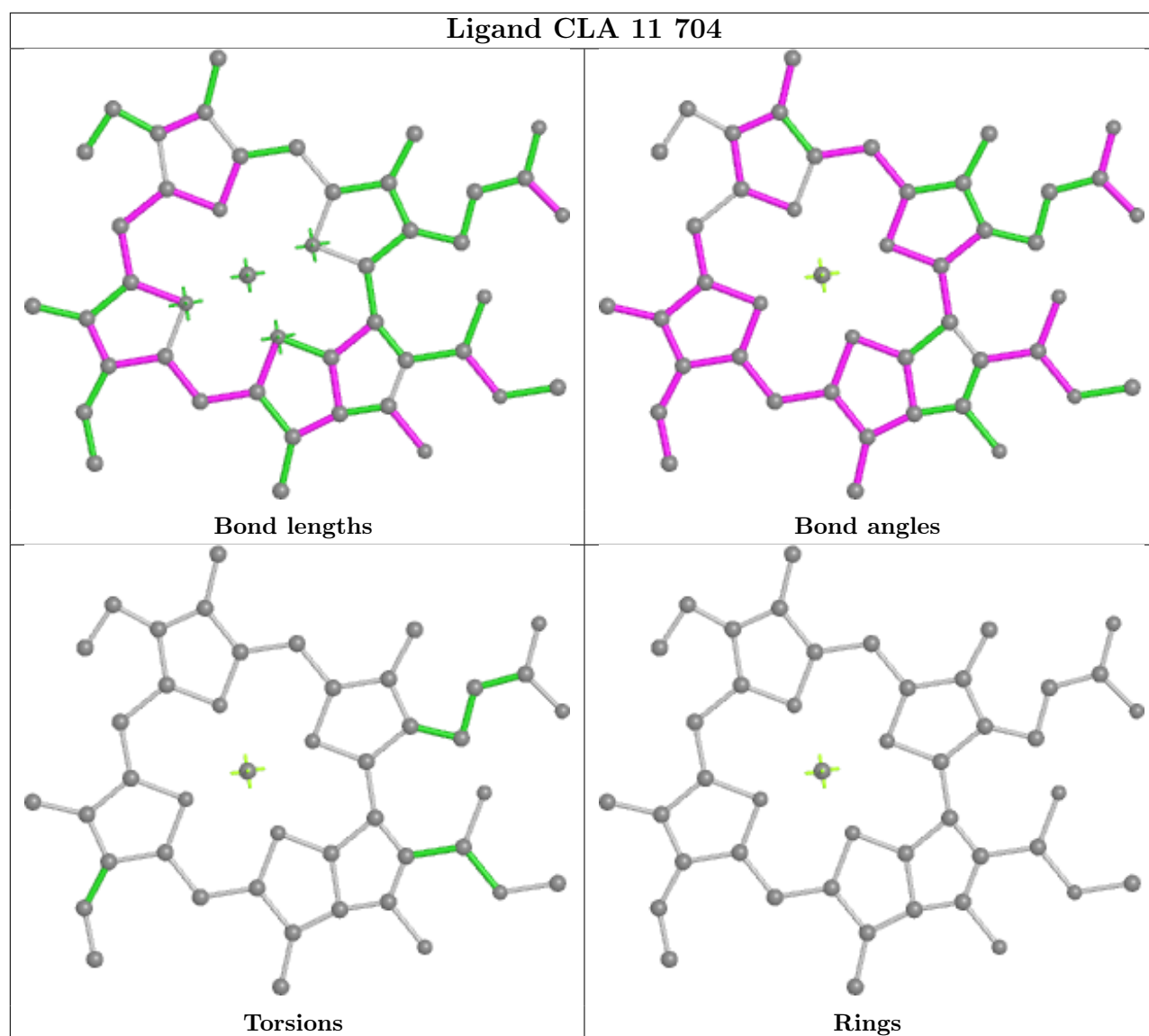
Ligand BCR A 851



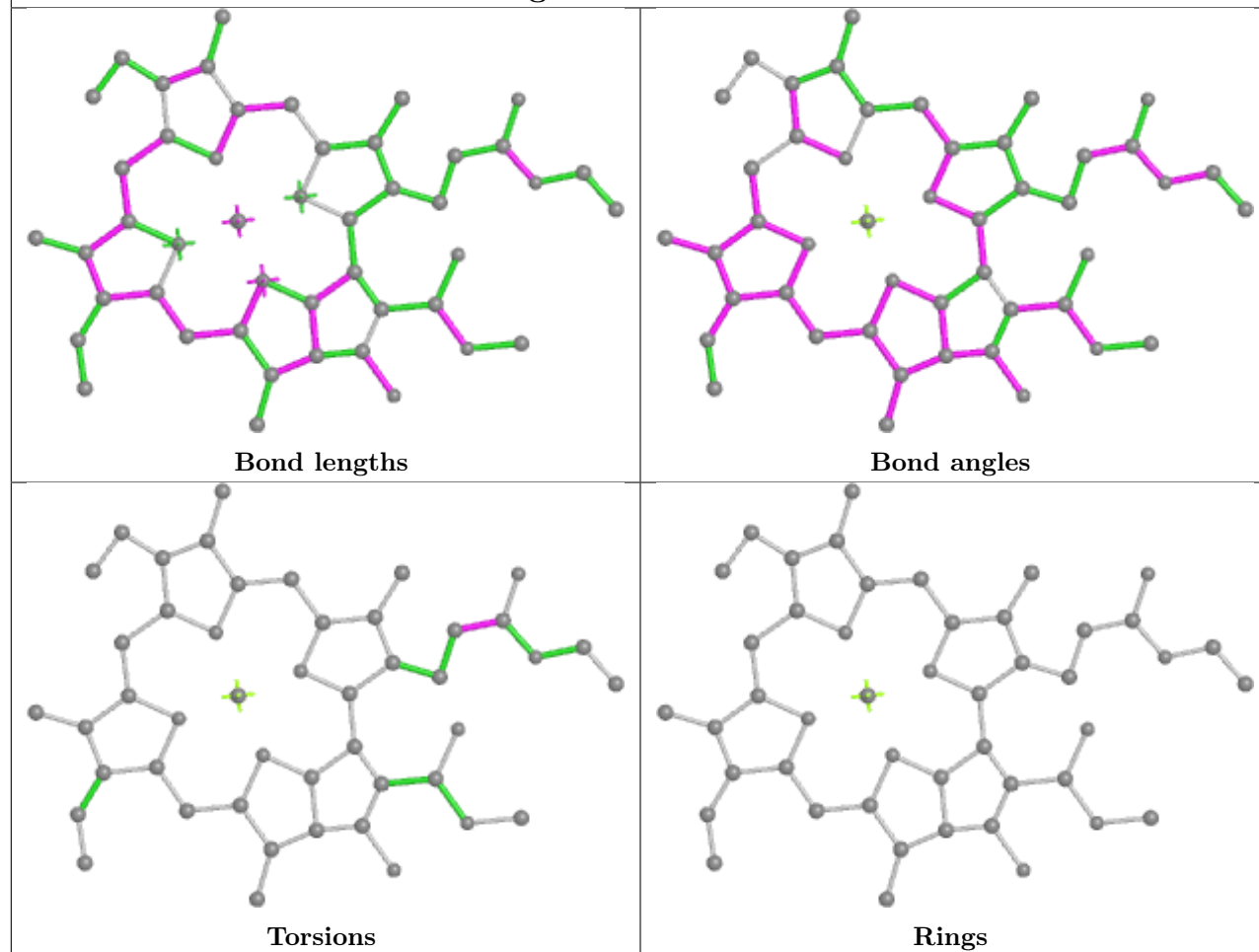




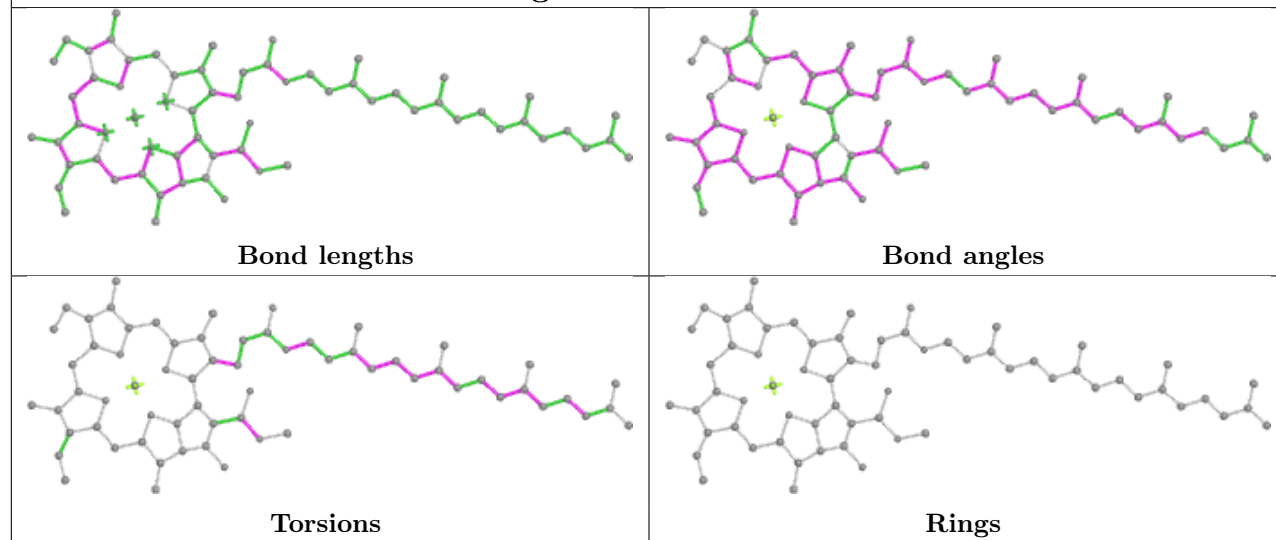




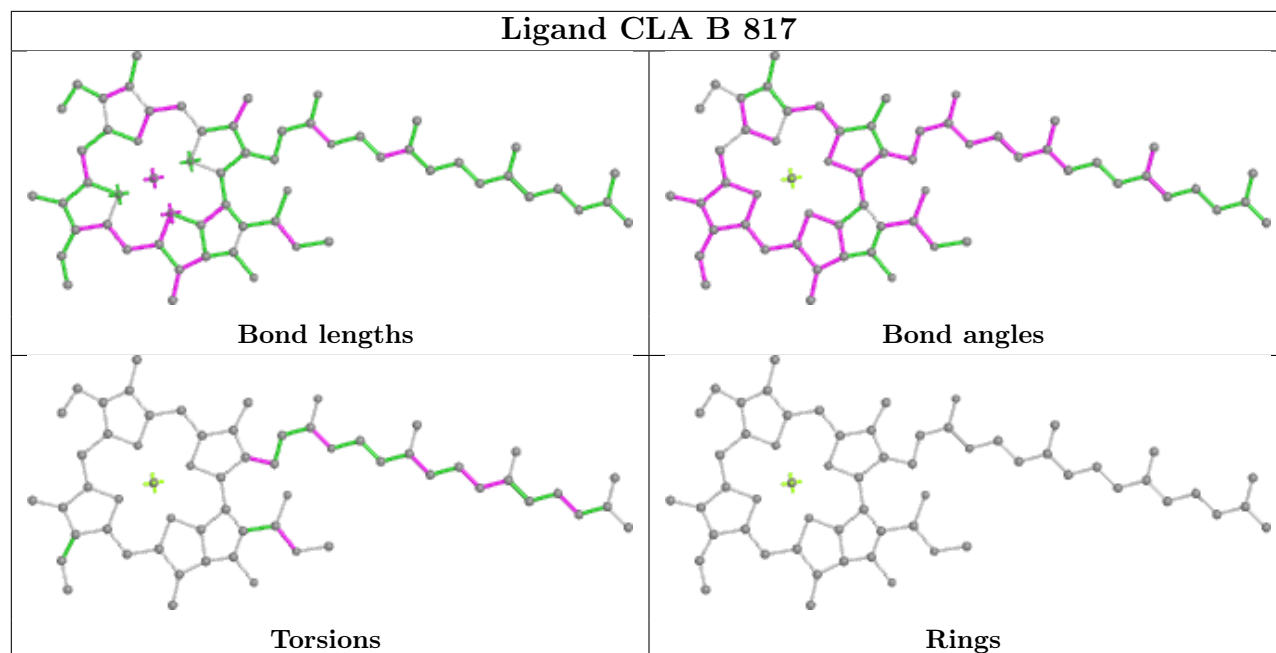
Ligand CLA 8 614



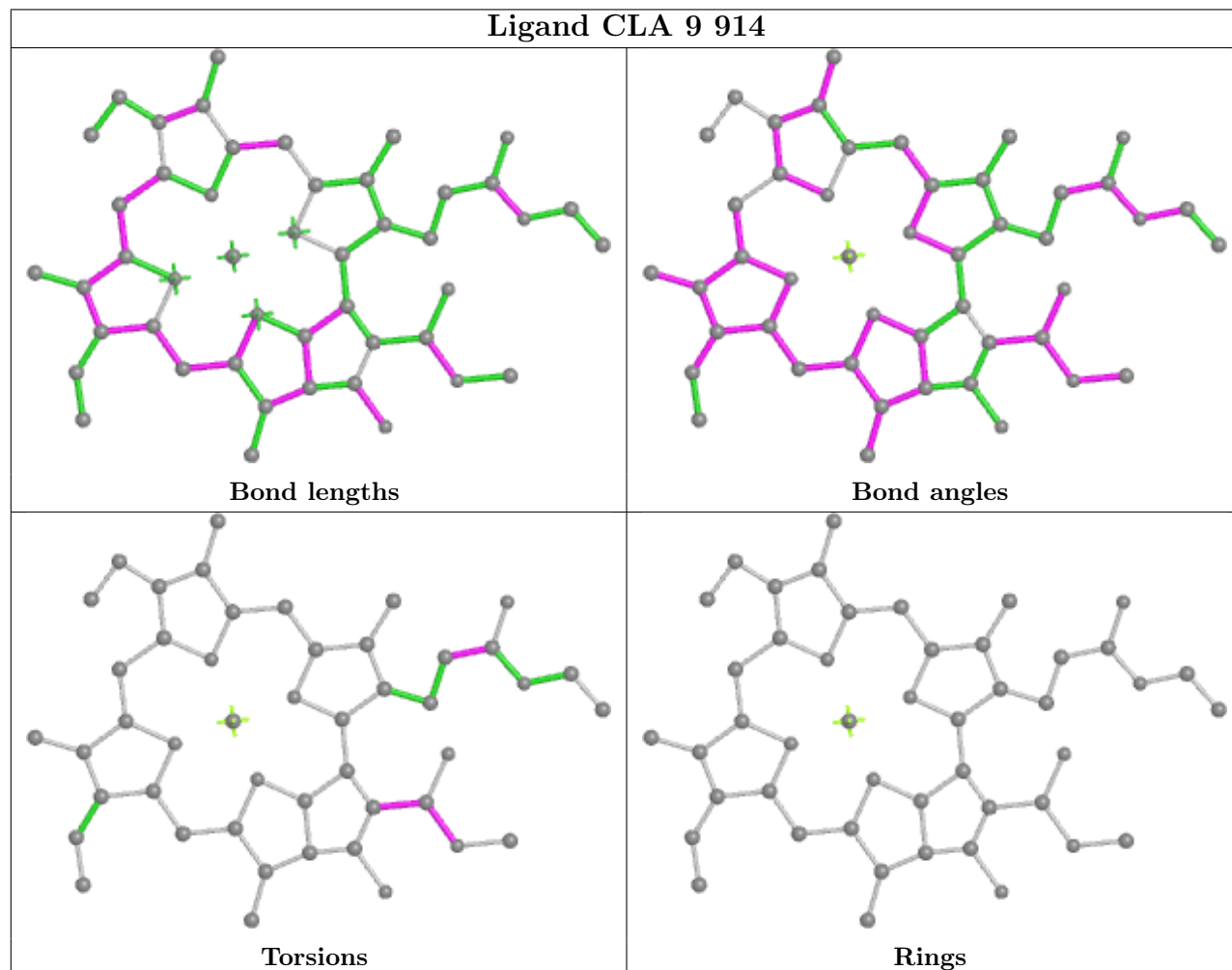
Ligand CLA A 829

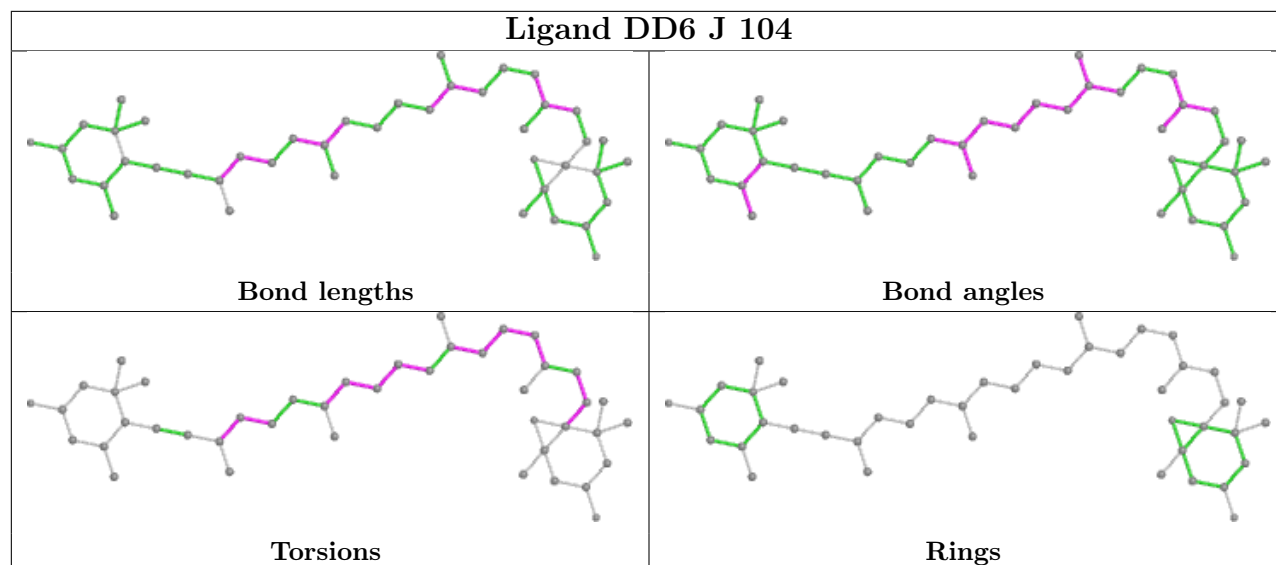
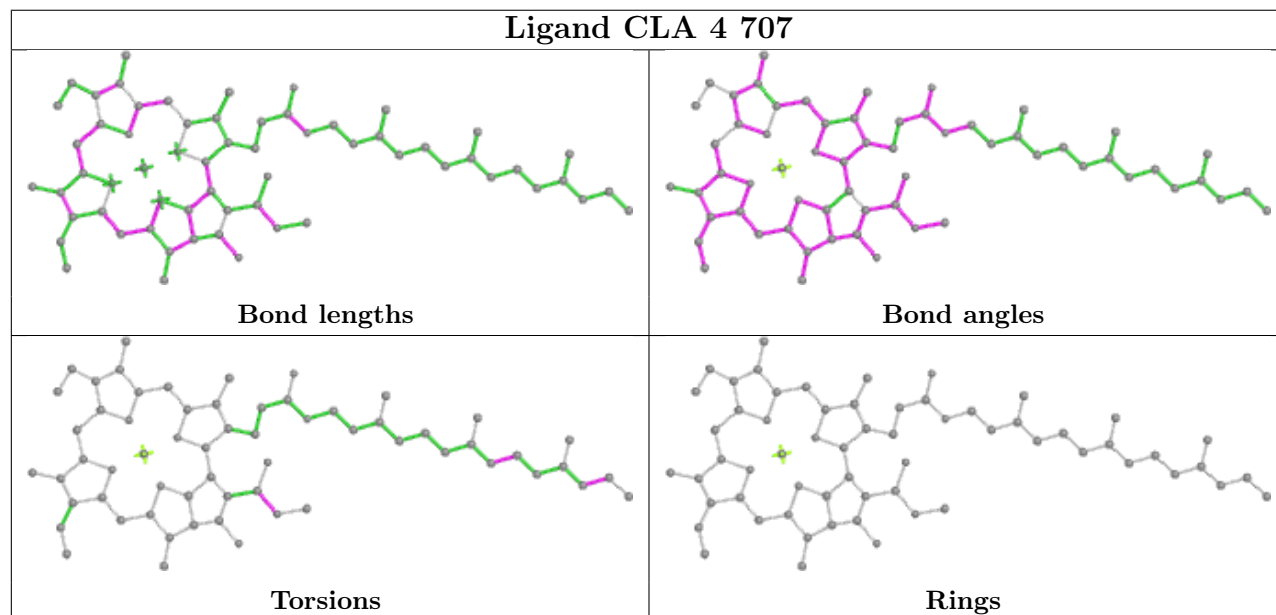


Ligand CLA B 817

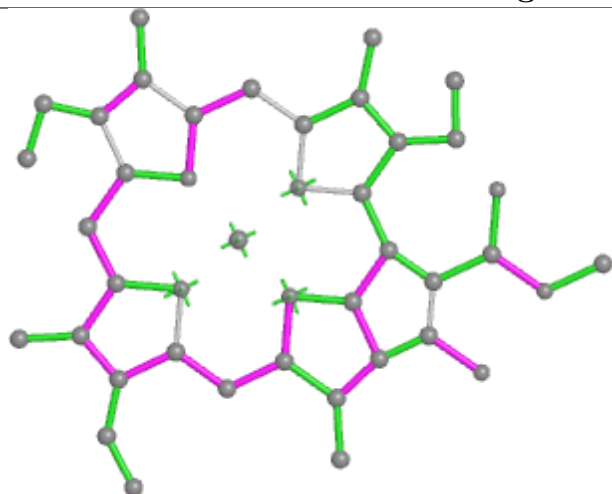


Ligand CLA 9 914

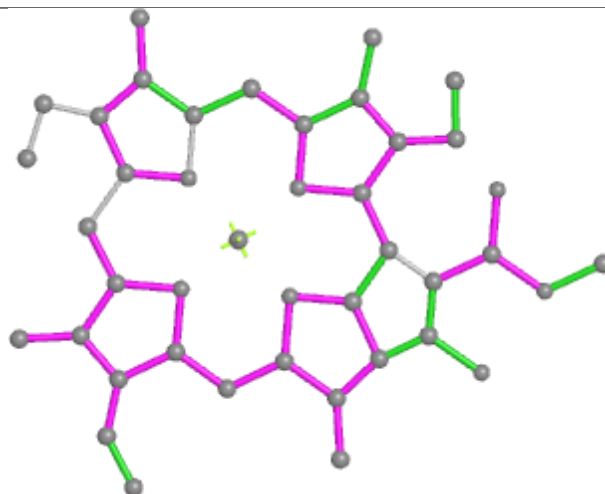


Ligand DD6 J 104**Ligand CLA 4 707**

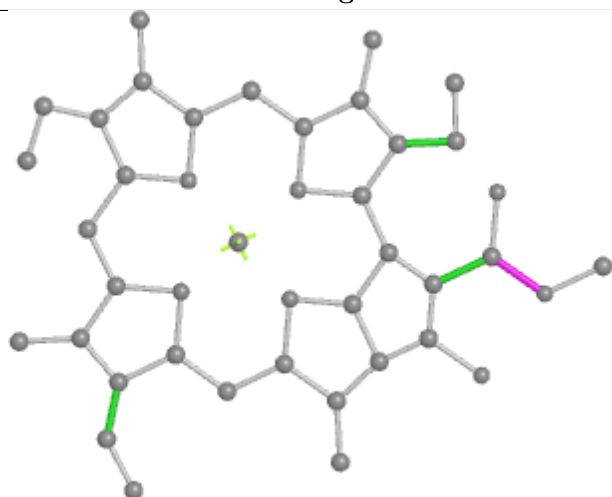
Ligand CLA 1 504



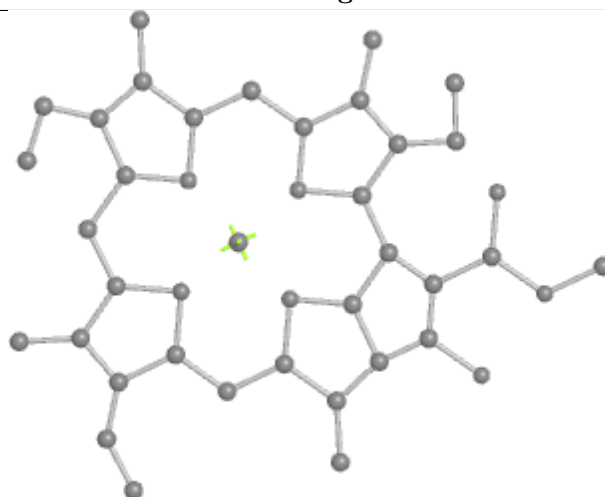
Bond lengths



Bond angles

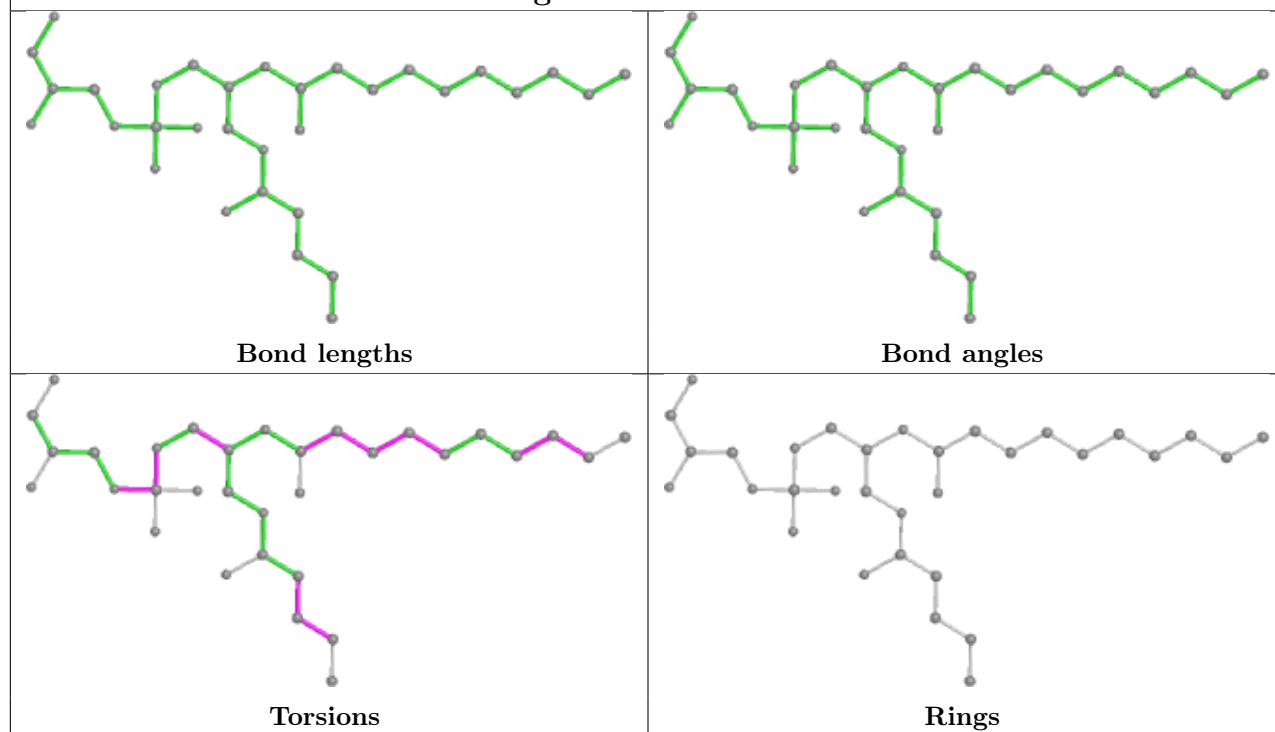


Torsions

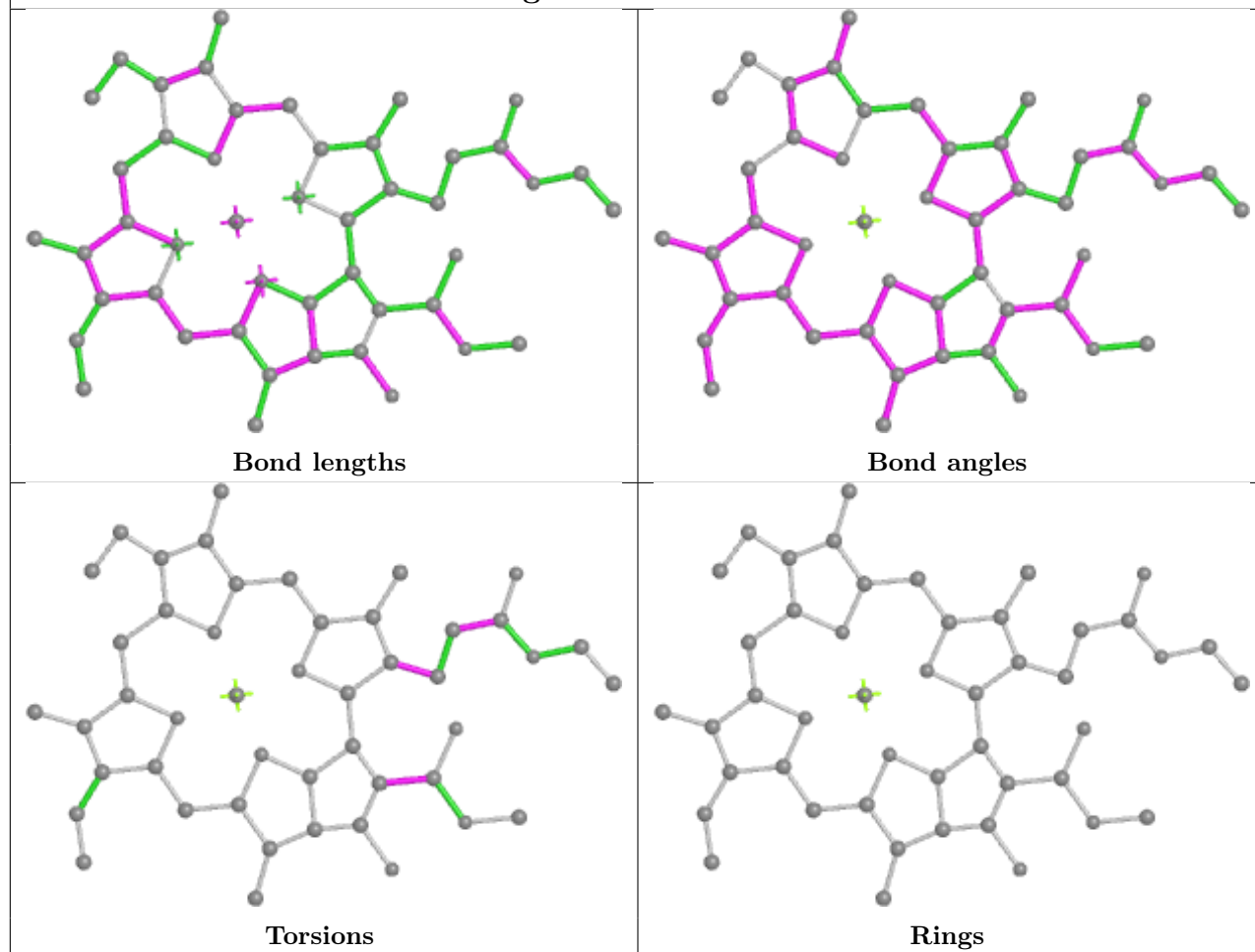


Rings

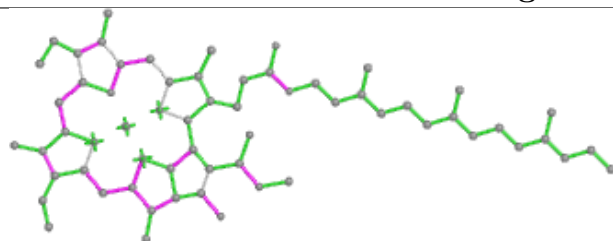
Ligand LHG 5 714



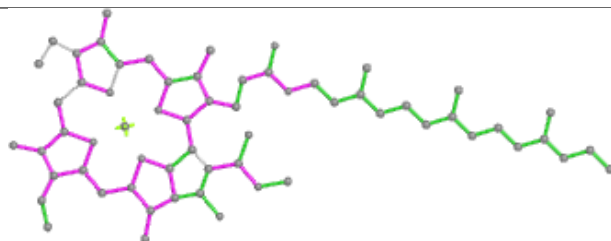
Ligand CLA B 819



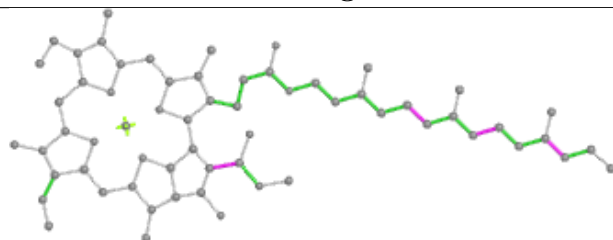
Ligand CLA 6 909



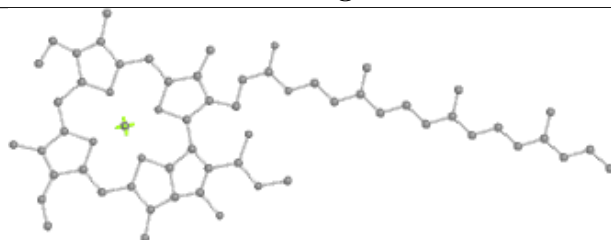
Bond lengths



Bond angles

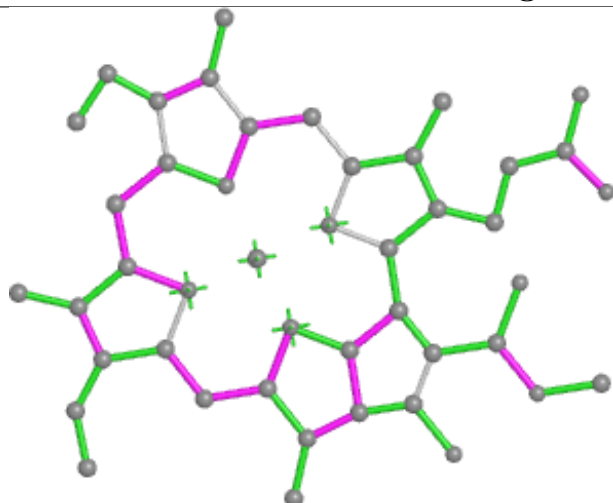


Torsions

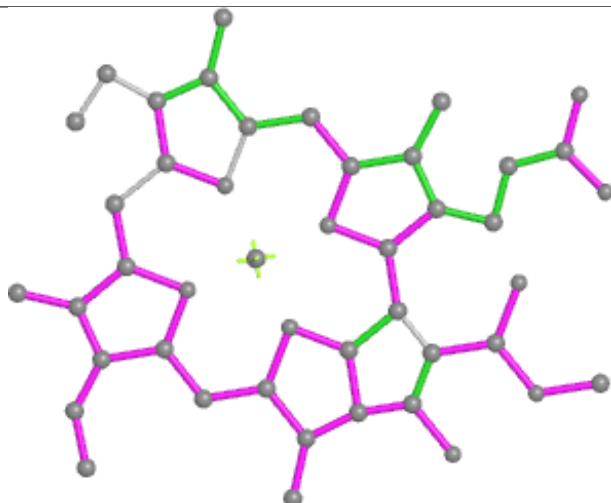


Rings

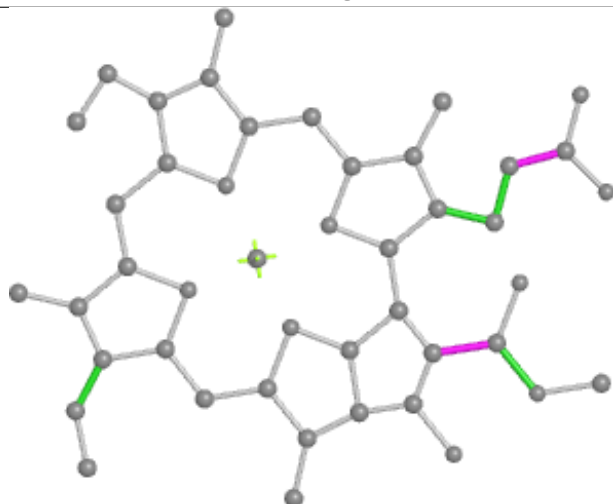
Ligand CLA 1 506



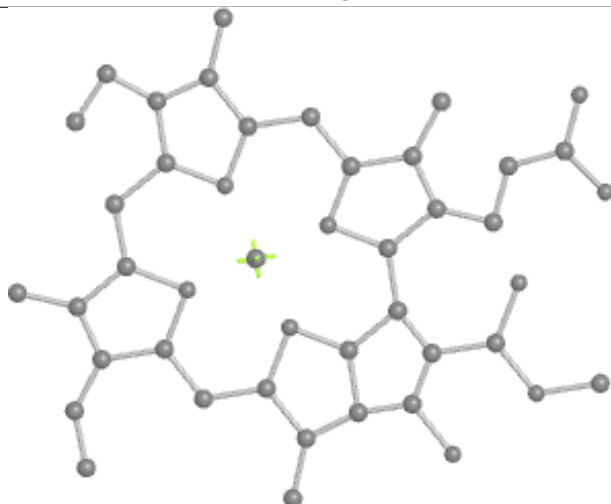
Bond lengths



Bond angles

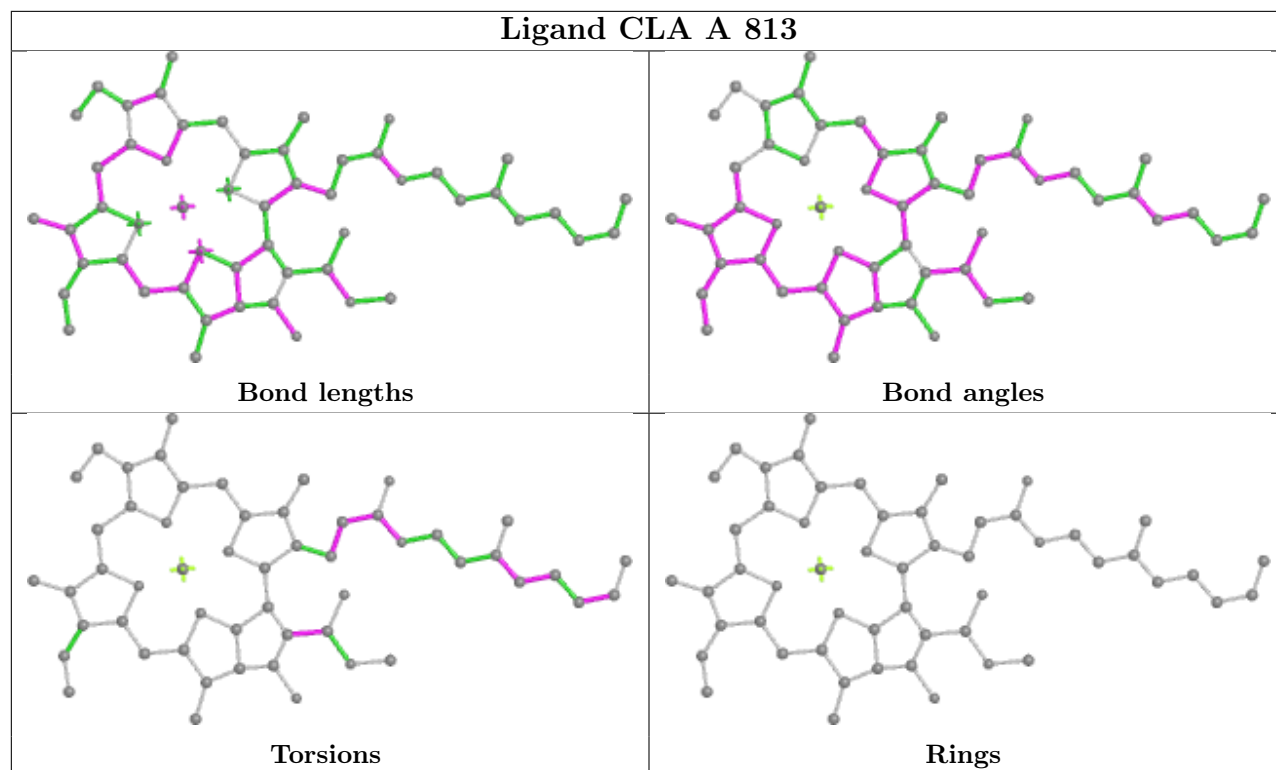


Torsions

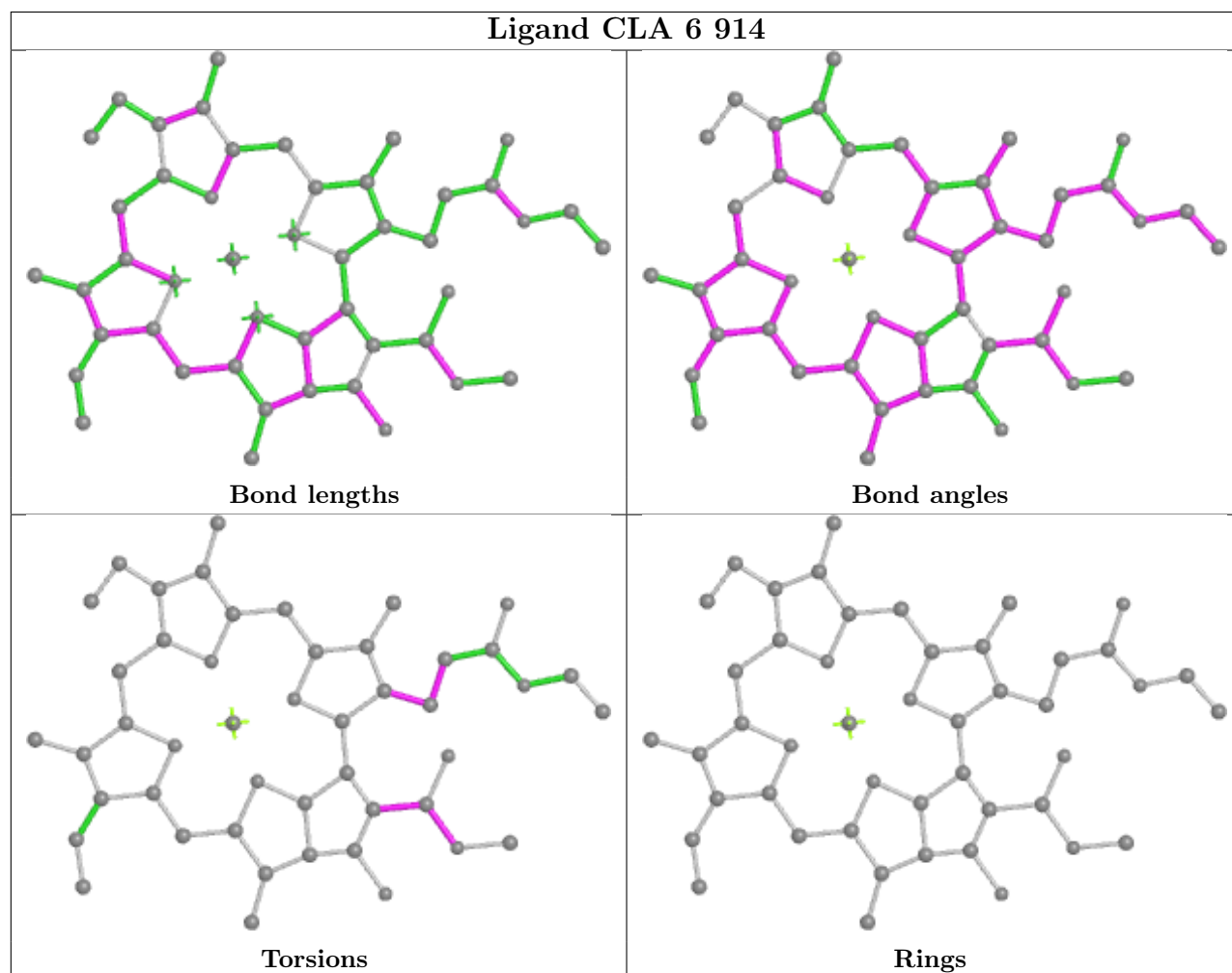


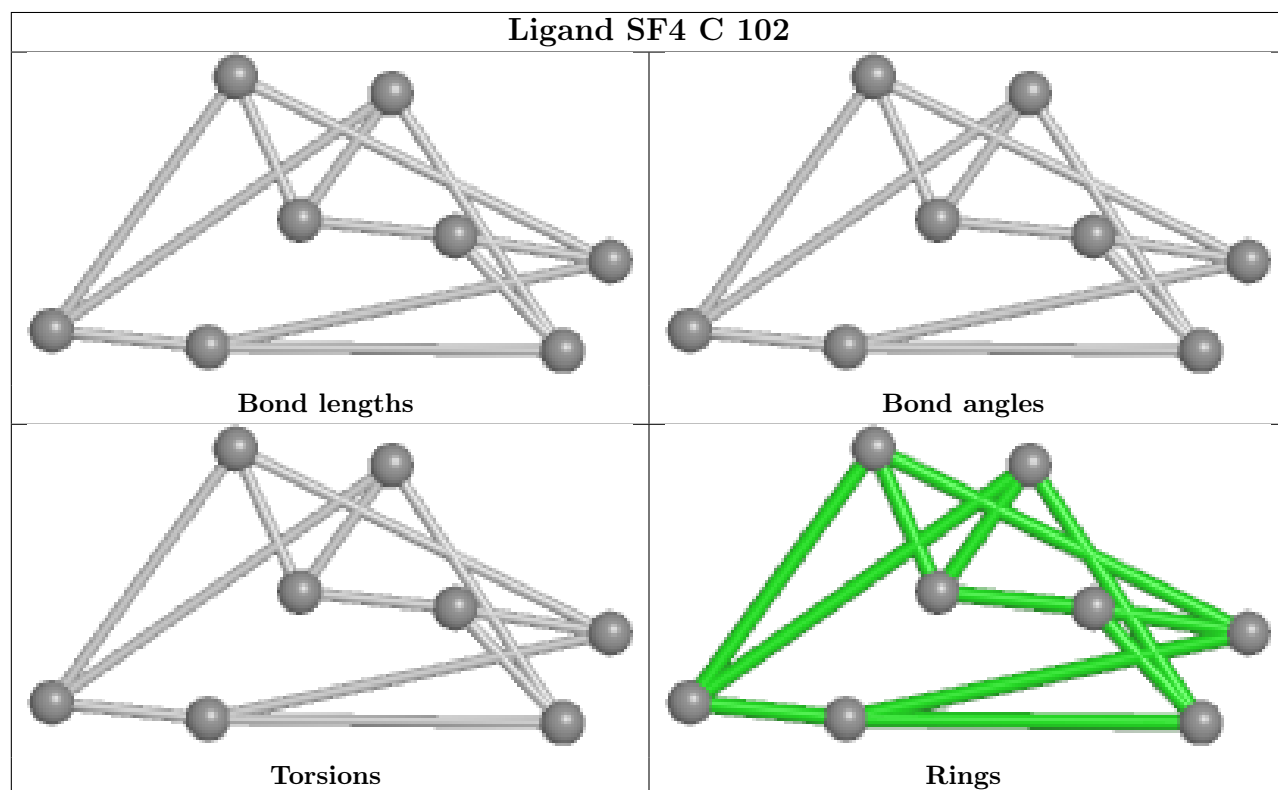
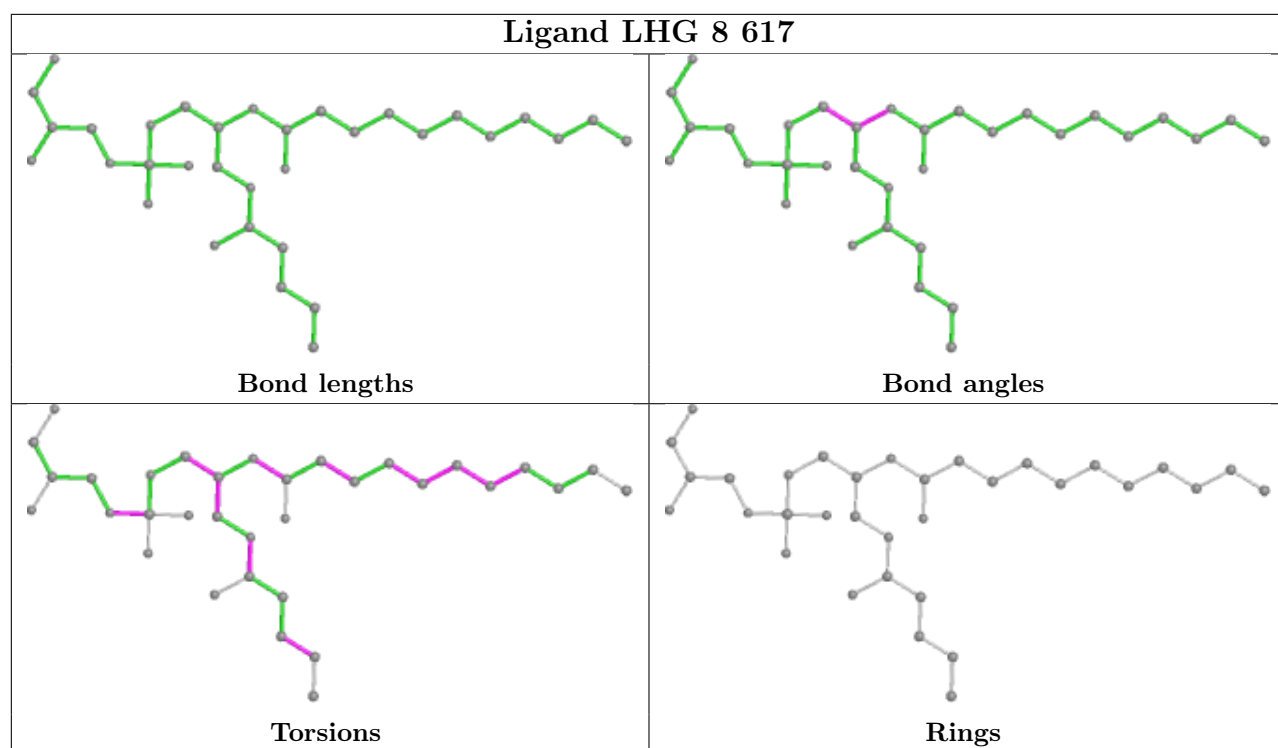
Rings

