



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:30 AM UTC

PDB ID : 7XQP / pdb_00007xqp
EMDB ID : EMD-33401
Title : PSI-LHCI-LHCII-Lhcb9 supercomplex of *Physcomitrella patens*
Authors : Zhang, S.; Tang, K.L.; Li, X.Y.; Wang, W.D.; Yan, Q.J.; Shen, L.L.; Kuang, T.Y.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on : 2022-05-08
Resolution : 2.68 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:

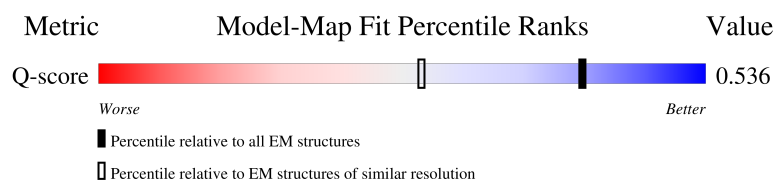
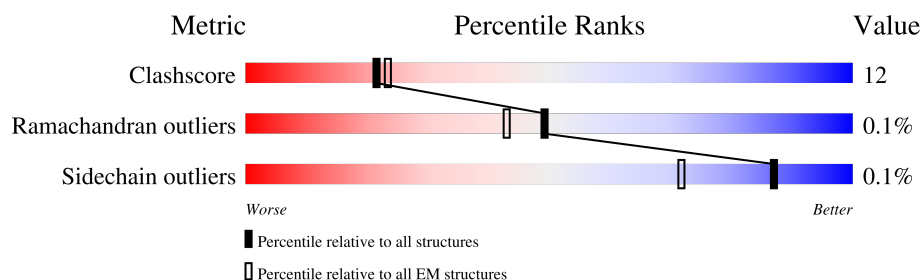
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.68 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	9255 (2.18 - 3.18)

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

Mol	Chain	Length	Quality of chain
1	A	742	 87% 13%
2	B	733	 86% 14%
3	C	80	 81% 19%
4	D	141	 87% 13%

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Mol	Chain	Length	Quality of chain
5	E	62	
6	F	159	
7	G	98	
8	H	95	
9	I	34	
10	J	41	
11	K	81	
12	L	163	
13	M	32	
14	O	89	
15	1	192	
15	5	192	
16	2	211	
16	6	211	
17	3	216	
17	7	216	
18	4	205	
18	8	205	
19	9	225	
20	a	227	
20	b	227	
20	c	227	

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	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	305	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-
21	CLA	1	314	X	-	-	-
21	CLA	1	315	X	-	-	-
21	CLA	1	316	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	X	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	401	X	-	-	-
21	CLA	3	402	X	-	-	-
21	CLA	3	403	X	-	-	-
21	CLA	3	404	X	-	-	-
21	CLA	3	405	X	-	-	-
21	CLA	3	406	X	-	-	-
21	CLA	3	408	X	-	-	-
21	CLA	3	409	X	-	X	-
21	CLA	3	410	X	-	-	-
21	CLA	3	411	X	-	-	-
21	CLA	3	412	X	-	-	-
21	CLA	3	413	X	-	-	-
21	CLA	3	414	X	-	-	-
21	CLA	3	415	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	4	613	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	605	X	-	-	-
21	CLA	5	607	X	-	-	-
21	CLA	5	608	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	608	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	7	401	X	-	-	-
21	CLA	7	402	X	-	-	-
21	CLA	7	403	X	-	-	-
21	CLA	7	404	X	-	-	-
21	CLA	7	405	X	-	-	-
21	CLA	7	408	X	-	-	-
21	CLA	7	409	X	-	-	-
21	CLA	7	410	X	-	-	-
21	CLA	7	411	X	-	-	-
21	CLA	7	412	X	-	-	-
21	CLA	7	413	X	-	-	-
21	CLA	7	414	X	-	-	-
21	CLA	8	601	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	X	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	8	618	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	852	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	F	302	X	-	-	-
21	CLA	F	304	X	-	-	-
21	CLA	F	305	X	-	-	-
21	CLA	G	202	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	H	201	X	-	-	-
21	CLA	J	102	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	202	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	L	302	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	O	201	X	-	-	-
21	CLA	O	202	X	-	-	-
21	CLA	O	203	X	-	-	-
21	CLA	O	204	X	-	-	-
21	CLA	a	602	X	-	-	-
21	CLA	a	603	X	-	-	-
21	CLA	a	604	X	-	-	-
21	CLA	a	610	X	-	-	-
21	CLA	a	611	X	-	-	-
21	CLA	a	612	X	-	-	-
21	CLA	a	613	X	-	-	-
21	CLA	a	614	X	-	-	-
21	CLA	b	303	X	-	-	-
21	CLA	b	304	X	-	-	-
21	CLA	b	305	X	-	-	-
21	CLA	b	311	X	-	-	-
21	CLA	b	312	X	-	-	-
21	CLA	b	313	X	-	-	-
21	CLA	b	314	X	-	-	-
21	CLA	b	315	X	-	-	-
21	CLA	c	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	c	603	X	-	-	-
21	CLA	c	604	X	-	-	-
21	CLA	c	610	X	-	-	-
21	CLA	c	611	X	-	-	-
21	CLA	c	612	X	-	-	-
21	CLA	c	613	X	-	-	-
21	CLA	c	614	X	-	-	-
24	BCR	K	205	-	-	X	-
29	CHL	1	302	X	-	-	-
29	CHL	1	307	X	-	-	-
29	CHL	2	601	X	-	-	-
29	CHL	2	602	X	-	-	-
29	CHL	2	605	X	-	-	-
29	CHL	2	606	X	-	-	-
29	CHL	2	607	X	-	-	-
29	CHL	2	614	X	-	-	-
29	CHL	3	407	X	-	-	-
29	CHL	4	605	X	-	-	-
29	CHL	4	606	X	-	-	-
29	CHL	4	607	X	-	-	-
29	CHL	4	614	X	-	-	-
29	CHL	5	601	X	-	-	-
29	CHL	5	606	X	-	-	-
29	CHL	6	601	X	-	-	-
29	CHL	6	602	X	-	-	-
29	CHL	6	605	X	-	-	-
29	CHL	6	606	X	-	-	-
29	CHL	6	607	X	-	-	-
29	CHL	6	614	X	-	-	-
29	CHL	7	406	X	-	-	-
29	CHL	8	605	X	-	-	-
29	CHL	8	606	X	-	-	-
29	CHL	8	607	X	-	-	-
29	CHL	8	613	X	-	-	-
29	CHL	9	601	X	-	-	-
29	CHL	9	605	X	-	-	-
29	CHL	9	606	X	-	-	-
29	CHL	9	607	X	-	-	-
29	CHL	9	608	X	-	-	-
29	CHL	9	609	X	-	-	-
29	CHL	a	601	X	-	-	-
29	CHL	a	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	a	606	X	-	-	-
29	CHL	a	607	X	-	-	-
29	CHL	a	608	X	-	-	-
29	CHL	a	609	X	-	-	-
29	CHL	b	302	X	-	-	-
29	CHL	b	306	X	-	-	-
29	CHL	b	307	X	-	-	-
29	CHL	b	308	X	-	-	-
29	CHL	b	309	X	-	-	-
29	CHL	b	310	X	-	-	-
29	CHL	c	601	X	-	-	-
29	CHL	c	605	X	-	-	-
29	CHL	c	606	X	-	-	-
29	CHL	c	607	X	-	-	-
29	CHL	c	608	X	-	-	-
29	CHL	c	609	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56417 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5836	3827	993	997	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1230	796	210	221	3		

- Molecule 7 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	95	Total	C	N	O	S	0	0
			740	476	125	138	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

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

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			566	356	98	109	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	163	Total	C	N	O	S	0	0
			1229	808	197	222	2		

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O	S	0	0
			238	155	38	44	1		

- Molecule 14 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	89	Total	C	N	O	S	0	0
			702	472	115	114	1		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1478	965	247	265	1		
15	5	192	Total	C	N	O	S	0	0
			1475	962	247	265	1		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	211	Total	C	N	O	S	0	0
			1632	1062	274	292	4		
16	6	205	Total	C	N	O	S	0	0
			1587	1035	265	283	4		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	216	Total	C	N	O	S	0	0
			1670	1094	269	300	7		
17	7	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	205	Total	C	N	O	S	0	0
			1592	1033	266	288	5		
18	8	204	Total	C	N	O	S	0	0
			1585	1029	265	286	5		

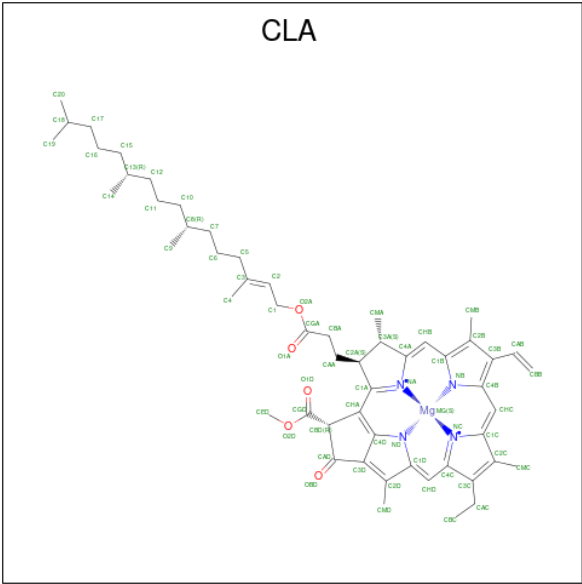
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	225	Total	C	N	O	S	0	0
			1747	1139	287	312	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	218	Total	C	N	O	S	0	0
			1651	1069	268	309	5		
20	b	218	Total	C	N	O	S	0	0
			1651	1069	268	309	5		
20	c	227	Total	C	N	O	P	S	0
			1727	1110	284	327	1	5	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 63	C 53	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	G	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	K	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	O	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 50	C 42	Mg 1	N 4	O 3	0
21	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	2	1	Total 51	C 42	Mg 1	N 4	O 4	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	7	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 54	C 45	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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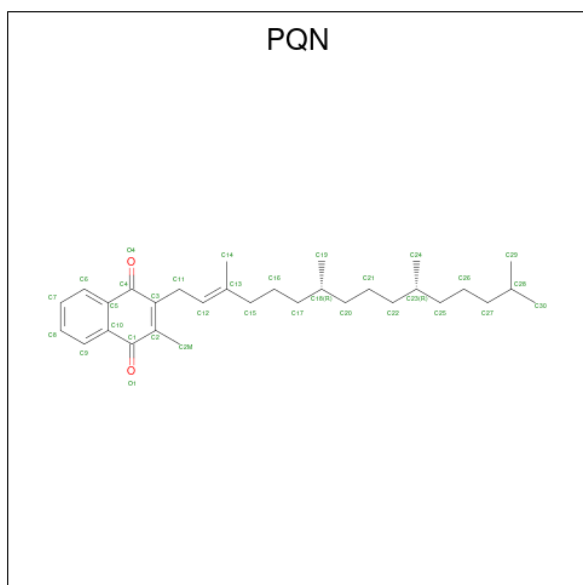
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	c	1	Total 44	C 35	Mg 1	N 4	O 4	0

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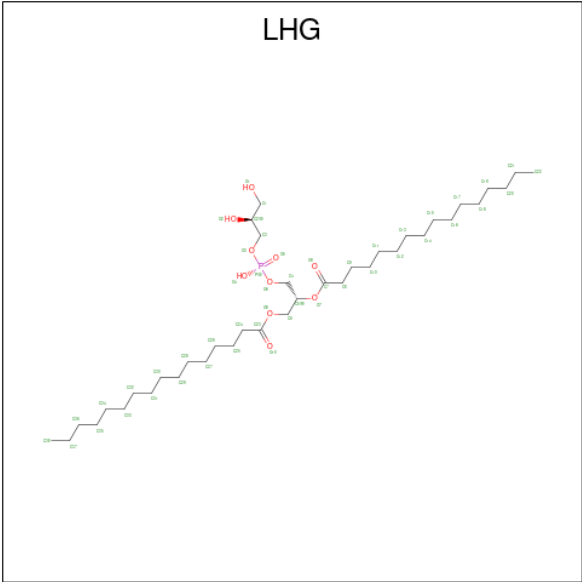
Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



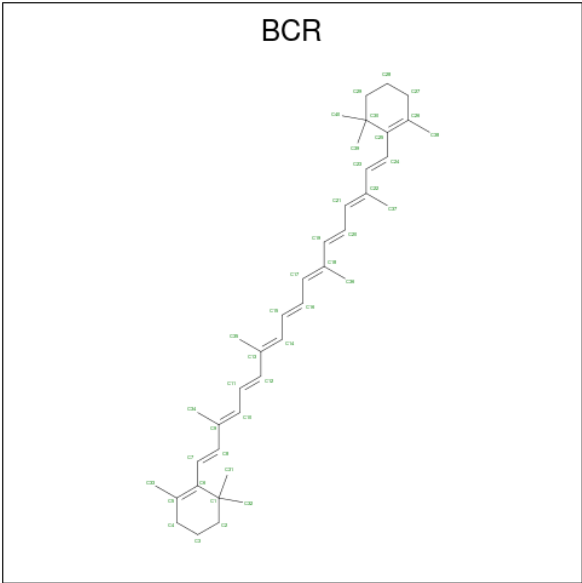
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			28	17	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	4	1	Total	C	O	P	0
			37	26	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	5	1	Total	C	O	P	0
			28	17	10	1	
23	6	1	Total	C	O	P	0
			35	24	10	1	
23	8	1	Total	C	O	P	0
			37	26	10	1	
23	9	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			49	38	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	c	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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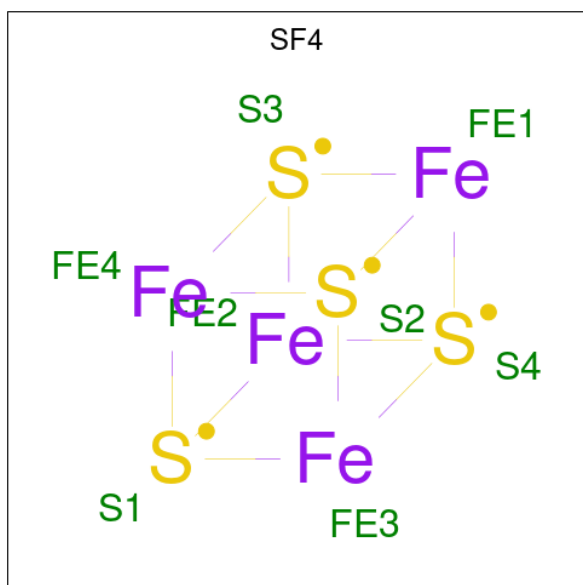
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	M	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	7	1	Total C 40 40	0

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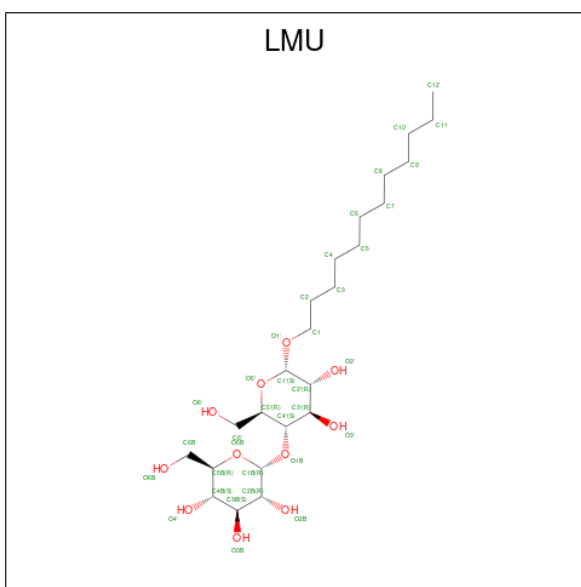
Mol	Chain	Residues	Atoms	AltConf
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



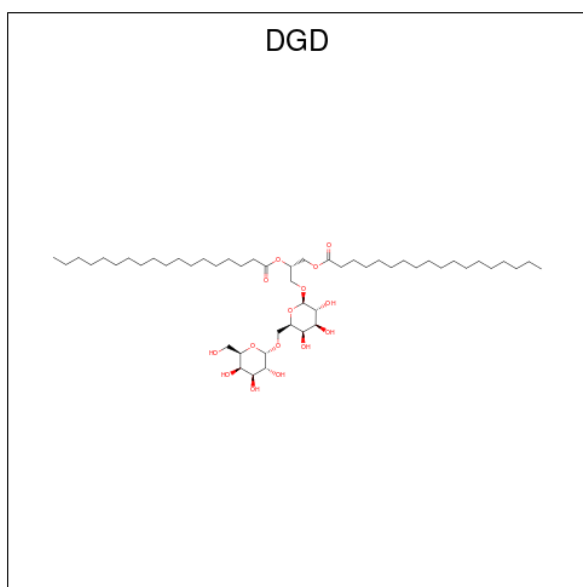
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).



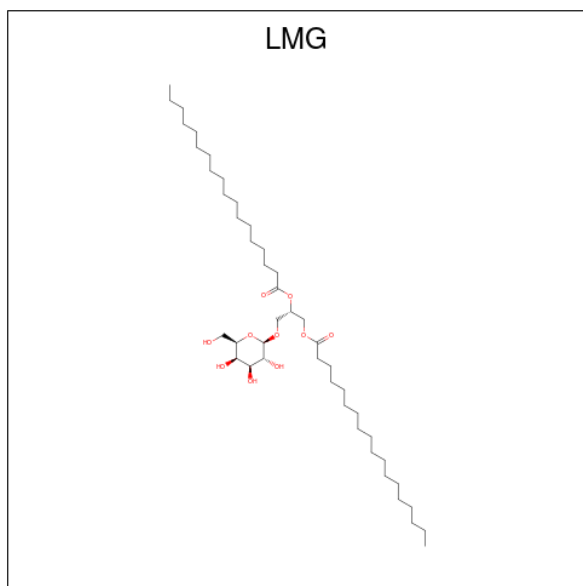
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total 35	C 24	O 11	0
26	A	1	Total 35	C 24	O 11	0
26	O	1	Total 35	C 24	O 11	0
26	3	1	Total 35	C 24	O 11	0
26	b	1	Total 35	C 24	O 11	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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



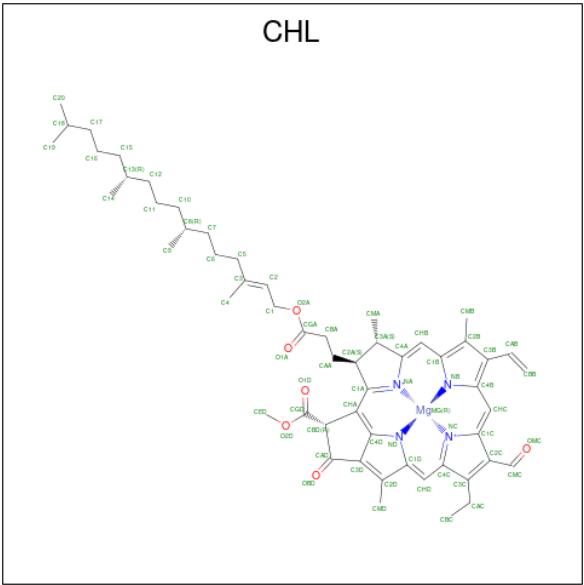
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			30	20	10	

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Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			13	7	6	
28	6	1	Total	C	O	0
			13	7	6	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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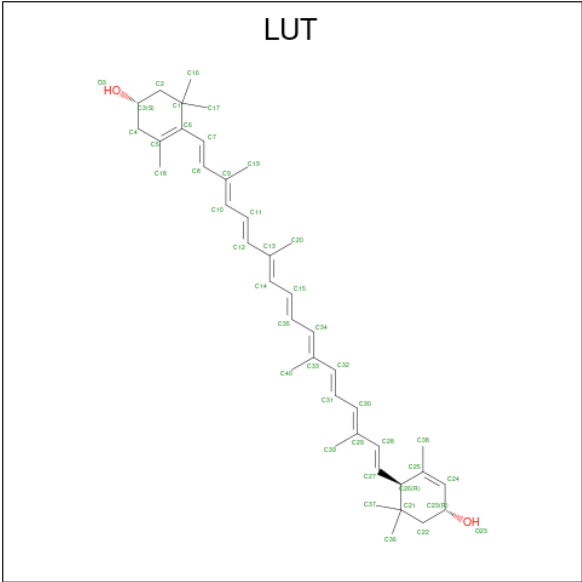
Mol	Chain	Residues	Atoms					AltConf
29	4	1	Total 41	C 32	Mg 1	N 4	O 4	0
29	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
29	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	6	1	Total 53	C 42	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	8	1	Total 41	C 32	Mg 1	N 4	O 4	0
29	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	8	1	Total 42	C 33	Mg 1	N 4	O 4	0
29	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			44	33	1	4	6	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



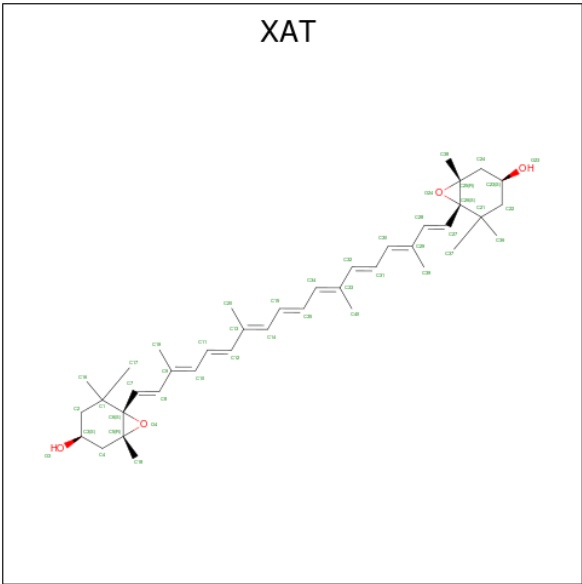
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	
30	5	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
30	c	1	Total	C	O	0
			42	40	2	
30	c	1	Total	C	O	0
			42	40	2	

- Molecule 31 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).



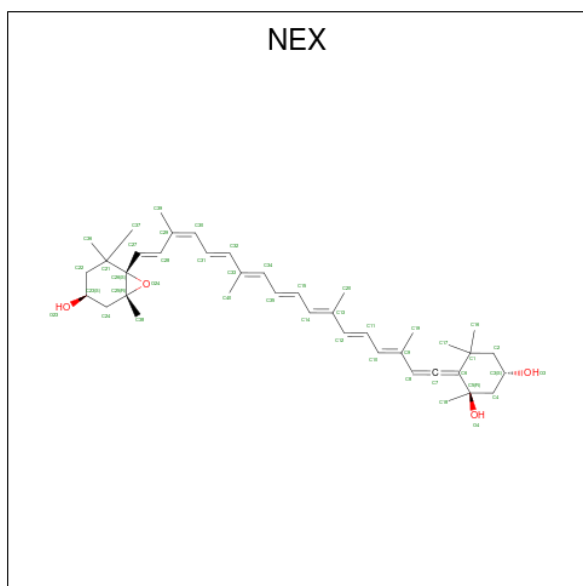
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			44	40	4	
31	2	1	Total	C	O	0
			44	40	4	
31	3	1	Total	C	O	0
			44	40	4	
31	4	1	Total	C	O	0
			44	40	4	
31	5	1	Total	C	O	0
			44	40	4	
31	6	1	Total	C	O	0
			44	40	4	
31	7	1	Total	C	O	0
			44	40	4	
31	8	1	Total	C	O	0
			44	40	4	
31	9	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			44	40	4	
31	c	1	Total	C	O	0
			44	40	4	

- Molecule 32 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).

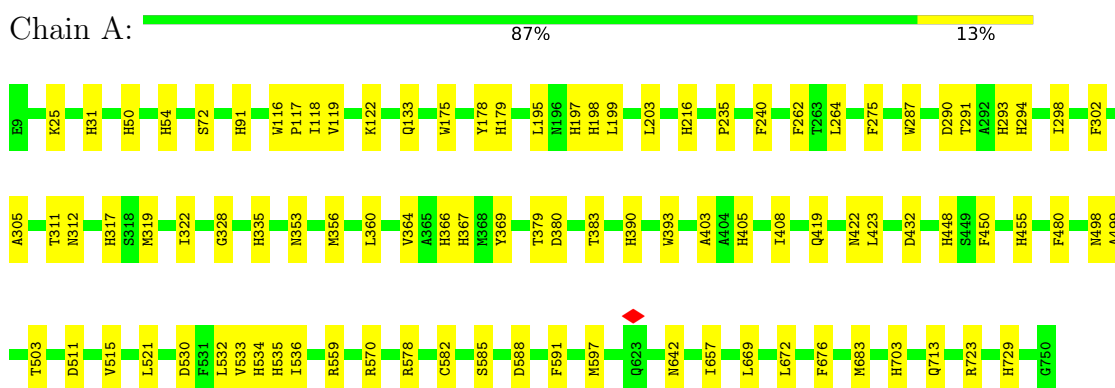


Mol	Chain	Residues	Atoms			AltConf
32	9	1	Total	C	O	0
			44	40	4	
32	b	1	Total	C	O	0
			44	40	4	
32	c	1	Total	C	O	0
			44	40	4	

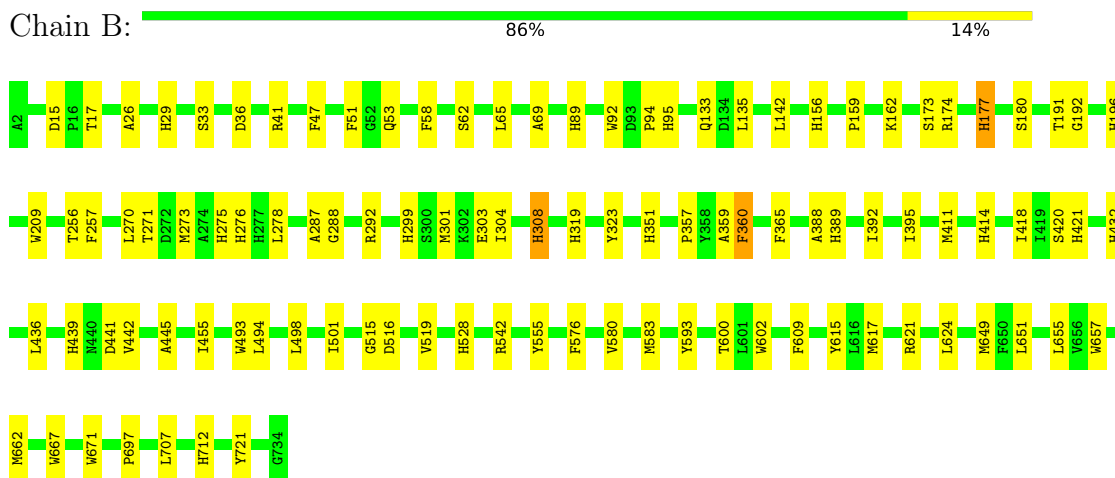
3 Residue-property plots

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

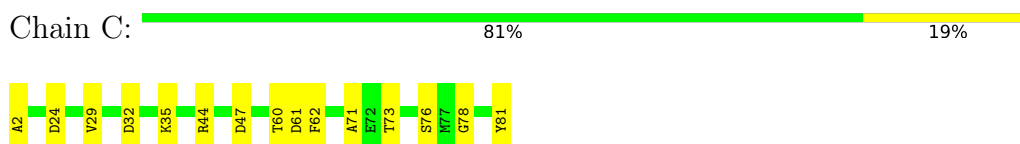
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Predicted protein PsaD

Chain D:  87% 13%



- Molecule 5: PsaE

Chain E:  85% 15%



- Molecule 6: PSI-F

Chain F:  89% 11%



- Molecule 7: PSI-G

Chain G:  85% 15% 5%



- Molecule 8: PsaH photosystem I reaction center subunit

Chain H:  93% 7%



- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  79% 21%



- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  88% 12%



- Molecule 11: PsaK

Chain K:  90% 10%



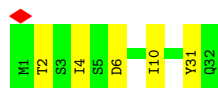
- Molecule 12: PSI subunit V

Chain L:  90% 10%



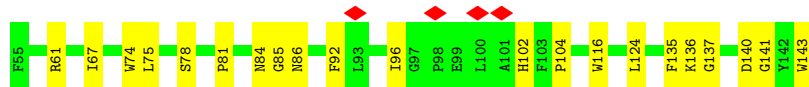
- Molecule 13: Photosystem I reaction center subunit XII

Chain M:  84% 16%



- Molecule 14: PsaO

Chain O:  76% 24%



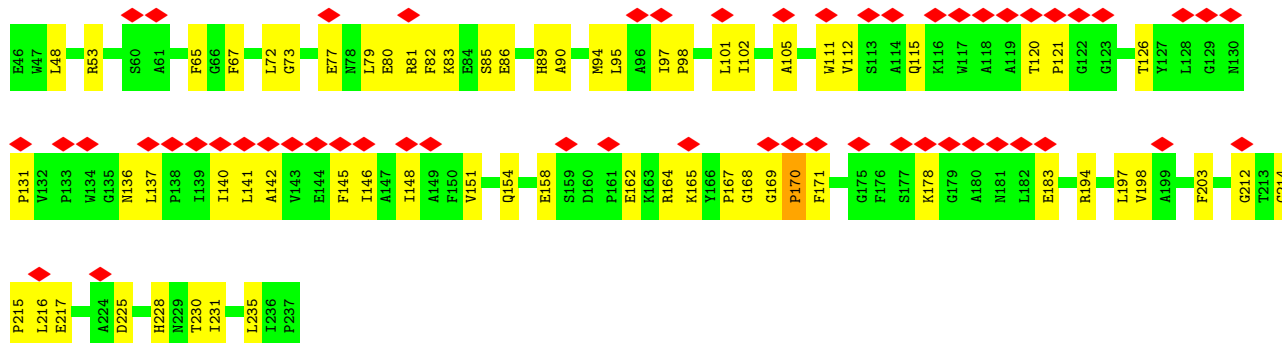
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 1:  84% 16%



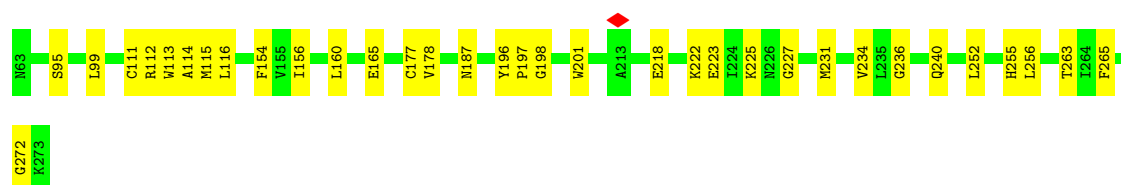
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5:  29% 66% 33%



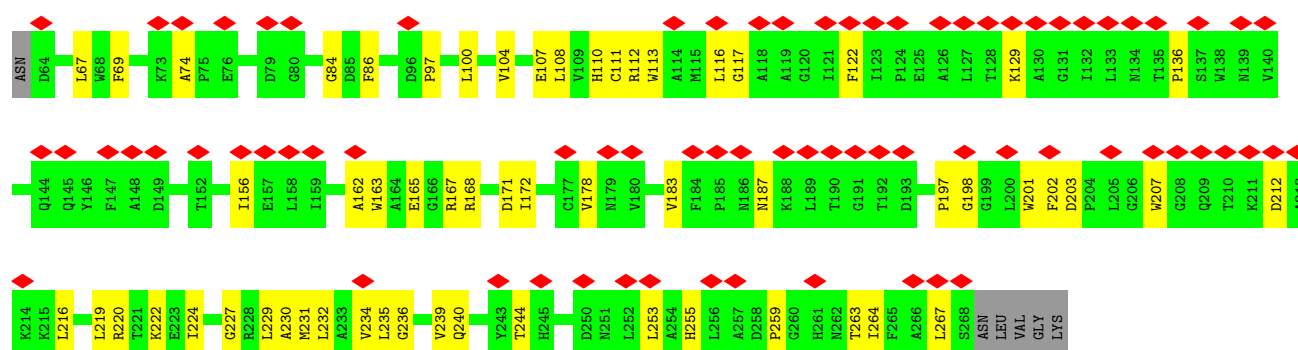
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  84% 16%



- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  36% 69% 28%



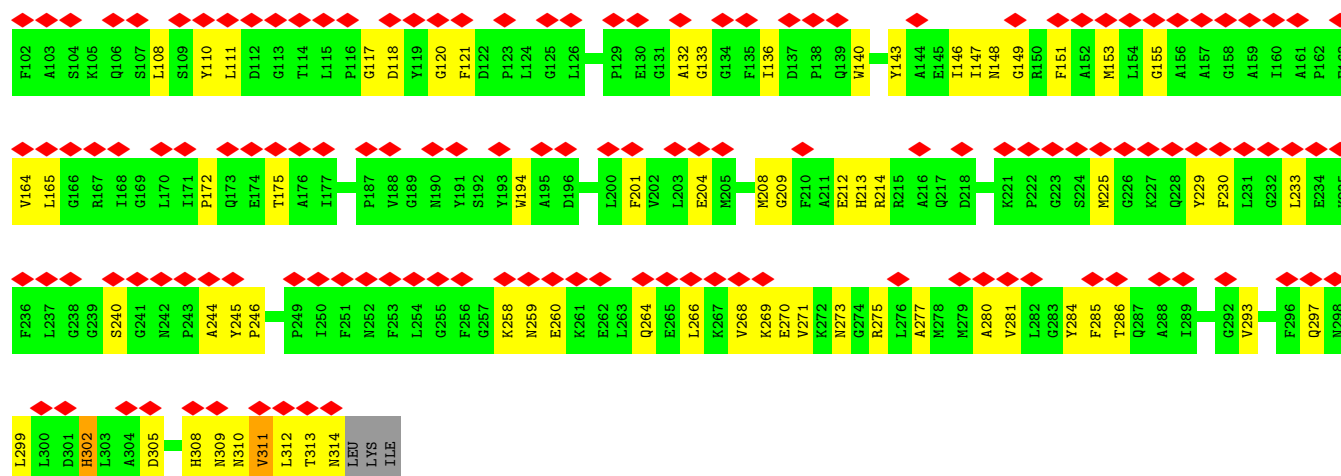
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 3:  89% 11%



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  62% 67% 31%



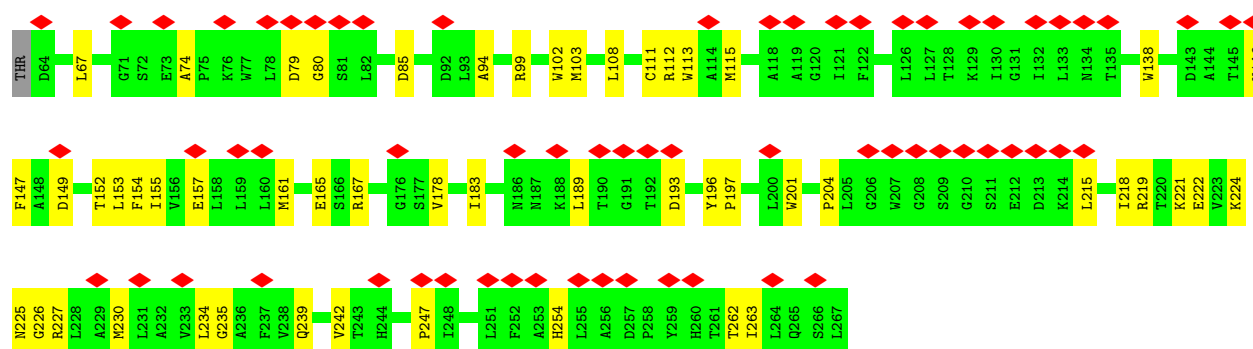
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:  85% 15%



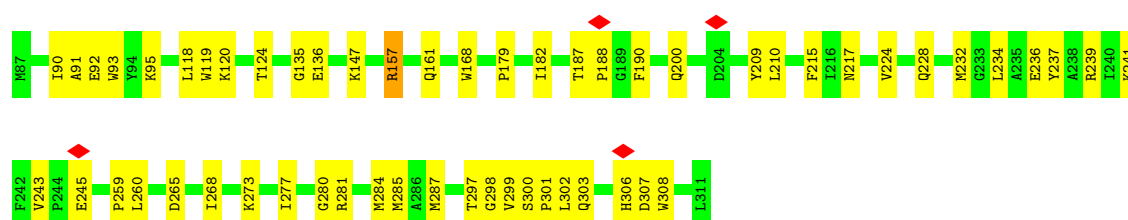
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  32% 74% 25%



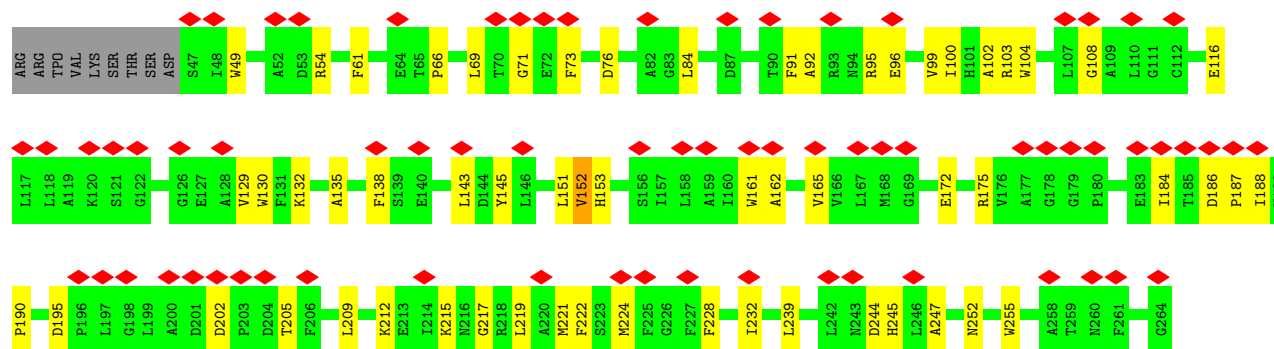
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9:  75% 24%



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain a:  31% 70% 26%

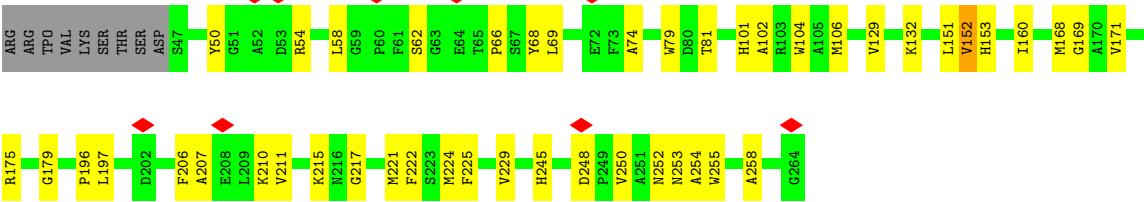


- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain b:

76%

20%



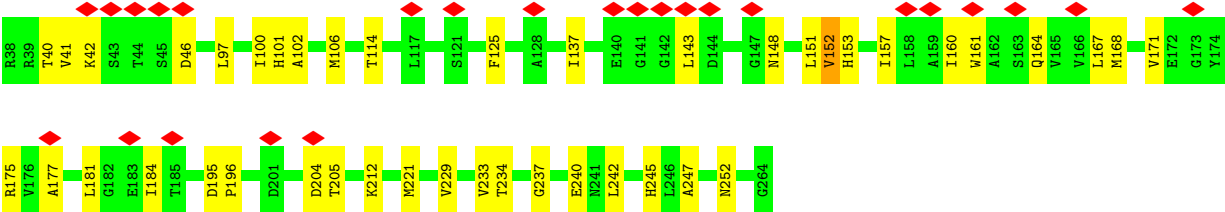
● Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain c:

11%

81%

19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83777	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 ($e^-/\text{\AA}^2$)	78	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.400	Depositor
Minimum map value	-1.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	486.72003, 486.72003, 486.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: CLA, SF4, LUT, NEX, LMU, BCR, TPO, CHL, PQN, LHG, LMG, DGD, XAT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/6031	0.33	0/8227
2	B	0.26	2/6063 (0.0%)	0.38	1/8274 (0.0%)
3	C	0.19	0/605	0.41	0/821
4	D	0.13	0/1132	0.38	1/1532 (0.1%)
5	E	0.12	0/498	0.23	0/677
6	F	0.15	0/1255	0.29	0/1696
7	G	0.20	0/767	0.38	0/1046
8	H	0.12	0/758	0.26	0/1022
9	I	0.15	0/273	0.37	0/373
10	J	0.14	0/334	0.25	0/457
11	K	0.13	0/572	0.23	0/773
12	L	0.14	0/1264	0.28	0/1727
13	M	0.24	0/239	0.26	0/322
14	O	0.17	0/729	0.37	0/997
15	1	0.20	0/1527	0.34	0/2088
15	5	0.18	0/1524	0.43	1/2084 (0.0%)
16	2	0.22	0/1683	0.41	0/2300
16	6	0.13	0/1638	0.31	0/2241
17	3	0.21	0/1721	0.40	0/2335
17	7	0.18	0/1695	0.39	0/2302
18	4	0.15	0/1641	0.29	0/2244
18	8	0.16	0/1634	0.31	0/2234
19	9	0.26	1/1801 (0.1%)	0.43	0/2451
20	a	0.18	0/1700	0.37	0/2316
20	b	0.15	0/1700	0.31	0/2316
20	c	0.14	0/1764	0.35	0/2399
All	All	0.19	3/40548 (0.0%)	0.35	3/55254 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	9	157	ARG	C-O	-6.48	1.16	1.24
2	B	177	HIS	CA-C	-5.34	1.46	1.52
2	B	308	HIS	CA-C	-5.26	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	PHE	CB-CA-C	9.86	119.59	109.83
4	D	173	LEU	N-CA-C	5.43	120.41	113.18
15	5	171	PHE	N-CA-C	-5.28	106.17	113.18

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	A	5836	0	5725	105	0
2	B	5849	0	5623	116	0
3	C	595	0	573	12	0
4	D	1104	0	1112	16	0
5	E	487	0	480	8	0
6	F	1230	0	1282	14	0
7	G	749	0	729	12	0
8	H	740	0	727	7	0
9	I	266	0	274	4	0
10	J	325	0	341	5	0
11	K	566	0	587	8	0
12	L	1229	0	1242	13	0
13	M	238	0	263	3	0
14	O	702	0	697	12	0
15	1	1478	0	1455	27	0
15	5	1475	0	1447	51	0
16	2	1632	0	1603	34	0
16	6	1587	0	1556	57	0
17	3	1670	0	1633	21	0
17	7	1644	0	1599	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	4	1592	0	1561	31	0
18	8	1585	0	1555	63	0
19	9	1747	0	1721	44	0
20	a	1651	0	1586	61	0
20	b	1651	0	1585	46	0
20	c	1727	0	1661	49	0
21	1	587	0	420	22	0
21	2	366	0	281	33	0
21	3	642	0	487	37	0
21	4	472	0	362	27	0
21	5	531	0	369	24	0
21	6	347	0	253	19	0
21	7	551	0	377	35	0
21	8	460	0	348	46	0
21	9	352	0	290	12	0
21	A	2422	0	2311	116	0
21	B	2312	0	2267	108	0
21	F	147	0	123	3	0
21	G	139	0	102	3	0
21	H	45	0	33	2	0
21	J	42	0	31	0	0
21	K	185	0	135	16	0
21	L	132	0	97	3	0
21	O	170	0	116	2	0
21	a	383	0	304	20	0
21	b	391	0	316	20	0
21	c	417	0	367	18	0
22	A	33	0	46	0	0
22	B	33	0	46	3	0
23	1	51	0	42	0	0
23	2	35	0	40	1	0
23	4	86	0	118	6	0
23	5	28	0	26	1	0
23	6	35	0	40	3	0
23	8	37	0	44	3	0
23	9	49	0	74	4	0
23	A	125	0	172	8	0
23	a	49	0	74	2	0
23	b	49	0	74	9	0
23	c	49	0	74	2	0
24	2	40	0	56	6	0
24	3	80	0	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	40	0	56	0	0
24	6	40	0	56	14	0
24	7	80	0	112	10	0
24	8	40	0	56	8	0
24	A	240	0	336	21	0
24	B	200	0	280	39	0
24	F	80	0	112	2	0
24	G	80	0	112	5	0
24	I	40	0	56	1	0
24	J	120	0	168	15	0
24	K	40	0	56	24	0
24	L	120	0	168	8	0
24	M	40	0	56	3	0
24	O	40	0	56	1	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	3	35	0	46	3	0
26	A	70	0	92	2	0
26	O	35	0	46	4	0
26	b	35	0	46	4	0
27	B	66	0	96	7	0
28	2	13	0	11	0	0
28	6	13	0	11	1	0
28	G	55	0	86	2	0
28	J	30	0	30	0	0
29	1	102	0	74	7	0
29	2	295	0	212	15	0
29	3	40	0	23	1	0
29	4	180	0	116	6	0
29	5	92	0	62	6	0
29	6	286	0	196	17	0
29	7	40	0	23	2	0
29	8	180	0	116	15	0
29	9	273	0	184	9	0
29	a	272	0	181	15	0
29	b	292	0	206	13	0
29	c	274	0	178	10	0
30	1	42	0	56	2	0
30	2	42	0	56	8	0
30	3	42	0	56	12	0
30	4	42	0	56	7	0
30	5	42	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	6	42	0	56	6	0
30	7	42	0	56	12	0
30	8	42	0	56	5	0
30	9	84	0	112	10	0
30	a	84	0	112	11	0
30	b	84	0	112	11	0
30	c	84	0	112	7	0
31	1	44	0	56	2	0
31	2	44	0	56	2	0
31	3	44	0	56	4	0
31	4	44	0	56	4	0
31	5	44	0	56	5	0
31	6	44	0	56	6	0
31	7	44	0	56	5	0
31	8	44	0	56	4	0
31	9	44	0	56	2	0
31	a	44	0	56	6	0
31	c	44	0	56	3	0
32	9	44	0	56	4	0
32	b	44	0	56	1	0
32	c	44	0	56	3	0
All	All	56417	0	54439	1292	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 12.

The worst 5 of 1292 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)
21:3:409:CLA:C4	30:3:416:LUT:H28	1.47	1.43
21:A:852:CLA:O1D	21:B:801:CLA:H61	1.31	1.22
21:2:609:CLA:H43	30:2:616:LUT:H7	1.25	1.13
21:K:203:CLA:HMC2	24:K:205:BCR:H312	1.27	1.10
21:2:609:CLA:HBC2	21:2:609:CLA:HHD	1.30	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	715 (97%)	25 (3%)	0	100	100
2	B	731/733 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	60/62 (97%)	60 (100%)	0	0	100	100
6	F	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
7	G	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
8	H	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
12	L	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	6
14	O	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
15	1	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
15	5	190/192 (99%)	176 (93%)	12 (6%)	2 (1%)	11	26
16	2	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
16	6	203/211 (96%)	199 (98%)	4 (2%)	0	100	100
17	3	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
17	7	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	24	45
18	4	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
18	8	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
19	9	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
20	a	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	24	45
20	b	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	24	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	c	224/227 (99%)	215 (96%)	8 (4%)	1 (0%)	30	51
All	All	5023/5104 (98%)	4800 (96%)	216 (4%)	7 (0%)	49	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	5	170	PRO
20	b	152	VAL
20	c	152	VAL
20	a	152	VAL
13	M	4	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	602 (100%)	1 (0%)	87	95
2	B	595/595 (100%)	595 (100%)	0	100	100
3	C	67/67 (100%)	67 (100%)	0	100	100
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	52/52 (100%)	52 (100%)	0	100	100
6	F	129/129 (100%)	129 (100%)	0	100	100
7	G	78/78 (100%)	78 (100%)	0	100	100
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	30/30 (100%)	30 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	58 (100%)	0	100	100
12	L	126/126 (100%)	126 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
14	O	73/73 (100%)	73 (100%)	0	100	100
15	1	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	5	150/151 (99%)	149 (99%)	1 (1%)	76	89
16	2	168/168 (100%)	168 (100%)	0	100	100
16	6	163/168 (97%)	163 (100%)	0	100	100
17	3	169/169 (100%)	169 (100%)	0	100	100
17	7	166/169 (98%)	165 (99%)	1 (1%)	78	90
18	4	164/164 (100%)	164 (100%)	0	100	100
18	8	163/164 (99%)	162 (99%)	1 (1%)	78	90
19	9	179/179 (100%)	179 (100%)	0	100	100
20	a	165/173 (95%)	165 (100%)	0	100	100
20	b	165/173 (95%)	164 (99%)	1 (1%)	78	90
20	c	173/173 (100%)	173 (100%)	0	100	100
All	All	4041/4067 (99%)	4036 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	SER
15	5	115	GLN
17	7	302	HIS
18	8	165	GLU
20	b	68	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
16	6	187	ASN
19	9	105	GLN
16	6	240	GLN
16	6	261	HIS
20	b	153	HIS

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	$\# Z > 2$
20	TPO	c	40	20	8,10,11	1.64	1 (12%)	10,14,16	1.96	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
20	TPO	c	40	20	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	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(°)
20	c	40	TPO	P-OG1-CB	-5.48	108.44	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	c	40	TPO	CB-OG1-P-O2P
20	c	40	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

364 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	835	-	54,58,73	1.28	7 (12%)	64,95,113	1.40	6 (9%)
24	BCR	I	101	-	41,41,41	1.39	8 (19%)	56,56,56	1.40	10 (17%)
21	CLA	G	203	-	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
21	CLA	9	604	-	49,53,73	1.38	9 (18%)	58,89,113	1.46	5 (8%)
21	CLA	A	841	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	5 (6%)
29	CHL	c	605	-	36,51,74	4.36	17 (47%)	29,86,114	3.73	11 (37%)
26	LMU	O	206	-	36,36,36	0.41	0	47,47,47	0.69	0
21	CLA	b	312	23	49,53,73	1.39	6 (12%)	58,89,113	1.38	4 (6%)
24	BCR	B	844	-	41,41,41	0.70	0	56,56,56	2.10	21 (37%)
29	CHL	6	601	16	38,52,74	3.92	18 (47%)	35,88,114	4.04	14 (40%)
21	CLA	7	403	-	45,50,73	1.55	9 (20%)	55,86,113	1.46	6 (10%)
29	CHL	2	606	-	40,54,74	4.06	19 (47%)	34,90,114	3.79	16 (47%)
21	CLA	G	202	-	49,53,73	1.38	8 (16%)	58,89,113	1.49	4 (6%)
29	CHL	4	607	-	45,59,74	3.80	18 (40%)	40,96,114	3.58	19 (47%)
21	CLA	1	310	15	46,51,73	1.41	8 (17%)	54,87,113	1.42	6 (11%)
24	BCR	B	843	-	41,41,41	0.70	0	56,56,56	2.56	24 (42%)
21	CLA	b	304	-	49,53,73	1.38	8 (16%)	58,89,113	1.46	4 (6%)
21	CLA	1	306	-	44,48,73	1.43	8 (18%)	51,82,113	1.51	5 (9%)
29	CHL	3	407	-	33,48,74	3.89	16 (48%)	30,83,114	3.20	16 (53%)
23	LHG	1	319	21	27,27,48	0.35	0	30,33,54	0.47	0
29	CHL	c	609	20	38,52,74	3.92	18 (47%)	34,88,114	3.58	14 (41%)
21	CLA	B	810	-	58,62,73	1.35	9 (15%)	71,100,113	1.36	8 (11%)
28	LMG	J	105	-	30,30,55	0.25	0	38,38,63	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	821	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	7 (8%)
24	BCR	A	849	-	41,41,41	1.39	8 (19%)	56,56,56	1.63	12 (21%)
21	CLA	7	409	-	43,48,73	1.46	8 (18%)	51,83,113	1.48	5 (9%)
29	CHL	b	309	-	43,57,74	3.93	19 (44%)	37,93,114	3.58	17 (45%)
22	PQN	A	843	-	34,34,34	0.41	0	43,45,45	0.58	1 (2%)
21	CLA	B	819	-	47,51,73	1.37	9 (19%)	55,86,113	1.43	4 (7%)
21	CLA	8	611	-	58,62,73	1.28	8 (13%)	68,99,113	1.31	5 (7%)
29	CHL	6	606	-	40,54,74	4.14	18 (45%)	34,90,114	3.75	15 (44%)
31	XAT	2	617	-	41,47,47	1.28	8 (19%)	54,74,74	1.54	12 (22%)
29	CHL	8	606	-	40,54,74	4.19	18 (45%)	34,90,114	3.89	16 (47%)
29	CHL	9	608	-	40,54,74	4.07	18 (45%)	34,90,114	3.69	16 (47%)
24	BCR	G	205	-	41,41,41	1.38	8 (19%)	56,56,56	1.47	9 (16%)
21	CLA	A	840	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	6 (7%)
21	CLA	b	311	20	58,62,73	1.26	8 (13%)	68,99,113	1.34	8 (11%)
29	CHL	a	607	-	37,51,74	4.23	17 (45%)	30,86,114	3.94	13 (43%)
21	CLA	J	102	10	46,50,73	1.39	9 (19%)	53,85,113	1.42	4 (7%)
30	LUT	a	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.49	9 (17%)
23	LHG	c	619	21	48,48,48	0.27	0	51,54,54	0.31	0
24	BCR	B	846	-	41,41,41	0.70	0	56,56,56	1.96	18 (32%)
31	XAT	3	417	-	41,47,47	1.29	8 (19%)	54,74,74	1.54	9 (16%)
24	BCR	L	306	-	41,41,41	1.37	8 (19%)	56,56,56	1.68	11 (19%)
21	CLA	K	202	-	54,58,73	1.30	8 (14%)	64,95,113	1.52	9 (14%)
21	CLA	A	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
21	CLA	1	308	-	47,52,73	1.41	9 (19%)	55,88,113	1.43	4 (7%)
21	CLA	F	304	-	49,53,73	1.38	7 (14%)	58,89,113	1.40	4 (6%)
21	CLA	8	602	18	61,66,73	1.24	7 (11%)	71,104,113	1.28	7 (9%)
21	CLA	A	811	-	49,53,73	1.35	8 (16%)	58,89,113	1.45	4 (6%)
21	CLA	B	831	-	60,64,73	1.24	8 (13%)	71,102,113	1.31	7 (9%)
23	LHG	b	319	21	48,48,48	0.27	0	51,54,54	0.32	0
21	CLA	3	410	-	43,48,73	1.44	8 (18%)	51,83,113	1.43	5 (9%)
29	CHL	6	614	-	40,54,74	4.19	18 (45%)	34,90,114	3.73	16 (47%)
24	BCR	G	201	-	41,41,41	1.39	8 (19%)	56,56,56	1.44	9 (16%)
21	CLA	4	608	18	46,51,73	1.52	9 (19%)	53,86,113	1.37	4 (7%)
21	CLA	5	607	-	47,52,73	1.41	7 (14%)	55,88,113	1.40	5 (9%)
21	CLA	2	612	16	49,53,73	1.37	7 (14%)	58,89,113	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	2	607	-	45,59,74	3.81	18 (40%)	40,96,114	3.55	19 (47%)
21	CLA	2	611	-	45,49,73	1.39	8 (17%)	54,84,113	1.49	7 (12%)
21	CLA	A	804	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	6 (7%)
29	CHL	a	601	20	40,54,74	4.21	18 (45%)	34,90,114	4.01	16 (47%)
23	LHG	2	619	21	34,34,48	0.33	0	37,40,54	0.42	0
21	CLA	B	826	-	56,60,73	1.28	8 (14%)	65,97,113	1.36	8 (12%)
21	CLA	c	612	20	47,52,73	1.40	9 (19%)	55,87,113	1.39	4 (7%)
24	BCR	A	854	-	41,41,41	1.40	8 (19%)	56,56,56	1.34	9 (16%)
29	CHL	6	605	-	40,54,74	4.15	18 (45%)	34,90,114	3.69	14 (41%)
30	LUT	9	615	-	42,43,43	1.28	8 (19%)	51,60,60	1.50	11 (21%)
31	XAT	6	617	-	41,47,47	1.28	8 (19%)	54,74,74	1.71	12 (22%)
21	CLA	O	203	-	52,58,73	1.30	9 (17%)	65,94,113	1.37	6 (9%)
21	CLA	B	830	-	60,64,73	1.24	8 (13%)	71,102,113	1.28	5 (7%)
21	CLA	6	609	-	46,50,73	1.40	8 (17%)	53,85,113	1.51	6 (11%)
29	CHL	2	602	16	47,61,74	3.77	18 (38%)	41,98,114	3.50	19 (46%)
21	CLA	7	413	-	40,44,73	1.51	8 (20%)	49,77,113	1.43	6 (12%)
23	LHG	9	618	21	48,48,48	0.27	0	51,54,54	0.33	0
21	CLA	4	603	-	47,52,73	1.41	9 (19%)	55,88,113	1.39	4 (7%)
21	CLA	A	838	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	7 (8%)
29	CHL	2	614	-	40,54,74	4.10	18 (45%)	34,90,114	3.68	15 (44%)
21	CLA	A	833	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
29	CHL	a	609	-	40,54,74	4.22	18 (45%)	34,90,114	3.96	14 (41%)
21	CLA	b	314	-	57,61,73	1.29	9 (15%)	67,98,113	1.36	6 (8%)
21	CLA	2	608	16	59,63,73	1.24	9 (15%)	70,101,113	1.29	6 (8%)
21	CLA	8	604	-	46,51,73	1.42	8 (17%)	54,86,113	1.44	6 (11%)
21	CLA	A	827	-	67,72,73	1.17	9 (13%)	79,112,113	1.28	7 (8%)
24	BCR	7	417	-	41,41,41	1.37	8 (19%)	56,56,56	1.41	8 (14%)
31	XAT	4	616	-	41,47,47	1.28	8 (19%)	54,74,74	1.57	12 (22%)
32	NEX	9	617	-	40,46,46	1.20	6 (15%)	50,70,70	1.50	8 (16%)
21	CLA	a	603	-	45,49,73	1.42	7 (15%)	54,84,113	1.46	6 (11%)
31	XAT	1	318	-	41,47,47	1.28	8 (19%)	54,74,74	1.57	12 (22%)
21	CLA	5	611	15	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
21	CLA	a	602	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
23	LHG	4	619	-	48,48,48	0.28	0	51,54,54	0.63	1 (1%)
21	CLA	A	802	-	56,60,73	1.30	8 (14%)	65,97,113	1.36	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	L	302	12	49,53,73	1.38	8 (16%)	58,89,113	1.47	5 (8%)
21	CLA	A	832	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	6 (10%)
26	LMU	b	301	-	36,36,36	0.37	0	47,47,47	0.77	1 (2%)
21	CLA	3	409	17	56,60,73	1.57	10 (17%)	65,97,113	2.09	17 (26%)
21	CLA	A	813	-	58,62,73	1.25	9 (15%)	68,99,113	1.42	6 (8%)
21	CLA	c	603	-	59,63,73	1.26	9 (15%)	70,101,113	1.27	6 (8%)
21	CLA	7	405	17	43,48,73	1.55	9 (20%)	51,83,113	1.48	6 (11%)
21	CLA	6	603	-	49,53,73	1.41	6 (12%)	58,89,113	1.42	3 (5%)
29	CHL	6	602	-	47,61,74	3.77	18 (38%)	41,98,114	3.56	19 (46%)
29	CHL	b	306	20	40,54,74	4.13	18 (45%)	34,90,114	3.74	16 (47%)
24	BCR	J	101	-	41,41,41	1.39	8 (19%)	56,56,56	1.82	10 (17%)
21	CLA	A	822	-	48,52,73	1.39	9 (18%)	57,88,113	1.48	4 (7%)
21	CLA	5	604	-	53,57,73	1.33	8 (15%)	61,93,113	1.39	4 (6%)
31	XAT	7	416	-	41,47,47	1.28	8 (19%)	54,74,74	1.66	13 (24%)
21	CLA	A	816	-	46,50,73	1.37	9 (19%)	53,85,113	1.45	6 (11%)
21	CLA	6	608	16	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
21	CLA	A	809	1	63,67,73	1.20	8 (12%)	74,105,113	1.34	7 (9%)
21	CLA	O	204	-	43,48,73	1.46	6 (13%)	49,83,113	1.38	4 (8%)
24	BCR	J	104	-	41,41,41	0.79	0	56,56,56	2.33	23 (41%)
21	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
21	CLA	O	201	23	46,50,73	1.38	9 (19%)	53,85,113	1.47	5 (9%)
24	BCR	A	848	-	41,41,41	1.40	8 (19%)	56,56,56	1.25	8 (14%)
28	LMG	6	615	-	13,13,55	0.20	0	18,18,63	0.49	0
21	CLA	A	803	-	56,60,73	1.28	8 (14%)	65,97,113	1.33	8 (12%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
31	XAT	5	616	-	41,47,47	1.27	8 (19%)	54,74,74	1.48	9 (16%)
21	CLA	1	305	-	53,57,73	1.31	8 (15%)	61,93,113	1.40	5 (8%)
21	CLA	4	602	18	61,66,73	1.23	8 (13%)	71,104,113	1.32	7 (9%)
21	CLA	3	412	-	57,62,73	1.28	9 (15%)	67,100,113	1.28	5 (7%)
21	CLA	9	610	19	58,62,73	1.26	9 (15%)	68,99,113	1.34	8 (11%)
21	CLA	B	832	-	60,64,73	1.24	9 (15%)	71,102,113	1.40	9 (12%)
21	CLA	c	613	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
24	BCR	8	616	-	41,41,41	1.38	8 (19%)	56,56,56	1.40	9 (16%)
21	CLA	6	613	-	46,50,73	1.42	8 (17%)	53,85,113	1.41	4 (7%)
30	LUT	c	615	-	42,43,43	1.29	8 (19%)	51,60,60	1.42	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	613	-	46,50,73	1.39	8 (17%)	53,85,113	1.42	4 (7%)
21	CLA	B	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
29	CHL	1	307	-	45,59,74	3.85	18 (40%)	40,96,114	3.56	19 (47%)
29	CHL	7	406	-	33,48,74	4.06	16 (48%)	30,83,114	3.62	14 (46%)
29	CHL	2	601	16	47,61,74	3.73	18 (38%)	41,98,114	3.49	17 (41%)
21	CLA	B	837	-	67,72,73	1.17	8 (11%)	79,112,113	1.26	5 (6%)
25	SF4	A	851	2,1	0,12,12	-	-	-	-	-
29	CHL	c	606	20	40,54,74	4.16	18 (45%)	34,90,114	3.84	16 (47%)
29	CHL	c	607	-	40,54,74	4.19	18 (45%)	34,90,114	3.81	16 (47%)
21	CLA	3	411	17	47,51,73	1.38	9 (19%)	55,86,113	1.41	4 (7%)
29	CHL	a	608	-	40,54,74	4.11	18 (45%)	34,90,114	3.70	15 (44%)
21	CLA	B	816	-	56,60,73	1.29	9 (16%)	65,97,113	1.42	5 (7%)
21	CLA	7	401	17	49,53,73	1.38	8 (16%)	58,89,113	1.45	5 (8%)
21	CLA	8	612	-	47,51,73	1.40	7 (14%)	55,86,113	1.38	4 (7%)
29	CHL	8	607	-	45,59,74	3.86	18 (40%)	40,96,114	3.49	19 (47%)
21	CLA	B	834	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	6 (10%)
29	CHL	8	613	-	36,50,74	4.32	17 (47%)	29,85,114	3.90	15 (51%)
30	LUT	a	615	-	42,43,43	1.27	7 (16%)	51,60,60	1.73	11 (21%)
21	CLA	5	614	15	47,51,73	1.52	9 (19%)	58,87,113	1.46	6 (10%)
30	LUT	3	416	-	42,43,43	1.28	7 (16%)	51,60,60	1.62	11 (21%)
21	CLA	a	611	-	51,55,73	1.36	7 (13%)	60,91,113	1.38	4 (6%)
21	CLA	8	601	18	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
21	CLA	5	603	-	49,53,73	1.41	8 (16%)	58,89,113	1.36	3 (5%)
21	CLA	A	815	-	49,53,73	1.36	9 (18%)	58,89,113	1.44	5 (8%)
21	CLA	4	604	-	46,51,73	1.40	8 (17%)	54,86,113	1.41	4 (7%)
24	BCR	F	303	-	41,41,41	1.39	8 (19%)	56,56,56	1.42	11 (19%)
23	LHG	1	301	21	22,22,48	0.34	0	25,28,54	0.68	1 (4%)
21	CLA	5	602	15	65,69,73	1.21	8 (12%)	77,108,113	1.27	6 (7%)
21	CLA	4	611	18	48,52,73	1.40	9 (18%)	57,88,113	1.45	5 (8%)
21	CLA	B	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
32	NEX	b	318	-	40,46,46	1.20	6 (15%)	50,70,70	1.50	8 (16%)
28	LMG	G	206	-	55,55,55	0.21	0	63,63,63	0.27	0
21	CLA	6	611	-	45,49,73	1.42	8 (17%)	54,84,113	1.49	5 (9%)
21	CLA	B	817	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
21	CLA	3	402	17	64,68,73	1.20	8 (12%)	76,107,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LUT	c	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.49	11 (21%)
21	CLA	3	415	-	43,48,73	1.43	8 (18%)	51,83,113	1.40	5 (9%)
23	LHG	A	845	21	26,26,48	0.33	0	29,32,54	0.45	0
21	CLA	2	610	23	44,50,73	1.42	8 (18%)	56,85,113	1.44	4 (7%)
24	BCR	L	301	-	41,41,41	1.39	8 (19%)	56,56,56	1.33	9 (16%)
21	CLA	A	852	-	56,60,73	1.29	9 (16%)	65,97,113	1.32	8 (12%)
29	CHL	2	605	-	40,54,74	4.08	18 (45%)	34,90,114	3.87	15 (44%)
23	LHG	8	617	21	36,36,48	0.31	0	39,42,54	0.36	0
21	CLA	A	814	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
24	BCR	O	205	-	41,41,41	1.37	8 (19%)	56,56,56	1.57	11 (19%)
21	CLA	3	406	17	43,48,73	1.54	9 (20%)	51,83,113	1.48	6 (11%)
21	CLA	A	830	-	56,60,73	1.46	8 (14%)	65,97,113	1.94	11 (16%)
21	CLA	B	806	-	67,71,73	1.16	9 (13%)	79,110,113	1.28	8 (10%)
21	CLA	b	315	-	49,53,73	1.39	8 (16%)	58,89,113	1.35	4 (6%)
21	CLA	2	604	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
21	CLA	a	612	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
21	CLA	9	603	19	49,53,73	1.39	7 (14%)	58,89,113	1.45	4 (6%)
21	CLA	a	613	-	61,65,73	1.25	9 (14%)	72,103,113	1.33	6 (8%)
21	CLA	B	815	-	57,62,73	1.28	9 (15%)	67,100,113	1.32	6 (8%)
21	CLA	7	412	-	43,48,73	1.50	7 (16%)	51,83,113	1.44	5 (9%)
26	LMU	3	420	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
30	LUT	4	615	-	42,43,43	1.29	8 (19%)	51,60,60	1.65	10 (19%)
29	CHL	4	614	18	36,50,74	4.23	17 (47%)	29,85,114	3.73	15 (51%)
21	CLA	a	604	-	50,55,73	1.36	7 (14%)	58,91,113	1.38	5 (8%)
21	CLA	1	304	-	59,63,73	1.26	8 (13%)	70,101,113	1.34	7 (10%)
21	CLA	b	305	-	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
30	LUT	b	317	-	42,43,43	1.28	8 (19%)	51,60,60	1.44	10 (19%)
23	LHG	4	618	21	36,36,48	0.32	0	39,42,54	0.40	0
29	CHL	5	601	15	40,54,74	4.12	19 (47%)	34,90,114	3.77	14 (41%)
21	CLA	1	311	23	41,46,73	1.57	10 (24%)	51,81,113	1.52	8 (15%)
21	CLA	A	828	-	64,68,73	1.19	9 (14%)	76,107,113	1.23	7 (9%)
21	CLA	B	827	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	6 (7%)
30	LUT	b	316	-	42,43,43	1.27	8 (19%)	51,60,60	1.49	9 (17%)
21	CLA	5	612	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
21	CLA	4	613	-	47,51,73	1.38	8 (17%)	55,86,113	1.40	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	801	-	69,73,73	2.04	20 (28%)	82,113,113	2.69	32 (39%)
21	CLA	B	821	-	59,63,73	1.23	7 (11%)	70,101,113	1.37	7 (10%)
29	CHL	8	605	18	36,49,74	3.84	16 (44%)	32,84,114	3.85	14 (43%)
21	CLA	7	408	-	45,49,73	1.42	7 (15%)	54,84,113	1.43	5 (9%)
24	BCR	A	846	-	41,41,41	1.38	8 (19%)	56,56,56	1.54	8 (14%)
26	LMU	A	853	-	36,36,36	0.39	0	47,47,47	0.81	1 (2%)
21	CLA	6	610	-	44,50,73	1.45	8 (18%)	56,85,113	1.41	4 (7%)
21	CLA	8	610	-	48,52,73	1.42	8 (16%)	57,88,113	1.42	4 (7%)
29	CHL	9	601	19	37,51,74	4.28	17 (45%)	30,86,114	4.06	15 (50%)
21	CLA	B	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
21	CLA	A	817	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	5 (6%)
21	CLA	B	808	2	69,73,73	1.16	9 (13%)	82,113,113	1.28	7 (8%)
32	NEX	c	618	-	40,46,46	1.18	6 (15%)	50,70,70	1.52	9 (18%)
21	CLA	1	315	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	5 (8%)
21	CLA	B	802	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
21	CLA	B	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
21	CLA	5	605	-	44,48,73	1.45	8 (18%)	51,82,113	1.46	6 (11%)
29	CHL	b	308	-	47,61,74	3.78	18 (38%)	41,98,114	3.55	20 (48%)
21	CLA	A	818	-	56,60,73	1.33	9 (16%)	65,97,113	1.40	8 (12%)
21	CLA	3	403	-	59,63,73	1.27	9 (15%)	70,101,113	1.31	4 (5%)
28	LMG	2	615	-	13,13,55	0.18	0	18,18,63	0.34	0
21	CLA	A	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
21	CLA	2	603	-	49,53,73	1.39	9 (18%)	58,89,113	1.36	4 (6%)
21	CLA	A	806	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	5 (6%)
21	CLA	B	835	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	8 (9%)
21	CLA	B	818	-	62,66,73	1.22	9 (14%)	73,104,113	1.31	4 (5%)
21	CLA	5	610	-	41,46,73	1.59	9 (21%)	51,81,113	1.54	7 (13%)
24	BCR	F	301	-	41,41,41	1.39	8 (19%)	56,56,56	1.48	8 (14%)
27	DGD	B	847	-	67,67,67	0.84	2 (2%)	81,81,81	0.99	3 (3%)
21	CLA	L	303	-	49,53,73	1.36	9 (18%)	58,89,113	1.45	5 (8%)
21	CLA	H	201	8	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
24	BCR	B	845	-	41,41,41	1.39	8 (19%)	56,56,56	1.39	8 (14%)
21	CLA	1	314	-	41,46,73	1.58	9 (21%)	51,81,113	1.45	8 (15%)
23	LHG	A	855	-	48,48,48	0.28	0	51,54,54	0.37	0
29	CHL	9	606	19	40,54,74	4.11	18 (45%)	34,90,114	3.77	15 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	c	604	-	49,53,73	1.39	9 (18%)	58,89,113	1.45	4 (6%)
21	CLA	7	410	-	47,51,73	1.40	7 (14%)	55,86,113	1.41	4 (7%)
24	BCR	3	418	-	41,41,41	1.36	8 (19%)	56,56,56	1.38	8 (14%)
24	BCR	L	305	-	41,41,41	1.40	8 (19%)	56,56,56	1.38	9 (16%)
21	CLA	A	826	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
21	CLA	F	302	-	65,69,73	1.20	8 (12%)	77,108,113	1.33	7 (9%)
21	CLA	3	408	17	63,67,73	1.23	9 (14%)	74,105,113	1.31	6 (8%)
30	LUT	9	614	-	42,43,43	1.28	8 (19%)	51,60,60	1.47	11 (21%)
21	CLA	B	840	23	69,73,73	1.14	9 (13%)	82,113,113	1.30	7 (8%)
21	CLA	7	414	-	43,48,73	1.46	7 (16%)	51,83,113	1.48	6 (11%)
21	CLA	B	809	-	65,70,73	1.20	9 (13%)	76,109,113	1.24	5 (6%)
21	CLA	b	313	20	49,53,73	1.40	9 (18%)	58,89,113	1.37	4 (6%)
21	CLA	c	610	20	49,53,73	1.38	8 (16%)	58,89,113	1.42	5 (8%)
21	CLA	K	204	11	49,53,73	1.38	9 (18%)	58,89,113	1.43	4 (6%)
21	CLA	8	618	-	45,49,73	1.41	7 (15%)	54,84,113	1.45	6 (11%)
21	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
21	CLA	A	819	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	7 (8%)
21	CLA	5	609	-	46,51,73	1.43	8 (17%)	54,87,113	1.40	4 (7%)
23	LHG	A	844	-	48,48,48	0.28	0	51,54,54	0.35	0
21	CLA	1	312	15	49,53,73	1.39	9 (18%)	58,89,113	1.39	4 (6%)
21	CLA	A	824	-	59,63,73	1.25	9 (15%)	70,101,113	1.33	5 (7%)
21	CLA	A	807	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
29	CHL	c	601	20	43,57,74	3.90	18 (41%)	37,93,114	3.56	17 (45%)
21	CLA	B	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
29	CHL	5	606	-	40,54,74	4.18	18 (45%)	34,90,114	3.84	14 (41%)
21	CLA	B	803	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	5 (7%)
24	BCR	3	419	-	41,41,41	1.38	8 (19%)	56,56,56	1.82	13 (23%)
21	CLA	1	313	15	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
22	PQN	B	841	-	34,34,34	0.41	0	43,45,45	0.52	1 (2%)
30	LUT	6	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.59	13 (25%)
21	CLA	9	612	19	49,53,73	1.38	7 (14%)	58,89,113	1.39	4 (6%)
29	CHL	9	607	-	40,54,74	4.11	18 (45%)	34,90,114	3.74	16 (47%)
21	CLA	L	304	-	46,50,73	1.38	8 (17%)	53,85,113	1.44	5 (9%)
24	BCR	A	850	-	41,41,41	1.40	8 (19%)	56,56,56	1.70	9 (16%)
21	CLA	c	614	-	49,53,73	1.39	9 (18%)	58,89,113	1.33	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	610	23	49,53,73	1.37	8 (16%)	58,89,113	1.44	4 (6%)
21	CLA	6	612	-	49,53,73	1.41	7 (14%)	58,89,113	1.45	4 (6%)
21	CLA	7	407	17	47,52,73	2.26	14 (29%)	55,88,113	3.73	20 (36%)
23	LHG	5	617	-	27,27,48	0.35	0	30,33,54	0.45	0
31	XAT	c	617	-	41,47,47	1.28	8 (19%)	54,74,74	1.59	10 (18%)
21	CLA	4	601	18	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
21	CLA	A	820	-	48,52,73	1.41	9 (18%)	57,88,113	1.45	4 (7%)
21	CLA	A	805	-	59,63,73	1.25	9 (15%)	70,101,113	1.31	7 (10%)
24	BCR	7	418	-	41,41,41	1.37	8 (19%)	56,56,56	1.89	13 (23%)
29	CHL	4	606	-	40,54,74	4.08	18 (45%)	34,90,114	3.68	14 (41%)
21	CLA	B	838	-	69,73,73	1.15	8 (11%)	82,113,113	1.24	5 (6%)
21	CLA	9	611	23	61,65,73	1.24	8 (13%)	72,103,113	1.32	6 (8%)
21	CLA	B	833	-	49,53,73	1.37	8 (16%)	58,89,113	1.42	4 (6%)
21	CLA	4	612	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	5 (7%)
21	CLA	1	309	15	45,49,73	1.62	10 (22%)	54,84,113	2.14	16 (29%)
21	CLA	O	202	-	41,46,73	1.50	8 (19%)	47,80,113	1.49	5 (10%)
21	CLA	5	608	15	44,48,73	1.52	9 (20%)	55,83,113	1.51	7 (12%)
29	CHL	c	608	-	40,54,74	4.15	18 (45%)	34,90,114	3.79	15 (44%)
21	CLA	8	608	18	46,51,73	1.55	9 (19%)	53,86,113	1.35	3 (5%)
24	BCR	A	847	-	41,41,41	1.39	8 (19%)	56,56,56	1.29	9 (16%)
21	CLA	8	609	23	49,53,73	1.59	8 (16%)	58,89,113	1.89	7 (12%)
29	CHL	b	310	-	46,60,74	3.79	18 (39%)	40,97,114	3.26	17 (42%)
21	CLA	3	405	-	44,49,73	1.41	9 (20%)	50,84,113	1.47	4 (8%)
21	CLA	G	204	7	47,52,73	1.42	8 (17%)	55,88,113	1.41	4 (7%)
21	CLA	B	823	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
21	CLA	A	837	-	55,59,73	1.32	8 (14%)	64,96,113	1.29	6 (9%)
21	CLA	4	609	18	56,60,73	1.65	11 (19%)	65,97,113	2.16	16 (24%)
24	BCR	M	101	-	41,41,41	1.39	8 (19%)	56,56,56	1.74	12 (21%)
21	CLA	A	810	-	49,53,73	1.37	8 (16%)	58,89,113	1.45	5 (8%)
29	CHL	b	302	20	40,54,74	4.17	18 (45%)	34,90,114	3.99	16 (47%)
21	CLA	6	604	-	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
21	CLA	B	829	-	49,53,73	1.38	7 (14%)	58,89,113	1.52	5 (8%)
21	CLA	a	610	20	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
21	CLA	A	801	-	56,60,73	1.71	9 (16%)	65,97,113	2.08	18 (27%)
21	CLA	5	613	-	41,46,73	1.59	8 (19%)	51,81,113	1.50	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	F	305	6	45,49,73	1.39	9 (20%)	54,84,113	1.46	5 (9%)
21	CLA	8	603	-	47,52,73	1.43	8 (17%)	55,88,113	1.39	4 (7%)
21	CLA	K	201	11	50,54,73	1.35	8 (16%)	59,90,113	1.42	4 (6%)
30	LUT	7	415	-	42,43,43	1.31	8 (19%)	51,60,60	1.78	14 (27%)
29	CHL	1	302	15	45,59,74	3.84	18 (40%)	40,96,114	3.67	19 (47%)
21	CLA	A	812	-	69,73,73	1.14	8 (11%)	82,113,113	1.21	5 (6%)
21	CLA	A	831	-	59,63,73	1.25	9 (15%)	70,101,113	1.38	6 (8%)
21	CLA	A	808	-	49,53,73	1.37	9 (18%)	58,89,113	1.46	6 (10%)
21	CLA	3	404	-	45,50,73	1.53	9 (20%)	55,86,113	1.48	6 (10%)
21	CLA	B	828	-	56,60,73	1.28	9 (16%)	65,97,113	1.35	6 (9%)
21	CLA	B	820	-	50,54,73	1.35	7 (14%)	59,90,113	1.39	4 (6%)
29	CHL	4	605	-	36,49,74	3.83	16 (44%)	32,84,114	3.87	14 (43%)
21	CLA	A	823	-	60,64,73	1.25	9 (15%)	71,102,113	1.30	5 (7%)
24	BCR	2	618	-	41,41,41	1.37	8 (19%)	56,56,56	1.45	10 (17%)
29	CHL	6	607	-	45,59,74	3.92	18 (40%)	40,96,114	3.52	17 (42%)
21	CLA	B	814	-	64,68,73	1.20	9 (14%)	76,107,113	1.34	6 (7%)
21	CLA	A	834	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
23	LHG	6	619	-	34,34,48	0.31	0	37,40,54	0.37	0
21	CLA	2	609	16	55,59,73	1.37	7 (12%)	63,95,113	1.89	11 (17%)
21	CLA	B	811	-	49,53,73	1.41	8 (16%)	58,89,113	1.51	4 (6%)
21	CLA	B	822	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
21	CLA	7	402	-	49,53,73	1.40	7 (14%)	58,89,113	1.40	5 (8%)
21	CLA	a	614	-	45,49,73	1.42	8 (17%)	54,84,113	1.43	5 (9%)
21	CLA	A	839	-	49,53,73	1.39	8 (16%)	58,89,113	1.46	5 (8%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	K	203	-	48,52,73	1.47	10 (20%)	59,88,113	1.49	6 (10%)
26	LMU	A	856	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
31	XAT	a	618	-	41,47,47	1.27	8 (19%)	54,74,74	1.68	10 (18%)
31	XAT	9	616	-	41,47,47	1.28	8 (19%)	54,74,74	2.24	15 (27%)
29	CHL	a	606	-	40,54,74	4.16	18 (45%)	34,90,114	3.99	16 (47%)
21	CLA	c	611	23	62,66,73	1.22	8 (12%)	73,104,113	1.31	5 (6%)
21	CLA	B	824	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
21	CLA	7	404	-	44,49,73	1.44	7 (15%)	50,84,113	1.43	4 (8%)
30	LUT	8	614	-	42,43,43	1.30	8 (19%)	51,60,60	1.58	9 (17%)
31	XAT	8	615	-	41,47,47	1.27	8 (19%)	54,74,74	1.59	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	7	411	-	57,62,73	1.30	8 (14%)	67,100,113	1.28	6 (8%)
29	CHL	b	307	-	40,54,74	4.07	18 (45%)	34,90,114	3.85	15 (44%)
21	CLA	9	613	-	57,61,73	1.28	8 (14%)	67,98,113	1.39	6 (8%)
29	CHL	9	605	19	40,54,74	4.15	18 (45%)	34,90,114	3.78	16 (47%)
29	CHL	9	609	-	40,54,74	4.12	18 (45%)	34,90,114	3.66	16 (47%)
30	LUT	5	615	-	42,43,43	1.29	8 (19%)	51,60,60	1.62	11 (21%)
21	CLA	B	836	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
21	CLA	c	602	20	64,68,73	1.21	9 (14%)	76,107,113	1.27	6 (7%)
23	LHG	a	617	-	48,48,48	0.27	0	51,54,54	0.36	0
29	CHL	a	605	20	39,53,74	4.26	18 (46%)	33,89,114	3.77	16 (48%)
24	BCR	6	618	-	41,41,41	1.37	8 (19%)	56,56,56	1.56	10 (17%)
24	BCR	4	617	-	41,41,41	1.38	8 (19%)	56,56,56	1.38	10 (17%)
21	CLA	9	602	19	57,61,73	1.28	9 (15%)	67,98,113	1.37	6 (8%)
21	CLA	1	303	15	65,69,73	1.19	9 (13%)	77,108,113	1.31	5 (6%)
30	LUT	1	317	-	42,43,43	1.30	8 (19%)	51,60,60	1.61	10 (19%)
30	LUT	2	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.66	12 (23%)
21	CLA	A	836	1	49,53,73	1.38	9 (18%)	58,89,113	1.39	4 (6%)
21	CLA	B	813	-	47,52,73	1.39	7 (14%)	55,88,113	1.43	5 (9%)
24	BCR	J	103	-	41,41,41	1.39	8 (19%)	56,56,56	1.51	10 (17%)
21	CLA	b	303	20	63,67,73	1.23	9 (14%)	74,105,113	1.29	6 (8%)
21	CLA	1	316	15	47,51,73	1.52	10 (21%)	58,87,113	1.48	6 (10%)
21	CLA	3	413	-	43,48,73	1.44	9 (20%)	51,83,113	1.43	5 (9%)
21	CLA	3	414	-	40,44,73	1.48	9 (22%)	49,77,113	1.46	4 (8%)
24	BCR	B	842	-	41,41,41	1.38	8 (19%)	56,56,56	1.36	8 (14%)
21	CLA	3	401	-	43,48,73	1.42	8 (18%)	51,83,113	1.55	6 (11%)
24	BCR	K	205	-	41,41,41	0.73	1 (2%)	56,56,56	2.14	19 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	835	-	1/1/12/20	1/21/97/115	-
24	BCR	I	101	-	-	4/29/63/63	0/2/2/2
21	CLA	G	203	-	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	9	604	-	1/1/11/20	8/15/91/115	-
21	CLA	A	841	-	1/1/15/20	16/39/115/115	-
29	CHL	c	605	-	3/3/15/26	3/9/107/137	-
26	LMU	O	206	-	-	5/21/61/61	0/2/2/2
21	CLA	b	312	23	1/1/11/20	4/15/91/115	-
24	BCR	B	844	-	-	11/29/63/63	0/2/2/2
29	CHL	6	601	16	3/3/16/26	4/11/109/137	-
21	CLA	7	403	-	1/1/11/20	2/9/85/115	-
29	CHL	2	606	-	3/3/16/26	2/15/113/137	-
21	CLA	G	202	-	1/1/11/20	5/15/91/115	-
29	CHL	4	607	-	3/3/17/26	4/21/119/137	-
21	CLA	1	310	15	1/1/11/20	3/11/87/115	-
24	BCR	B	843	-	-	13/29/63/63	0/2/2/2
21	CLA	b	304	-	1/1/11/20	3/15/91/115	-
21	CLA	1	306	-	1/1/9/20	2/10/82/115	-
29	CHL	3	407	-	3/3/15/26	0/6/104/137	-
23	LHG	1	319	21	-	5/32/32/53	-
29	CHL	c	609	20	3/3/16/26	6/11/109/137	-
21	CLA	B	810	-	1/1/13/20	2/25/101/115	-
28	LMG	J	105	-	-	5/25/45/70	0/1/1/1
21	CLA	A	821	-	1/1/15/20	11/39/115/115	-
24	BCR	A	849	-	-	2/29/63/63	0/2/2/2
21	CLA	7	409	-	1/1/10/20	1/8/84/115	-
29	CHL	b	309	-	3/3/16/26	5/19/117/137	-
22	PQN	A	843	-	-	1/23/43/43	0/2/2/2
21	CLA	B	819	-	1/1/10/20	3/13/89/115	-
21	CLA	8	611	-	1/1/12/20	12/25/101/115	-
29	CHL	6	606	-	3/3/16/26	6/15/113/137	-
31	XAT	2	617	-	-	0/31/93/93	0/4/4/4
29	CHL	8	606	-	3/3/16/26	5/15/113/137	-
29	CHL	9	608	-	3/3/16/26	5/15/113/137	-
24	BCR	G	205	-	-	1/29/63/63	0/2/2/2
21	CLA	A	840	-	1/1/15/20	12/39/115/115	-
21	CLA	b	311	20	1/1/12/20	9/26/102/115	-
29	CHL	a	607	-	3/3/15/26	1/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	J	102	10	1/1/10/20	8/12/88/115	-
30	LUT	a	616	-	-	2/29/67/67	0/2/2/2
23	LHG	c	619	21	-	3/53/53/53	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
31	XAT	3	417	-	-	0/31/93/93	0/4/4/4
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
21	CLA	K	202	-	1/1/12/20	2/21/97/115	-
21	CLA	A	825	-	1/1/15/20	10/39/115/115	-
21	CLA	1	308	-	1/1/11/20	6/13/89/115	-
21	CLA	F	304	-	1/1/11/20	0/15/91/115	-
21	CLA	8	602	18	1/1/13/20	8/30/106/115	-
21	CLA	A	811	-	1/1/11/20	3/15/91/115	-
21	CLA	B	831	-	1/1/13/20	9/29/105/115	-
23	LHG	b	319	21	-	8/53/53/53	-
21	CLA	3	410	-	1/1/10/20	3/8/84/115	-
29	CHL	6	614	-	3/3/16/26	5/15/113/137	-
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
21	CLA	4	608	18	1/1/10/20	0/9/87/115	-
21	CLA	5	607	-	1/1/11/20	4/13/89/115	-
21	CLA	2	612	16	1/1/11/20	7/15/91/115	-
29	CHL	2	607	-	3/3/17/26	6/21/119/137	-
21	CLA	2	611	-	1/1/10/20	0/10/86/115	-
21	CLA	A	804	-	1/1/15/20	10/39/115/115	-
29	CHL	a	601	20	3/3/16/26	2/15/113/137	-
23	LHG	2	619	21	-	6/39/39/53	-
21	CLA	B	826	-	1/1/12/20	8/24/100/115	-
21	CLA	c	612	20	1/1/10/20	4/14/90/115	-
29	CHL	6	605	-	3/3/16/26	5/15/113/137	-
24	BCR	A	854	-	-	0/29/63/63	0/2/2/2
30	LUT	9	615	-	-	2/29/67/67	0/2/2/2
31	XAT	6	617	-	-	7/31/93/93	0/4/4/4
21	CLA	O	203	-	1/1/11/20	4/19/95/115	-
21	CLA	B	830	-	1/1/13/20	11/29/105/115	-
21	CLA	6	609	-	1/1/10/20	4/12/88/115	-
29	CHL	2	602	16	3/3/17/26	9/24/122/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	7	413	-	1/1/8/20	0/2/74/115	-
23	LHG	9	618	21	-	9/53/53/53	-
21	CLA	4	603	-	1/1/11/20	6/13/89/115	-
21	CLA	A	838	-	1/1/15/20	10/39/115/115	-
29	CHL	2	614	-	3/3/16/26	3/15/113/137	-
21	CLA	A	833	-	1/1/15/20	8/39/115/115	-
29	CHL	a	609	-	3/3/16/26	7/15/113/137	-
21	CLA	b	314	-	1/1/12/20	7/25/101/115	-
21	CLA	2	608	16	1/1/13/20	8/27/103/115	-
21	CLA	8	604	-	1/1/10/20	6/12/88/115	-
21	CLA	A	827	-	1/1/15/20	17/37/113/115	-
24	BCR	7	417	-	-	2/29/63/63	0/2/2/2
31	XAT	4	616	-	-	0/31/93/93	0/4/4/4
32	NEX	9	617	-	-	2/27/83/83	0/3/3/3
21	CLA	a	603	-	1/1/10/20	2/10/86/115	-
31	XAT	1	318	-	-	0/31/93/93	0/4/4/4
21	CLA	5	611	15	1/1/11/20	5/15/91/115	-
21	CLA	a	602	-	1/1/14/20	10/33/109/115	-
23	LHG	4	619	-	-	10/53/53/53	-
21	CLA	A	802	-	1/1/12/20	3/24/100/115	-
21	CLA	L	302	12	1/1/11/20	7/15/91/115	-
21	CLA	A	832	-	1/1/11/20	5/15/91/115	-
26	LMU	b	301	-	-	6/21/61/61	0/2/2/2
21	CLA	3	409	17	1/1/12/20	10/24/100/115	-
21	CLA	A	813	-	1/1/12/20	4/26/102/115	-
21	CLA	c	603	-	1/1/13/20	6/27/103/115	-
21	CLA	7	405	17	1/1/10/20	2/8/84/115	-
21	CLA	6	603	-	1/1/11/20	7/15/91/115	-
29	CHL	6	602	-	3/3/17/26	10/24/122/137	-
29	CHL	b	306	20	3/3/16/26	6/15/113/137	-
24	BCR	J	101	-	-	7/29/63/63	0/2/2/2
21	CLA	A	822	-	1/1/11/20	3/13/89/115	-
21	CLA	5	604	-	1/1/11/20	6/20/96/115	-
31	XAT	7	416	-	-	0/31/93/93	0/4/4/4
21	CLA	A	816	-	1/1/10/20	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	608	16	1/1/11/20	7/15/91/115	-
21	CLA	A	809	1	1/1/13/20	5/32/108/115	-
21	CLA	O	204	-	1/1/10/20	2/8/84/115	-
24	BCR	J	104	-	-	9/29/63/63	0/2/2/2
21	CLA	A	842	-	1/1/15/20	14/39/115/115	-
21	CLA	O	201	23	1/1/10/20	2/12/88/115	-
24	BCR	A	848	-	-	1/29/63/63	0/2/2/2
28	LMG	6	615	-	-	3/4/24/70	0/1/1/1
21	CLA	A	803	-	1/1/12/20	6/24/100/115	-
25	SF4	C	102	3	-	-	0/6/5/5
31	XAT	5	616	-	-	3/31/93/93	0/4/4/4
21	CLA	1	305	-	1/1/11/20	9/20/96/115	-
21	CLA	4	602	18	1/1/13/20	10/30/106/115	-
21	CLA	3	412	-	1/1/13/20	11/25/101/115	-
21	CLA	9	610	19	1/1/12/20	3/26/102/115	-
21	CLA	B	832	-	1/1/13/20	7/29/105/115	-
21	CLA	c	613	-	1/1/15/20	9/39/115/115	-
24	BCR	8	616	-	-	6/29/63/63	0/2/2/2
21	CLA	6	613	-	1/1/10/20	5/12/88/115	-
30	LUT	c	615	-	-	0/29/67/67	0/2/2/2
21	CLA	2	613	-	1/1/10/20	3/12/88/115	-
21	CLA	B	805	-	1/1/15/20	18/39/115/115	-
29	CHL	1	307	-	3/3/17/26	2/21/119/137	-
29	CHL	7	406	-	3/3/15/26	0/6/104/137	-
29	CHL	2	601	16	3/3/17/26	8/24/122/137	-
21	CLA	B	837	-	1/1/15/20	10/37/113/115	-
25	SF4	A	851	2,1	-	-	0/6/5/5
29	CHL	c	606	20	3/3/16/26	4/15/113/137	-
29	CHL	c	607	-	3/3/16/26	3/15/113/137	-
21	CLA	3	411	17	1/1/10/20	2/13/89/115	-
29	CHL	a	608	-	3/3/16/26	7/15/113/137	-
21	CLA	B	816	-	1/1/12/20	5/24/100/115	-
21	CLA	7	401	17	1/1/11/20	8/15/91/115	-
21	CLA	8	612	-	1/1/10/20	3/13/89/115	-
29	CHL	8	607	-	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	834	-	1/1/11/20	5/15/91/115	-
29	CHL	8	613	-	3/3/15/26	2/10/108/137	-
30	LUT	a	615	-	-	4/29/67/67	0/2/2/2
21	CLA	5	614	15	1/1/11/20	5/11/87/115	-
30	LUT	3	416	-	-	5/29/67/67	0/2/2/2
21	CLA	a	611	-	1/1/11/20	6/18/94/115	-
21	CLA	8	601	18	1/1/11/20	9/15/91/115	-
21	CLA	5	603	-	1/1/11/20	6/15/91/115	-
21	CLA	A	815	-	1/1/11/20	5/15/91/115	-
21	CLA	4	604	-	1/1/10/20	2/12/88/115	-
24	BCR	F	303	-	-	0/29/63/63	0/2/2/2
23	LHG	1	301	21	-	7/26/26/53	-
21	CLA	5	602	15	1/1/14/20	15/35/111/115	-
21	CLA	4	611	18	1/1/11/20	4/13/89/115	-
21	CLA	B	839	-	1/1/15/20	10/39/115/115	-
32	NEX	b	318	-	-	2/27/83/83	0/3/3/3
28	LMG	G	206	-	-	9/50/70/70	0/1/1/1
21	CLA	6	611	-	1/1/10/20	6/10/86/115	-
21	CLA	B	817	-	1/1/15/20	20/39/115/115	-
21	CLA	3	402	17	1/1/14/20	5/33/109/115	-
30	LUT	c	616	-	-	0/29/67/67	0/2/2/2
21	CLA	3	415	-	1/1/10/20	0/8/84/115	-
23	LHG	A	845	21	-	5/31/31/53	-
21	CLA	2	610	23	1/1/10/20	2/9/85/115	-
24	BCR	L	301	-	-	4/29/63/63	0/2/2/2
21	CLA	A	852	-	1/1/12/20	6/24/100/115	-
29	CHL	2	605	-	3/3/16/26	3/15/113/137	-
23	LHG	8	617	21	-	9/41/41/53	-
21	CLA	A	814	-	1/1/15/20	8/39/115/115	-
24	BCR	O	205	-	-	6/29/63/63	0/2/2/2
21	CLA	3	406	17	1/1/10/20	0/8/84/115	-
21	CLA	A	830	-	1/1/12/20	4/24/100/115	-
21	CLA	B	806	-	1/1/14/20	7/37/113/115	-
21	CLA	b	315	-	1/1/11/20	11/15/91/115	-
21	CLA	2	604	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	a	612	-	1/1/11/20	6/15/91/115	-
21	CLA	9	603	19	1/1/11/20	5/15/91/115	-
21	CLA	a	613	-	1/1/13/20	5/30/106/115	-
21	CLA	B	815	-	1/1/13/20	5/25/101/115	-
21	CLA	7	412	-	1/1/10/20	2/8/84/115	-
26	LMU	3	420	-	-	3/21/61/61	0/2/2/2
30	LUT	4	615	-	-	4/29/67/67	0/2/2/2
29	CHL	4	614	18	3/3/15/26	2/10/108/137	-
21	CLA	a	604	-	1/1/11/20	9/17/93/115	-
21	CLA	1	304	-	1/1/13/20	6/27/103/115	-
21	CLA	b	305	-	1/1/11/20	5/15/91/115	-
30	LUT	b	317	-	-	2/29/67/67	0/2/2/2
29	CHL	5	601	15	3/3/16/26	5/15/113/137	-
23	LHG	4	618	21	-	9/41/41/53	-
21	CLA	1	311	23	1/1/10/20	2/4/80/115	-
21	CLA	A	828	-	1/1/14/20	14/33/109/115	-
21	CLA	B	827	-	1/1/15/20	10/39/115/115	-
30	LUT	b	316	-	-	2/29/67/67	0/2/2/2
21	CLA	5	612	-	1/1/11/20	5/15/91/115	-
21	CLA	4	613	-	1/1/10/20	2/13/89/115	-
21	CLA	B	801	-	1/1/15/20	14/39/115/115	-
21	CLA	B	821	-	1/1/13/20	4/27/103/115	-
29	CHL	8	605	18	3/3/15/26	2/10/106/137	-
21	CLA	7	408	-	1/1/10/20	4/10/86/115	-
24	BCR	A	846	-	-	4/29/63/63	0/2/2/2
26	LMU	A	853	-	-	0/21/61/61	0/2/2/2
21	CLA	6	610	-	1/1/10/20	1/9/85/115	-
21	CLA	8	610	-	1/1/11/20	7/13/89/115	-
29	CHL	9	601	19	3/3/15/26	2/12/110/137	-
21	CLA	B	812	-	1/1/15/20	18/39/115/115	-
21	CLA	A	817	-	1/1/15/20	17/39/115/115	-
21	CLA	B	808	2	1/1/15/20	7/39/115/115	-
32	NEX	c	618	-	-	2/27/83/83	0/3/3/3
21	CLA	1	315	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	802	-	1/1/15/20	19/39/115/115	-
21	CLA	B	804	-	1/1/15/20	13/39/115/115	-
21	CLA	5	605	-	1/1/9/20	6/10/82/115	-
29	CHL	b	308	-	3/3/17/26	6/24/122/137	-
21	CLA	A	818	-	1/1/12/20	7/24/100/115	-
21	CLA	3	403	-	1/1/13/20	8/27/103/115	-
28	LMG	2	615	-	-	1/4/24/70	0/1/1/1
21	CLA	A	829	-	1/1/15/20	9/39/115/115	-
21	CLA	2	603	-	1/1/11/20	7/15/91/115	-
21	CLA	A	806	-	1/1/15/20	18/39/115/115	-
21	CLA	B	835	-	1/1/15/20	6/39/115/115	-
21	CLA	B	818	-	1/1/13/20	9/31/107/115	-
21	CLA	5	610	-	1/1/10/20	0/4/80/115	-
24	BCR	F	301	-	-	0/29/63/63	0/2/2/2
27	DGD	B	847	-	-	16/55/95/95	0/2/2/2
21	CLA	L	303	-	1/1/11/20	3/15/91/115	-
21	CLA	H	201	8	1/1/11/20	6/15/91/115	-
24	BCR	B	845	-	-	2/29/63/63	0/2/2/2
21	CLA	1	314	-	1/1/10/20	1/4/80/115	-
23	LHG	A	855	-	-	7/53/53/53	-
29	CHL	9	606	19	3/3/16/26	5/15/113/137	-
21	CLA	c	604	-	1/1/11/20	5/15/91/115	-
21	CLA	7	410	-	1/1/10/20	5/13/89/115	-
24	BCR	3	418	-	-	4/29/63/63	0/2/2/2
24	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	A	826	-	1/1/15/20	8/39/115/115	-
21	CLA	F	302	-	1/1/14/20	11/35/111/115	-
21	CLA	3	408	17	1/1/13/20	6/32/108/115	-
30	LUT	9	614	-	-	2/29/67/67	0/2/2/2
21	CLA	B	840	23	1/1/15/20	4/39/115/115	-
21	CLA	7	414	-	1/1/10/20	1/8/84/115	-
21	CLA	B	809	-	1/1/14/20	13/35/111/115	-
21	CLA	b	313	20	1/1/11/20	8/15/91/115	-
21	CLA	c	610	20	1/1/11/20	5/15/91/115	-
21	CLA	K	204	11	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	8	618	-	1/1/10/20	4/10/86/115	-
21	CLA	B	825	-	1/1/15/20	9/39/115/115	-
21	CLA	A	819	-	1/1/15/20	15/39/115/115	-
21	CLA	5	609	-	1/1/11/20	5/11/87/115	-
23	LHG	A	844	-	-	8/53/53/53	-
21	CLA	1	312	15	1/1/11/20	5/15/91/115	-
21	CLA	A	824	-	1/1/13/20	11/27/103/115	-
21	CLA	A	807	1	1/1/15/20	11/39/115/115	-
29	CHL	c	601	20	3/3/16/26	6/19/117/137	-
21	CLA	B	807	-	1/1/15/20	17/39/115/115	-
29	CHL	5	606	-	3/3/16/26	5/15/113/137	-
21	CLA	B	803	-	1/1/13/20	7/27/103/115	-
24	BCR	3	419	-	-	8/29/63/63	0/2/2/2
21	CLA	1	313	15	1/1/11/20	5/15/91/115	-
22	PQN	B	841	-	-	1/23/43/43	0/2/2/2
30	LUT	6	616	-	-	2/29/67/67	0/2/2/2
21	CLA	9	612	19	1/1/11/20	4/15/91/115	-
29	CHL	9	607	-	3/3/16/26	9/15/113/137	-
21	CLA	L	304	-	1/1/10/20	3/12/88/115	-
24	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	CLA	c	614	-	1/1/11/20	5/15/91/115	-
21	CLA	4	610	23	1/1/11/20	2/15/91/115	-
21	CLA	6	612	-	1/1/11/20	7/15/91/115	-
21	CLA	7	407	17	-	5/13/89/115	-
23	LHG	5	617	-	-	6/32/32/53	-
31	XAT	c	617	-	-	1/31/93/93	0/4/4/4
21	CLA	4	601	18	1/1/11/20	3/15/91/115	-
21	CLA	A	820	-	1/1/11/20	2/13/89/115	-
21	CLA	A	805	-	1/1/13/20	6/27/103/115	-
24	BCR	7	418	-	-	6/29/63/63	0/2/2/2
29	CHL	4	606	-	3/3/16/26	4/15/113/137	-
21	CLA	B	838	-	1/1/15/20	9/39/115/115	-
21	CLA	9	611	23	1/1/13/20	9/30/106/115	-
21	CLA	B	833	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	612	-	1/1/13/20	7/27/103/115	-
21	CLA	1	309	15	1/1/10/20	2/10/86/115	-
21	CLA	O	202	-	1/1/9/20	2/6/78/115	-
21	CLA	5	608	15	1/1/10/20	2/8/84/115	-
29	CHL	c	608	-	3/3/16/26	8/15/113/137	-
21	CLA	8	608	18	1/1/10/20	5/9/87/115	-
24	BCR	A	847	-	-	0/29/63/63	0/2/2/2
21	CLA	8	609	23	1/1/11/20	7/15/91/115	-
29	CHL	b	310	-	3/3/17/26	1/22/120/137	-
21	CLA	3	405	-	1/1/10/20	3/10/86/115	-
21	CLA	G	204	7	1/1/11/20	4/13/89/115	-
21	CLA	B	823	-	1/1/15/20	10/39/115/115	-
21	CLA	A	837	-	1/1/12/20	9/23/99/115	-
21	CLA	4	609	18	-	10/24/100/115	-
24	BCR	M	101	-	-	8/29/63/63	0/2/2/2
21	CLA	A	810	-	1/1/11/20	4/15/91/115	-
29	CHL	b	302	20	3/3/16/26	4/15/113/137	-
21	CLA	6	604	-	1/1/11/20	4/15/91/115	-
21	CLA	B	829	-	1/1/11/20	1/15/91/115	-
21	CLA	a	610	20	1/1/11/20	4/15/91/115	-
21	CLA	A	801	-	-	7/24/100/115	-
21	CLA	5	613	-	1/1/10/20	1/4/80/115	-
21	CLA	F	305	6	1/1/10/20	2/10/86/115	-
21	CLA	8	603	-	1/1/11/20	3/13/89/115	-
21	CLA	K	201	11	1/1/11/20	6/17/93/115	-
30	LUT	7	415	-	-	6/29/67/67	0/2/2/2
29	CHL	1	302	15	3/3/17/26	7/21/119/137	-
21	CLA	A	812	-	1/1/15/20	4/39/115/115	-
21	CLA	A	831	-	1/1/13/20	6/27/103/115	-
21	CLA	A	808	-	1/1/11/20	2/15/91/115	-
21	CLA	3	404	-	1/1/11/20	0/9/85/115	-
21	CLA	B	828	-	1/1/12/20	7/24/100/115	-
21	CLA	B	820	-	1/1/11/20	4/17/93/115	-
29	CHL	4	605	-	3/3/15/26	2/10/106/137	-
21	CLA	A	823	-	1/1/13/20	8/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	6	607	-	3/3/17/26	4/21/119/137	-
24	BCR	2	618	-	-	2/29/63/63	0/2/2/2
21	CLA	B	814	-	1/1/14/20	9/33/109/115	-
21	CLA	A	834	-	1/1/15/20	10/39/115/115	-
23	LHG	6	619	-	-	3/39/39/53	-
21	CLA	2	609	16	1/1/11/20	9/22/98/115	-
21	CLA	B	811	-	1/1/11/20	3/15/91/115	-
21	CLA	B	822	-	1/1/11/20	4/15/91/115	-
21	CLA	7	402	-	1/1/11/20	9/15/91/115	-
21	CLA	a	614	-	1/1/10/20	2/10/86/115	-
21	CLA	A	839	-	1/1/11/20	0/15/91/115	-
25	SF4	C	101	3	-	-	0/6/5/5
21	CLA	K	203	-	1/1/11/20	4/13/89/115	-
26	LMU	A	856	-	-	3/21/61/61	0/2/2/2
31	XAT	a	618	-	-	1/31/93/93	0/4/4/4
31	XAT	9	616	-	-	8/31/93/93	0/4/4/4
29	CHL	a	606	-	3/3/16/26	3/15/113/137	-
21	CLA	c	611	23	1/1/13/20	11/31/107/115	-
21	CLA	B	824	-	1/1/15/20	8/39/115/115	-
21	CLA	7	404	-	1/1/10/20	2/10/86/115	-
30	LUT	8	614	-	-	4/29/67/67	0/2/2/2
31	XAT	8	615	-	-	0/31/93/93	0/4/4/4
21	CLA	7	411	-	1/1/13/20	8/25/101/115	-
29	CHL	b	307	-	3/3/16/26	2/15/113/137	-
21	CLA	9	613	-	1/1/12/20	7/25/101/115	-
29	CHL	9	605	19	3/3/16/26	4/15/113/137	-
29	CHL	9	609	-	3/3/16/26	4/15/113/137	-
30	LUT	5	615	-	-	7/29/67/67	0/2/2/2
21	CLA	B	836	-	1/1/15/20	14/39/115/115	-
21	CLA	c	602	20	1/1/14/20	7/33/109/115	-
23	LHG	a	617	-	-	10/53/53/53	-
29	CHL	a	605	20	3/3/16/26	4/13/111/137	-
24	BCR	6	618	-	-	4/29/63/63	0/2/2/2
24	BCR	4	617	-	-	2/29/63/63	0/2/2/2
21	CLA	9	602	19	1/1/12/20	4/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	303	15	1/1/14/20	17/35/111/115	-
30	LUT	1	317	-	-	3/29/67/67	0/2/2/2
30	LUT	2	616	-	-	4/29/67/67	0/2/2/2
21	CLA	A	836	1	1/1/11/20	2/15/91/115	-
21	CLA	B	813	-	1/1/11/20	2/13/89/115	-
24	BCR	J	103	-	-	3/29/63/63	0/2/2/2
21	CLA	b	303	20	1/1/13/20	10/32/108/115	-
21	CLA	1	316	15	1/1/11/20	3/11/87/115	-
21	CLA	3	413	-	1/1/10/20	2/8/84/115	-
21	CLA	3	414	-	1/1/8/20	2/2/74/115	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
21	CLA	3	401	-	1/1/10/20	1/8/84/115	-
24	BCR	K	205	-	-	3/29/63/63	0/2/2/2

