



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:48 AM UTC

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:

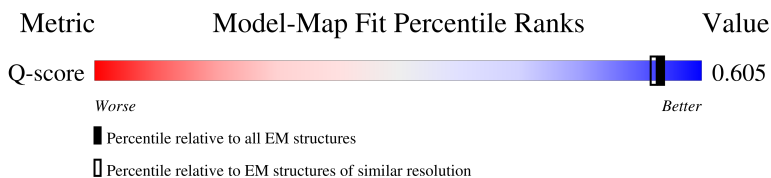
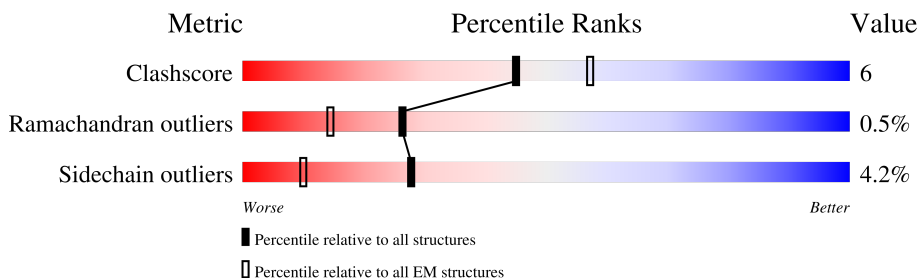
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

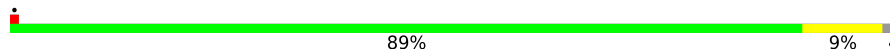
The reported resolution of this entry is 2.83 Å.

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.



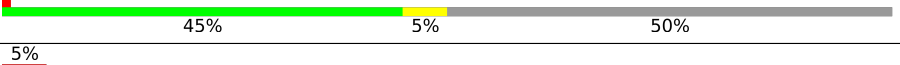
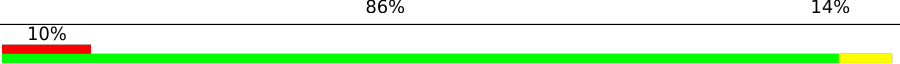
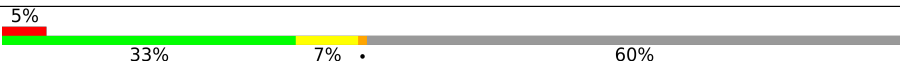
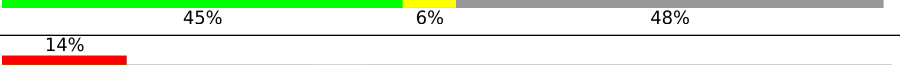
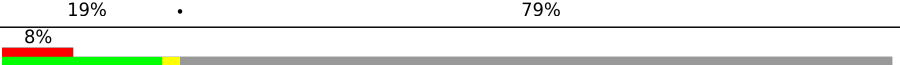
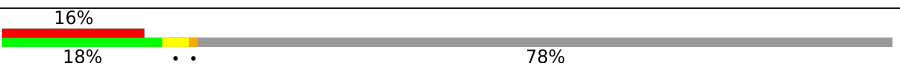
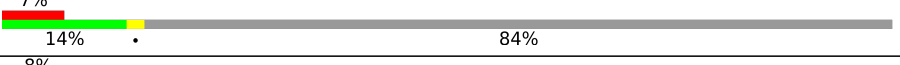
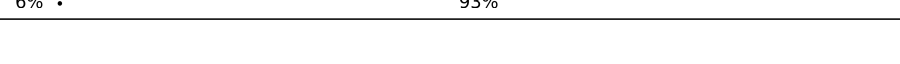
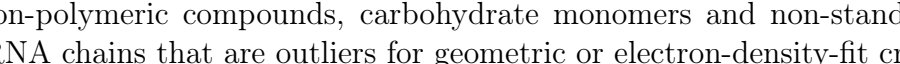
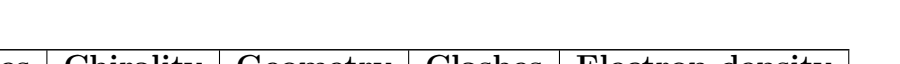
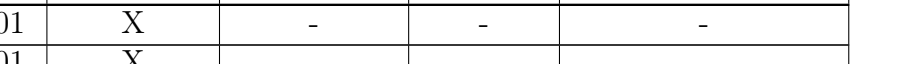
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	-	-	-
21	CLA	5	701	X	-	-	-
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		

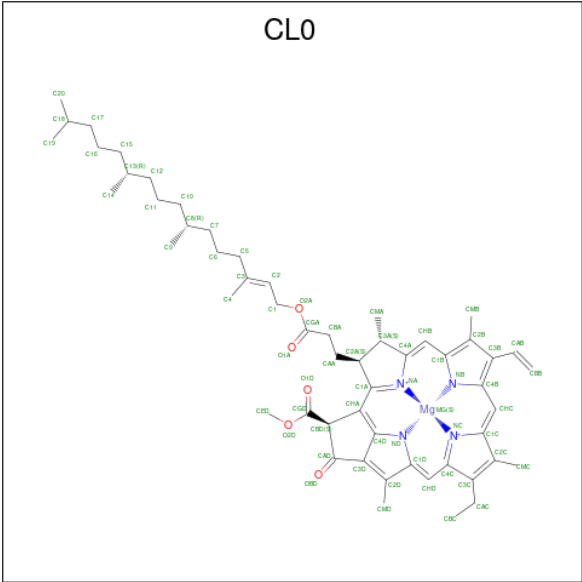
- Molecule 18 is a protein called LHCI-10.

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.

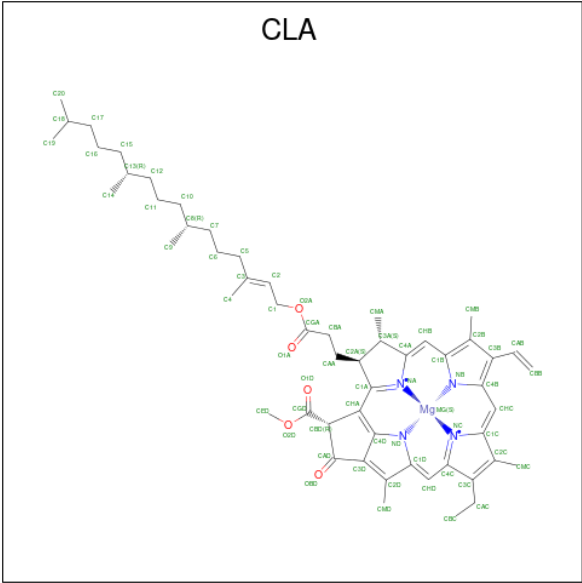
Mol	Chain	Residues	Atoms					AltConf	Trace
19	11	171	Total	C	N	O	S	0	0
			1277	822	219	232	4		
19	12	150	Total	C	N	O	S	0	0
			1127	726	190	207	4		
19	13	78	Total	C	N	O	S	0	0
			594	386	103	101	4		

- 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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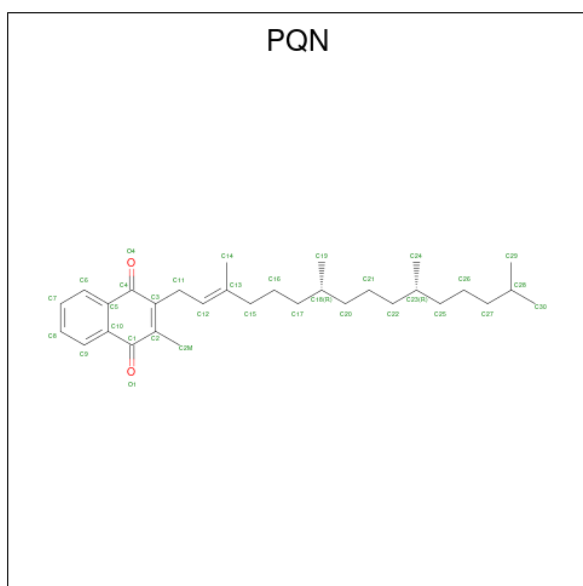
Mol	Chain	Residues	Atoms					AltConf
21	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	10	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	11	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	11	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	11	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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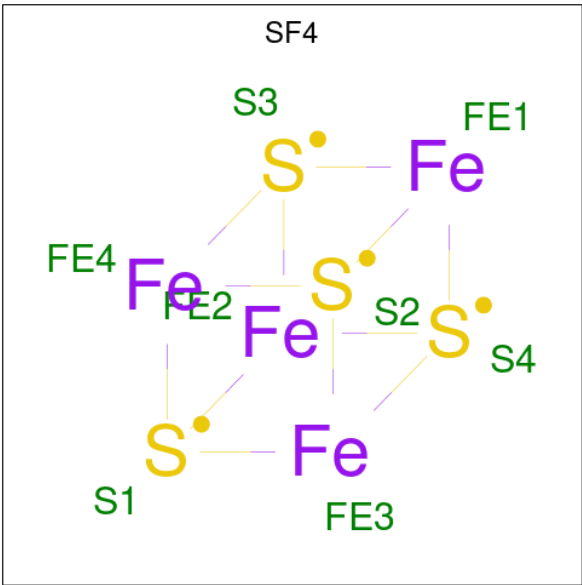
Mol	Chain	Residues	Atoms					AltConf
21	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	13	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	13	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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



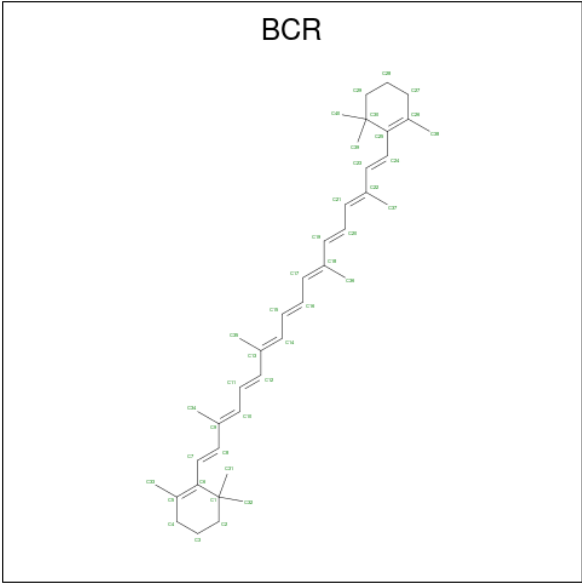
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O		0
			33	31	2		
22	B	1	Total	C	O		0
			31	29	2		

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



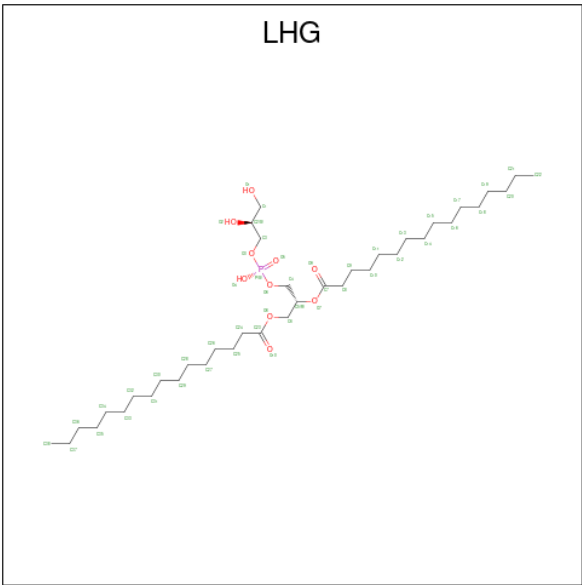
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	
23	C	1	Total	Fe	S	0
			8	4	4	

- 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).

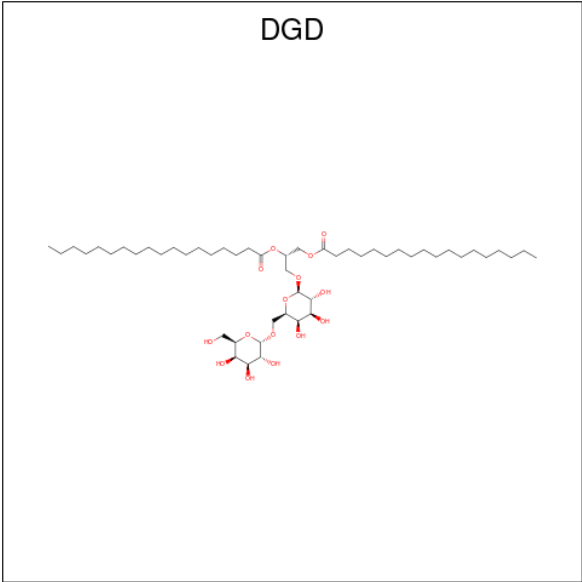


Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			27	16	10	1	
25	B	1	Total	C	O	P	0
			23	12	10	1	
25	1	1	Total	C	O	P	0
			36	25	10	1	
25	2	1	Total	C	O	P	0
			30	19	10	1	
25	3	1	Total	C	O	P	0
			25	14	10	1	
25	4	1	Total	C	O	P	0
			19	10	8	1	
25	5	1	Total	C	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).

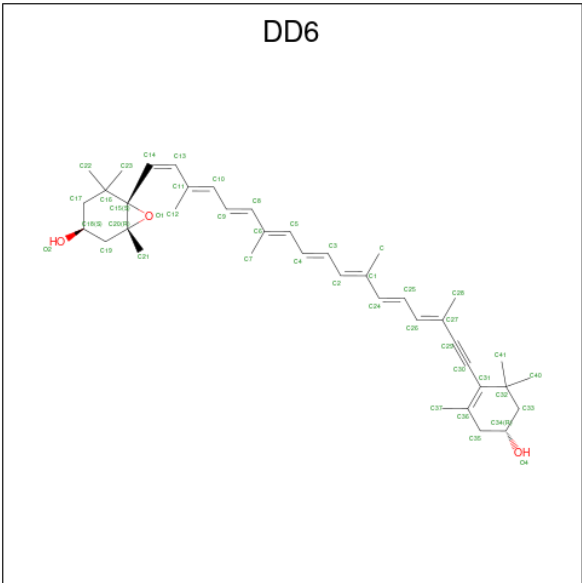
Mol	Chain	Residues	Atoms	AltConf
26	A	7	Total C 97 97	0
26	B	5	Total C 62 62	0
26	D	1	Total C 6 6	0
26	F	1	Total C 9 9	0
26	M	2	Total C 20 20	0
26	1	4	Total C 42 42	0
26	2	5	Total C 42 42	0
26	6	4	Total C 47 47	0
26	7	6	Total C 67 67	0
26	8	4	Total C 46 46	0
26	9	1	Total C 15 15	0
26	10	2	Total C 26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

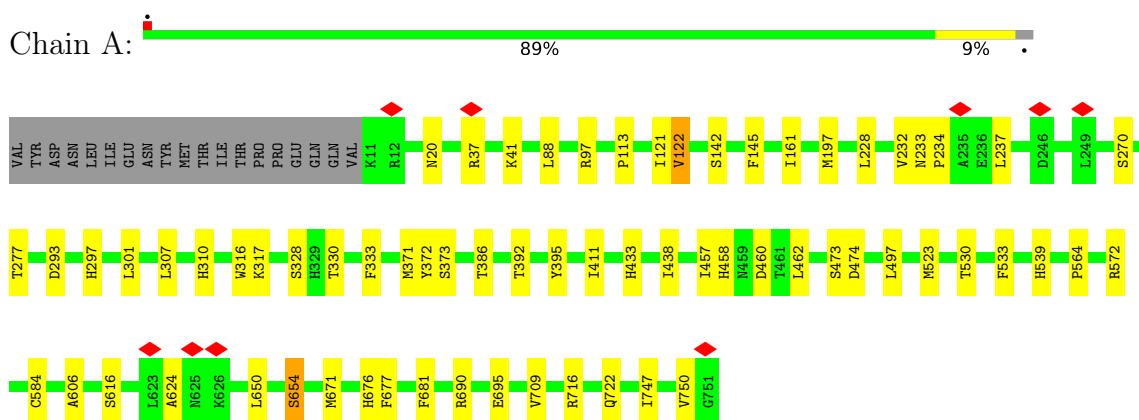
- Molecule 29 is water.

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	

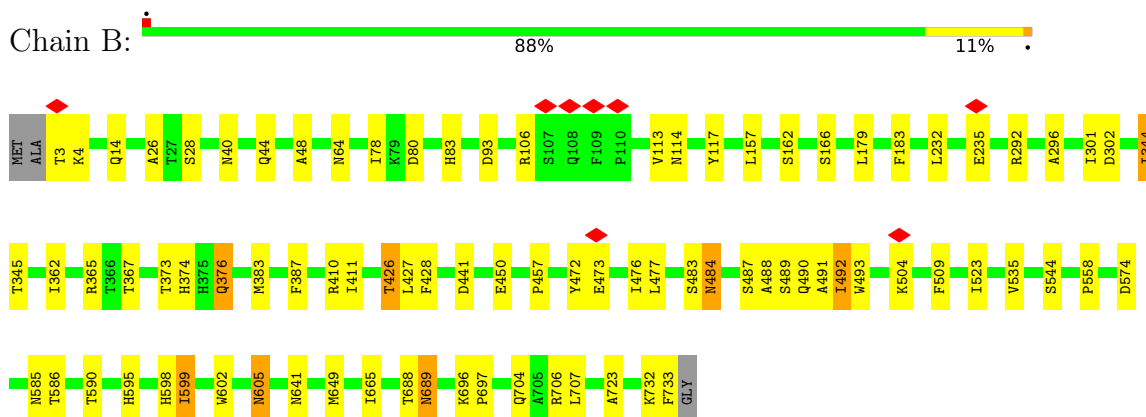
3 Residue-property plots

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.

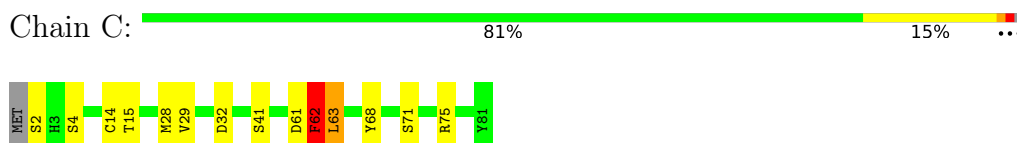
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



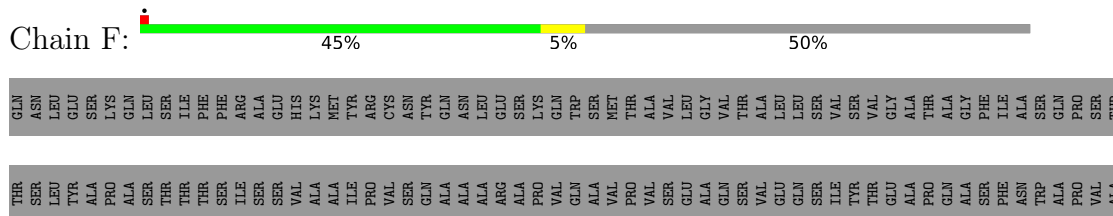
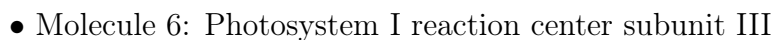
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

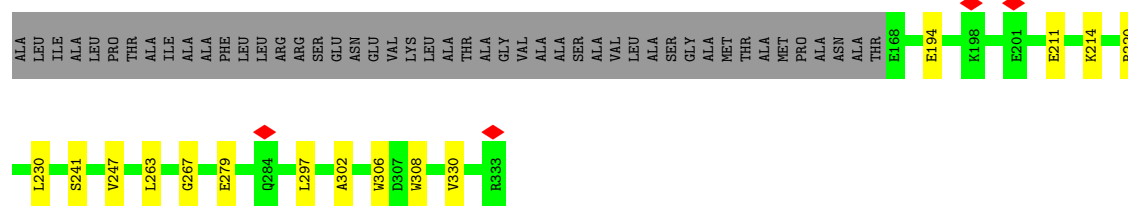


- Molecule 3: Photosystem I iron-sulfur center

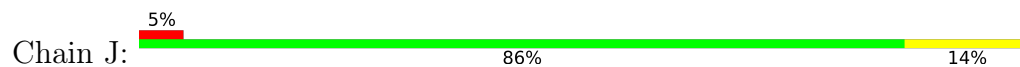


- Molecule 4: Photosystem I reaction center subunit II

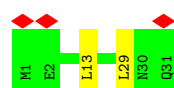




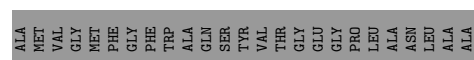
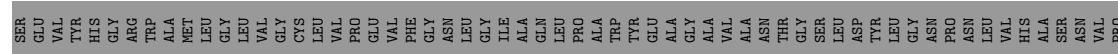
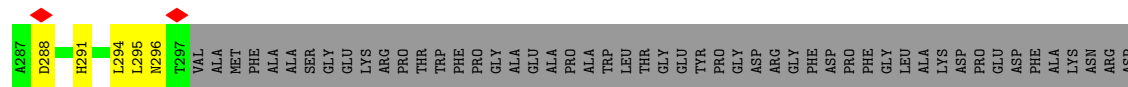
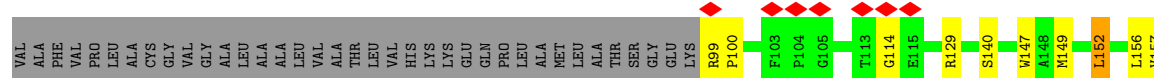
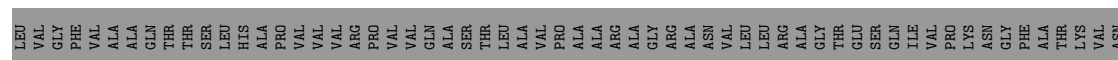
- Molecule 7: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 9: LHCI-1



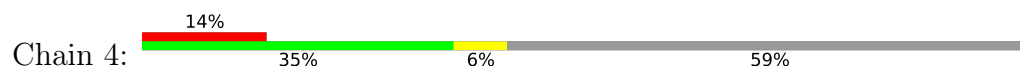
- Molecule 10: LHCI-2



- Molecule 11: LHCI-3

[illegible]

- Molecule 12: LHCI-4



PRO	LEU	LYS	LEU	PRO	ILE	ASP	VAL	SER	GLU	GLY	ALA	GLN	PHE	TRP	VAL	GLY	ARG	GLY	LEU	THR	ASP	GLY	THR	LEU	THR	MET	LEU	PRO	ILE
PRO	LEU	LYS	LEU	PRO	ILE	ASP	VAL	SER	GLU	GLY	ALA	GLN	PHE	TRP	VAL	GLY	ARG	GLY	LEU	THR	ASP	GLY	THR	LEU	THR	MET	LEU	PRO	ILE

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

- Molecule 15: LHCI-7

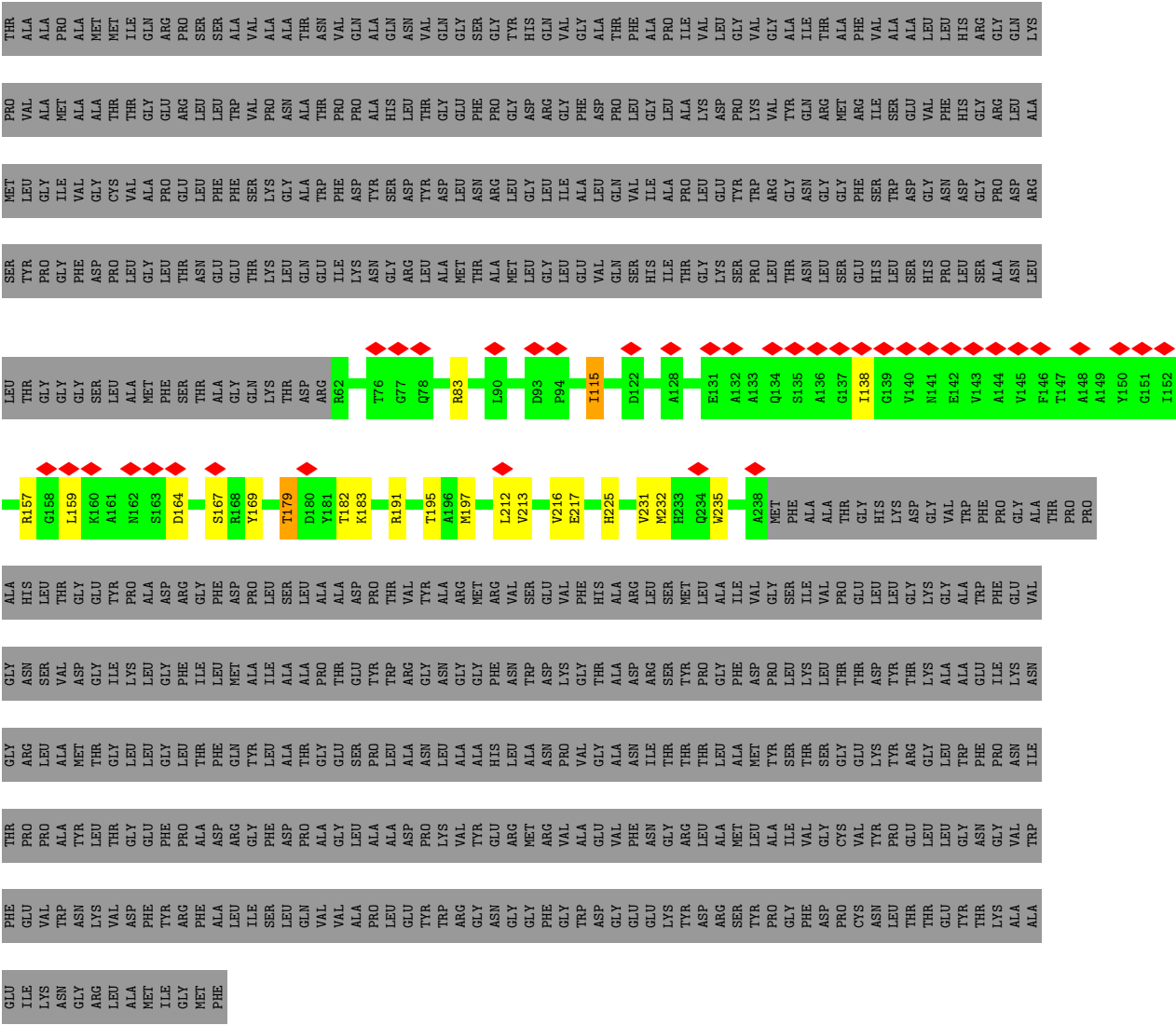
[illegible]

PRO
VAL
ALA
MET
PHE
ALA
THR
THR

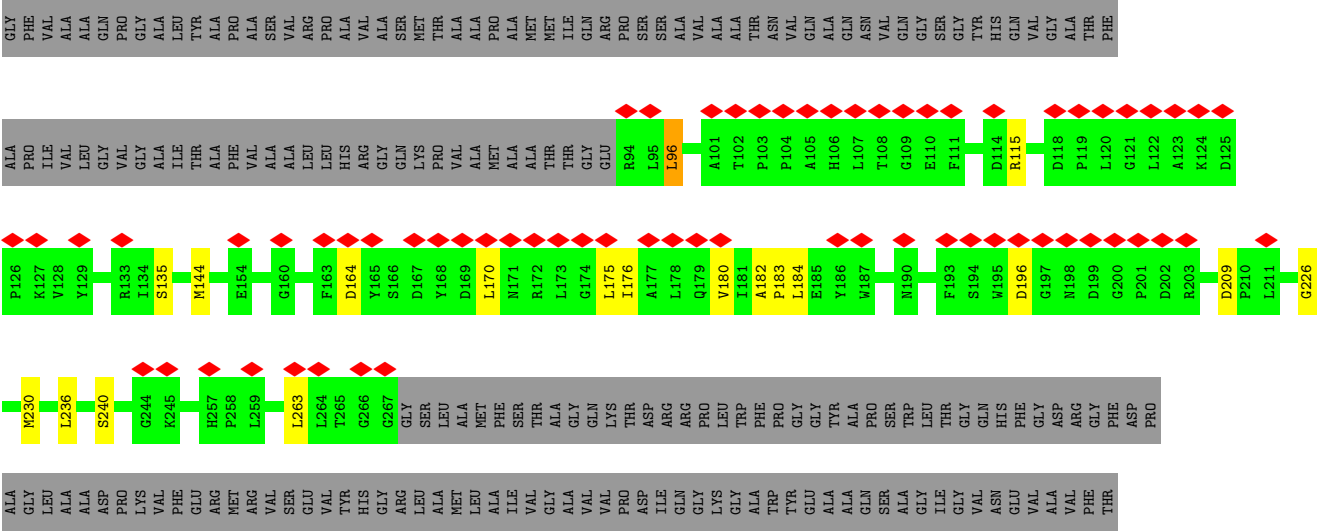
- Molecule 16: LHCI-8



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



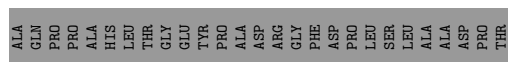
● Molecule 17: LHCI-9



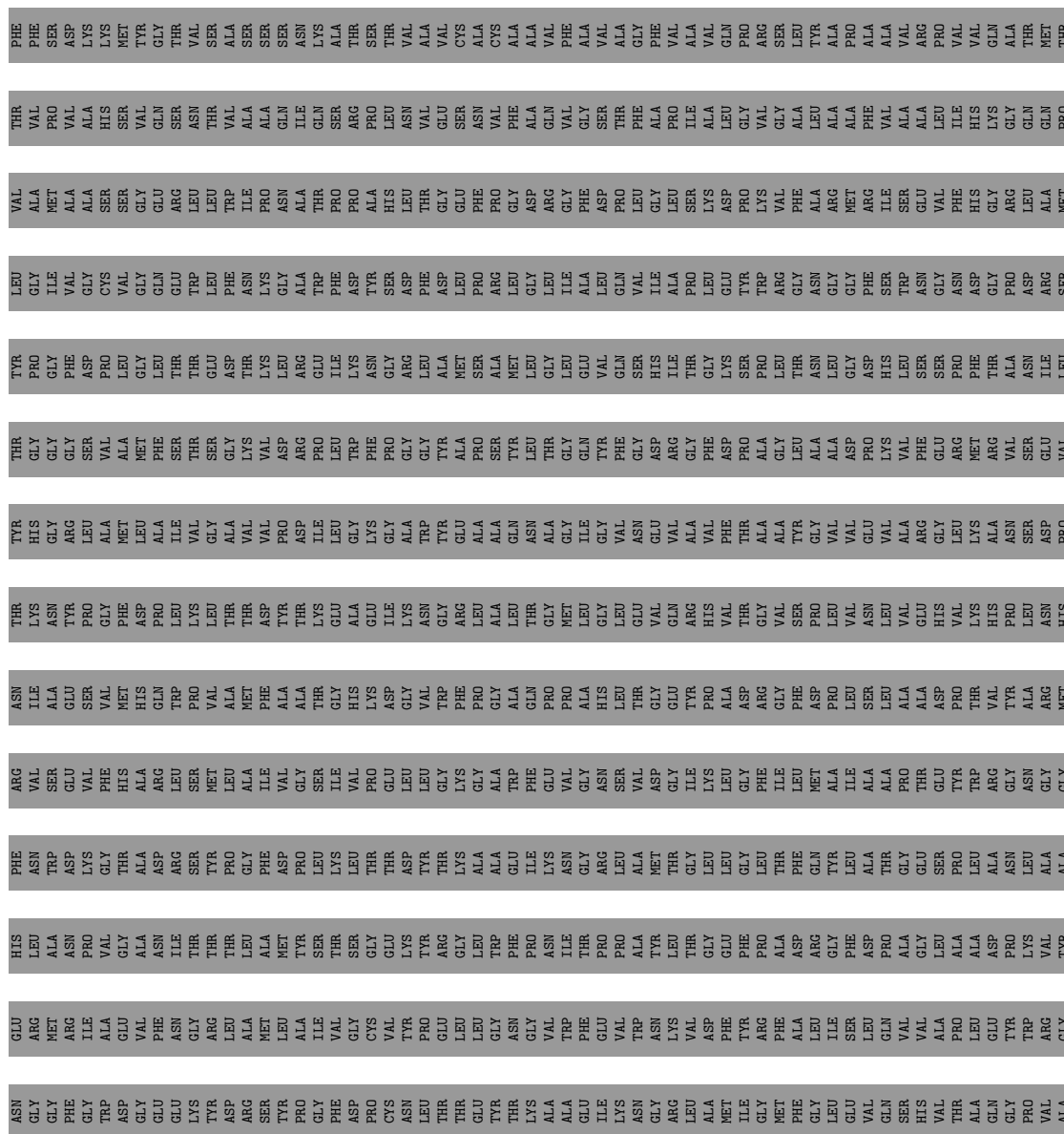
[illegible]

- Molecule 18: LHCI-10

[illegible]

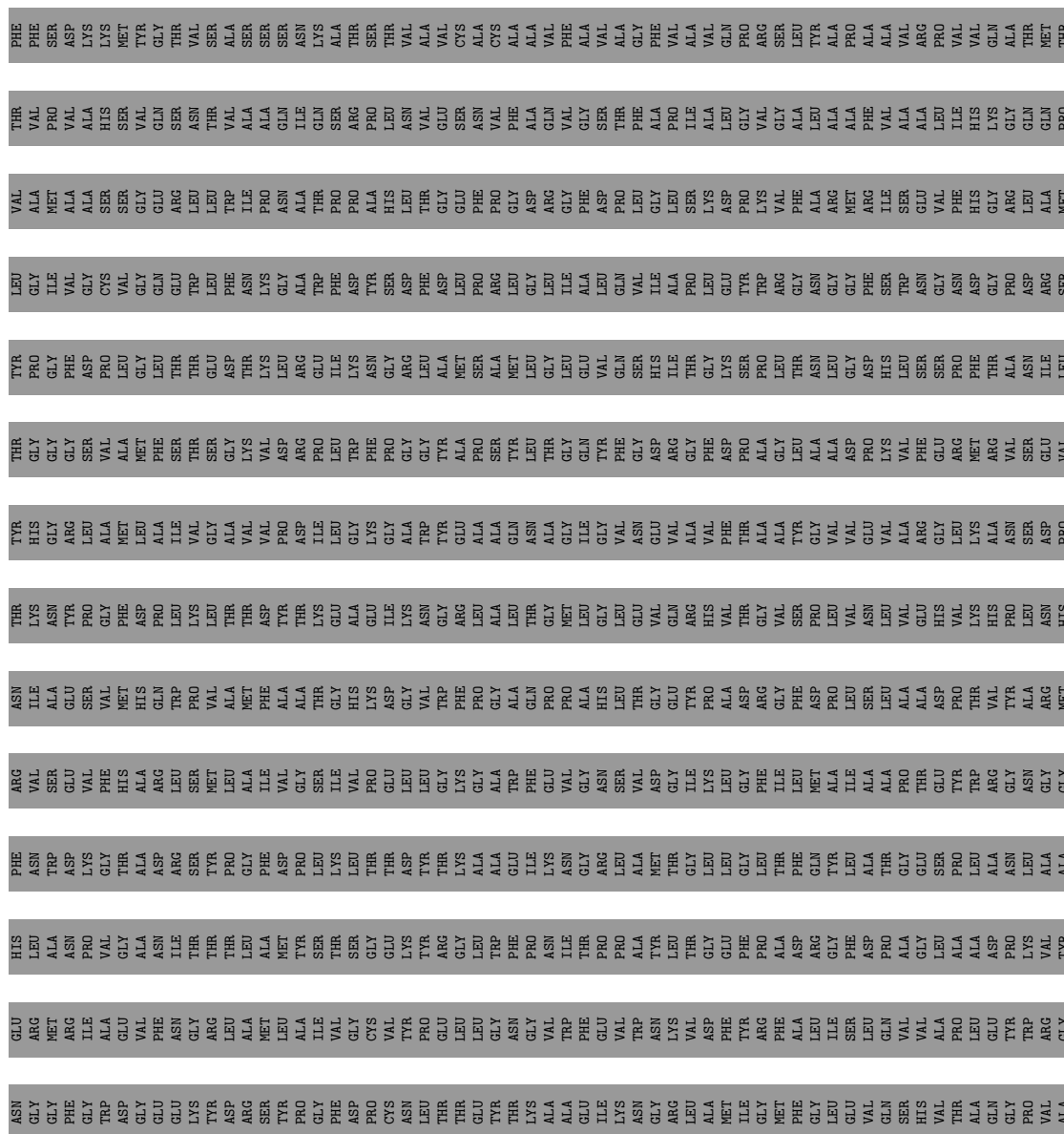


Chain 11: 7% 14% 84%





- 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, CL0, BCR, UNL, DD6, LHG, PQN, 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	48
2	B	729/734 (99%)	700 (96%)	26 (4%)	3 (0%)	30	48
3	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	9	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%)	24	43
11	3	220/431 (51%)	204 (93%)	14 (6%)	2 (1%)	14	27
12	4	167/411 (41%)	152 (91%)	12 (7%)	3 (2%)	6	14
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%)	11	23
16	8	175/828 (21%)	166 (95%)	8 (5%)	1 (1%)	21	39
17	9	172/873 (20%)	164 (95%)	8 (5%)	0	100	100
18	10	138/643 (22%)	125 (91%)	11 (8%)	2 (1%)	9	18
19	11	169/1048 (16%)	157 (93%)	12 (7%)	0	100	100
19	12	148/1048 (14%)	135 (91%)	10 (7%)	3 (2%)	6	12
19	13	72/1048 (7%)	67 (93%)	5 (7%)	0	100	100
All	All	4204/12034 (35%)	3978 (95%)	205 (5%)	21 (0%)	26	43

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%)	47	70
2	B	608/609 (100%)	590 (97%)	18 (3%)	36	60
3	C	69/70 (99%)	65 (94%)	4 (6%)	18	38
4	D	154/557 (28%)	146 (95%)	8 (5%)	21	43
5	E	53/127 (42%)	52 (98%)	1 (2%)	50	73
6	F	132/259 (51%)	129 (98%)	3 (2%)	44	68
7	J	34/34 (100%)	32 (94%)	2 (6%)	18	37
8	M	26/26 (100%)	26 (100%)	0	100	100
9	1	152/372 (41%)	140 (92%)	12 (8%)	11	25
10	2	166/465 (36%)	160 (96%)	6 (4%)	31	56
11	3	174/343 (51%)	168 (97%)	6 (3%)	32	57
12	4	131/310 (42%)	122 (93%)	9 (7%)	14	30
13	5	125/186 (67%)	118 (94%)	7 (6%)	19	40
14	6	140/688 (20%)	131 (94%)	9 (6%)	16	33
15	7	142/471 (30%)	139 (98%)	3 (2%)	47	70
16	8	136/633 (22%)	130 (96%)	6 (4%)	25	49
17	9	142/672 (21%)	133 (94%)	9 (6%)	16	34
18	10	111/497 (22%)	101 (91%)	10 (9%)	9	20
19	11	123/803 (15%)	117 (95%)	6 (5%)	22	45
19	12	110/803 (14%)	107 (97%)	3 (3%)	39	63
19	13	57/803 (7%)	50 (88%)	7 (12%)	4	9
All	All	3407/9369 (36%)	3265 (96%)	142 (4%)	28	51

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

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

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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	7	713	15	51,55,73	2.31	20 (39%)	60,91,113	3.05	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	811	1	49,53,73	2.24	16 (32%)	58,89,113	3.19	30 (51%)
21	CLA	2	516	29	49,53,73	2.33	20 (40%)	58,89,113	2.82	25 (43%)
21	CLA	B	818	29	69,73,73	1.93	17 (24%)	82,113,113	2.66	31 (37%)
21	CLA	B	834	2	64,68,73	2.19	18 (28%)	76,107,113	2.88	36 (47%)
21	CLA	B	816	2	63,67,73	2.08	21 (33%)	74,105,113	2.88	36 (48%)
21	CLA	3	715	11	49,53,73	2.35	16 (32%)	58,89,113	3.11	30 (51%)
21	CLA	7	702	15	51,55,73	2.16	21 (41%)	60,91,113	3.16	30 (50%)
21	CLA	B	826	2	69,73,73	1.85	22 (31%)	82,113,113	2.84	32 (39%)
21	CLA	5	704	29	54,58,73	2.36	17 (31%)	64,95,113	2.95	32 (50%)
21	CLA	B	812	2	69,73,73	1.75	17 (24%)	82,113,113	2.59	31 (37%)
21	CLA	8	604	16	64,68,73	1.94	17 (26%)	76,107,113	2.70	30 (39%)
21	CLA	8	611	16	49,53,73	2.40	18 (36%)	58,89,113	3.05	31 (53%)
21	CLA	12	505	19	51,55,73	2.26	17 (33%)	60,91,113	2.91	33 (55%)
28	DD6	1	518	-	40,45,45	1.31	5 (12%)	51,67,67	1.41	8 (15%)
28	DD6	6	915	-	40,45,45	1.30	7 (17%)	51,67,67	1.56	13 (25%)
24	BCR	A	847	-	41,41,41	1.42	9 (21%)	56,56,56	1.58	8 (14%)
21	CLA	A	815	1	64,68,73	1.87	16 (25%)	76,107,113	3.09	37 (48%)
21	CLA	1	513	9	64,68,73	2.02	19 (29%)	75,106,113	2.66	29 (38%)
21	CLA	A	831	1	69,73,73	1.73	16 (23%)	82,113,113	2.86	32 (39%)
21	CLA	3	708	25	47,51,73	2.30	16 (34%)	55,86,113	3.06	29 (52%)
21	CLA	A	808	1	55,59,73	2.19	21 (38%)	64,96,113	2.92	29 (45%)
21	CLA	7	712	15	49,53,73	2.30	19 (38%)	58,89,113	3.19	34 (58%)
21	CLA	9	907	17	51,55,73	2.36	18 (35%)	60,91,113	3.39	33 (55%)
21	CLA	9	902	17	46,50,73	2.30	20 (43%)	53,85,113	2.94	27 (50%)
21	CLA	7	708	15	66,70,73	2.01	16 (24%)	78,109,113	2.62	34 (43%)
21	CLA	10	704	18	64,68,73	2.13	20 (31%)	76,107,113	2.72	29 (38%)
21	CLA	B	837	29	49,53,73	2.36	17 (34%)	58,89,113	2.77	28 (48%)
21	CLA	A	837	1	49,53,73	2.36	19 (38%)	58,89,113	3.09	30 (51%)
28	DD6	2	520	-	40,45,45	1.32	8 (20%)	51,67,67	1.49	9 (17%)
21	CLA	9	908	17	66,70,73	2.11	20 (30%)	78,109,113	2.64	31 (39%)
21	CLA	A	802	29	69,73,73	1.90	21 (30%)	82,113,113	2.68	36 (43%)
25	LHG	1	521	21	35,35,48	0.39	0	38,41,54	0.91	2 (5%)
21	CLA	3	710	11	59,63,73	2.07	15 (25%)	70,101,113	2.78	30 (42%)
21	CLA	5	702	13	64,68,73	1.98	18 (28%)	76,107,113	2.51	31 (40%)
21	CLA	13	501	19	49,53,73	2.43	22 (44%)	58,89,113	3.00	30 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	J	101	7	49,53,73	2.40	21 (42%)	58,89,113	3.27	36 (62%)
21	CLA	B	831	2	69,73,73	1.92	19 (27%)	82,113,113	2.83	33 (40%)
21	CLA	B	839	25	69,73,73	1.96	21 (30%)	82,113,113	2.77	35 (42%)
21	CLA	11	708	25	47,51,73	2.33	21 (44%)	55,86,113	3.16	31 (56%)
25	LHG	8	617	21	32,32,48	0.41	0	35,38,54	1.00	1 (2%)
28	DD6	12	510	-	40,45,45	1.29	6 (15%)	51,67,67	2.01	14 (27%)
21	CLA	3	712	29	49,53,73	2.45	20 (40%)	58,89,113	2.93	30 (51%)
21	CLA	8	607	29	51,55,73	2.20	20 (39%)	60,91,113	3.02	31 (51%)
21	CLA	9	904	17	49,53,73	2.40	18 (36%)	58,89,113	2.95	30 (51%)
21	CLA	7	710	15	49,53,73	2.35	17 (34%)	58,89,113	3.11	29 (50%)
21	CLA	B	805	2	69,73,73	2.00	15 (21%)	82,113,113	2.34	31 (37%)
21	CLA	B	820	2	49,53,73	2.34	17 (34%)	58,89,113	3.07	24 (41%)
21	CLA	9	910	17	49,53,73	2.32	18 (36%)	58,89,113	3.37	34 (58%)
24	BCR	B	846	-	41,41,41	1.51	9 (21%)	56,56,56	1.36	10 (17%)
21	CLA	2	503	10	49,53,73	2.34	18 (36%)	58,89,113	3.06	29 (50%)
25	LHG	9	917	21	33,33,48	0.40	0	36,39,54	0.84	1 (2%)
21	CLA	A	830	1	69,73,73	1.97	18 (26%)	82,113,113	2.58	36 (43%)
21	CLA	A	806	1	69,73,73	1.98	20 (28%)	82,113,113	2.55	35 (42%)
21	CLA	A	843	29	56,60,73	2.03	19 (33%)	65,97,113	2.93	35 (53%)
21	CLA	6	914	14	51,55,73	2.28	19 (37%)	60,91,113	3.05	33 (55%)
24	BCR	F	405	-	41,41,41	1.51	7 (17%)	56,56,56	1.92	13 (23%)
21	CLA	F	404	6	49,53,73	2.27	18 (36%)	58,89,113	3.10	29 (50%)
23	SF4	C	102	3	0,12,12	-	-	-	-	-
21	CLA	A	824	1	55,59,73	2.04	18 (32%)	64,96,113	3.16	33 (51%)
24	BCR	A	849	-	41,41,41	1.69	7 (17%)	56,56,56	1.58	13 (23%)
21	CLA	2	508	10	51,55,73	2.28	16 (31%)	60,91,113	3.00	33 (55%)
21	CLA	4	708	25	47,51,73	2.35	20 (42%)	55,86,113	3.00	28 (50%)
21	CLA	12	501	19	64,68,73	2.10	16 (25%)	76,107,113	2.76	35 (46%)
21	CLA	6	910	25	47,51,73	2.33	19 (40%)	55,86,113	3.28	31 (56%)
21	CLA	2	504	10	64,68,73	1.96	15 (23%)	76,107,113	2.63	35 (46%)
21	CLA	B	823	29	58,62,73	2.11	18 (31%)	68,99,113	2.86	30 (44%)
21	CLA	3	714	29	49,53,73	2.34	18 (36%)	58,89,113	2.97	30 (51%)
21	CLA	11	706	19	69,73,73	1.99	17 (24%)	82,113,113	2.65	34 (41%)
21	CLA	4	706	12	51,55,73	2.34	17 (33%)	60,91,113	2.86	30 (50%)
21	CLA	12	503	-	49,53,73	2.42	20 (40%)	58,89,113	3.10	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	854	21	26,26,48	0.46	0	29,32,54	1.27	5 (17%)
21	CLA	A	820	1	69,73,73	1.83	22 (31%)	82,113,113	2.89	34 (41%)
21	CLA	B	806	2	69,73,73	1.84	18 (26%)	82,113,113	2.62	39 (47%)
21	CLA	4	709	12	49,53,73	2.47	21 (42%)	58,89,113	3.19	31 (53%)
21	CLA	A	805	1	63,67,73	1.96	19 (30%)	74,105,113	2.94	34 (45%)
21	CLA	1	509	9	51,55,73	2.36	20 (39%)	60,91,113	3.02	30 (50%)
21	CLA	2	506	29	54,58,73	2.22	17 (31%)	64,95,113	2.85	33 (51%)
21	CLA	A	803	-	69,73,73	1.93	18 (26%)	82,113,113	2.77	33 (40%)
21	CLA	A	812	1	69,73,73	1.79	18 (26%)	82,113,113	2.74	36 (43%)
21	CLA	1	514	9	49,53,73	2.40	19 (38%)	58,89,113	2.95	29 (50%)
21	CLA	13	502	-	51,55,73	2.37	20 (39%)	60,91,113	2.92	31 (51%)
28	DD6	12	509	-	40,45,45	1.23	7 (17%)	51,67,67	1.42	7 (13%)
21	CLA	B	825	2	69,73,73	1.87	15 (21%)	82,113,113	2.54	37 (45%)
28	DD6	4	713	-	40,45,45	1.31	7 (17%)	51,67,67	1.56	9 (17%)
21	CLA	7	703	15	64,68,73	2.09	19 (29%)	76,107,113	2.80	29 (38%)
21	CLA	A	862	29	69,73,73	1.80	19 (27%)	82,113,113	3.15	40 (48%)
21	CLA	10	711	18	49,53,73	2.46	18 (36%)	58,89,113	3.03	30 (51%)
24	BCR	B	843	-	41,41,41	1.41	8 (19%)	56,56,56	1.43	10 (17%)
21	CLA	9	905	29	54,58,73	2.29	17 (31%)	64,95,113	2.87	32 (50%)
21	CLA	4	707	12	66,70,73	2.09	18 (27%)	78,109,113	2.69	37 (47%)
21	CLA	11	710	19	49,53,73	2.33	19 (38%)	58,89,113	3.19	30 (51%)
21	CLA	8	609	16	66,70,73	2.15	18 (27%)	78,109,113	2.60	28 (35%)
21	CLA	A	819	1	58,62,73	2.12	20 (34%)	68,99,113	2.76	34 (50%)
21	CLA	A	827	29	64,68,73	1.98	20 (31%)	76,107,113	2.79	33 (43%)
21	CLA	1	508	29	51,55,73	2.33	20 (39%)	60,91,113	3.26	34 (56%)
21	CLA	5	709	13	49,53,73	2.39	17 (34%)	58,89,113	3.05	29 (50%)
28	DD6	7	716	-	40,45,45	1.35	5 (12%)	51,67,67	1.50	9 (17%)
21	CLA	1	511	25	47,51,73	2.33	19 (40%)	55,86,113	3.07	27 (49%)
28	DD6	9	916	-	40,45,45	1.32	7 (17%)	51,67,67	1.63	10 (19%)
21	CLA	2	513	10	49,53,73	2.41	18 (36%)	58,89,113	3.04	29 (50%)
28	DD6	8	616	-	40,45,45	1.32	5 (12%)	51,67,67	1.50	9 (17%)
21	CLA	3	706	11	51,55,73	2.31	18 (35%)	60,91,113	3.05	32 (53%)
21	CLA	8	606	29	49,53,73	2.32	21 (42%)	58,89,113	3.03	24 (41%)
21	CLA	F	401	29	55,59,73	2.13	17 (30%)	64,96,113	3.00	28 (43%)
21	CLA	10	712	18	51,55,73	2.38	20 (39%)	60,91,113	2.99	28 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	828	2	69,73,73	1.79	20 (28%)	82,113,113	2.90	31 (37%)
21	CLA	1	510	9	66,70,73	1.98	20 (30%)	78,109,113	2.53	29 (37%)
21	CLA	7	714	15	51,55,73	2.25	17 (33%)	60,91,113	3.03	31 (51%)
21	CLA	9	913	17	51,55,73	2.37	22 (43%)	60,91,113	3.05	31 (51%)
28	DD6	J	104	-	40,45,45	1.33	8 (20%)	51,67,67	1.56	8 (15%)
21	CLA	A	844	25	69,73,73	2.00	20 (28%)	82,113,113	2.82	36 (43%)
21	CLA	3	709	11	49,53,73	2.25	18 (36%)	58,89,113	3.01	31 (53%)
24	BCR	B	845	-	41,41,41	1.49	7 (17%)	56,56,56	1.46	8 (14%)
21	CLA	A	841	1	69,73,73	1.74	18 (26%)	82,113,113	2.76	30 (36%)
25	LHG	10	713	21	31,31,48	0.32	0	34,37,54	0.95	2 (5%)
21	CLA	B	836	2	51,55,73	2.08	20 (39%)	60,91,113	3.47	37 (61%)
21	CLA	A	842	1	69,73,73	1.89	20 (28%)	82,113,113	2.61	28 (34%)
21	CLA	5	707	13	59,63,73	2.25	20 (33%)	70,101,113	2.91	34 (48%)
28	DD6	11	712	-	40,45,45	1.28	7 (17%)	51,67,67	1.33	8 (15%)
21	CLA	A	833	1	69,73,73	1.89	19 (27%)	82,113,113	2.71	32 (39%)
21	CLA	A	838	1	55,59,73	2.14	21 (38%)	64,96,113	2.85	32 (50%)
21	CLA	9	906	29	51,55,73	2.35	18 (35%)	60,91,113	3.03	29 (48%)
28	DD6	6	916	-	40,45,45	1.24	4 (10%)	51,67,67	1.52	7 (13%)
21	CLA	4	705	29	51,55,73	2.26	20 (39%)	60,91,113	3.08	31 (51%)
21	CLA	B	801	2	69,73,73	2.03	22 (31%)	82,113,113	2.49	33 (40%)
21	CLA	13	503	19	51,55,73	2.31	17 (33%)	60,91,113	2.99	28 (46%)
21	CLA	A	839	1	69,73,73	1.84	18 (26%)	82,113,113	2.87	37 (45%)
21	CLA	4	710	12	49,53,73	2.37	20 (40%)	58,89,113	3.05	28 (48%)
21	CLA	10	703	18	45,49,73	2.50	20 (44%)	54,84,113	3.05	31 (57%)
25	LHG	3	719	21	24,24,48	0.39	0	27,30,54	0.59	0
21	CLA	11	702	19	64,68,73	2.04	18 (28%)	76,107,113	2.57	33 (43%)
21	CLA	1	512	9	49,53,73	2.36	17 (34%)	58,89,113	3.08	33 (56%)
21	CLA	A	832	1	54,58,73	2.07	13 (24%)	64,95,113	3.17	39 (60%)
21	CLA	10	705	18	49,53,73	2.42	20 (40%)	58,89,113	3.27	28 (48%)
24	BCR	B	844	-	41,41,41	1.47	7 (17%)	56,56,56	1.47	10 (17%)
27	DGD	B	847	-	58,58,67	1.02	4 (6%)	72,72,81	1.34	9 (12%)
21	CLA	B	804	2	69,73,73	1.91	21 (30%)	82,113,113	2.73	36 (43%)
21	CLA	B	833	2	49,53,73	2.23	19 (38%)	58,89,113	3.27	35 (60%)
21	CLA	1	516	9	49,53,73	2.35	20 (40%)	58,89,113	2.93	29 (50%)
21	CLA	A	836	1	58,62,73	1.89	17 (29%)	68,99,113	2.81	32 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	838	2	49,53,73	1.93	17 (34%)	58,89,113	3.36	32 (55%)
21	CLA	6	911	14	49,53,73	2.40	15 (30%)	58,89,113	3.11	31 (53%)
21	CLA	12	508	19	49,53,73	2.46	21 (42%)	58,89,113	3.08	29 (50%)
21	CLA	B	803	2	58,62,73	2.09	19 (32%)	68,99,113	3.09	32 (47%)
21	CLA	2	512	10	59,63,73	2.11	19 (32%)	70,101,113	2.88	28 (40%)
21	CLA	3	701	11	45,49,73	2.39	19 (42%)	54,84,113	3.18	28 (51%)
22	PQN	A	845	-	34,34,34	1.71	3 (8%)	43,45,45	1.46	7 (16%)
28	DD6	3	717	-	40,45,45	1.47	6 (15%)	51,67,67	1.95	12 (23%)
28	DD6	4	712	-	40,45,45	1.33	6 (15%)	51,67,67	1.57	11 (21%)
21	CLA	7	706	29	51,55,73	2.24	20 (39%)	60,91,113	2.99	32 (53%)
21	CLA	A	814	1	64,68,73	2.13	20 (31%)	76,107,113	2.51	29 (38%)
21	CLA	A	816	1	49,53,73	2.23	15 (30%)	58,89,113	3.12	31 (53%)
21	CLA	7	705	29	54,58,73	2.19	17 (31%)	64,95,113	2.99	32 (50%)
21	CLA	2	514	29	49,53,73	2.44	19 (38%)	58,89,113	2.90	30 (51%)
21	CLA	3	707	11	66,70,73	1.96	17 (25%)	78,109,113	2.63	33 (42%)
21	CLA	5	705	29	51,55,73	2.35	20 (39%)	60,91,113	2.94	33 (55%)
21	CLA	A	813	1	58,62,73	2.16	21 (36%)	68,99,113	2.73	30 (44%)
25	LHG	7	717	21	47,47,48	0.54	0	50,53,54	1.03	3 (6%)
21	CLA	6	906	14	54,58,73	2.31	18 (33%)	64,95,113	3.06	33 (51%)
21	CLA	12	506	19	59,63,73	2.23	19 (32%)	70,101,113	2.78	31 (44%)
25	LHG	2	521	21	29,29,48	0.39	0	32,35,54	1.25	4 (12%)
21	CLA	A	804	1	69,73,73	1.78	16 (23%)	82,113,113	2.70	33 (40%)
28	DD6	3	718	-	40,45,45	1.30	6 (15%)	51,67,67	1.51	10 (19%)
28	DD6	11	713	-	40,45,45	1.33	8 (20%)	51,67,67	1.58	10 (19%)
21	CLA	4	703	12	49,53,73	2.28	19 (38%)	58,89,113	3.12	29 (50%)
21	CLA	A	817	29	53,57,73	2.06	18 (33%)	61,93,113	2.98	29 (47%)
21	CLA	10	706	-	45,49,73	2.45	18 (40%)	54,84,113	3.14	30 (55%)
21	CLA	B	815	2	59,63,73	2.12	20 (33%)	70,101,113	2.61	31 (44%)
21	CLA	6	904	14	64,68,73	2.06	19 (29%)	76,107,113	2.66	36 (47%)
21	CLA	11	707	19	58,62,73	2.28	19 (32%)	68,99,113	2.70	30 (44%)
21	CLA	12	504	-	45,49,73	2.52	18 (40%)	54,84,113	2.92	30 (55%)
24	BCR	J	102	-	41,41,41	1.46	7 (17%)	56,56,56	1.49	8 (14%)
28	DD6	2	519	-	40,45,45	1.41	7 (17%)	51,67,67	1.67	12 (23%)
21	CLA	10	710	18	59,63,73	2.19	17 (28%)	70,101,113	2.74	31 (44%)
21	CLA	3	702	11	64,68,73	1.96	18 (28%)	76,107,113	2.88	34 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	825	1	63,67,73	1.88	18 (28%)	74,105,113	2.70	31 (41%)
21	CLA	6	908	14	49,53,73	2.23	19 (38%)	58,89,113	3.22	34 (58%)
21	CLA	1	517	29	49,53,73	2.43	20 (40%)	58,89,113	2.93	28 (48%)
21	CLA	2	505	10	49,53,73	2.32	17 (34%)	58,89,113	2.87	30 (51%)
21	CLA	1	501	29	49,53,73	2.39	17 (34%)	58,89,113	3.08	31 (53%)
21	CLA	4	711	29	49,53,73	2.28	17 (34%)	58,89,113	2.93	32 (55%)
21	CLA	6	912	14	49,53,73	2.43	18 (36%)	58,89,113	2.98	30 (51%)
21	CLA	8	614	16	51,55,73	2.30	19 (37%)	60,91,113	2.94	29 (48%)
24	BCR	A	850	-	41,41,41	1.40	7 (17%)	56,56,56	1.49	13 (23%)
24	BCR	B	841	-	41,41,41	1.34	6 (14%)	56,56,56	1.48	9 (16%)
21	CLA	12	507	19	49,53,73	2.44	20 (40%)	58,89,113	3.20	30 (51%)
21	CLA	B	829	2	49,53,73	2.34	15 (30%)	58,89,113	3.33	33 (56%)
21	CLA	2	515	10	49,53,73	2.40	19 (38%)	58,89,113	3.06	31 (53%)
24	BCR	B	842	-	41,41,41	1.40	7 (17%)	56,56,56	1.53	11 (19%)
21	CLA	B	819	2	51,55,73	2.29	22 (43%)	60,91,113	3.01	32 (53%)
21	CLA	1	515	29	49,53,73	2.39	17 (34%)	58,89,113	2.95	30 (51%)
21	CLA	3	711	11	49,53,73	2.36	17 (34%)	58,89,113	3.05	28 (48%)
21	CLA	B	835	2	69,73,73	1.96	19 (27%)	82,113,113	2.51	35 (42%)
21	CLA	B	832	2	62,66,73	2.05	16 (25%)	73,104,113	2.99	37 (50%)
21	CLA	B	814	2	49,53,73	2.26	20 (40%)	58,89,113	3.02	31 (53%)
28	DD6	7	715	-	40,45,45	1.33	6 (15%)	51,67,67	1.45	7 (13%)
21	CLA	B	813	2	69,73,73	2.03	21 (30%)	82,113,113	2.55	28 (34%)
21	CLA	9	911	17	59,63,73	2.16	20 (33%)	70,101,113	2.80	29 (41%)
21	CLA	8	613	16	49,53,73	2.39	19 (38%)	58,89,113	3.13	32 (55%)
21	CLA	B	808	2	49,53,73	2.23	21 (42%)	58,89,113	2.91	31 (53%)
21	CLA	5	703	13	49,53,73	2.17	17 (34%)	58,89,113	2.89	29 (50%)
25	LHG	B	848	21	22,22,48	0.37	0	25,28,54	1.09	2 (8%)
21	CLA	B	830	2	53,57,73	2.35	20 (37%)	61,93,113	3.15	35 (57%)
21	CLA	10	708	25	47,51,73	2.34	18 (38%)	55,86,113	3.12	28 (50%)
21	CLA	4	704	29	54,58,73	2.27	18 (33%)	64,95,113	2.86	31 (48%)
24	BCR	F	402	-	41,41,41	1.43	6 (14%)	56,56,56	1.62	10 (17%)
21	CLA	B	802	-	69,73,73	1.93	19 (27%)	82,113,113	2.74	37 (45%)
21	CLA	11	711	19	49,53,73	2.46	21 (42%)	58,89,113	3.07	30 (51%)
21	CLA	2	507	29	51,55,73	2.17	18 (35%)	60,91,113	3.06	31 (51%)
21	CLA	B	824	29	50,54,73	2.11	20 (40%)	59,90,113	3.18	31 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	817	2	64,68,73	1.93	18 (28%)	76,107,113	2.89	41 (53%)
21	CLA	6	905	14	49,53,73	2.25	19 (38%)	58,89,113	2.89	29 (50%)
21	CLA	9	914	17	51,55,73	2.42	18 (35%)	60,91,113	2.97	29 (48%)
21	CLA	B	821	2	59,63,73	2.12	18 (30%)	70,101,113	3.04	35 (50%)
21	CLA	B	822	2	49,53,73	2.27	20 (40%)	58,89,113	2.85	33 (56%)
21	CLA	4	702	12	59,63,73	2.11	18 (30%)	70,101,113	2.89	28 (40%)
23	SF4	A	846	2,1	0,12,12	-	-	-		
21	CLA	11	705	-	51,55,73	2.33	19 (37%)	60,91,113	2.87	33 (55%)
25	LHG	5	714	21	31,31,48	0.35	0	34,37,54	0.63	0
21	CLA	2	511	10	49,53,73	2.50	19 (38%)	58,89,113	3.16	32 (55%)
21	CLA	5	701	13	49,53,73	2.30	19 (38%)	58,89,113	2.88	32 (55%)
21	CLA	F	403	29	49,53,73	2.32	17 (34%)	58,89,113	2.96	30 (51%)
21	CLA	10	707	18	52,56,73	2.36	19 (36%)	61,92,113	2.95	32 (52%)
21	CLA	A	835	1	49,53,73	2.28	20 (40%)	58,89,113	3.11	29 (50%)
21	CLA	1	507	29	54,58,73	2.28	17 (31%)	64,95,113	2.77	30 (46%)
21	CLA	2	509	10	66,70,73	1.96	18 (27%)	78,109,113	2.64	26 (33%)
21	CLA	1	505	9	64,68,73	2.05	16 (25%)	76,107,113	2.45	28 (36%)
21	CLA	9	909	25	47,51,73	2.32	18 (38%)	55,86,113	3.13	27 (49%)
21	CLA	9	912	17	49,53,73	2.38	20 (40%)	58,89,113	3.09	28 (48%)
21	CLA	A	809	1	69,73,73	2.00	18 (26%)	82,113,113	2.60	35 (42%)
21	CLA	12	502	19	49,53,73	2.40	18 (36%)	58,89,113	3.01	32 (55%)
25	LHG	6	917	21	27,27,48	0.36	0	30,33,54	1.22	4 (13%)
21	CLA	A	822	29	69,73,73	1.94	19 (27%)	82,113,113	2.44	35 (42%)
28	DD6	2	518	-	40,45,45	1.25	7 (17%)	51,67,67	1.71	12 (23%)
21	CLA	A	829	1	69,73,73	1.75	17 (24%)	82,113,113	2.77	39 (47%)
21	CLA	6	913	14	49,53,73	2.41	19 (38%)	58,89,113	2.97	29 (50%)
21	CLA	8	605	16	49,53,73	2.38	19 (38%)	58,89,113	2.94	26 (44%)
21	CLA	11	704	29	49,53,73	2.38	18 (36%)	58,89,113	3.06	28 (48%)
21	CLA	2	517	-	49,53,73	2.51	20 (40%)	58,89,113	2.98	26 (44%)
21	CLA	B	827	2	69,73,73	1.87	16 (23%)	82,113,113	2.69	37 (45%)
21	CLA	3	704	29	46,50,73	2.22	20 (43%)	53,85,113	3.20	29 (54%)
21	CLA	A	828	1	69,73,73	1.74	17 (24%)	82,113,113	2.74	34 (41%)
22	PQN	B	840	-	32,32,34	1.74	5 (15%)	40,42,45	1.84	10 (25%)
21	CLA	A	840	1	51,55,73	2.19	19 (37%)	60,91,113	3.78	36 (60%)
21	CLA	3	703	11	49,53,73	2.39	17 (34%)	58,89,113	3.01	32 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	1	519	-	40,45,45	1.29	6 (15%)	51,67,67	1.53	8 (15%)
21	CLA	5	706	13	49,53,73	2.42	17 (34%)	58,89,113	3.04	32 (55%)
21	CLA	6	907	29	51,55,73	2.28	20 (39%)	60,91,113	3.00	34 (56%)
21	CLA	A	807	1	69,73,73	2.04	20 (28%)	82,113,113	2.74	40 (48%)
21	CLA	A	810	1	69,73,73	1.93	20 (28%)	82,113,113	2.77	28 (34%)
21	CLA	7	711	15	69,73,73	1.89	16 (23%)	82,113,113	2.41	29 (35%)
21	CLA	5	711	13	49,53,73	2.47	20 (40%)	58,89,113	2.98	28 (48%)
21	CLA	5	708	25	47,51,73	2.36	17 (36%)	55,86,113	3.11	24 (43%)
21	CLA	A	823	1	49,53,73	2.09	16 (32%)	58,89,113	3.15	30 (51%)
28	DD6	5	713	-	40,45,45	1.58	10 (25%)	51,67,67	1.87	13 (25%)
21	CLA	6	903	14	51,55,73	2.38	21 (41%)	60,91,113	3.15	32 (53%)
25	LHG	A	853	-	48,48,48	0.71	1 (2%)	51,54,54	0.68	1 (1%)
25	LHG	4	714	21	18,18,48	0.58	0	21,23,54	0.86	1 (4%)
21	CLA	11	709	19	49,53,73	2.41	19 (38%)	58,89,113	2.96	30 (51%)
21	CLA	A	834	1	49,53,73	2.21	16 (32%)	58,89,113	3.34	32 (55%)
21	CLA	11	703	19	69,73,73	1.98	19 (27%)	82,113,113	2.66	32 (39%)
21	CLA	A	818	1	58,62,73	2.10	17 (29%)	68,99,113	2.83	33 (48%)
28	DD6	8	615	-	40,45,45	1.33	5 (12%)	51,67,67	1.39	8 (15%)
21	CLA	2	510	25	47,51,73	2.25	18 (38%)	55,86,113	3.35	30 (54%)
21	CLA	8	612	16	69,73,73	1.94	20 (28%)	82,113,113	2.56	32 (39%)
21	CLA	6	909	14	66,70,73	2.03	17 (25%)	78,109,113	2.67	29 (37%)
25	LHG	11	714	21	29,29,48	0.36	0	32,35,54	0.73	1 (3%)
28	DD6	5	712	-	40,45,45	1.35	6 (15%)	51,67,67	1.40	6 (11%)
21	CLA	5	710	13	54,58,73	2.29	17 (31%)	64,95,113	3.15	31 (48%)
21	CLA	B	807	2	69,73,73	1.84	20 (28%)	82,113,113	2.60	34 (41%)
21	CLA	B	810	2	49,53,73	2.26	20 (40%)	58,89,113	3.12	31 (53%)
21	CLA	A	821	1	65,69,73	1.82	16 (24%)	77,108,113	2.92	30 (38%)
21	CLA	B	809	2	49,53,73	2.35	20 (40%)	58,89,113	2.97	32 (55%)
21	CLA	7	709	25	47,51,73	2.26	20 (42%)	55,86,113	2.99	34 (61%)
21	CLA	9	903	17	64,68,73	2.21	16 (25%)	76,107,113	2.84	34 (44%)
21	CLA	11	701	19	45,49,73	2.43	20 (44%)	54,84,113	3.12	31 (57%)
24	BCR	A	852	-	41,41,41	1.57	6 (14%)	56,56,56	1.35	6 (10%)
21	CLA	7	707	15	51,55,73	2.21	15 (29%)	60,91,113	2.78	27 (45%)
24	BCR	A	851	-	41,41,41	1.62	11 (26%)	56,56,56	1.27	8 (14%)
23	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	811	2	49,53,73	2.28	20 (40%)	58,89,113	3.15	29 (50%)
24	BCR	J	103	-	41,41,41	1.38	8 (19%)	56,56,56	1.52	7 (12%)
28	DD6	3	716	-	40,45,45	1.23	4 (10%)	51,67,67	1.55	7 (13%)
28	DD6	9	915	-	40,45,45	1.34	8 (20%)	51,67,67	1.60	10 (19%)
21	CLA	1	506	9	49,53,73	2.37	16 (32%)	58,89,113	2.87	32 (55%)
28	DD6	1	520	-	40,45,45	1.34	7 (17%)	51,67,67	1.51	9 (17%)
21	CLA	8	610	25	47,51,73	2.17	17 (36%)	55,86,113	3.06	32 (58%)
21	CLA	7	704	15	49,53,73	2.26	19 (38%)	58,89,113	3.06	31 (53%)
24	BCR	M	102	-	41,41,41	1.45	8 (19%)	56,56,56	1.46	7 (12%)
21	CLA	3	705	29	51,55,73	2.28	19 (37%)	60,91,113	3.13	29 (48%)
21	CLA	3	713	11	49,53,73	2.40	19 (38%)	58,89,113	3.13	30 (51%)
21	CLA	A	826	29	69,73,73	1.96	19 (27%)	82,113,113	2.61	34 (41%)
21	CLA	8	608	16	51,55,73	2.35	17 (33%)	60,91,113	3.00	33 (55%)
24	BCR	A	848	-	41,41,41	1.44	7 (17%)	56,56,56	1.64	11 (19%)
21	CLA	4	701	-	45,49,73	2.35	19 (42%)	54,84,113	3.50	31 (57%)
21	CLA	10	709	18	49,53,73	2.32	19 (38%)	58,89,113	3.13	31 (53%)
21	CLA	1	504	9	46,50,73	2.40	19 (41%)	53,85,113	3.02	27 (50%)
20	CL0	A	801	1	58,73,73	2.98	19 (32%)	60,113,113	3.11	21 (35%)
21	CLA	8	603	16	51,55,73	2.20	16 (31%)	60,91,113	3.24	31 (51%)

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	7	713	15	1/1/11/20	0/18/94/115	-
21	CLA	A	811	1	1/1/11/20	3/15/91/115	-
21	CLA	2	516	29	-	1/15/91/115	-
21	CLA	B	818	29	1/1/15/20	4/39/115/115	-
21	CLA	B	834	2	1/1/14/20	8/33/109/115	-
21	CLA	B	816	2	1/1/13/20	5/32/108/115	-
21	CLA	3	715	11	1/1/11/20	3/15/91/115	-
21	CLA	7	702	15	1/1/11/20	6/18/94/115	-
21	CLA	B	826	2	1/1/15/20	13/39/115/115	-
21	CLA	8	611	16	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	812	2	1/1/15/20	15/39/115/115	-
21	CLA	8	604	16	1/1/14/20	5/33/109/115	-
21	CLA	12	505	19	1/1/11/20	3/18/94/115	-
21	CLA	5	704	29	-	3/21/97/115	-
28	DD6	1	518	-	-	14/26/80/80	0/3/3/3
28	DD6	6	915	-	-	3/26/80/80	0/3/3/3
24	BCR	A	847	-	-	4/29/63/63	0/2/2/2
21	CLA	A	815	1	1/1/14/20	15/33/109/115	-
21	CLA	7	712	15	1/1/11/20	1/15/91/115	-
21	CLA	A	831	1	1/1/15/20	8/39/115/115	-
21	CLA	3	708	25	1/1/10/20	5/13/89/115	-
21	CLA	A	808	1	1/1/12/20	4/23/99/115	-
21	CLA	10	704	18	1/1/14/20	6/33/109/115	-
21	CLA	9	907	17	1/1/11/20	2/18/94/115	-
21	CLA	9	902	17	1/1/10/20	2/12/88/115	-
21	CLA	7	708	15	1/1/14/20	8/36/112/115	-
21	CLA	1	513	9	-	9/31/107/115	-
21	CLA	B	837	29	1/1/11/20	5/15/91/115	-
21	CLA	A	837	1	-	4/15/91/115	-
28	DD6	2	520	-	-	10/26/80/80	0/3/3/3
21	CLA	9	908	17	1/1/14/20	5/36/112/115	-
21	CLA	A	802	29	1/1/15/20	3/39/115/115	-
25	LHG	1	521	21	-	14/40/40/53	-
21	CLA	5	702	13	1/1/14/20	5/33/109/115	-
21	CLA	3	710	11	-	9/27/103/115	-
21	CLA	13	501	19	1/1/11/20	5/15/91/115	-
21	CLA	J	101	7	1/1/11/20	4/15/91/115	-
21	CLA	B	831	2	1/1/15/20	13/39/115/115	-
21	CLA	11	708	25	1/1/10/20	5/13/89/115	-
25	LHG	8	617	21	-	15/37/37/53	-
28	DD6	12	510	-	-	11/26/80/80	0/3/3/3
21	CLA	3	712	29	1/1/11/20	6/15/91/115	-
21	CLA	9	904	17	1/1/11/20	2/15/91/115	-
21	CLA	8	607	29	-	0/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	7	710	15	1/1/11/20	5/15/91/115	-
21	CLA	B	805	2	1/1/15/20	13/39/115/115	-
21	CLA	B	820	2	-	5/15/91/115	-
21	CLA	9	910	17	1/1/11/20	4/15/91/115	-
24	BCR	B	846	-	-	0/29/63/63	0/2/2/2
21	CLA	2	503	10	1/1/11/20	1/15/91/115	-
25	LHG	9	917	21	-	21/38/38/53	-
21	CLA	A	830	1	1/1/15/20	10/39/115/115	-
21	CLA	A	806	1	1/1/15/20	12/39/115/115	-
21	CLA	A	843	29	1/1/12/20	2/24/100/115	-
21	CLA	6	914	14	-	6/18/94/115	-
24	BCR	F	405	-	-	5/29/63/63	0/2/2/2
21	CLA	F	404	6	1/1/11/20	4/15/91/115	-
20	CL0	A	801	1	3/3/20/25	6/37/135/135	-
23	SF4	C	102	3	-	-	0/6/5/5
21	CLA	A	824	1	-	7/23/99/115	-
24	BCR	A	849	-	-	3/29/63/63	0/2/2/2
21	CLA	2	508	10	1/1/11/20	2/18/94/115	-
21	CLA	4	708	25	1/1/10/20	0/13/89/115	-
21	CLA	12	501	19	1/1/14/20	5/33/109/115	-
21	CLA	6	910	25	1/1/10/20	3/13/89/115	-
21	CLA	2	504	10	1/1/14/20	13/33/109/115	-
21	CLA	B	823	29	1/1/12/20	8/26/102/115	-
21	CLA	3	714	29	1/1/11/20	2/15/91/115	-
21	CLA	11	706	19	1/1/15/20	10/39/115/115	-
21	CLA	4	706	12	1/1/11/20	3/18/94/115	-
21	CLA	12	503	-	1/1/11/20	1/15/91/115	-
25	LHG	A	854	21	-	13/31/31/53	-
21	CLA	A	820	1	1/1/15/20	13/39/115/115	-
21	CLA	B	806	2	1/1/15/20	9/39/115/115	-
21	CLA	4	709	12	1/1/11/20	4/15/91/115	-
21	CLA	A	805	1	1/1/13/20	11/32/108/115	-
21	CLA	1	509	9	1/1/11/20	2/18/94/115	-
21	CLA	2	506	29	1/1/12/20	4/21/97/115	-
21	CLA	A	803	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	812	1	1/1/15/20	5/39/115/115	-
21	CLA	1	514	9	1/1/11/20	1/15/91/115	-
21	CLA	13	502	-	1/1/11/20	3/18/94/115	-
28	DD6	12	509	-	-	3/26/80/80	0/3/3/3
21	CLA	B	825	2	1/1/15/20	3/39/115/115	-
28	DD6	4	713	-	-	14/26/80/80	0/3/3/3
21	CLA	7	703	15	-	11/33/109/115	-
21	CLA	A	862	29	1/1/15/20	10/39/115/115	-
21	CLA	10	711	18	1/1/11/20	1/15/91/115	-
24	BCR	B	843	-	-	6/29/63/63	0/2/2/2
21	CLA	9	905	29	1/1/12/20	5/21/97/115	-
21	CLA	4	707	12	1/1/14/20	4/36/112/115	-
21	CLA	11	710	19	-	4/15/91/115	-
21	CLA	8	609	16	1/1/14/20	4/36/112/115	-
21	CLA	A	819	1	1/1/12/20	8/26/102/115	-
21	CLA	A	827	29	1/1/14/20	8/33/109/115	-
21	CLA	1	508	29	-	2/18/94/115	-
21	CLA	5	709	13	1/1/11/20	2/15/91/115	-
28	DD6	7	716	-	-	2/26/80/80	0/3/3/3
21	CLA	1	511	25	1/1/10/20	2/13/89/115	-
28	DD6	9	916	-	-	10/26/80/80	0/3/3/3
21	CLA	2	513	10	1/1/11/20	5/15/91/115	-
28	DD6	8	616	-	-	7/26/80/80	0/3/3/3
21	CLA	3	706	11	1/1/11/20	6/18/94/115	-
21	CLA	8	606	29	1/1/11/20	0/15/91/115	-
21	CLA	F	401	29	1/1/12/20	7/23/99/115	-
21	CLA	10	712	18	1/1/11/20	3/18/94/115	-
21	CLA	B	828	2	1/1/15/20	7/39/115/115	-
21	CLA	1	510	9	1/1/14/20	9/36/112/115	-
21	CLA	7	714	15	1/1/11/20	2/18/94/115	-
21	CLA	9	913	17	-	4/18/94/115	-
28	DD6	J	104	-	-	16/26/80/80	0/3/3/3
21	CLA	A	844	25	1/1/15/20	14/39/115/115	-
21	CLA	3	709	11	1/1/11/20	4/15/91/115	-
24	BCR	B	845	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	841	1	1/1/15/20	6/39/115/115	-
25	LHG	10	713	21	-	16/36/36/53	-
21	CLA	B	836	2	1/1/11/20	1/18/94/115	-
21	CLA	A	842	1	1/1/15/20	13/39/115/115	-
21	CLA	5	707	13	1/1/13/20	6/27/103/115	-
28	DD6	11	712	-	-	4/26/80/80	0/3/3/3
21	CLA	A	833	1	1/1/15/20	5/39/115/115	-
21	CLA	A	838	1	1/1/12/20	4/23/99/115	-
21	CLA	9	906	29	-	2/18/94/115	-
28	DD6	6	916	-	-	6/26/80/80	0/3/3/3
21	CLA	4	705	29	-	3/18/94/115	-
21	CLA	B	801	2	1/1/15/20	3/39/115/115	-
21	CLA	13	503	19	1/1/11/20	2/18/94/115	-
21	CLA	A	839	1	1/1/15/20	14/39/115/115	-
21	CLA	4	710	12	-	5/15/91/115	-
21	CLA	10	703	18	1/1/10/20	2/10/86/115	-
25	LHG	3	719	21	-	9/28/28/53	-
21	CLA	11	702	19	1/1/14/20	7/33/109/115	-
21	CLA	1	512	9	1/1/11/20	2/15/91/115	-
21	CLA	A	832	1	-	4/21/97/115	-
21	CLA	10	705	18	1/1/11/20	2/15/91/115	-
24	BCR	B	844	-	-	2/29/63/63	0/2/2/2
27	DGD	B	847	-	-	23/46/86/95	0/2/2/2
21	CLA	B	804	2	1/1/15/20	11/39/115/115	-
21	CLA	B	833	2	1/1/11/20	9/15/91/115	-
21	CLA	1	516	9	1/1/11/20	1/15/91/115	-
21	CLA	A	836	1	-	5/26/102/115	-
21	CLA	B	838	2	-	2/15/91/115	-
21	CLA	6	911	14	1/1/11/20	2/15/91/115	-
21	CLA	12	508	19	1/1/11/20	5/15/91/115	-
21	CLA	B	803	2	1/1/12/20	13/26/102/115	-
21	CLA	2	512	10	-	13/27/103/115	-
21	CLA	3	701	11	1/1/10/20	2/10/86/115	-
22	PQN	A	845	-	-	8/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	3	717	-	-	9/26/80/80	0/3/3/3
28	DD6	4	712	-	-	3/26/80/80	0/3/3/3
21	CLA	7	706	29	-	5/18/94/115	-
21	CLA	A	814	1	1/1/14/20	3/33/109/115	-
21	CLA	A	816	1	-	1/15/91/115	-
21	CLA	7	705	29	1/1/12/20	3/21/97/115	-
21	CLA	2	514	29	1/1/11/20	5/15/91/115	-
21	CLA	3	707	11	1/1/14/20	4/36/112/115	-
21	CLA	5	705	29	1/1/11/20	4/18/94/115	-
21	CLA	A	813	1	1/1/12/20	9/26/102/115	-
25	LHG	7	717	21	-	20/52/52/53	-
21	CLA	6	906	14	1/1/12/20	5/21/97/115	-
21	CLA	12	506	19	1/1/13/20	5/27/103/115	-
25	LHG	2	521	21	-	15/34/34/53	-
21	CLA	A	804	1	1/1/15/20	13/39/115/115	-
28	DD6	3	718	-	-	7/26/80/80	0/3/3/3
28	DD6	11	713	-	-	9/26/80/80	0/3/3/3
21	CLA	4	703	12	1/1/11/20	7/15/91/115	-
21	CLA	A	817	29	-	2/20/96/115	-
21	CLA	10	706	-	1/1/10/20	2/10/86/115	-
21	CLA	B	815	2	1/1/13/20	8/27/103/115	-
21	CLA	6	904	14	1/1/14/20	5/33/109/115	-
21	CLA	11	707	19	1/1/12/20	2/26/102/115	-
21	CLA	12	504	-	1/1/10/20	0/10/86/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
28	DD6	2	519	-	-	4/26/80/80	0/3/3/3
21	CLA	10	710	18	1/1/13/20	2/27/103/115	-
21	CLA	3	702	11	-	7/33/109/115	-
21	CLA	A	825	1	-	10/32/108/115	-
21	CLA	6	908	14	1/1/11/20	1/15/91/115	-
21	CLA	6	912	14	1/1/11/20	4/15/91/115	-
21	CLA	2	505	10	1/1/11/20	6/15/91/115	-
21	CLA	1	501	29	1/1/11/20	2/15/91/115	-
21	CLA	4	711	29	1/1/11/20	4/15/91/115	-
21	CLA	1	517	29	-	1/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	614	16	-	2/18/94/115	-
24	BCR	A	850	-	-	6/29/63/63	0/2/2/2
24	BCR	B	841	-	-	2/29/63/63	0/2/2/2
21	CLA	12	507	19	1/1/11/20	2/15/91/115	-
21	CLA	B	829	2	-	5/15/91/115	-
21	CLA	2	515	10	1/1/11/20	2/15/91/115	-
24	BCR	B	842	-	-	11/29/63/63	0/2/2/2
21	CLA	3	711	11	1/1/11/20	4/15/91/115	-
21	CLA	1	515	29	1/1/11/20	1/15/91/115	-
21	CLA	B	819	2	-	6/18/94/115	-
21	CLA	B	835	2	1/1/15/20	13/39/115/115	-
21	CLA	B	832	2	1/1/13/20	11/31/107/115	-
21	CLA	B	814	2	1/1/11/20	2/15/91/115	-
28	DD6	7	715	-	-	12/26/80/80	0/3/3/3
21	CLA	B	813	2	1/1/15/20	10/39/115/115	-
21	CLA	9	911	17	1/1/13/20	8/27/103/115	-
21	CLA	8	613	16	1/1/11/20	5/15/91/115	-
21	CLA	B	808	2	1/1/11/20	2/15/91/115	-
21	CLA	5	703	13	1/1/11/20	4/15/91/115	-
25	LHG	B	848	21	-	11/26/26/53	-
21	CLA	B	830	2	1/1/11/20	7/20/96/115	-
21	CLA	10	708	25	1/1/10/20	2/13/89/115	-
21	CLA	4	704	29	1/1/12/20	0/21/97/115	-
24	BCR	F	402	-	-	1/29/63/63	0/2/2/2
21	CLA	B	802	-	1/1/15/20	9/39/115/115	-
21	CLA	11	711	19	1/1/11/20	4/15/91/115	-
21	CLA	2	507	29	-	5/18/94/115	-
21	CLA	B	824	29	1/1/11/20	4/17/93/115	-
21	CLA	B	817	2	1/1/14/20	12/33/109/115	-
21	CLA	6	905	14	1/1/11/20	5/15/91/115	-
21	CLA	9	914	17	1/1/11/20	4/18/94/115	-
21	CLA	B	821	2	1/1/13/20	6/27/103/115	-
21	CLA	B	822	2	1/1/11/20	3/15/91/115	-
21	CLA	4	702	12	-	5/27/103/115	-
25	LHG	5	714	21	-	14/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	11	705	-	1/1/11/20	5/18/94/115	-
23	SF4	A	846	2,1	-	-	0/6/5/5
21	CLA	2	511	10	1/1/11/20	4/15/91/115	-
21	CLA	5	701	13	1/1/11/20	6/15/91/115	-
21	CLA	F	403	29	1/1/11/20	5/15/91/115	-
21	CLA	10	707	18	1/1/11/20	7/19/95/115	-
21	CLA	2	509	10	1/1/14/20	5/36/112/115	-
21	CLA	1	507	29	1/1/12/20	2/21/97/115	-
21	CLA	9	909	25	1/1/10/20	3/13/89/115	-
21	CLA	1	505	9	1/1/14/20	9/33/109/115	-
21	CLA	A	835	1	-	5/15/91/115	-
21	CLA	9	912	17	1/1/11/20	3/15/91/115	-
21	CLA	A	809	1	1/1/15/20	14/39/115/115	-
21	CLA	12	502	19	1/1/11/20	4/15/91/115	-
25	LHG	6	917	21	-	11/32/32/53	-
21	CLA	A	822	29	-	11/39/115/115	-
28	DD6	2	518	-	-	2/26/80/80	0/3/3/3
21	CLA	A	829	1	1/1/15/20	17/39/115/115	-
21	CLA	6	913	14	1/1/11/20	5/15/91/115	-
21	CLA	8	605	16	1/1/11/20	2/15/91/115	-
21	CLA	11	704	29	1/1/11/20	0/15/91/115	-
21	CLA	2	517	-	1/1/11/20	1/15/91/115	-
21	CLA	B	827	2	1/1/15/20	12/39/115/115	-
21	CLA	3	704	29	1/1/10/20	1/12/88/115	-
21	CLA	A	828	1	1/1/15/20	11/39/115/115	-
22	PQN	B	840	-	-	4/21/41/43	0/2/2/2
21	CLA	A	840	1	1/1/11/20	8/18/94/115	-
21	CLA	3	703	11	1/1/11/20	4/15/91/115	-
28	DD6	1	519	-	-	2/26/80/80	0/3/3/3
21	CLA	5	706	13	1/1/11/20	1/15/91/115	-
21	CLA	6	907	29	-	1/18/94/115	-
21	CLA	A	807	1	1/1/15/20	9/39/115/115	-
21	CLA	7	711	15	1/1/15/20	7/39/115/115	-
21	CLA	A	810	1	-	14/39/115/115	-
21	CLA	5	711	13	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	708	25	1/1/10/20	3/13/89/115	-
21	CLA	A	823	1	-	3/15/91/115	-
28	DD6	5	713	-	-	5/26/80/80	0/3/3/3
21	CLA	6	903	14	1/1/11/20	6/18/94/115	-
25	LHG	A	853	-	-	19/53/53/53	-
25	LHG	4	714	21	-	7/19/19/53	-
21	CLA	11	709	19	1/1/11/20	3/15/91/115	-
21	CLA	A	834	1	1/1/11/20	4/15/91/115	-
21	CLA	11	703	19	1/1/15/20	13/39/115/115	-
21	CLA	A	818	1	1/1/12/20	11/26/102/115	-
28	DD6	8	615	-	-	12/26/80/80	0/3/3/3
21	CLA	2	510	25	1/1/10/20	3/13/89/115	-
21	CLA	8	612	16	-	11/39/115/115	-
21	CLA	6	909	14	1/1/14/20	4/36/112/115	-
25	LHG	11	714	21	-	11/34/34/53	-
28	DD6	5	712	-	-	3/26/80/80	0/3/3/3
21	CLA	5	710	13	-	6/21/97/115	-
21	CLA	B	807	2	1/1/15/20	11/39/115/115	-
21	CLA	B	810	2	1/1/11/20	3/15/91/115	-
21	CLA	A	821	1	1/1/14/20	12/35/111/115	-
21	CLA	B	809	2	1/1/11/20	4/15/91/115	-
21	CLA	7	709	25	1/1/10/20	2/13/89/115	-
21	CLA	9	903	17	1/1/14/20	5/33/109/115	-
21	CLA	11	701	19	1/1/10/20	2/10/86/115	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	7	707	15	1/1/11/20	2/18/94/115	-
24	BCR	A	851	-	-	0/29/63/63	0/2/2/2
23	SF4	C	101	3	-	-	0/6/5/5
21	CLA	B	811	2	-	3/15/91/115	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2
28	DD6	3	716	-	-	4/26/80/80	0/3/3/3
28	DD6	9	915	-	-	12/26/80/80	0/3/3/3
21	CLA	1	506	9	1/1/11/20	4/15/91/115	-
28	DD6	1	520	-	-	14/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	610	25	1/1/10/20	3/13/89/115	-
21	CLA	7	704	15	1/1/11/20	2/15/91/115	-
24	BCR	M	102	-	-	2/29/63/63	0/2/2/2
21	CLA	3	705	29	1/1/11/20	2/18/94/115	-
21	CLA	3	713	11	1/1/11/20	5/15/91/115	-
21	CLA	A	826	29	1/1/15/20	13/39/115/115	-
21	CLA	8	608	16	1/1/11/20	1/18/94/115	-
24	BCR	A	848	-	-	6/29/63/63	0/2/2/2
21	CLA	4	701	-	-	2/10/86/115	-
21	CLA	10	709	18	1/1/11/20	2/15/91/115	-
21	CLA	1	504	9	1/1/10/20	1/12/88/115	-
21	CLA	B	839	25	1/1/15/20	14/39/115/115	-
21	CLA	8	603	16	1/1/11/20	6/18/94/115	-

The worst 5 of 4696 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	801	CL0	C1D-C2D	8.79	1.49	1.39
20	A	801	CL0	C3A-C2A	-8.57	1.47	1.54
20	A	801	CL0	CBD-CGD	-8.05	1.42	1.52
21	A	807	CLA	C1B-NB	-7.57	1.27	1.37
21	B	801	CLA	C1B-NB	-7.52	1.28	1.37

The worst 5 of 7891 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	801	CL0	O2D-CGD-CBD	13.44	125.72	110.95
21	A	834	CLA	C1D-ND-C4D	-12.01	97.88	106.31
21	A	827	CLA	C1D-ND-C4D	-11.88	97.98	106.31
21	9	907	CLA	C1D-ND-C4D	-11.74	98.07	106.31
21	A	823	CLA	C1D-ND-C4D	-11.49	98.25	106.31

5 of 198 chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
21	A	804	CLA	ND

5 of 1751 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	804	CLA	C1A-C2A-CAA-CBA
21	A	804	CLA	CHA-CBD-CGD-O1D
21	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

214 monomers are involved in 397 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	7	713	CLA	3	0
21	A	811	CLA	1	0
21	B	818	CLA	1	0
21	B	834	CLA	2	0
21	B	816	CLA	3	0
21	3	715	CLA	1	0
21	B	826	CLA	2	0
21	B	812	CLA	2	0
21	8	604	CLA	2	0
21	8	611	CLA	1	0
21	12	505	CLA	1	0
28	1	518	DD6	1	0
28	6	915	DD6	1	0
24	A	847	BCR	3	0
21	1	513	CLA	2	0
21	A	831	CLA	3	0
21	3	708	CLA	2	0
21	A	808	CLA	1	0
21	9	907	CLA	1	0
21	9	902	CLA	2	0
21	7	708	CLA	4	0
21	10	704	CLA	2	0
21	A	837	CLA	1	0
21	A	802	CLA	2	0
21	3	710	CLA	2	0
21	5	702	CLA	2	0
21	13	501	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	101	CLA	1	0
21	B	831	CLA	6	0
21	B	839	CLA	2	0
21	11	708	CLA	1	0
21	3	712	CLA	1	0
21	8	607	CLA	1	0
21	7	710	CLA	1	0
21	B	805	CLA	1	0
21	9	910	CLA	2	0
21	2	503	CLA	2	0
21	A	830	CLA	2	0
21	A	806	CLA	2	0
21	A	843	CLA	1	0
21	6	914	CLA	1	0
24	F	405	BCR	4	0
21	F	404	CLA	1	0
21	A	824	CLA	1	0
24	A	849	BCR	3	0
21	2	508	CLA	2	0
21	4	708	CLA	2	0
21	6	910	CLA	2	0
21	2	504	CLA	1	0
21	B	823	CLA	3	0
21	3	714	CLA	1	0
21	4	706	CLA	1	0
21	A	820	CLA	3	0
21	B	806	CLA	1	0
21	4	709	CLA	1	0
21	A	805	CLA	1	0
21	1	509	CLA	1	0
21	2	506	CLA	1	0
21	A	803	CLA	5	0
21	A	812	CLA	2	0
21	1	514	CLA	2	0
21	13	502	CLA	1	0
21	B	825	CLA	2	0
21	7	703	CLA	3	0
21	A	862	CLA	7	0
21	10	711	CLA	1	0
21	11	710	CLA	1	0
21	8	609	CLA	2	0
21	A	819	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	827	CLA	1	0
21	1	508	CLA	2	0
21	5	709	CLA	1	0
21	1	511	CLA	1	0
21	2	513	CLA	2	0
21	3	706	CLA	2	0
21	F	401	CLA	2	0
21	10	712	CLA	2	0
21	B	828	CLA	2	0
21	1	510	CLA	1	0
21	7	714	CLA	1	0
21	9	913	CLA	3	0
21	A	844	CLA	5	0
21	3	709	CLA	1	0
24	B	845	BCR	6	0
21	A	841	CLA	1	0
21	A	842	CLA	5	0
21	5	707	CLA	5	0
21	A	833	CLA	3	0
21	A	838	CLA	1	0
21	B	801	CLA	2	0
21	13	503	CLA	1	0
21	A	839	CLA	4	0
21	4	710	CLA	2	0
25	3	719	LHG	1	0
21	1	512	CLA	1	0
21	A	832	CLA	1	0
24	B	844	BCR	2	0
27	B	847	DGD	3	0
21	B	804	CLA	3	0
21	B	833	CLA	1	0
21	1	516	CLA	2	0
21	A	836	CLA	1	0
21	B	838	CLA	2	0
21	6	911	CLA	2	0
21	12	508	CLA	1	0
21	B	803	CLA	2	0
21	3	701	CLA	2	0
22	A	845	PQN	2	0
28	4	712	DD6	2	0
21	7	705	CLA	1	0
21	2	514	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	707	CLA	3	0
21	A	813	CLA	2	0
21	12	506	CLA	4	0
25	2	521	LHG	1	0
21	A	804	CLA	3	0
28	11	713	DD6	1	0
21	A	817	CLA	3	0
21	10	706	CLA	2	0
21	B	815	CLA	2	0
21	6	904	CLA	2	0
21	11	707	CLA	3	0
21	12	504	CLA	4	0
24	J	102	BCR	7	0
21	3	702	CLA	1	0
21	A	825	CLA	1	0
21	6	908	CLA	1	0
21	1	517	CLA	3	0
21	2	505	CLA	3	0
21	4	711	CLA	2	0
21	6	912	CLA	1	0
24	A	850	BCR	1	0
24	B	841	BCR	3	0
21	12	507	CLA	1	0
21	B	829	CLA	5	0
21	2	515	CLA	1	0
24	B	842	BCR	2	0
21	B	819	CLA	1	0
21	1	515	CLA	2	0
21	3	711	CLA	1	0
21	B	835	CLA	8	0
21	9	911	CLA	1	0
21	8	613	CLA	1	0
21	B	830	CLA	3	0
21	10	708	CLA	1	0
21	4	704	CLA	1	0
24	F	402	BCR	1	0
21	B	802	CLA	2	0
21	11	711	CLA	1	0
21	2	507	CLA	4	0
21	B	824	CLA	1	0
21	B	817	CLA	1	0
21	9	914	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	821	CLA	1	0
21	4	702	CLA	2	0
21	11	705	CLA	2	0
21	2	511	CLA	6	0
21	5	701	CLA	1	0
21	F	403	CLA	2	0
21	10	707	CLA	2	0
21	A	835	CLA	1	0
21	1	507	CLA	2	0
21	2	509	CLA	4	0
21	1	505	CLA	2	0
21	9	909	CLA	1	0
21	A	809	CLA	2	0
21	12	502	CLA	1	0
21	A	822	CLA	1	0
21	A	829	CLA	6	0
21	6	913	CLA	1	0
21	2	517	CLA	1	0
21	B	827	CLA	4	0
21	3	704	CLA	1	0
21	A	828	CLA	2	0
21	A	840	CLA	1	0
21	3	703	CLA	1	0
21	5	706	CLA	2	0
21	6	907	CLA	1	0
21	A	807	CLA	2	0
21	A	810	CLA	4	0
21	5	711	CLA	1	0
21	5	708	CLA	2	0
21	A	823	CLA	3	0
21	6	903	CLA	1	0
25	A	853	LHG	1	0
25	4	714	LHG	3	0
21	11	709	CLA	1	0
21	A	834	CLA	1	0
21	11	703	CLA	3	0
21	A	818	CLA	2	0
21	2	510	CLA	4	0
21	8	612	CLA	3	0
21	6	909	CLA	2	0
21	B	807	CLA	2	0
21	A	821	CLA	4	0

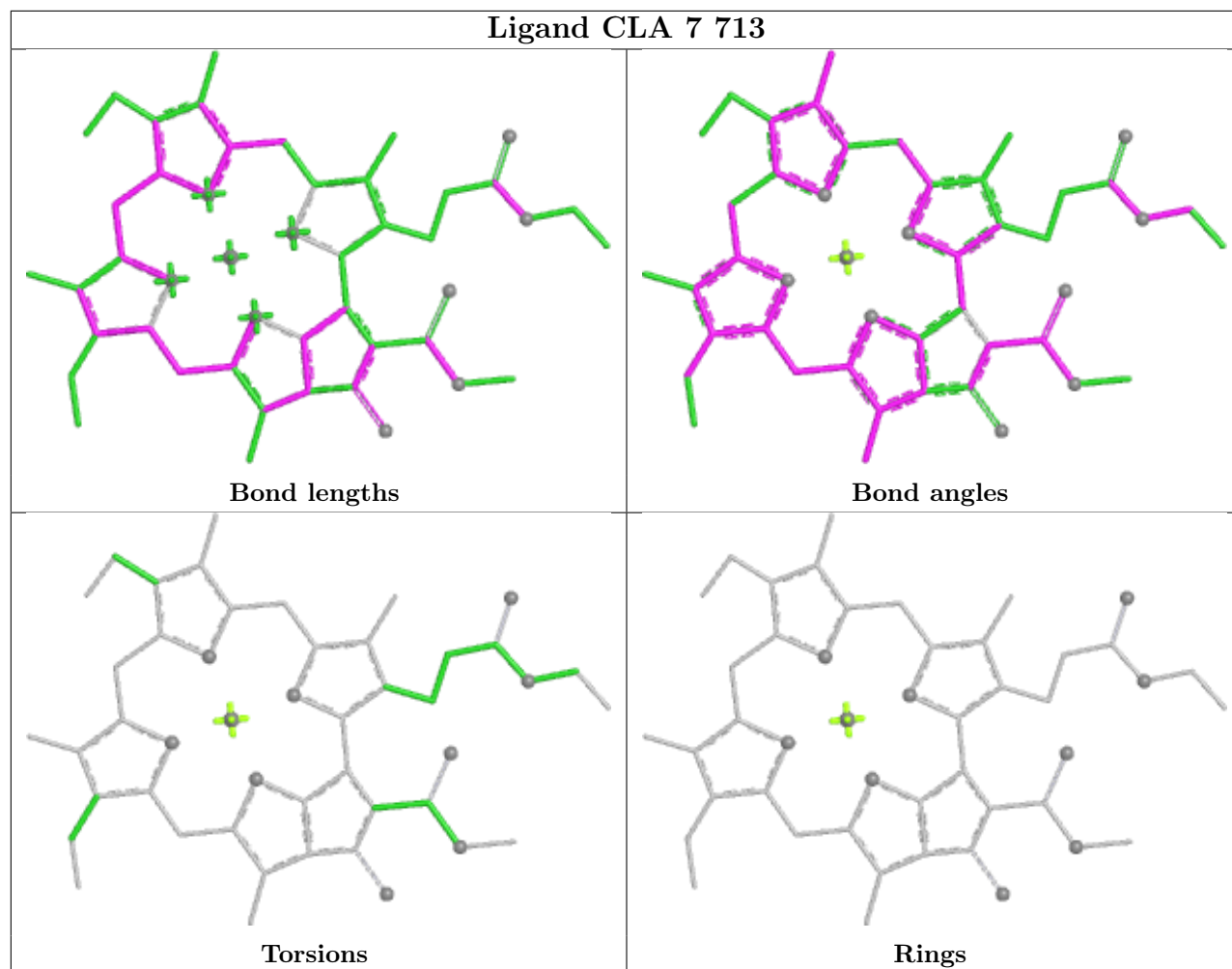
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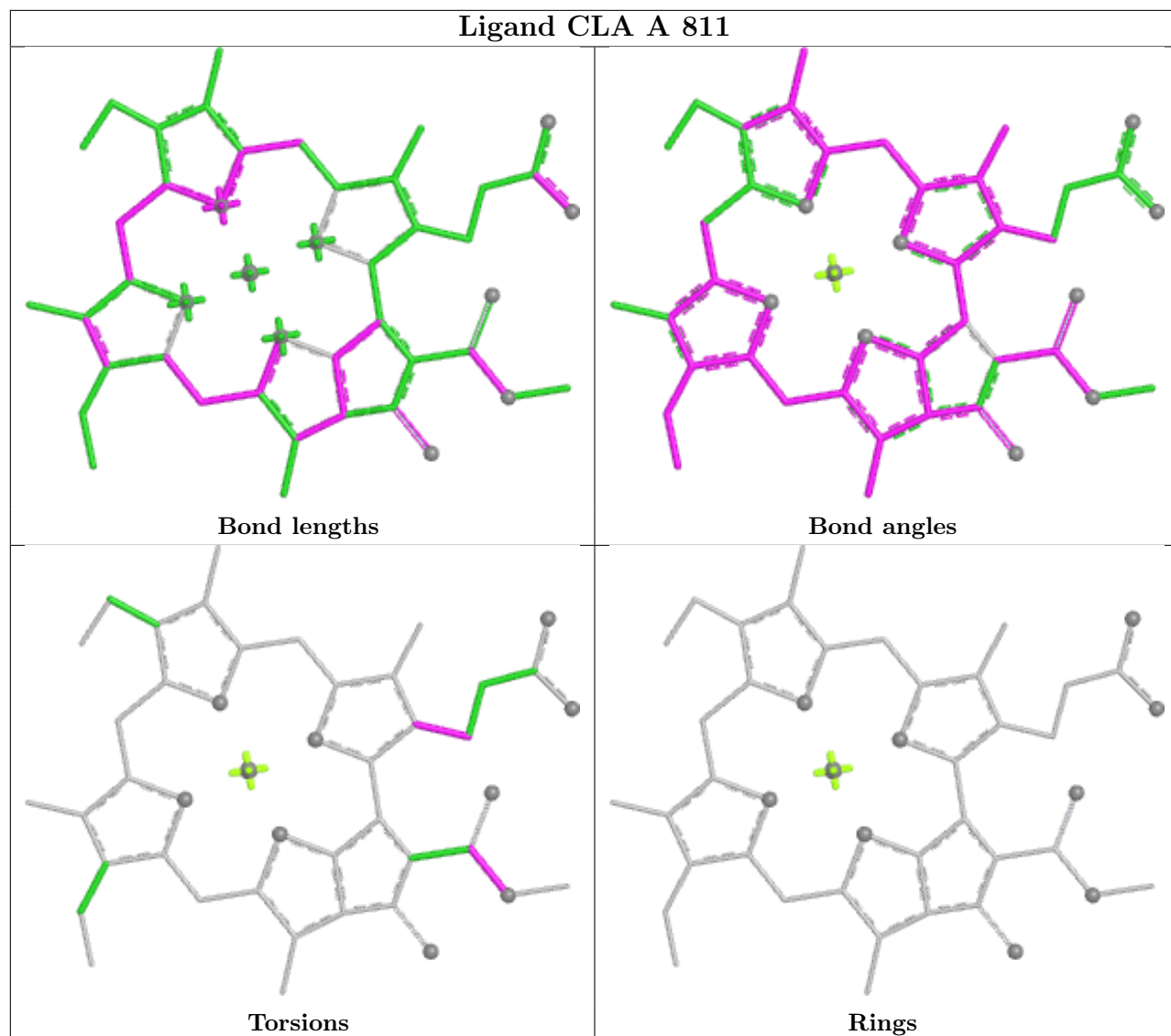
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	11	701	CLA	1	0
24	A	852	BCR	9	0
21	7	707	CLA	1	0
24	A	851	BCR	3	0
21	B	811	CLA	1	0
24	J	103	BCR	1	0
28	3	716	DD6	1	0
21	1	506	CLA	1	0
24	M	102	BCR	2	0
21	3	705	CLA	2	0
21	3	713	CLA	1	0
21	A	826	CLA	3	0
24	A	848	BCR	3	0
21	4	701	CLA	3	0
21	10	709	CLA	1	0
21	1	504	CLA	2	0
20	A	801	CL0	2	0
21	8	603	CLA	1	0

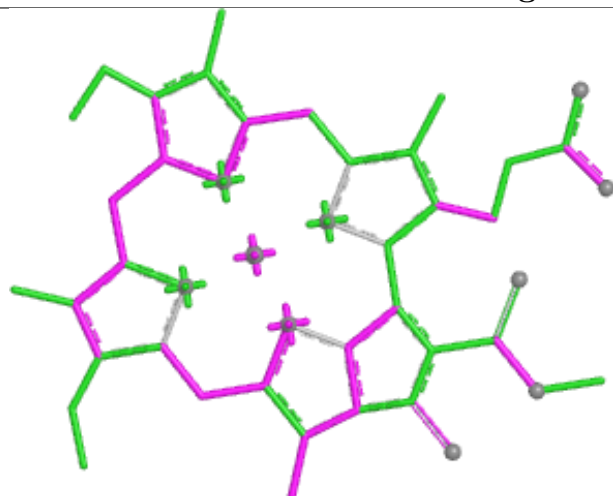
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA 7 713

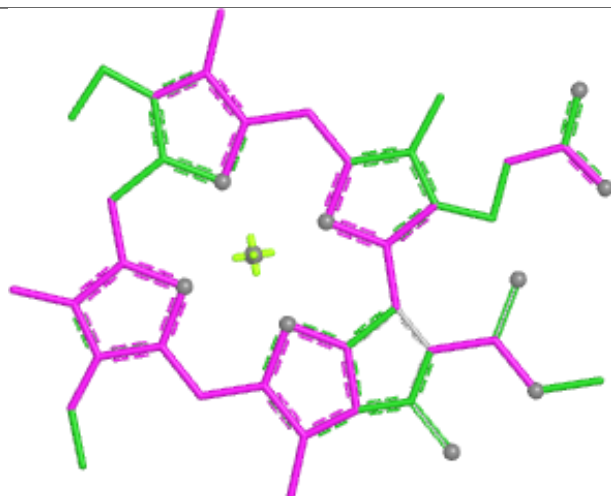




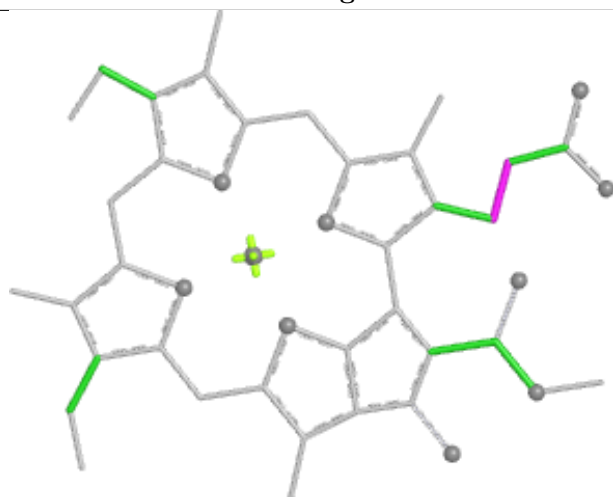
Ligand CLA 2 516



Bond lengths



Bond angles

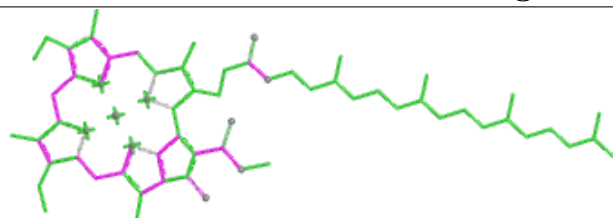


Torsions

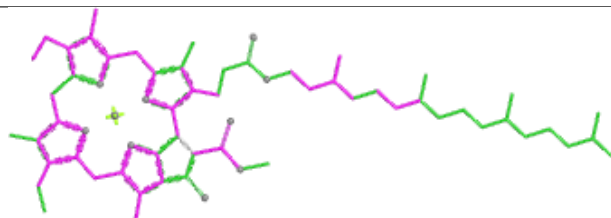


Rings

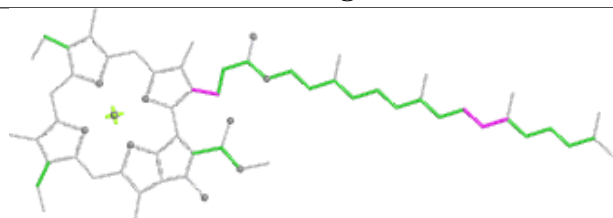
Ligand CLA B 818



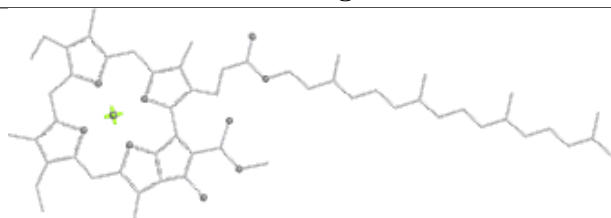
Bond lengths



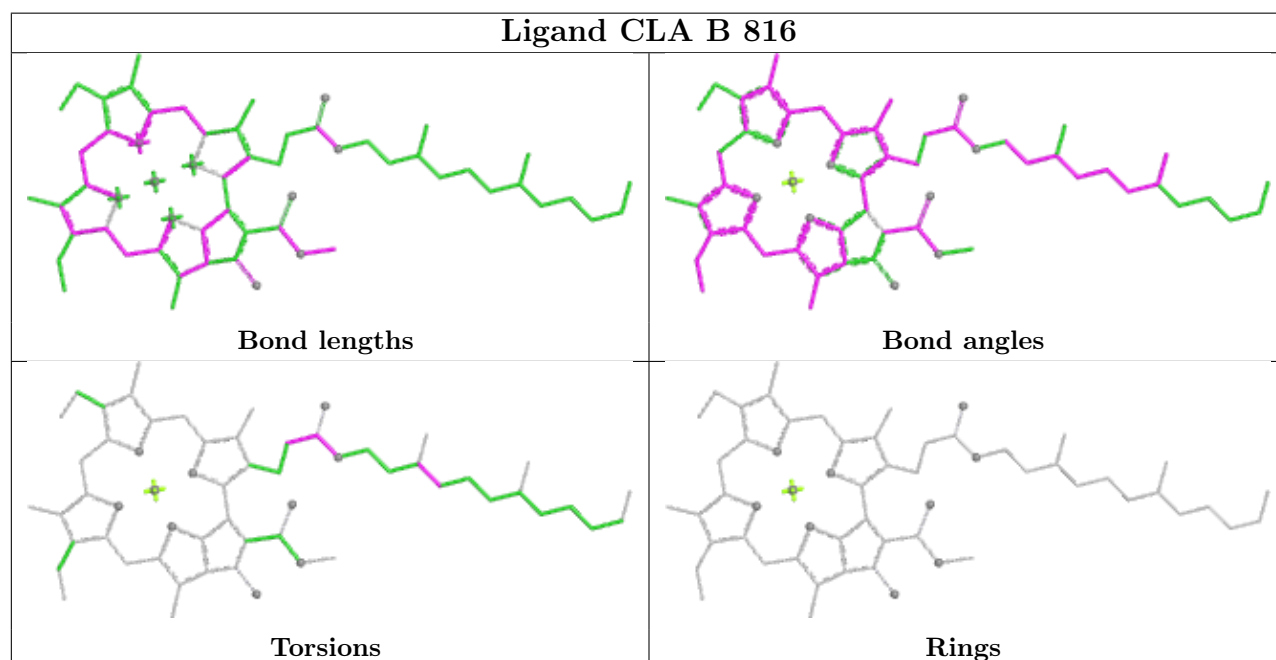
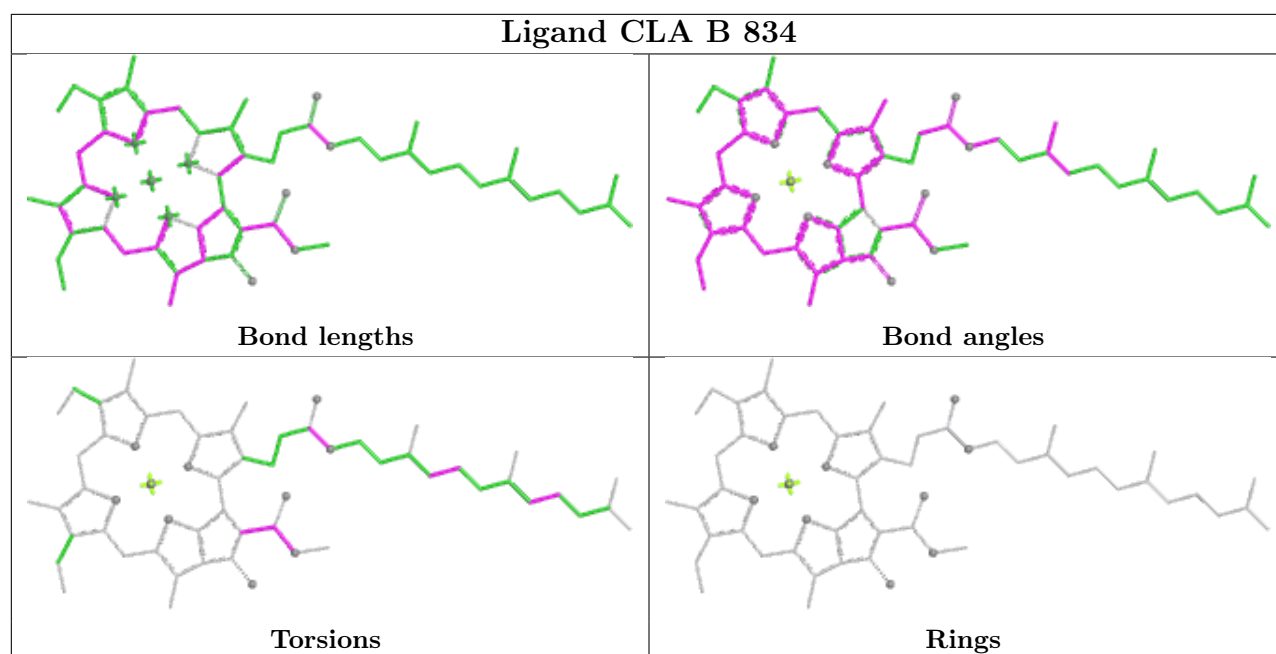
Bond angles



