



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:36 PM UTC

PDB ID : 8HTU / pdb_00008htu
EMDB ID : EMD-35018
Title : Cryo-EM structure of PpPSI-L
Authors : Li, M.; Pan, X.W.; Sun, H.Y.
Deposited on : 2022-12-21
Resolution : 2.87 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

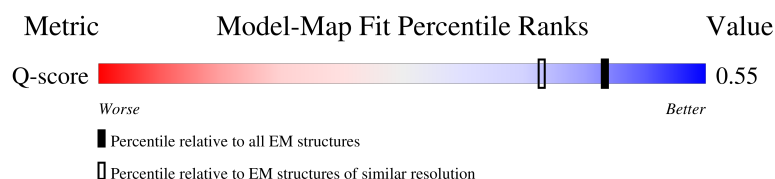
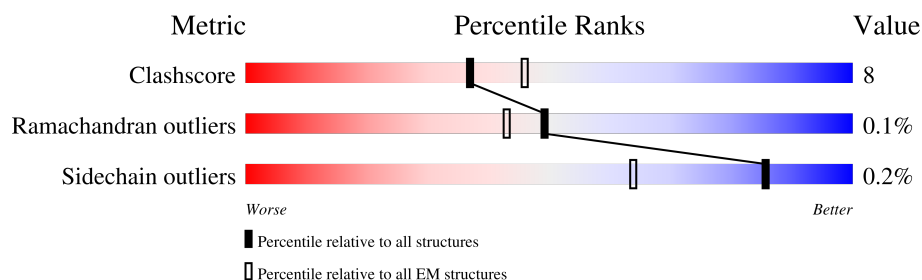
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.87 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.



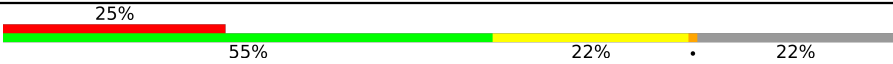
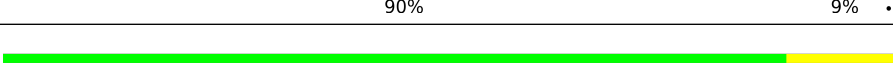
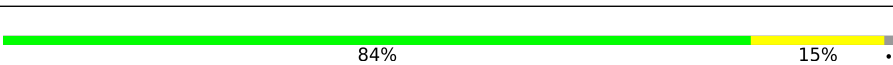
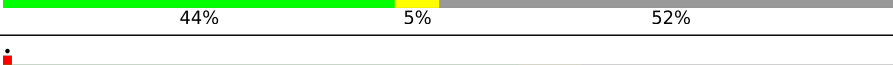
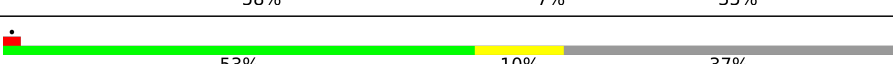
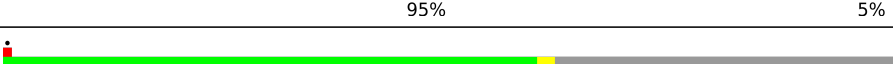
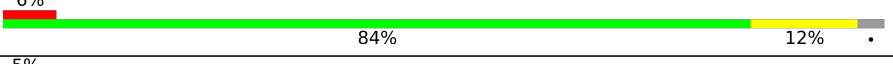
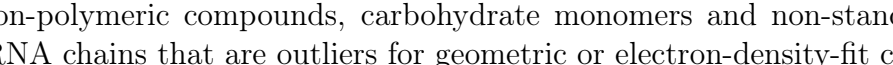
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	U	265	8% 70% 12% 17%
1	V	265	20% 69% 12% 19%
1	W	265	16% 72% 14% 14%
2	1	245	• 70% 9% 21%

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Mol	Chain	Length	Quality of chain
2	5	245	
3	2	273	
3	6	273	
4	3	323	
4	7	323	
5	4	270	
5	8	270	
6	A	750	
7	B	734	
8	C	81	
9	D	210	
10	E	132	
11	F	246	
12	G	155	
13	H	139	
14	I	36	
15	J	41	
16	K	132	
17	L	223	
18	M	32	
19	O	143	
20	9	311	

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
21	CHL	1	601	X	-	-	-
21	CHL	1	607	X	-	-	-
21	CHL	2	601	X	-	-	-
21	CHL	2	602	X	-	-	-
21	CHL	2	606	X	-	-	-
21	CHL	2	607	X	-	-	-
21	CHL	2	608	X	-	-	-
21	CHL	2	618	X	-	-	-
21	CHL	3	608	X	-	-	-
21	CHL	4	606	X	-	-	-
21	CHL	4	607	X	-	-	-
21	CHL	4	608	X	-	-	-
21	CHL	4	618	X	-	-	-
21	CHL	5	601	X	-	-	-
21	CHL	5	607	X	-	-	-
21	CHL	6	601	X	-	-	-
21	CHL	6	602	X	-	-	-
21	CHL	6	606	X	-	-	-
21	CHL	6	607	X	-	-	-
21	CHL	6	608	X	-	-	-
21	CHL	6	618	X	-	-	-
21	CHL	7	608	X	-	-	-
21	CHL	8	606	X	-	-	-
21	CHL	8	607	X	-	-	-
21	CHL	8	608	X	-	-	-
21	CHL	8	618	X	-	-	-
21	CHL	9	601	X	-	-	-
21	CHL	9	605	X	-	-	-
21	CHL	9	606	X	-	-	-
21	CHL	9	607	X	-	-	-
21	CHL	9	608	X	-	-	-
21	CHL	U	601	X	-	-	-
21	CHL	U	605	X	-	-	-
21	CHL	U	606	X	-	-	-
21	CHL	U	607	X	-	-	-
21	CHL	U	608	X	-	-	-
21	CHL	U	609	X	-	-	-
21	CHL	V	601	X	-	-	-
21	CHL	V	605	X	-	-	-
21	CHL	V	606	X	-	-	-
21	CHL	V	607	X	-	-	-
21	CHL	V	608	X	-	-	-
21	CHL	V	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	W	601	X	-	-	-
21	CHL	W	605	X	-	-	-
21	CHL	W	606	X	-	-	-
21	CHL	W	607	X	-	-	-
21	CHL	W	608	X	-	-	-
21	CHL	W	609	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	2	614	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	608	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	6	614	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	607	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	617	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	613	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	610	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	302	X	-	-	-
22	CLA	L	303	X	-	-	-
22	CLA	L	304	X	-	-	-
22	CLA	O	2001	X	-	-	-
22	CLA	O	2002	X	-	-	-
22	CLA	O	2003	X	-	-	-
22	CLA	U	602	X	-	-	-
22	CLA	U	603	X	-	-	-
22	CLA	U	604	X	-	-	-
22	CLA	U	610	X	-	-	-
22	CLA	U	611	X	-	-	-
22	CLA	U	612	X	-	-	-
22	CLA	U	613	X	-	-	-
22	CLA	U	614	X	-	-	-
22	CLA	V	603	X	-	-	-
22	CLA	V	604	X	-	-	-
22	CLA	V	610	X	-	-	-
22	CLA	V	611	X	-	-	-
22	CLA	V	612	X	-	-	-
22	CLA	V	613	X	-	-	-
22	CLA	V	614	X	-	-	-
22	CLA	W	602	X	-	-	-
22	CLA	W	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	W	604	X	-	-	-
22	CLA	W	610	X	-	-	-
22	CLA	W	611	X	-	-	-
22	CLA	W	612	X	-	-	-
22	CLA	W	613	X	-	-	-
22	CLA	W	614	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 57715 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
1	U	219	Total	C	N	O	S	0	0	
			1659	1073	270	311	5			
1	V	215	Total	C	N	O	S	0	0	
			1630	1052	265	308	5			
1	W	228	Total	C	N	O	P	S	0	0
			1734	1113	286	329	1	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	193	Total	C	N	O	S	0	0
			1478	964	248	265	1		
2	5	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	211	Total	C	N	O	S	0	0
			1625	1055	273	293	4		
3	6	205	Total	C	N	O	S	0	0
			1583	1029	265	285	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	222	Total	C	N	O	S	0	0
			1719	1125	281	306	7		
4	7	219	Total	C	N	O	S	0	0
			1687	1105	274	301	7		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	206	Total	C	N	O	S	0	0
			1600	1040	267	288	5		
5	8	204	Total	C	N	O	S	0	0
			1582	1028	265	284	5		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

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

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	733	Total	C	N	O	S	0	0
			5850	3839	996	999	16		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	142	Total	C	N	O	S	0	0
			1114	714	197	200	3		

- Molecule 10 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	64	Total	C	N	O	0	0
			507	322	90	95		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	161	Total	C	N	O	S	0	0
			1251	808	217	223	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	97	Total	C	N	O	0	0
			740	478	127	135		

- Molecule 13 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	95	Total	C	N	O	S	0	0
			736	472	125	138	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

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

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 16 is a protein called Photosystem I subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	81	Total	C	N	O	S	0	0
			565	356	98	108	3		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	163	Total	C	N	O	S	0	0
			1228	809	197	220	2		

- Molecule 18 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	M	31	Total	C	N	O	0	0
			230	150	37	43		

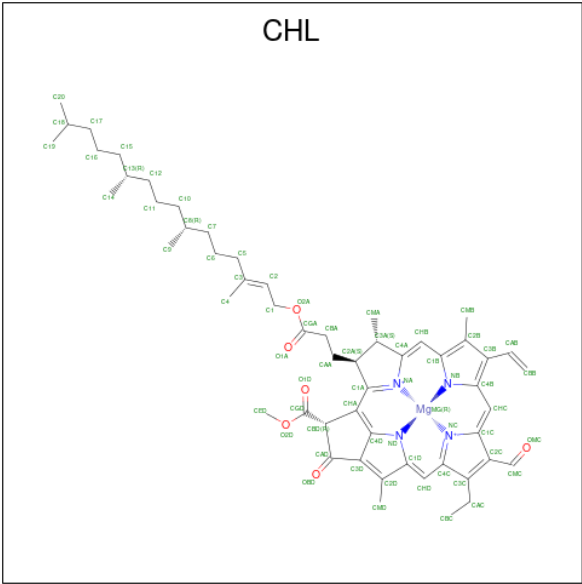
- Molecule 19 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	90	Total	C	N	O	S	0	0
			711	477	117	116	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	221	Total	C	N	O	S	0	0
			1713	1113	283	308	9		

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
21	U	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	U	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	U	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
21	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	V	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	V	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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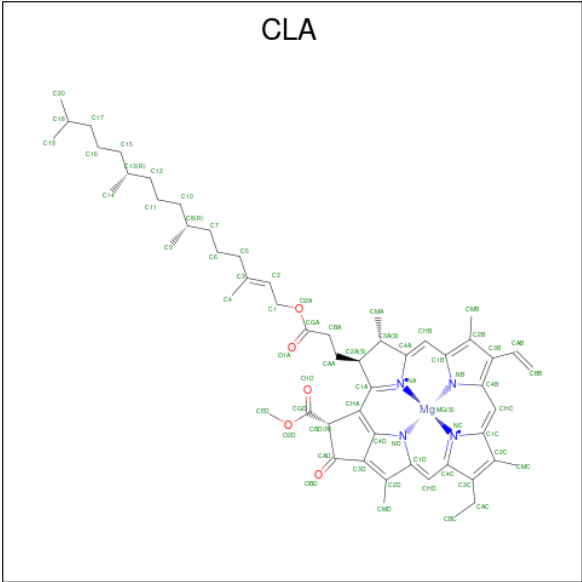
Mol	Chain	Residues	Atoms					AltConf
21	V	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	V	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	V	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	V	1	Total 40	C 33	Mg 1	N 4	O 2	0
21	W	1	Total 63	C 53	Mg 1	N 4	O 5	0
21	W	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	W	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	W	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	W	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	W	1	Total 40	C 33	Mg 1	N 4	O 2	0
21	1	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
21	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	3	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	4	1	Total 47	C 36	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
21	5	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	6	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	6	1	Total 47	C 36	Mg 1	N 4	O 6	0
21	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	9	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	9	1	Total 38	C 31	Mg 1	N 4	O 2	0
21	9	1	Total 44	C 35	Mg 1	N 4	O 4	0
21	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	9	1	Total 43	C 34	Mg 1	N 4	O 4	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	V	1	Total	C	Mg	N	O	0
			38	30	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	V	1	Total	C	Mg	N	O	0
			56	47	1	4	4	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	B	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	H	1	Total 38	C 32	Mg 1	N 4	O 1	0
22	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	K	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N		0
			27	22	1	4		
22	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	O	1	Total	C	Mg	N		0
			27	22	1	4		
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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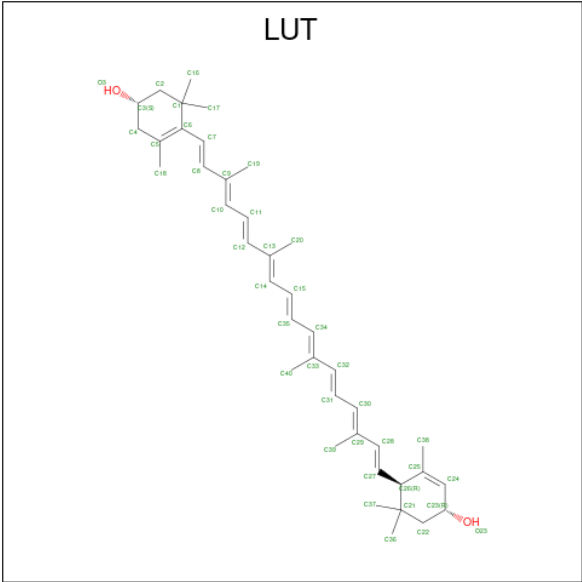
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



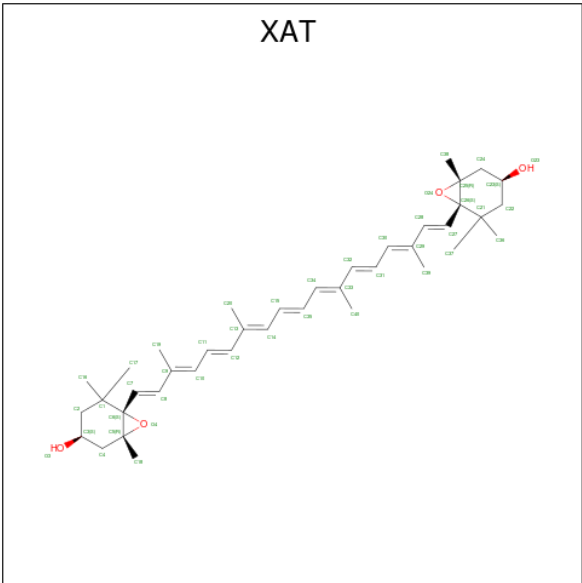
Mol	Chain	Residues	Atoms			AltConf
23	U	1	Total	C	O	0
			42	40	2	
23	U	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	W	1	Total	C	O	0
			42	40	2	
23	W	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	5	1	Total	C	O	0
			42	40	2	
23	6	1	Total	C	O	0
			42	40	2	
23	7	1	Total	C	O	0
			42	40	2	
23	8	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
23	9	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	
23	9	1	Total	C	O	0
			42	40	2	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



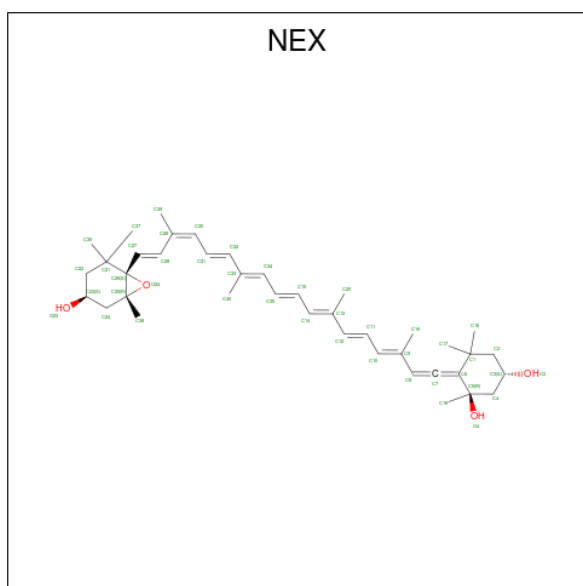
Mol	Chain	Residues	Atoms			AltConf
24	U	1	Total	C	O	0
			44	40	4	
24	V	1	Total	C	O	0
			44	40	4	
24	W	1	Total	C	O	0
			44	40	4	
24	1	1	Total	C	O	0
			44	40	4	
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	5	1	Total	C	O	0
			44	40	4	

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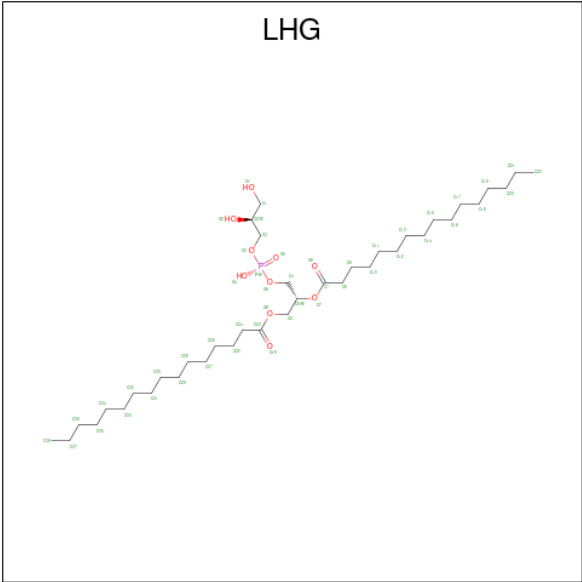
Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total	C	O	0
			44	40	4	
24	7	1	Total	C	O	0
			44	40	4	
24	8	1	Total	C	O	0
			44	40	4	

- Molecule 25 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
25	U	1	Total	C	O	0
			44	40	4	
25	V	1	Total	C	O	0
			44	40	4	
25	W	1	Total	C	O	0
			44	40	4	
25	9	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



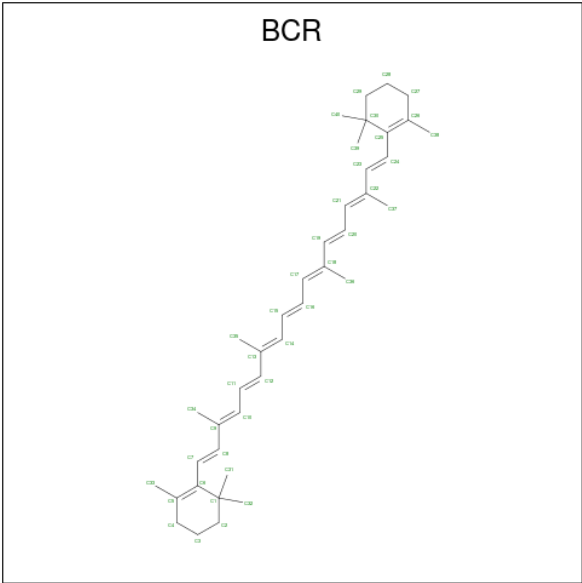
Mol	Chain	Residues	Atoms				AltConf
26	U	1	Total	C	O	P	0
			45	34	10	1	
26	V	1	Total	C	O	P	0
			42	31	10	1	
26	W	1	Total	C	O	P	0
			45	34	10	1	
26	1	1	Total	C	O	P	0
			49	38	10	1	
26	2	1	Total	C	O	P	0
			32	21	10	1	
26	3	1	Total	C	O	P	0
			32	21	10	1	
26	4	1	Total	C	O	P	0
			38	27	10	1	
26	A	1	Total	C	O	P	0
			47	36	10	1	
26	A	1	Total	C	O	P	0
			31	20	10	1	
26	B	1	Total	C	O	P	0
			35	24	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			32	21	10	1	
26	7	1	Total	C	O	P	0
			34	23	10	1	
26	8	1	Total	C	O	P	0
			38	27	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	9	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
27	1	1	Total	C	0
			40	40	
27	2	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	3	1	Total	C	0
			40	40	
27	4	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	

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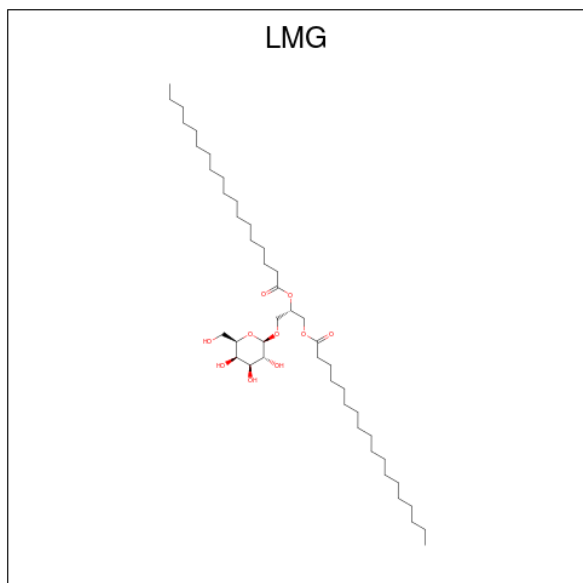
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 39 39	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	G	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	M	1	Total C 40 40	0
27	O	1	Total C 40 40	0
27	6	1	Total C 40 40	0
27	7	1	Total C 40 40	0

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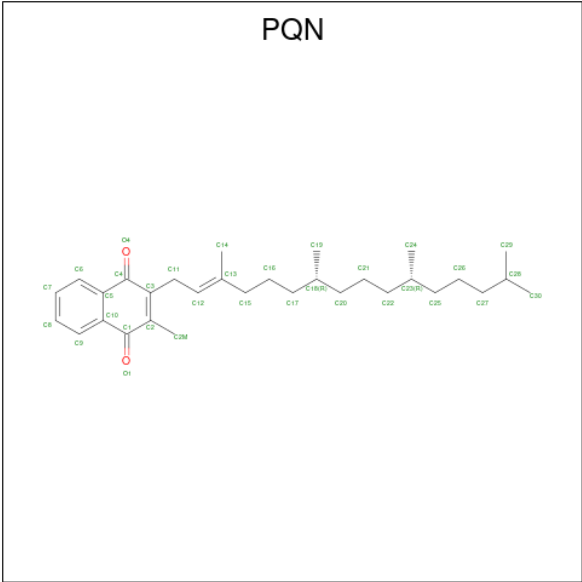
Mol	Chain	Residues	Atoms		AltConf
27	7	1	Total	C	0
			40	40	
27	8	1	Total	C	0
			40	40	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



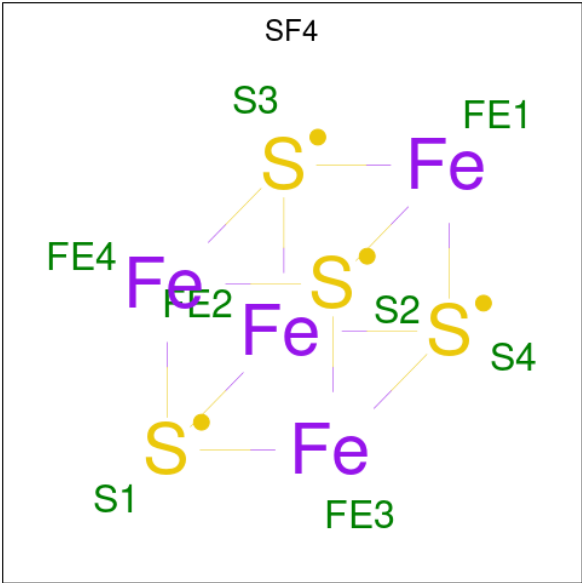
Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			47	37	10	
28	A	1	Total	C	O	0
			34	24	10	
28	G	1	Total	C	O	0
			32	22	10	
28	J	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			35	25	10	
28	L	1	Total	C	O	0
			44	34	10	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



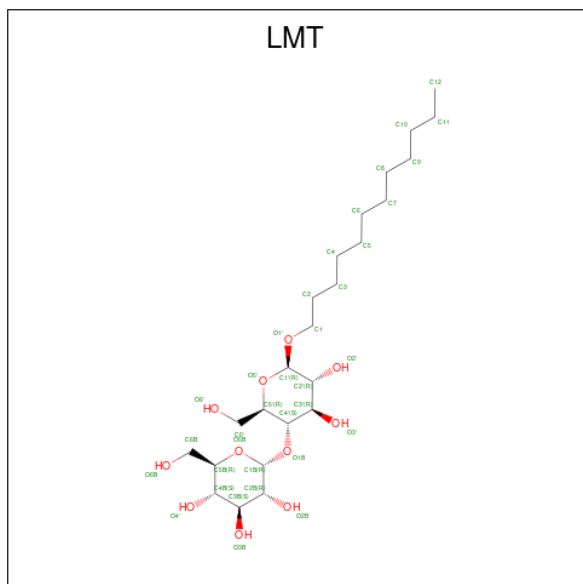
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	

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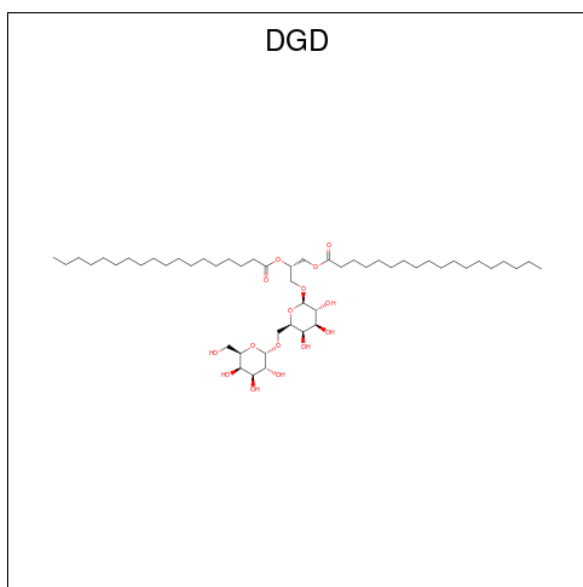
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
30	C	1	8	4	4	0

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	35	24	11	0
31	B	1	31	20	11	0
31	G	1	35	24	11	0
31	K	1	35	24	11	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

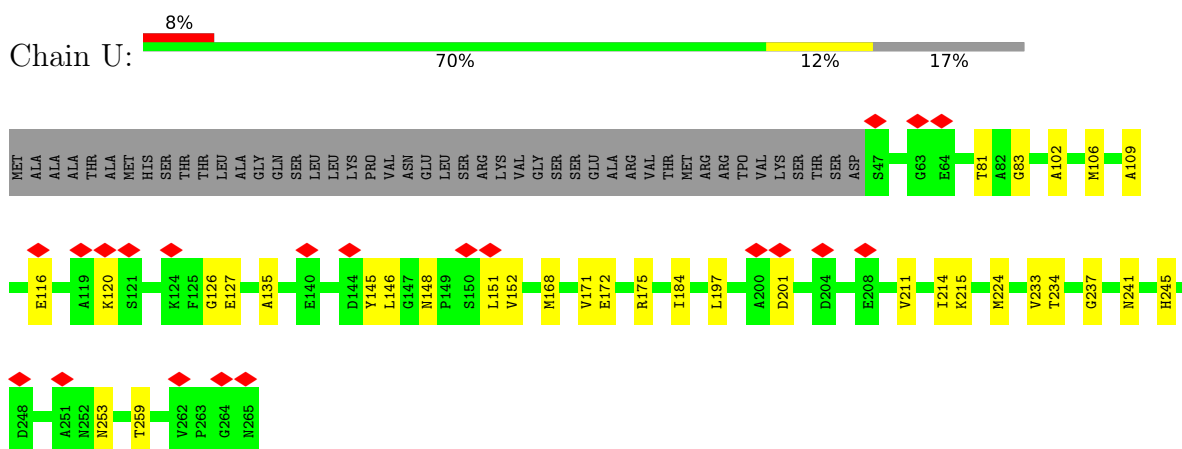
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	A	2	Total	O	0
			2	2	

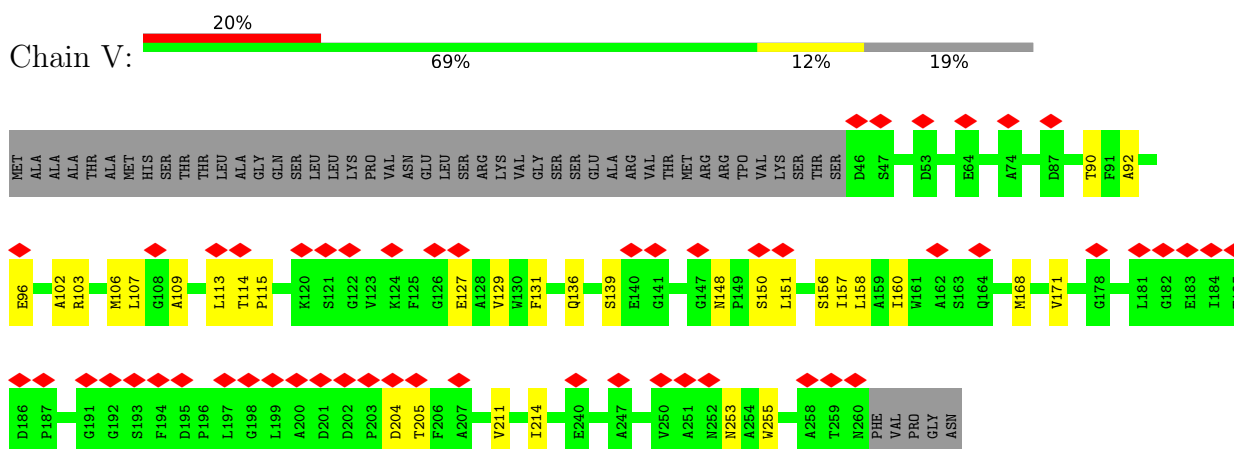
3 Residue-property plots

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.

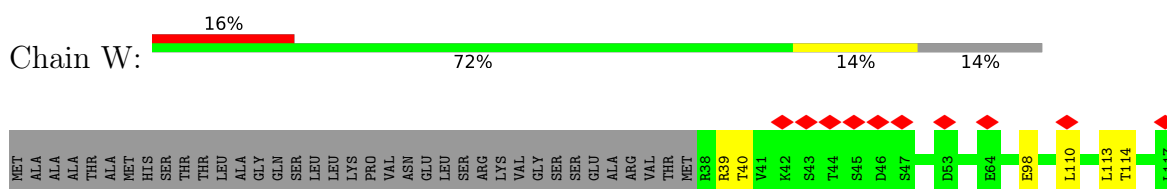
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

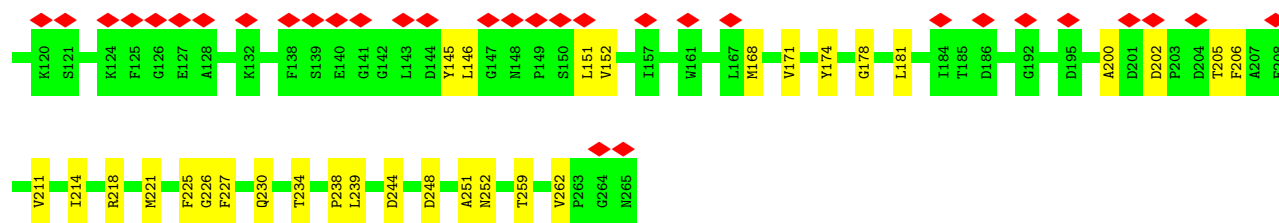


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



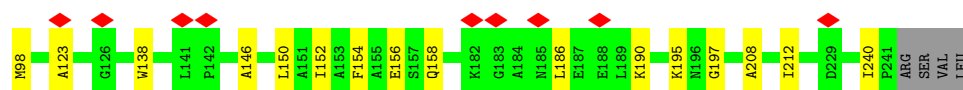
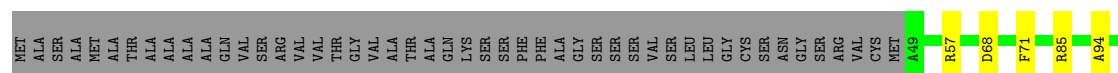
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic





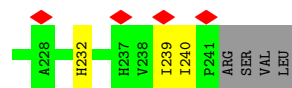
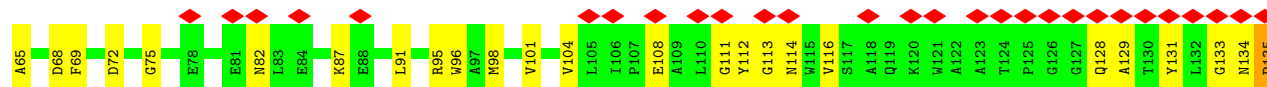
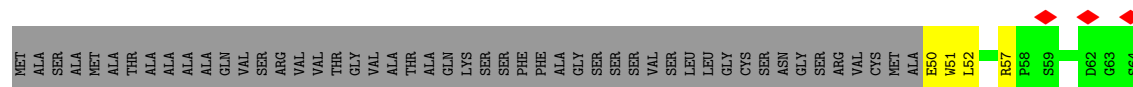
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 70% 9% 21%



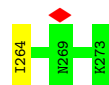
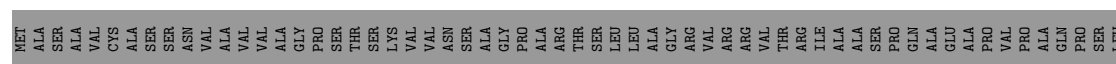
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 25% 55% 22% 22%

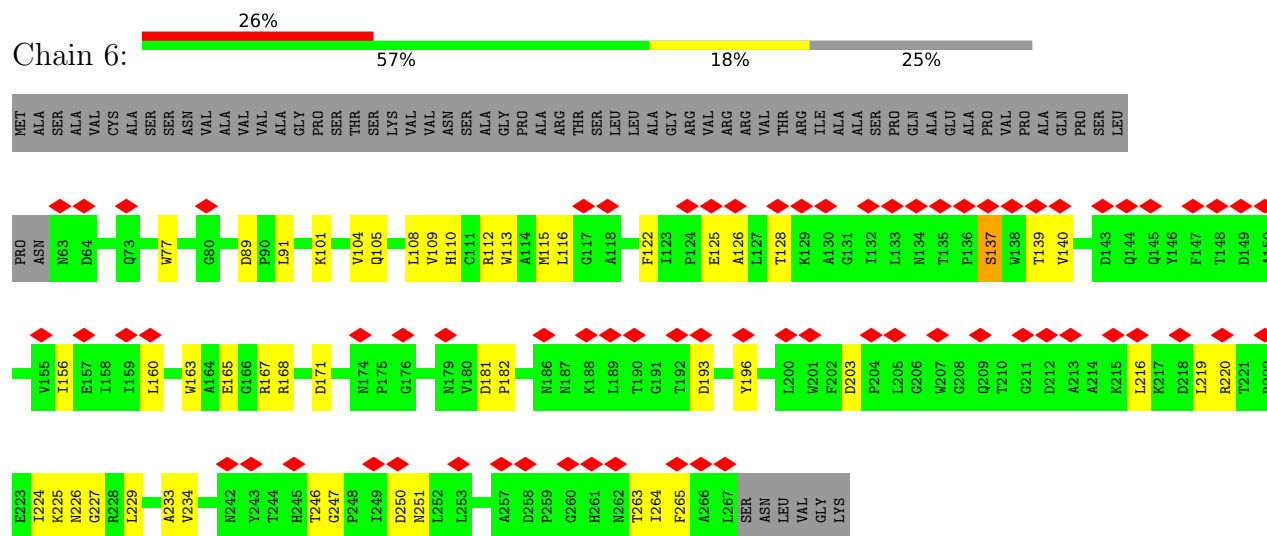


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

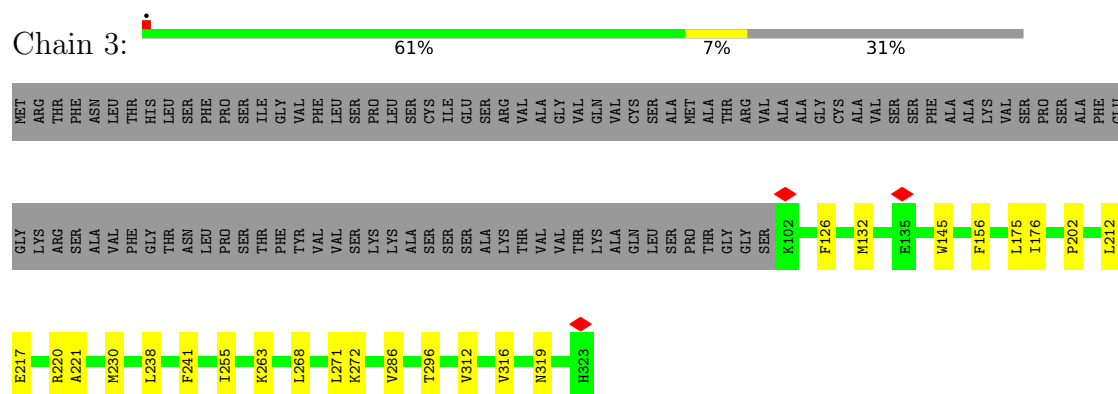
Chain 2: 66% 11% 23%



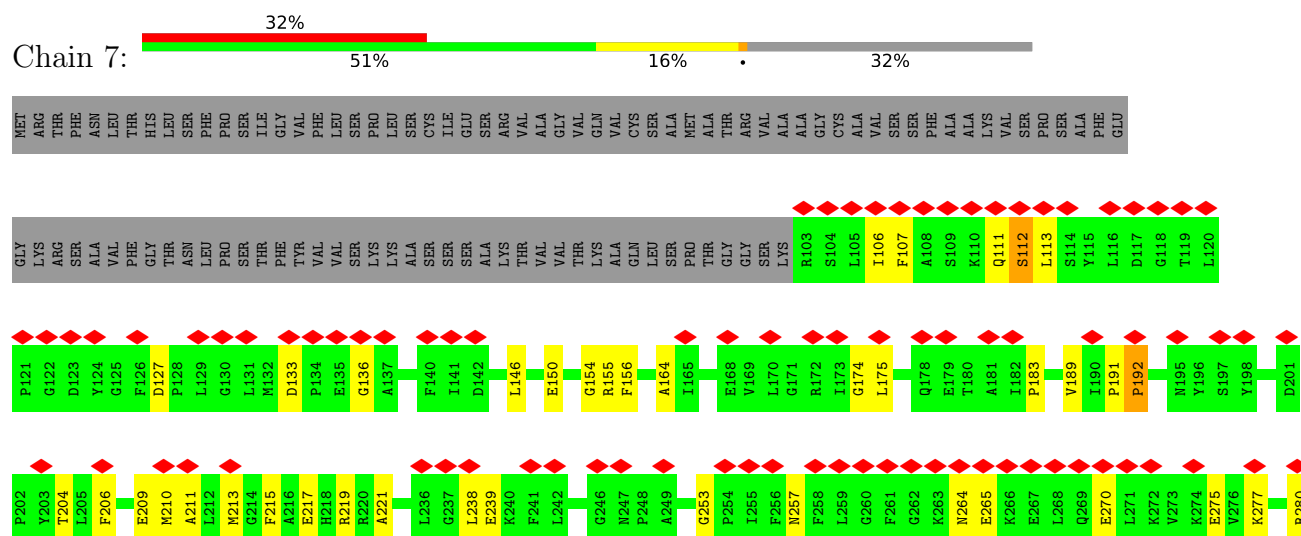
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

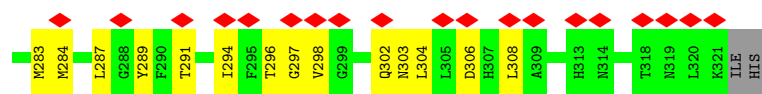


- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

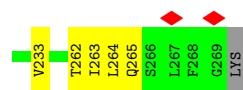
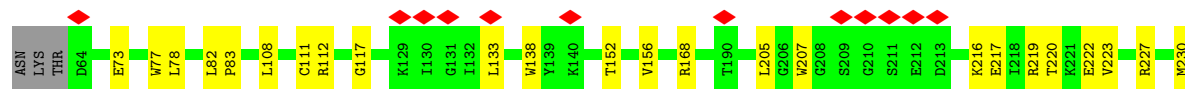


- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

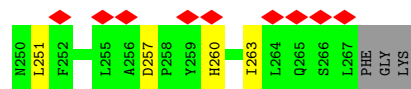
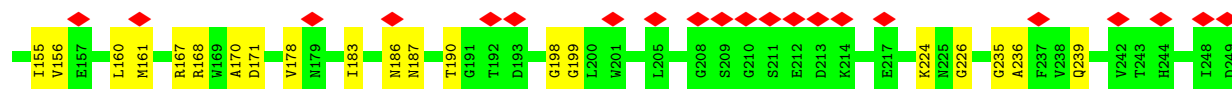




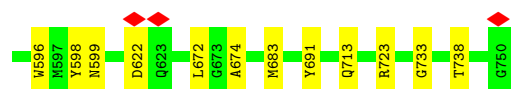
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

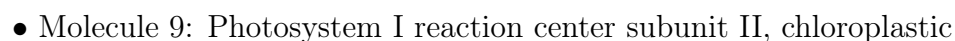


- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

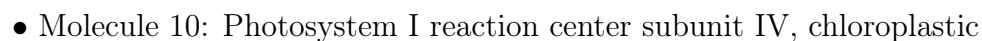
12%



15%



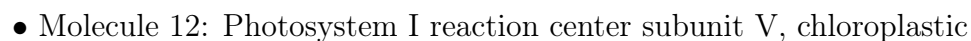
32%



52%



35%



Chain G:  53% 10% 37%

MET ALA SER CYS ALA ALA SER MET THR THR VAL ALA ALA SER LEU LEU LYS ALA ASN PHE SER PHE SER GLY LEU ARG ARG GLY THR LYS VAL ASP SER ILE ALA MET SER ARG SER SER PHE SER ALA SER LYS THR ALA ILE LYS SER SER GLY VAL THR CYS GLU N90

T61 G76 Q84 R85 V88 V95 T100 D103 Q110 F111 V112 K117 G123 F124 T125 I126 W132 T146 Q154 F155

- Molecule 13: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  7% 60% 9% 32%

MET ALA ALA ALA SER ALA THR MET VAL SER GLY LEU ALA GLY SER SER LEU ALA GLN LYS PHE LYS ILE ALA ALA PRO LYS SER VAL SER VAL ARG SER PRO SER LYS VAL GLY ILE SER ALA K45 Y46 G47 E48 F53 Y76 F84 F87 A88 G89 A90 F91

T92 K93 R94 G95 L96 G104 T108 L112 S116 D119 M133 G134 K139

- Molecule 14: Photosystem I reaction center subunit VIII

Chain I:  81% 14% 6%

H1 T9 L13 F18 P19 E34 ILE

- Molecule 15: Photosystem I reaction center subunit IX

Chain J:  95% 5%

H1 E28 R31 L41

- Molecule 16: Photosystem I subunit X

Chain K:  60% 39%

MET ALA ALA MET THR THR MET THR VAL ALA THR VAL ARG GLN PHE GLU GLY LEU LYS ALA ALA THR THR THR SER PHE SER LYS PRO ASN LEU SER LEU ALA ALA ARG LYS THR THR ALA GLY LYS GLY ALA LEU LEU ASP Y50 M68 D92 V117 A130 GLY LEU

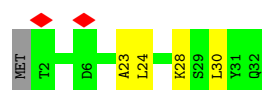
- Molecule 17: PSI subunit V

Chain L:  67% 6% 27%

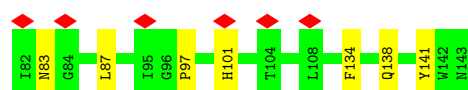
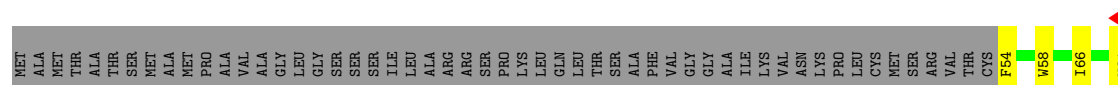
MET ALA ALA ALA MET THR ARG ALA GLY THR LEU LEU ALA MET GLU ARG VAL GLN ARG VAL SER LYS THR THR THR GLY ALA VAL SER ASN THR PHE LEU GLY ASN ARG GLY ARG ALA THR SER ALA PRO GLN ARG ALA CYS ASP LEU ARG VAL LYS VAL MET VAL VAL ARG GLY ALA

E61 V65 I66 E67 P68 L69 E79 T80 P81 S85 E110 L125 R135 T148 M152 V222 K223

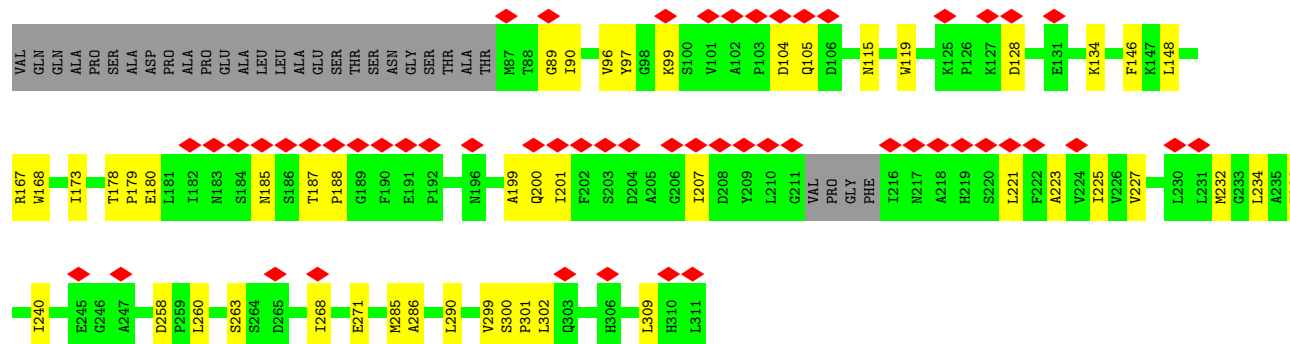
Chain M: 6% 84% 12%



Chain O:



Chain 9:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0188	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: XAT, LMG, TPO, LHG, NEX, SF4, CLA, DGD, LMT, LUT, BCR, PQN, CHL

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	U	0.16	0/1708	0.32	0/2327
1	V	0.15	0/1677	0.28	0/2284
1	W	0.15	0/1770	0.30	0/2406
2	1	0.21	0/1527	0.39	0/2088
2	5	0.18	0/1522	0.47	2/2081 (0.1%)
3	2	0.15	0/1676	0.31	0/2296
3	6	0.21	0/1634	0.38	0/2240
4	3	0.16	0/1770	0.32	0/2400
4	7	0.27	1/1738 (0.1%)	0.50	4/2360 (0.2%)
5	4	0.15	0/1650	0.32	0/2255
5	8	0.13	0/1631	0.30	0/2230
6	A	0.19	0/6032	0.32	0/8227
7	B	0.16	0/6064	0.31	1/8274 (0.0%)
8	C	0.14	0/605	0.30	0/821
9	D	0.13	0/1142	0.31	0/1546
10	E	0.13	0/518	0.28	0/704
11	F	0.20	0/1277	0.36	0/1725
12	G	0.12	0/758	0.25	0/1034
13	H	0.16	0/753	0.28	0/1013
14	I	0.25	0/273	0.40	0/373
15	J	0.16	0/334	0.29	0/457
16	K	0.13	0/571	0.22	0/773
17	L	0.20	0/1263	0.33	0/1725
18	M	0.19	0/231	0.27	0/312
19	O	0.19	0/738	0.39	0/1009
20	9	0.18	0/1764	0.42	1/2397 (0.0%)
All	All	0.18	1/40626 (0.0%)	0.34	8/55357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	7	183	PRO	CG-CD	-7.87	1.24	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7	183	PRO	N-CD-CG	-11.22	86.37	103.20
4	7	183	PRO	CA-N-CD	-6.75	102.55	112.00
4	7	192	PRO	CA-N-CD	-5.89	103.75	112.00
7	B	479	SER	N-CA-C	-5.75	106.25	113.72
4	7	183	PRO	CA-CB-CG	-5.72	93.63	104.50

There are no chirality outliers.

There are no planarity outliers.

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	U	1659	0	1592	31	0
1	V	1630	0	1562	22	0
1	W	1734	0	1665	21	0
2	1	1478	0	1453	16	0
2	5	1473	0	1448	58	0
3	2	1625	0	1584	24	0
3	6	1583	0	1537	42	0
4	3	1719	0	1685	23	0
4	7	1687	0	1651	47	0
5	4	1600	0	1567	25	0
5	8	1582	0	1553	37	0
6	A	5837	0	5725	61	0
7	B	5850	0	5622	61	0
8	C	595	0	573	10	0
9	D	1114	0	1116	12	0
10	E	507	0	503	4	0
11	F	1251	0	1303	13	0
12	G	740	0	723	14	0
13	H	736	0	721	7	0
14	I	266	0	274	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	325	0	341	1	0
16	K	565	0	587	2	0
17	L	1228	0	1238	11	0
18	M	230	0	251	4	0
19	O	711	0	705	9	0
20	9	1713	0	1675	46	0
21	1	103	0	78	2	0
21	2	289	0	210	10	0
21	3	56	0	47	1	0
21	4	182	0	122	7	0
21	5	90	0	61	5	0
21	6	310	0	243	9	0
21	7	46	0	31	3	0
21	8	186	0	128	6	0
21	9	207	0	132	17	0
21	U	319	0	267	8	0
21	V	263	0	168	3	0
21	W	259	0	156	2	0
22	1	645	0	581	4	0
22	2	400	0	322	6	0
22	3	745	0	719	14	0
22	4	532	0	474	12	0
22	5	568	0	442	15	0
22	6	416	0	357	8	0
22	7	626	0	498	16	0
22	8	526	0	448	16	0
22	9	401	0	348	9	0
22	A	2769	0	2877	40	0
22	B	2419	0	2498	39	0
22	F	155	0	137	3	0
22	G	141	0	105	4	0
22	H	38	0	26	0	0
22	J	50	0	39	0	0
22	K	204	0	183	3	0
22	L	190	0	203	3	0
22	O	109	0	55	3	0
22	U	464	0	467	7	0
22	V	387	0	306	5	0
22	W	383	0	308	1	0
23	1	42	0	56	2	0
23	2	42	0	56	4	0
23	3	42	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	4	42	0	56	1	0
23	5	42	0	56	3	0
23	6	42	0	56	2	0
23	7	42	0	56	2	0
23	8	42	0	56	2	0
23	9	126	0	168	15	0
23	U	84	0	112	6	0
23	V	84	0	112	3	0
23	W	84	0	112	3	0
24	1	44	0	56	3	0
24	2	44	0	56	7	0
24	3	44	0	56	5	0
24	4	44	0	56	11	0
24	5	44	0	56	7	0
24	6	44	0	56	5	0
24	7	44	0	56	3	0
24	8	44	0	56	3	0
24	U	44	0	56	0	0
24	V	44	0	56	0	0
24	W	44	0	56	1	0
25	9	44	0	56	4	0
25	U	44	0	56	1	0
25	V	44	0	56	2	0
25	W	44	0	56	2	0
26	1	49	0	74	2	0
26	2	32	0	34	0	0
26	3	32	0	34	0	0
26	4	38	0	46	3	0
26	5	37	0	44	0	0
26	6	32	0	34	2	0
26	7	34	0	38	0	0
26	8	38	0	46	0	0
26	9	28	0	26	0	0
26	A	78	0	99	0	0
26	B	35	0	40	0	0
26	U	45	0	60	1	0
26	V	42	0	54	0	0
26	W	45	0	60	1	0
27	1	40	0	56	1	0
27	2	40	0	56	4	0
27	3	80	0	112	13	0
27	4	40	0	56	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	6	40	0	56	5	0
27	7	80	0	112	10	0
27	8	40	0	56	8	0
27	A	239	0	333	27	0
27	B	280	0	392	30	0
27	F	40	0	56	3	0
27	G	40	0	56	4	0
27	I	40	0	56	4	0
27	J	40	0	56	4	0
27	K	80	0	112	11	0
27	L	120	0	168	13	0
27	M	40	0	56	5	0
27	O	40	0	56	5	0
28	2	47	0	67	0	0
28	A	34	0	38	0	0
28	G	32	0	34	2	0
28	J	90	0	126	0	0
28	L	44	0	58	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	A	35	0	46	0	0
31	B	31	0	35	0	0
31	G	35	0	46	0	0
31	K	35	0	46	0	0
32	B	66	0	96	0	0
33	A	2	0	0	0	0
All	All	57715	0	56700	868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 868 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)
27:L:305:BCR:HC8	27:L:305:BCR:H331	1.56	0.86
4:7:164:ALA:HB2	24:7:619:XAT:H163	1.58	0.85
22:B:823:CLA:CBC	27:B:1609:BCR:H343	2.11	0.81
2:5:108:GLU:HB3	2:5:220:LEU:HD21	1.63	0.79
2:5:52:LEU:HD21	21:5:601:CHL:HMA3	1.68	0.76

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	U	217/265 (82%)	208 (96%)	9 (4%)	0	100	100
1	V	213/265 (80%)	207 (97%)	6 (3%)	0	100	100
1	W	225/265 (85%)	215 (96%)	9 (4%)	1 (0%)	30	56
2	1	191/245 (78%)	183 (96%)	8 (4%)	0	100	100
2	5	190/245 (78%)	166 (87%)	23 (12%)	1 (0%)	24	51
3	2	209/273 (77%)	200 (96%)	9 (4%)	0	100	100
3	6	203/273 (74%)	190 (94%)	13 (6%)	0	100	100
4	3	220/323 (68%)	213 (97%)	7 (3%)	0	100	100
4	7	217/323 (67%)	203 (94%)	13 (6%)	1 (0%)	24	51
5	4	204/270 (76%)	192 (94%)	12 (6%)	0	100	100
5	8	202/270 (75%)	187 (93%)	15 (7%)	0	100	100
6	A	740/750 (99%)	716 (97%)	23 (3%)	1 (0%)	48	74
7	B	731/734 (100%)	714 (98%)	17 (2%)	0	100	100
8	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
9	D	140/210 (67%)	133 (95%)	7 (5%)	0	100	100
10	E	62/132 (47%)	62 (100%)	0	0	100	100
11	F	159/246 (65%)	152 (96%)	6 (4%)	1 (1%)	21	48
12	G	95/155 (61%)	91 (96%)	4 (4%)	0	100	100
13	H	93/139 (67%)	90 (97%)	3 (3%)	0	100	100
14	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
15	J	39/41 (95%)	39 (100%)	0	0	100	100
16	K	79/132 (60%)	79 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	L	161/223 (72%)	155 (96%)	6 (4%)	0	100	100
18	M	29/32 (91%)	29 (100%)	0	0	100	100
19	O	88/143 (62%)	81 (92%)	7 (8%)	0	100	100
20	9	217/311 (70%)	190 (88%)	26 (12%)	1 (0%)	24	51
All	All	5034/6382 (79%)	4800 (95%)	228 (4%)	6 (0%)	49	74

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	315	ILE
2	5	135	PRO
4	7	112	SER
11	F	88	ALA
1	W	39	ARG

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	U	166/203 (82%)	165 (99%)	1 (1%)	78	92
1	V	163/203 (80%)	163 (100%)	0	100	100
1	W	173/203 (85%)	173 (100%)	0	100	100
2	1	148/186 (80%)	148 (100%)	0	100	100
2	5	148/186 (80%)	148 (100%)	0	100	100
3	2	167/213 (78%)	167 (100%)	0	100	100
3	6	162/213 (76%)	160 (99%)	2 (1%)	63	84
4	3	174/256 (68%)	174 (100%)	0	100	100
4	7	170/256 (66%)	170 (100%)	0	100	100
5	4	164/210 (78%)	164 (100%)	0	100	100
5	8	162/210 (77%)	162 (100%)	0	100	100
6	A	603/611 (99%)	602 (100%)	1 (0%)	87	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	B	595/596 (100%)	594 (100%)	1 (0%)	87	96
8	C	67/68 (98%)	67 (100%)	0	100	100
9	D	115/157 (73%)	115 (100%)	0	100	100
10	E	56/105 (53%)	56 (100%)	0	100	100
11	F	132/193 (68%)	131 (99%)	1 (1%)	73	89
12	G	77/121 (64%)	77 (100%)	0	100	100
13	H	75/103 (73%)	74 (99%)	1 (1%)	61	84
14	I	30/32 (94%)	30 (100%)	0	100	100
15	J	35/35 (100%)	35 (100%)	0	100	100
16	K	58/95 (61%)	58 (100%)	0	100	100
17	L	124/165 (75%)	123 (99%)	1 (1%)	73	89
18	M	26/27 (96%)	26 (100%)	0	100	100
19	O	74/115 (64%)	74 (100%)	0	100	100
20	9	174/243 (72%)	173 (99%)	1 (1%)	78	92
All	All	4038/5005 (81%)	4029 (100%)	9 (0%)	85	96

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

Mol	Chain	Res	Type
3	6	226	ASN
20	9	134	LYS
11	F	87	VAL
13	H	119	ASP
17	L	135	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
7	B	158	GLN
4	7	302	GLN
7	B	502	ASN
19	O	85	ASN
7	B	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	W	40	1	8,10,11	1.64	1 (12%)	10,14,16	2.03	1 (10%)

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
1	TPO	W	40	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	40	TPO	P-O1P	3.50	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	40	TPO	P-OG1-CB	-5.76	107.66	123.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

366 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	L	304	-	64,68,73	1.20	7 (10%)	76,107,113	1.15	5 (6%)
22	CLA	7	606	-	50,54,73	1.35	7 (14%)	59,90,113	1.24	4 (6%)
22	CLA	B	816	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	4 (4%)
22	CLA	1	614	-	53,57,73	1.33	7 (13%)	63,94,113	1.16	4 (6%)
22	CLA	A	803	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	5 (6%)
22	CLA	3	609	4	69,73,73	1.16	6 (8%)	82,113,113	1.24	6 (7%)
21	CHL	4	608	-	40,54,74	4.22	18 (45%)	34,90,114	2.69	10 (29%)
22	CLA	U	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.13	6 (7%)
22	CLA	A	825	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	7 (8%)
26	LHG	9	2630	22	27,27,48	1.31	2 (7%)	30,33,54	0.99	3 (10%)
22	CLA	6	614	-	54,58,73	1.33	7 (12%)	64,95,113	1.27	6 (9%)
22	CLA	B	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	5 (6%)
22	CLA	A	824	-	66,70,73	1.19	7 (10%)	78,109,113	1.16	6 (7%)
22	CLA	B	819	-	64,68,73	1.21	7 (10%)	76,107,113	1.23	7 (9%)
22	CLA	F	304	11	45,51,73	1.41	9 (20%)	51,81,113	2.01	5 (9%)
21	CHL	8	618	5	37,51,74	4.33	18 (48%)	30,86,114	3.08	13 (43%)
22	CLA	U	613	1	69,73,73	1.17	6 (8%)	82,113,113	1.12	4 (4%)
22	CLA	W	614	-	42,47,73	1.55	8 (19%)	52,82,113	1.24	5 (9%)
21	CHL	4	607	-	41,55,74	4.19	18 (43%)	35,91,114	2.77	13 (37%)
22	CLA	A	842	-	59,63,73	1.26	7 (11%)	70,101,113	1.22	6 (8%)
26	LHG	V	2630	22	41,41,48	1.02	2 (4%)	44,47,54	0.98	2 (4%)
22	CLA	B	804	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	2	621	-	41,41,41	0.79	0	56,56,56	2.11	20 (35%)
27	BCR	8	621	-	41,41,41	0.81	0	56,56,56	2.32	19 (33%)
26	LHG	3	630	22	31,31,48	1.16	2 (6%)	34,37,54	1.07	2 (5%)
21	CHL	9	601	20	32,47,74	4.55	17 (53%)	24,81,114	2.65	8 (33%)
32	DGD	B	850	-	67,67,67	0.90	2 (2%)	81,81,81	0.96	3 (3%)
22	CLA	B	838	-	51,55,73	1.33	7 (13%)	60,91,113	1.27	6 (10%)
23	LUT	6	619	-	42,43,43	0.73	0	51,60,60	1.66	11 (21%)
22	CLA	A	819	-	66,70,73	1.17	8 (12%)	78,109,113	1.17	7 (8%)
22	CLA	3	611	26	59,63,73	1.27	6 (10%)	70,101,113	1.13	4 (5%)
27	BCR	A	849	-	41,41,41	0.78	1 (2%)	56,56,56	2.00	17 (30%)
26	LHG	A	847	22	30,30,48	1.16	2 (6%)	33,36,54	1.25	3 (9%)
31	LMT	A	857	-	36,36,36	0.76	0	47,47,47	1.37	7 (14%)
21	CHL	6	602	3	50,64,74	3.83	19 (38%)	46,102,114	2.69	12 (26%)
22	CLA	B	814	-	69,73,73	1.15	7 (10%)	82,113,113	1.24	9 (10%)
26	LHG	B	851	22	34,34,48	1.12	2 (5%)	37,40,54	1.02	2 (5%)
27	BCR	6	621	-	41,41,41	0.82	0	56,56,56	2.43	19 (33%)
22	CLA	A	826	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	5 (6%)
22	CLA	3	612	4	69,73,73	1.16	6 (8%)	82,113,113	1.10	5 (6%)
24	XAT	6	620	-	41,47,47	1.27	2 (4%)	54,74,74	6.47	29 (53%)
22	CLA	B	836	-	56,60,73	1.27	7 (12%)	65,97,113	1.25	7 (10%)
22	CLA	3	615	-	57,61,73	1.29	7 (12%)	67,98,113	1.24	5 (7%)
22	CLA	5	606	2	49,53,73	1.39	8 (16%)	58,89,113	1.21	3 (5%)
22	CLA	A	839	-	64,68,73	1.20	7 (10%)	76,107,113	1.18	6 (7%)
22	CLA	7	603	4	49,53,73	1.42	7 (14%)	58,89,113	1.22	3 (5%)
22	CLA	1	608	-	49,53,73	1.39	7 (14%)	58,89,113	1.23	5 (8%)
27	BCR	G	205	-	41,41,41	0.77	0	56,56,56	1.93	19 (33%)
27	BCR	A	851	-	41,41,41	0.77	1 (2%)	56,56,56	2.17	25 (44%)
22	CLA	8	604	-	54,58,73	1.33	5 (9%)	64,95,113	1.21	6 (9%)
22	CLA	5	604	-	45,49,73	1.43	7 (15%)	54,84,113	1.19	2 (3%)
22	CLA	W	613	1	64,68,73	1.21	7 (10%)	76,107,113	1.13	4 (5%)
22	CLA	7	614	-	45,49,73	1.42	6 (13%)	54,84,113	1.29	5 (9%)
22	CLA	B	822	-	64,68,73	1.21	7 (10%)	76,107,113	1.23	8 (10%)
23	LUT	W	2621	-	42,43,43	0.76	0	51,60,60	1.71	9 (17%)
22	CLA	2	603	-	50,54,73	1.36	7 (14%)	59,90,113	1.32	4 (6%)
22	CLA	2	604	-	54,58,73	1.30	6 (11%)	64,95,113	1.25	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	840	-	54,58,73	1.29	6 (11%)	64,95,113	1.26	4 (6%)
22	CLA	4	604	-	59,63,73	1.26	7 (11%)	70,101,113	1.25	4 (5%)
22	CLA	4	613	5	59,63,73	1.26	7 (11%)	70,101,113	1.14	6 (8%)
22	CLA	B	820	-	59,63,73	1.25	7 (11%)	70,101,113	1.20	5 (7%)
22	CLA	U	604	-	56,60,73	1.29	7 (12%)	65,97,113	1.22	5 (7%)
22	CLA	1	604	-	54,58,73	1.31	7 (12%)	64,95,113	1.24	5 (7%)
22	CLA	A	818	-	69,73,73	1.16	7 (10%)	82,113,113	1.09	7 (8%)
21	CHL	V	609	1	33,48,74	4.50	17 (51%)	25,82,114	2.86	10 (40%)
21	CHL	W	609	1	33,48,74	4.43	16 (48%)	25,82,114	2.91	10 (40%)
22	CLA	G	201	-	49,53,73	1.38	7 (14%)	58,89,113	1.17	4 (6%)
21	CHL	U	605	1	33,46,74	4.16	16 (48%)	30,81,114	2.42	10 (33%)
26	LHG	4	630	22	37,37,48	1.03	2 (5%)	40,43,54	1.23	6 (15%)
22	CLA	A	821	-	59,63,73	1.25	7 (11%)	70,101,113	1.13	4 (5%)
26	LHG	8	630	22	37,37,48	1.07	2 (5%)	40,43,54	1.11	4 (10%)
22	CLA	B	824	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
22	CLA	B	841	26	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
22	CLA	B	833	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	5 (6%)
22	CLA	K	204	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	4 (4%)
22	CLA	3	602	4	69,73,73	1.16	6 (8%)	82,113,113	1.09	5 (6%)
22	CLA	V	610	1	43,47,73	1.56	8 (18%)	54,82,113	1.29	6 (11%)
22	CLA	B	835	-	49,53,73	1.36	5 (10%)	58,89,113	1.24	7 (12%)
22	CLA	B	827	-	60,64,73	1.22	6 (10%)	71,102,113	1.21	4 (5%)
21	CHL	2	601	3	40,54,74	4.24	19 (47%)	34,90,114	3.01	12 (35%)
22	CLA	4	601	5	54,58,73	1.31	7 (12%)	64,95,113	1.25	7 (10%)
22	CLA	L	303	-	69,73,73	1.15	7 (10%)	82,113,113	1.13	7 (8%)
22	CLA	5	612	2	50,54,73	1.40	7 (14%)	59,90,113	1.16	3 (5%)
22	CLA	A	802	-	69,73,73	1.15	7 (10%)	82,113,113	1.05	4 (4%)
21	CHL	2	606	-	40,54,74	4.18	18 (45%)	34,90,114	2.97	13 (38%)
22	CLA	A	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	6 (7%)
22	CLA	A	837	6	69,73,73	1.18	7 (10%)	82,113,113	1.12	3 (3%)
23	LUT	9	621	-	42,43,43	0.81	0	51,60,60	1.73	13 (25%)
21	CHL	U	601	1	57,71,74	3.14	16 (28%)	60,111,114	2.05	14 (23%)
27	BCR	A	852	-	41,41,41	0.72	1 (2%)	56,56,56	2.29	25 (44%)
22	CLA	A	838	-	59,63,73	1.25	6 (10%)	70,101,113	1.21	6 (8%)
22	CLA	H	201	-	40,46,73	1.48	6 (15%)	52,80,113	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	609	4	61,65,73	1.30	7 (11%)	72,103,113	1.16	6 (8%)
26	LHG	1	630	22	48,48,48	0.93	2 (4%)	51,54,54	0.97	3 (5%)
26	LHG	U	2630	22	44,44,48	0.98	2 (4%)	47,50,54	0.97	2 (4%)
21	CHL	V	606	-	33,46,74	4.12	16 (48%)	30,81,114	2.36	10 (33%)
21	CHL	6	601	3	60,74,74	3.49	19 (31%)	58,114,114	2.29	13 (22%)
22	CLA	8	610	5	59,63,73	1.26	7 (11%)	70,101,113	1.14	6 (8%)
27	BCR	L	306	-	41,41,41	0.71	0	56,56,56	2.09	21 (37%)
22	CLA	5	610	2	59,63,73	1.25	7 (11%)	70,101,113	1.11	5 (7%)
22	CLA	6	603	-	50,54,73	1.37	6 (12%)	59,90,113	1.31	4 (6%)
28	LMG	J	103	-	55,55,55	0.88	2 (3%)	63,63,63	1.01	4 (6%)
22	CLA	W	610	1	69,73,73	1.17	6 (8%)	82,113,113	1.19	7 (8%)
24	XAT	4	620	-	41,47,47	1.05	1 (2%)	54,74,74	4.69	23 (42%)
22	CLA	5	603	-	49,53,73	1.40	6 (12%)	58,89,113	1.26	4 (6%)
22	CLA	W	603	-	42,47,73	1.47	7 (16%)	50,82,113	1.23	6 (12%)
23	LUT	9	624	-	42,43,43	0.80	0	51,60,60	3.54	26 (50%)
22	CLA	B	808	-	69,73,73	1.16	8 (11%)	82,113,113	1.10	6 (7%)
22	CLA	4	610	5	65,69,73	1.24	7 (10%)	77,108,113	1.12	6 (7%)
21	CHL	V	607	-	35,48,74	4.04	16 (45%)	31,83,114	3.07	12 (38%)
22	CLA	4	603	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	5 (6%)
22	CLA	1	610	2	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
23	LUT	U	2621	-	42,43,43	0.78	0	51,60,60	1.78	12 (23%)
21	CHL	W	608	-	35,48,74	4.01	16 (45%)	31,83,114	2.69	11 (35%)
31	LMT	B	849	-	32,32,36	0.64	0	43,43,47	1.32	7 (16%)
22	CLA	G	203	-	54,58,73	1.32	7 (12%)	64,95,113	1.25	5 (7%)
22	CLA	A	820	-	69,73,73	1.14	7 (10%)	82,113,113	1.13	7 (8%)
22	CLA	A	829	-	64,68,73	1.18	5 (7%)	76,107,113	1.23	8 (10%)
22	CLA	4	602	5	69,73,73	1.15	7 (10%)	82,113,113	1.09	6 (7%)
22	CLA	5	608	-	54,58,73	1.31	7 (12%)	64,95,113	1.28	5 (7%)
22	CLA	U	610	1	69,73,73	1.16	7 (10%)	82,113,113	1.14	7 (8%)
21	CHL	9	607	-	37,51,74	4.31	17 (45%)	30,86,114	3.03	11 (36%)
22	CLA	B	813	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	6 (7%)
22	CLA	W	612	1	41,46,73	1.56	7 (17%)	51,81,113	1.31	7 (13%)
22	CLA	7	617	-	50,54,73	1.36	6 (12%)	59,90,113	1.21	5 (8%)
27	BCR	B	848	-	41,41,41	0.71	0	56,56,56	1.99	17 (30%)
29	PQN	B	842	-	34,34,34	0.61	1 (2%)	43,45,45	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	827	33	69,73,73	1.17	7 (10%)	82,113,113	1.13	6 (7%)
21	CHL	8	607	-	40,54,74	4.26	18 (45%)	34,90,114	2.91	11 (32%)
22	CLA	B	807	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	5 (6%)
21	CHL	U	608	-	35,48,74	4.02	16 (45%)	31,83,114	2.65	11 (35%)
22	CLA	L	302	17	69,73,73	1.17	7 (10%)	82,113,113	1.11	6 (7%)
21	CHL	5	607	2	32,47,74	4.60	18 (56%)	24,81,114	2.67	8 (33%)
22	CLA	7	612	4	49,53,73	1.39	7 (14%)	58,89,113	1.28	3 (5%)
21	CHL	6	608	-	42,56,74	4.11	18 (42%)	36,92,114	2.82	13 (36%)
22	CLA	7	615	-	43,48,73	1.45	7 (16%)	51,83,113	1.22	4 (7%)
21	CHL	2	602	3	55,69,74	3.64	19 (34%)	52,108,114	2.42	16 (30%)
22	CLA	7	607	4	49,53,73	1.39	7 (14%)	58,89,113	1.27	3 (5%)
21	CHL	9	606	-	38,52,74	4.26	18 (47%)	31,87,114	3.14	12 (38%)
22	CLA	B	831	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	7 (8%)
22	CLA	3	604	-	59,63,73	1.24	6 (10%)	70,101,113	1.20	6 (8%)
31	LMT	G	206	-	36,36,36	0.64	0	47,47,47	1.27	6 (12%)
22	CLA	A	801	-	69,73,73	1.16	6 (8%)	82,113,113	1.42	11 (13%)
23	LUT	2	619	-	42,43,43	1.30	7 (16%)	51,60,60	1.48	11 (21%)
23	LUT	8	619	-	42,43,43	0.75	1 (2%)	51,60,60	1.76	13 (25%)
22	CLA	V	614	-	49,53,73	1.38	7 (14%)	58,89,113	1.20	5 (8%)
28	LMG	J	104	-	35,35,55	1.15	2 (5%)	43,43,63	1.02	2 (4%)
21	CHL	U	609	1	60,74,74	3.43	18 (30%)	58,114,114	2.35	15 (25%)
22	CLA	3	613	4	69,73,73	1.17	8 (11%)	82,113,113	1.18	7 (8%)
22	CLA	5	616	2	50,54,73	1.39	7 (14%)	59,90,113	1.16	3 (5%)
22	CLA	9	610	20	59,63,73	1.25	7 (11%)	70,101,113	1.15	6 (8%)
22	CLA	B	810	-	69,73,73	1.15	7 (10%)	82,113,113	1.19	6 (7%)
22	CLA	A	822	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	4 (4%)
22	CLA	7	611	26	45,49,73	1.43	7 (15%)	54,84,113	1.18	4 (7%)
27	BCR	L	305	-	41,41,41	0.66	0	56,56,56	2.01	22 (39%)
22	CLA	A	836	-	59,66,73	1.44	9 (15%)	65,99,113	1.51	8 (12%)
22	CLA	6	611	26	49,53,73	1.37	7 (14%)	58,89,113	1.31	4 (6%)
27	BCR	J	102	-	41,41,41	0.73	0	56,56,56	2.26	18 (32%)
22	CLA	A	810	6	69,73,73	1.15	7 (10%)	82,113,113	1.18	6 (7%)
23	LUT	5	617	-	42,43,43	1.31	8 (19%)	51,60,60	1.67	11 (21%)
21	CHL	V	605	1	36,50,74	4.41	18 (50%)	29,85,114	3.30	10 (34%)
22	CLA	8	609	5	59,63,73	1.27	8 (13%)	70,101,113	1.25	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	B	844	-	41,41,41	0.72	0	56,56,56	2.05	23 (41%)
22	CLA	V	604	-	54,58,73	1.32	7 (12%)	64,95,113	1.24	6 (9%)
21	CHL	W	607	-	35,48,74	4.05	17 (48%)	31,83,114	2.95	12 (38%)
22	CLA	A	845	26	69,73,73	1.17	7 (10%)	82,113,113	1.06	5 (6%)
22	CLA	7	610	4	59,63,73	1.28	6 (10%)	70,101,113	1.21	4 (5%)
24	XAT	2	620	-	41,47,47	0.96	2 (4%)	54,74,74	2.33	22 (40%)
24	XAT	V	2622	-	41,47,47	1.13	1 (2%)	54,74,74	5.41	23 (42%)
22	CLA	8	601	5	54,58,73	1.32	8 (14%)	64,95,113	1.19	4 (6%)
22	CLA	2	613	3	61,65,73	1.24	6 (9%)	72,103,113	1.25	6 (8%)
22	CLA	1	616	2	49,53,73	1.39	6 (12%)	58,89,113	1.25	3 (5%)
22	CLA	A	831	-	69,73,73	1.15	7 (10%)	82,113,113	1.09	5 (6%)
23	LUT	V	2620	-	42,43,43	0.75	0	51,60,60	1.79	15 (29%)
21	CHL	4	618	5	37,51,74	4.27	18 (48%)	30,86,114	3.02	13 (43%)
22	CLA	9	609	20	49,53,73	2.33	18 (36%)	58,89,113	3.03	26 (44%)
22	CLA	8	612	5	50,54,73	1.37	7 (14%)	59,90,113	1.16	3 (5%)
22	CLA	A	834	-	69,73,73	1.17	7 (10%)	82,113,113	1.12	5 (6%)
22	CLA	A	808	-	64,68,73	1.21	7 (10%)	76,107,113	1.14	5 (6%)
22	CLA	2	609	3	50,54,73	1.34	7 (14%)	59,90,113	1.25	4 (6%)
22	CLA	3	617	-	57,63,73	1.89	8 (14%)	62,98,113	2.03	9 (14%)
26	LHG	2	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.06	2 (5%)
22	CLA	W	604	-	46,50,73	1.40	7 (15%)	53,85,113	1.25	3 (5%)
22	CLA	6	613	3	69,73,73	1.17	5 (7%)	82,113,113	1.08	4 (4%)
22	CLA	2	611	26	49,53,73	1.38	6 (12%)	58,89,113	1.26	4 (6%)
22	CLA	8	611	26	59,63,73	1.27	6 (10%)	70,101,113	1.10	4 (5%)
22	CLA	A	813	-	59,63,73	1.24	7 (11%)	70,101,113	1.24	6 (8%)
23	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.66	12 (23%)
27	BCR	A	848	-	41,41,41	0.79	0	56,56,56	1.92	17 (30%)
27	BCR	B	845	-	41,41,41	0.73	0	56,56,56	2.49	22 (39%)
21	CHL	V	601	1	57,71,74	3.13	16 (28%)	60,111,114	2.22	16 (26%)
22	CLA	A	854	-	64,68,73	1.20	8 (12%)	76,107,113	1.16	5 (6%)
27	BCR	L	301	-	41,41,41	0.73	0	56,56,56	2.26	17 (30%)
22	CLA	V	611	26	43,48,73	1.54	7 (16%)	51,83,113	1.28	5 (9%)
22	CLA	5	611	26	50,54,73	1.37	7 (14%)	59,90,113	1.22	4 (6%)
22	CLA	A	806	-	69,73,73	1.15	6 (8%)	82,113,113	1.16	6 (7%)
27	BCR	I	101	-	41,41,41	0.76	1 (2%)	56,56,56	1.78	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	825	-	69,73,73	1.15	7 (10%)	82,113,113	1.19	5 (6%)
22	CLA	2	612	3	49,53,73	1.38	7 (14%)	58,89,113	1.25	4 (6%)
22	CLA	A	807	6	69,73,73	1.15	8 (11%)	82,113,113	1.13	4 (4%)
22	CLA	1	606	-	49,53,73	1.39	6 (12%)	58,89,113	1.24	4 (6%)
27	BCR	A	850	-	41,41,41	0.76	0	56,56,56	1.82	15 (26%)
22	CLA	B	806	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	6 (7%)
22	CLA	F	303	-	49,53,73	1.36	7 (14%)	58,89,113	1.28	5 (8%)
27	BCR	7	621	-	41,41,41	0.74	0	56,56,56	2.22	21 (37%)
21	CHL	6	606	-	40,54,74	4.19	18 (45%)	34,90,114	3.11	11 (32%)
27	BCR	7	620	-	41,41,41	0.68	0	56,56,56	2.11	20 (35%)
31	LMT	K	208	-	36,36,36	0.60	0	47,47,47	1.28	6 (12%)
22	CLA	A	833	-	59,63,73	1.24	7 (11%)	70,101,113	1.19	7 (10%)
22	CLA	4	612	5	49,53,73	1.38	6 (12%)	58,89,113	1.25	4 (6%)
22	CLA	5	609	2	45,49,73	1.44	8 (17%)	54,84,113	1.21	4 (7%)
21	CHL	W	601	1	57,71,74	3.14	16 (28%)	60,111,114	2.09	14 (23%)
21	CHL	3	608	-	50,64,74	3.71	19 (38%)	46,102,114	2.51	13 (28%)
22	CLA	2	610	3	64,68,73	1.20	7 (10%)	76,107,113	1.09	5 (6%)
24	XAT	3	619	-	41,47,47	0.91	1 (2%)	54,74,74	2.61	22 (40%)
22	CLA	B	839	-	69,73,73	1.15	7 (10%)	82,113,113	1.11	5 (6%)
22	CLA	2	614	-	54,58,73	1.32	7 (12%)	64,95,113	1.22	5 (7%)
22	CLA	3	607	4	54,58,73	1.30	8 (14%)	64,95,113	1.23	7 (10%)
27	BCR	F	305	-	41,41,41	0.70	0	56,56,56	2.12	18 (32%)
29	PQN	A	844	-	34,34,34	0.49	0	43,45,45	0.91	4 (9%)
21	CHL	6	618	3	41,55,74	4.11	18 (43%)	35,91,114	2.94	13 (37%)
22	CLA	9	604	-	47,51,73	1.39	7 (14%)	55,86,113	1.16	3 (5%)
22	CLA	A	835	-	69,73,73	1.16	7 (10%)	82,113,113	1.09	5 (6%)
22	CLA	1	611	26	69,73,73	1.18	7 (10%)	82,113,113	1.17	8 (9%)
21	CHL	6	607	-	41,55,74	4.20	19 (46%)	35,91,114	2.92	13 (37%)
22	CLA	B	828	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
24	XAT	W	2622	-	41,47,47	0.92	1 (2%)	54,74,74	2.42	18 (33%)
22	CLA	G	204	12	50,54,73	1.36	7 (14%)	59,90,113	1.21	3 (5%)
21	CHL	5	601	2	45,59,74	4.00	18 (40%)	40,96,114	2.76	15 (37%)
22	CLA	8	603	-	59,63,73	1.27	7 (11%)	70,101,113	1.22	3 (4%)
22	CLA	1	609	2	69,73,73	1.19	8 (11%)	82,113,113	1.12	7 (8%)
22	CLA	B	809	7	69,73,73	1.17	7 (10%)	82,113,113	1.17	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	K	202	-	41,41,41	0.69	0	56,56,56	2.04	20 (35%)
23	LUT	W	2620	-	42,43,43	0.80	0	51,60,60	1.72	12 (23%)
27	BCR	3	621	-	41,41,41	0.81	1 (2%)	56,56,56	2.29	21 (37%)
27	BCR	A	856	-	40,40,41	0.71	0	54,54,56	1.71	14 (25%)
27	BCR	B	1609	-	41,41,41	0.76	0	56,56,56	3.23	26 (46%)
23	LUT	9	620	-	42,43,43	0.73	0	51,60,60	1.88	14 (27%)
22	CLA	7	613	4	59,63,73	1.27	6 (10%)	70,101,113	1.15	4 (5%)
22	CLA	B	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	6 (7%)
21	CHL	8	608	-	45,59,74	3.98	18 (40%)	40,96,114	2.77	16 (40%)
22	CLA	6	610	3	64,68,73	1.20	7 (10%)	76,107,113	1.11	4 (5%)
22	CLA	5	614	-	47,51,73	1.38	6 (12%)	55,86,113	1.22	4 (7%)
22	CLA	9	613	20	56,60,73	1.31	7 (12%)	65,97,113	1.22	6 (9%)
21	CHL	V	608	-	35,48,74	4.01	17 (48%)	31,83,114	2.68	13 (41%)
28	LMG	A	860	-	34,34,55	1.14	2 (5%)	42,42,63	1.11	2 (4%)
21	CHL	1	601	2	50,64,74	3.79	18 (36%)	46,102,114	2.56	14 (30%)
25	NEX	9	623	-	40,46,46	1.20	3 (7%)	50,70,70	2.04	13 (26%)
22	CLA	1	603	-	59,63,73	1.27	7 (11%)	70,101,113	1.29	6 (8%)
22	CLA	9	612	20	41,47,73	1.44	8 (19%)	51,81,113	1.18	4 (7%)
24	XAT	U	2622	-	41,47,47	0.93	1 (2%)	54,74,74	2.40	16 (29%)
22	CLA	U	603	-	69,73,73	1.18	6 (8%)	82,113,113	1.18	3 (3%)
26	LHG	7	630	22	33,33,48	1.14	2 (6%)	36,39,54	1.10	3 (8%)
21	CHL	U	607	-	60,74,74	3.43	18 (30%)	58,114,114	2.43	16 (27%)
22	CLA	O	2002	-	59,63,73	1.26	7 (11%)	70,101,113	1.11	4 (5%)
23	LUT	U	2620	-	42,43,43	0.73	0	51,60,60	1.77	13 (25%)
24	XAT	5	618	-	41,47,47	0.93	2 (4%)	54,74,74	2.66	27 (50%)
22	CLA	B	837	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	7 (8%)
22	CLA	9	611	26	69,73,73	1.18	7 (10%)	82,113,113	1.15	5 (6%)
30	SF4	C	102	8	0,12,12	-	-	-	-	-
22	CLA	V	612	1	41,46,73	1.58	8 (19%)	51,81,113	1.41	5 (9%)
26	LHG	W	2630	22	44,44,48	0.98	2 (4%)	47,50,54	0.98	2 (4%)
27	BCR	3	620	-	41,41,41	0.72	0	56,56,56	2.12	19 (33%)
21	CHL	1	607	-	41,55,74	4.20	18 (43%)	35,91,114	2.71	12 (34%)
25	NEX	U	2623	-	40,46,46	1.18	4 (10%)	50,70,70	2.31	17 (34%)
22	CLA	B	818	-	68,72,73	1.16	7 (10%)	80,111,113	1.15	5 (6%)
27	BCR	O	2004	-	41,41,41	0.77	0	56,56,56	2.13	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	823	-	56,62,73	1.23	6 (10%)	65,99,113	1.22	6 (9%)
21	CHL	4	606	-	40,54,74	4.20	18 (45%)	34,90,114	3.10	12 (35%)
22	CLA	B	811	-	65,69,73	1.21	7 (10%)	77,108,113	1.10	5 (6%)
23	LUT	7	618	-	42,43,43	0.80	0	51,60,60	1.69	10 (19%)
22	CLA	3	606	-	50,54,73	1.35	7 (14%)	59,90,113	1.26	3 (5%)
22	CLA	8	613	5	59,63,73	1.27	6 (10%)	70,101,113	1.20	4 (5%)
21	CHL	W	605	1	33,46,74	4.16	16 (48%)	30,81,114	2.40	10 (33%)
22	CLA	B	805	-	69,73,73	1.16	7 (10%)	82,113,113	1.19	8 (9%)
27	BCR	4	621	-	41,41,41	0.81	0	56,56,56	3.13	16 (28%)
22	CLA	K	201	16	46,50,73	1.41	7 (15%)	53,85,113	1.34	4 (7%)
22	CLA	B	829	-	69,73,73	1.17	6 (8%)	82,113,113	1.08	3 (3%)
22	CLA	9	602	20	64,68,73	1.20	8 (12%)	76,107,113	1.27	7 (9%)
22	CLA	B	832	-	69,73,73	1.17	7 (10%)	82,113,113	1.18	8 (9%)
21	CHL	W	606	-	33,46,74	4.15	16 (48%)	30,81,114	2.40	9 (30%)
22	CLA	K	206	16	46,50,73	1.41	7 (15%)	53,85,113	1.25	4 (7%)
22	CLA	3	614	-	49,53,73	1.38	7 (14%)	58,89,113	1.27	5 (8%)
22	CLA	V	603	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	3 (3%)
22	CLA	A	809	6	60,64,73	1.23	7 (11%)	71,102,113	1.21	6 (8%)
27	BCR	B	847	-	41,41,41	0.76	0	56,56,56	2.16	18 (32%)
22	CLA	V	613	1	60,64,73	1.24	6 (10%)	70,101,113	1.24	6 (8%)
22	CLA	V	602	1	63,67,73	1.22	6 (9%)	74,105,113	1.16	7 (9%)
22	CLA	A	817	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	6 (7%)
22	CLA	B	821	-	54,58,73	1.32	7 (12%)	64,95,113	1.19	5 (7%)
27	BCR	K	205	-	41,41,41	0.83	1 (2%)	56,56,56	2.39	24 (42%)
22	CLA	A	843	-	69,73,73	1.16	8 (11%)	82,113,113	1.14	6 (7%)
25	NEX	V	2623	-	40,46,46	0.95	3 (7%)	50,70,70	2.45	18 (36%)
22	CLA	B	830	-	49,53,73	1.39	7 (14%)	58,89,113	1.20	5 (8%)
22	CLA	A	804	-	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
22	CLA	5	613	2	54,58,73	1.32	6 (11%)	64,95,113	1.23	7 (10%)
23	LUT	V	2621	-	42,43,43	0.78	0	51,60,60	1.74	12 (23%)
21	CHL	7	608	-	40,54,74	4.19	18 (45%)	34,90,114	2.95	13 (38%)
22	CLA	9	603	20	46,50,73	1.43	6 (13%)	53,85,113	1.26	3 (5%)
21	CHL	2	607	-	41,55,74	4.19	18 (43%)	35,91,114	2.93	12 (34%)
22	CLA	A	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.09	5 (6%)
22	CLA	4	609	5	49,53,73	1.36	7 (14%)	58,89,113	1.23	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	XAT	7	619	-	41,47,47	1.30	3 (7%)	54,74,74	5.80	20 (37%)
26	LHG	5	630	22	36,36,48	1.08	2 (5%)	39,42,54	1.08	3 (7%)
22	CLA	3	610	4	64,68,73	1.22	7 (10%)	76,107,113	1.14	5 (6%)
23	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.89	16 (31%)
22	CLA	7	602	4	64,68,73	1.23	6 (9%)	76,107,113	1.32	7 (9%)
26	LHG	A	846	-	46,46,48	0.96	2 (4%)	49,52,54	1.00	3 (6%)
28	LMG	2	631	-	47,47,55	0.98	2 (4%)	55,55,63	0.99	4 (7%)
21	CHL	8	606	-	40,54,74	4.24	19 (47%)	34,90,114	3.04	12 (35%)
22	CLA	3	603	4	69,73,73	1.17	7 (10%)	82,113,113	1.14	5 (6%)
25	NEX	W	2623	-	40,46,46	1.05	3 (7%)	50,70,70	2.74	18 (36%)
22	CLA	A	832	-	59,63,73	1.26	8 (13%)	70,101,113	1.28	5 (7%)
30	SF4	C	101	8	0,12,12	-	-	-	-	-
22	CLA	A	830	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	7 (8%)
22	CLA	4	611	26	49,53,73	1.40	8 (16%)	58,89,113	1.25	3 (5%)
27	BCR	M	2001	-	41,41,41	0.65	0	56,56,56	2.19	22 (39%)
22	CLA	B	823	-	49,53,73	1.38	6 (12%)	58,89,113	1.31	5 (8%)
30	SF4	A	853	6,7	0,12,12	-	-	-	-	-
22	CLA	6	609	3	59,63,73	1.26	7 (11%)	70,101,113	1.15	7 (10%)
22	CLA	A	811	-	59,63,73	1.25	7 (11%)	70,101,113	1.15	4 (5%)
22	CLA	1	612	2	50,54,73	1.35	7 (14%)	59,90,113	1.20	4 (6%)
22	CLA	U	611	26	49,53,73	1.39	6 (12%)	58,89,113	1.19	3 (5%)
23	LUT	3	618	-	42,43,43	0.77	1 (2%)	51,60,60	1.71	13 (25%)
22	CLA	O	2001	-	27,35,73	1.81	6 (22%)	32,60,113	1.41	3 (9%)
22	CLA	A	815	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
22	CLA	A	816	-	49,53,73	1.35	6 (12%)	58,89,113	1.30	5 (8%)
22	CLA	8	602	5	64,68,73	1.22	6 (9%)	76,107,113	1.12	5 (6%)
21	CHL	2	618	3	37,51,74	4.37	17 (45%)	30,86,114	3.05	13 (43%)
21	CHL	U	606	-	40,54,74	4.18	18 (45%)	34,90,114	3.09	12 (35%)
22	CLA	B	815	-	49,53,73	1.37	8 (16%)	58,89,113	1.22	4 (6%)
22	CLA	F	301	33	69,73,73	1.16	8 (11%)	82,113,113	1.10	5 (6%)
22	CLA	U	612	1	69,73,73	1.17	7 (10%)	82,113,113	1.07	4 (4%)
22	CLA	O	2003	-	27,35,73	1.83	6 (22%)	32,60,113	1.32	3 (9%)
24	XAT	8	620	-	41,47,47	1.29	6 (14%)	54,74,74	1.86	16 (29%)
27	BCR	B	843	-	41,41,41	0.70	0	56,56,56	2.20	22 (39%)
26	LHG	6	630	22	31,31,48	1.17	2 (6%)	34,37,54	1.09	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	826	-	69,73,73	1.17	7 (10%)	82,113,113	1.14	6 (7%)
22	CLA	B	802	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	5 (6%)
22	CLA	4	614	-	50,54,73	1.35	7 (14%)	59,90,113	1.21	4 (6%)
22	CLA	A	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	8 (9%)
27	BCR	1	619	-	41,41,41	0.69	0	56,56,56	2.60	27 (48%)
21	CHL	9	605	-	31,46,74	4.35	16 (51%)	25,80,114	2.75	8 (32%)
22	CLA	1	613	2	54,58,73	1.31	7 (12%)	64,95,113	1.22	4 (6%)
28	LMG	L	307	-	44,44,55	1.00	2 (4%)	52,52,63	0.93	2 (3%)
22	CLA	J	101	15	54,58,73	1.32	7 (12%)	64,95,113	1.27	6 (9%)
22	CLA	K	203	-	59,63,73	1.26	7 (11%)	70,101,113	1.17	6 (8%)
22	CLA	7	604	-	54,58,73	1.32	7 (12%)	64,95,113	1.23	6 (9%)
21	CHL	9	608	-	37,51,74	4.28	19 (51%)	30,86,114	3.00	11 (36%)
28	LMG	G	202	-	32,32,55	1.22	3 (9%)	40,40,63	1.16	2 (5%)
22	CLA	U	614	-	46,50,73	1.40	7 (15%)	53,85,113	1.13	3 (5%)
22	CLA	8	614	-	49,53,73	1.39	7 (14%)	58,89,113	1.26	5 (8%)
24	XAT	1	618	-	41,47,47	0.94	2 (4%)	54,74,74	2.49	25 (46%)
27	BCR	B	801	-	41,41,41	0.73	0	56,56,56	1.92	16 (28%)
22	CLA	W	602	1	64,68,73	1.21	8 (12%)	76,107,113	1.13	4 (5%)
21	CHL	2	608	-	40,54,74	4.29	18 (45%)	34,90,114	2.73	12 (35%)
22	CLA	B	817	-	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
22	CLA	6	612	3	49,53,73	1.40	6 (12%)	58,89,113	1.21	4 (6%)
22	CLA	6	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.22	4 (6%)
22	CLA	A	812	-	69,73,73	1.14	8 (11%)	82,113,113	1.10	4 (4%)
22	CLA	A	814	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
22	CLA	1	602	2	69,73,73	1.16	7 (10%)	82,113,113	1.10	5 (6%)
22	CLA	B	840	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	5 (6%)
22	CLA	5	602	2	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
22	CLA	W	611	26	43,48,73	1.54	8 (18%)	51,83,113	1.25	5 (9%)
22	CLA	B	812	-	46,52,73	1.36	6 (13%)	53,87,113	1.28	5 (9%)

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
22	CLA	L	304	-	1/1/14/20	15/33/109/115	-
22	CLA	7	606	-	1/1/11/20	9/17/93/115	-
22	CLA	B	816	-	1/1/15/20	9/39/115/115	-
22	CLA	1	614	-	1/1/12/20	11/19/95/115	-
22	CLA	A	803	-	1/1/15/20	8/39/115/115	-
22	CLA	3	609	4	1/1/15/20	14/39/115/115	-
21	CHL	4	608	-	3/3/16/26	5/15/113/137	-
22	CLA	U	602	1	1/1/15/20	11/39/115/115	-
22	CLA	A	825	-	-	17/39/115/115	-
26	LHG	9	2630	22	-	13/32/32/53	-
22	CLA	6	614	-	1/1/12/20	4/21/97/115	-
22	CLA	B	834	-	1/1/15/20	13/39/115/115	-
22	CLA	A	824	-	1/1/14/20	14/36/112/115	-
22	CLA	B	819	-	1/1/14/20	14/33/109/115	-
22	CLA	F	304	11	1/1/8/20	7/20/73/115	-
21	CHL	8	618	5	3/3/15/26	0/12/110/137	-
22	CLA	U	613	1	1/1/15/20	9/39/115/115	-
22	CLA	W	614	-	1/1/10/20	1/6/82/115	-
21	CHL	4	607	-	3/3/16/26	3/17/115/137	-
22	CLA	A	842	-	1/1/13/20	8/27/103/115	-
26	LHG	V	2630	22	-	7/46/46/53	-
22	CLA	B	804	-	1/1/15/20	8/39/115/115	-
27	BCR	2	621	-	-	6/29/63/63	0/2/2/2
27	BCR	8	621	-	-	4/29/63/63	0/2/2/2
26	LHG	3	630	22	-	7/36/36/53	-
21	CHL	9	601	20	3/3/14/26	1/4/102/137	-
32	DGD	B	850	-	-	17/55/95/95	0/2/2/2
22	CLA	B	838	-	-	5/18/94/115	-
23	LUT	6	619	-	-	2/29/67/67	0/2/2/2
22	CLA	A	819	-	1/1/14/20	8/36/112/115	-
22	CLA	3	611	26	1/1/13/20	12/27/103/115	-
27	BCR	A	849	-	-	4/29/63/63	0/2/2/2
26	LHG	A	847	22	-	14/35/35/53	-
31	LMT	A	857	-	-	7/21/61/61	0/2/2/2
21	CHL	6	602	3	3/3/18/26	9/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	814	-	1/1/15/20	12/39/115/115	-
26	LHG	B	851	22	-	9/39/39/53	-
27	BCR	6	621	-	-	6/29/63/63	0/2/2/2
22	CLA	A	826	-	1/1/15/20	10/39/115/115	-
22	CLA	3	612	4	1/1/15/20	14/39/115/115	-
24	XAT	6	620	-	-	3/31/93/93	0/4/4/4
22	CLA	B	836	-	1/1/12/20	9/24/100/115	-
22	CLA	3	615	-	1/1/12/20	4/25/101/115	-
22	CLA	5	606	2	1/1/11/20	2/15/91/115	-
22	CLA	A	839	-	1/1/14/20	8/33/109/115	-
22	CLA	7	603	4	1/1/11/20	6/15/91/115	-
22	CLA	1	608	-	1/1/11/20	5/15/91/115	-
27	BCR	G	205	-	-	4/29/63/63	0/2/2/2
27	BCR	A	851	-	-	1/29/63/63	0/2/2/2
22	CLA	8	604	-	1/1/12/20	6/21/97/115	-
22	CLA	5	604	-	1/1/10/20	2/10/86/115	-
22	CLA	W	613	1	1/1/14/20	7/33/109/115	-
22	CLA	7	614	-	1/1/10/20	4/10/86/115	-
22	CLA	B	822	-	1/1/14/20	16/33/109/115	-
23	LUT	W	2621	-	-	2/29/67/67	0/2/2/2
22	CLA	2	603	-	1/1/11/20	5/17/93/115	-
22	CLA	2	604	-	1/1/12/20	4/21/97/115	-
22	CLA	A	840	-	1/1/12/20	8/21/97/115	-
22	CLA	4	604	-	1/1/13/20	7/27/103/115	-
22	CLA	4	613	5	1/1/13/20	6/27/103/115	-
22	CLA	B	820	-	1/1/13/20	12/27/103/115	-
22	CLA	U	604	-	1/1/12/20	8/24/100/115	-
22	CLA	A	818	-	1/1/15/20	5/39/115/115	-
22	CLA	1	604	-	-	10/21/97/115	-
21	CHL	V	609	1	3/3/14/26	2/6/104/137	-
21	CHL	W	609	1	3/3/14/26	3/6/104/137	-
22	CLA	G	201	-	1/1/11/20	6/15/91/115	-
21	CHL	U	605	1	3/3/15/26	0/4/100/137	-
26	LHG	4	630	22	-	20/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	821	-	1/1/13/20	4/27/103/115	-
26	LHG	8	630	22	-	8/42/42/53	-
22	CLA	B	824	-	1/1/15/20	9/39/115/115	-
22	CLA	B	841	26	1/1/15/20	8/39/115/115	-
22	CLA	B	833	-	1/1/15/20	14/39/115/115	-
22	CLA	K	204	-	1/1/15/20	14/39/115/115	-
22	CLA	3	602	4	1/1/15/20	7/39/115/115	-
22	CLA	V	610	1	1/1/10/20	2/6/82/115	-
22	CLA	B	835	-	1/1/11/20	2/15/91/115	-
22	CLA	B	827	-	1/1/13/20	12/29/105/115	-
21	CHL	2	601	3	3/3/16/26	3/15/113/137	-
22	CLA	4	601	5	1/1/12/20	9/21/97/115	-
22	CLA	L	303	-	1/1/15/20	11/39/115/115	-
22	CLA	5	612	2	1/1/11/20	8/17/93/115	-
22	CLA	A	802	-	1/1/15/20	8/39/115/115	-
21	CHL	2	606	-	3/3/16/26	6/15/113/137	-
22	CLA	A	828	-	1/1/15/20	11/39/115/115	-
22	CLA	A	837	6	-	17/39/115/115	-
23	LUT	9	621	-	-	1/29/67/67	0/2/2/2
21	CHL	U	601	1	3/3/20/26	17/35/131/137	-
27	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	A	838	-	1/1/13/20	9/27/103/115	-
22	CLA	H	201	-	1/1/9/20	2/4/80/115	-
22	CLA	7	609	4	1/1/13/20	10/30/106/115	-
26	LHG	1	630	22	-	22/53/53/53	-
26	LHG	U	2630	22	-	10/49/49/53	-
21	CHL	V	606	-	3/3/15/26	2/4/100/137	-
21	CHL	6	601	3	3/3/20/26	13/39/137/137	-
22	CLA	8	610	5	1/1/13/20	6/27/103/115	-
27	BCR	L	306	-	-	3/29/63/63	0/2/2/2
22	CLA	5	610	2	1/1/13/20	4/27/103/115	-
22	CLA	6	603	-	1/1/11/20	7/17/93/115	-
28	LMG	J	103	-	-	12/50/70/70	0/1/1/1
22	CLA	W	610	1	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	4	620	-	-	3/31/93/93	0/4/4/4
22	CLA	5	603	-	1/1/11/20	8/15/91/115	-
22	CLA	W	603	-	1/1/10/20	3/6/82/115	-
23	LUT	9	624	-	-	3/29/67/67	0/2/2/2
22	CLA	B	808	-	1/1/15/20	12/39/115/115	-
22	CLA	4	610	5	1/1/14/20	11/35/111/115	-
21	CHL	V	607	-	3/3/15/26	2/8/104/137	-
22	CLA	4	603	-	1/1/15/20	15/39/115/115	-
22	CLA	1	610	2	1/1/15/20	11/39/115/115	-
23	LUT	U	2621	-	-	1/29/67/67	0/2/2/2
21	CHL	W	608	-	3/3/15/26	1/8/104/137	-
31	LMT	B	849	-	-	5/17/57/61	0/2/2/2
22	CLA	G	203	-	1/1/12/20	7/21/97/115	-
22	CLA	A	820	-	1/1/15/20	9/39/115/115	-
22	CLA	A	829	-	1/1/14/20	7/33/109/115	-
22	CLA	4	602	5	1/1/15/20	17/39/115/115	-
22	CLA	5	608	-	1/1/12/20	6/21/97/115	-
22	CLA	U	610	1	1/1/15/20	13/39/115/115	-
21	CHL	9	607	-	3/3/15/26	1/12/110/137	-
22	CLA	B	813	-	1/1/15/20	12/39/115/115	-
22	CLA	W	612	1	1/1/10/20	2/4/80/115	-
22	CLA	7	617	-	1/1/11/20	7/17/93/115	-
27	BCR	B	848	-	-	3/29/63/63	0/2/2/2
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
22	CLA	A	827	33	-	13/39/115/115	-
21	CHL	8	607	-	3/3/16/26	3/15/113/137	-
22	CLA	B	807	-	-	4/39/115/115	-
21	CHL	U	608	-	3/3/15/26	3/8/104/137	-
22	CLA	L	302	17	1/1/15/20	22/39/115/115	-
21	CHL	5	607	2	3/3/14/26	0/4/102/137	-
22	CLA	7	612	4	1/1/11/20	4/15/91/115	-
21	CHL	6	608	-	3/3/16/26	4/18/116/137	-
22	CLA	7	615	-	1/1/10/20	2/8/84/115	-
21	CHL	2	602	3	3/3/19/26	10/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	607	4	1/1/11/20	2/15/91/115	-
21	CHL	9	606	-	3/3/15/26	3/13/111/137	-
22	CLA	B	831	-	1/1/15/20	14/39/115/115	-
22	CLA	3	604	-	1/1/13/20	8/27/103/115	-
31	LMT	G	206	-	-	7/21/61/61	0/2/2/2
22	CLA	A	801	-	1/1/15/20	12/39/115/115	-
23	LUT	2	619	-	-	12/29/67/67	0/2/2/2
23	LUT	8	619	-	-	1/29/67/67	0/2/2/2
22	CLA	V	614	-	1/1/11/20	4/15/91/115	-
28	LMG	J	104	-	-	6/30/50/70	0/1/1/1
21	CHL	U	609	1	3/3/20/26	20/39/137/137	-
22	CLA	3	613	4	1/1/15/20	13/39/115/115	-
22	CLA	5	616	2	1/1/11/20	4/17/93/115	-
22	CLA	9	610	20	1/1/13/20	9/27/103/115	-
22	CLA	B	810	-	1/1/15/20	16/39/115/115	-
22	CLA	A	822	-	1/1/15/20	11/39/115/115	-
22	CLA	7	611	26	1/1/10/20	4/10/86/115	-
27	BCR	L	305	-	-	2/29/63/63	0/2/2/2
22	CLA	A	836	-	1/1/14/20	12/37/105/115	-
22	CLA	6	611	26	1/1/11/20	6/15/91/115	-
27	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	CLA	A	810	6	1/1/15/20	17/39/115/115	-
23	LUT	5	617	-	-	14/29/67/67	0/2/2/2
21	CHL	V	605	1	3/3/15/26	2/10/108/137	-
22	CLA	8	609	5	1/1/13/20	8/27/103/115	-
27	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	CLA	V	604	-	1/1/12/20	7/21/97/115	-
21	CHL	W	607	-	3/3/15/26	4/8/104/137	-
22	CLA	A	845	26	1/1/15/20	11/39/115/115	-
22	CLA	7	610	4	1/1/13/20	7/27/103/115	-
24	XAT	2	620	-	-	0/31/93/93	0/4/4/4
24	XAT	V	2622	-	-	2/31/93/93	0/4/4/4
22	CLA	8	601	5	1/1/12/20	4/21/97/115	-
22	CLA	2	613	3	1/1/13/20	12/30/106/115	-
22	CLA	1	616	2	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	831	-	1/1/15/20	10/39/115/115	-
23	LUT	V	2620	-	-	1/29/67/67	0/2/2/2
21	CHL	4	618	5	3/3/15/26	2/12/110/137	-
22	CLA	9	609	20	1/1/11/20	4/15/91/115	-
22	CLA	8	612	5	1/1/11/20	8/17/93/115	-
22	CLA	A	834	-	1/1/15/20	11/39/115/115	-
22	CLA	A	808	-	1/1/14/20	6/33/109/115	-
22	CLA	2	609	3	1/1/11/20	7/17/93/115	-
22	CLA	3	617	-	1/1/13/20	13/29/102/115	-
26	LHG	2	630	22	-	7/36/36/53	-
22	CLA	W	604	-	1/1/10/20	2/12/88/115	-
22	CLA	6	613	3	1/1/15/20	10/39/115/115	-
22	CLA	2	611	26	1/1/11/20	7/15/91/115	-
22	CLA	8	611	26	1/1/13/20	4/27/103/115	-
22	CLA	A	813	-	1/1/13/20	6/27/103/115	-
23	LUT	1	617	-	-	0/29/67/67	0/2/2/2
27	BCR	A	848	-	-	4/29/63/63	0/2/2/2
27	BCR	B	845	-	-	9/29/63/63	0/2/2/2
21	CHL	V	601	1	3/3/20/26	19/35/131/137	-
22	CLA	A	854	-	1/1/14/20	17/33/109/115	-
27	BCR	L	301	-	-	6/29/63/63	0/2/2/2
22	CLA	V	611	26	1/1/10/20	2/8/84/115	-
22	CLA	5	611	26	1/1/11/20	4/17/93/115	-
22	CLA	A	806	-	1/1/15/20	13/39/115/115	-
27	BCR	I	101	-	-	3/29/63/63	0/2/2/2
22	CLA	B	825	-	1/1/15/20	9/39/115/115	-
22	CLA	2	612	3	1/1/11/20	7/15/91/115	-
22	CLA	A	807	6	1/1/15/20	16/39/115/115	-
22	CLA	1	606	-	1/1/11/20	6/15/91/115	-
27	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	B	806	-	1/1/15/20	16/39/115/115	-
22	CLA	F	303	-	1/1/11/20	2/15/91/115	-
27	BCR	7	621	-	-	1/29/63/63	0/2/2/2
21	CHL	6	606	-	3/3/16/26	7/15/113/137	-
27	BCR	7	620	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	K	208	-	-	7/21/61/61	0/2/2/2
22	CLA	A	833	-	1/1/13/20	8/27/103/115	-
22	CLA	4	612	5	1/1/11/20	6/15/91/115	-
22	CLA	5	609	2	1/1/10/20	5/10/86/115	-
21	CHL	W	601	1	3/3/20/26	15/35/131/137	-
21	CHL	3	608	-	3/3/18/26	10/27/125/137	-
22	CLA	2	610	3	1/1/14/20	5/33/109/115	-
24	XAT	3	619	-	-	0/31/93/93	0/4/4/4
22	CLA	B	839	-	1/1/15/20	7/39/115/115	-
22	CLA	2	614	-	1/1/12/20	3/21/97/115	-
22	CLA	3	607	4	1/1/12/20	9/21/97/115	-
27	BCR	F	305	-	-	5/29/63/63	0/2/2/2
29	PQN	A	844	-	-	7/23/43/43	0/2/2/2
21	CHL	6	618	3	3/3/16/26	9/17/115/137	-
22	CLA	9	604	-	1/1/10/20	2/13/89/115	-
22	CLA	A	835	-	1/1/15/20	13/39/115/115	-
22	CLA	1	611	26	1/1/15/20	16/39/115/115	-
21	CHL	6	607	-	3/3/16/26	5/17/115/137	-
22	CLA	B	828	-	1/1/15/20	12/39/115/115	-
24	XAT	W	2622	-	-	1/31/93/93	0/4/4/4
22	CLA	G	204	12	1/1/11/20	4/17/93/115	-
21	CHL	5	601	2	3/3/17/26	4/21/119/137	-
22	CLA	8	603	-	1/1/13/20	9/27/103/115	-
22	CLA	1	609	2	1/1/15/20	14/39/115/115	-
22	CLA	B	809	7	1/1/15/20	11/39/115/115	-
27	BCR	K	202	-	-	4/29/63/63	0/2/2/2
23	LUT	W	2620	-	-	1/29/67/67	0/2/2/2
27	BCR	3	621	-	-	0/29/63/63	0/2/2/2
27	BCR	A	856	-	-	1/27/61/63	0/2/2/2
27	BCR	B	1609	-	-	5/29/63/63	0/2/2/2
23	LUT	9	620	-	-	1/29/67/67	0/2/2/2
22	CLA	7	613	4	1/1/13/20	8/27/103/115	-
22	CLA	B	803	-	1/1/15/20	12/39/115/115	-
21	CHL	8	608	-	3/3/17/26	4/21/119/137	-
22	CLA	6	610	3	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	614	-	1/1/10/20	3/13/89/115	-
22	CLA	9	613	20	1/1/12/20	3/24/100/115	-
21	CHL	V	608	-	3/3/15/26	2/8/104/137	-
28	LMG	A	860	-	-	12/29/49/70	0/1/1/1
21	CHL	1	601	2	3/3/18/26	8/27/125/137	-
25	NEX	9	623	-	-	2/27/83/83	0/3/3/3
22	CLA	1	603	-	1/1/13/20	11/27/103/115	-
22	CLA	9	612	20	1/1/9/20	1/6/82/115	-
24	XAT	U	2622	-	-	1/31/93/93	0/4/4/4
22	CLA	U	603	-	1/1/15/20	10/39/115/115	-
26	LHG	7	630	22	-	11/38/38/53	-
21	CHL	U	607	-	3/3/20/26	14/39/137/137	-
22	CLA	O	2002	-	1/1/13/20	12/27/103/115	-
23	LUT	U	2620	-	-	0/29/67/67	0/2/2/2
24	XAT	5	618	-	-	5/31/93/93	0/4/4/4
22	CLA	B	837	-	1/1/15/20	8/39/115/115	-
22	CLA	9	611	26	1/1/15/20	14/39/115/115	-
30	SF4	C	102	8	-	-	0/6/5/5
22	CLA	V	612	1	1/1/10/20	1/4/80/115	-
26	LHG	W	2630	22	-	13/49/49/53	-
27	BCR	3	620	-	-	2/29/63/63	0/2/2/2
21	CHL	1	607	-	3/3/16/26	7/17/115/137	-
25	NEX	U	2623	-	-	3/27/83/83	0/3/3/3
22	CLA	B	818	-	1/1/14/20	15/38/114/115	-
27	BCR	O	2004	-	-	5/29/63/63	0/2/2/2
22	CLA	A	823	-	1/1/13/20	8/27/103/115	-
21	CHL	4	606	-	3/3/16/26	1/15/113/137	-
22	CLA	B	811	-	1/1/14/20	7/35/111/115	-
23	LUT	7	618	-	-	1/29/67/67	0/2/2/2
22	CLA	3	606	-	1/1/11/20	10/17/93/115	-
22	CLA	8	613	5	1/1/13/20	6/27/103/115	-
21	CHL	W	605	1	3/3/15/26	0/4/100/137	-
22	CLA	B	805	-	1/1/15/20	10/39/115/115	-
27	BCR	4	621	-	-	7/29/63/63	0/2/2/2
22	CLA	K	201	16	1/1/10/20	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	829	-	1/1/15/20	7/39/115/115	-
22	CLA	9	602	20	1/1/14/20	10/33/109/115	-
22	CLA	B	832	-	-	10/39/115/115	-
21	CHL	W	606	-	3/3/15/26	0/4/100/137	-
22	CLA	K	206	16	1/1/10/20	4/12/88/115	-
22	CLA	3	614	-	1/1/11/20	6/15/91/115	-
22	CLA	V	603	-	1/1/14/20	12/33/109/115	-
22	CLA	A	809	6	1/1/13/20	6/29/105/115	-
27	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	V	613	1	1/1/12/20	12/28/104/115	-
22	CLA	V	602	1	-	8/32/108/115	-
22	CLA	A	817	-	1/1/15/20	14/39/115/115	-
22	CLA	B	821	-	1/1/12/20	6/21/97/115	-
27	BCR	K	205	-	-	3/29/63/63	0/2/2/2
22	CLA	A	843	-	1/1/15/20	15/39/115/115	-
25	NEX	V	2623	-	-	2/27/83/83	0/3/3/3
22	CLA	B	830	-	1/1/11/20	6/15/91/115	-
22	CLA	A	804	-	1/1/15/20	19/39/115/115	-
22	CLA	5	613	2	-	9/21/97/115	-
23	LUT	V	2621	-	-	2/29/67/67	0/2/2/2
21	CHL	7	608	-	3/3/16/26	3/15/113/137	-
22	CLA	9	603	20	1/1/10/20	5/12/88/115	-
21	CHL	2	607	-	3/3/16/26	1/17/115/137	-
22	CLA	A	841	-	1/1/15/20	11/39/115/115	-
22	CLA	4	609	5	1/1/11/20	6/15/91/115	-
24	XAT	7	619	-	-	6/31/93/93	0/4/4/4
26	LHG	5	630	22	-	4/41/41/53	-
22	CLA	3	610	4	1/1/14/20	9/33/109/115	-
23	LUT	4	619	-	-	0/29/67/67	0/2/2/2
22	CLA	7	602	4	-	10/33/109/115	-
26	LHG	A	846	-	-	10/51/51/53	-
28	LMG	2	631	-	-	12/42/62/70	0/1/1/1
21	CHL	8	606	-	3/3/16/26	0/15/113/137	-
22	CLA	3	603	4	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	NEX	W	2623	-	-	7/27/83/83	0/3/3/3
22	CLA	A	832	-	1/1/13/20	7/27/103/115	-
30	SF4	C	101	8	-	-	0/6/5/5
22	CLA	A	830	-	1/1/15/20	16/39/115/115	-
22	CLA	4	611	26	1/1/11/20	4/15/91/115	-
27	BCR	M	2001	-	-	5/29/63/63	0/2/2/2
22	CLA	B	823	-	1/1/11/20	3/15/91/115	-
30	SF4	A	853	6,7	-	-	0/6/5/5
22	CLA	6	609	3	1/1/13/20	2/27/103/115	-
22	CLA	A	811	-	1/1/13/20	8/27/103/115	-
22	CLA	1	612	2	1/1/11/20	2/17/93/115	-
22	CLA	U	611	26	1/1/11/20	8/15/91/115	-
23	LUT	3	618	-	-	1/29/67/67	0/2/2/2
22	CLA	O	2001	-	1/1/5/20	-	-
22	CLA	A	815	-	1/1/15/20	13/39/115/115	-
22	CLA	A	816	-	1/1/11/20	5/15/91/115	-
22	CLA	8	602	5	1/1/14/20	8/33/109/115	-
21	CHL	2	618	3	3/3/15/26	2/12/110/137	-
21	CHL	U	606	-	3/3/16/26	7/15/113/137	-
22	CLA	B	815	-	1/1/11/20	3/15/91/115	-
22	CLA	F	301	33	1/1/15/20	14/39/115/115	-
22	CLA	U	612	1	1/1/15/20	12/39/115/115	-
22	CLA	O	2003	-	1/1/5/20	-	-
24	XAT	8	620	-	-	17/31/93/93	0/4/4/4
27	BCR	B	843	-	-	5/29/63/63	0/2/2/2
26	LHG	6	630	22	-	8/36/36/53	-
22	CLA	B	826	-	1/1/15/20	9/39/115/115	-
22	CLA	B	802	-	1/1/15/20	10/39/115/115	-
22	CLA	4	614	-	1/1/11/20	6/17/93/115	-
22	CLA	A	805	-	-	16/39/115/115	-
27	BCR	1	619	-	-	6/29/63/63	0/2/2/2
21	CHL	9	605	-	3/3/14/26	0/2/100/137	-
22	CLA	1	613	2	1/1/12/20	7/21/97/115	-
28	LMG	L	307	-	-	14/39/59/70	0/1/1/1
22	CLA	J	101	15	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	203	-	1/1/13/20	10/27/103/115	-
22	CLA	7	604	-	1/1/12/20	6/21/97/115	-
21	CHL	9	608	-	3/3/15/26	0/12/110/137	-
28	LMG	G	202	-	-	9/27/47/70	0/1/1/1
22	CLA	U	614	-	1/1/10/20	2/12/88/115	-
22	CLA	8	614	-	1/1/11/20	9/15/91/115	-
24	XAT	1	618	-	-	0/31/93/93	0/4/4/4
27	BCR	B	801	-	-	4/29/63/63	0/2/2/2
22	CLA	W	602	1	1/1/14/20	4/33/109/115	-
21	CHL	2	608	-	3/3/16/26	3/15/113/137	-
22	CLA	B	817	-	1/1/15/20	15/39/115/115	-
22	CLA	6	612	3	1/1/11/20	6/15/91/115	-
22	CLA	6	604	-	1/1/12/20	4/21/97/115	-
22	CLA	A	812	-	1/1/15/20	10/39/115/115	-
22	CLA	A	814	-	1/1/15/20	19/39/115/115	-
22	CLA	1	602	2	1/1/15/20	14/39/115/115	-
22	CLA	B	840	-	1/1/15/20	14/39/115/115	-
22	CLA	5	602	2	1/1/14/20	14/33/109/115	-
22	CLA	W	611	26	1/1/10/20	1/8/84/115	-
22	CLA	B	812	-	1/1/11/20	4/15/91/115	-

The worst 5 of 2507 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	601	CHL	C2C-C3C	10.61	1.46	1.36
21	6	607	CHL	C2C-C3C	10.59	1.46	1.36
21	1	607	CHL	C2C-C3C	10.59	1.46	1.36
21	V	609	CHL	C2C-C3C	10.58	1.46	1.36
21	9	601	CHL	C2C-C3C	10.56	1.46	1.36

The worst 5 of 3026 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	2622	XAT	O4-C5-C4	-23.41	91.55	113.49
24	4	620	XAT	O4-C5-C4	-22.54	92.37	113.49
24	7	619	XAT	O4-C5-C18	-21.79	90.69	115.05
24	6	620	XAT	O4-C5-C4	-20.96	93.85	113.49
24	7	619	XAT	O24-C25-C24	-20.37	94.40	113.49

5 of 357 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	U	601	CHL	ND
21	U	601	CHL	NA
21	U	601	CHL	NC
21	U	605	CHL	ND
21	U	605	CHL	NA

5 of 2623 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	U	601	CHL	CAD-CBD-CGD-O2D
21	U	606	CHL	C1A-C2A-CAA-CBA
21	U	607	CHL	C1A-C2A-CAA-CBA
21	U	607	CHL	C3A-C2A-CAA-CBA
21	U	608	CHL	CHA-CBD-CGD-O2D

There are no ring outliers.