The worst 5 of 3213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	601	CHL	C2C-C3C	12.04	1.48	1.36
29	c	605	CHL	C2C-C3C	12.02	1.48	1.36
29	9	601	CHL	C2C-C3C	12.00	1.48	1.36
29	a	606	CHL	C2C-C3C	11.98	1.48	1.36
29	a	609	CHL	C2C-C3C	11.97	1.48	1.36

The worst 5 of 2790 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	407	CLA	CAC-C3C-C4C	16.77	146.62	124.79
29	a	601	CHL	C4D-ND-C1D	10.89	113.49	105.22
29	9	601	CHL	C4D-ND-C1D	10.87	113.47	105.22
29	c	609	CHL	C4D-ND-C1D	10.83	113.44	105.22
29	a	609	CHL	C4D-ND-C1D	10.80	113.41	105.22

5 of 368 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	802	CLA	ND
21	A	803	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	806	CLA	ND

5 of 1947 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	801	CLA	CBD-CGD-O2D-CED
21	A	802	CLA	C4B-C3B-CAB-CBB
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

307 monomers are involved in 867 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	835	CLA	2	0
24	I	101	BCR	1	0
21	A	841	CLA	4	0
29	c	605	CHL	1	0
26	O	206	LMU	4	0
21	b	312	CLA	3	0
24	B	844	BCR	6	0
29	6	601	CHL	3	0
29	2	606	CHL	2	0
21	G	202	CLA	2	0
29	4	607	CHL	4	0
21	1	310	CLA	1	0
24	B	843	BCR	20	0
21	b	304	CLA	4	0
21	1	306	CLA	2	0
29	3	407	CHL	1	0
29	c	609	CHL	3	0
21	B	810	CLA	1	0
21	A	821	CLA	7	0
24	A	849	BCR	4	0
29	b	309	CHL	3	0
21	B	819	CLA	1	0
21	8	611	CLA	5	0
29	6	606	CHL	1	0
31	2	617	XAT	2	0
29	8	606	CHL	2	0
29	9	608	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	205	BCR	2	0
21	A	840	CLA	8	0
21	b	311	CLA	6	0
29	a	607	CHL	5	0
30	a	616	LUT	7	0
23	c	619	LHG	2	0
24	B	846	BCR	8	0
31	3	417	XAT	4	0
24	L	306	BCR	3	0
21	K	202	CLA	1	0
21	A	825	CLA	3	0
21	1	308	CLA	1	0
21	F	304	CLA	2	0
21	8	602	CLA	4	0
21	B	831	CLA	6	0
23	b	319	LHG	9	0
29	6	614	CHL	4	0
24	G	201	BCR	4	0
21	5	607	CLA	3	0
29	2	607	CHL	3	0
21	A	804	CLA	3	0
29	a	601	CHL	1	0
23	2	619	LHG	1	0
21	B	826	CLA	1	0
21	c	612	CLA	2	0
24	A	854	BCR	13	0
29	6	605	CHL	1	0
30	9	615	LUT	7	0
31	6	617	XAT	6	0
21	O	203	CLA	1	0
21	B	830	CLA	4	0
21	6	609	CLA	4	0
29	2	602	CHL	3	0
23	9	618	LHG	4	0
21	A	838	CLA	3	0
29	2	614	CHL	5	0
21	A	833	CLA	5	0
29	a	609	CHL	3	0
21	b	314	CLA	4	0
21	2	608	CLA	2	0
21	8	604	CLA	3	0
21	A	827	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	417	BCR	7	0
31	4	616	XAT	4	0
32	9	617	NEX	4	0
31	1	318	XAT	2	0
21	a	602	CLA	5	0
23	4	619	LHG	1	0
21	A	802	CLA	4	0
21	L	302	CLA	2	0
21	A	832	CLA	1	0
26	b	301	LMU	4	0
21	3	409	CLA	21	0
21	A	813	CLA	1	0
21	c	603	CLA	4	0
21	6	603	CLA	2	0
29	6	602	CHL	3	0
29	b	306	CHL	2	0
24	J	101	BCR	4	0
21	A	822	CLA	3	0
21	5	604	CLA	2	0
31	7	416	XAT	5	0
21	A	816	CLA	1	0
21	6	608	CLA	2	0
21	A	809	CLA	1	0
24	J	104	BCR	8	0
21	A	842	CLA	7	0
28	6	615	LMG	1	0
21	A	803	CLA	2	0
31	5	616	XAT	5	0
21	4	602	CLA	5	0
21	3	412	CLA	1	0
21	9	610	CLA	1	0
21	B	832	CLA	4	0
21	c	613	CLA	4	0
24	8	616	BCR	8	0
21	6	613	CLA	1	0
30	c	615	LUT	3	0
21	2	613	CLA	2	0
21	B	805	CLA	4	0
29	1	307	CHL	5	0
29	7	406	CHL	2	0
29	2	601	CHL	2	0
21	B	837	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	606	CHL	2	0
29	c	607	CHL	1	0
21	3	411	CLA	1	0
29	a	608	CHL	3	0
21	B	816	CLA	5	0
21	7	401	CLA	7	0
21	8	612	CLA	2	0
29	8	607	CHL	5	0
29	8	613	CHL	4	0
30	a	615	LUT	4	0
21	5	614	CLA	1	0
30	3	416	LUT	12	0
21	a	611	CLA	4	0
21	5	603	CLA	3	0
21	5	602	CLA	10	0
21	4	611	CLA	1	0
21	B	839	CLA	4	0
32	b	318	NEX	1	0
28	G	206	LMG	2	0
21	6	611	CLA	1	0
21	B	817	CLA	8	0
21	3	402	CLA	1	0
30	c	616	LUT	4	0
21	3	415	CLA	2	0
23	A	845	LHG	1	0
21	2	610	CLA	2	0
24	L	301	BCR	3	0
21	A	852	CLA	6	0
23	8	617	LHG	3	0
21	A	814	CLA	1	0
24	O	205	BCR	1	0
21	A	830	CLA	3	0
21	B	806	CLA	2	0
21	b	315	CLA	1	0
21	2	604	CLA	3	0
21	a	612	CLA	1	0
21	a	613	CLA	3	0
21	B	815	CLA	2	0
26	3	420	LMU	3	0
30	4	615	LUT	7	0
29	4	614	CHL	1	0
21	a	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	304	CLA	2	0
30	b	317	LUT	5	0
23	4	618	LHG	5	0
29	5	601	CHL	3	0
21	A	828	CLA	3	0
21	B	827	CLA	9	0
30	b	316	LUT	6	0
21	5	612	CLA	1	0
21	4	613	CLA	2	0
21	B	801	CLA	9	0
21	B	821	CLA	1	0
29	8	605	CHL	4	0
21	7	408	CLA	2	0
24	A	846	BCR	1	0
21	6	610	CLA	1	0
21	8	610	CLA	1	0
29	9	601	CHL	2	0
21	B	812	CLA	1	0
21	A	817	CLA	3	0
21	B	808	CLA	2	0
32	c	618	NEX	3	0
21	1	315	CLA	1	0
21	B	802	CLA	3	0
21	B	804	CLA	2	0
21	5	605	CLA	2	0
29	b	308	CHL	2	0
21	A	818	CLA	7	0
21	A	829	CLA	2	0
21	2	603	CLA	1	0
21	A	806	CLA	3	0
21	B	835	CLA	2	0
21	B	818	CLA	1	0
24	F	301	BCR	2	0
27	B	847	DGD	7	0
21	L	303	CLA	1	0
21	H	201	CLA	2	0
24	B	845	BCR	3	0
21	1	314	CLA	1	0
23	A	855	LHG	4	0
29	9	606	CHL	1	0
21	c	604	CLA	3	0
21	7	410	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	418	BCR	6	0
24	L	305	BCR	2	0
21	A	826	CLA	2	0
21	F	302	CLA	1	0
21	3	408	CLA	5	0
30	9	614	LUT	3	0
21	B	840	CLA	1	0
21	B	809	CLA	4	0
21	c	610	CLA	2	0
21	K	204	CLA	1	0
21	8	618	CLA	2	0
21	B	825	CLA	2	0
21	A	819	CLA	6	0
21	5	609	CLA	2	0
23	A	844	LHG	3	0
21	1	312	CLA	1	0
21	A	824	CLA	3	0
21	A	807	CLA	2	0
21	B	807	CLA	5	0
29	5	606	CHL	3	0
21	B	803	CLA	2	0
24	3	419	BCR	1	0
21	1	313	CLA	1	0
22	B	841	PQN	3	0
30	6	616	LUT	6	0
21	9	612	CLA	1	0
29	9	607	CHL	1	0
24	A	850	BCR	1	0
21	c	614	CLA	2	0
21	6	612	CLA	2	0
21	7	407	CLA	18	0
23	5	617	LHG	1	0
31	c	617	XAT	3	0
21	4	601	CLA	2	0
21	A	820	CLA	1	0
21	A	805	CLA	4	0
24	7	418	BCR	4	0
29	4	606	CHL	1	0
21	B	838	CLA	1	0
21	9	611	CLA	5	0
21	4	612	CLA	1	0
21	1	309	CLA	10	0

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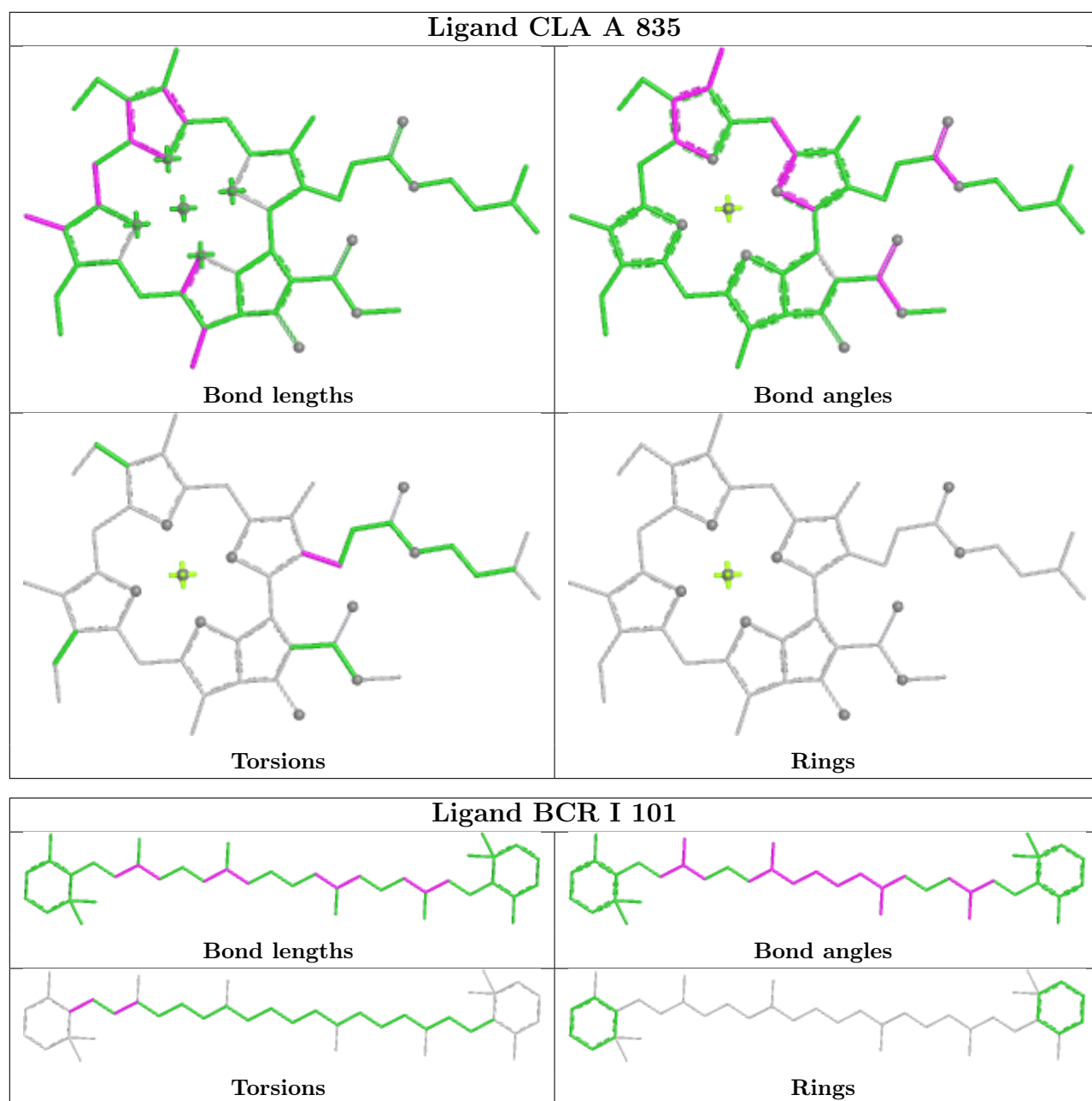
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21	O	202	CLA	1	0
29	c	608	CHL	3	0
21	8	608	CLA	2	0
24	A	847	BCR	3	0
21	8	609	CLA	26	0
29	b	310	CHL	3	0
21	G	204	CLA	1	0
21	B	823	CLA	3	0
21	A	837	CLA	3	0
21	4	609	CLA	16	0
24	M	101	BCR	3	0
21	A	810	CLA	4	0
29	b	302	CHL	2	0
21	6	604	CLA	7	0
21	B	829	CLA	1	0
21	a	610	CLA	5	0
21	A	801	CLA	1	0
21	8	603	CLA	1	0
21	K	201	CLA	5	0
30	7	415	LUT	12	0
29	1	302	CHL	2	0
21	A	812	CLA	5	0
21	A	831	CLA	1	0
21	A	808	CLA	2	0
21	3	404	CLA	4	0
21	B	828	CLA	3	0
21	A	823	CLA	1	0
24	2	618	BCR	6	0
29	6	607	CHL	5	0
21	B	814	CLA	4	0
21	A	834	CLA	4	0
23	6	619	LHG	3	0
21	2	609	CLA	23	0
21	B	811	CLA	1	0
21	B	822	CLA	2	0
21	7	402	CLA	9	0
21	a	614	CLA	1	0
21	K	203	CLA	9	0
26	A	856	LMU	2	0
31	a	618	XAT	6	0
31	9	616	XAT	2	0
29	a	606	CHL	2	0

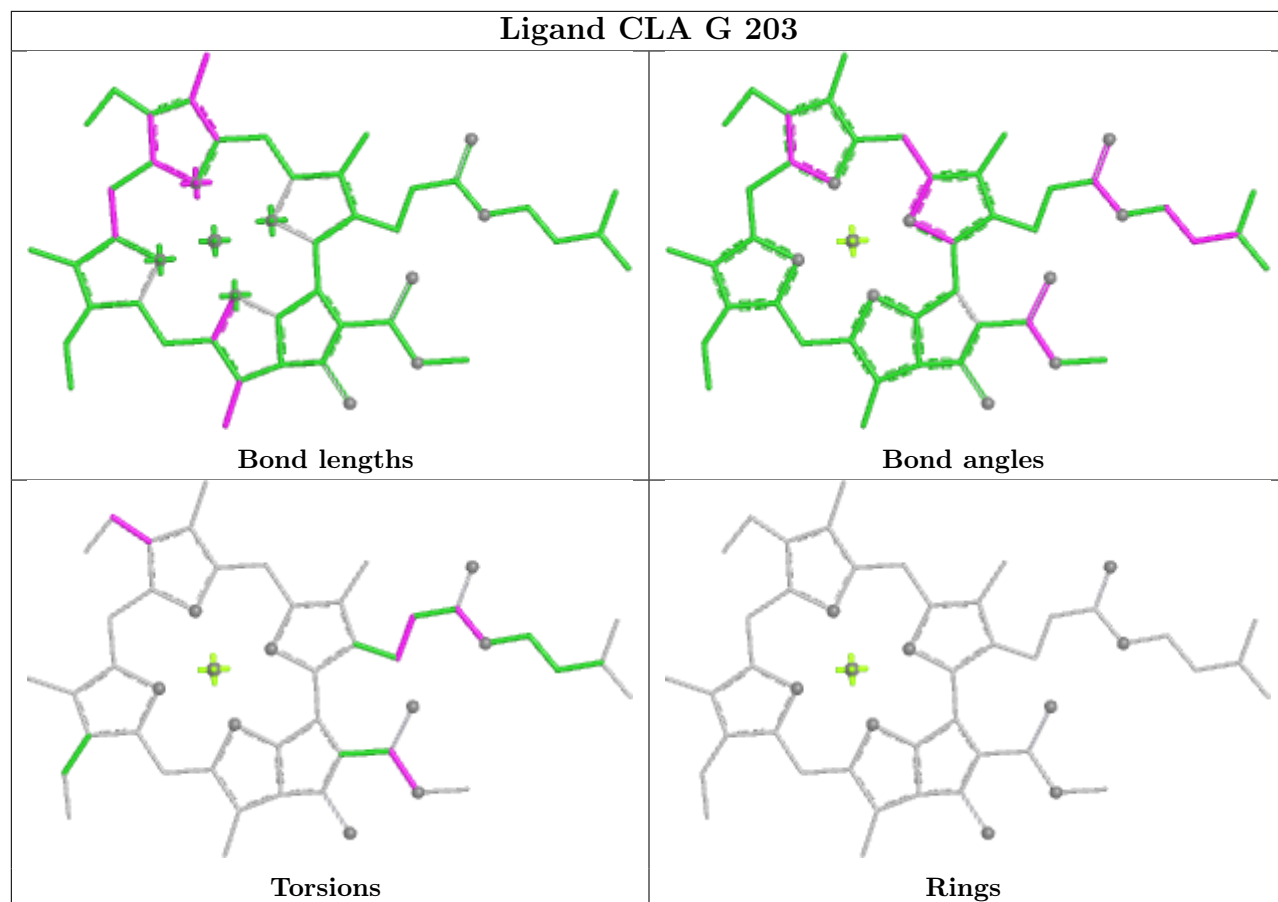
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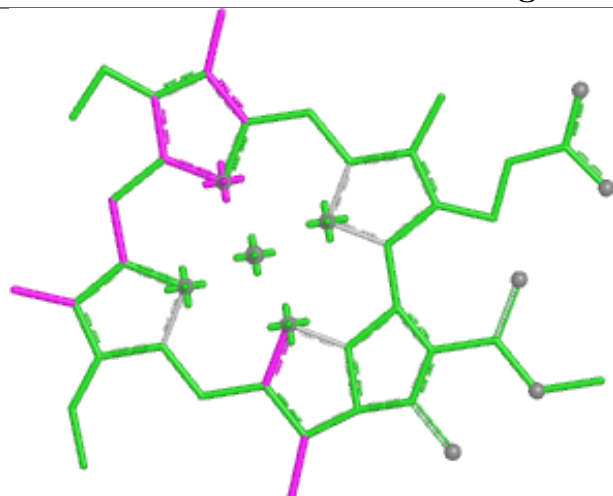
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	B	824	CLA	3	0
21	7	404	CLA	3	0
30	8	614	LUT	5	0
31	8	615	XAT	4	0
21	7	411	CLA	2	0
29	b	307	CHL	2	0
21	9	613	CLA	2	0
29	9	605	CHL	2	0
29	9	609	CHL	2	0
30	5	615	LUT	2	0
21	B	836	CLA	4	0
21	c	602	CLA	3	0
23	a	617	LHG	2	0
29	a	605	CHL	1	0
24	6	618	BCR	14	0
21	9	602	CLA	3	0
21	1	303	CLA	2	0
30	1	317	LUT	2	0
30	2	616	LUT	8	0
21	A	836	CLA	1	0
21	B	813	CLA	3	0
24	J	103	BCR	3	0
21	b	303	CLA	3	0
21	3	413	CLA	1	0
24	B	842	BCR	3	0
21	3	401	CLA	2	0
24	K	205	BCR	24	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.

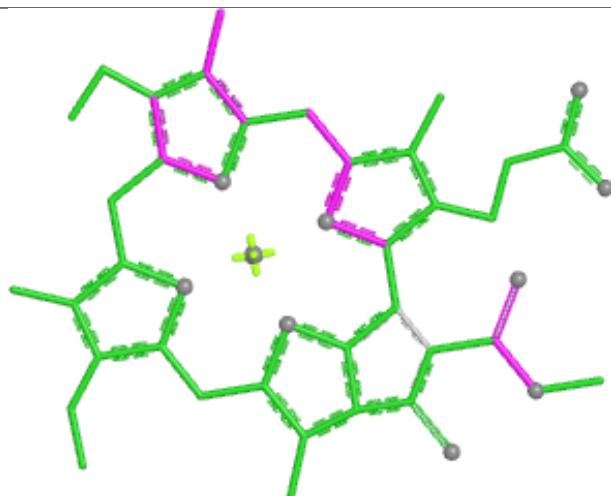




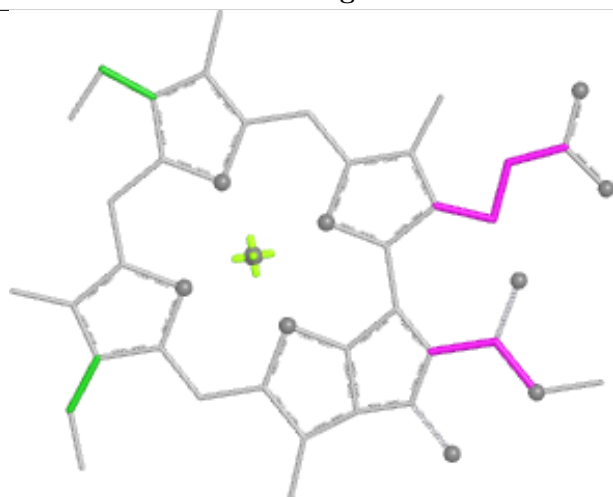
Ligand CLA 9 604



Bond lengths



Bond angles

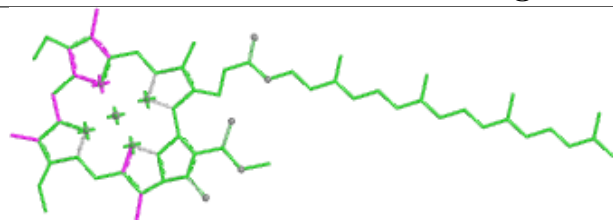


Torsions

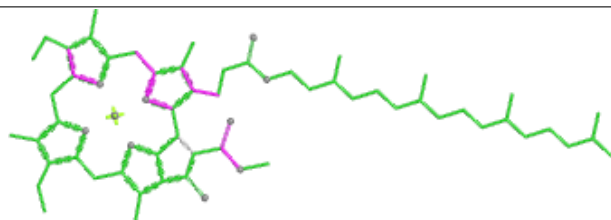


Rings

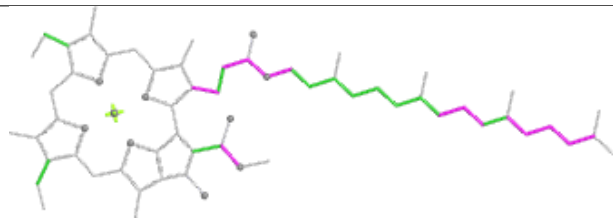
Ligand CLA A 841



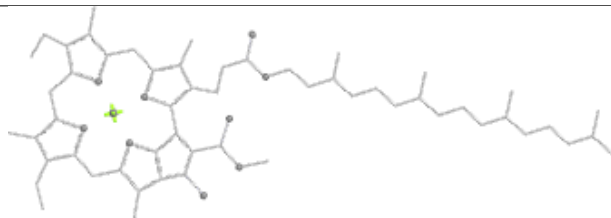
Bond lengths



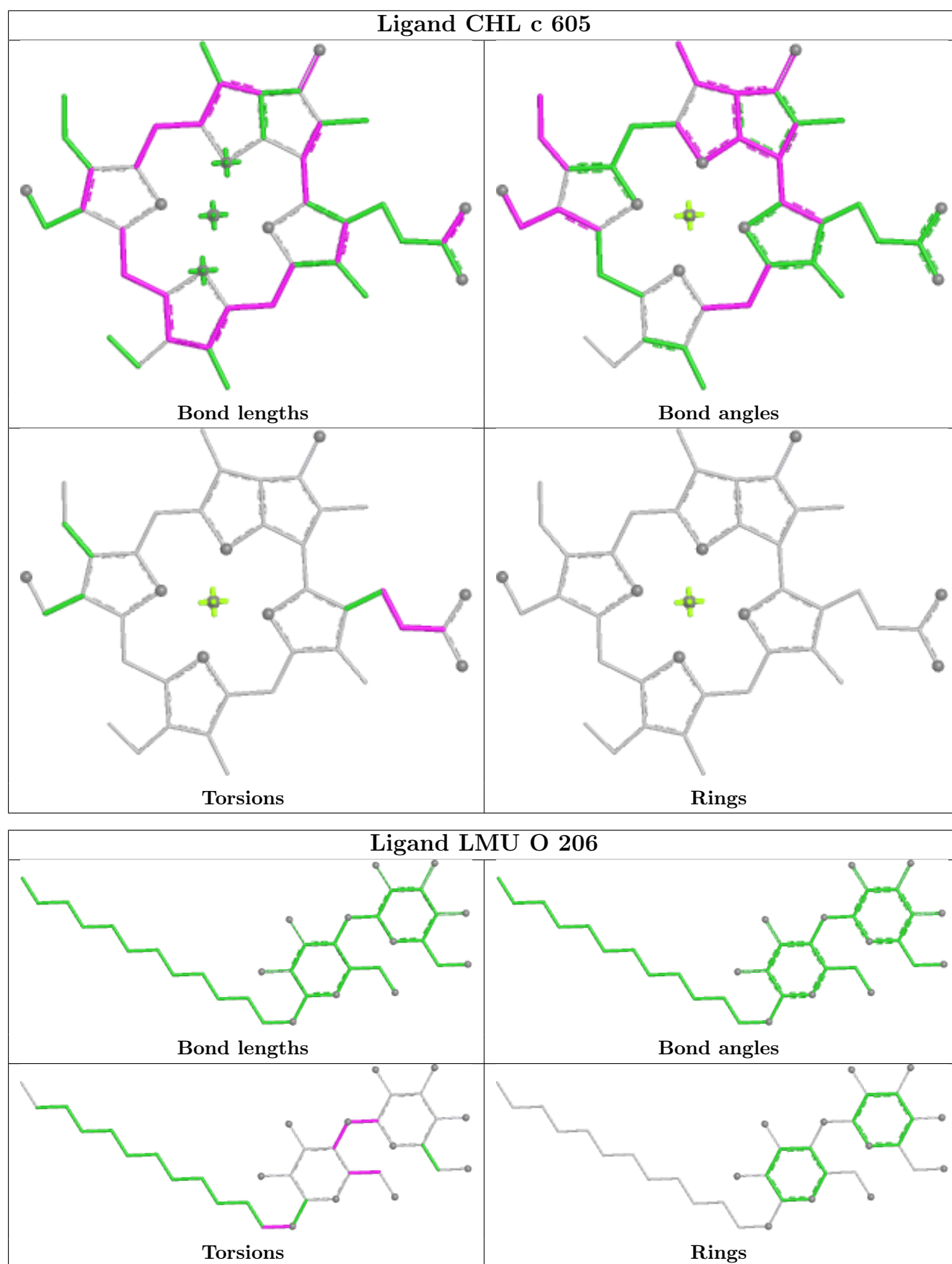
Bond angles



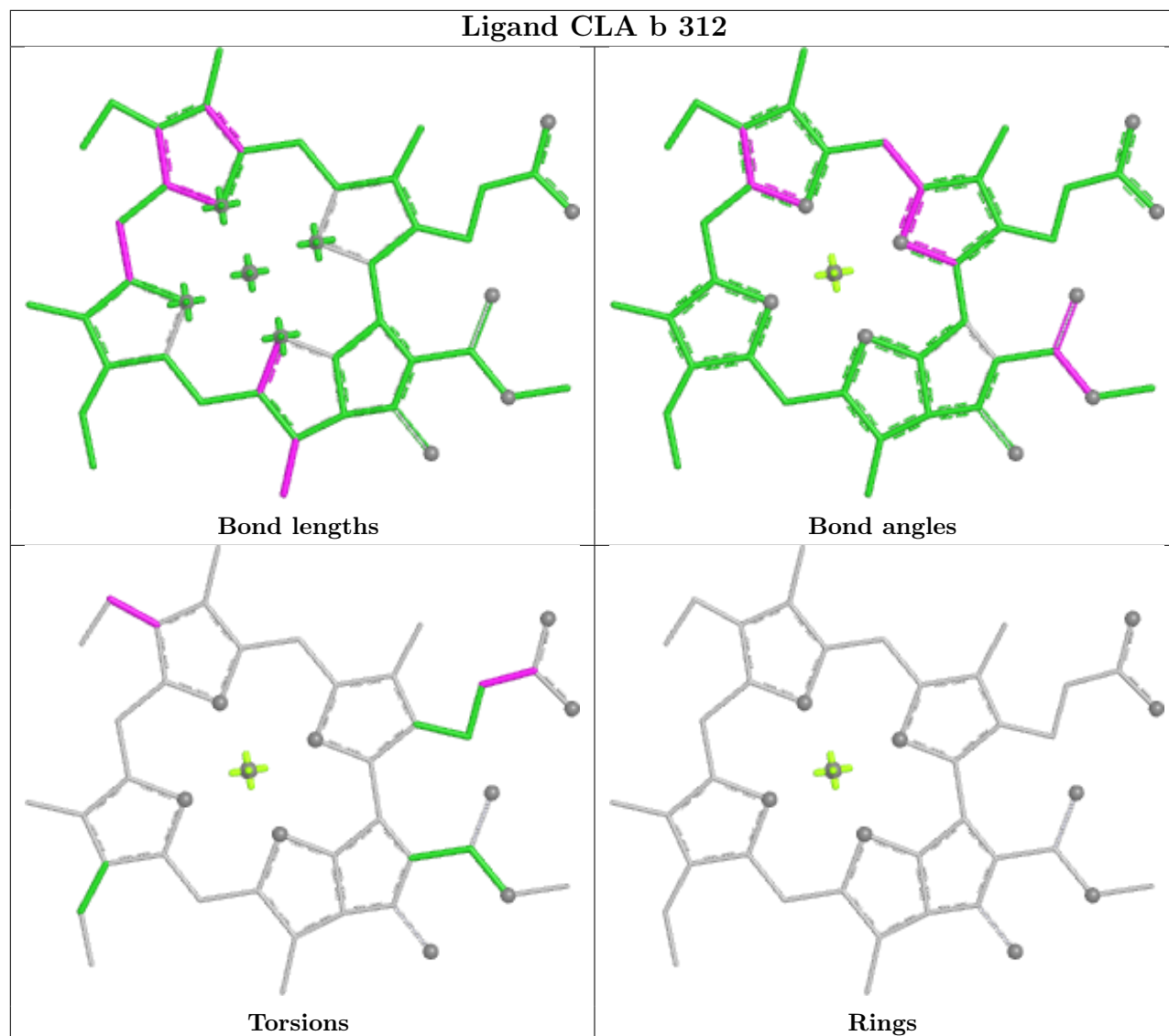
Torsions



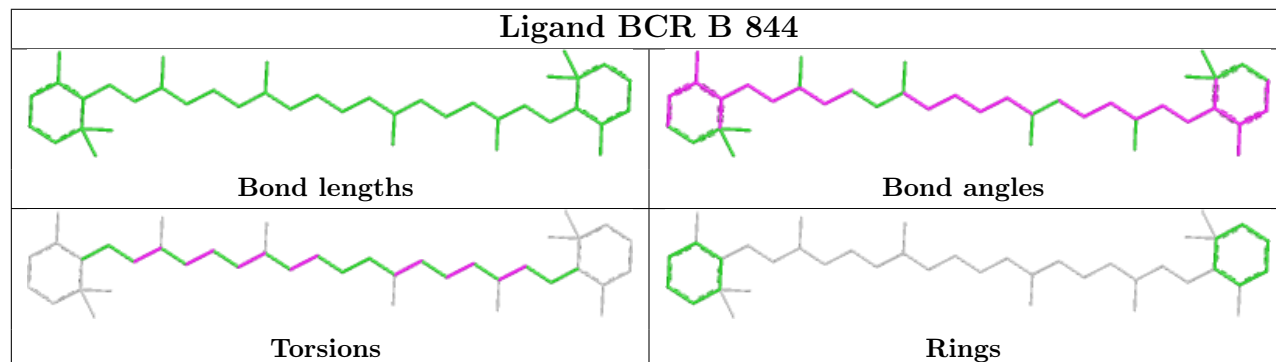
Rings



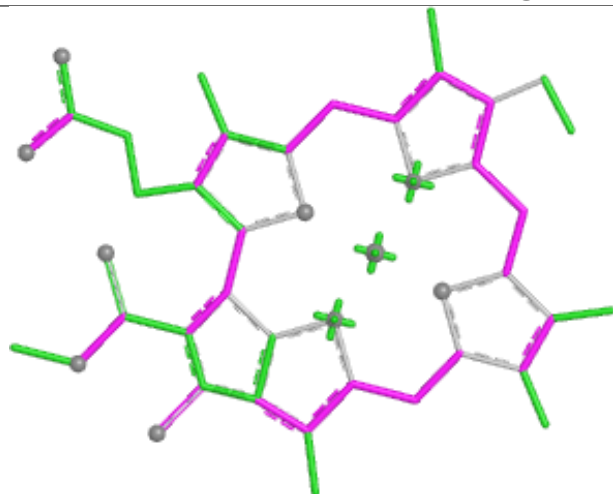
Ligand CLA b 312



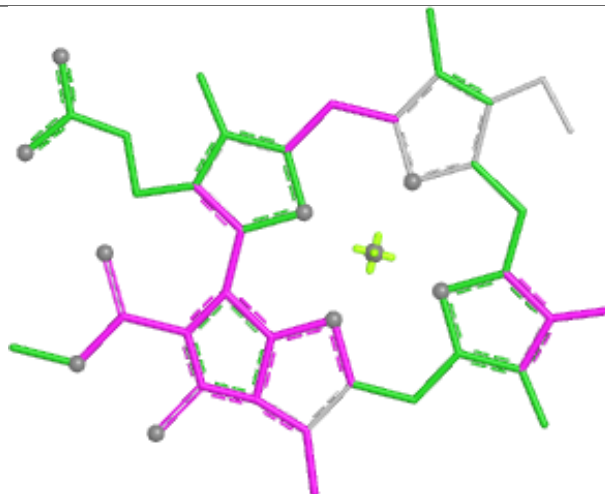
Ligand BCR B 844



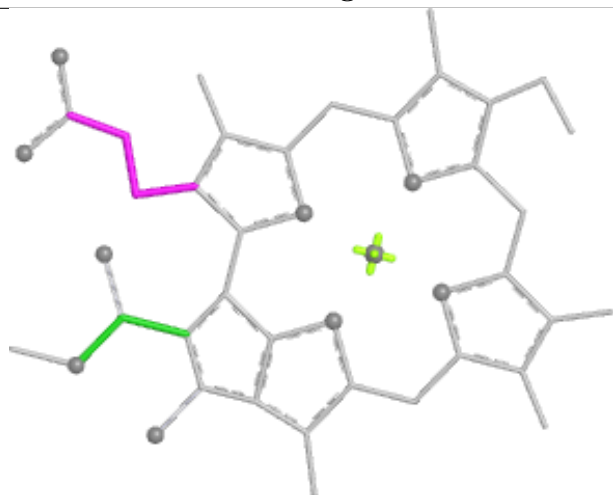
Ligand CHL 6 601



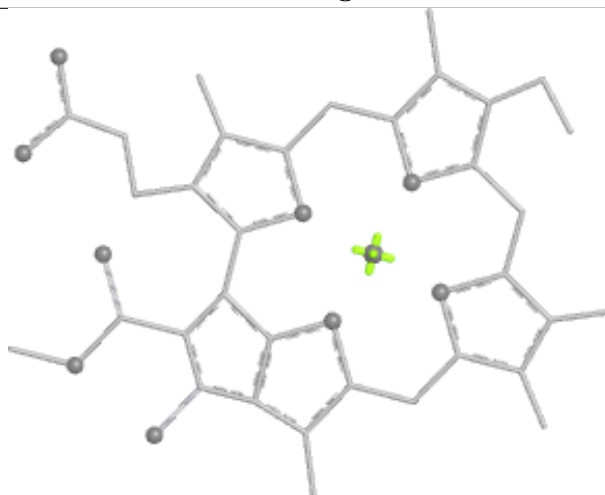
Bond lengths



Bond angles

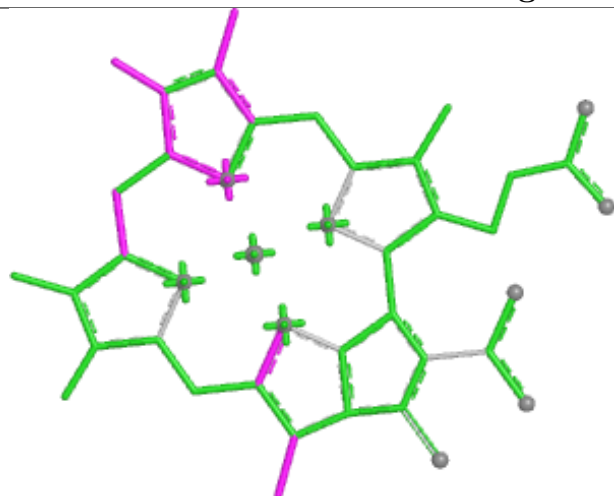


Torsions

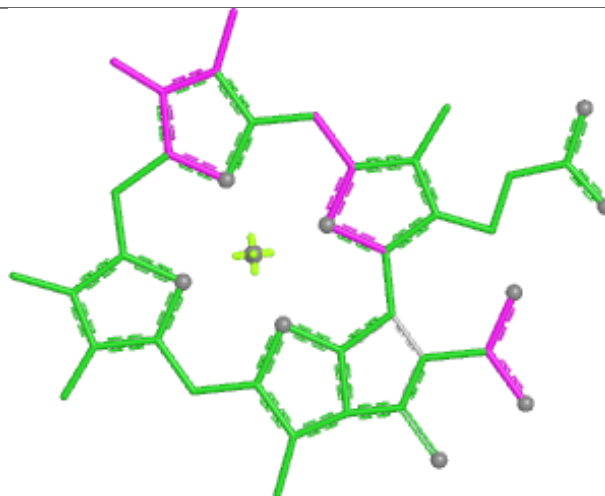


Rings

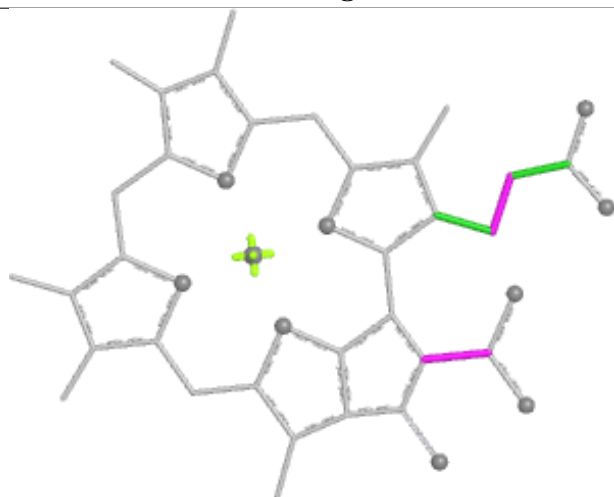
Ligand CLA 7 403



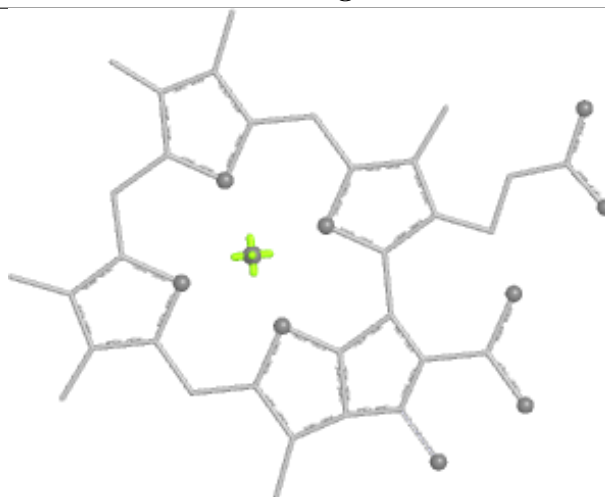
Bond lengths



Bond angles

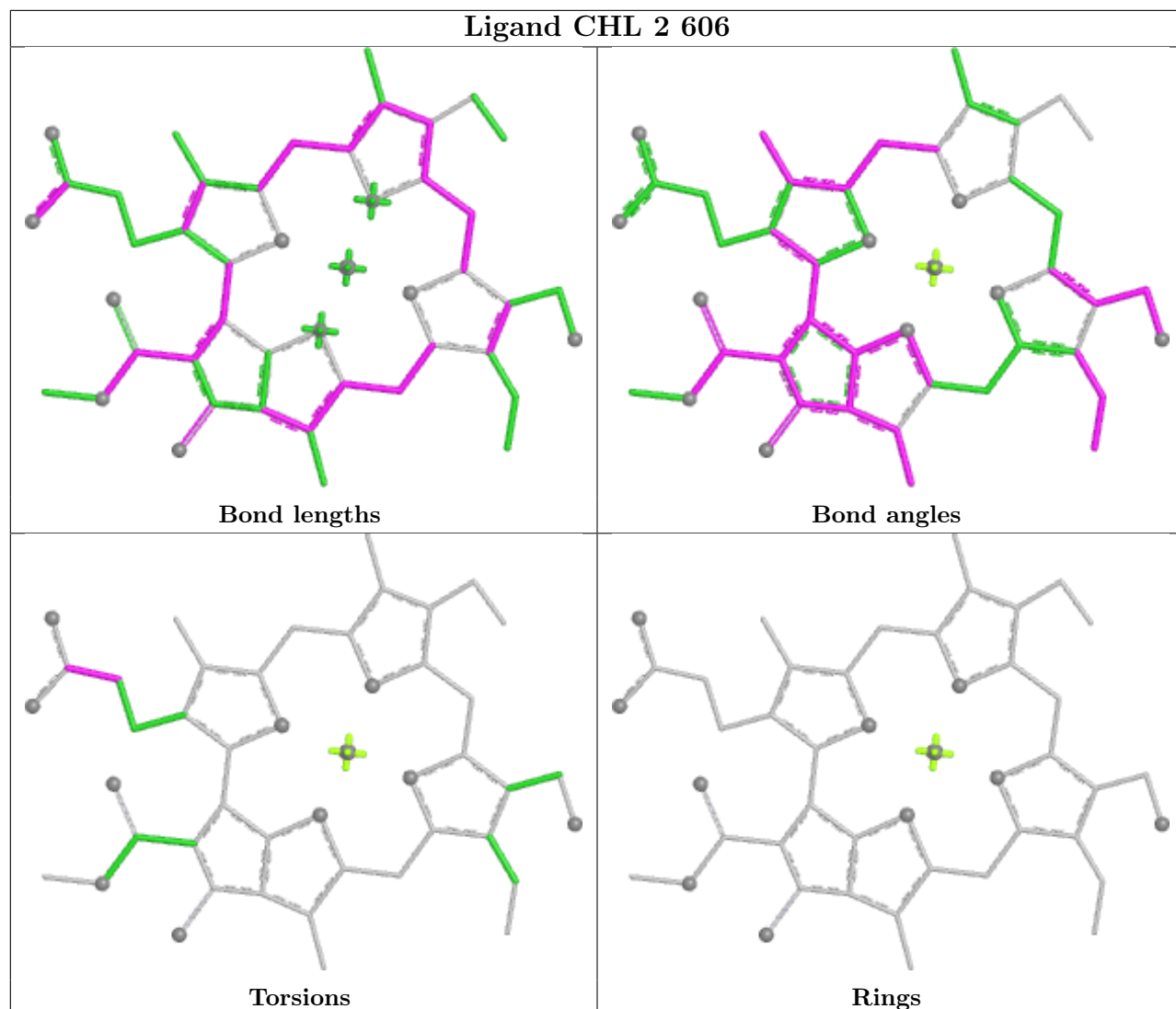


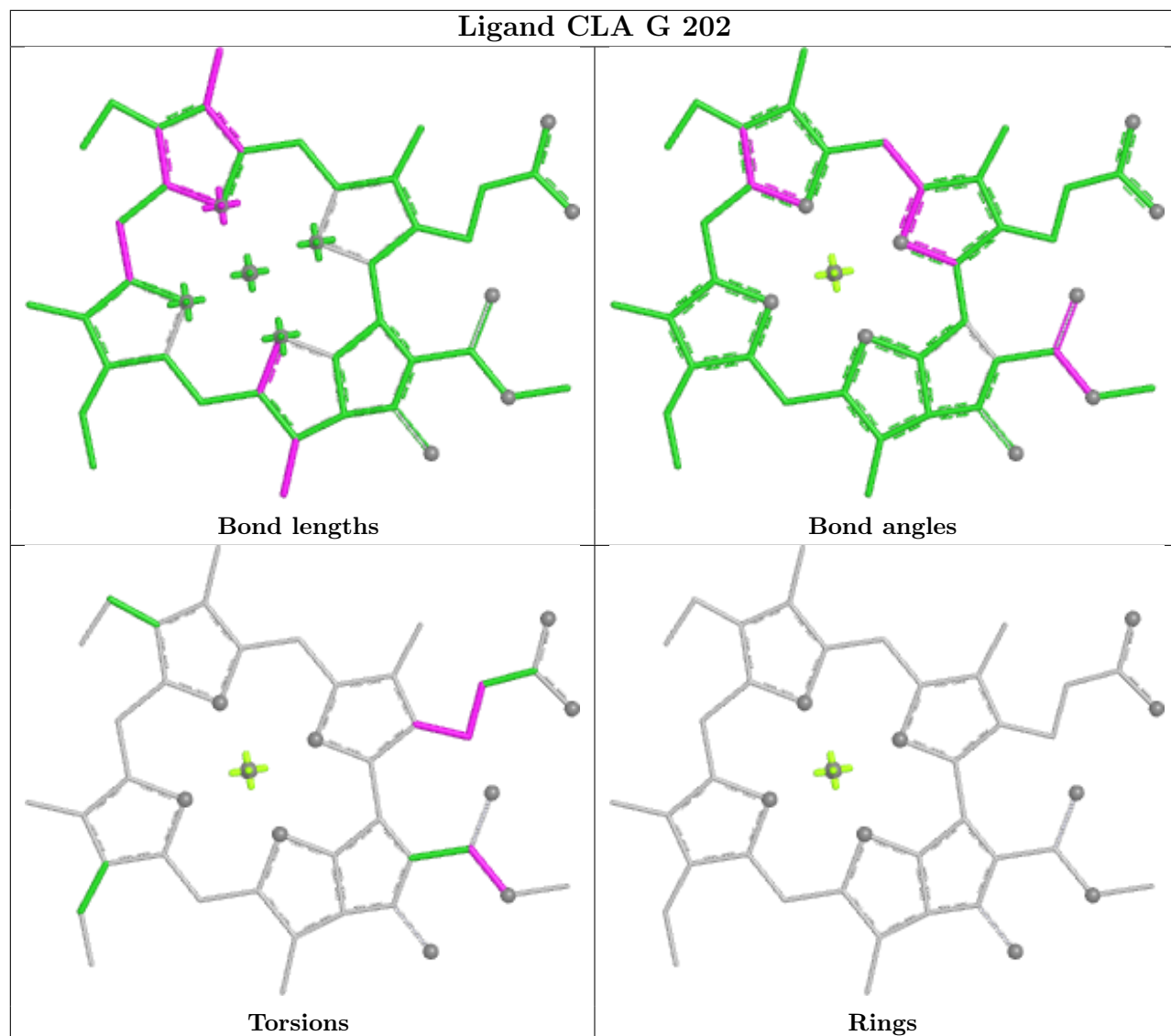
Torsions

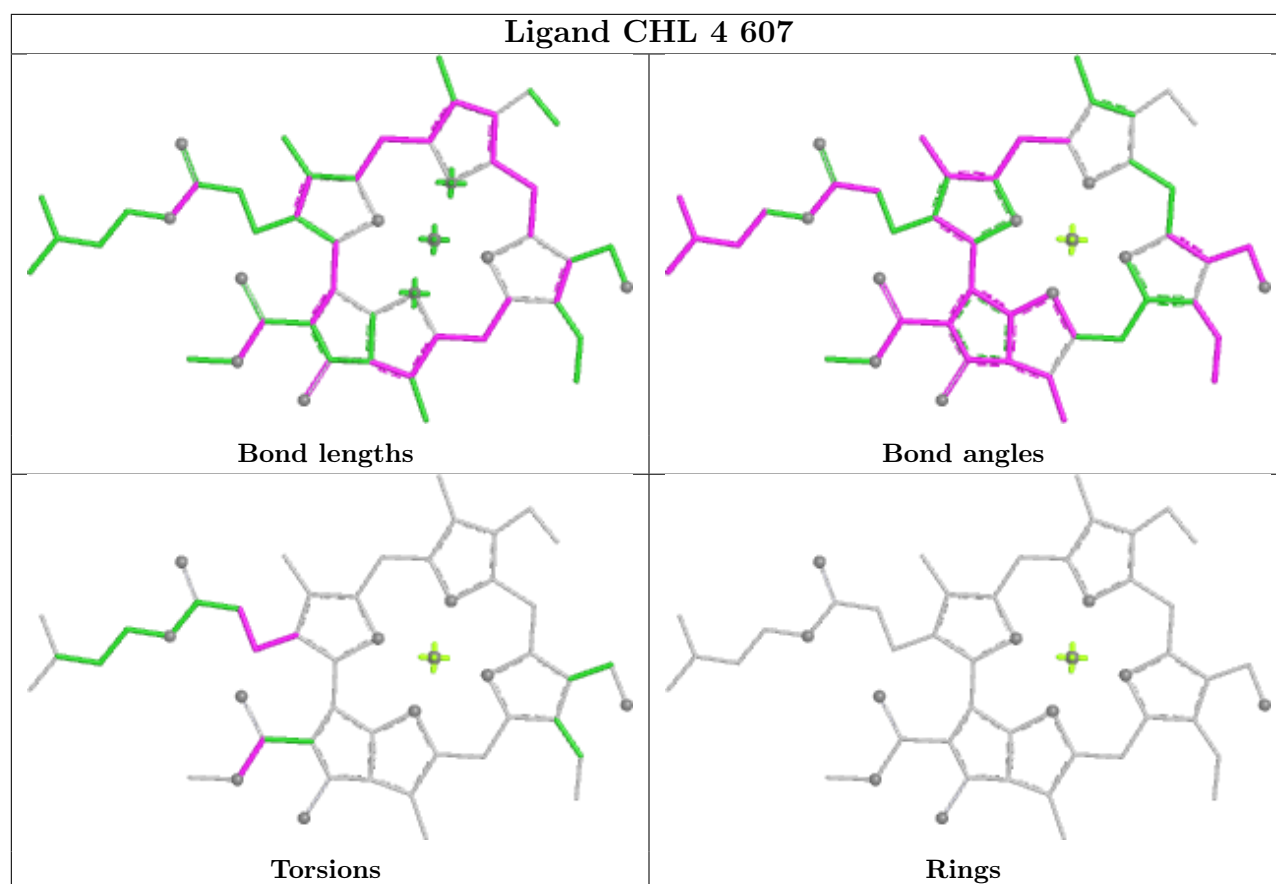


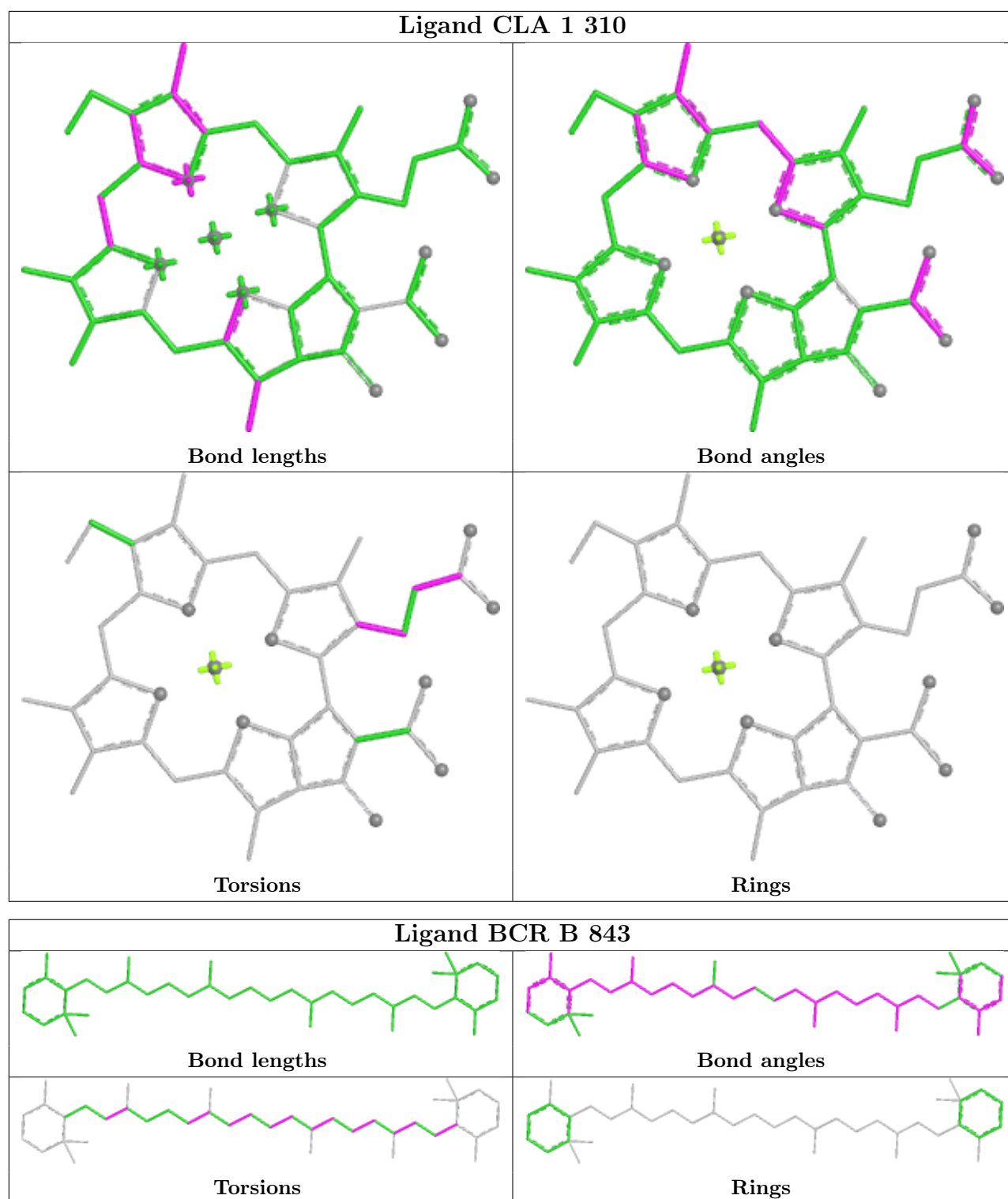
Rings

Ligand CHL 2 606

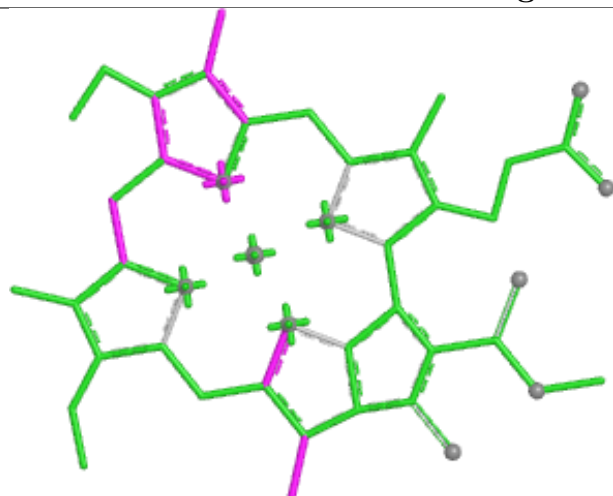




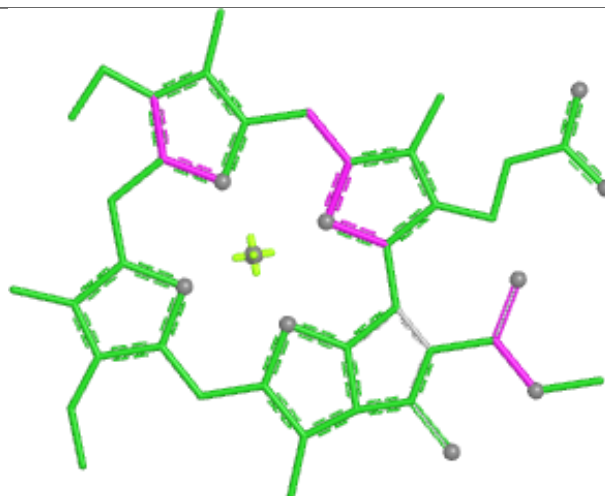




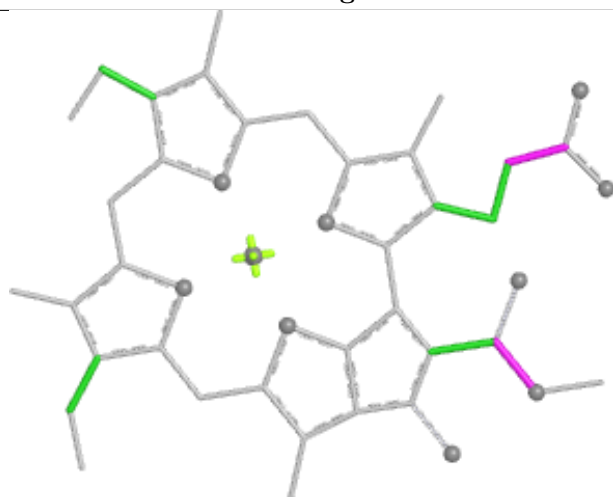
Ligand CLA b 304



Bond lengths



Bond angles

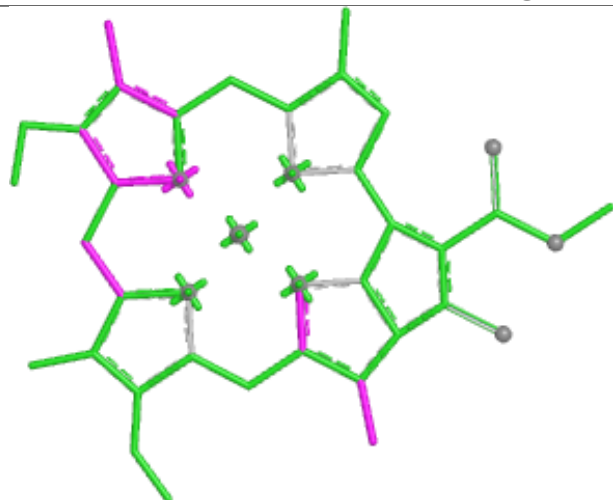


Torsions

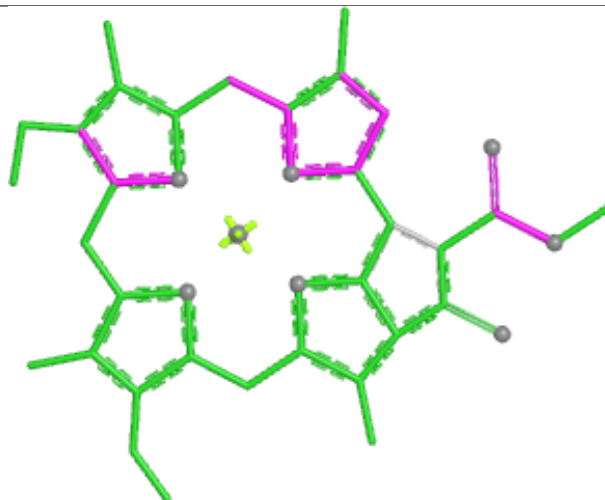


Rings

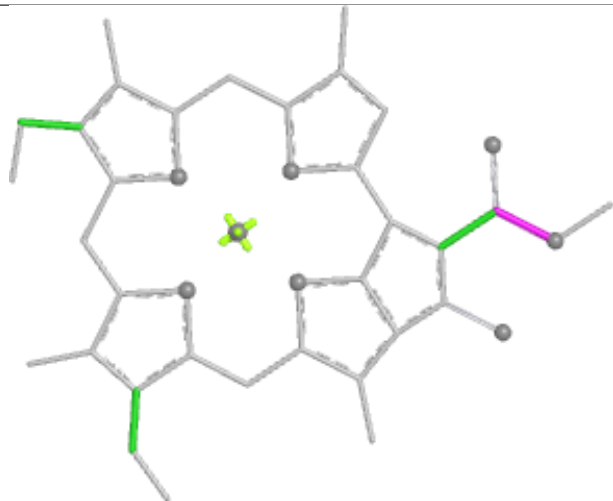
Ligand CLA 1 306



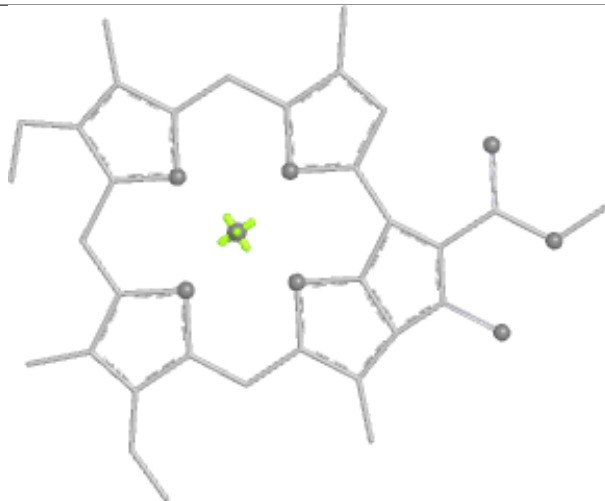
Bond lengths



Bond angles

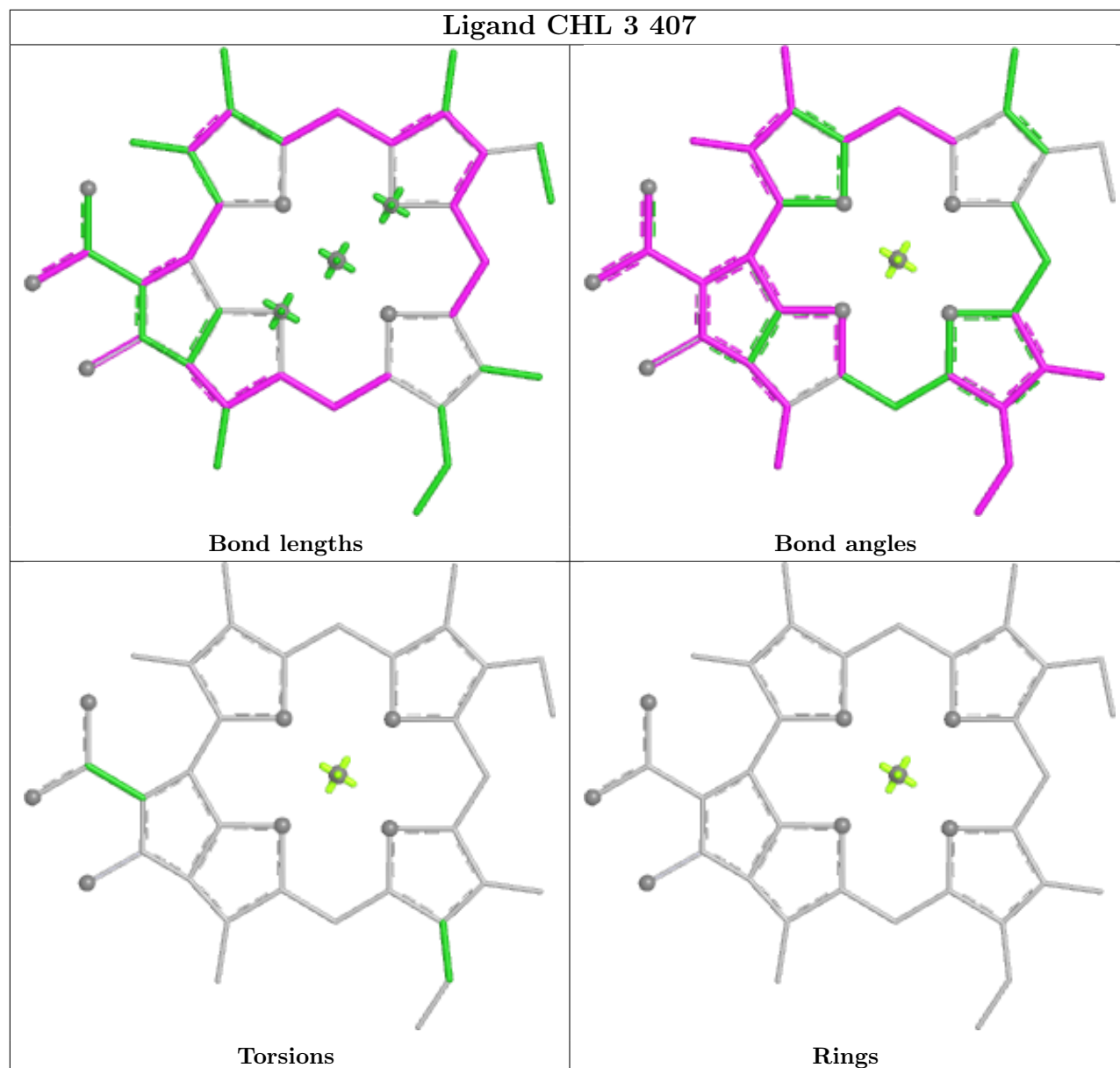


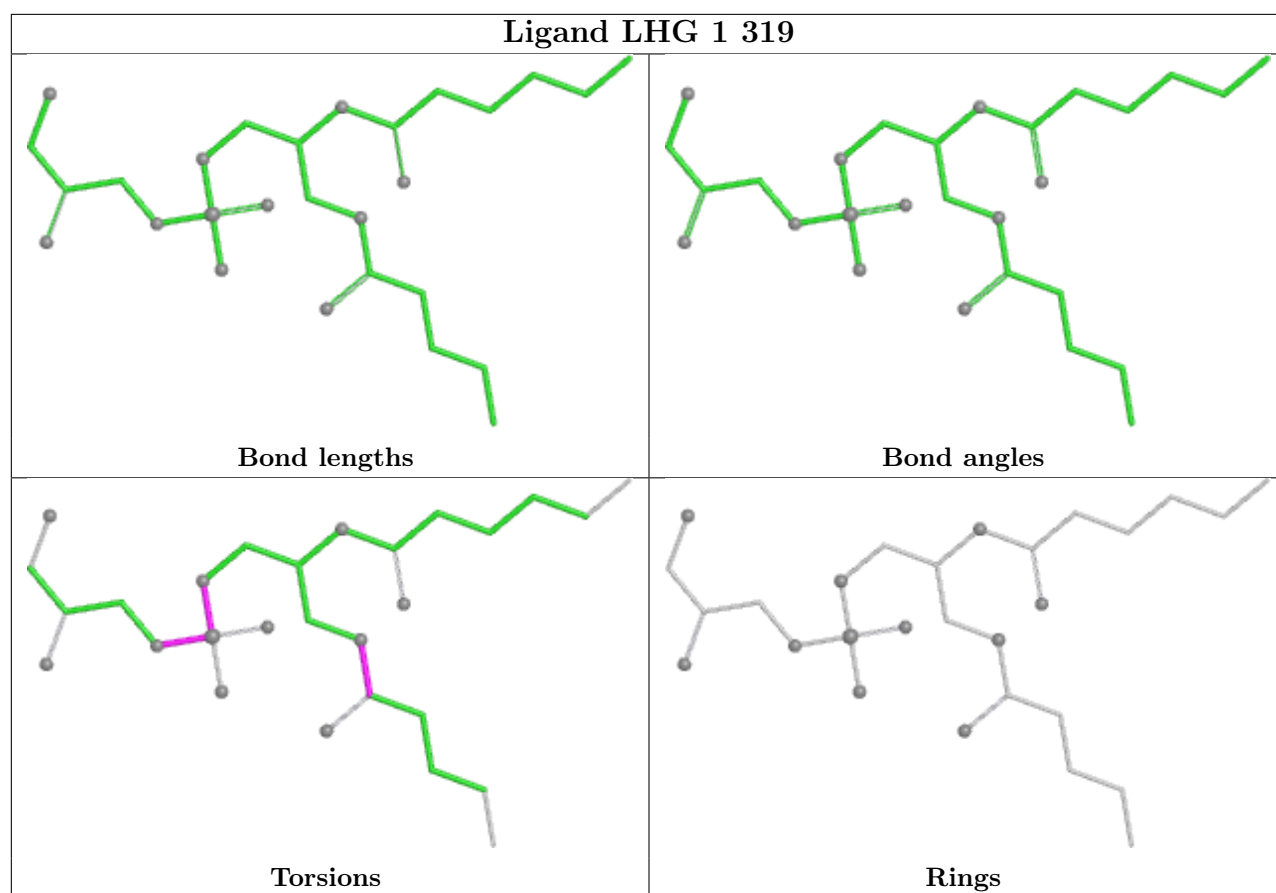
Torsions



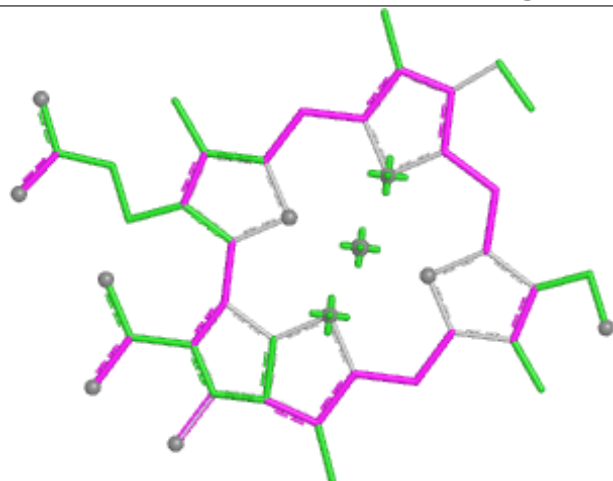
Rings

Ligand CHL 3 407

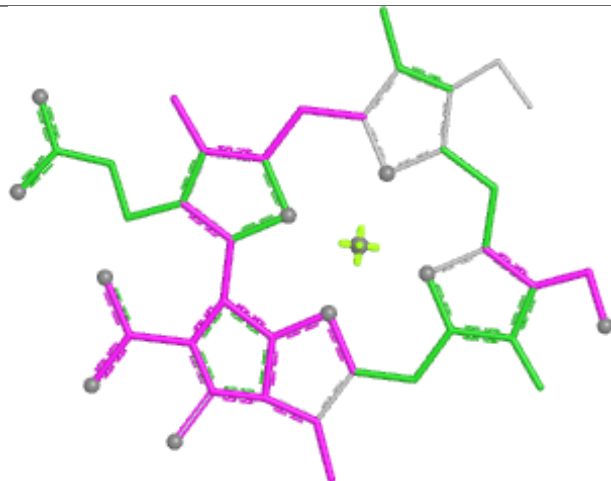




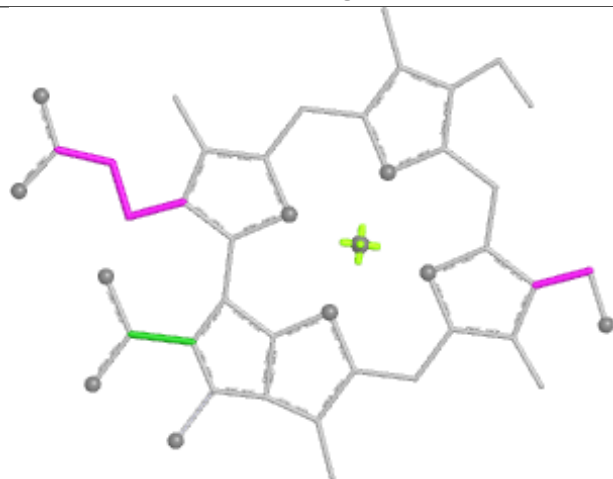
Ligand CHL c 609



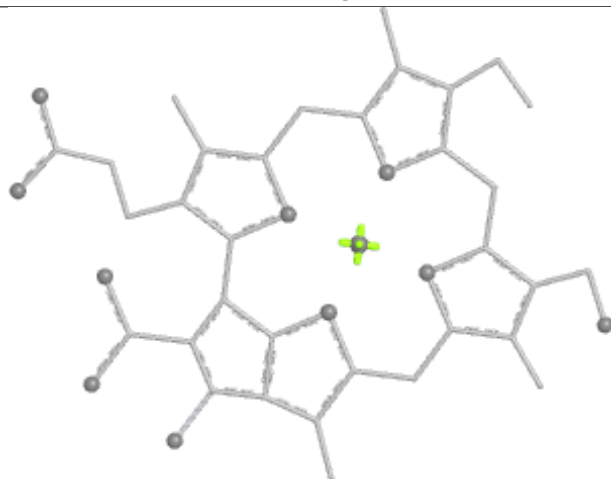
Bond lengths



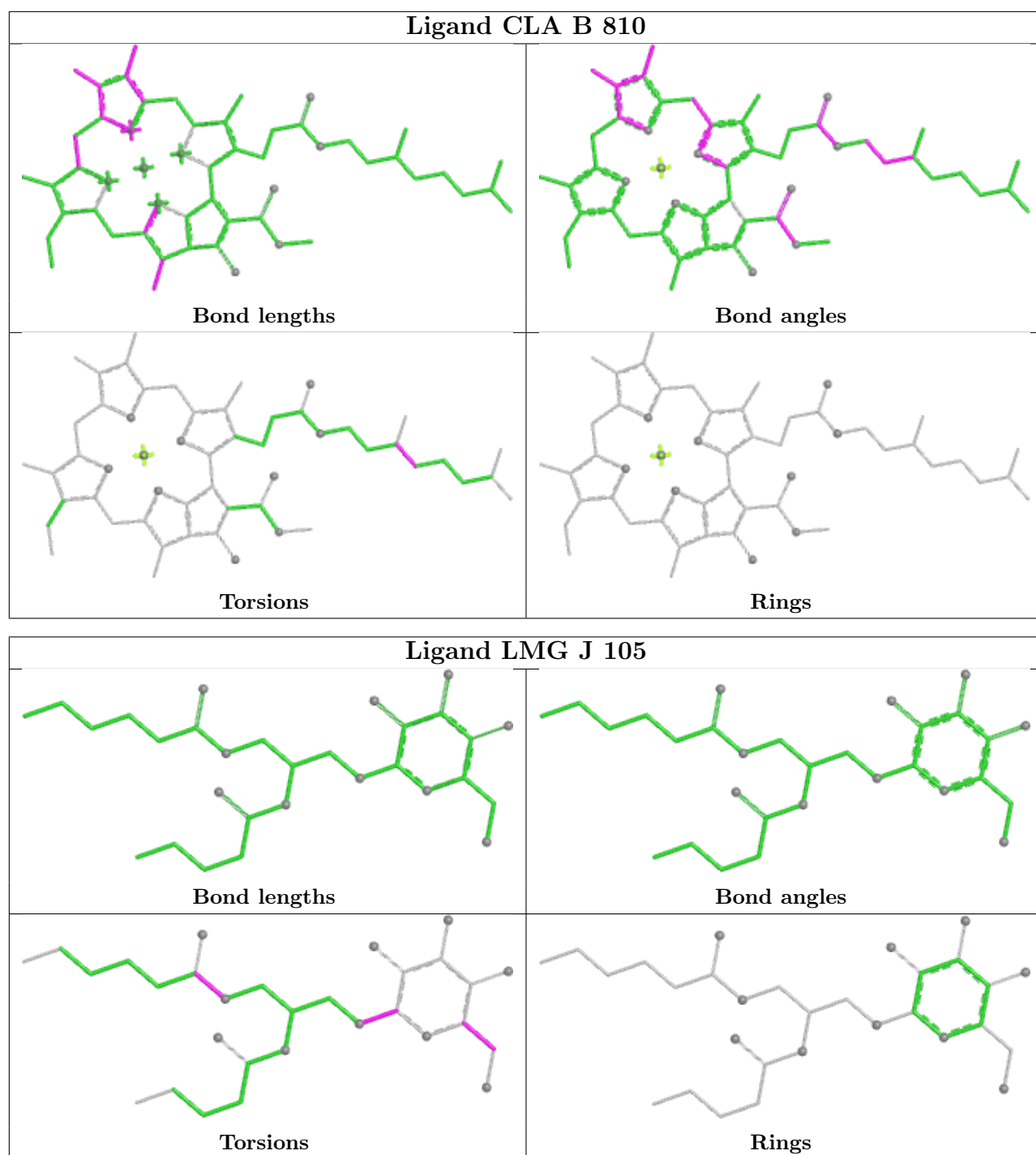
Bond angles

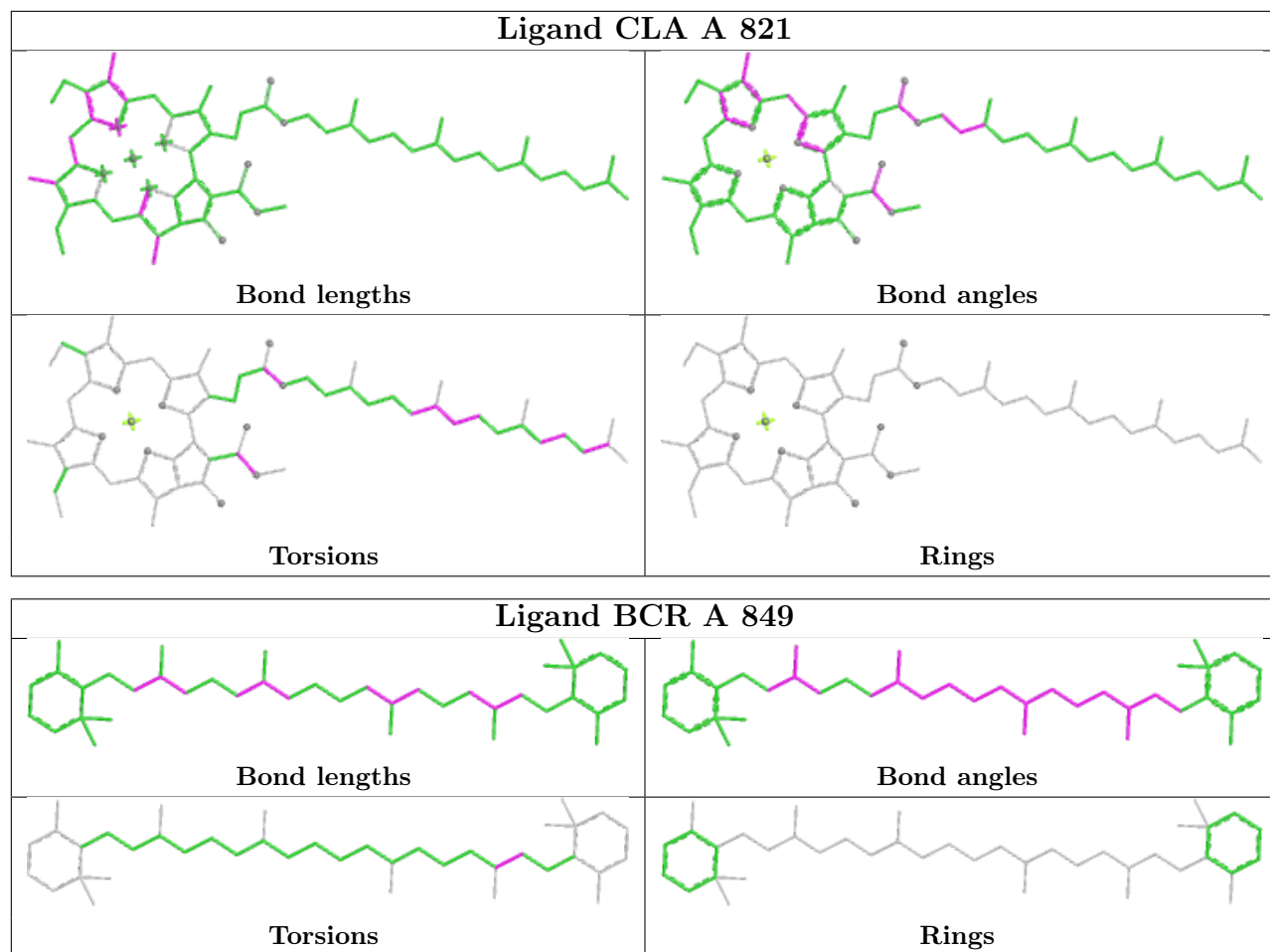


Torsions

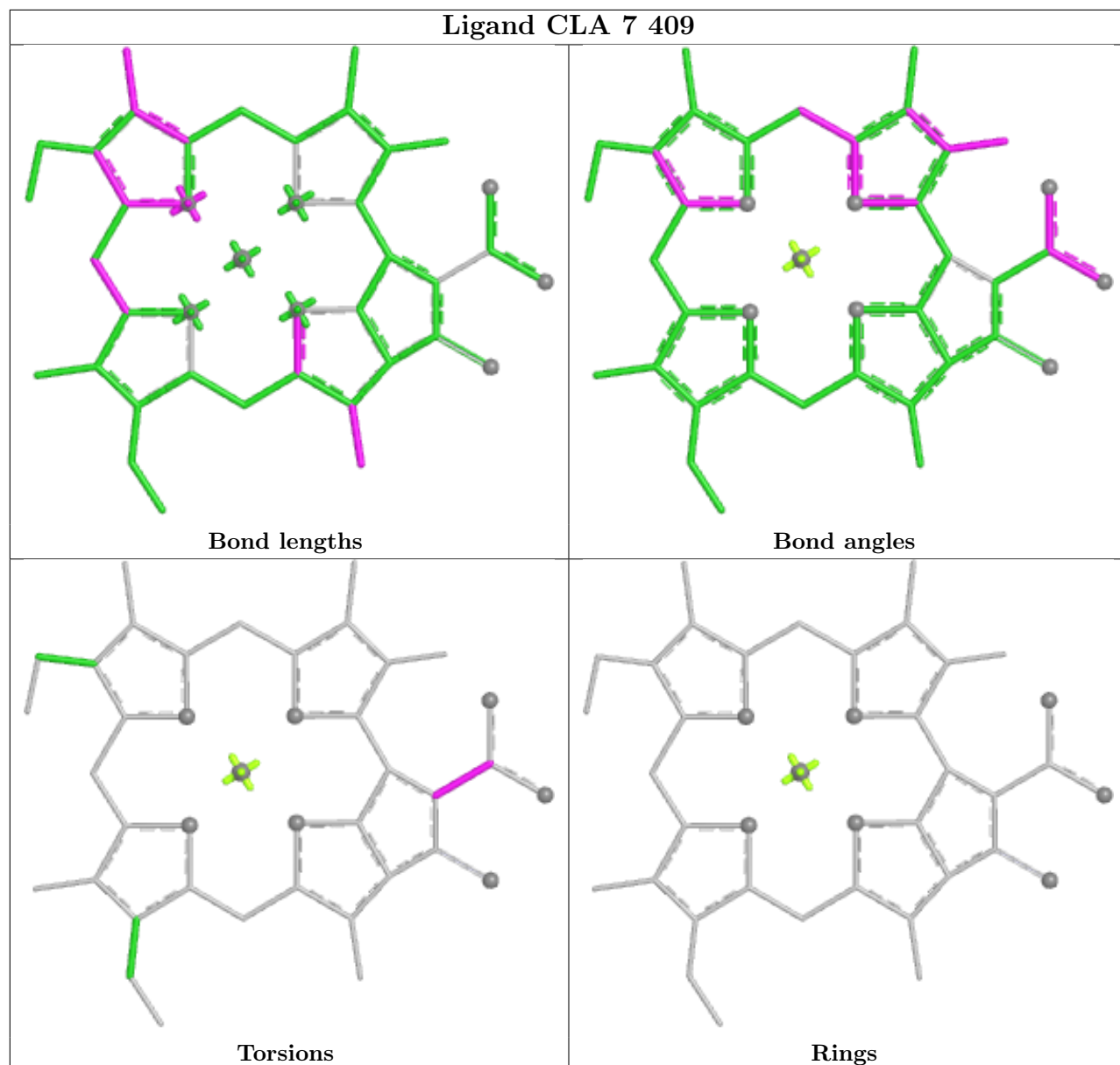


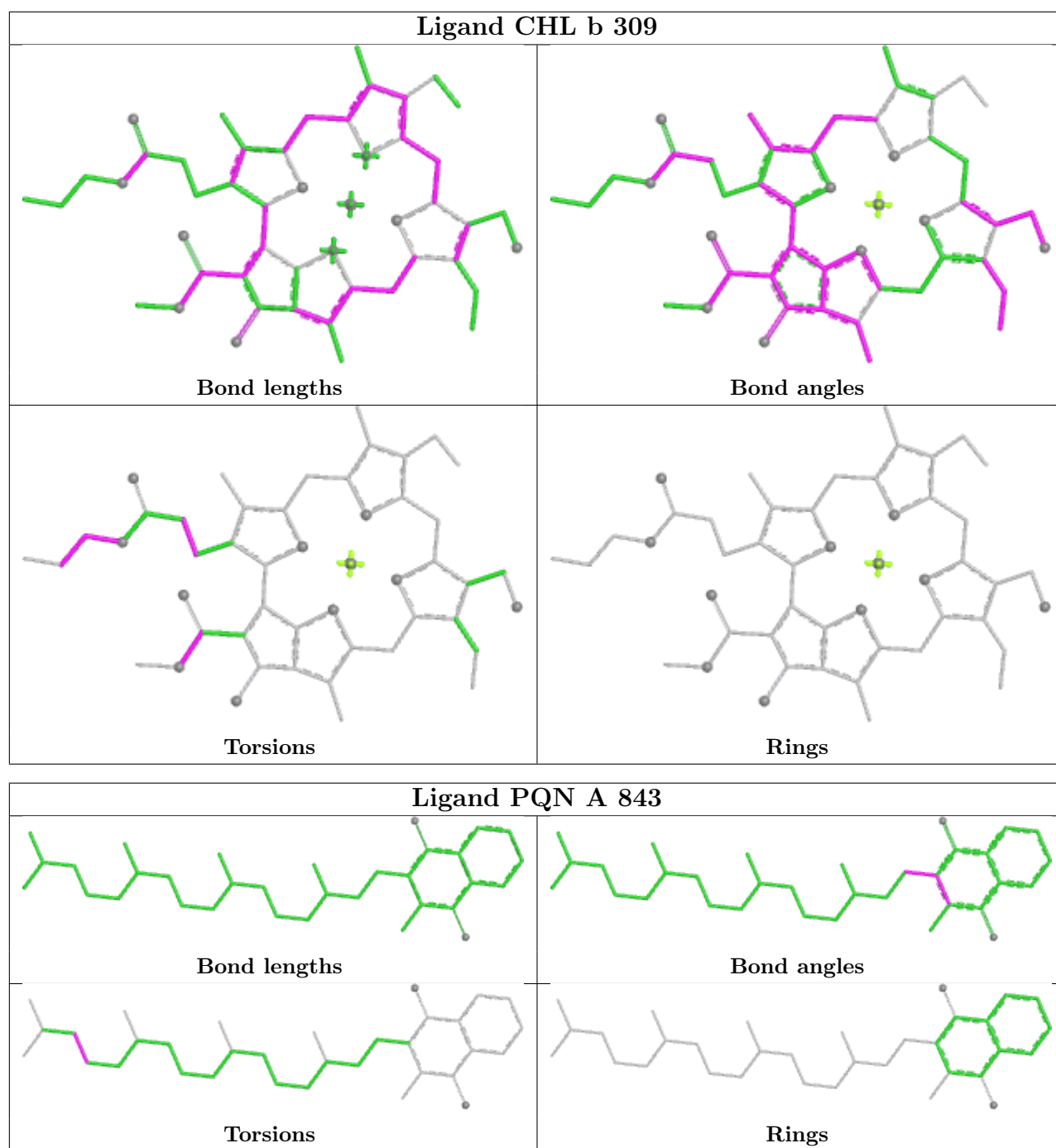
Rings



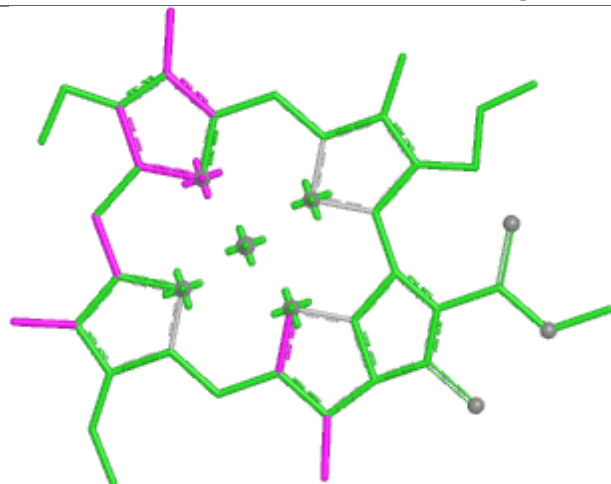


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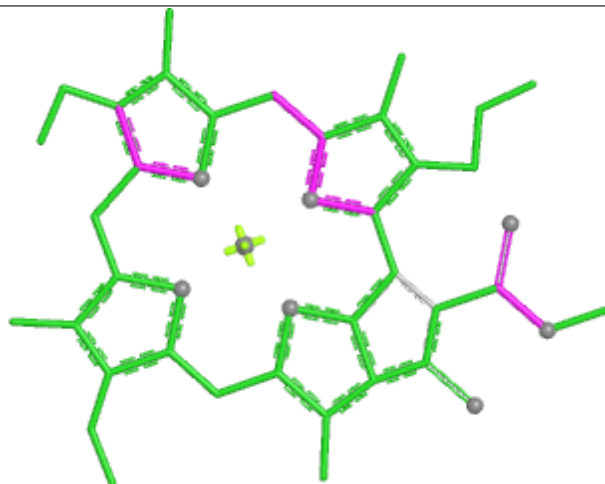