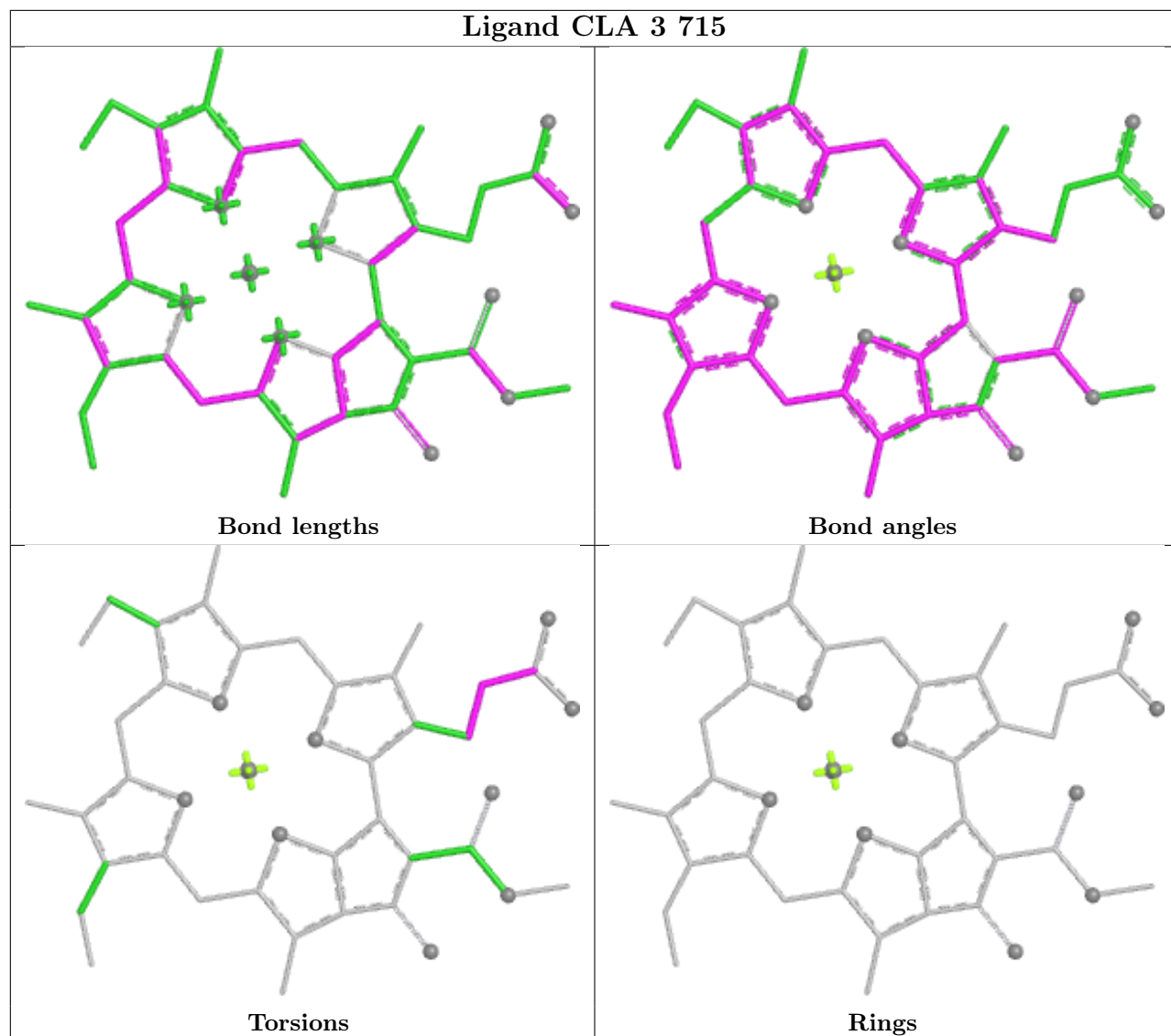
Torsions



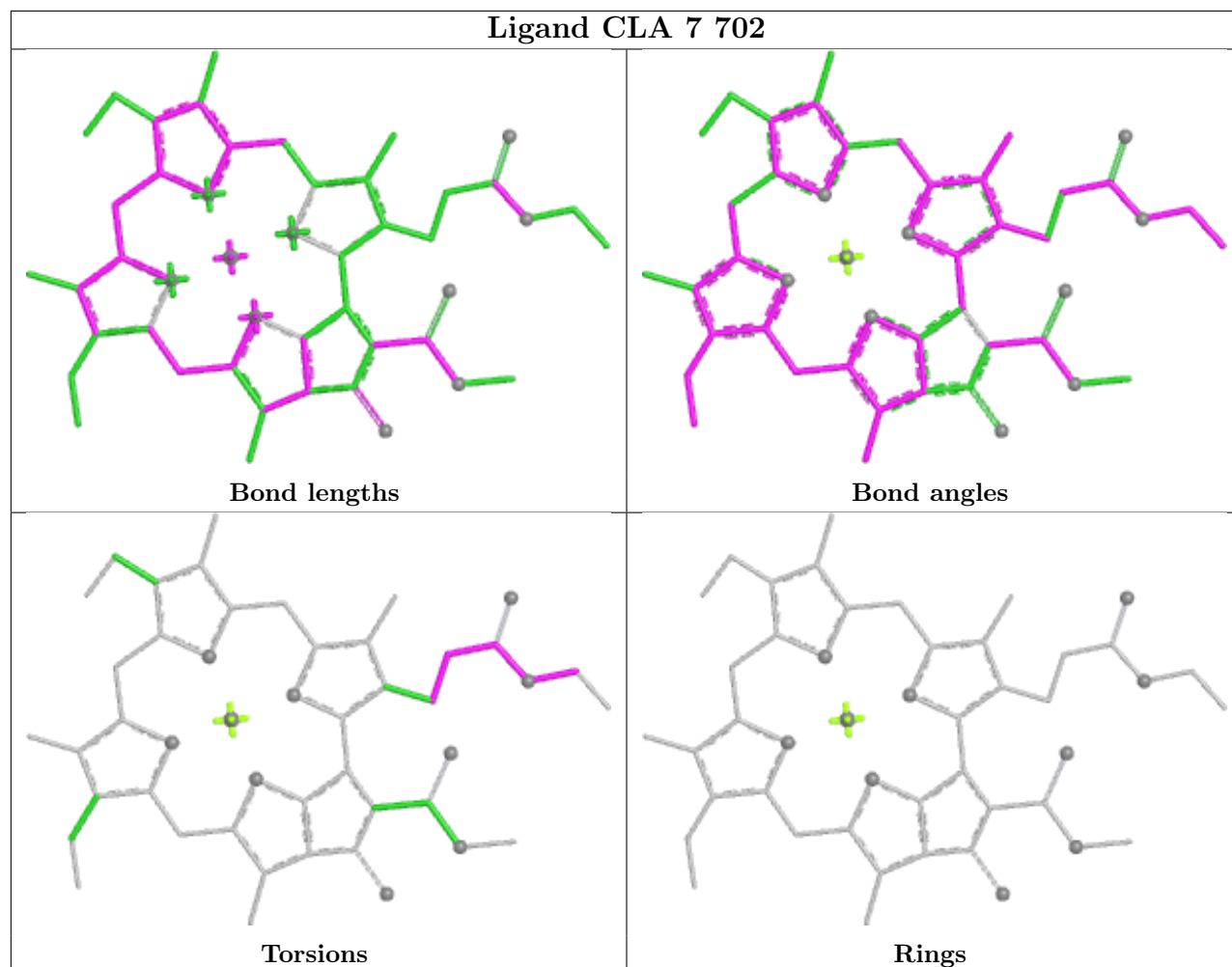
Rings



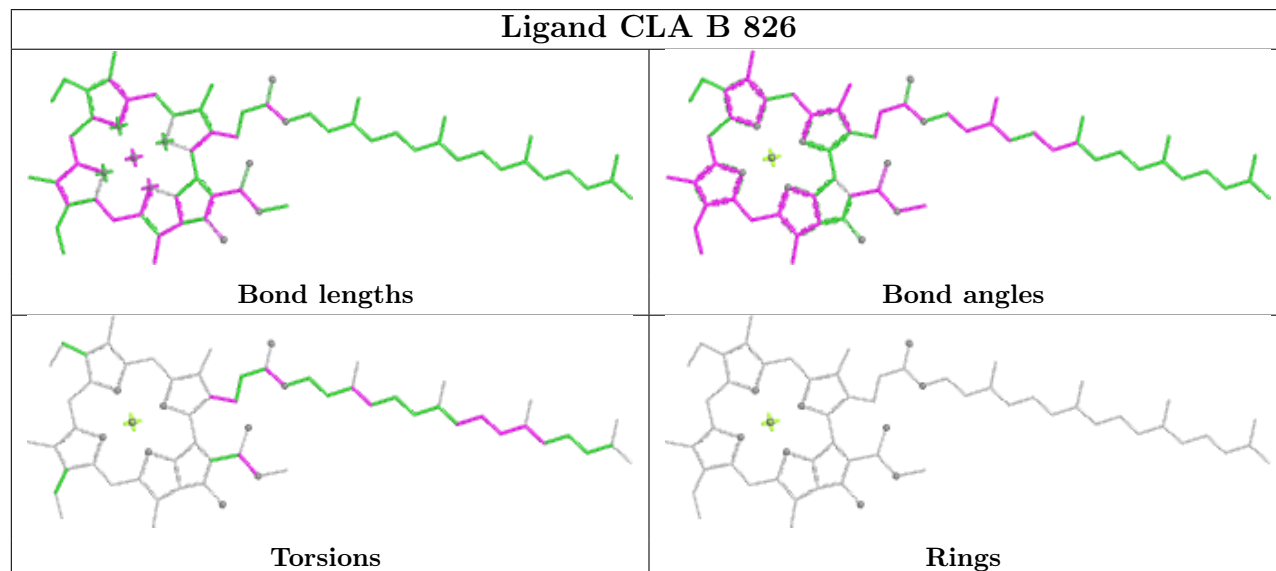
Ligand CLA 3 715



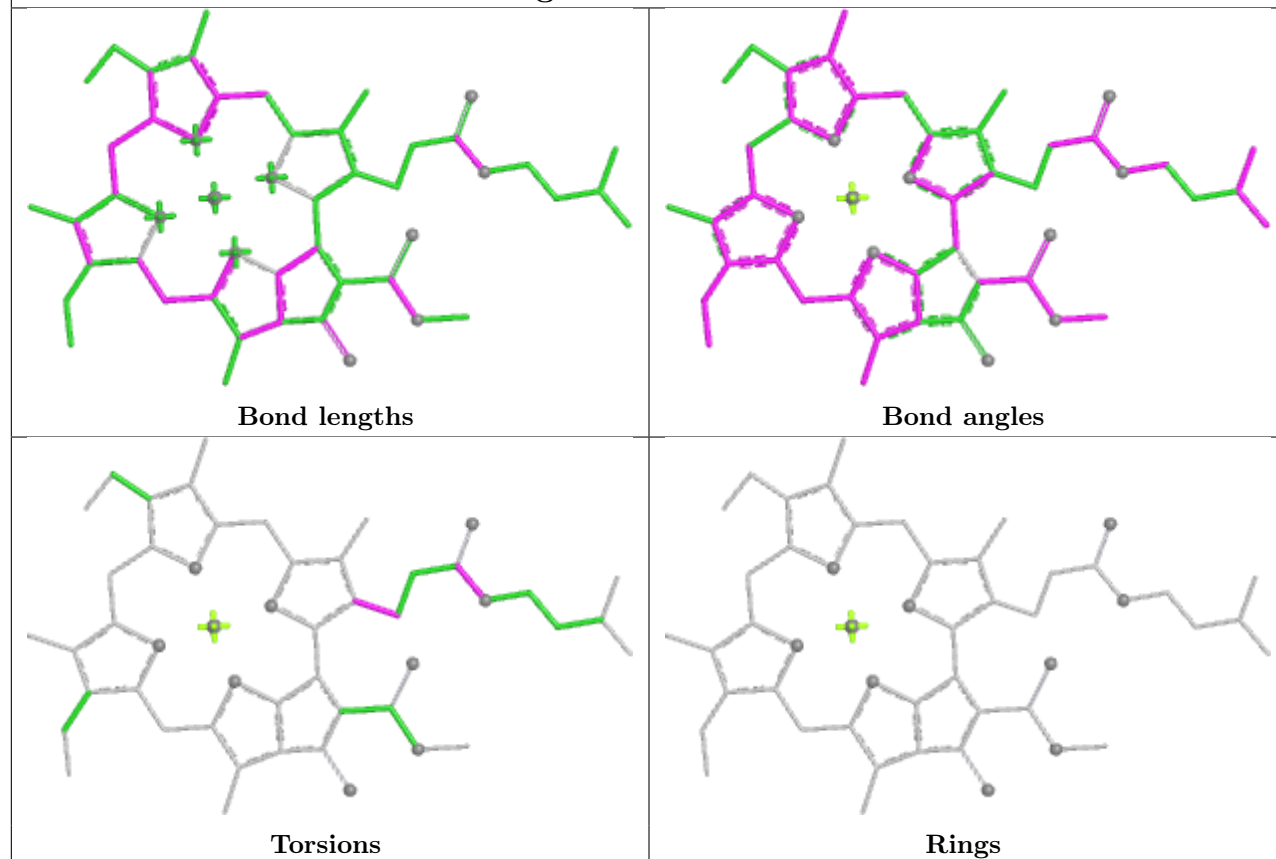
Ligand CLA 7 702



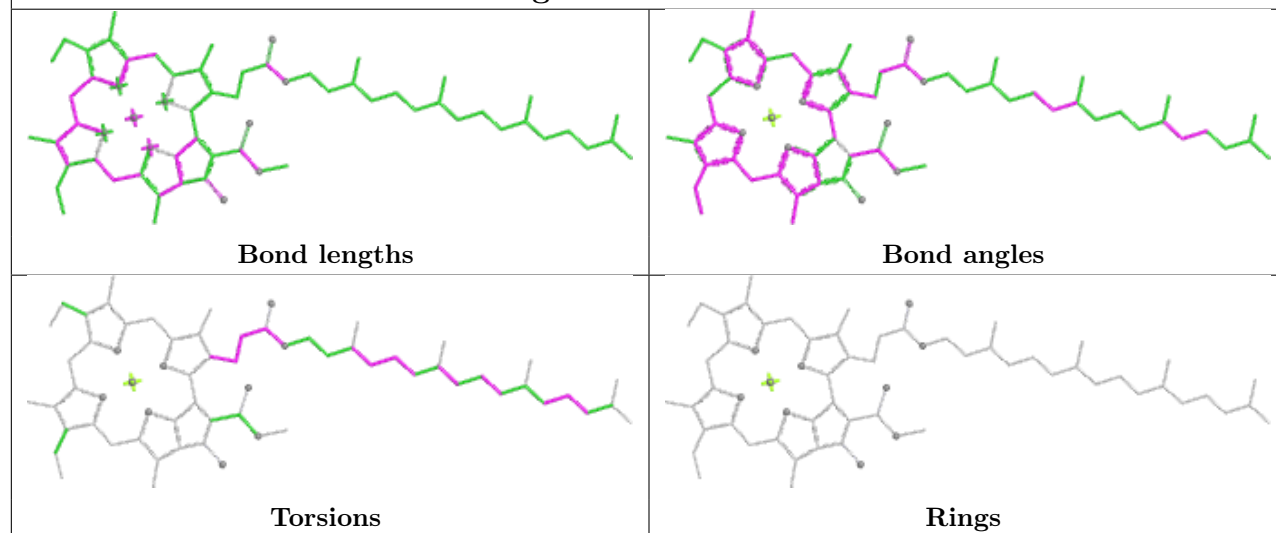
Ligand CLA B 826



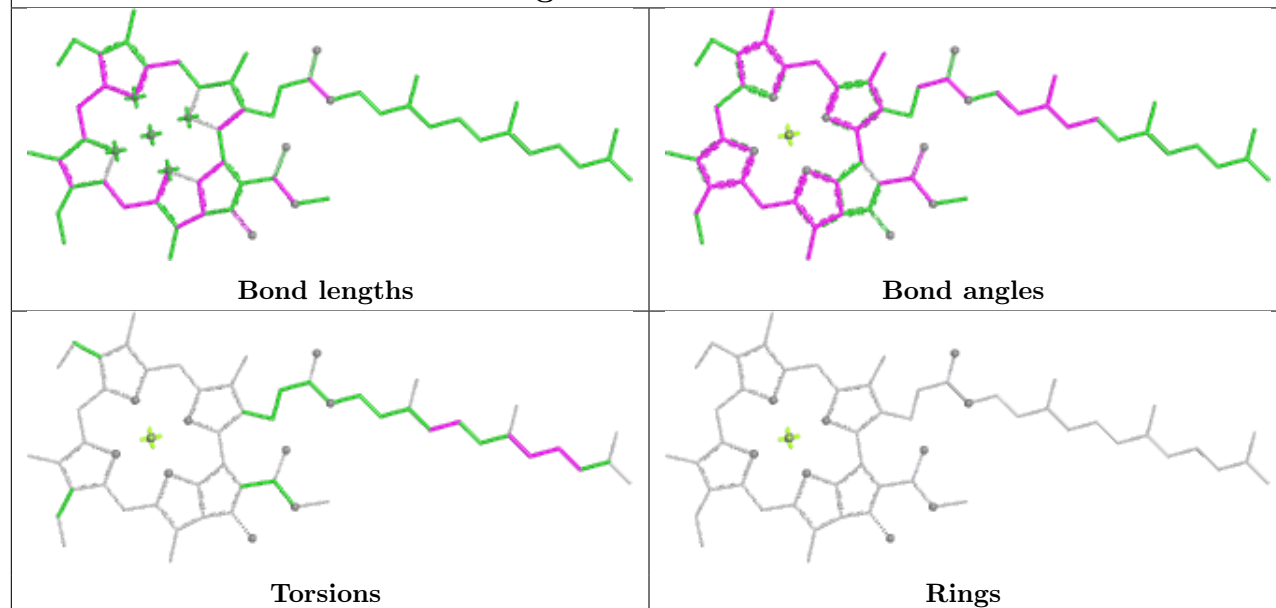
Ligand CLA 5 704



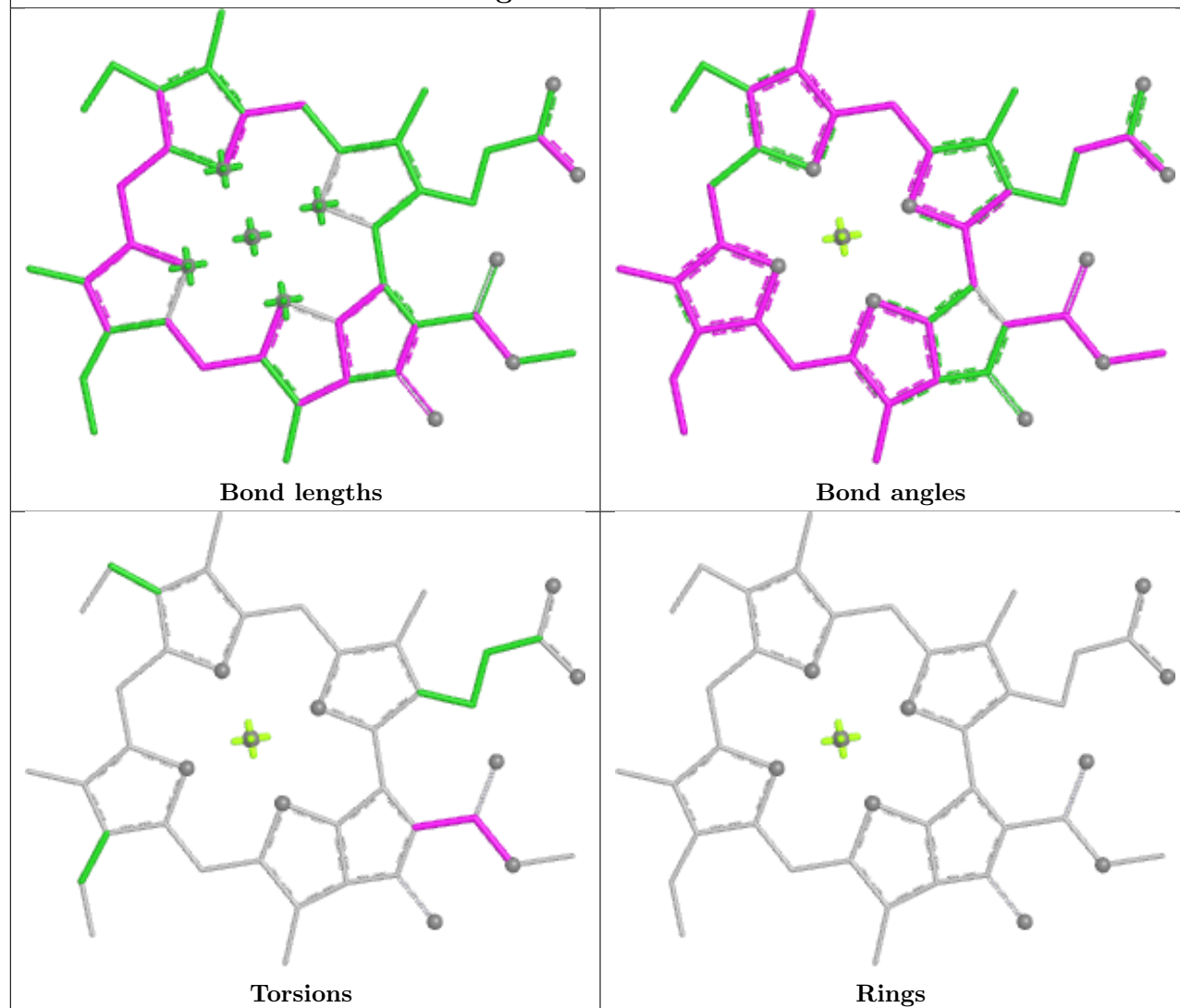
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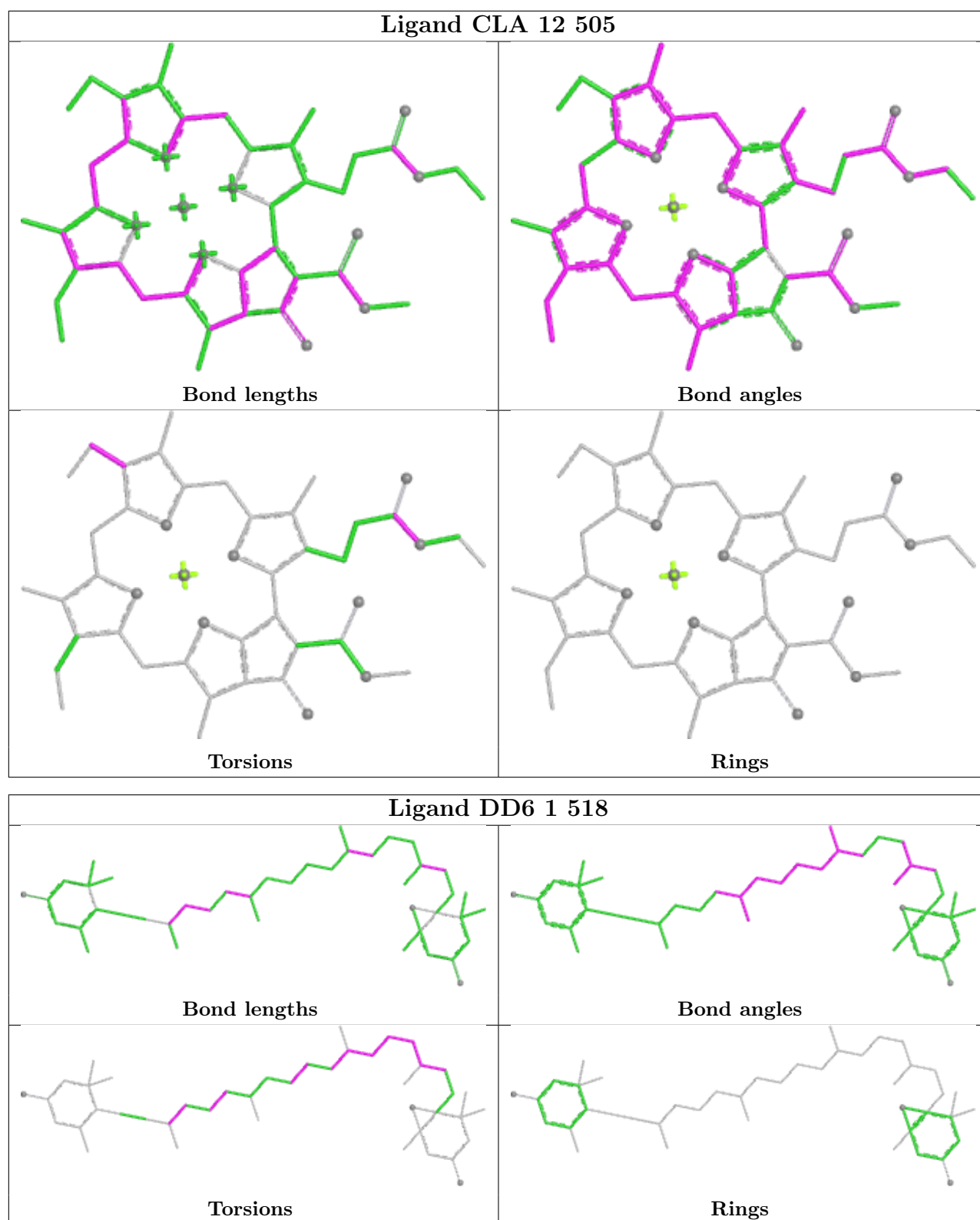


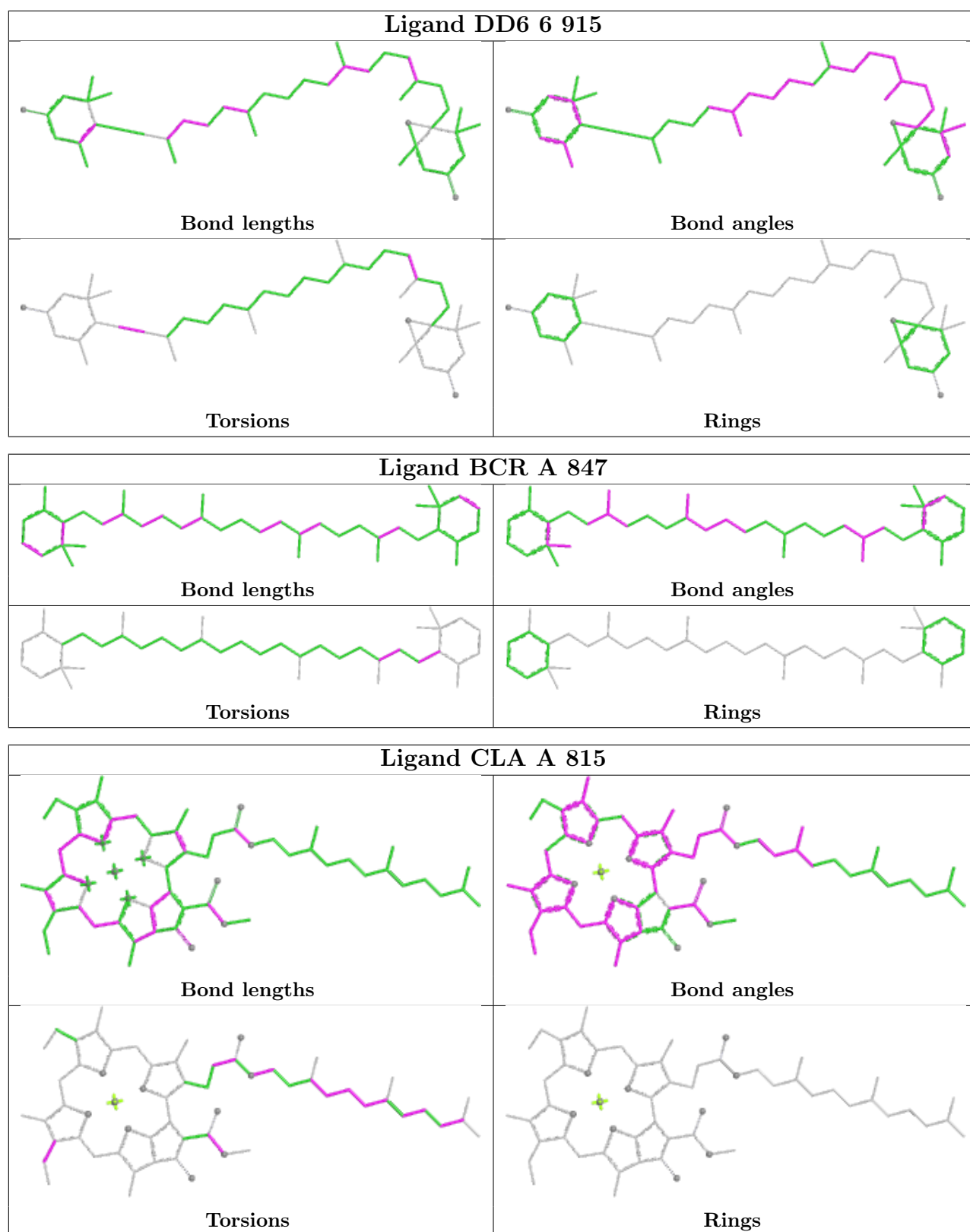
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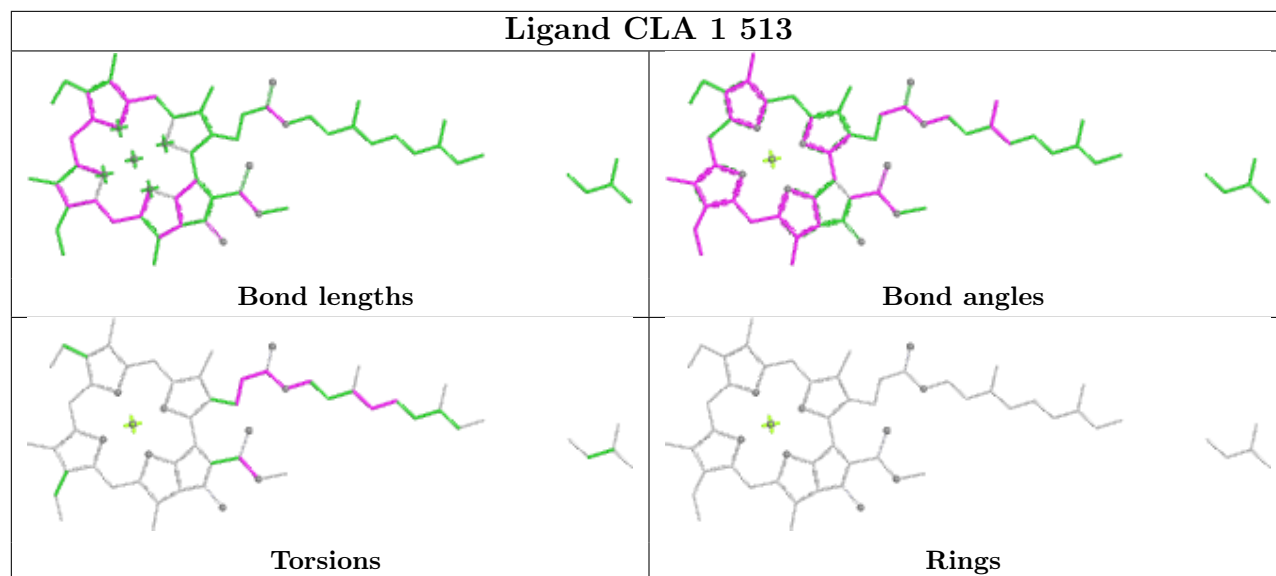
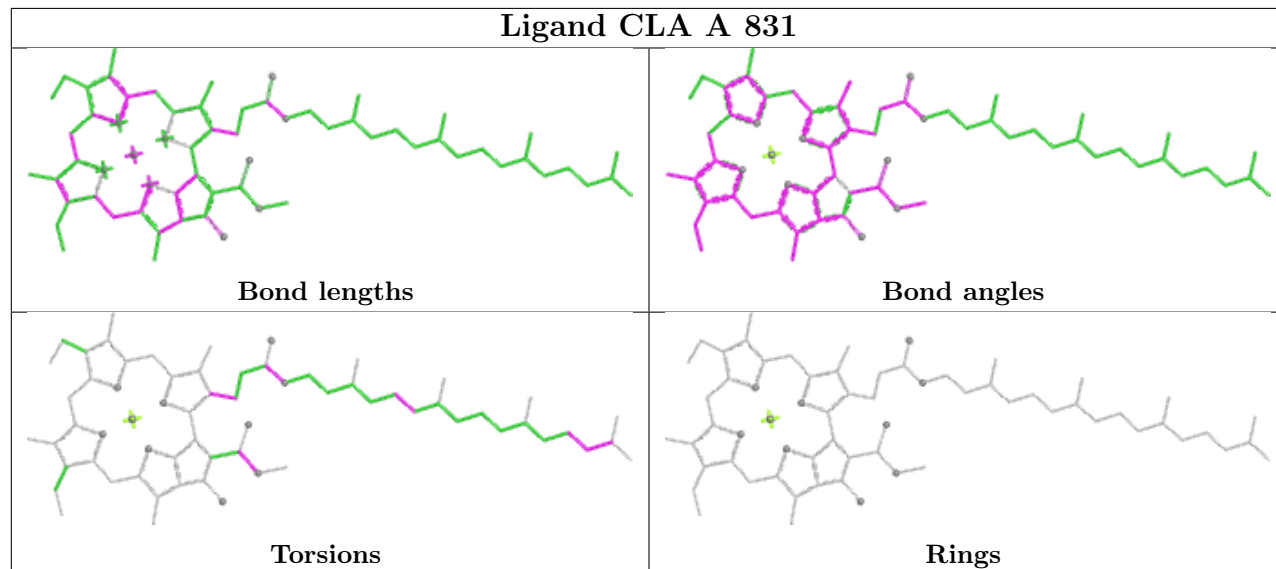


Ligand CLA 8 611

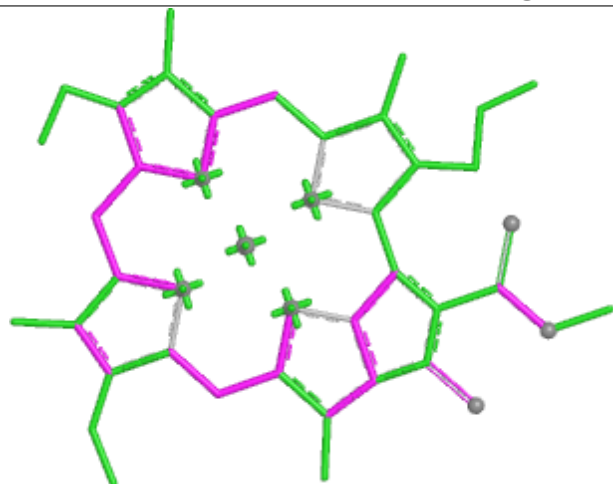




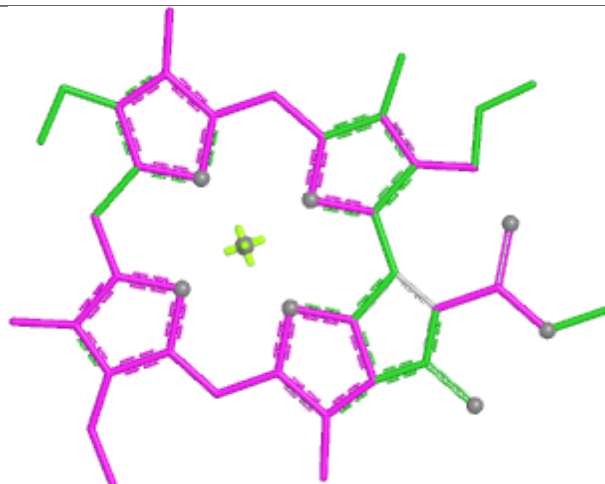


Ligand CLA 1 513**Ligand CLA A 831**

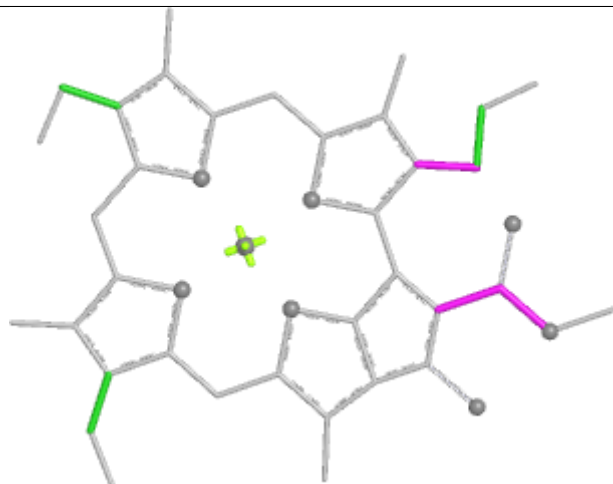
Ligand CLA 3 708



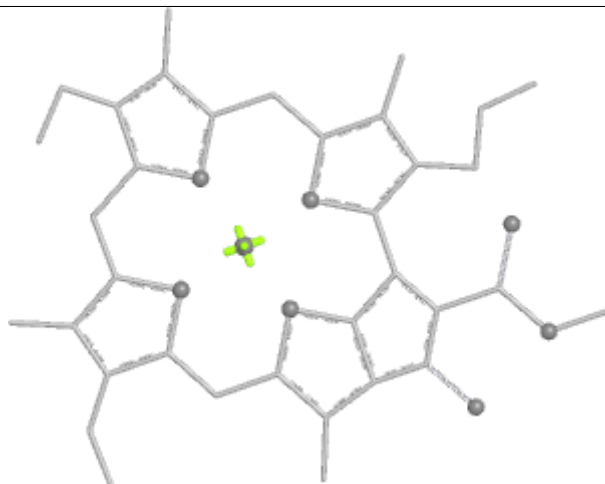
Bond lengths



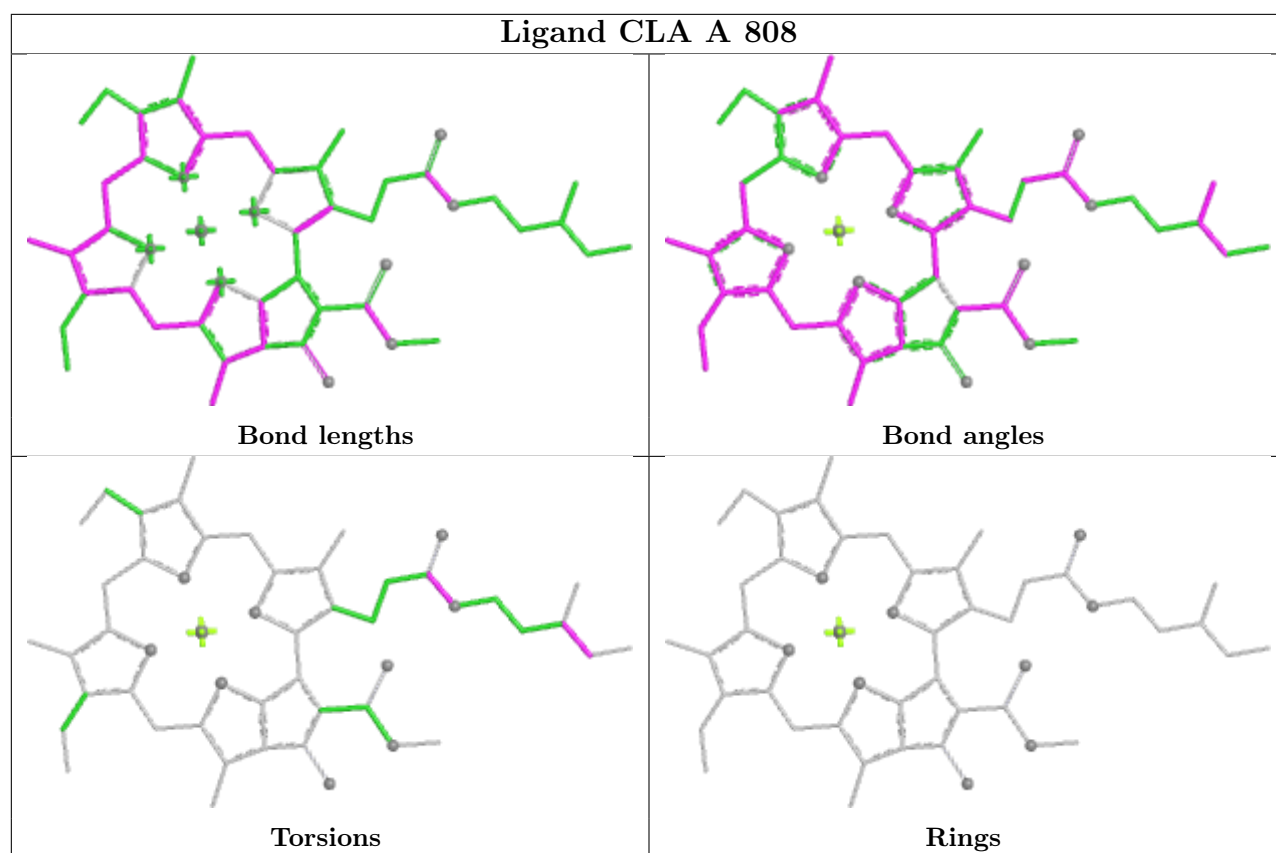
Bond angles



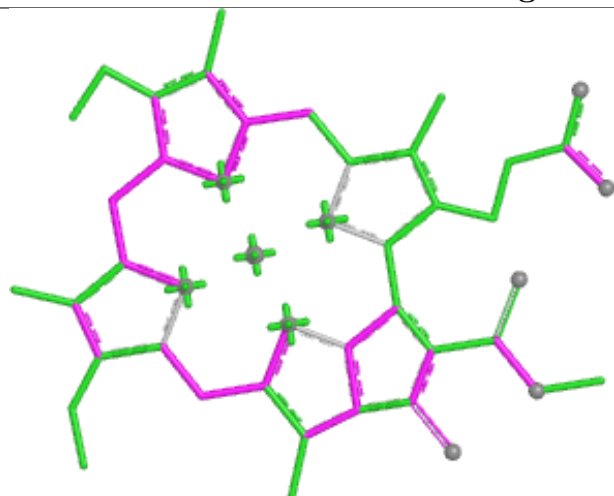
Torsions



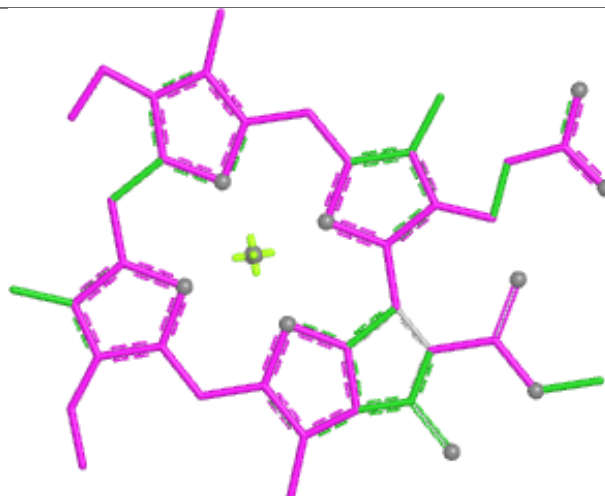
Rings



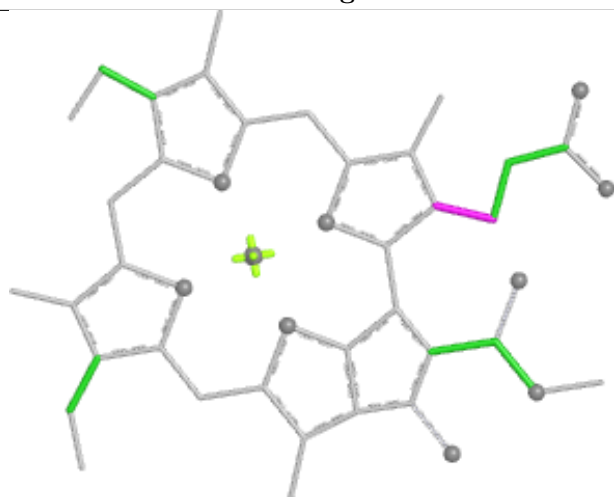
Ligand CLA 7 712



Bond lengths



Bond angles

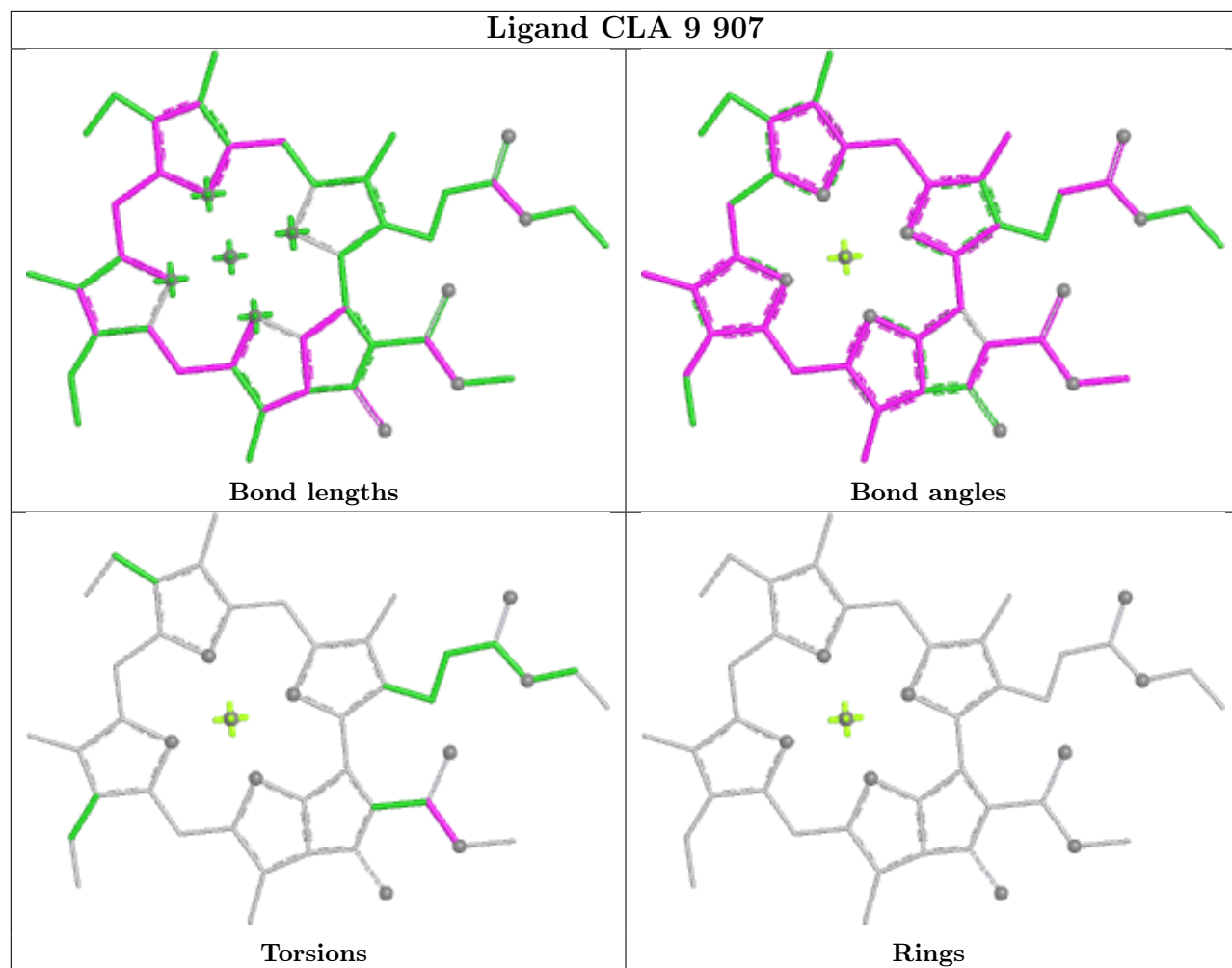


Torsions

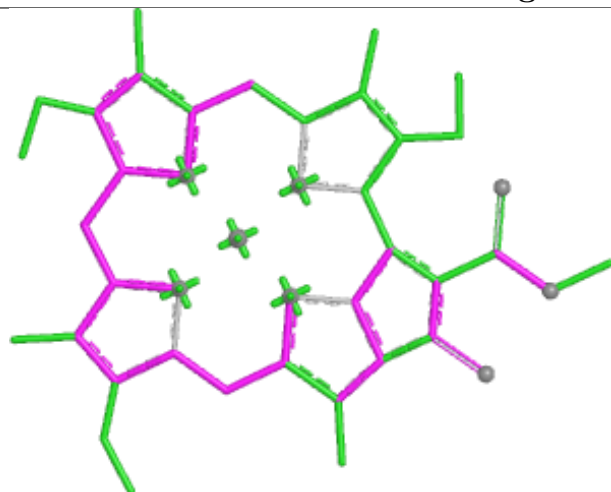


Rings

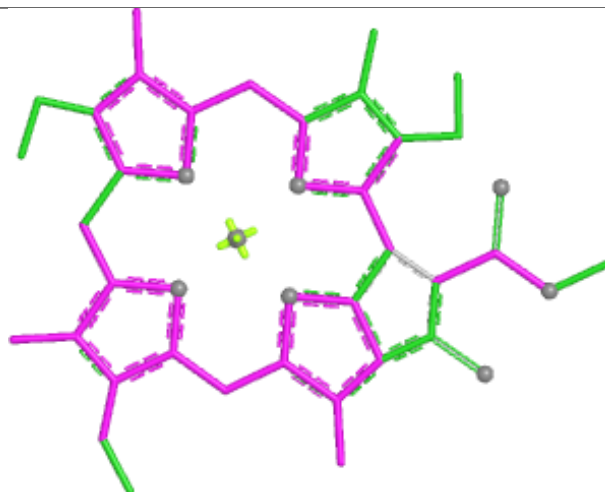
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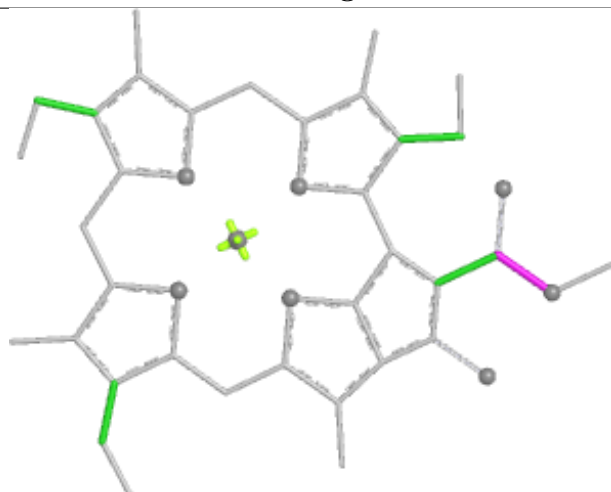
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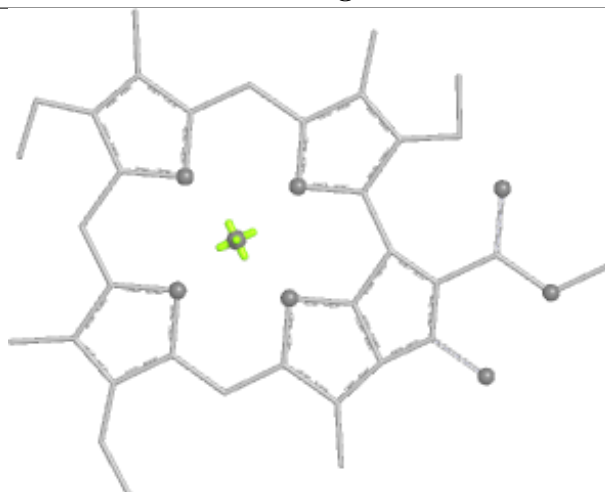
Bond lengths



Bond angles

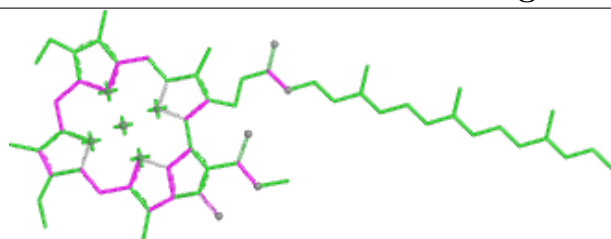


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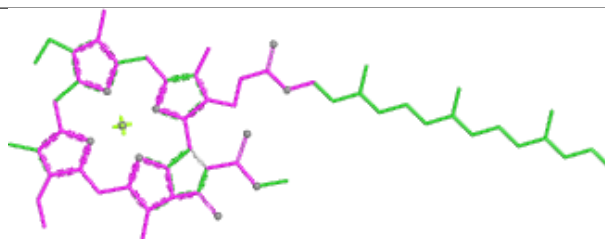


Rings

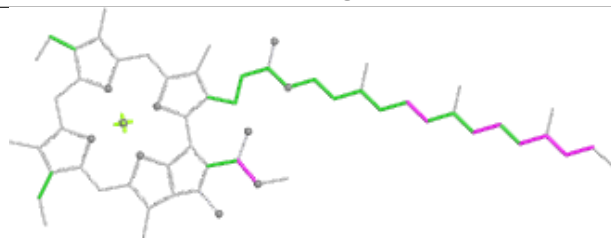
Ligand CLA 7 708



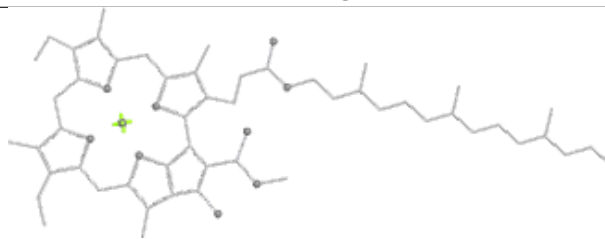
Bond lengths



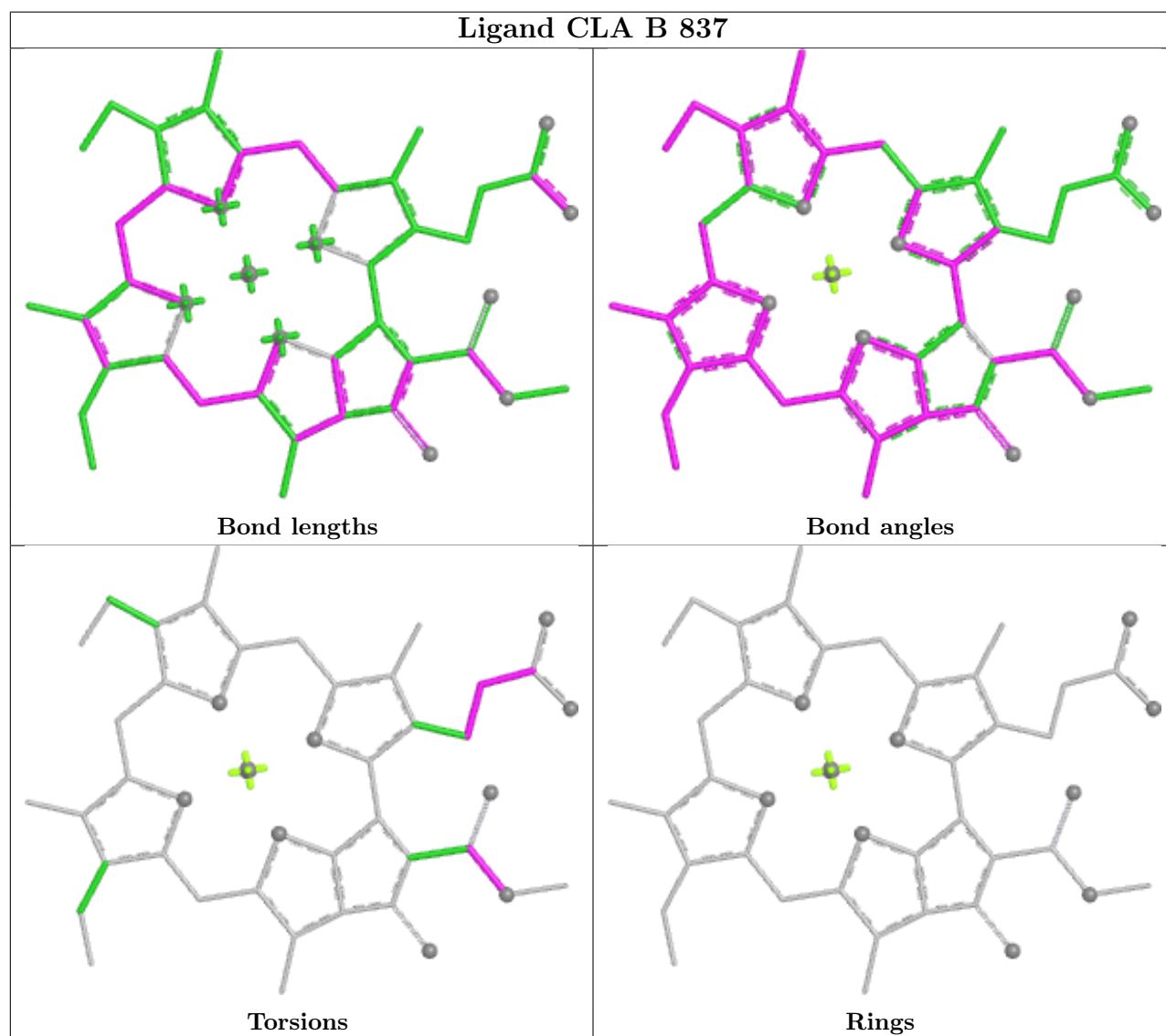
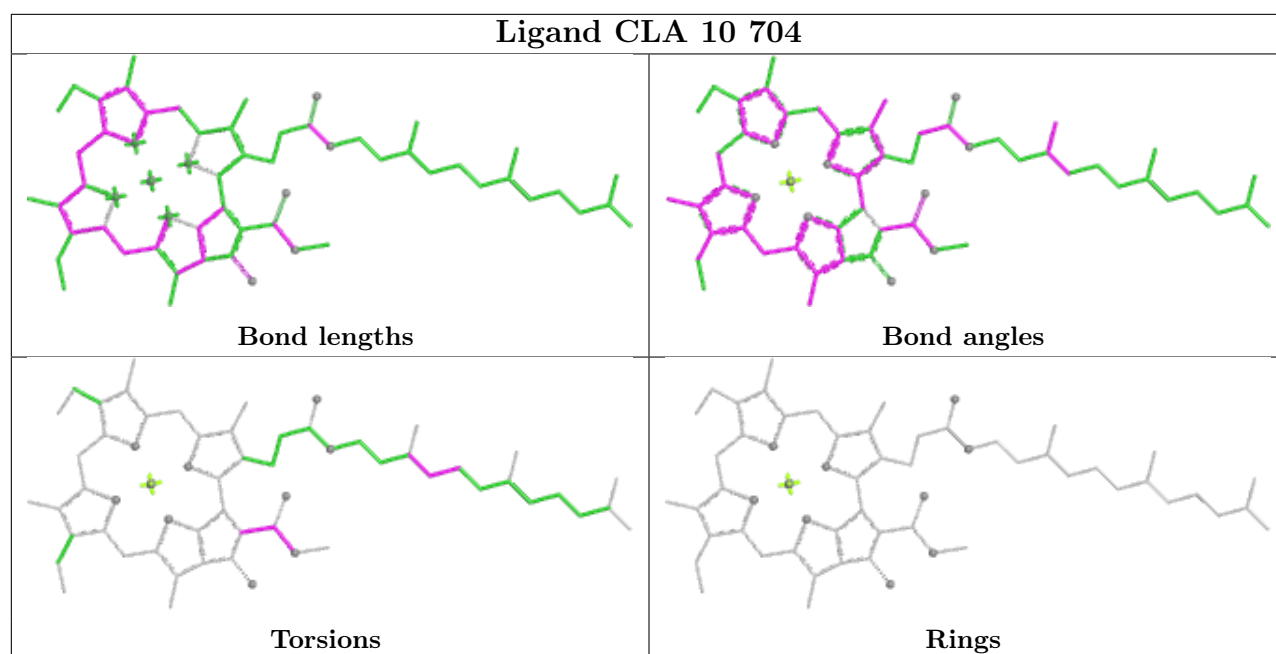
Bond angles

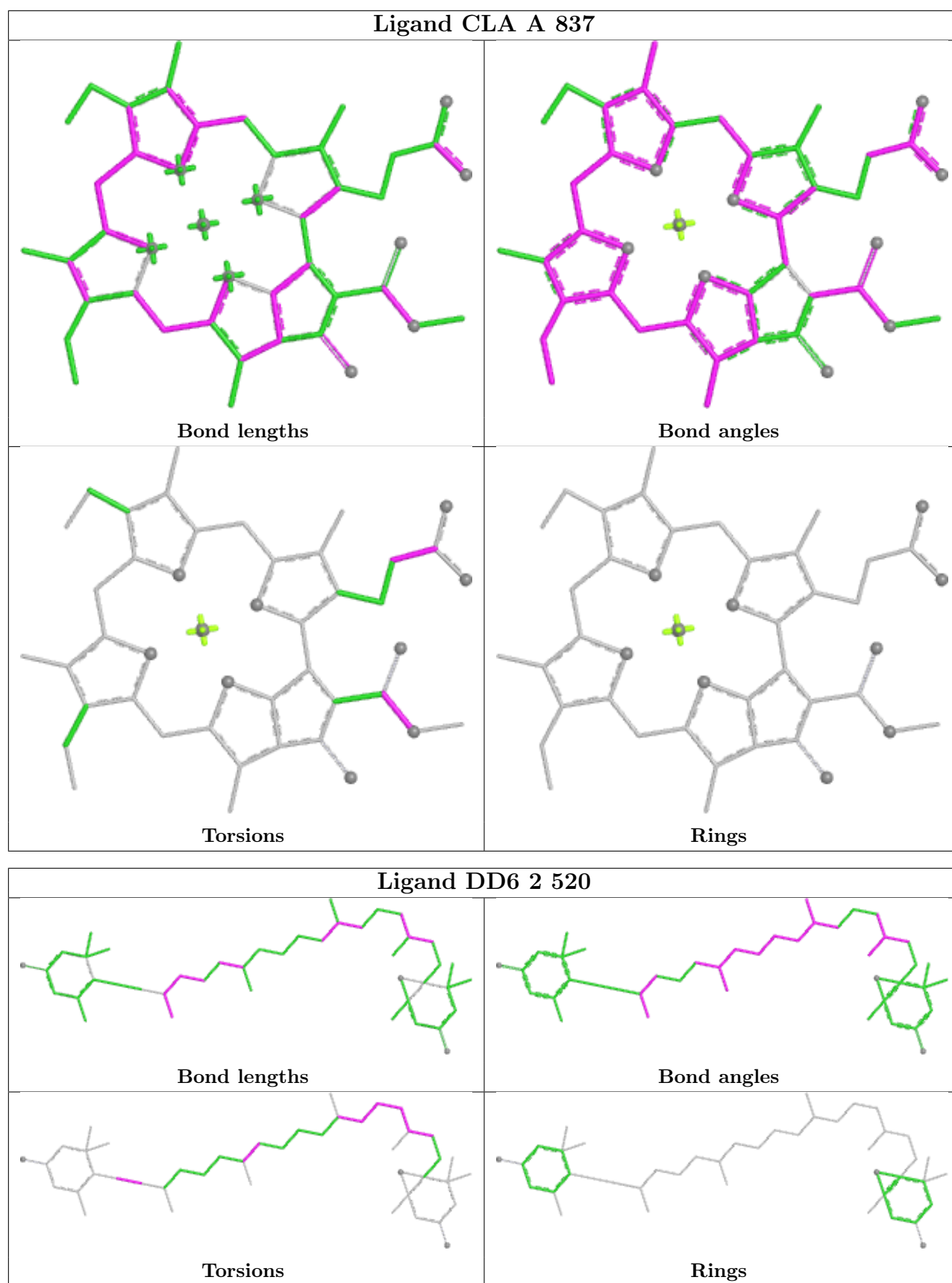


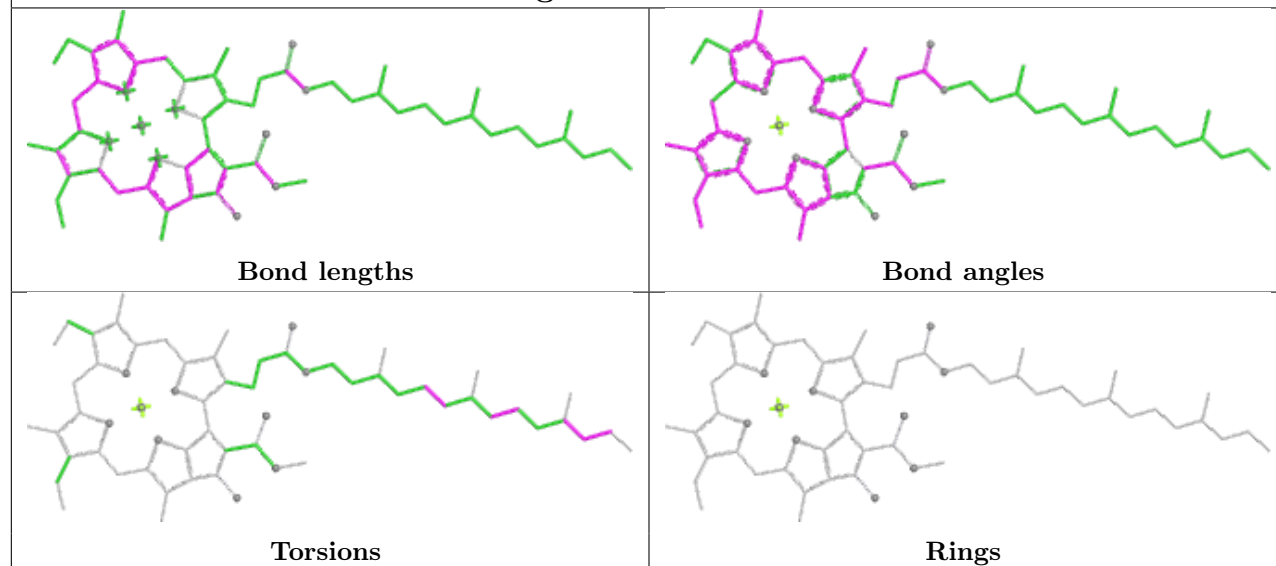
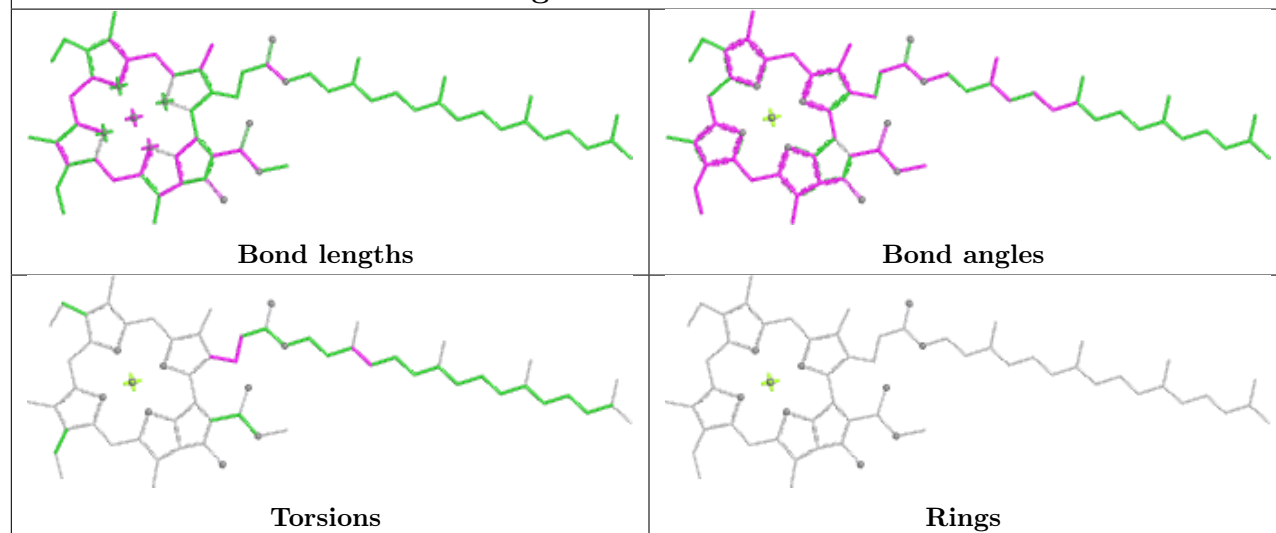
Torsions

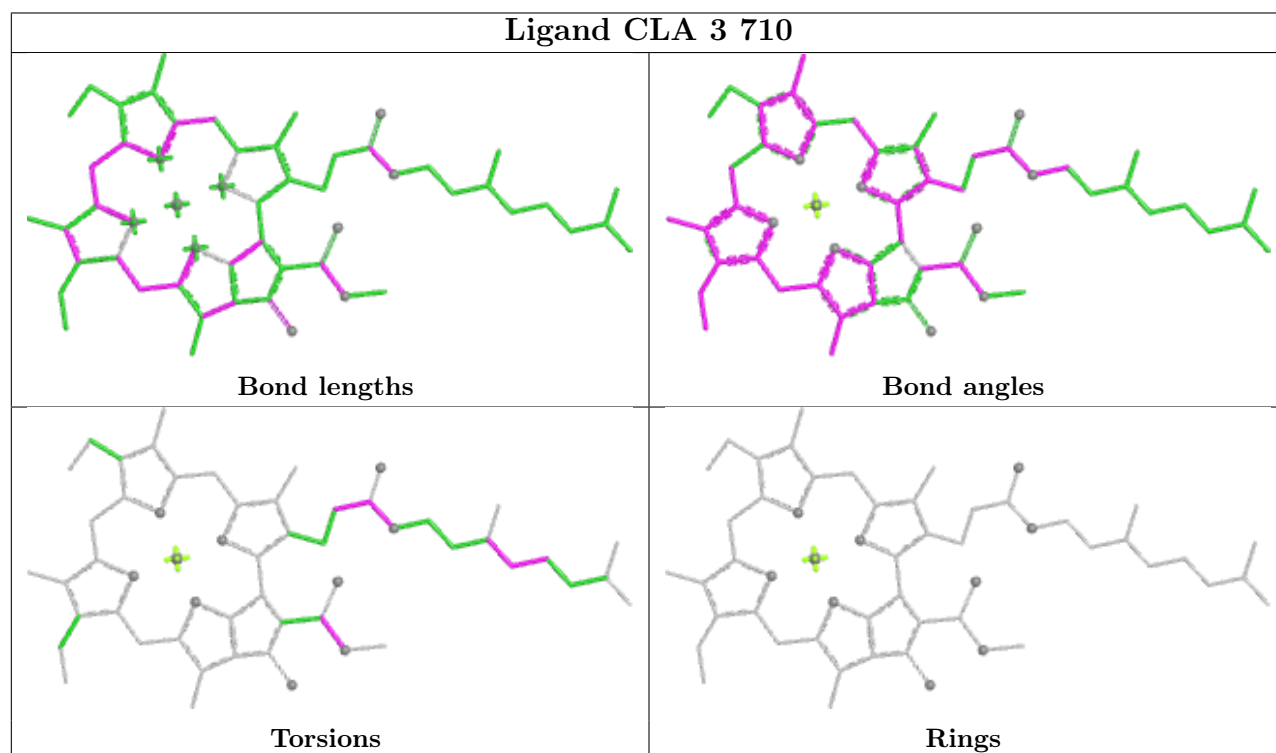
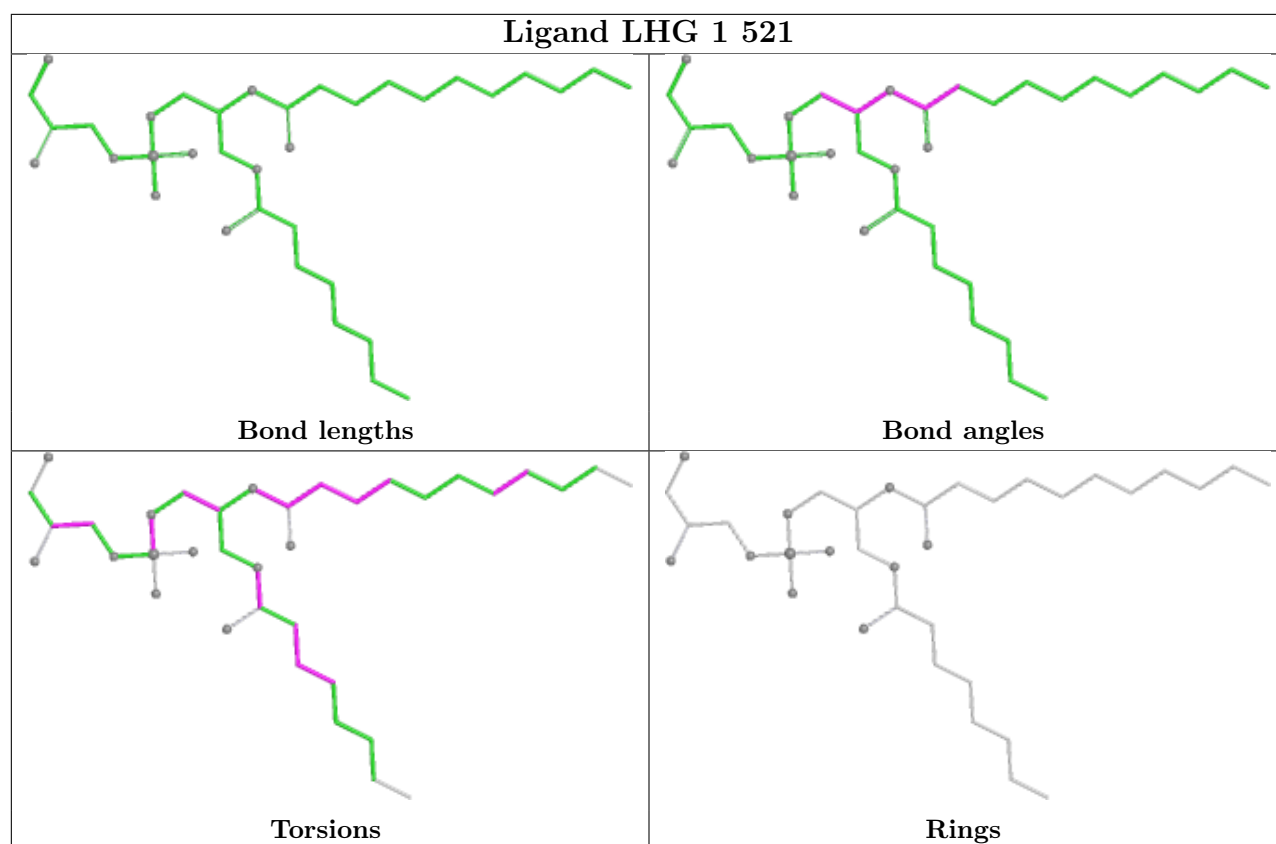


Rings

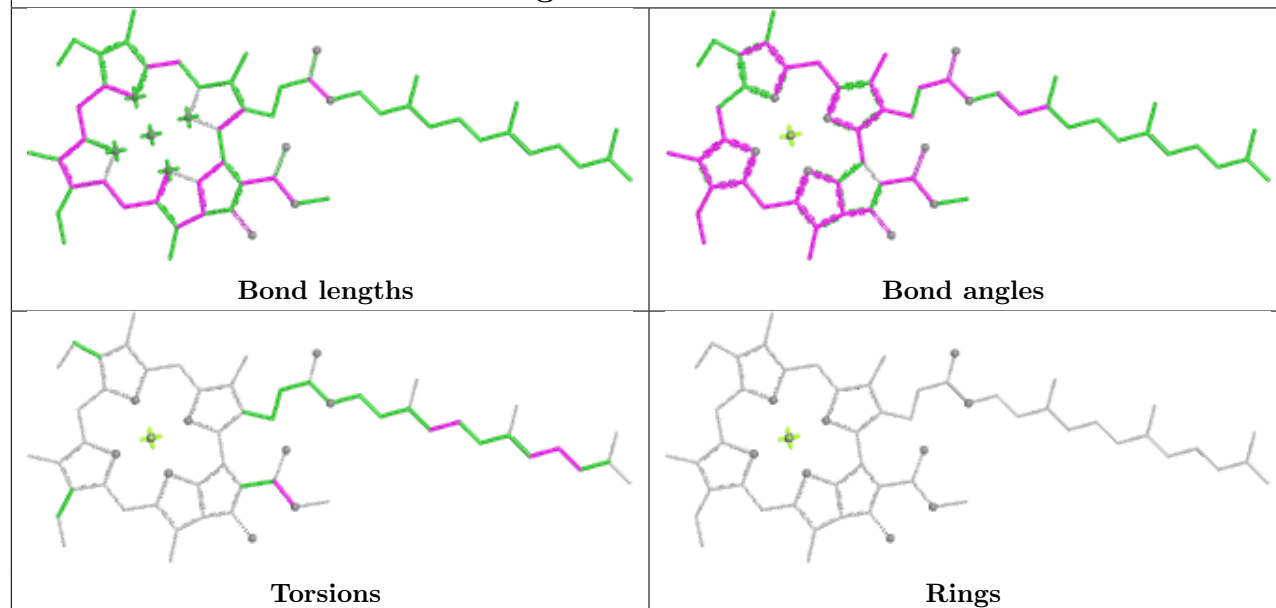




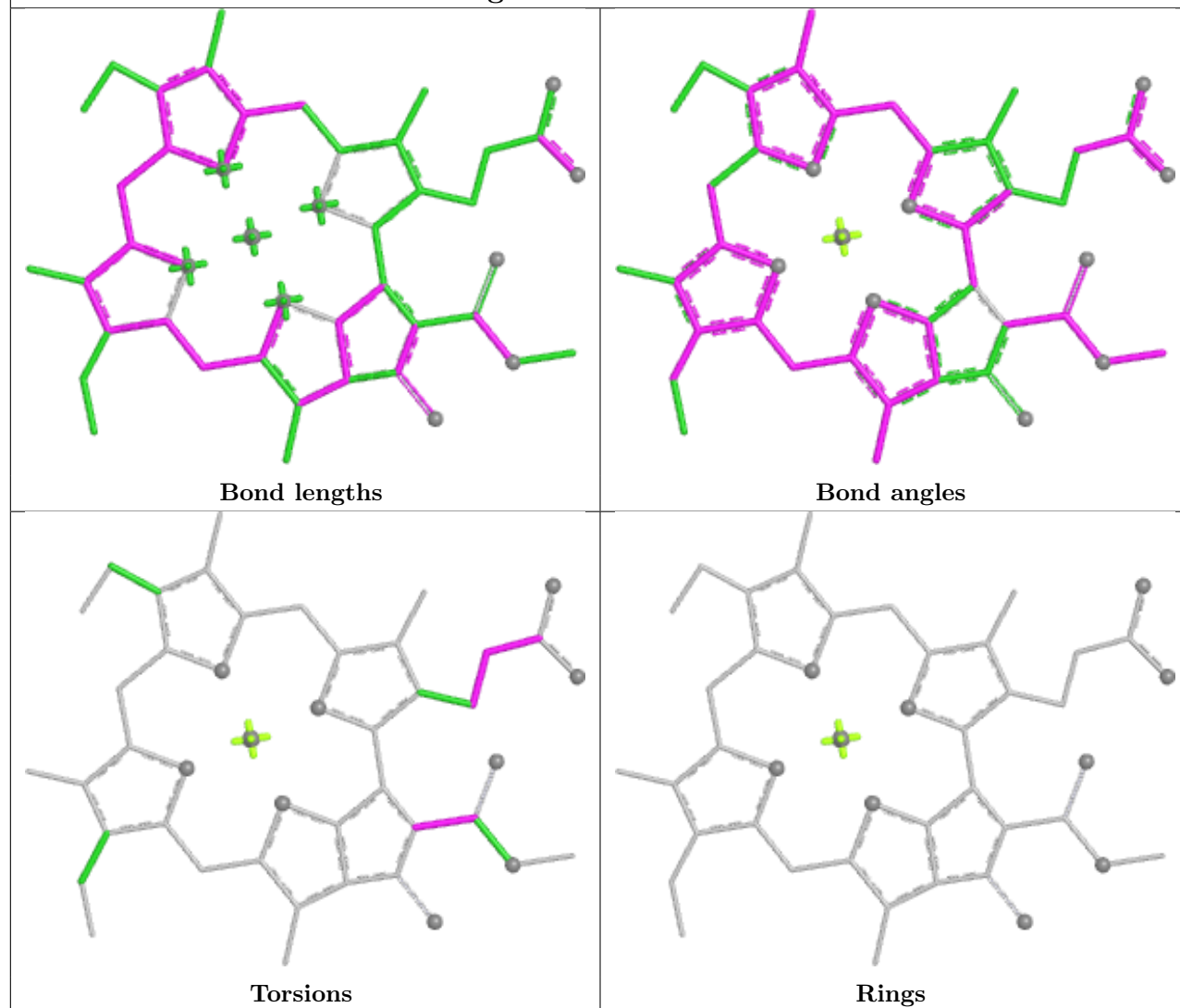
Ligand CLA 9 908**Ligand CLA A 802**



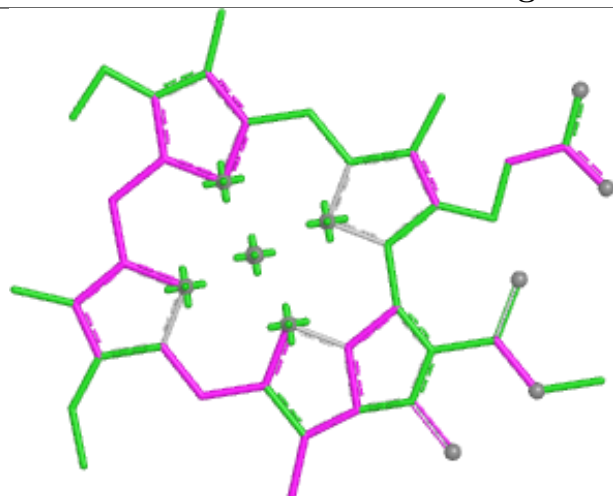
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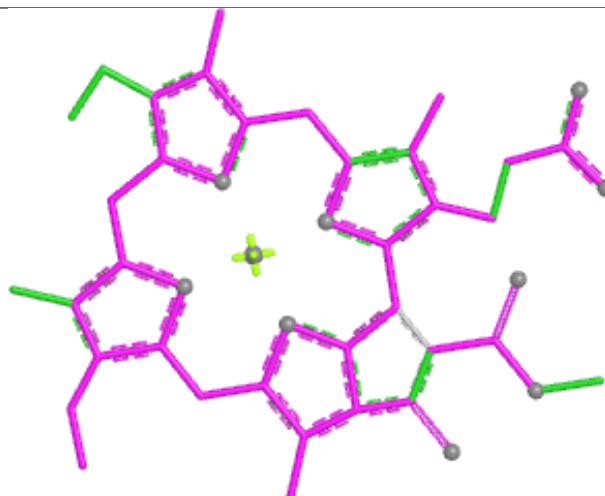
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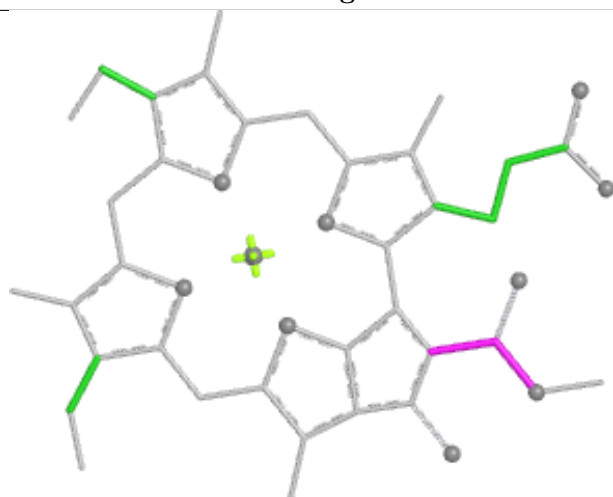
Ligand CLA J 101



Bond lengths



Bond angles

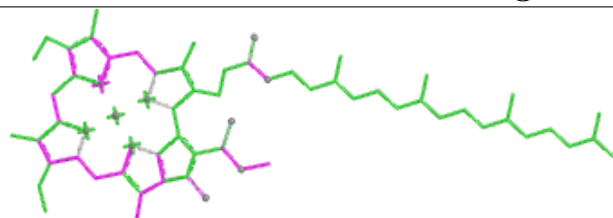


Torsions

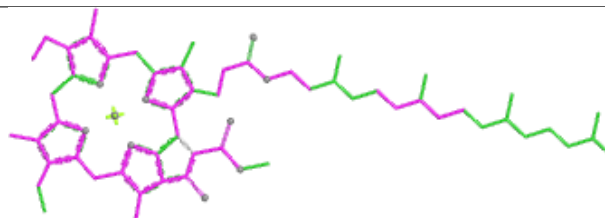


Rings

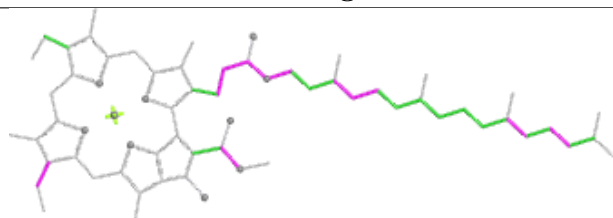
Ligand CLA B 831



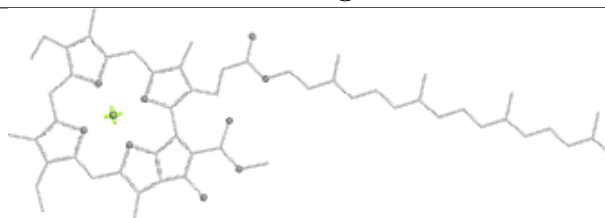
Bond lengths



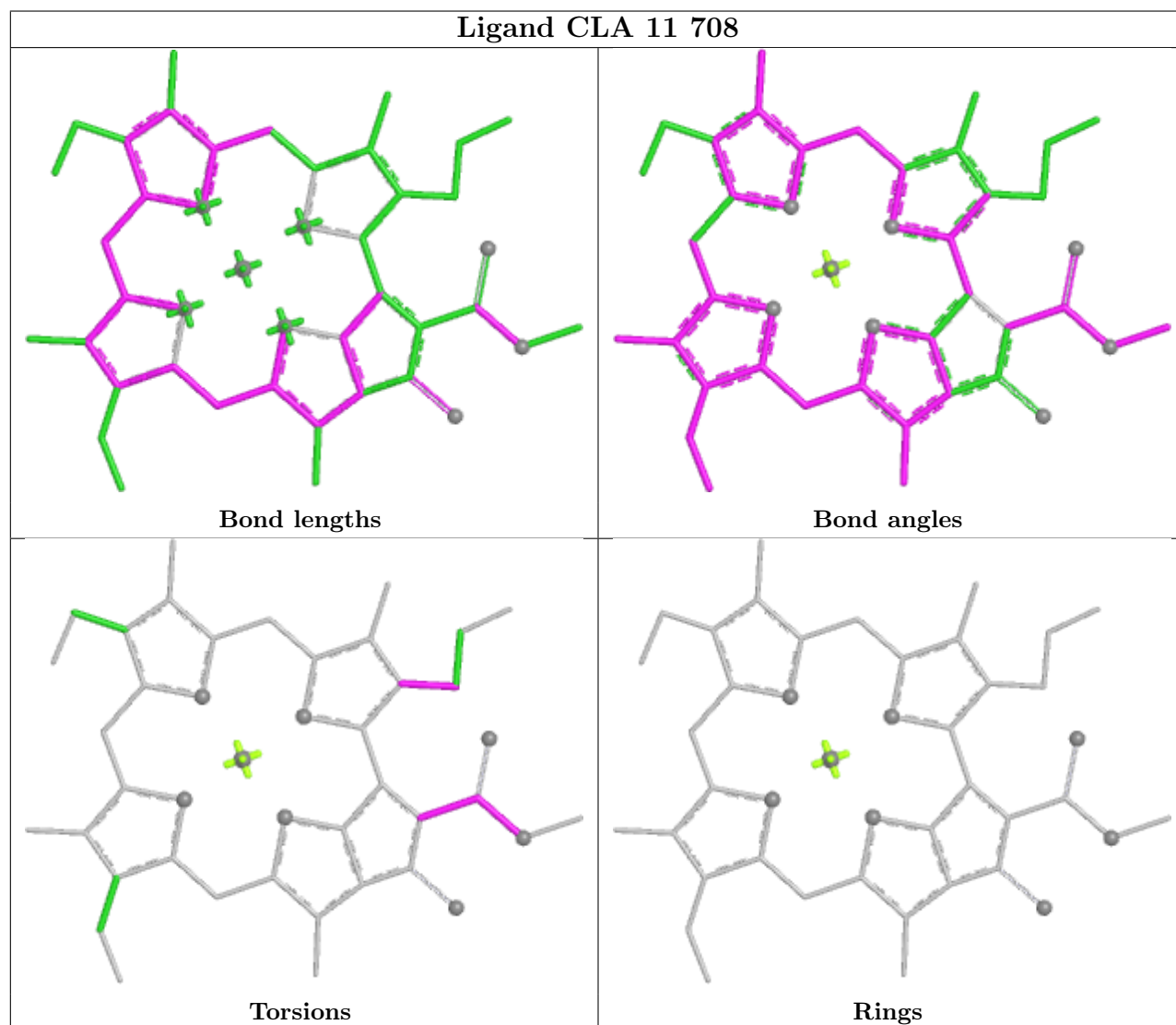
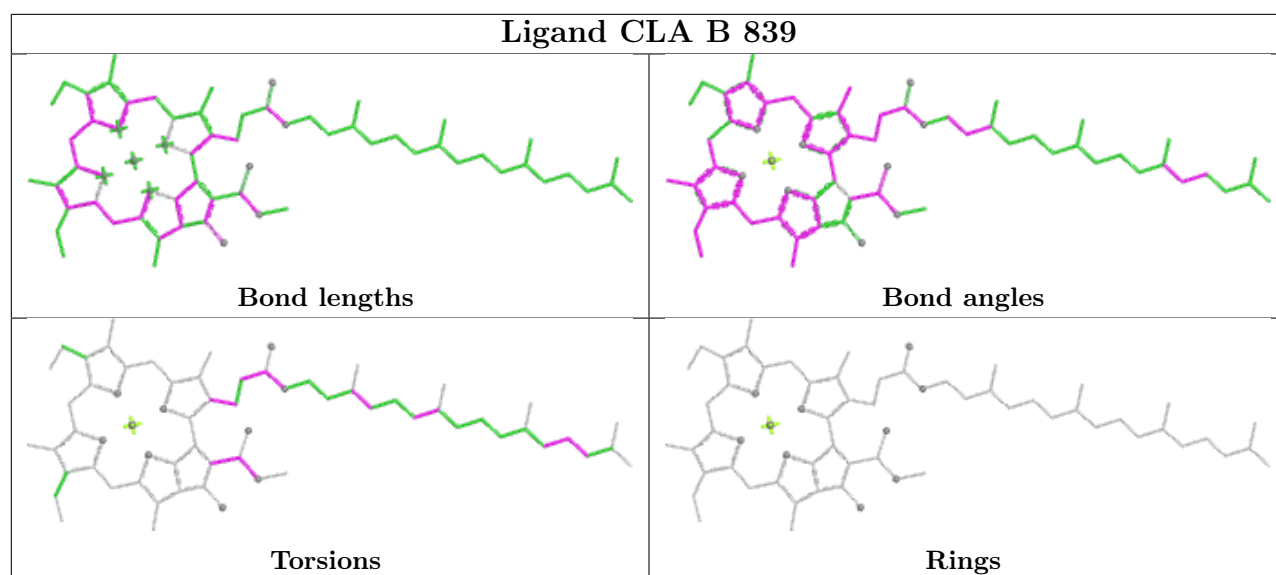
Bond angles

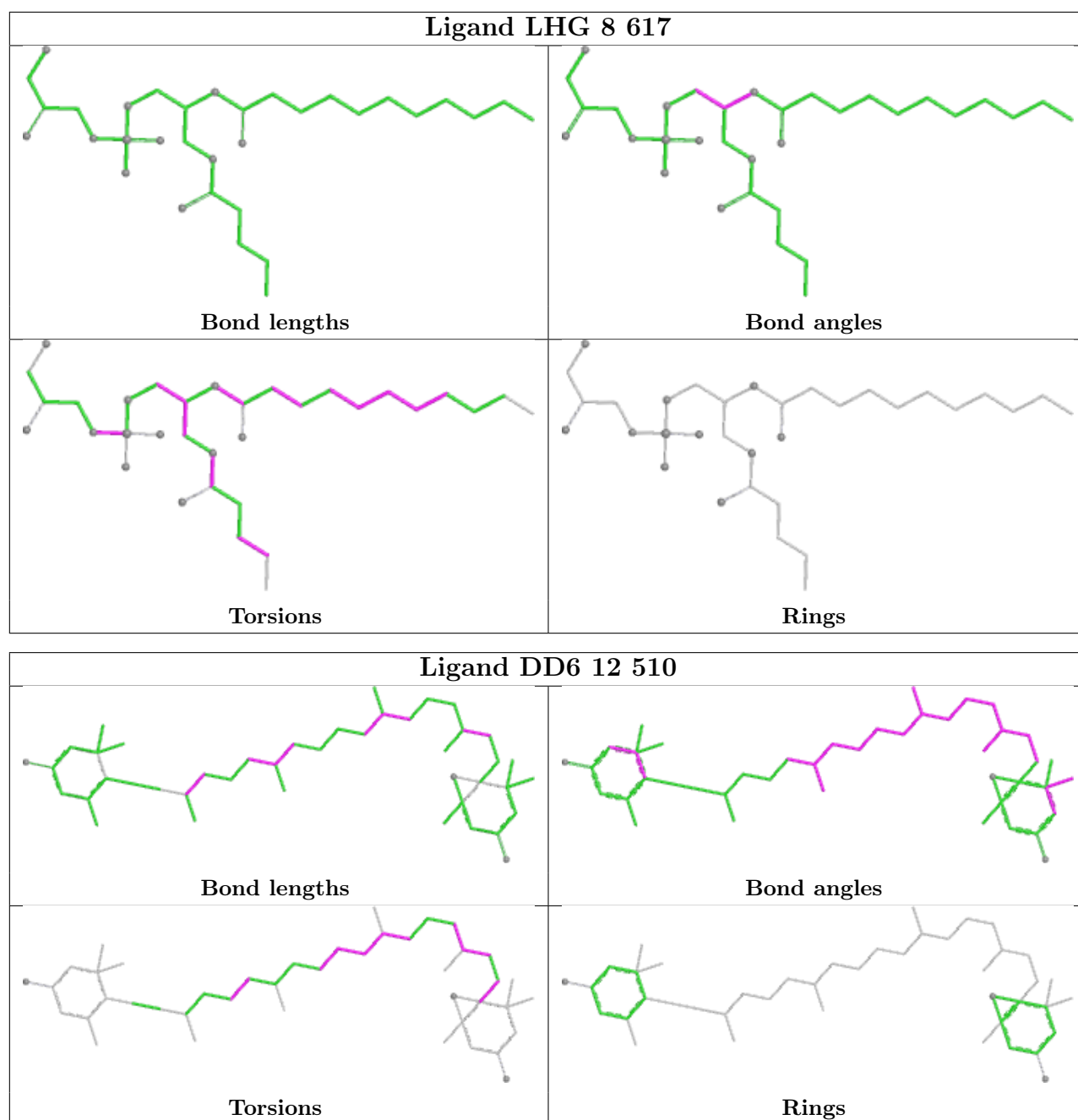


Torsions

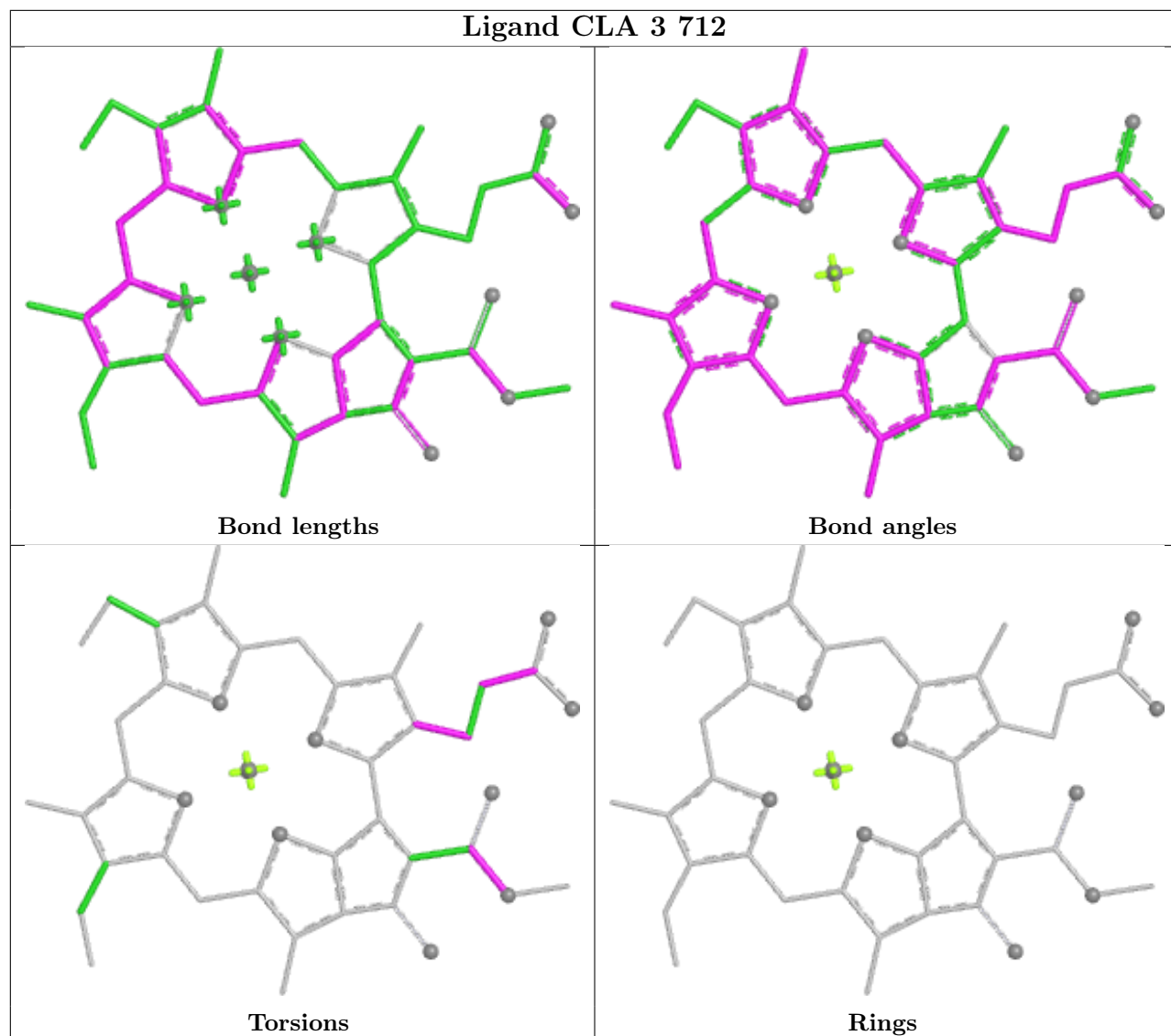


Rings

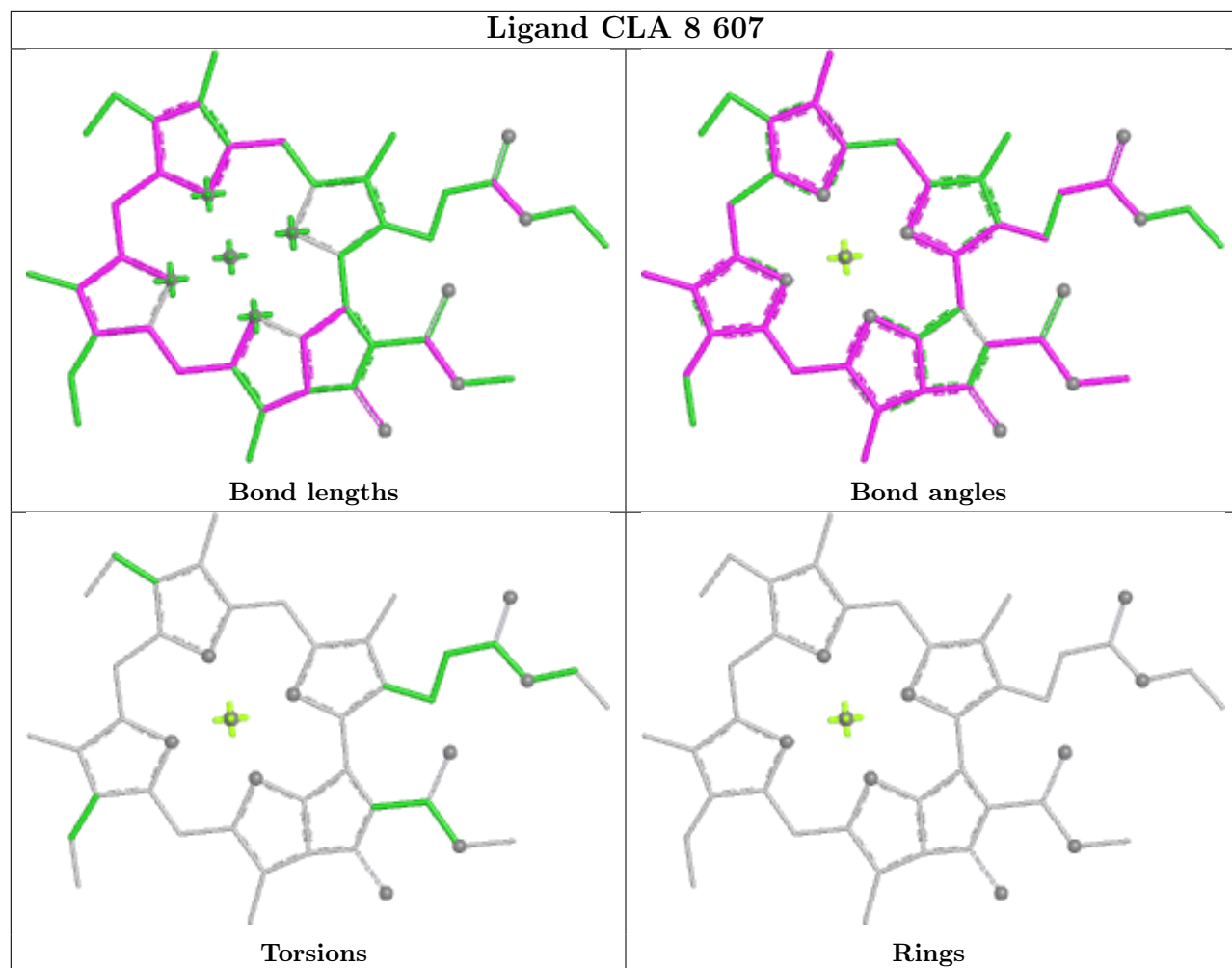




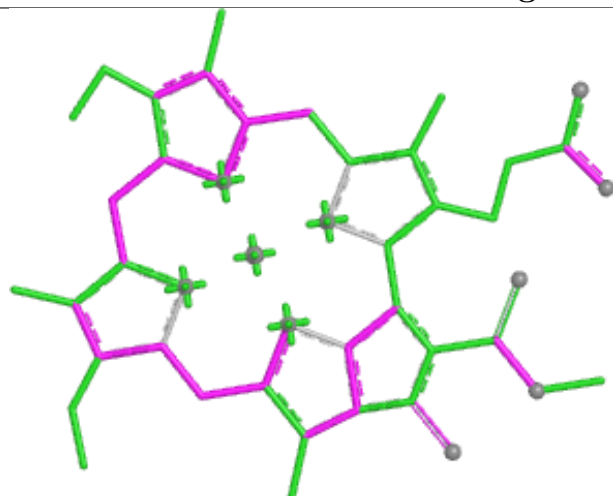
Ligand CLA 3 712



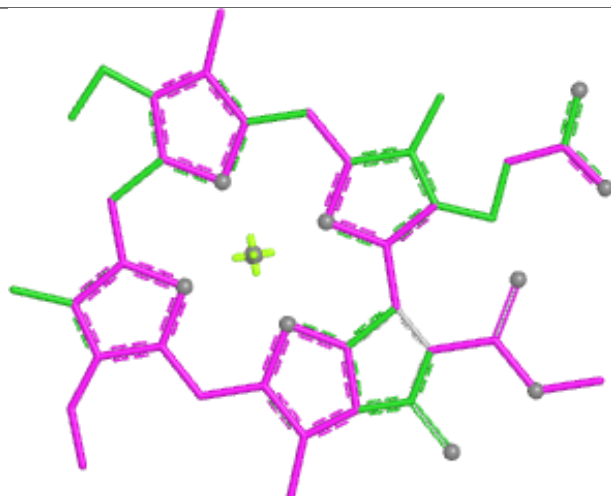
Ligand CLA 8 607



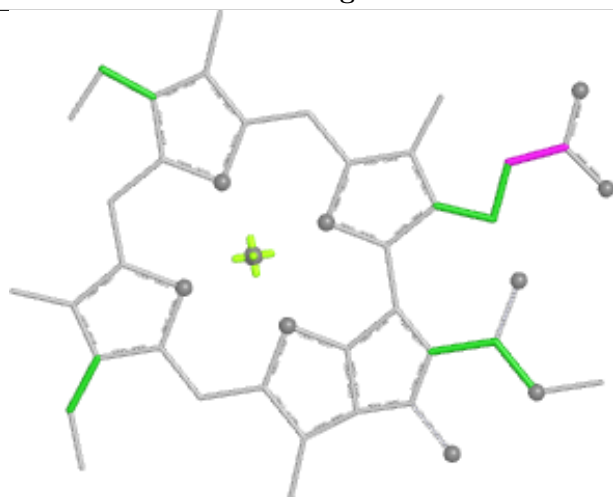
Ligand CLA 9 904



Bond lengths



Bond angles

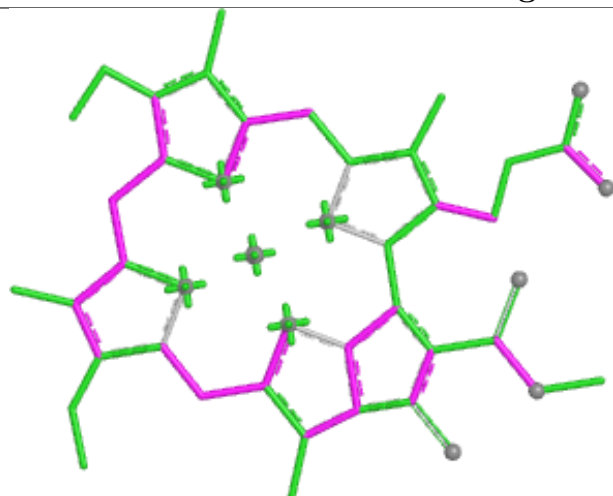


Torsions

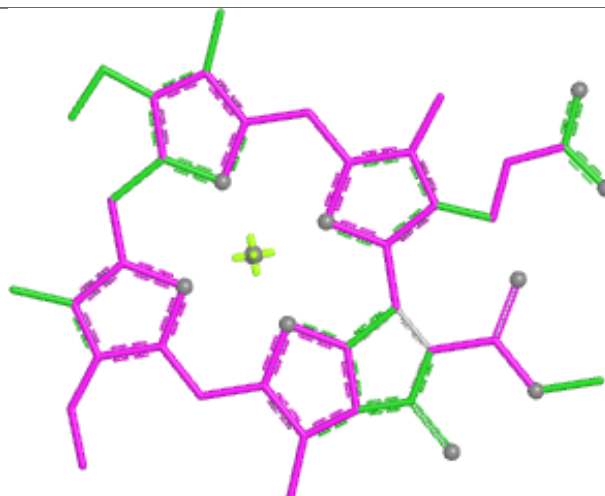


Rings

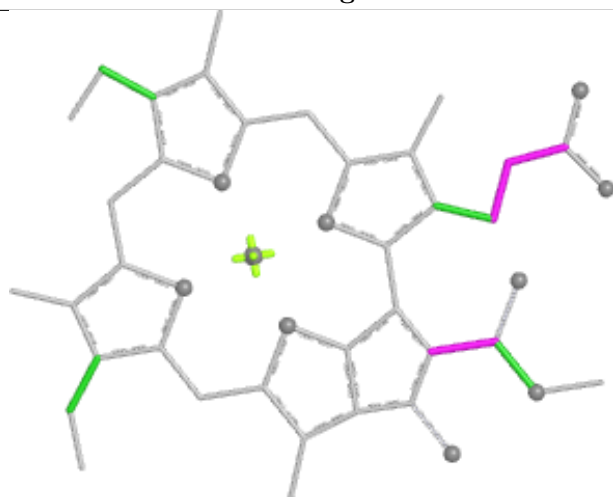
Ligand CLA 7 710



Bond lengths



Bond angles

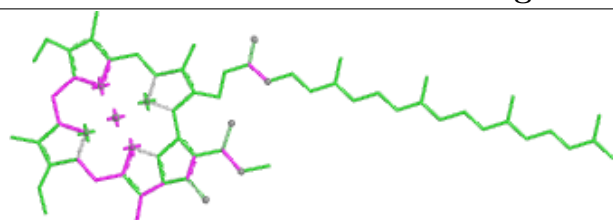


Torsions

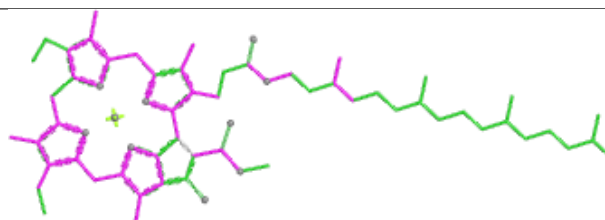


Rings

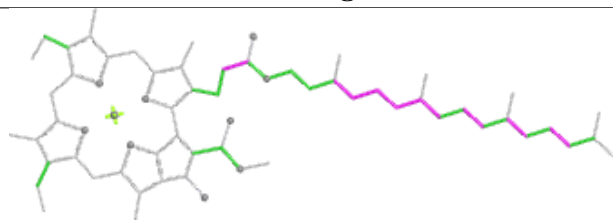
Ligand CLA B 805



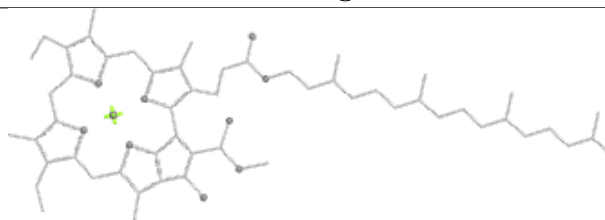
Bond lengths



Bond angles

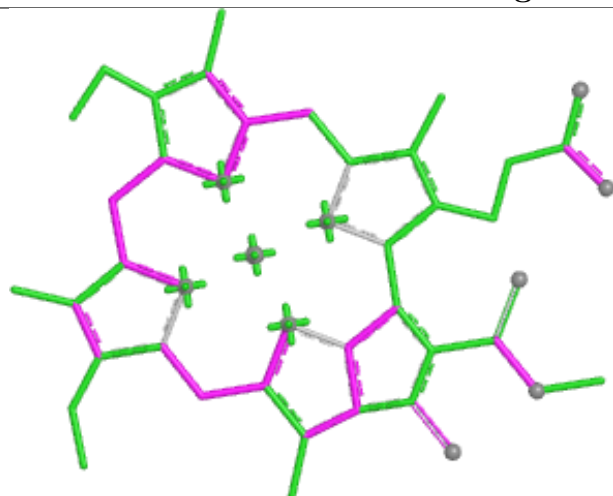


Torsions

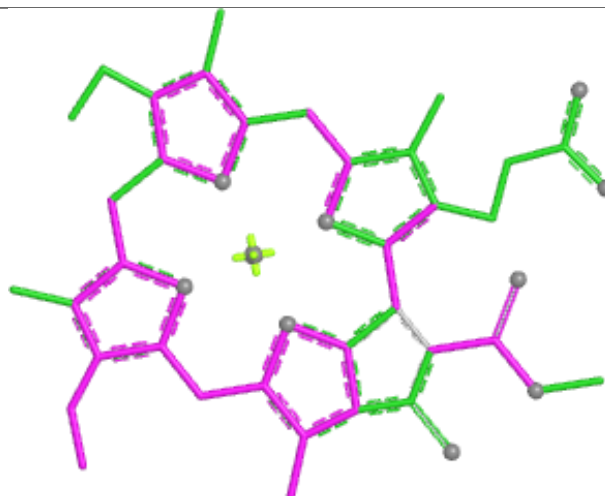


Rings

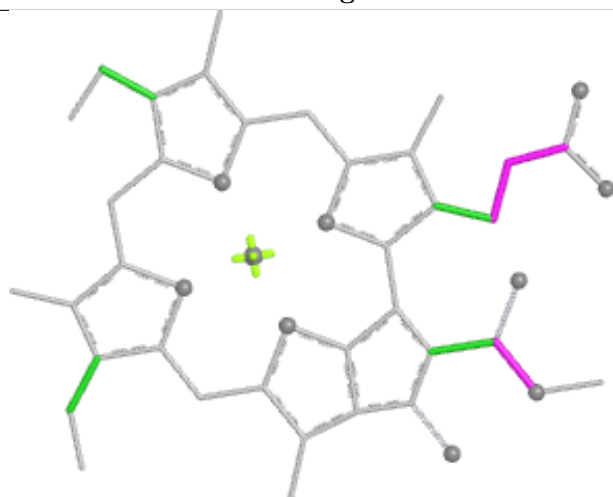
Ligand CLA B 820



Bond lengths



Bond angles

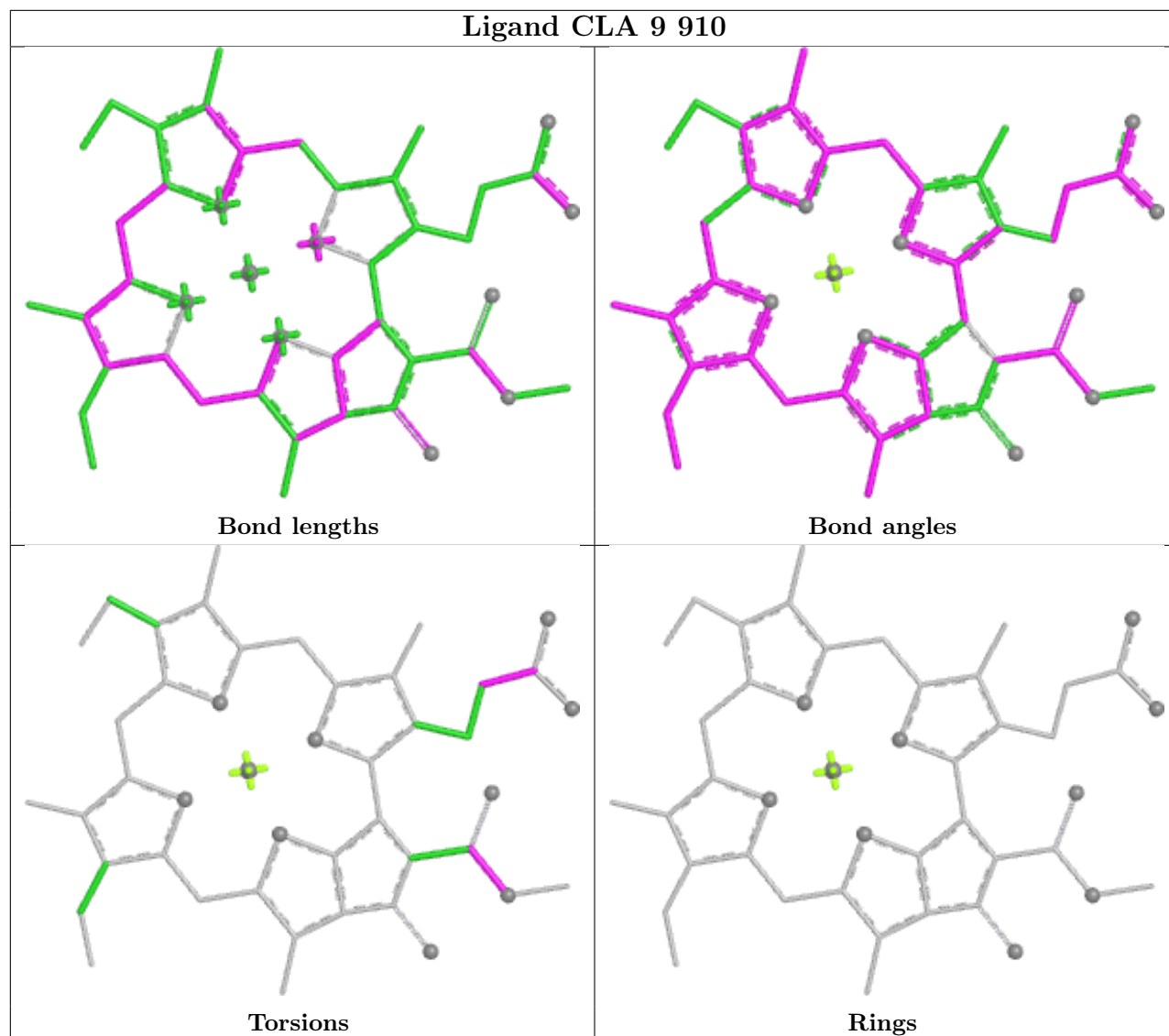


Torsions

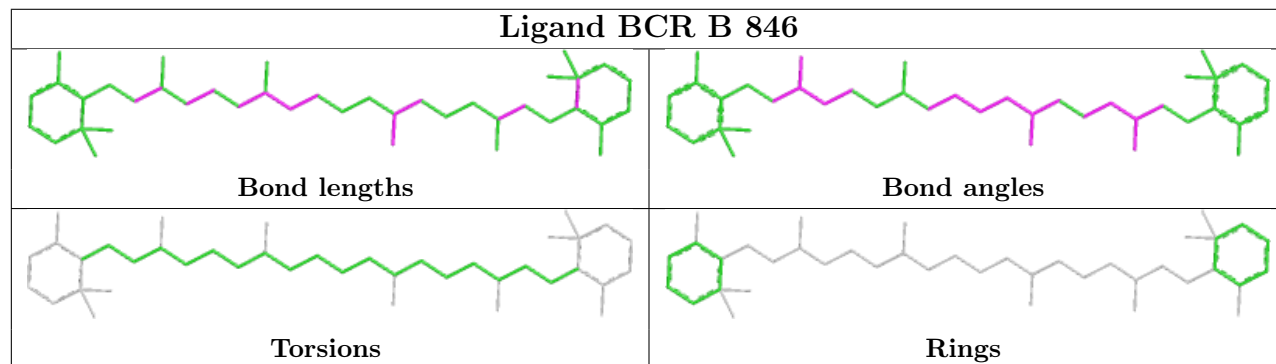


Rings

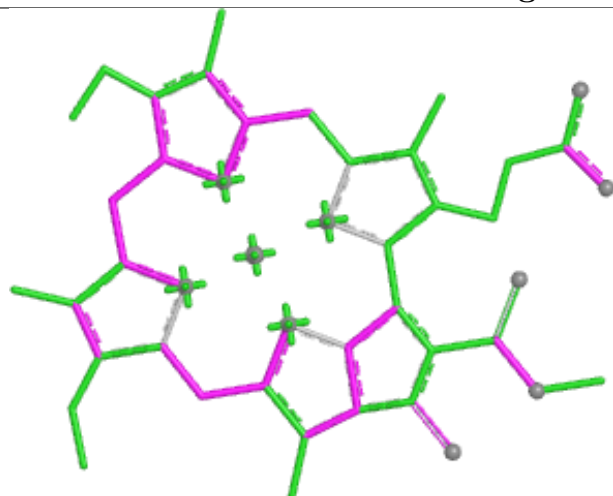
Ligand CLA 9 910



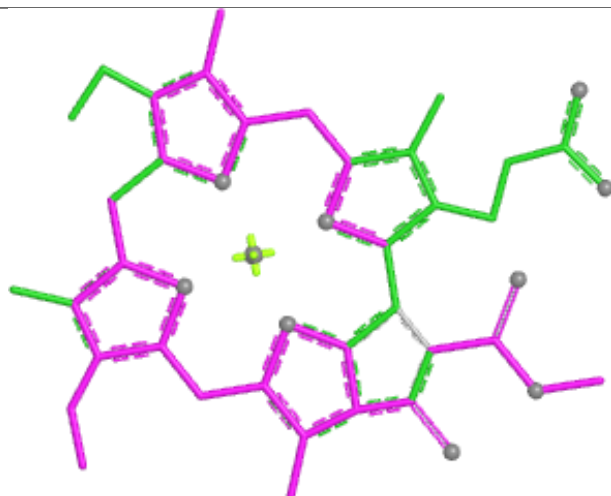
Ligand BCR B 846



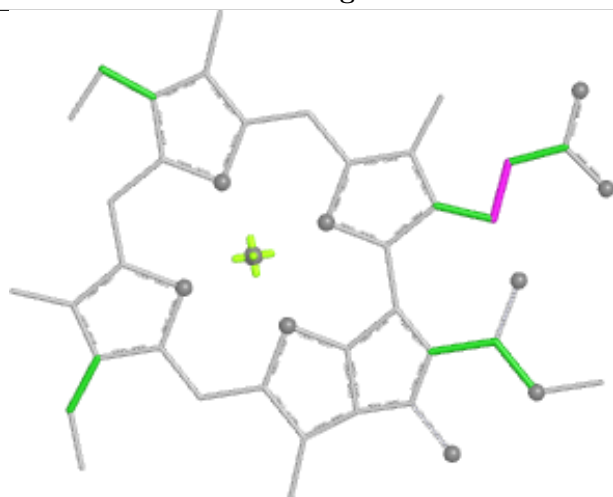
Ligand CLA 2 503



Bond lengths



Bond angles

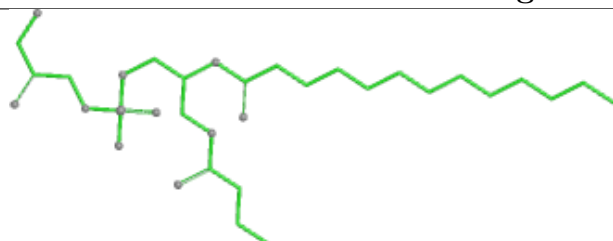


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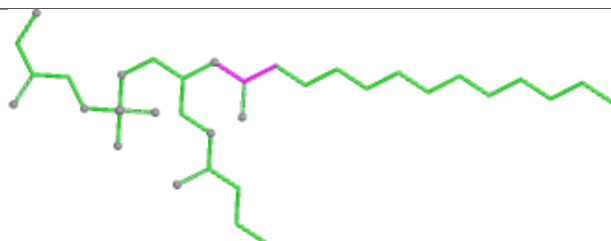