226 monomers are involved in 491 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	304	CLA	2	0
22	7	606	CLA	2	0
22	A	803	CLA	5	0
22	3	609	CLA	2	0
21	4	608	CHL	3	0
22	A	825	CLA	1	0
22	B	819	CLA	1	0
22	F	304	CLA	1	0
21	8	618	CHL	2	0
21	4	607	CHL	1	0
22	B	804	CLA	2	0
27	2	621	BCR	4	0
27	8	621	BCR	8	0
21	9	601	CHL	2	0
22	B	838	CLA	1	0
23	6	619	LUT	2	0
22	A	819	CLA	1	0
27	A	849	BCR	1	0
22	B	814	CLA	1	0
27	6	621	BCR	5	0
22	3	612	CLA	2	0
24	6	620	XAT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	836	CLA	1	0
22	5	606	CLA	2	0
27	G	205	BCR	4	0
27	A	851	BCR	11	0
22	8	604	CLA	2	0
22	5	604	CLA	1	0
22	B	822	CLA	1	0
23	W	2621	LUT	1	0
22	2	604	CLA	2	0
22	4	604	CLA	3	0
22	U	604	CLA	2	0
21	V	609	CHL	2	0
21	W	609	CHL	1	0
22	G	201	CLA	4	0
26	4	630	LHG	3	0
22	B	824	CLA	1	0
22	B	833	CLA	2	0
22	K	204	CLA	2	0
22	V	610	CLA	2	0
22	B	827	CLA	1	0
21	2	601	CHL	1	0
22	4	601	CLA	1	0
22	L	303	CLA	1	0
22	5	612	CLA	1	0
22	A	802	CLA	3	0
21	2	606	CHL	3	0
22	A	828	CLA	3	0
22	A	837	CLA	3	0
23	9	621	LUT	4	0
27	A	852	BCR	8	0
22	7	609	CLA	4	0
26	1	630	LHG	2	0
26	U	2630	LHG	1	0
21	6	601	CHL	1	0
22	8	610	CLA	2	0
27	L	306	BCR	5	0
22	5	610	CLA	1	0
24	4	620	XAT	11	0
22	5	603	CLA	2	0
23	9	624	LUT	7	0
22	B	808	CLA	2	0
22	4	610	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	U	2621	LUT	4	0
21	W	608	CHL	1	0
22	A	829	CLA	1	0
22	4	602	CLA	2	0
22	U	610	CLA	2	0
21	9	607	CHL	2	0
22	B	813	CLA	3	0
27	B	848	BCR	1	0
22	A	827	CLA	2	0
21	8	607	CHL	1	0
22	B	807	CLA	1	0
21	5	607	CHL	1	0
21	6	608	CHL	4	0
21	2	602	CHL	2	0
22	7	607	CLA	1	0
21	9	606	CHL	8	0
22	B	831	CLA	1	0
22	3	604	CLA	1	0
22	A	801	CLA	3	0
23	2	619	LUT	4	0
23	8	619	LUT	2	0
21	U	609	CHL	2	0
22	3	613	CLA	2	0
22	B	810	CLA	1	0
27	L	305	BCR	4	0
22	A	836	CLA	3	0
27	J	102	BCR	4	0
22	A	810	CLA	3	0
23	5	617	LUT	3	0
21	V	605	CHL	1	0
22	8	609	CLA	2	0
27	B	844	BCR	2	0
22	A	845	CLA	1	0
22	7	610	CLA	1	0
24	2	620	XAT	7	0
22	8	601	CLA	1	0
22	2	613	CLA	1	0
23	V	2620	LUT	2	0
21	4	618	CHL	1	0
22	9	609	CLA	3	0
22	3	617	CLA	1	0
22	2	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	611	CLA	1	0
23	1	617	LUT	2	0
27	A	848	BCR	2	0
27	B	845	BCR	6	0
22	A	854	CLA	3	0
27	L	301	BCR	4	0
22	5	611	CLA	1	0
27	I	101	BCR	4	0
22	B	825	CLA	1	0
22	1	606	CLA	1	0
22	B	806	CLA	3	0
22	F	303	CLA	1	0
27	7	621	BCR	3	0
21	6	606	CHL	1	0
27	7	620	BCR	7	0
22	5	609	CLA	6	0
21	3	608	CHL	1	0
22	2	610	CLA	1	0
24	3	619	XAT	5	0
22	B	839	CLA	2	0
22	2	614	CLA	1	0
22	3	607	CLA	1	0
27	F	305	BCR	3	0
21	6	618	CHL	2	0
22	A	835	CLA	1	0
22	1	611	CLA	2	0
21	6	607	CHL	1	0
22	B	828	CLA	3	0
24	W	2622	XAT	1	0
21	5	601	CHL	4	0
22	1	609	CLA	1	0
27	K	202	BCR	7	0
23	W	2620	LUT	2	0
27	3	621	BCR	4	0
27	A	856	BCR	5	0
27	B	1609	BCR	8	0
23	9	620	LUT	4	0
22	7	613	CLA	2	0
22	B	803	CLA	4	0
21	8	608	CHL	2	0
22	6	610	CLA	4	0
21	1	601	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	9	623	NEX	4	0
22	9	612	CLA	1	0
21	U	607	CHL	4	0
22	O	2002	CLA	3	0
23	U	2620	LUT	2	0
24	5	618	XAT	7	0
22	B	837	CLA	1	0
22	9	611	CLA	2	0
26	W	2630	LHG	1	0
27	3	620	BCR	9	0
21	1	607	CHL	1	0
25	U	2623	NEX	1	0
22	B	818	CLA	1	0
27	O	2004	BCR	5	0
21	4	606	CHL	2	0
23	7	618	LUT	2	0
22	3	606	CLA	3	0
22	8	613	CLA	3	0
22	B	805	CLA	1	0
27	4	621	BCR	11	0
22	K	201	CLA	1	0
22	9	602	CLA	3	0
22	3	614	CLA	1	0
22	A	809	CLA	4	0
27	B	847	BCR	4	0
22	V	613	CLA	1	0
22	V	602	CLA	2	0
22	B	821	CLA	1	0
27	K	205	BCR	4	0
22	A	843	CLA	1	0
25	V	2623	NEX	2	0
22	5	613	CLA	1	0
23	V	2621	LUT	1	0
21	7	608	CHL	3	0
21	2	607	CHL	2	0
22	A	841	CLA	1	0
22	4	609	CLA	1	0
24	7	619	XAT	3	0
22	3	610	CLA	1	0
23	4	619	LUT	1	0
22	7	602	CLA	6	0
21	8	606	CHL	1	0

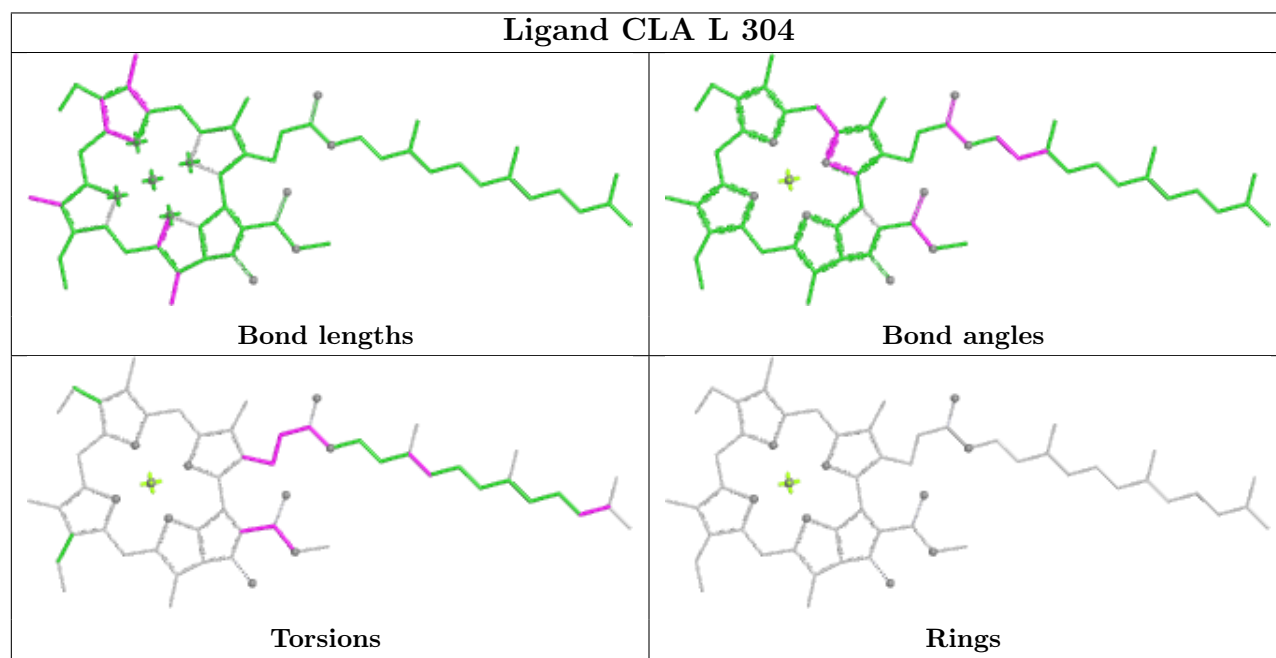
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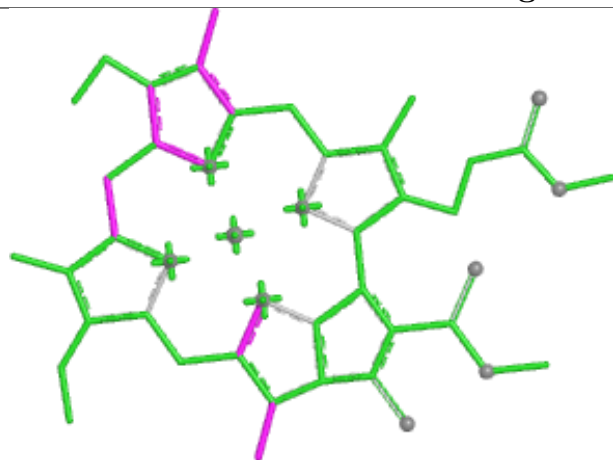
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25	W	2623	NEX	2	0
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22	A	830	CLA	1	0
22	4	611	CLA	1	0
27	M	2001	BCR	5	0
22	B	823	CLA	3	0
22	6	609	CLA	2	0
22	A	816	CLA	1	0
22	8	602	CLA	4	0
21	2	618	CHL	1	0
21	U	606	CHL	2	0
22	B	815	CLA	2	0
22	F	301	CLA	1	0
24	8	620	XAT	3	0
27	B	843	BCR	4	0
26	6	630	LHG	2	0
22	B	802	CLA	1	0
22	4	614	CLA	1	0
27	1	619	BCR	1	0
21	9	605	CHL	2	0
21	9	608	CHL	3	0
28	G	202	LMG	2	0
22	U	614	CLA	3	0
22	8	614	CLA	1	0
24	1	618	XAT	3	0
27	B	801	BCR	5	0
21	2	608	CHL	2	0
22	B	817	CLA	1	0
22	6	612	CLA	1	0
22	6	604	CLA	1	0
22	A	814	CLA	1	0
22	B	840	CLA	1	0
22	5	602	CLA	1	0
22	W	611	CLA	1	0
22	B	812	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

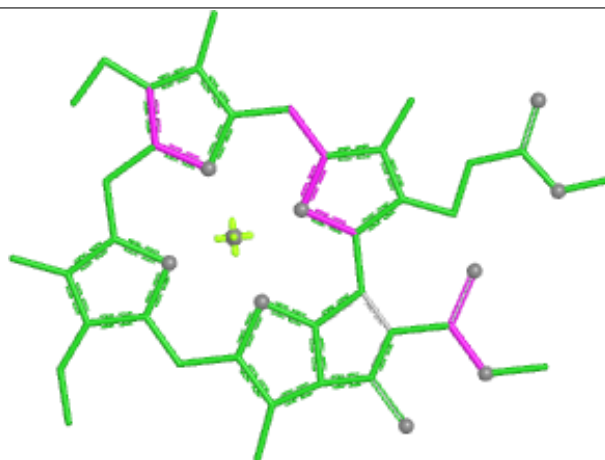
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



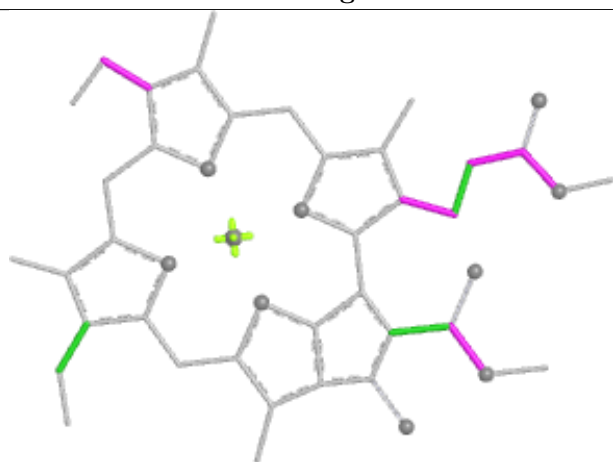
Ligand CLA 7 606



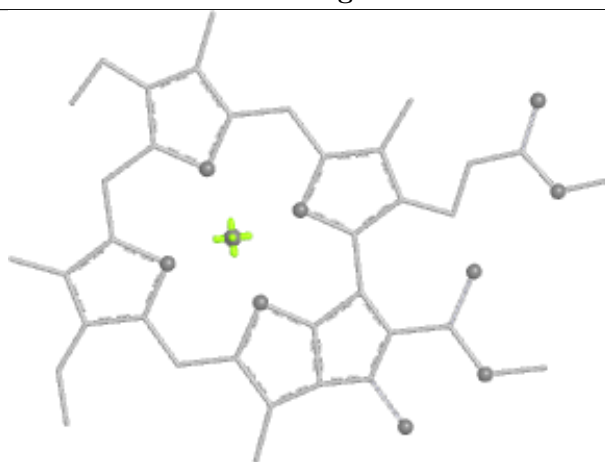
Bond lengths



Bond angles

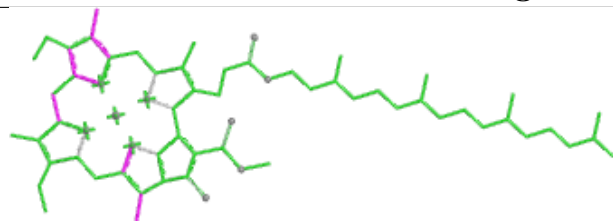


Torsions

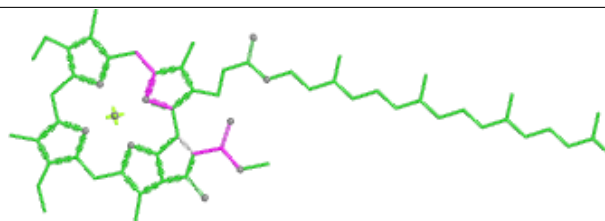


Rings

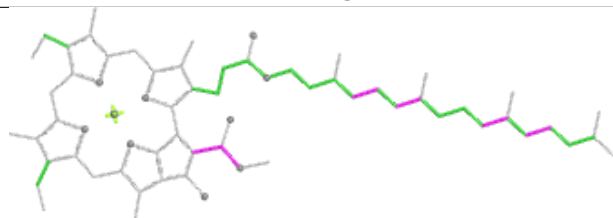
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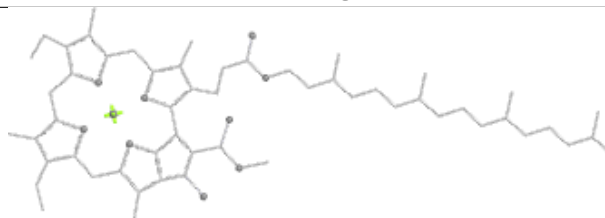
Bond lengths



Bond angles

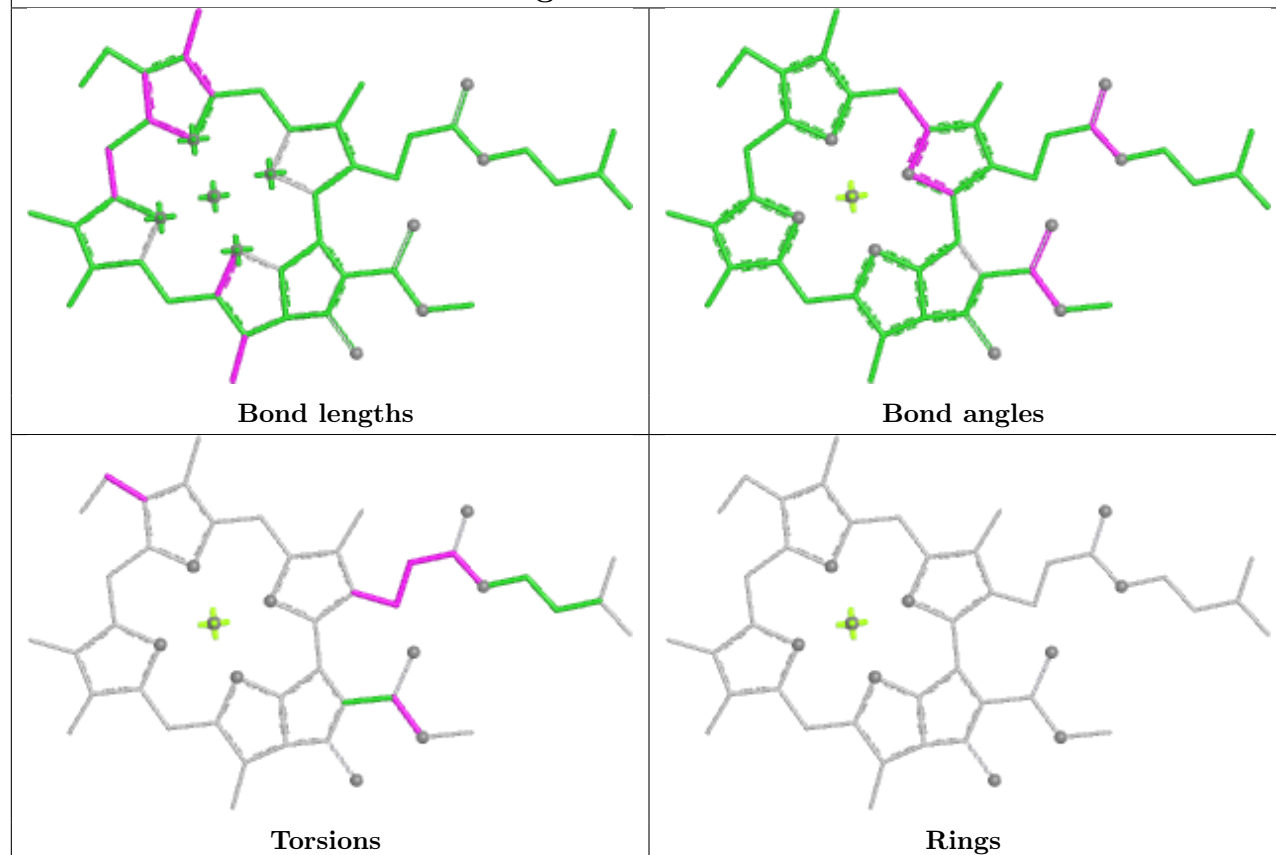


Torsions

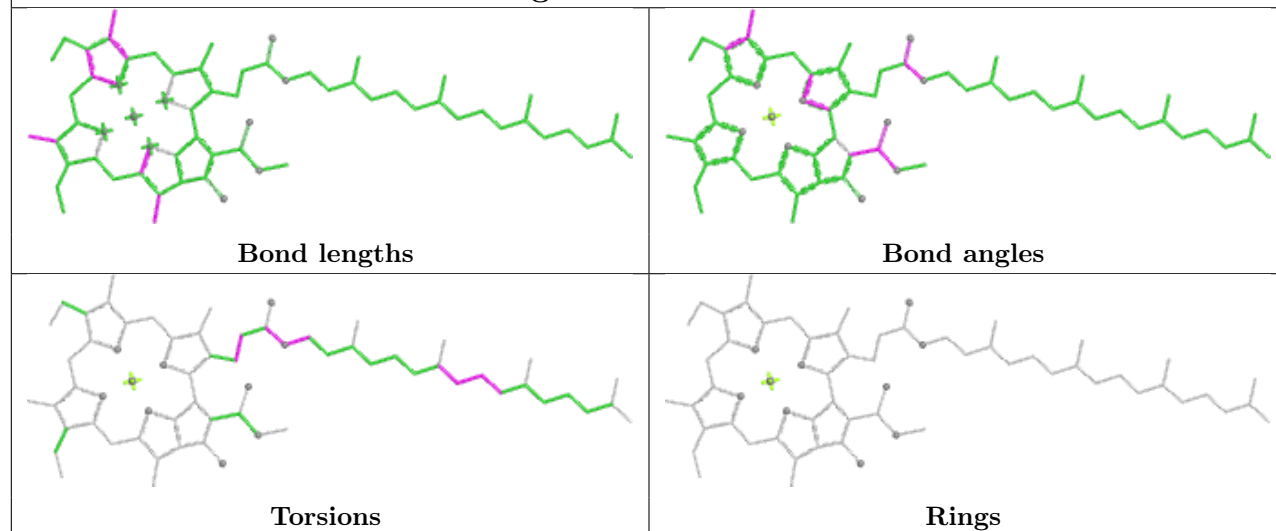


Rings

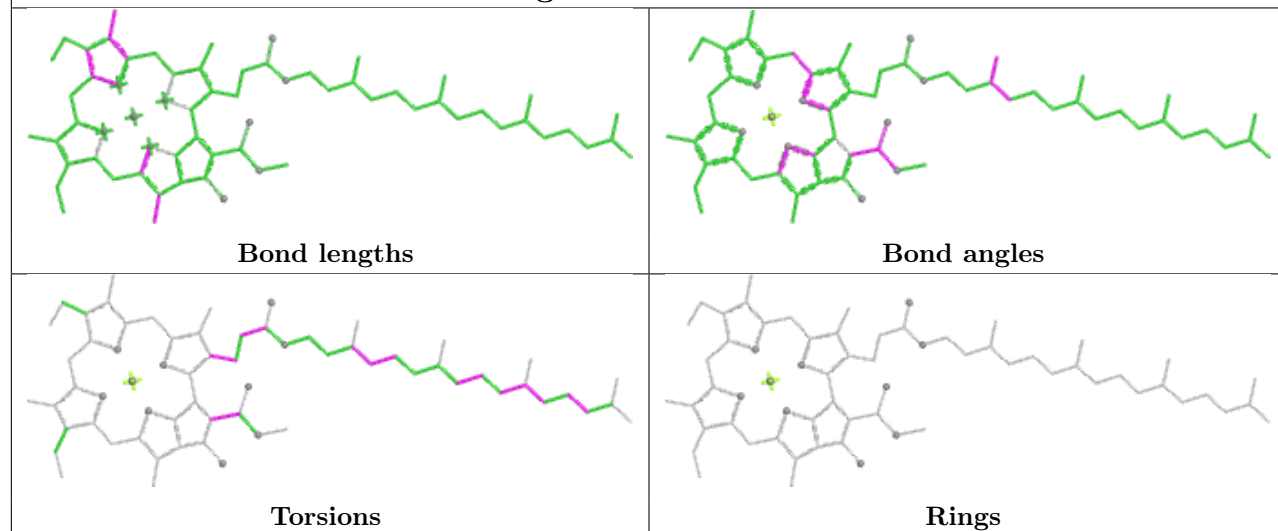
Ligand CLA 1 614



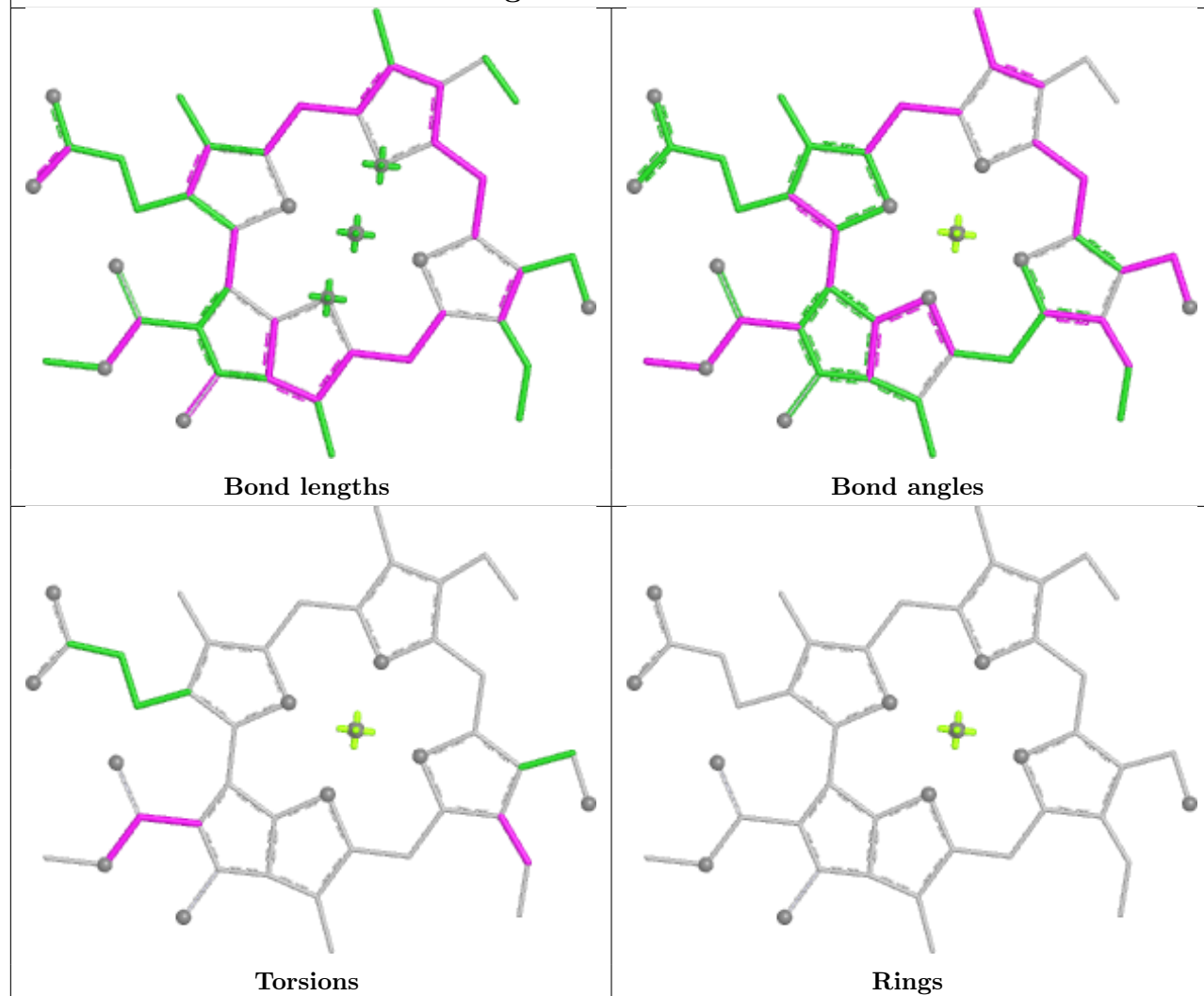
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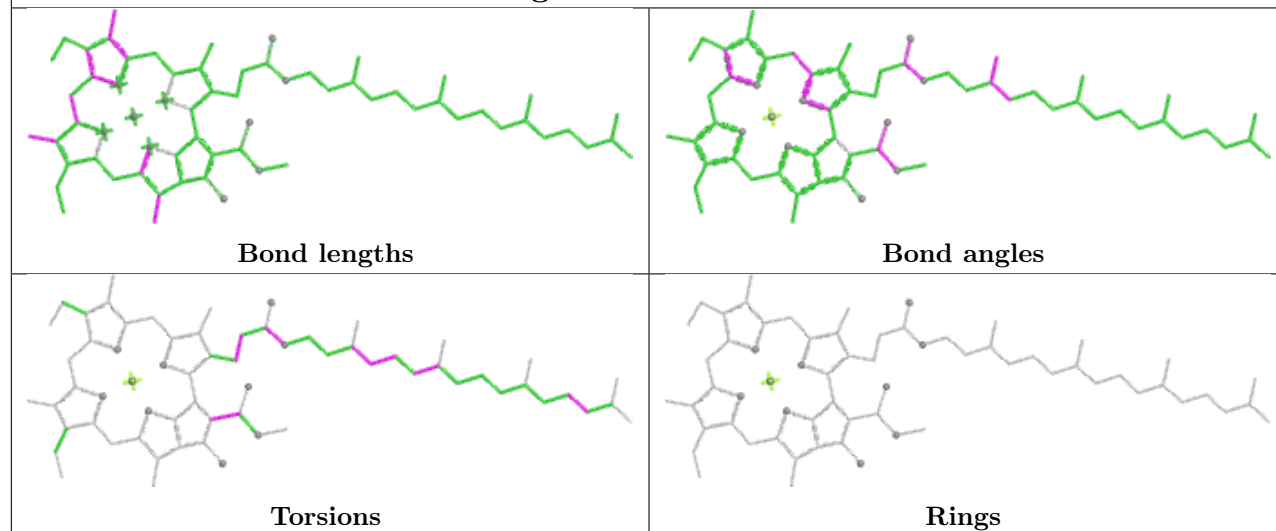
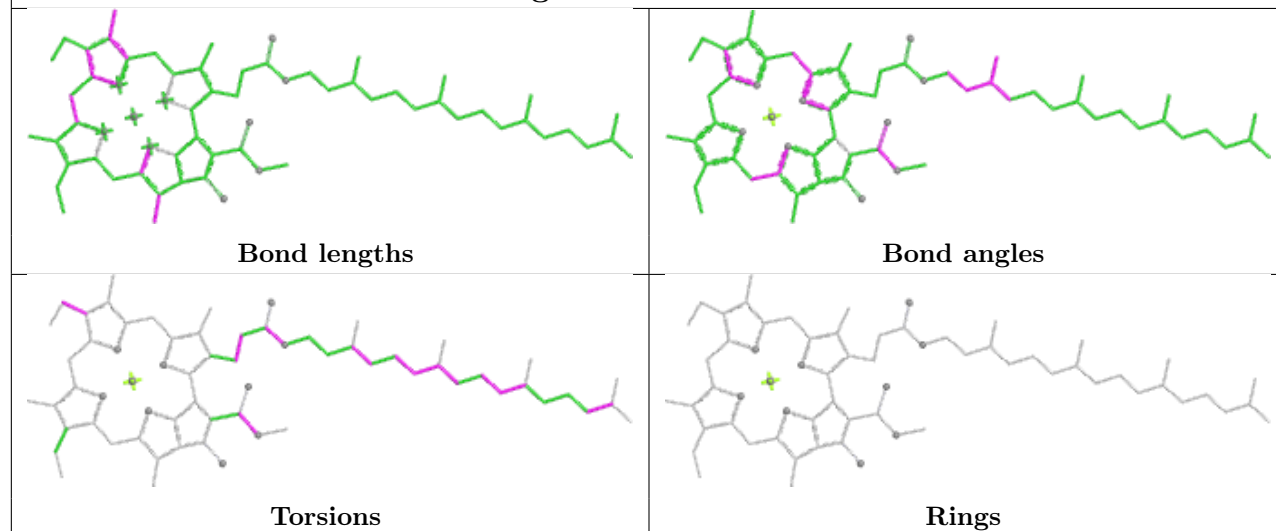


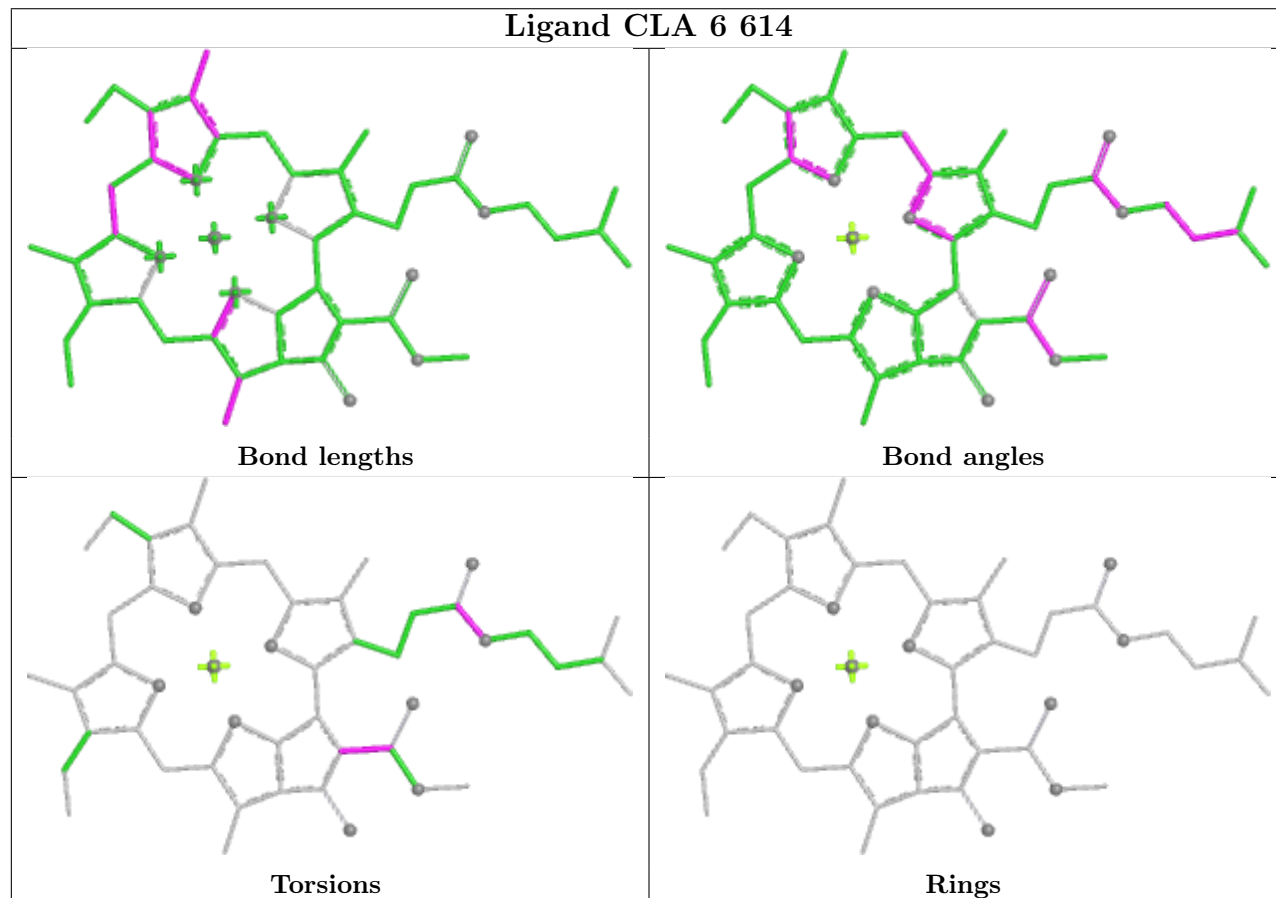
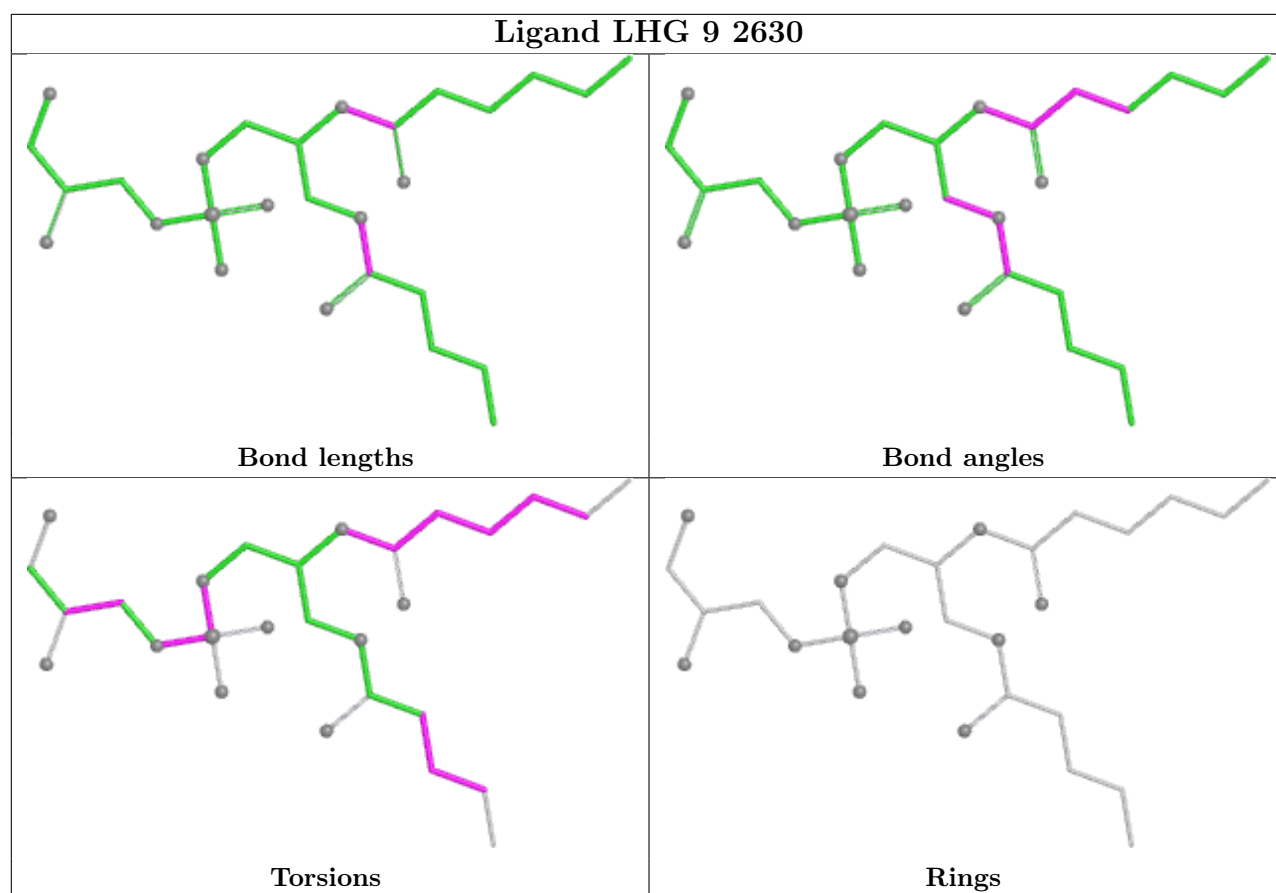
Ligand CLA 3 609

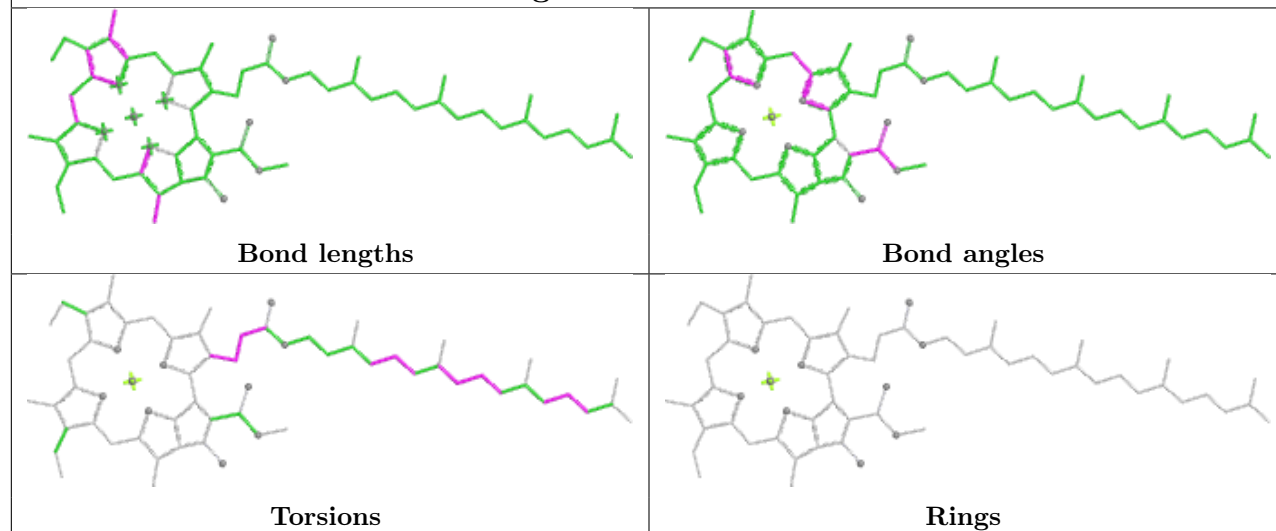
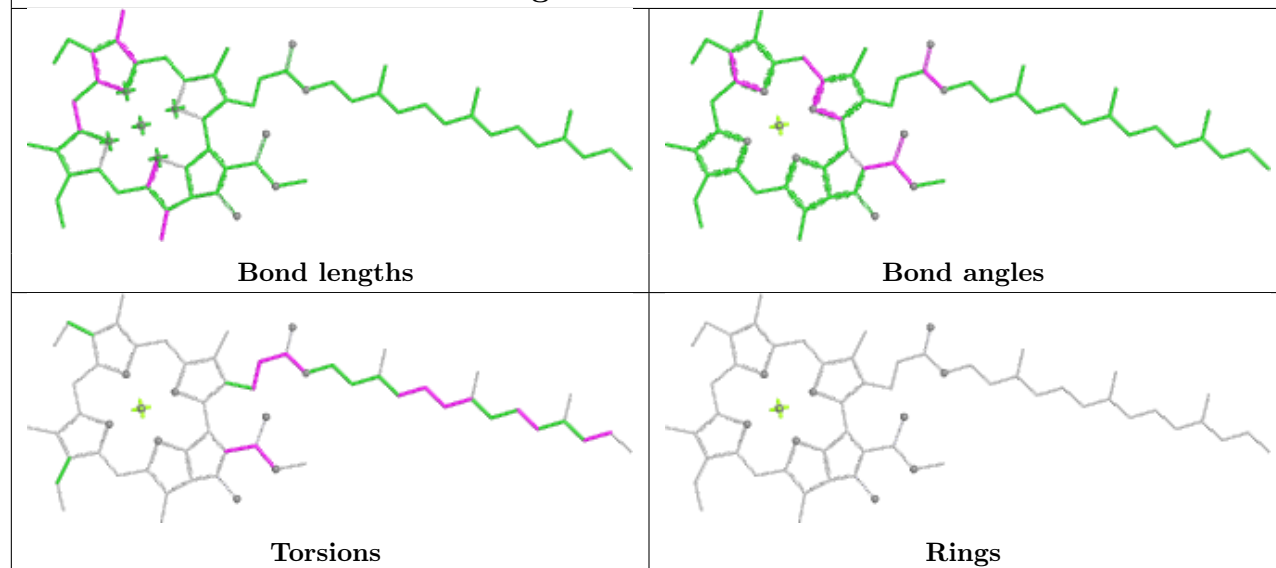


Ligand CHL 4 608

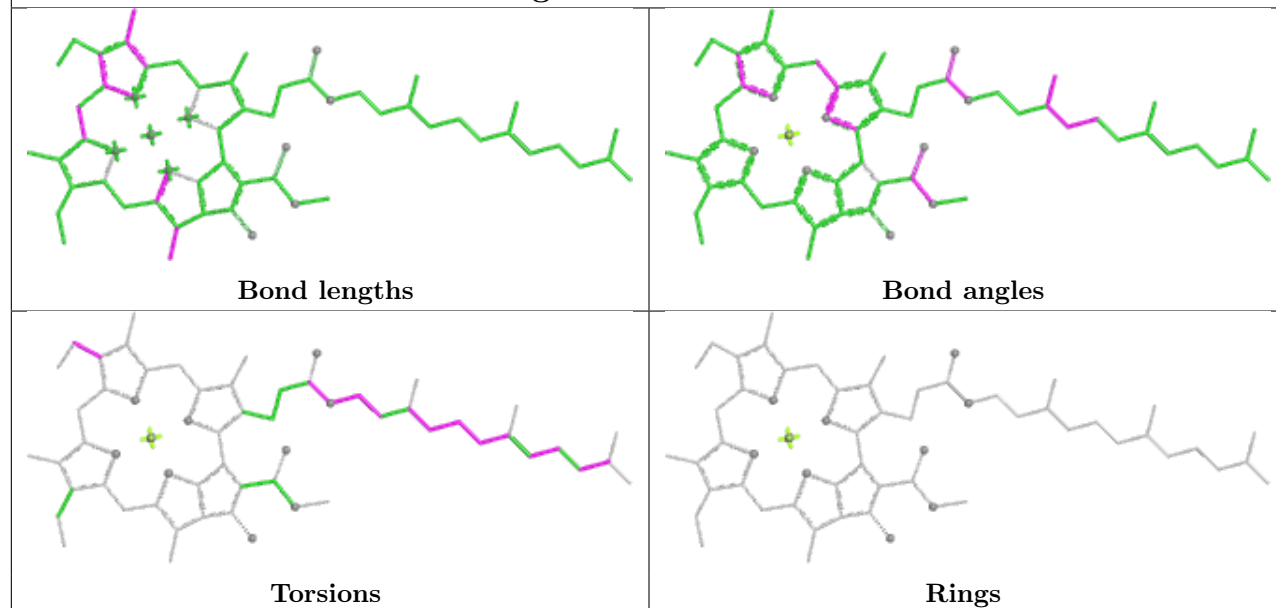


Ligand CLA U 602**Ligand CLA A 825**

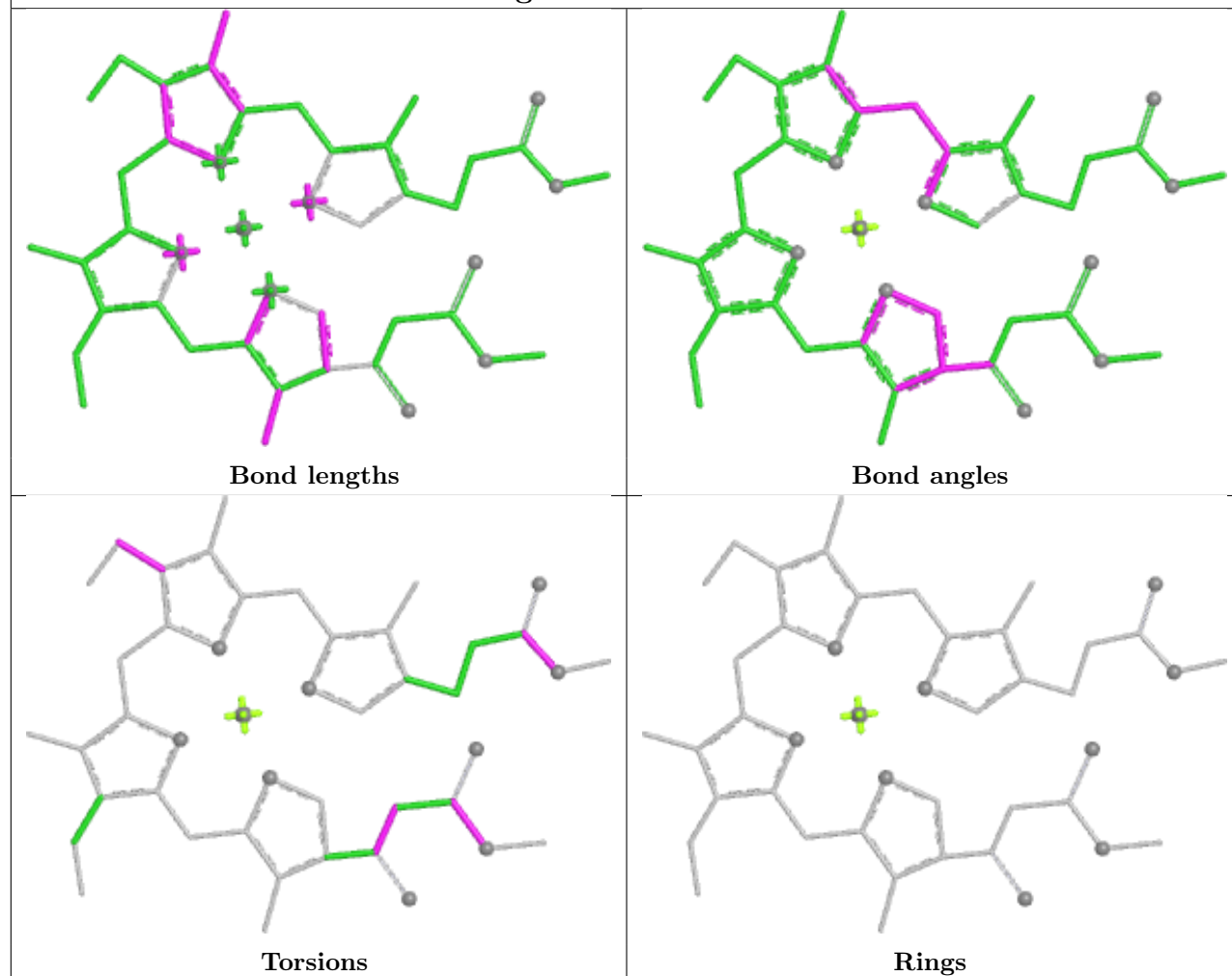


Ligand CLA B 834**Ligand CLA A 824**

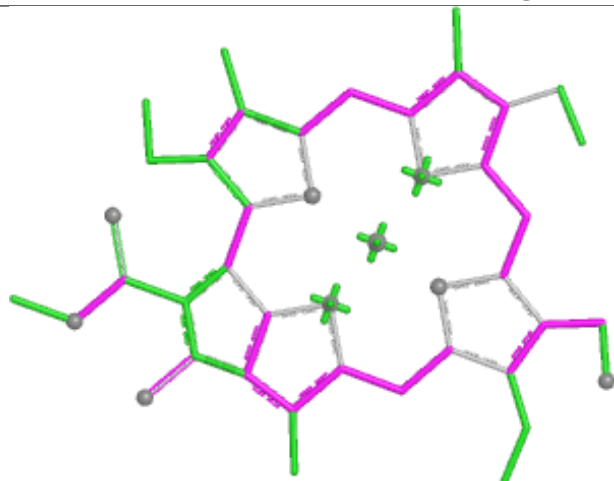
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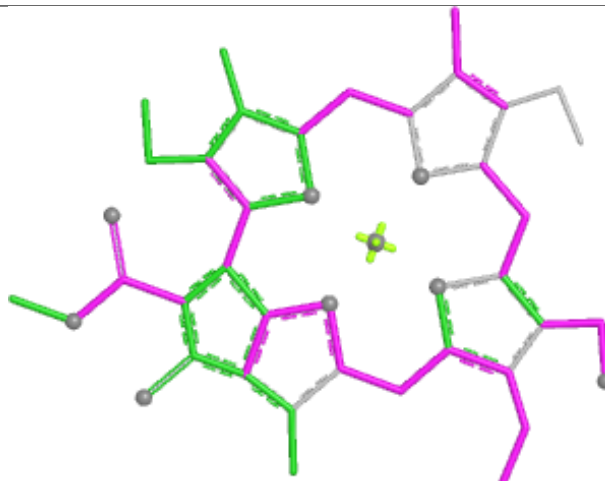
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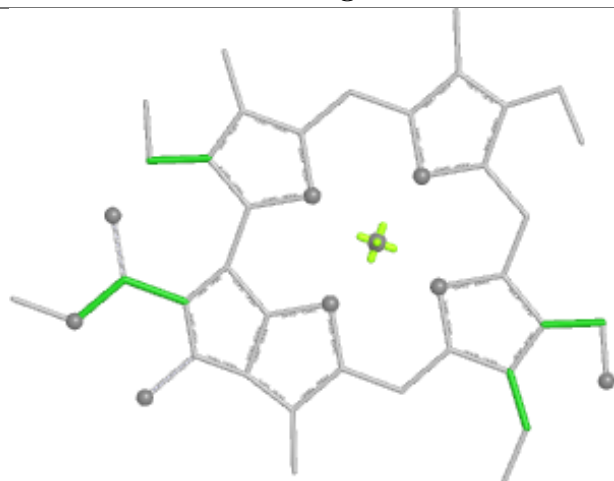
Ligand CHL 8 618



Bond lengths



Bond angles

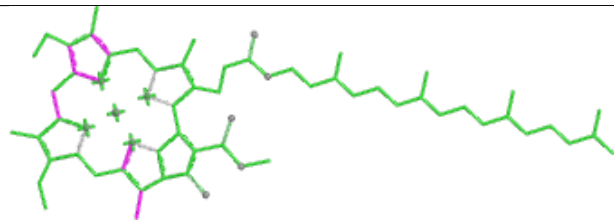


Torsions

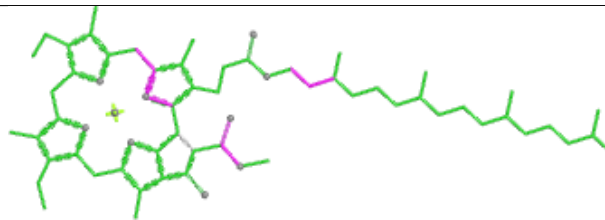


Rings

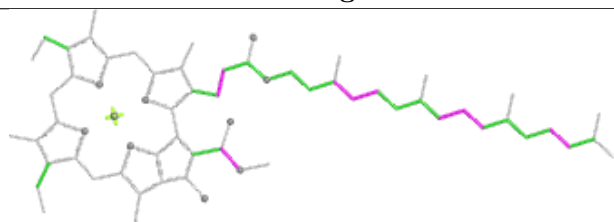
Ligand CLA U 613



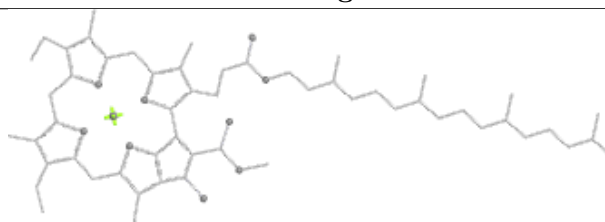
Bond lengths



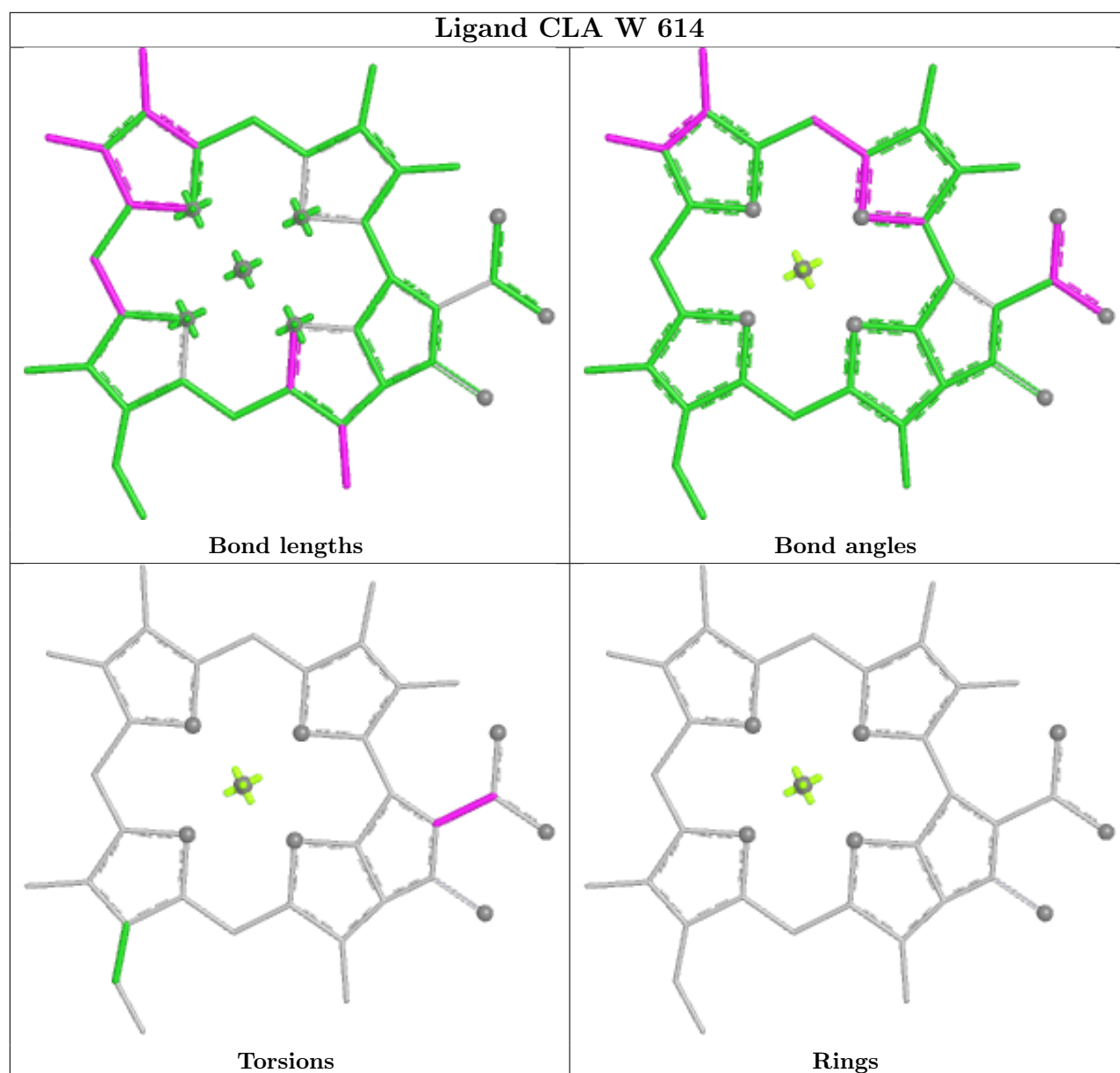
Bond angles



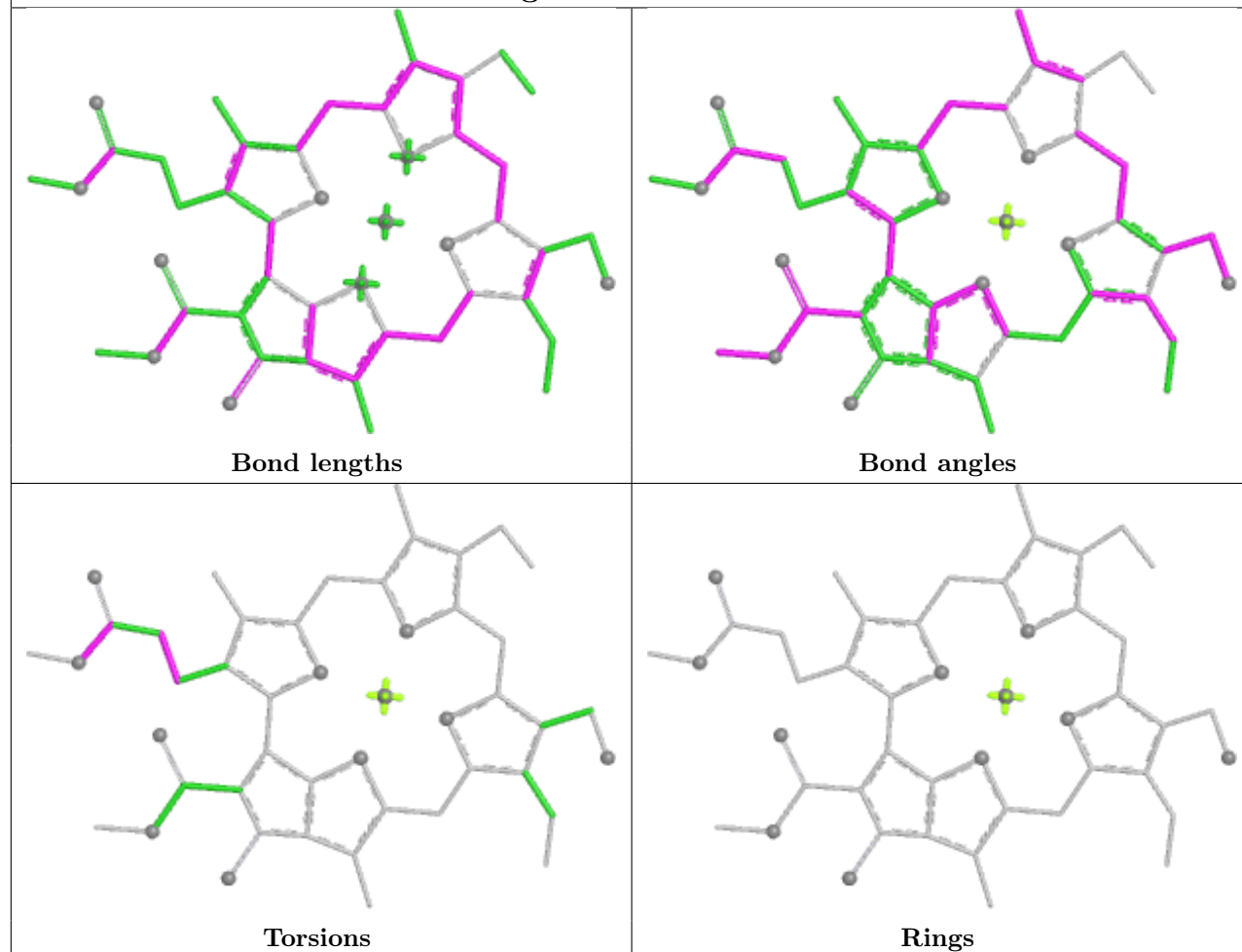
Torsions



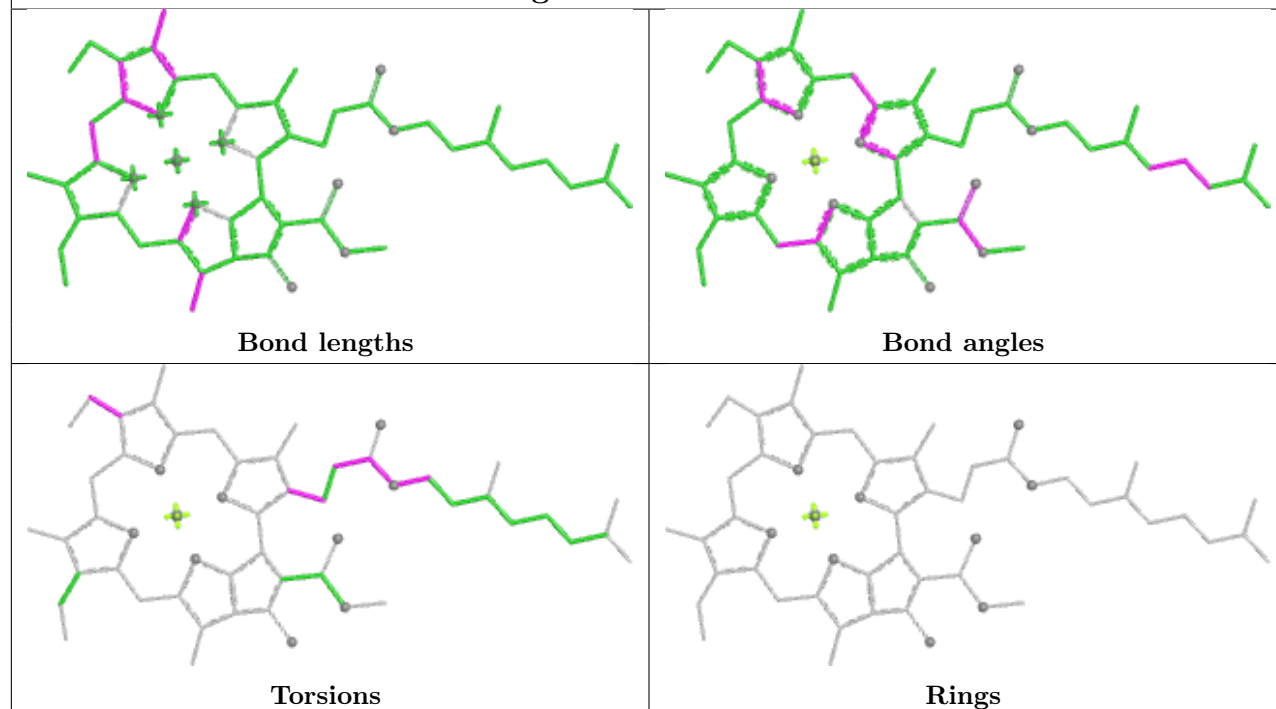
Rings

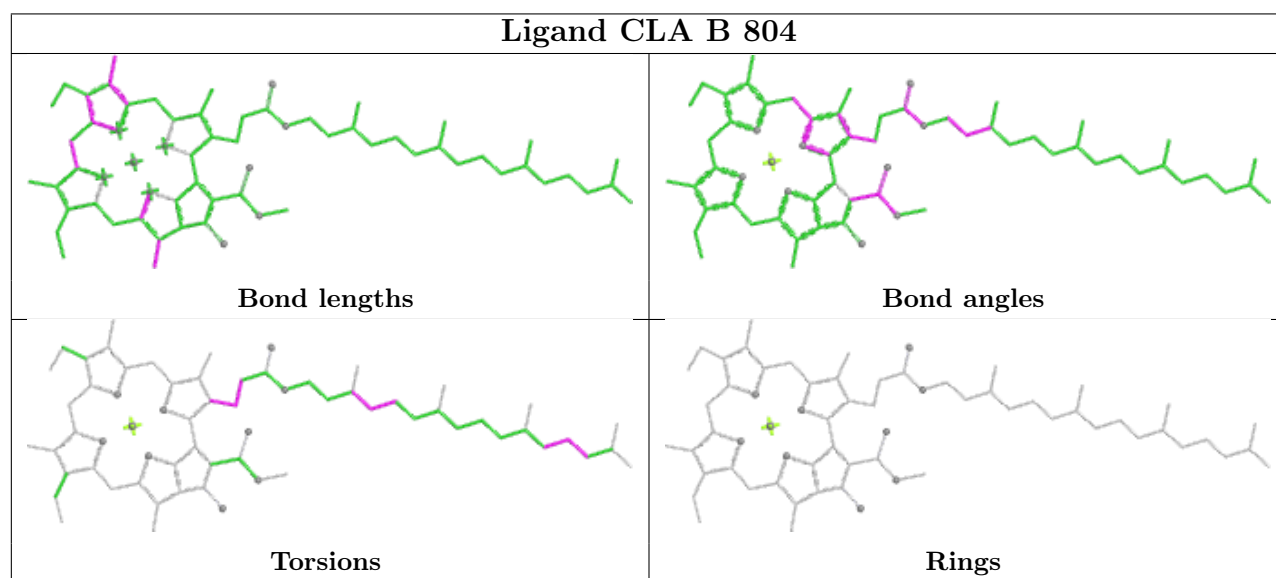
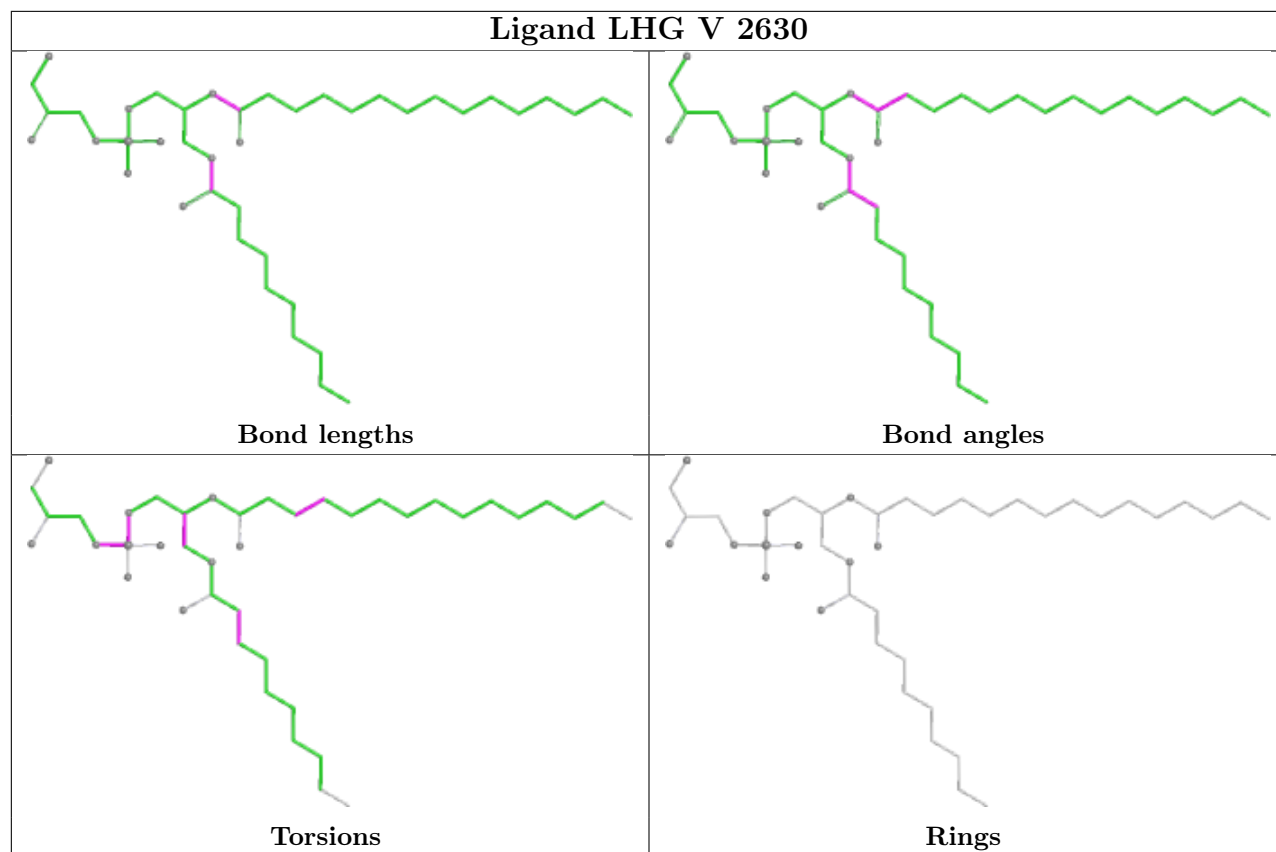


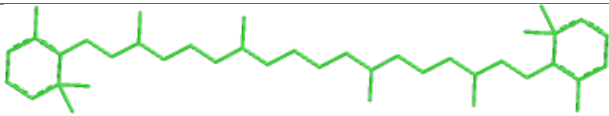
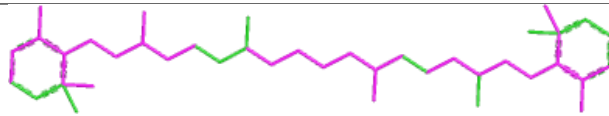
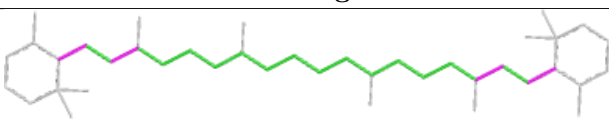
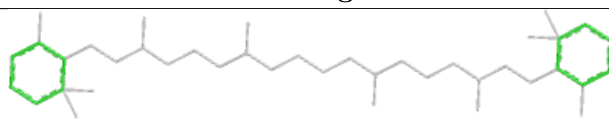
Ligand CHL 4 607

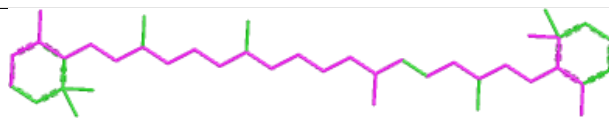
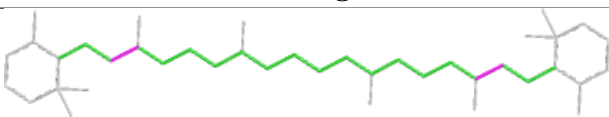
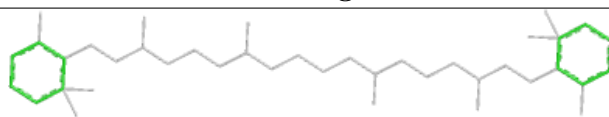


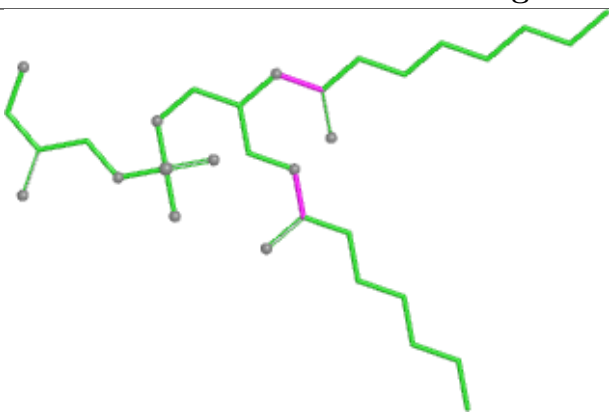
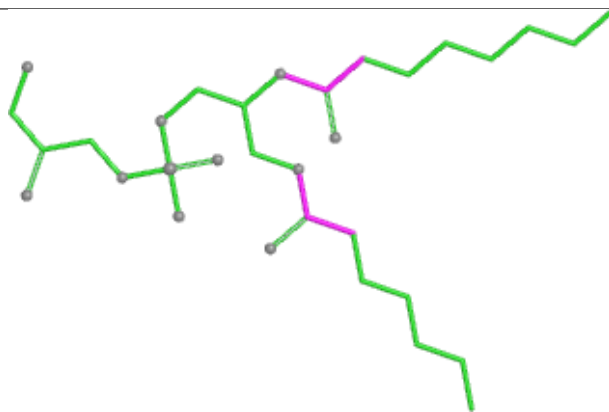
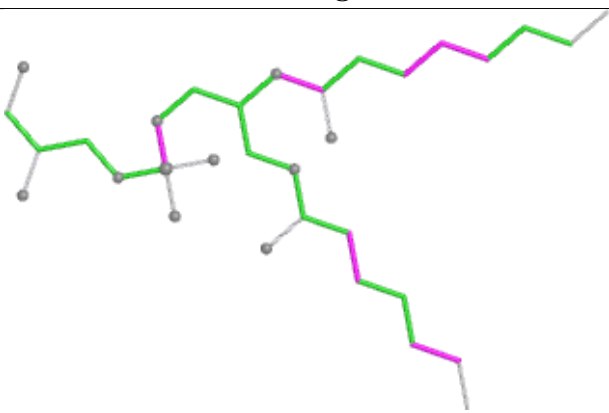
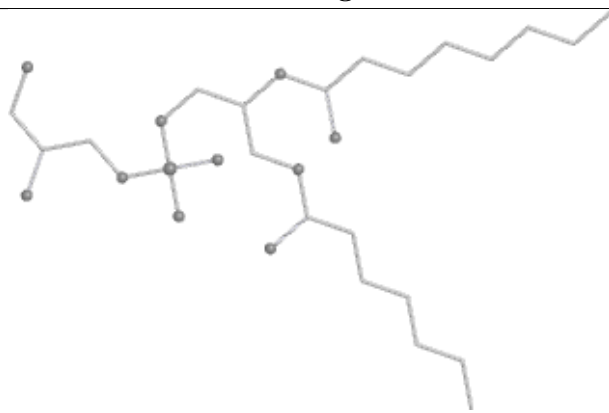
Ligand CLA A 842



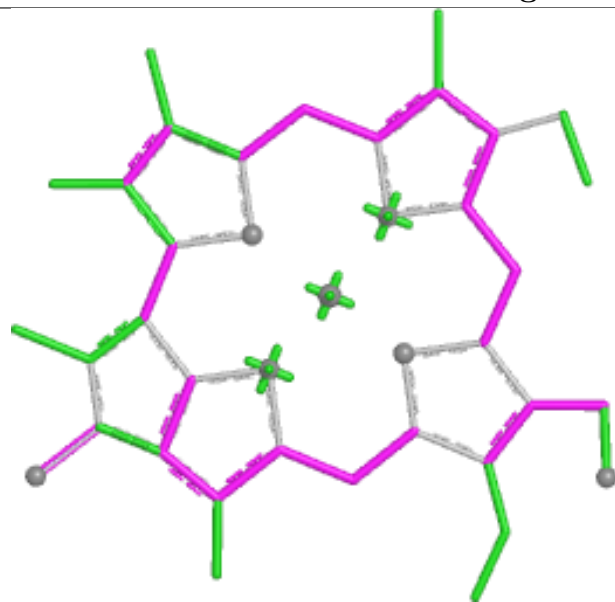


Ligand BCR 2 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 8 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG 3 630	
	
Bond lengths	Bond angles
	
Torsions	Rings

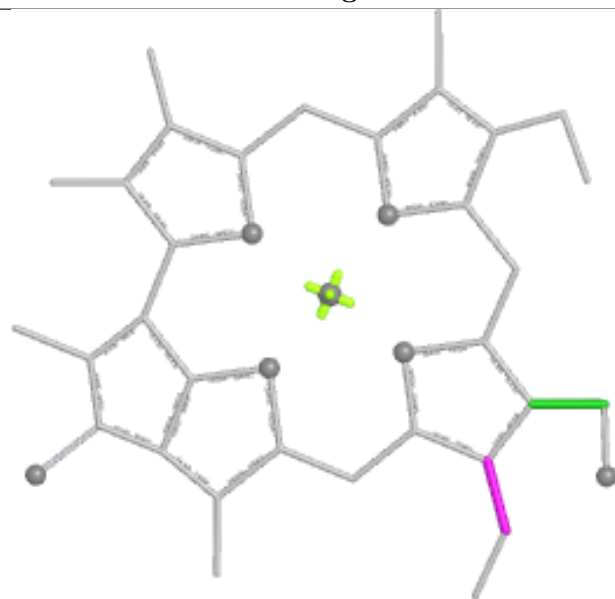
Ligand CHL 9 601



Bond lengths



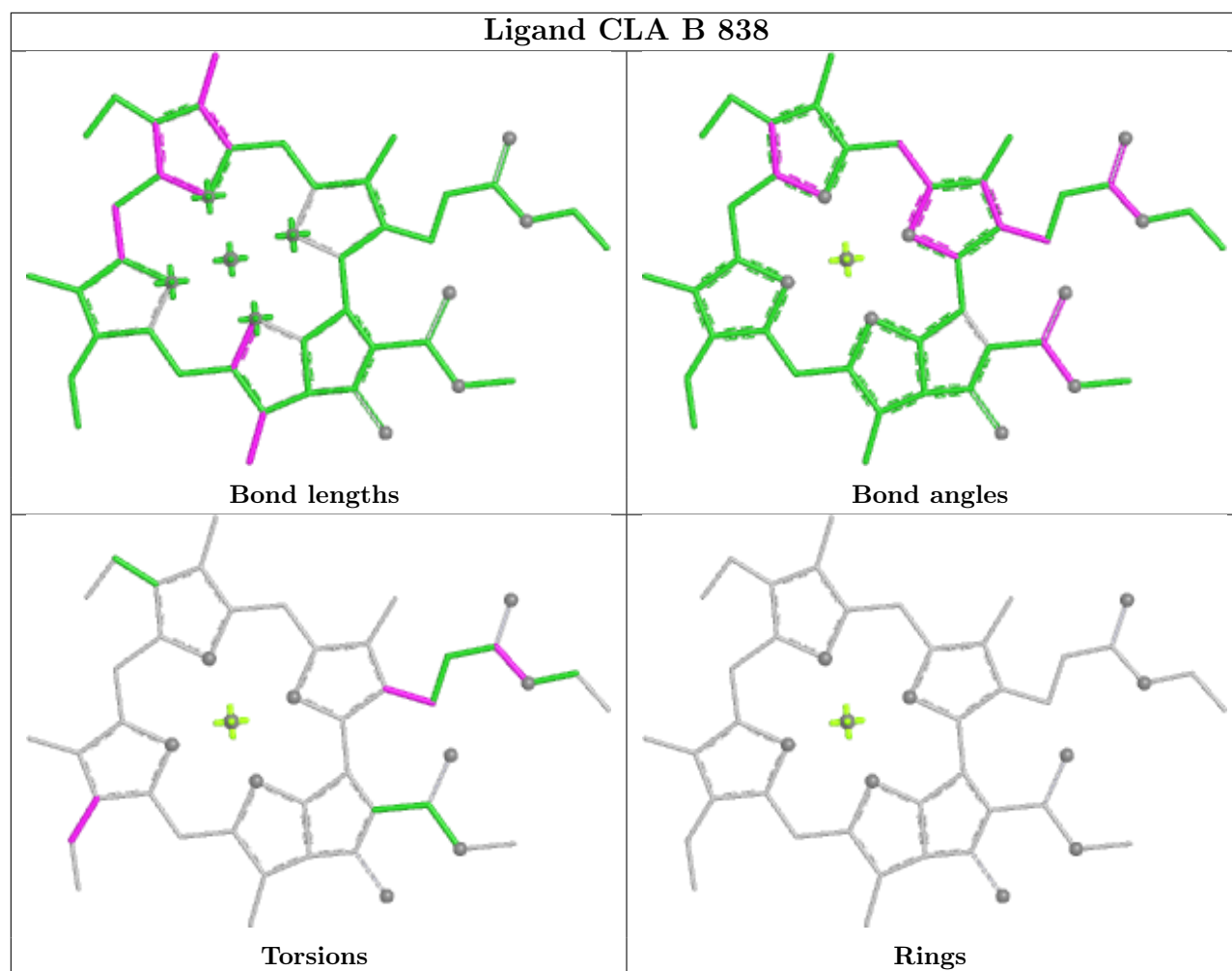
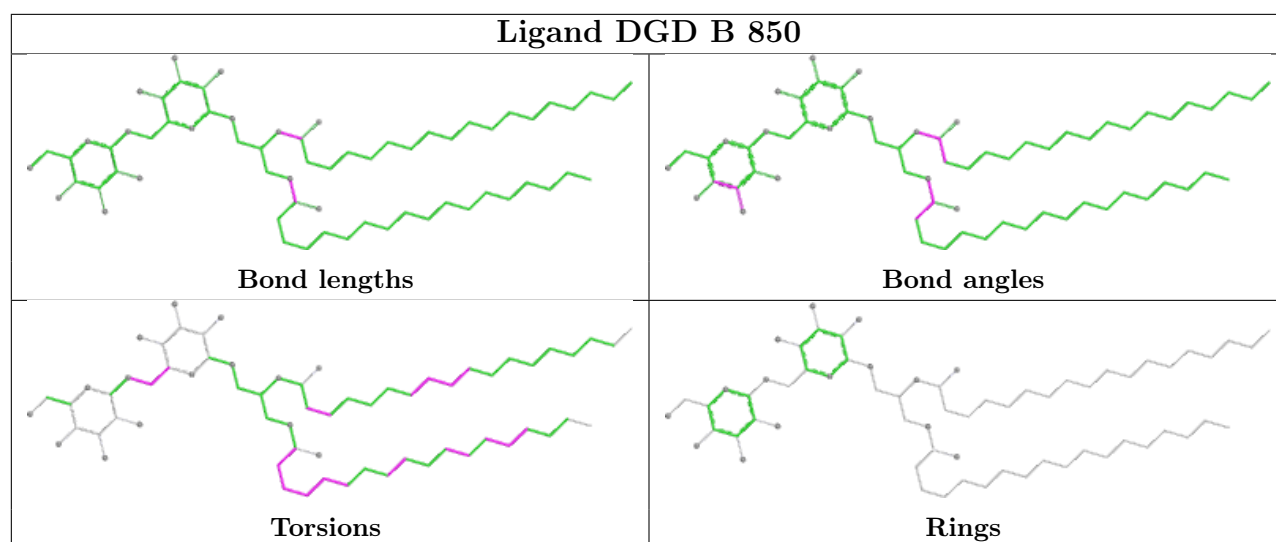
Bond angles

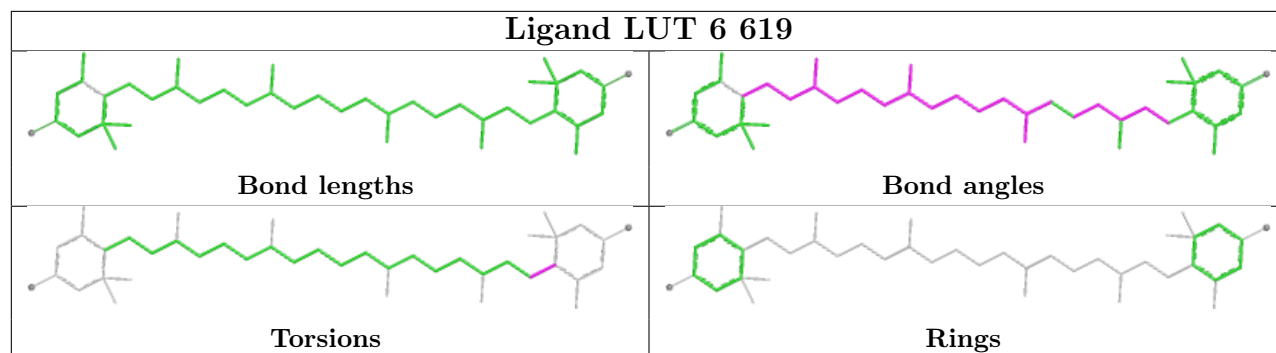
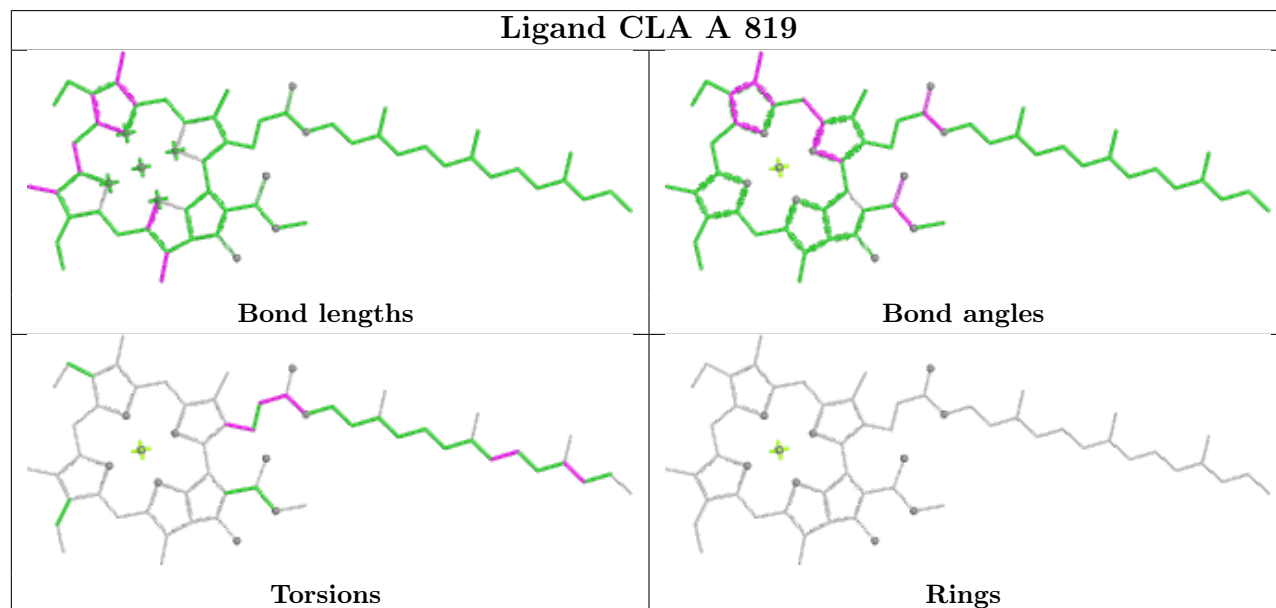
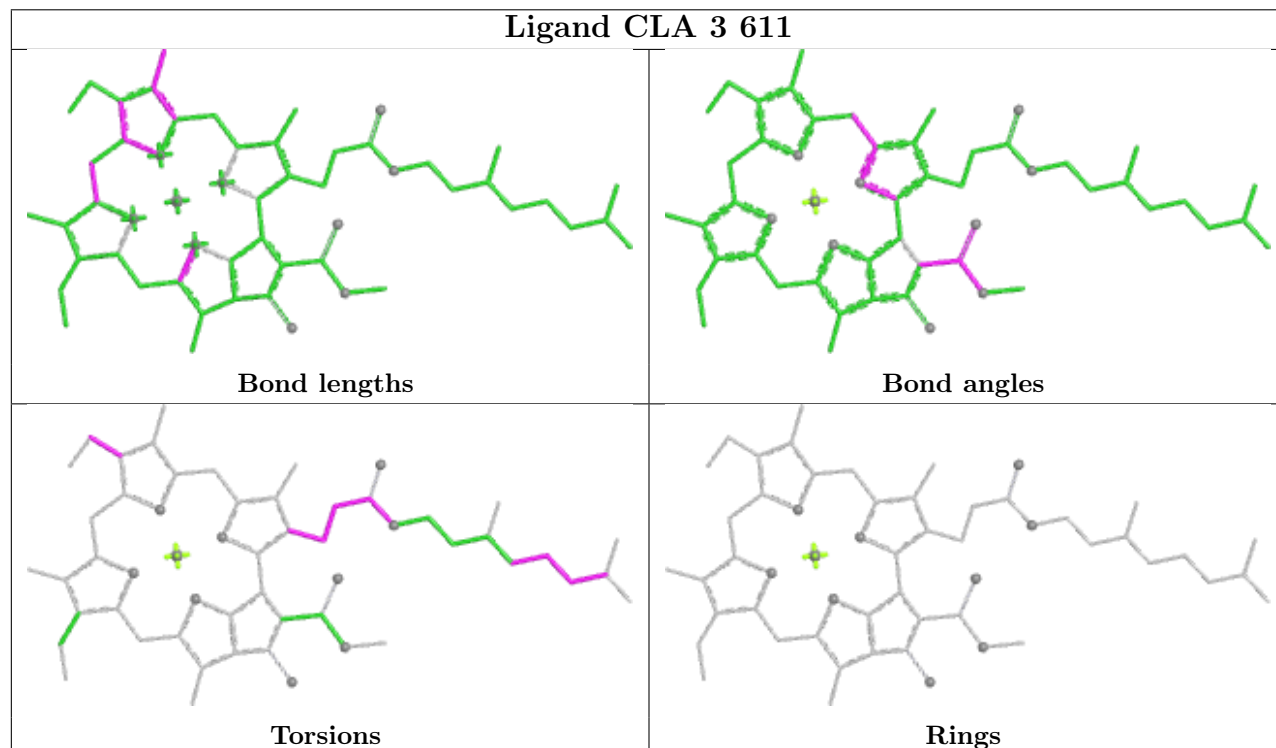


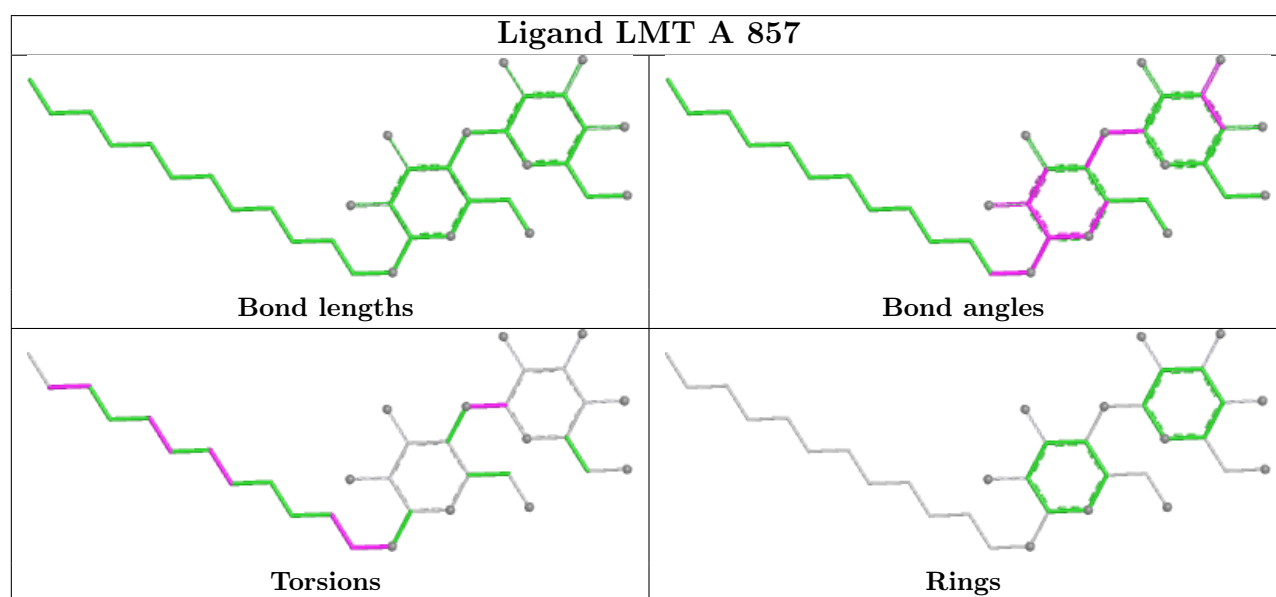
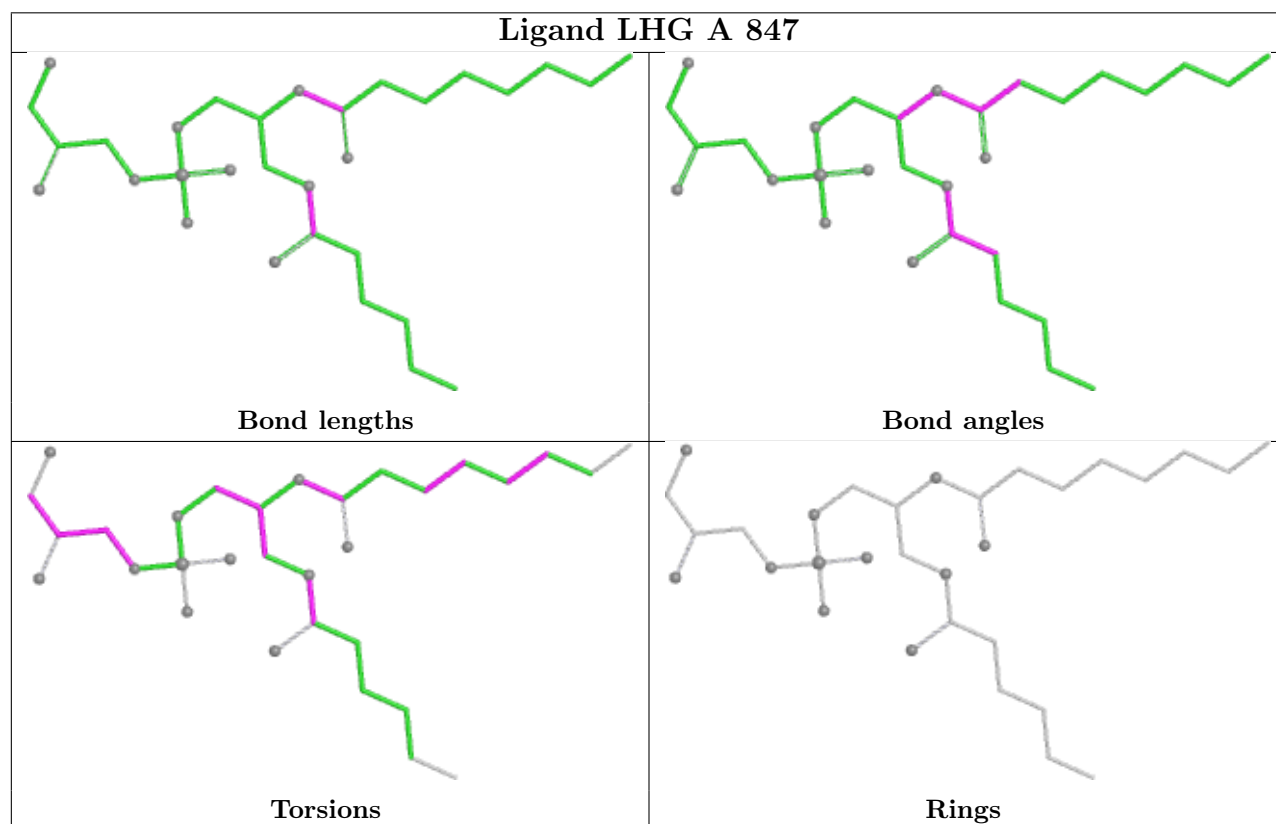
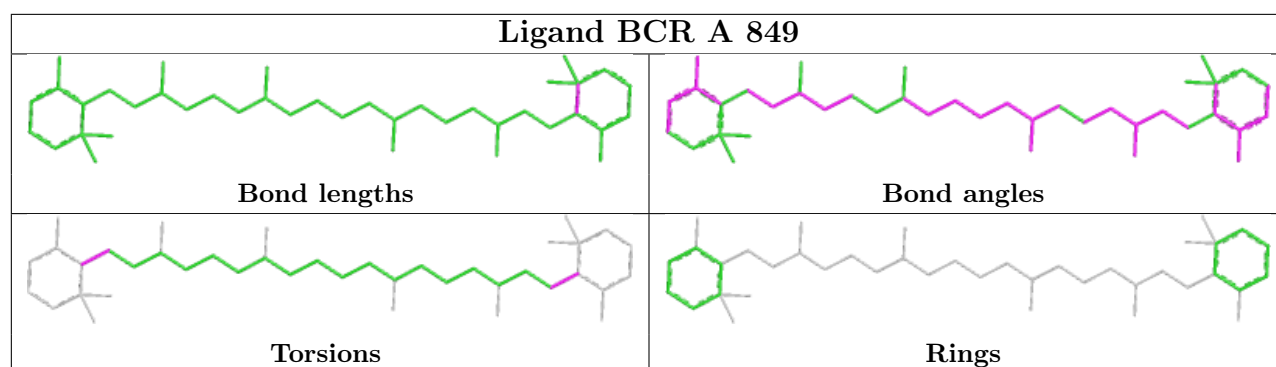
Torsions

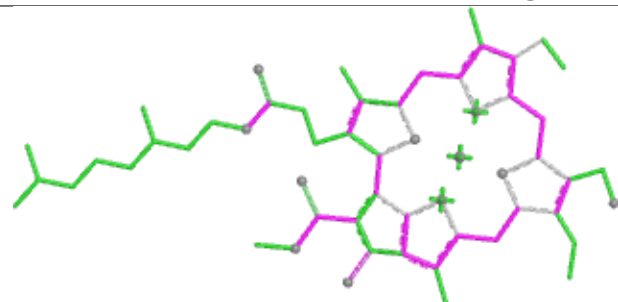
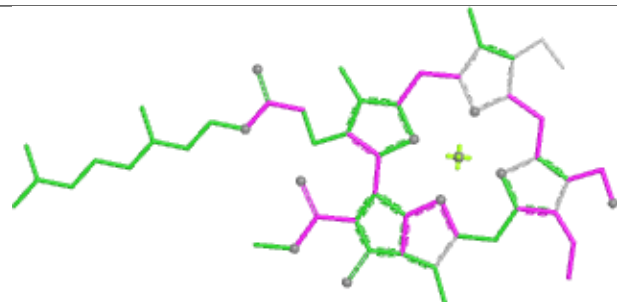
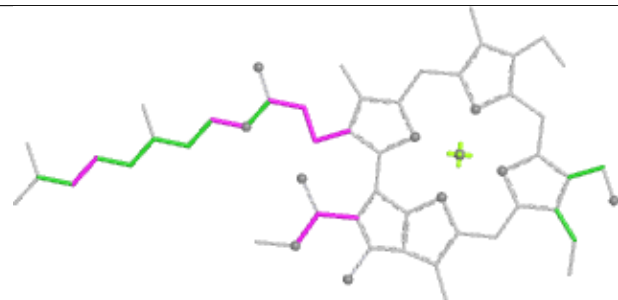
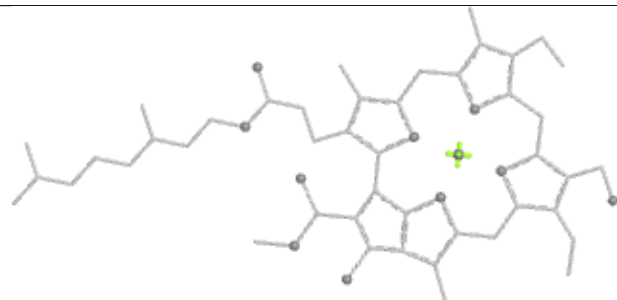
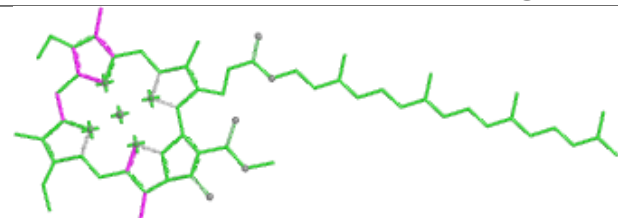
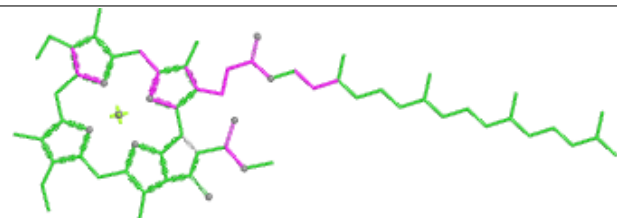
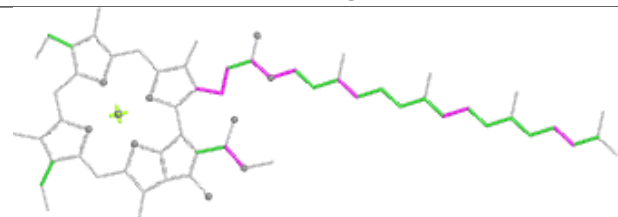
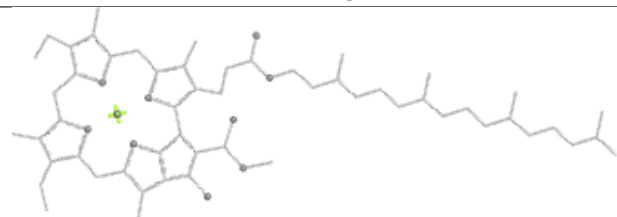


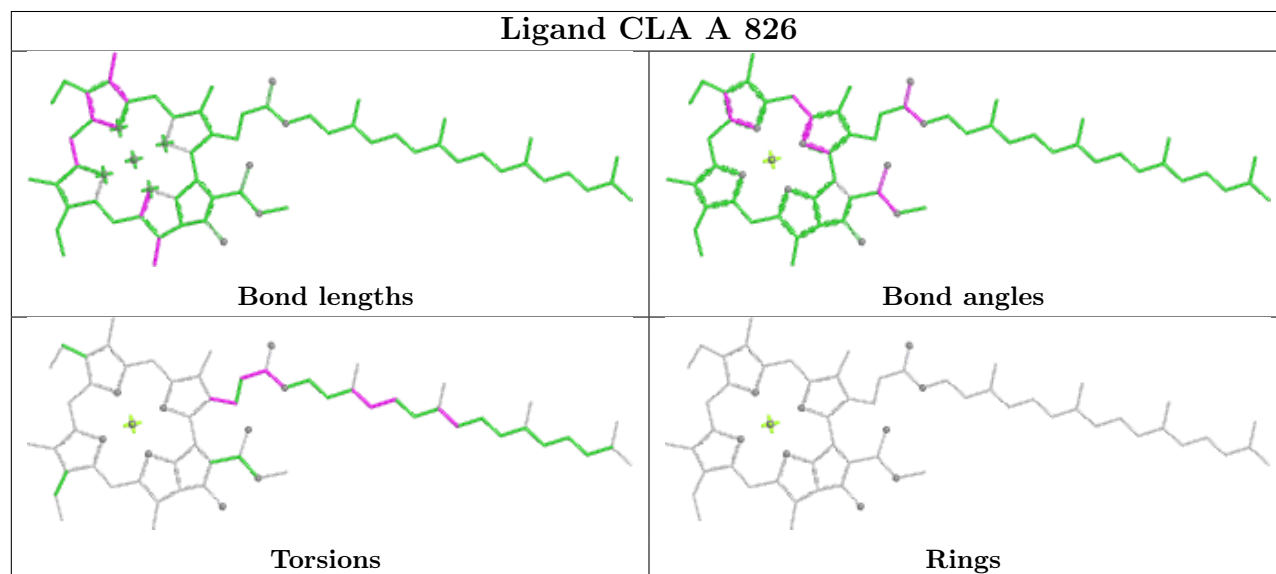
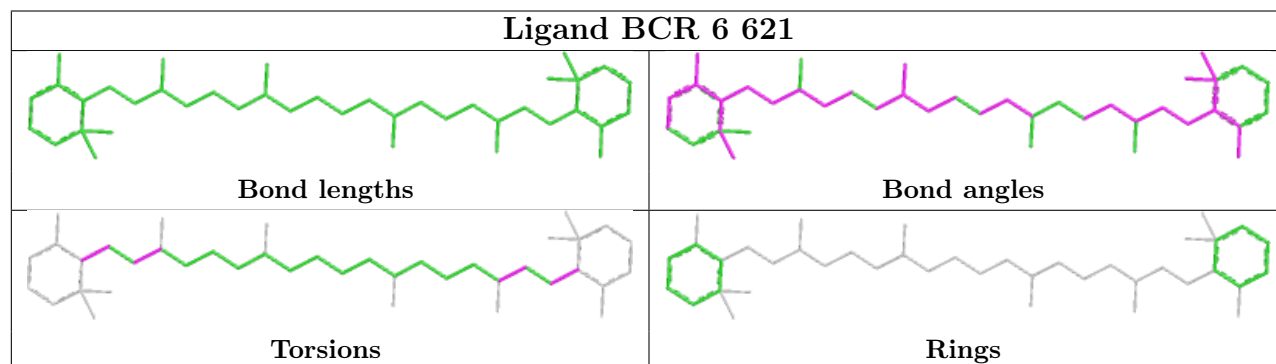
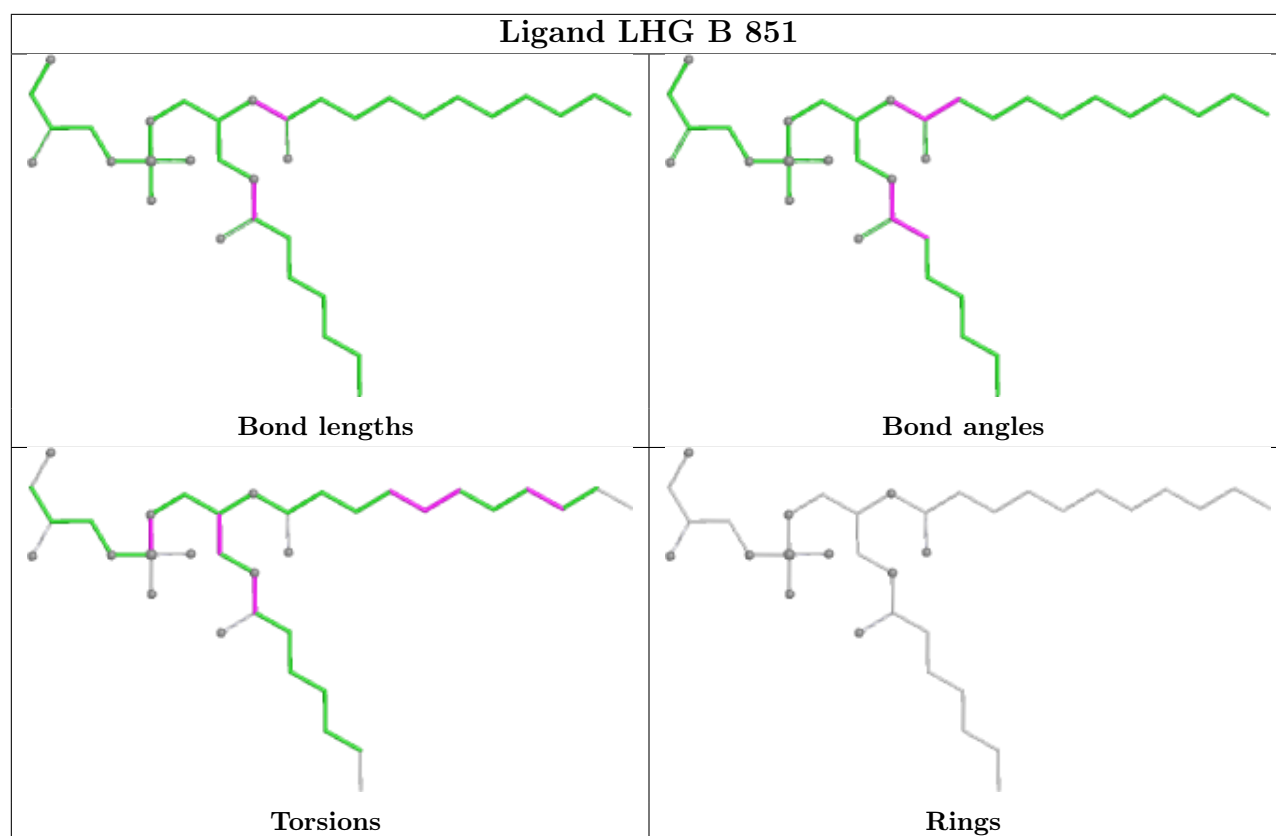
Rings



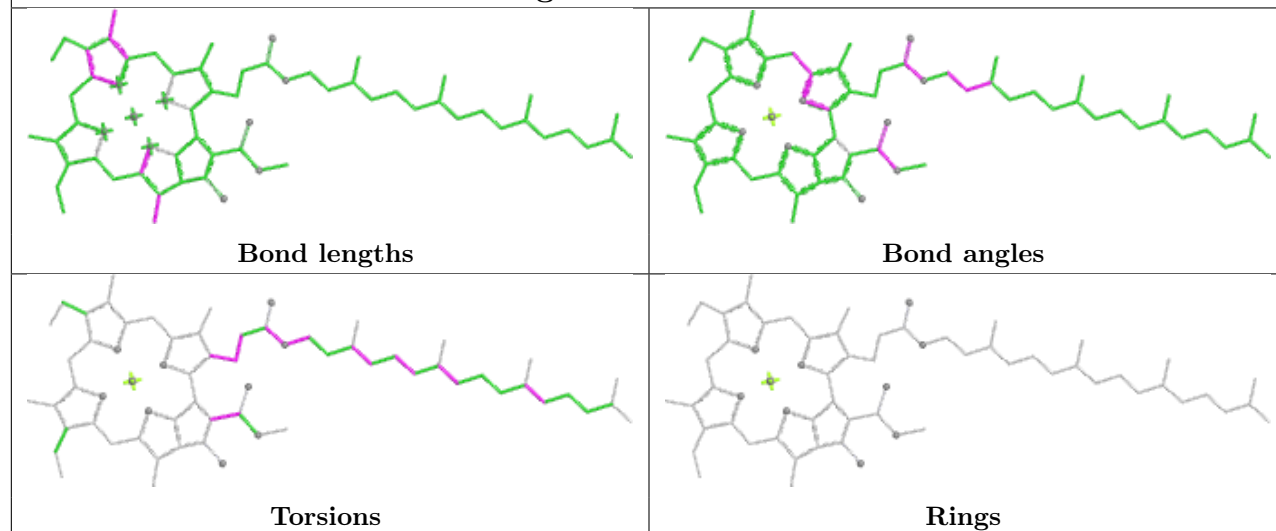
Ligand LUT 6 619**Ligand CLA A 819****Ligand CLA 3 611**



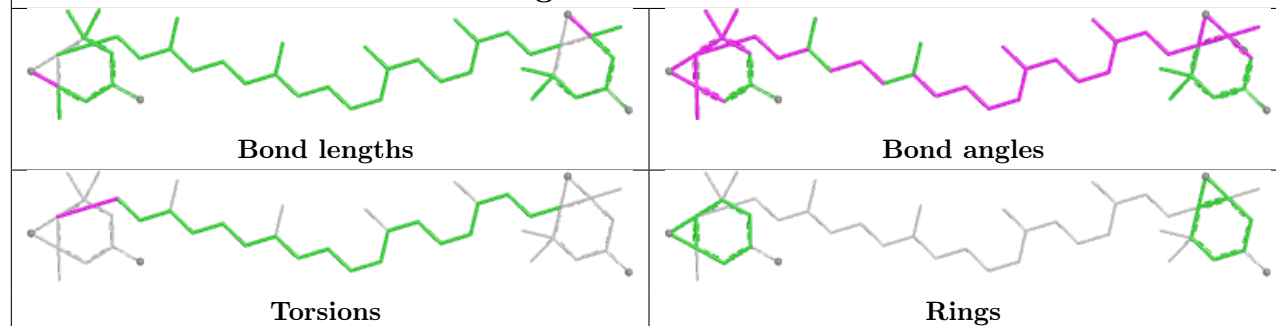
Ligand CHL 6 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 814****Bond lengths****Bond angles****Torsions****Rings**



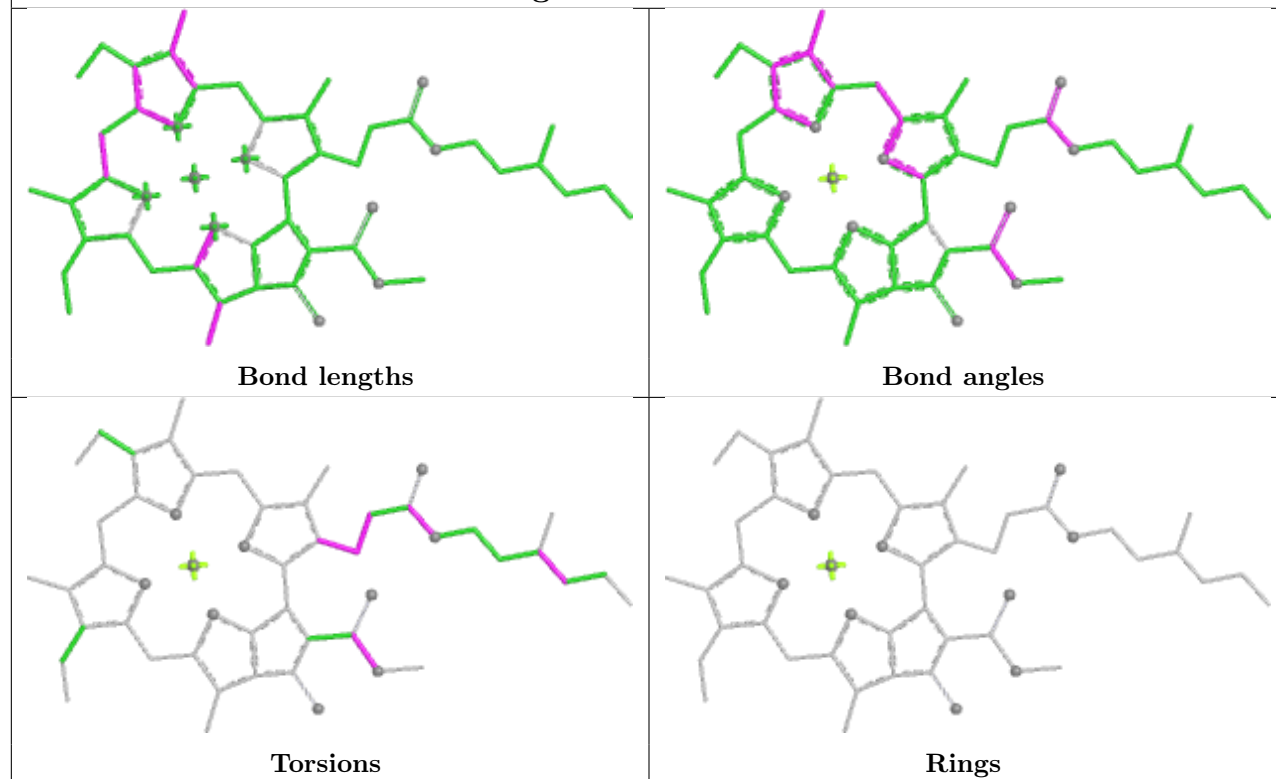
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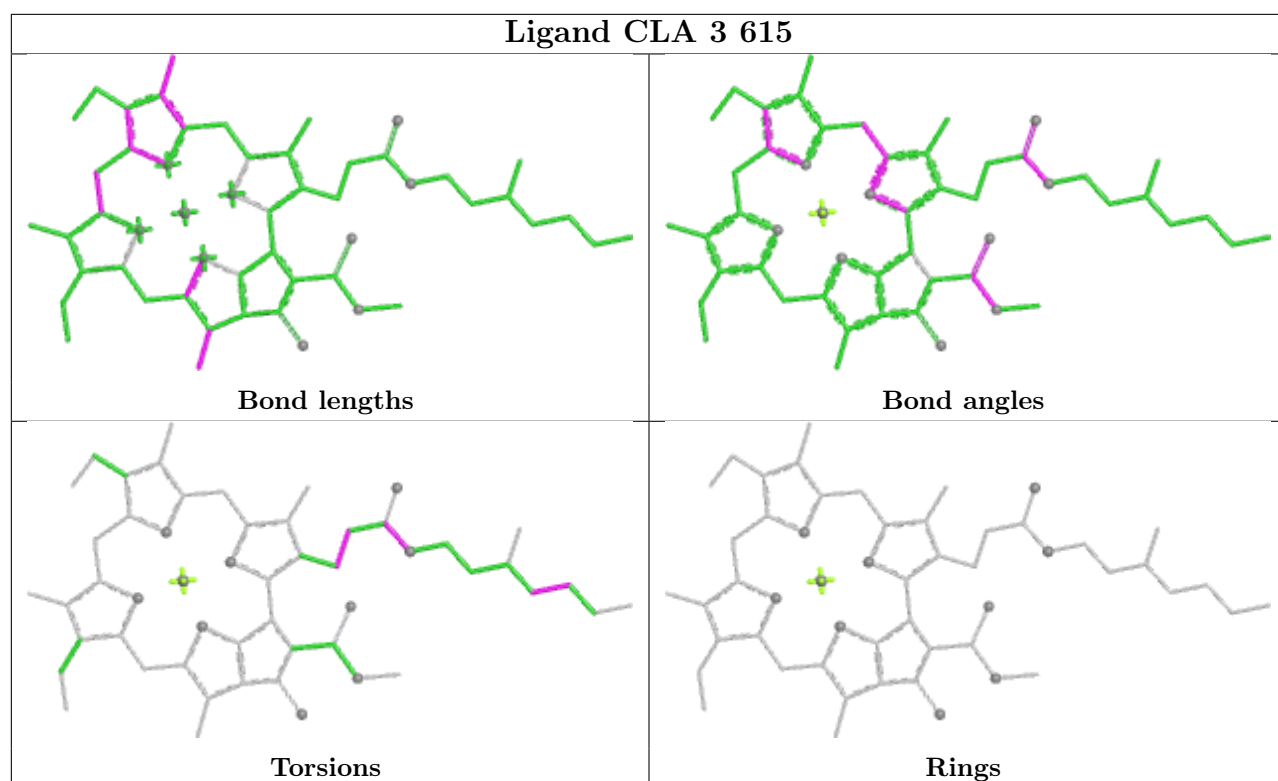


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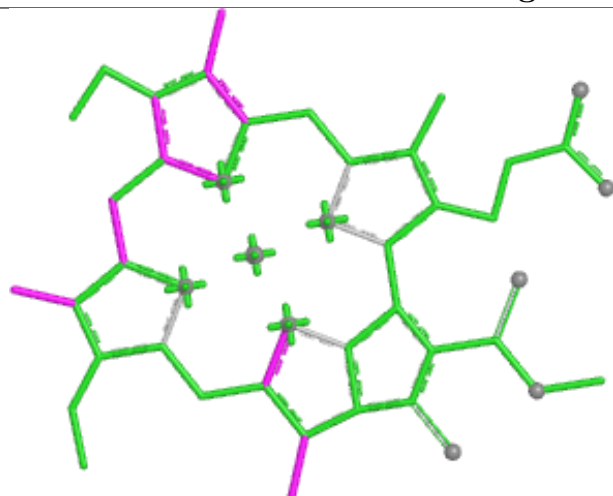


Ligand CLA B 836

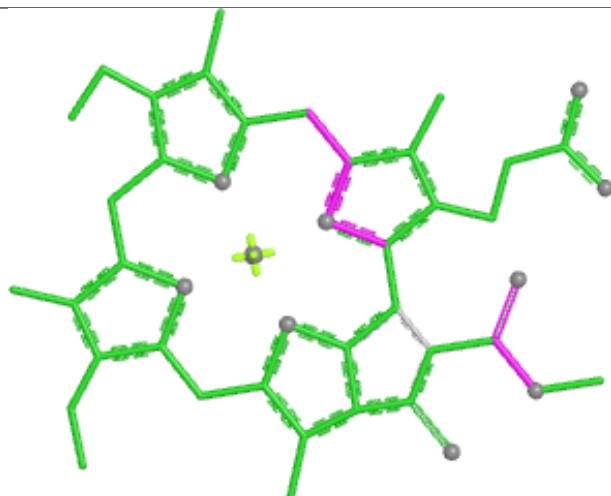




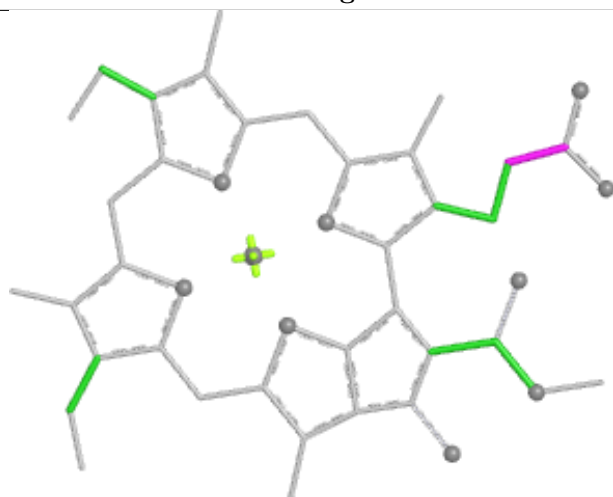
Ligand CLA 5 606



Bond lengths



Bond angles

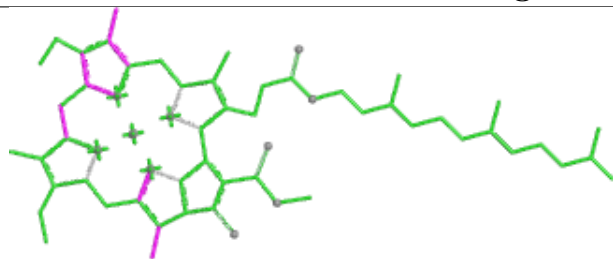


Torsions

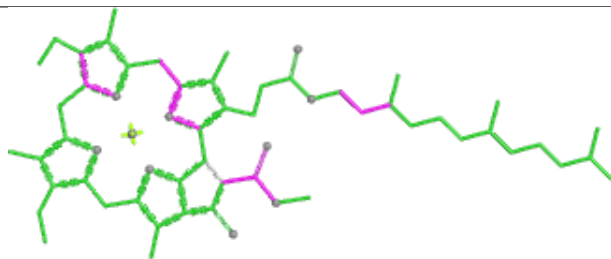


Rings

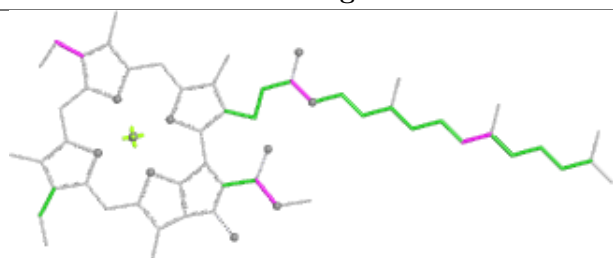
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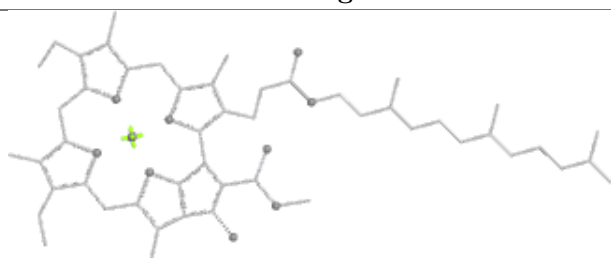
Bond lengths



Bond angles

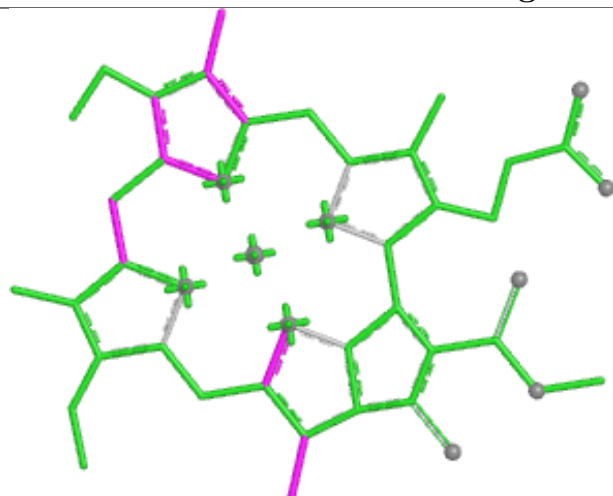


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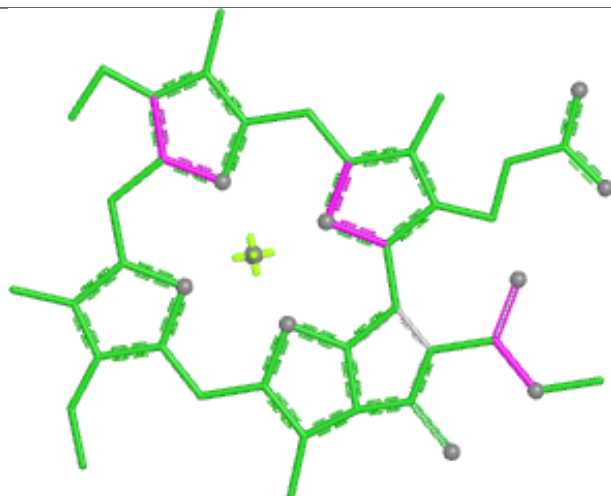


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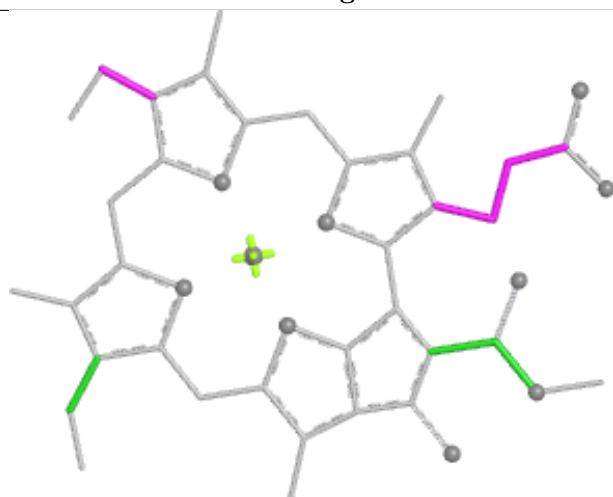
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Bond lengths



Bond angles

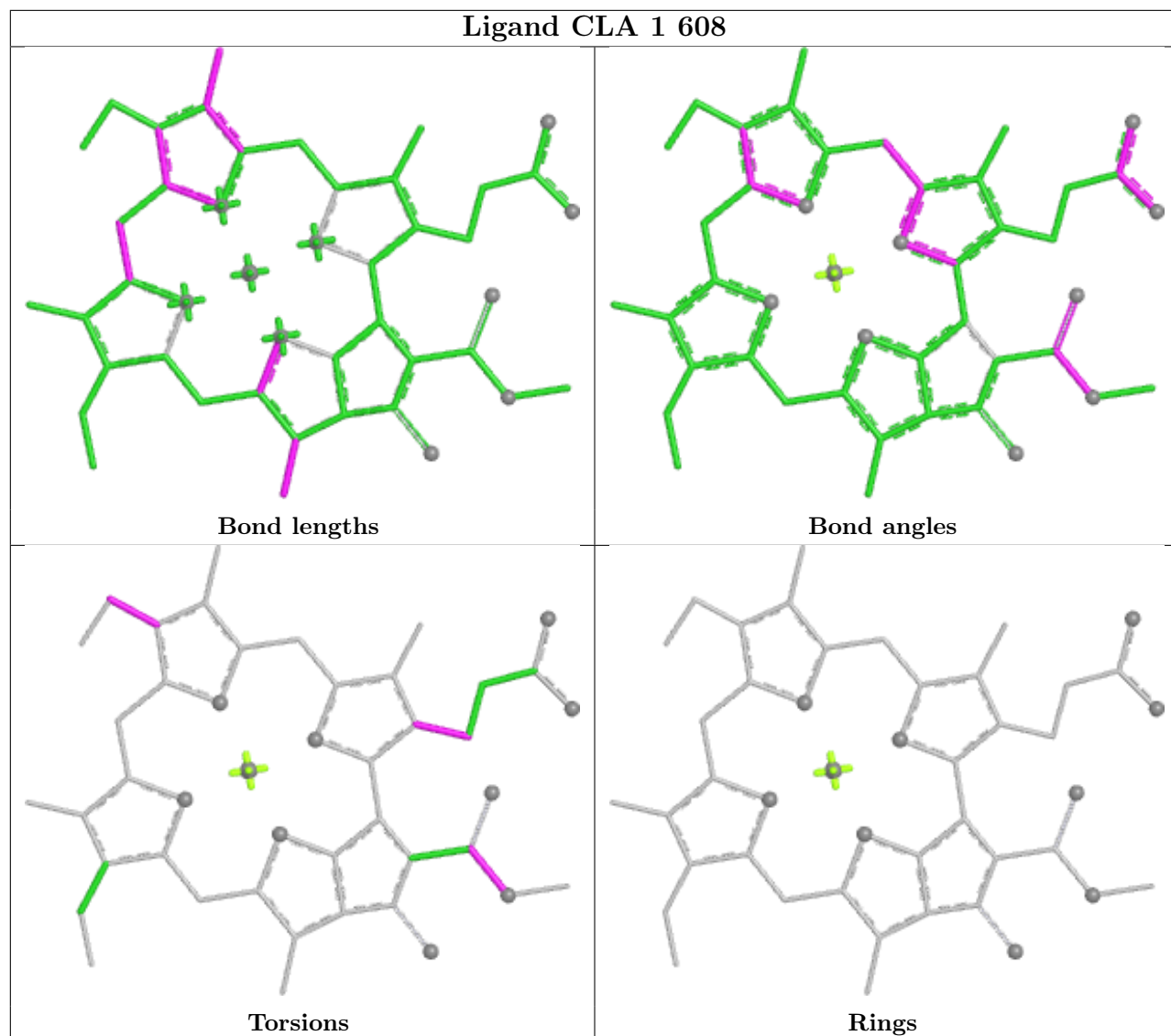


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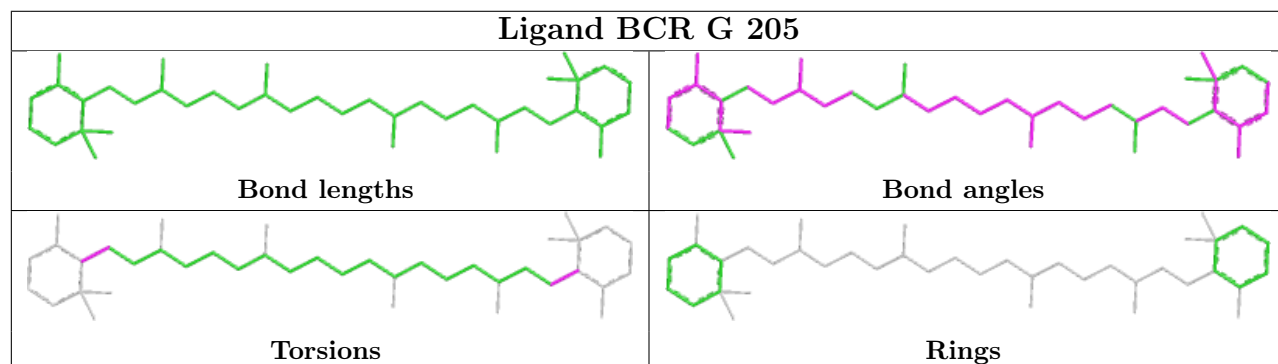


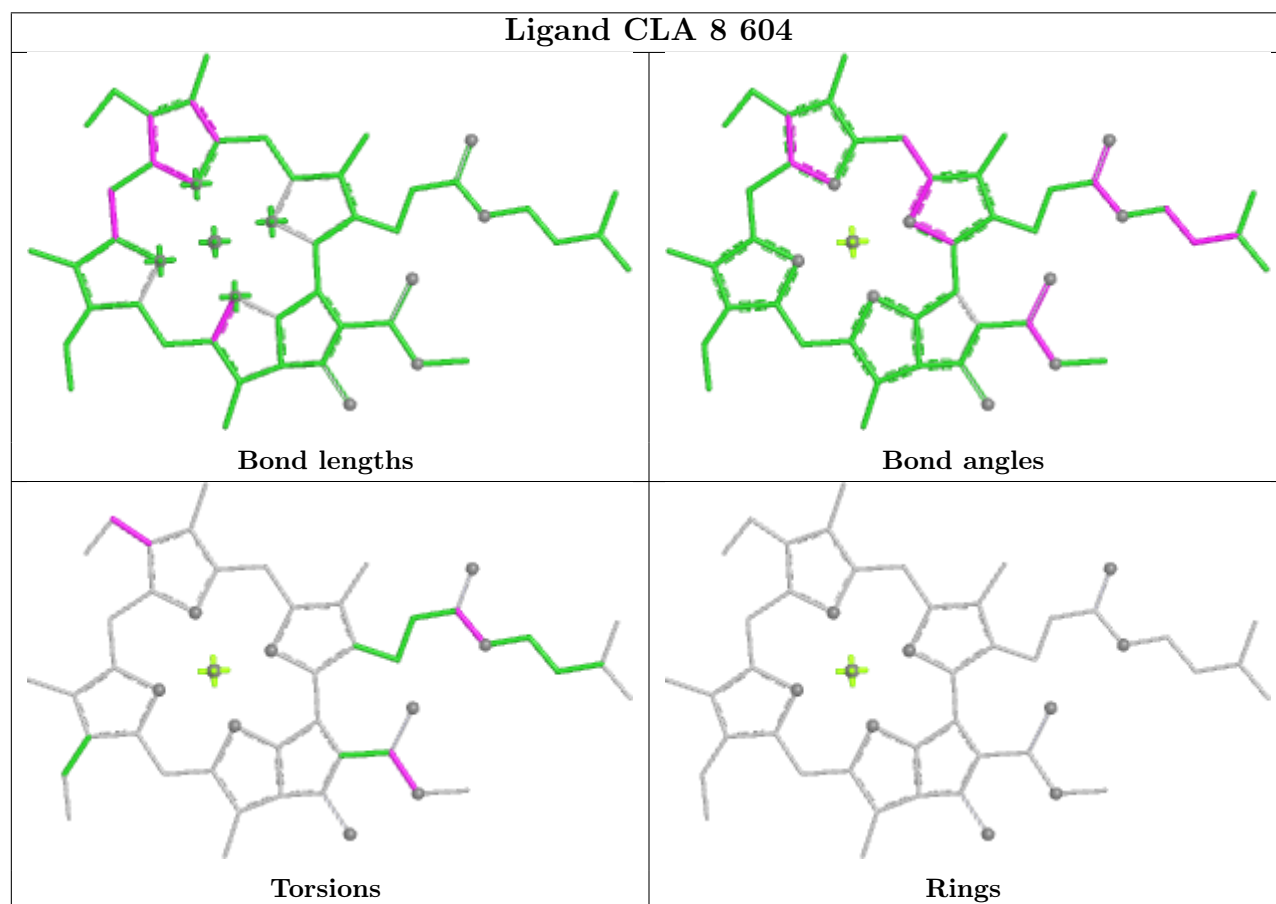
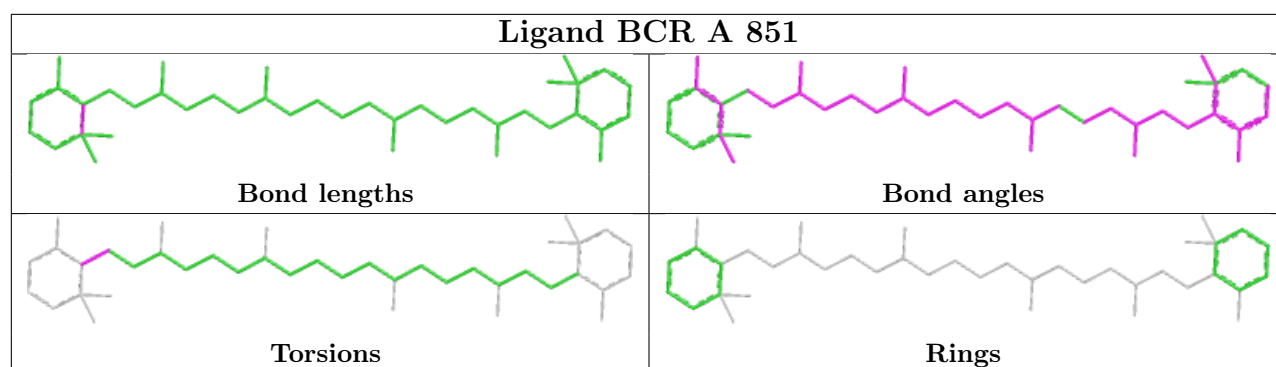
Rings

Ligand CLA 1 608

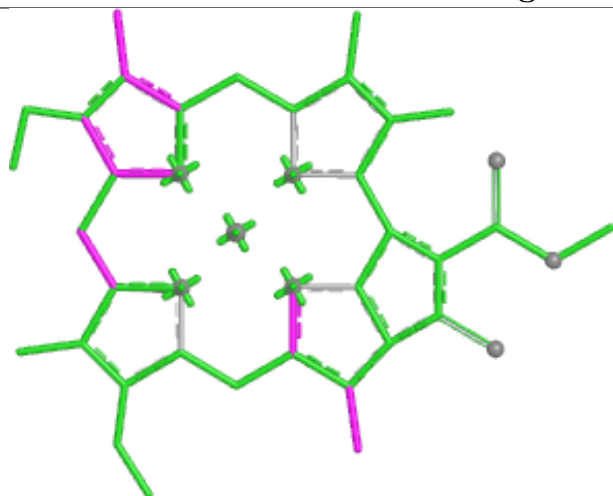


Ligand BCR G 205

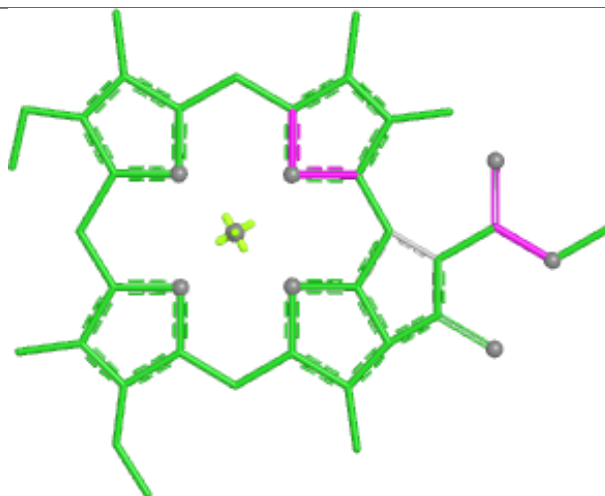




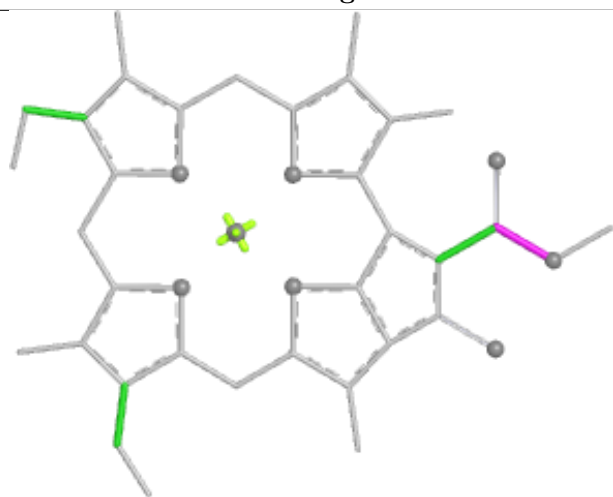
Ligand CLA 5 604



Bond lengths



Bond angles

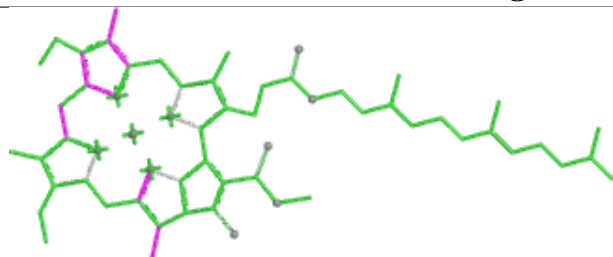


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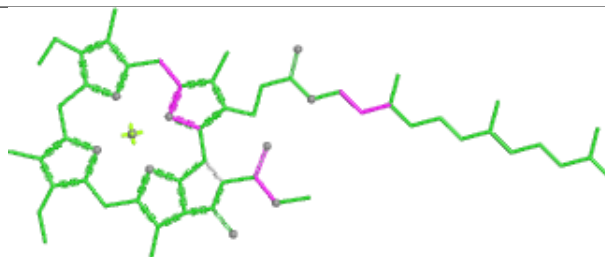


Rings

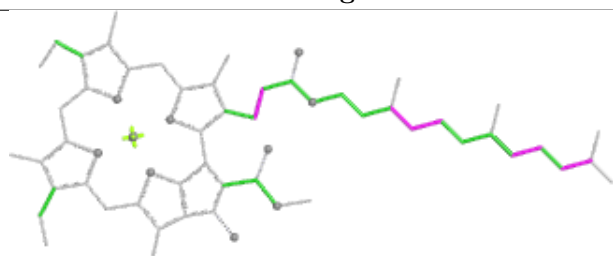
Ligand CLA W 613



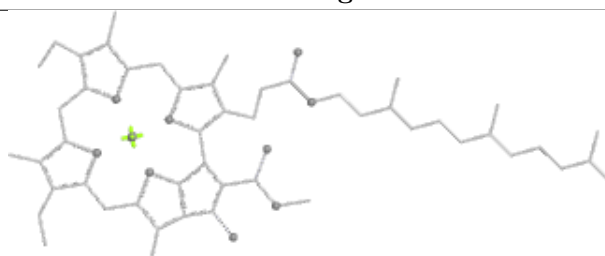
Bond lengths



Bond angles

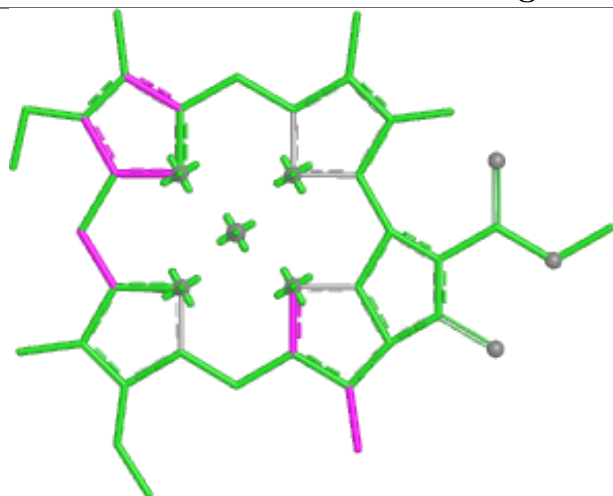


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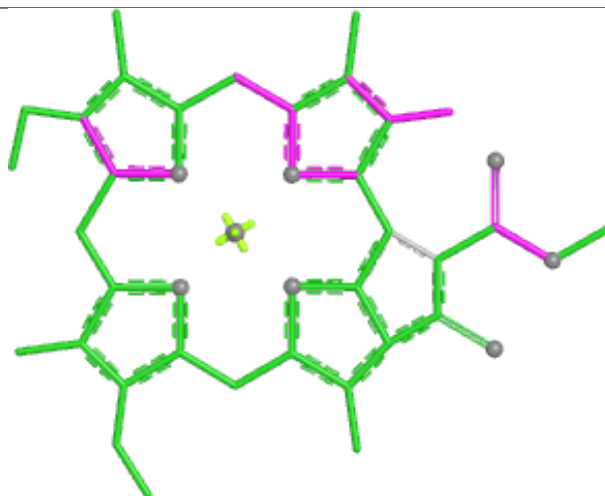


Rings

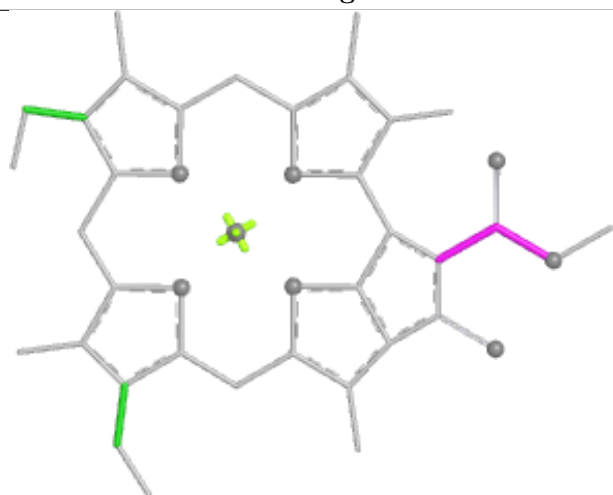
Ligand CLA 7 614



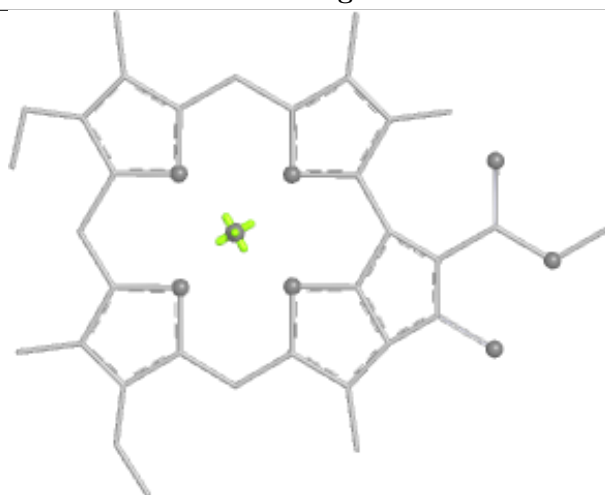
Bond lengths



Bond angles

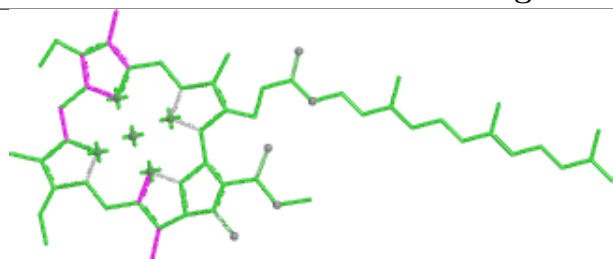


Torsions

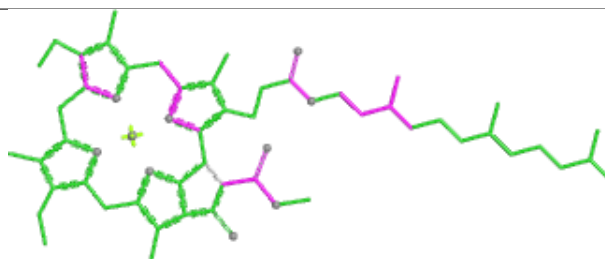


Rings

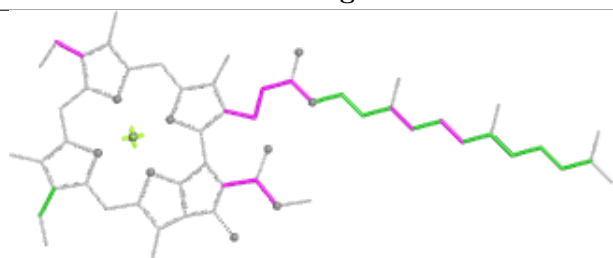
Ligand CLA B 822



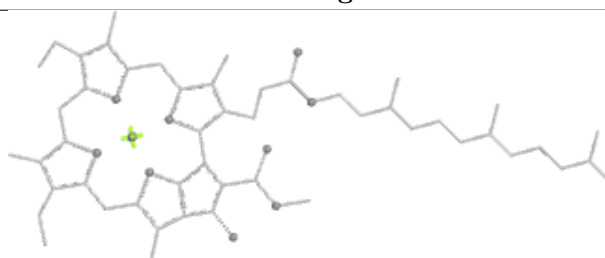
Bond lengths



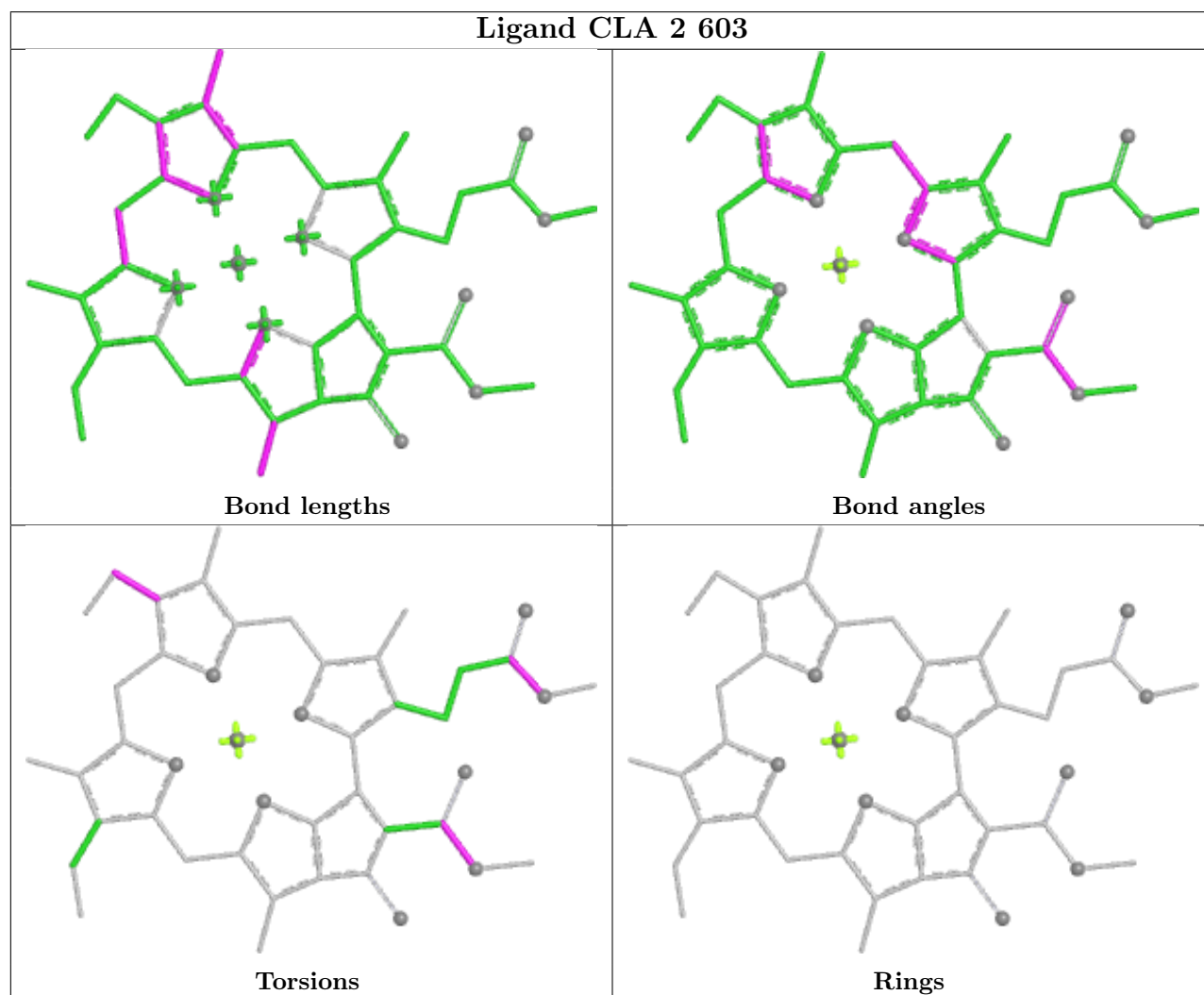
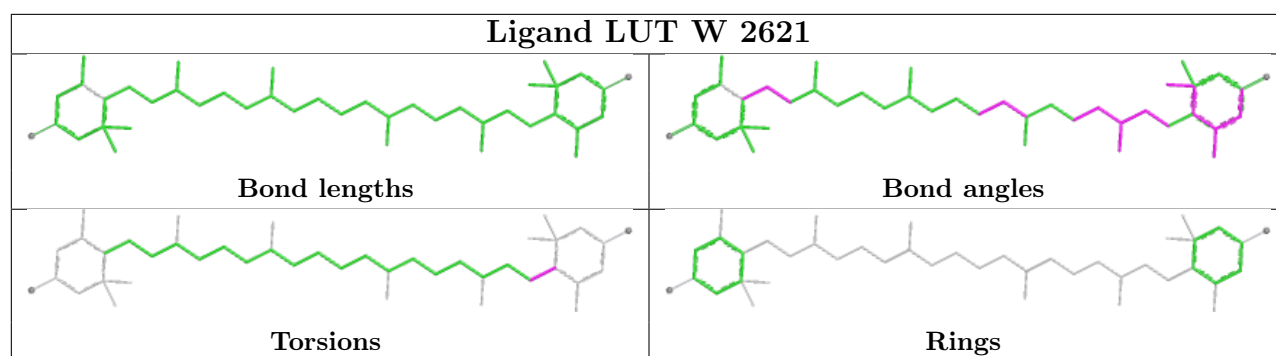
Bond angles