Ligand CLA A 813

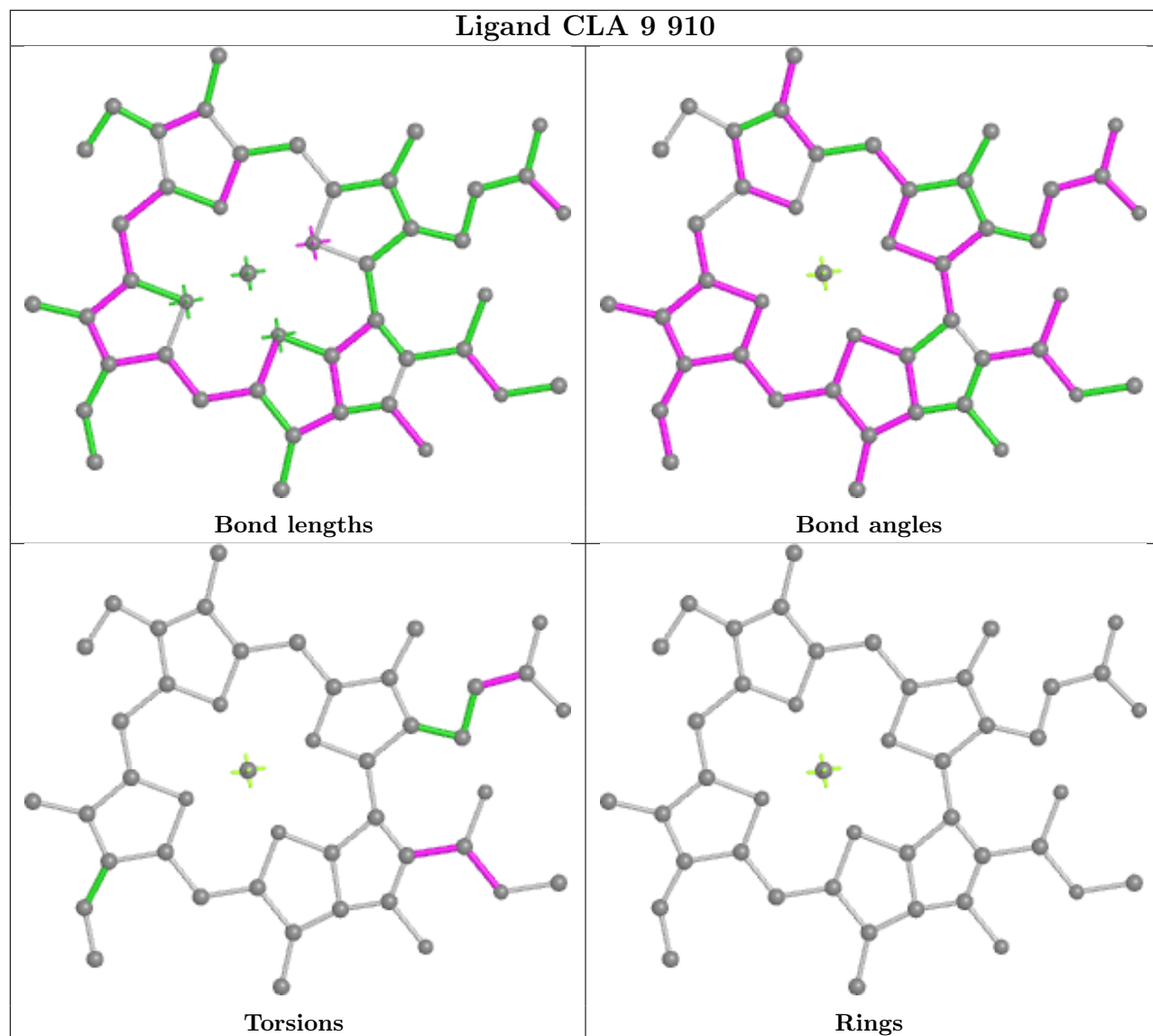


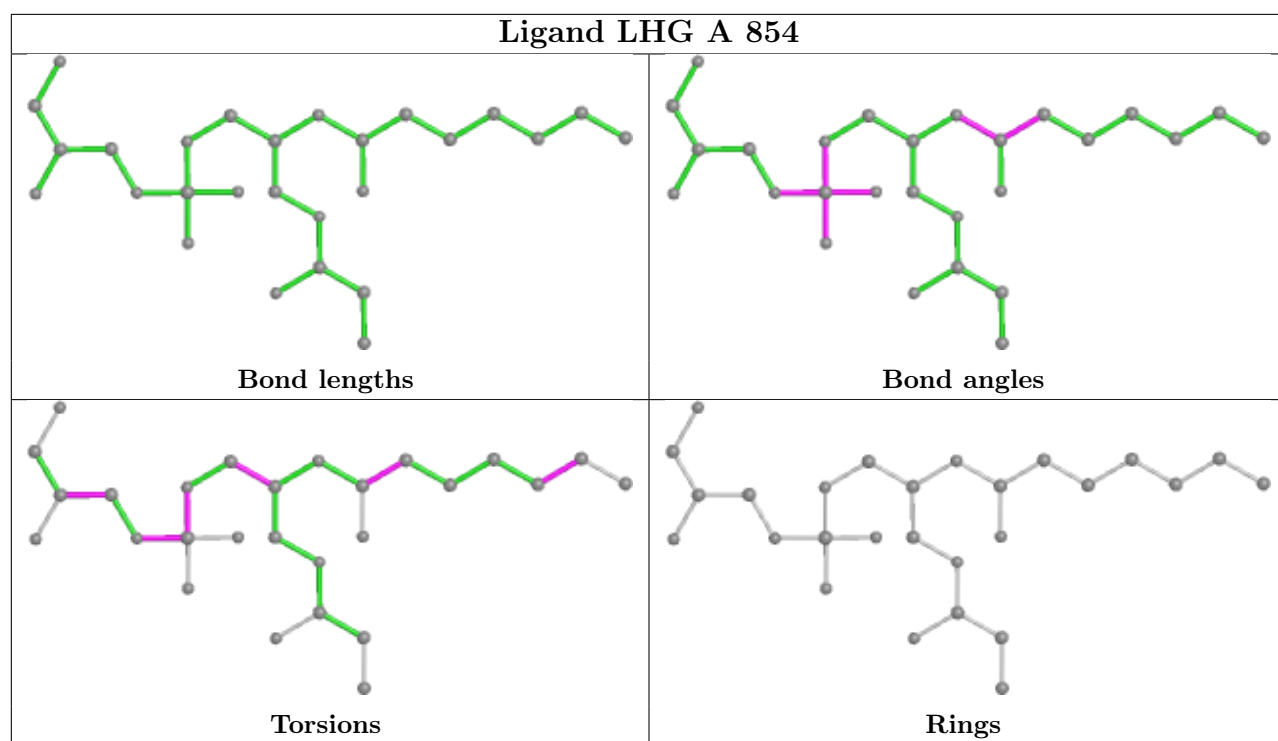
Ligand CLA 6 914



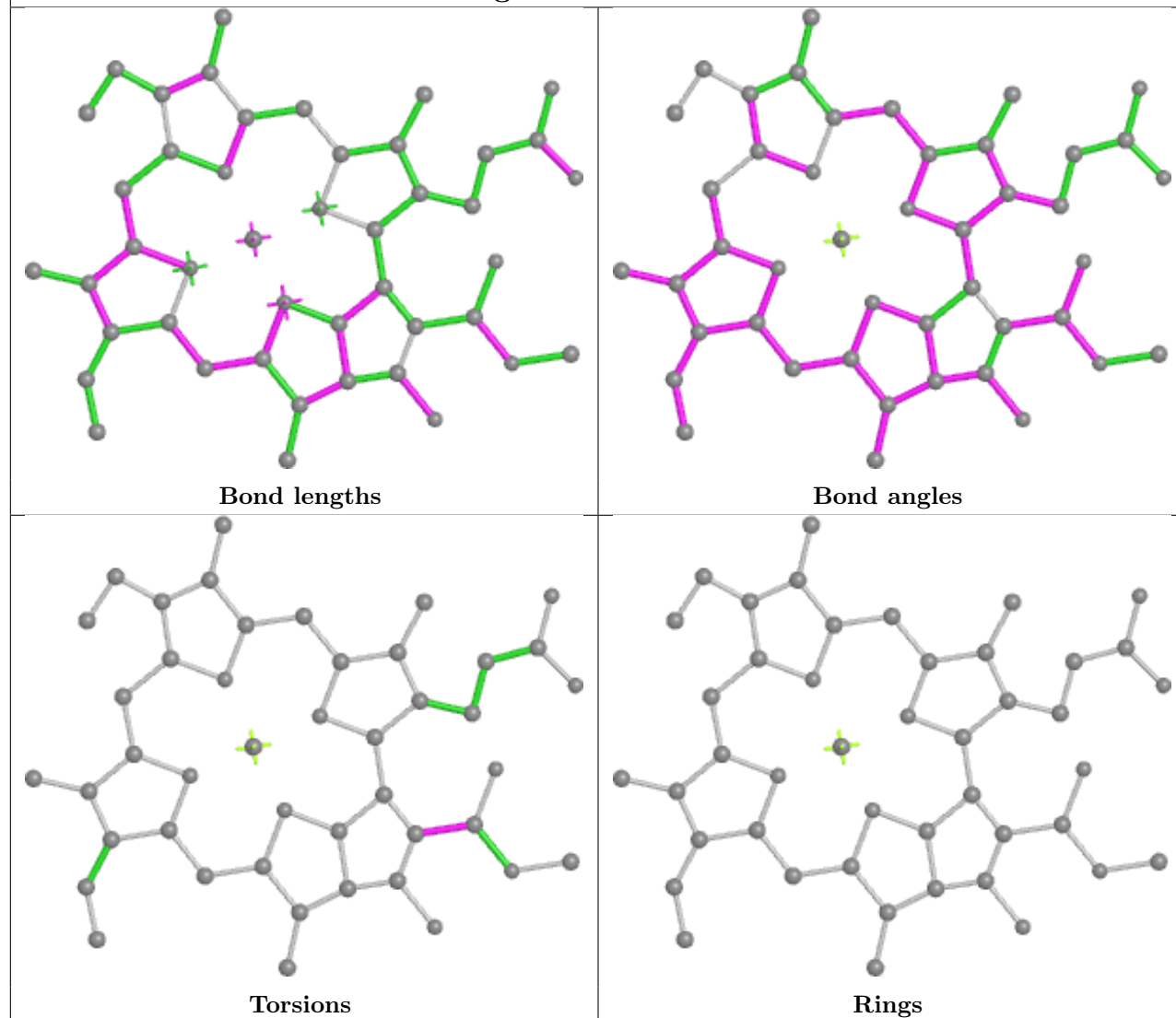


Ligand CLA 9 910

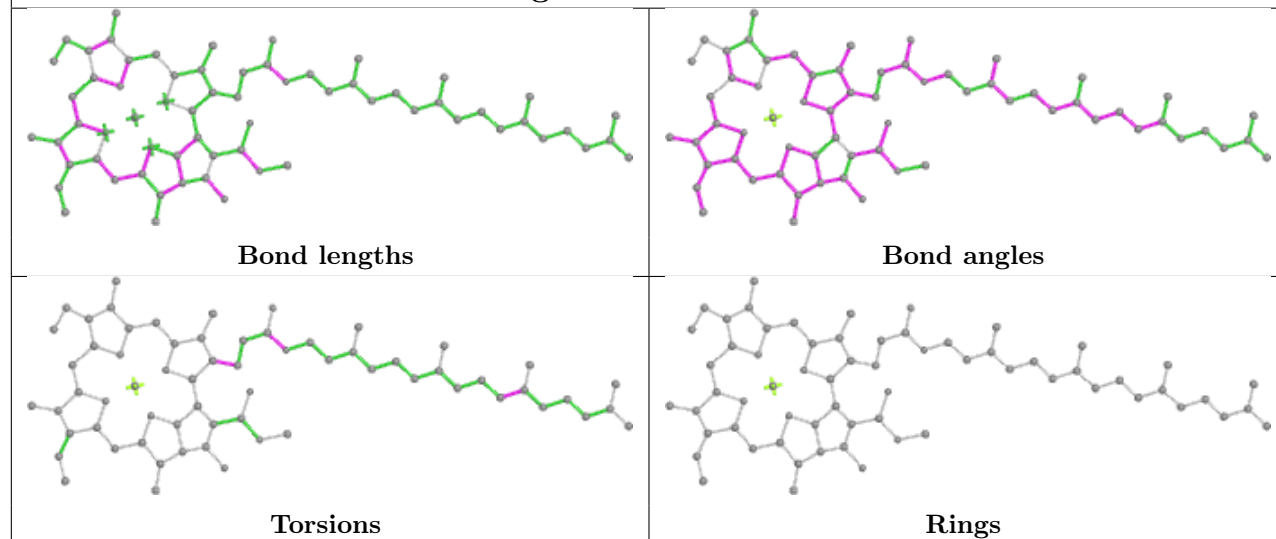


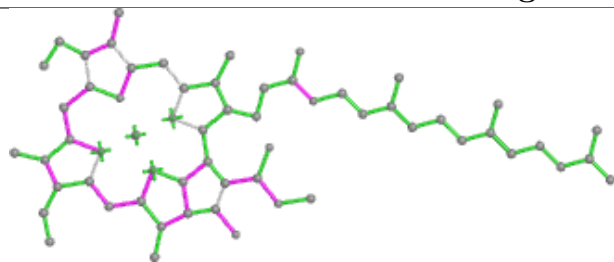


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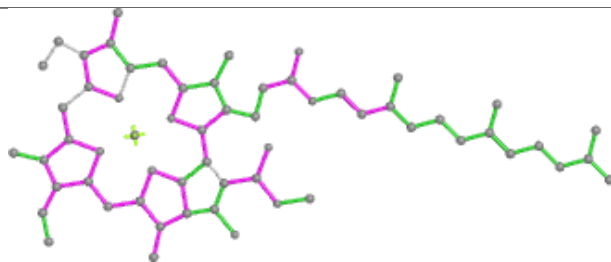


Ligand CLA A 812

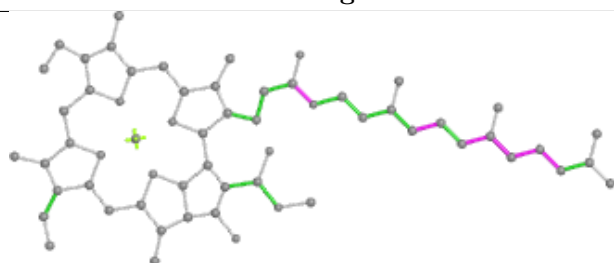


Ligand CLA 7 703

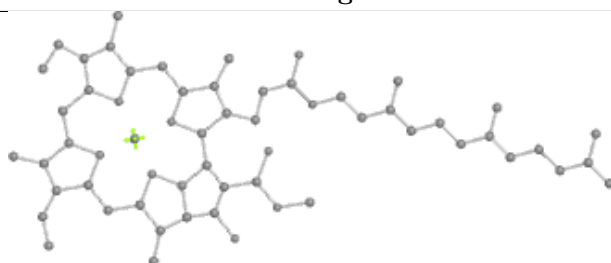
Bond lengths



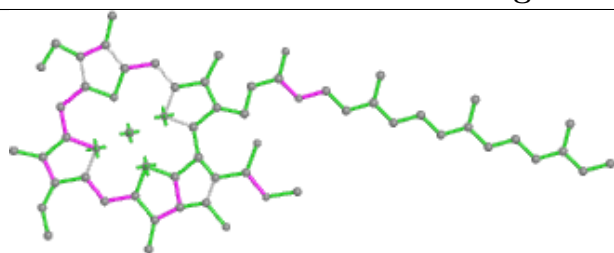
Bond angles



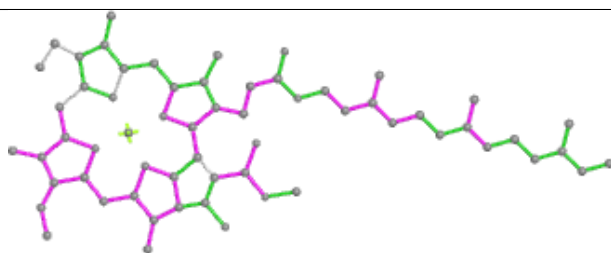
Torsions



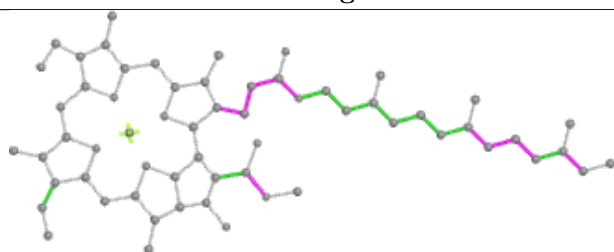
Rings

Ligand CLA A 821

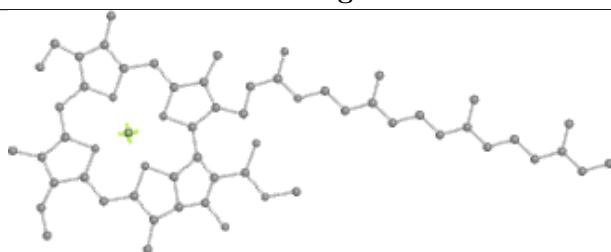
Bond lengths



Bond angles

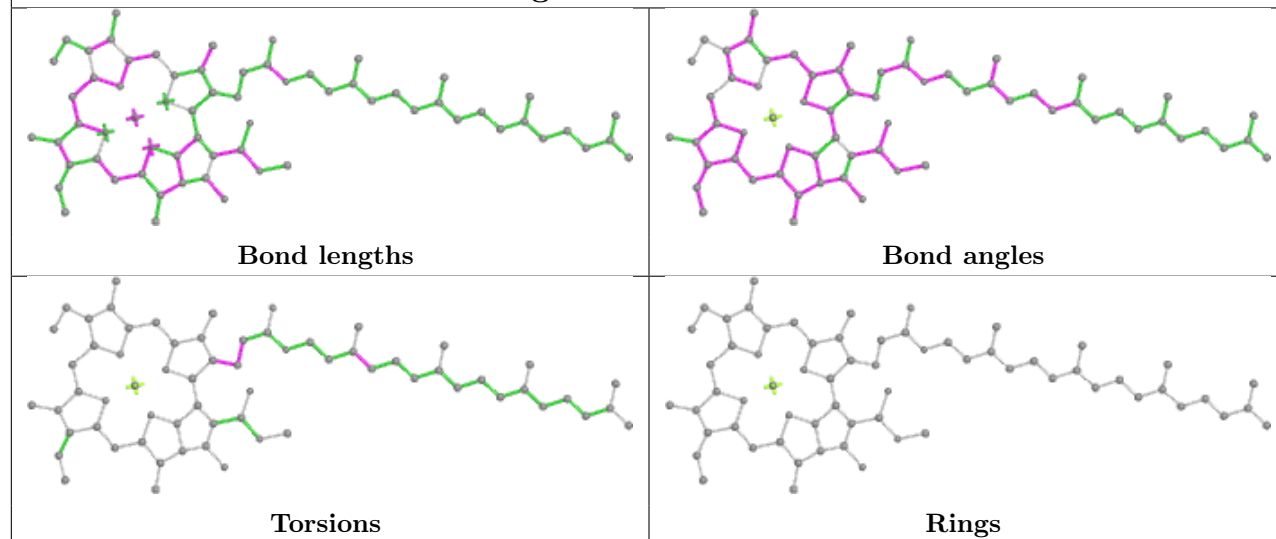


Torsions

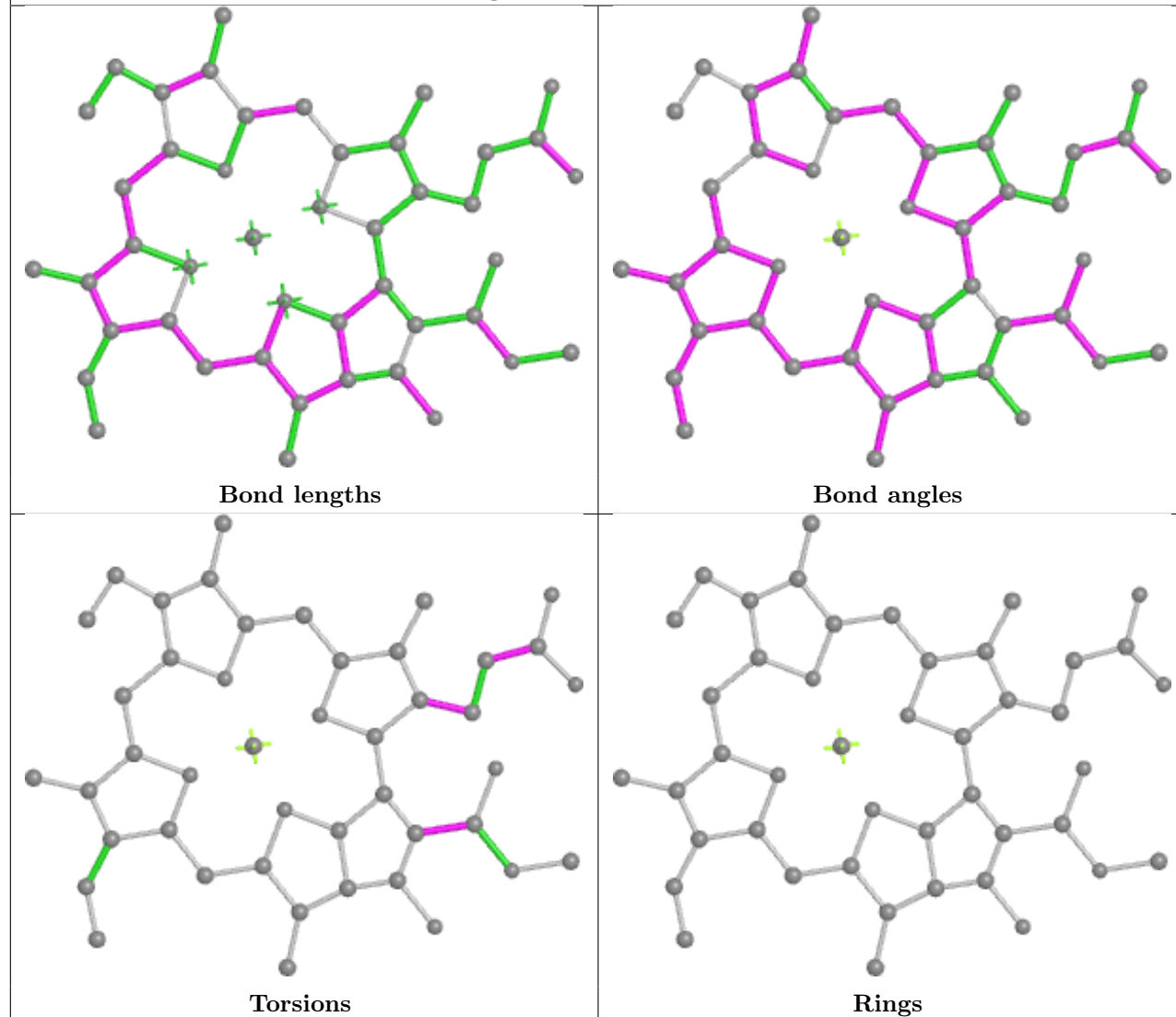


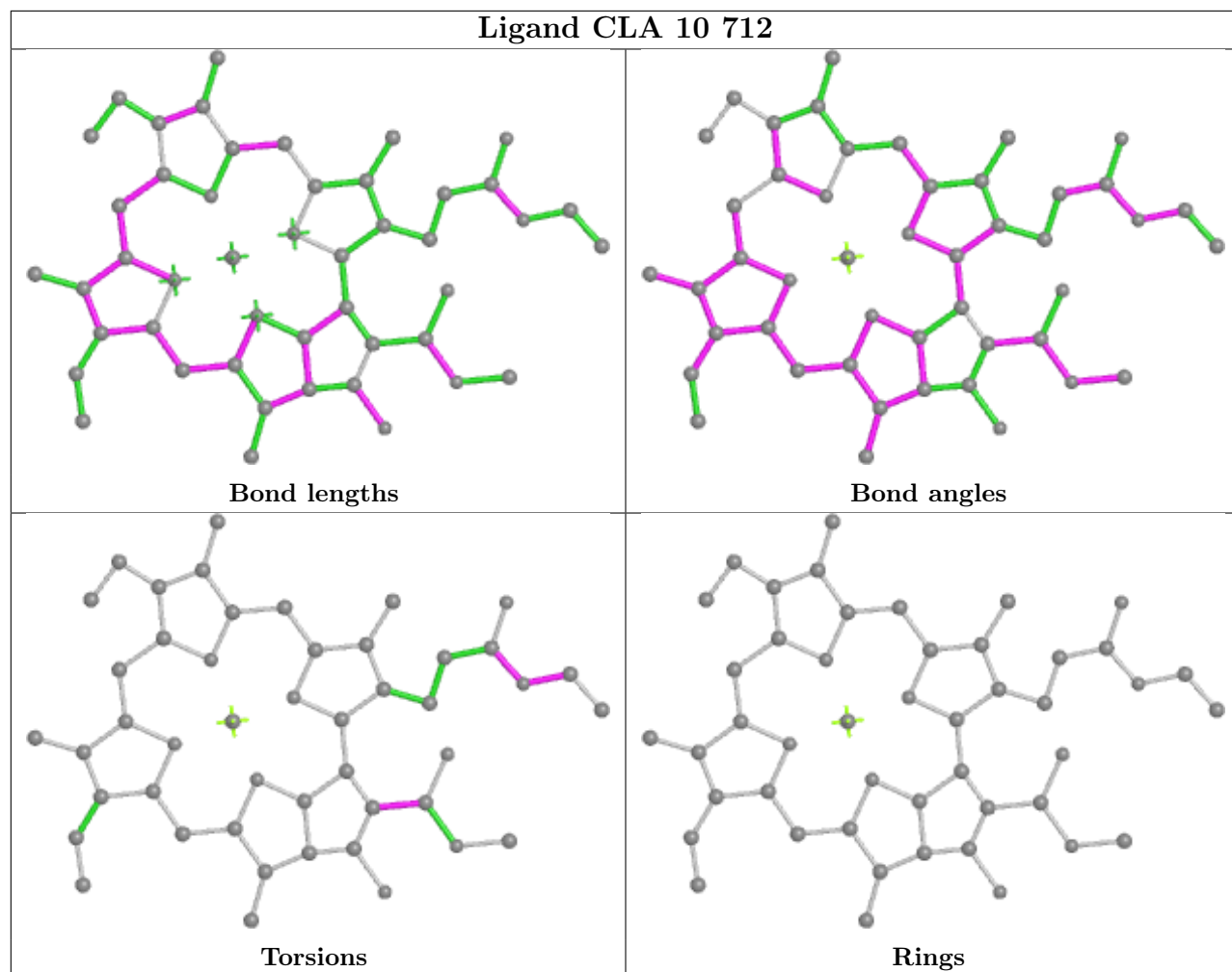
Rings

Ligand CLA A 802

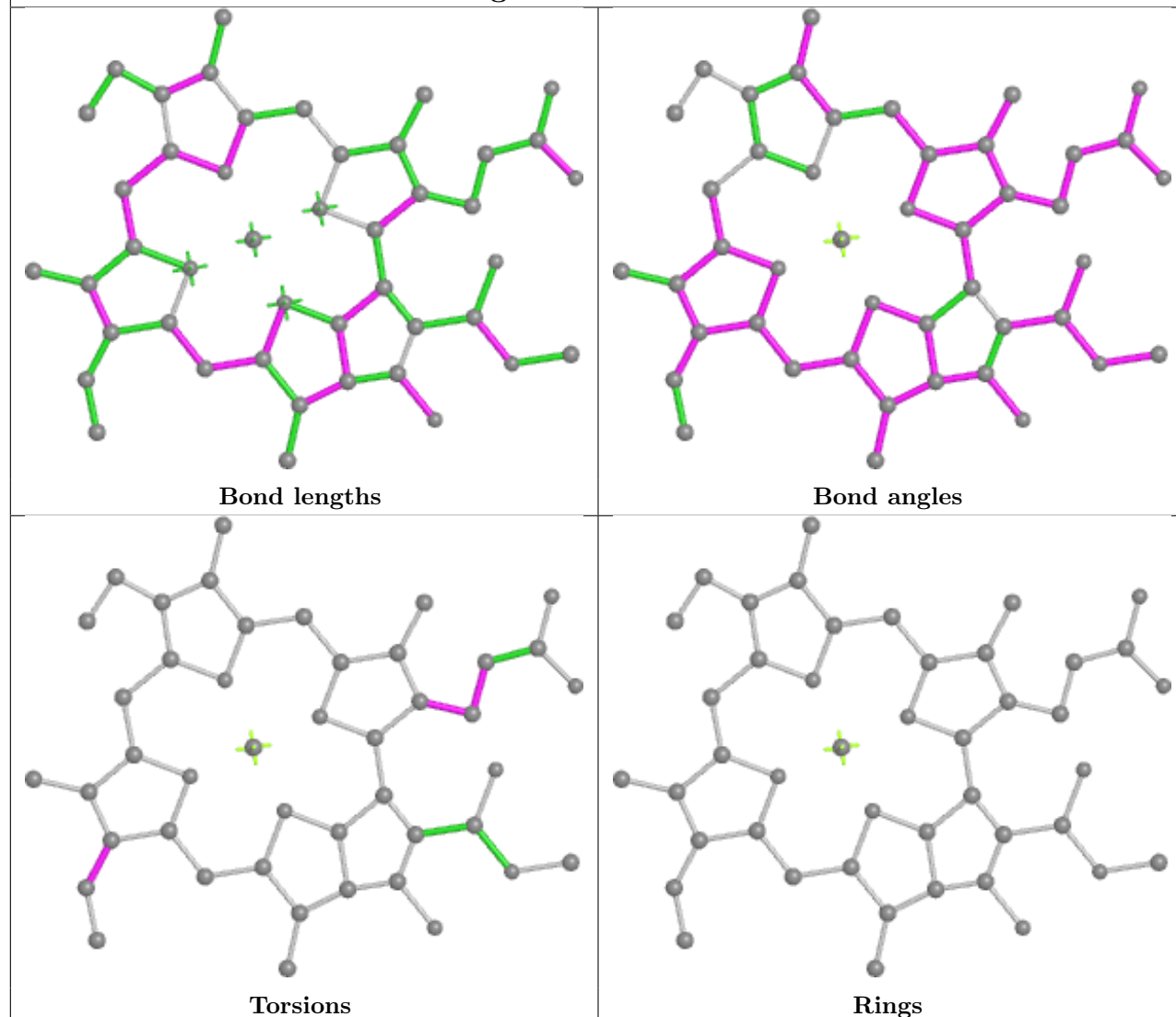


Ligand CLA 11 711

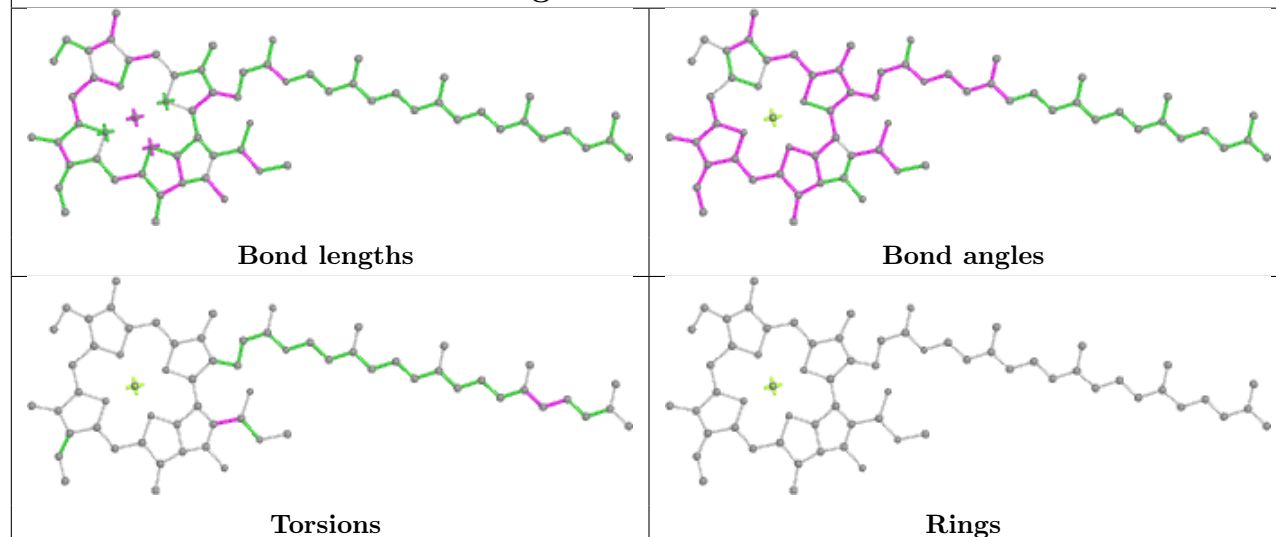




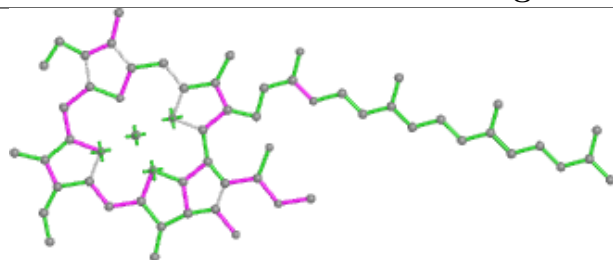
Ligand CLA B 829



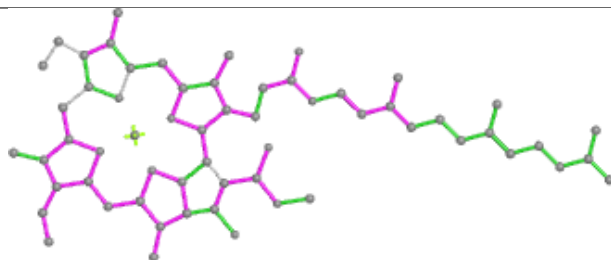
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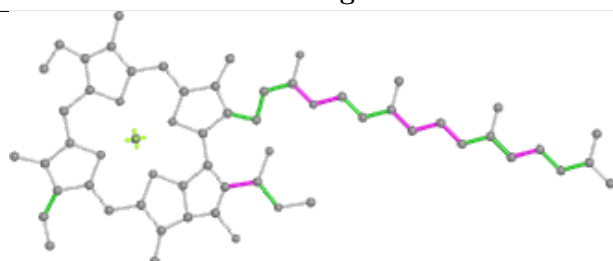
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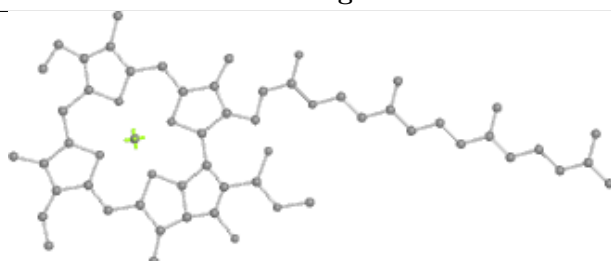
Bond lengths



Bond angles

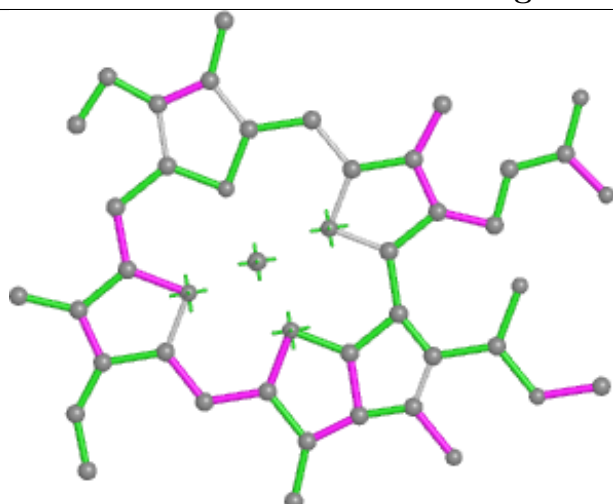


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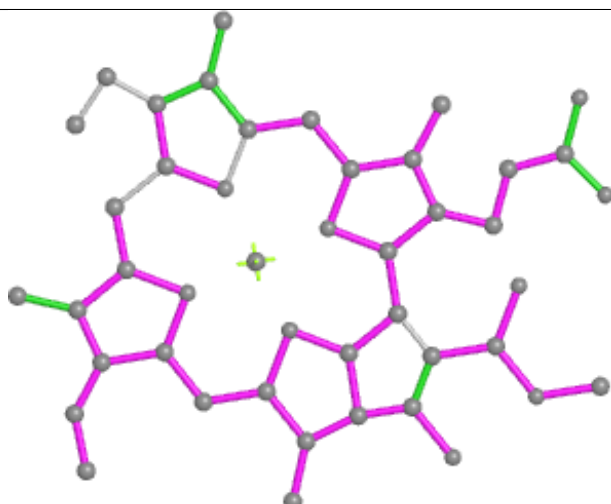