Rings

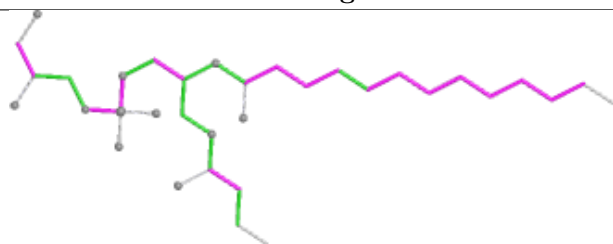
Ligand LHG 9 917



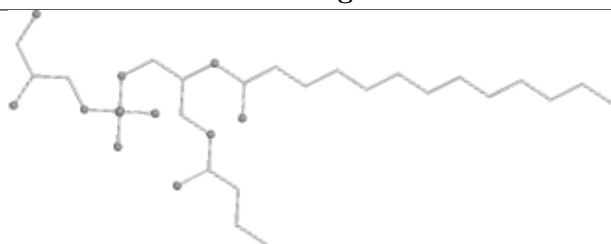
Bond lengths



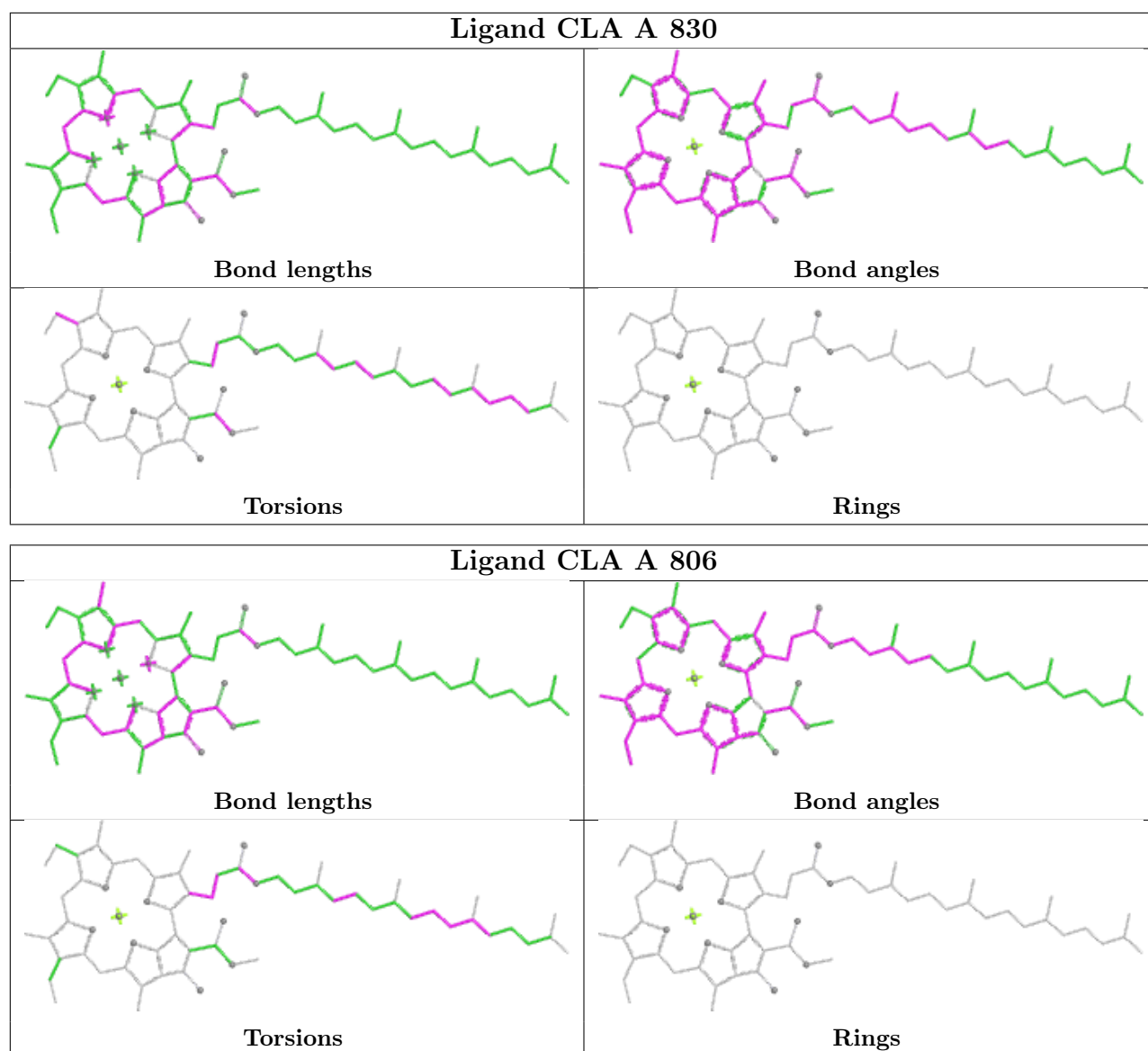
Bond angles

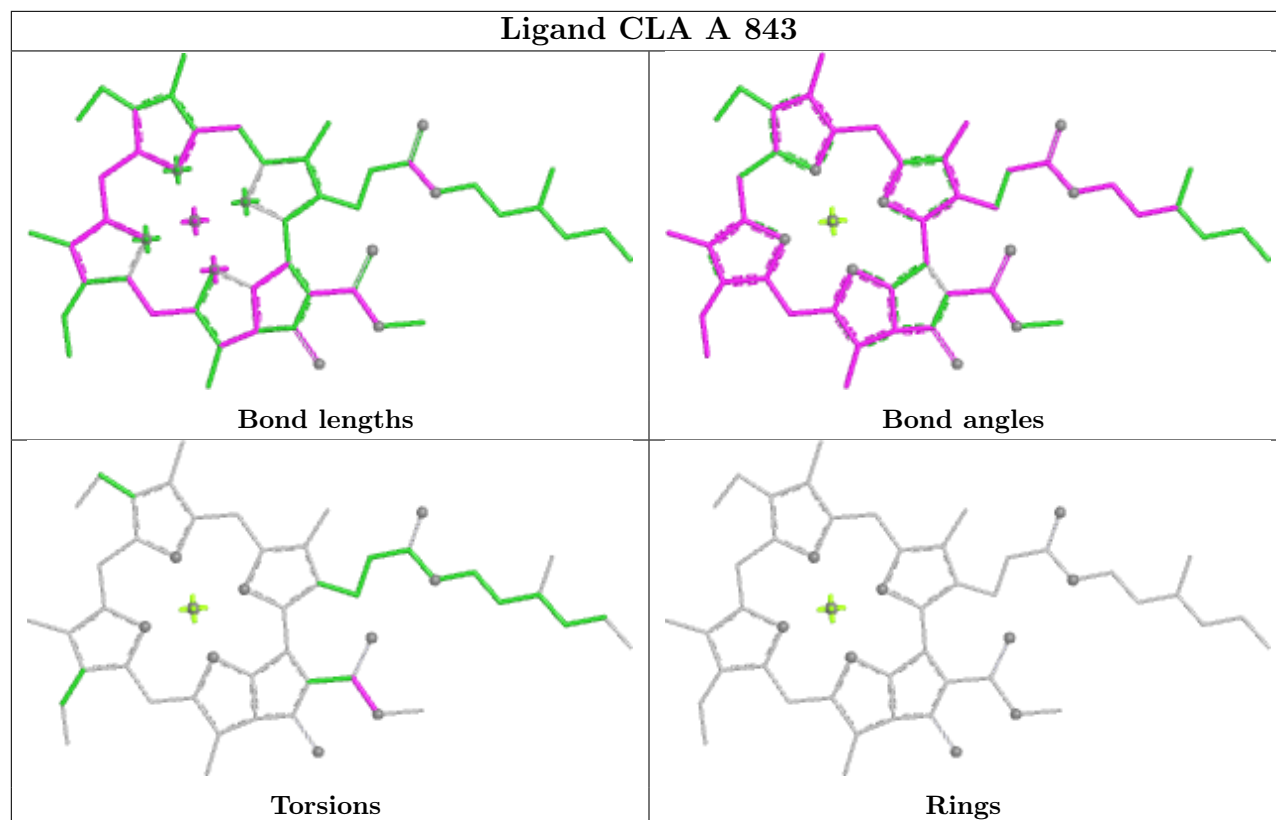


Torsions

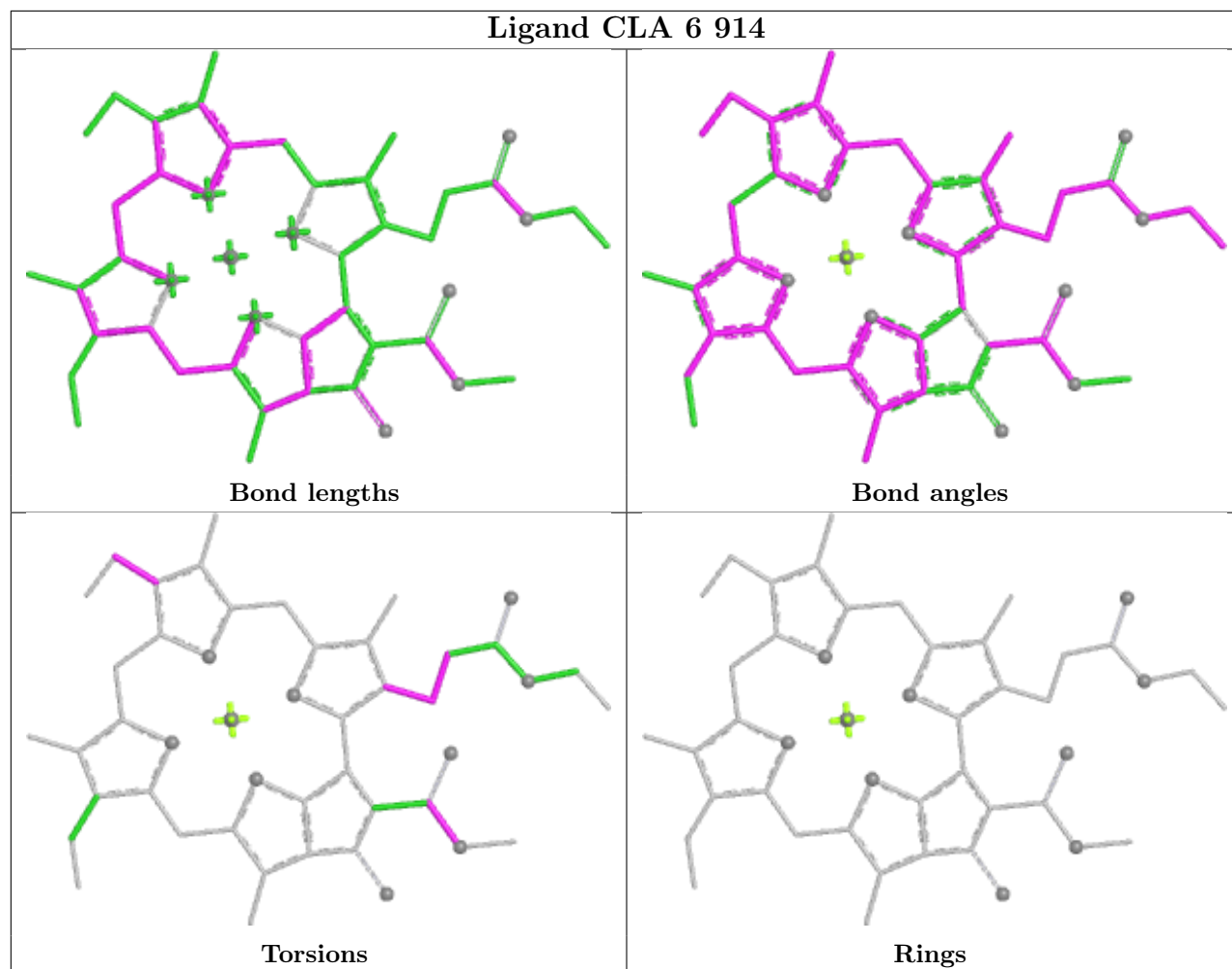


Rings

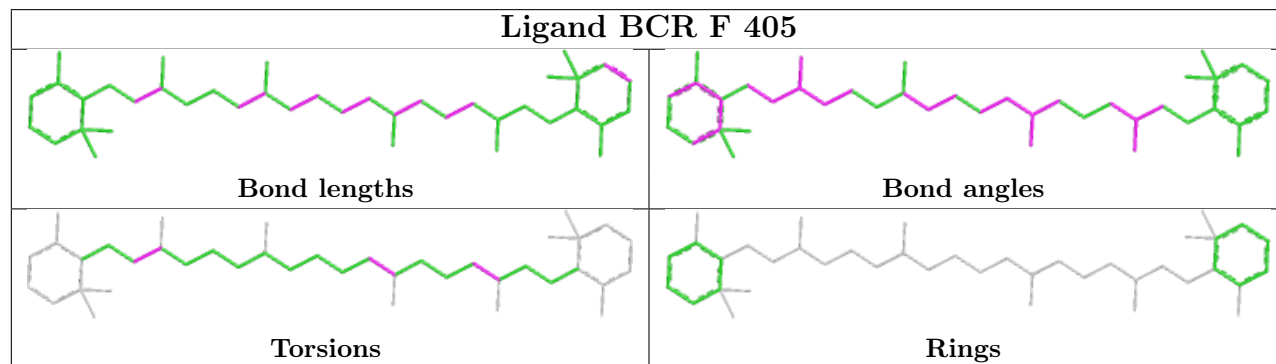




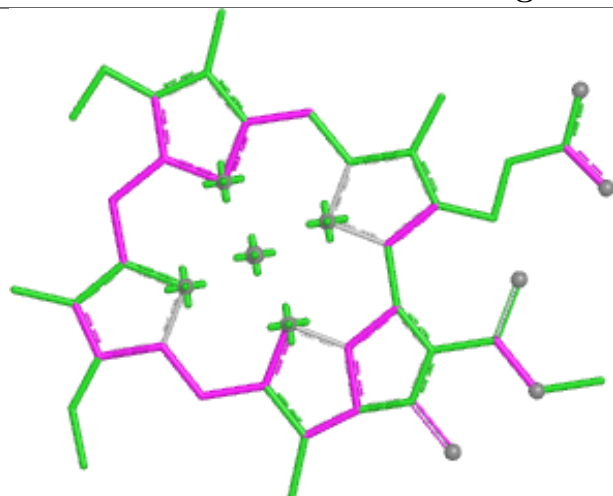
Ligand CLA 6 914



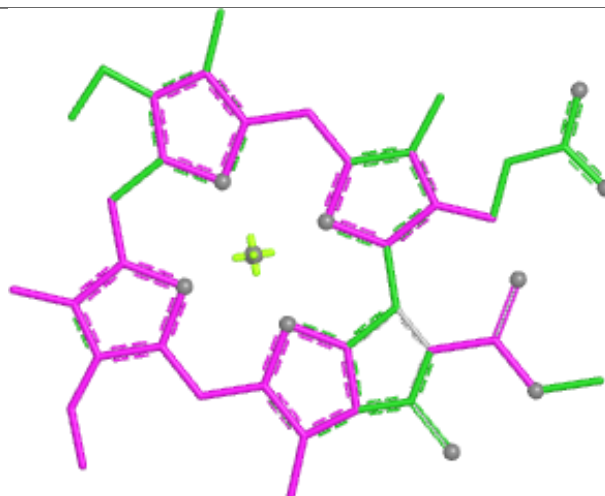
Ligand BCR F 405



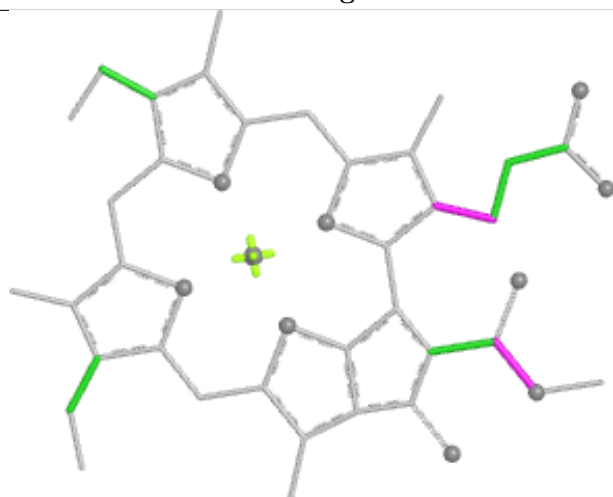
Ligand CLA F 404



Bond lengths



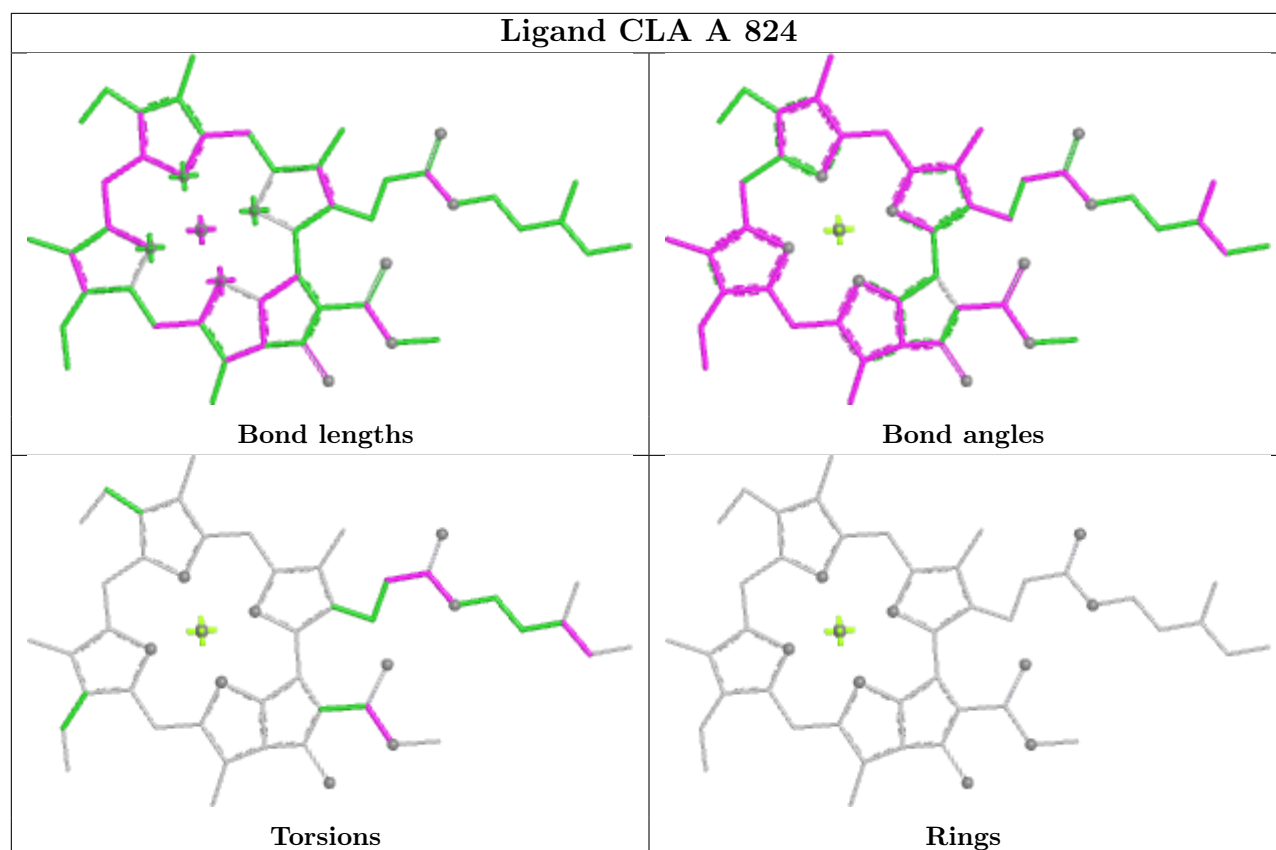
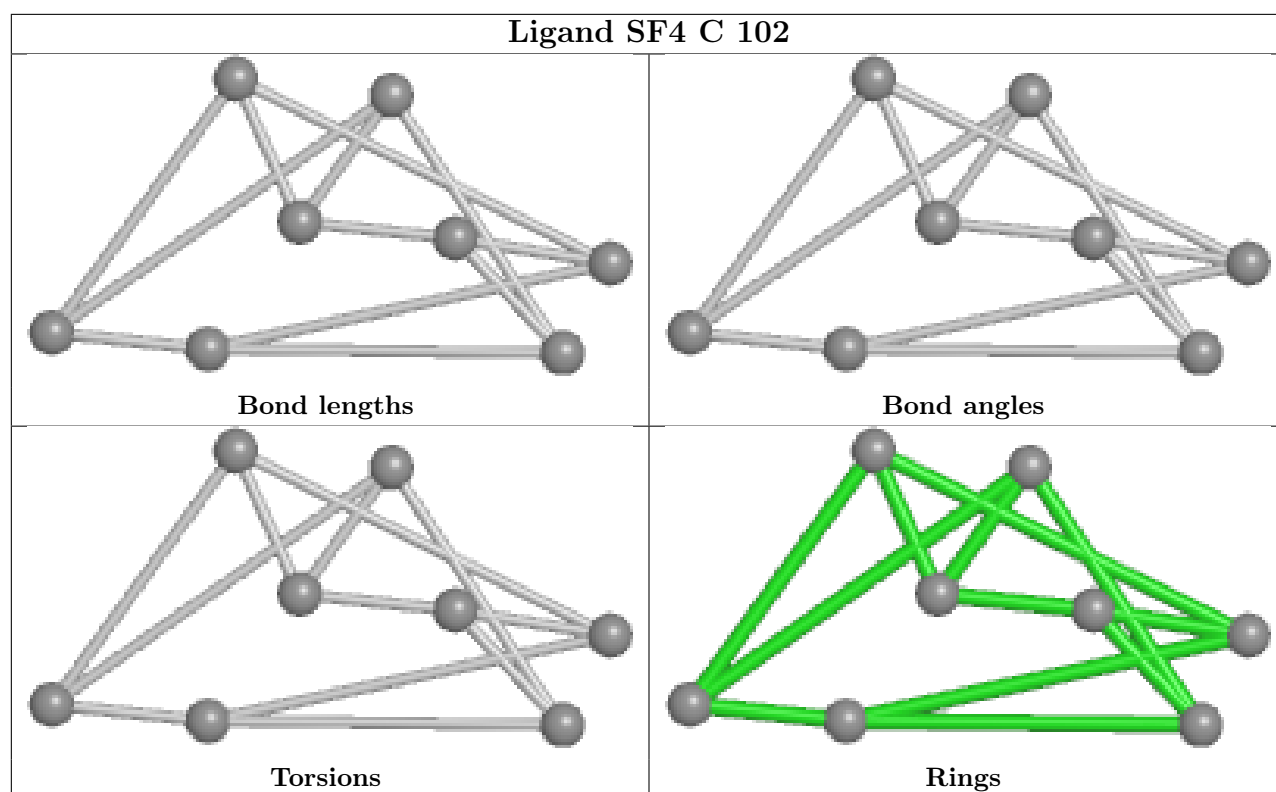
Bond angles

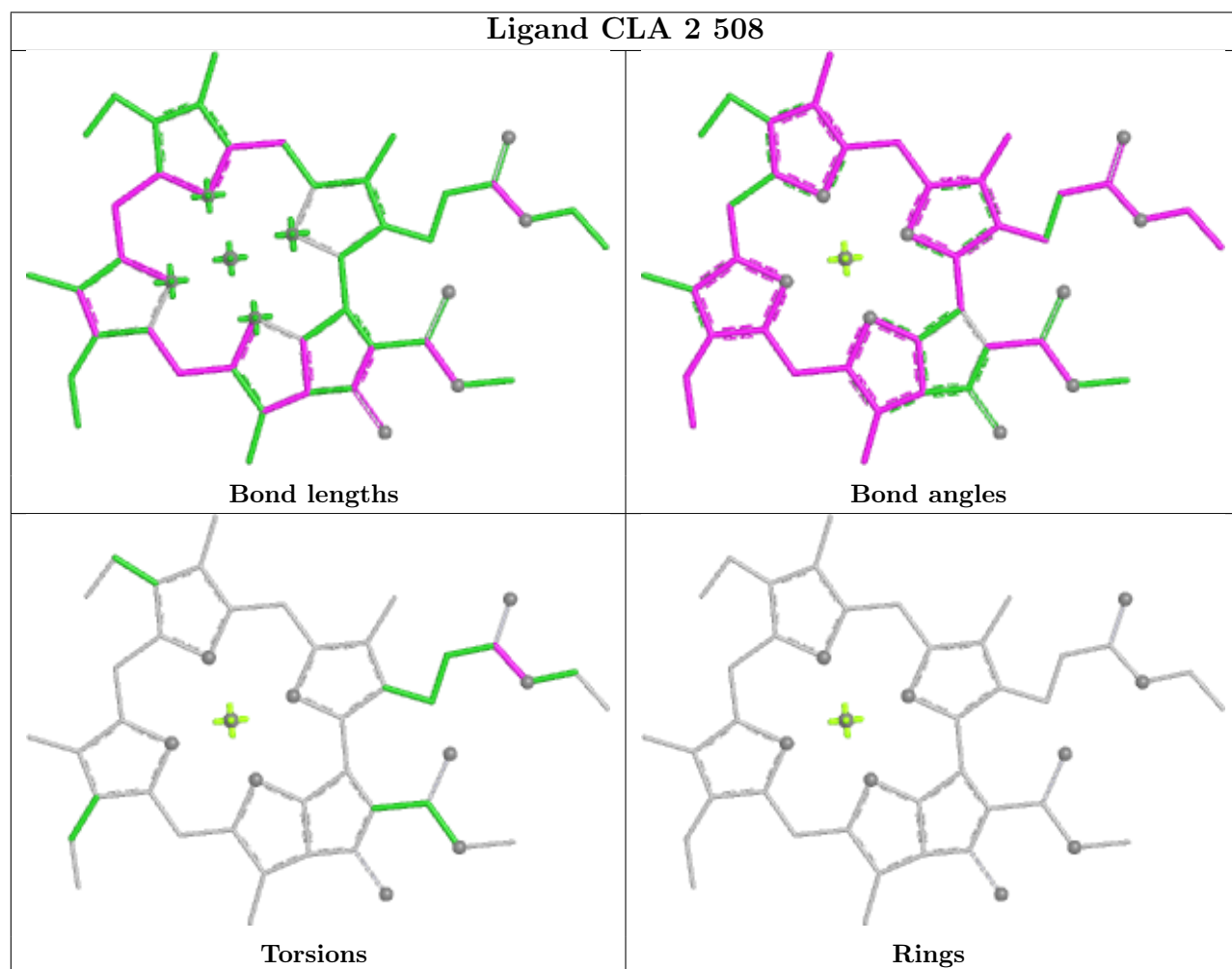
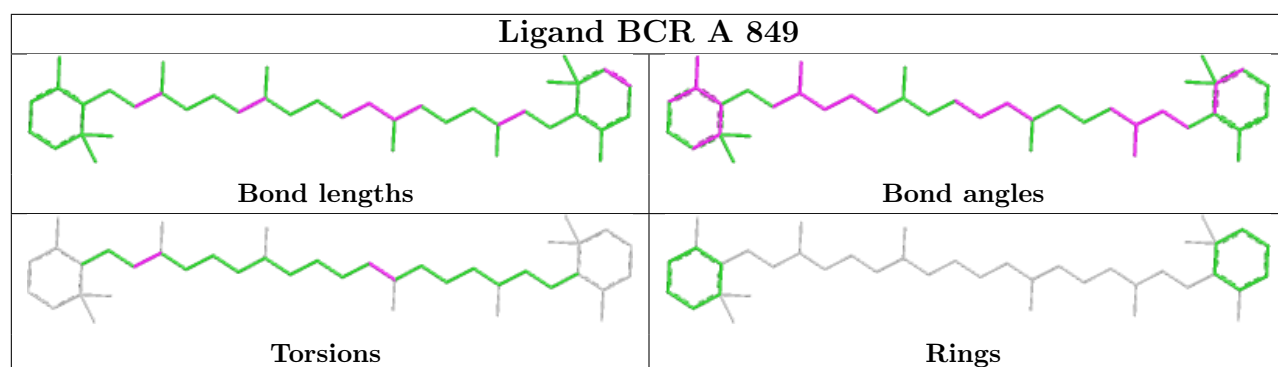


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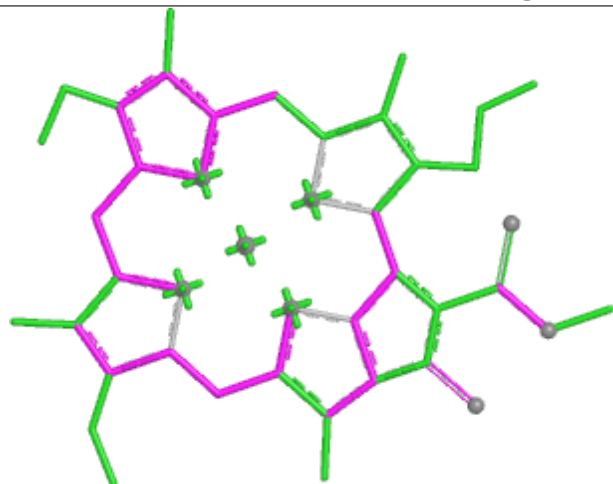


Rings

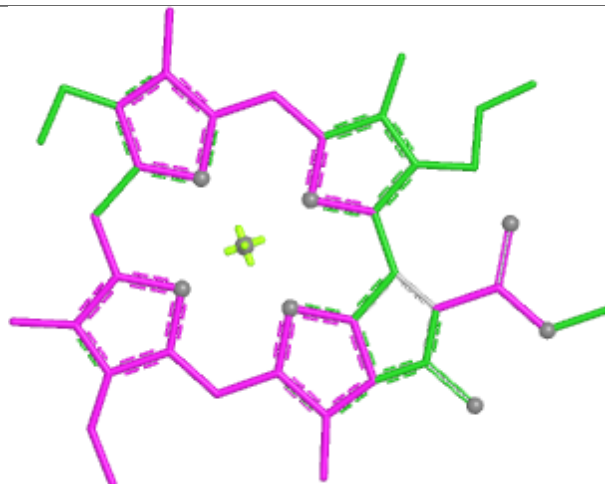




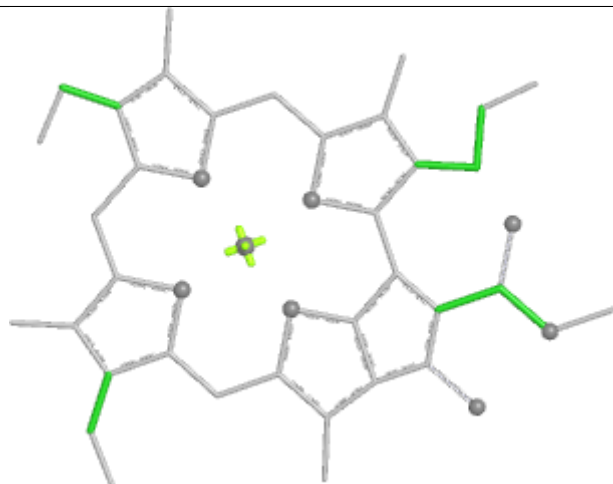
Ligand CLA 4 708



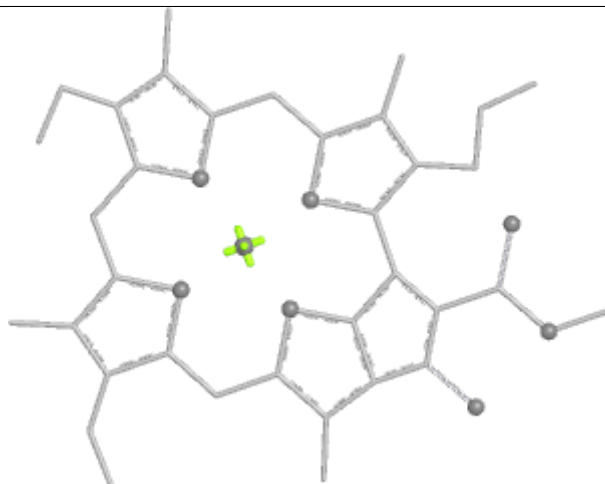
Bond lengths



Bond angles

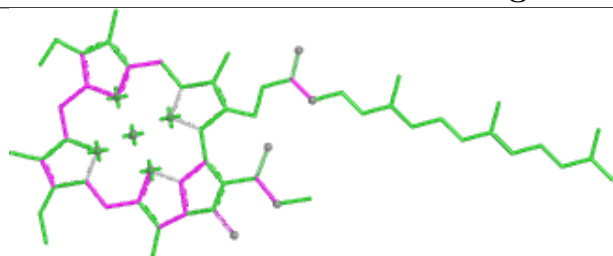


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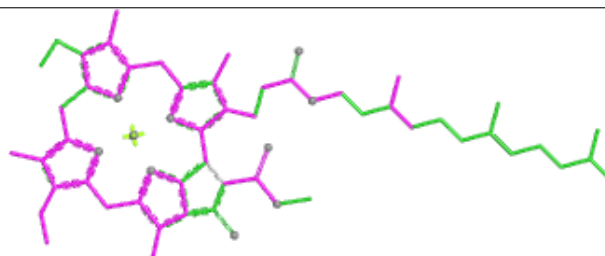


Rings

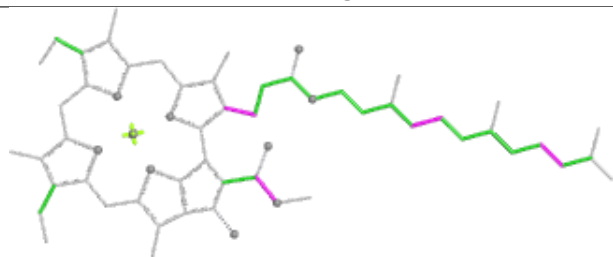
Ligand CLA 12 501



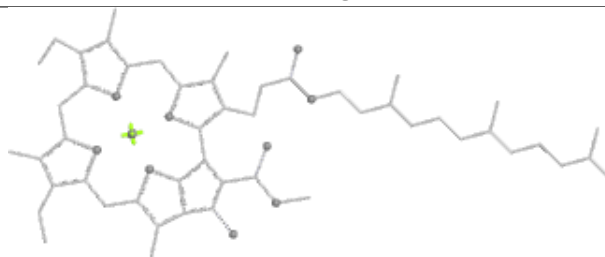
Bond lengths



Bond angles

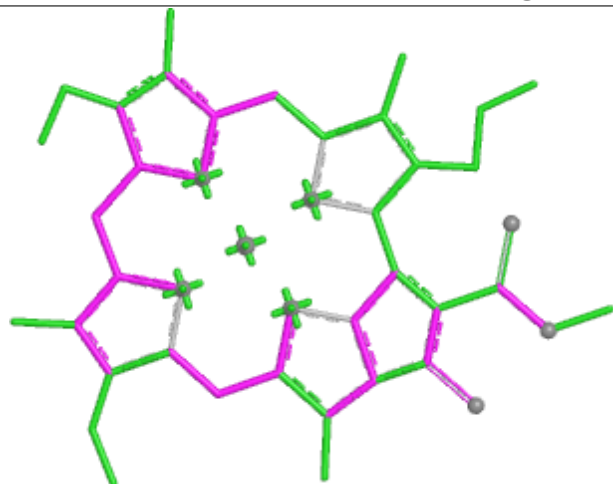


Torsions

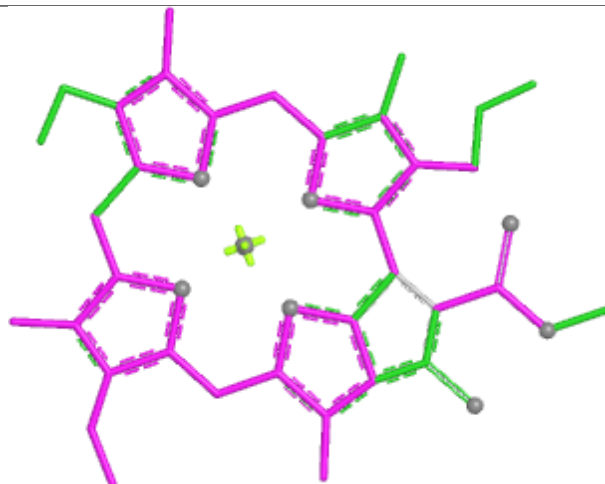


Rings

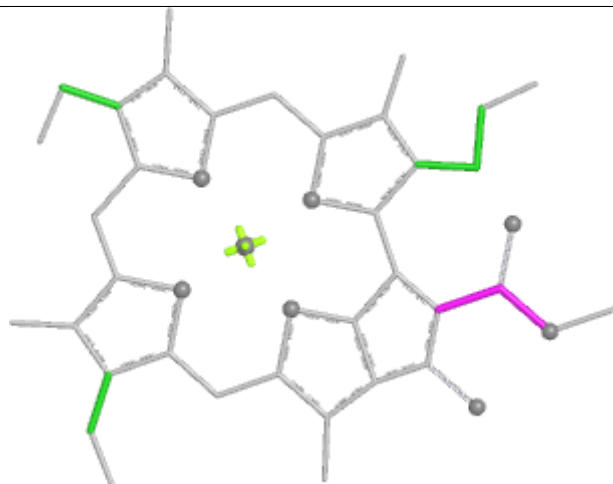
Ligand CLA 6 910



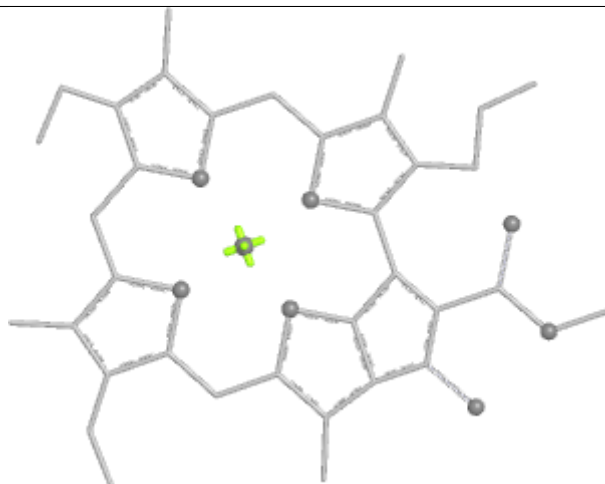
Bond lengths



Bond angles

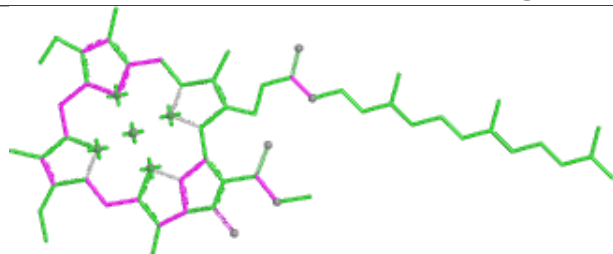


Torsions

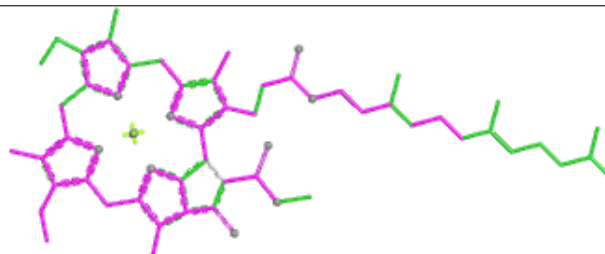


Rings

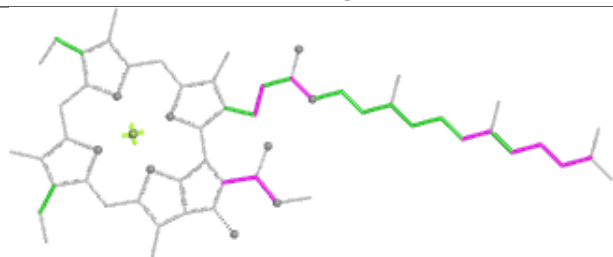
Ligand CLA 2 504



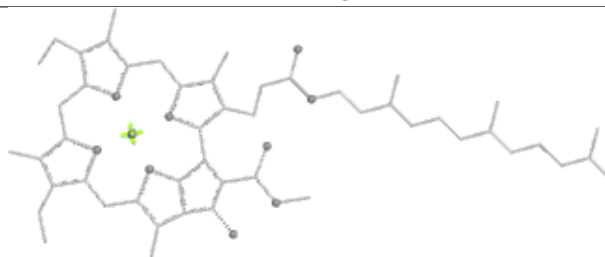
Bond lengths



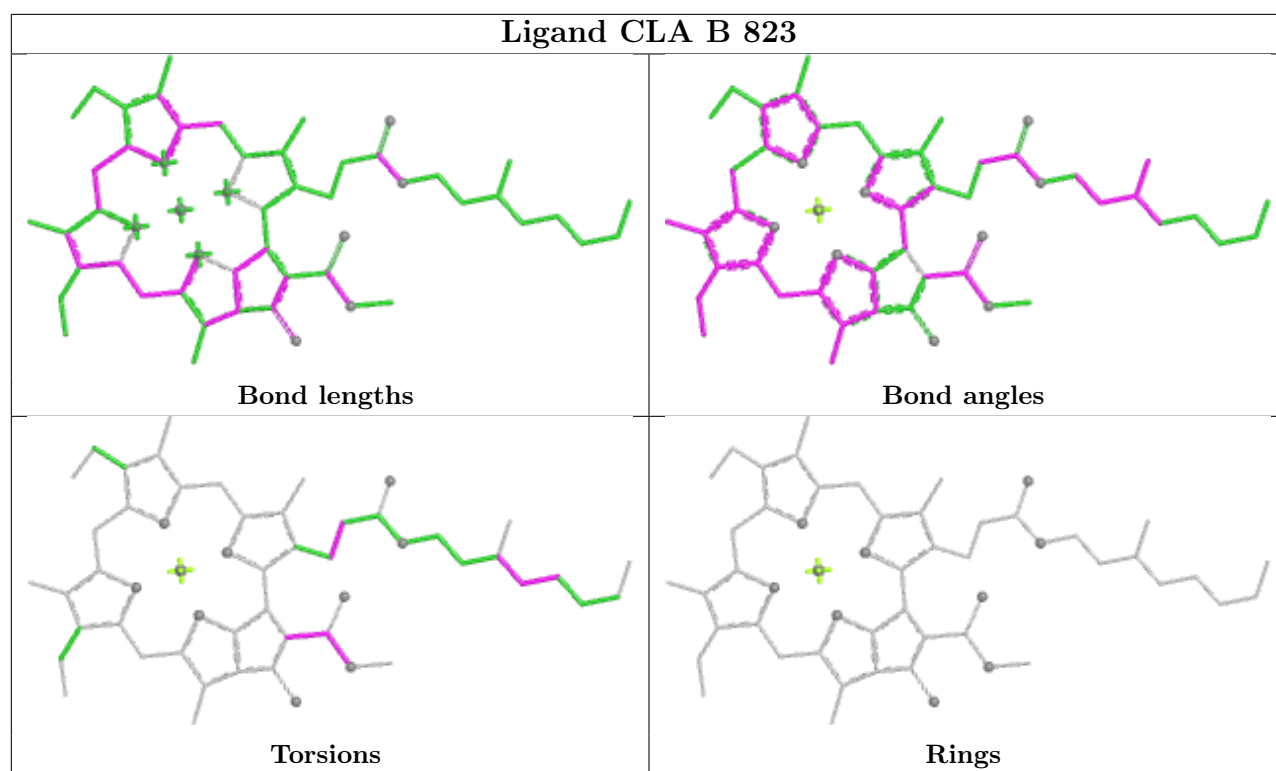
Bond angles



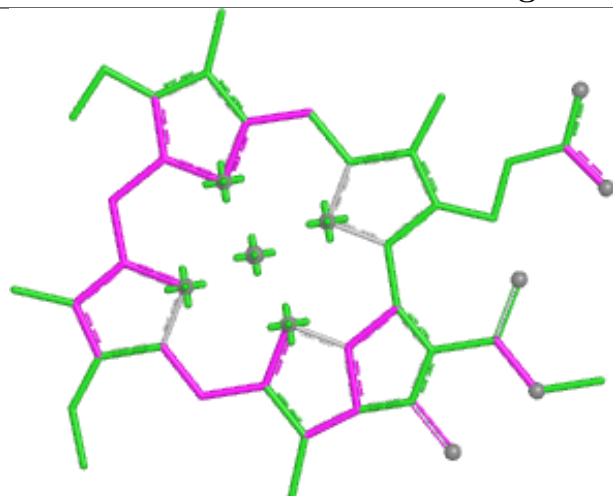
Torsions



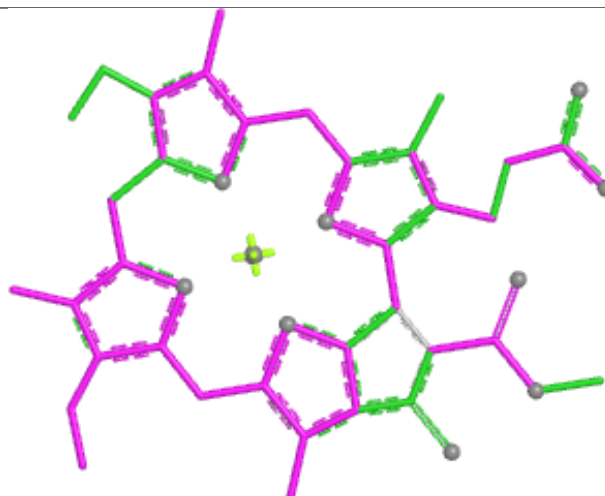
Rings



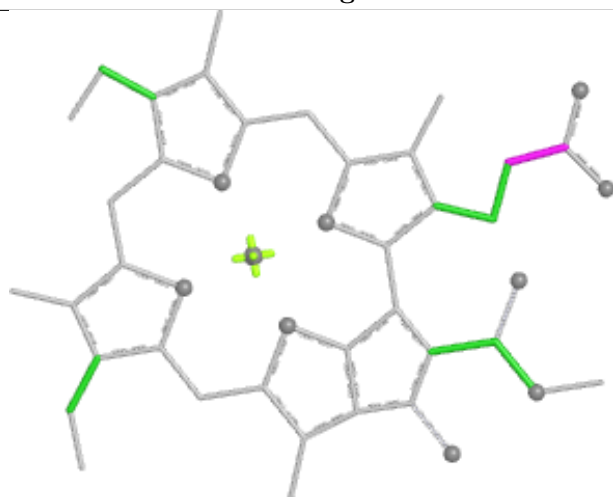
Ligand CLA 3 714



Bond lengths



Bond angles

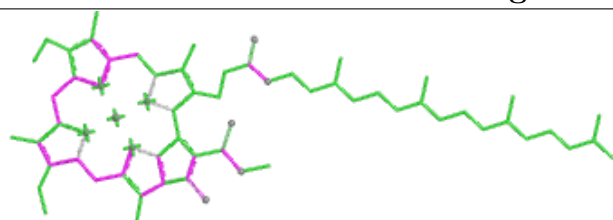


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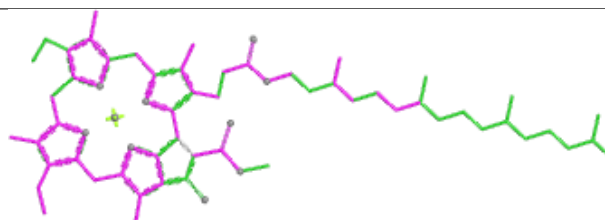


Rings

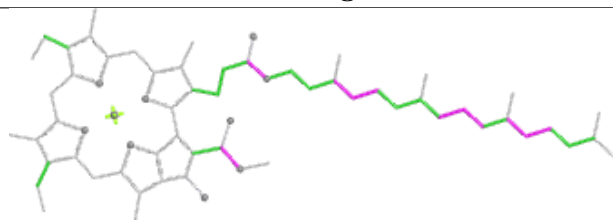
Ligand CLA 11 706



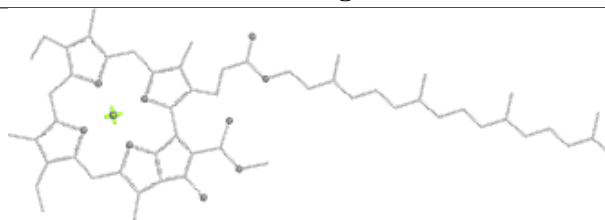
Bond lengths



Bond angles

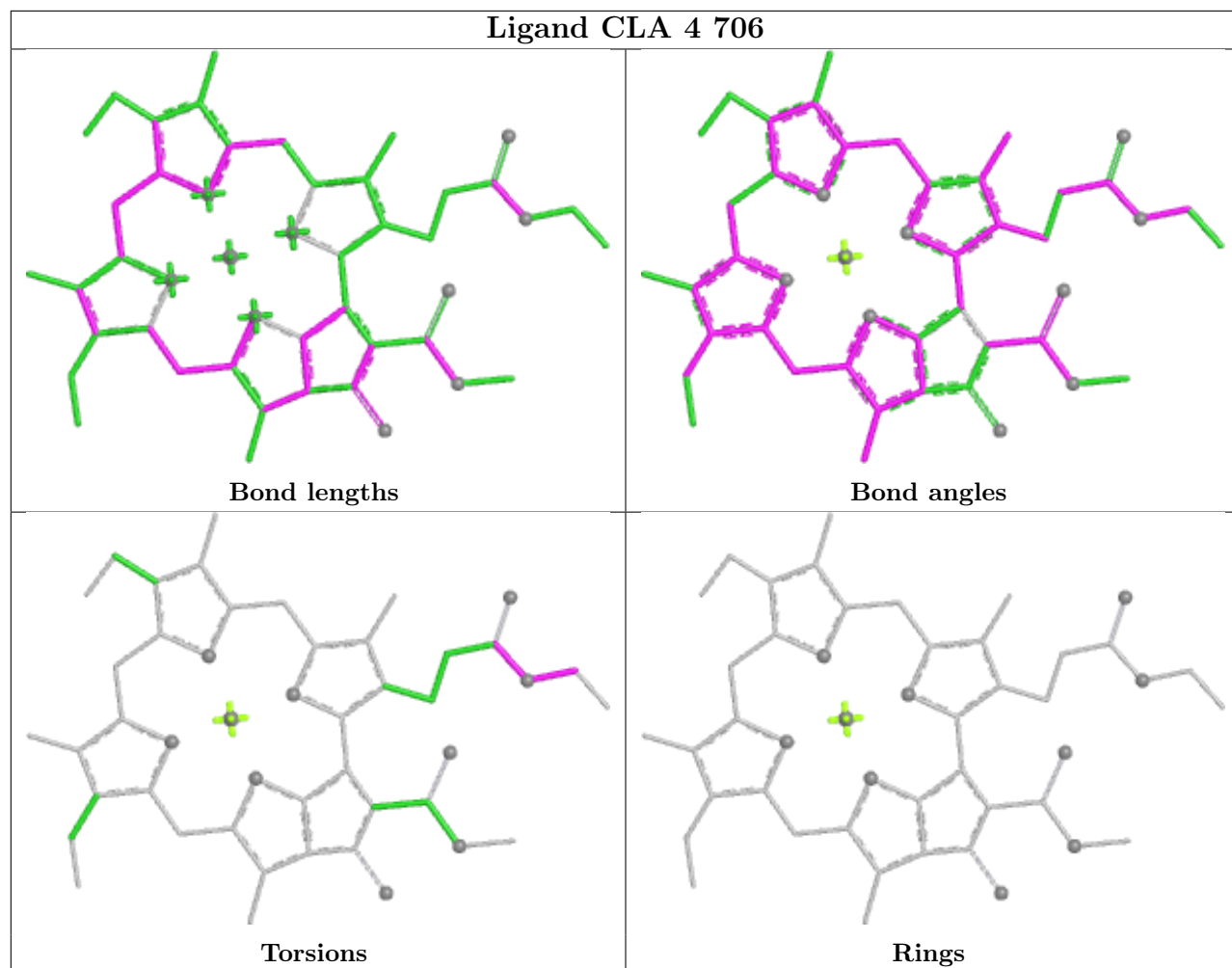


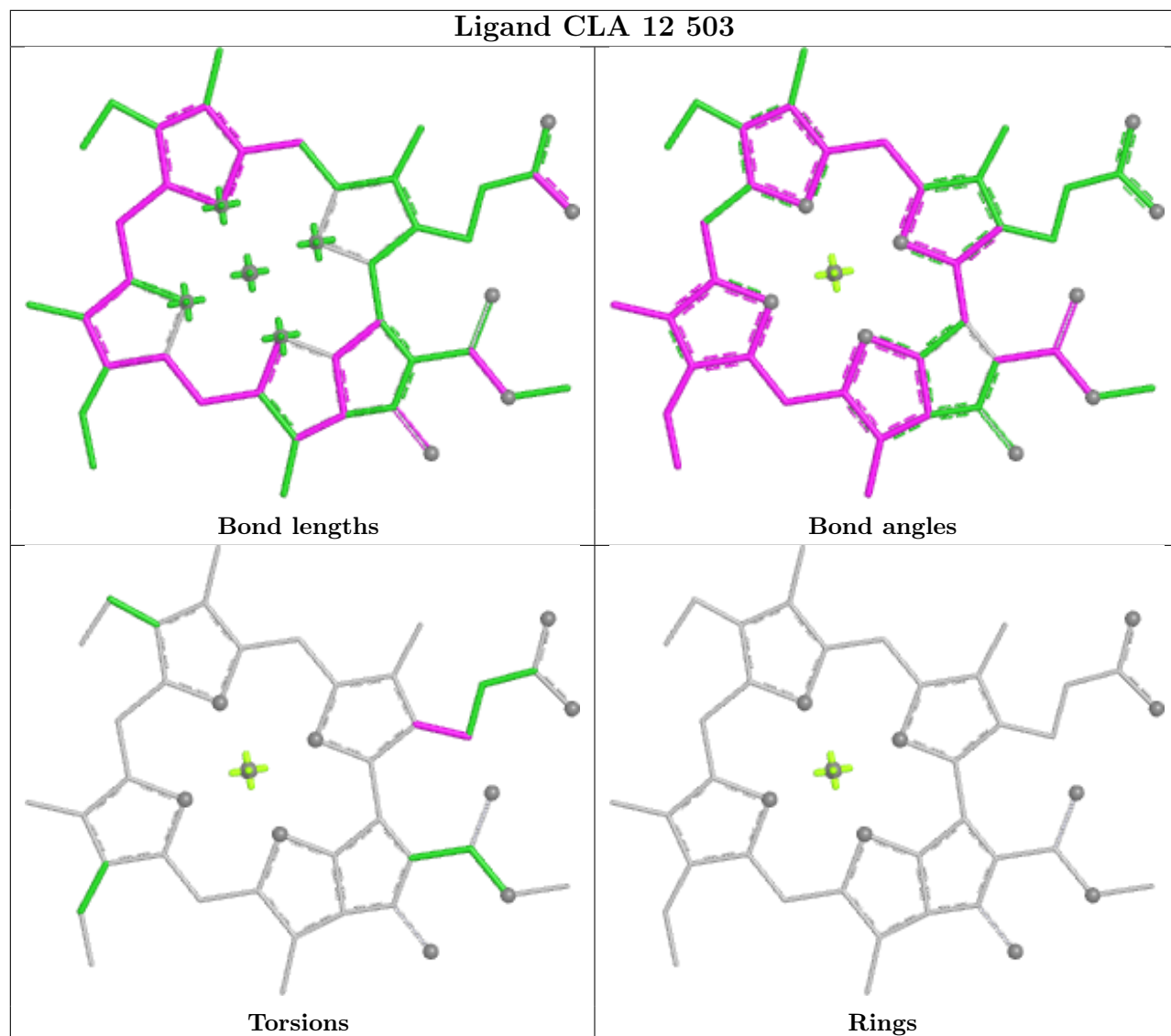
Torsions

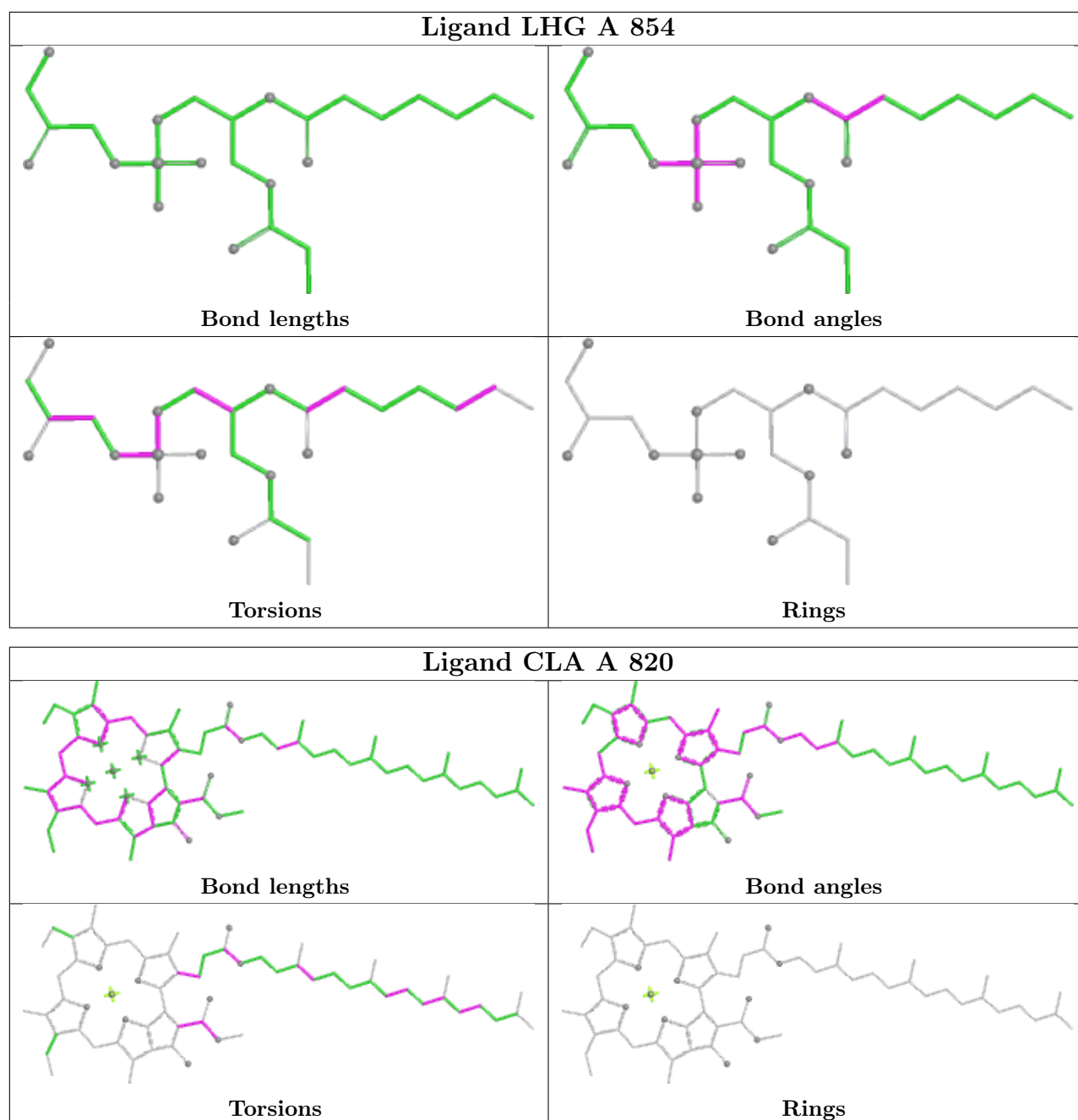


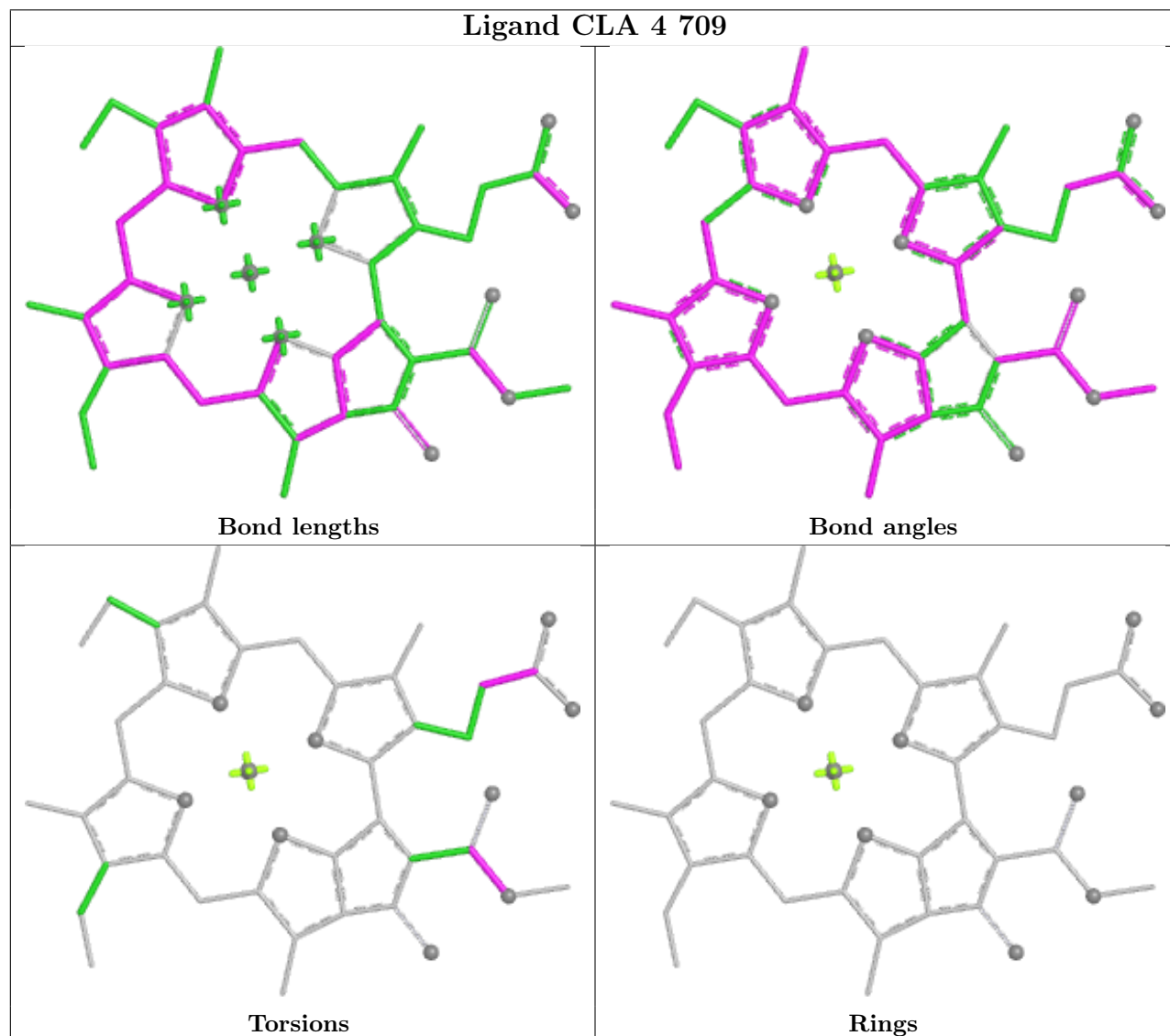
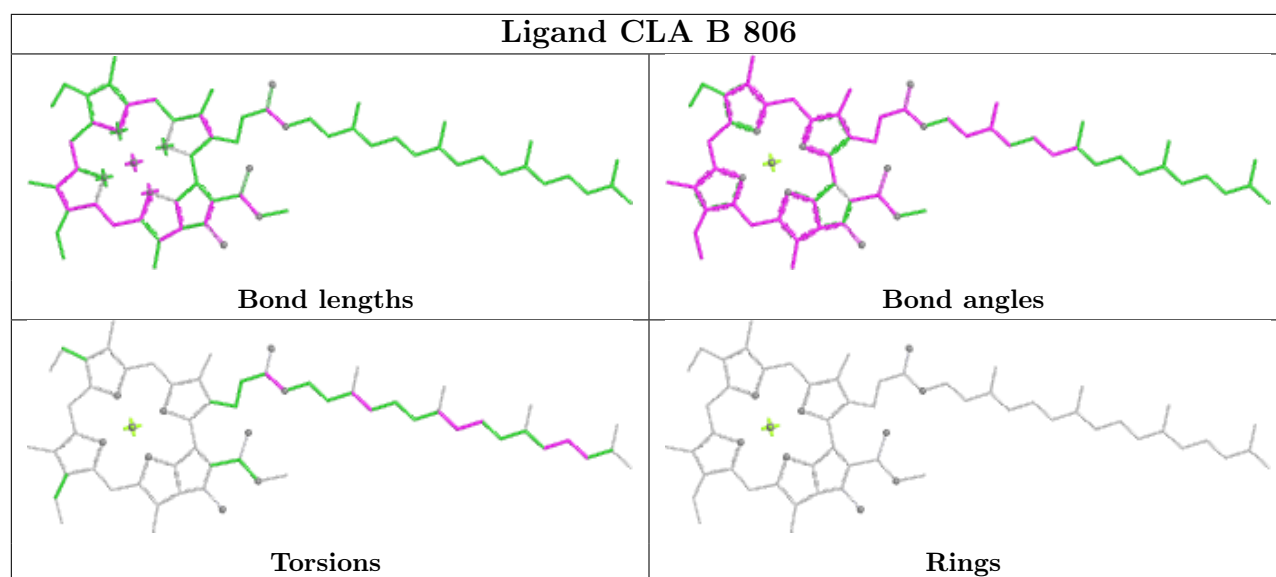
Rings

Ligand CLA 4 706

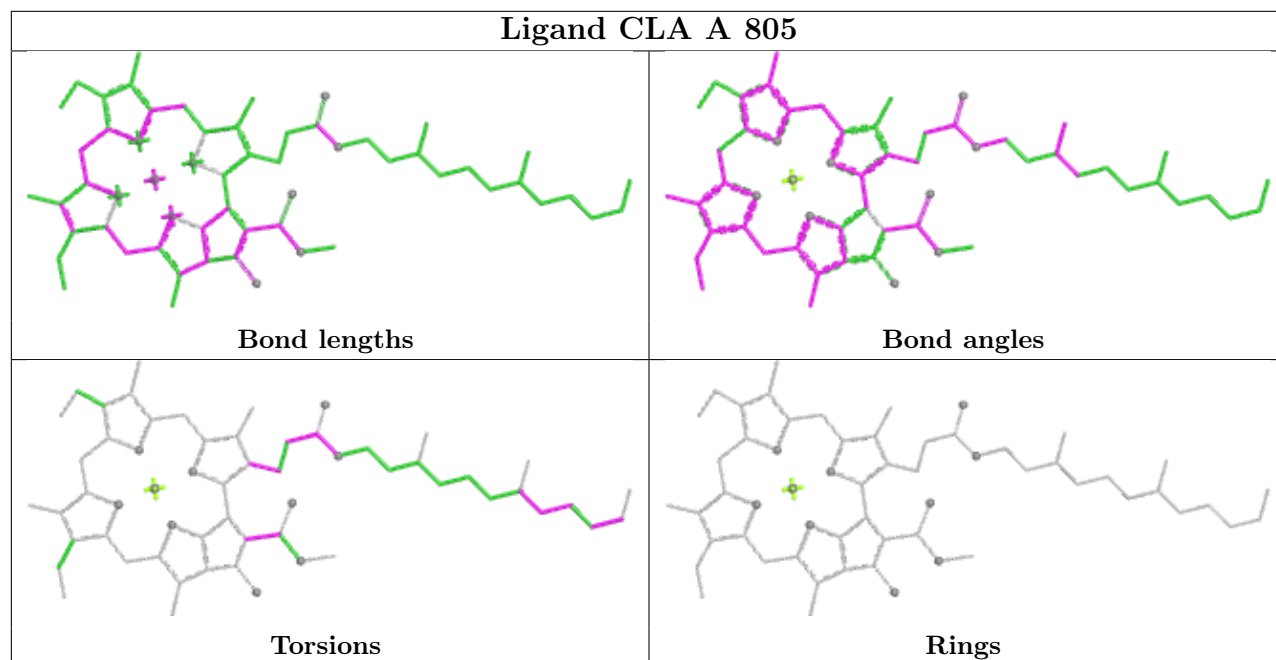




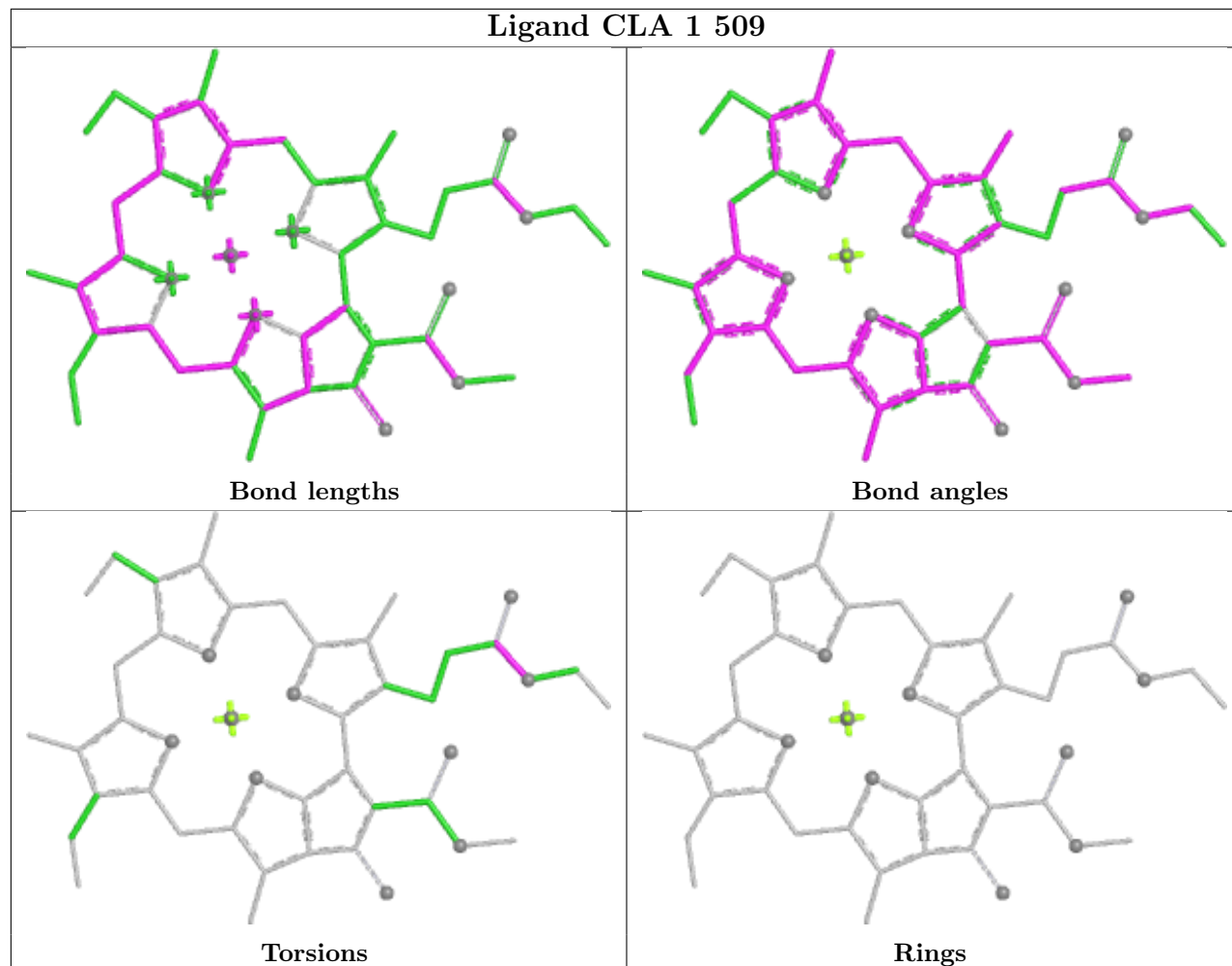




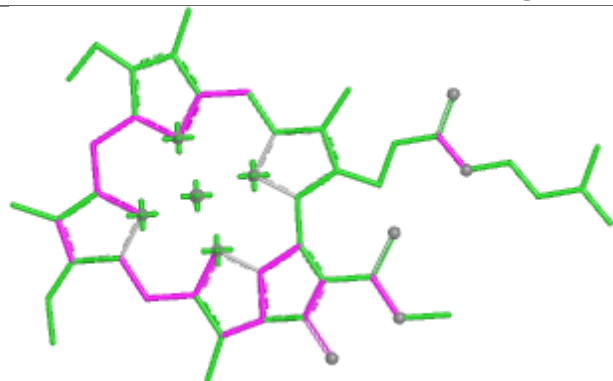
Ligand CLA A 805



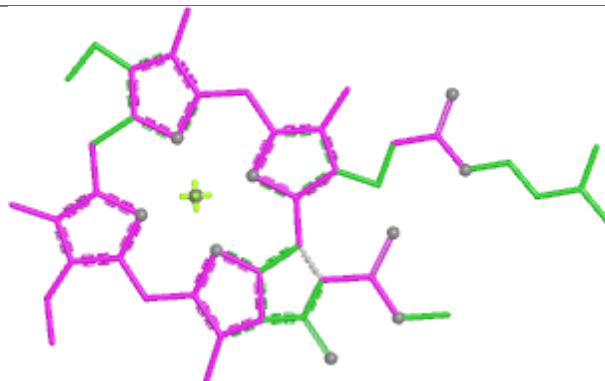
Ligand CLA 1 509



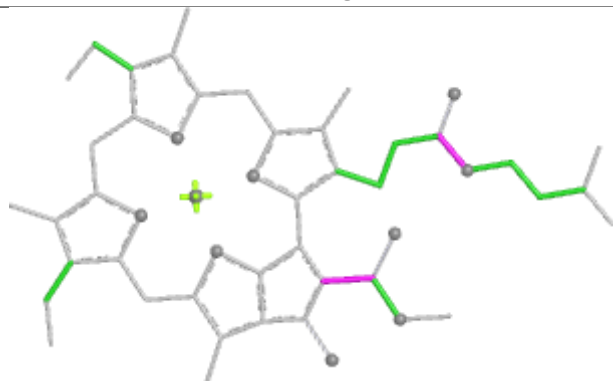
Ligand CLA 2 506



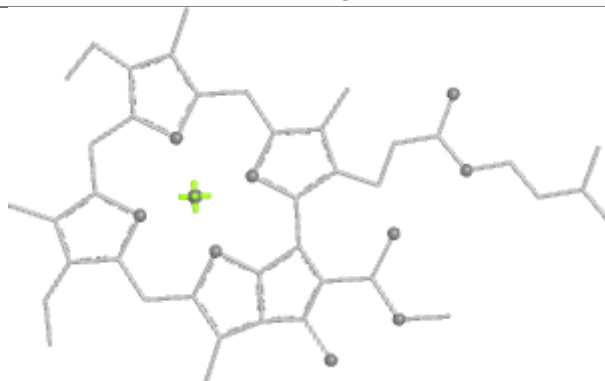
Bond lengths



Bond angles

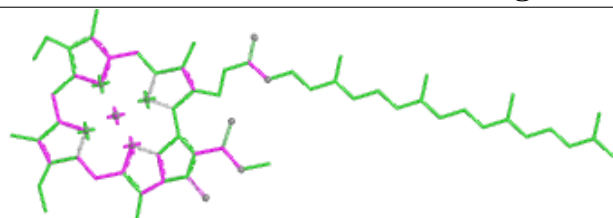


Torsions

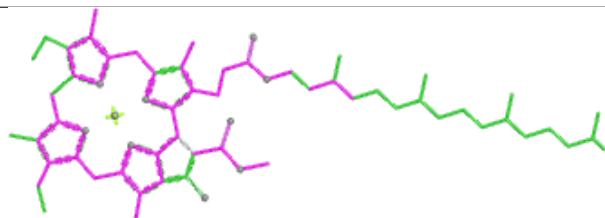


Rings

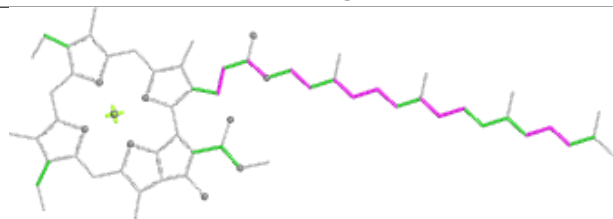
Ligand CLA A 803



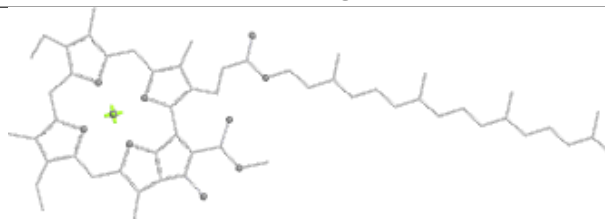
Bond lengths



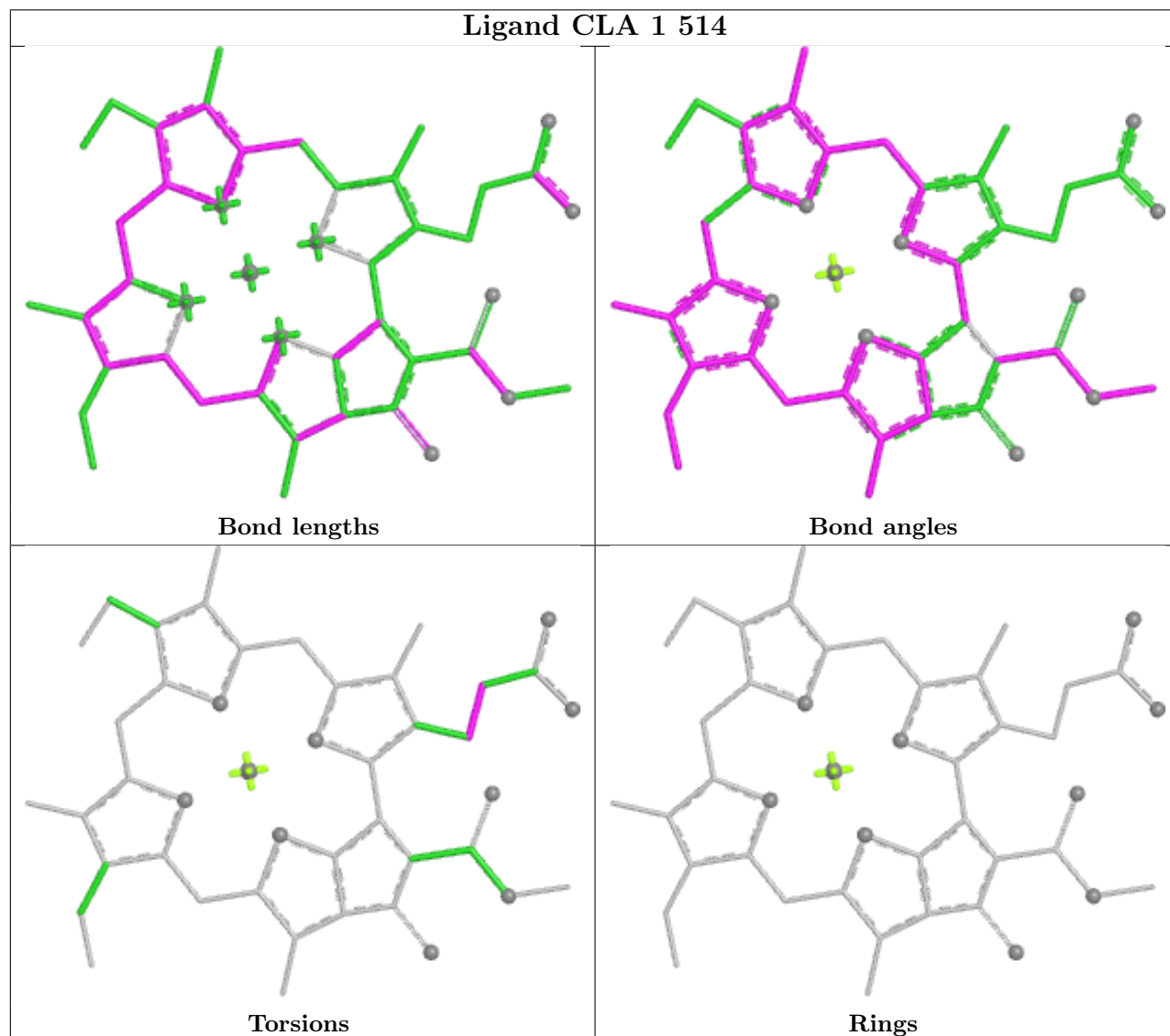
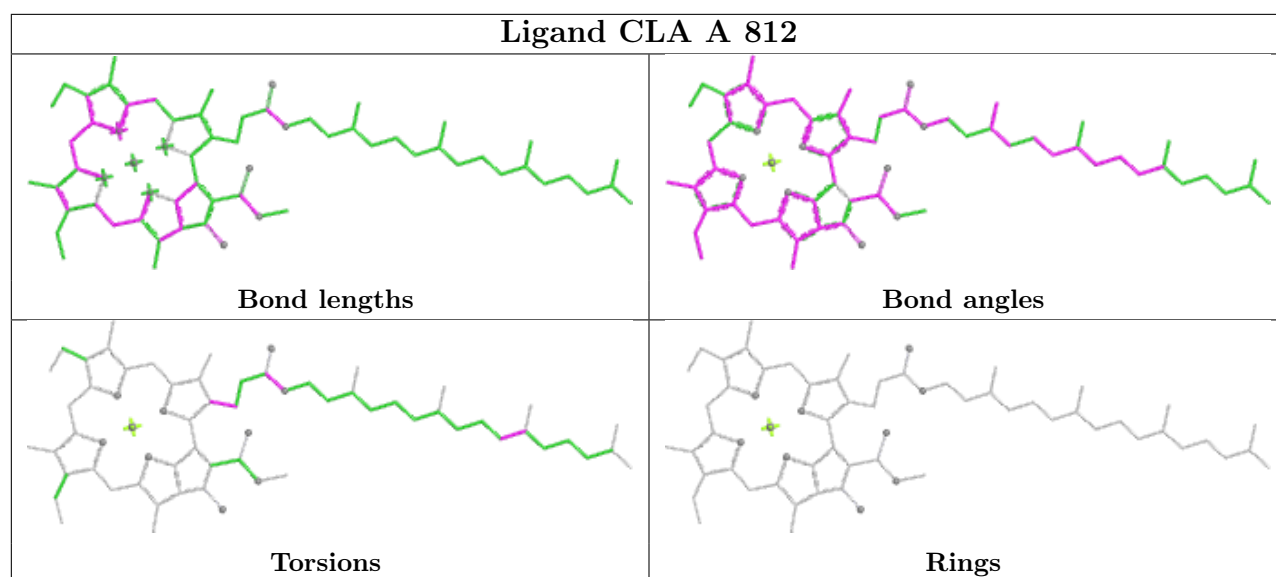
Bond angles

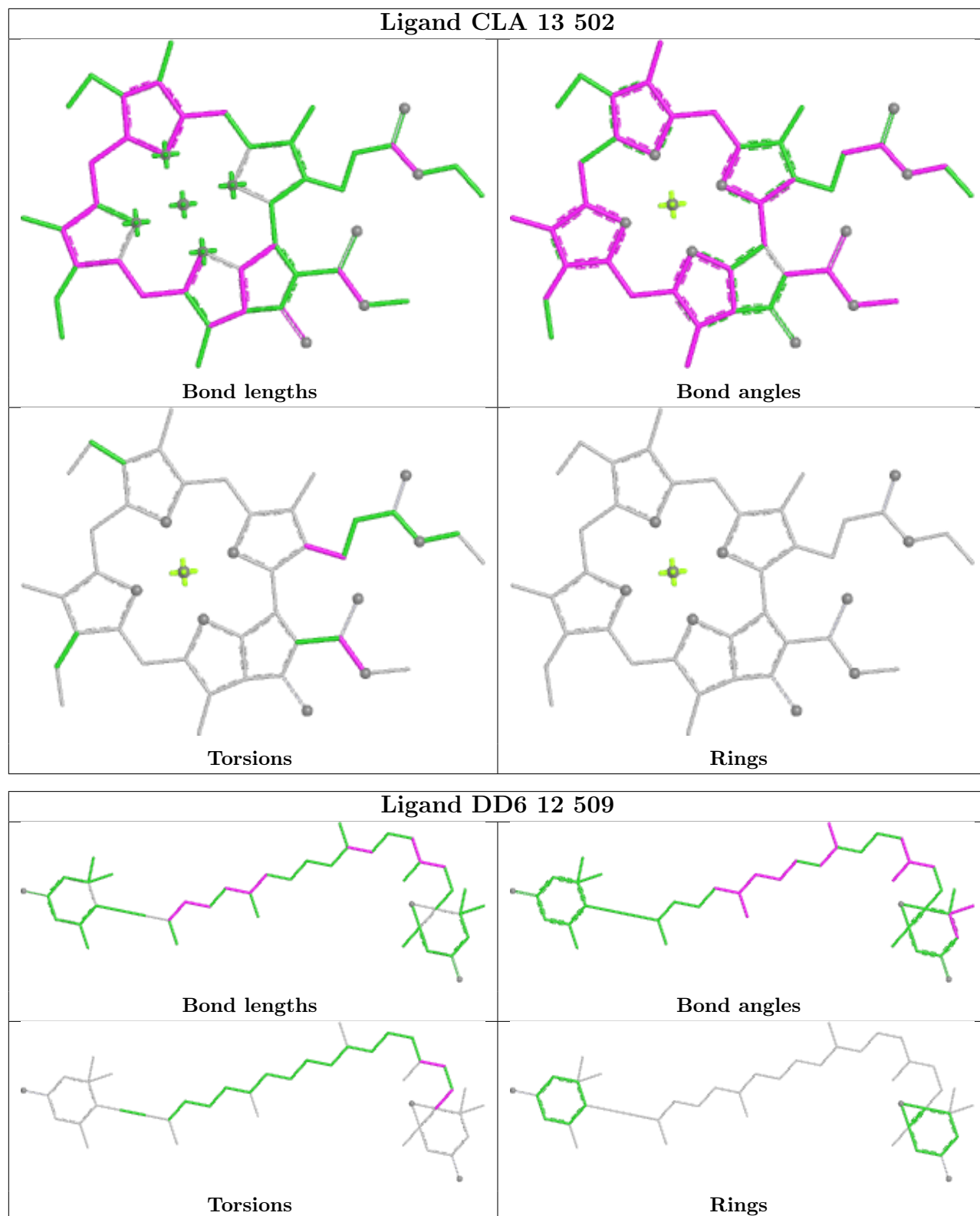


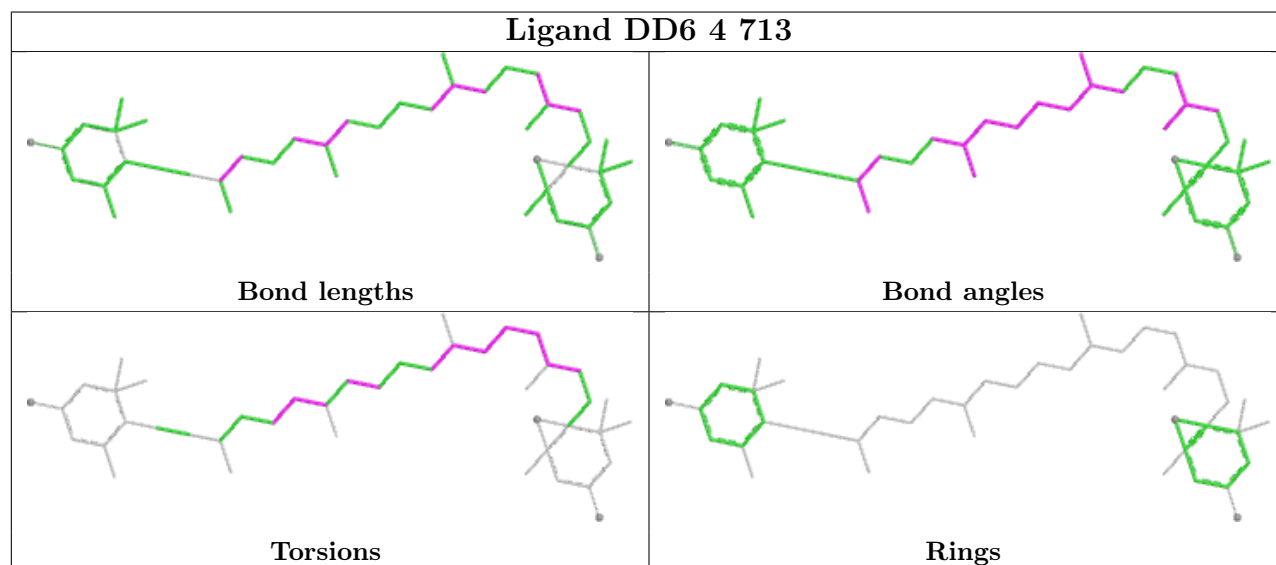
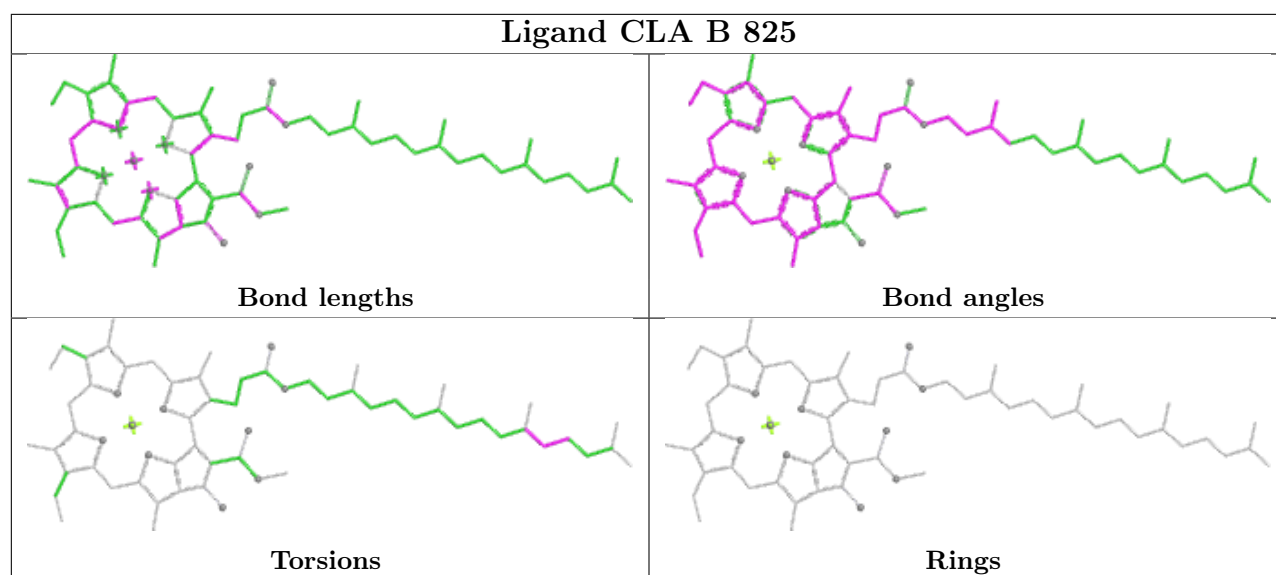
Torsions

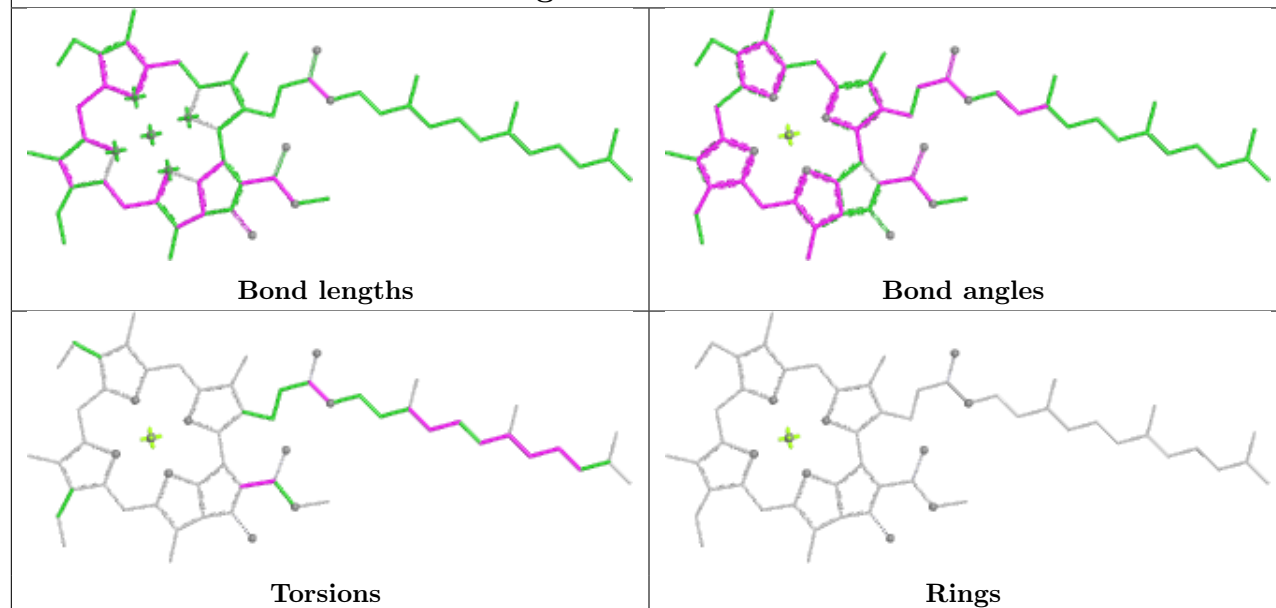
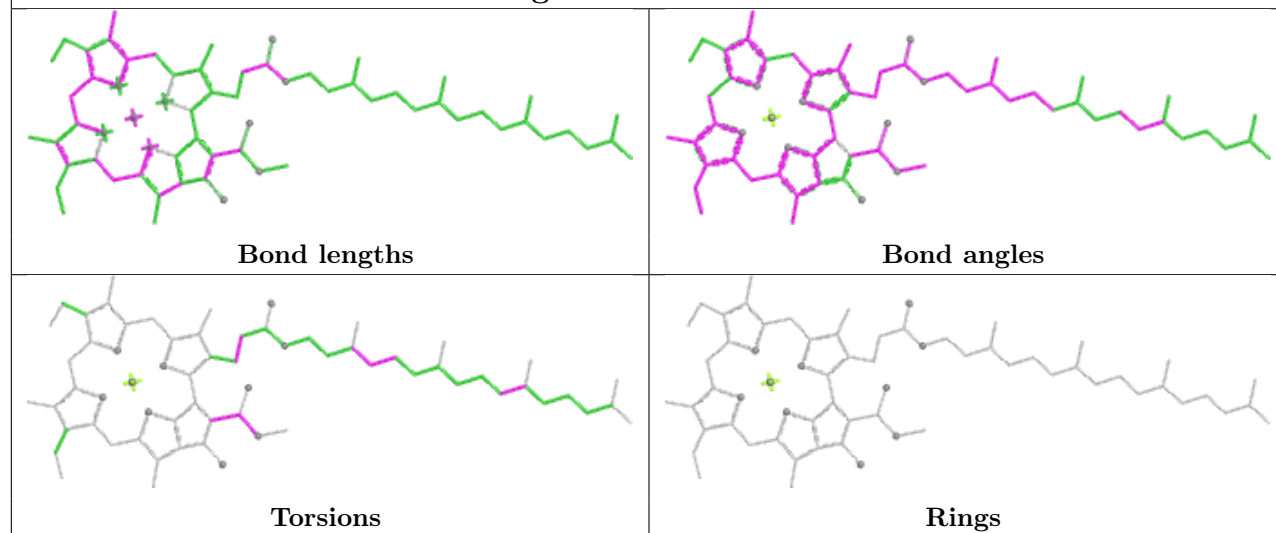


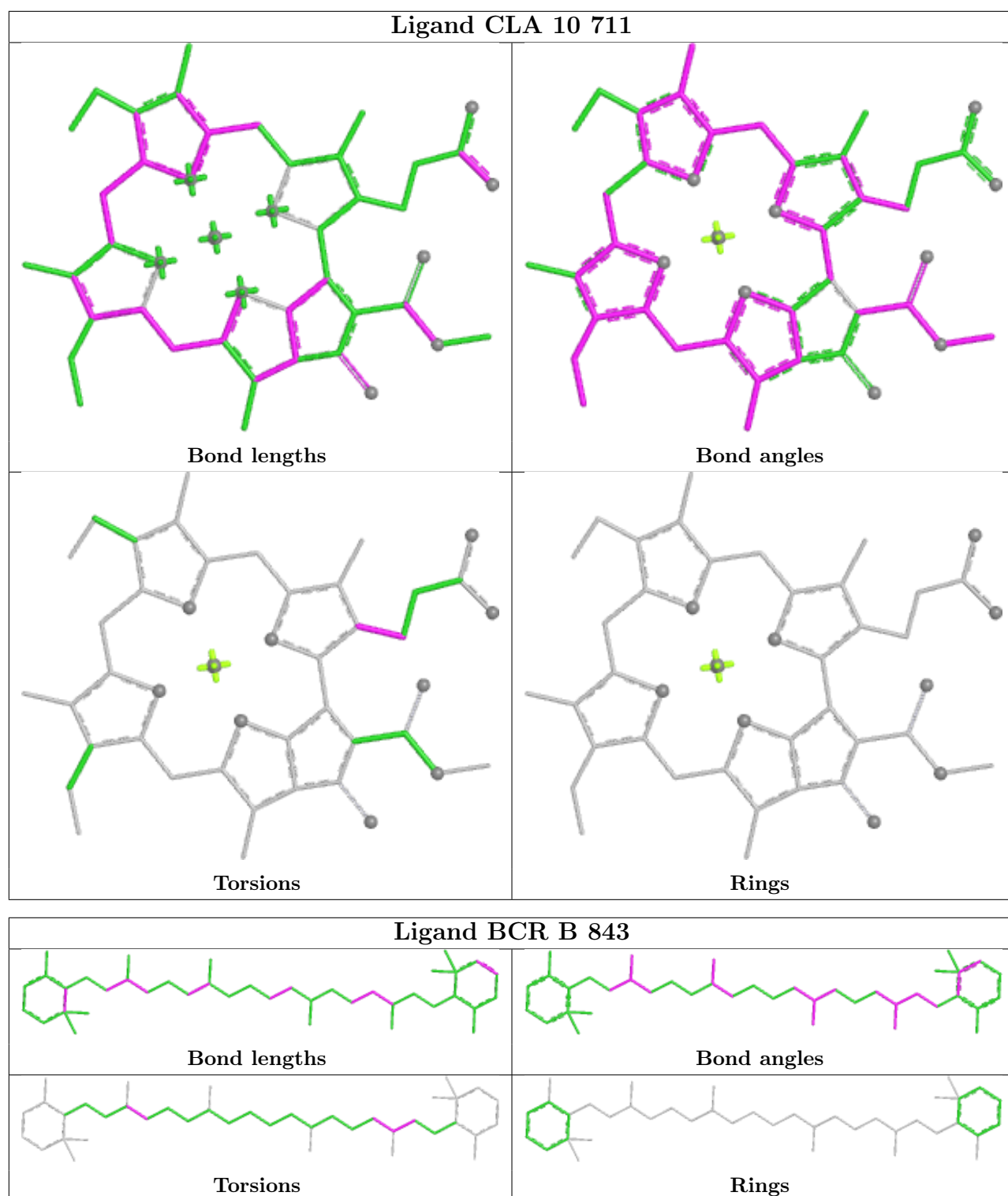
Rings



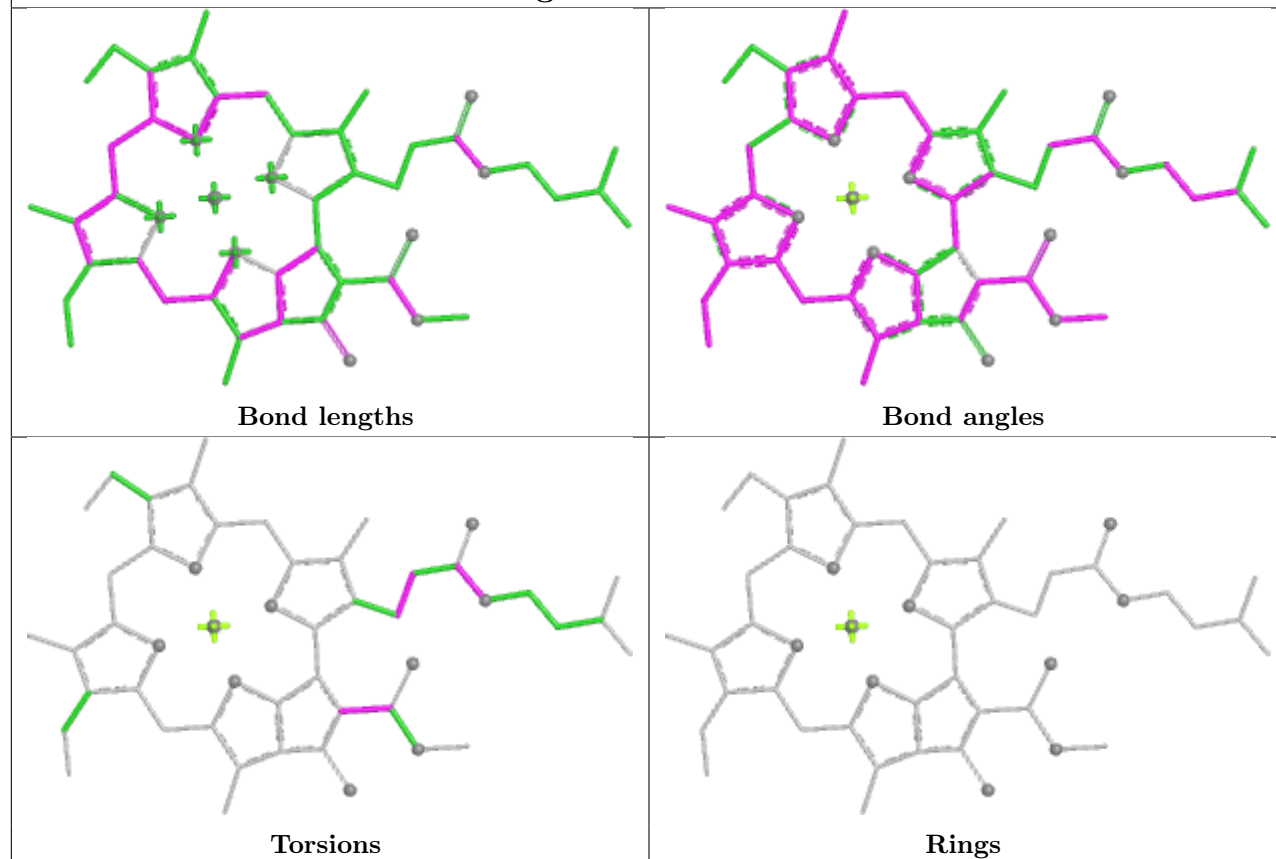




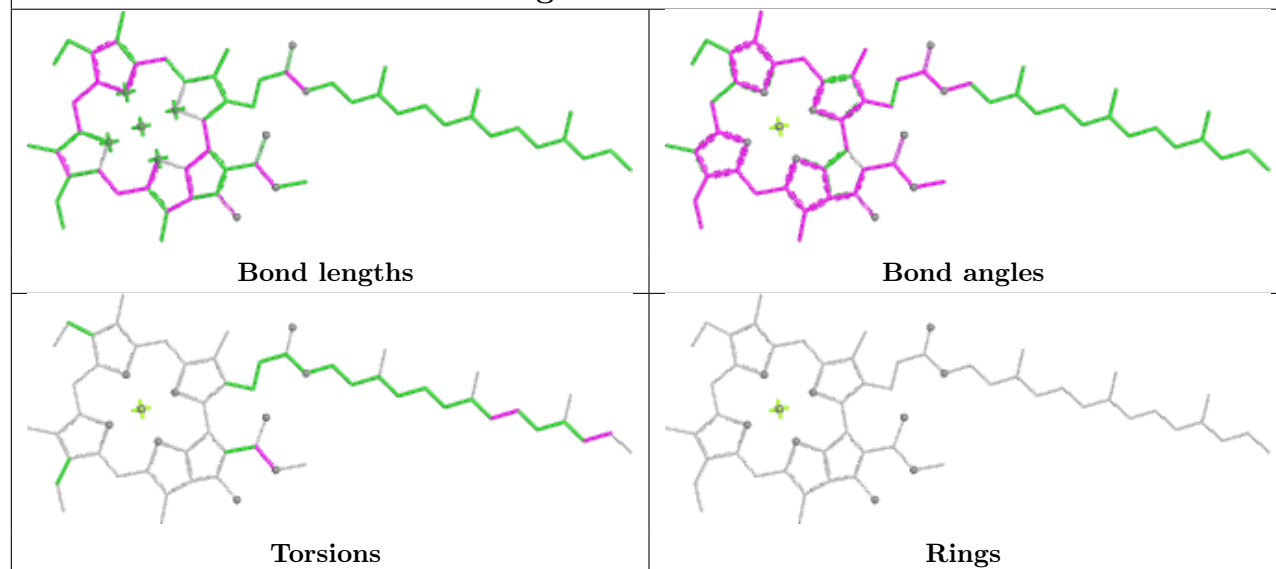
Ligand CLA 7 703**Ligand CLA A 862**

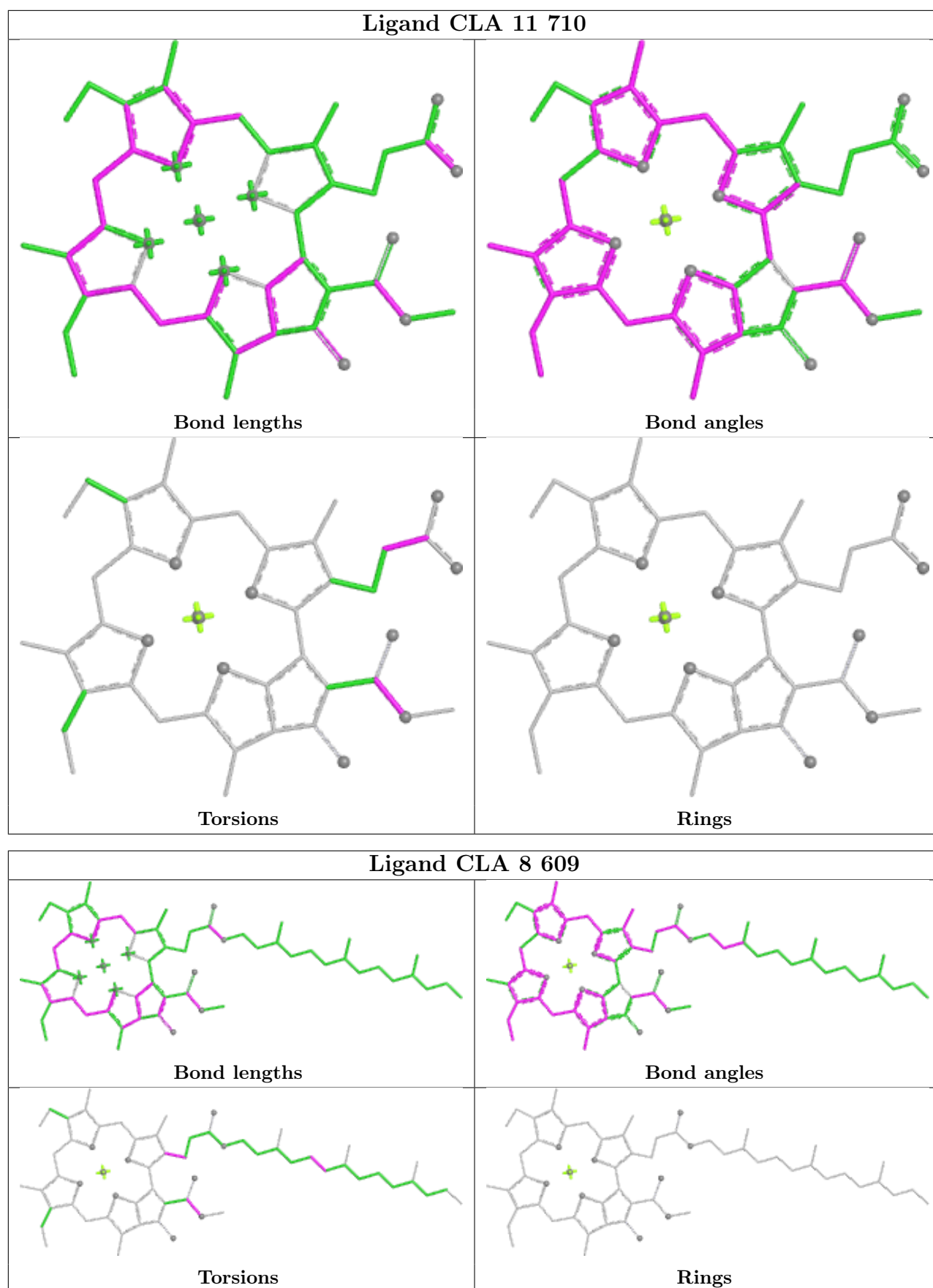


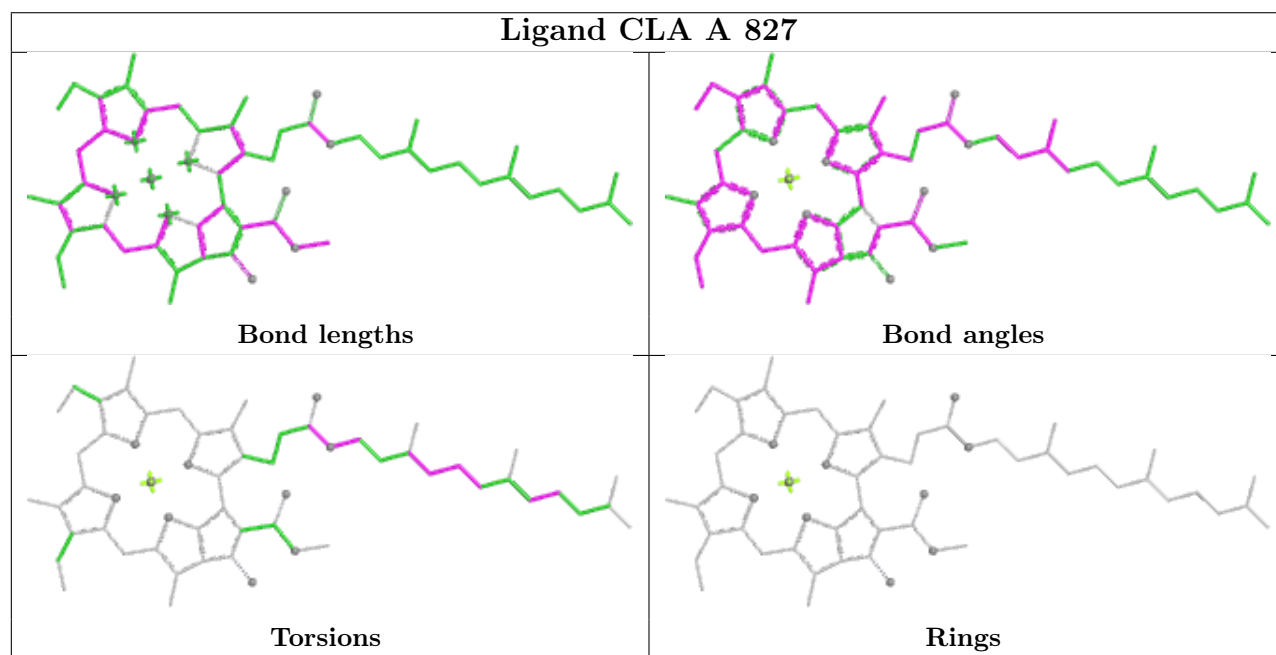
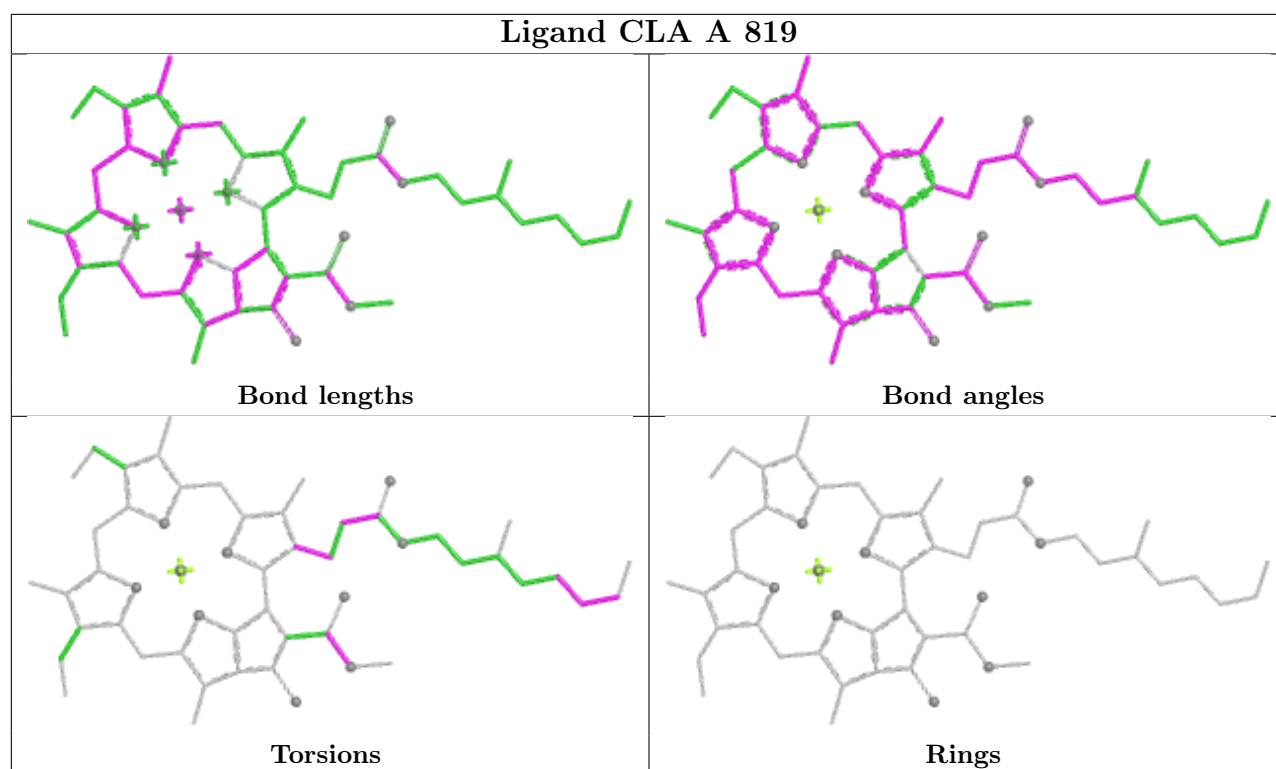
Ligand CLA 9 905