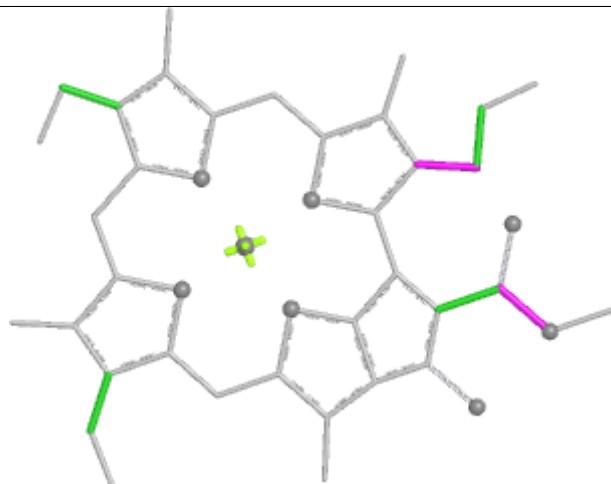
Ligand CLA B 819



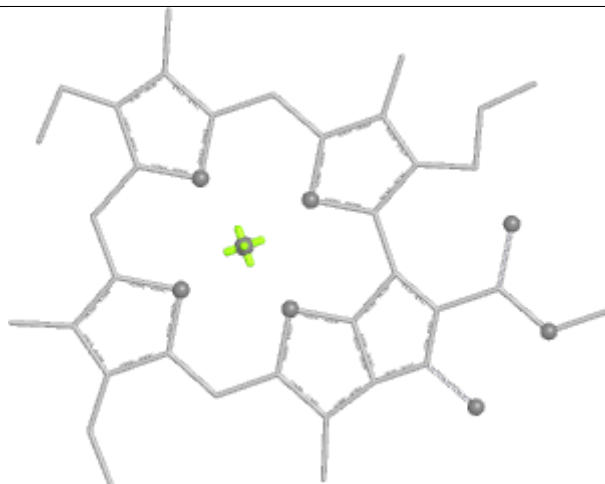
Bond lengths



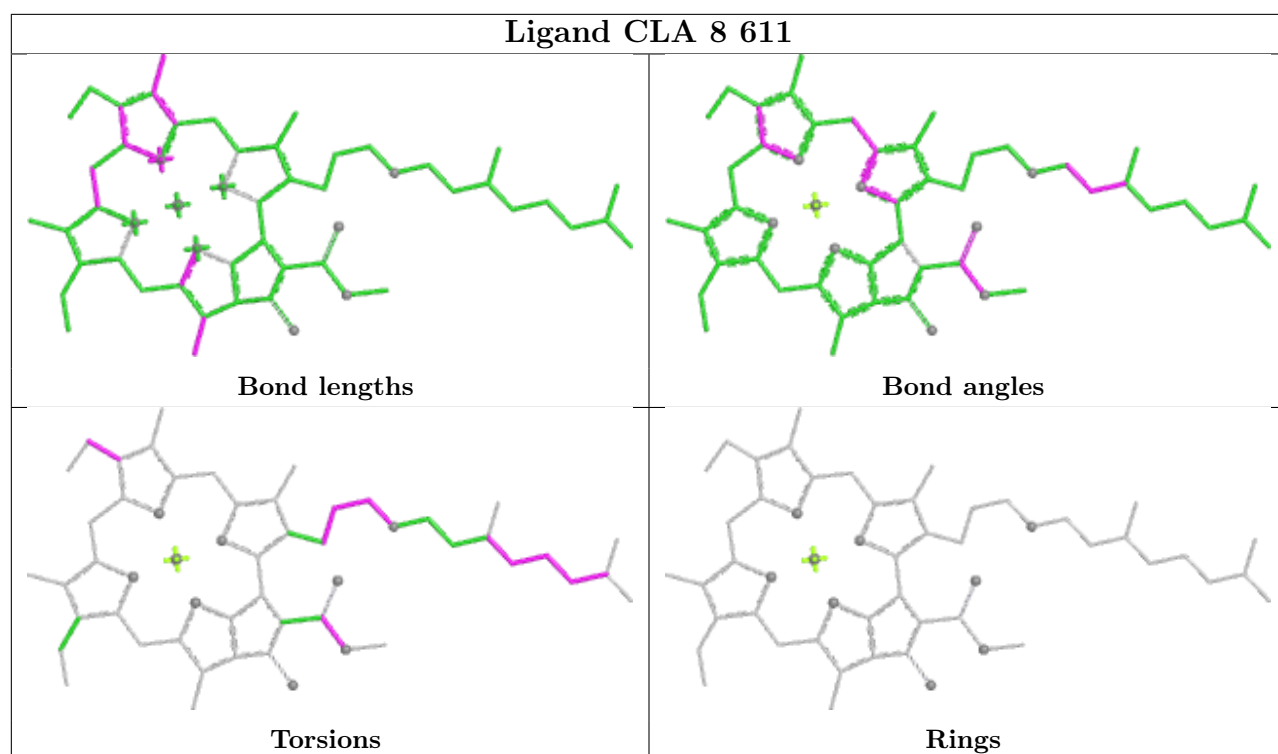
Bond angles



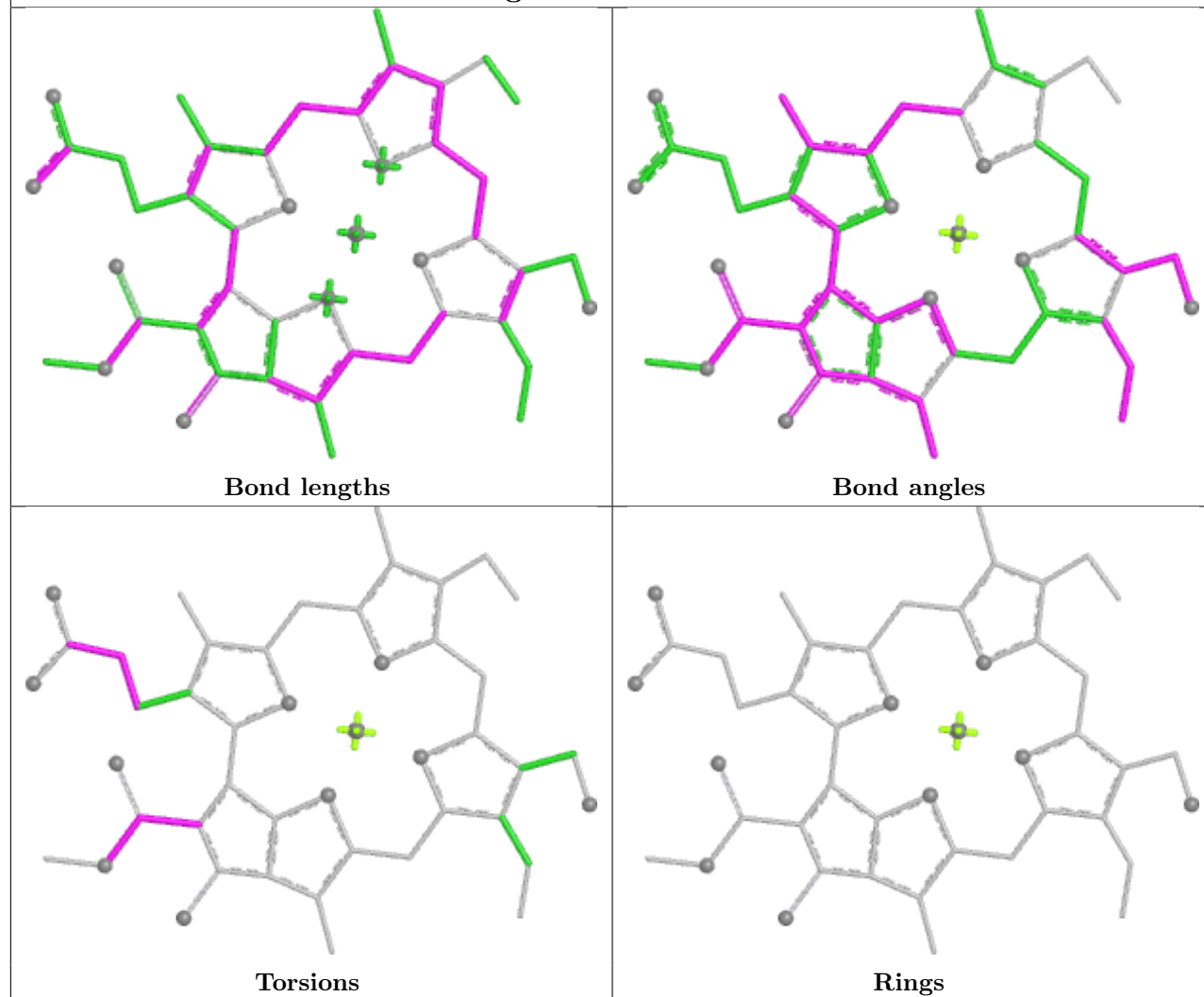
Torsions



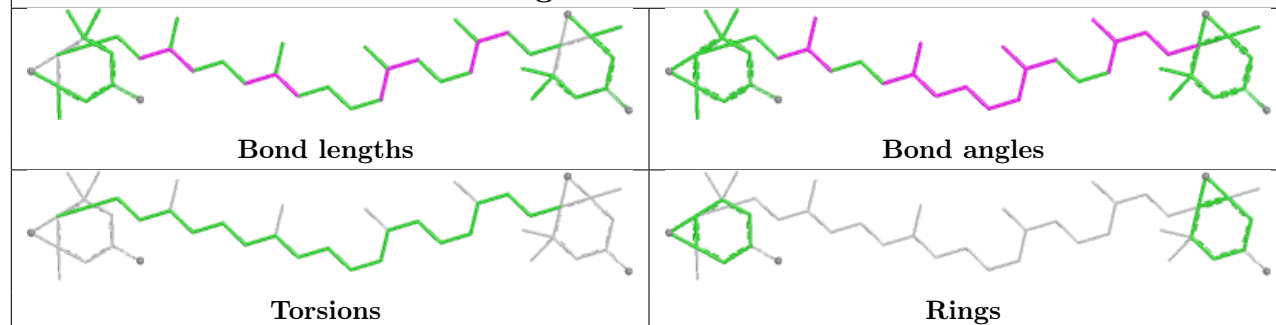
Rings



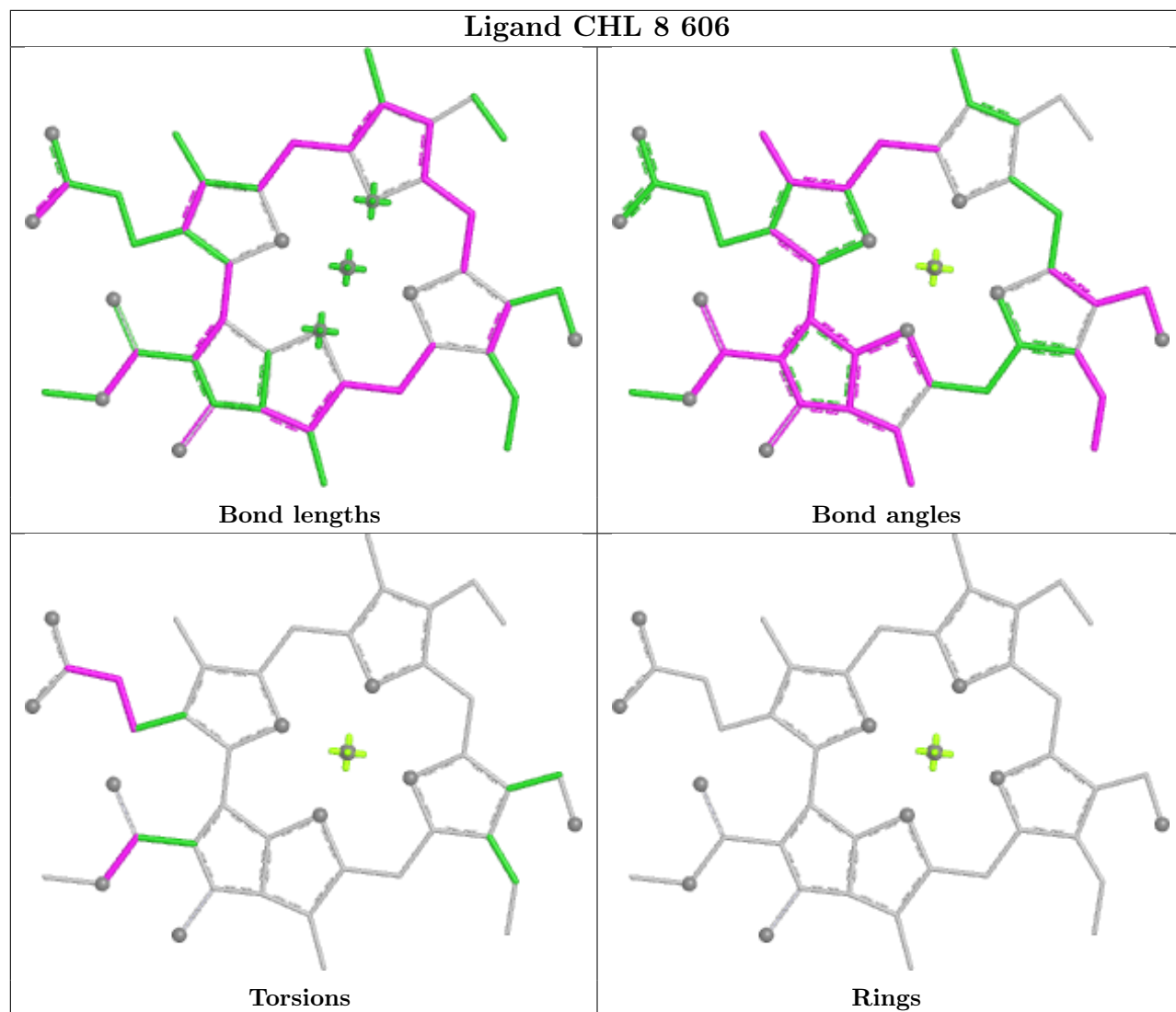
Ligand CHL 6 606



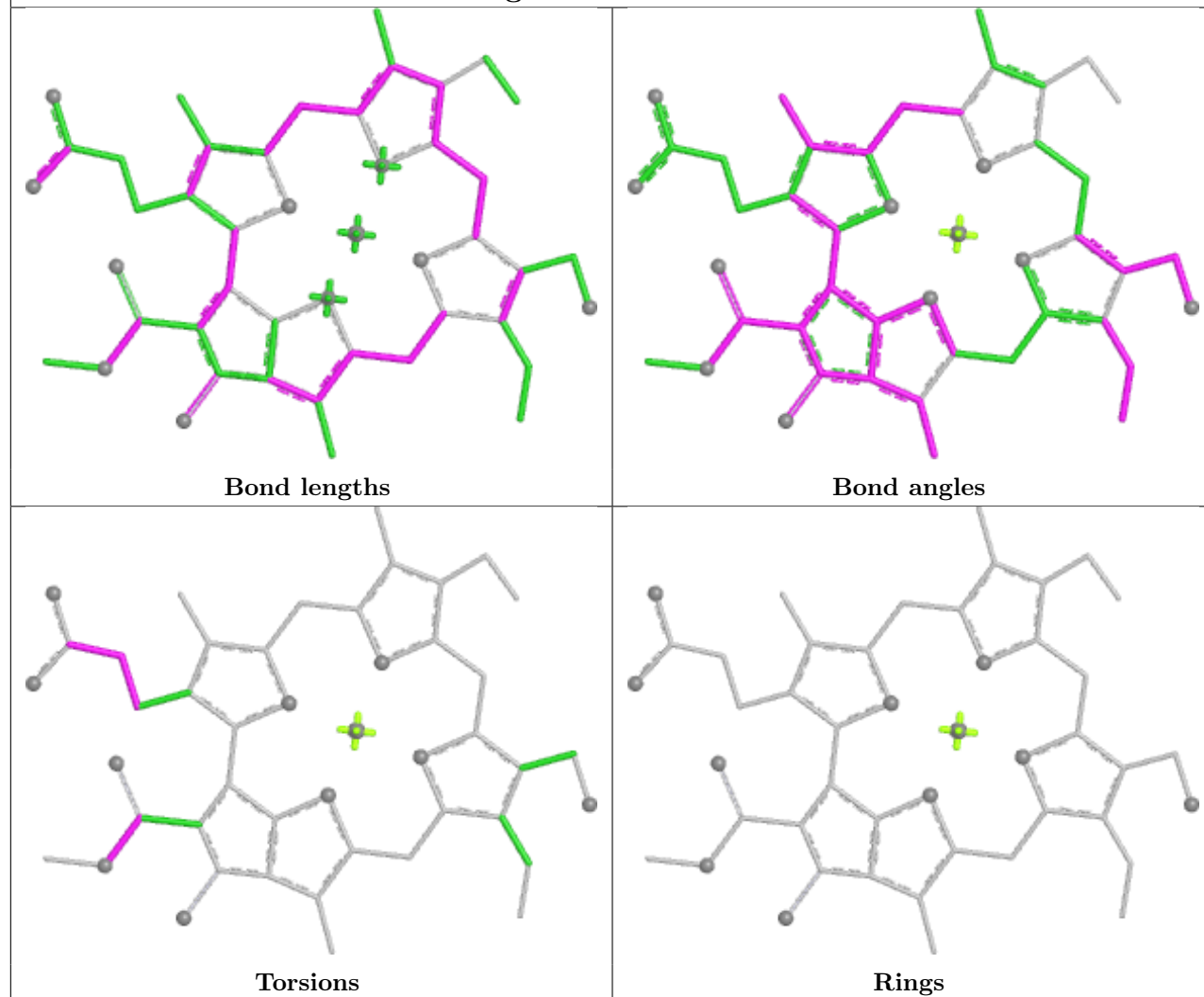
Ligand XAT 2 617



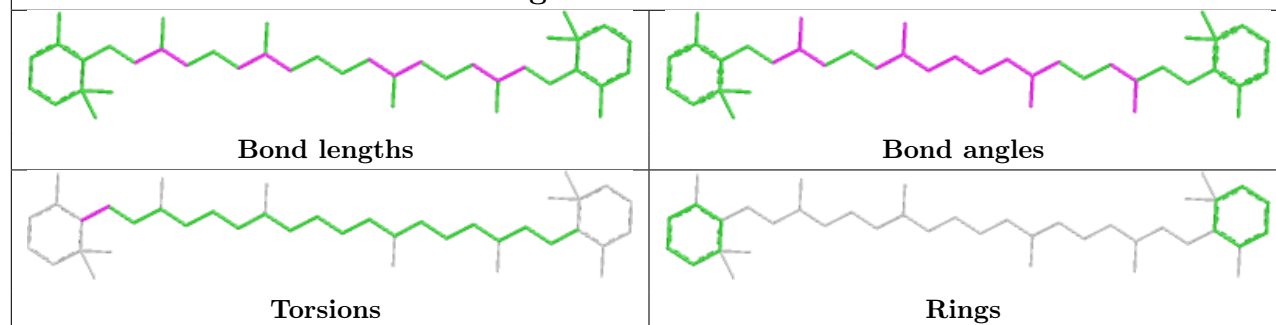
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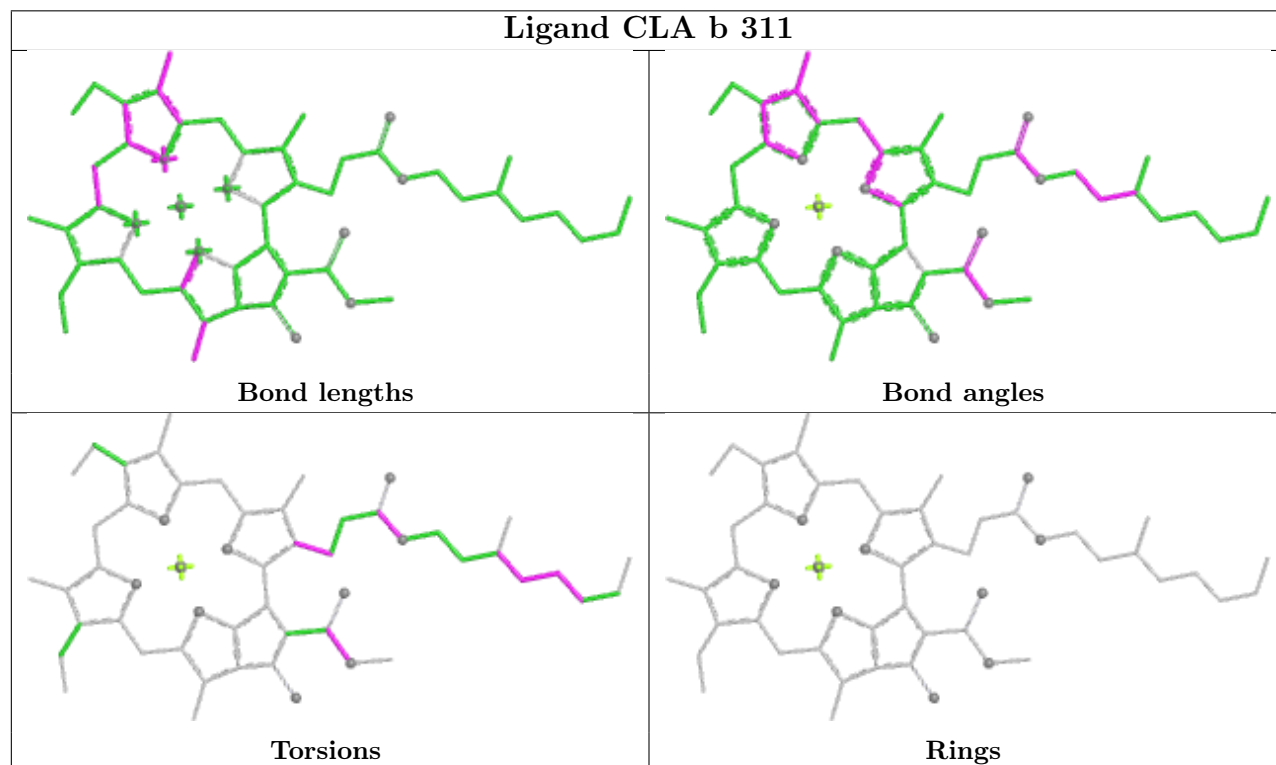
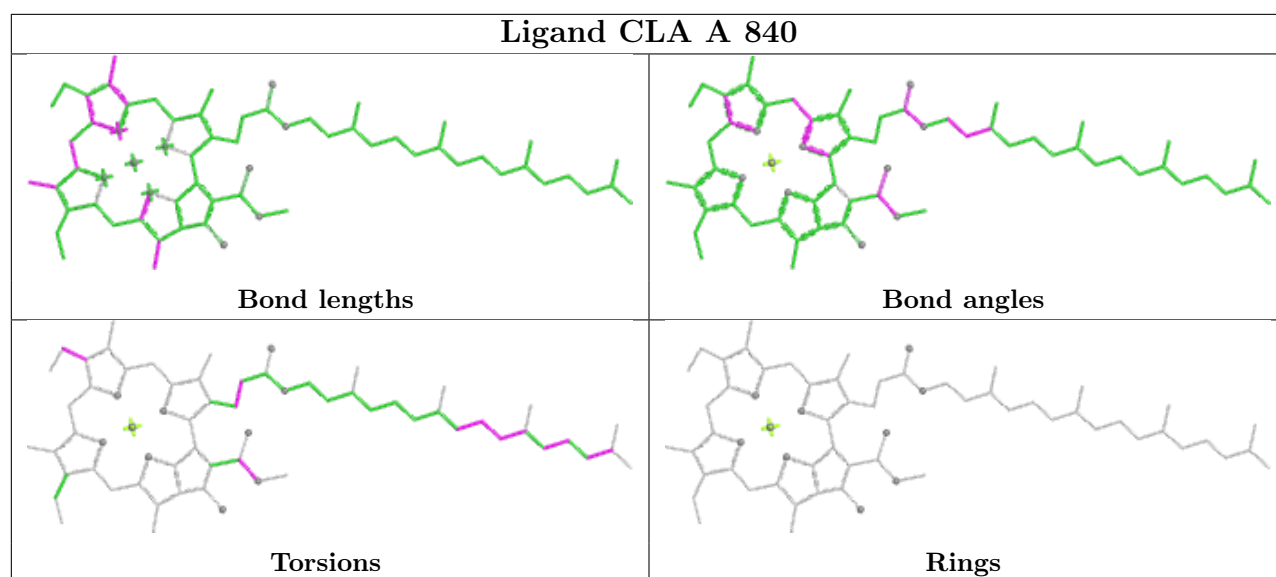


Ligand CHL 9 608

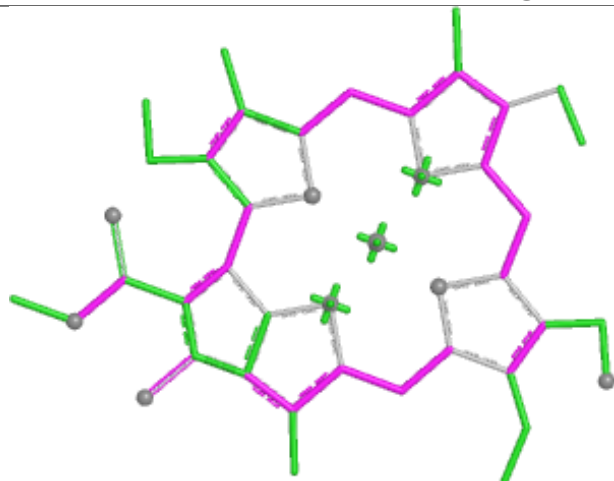


Ligand BCR G 205

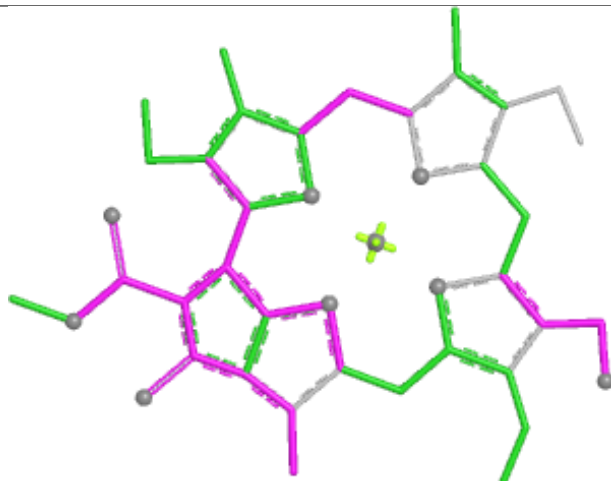




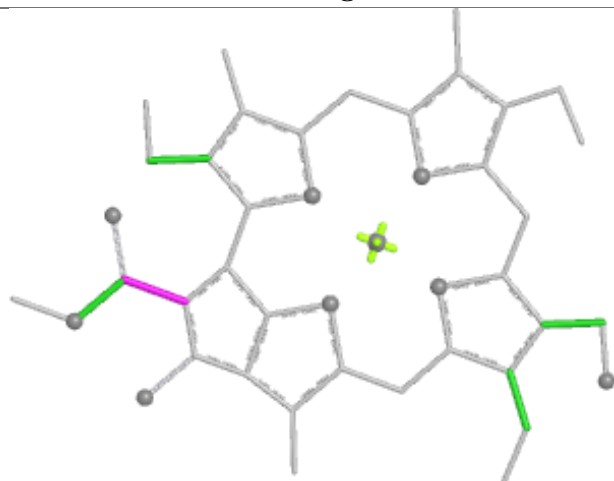
Ligand CHL a 607



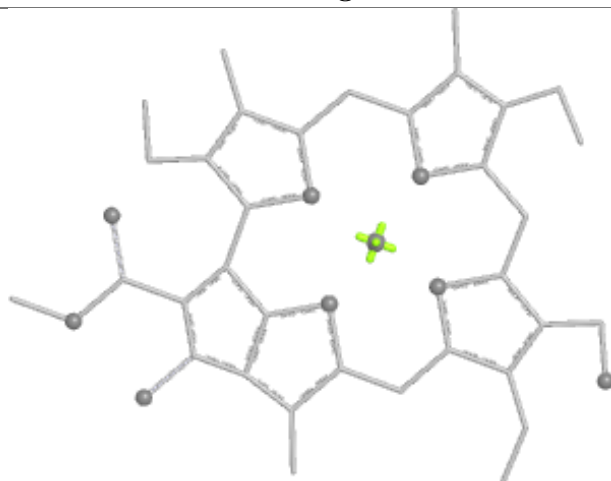
Bond lengths



Bond angles

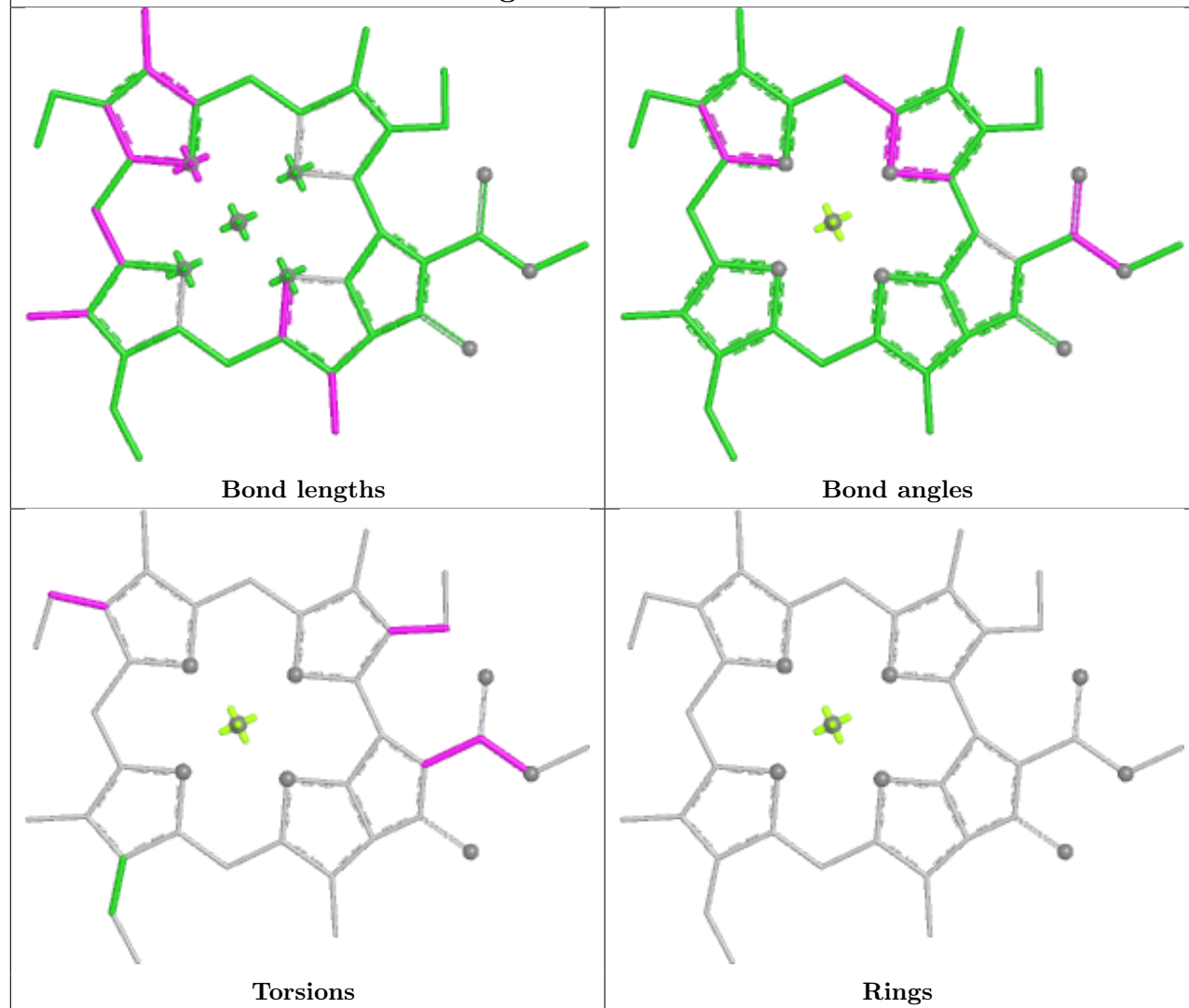


Torsions

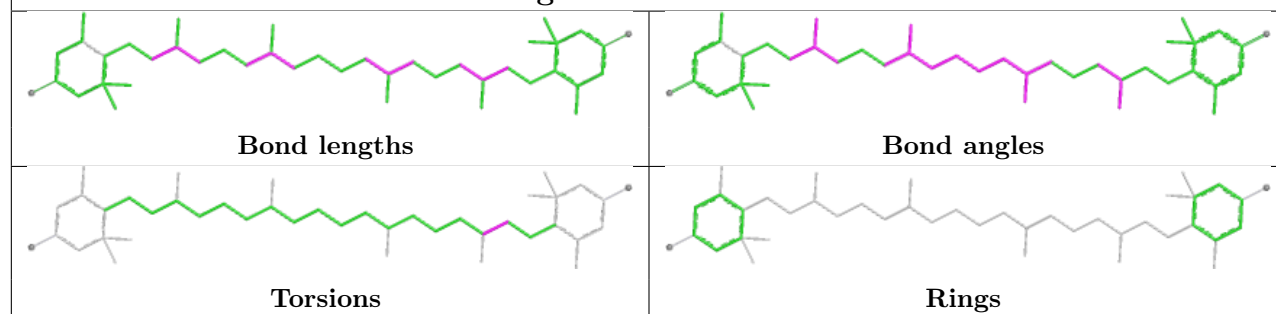


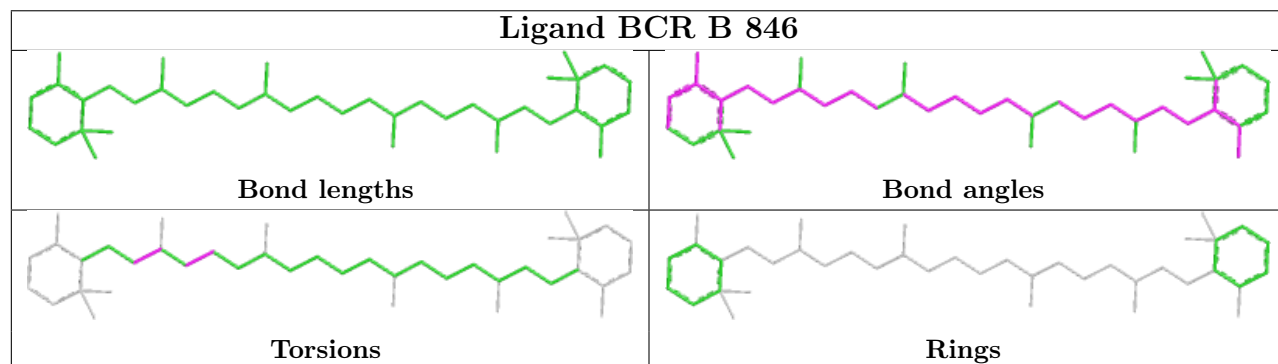
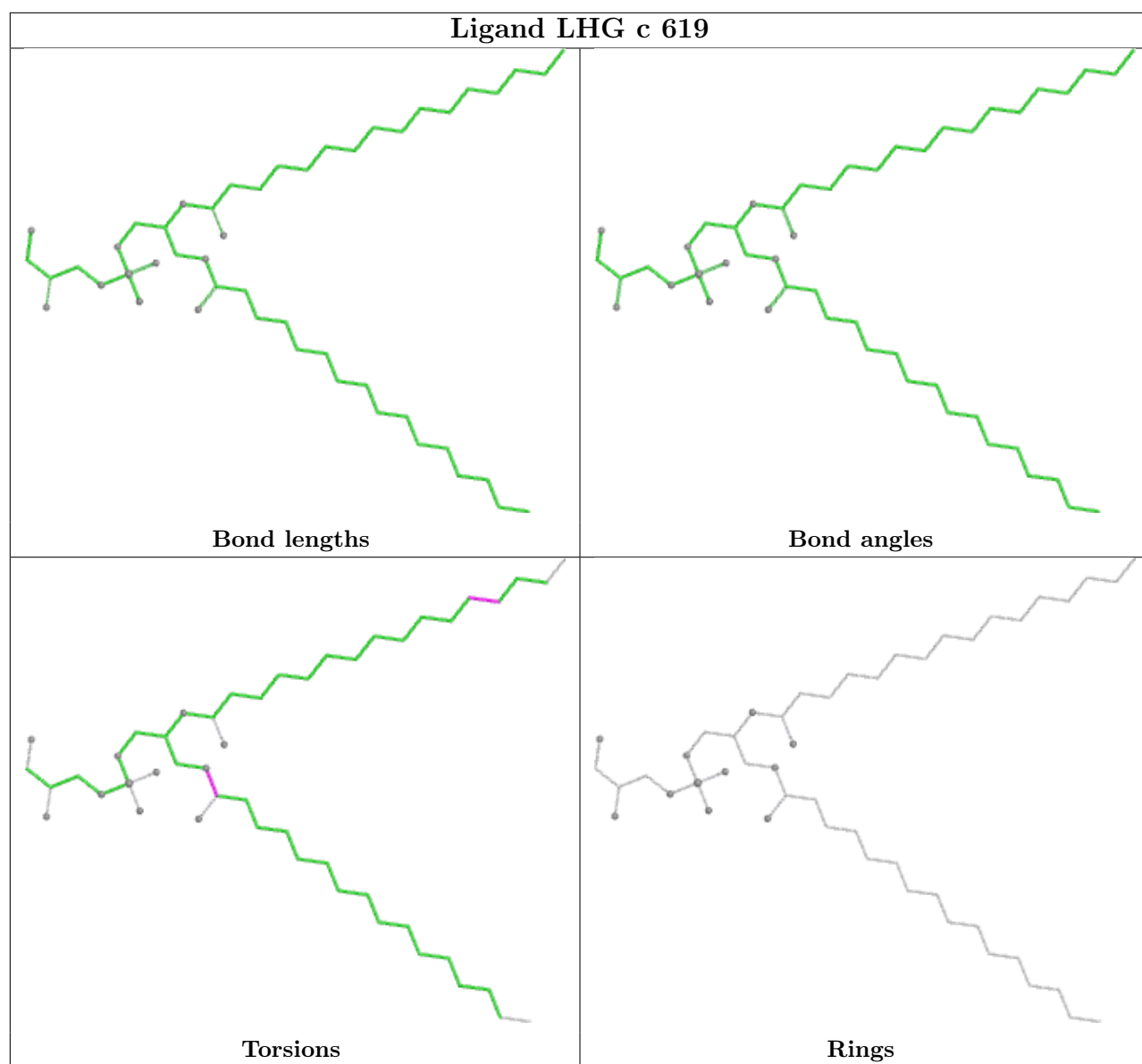
Rings

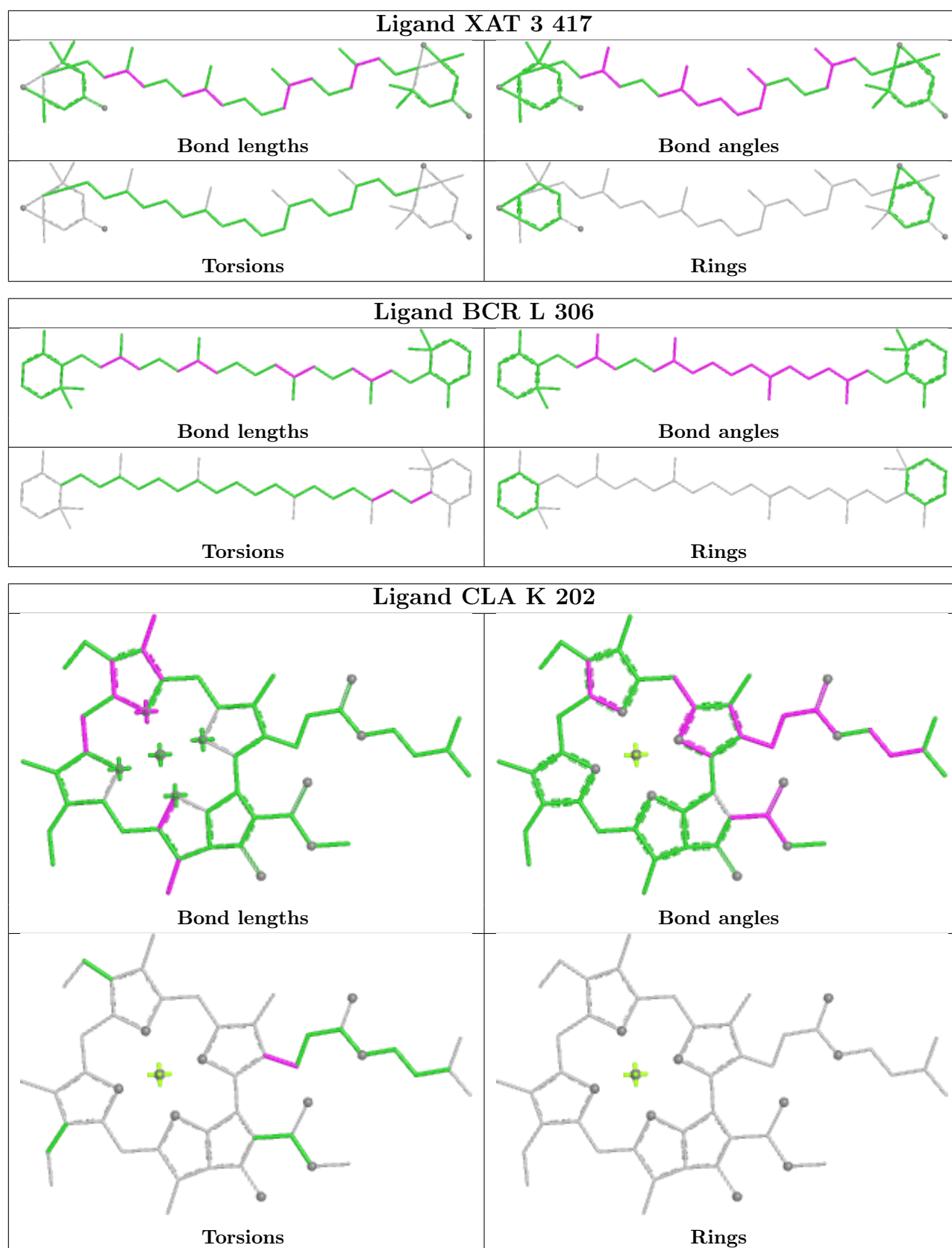
Ligand CLA J 102

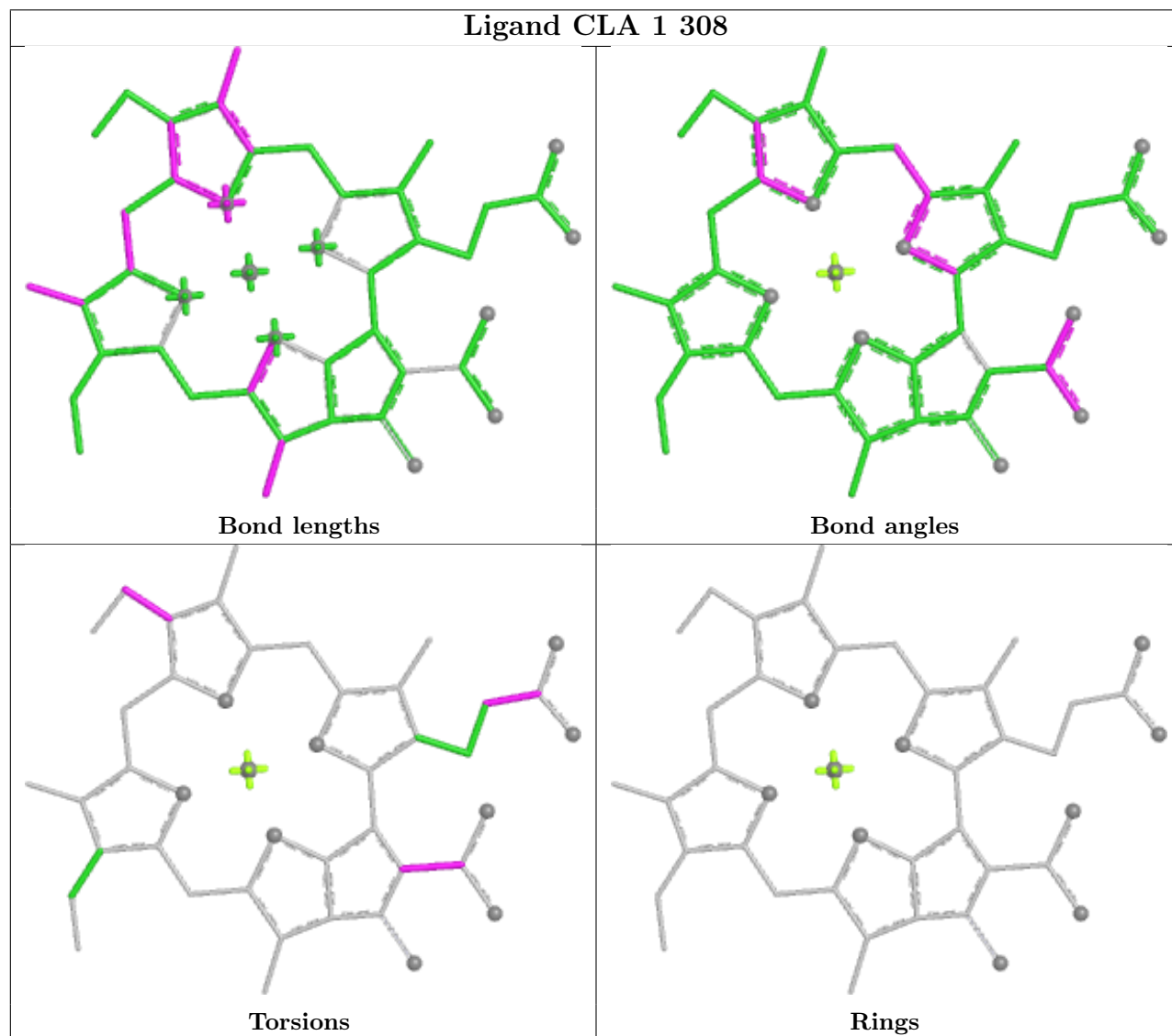
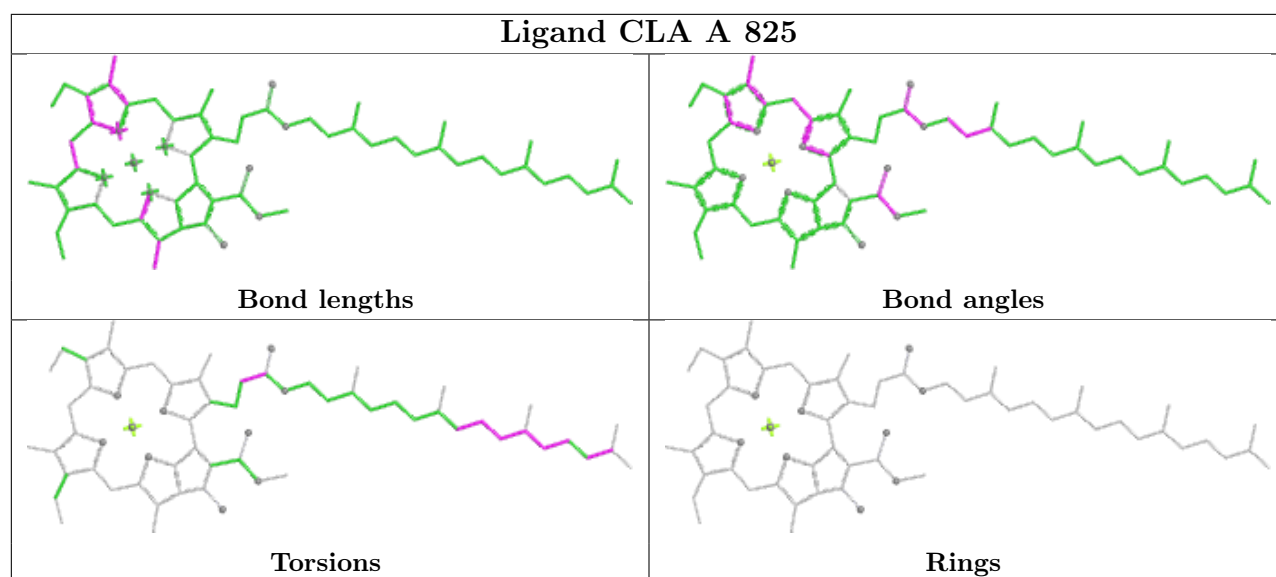