Rings

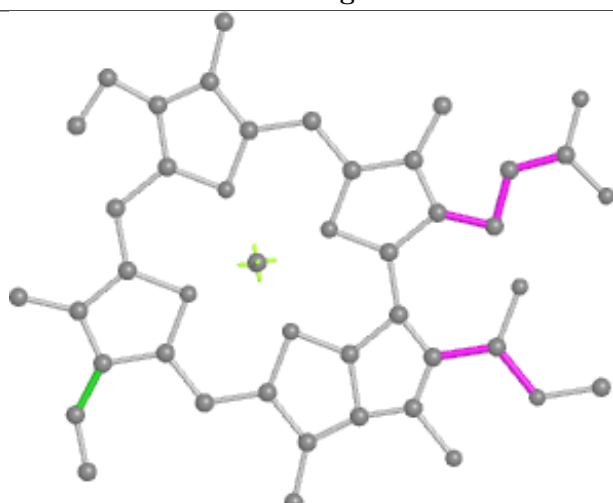
Ligand CLA B 833



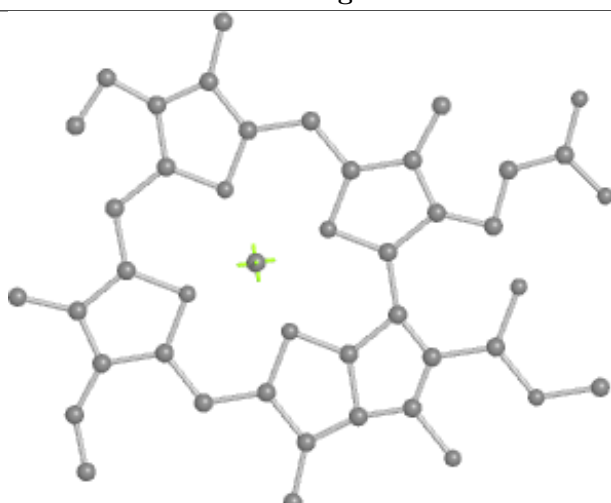
Bond lengths



Bond angles

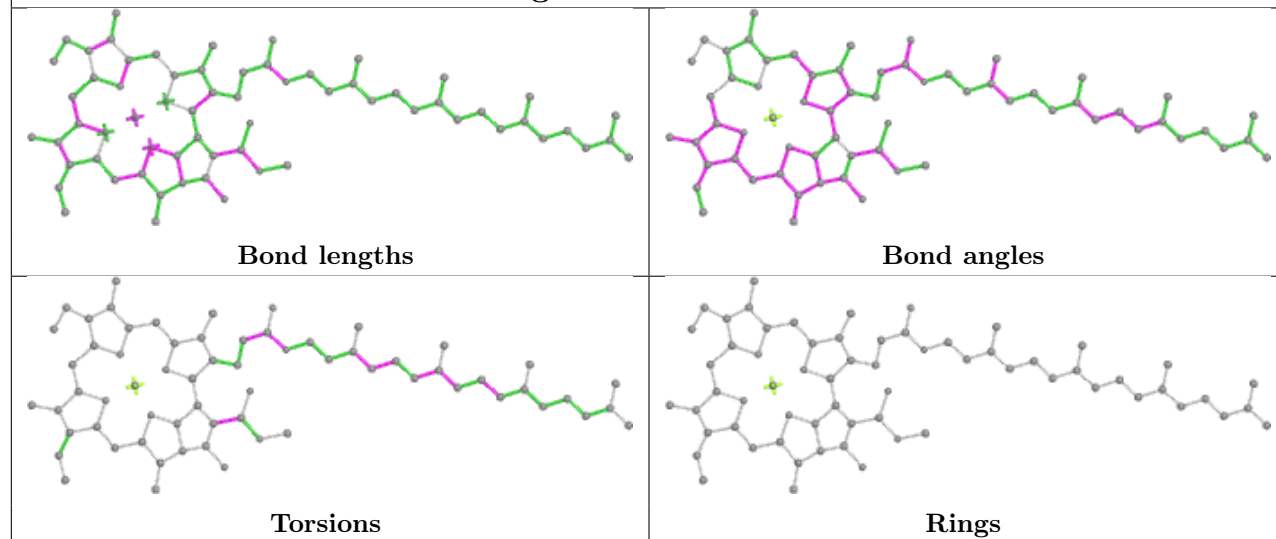


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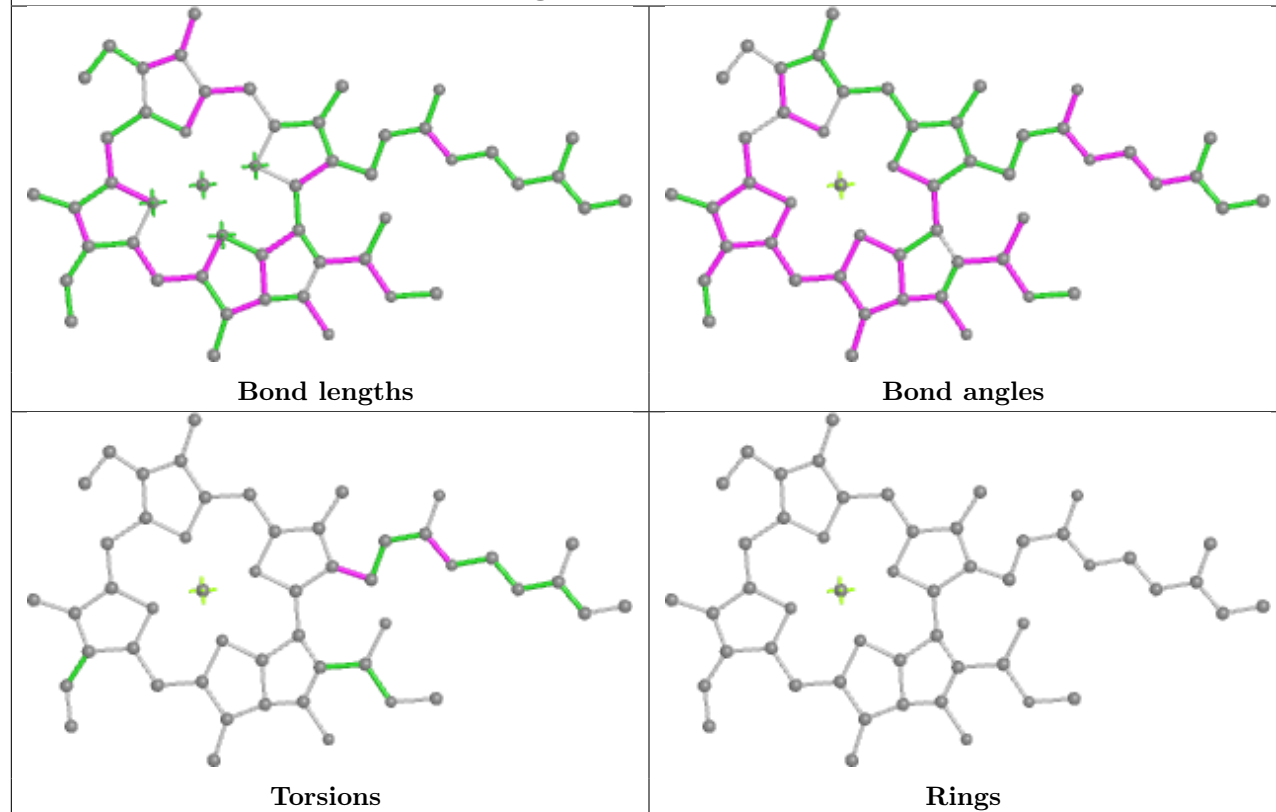


Rings

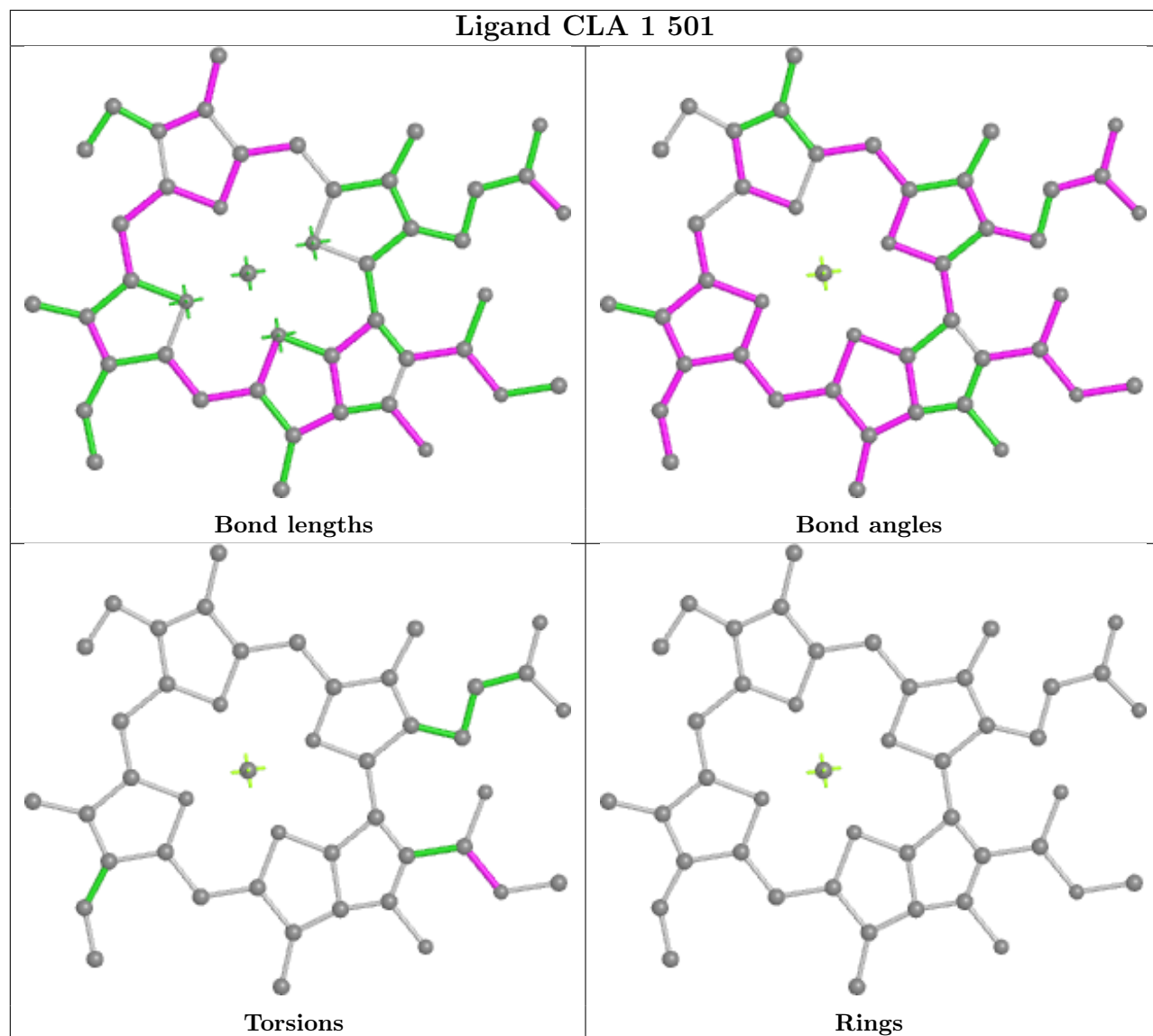
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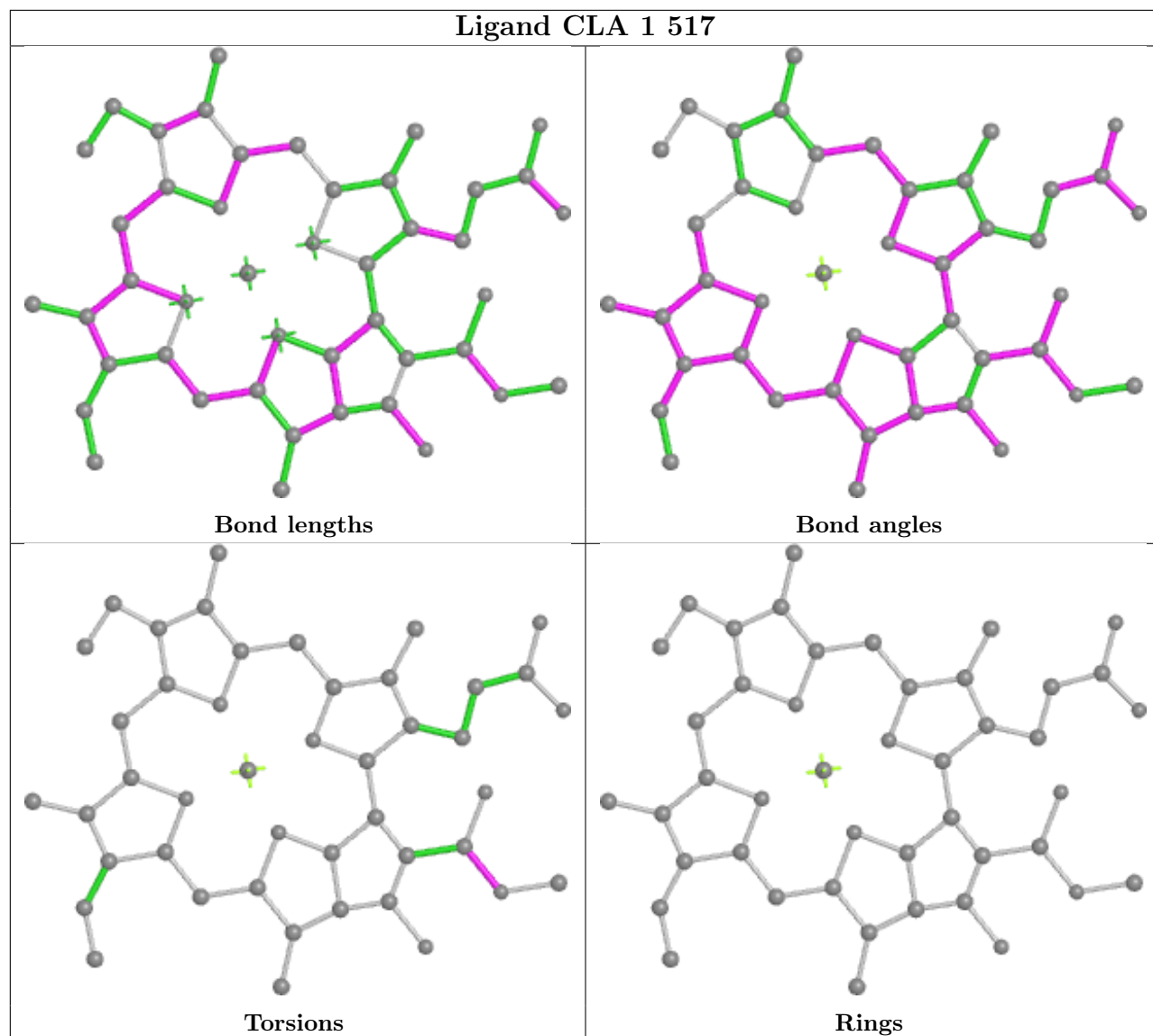
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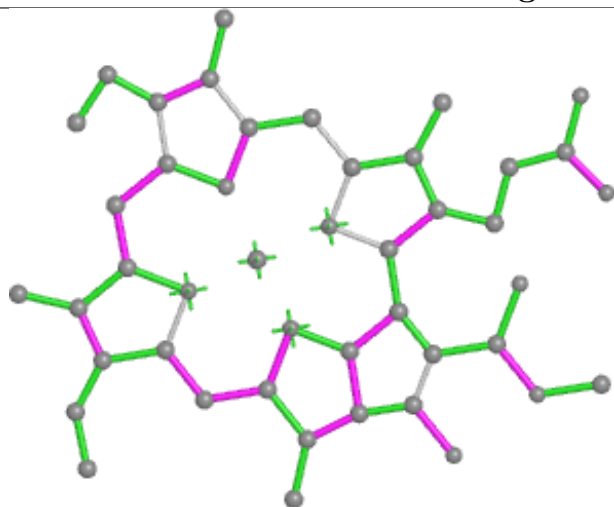
Ligand CLA 1 501



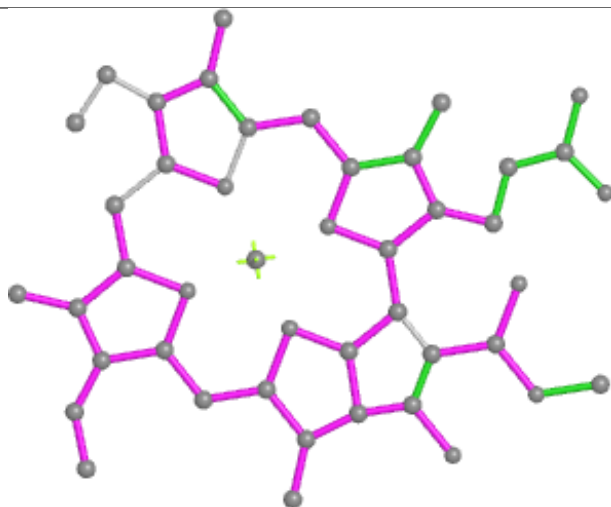
Ligand CLA 1 517



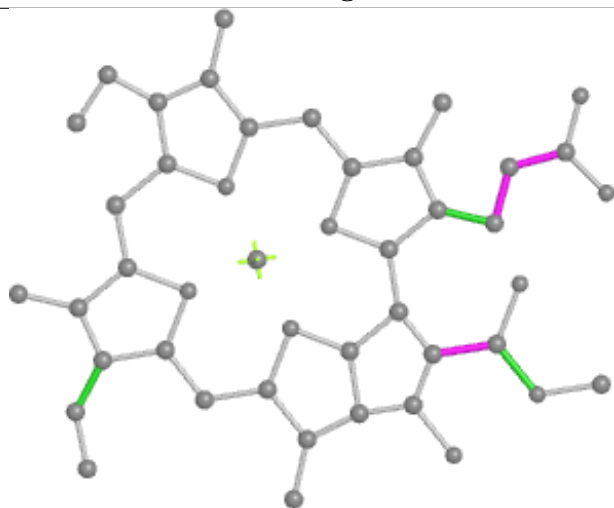
Ligand CLA 3 715



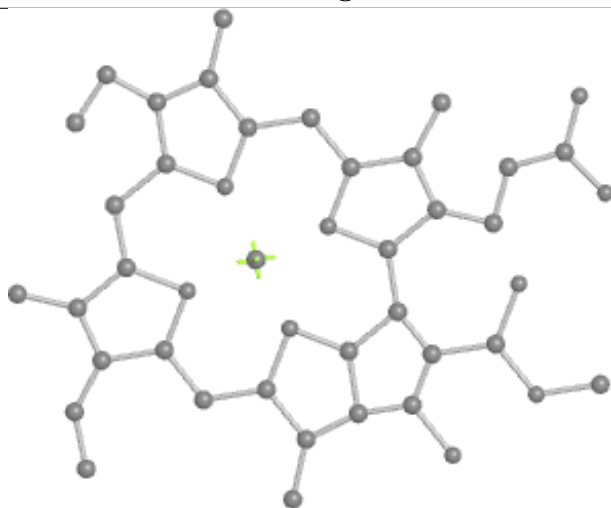
Bond lengths



Bond angles

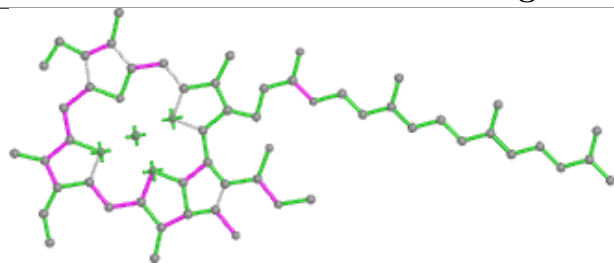


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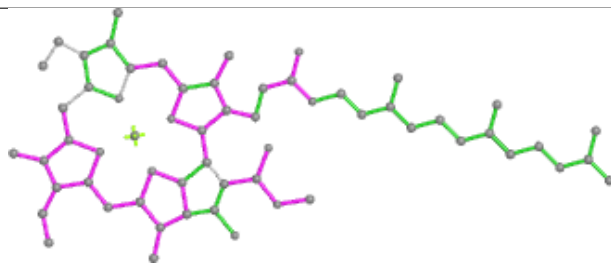


Rings

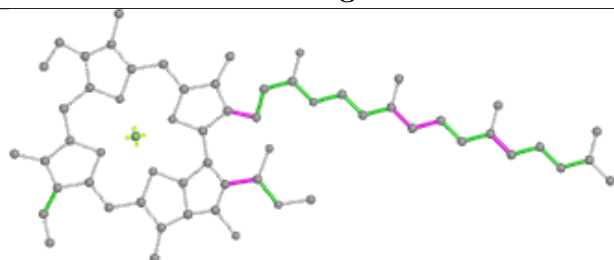
Ligand CLA 9 903



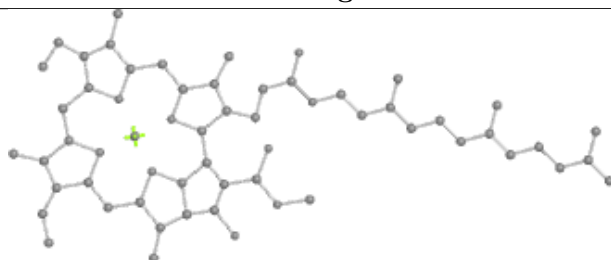
Bond lengths



Bond angles

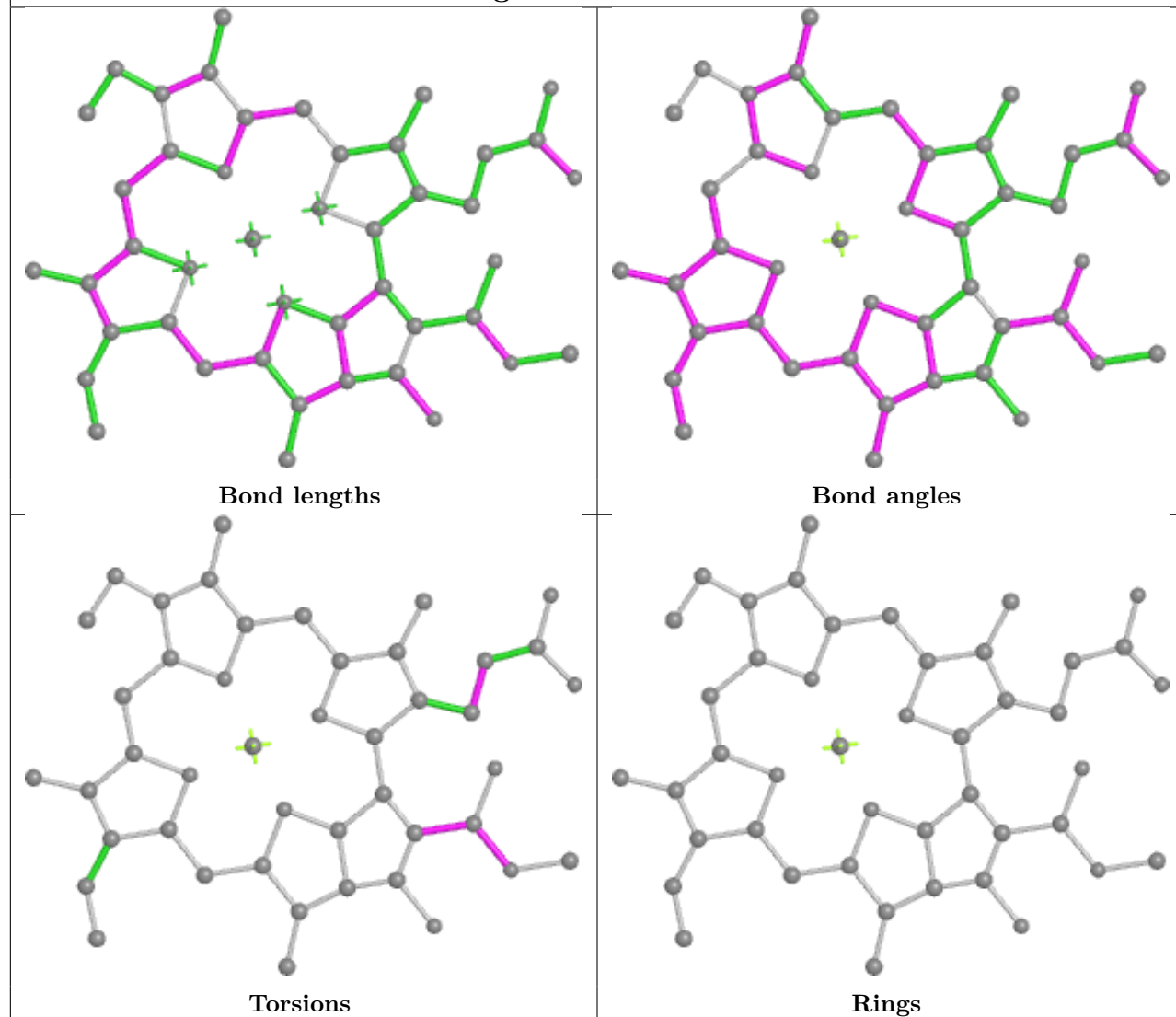


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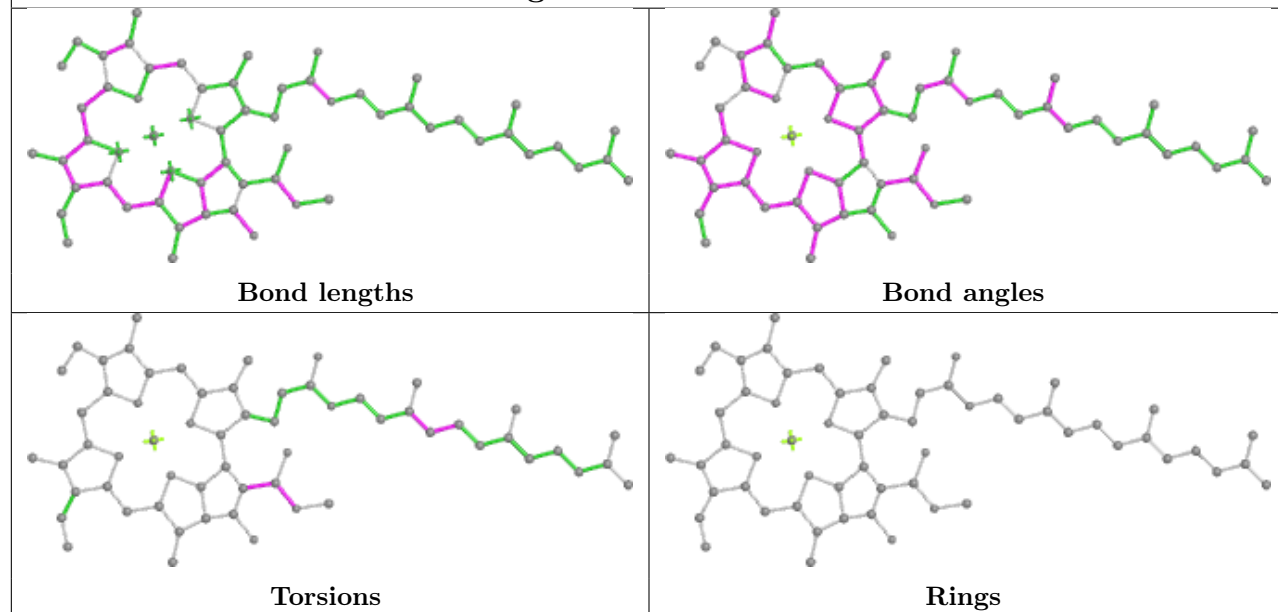


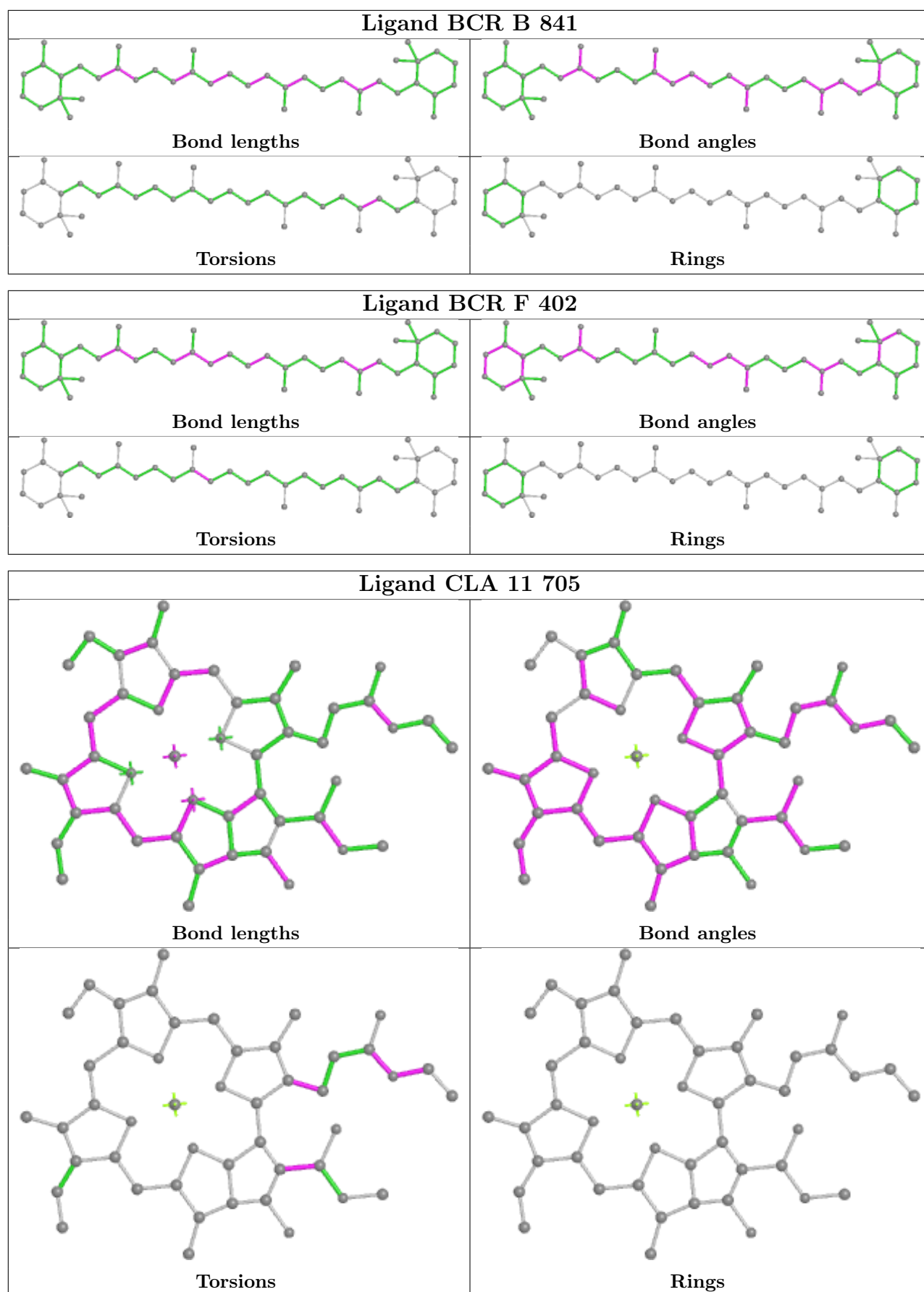
Rings

Ligand CLA 2 513

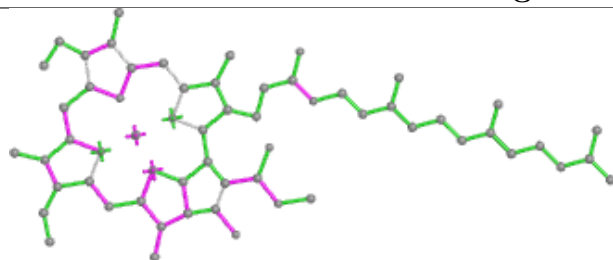


Ligand CLA 10 704

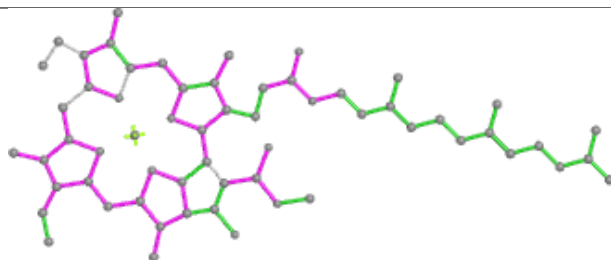




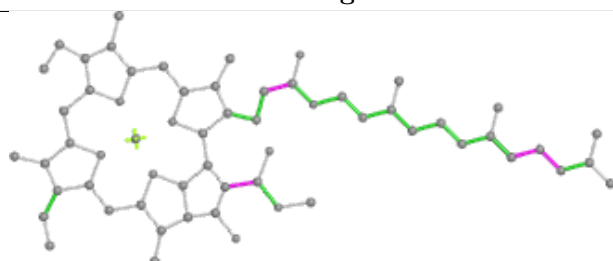
Ligand CLA A 814



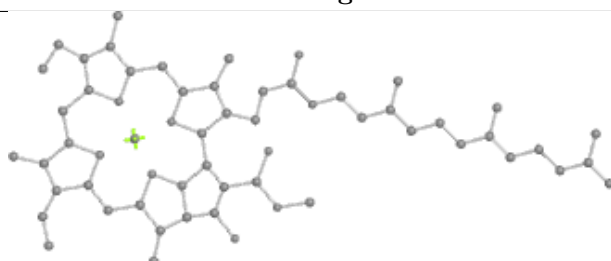
Bond lengths



Bond angles

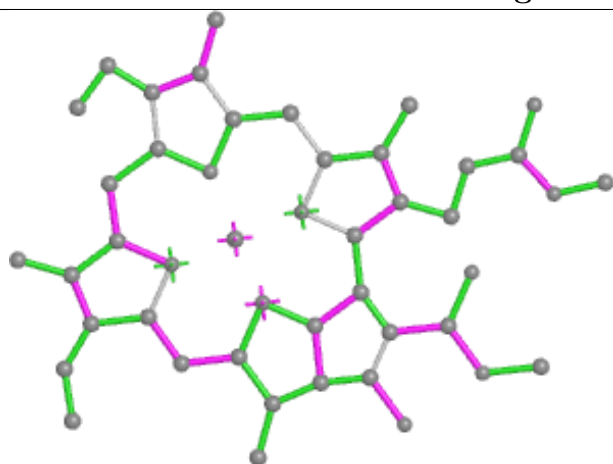


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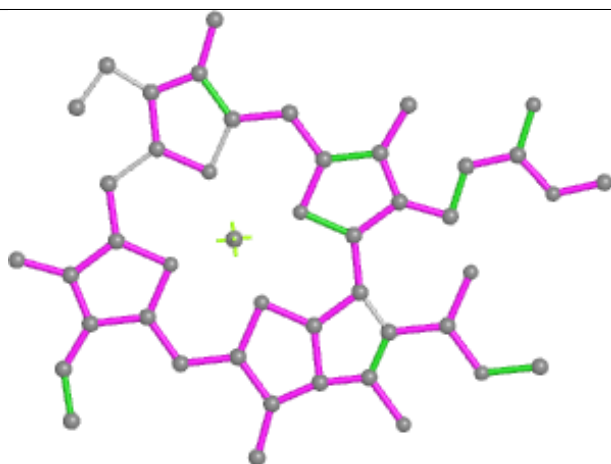


Rings

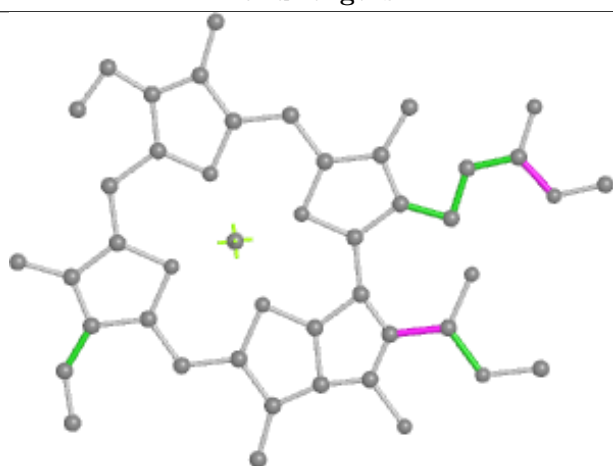
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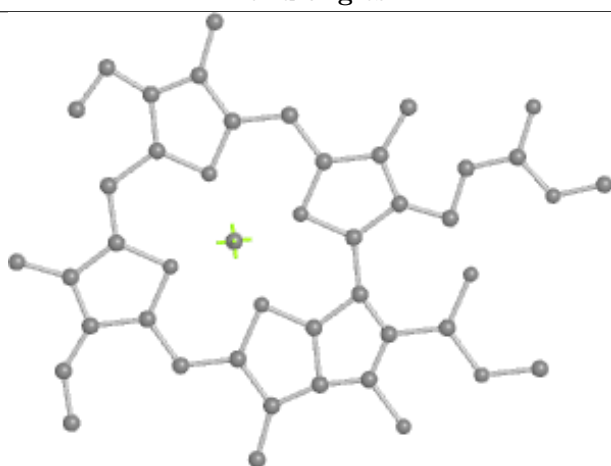
Bond lengths



Bond angles

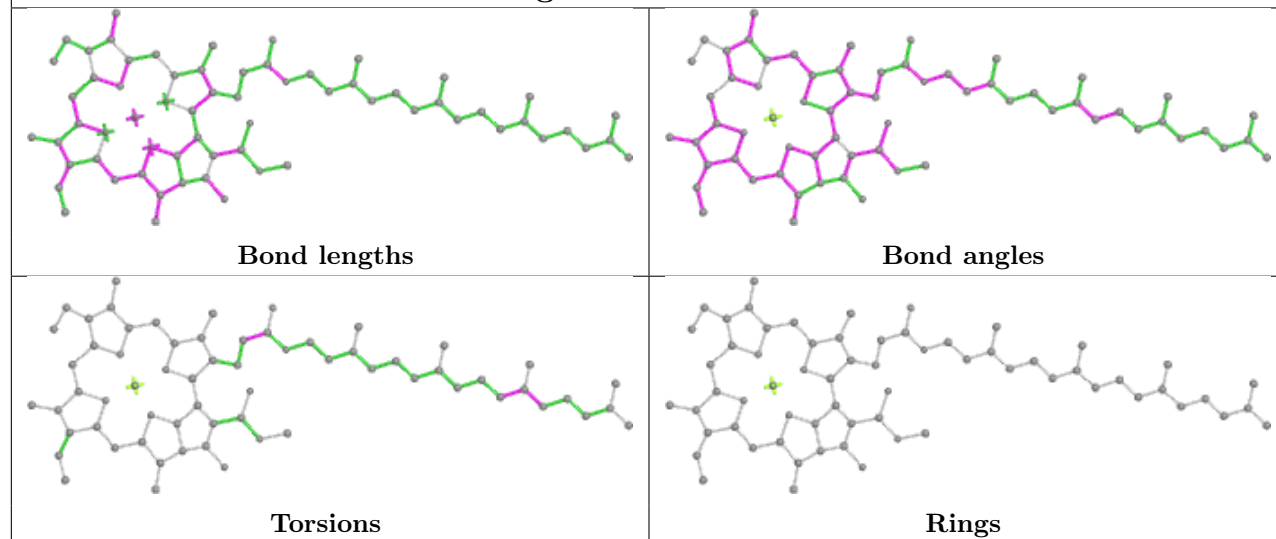


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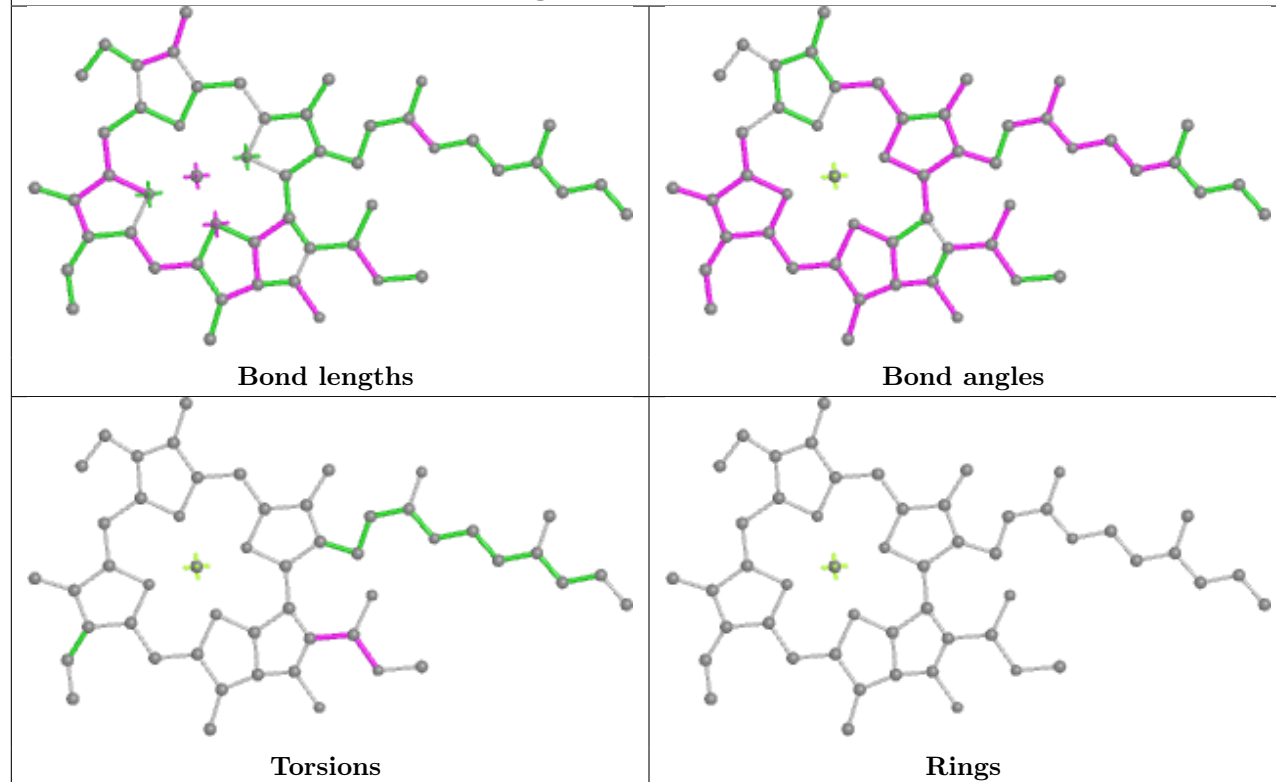