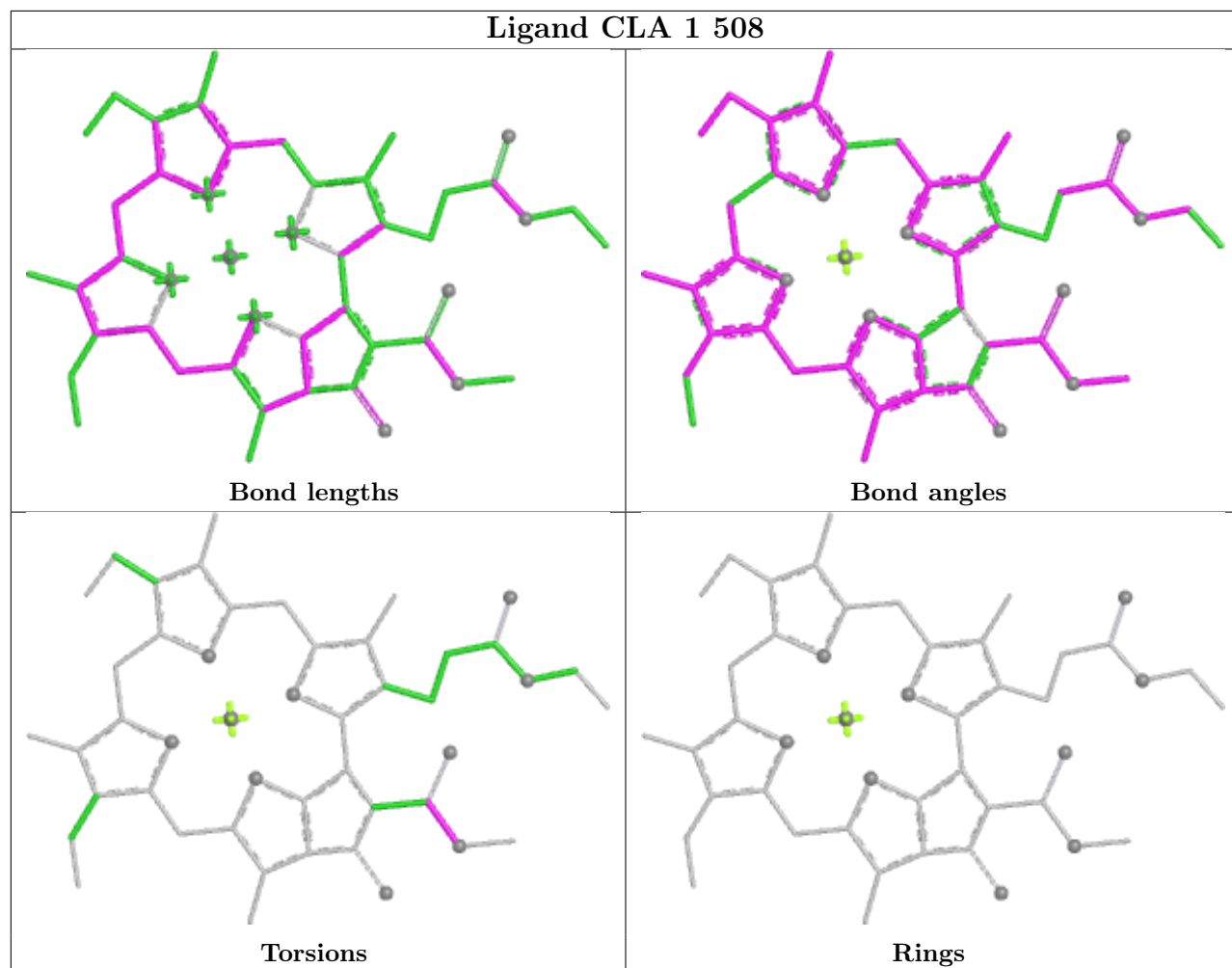
Ligand CLA 4 707



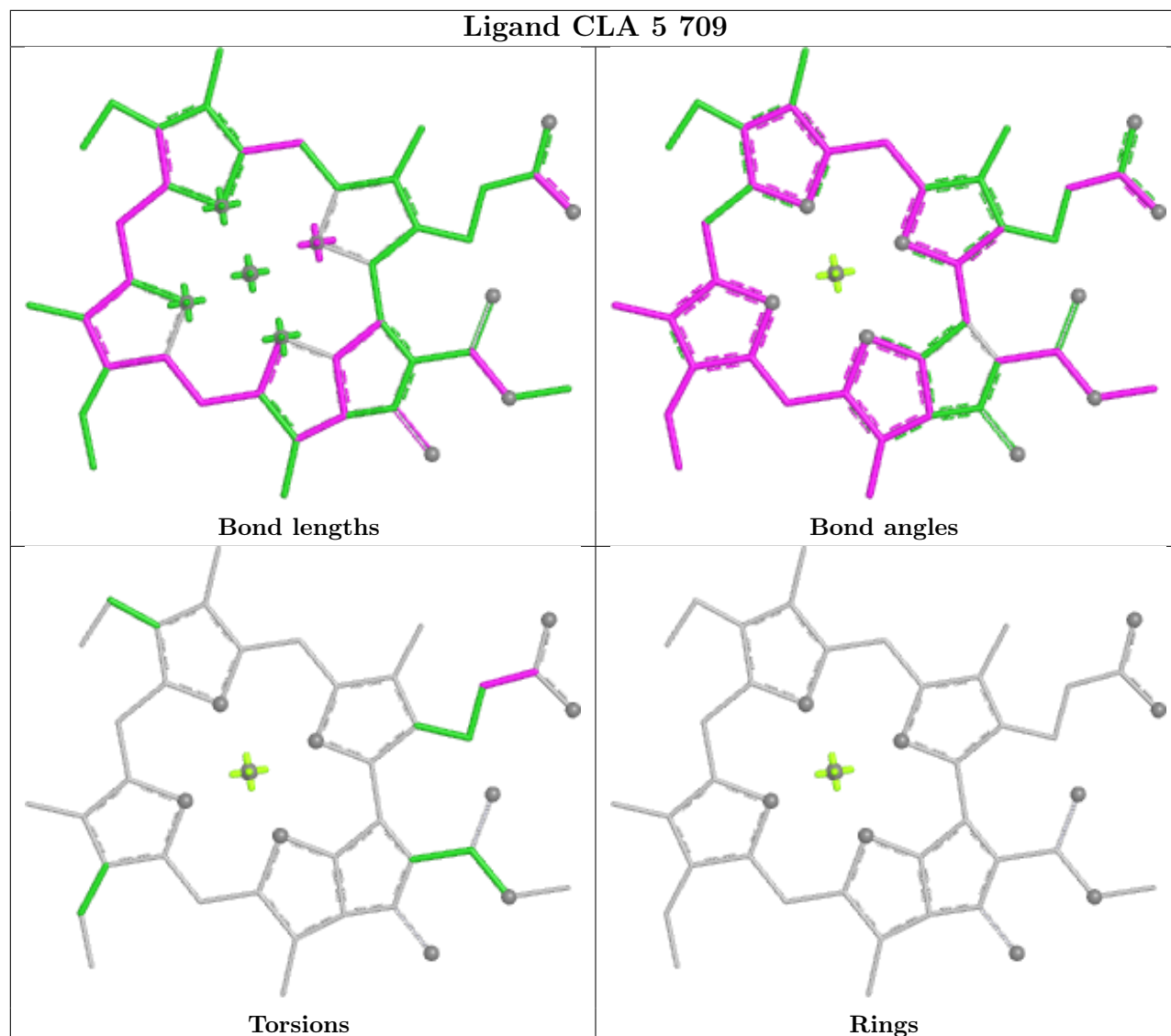




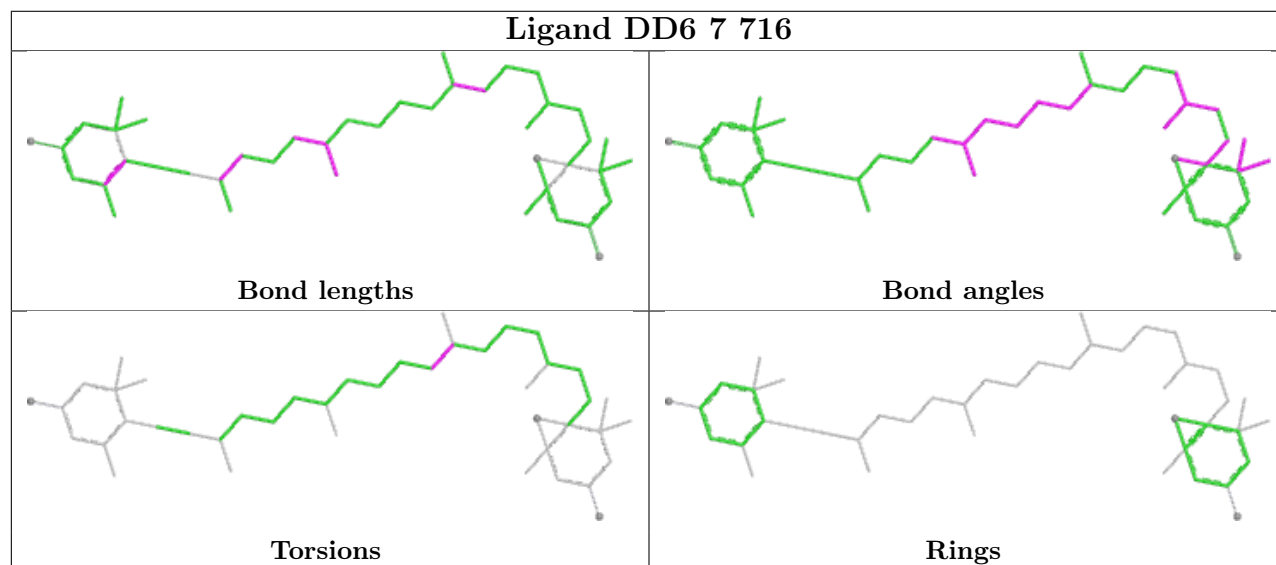
Ligand CLA 1 508

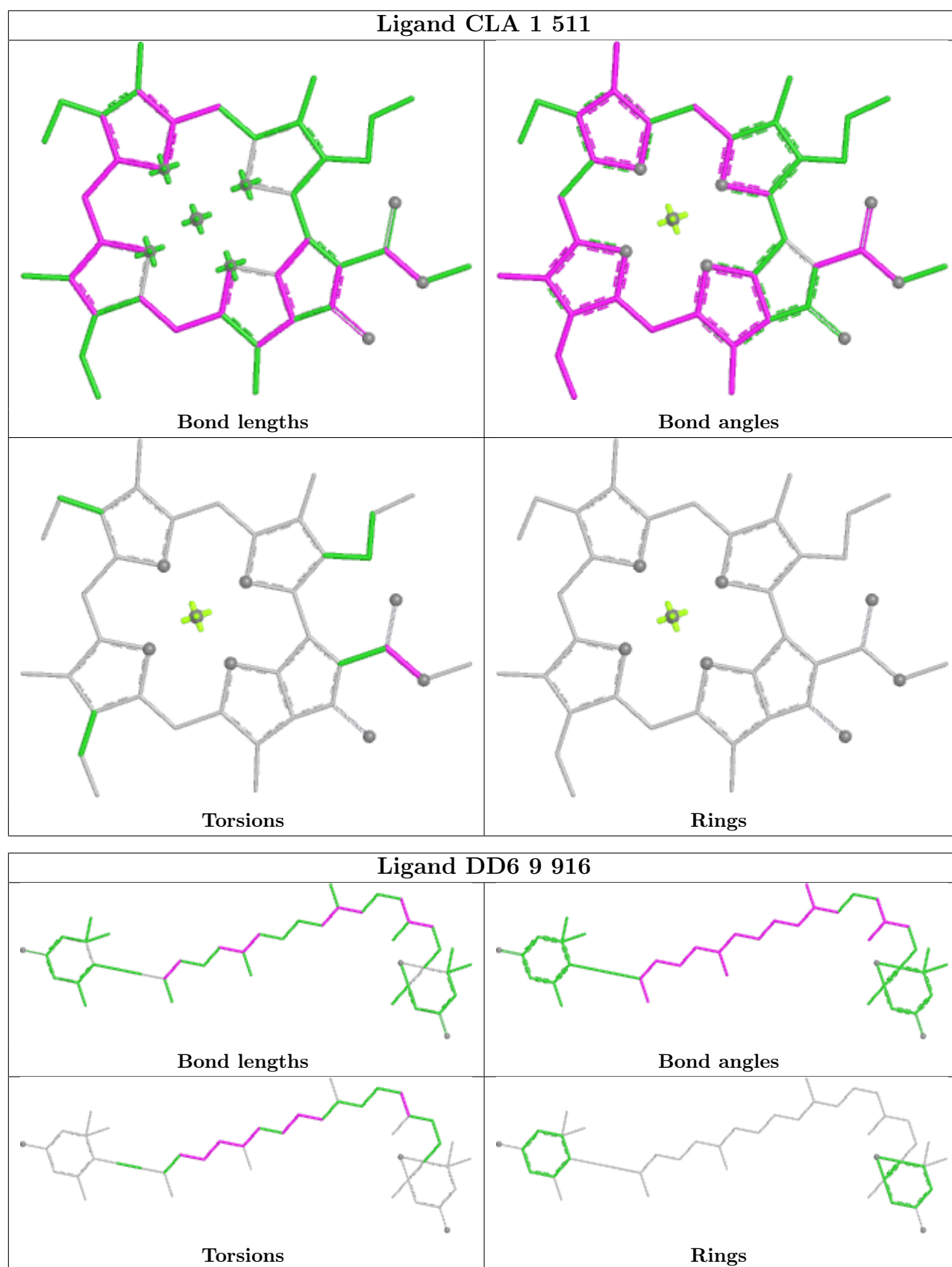


Ligand CLA 5 709

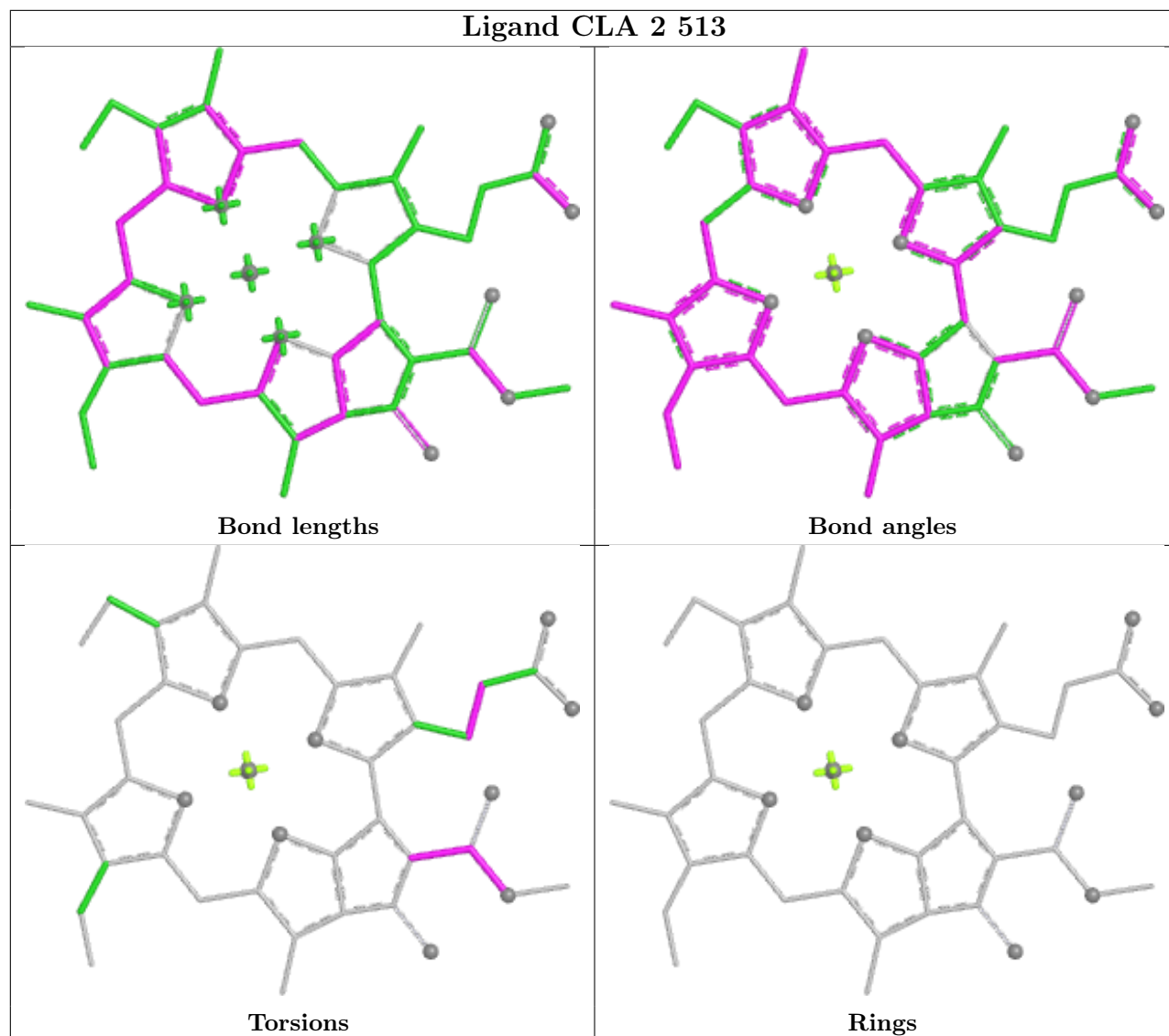


Ligand DD6 7 716

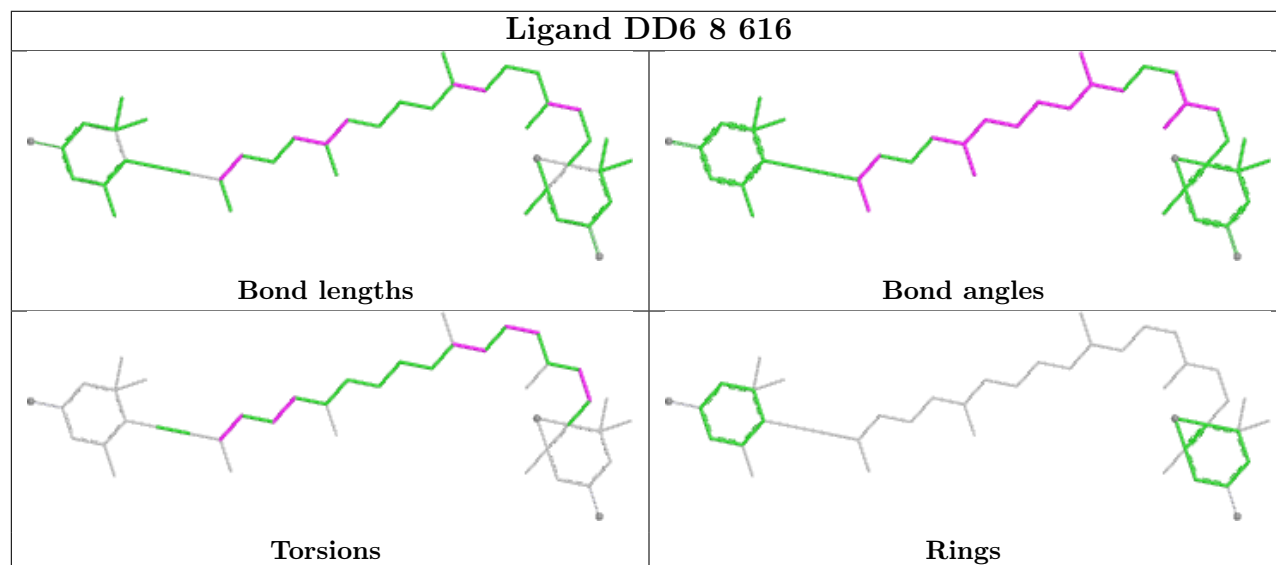




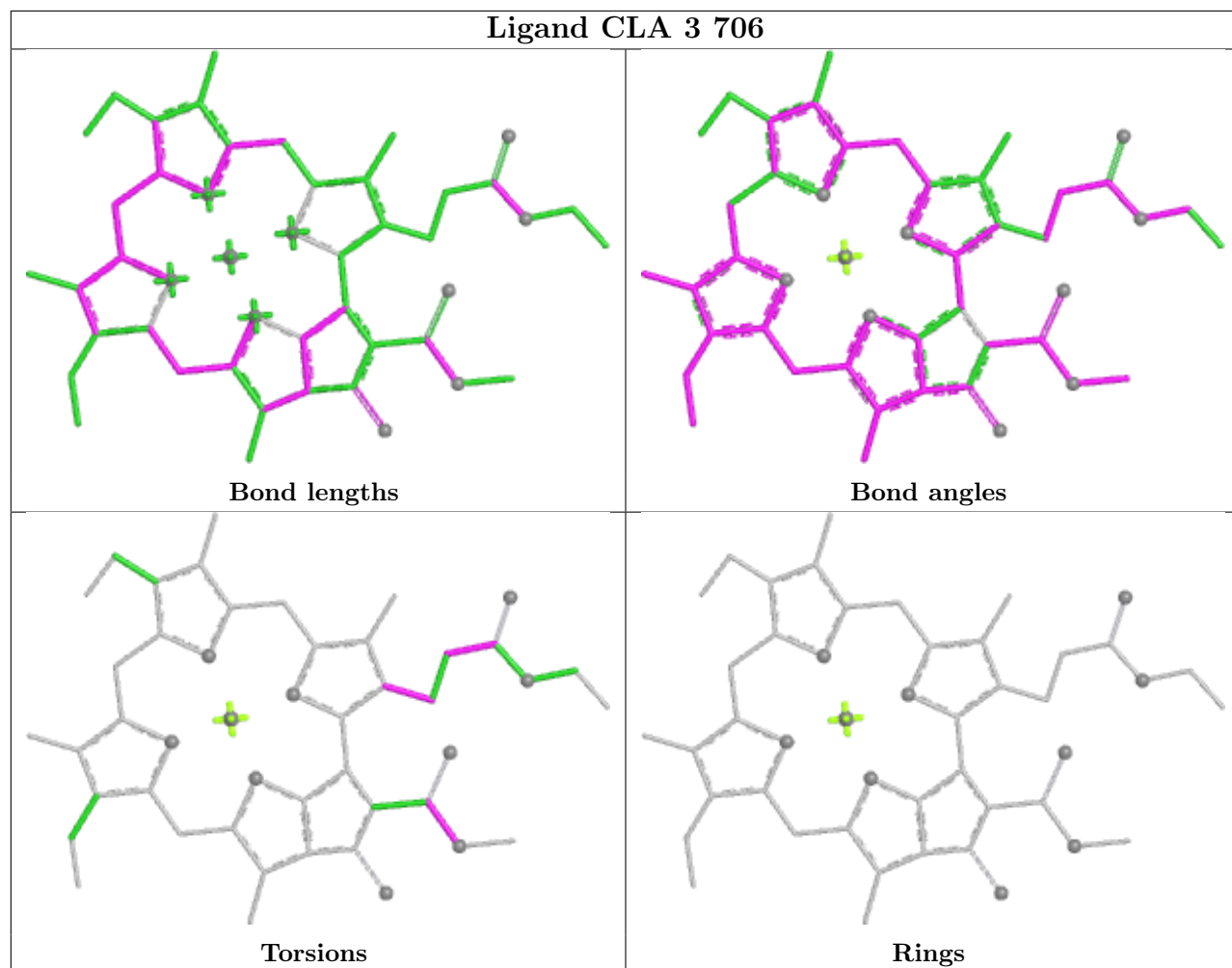
Ligand CLA 2 513



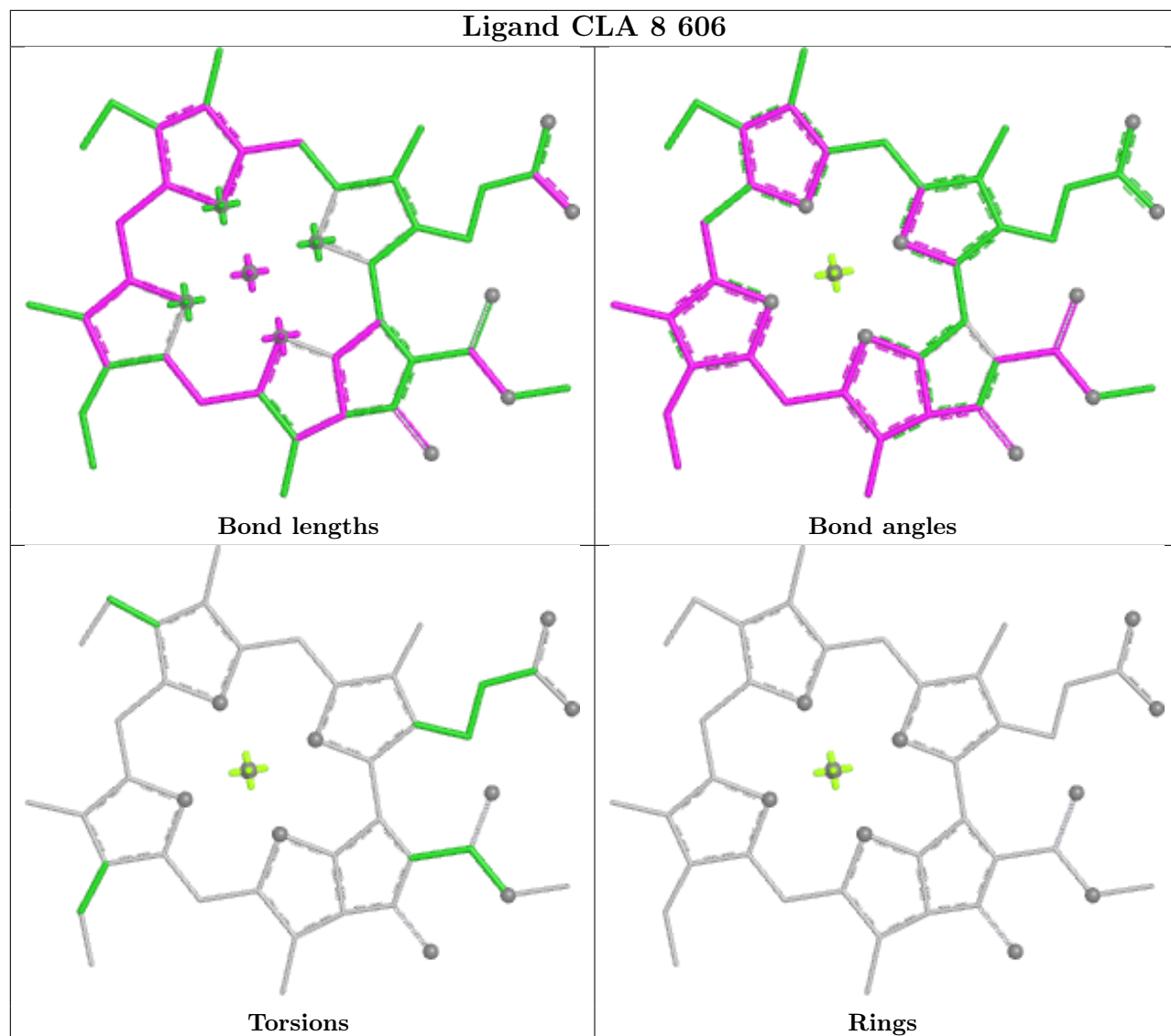
Ligand DD6 8 616

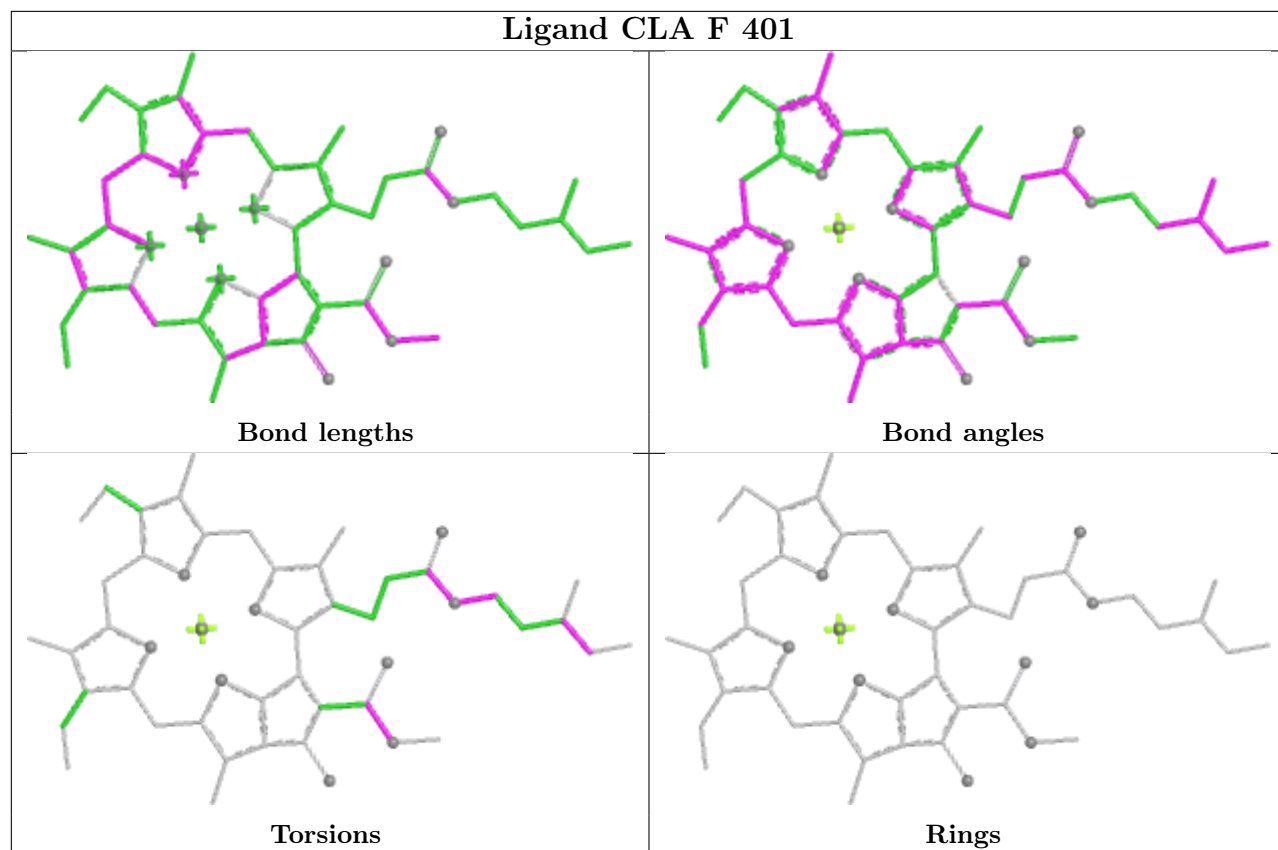


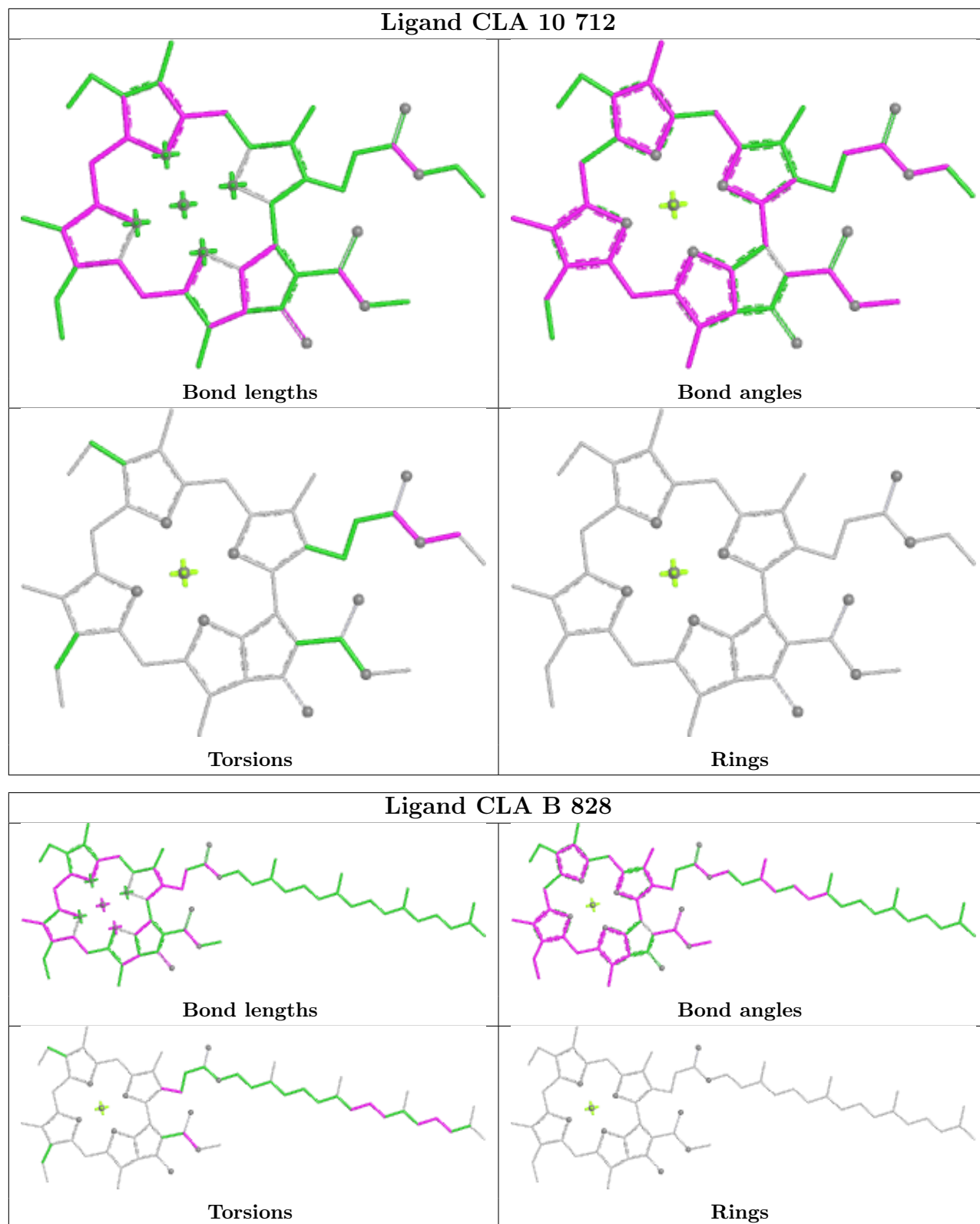
Ligand CLA 3 706



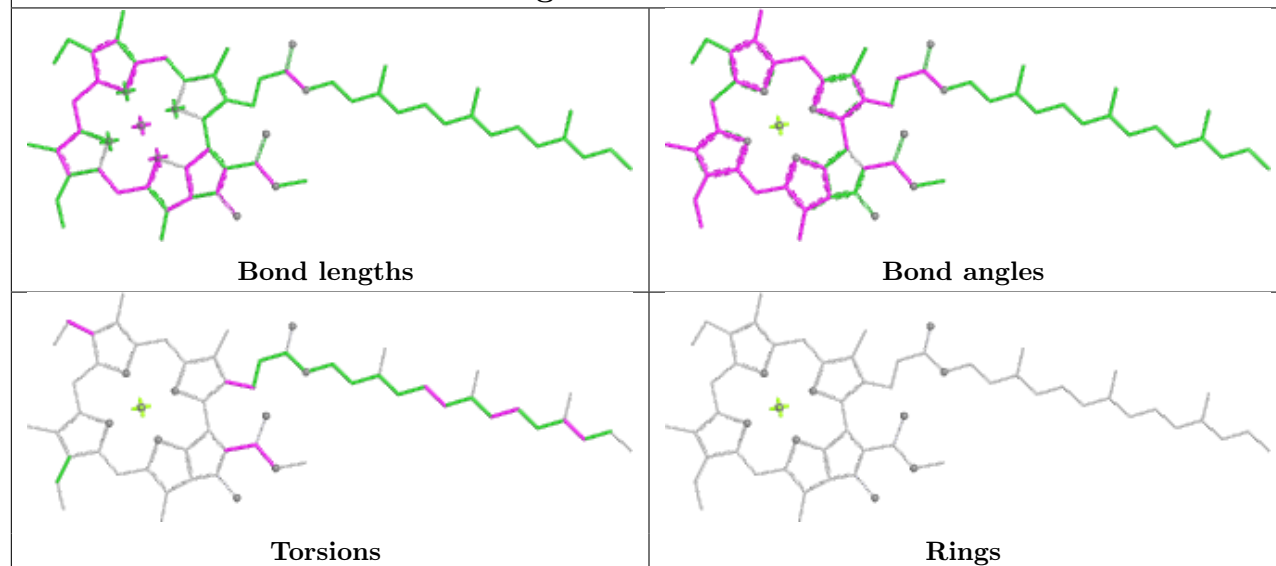
Ligand CLA 8 606



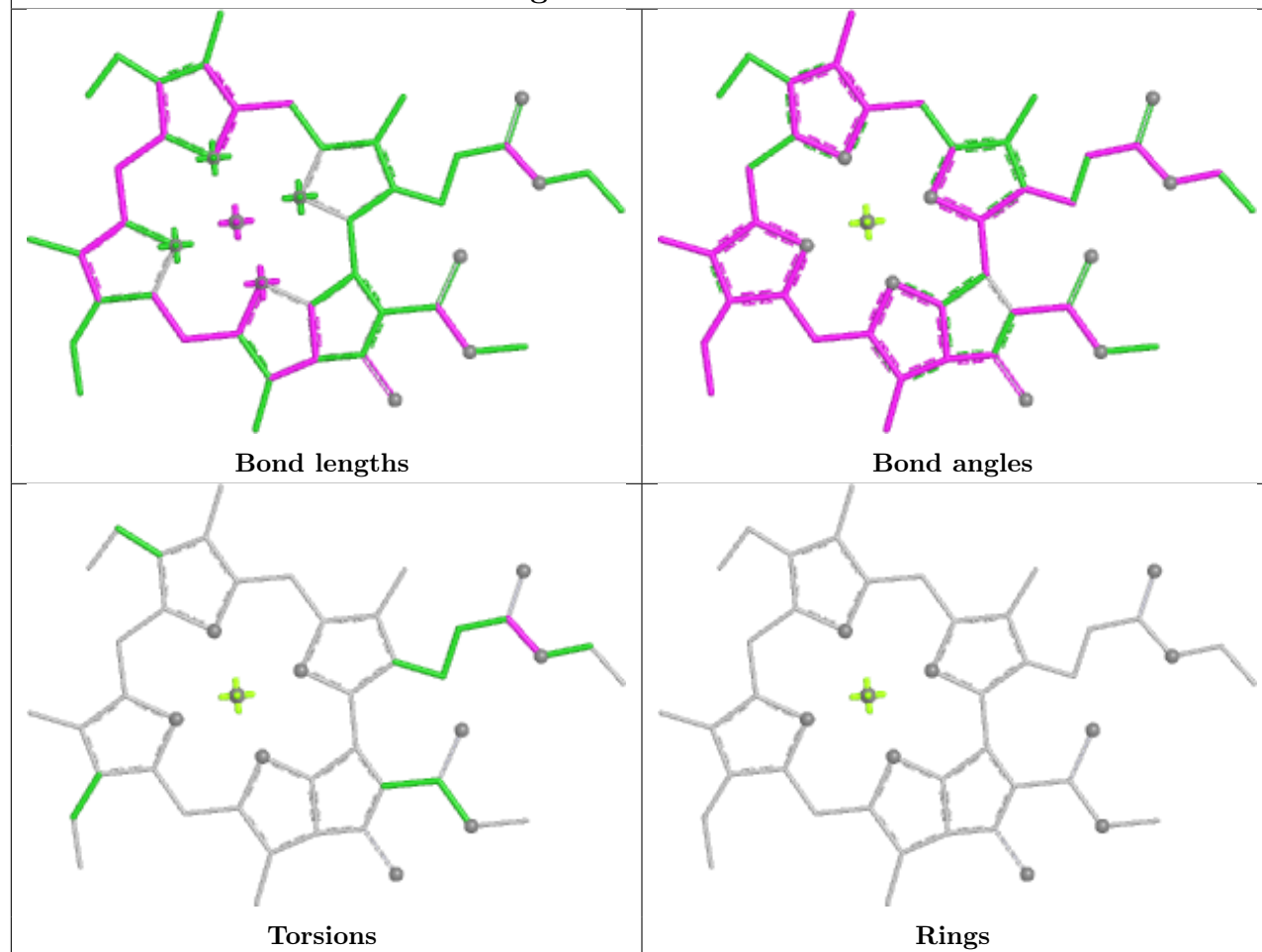




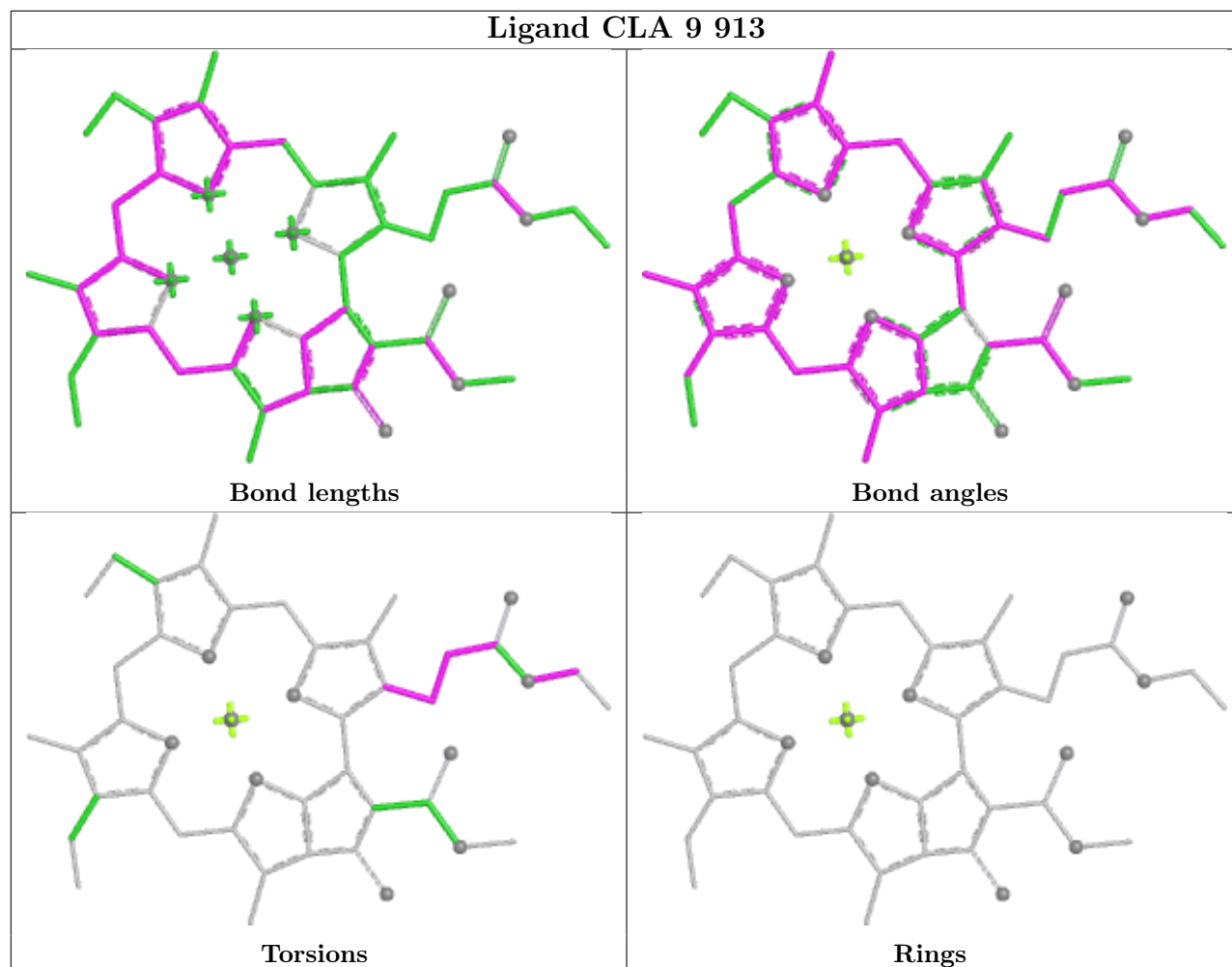
Ligand CLA 1 510



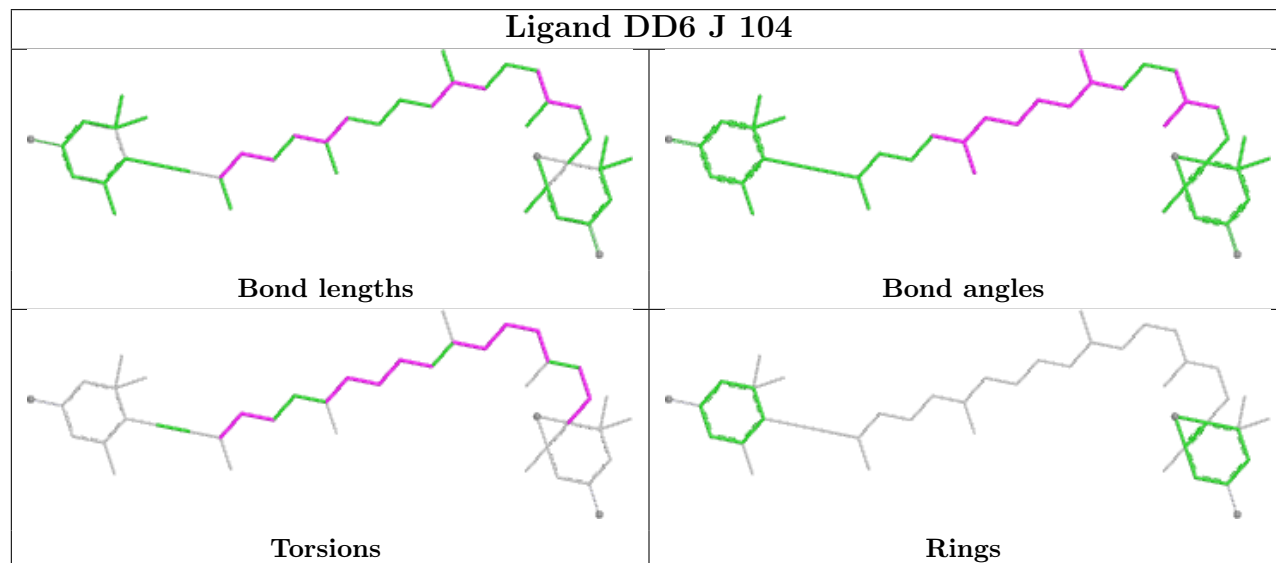
Ligand CLA 7 714

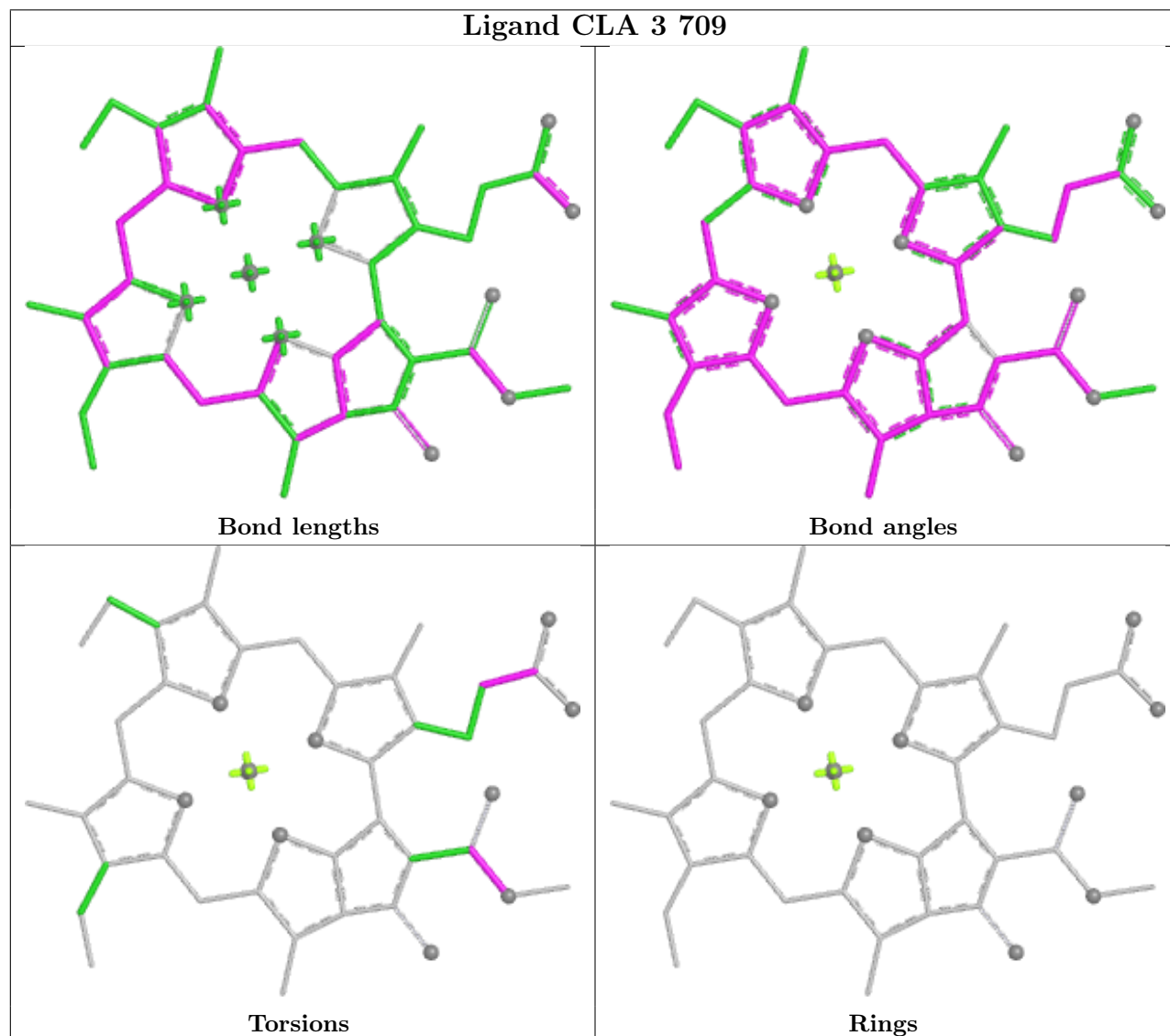
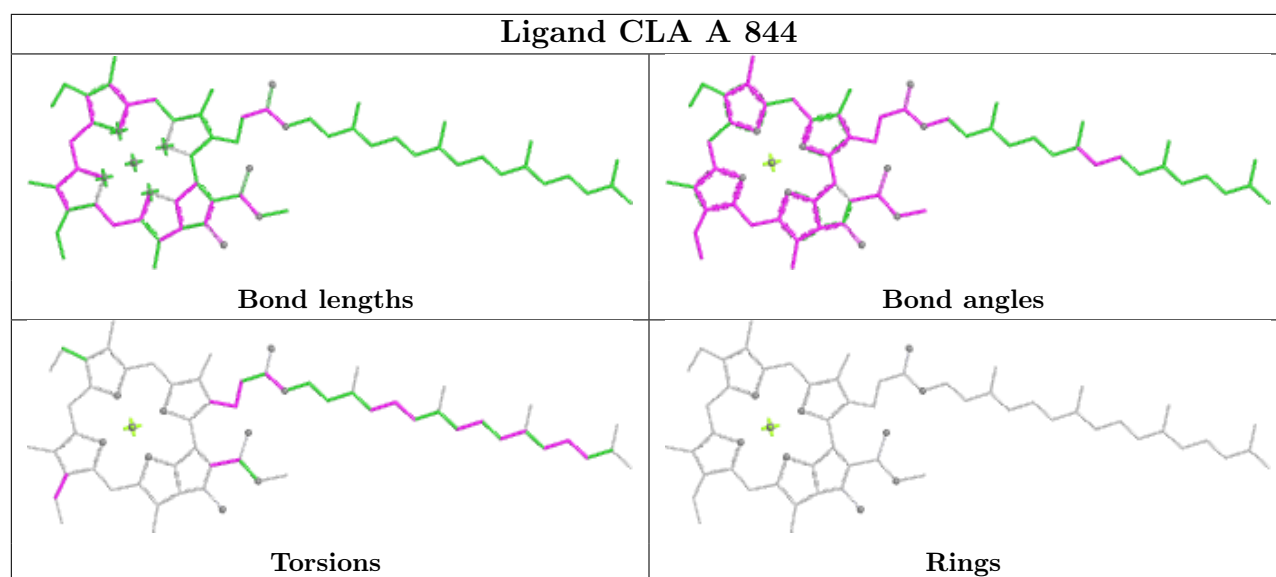


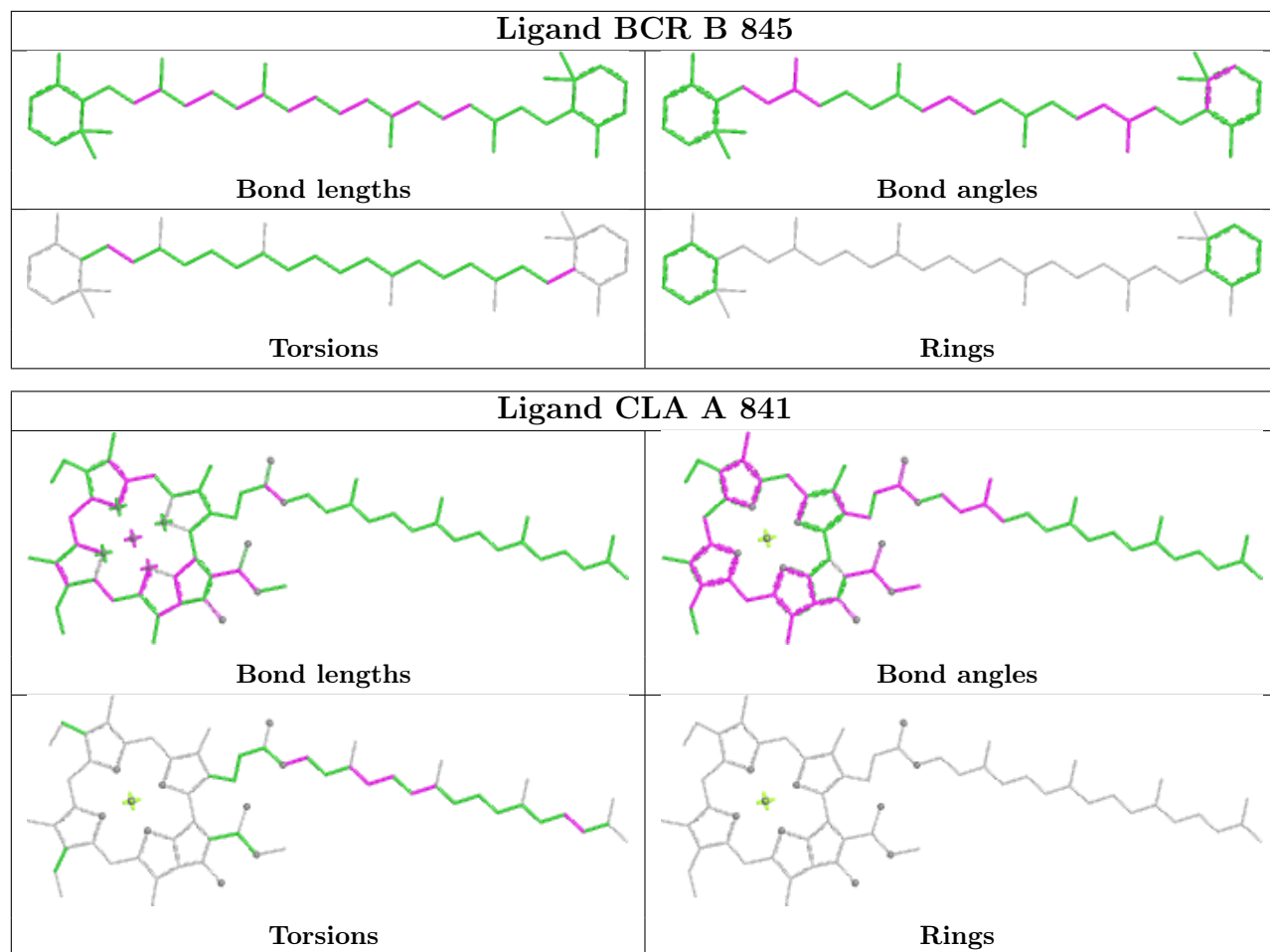
Ligand CLA 9 913

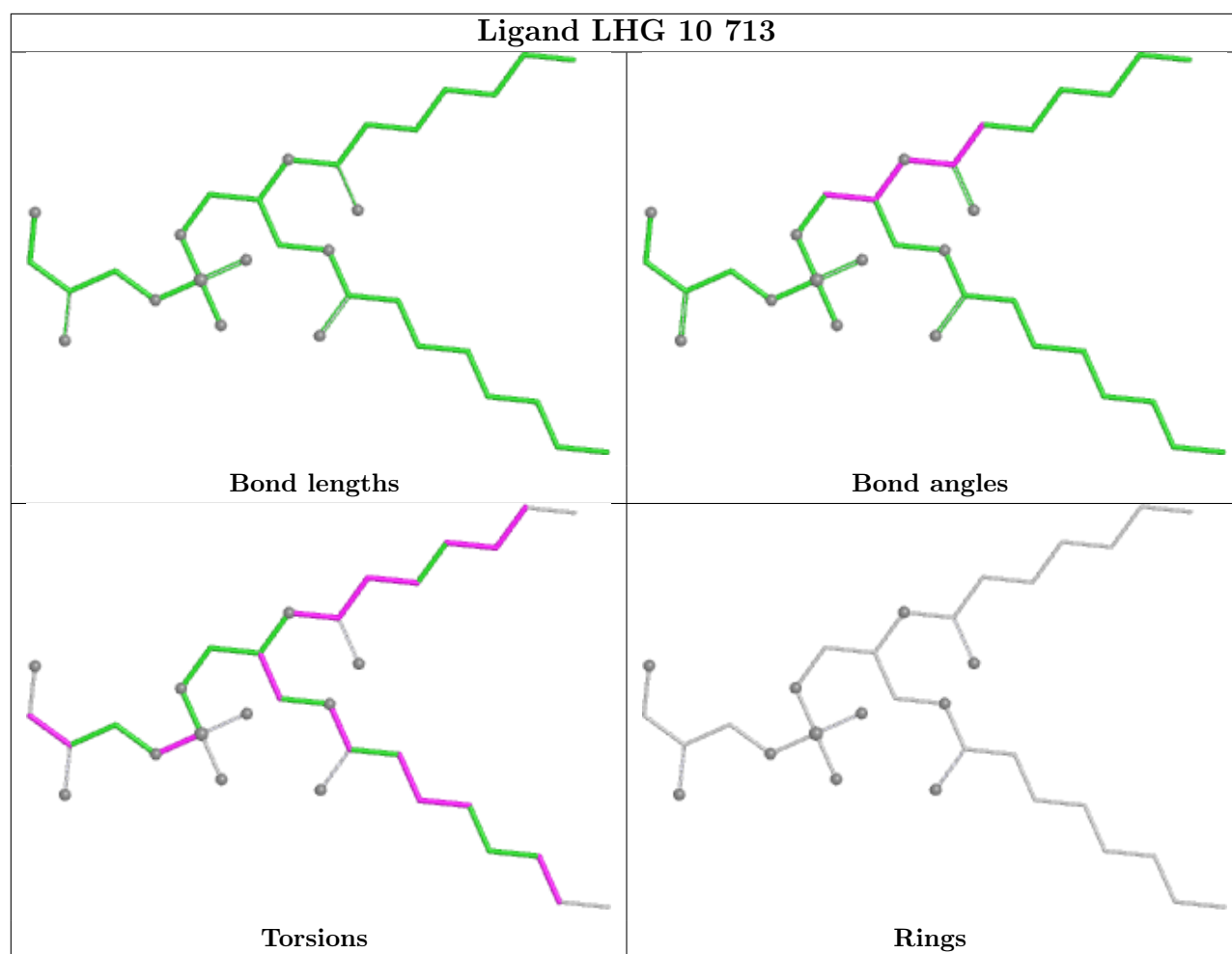


Ligand DD6 J 104

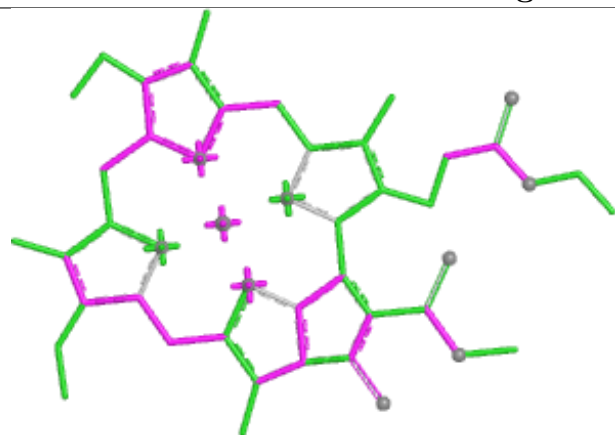




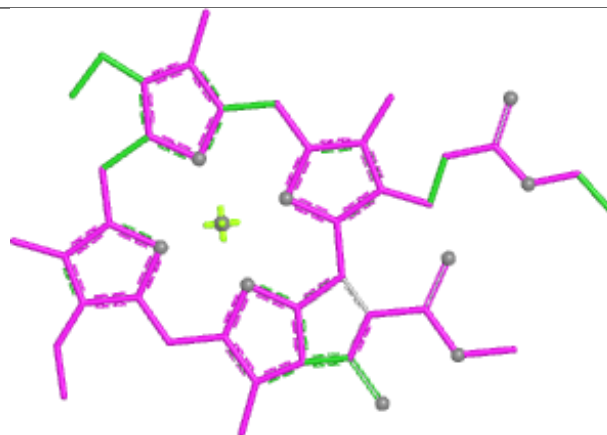




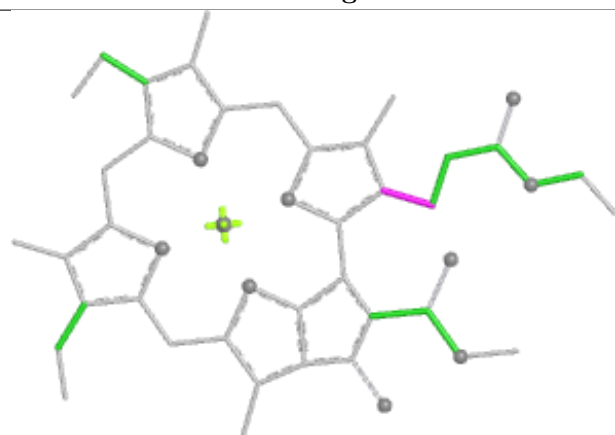
Ligand CLA B 836



Bond lengths



Bond angles

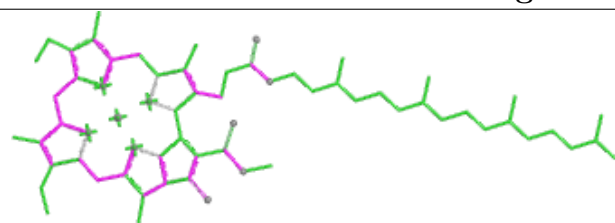


Torsions

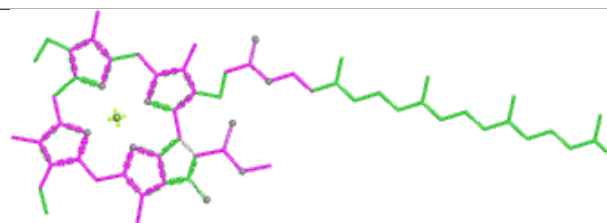


Rings

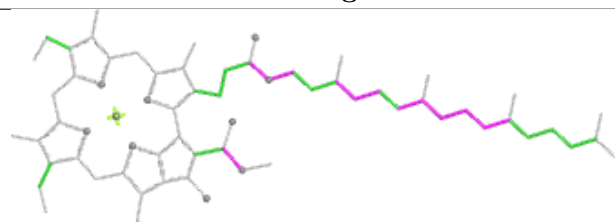
Ligand CLA A 842



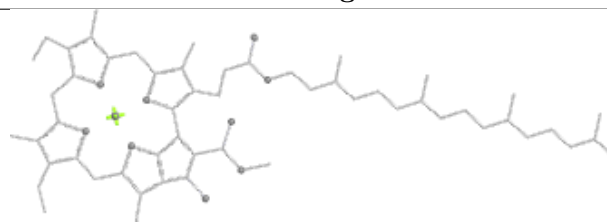
Bond lengths



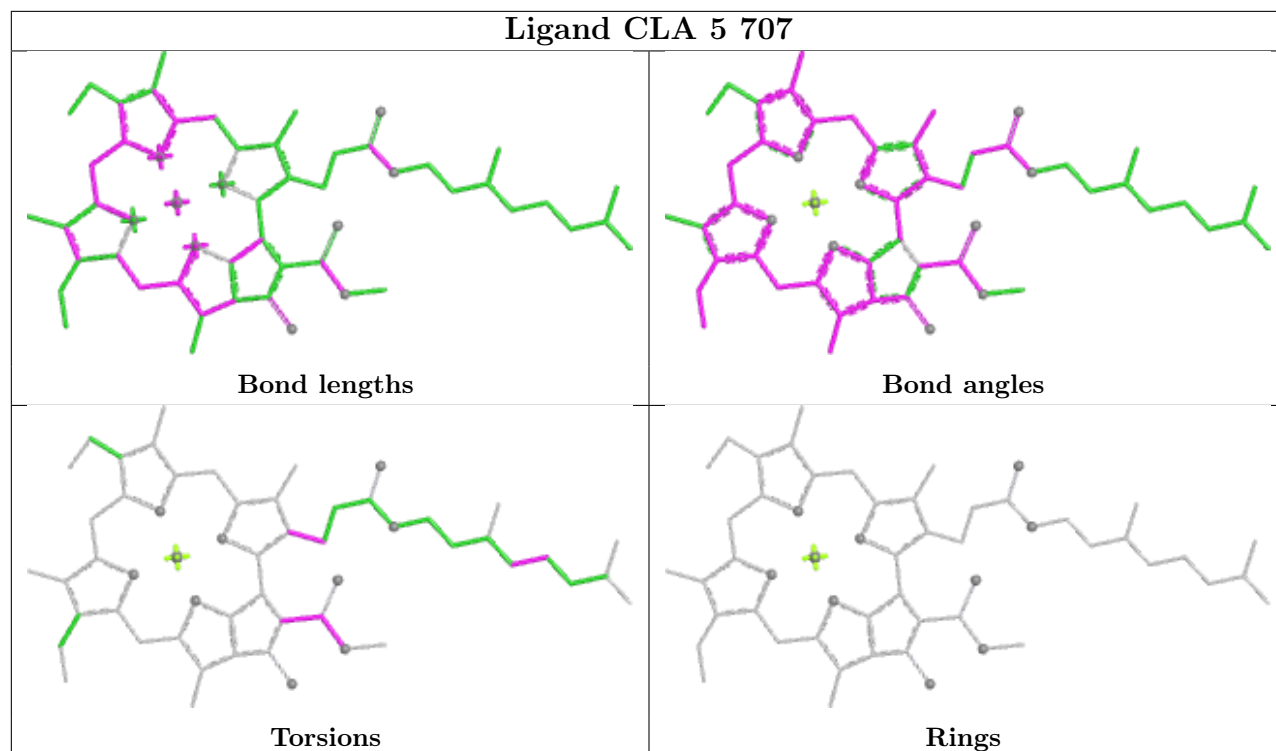
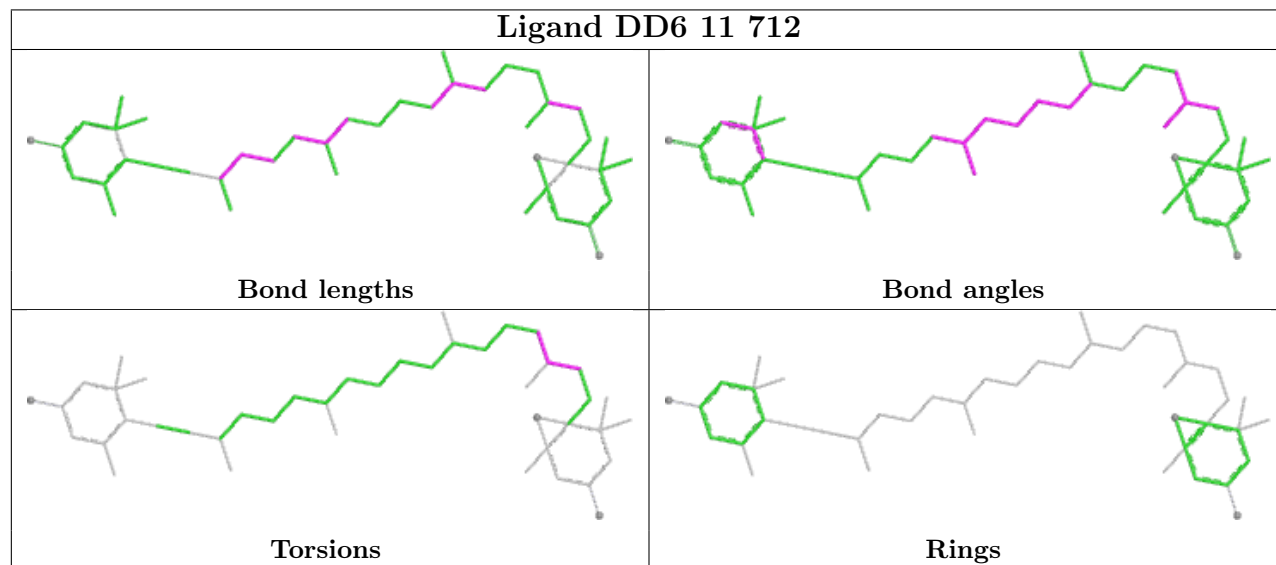
Bond angles

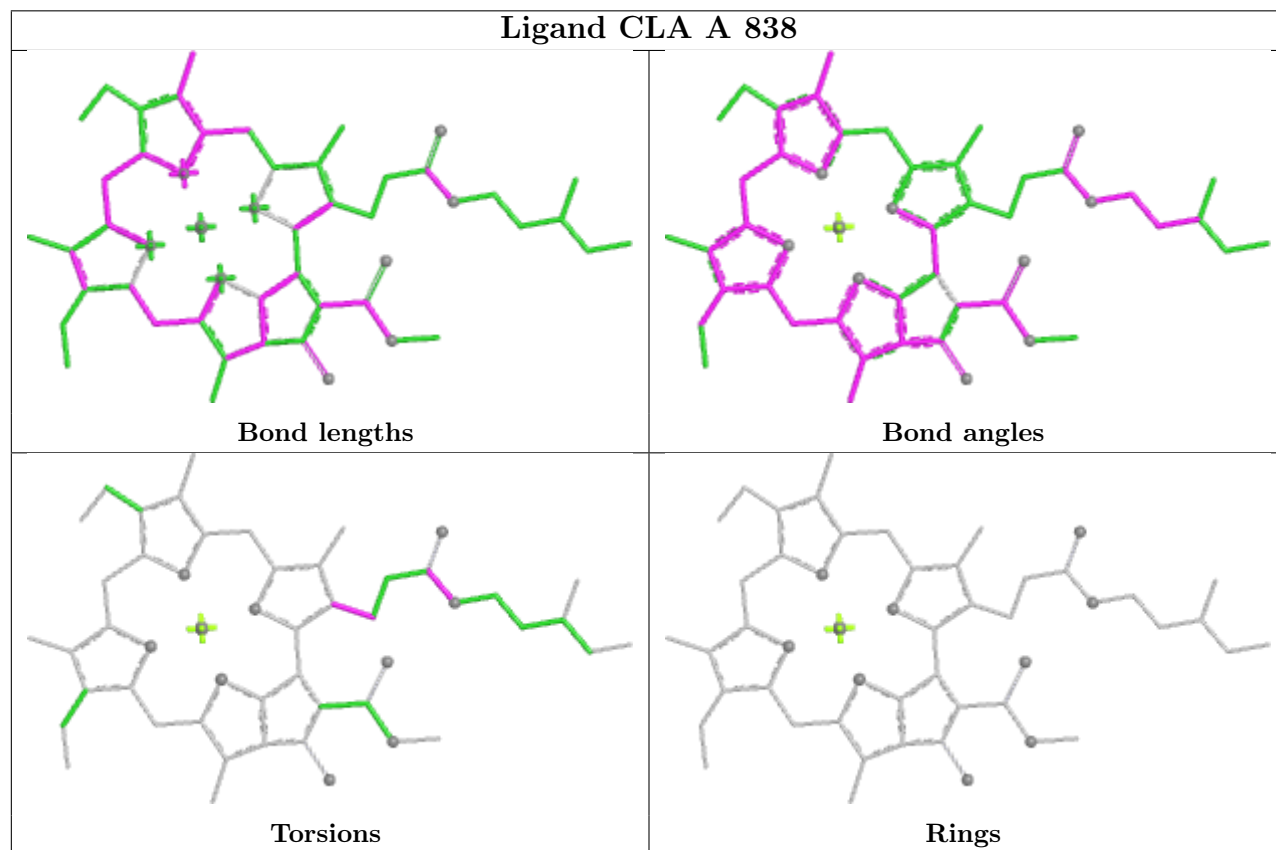
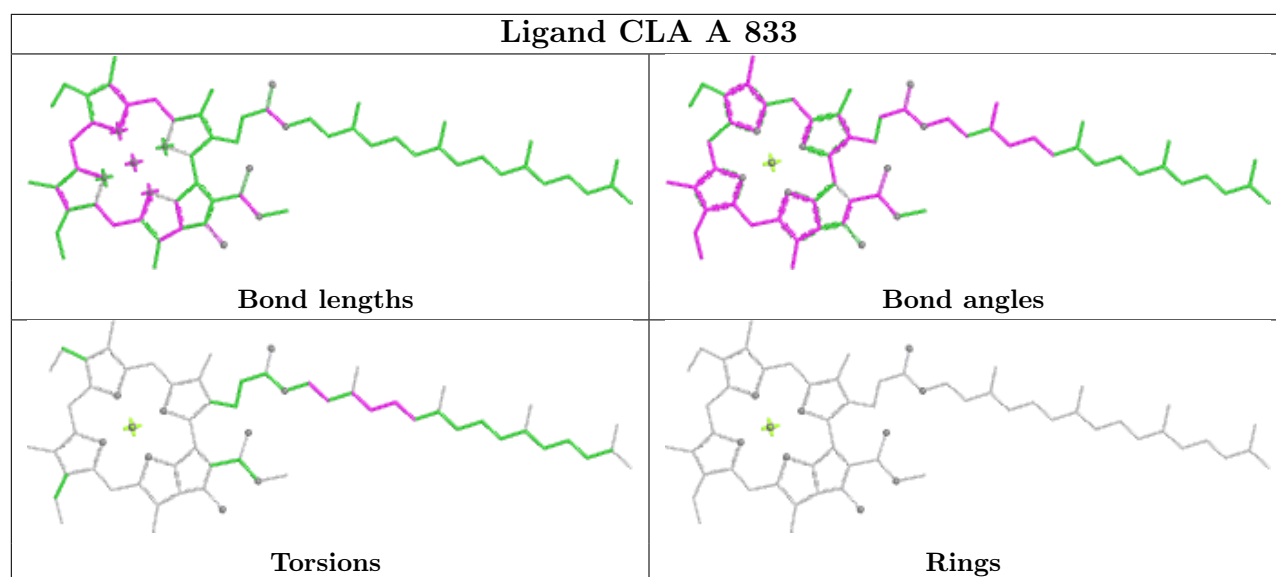


Torsions

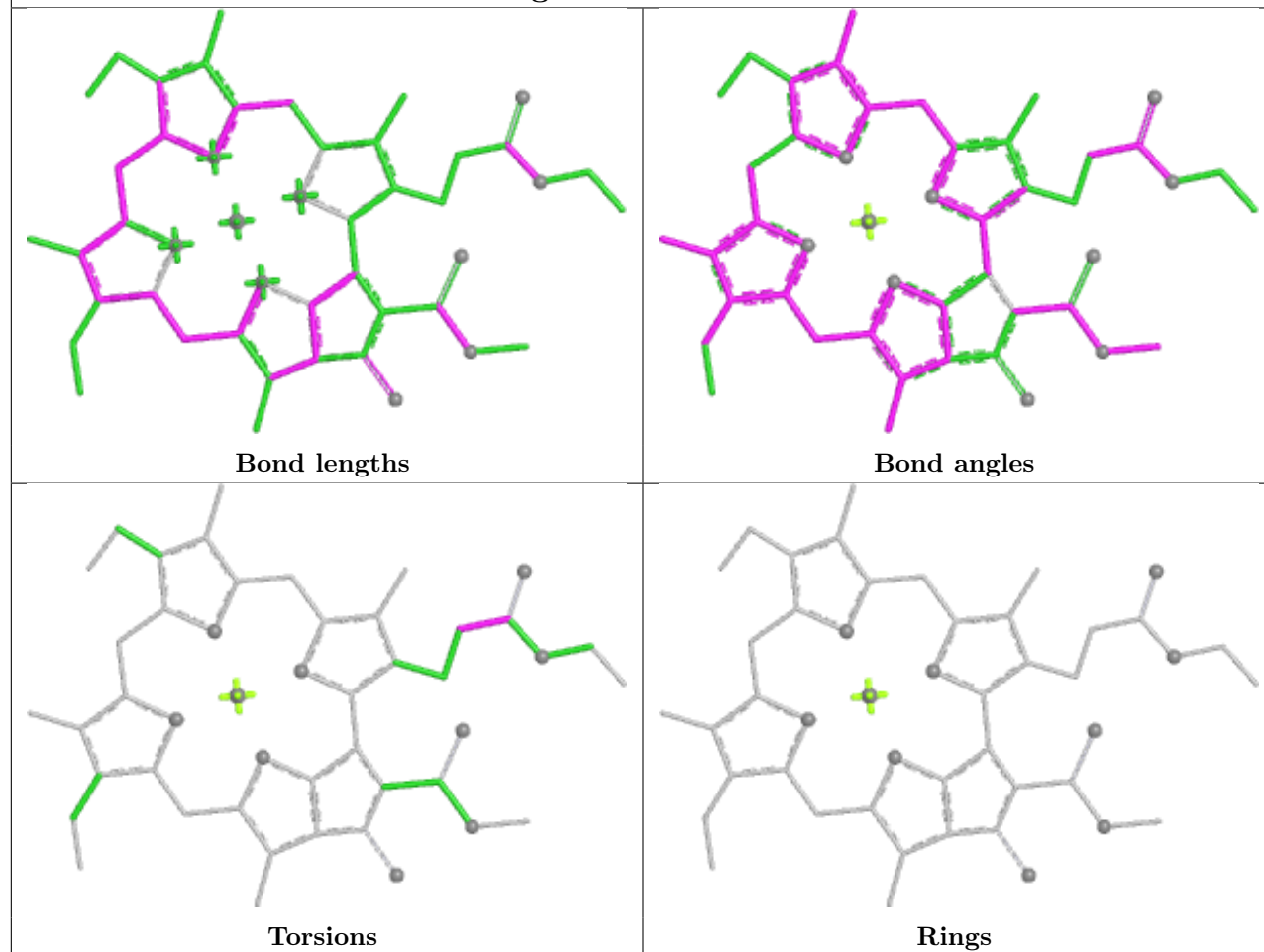


Rings

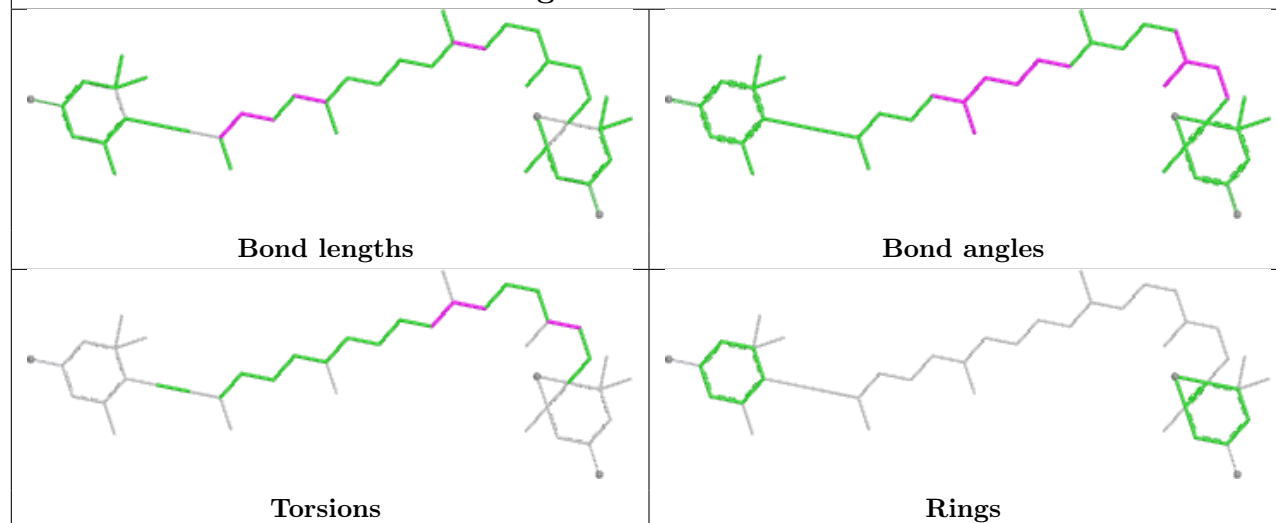
Ligand CLA 5 707**Ligand DD6 11 712**



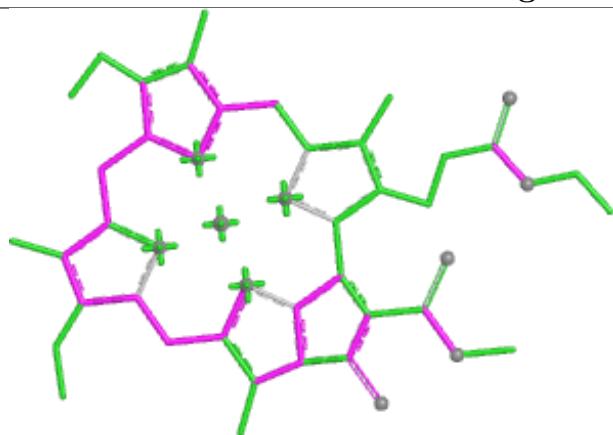
Ligand CLA 9 906



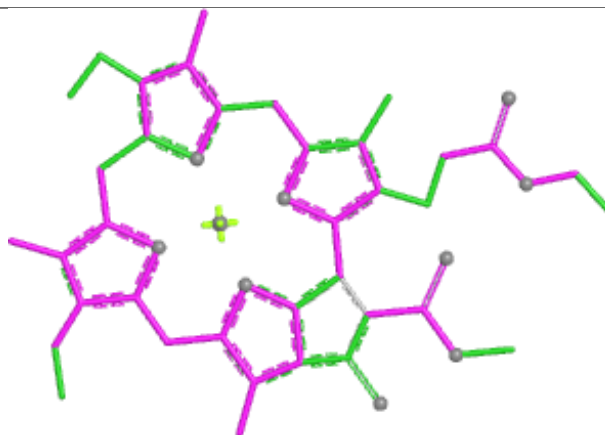
Ligand DD6 6 916



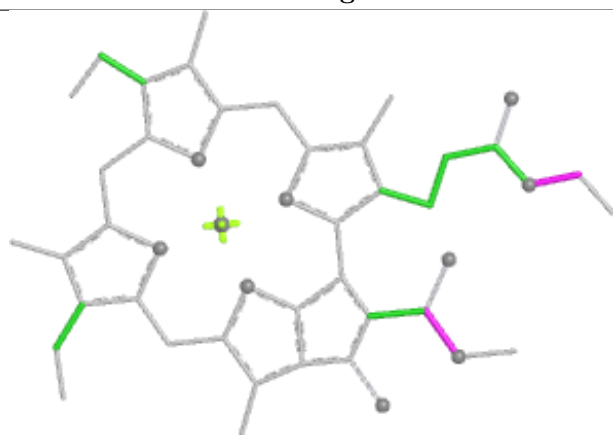
Ligand CLA 4 705



Bond lengths



Bond angles

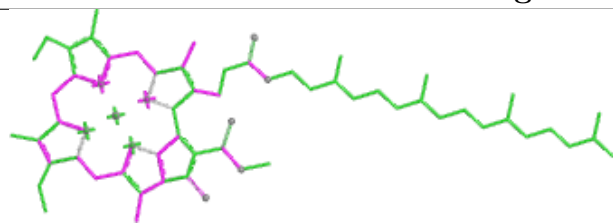


Torsions

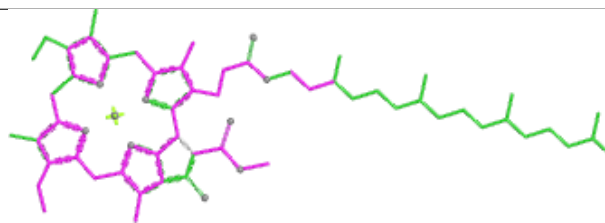


Rings

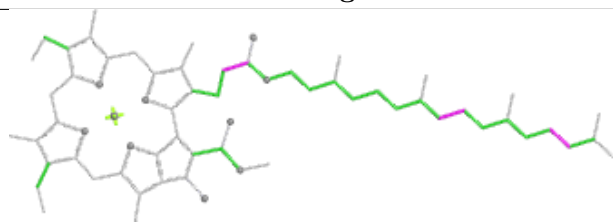
Ligand CLA B 801



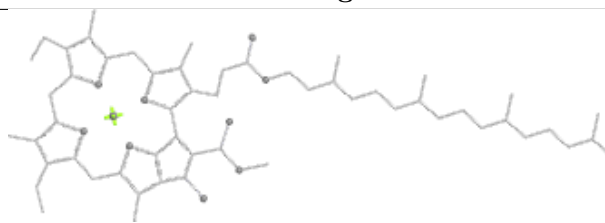
Bond lengths



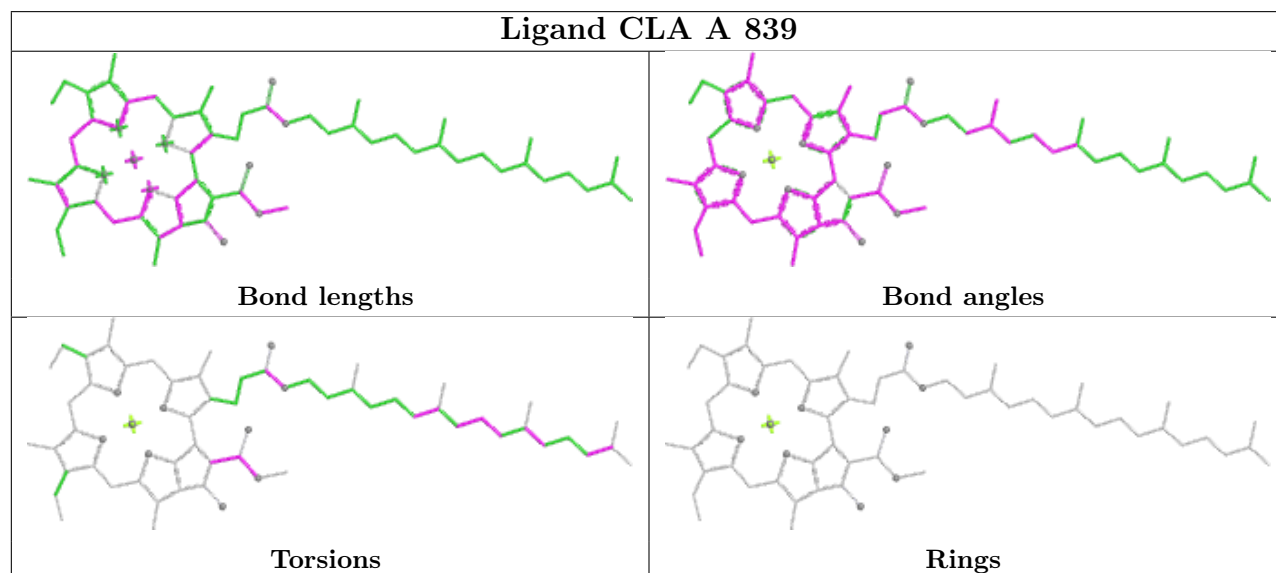
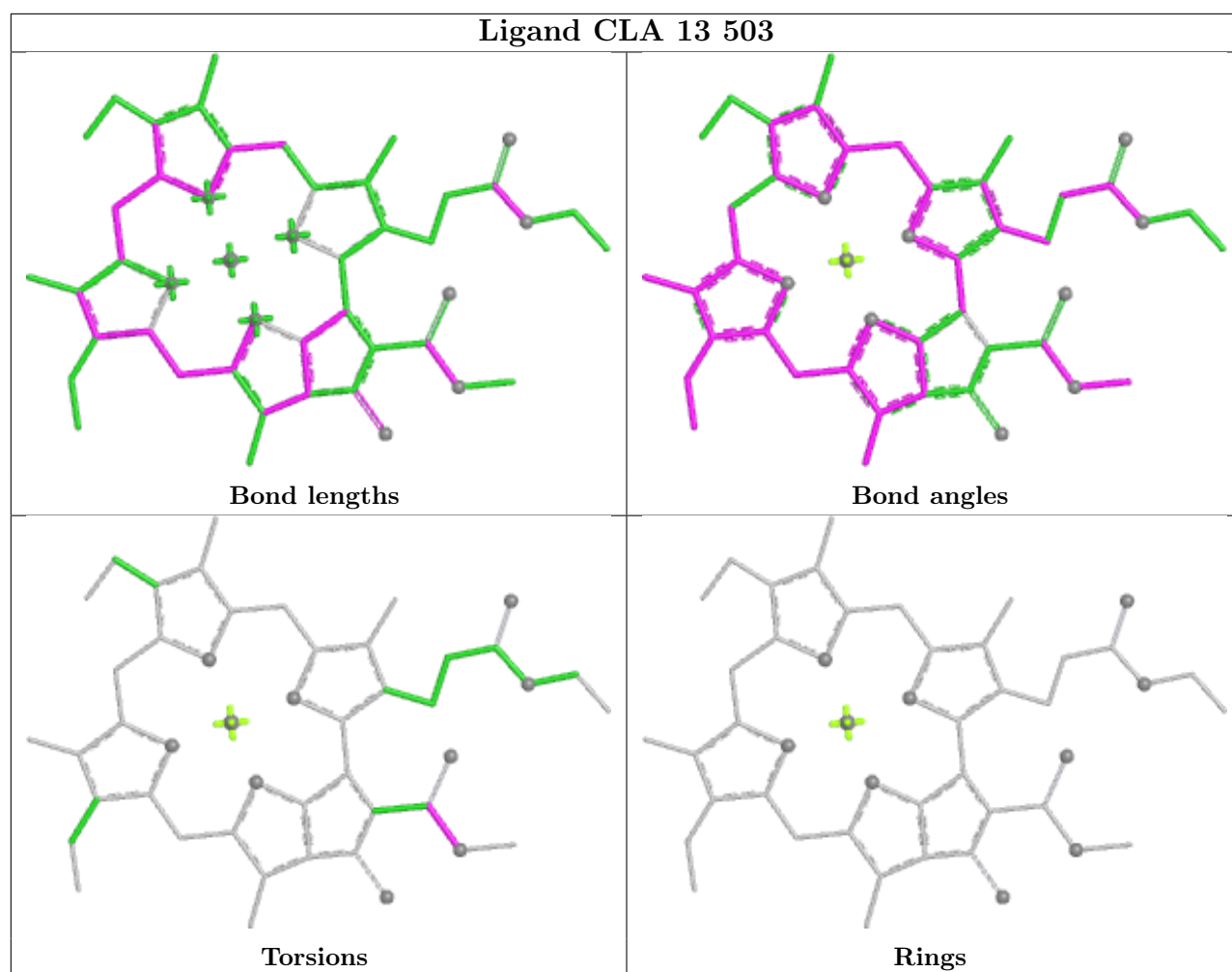
Bond angles



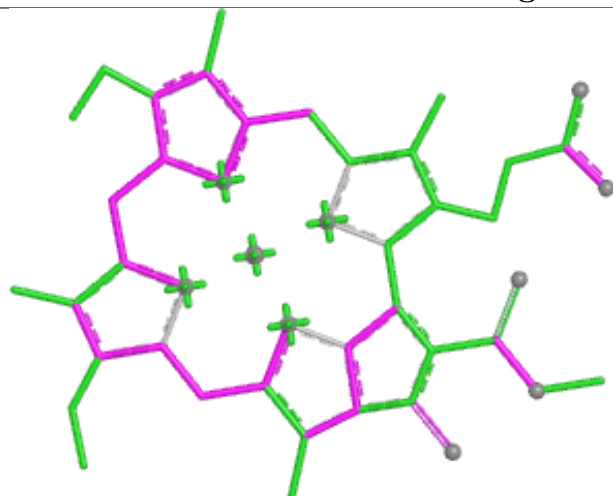
Torsions



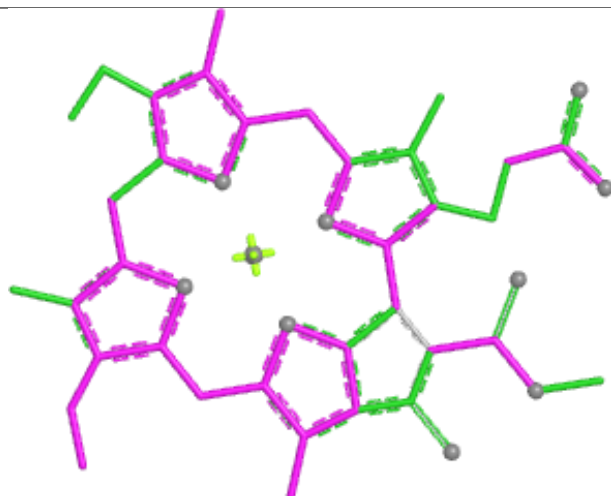
Rings



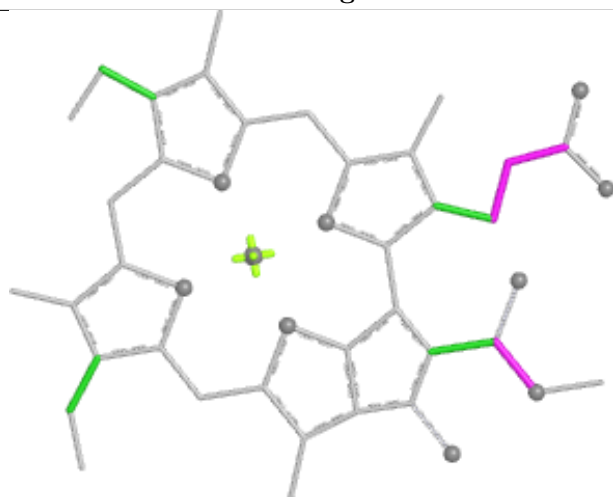
Ligand CLA 4 710



Bond lengths



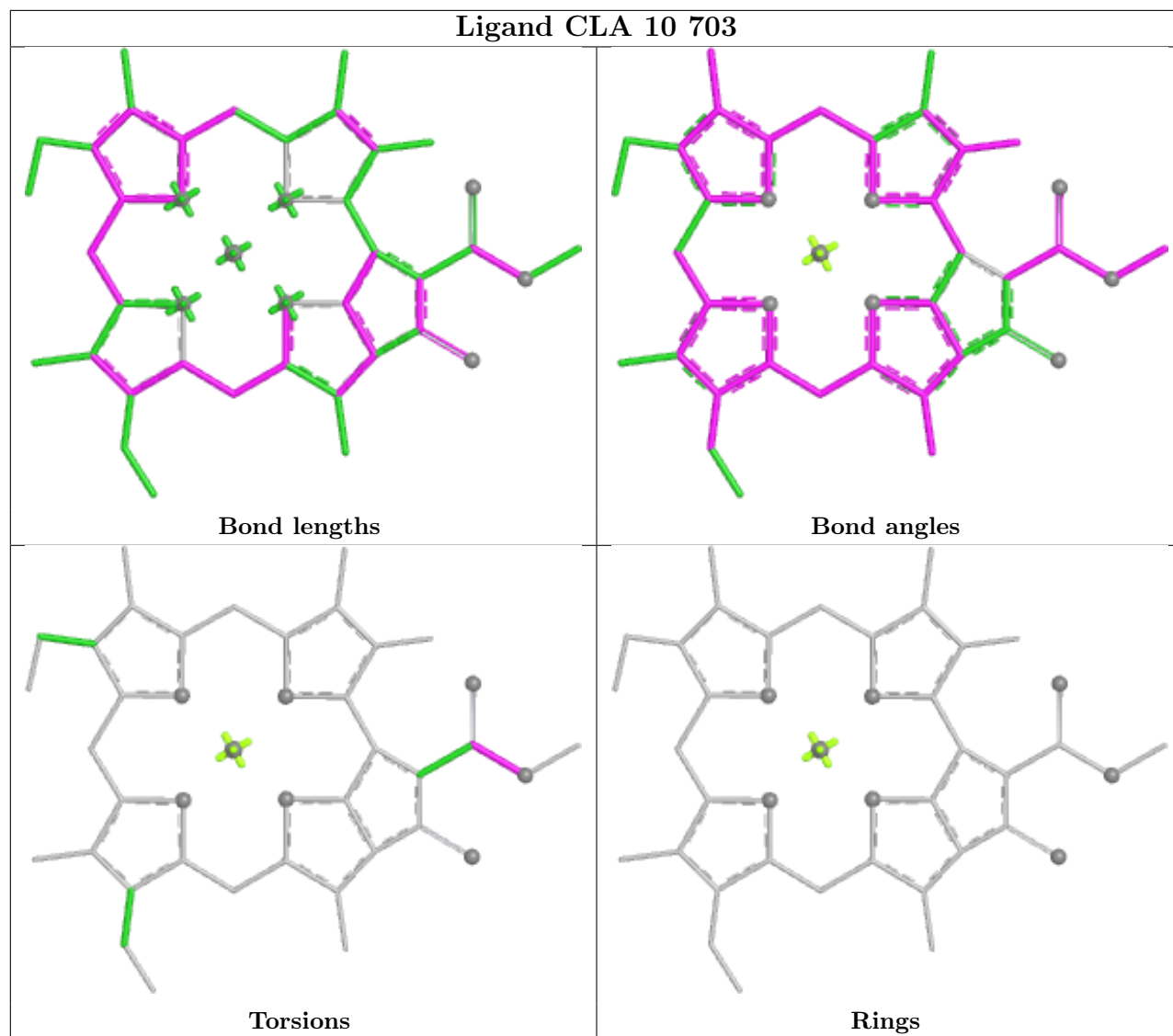
Bond angles

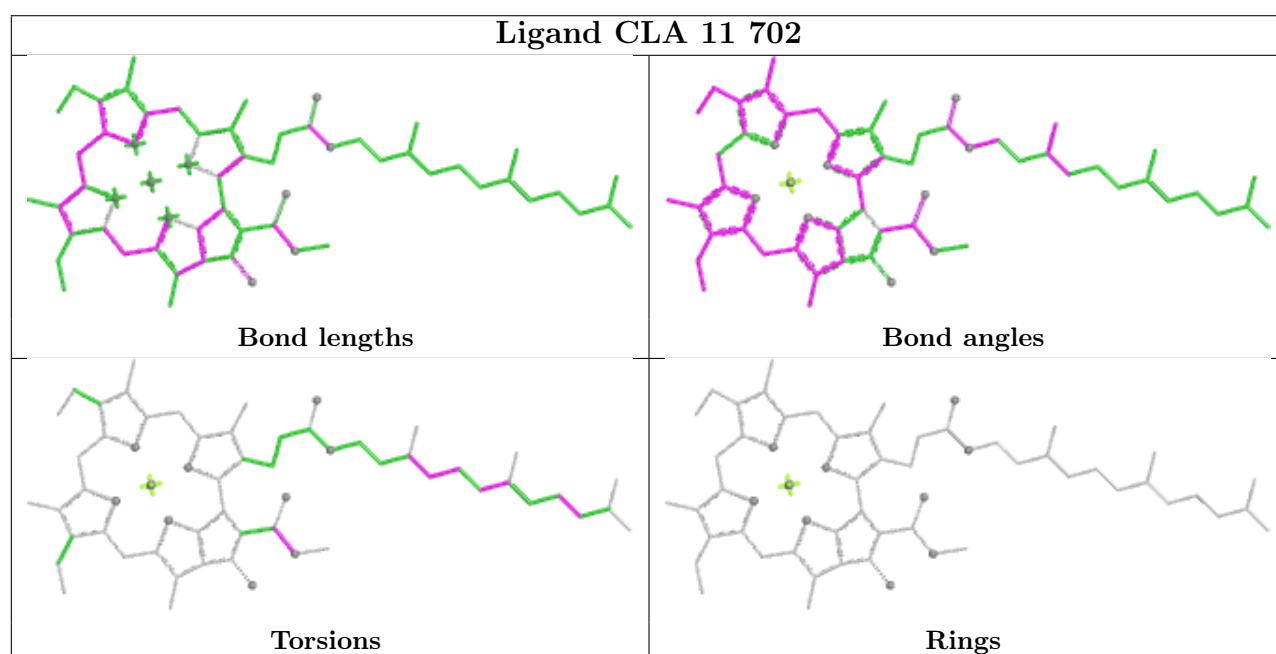
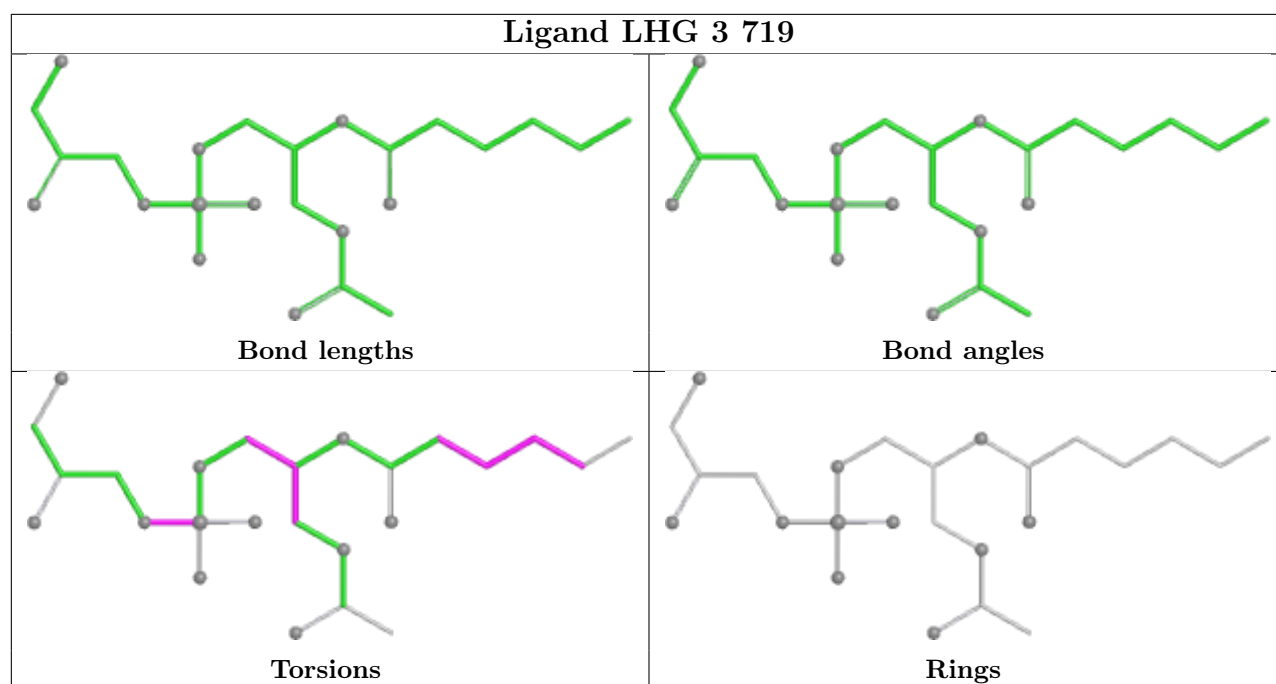


Torsions

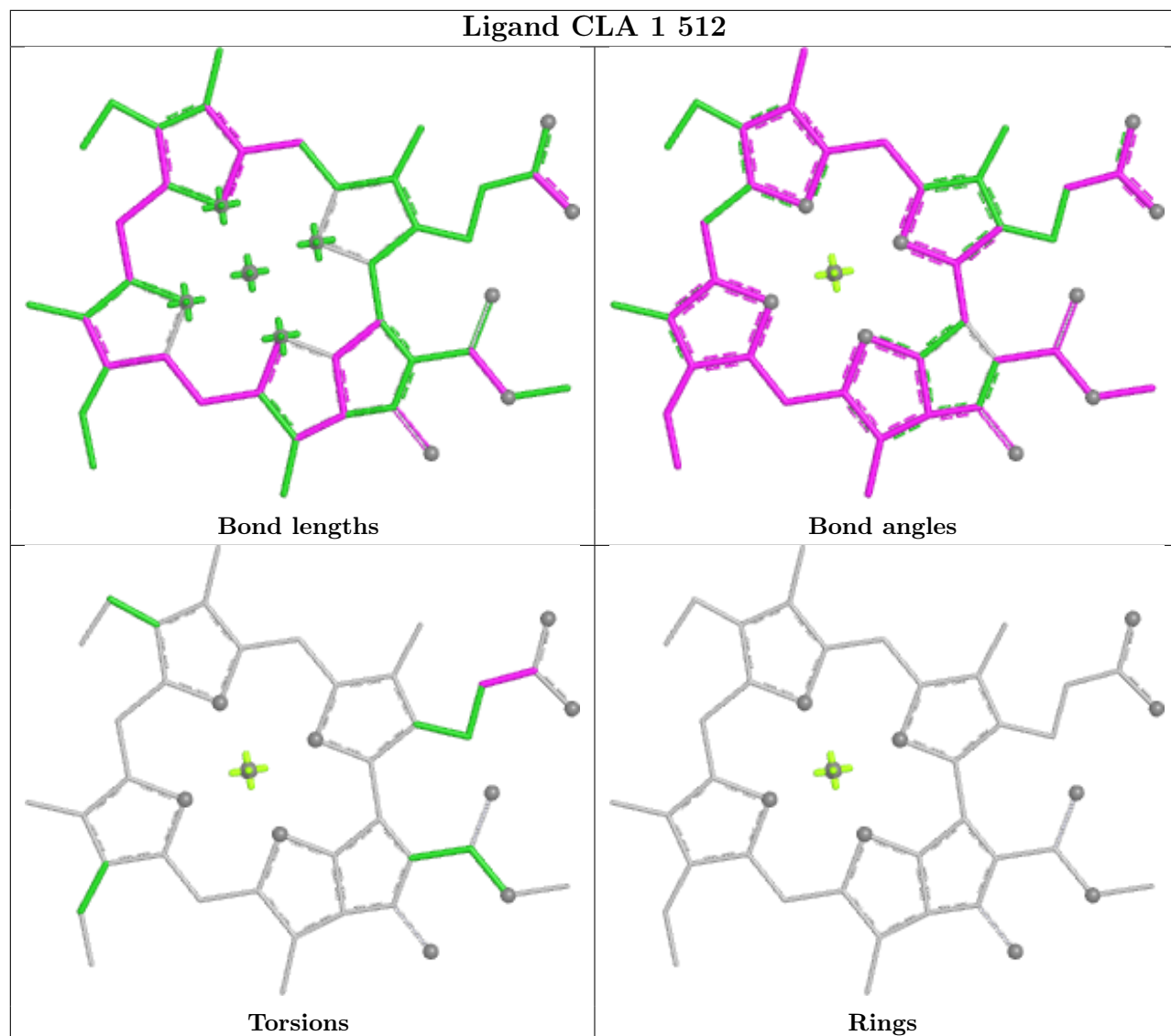


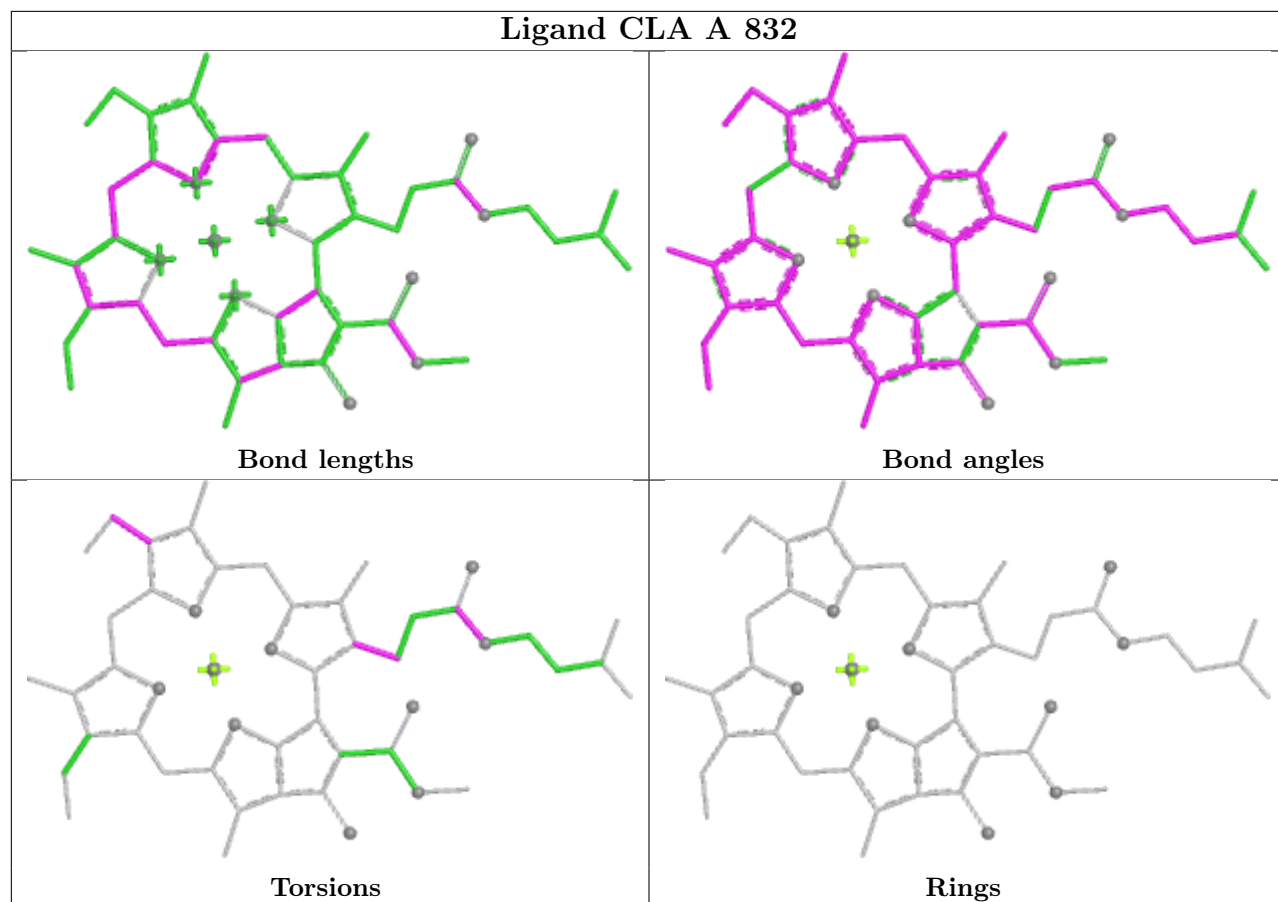
Rings

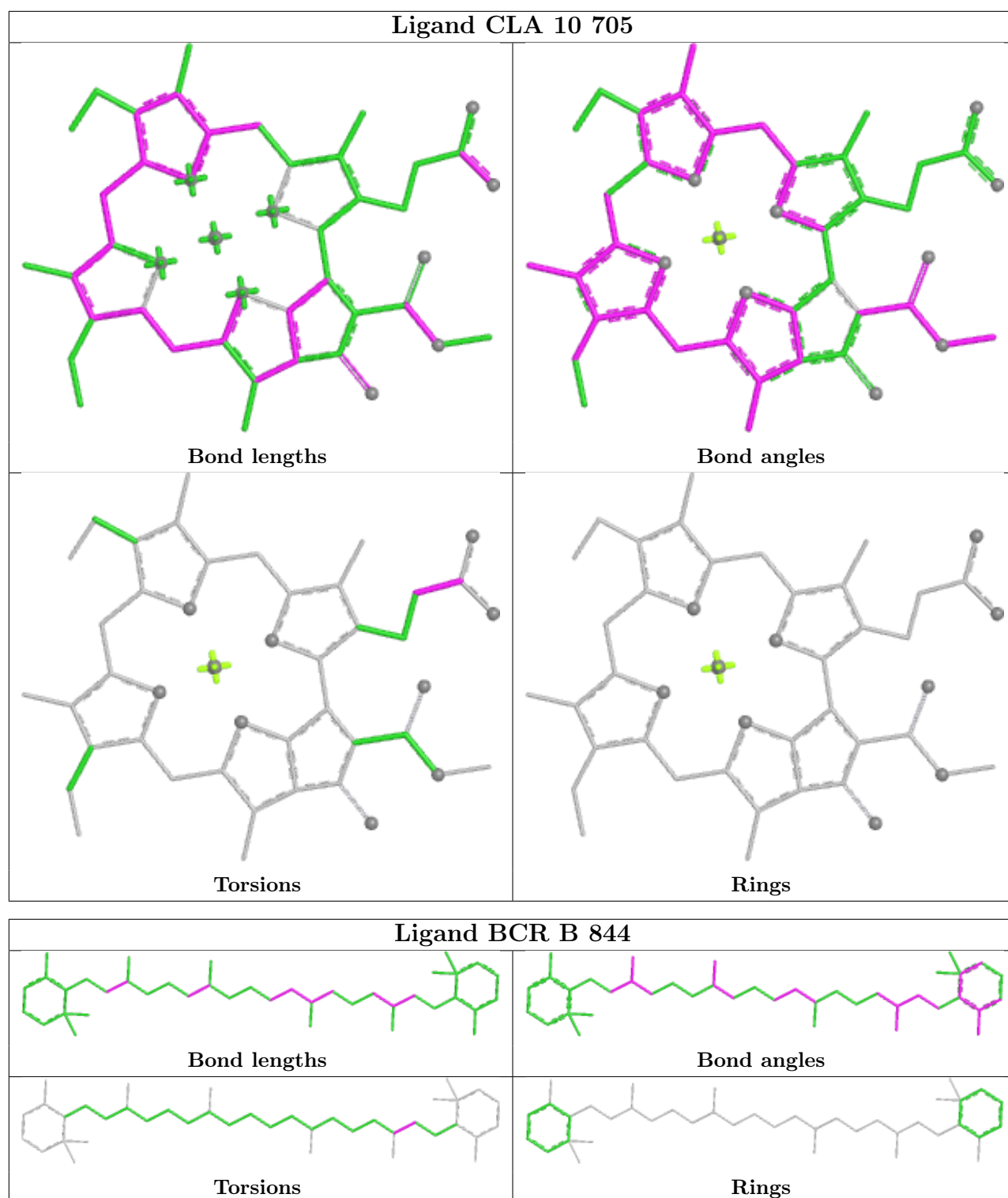


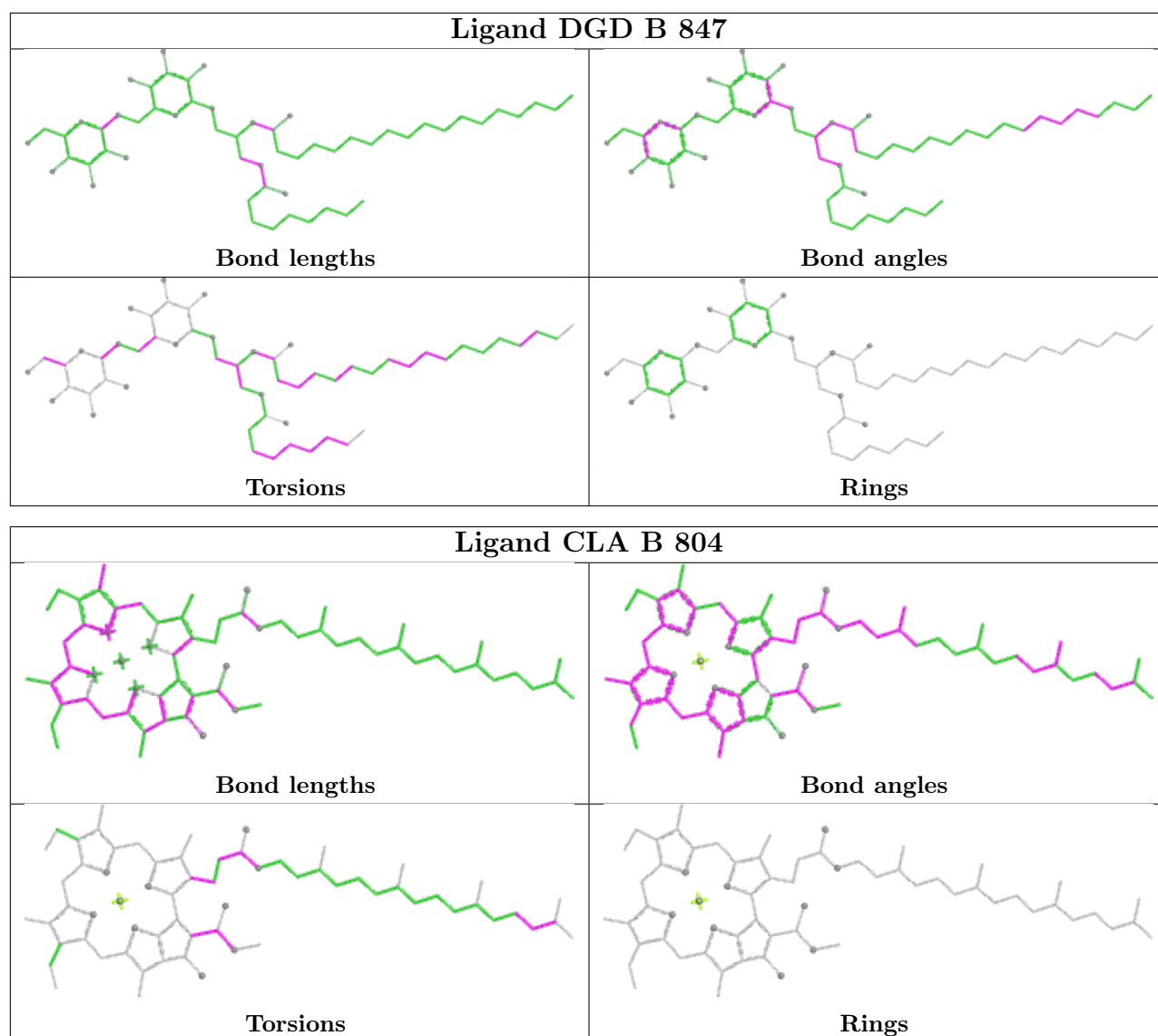


Ligand CLA 1 512

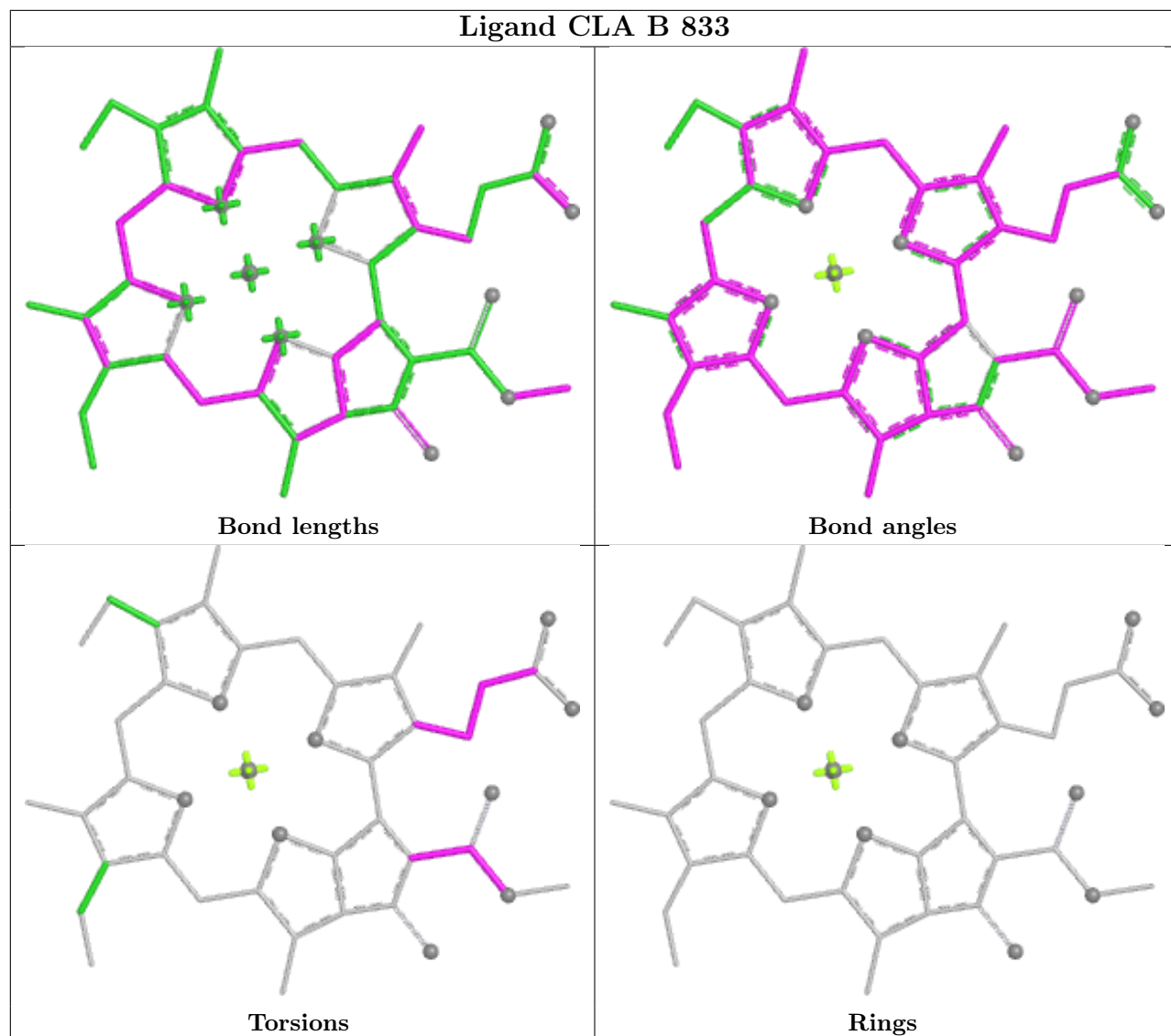




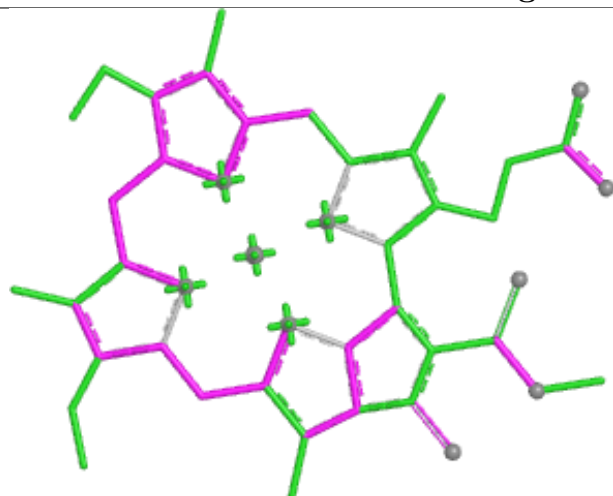




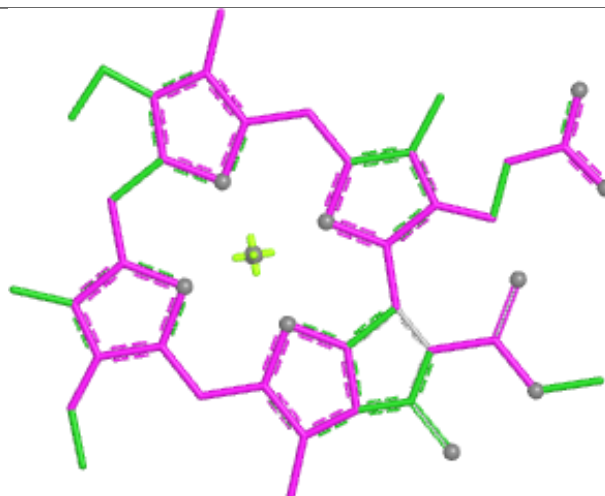
Ligand CLA B 833



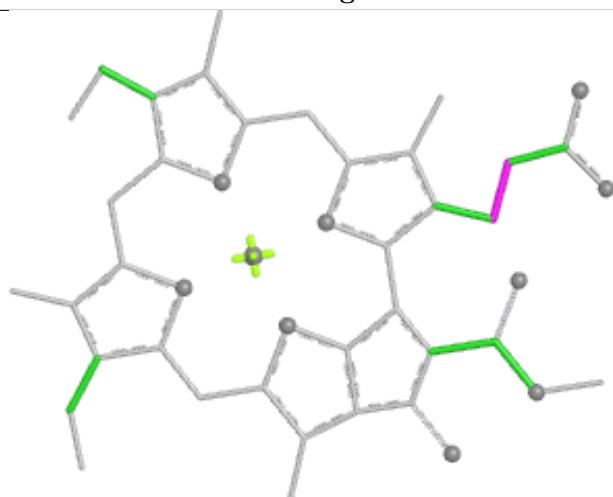
Ligand CLA 1 516



Bond lengths



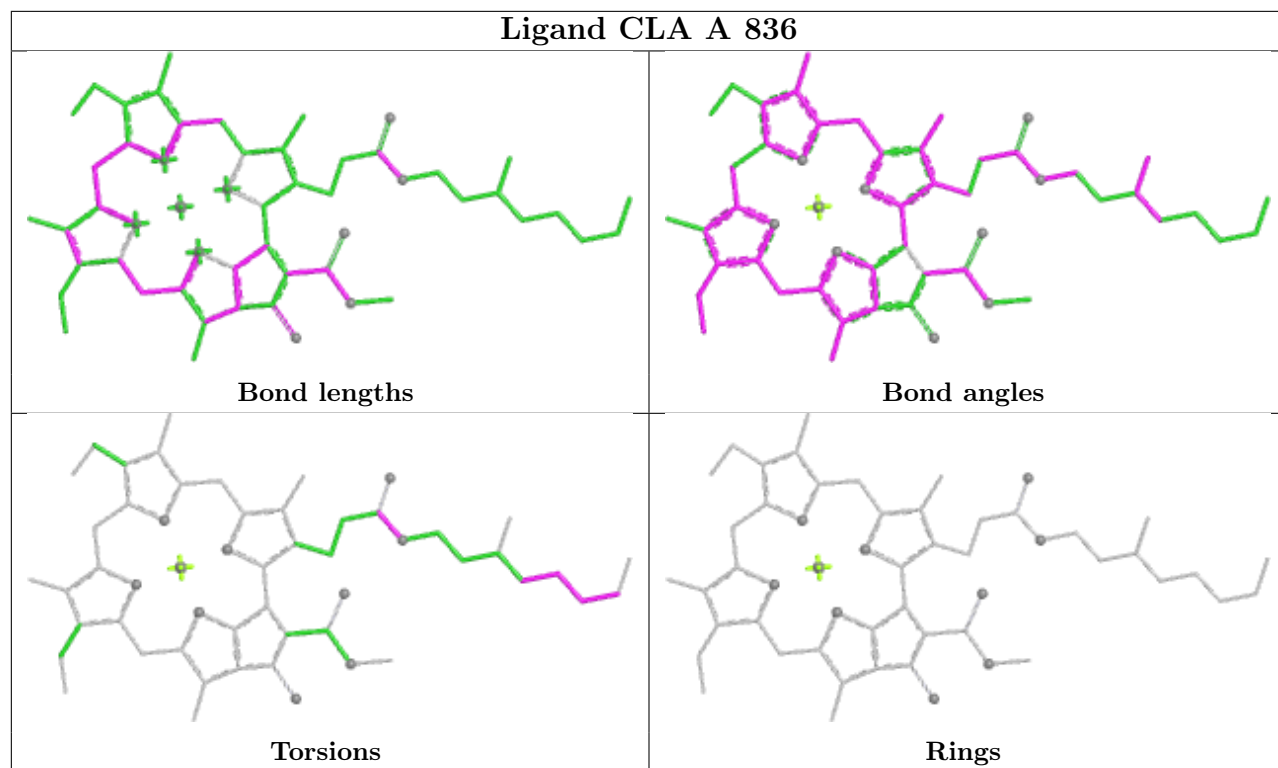
Bond angles



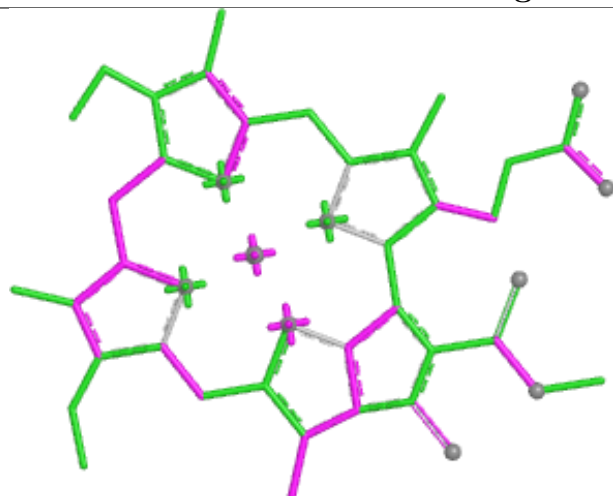
Torsions



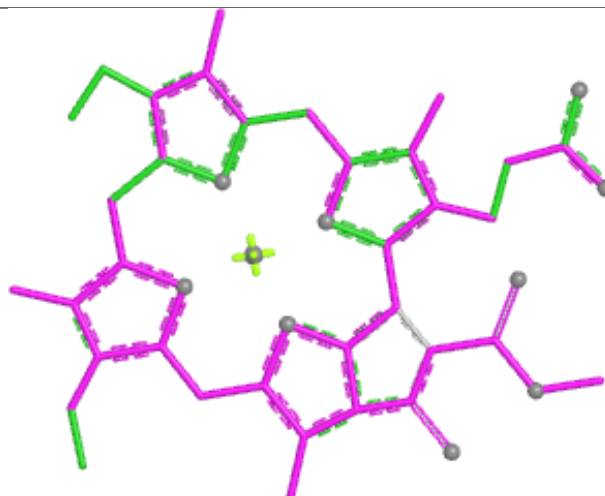
Rings



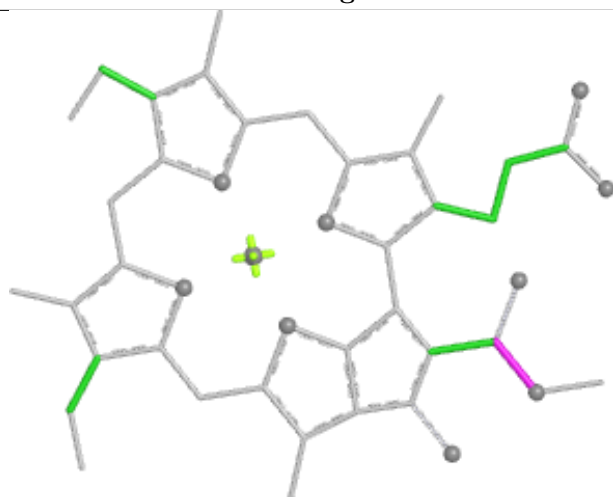
Ligand CLA B 838



Bond lengths



Bond angles

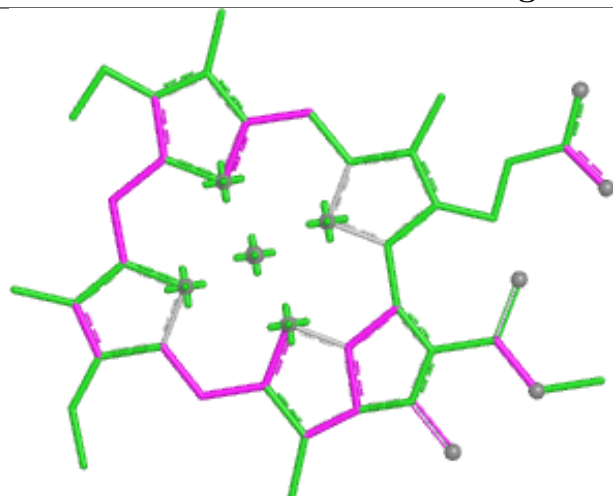


Torsions

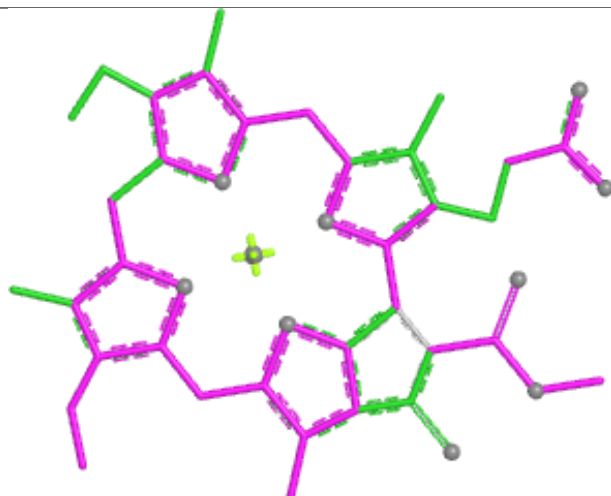


Rings

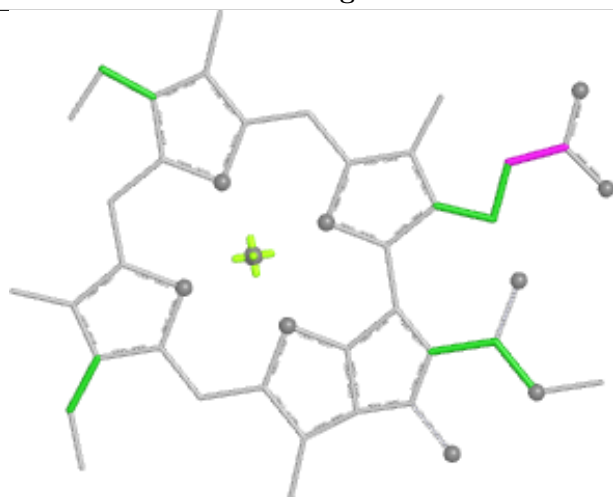
Ligand CLA 6 911



Bond lengths



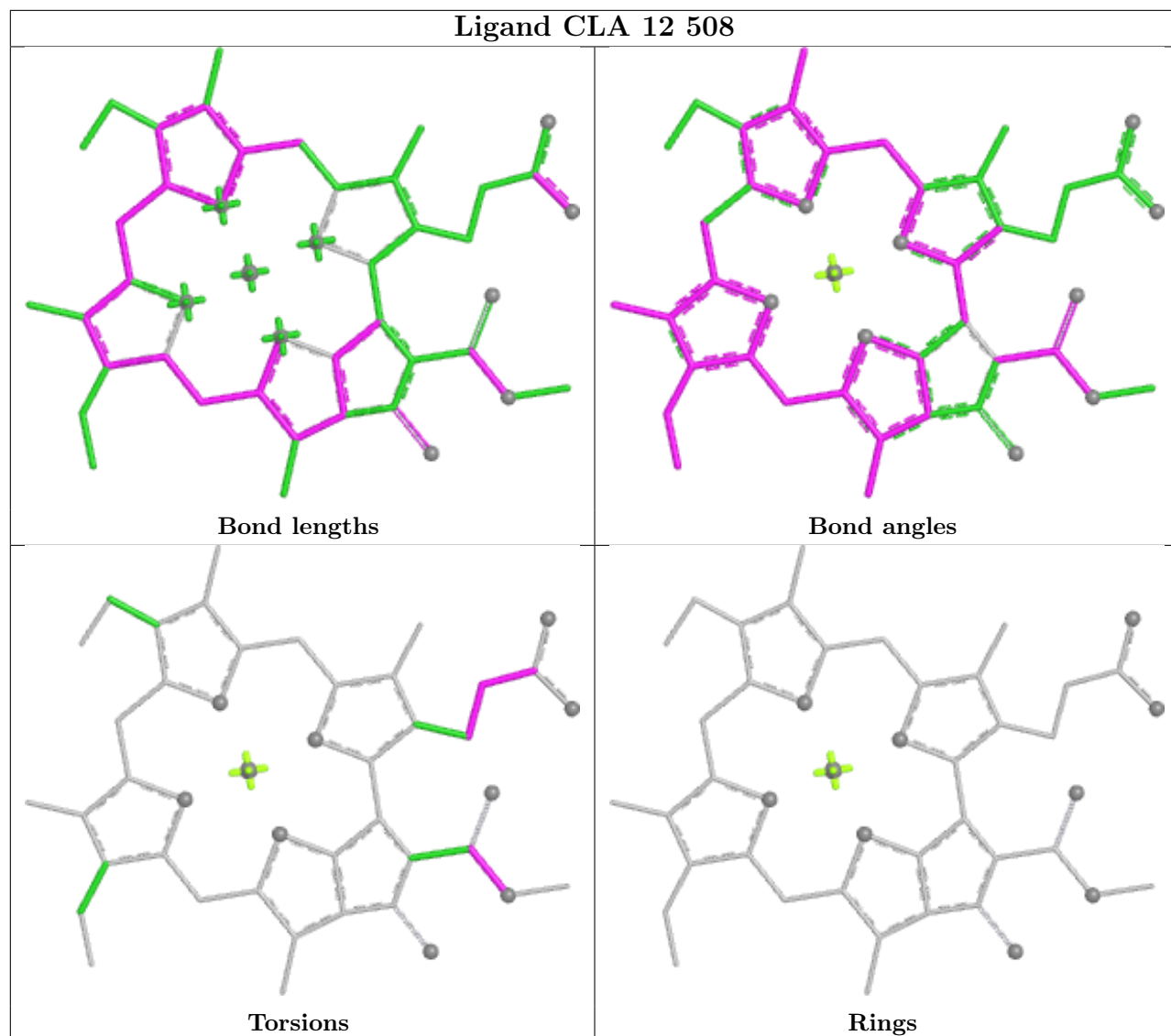
Bond angles



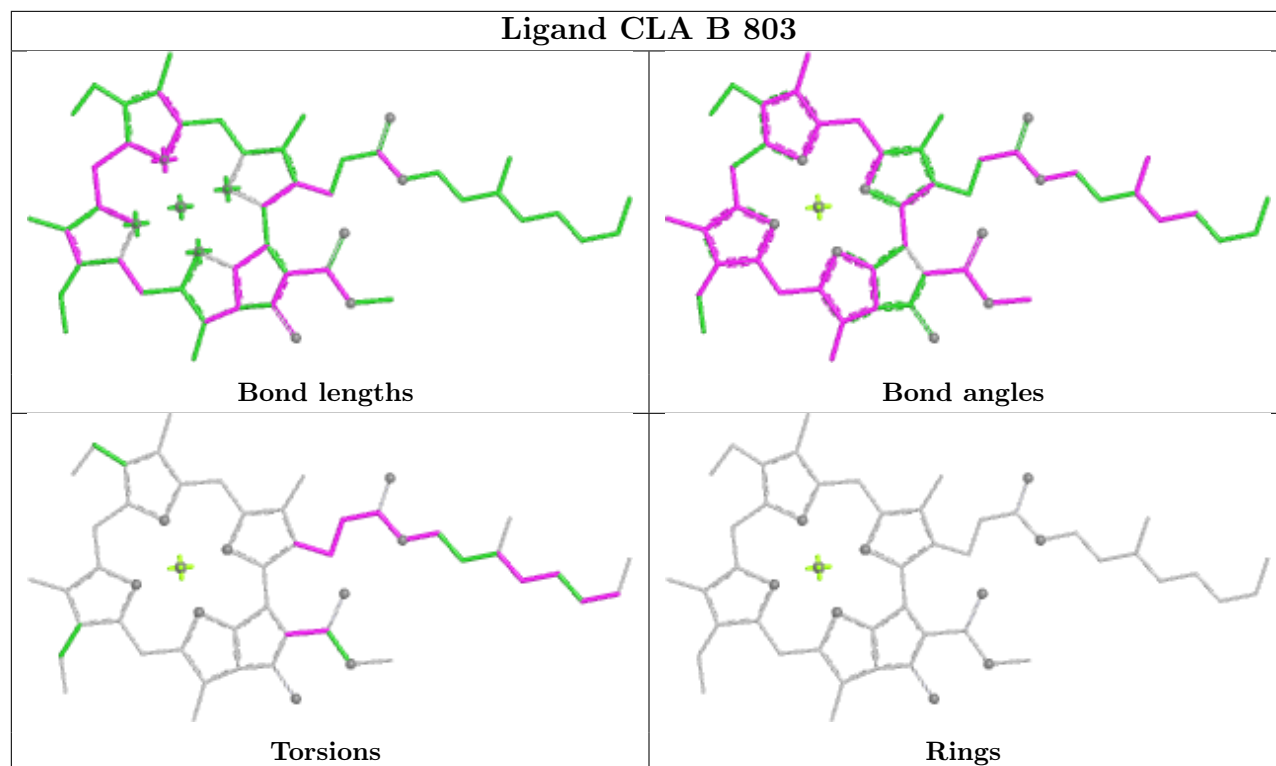
Torsions



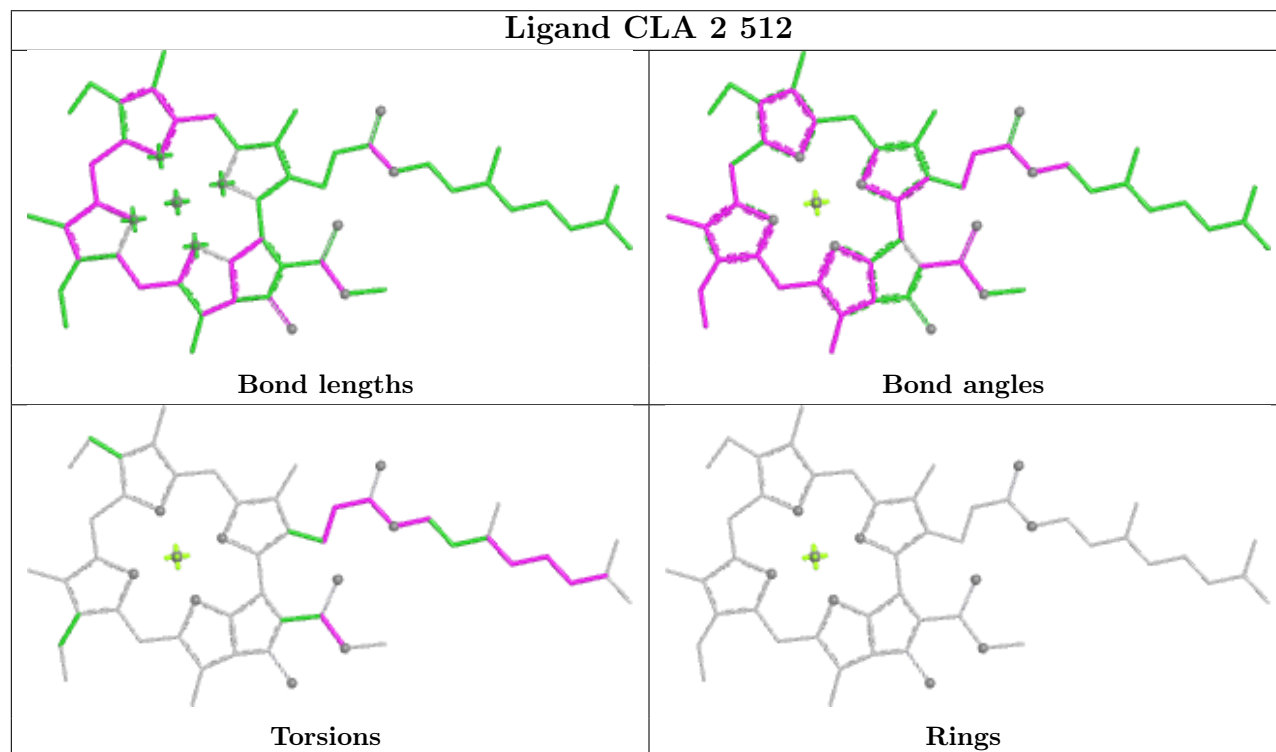
Rings



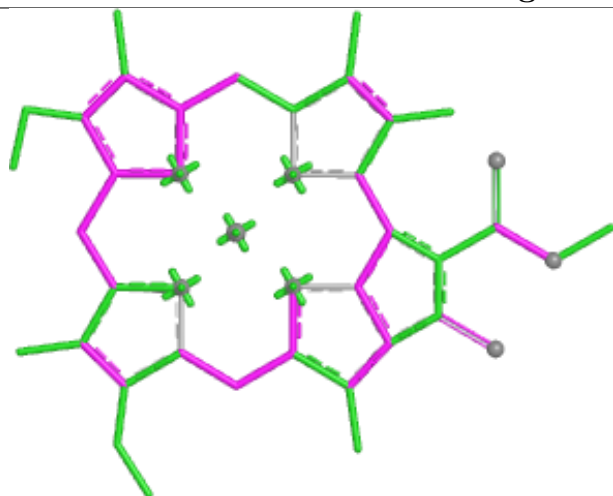
Ligand CLA B 803



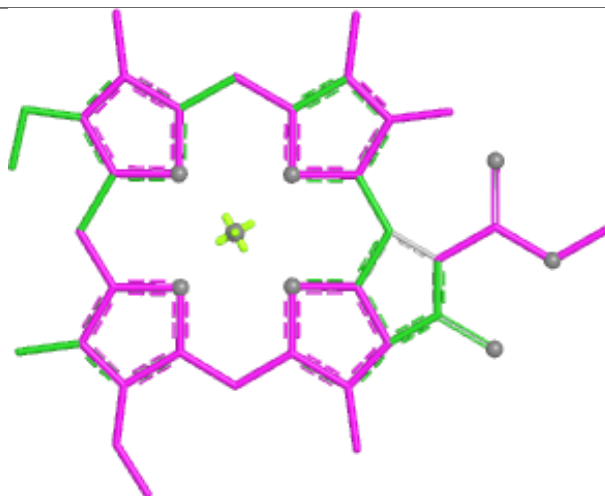
Ligand CLA 2 512



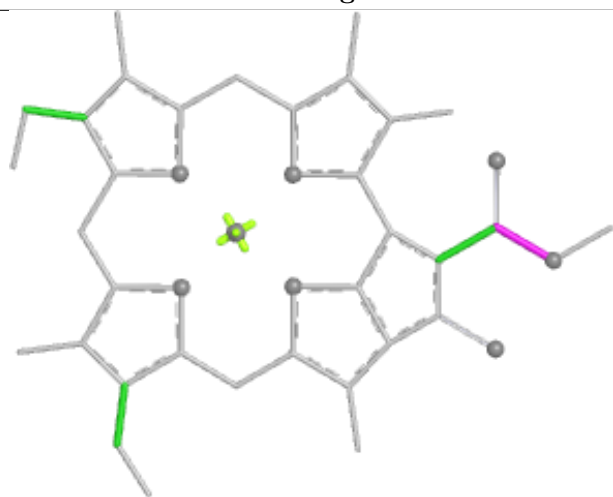
Ligand CLA 3 701



Bond lengths



Bond angles

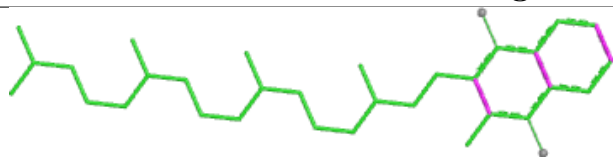


Torsions

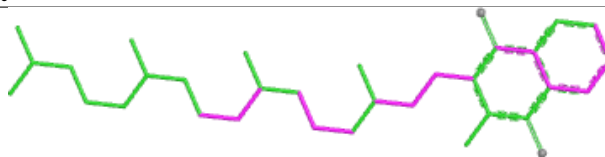


Rings

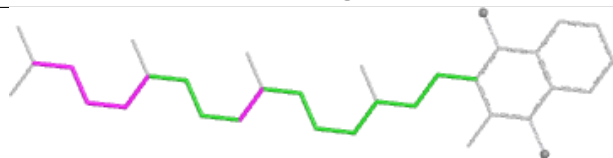
Ligand PQN A 845



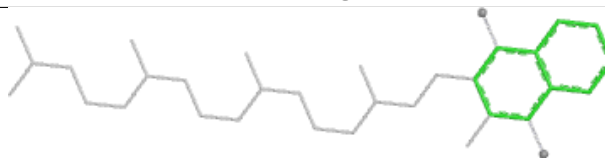
Bond lengths



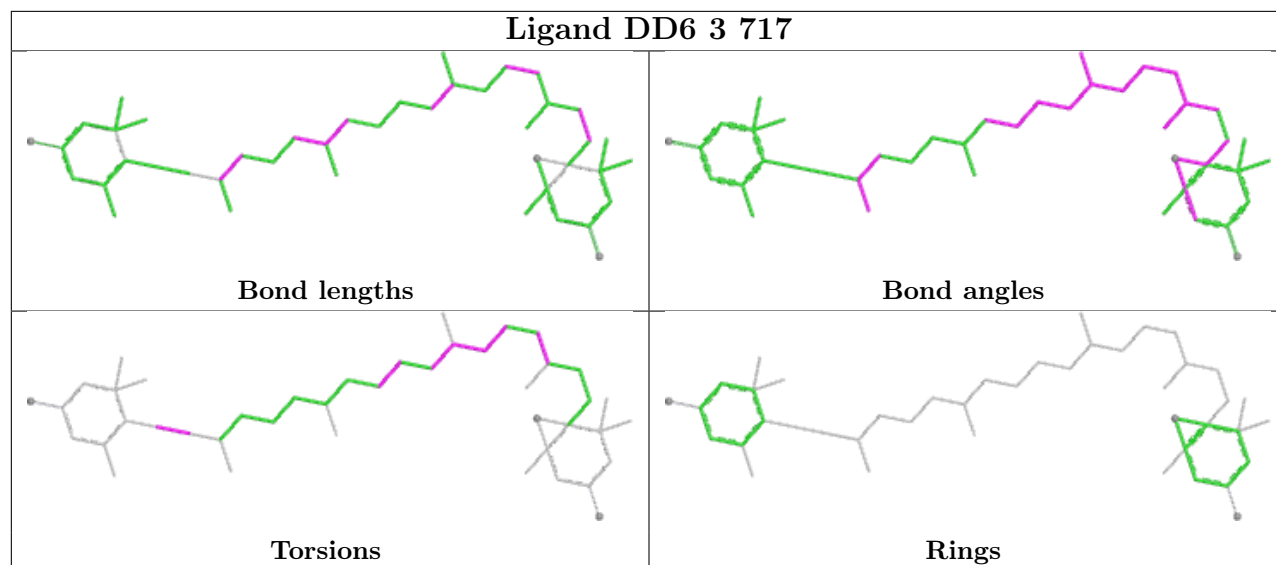
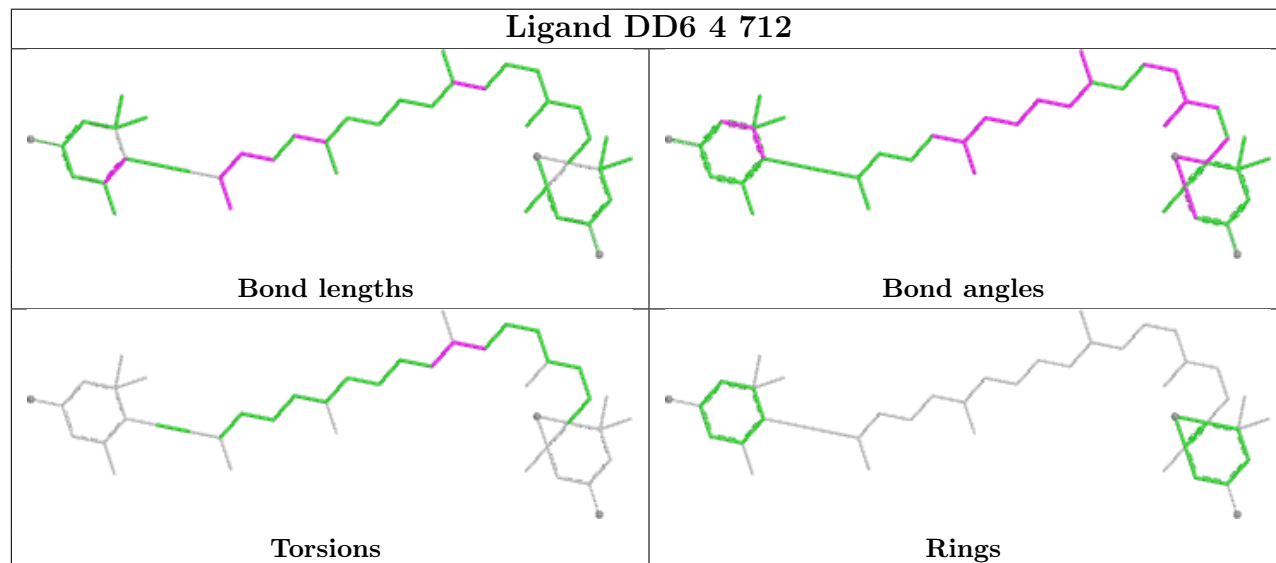
Bond angles