Ligand LUT a 616

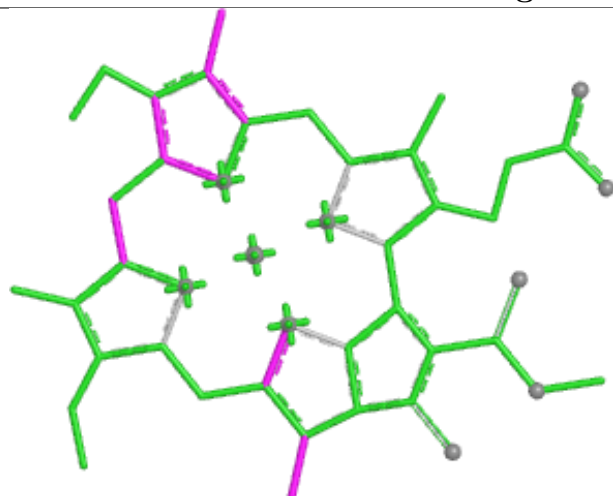




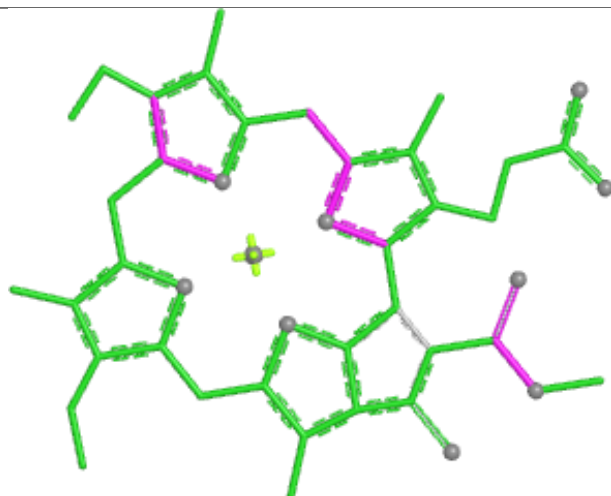




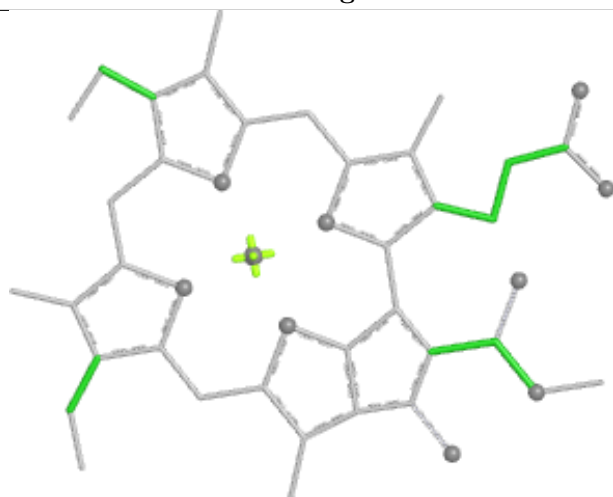
Ligand CLA F 304



Bond lengths



Bond angles

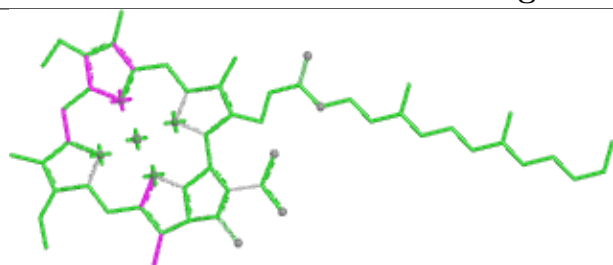


Torsions

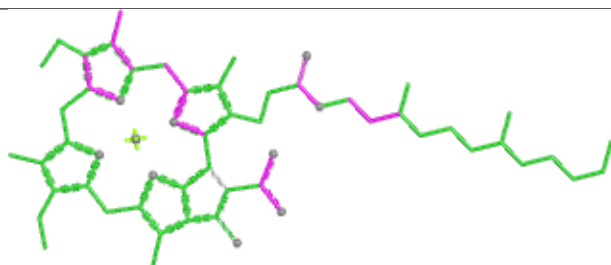


Rings

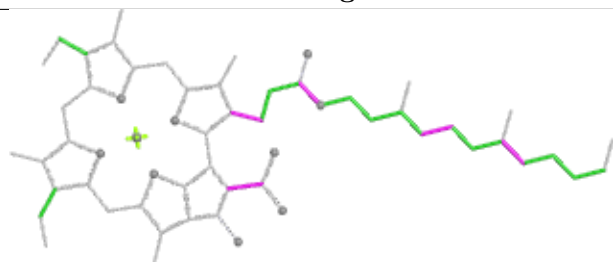
Ligand CLA 8 602



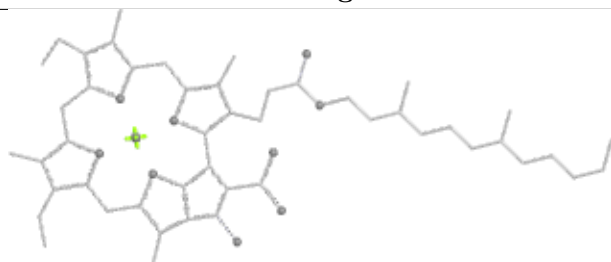
Bond lengths



Bond angles

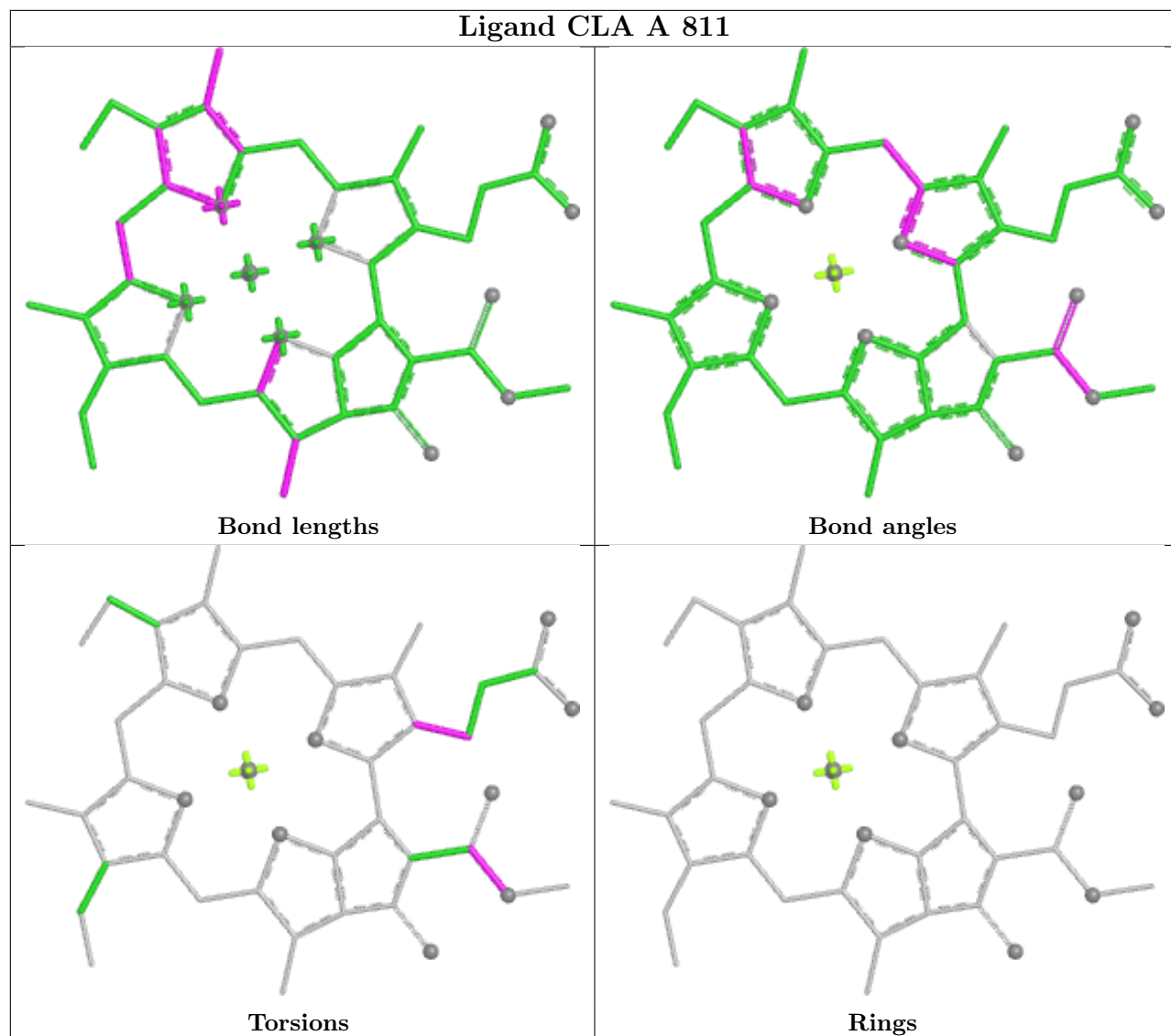


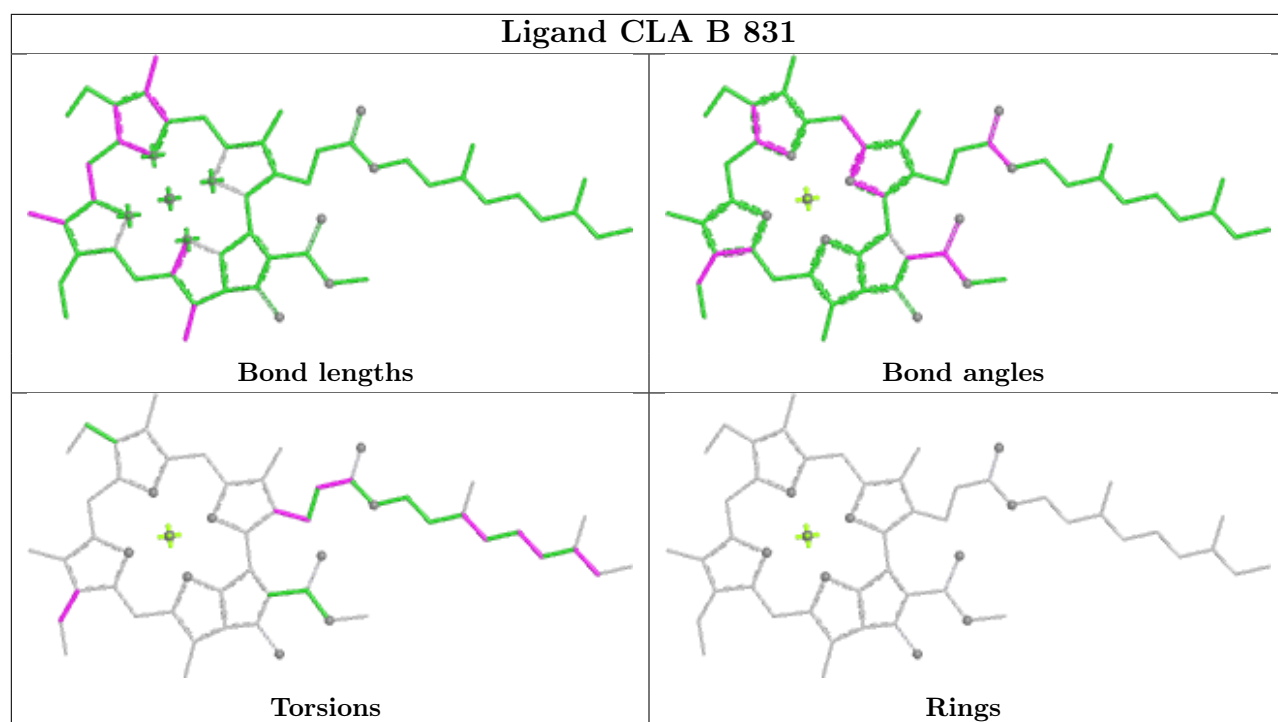
Torsions

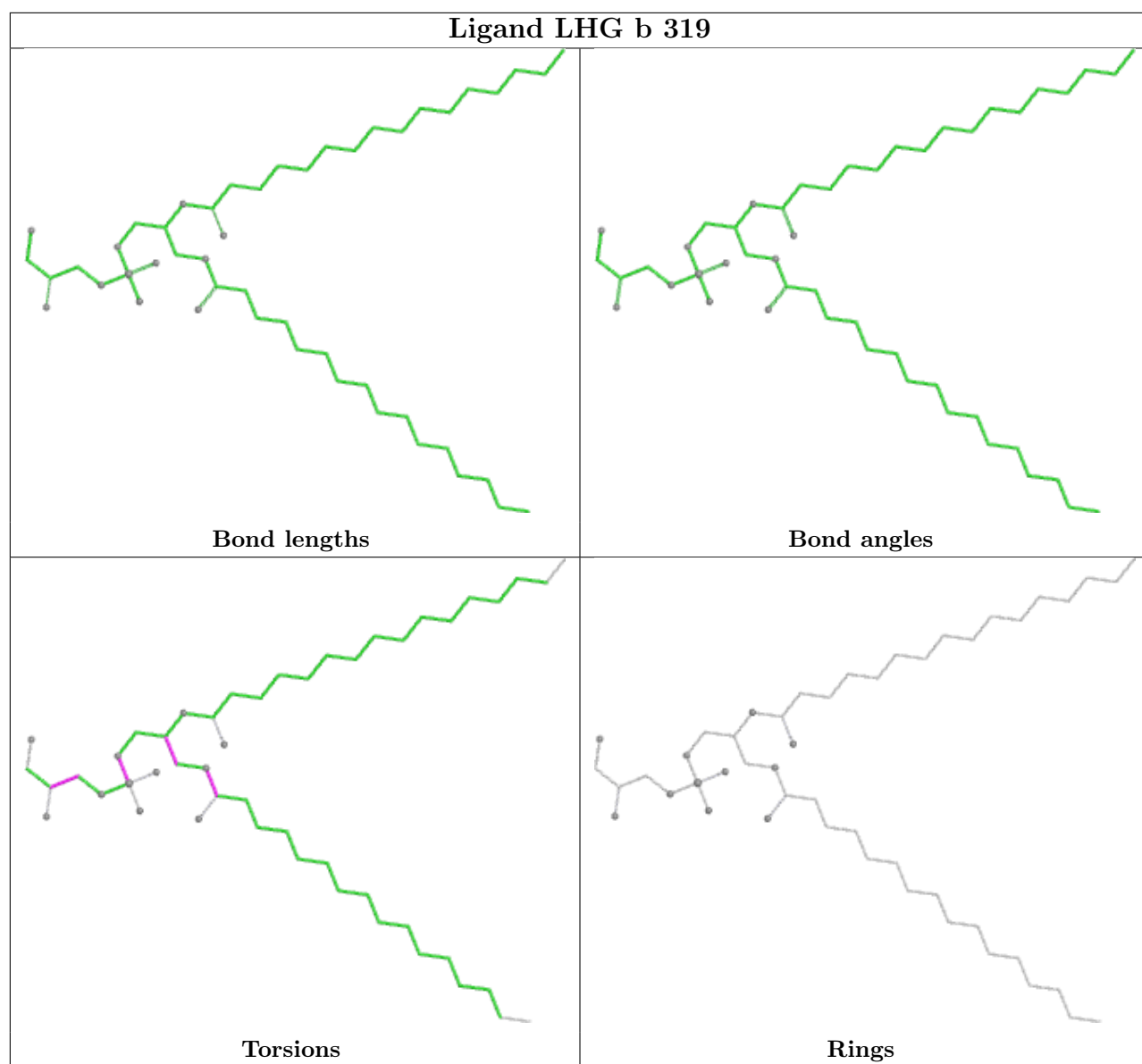


Rings

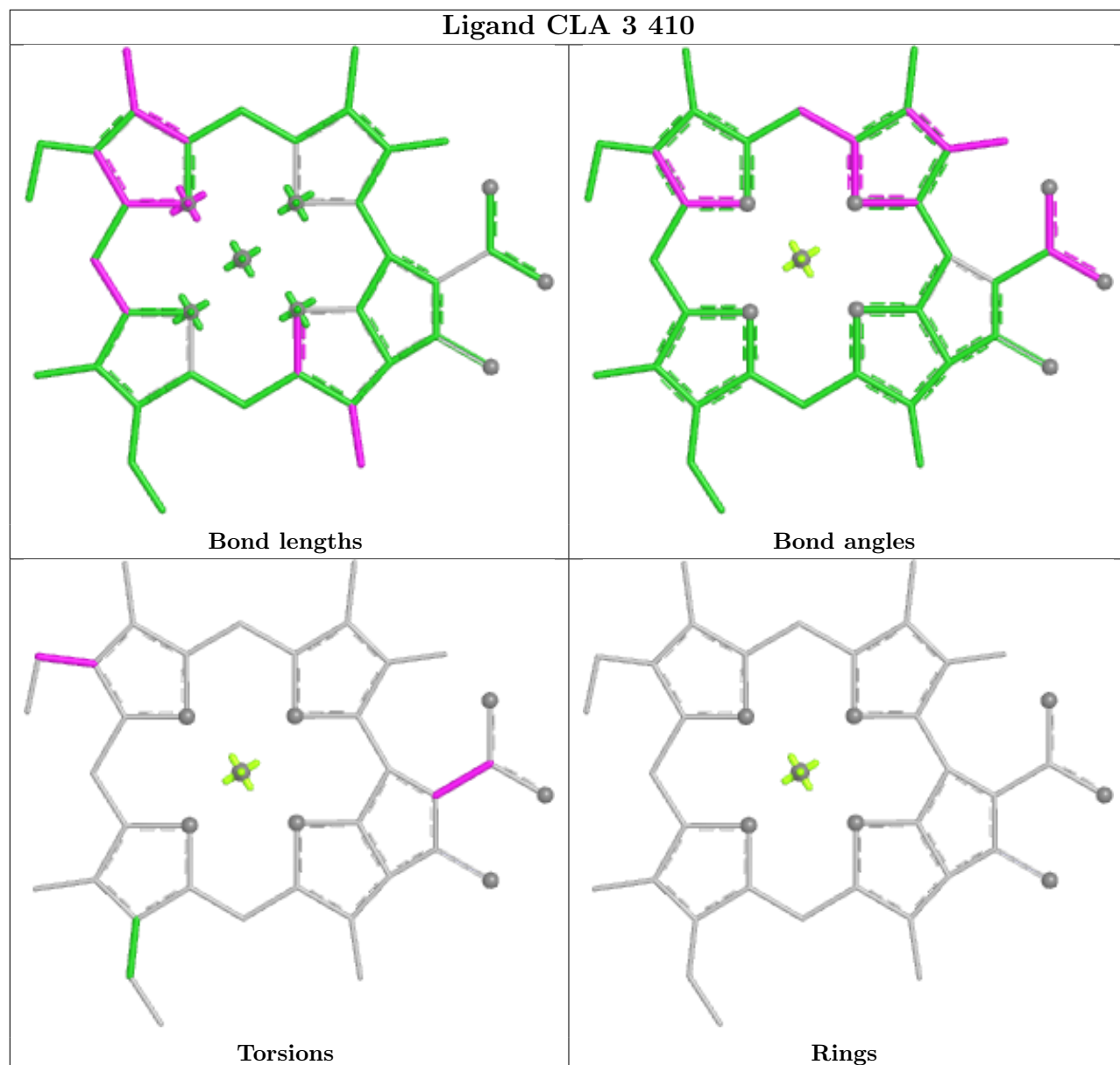
Ligand CLA A 811



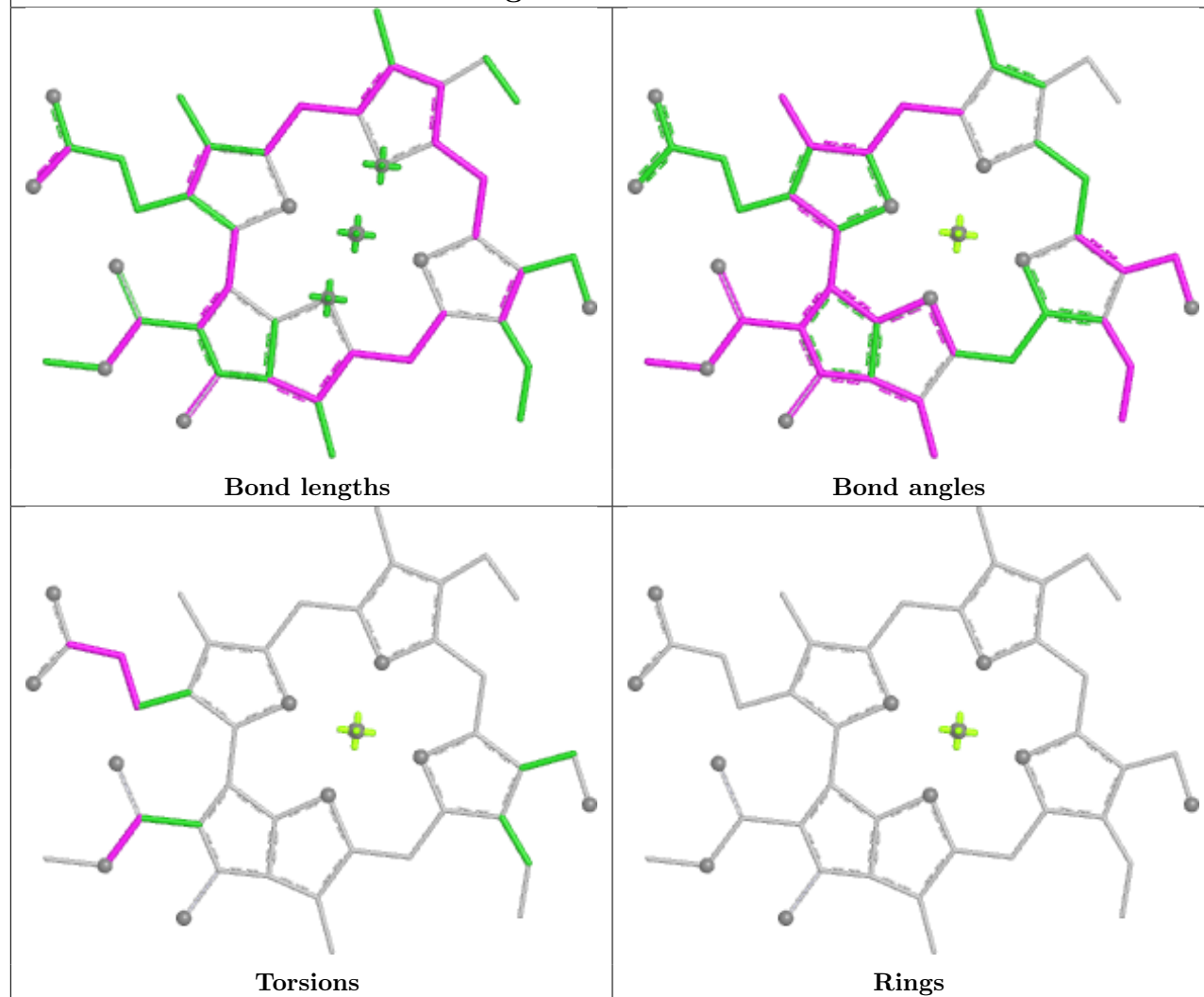




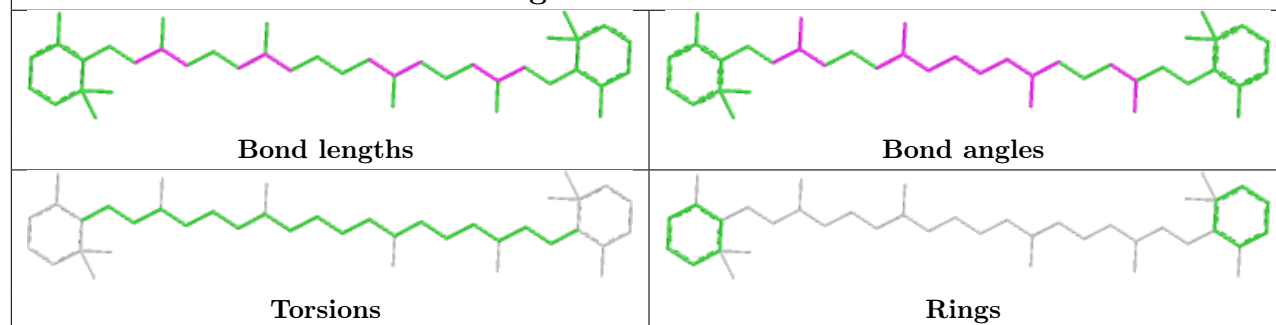
Ligand CLA 3 410



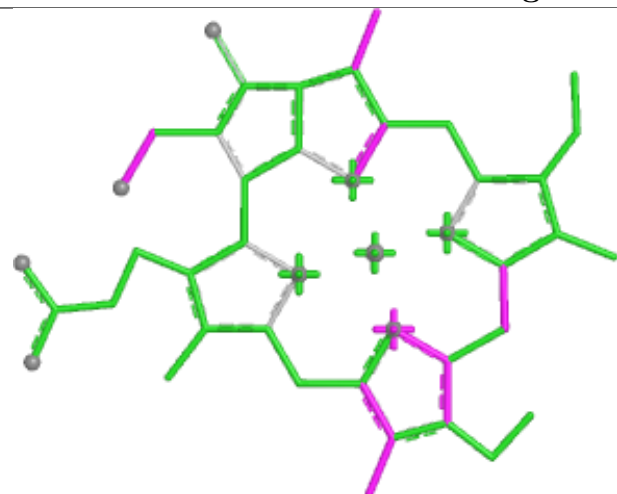
Ligand CHL 6 614



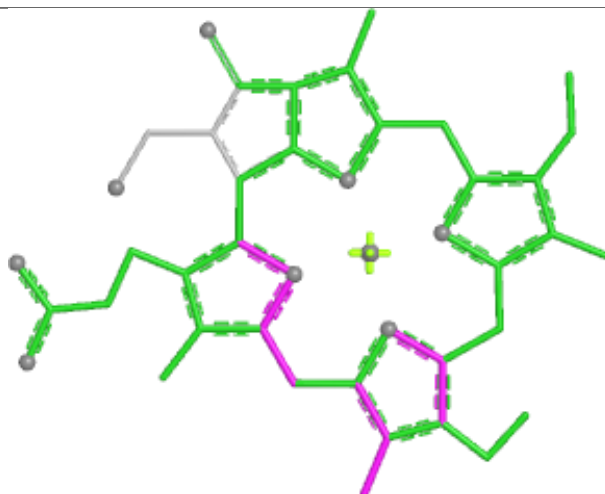
Ligand BCR G 201



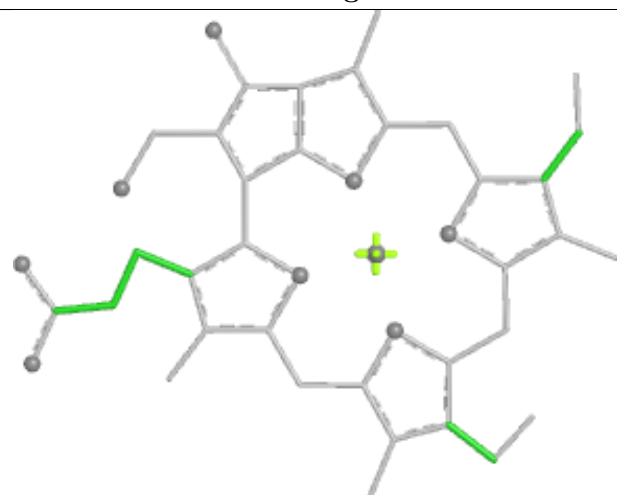
Ligand CLA 4 608



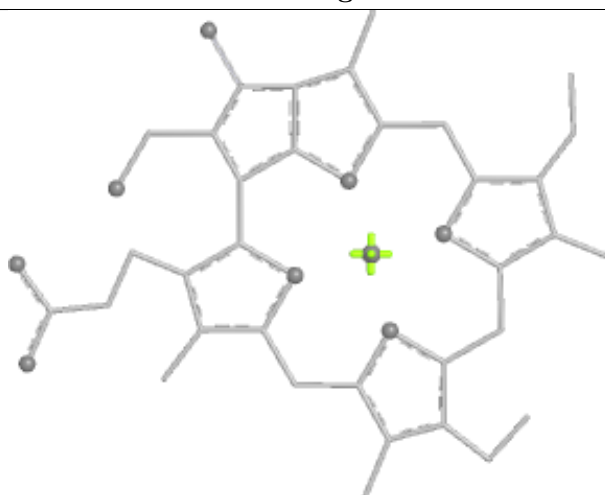
Bond lengths



Bond angles

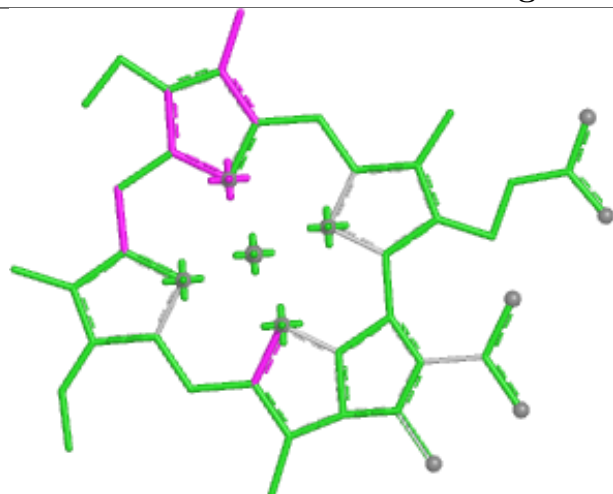


Torsions

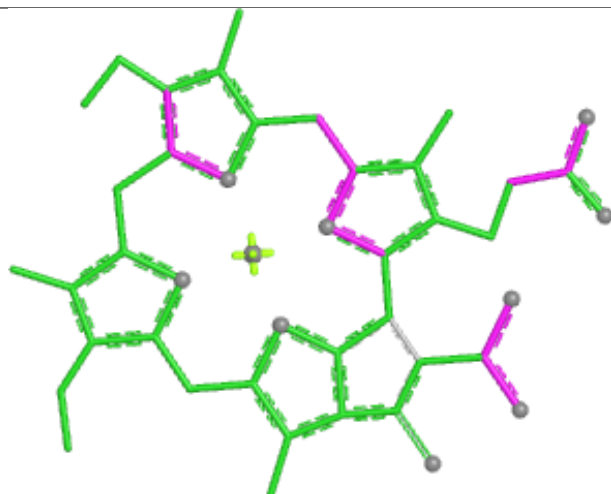


Rings

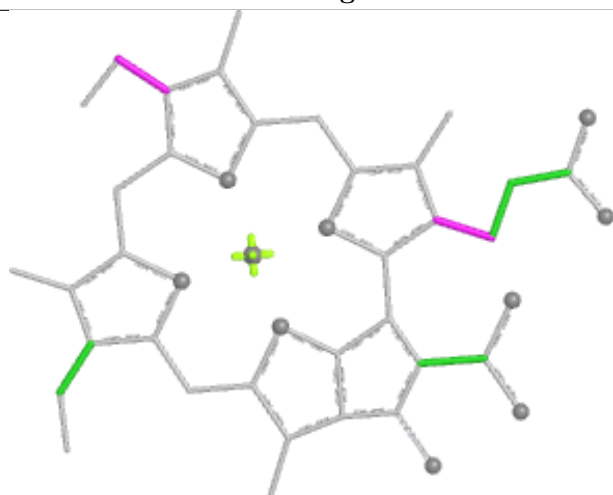
Ligand CLA 5 607



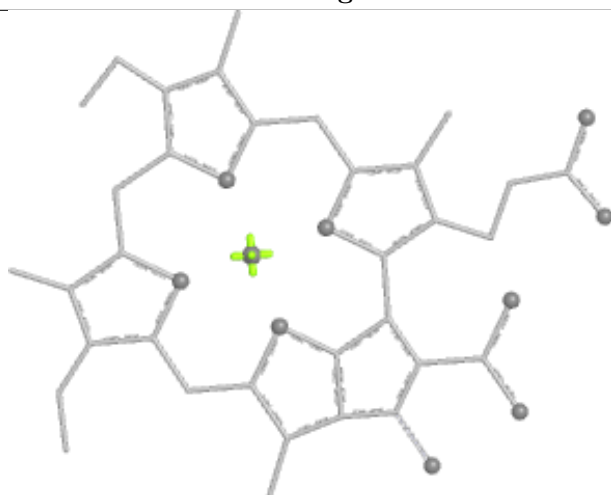
Bond lengths



Bond angles

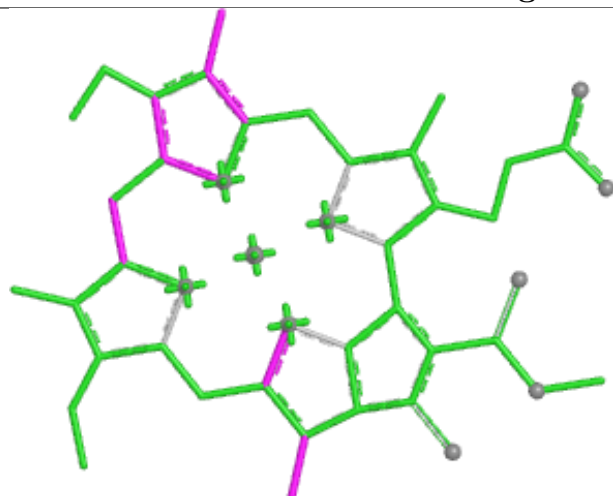


Torsions

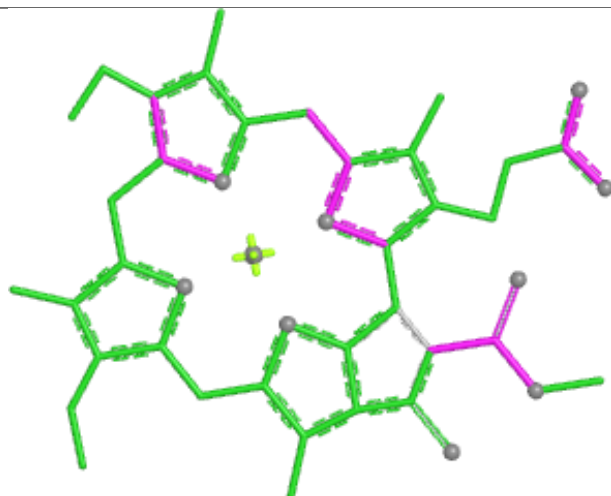


Rings

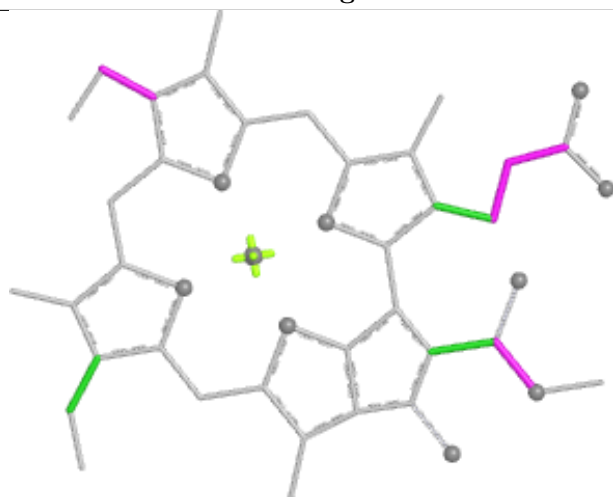
Ligand CLA 2 612



Bond lengths



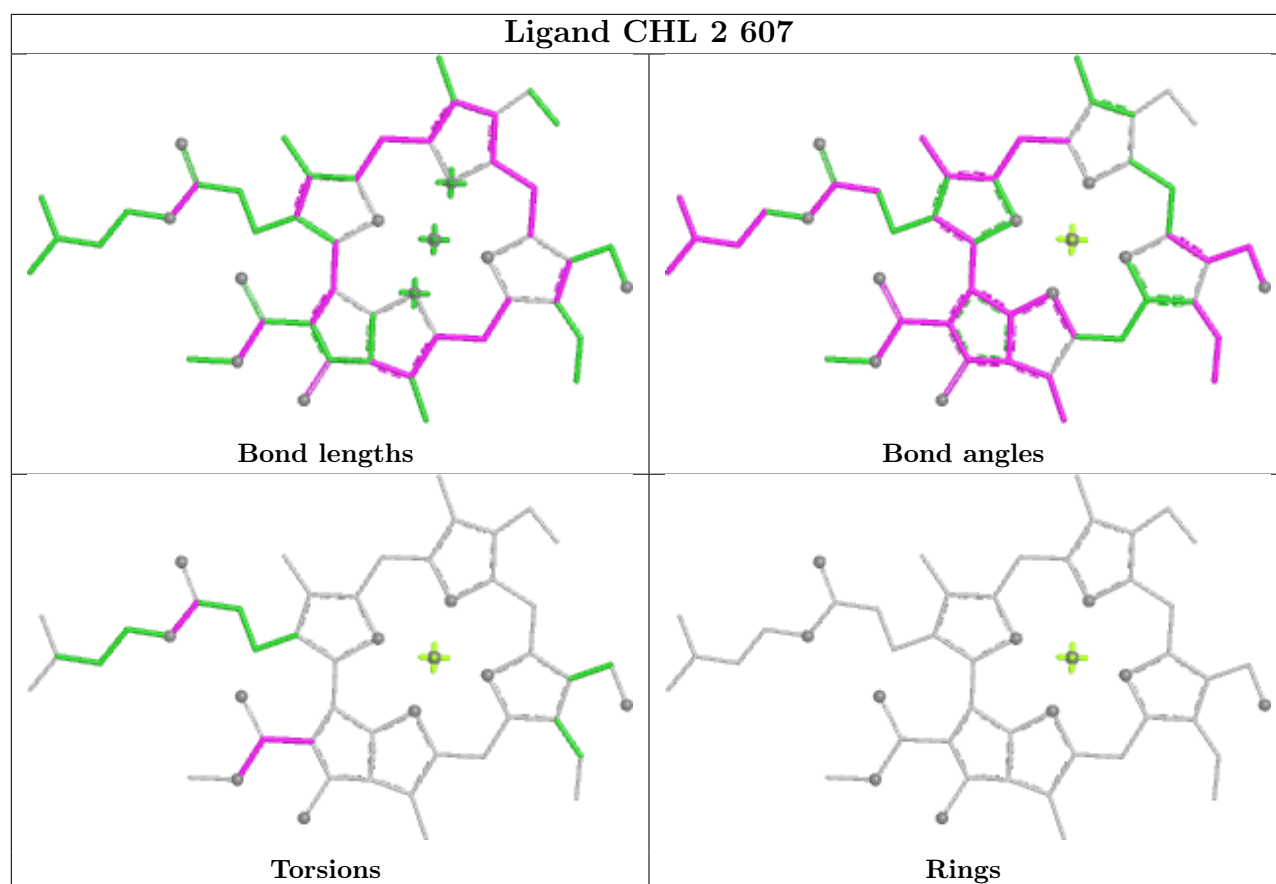
Bond angles



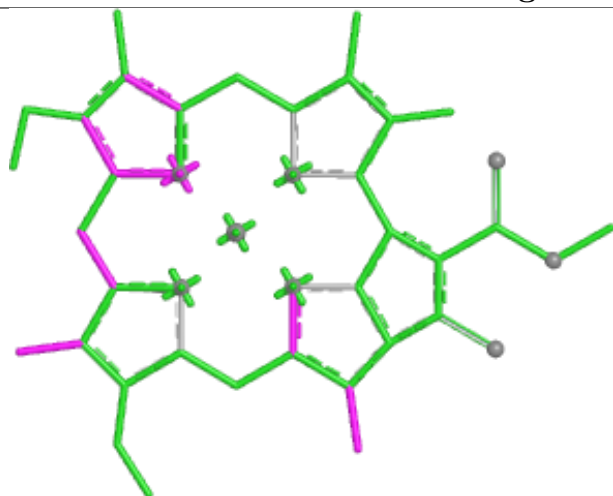
Torsions



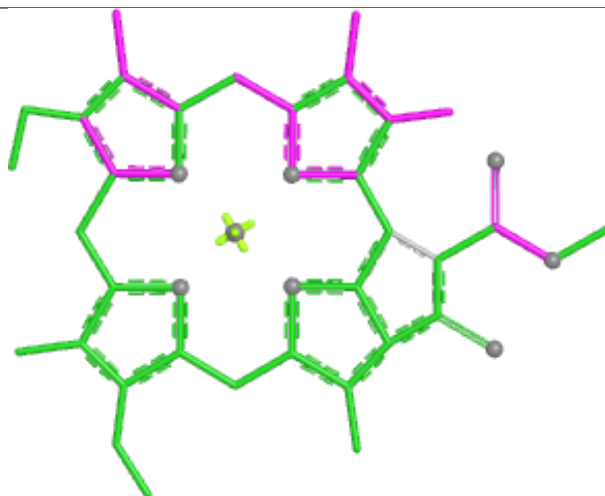
Rings



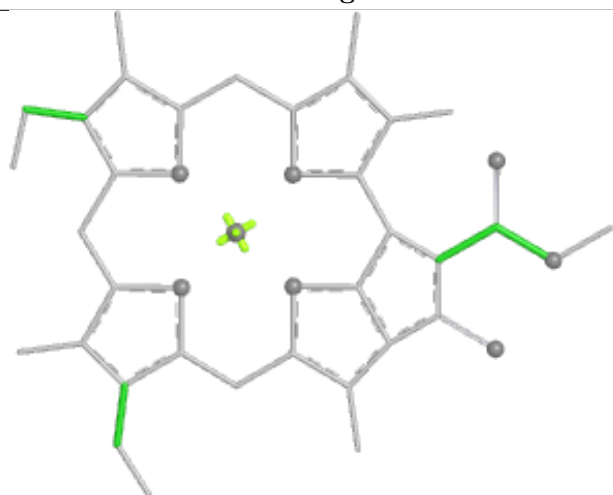
Ligand CLA 2 611



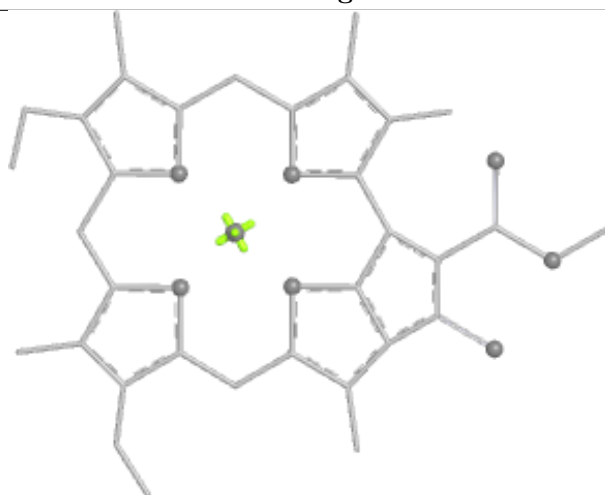
Bond lengths



Bond angles

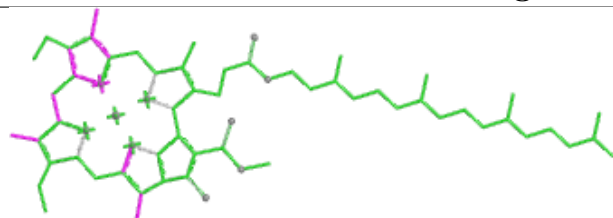


Torsions

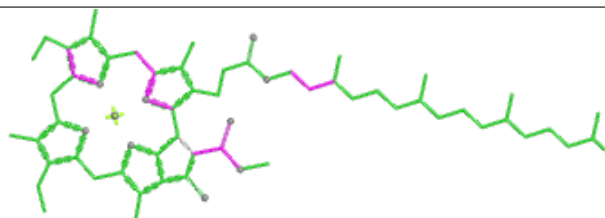


Rings

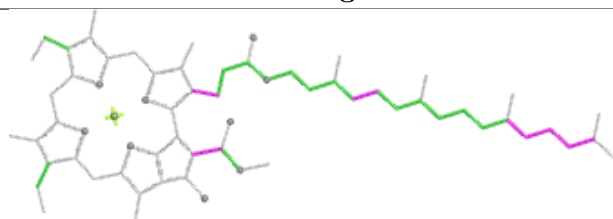
Ligand CLA A 804



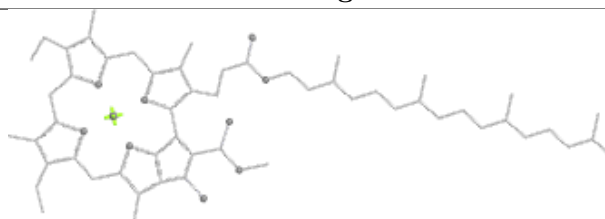
Bond lengths



Bond angles

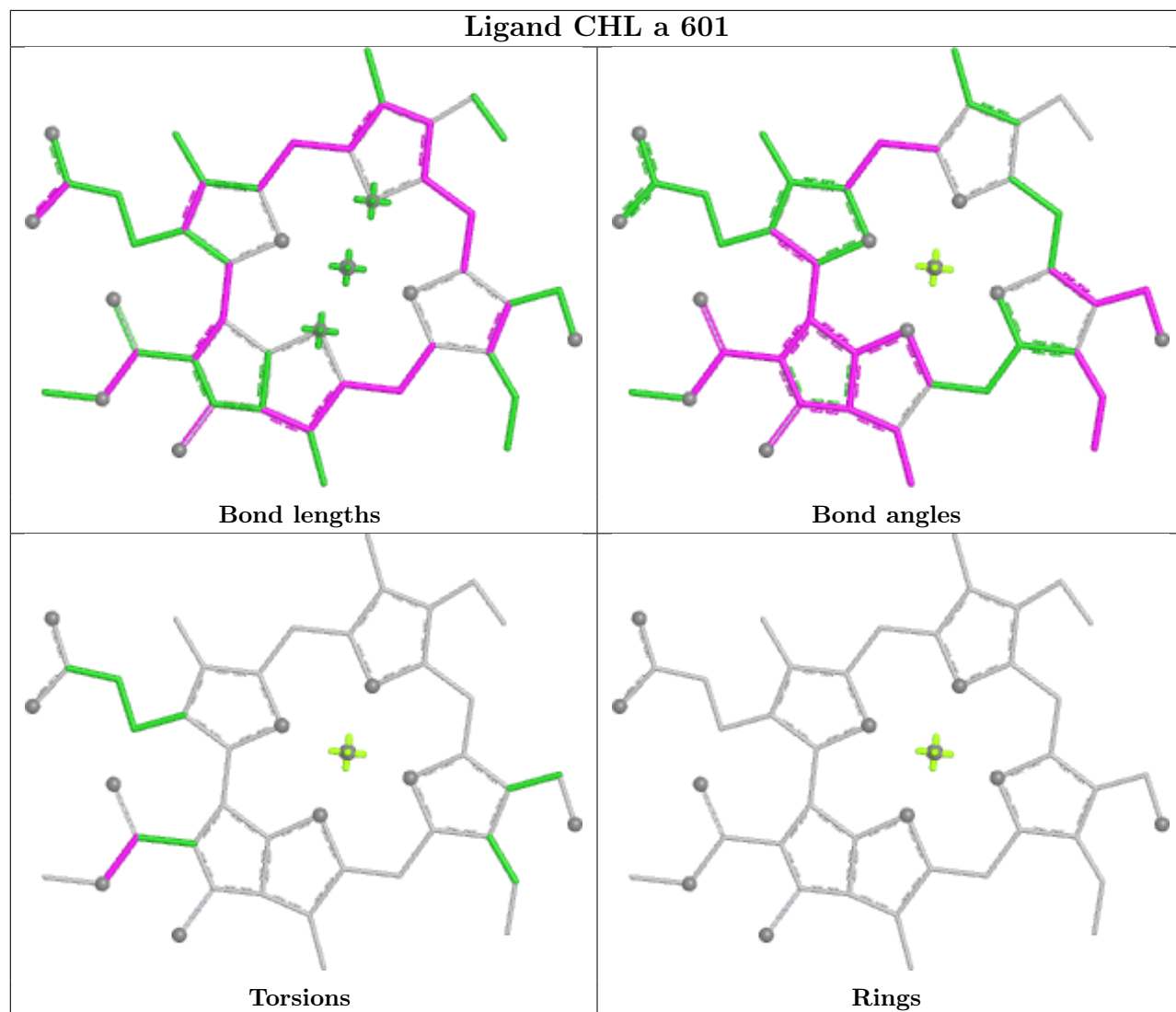


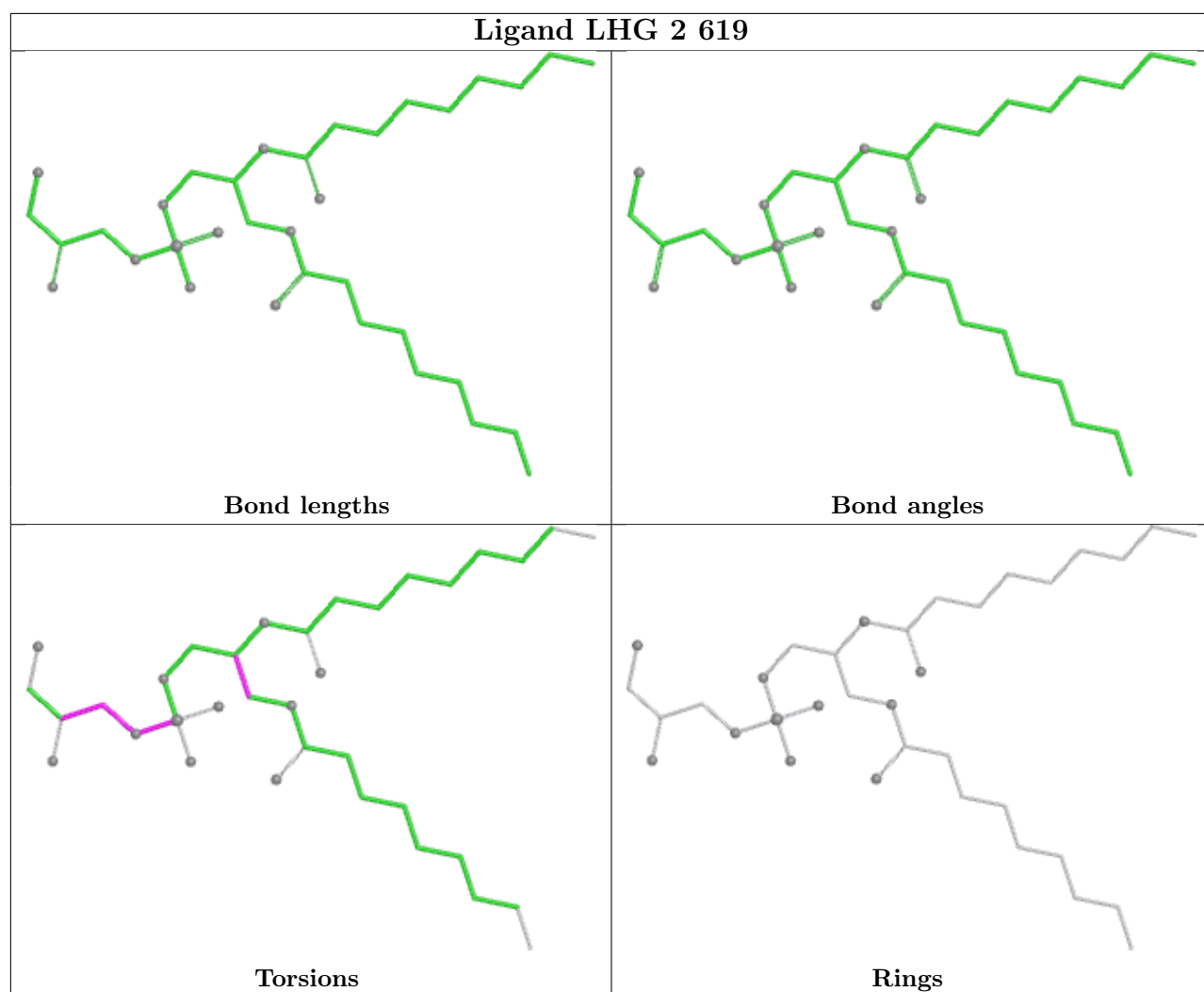
Torsions

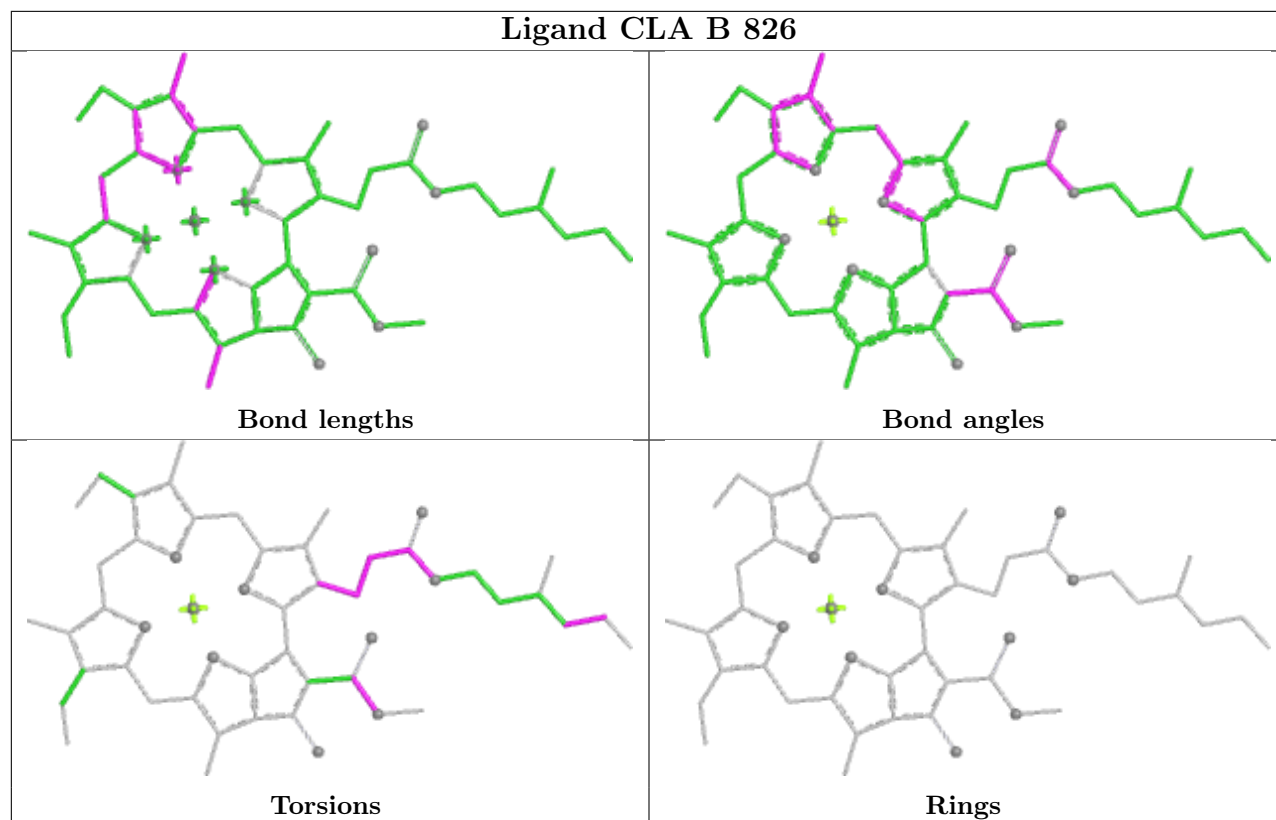


Rings

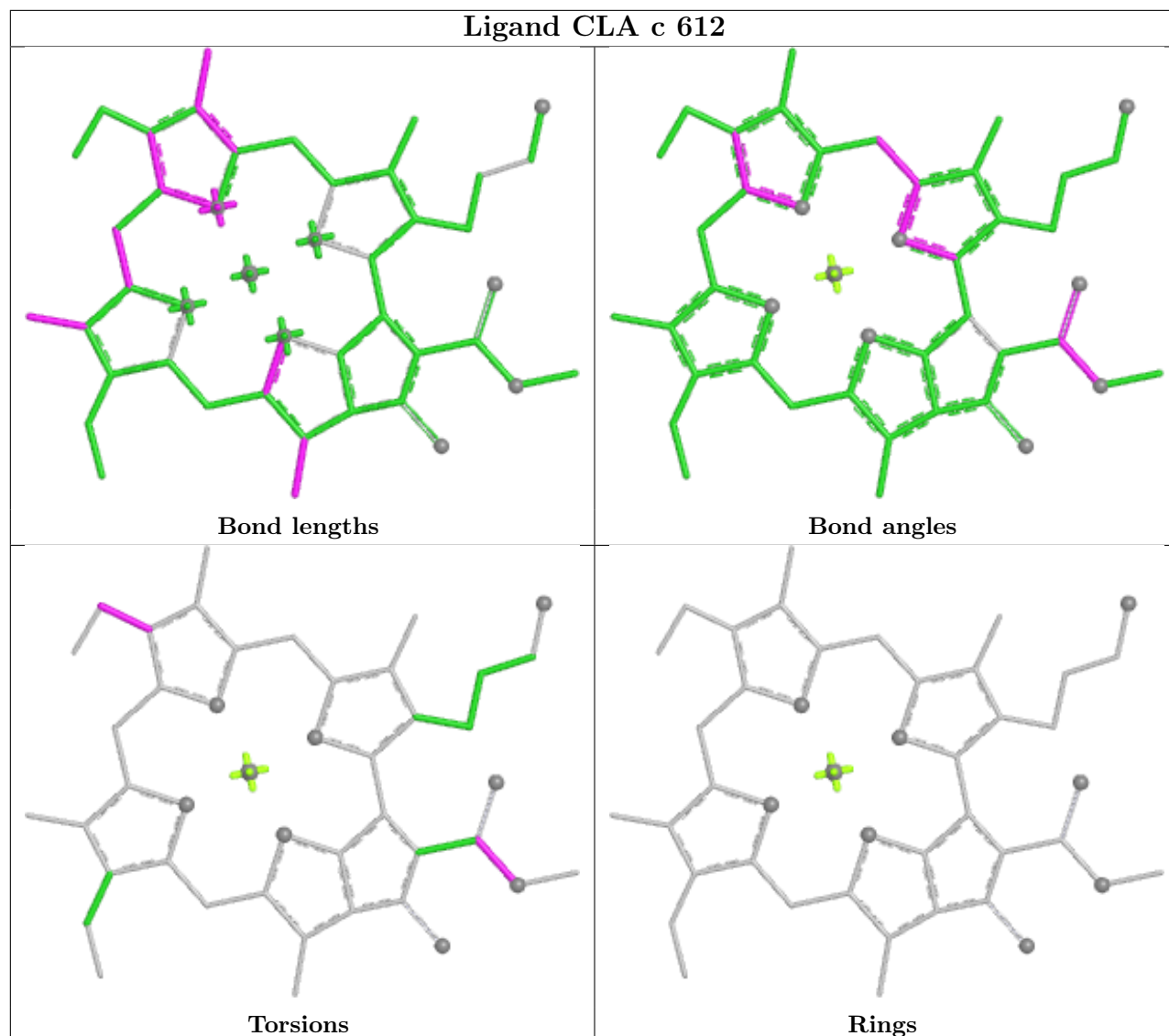
Ligand CHL a 601



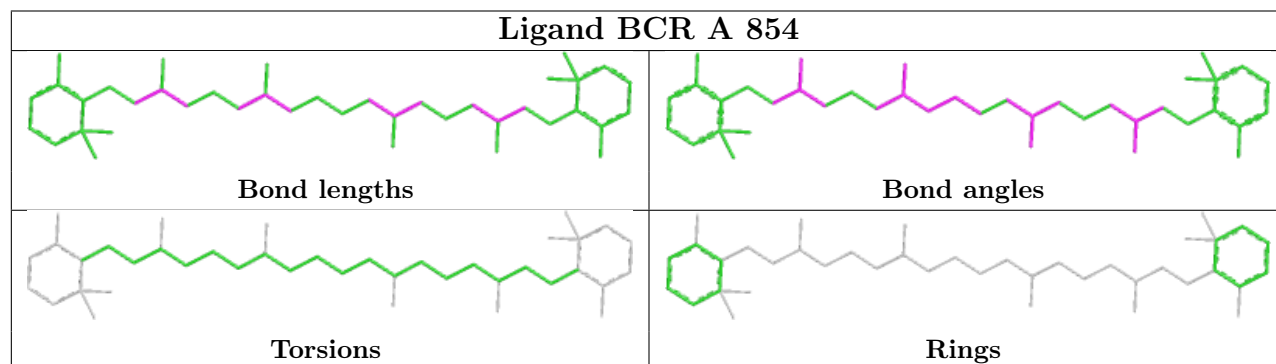




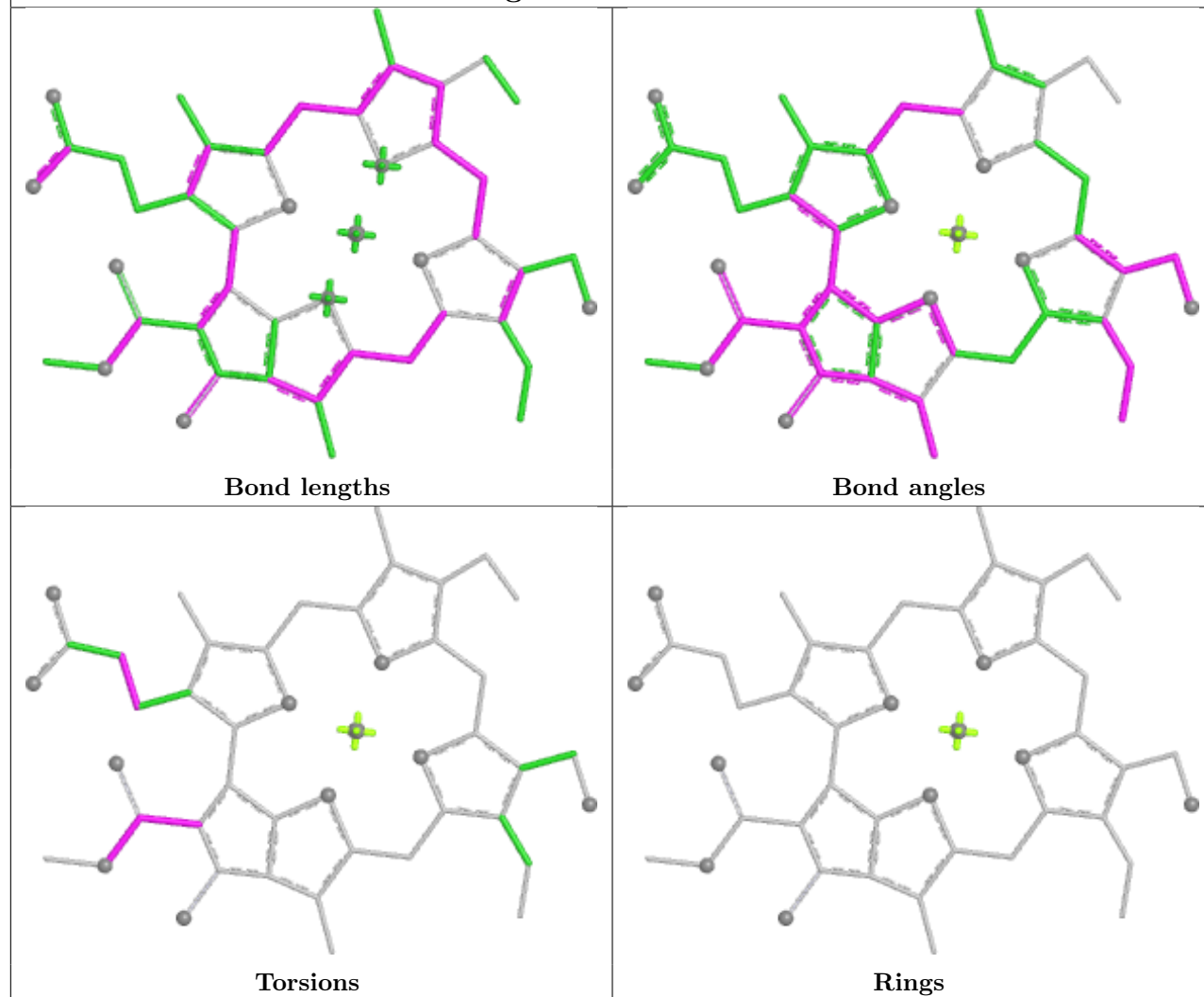
Ligand CLA c 612



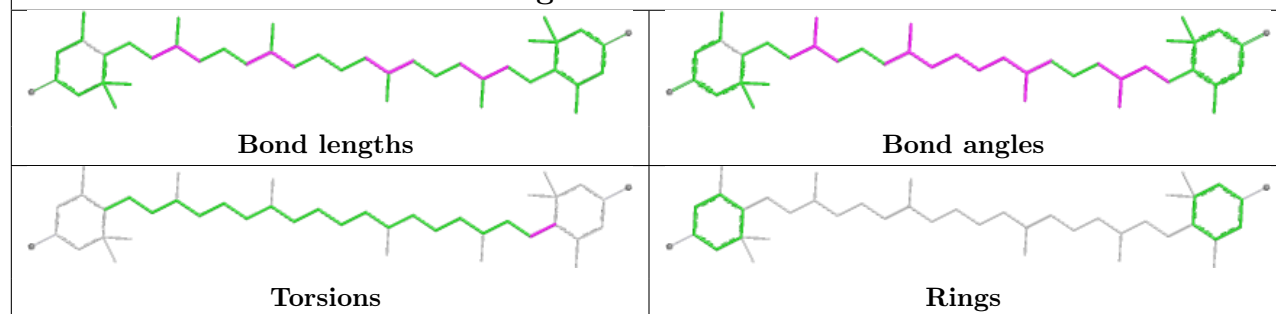
Ligand BCR A 854

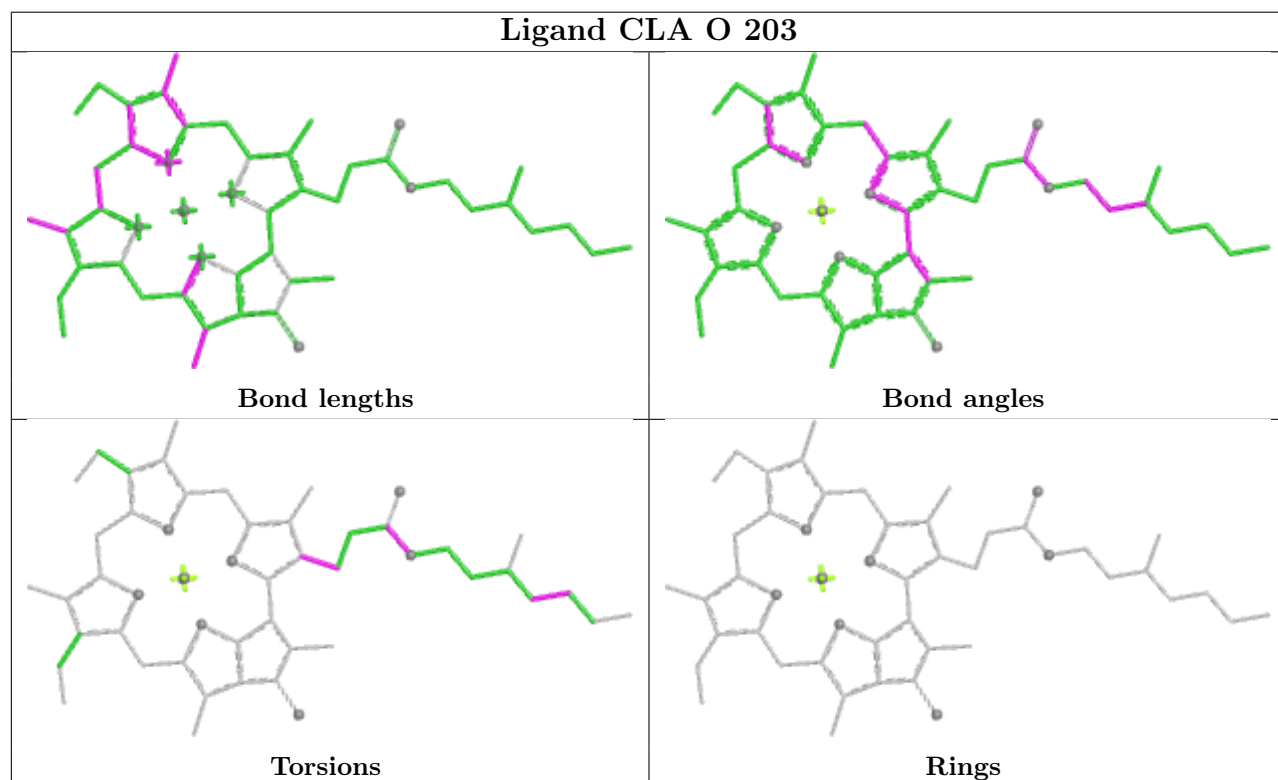
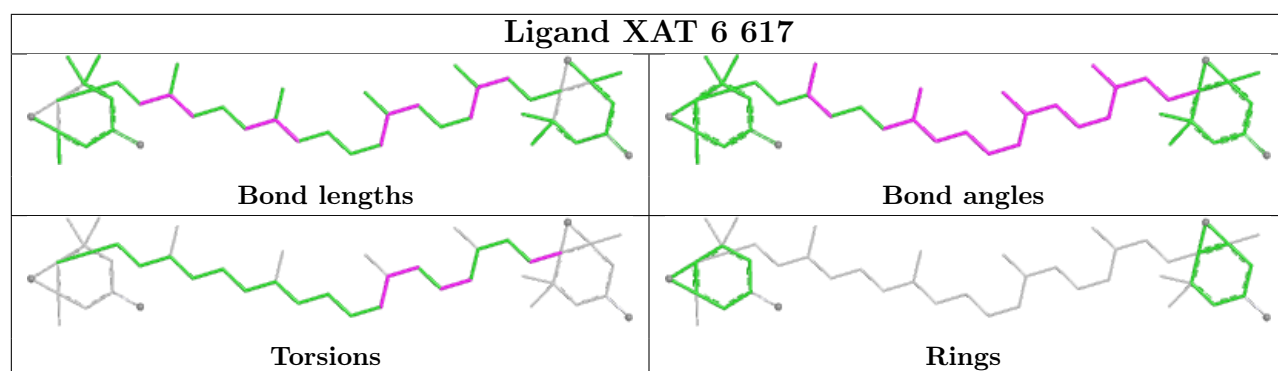