Rings

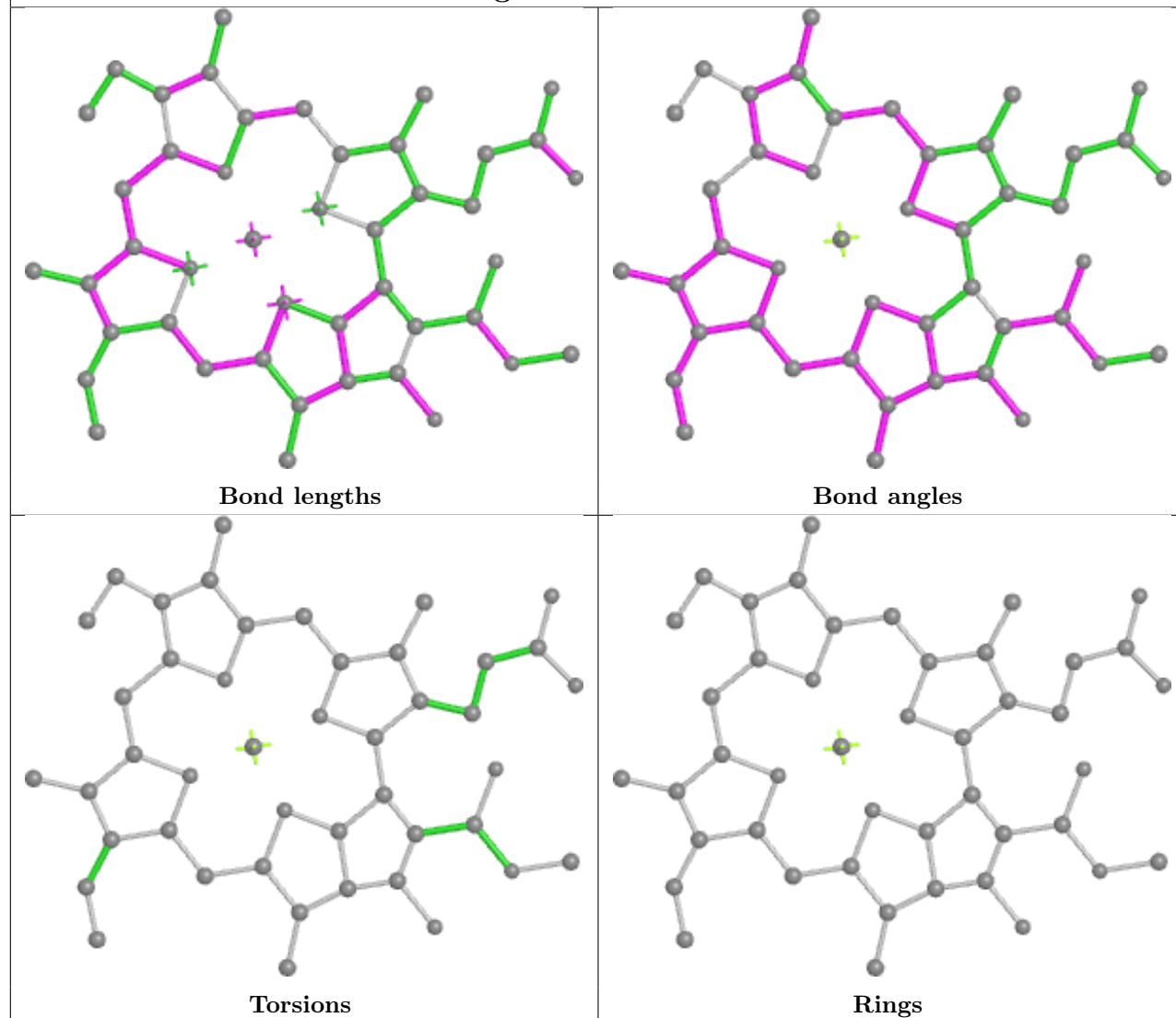
Ligand CL0 A 801



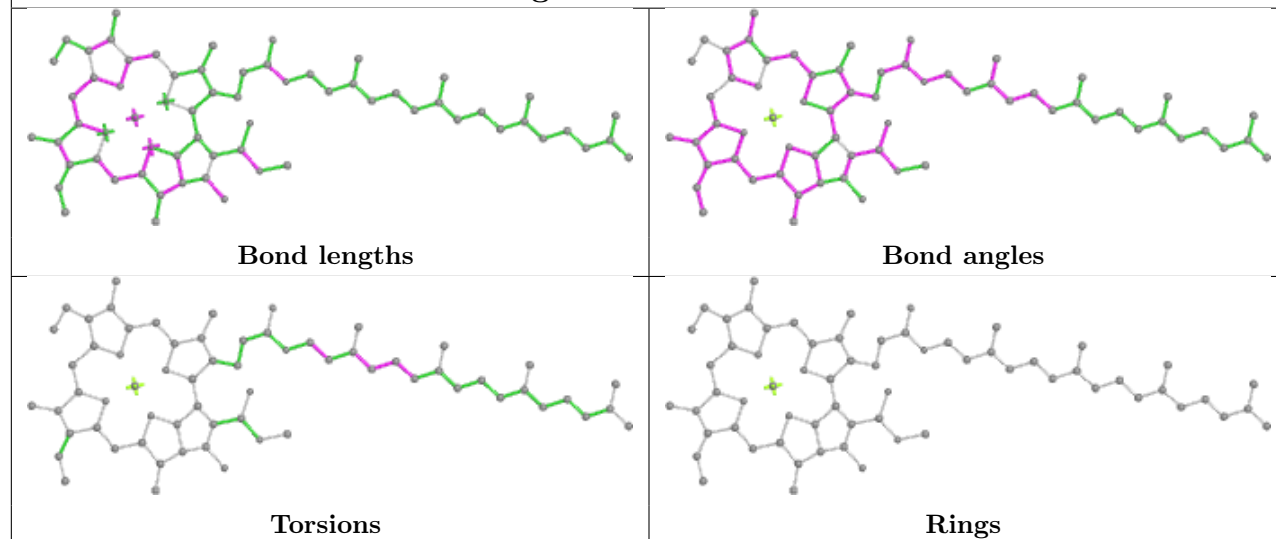
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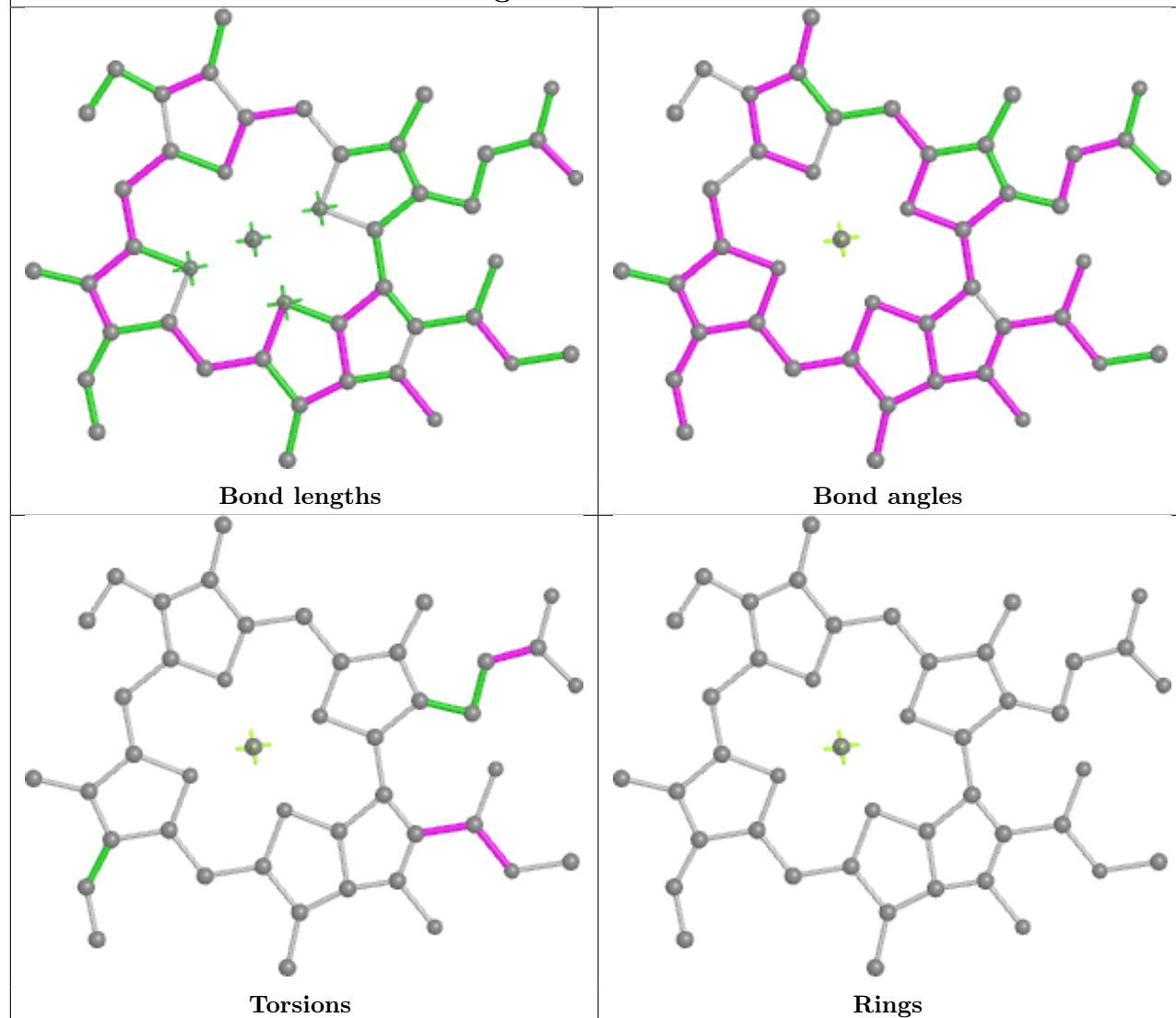
Ligand CLA 8 606



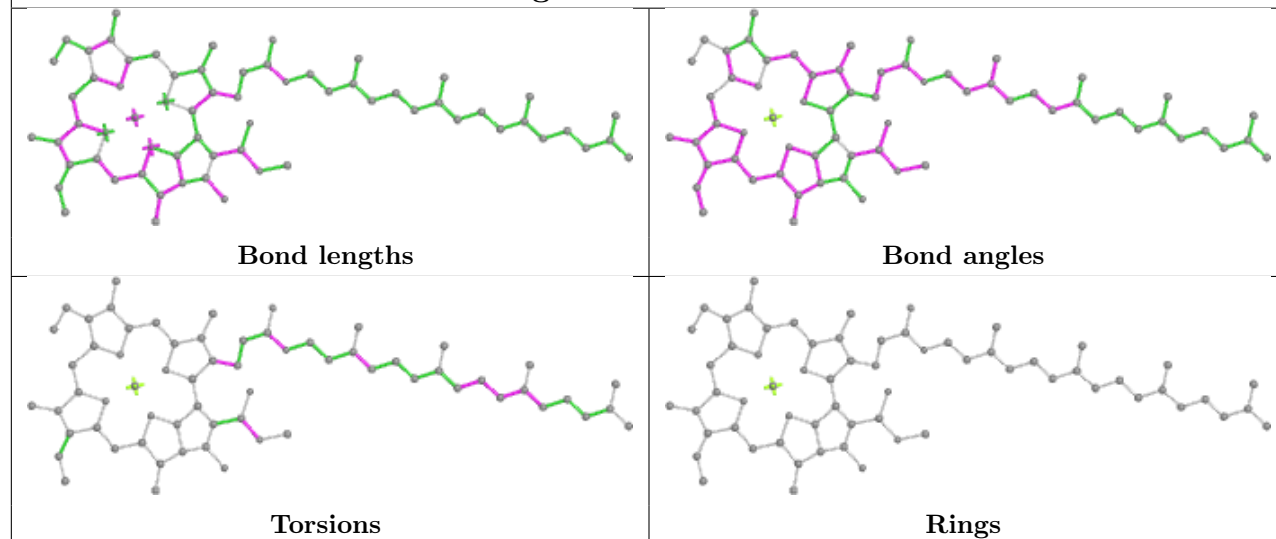
Ligand CLA A 833



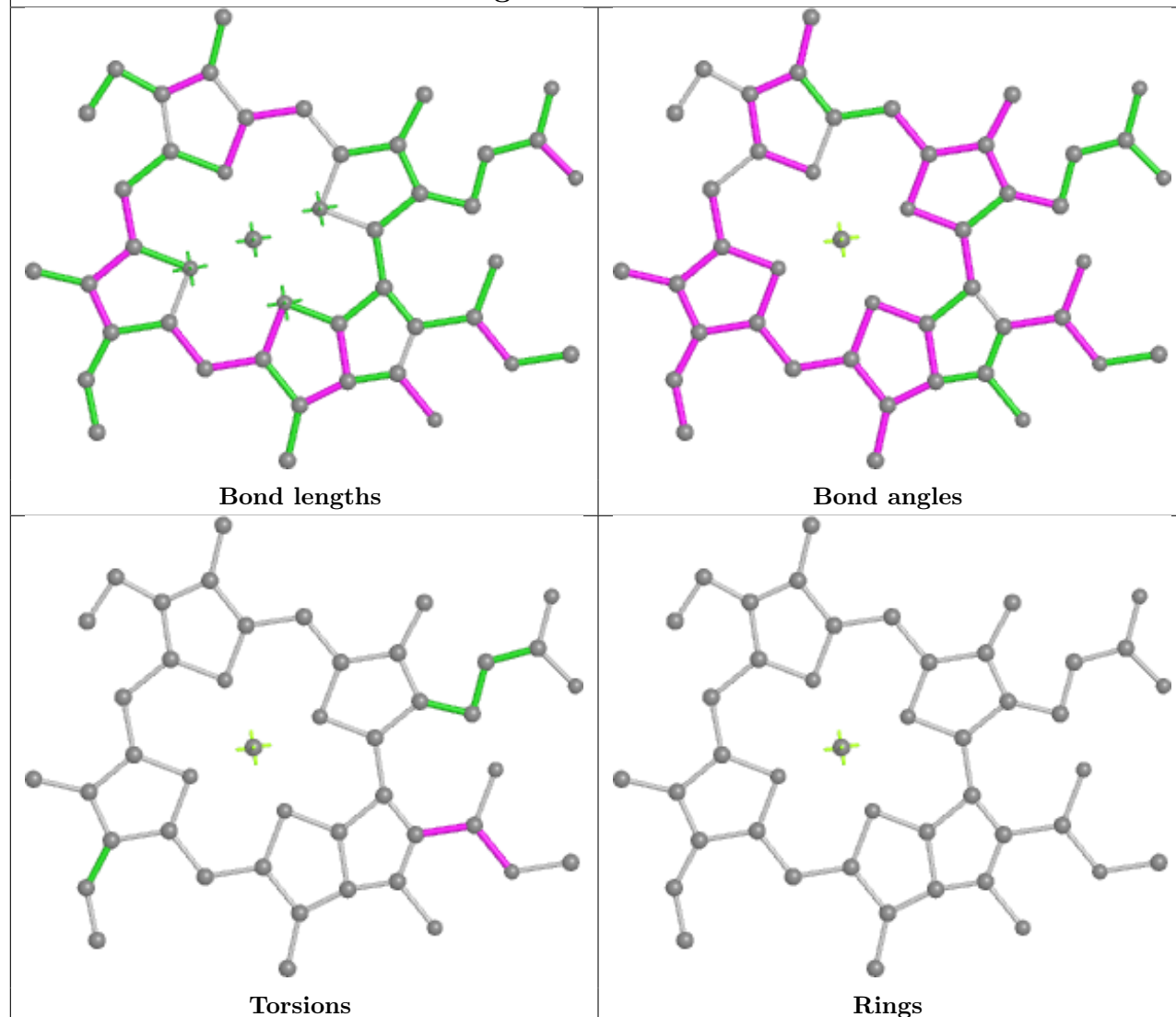
Ligand CLA 3 709



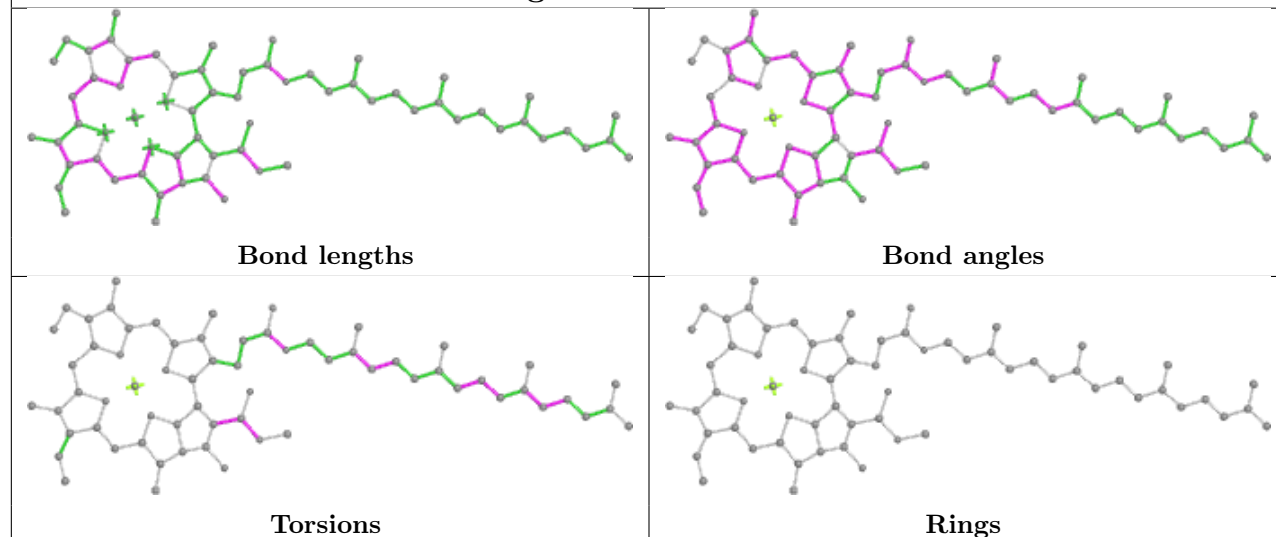
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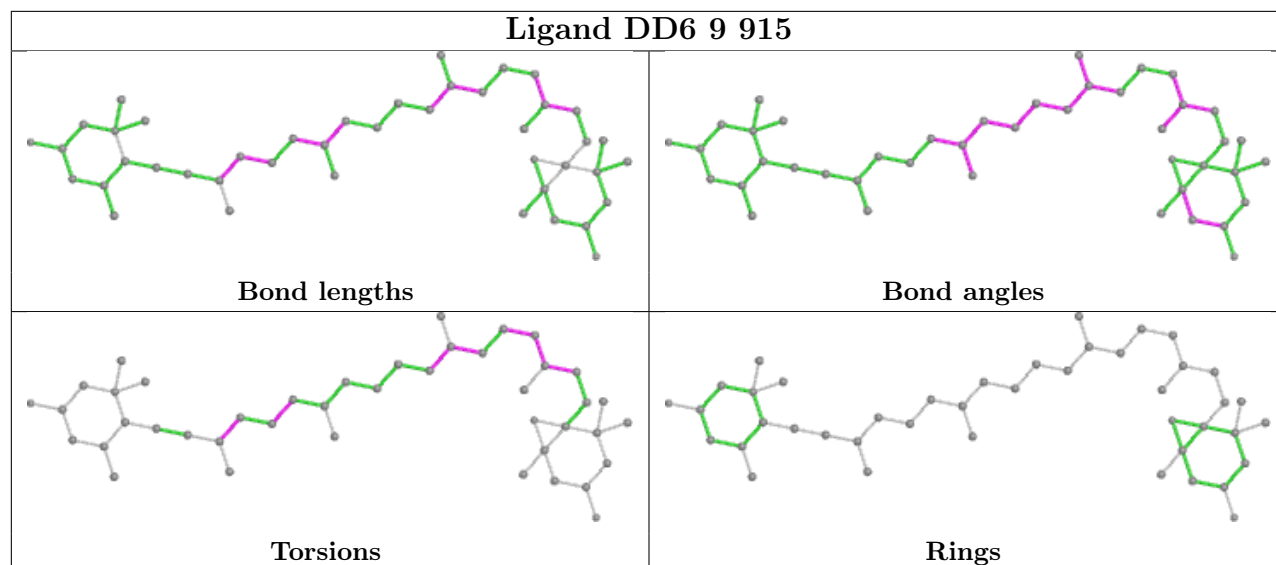
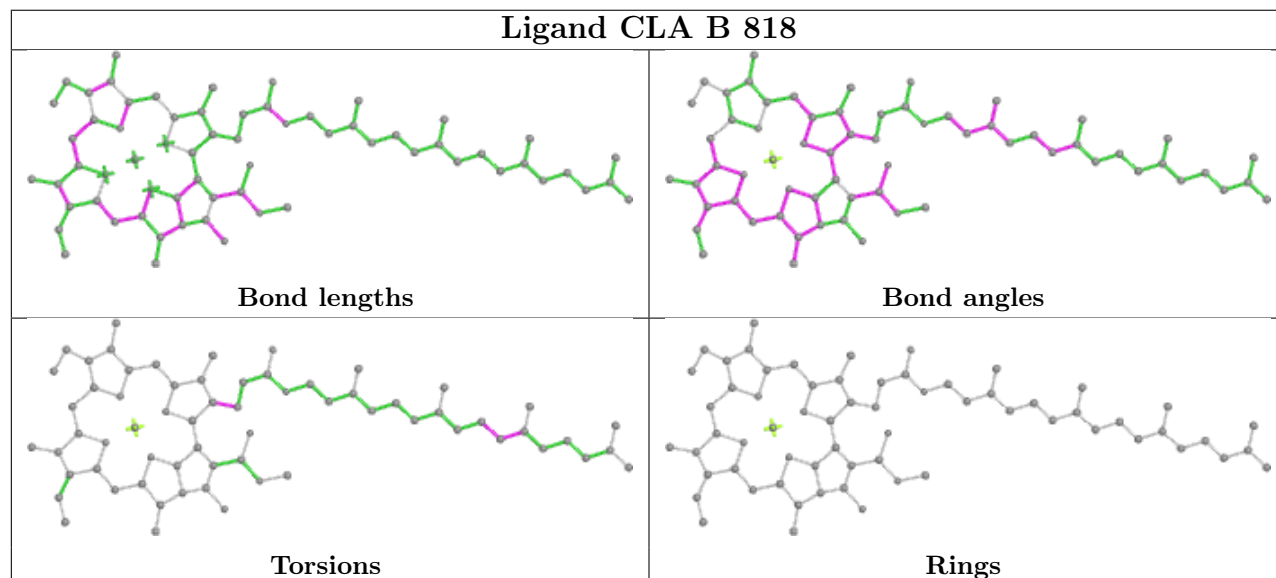
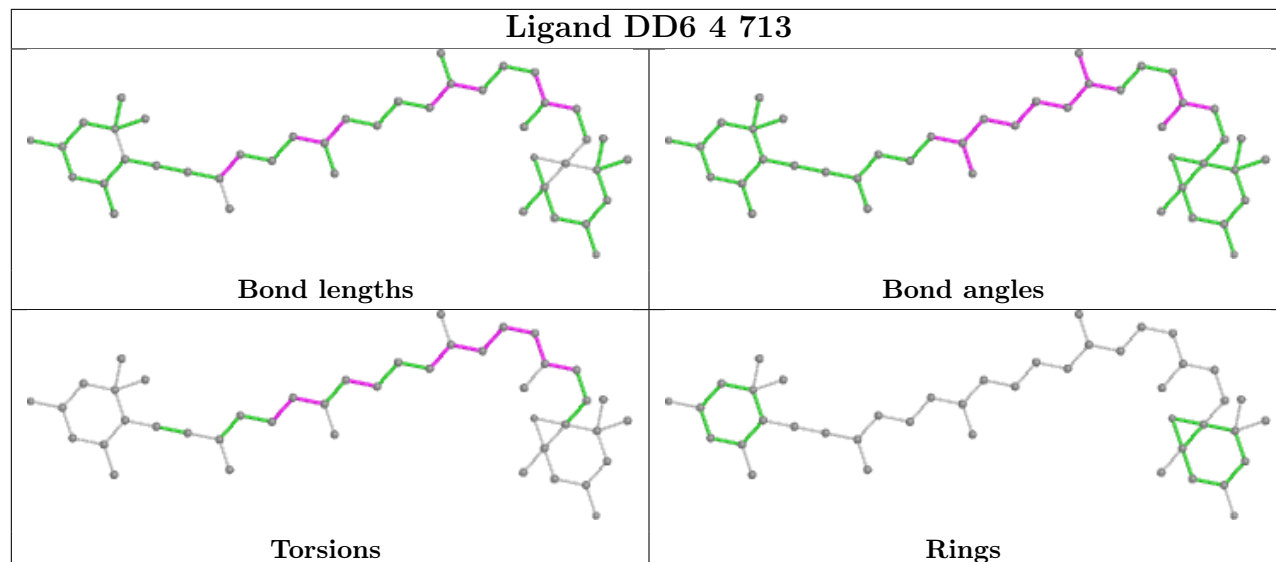


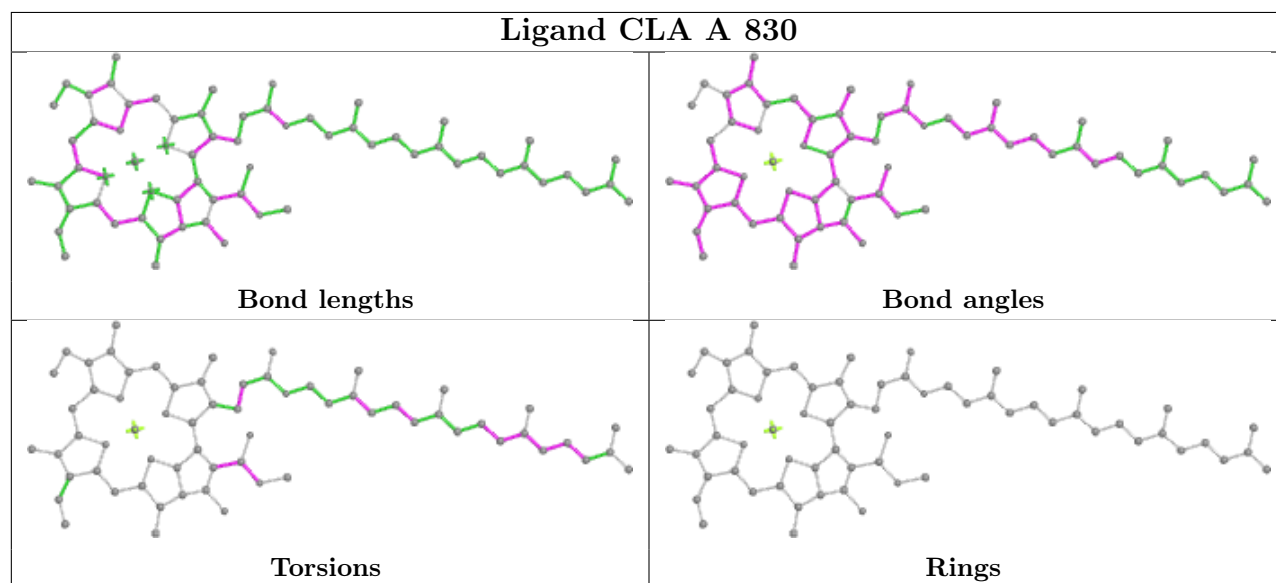
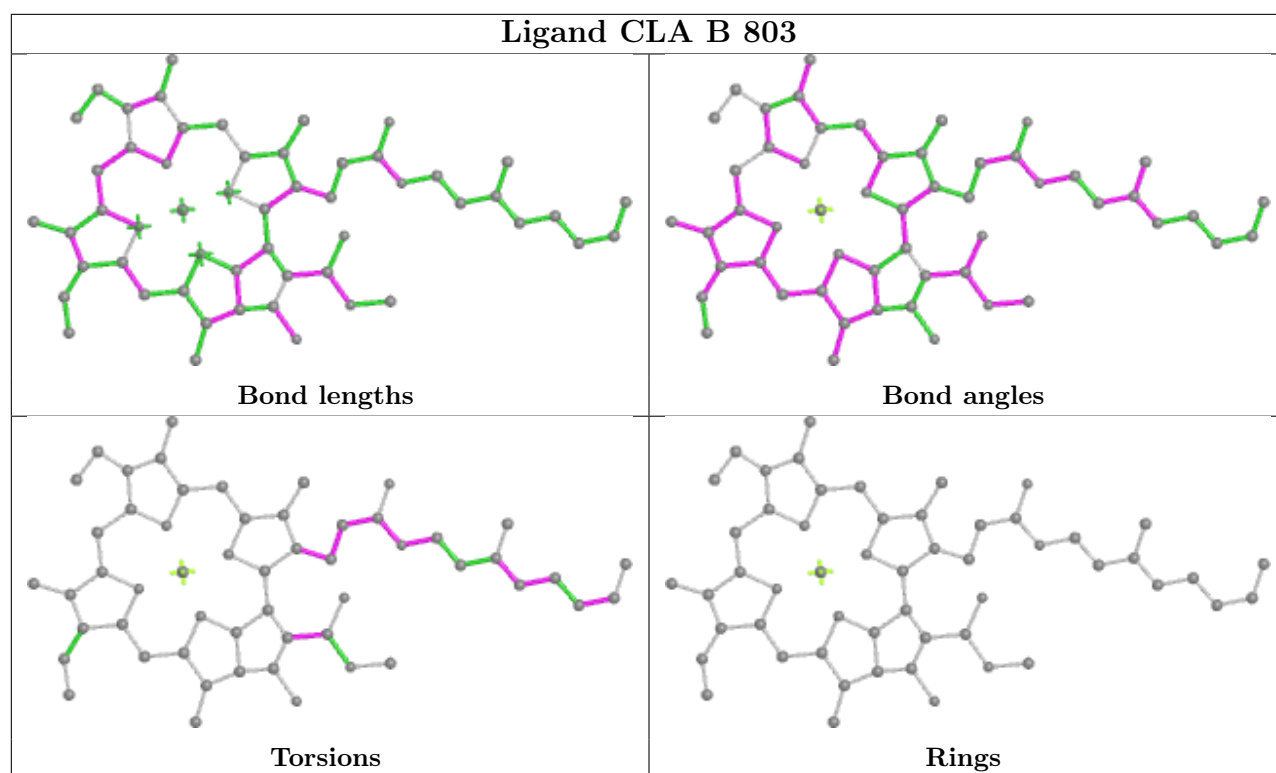
Ligand CLA 5 706



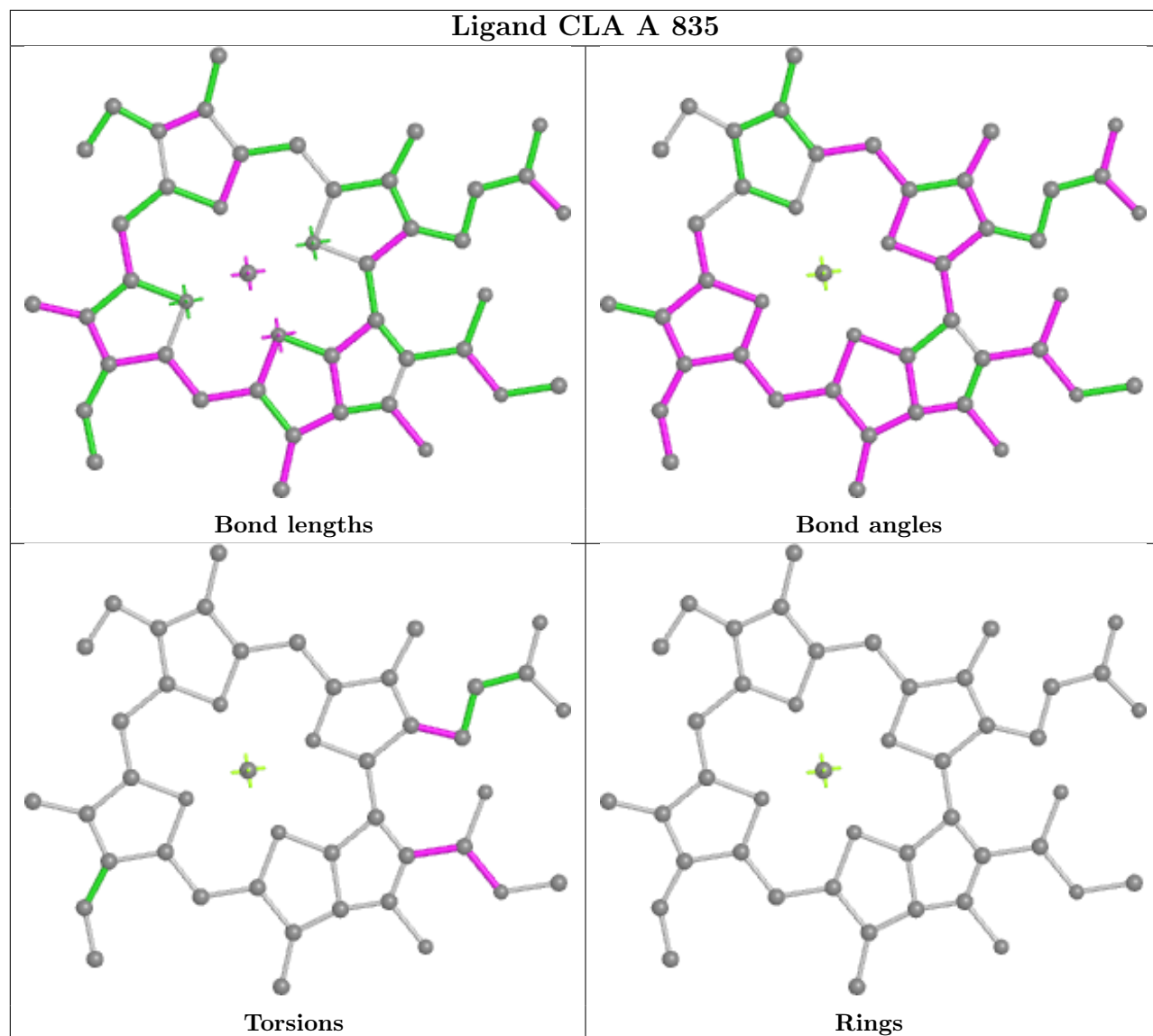
Ligand CLA 11 706

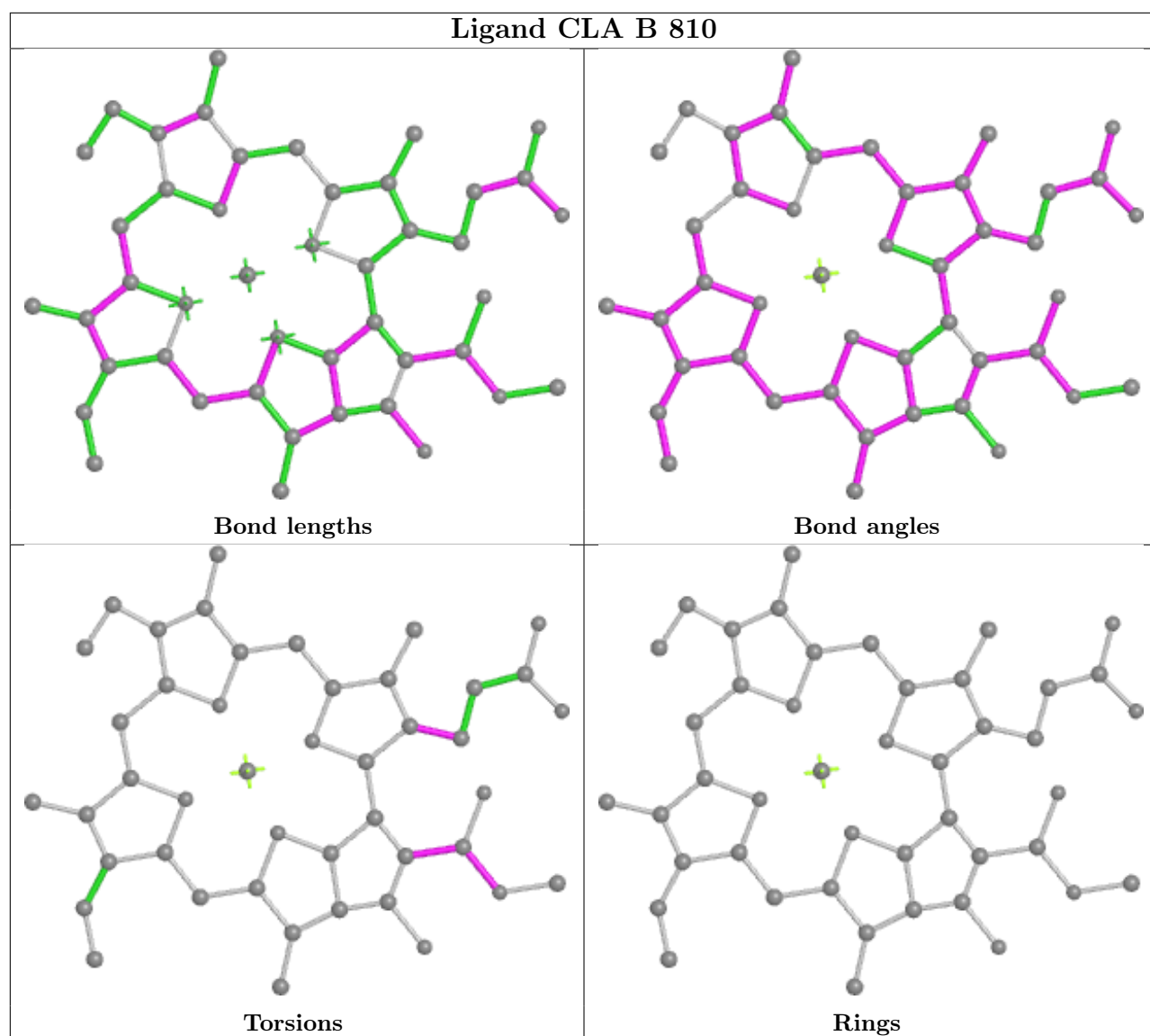


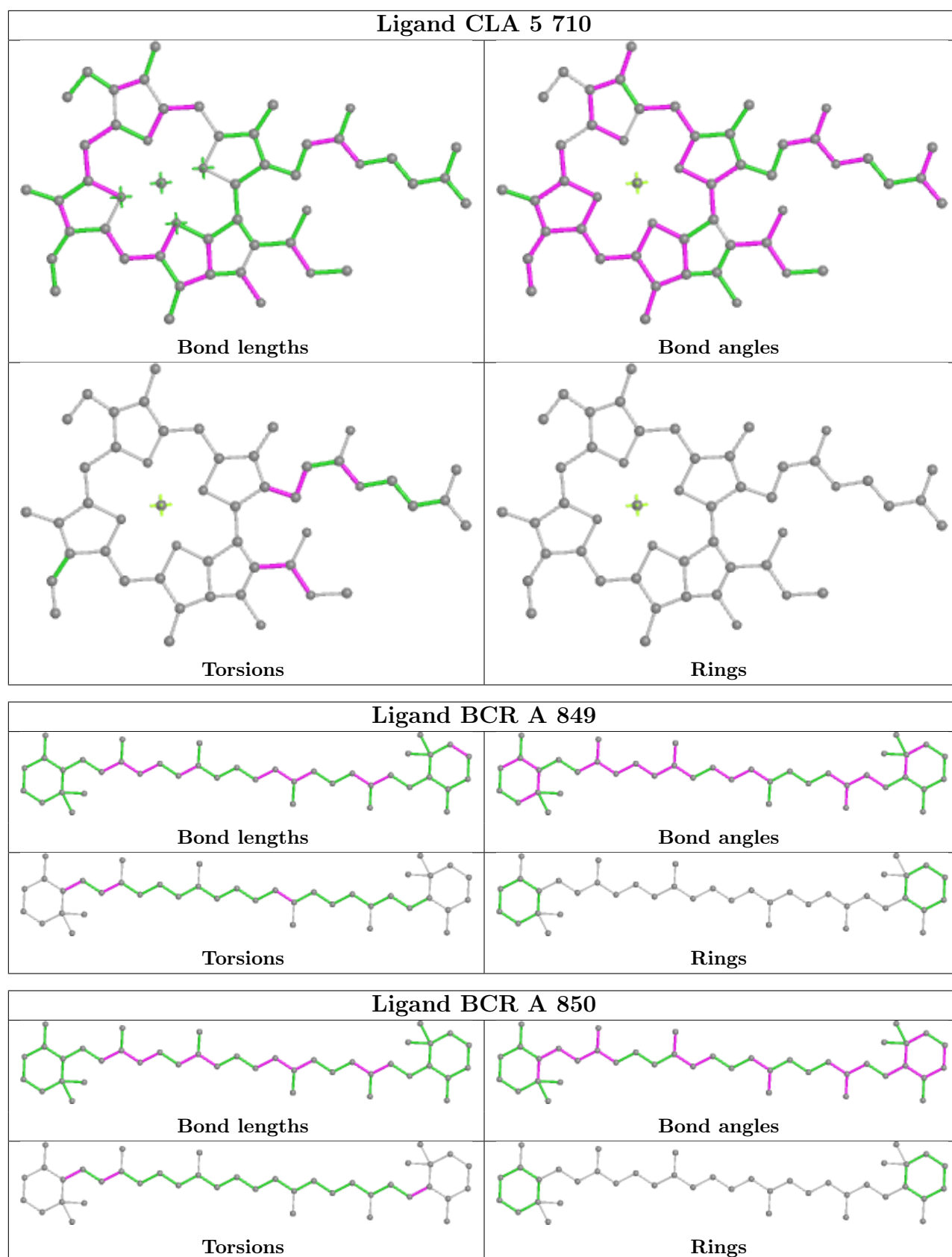
Ligand DD6 9 915**Ligand CLA B 818****Ligand DD6 4 713**