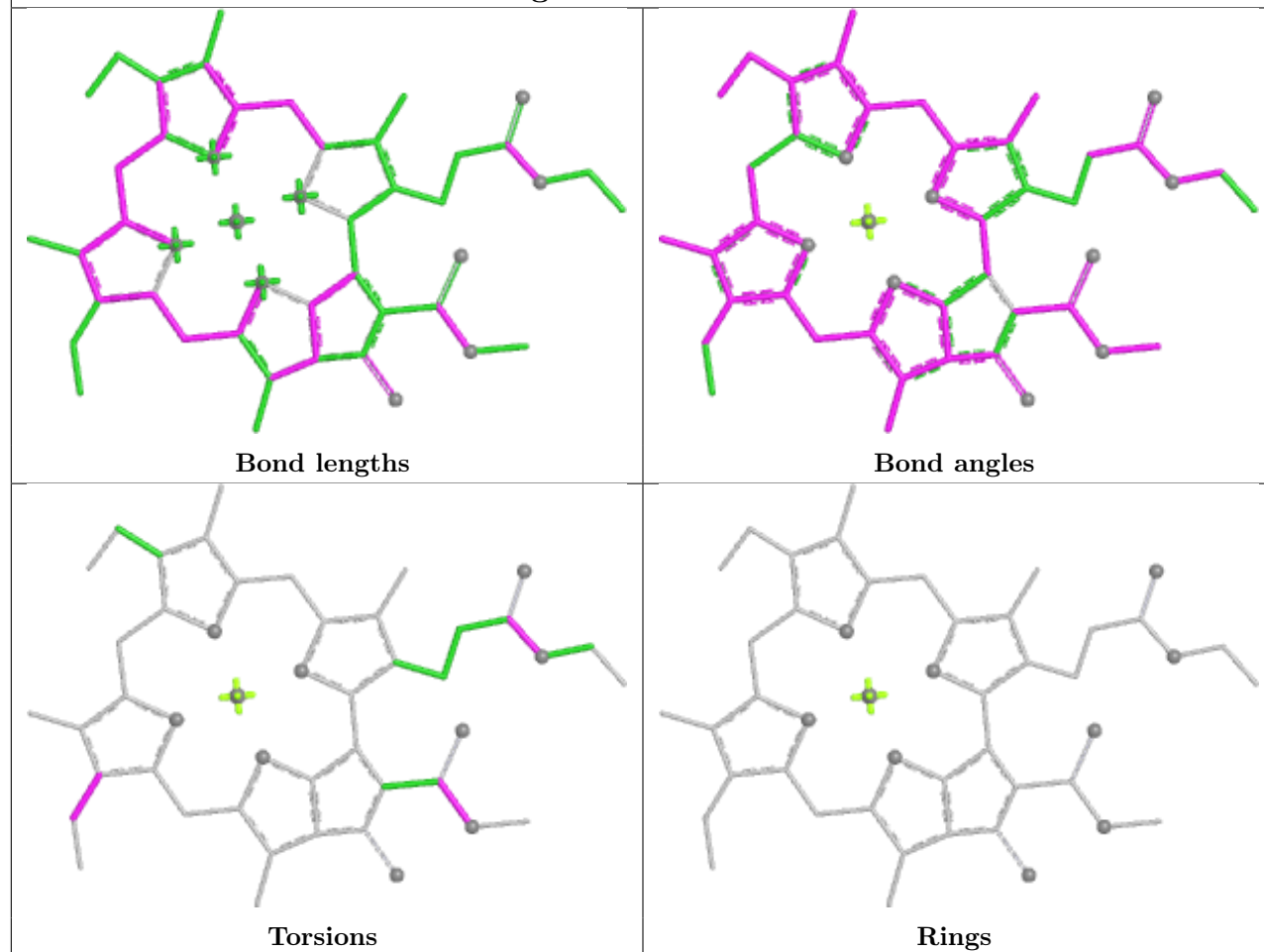
Torsions



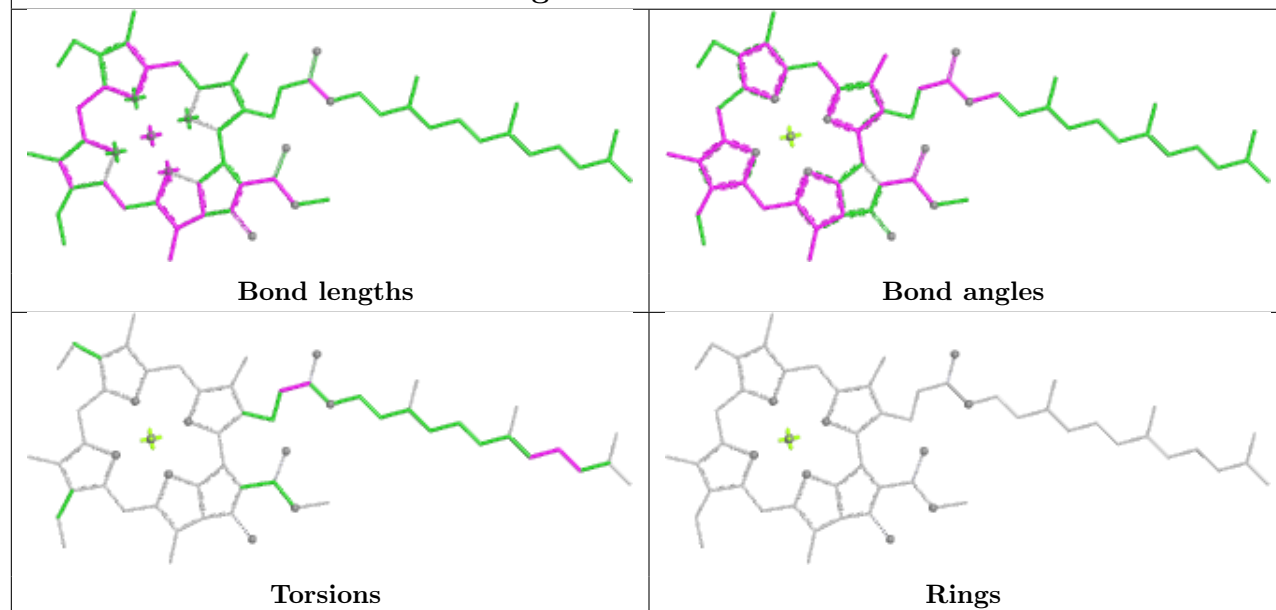
Rings

Ligand DD6 3 717**Ligand DD6 4 712**

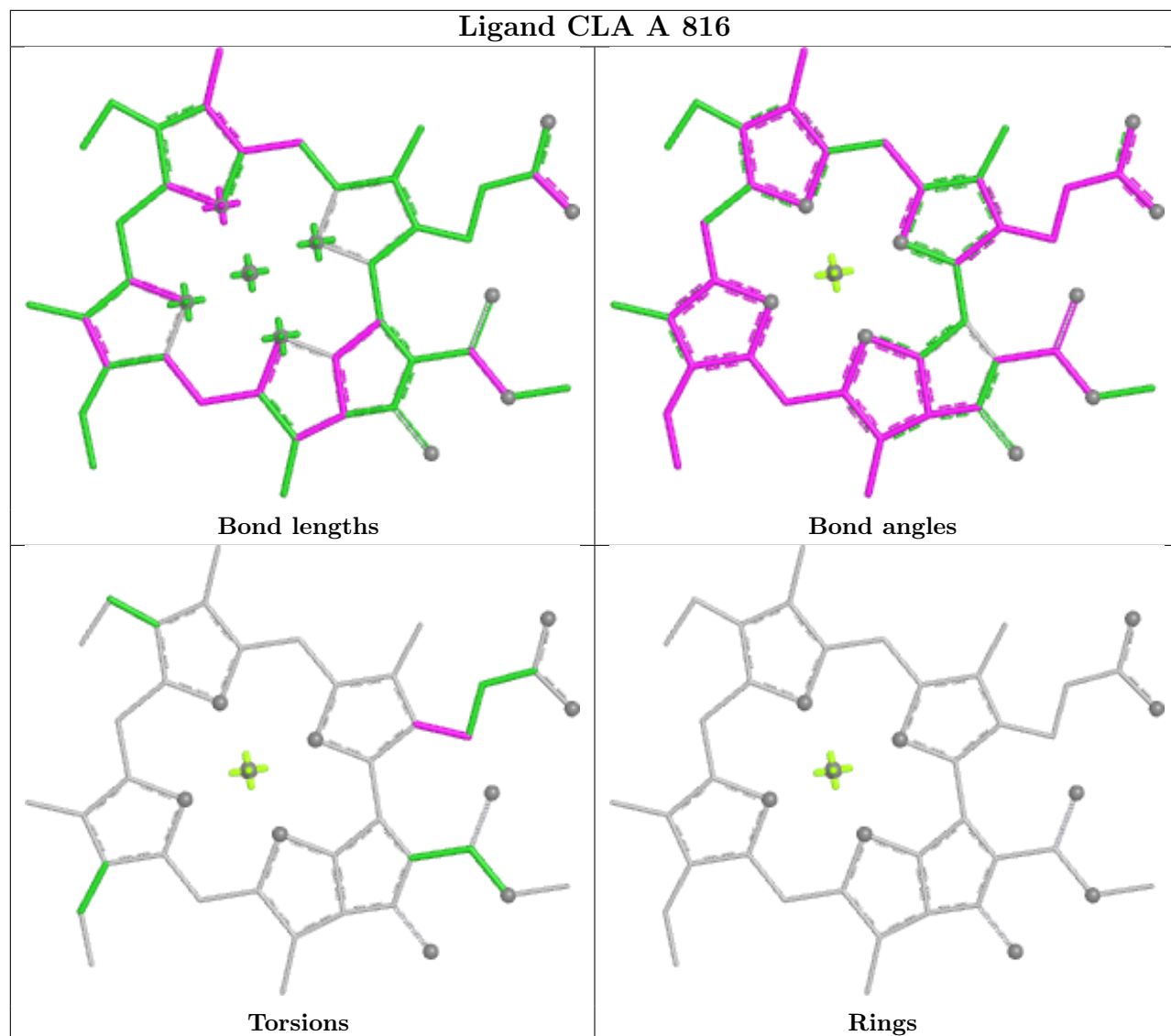
Ligand CLA 7 706

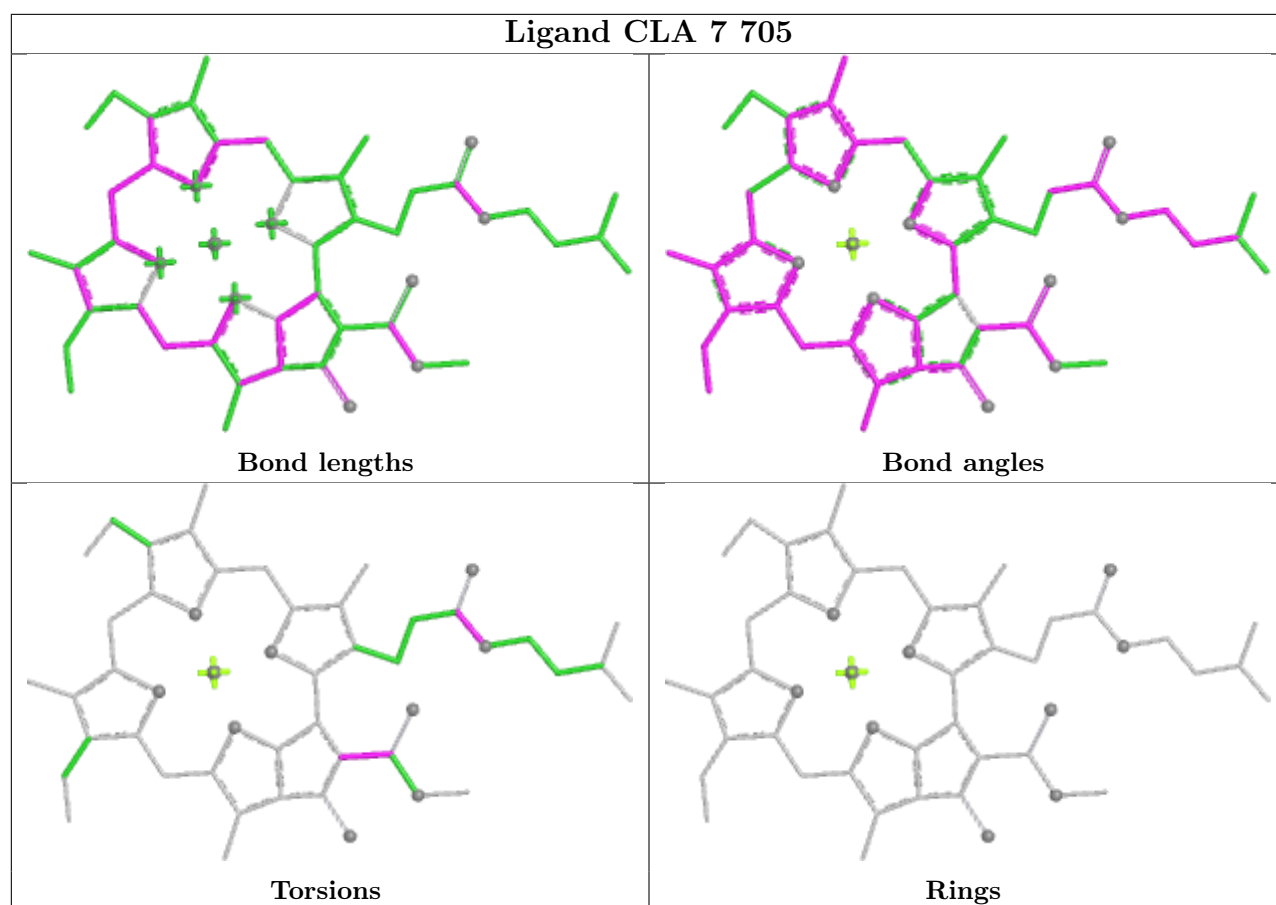


Ligand CLA A 814

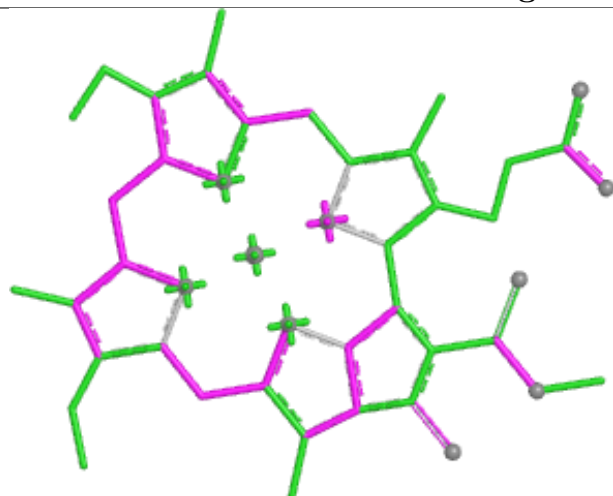


Ligand CLA A 816

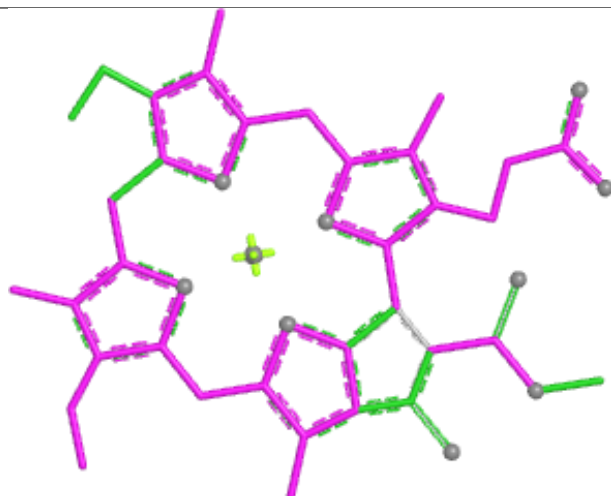




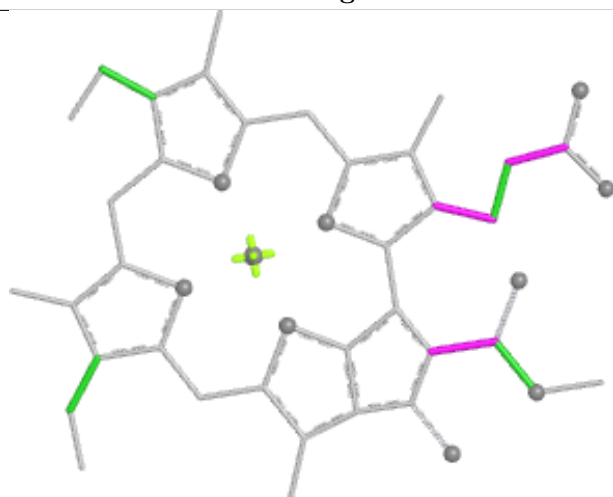
Ligand CLA 2 514



Bond lengths



Bond angles

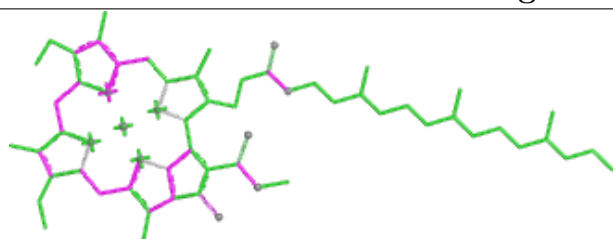


Torsions

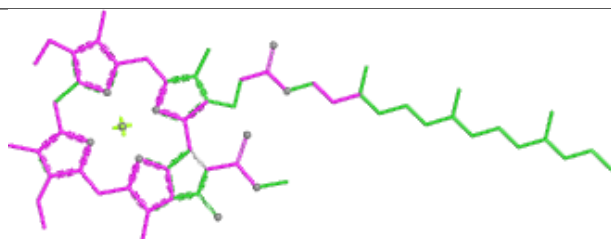


Rings

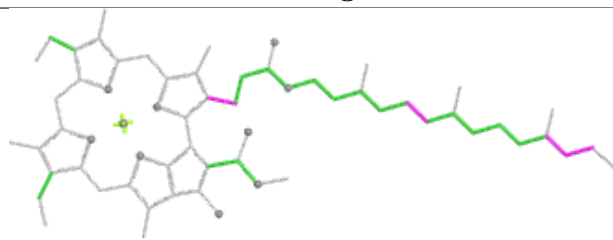
Ligand CLA 3 707



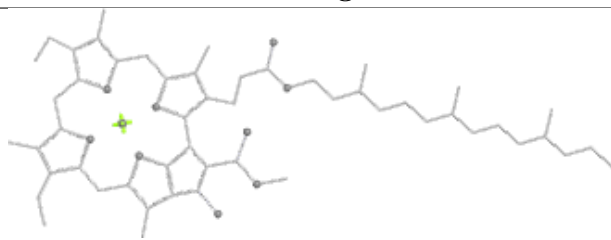
Bond lengths



Bond angles

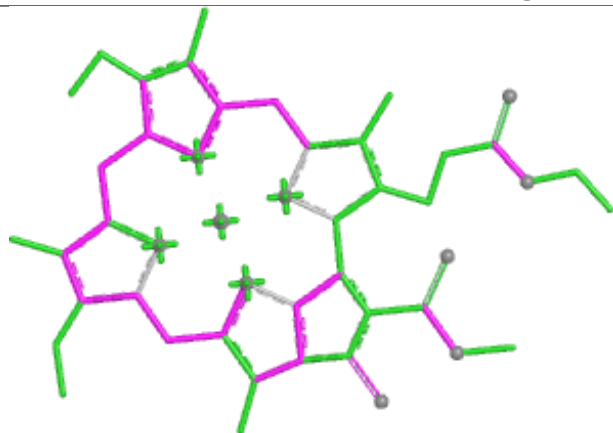


Torsions

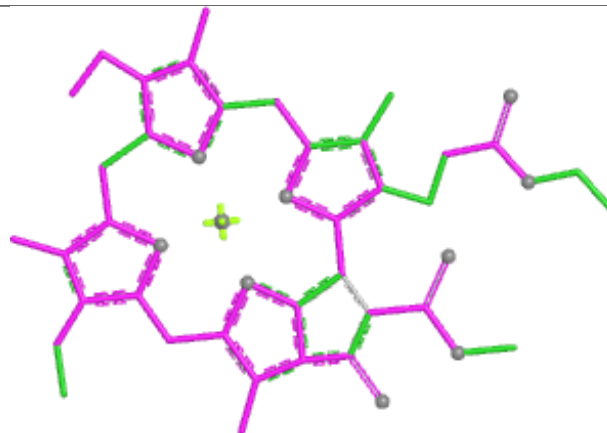


Rings

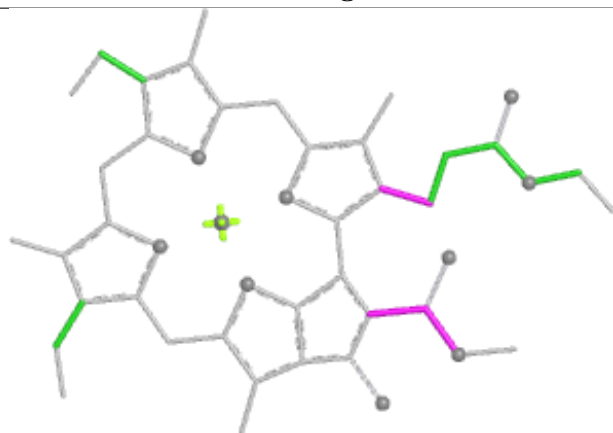
Ligand CLA 5 705



Bond lengths



Bond angles

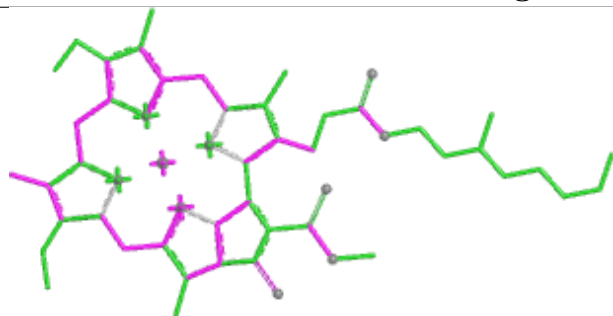


Torsions

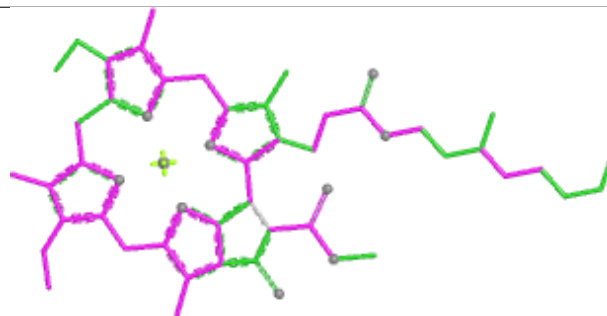


Rings

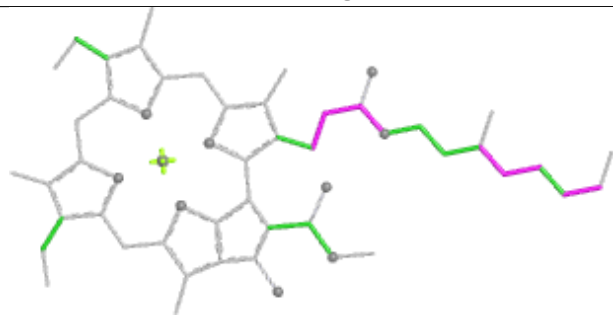
Ligand CLA A 813



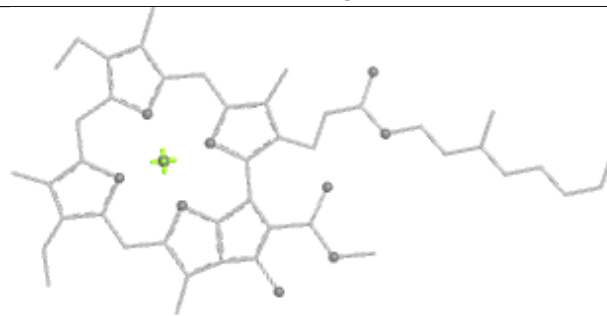
Bond lengths



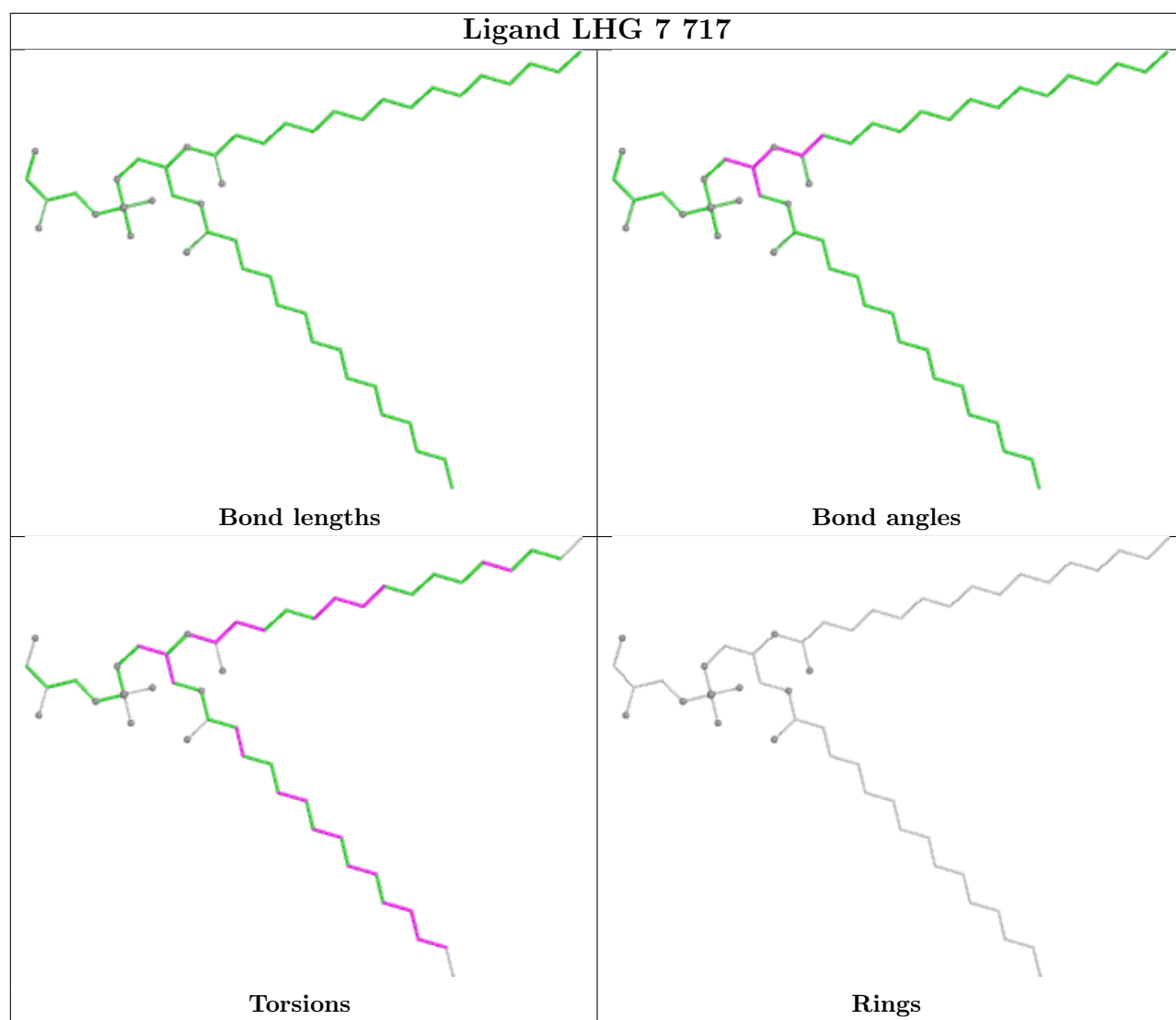
Bond angles



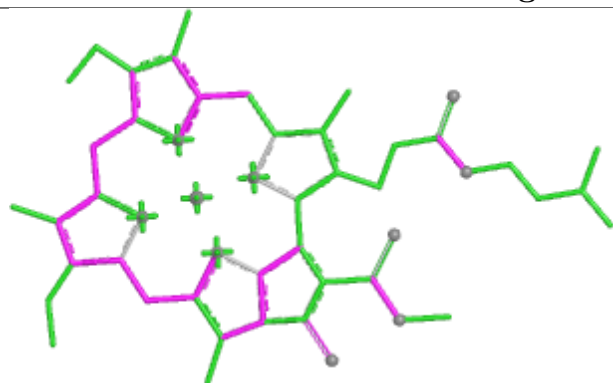
Torsions



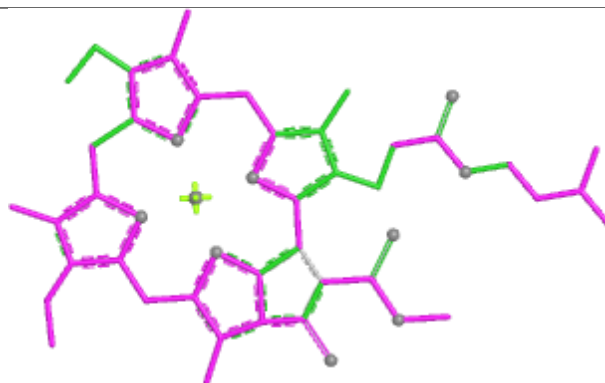
Rings



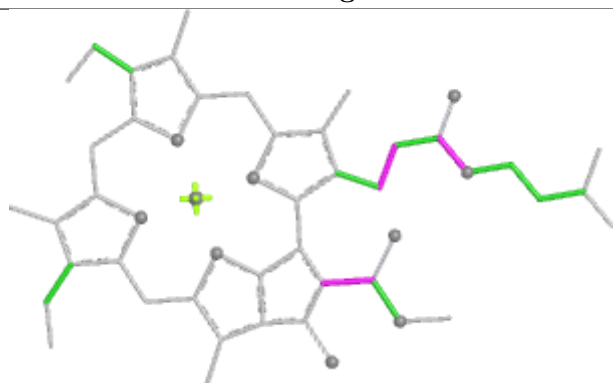
Ligand CLA 6 906



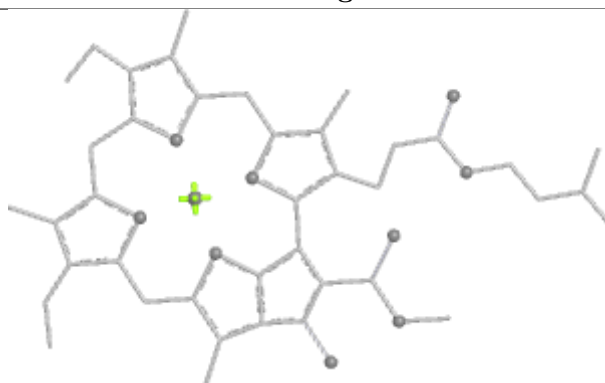
Bond lengths



Bond angles

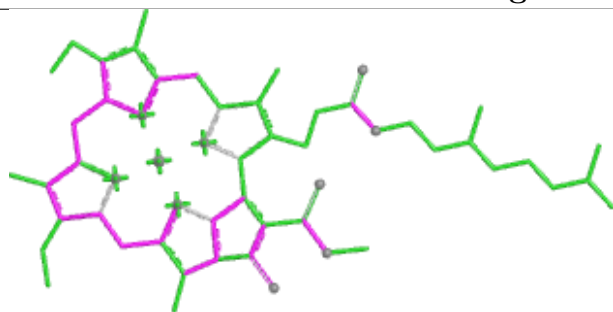


Torsions

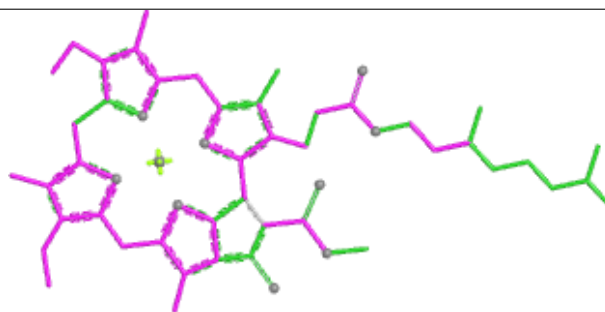


Rings

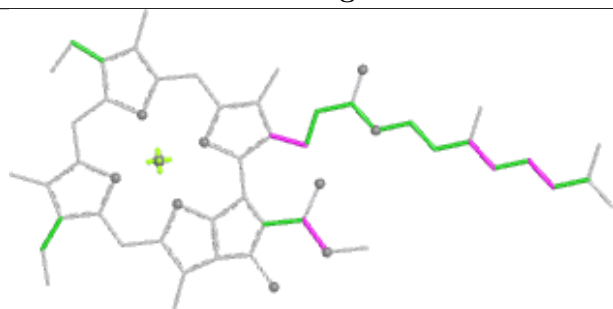
Ligand CLA 12 506



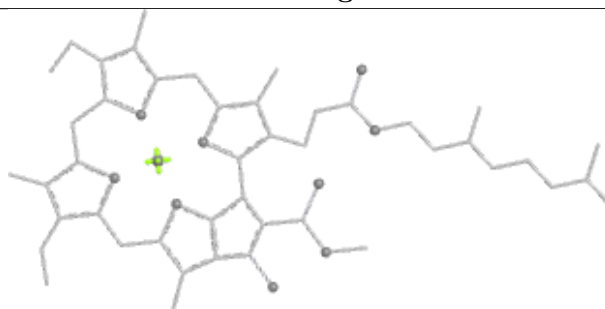
Bond lengths



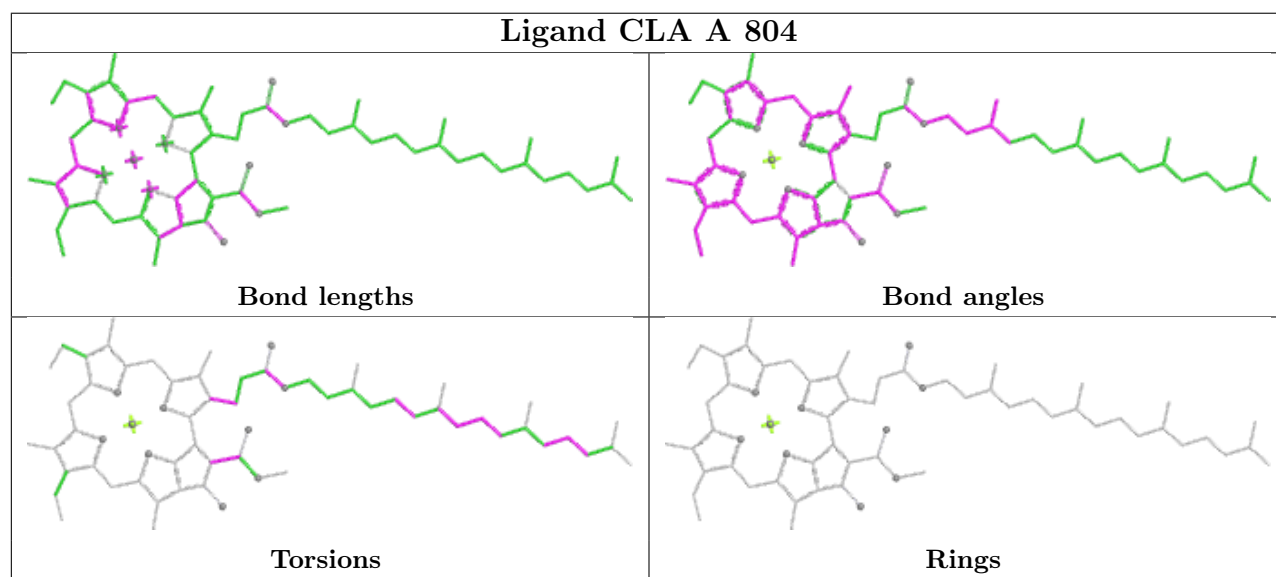
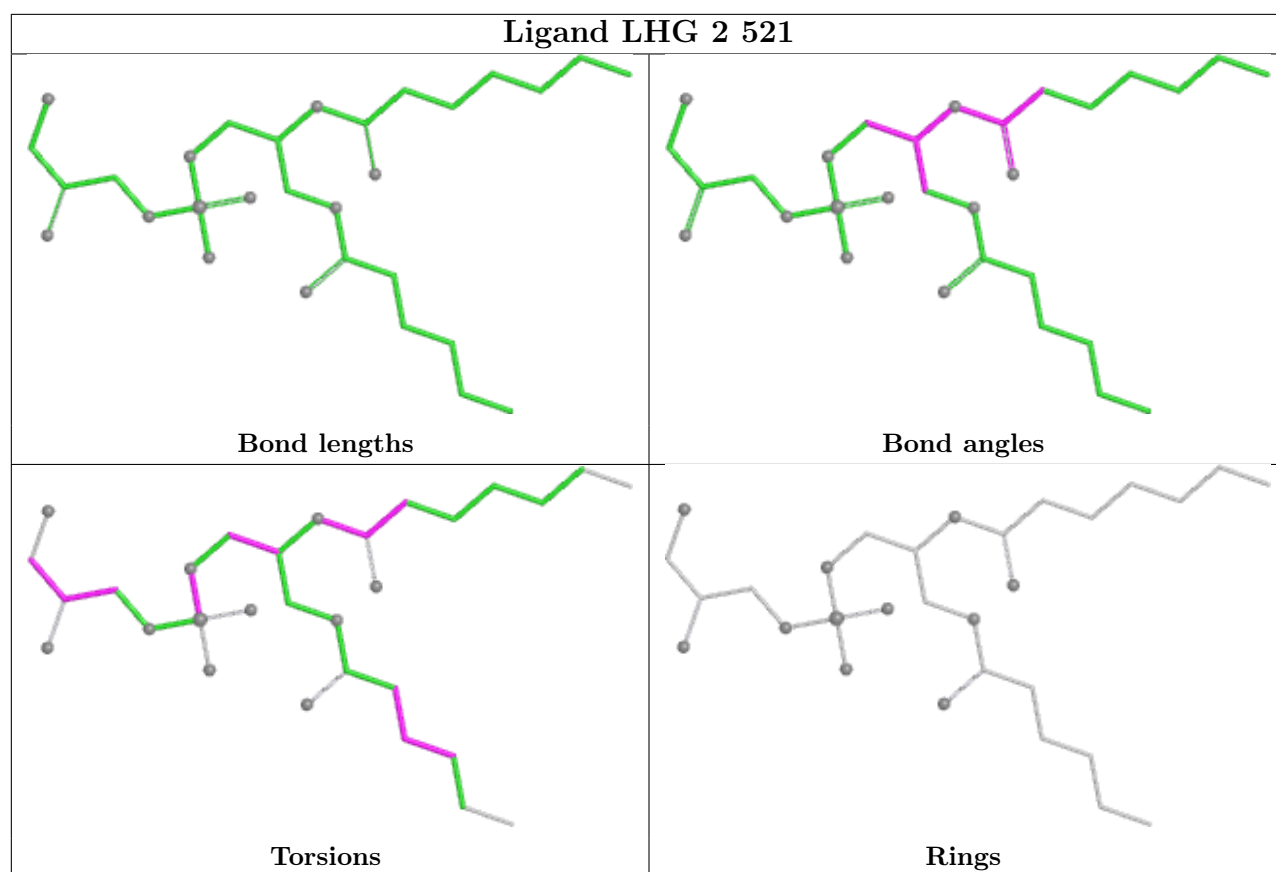
Bond angles

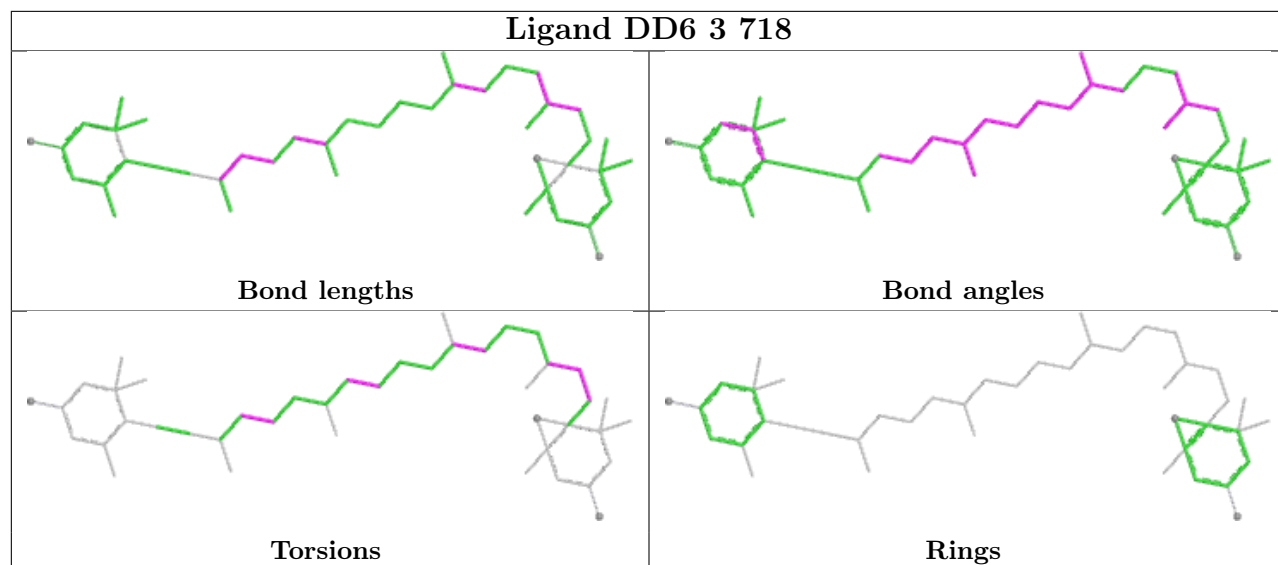
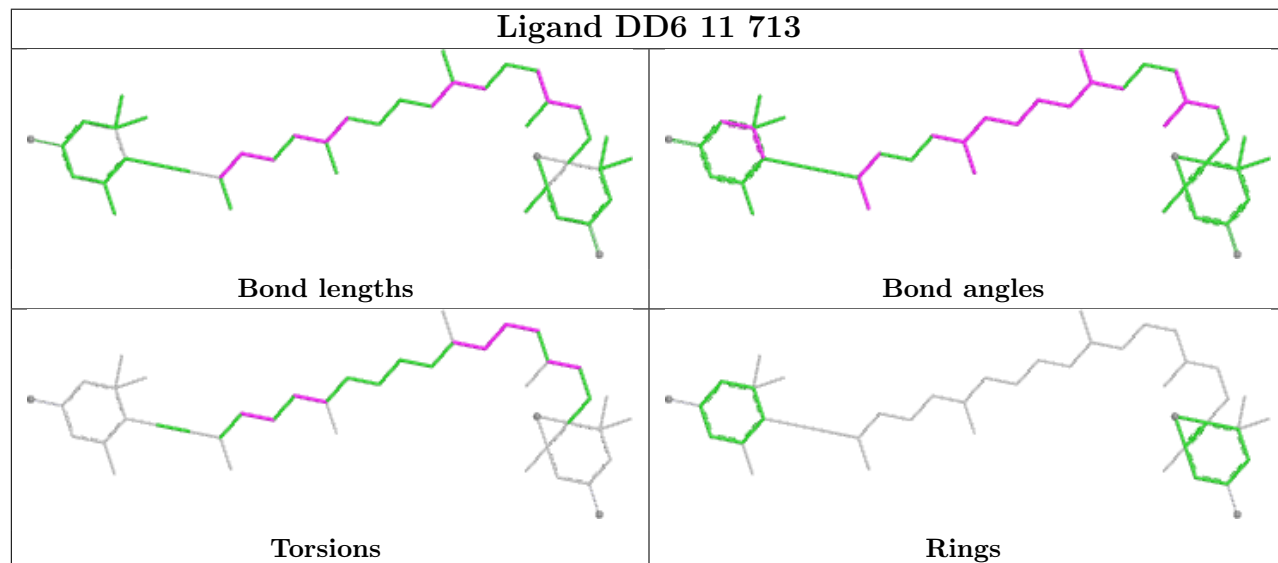


Torsions

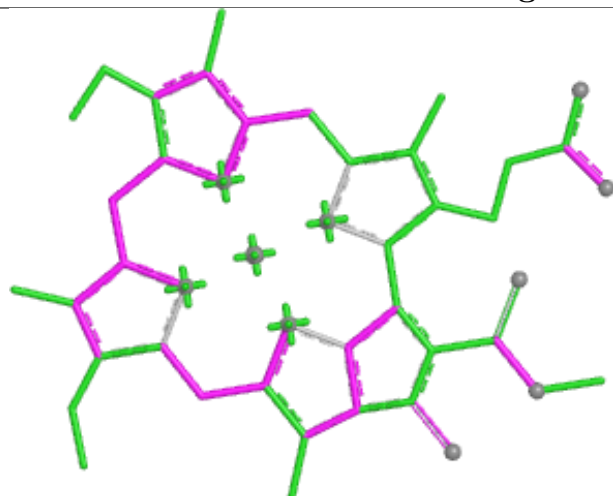


Rings

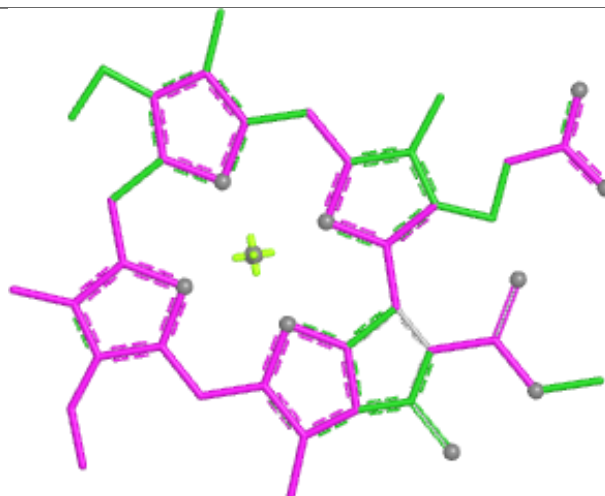


Ligand DD6 3 718**Ligand DD6 11 713**

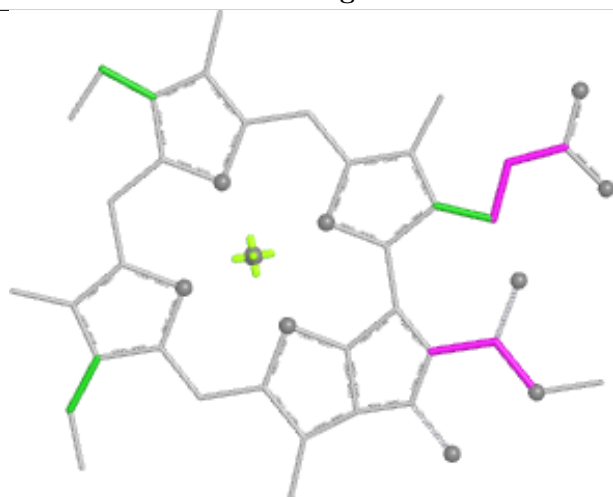
Ligand CLA 4 703



Bond lengths



Bond angles

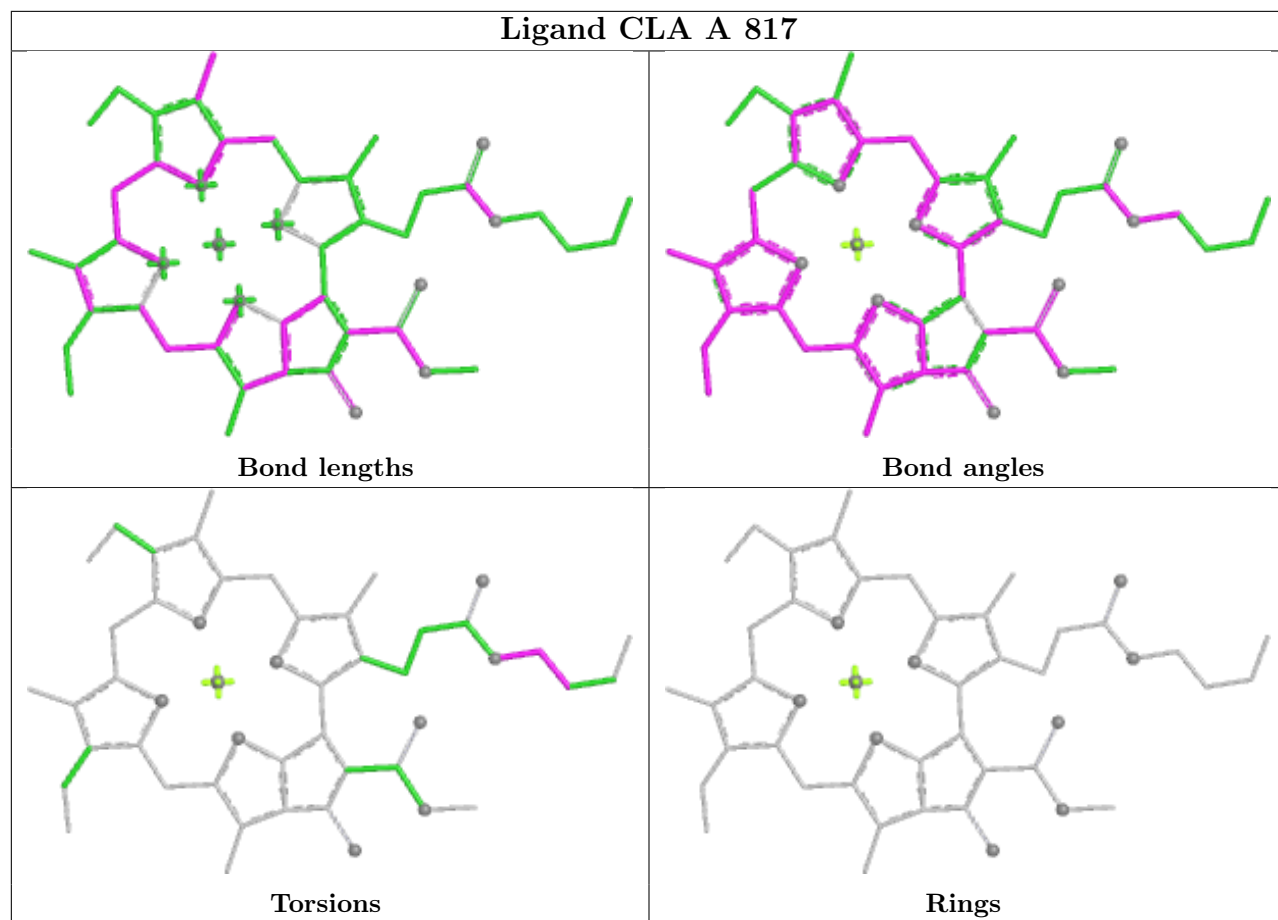


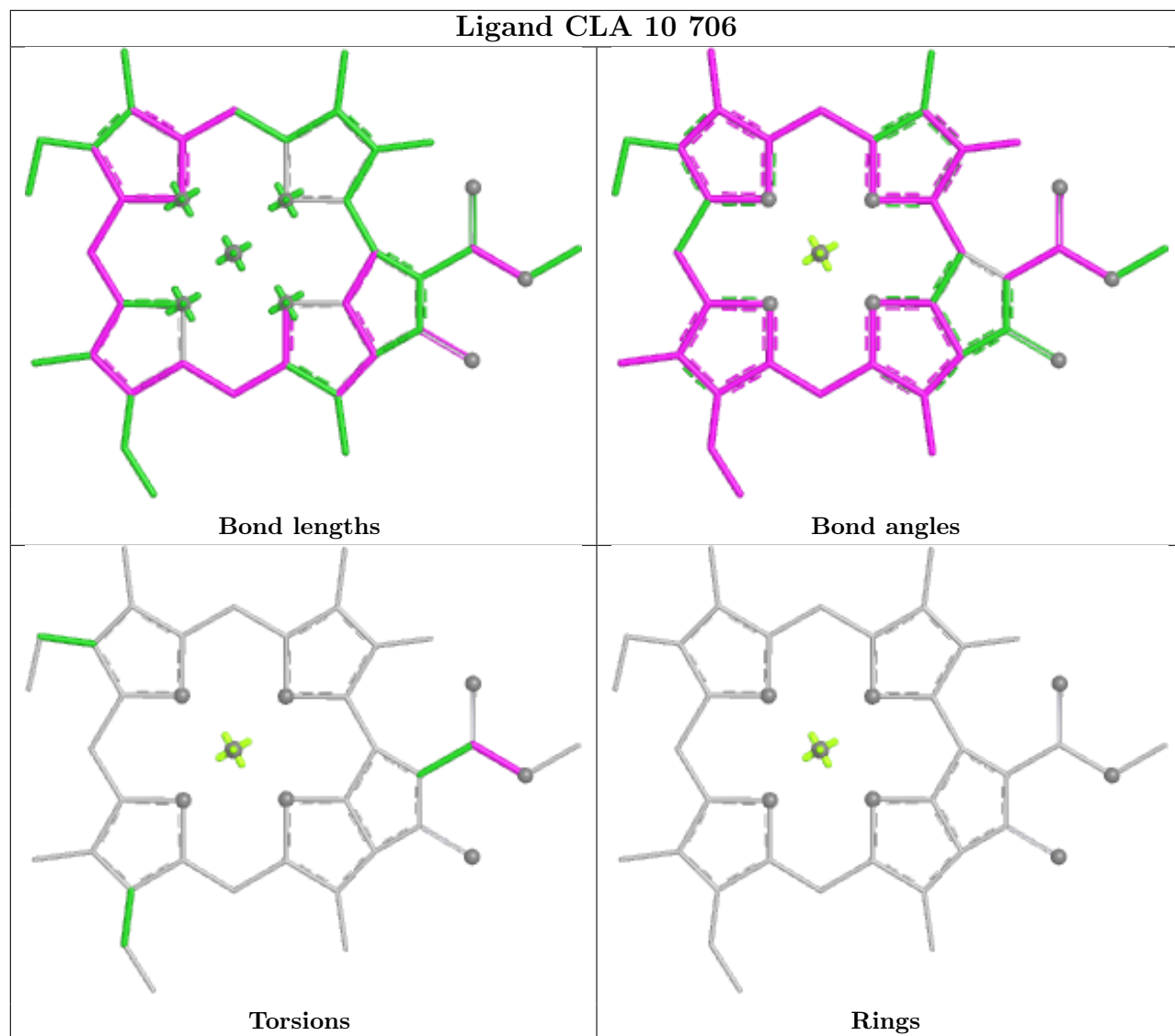
Torsions



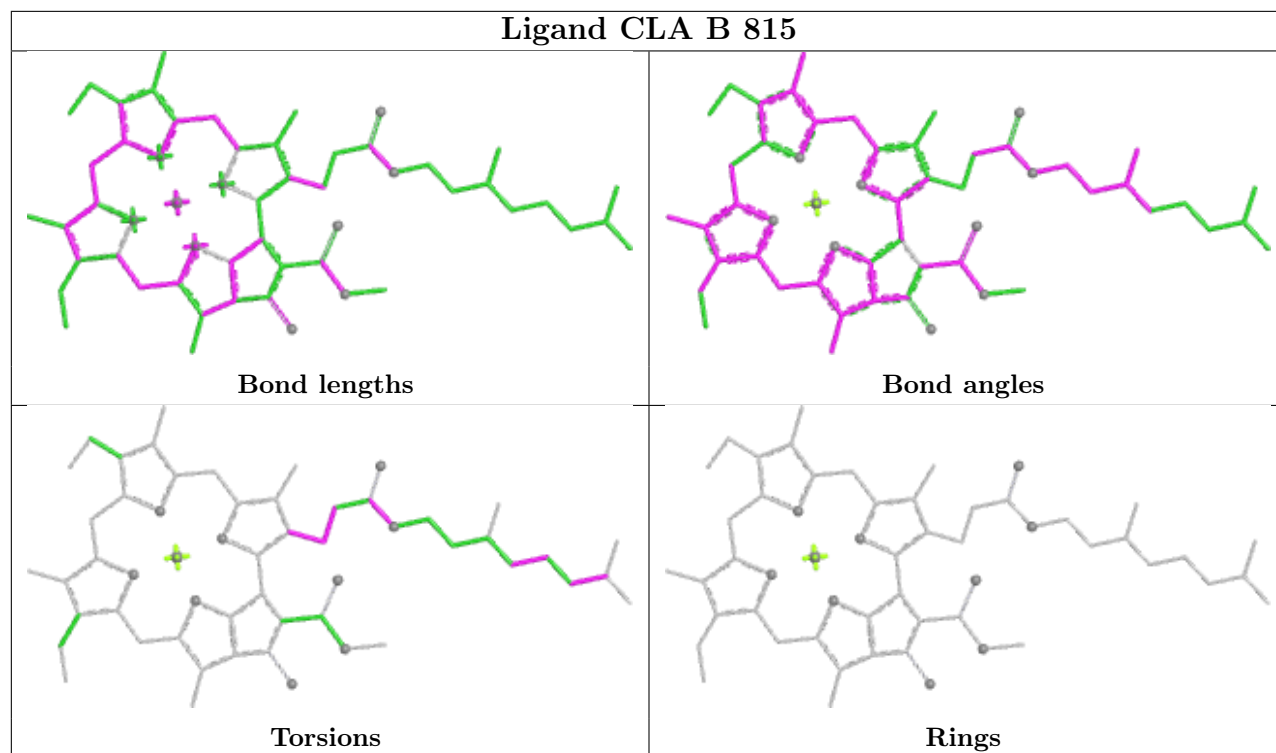
Rings

Ligand CLA A 817

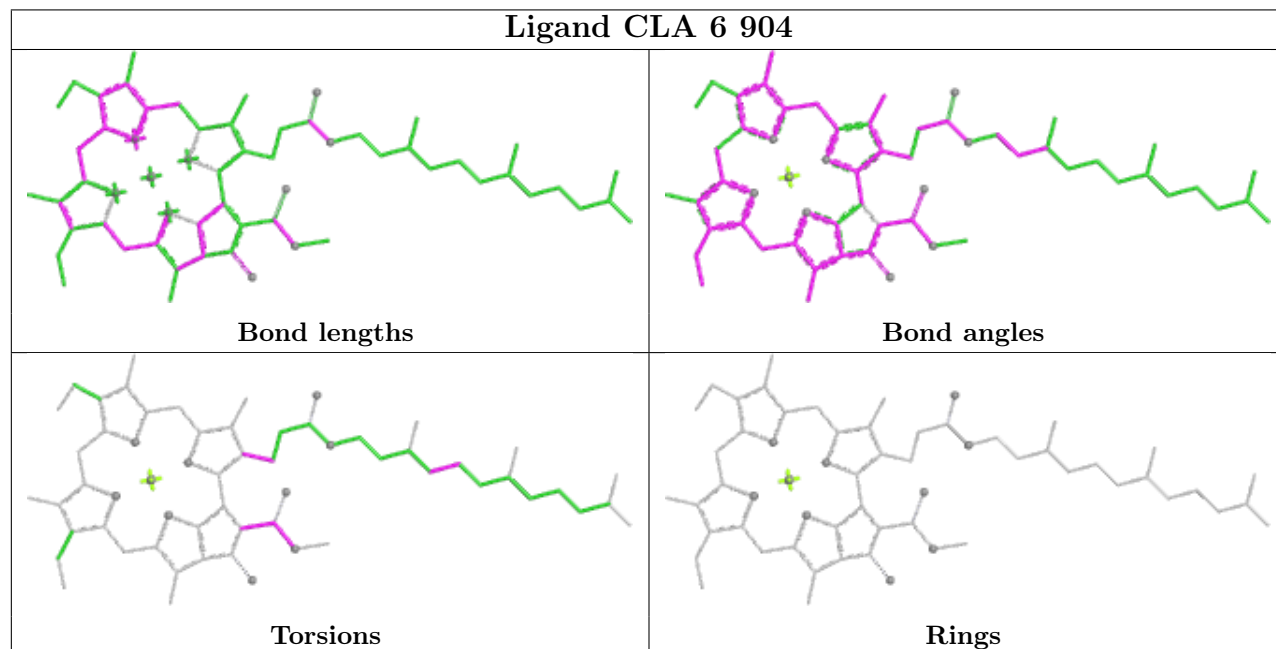


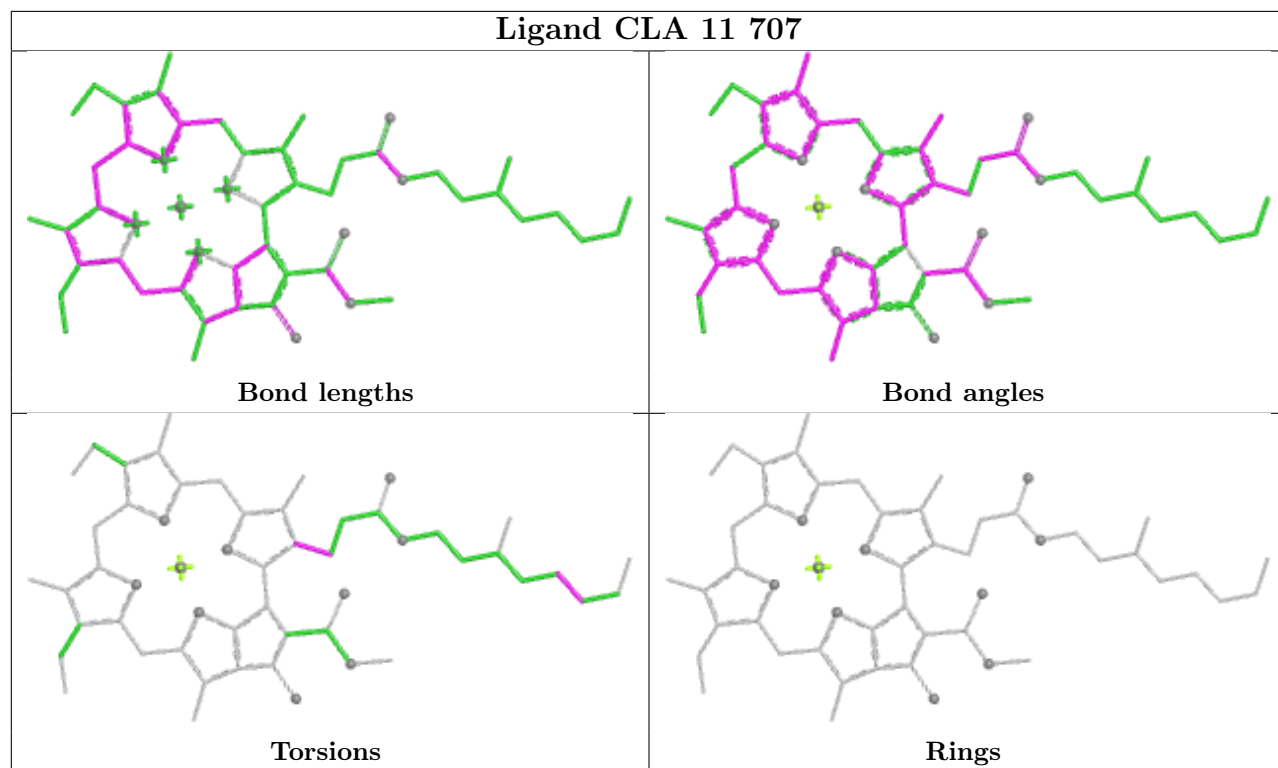


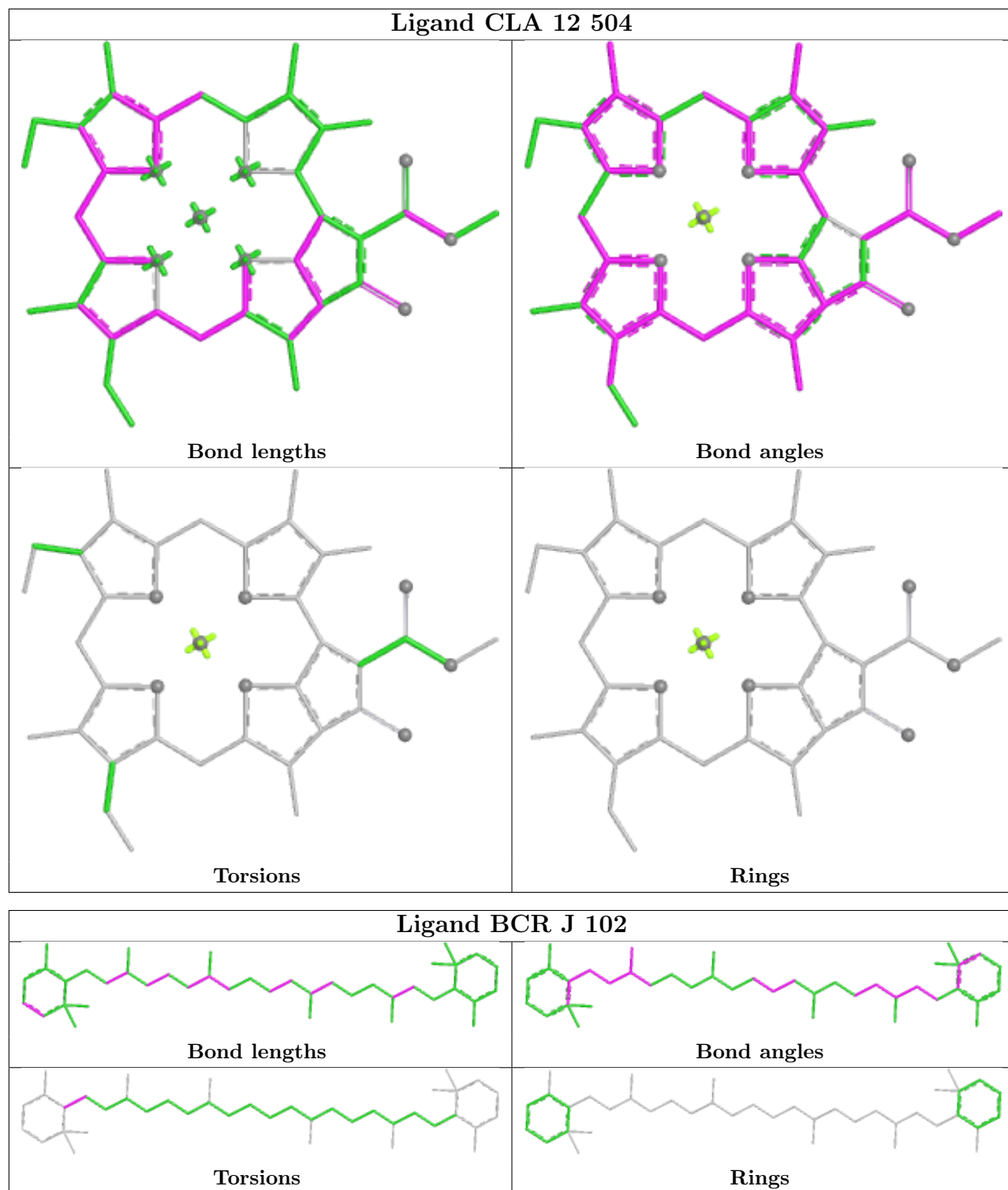
Ligand CLA B 815

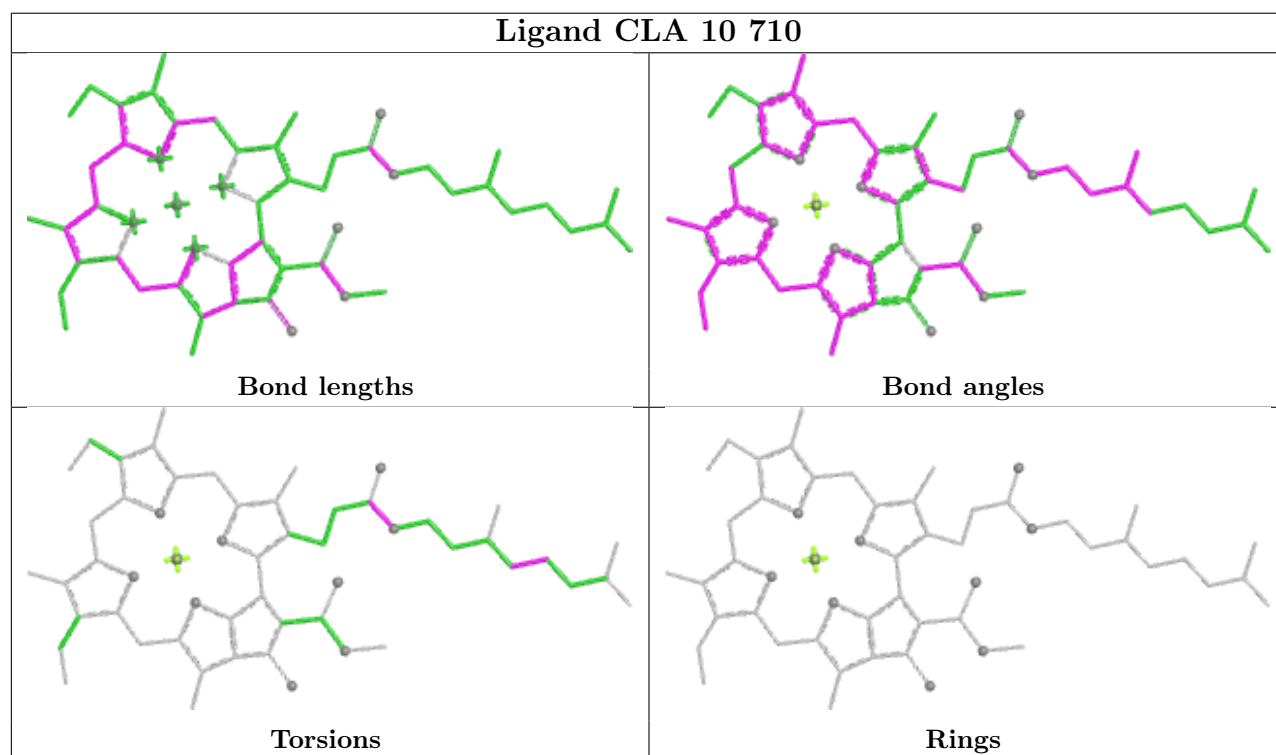
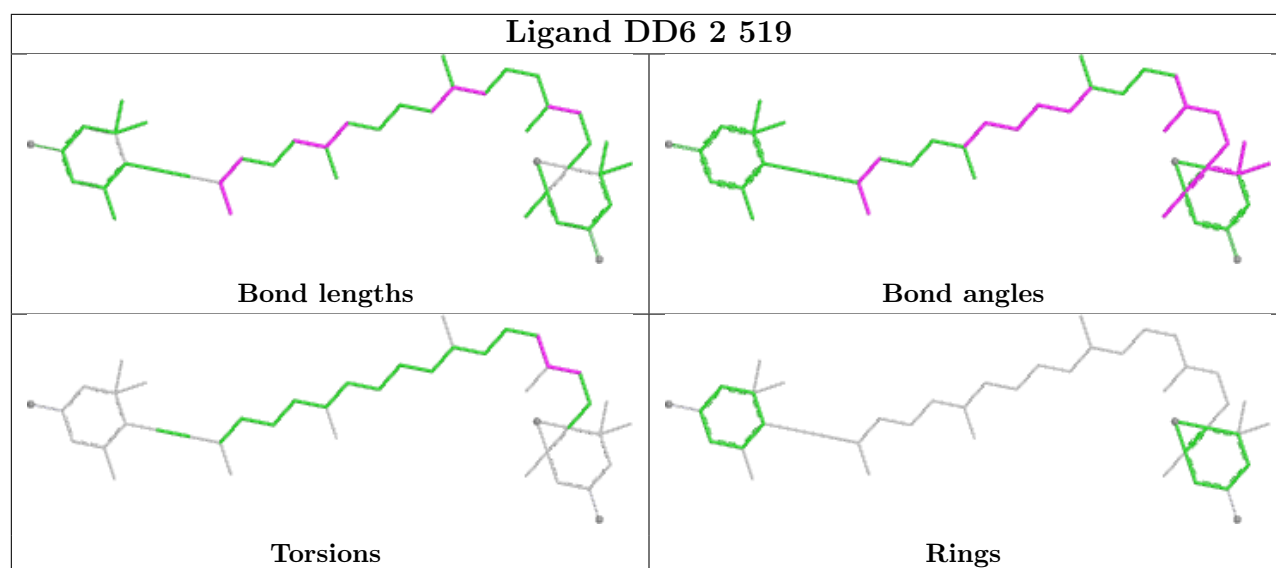


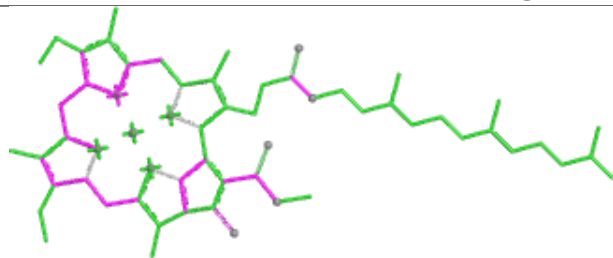
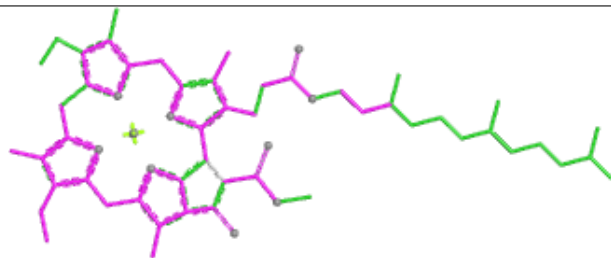
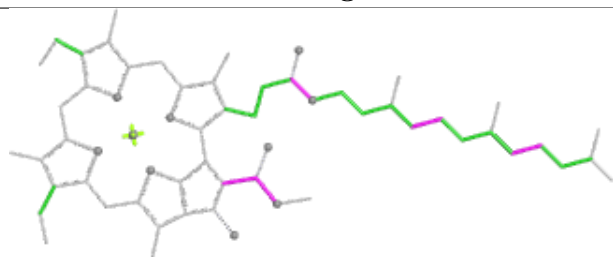
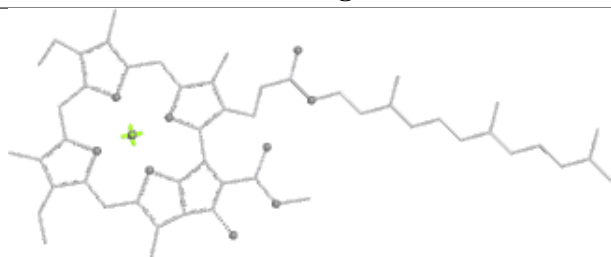
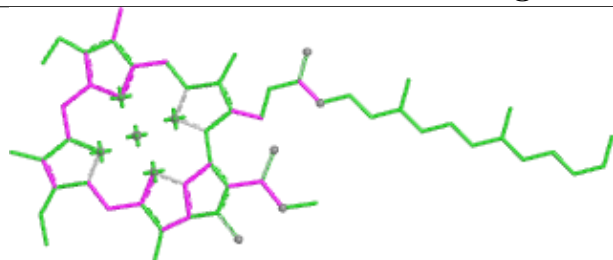
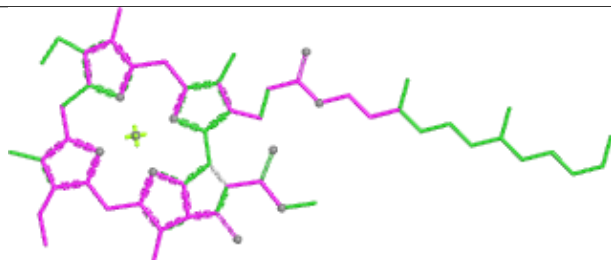
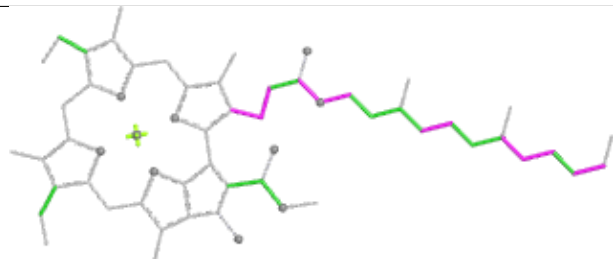
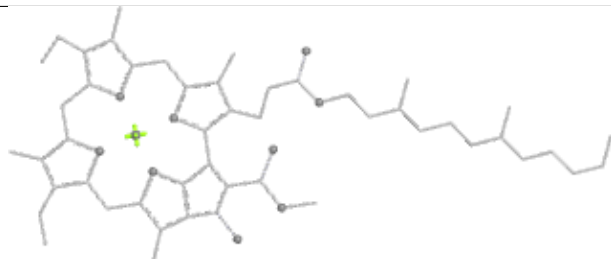
Ligand CLA 6 904



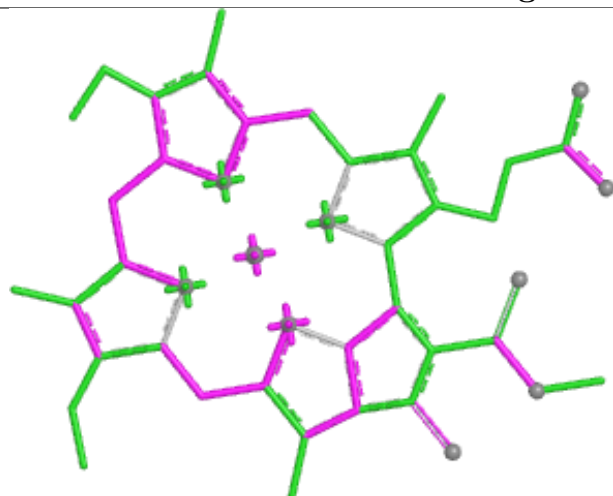




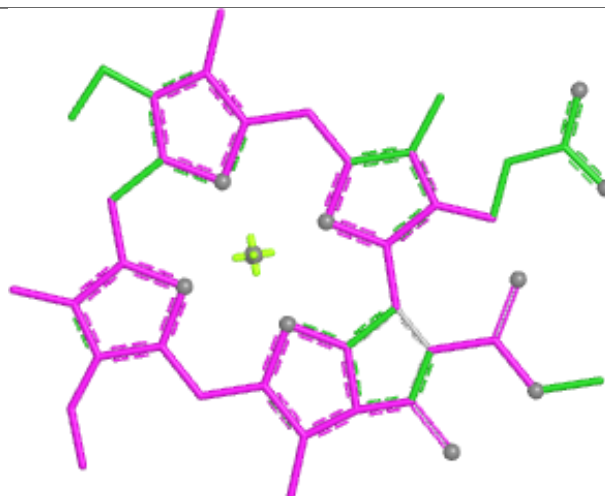


Ligand CLA 3 702**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 825****Bond lengths****Bond angles****Torsions****Rings**

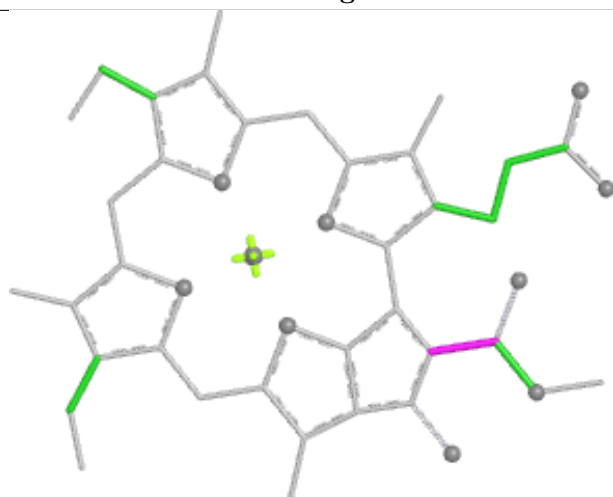
Ligand CLA 6 908



Bond lengths



Bond angles

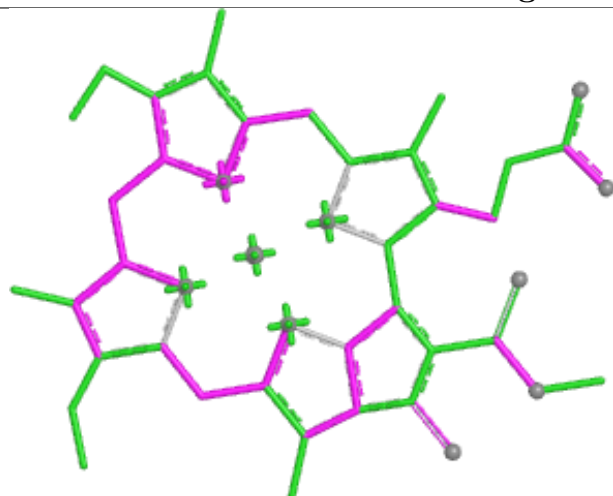


Torsions

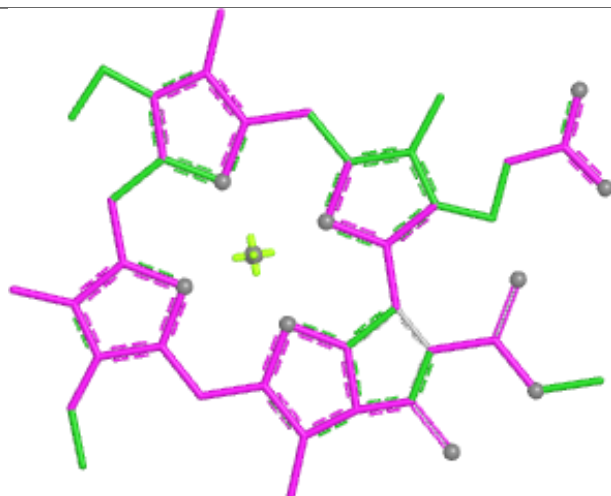


Rings

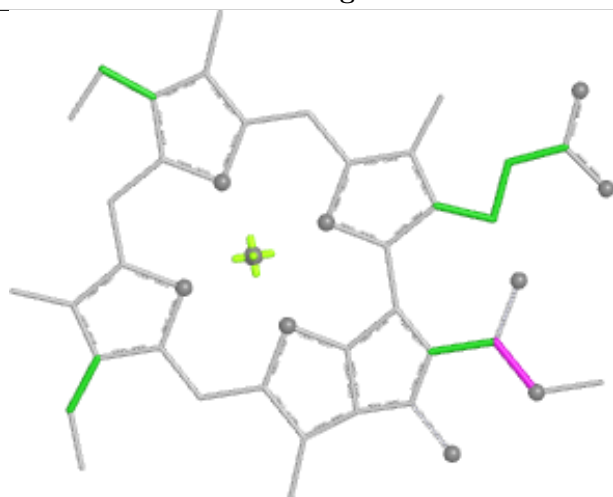
Ligand CLA 1 517



Bond lengths



Bond angles

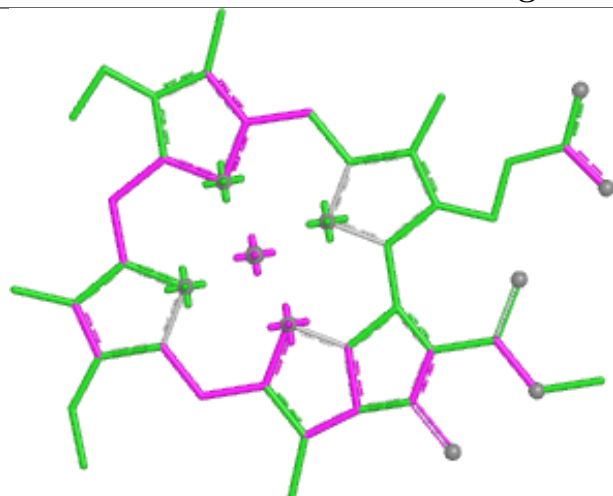


Torsions

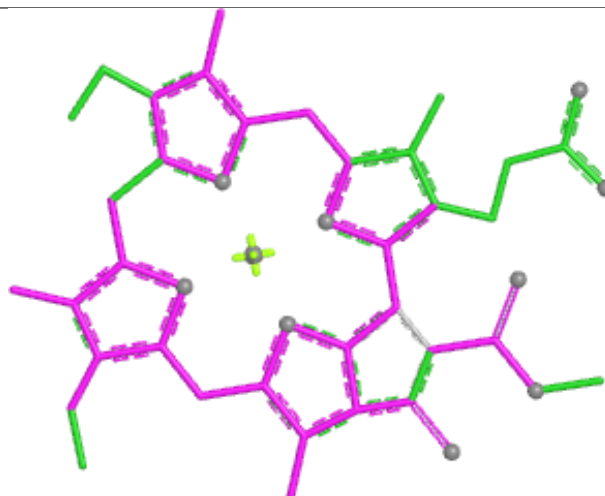


Rings

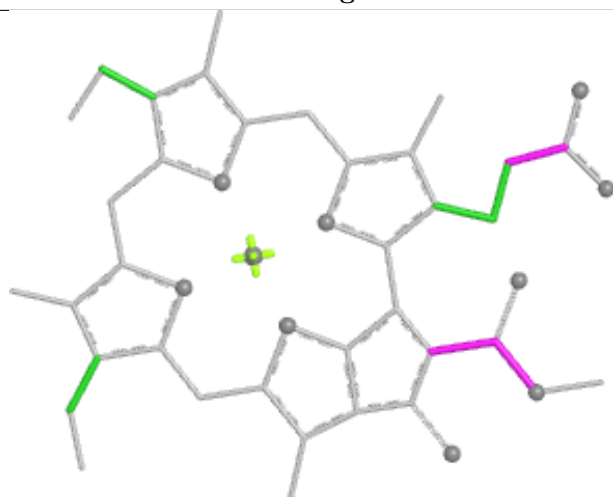
Ligand CLA 2 505



Bond lengths



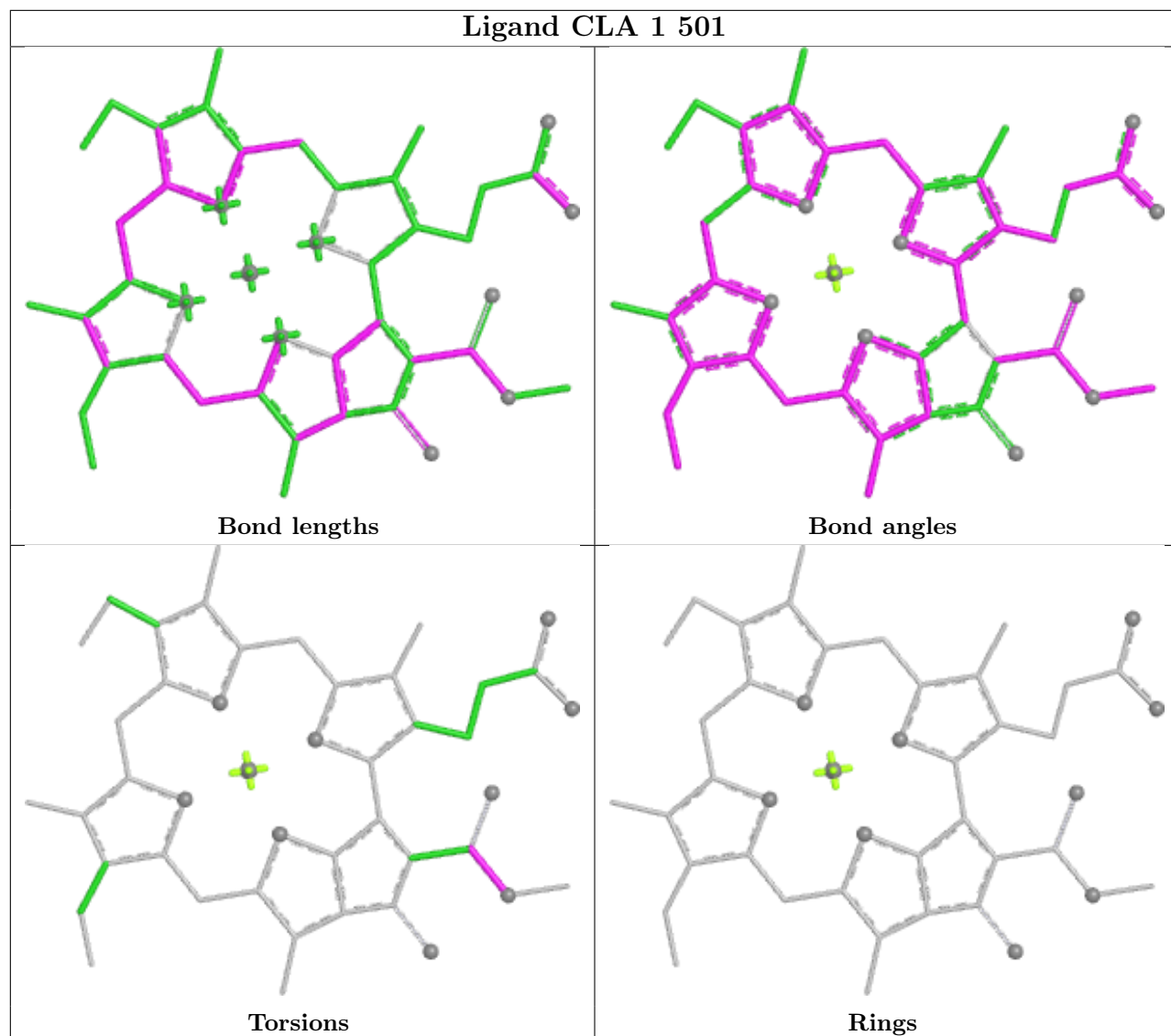
Bond angles



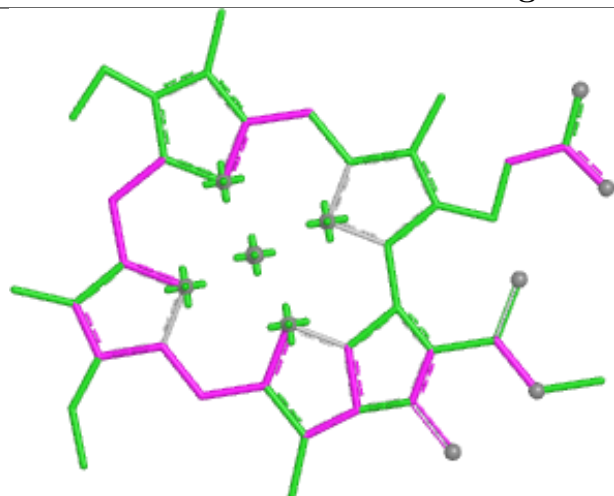
Torsions



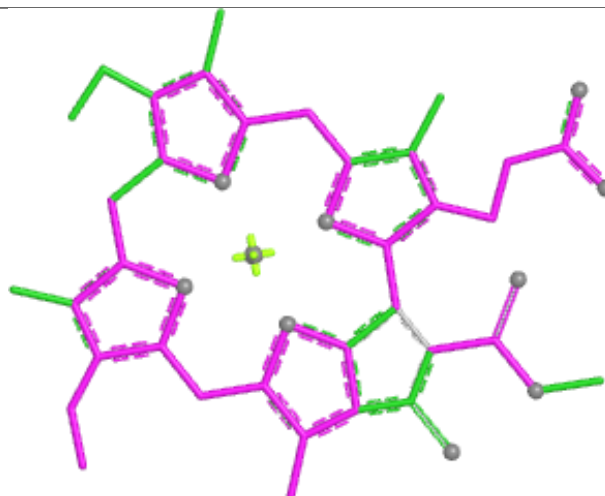
Rings



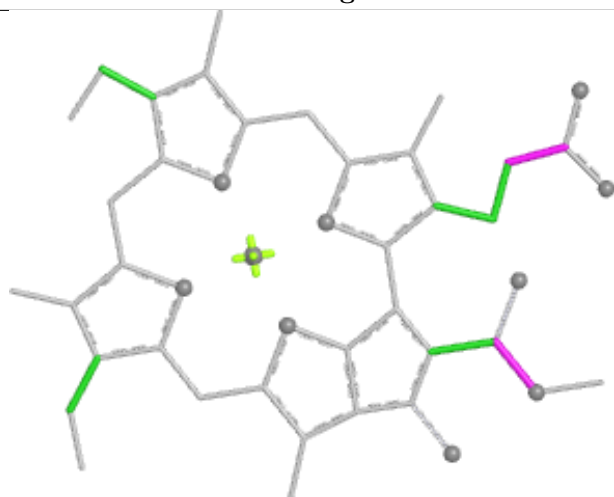
Ligand CLA 4 711



Bond lengths



Bond angles

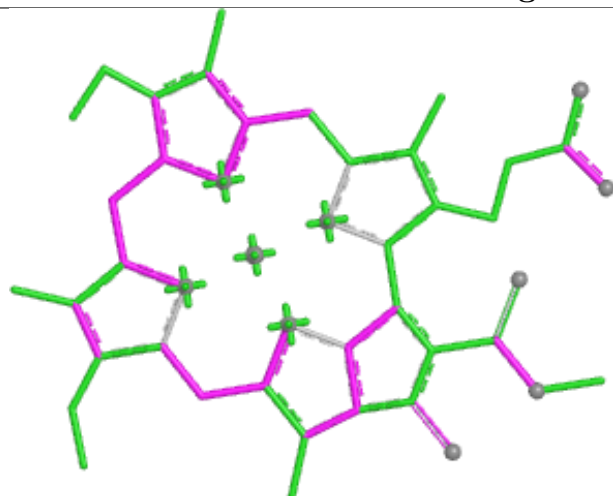


Torsions

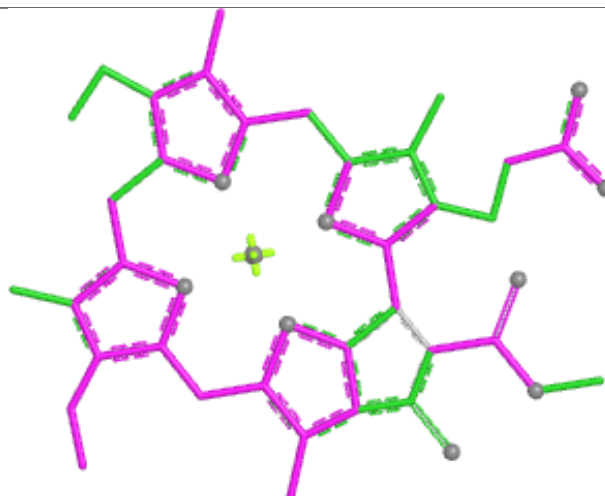


Rings

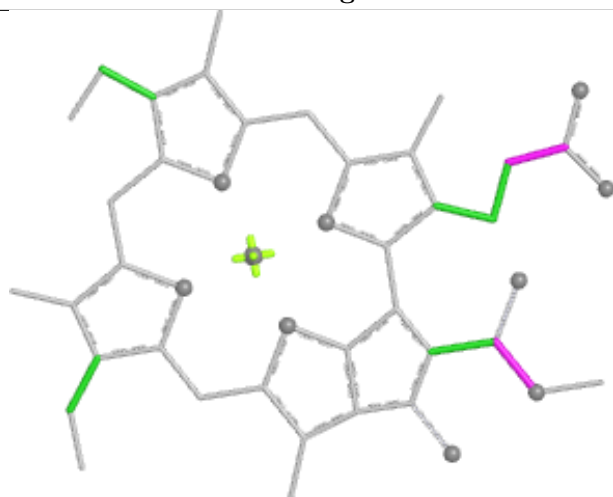
Ligand CLA 6 912



Bond lengths



Bond angles

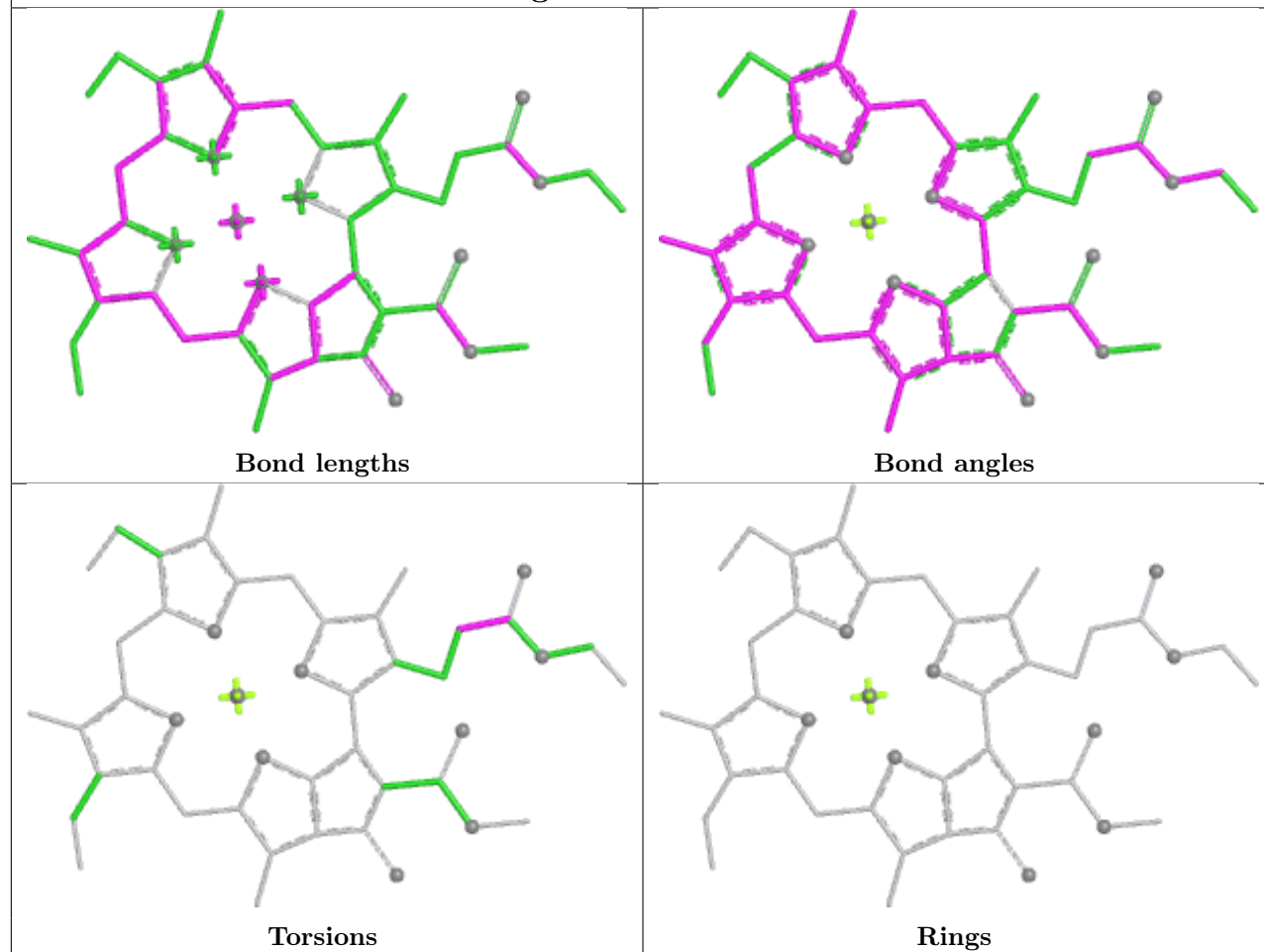


Torsions

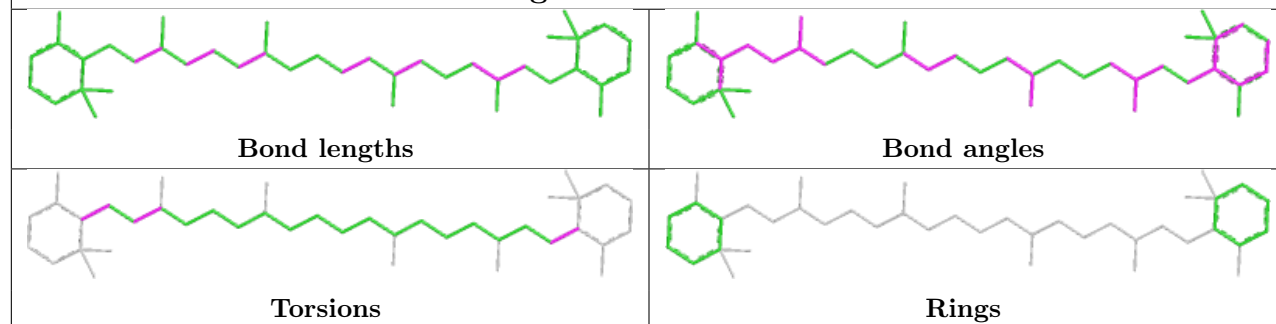


Rings

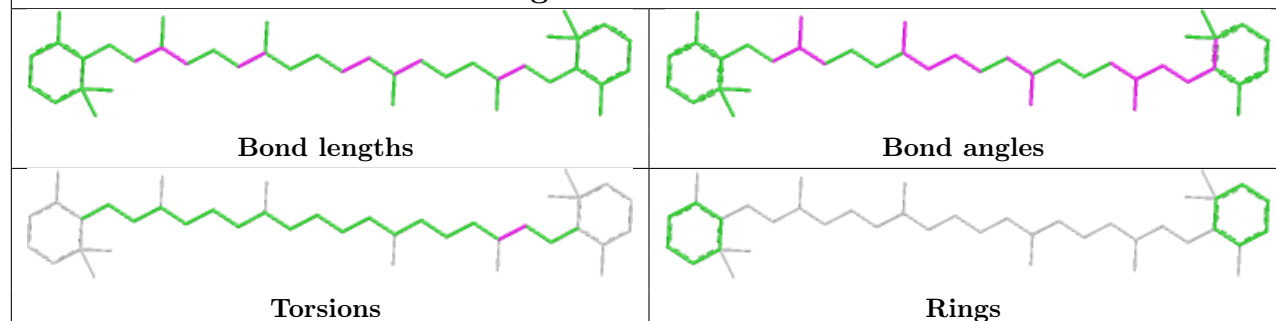
Ligand CLA 8 614

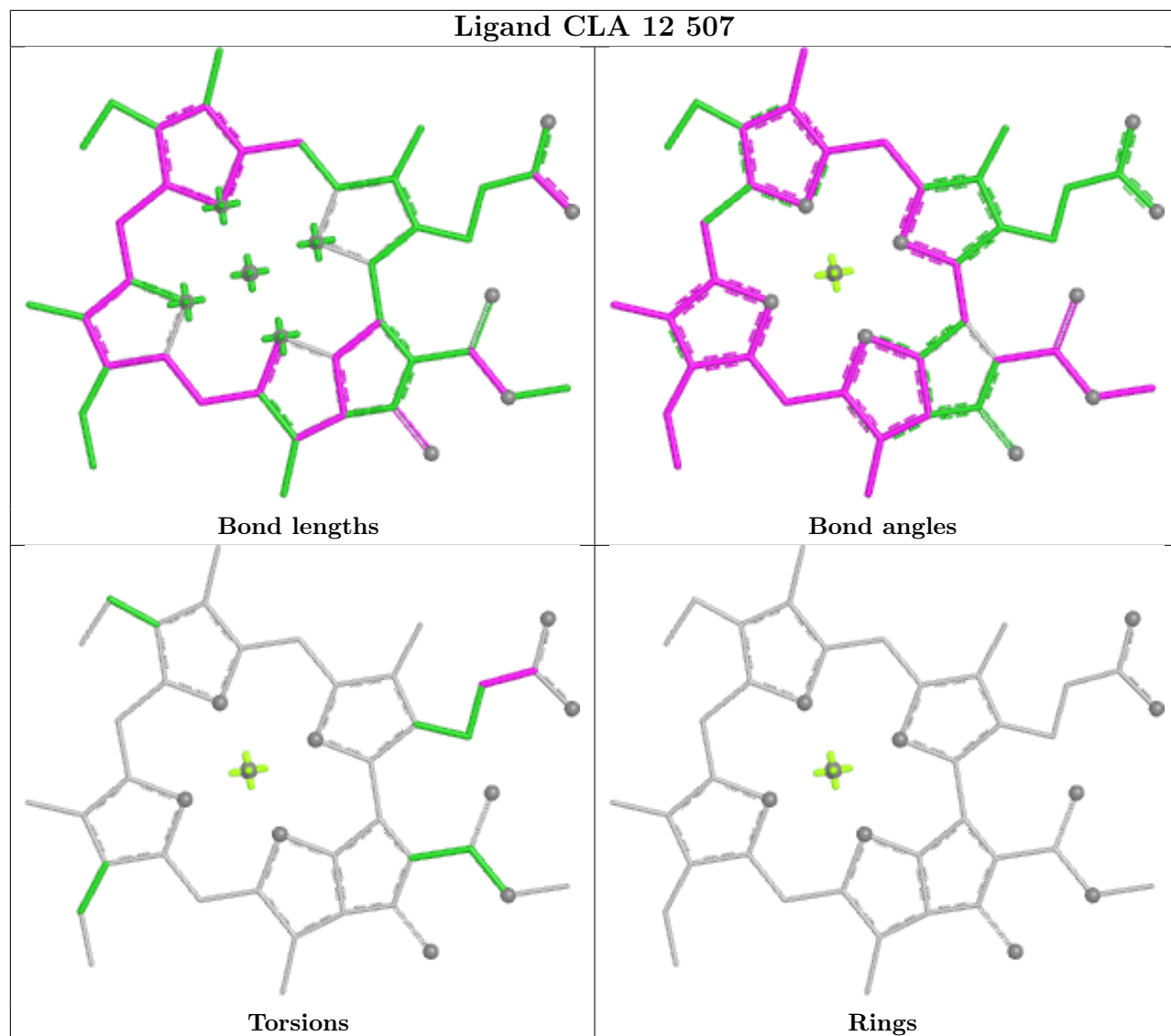


Ligand BCR A 850

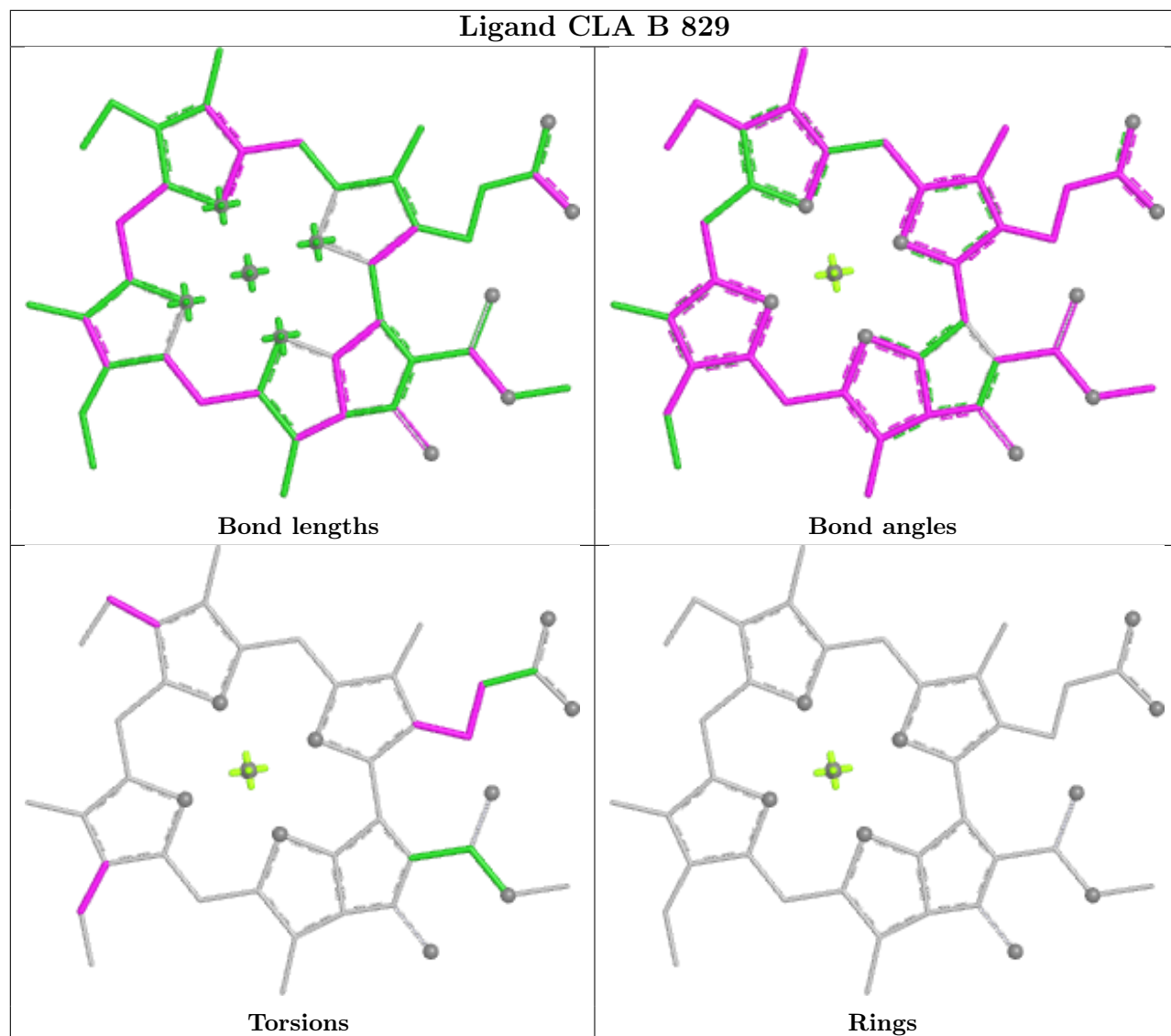


Ligand BCR B 841

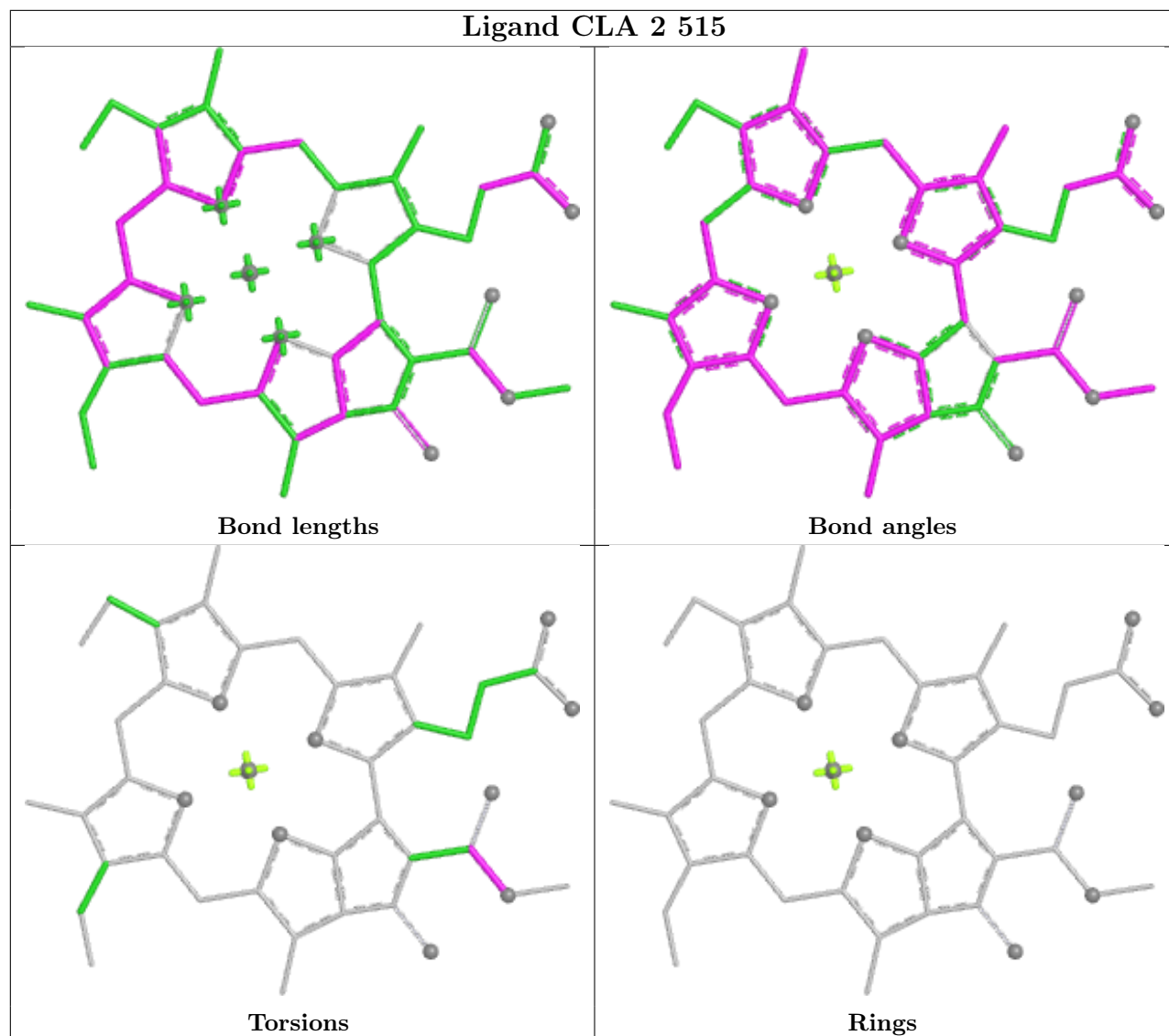




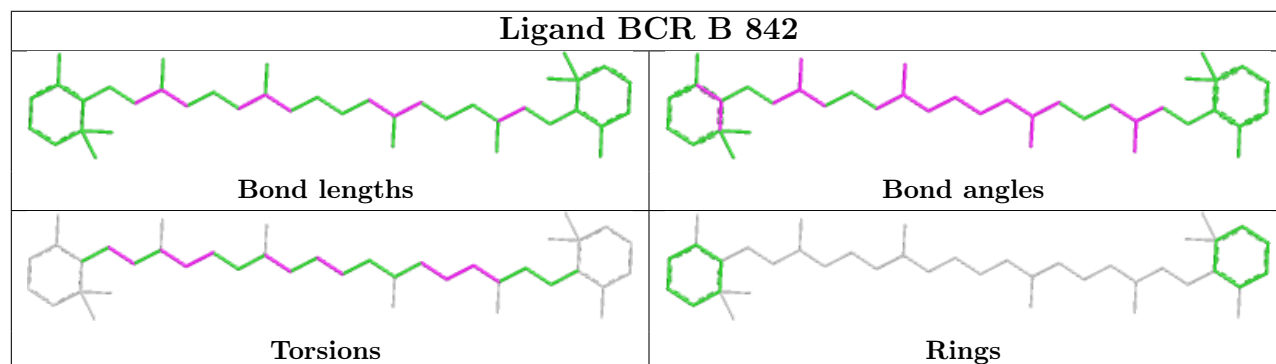
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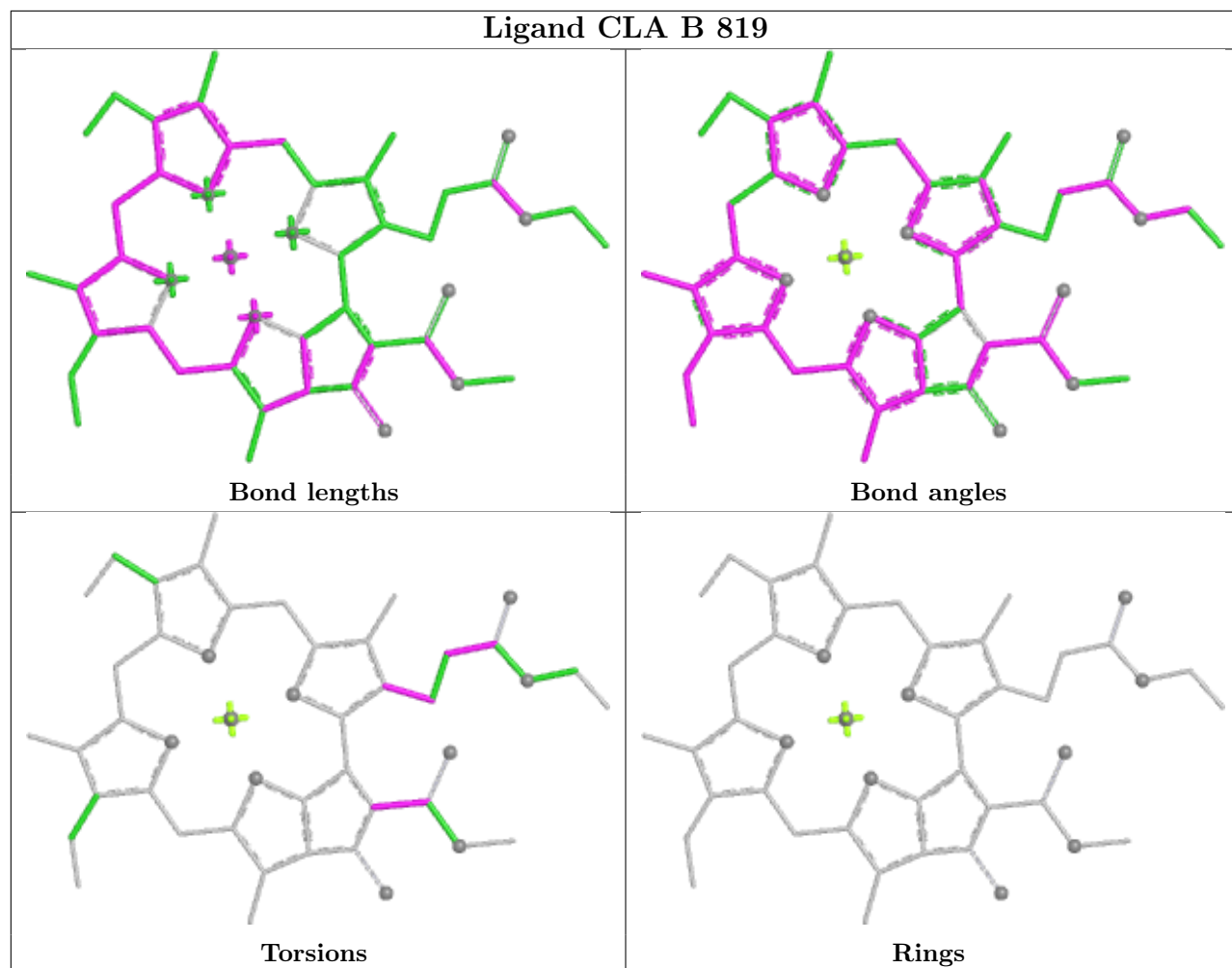
Ligand CLA 2 515