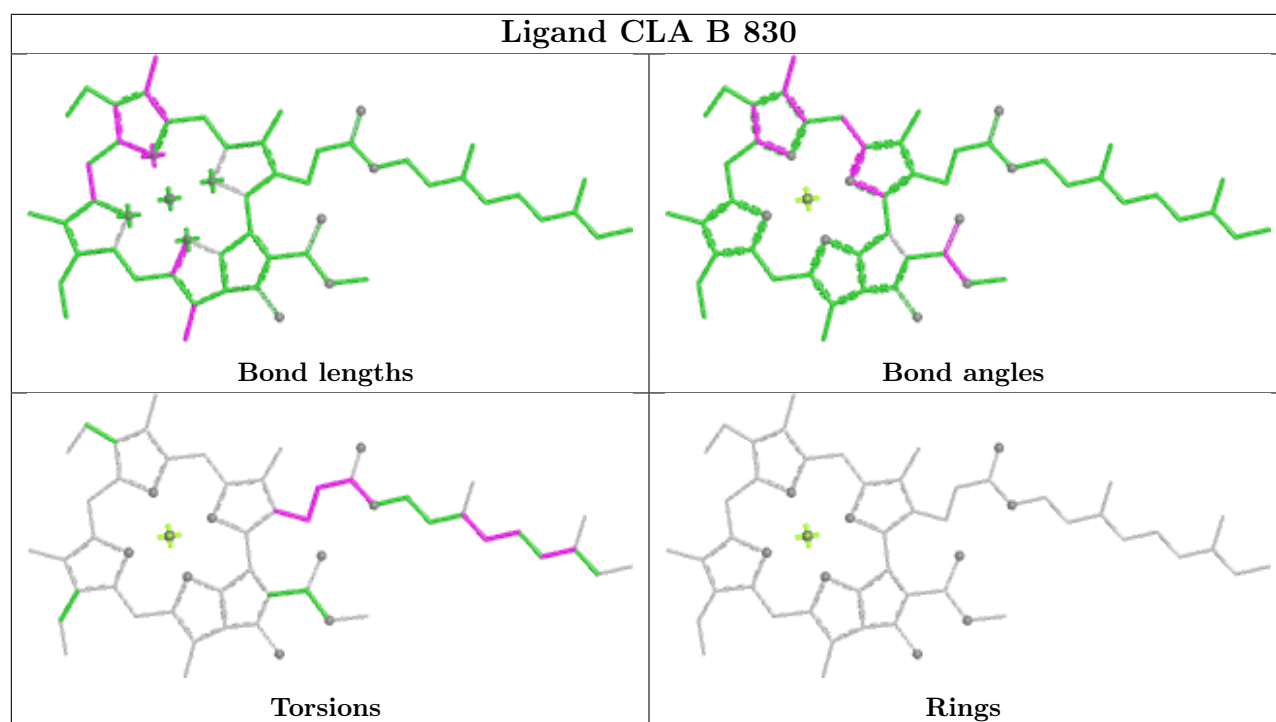
Ligand CHL 6 605



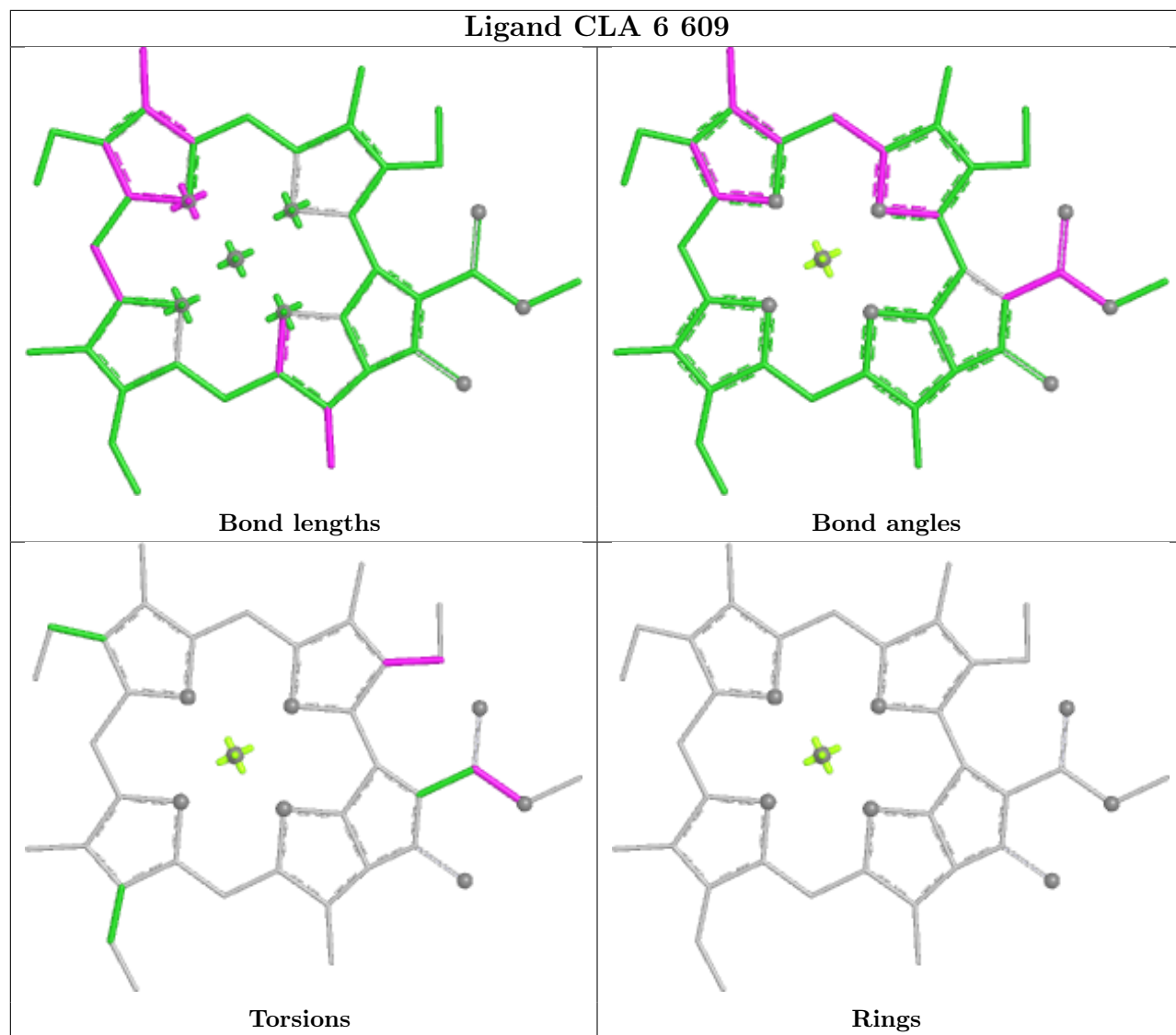
Ligand LUT 9 615

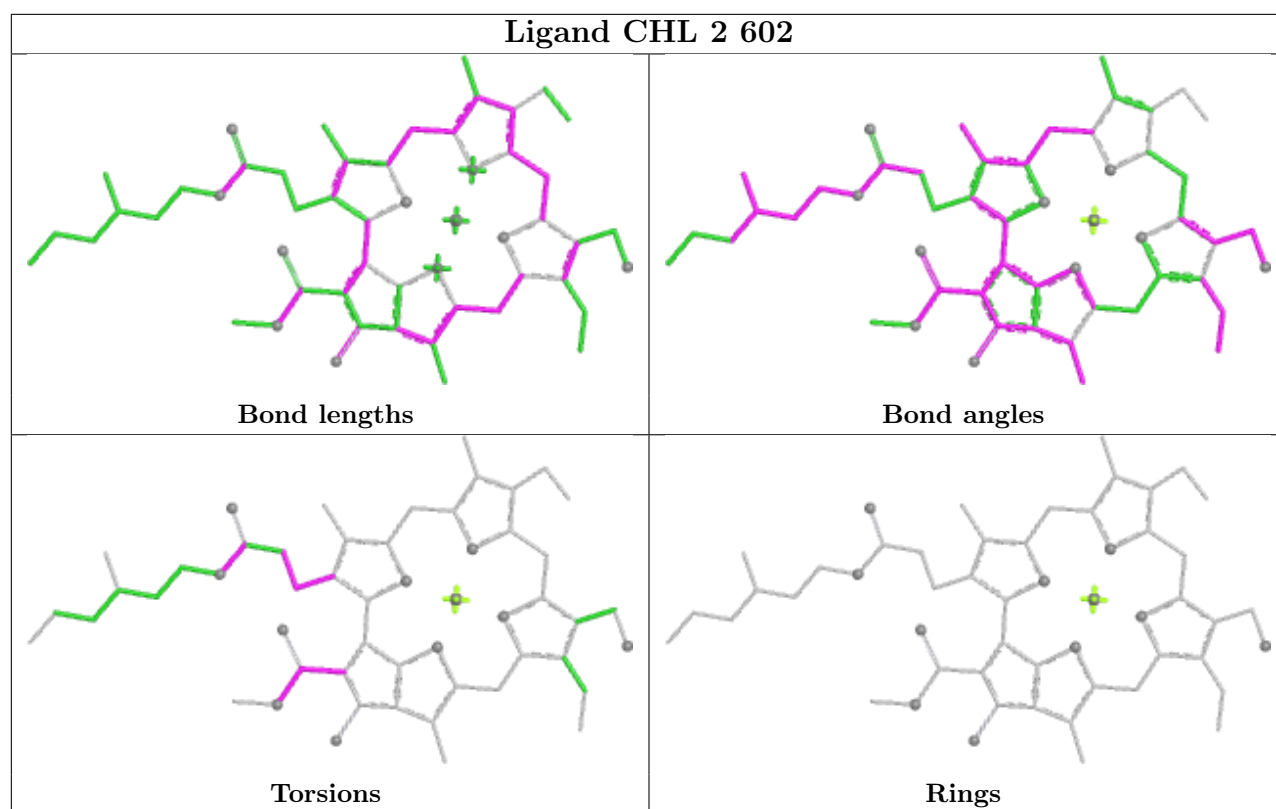




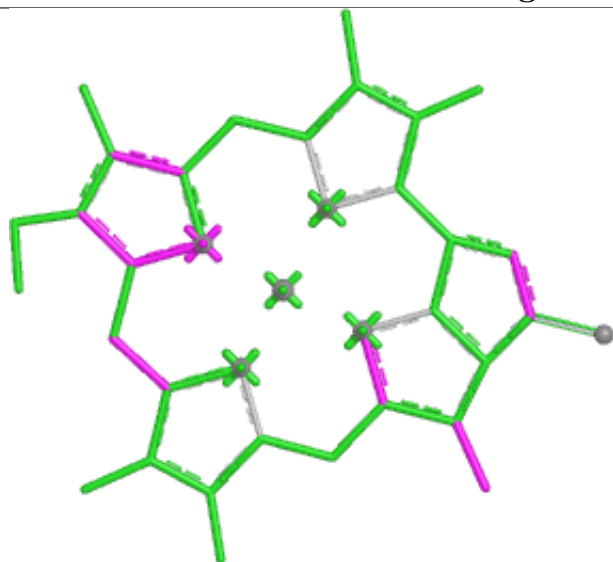


Ligand CLA 6 609

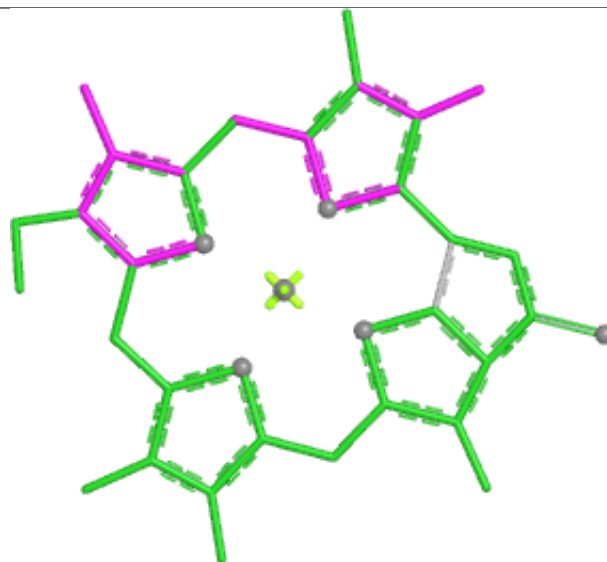




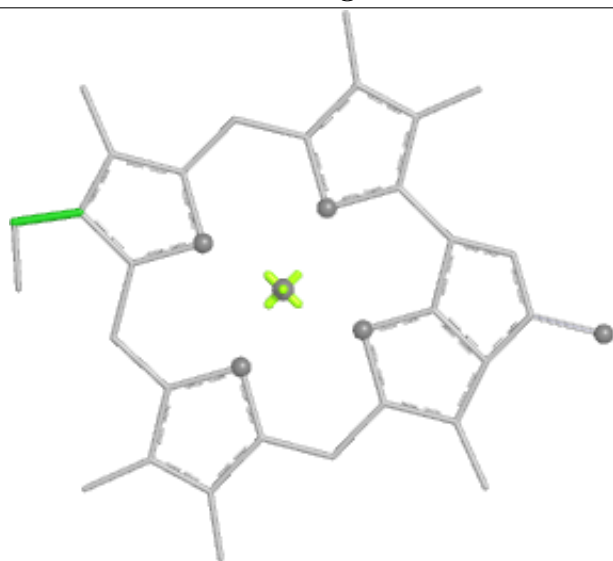
Ligand CLA 7 413



Bond lengths



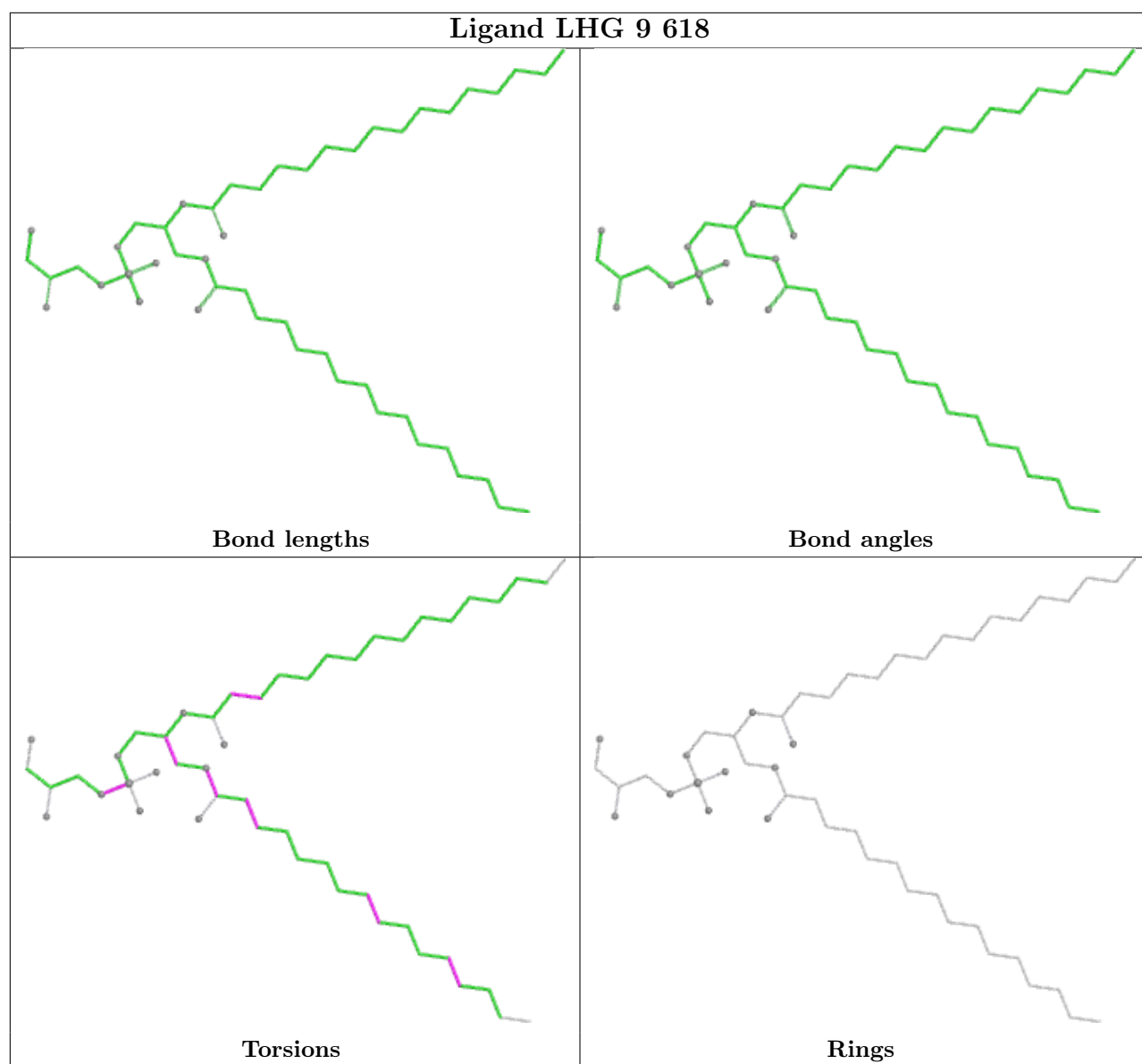
Bond angles



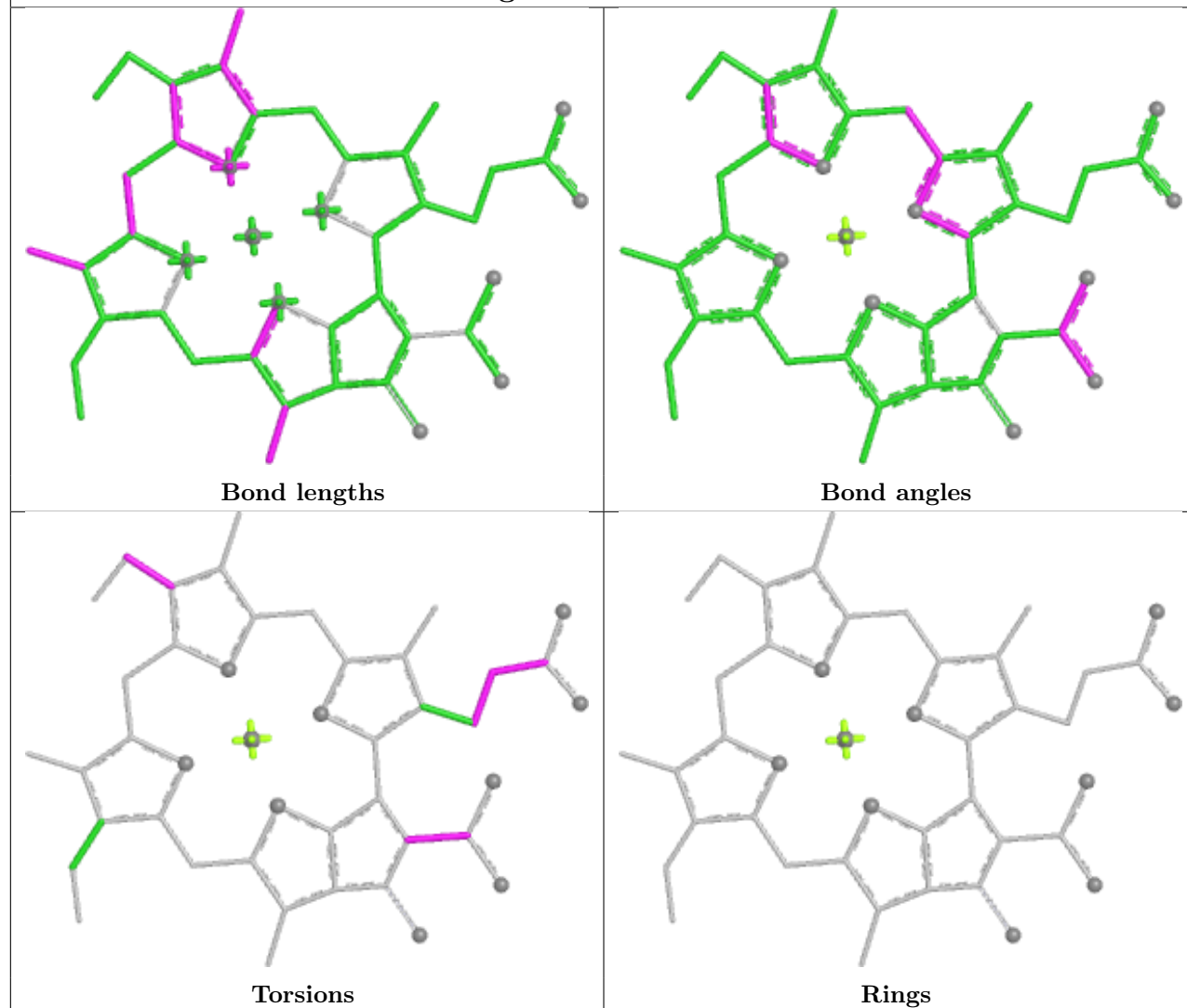
Torsions



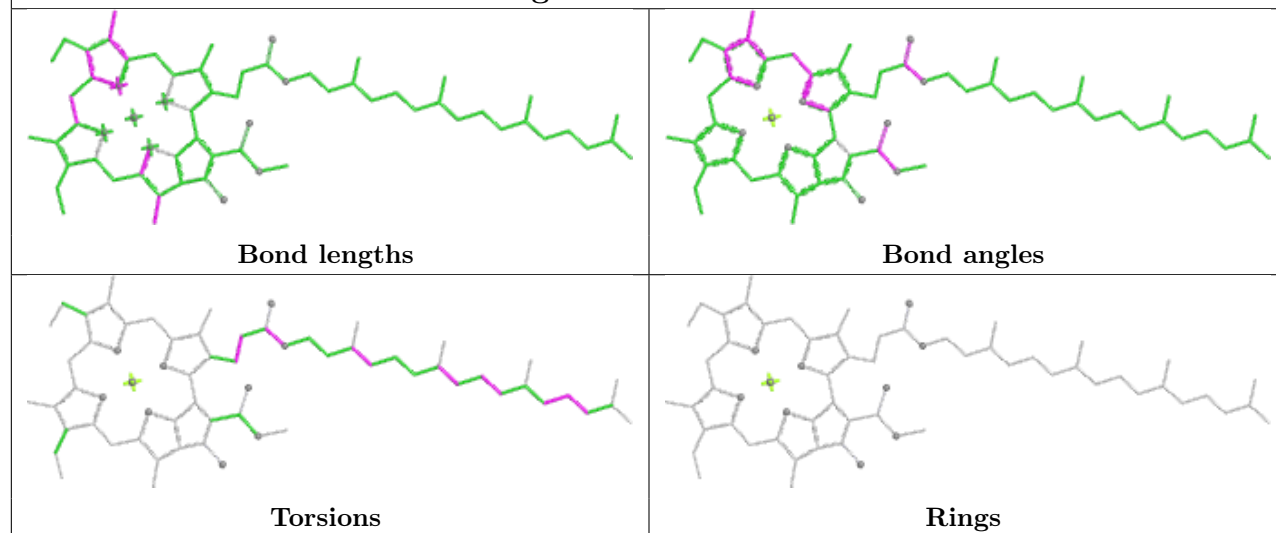
Rings



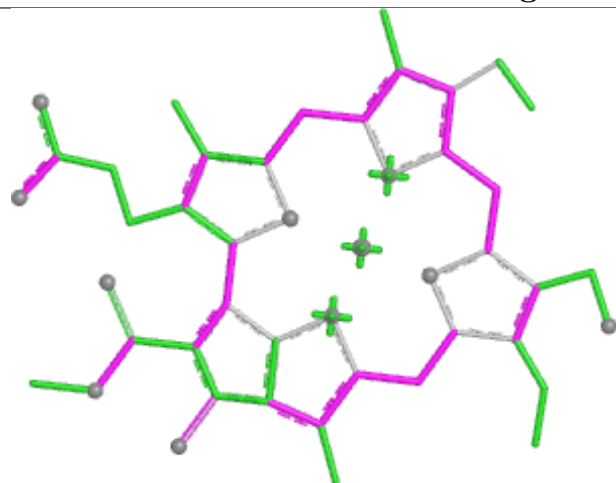
Ligand CLA 4 603



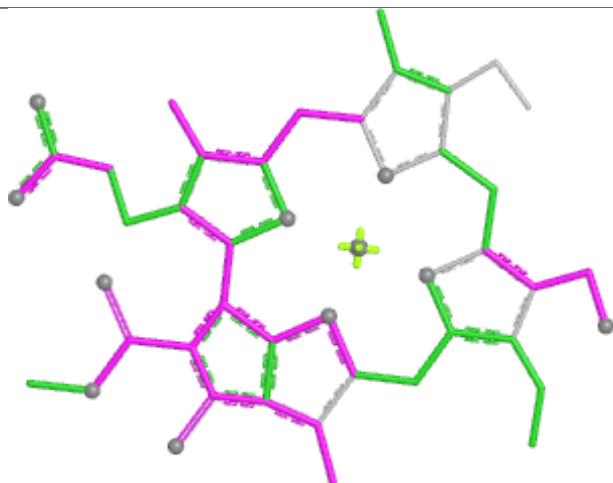
Ligand CLA A 838



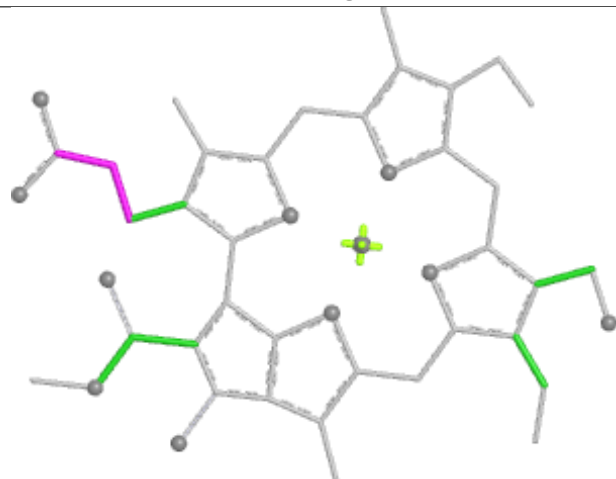
Ligand CHL 2 614



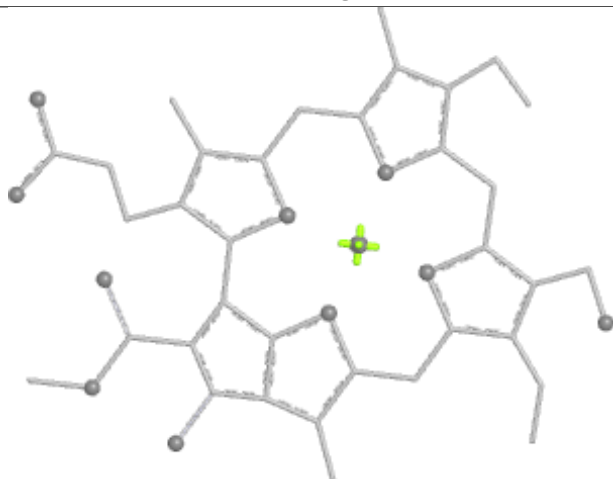
Bond lengths



Bond angles

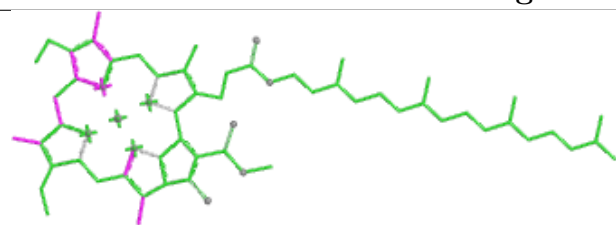


Torsions

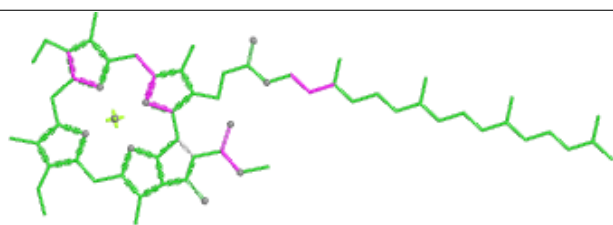


Rings

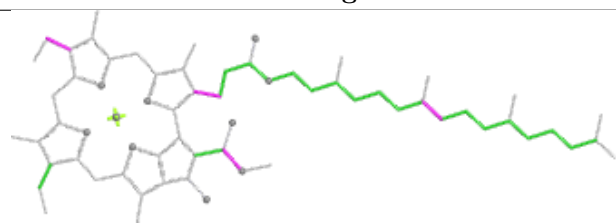
Ligand CLA A 833



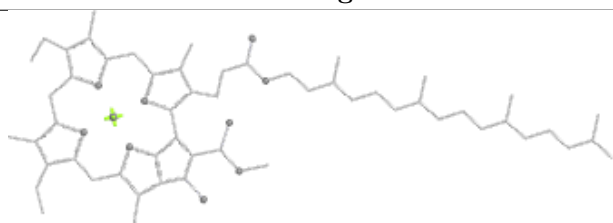
Bond lengths



Bond angles

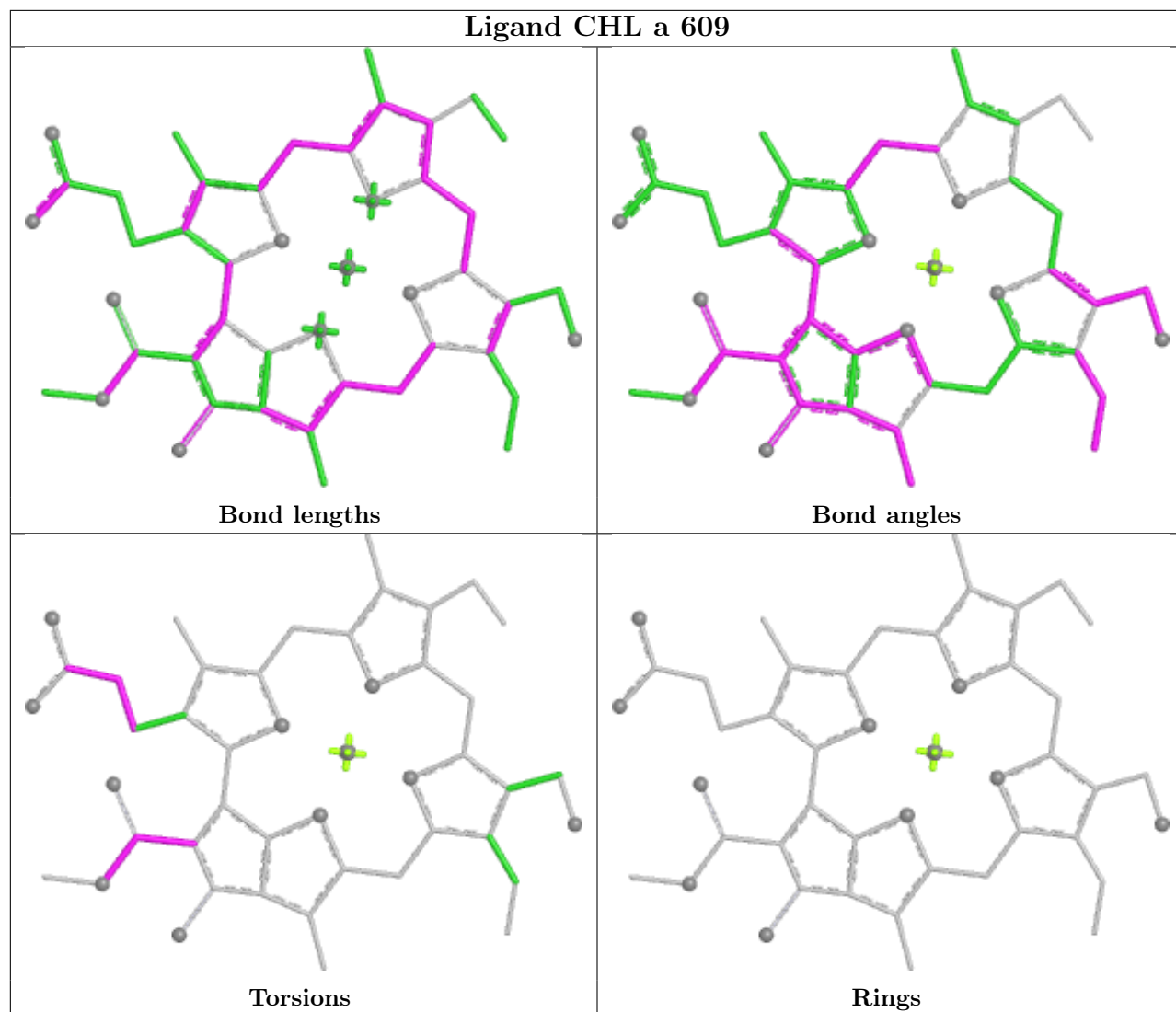


Torsions

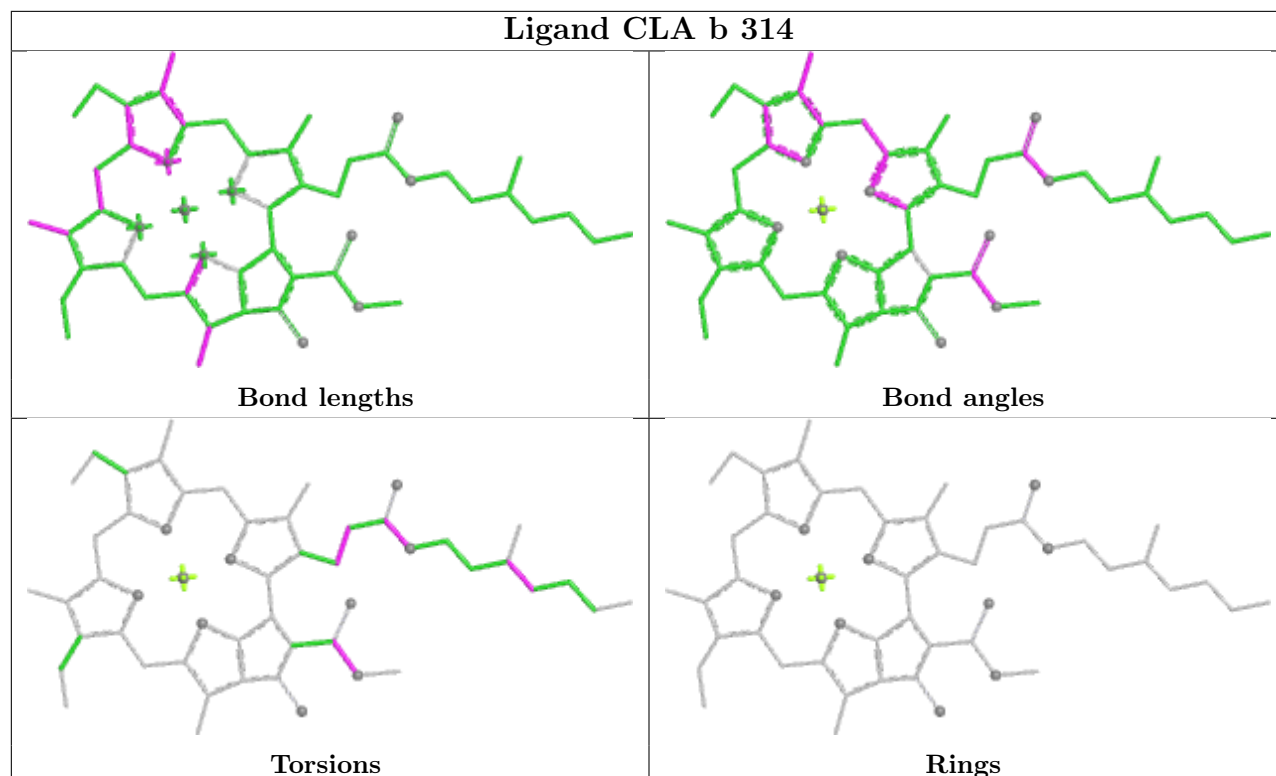


Rings

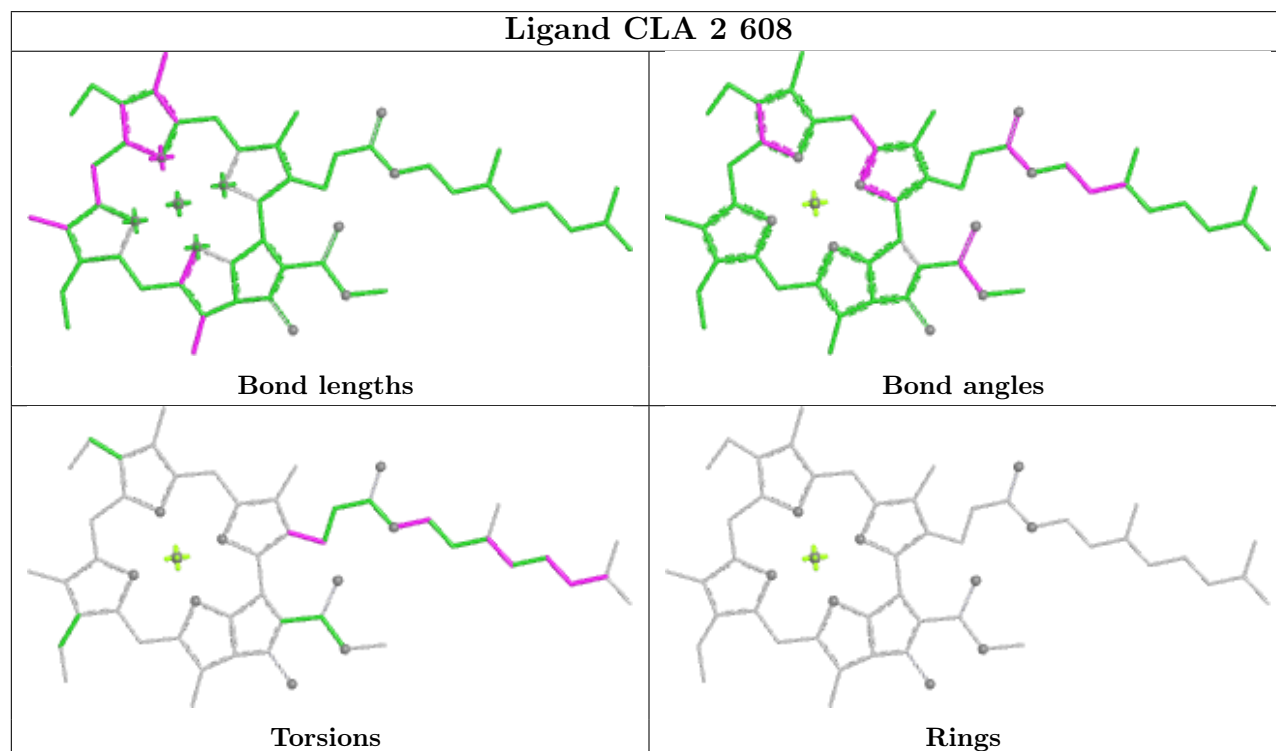
Ligand CHL a 609



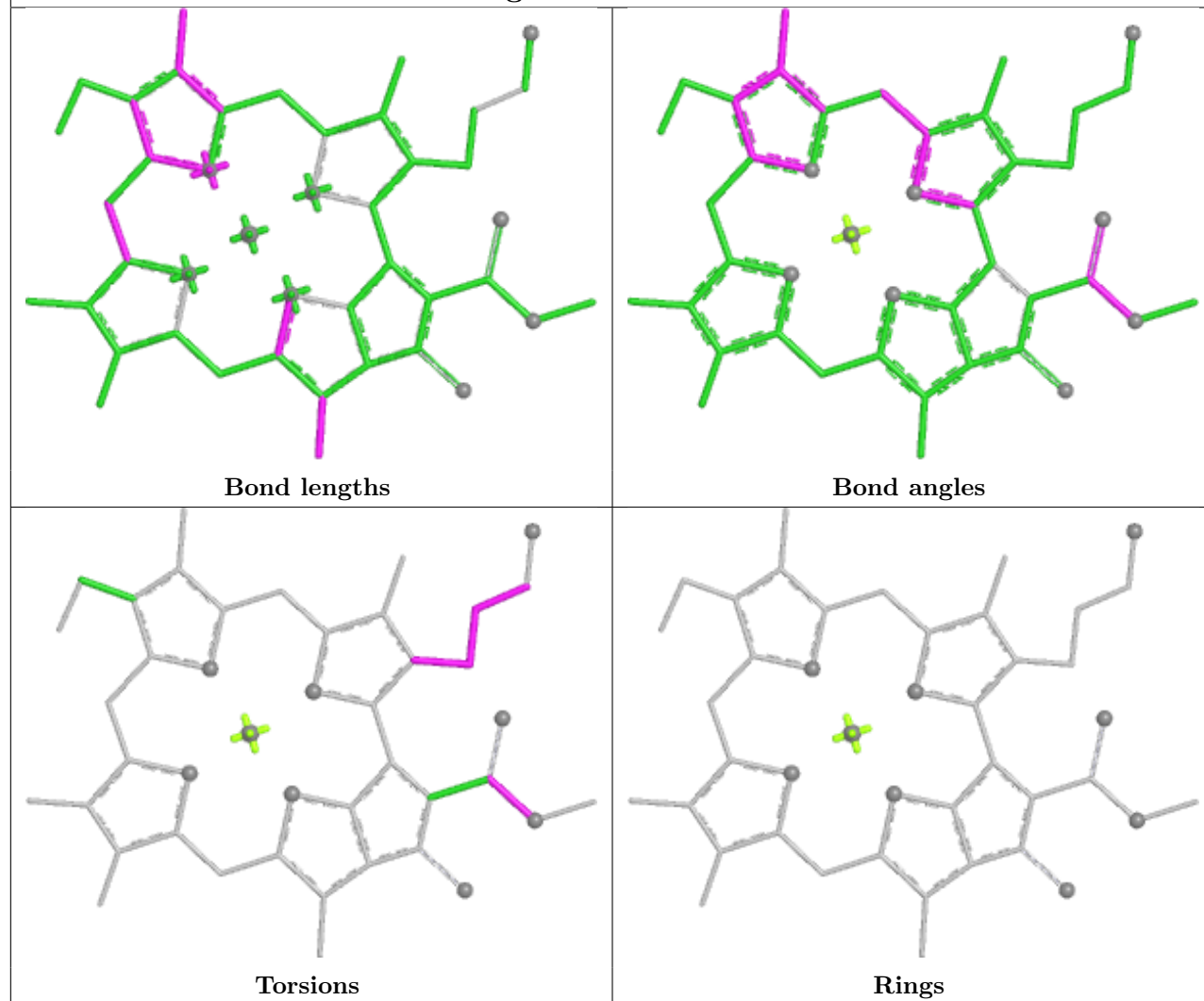
Ligand CLA b 314



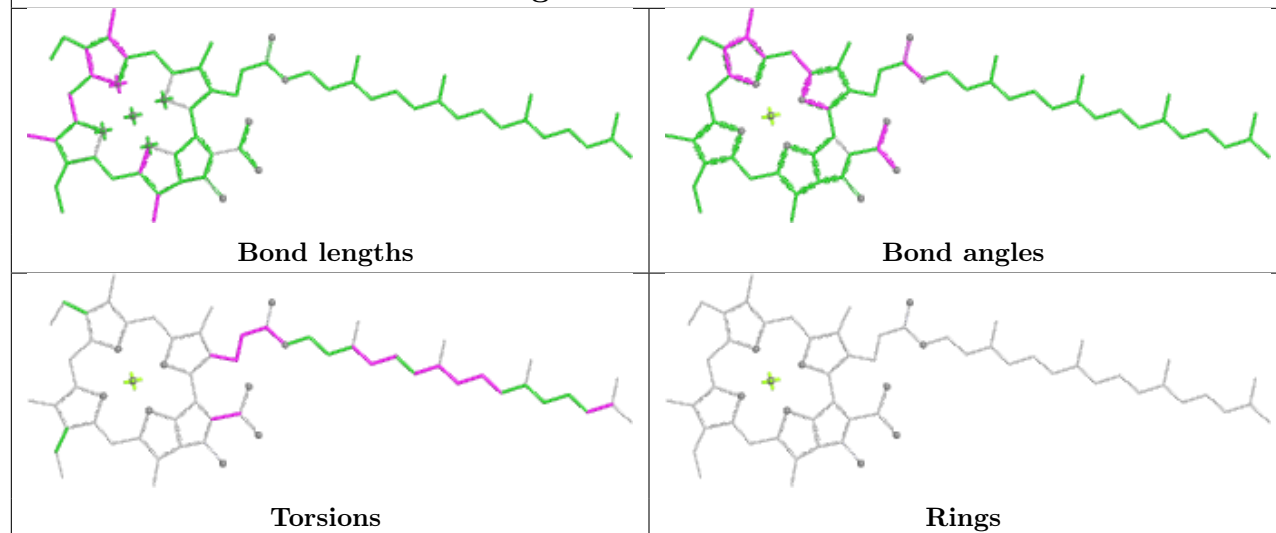
Ligand CLA 2 608

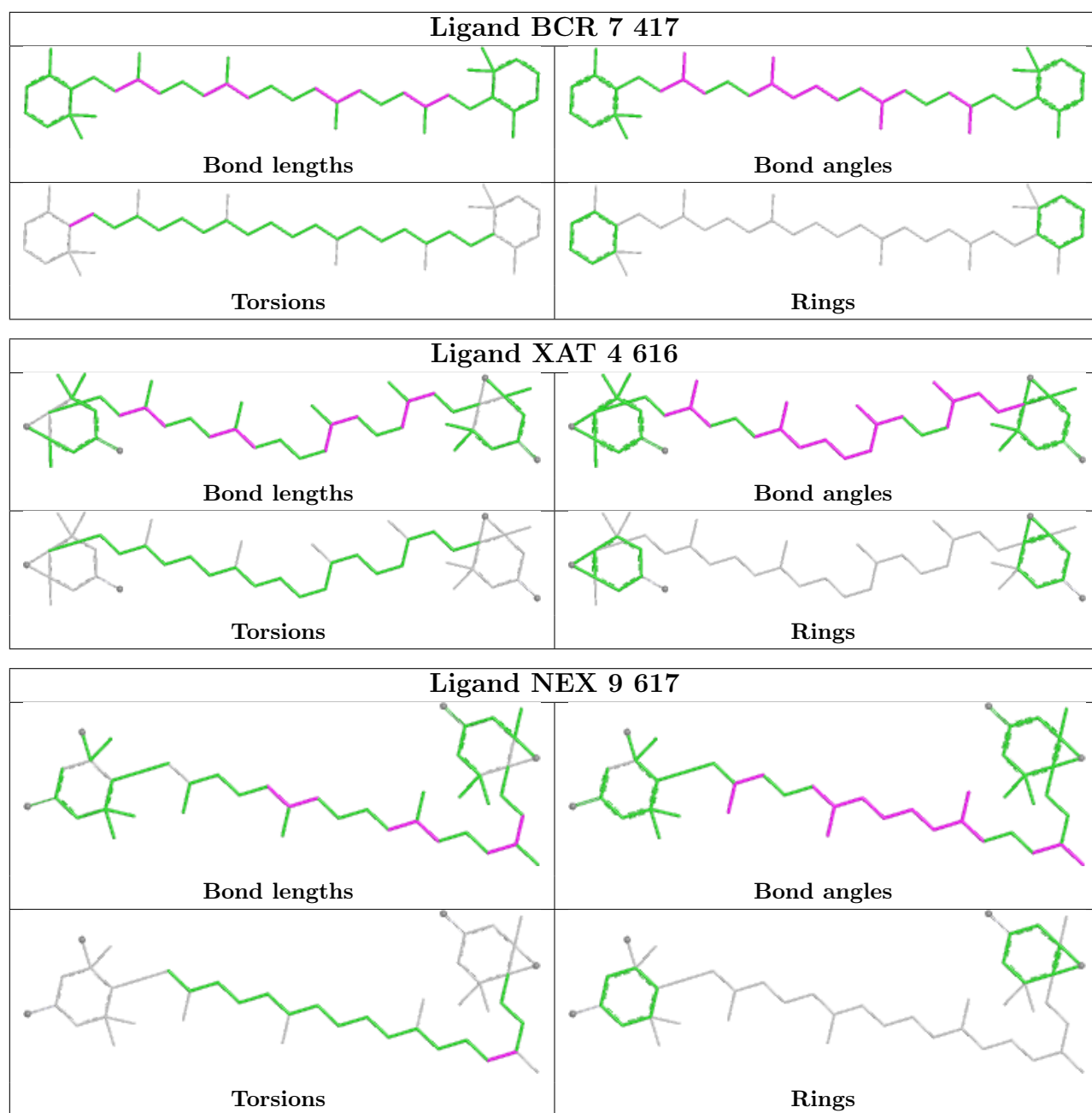


Ligand CLA 8 604

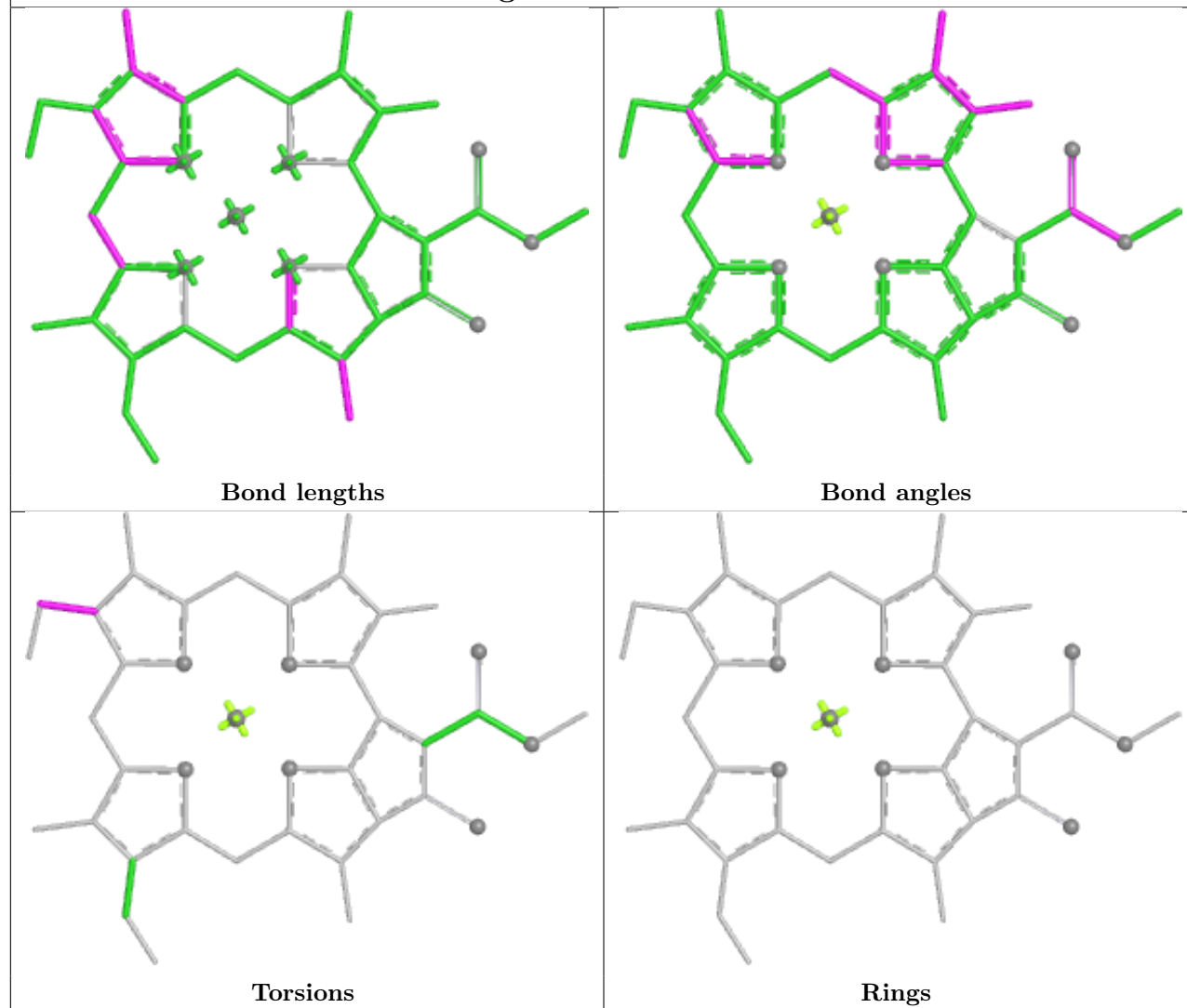


Ligand CLA A 827

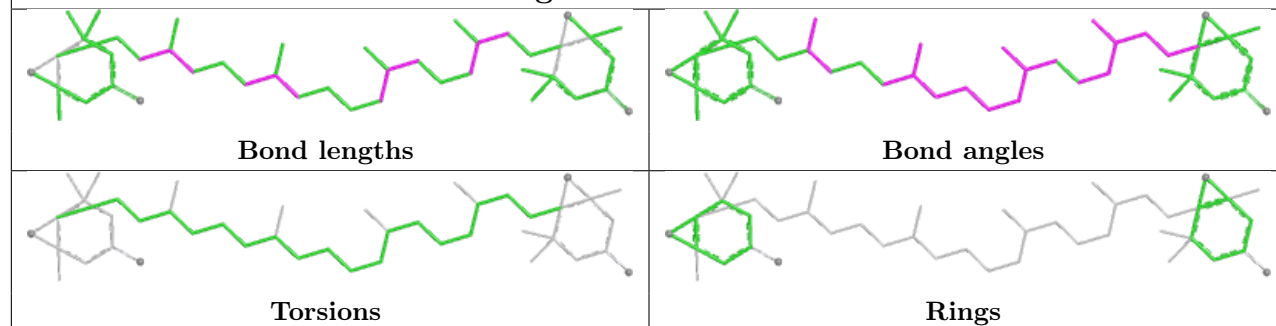




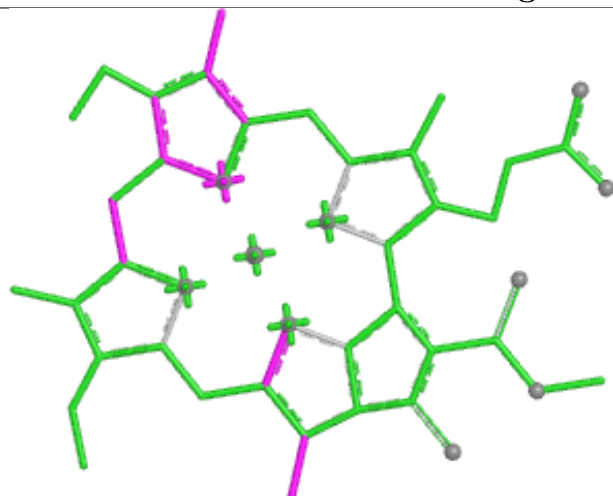
Ligand CLA a 603



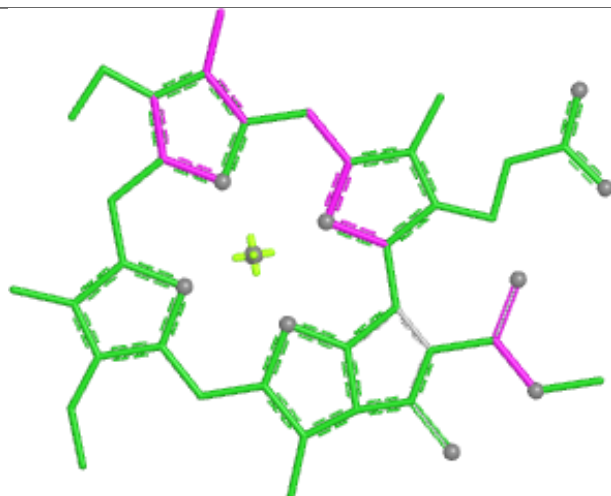
Ligand XAT 1 318



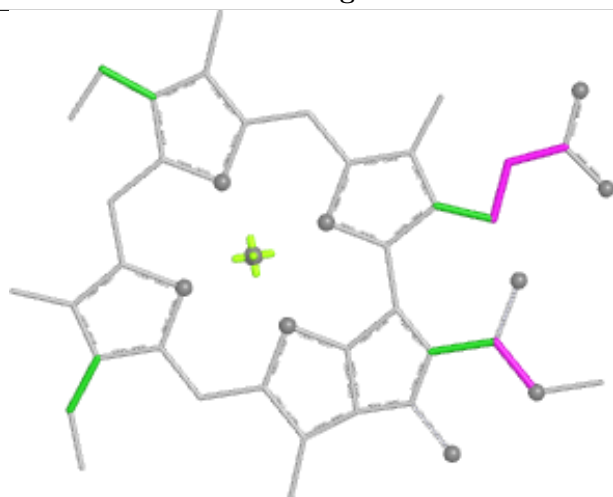
Ligand CLA 5 611



Bond lengths



Bond angles

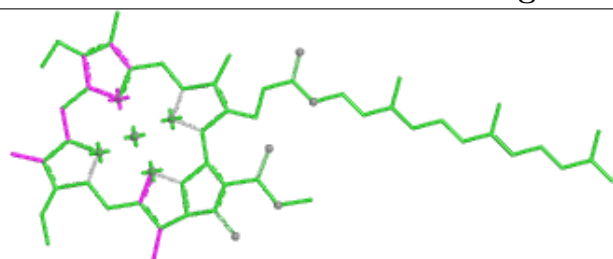


Torsions

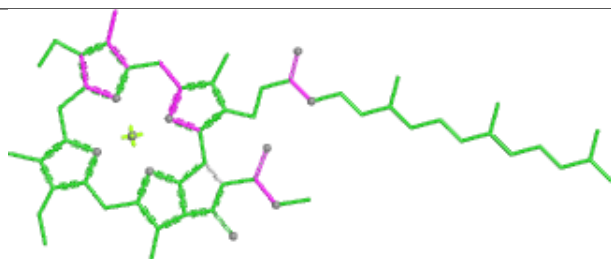


Rings

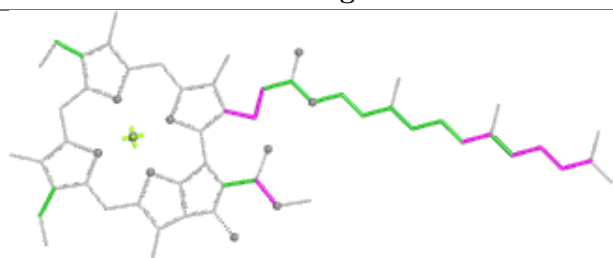
Ligand CLA a 602



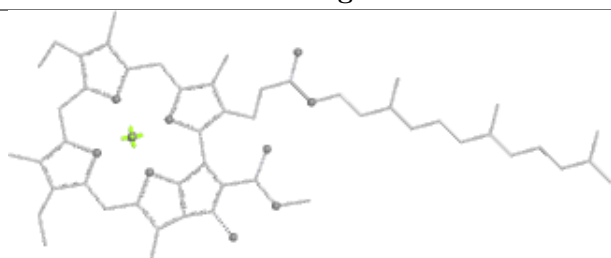
Bond lengths



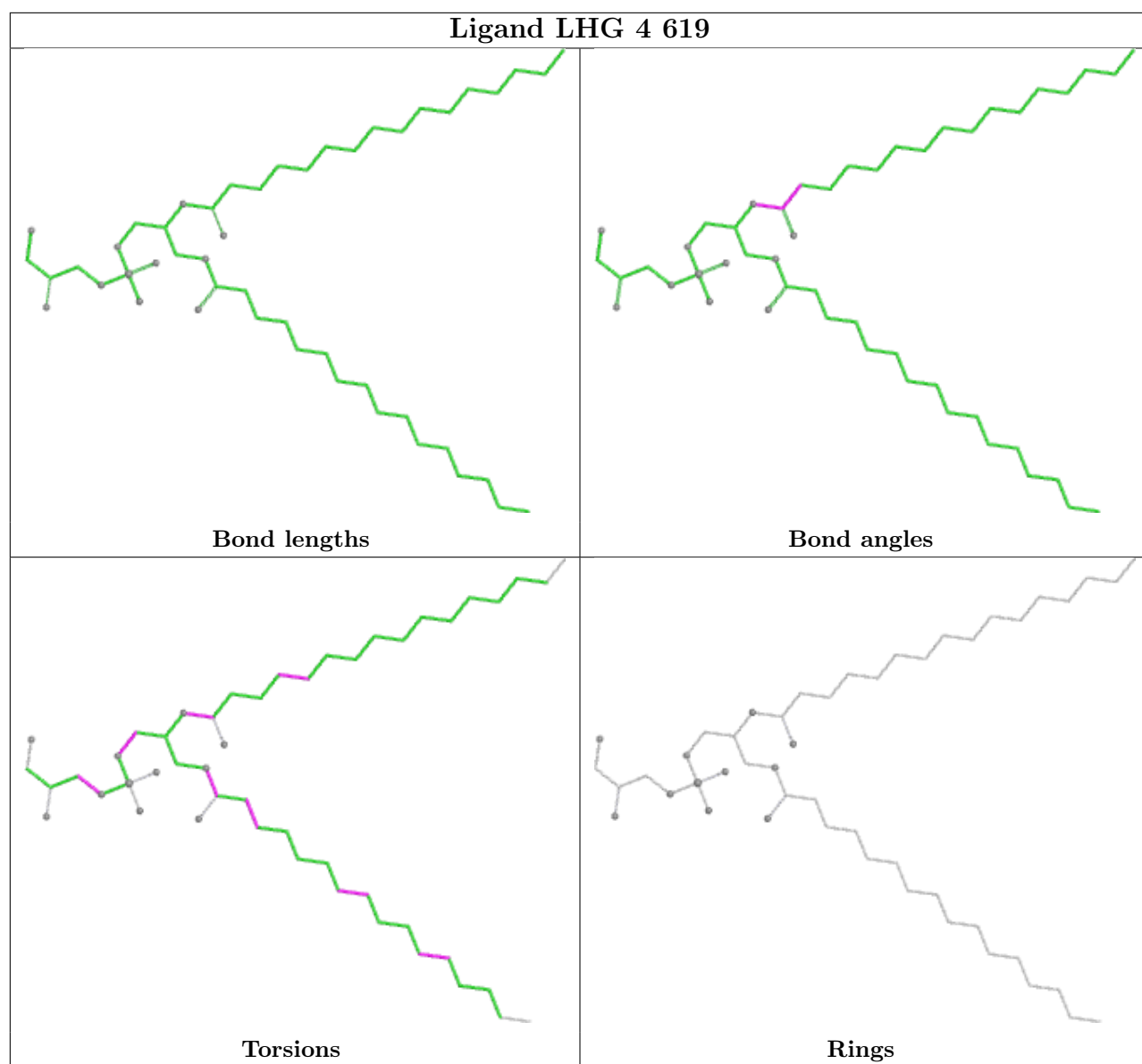
Bond angles

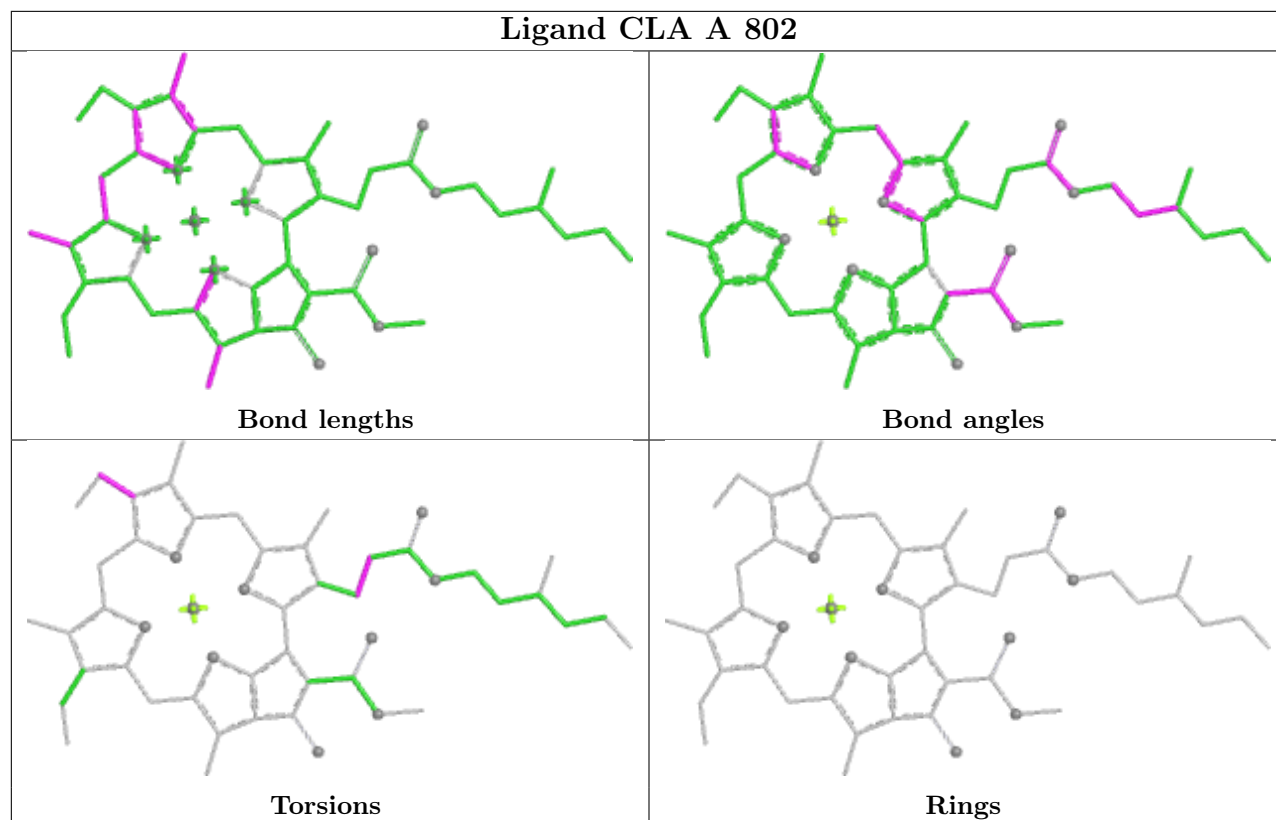


Torsions

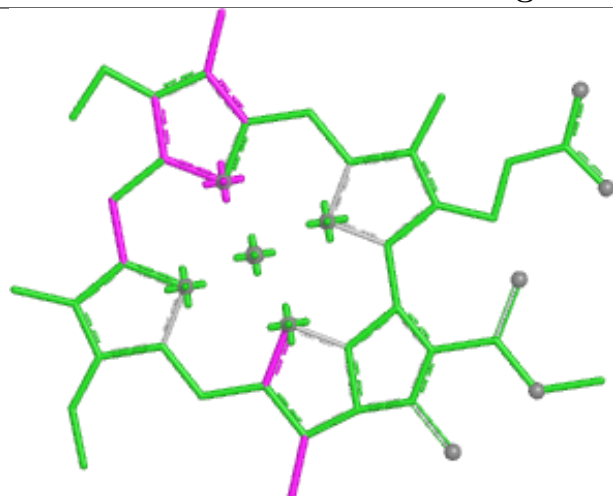


Rings

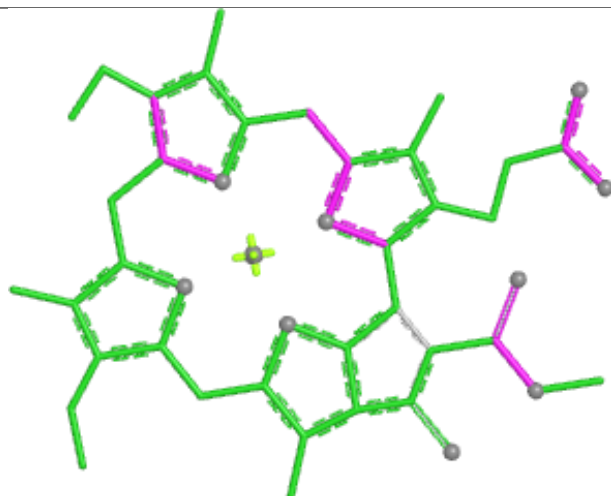




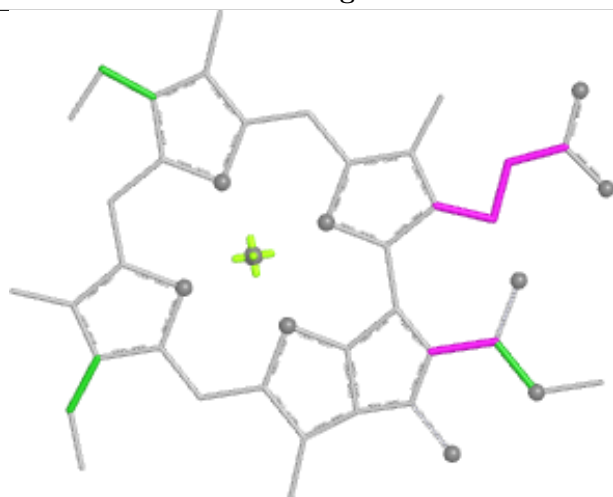
Ligand CLA L 302



Bond lengths



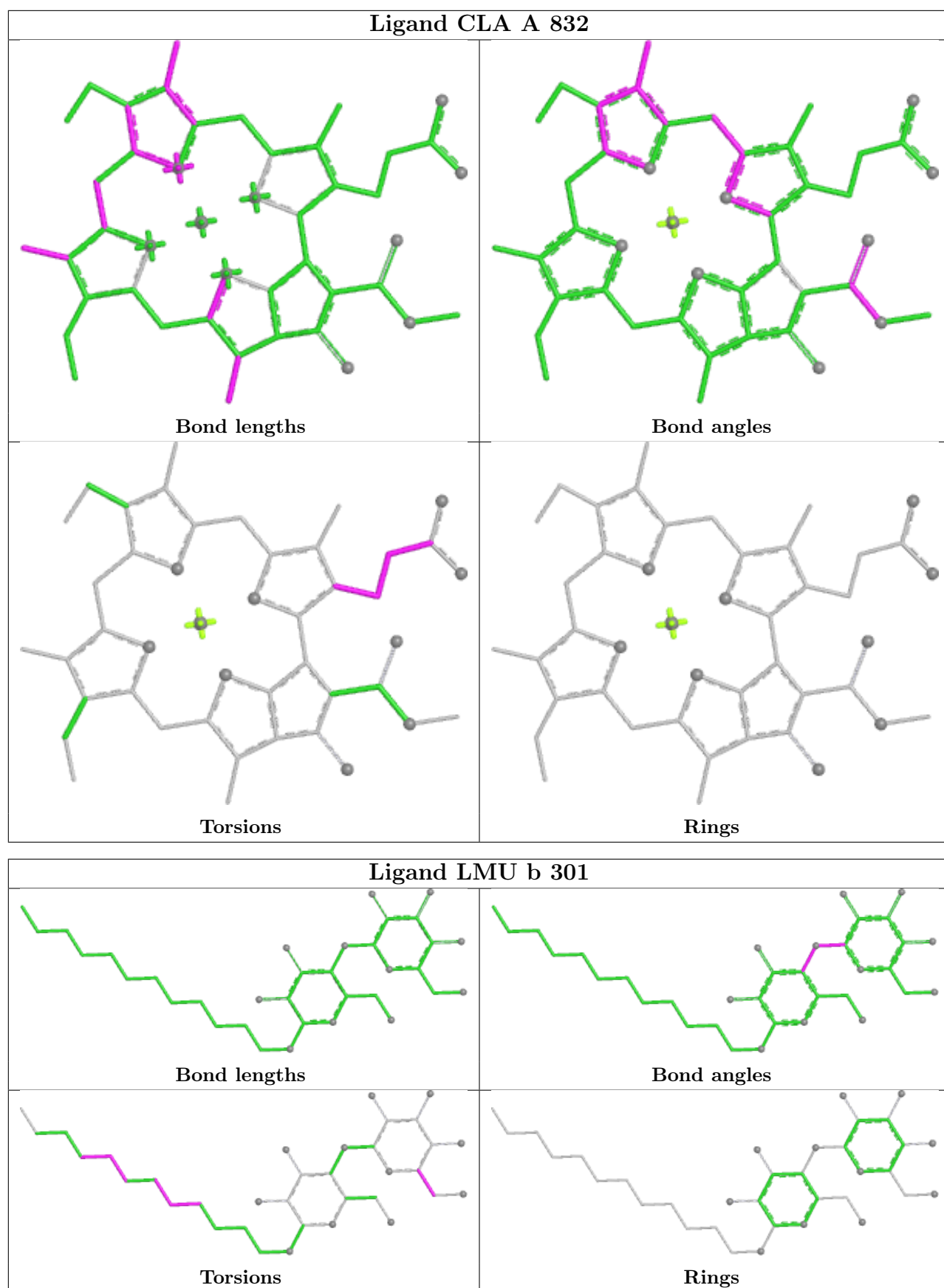
Bond angles



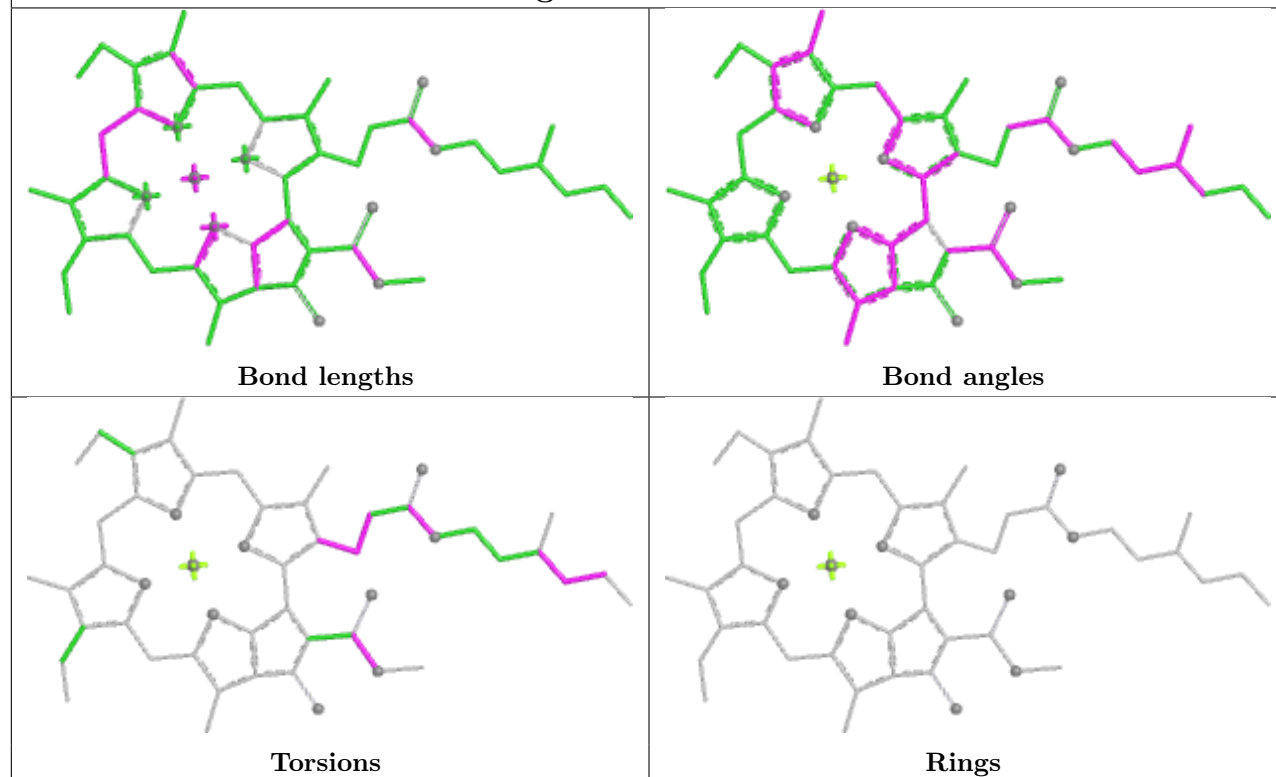
Torsions



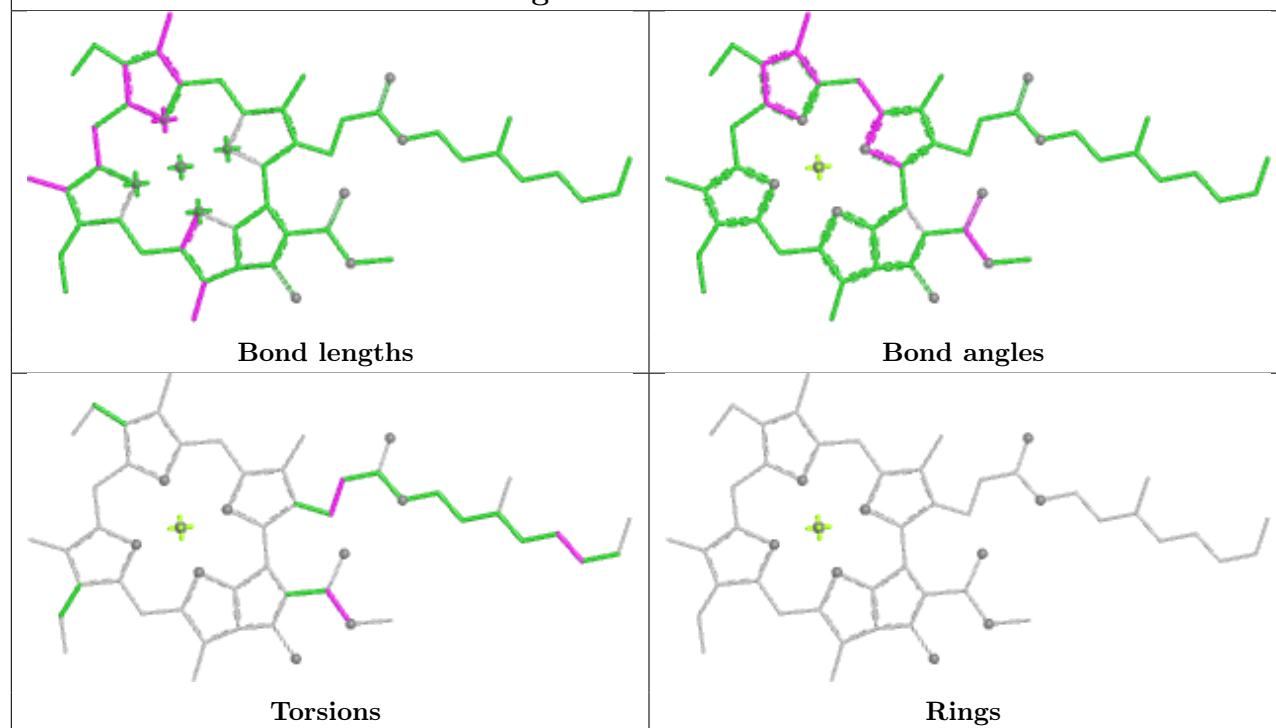
Rings

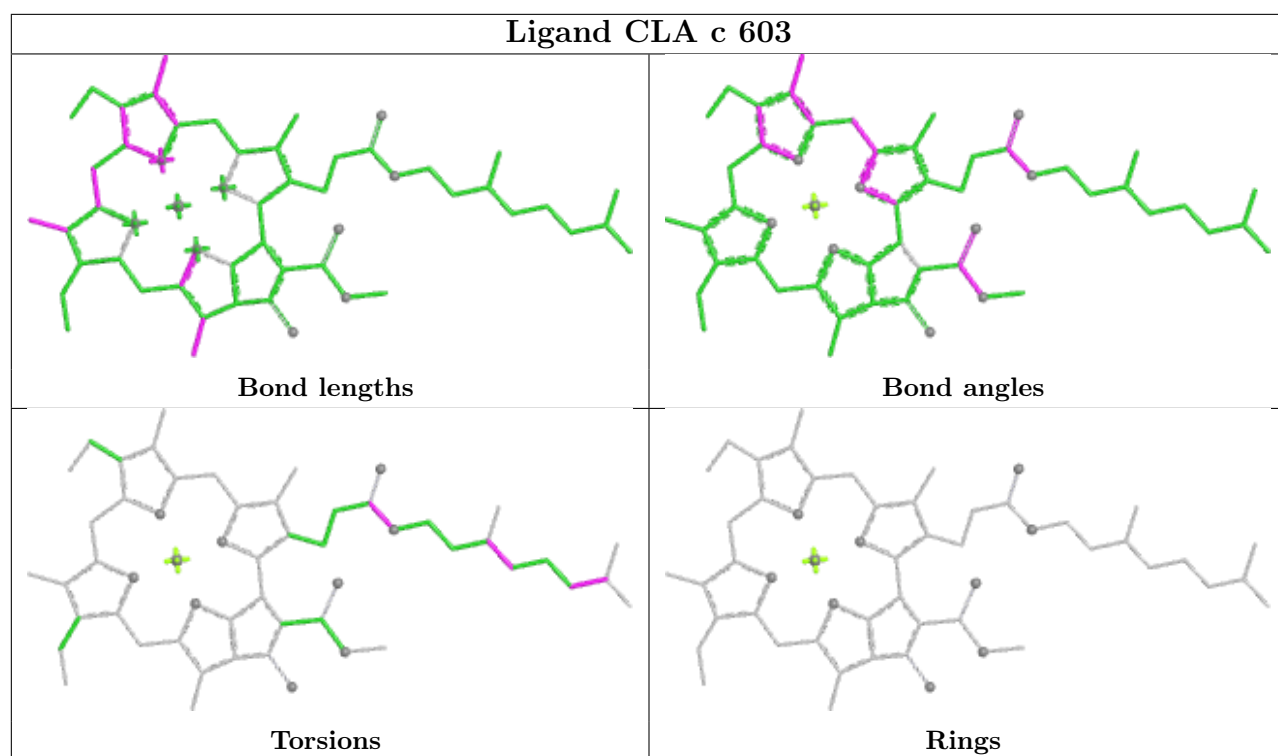


Ligand CLA 3 409

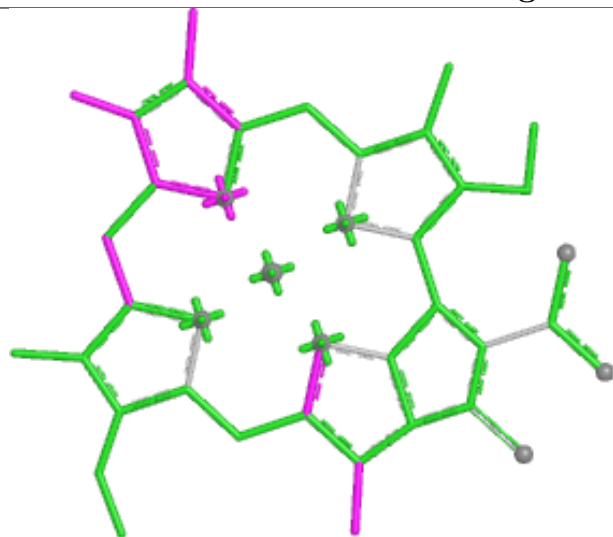


Ligand CLA A 813

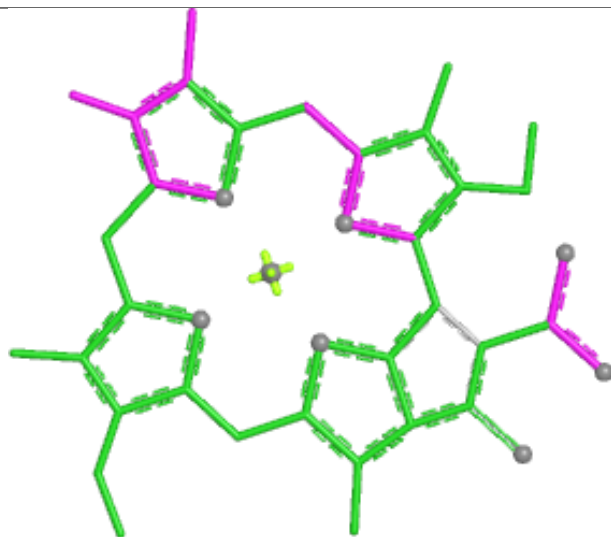




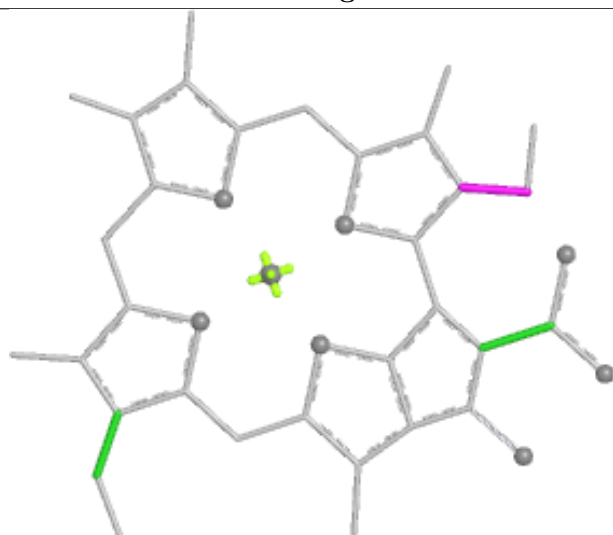
Ligand CLA 7 405



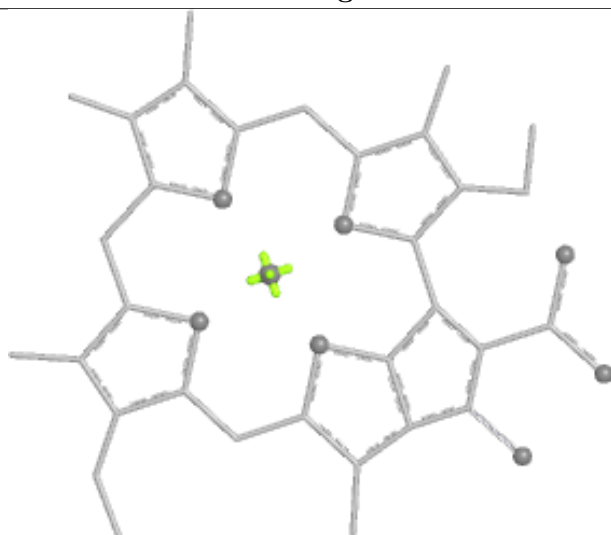
Bond lengths



Bond angles

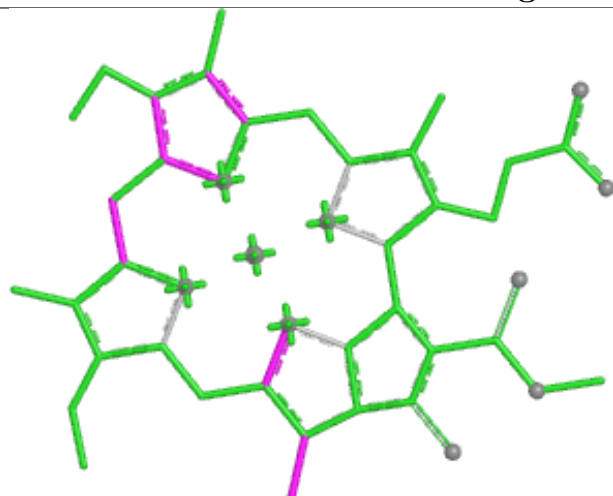


Torsions

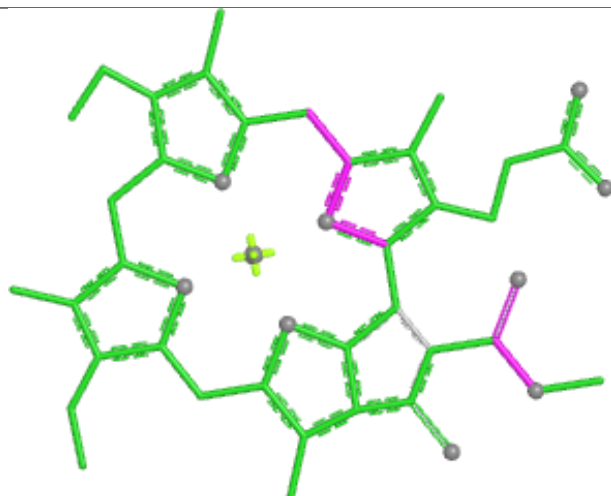


Rings

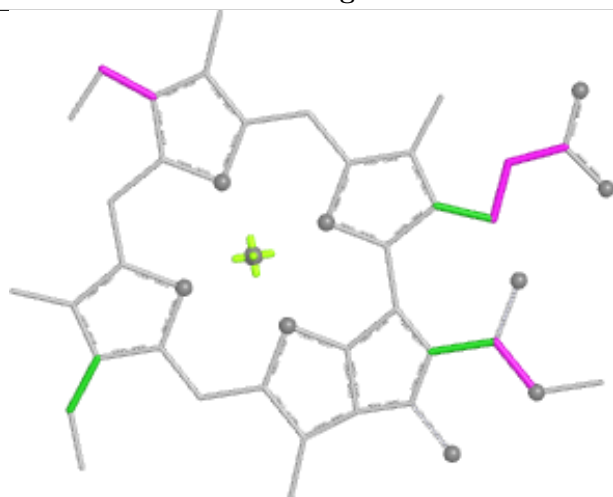
Ligand CLA 6 603



Bond lengths



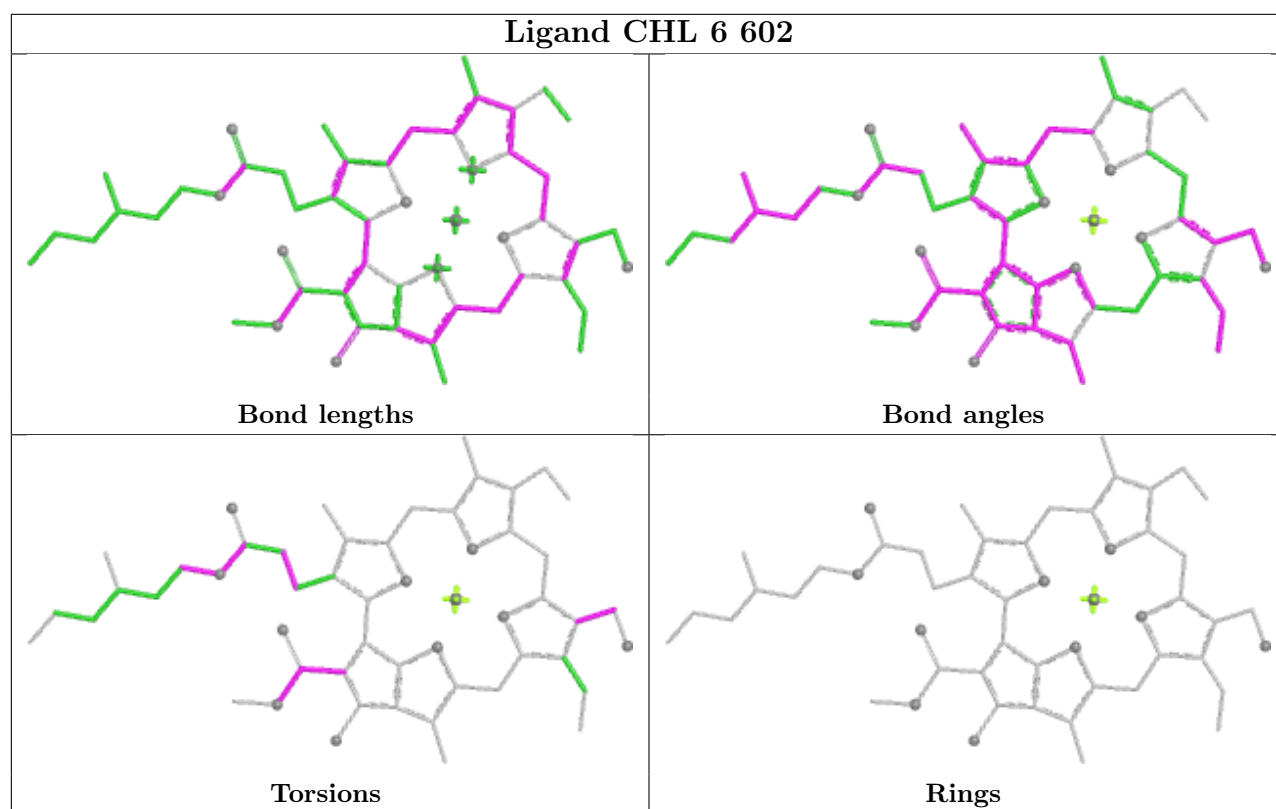
Bond angles

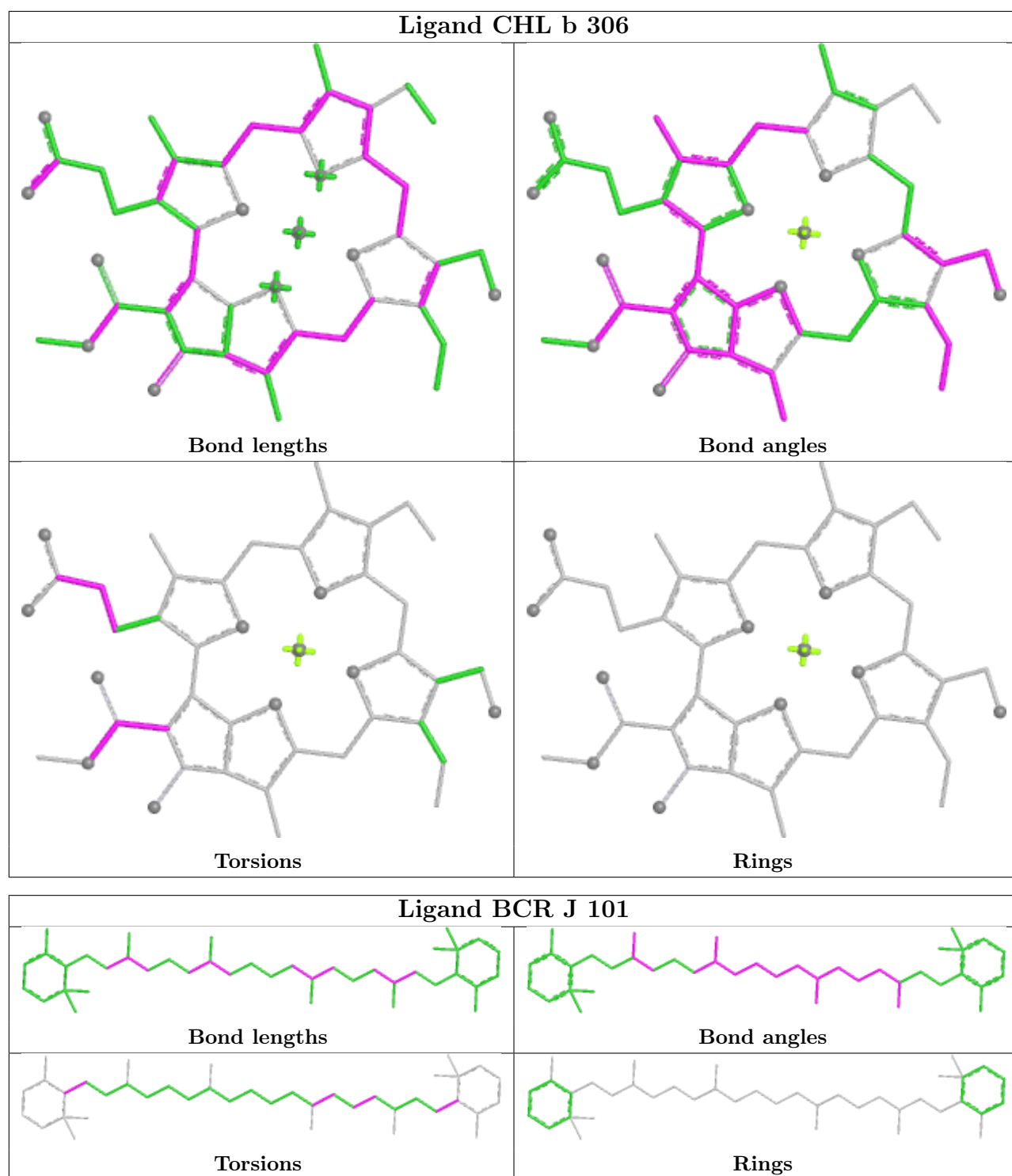


Torsions

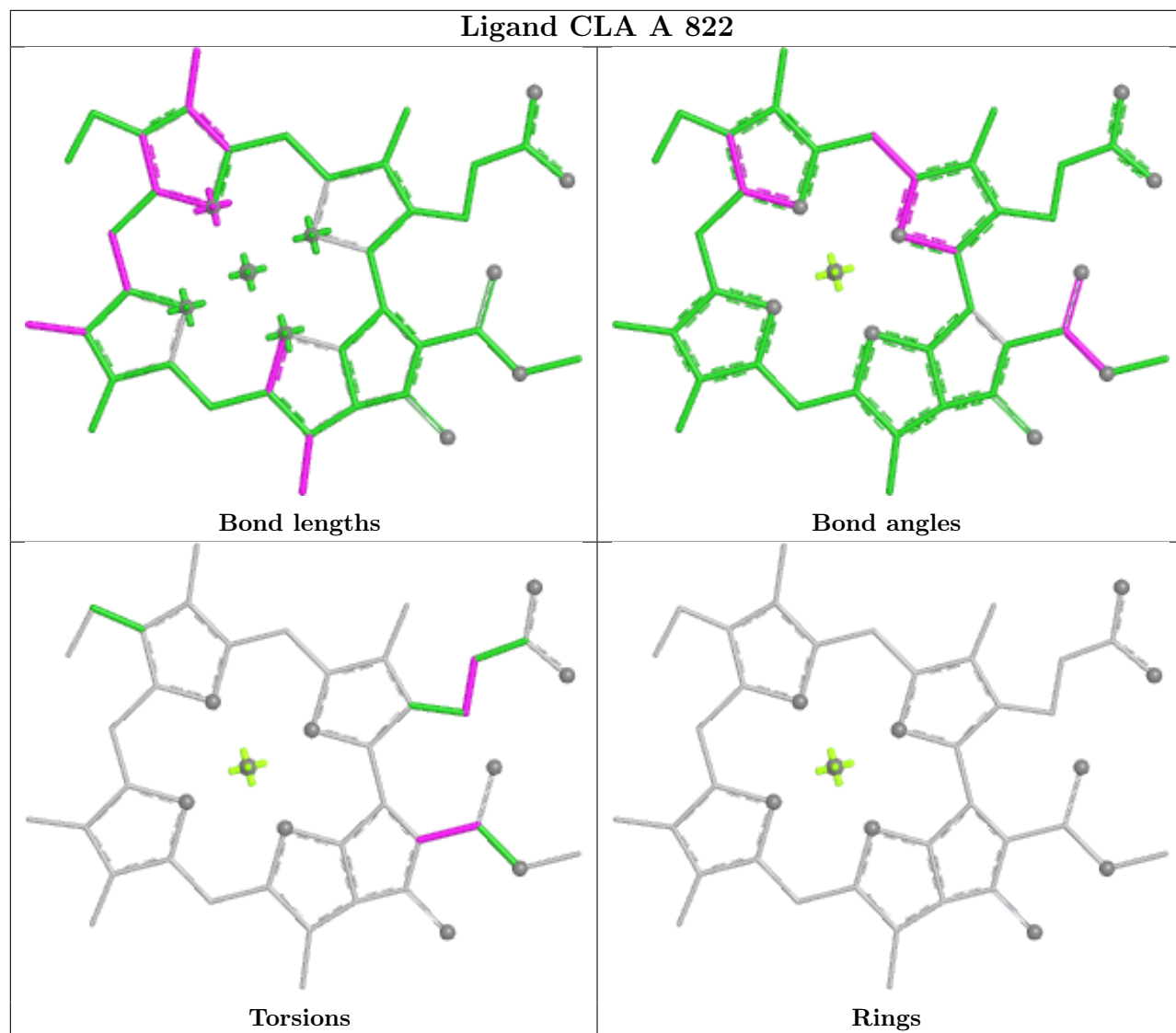


Rings

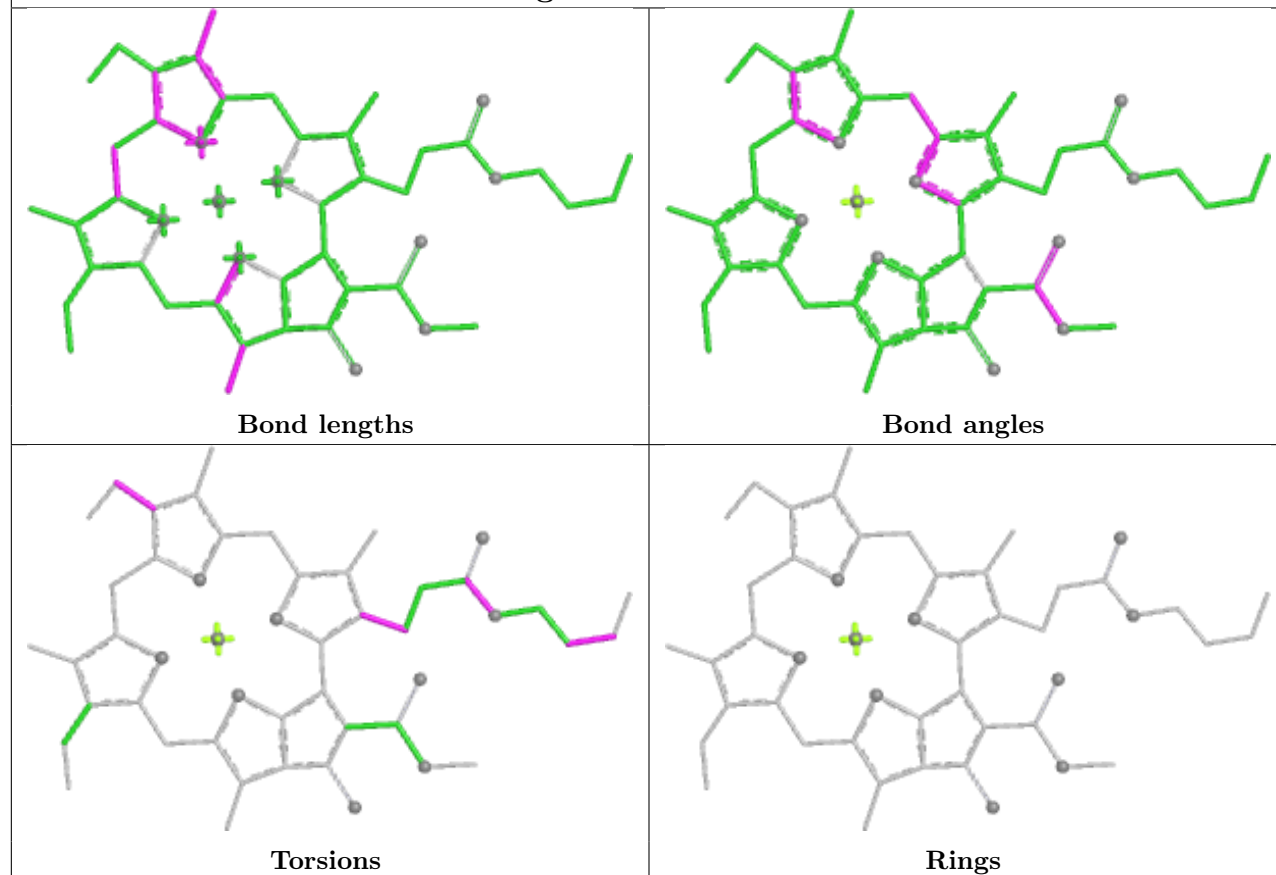




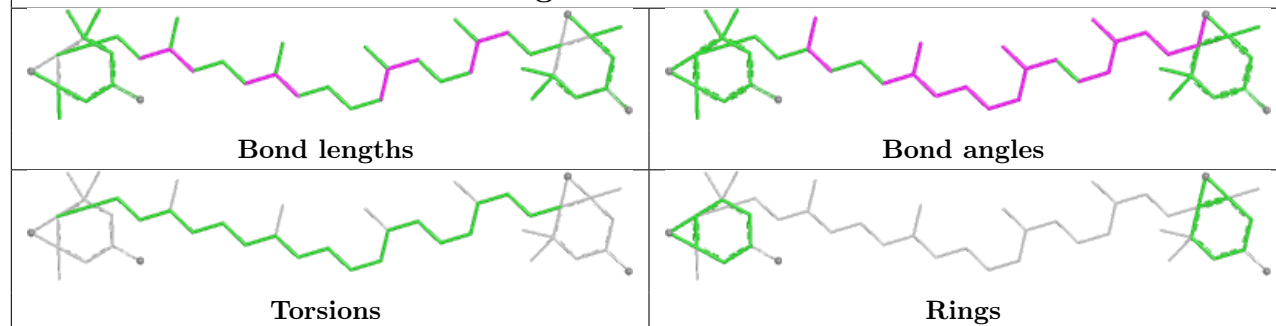
Ligand CLA A 822



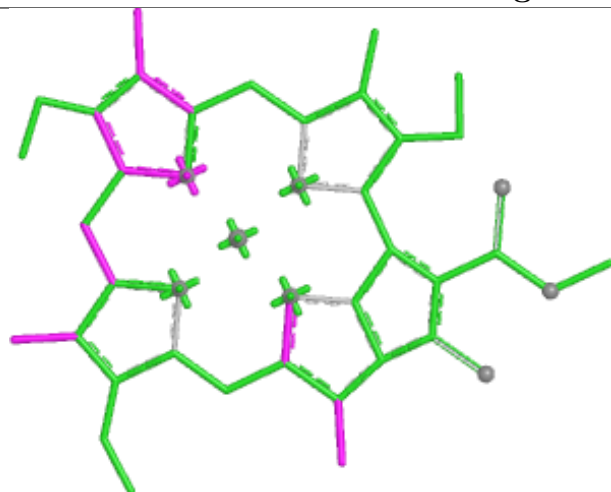
Ligand CLA 5 604



Ligand XAT 7 416



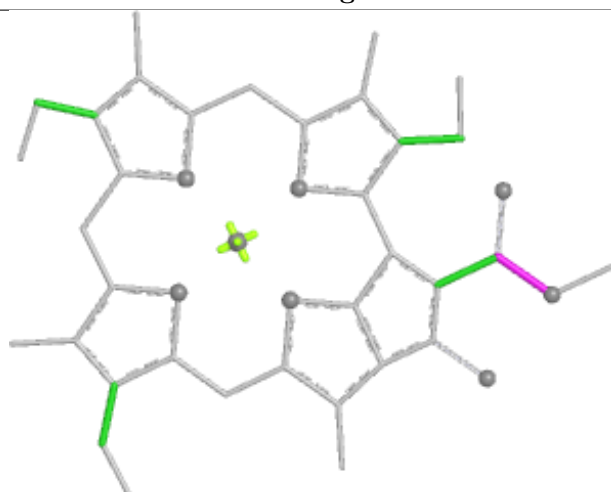
Ligand CLA A 816



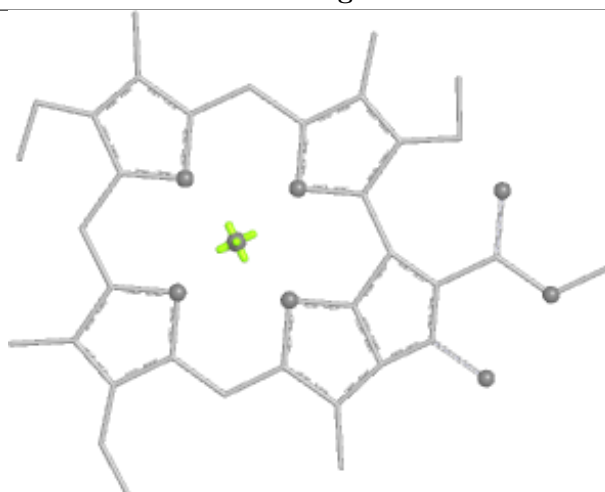
Bond lengths



Bond angles

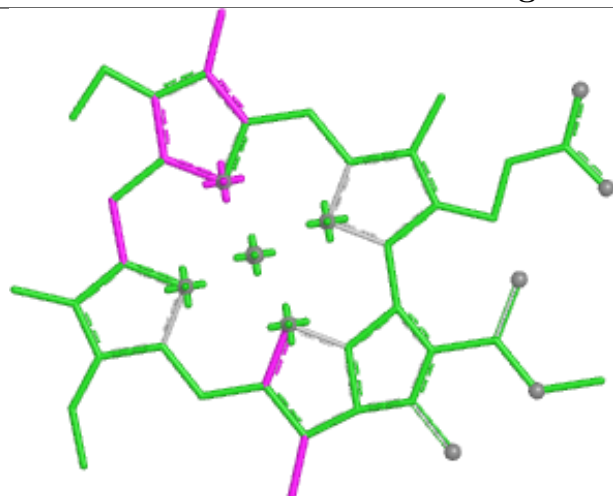


Torsions

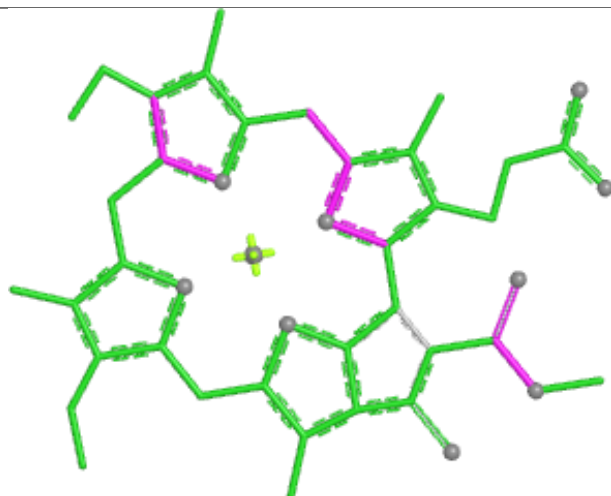


Rings

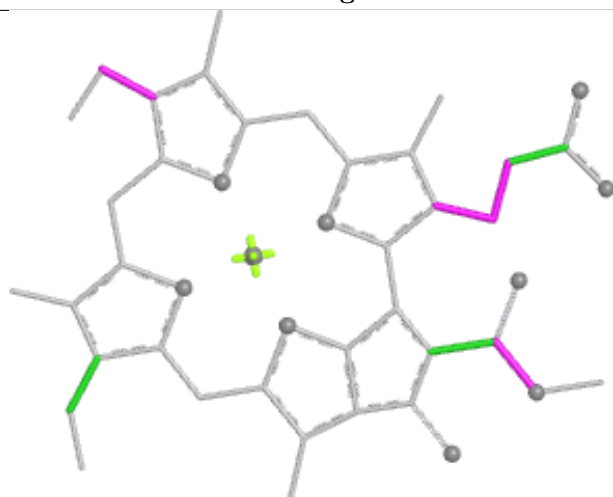
Ligand CLA 6 608



Bond lengths



Bond angles

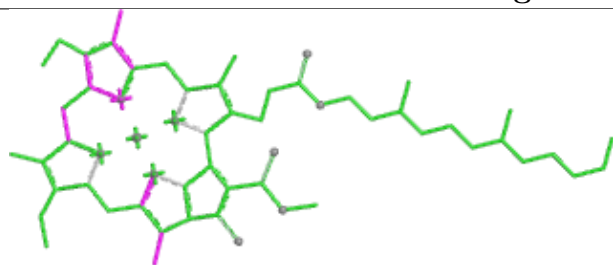


Torsions

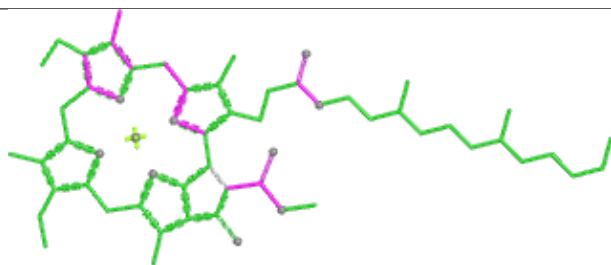


Rings

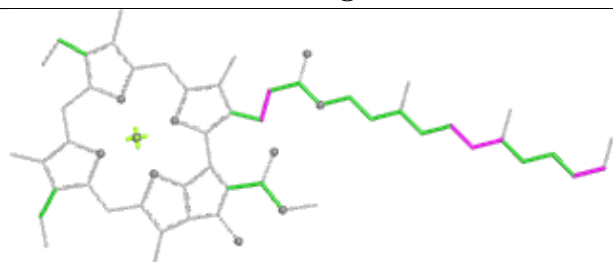
Ligand CLA A 809



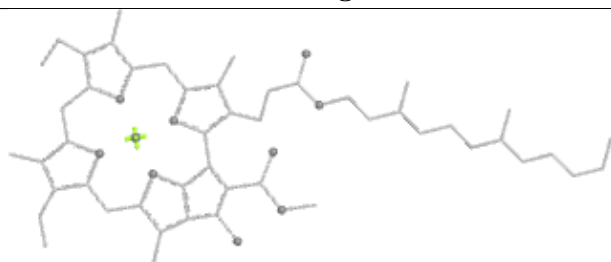
Bond lengths



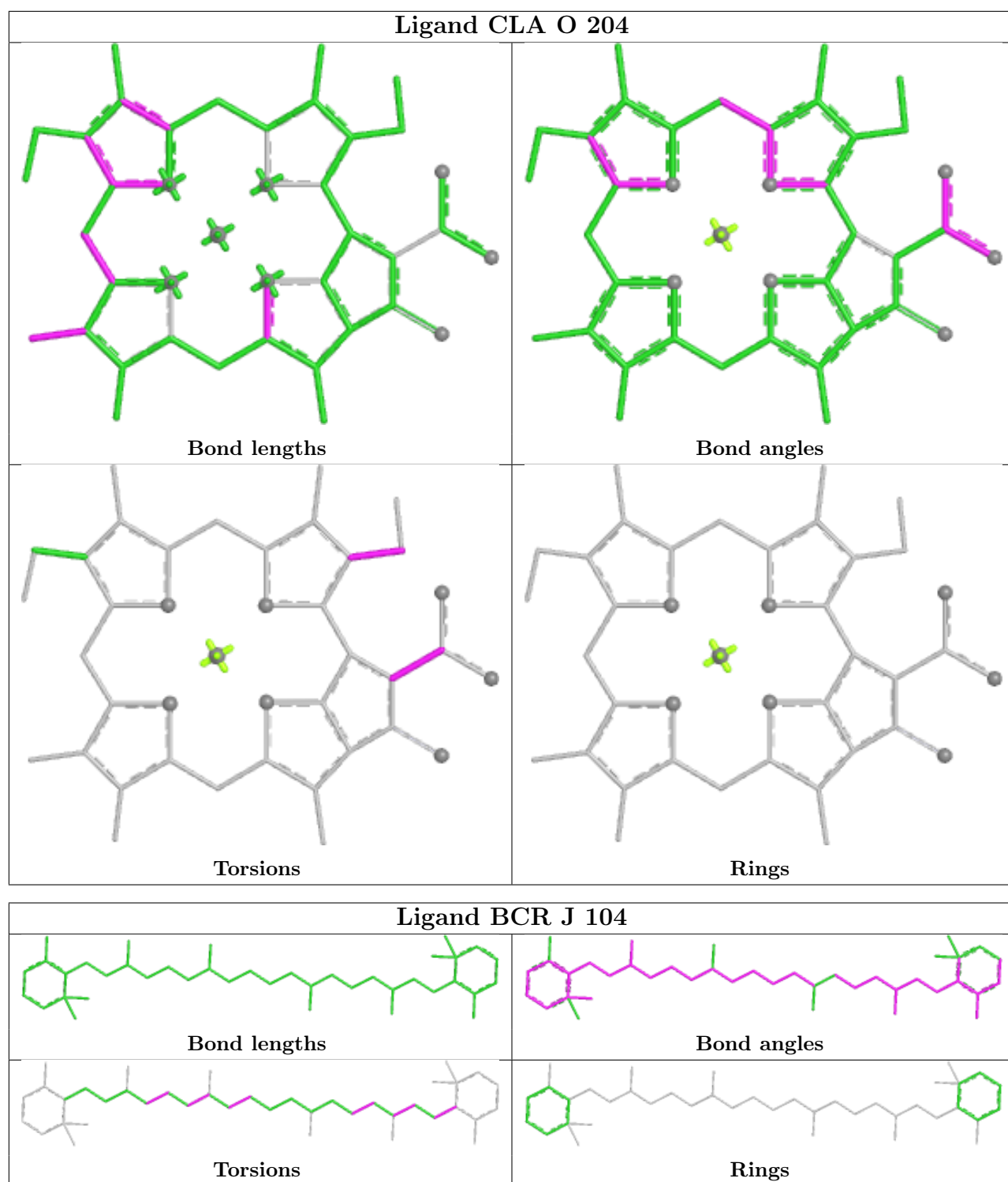
Bond angles

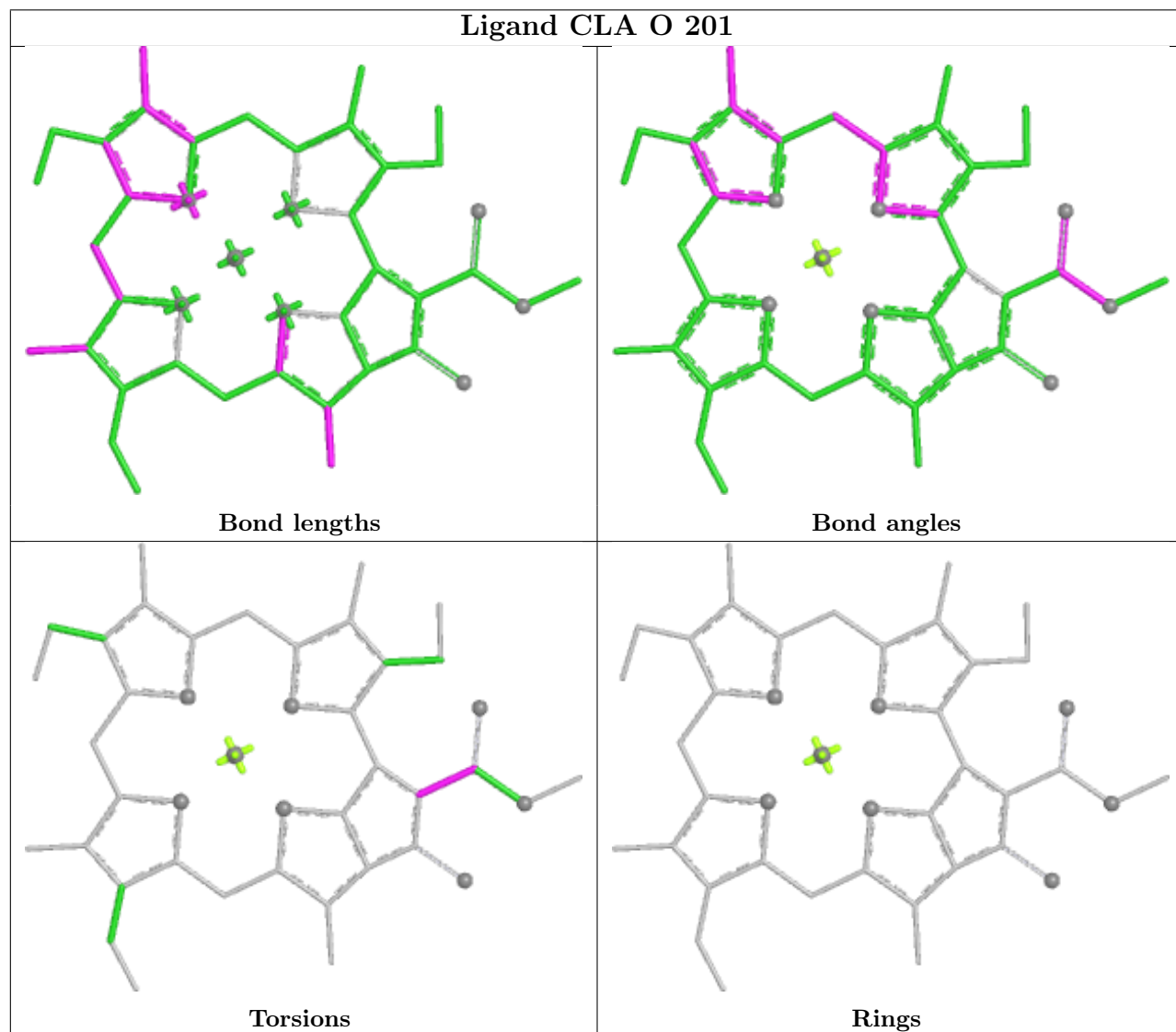
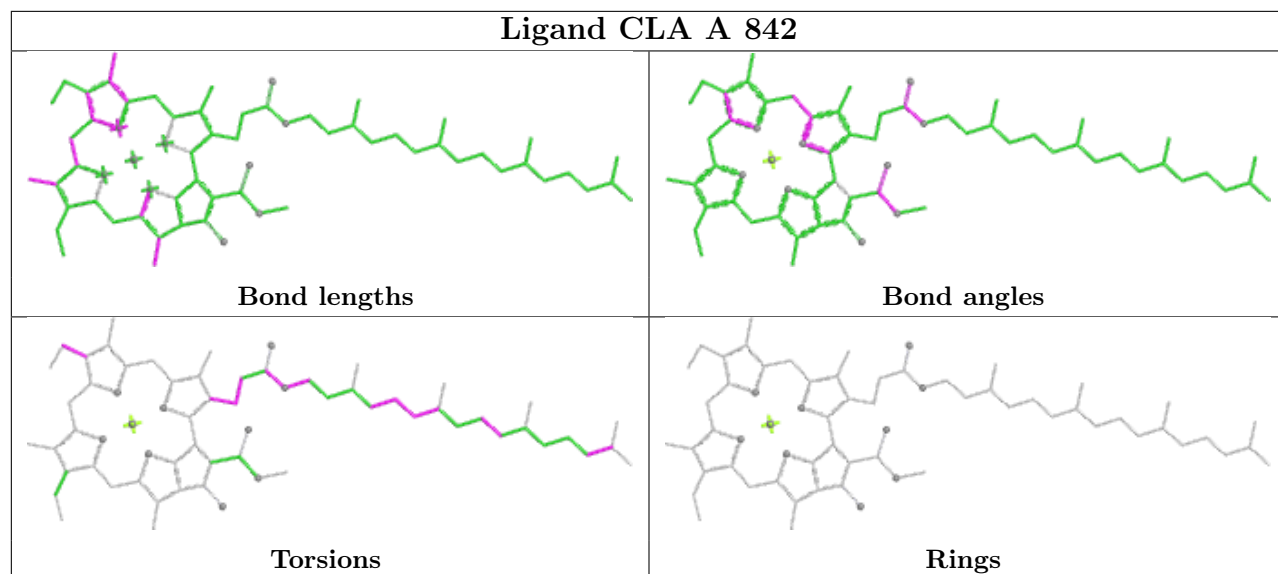


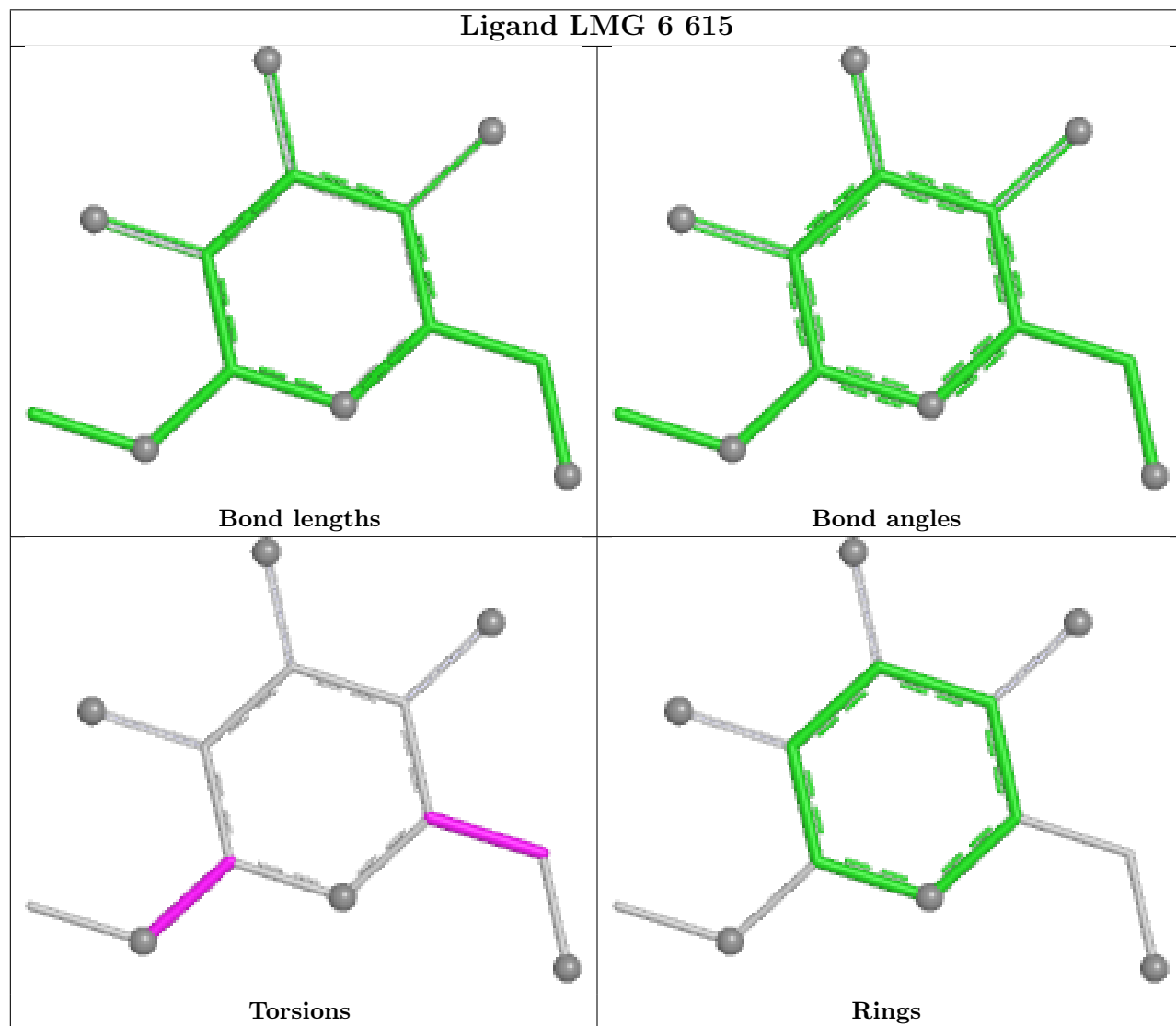
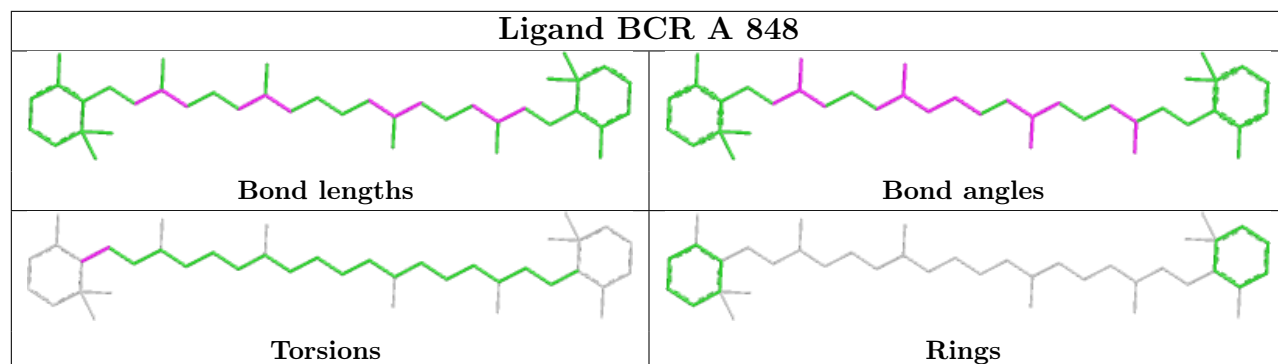
Torsions

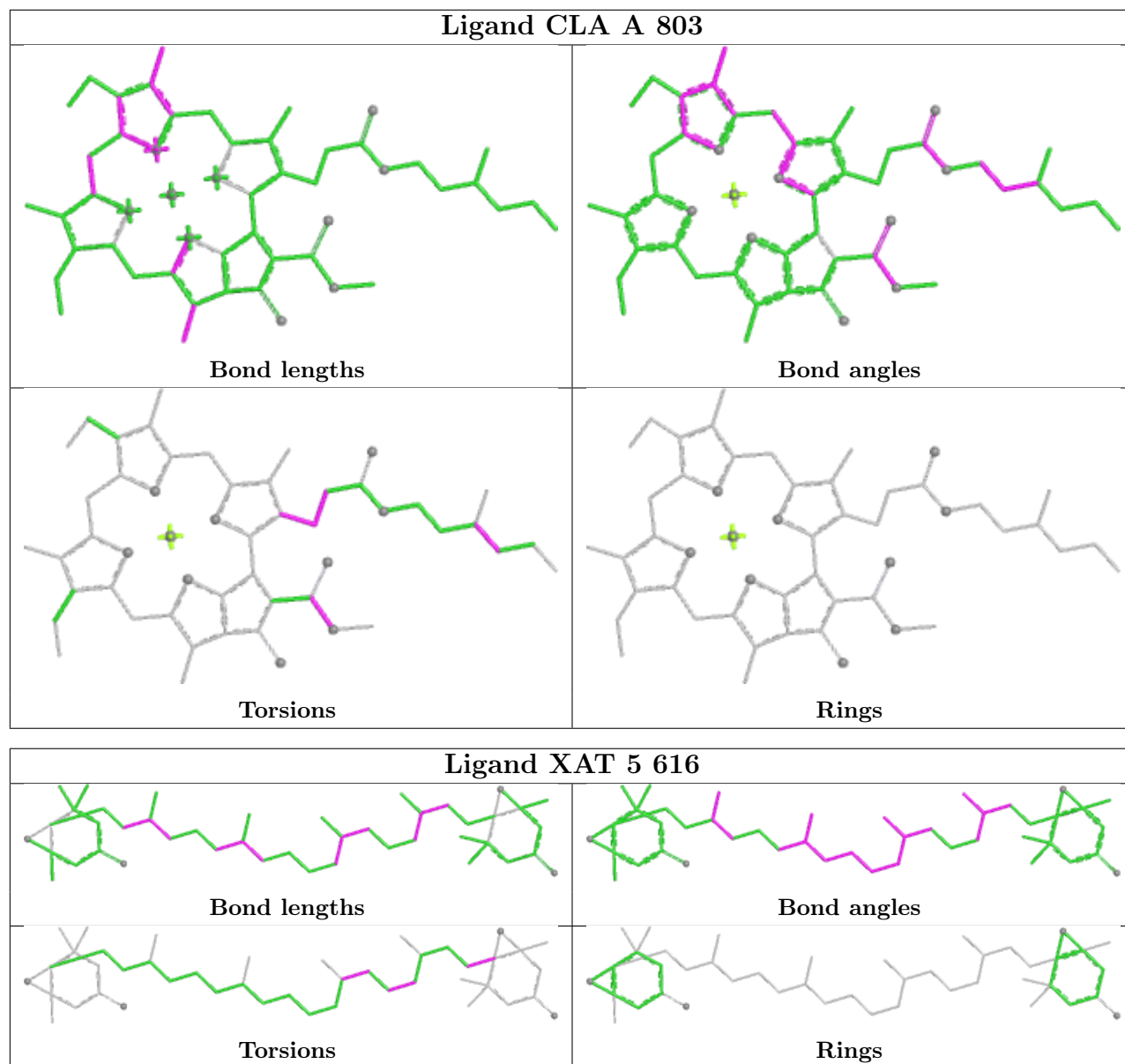


Rings

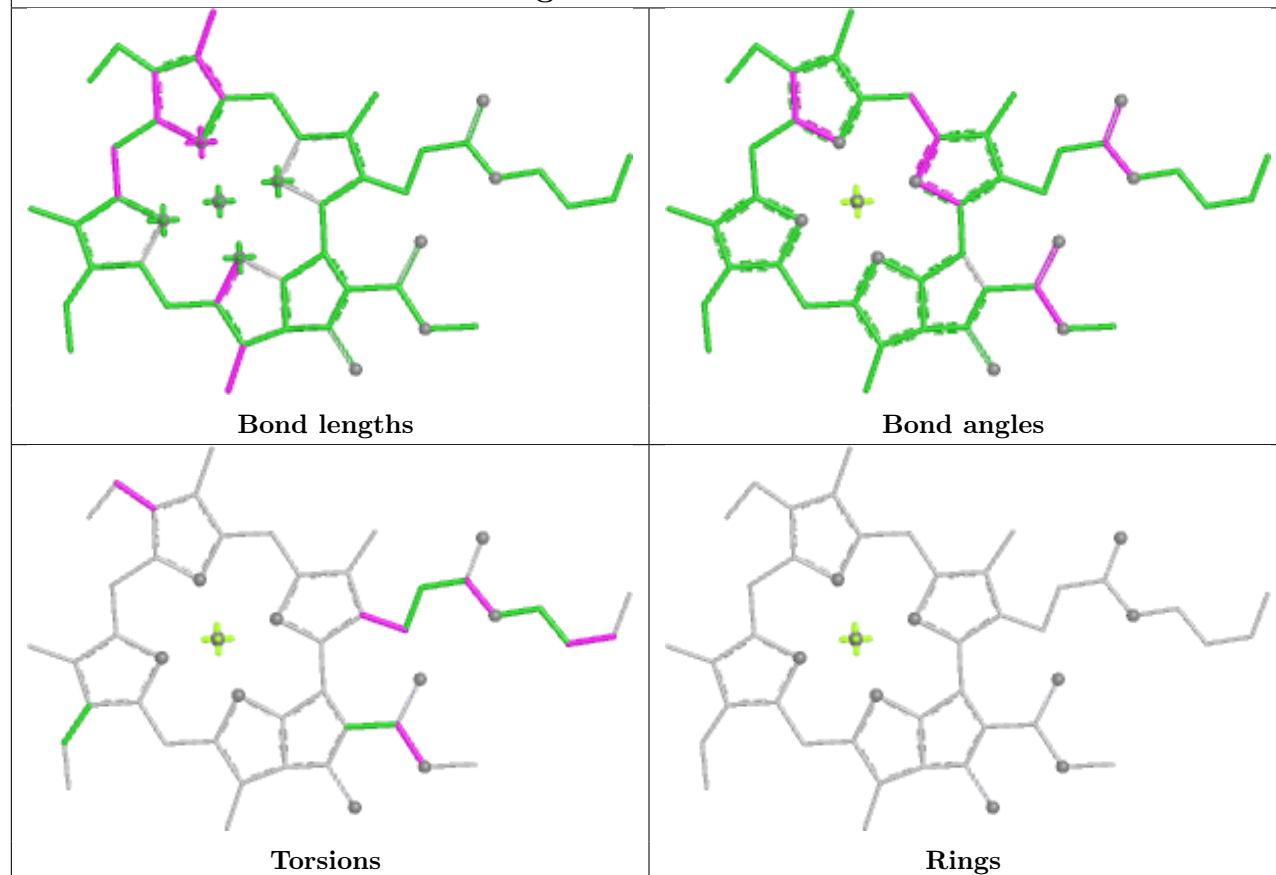




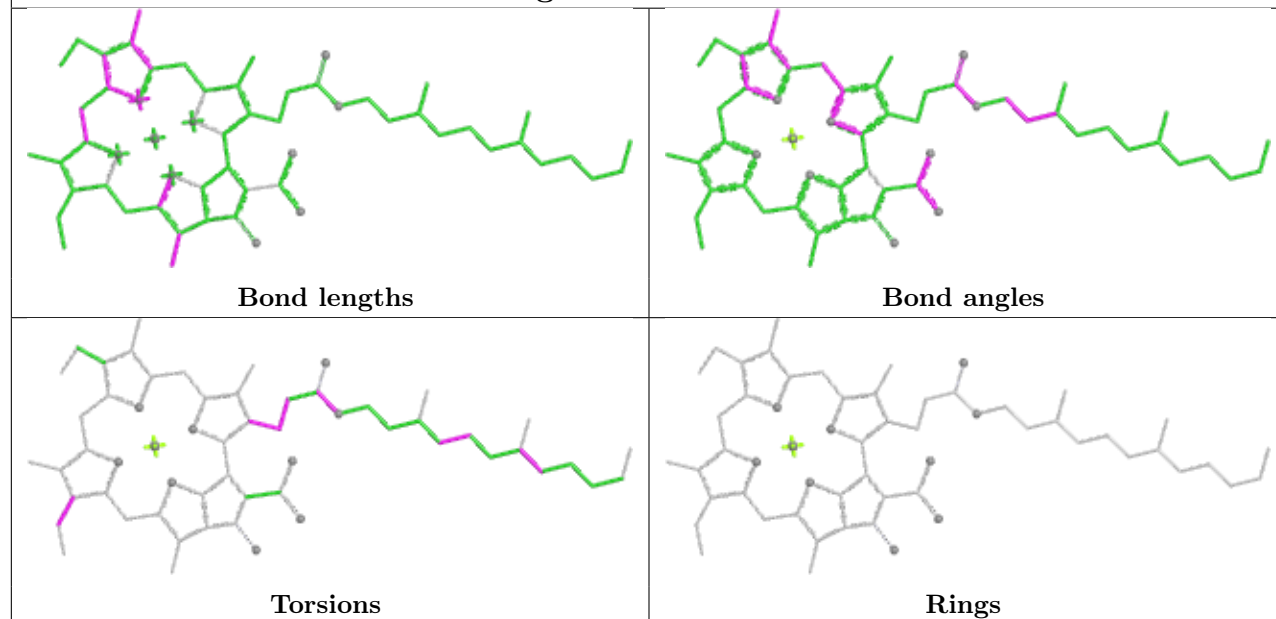




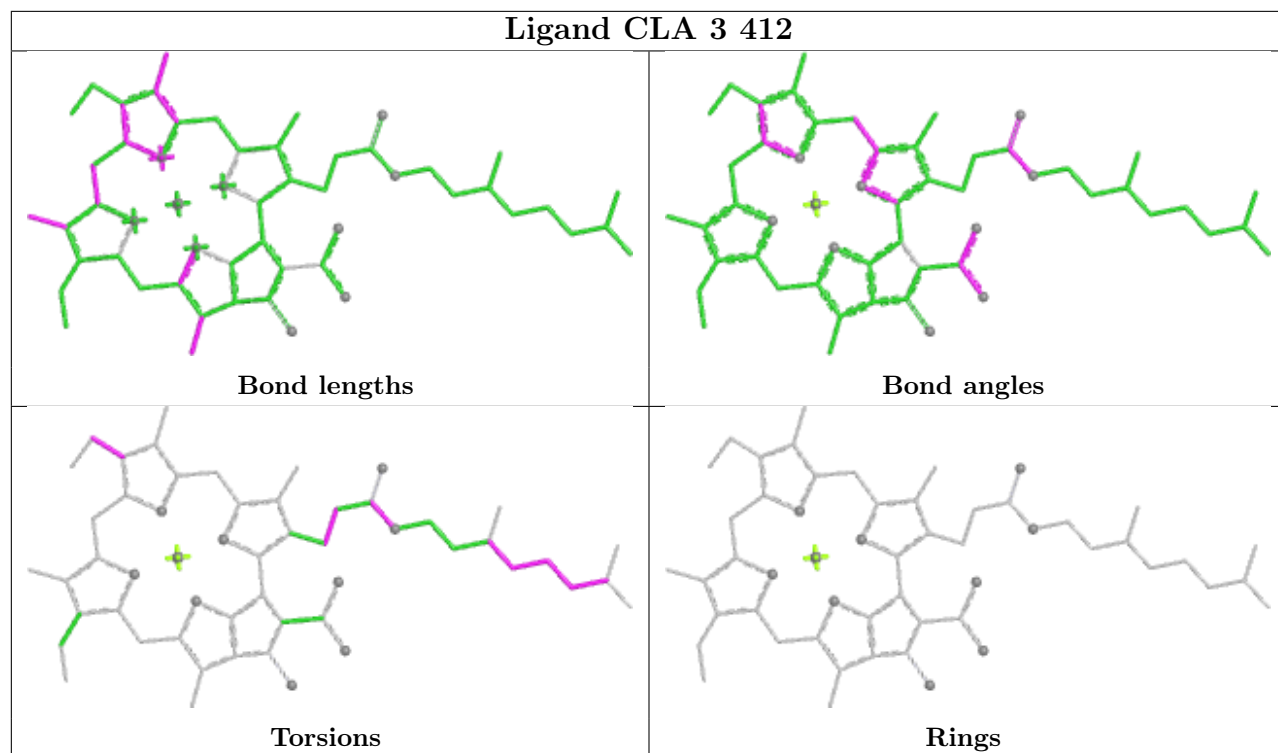
Ligand CLA 1 305



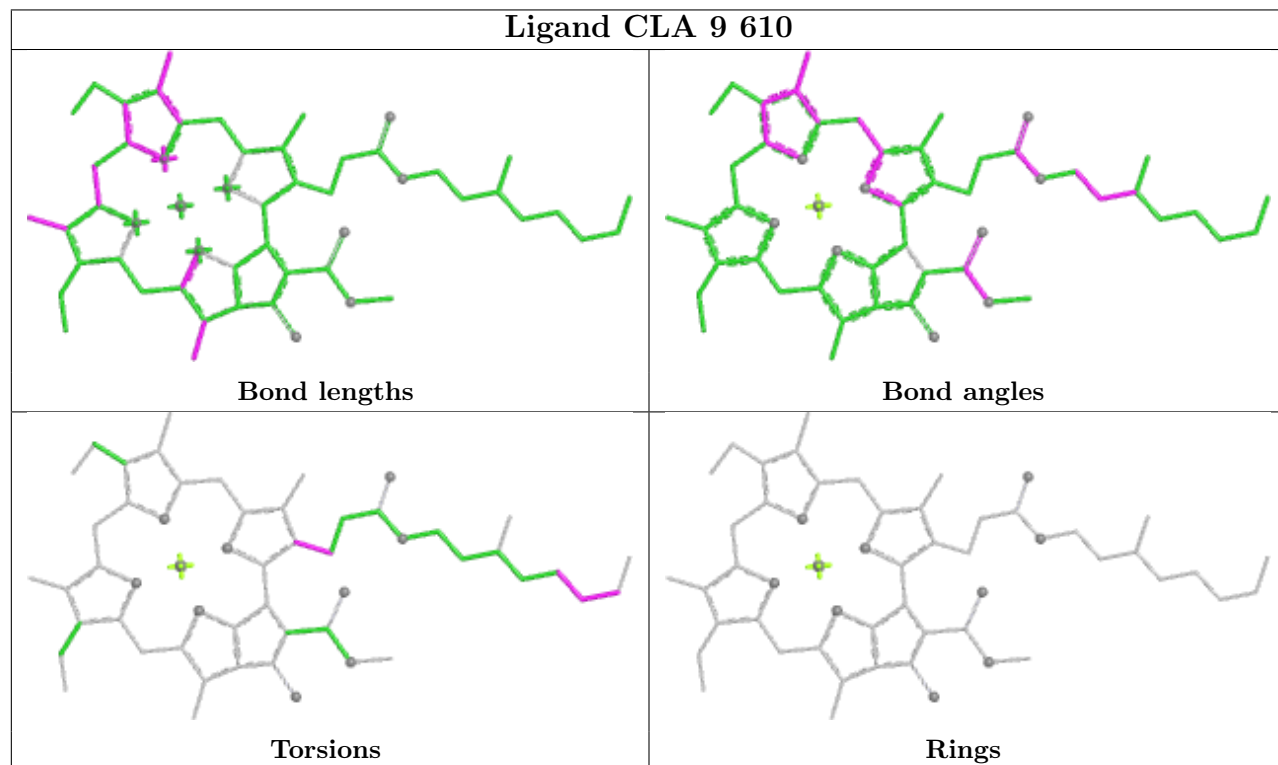
Ligand CLA 4 602

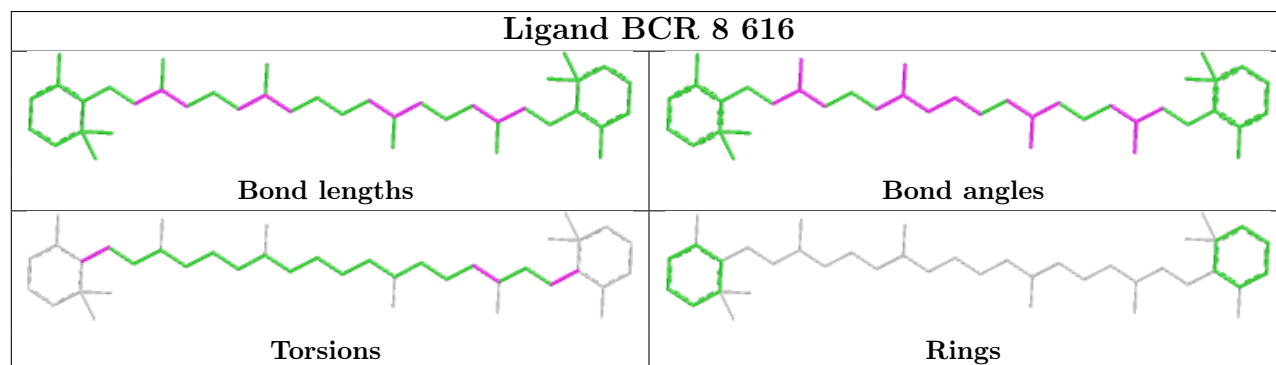
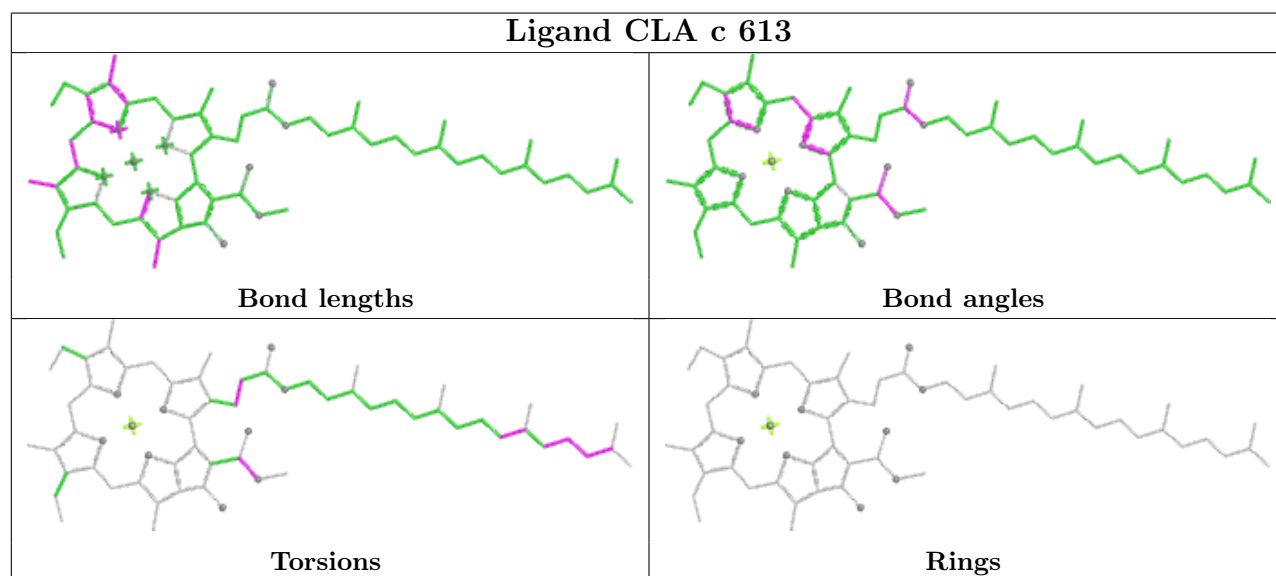
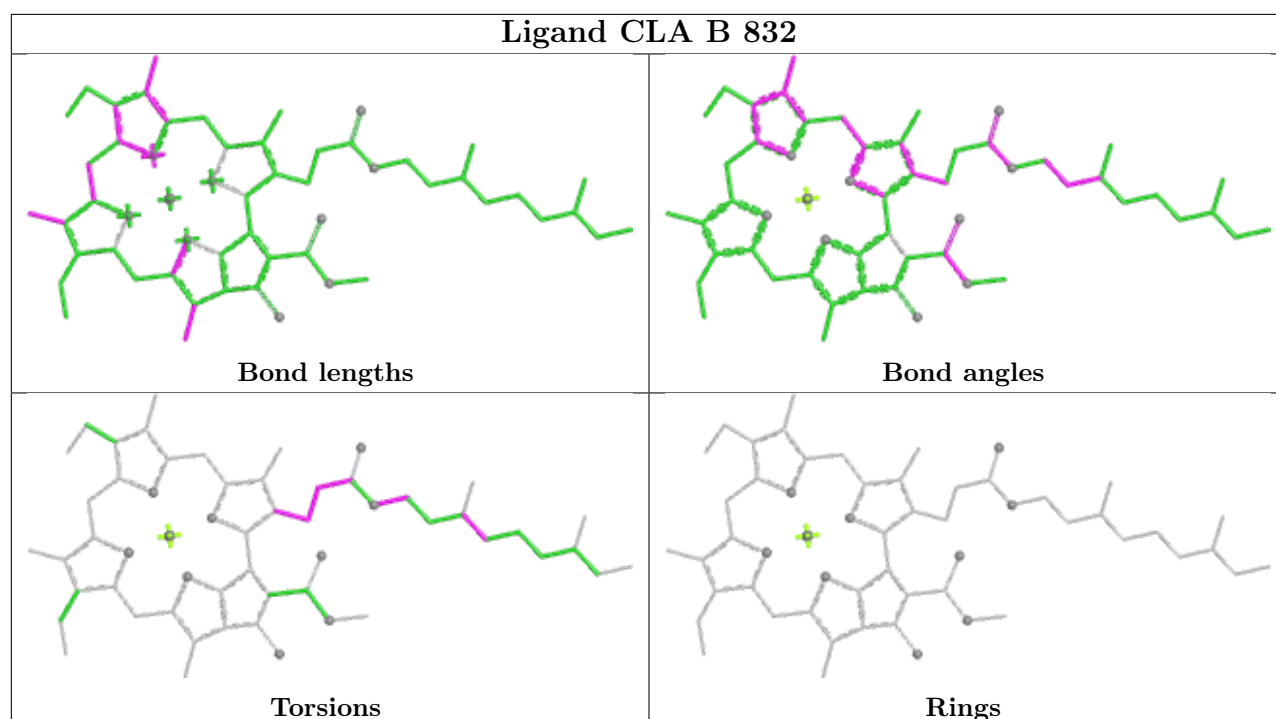


Ligand CLA 3 412

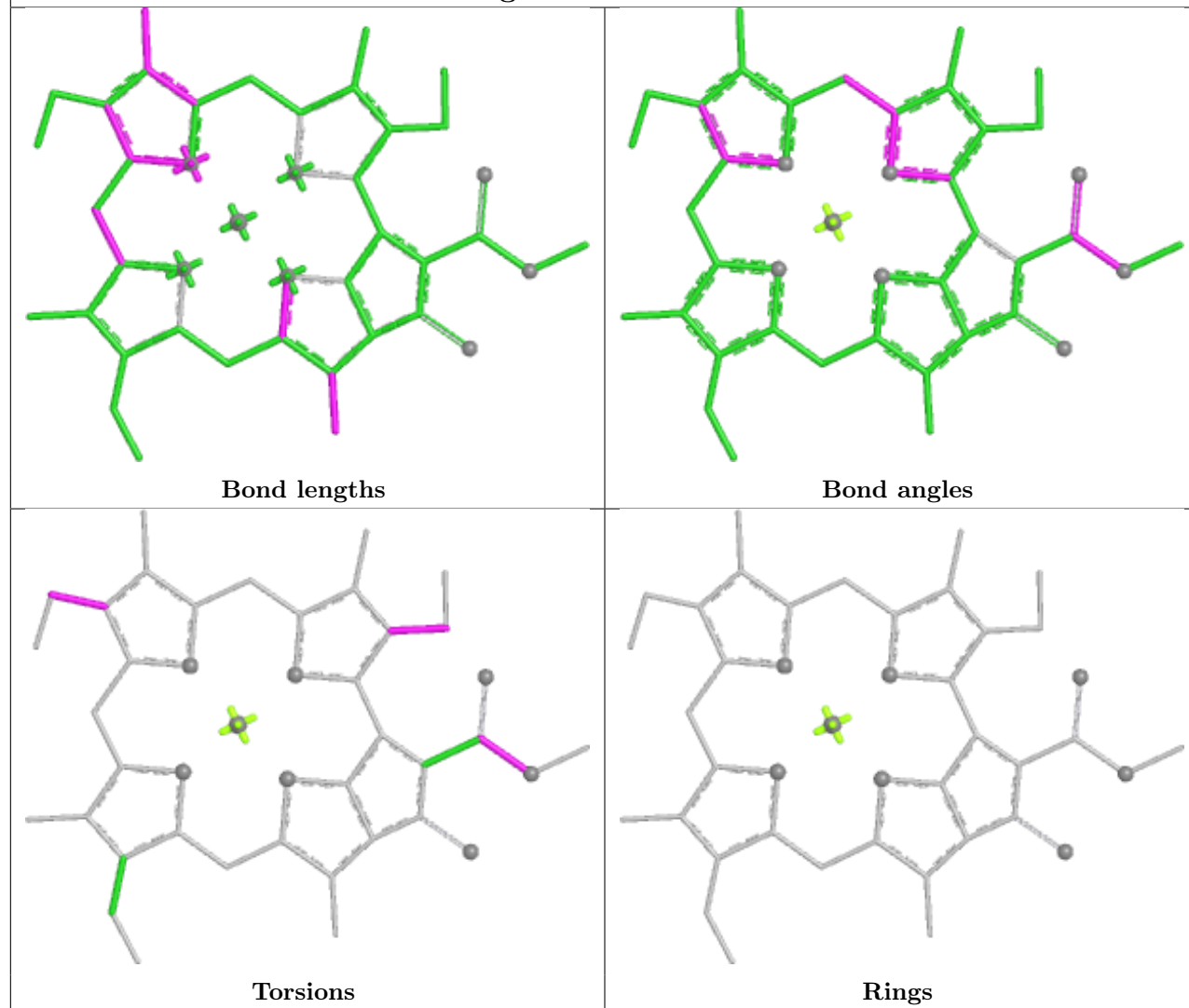


Ligand CLA 9 610

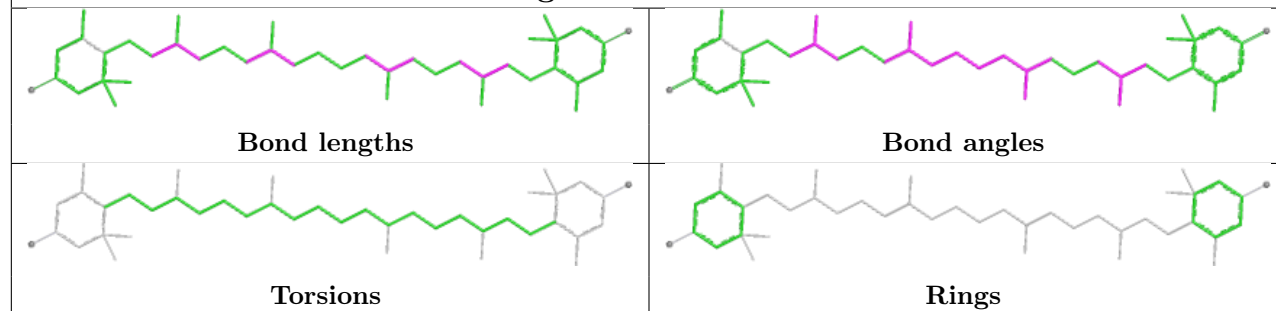




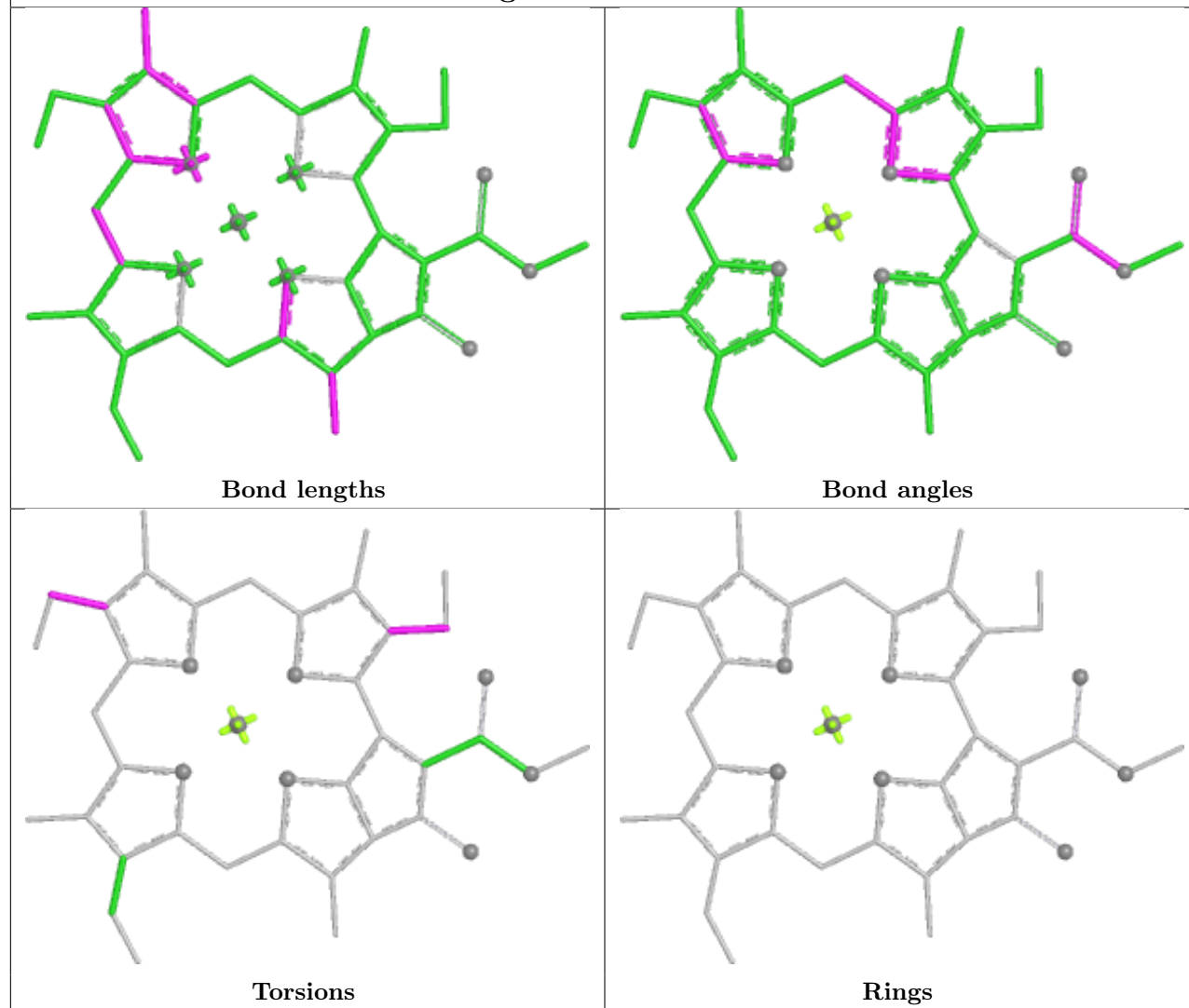
Ligand CLA 6 613



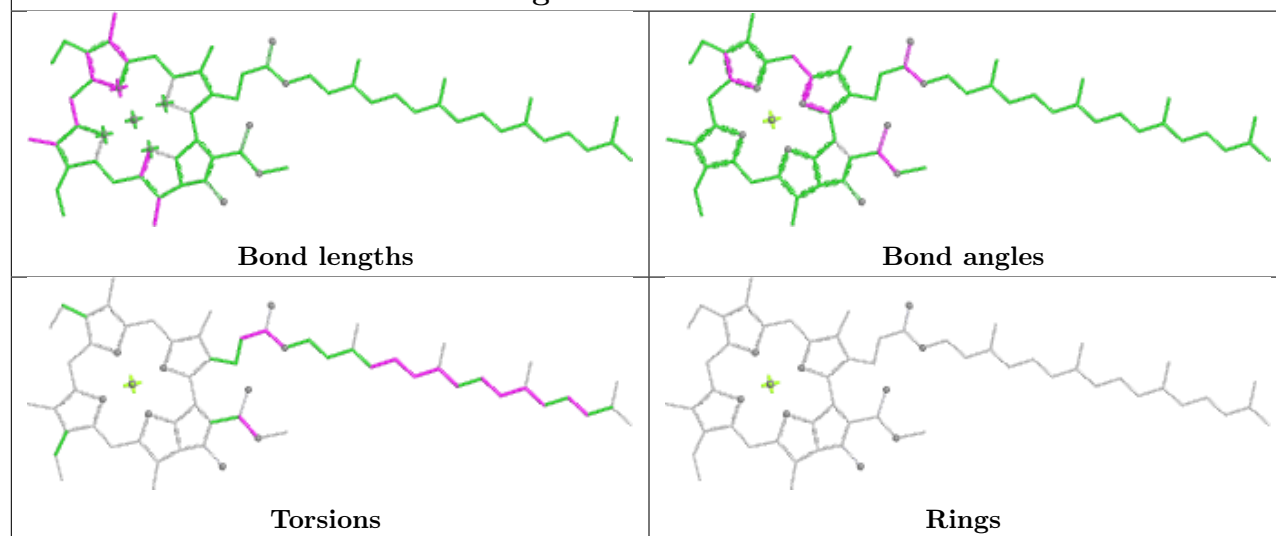
Ligand LUT c 615

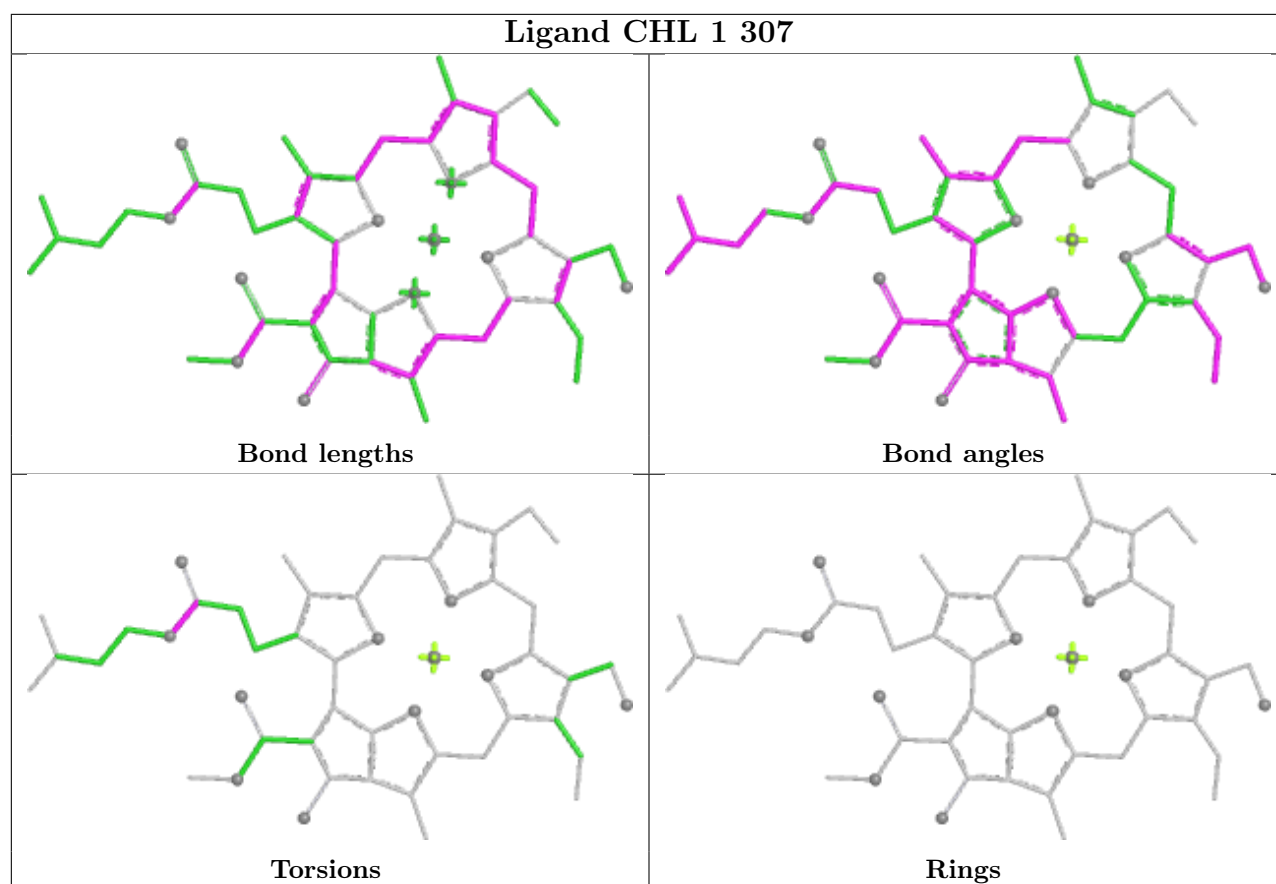


Ligand CLA 2 613

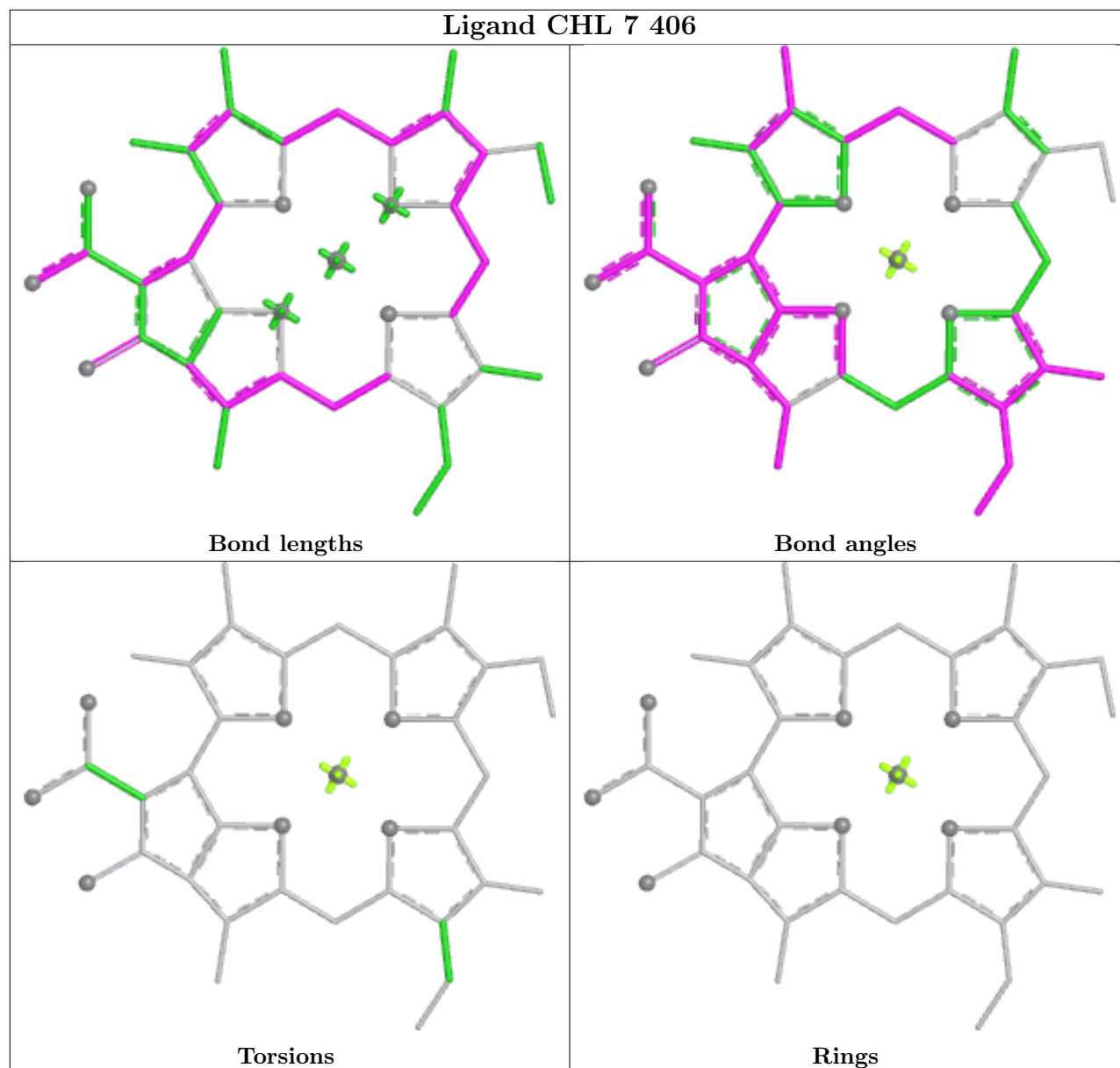


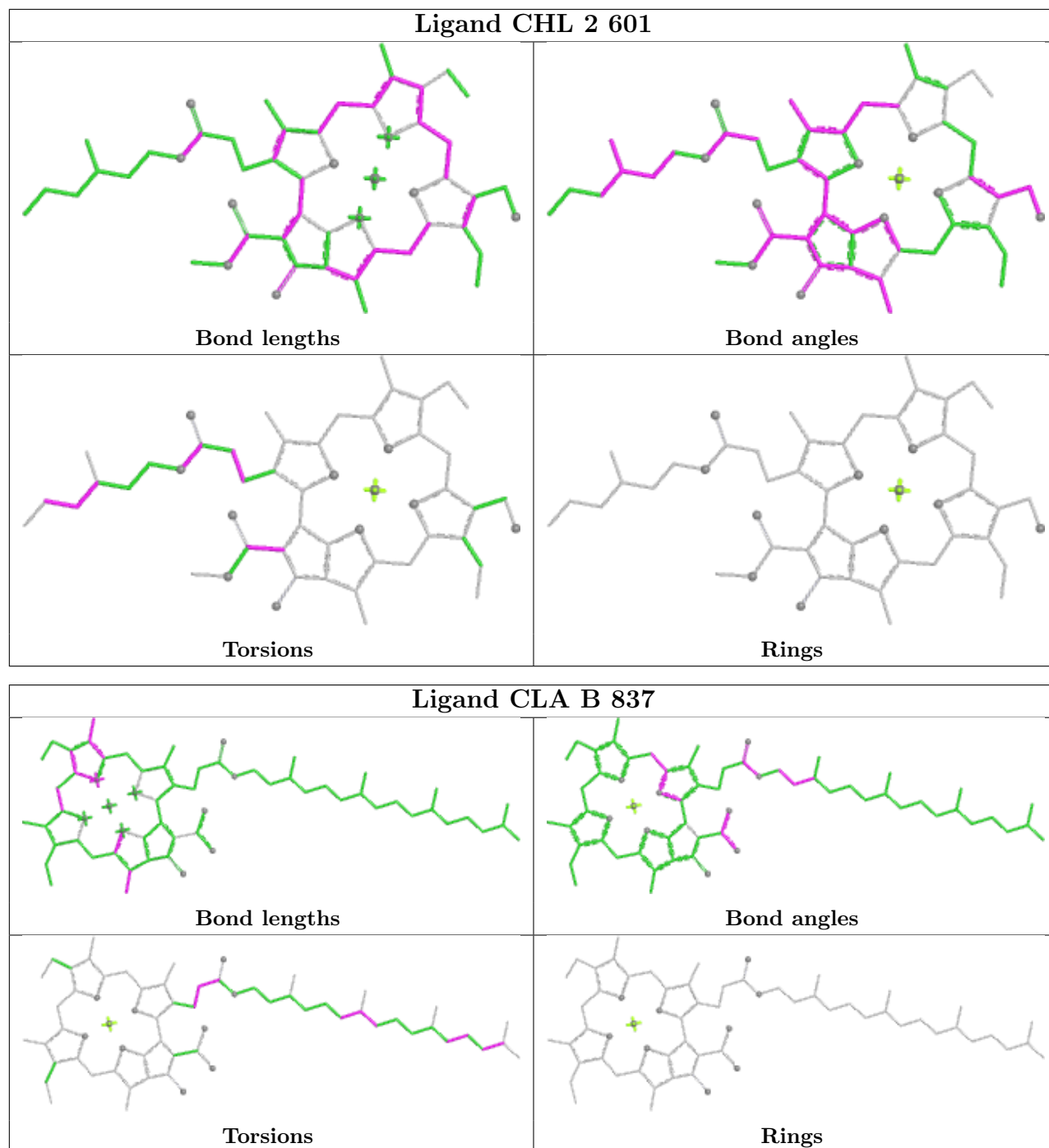
Ligand CLA B 805



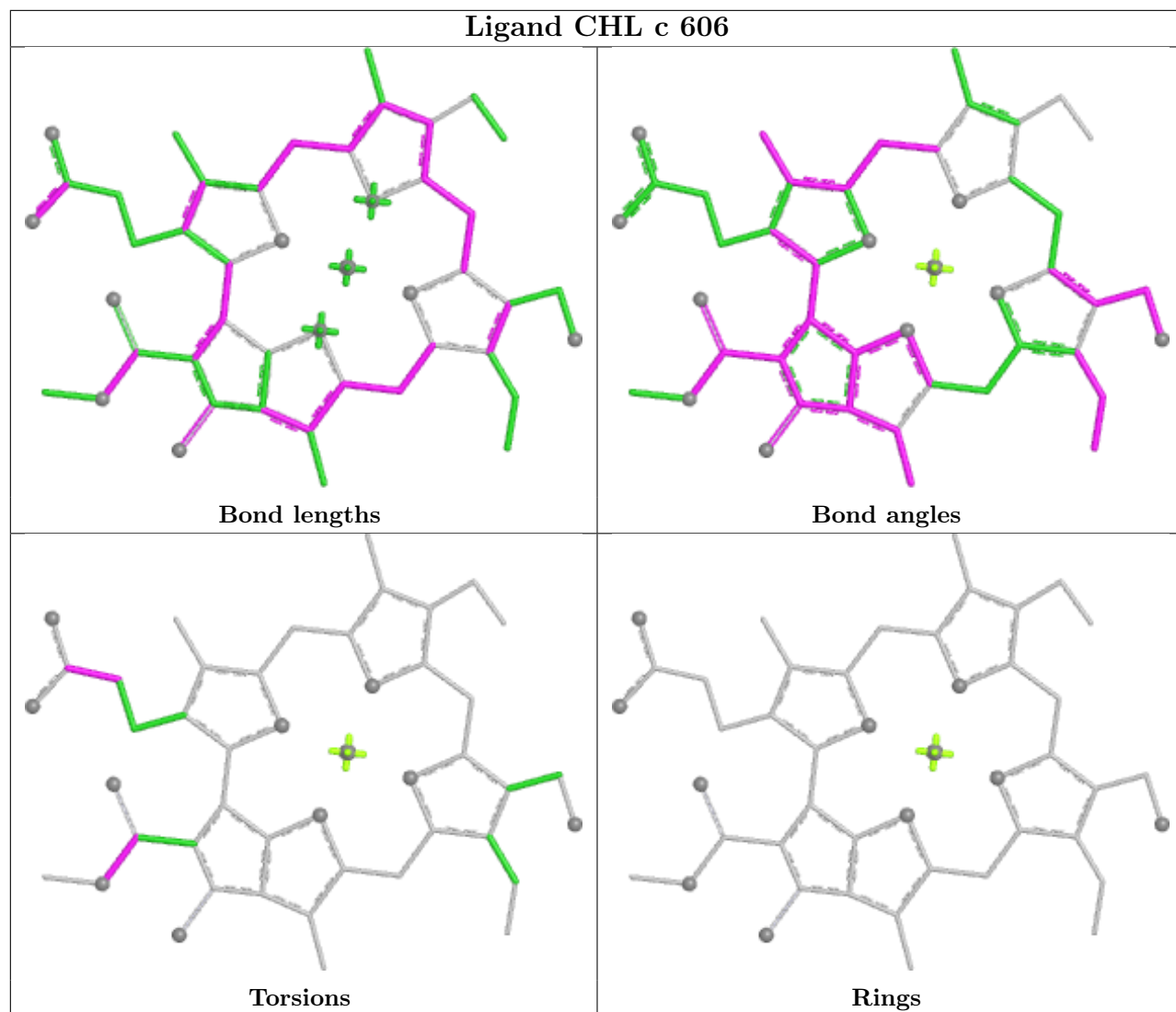


Ligand CHL 7 406

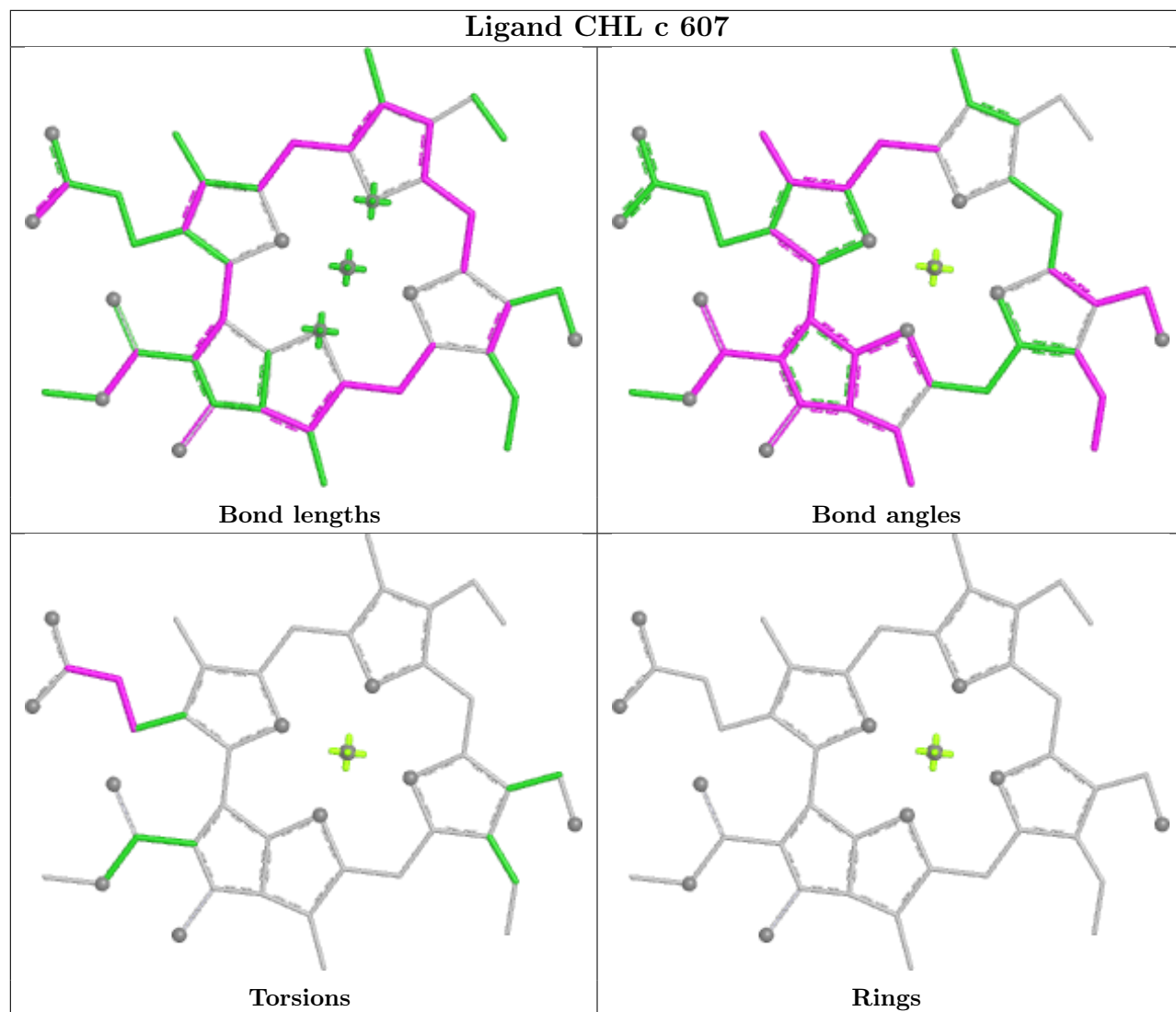




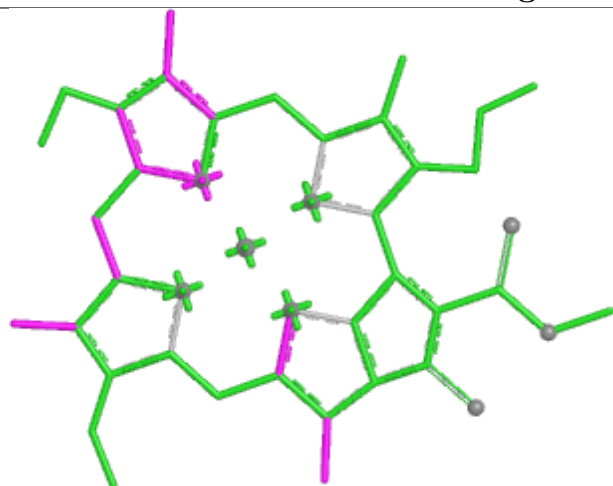
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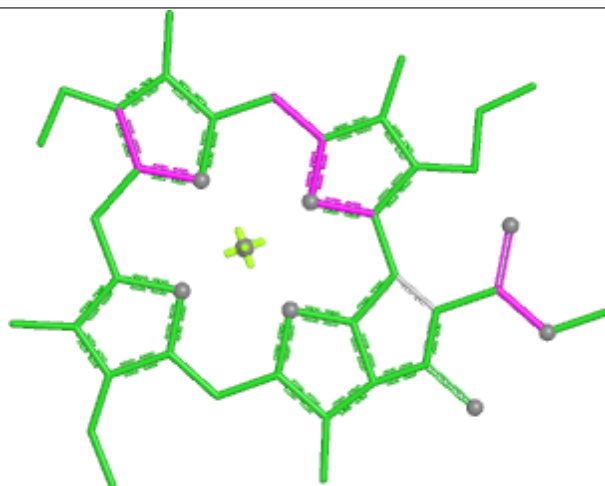
Ligand CHL c 607