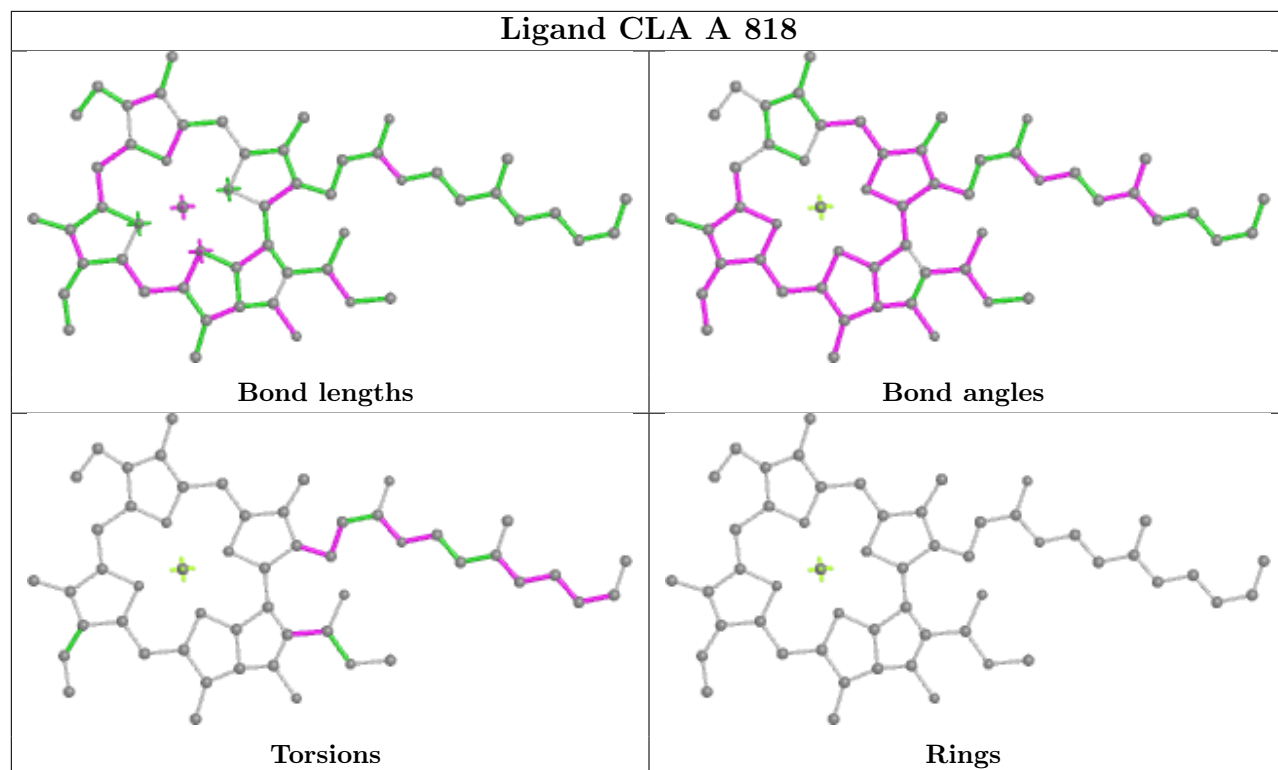


Ligand CLA A 835

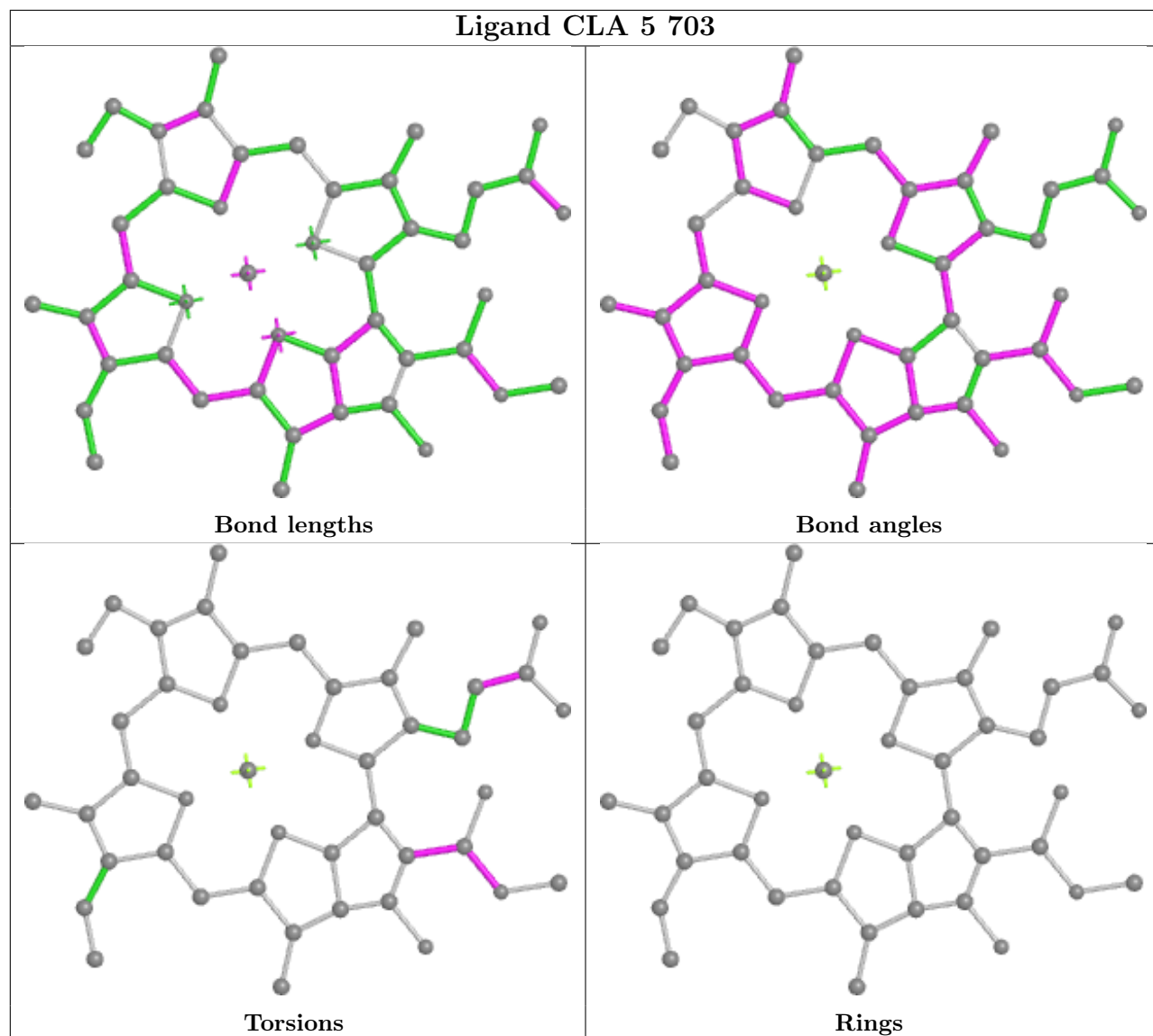




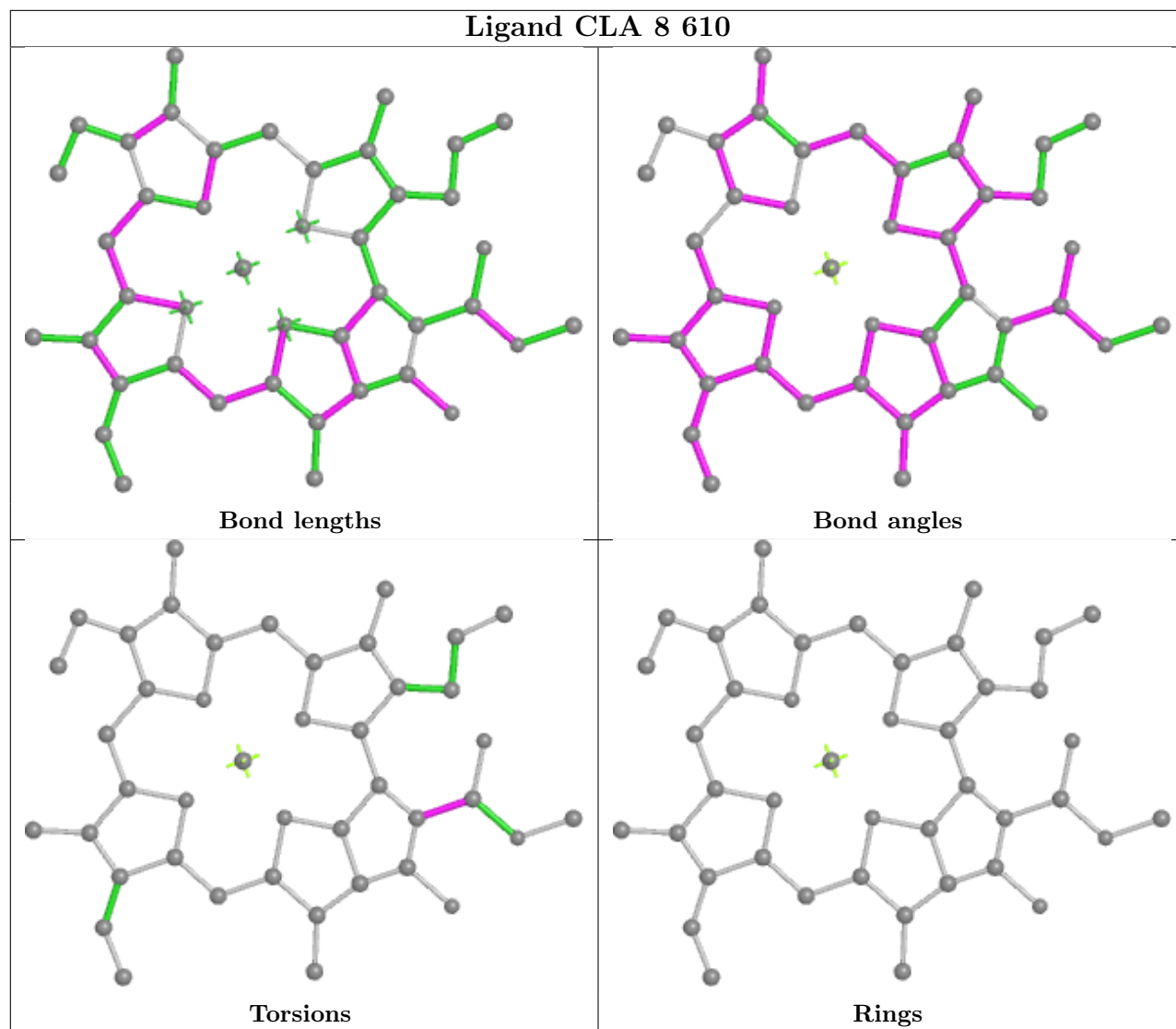


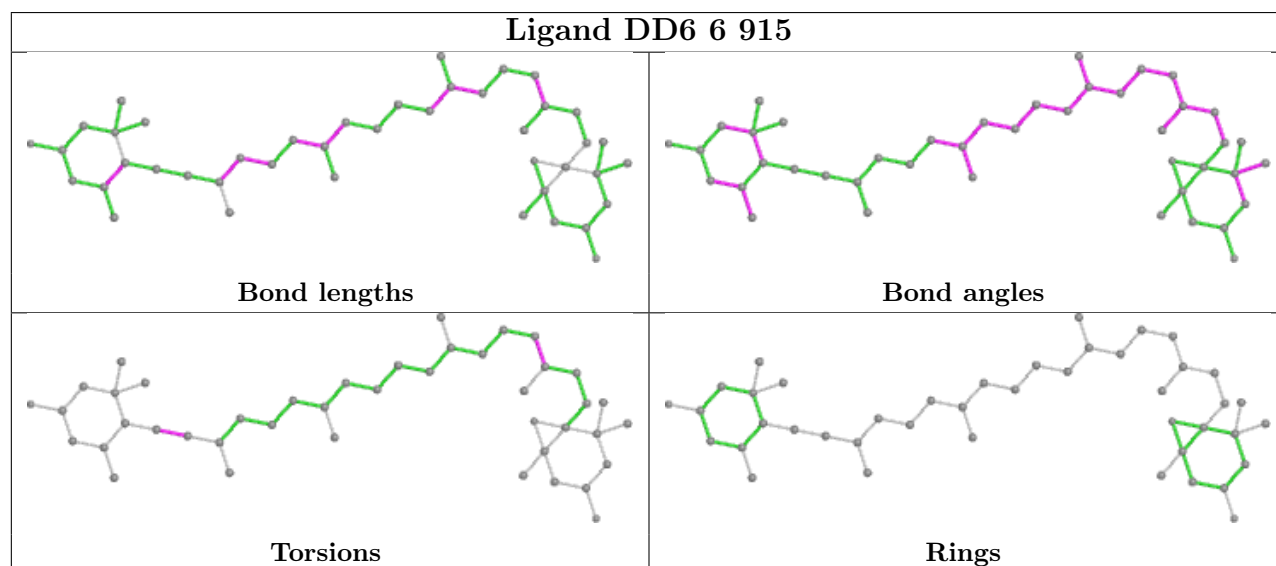
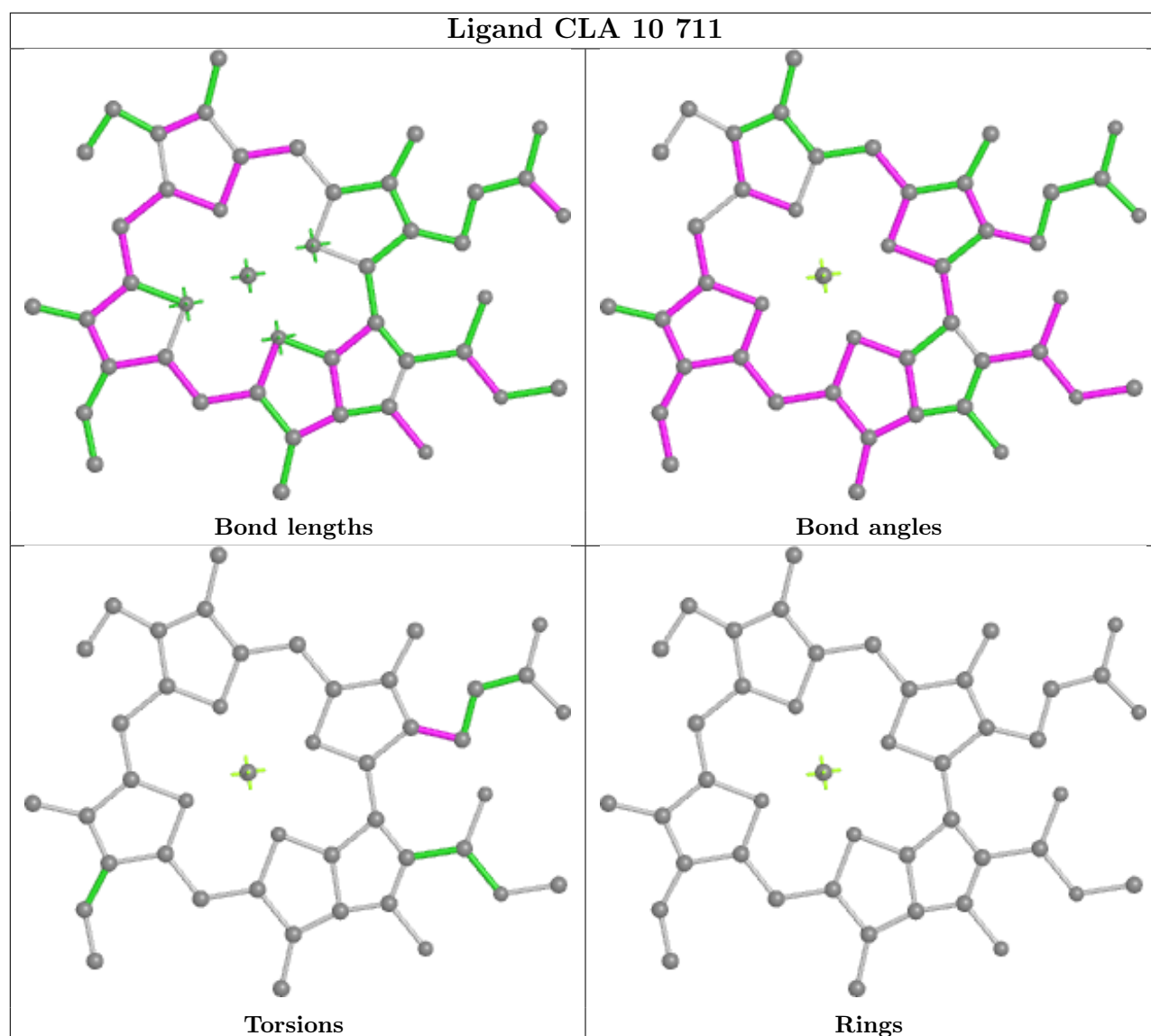


Ligand CLA 5 703

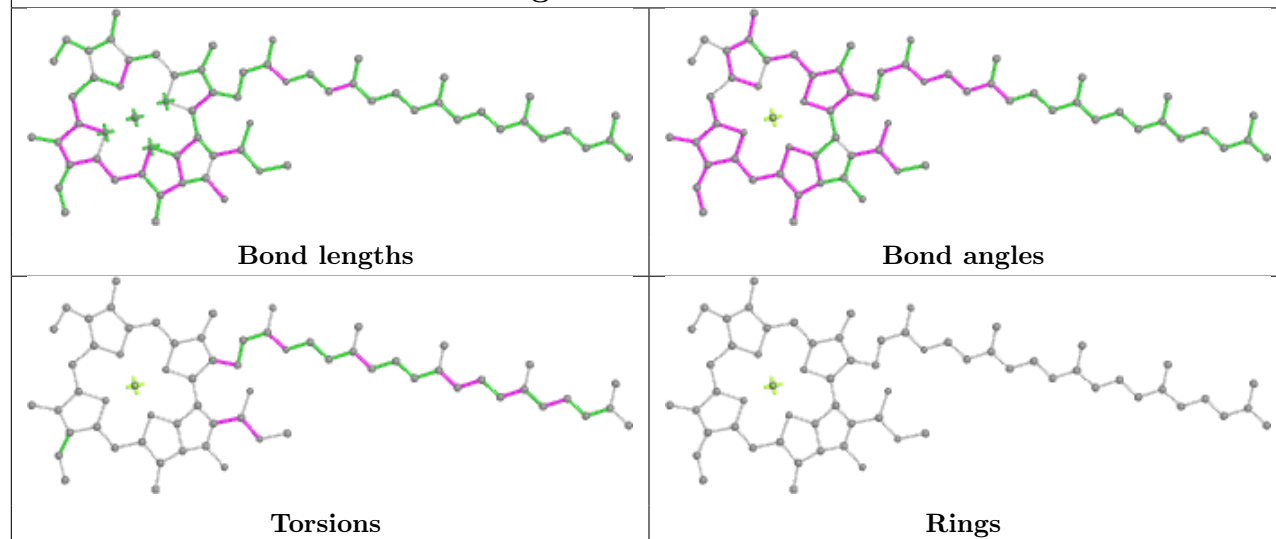


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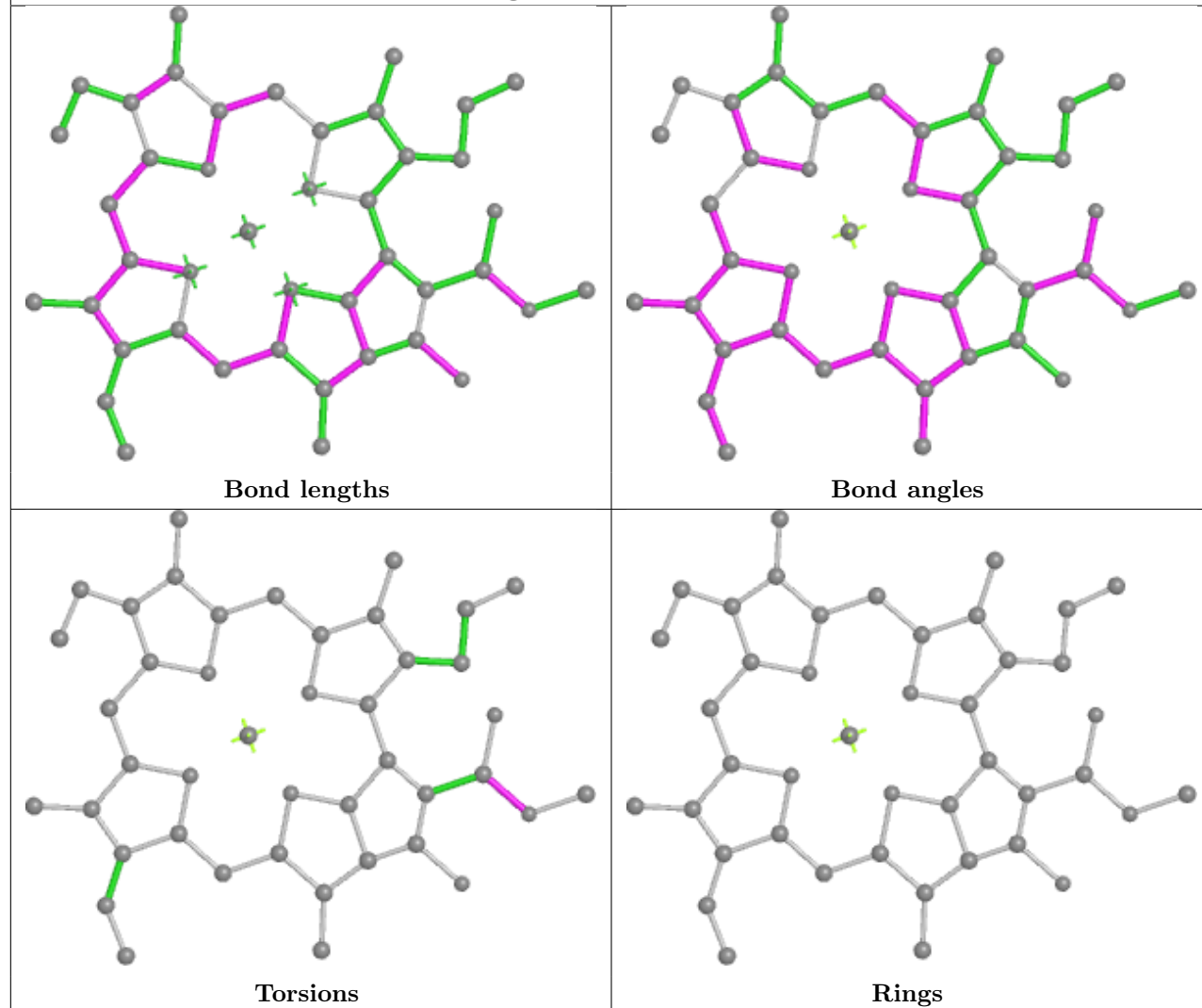




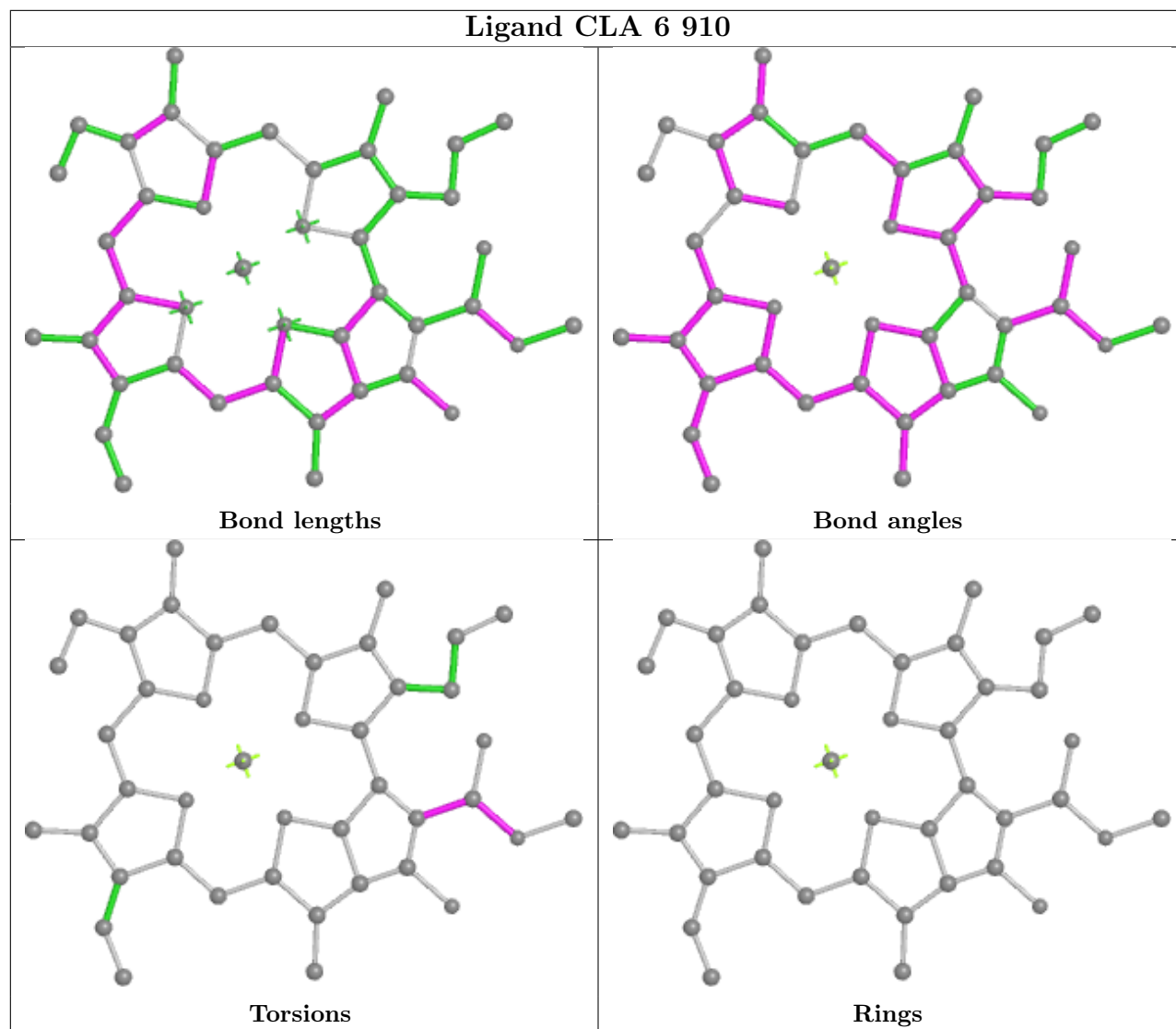
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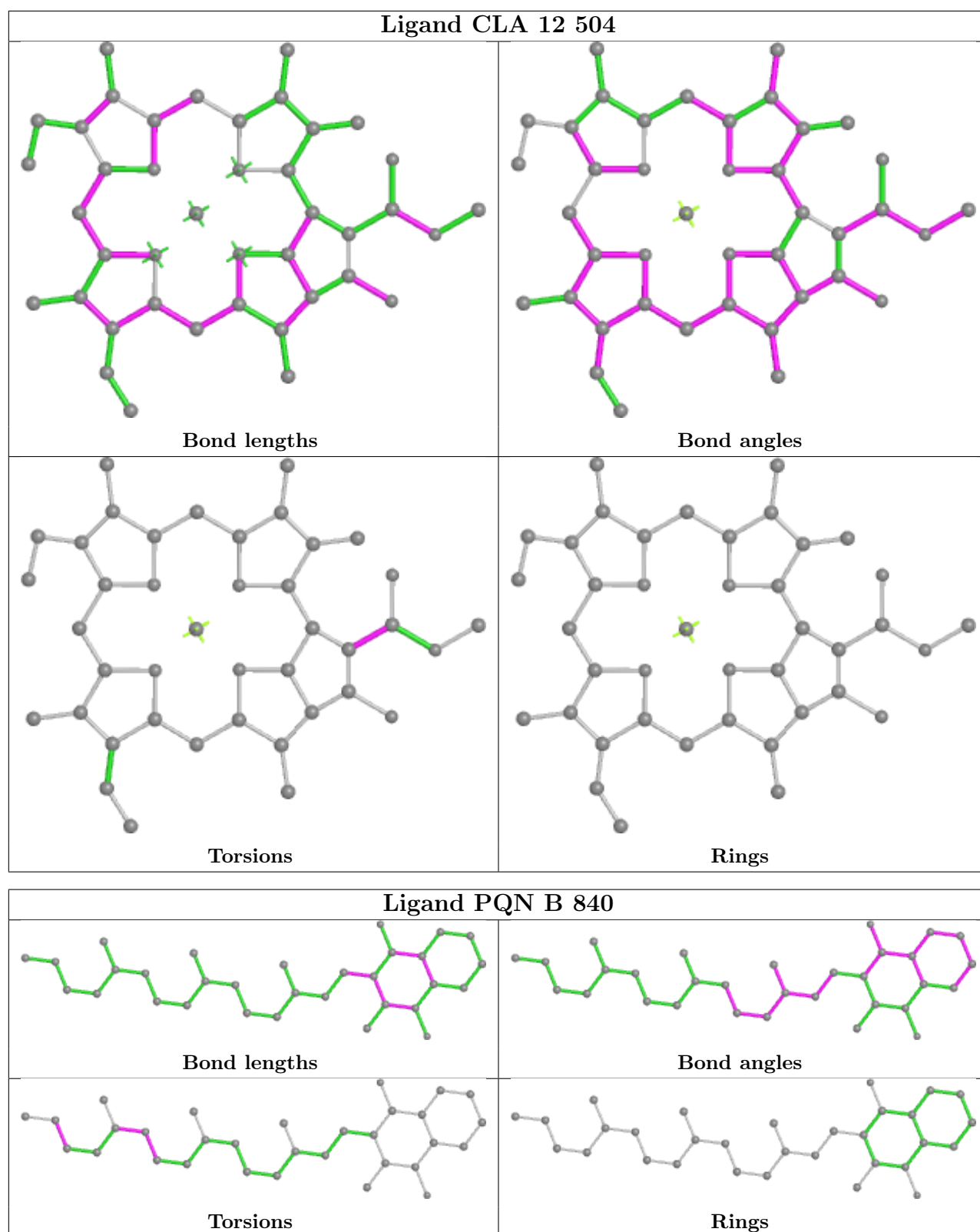


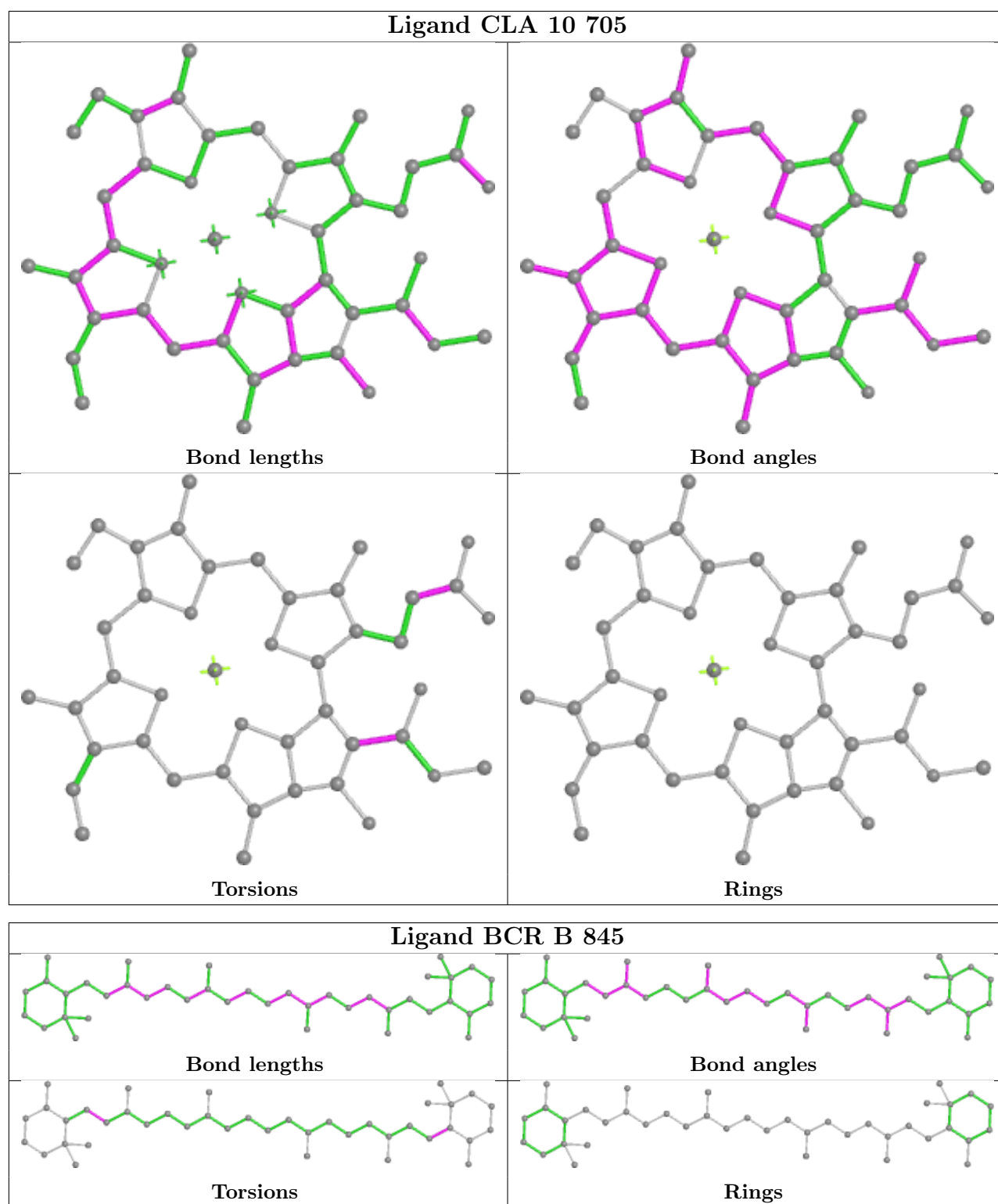
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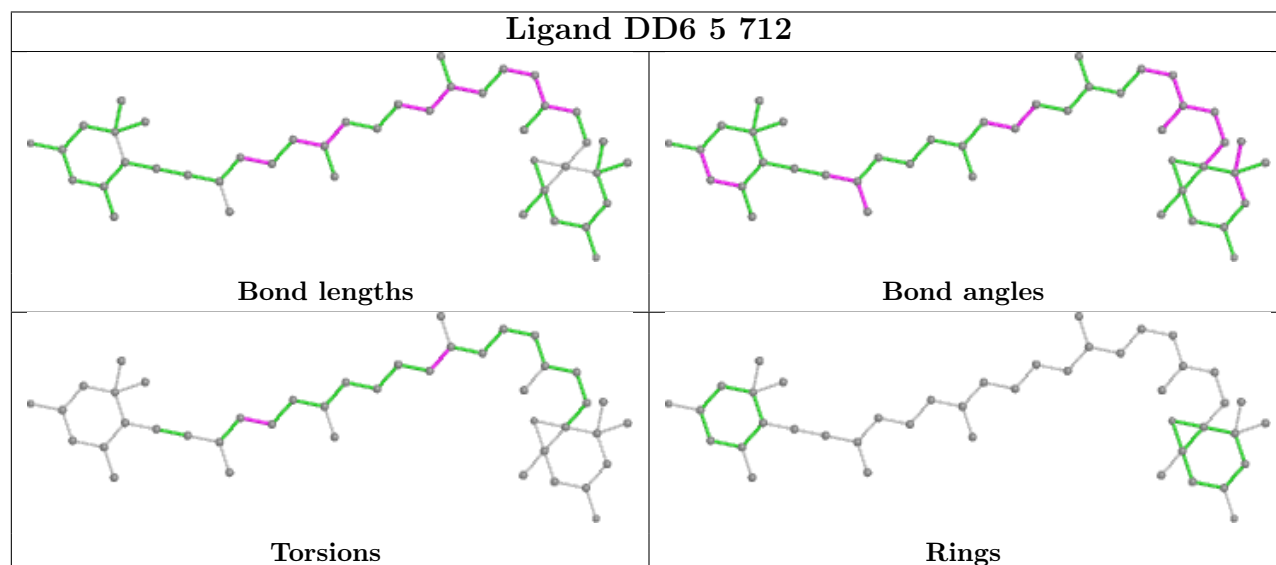
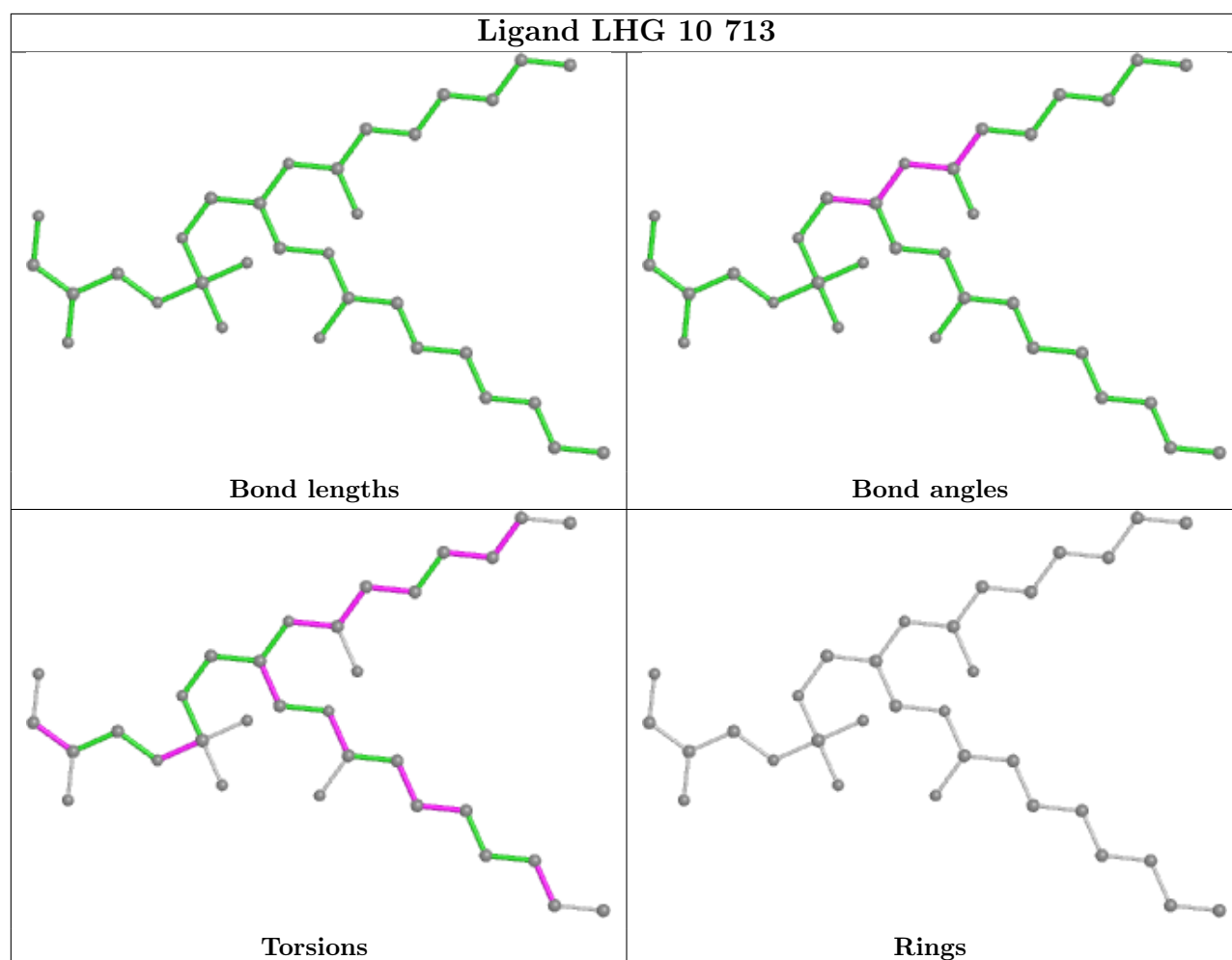