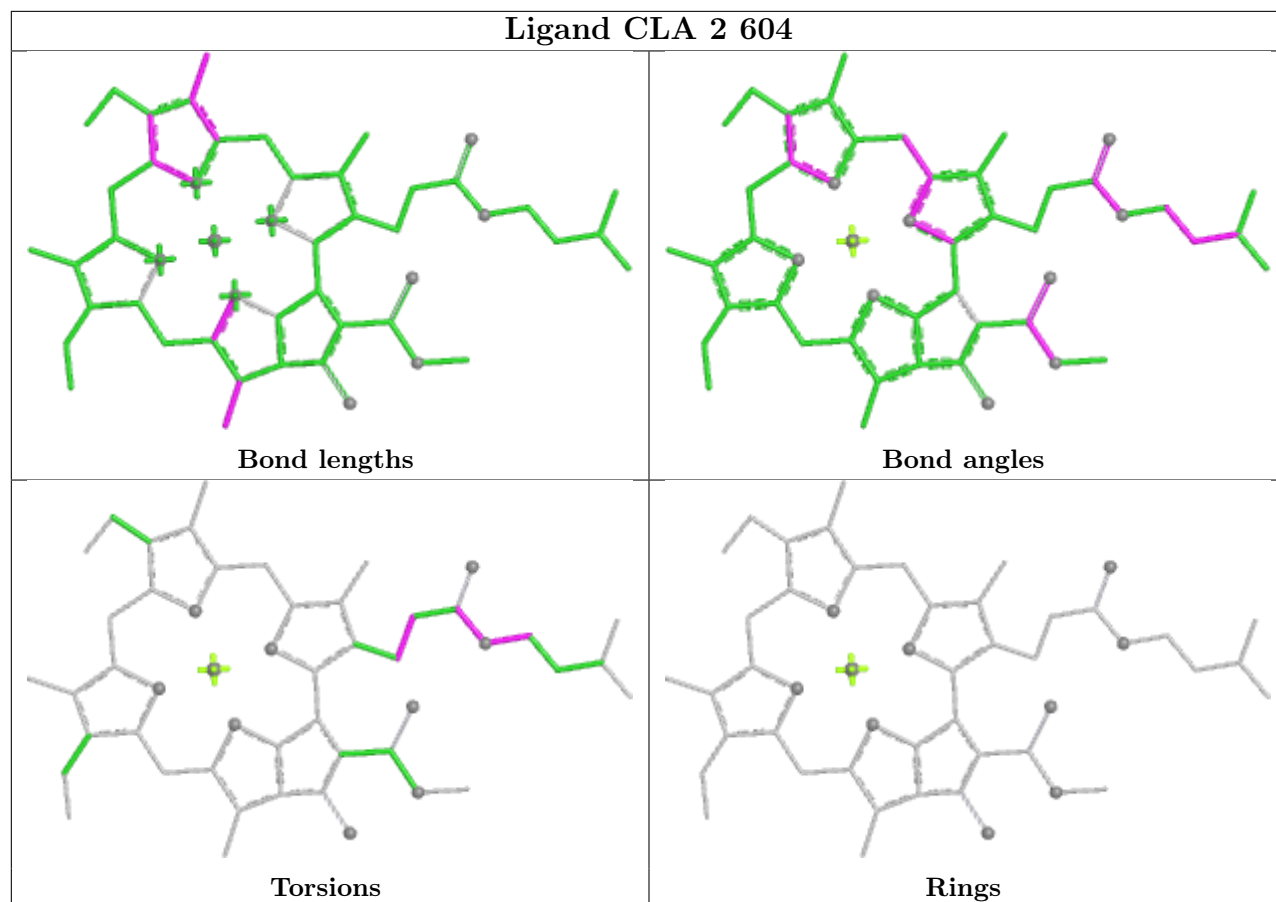
Torsions



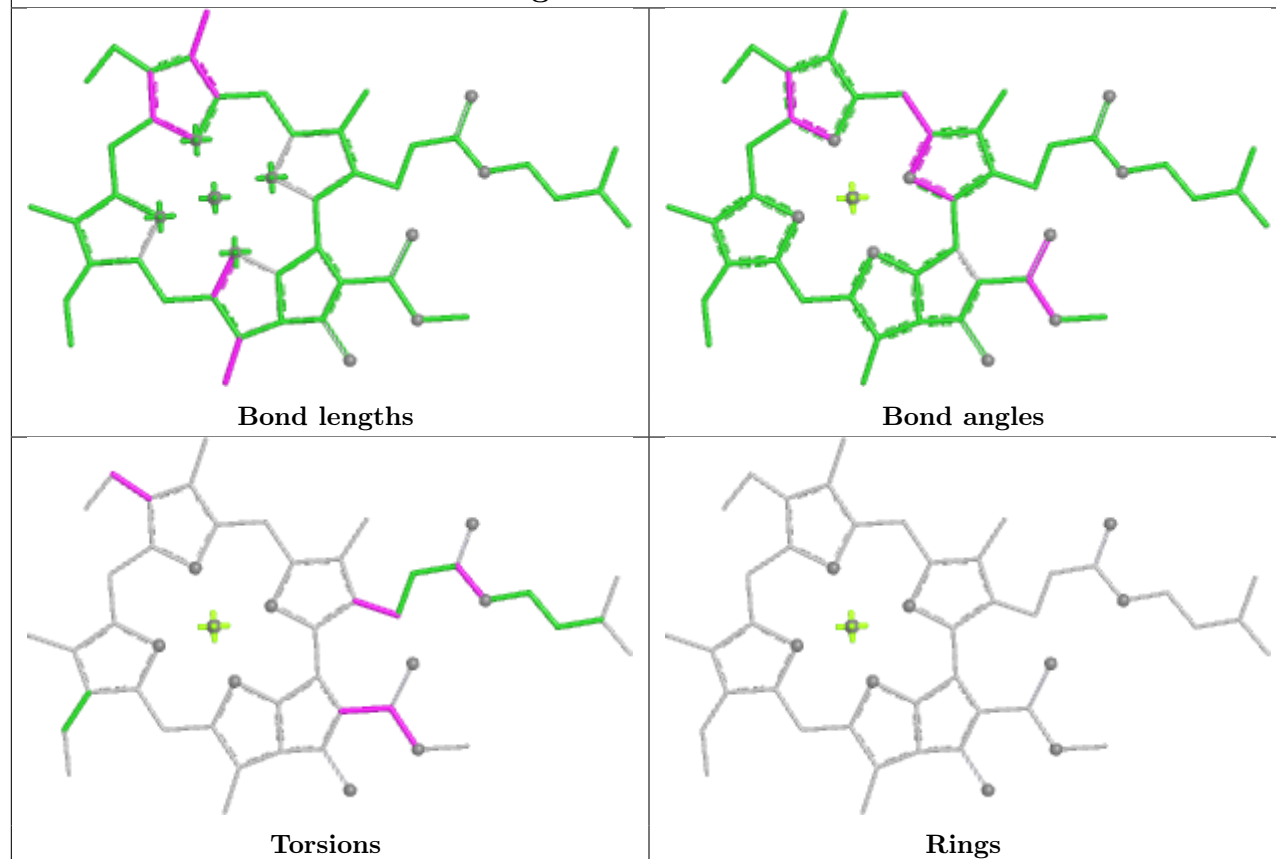
Rings



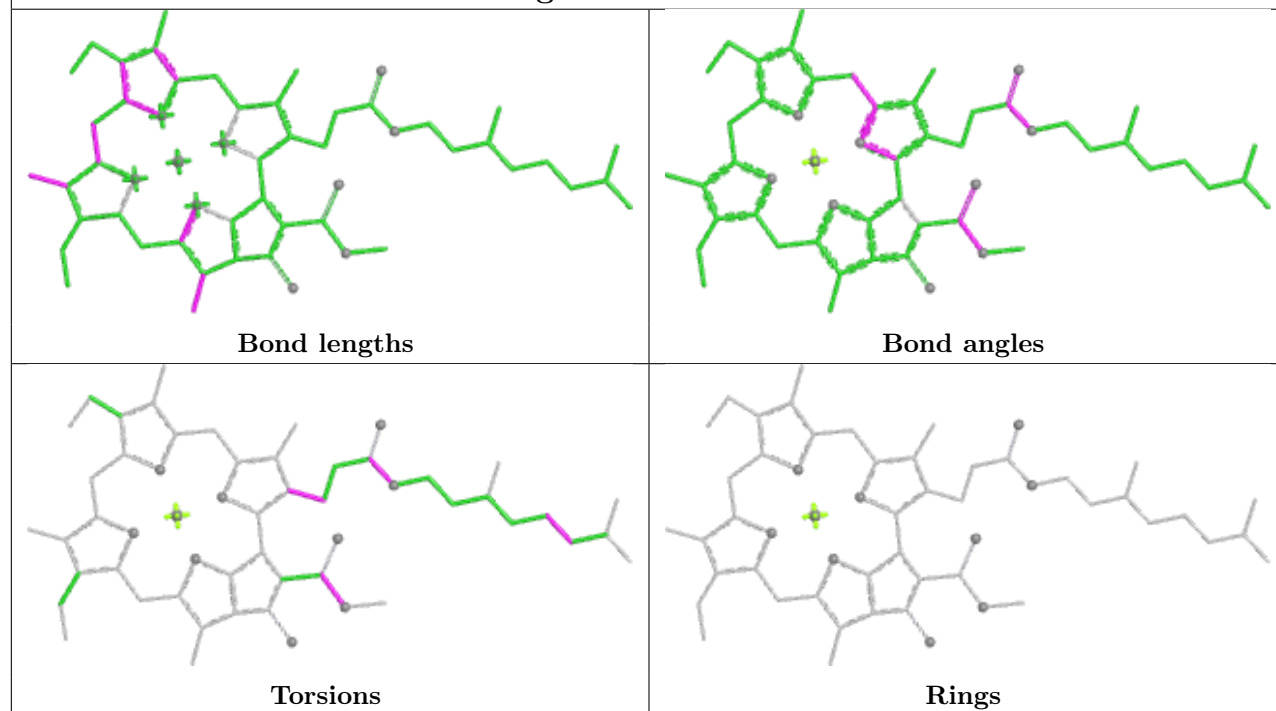
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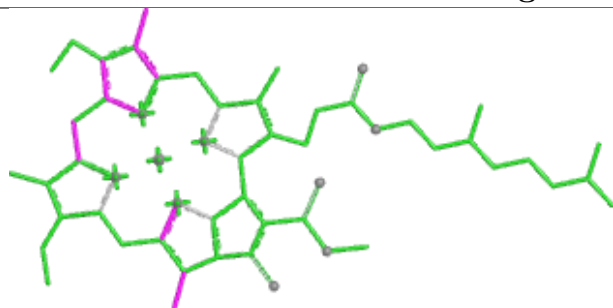


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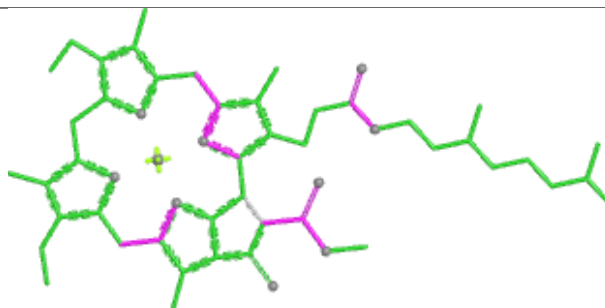


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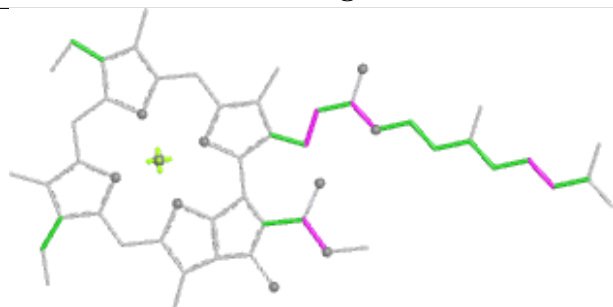


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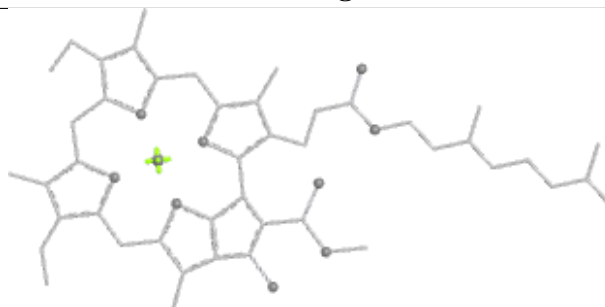
Bond lengths



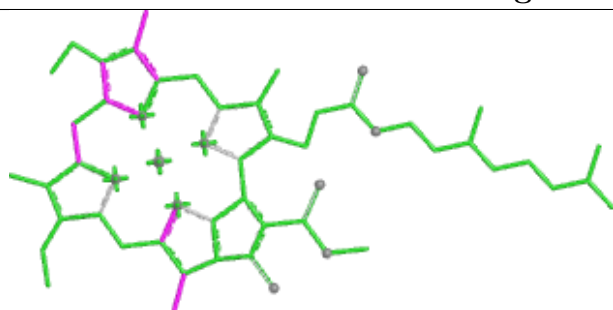
Bond angles



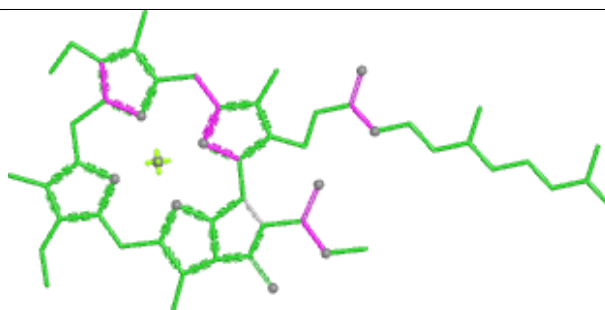
Torsions



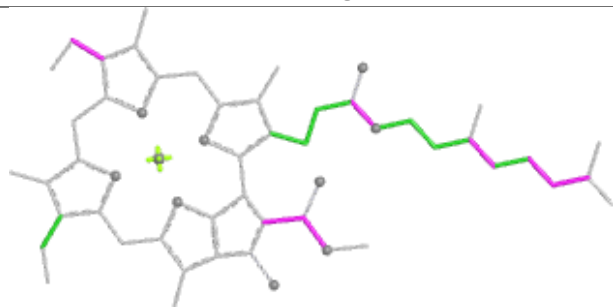
Rings

Ligand CLA B 820

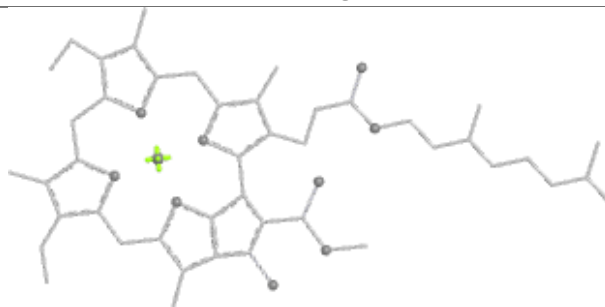
Bond lengths



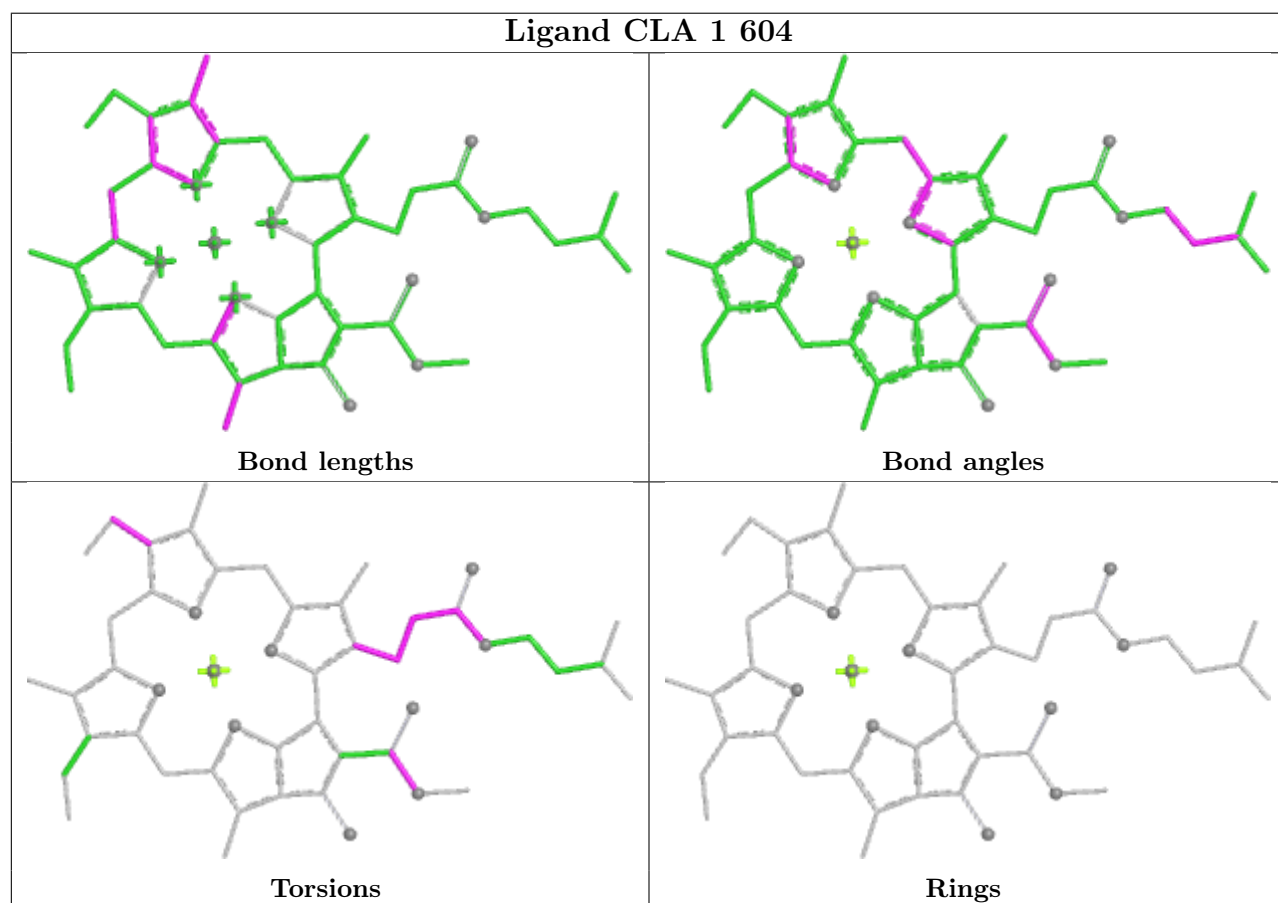
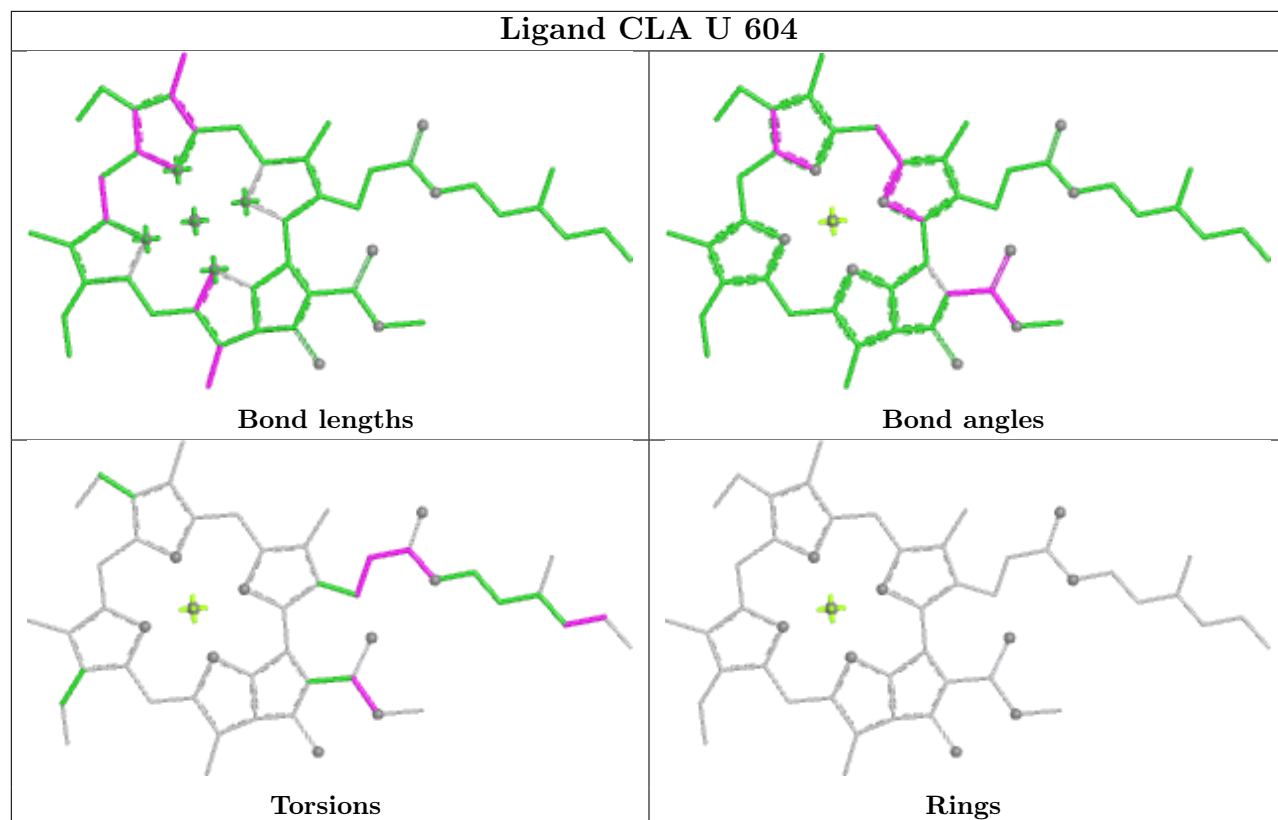
Bond angles

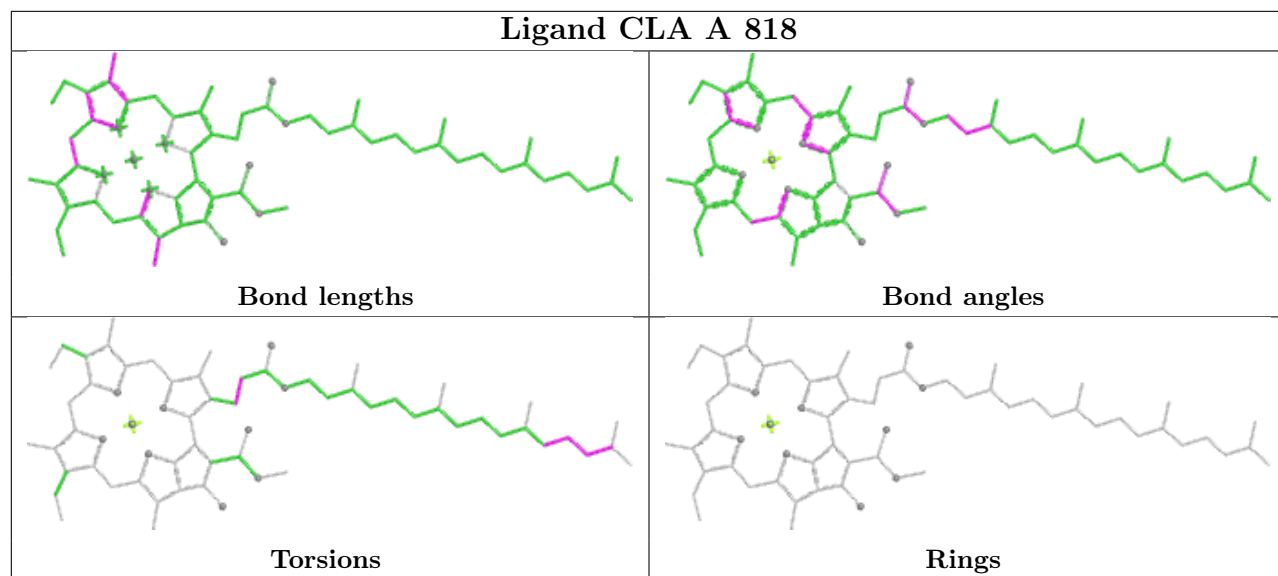


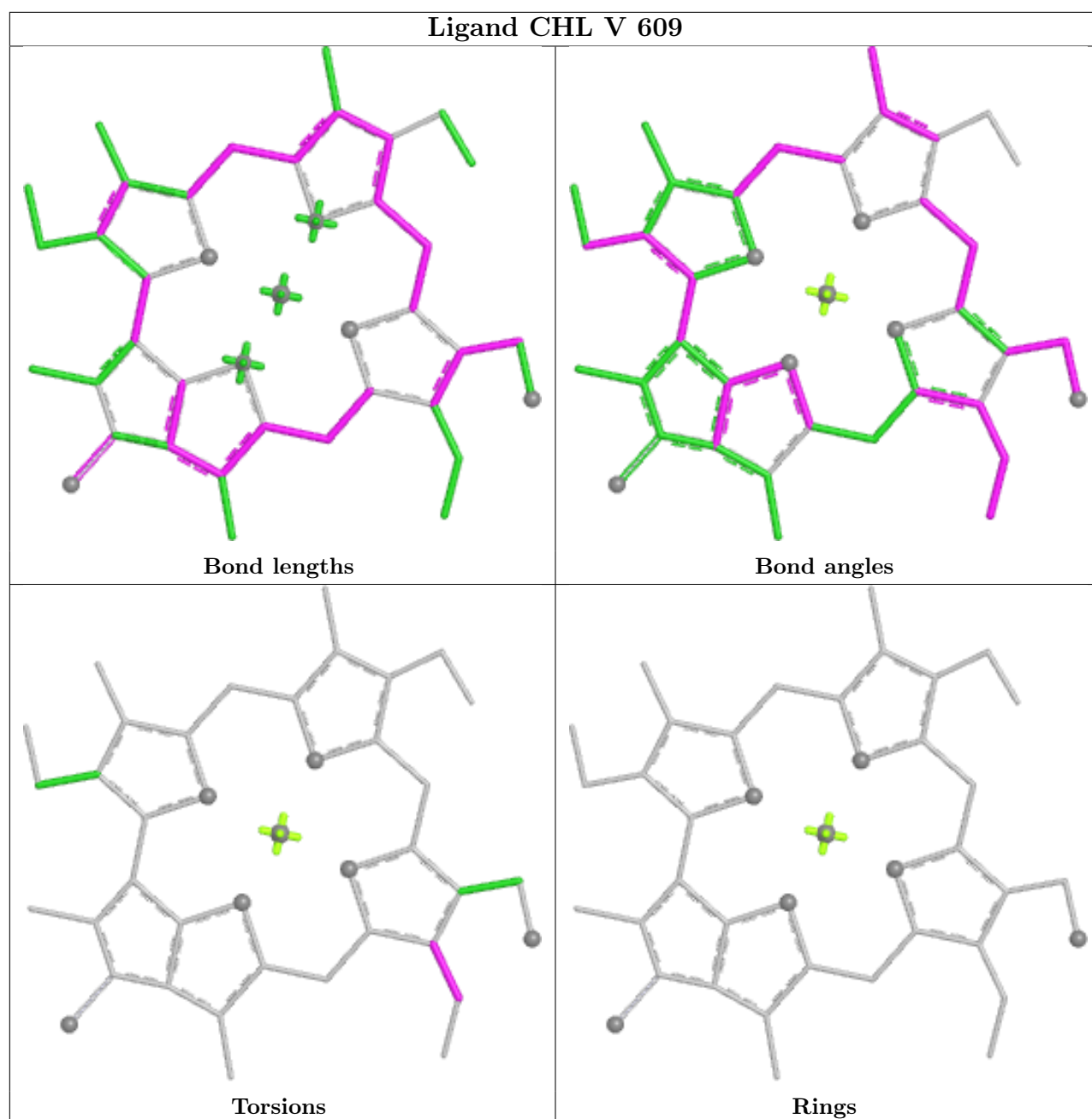
Torsions

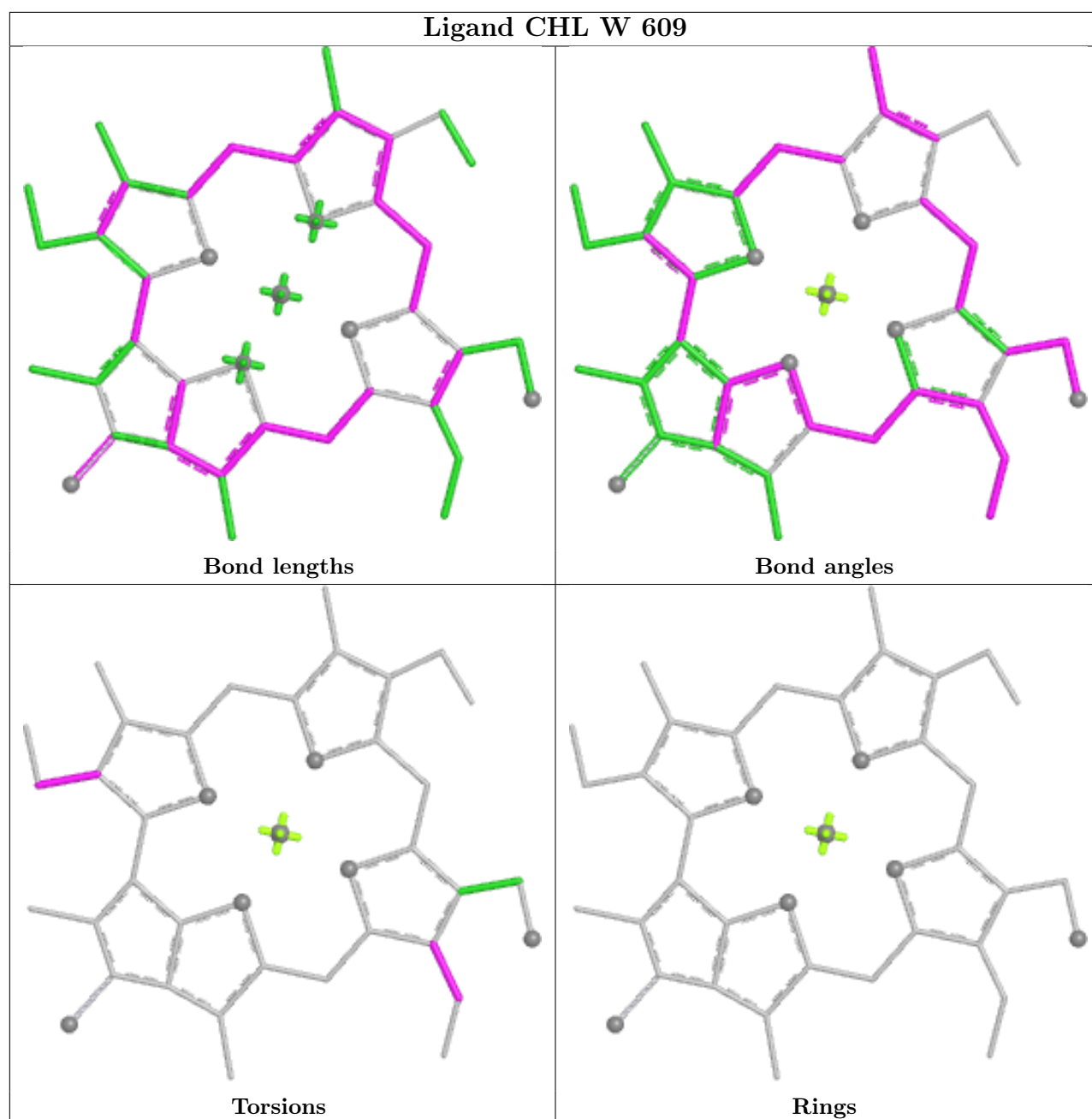


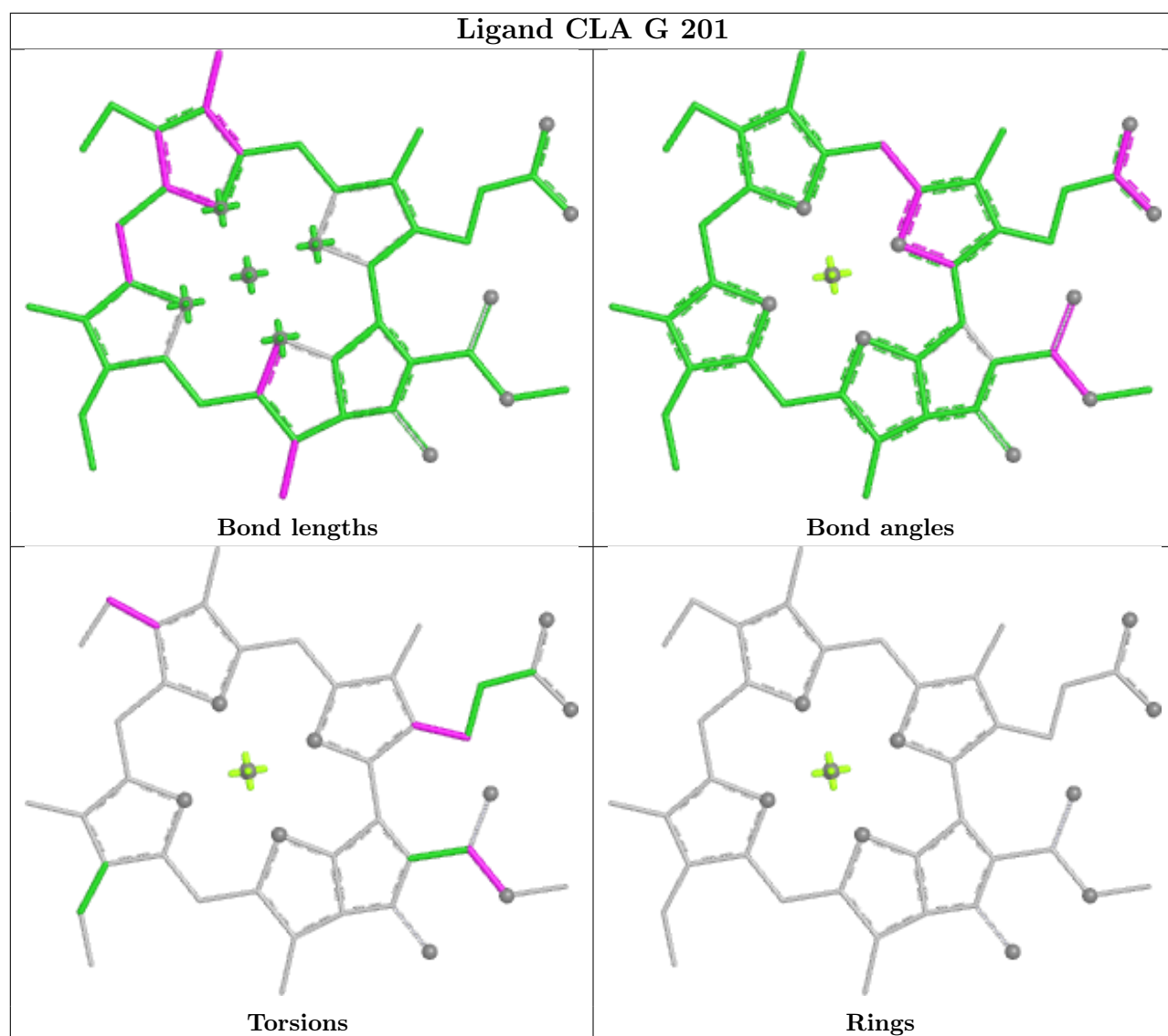
Rings

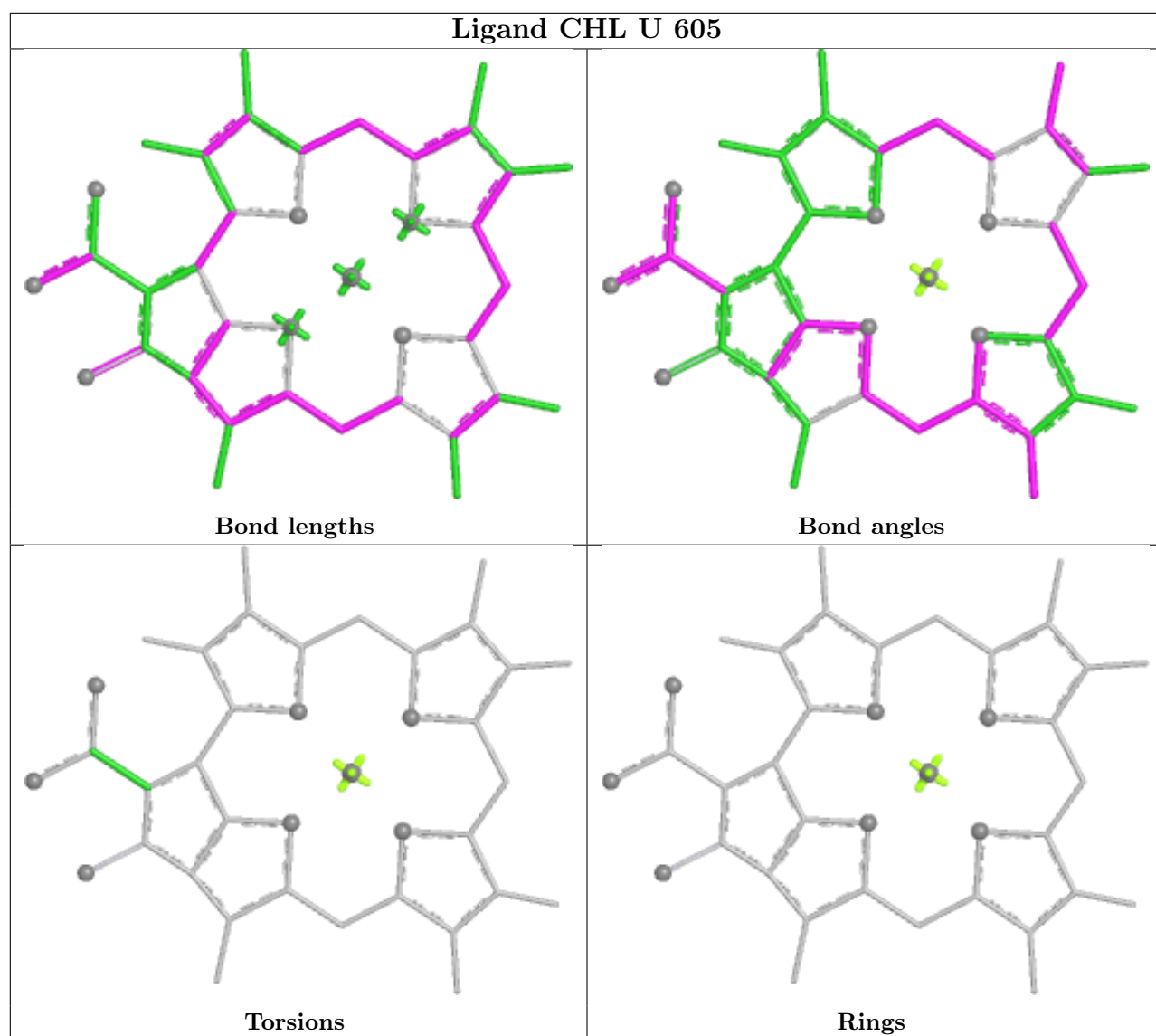




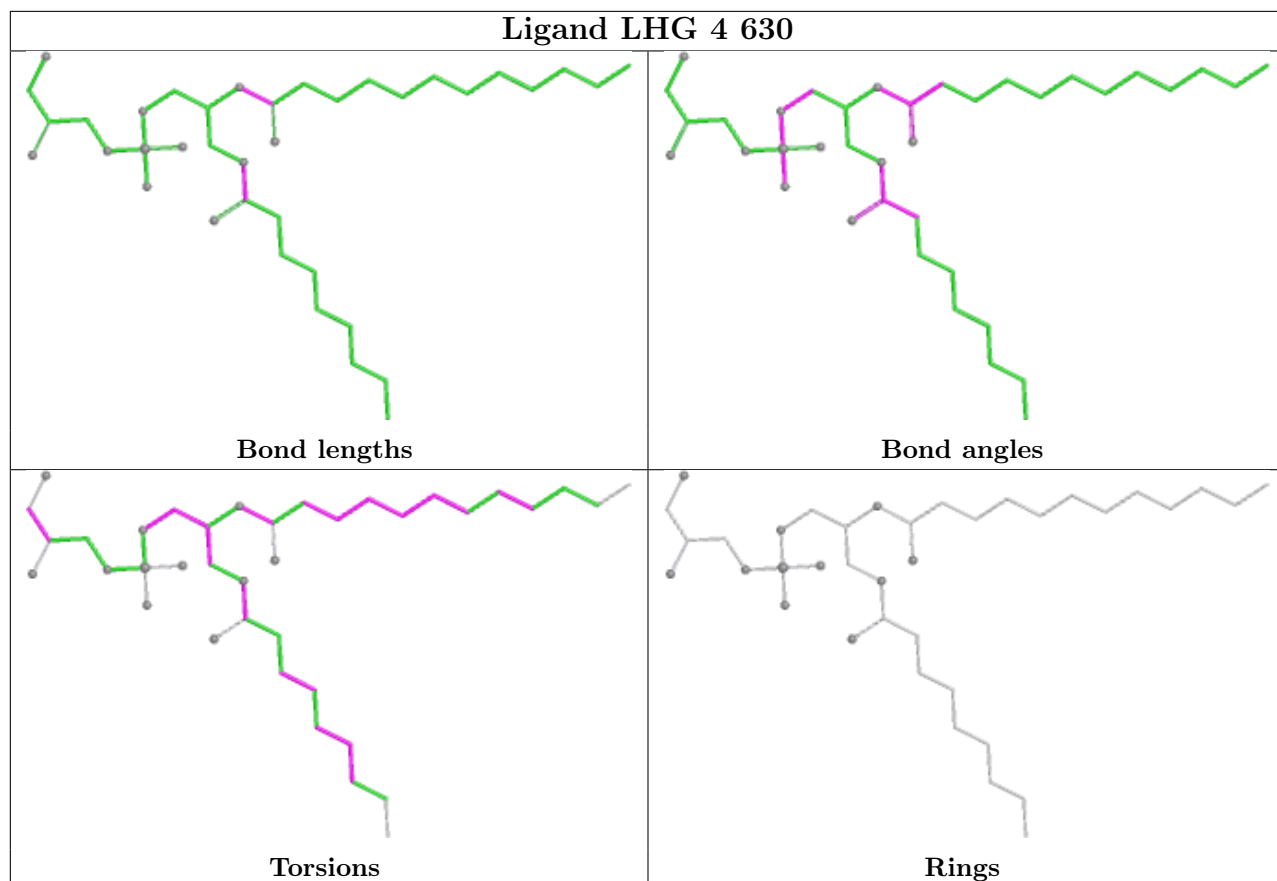




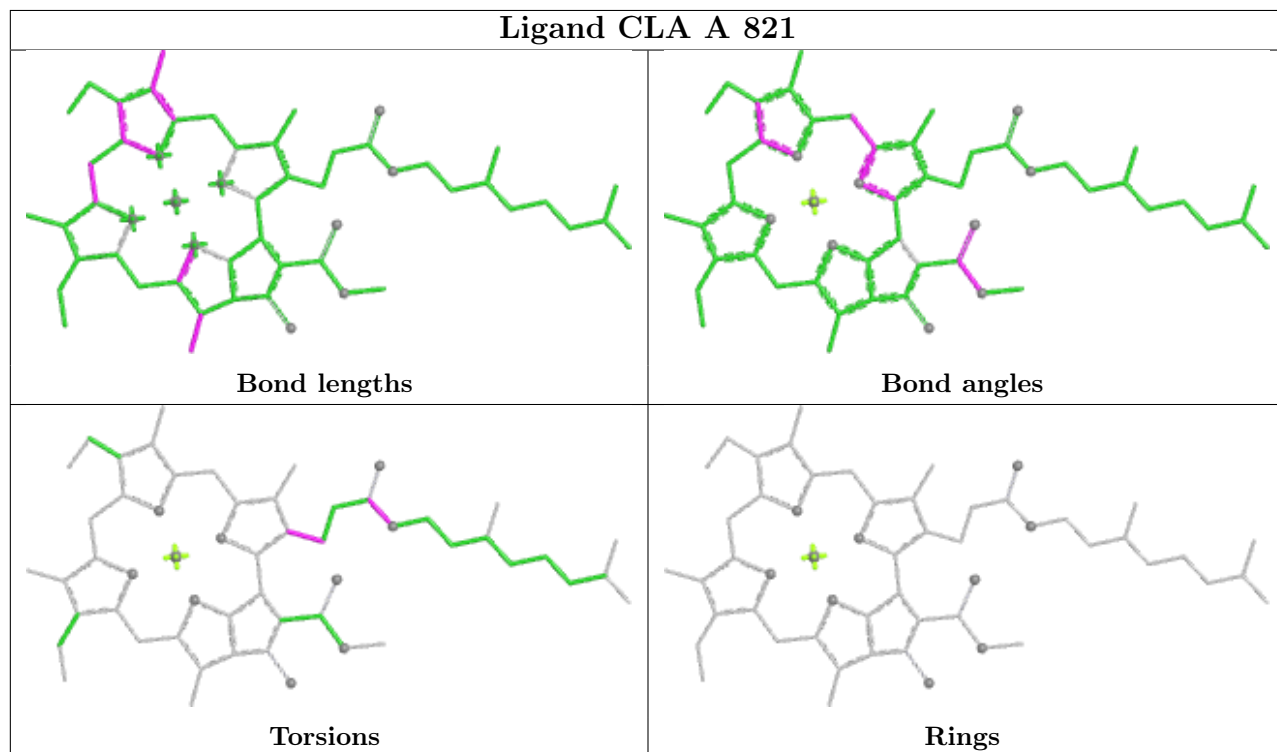


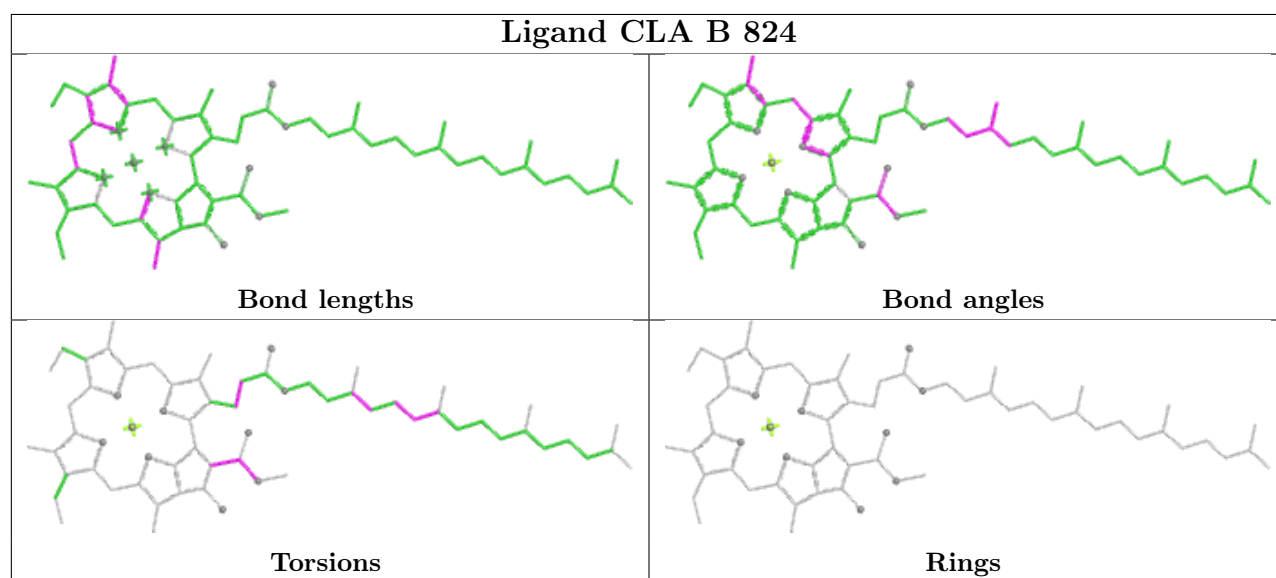
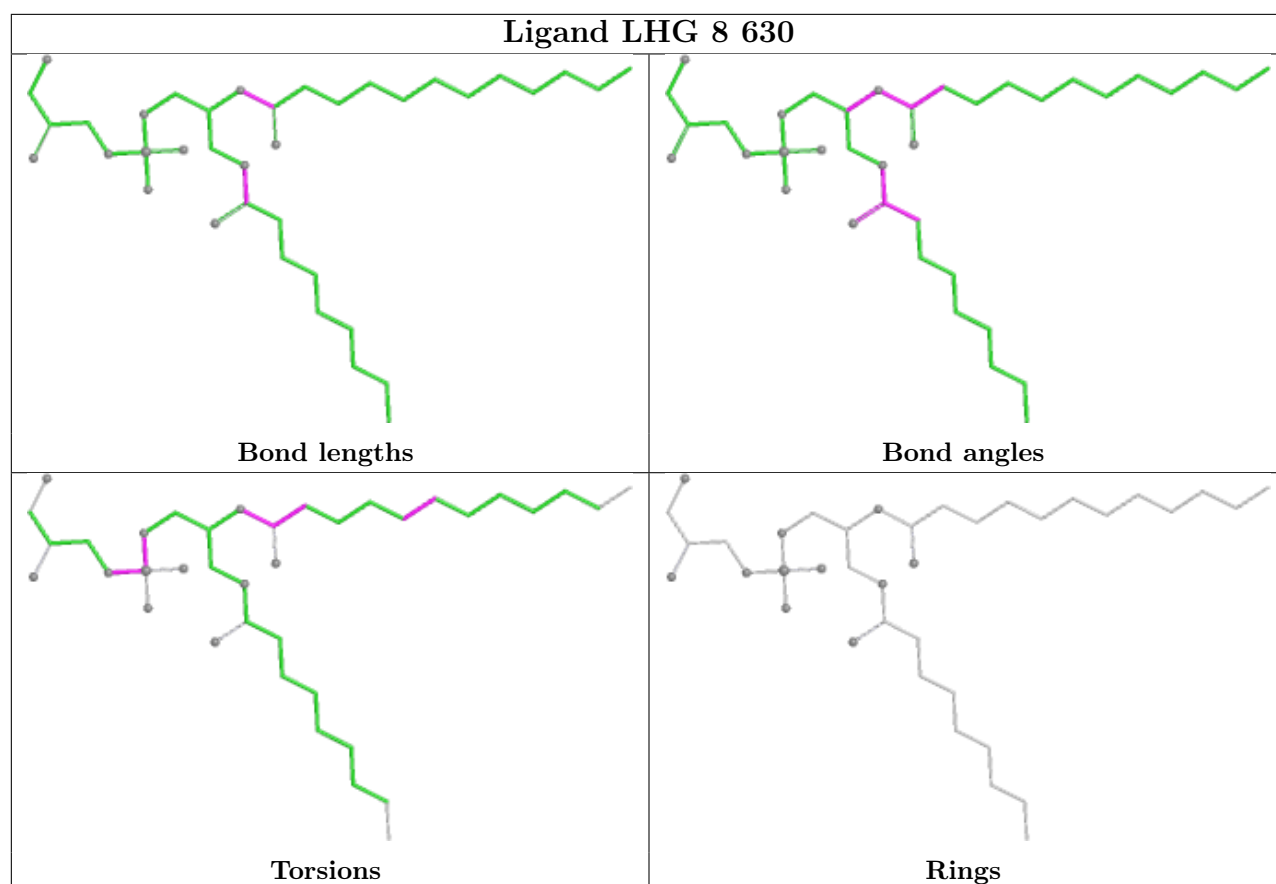


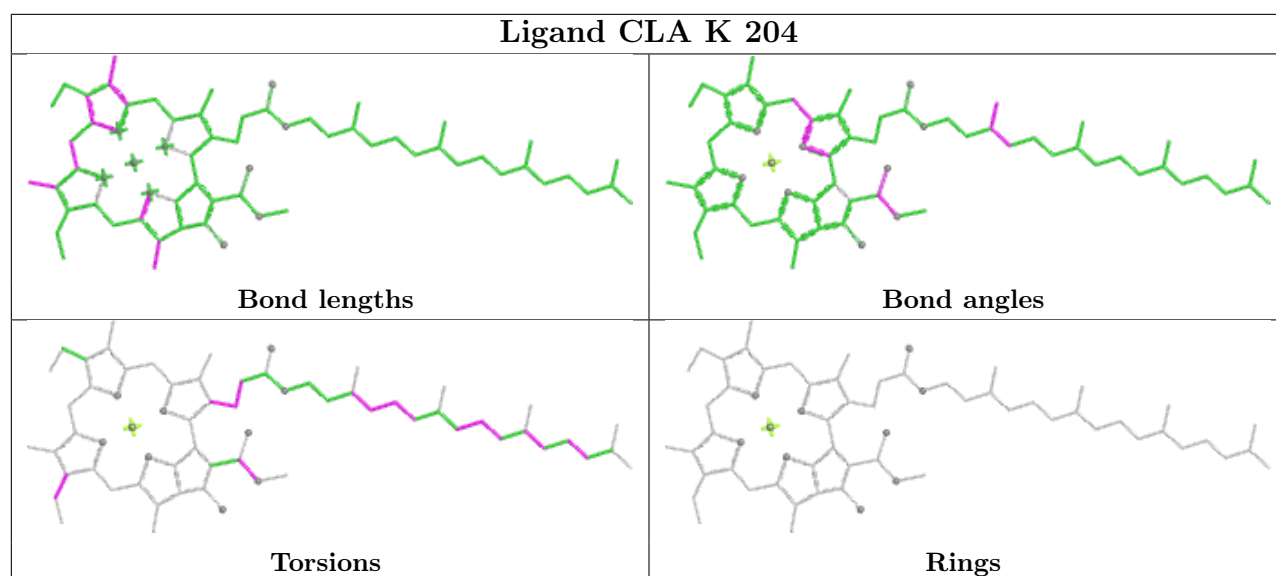
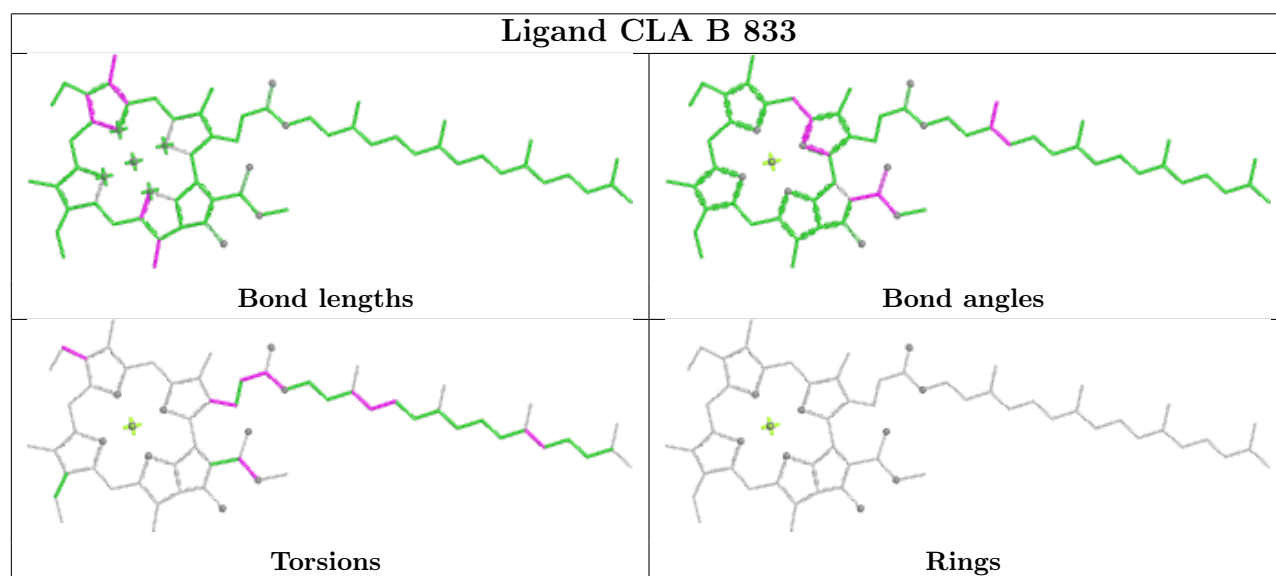
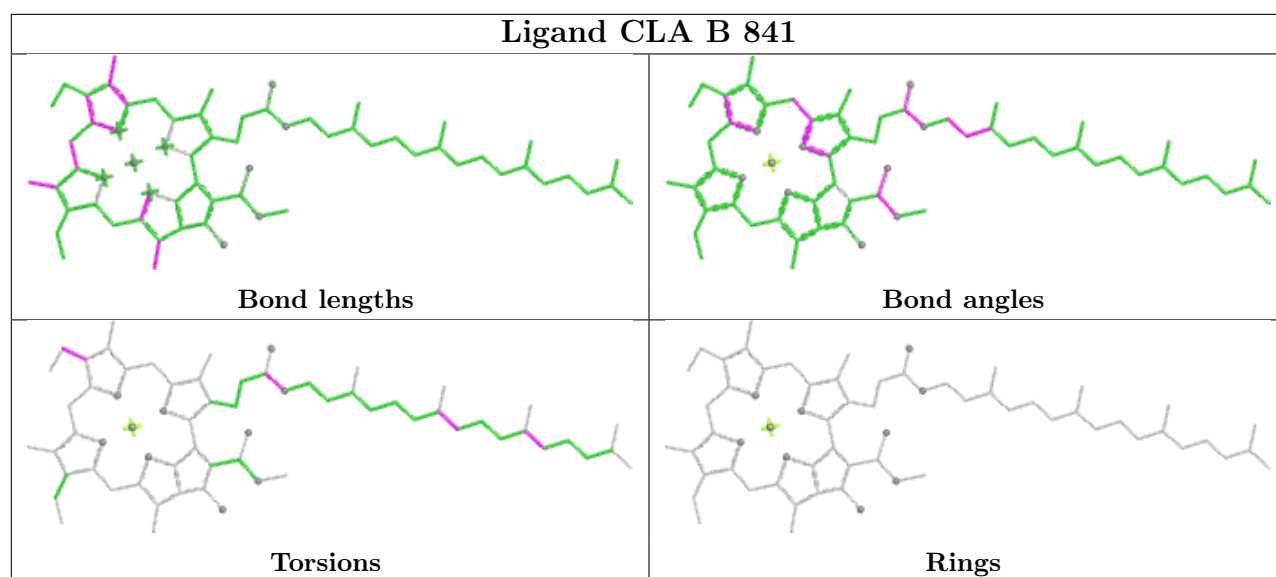
Ligand LHG 4 630



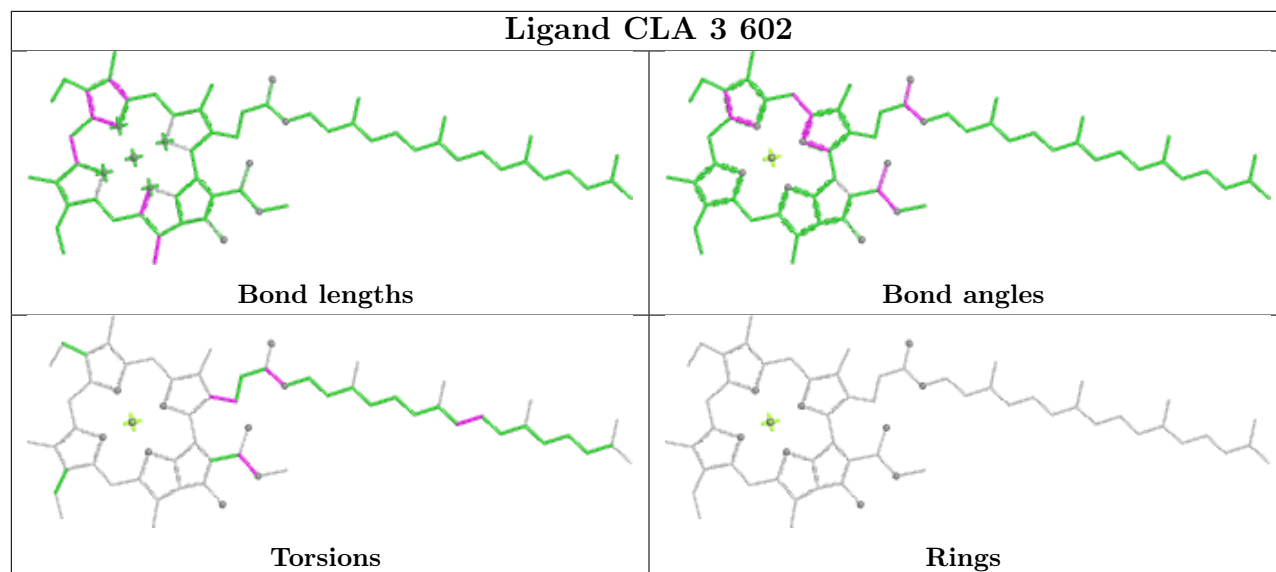
Ligand CLA A 821



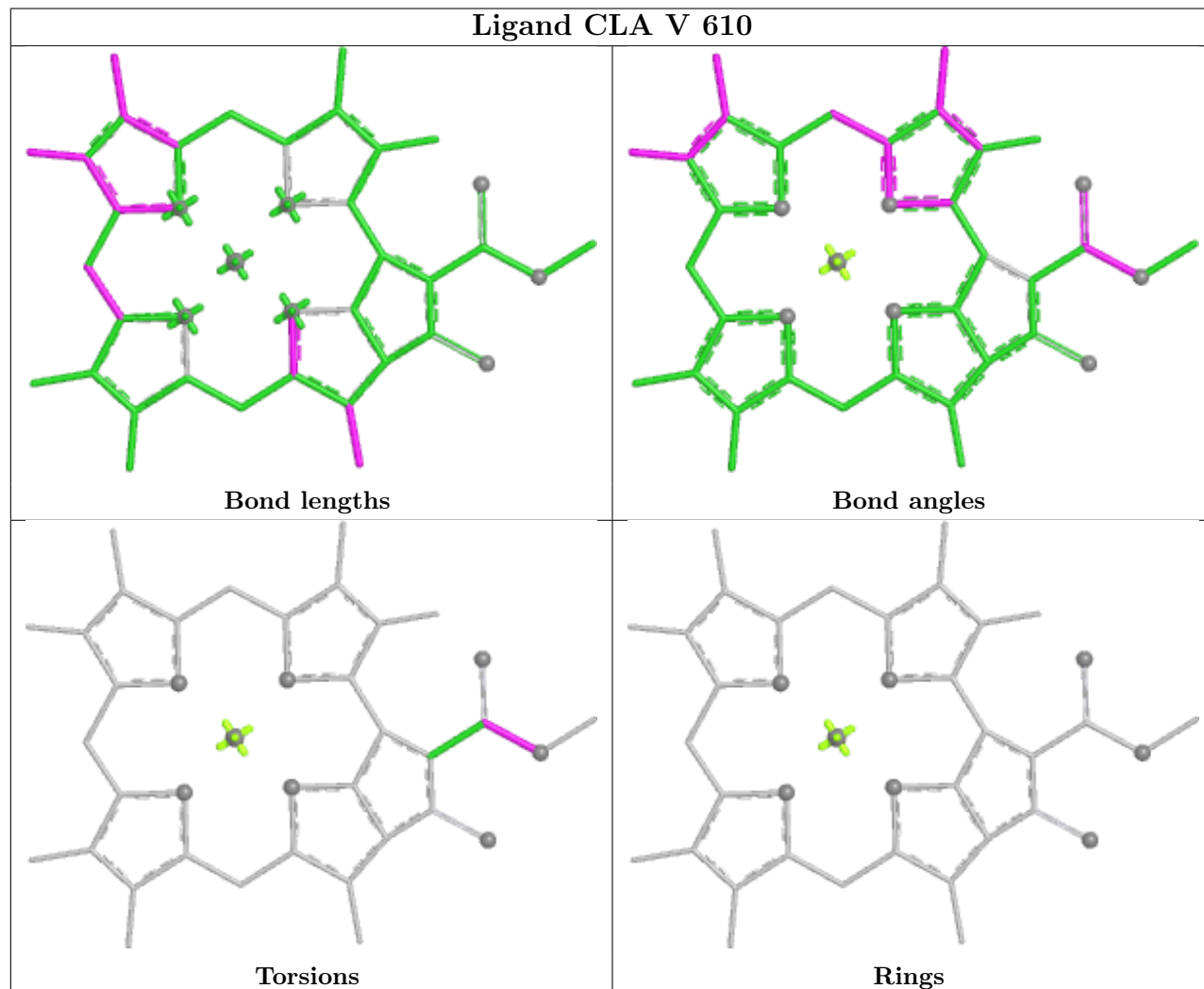




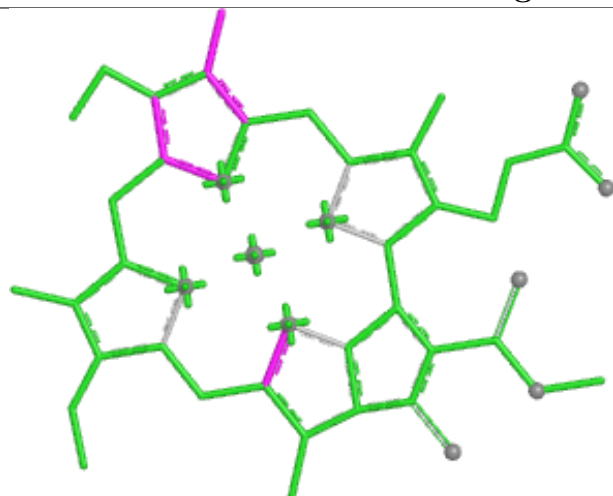
Ligand CLA 3 602



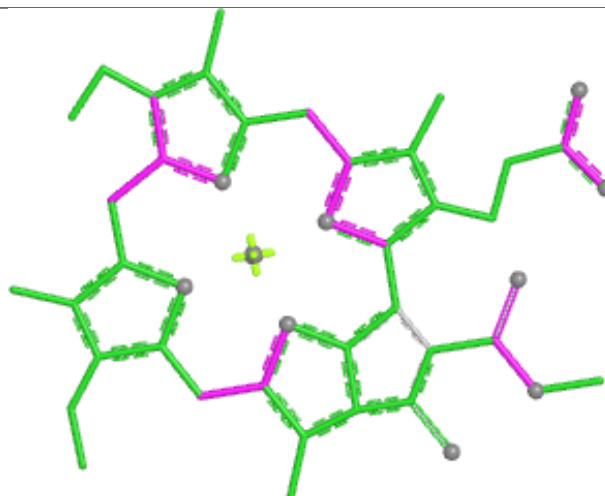
Ligand CLA V 610



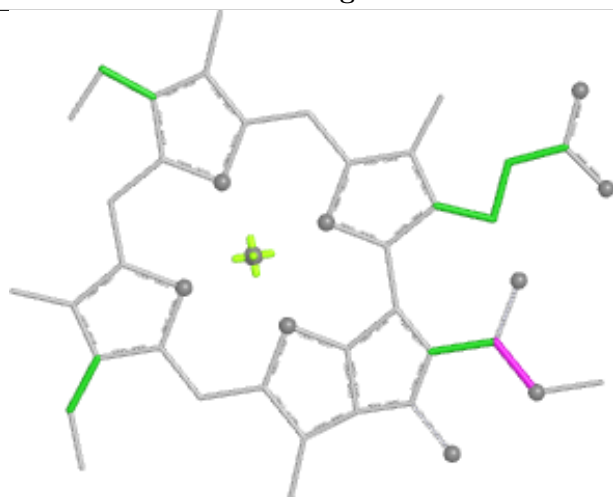
Ligand CLA B 835



Bond lengths



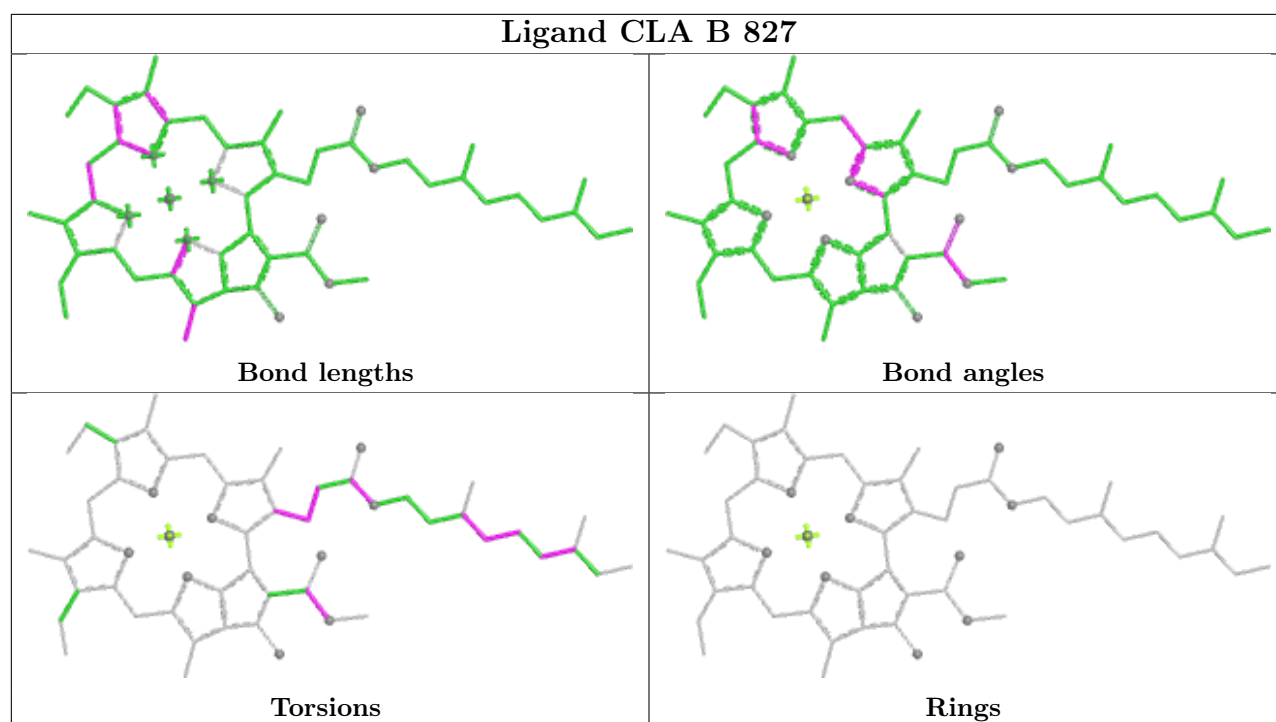
Bond angles



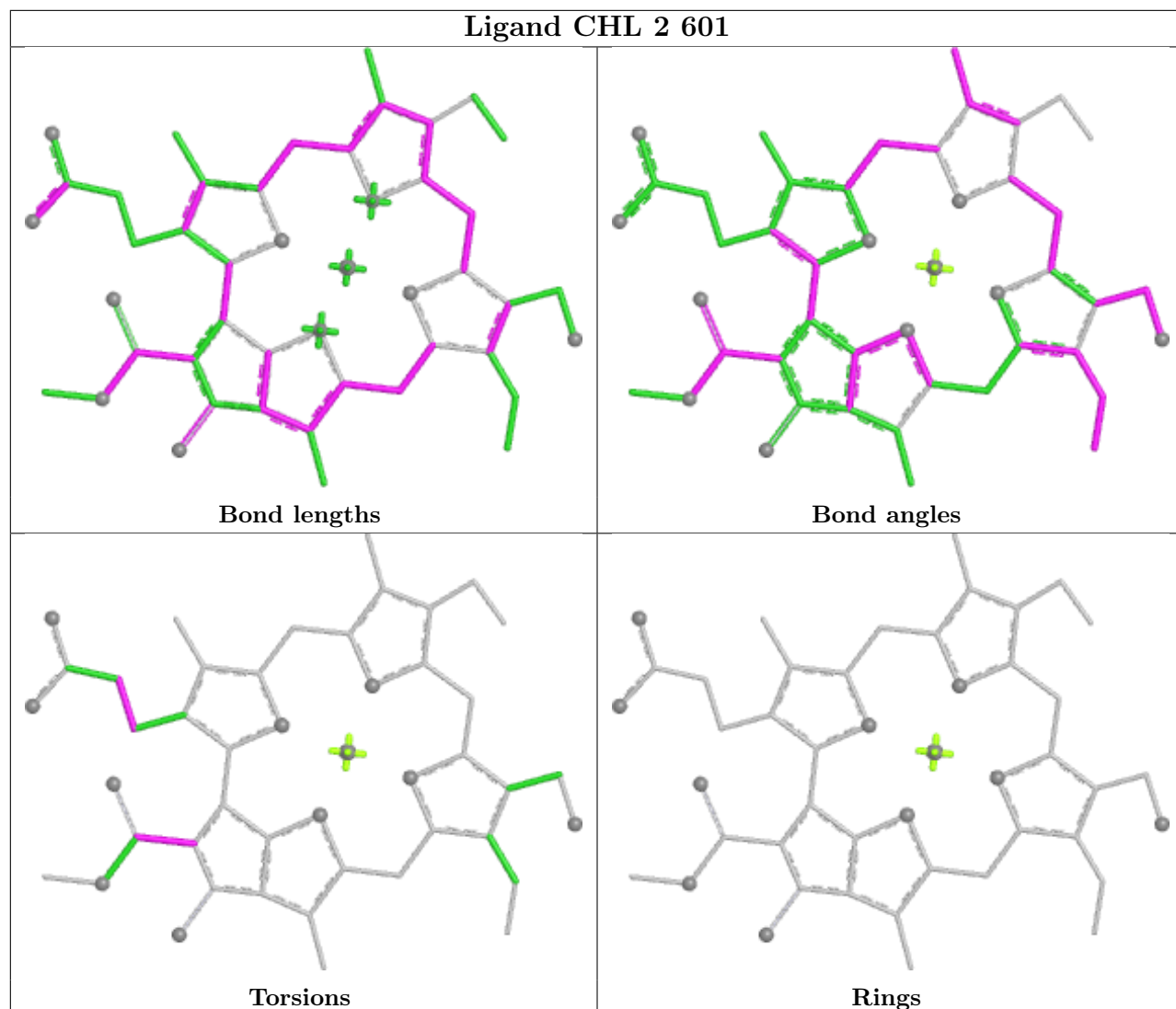
Torsions



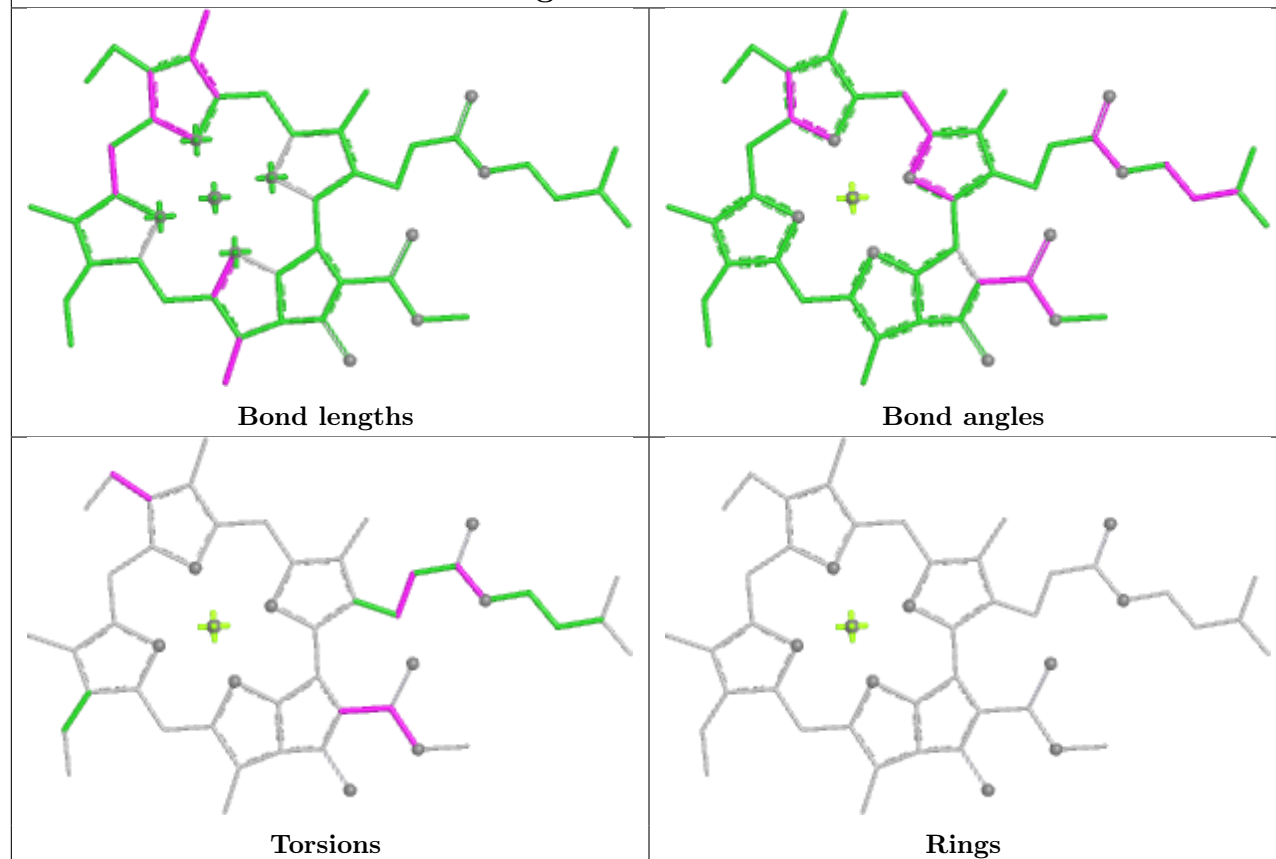
Rings



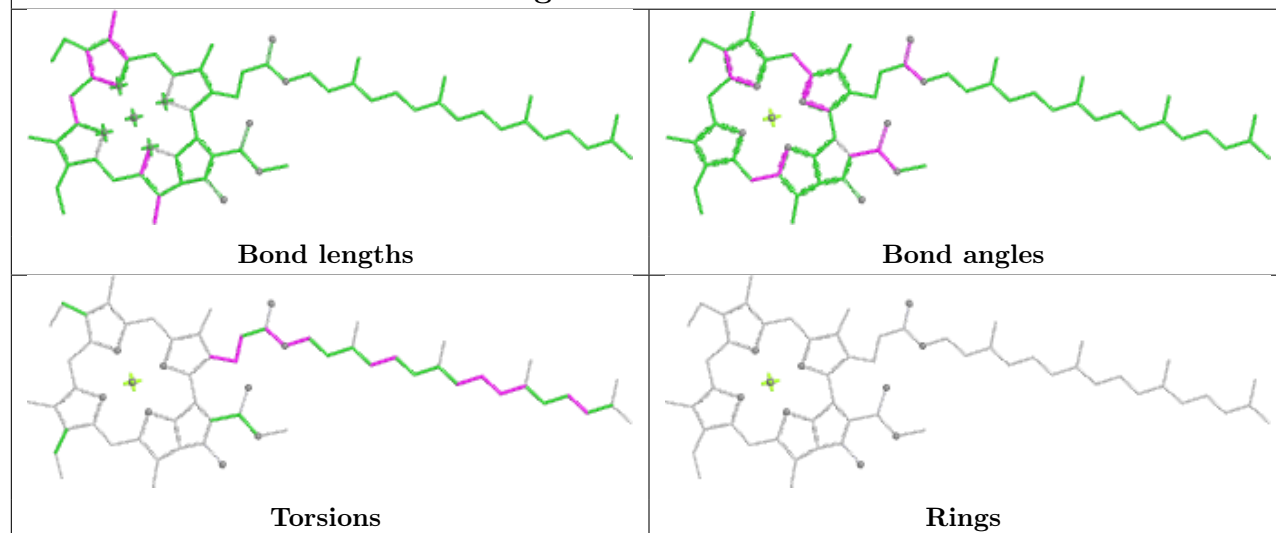
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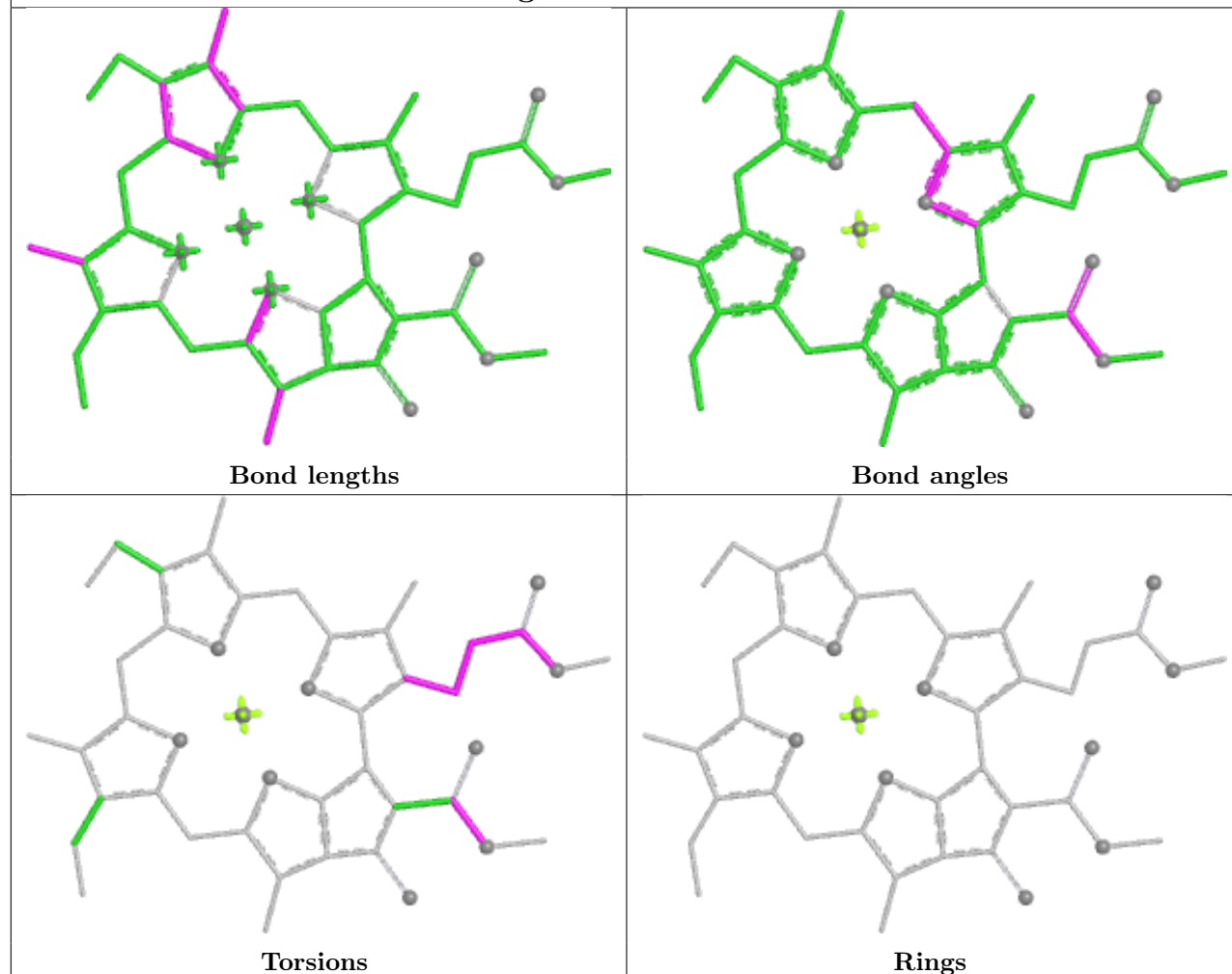
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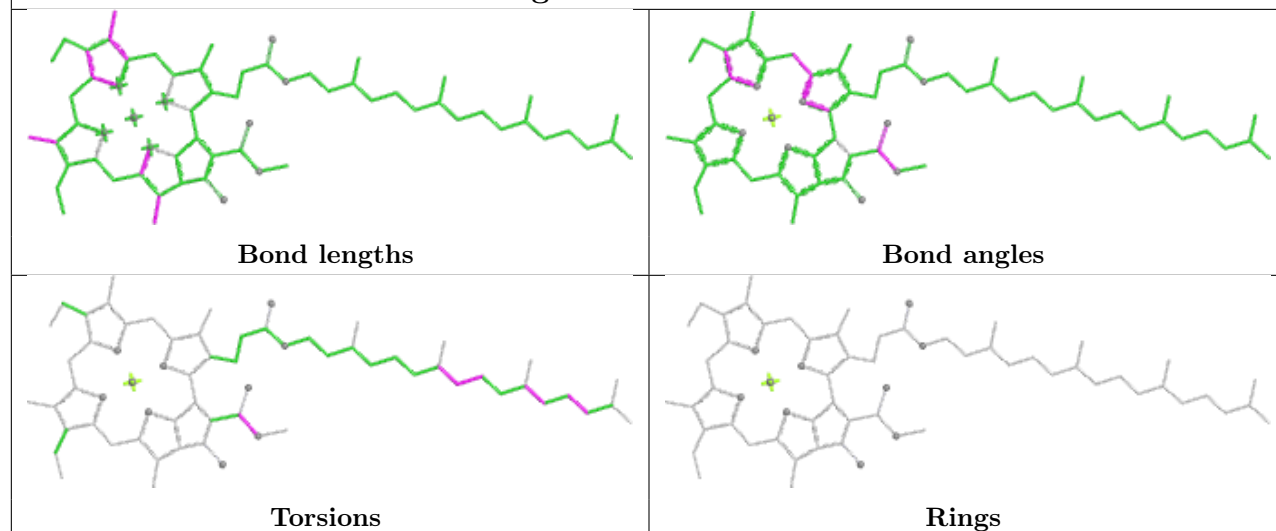
Ligand CLA L 303



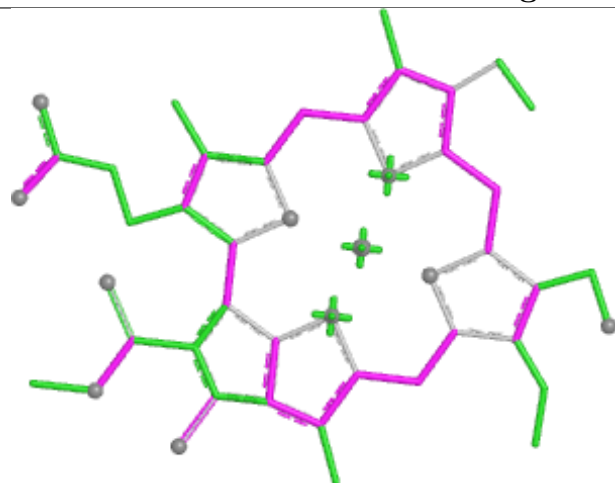
Ligand CLA 5 612



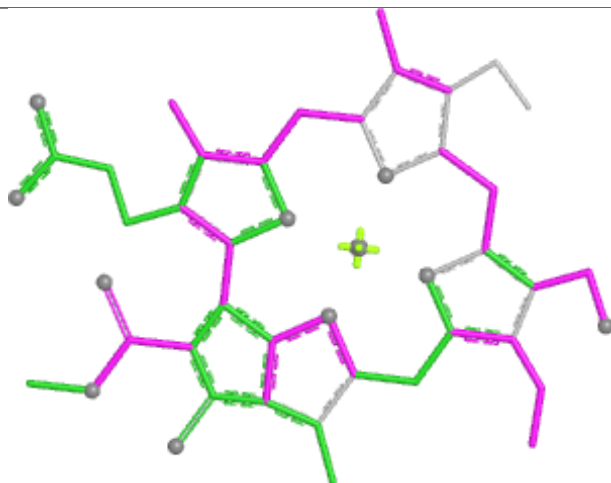
Ligand CLA A 802



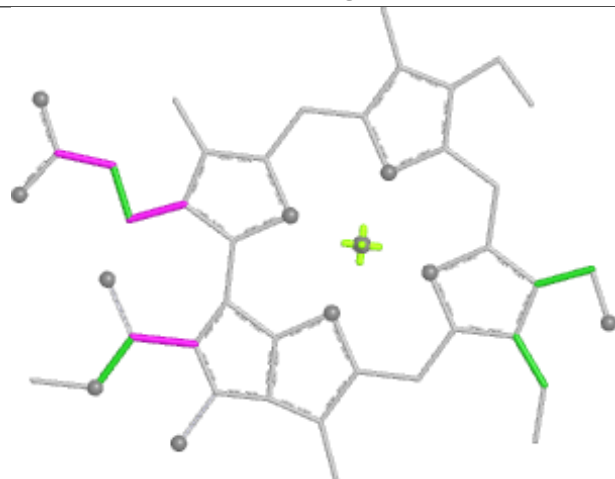
Ligand CHL 2 606



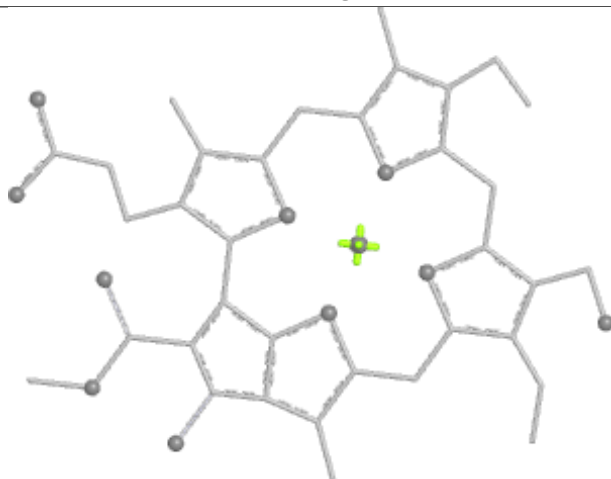
Bond lengths



Bond angles

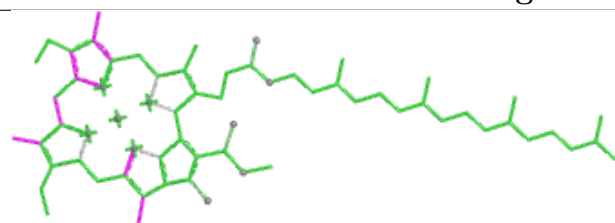


Torsions

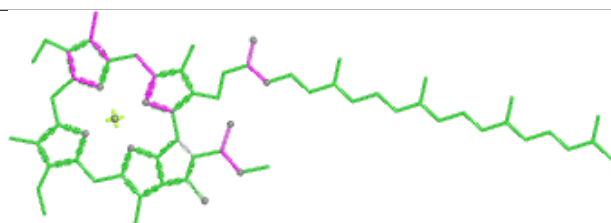


Rings

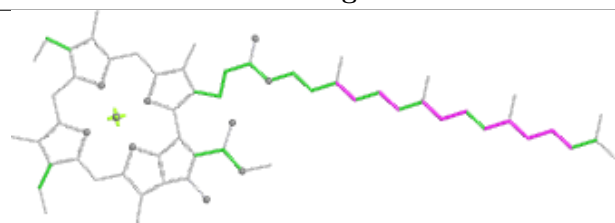
Ligand CLA A 828



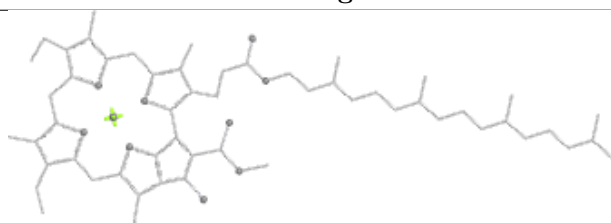
Bond lengths



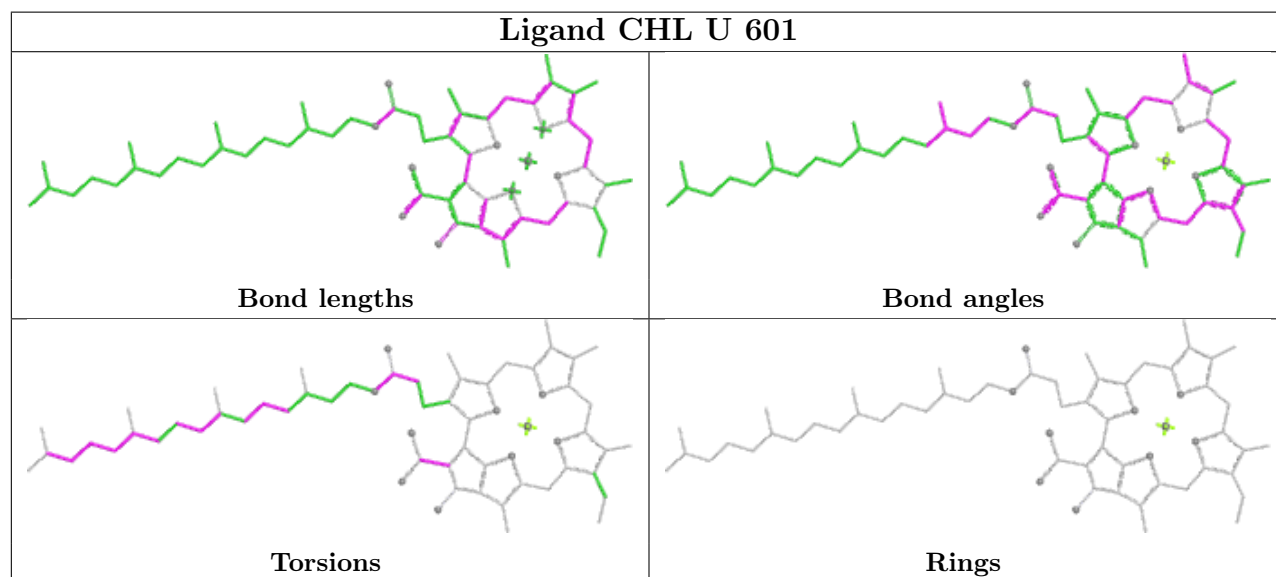
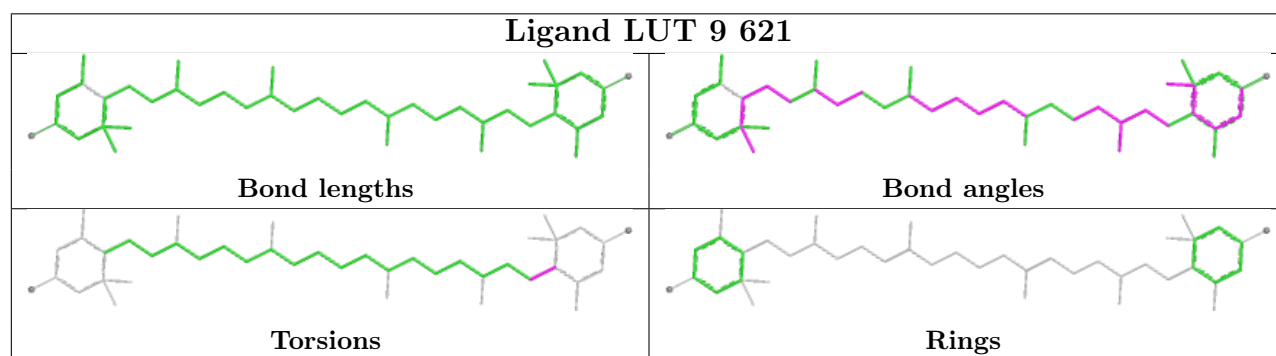
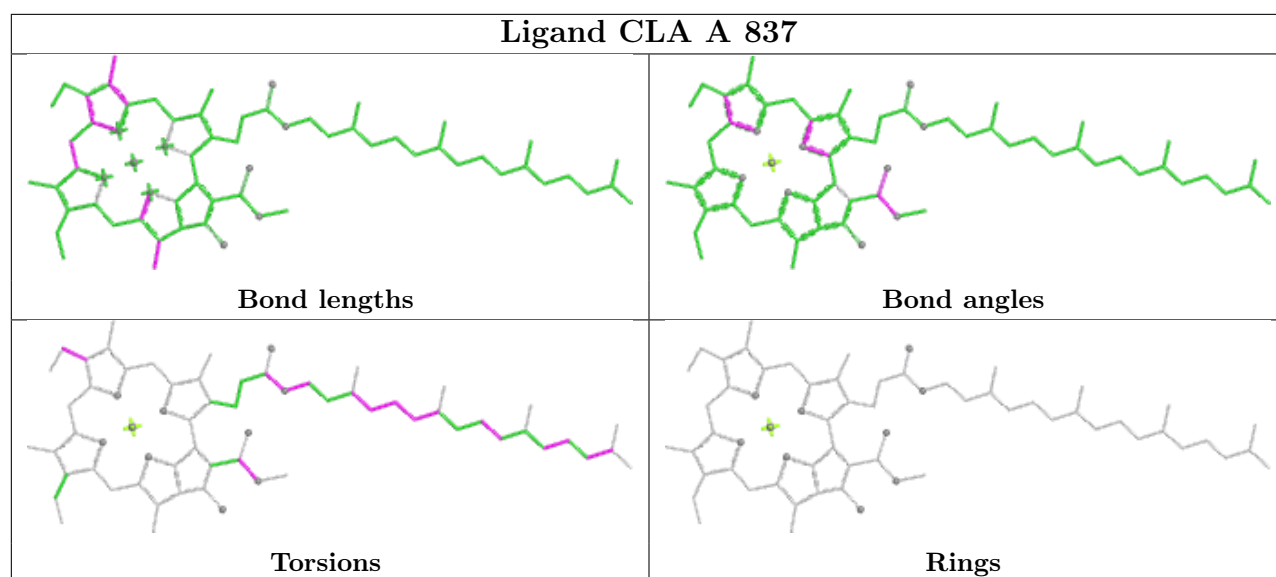
Bond angles

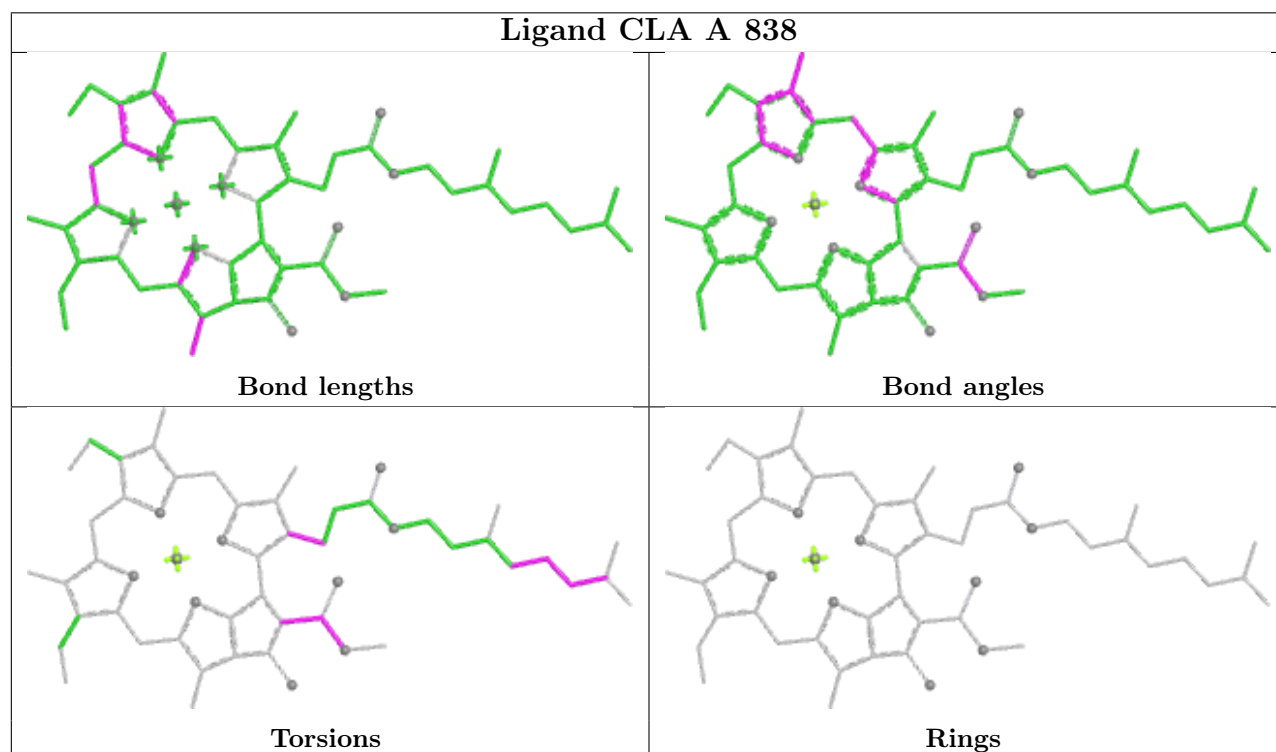
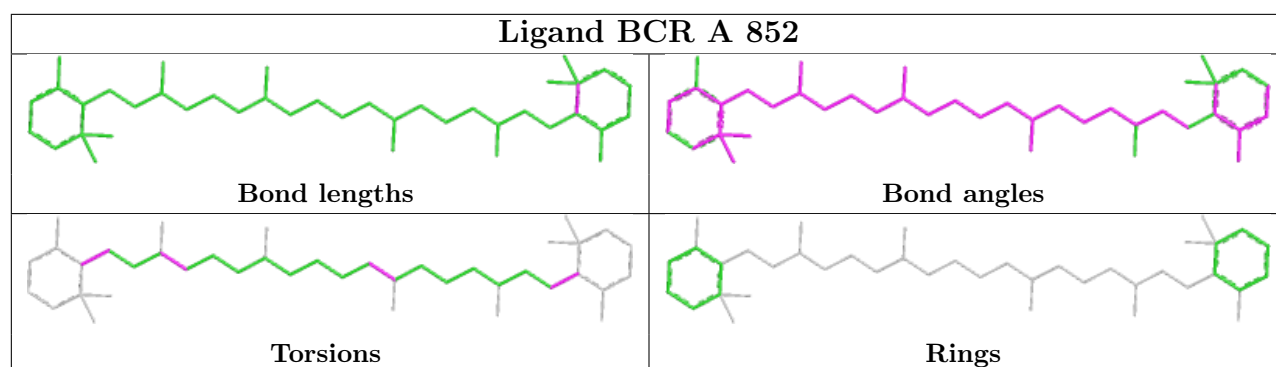


Torsions

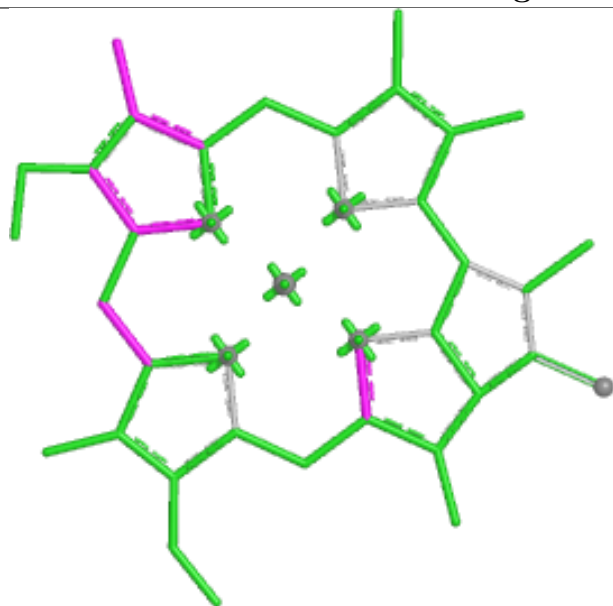


Rings

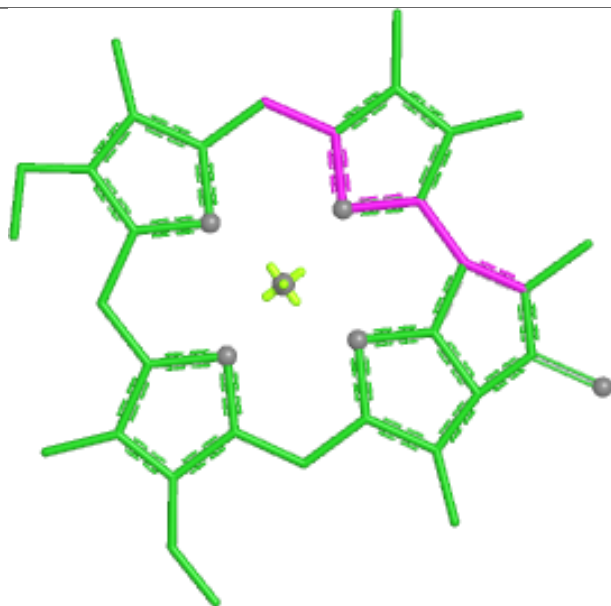




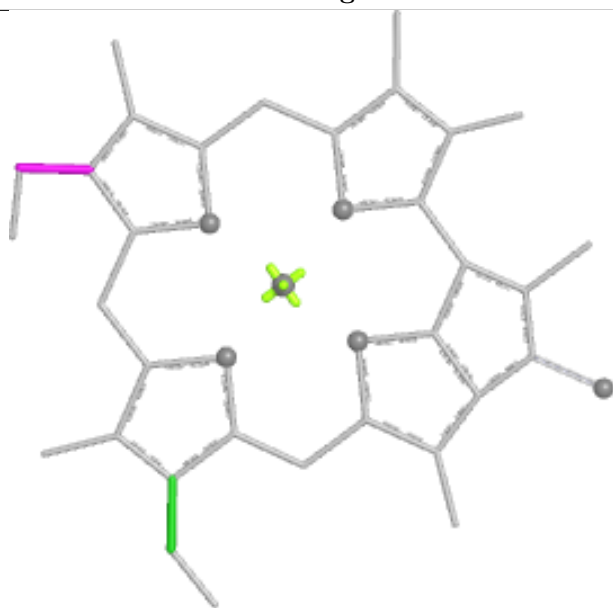
Ligand CLA H 201



Bond lengths



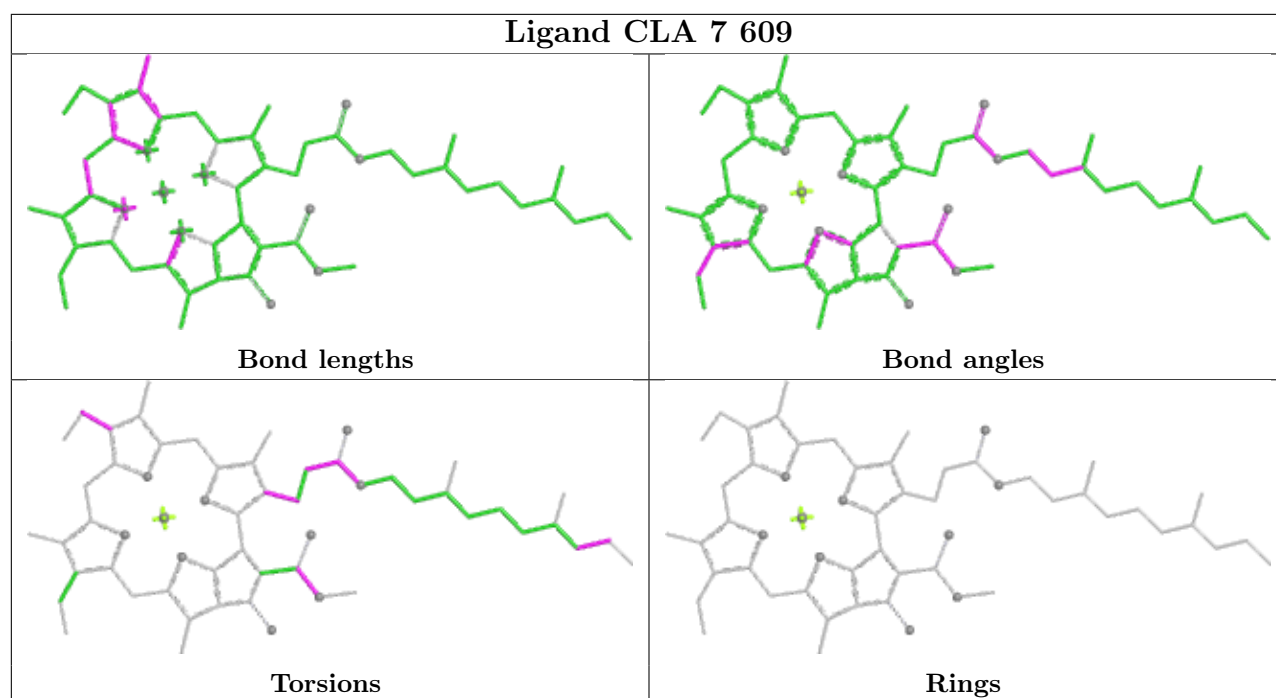
Bond angles

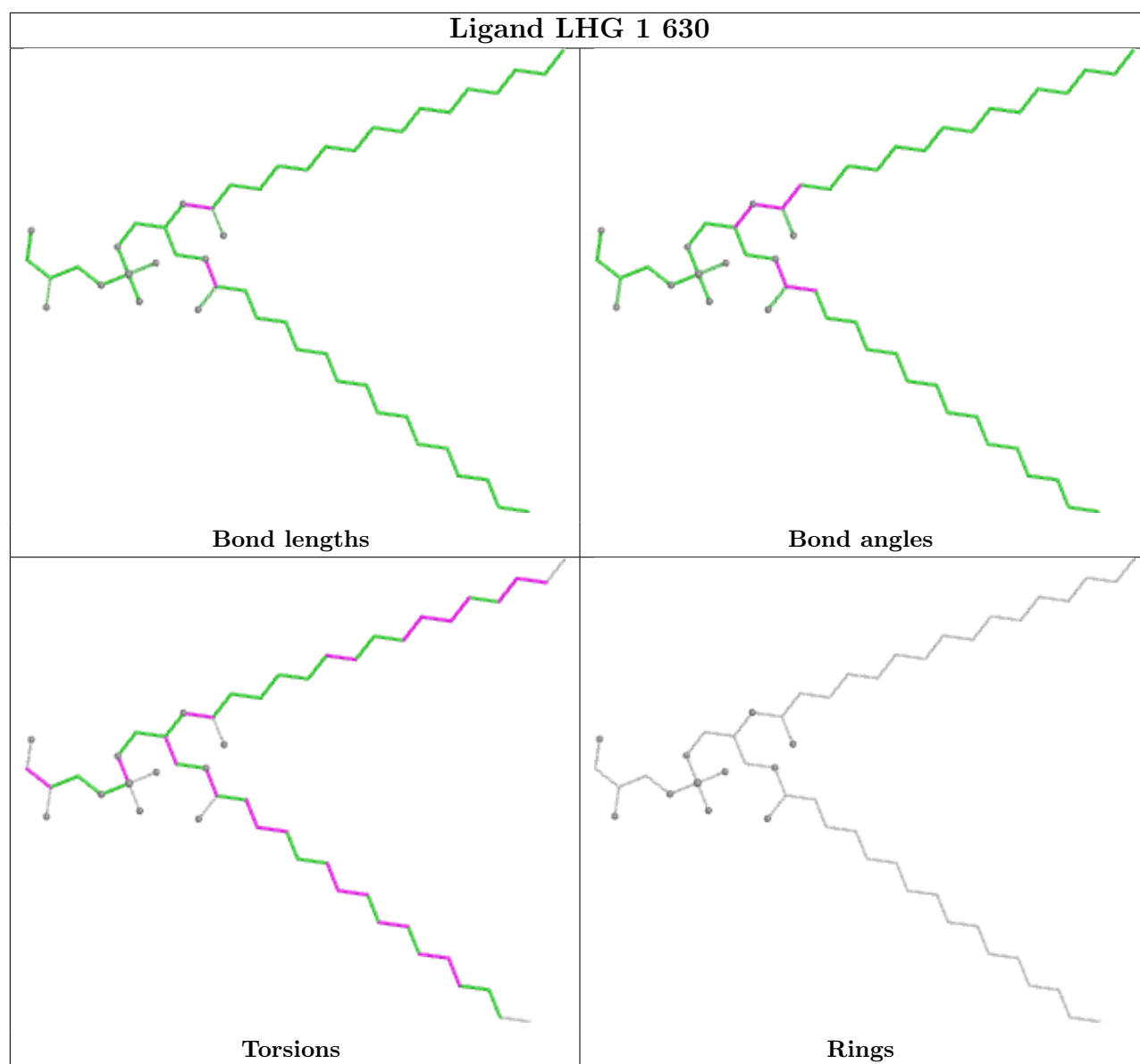


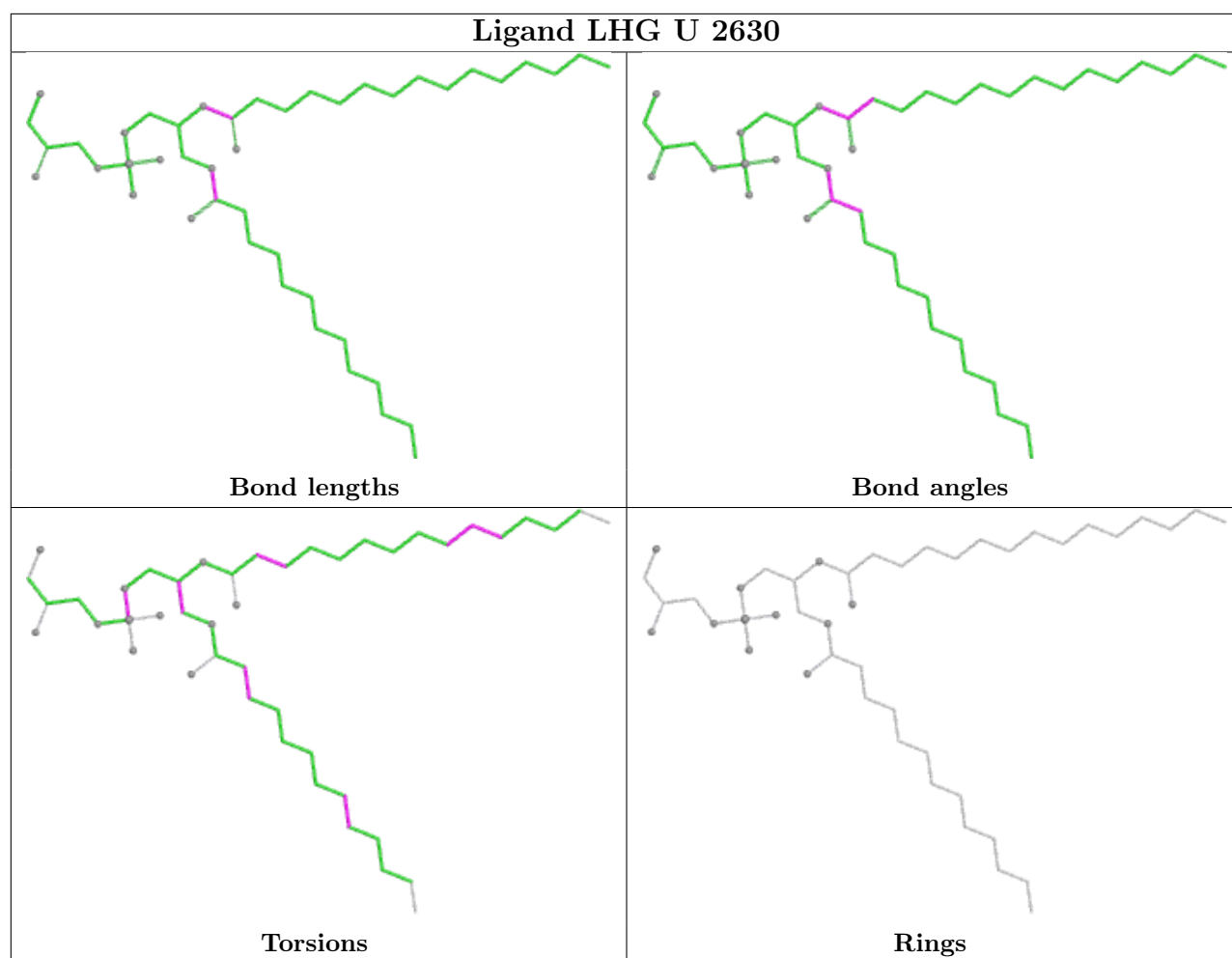
Torsions

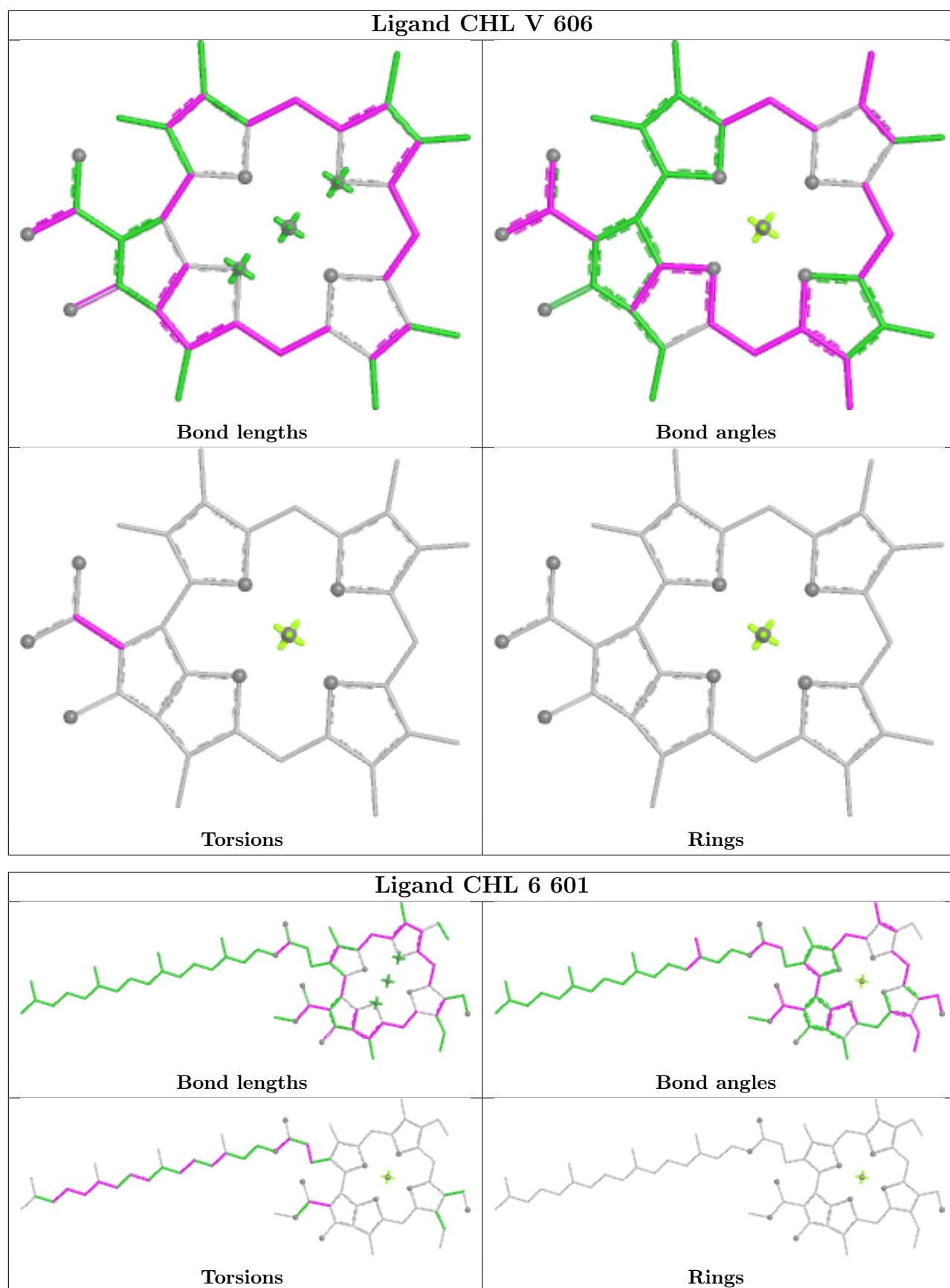


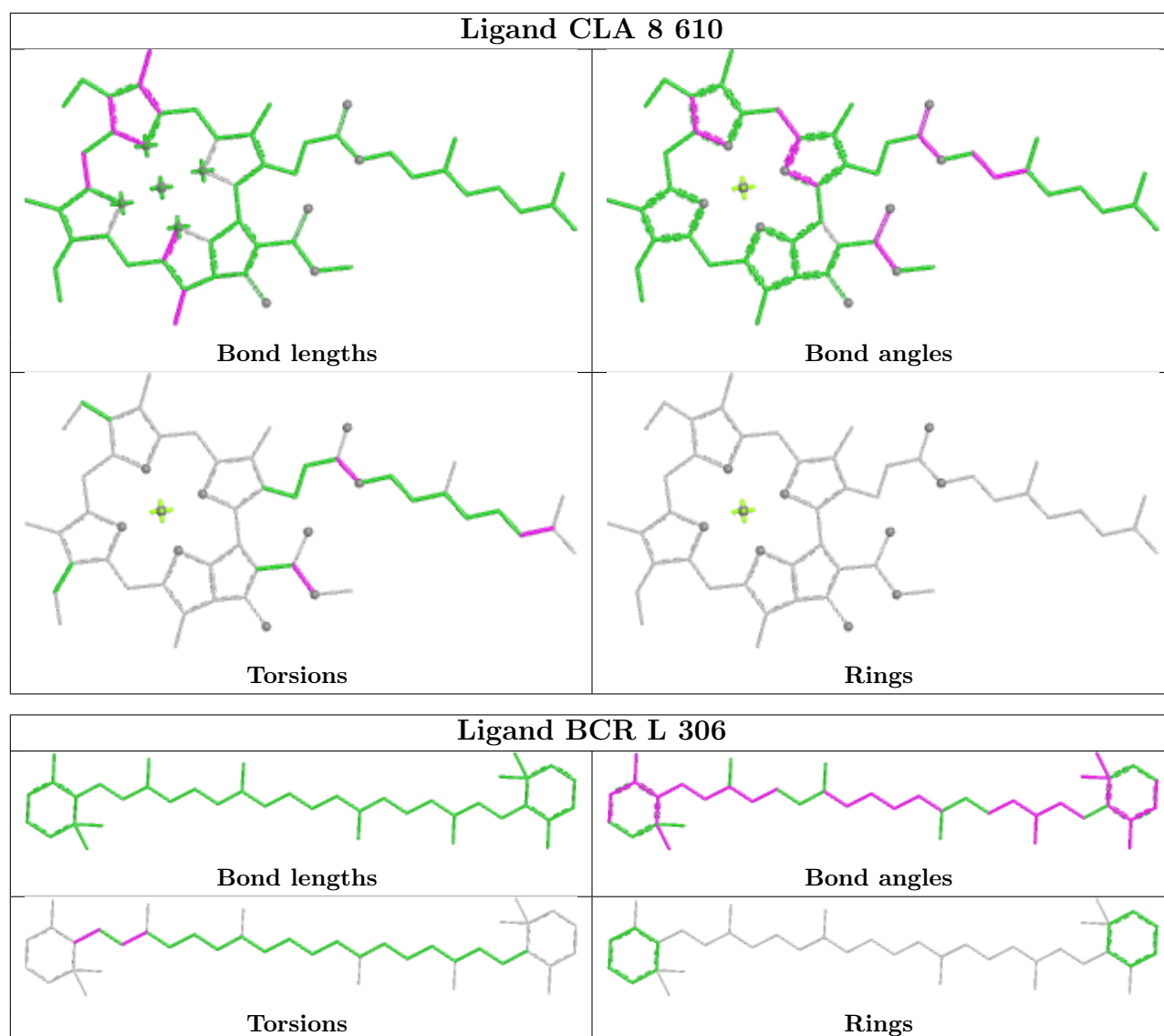
Rings

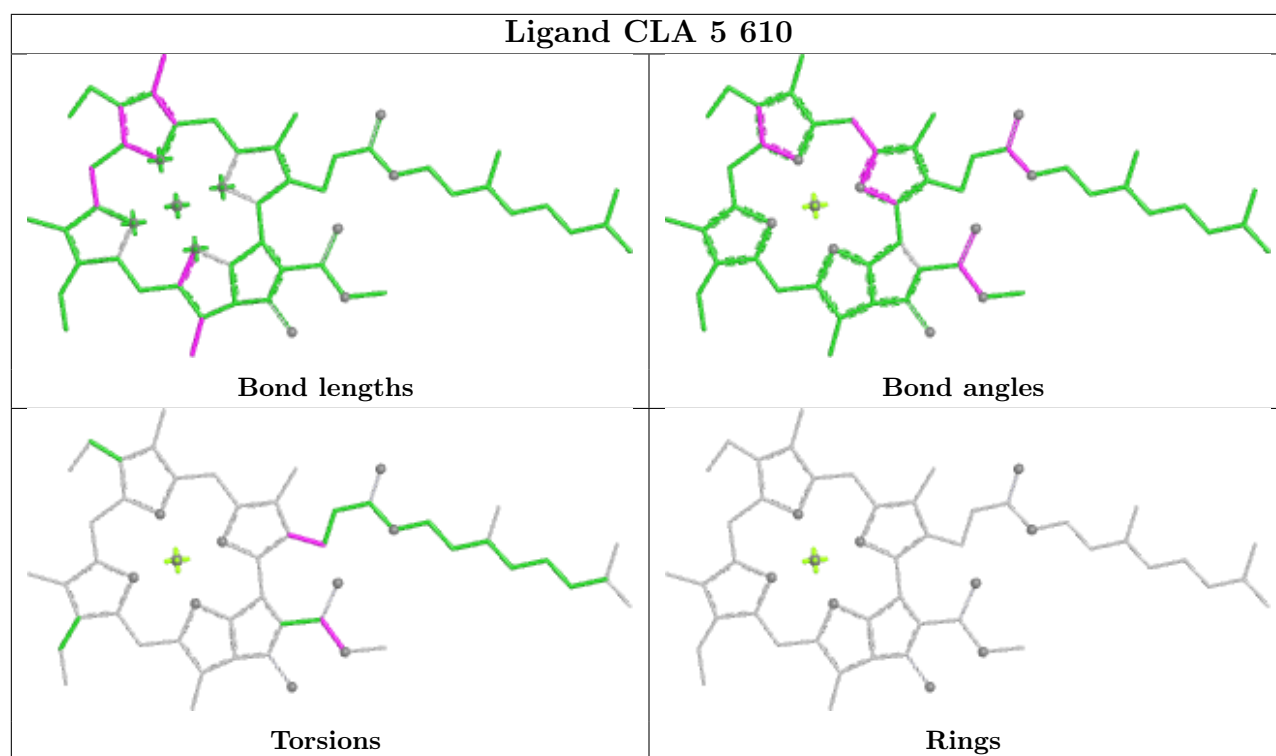




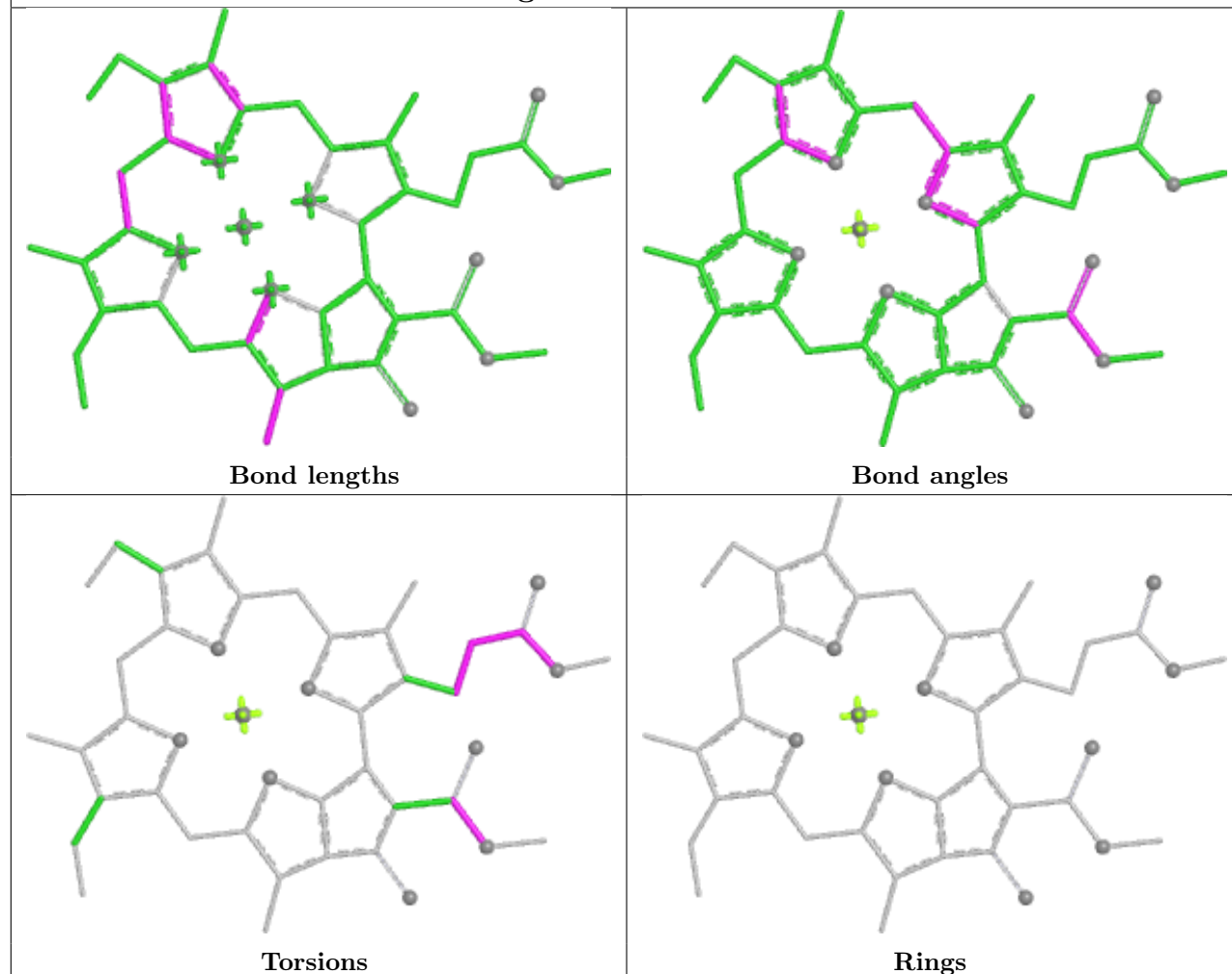




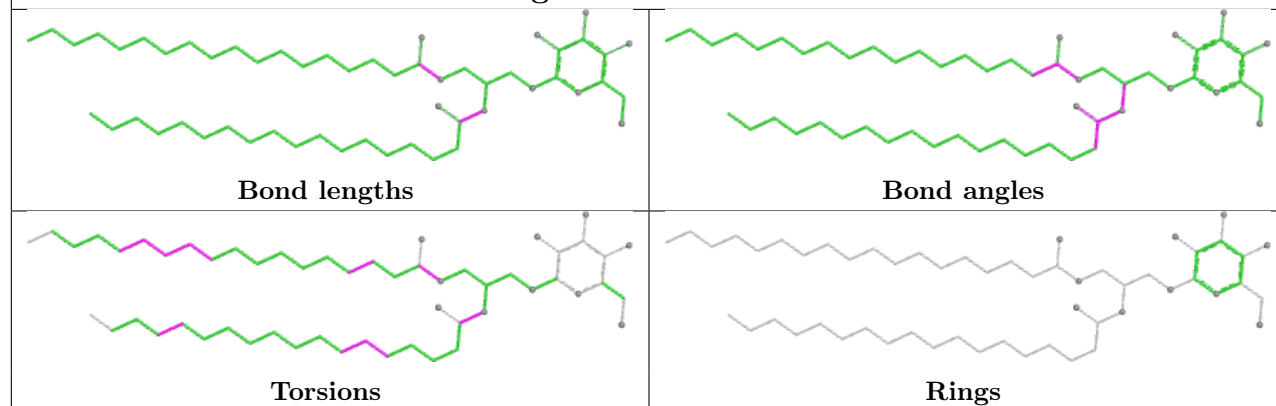


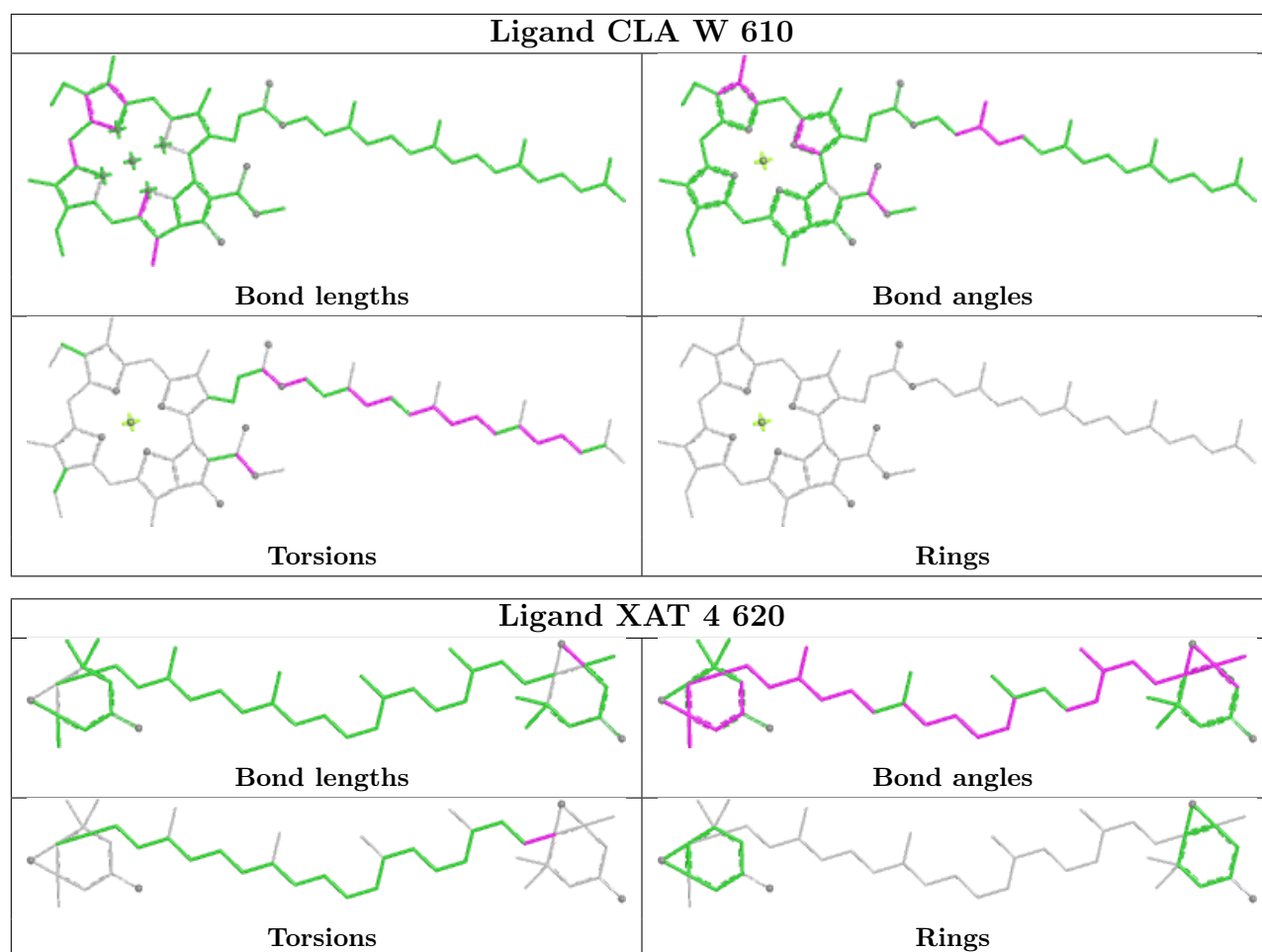


Ligand CLA 6 603

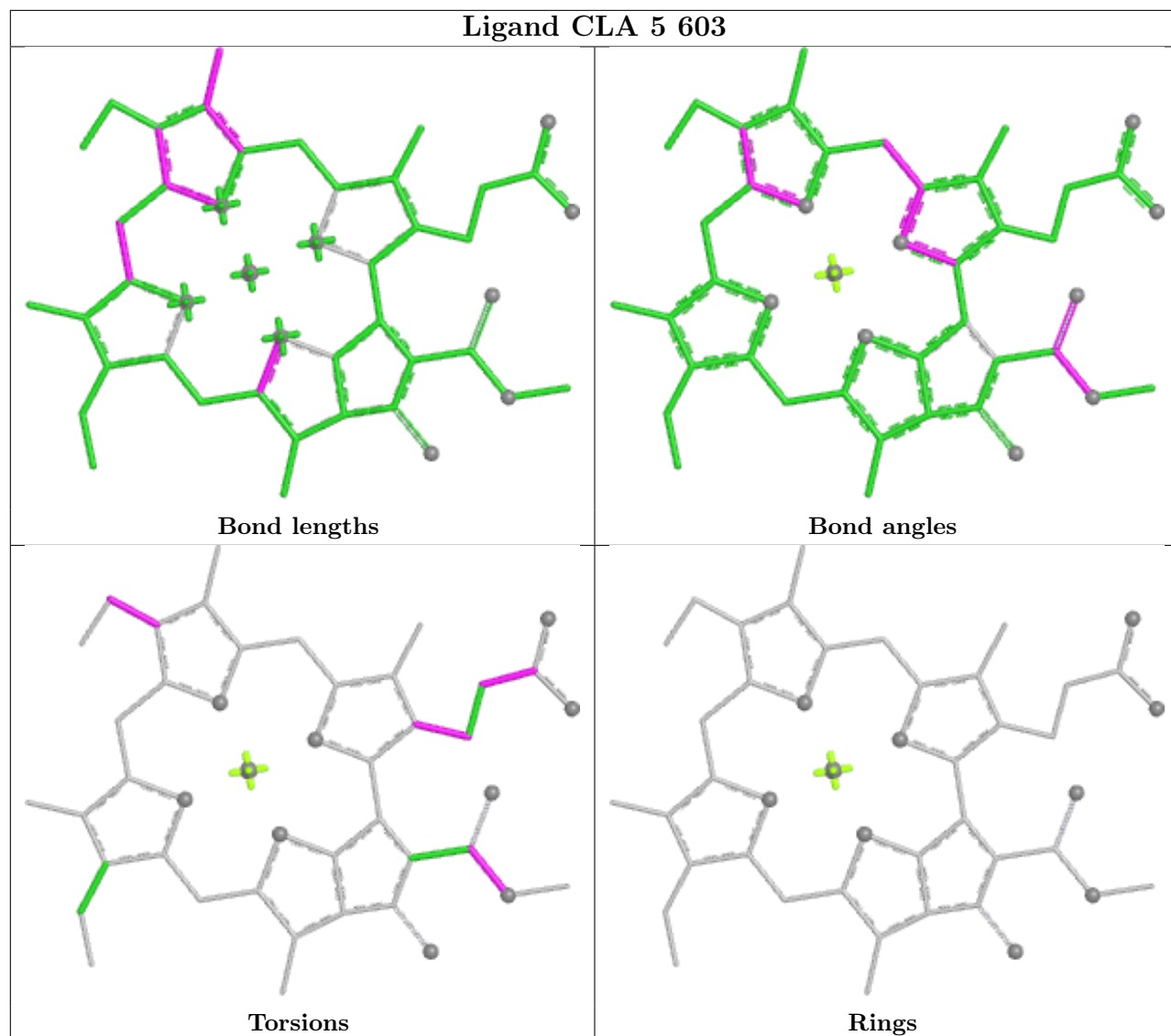


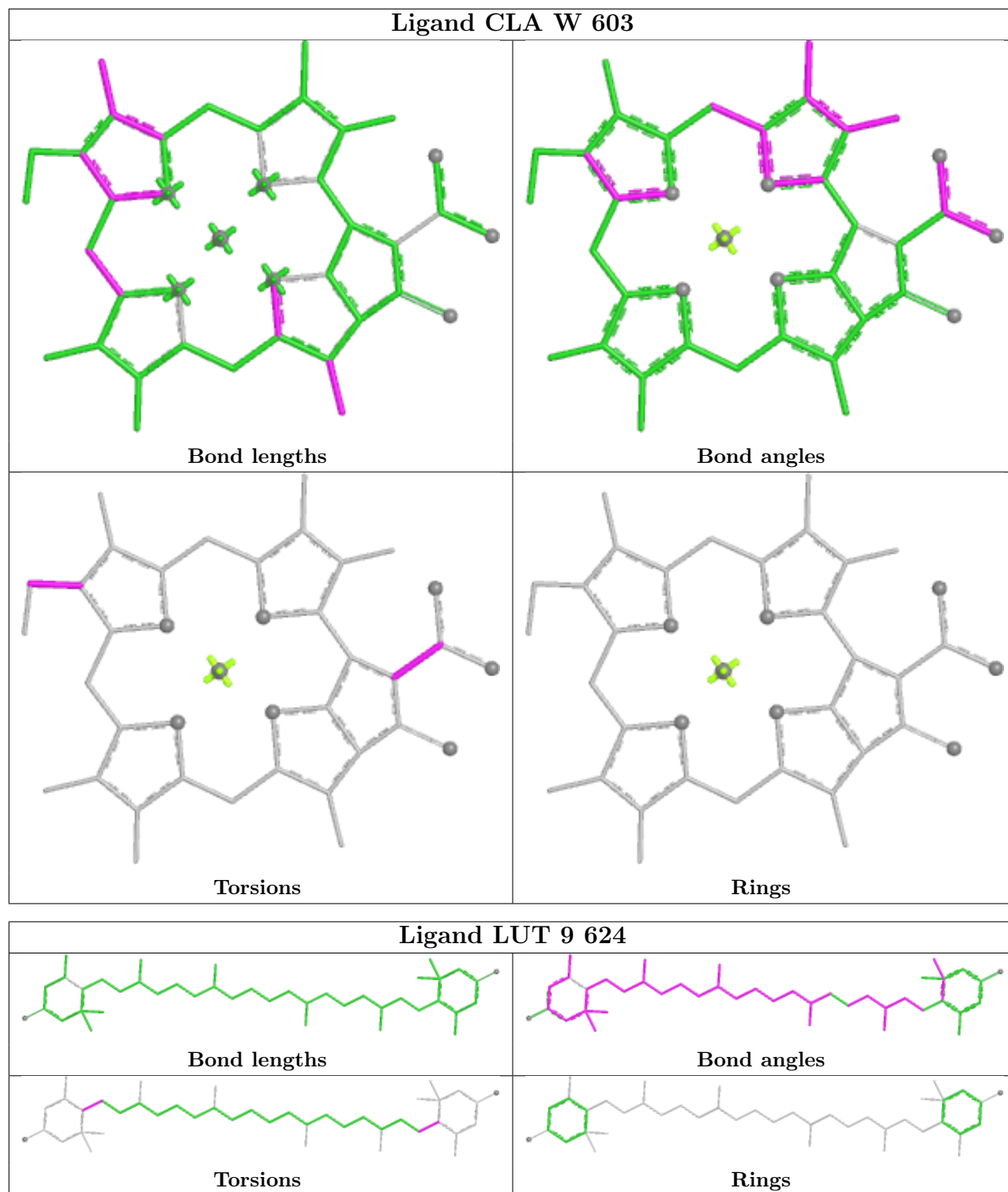
Ligand LMG J 103

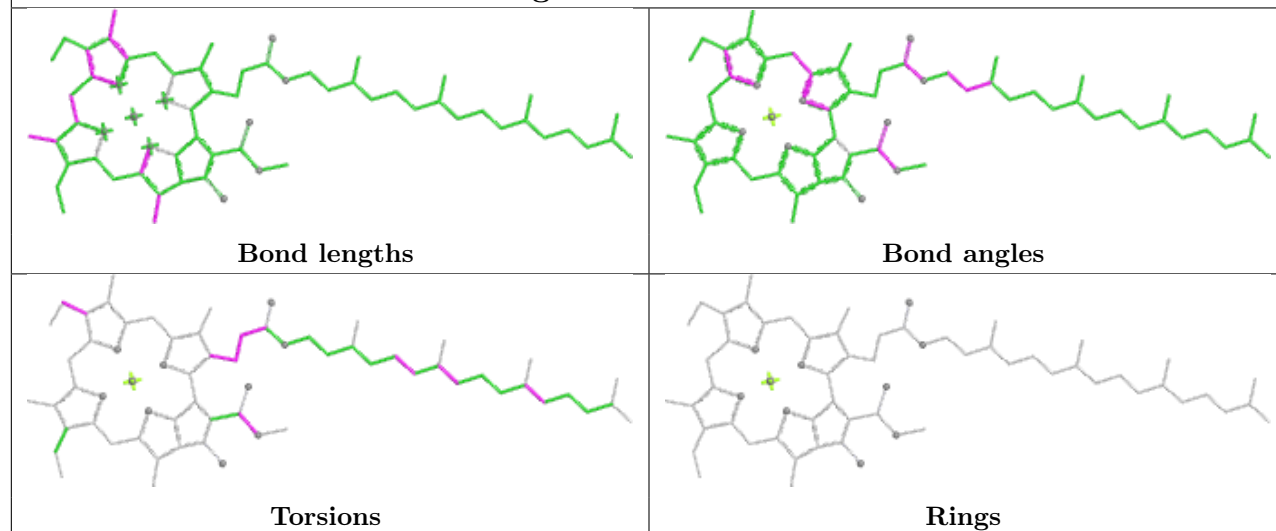
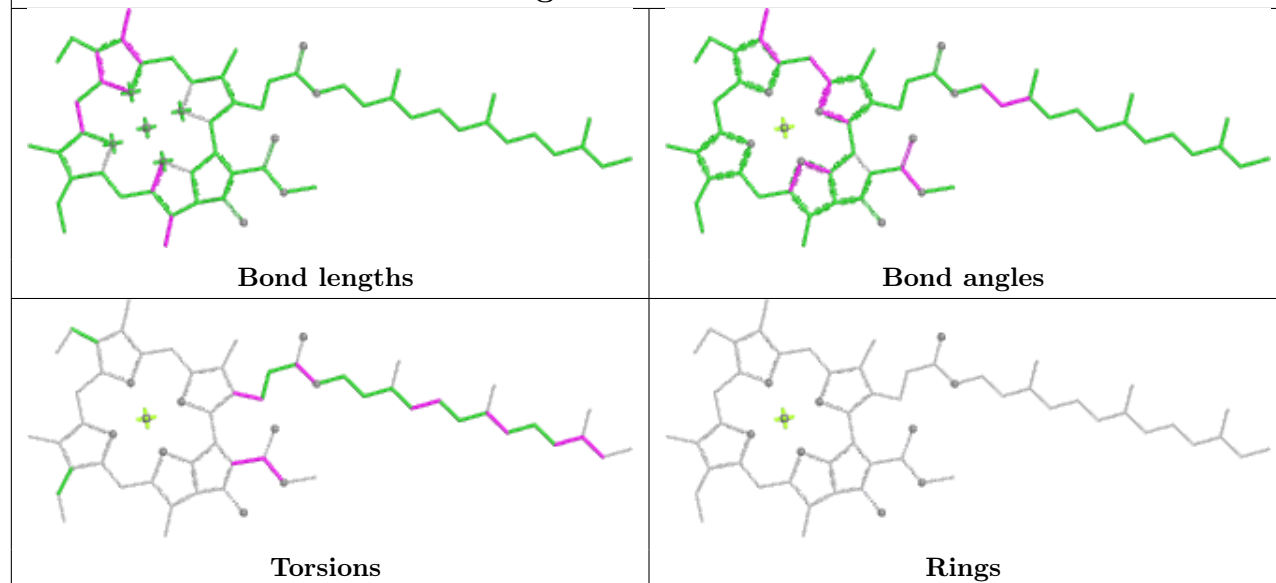