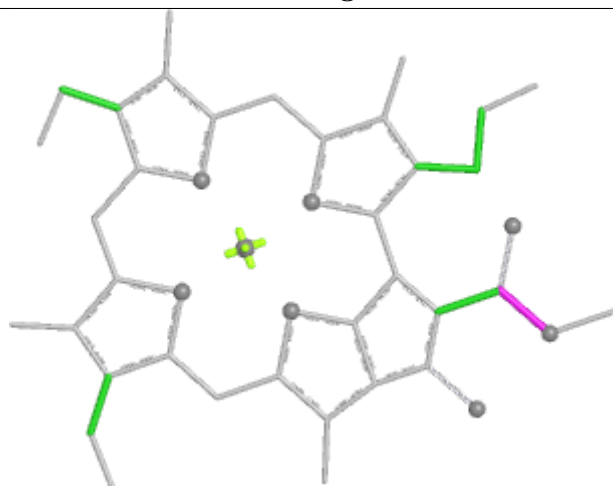
Ligand CLA 3 411



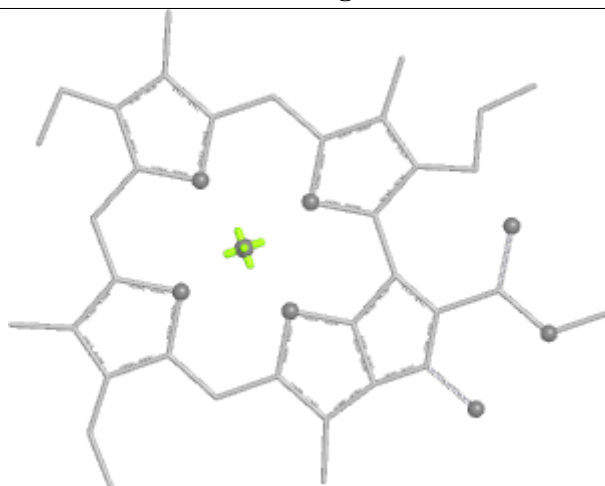
Bond lengths



Bond angles

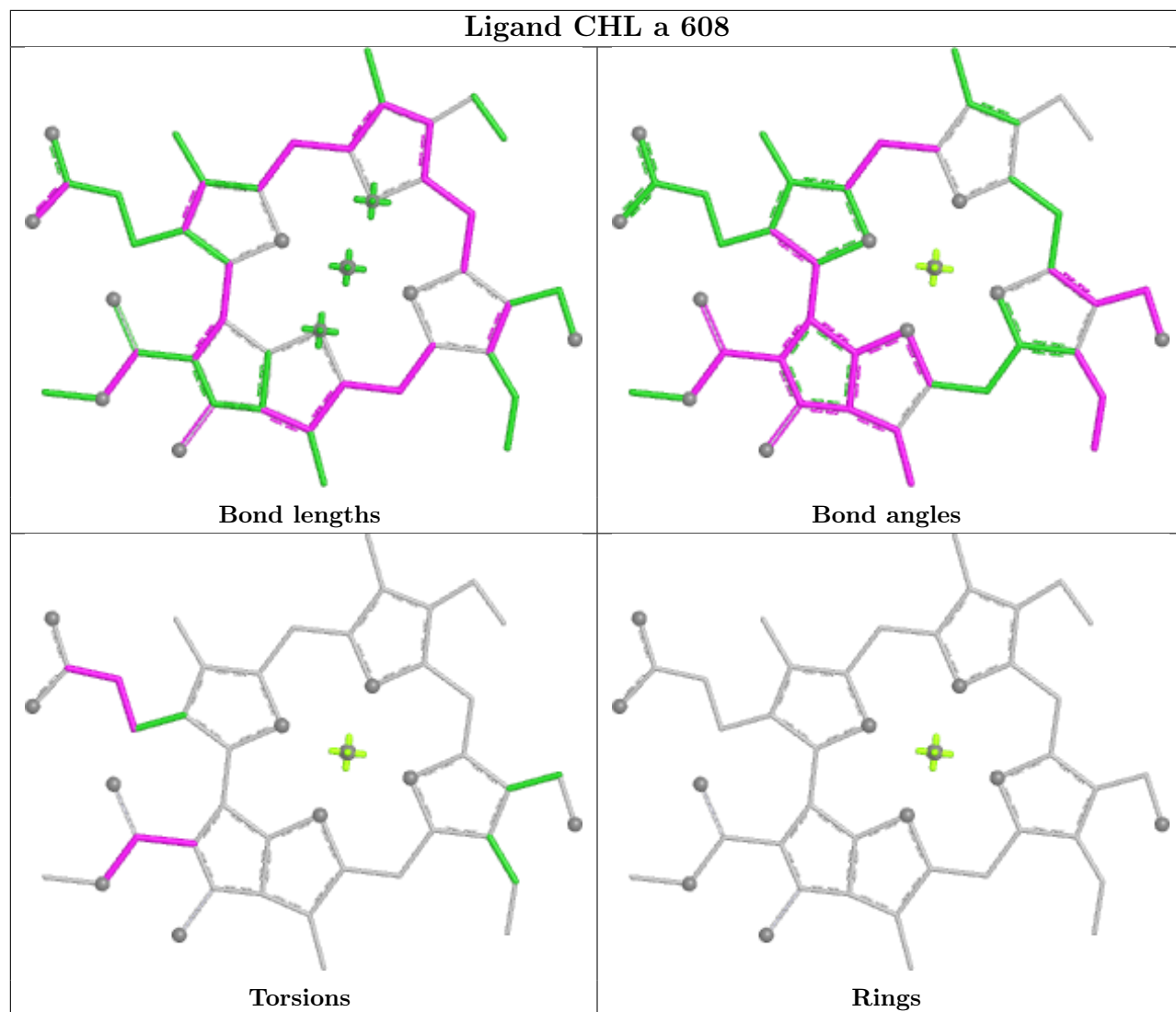


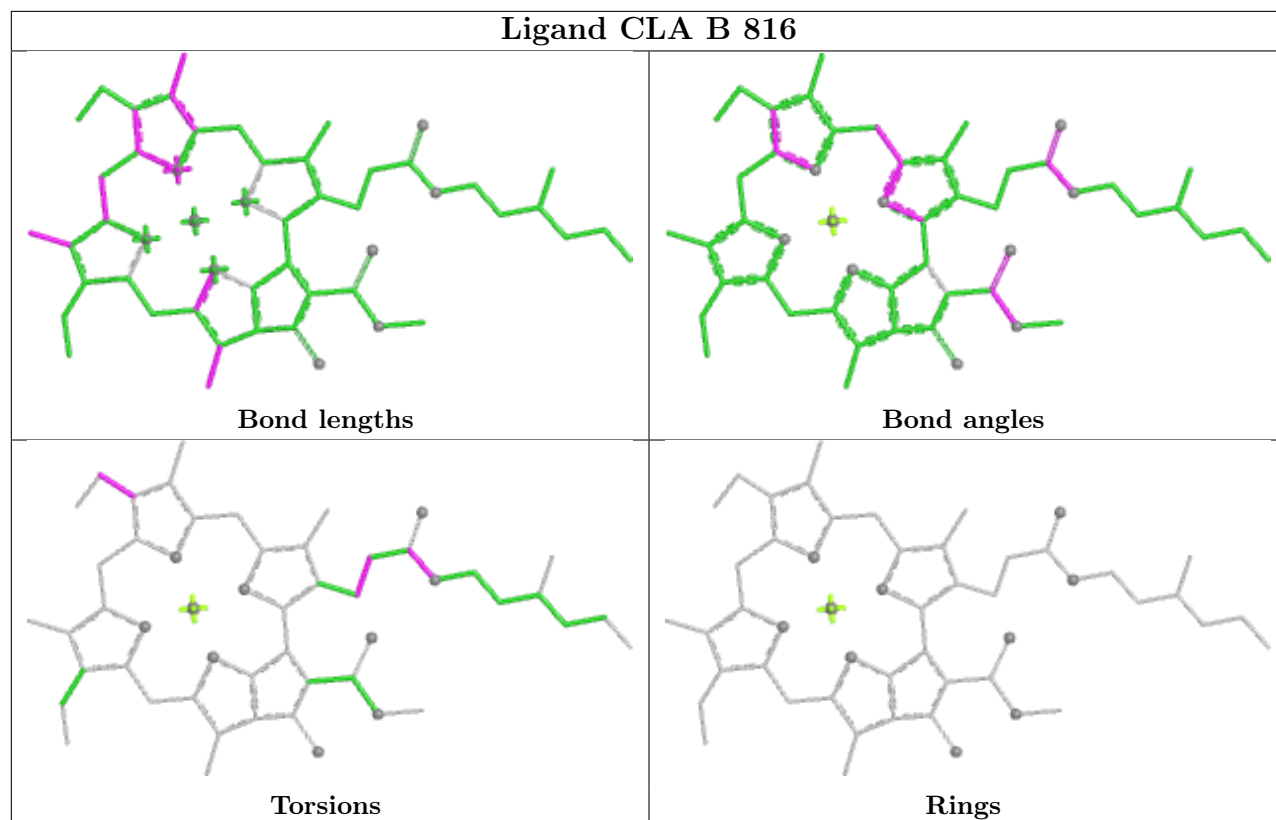
Torsions



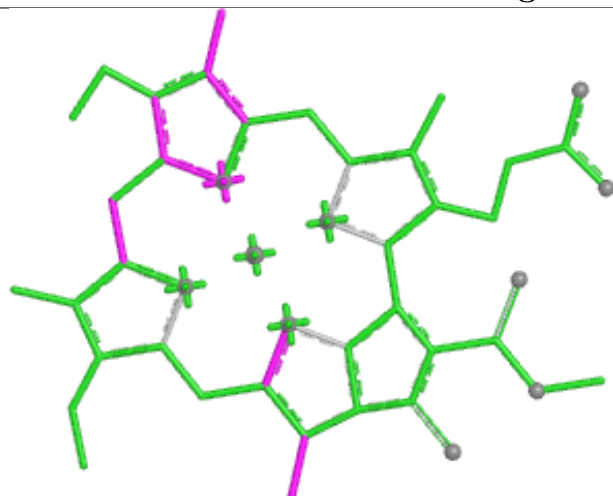
Rings

Ligand CHL a 608

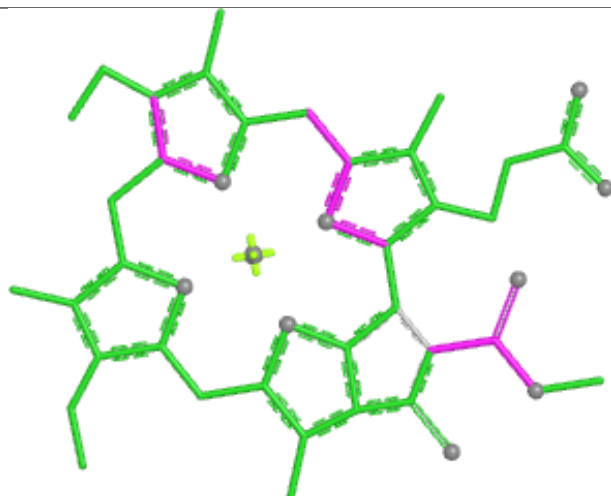




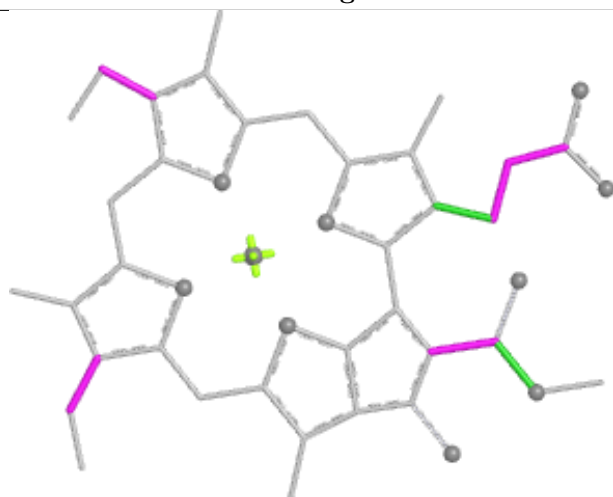
Ligand CLA 7 401



Bond lengths



Bond angles

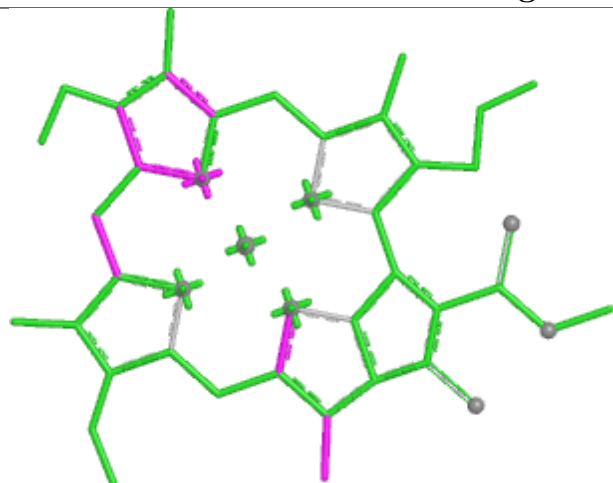


Torsions

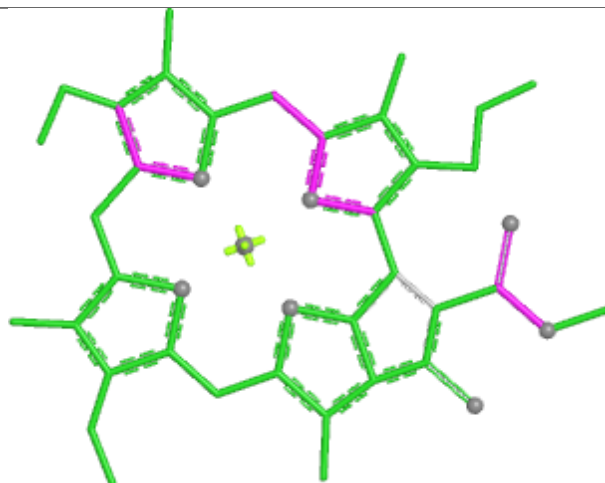


Rings

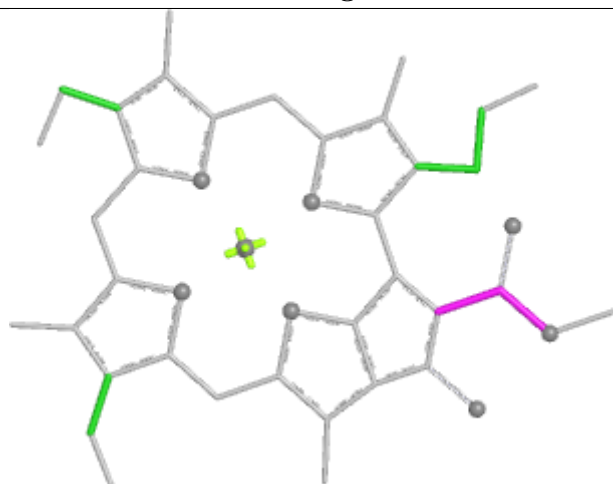
Ligand CLA 8 612



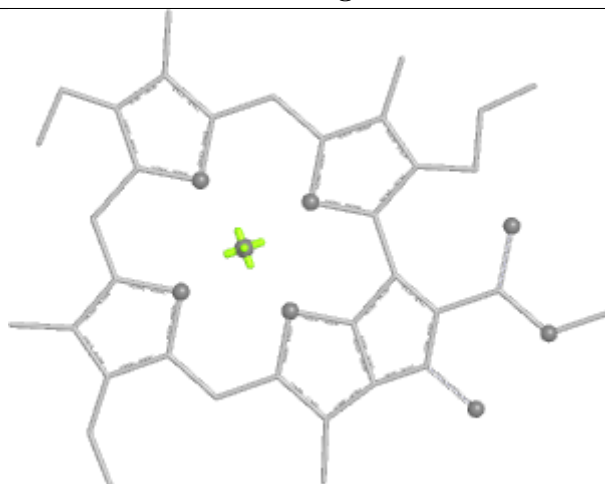
Bond lengths



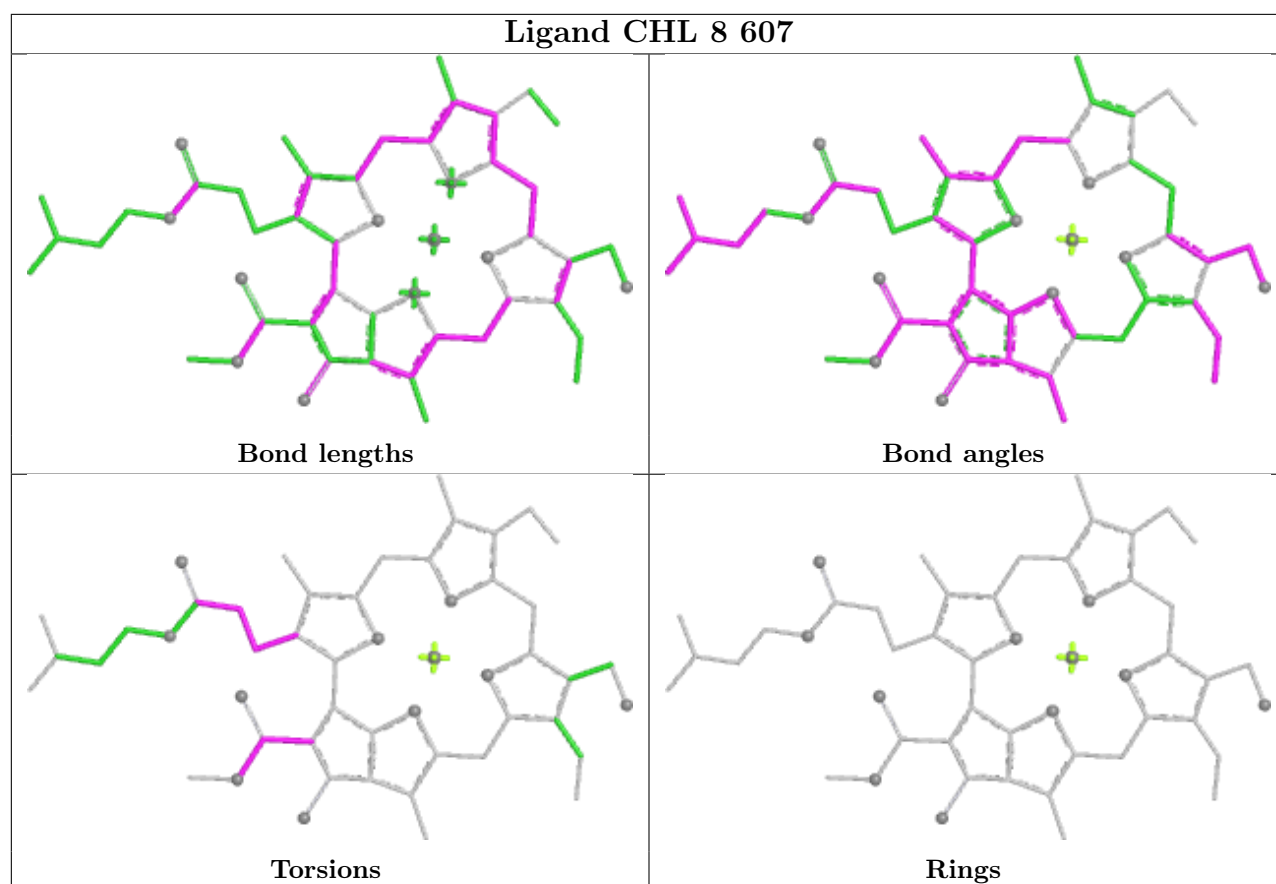
Bond angles



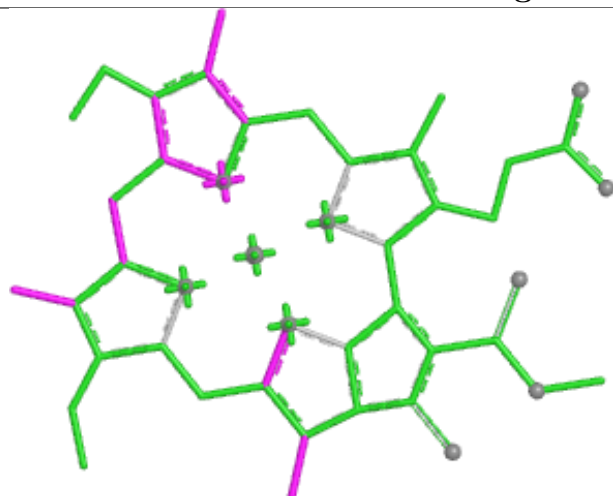
Torsions



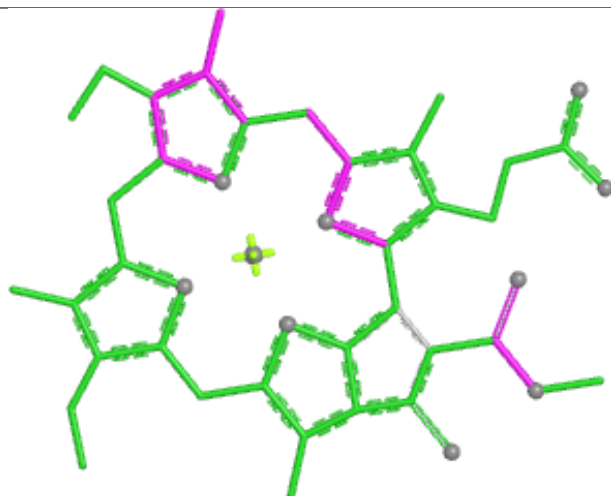
Rings



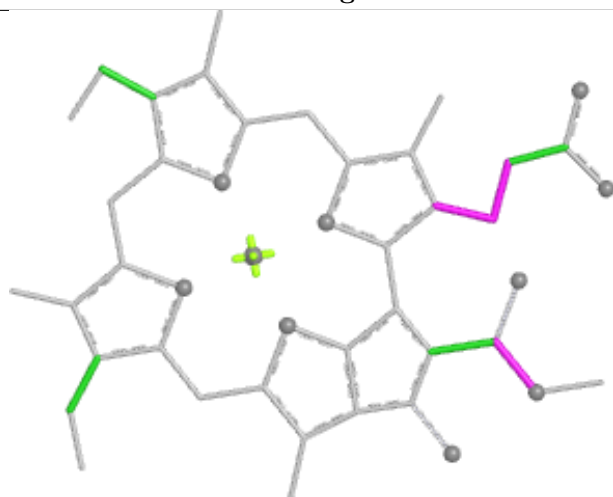
Ligand CLA B 834



Bond lengths



Bond angles

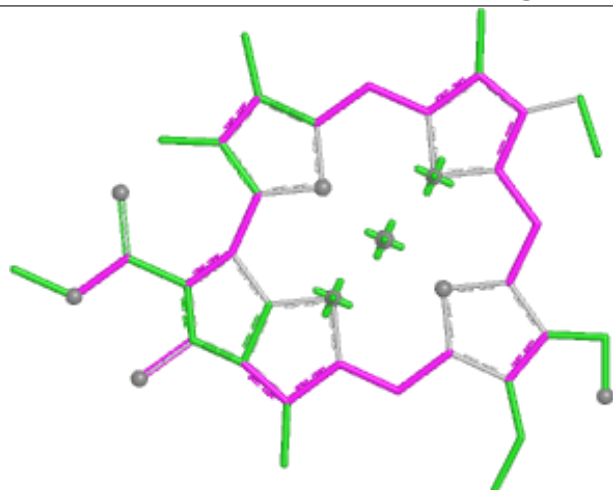


Torsions

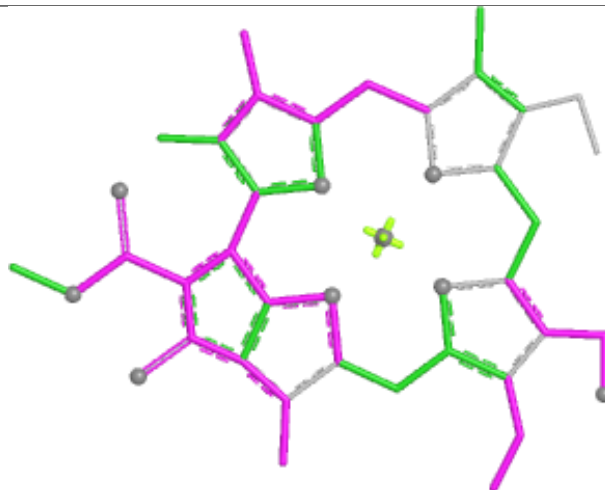


Rings

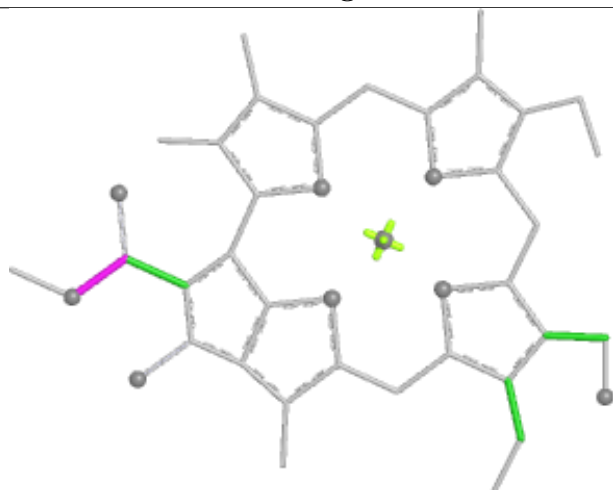
Ligand CHL 8 613



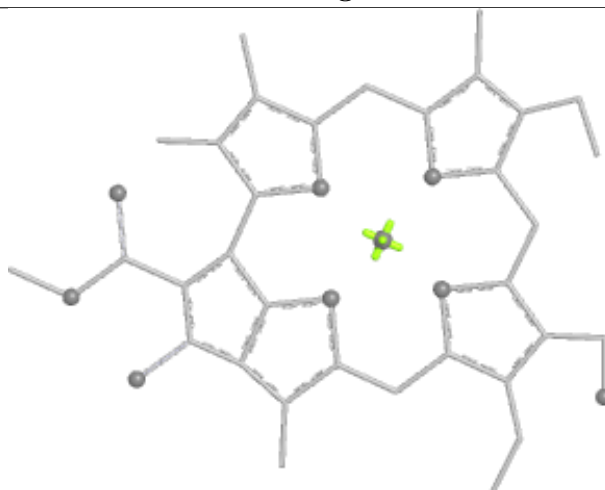
Bond lengths



Bond angles

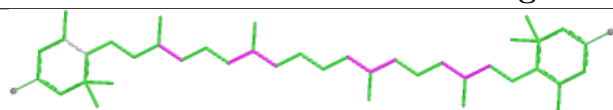


Torsions

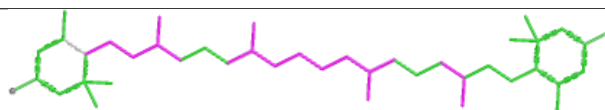


Rings

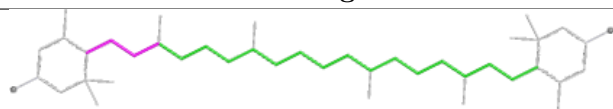
Ligand LUT a 615



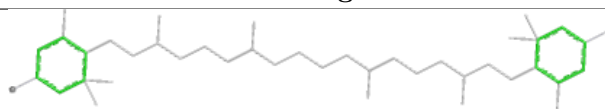
Bond lengths



Bond angles

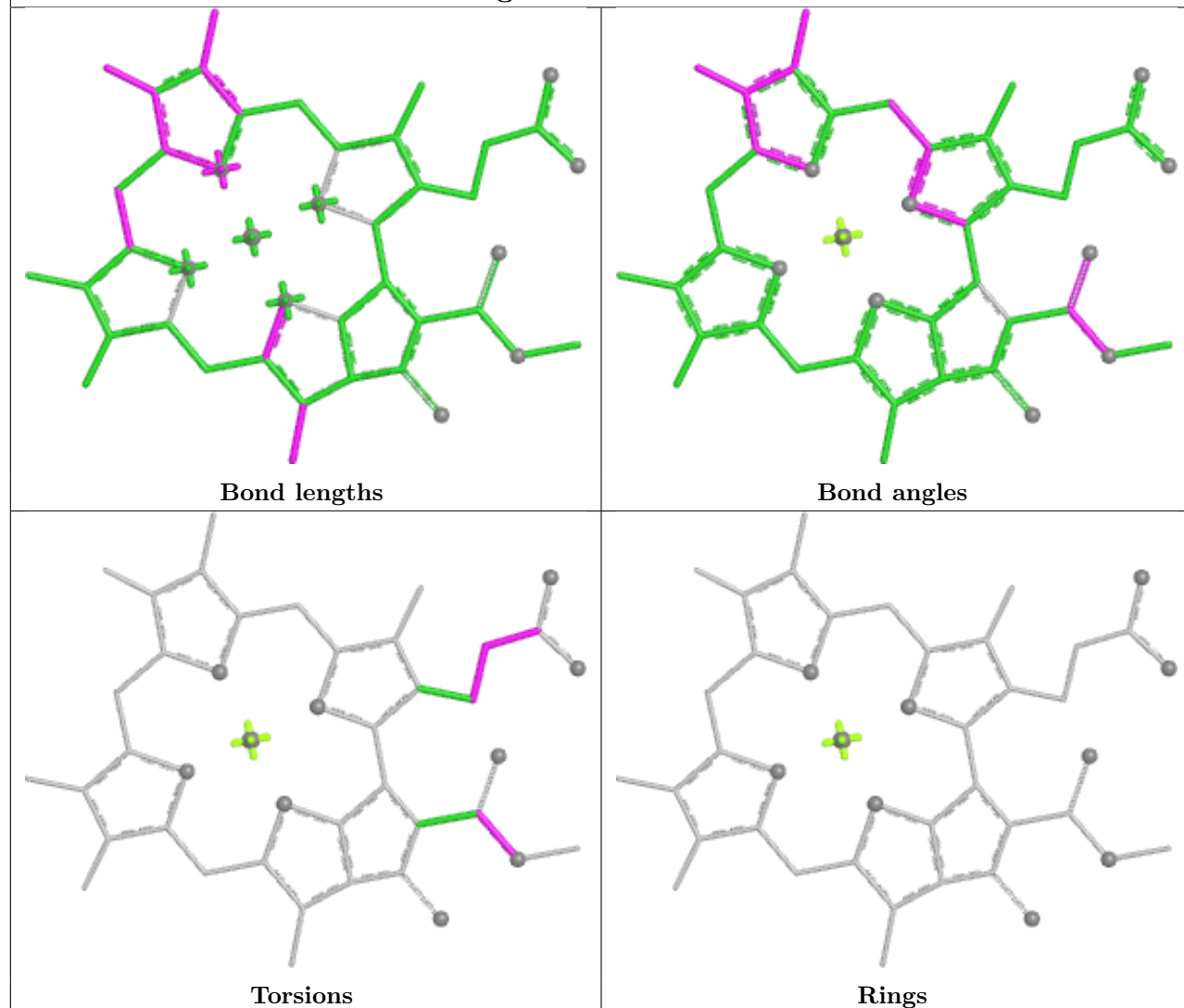


Torsions

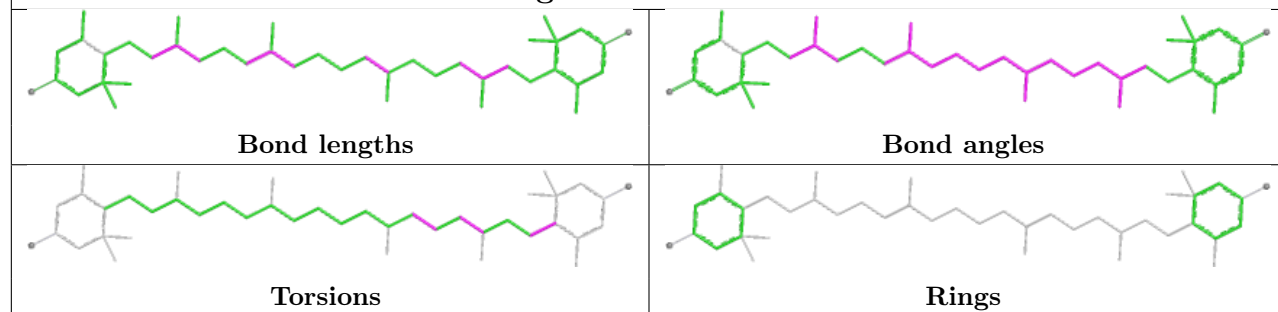


Rings

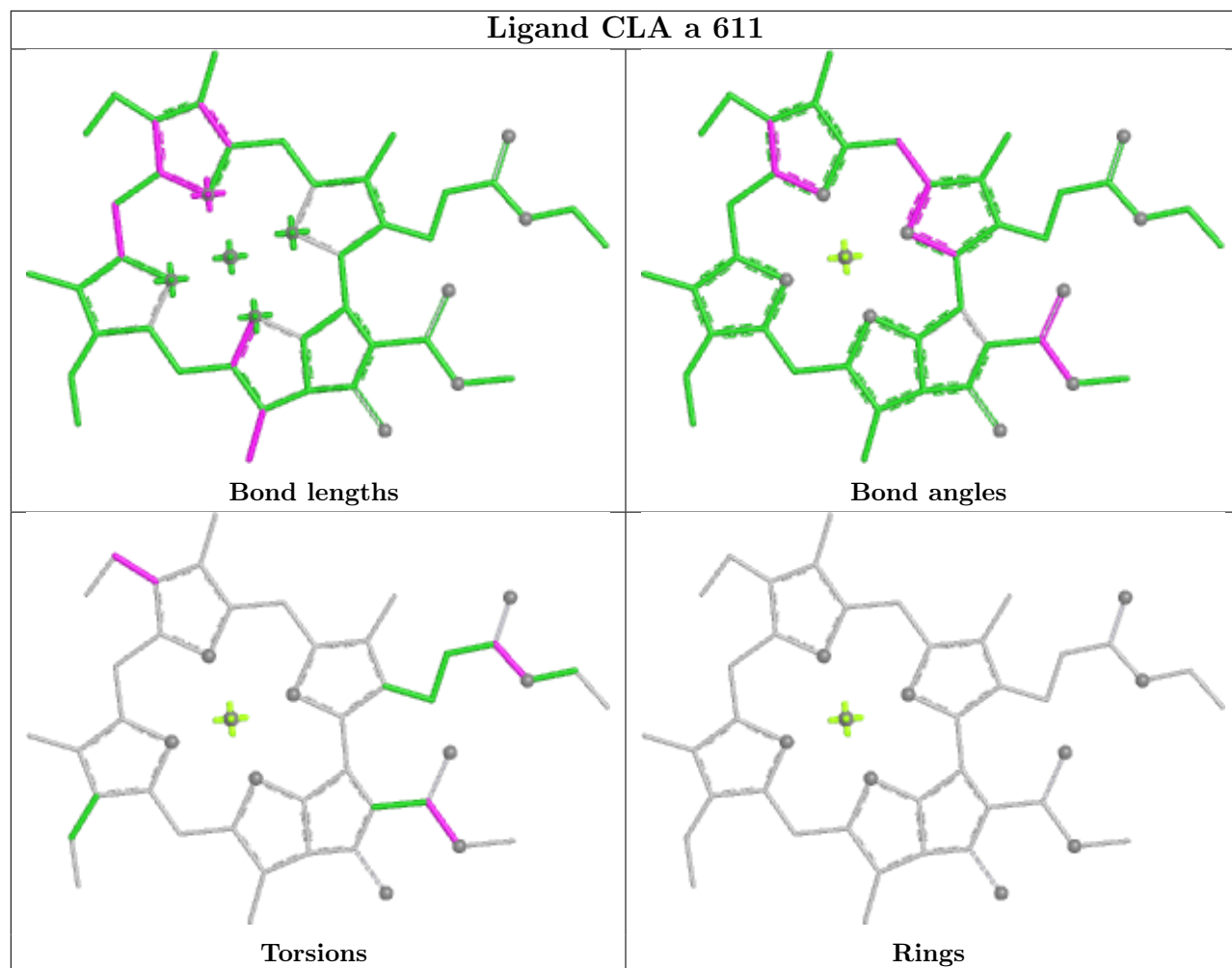
Ligand CLA 5 614



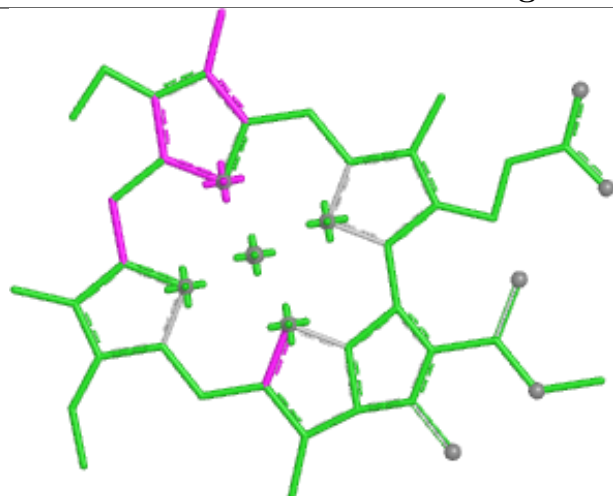
Ligand LUT 3 416



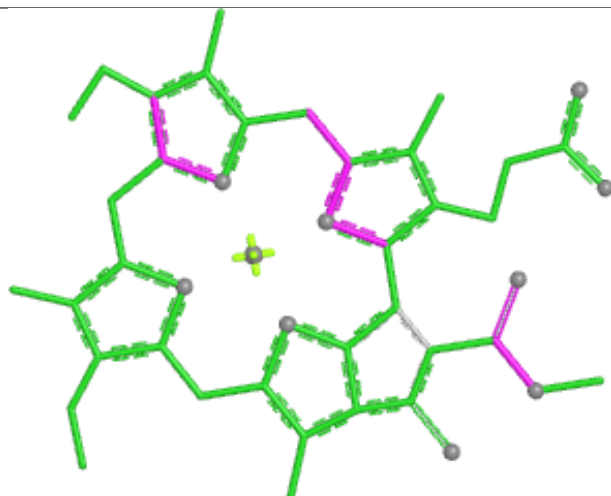
Ligand CLA a 611



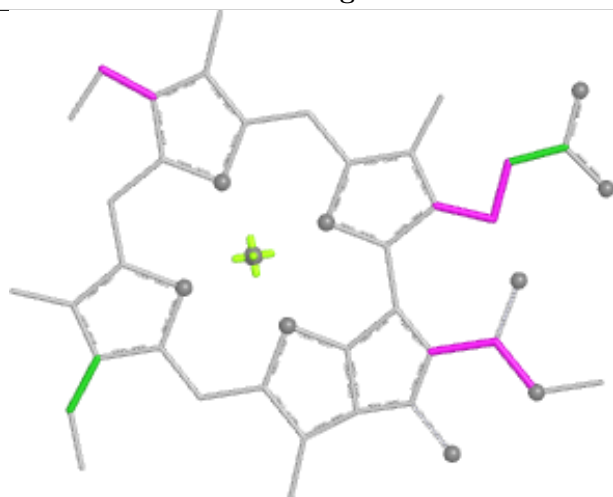
Ligand CLA 8 601



Bond lengths



Bond angles

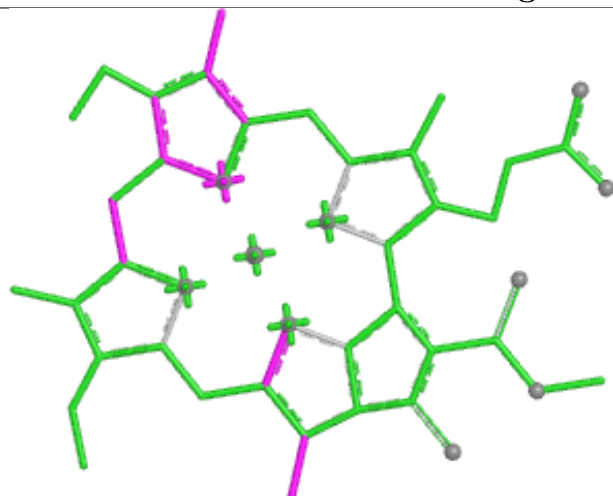


Torsions

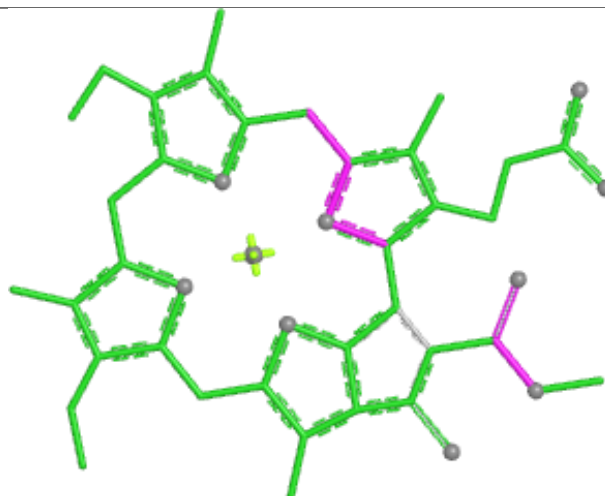


Rings

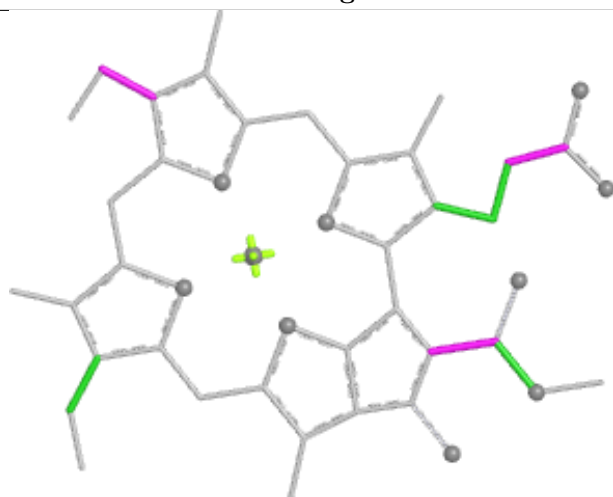
Ligand CLA 5 603



Bond lengths



Bond angles

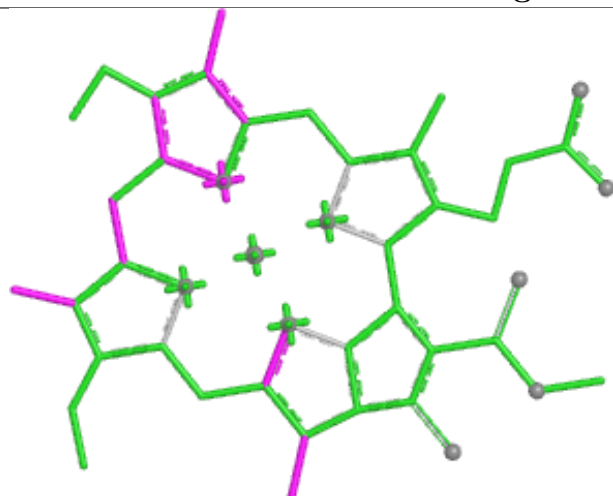


Torsions

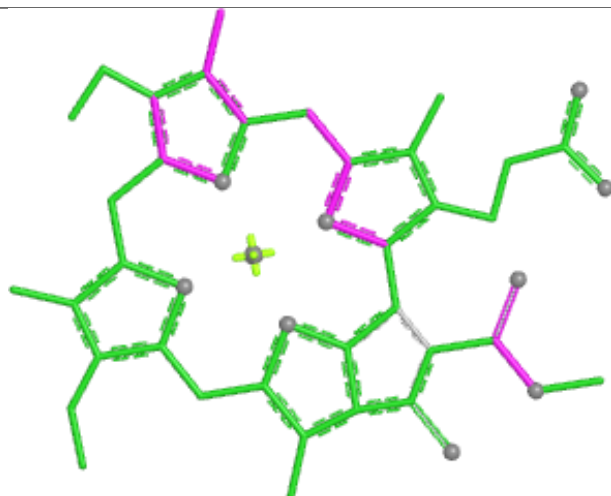


Rings

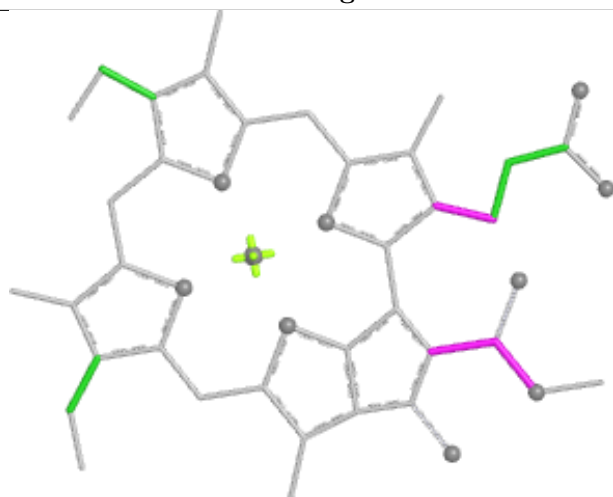
Ligand CLA A 815



Bond lengths



Bond angles

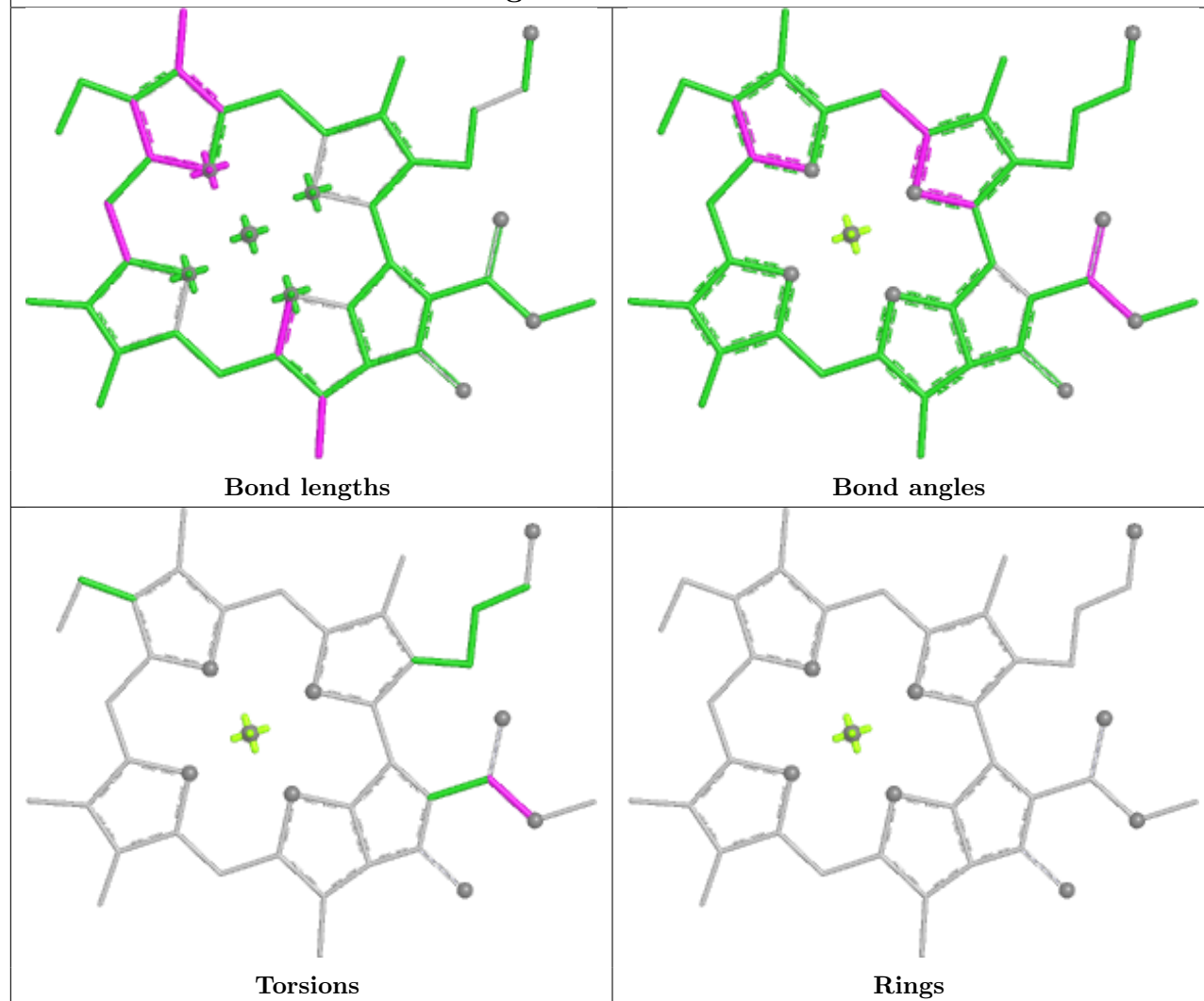


Torsions

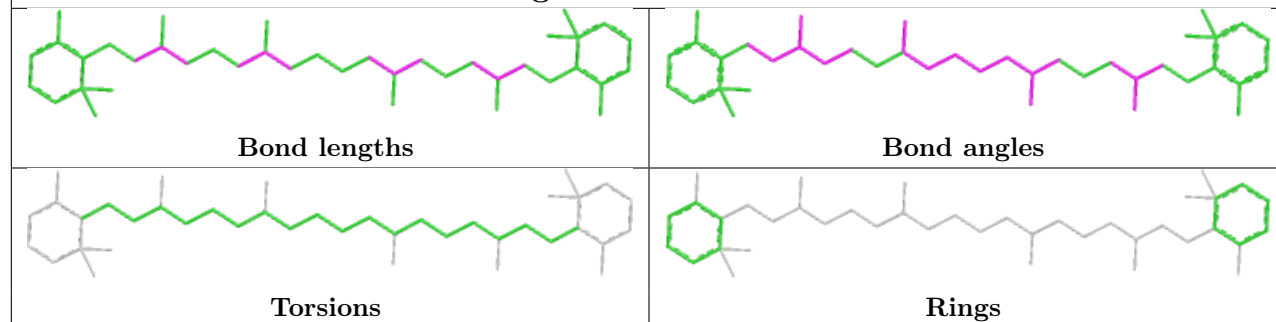


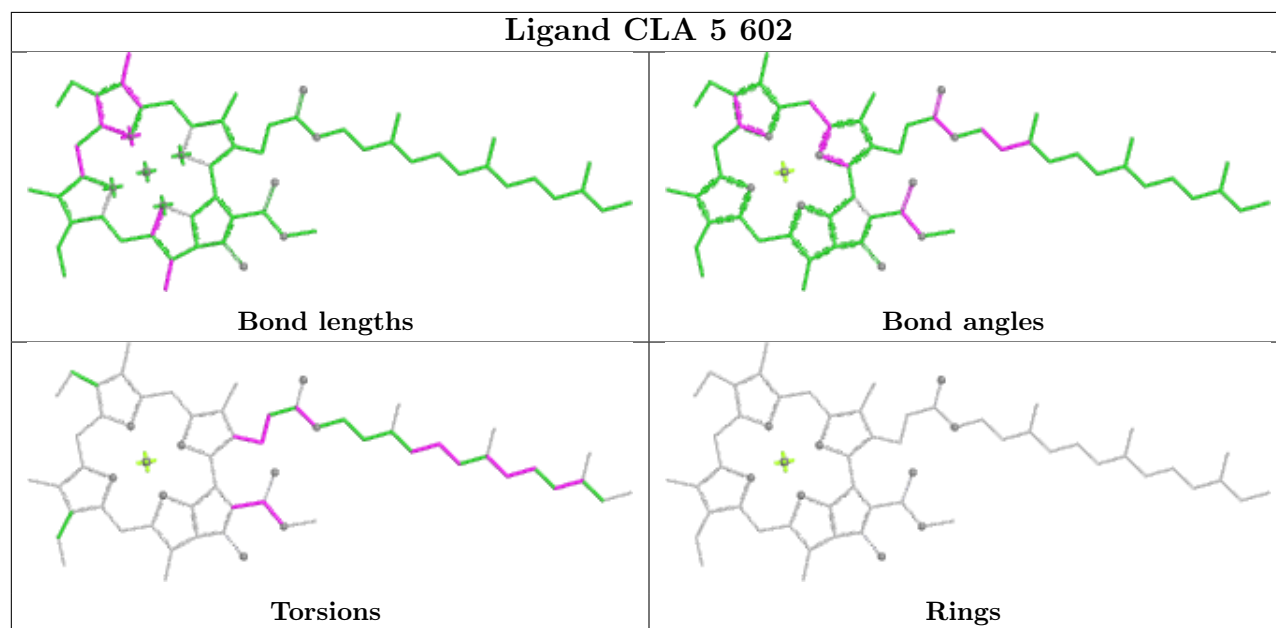
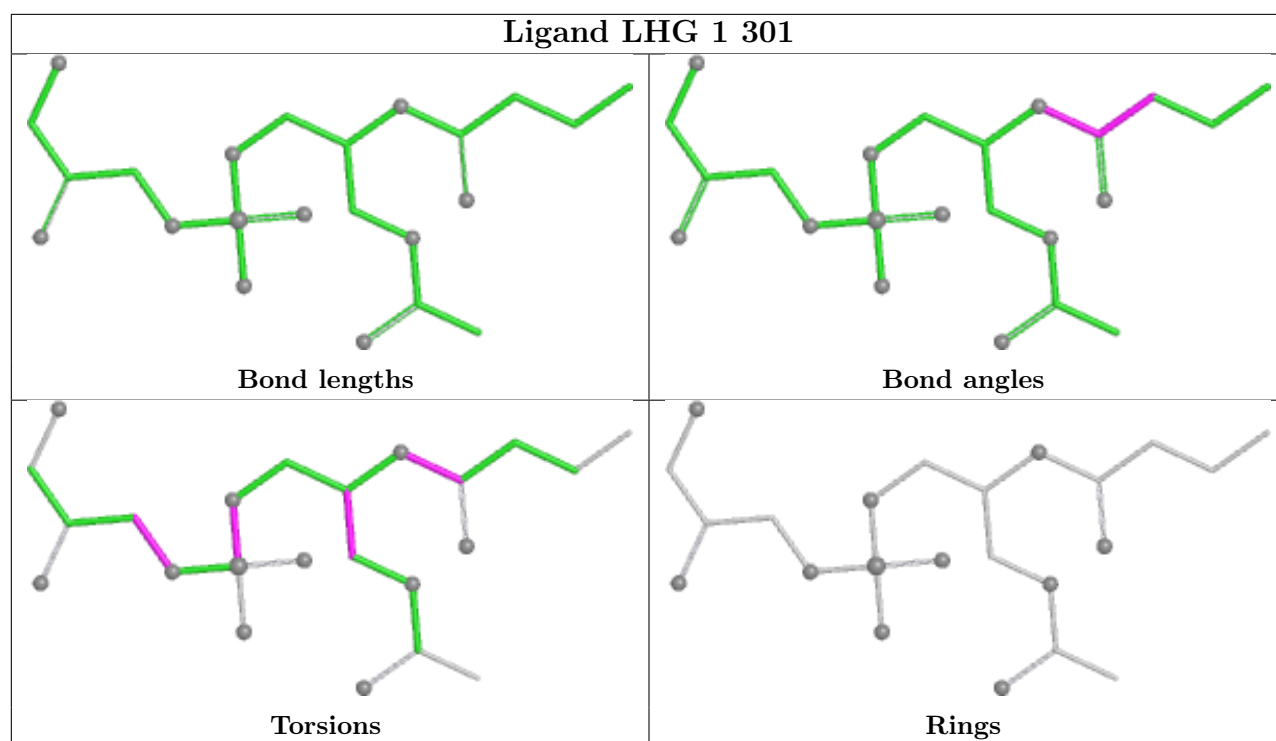
Rings

Ligand CLA 4 604

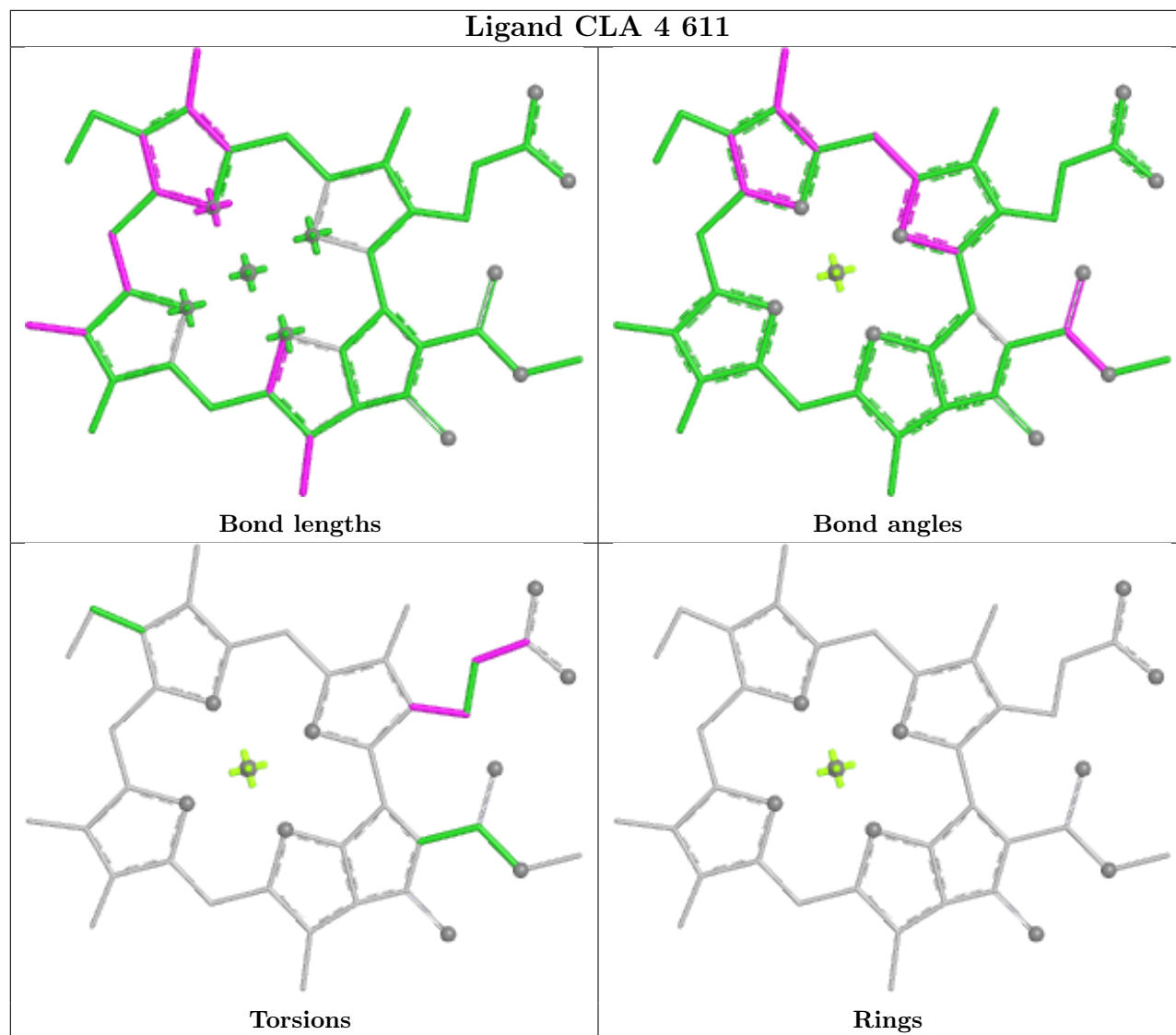


Ligand BCR F 303

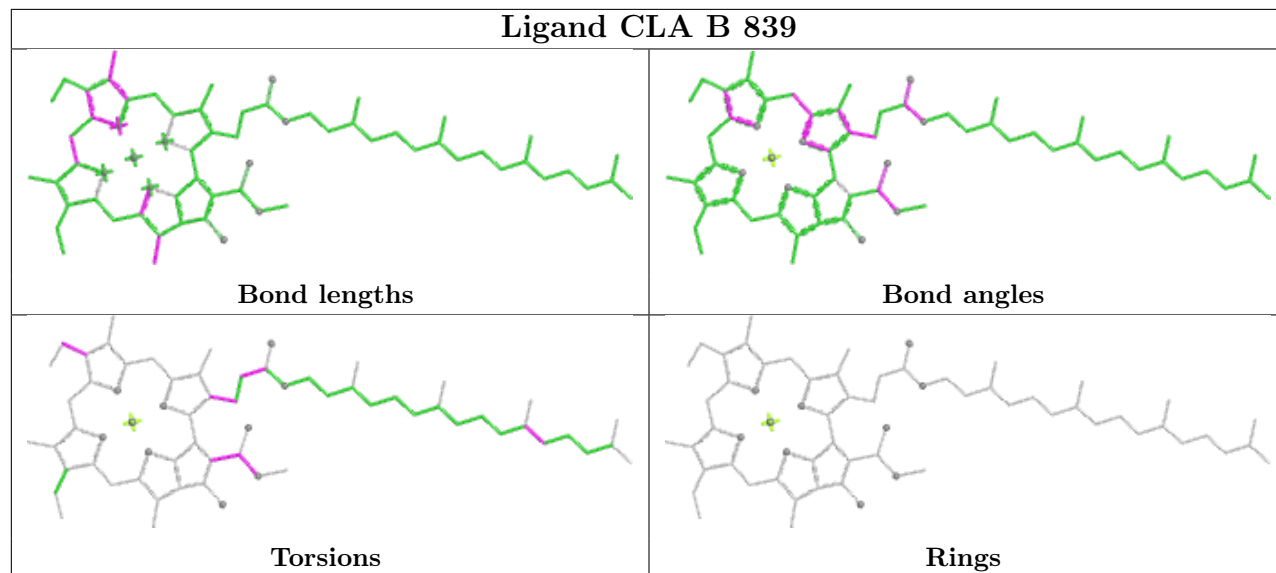


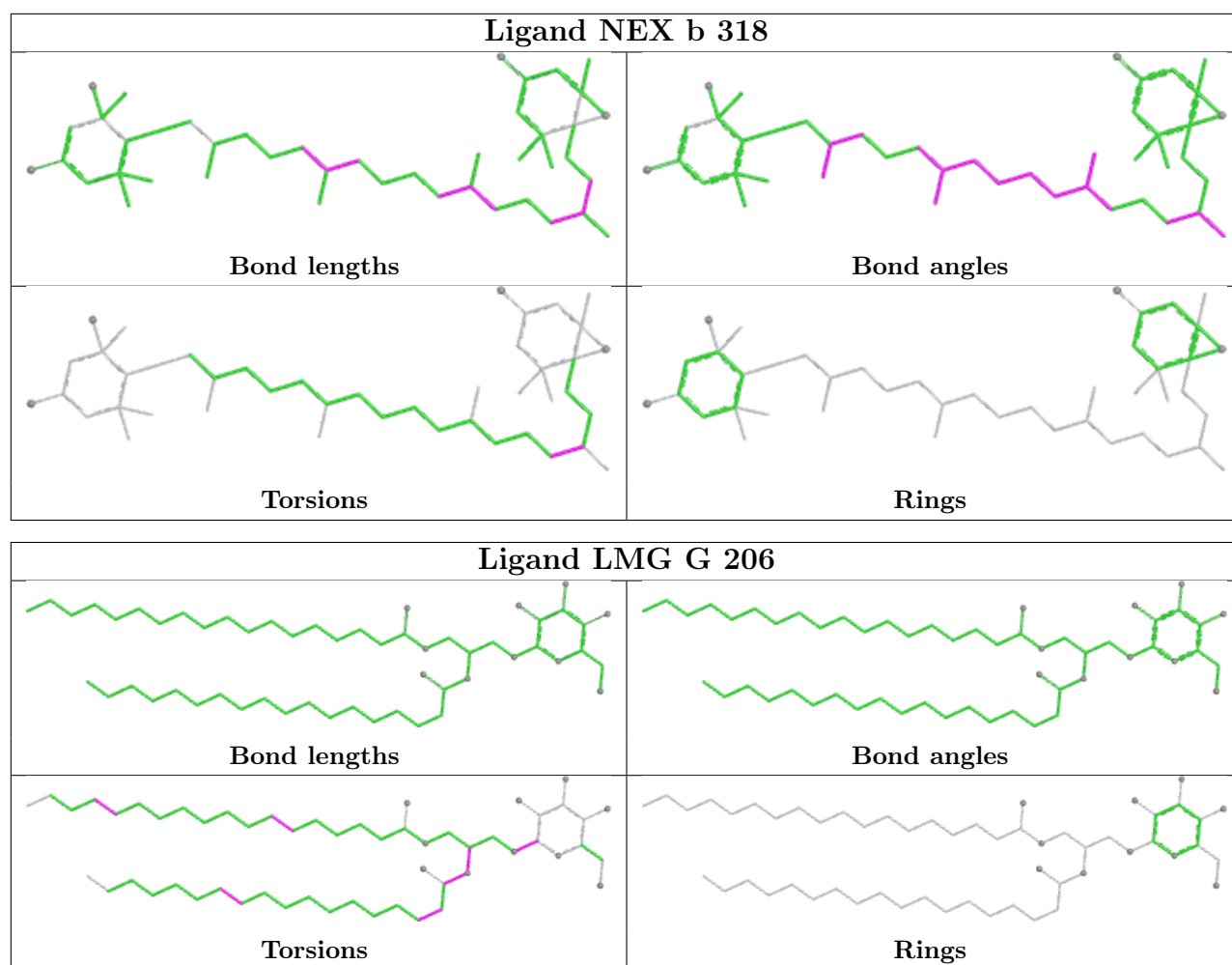


Ligand CLA 4 611

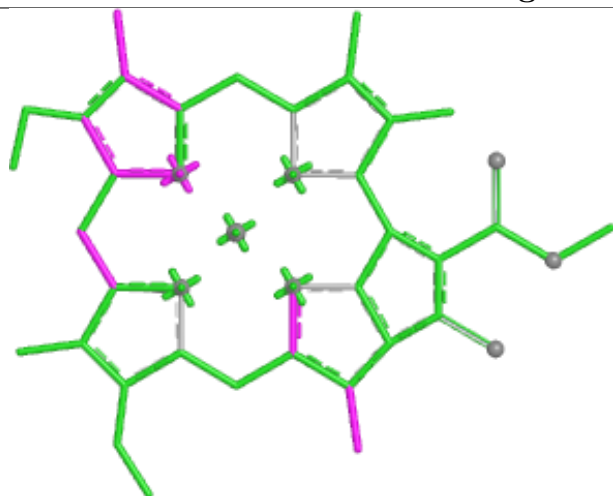


Ligand CLA B 839

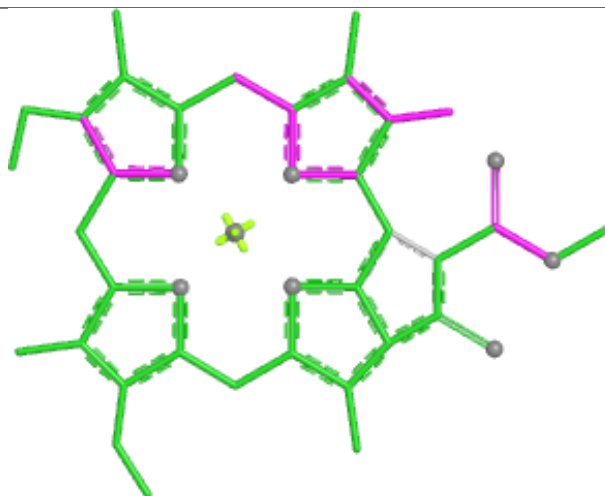




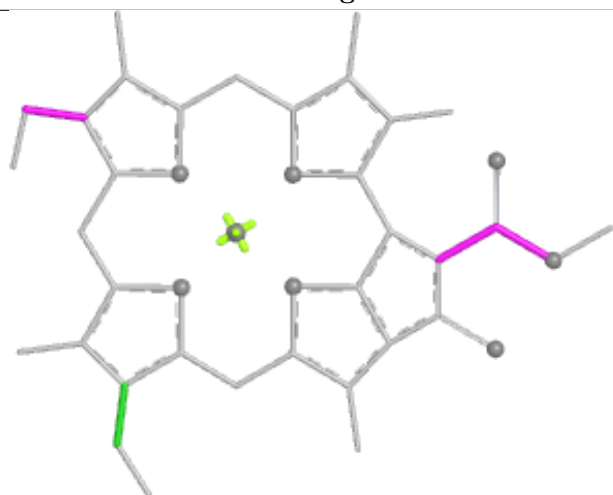
Ligand CLA 6 611



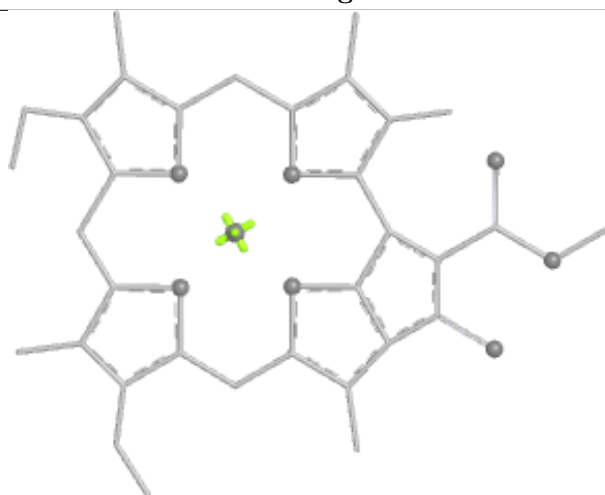
Bond lengths



Bond angles

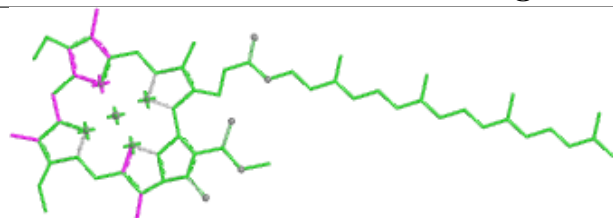


Torsions

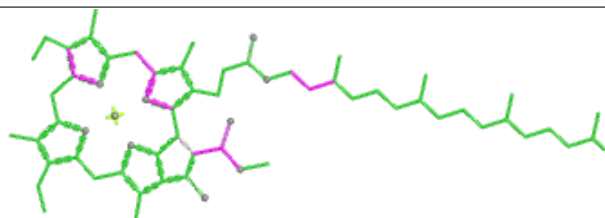


Rings

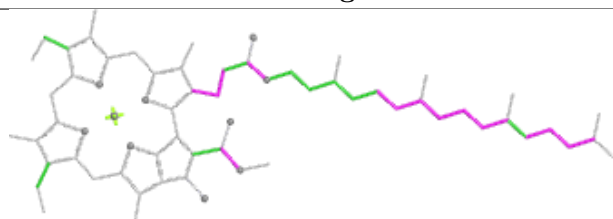
Ligand CLA B 817



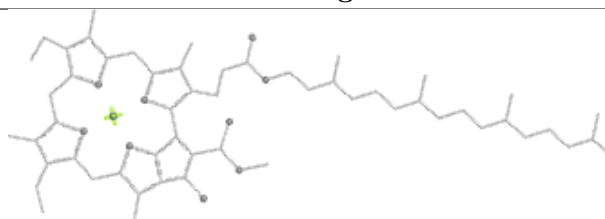
Bond lengths



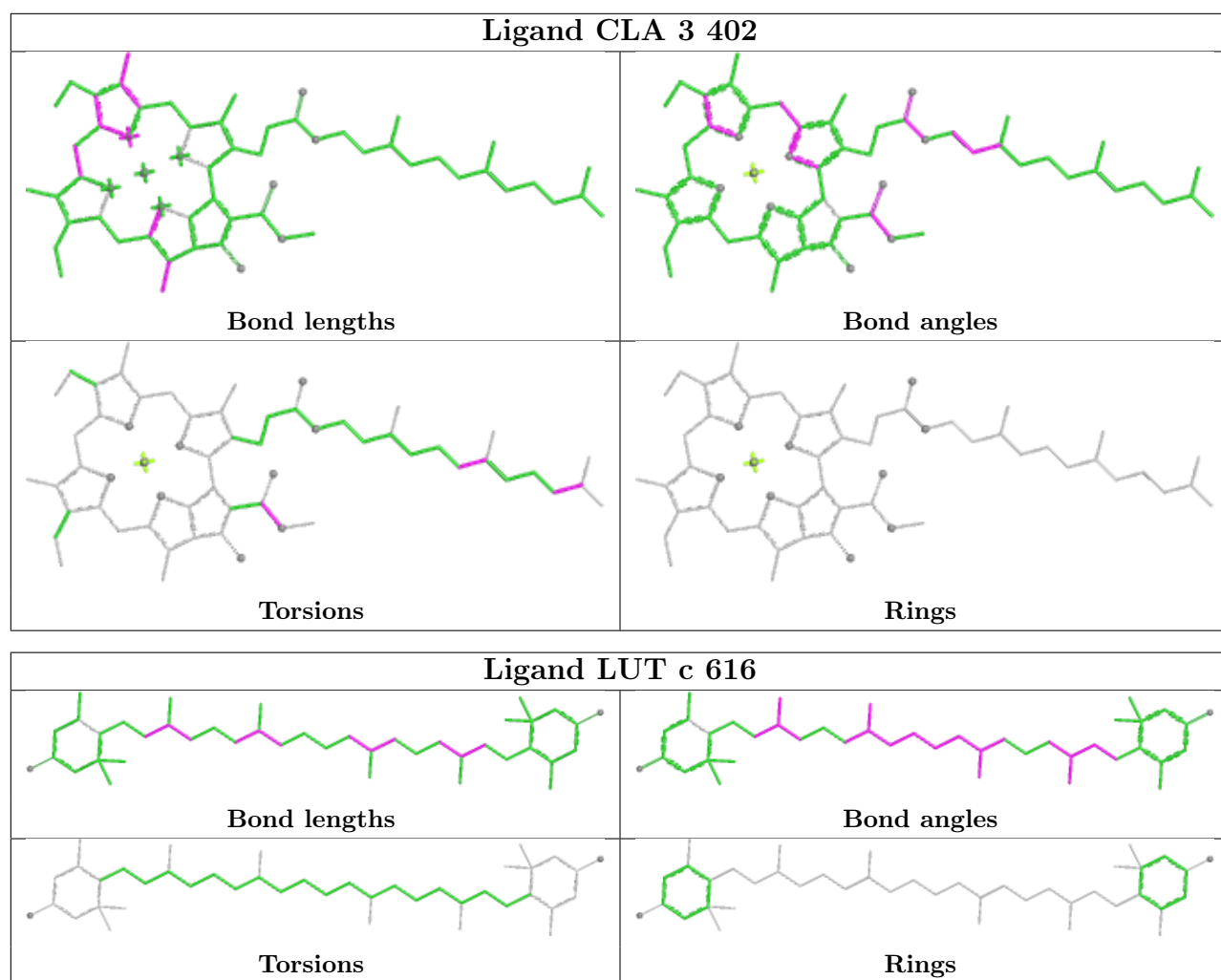
Bond angles



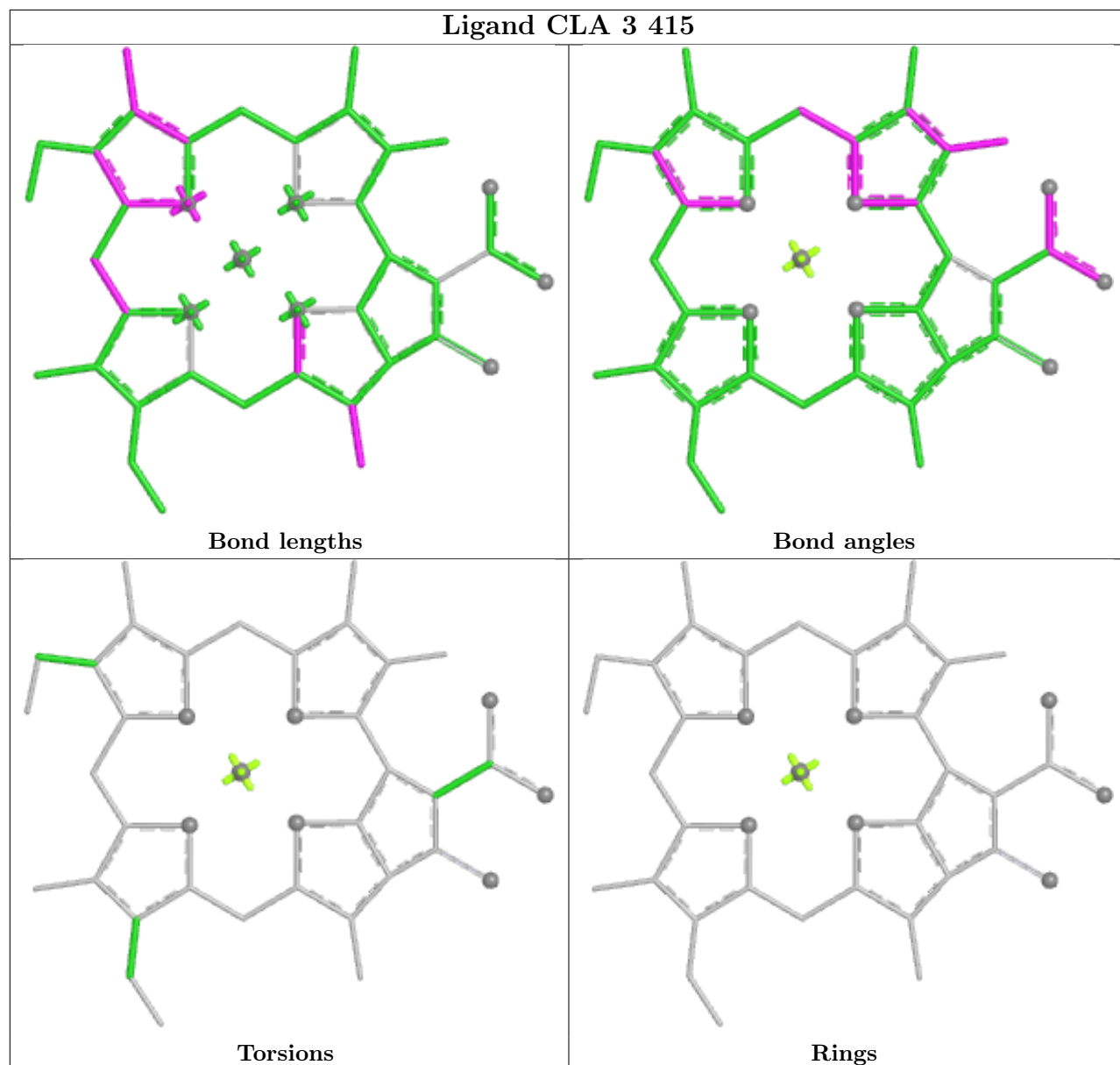
Torsions

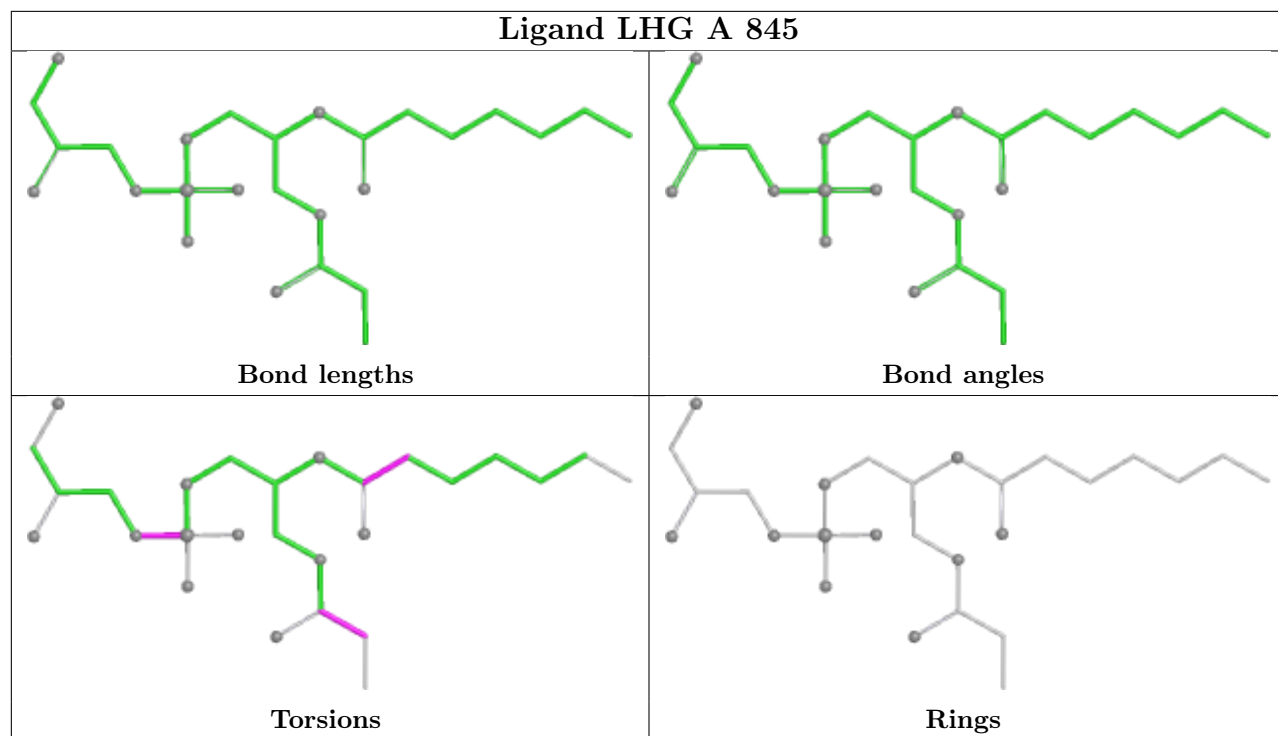


Rings

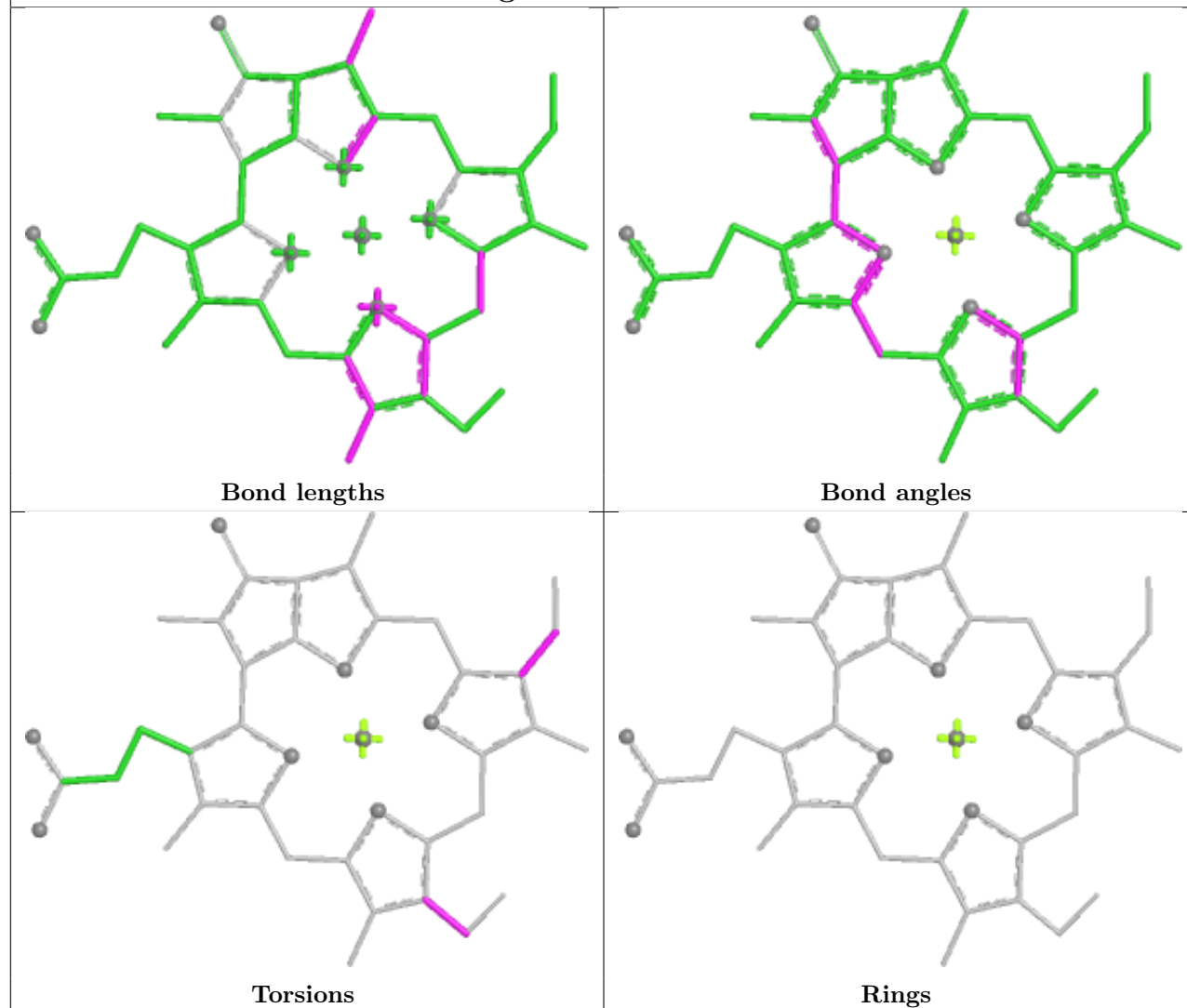


Ligand CLA 3 415

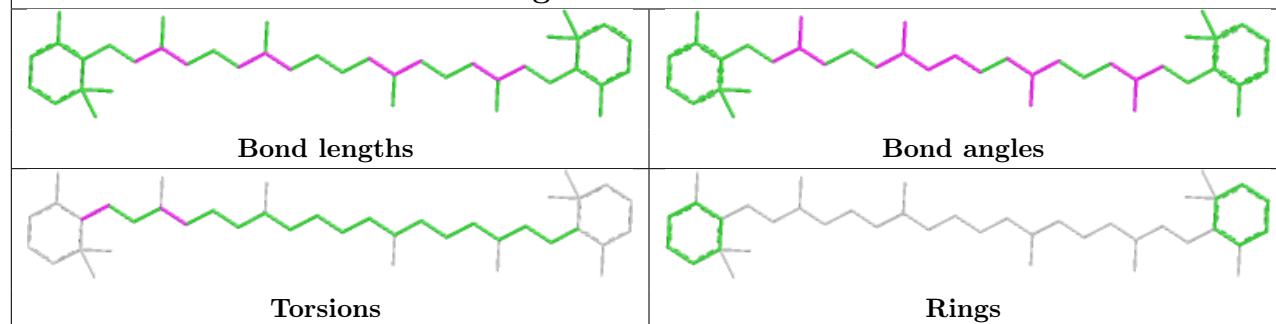


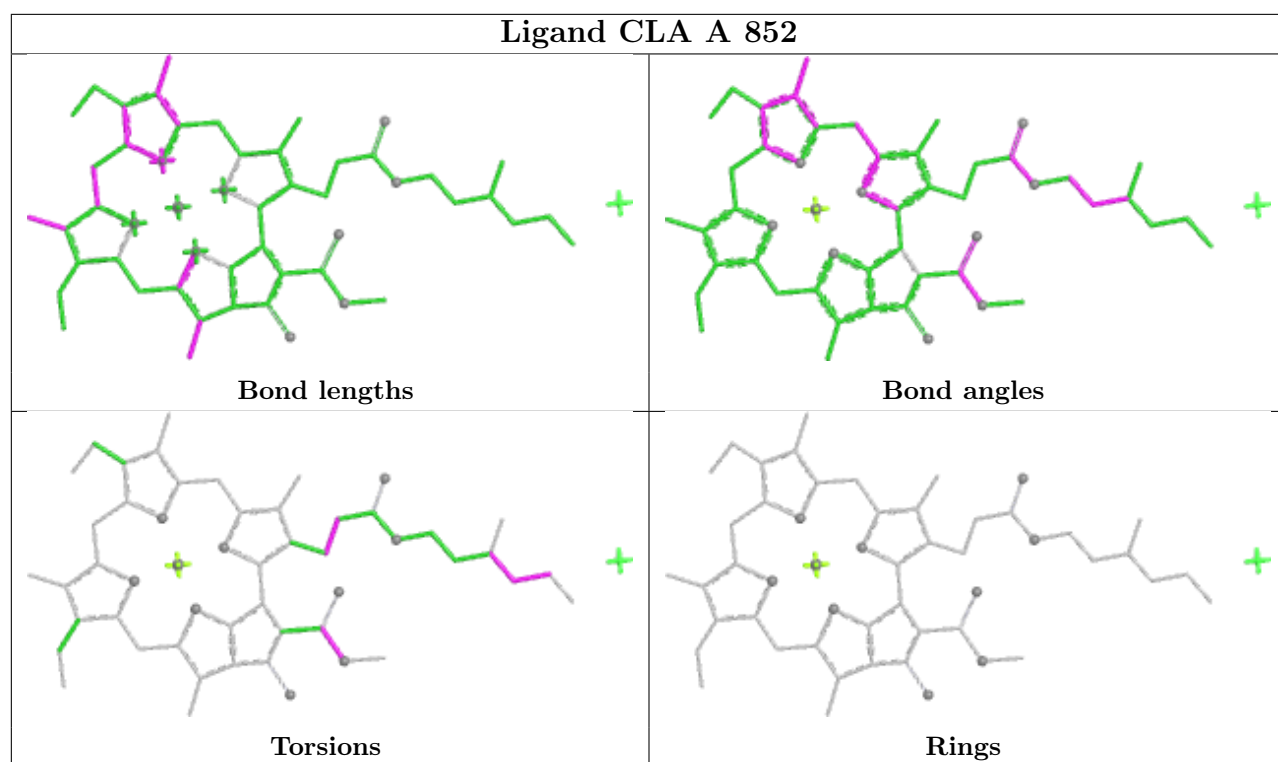


Ligand CLA 2 610

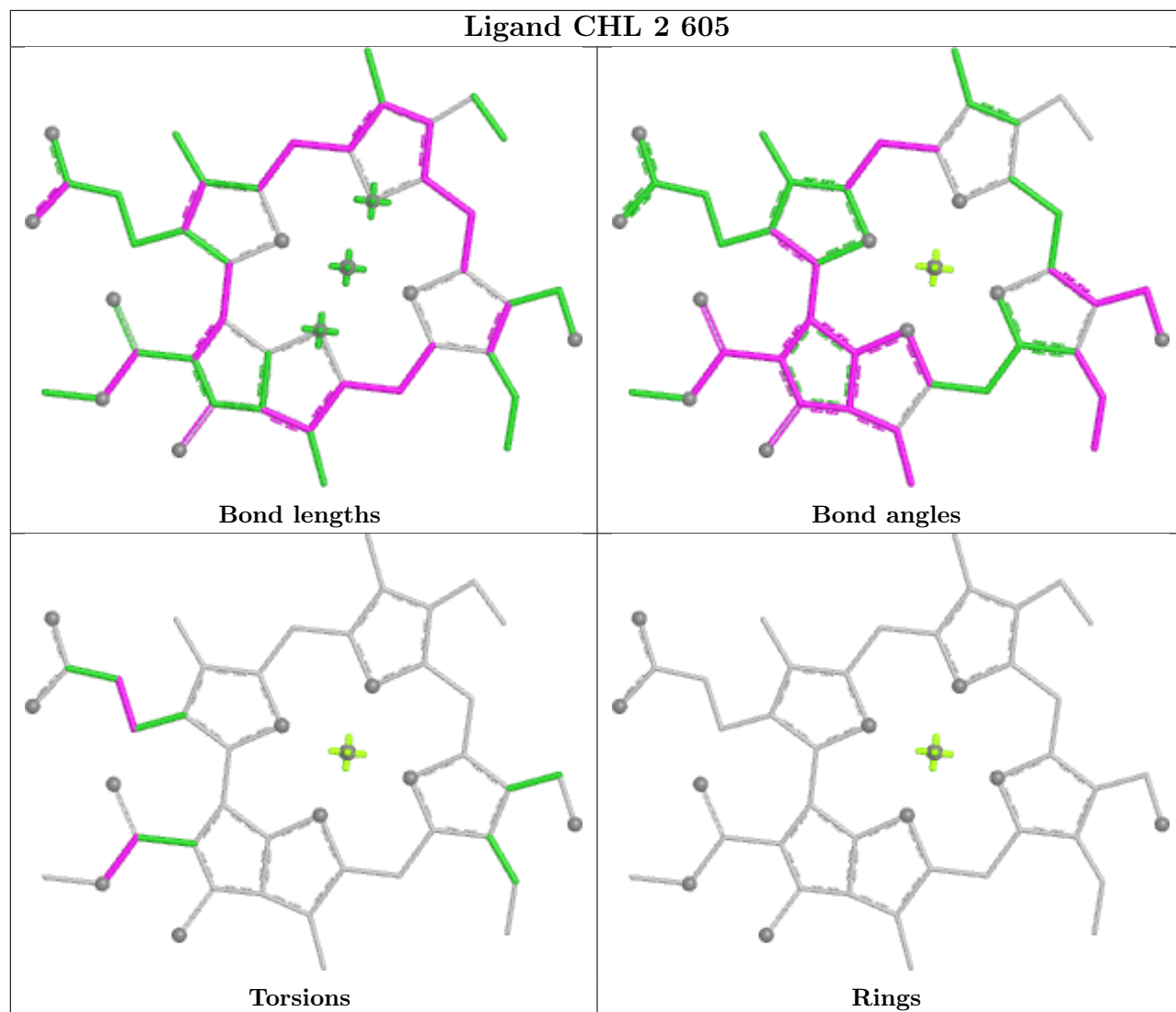


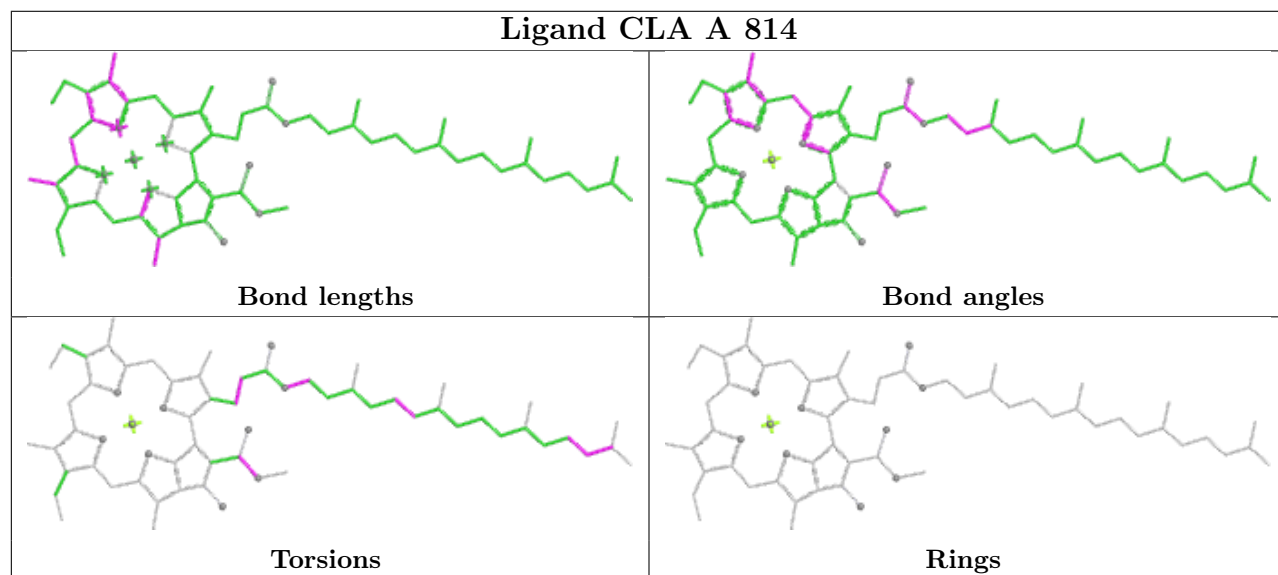
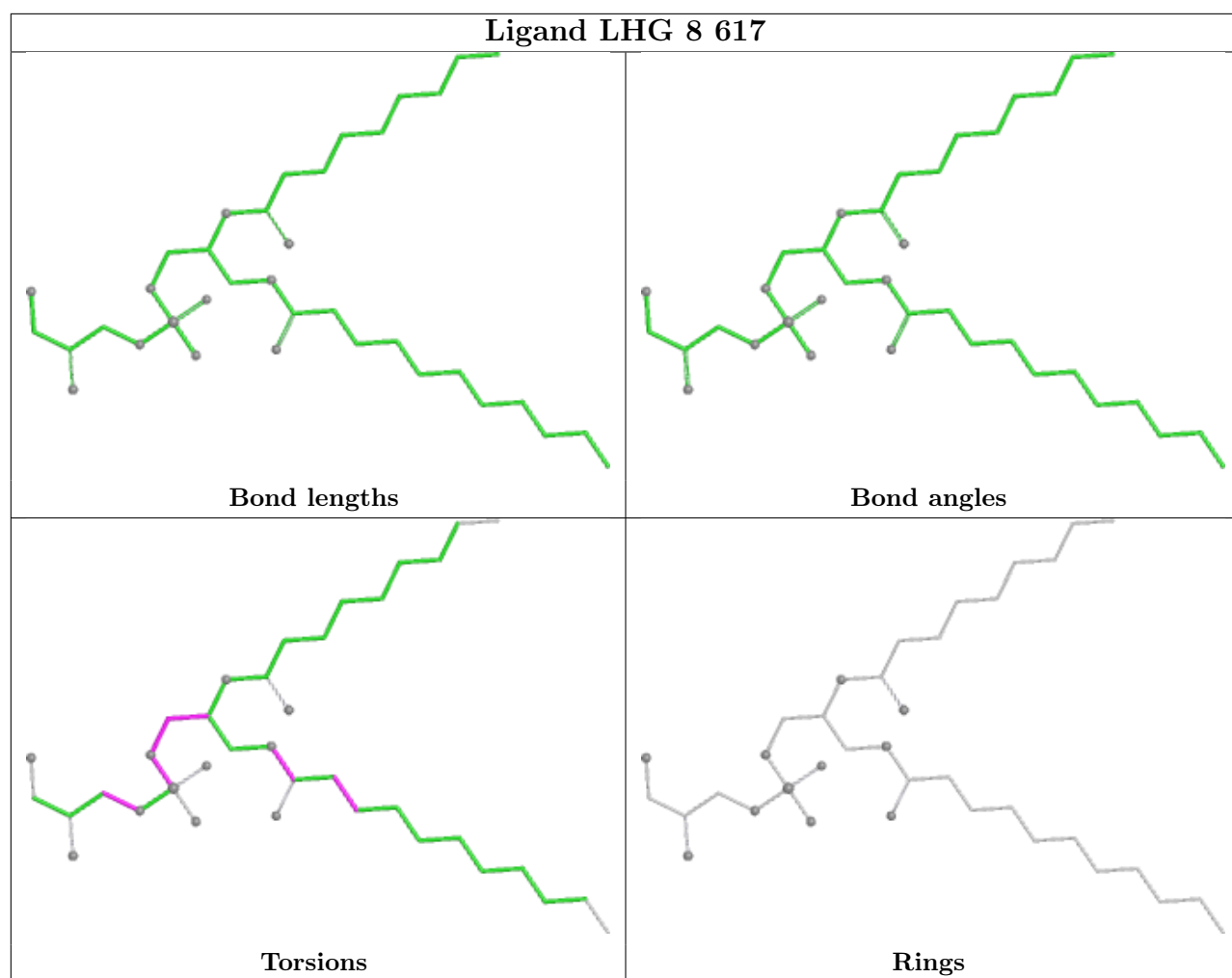
Ligand BCR L 301