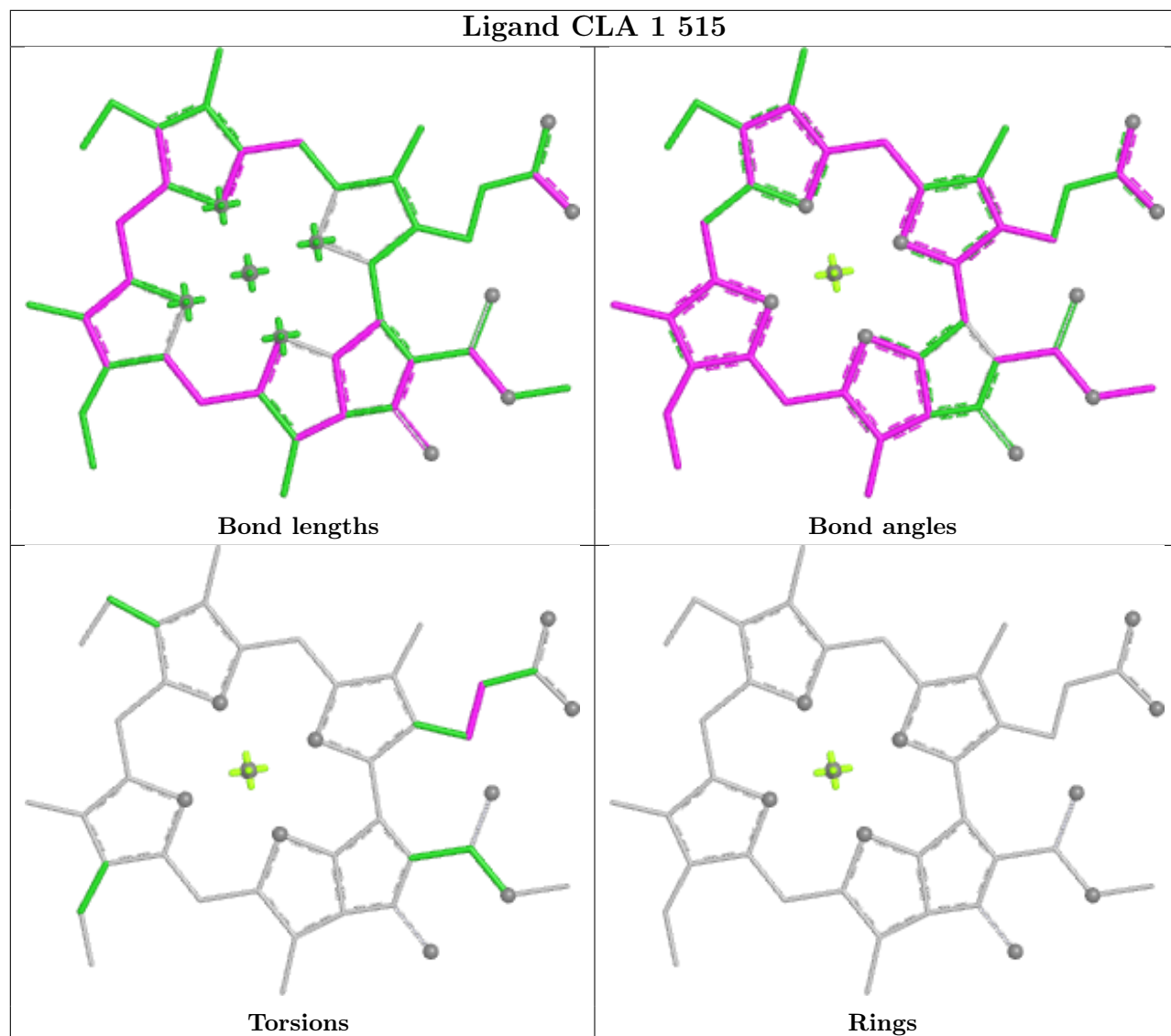
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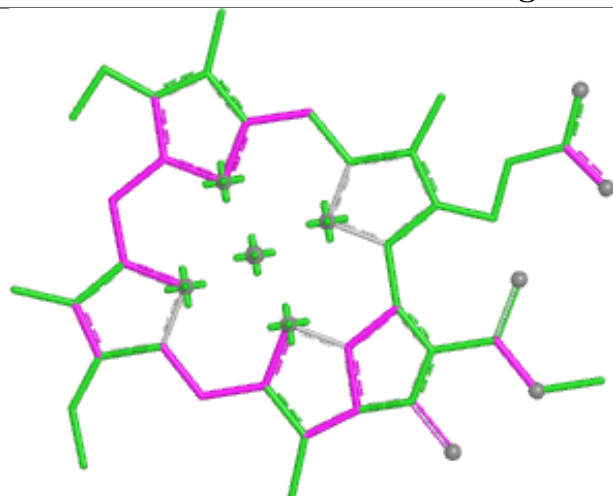
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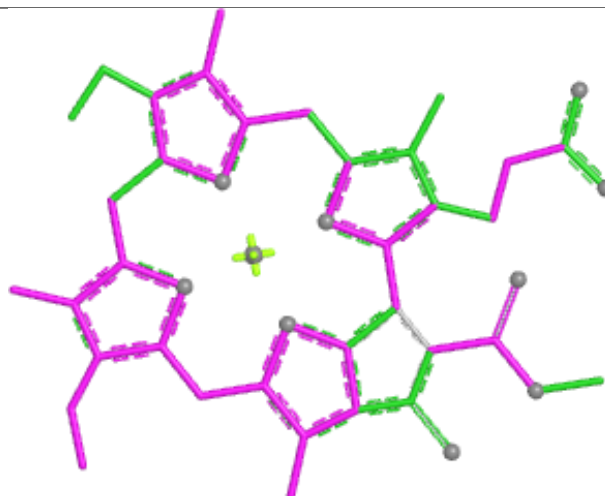
Ligand CLA 1 515



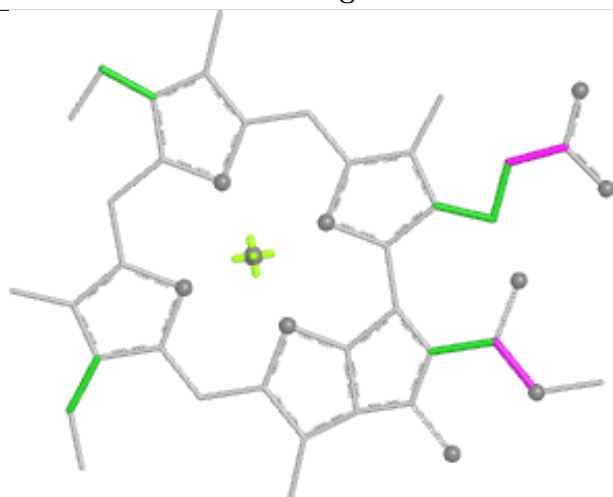
Ligand CLA 3 711



Bond lengths



Bond angles

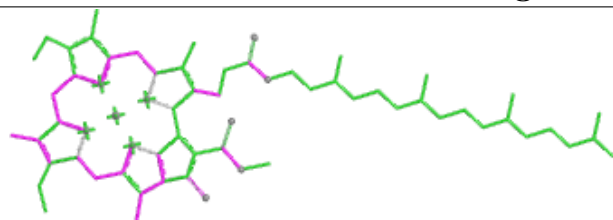


Torsions

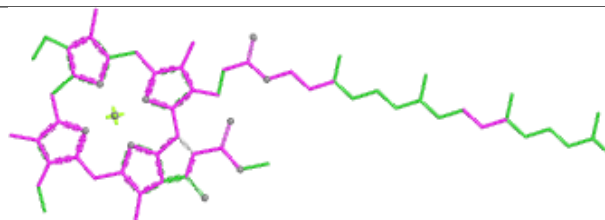


Rings

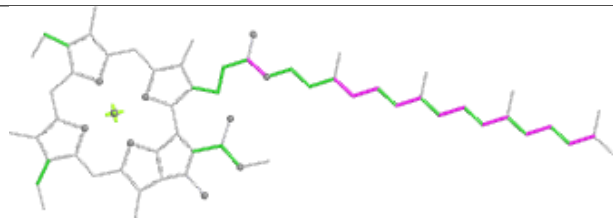
Ligand CLA B 835



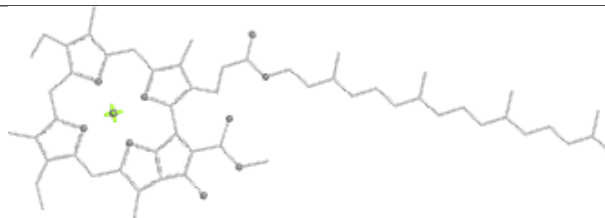
Bond lengths



Bond angles

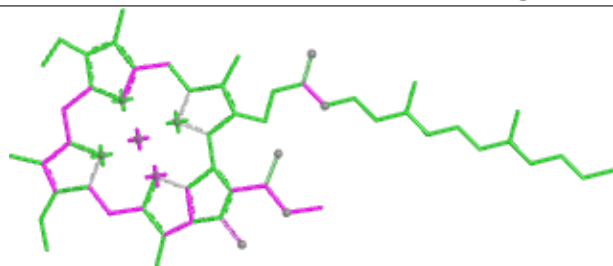


Torsions

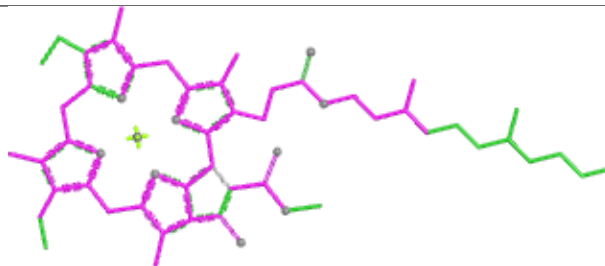


Rings

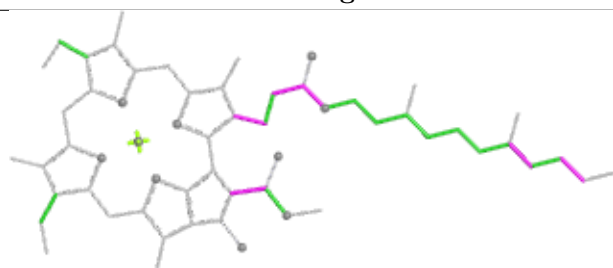
Ligand CLA B 832



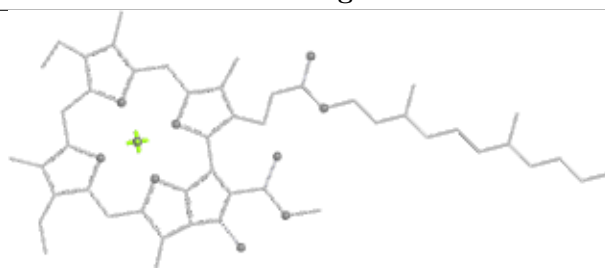
Bond lengths



Bond angles

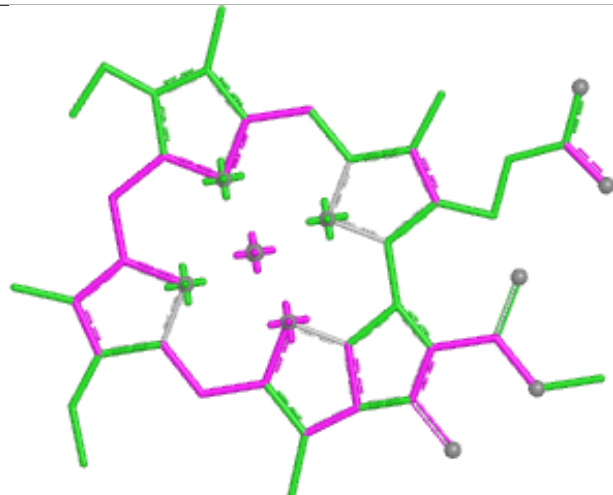


Torsions

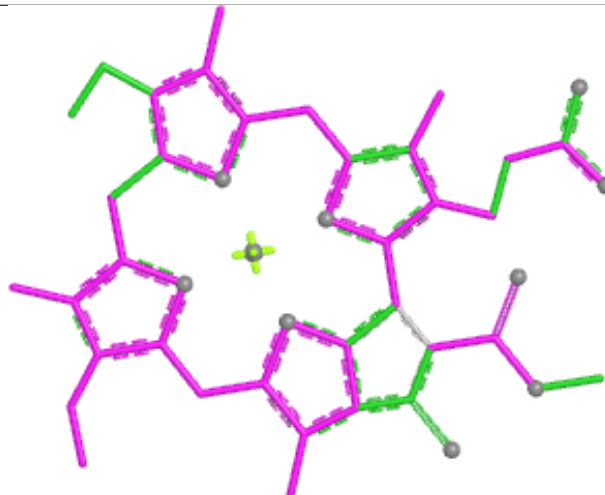


Rings

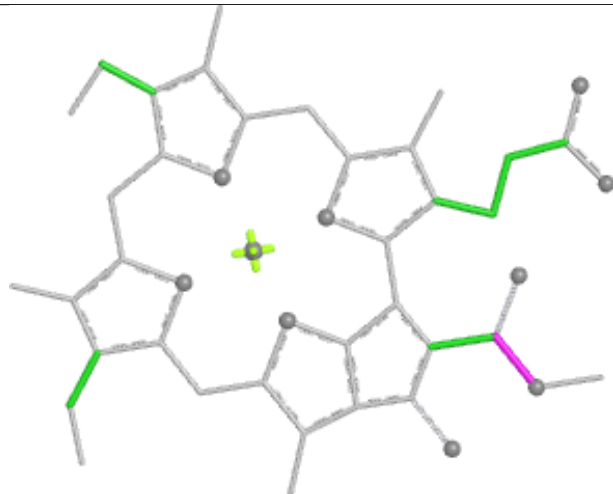
Ligand CLA B 814



Bond lengths



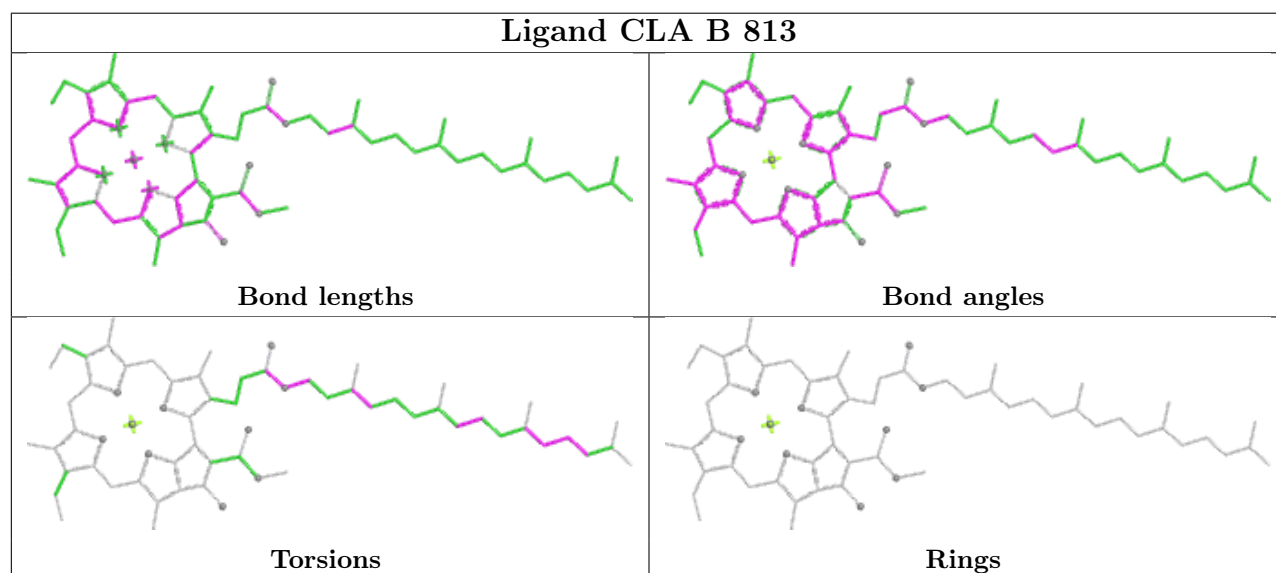
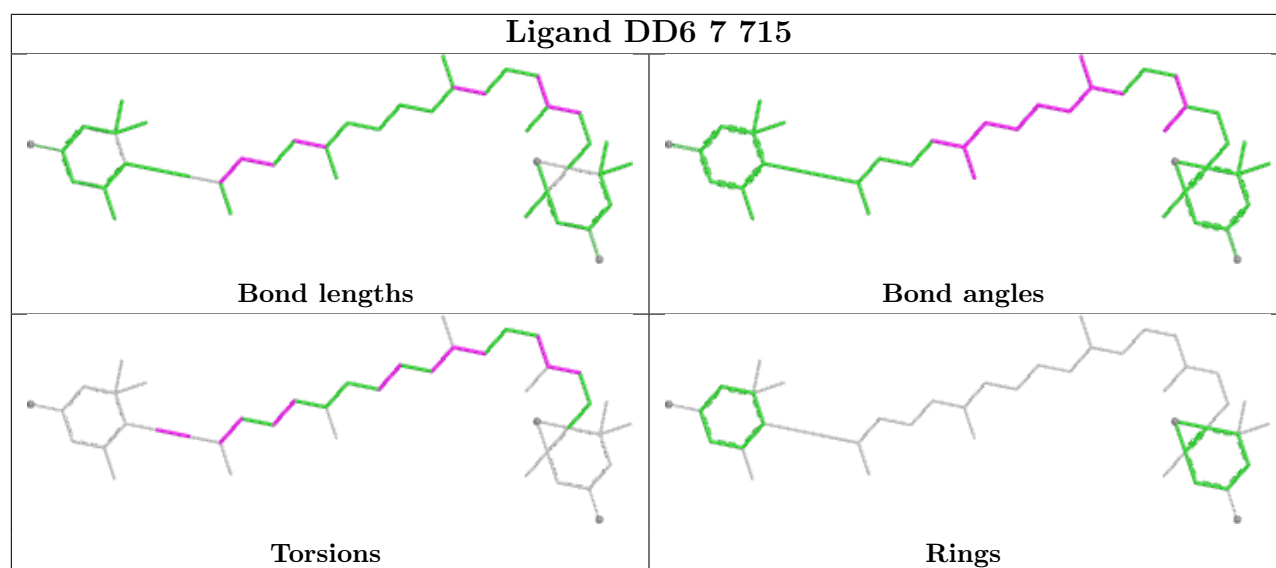
Bond angles

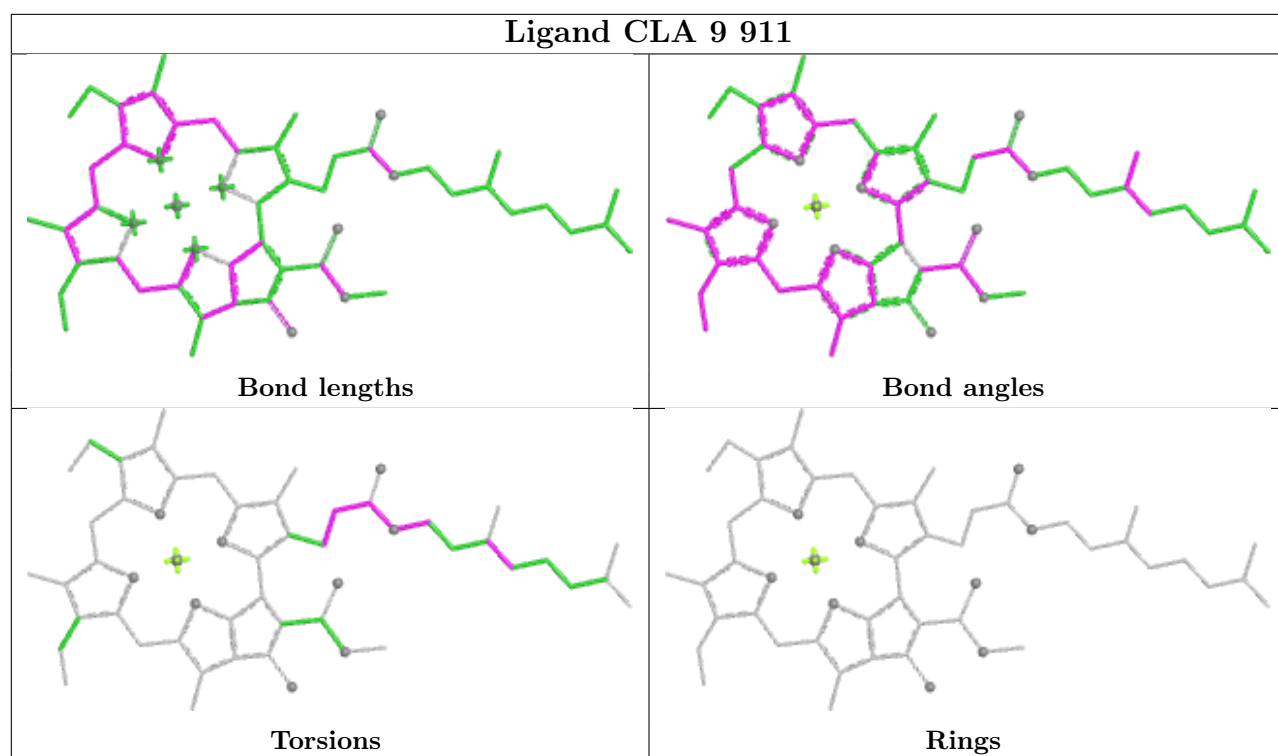


Torsions

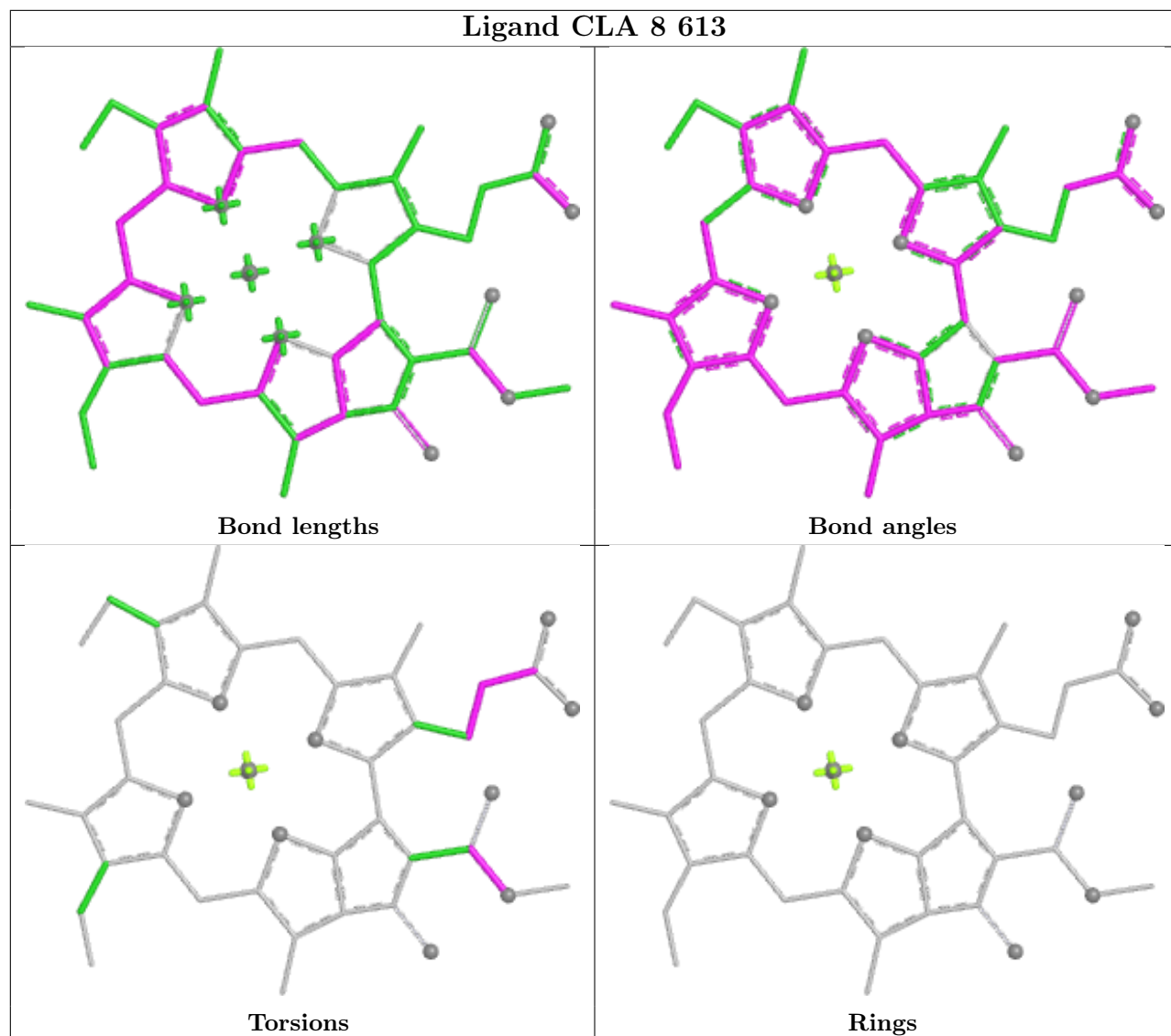


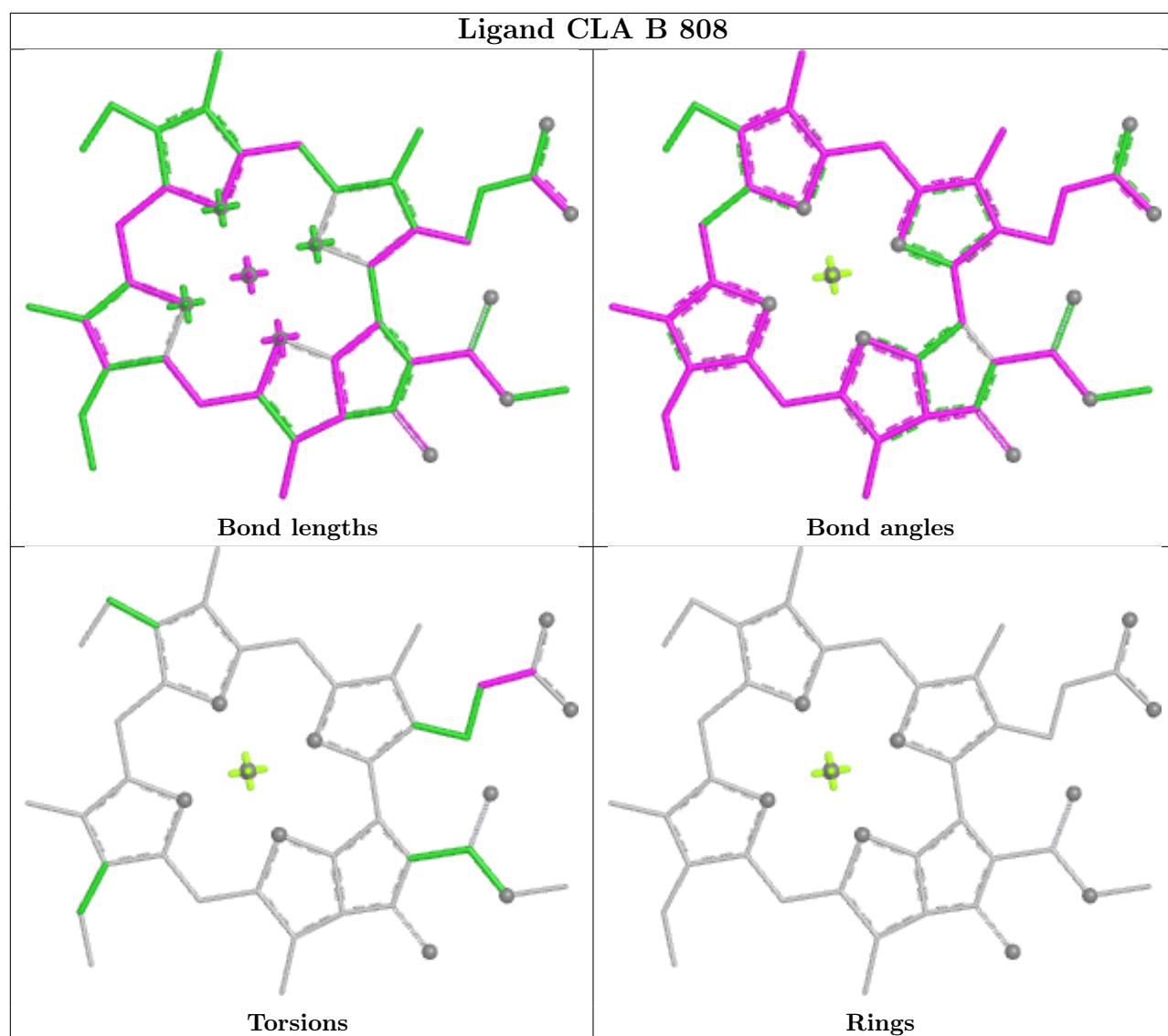
Rings



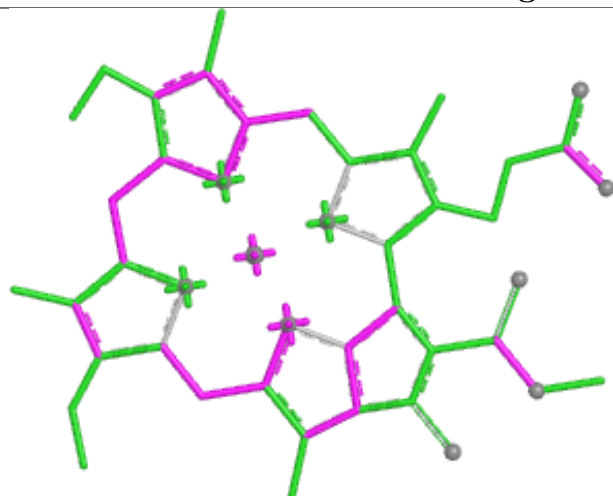


Ligand CLA 8 613

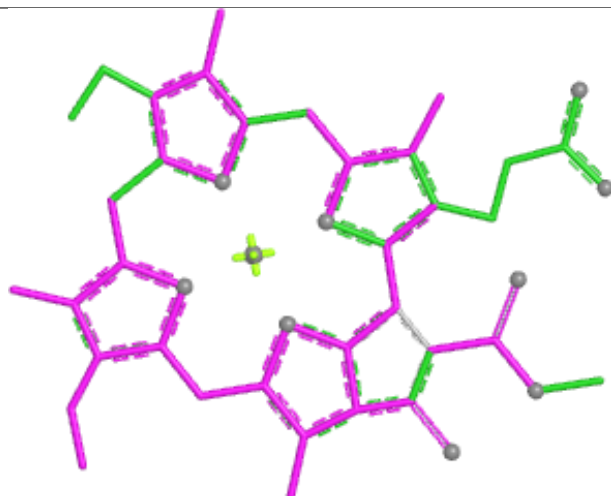




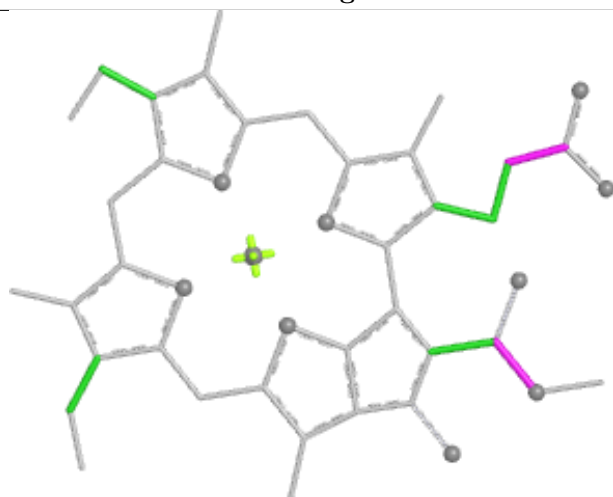
Ligand CLA 5 703



Bond lengths



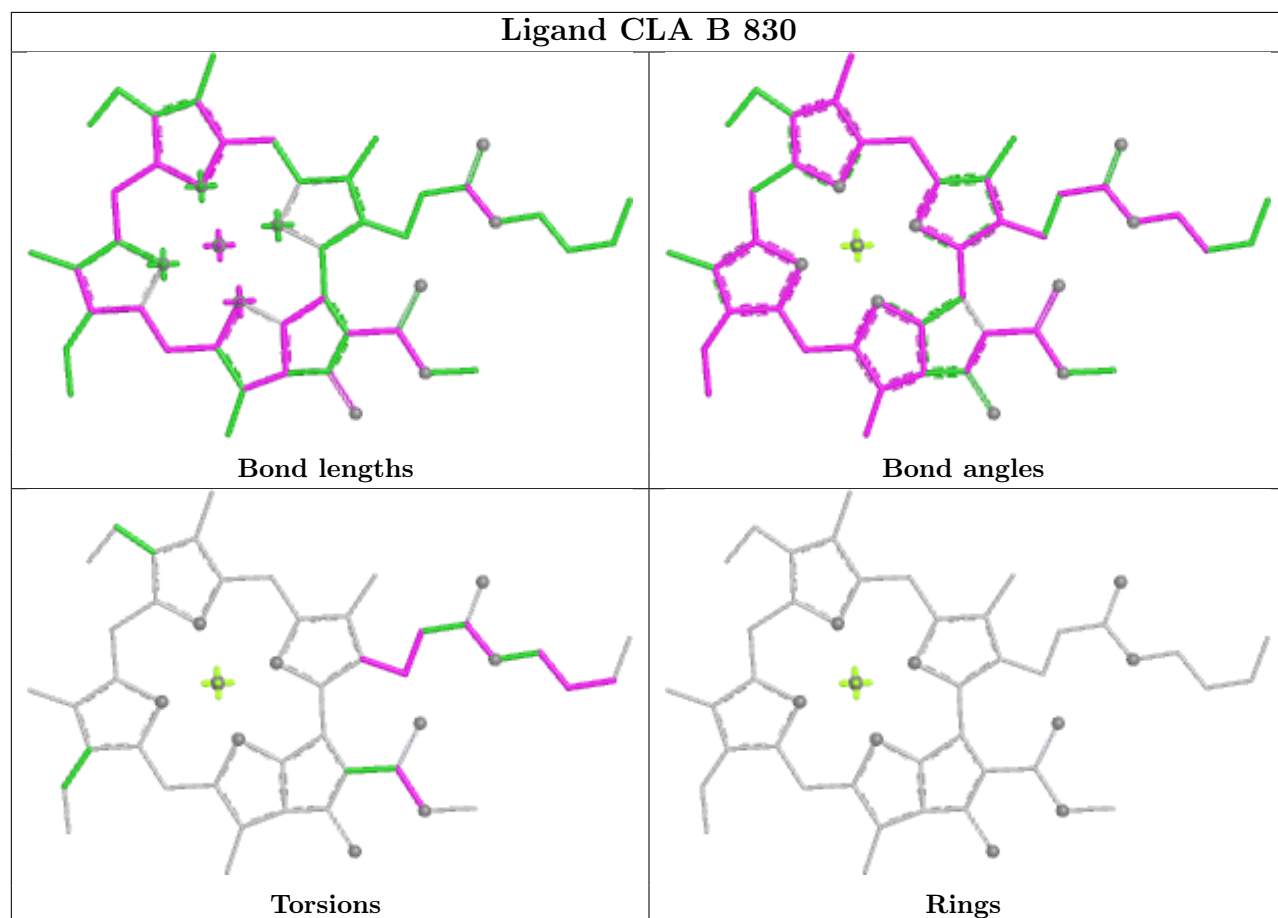
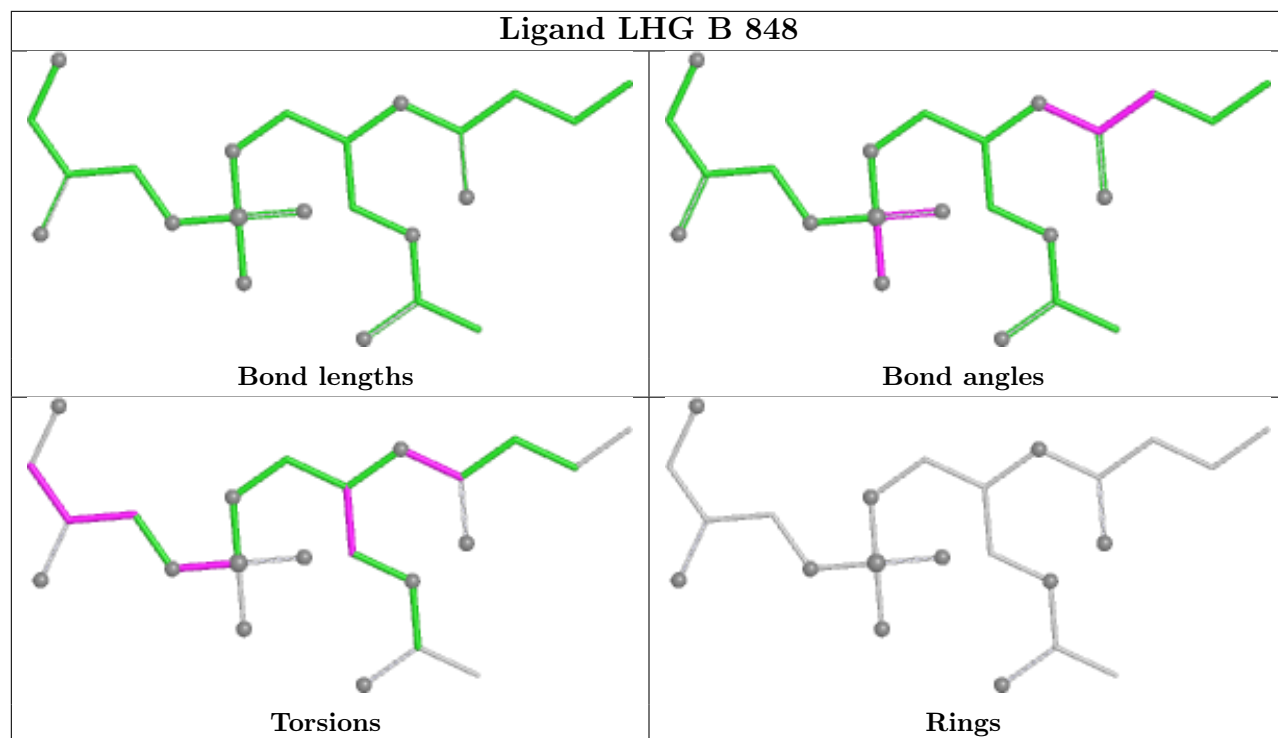
Bond angles

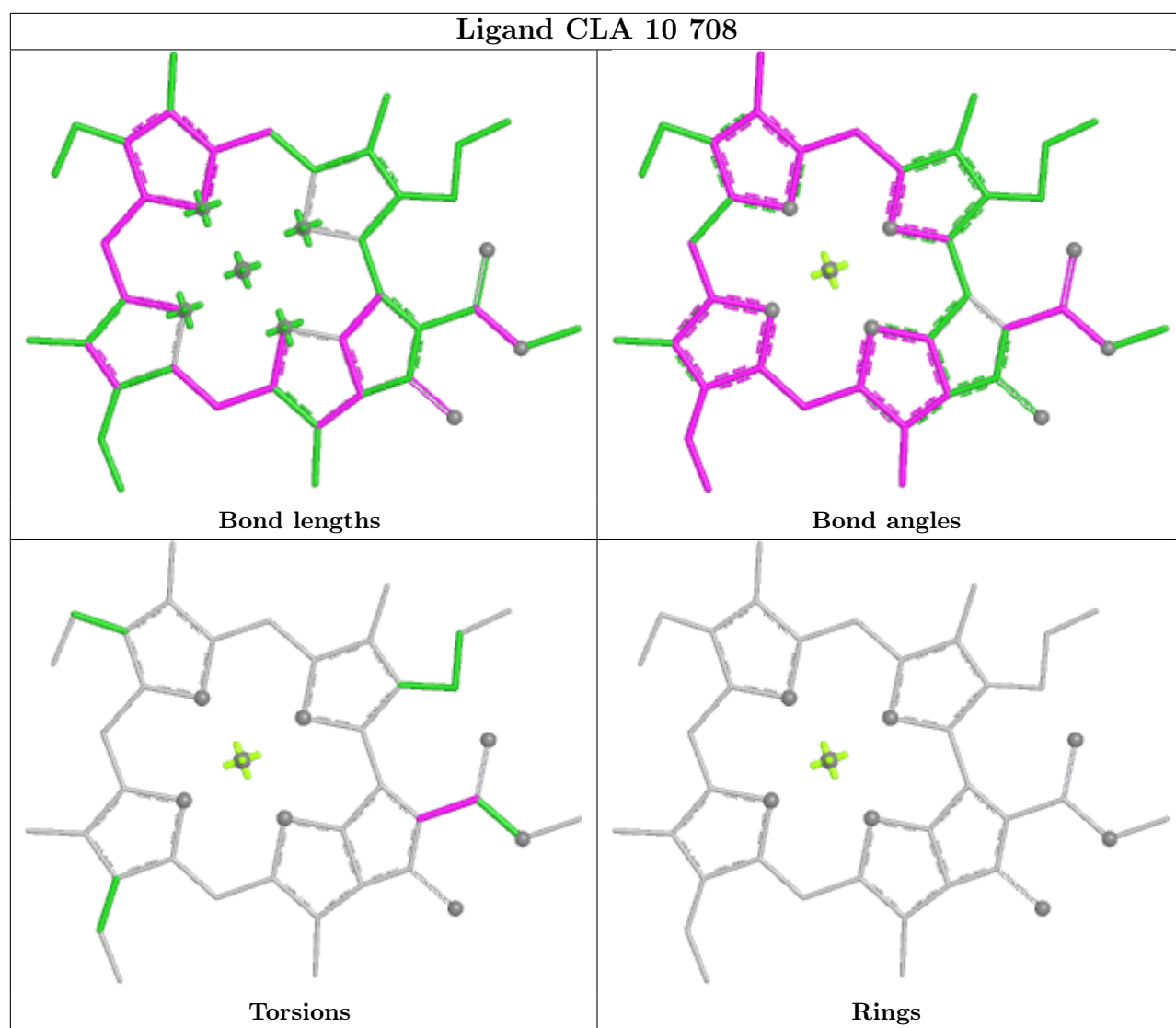


Torsions

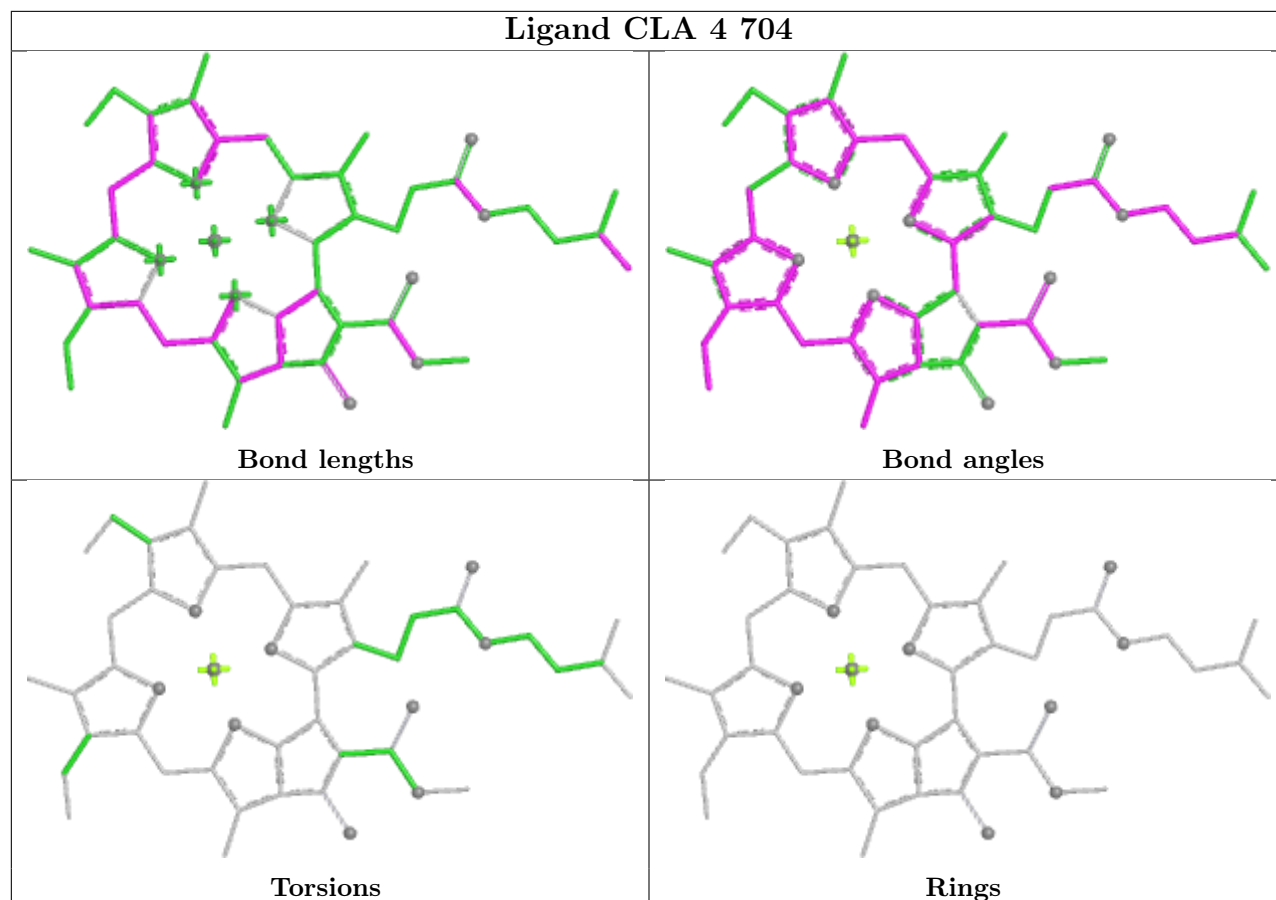


Rings

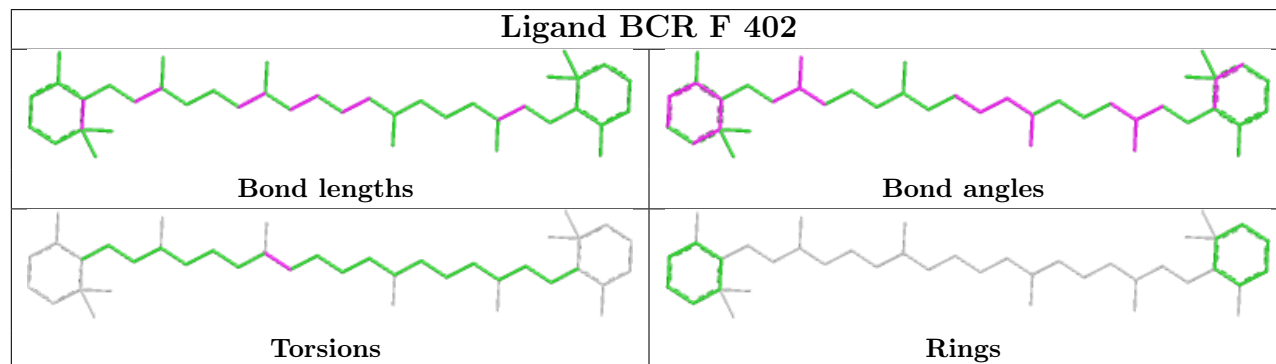


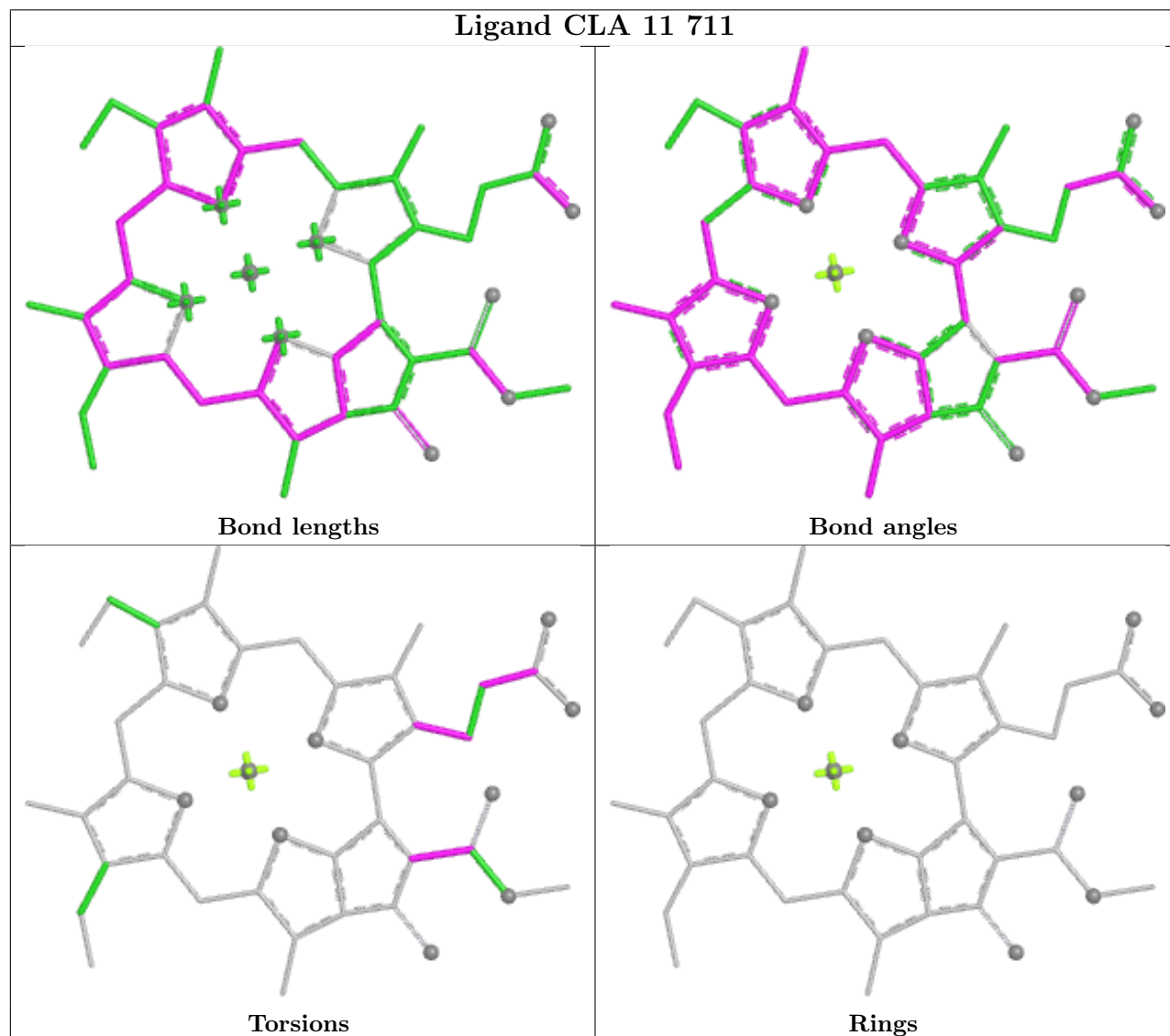
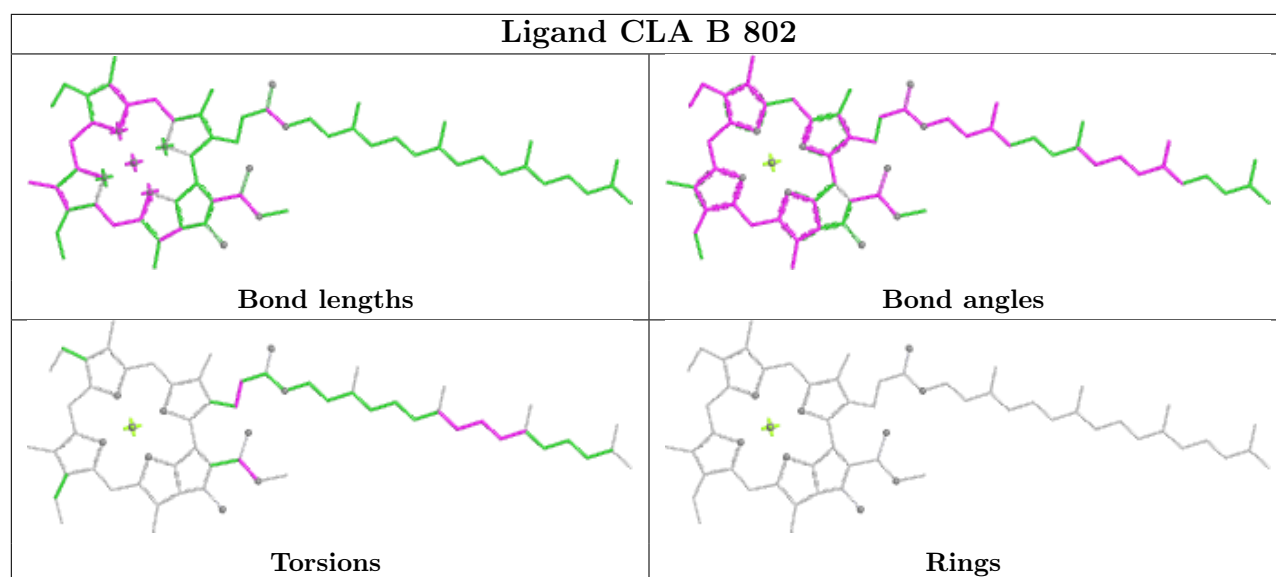


Ligand CLA 4 704

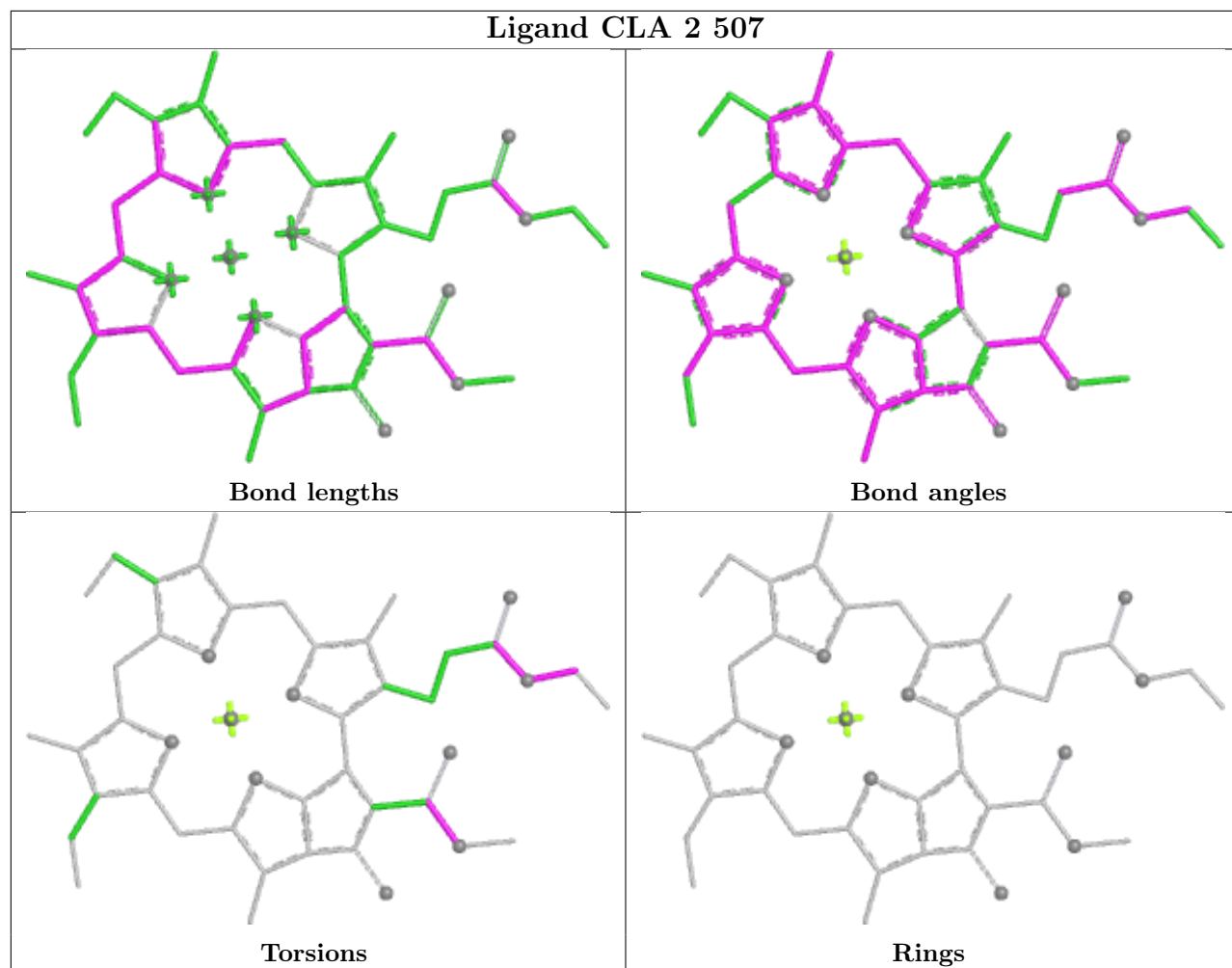


Ligand BCR F 402

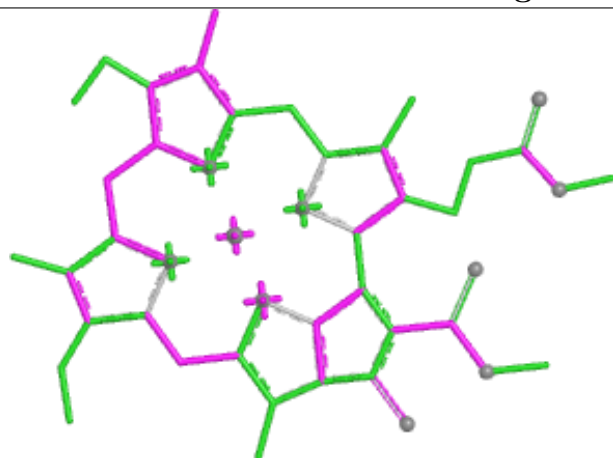




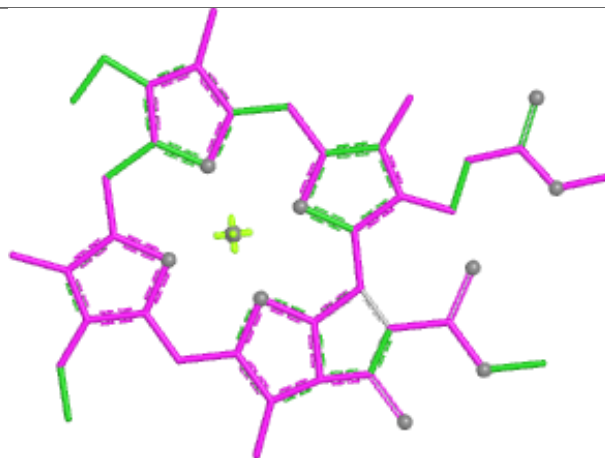
Ligand CLA 2 507



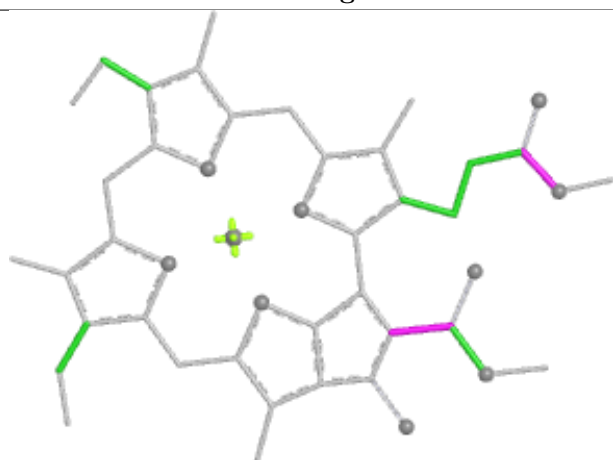
Ligand CLA B 824



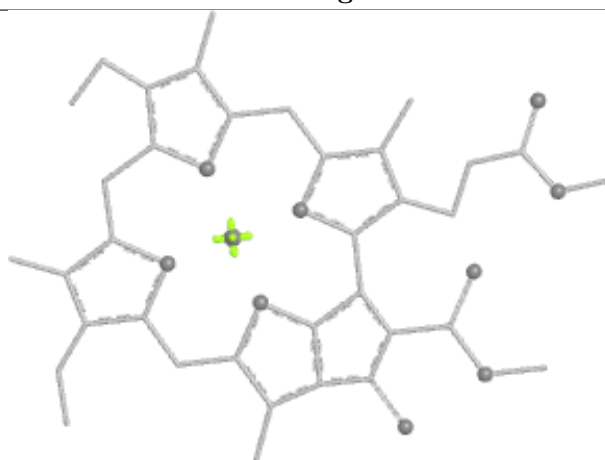
Bond lengths



Bond angles

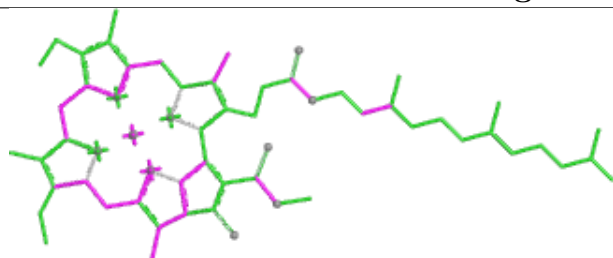


Torsions

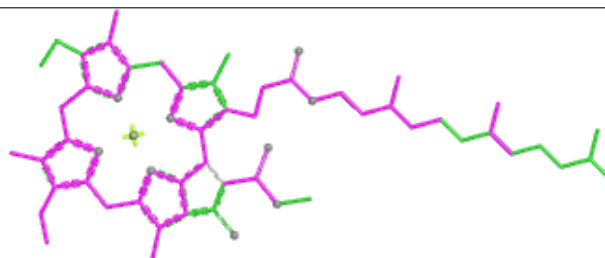


Rings

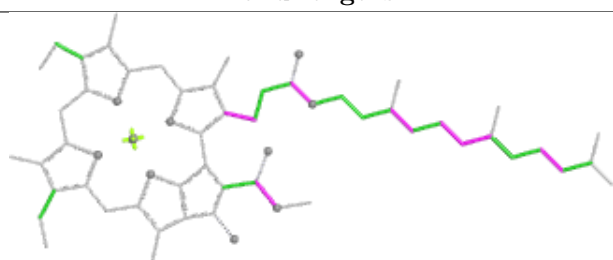
Ligand CLA B 817



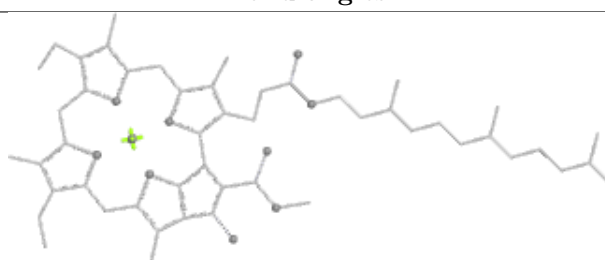
Bond lengths



Bond angles

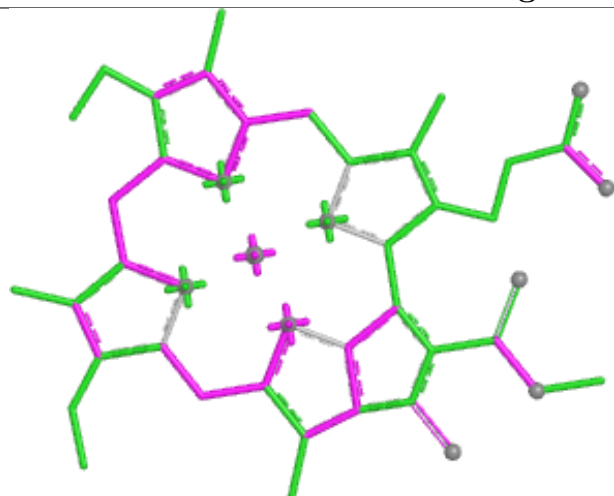


Torsions

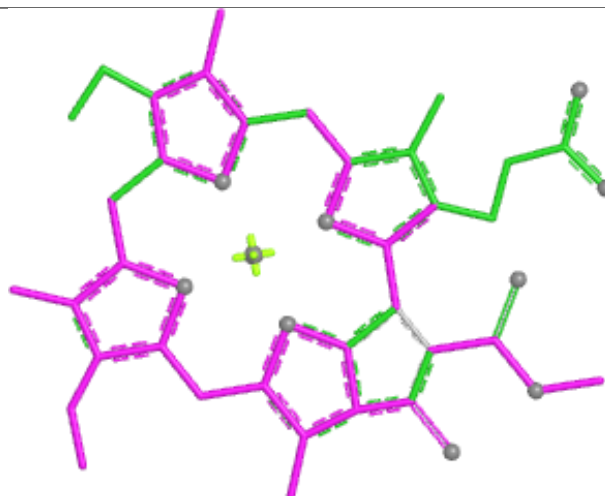


Rings

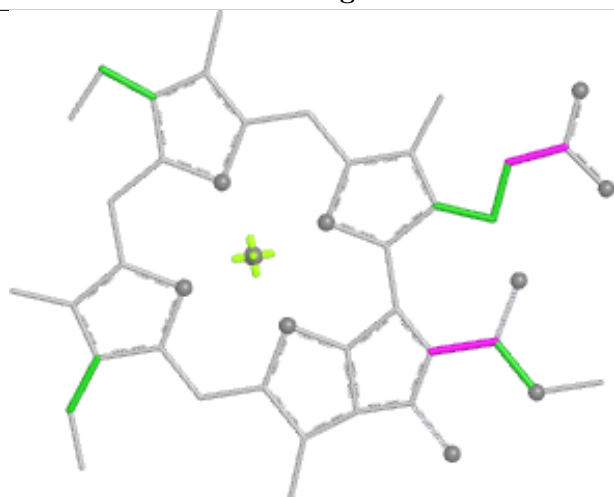
Ligand CLA 6 905



Bond lengths



Bond angles

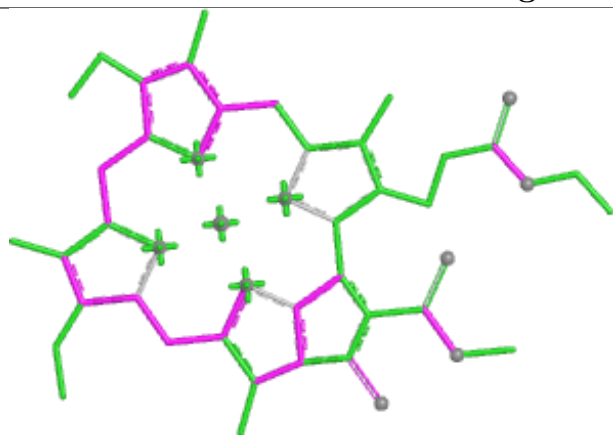


Torsions

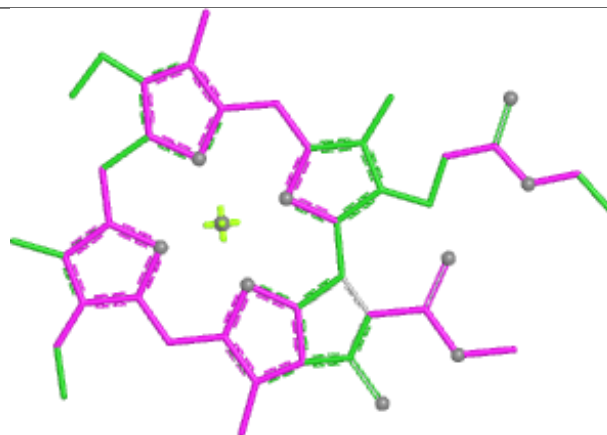


Rings

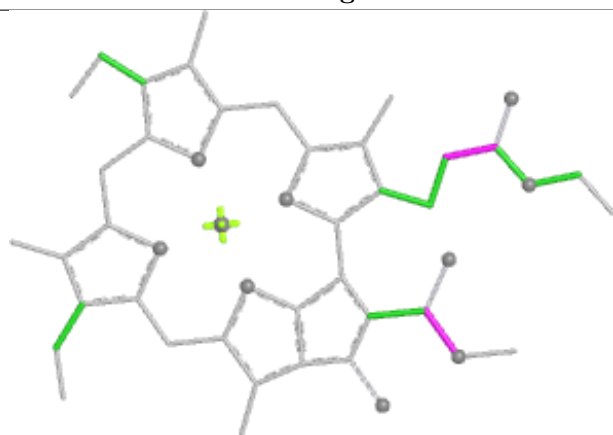
Ligand CLA 9 914



Bond lengths



Bond angles

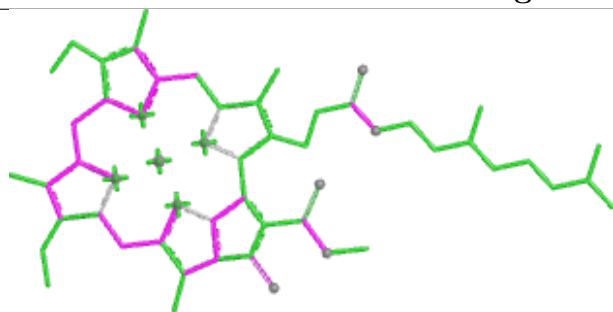


Torsions

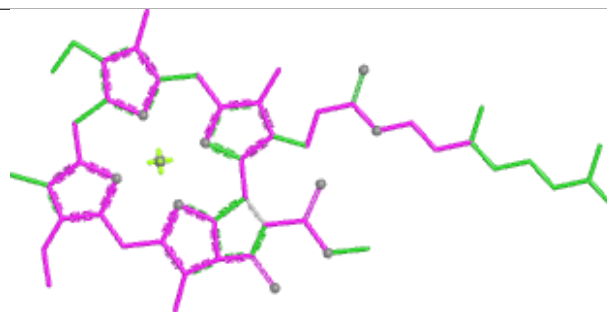


Rings

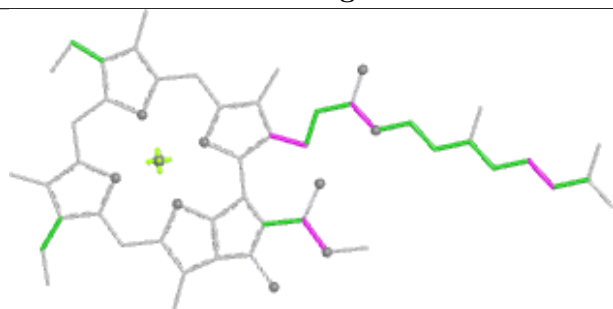
Ligand CLA B 821



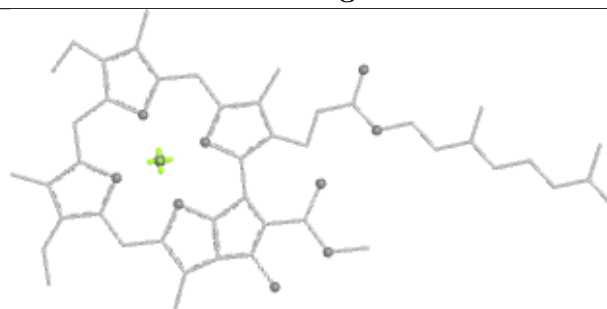
Bond lengths



Bond angles

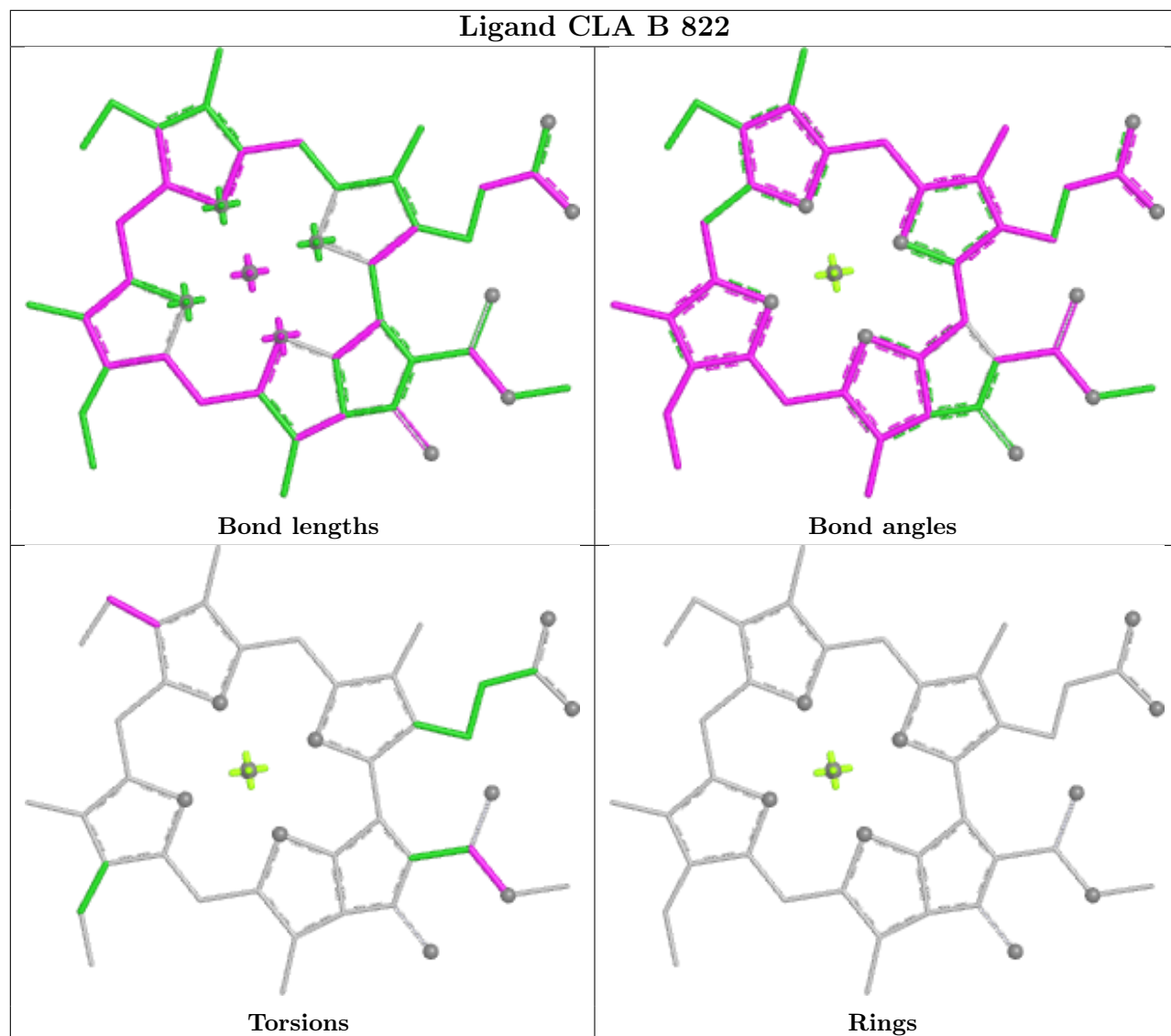


Torsions

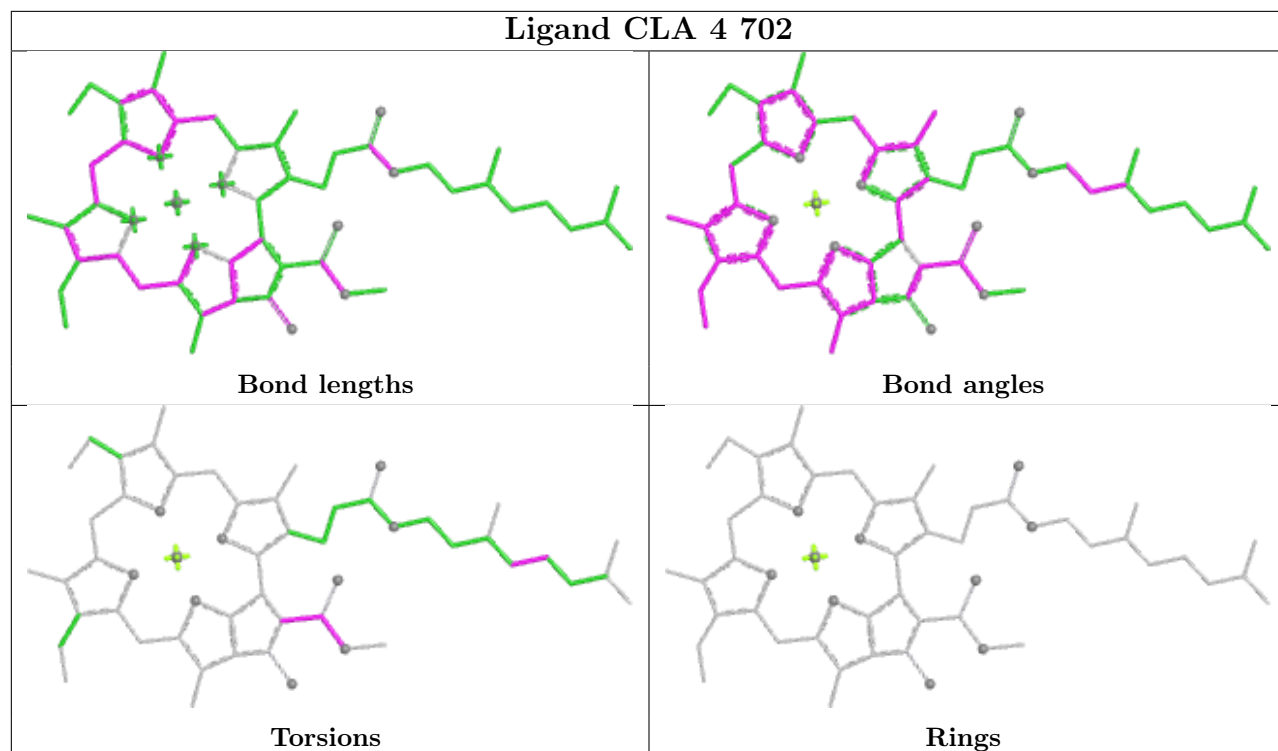


Rings

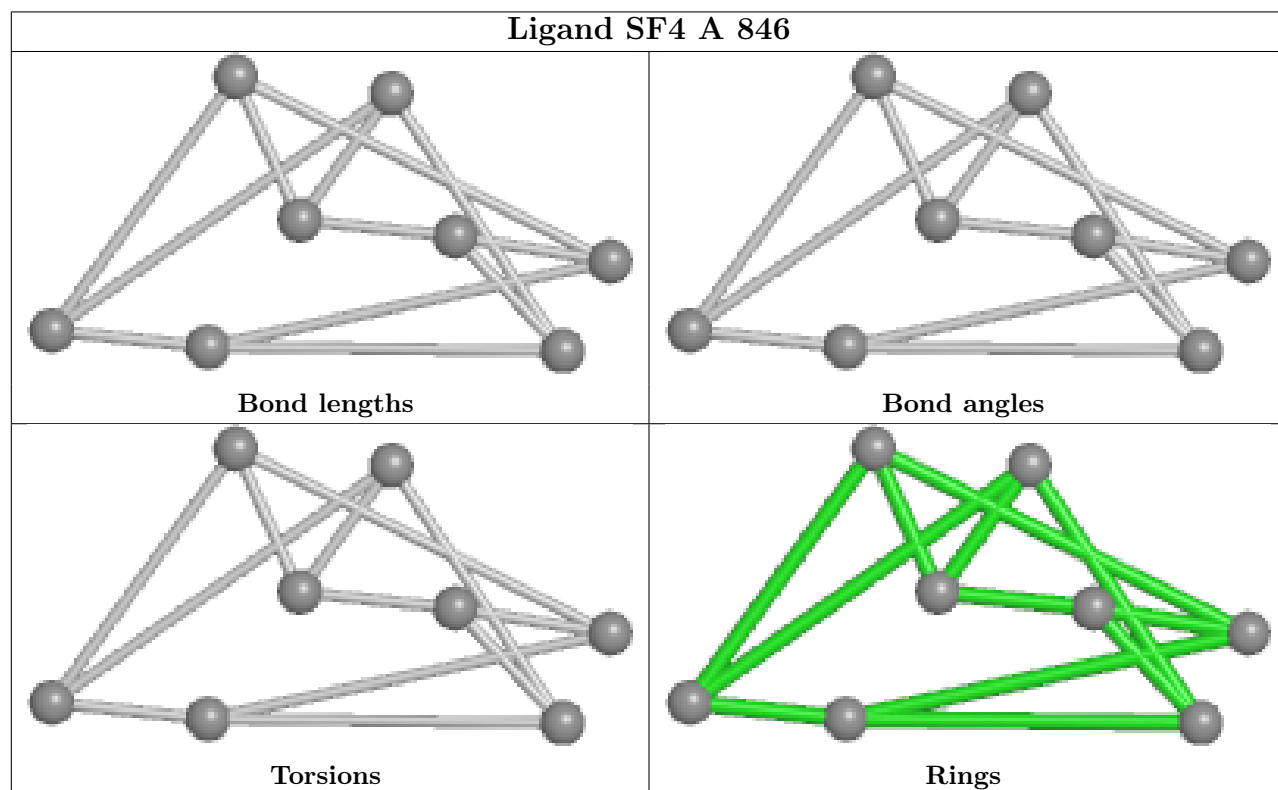
Ligand CLA B 822

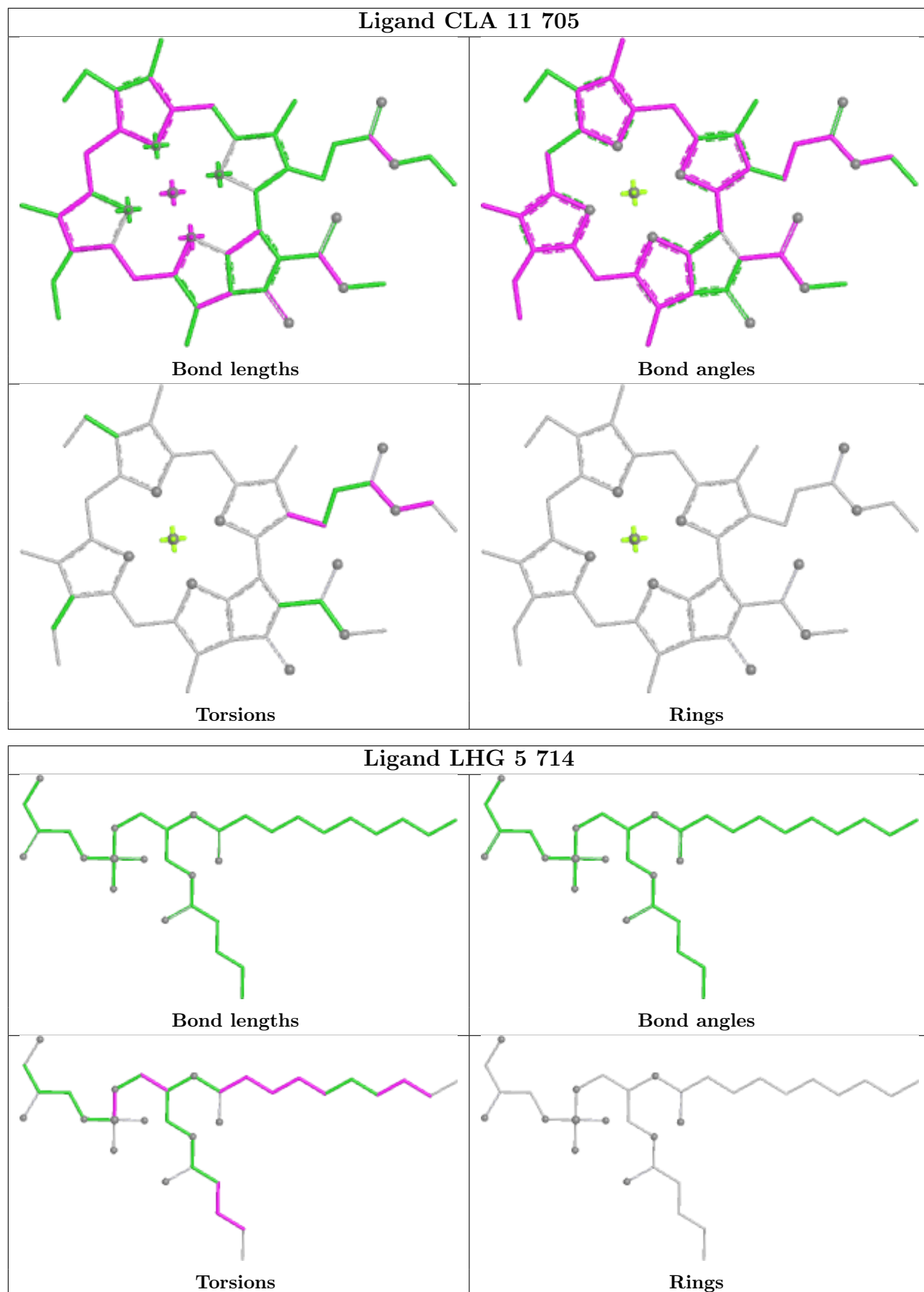


Ligand CLA 4 702

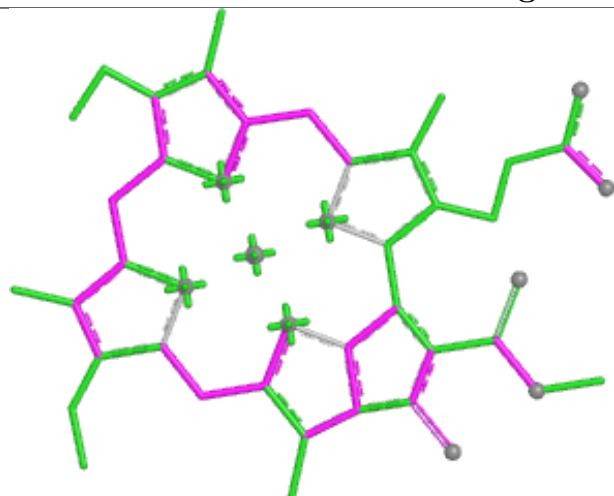


Ligand SF4 A 846

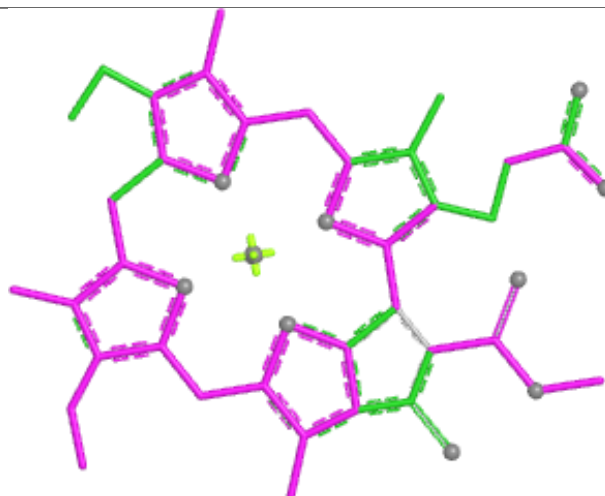




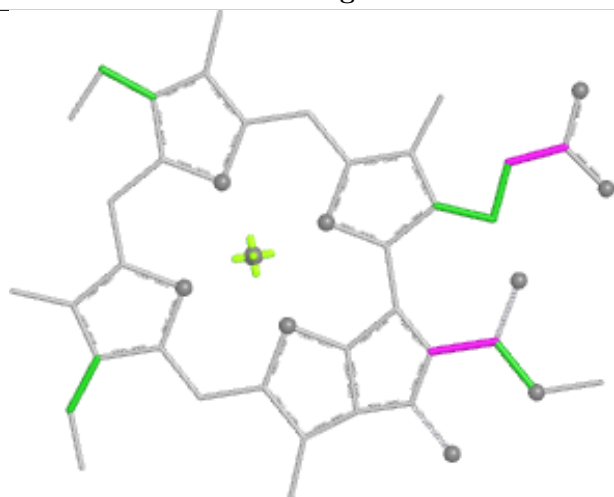
Ligand CLA 2 511



Bond lengths



Bond angles

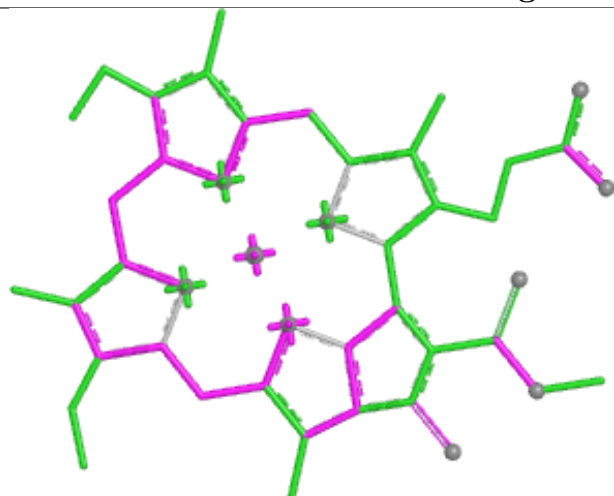


Torsions

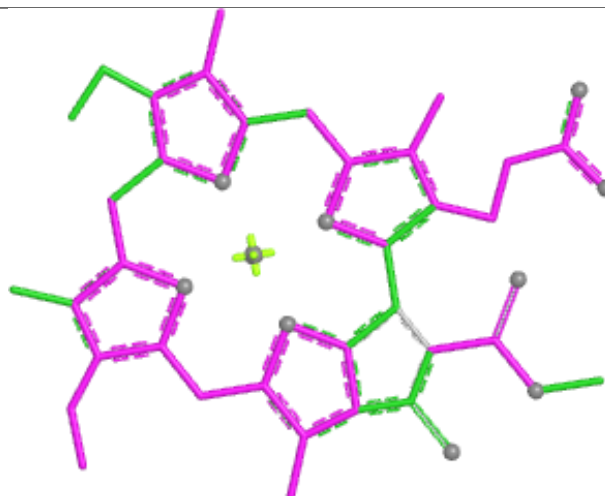


Rings

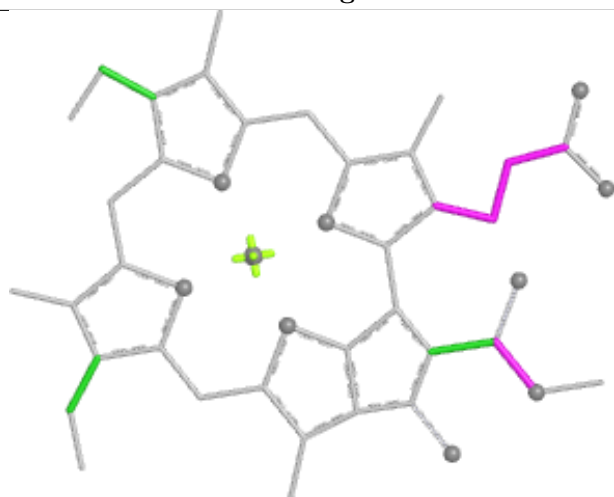
Ligand CLA 5 701



Bond lengths



Bond angles

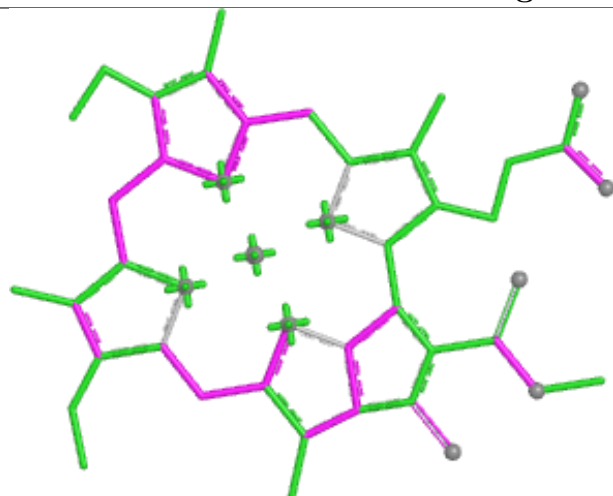


Torsions

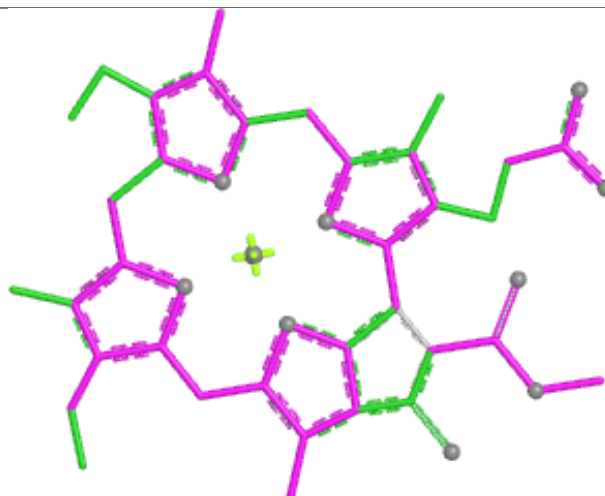


Rings

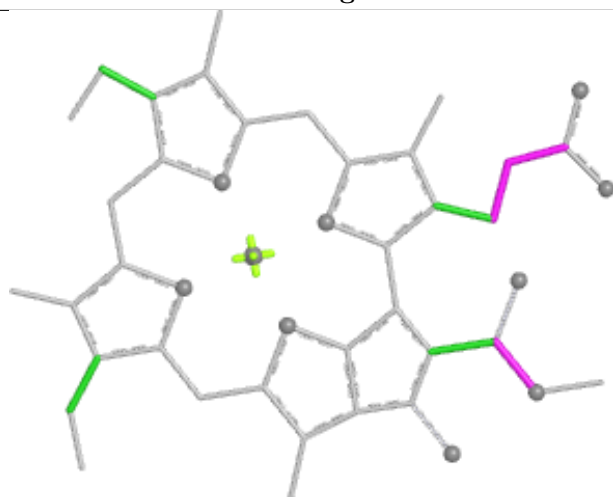
Ligand CLA F 403



Bond lengths



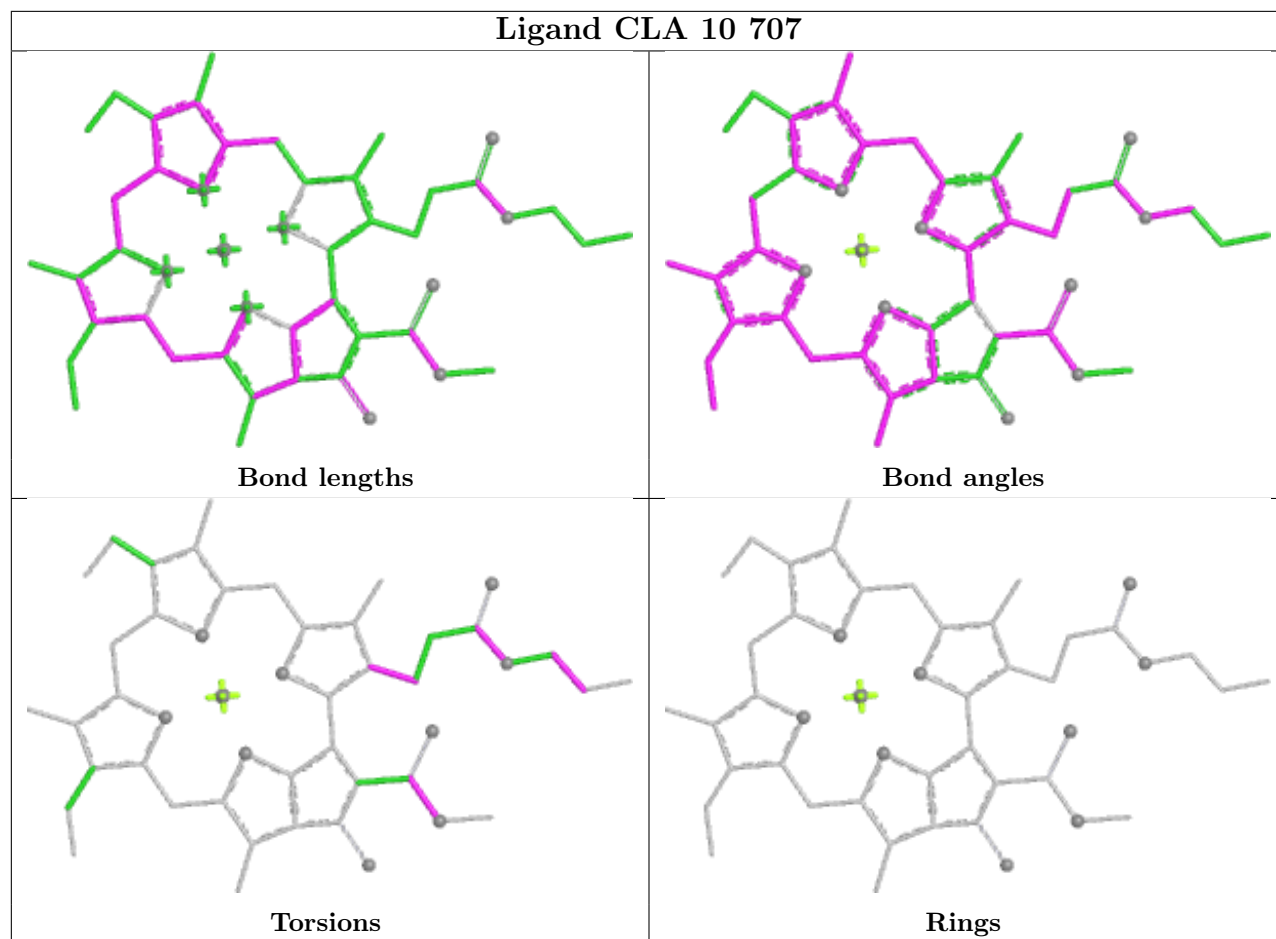
Bond angles



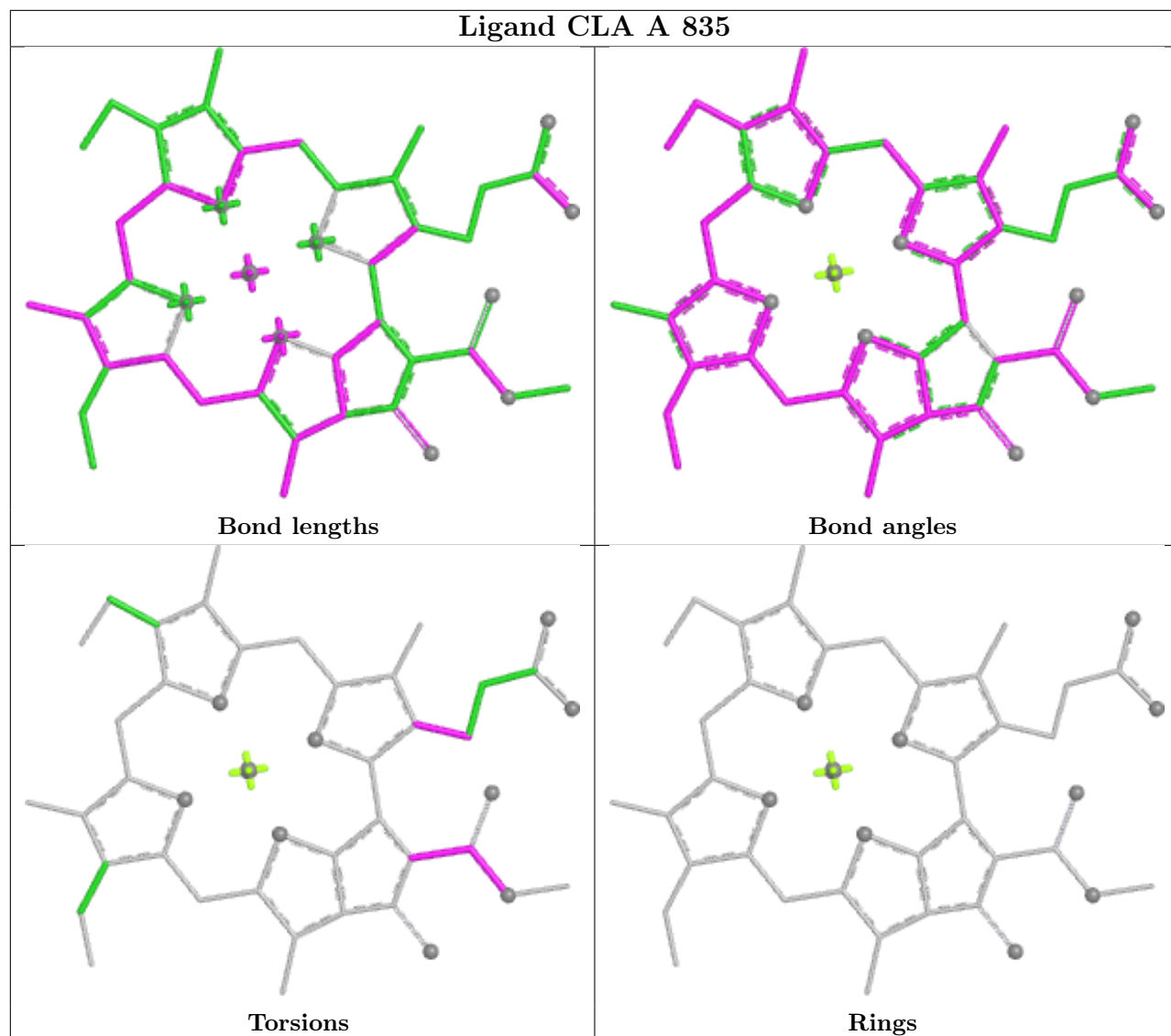
Torsions



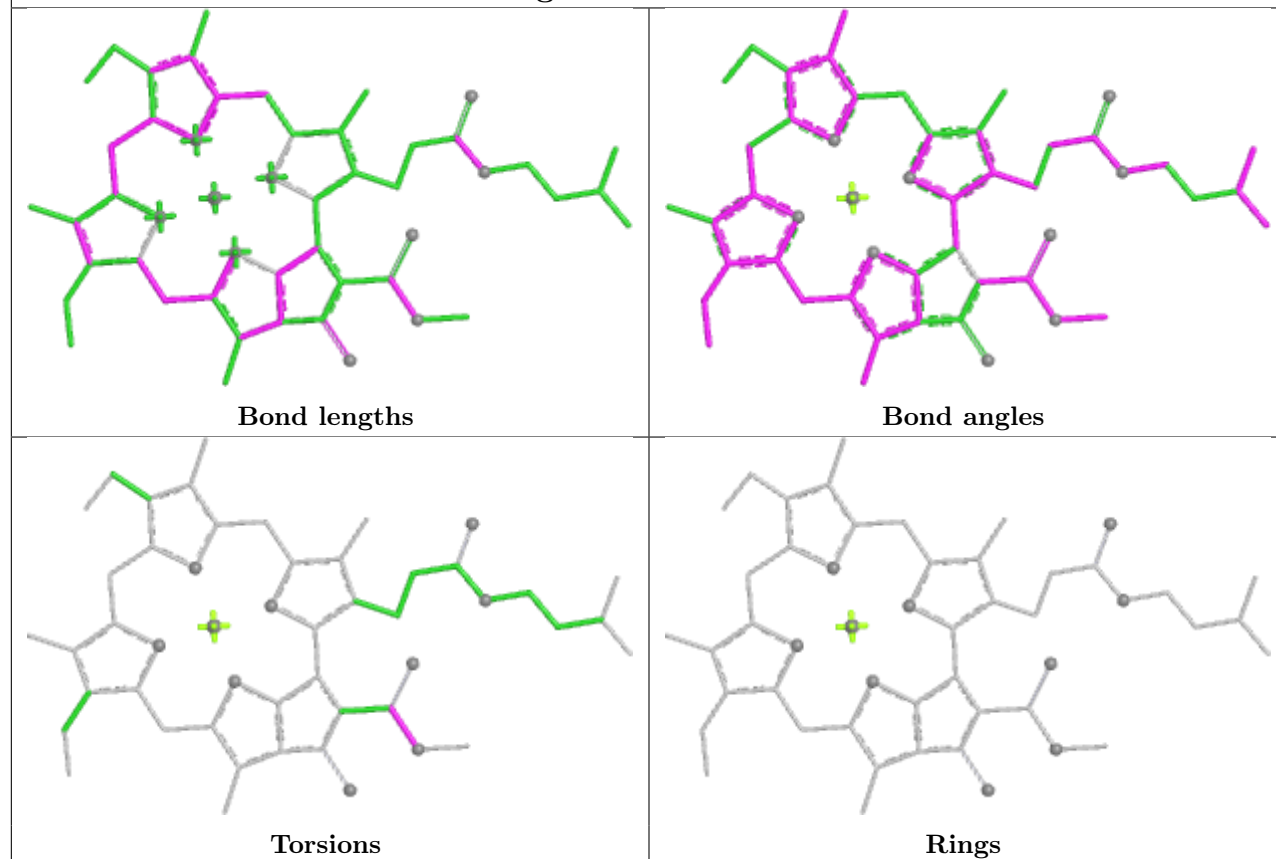
Rings



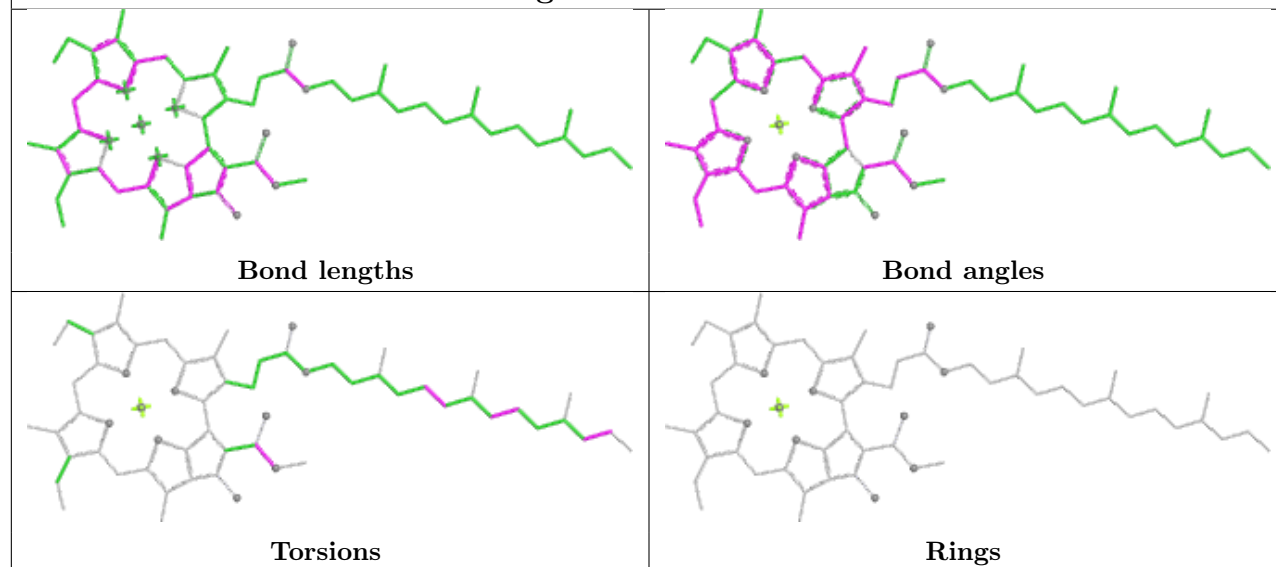
Ligand CLA A 835



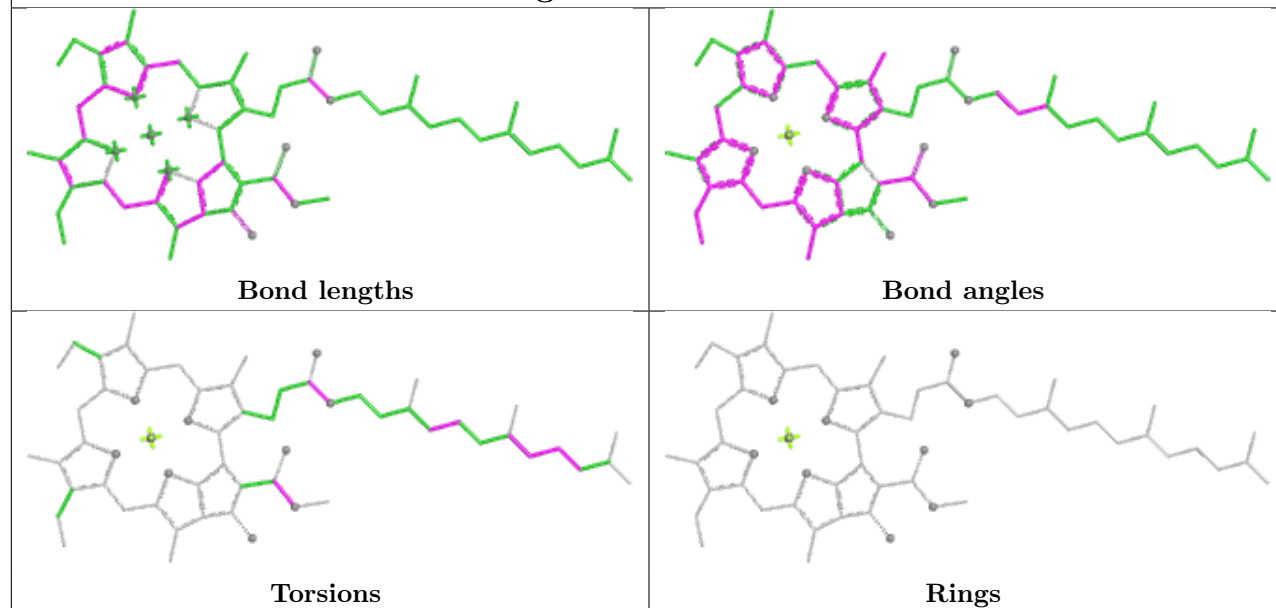
Ligand CLA 1 507



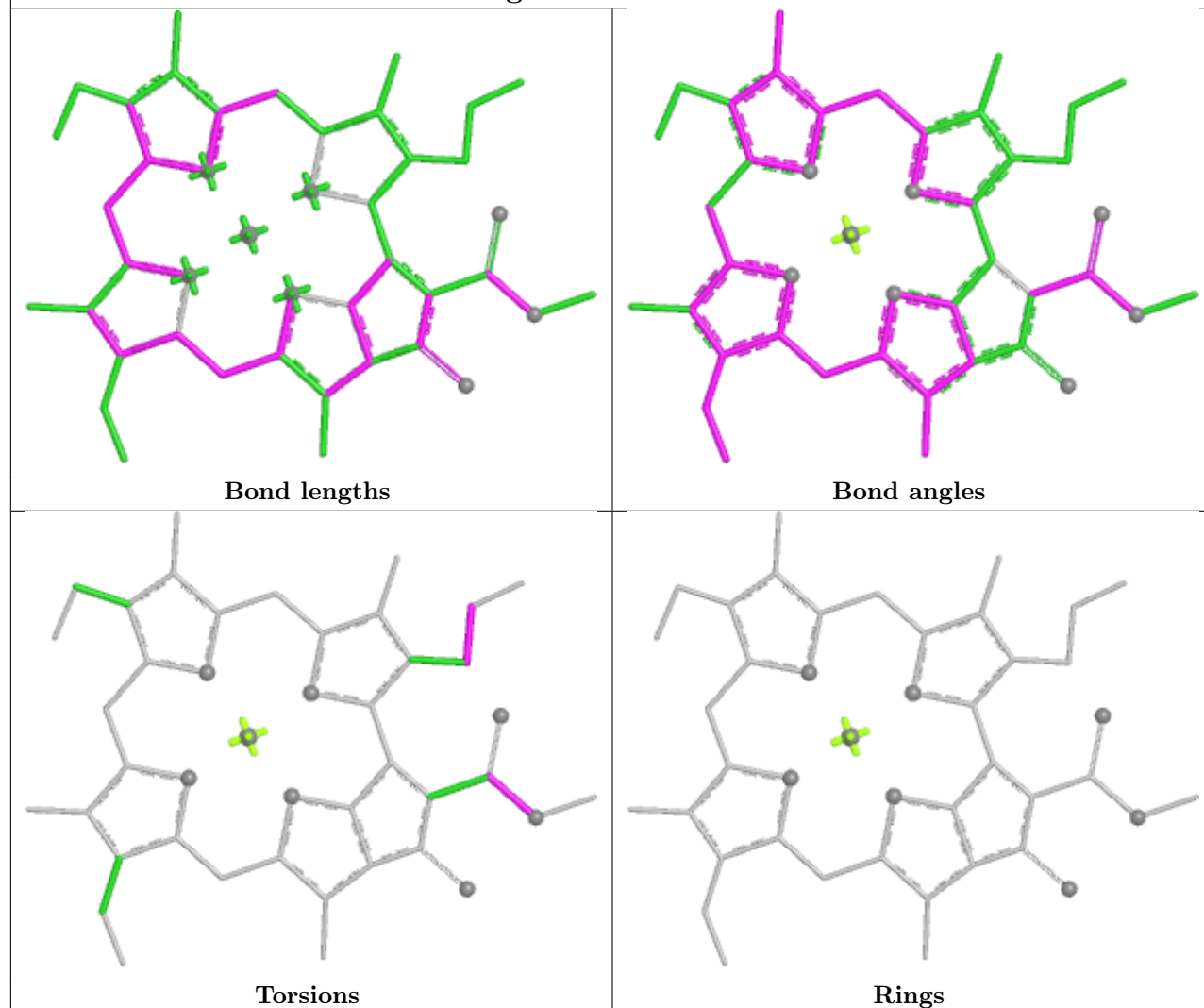
Ligand CLA 2 509



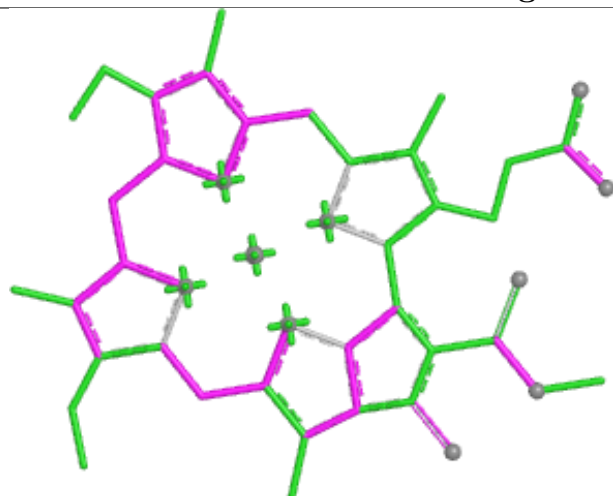
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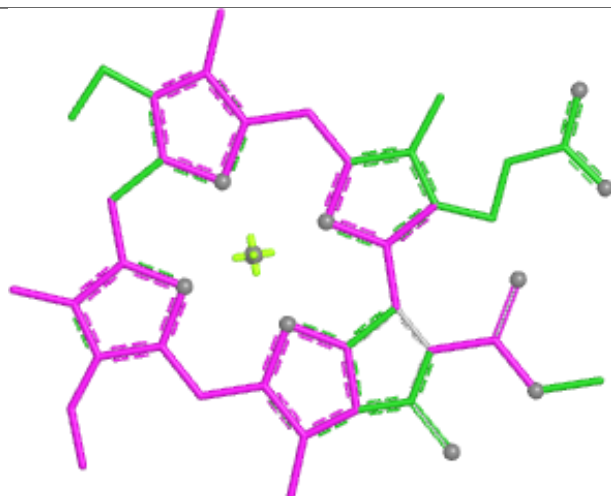
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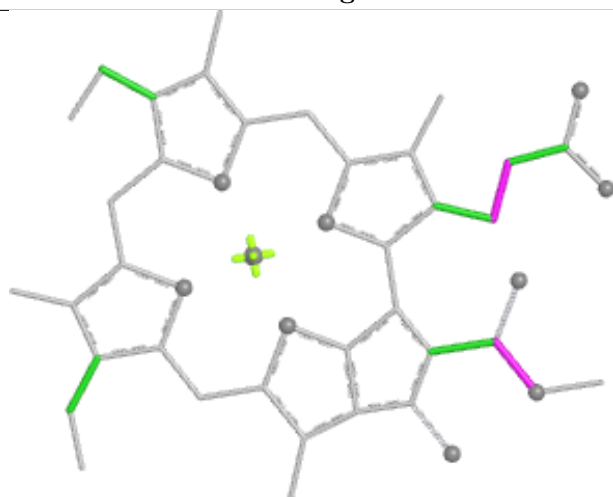
Ligand CLA 9 912