Ligand CLA 6 910

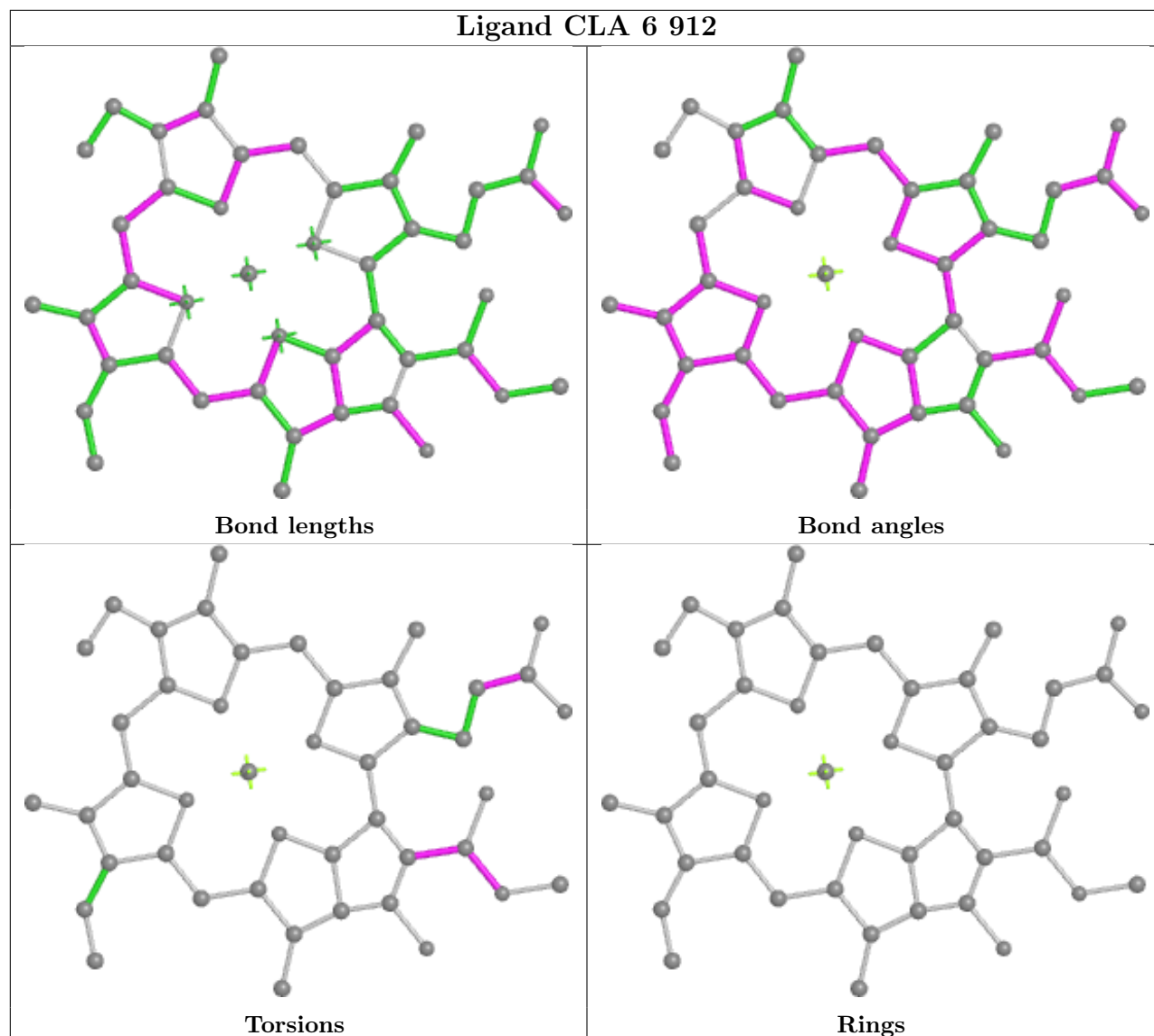




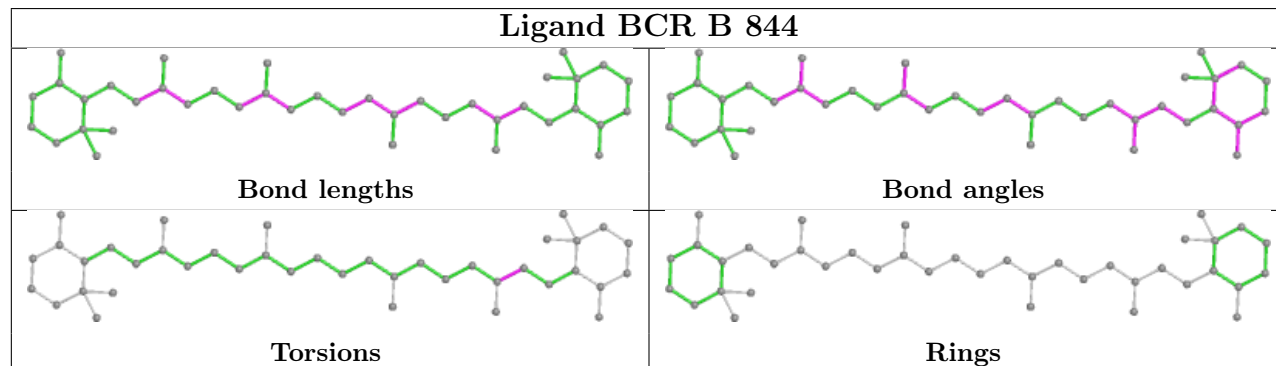


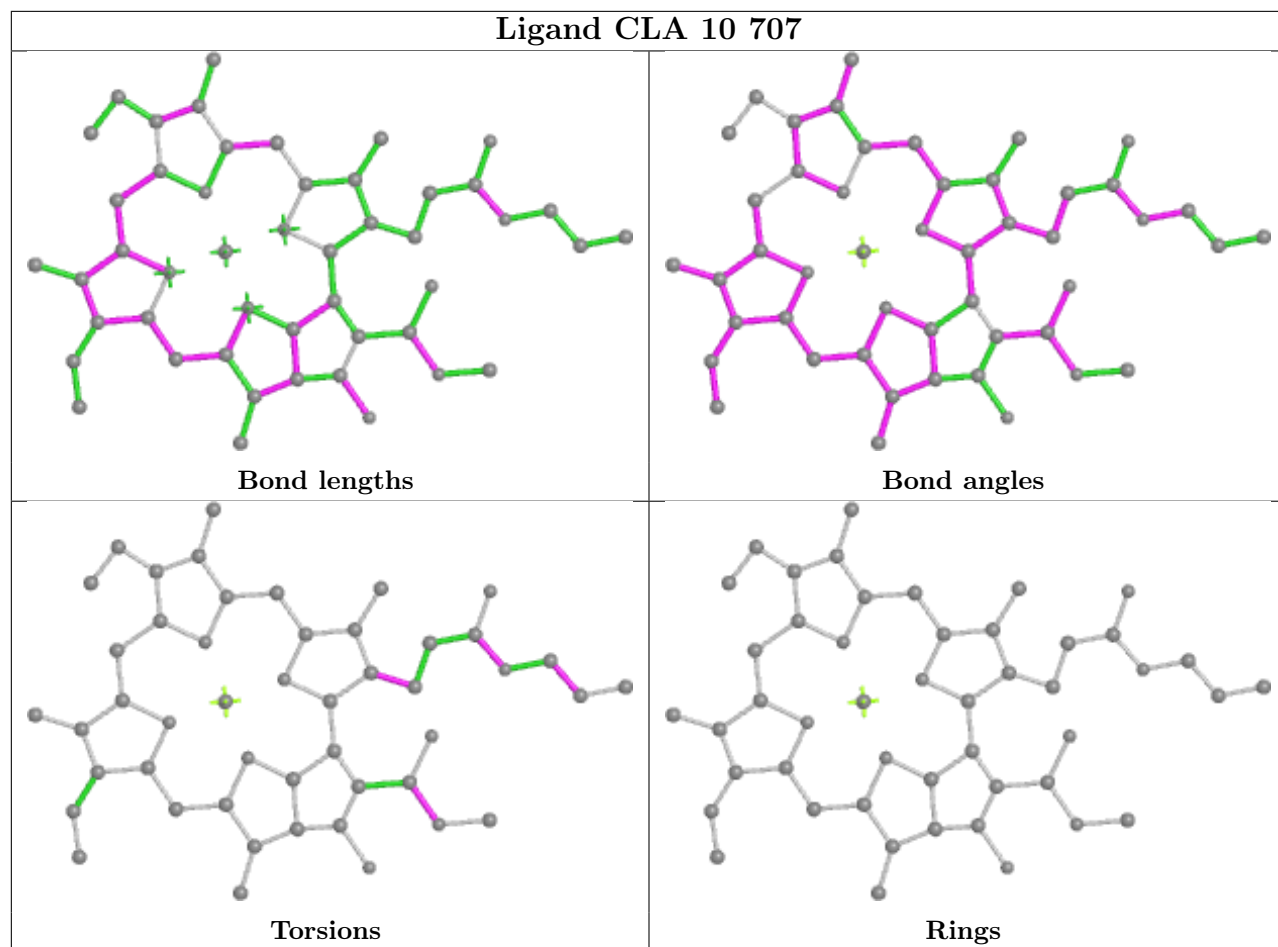


Ligand CLA 6 912

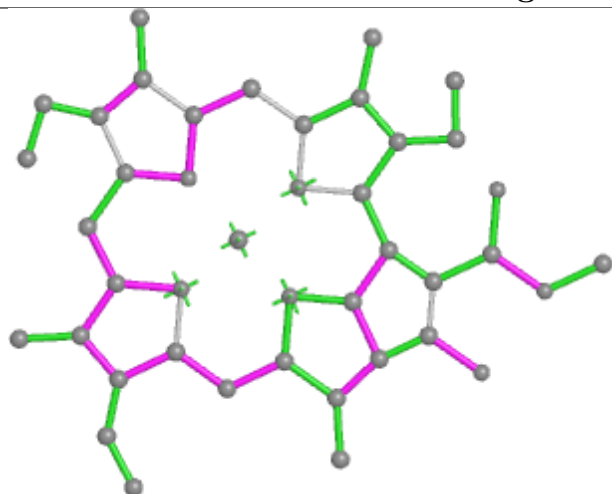


Ligand BCR B 844

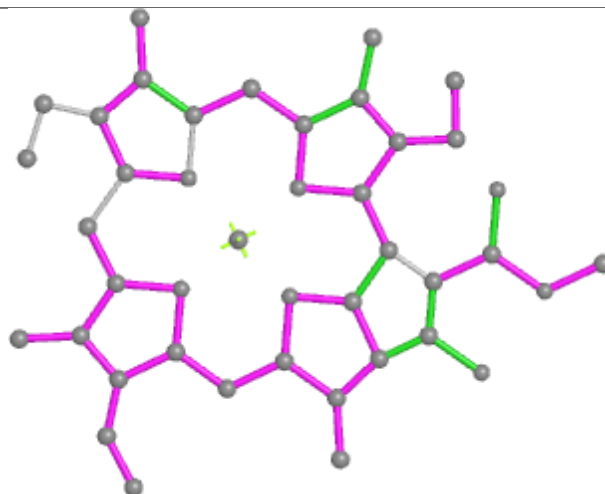




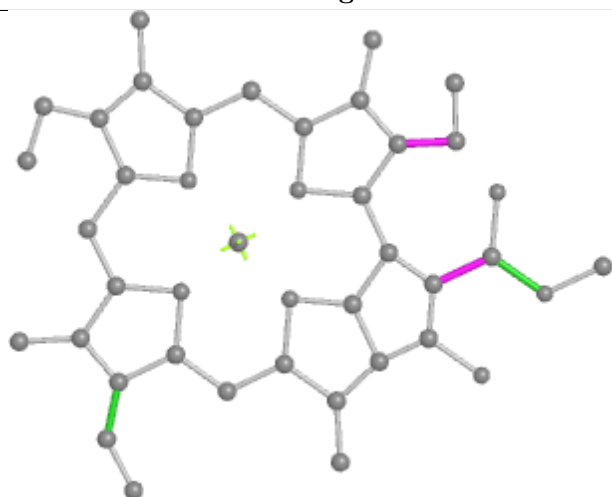
Ligand CLA 3 704



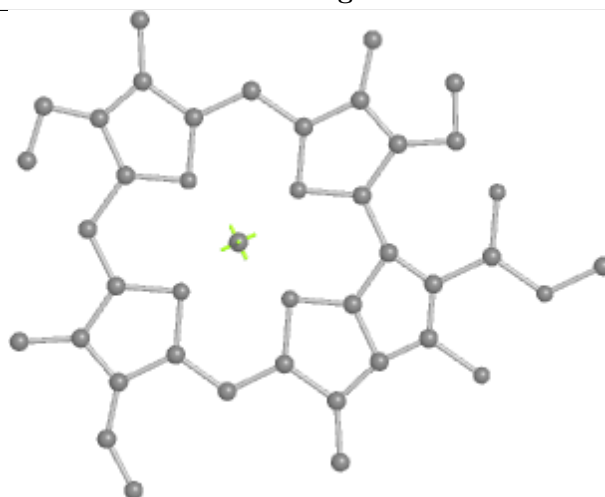
Bond lengths



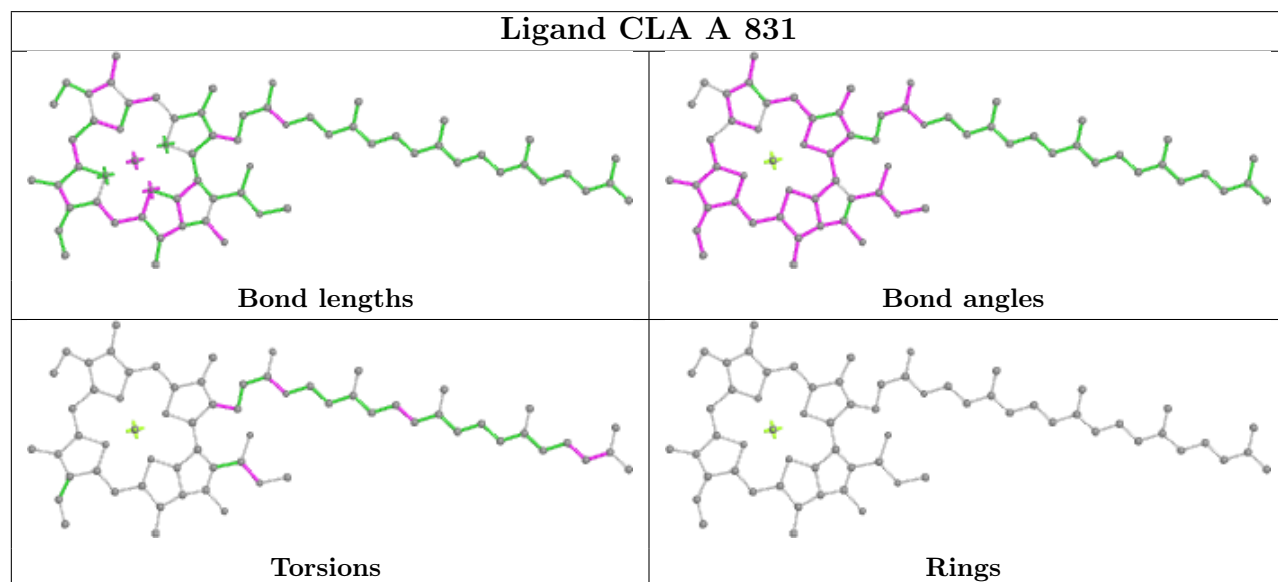
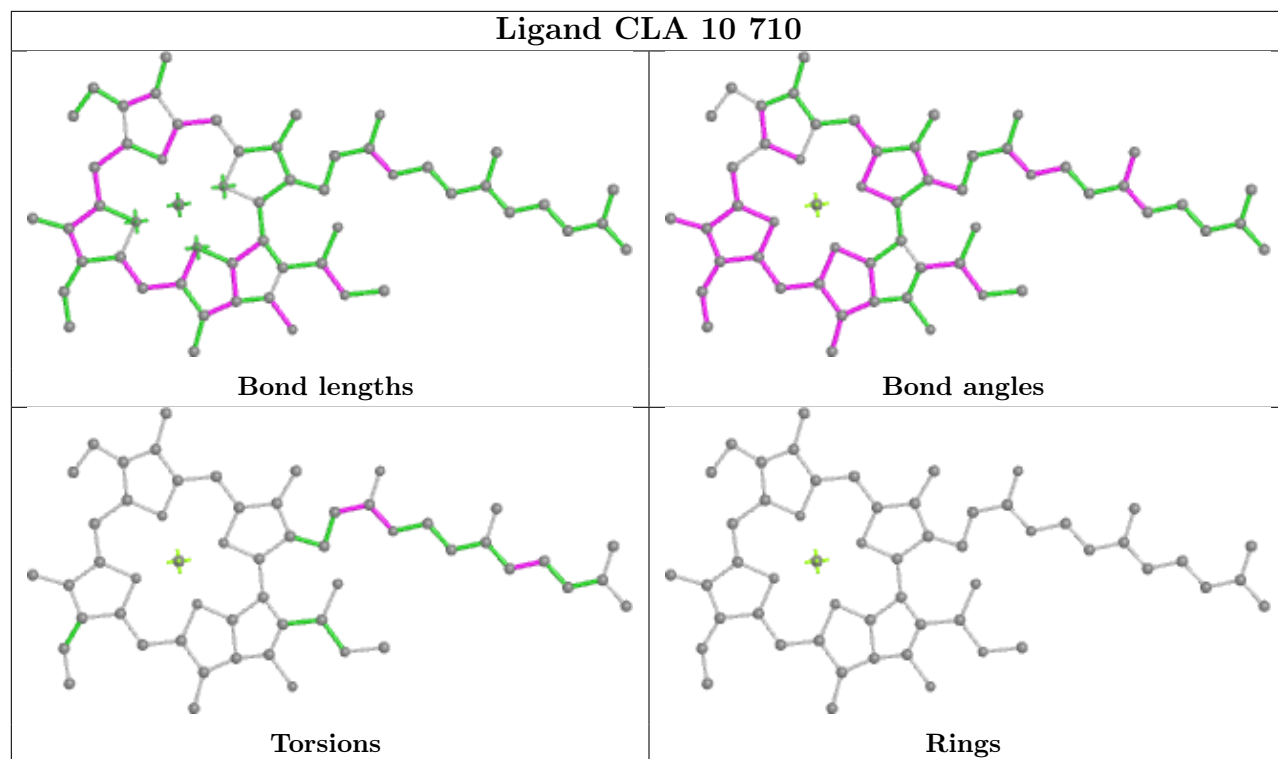
Bond angles

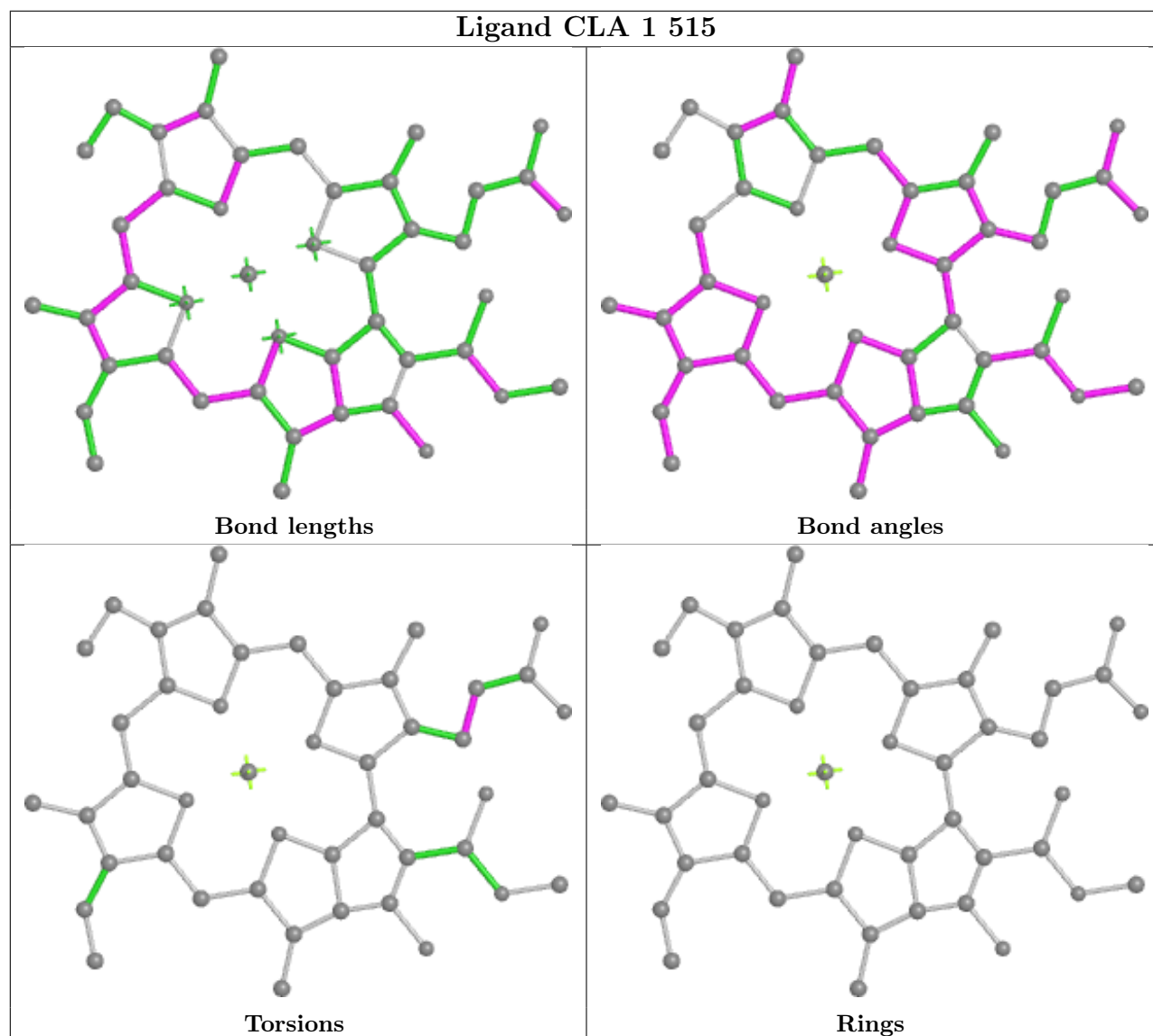
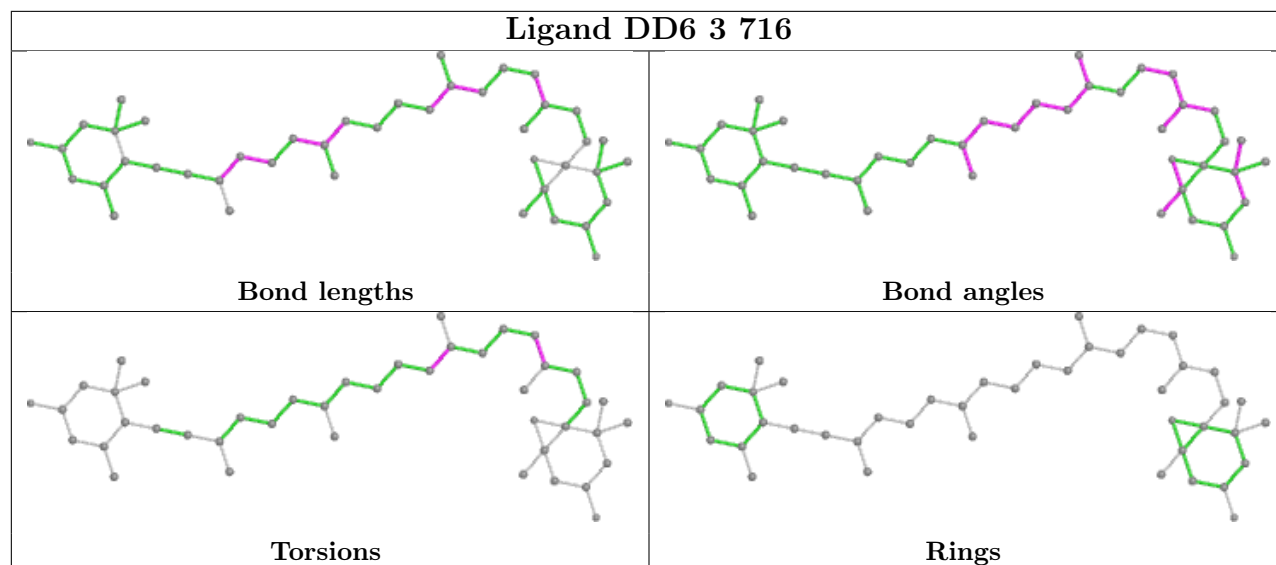


Torsions

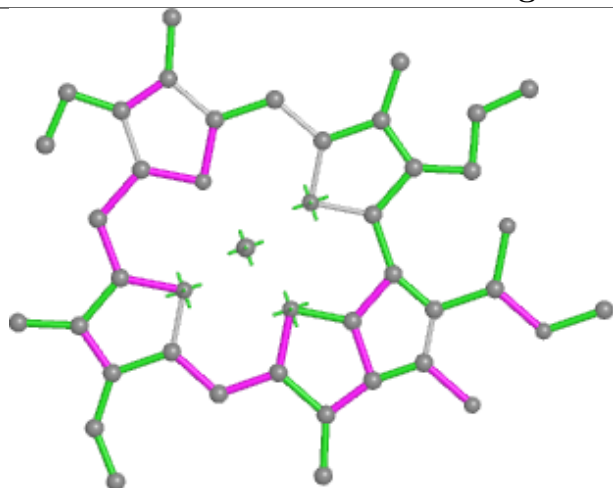


Rings

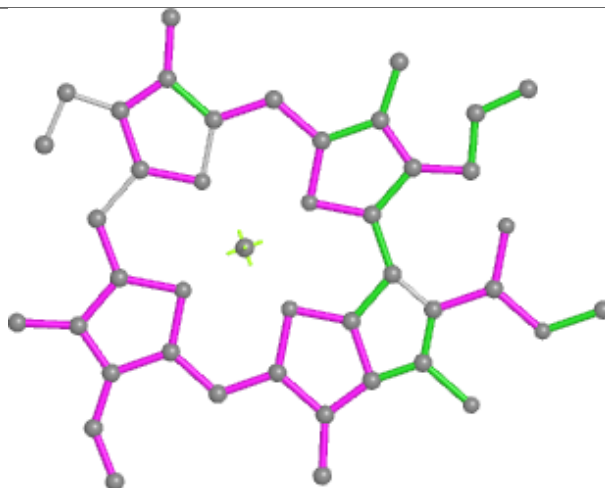




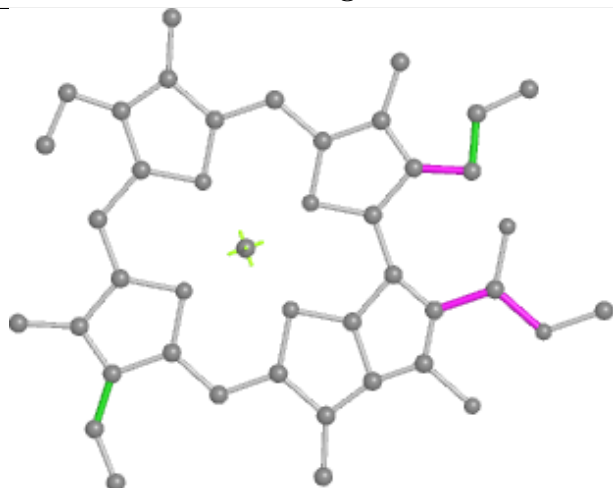
Ligand CLA 3 708



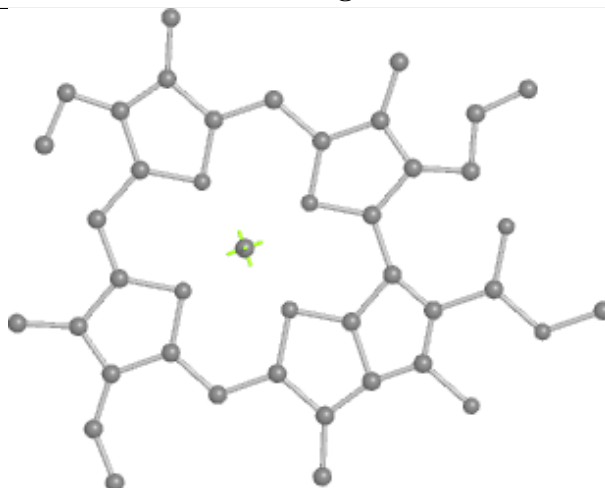
Bond lengths



Bond angles

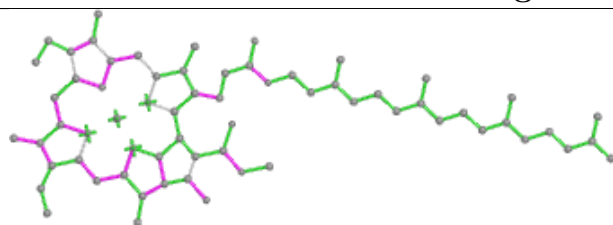


Torsions

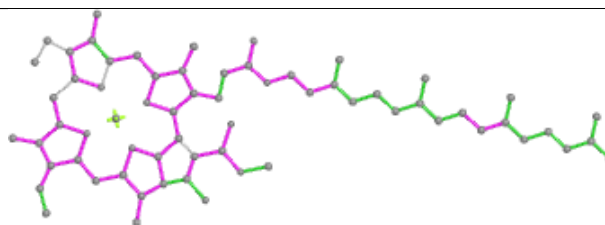


Rings

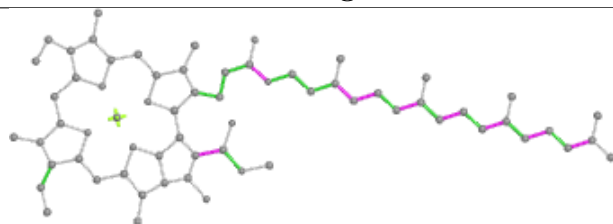
Ligand CLA B 835



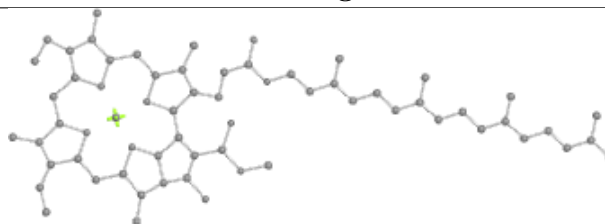
Bond lengths



Bond angles

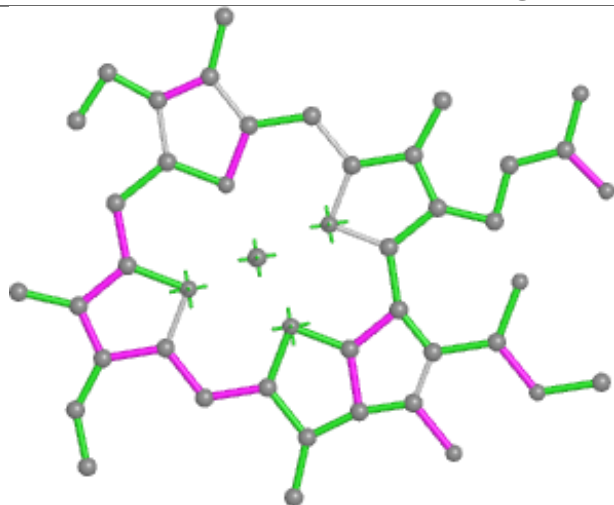


Torsions

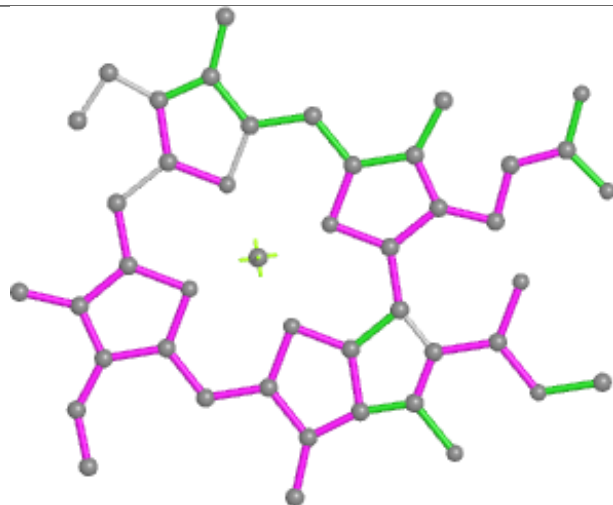


Rings

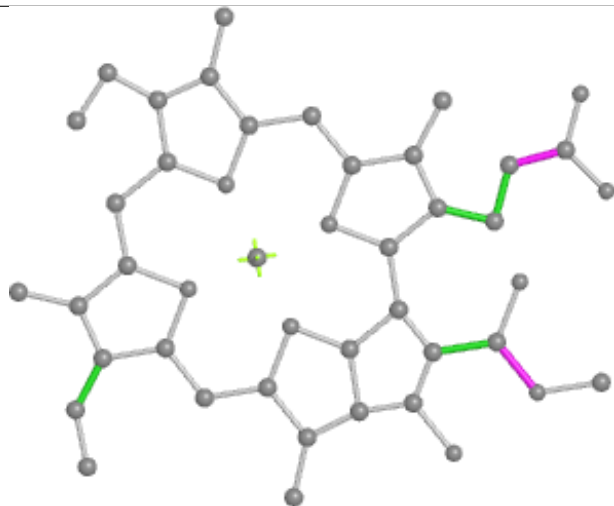
Ligand CLA A 834



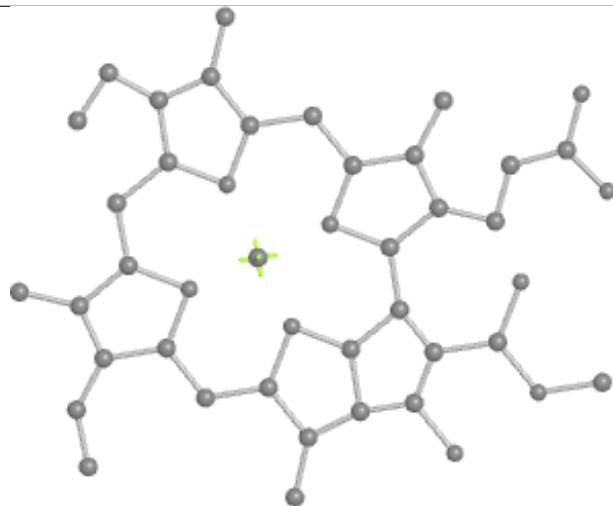
Bond lengths



Bond angles

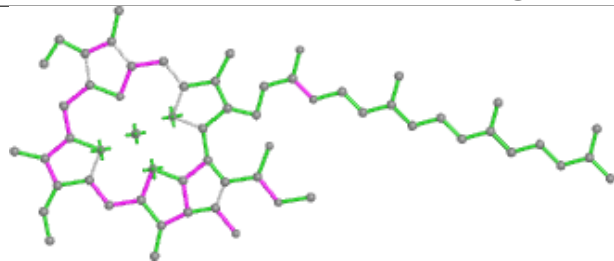


Torsions

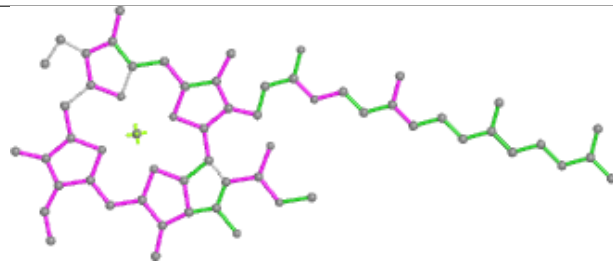


Rings

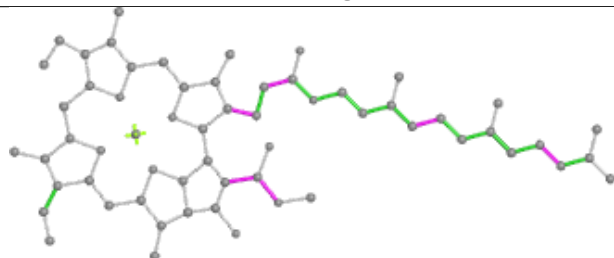
Ligand CLA 12 501



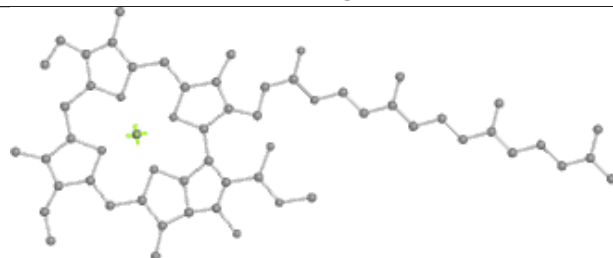
Bond lengths



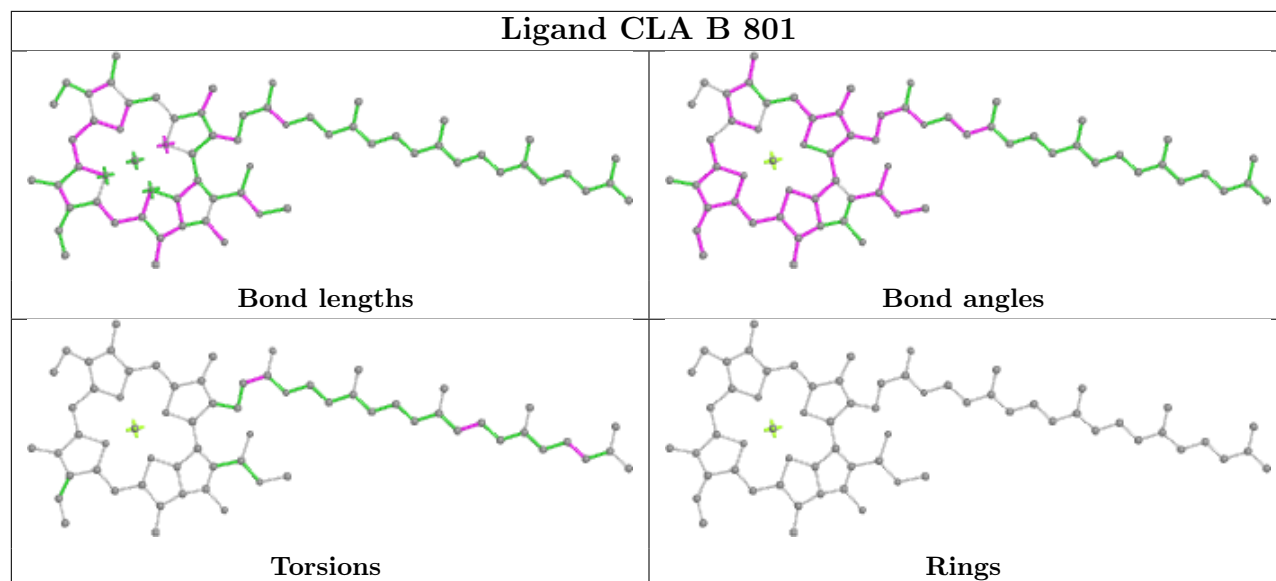
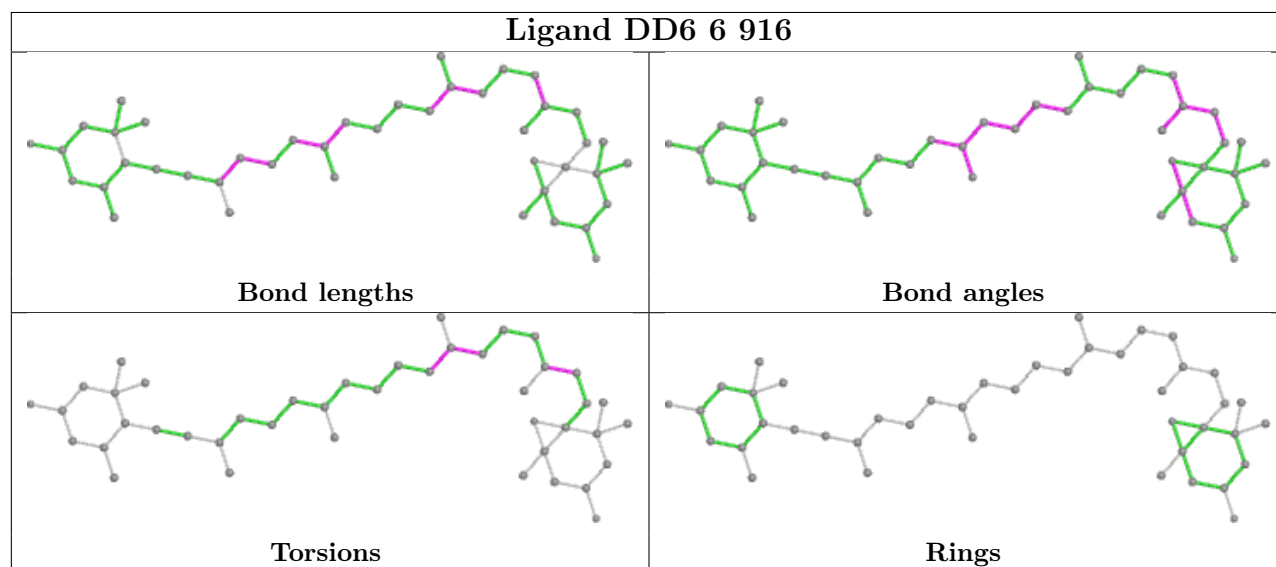
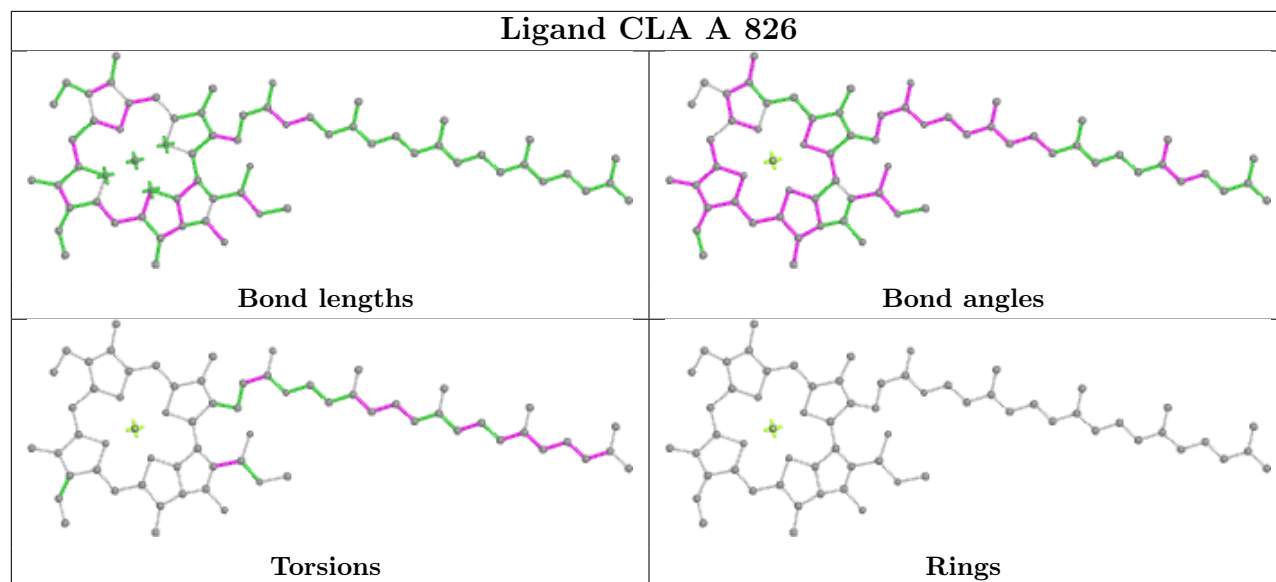
Bond angles