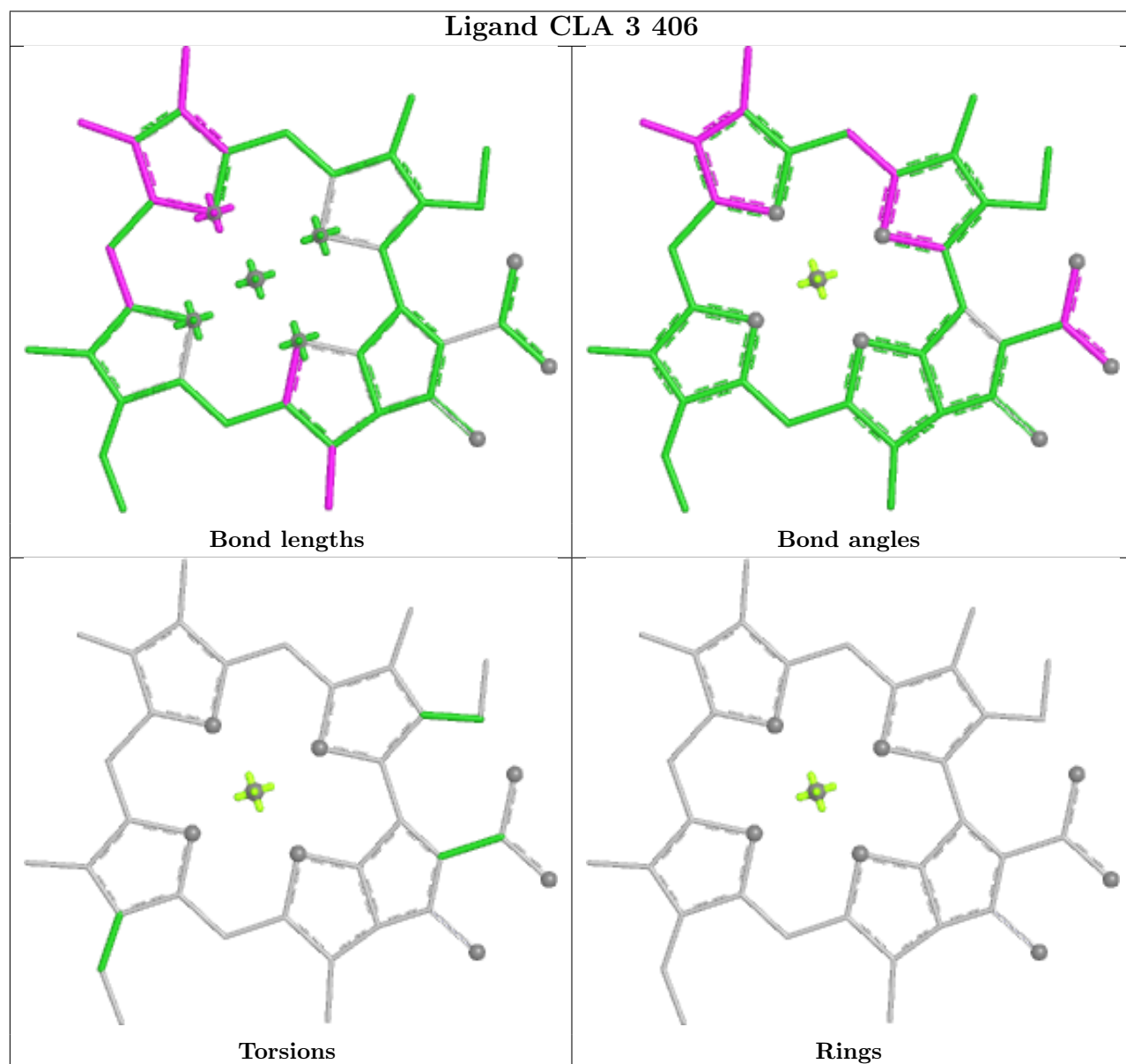
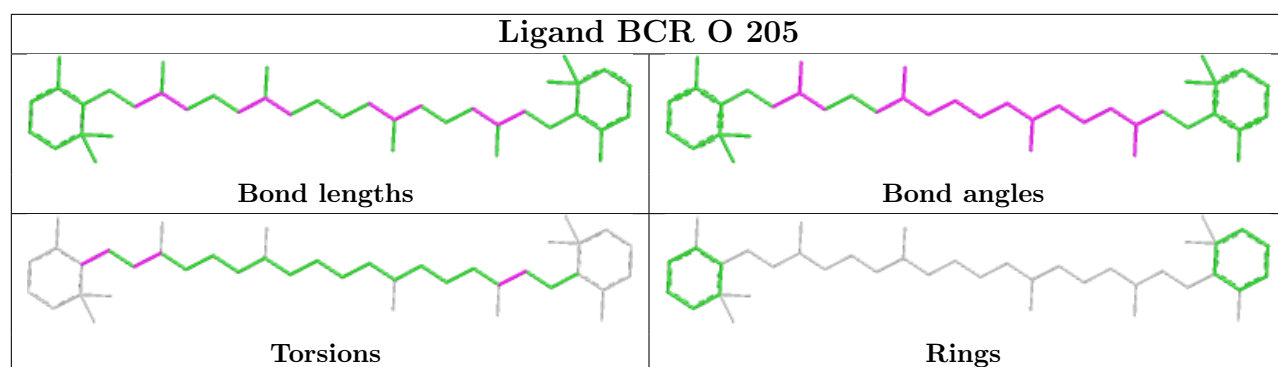




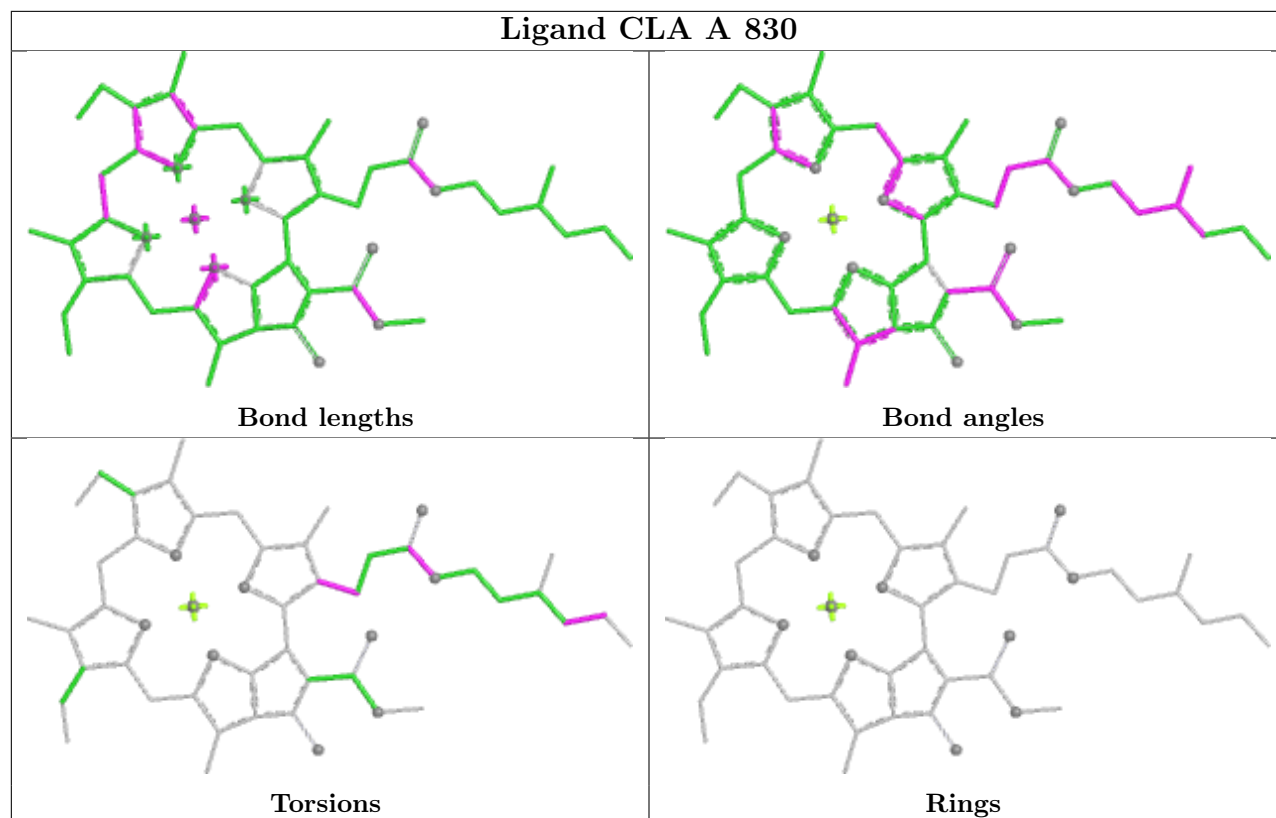
Ligand CHL 2 605



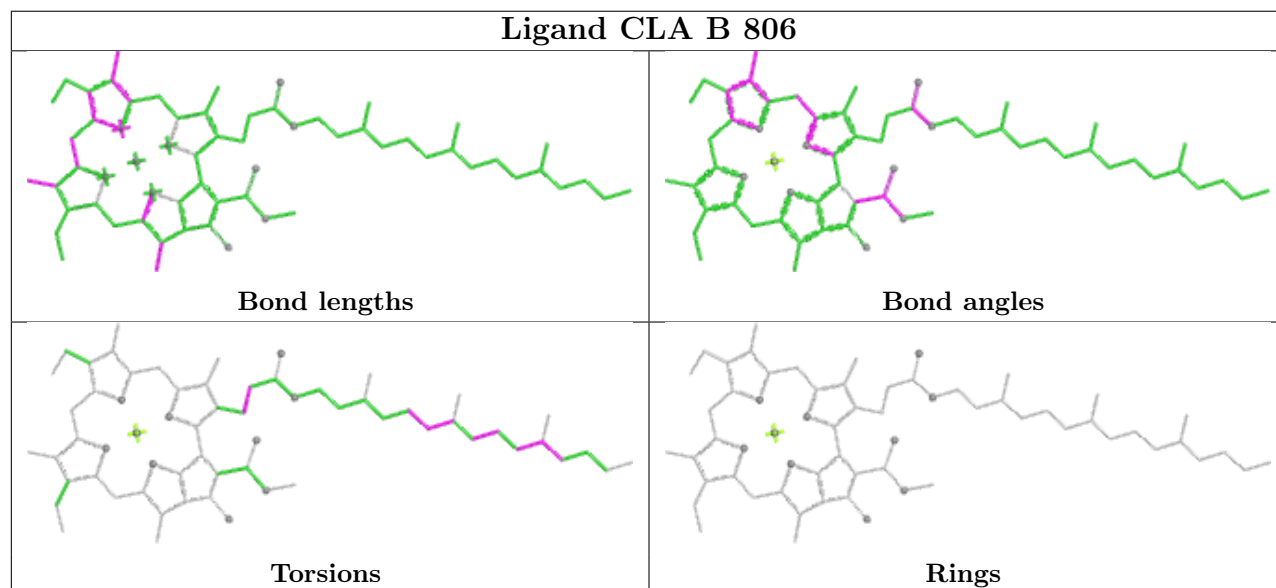




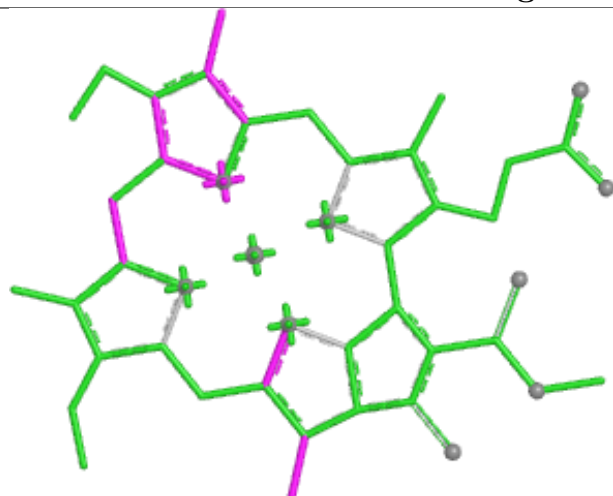
Ligand CLA A 830



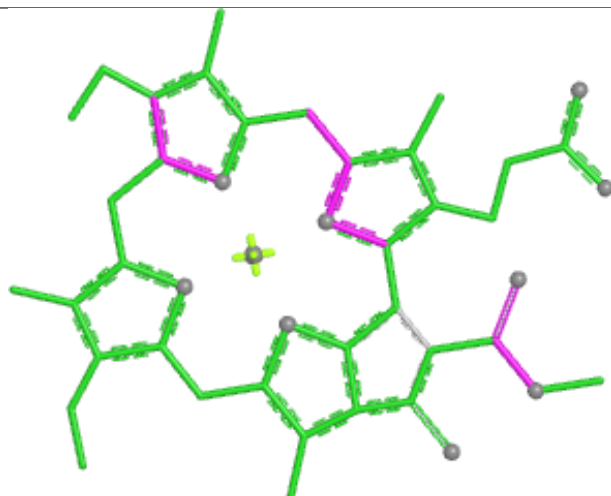
Ligand CLA B 806



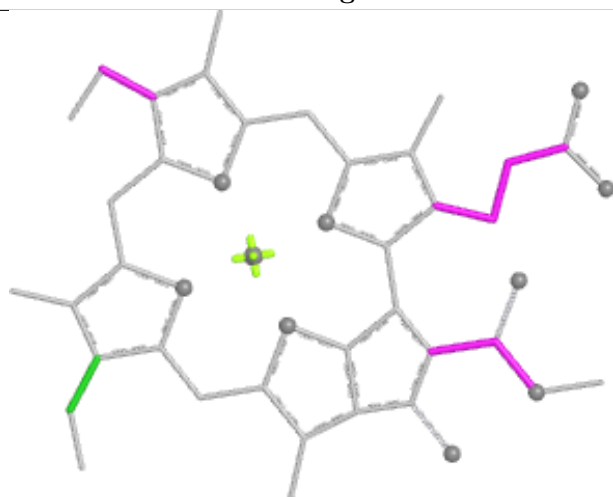
Ligand CLA b 315



Bond lengths



Bond angles

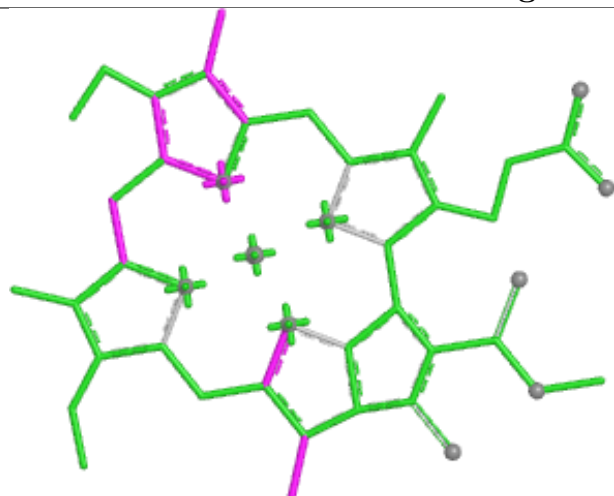


Torsions

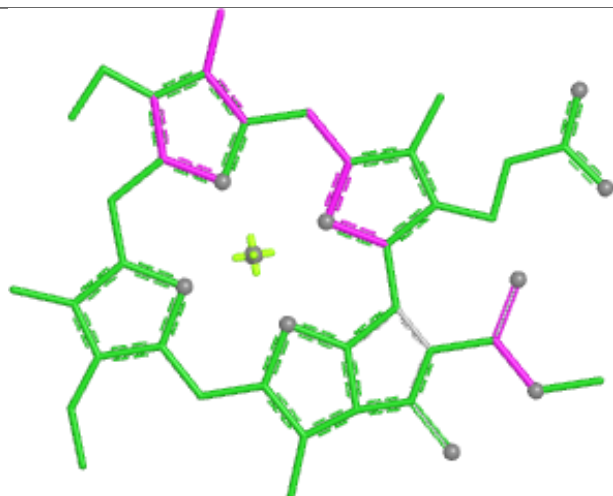


Rings

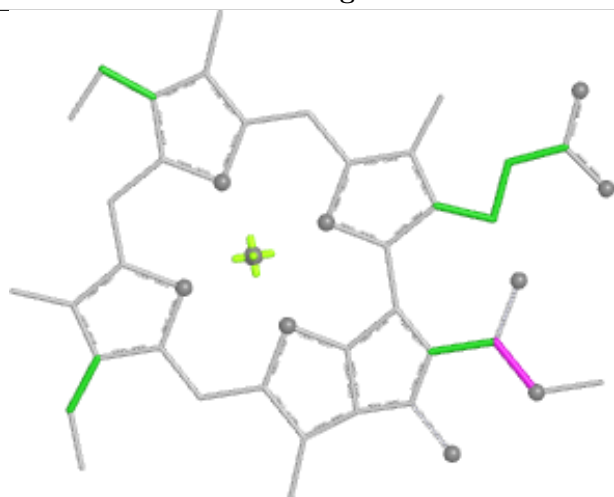
Ligand CLA 2 604



Bond lengths



Bond angles

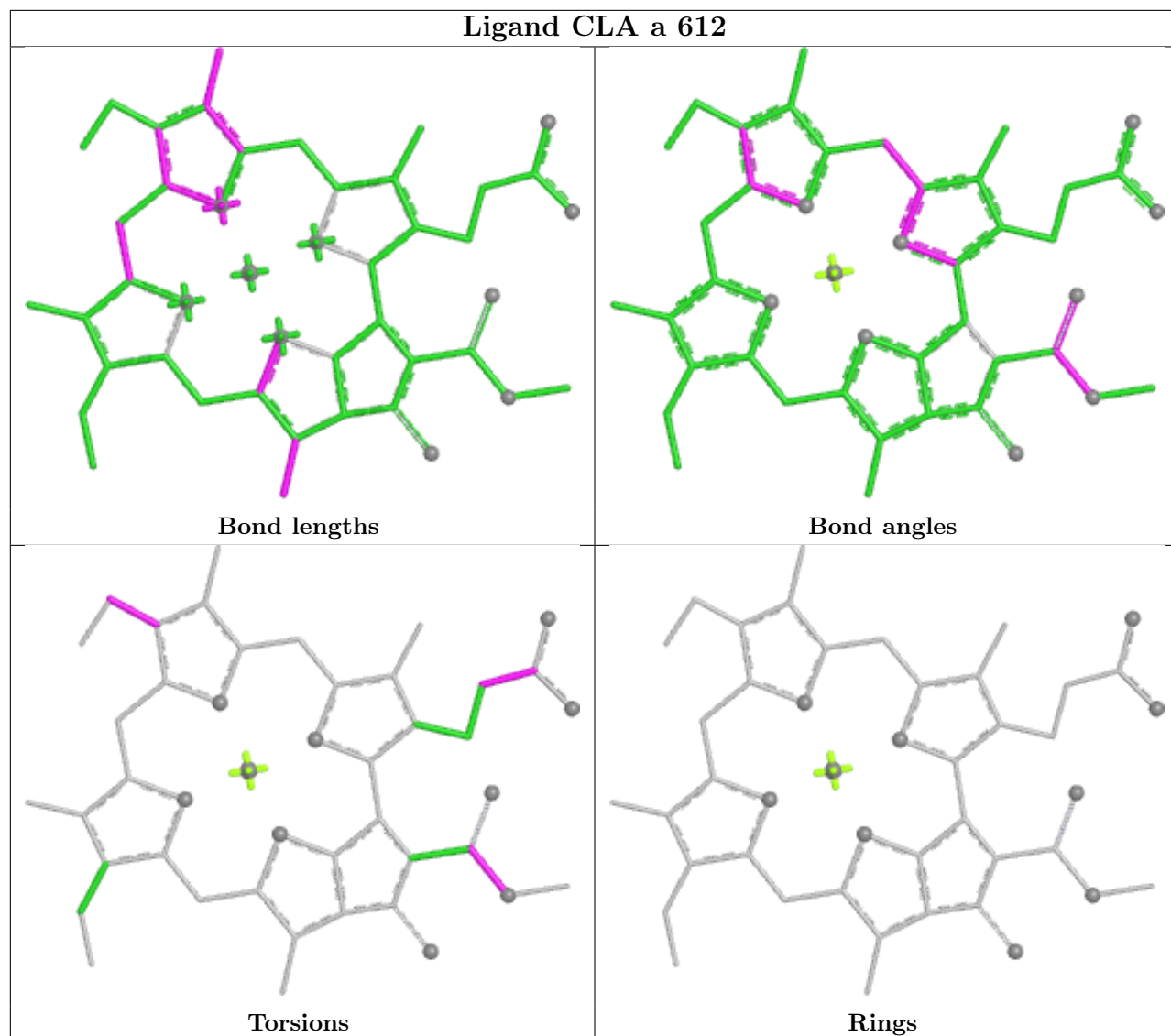


Torsions

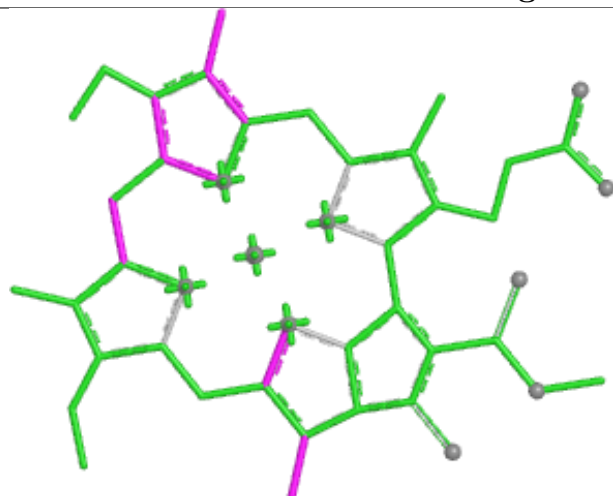


Rings

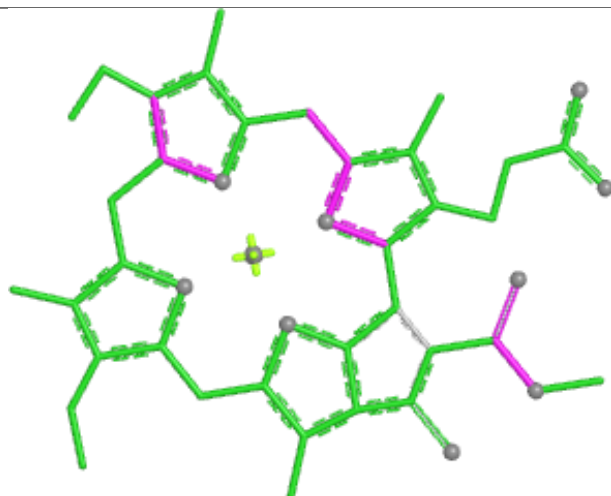
Ligand CLA a 612



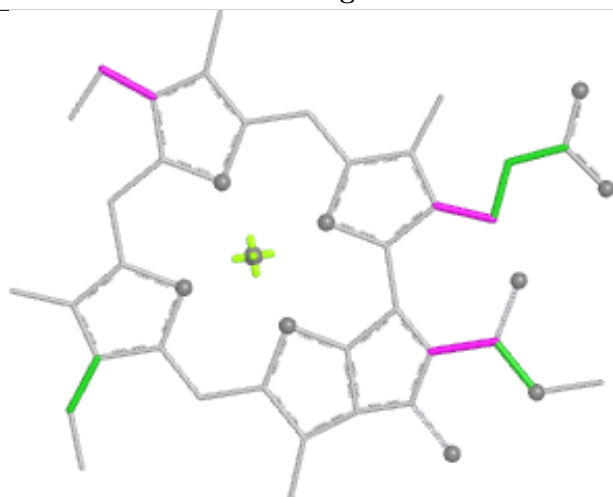
Ligand CLA 9 603



Bond lengths



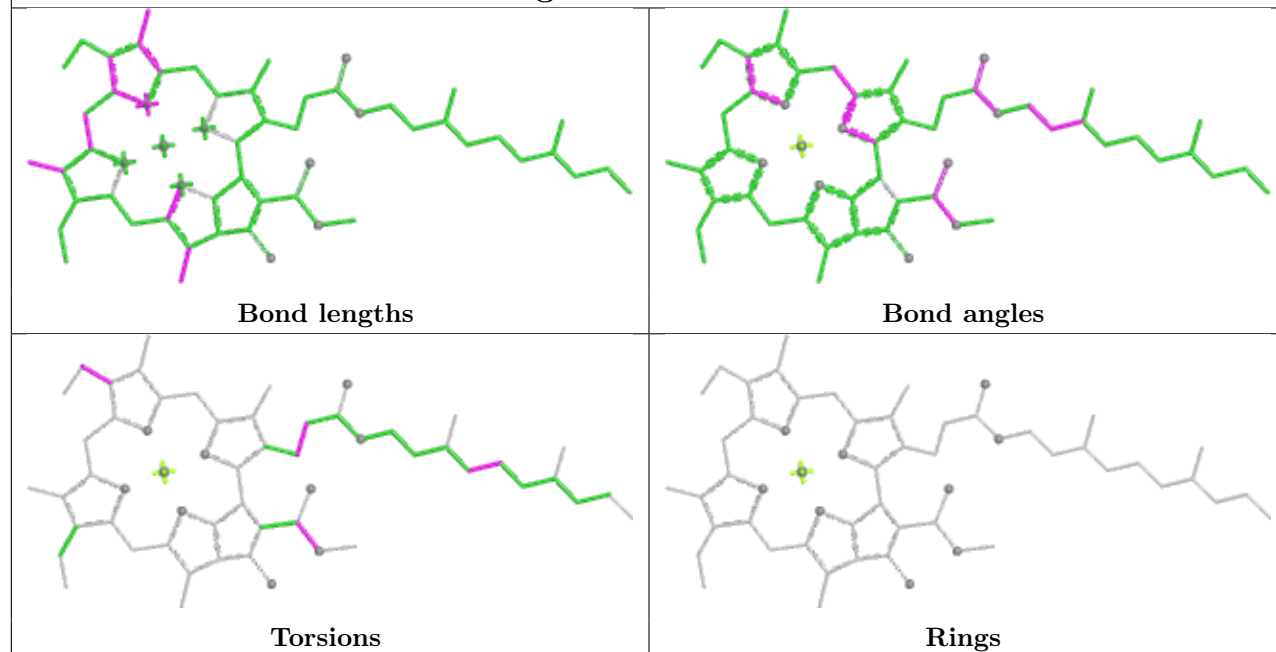
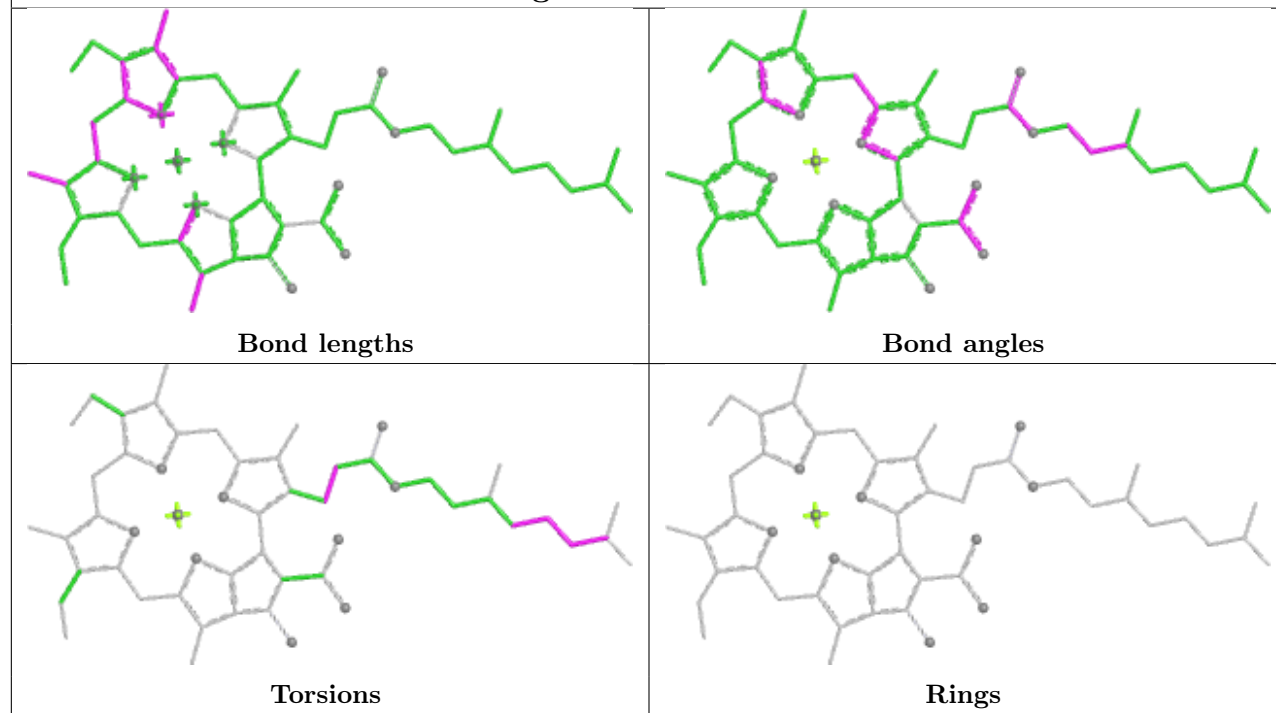
Bond angles



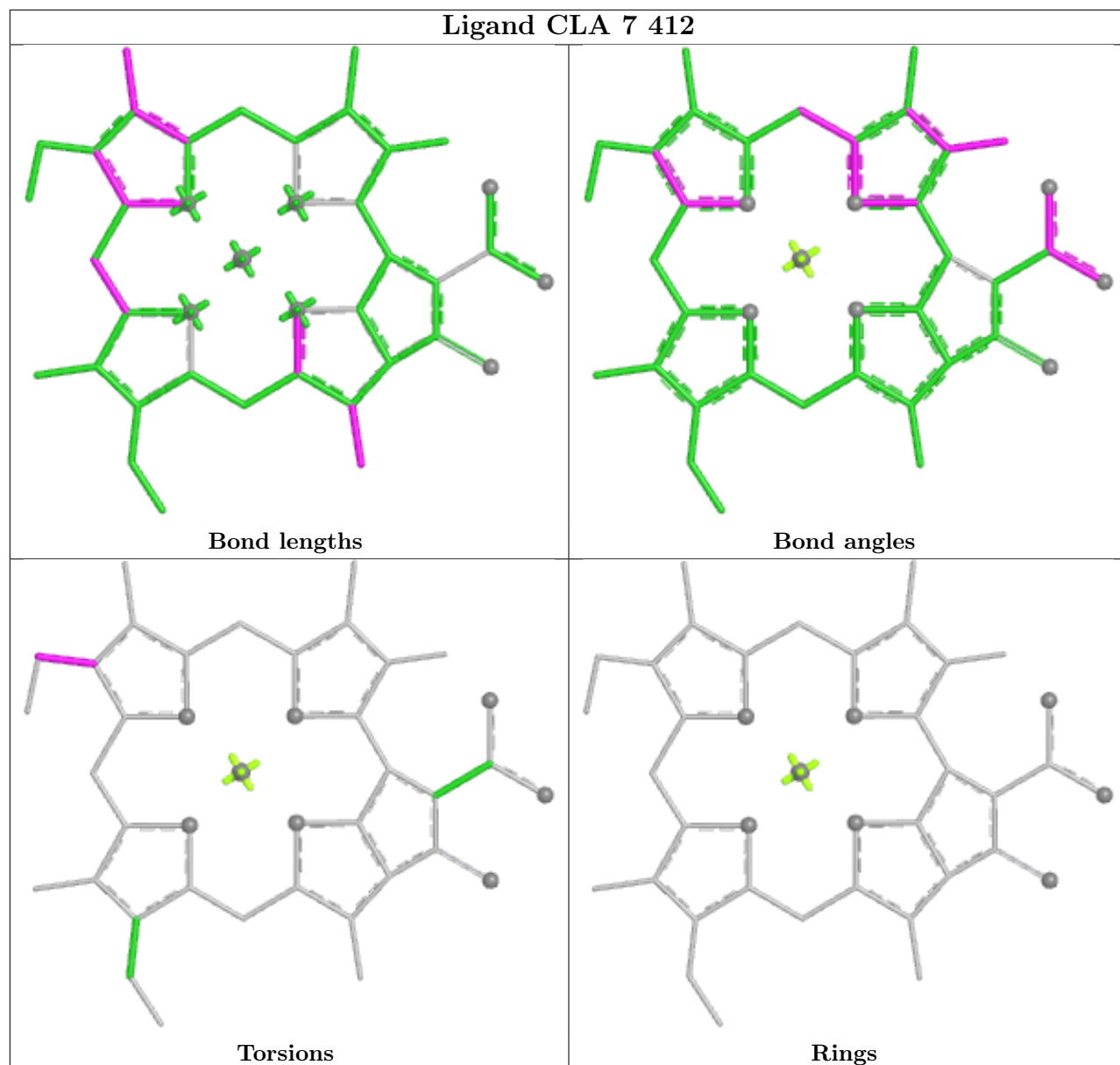
Torsions

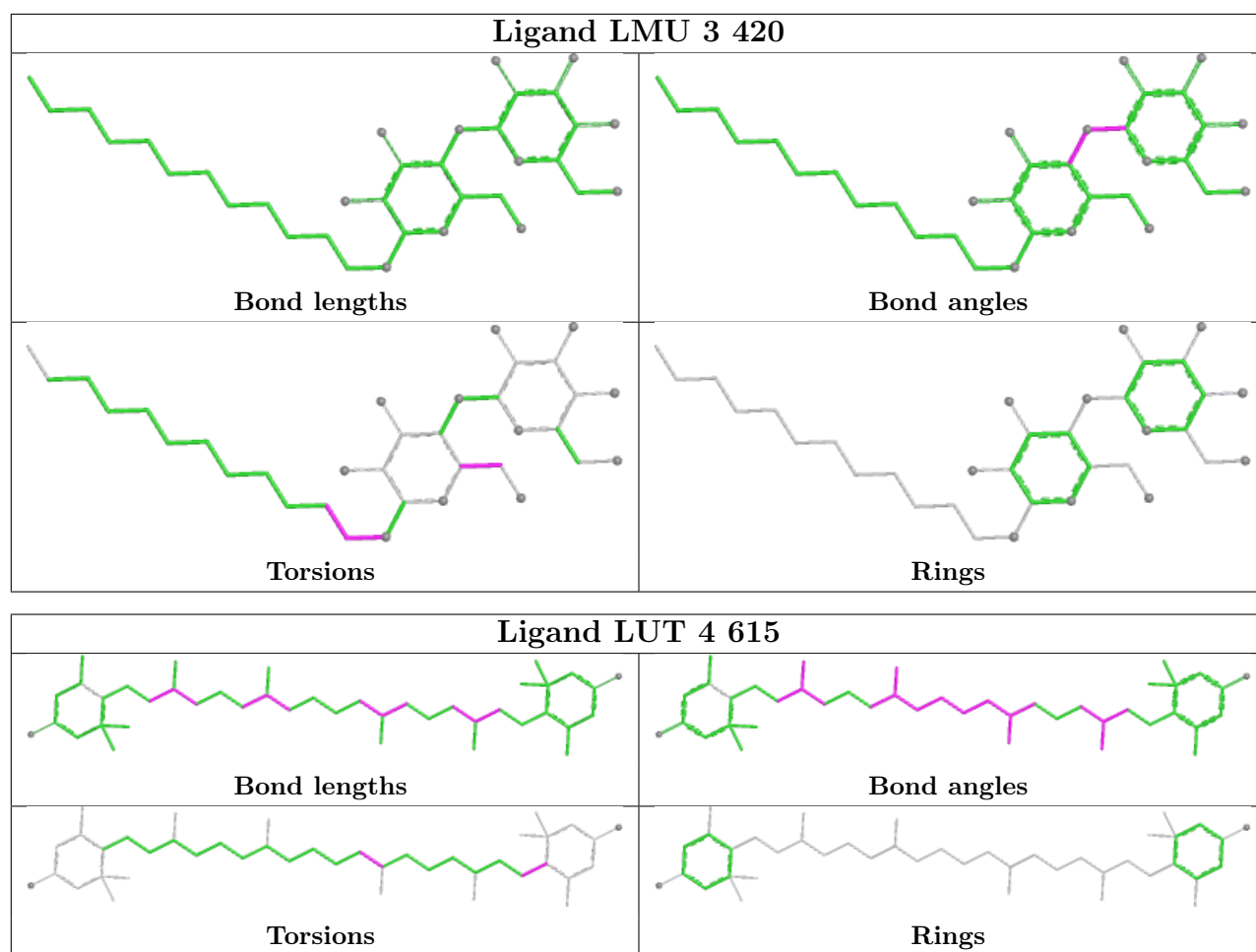


Rings

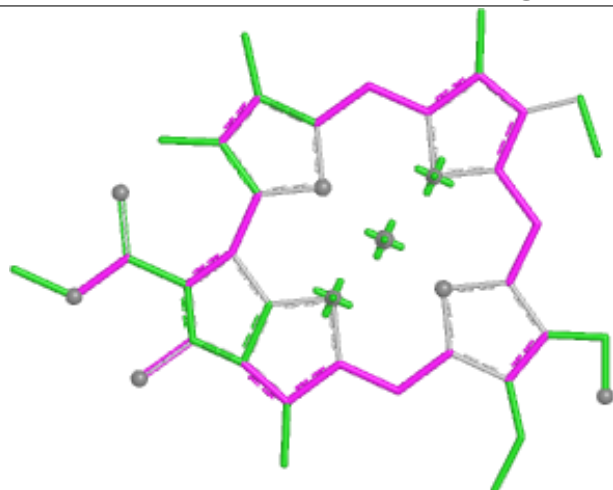
Ligand CLA a 613**Ligand CLA B 815**

Ligand CLA 7 412

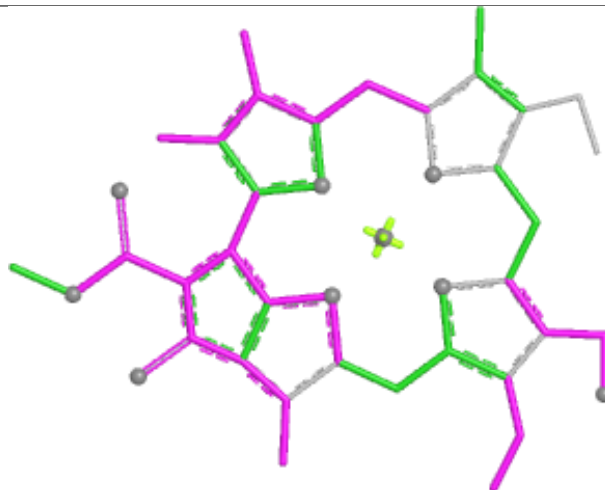




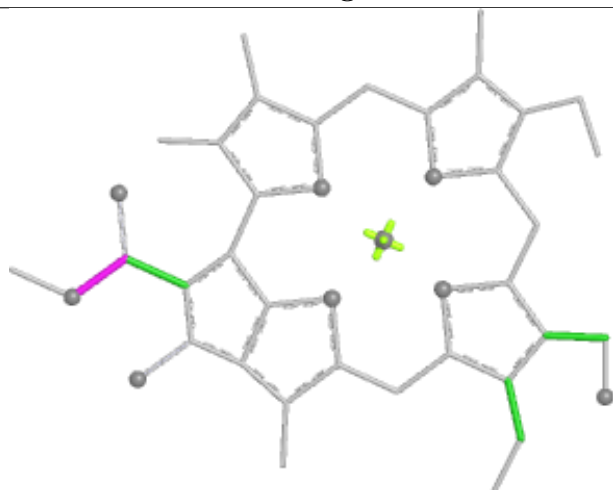
Ligand CHL 4 614



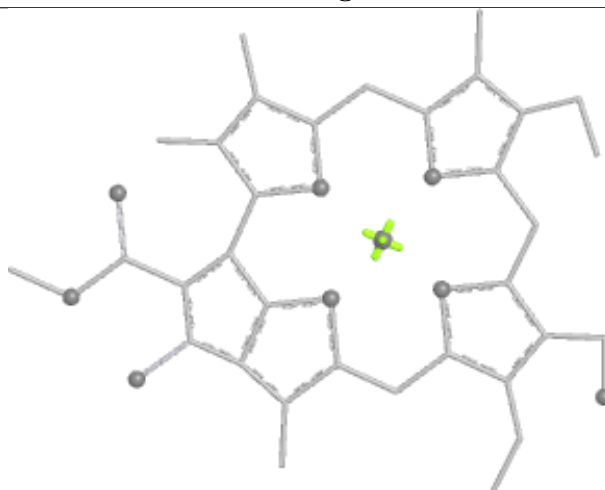
Bond lengths



Bond angles

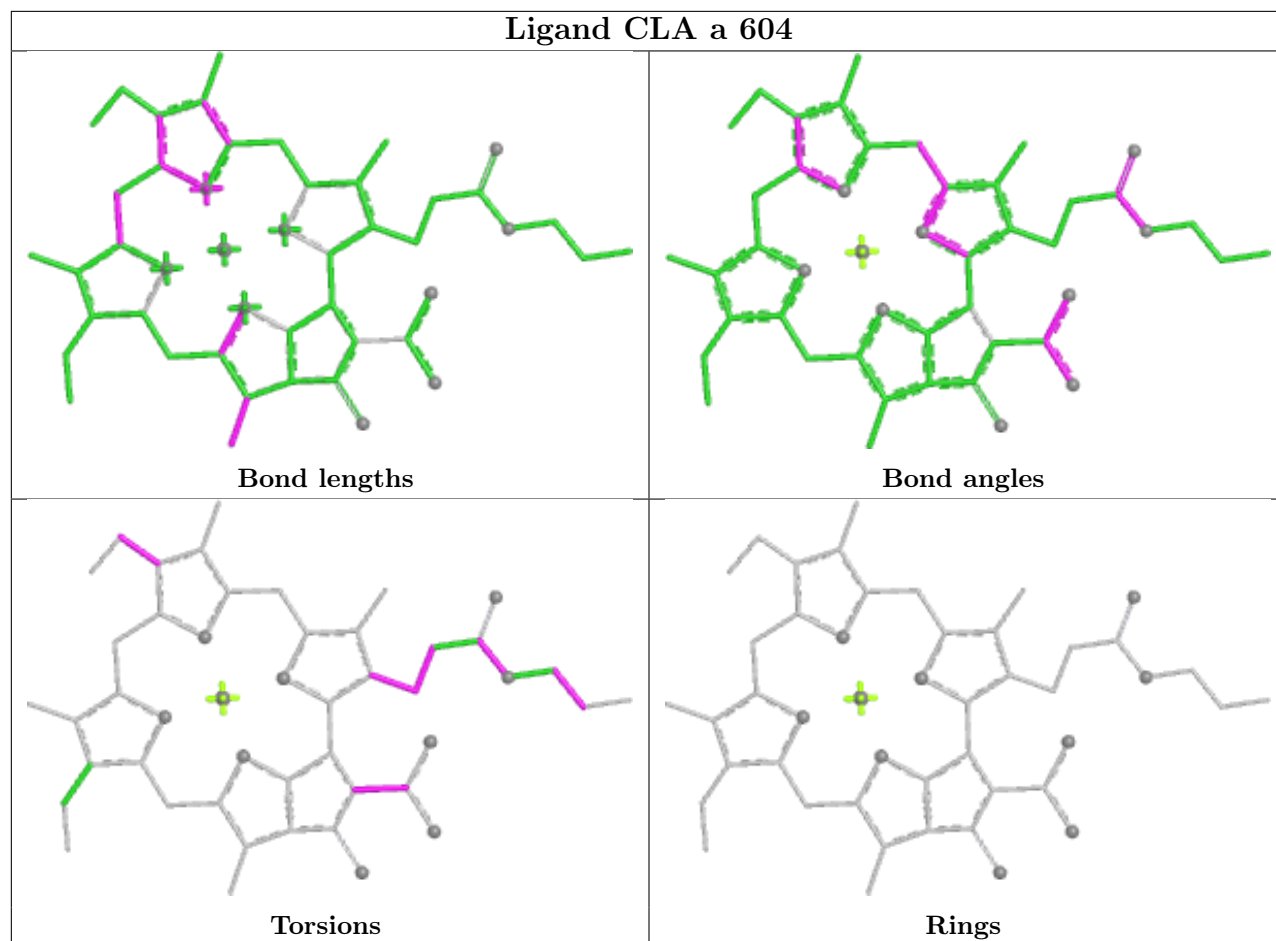


Torsions

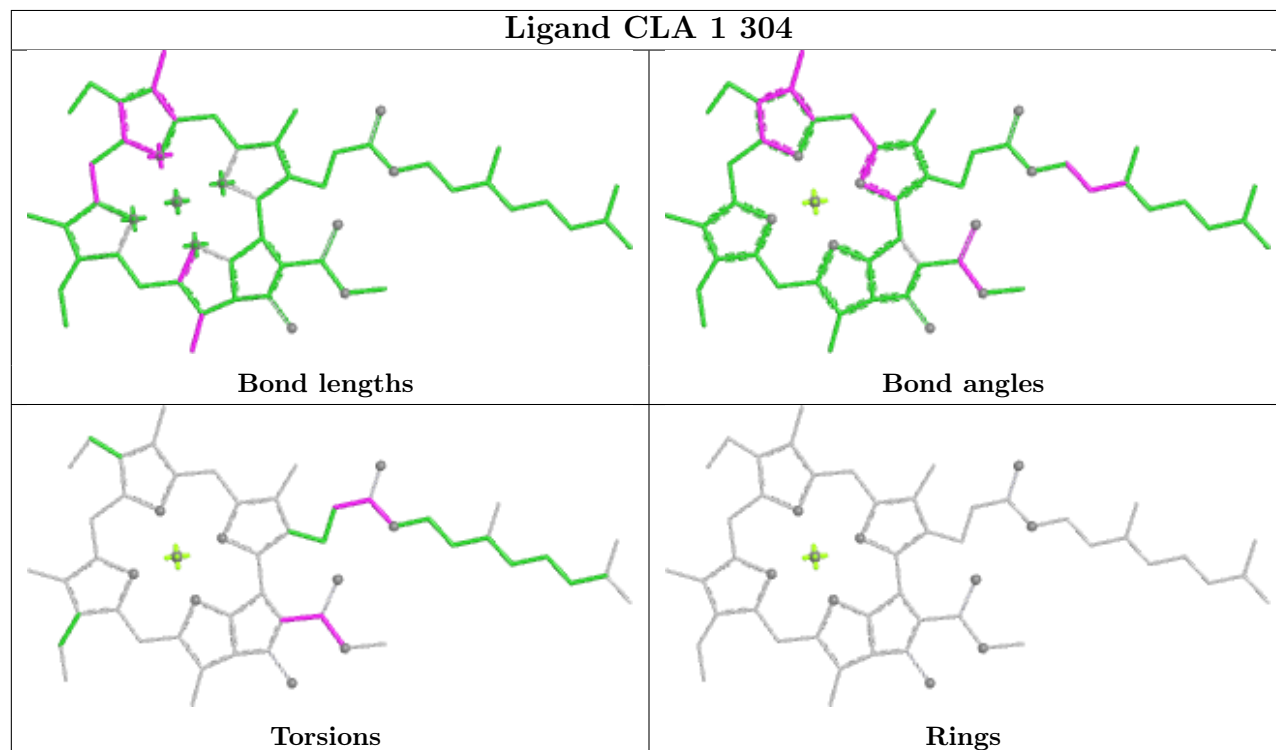


Rings

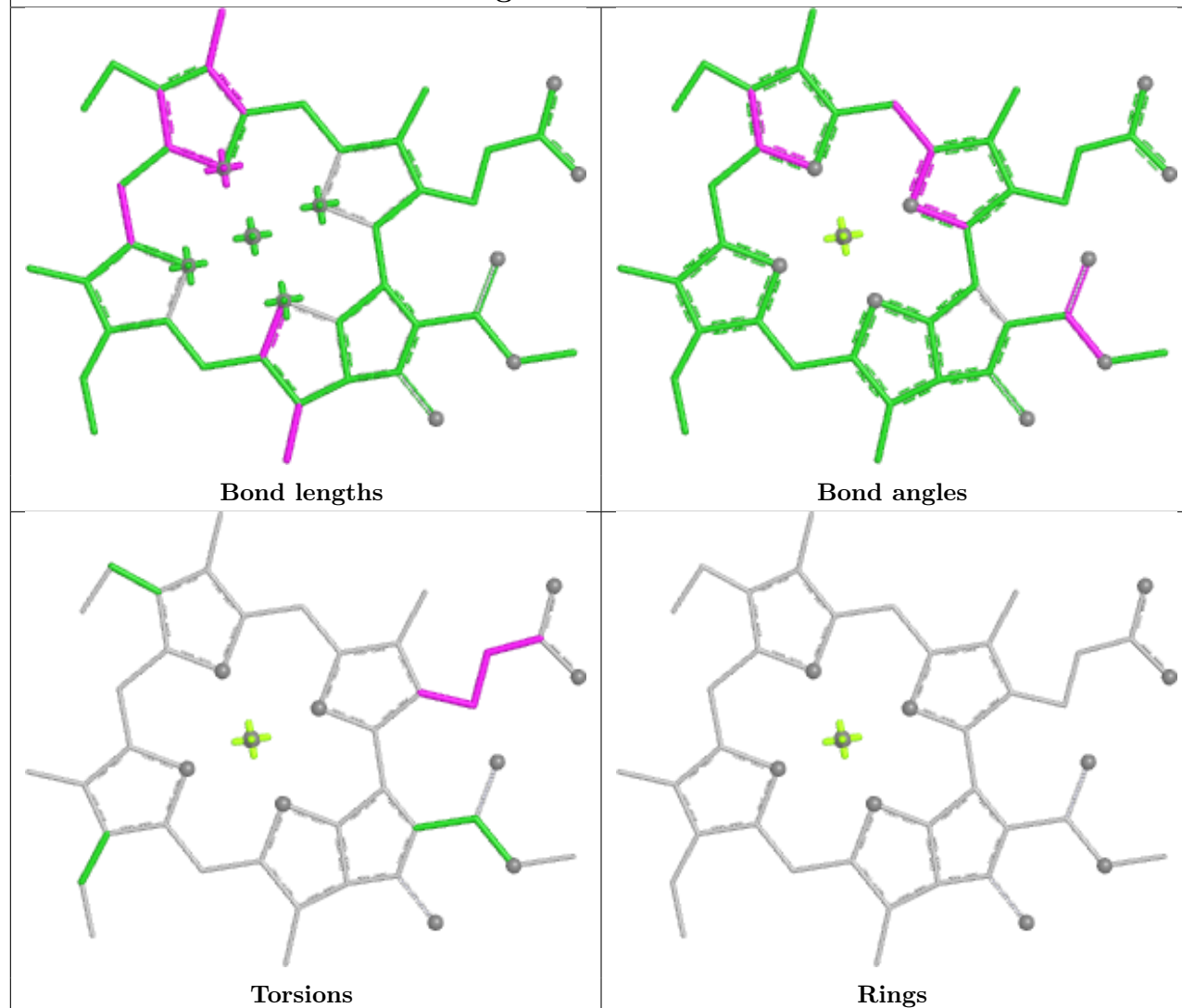
Ligand CLA a 604



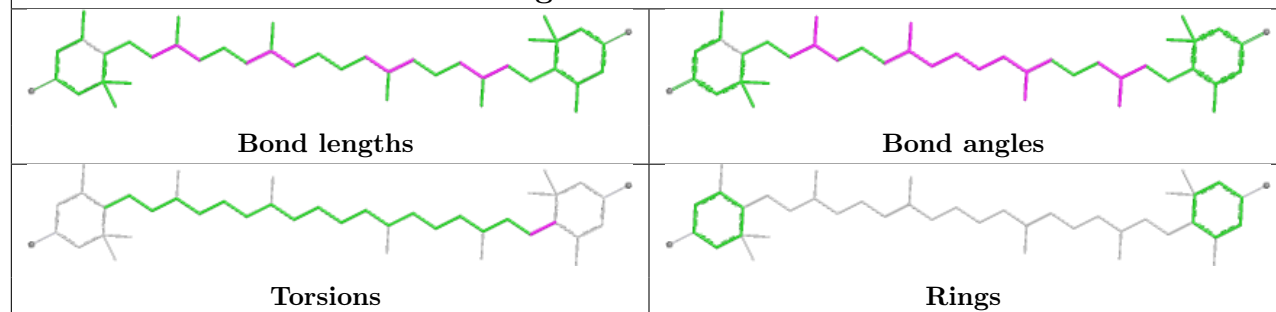
Ligand CLA 1 304

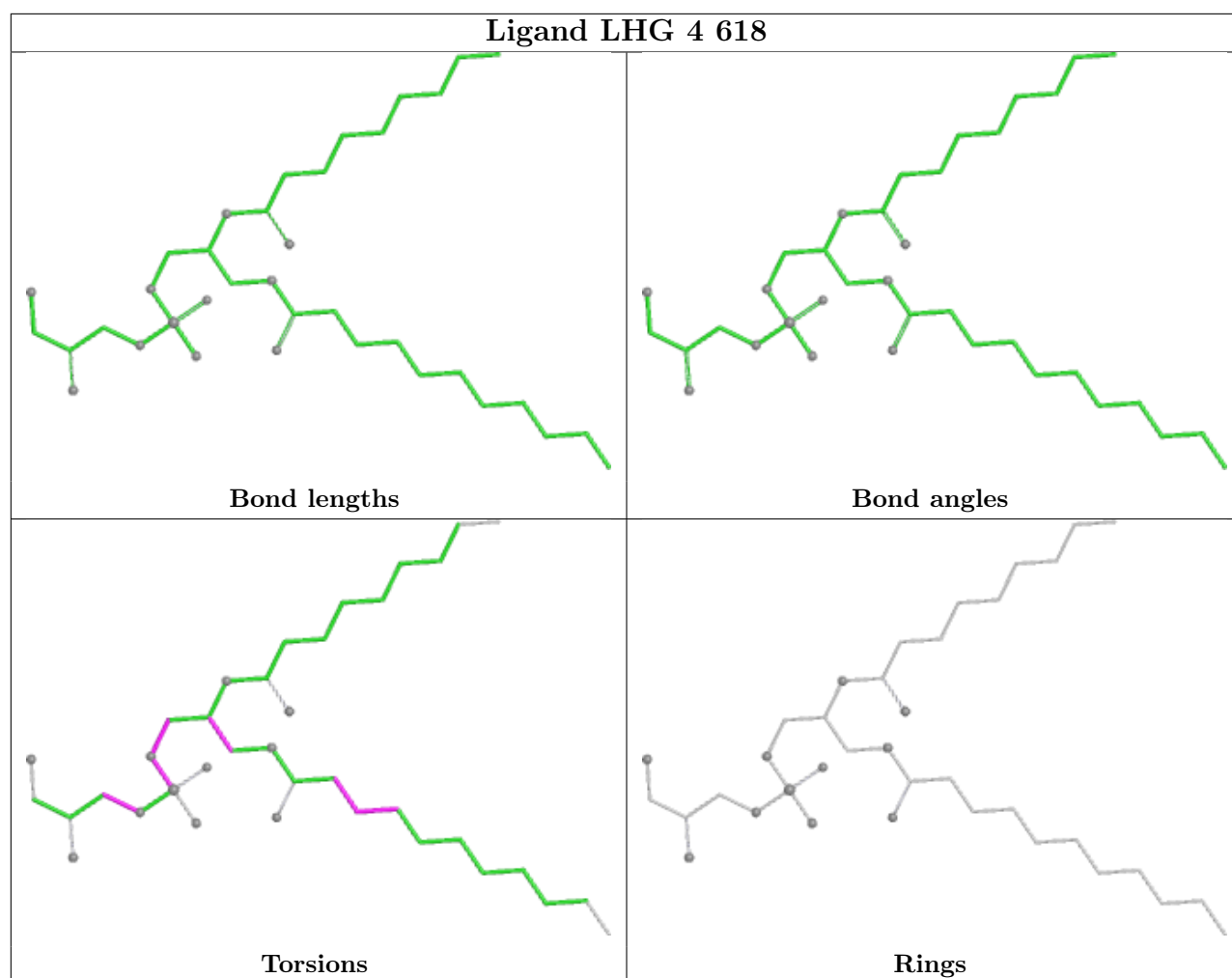


Ligand CLA b 305

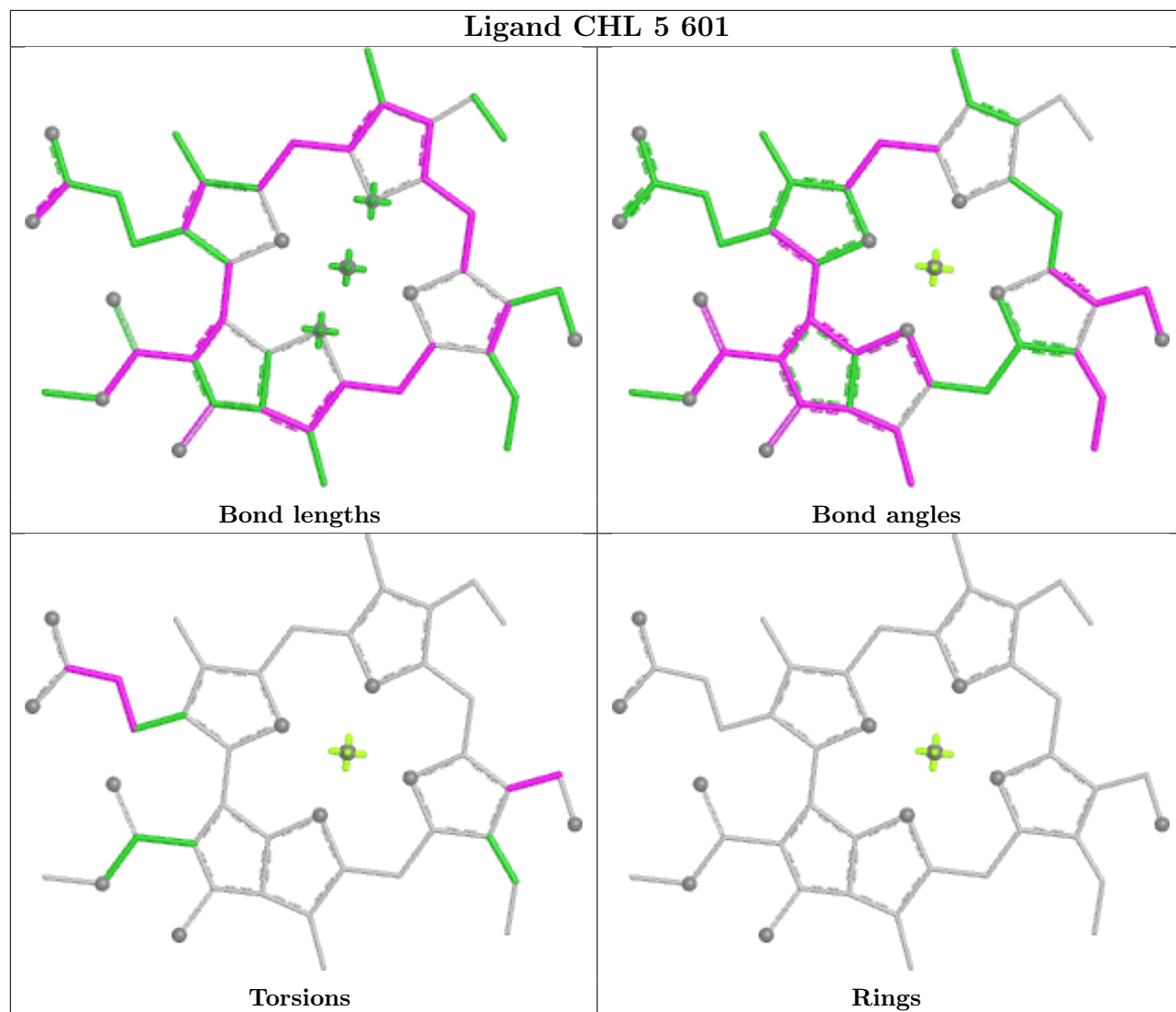


Ligand LUT b 317

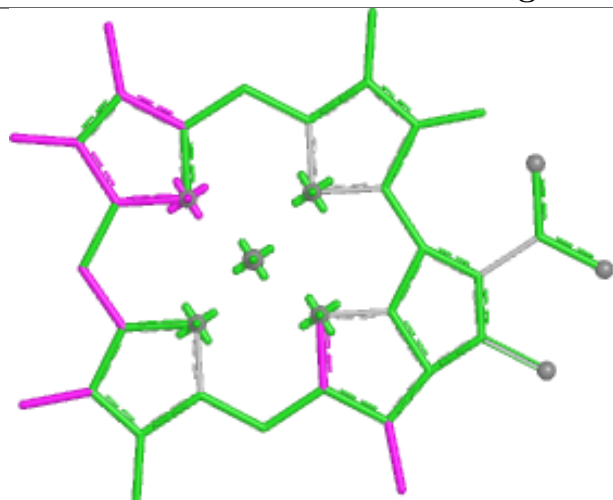




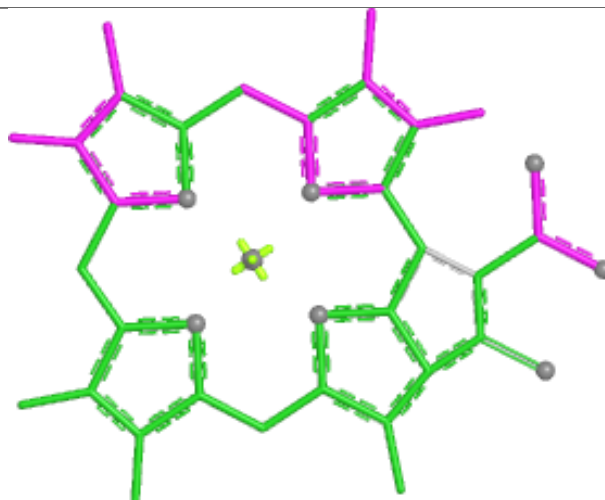
Ligand CHL 5 601



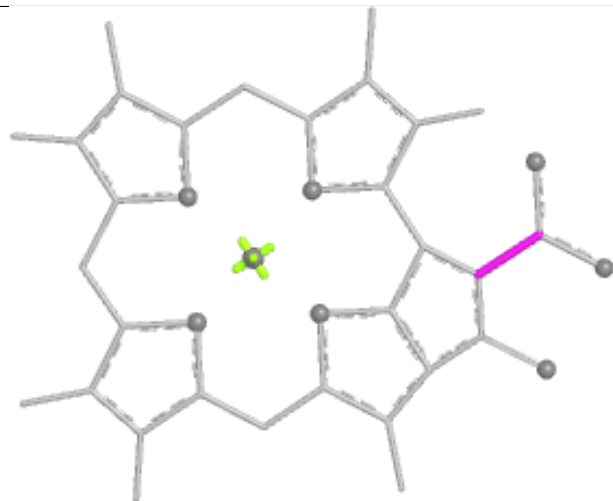
Ligand CLA 1 311



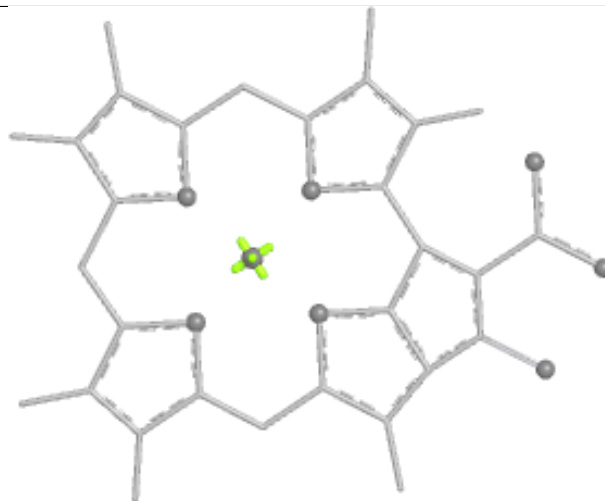
Bond lengths



Bond angles

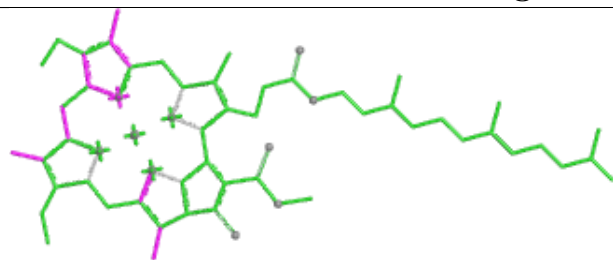


Torsions

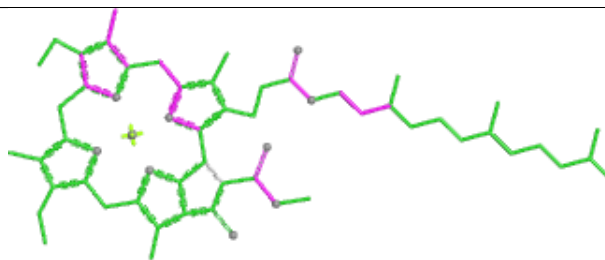


Rings

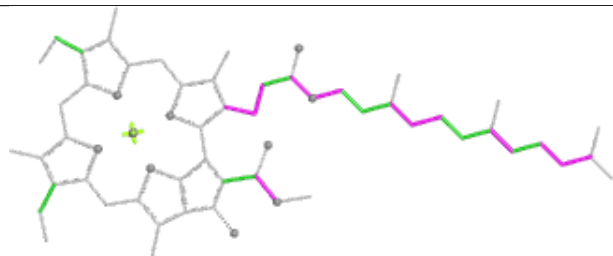
Ligand CLA A 828



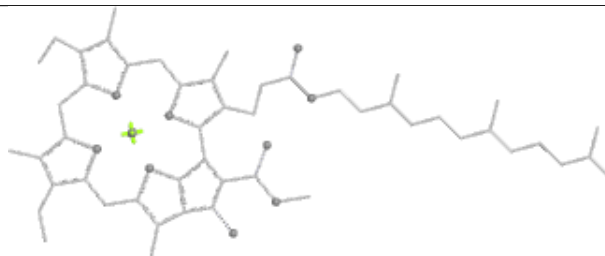
Bond lengths



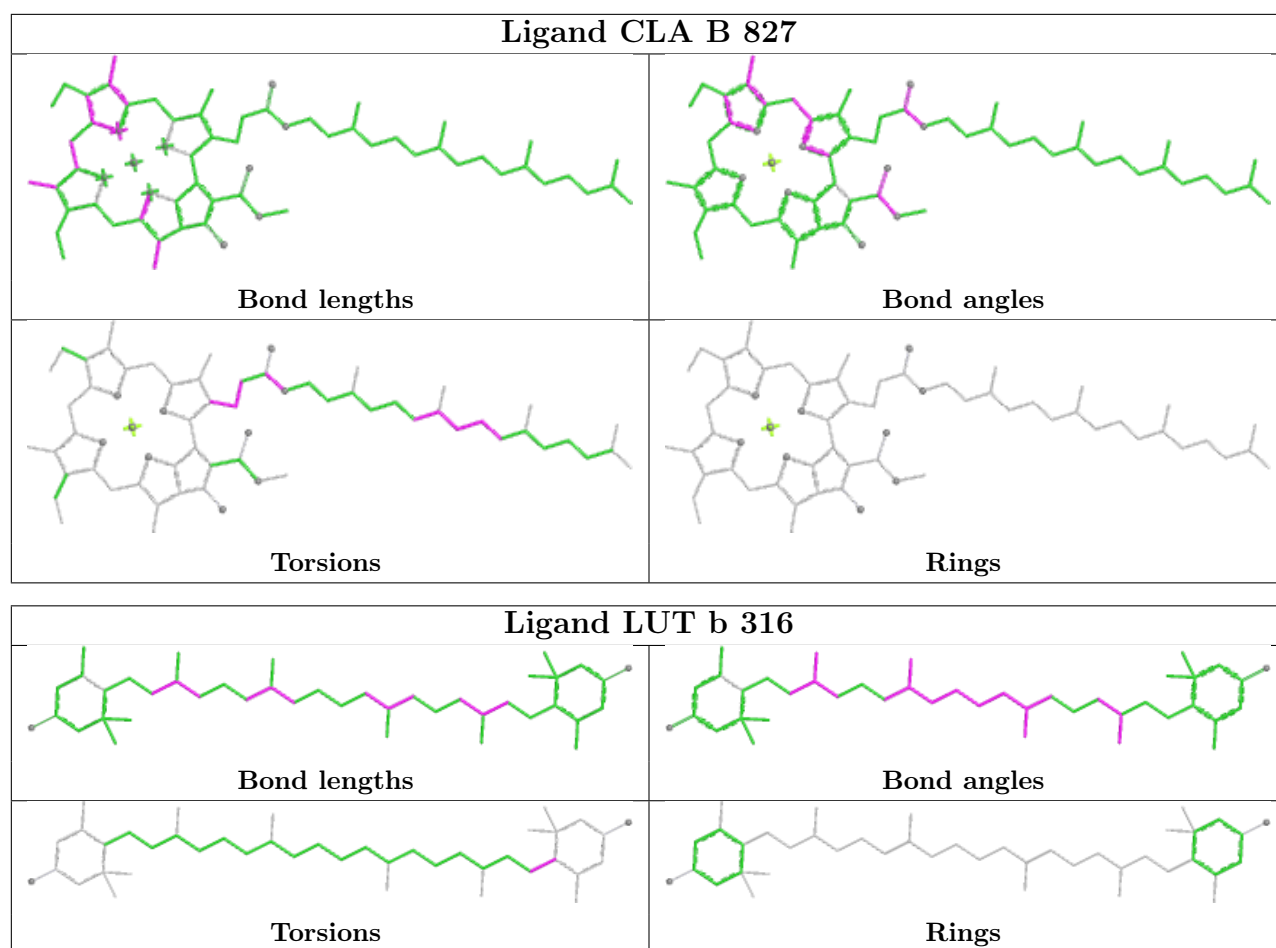
Bond angles



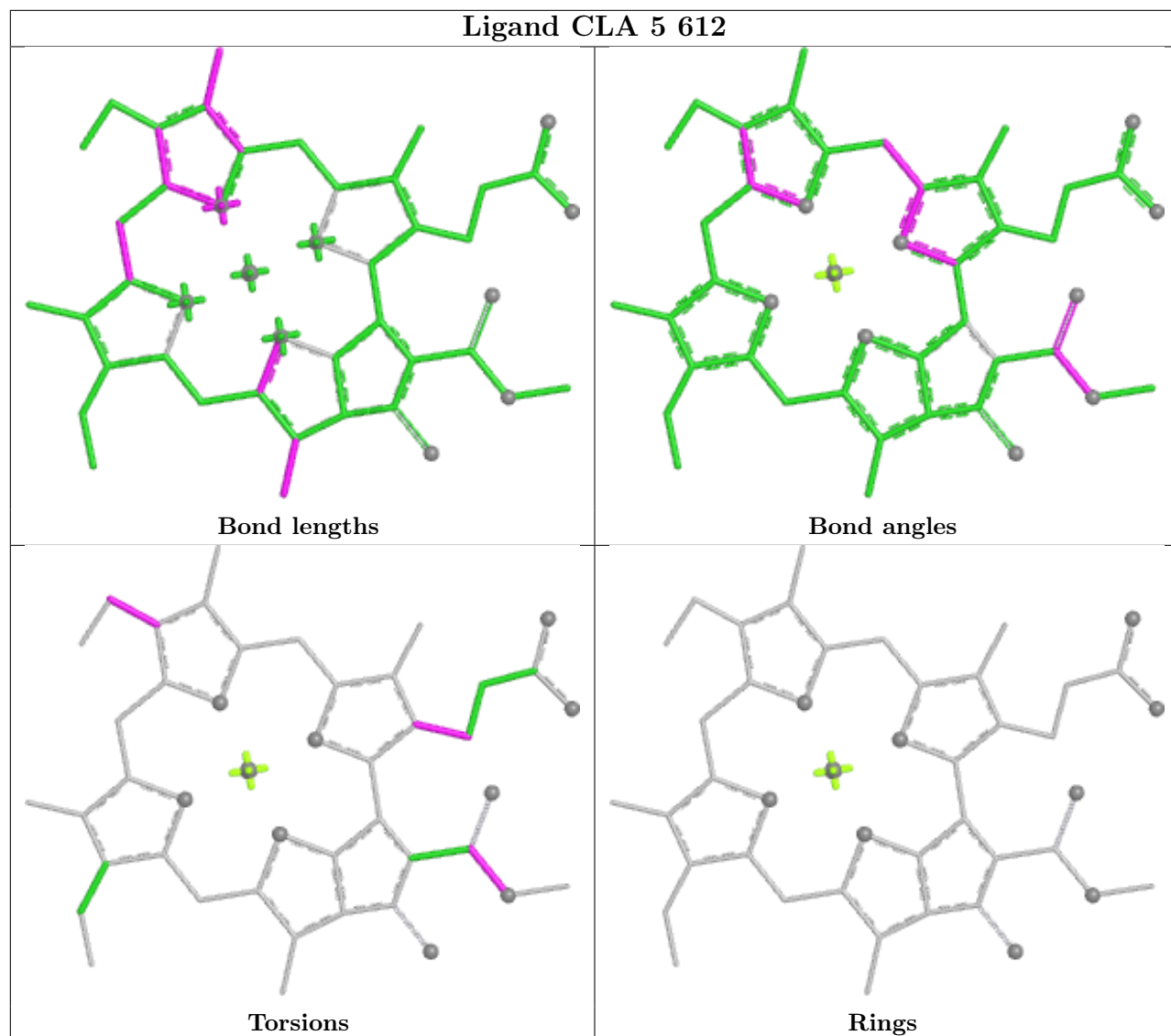
Torsions



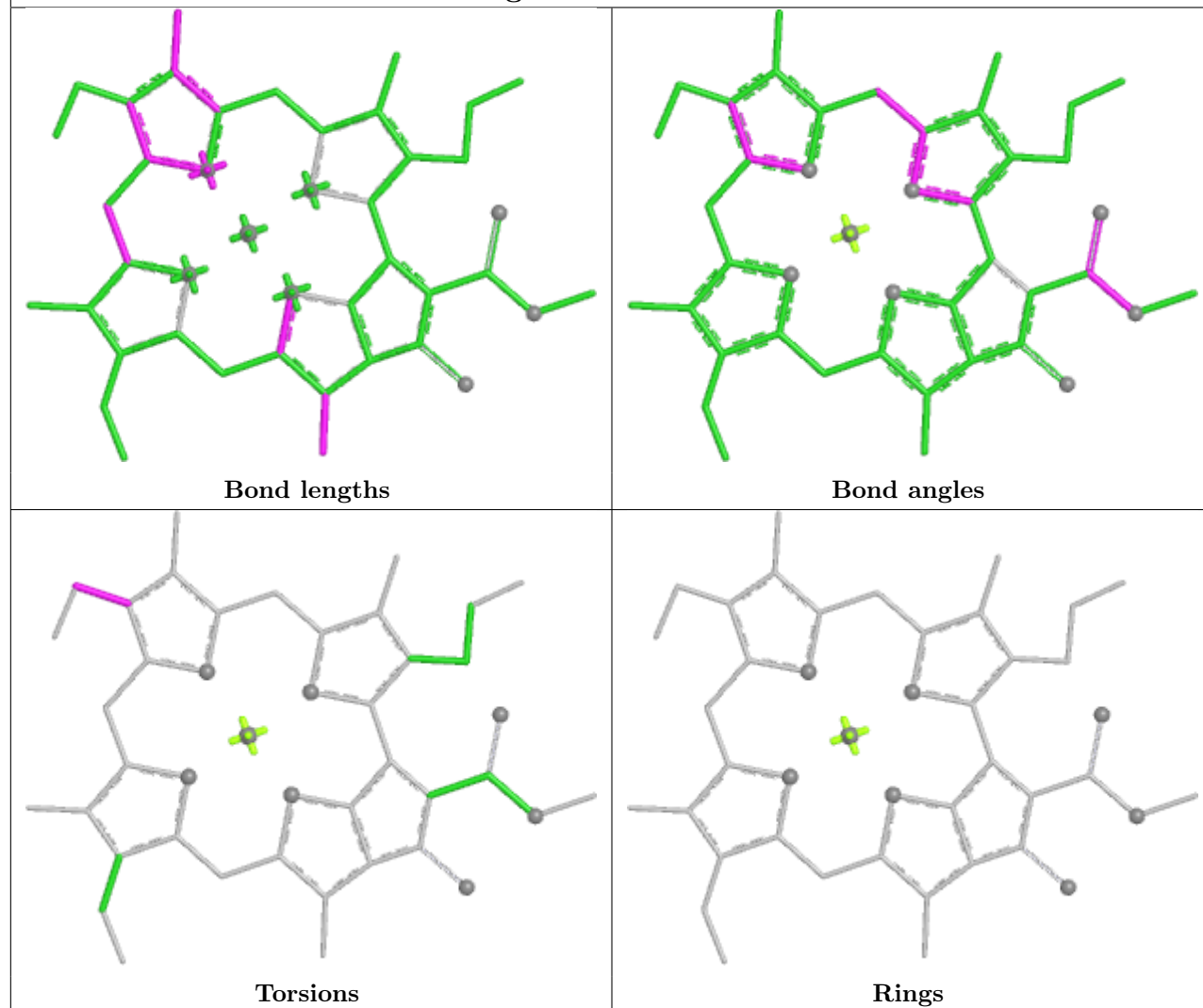
Rings



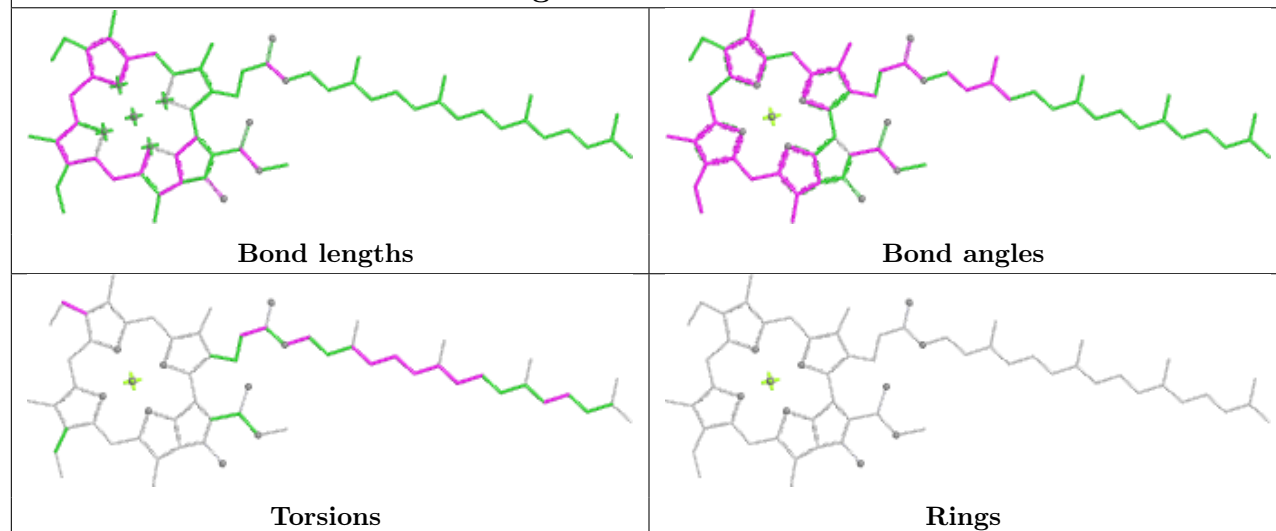
Ligand CLA 5 612

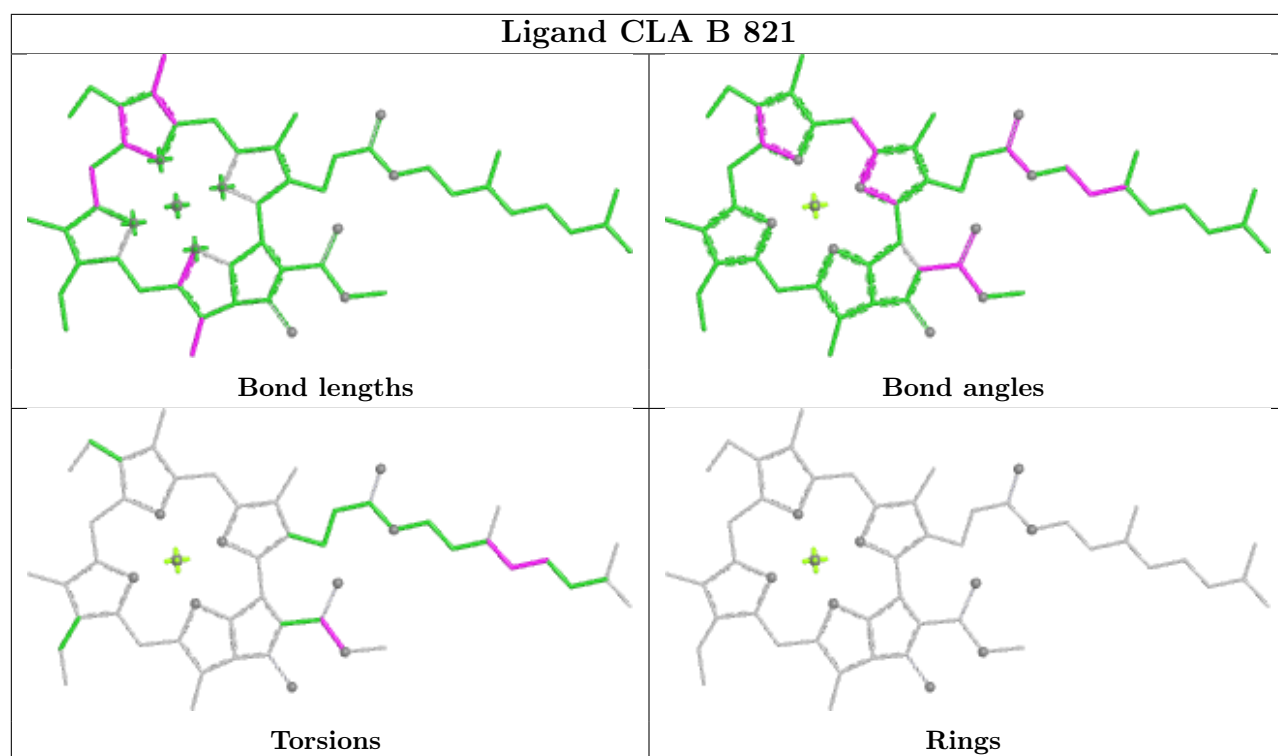


Ligand CLA 4 613

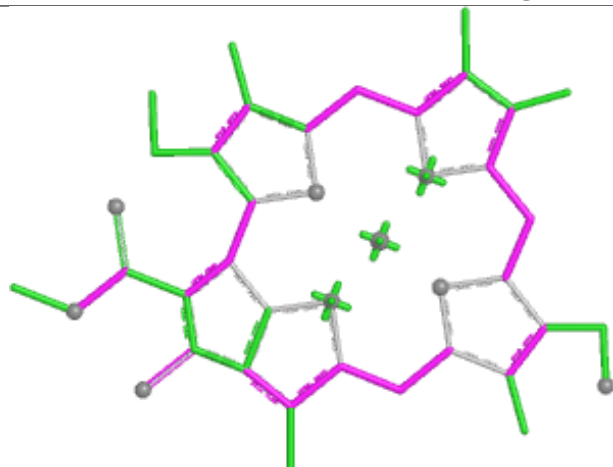


Ligand CLA B 801

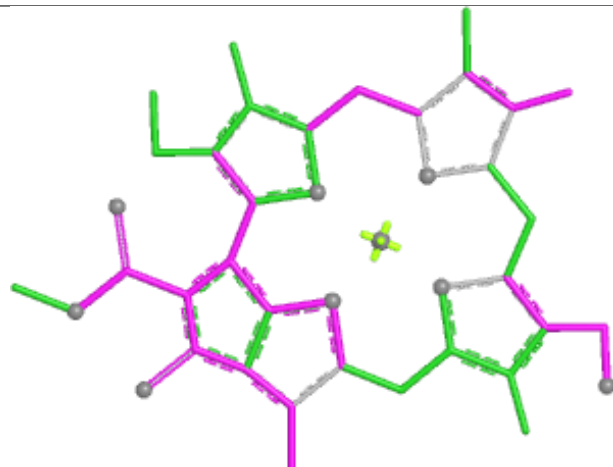




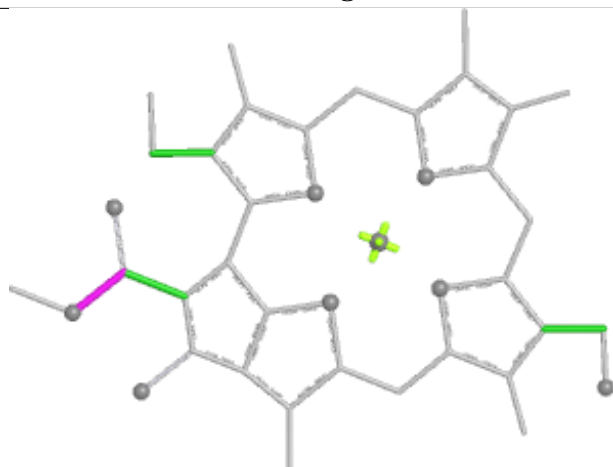
Ligand CHL 8 605



Bond lengths



Bond angles

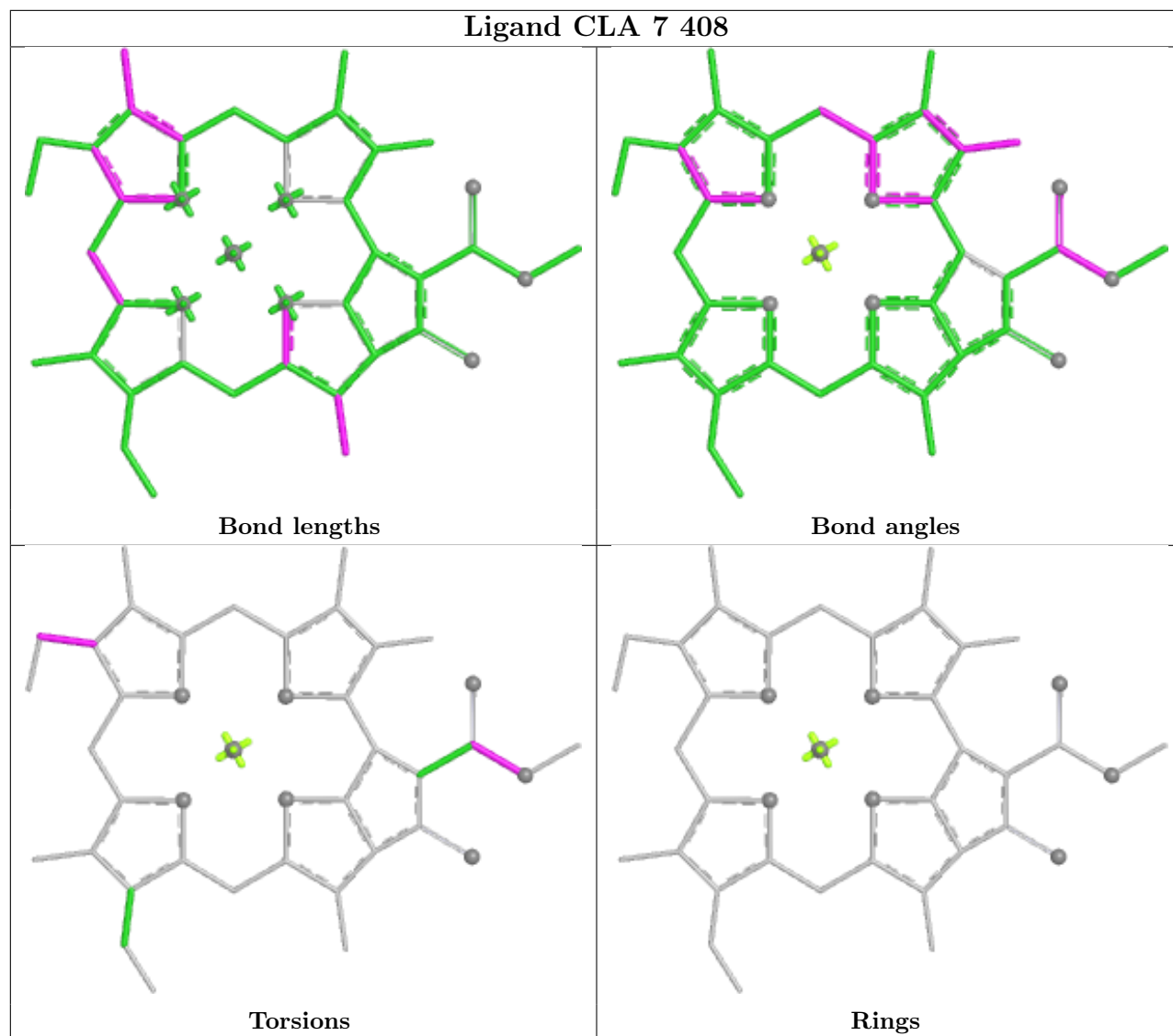


Torsions

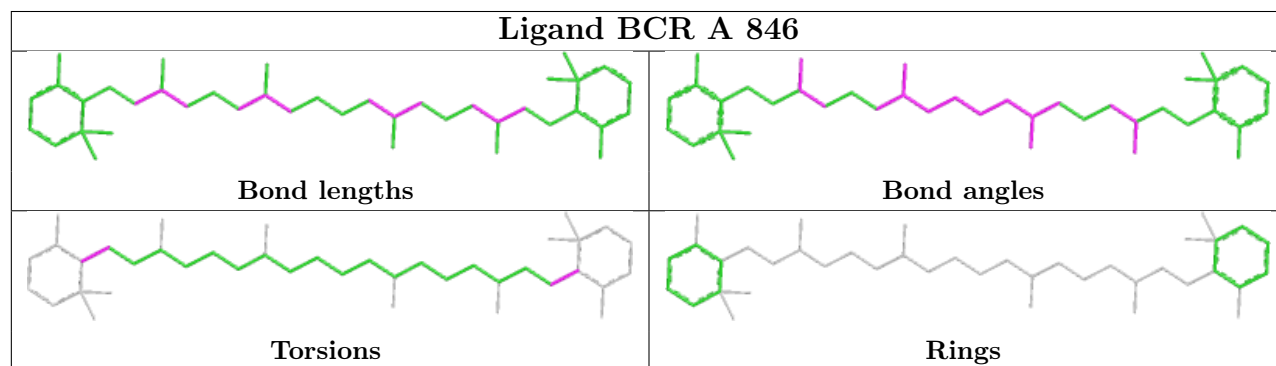


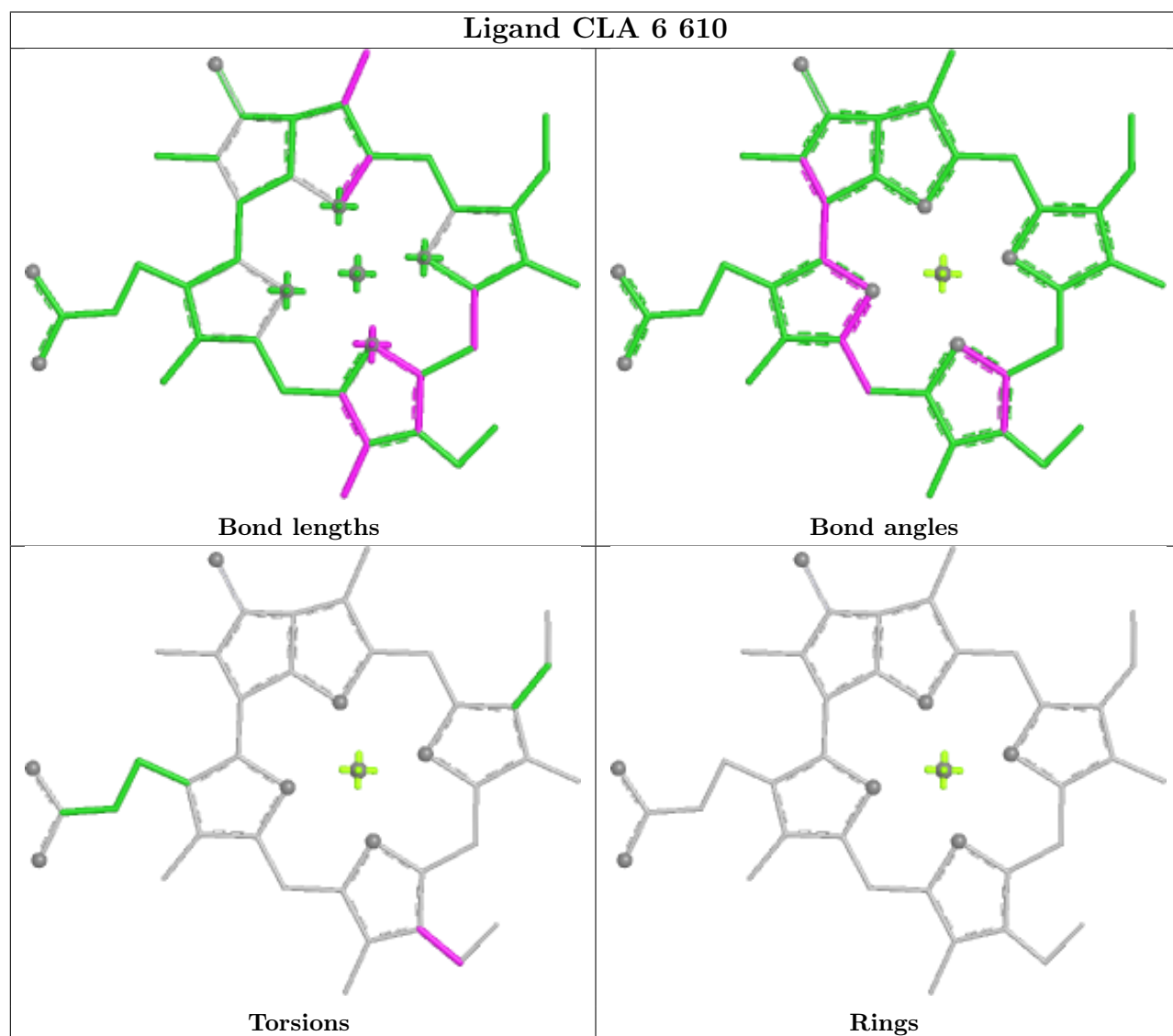
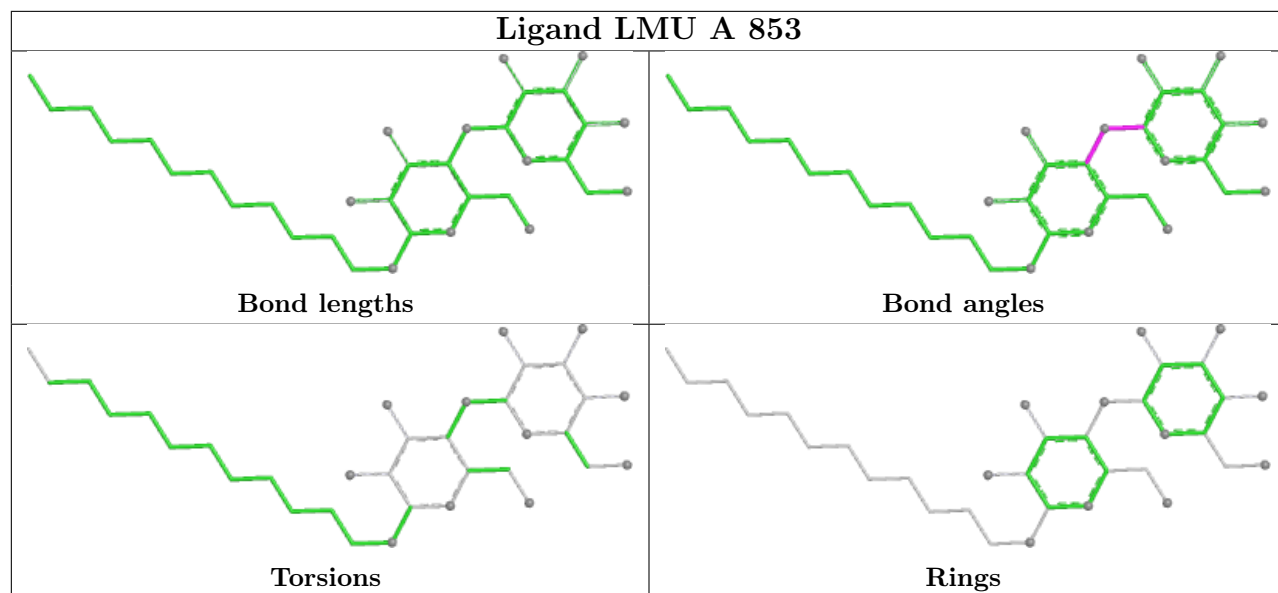
Rings