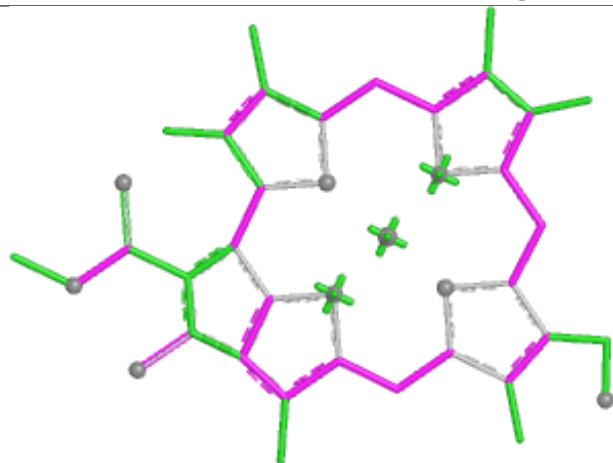
Ligand CLA 5 603



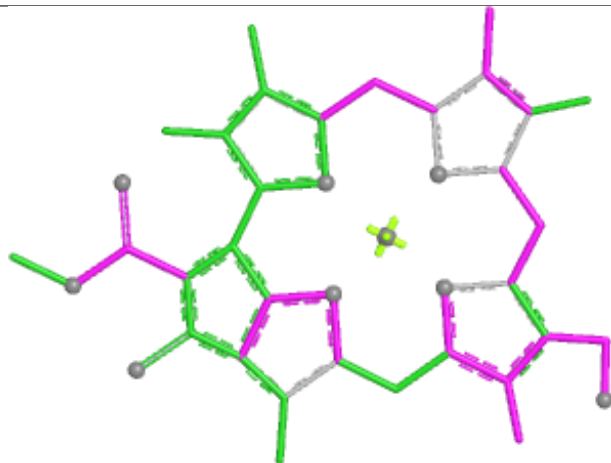


Ligand CLA B 808**Ligand CLA 4 610**

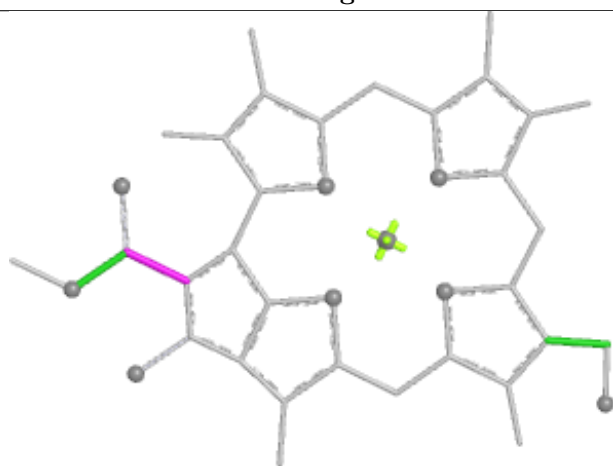
Ligand CHL V 607



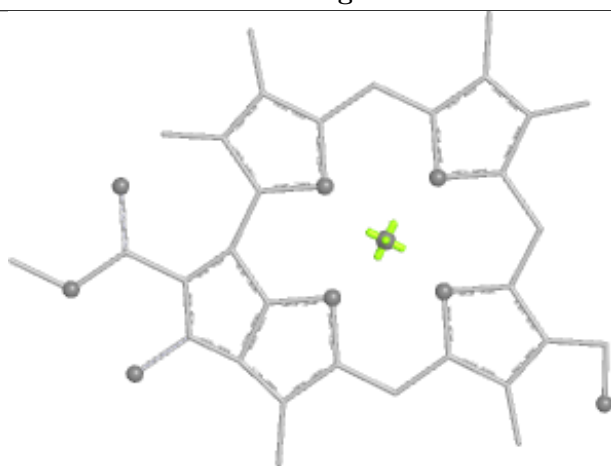
Bond lengths



Bond angles

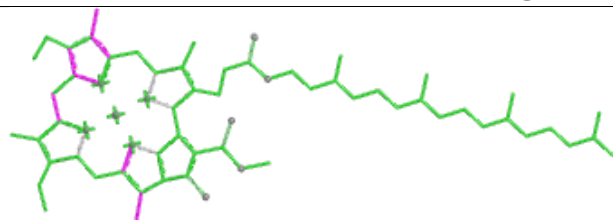


Torsions

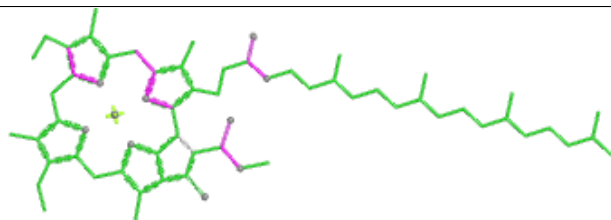


Rings

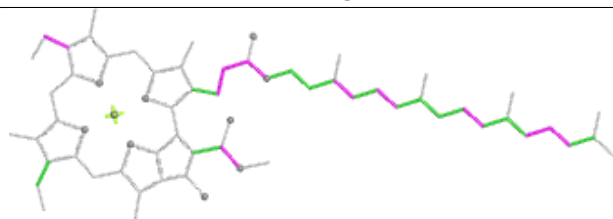
Ligand CLA 4 603



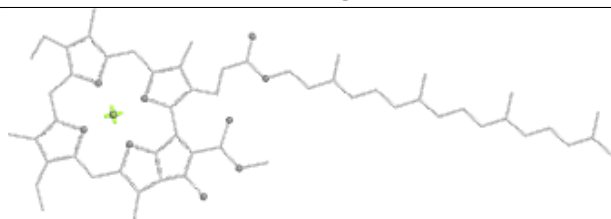
Bond lengths



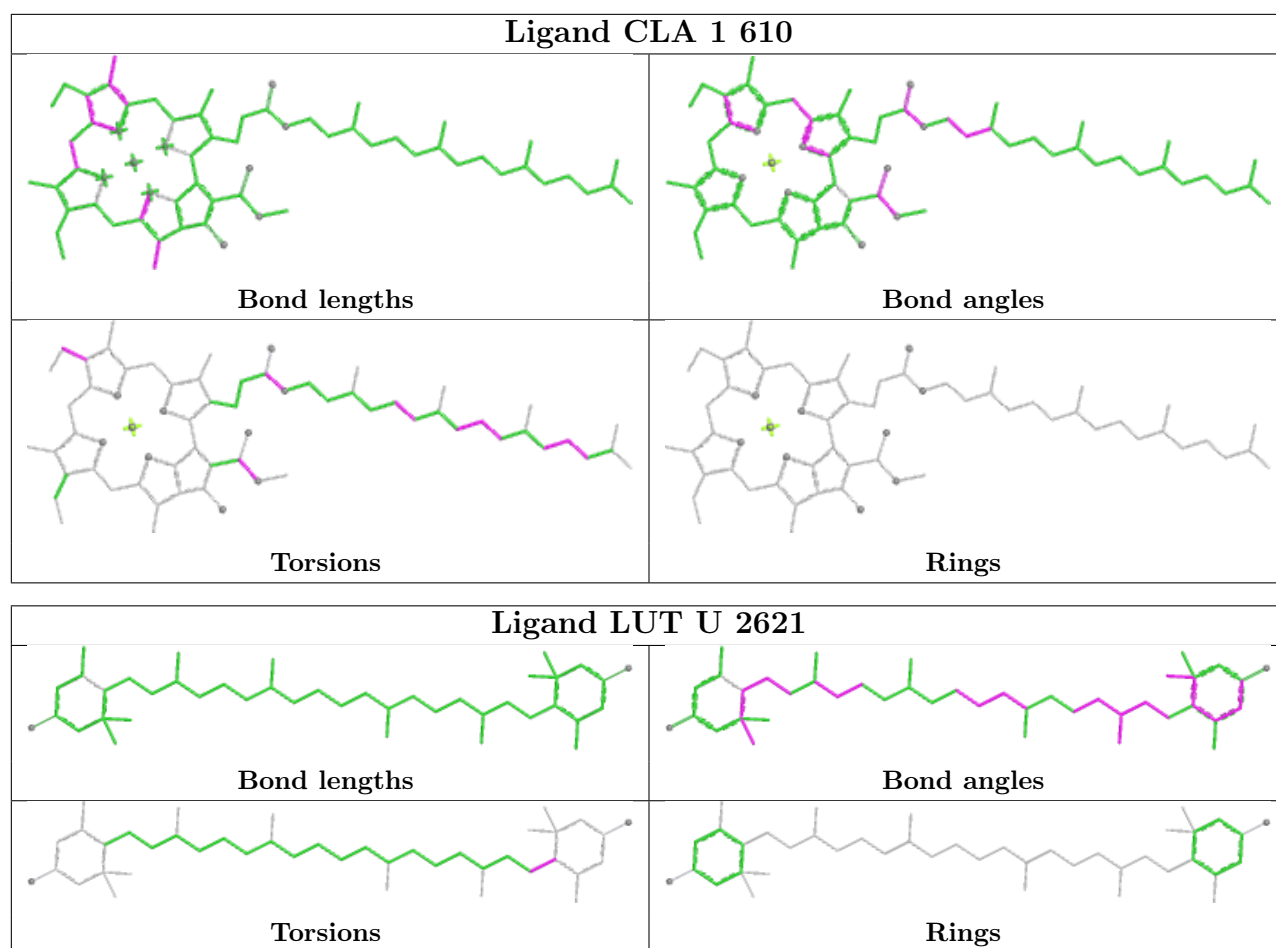
Bond angles

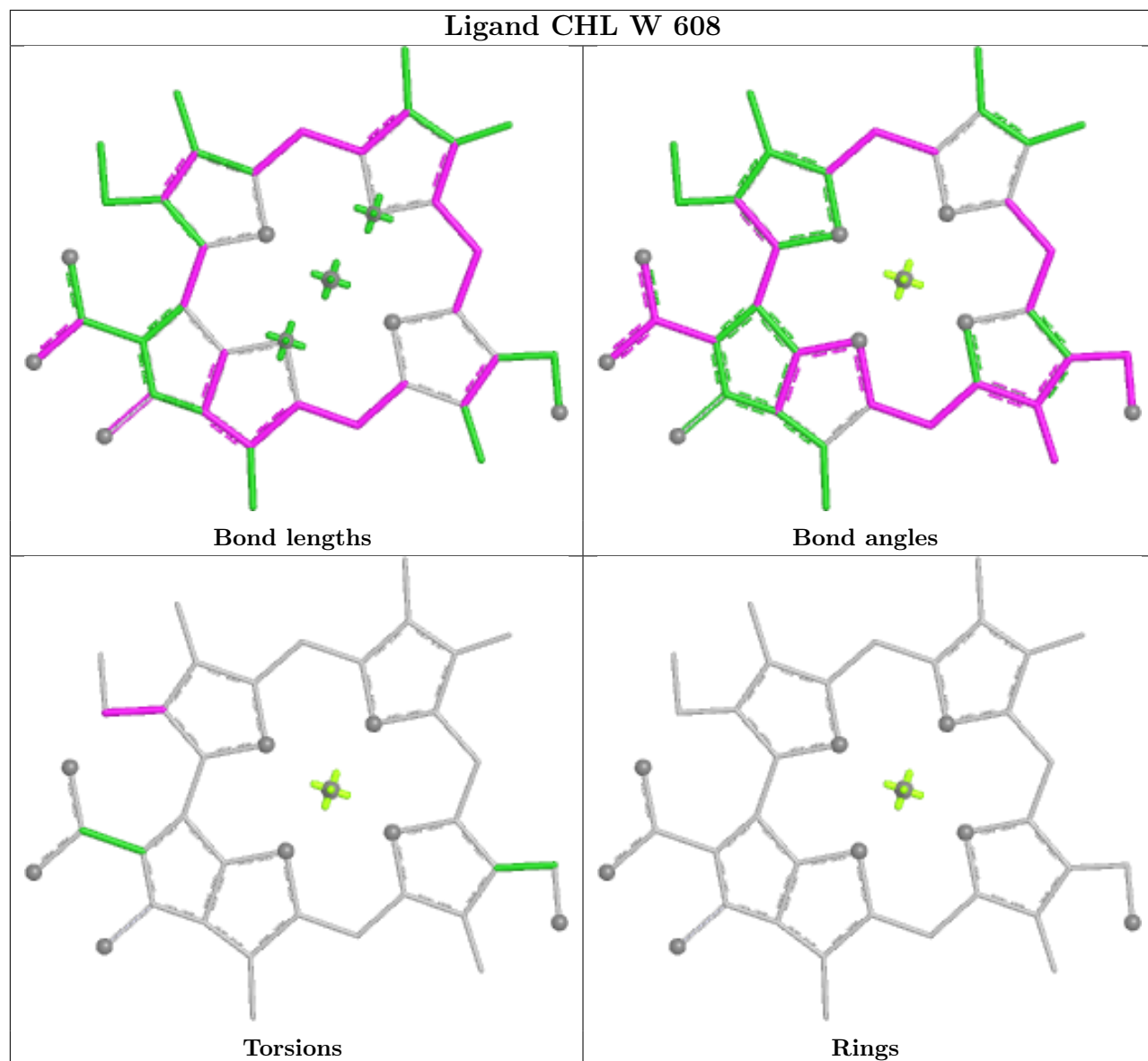


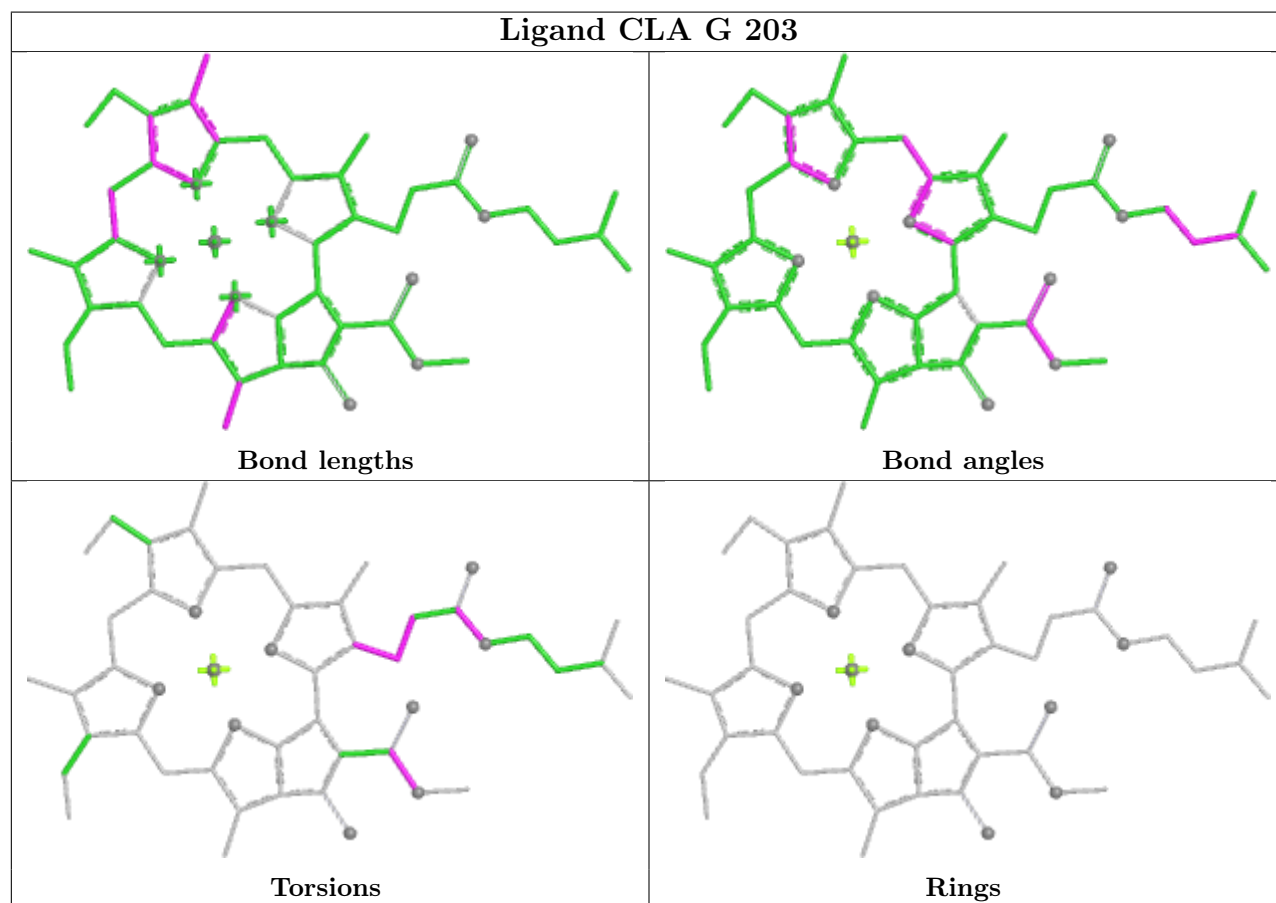
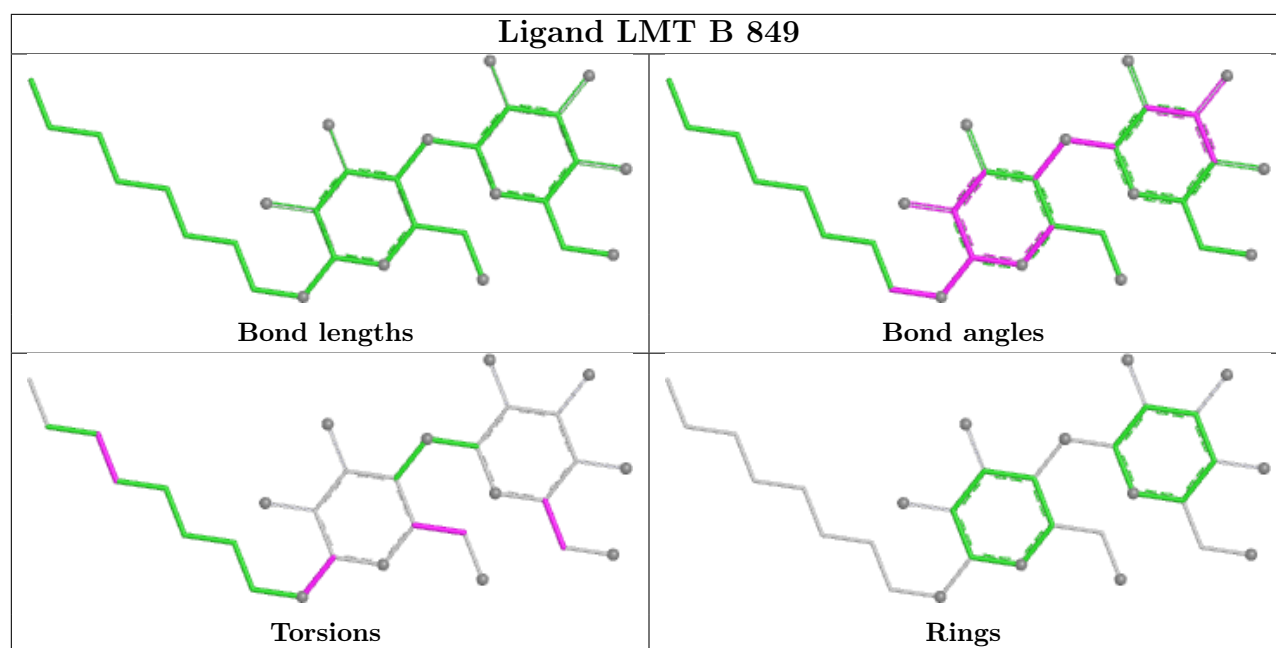
Torsions

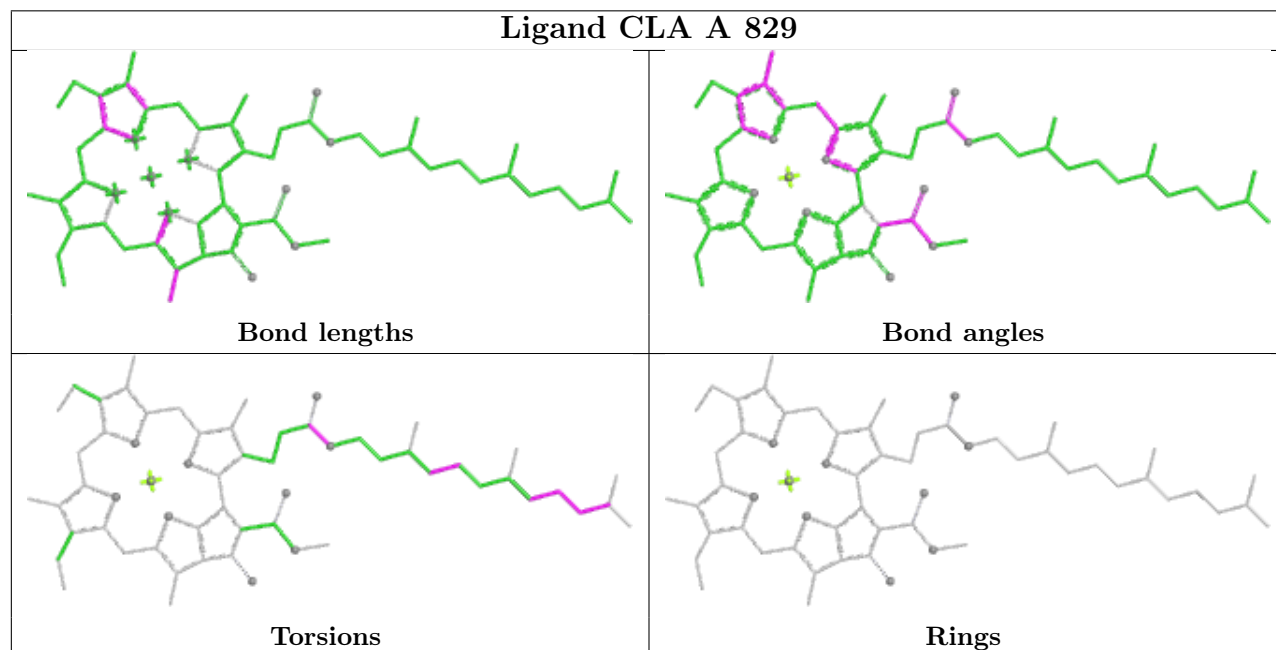
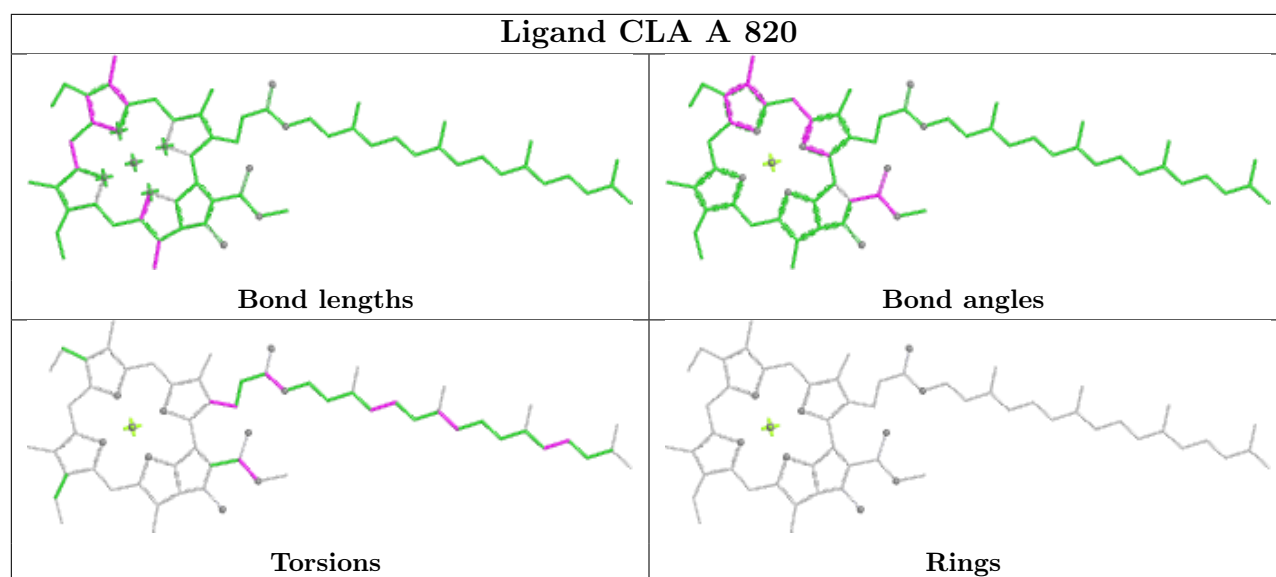


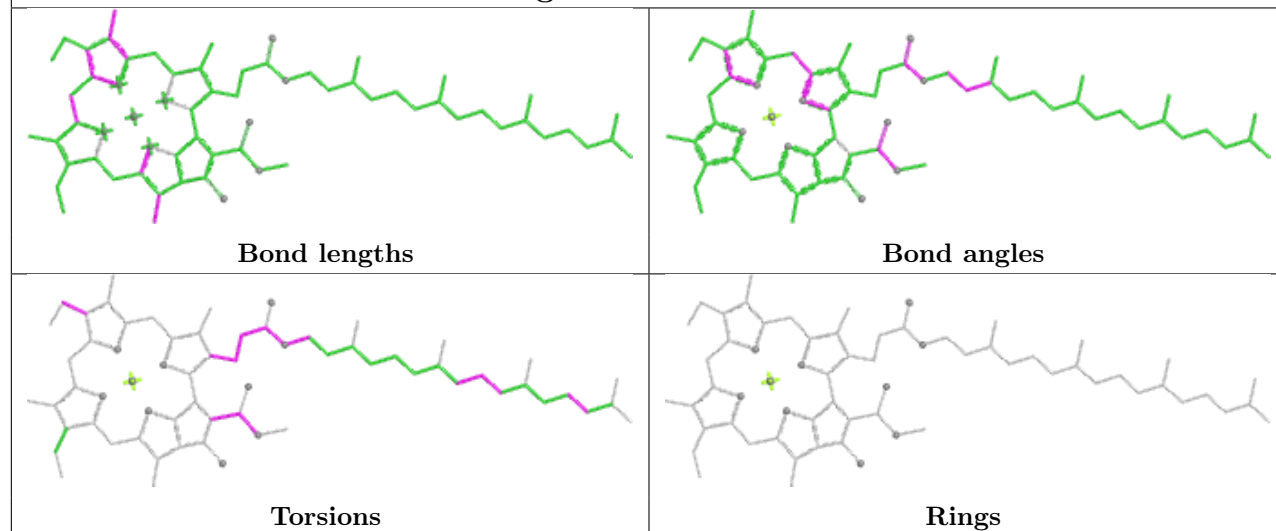
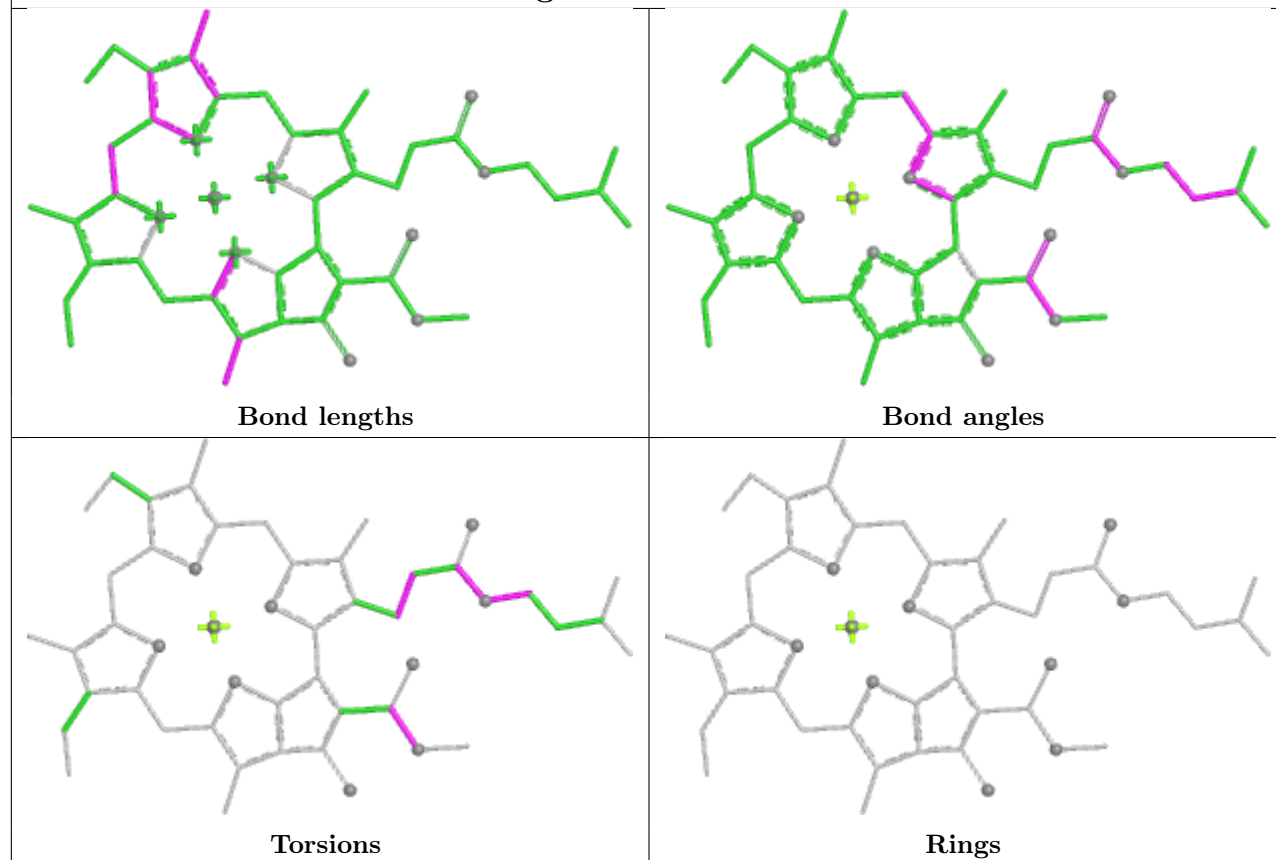
Rings



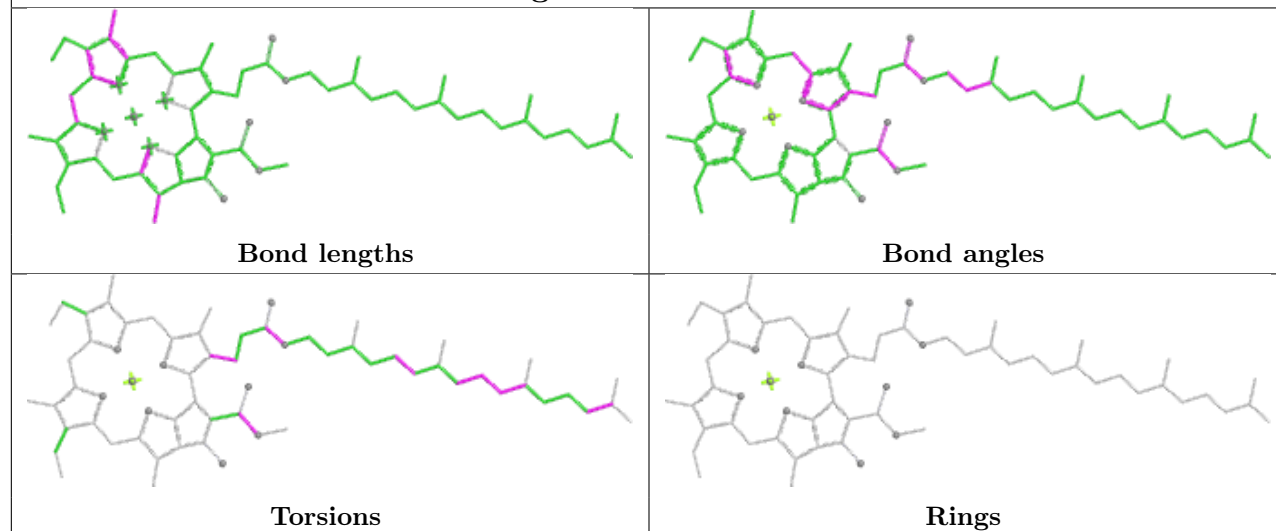




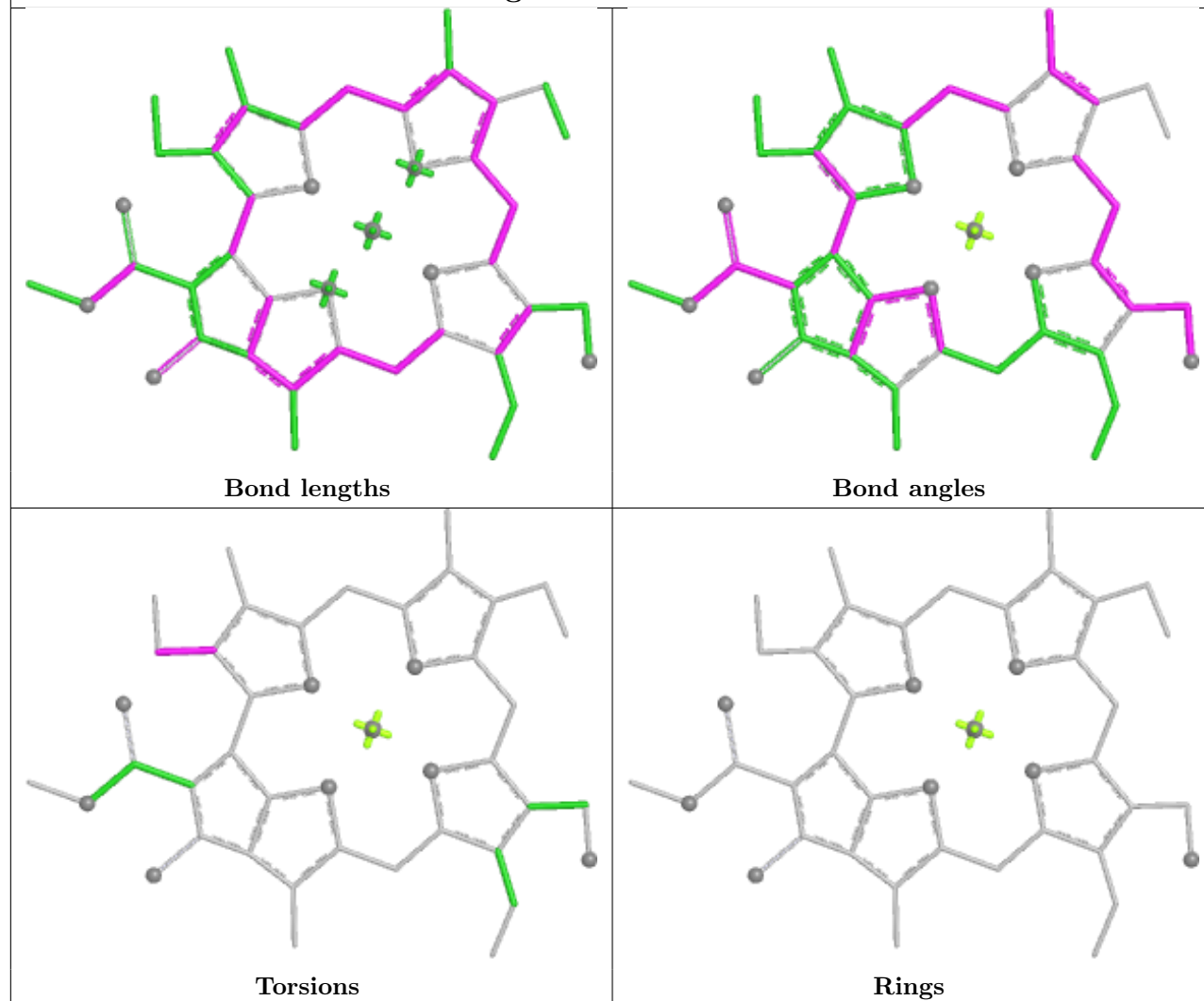


Ligand CLA 4 602**Ligand CLA 5 608**

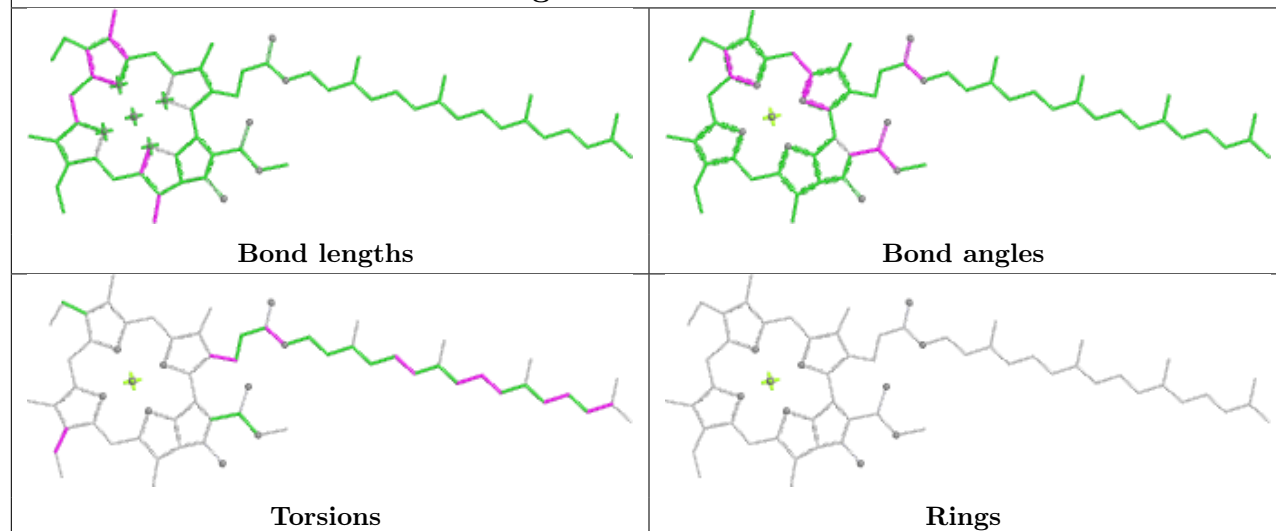
Ligand CLA U 610



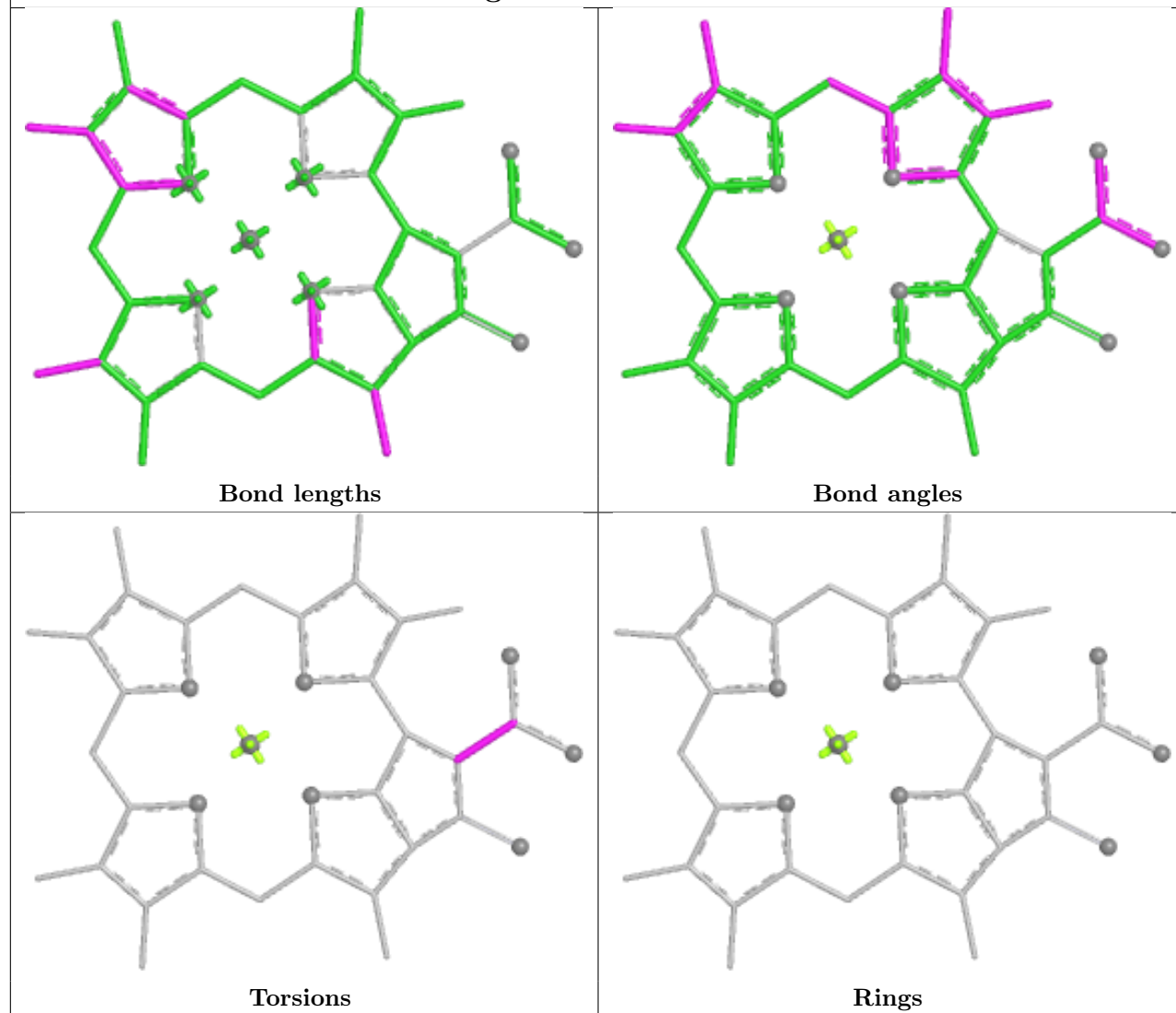
Ligand CHL 9 607



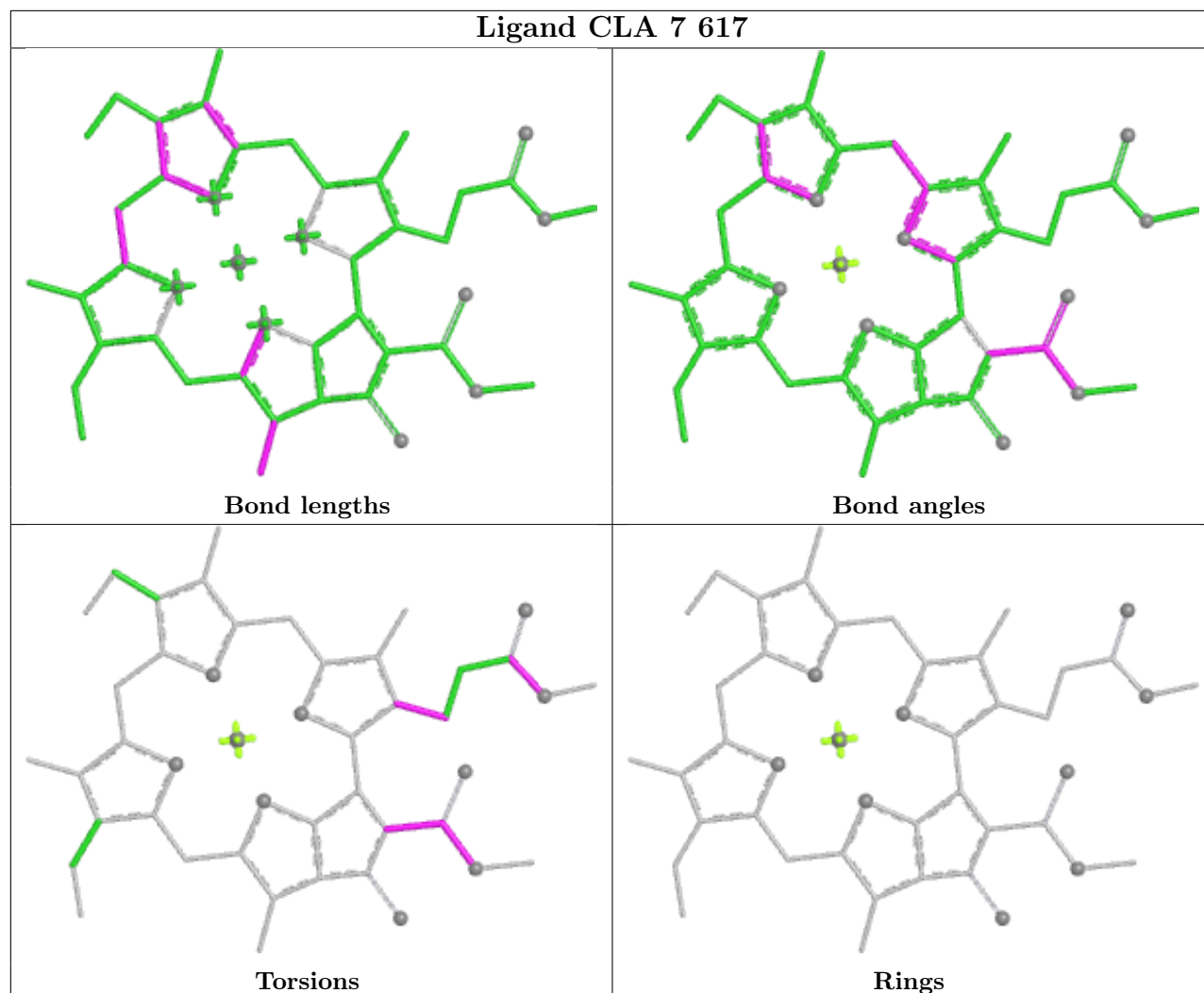
Ligand CLA B 813



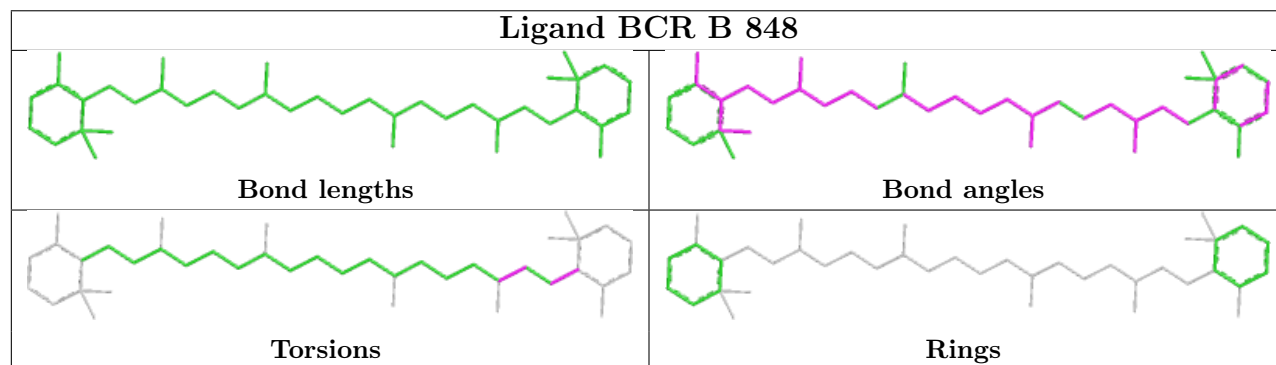
Ligand CLA W 612

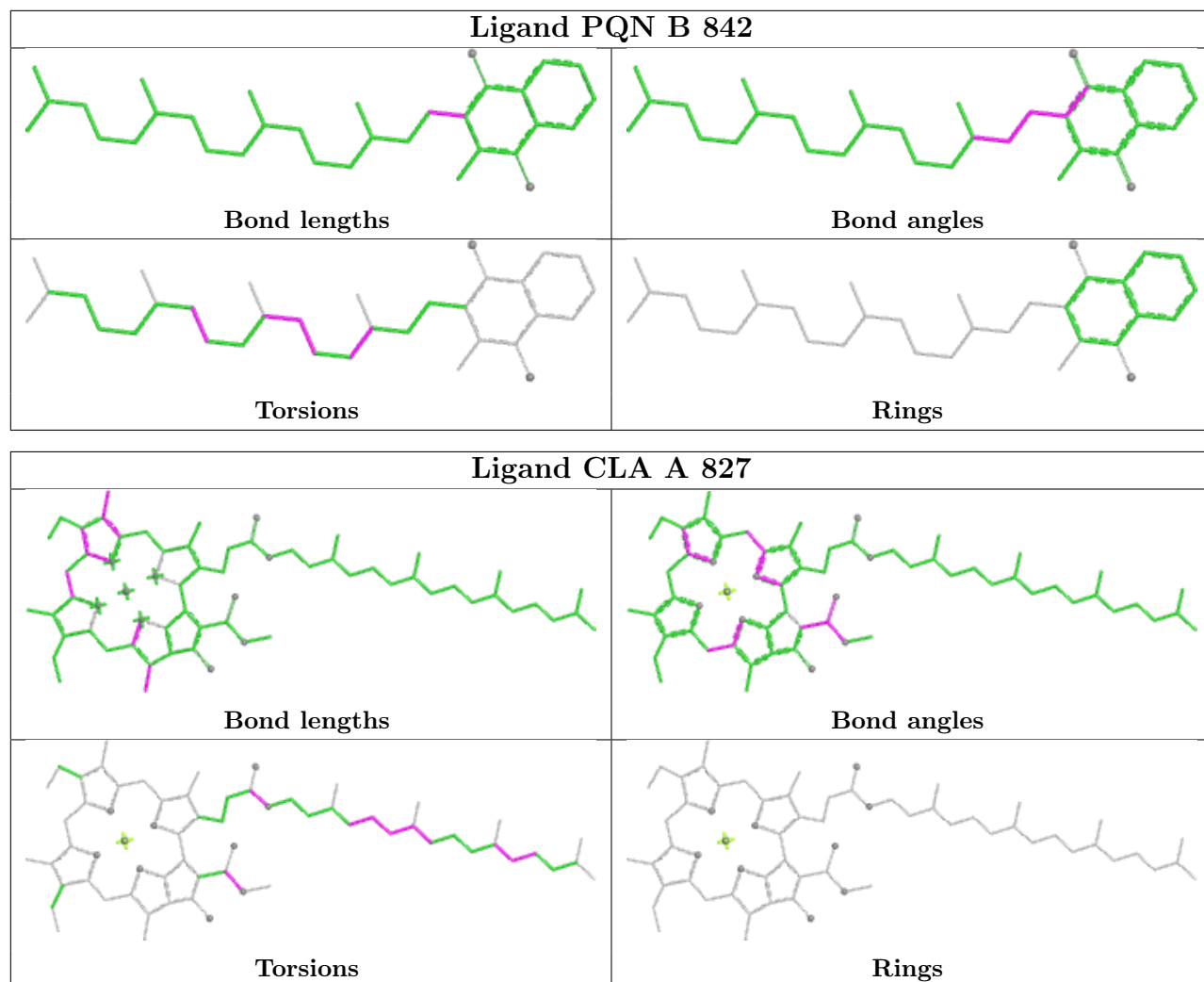


Ligand CLA 7 617

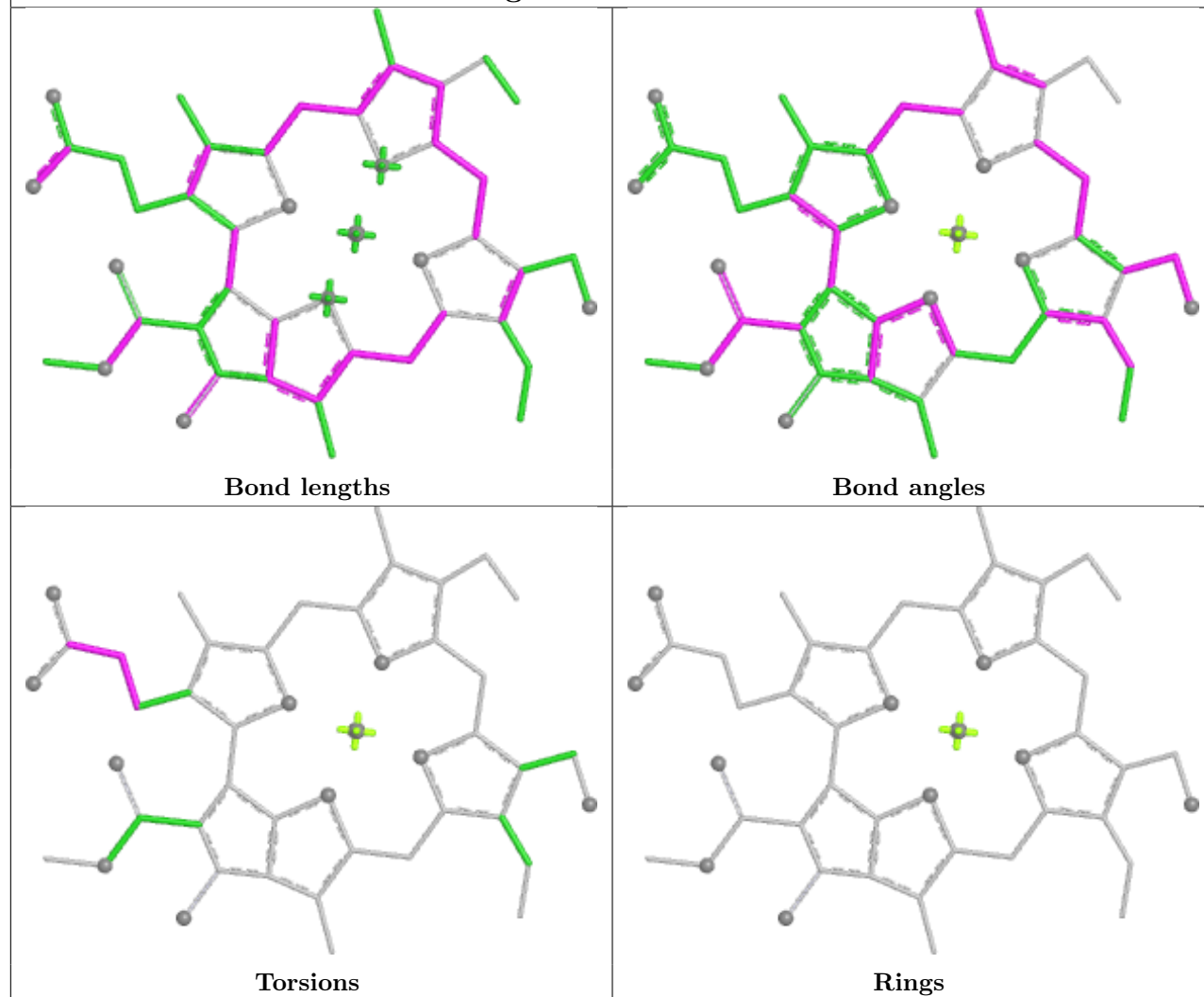


Ligand BCR B 848

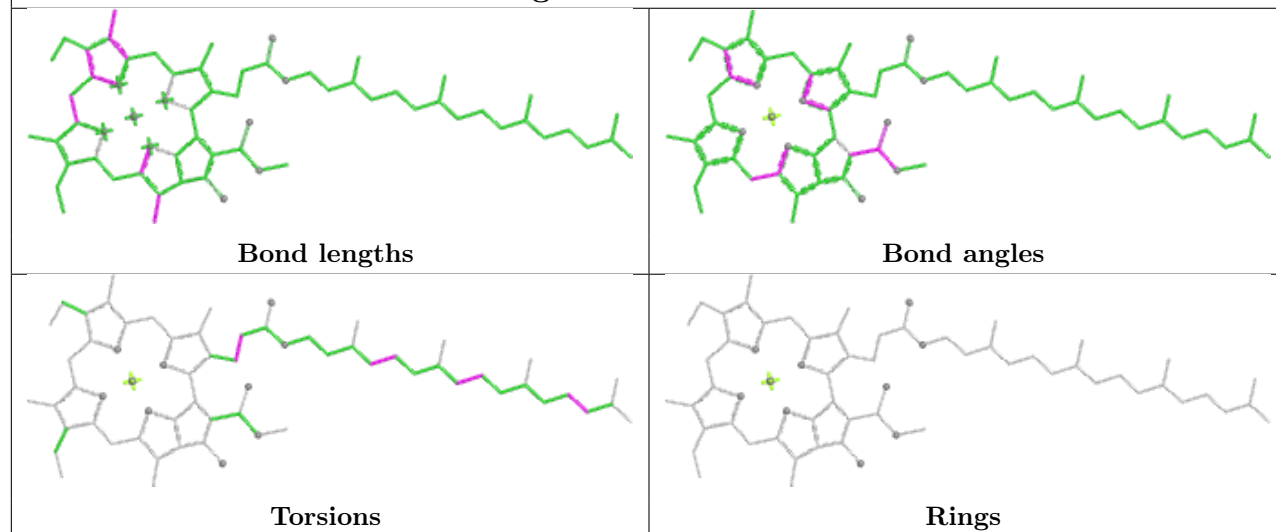




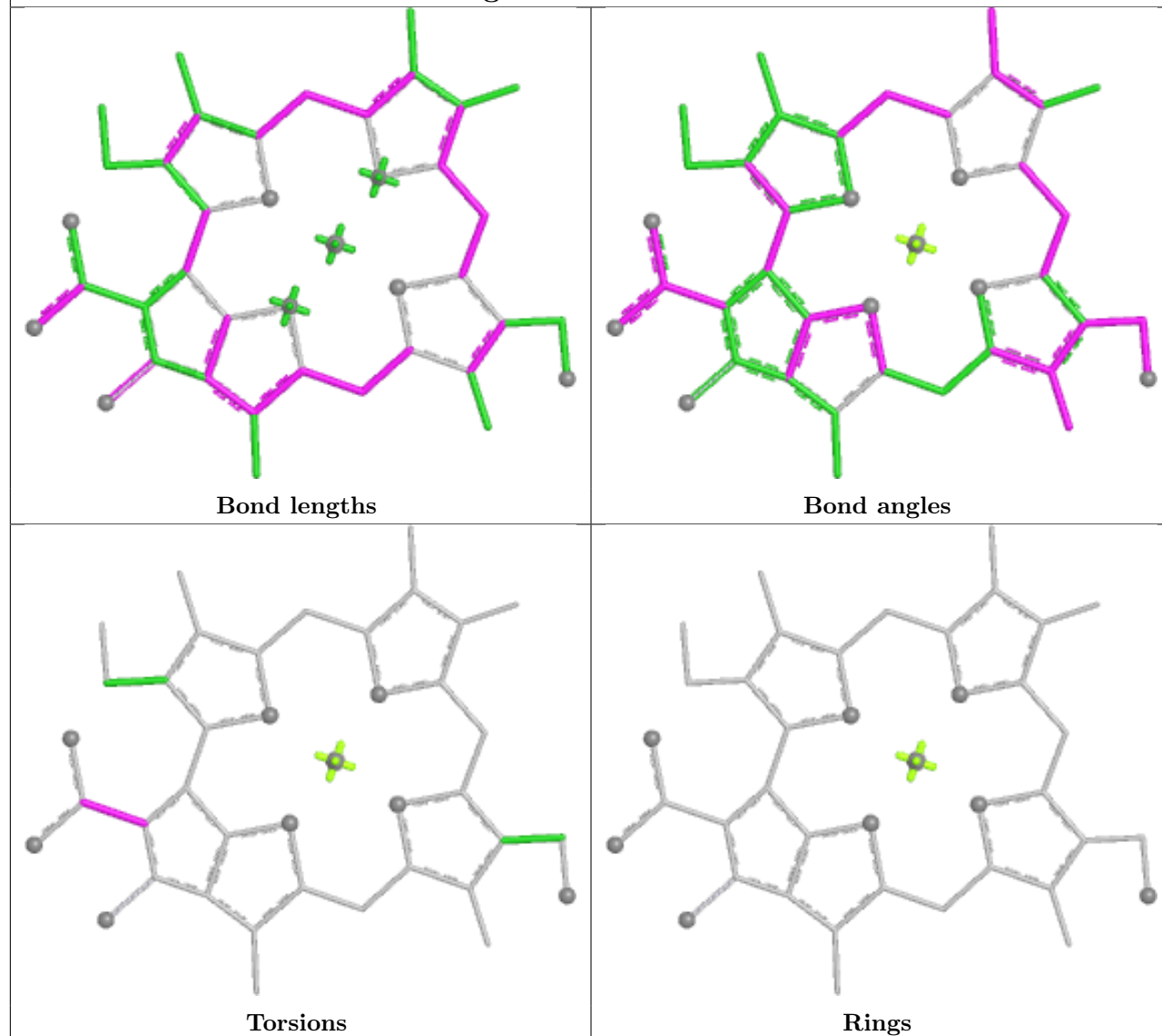
Ligand CHL 8 607



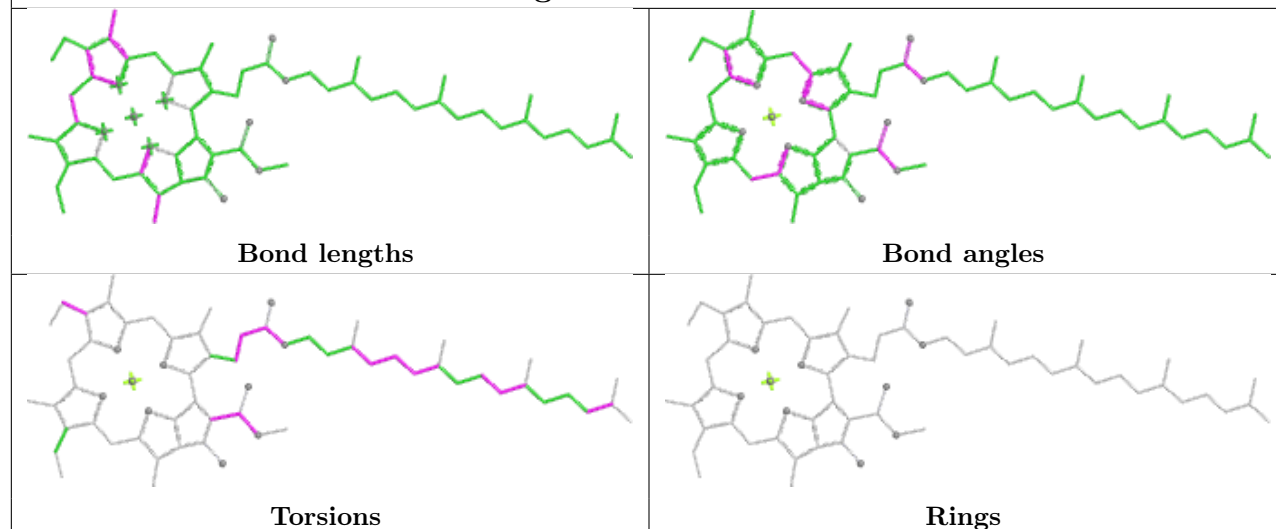
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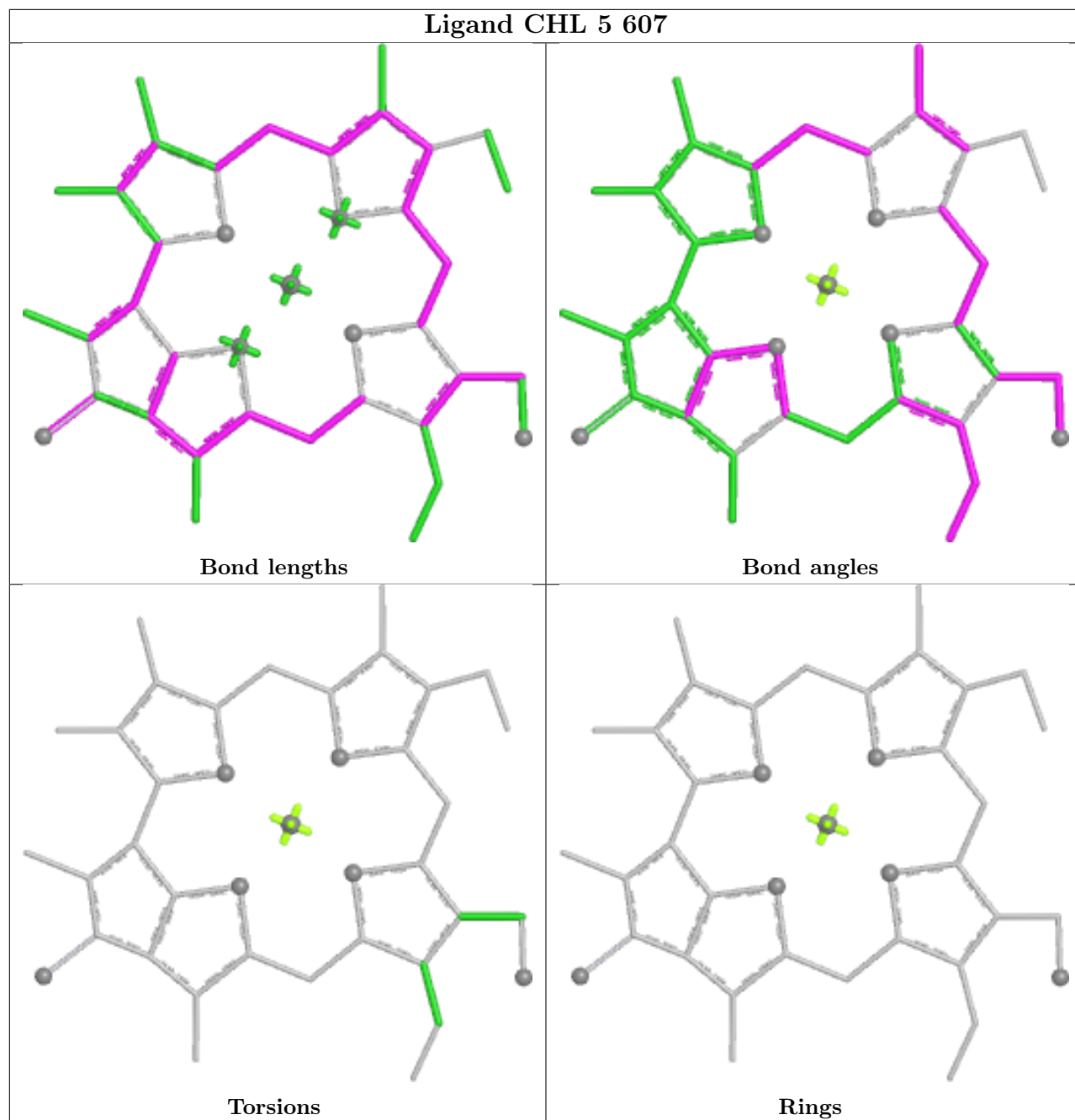
Ligand CHL U 608



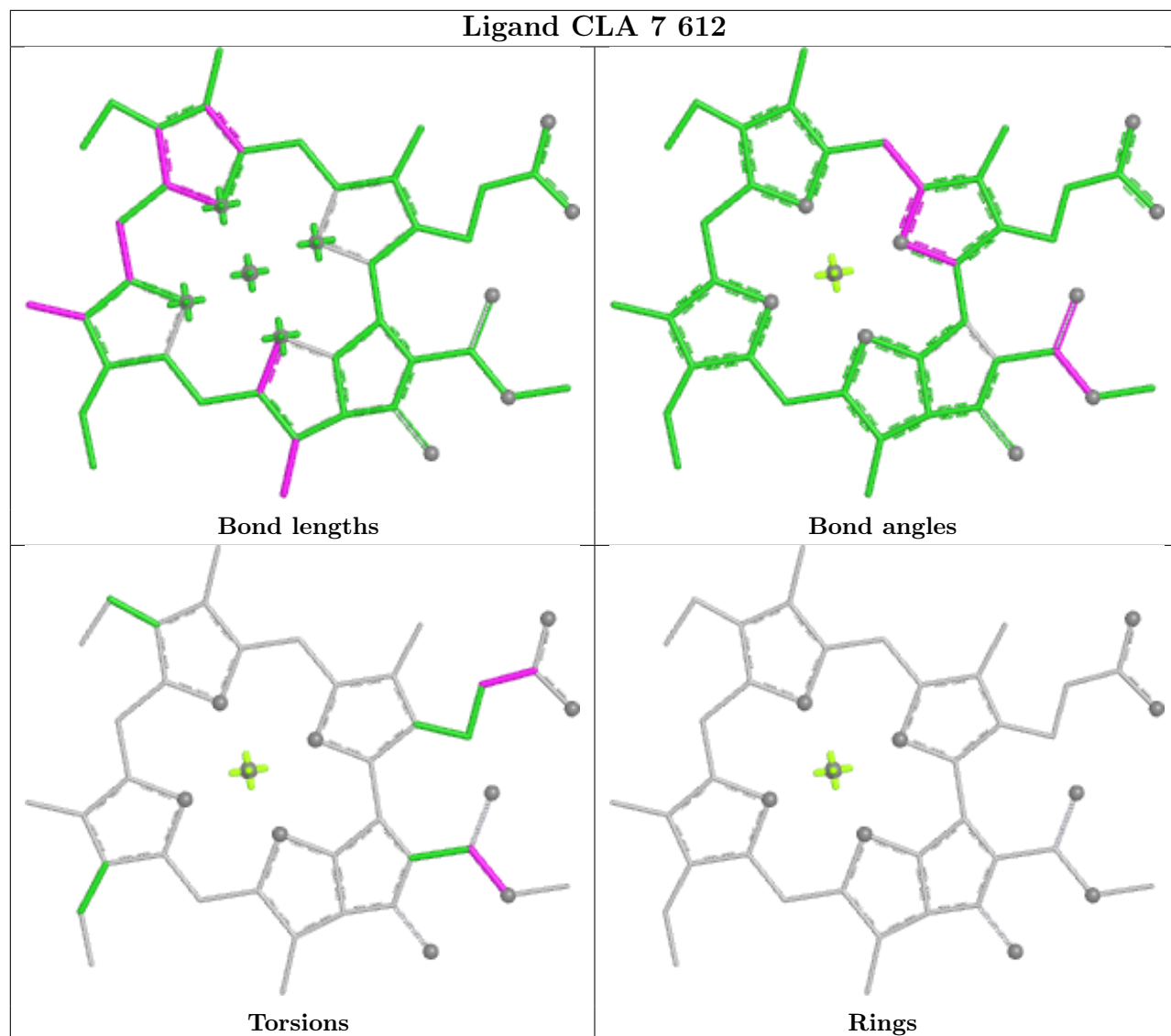
Ligand CLA L 302



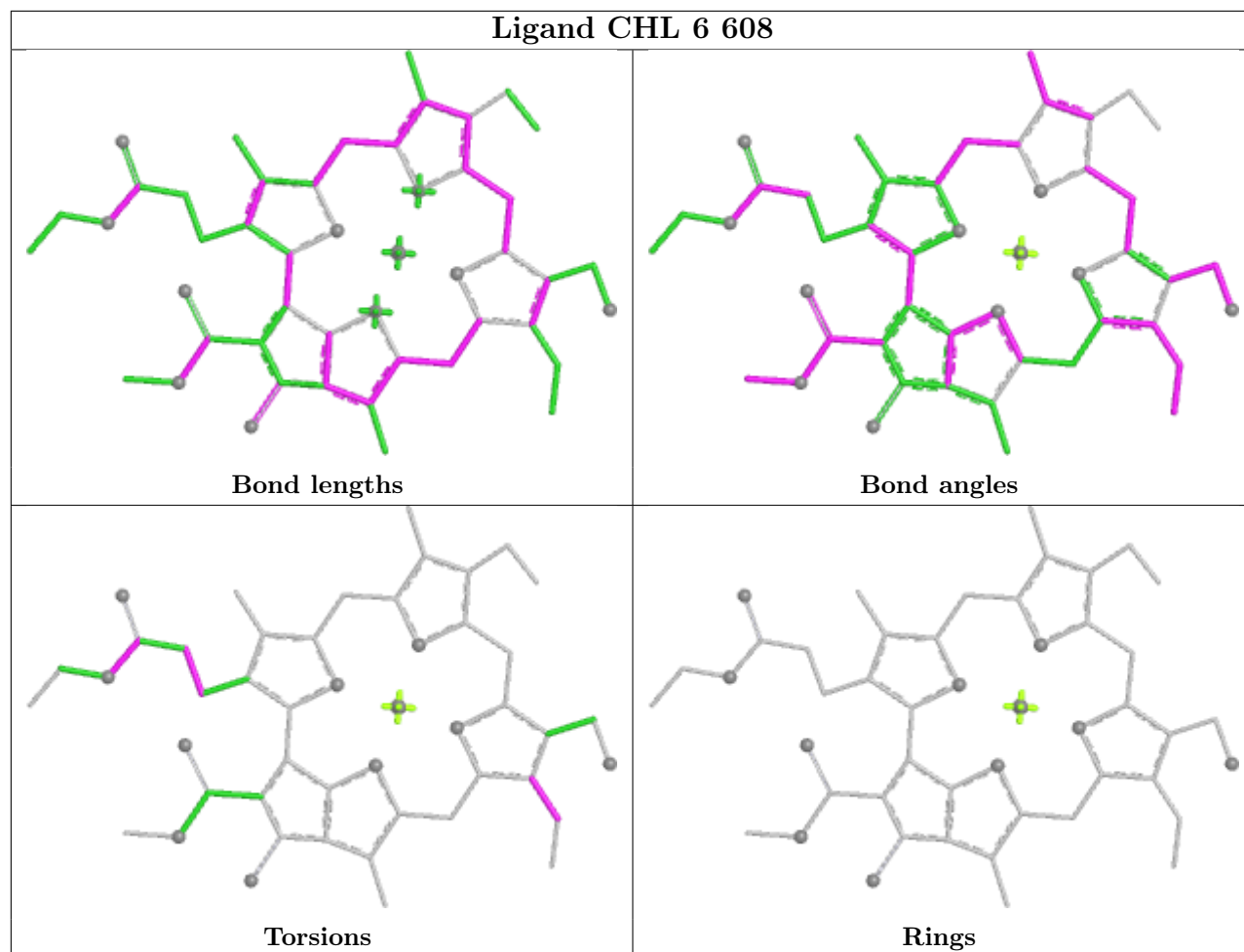
Ligand CHL 5 607



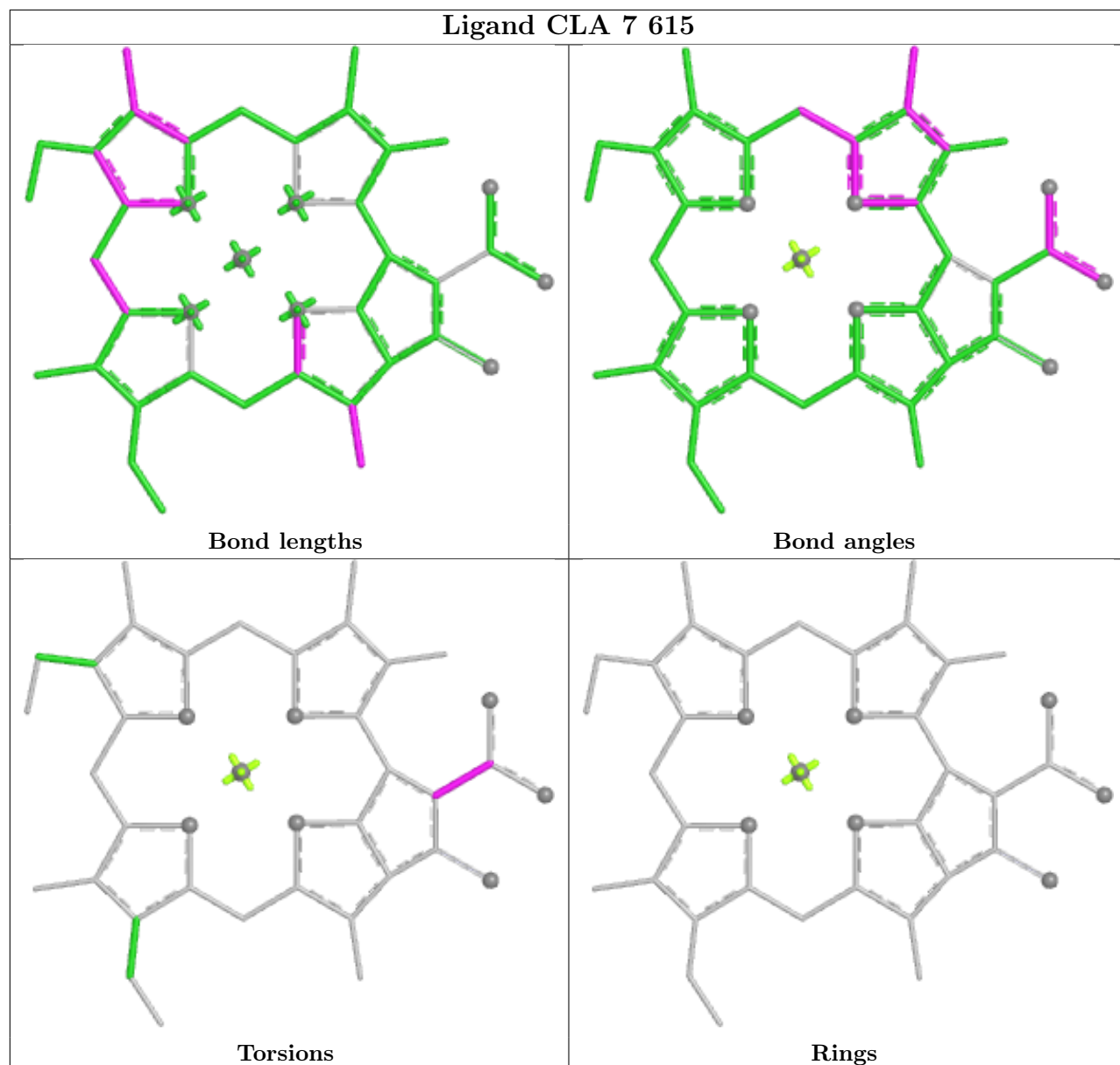
Ligand CLA 7 612



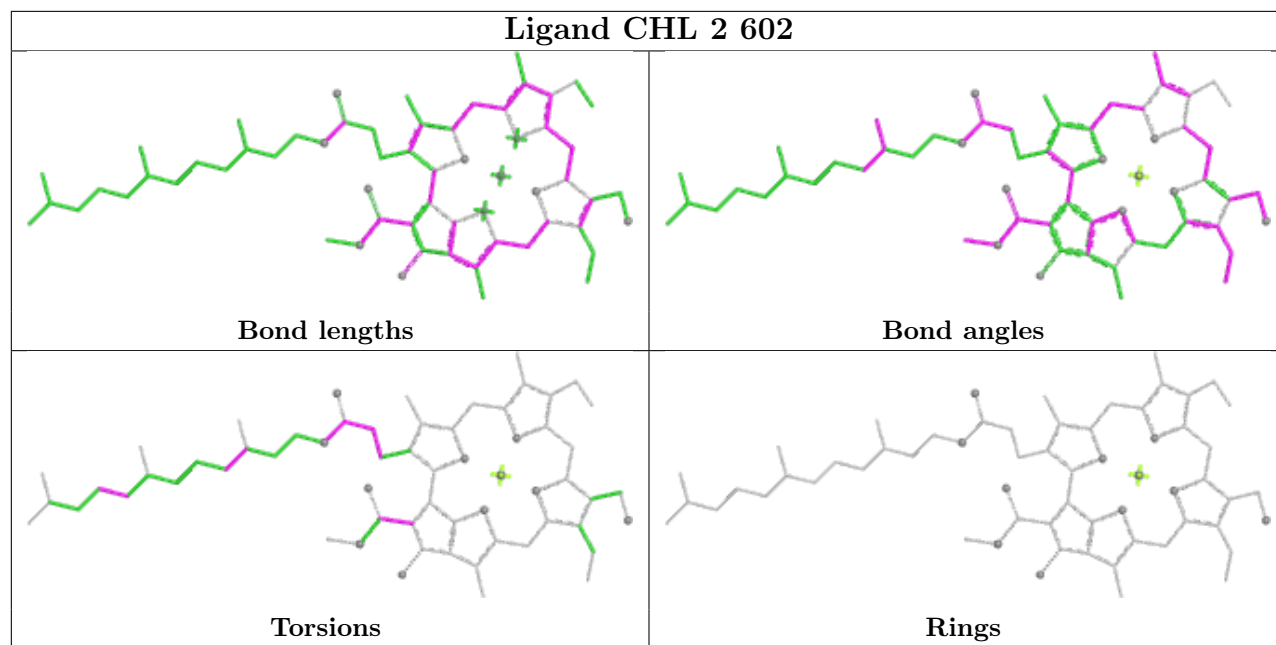
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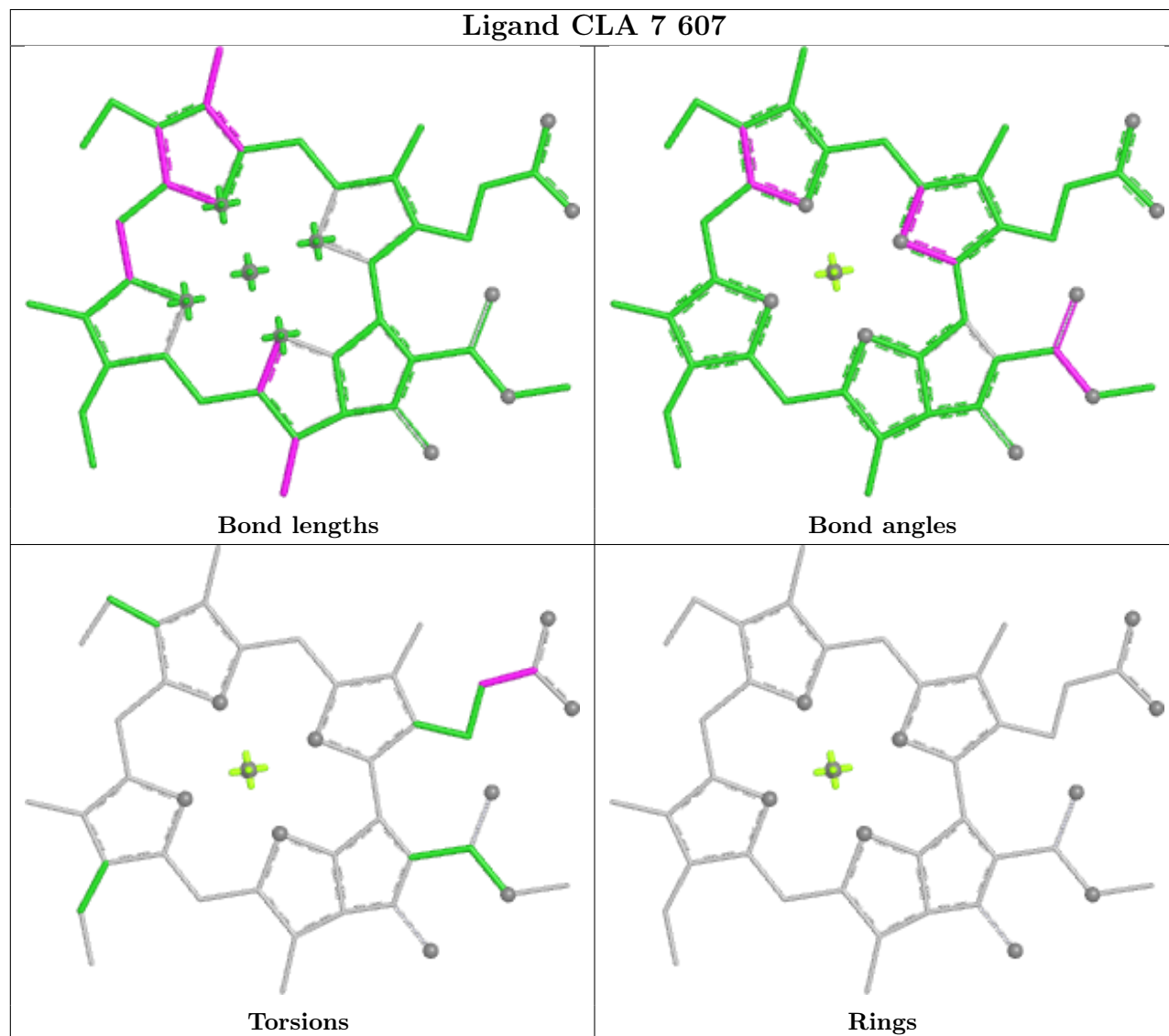
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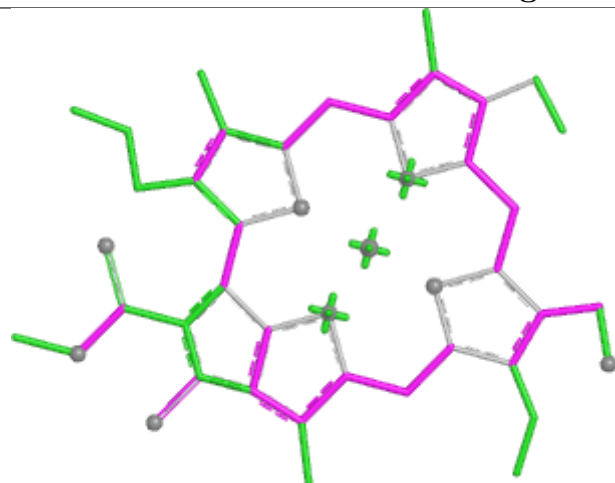
Ligand CHL 2 602



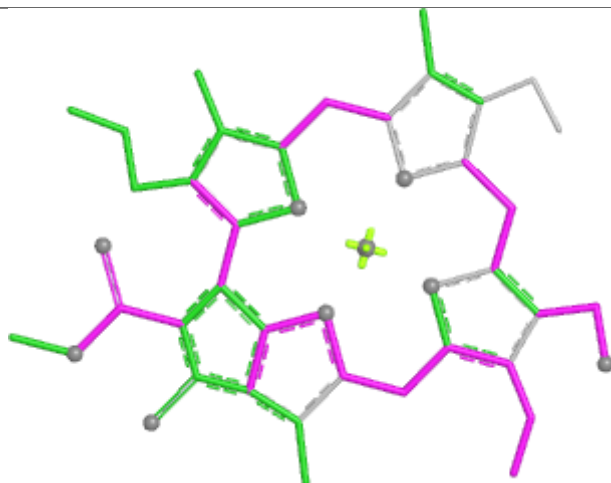
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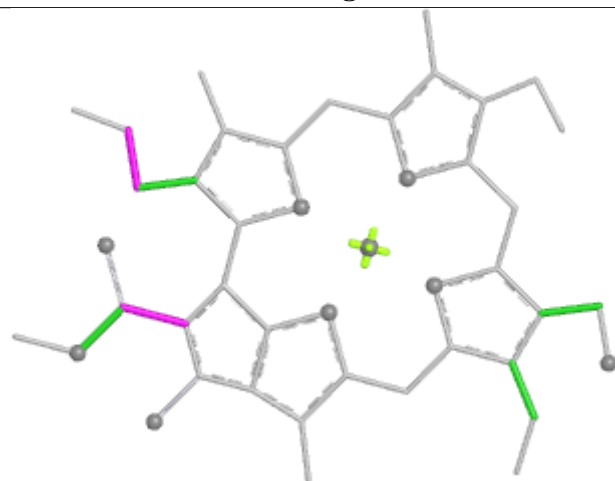
Ligand CHL 9 606



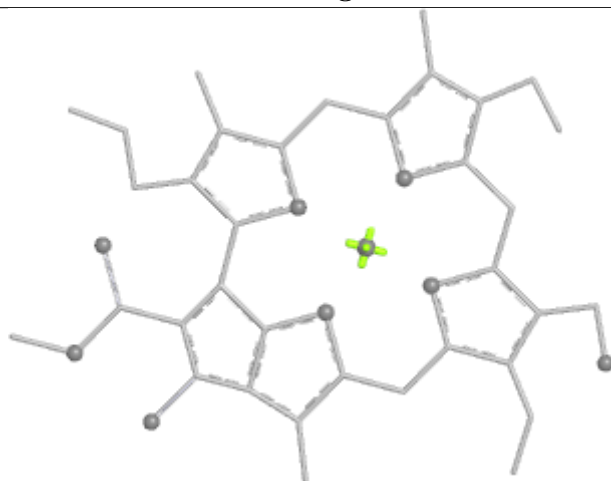
Bond lengths



Bond angles

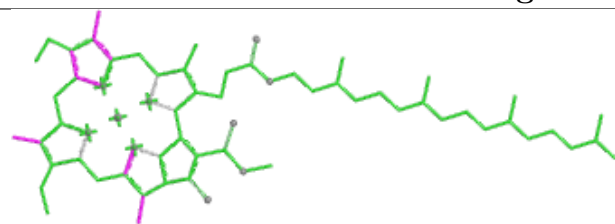


Torsions

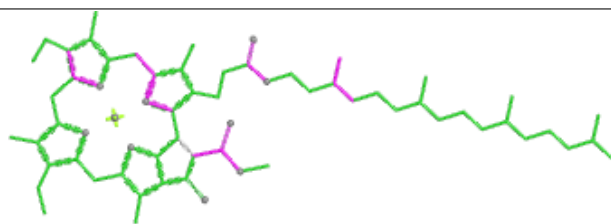


Rings

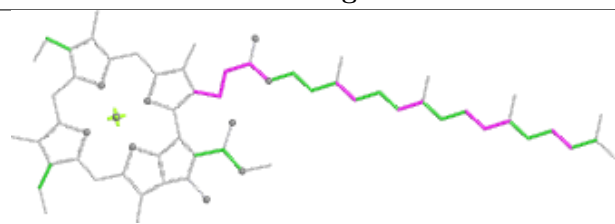
Ligand CLA B 831



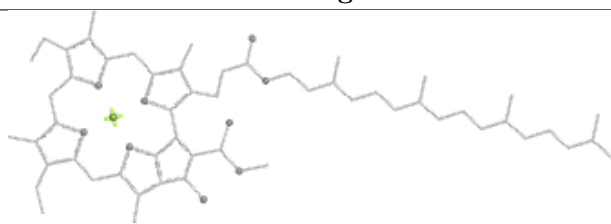
Bond lengths



Bond angles

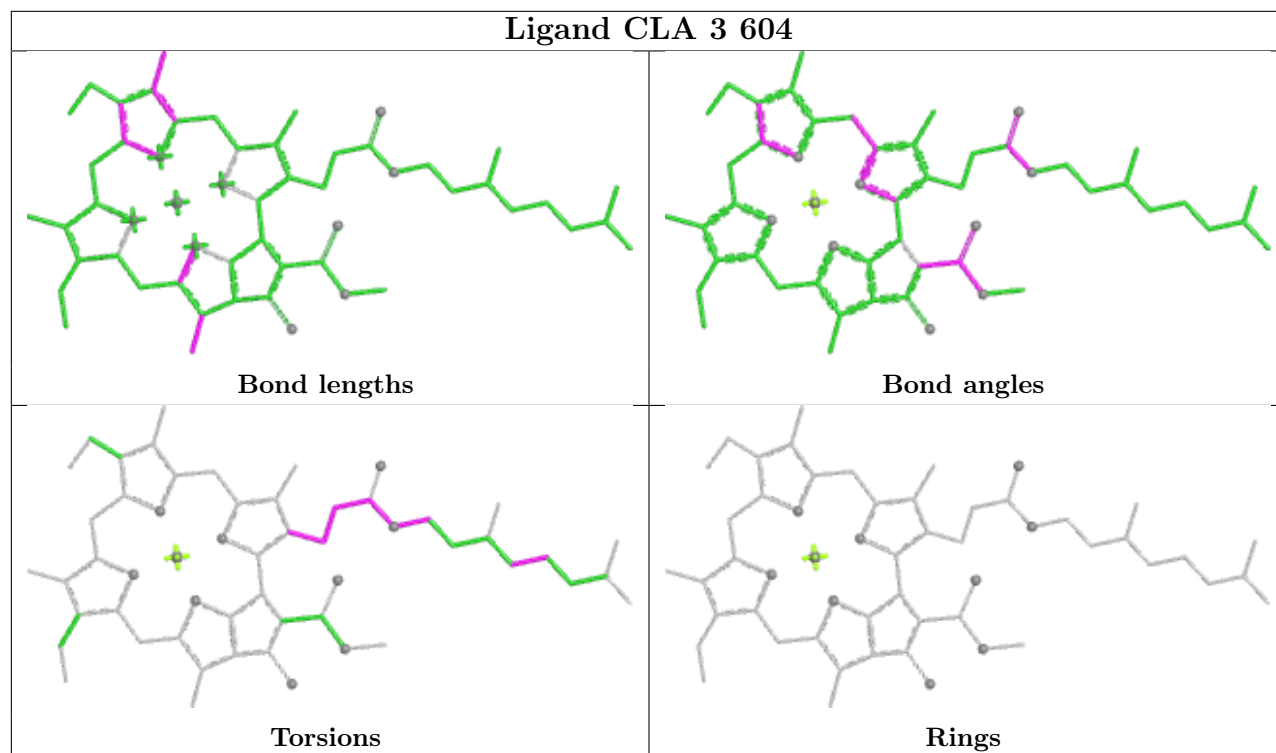


Torsions

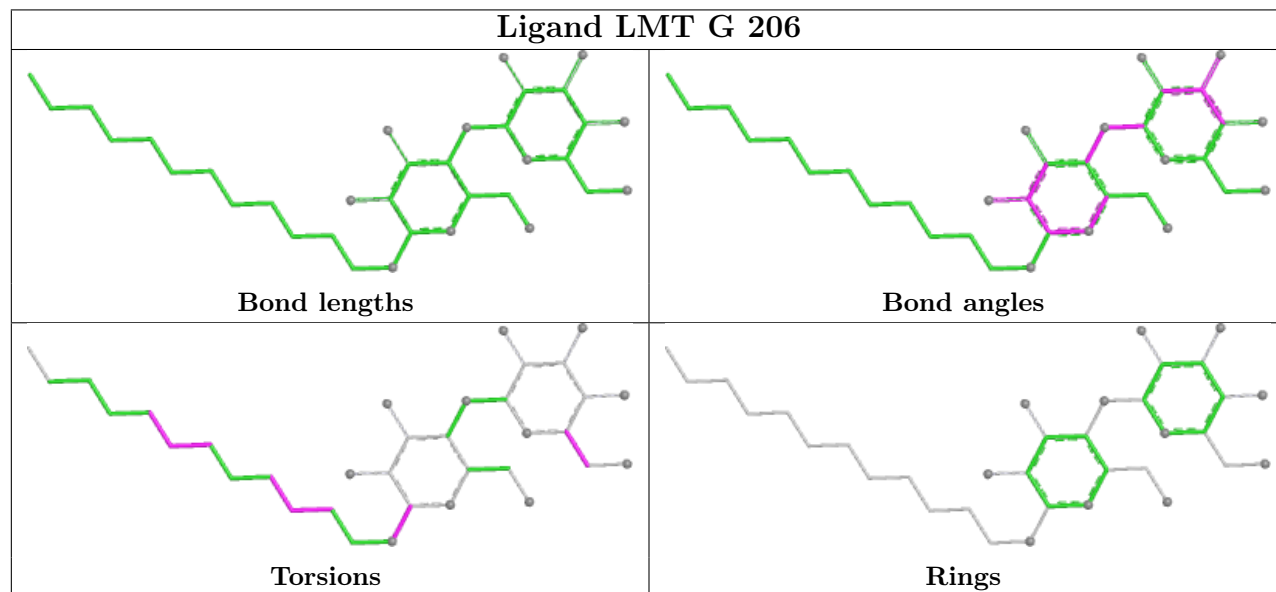


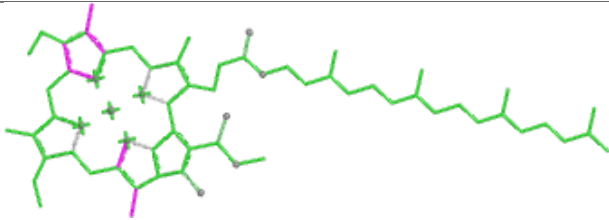
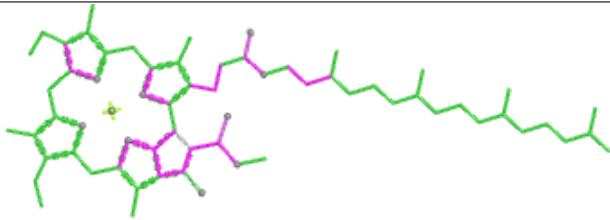
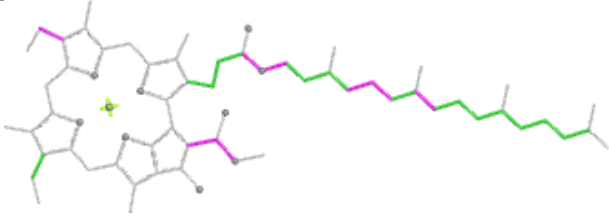
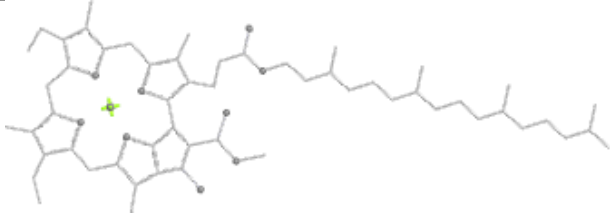
Rings

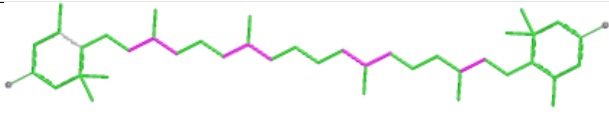
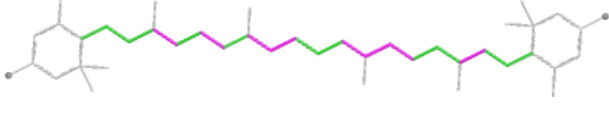
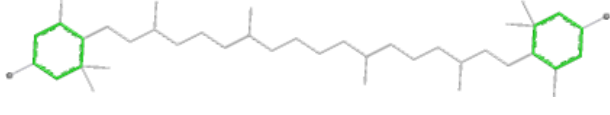
Ligand CLA 3 604

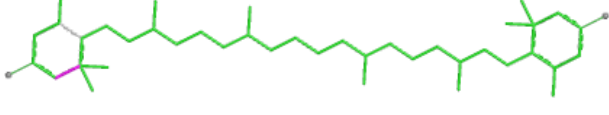
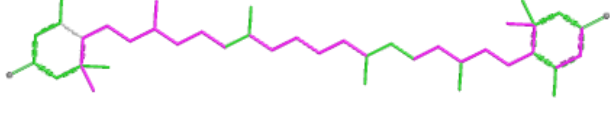
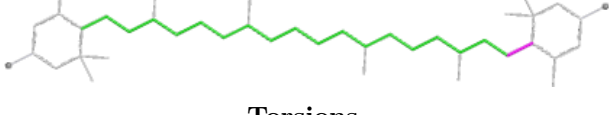
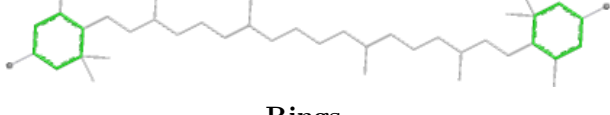


Ligand LMT G 206

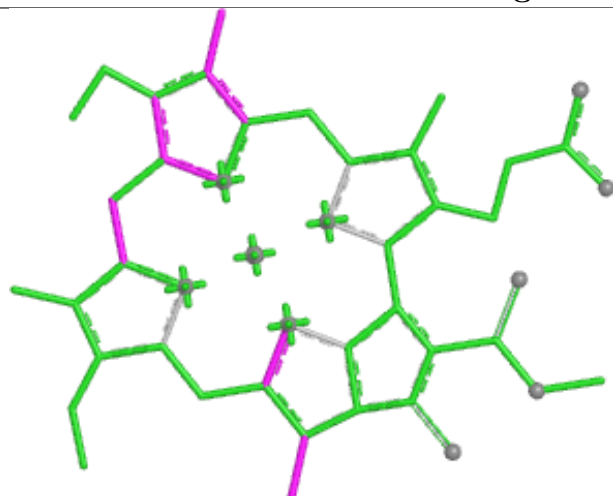


Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

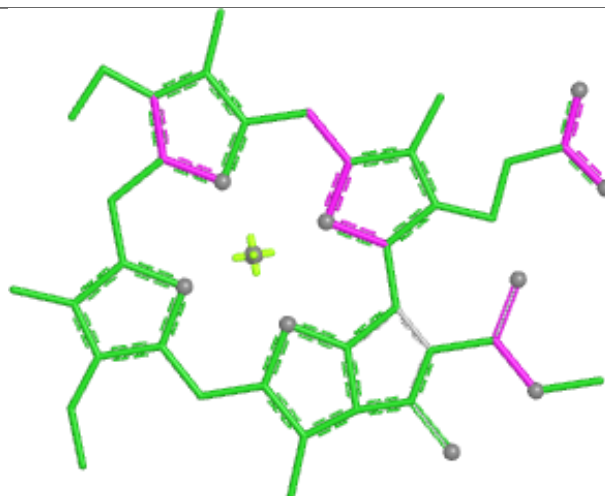
Ligand LUT 2 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

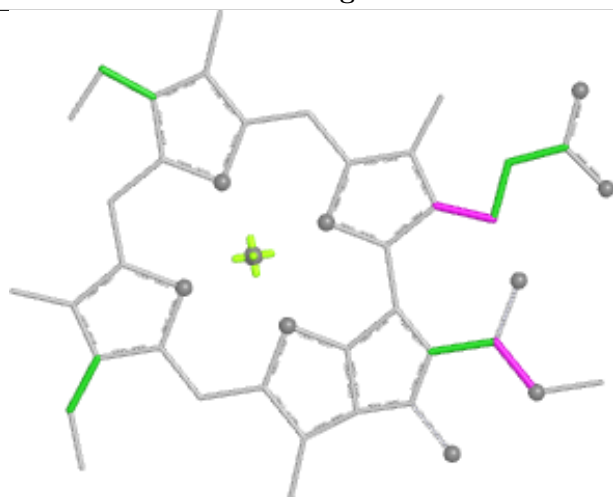
Ligand CLA V 614



Bond lengths



Bond angles

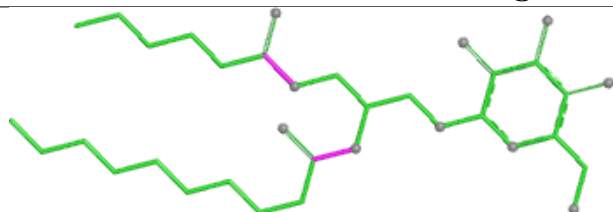


Torsions

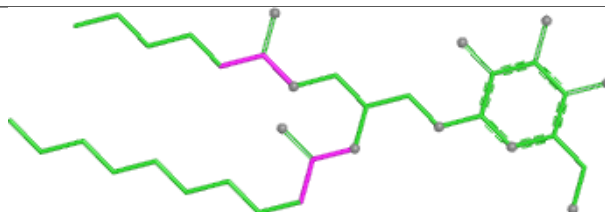


Rings

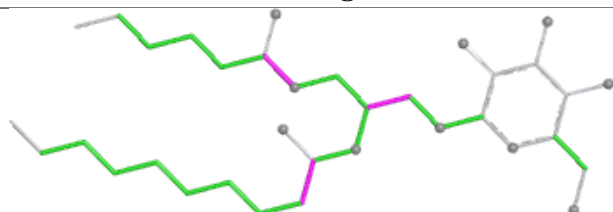
Ligand LMG J 104



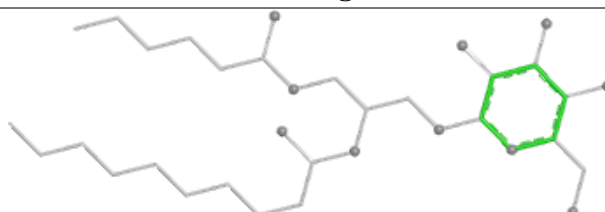
Bond lengths



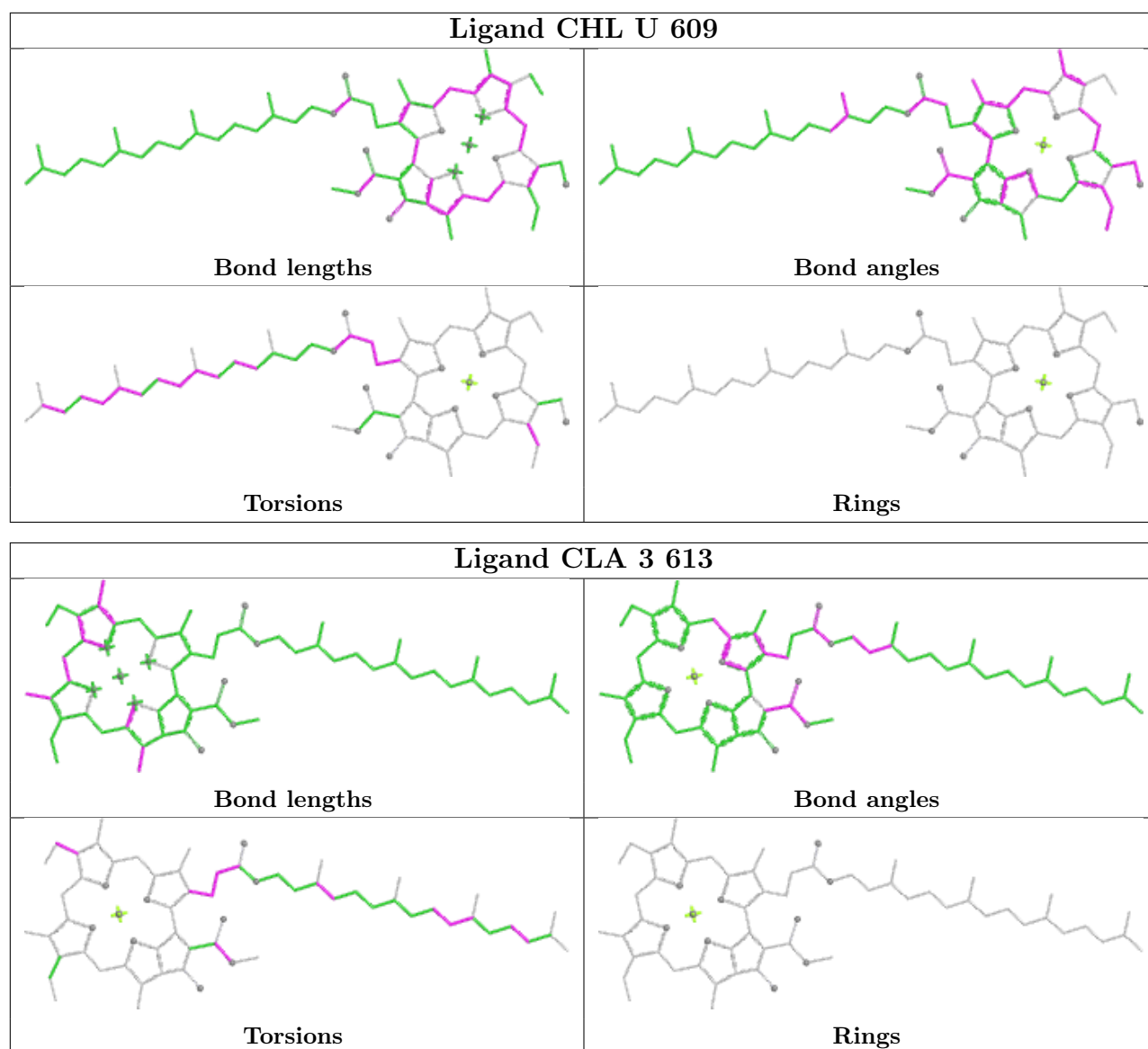
Bond angles



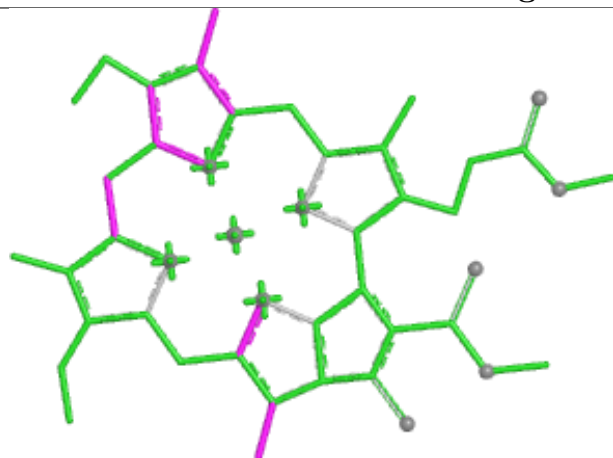
Torsions



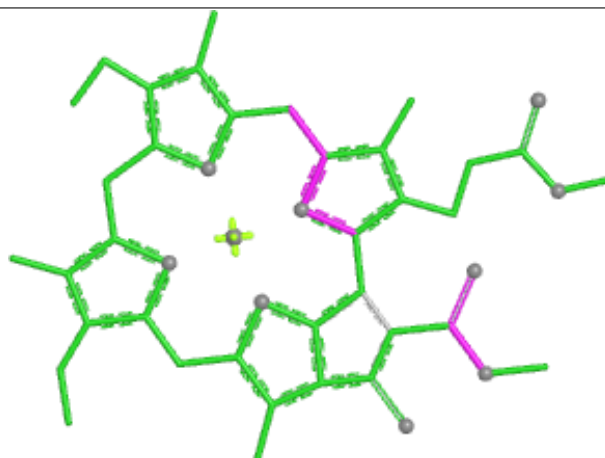
Rings



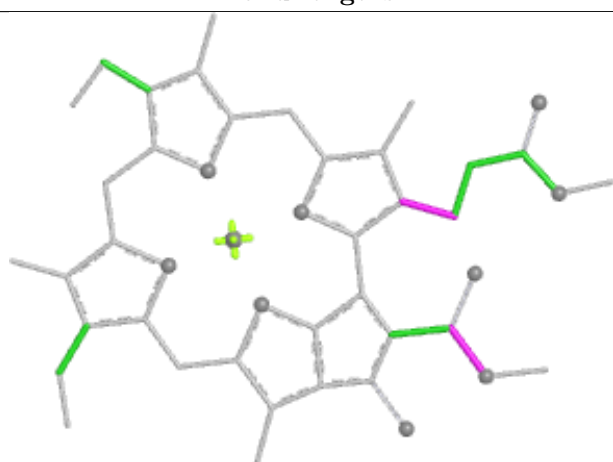
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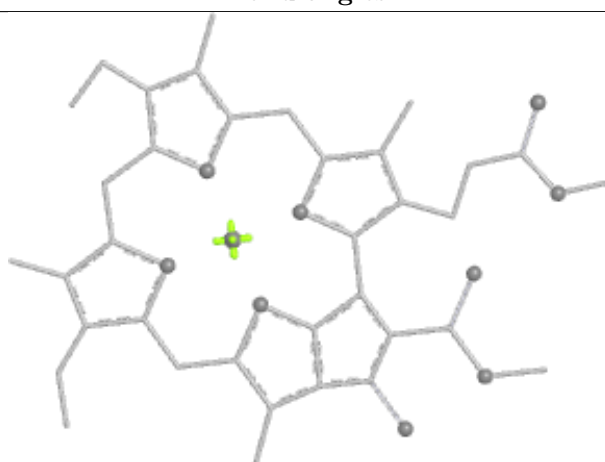
Bond lengths



Bond angles

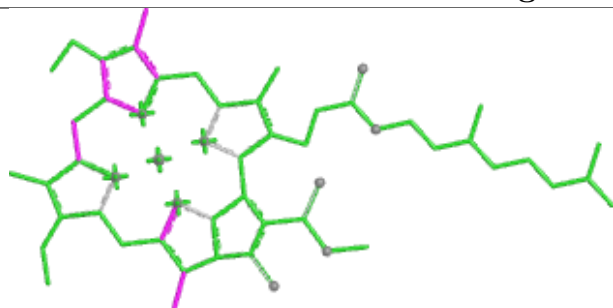


Torsions

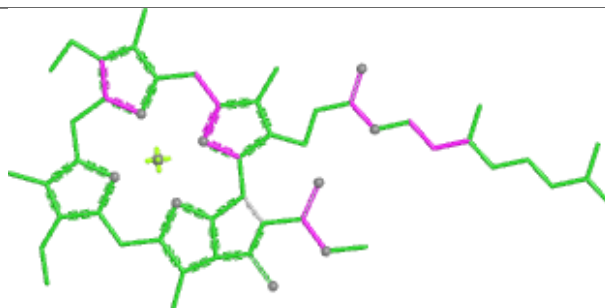


Rings

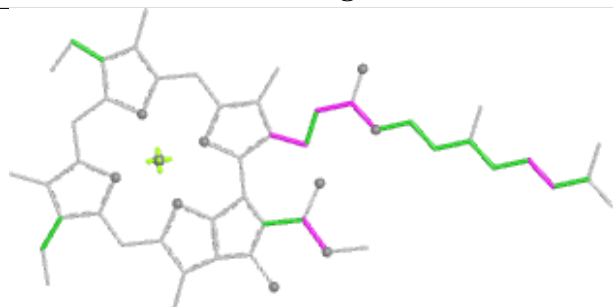
Ligand CLA 9 610



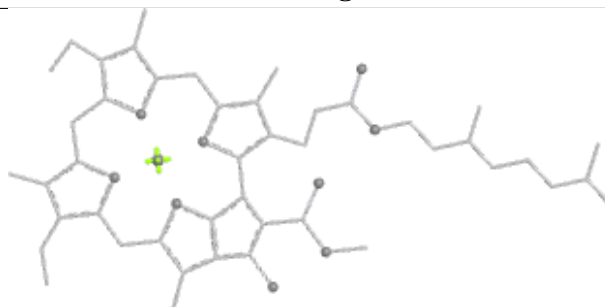
Bond lengths



Bond angles

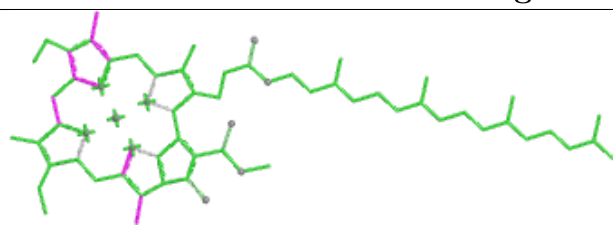


Torsions

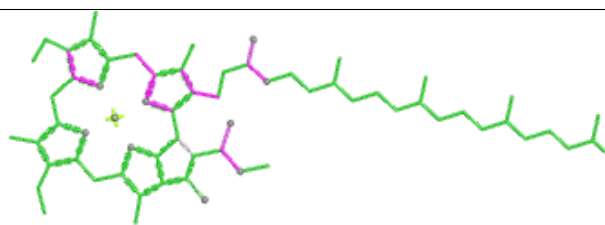


Rings

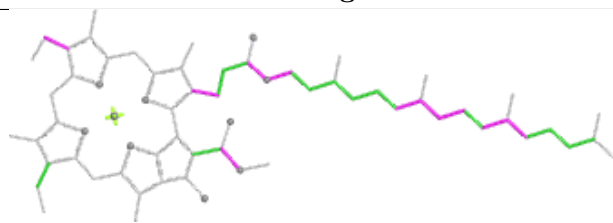
Ligand CLA B 810



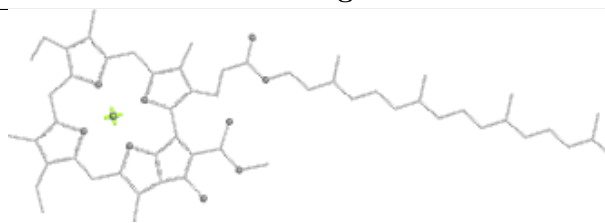
Bond lengths



Bond angles

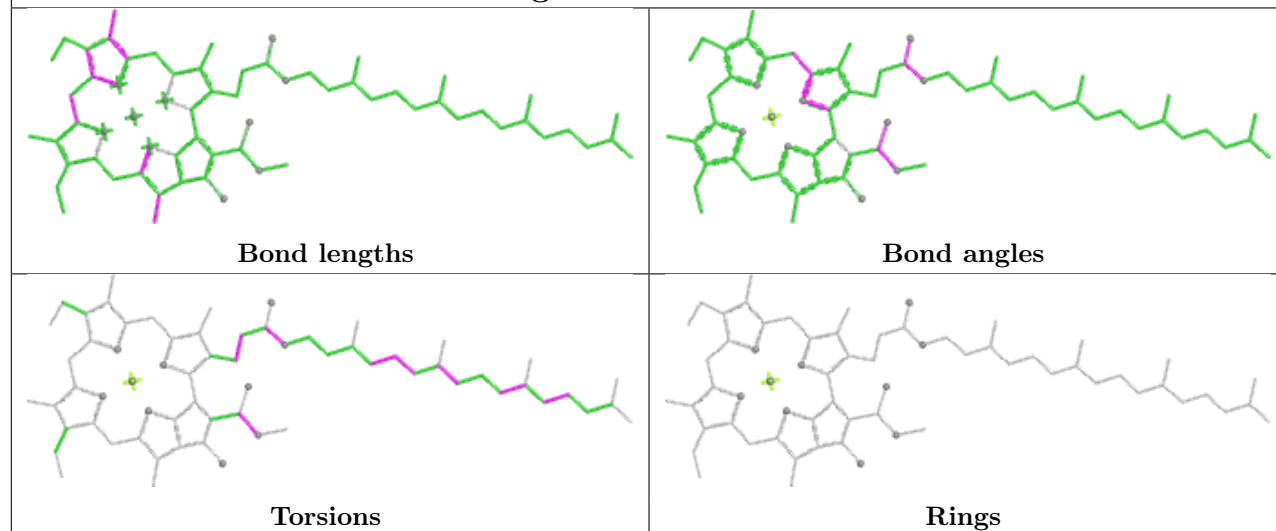


Torsions

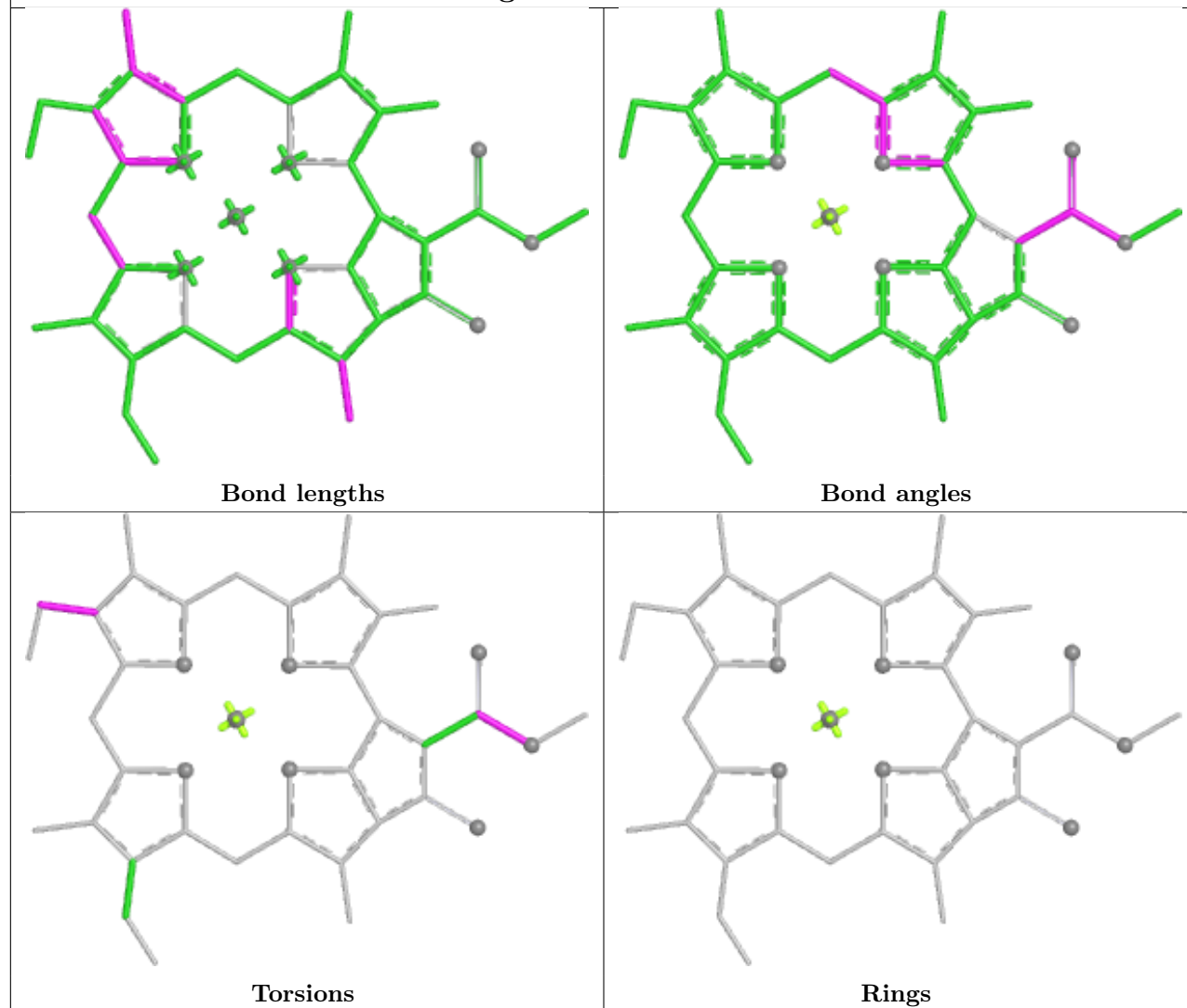


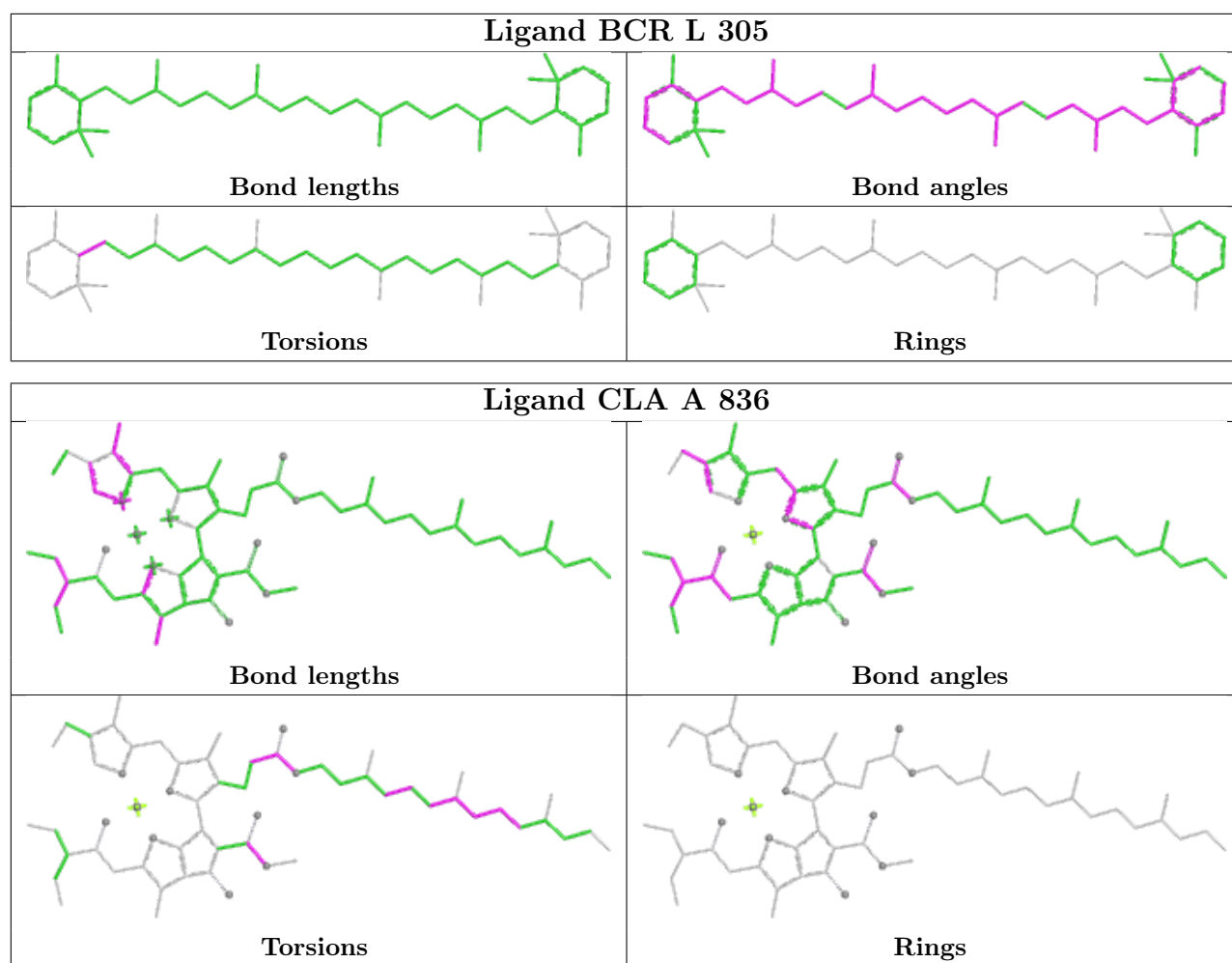
Rings

Ligand CLA A 822

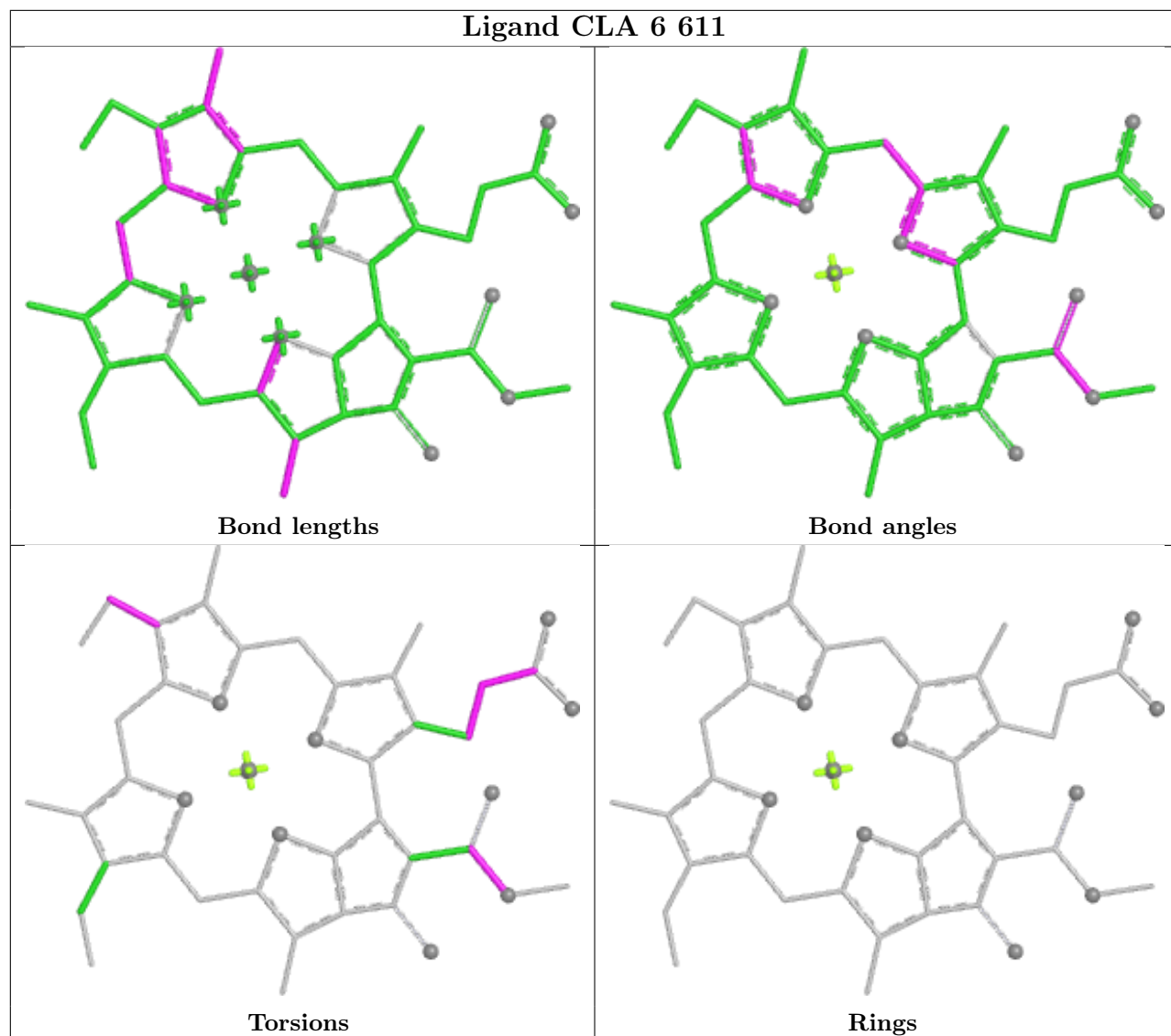


Ligand CLA 7 611

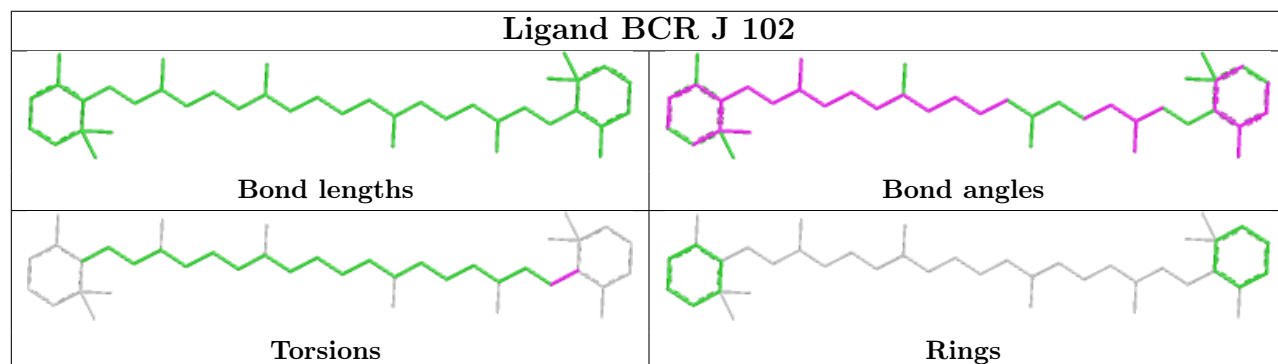


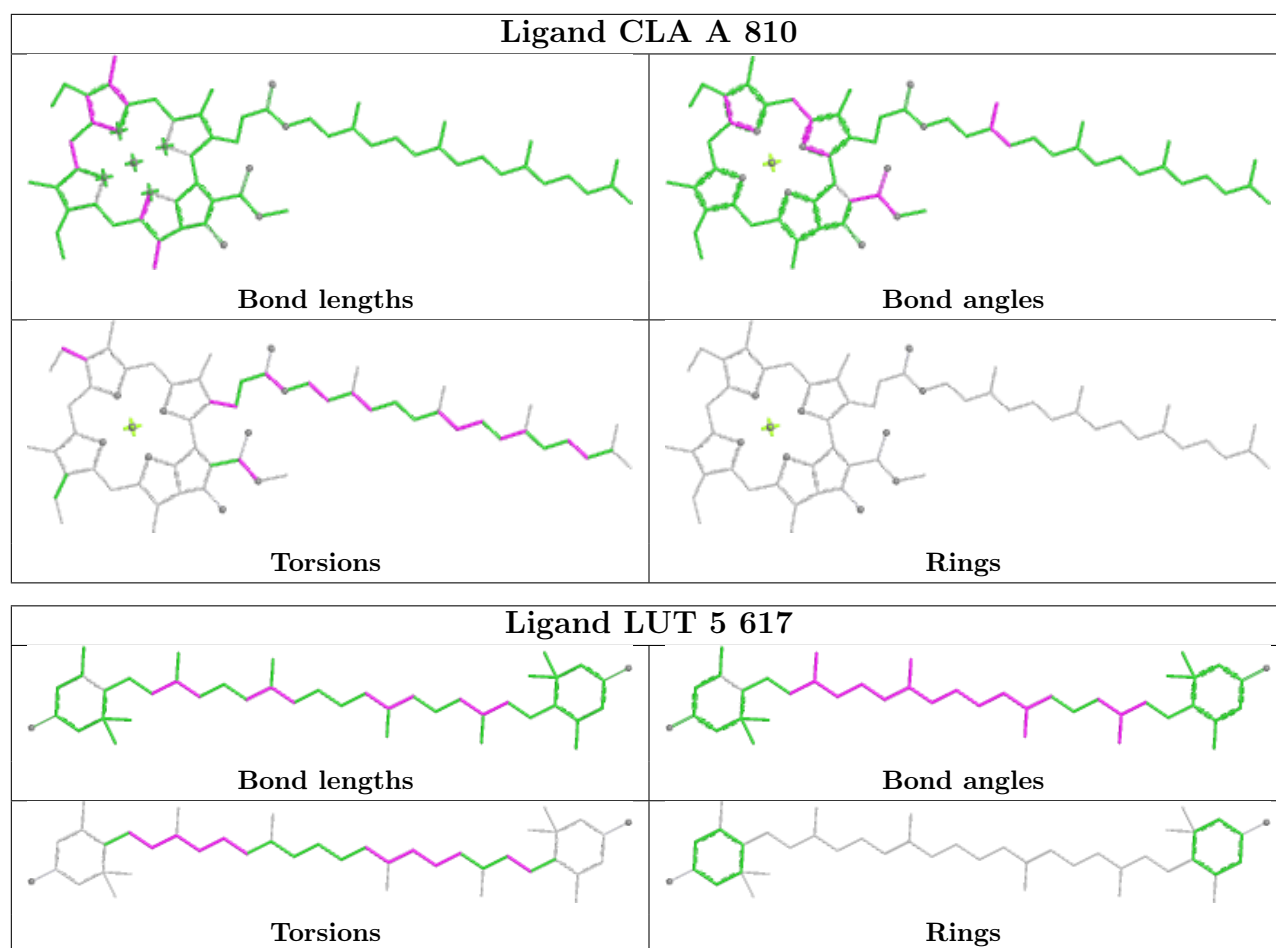


Ligand CLA 6 611

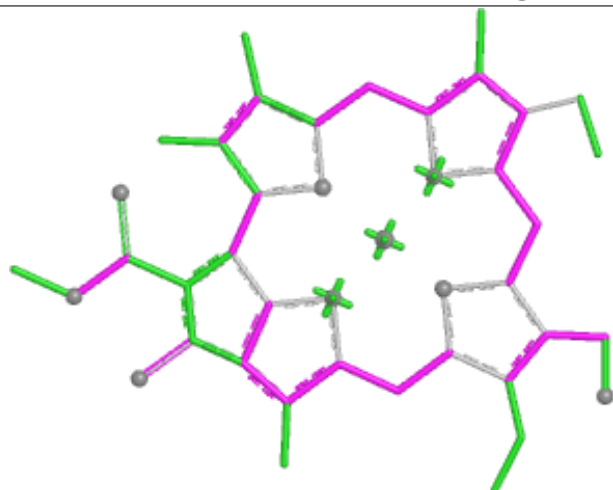


Ligand BCR J 102

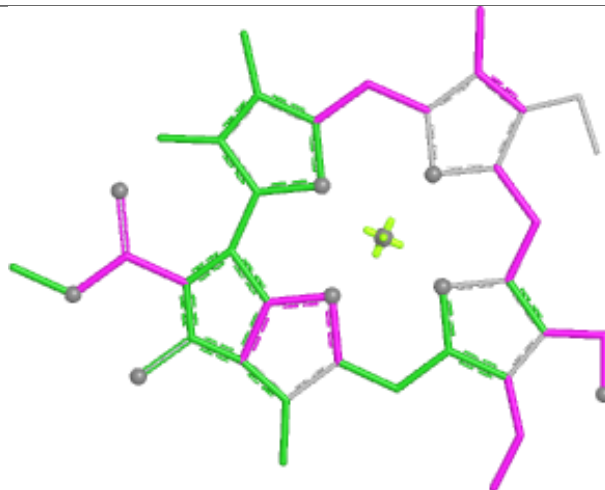




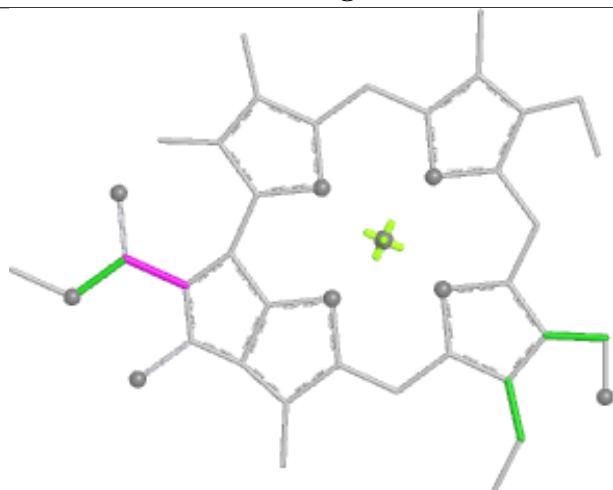
Ligand CHL V 605



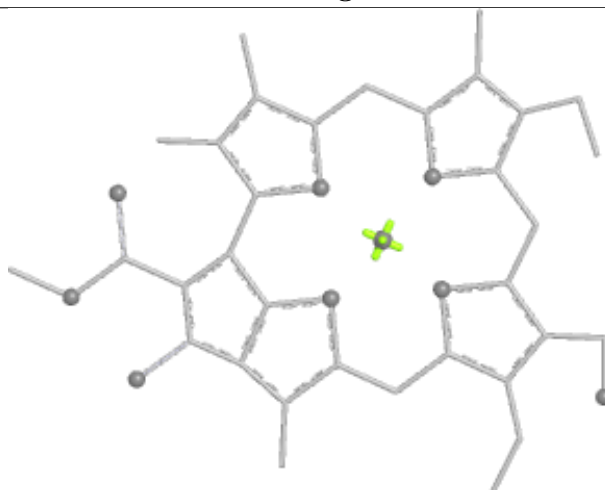
Bond lengths



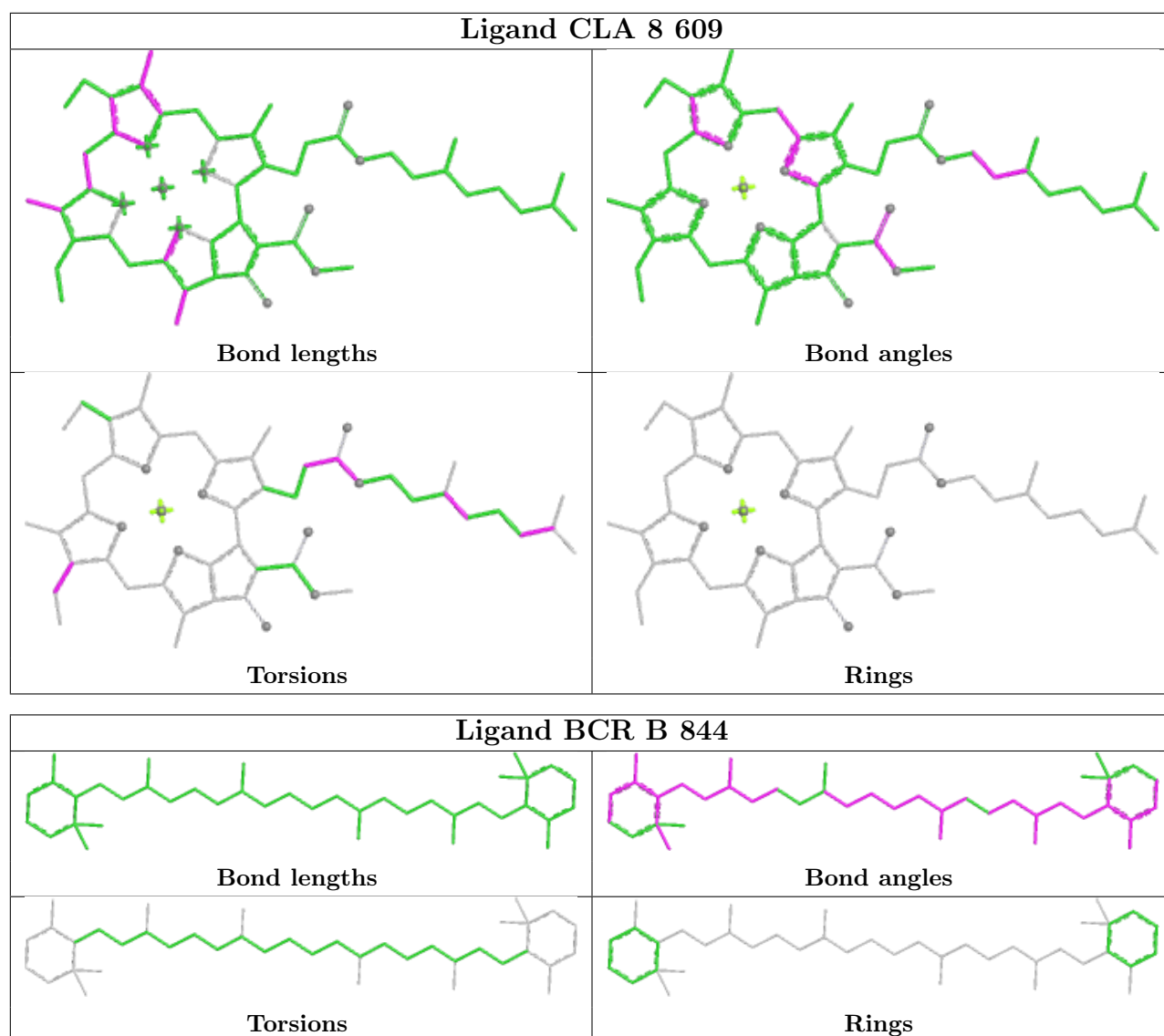
Bond angles

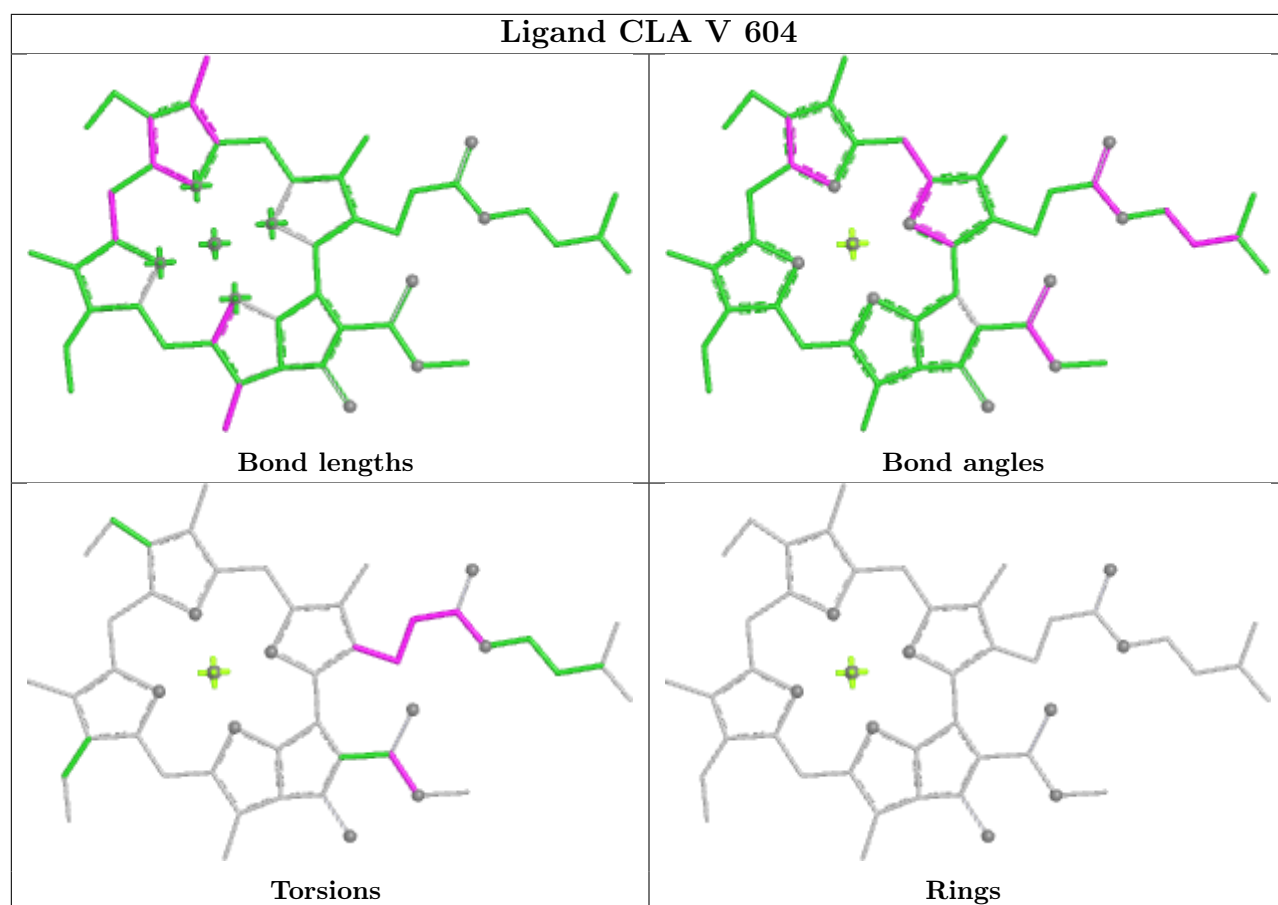


Torsions

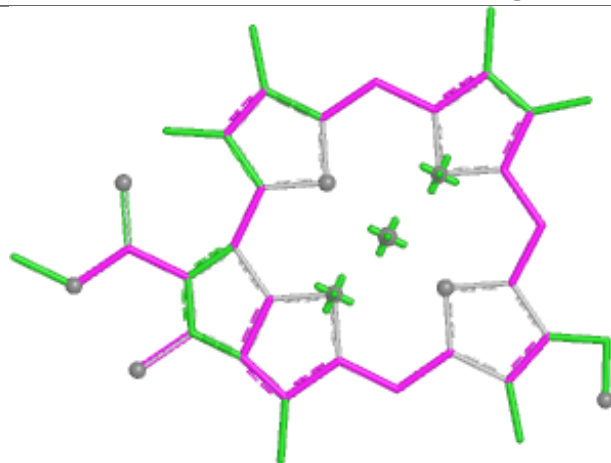


Rings

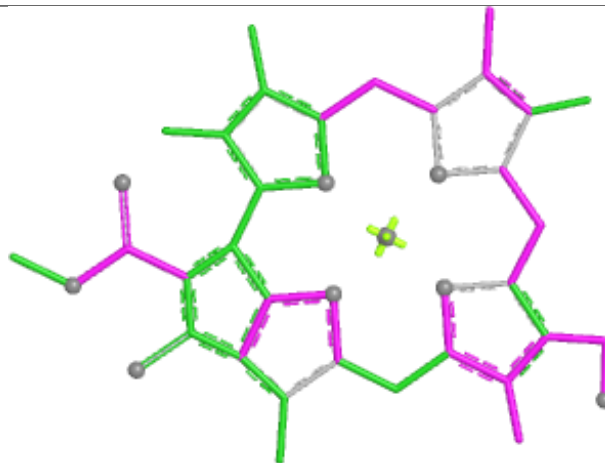




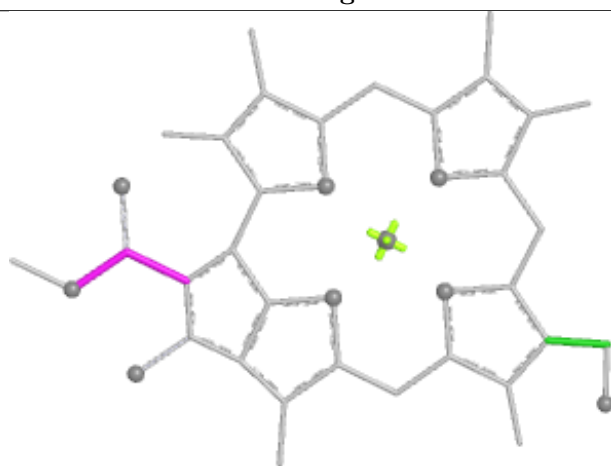
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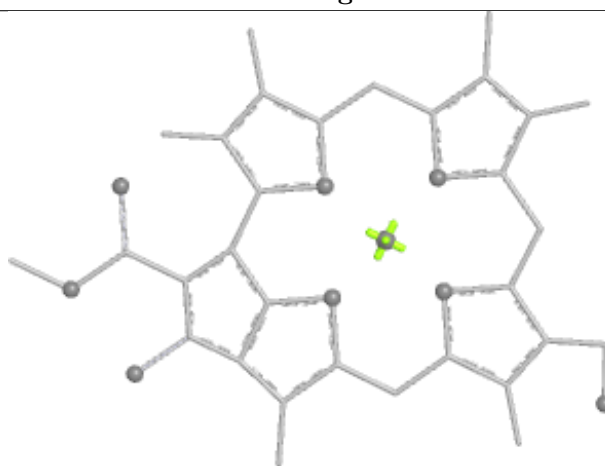
Bond lengths