Bond lengths



Bond angles

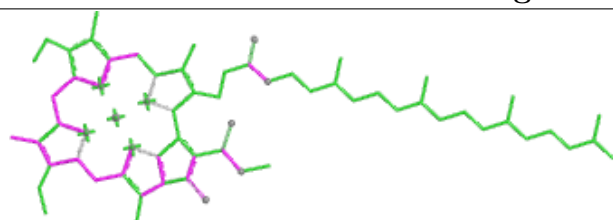


Torsions

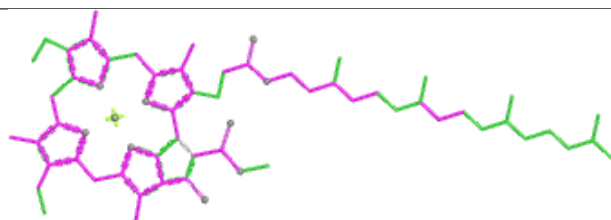


Rings

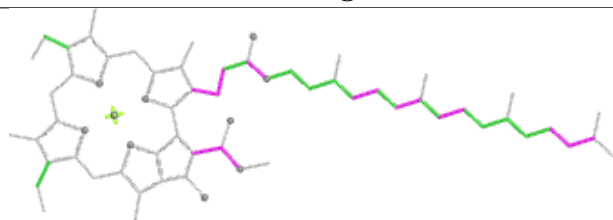
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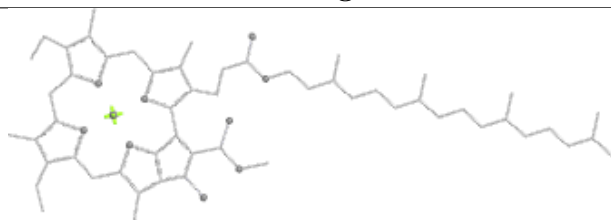
Bond lengths



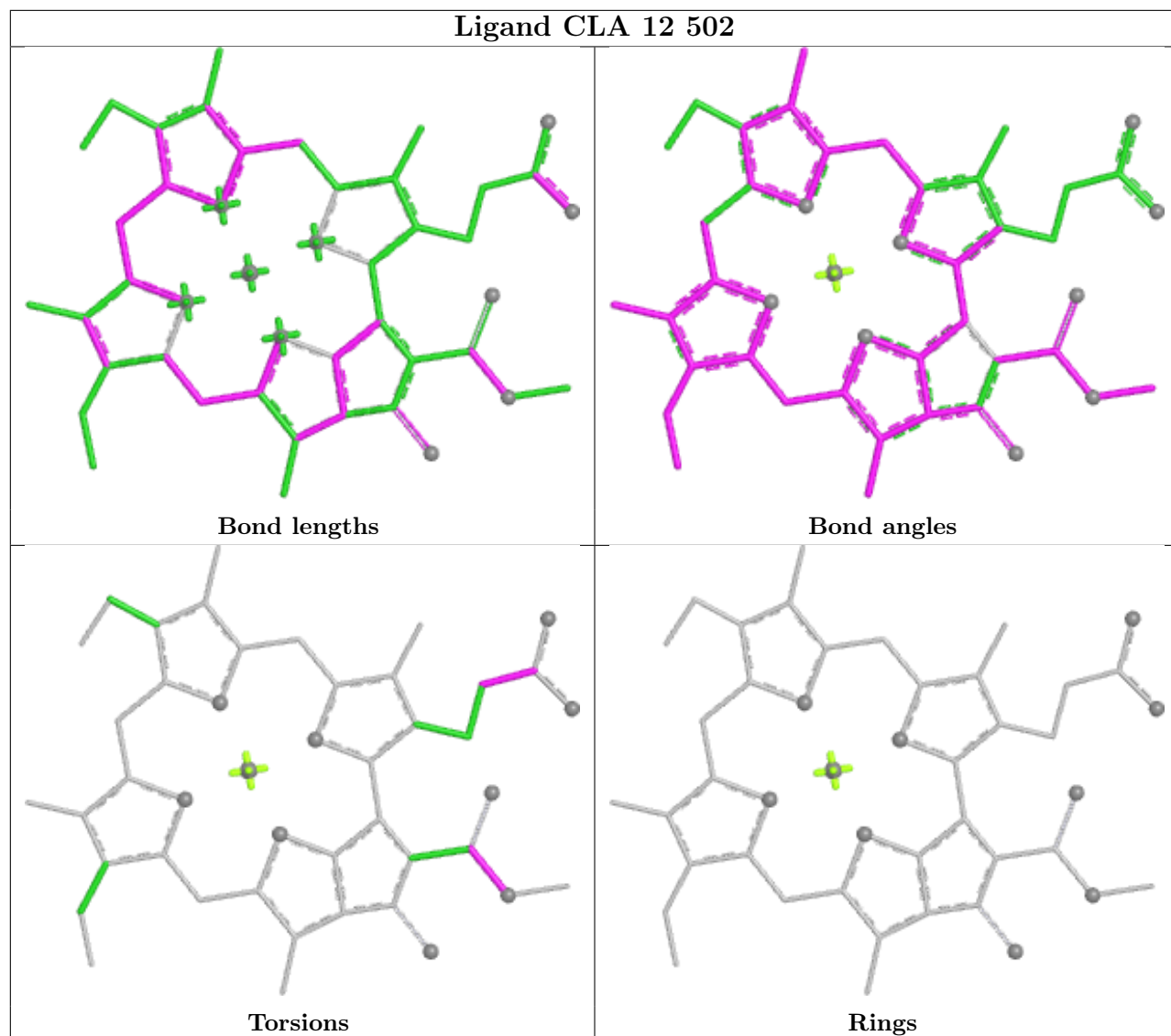
Bond angles

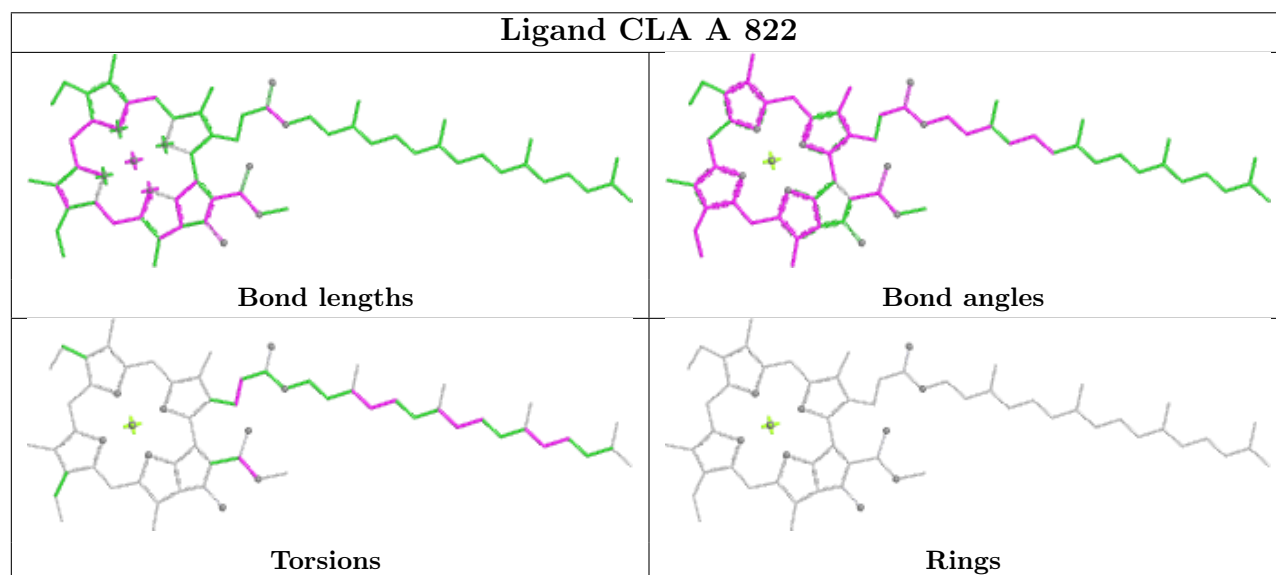
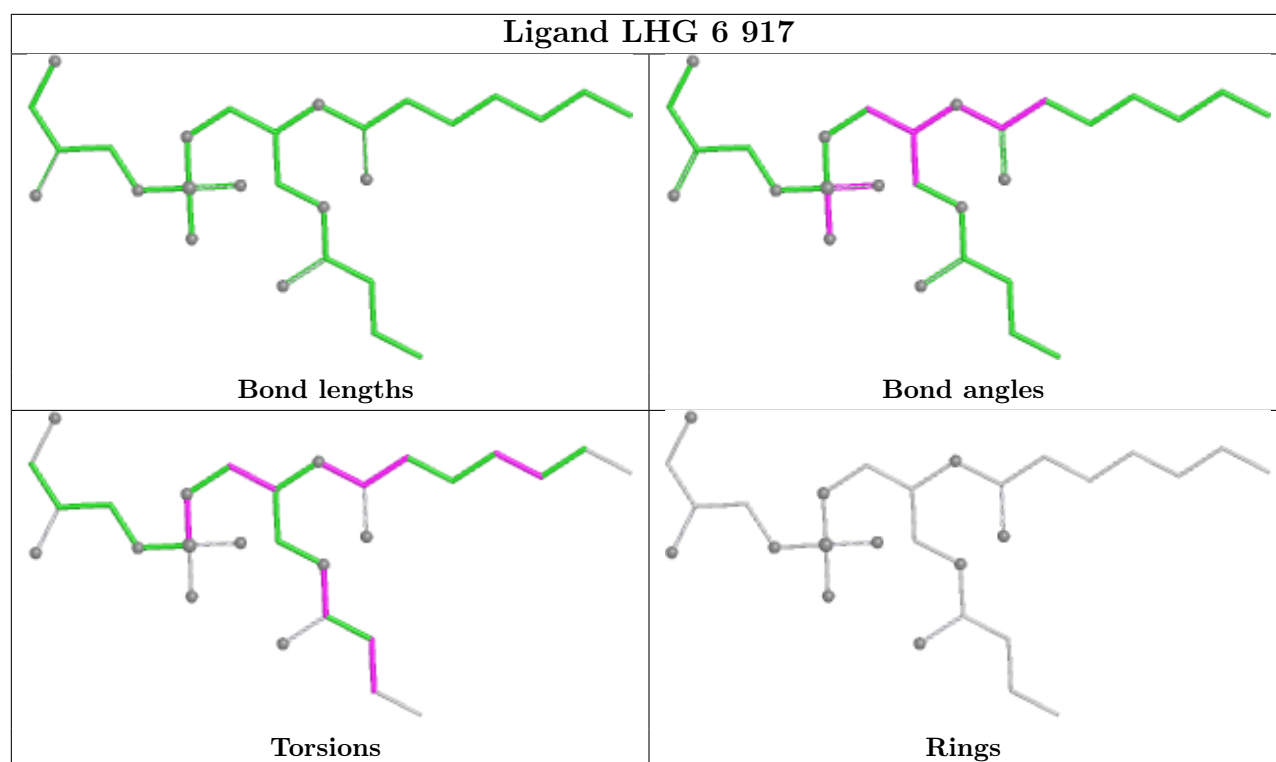


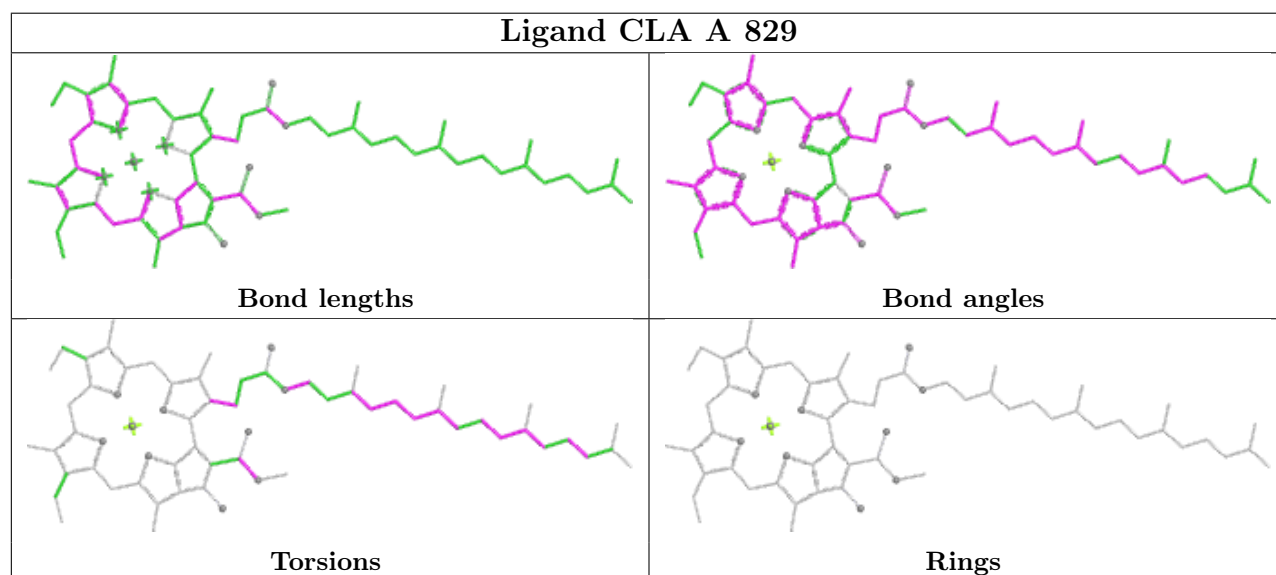
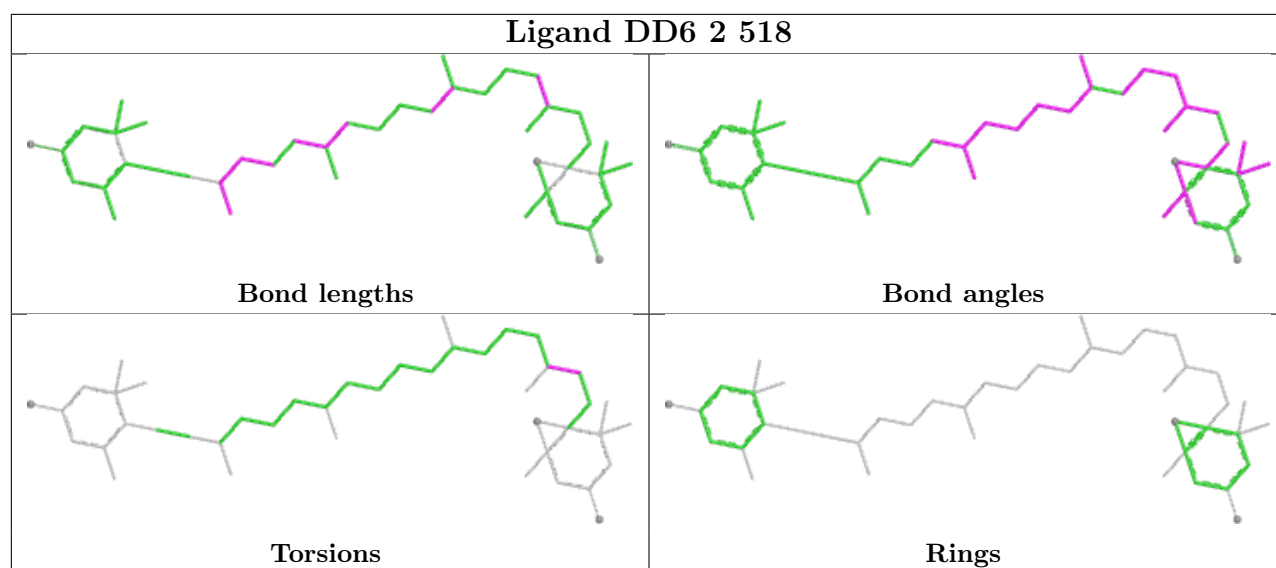
Torsions



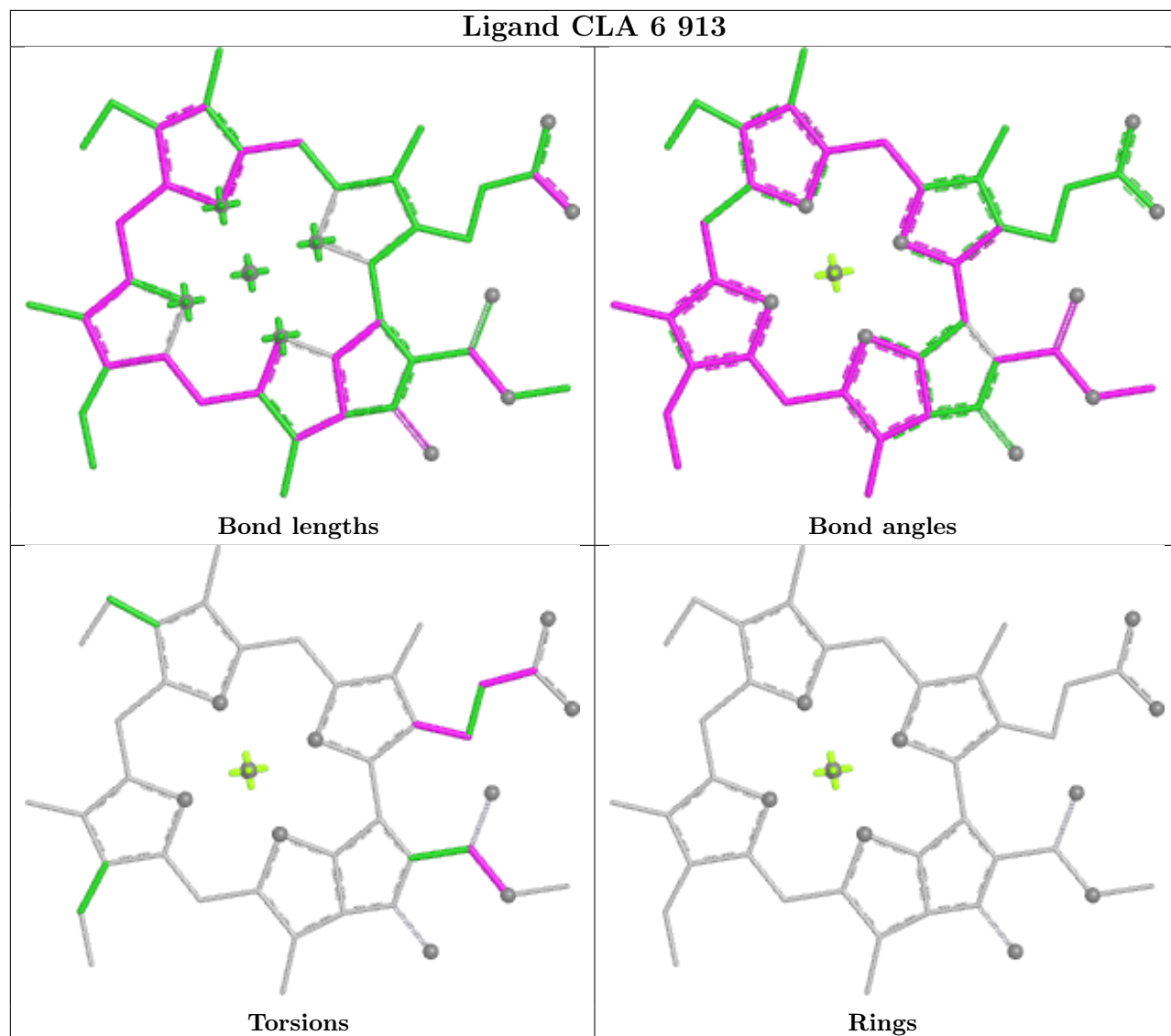
Rings



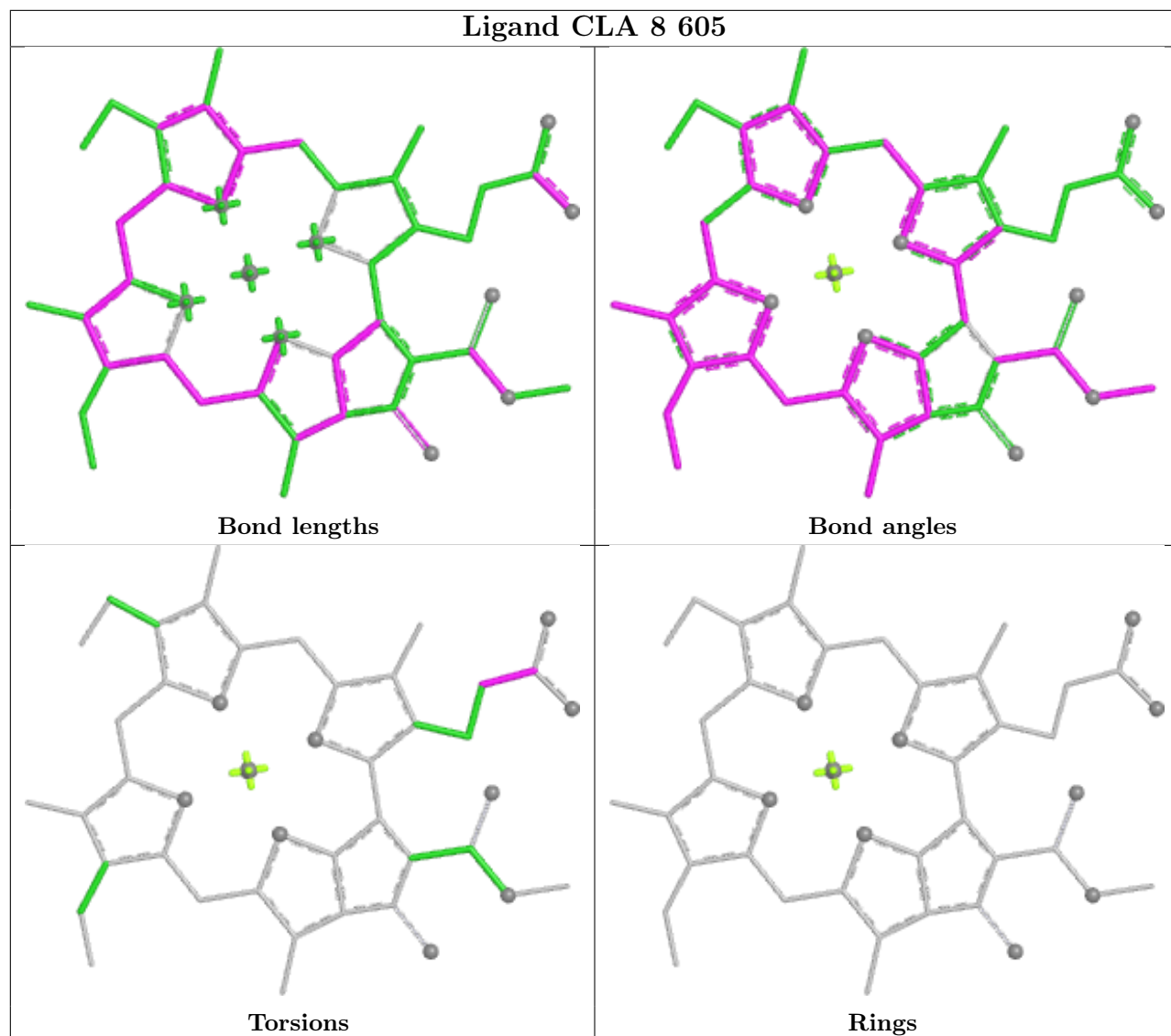


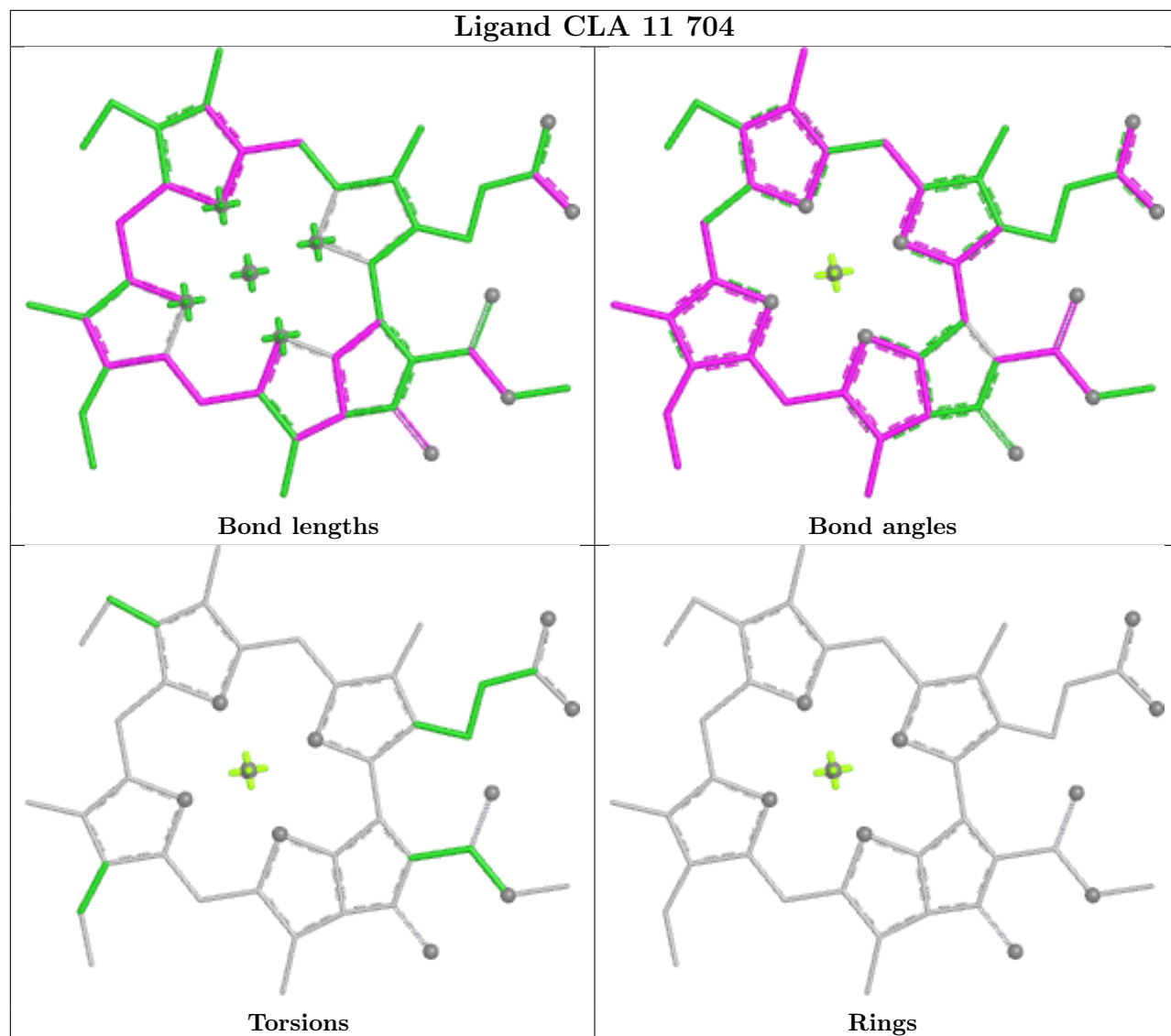


Ligand CLA 6 913

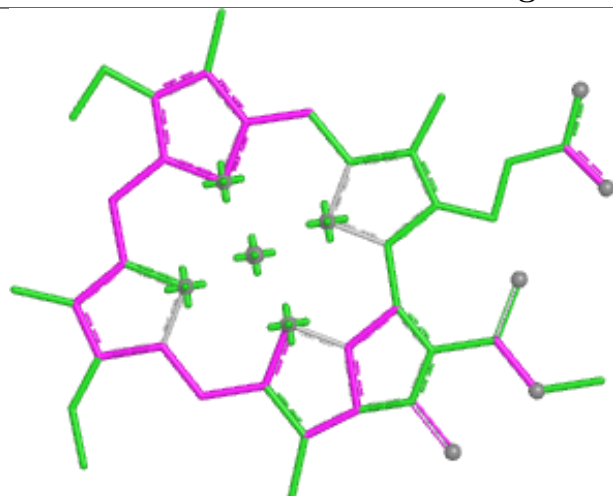


Ligand CLA 8 605

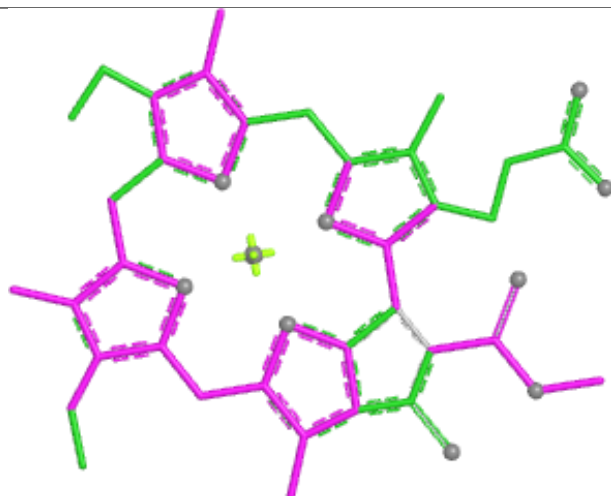




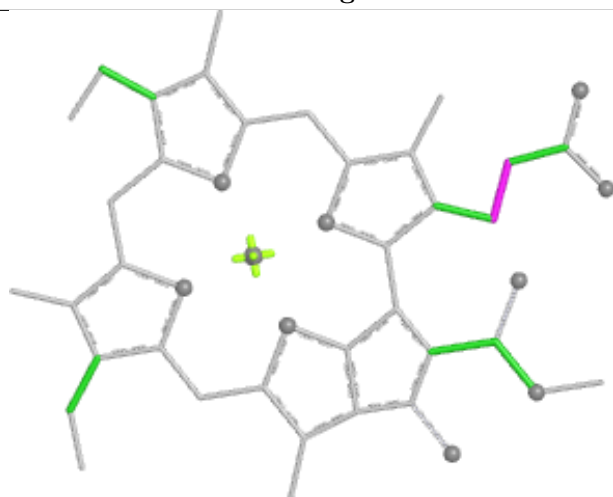
Ligand CLA 2 517



Bond lengths



Bond angles

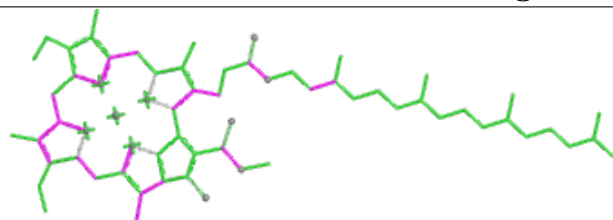


Torsions

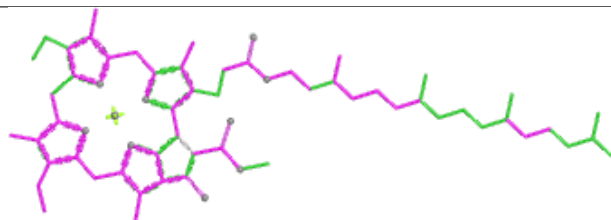


Rings

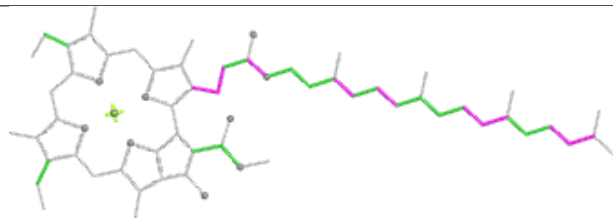
Ligand CLA B 827



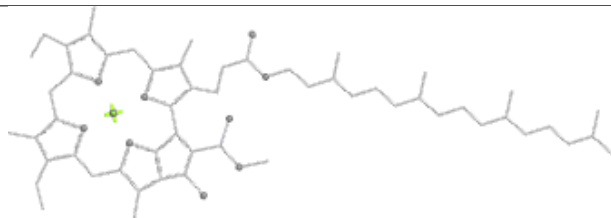
Bond lengths



Bond angles

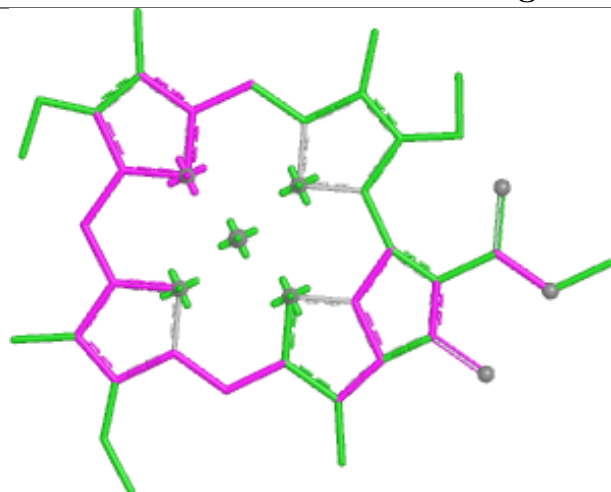


Torsions



Rings

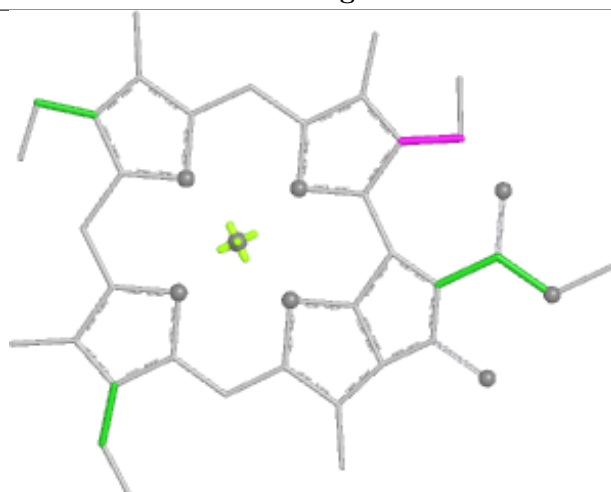
Ligand CLA 3 704



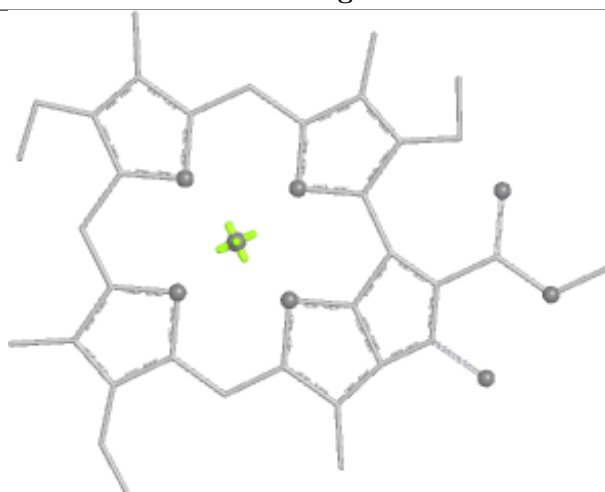
Bond lengths



Bond angles

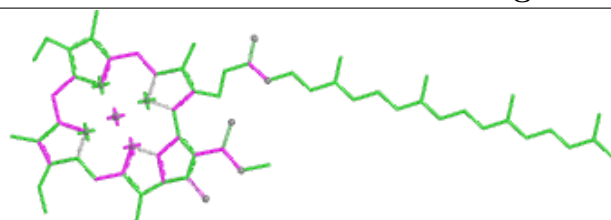


Torsions

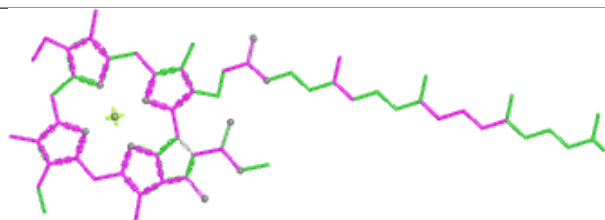


Rings

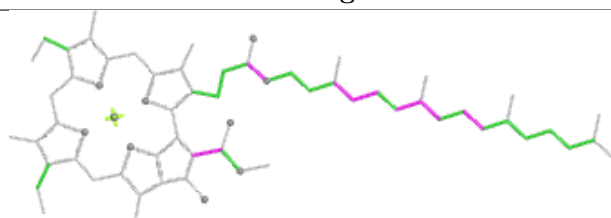
Ligand CLA A 828



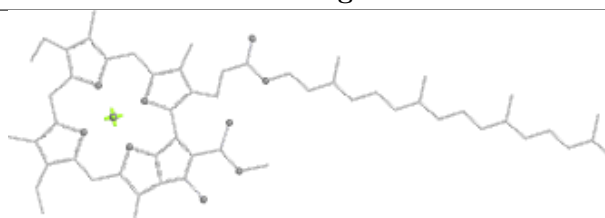
Bond lengths



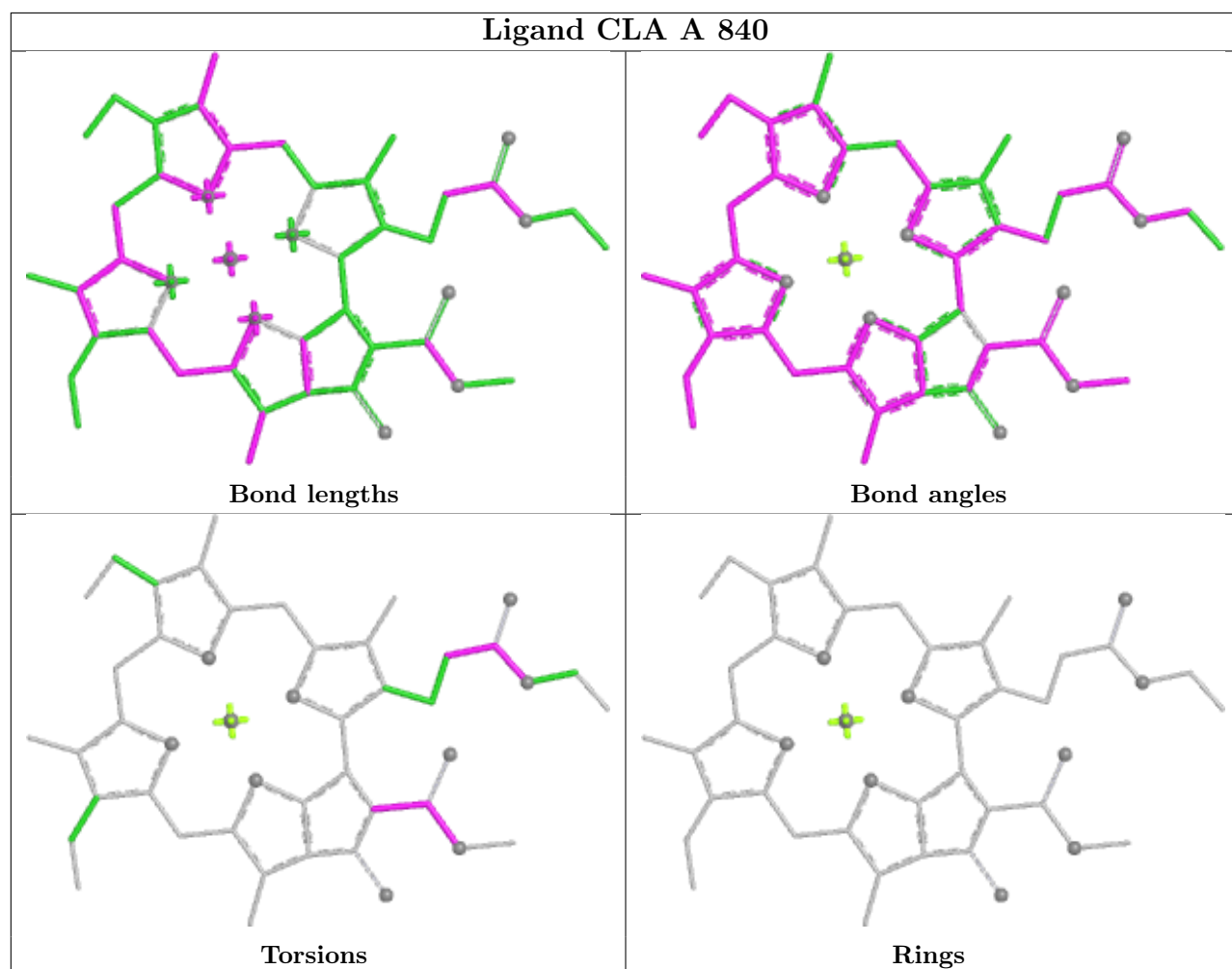
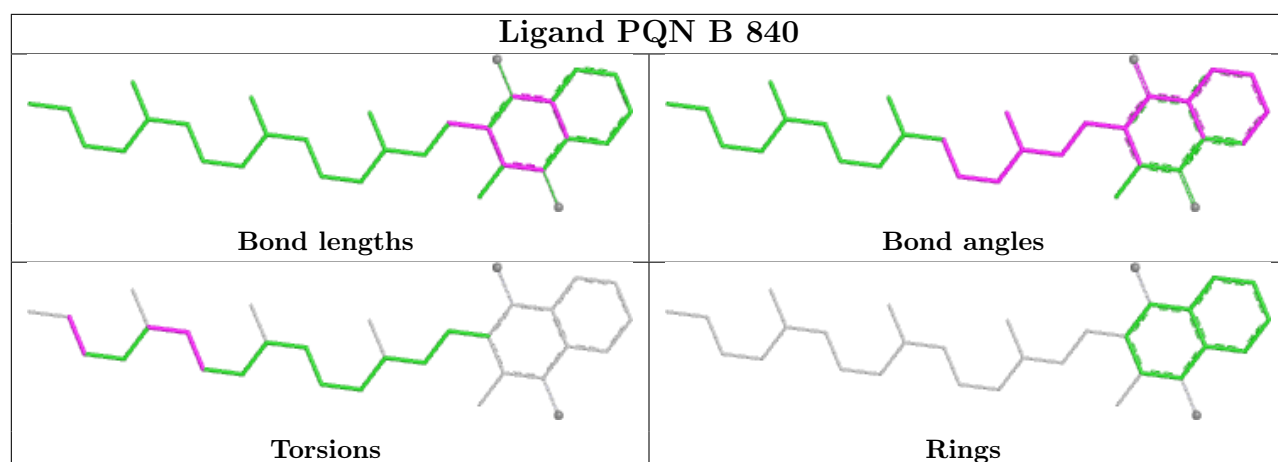
Bond angles



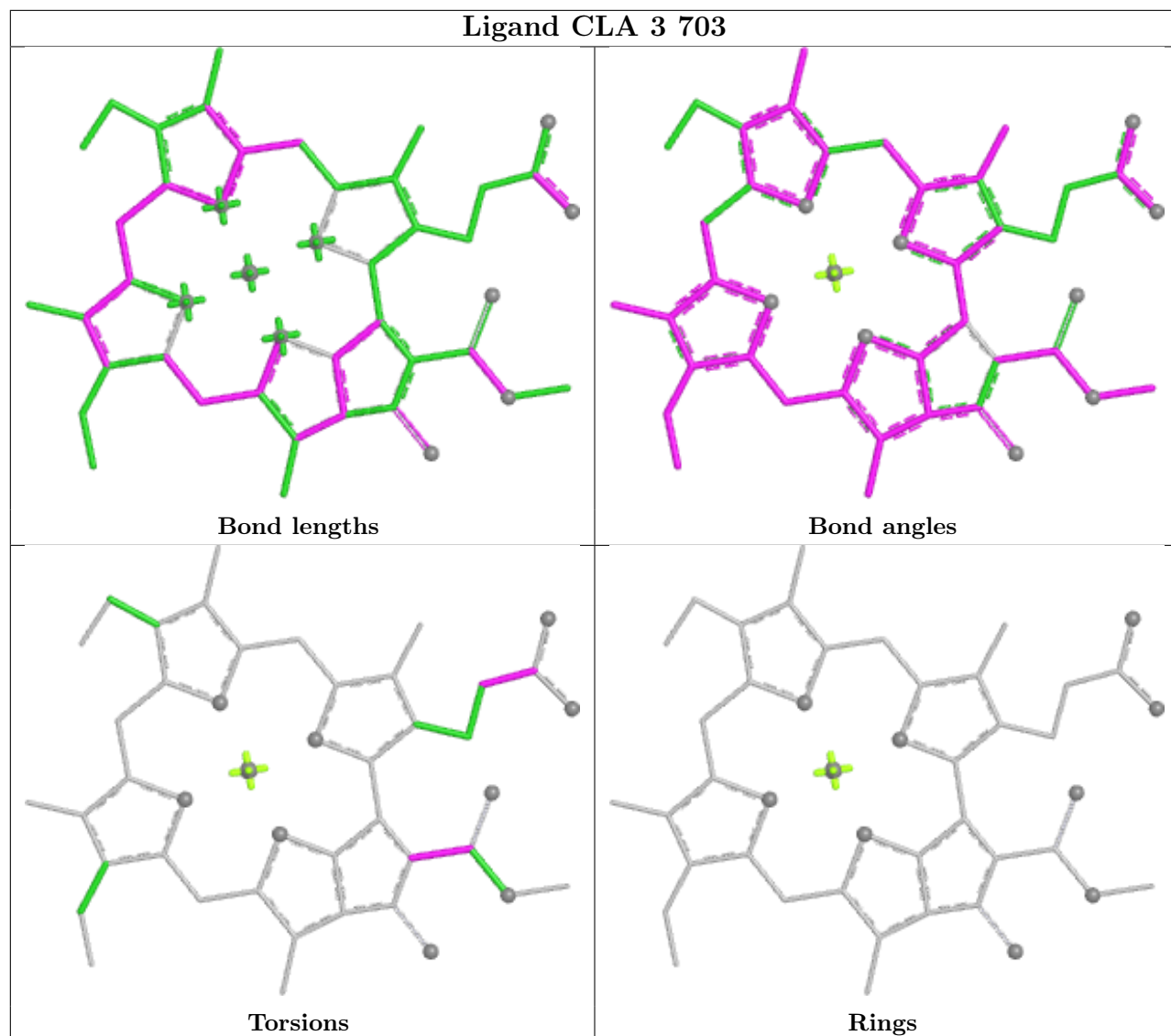
Torsions



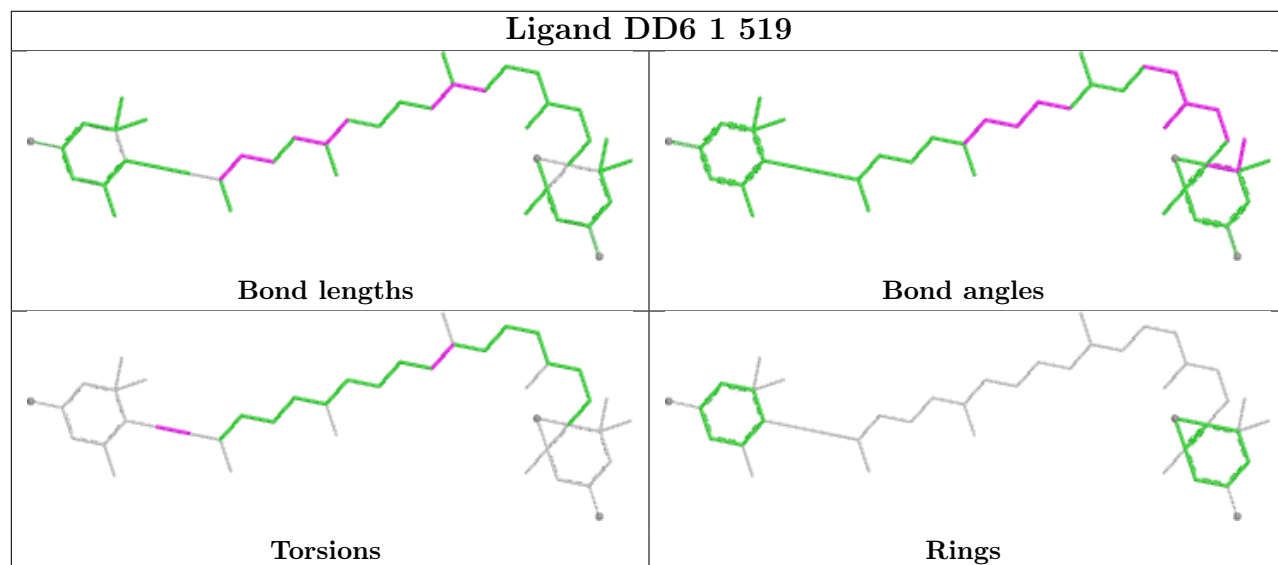
Rings



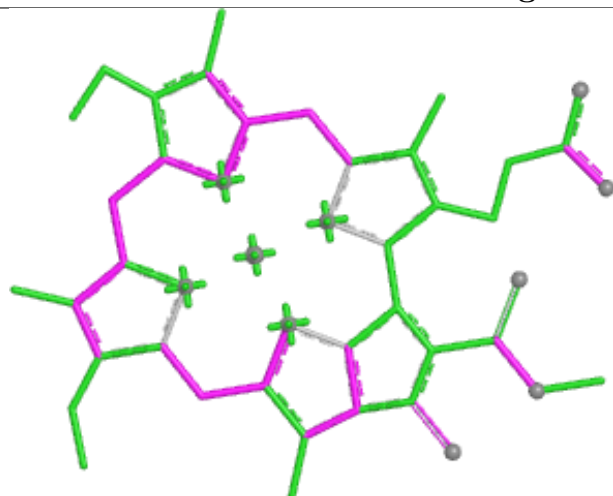
Ligand CLA 3 703



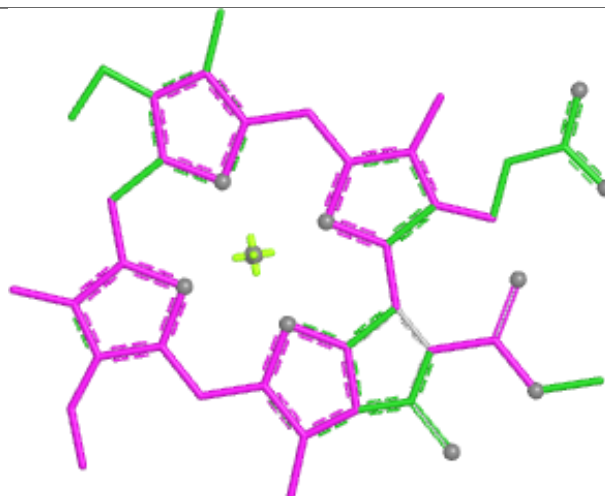
Ligand DD6 1 519



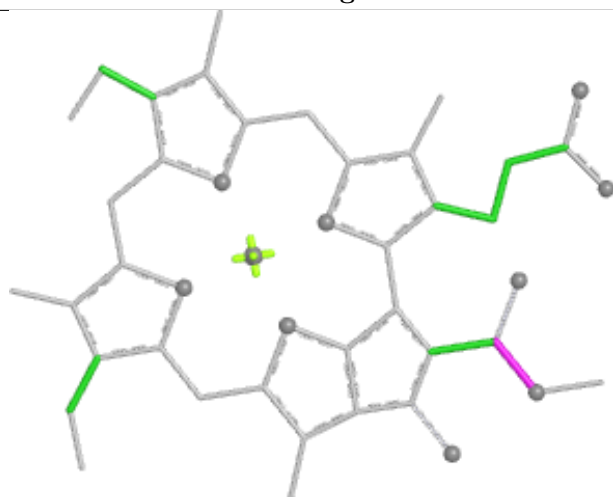
Ligand CLA 5 706



Bond lengths



Bond angles

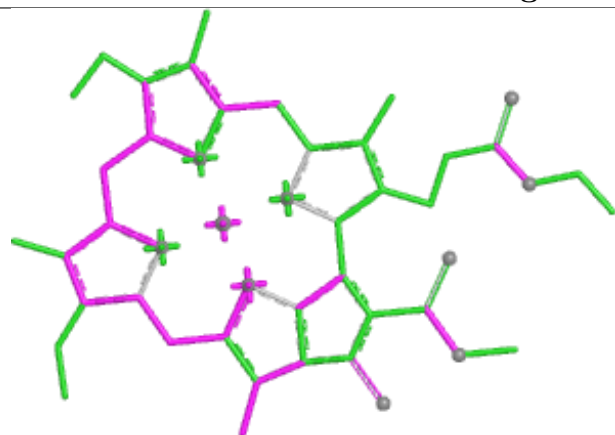


Torsions

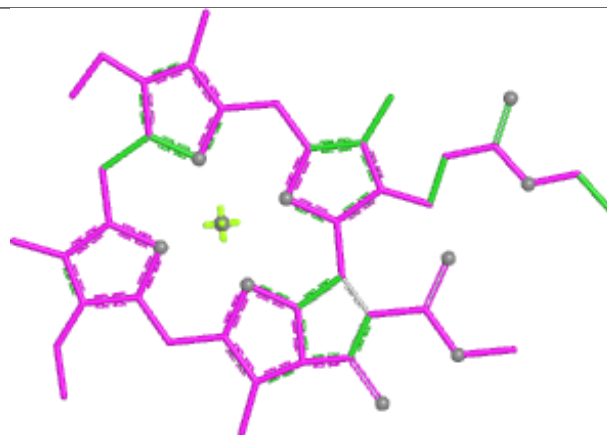


Rings

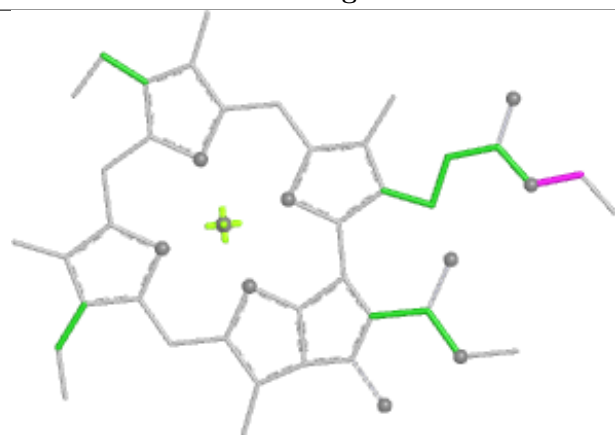
Ligand CLA 6 907



Bond lengths



Bond angles

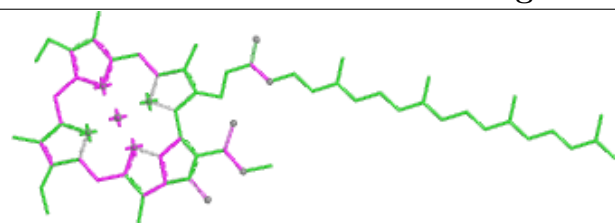


Torsions

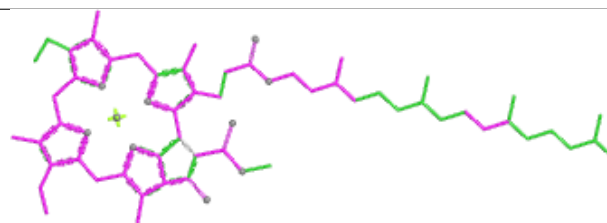


Rings

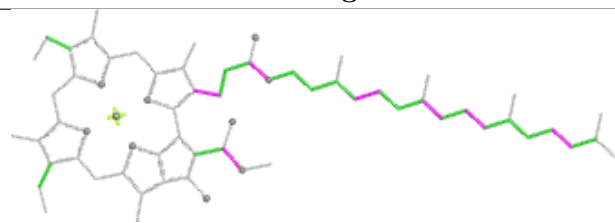
Ligand CLA A 807



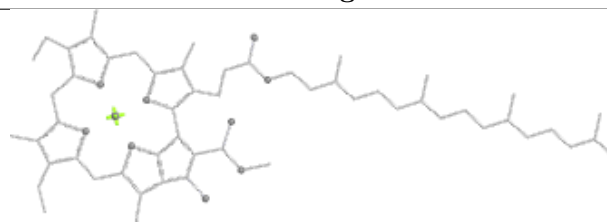
Bond lengths



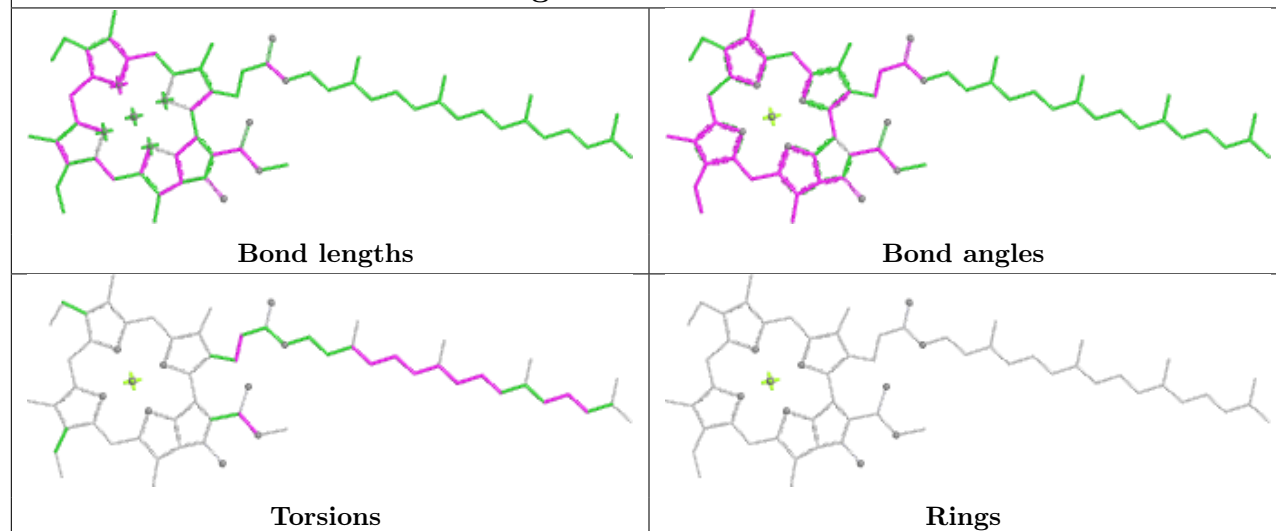
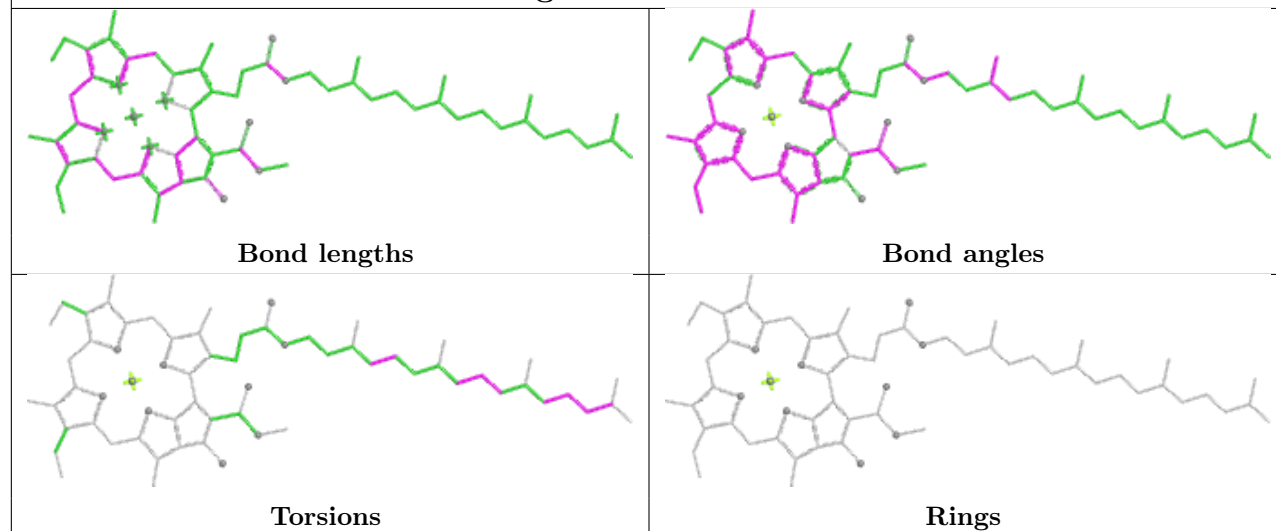
Bond angles



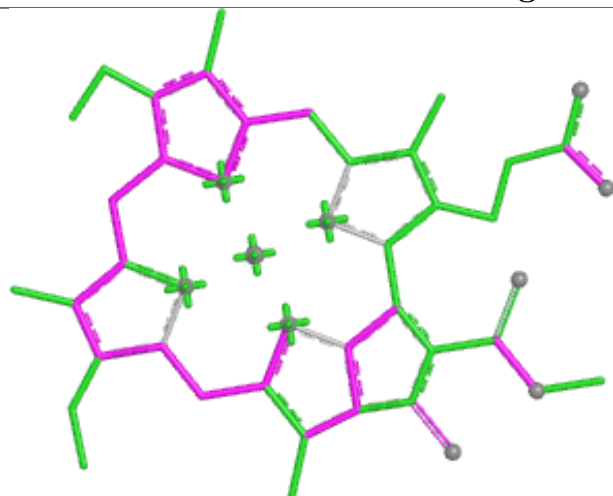
Torsions



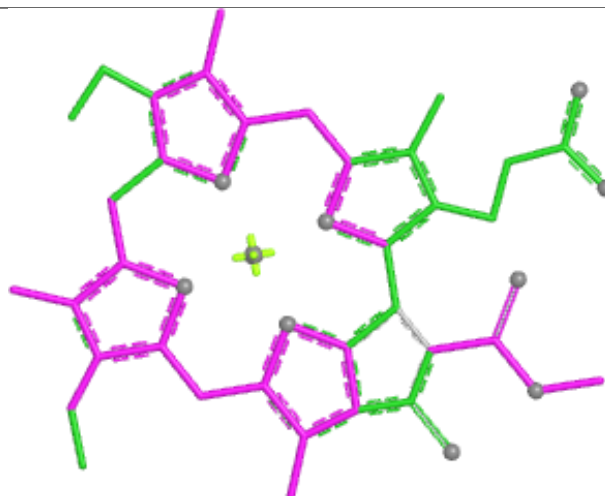
Rings

Ligand CLA A 810**Ligand CLA 7 711**

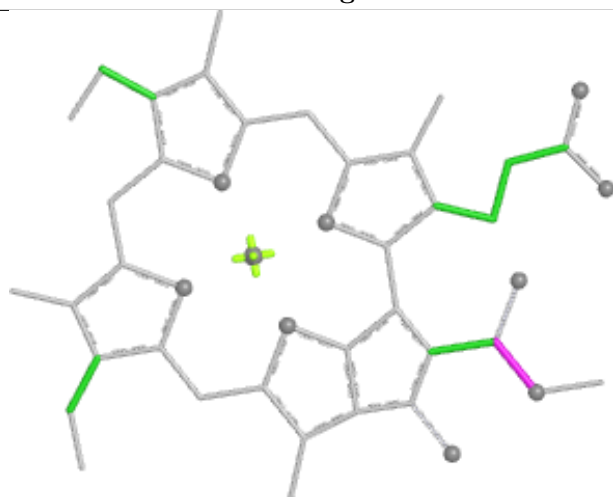
Ligand CLA 5 711



Bond lengths



Bond angles

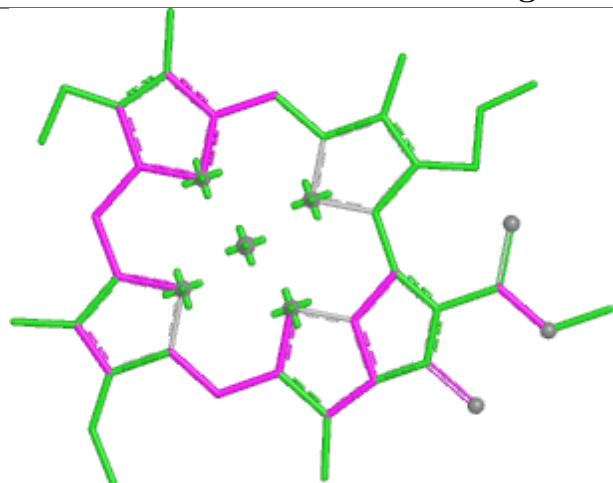


Torsions

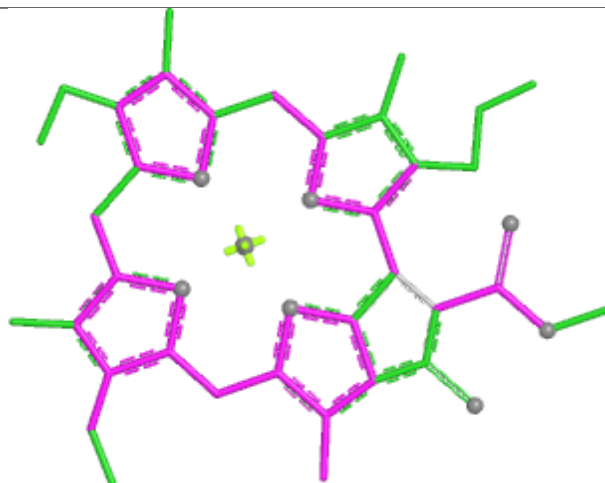


Rings

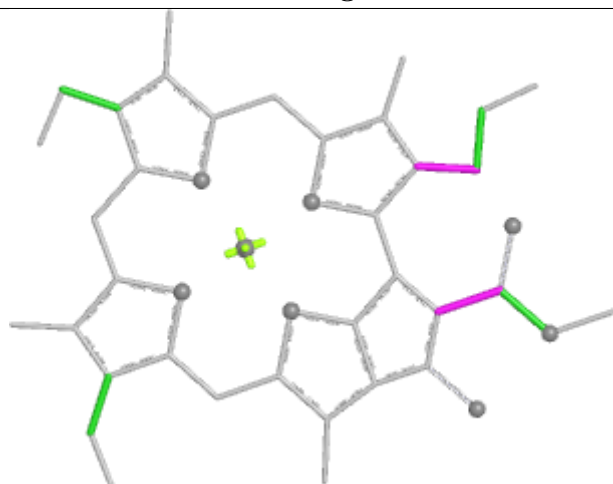
Ligand CLA 5 708



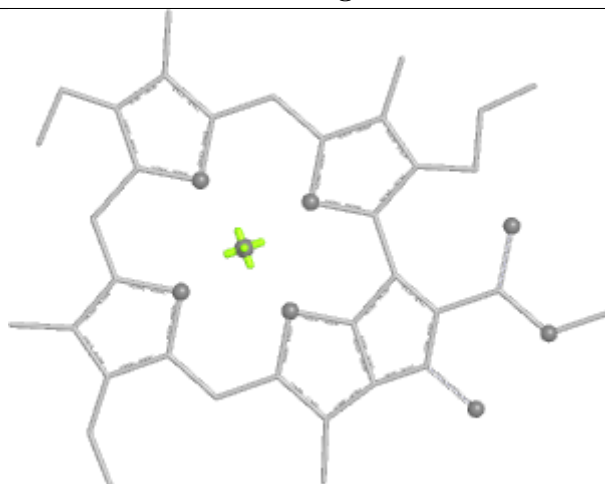
Bond lengths



Bond angles

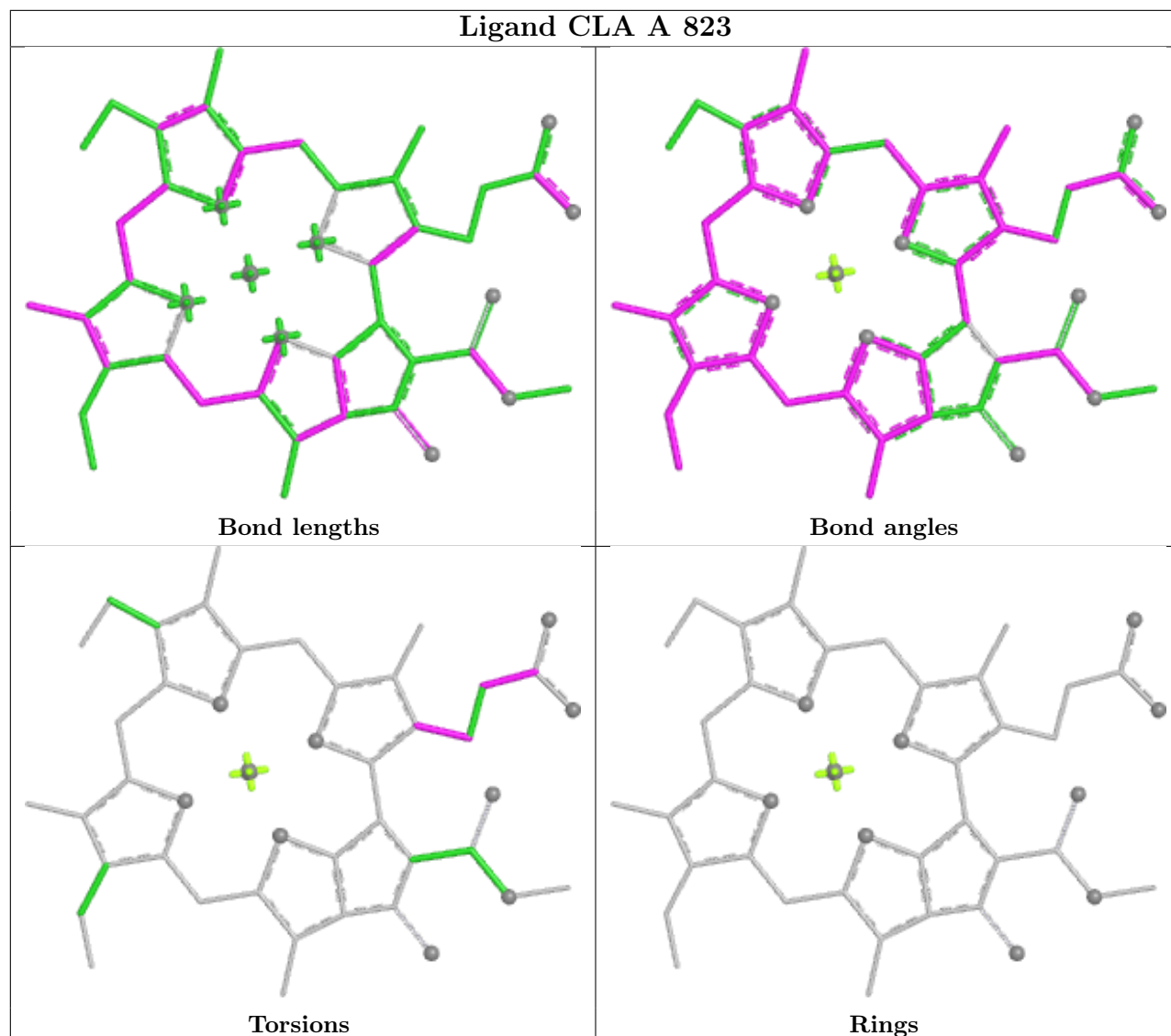


Torsions

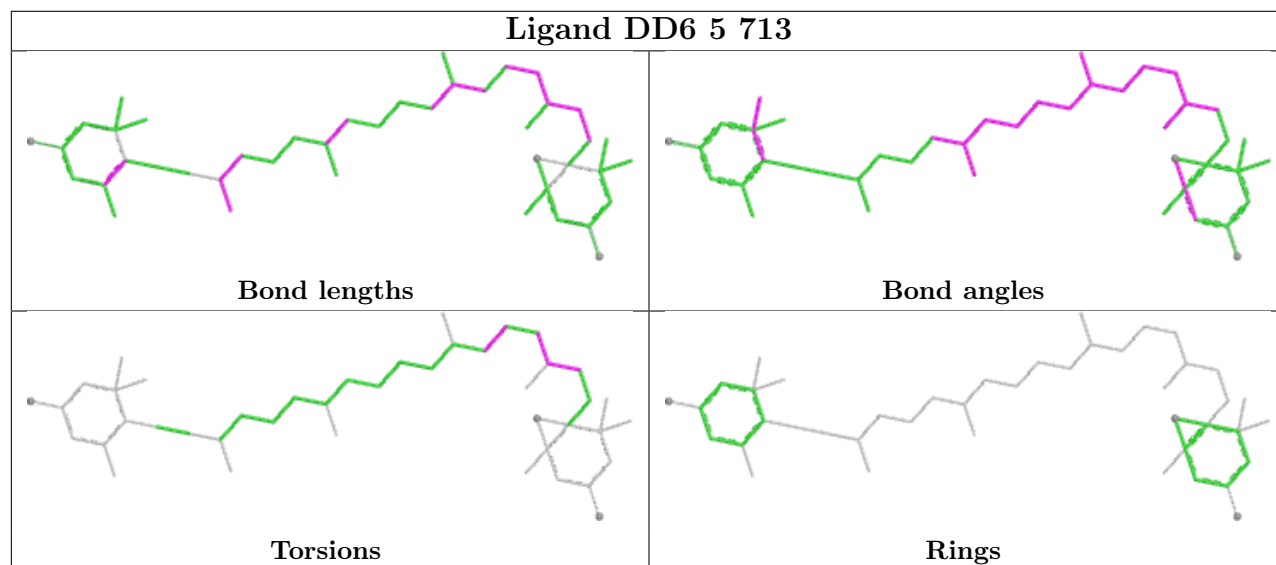


Rings

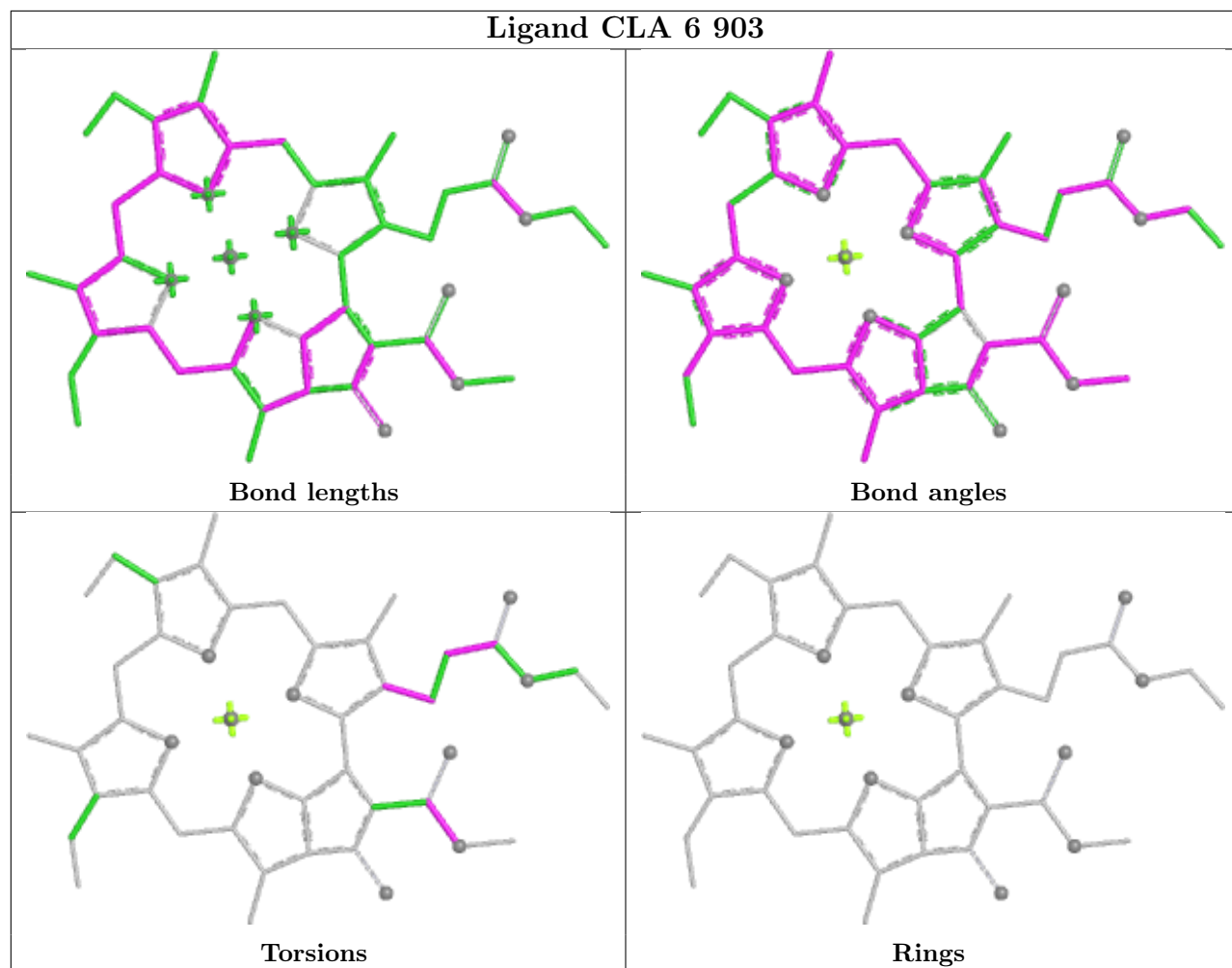
Ligand CLA A 823

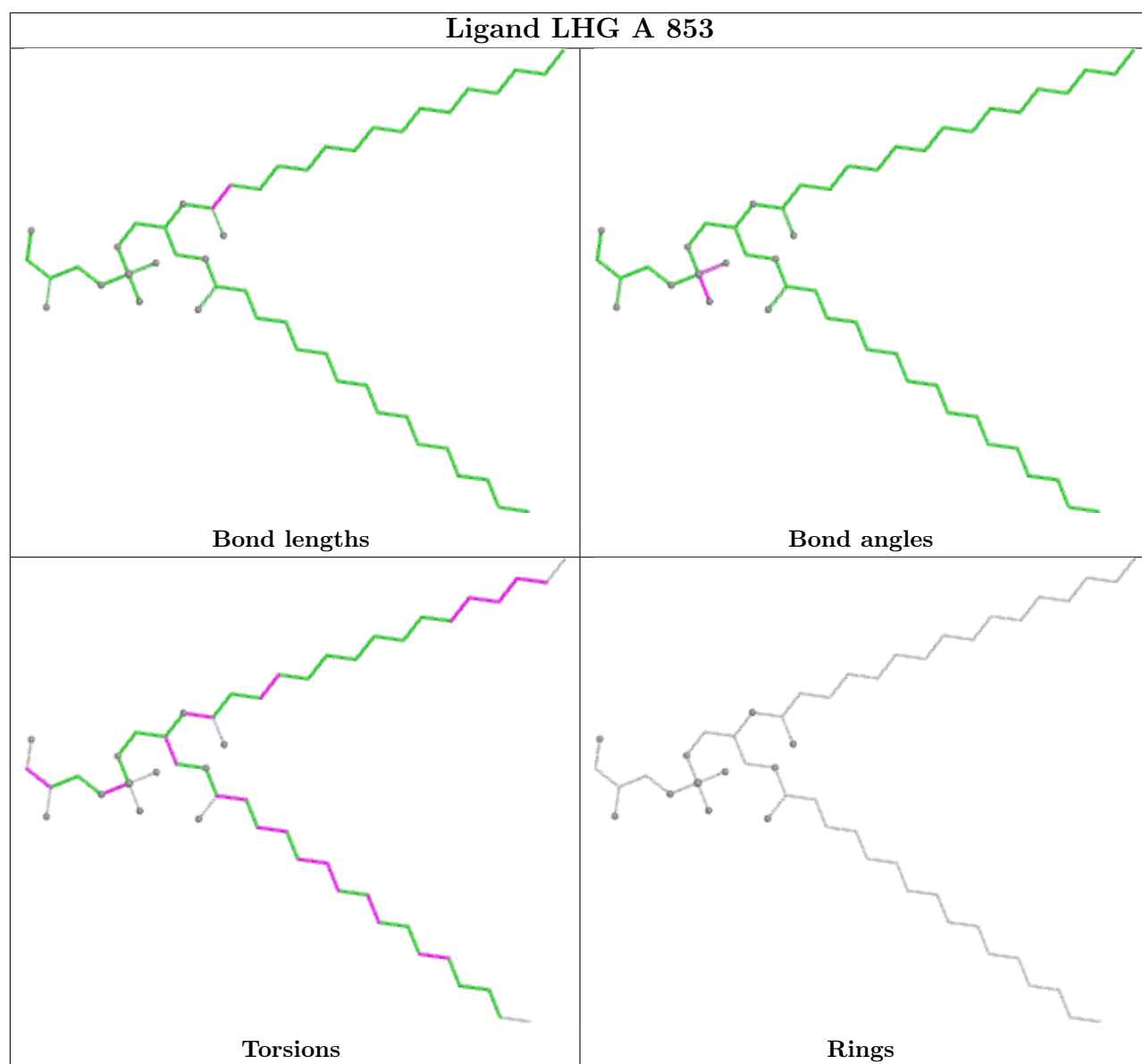


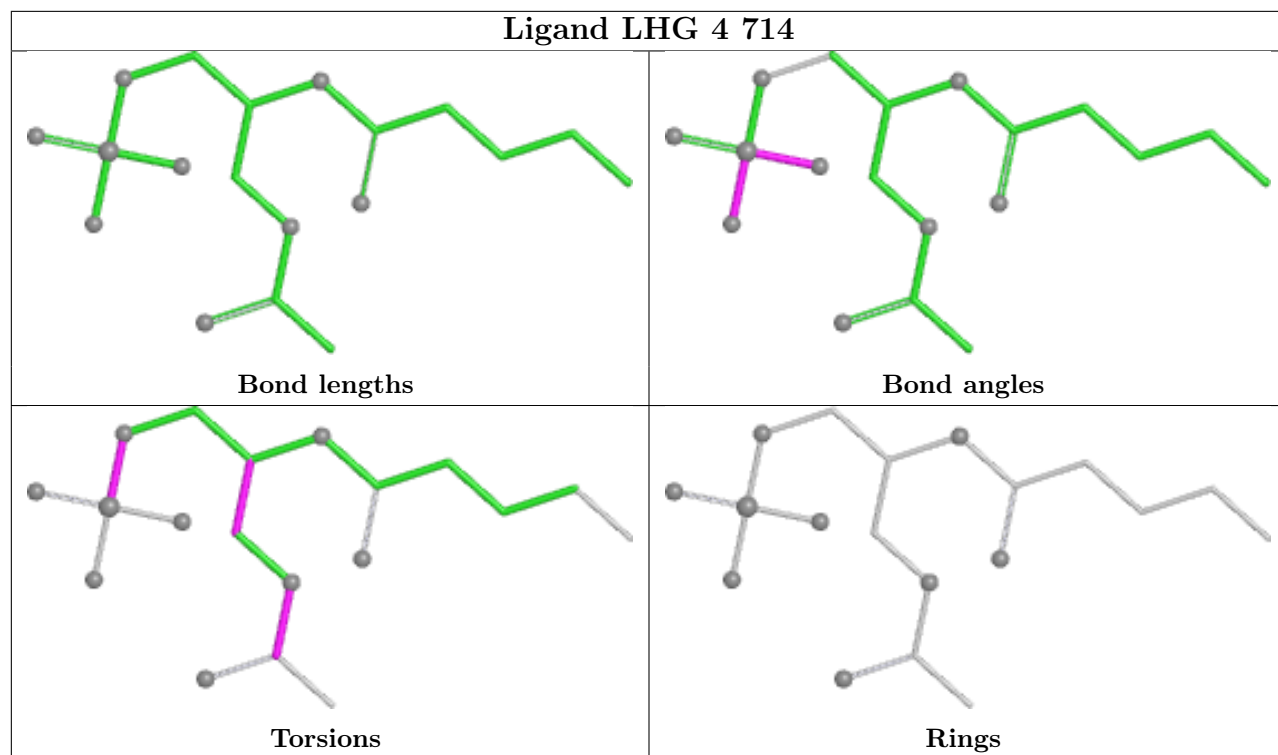
Ligand DD6 5 713

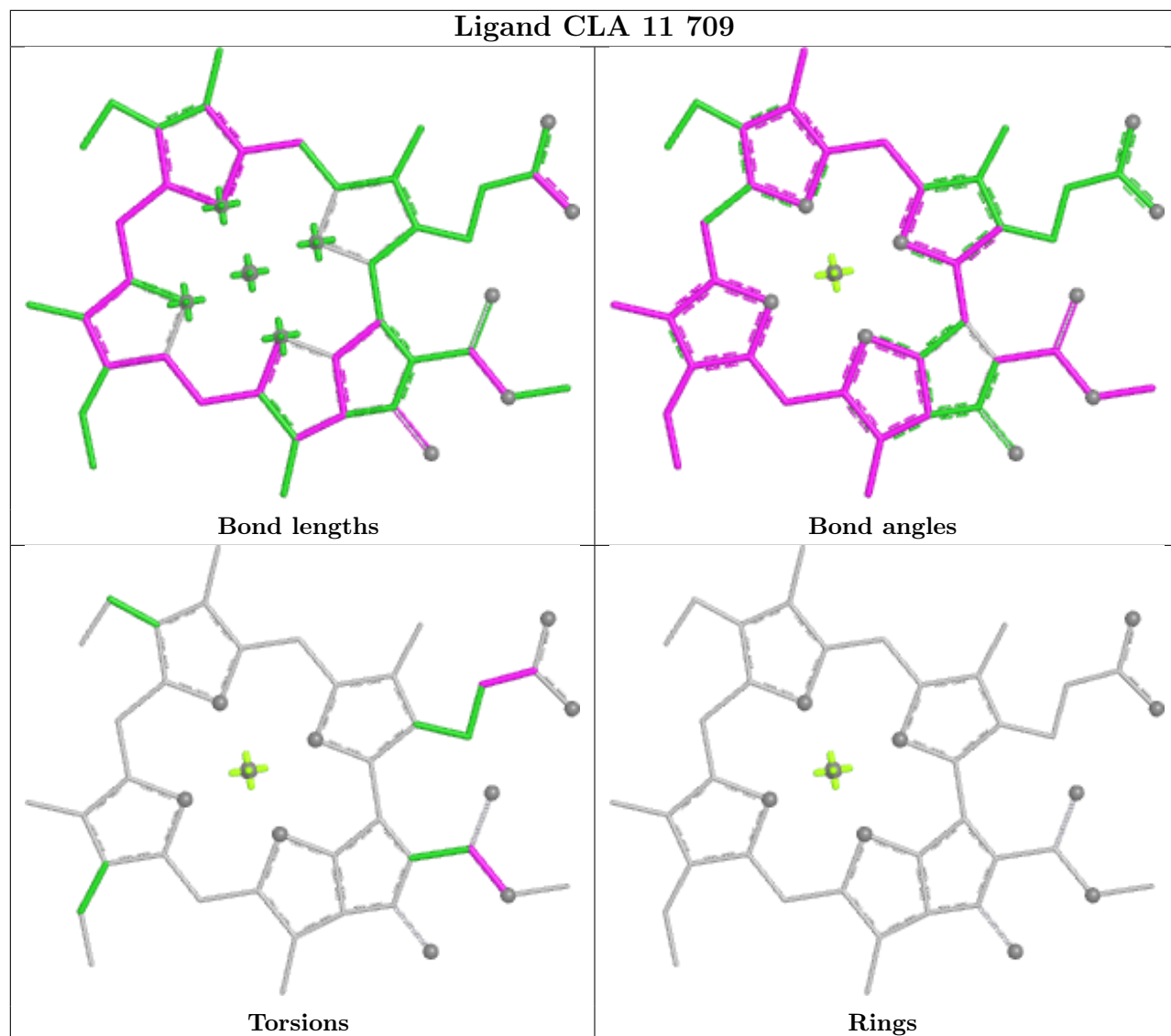


Ligand CLA 6 903

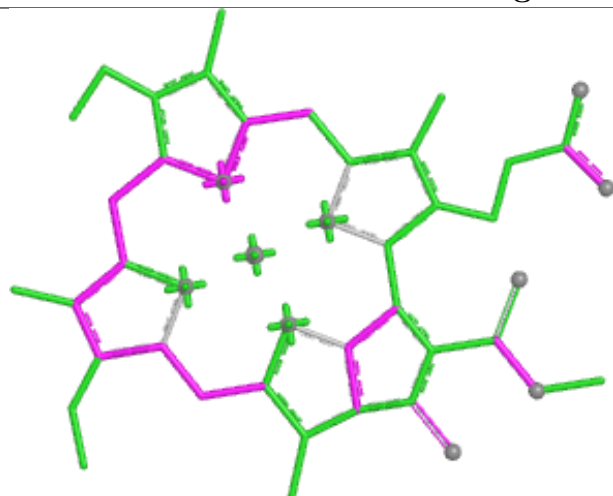




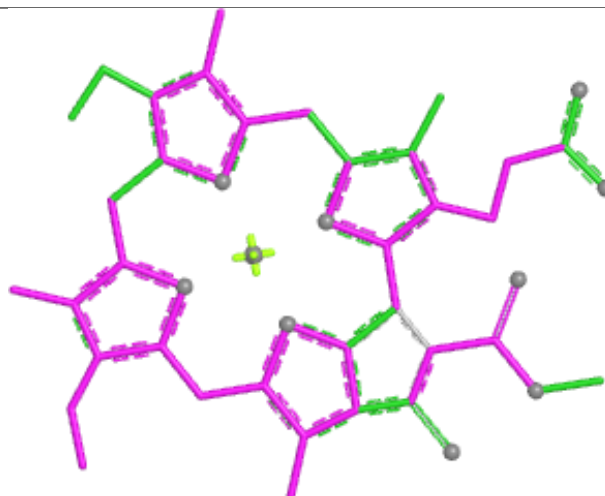




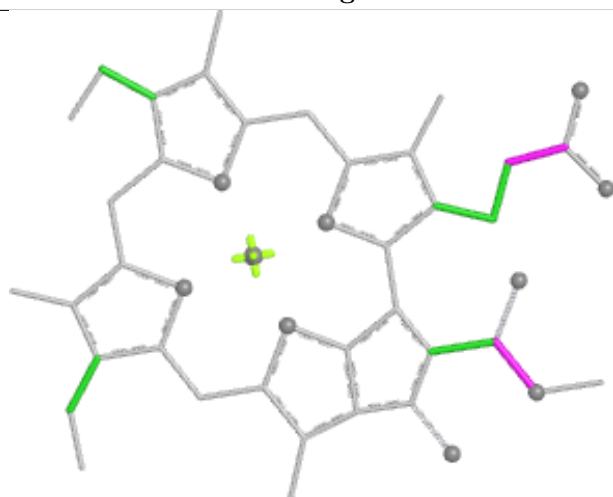
Ligand CLA A 834



Bond lengths



Bond angles

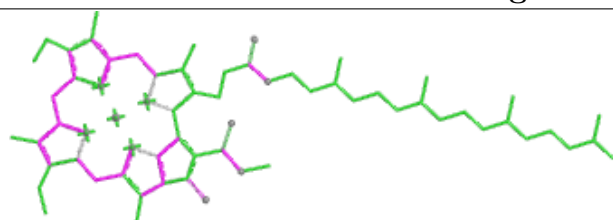


Torsions

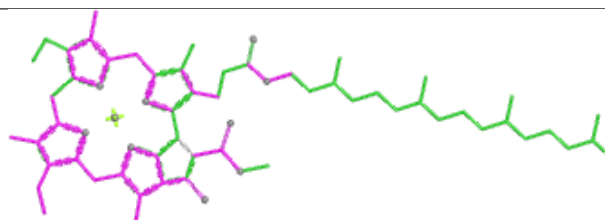


Rings

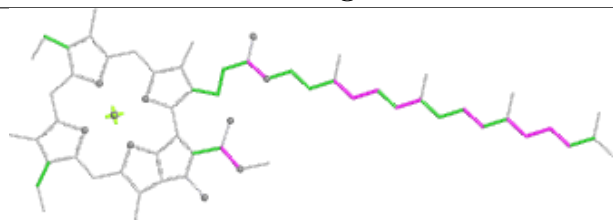
Ligand CLA 11 703



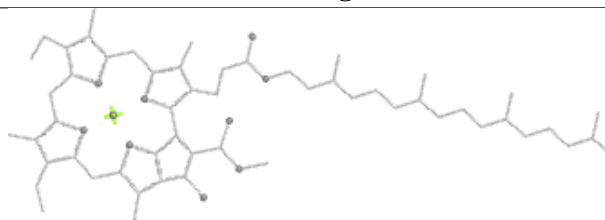
Bond lengths



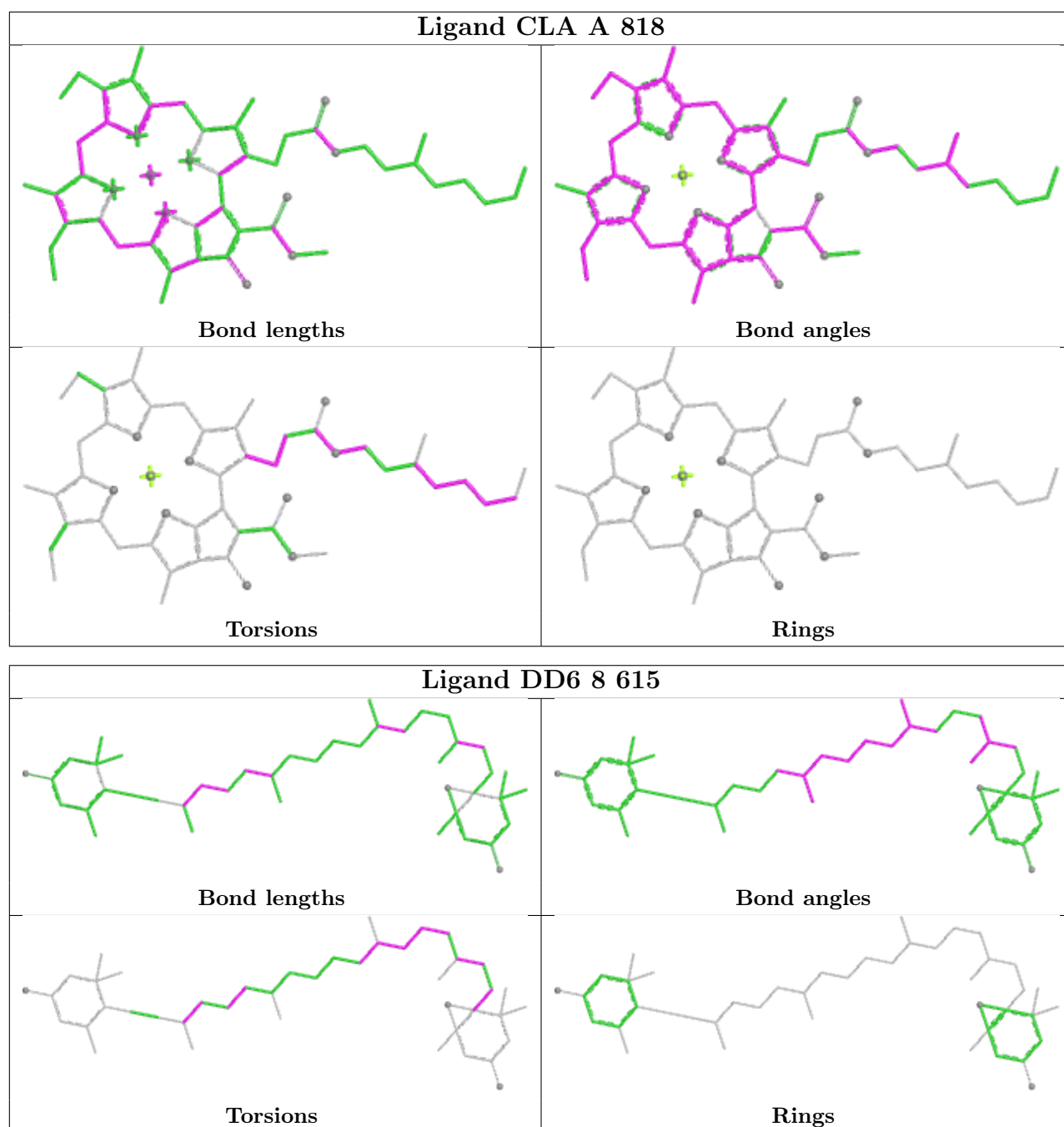
Bond angles



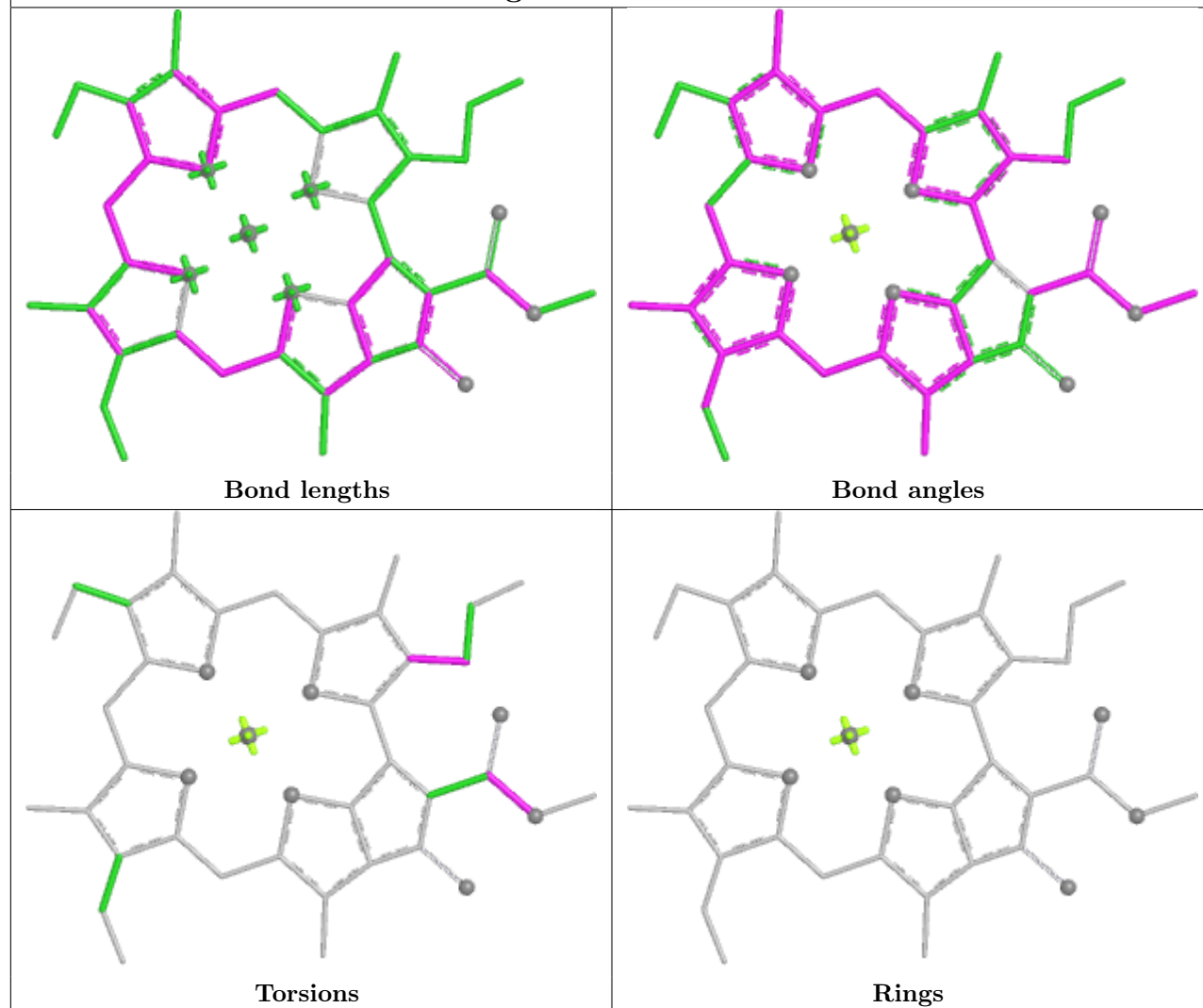
Torsions



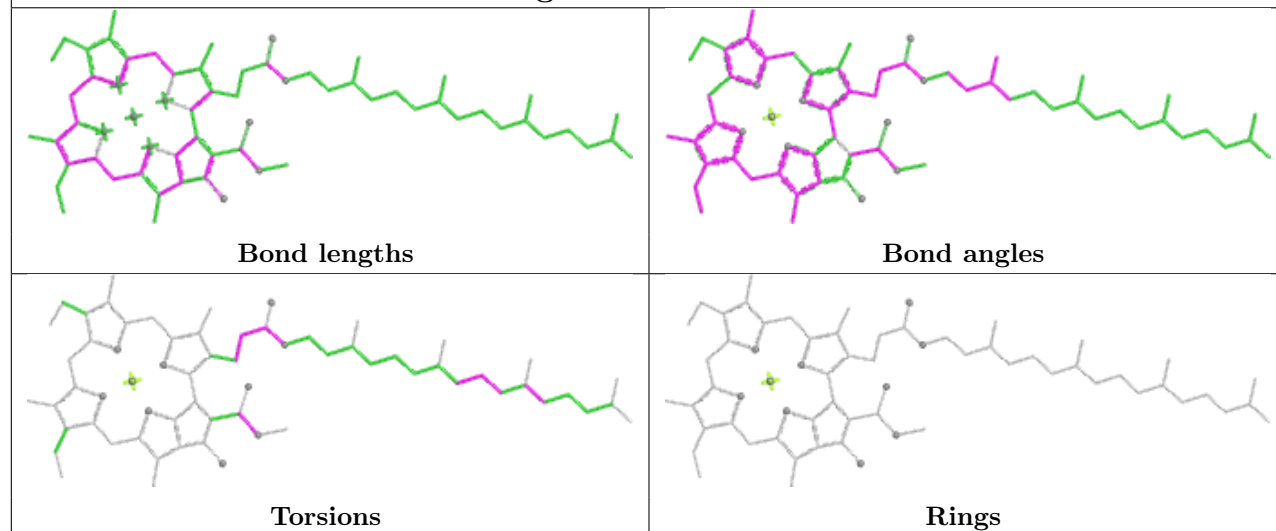
Rings



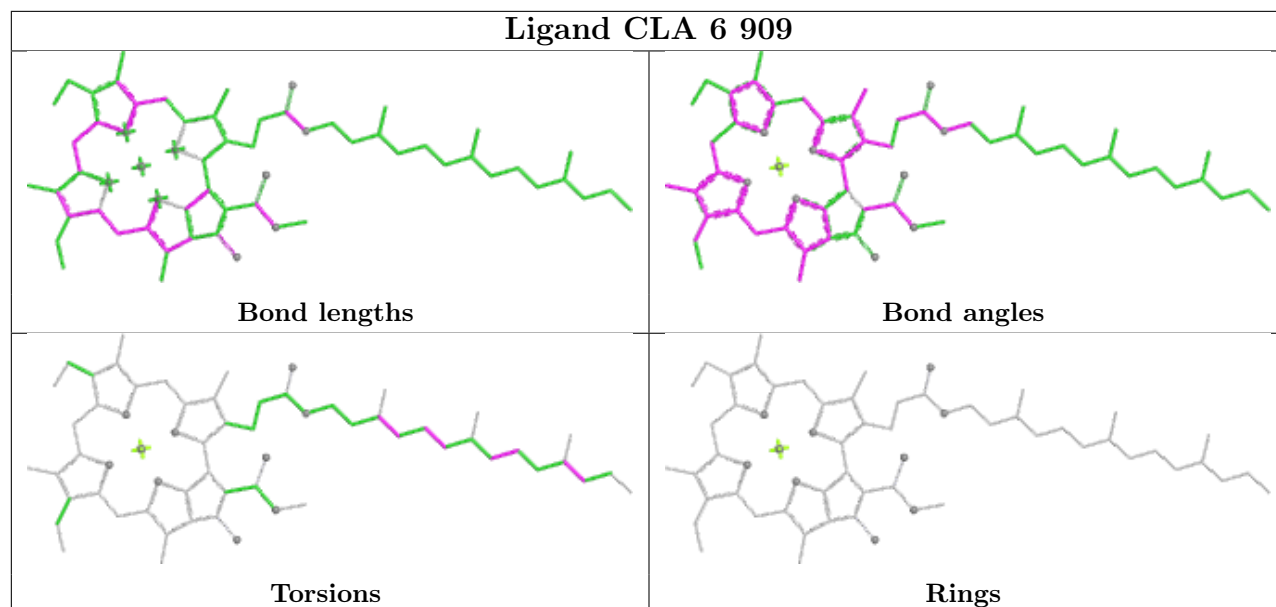
Ligand CLA 2 510



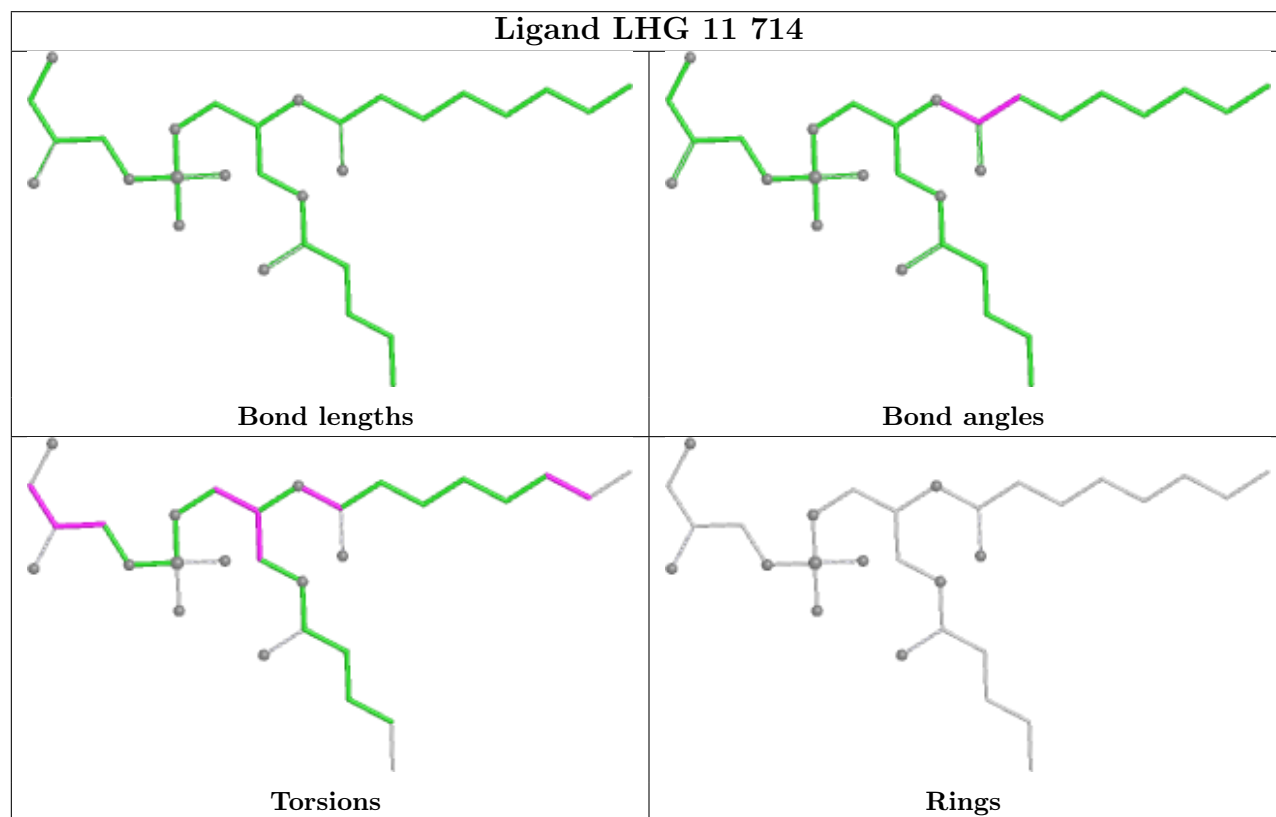
Ligand CLA 8 612

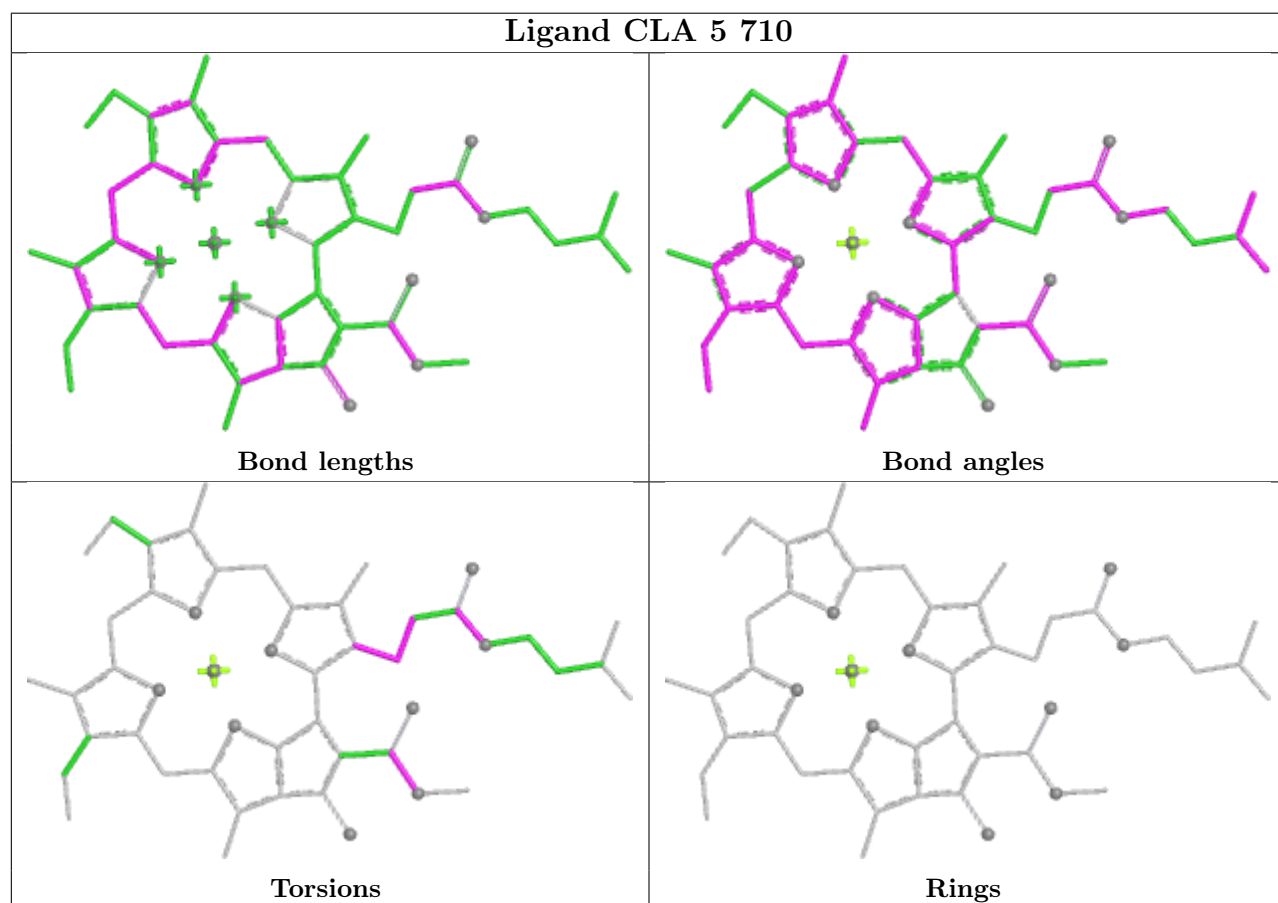
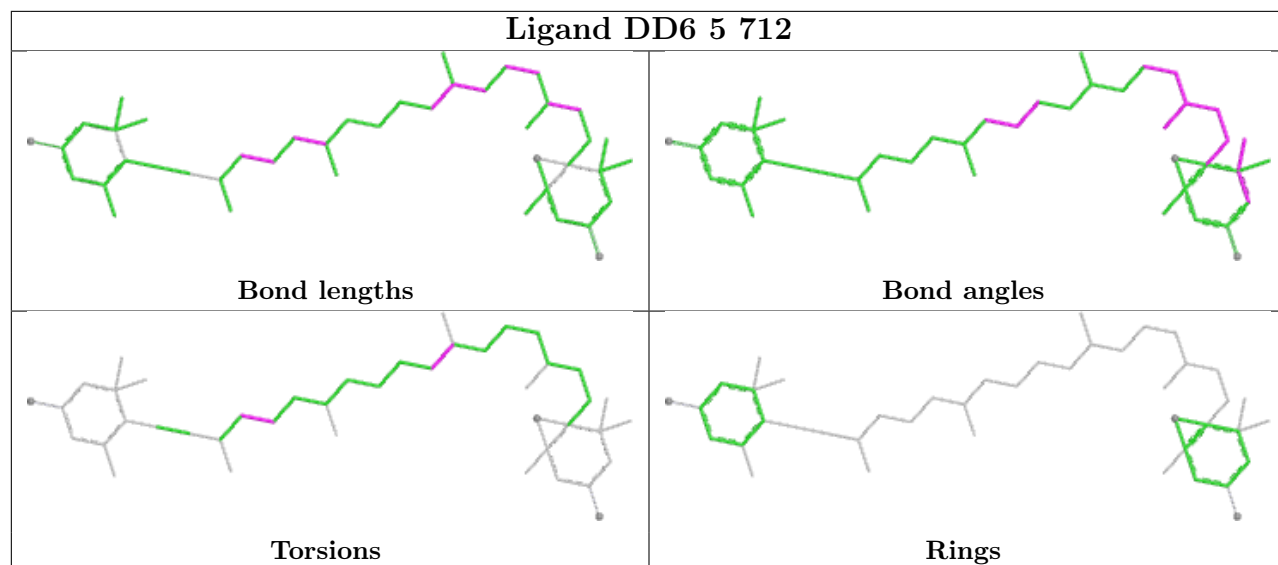


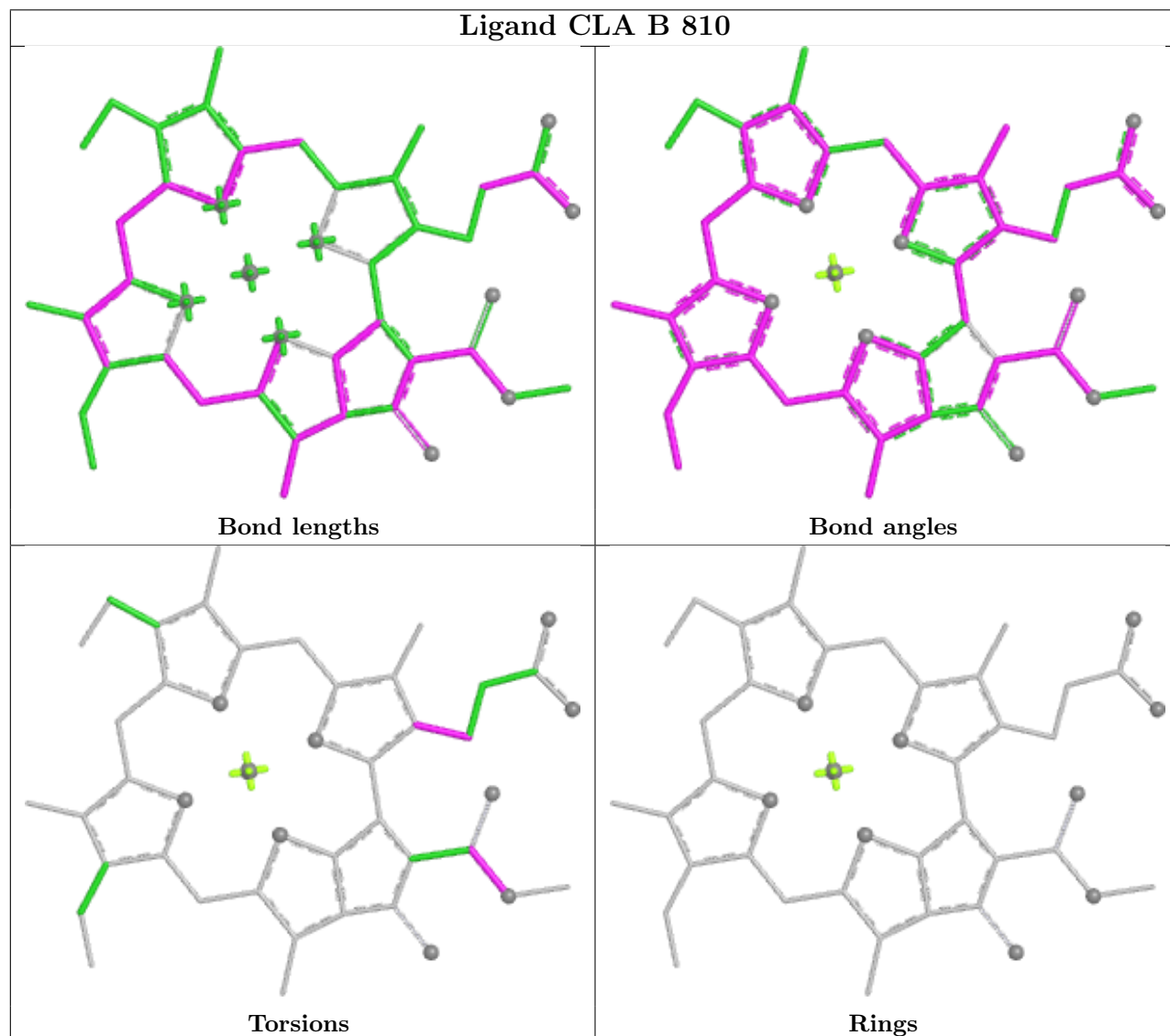
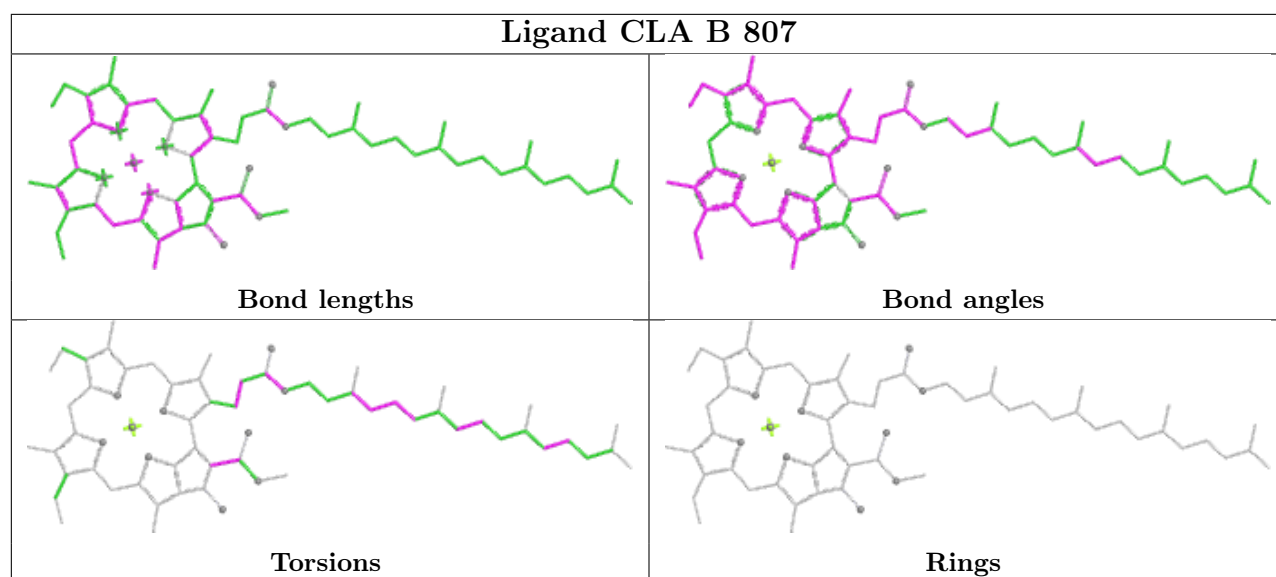
Ligand CLA 6 909