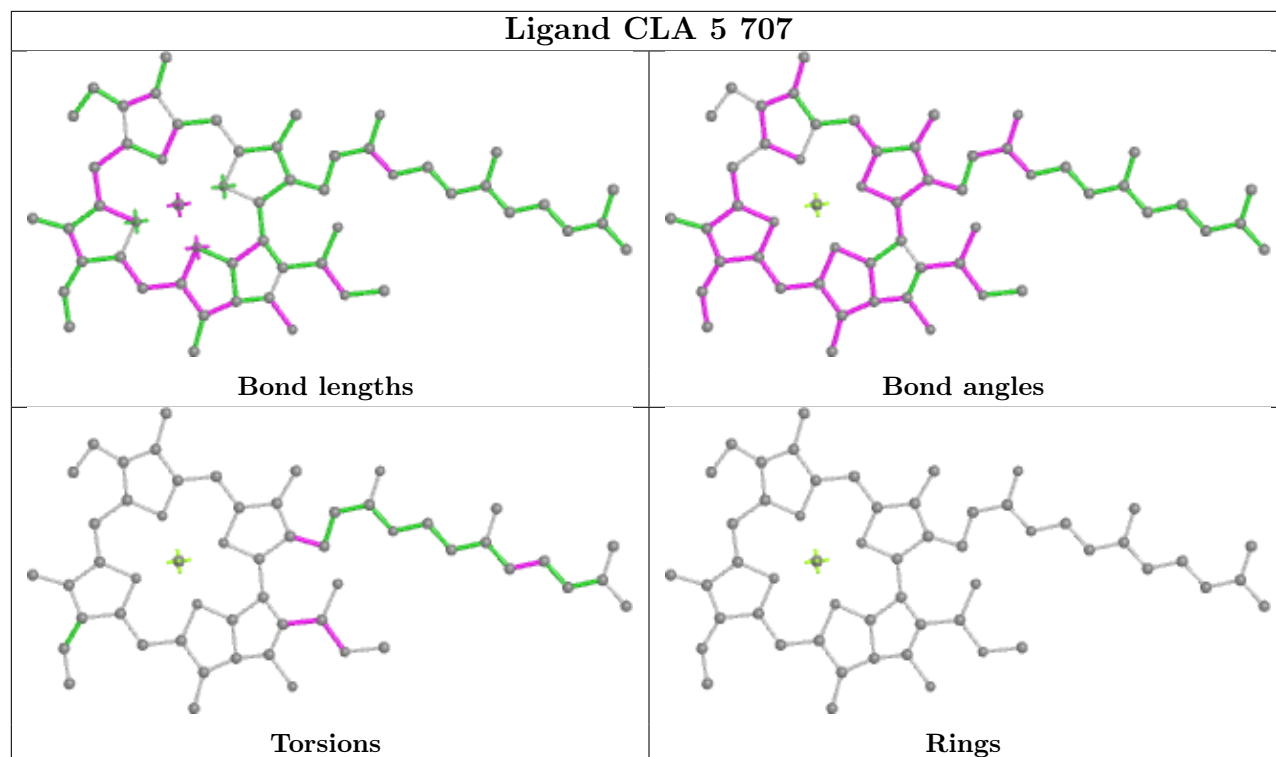
Torsions



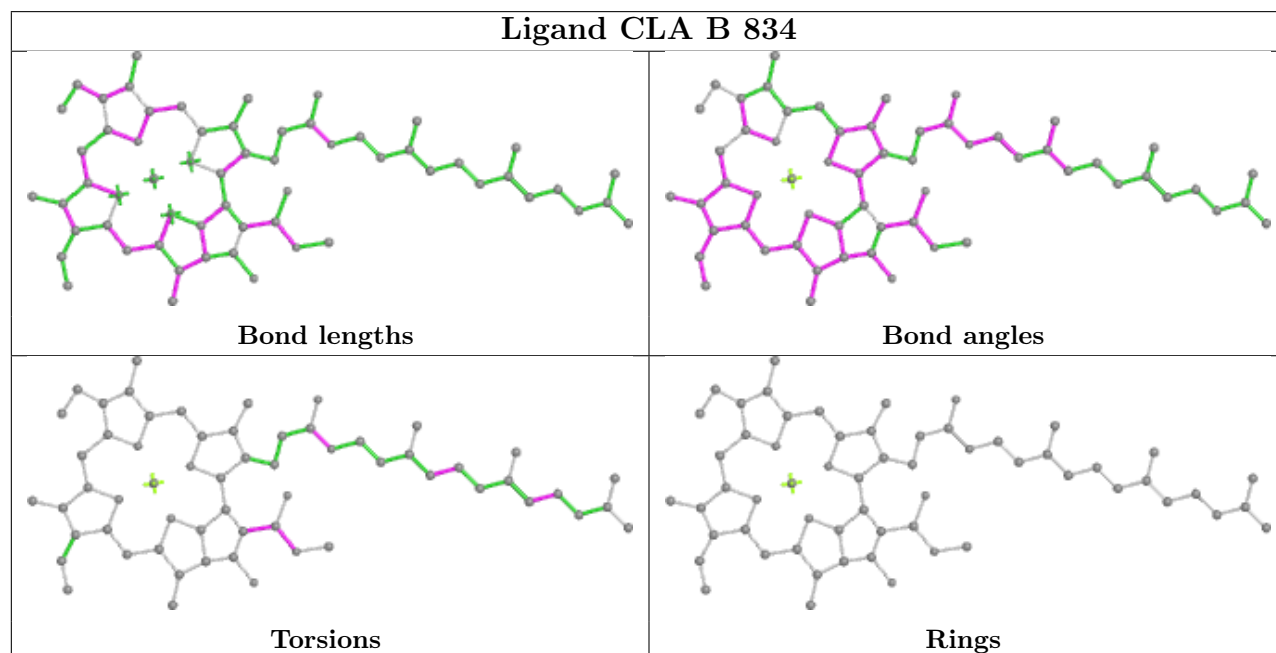
Rings



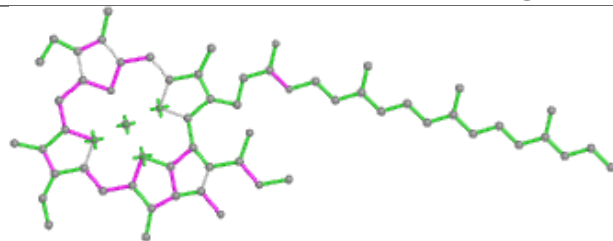
Ligand CLA 5 707



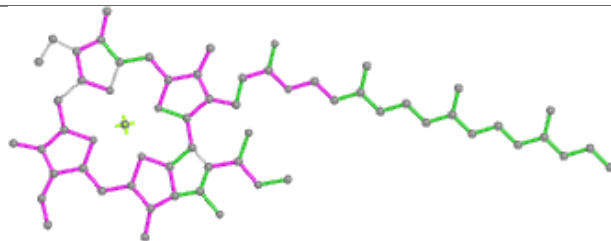
Ligand CLA B 834



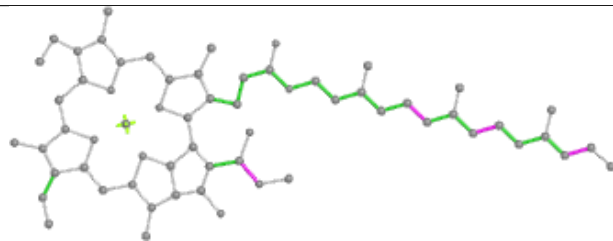
Ligand CLA 2 509



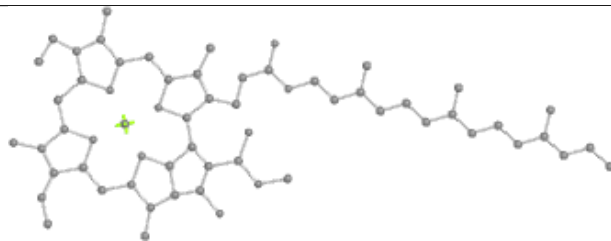
Bond lengths



Bond angles

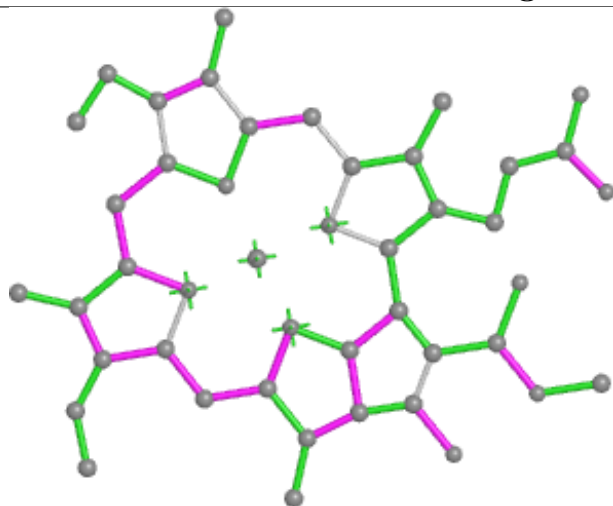


Torsions

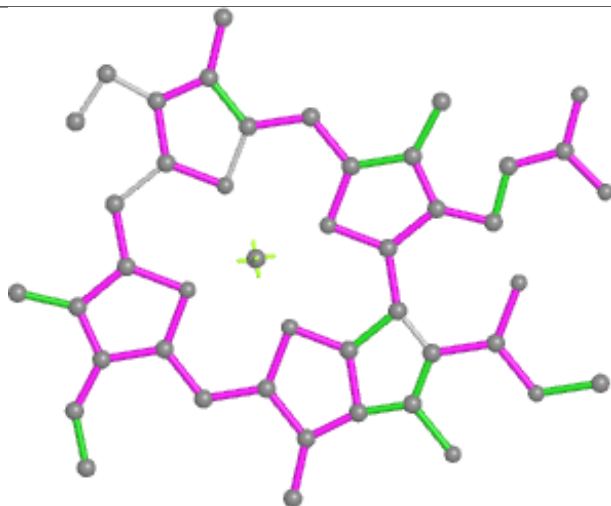


Rings

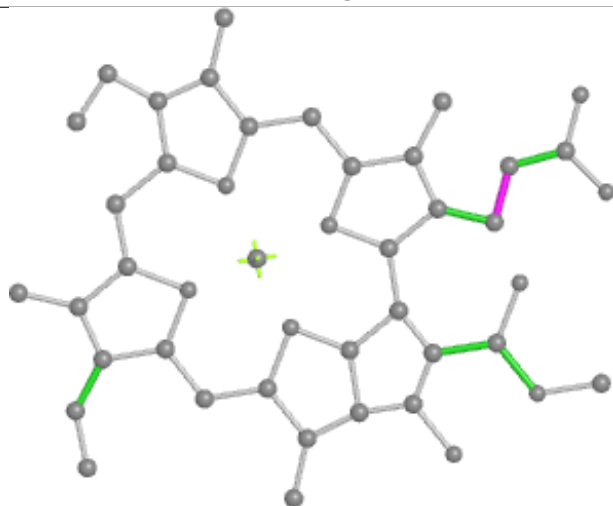
Ligand CLA 1 516



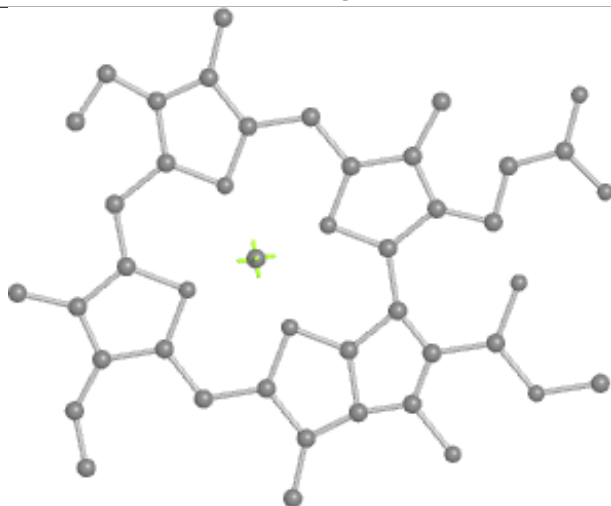
Bond lengths



Bond angles

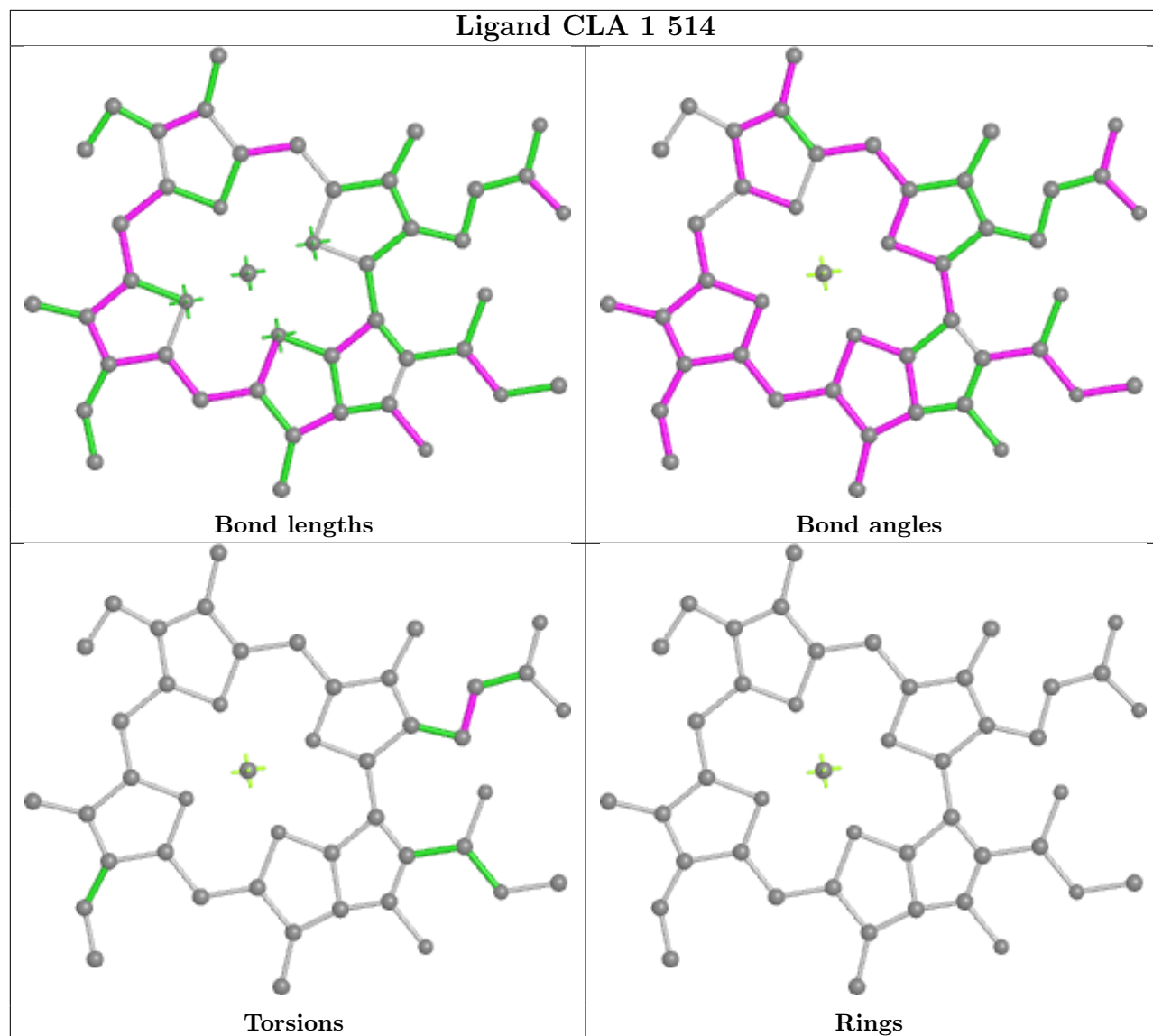


Torsions

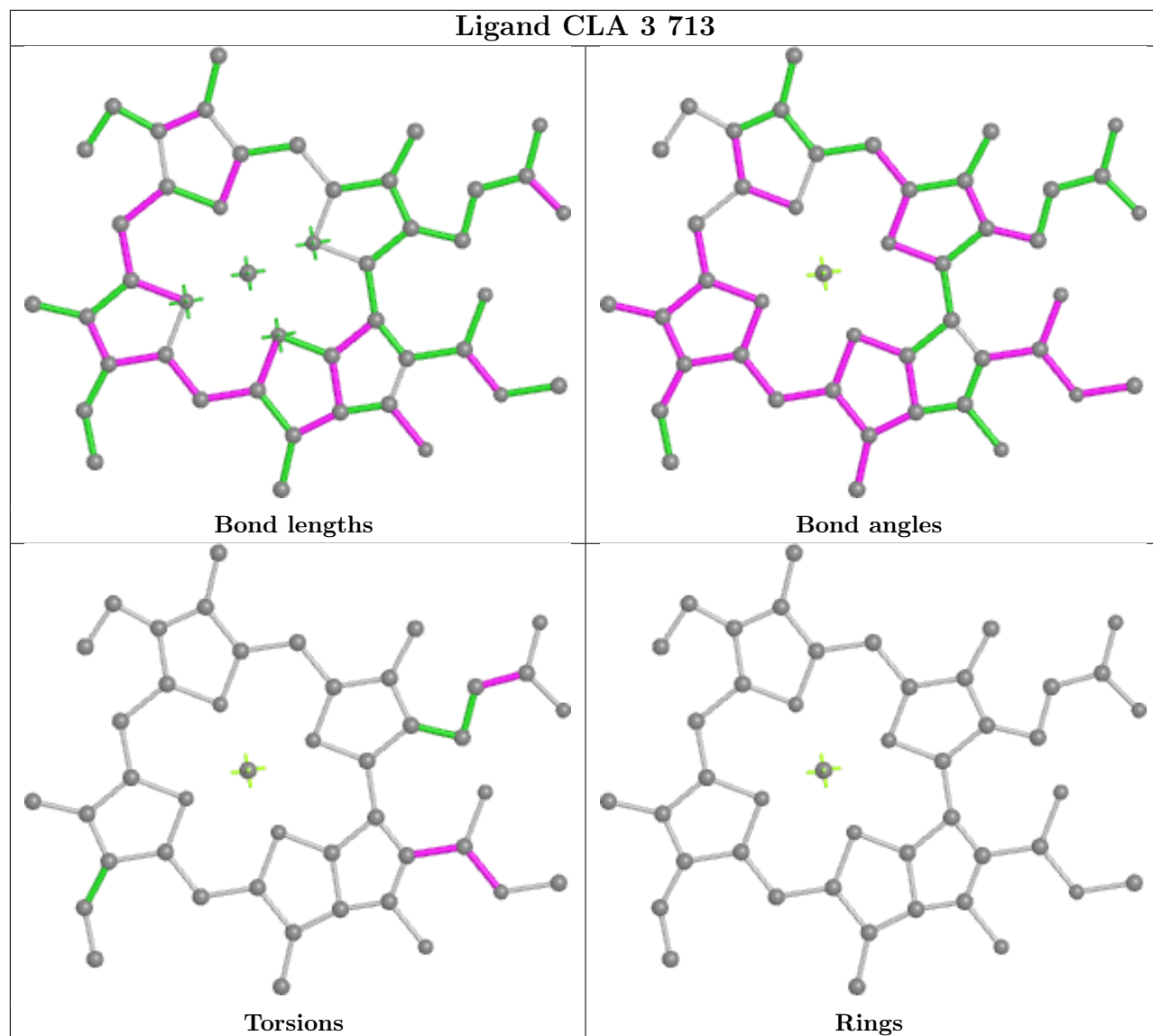


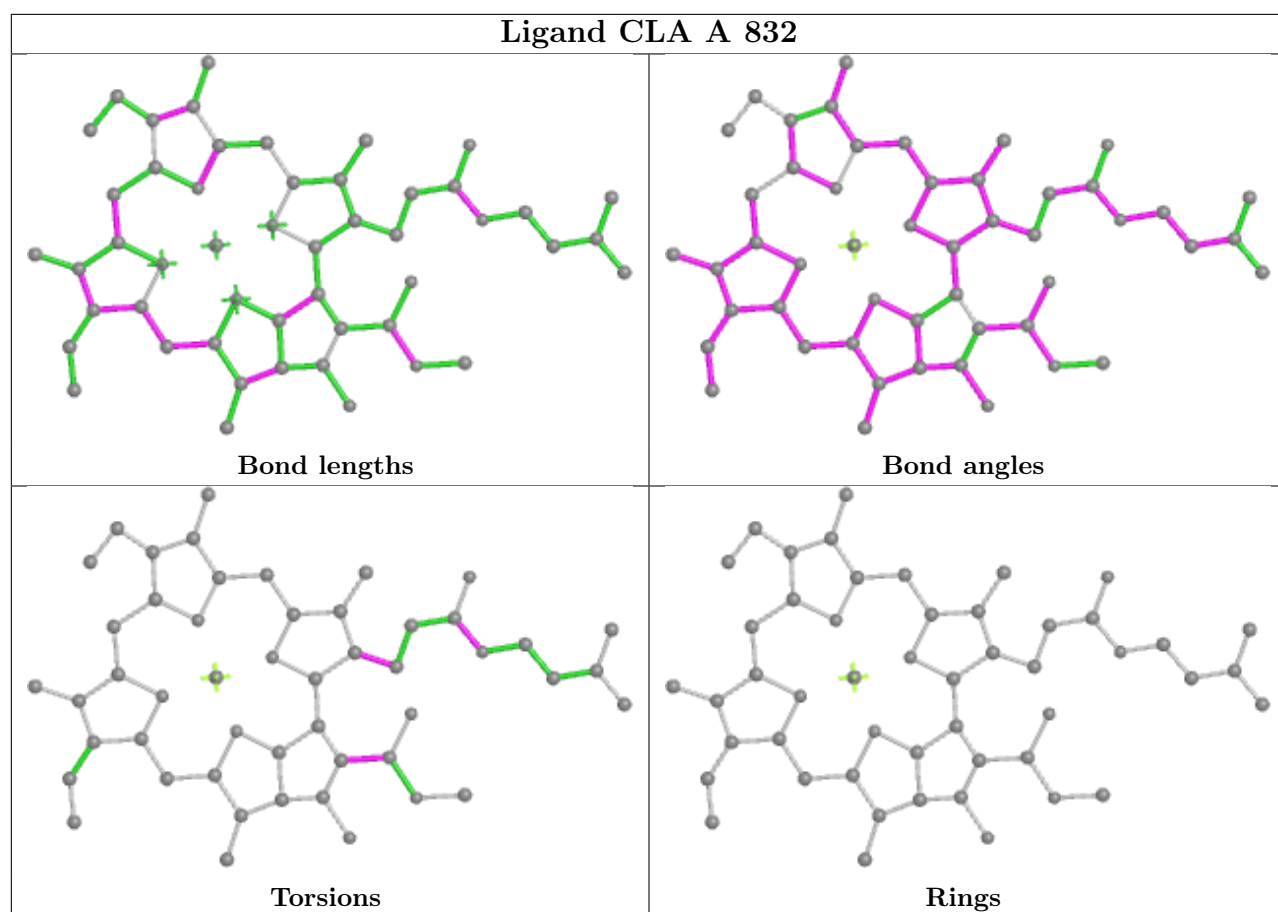
Rings

Ligand CLA 1 514

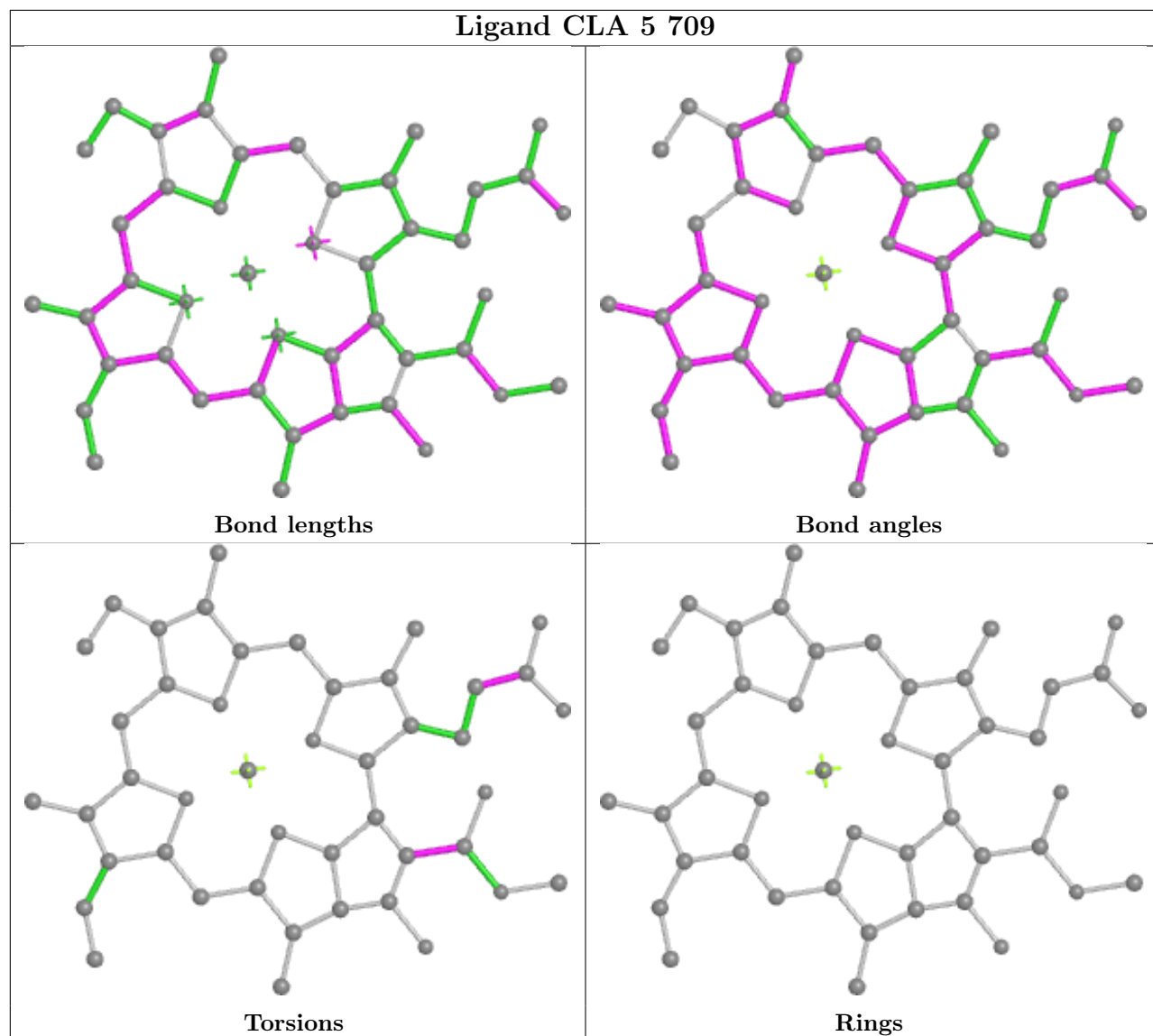


Ligand CLA 3 713

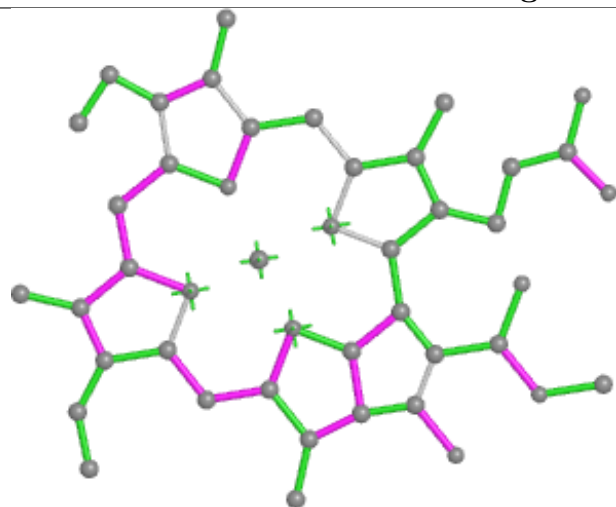




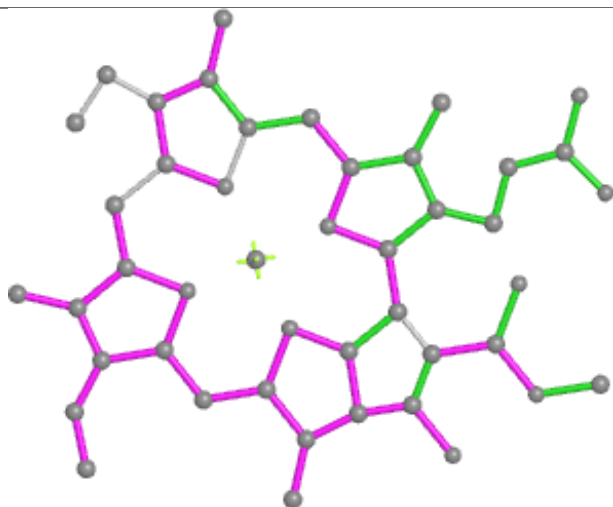
Ligand CLA 5 709



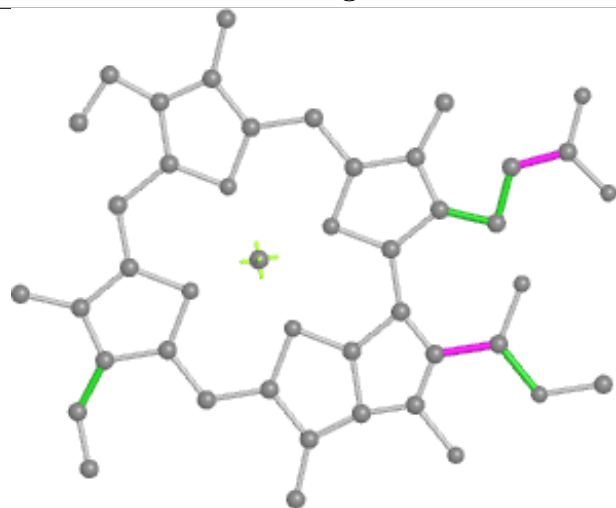
Ligand CLA 7 704



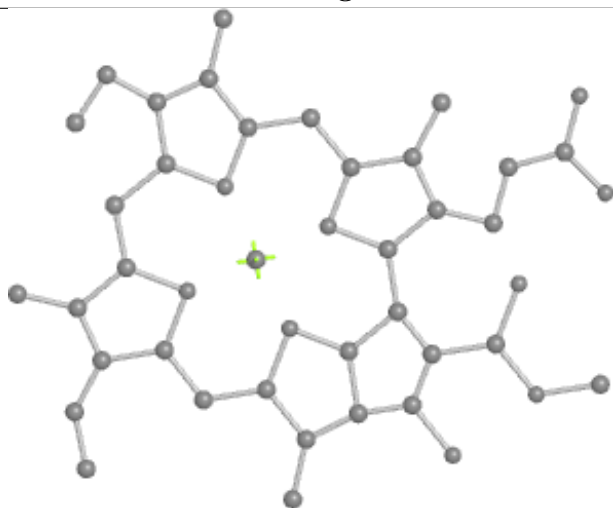
Bond lengths



Bond angles

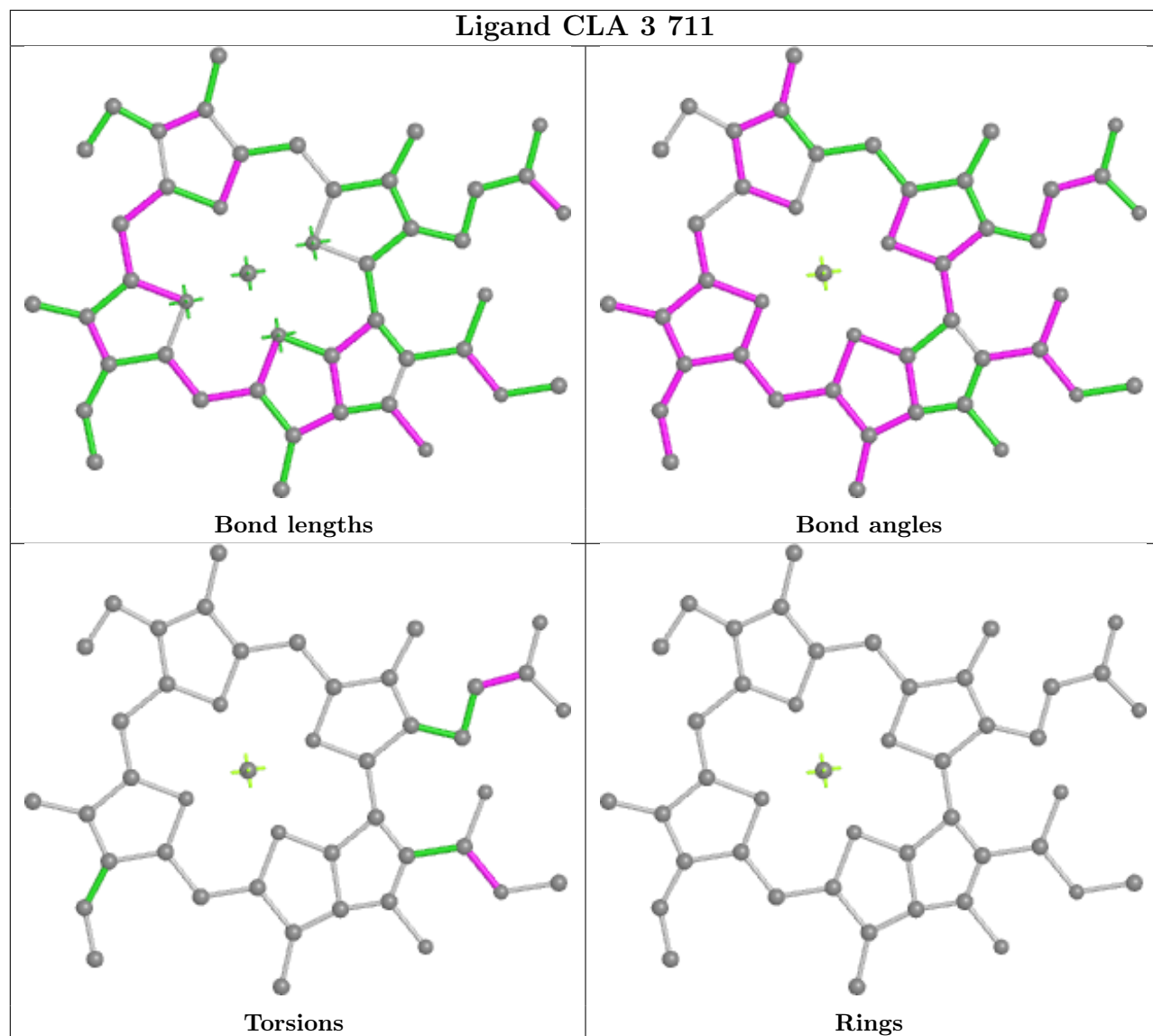


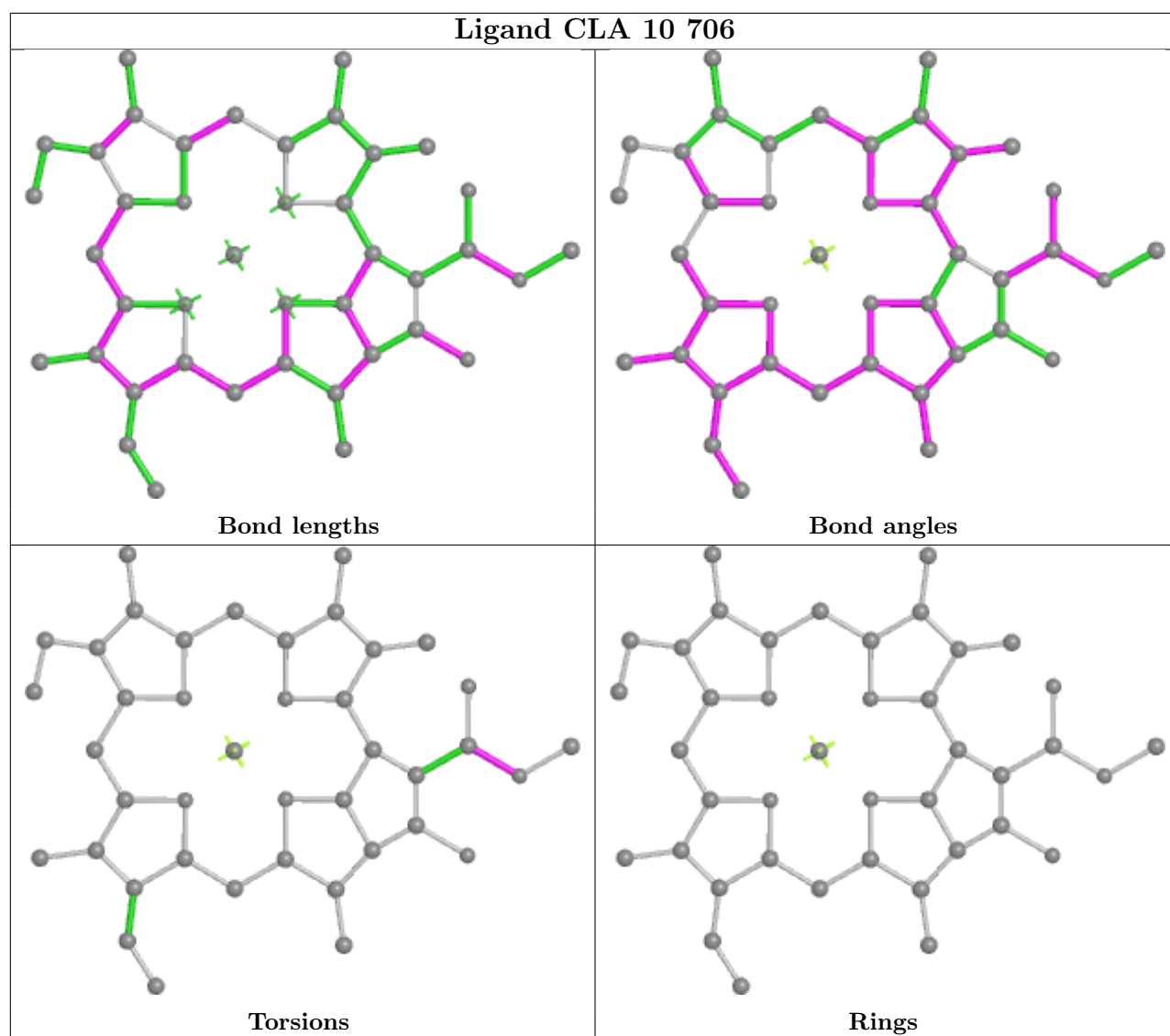
Torsions

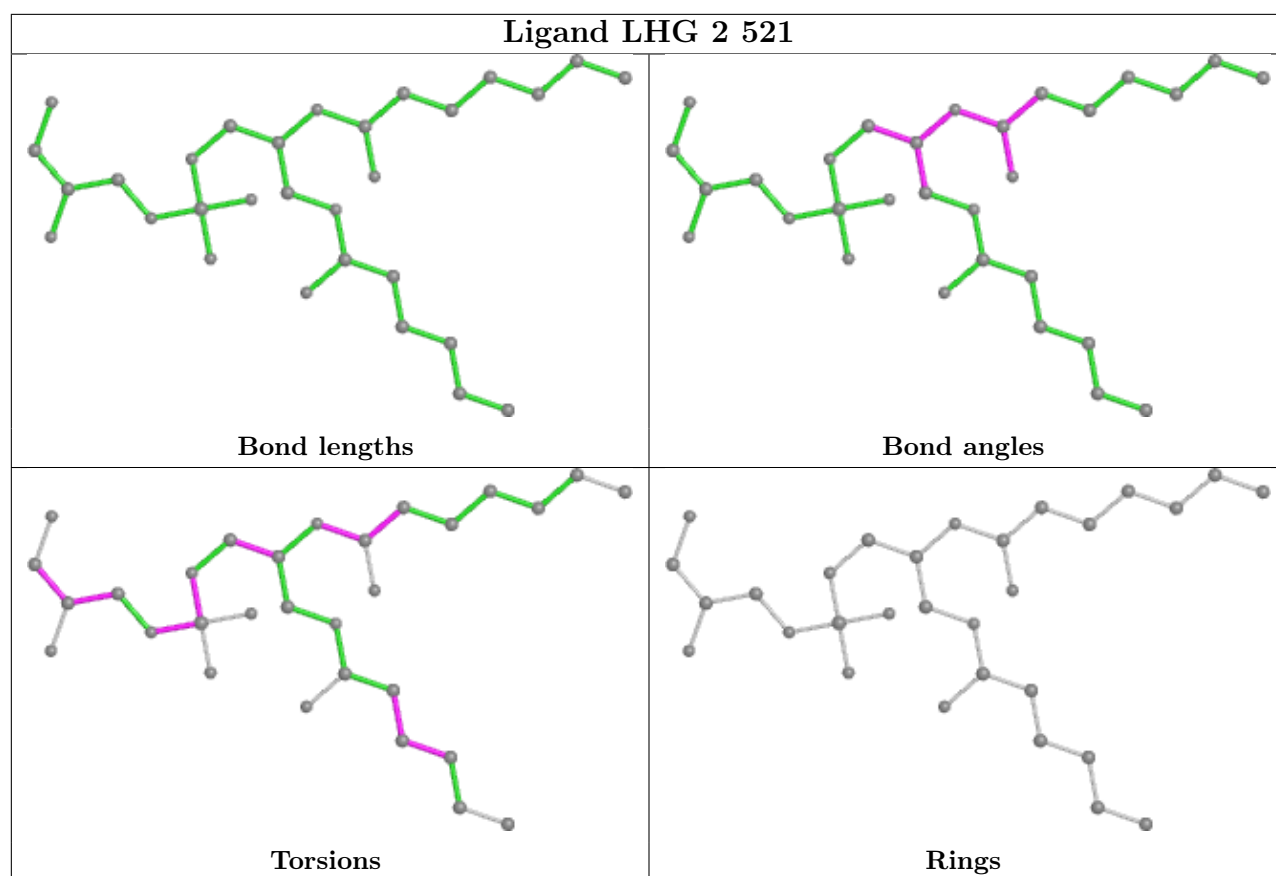


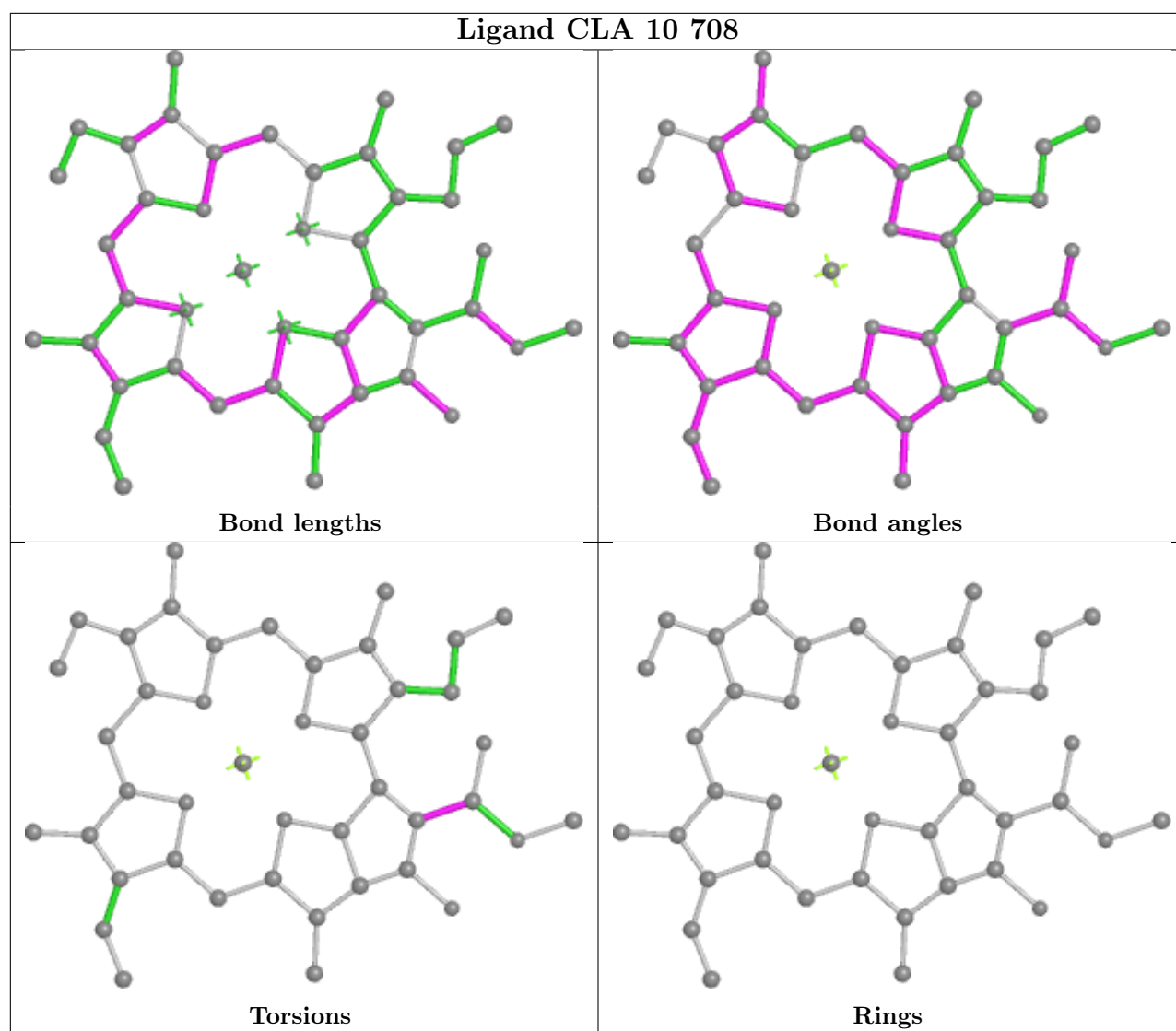
Rings

Ligand CLA 3 711

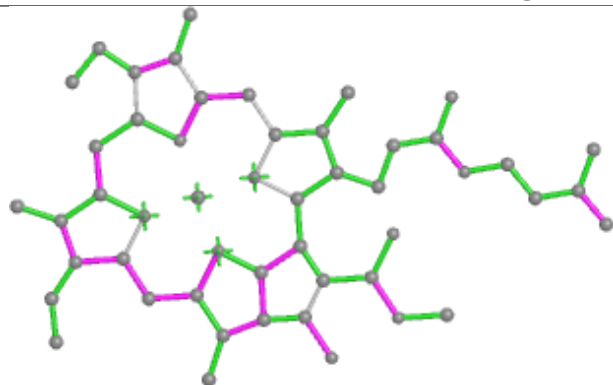




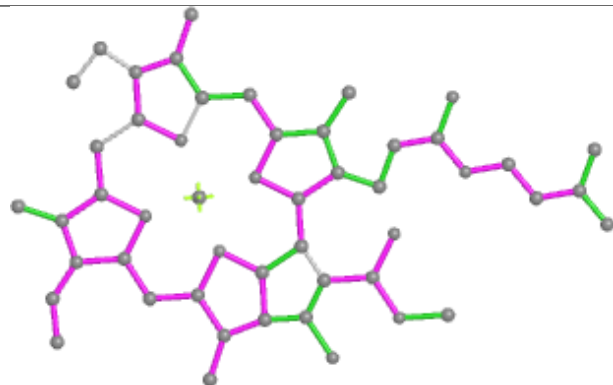




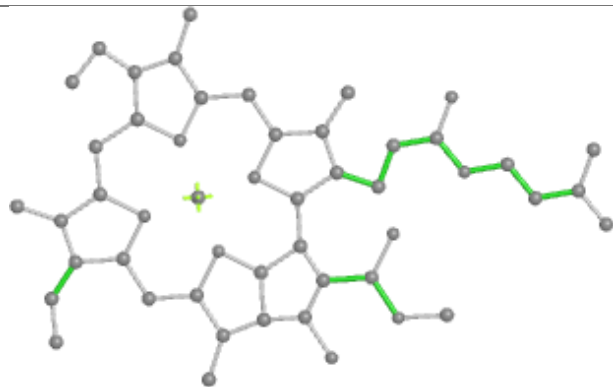
Ligand CLA 4 704



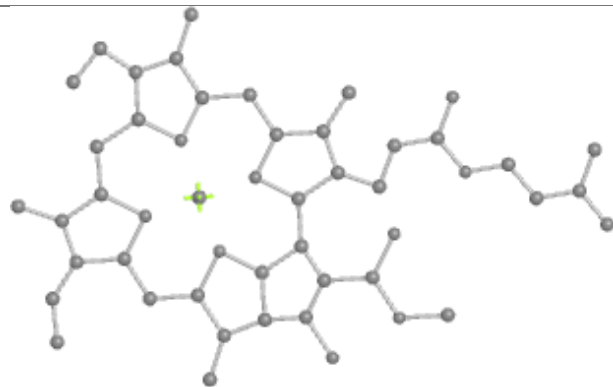
Bond lengths



Bond angles

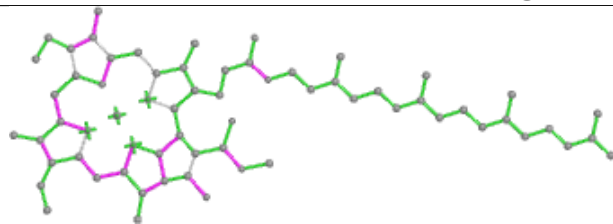


Torsions

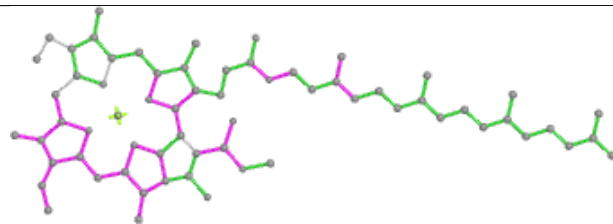


Rings

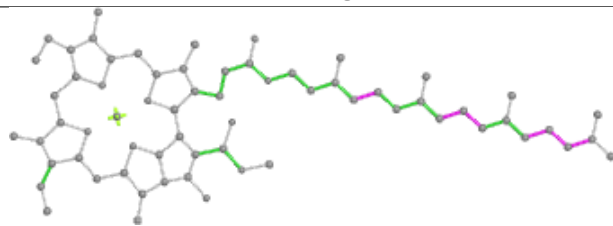
Ligand CLA 7 711



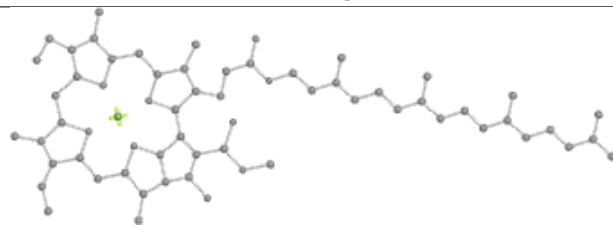
Bond lengths



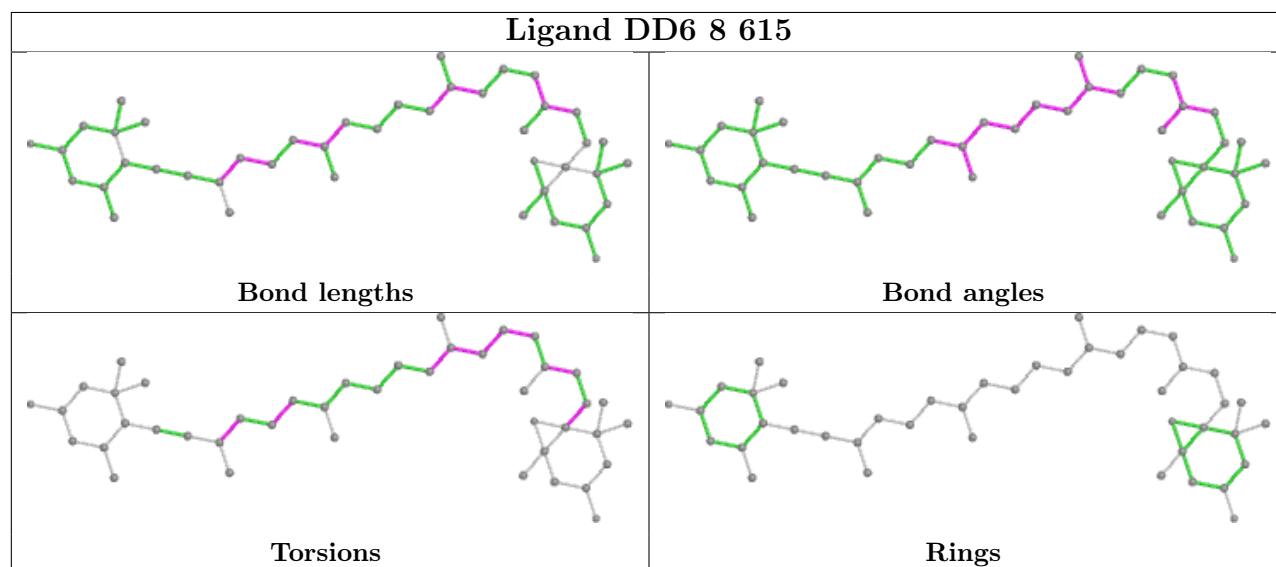
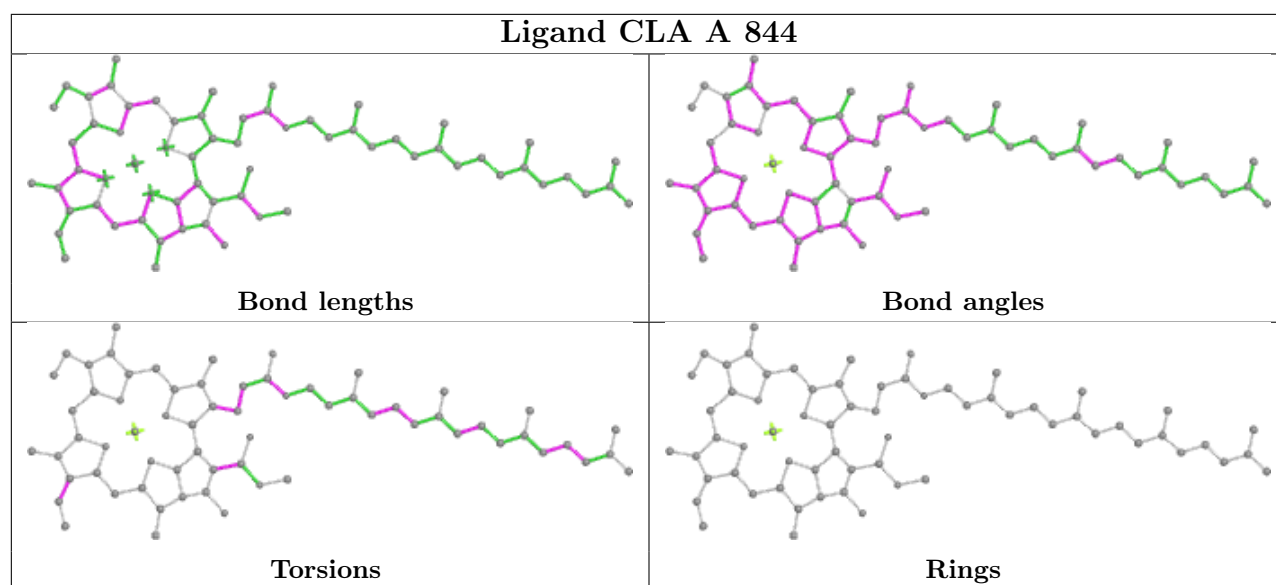
Bond angles

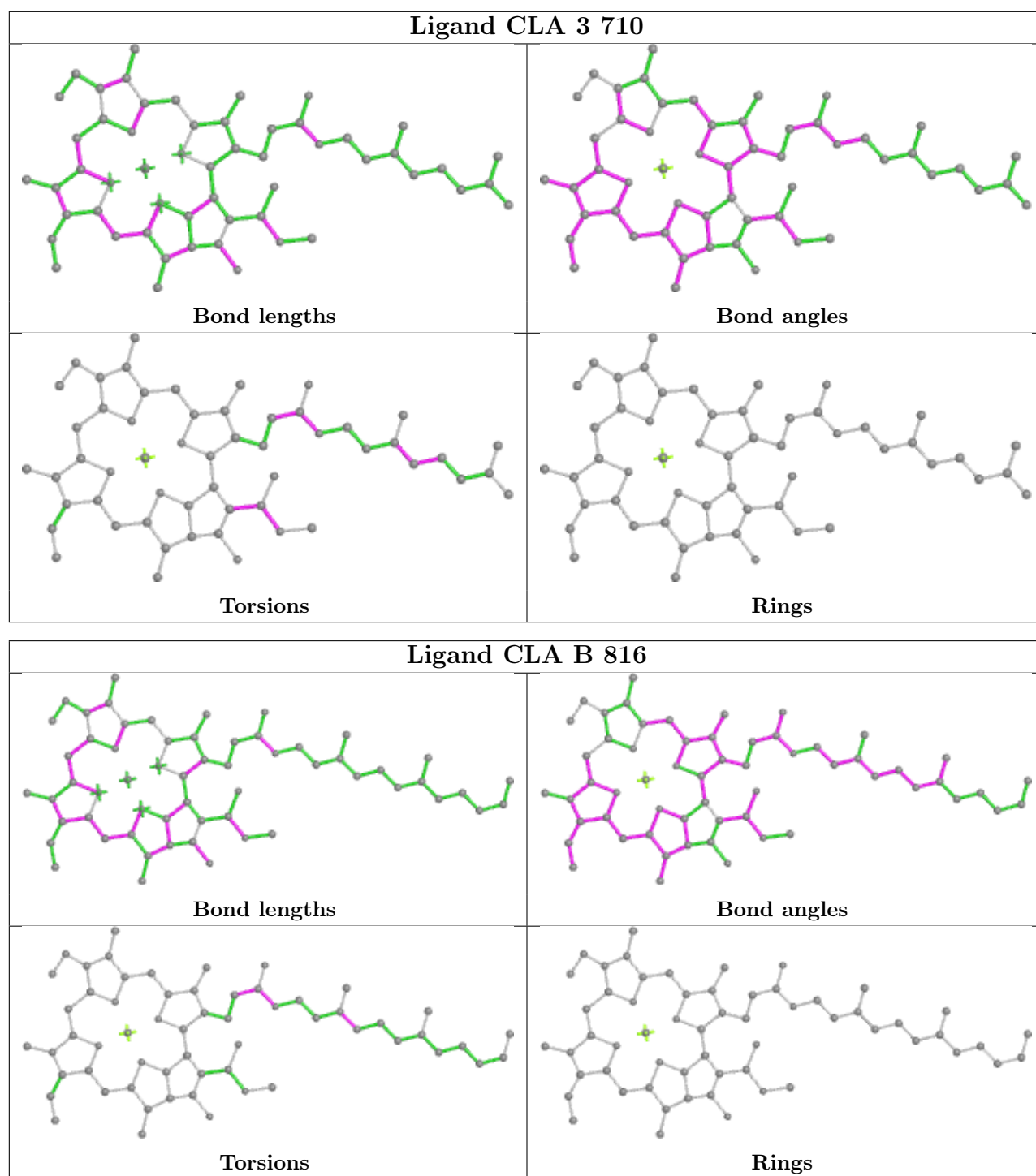


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

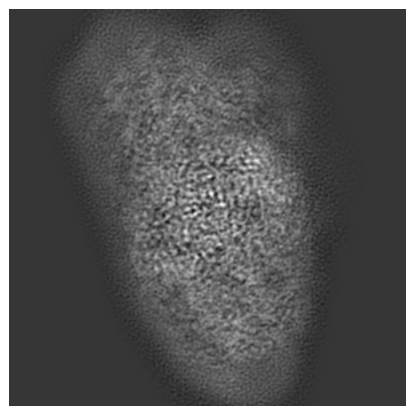
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65026. These allow visual inspection of the internal detail of the map and identification of artifacts.