Bond angles

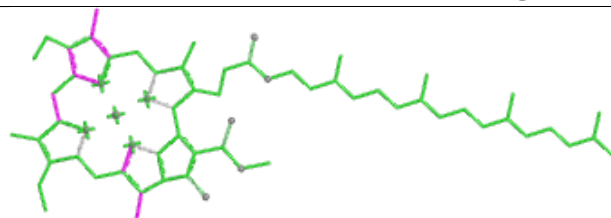


Torsions

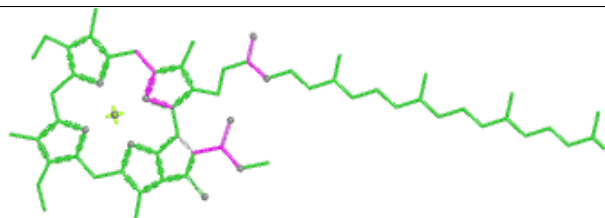


Rings

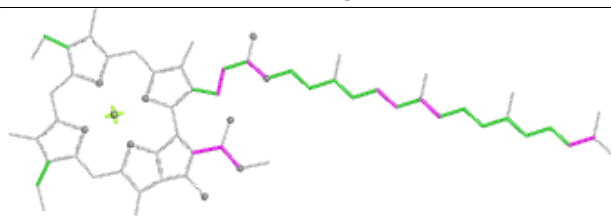
Ligand CLA A 845



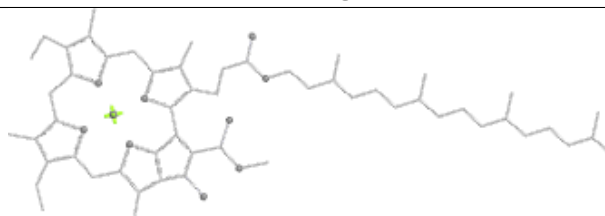
Bond lengths



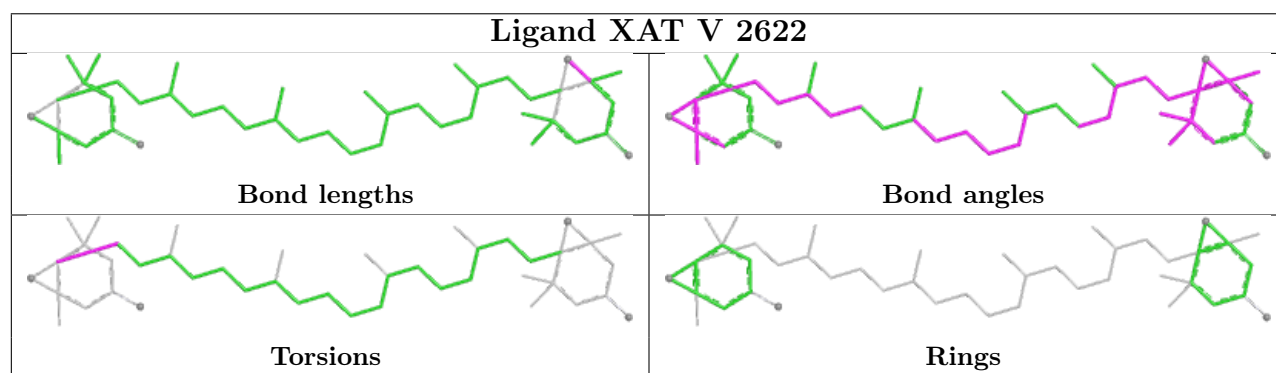
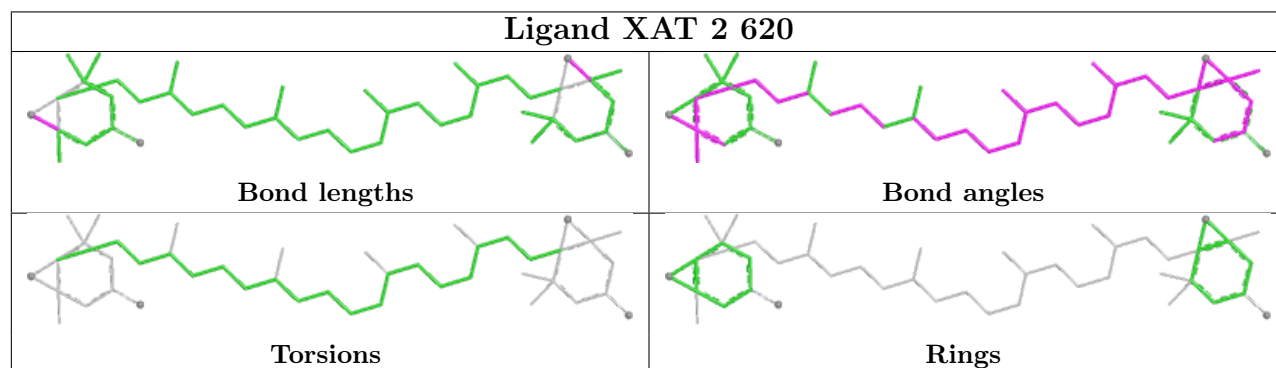
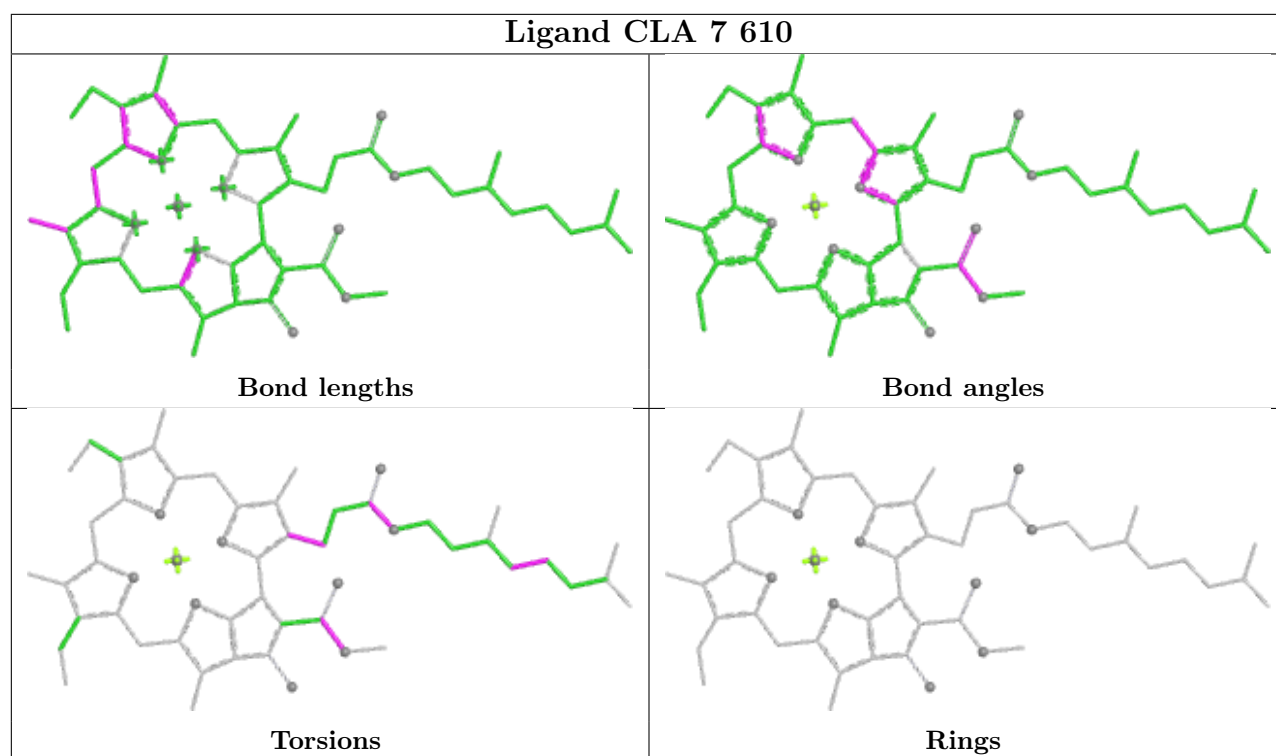
Bond angles



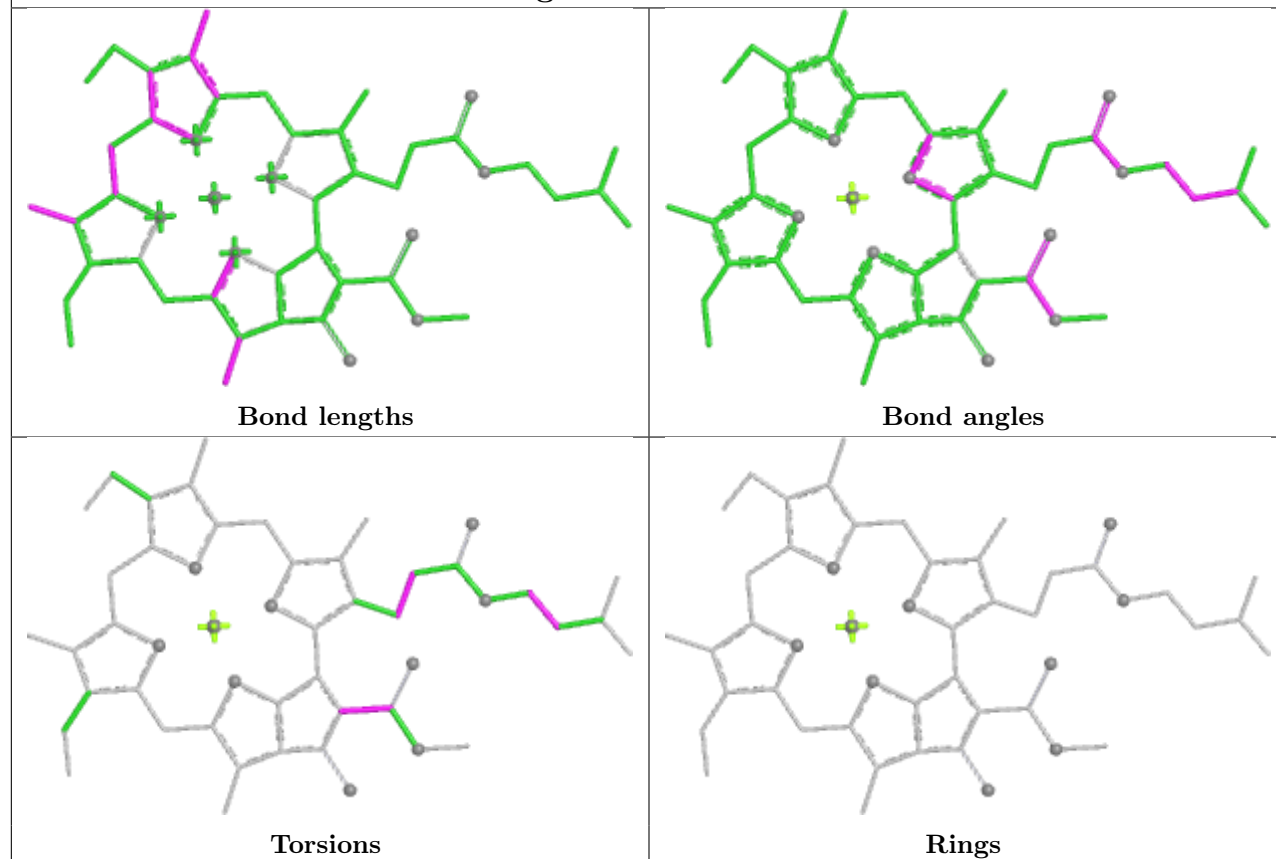
Torsions



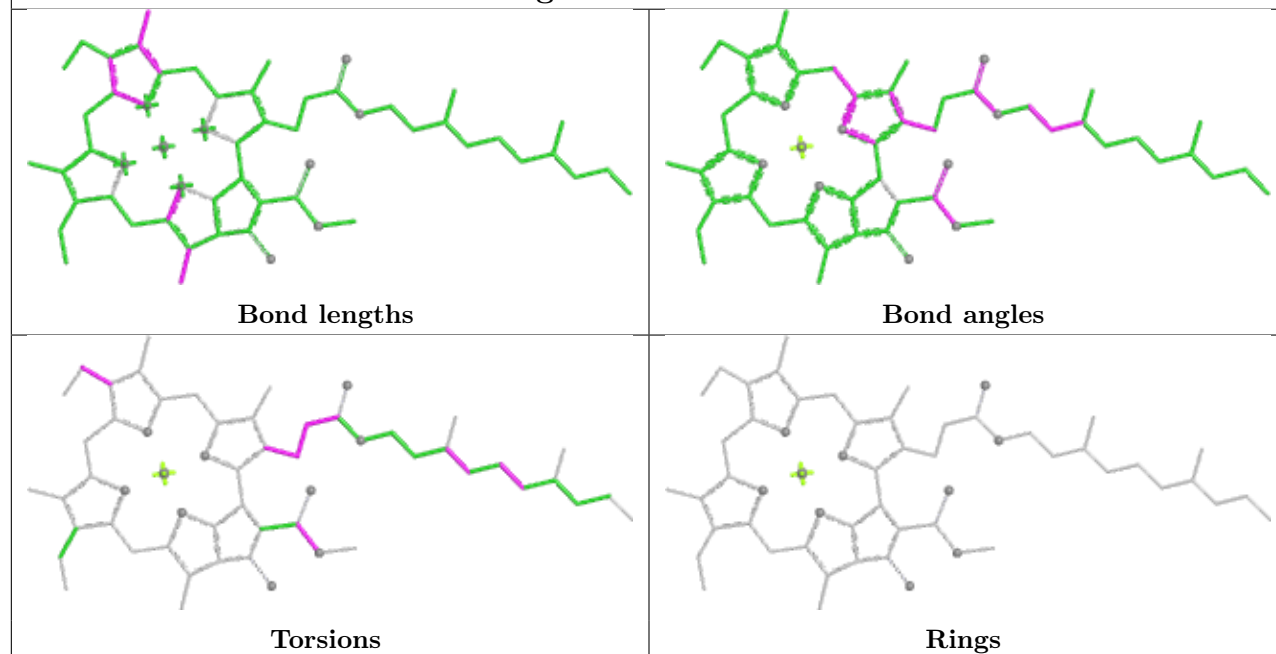
Rings



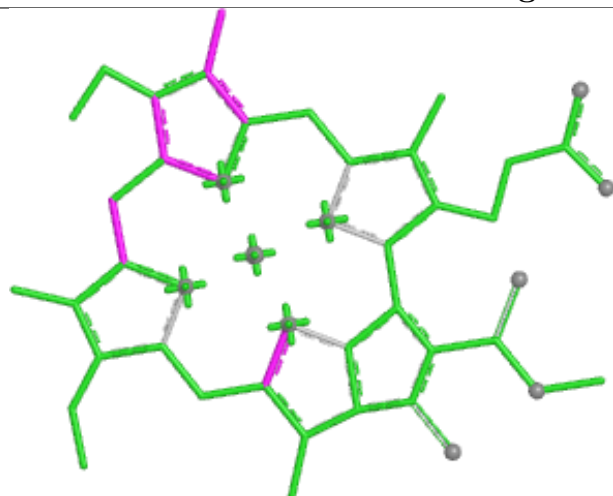
Ligand CLA 8 601



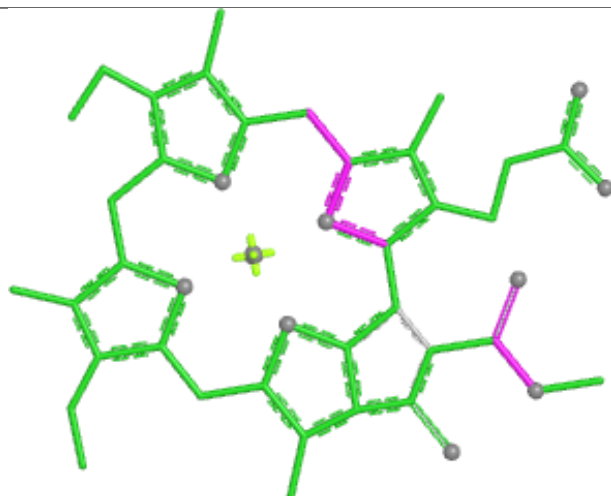
Ligand CLA 2 613



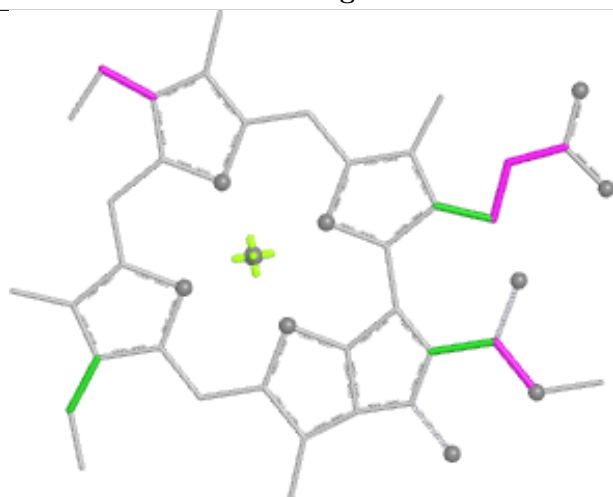
Ligand CLA 1 616



Bond lengths



Bond angles

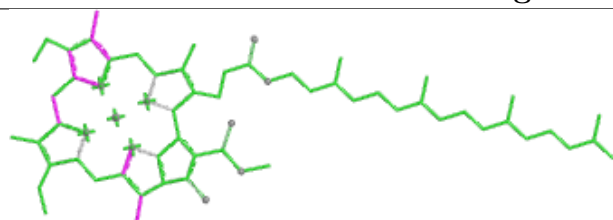


Torsions

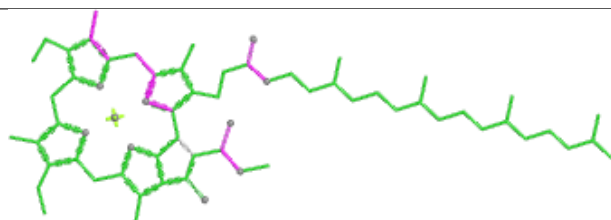


Rings

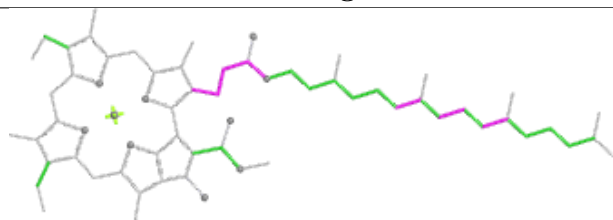
Ligand CLA A 831



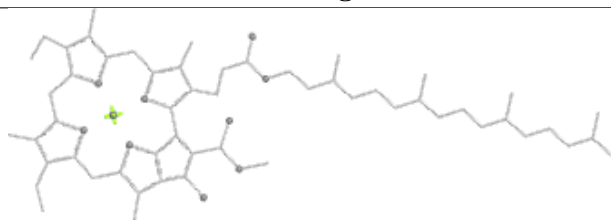
Bond lengths



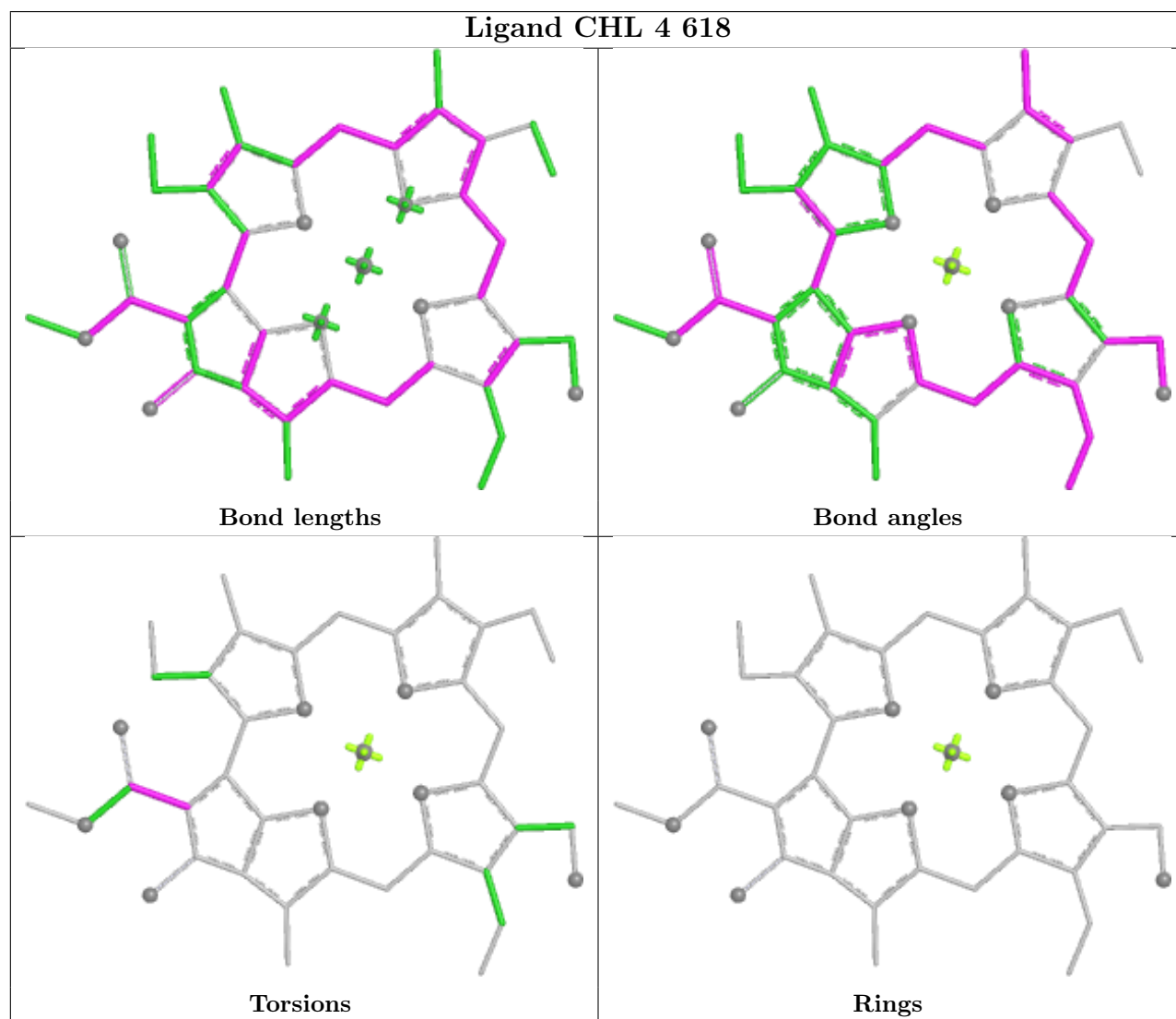
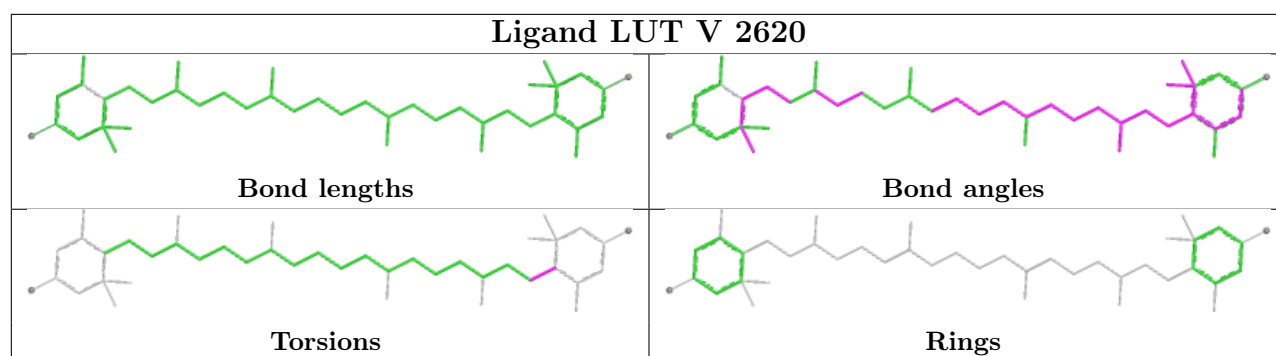
Bond angles



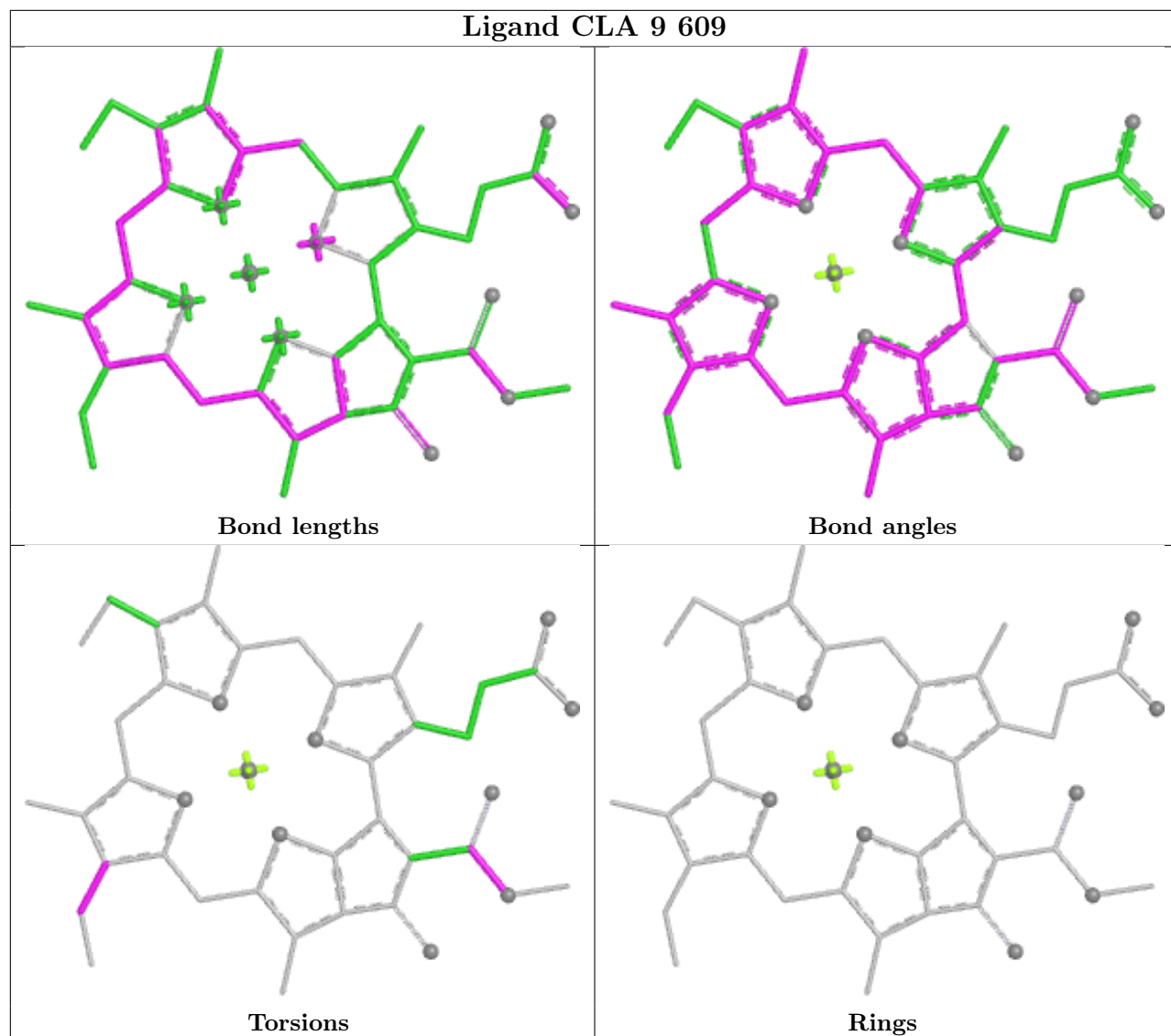
Torsions



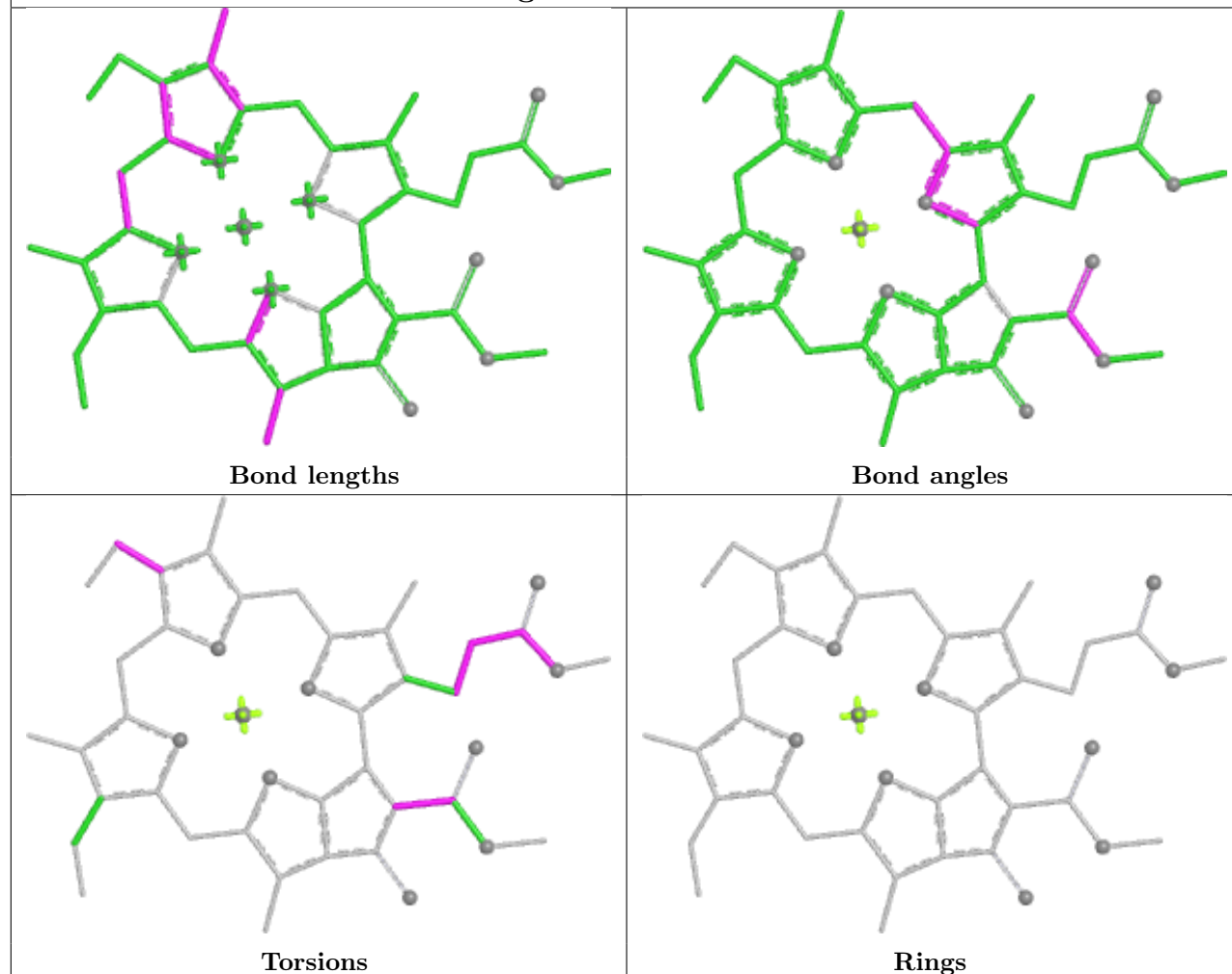
Rings



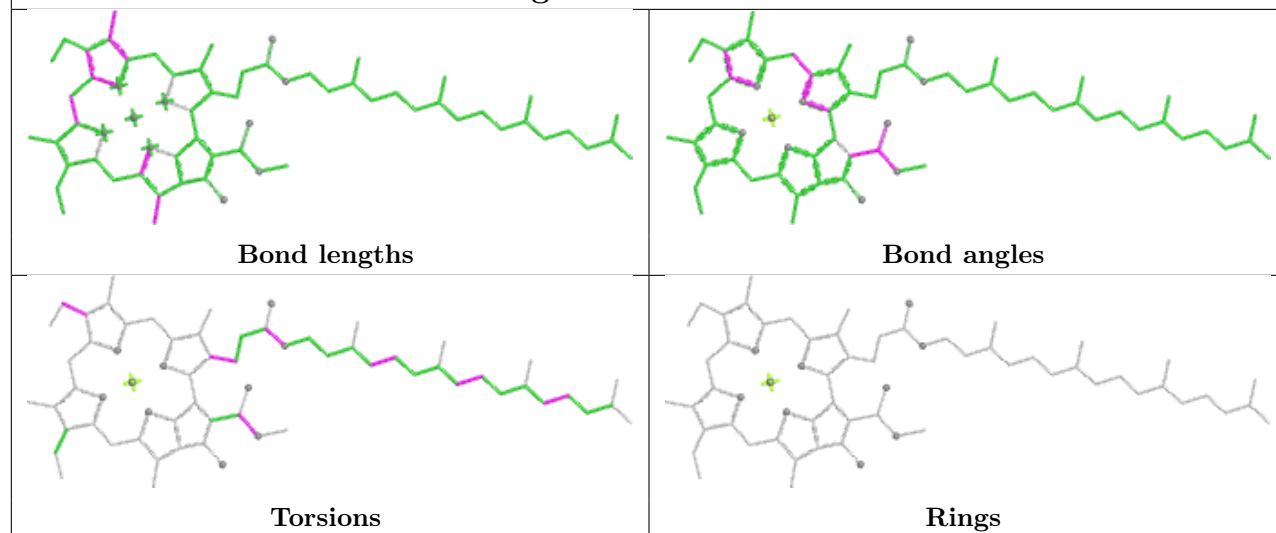
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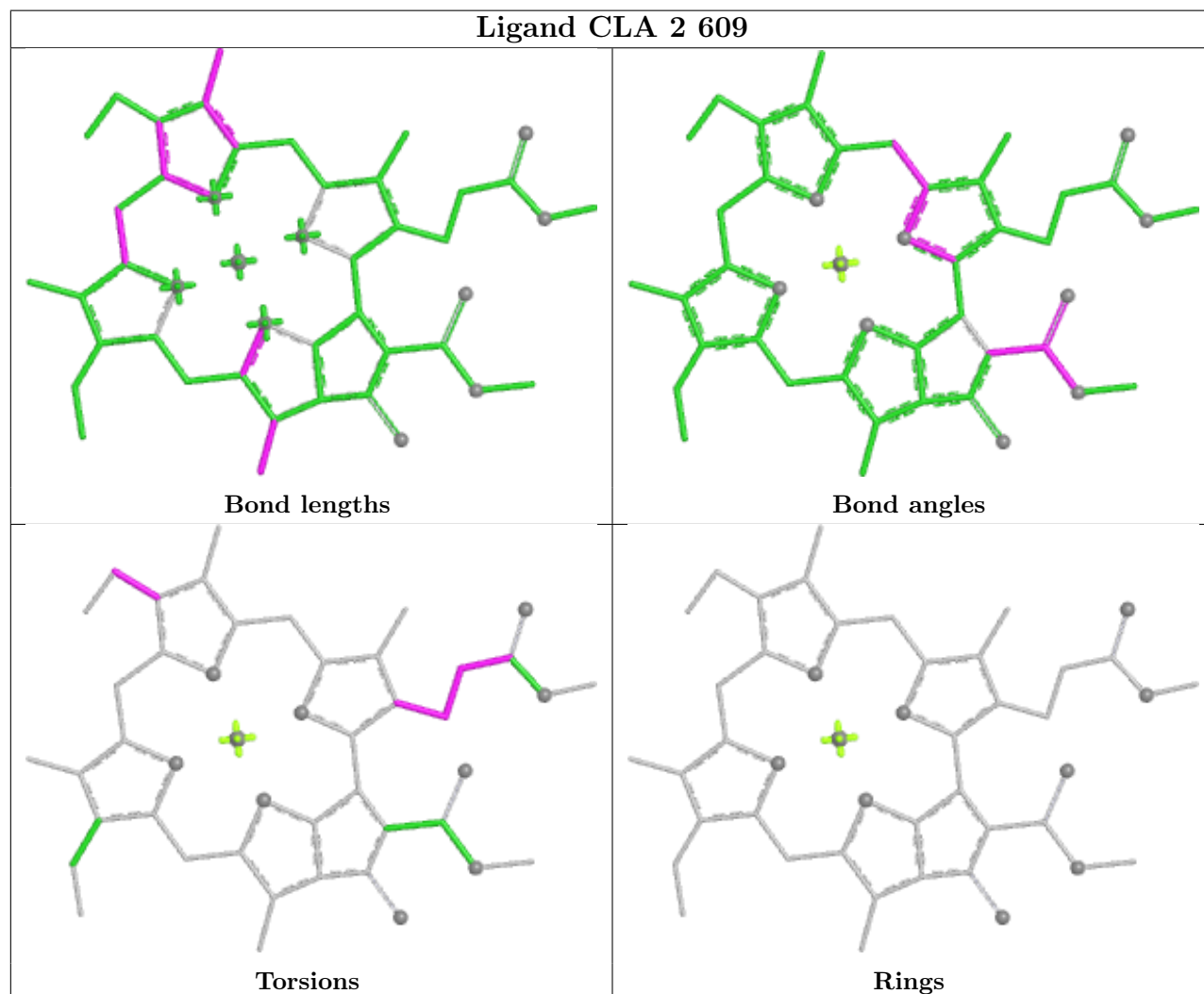
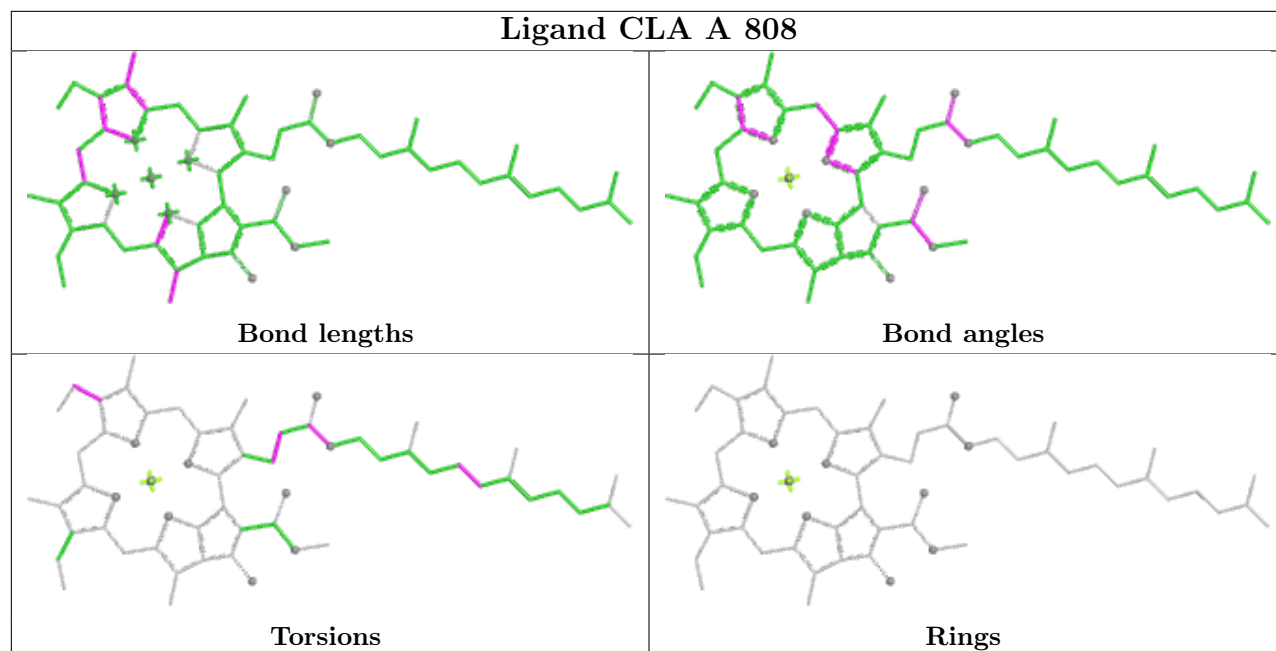


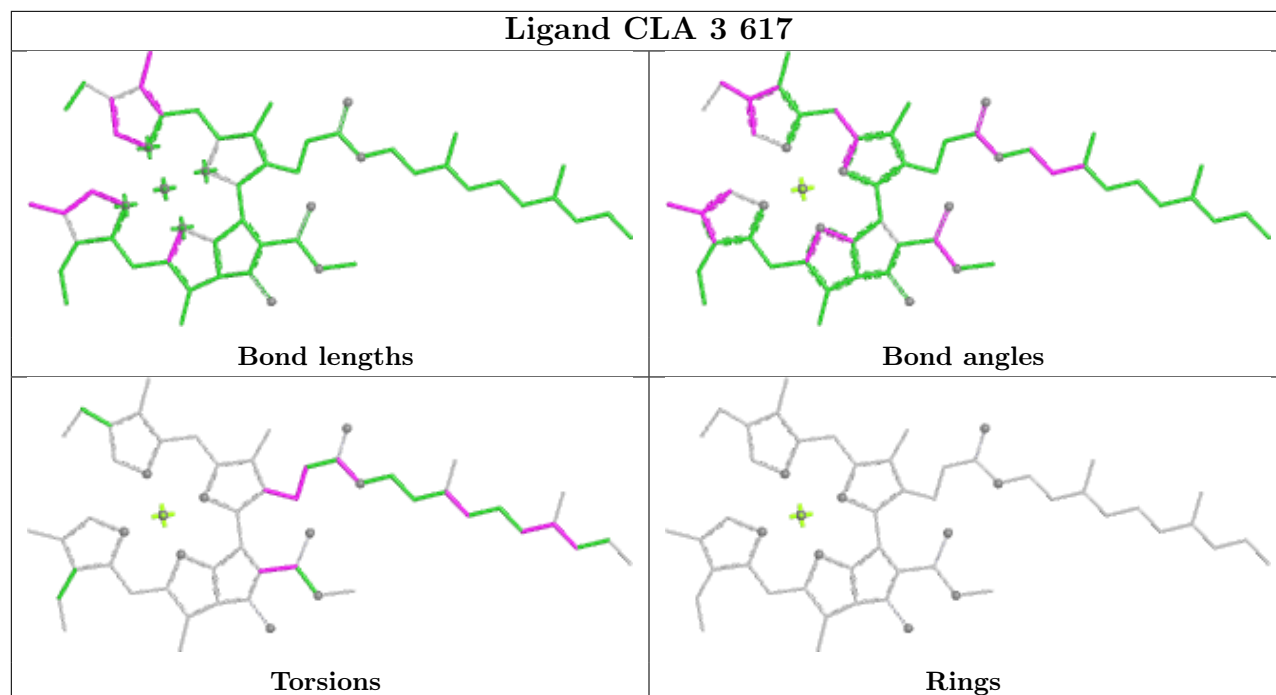
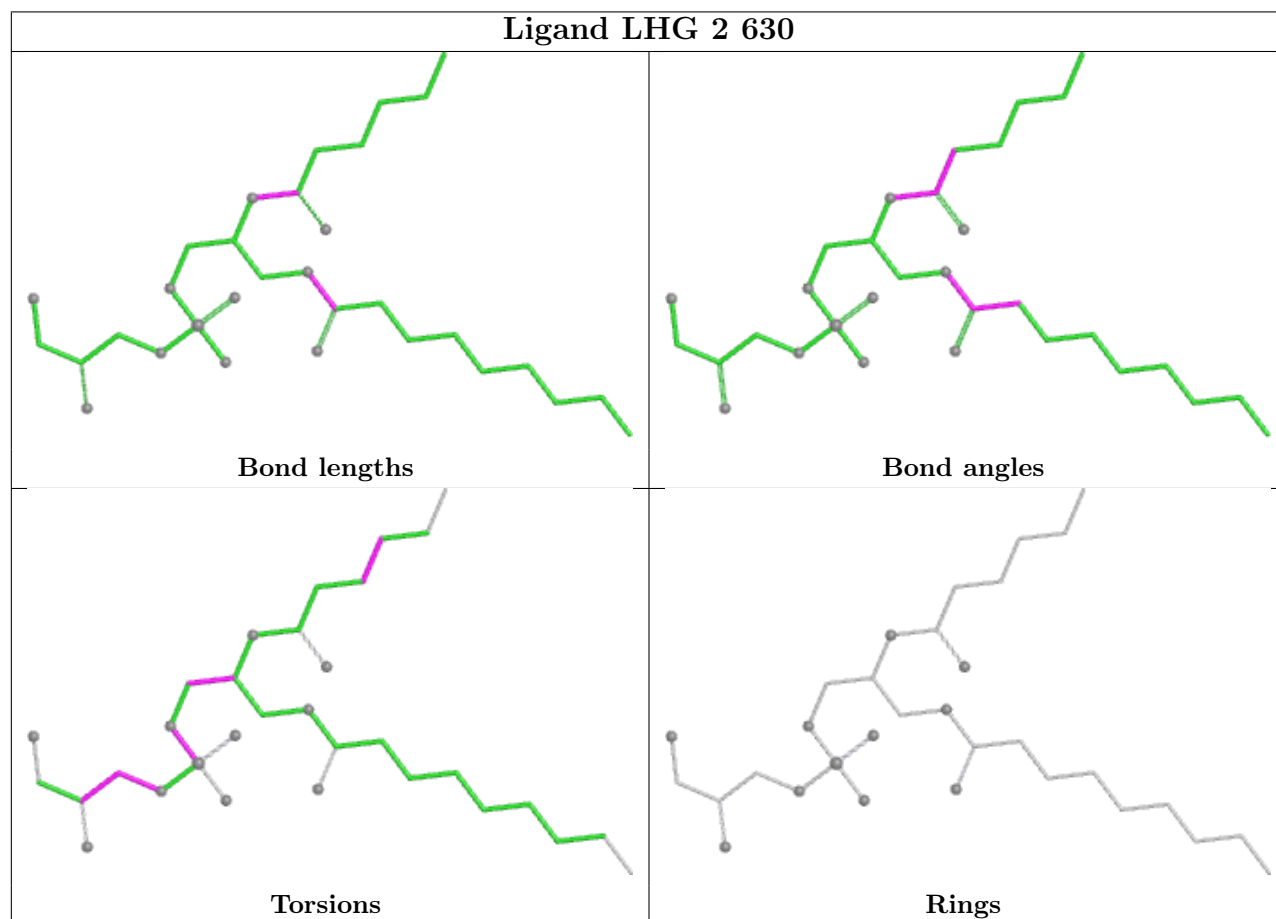
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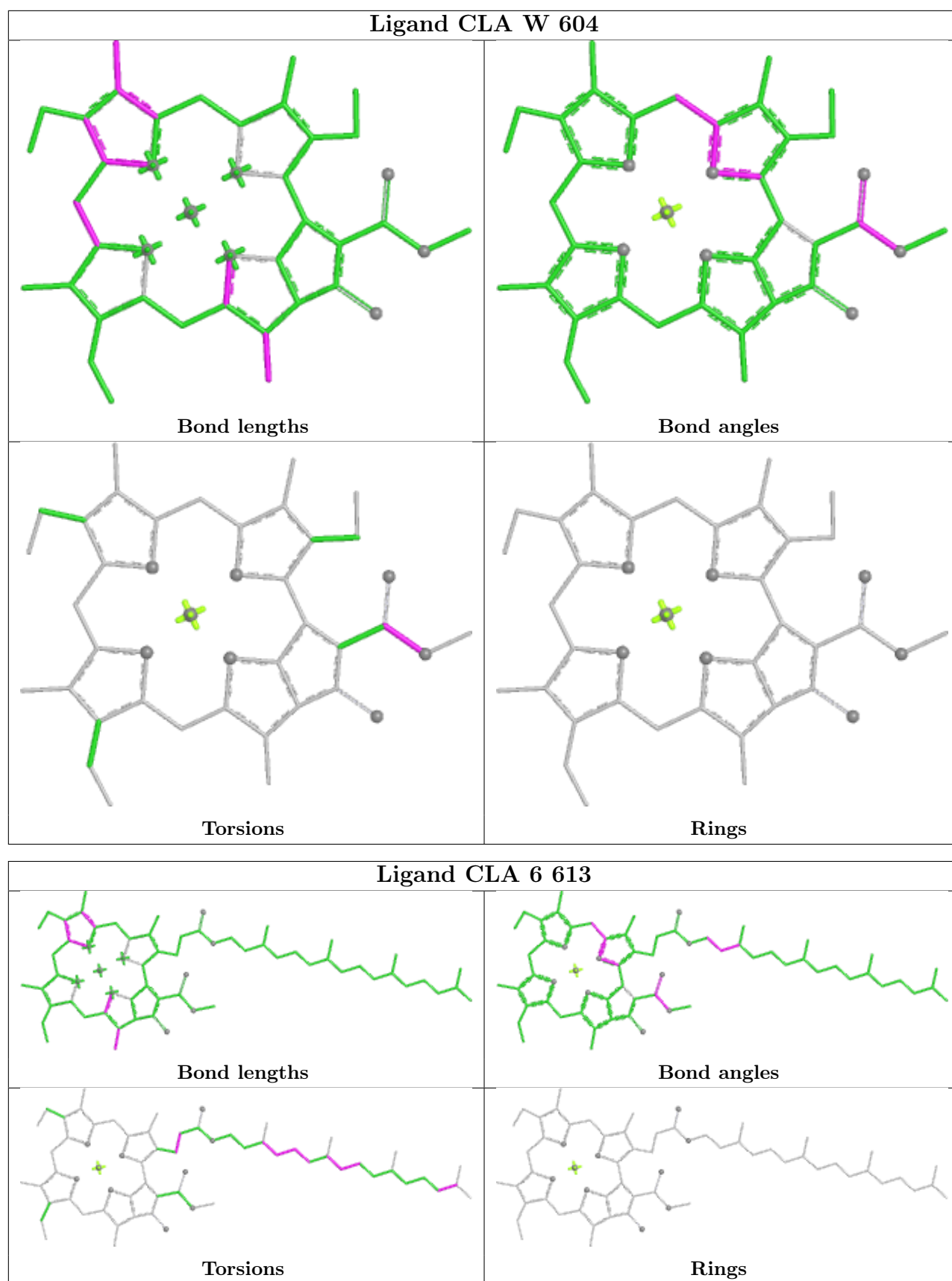


Ligand CLA A 834

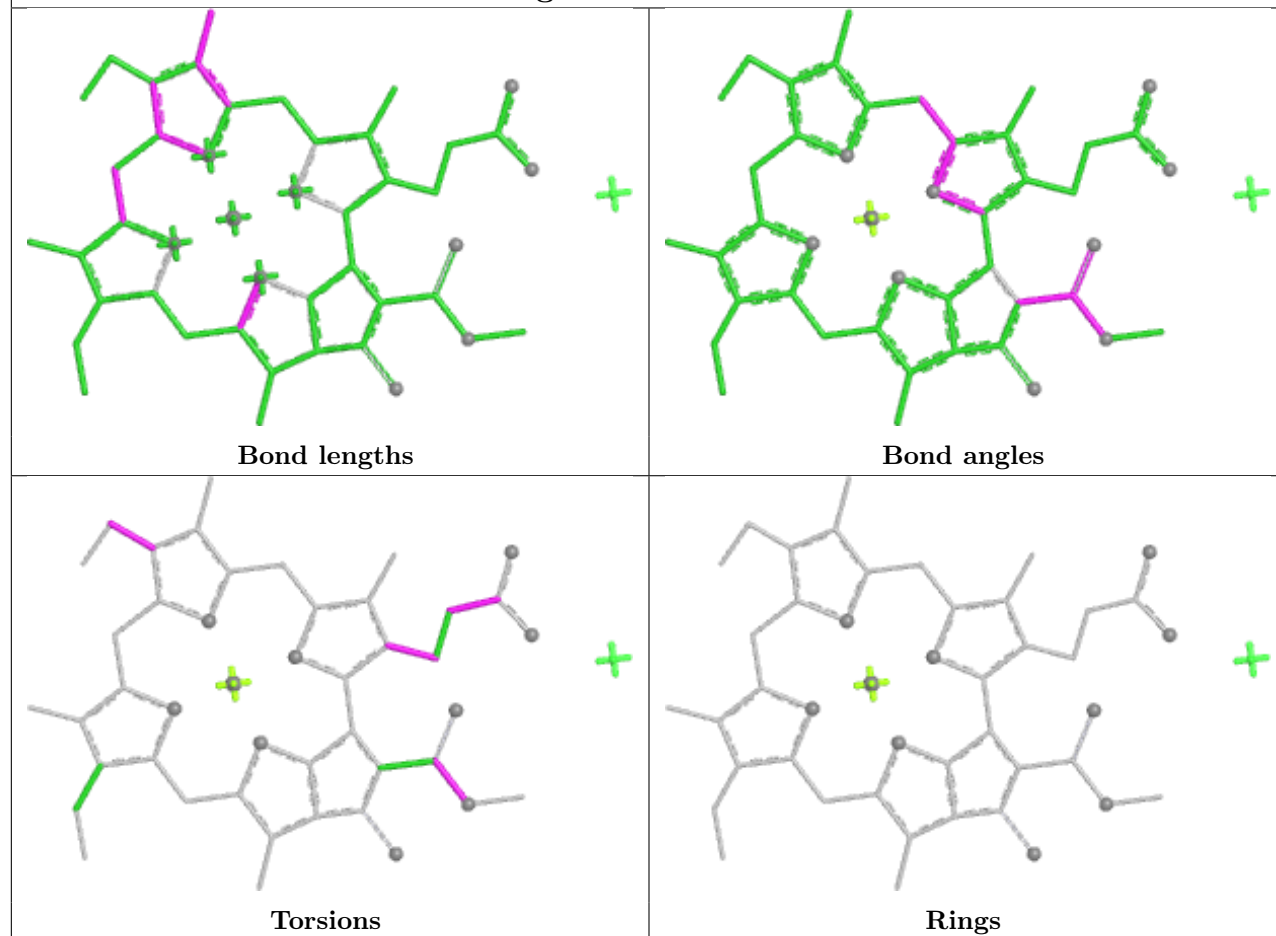




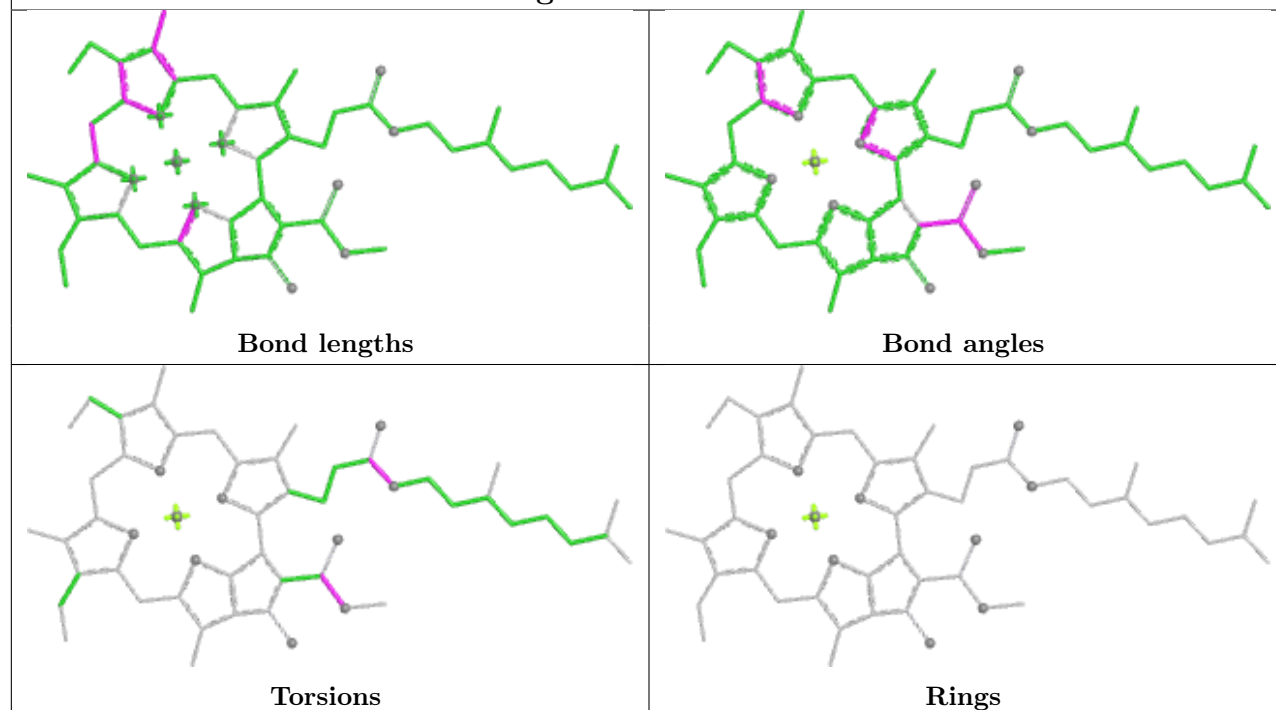
Ligand CLA 3 617**Ligand LHG 2 630**



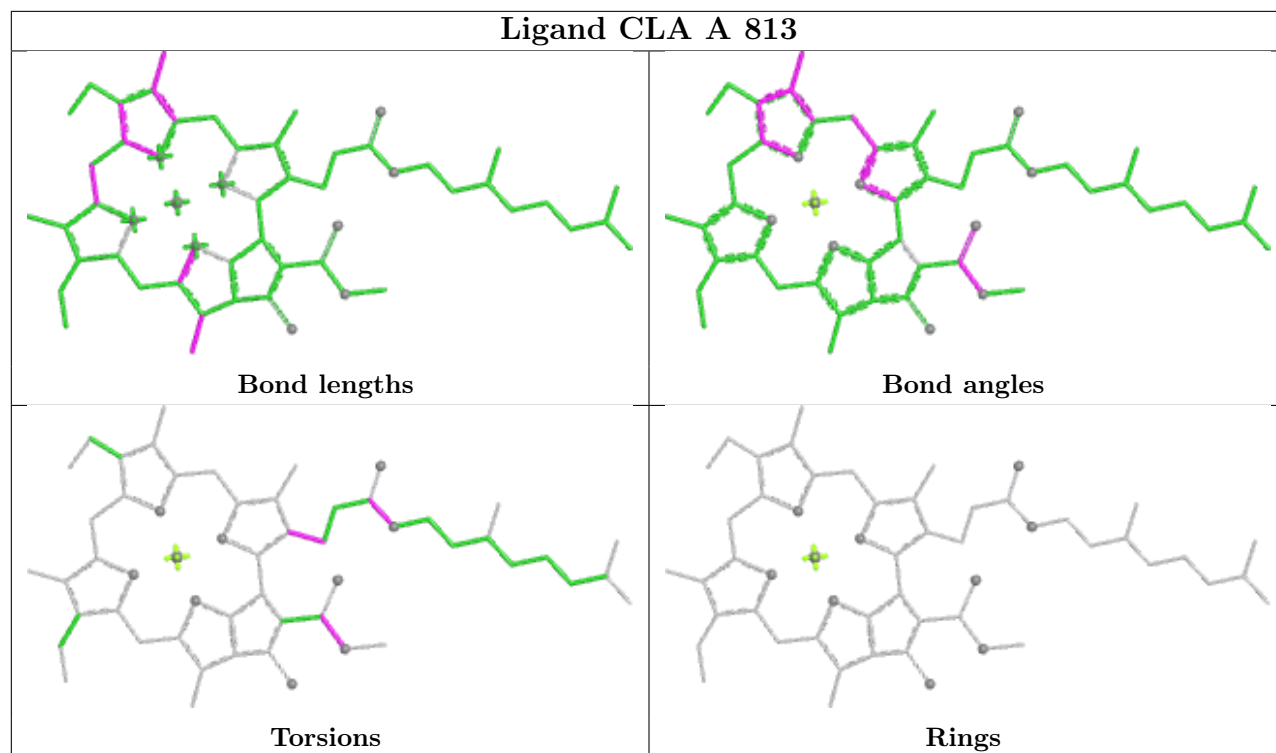
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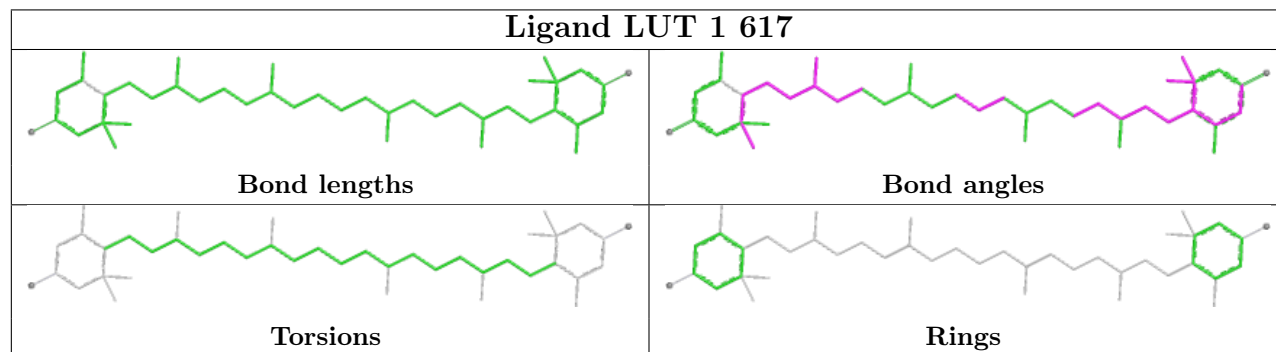
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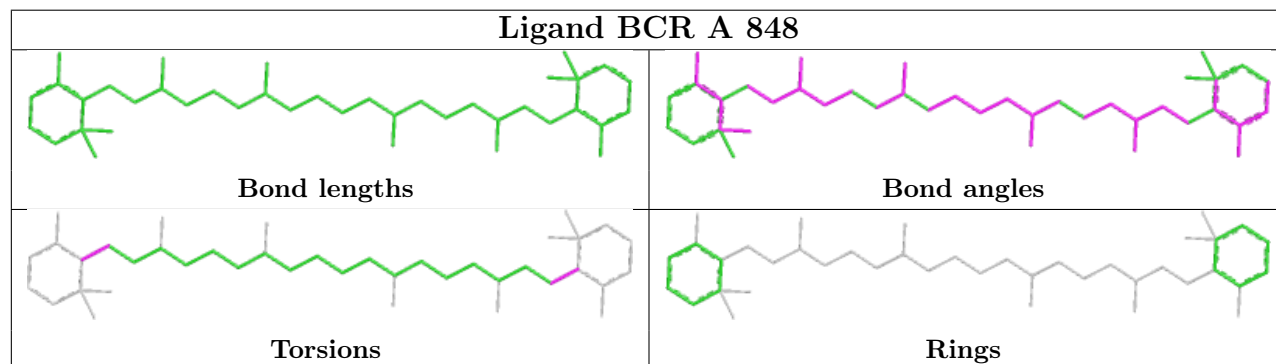
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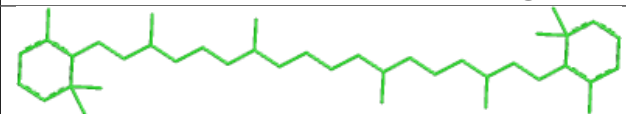
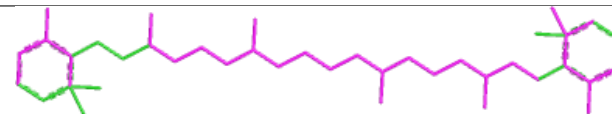
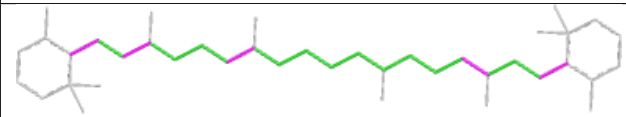
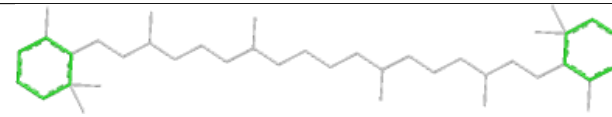


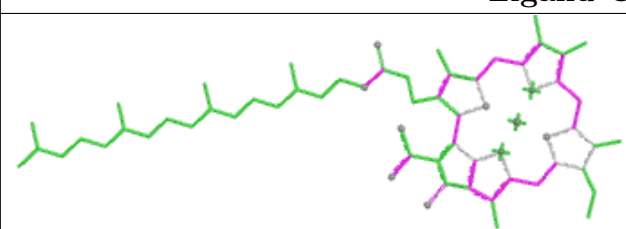
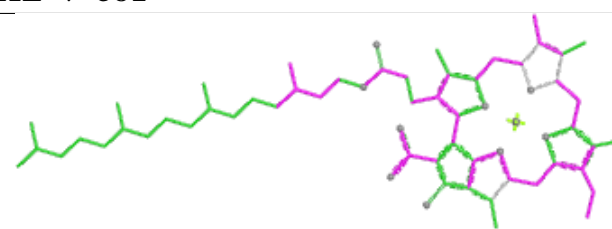
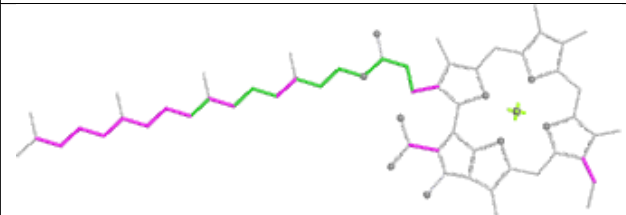
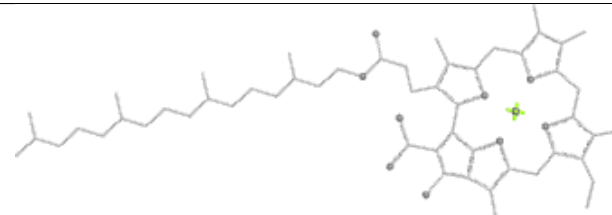
Ligand LUT 1 617

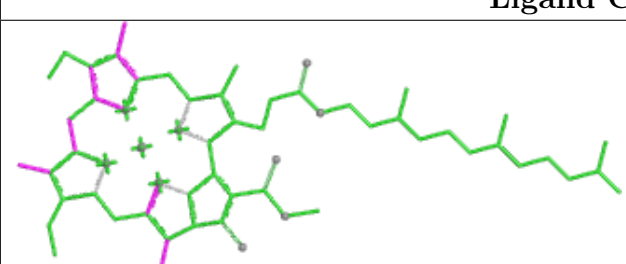
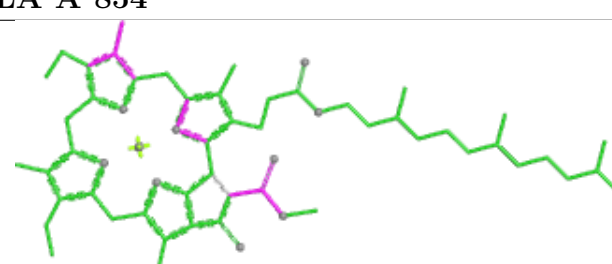
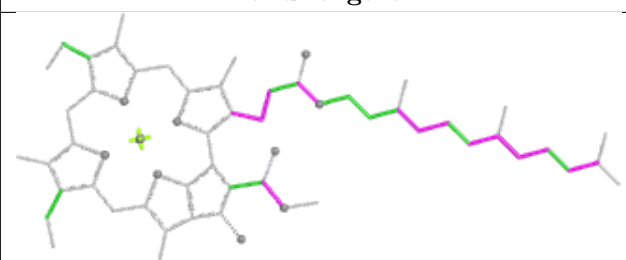
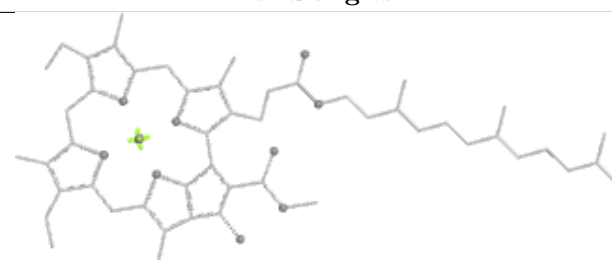


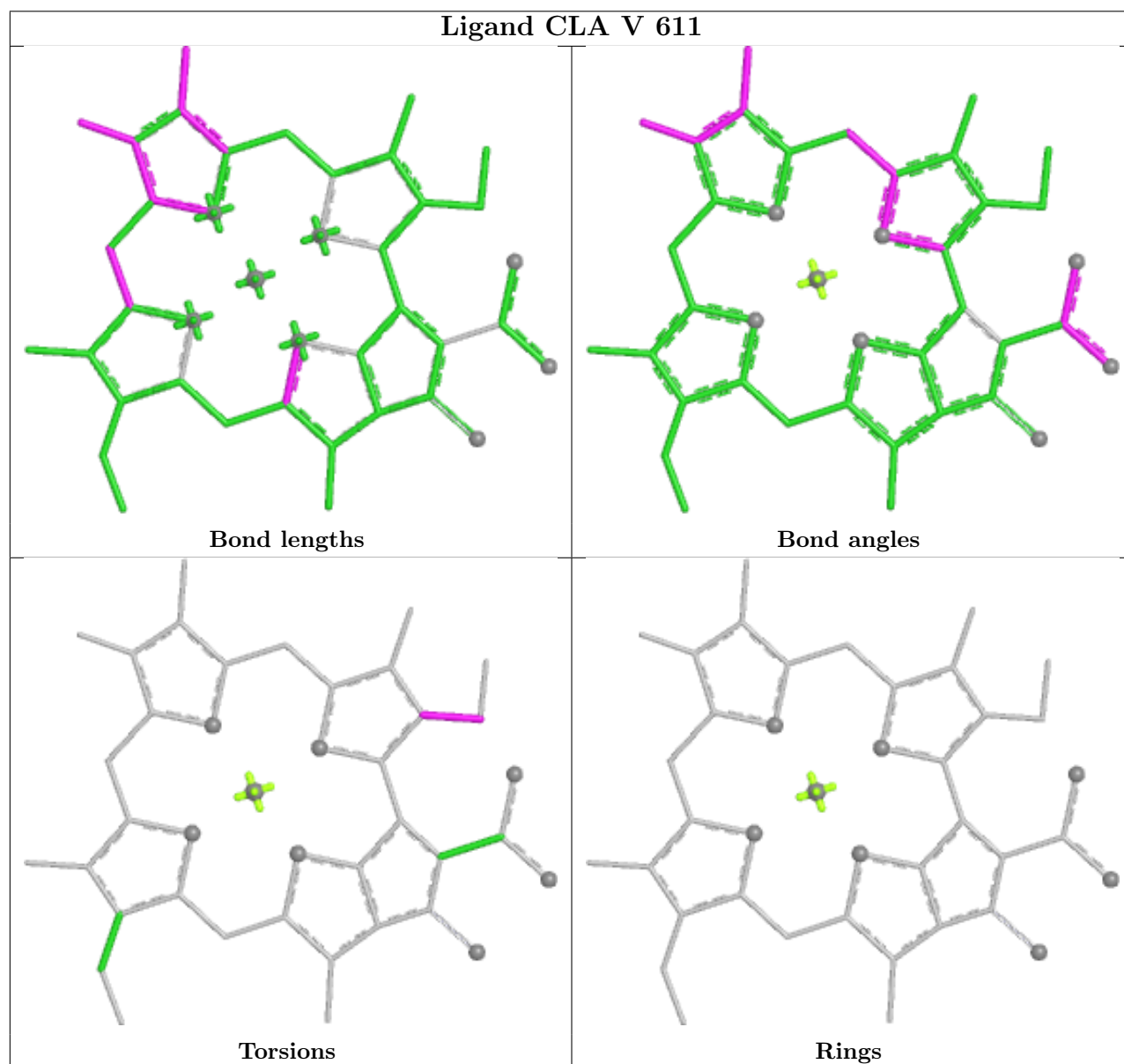
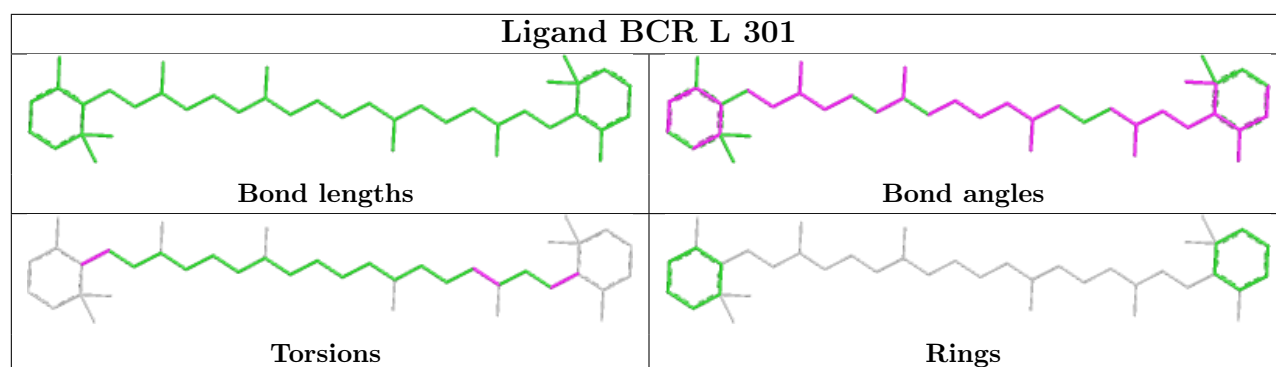
Ligand BCR A 848



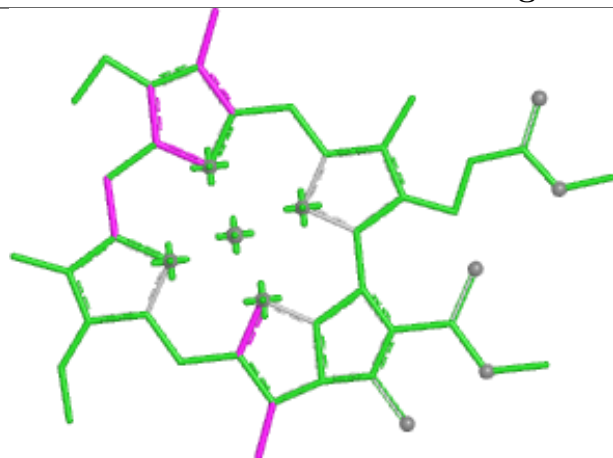
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL V 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

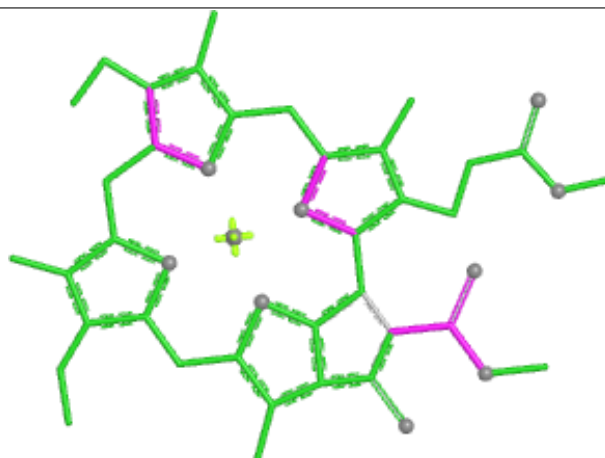
Ligand CLA A 854	
	
Bond lengths	Bond angles
	
Torsions	Rings



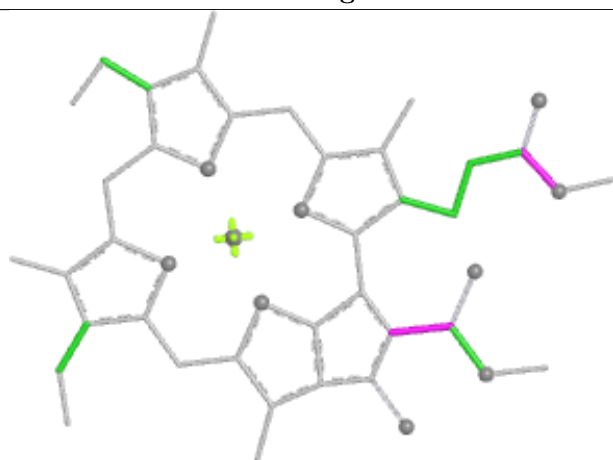
Ligand CLA 5 611



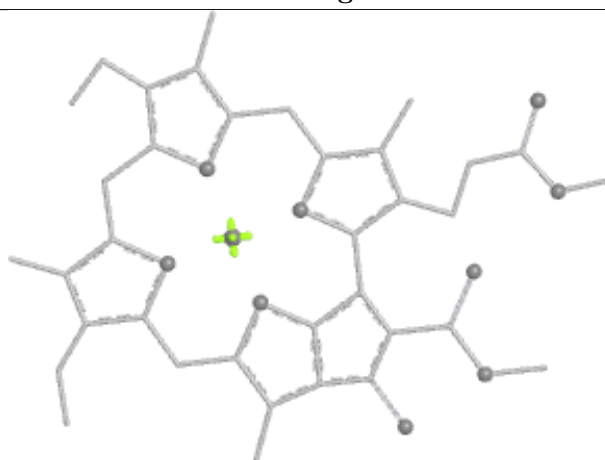
Bond lengths



Bond angles

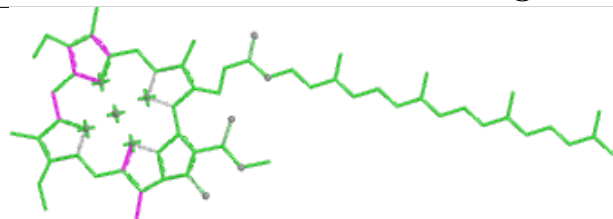


Torsions

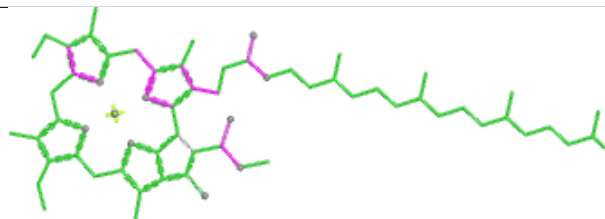


Rings

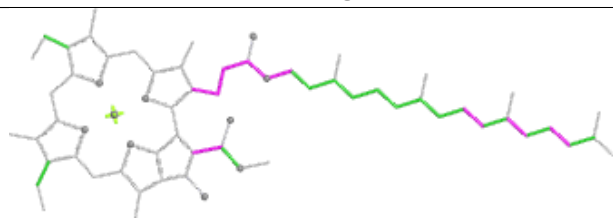
Ligand CLA A 806



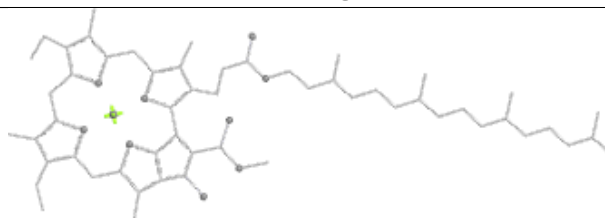
Bond lengths



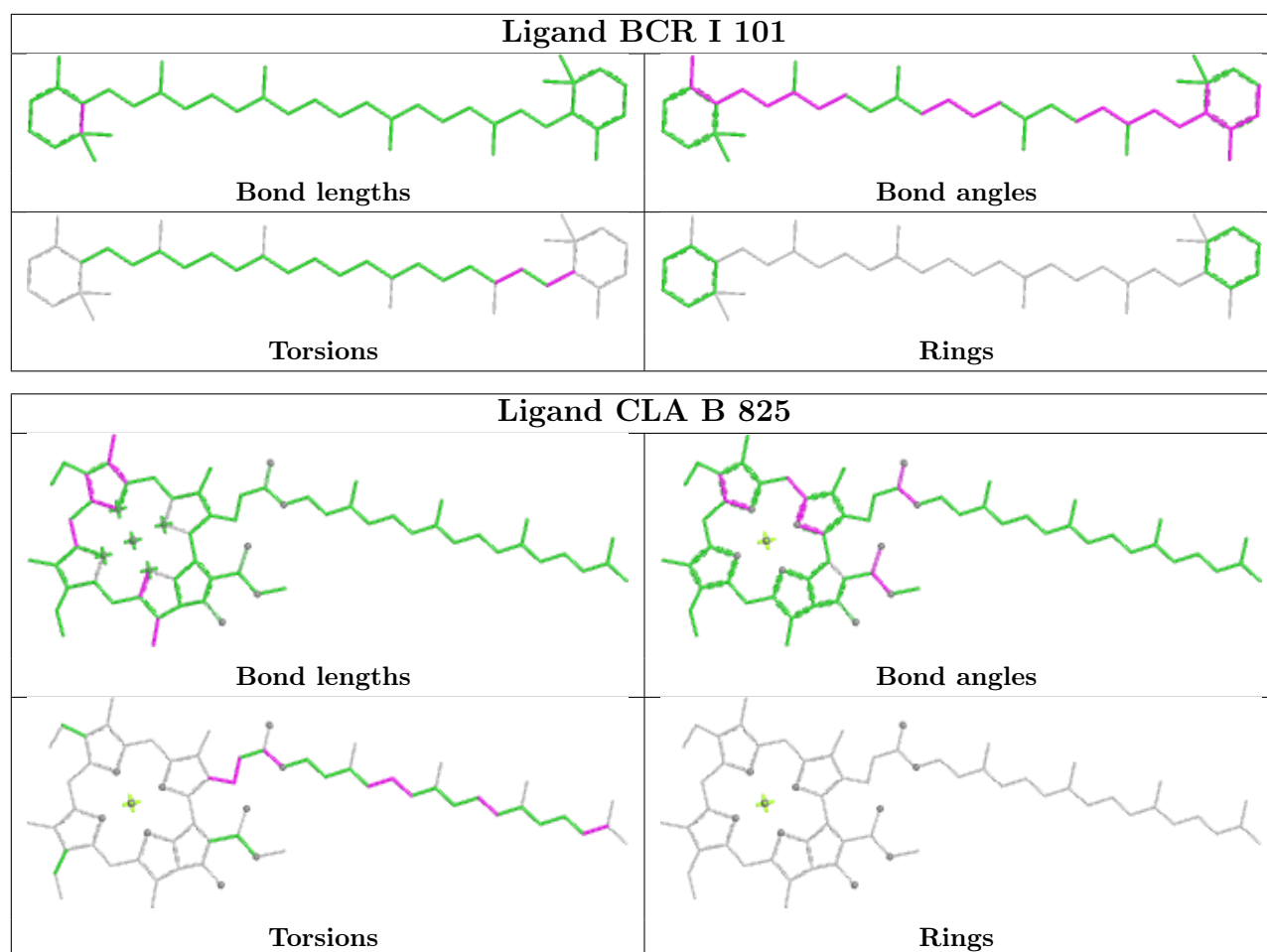
Bond angles



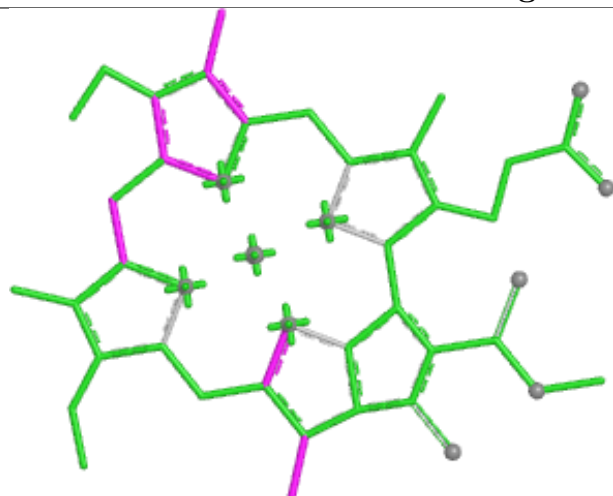
Torsions



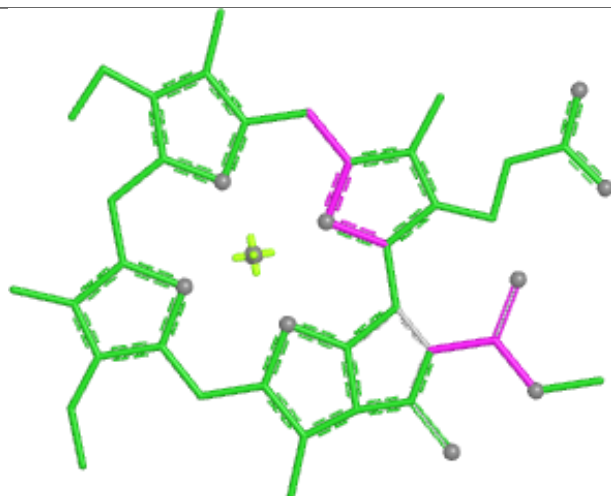
Rings



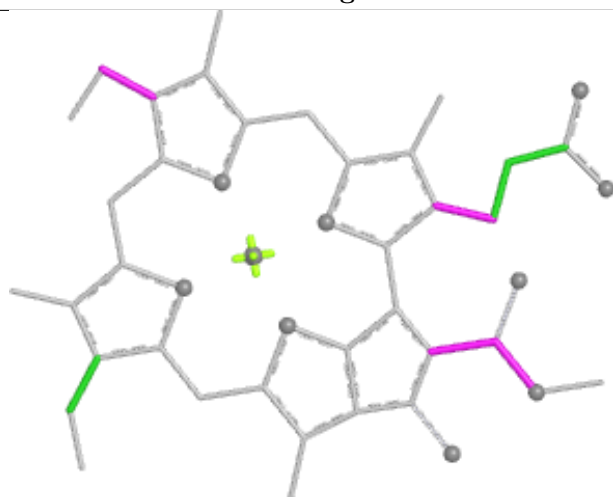
Ligand CLA 2 612



Bond lengths



Bond angles

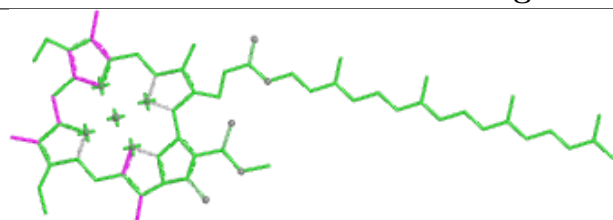


Torsions

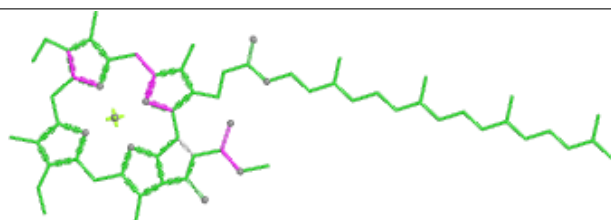


Rings

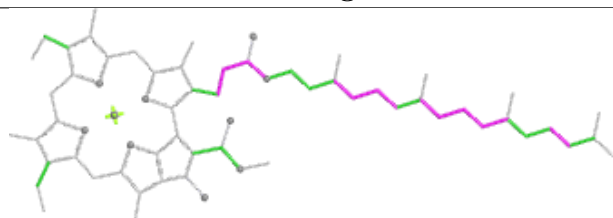
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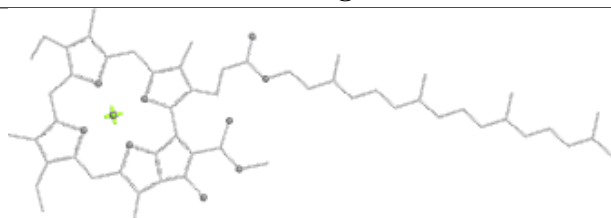
Bond lengths



Bond angles

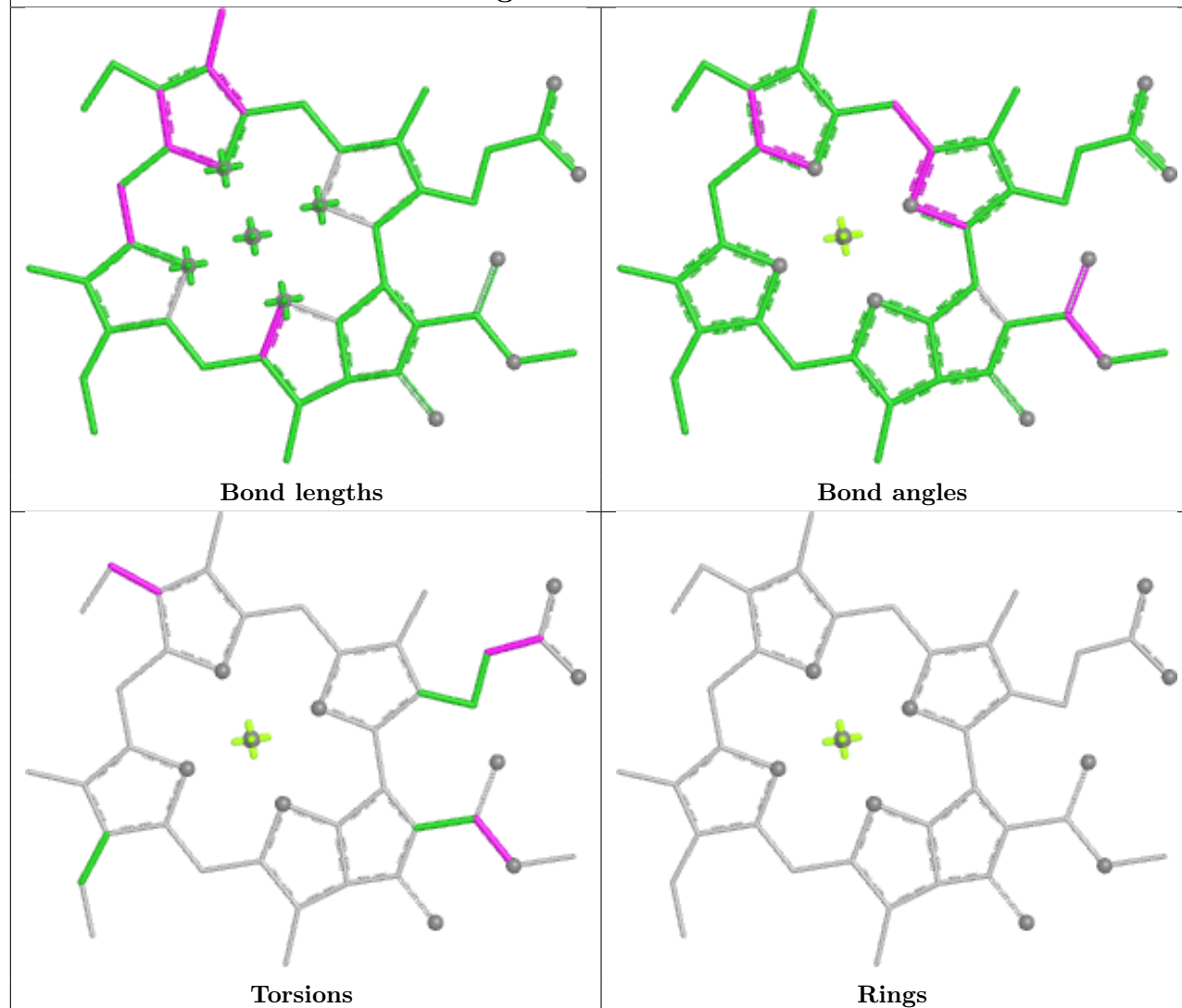


Torsions

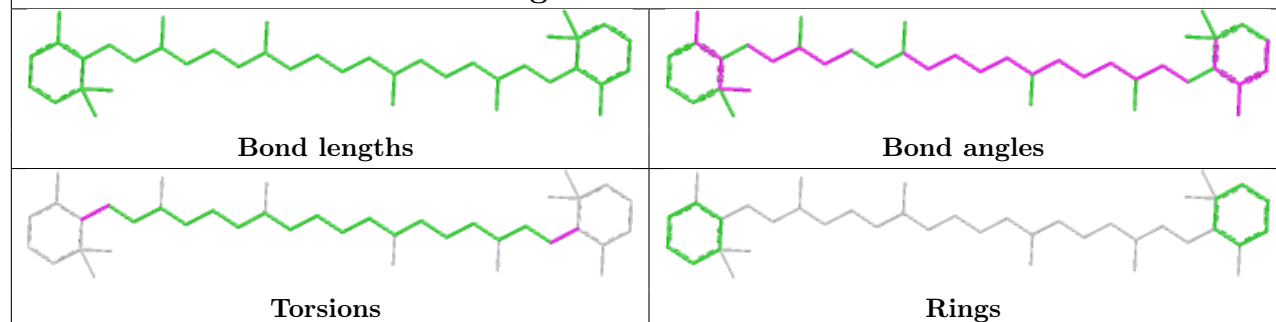


Rings

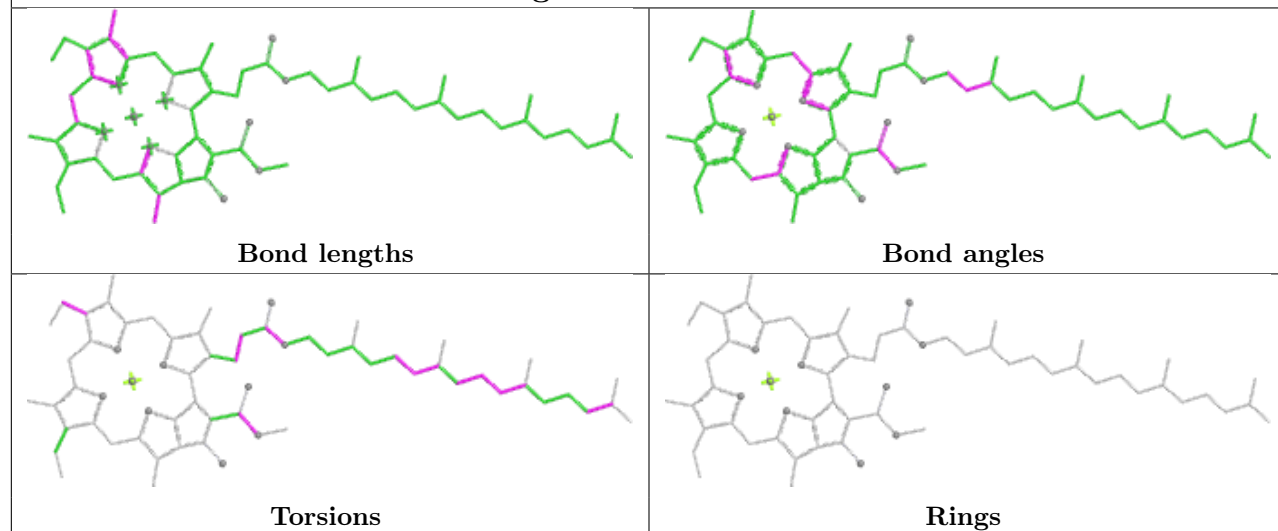
Ligand CLA 1 606



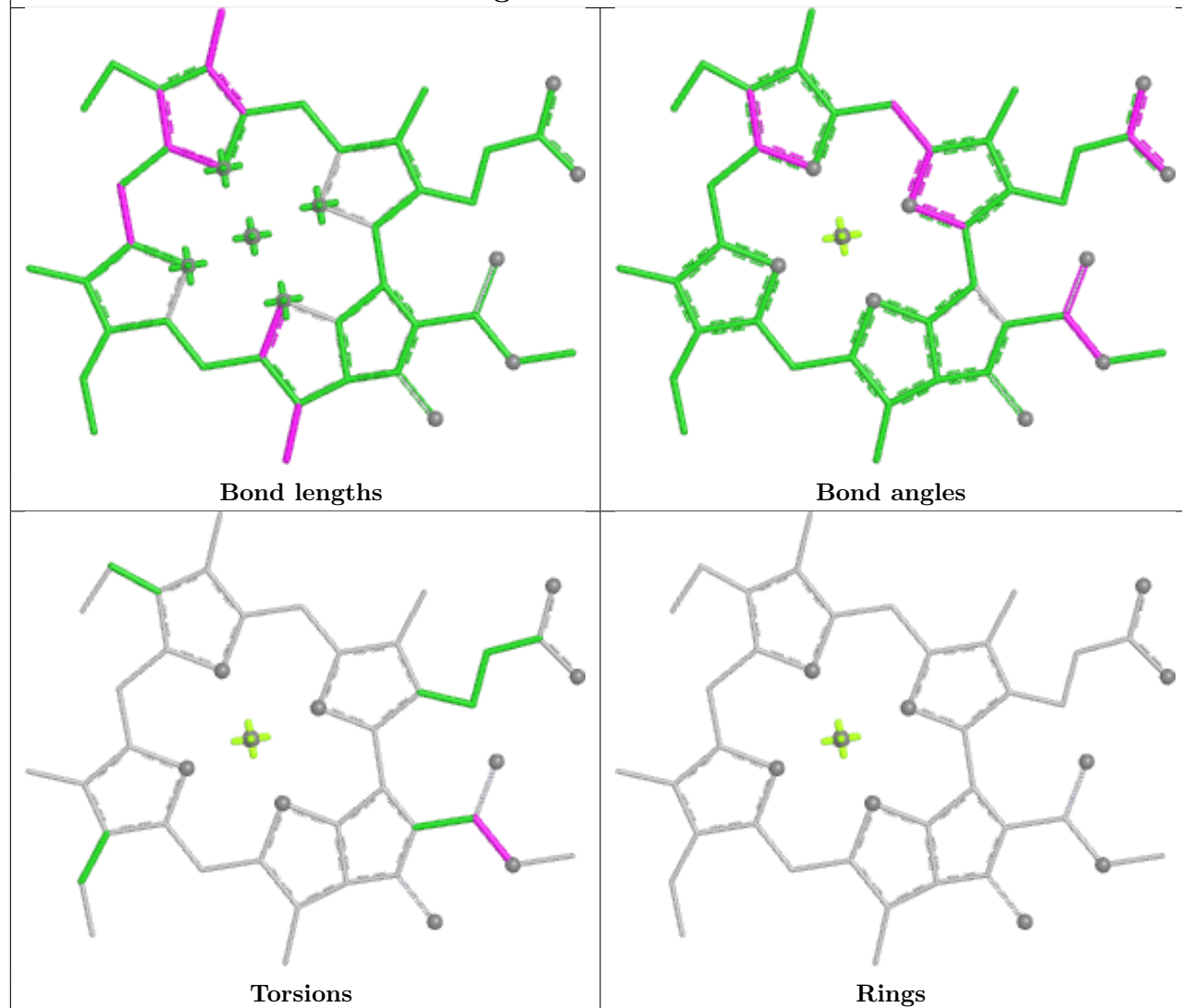
Ligand BCR A 850

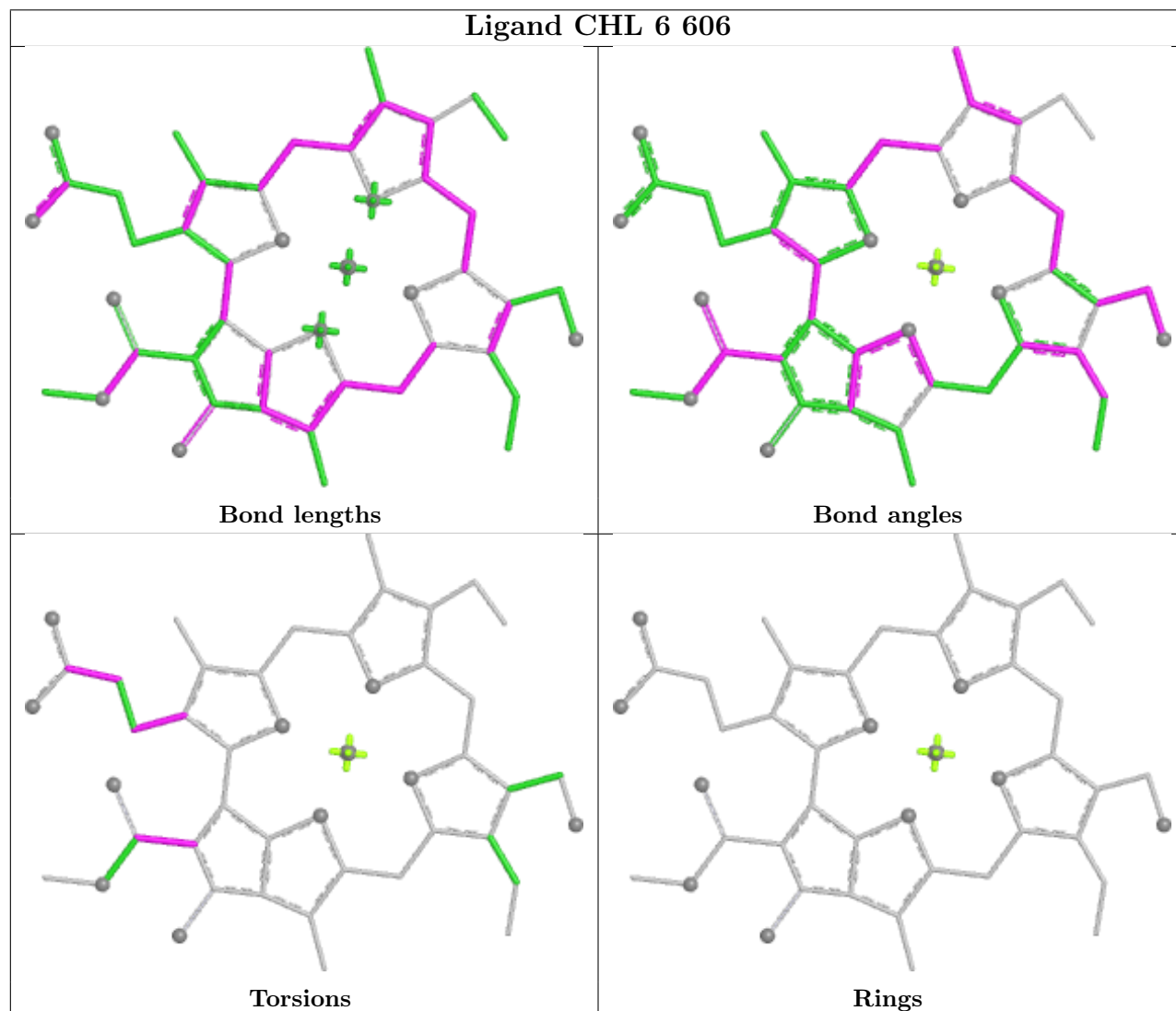
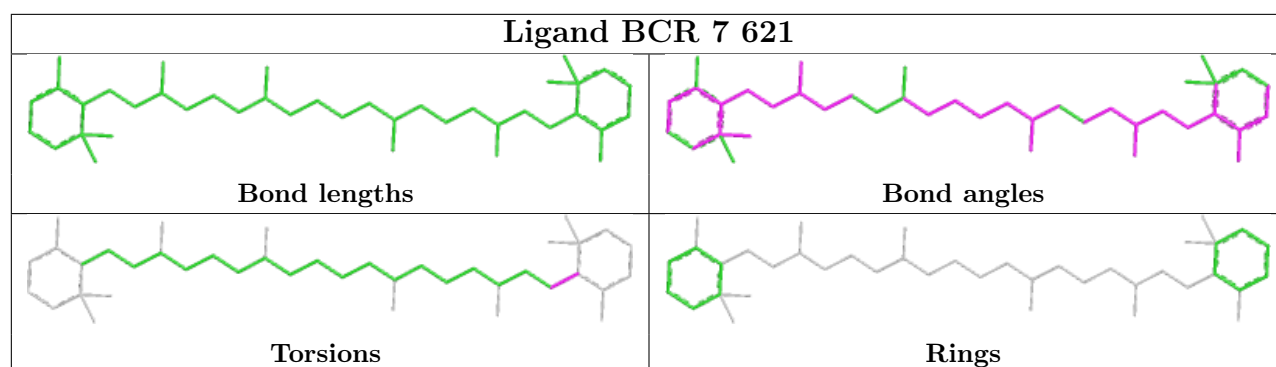


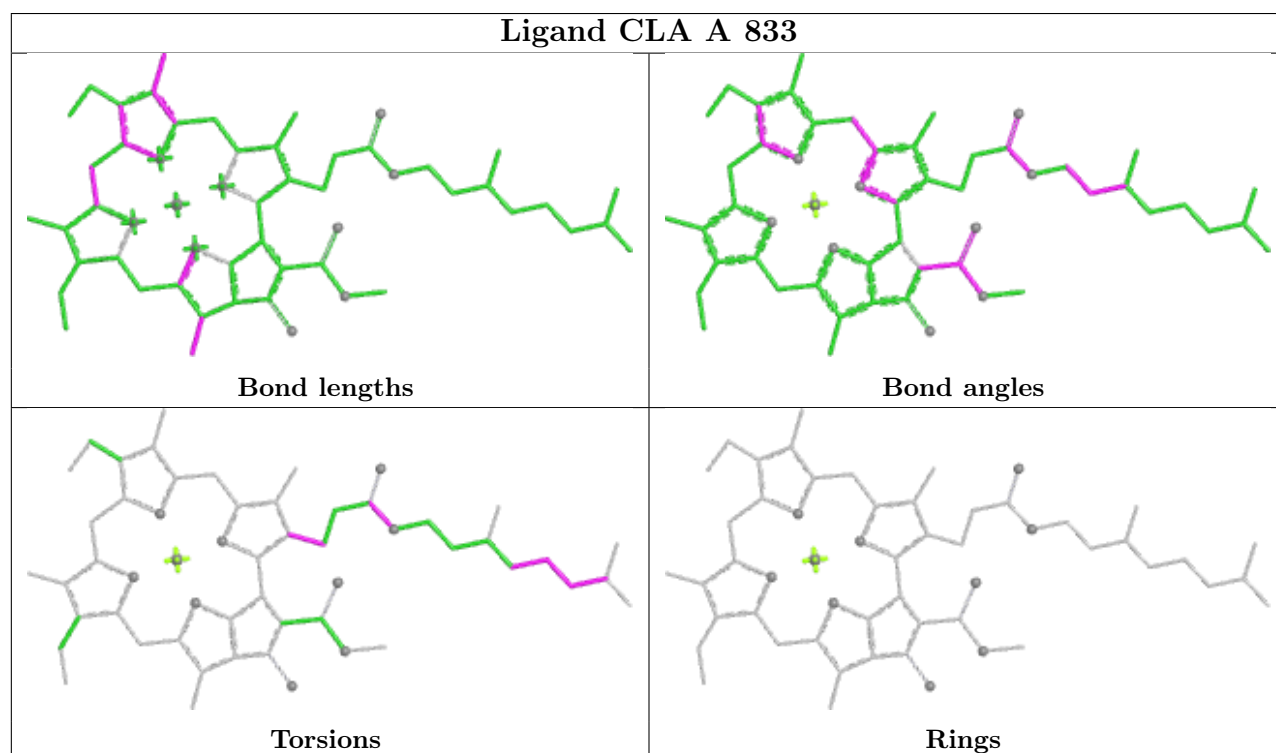
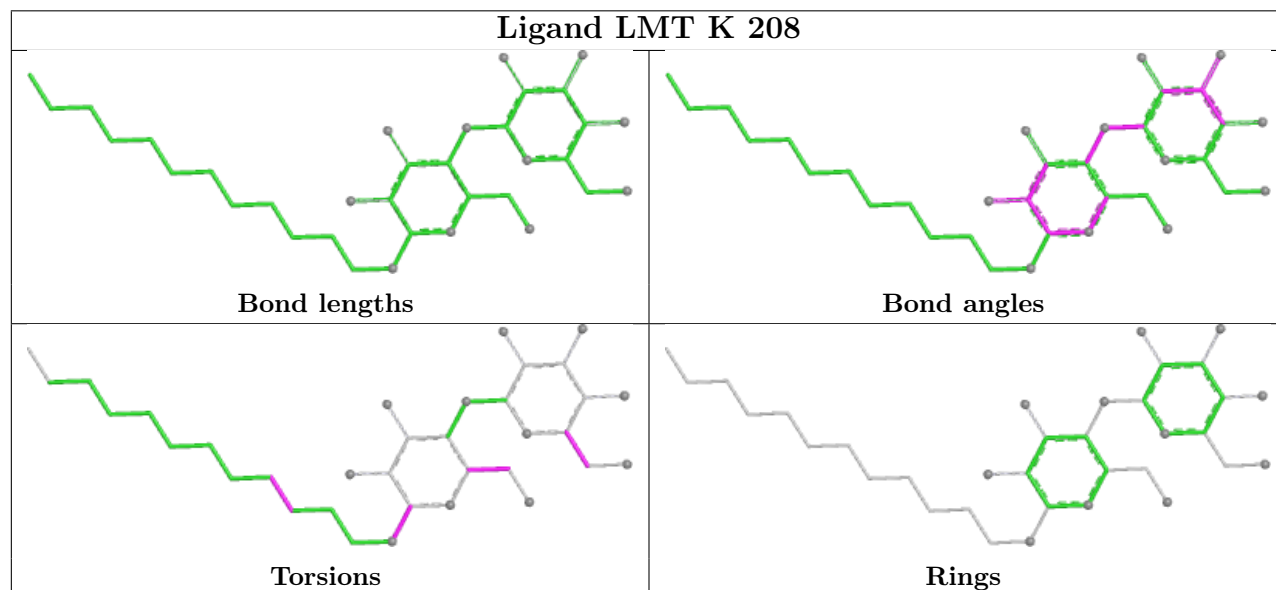
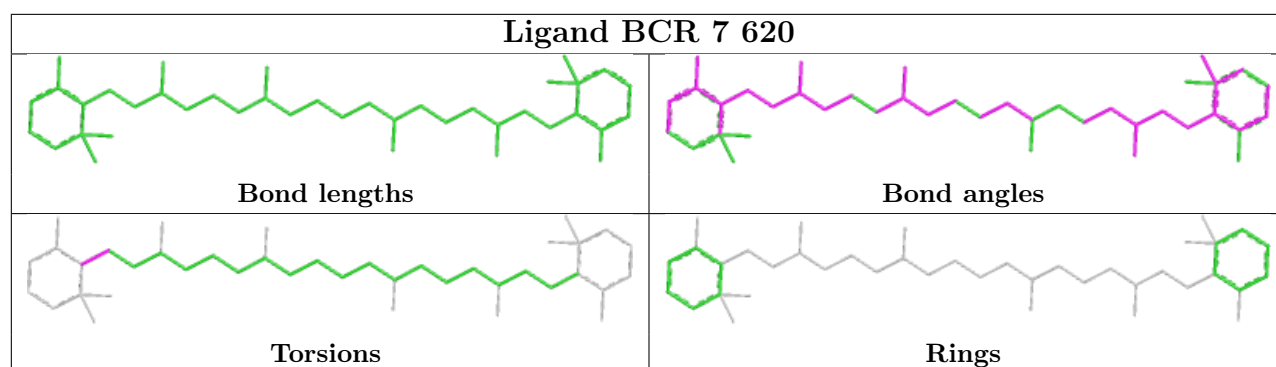
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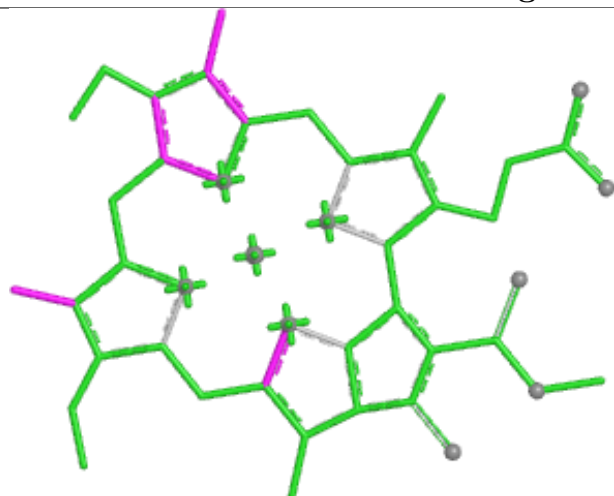
Ligand CLA F 303



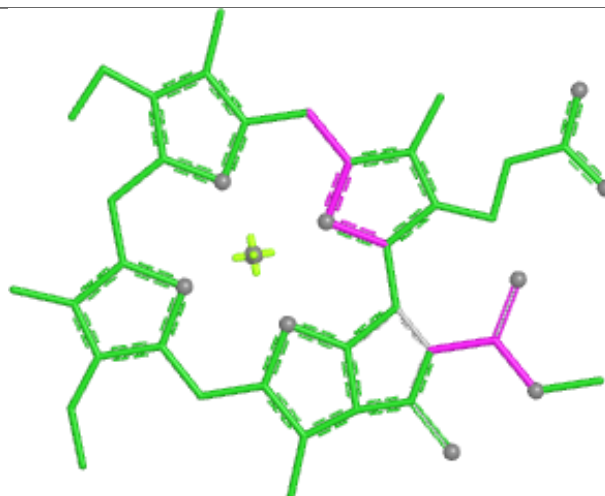




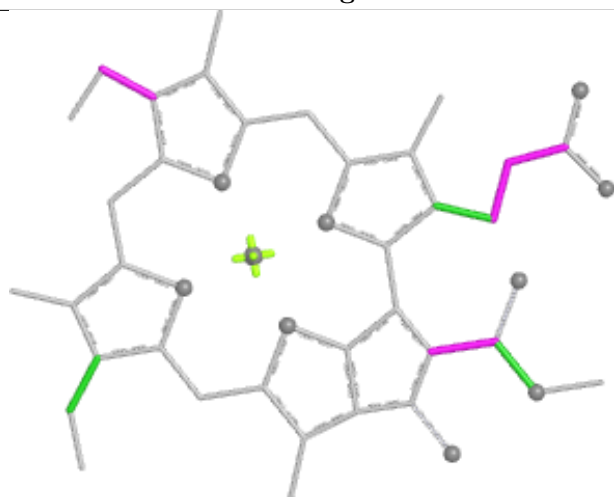
Ligand CLA 4 612



Bond lengths



Bond angles

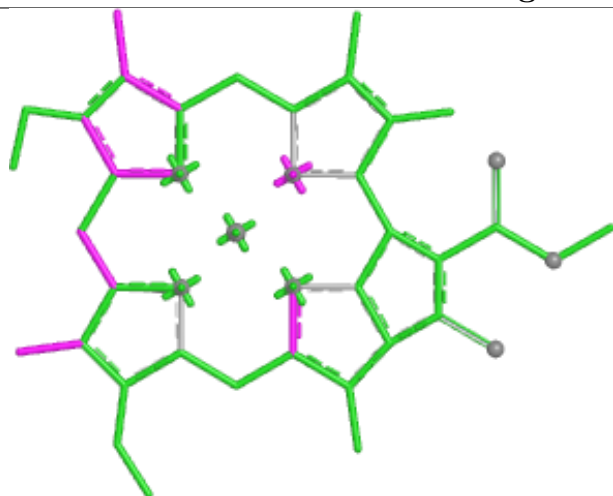


Torsions

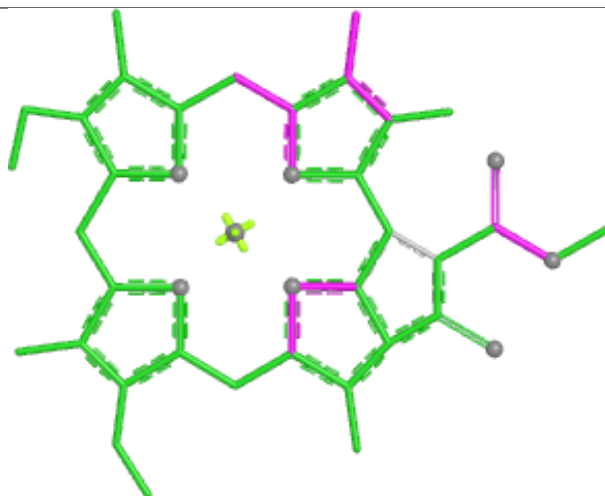


Rings

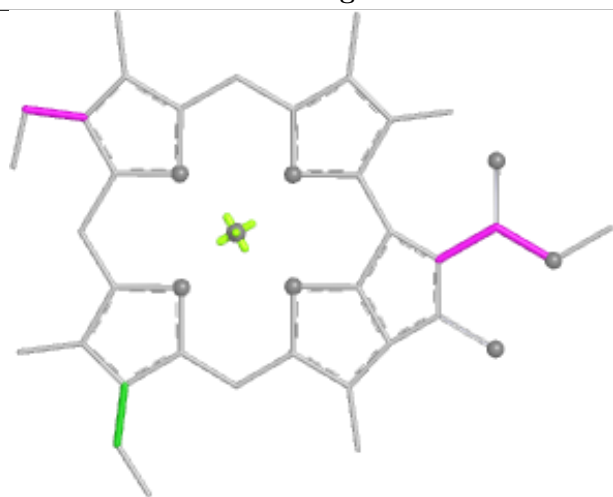
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Bond lengths



Bond angles

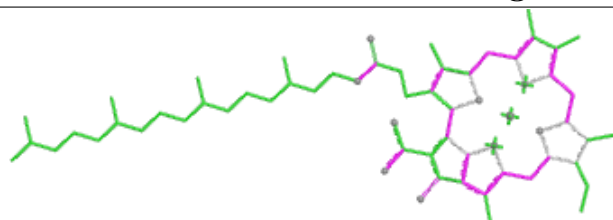


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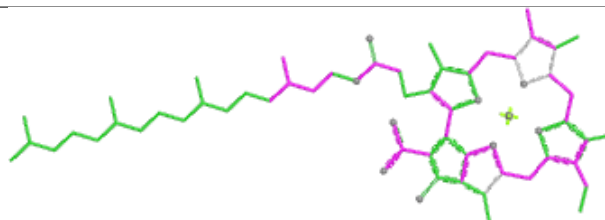