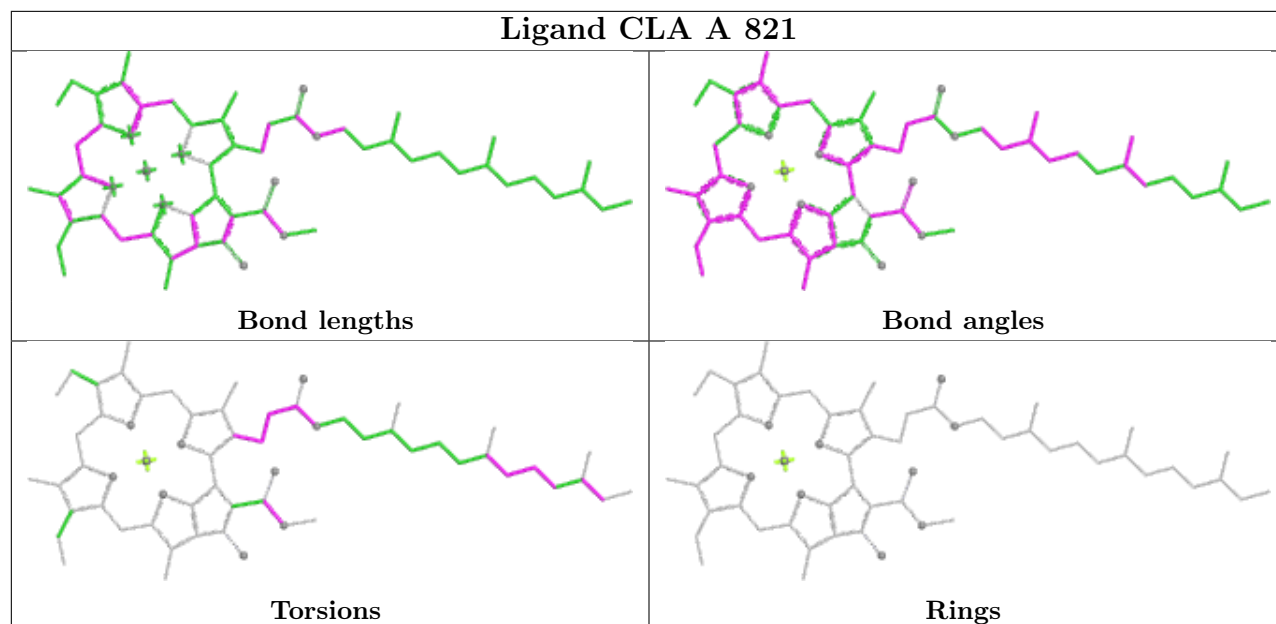
Ligand LHG 11 714



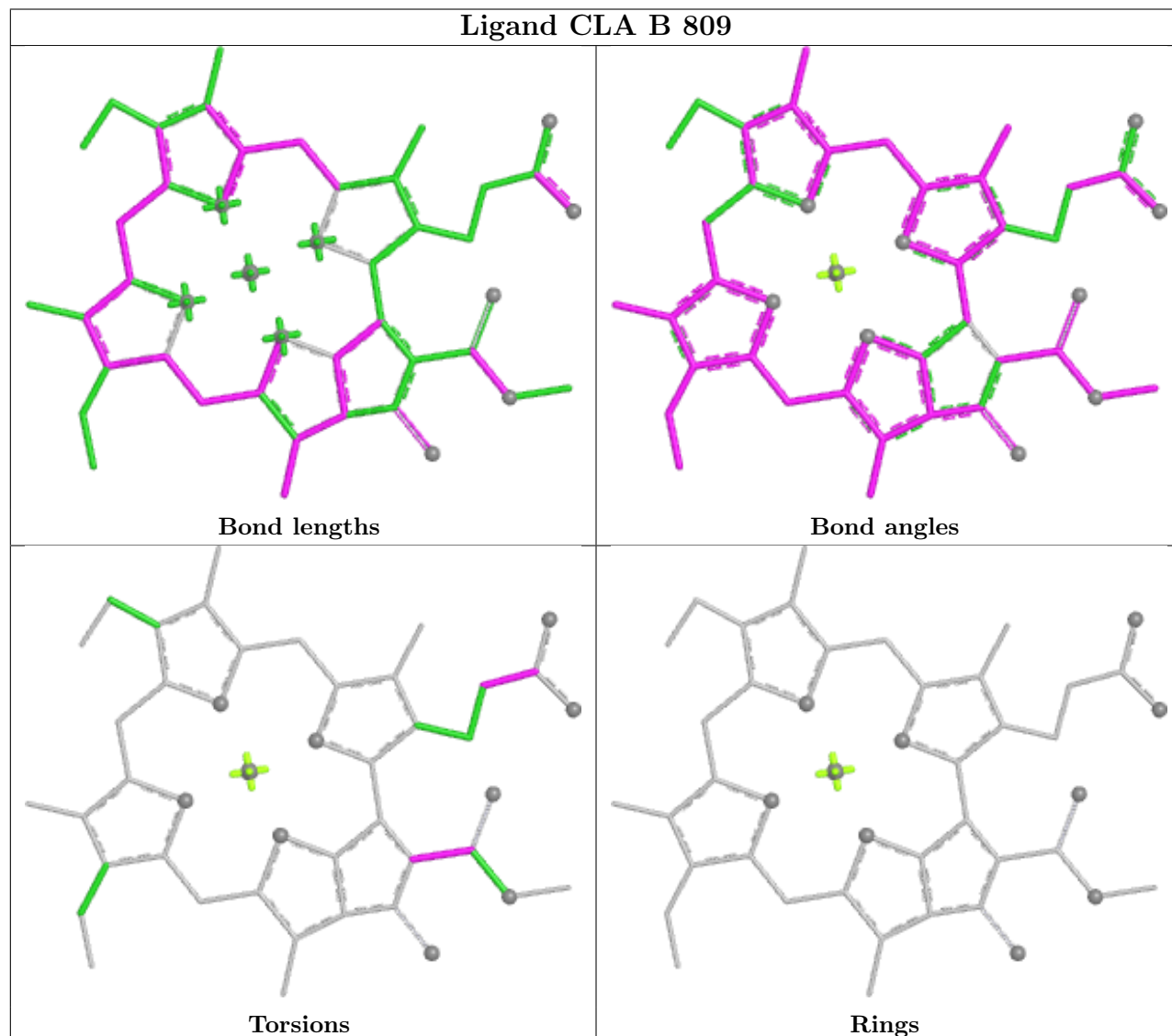




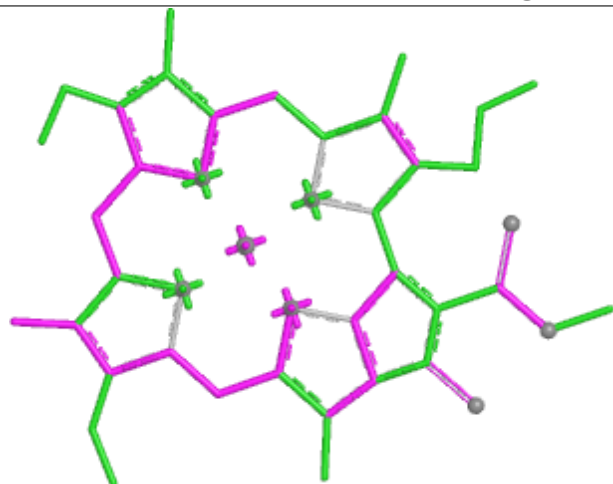
Ligand CLA A 821



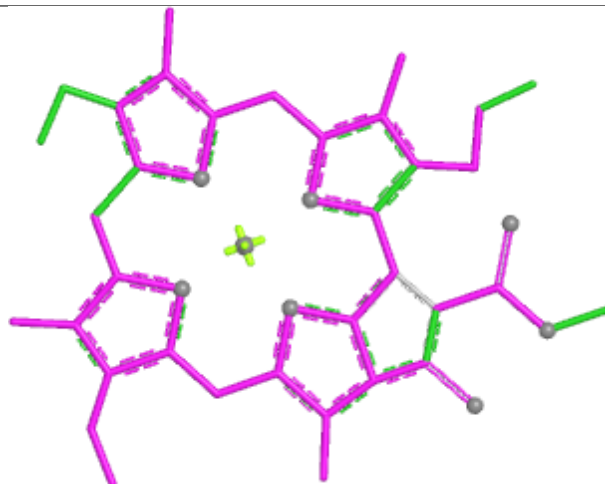
Ligand CLA B 809



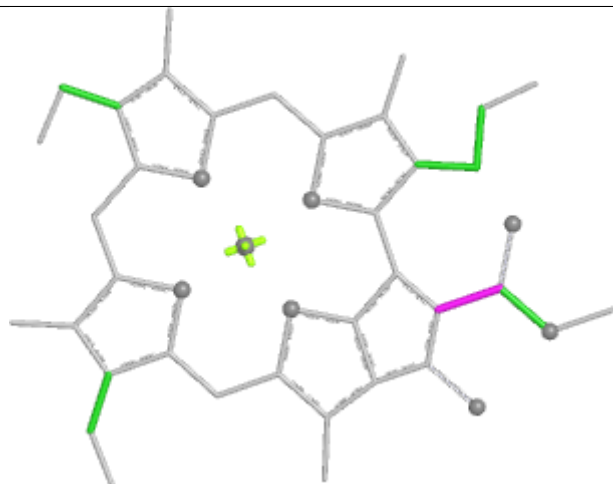
Ligand CLA 7 709



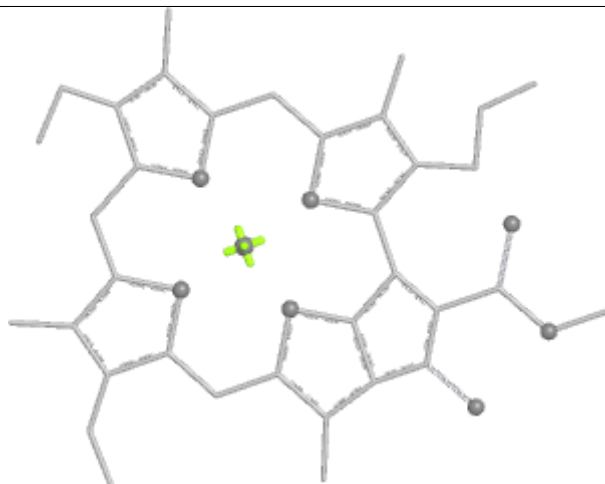
Bond lengths



Bond angles

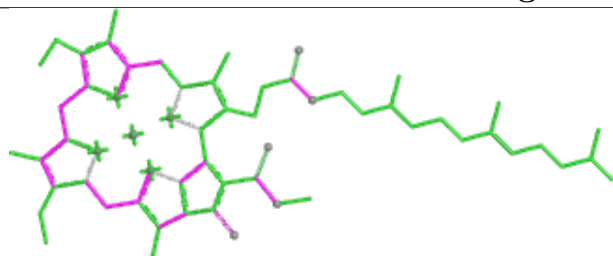


Torsions

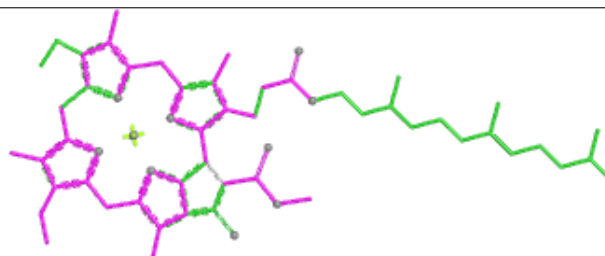


Rings

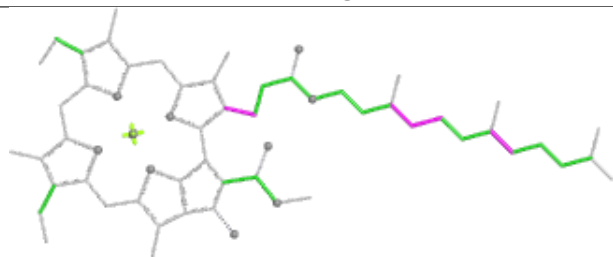
Ligand CLA 9 903



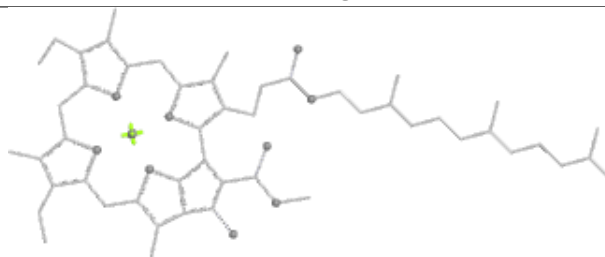
Bond lengths



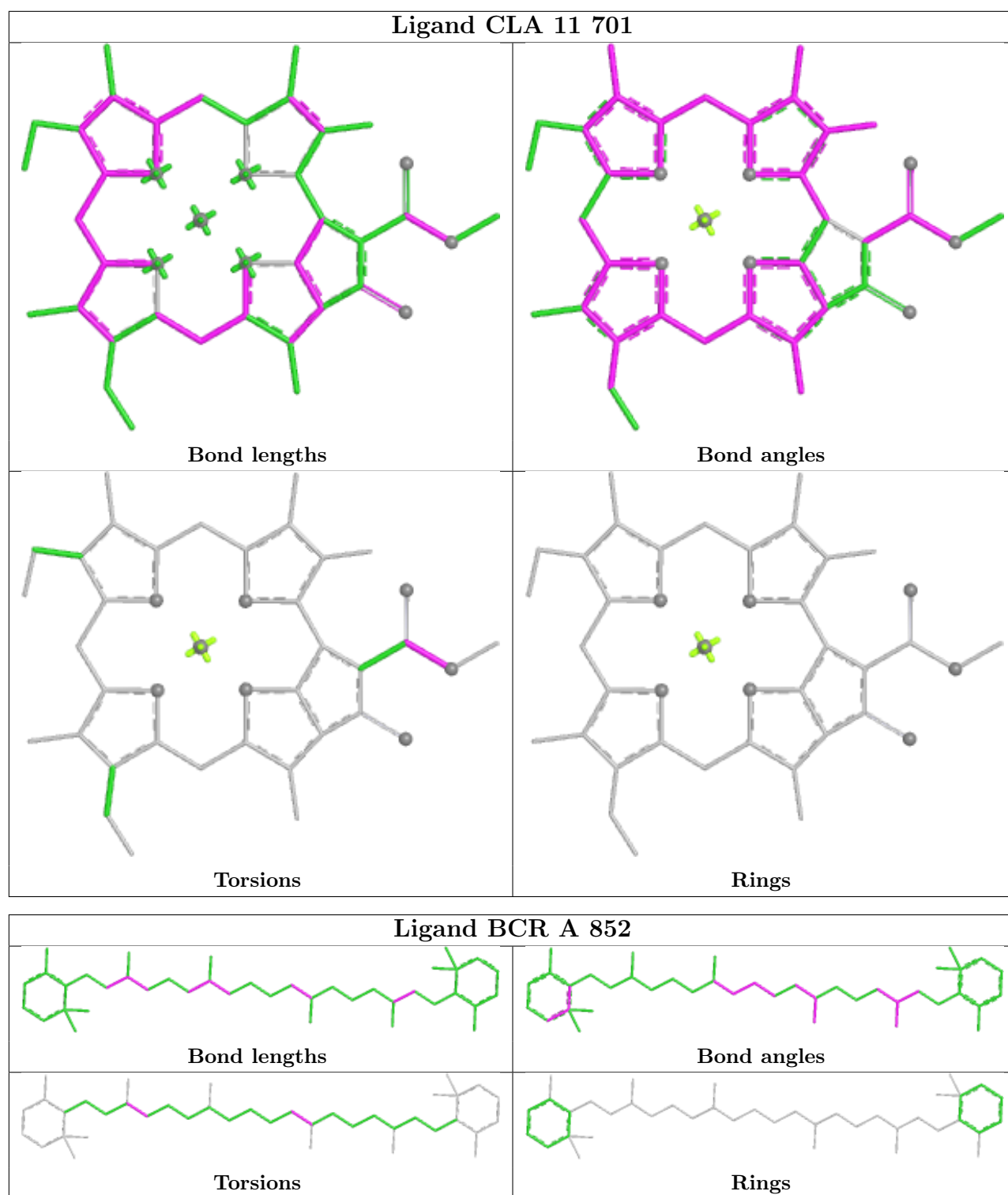
Bond angles



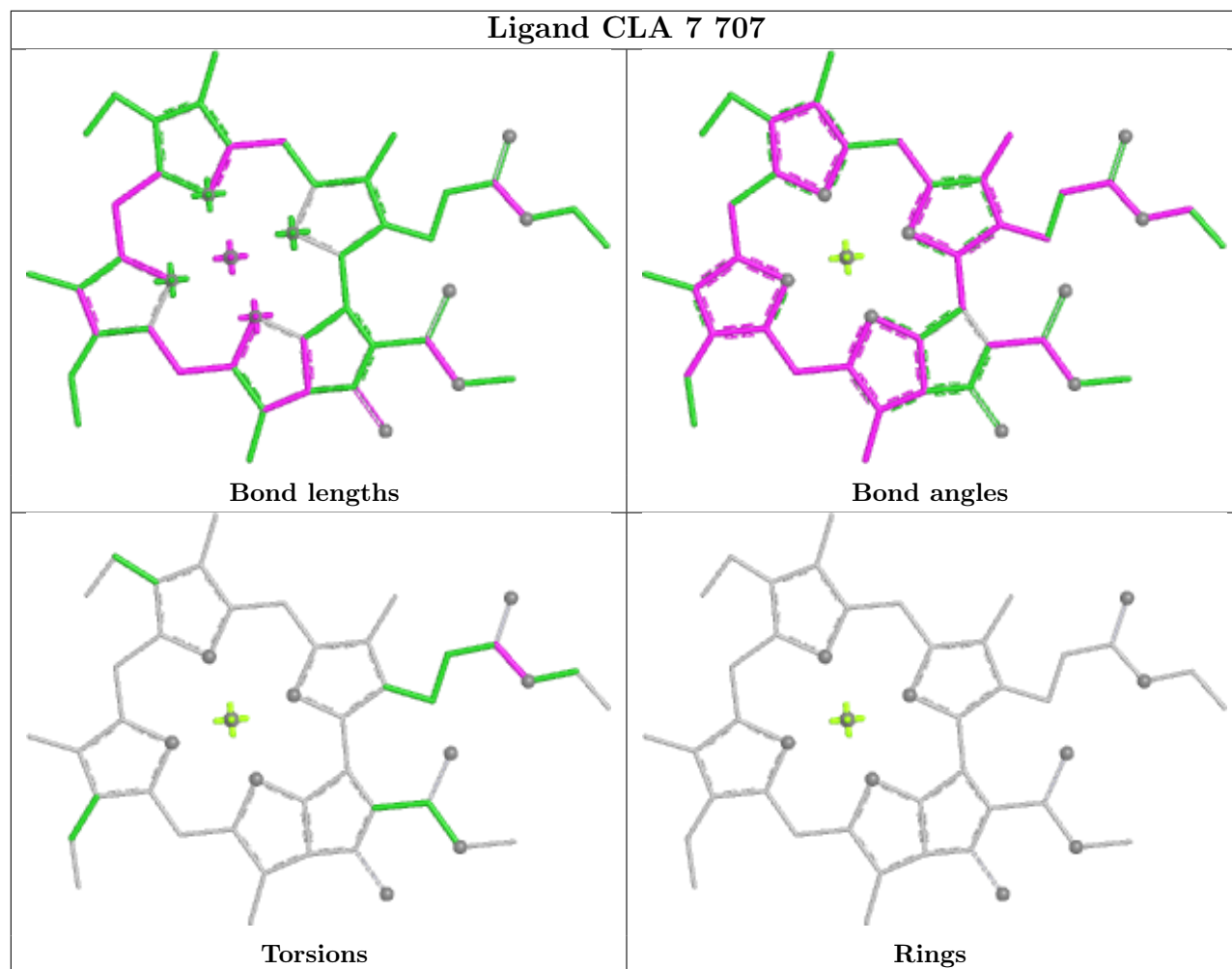
Torsions



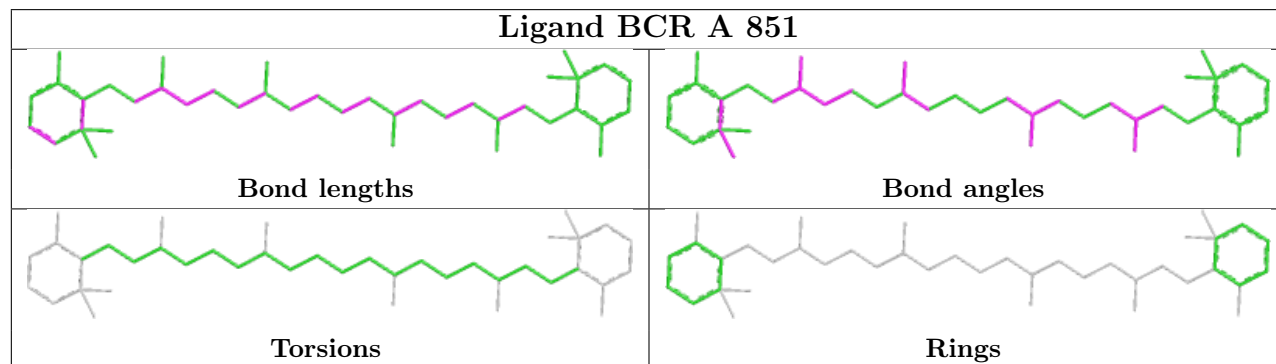
Rings

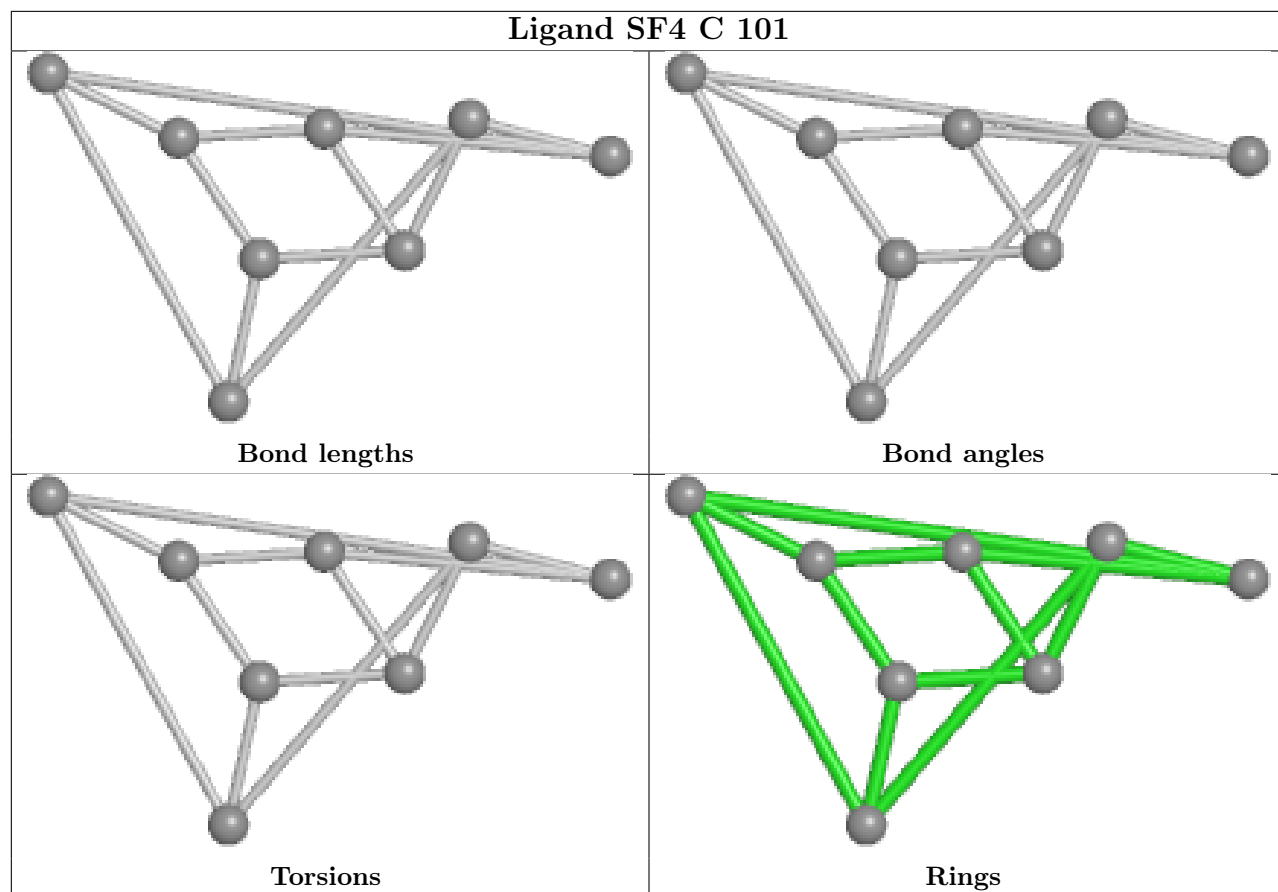


Ligand CLA 7 707

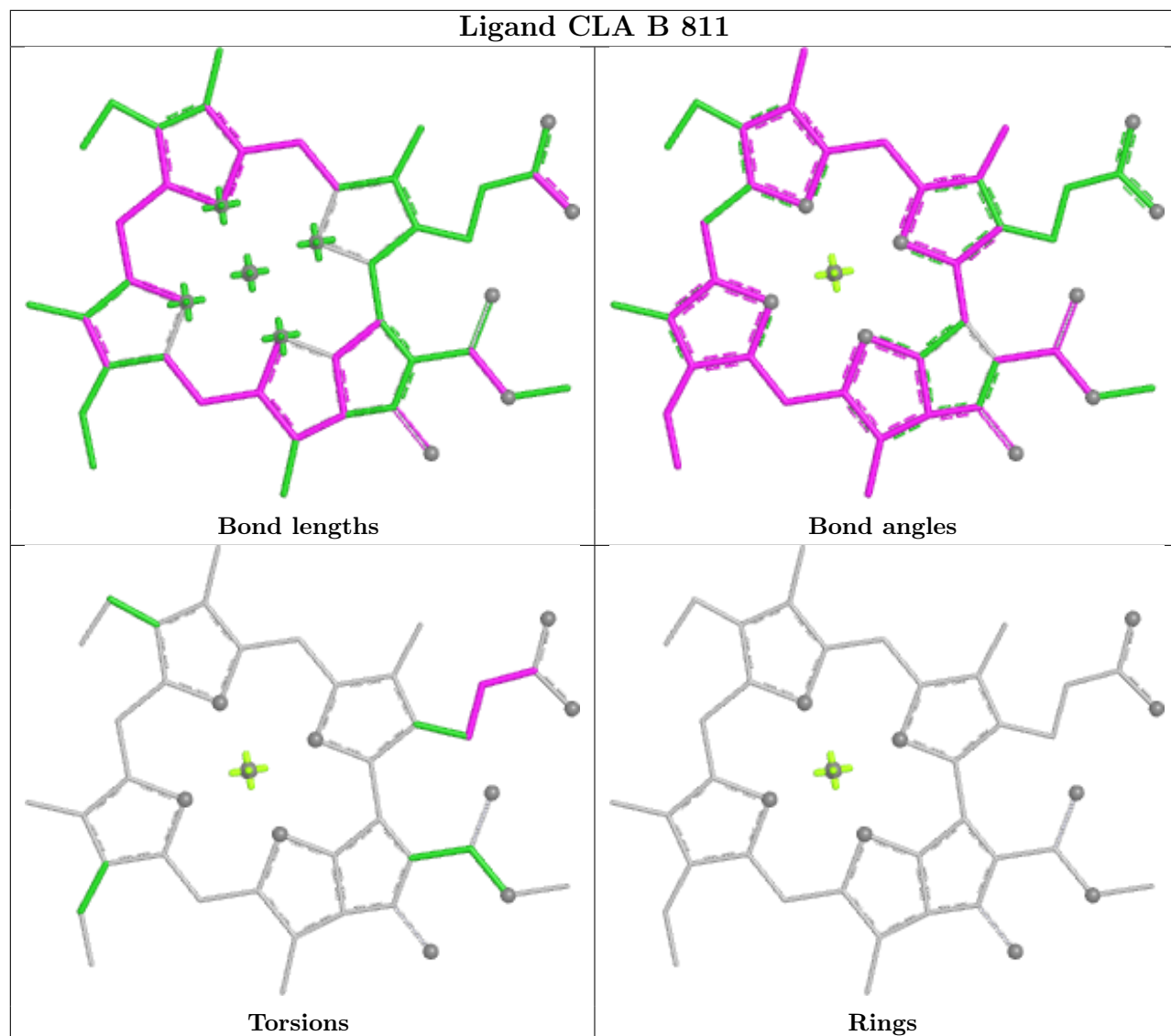


Ligand BCR A 851

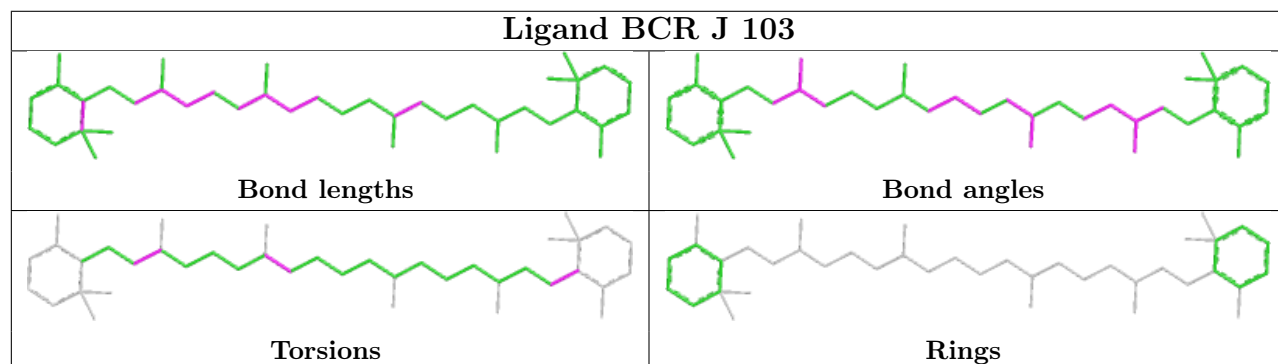


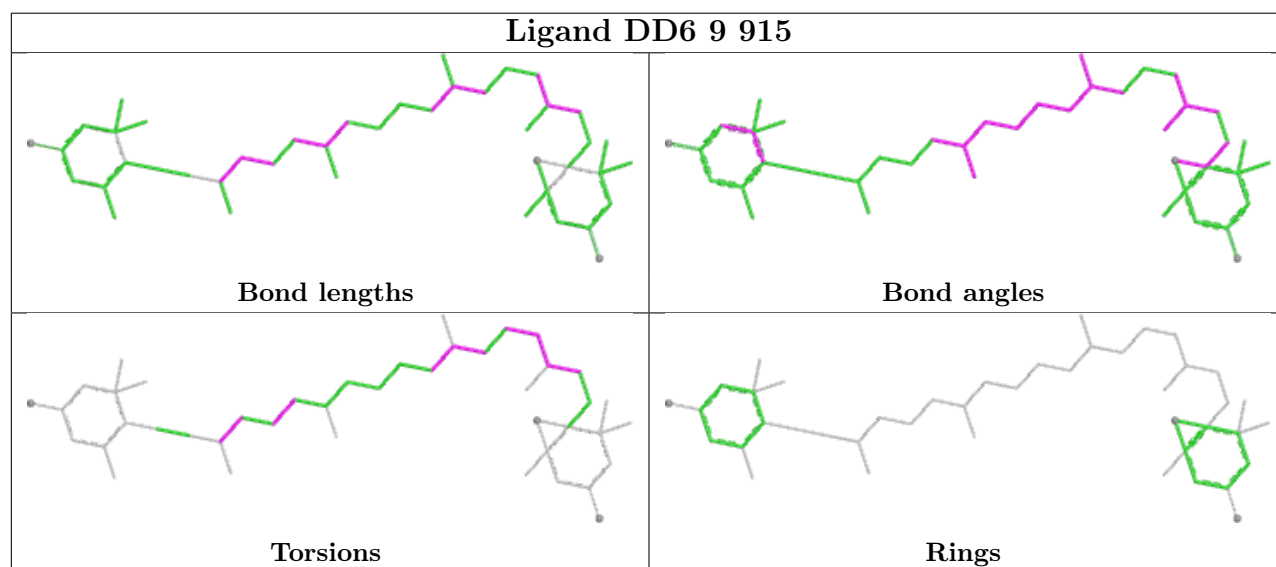
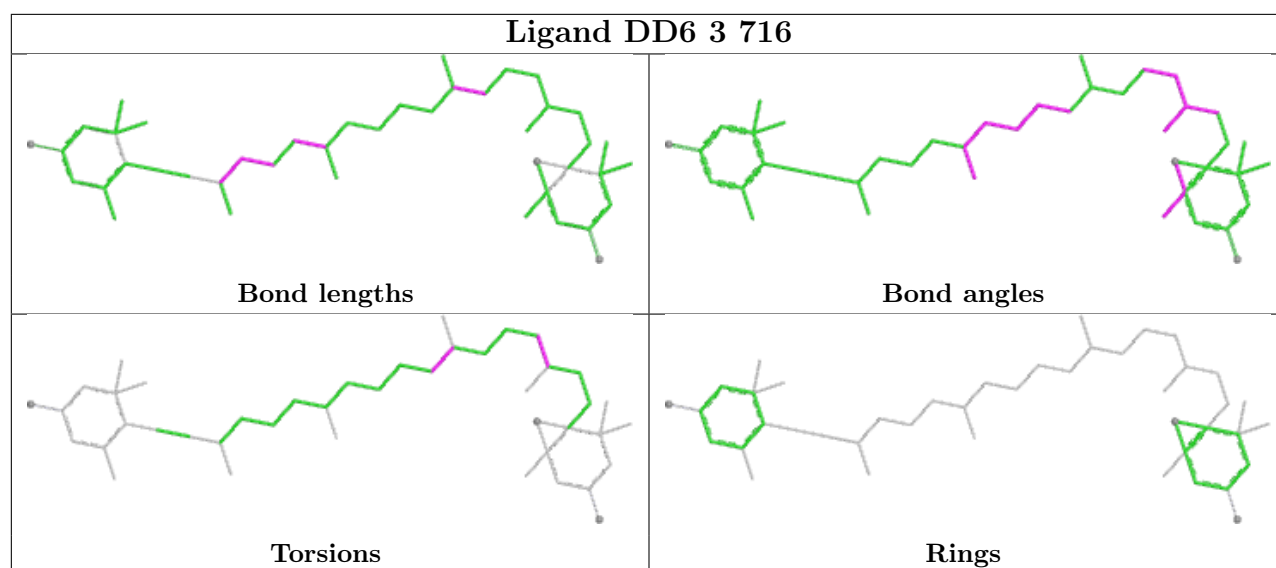


Ligand CLA B 811

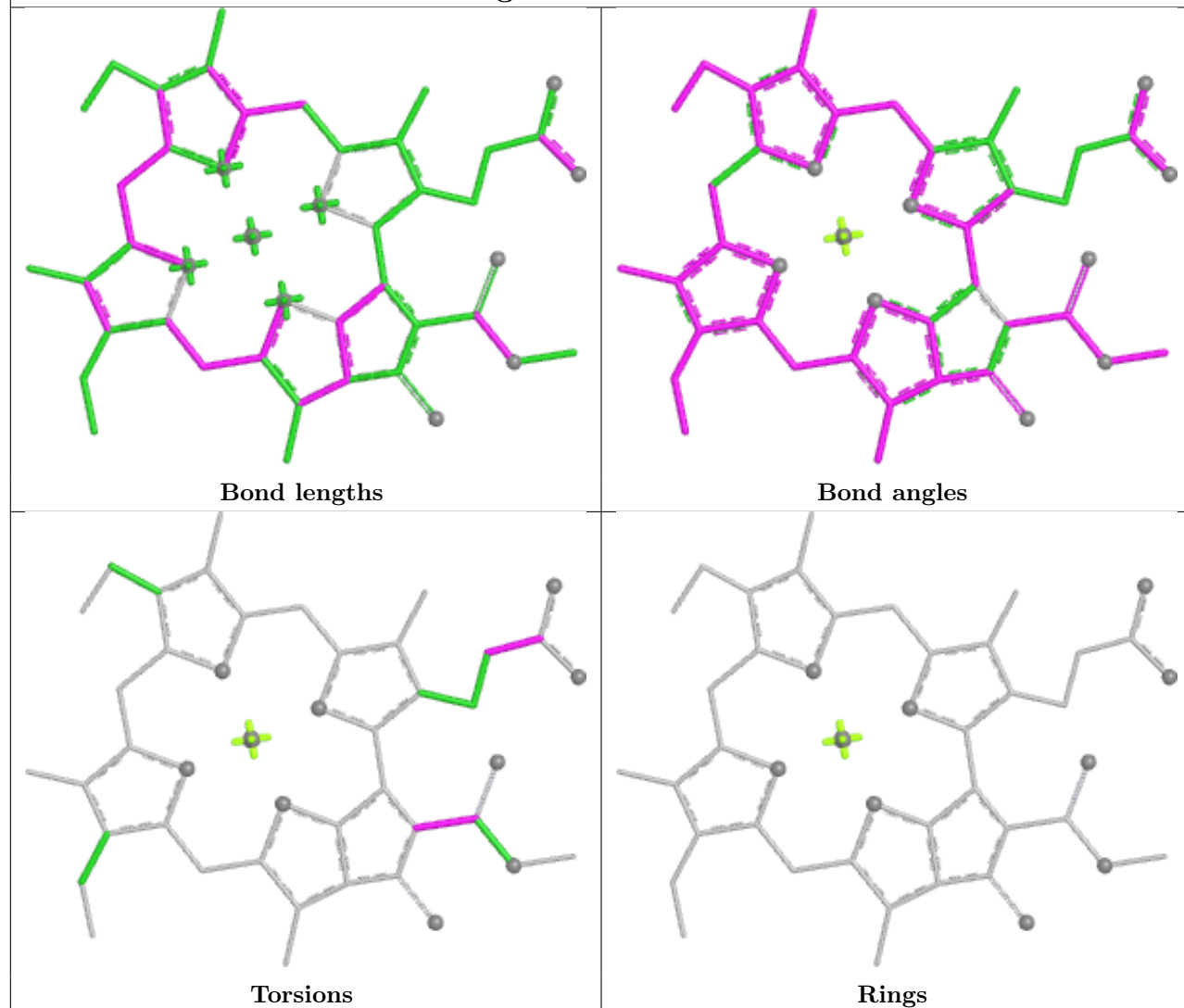


Ligand BCR J 103

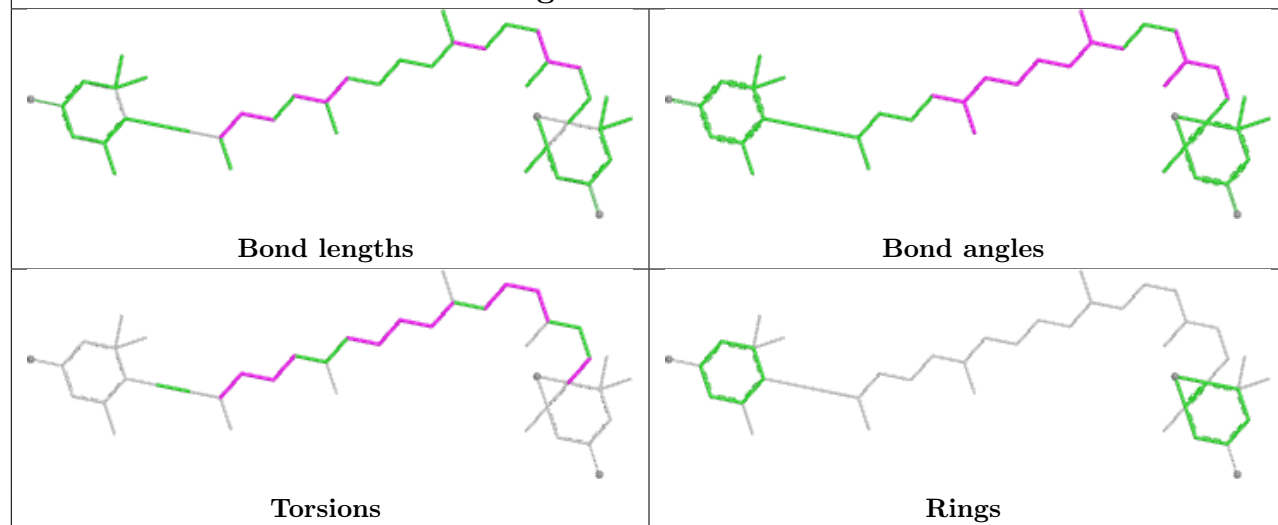




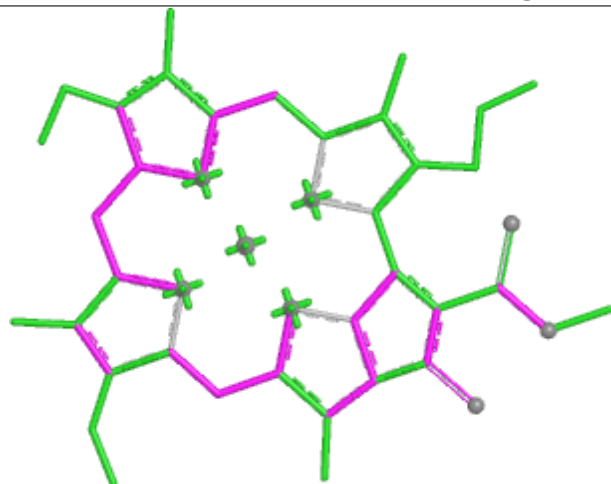
Ligand CLA 1 506



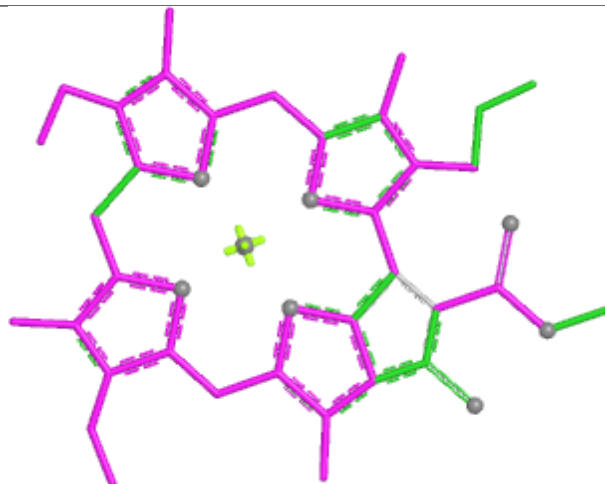
Ligand DD6 1 520



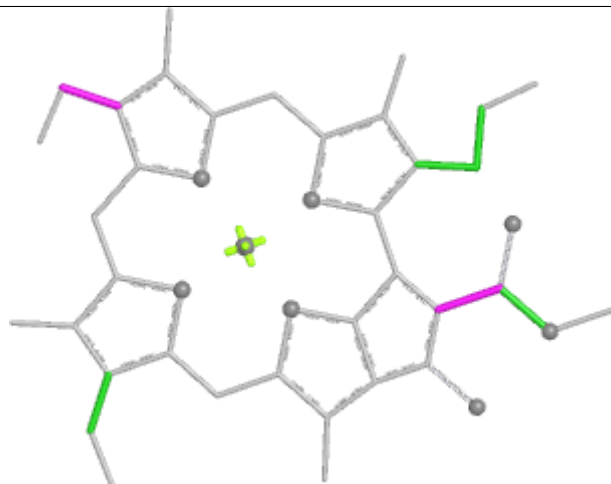
Ligand CLA 8 610



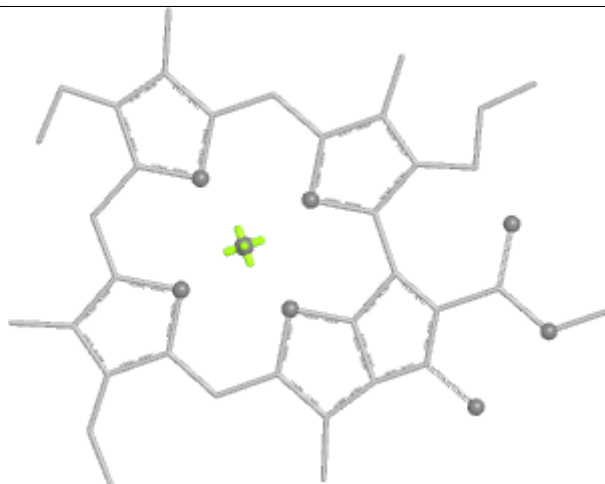
Bond lengths



Bond angles

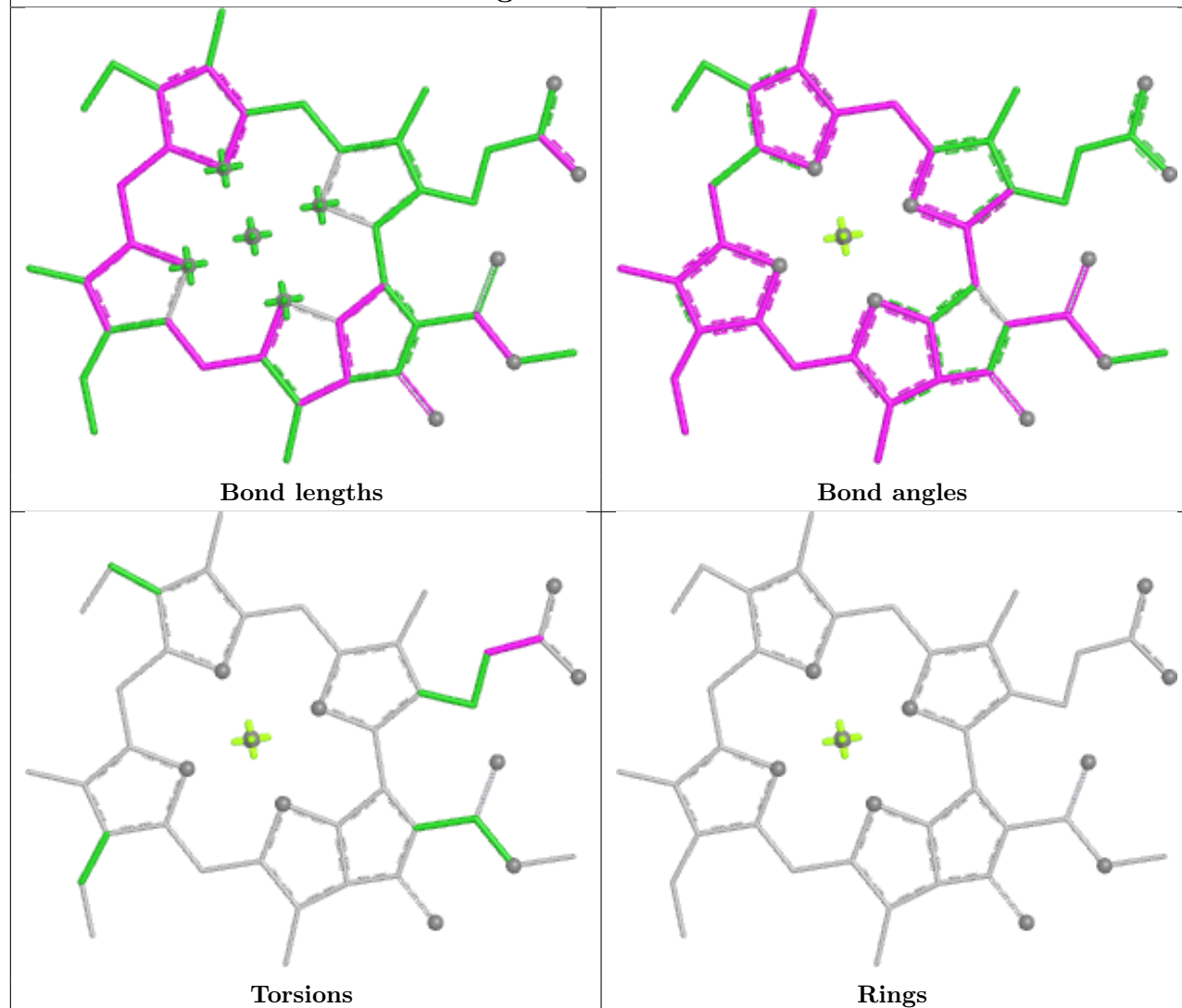


Torsions

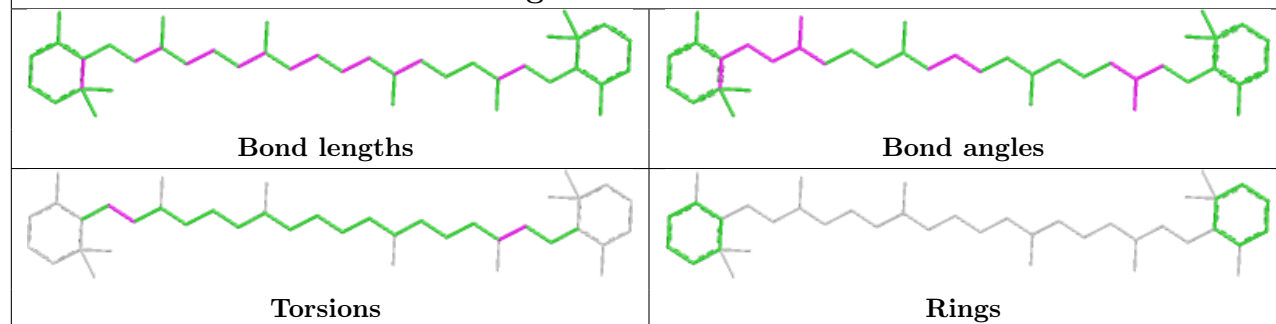


Rings

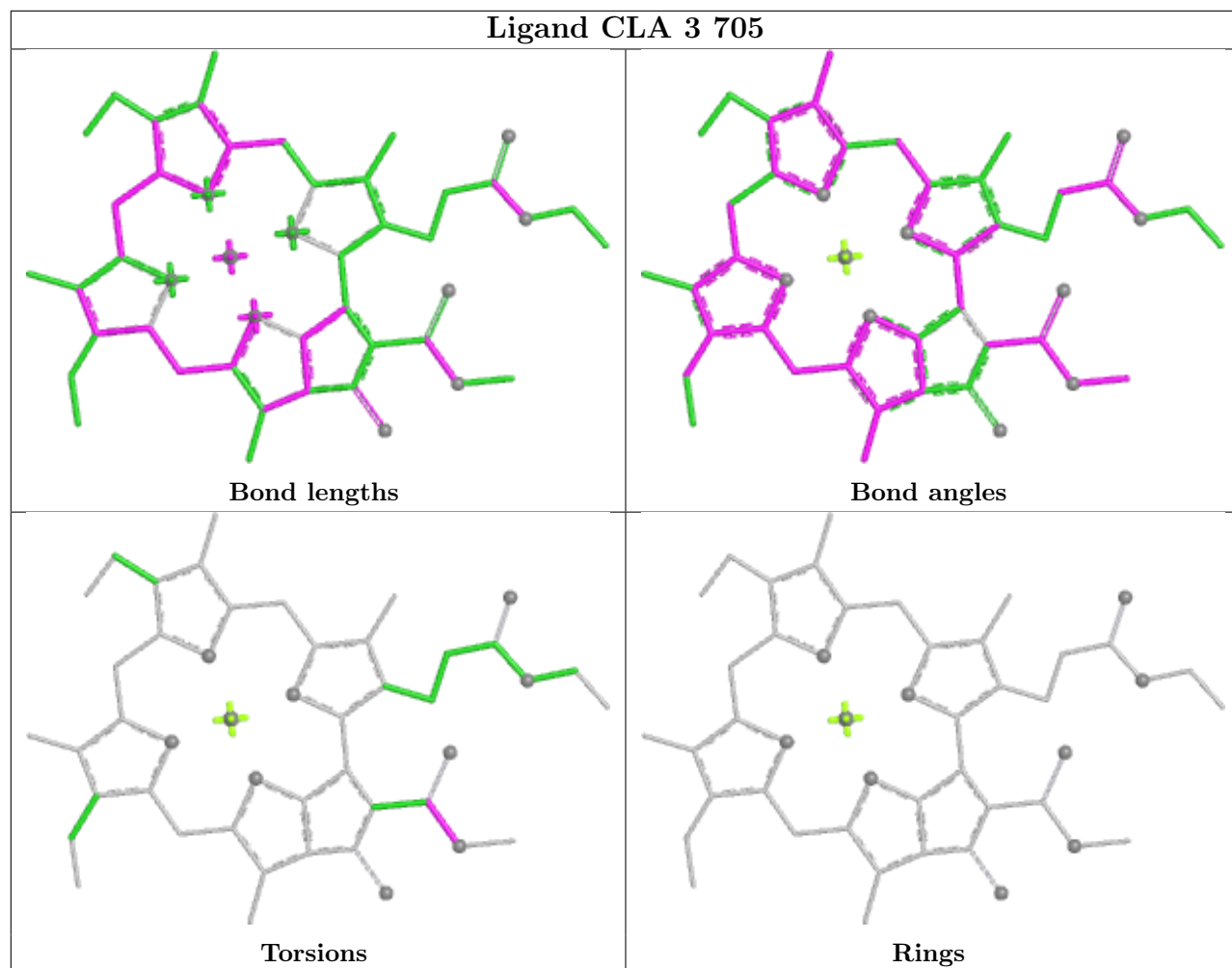
Ligand CLA 7 704



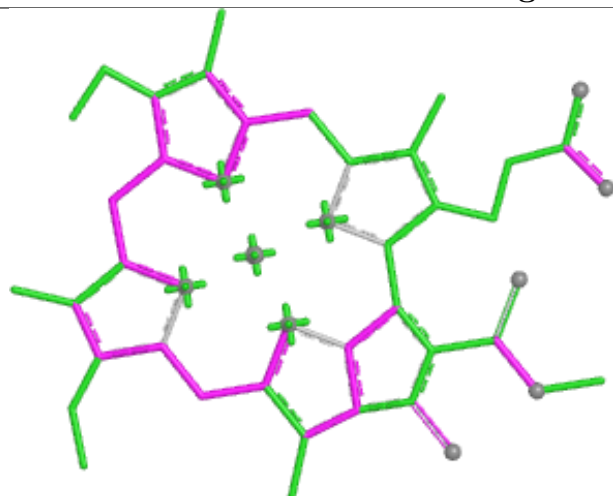
Ligand BCR M 102



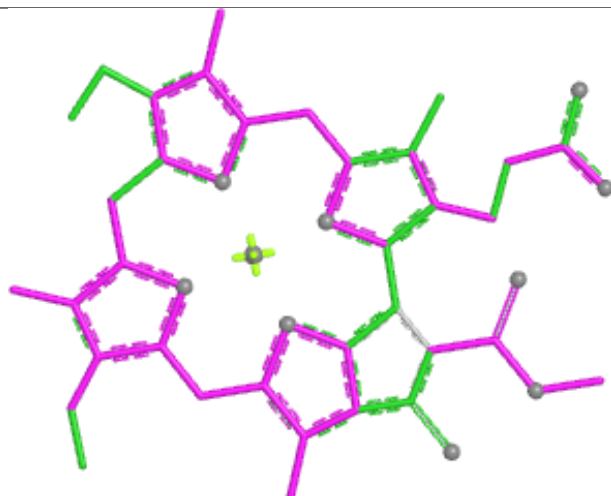
Ligand CLA 3 705



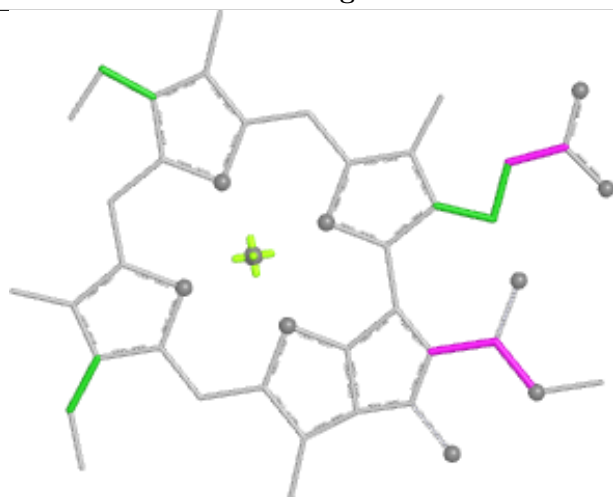
Ligand CLA 3 713



Bond lengths



Bond angles

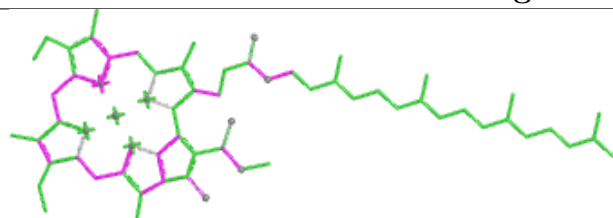


Torsions

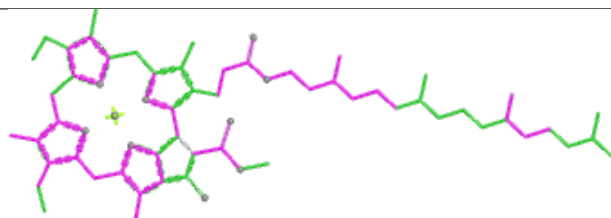


Rings

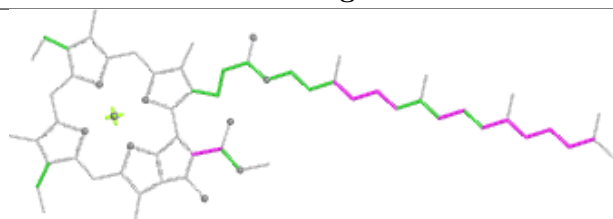
Ligand CLA A 826



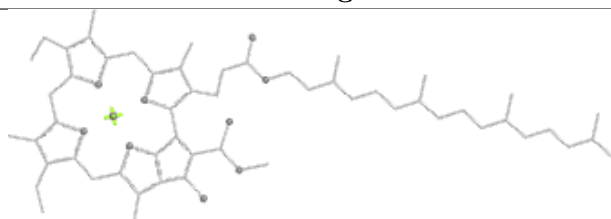
Bond lengths



Bond angles

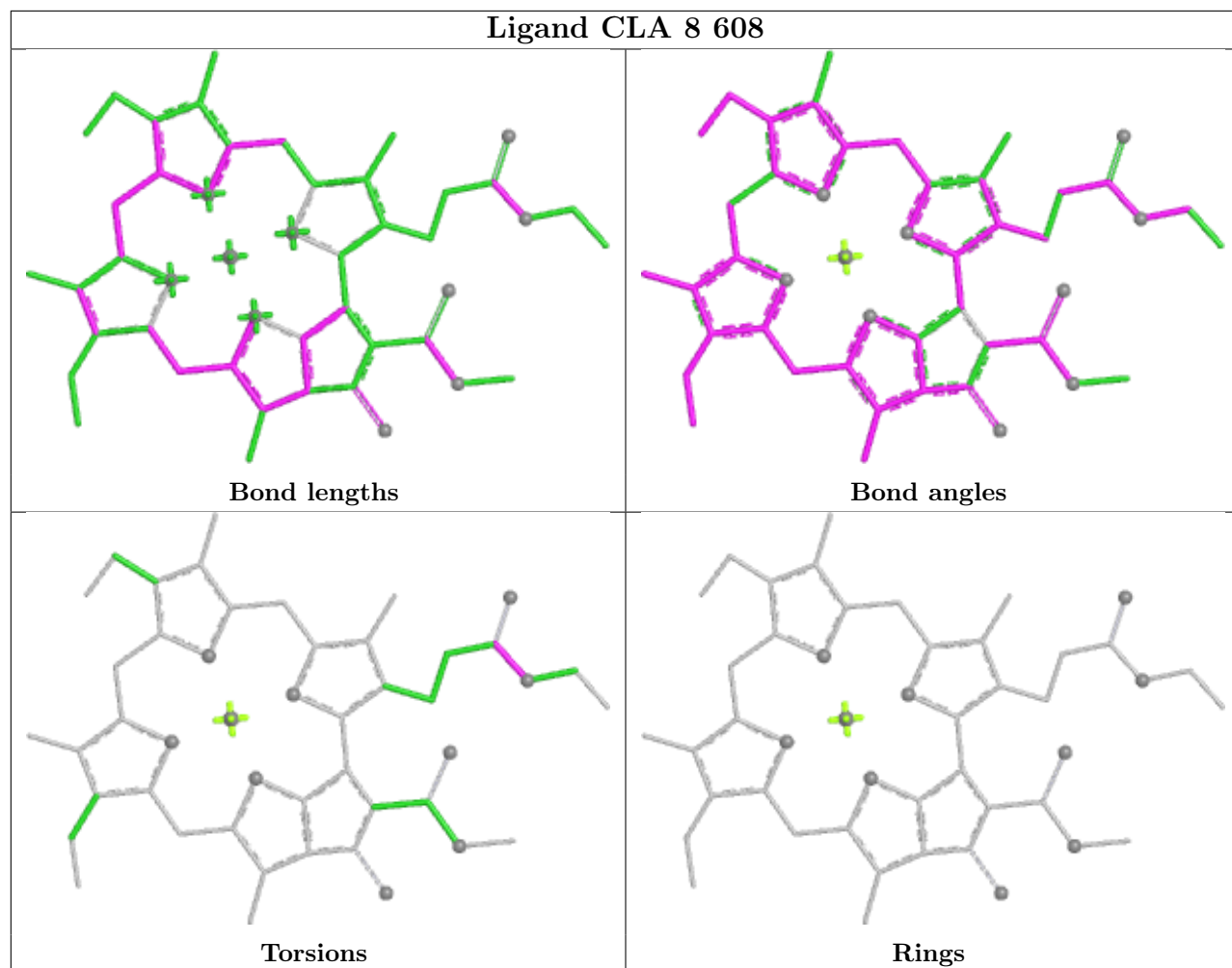


Torsions

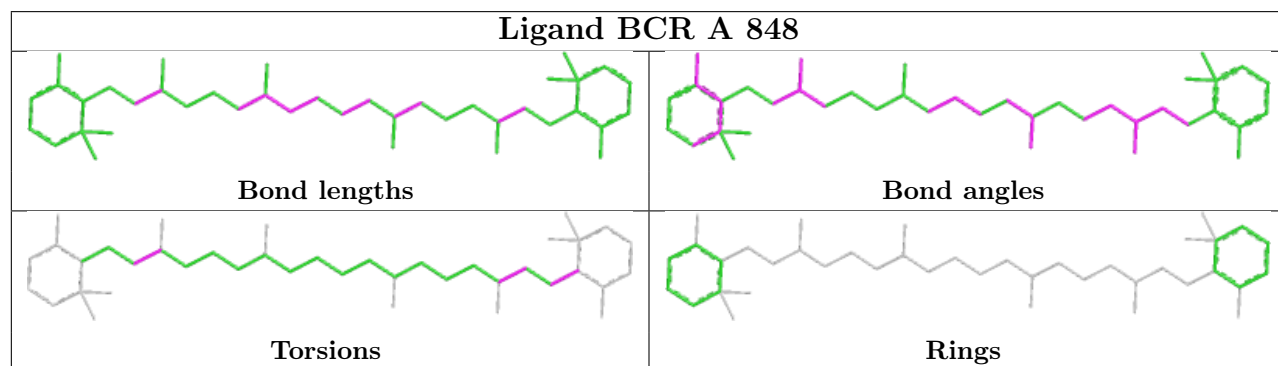


Rings

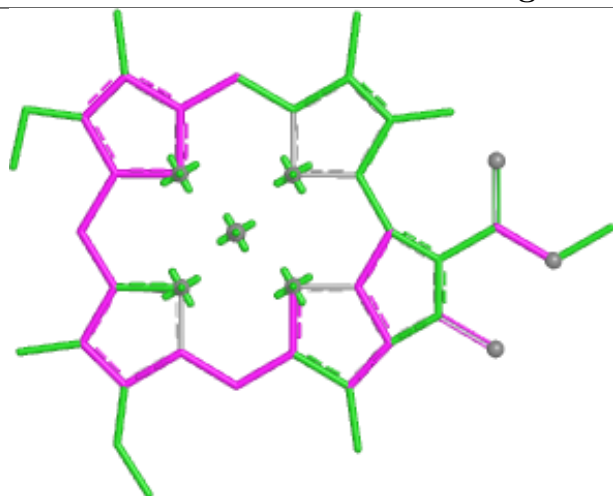
Ligand CLA 8 608



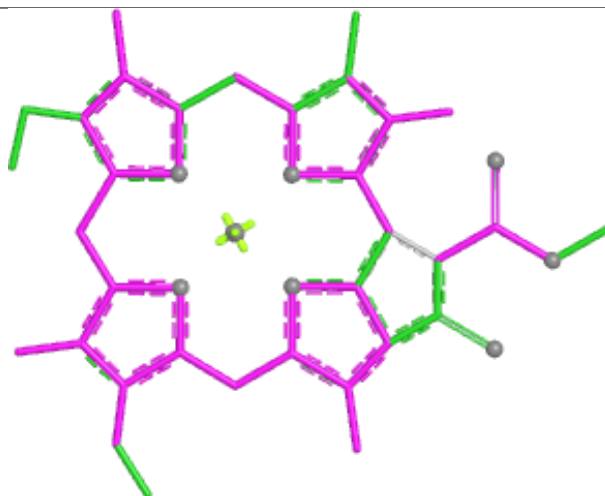
Ligand BCR A 848



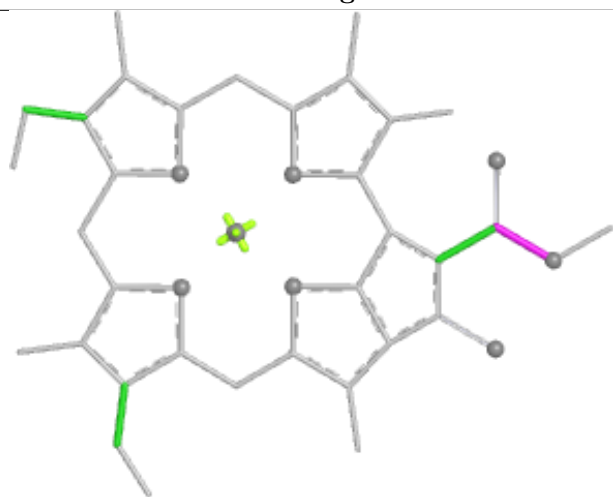
Ligand CLA 4 701



Bond lengths



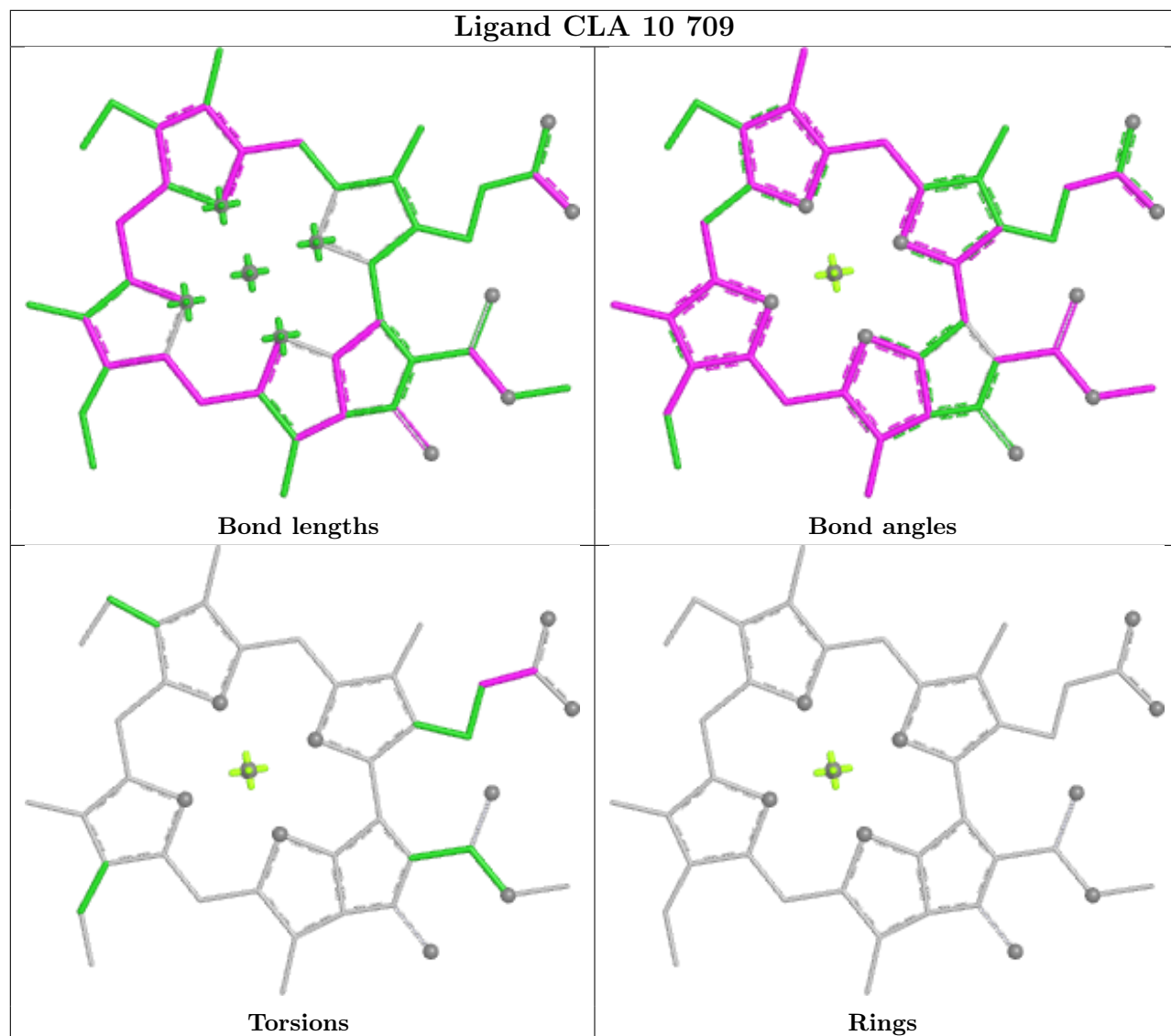
Bond angles



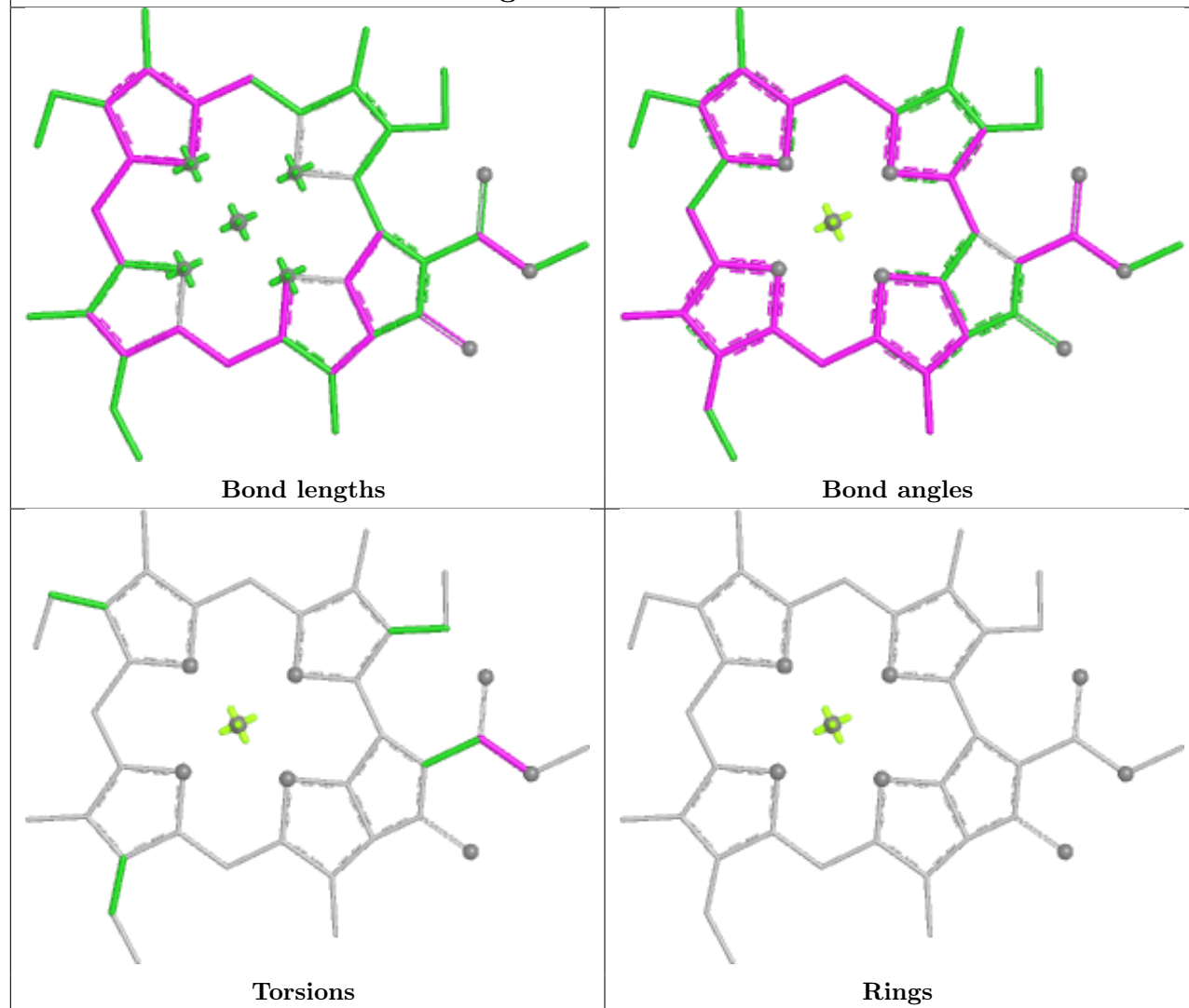
Torsions



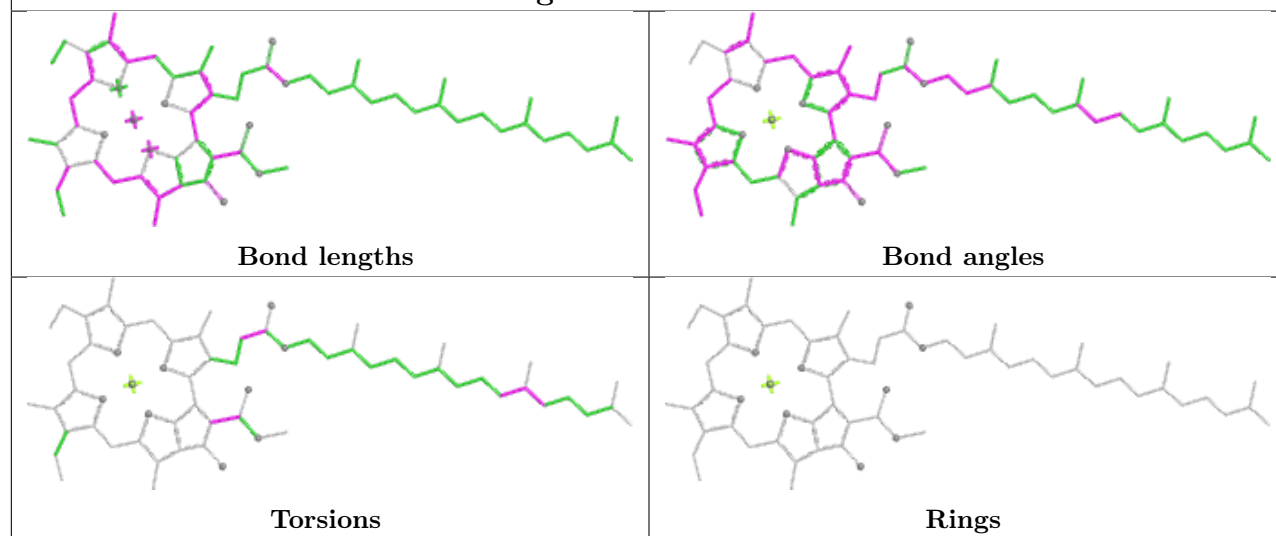
Rings

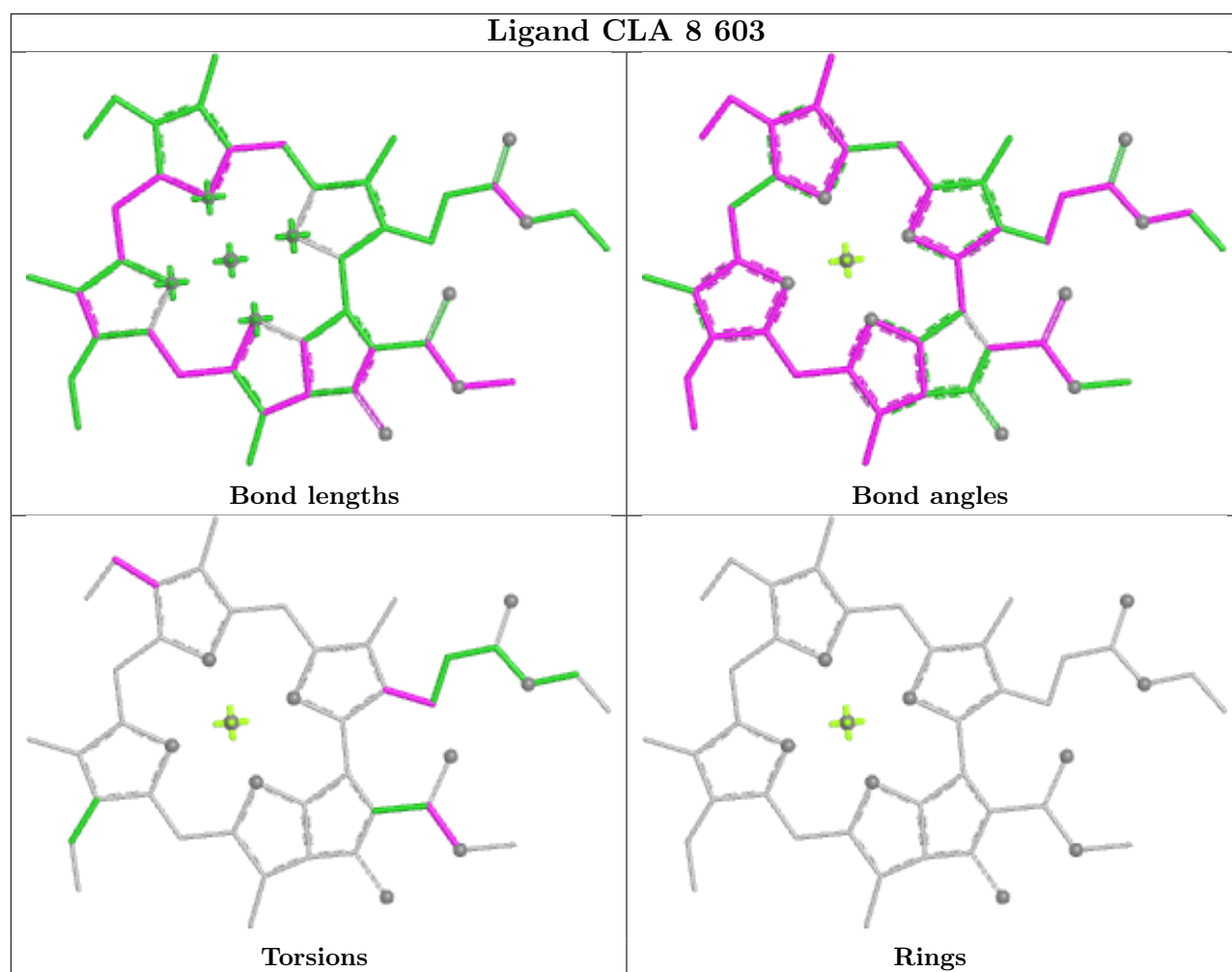


Ligand CLA 1 504



Ligand CL0 A 801





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.

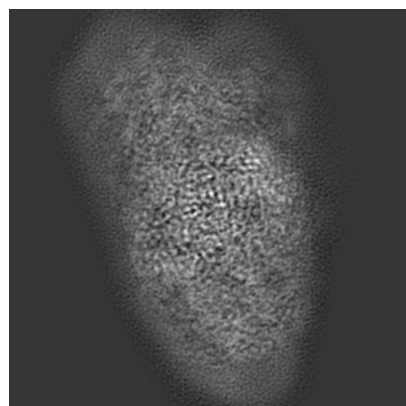
6 Map visualisation [i](#)

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.

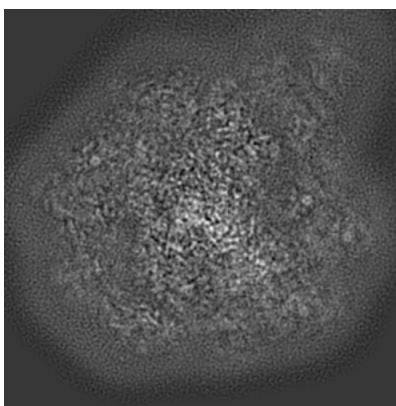
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

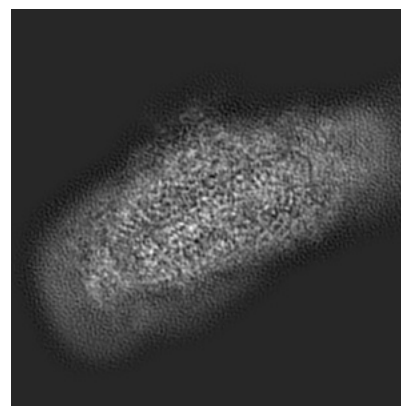
6.1.1 Primary map



X

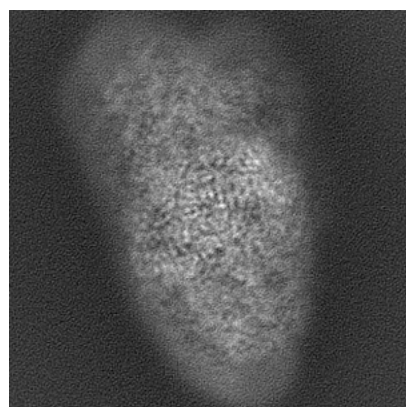


Y

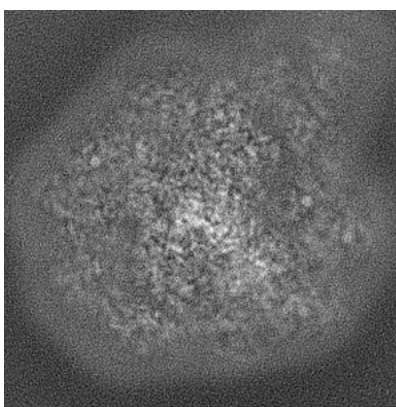


Z

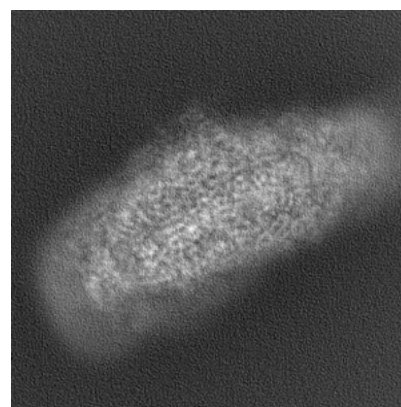
6.1.2 Raw map



X



Y

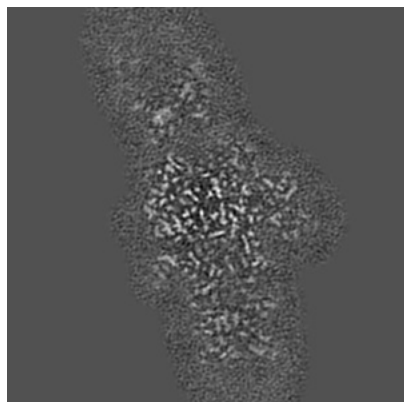


Z

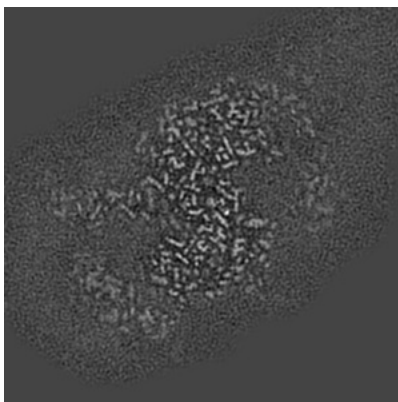
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

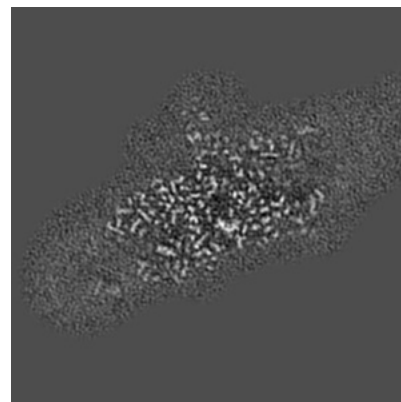
6.2.1 Primary map



X Index: 144

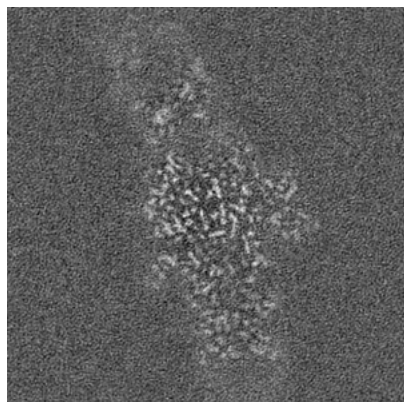


Y Index: 144

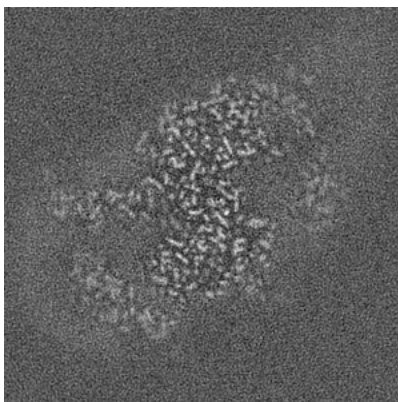


Z Index: 144

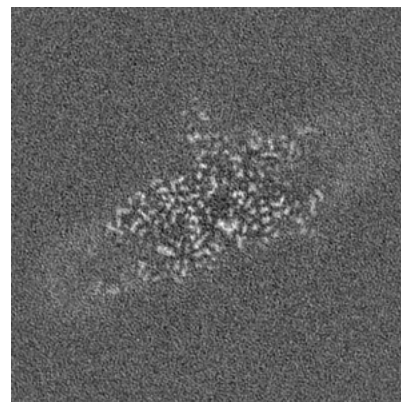
6.2.2 Raw map



X Index: 144



Y Index: 144

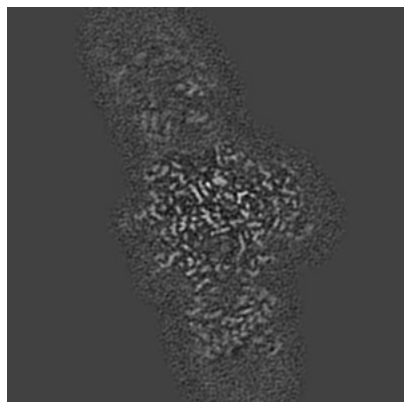


Z Index: 144

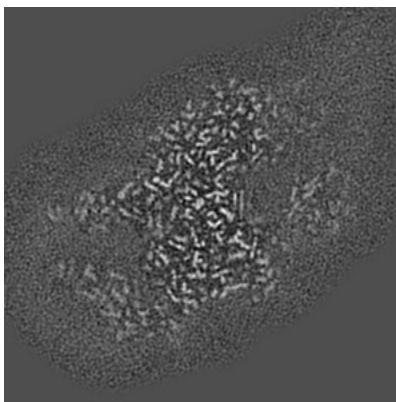
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

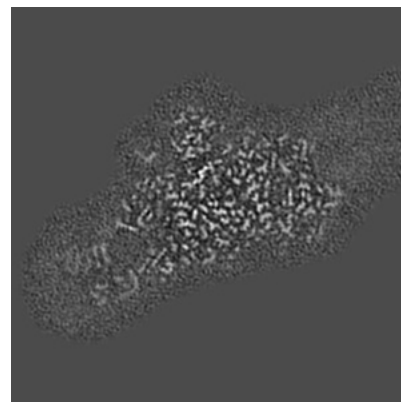
6.3.1 Primary map



X Index: 139

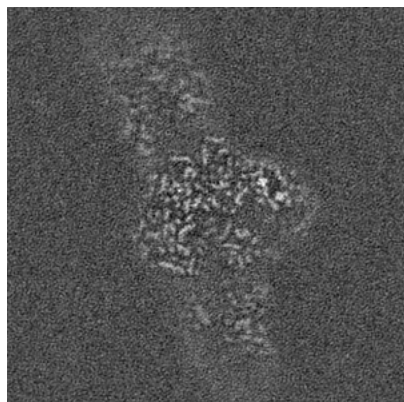


Y Index: 139

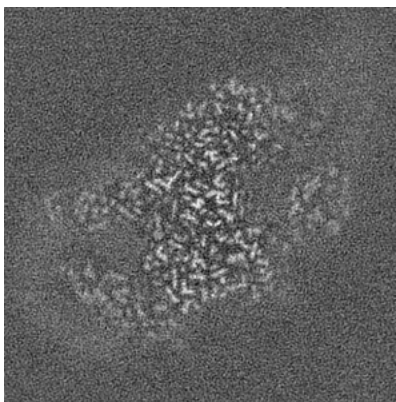


Z Index: 154

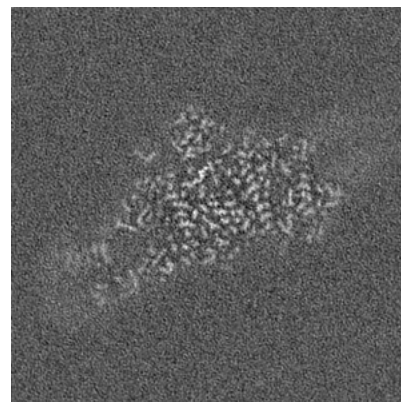
6.3.2 Raw map



X Index: 129



Y Index: 140

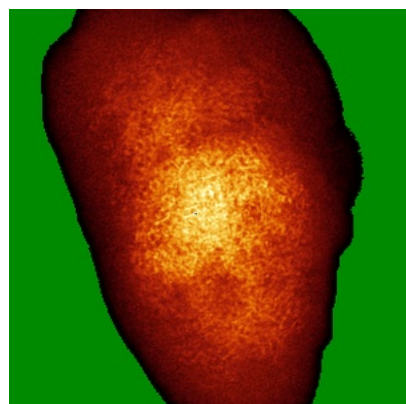


Z Index: 154

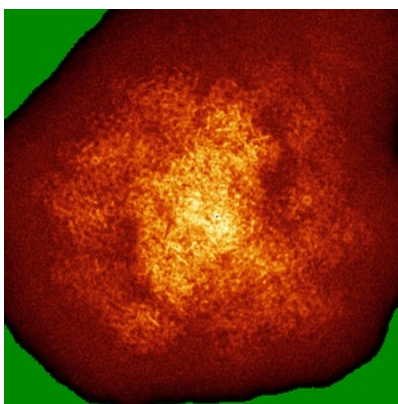
The images above show the largest variance slices of the map in three orthogonal directions.

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

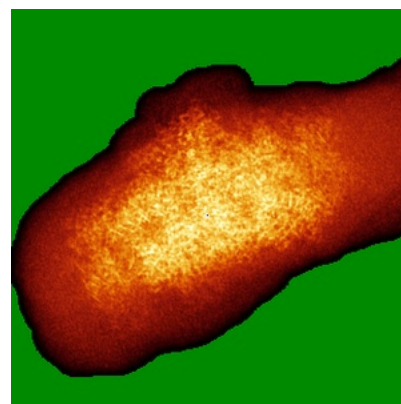
6.4.1 Primary map



X

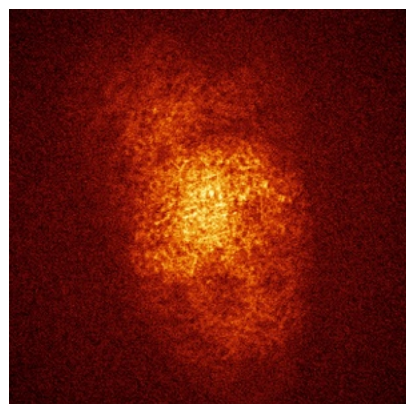


Y

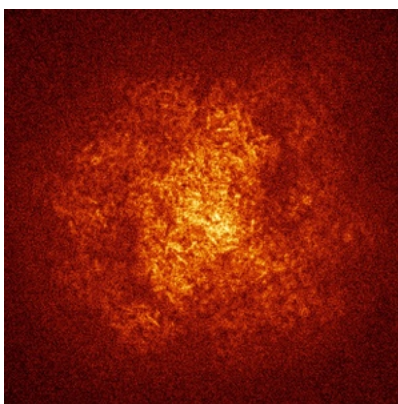


Z

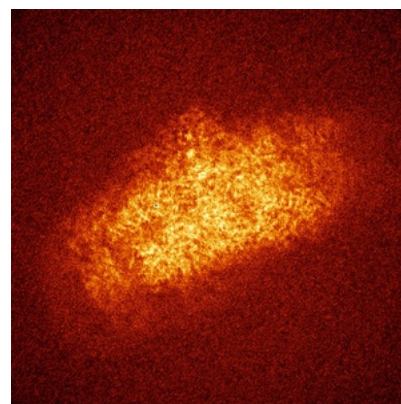
6.4.2 Raw map



X



Y

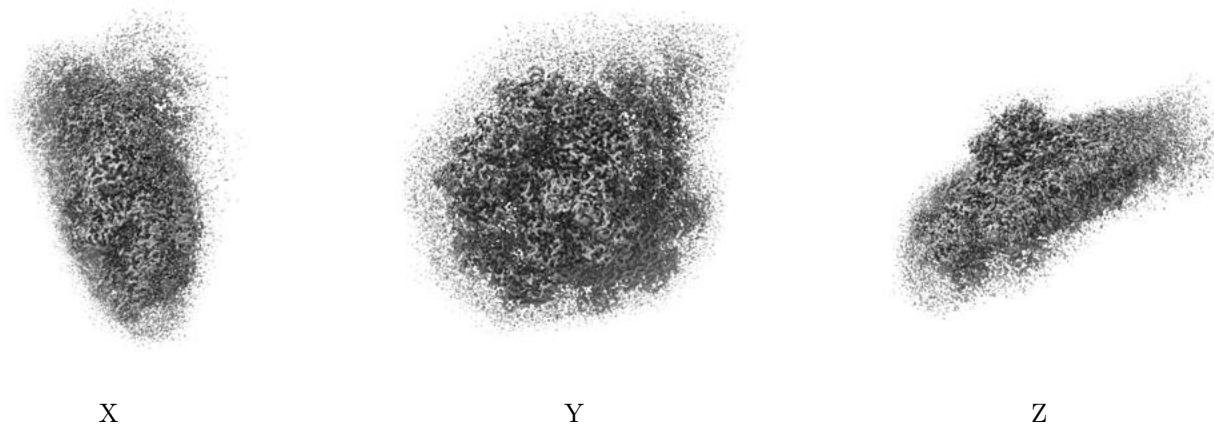


Z

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.

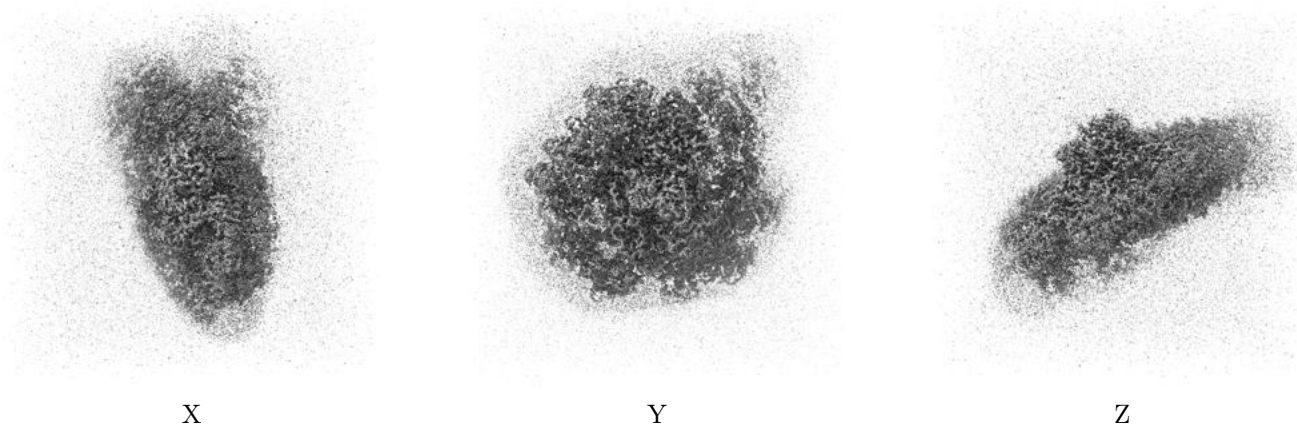
6.5 Orthogonal surface views [i](#)

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.

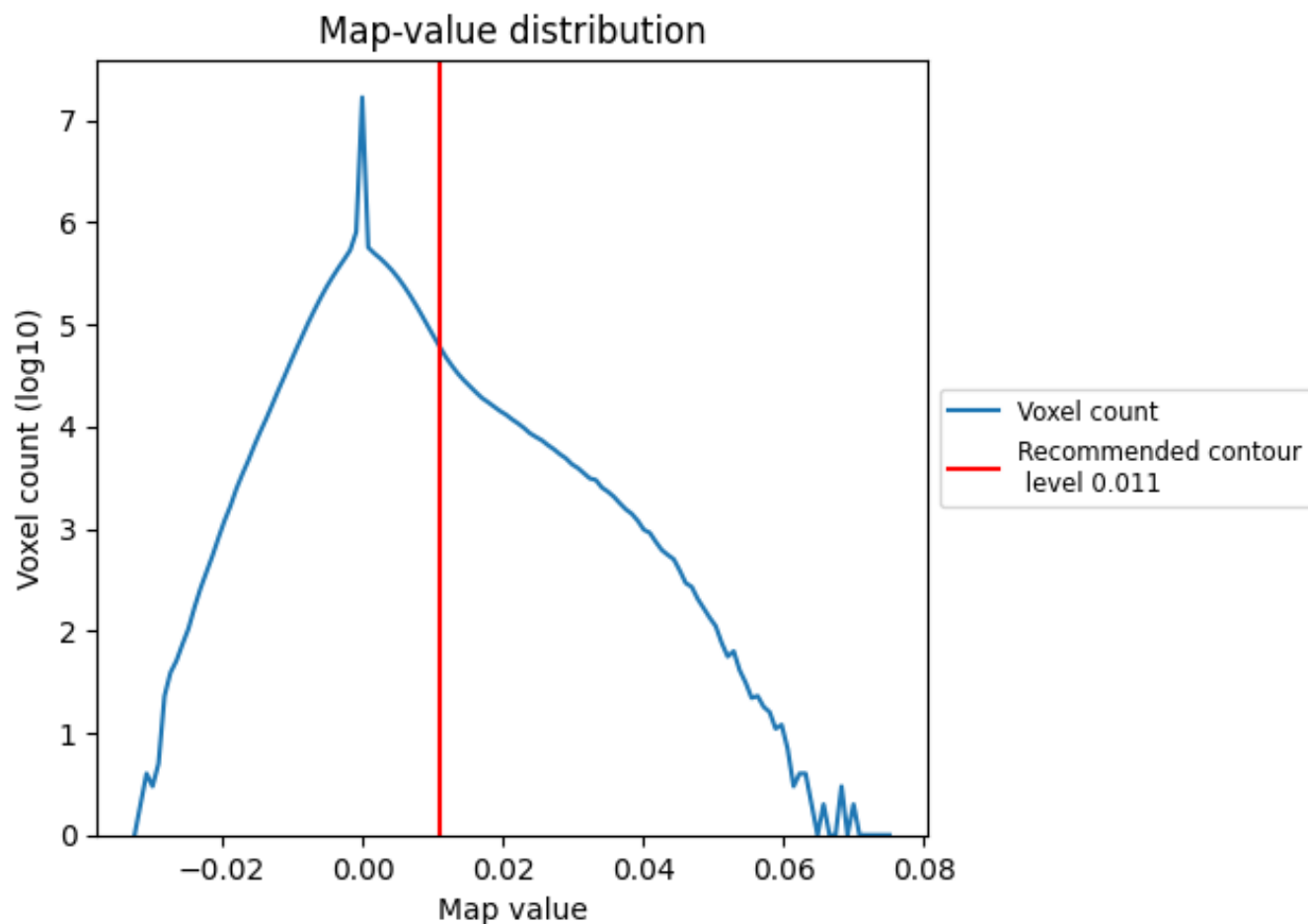
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

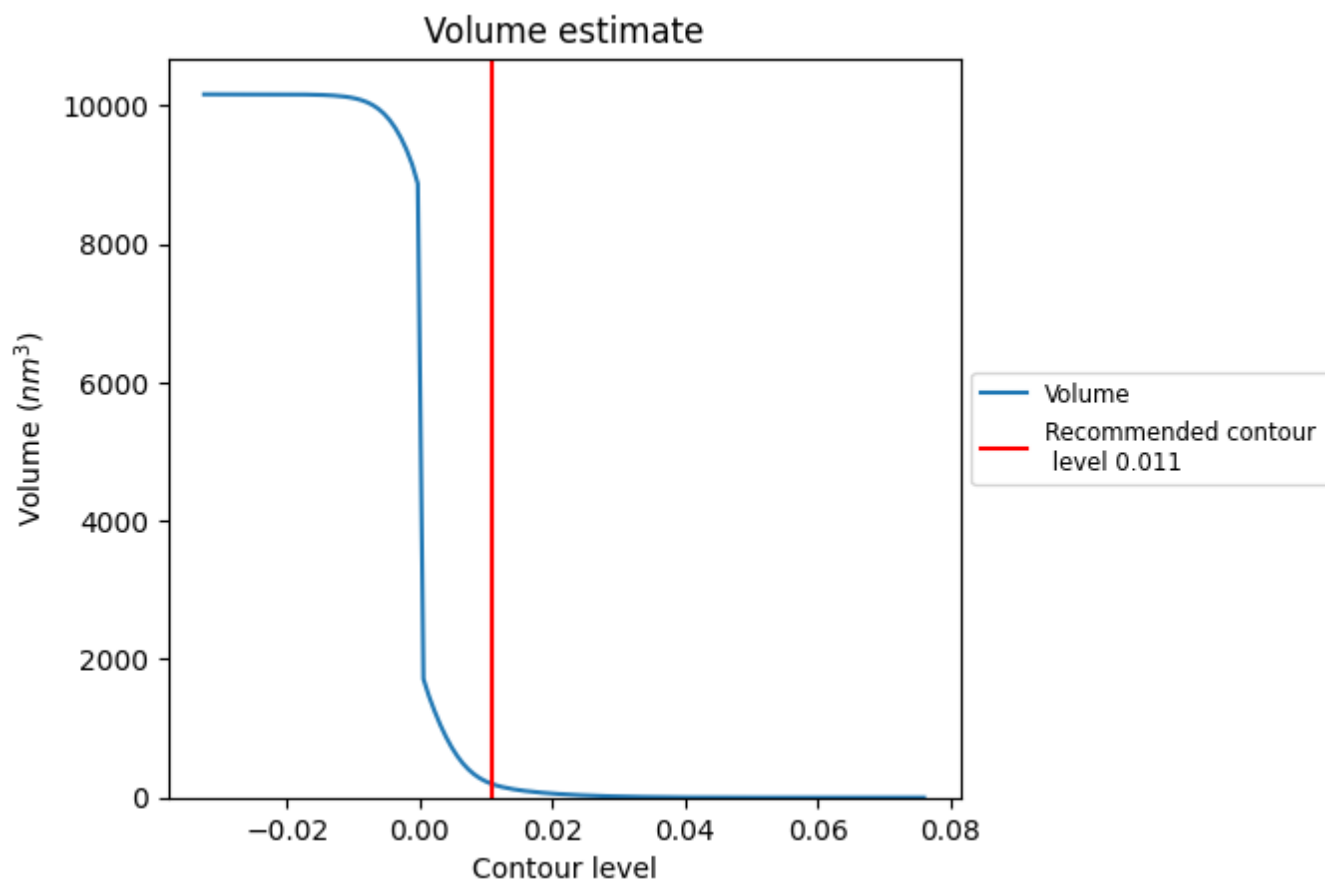
This section contains the results of statistical analysis of the map.

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.

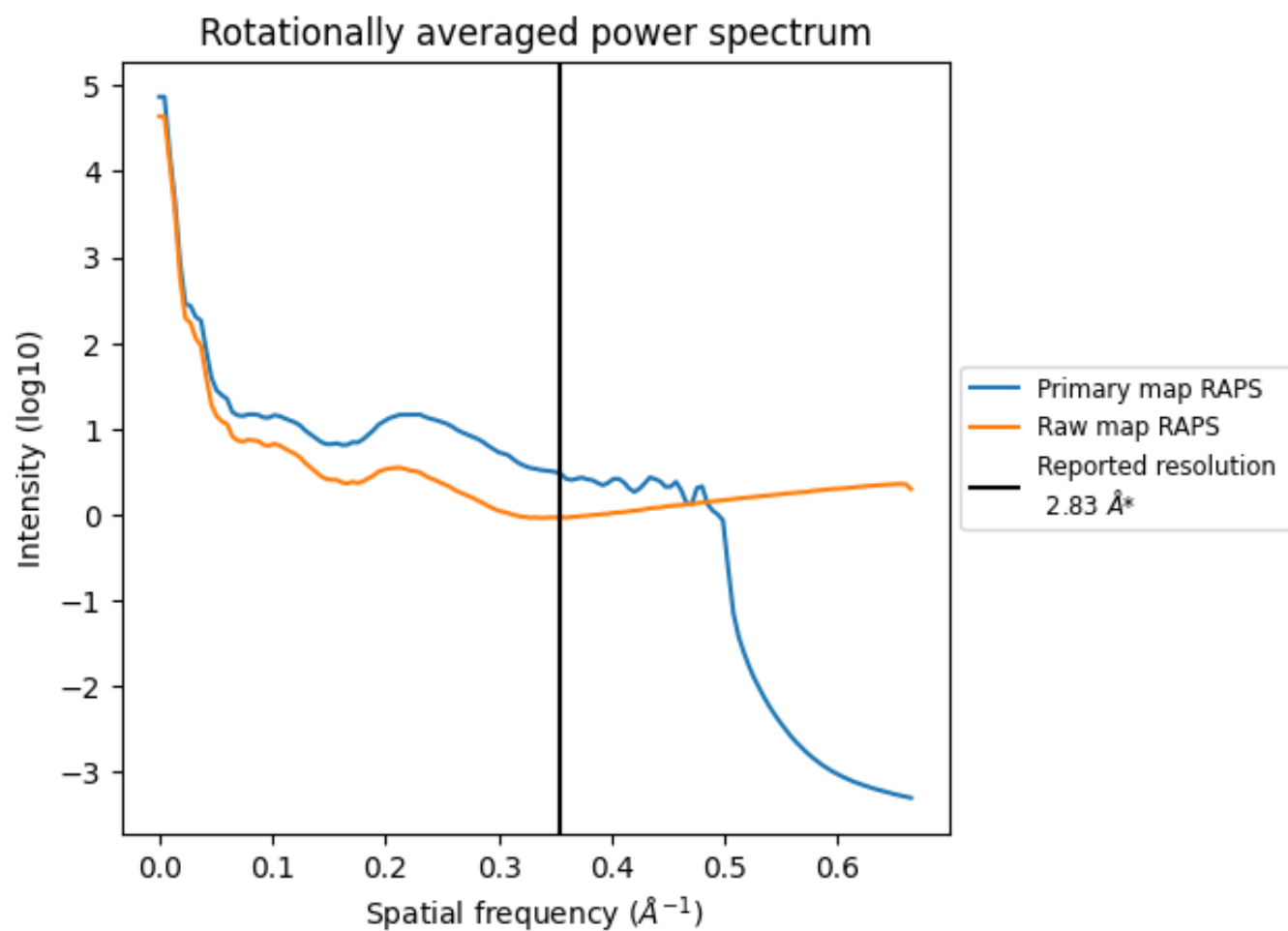
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; 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 ⓘ

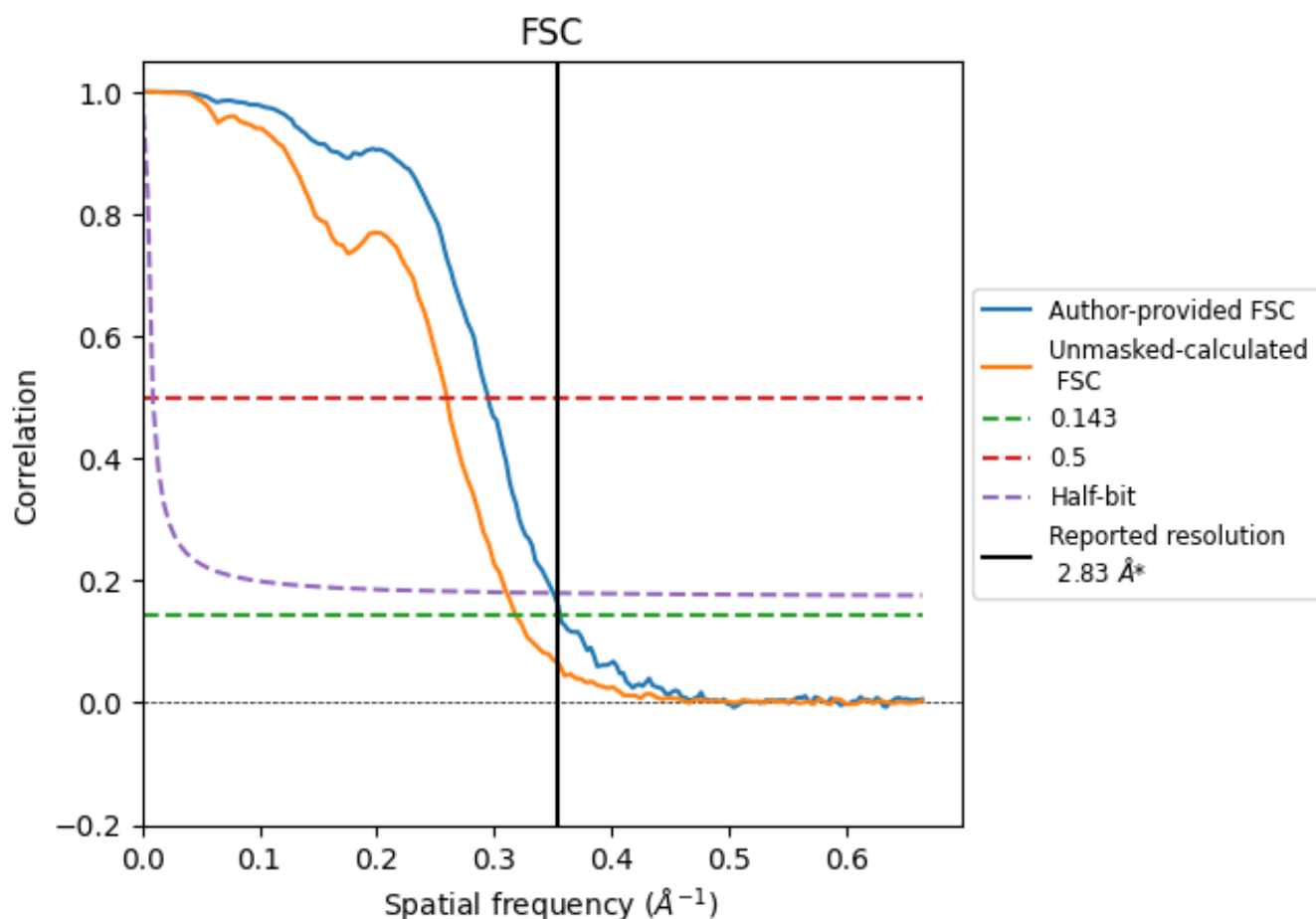


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

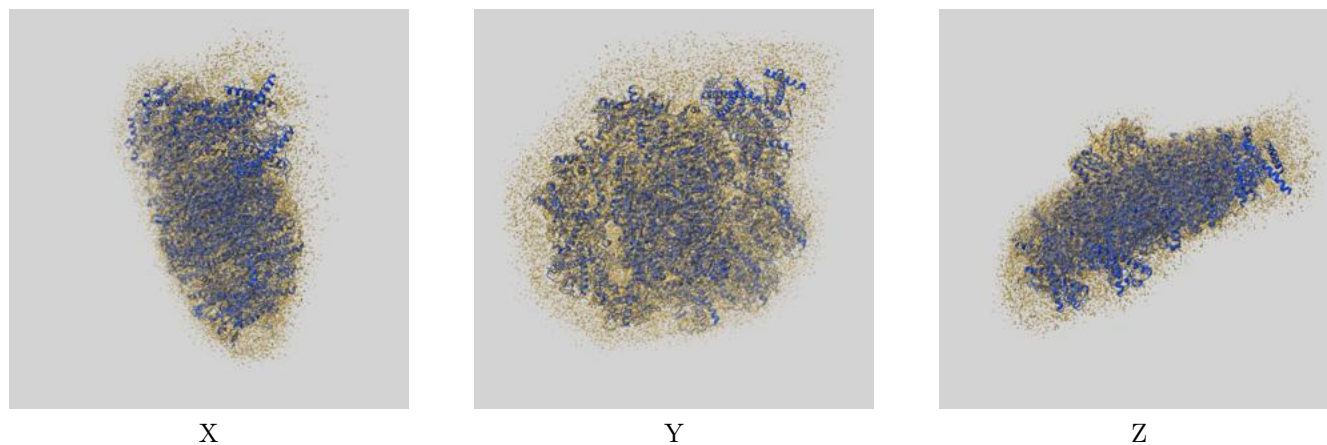
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.81	3.39	2.85
Unmasked-calculated*	3.14	3.85	3.22

*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](#)

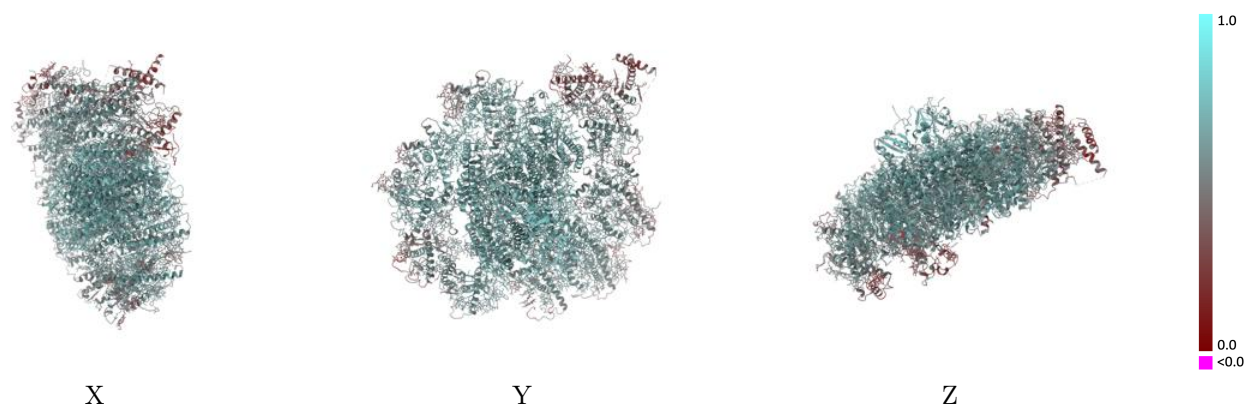
This section contains information regarding the fit between EMDB map EMD-65026 and PDB model 9VFJ. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



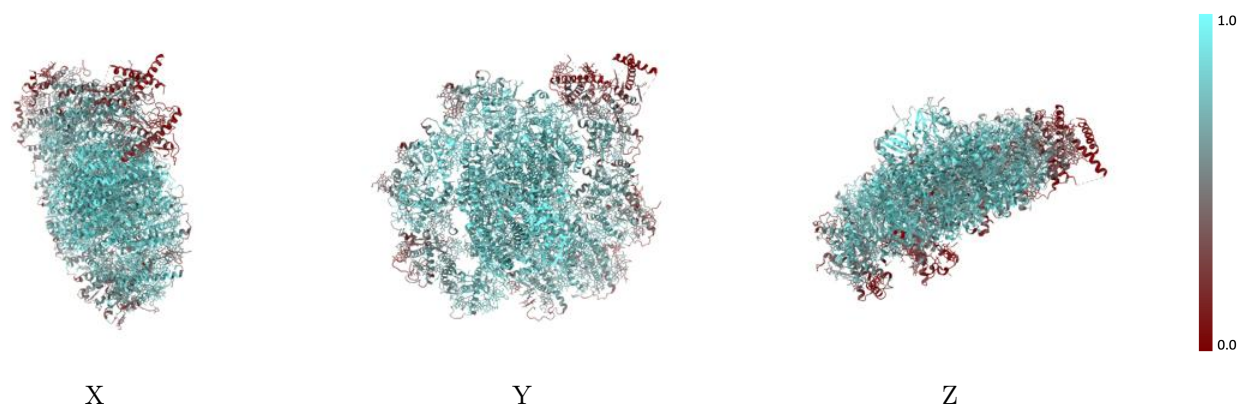
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



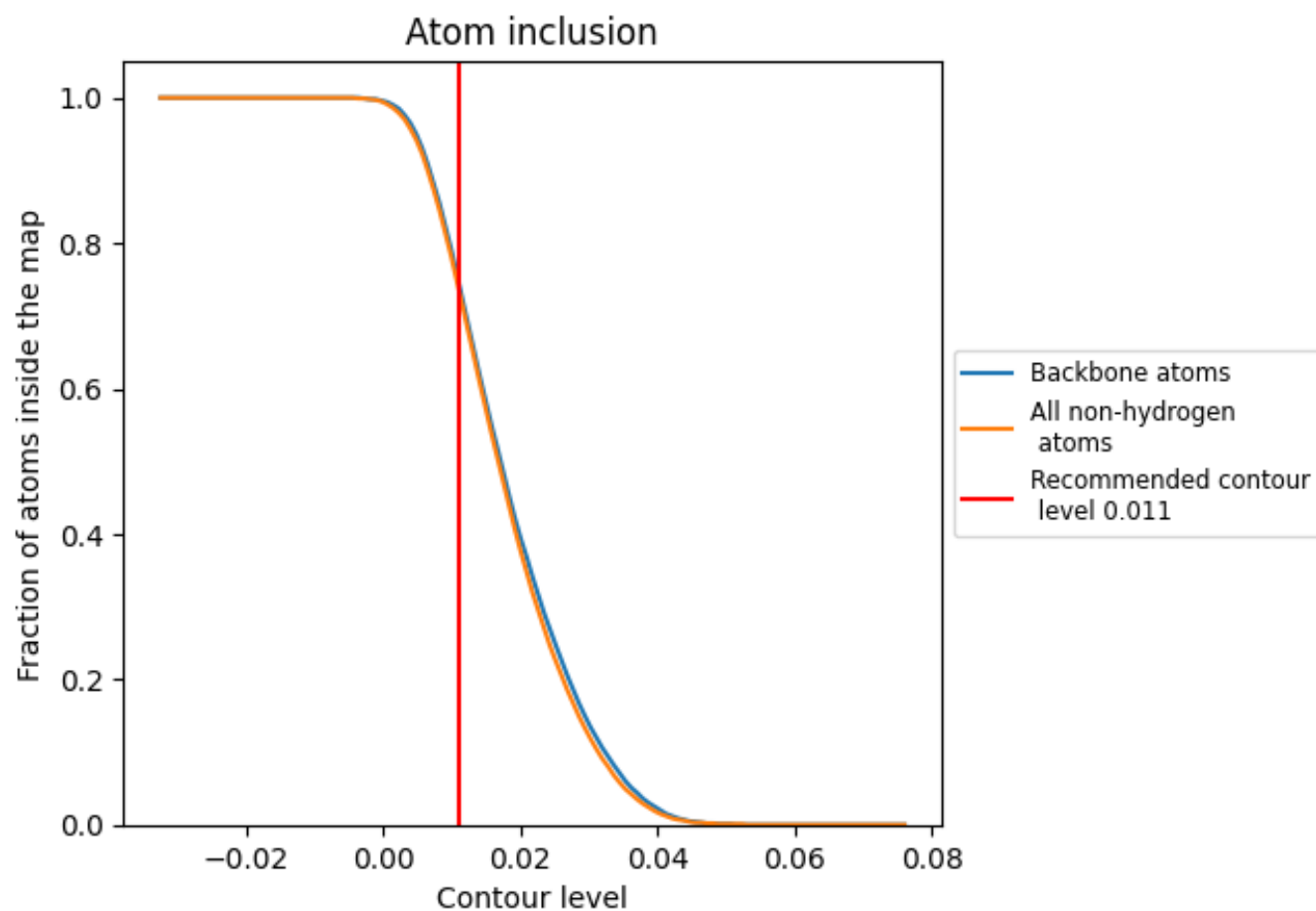
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