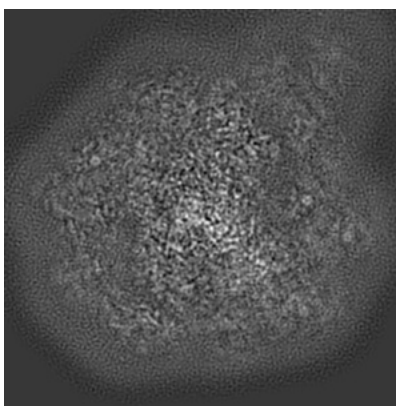
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

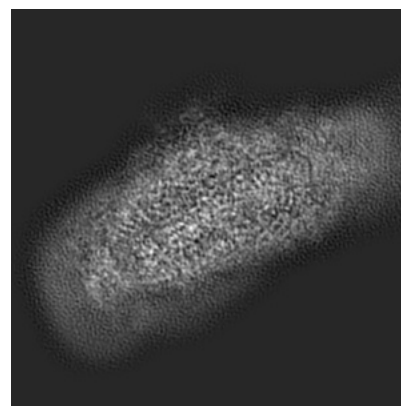
6.1.1 Primary map



X

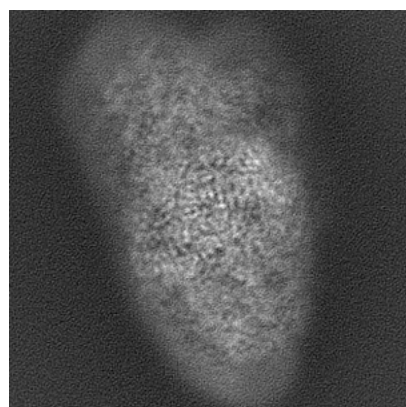


Y

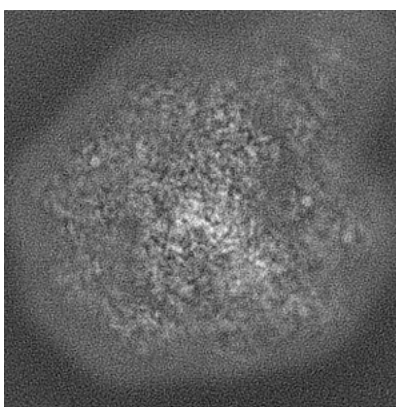


Z

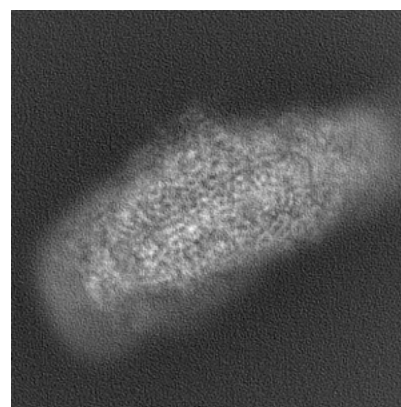
6.1.2 Raw map



X



Y

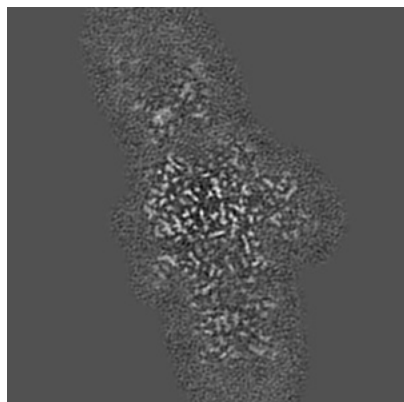


Z

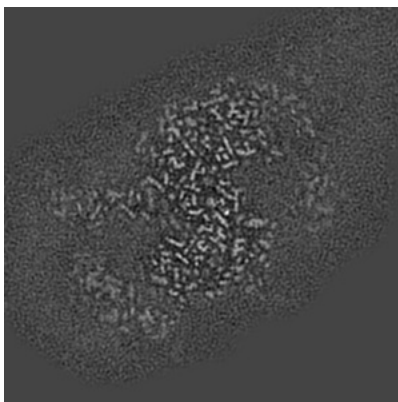
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

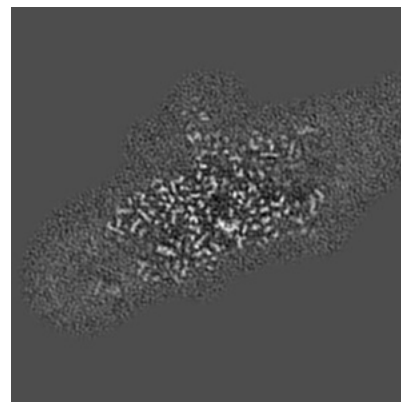
6.2.1 Primary map



X Index: 144

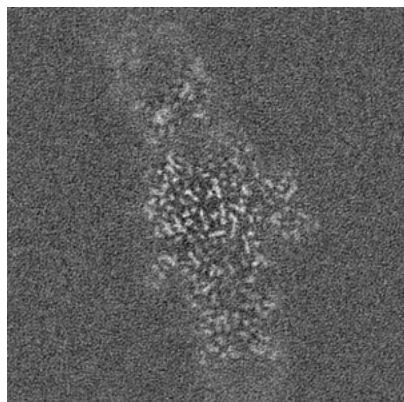


Y Index: 144

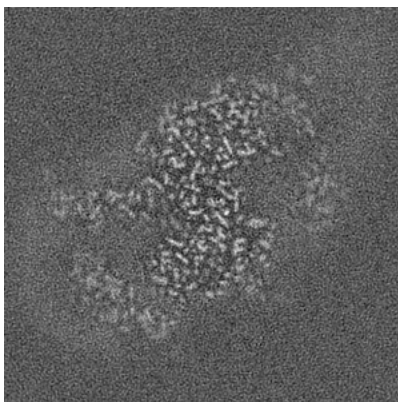


Z Index: 144

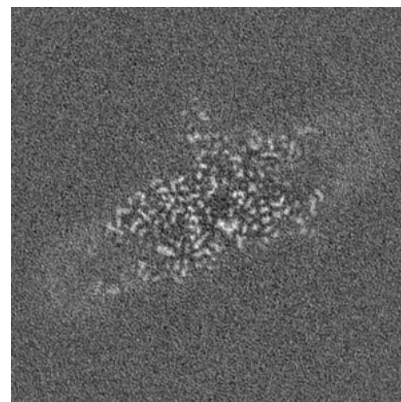
6.2.2 Raw map



X Index: 144



Y Index: 144

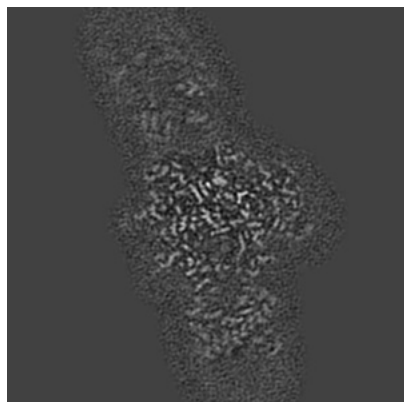


Z Index: 144

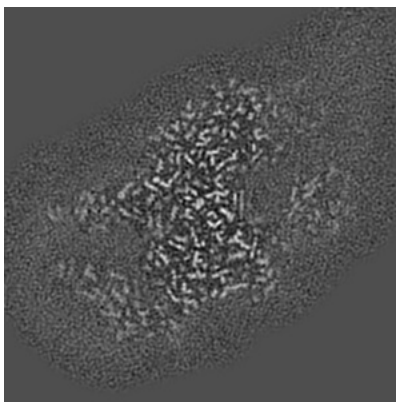
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

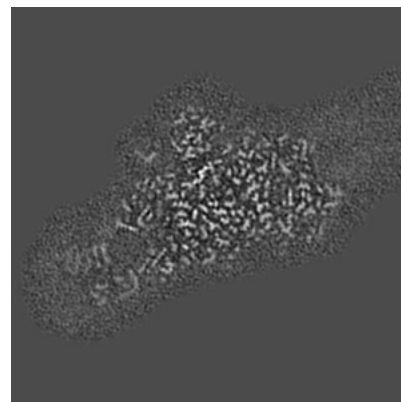
6.3.1 Primary map



X Index: 139

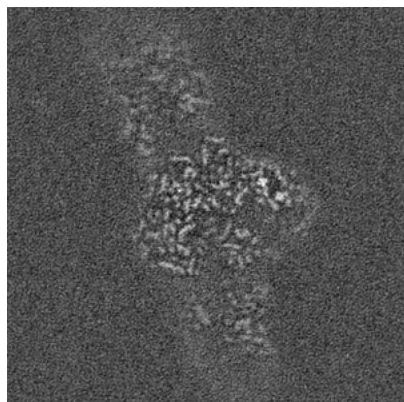


Y Index: 139

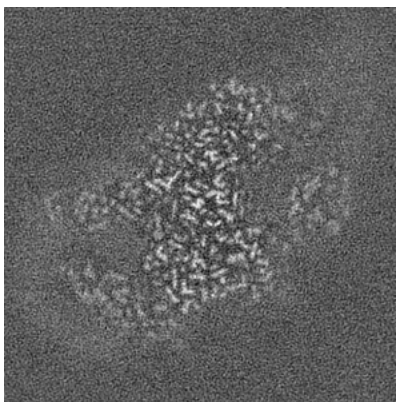


Z Index: 154

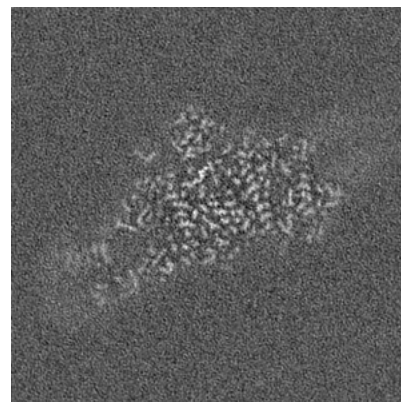
6.3.2 Raw map



X Index: 129



Y Index: 140

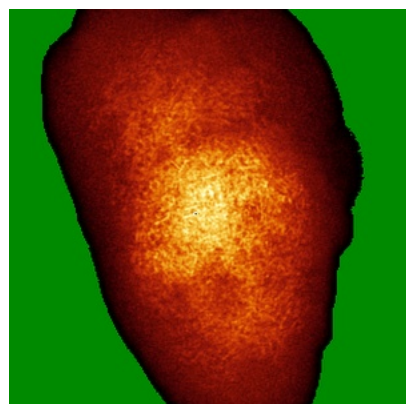


Z Index: 154

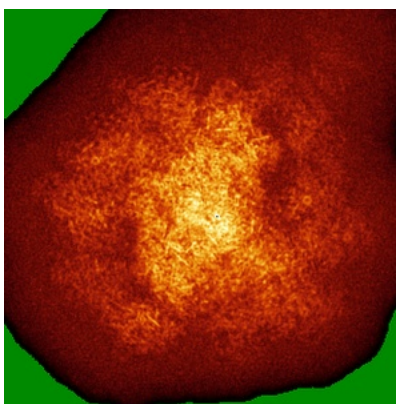
The images above show the largest variance slices of the map in three orthogonal directions.

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

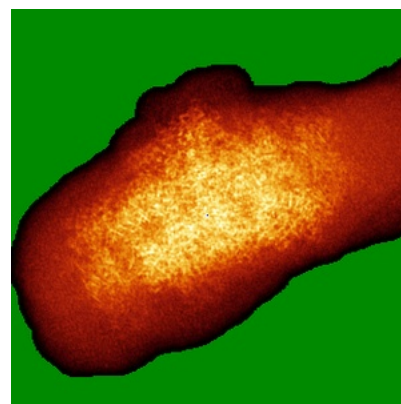
6.4.1 Primary map



X

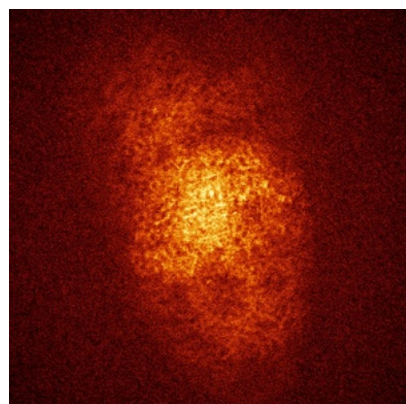


Y

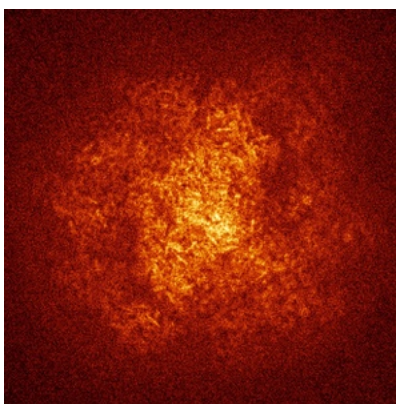


Z

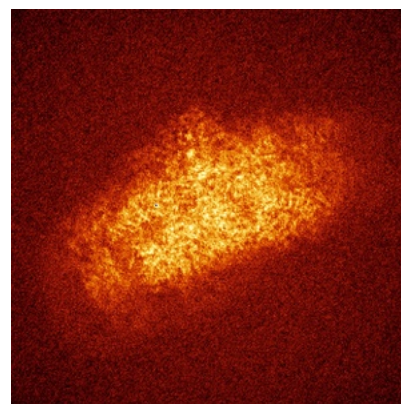
6.4.2 Raw map



X



Y

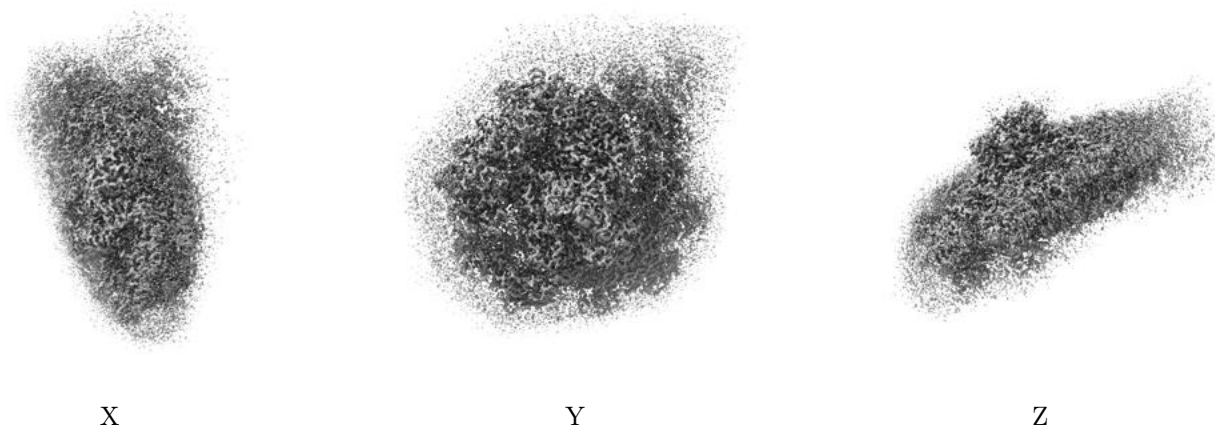


Z

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.

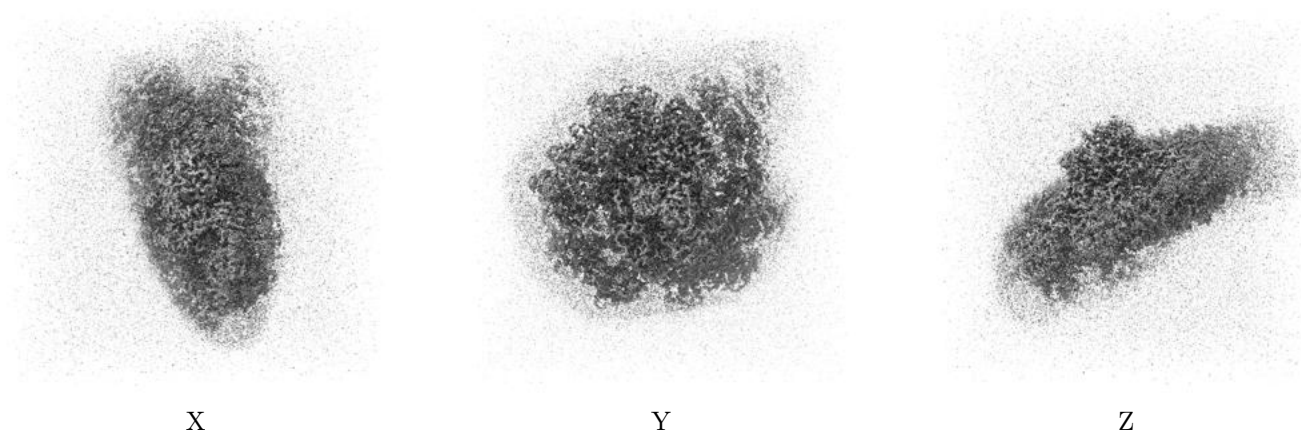
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

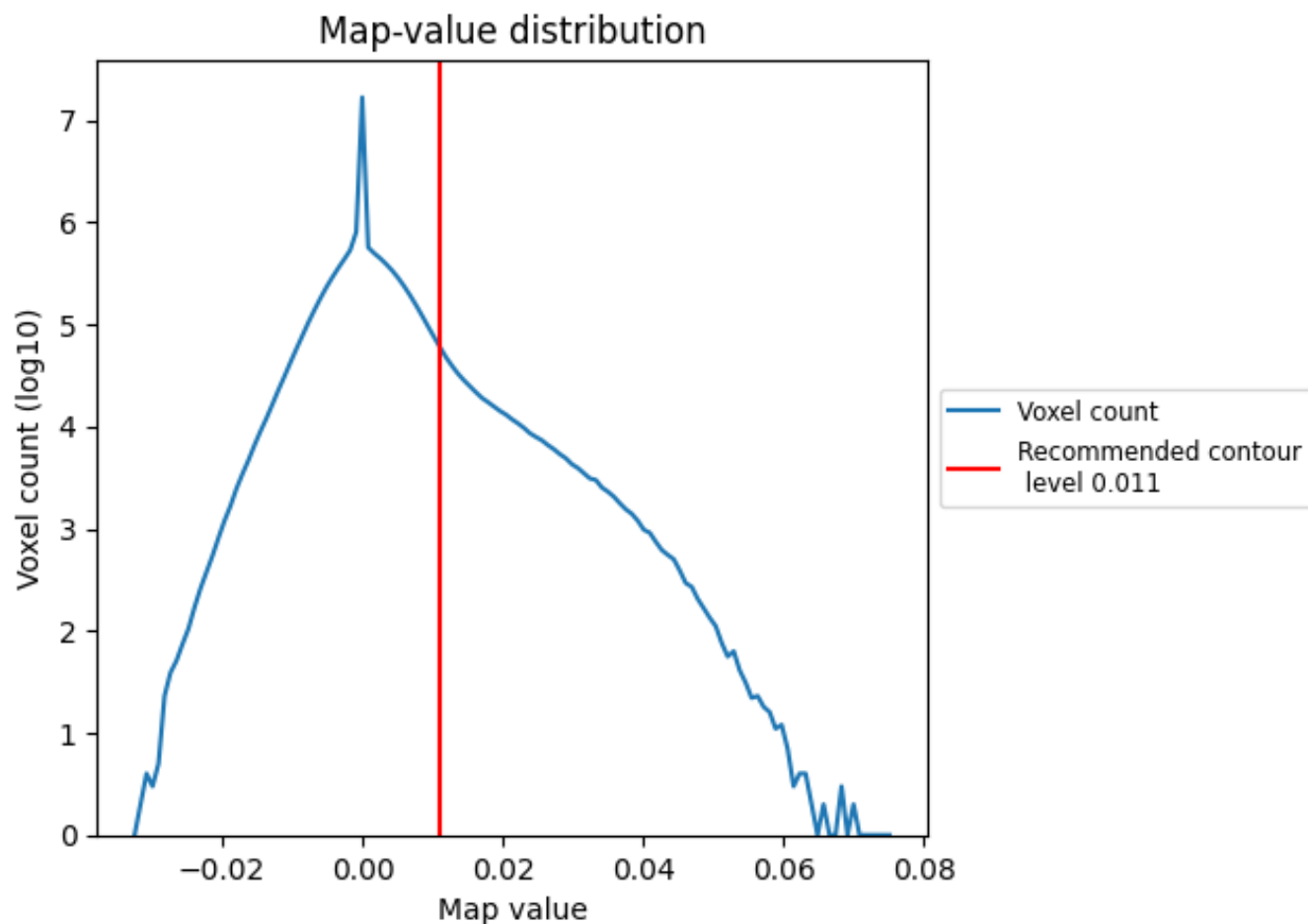
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

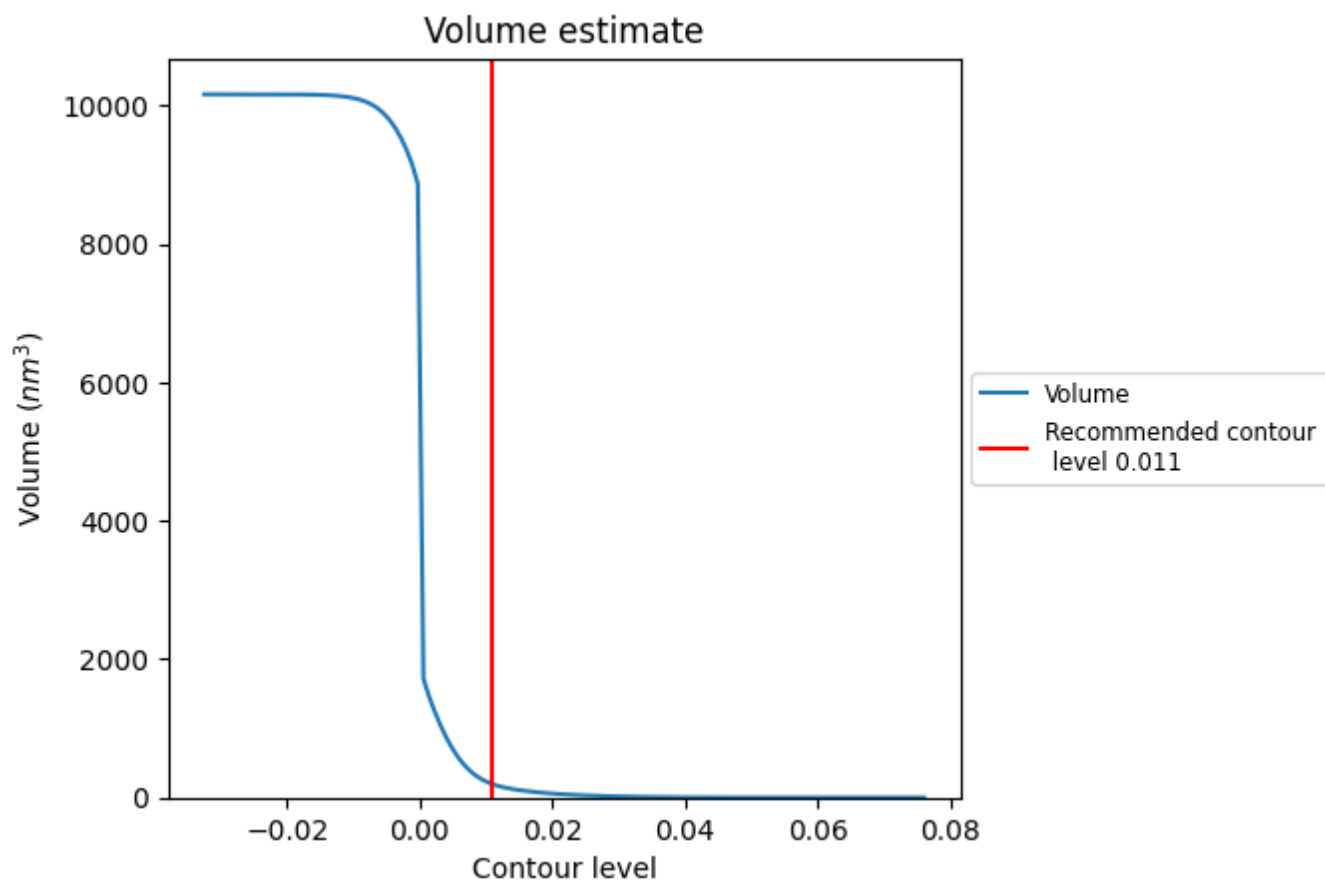
This section contains the results of statistical analysis of the map.

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.

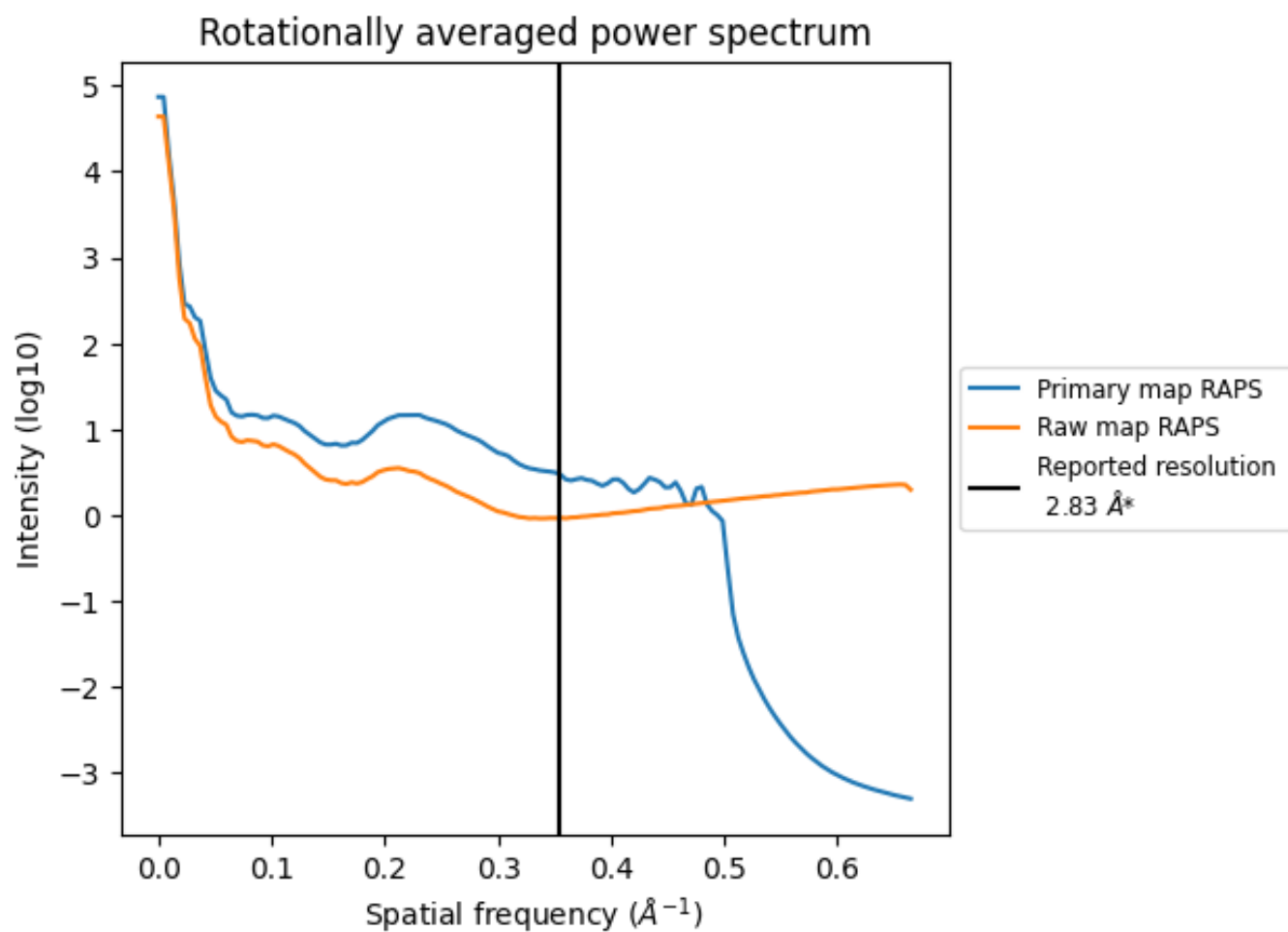
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm^3 ; this corresponds to an approximate mass of 175 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 ⓘ

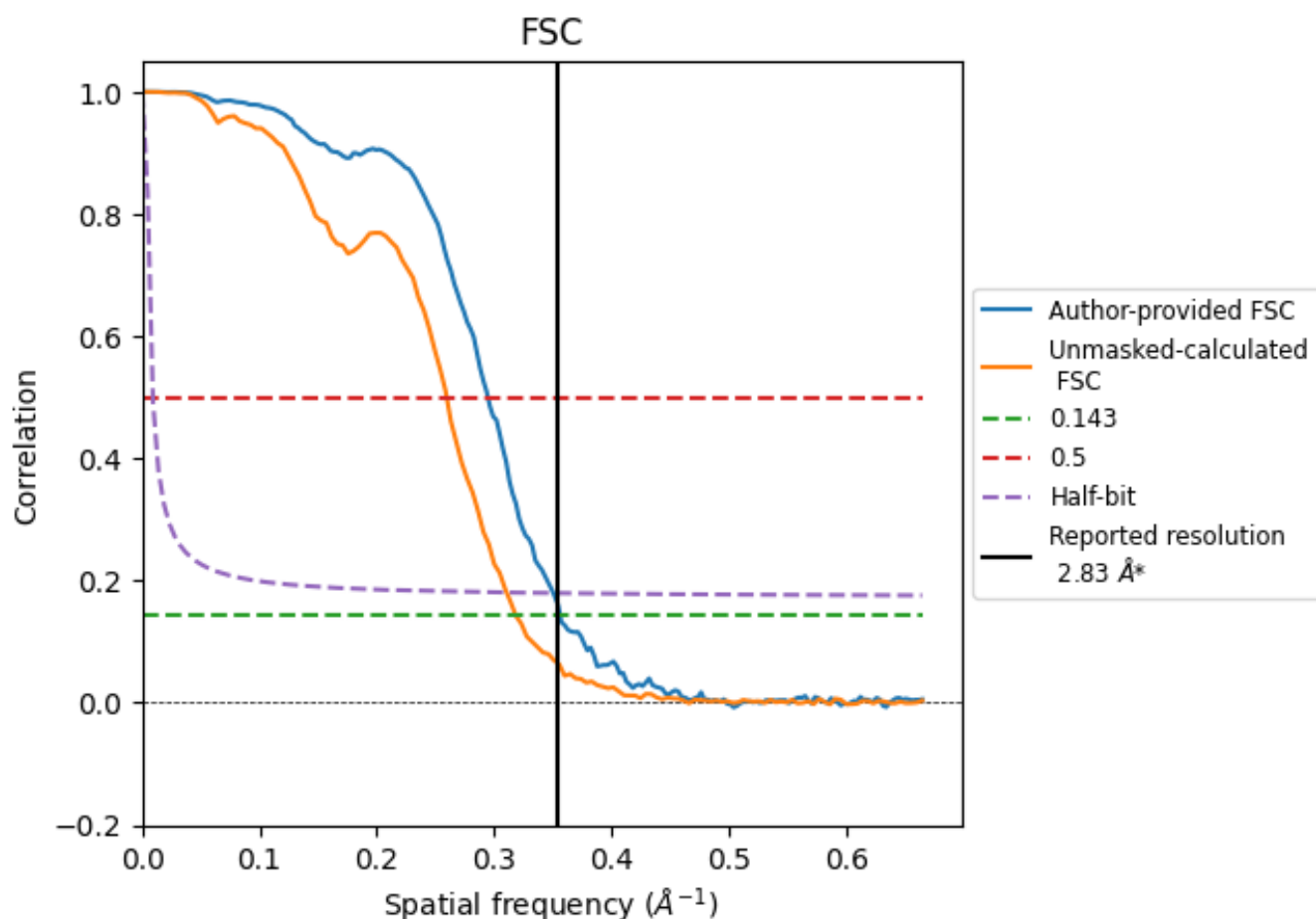


*Reported resolution corresponds to spatial frequency of 0.353 \AA^{-1}

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 0.353 \AA^{-1}

8.2 Resolution estimates [i](#)

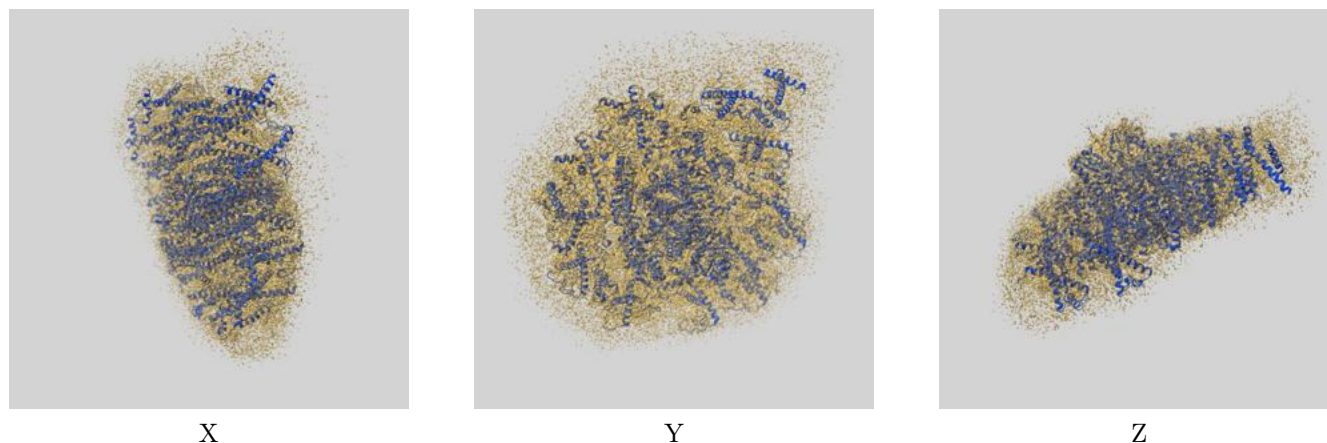
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.81	3.39	2.85
Unmasked-calculated*	3.14	3.85	3.22

*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 3.14 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

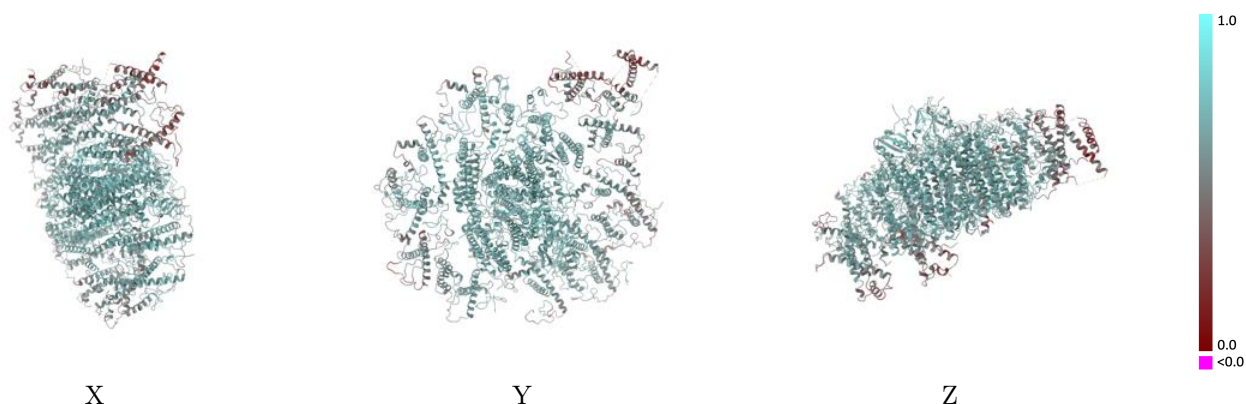
This section contains information regarding the fit between EMDB map EMD-65026 and PDB model 9VFJ. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



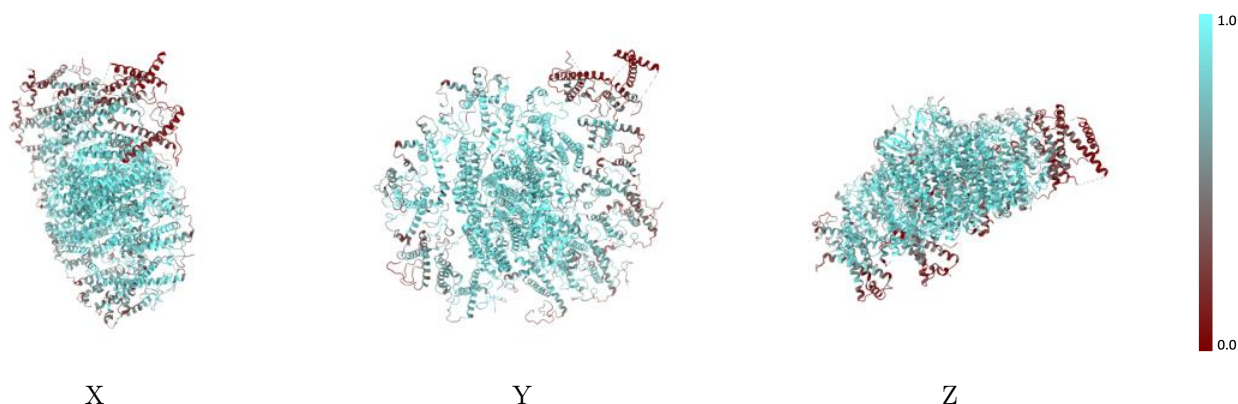
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



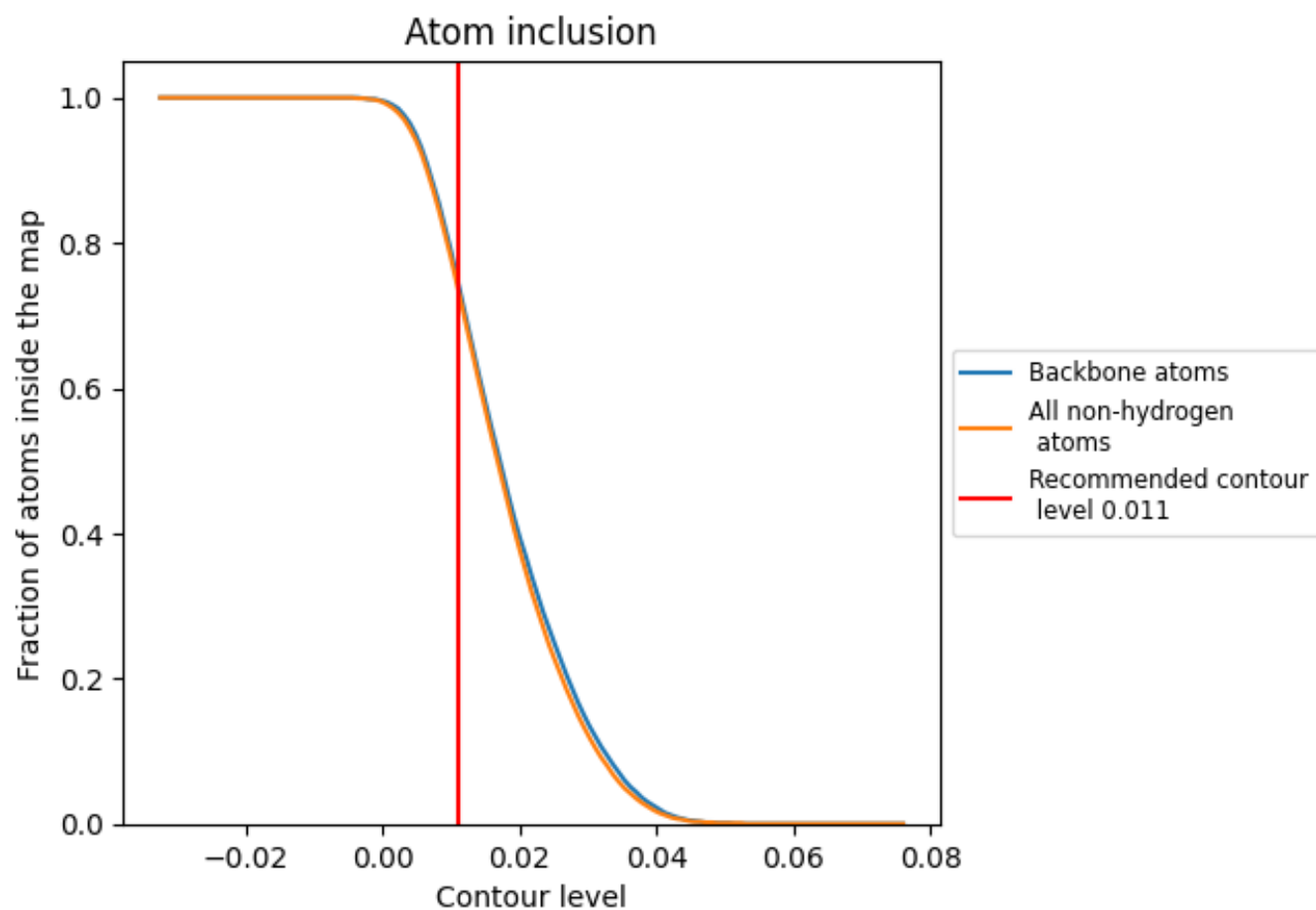
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7360	 0.6050
1	 0.6770	 0.5760
10	 0.3090	 0.4220
11	 0.5030	 0.4990
12	 0.3990	 0.4450
13	 0.1900	 0.3910
2	 0.7590	 0.6050
3	 0.6850	 0.5760
4	 0.5140	 0.4940
5	 0.7340	 0.5930
6	 0.6070	 0.5390
7	 0.8140	 0.6320
8	 0.6480	 0.5640
9	 0.5320	 0.5300
A	 0.9130	 0.6890
B	 0.9010	 0.6820
C	 0.9420	 0.6960
D	 0.7840	 0.6280
E	 0.7630	 0.6290
F	 0.8350	 0.6510
J	 0.8400	 0.6600
M	 0.7410	 0.6100