Rings

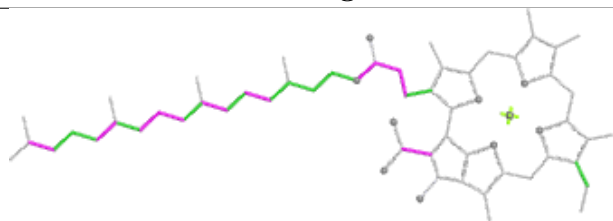
Ligand CHL W 601



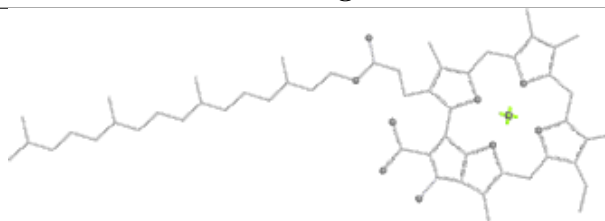
Bond lengths



Bond angles

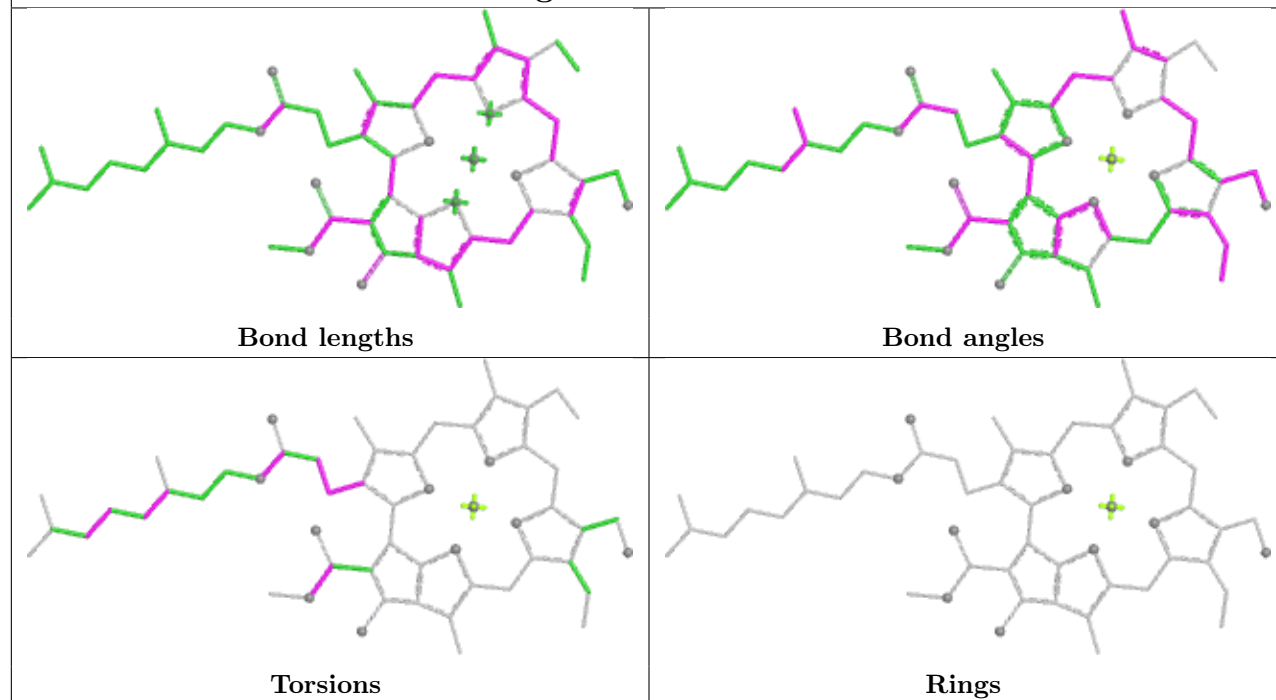


Torsions

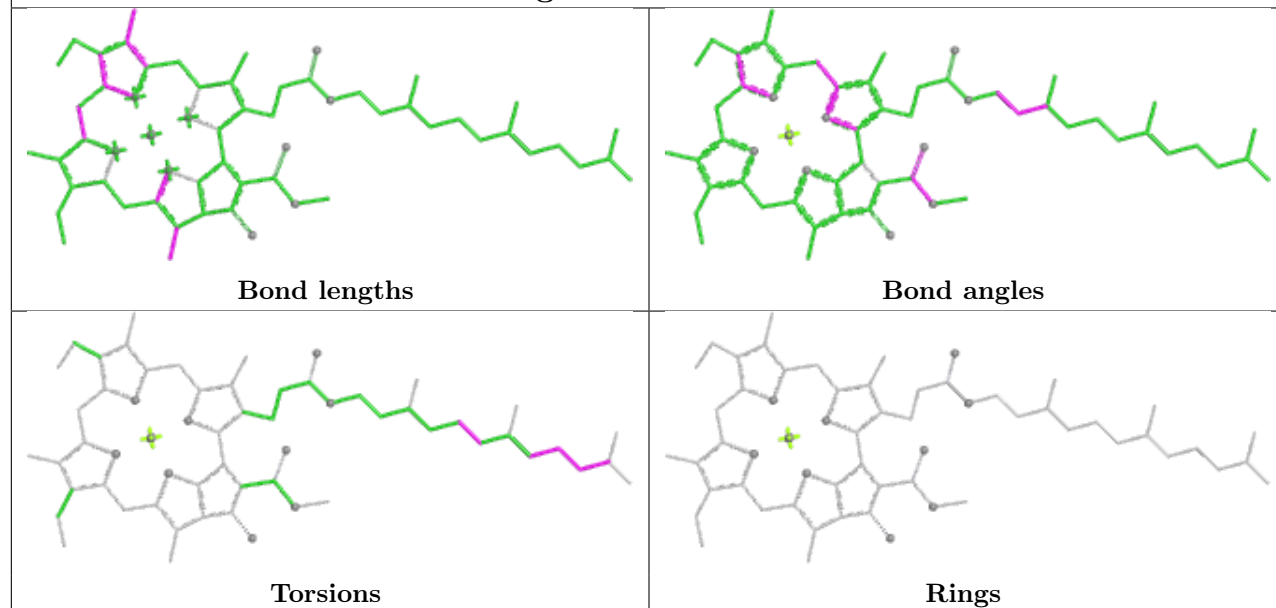


Rings

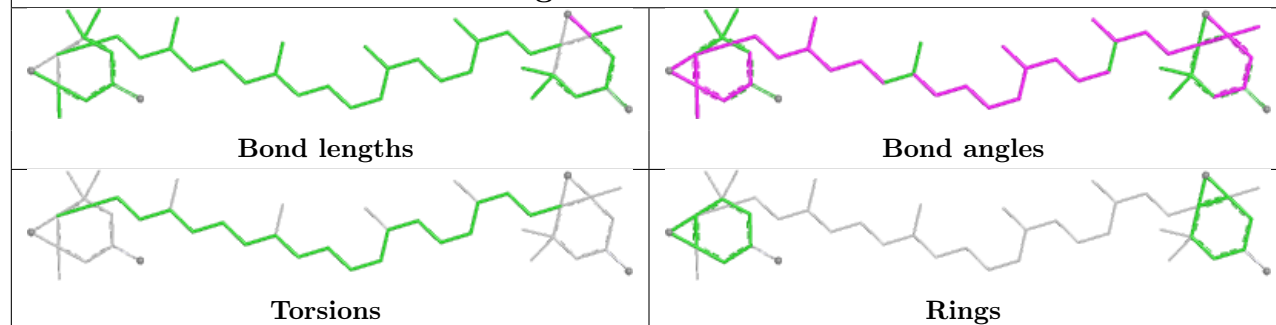
Ligand CHL 3 608

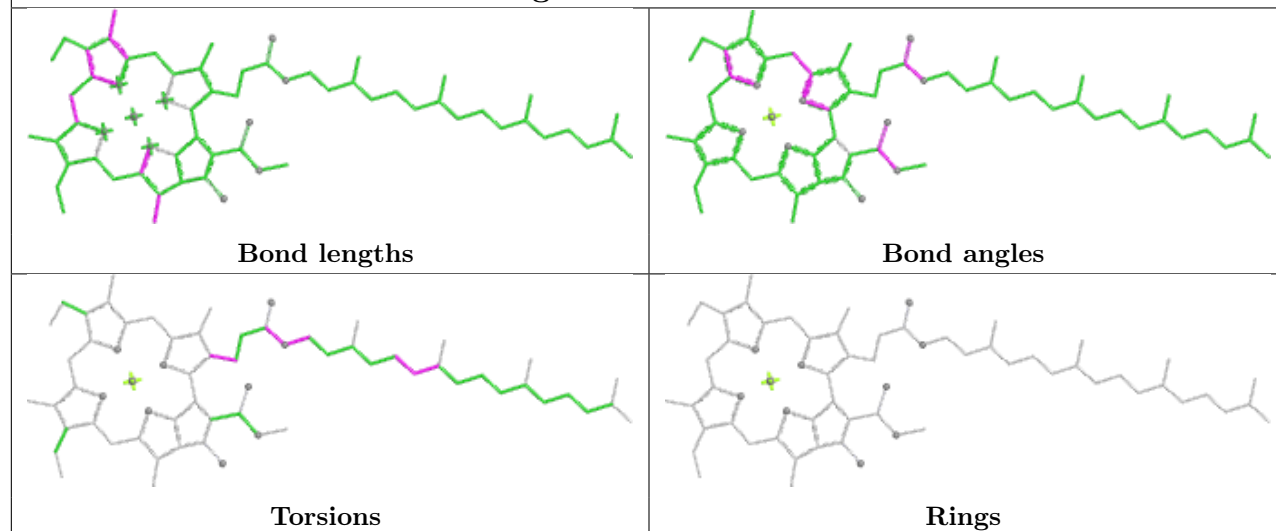
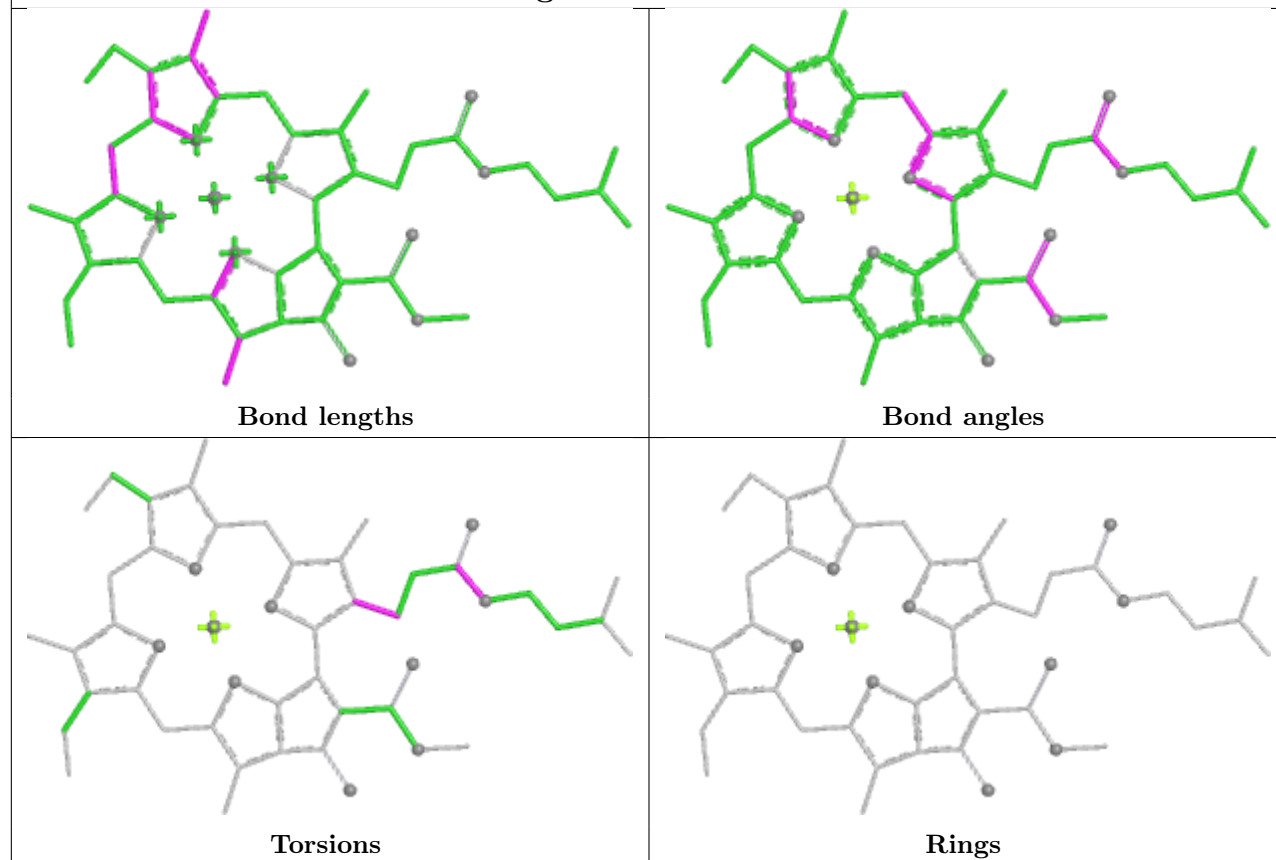


Ligand CLA 2 610

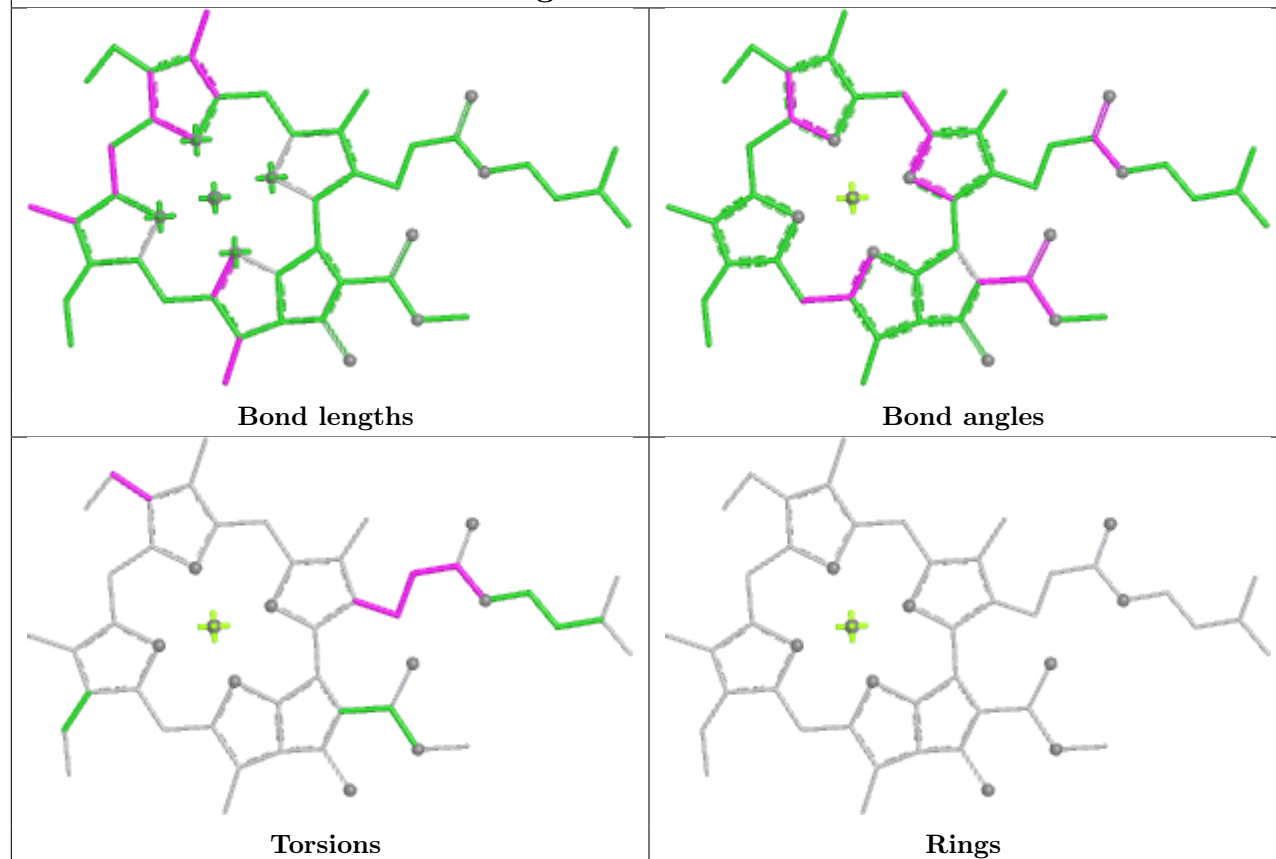


Ligand XAT 3 619

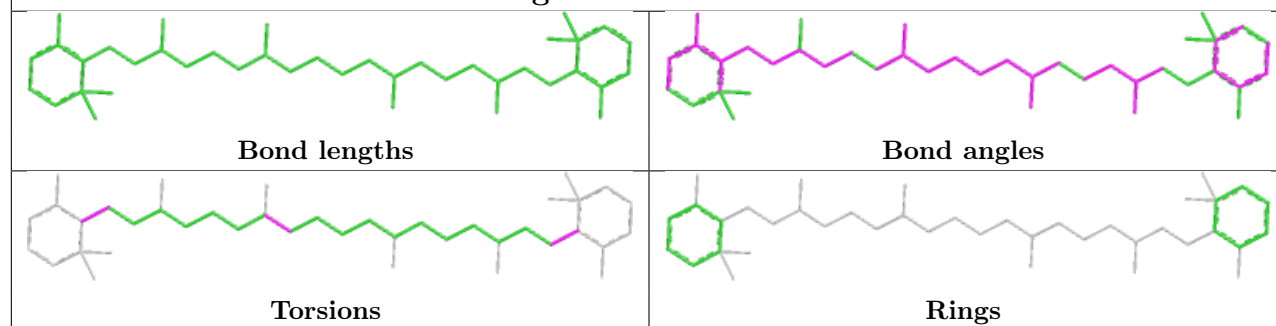


Ligand CLA B 839**Ligand CLA 2 614**

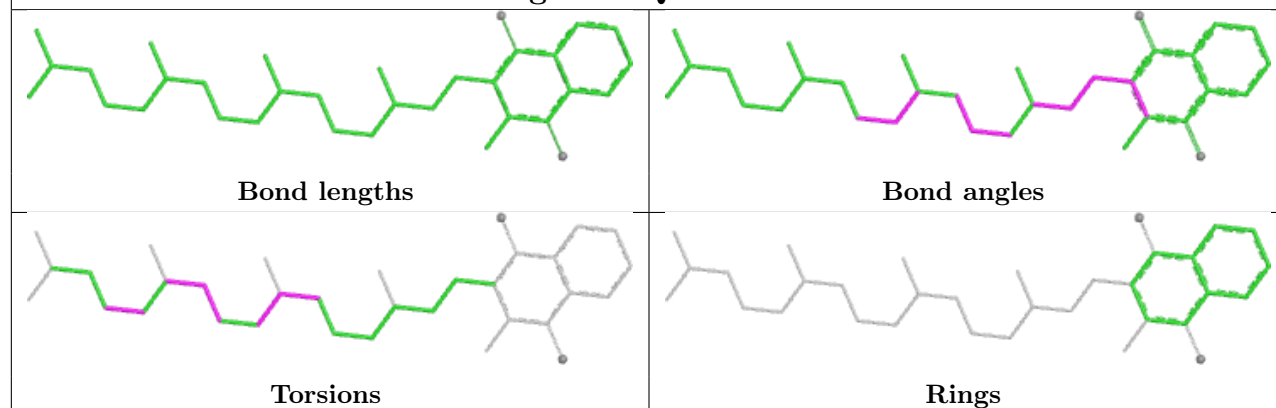
Ligand CLA 3 607



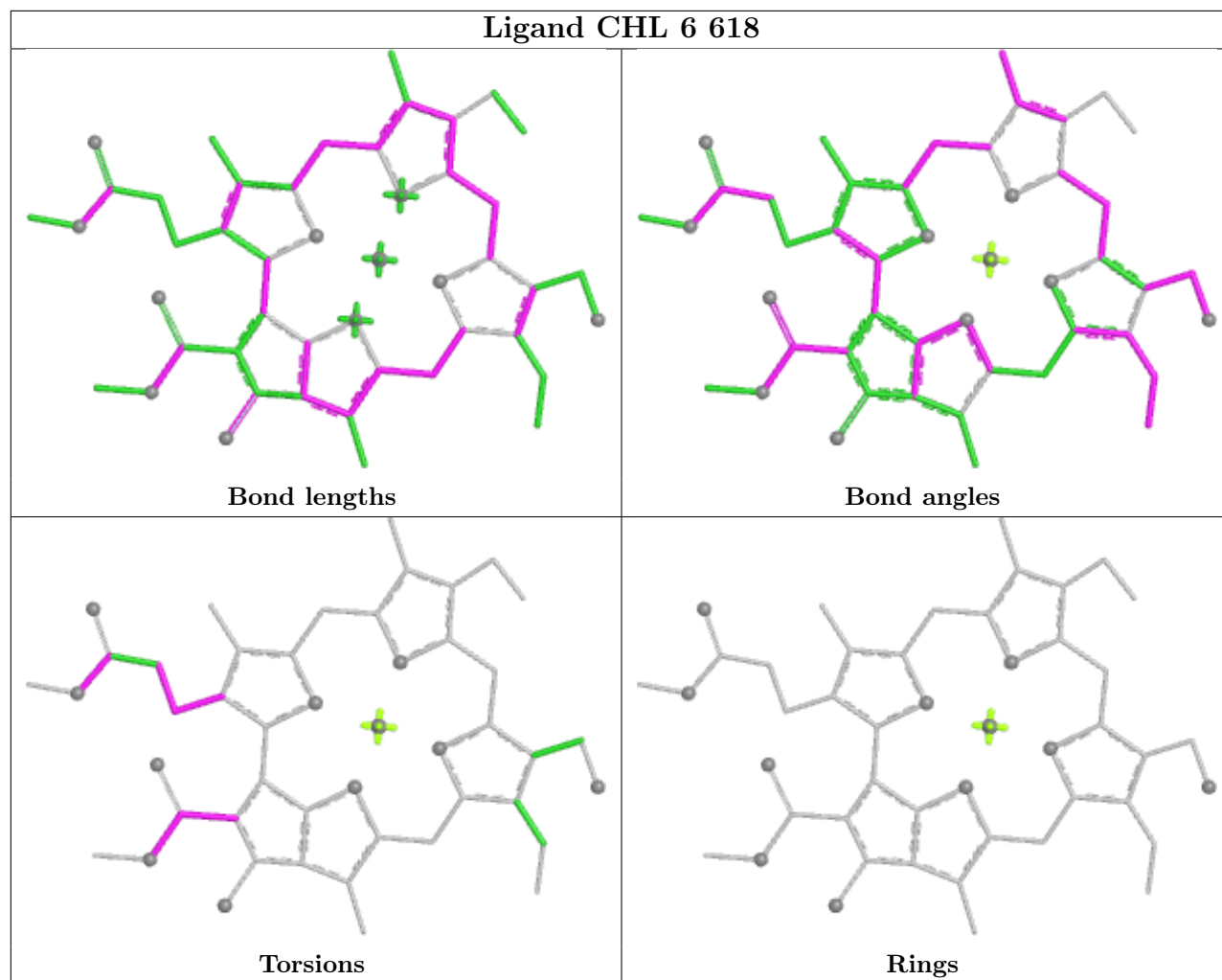
Ligand BCR F 305



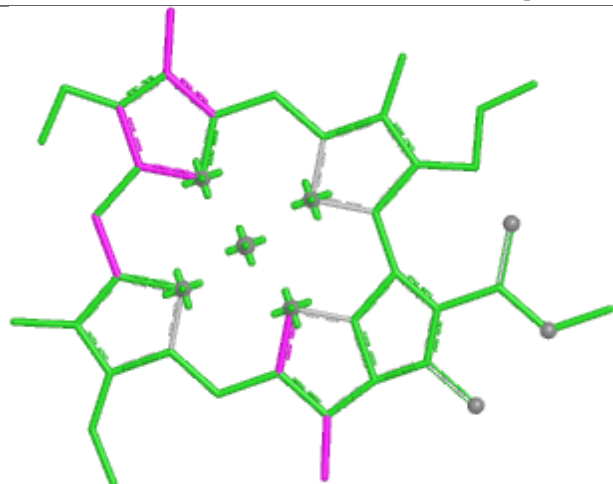
Ligand PQN A 844



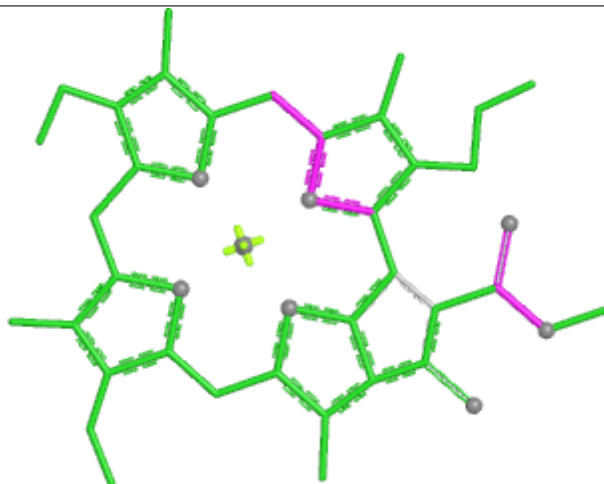
Ligand CHL 6 618



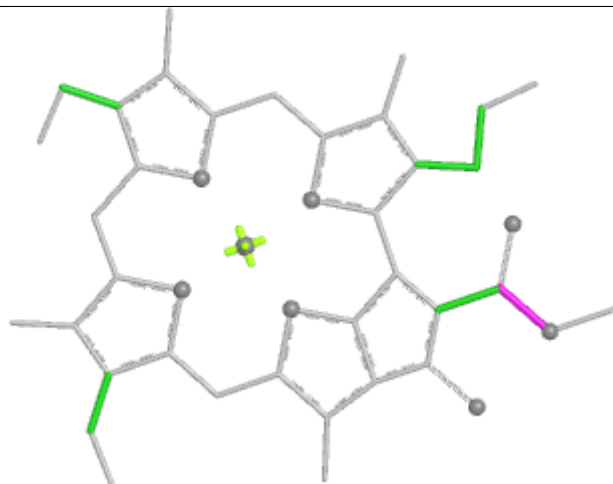
Ligand CLA 9 604



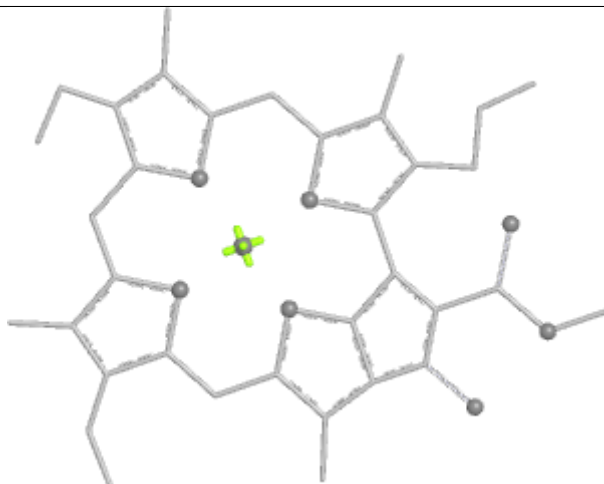
Bond lengths



Bond angles

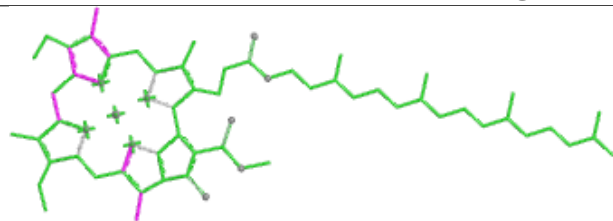


Torsions

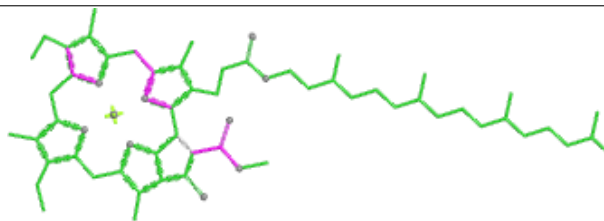


Rings

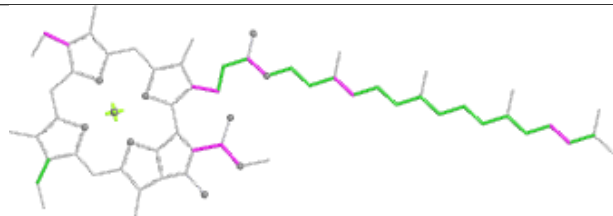
Ligand CLA A 835



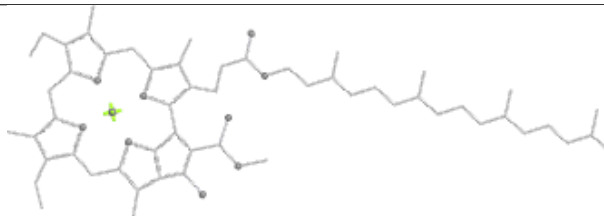
Bond lengths



Bond angles

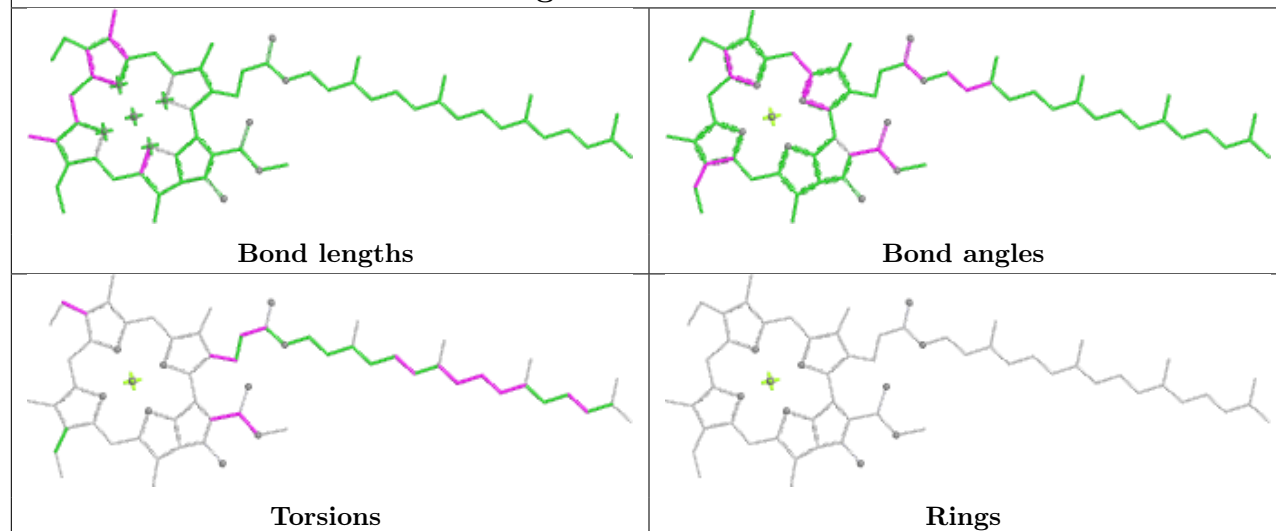


Torsions

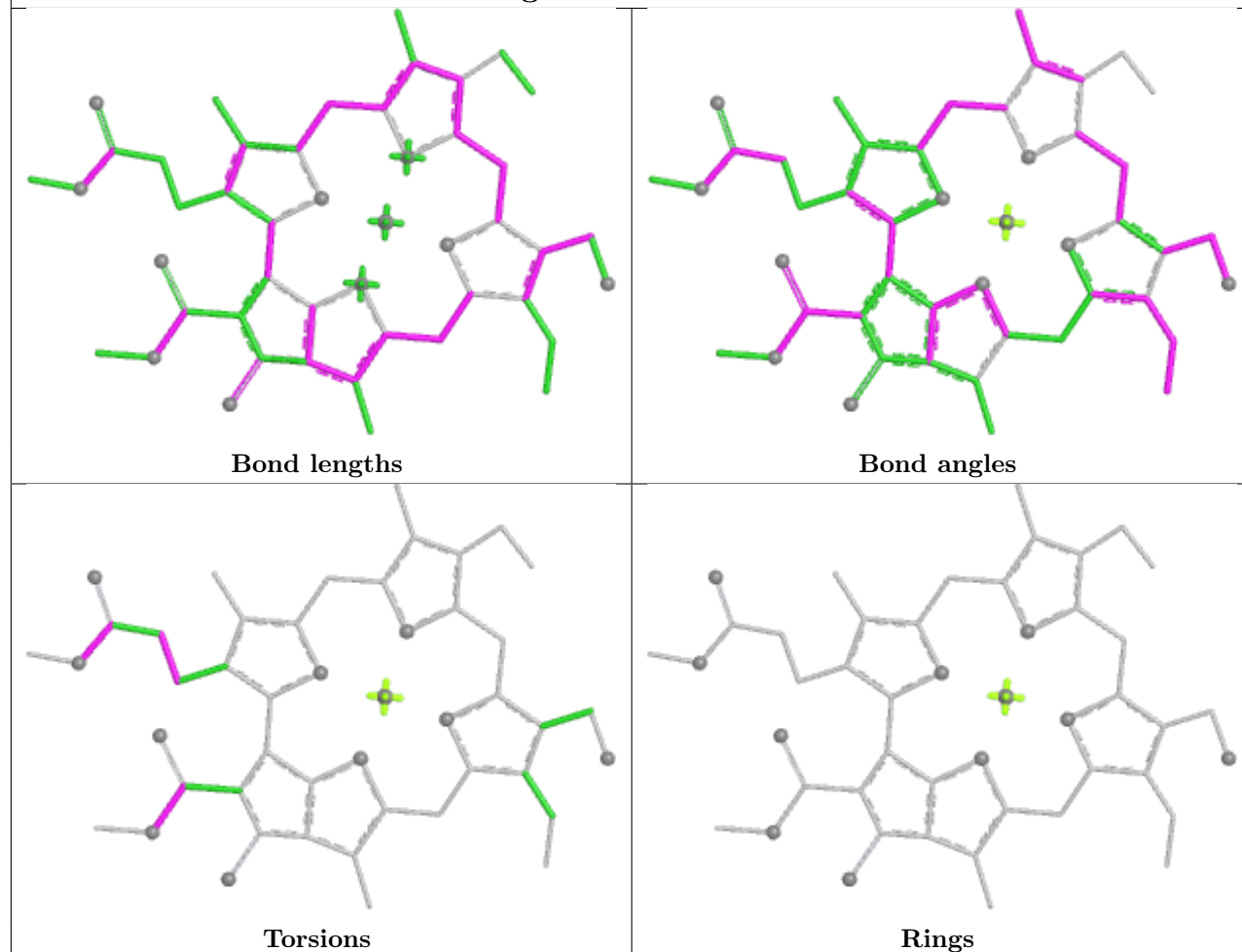


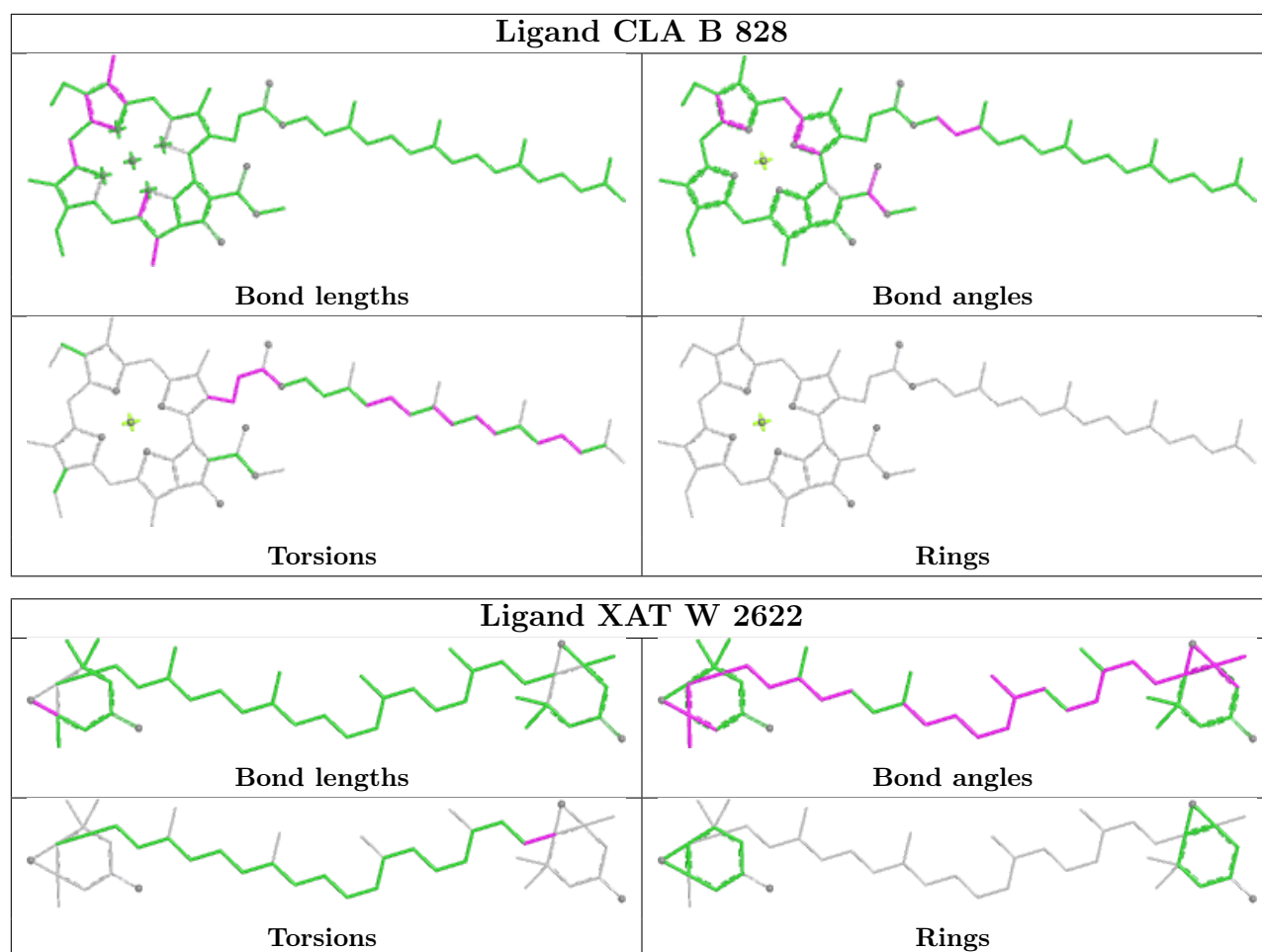
Rings

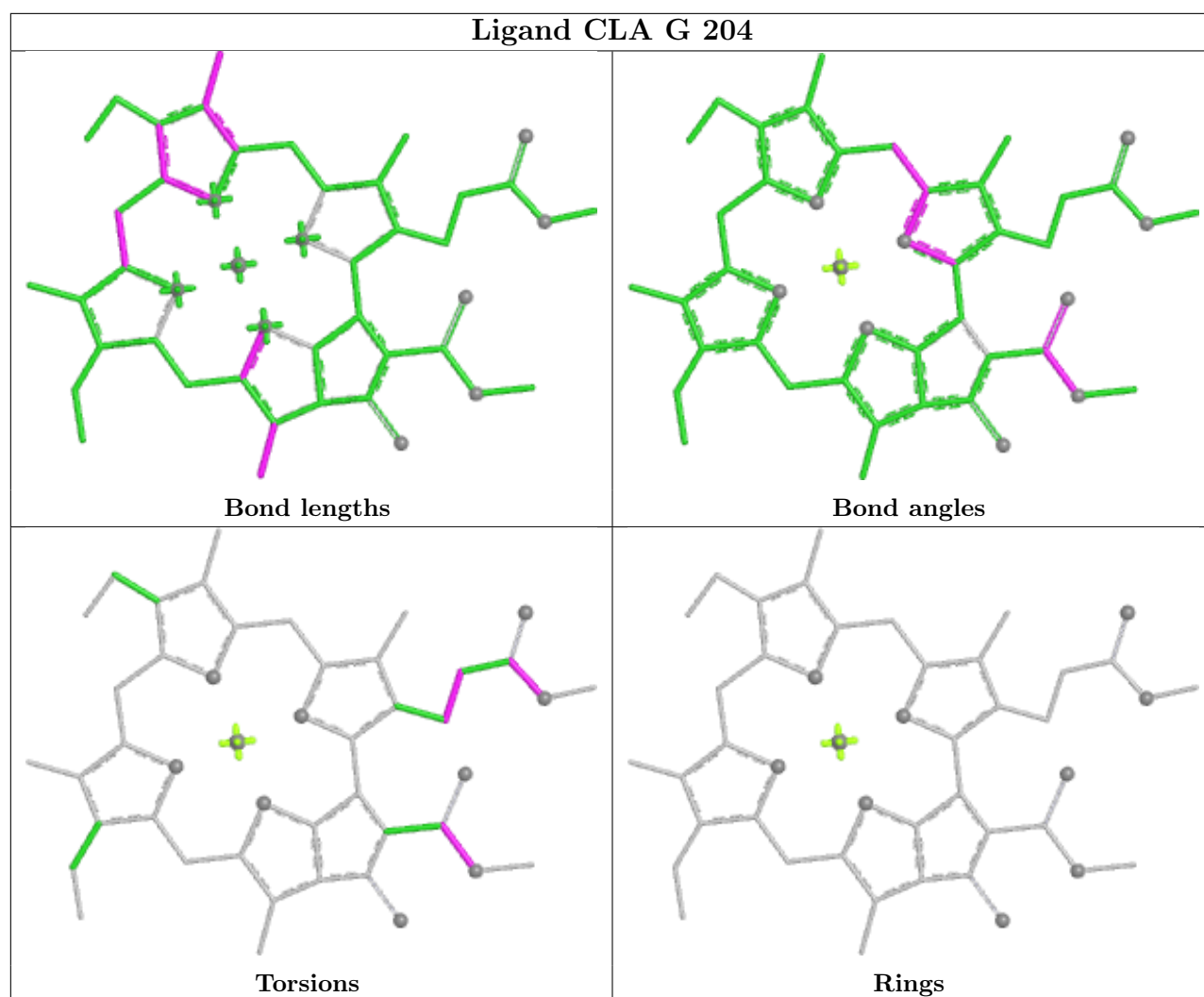
Ligand CLA 1 611



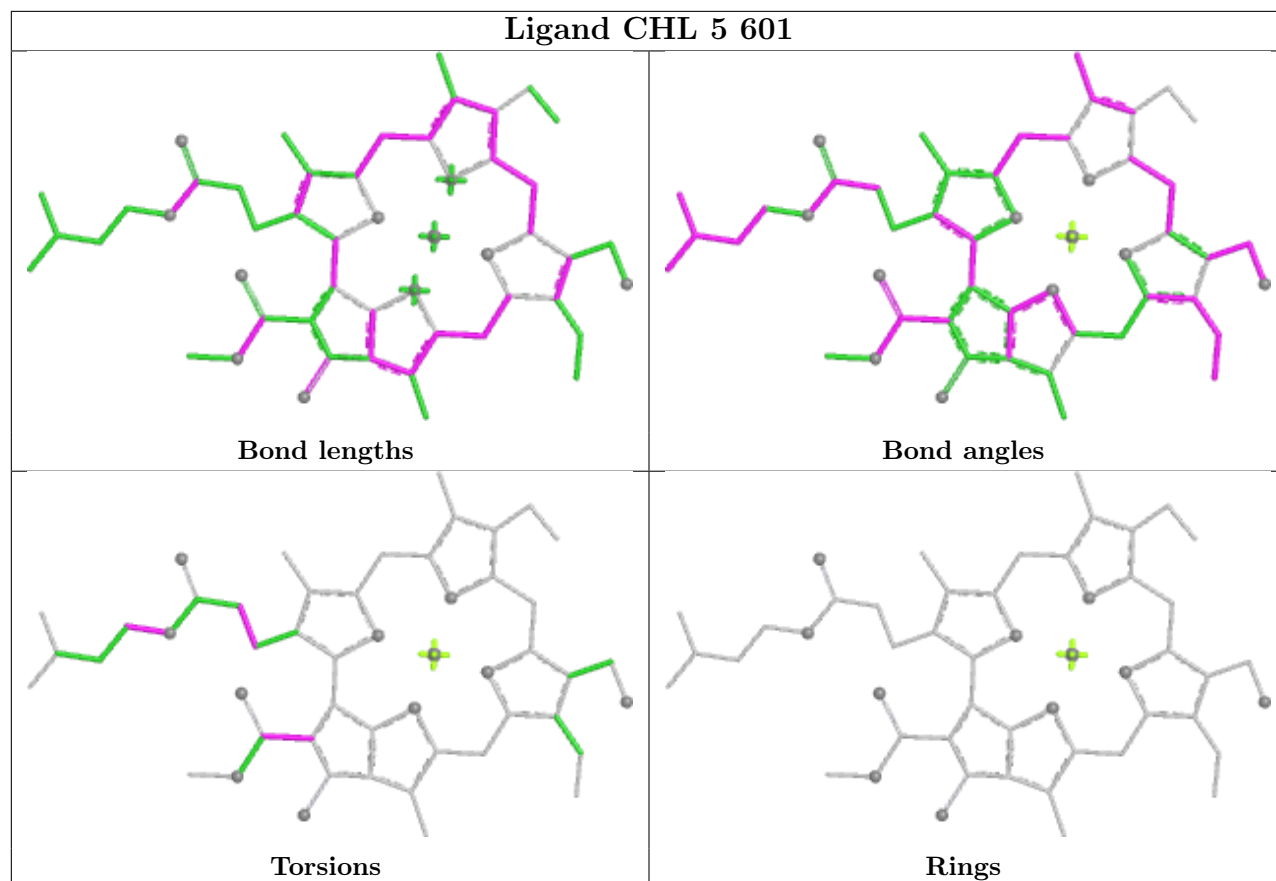
Ligand CHL 6 607



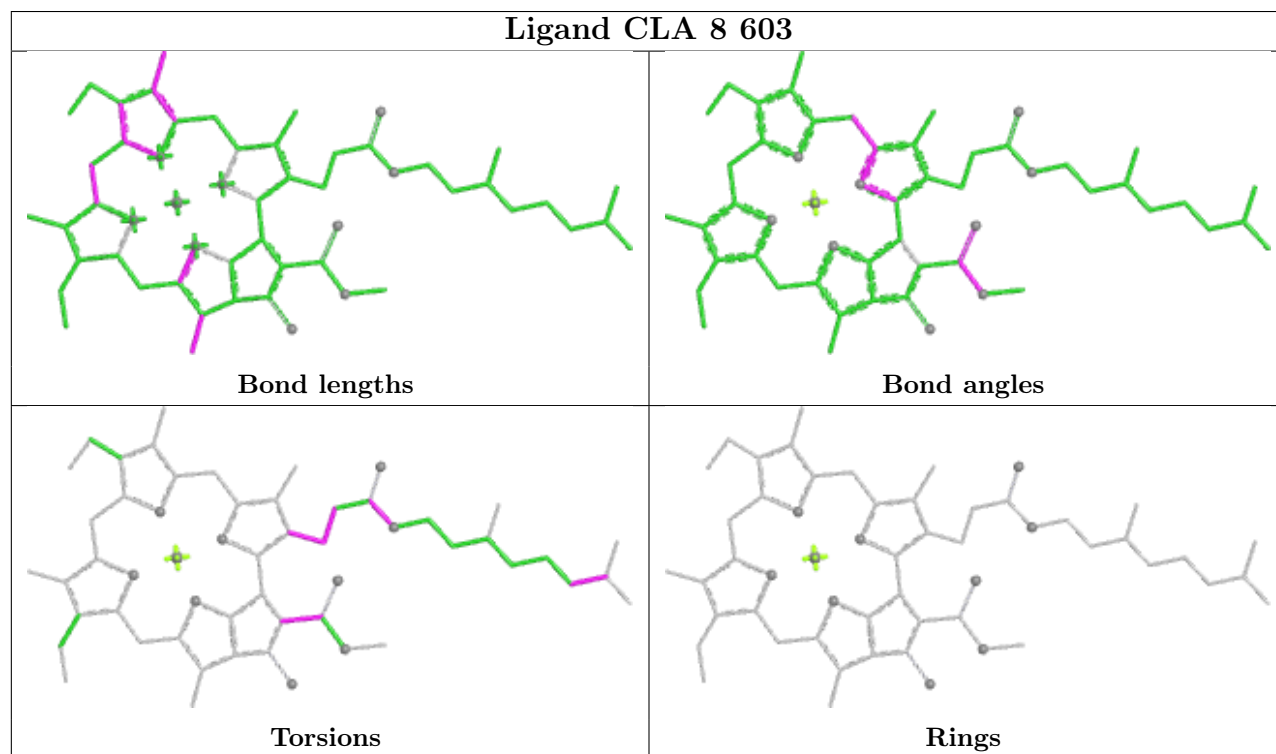


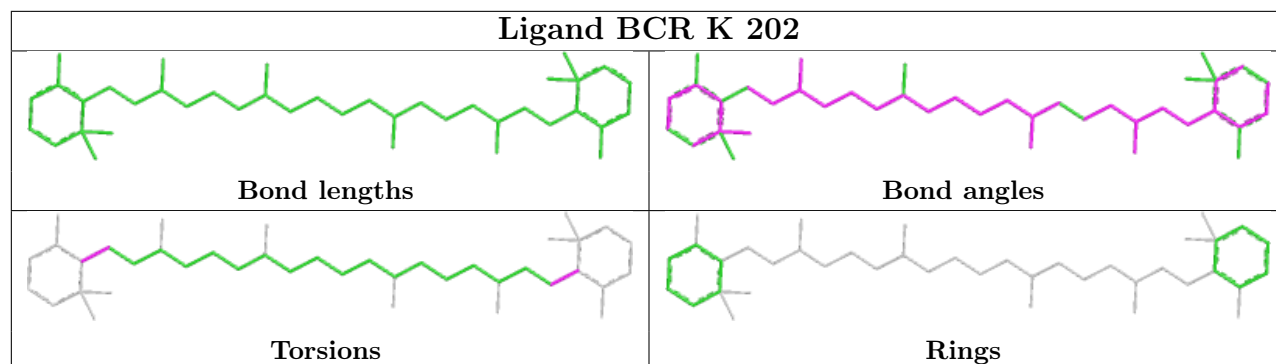
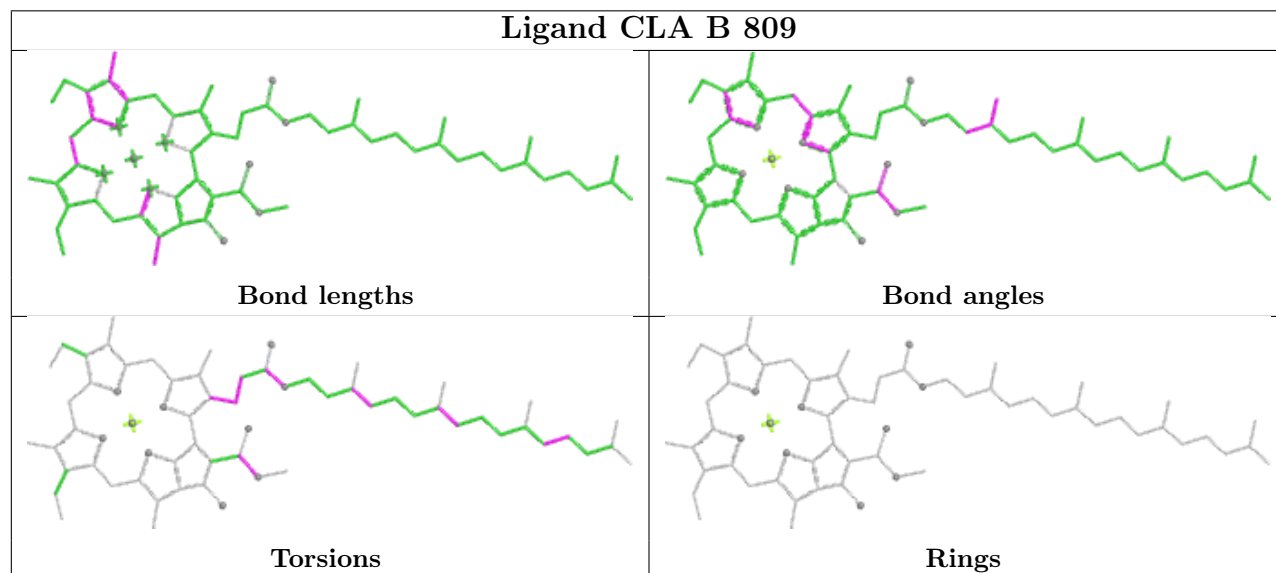
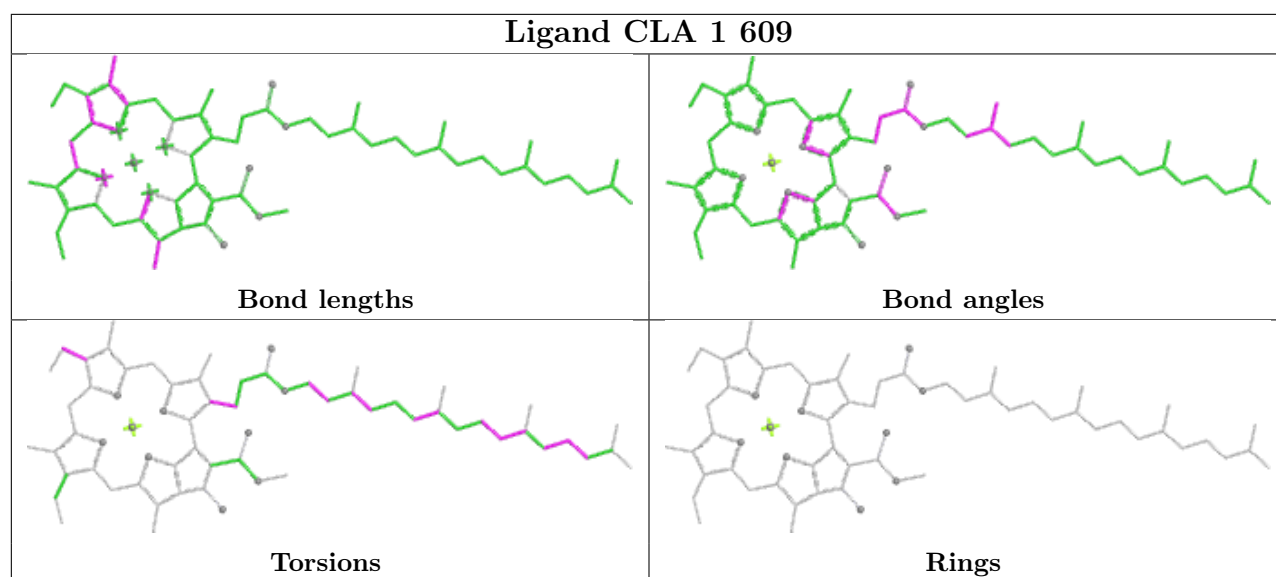


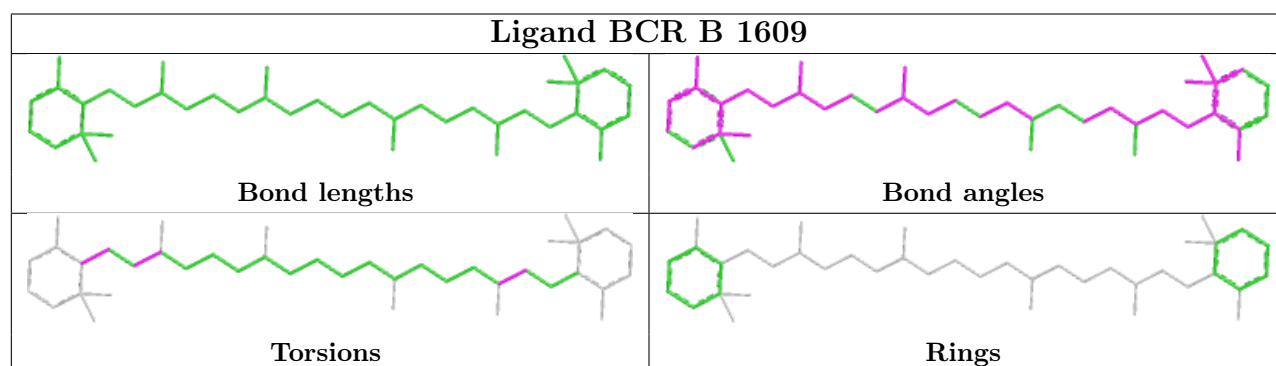
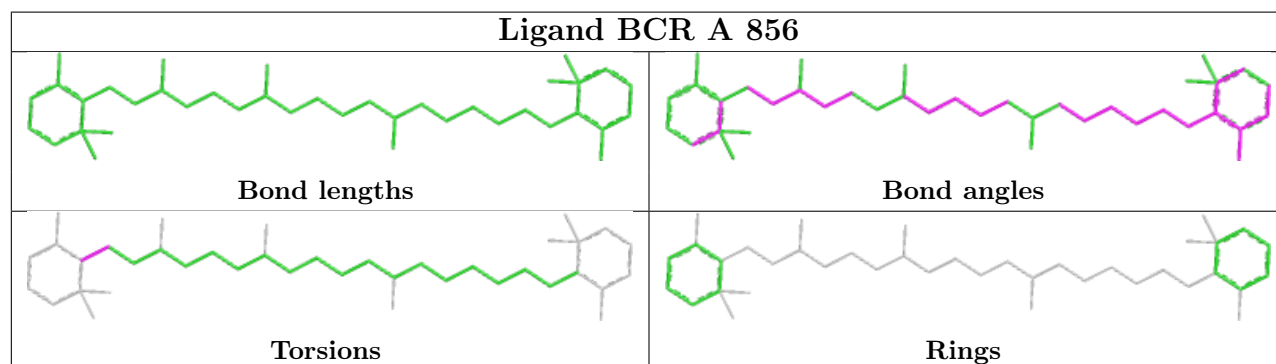
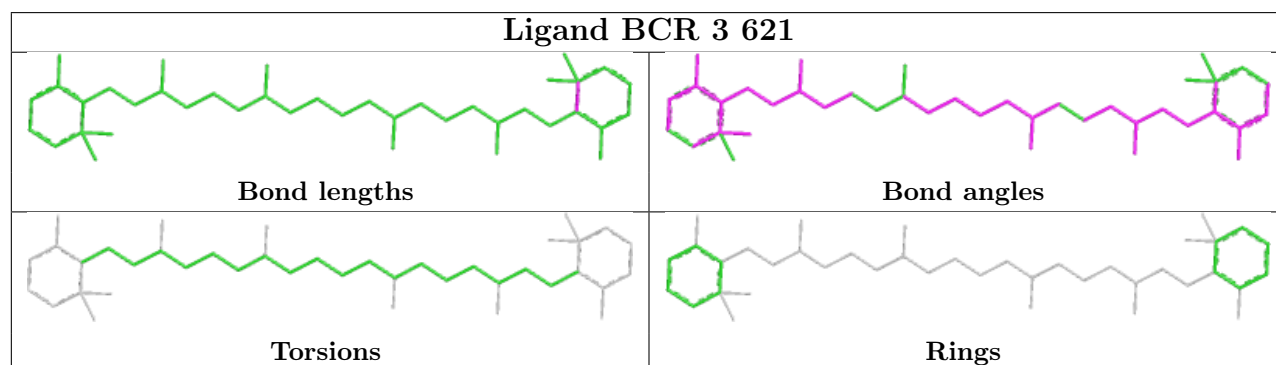
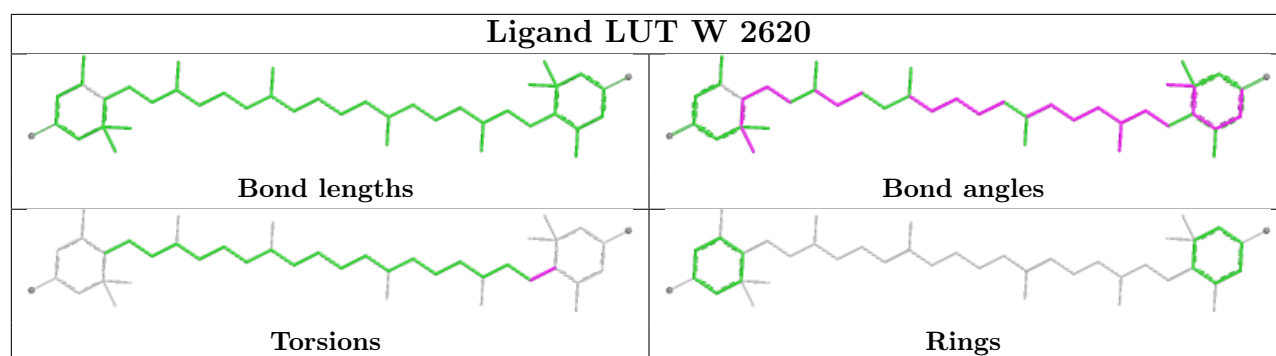
Ligand CHL 5 601



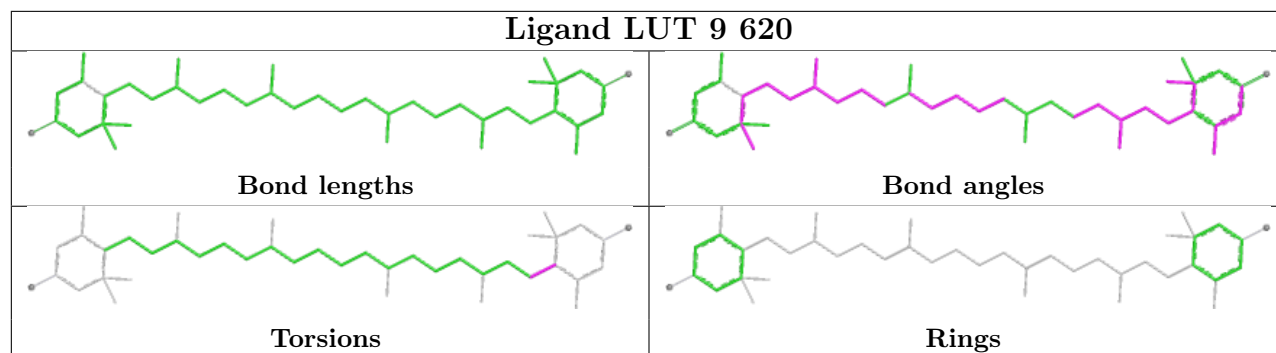
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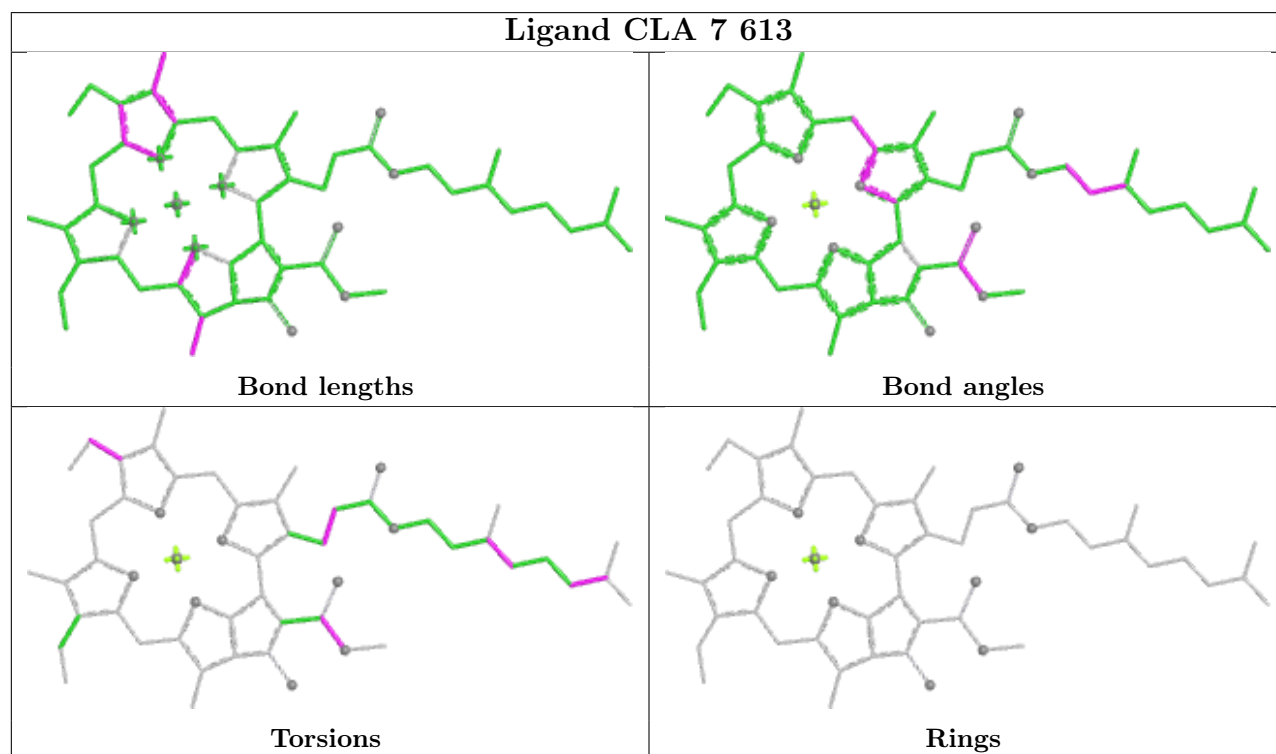




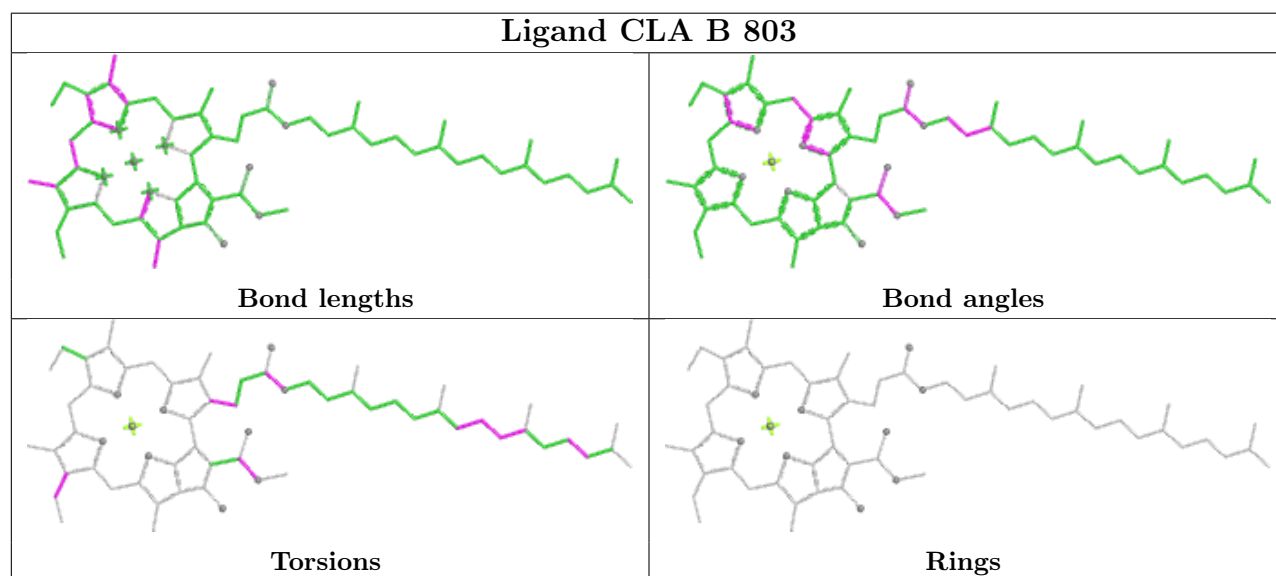
Ligand LUT 9 620



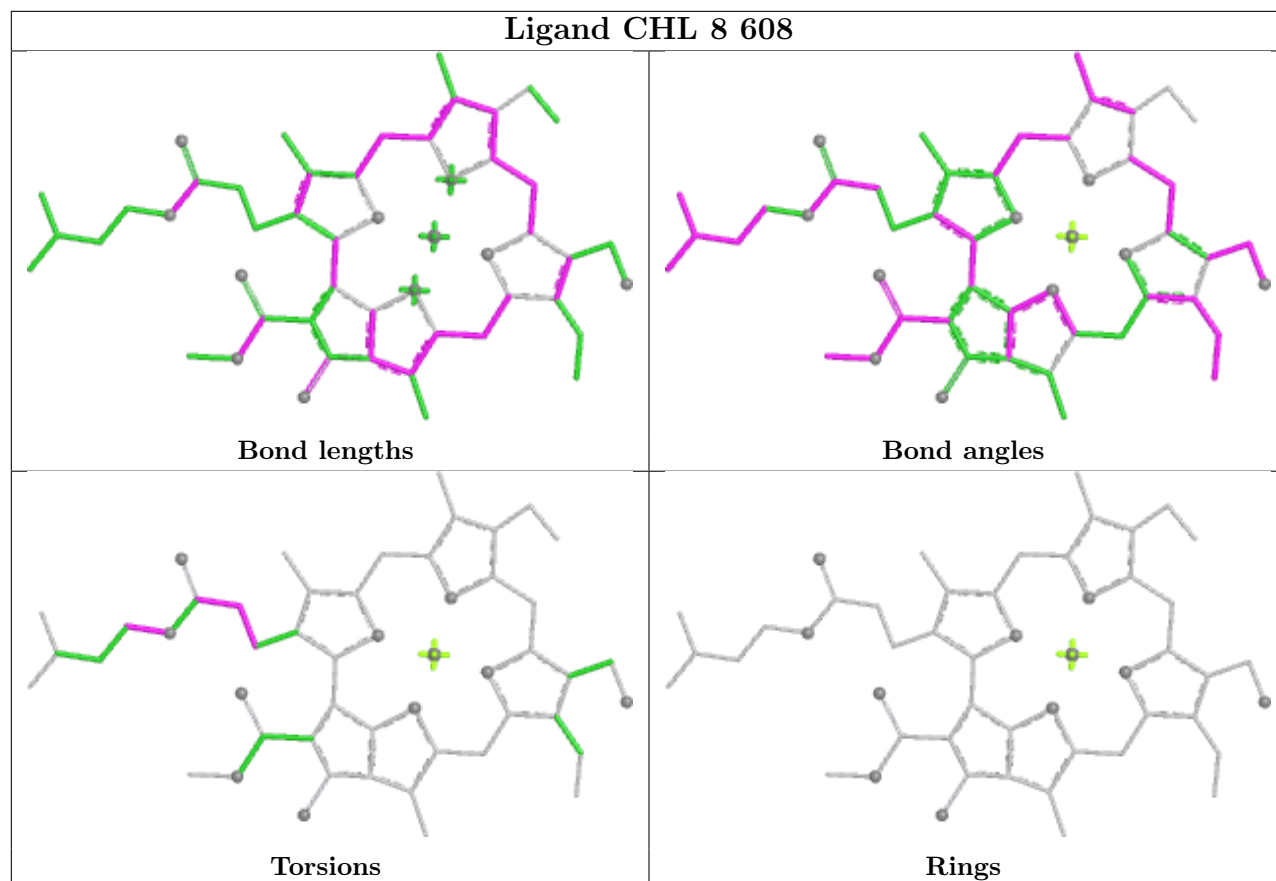
Ligand CLA 7 613



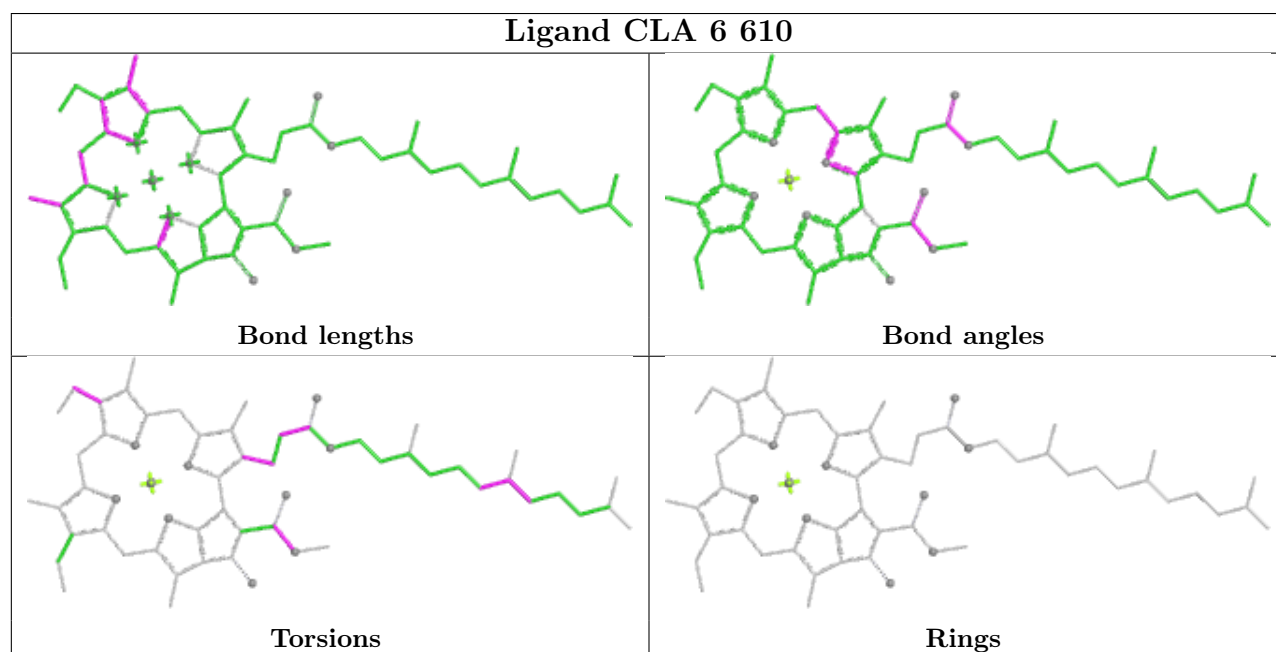
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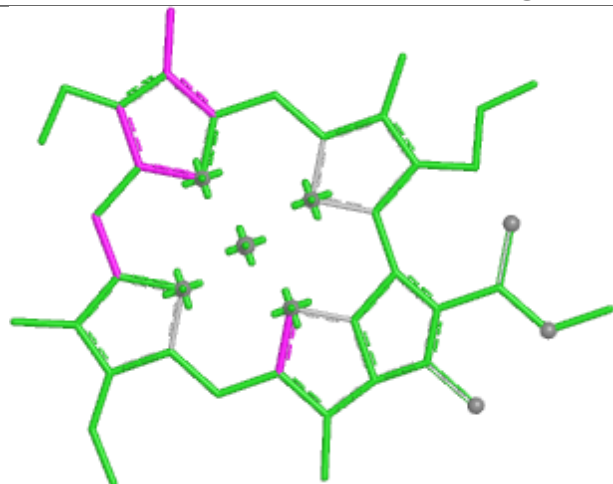
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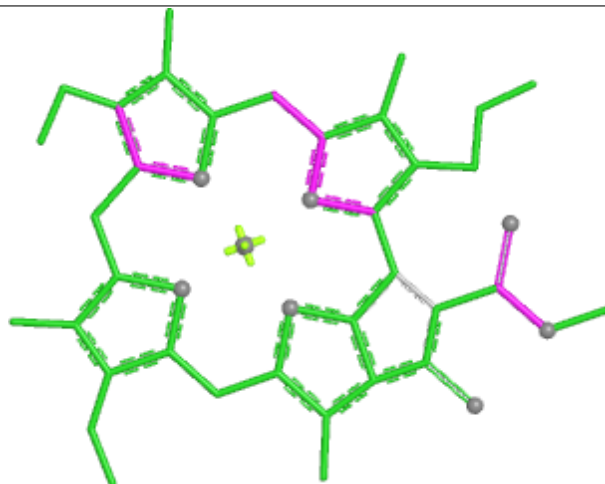
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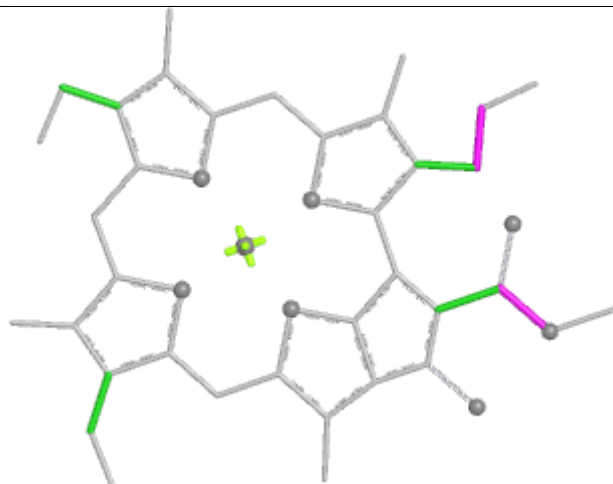
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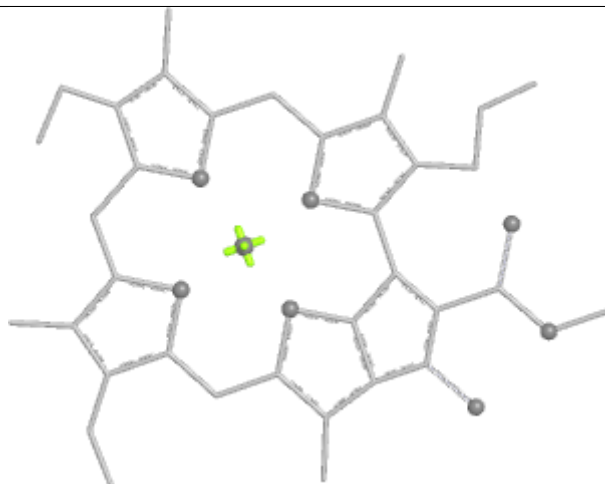
Bond lengths



Bond angles

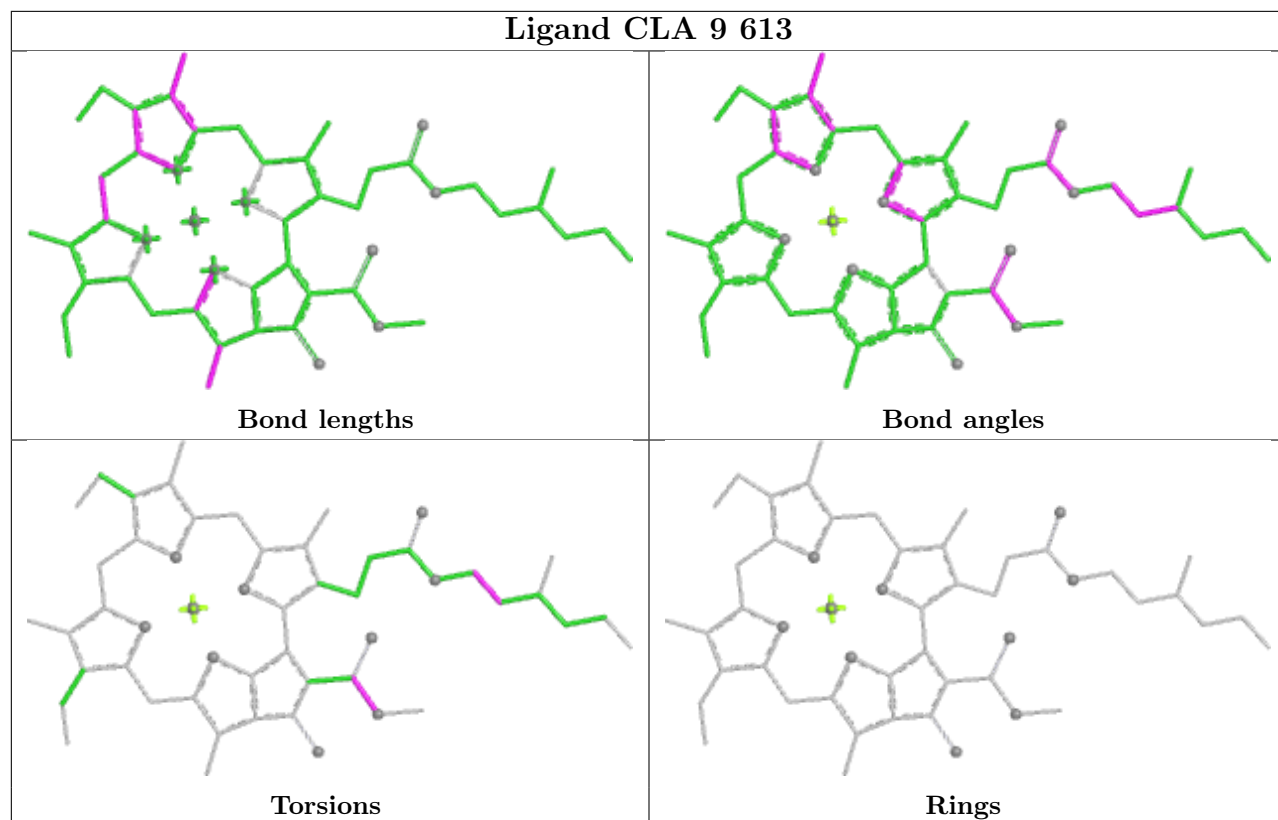


Torsions

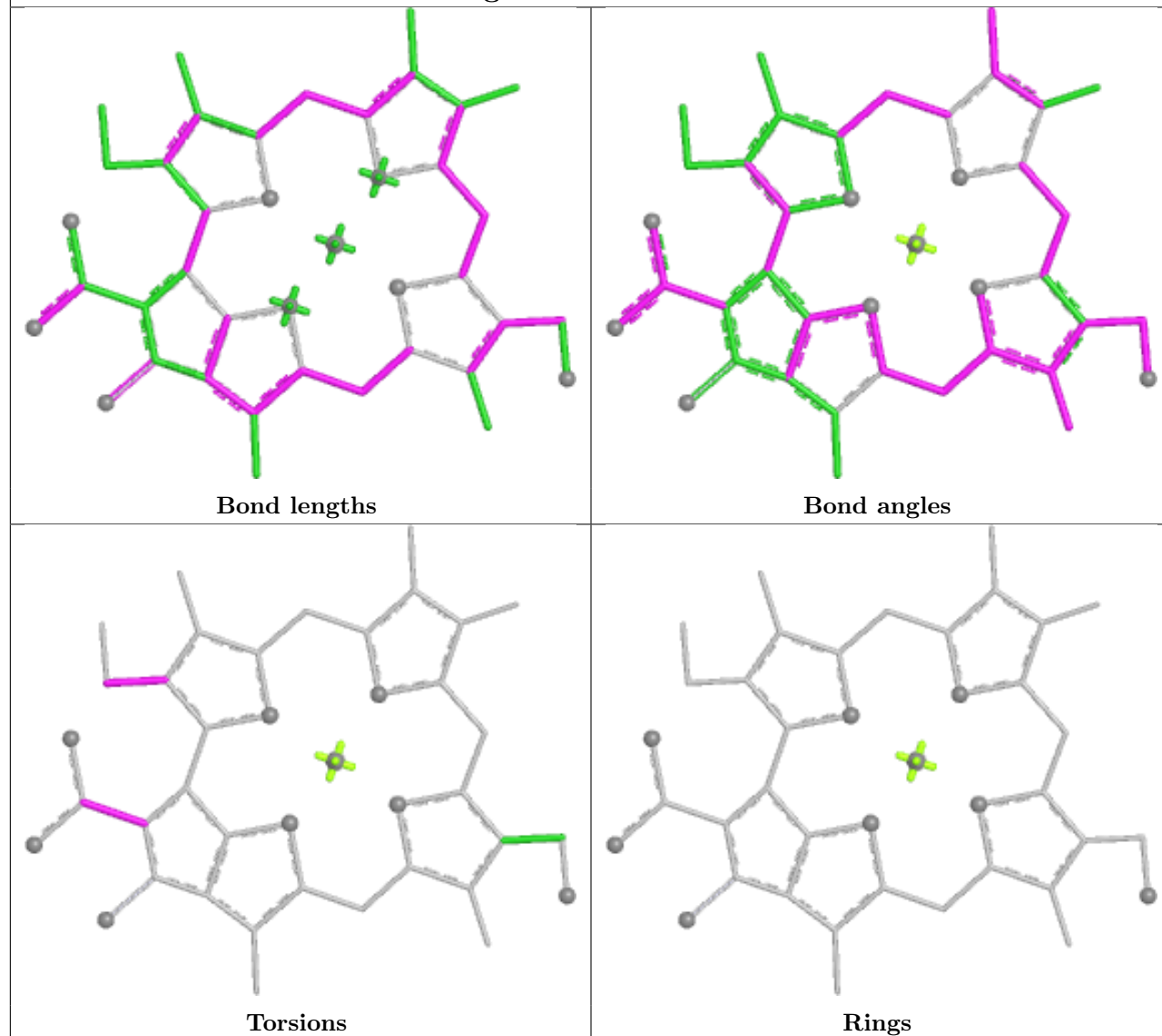


Rings

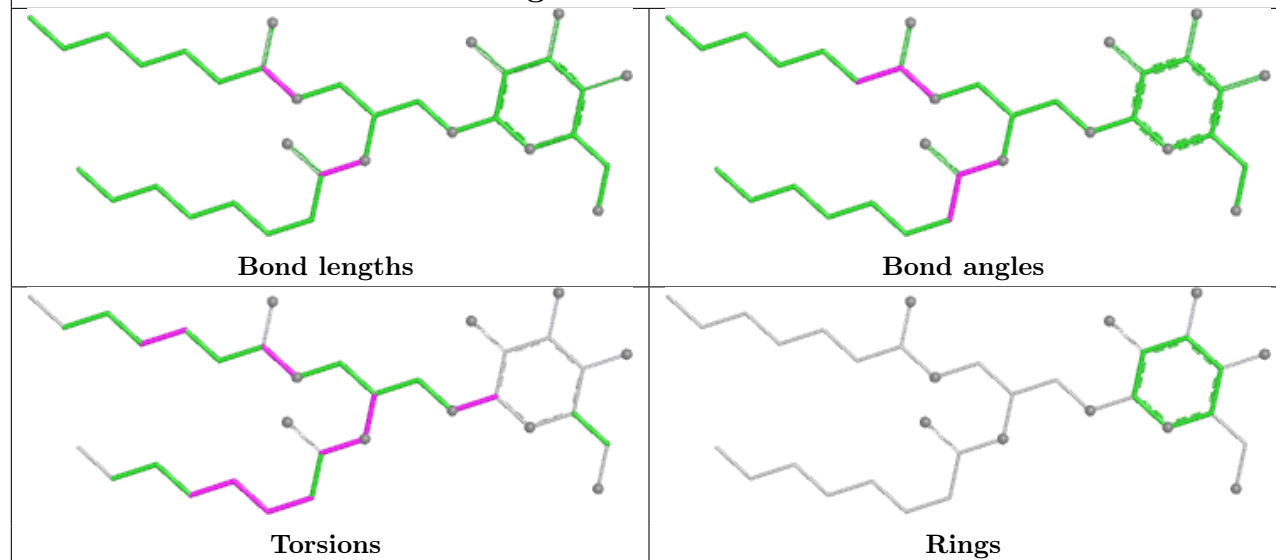
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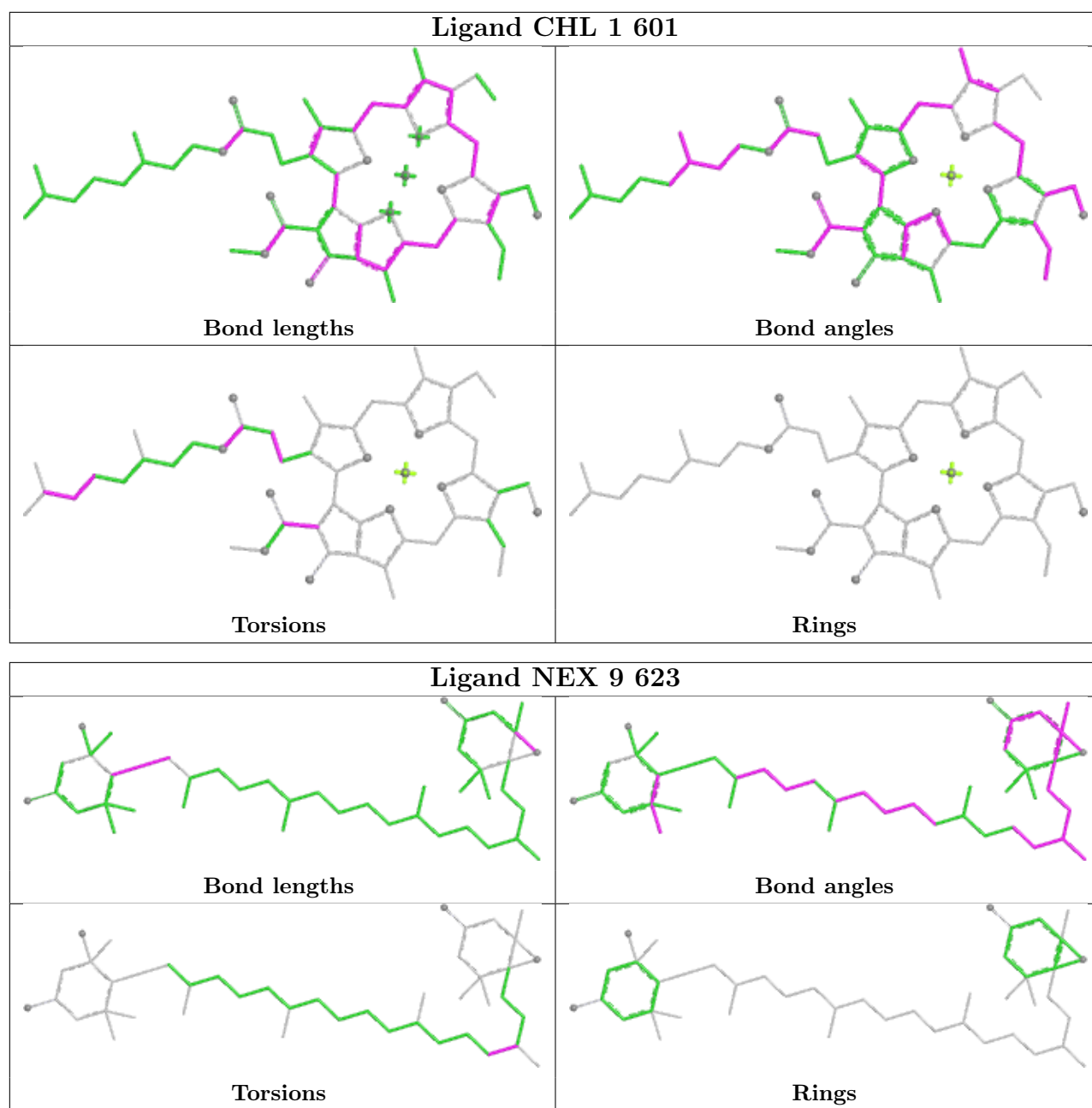


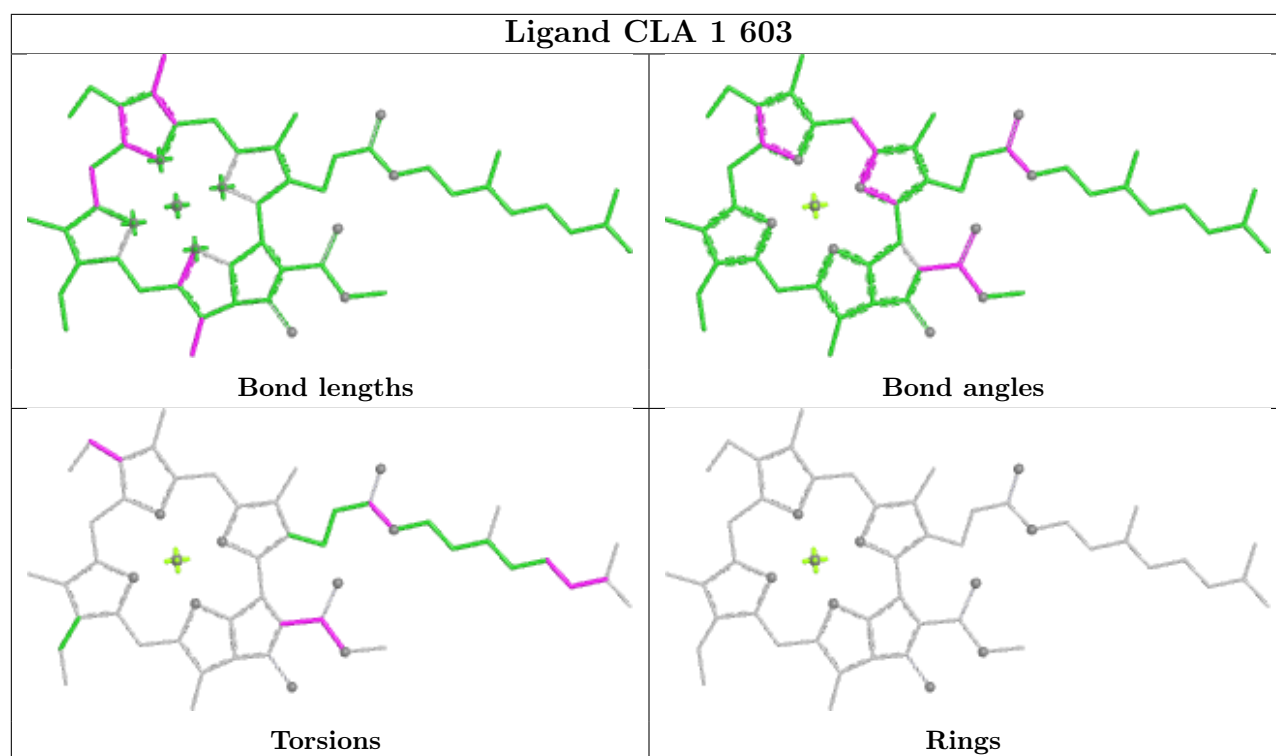
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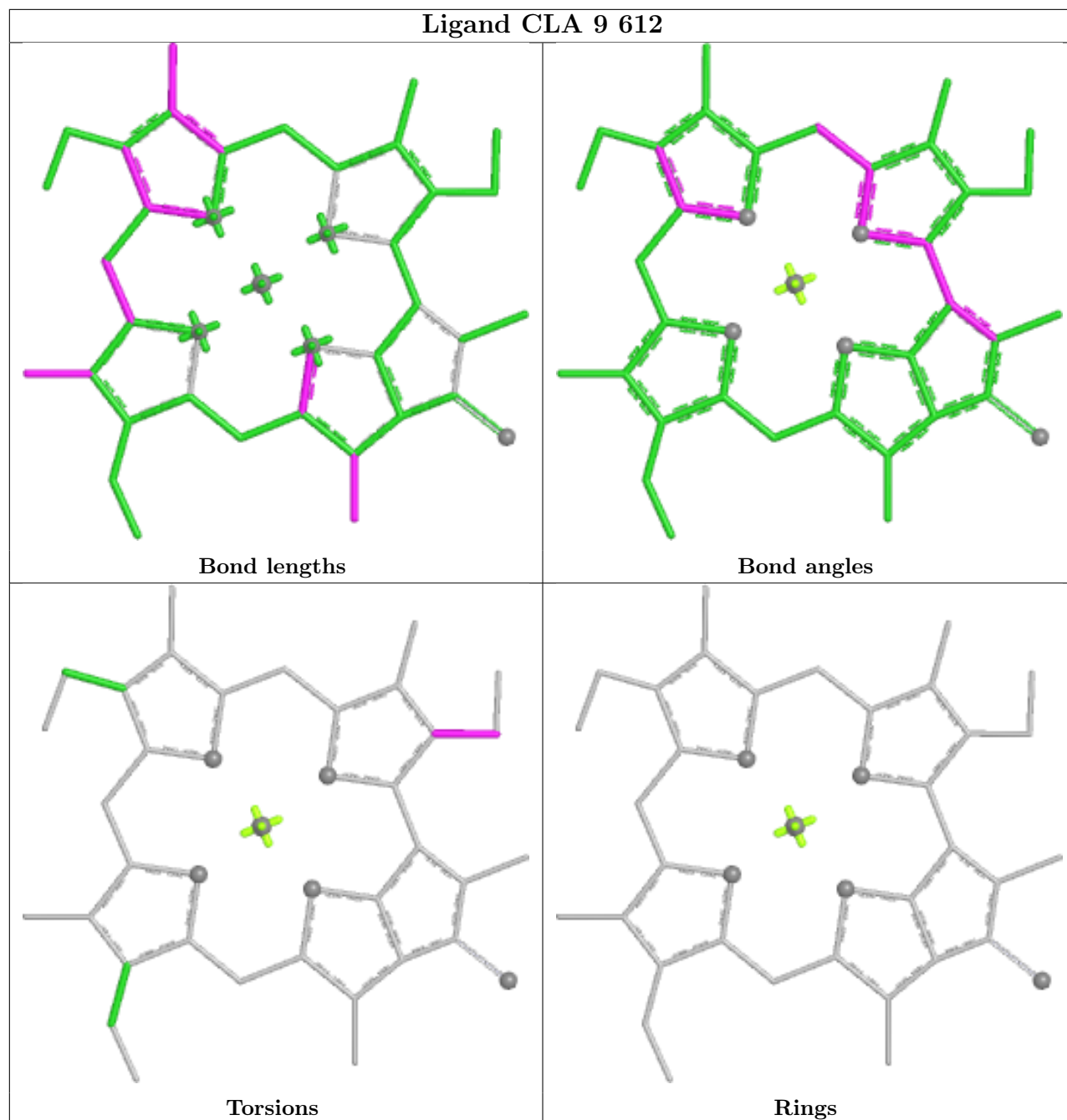
Ligand LMG A 860



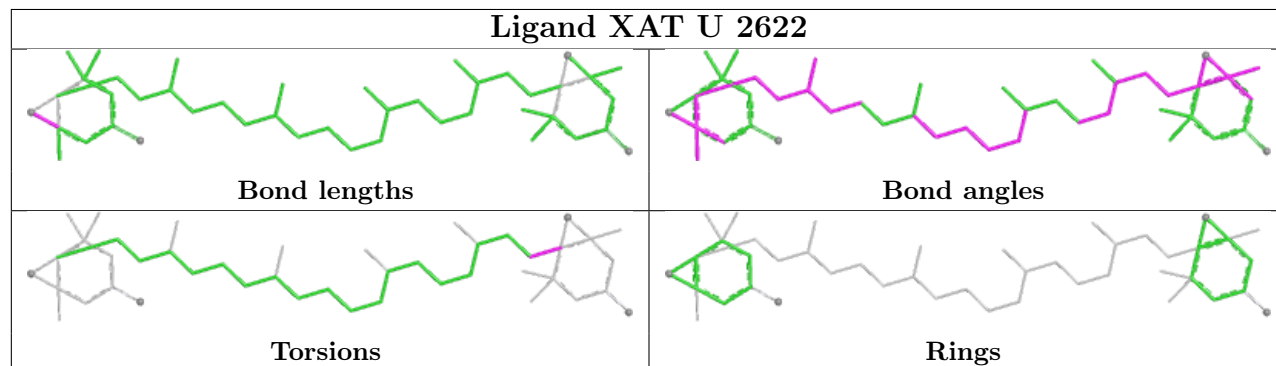


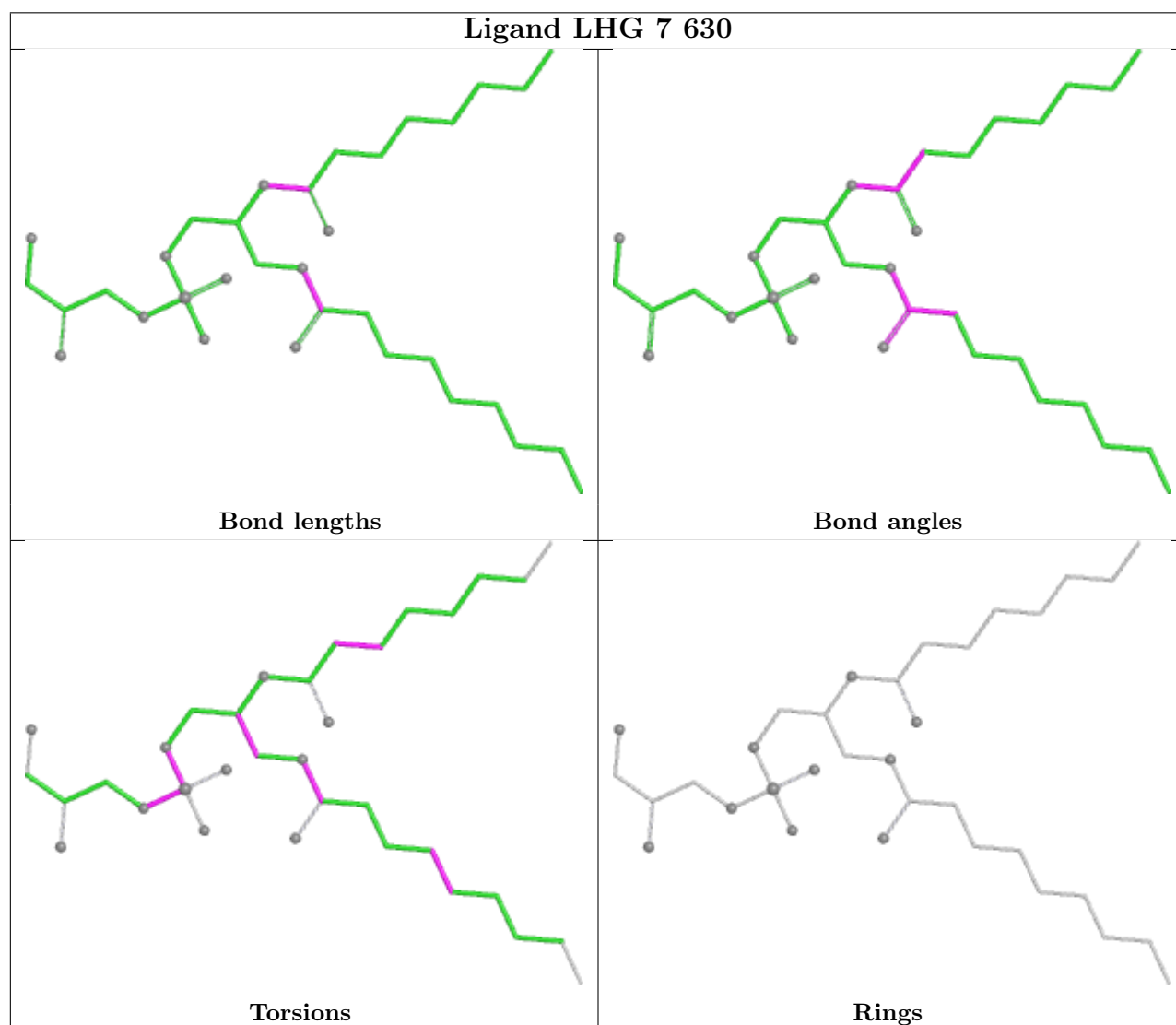
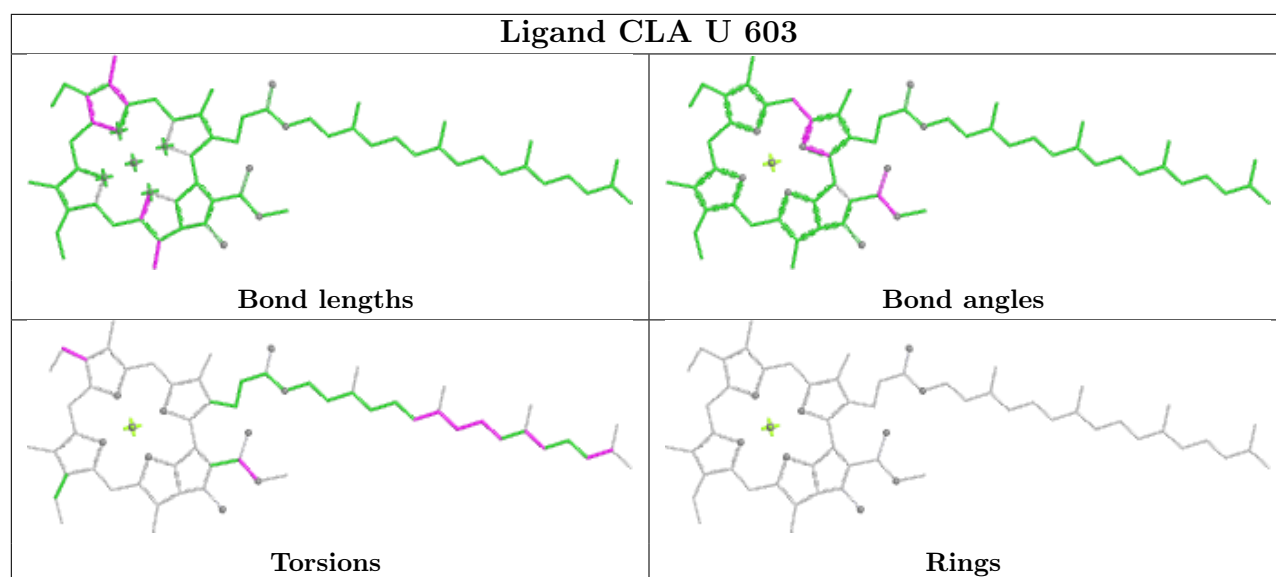


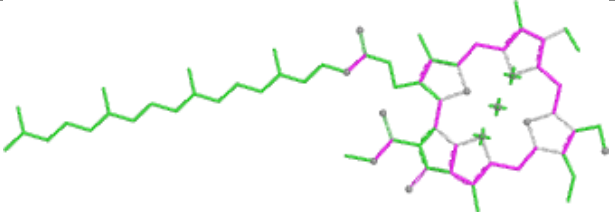
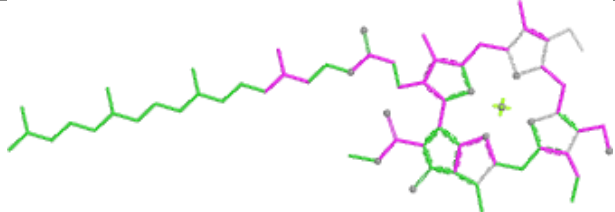
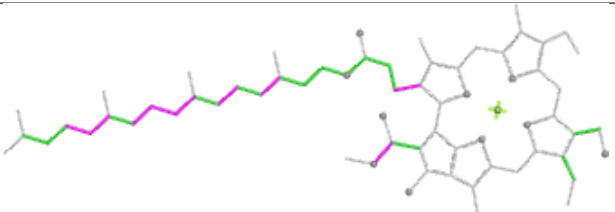
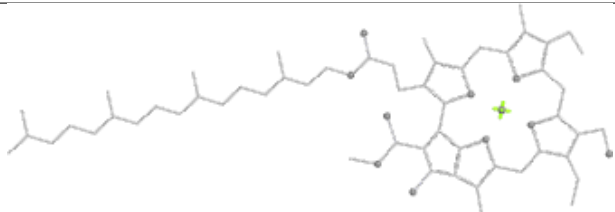
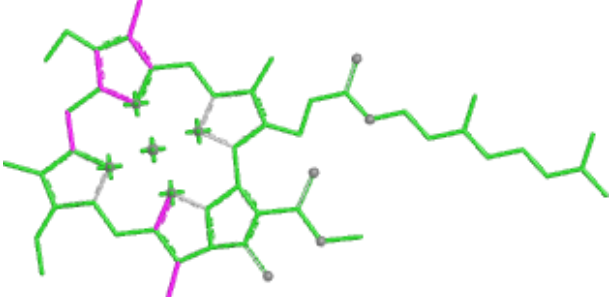
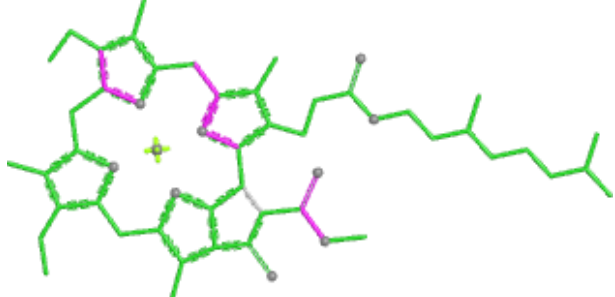
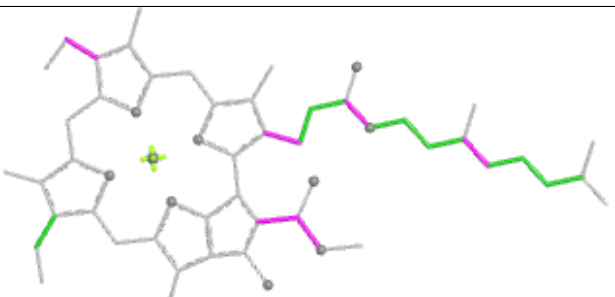
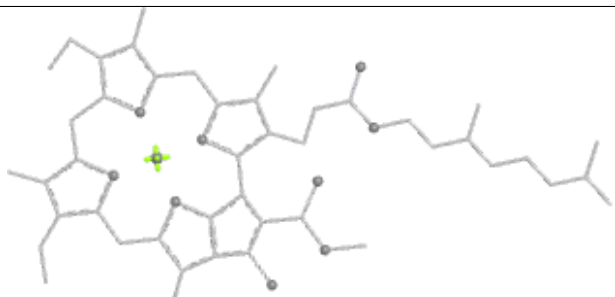
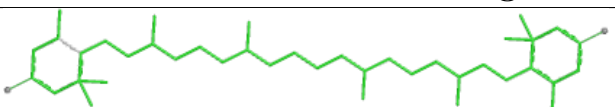
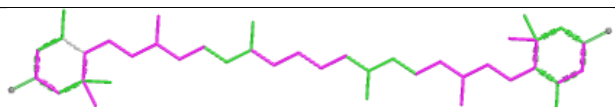
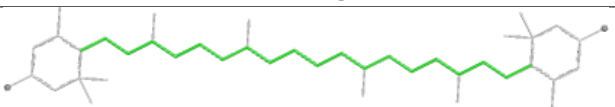
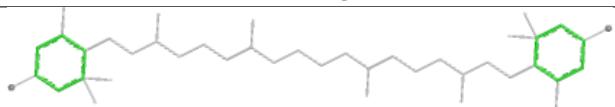
Ligand CLA 9 612

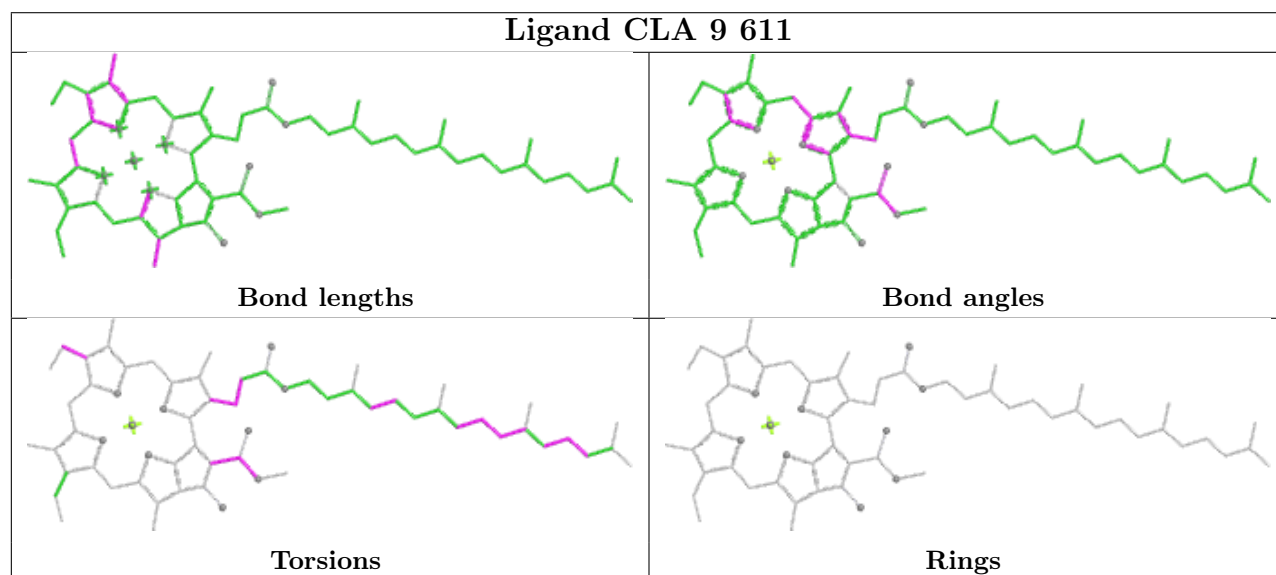
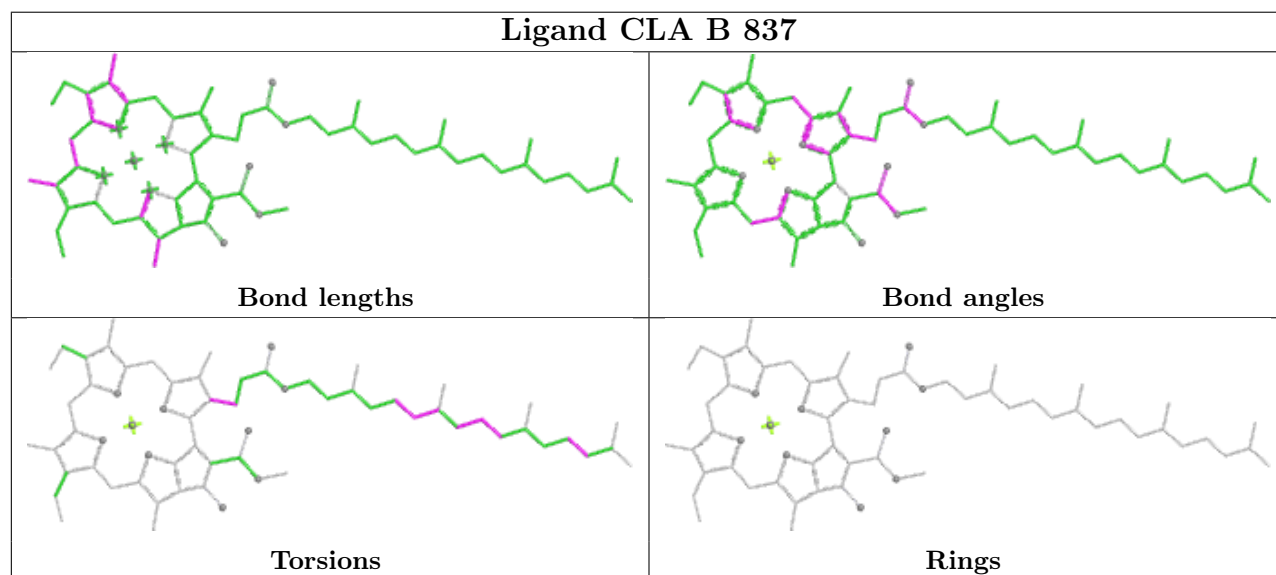
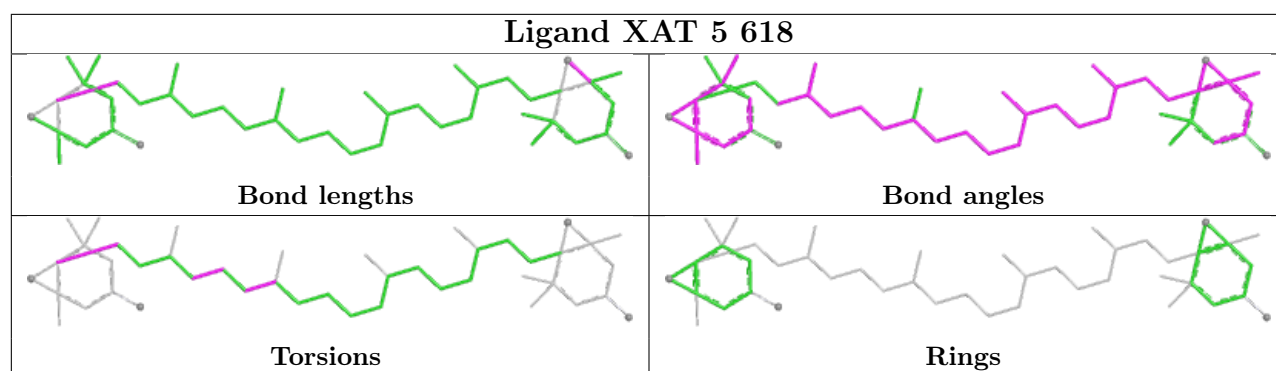


Ligand XAT U 2622

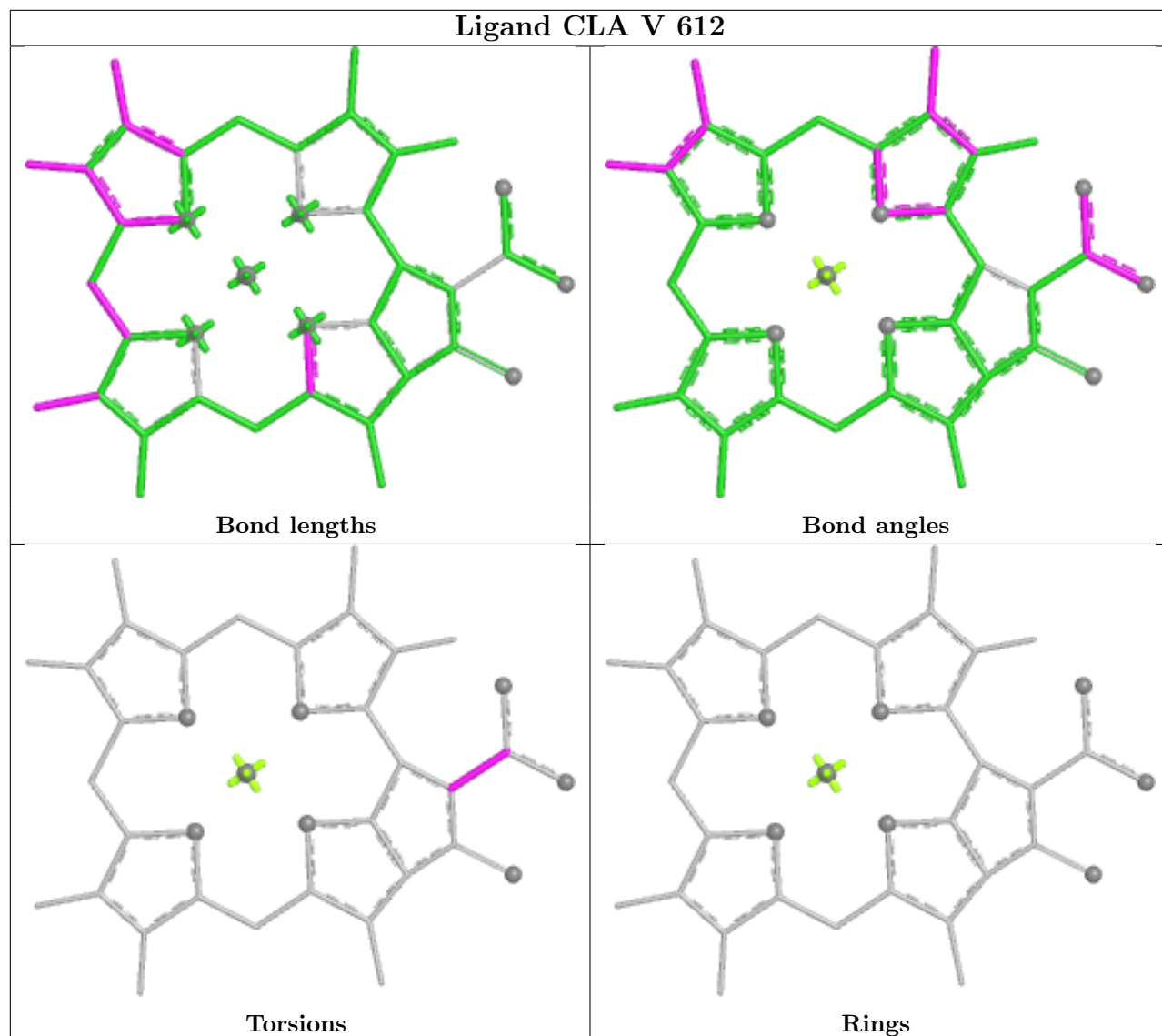


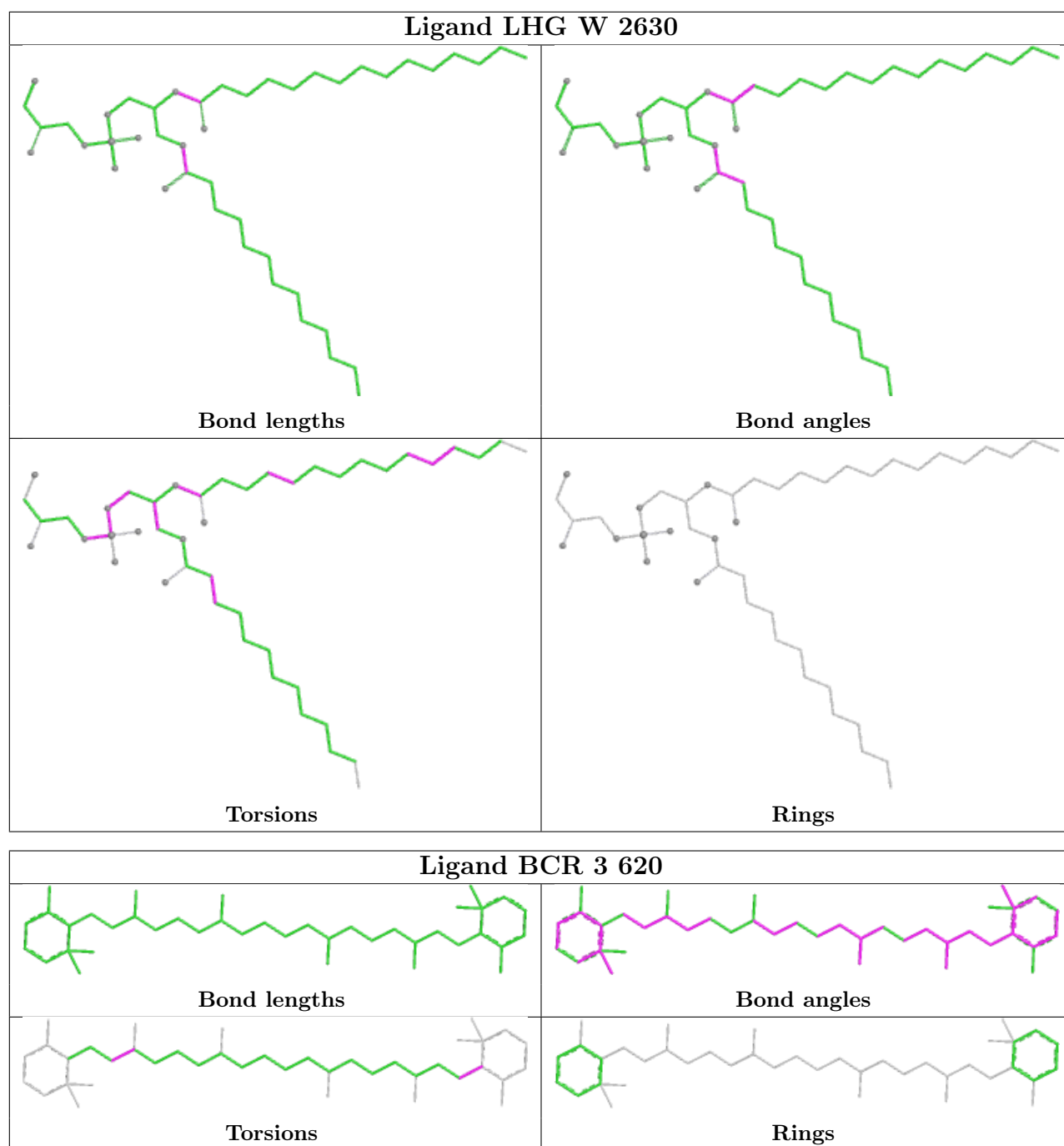


Ligand CHL U 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA O 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT U 2620	
 Bond lengths	 Bond angles
 Torsions	 Rings

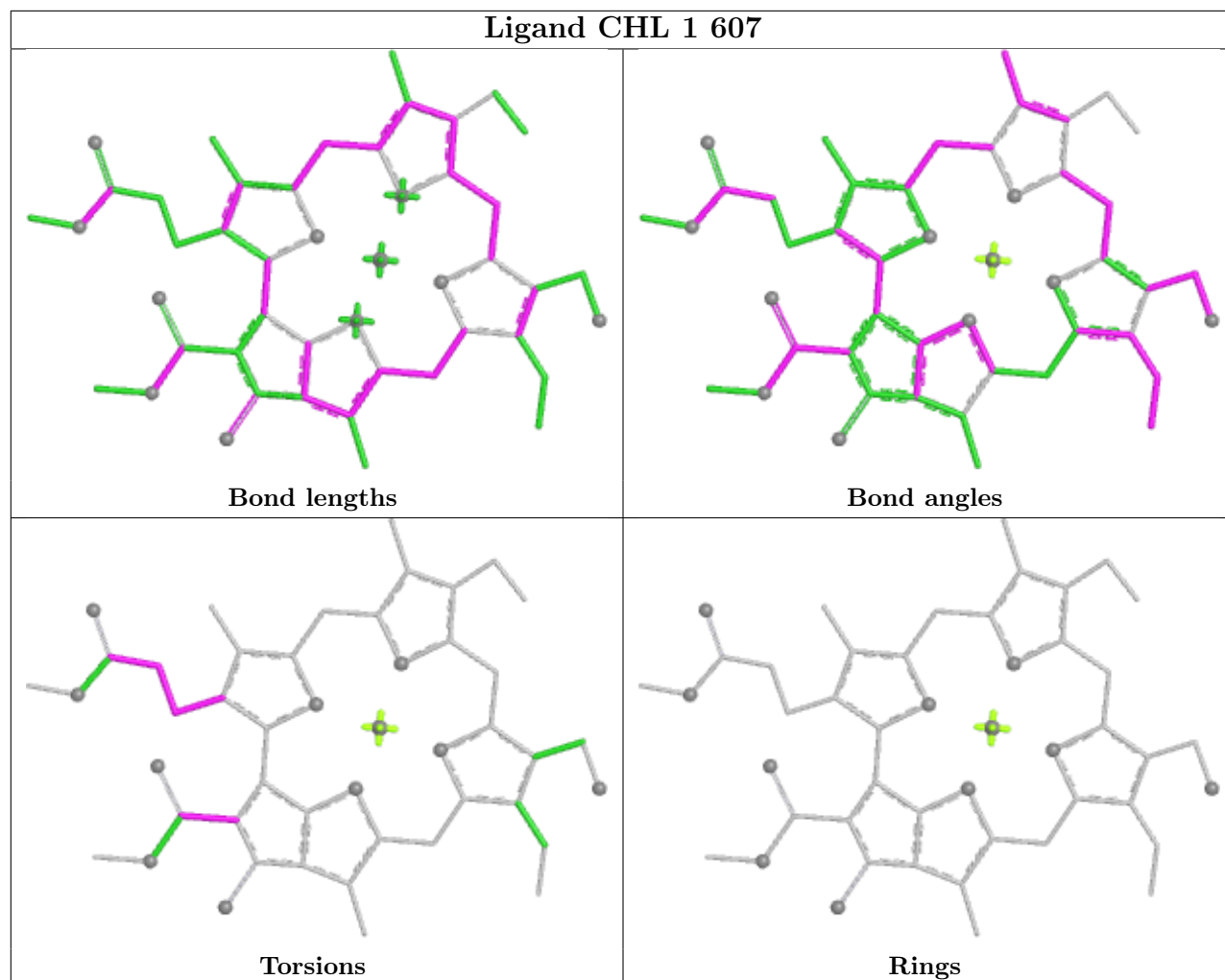


Ligand CLA V 612

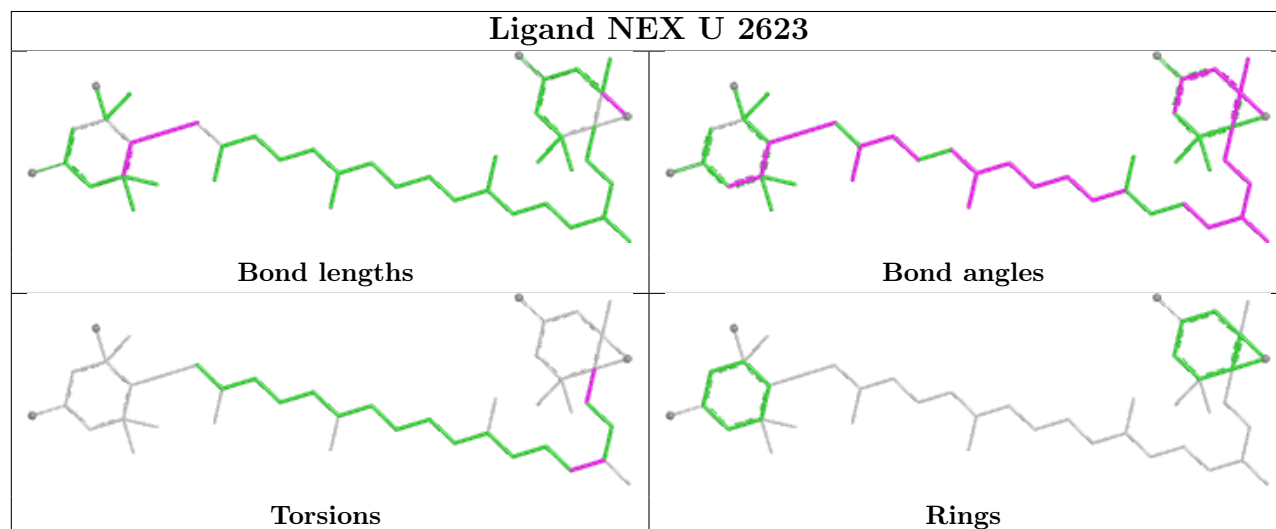


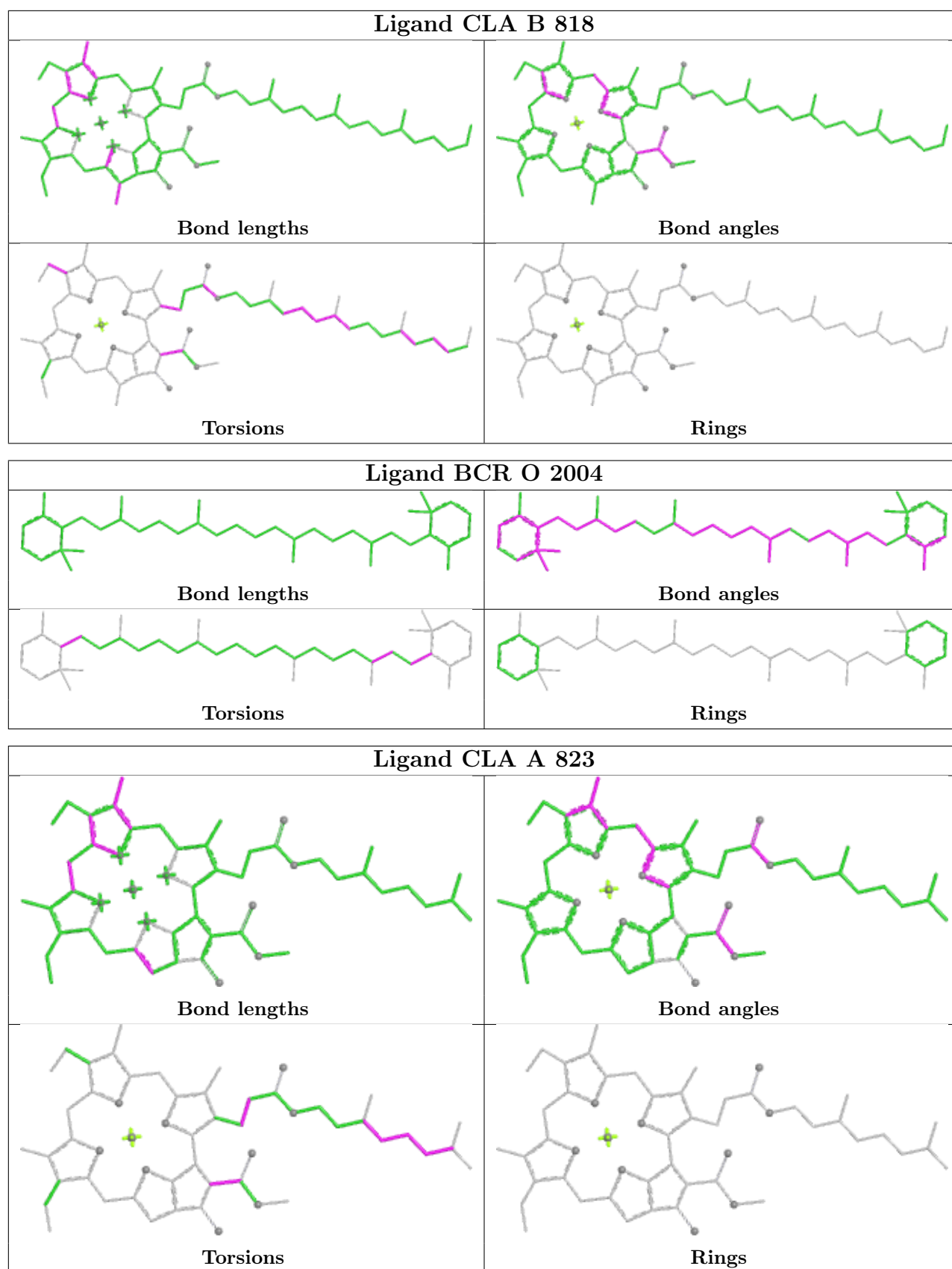


Ligand CHL 1 607

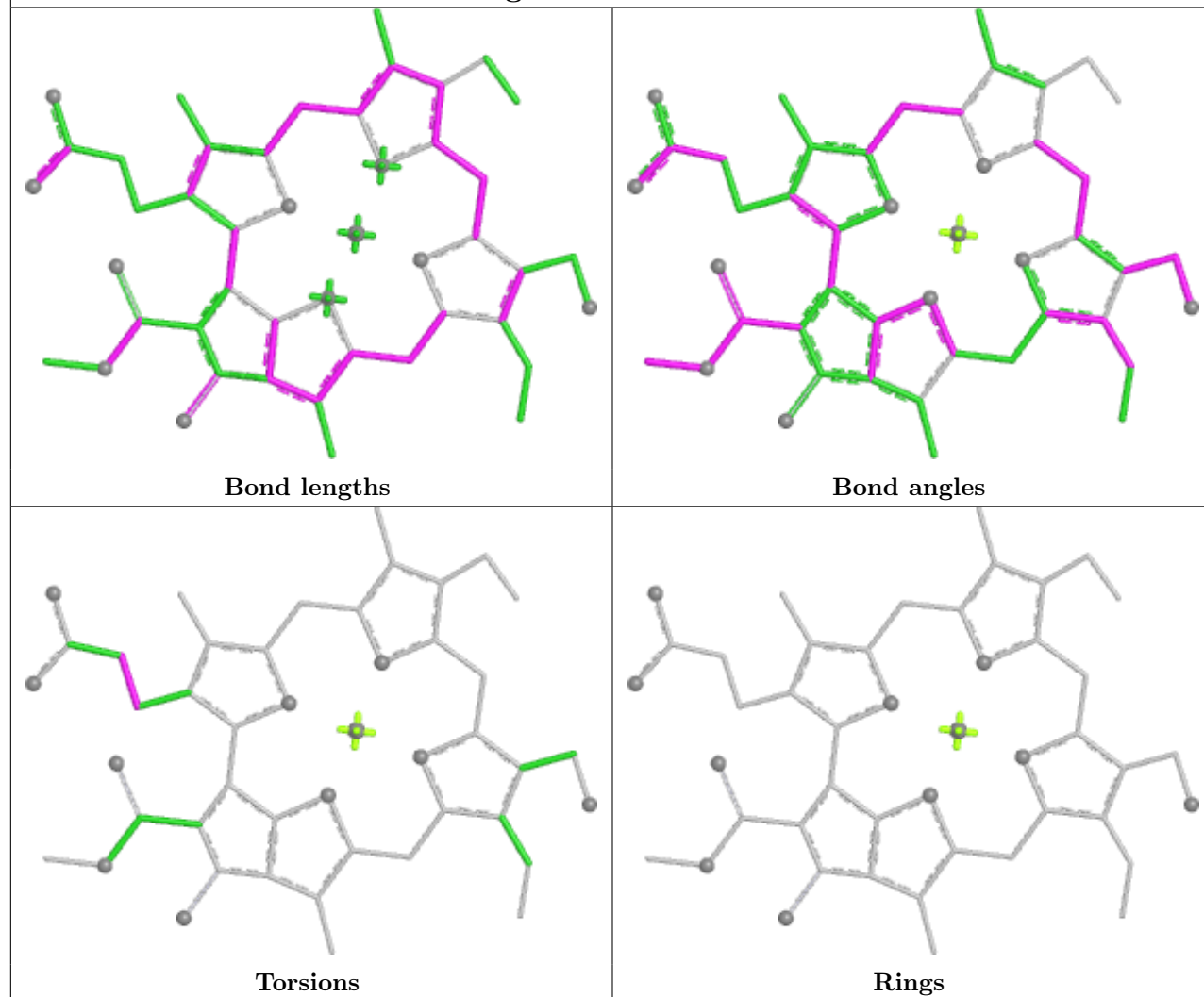


Ligand NEX U 2623

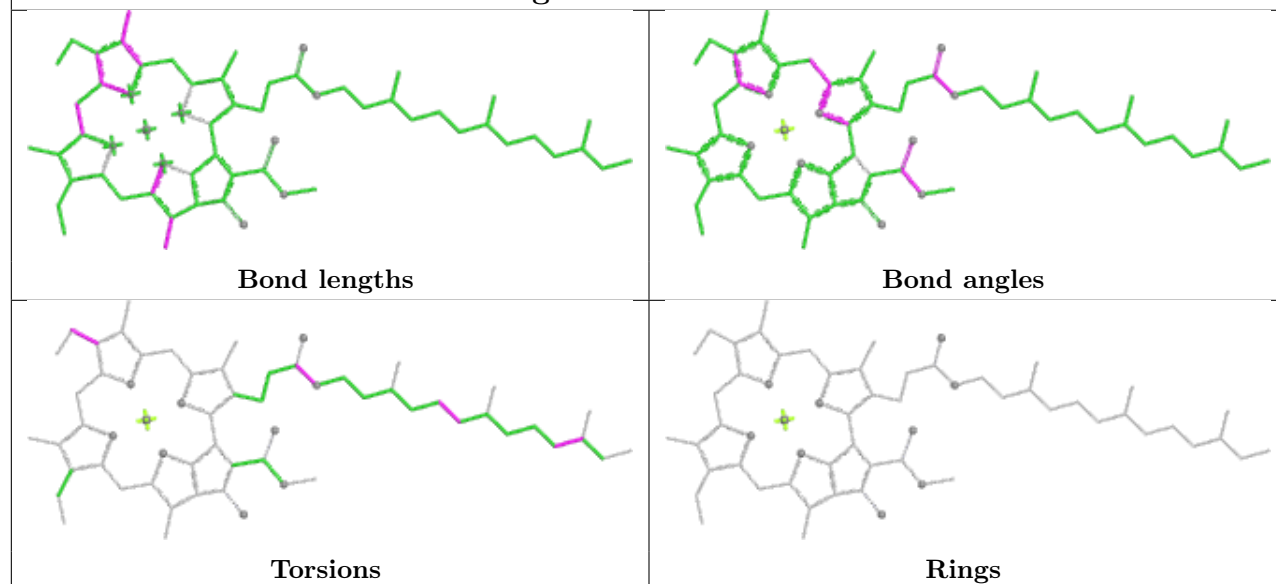


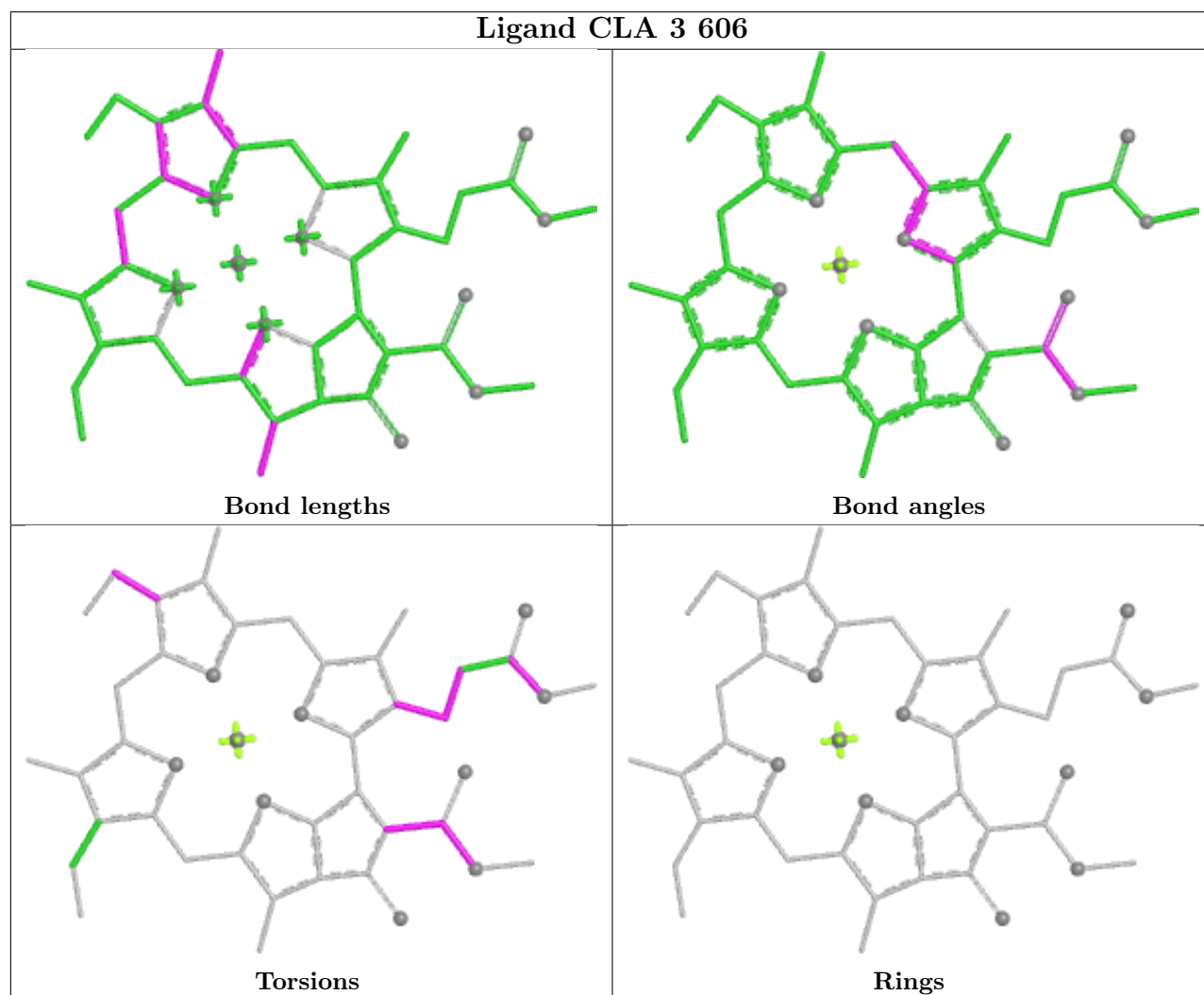
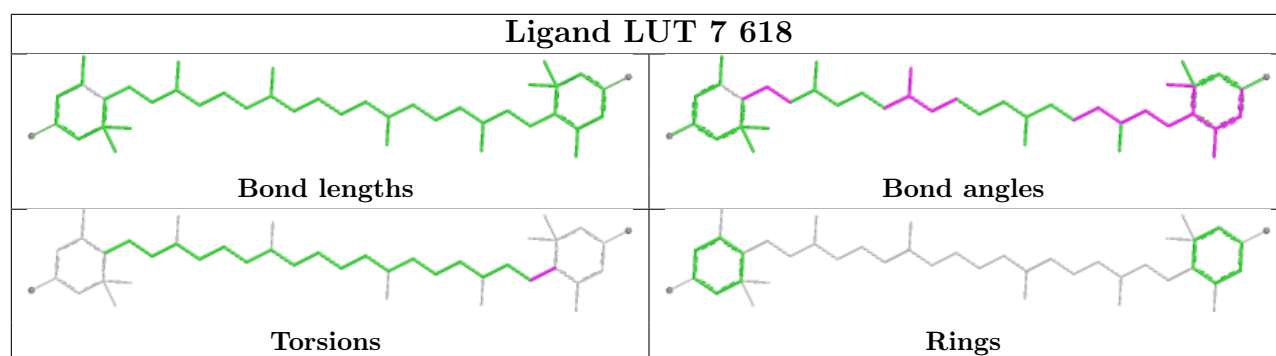


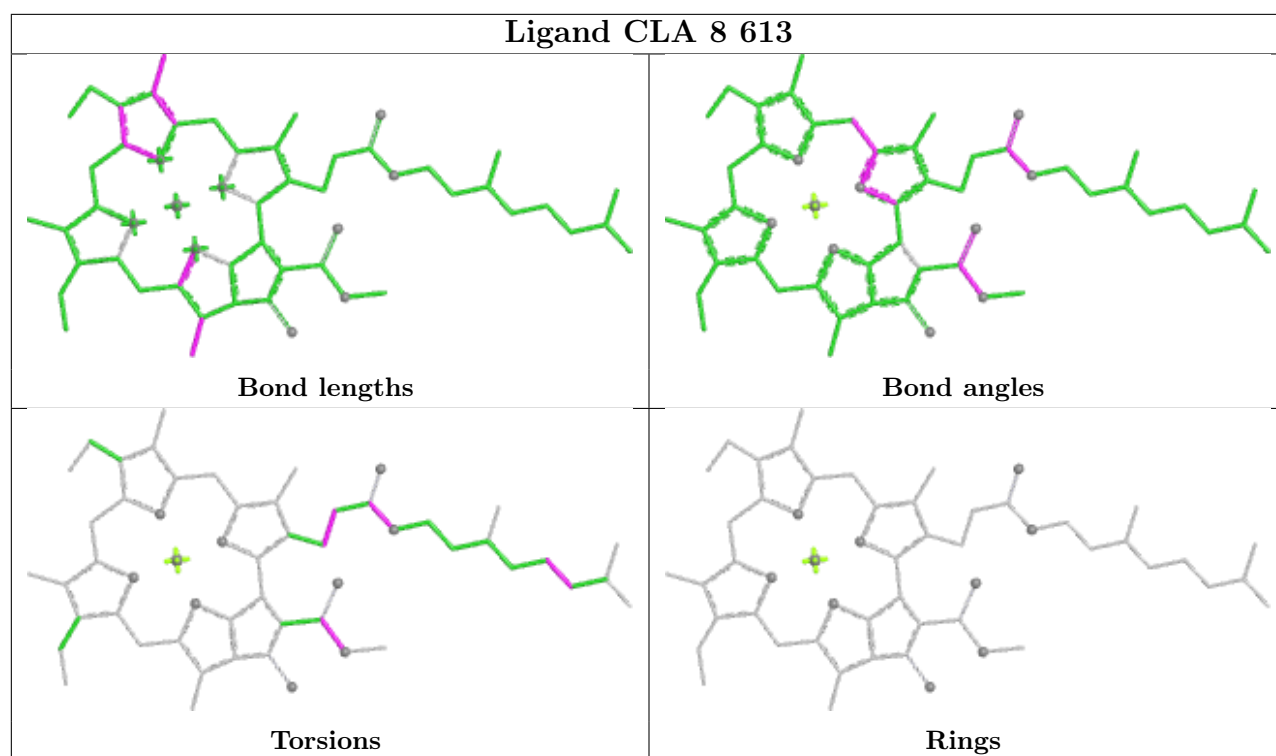
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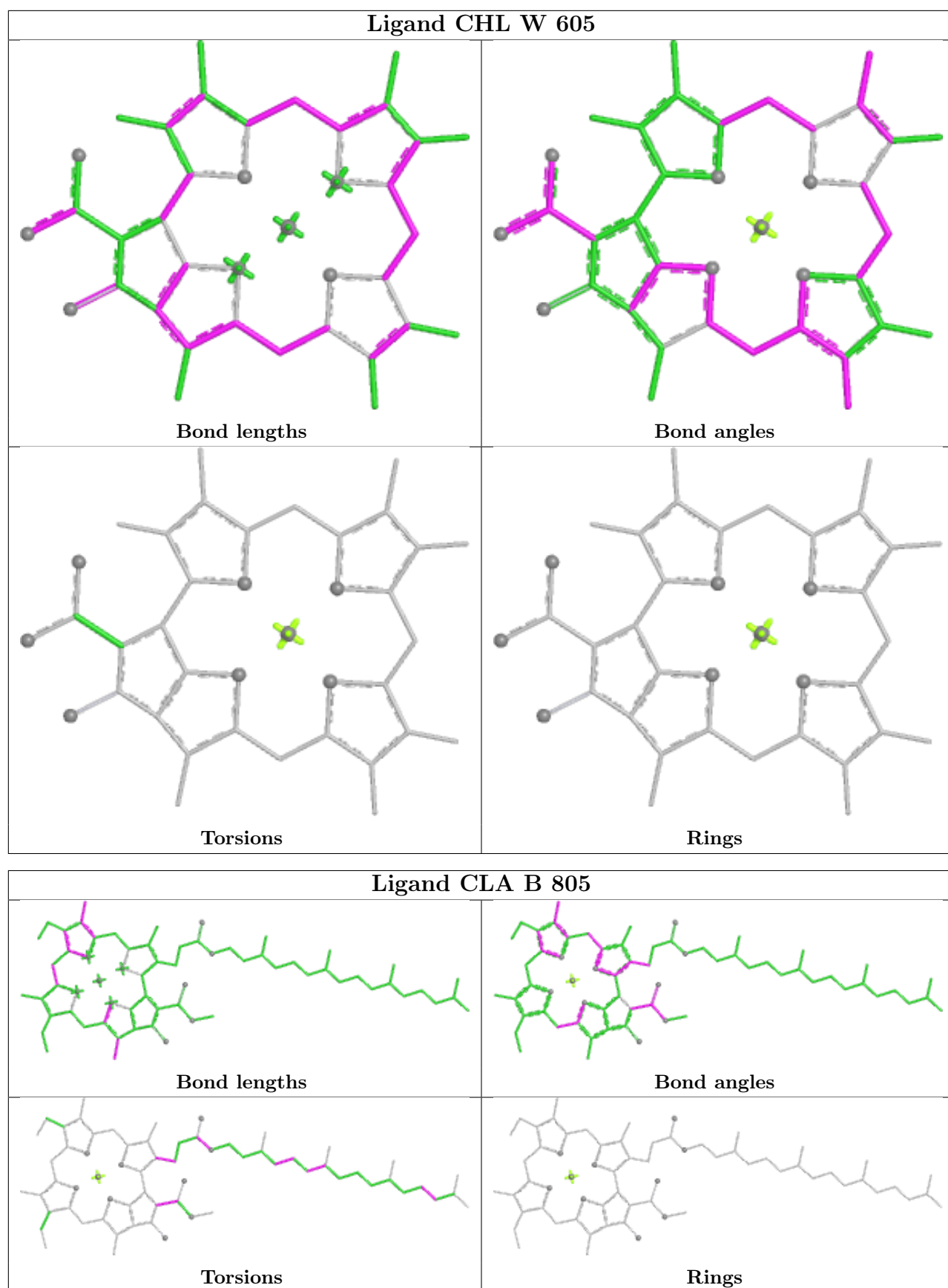


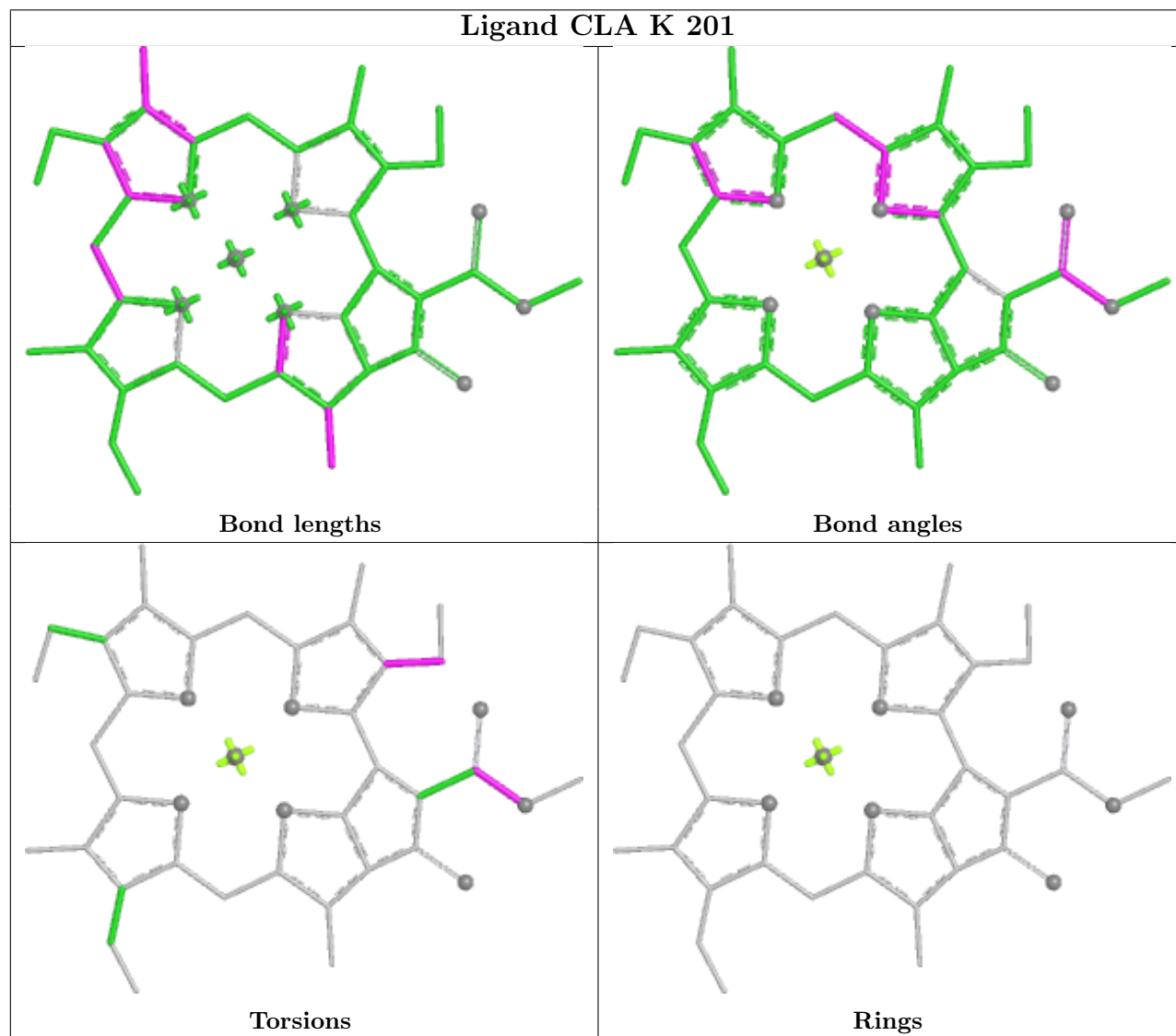
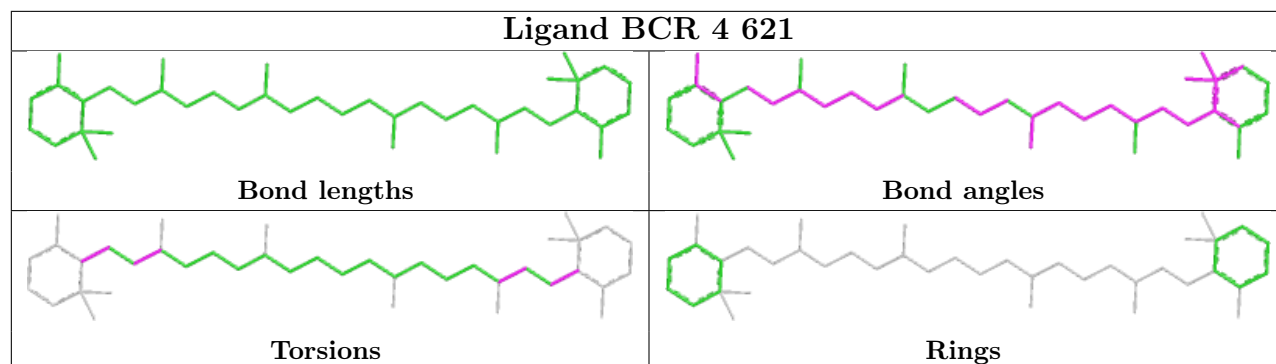
Ligand CLA B 811

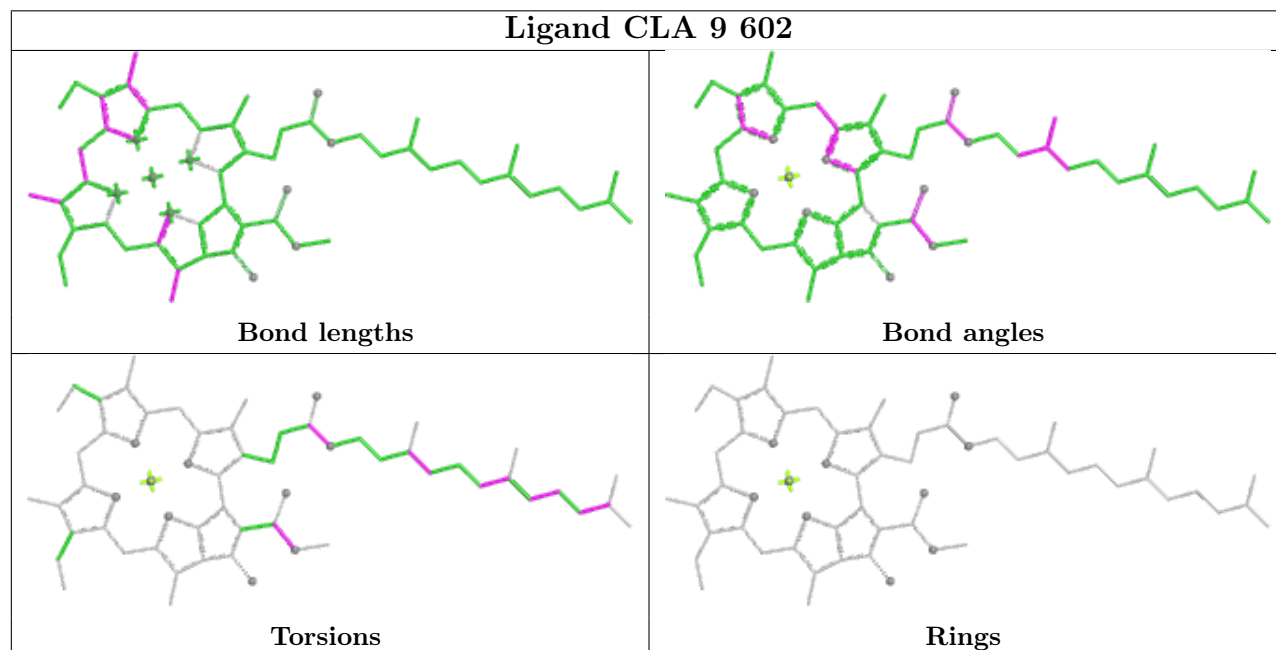
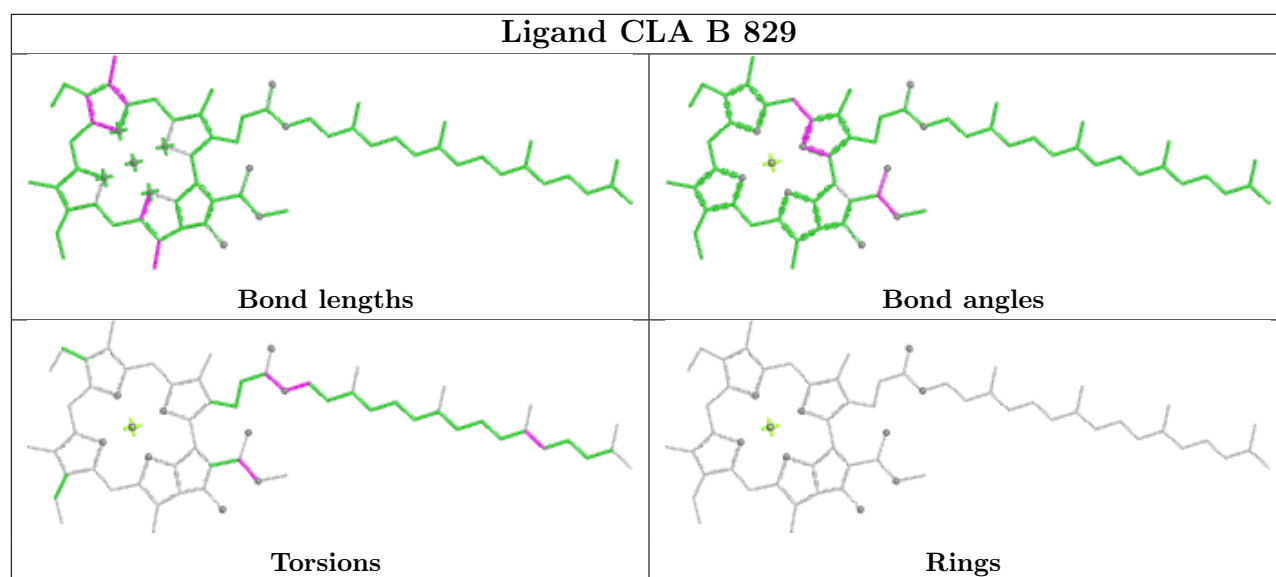




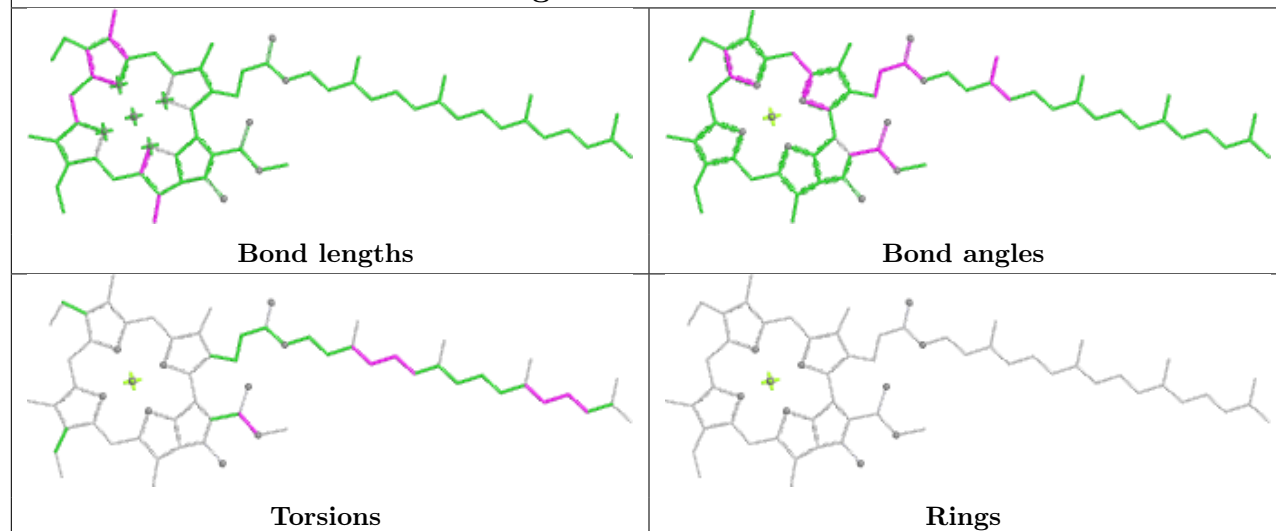




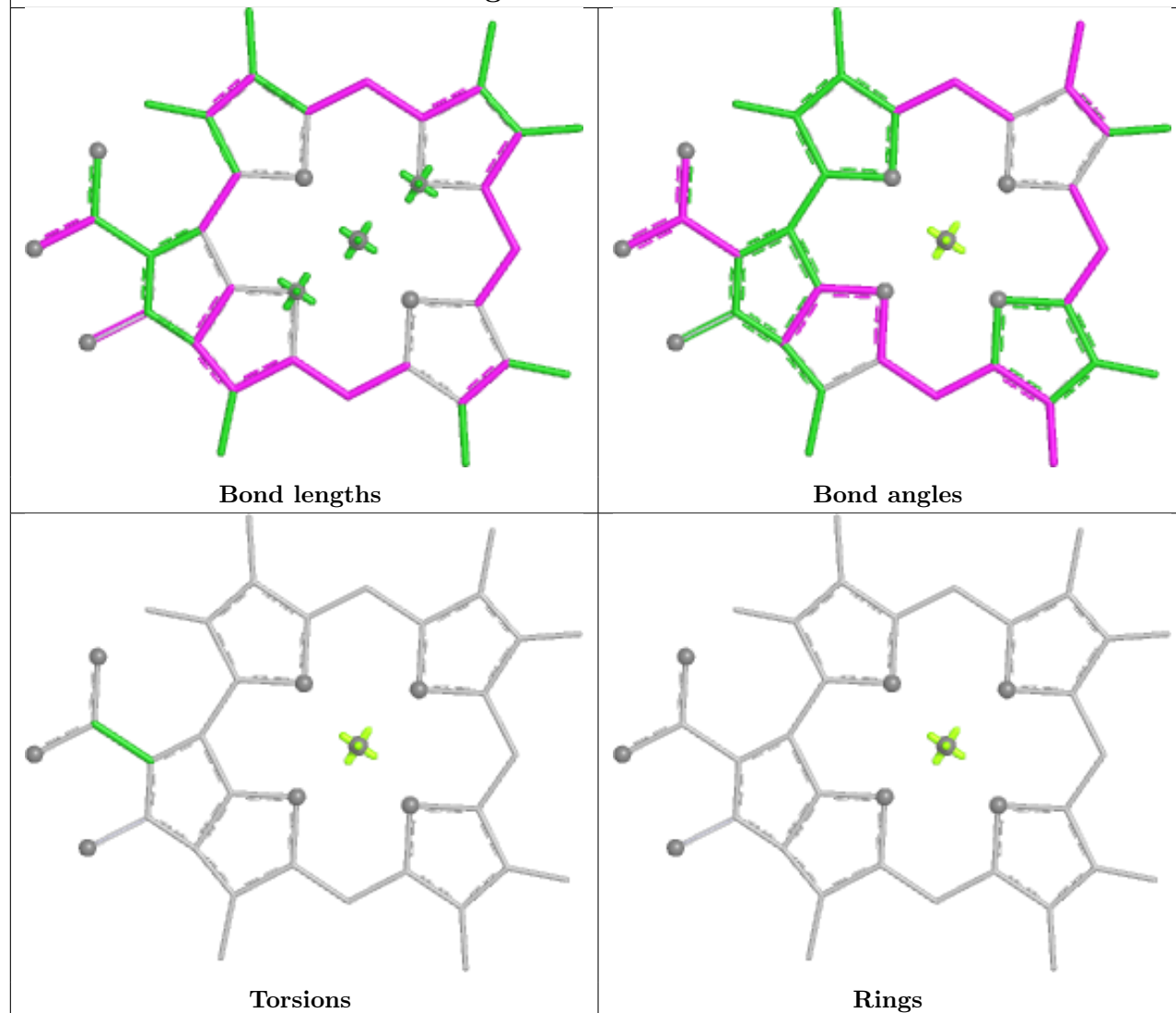




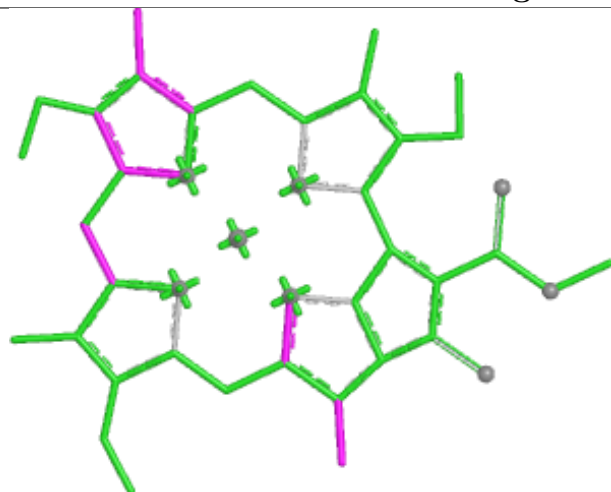
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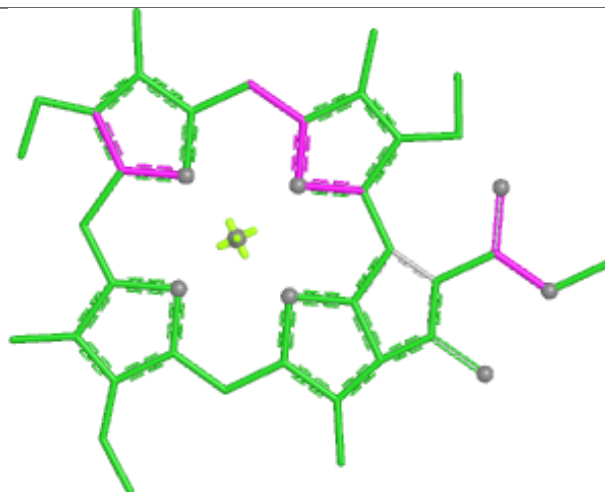
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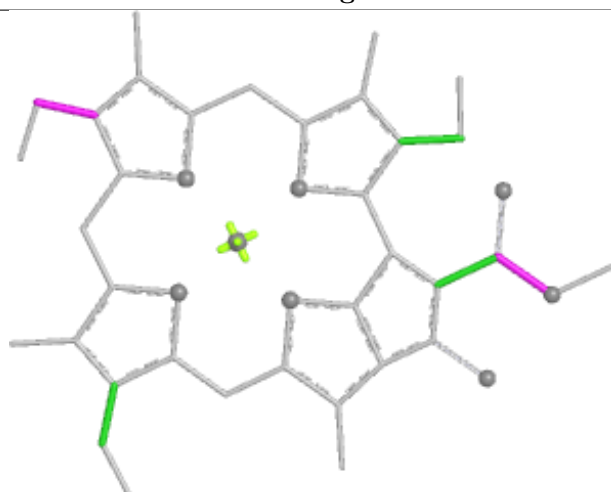
Ligand CLA K 206



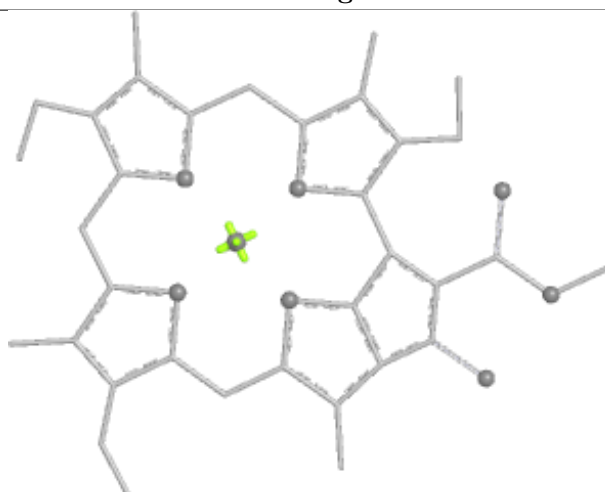
Bond lengths



Bond angles

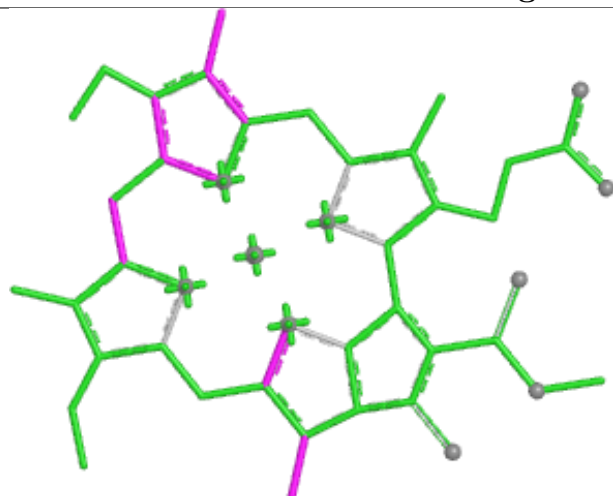


Torsions

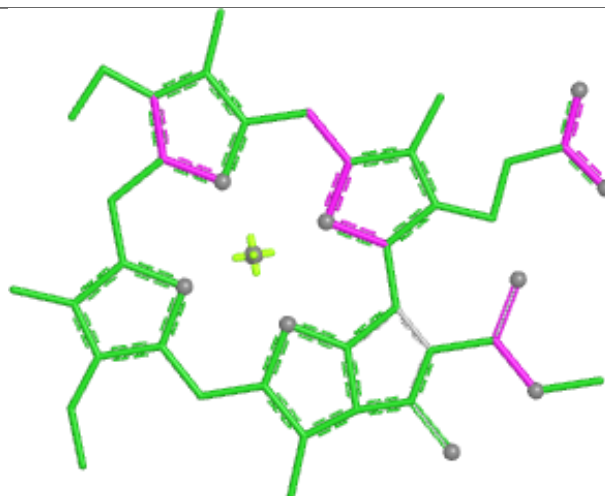


Rings

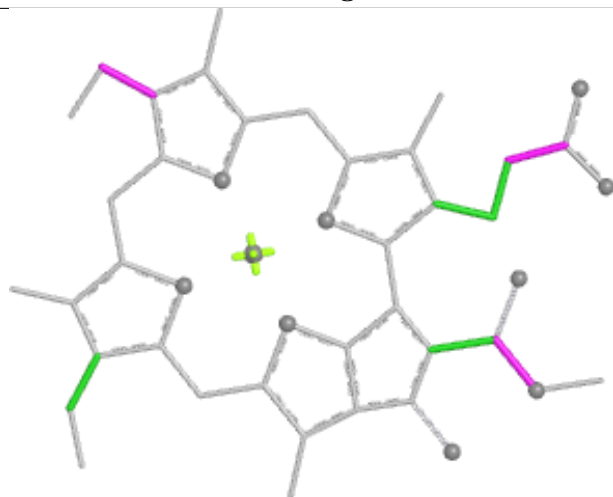
Ligand CLA 3 614



Bond lengths



Bond angles

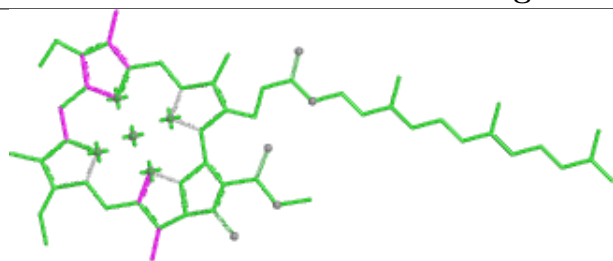


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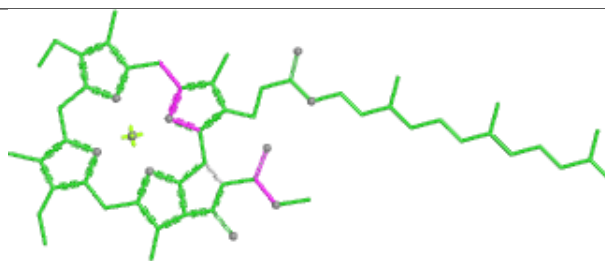


Rings

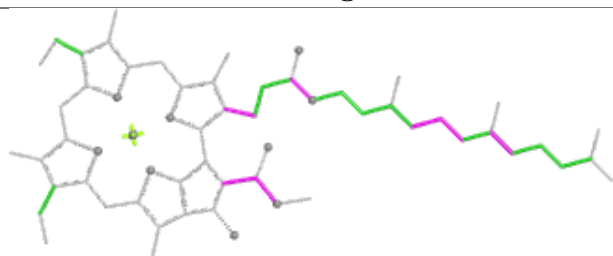
Ligand CLA V 603



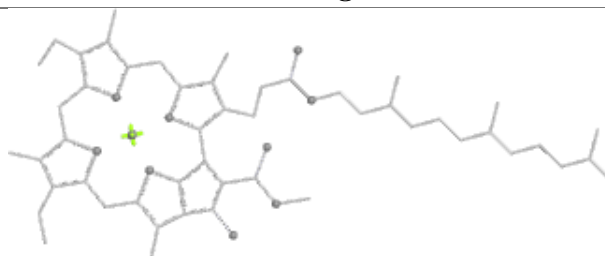
Bond lengths



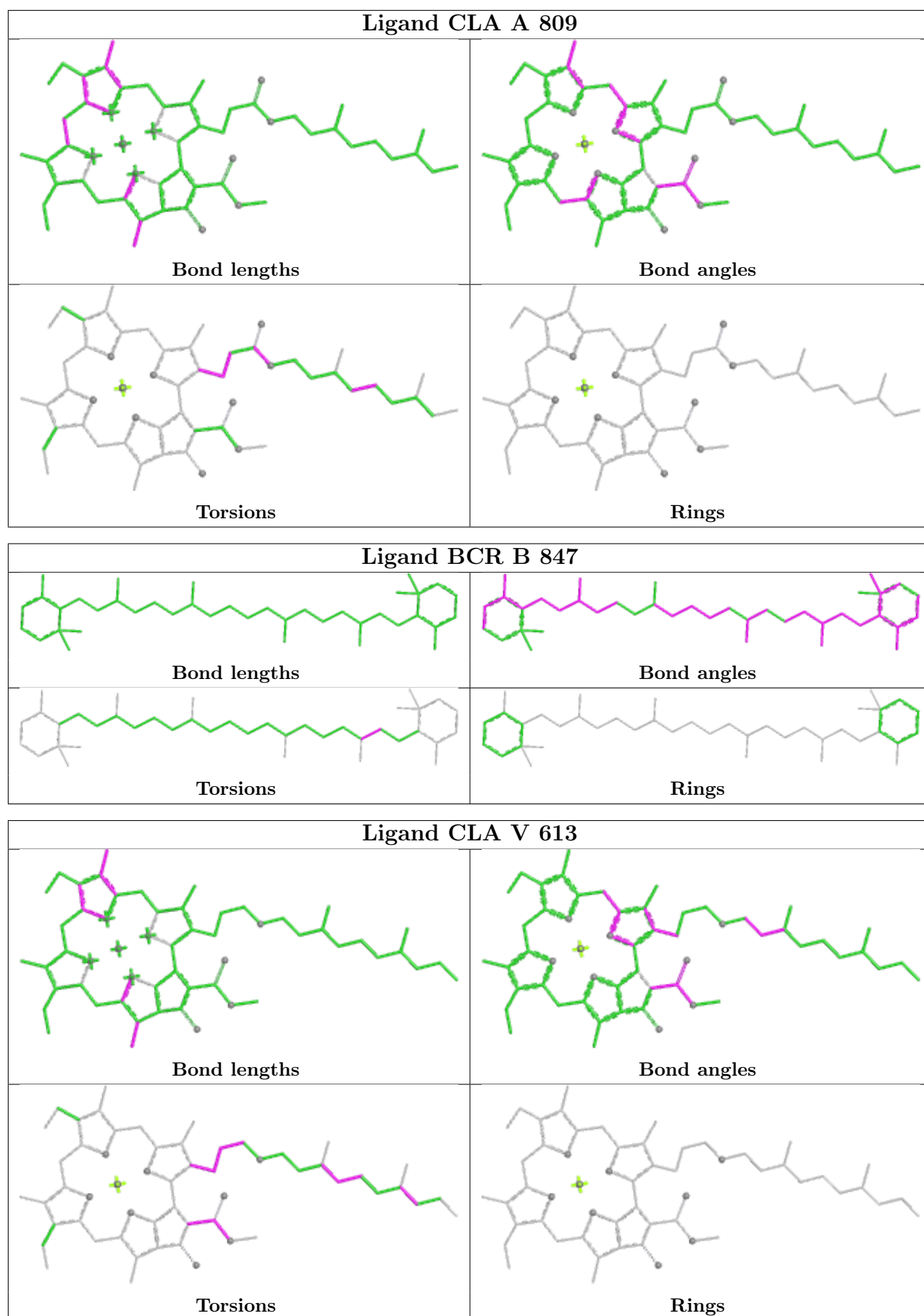
Bond angles

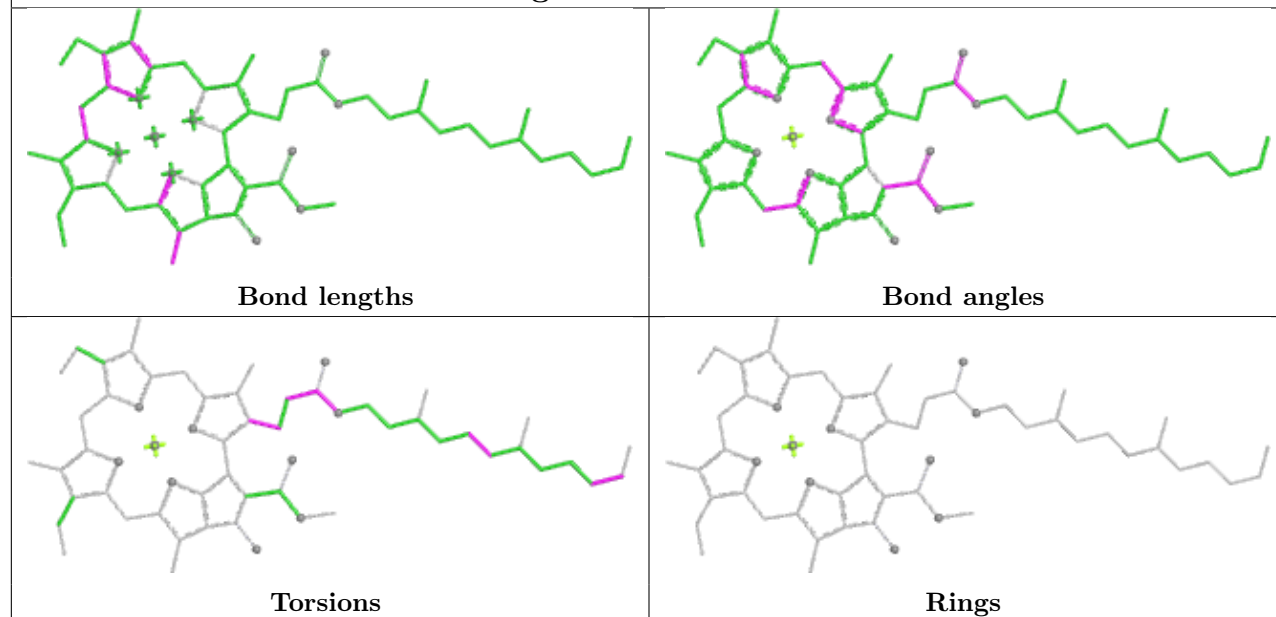
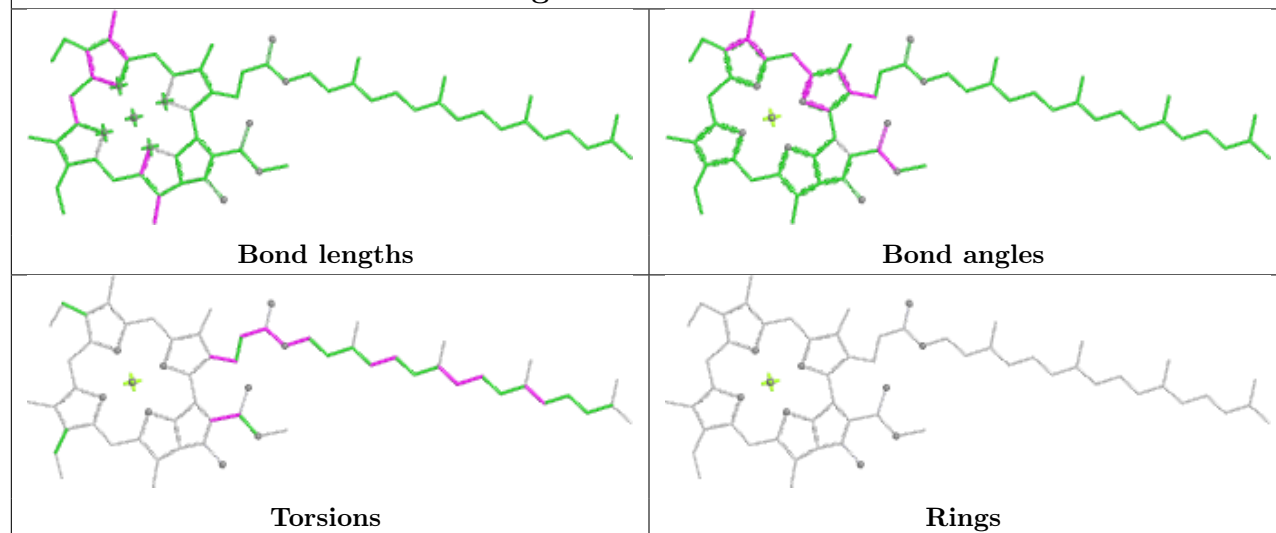


Torsions

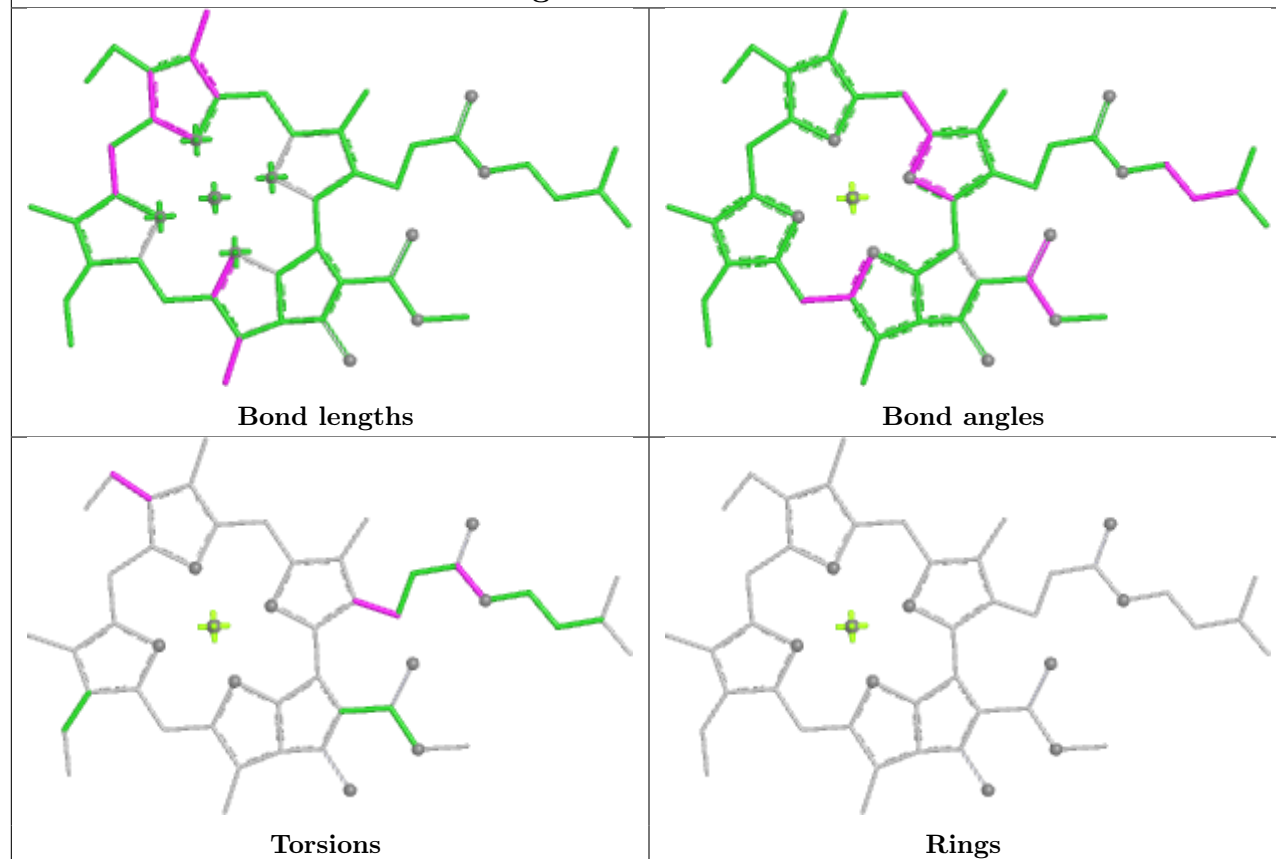


Rings

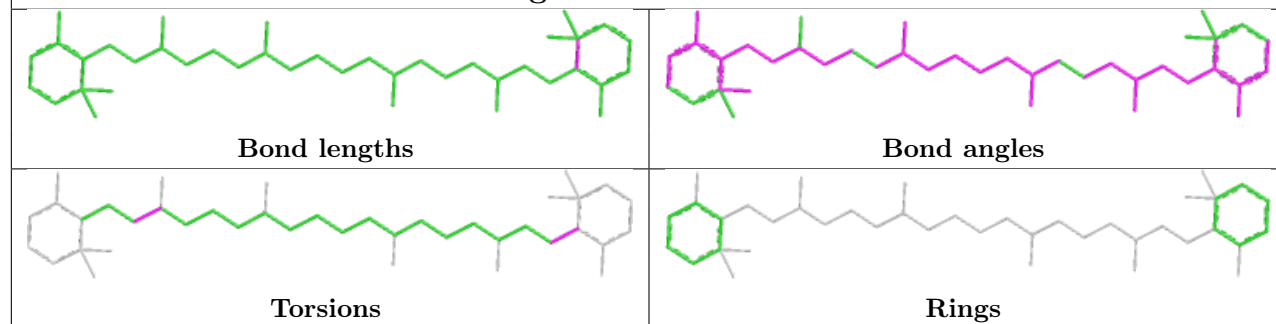


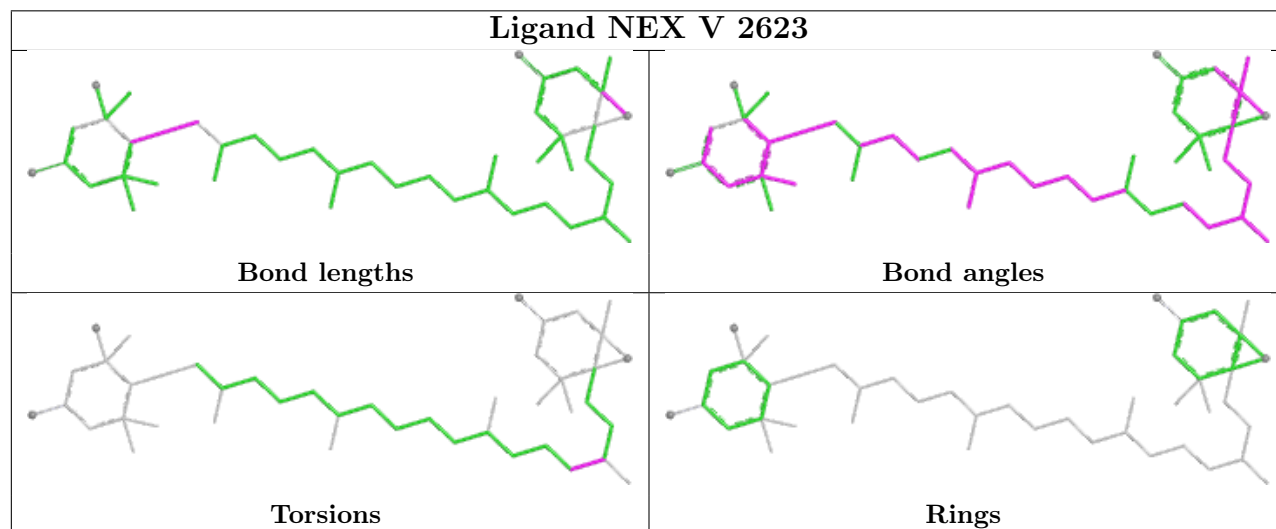
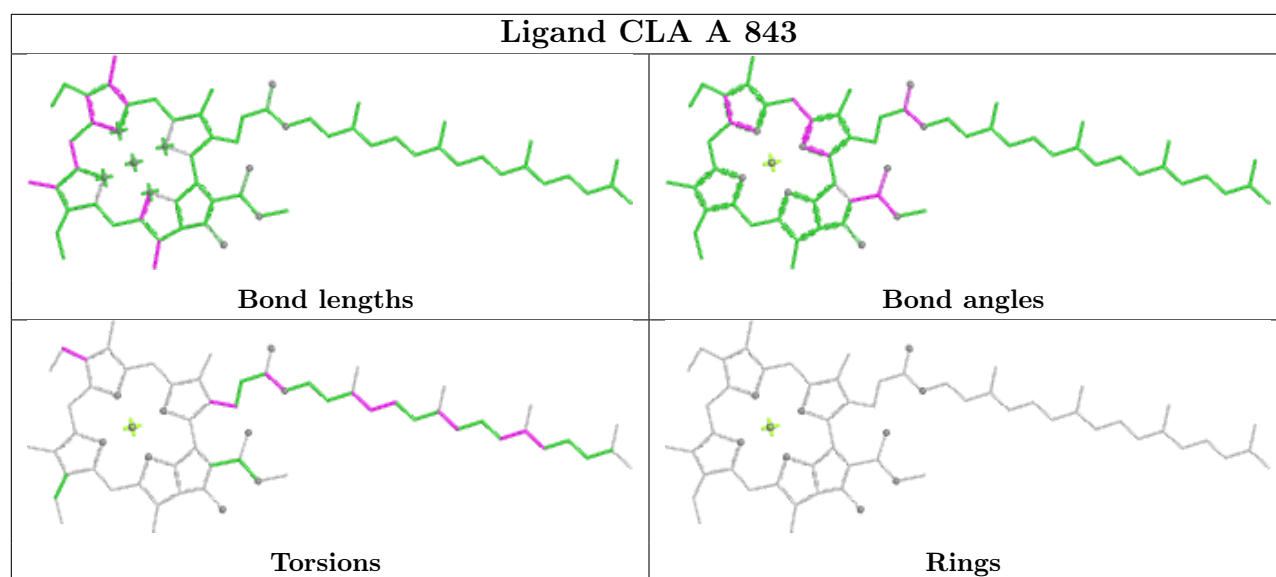
Ligand CLA V 602**Ligand CLA A 817**

Ligand CLA B 821

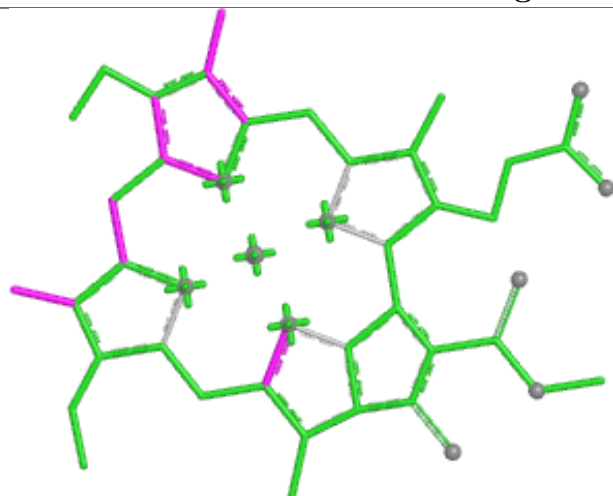


Ligand BCR K 205

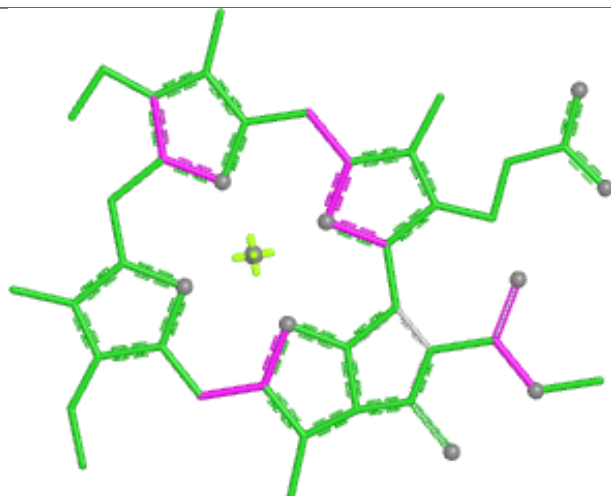




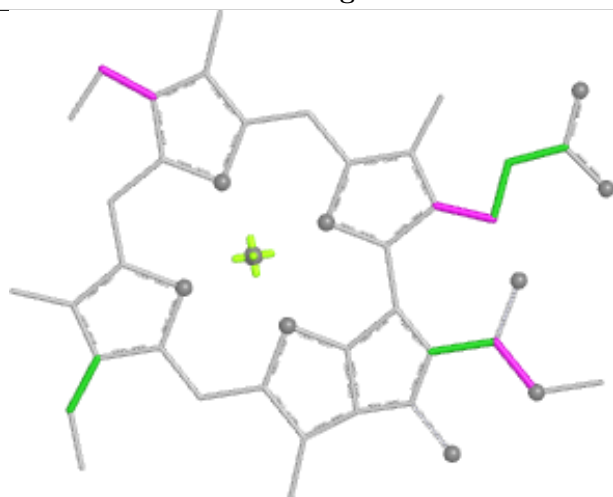
Ligand CLA B 830



Bond lengths



Bond angles

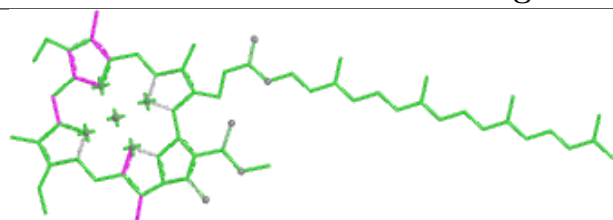


Torsions

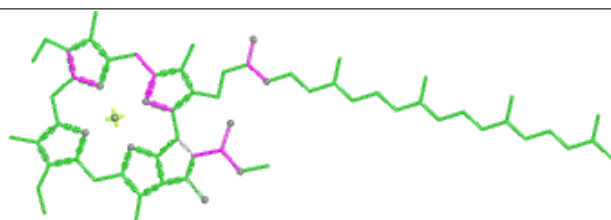


Rings

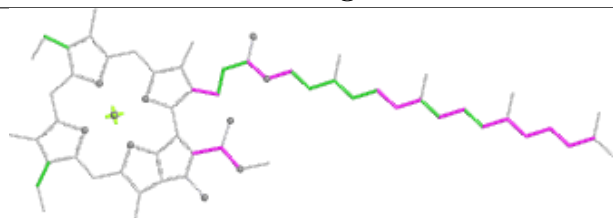
Ligand CLA A 804



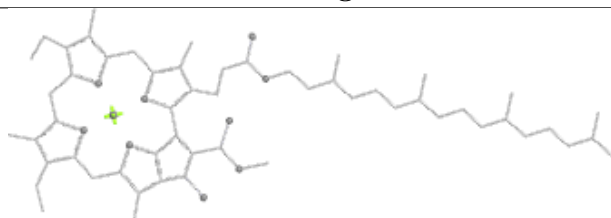
Bond lengths



Bond angles

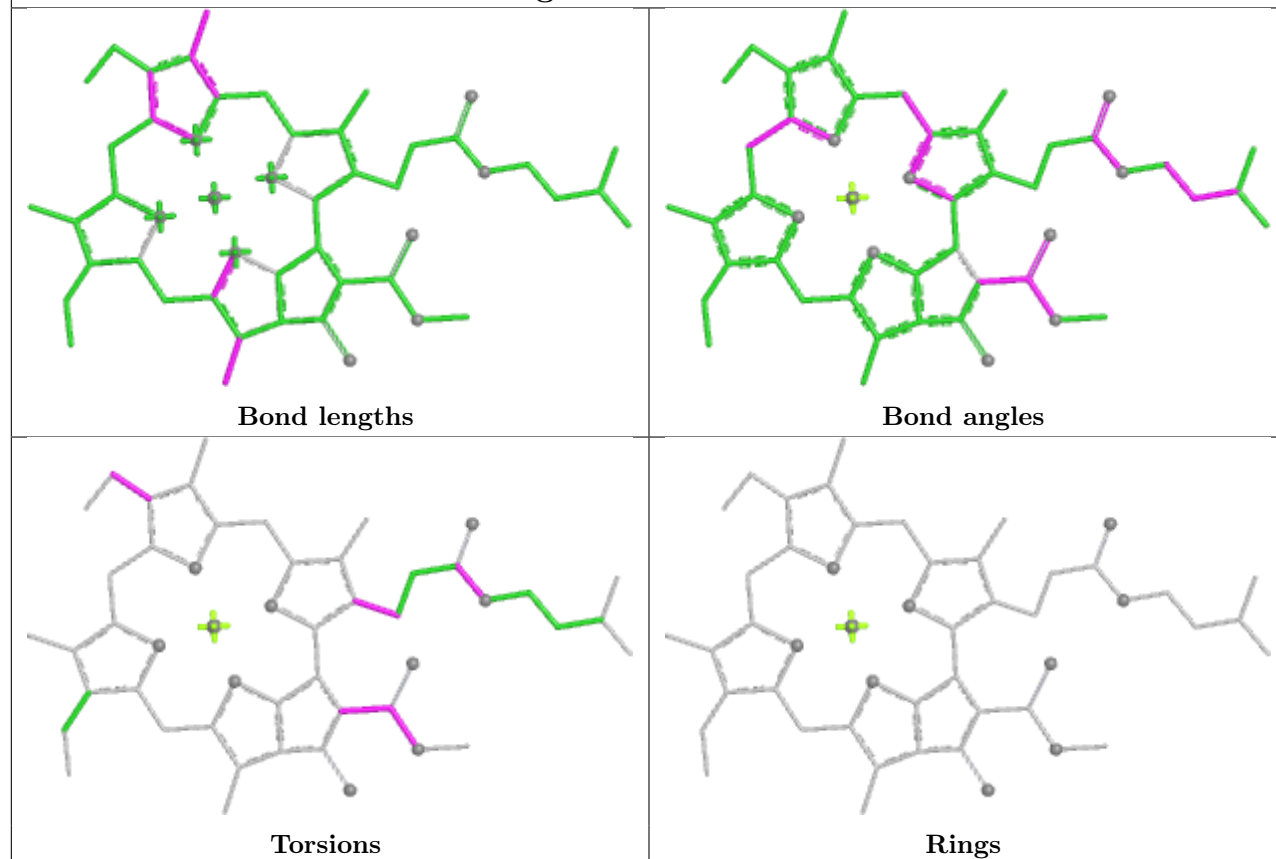


Torsions

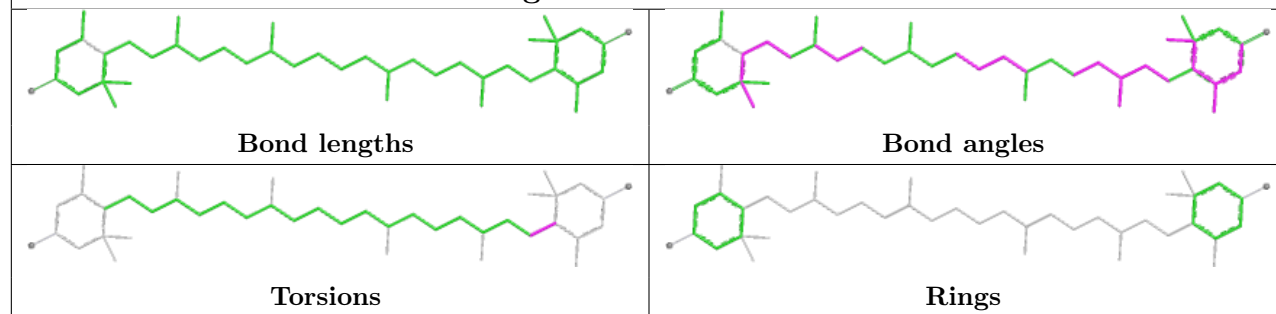


Rings

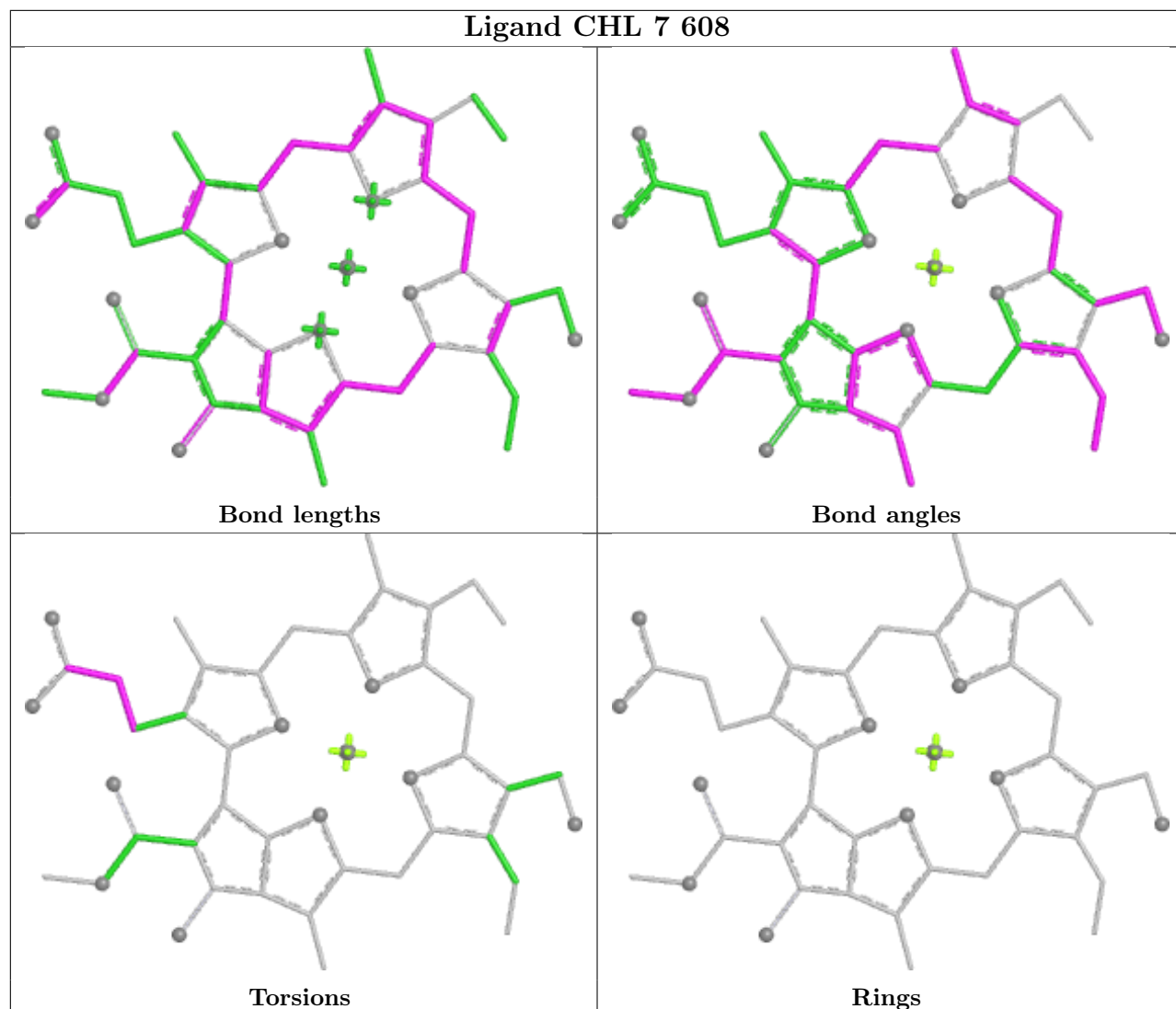
Ligand CLA 5 613



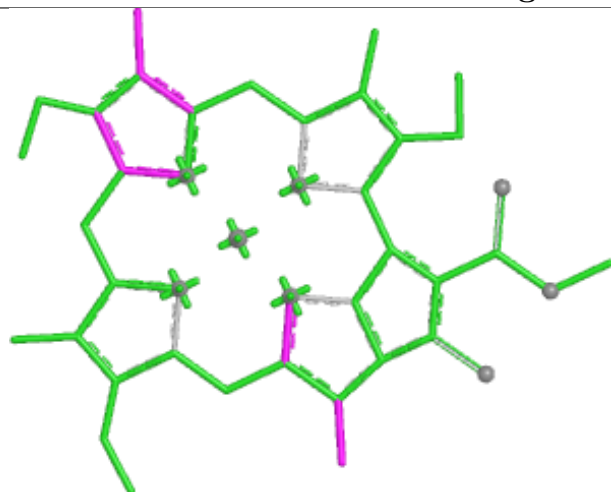
Ligand LUT V 2621



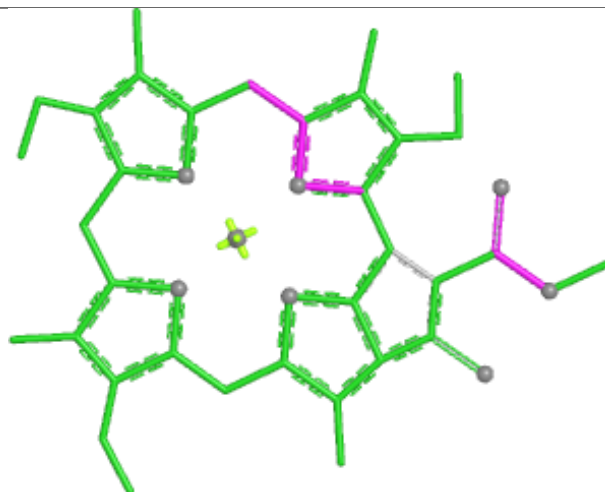
Ligand CHL 7 608



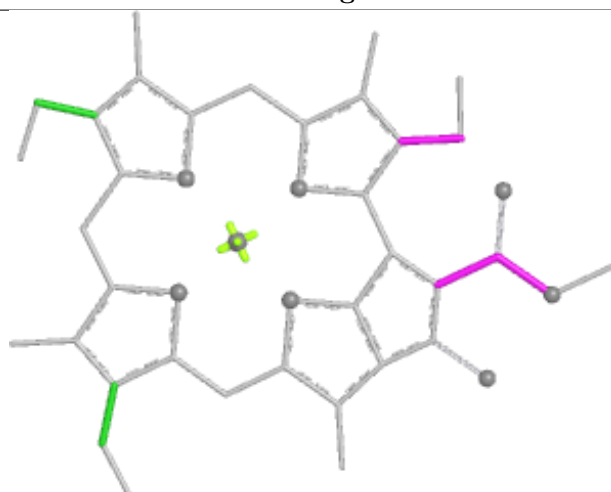
Ligand CLA 9 603



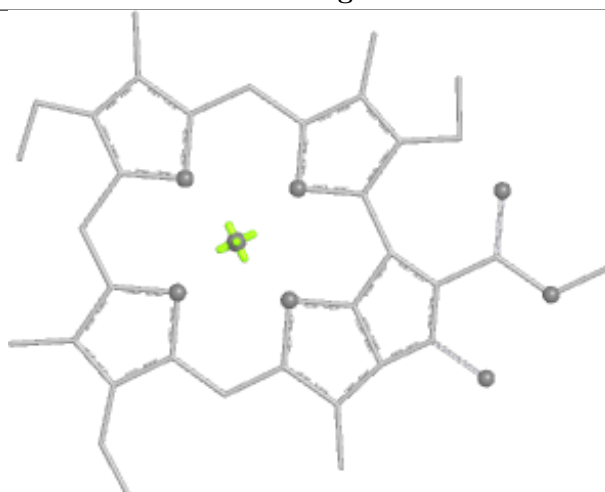
Bond lengths



Bond angles

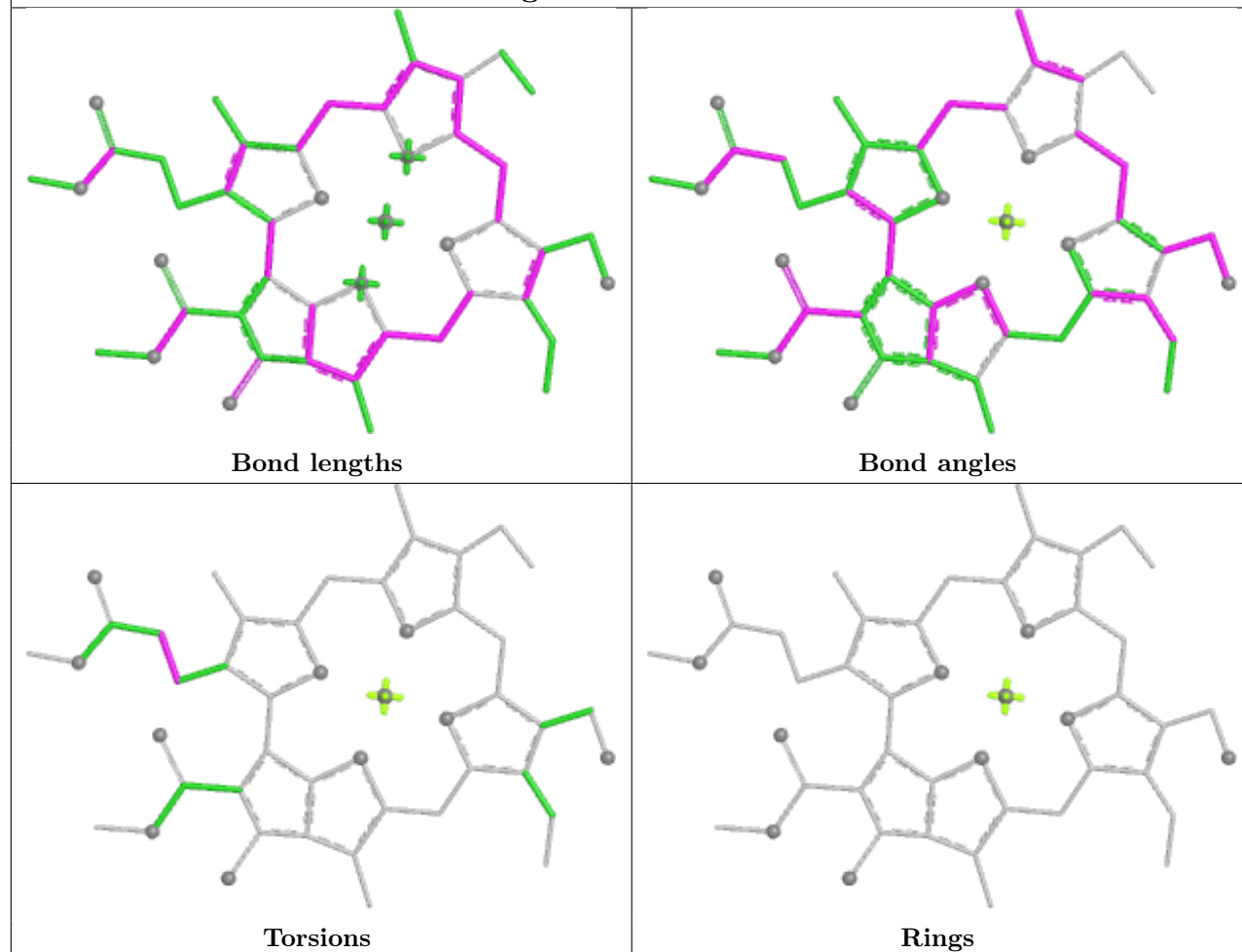


Torsions

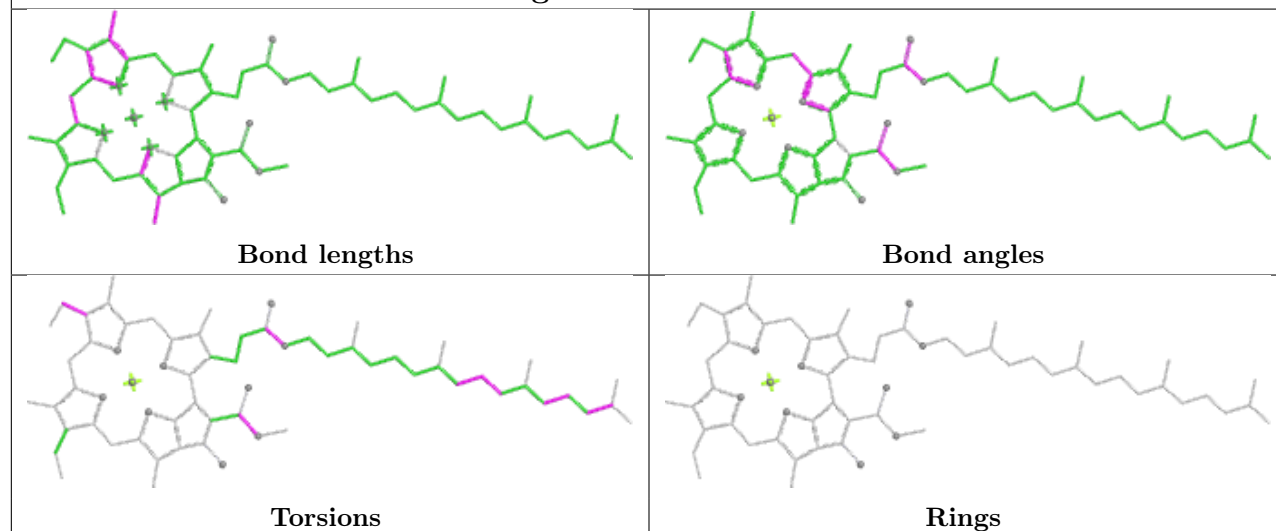


Rings

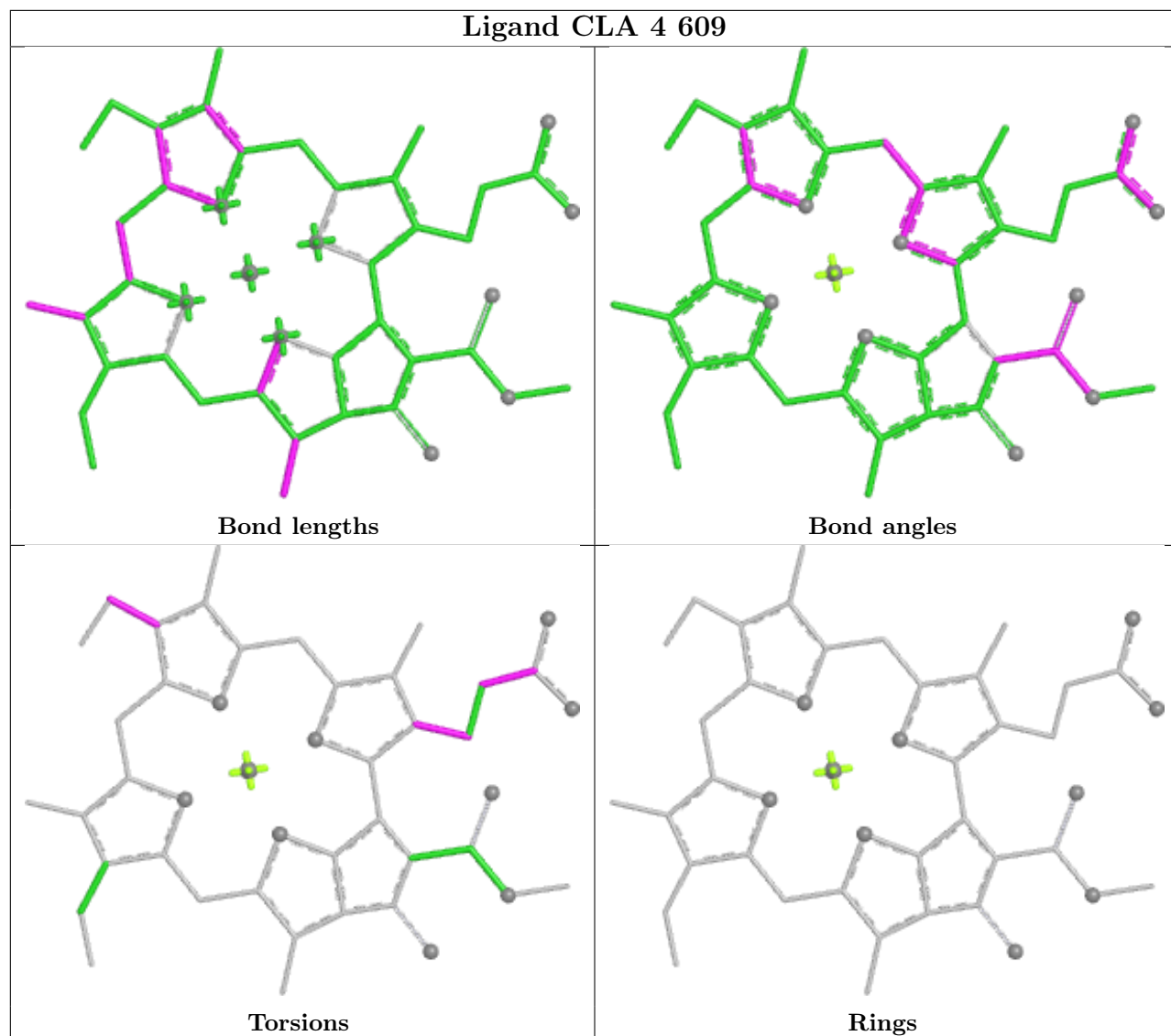
Ligand CHL 2 607



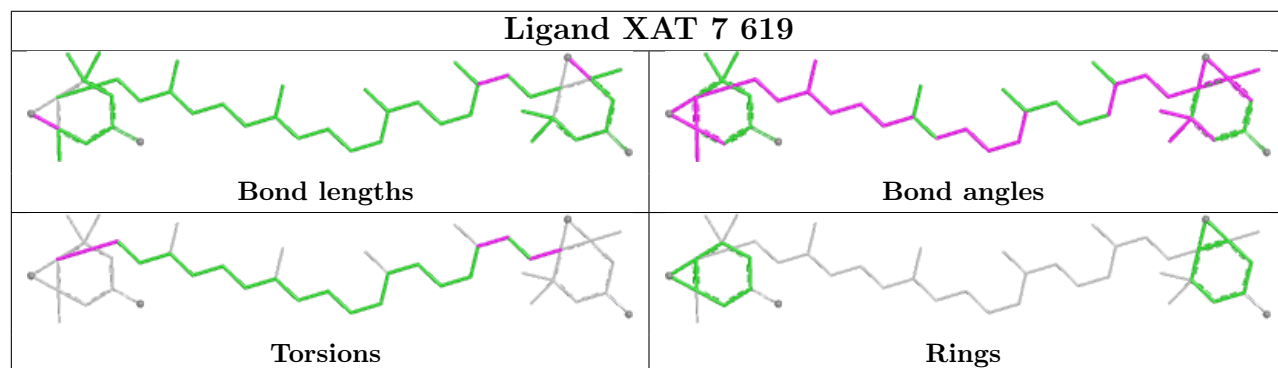
Ligand CLA A 841



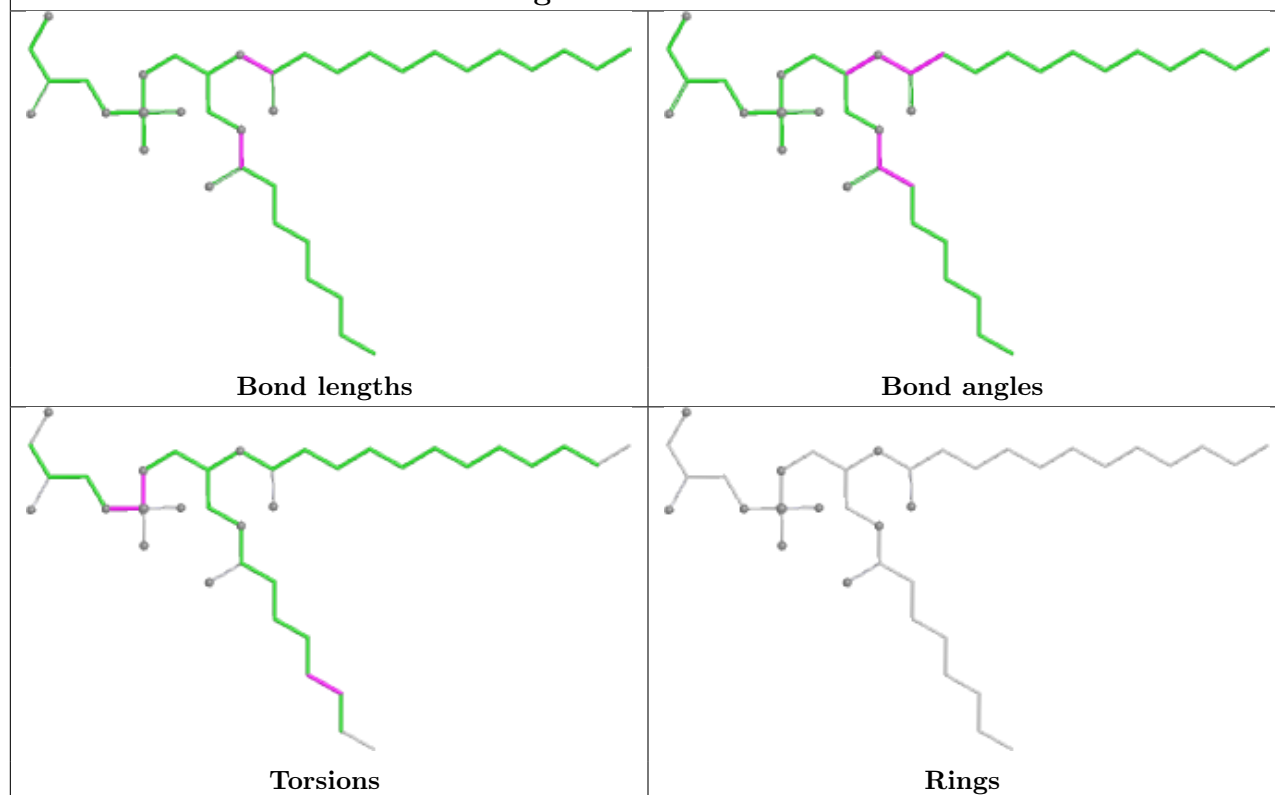
Ligand CLA 4 609



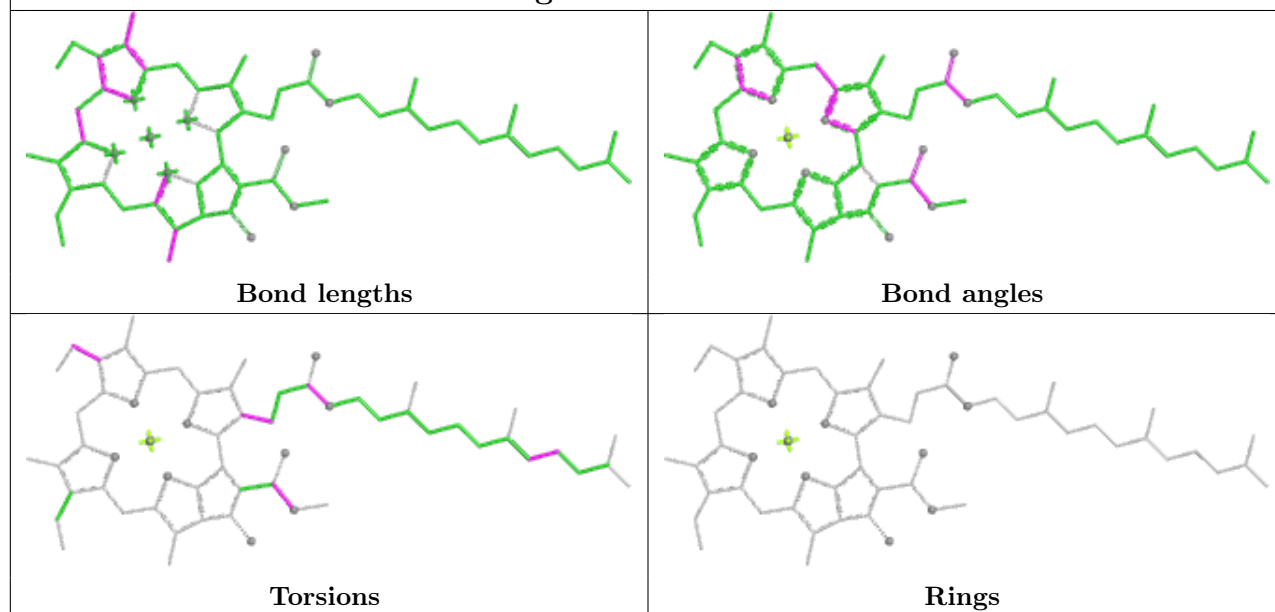
Ligand XAT 7 619

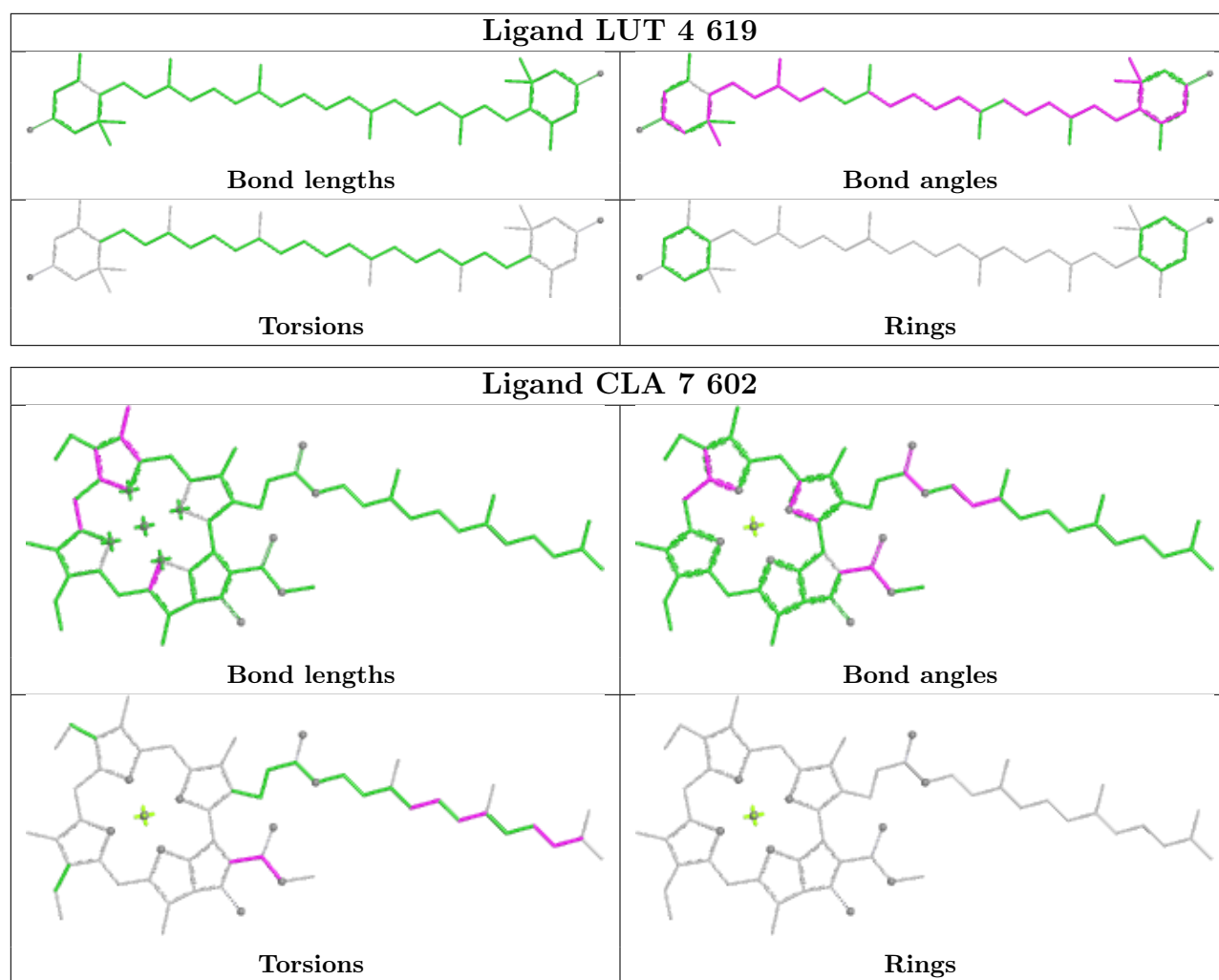


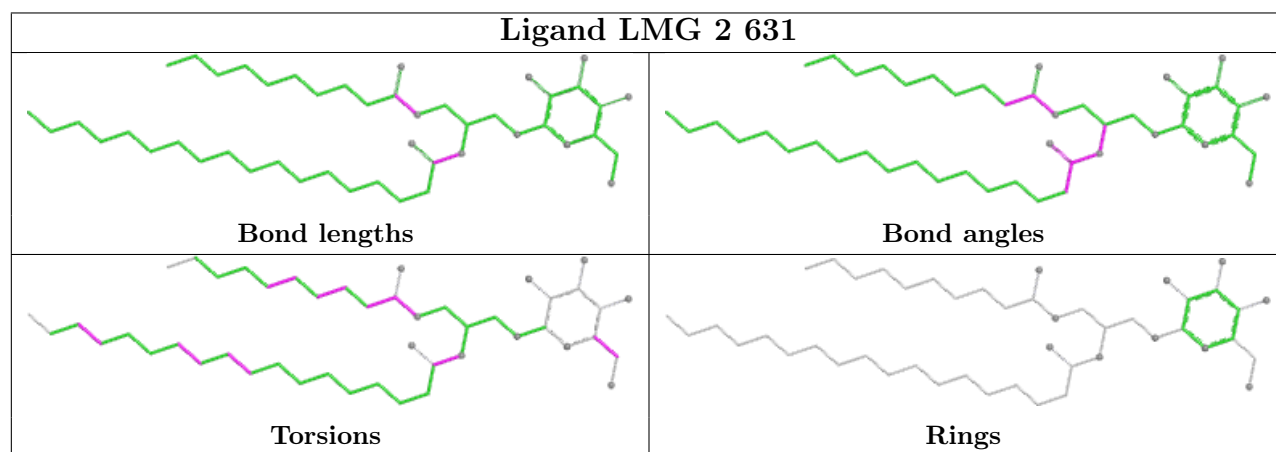
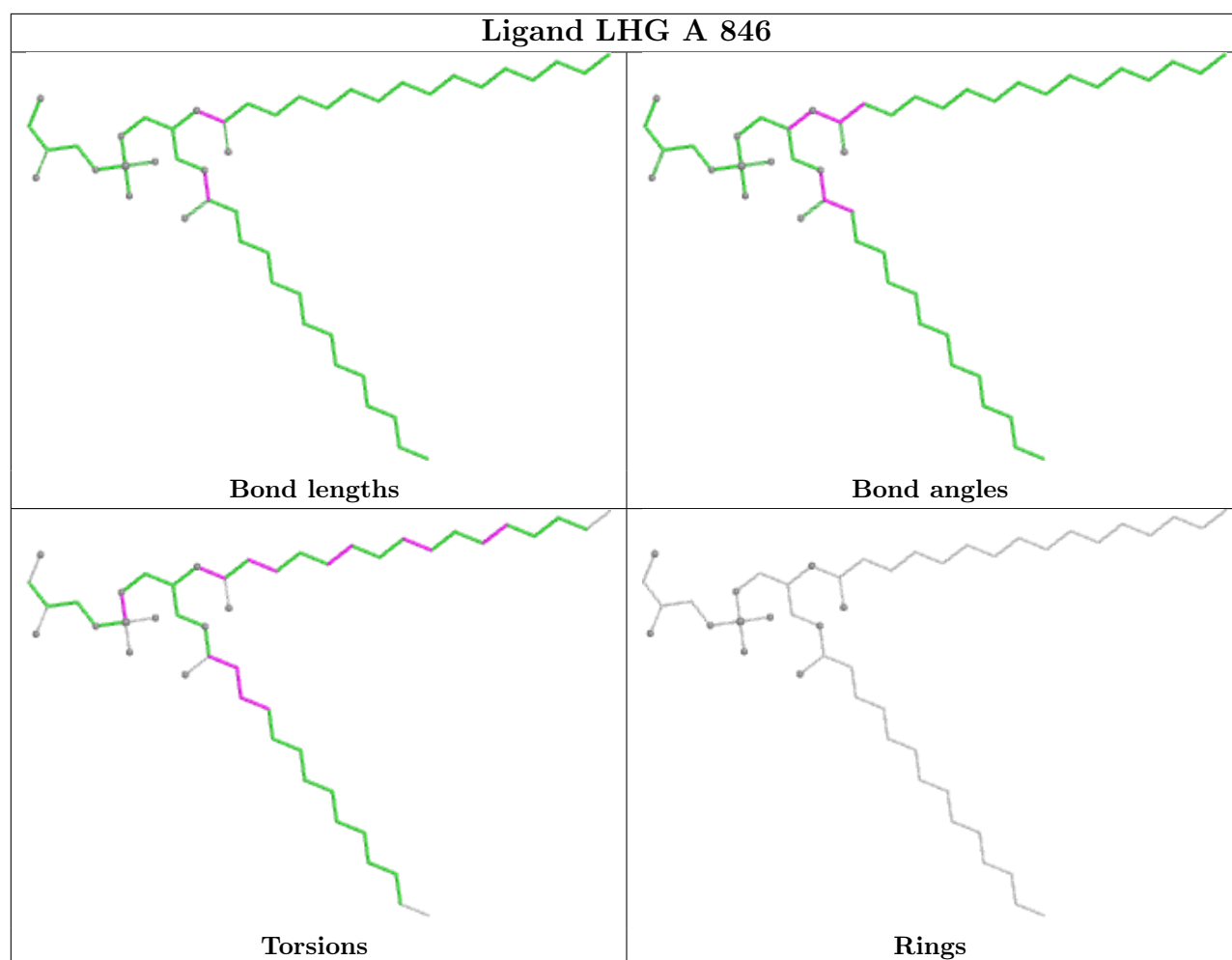
Ligand LHG 5 630



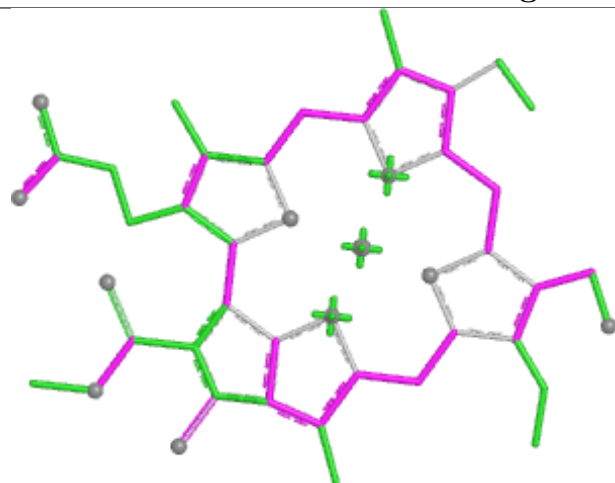
Ligand CLA 3 610



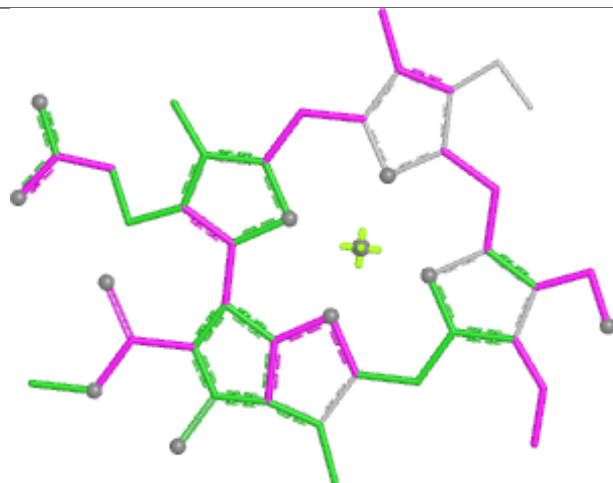




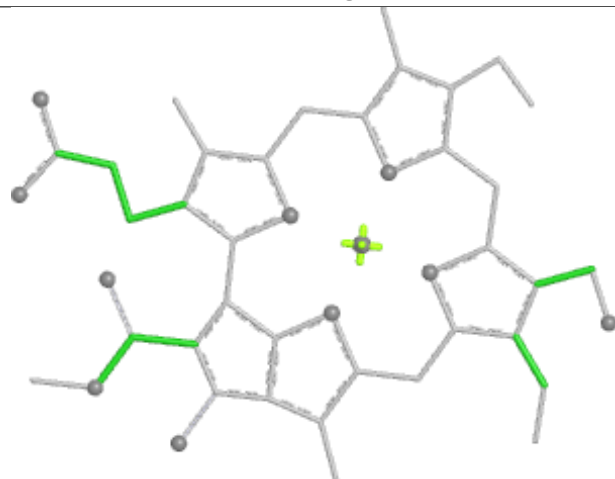
Ligand CHL 8 606



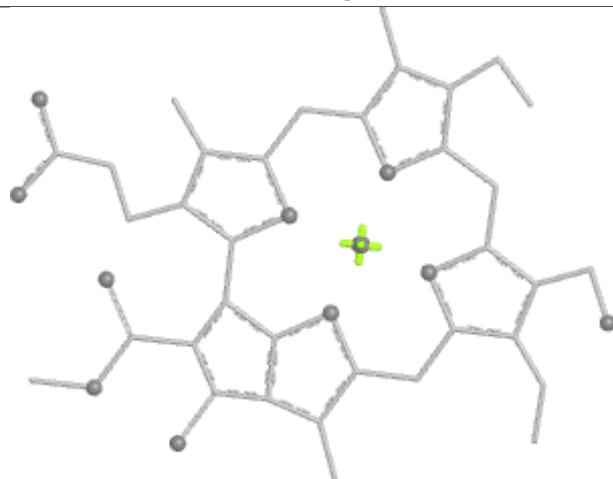
Bond lengths



Bond angles

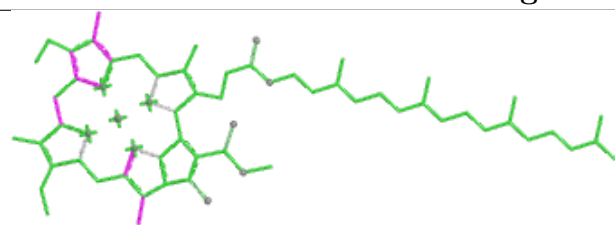


Torsions

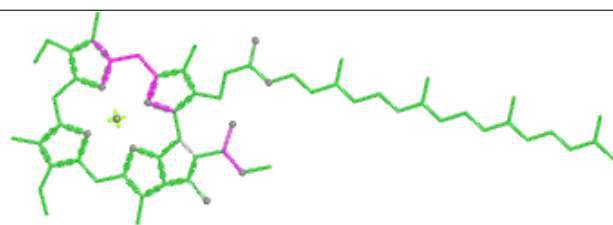


Rings

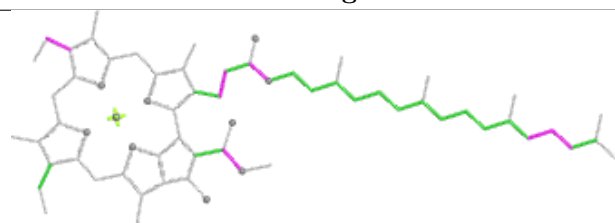
Ligand CLA 3 603



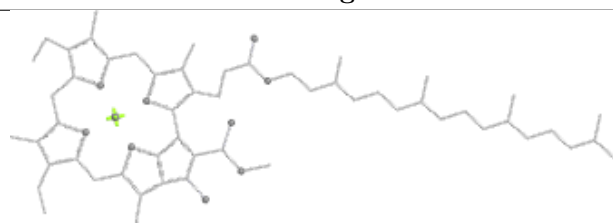
Bond lengths



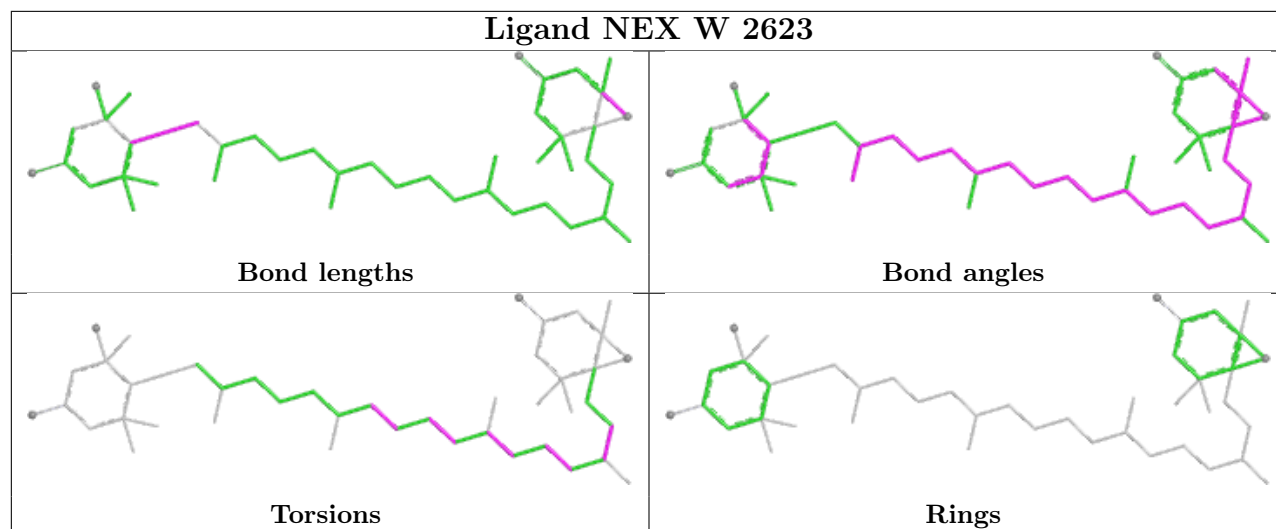
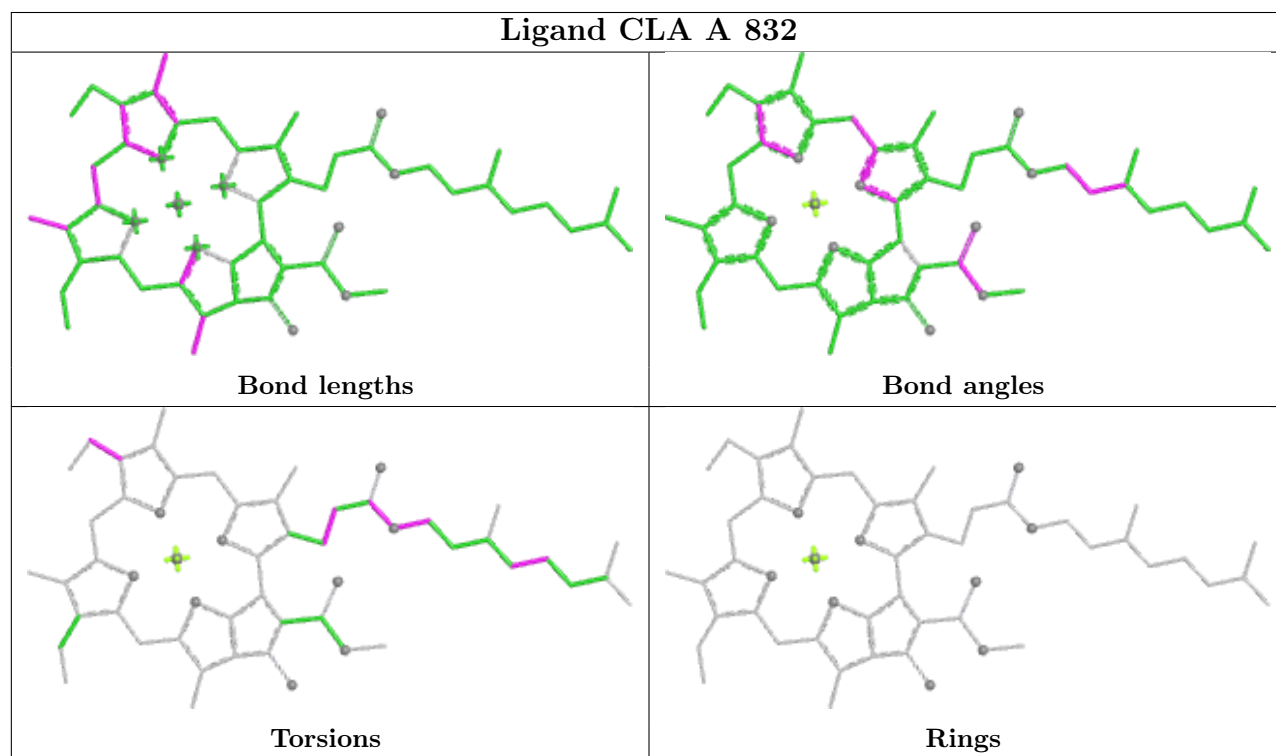
Bond angles



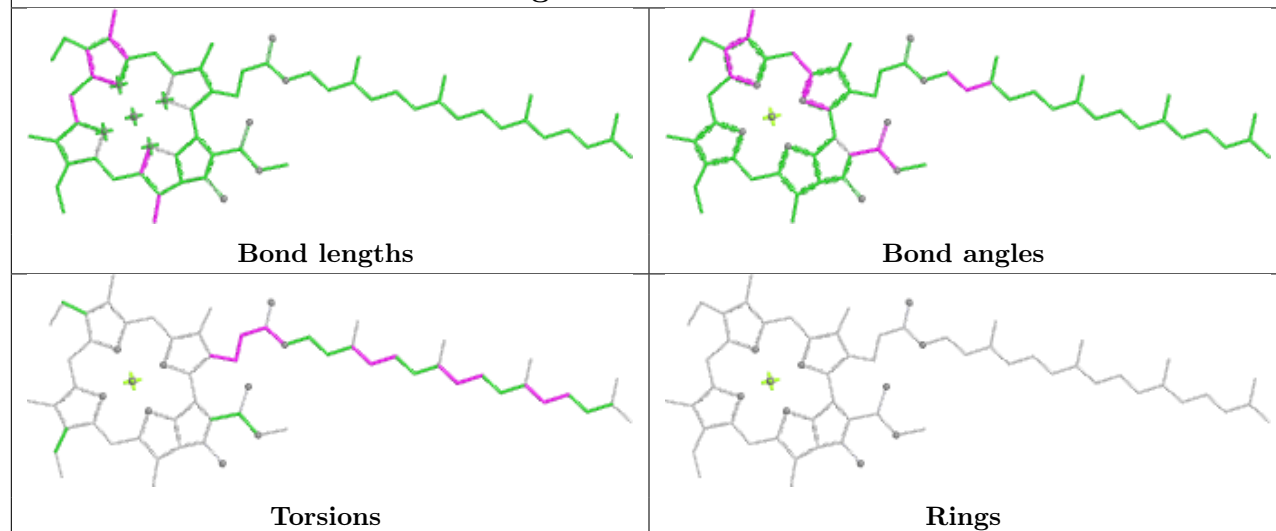
Torsions



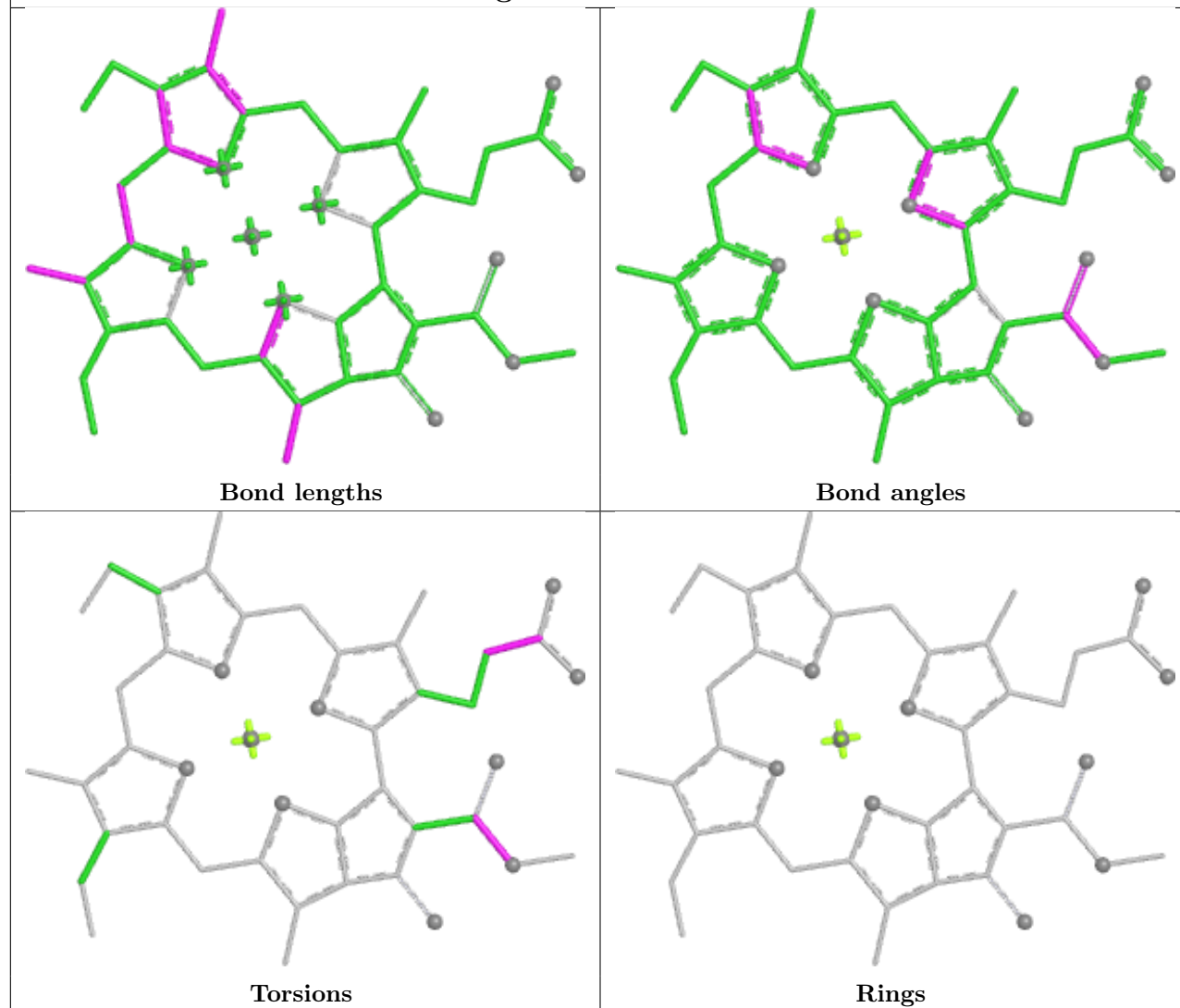
Rings

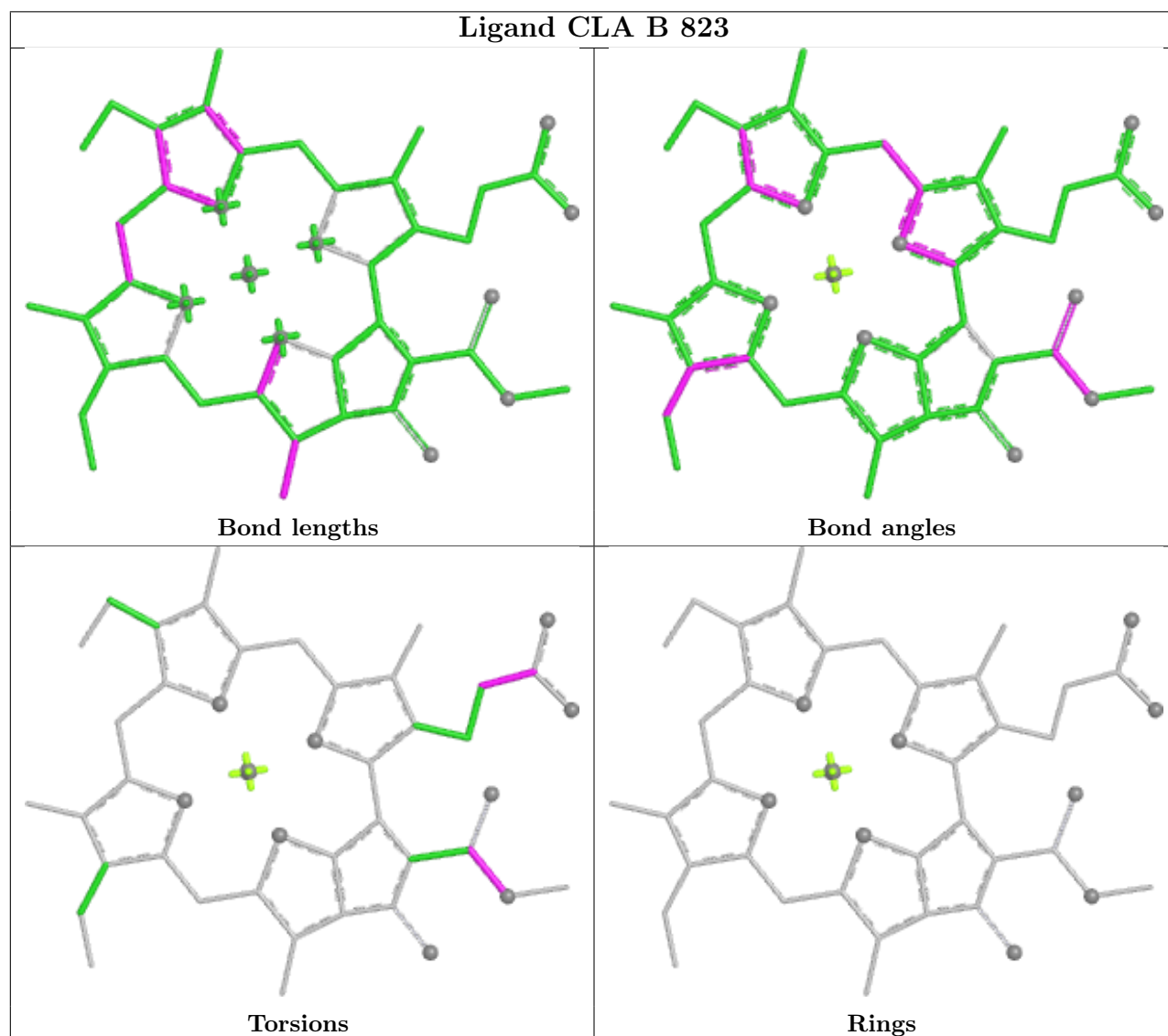
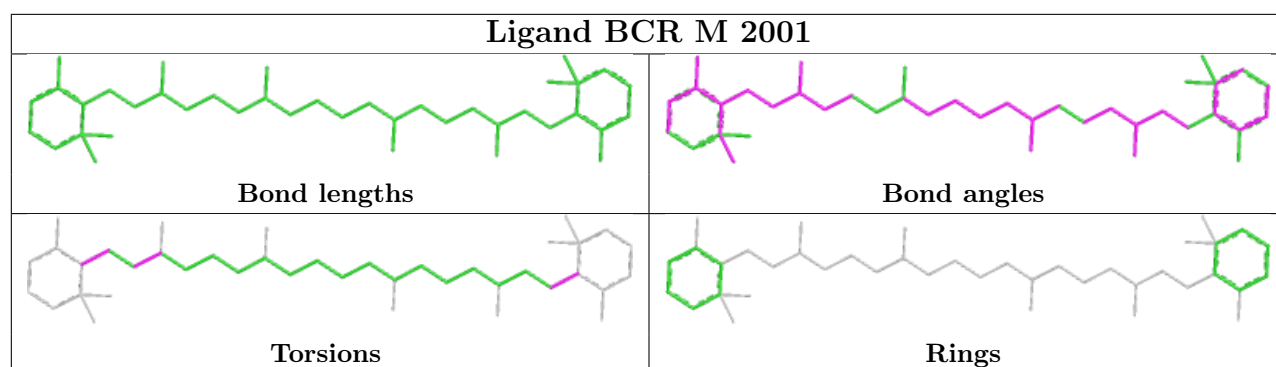
Ligand NEX W 2623**Ligand CLA A 832**

Ligand CLA A 830

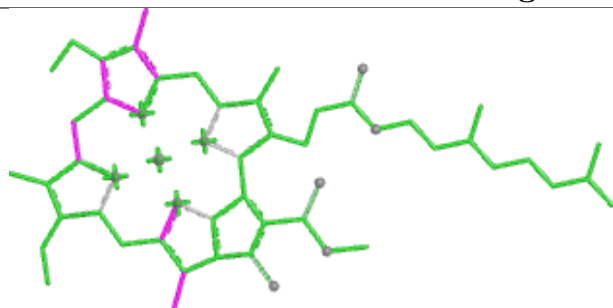


Ligand CLA 4 611

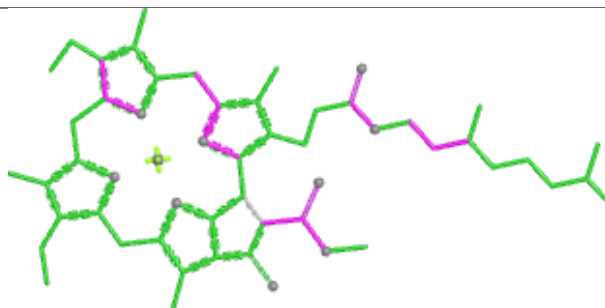




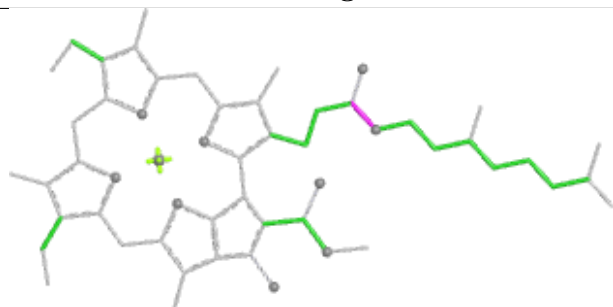
Ligand CLA 6 609



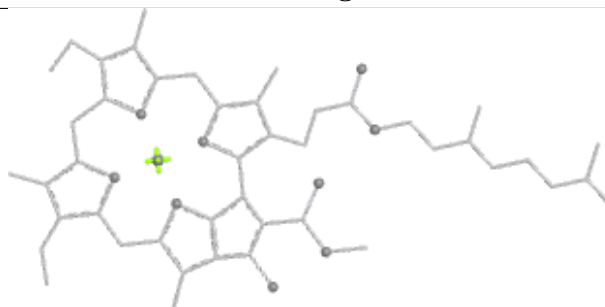
Bond lengths



Bond angles

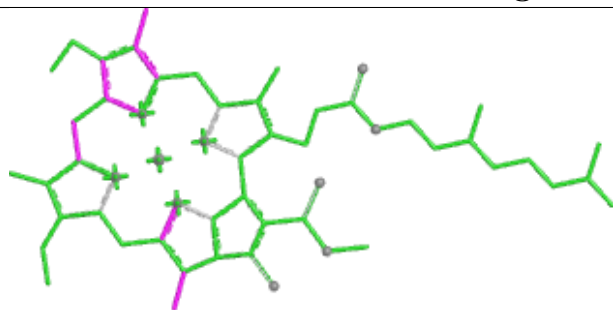


Torsions

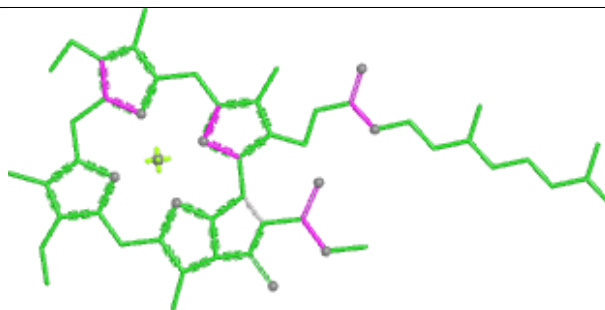


Rings

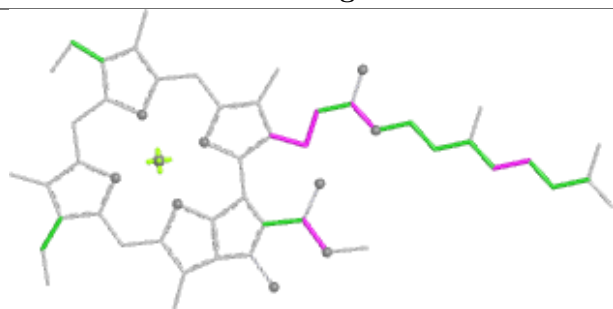
Ligand CLA A 811



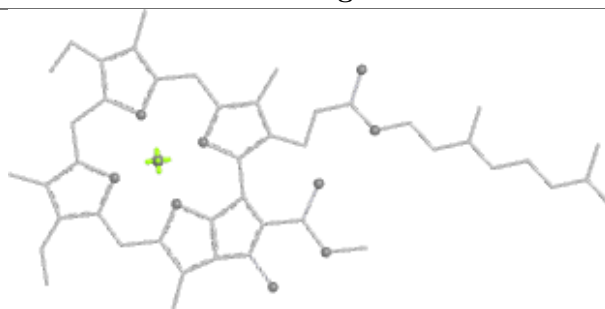
Bond lengths



Bond angles

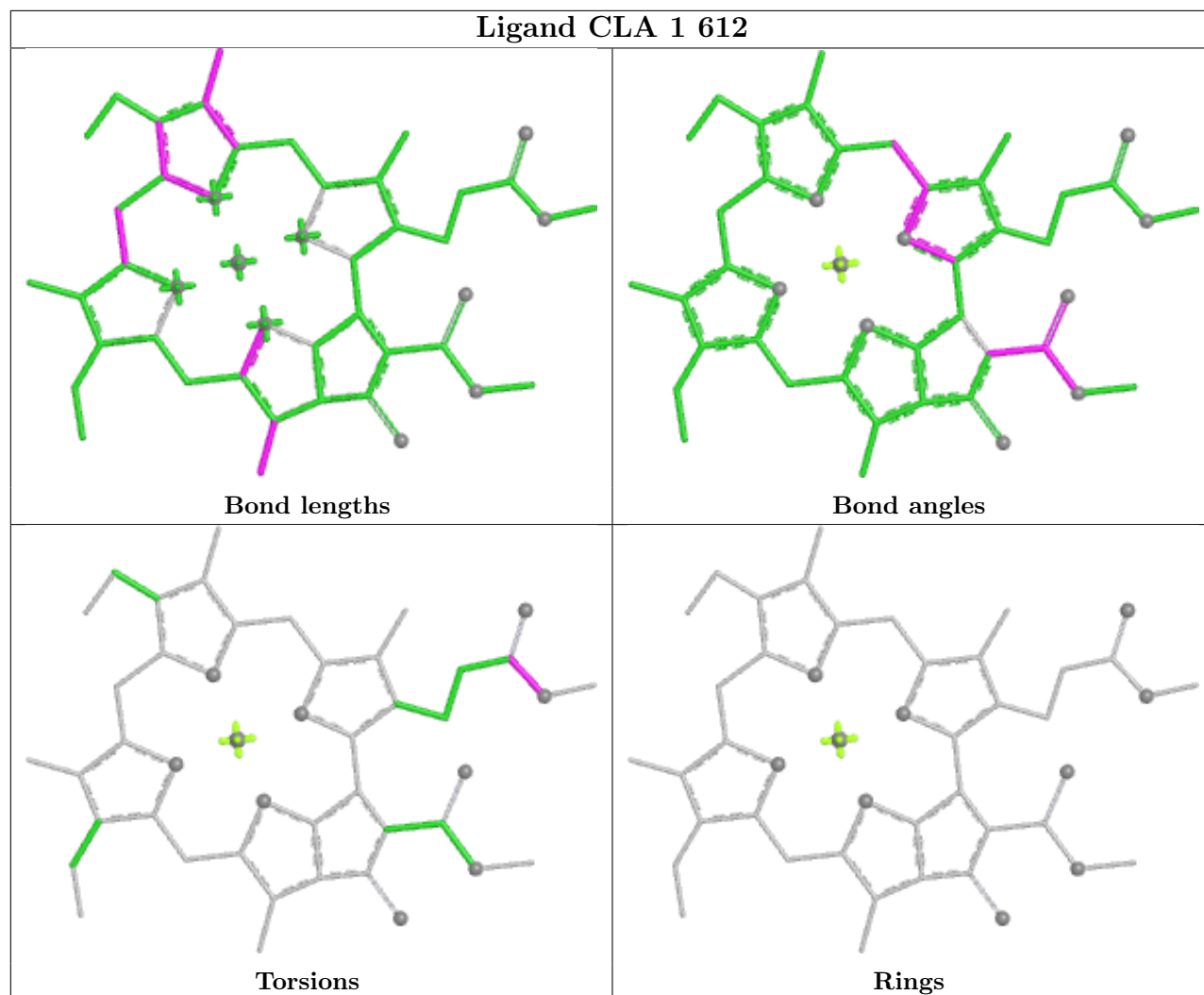


Torsions

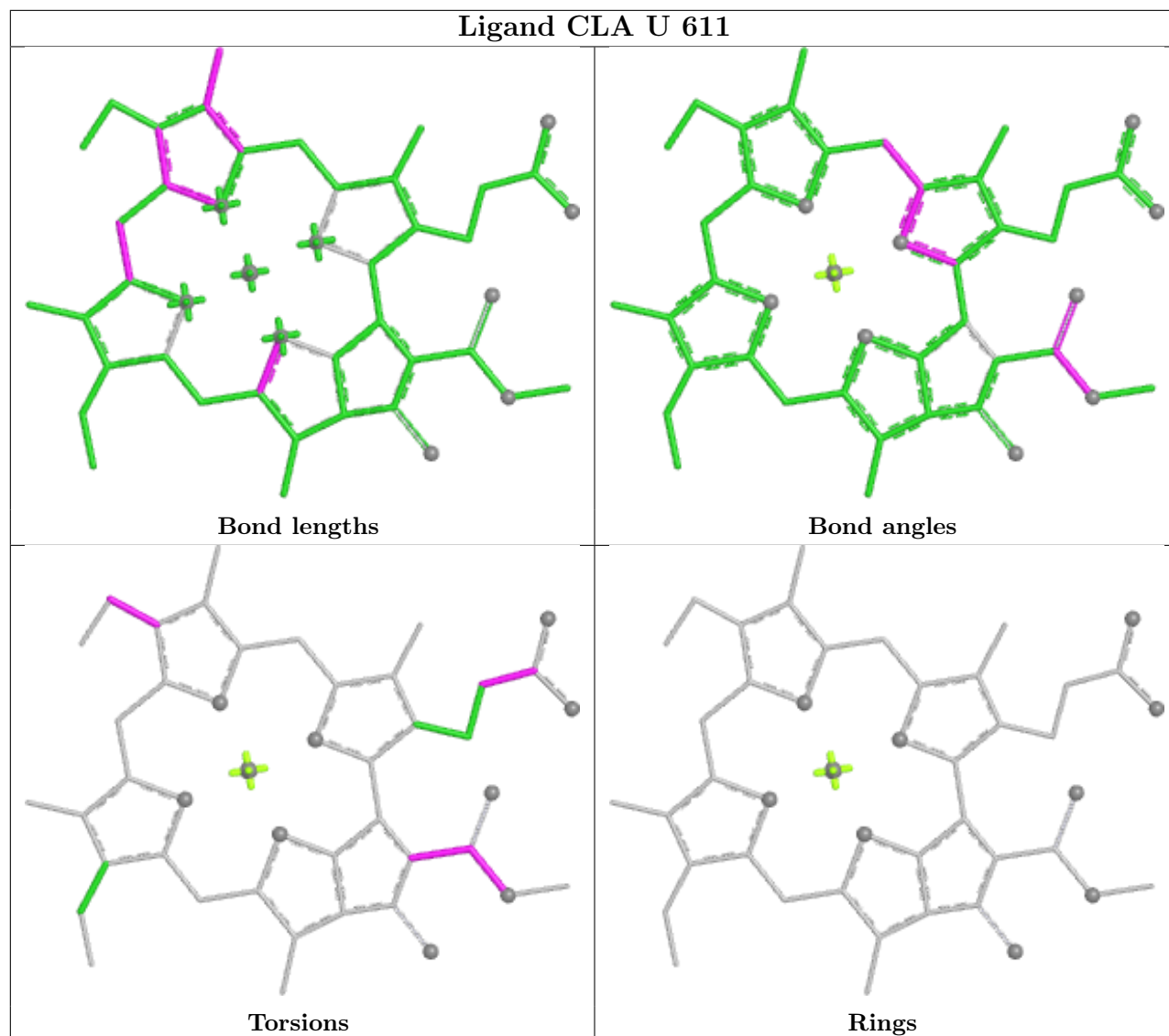


Rings

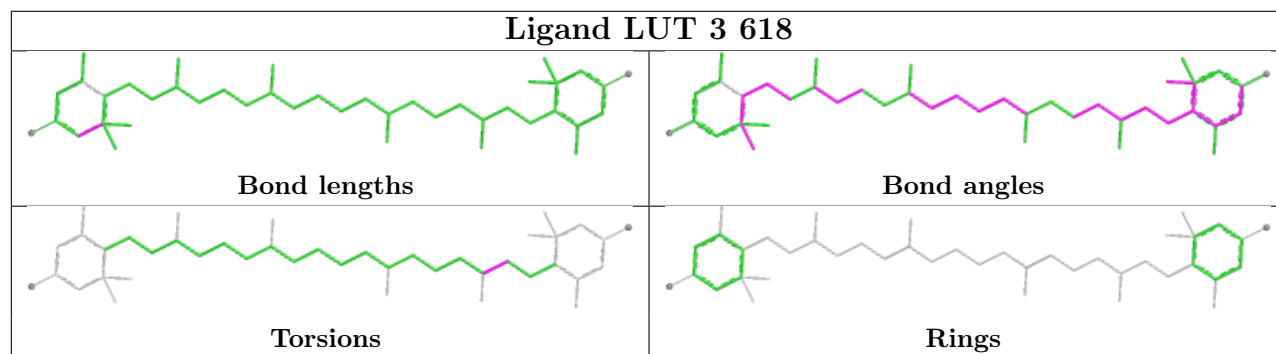
Ligand CLA 1 612



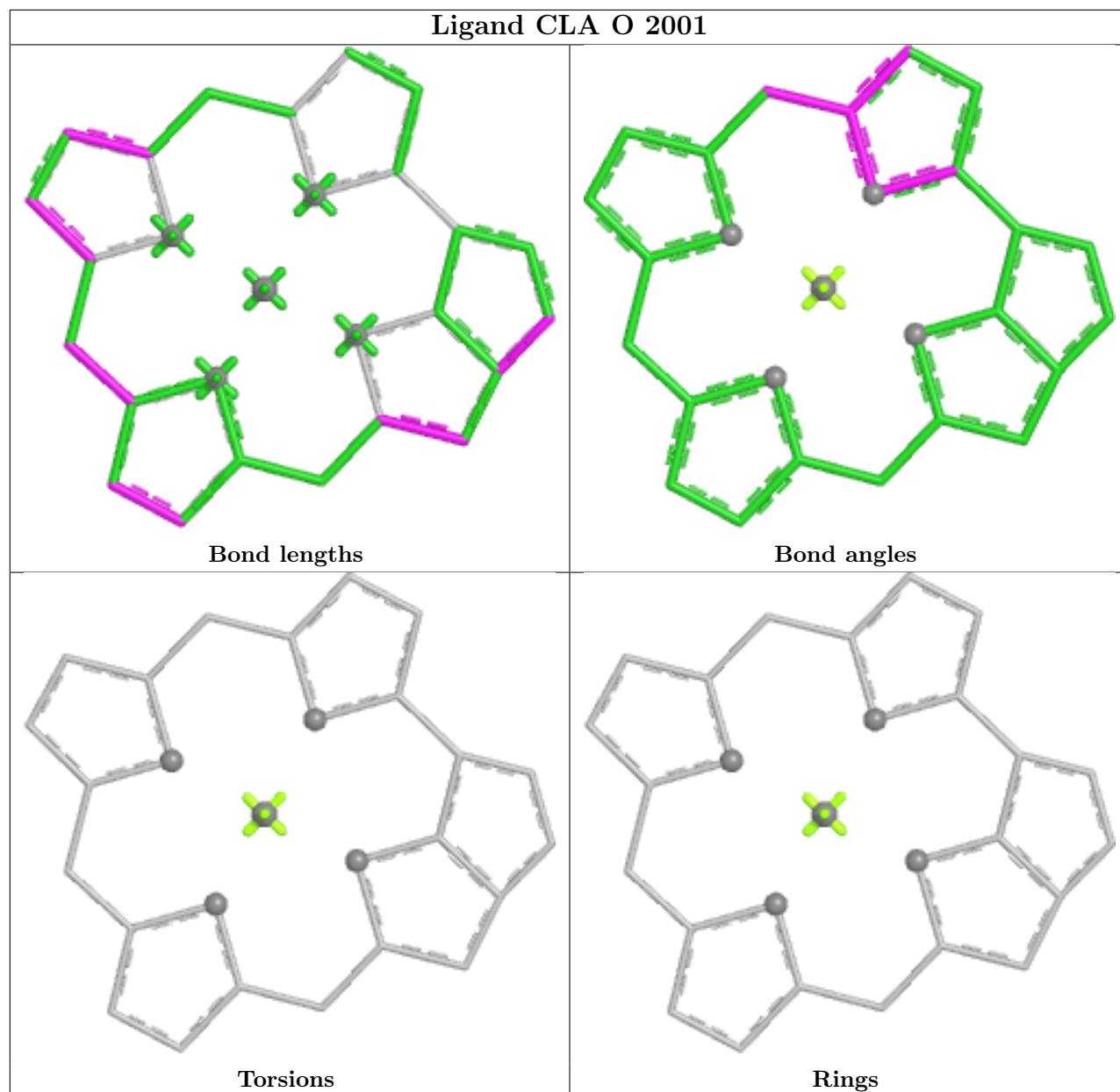
Ligand CLA U 611

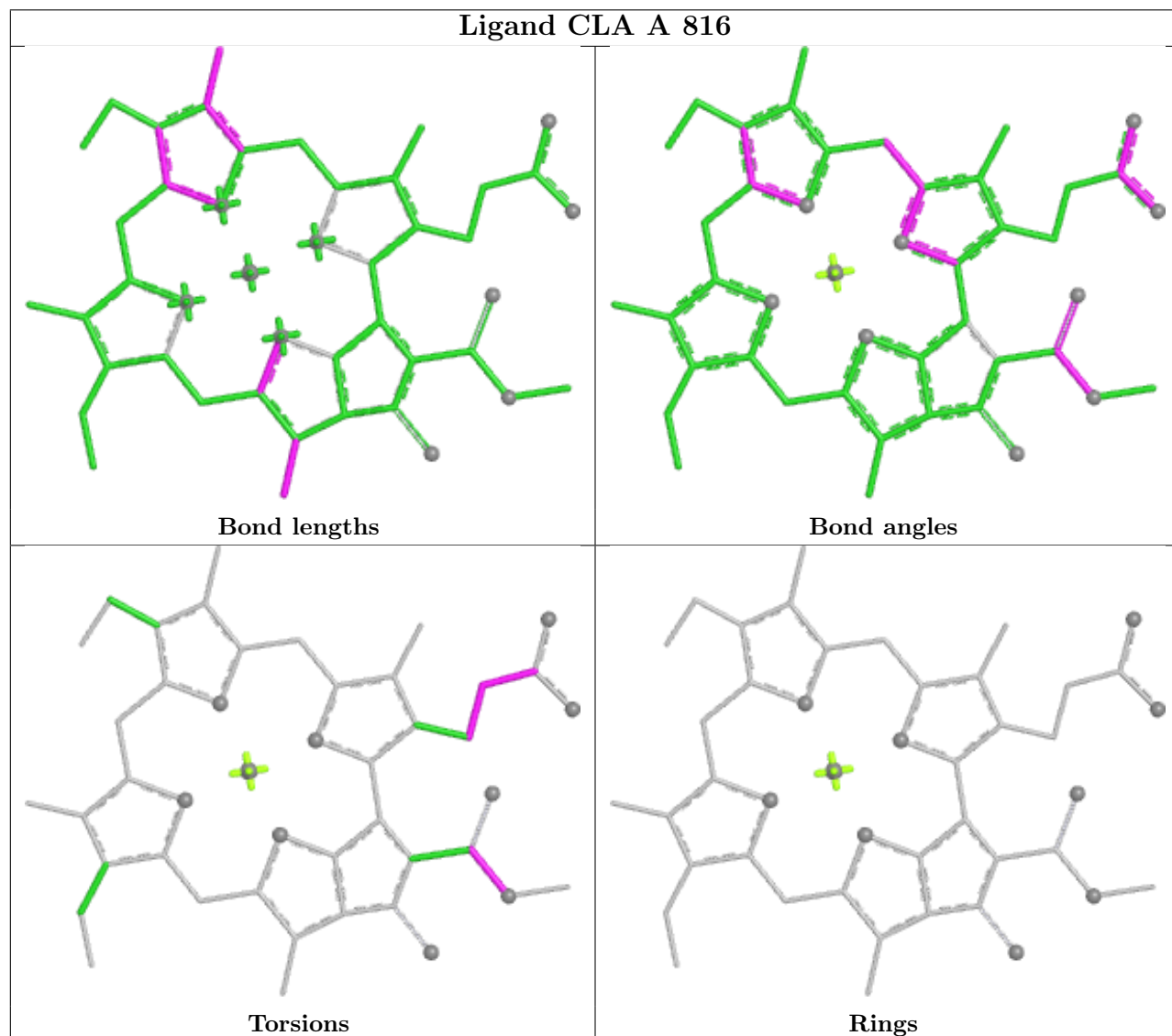
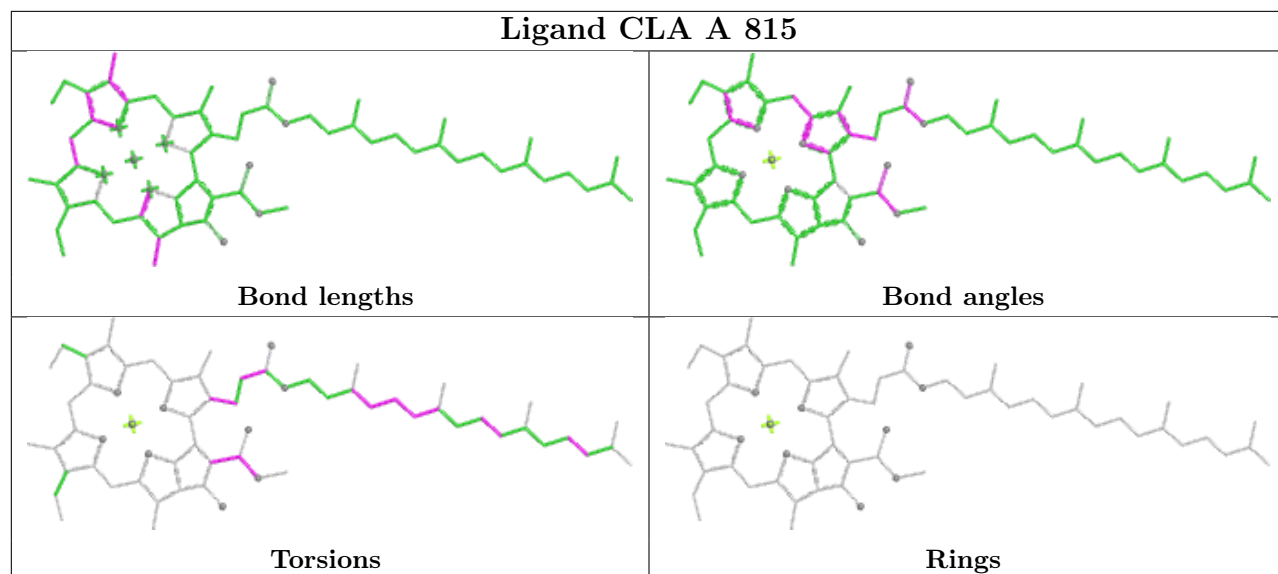


Ligand LUT 3 618

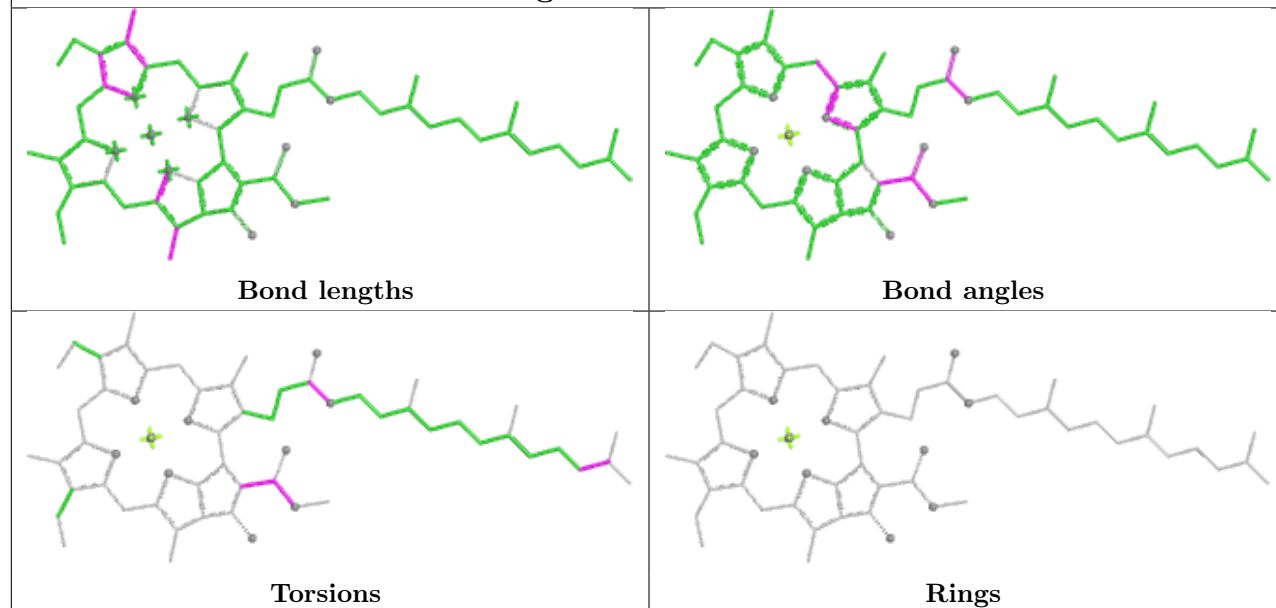


Ligand CLA O 2001

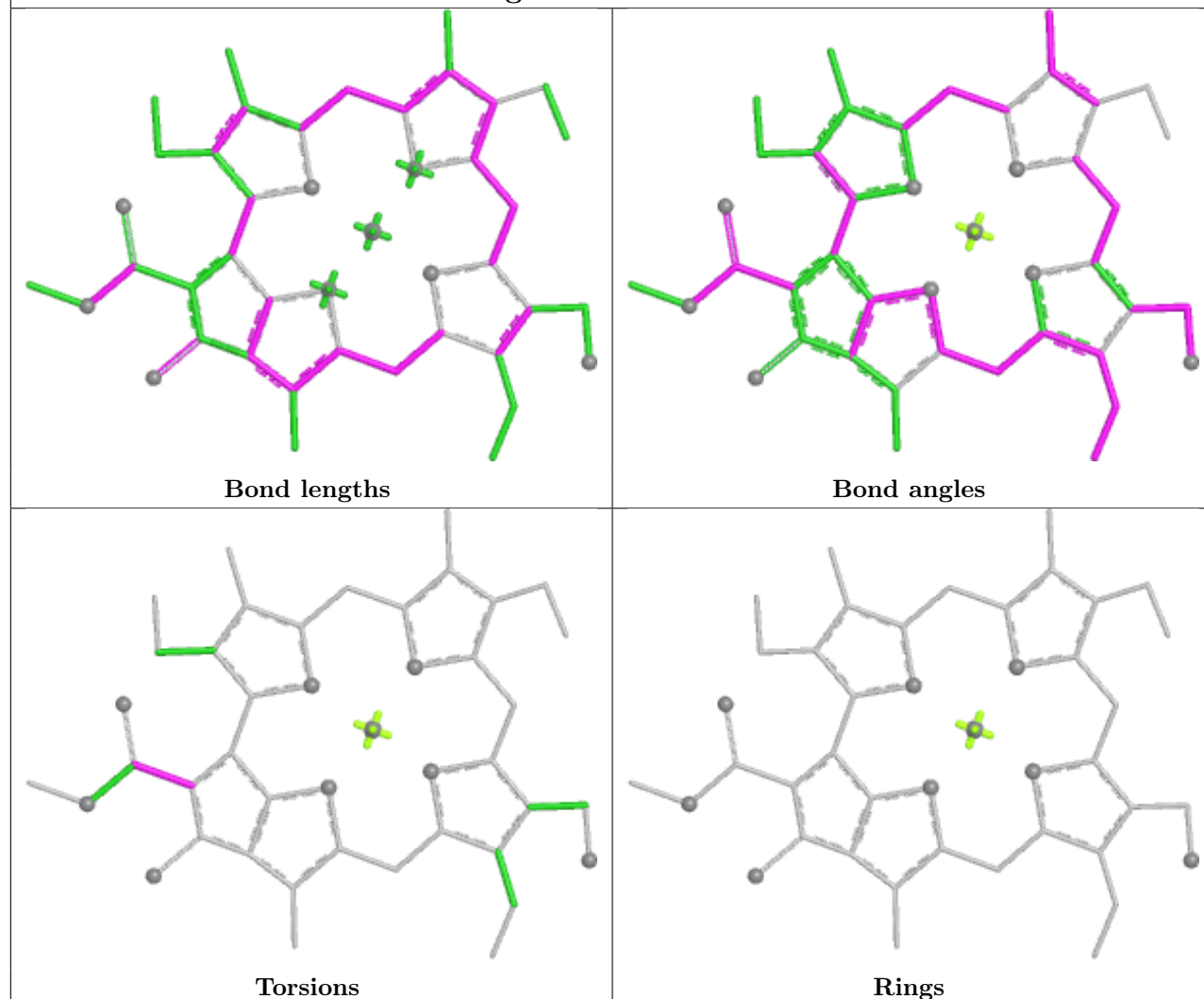


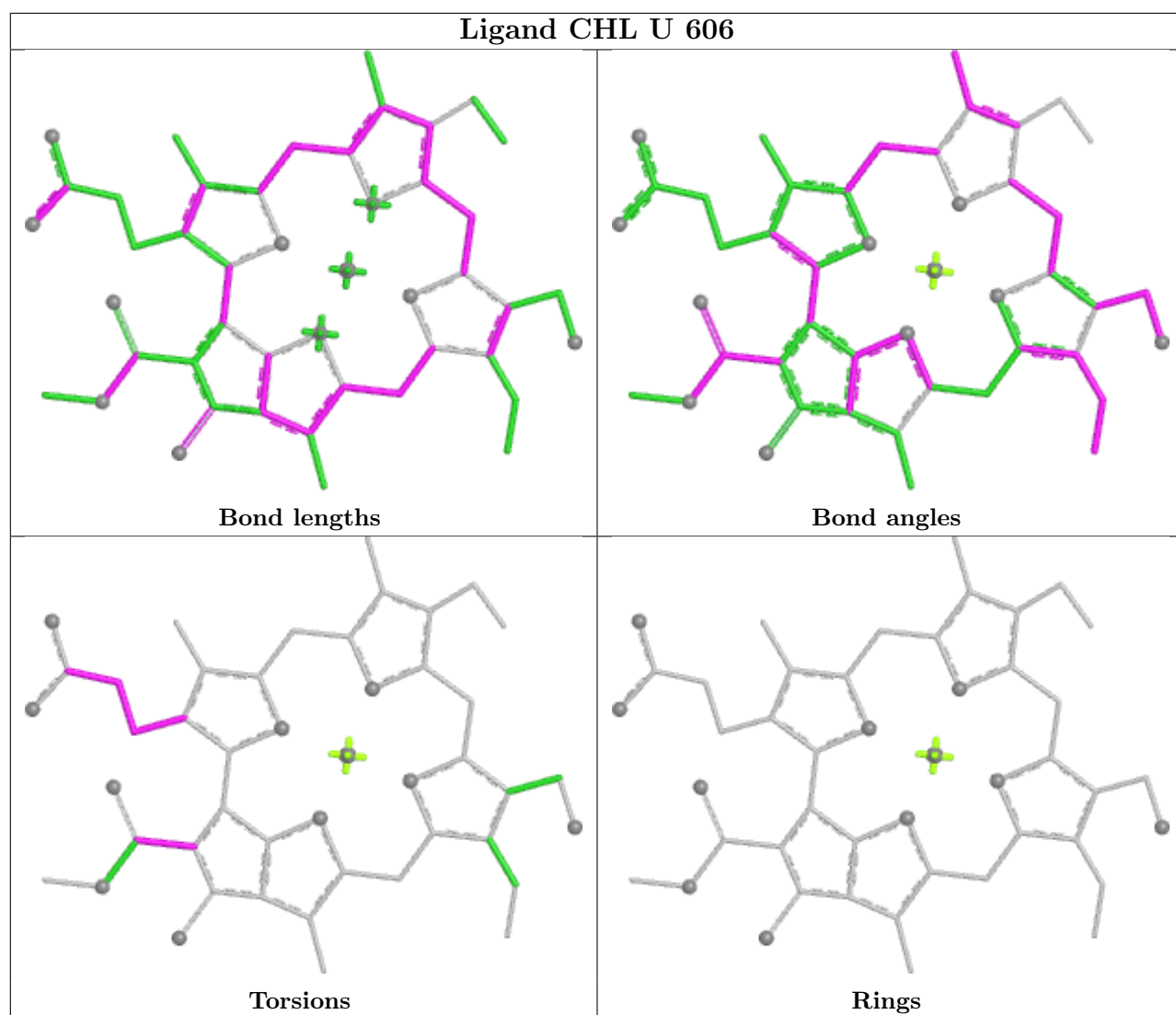


Ligand CLA 8 602

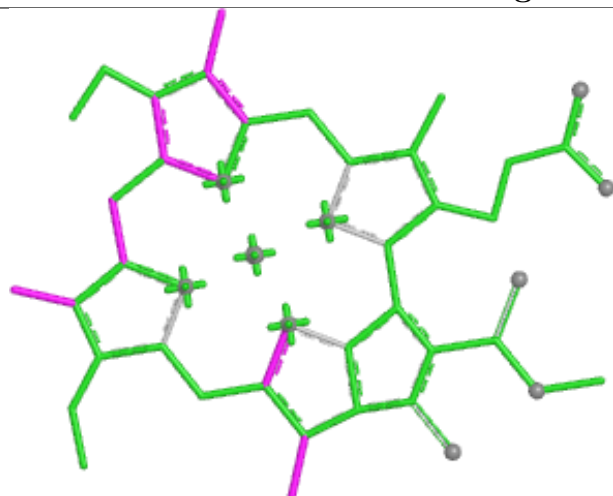


Ligand CHL 2 618

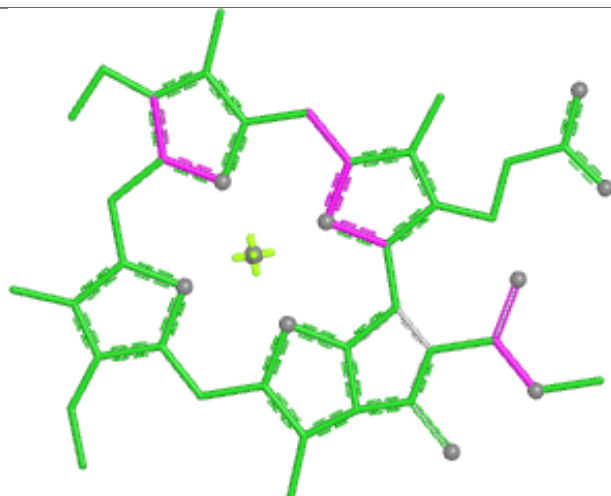




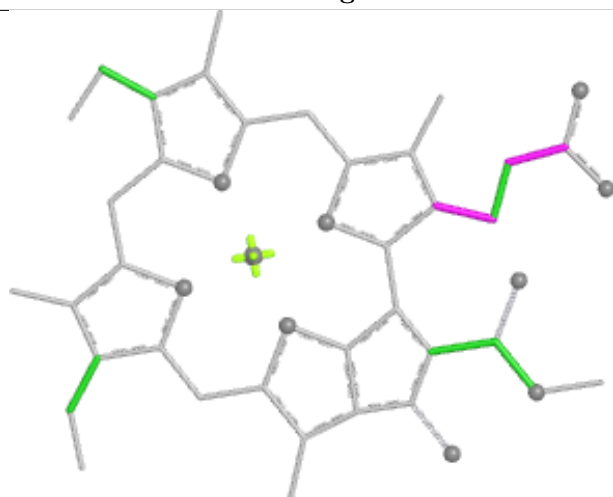
Ligand CLA B 815



Bond lengths



Bond angles

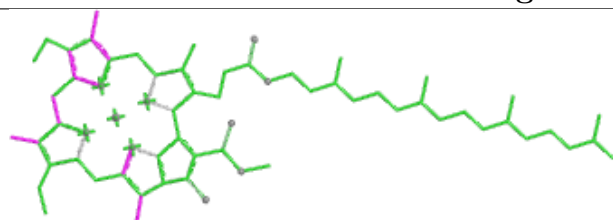


Torsions

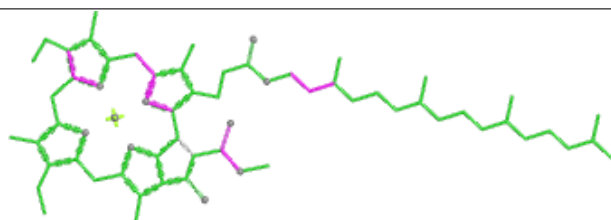


Rings

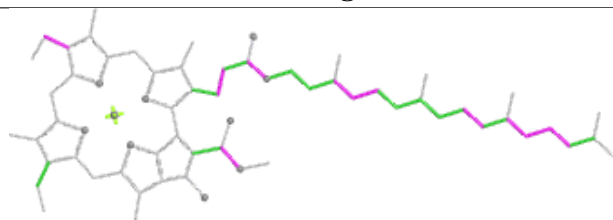
Ligand CLA F 301



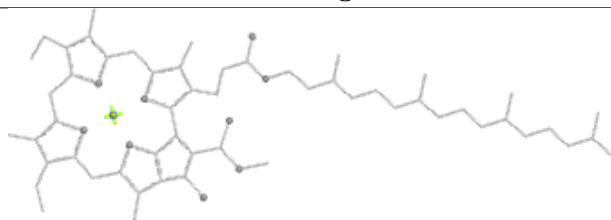
Bond lengths



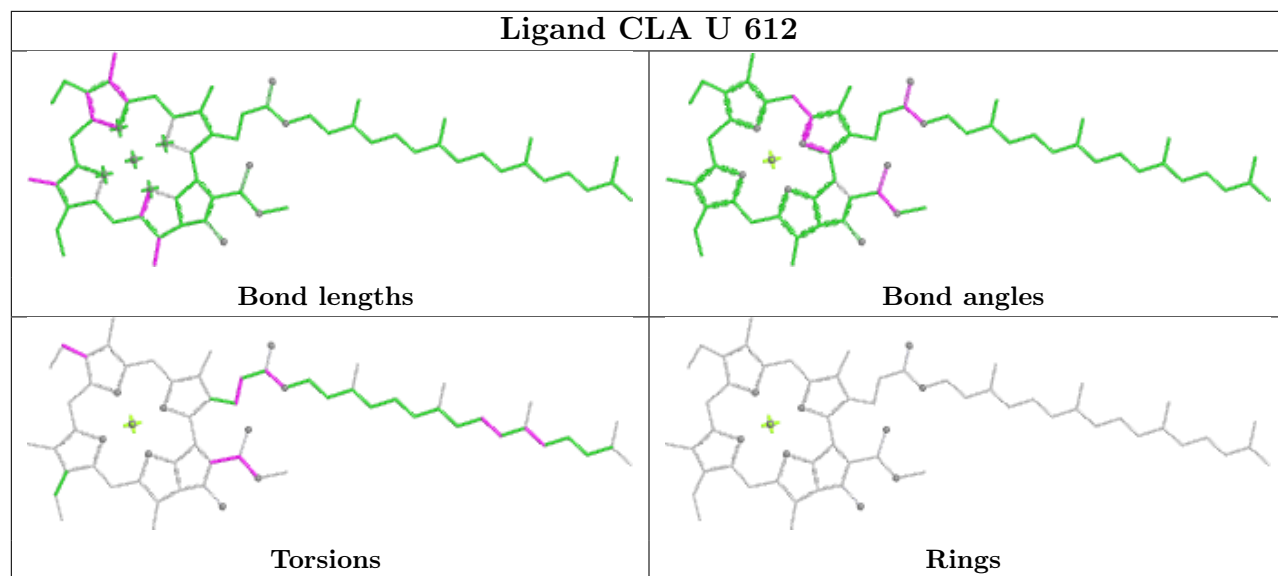
Bond angles

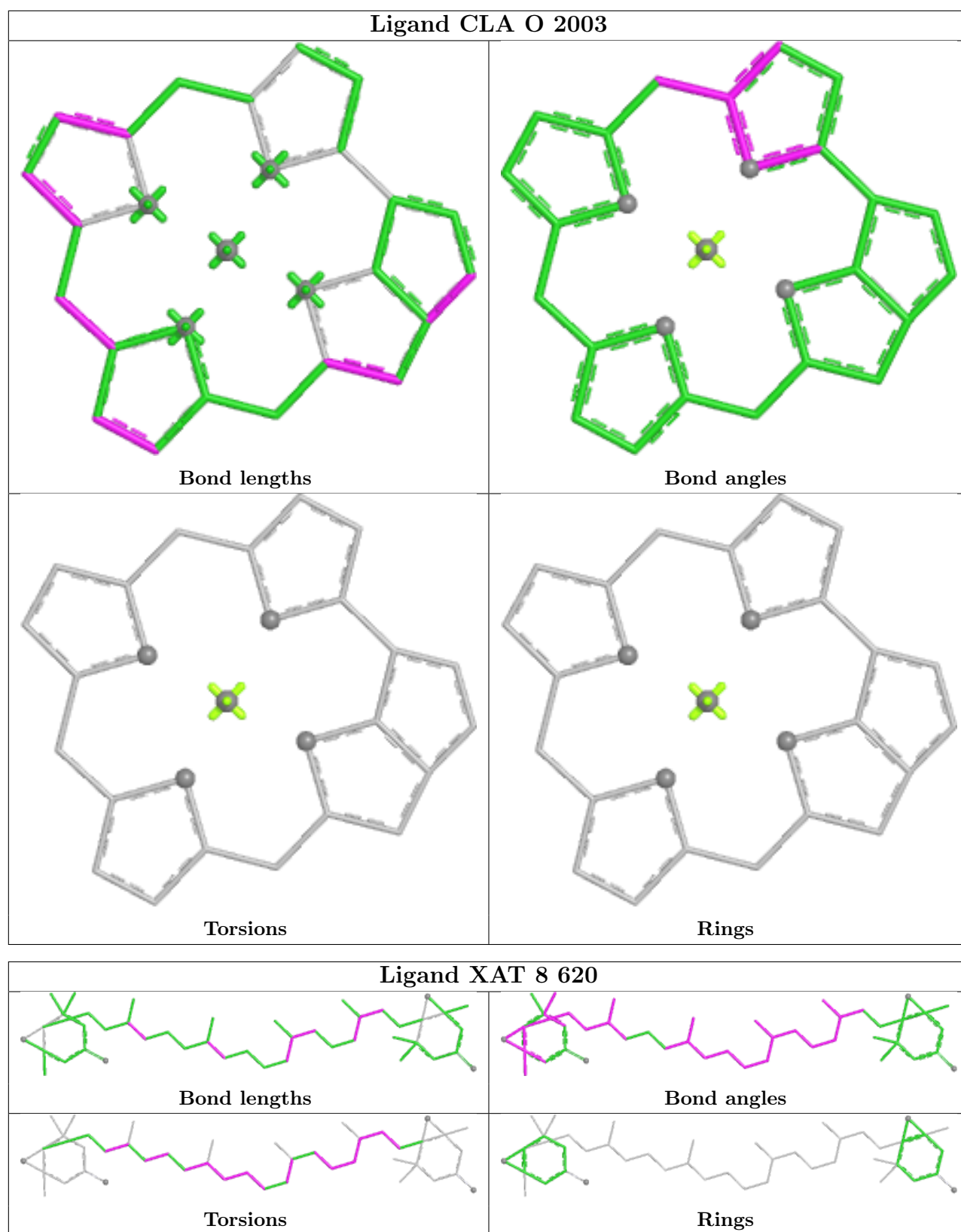


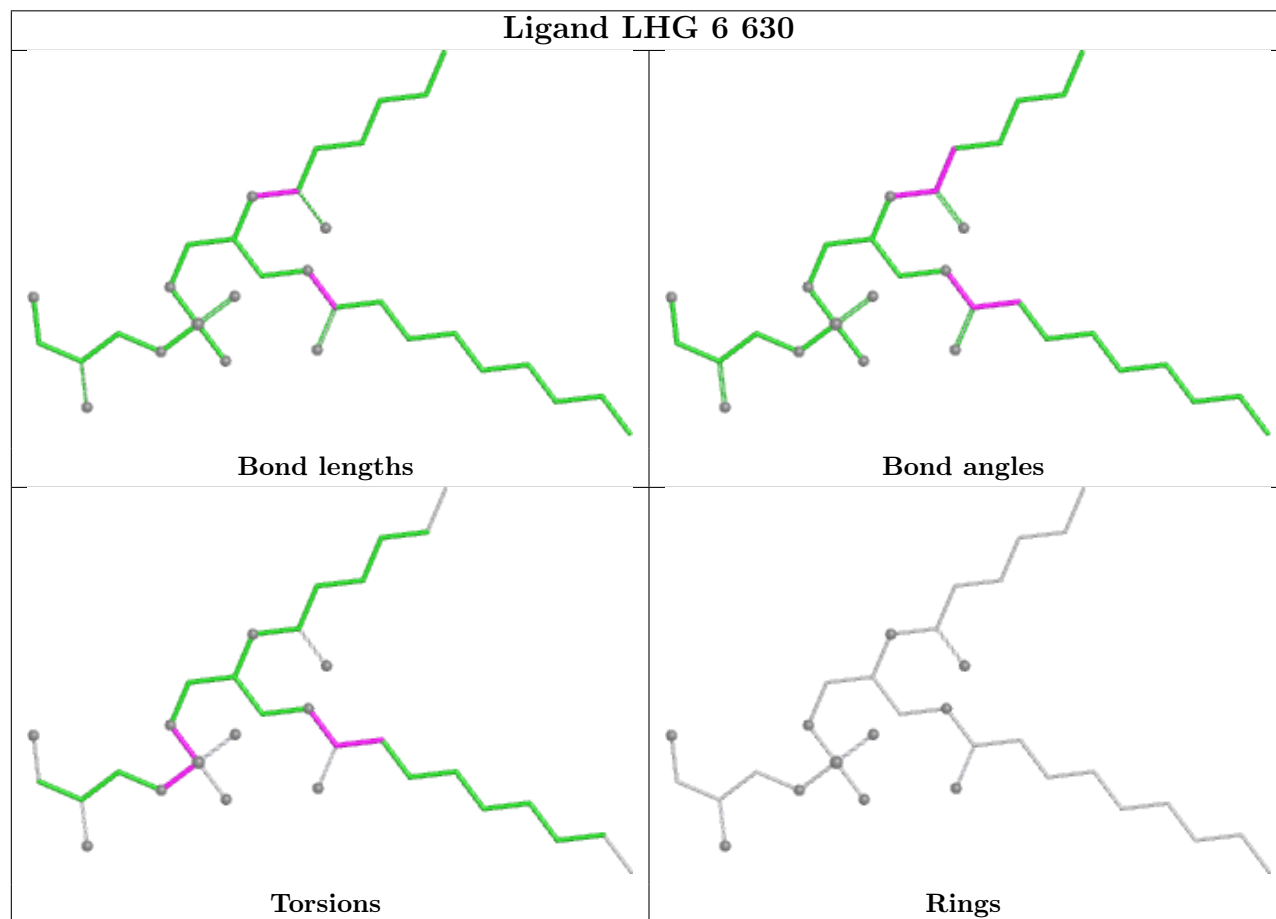
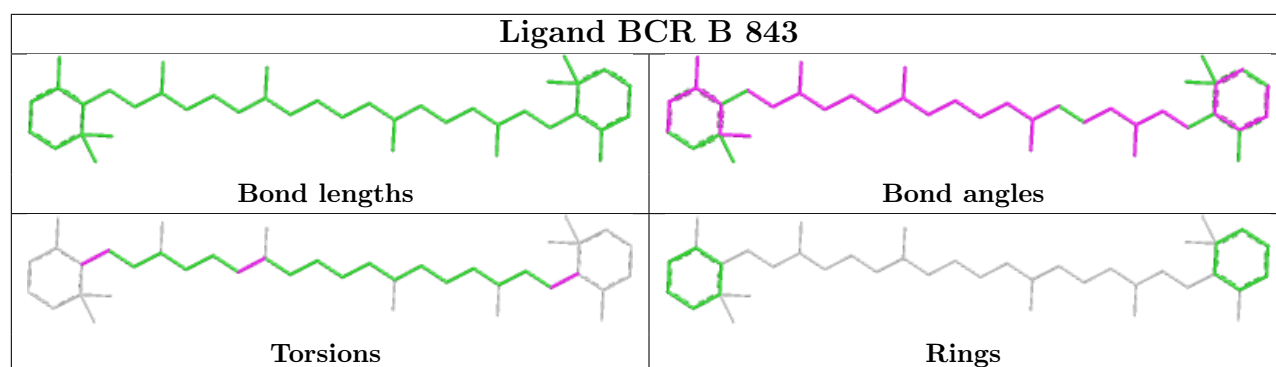
Torsions

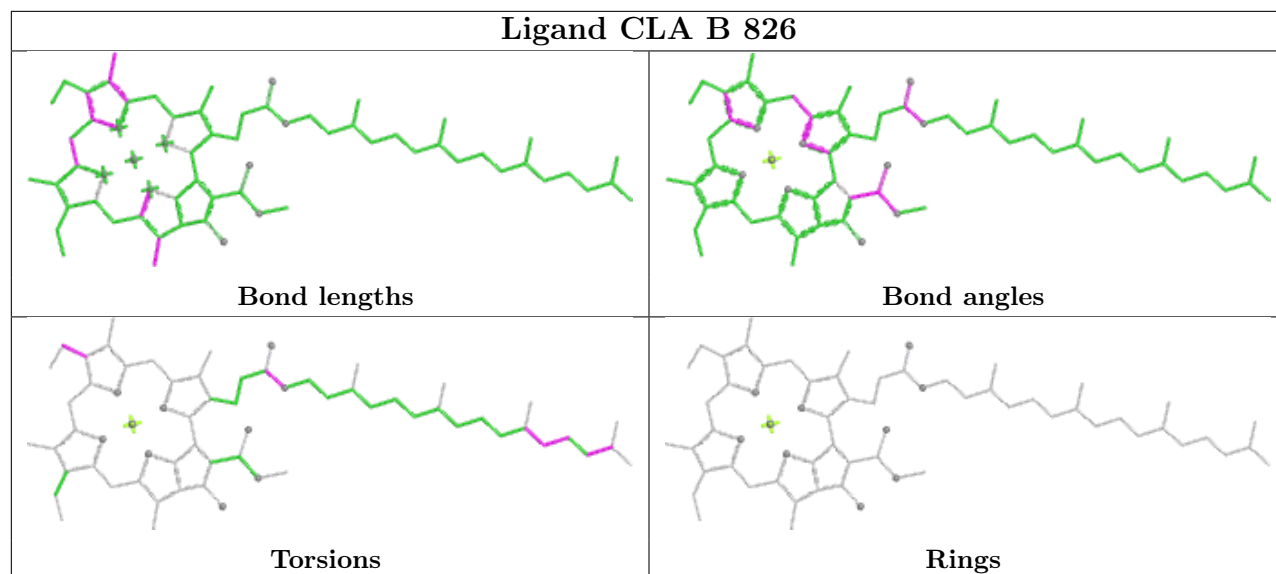
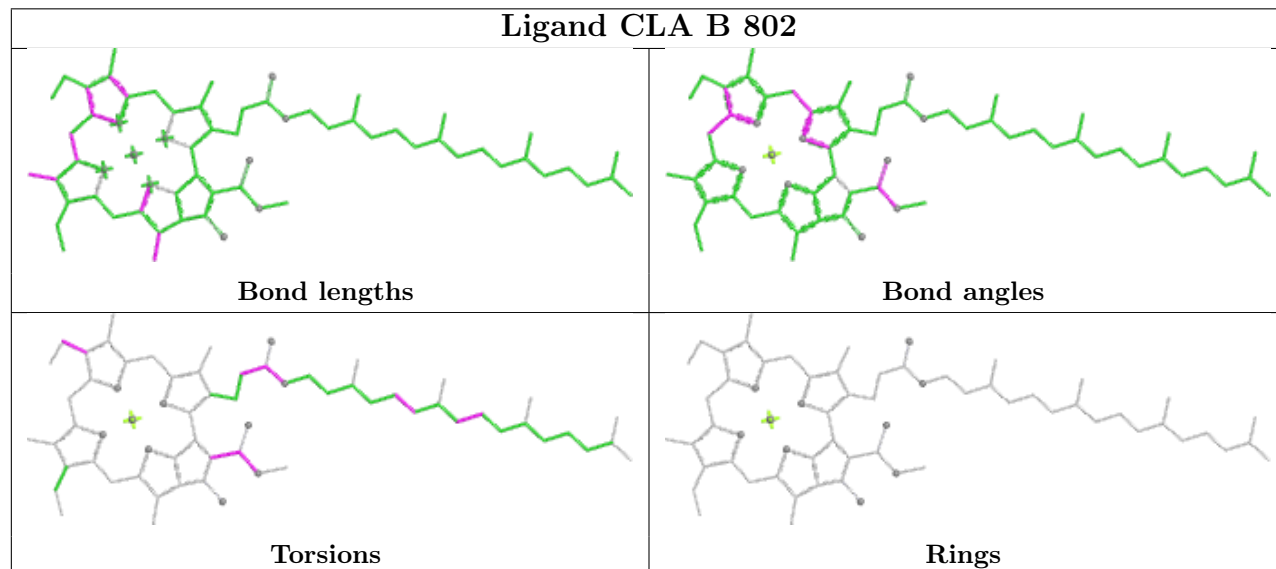


Rings

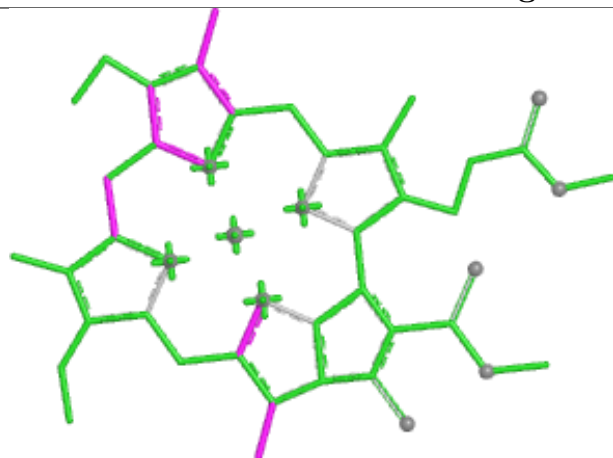




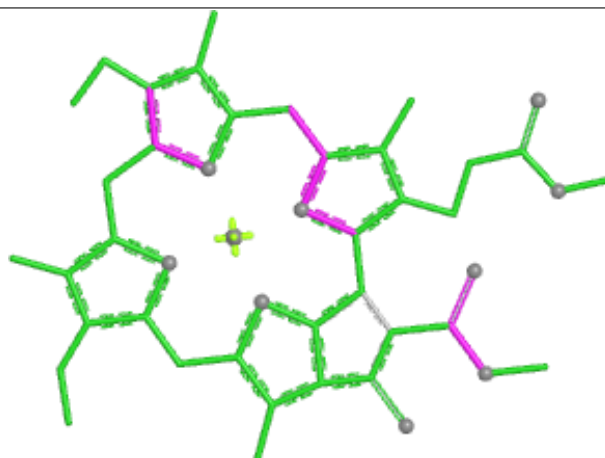


Ligand CLA B 826**Ligand CLA B 802**

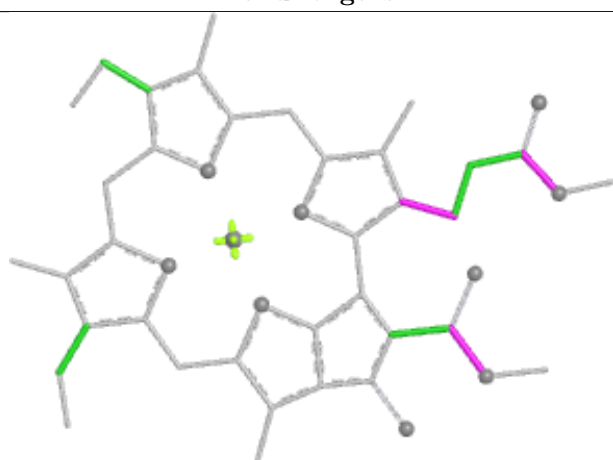
Ligand CLA 4 614



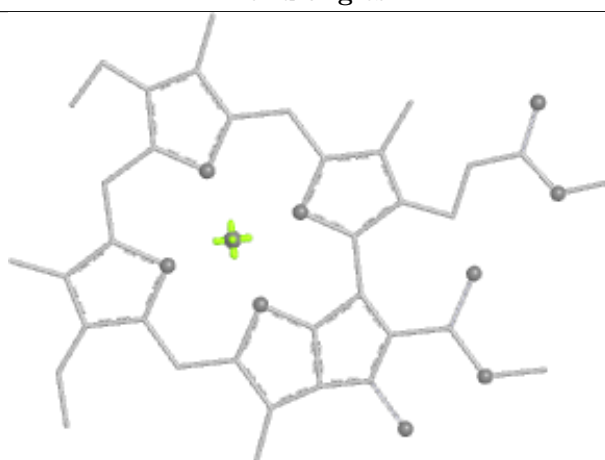
Bond lengths



Bond angles

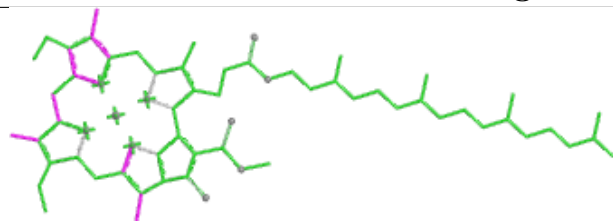


Torsions

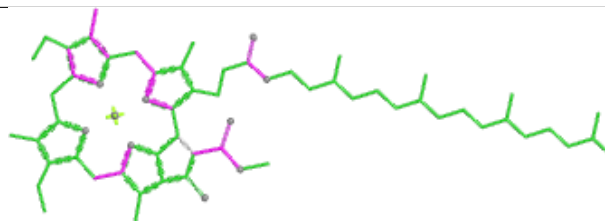


Rings

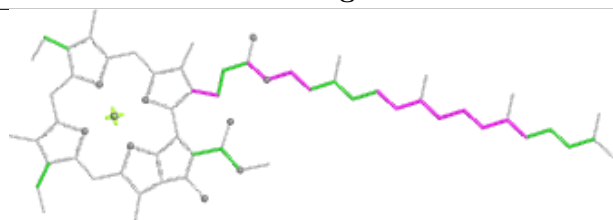
Ligand CLA A 805



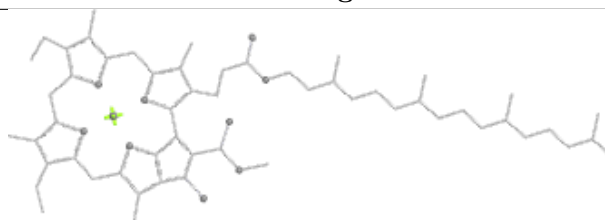
Bond lengths



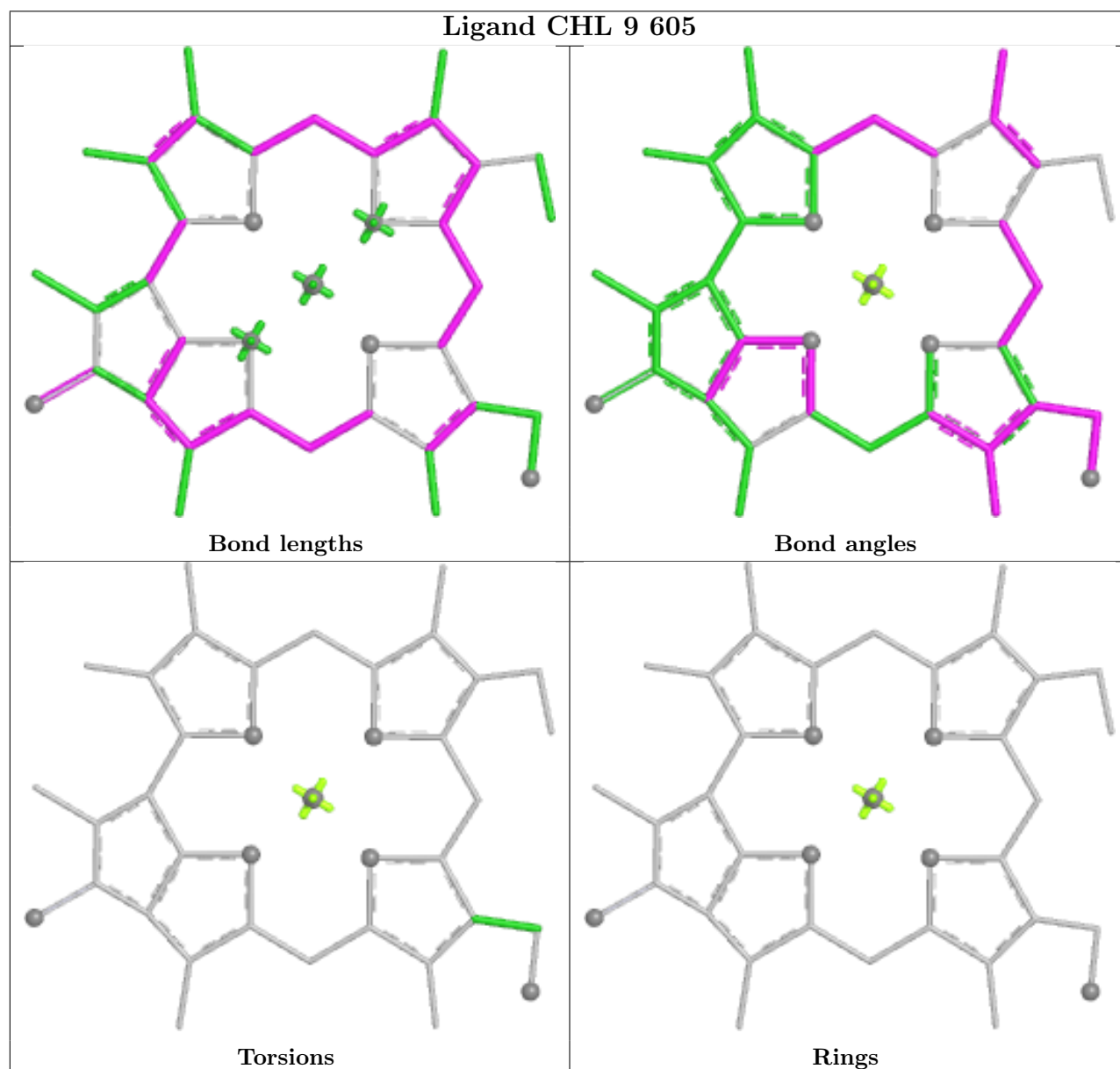
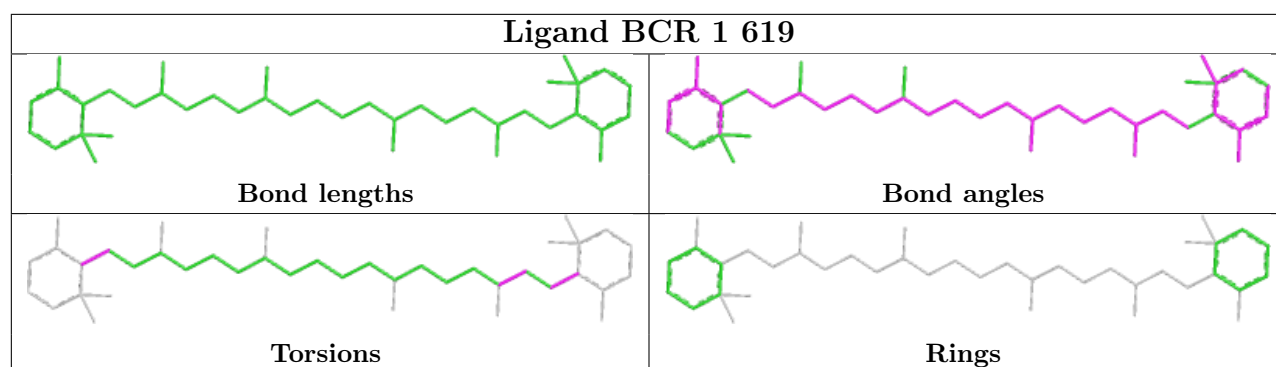
Bond angles



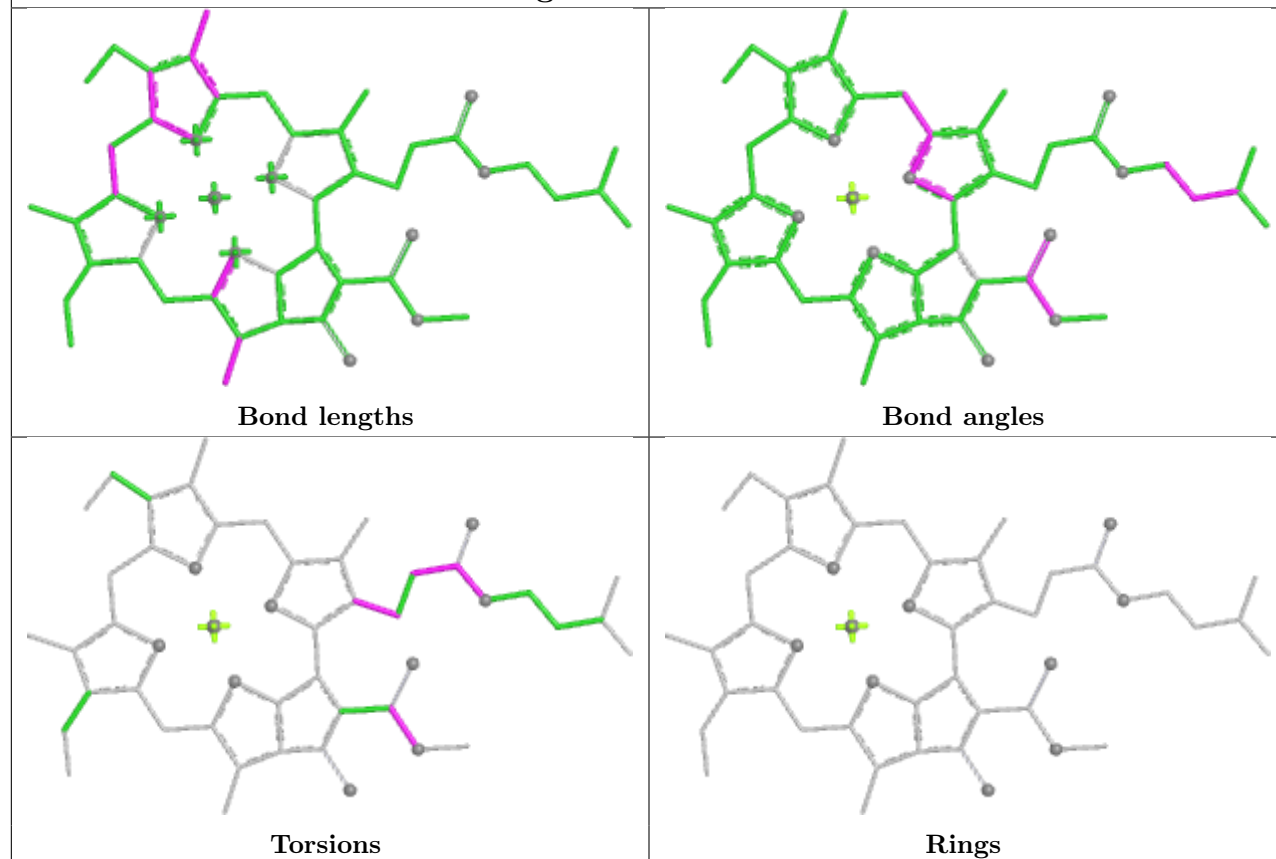
Torsions



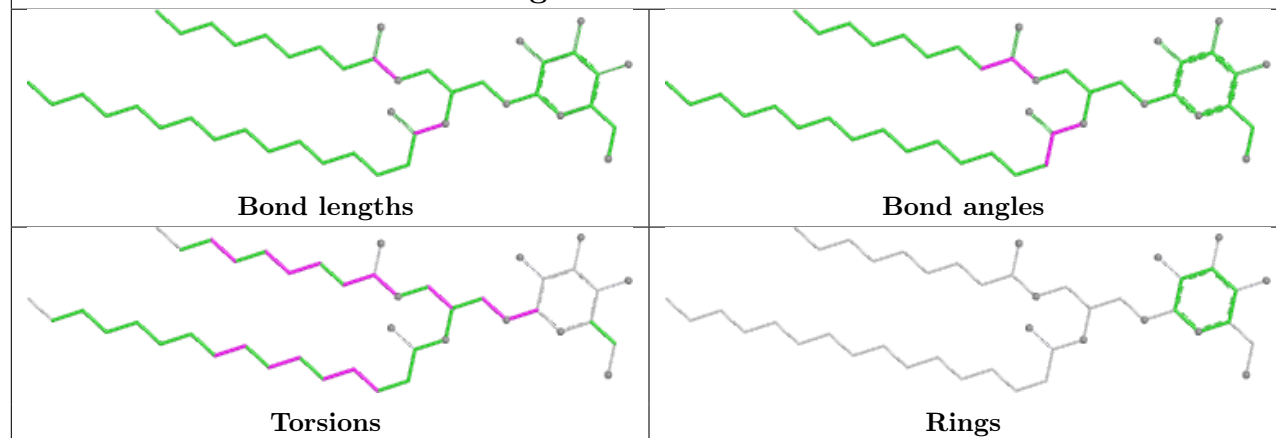
Rings



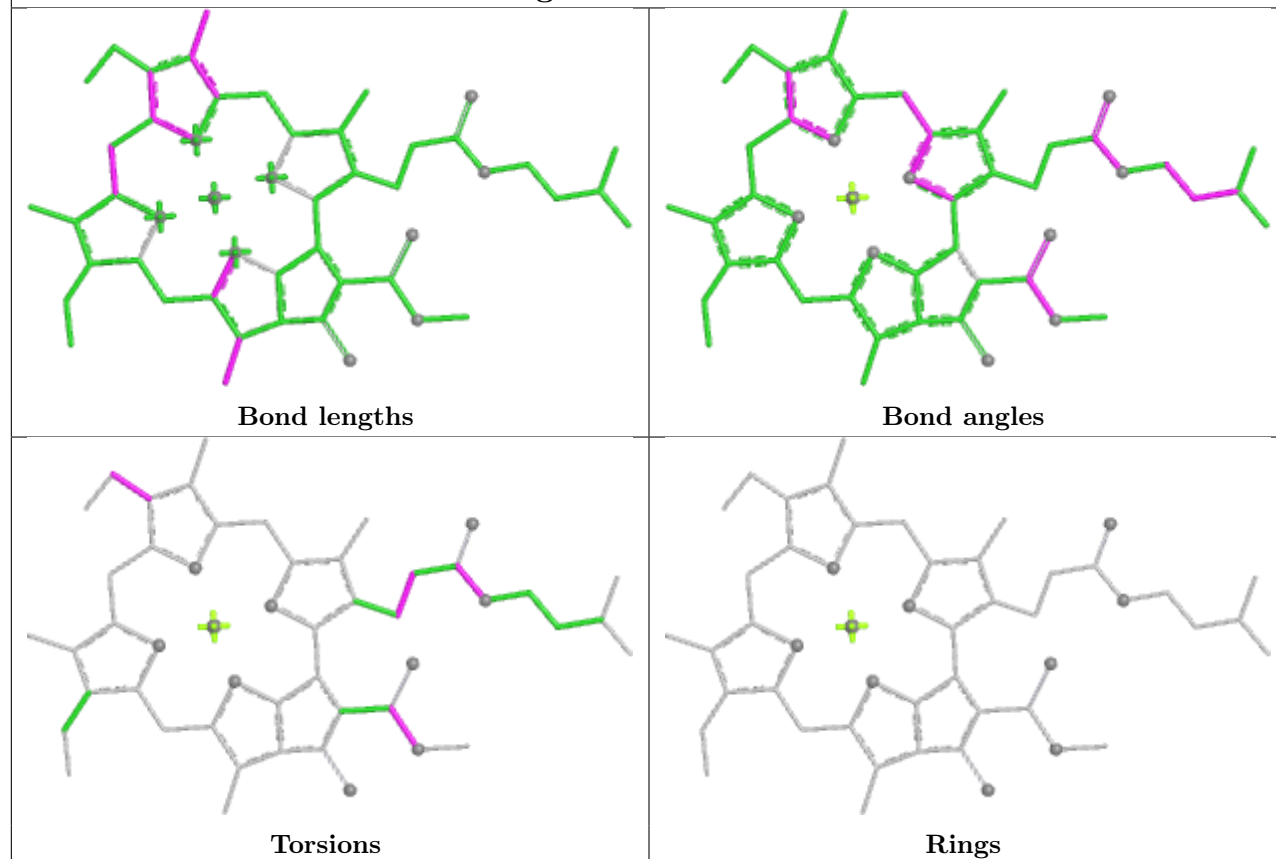
Ligand CLA 1 613



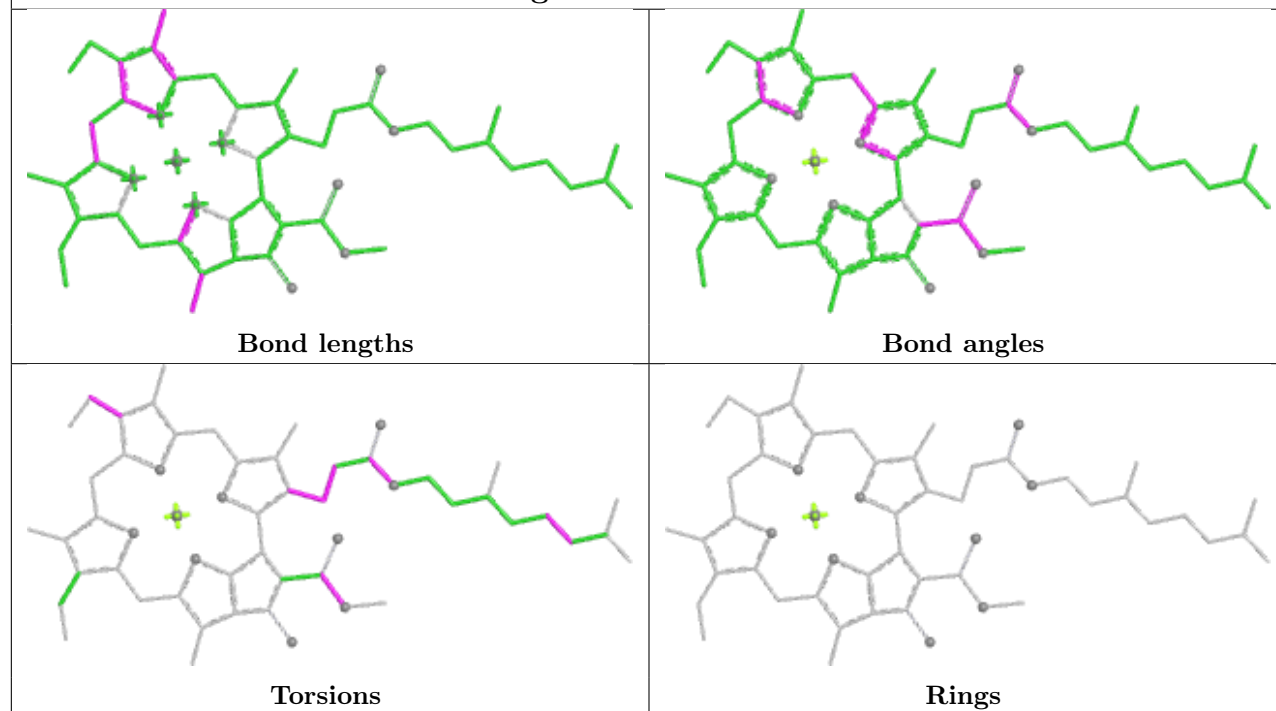
Ligand LMG L 307



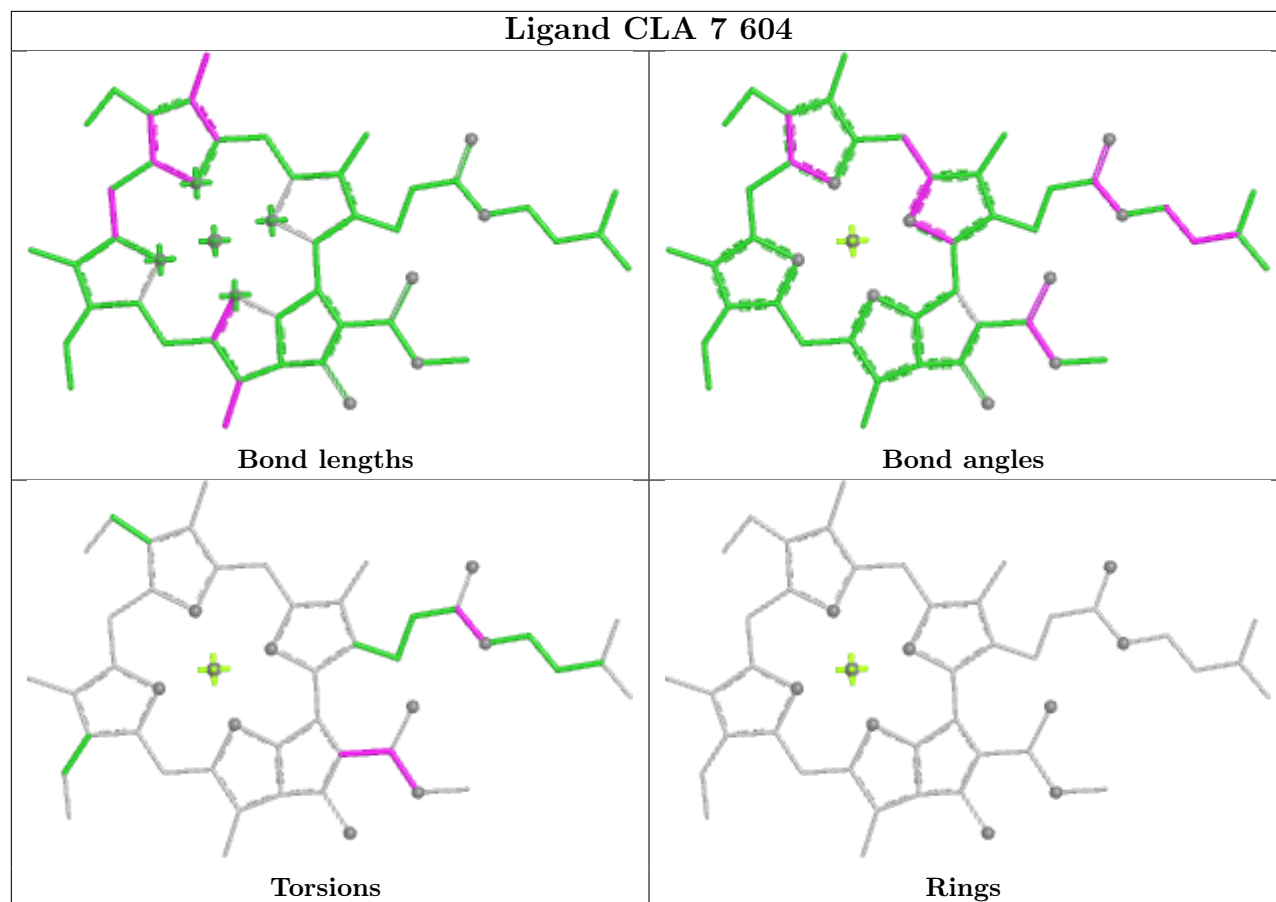
Ligand CLA J 101



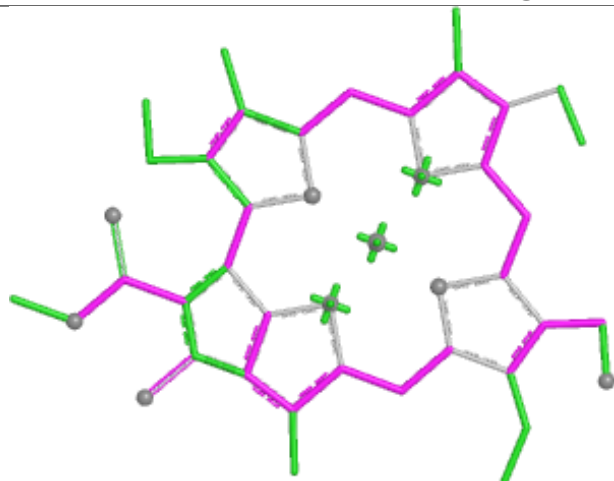
Ligand CLA K 203



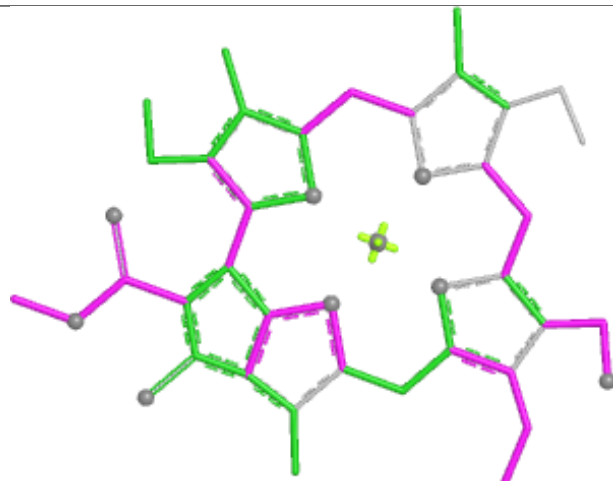
Ligand CLA 7 604



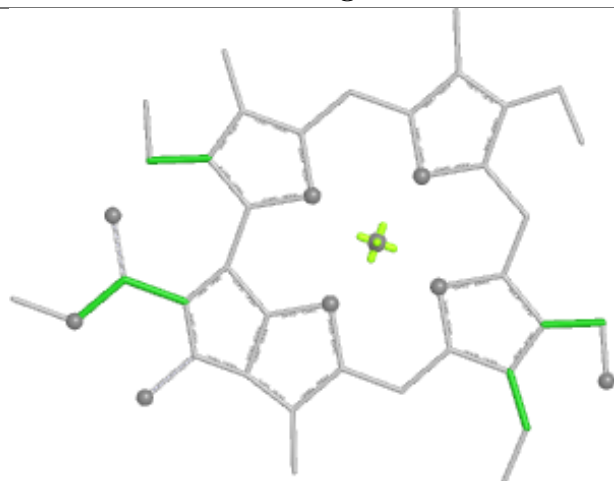
Ligand CHL 9 608



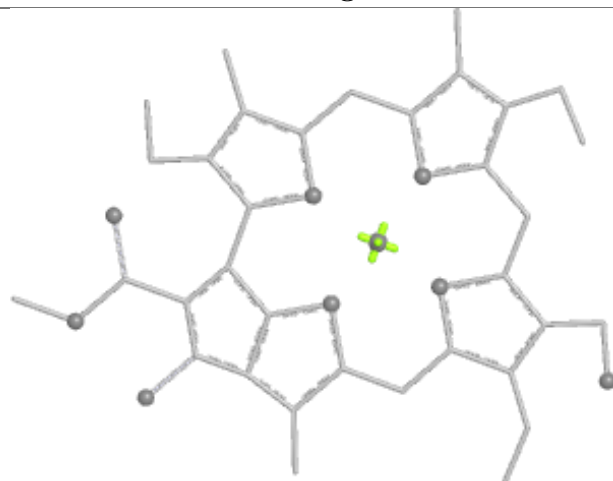
Bond lengths



Bond angles

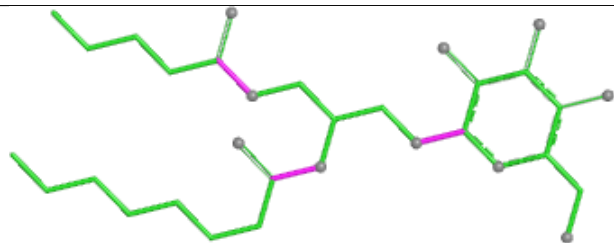


Torsions

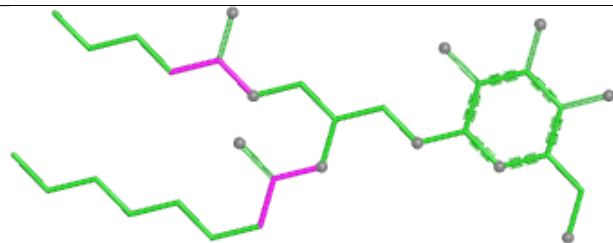


Rings

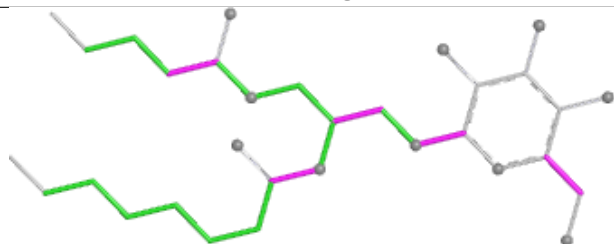
Ligand LMG G 202



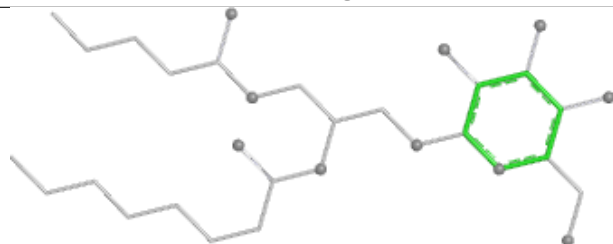
Bond lengths



Bond angles

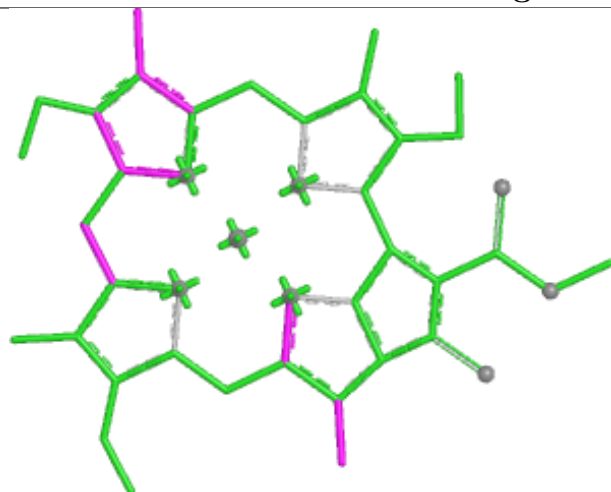


Torsions

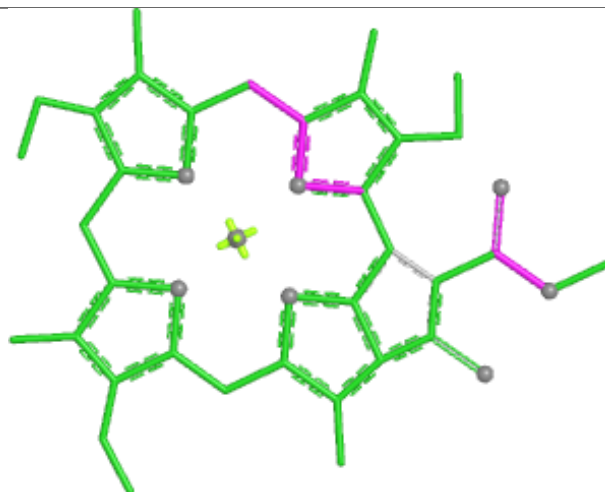


Rings

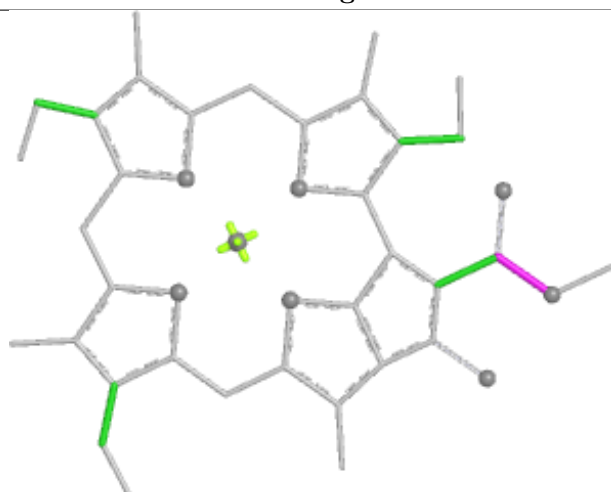
Ligand CLA U 614



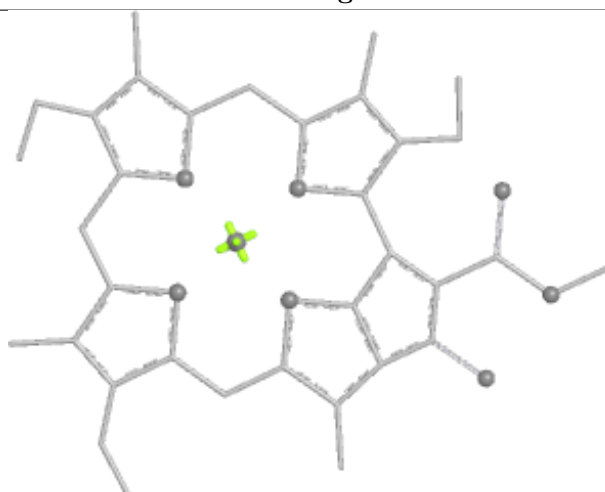
Bond lengths



Bond angles

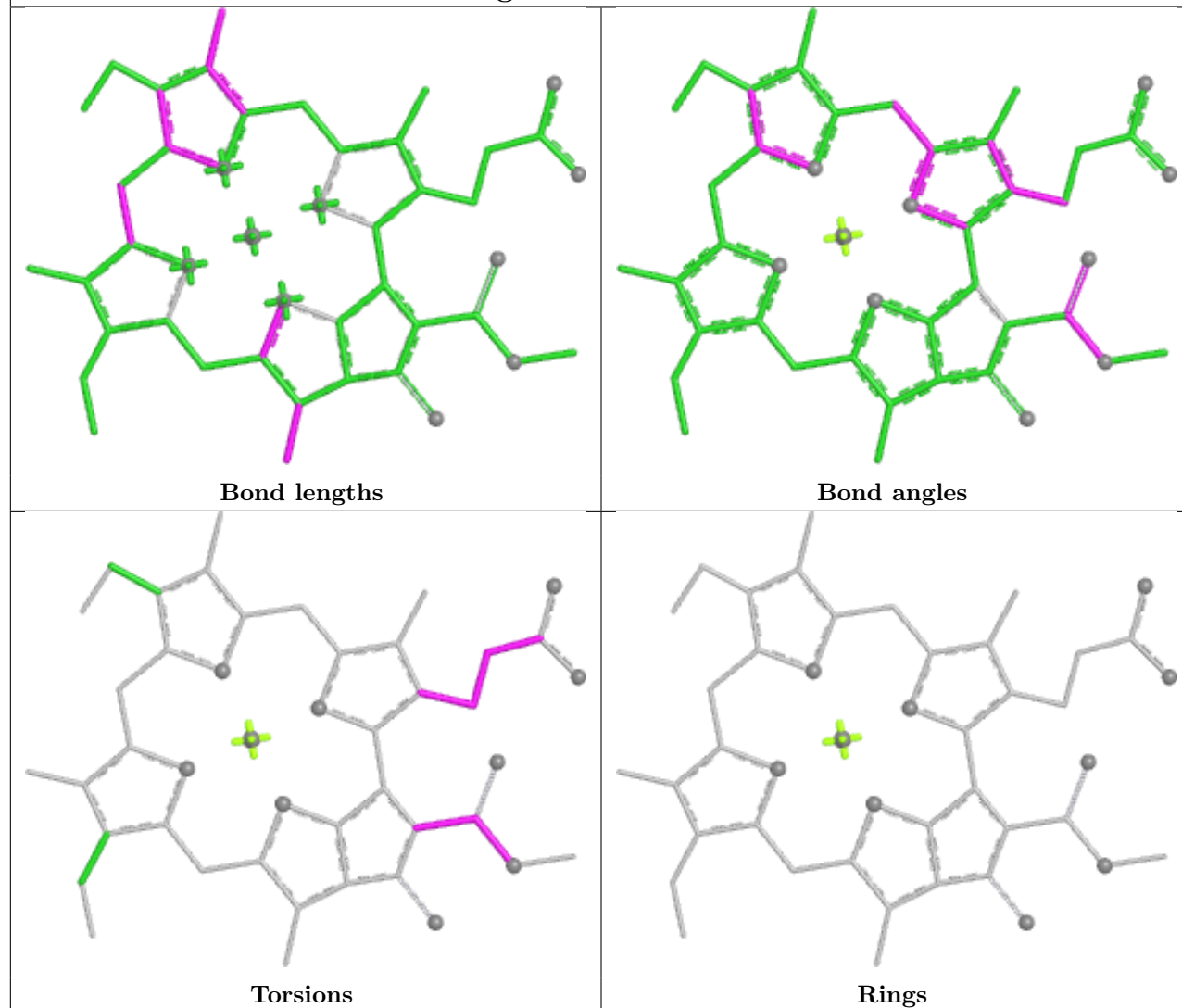


Torsions

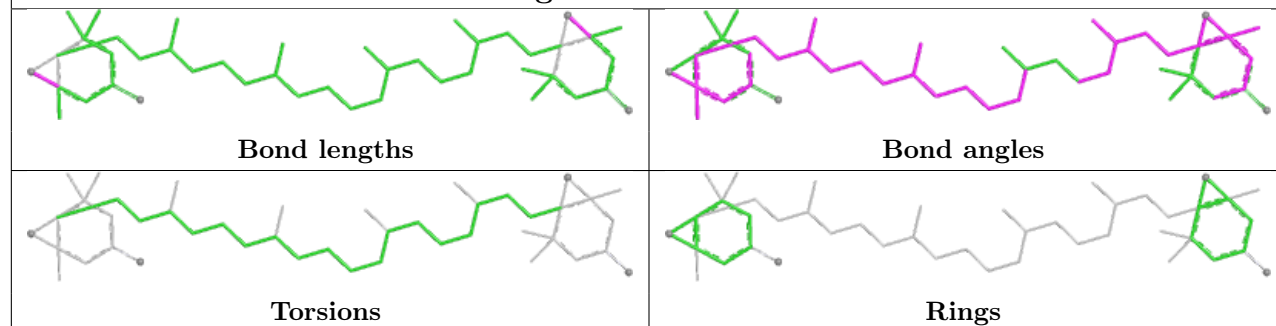


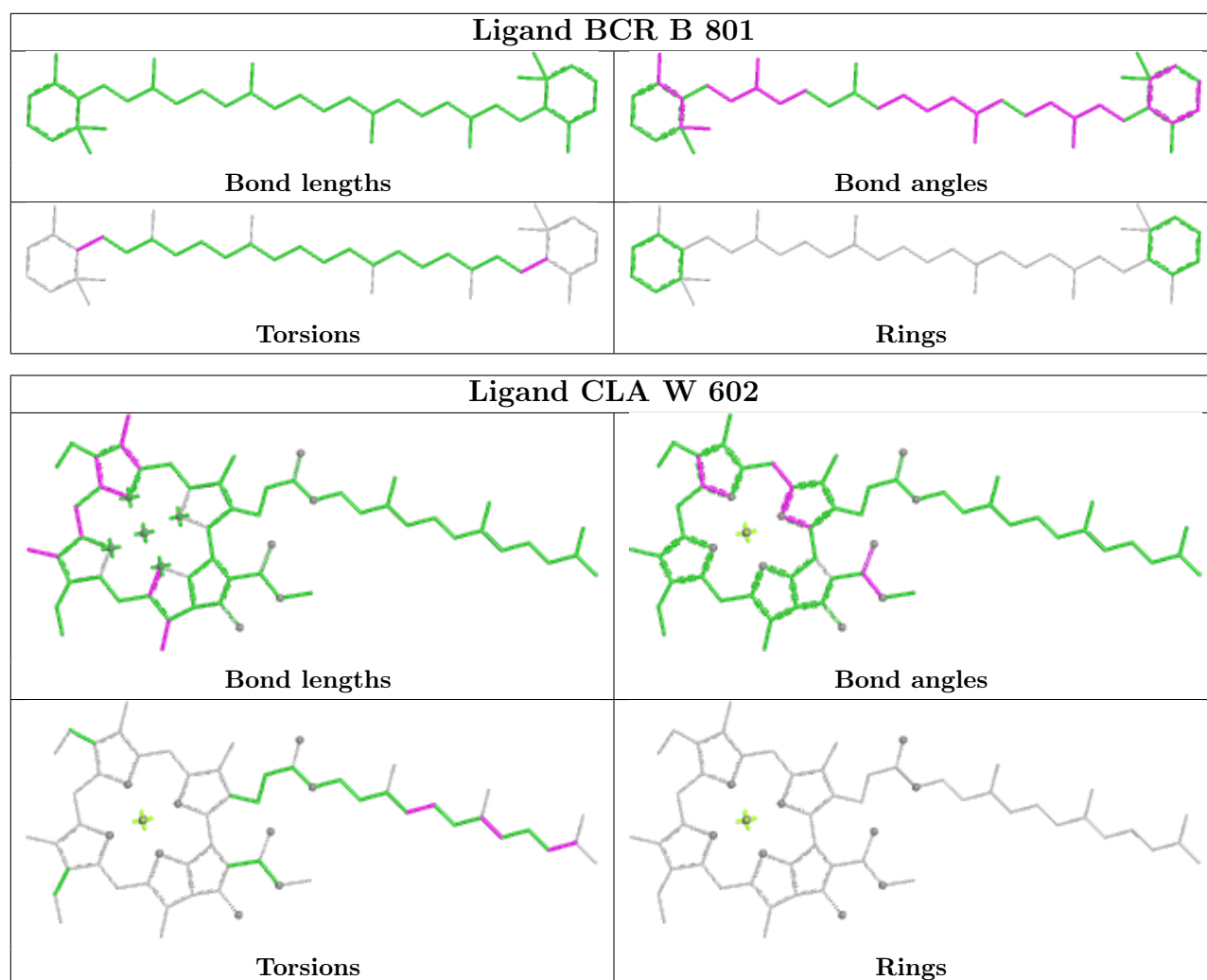
Rings

Ligand CLA 8 614

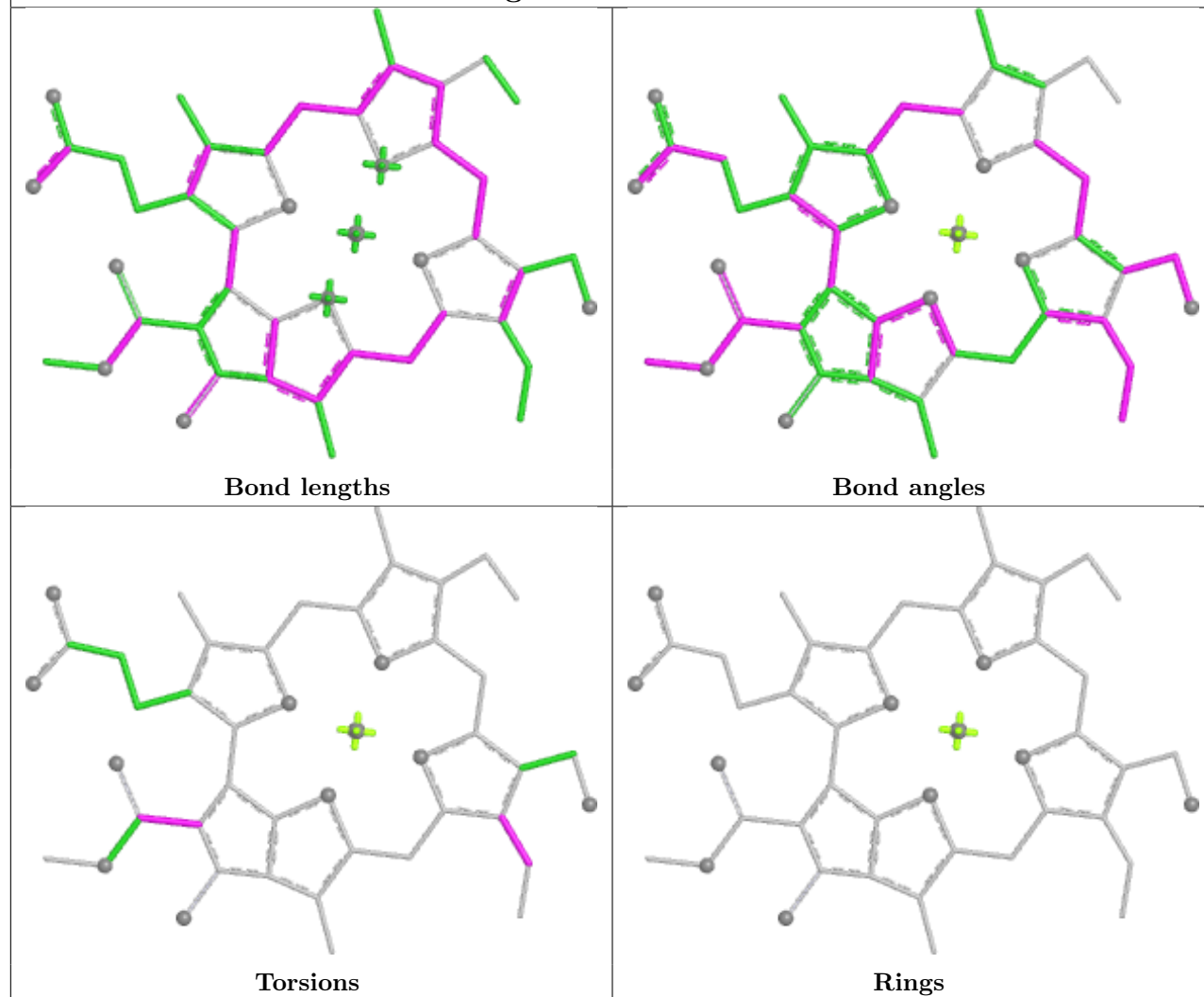


Ligand XAT 1 618

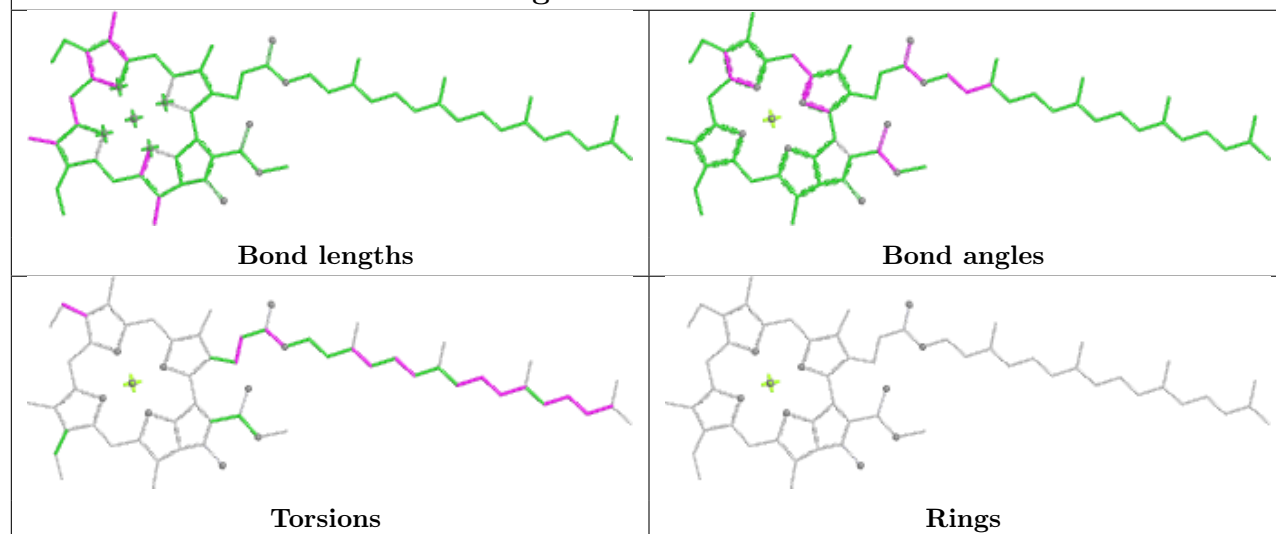




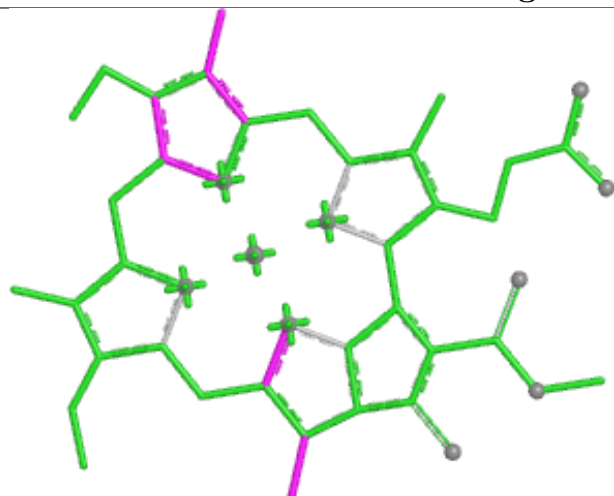
Ligand CHL 2 608



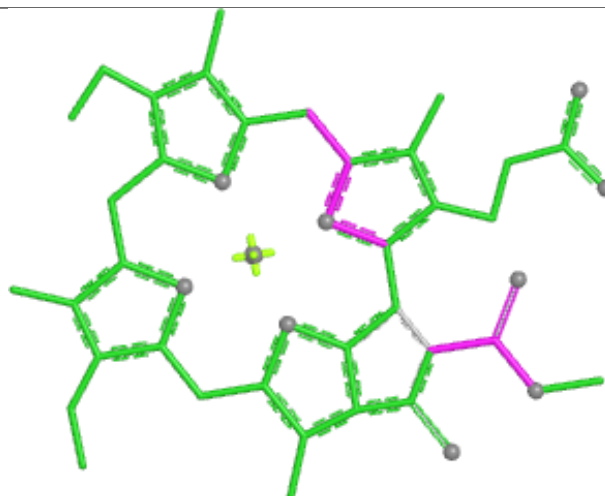
Ligand CLA B 817



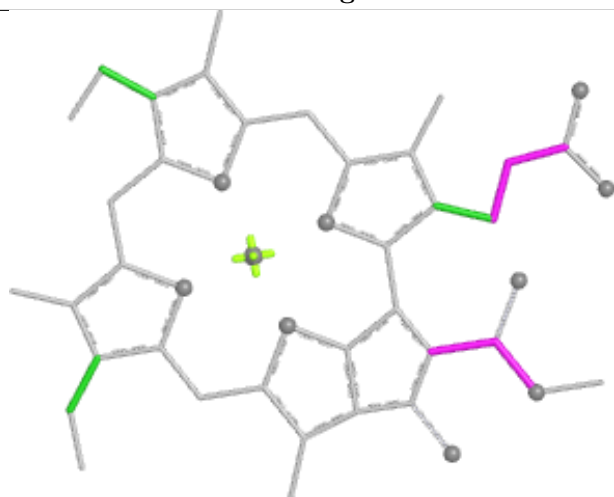
Ligand CLA 6 612



Bond lengths



Bond angles

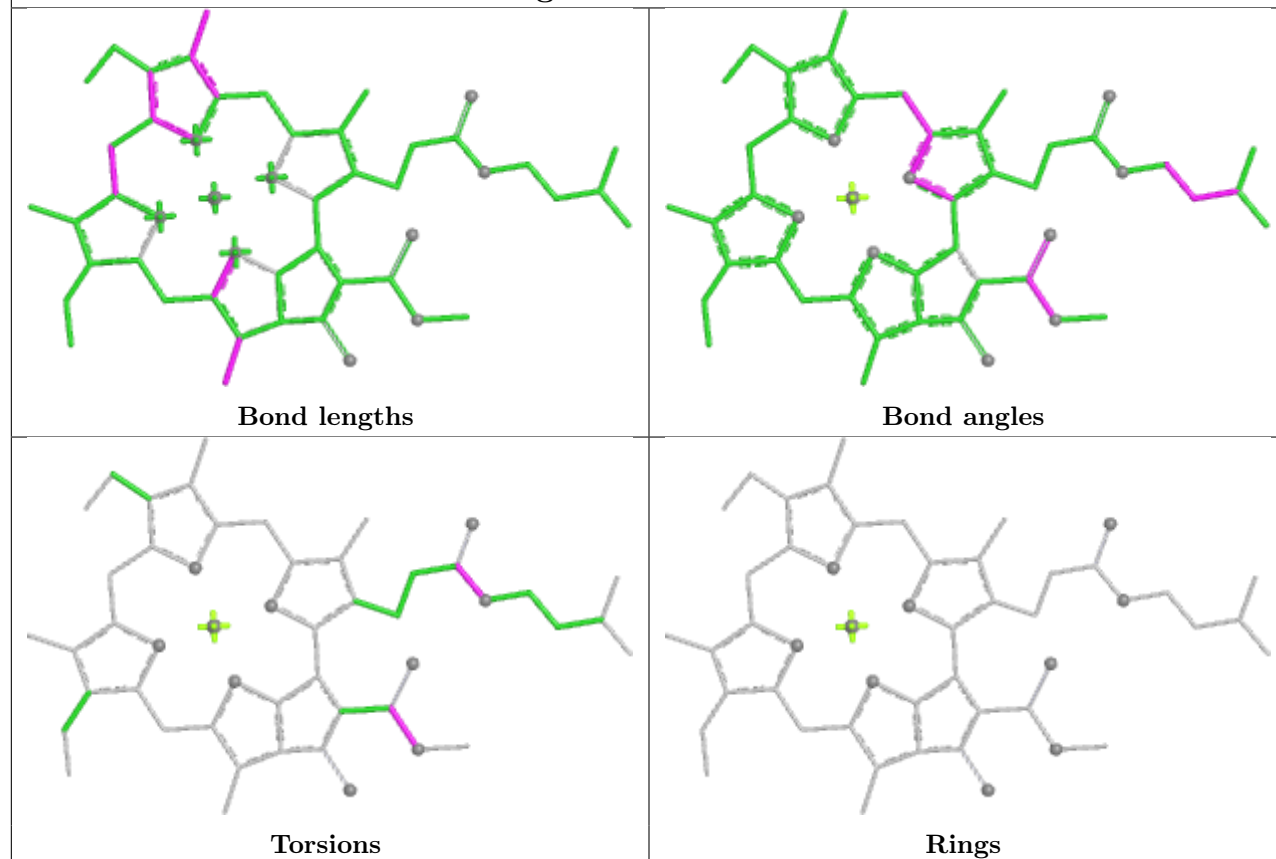


Torsions

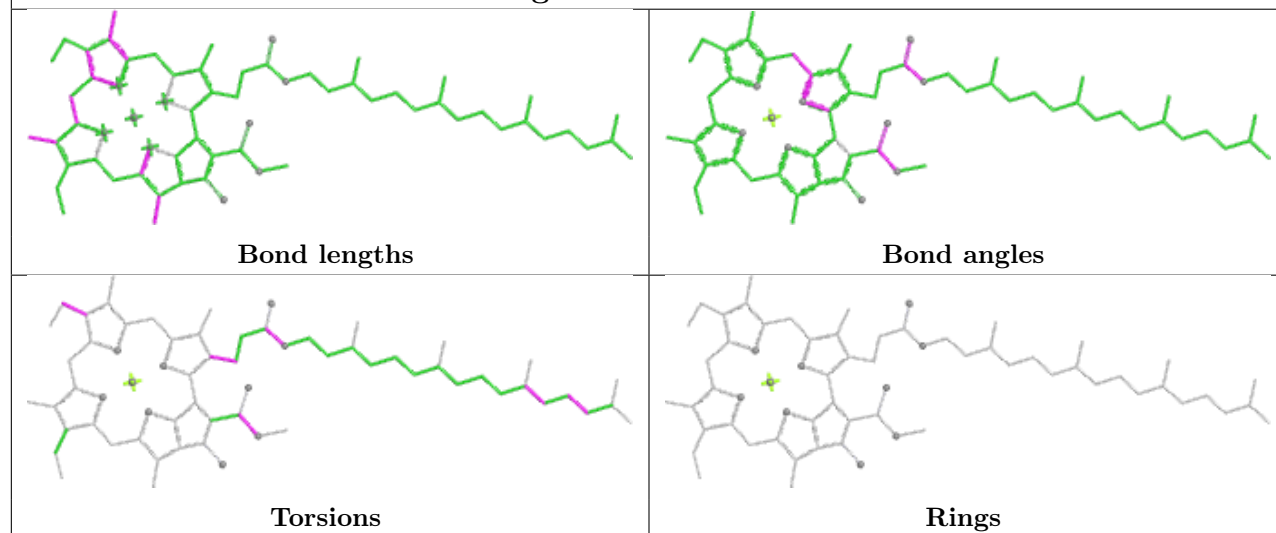


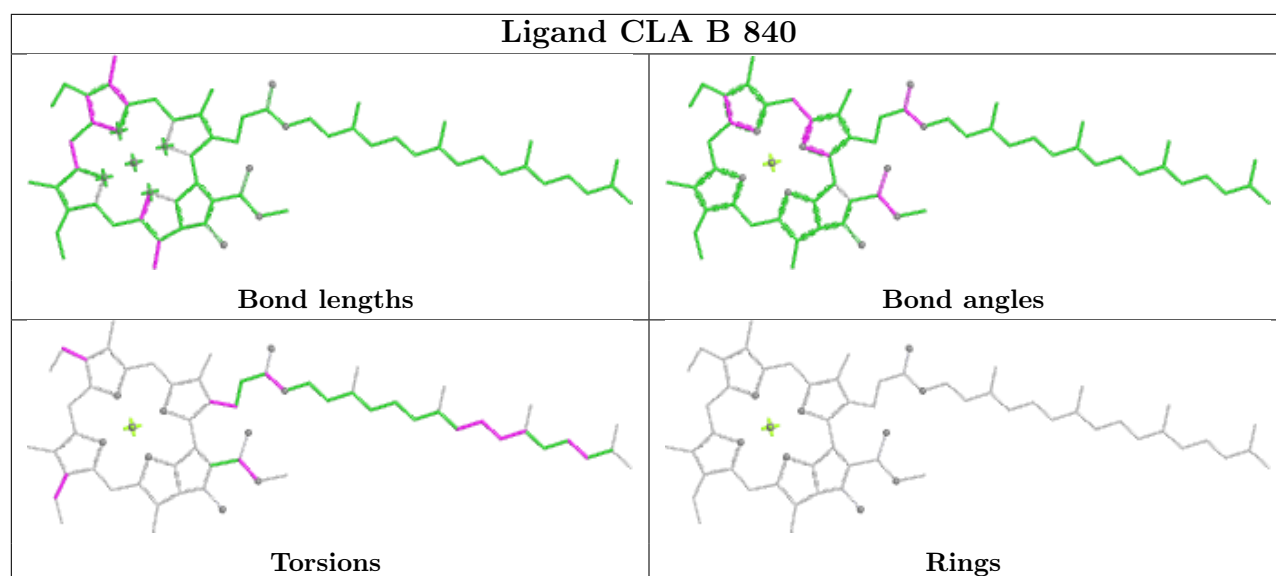
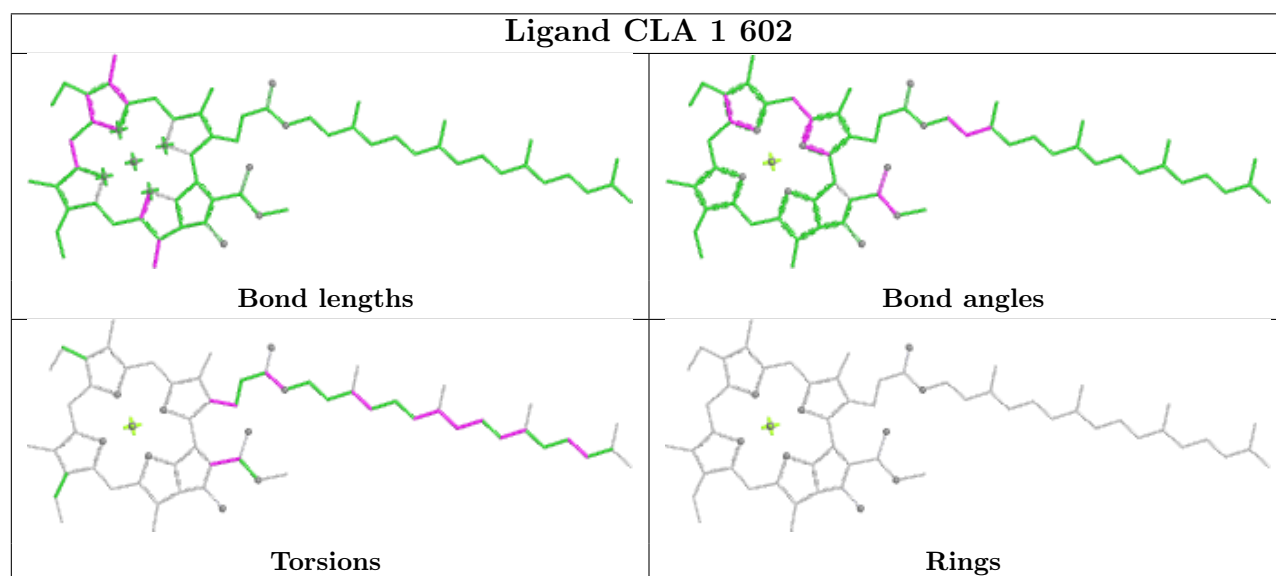
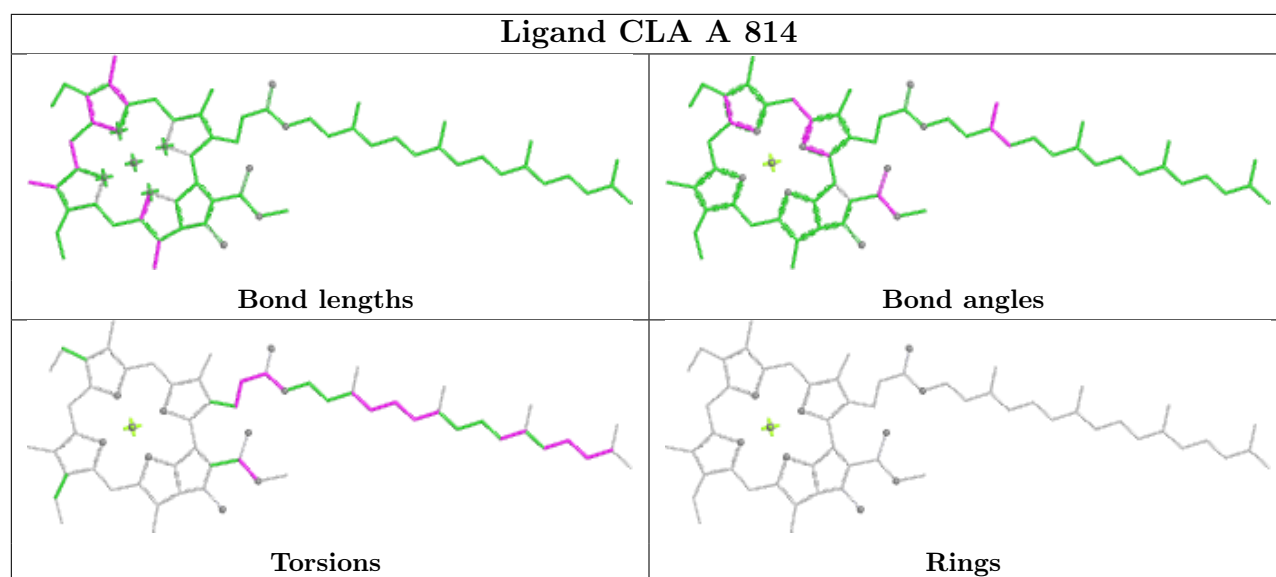
Rings

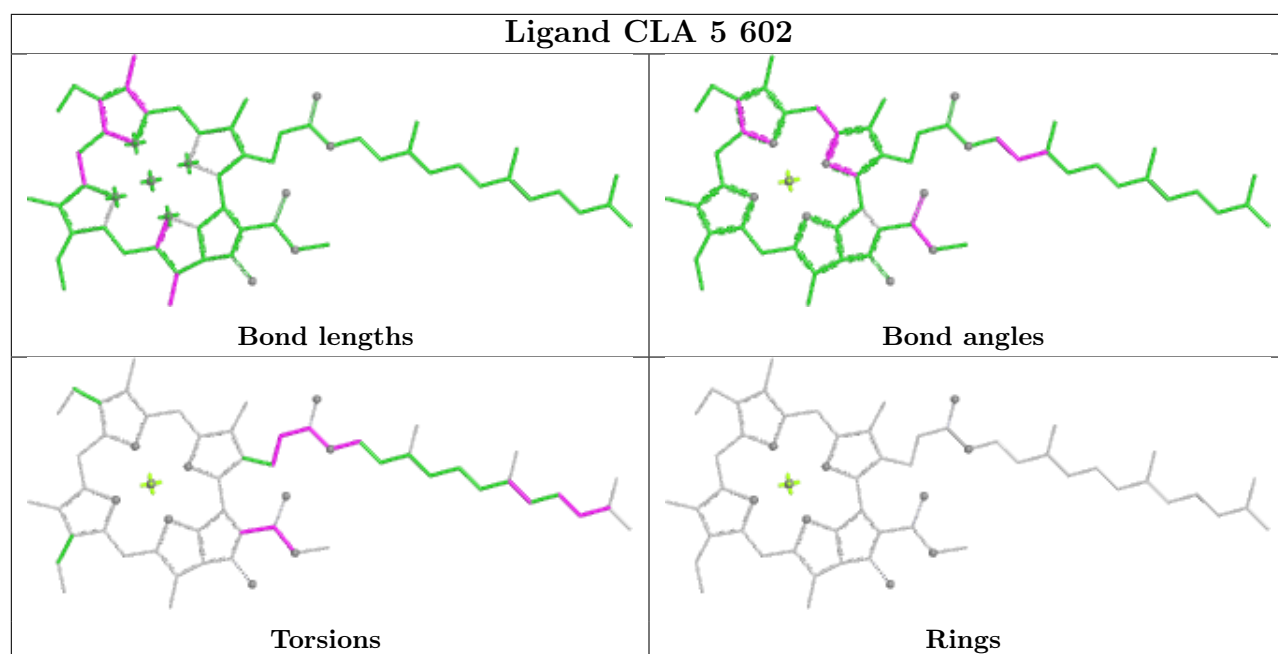
Ligand CLA 6 604

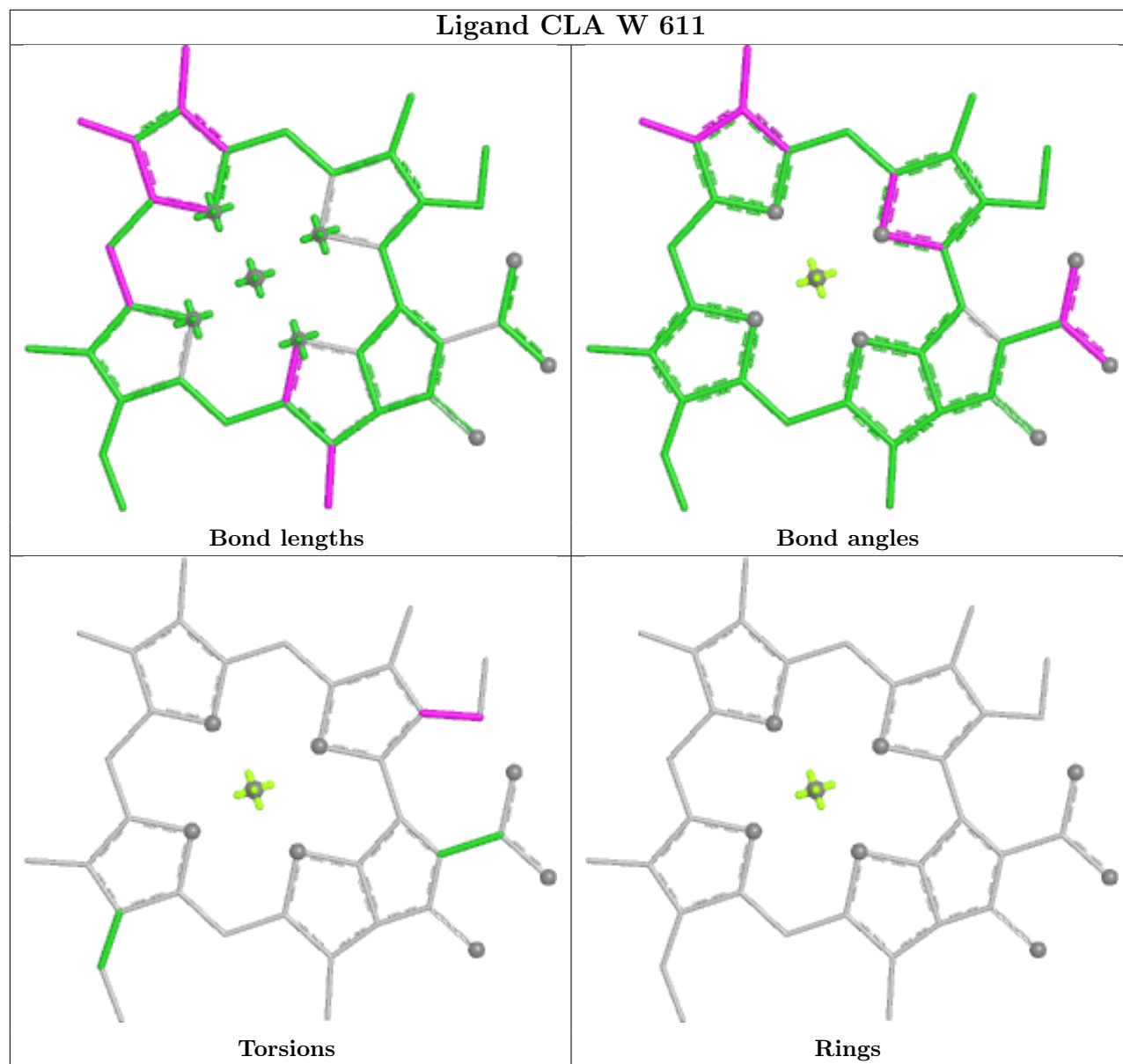


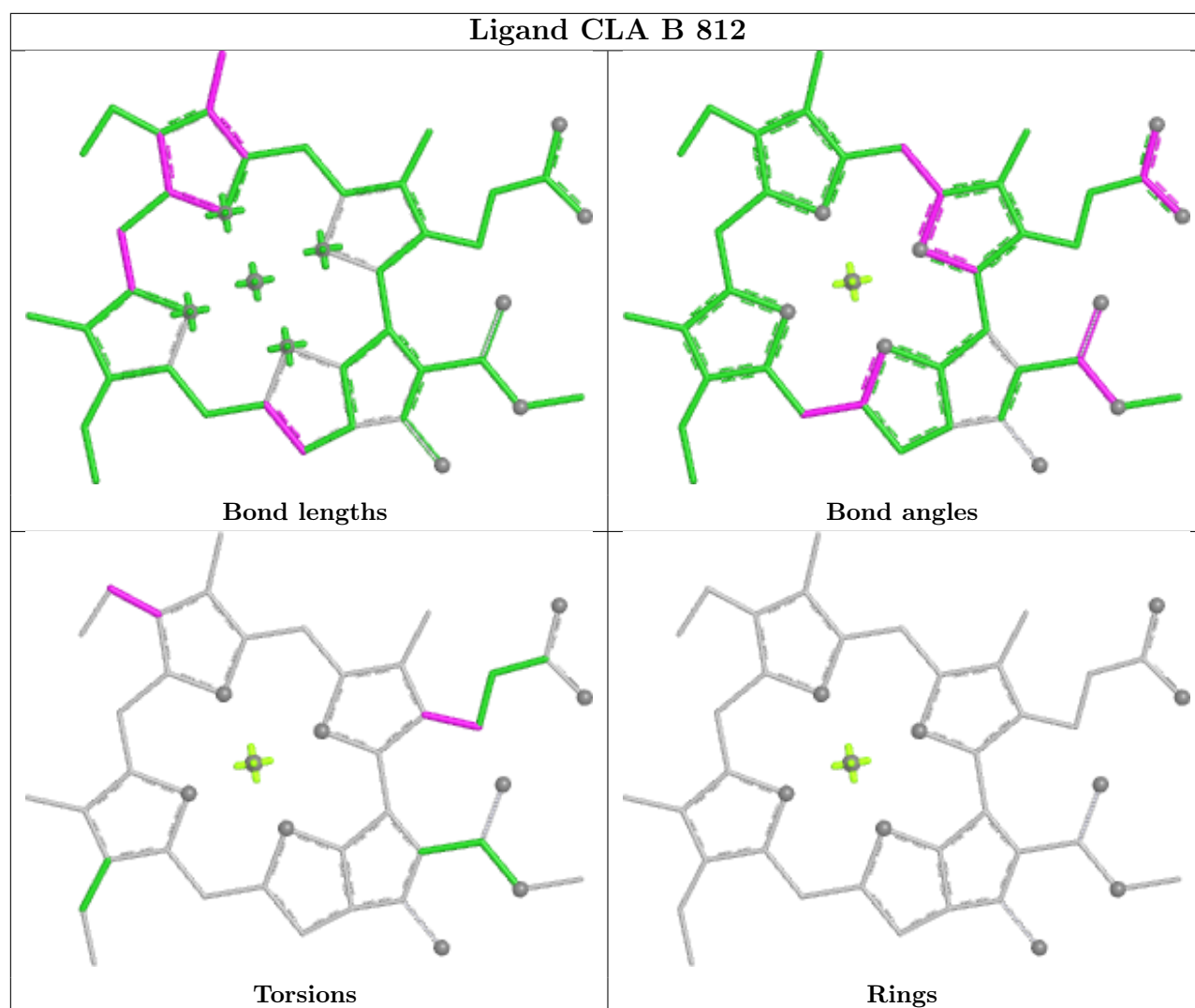
Ligand CLA A 812











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.

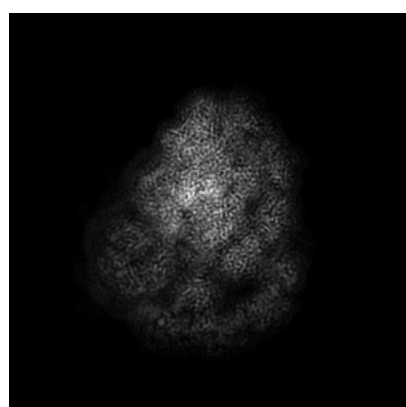
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35018. These allow visual inspection of the internal detail of the map and identification of artifacts.

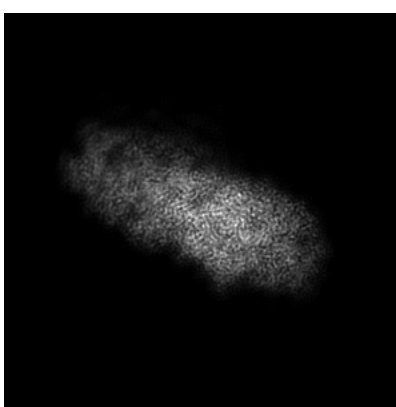
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

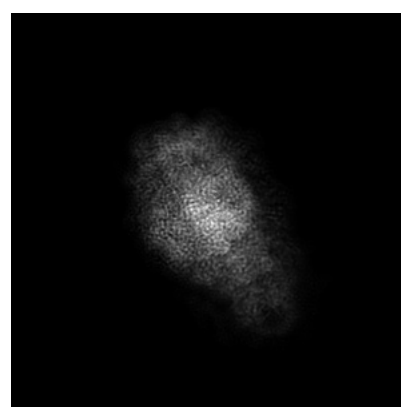
6.1.1 Primary map



X



Y

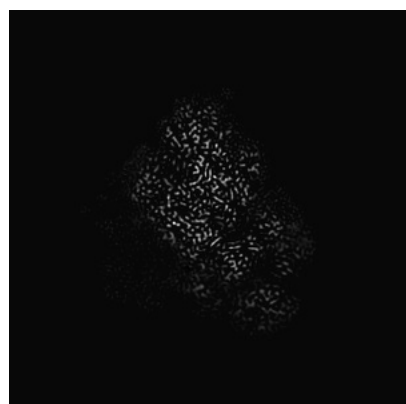


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

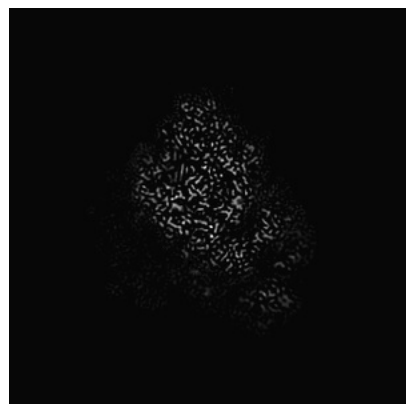


Z Index: 160

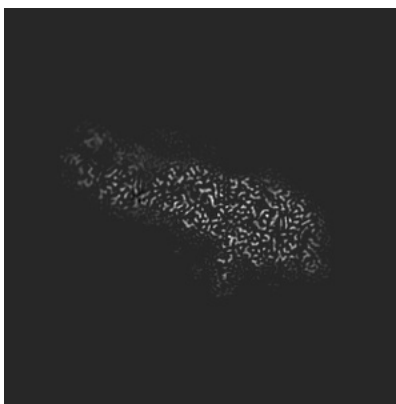
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 158



Y Index: 151

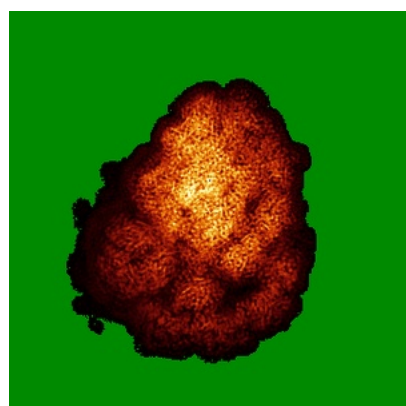


Z Index: 175

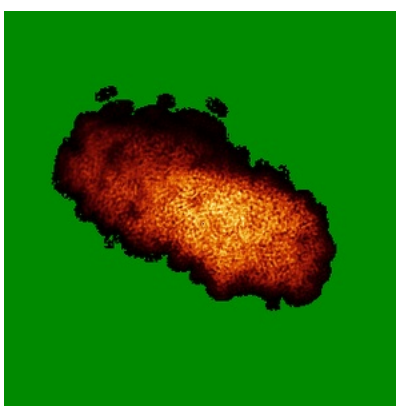
The images above show the largest variance slices of the map in three orthogonal directions.

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

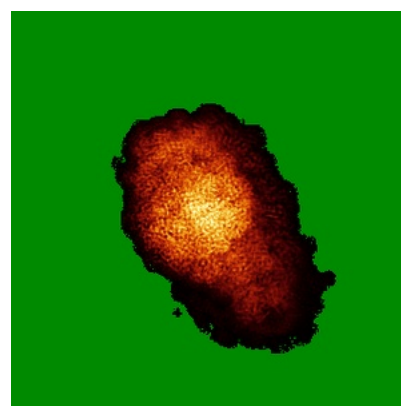
6.4.1 Primary map



X



Y

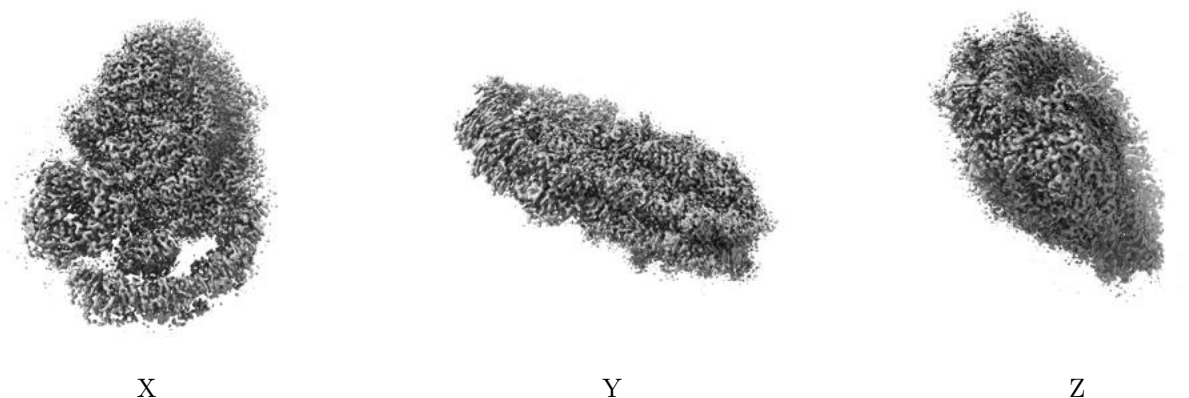


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

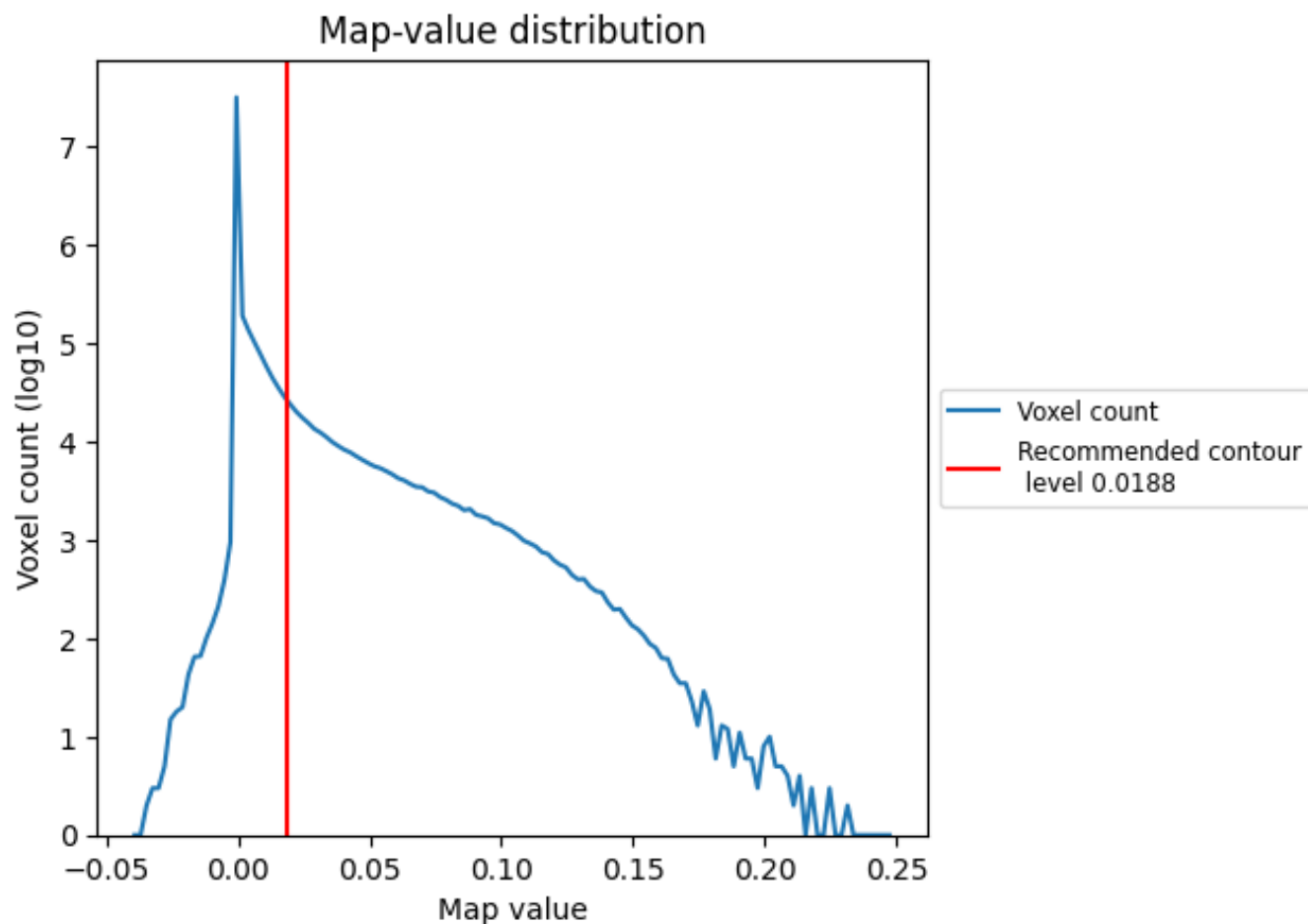
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

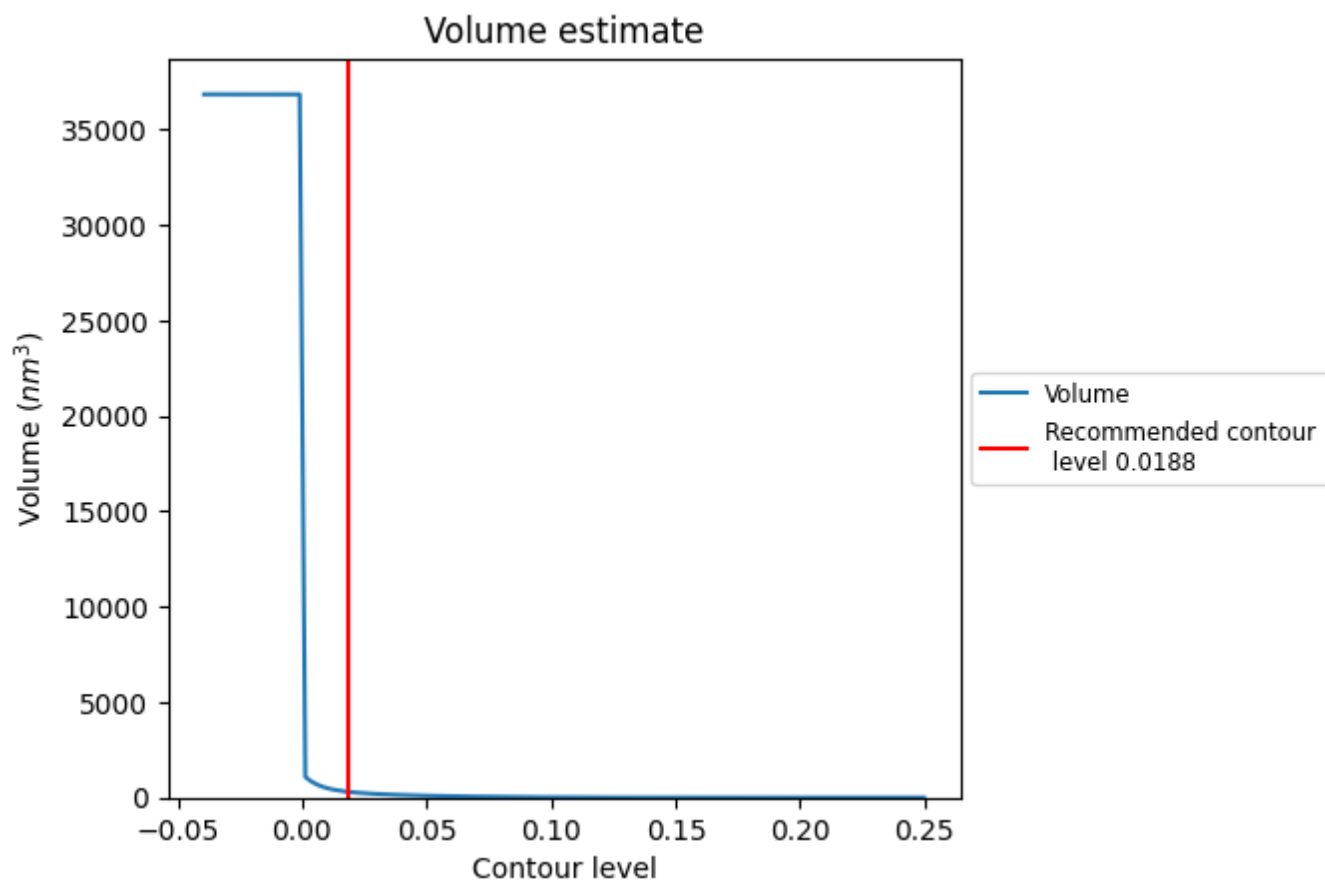
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

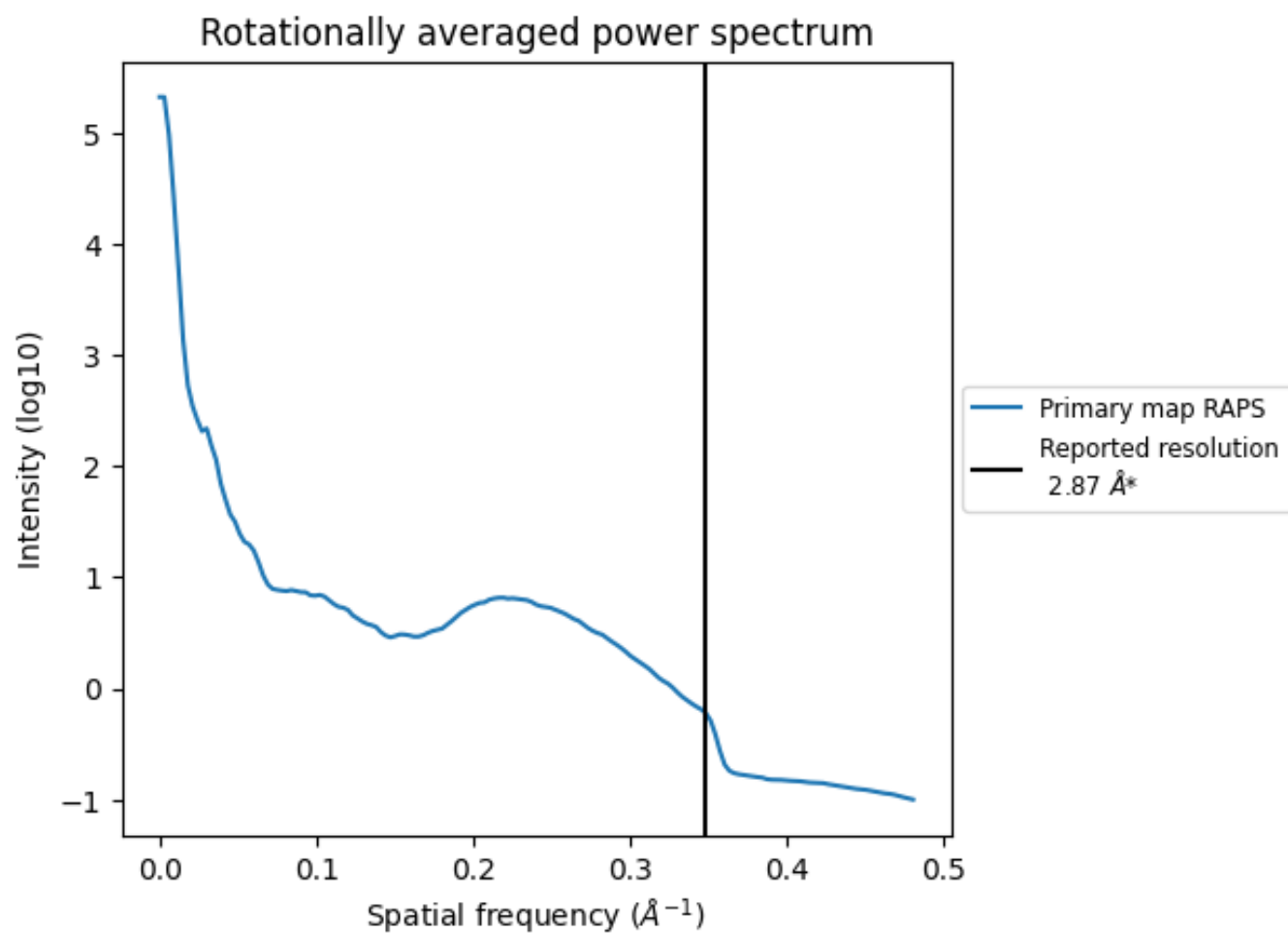
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm^3 ; this corresponds to an approximate mass of 267 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 0.348 Å⁻¹

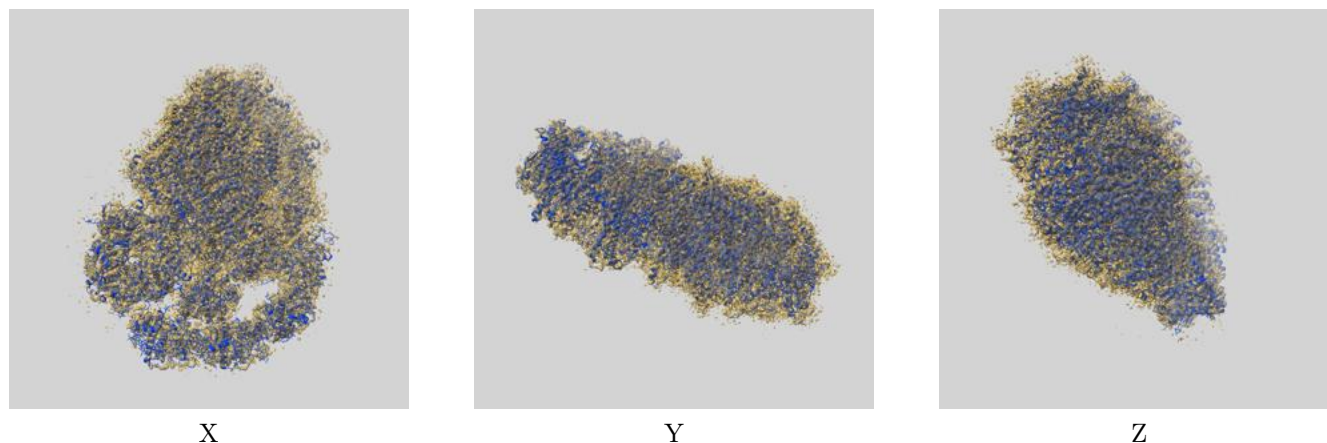
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

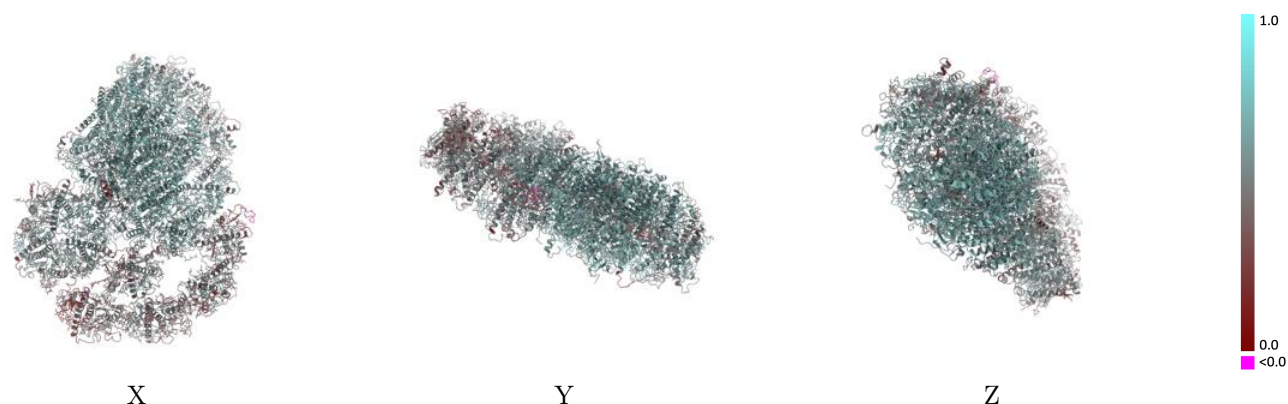
This section contains information regarding the fit between EMDB map EMD-35018 and PDB model 8HTU. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



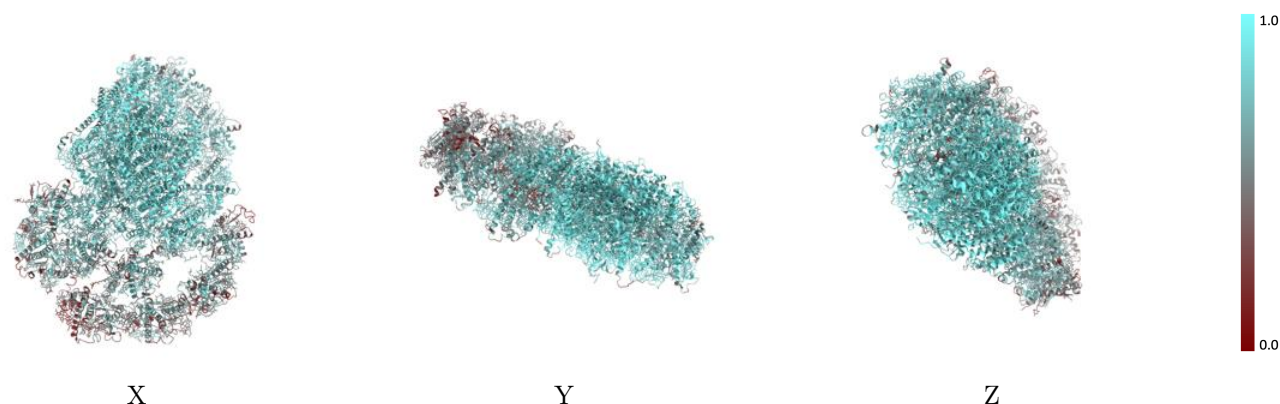
The images above show the 3D surface view of the map at the recommended contour level 0.0188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



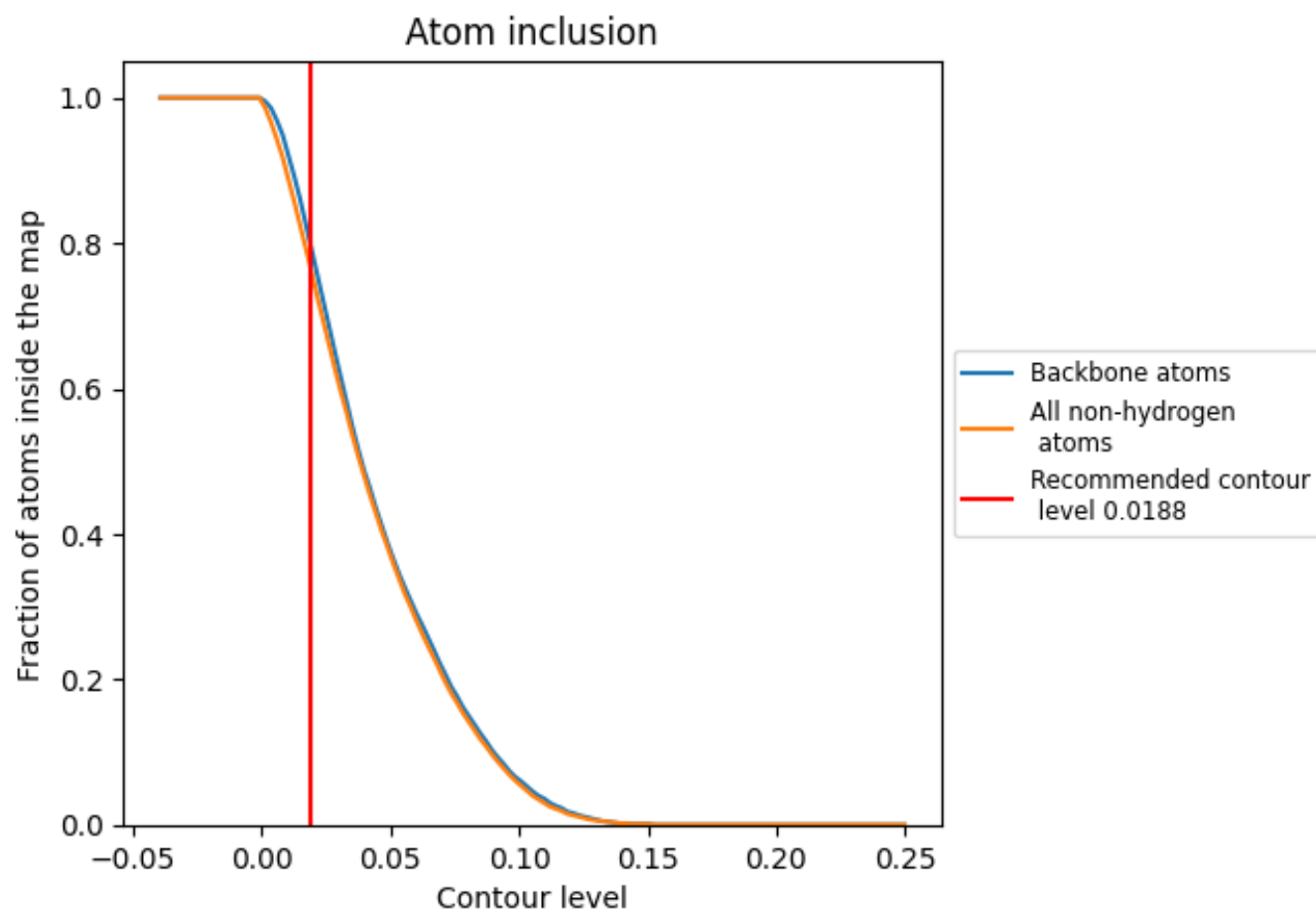
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0188).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.5500
1	 0.7560	 0.5390
2	 0.8540	 0.5860
3	 0.8550	 0.5880
4	 0.7930	 0.5400
5	 0.5530	 0.4110
6	 0.5150	 0.4410
7	 0.4180	 0.3830
8	 0.5530	 0.4610
9	 0.6210	 0.4420
A	 0.9310	 0.6320
B	 0.9210	 0.6270
C	 0.9460	 0.6200
D	 0.8850	 0.5910
E	 0.8660	 0.6050
F	 0.8630	 0.5990
G	 0.7240	 0.5410
H	 0.7350	 0.5080
I	 0.9010	 0.5910
J	 0.8490	 0.5860
K	 0.8640	 0.5880
L	 0.8690	 0.5870
M	 0.7750	 0.5580
O	 0.7840	 0.4770
U	 0.6840	 0.5290
V	 0.5640	 0.4930
W	 0.6720	 0.5220