Ligand CLA 7 408

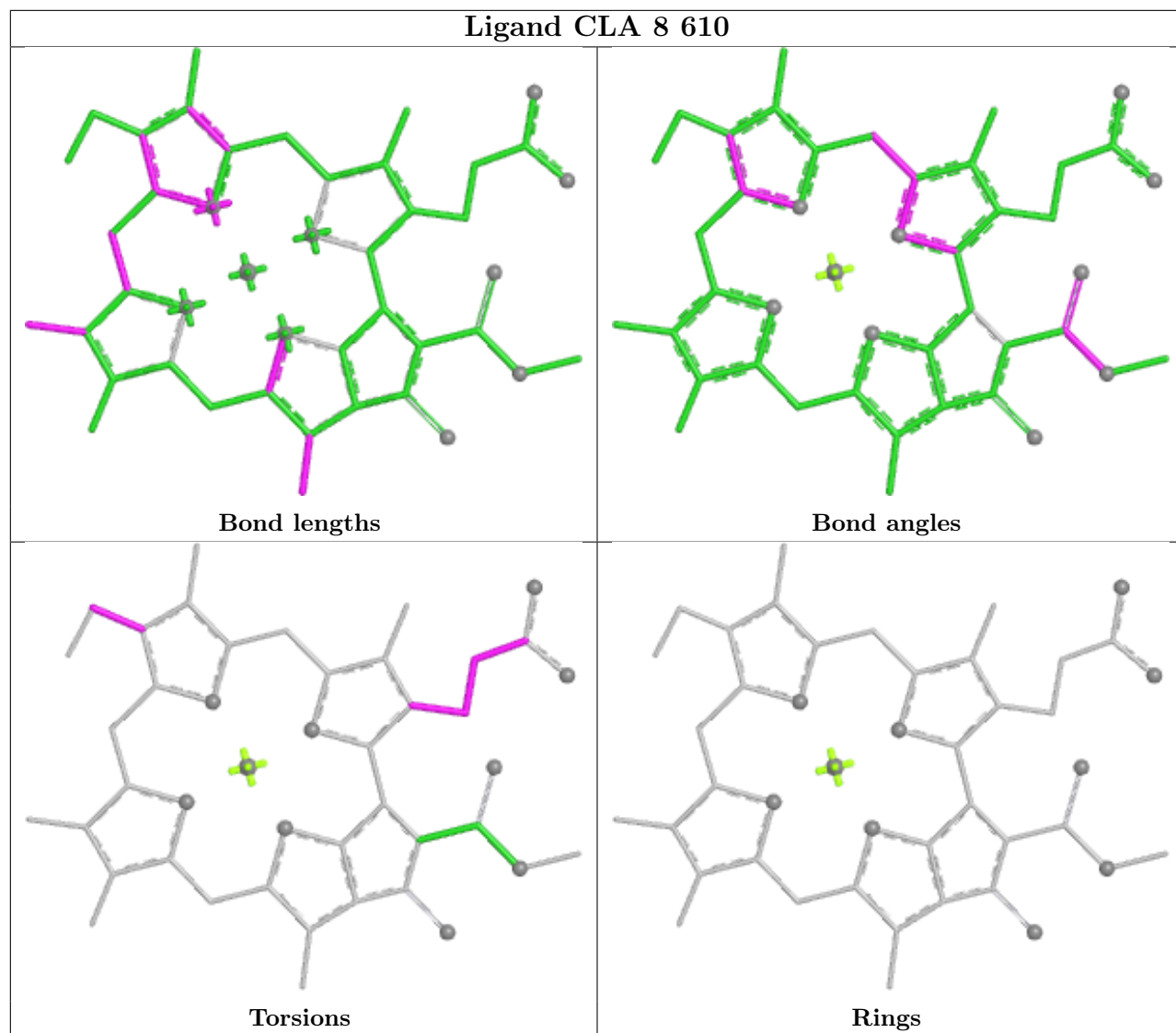


Ligand BCR A 846

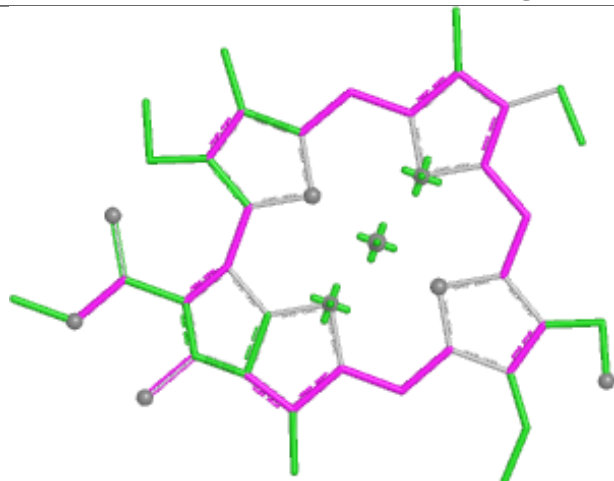




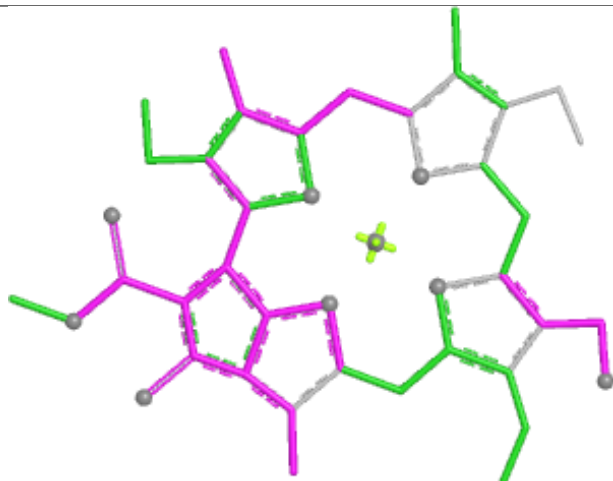
Ligand CLA 8 610



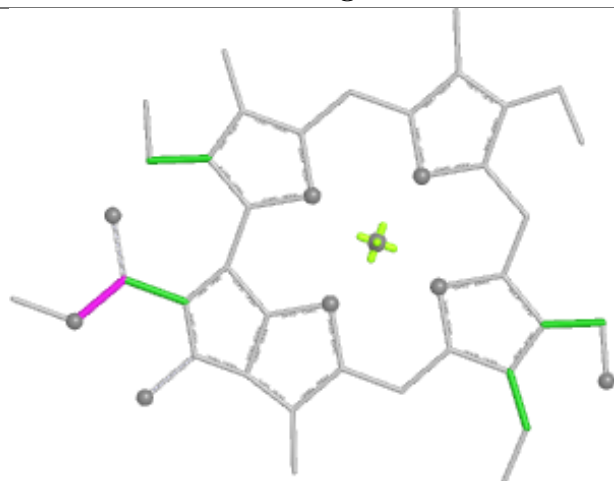
Ligand CHL 9 601



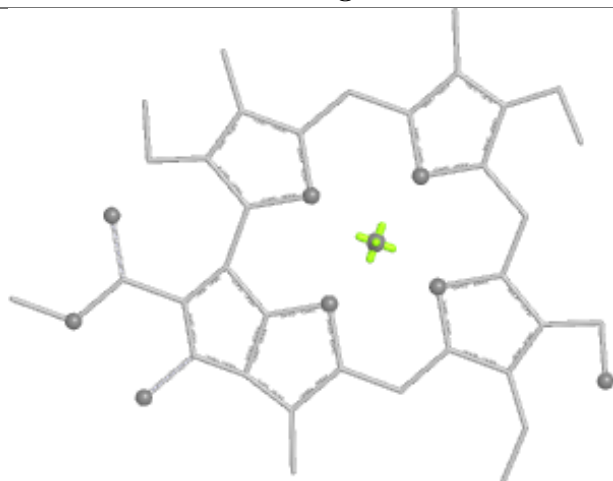
Bond lengths



Bond angles

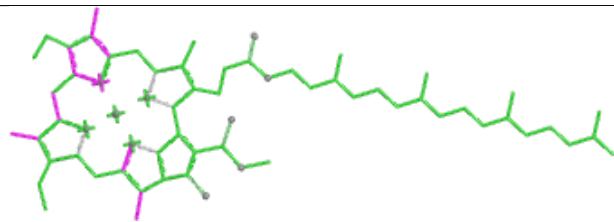


Torsions

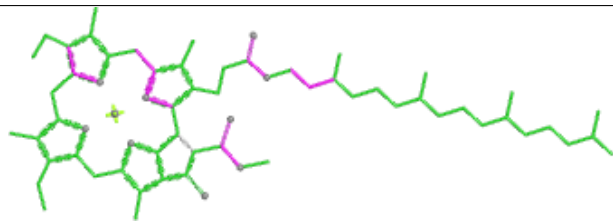


Rings

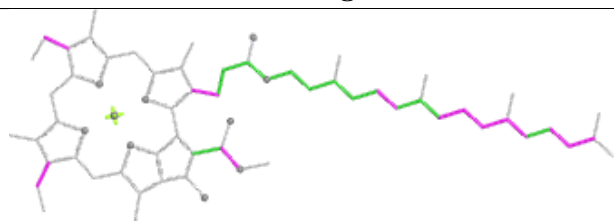
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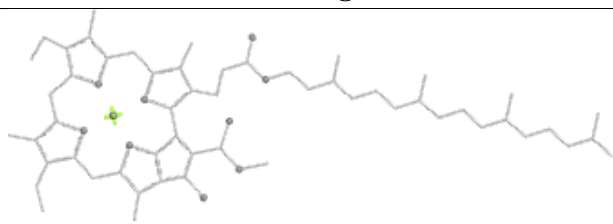
Bond lengths



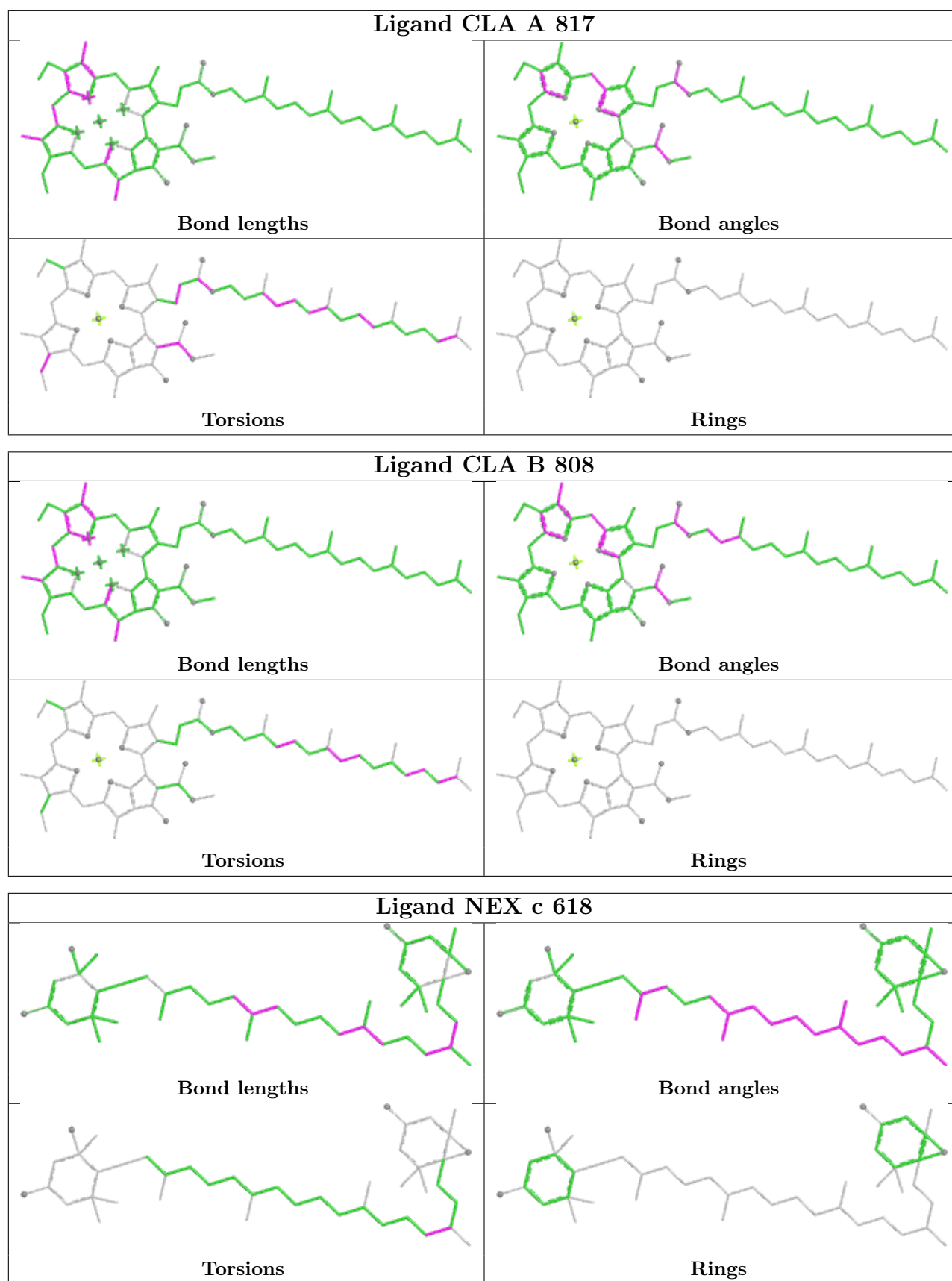
Bond angles



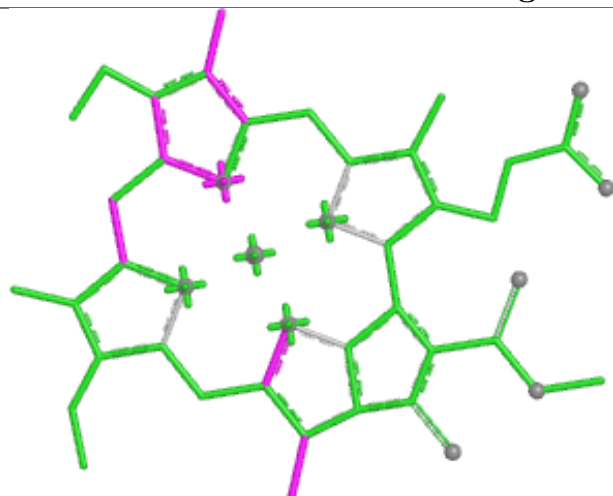
Torsions



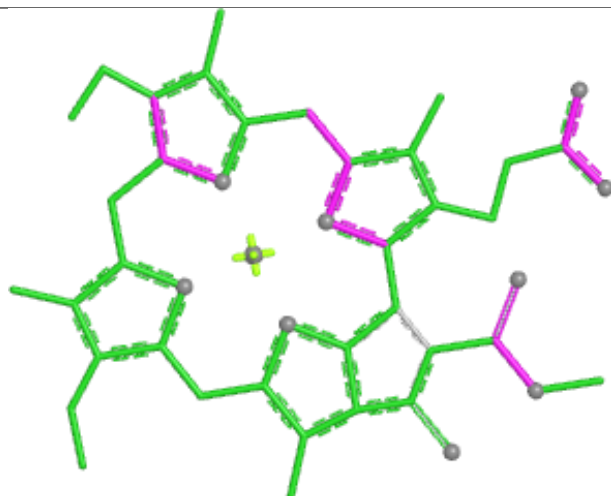
Rings



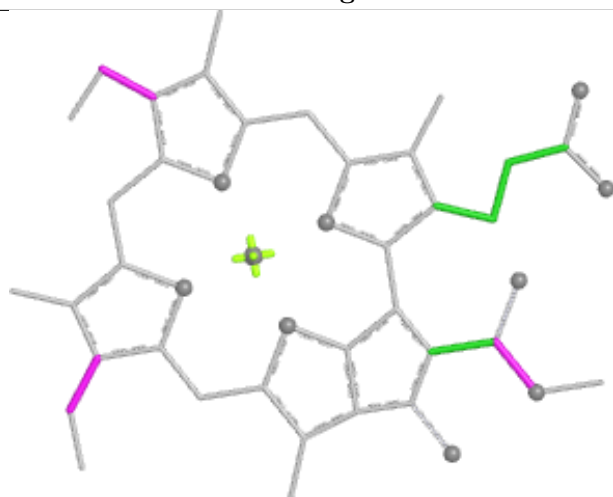
Ligand CLA 1 315



Bond lengths



Bond angles

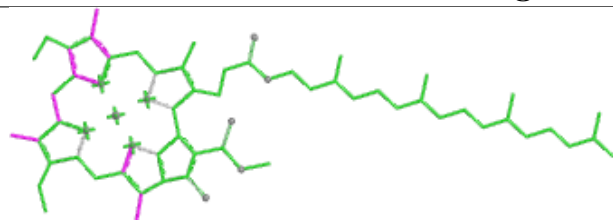


Torsions

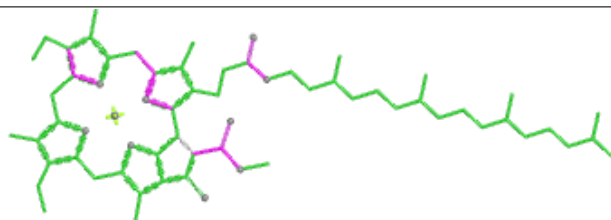


Rings

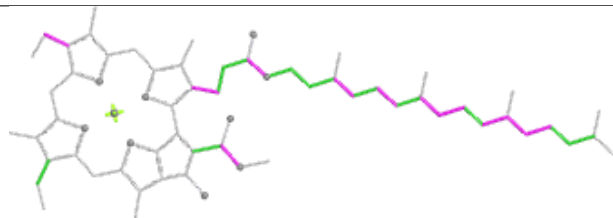
Ligand CLA B 802



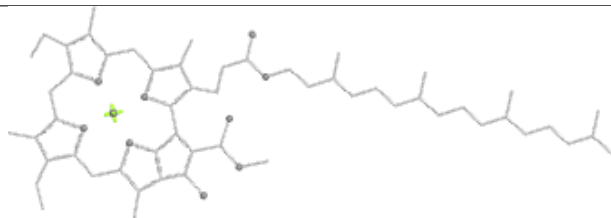
Bond lengths



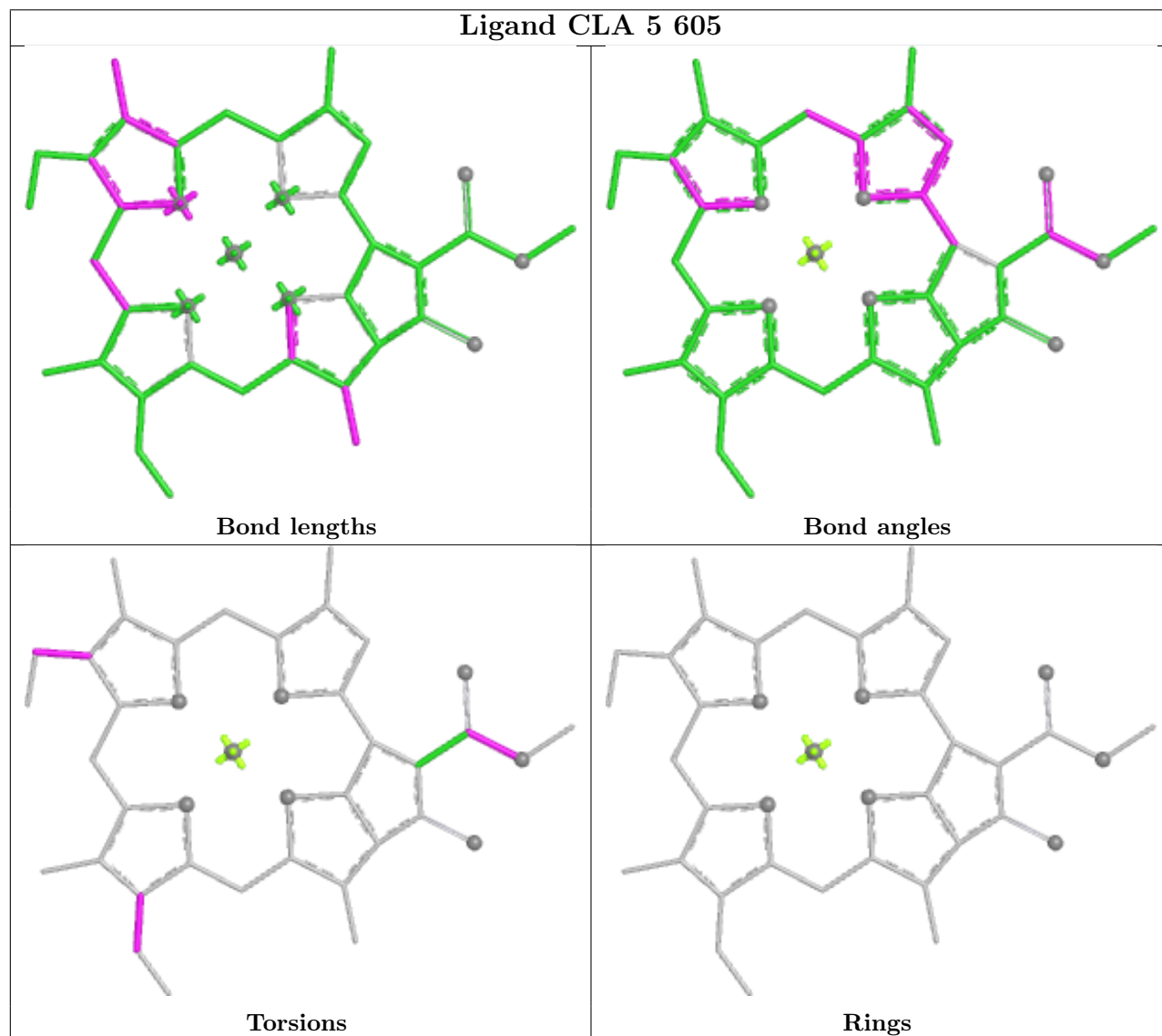
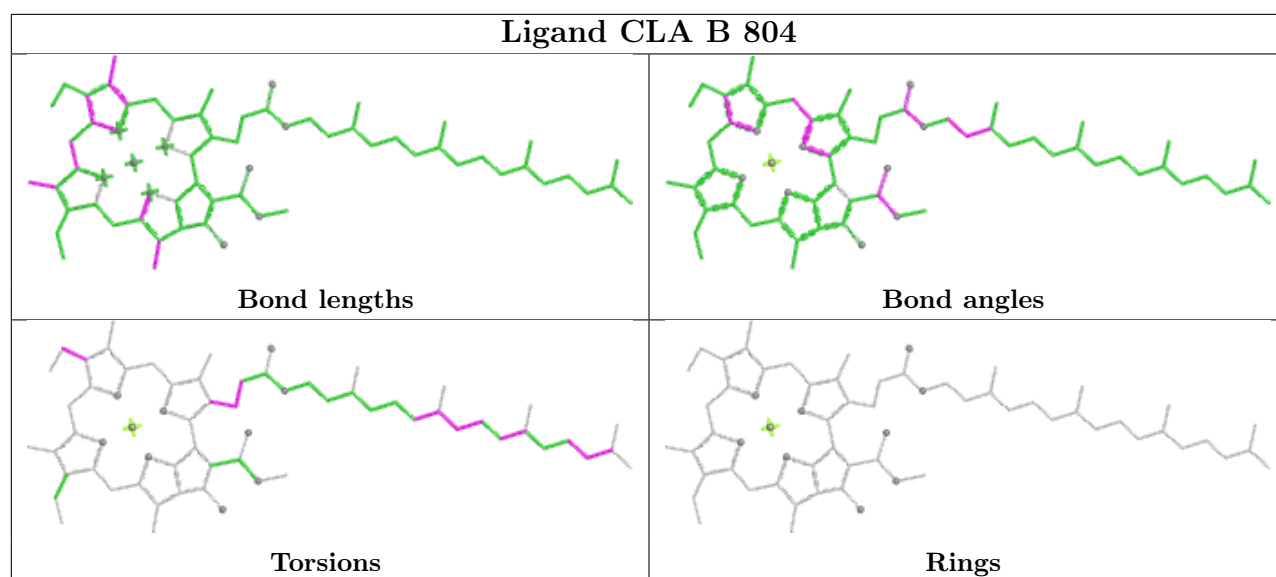
Bond angles

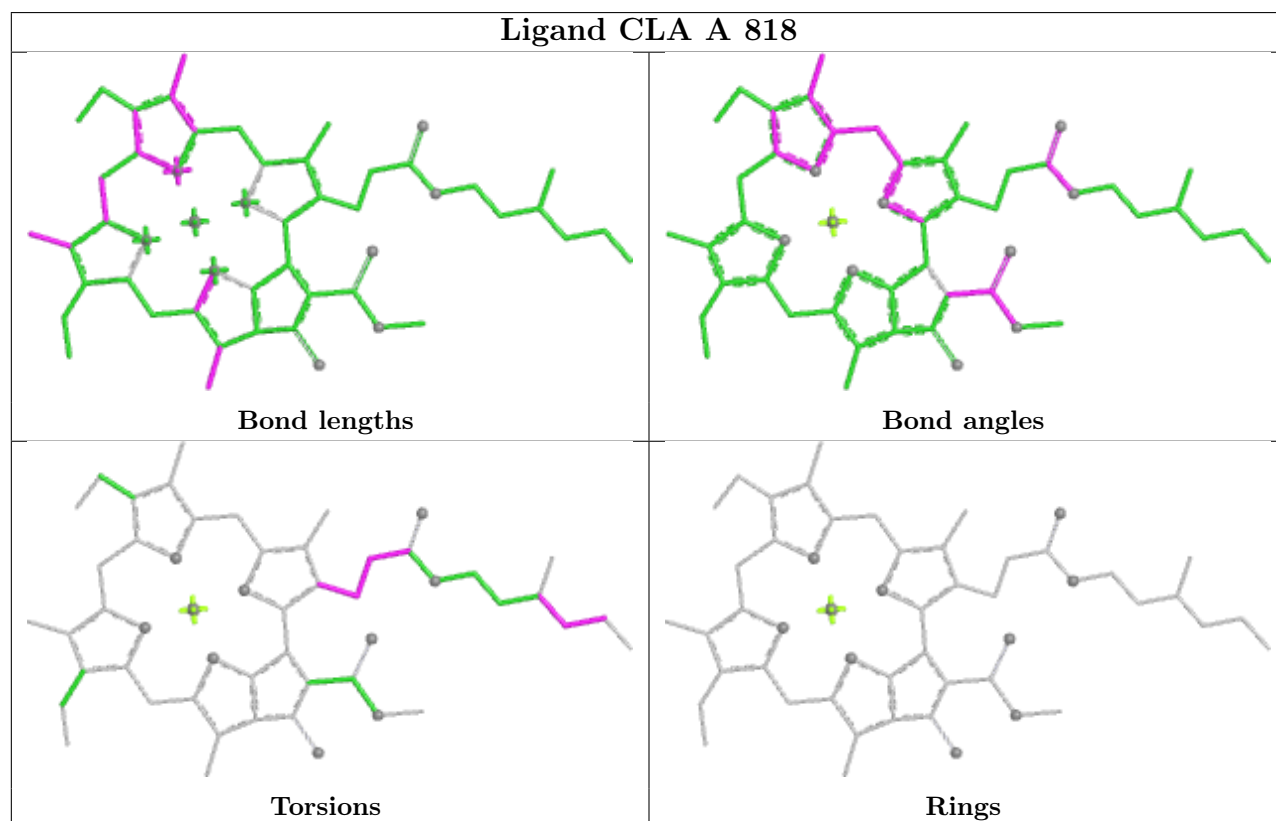
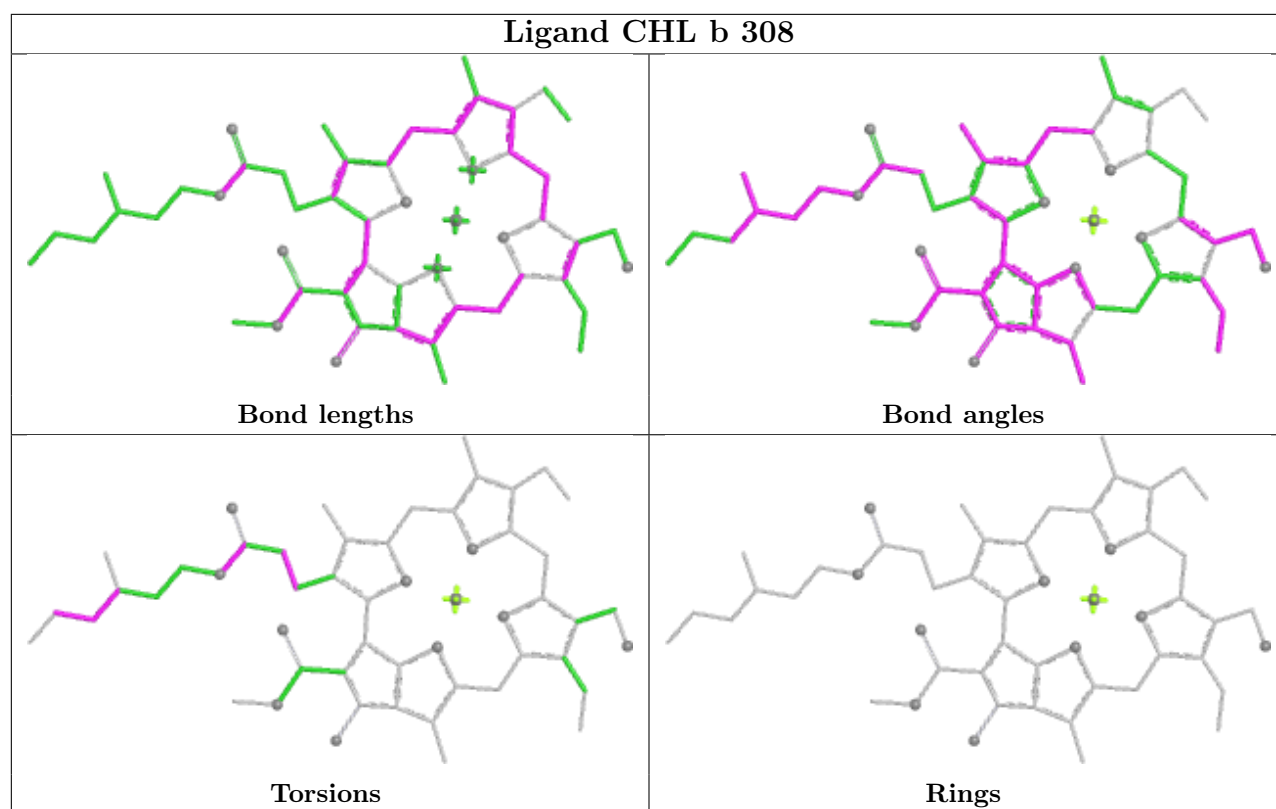


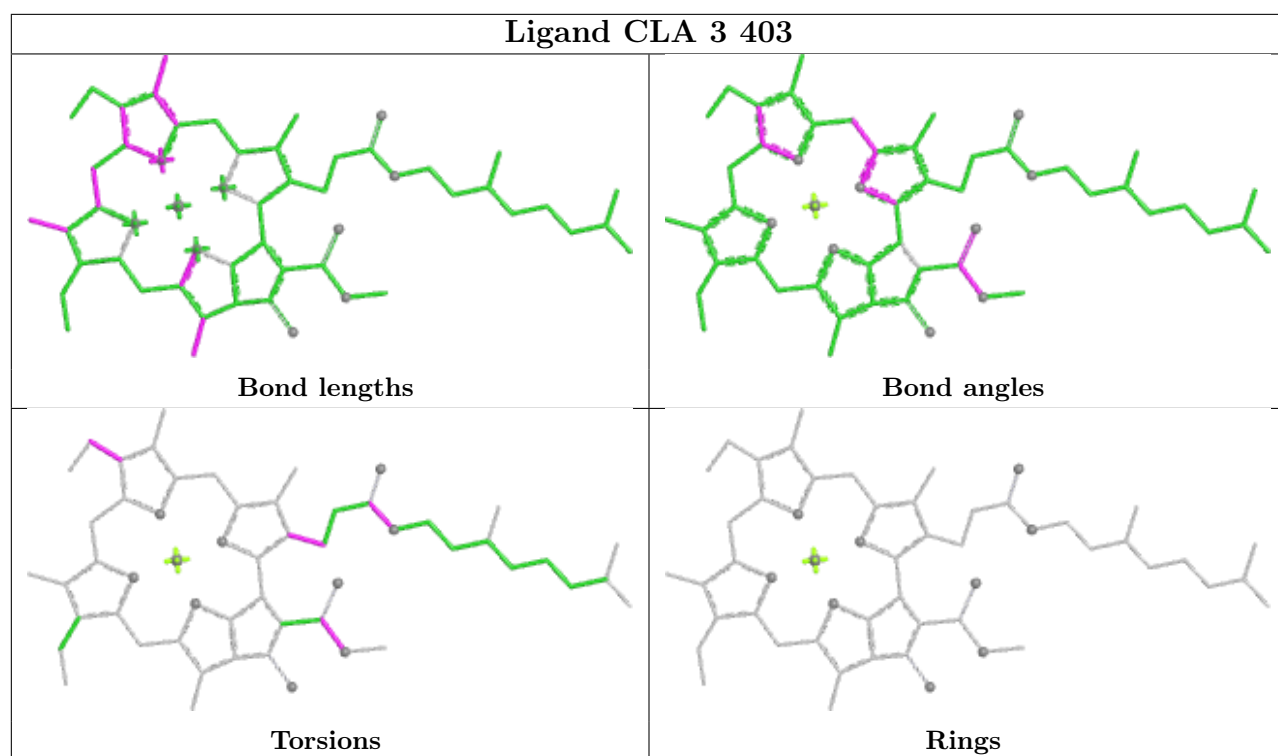
Torsions

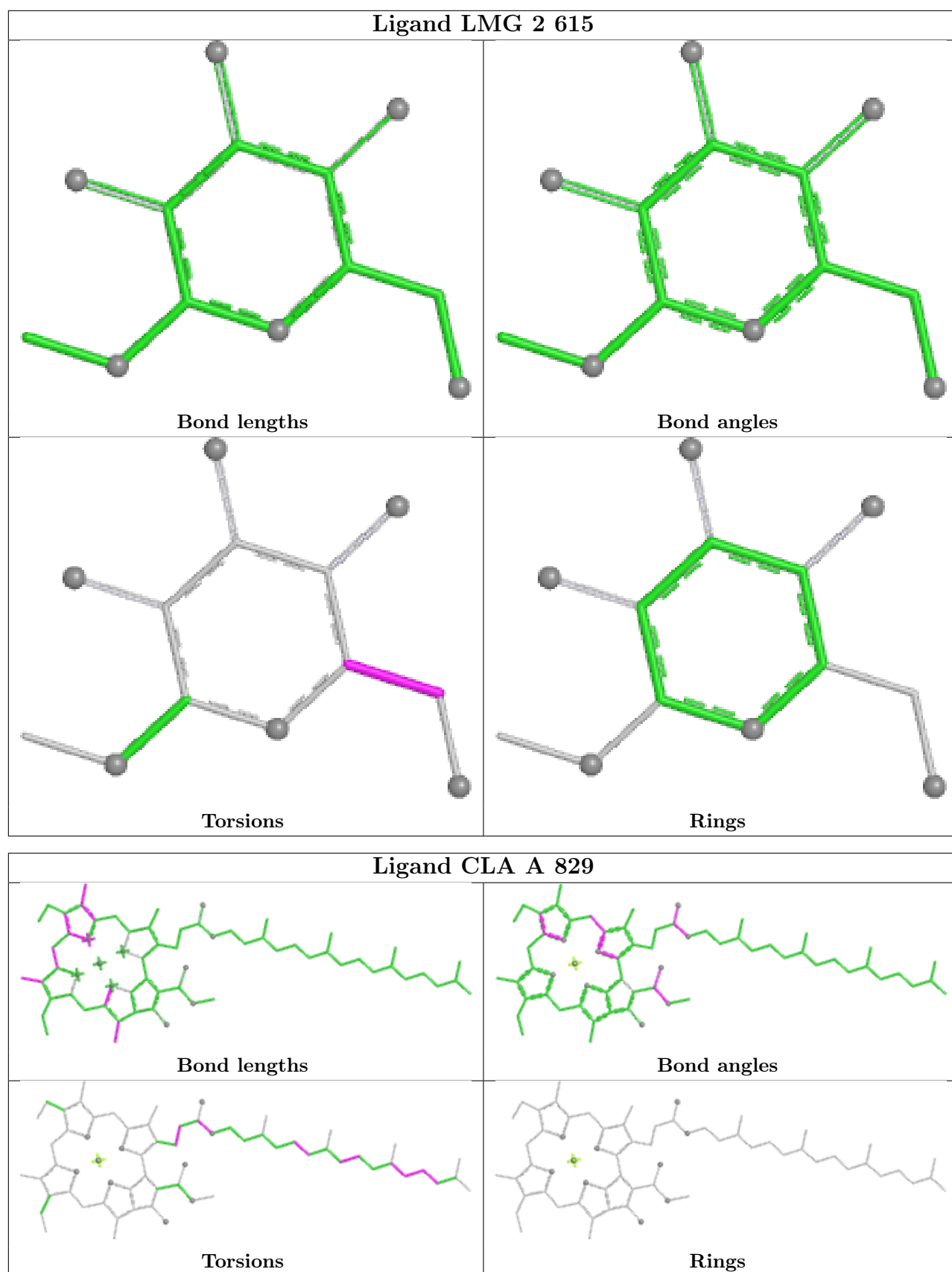


Rings

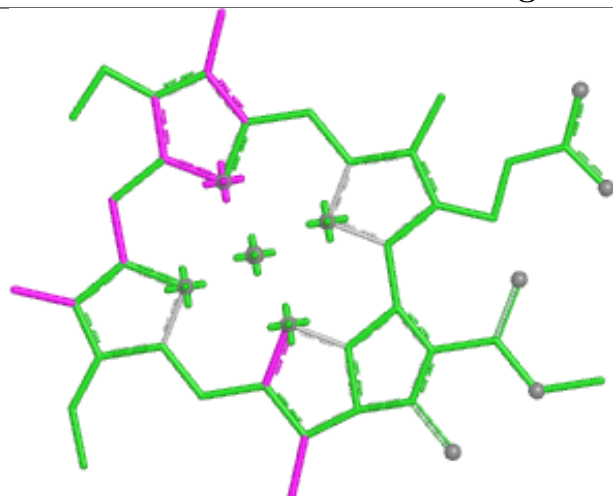




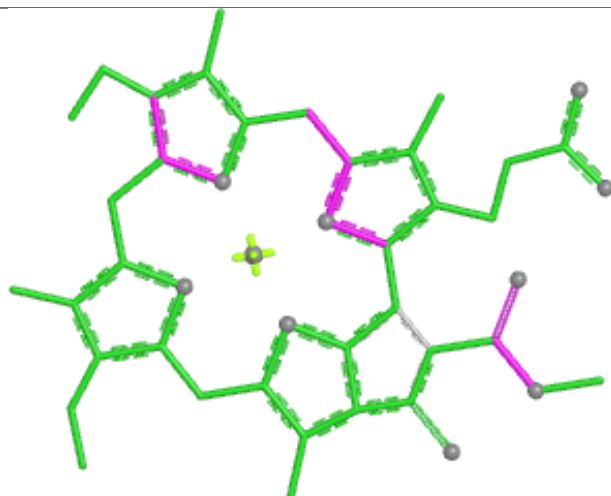




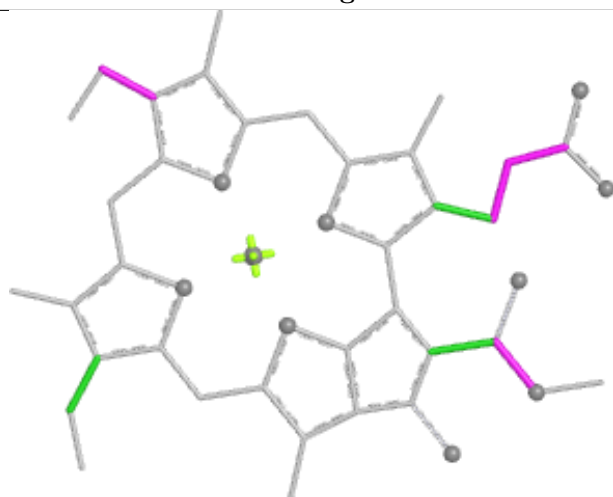
Ligand CLA 2 603



Bond lengths



Bond angles

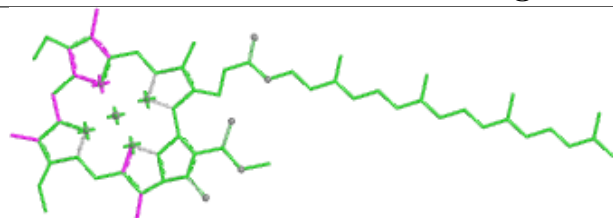


Torsions

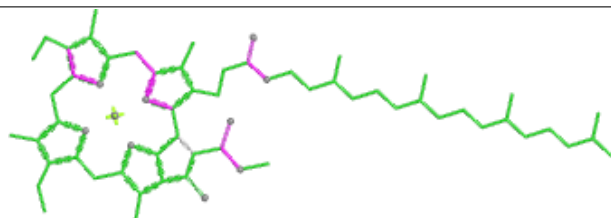


Rings

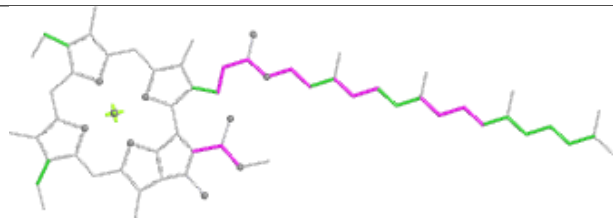
Ligand CLA A 806



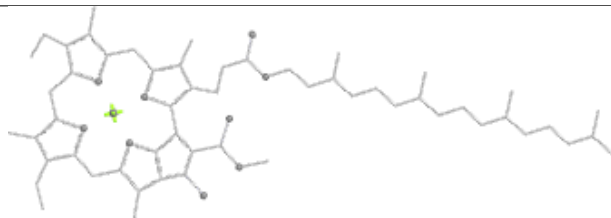
Bond lengths



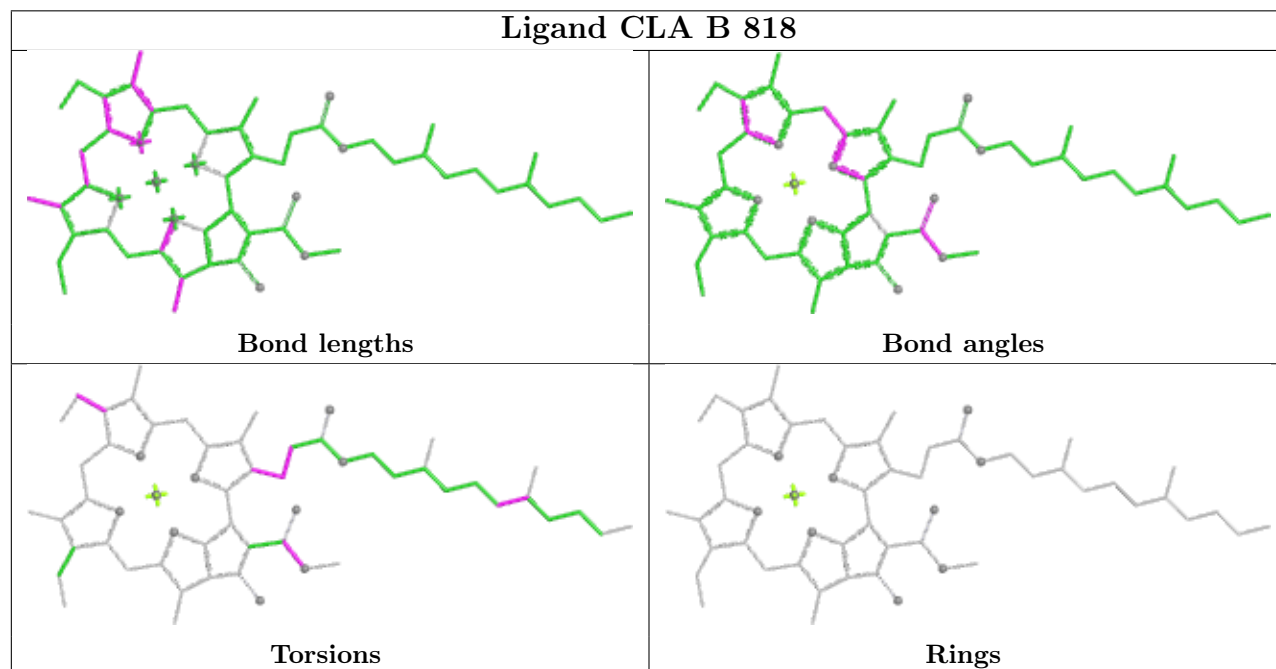
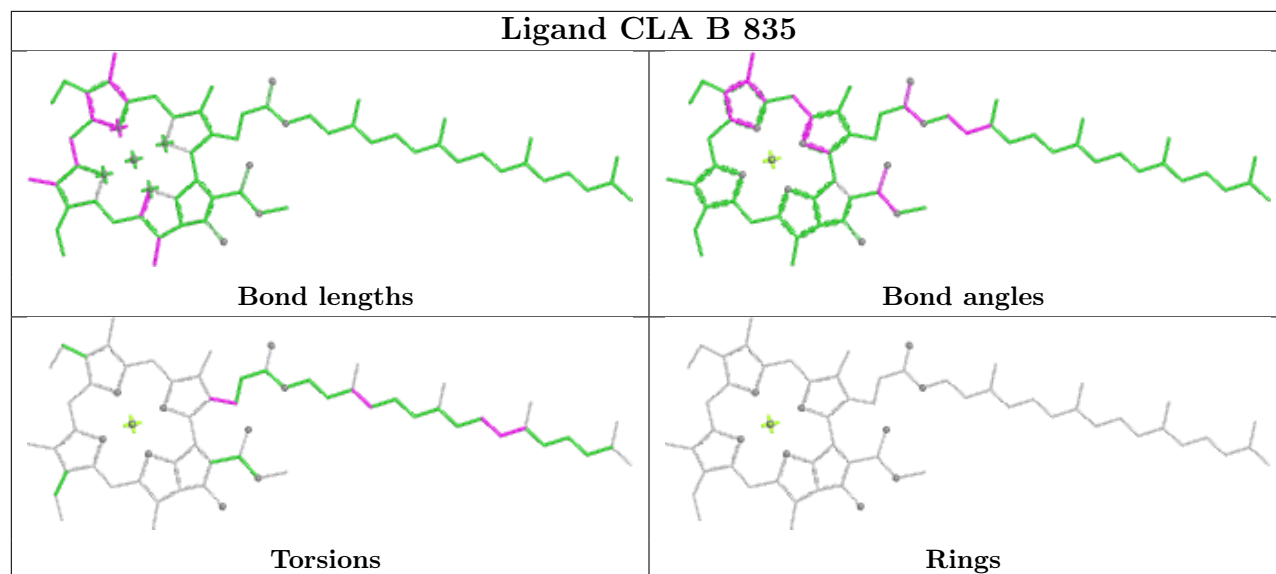
Bond angles



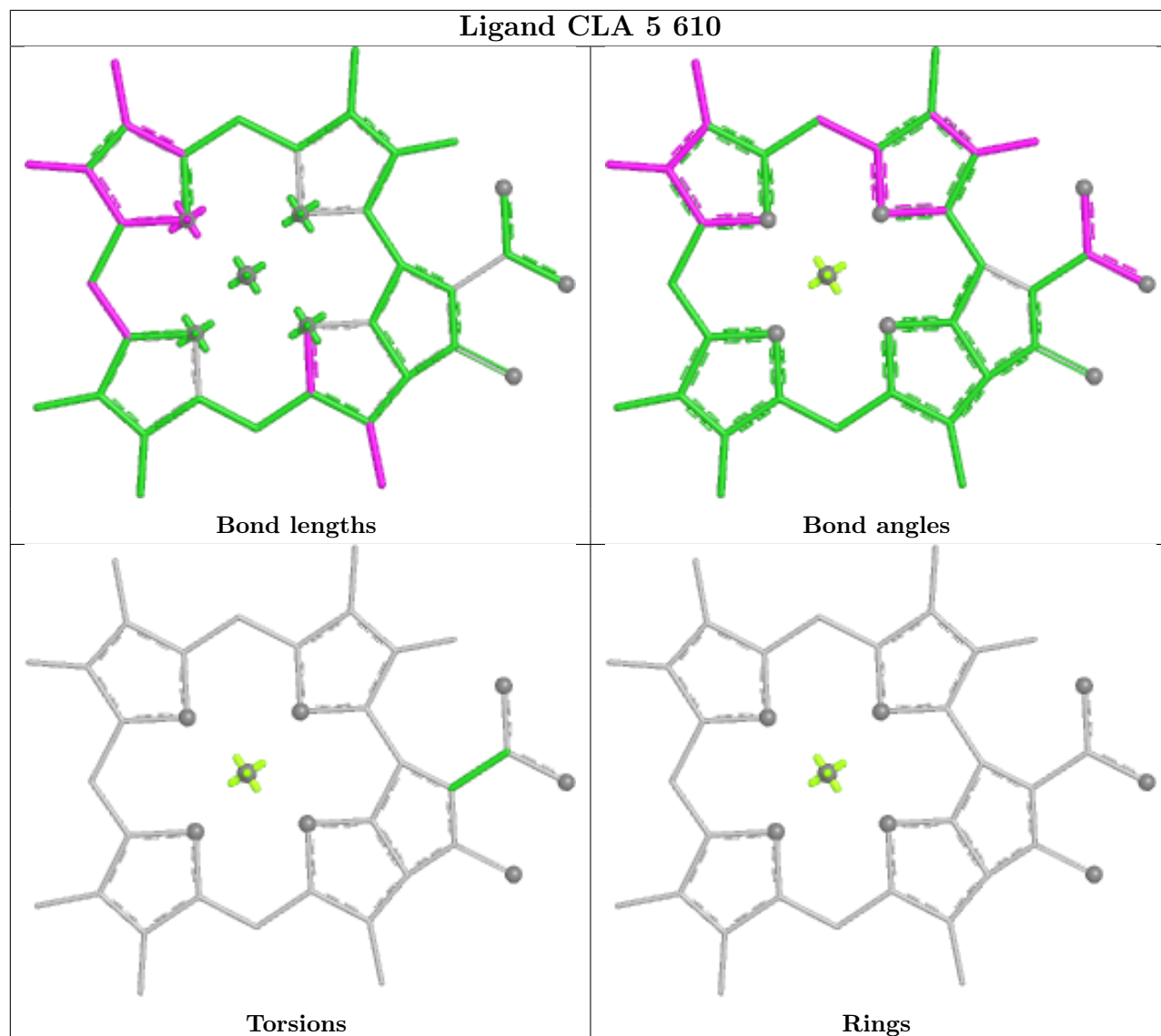
Torsions



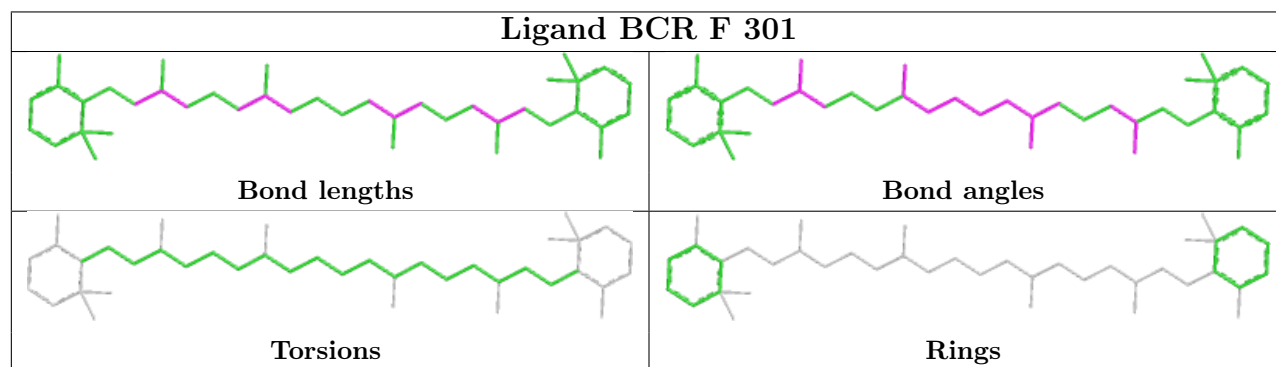
Rings

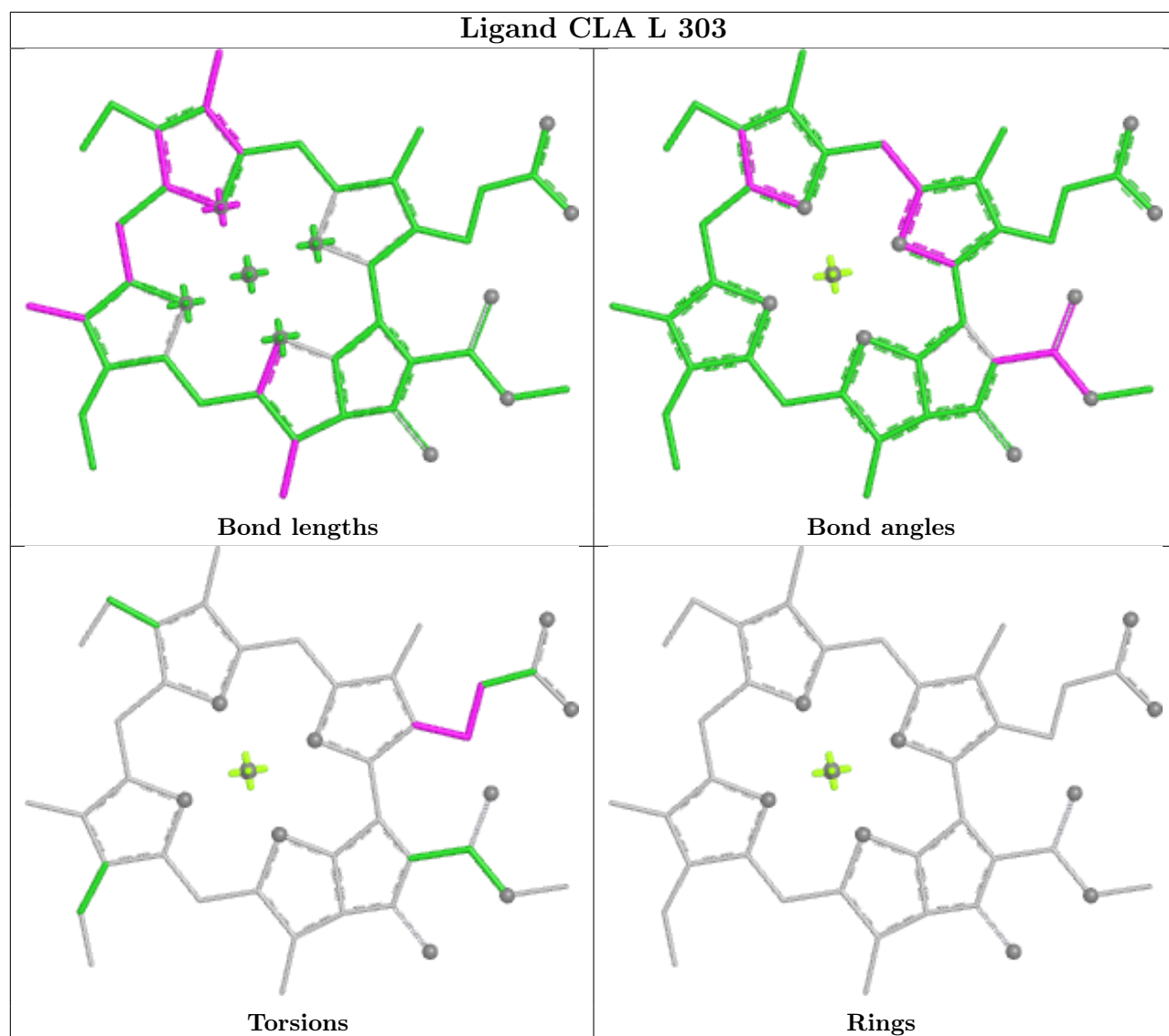
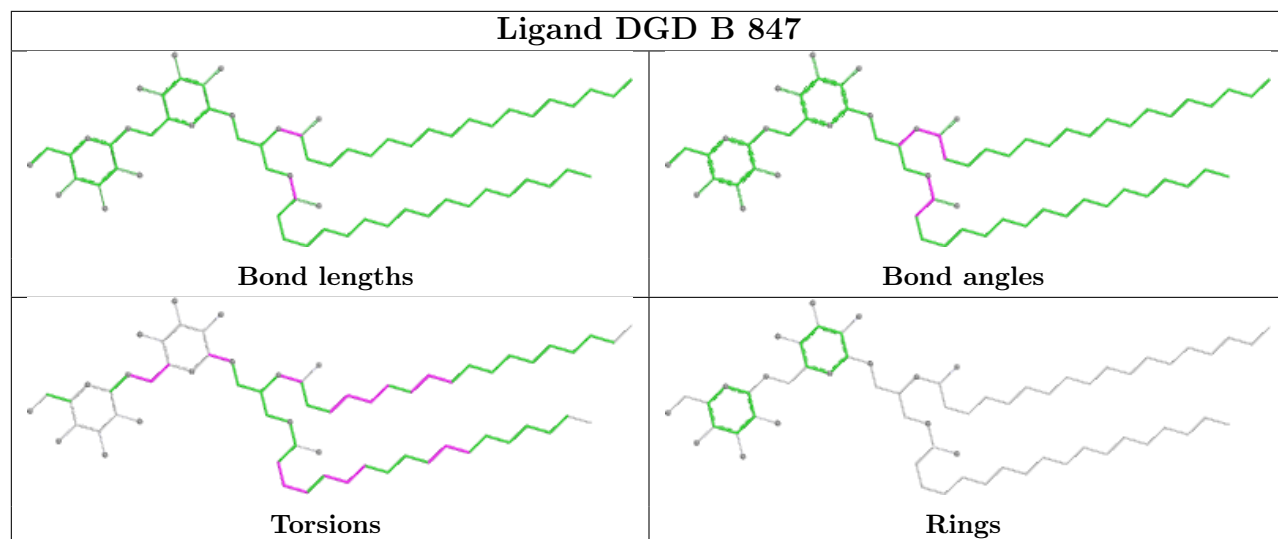


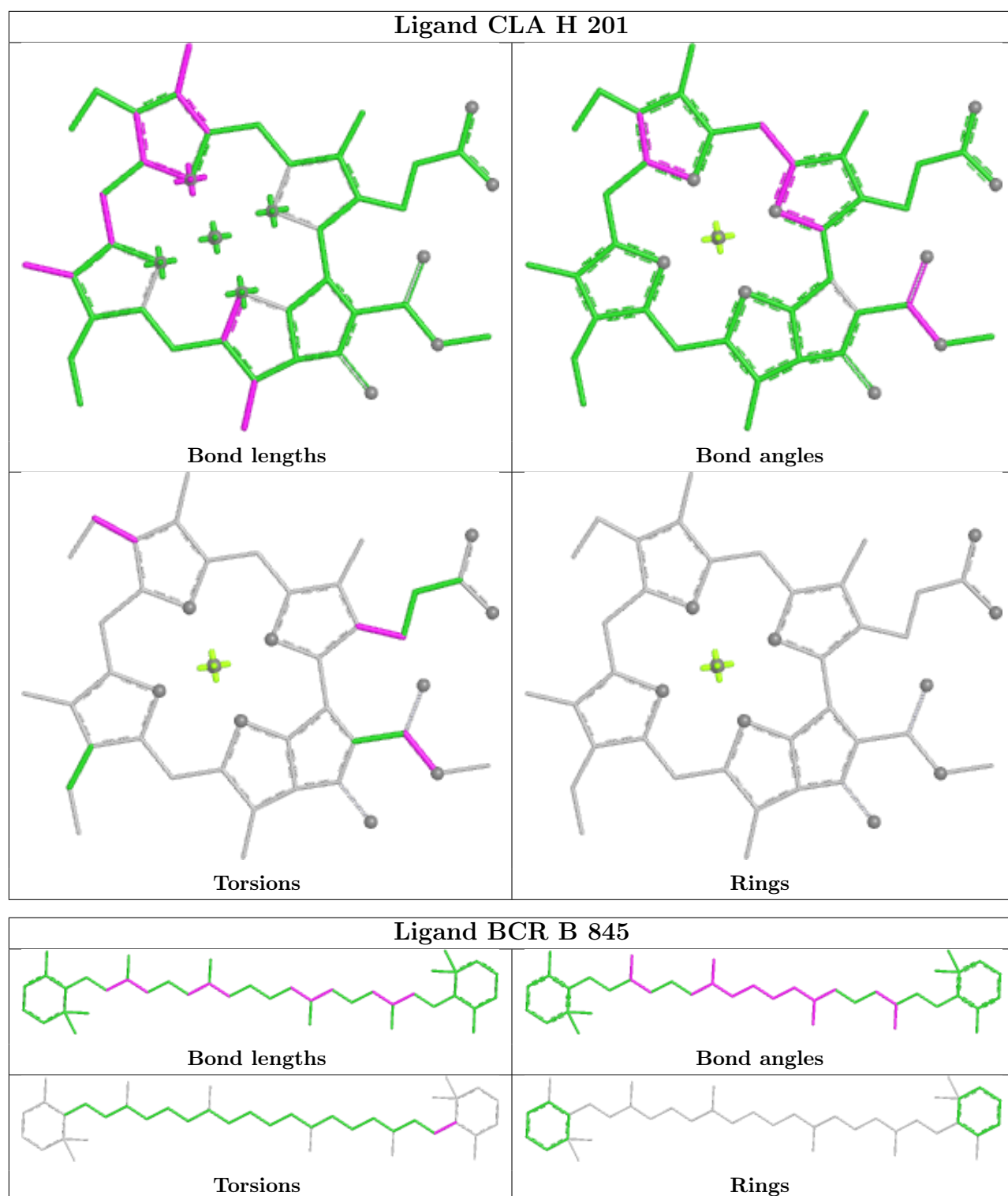
Ligand CLA 5 610



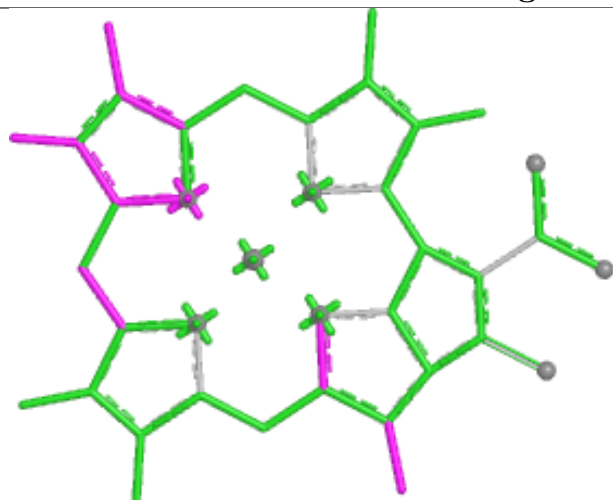
Ligand BCR F 301



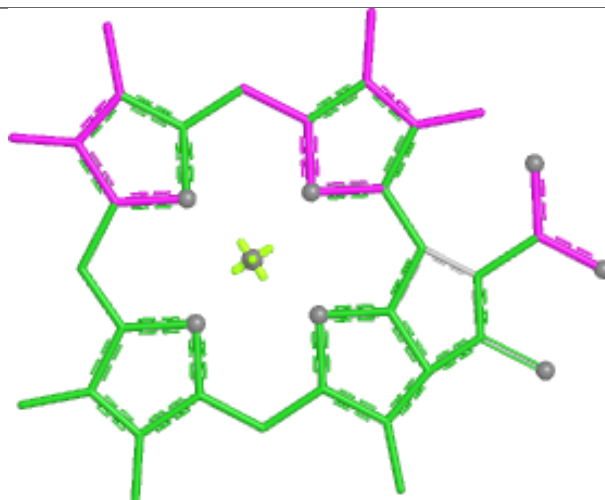




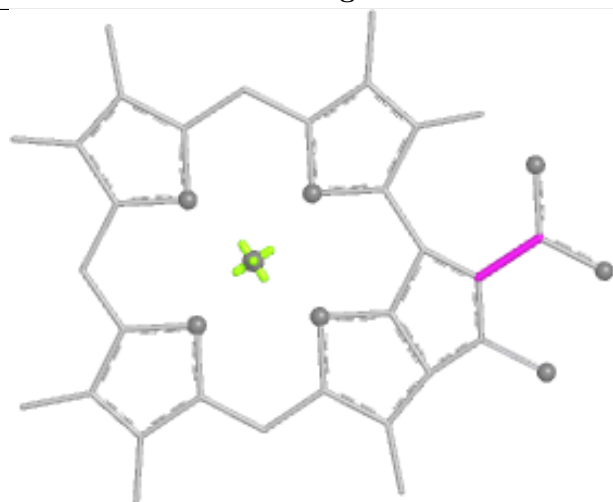
Ligand CLA 1 314



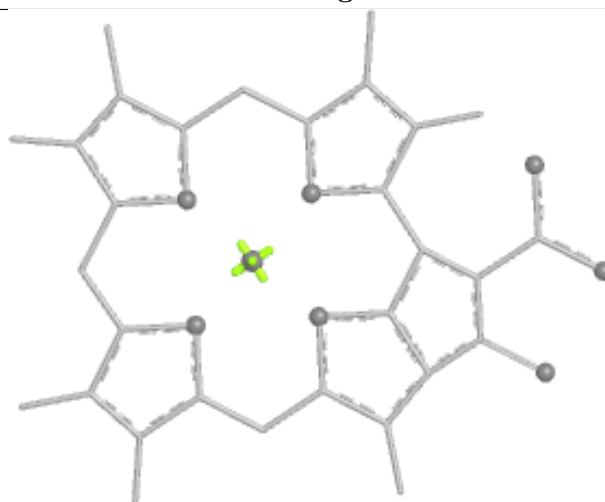
Bond lengths



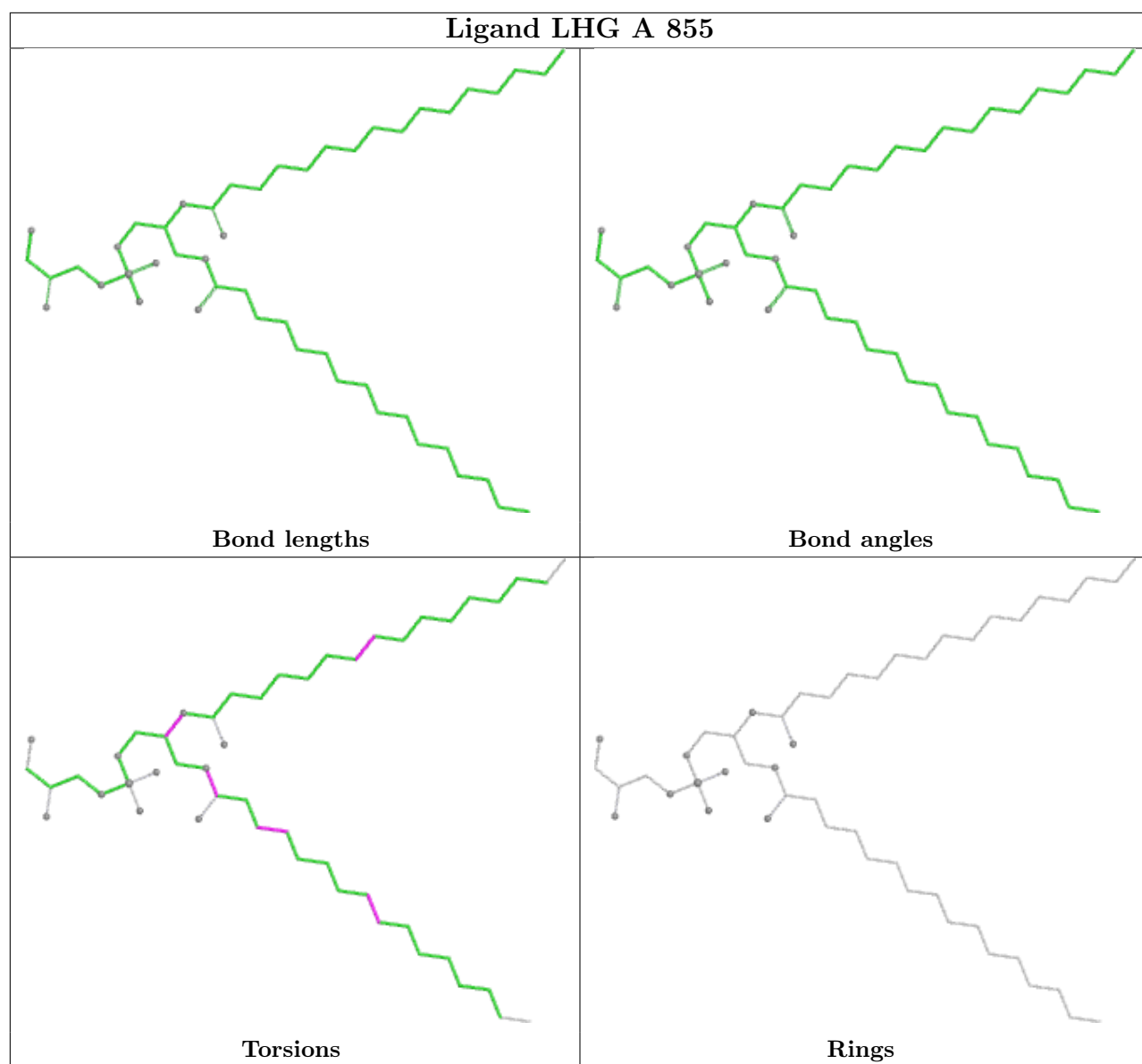
Bond angles



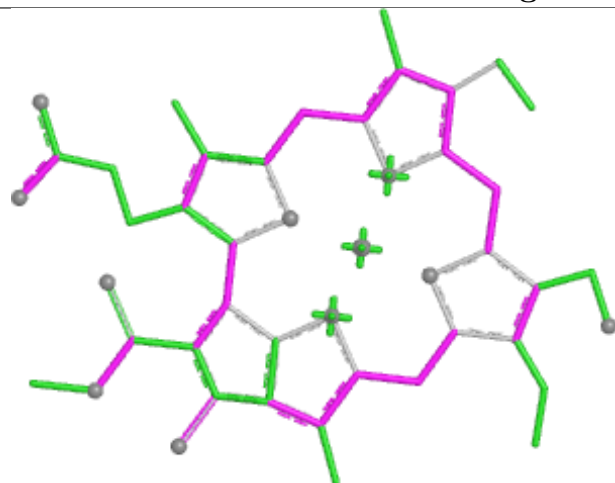
Torsions



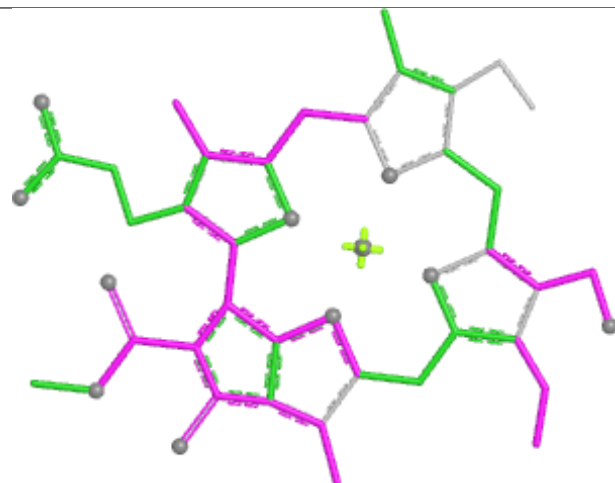
Rings



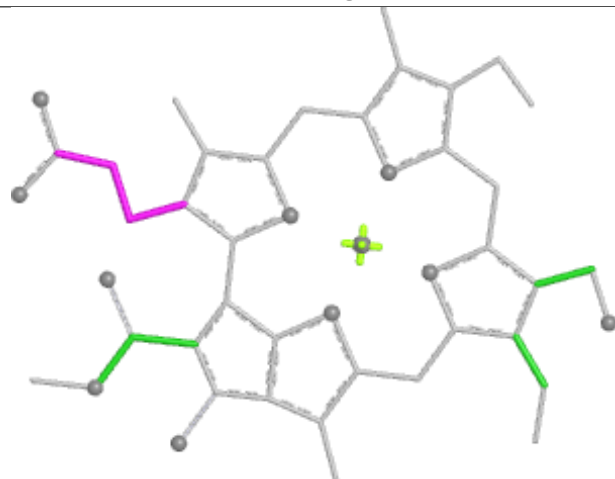
Ligand CHL 9 606



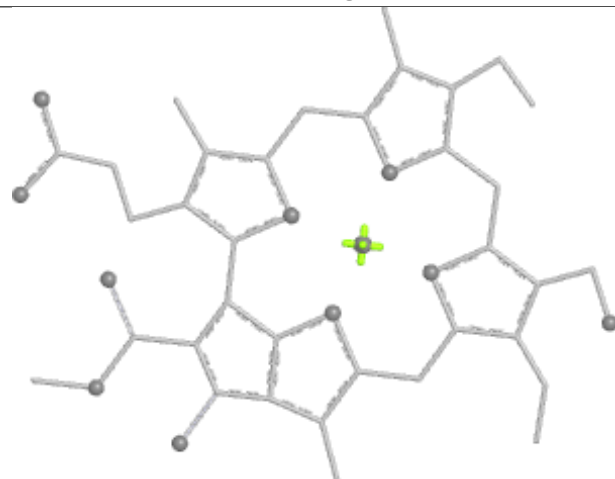
Bond lengths



Bond angles

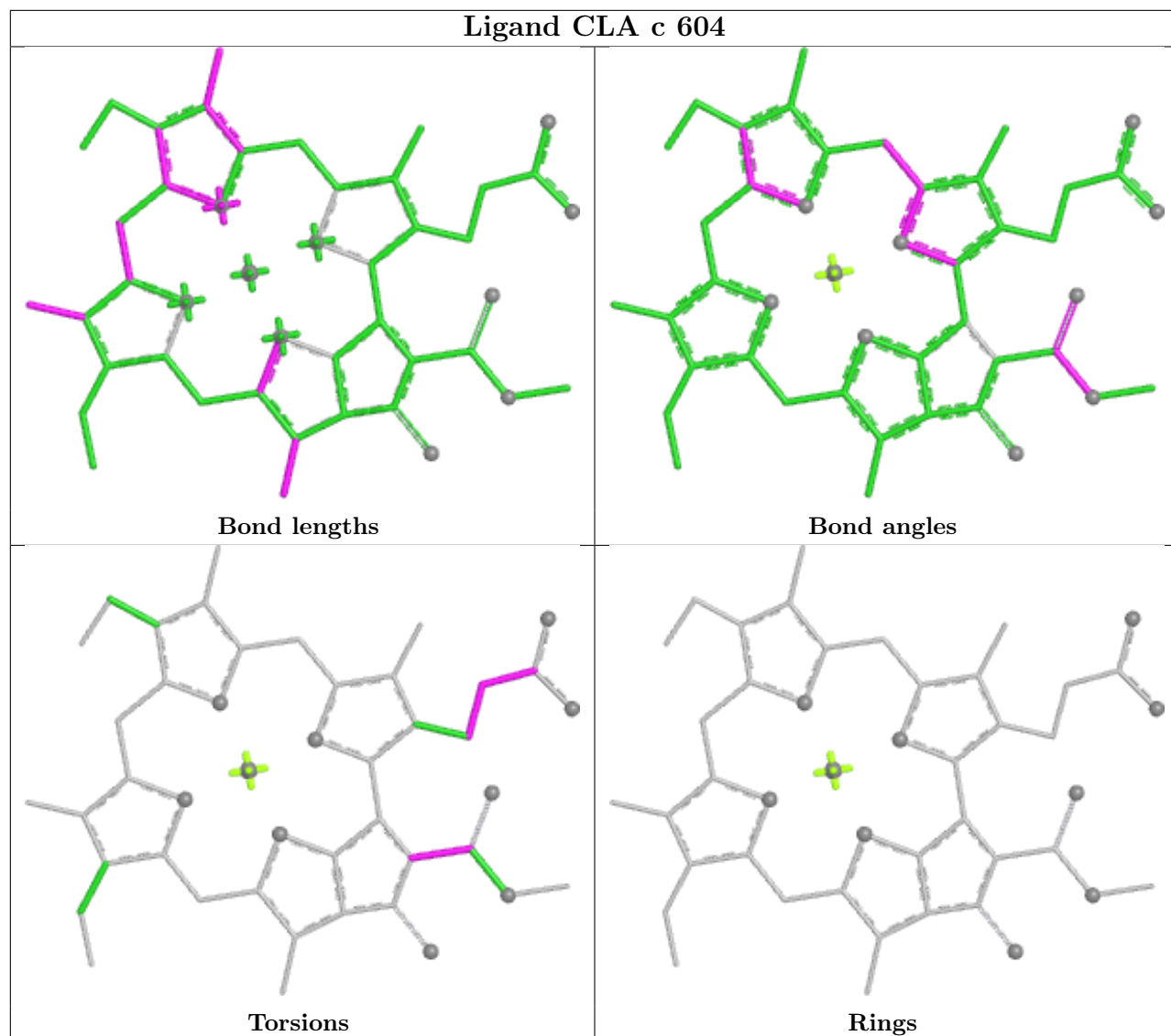


Torsions

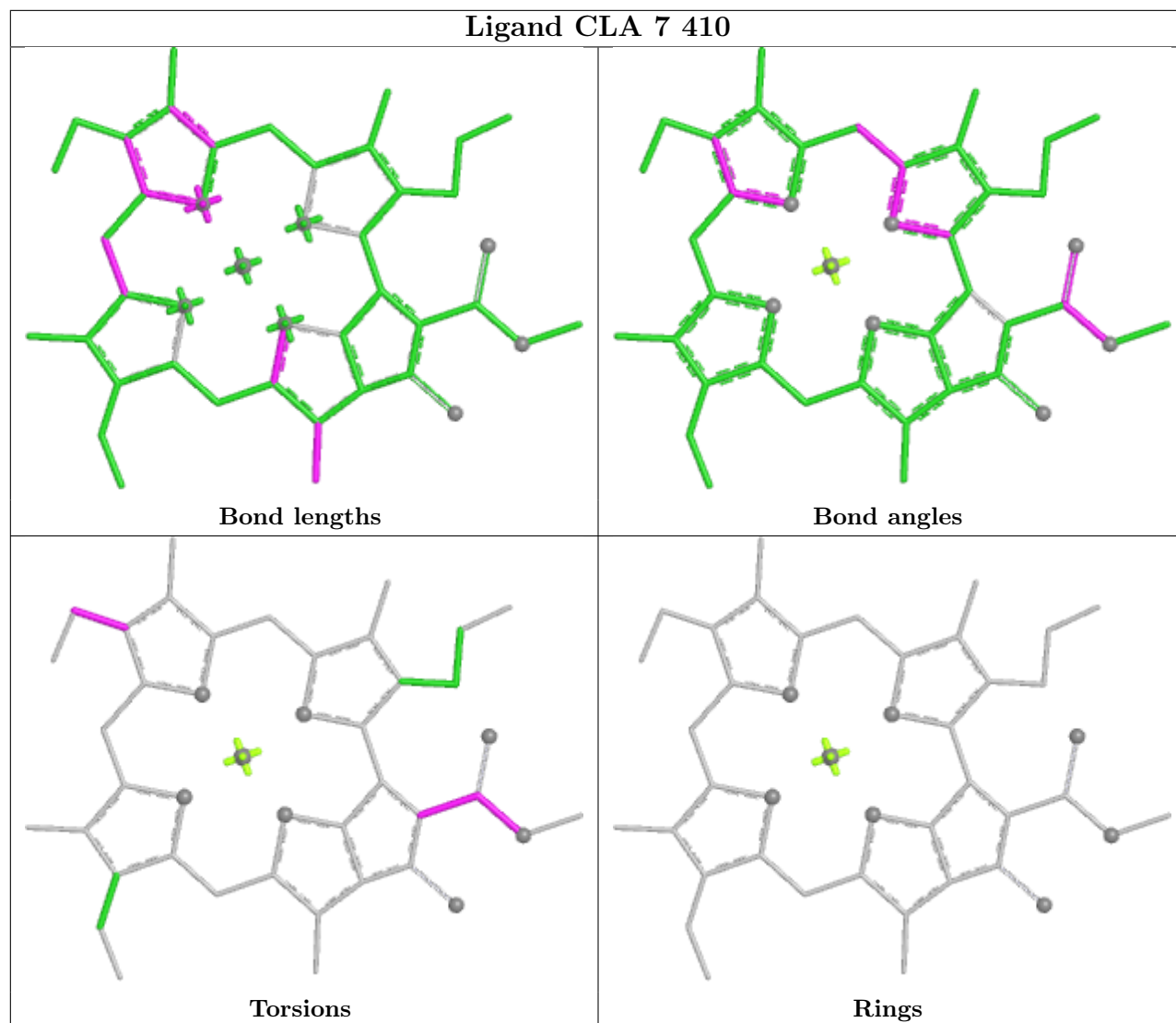


Rings

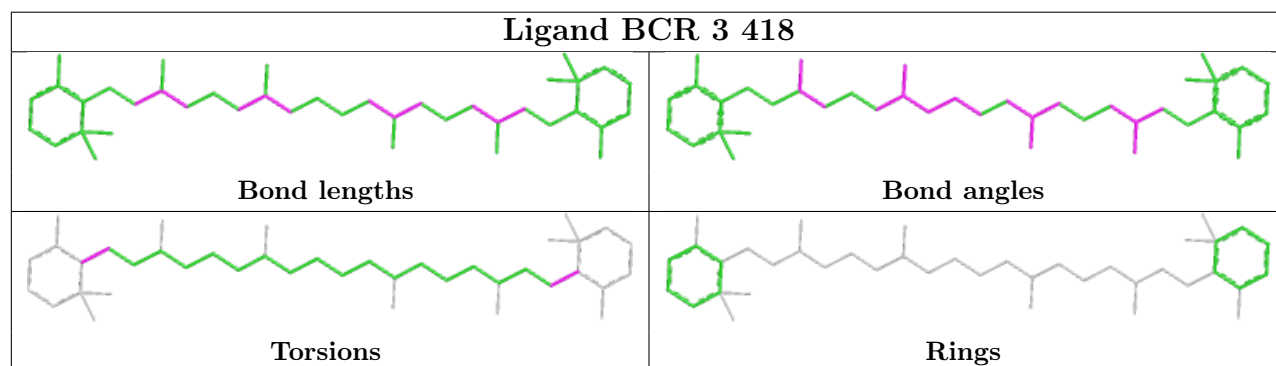
Ligand CLA c 604

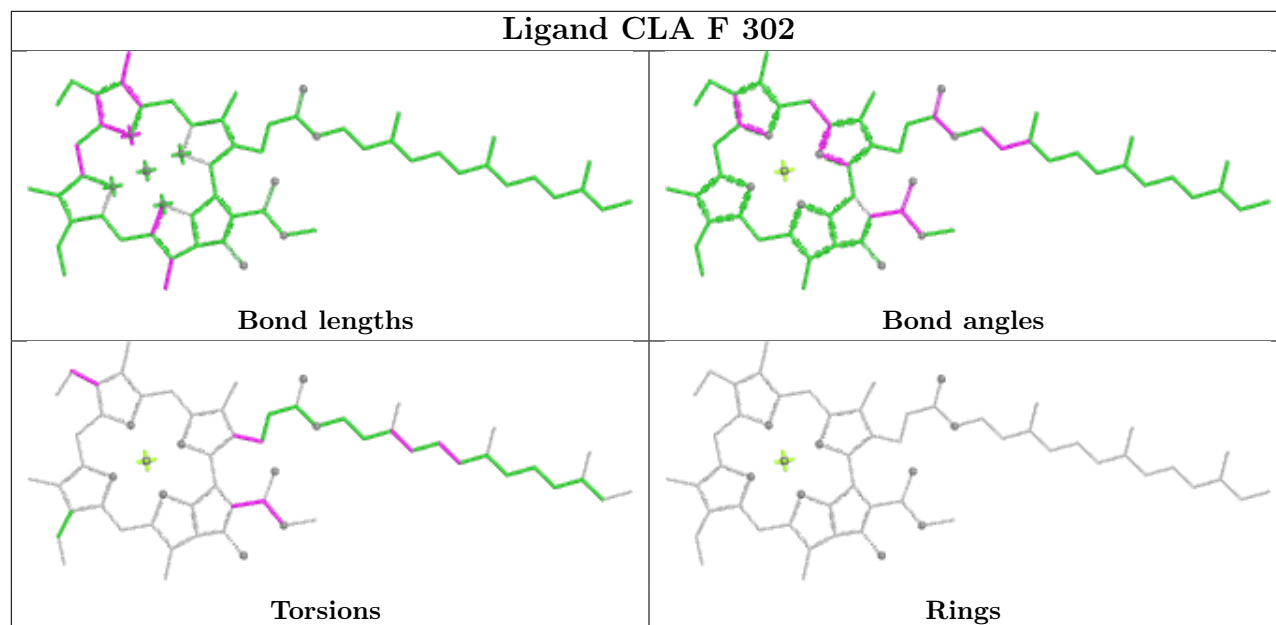
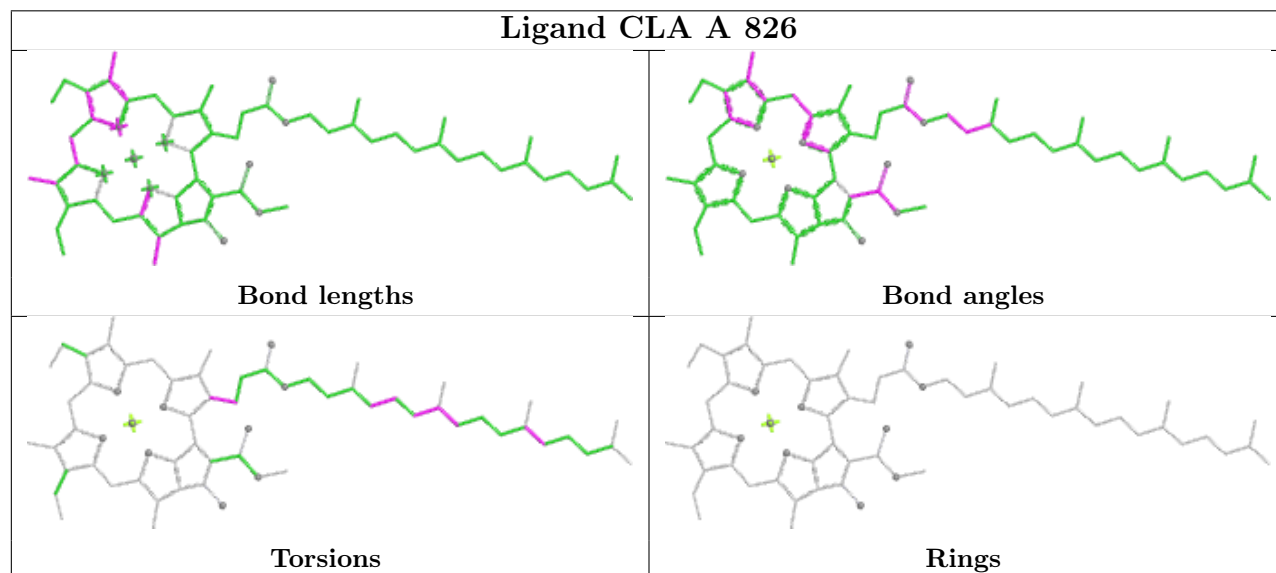
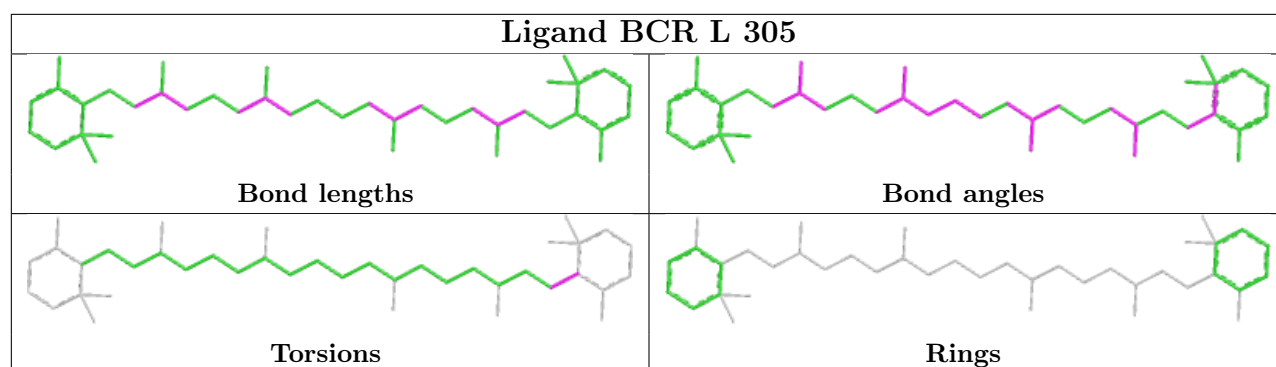


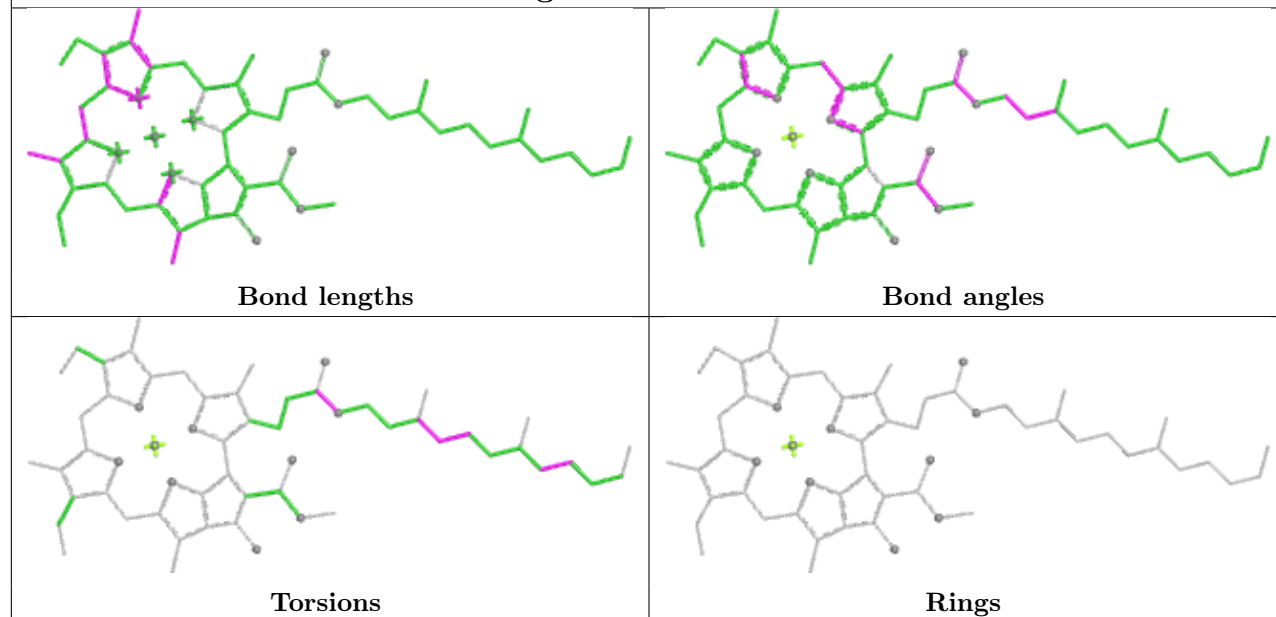
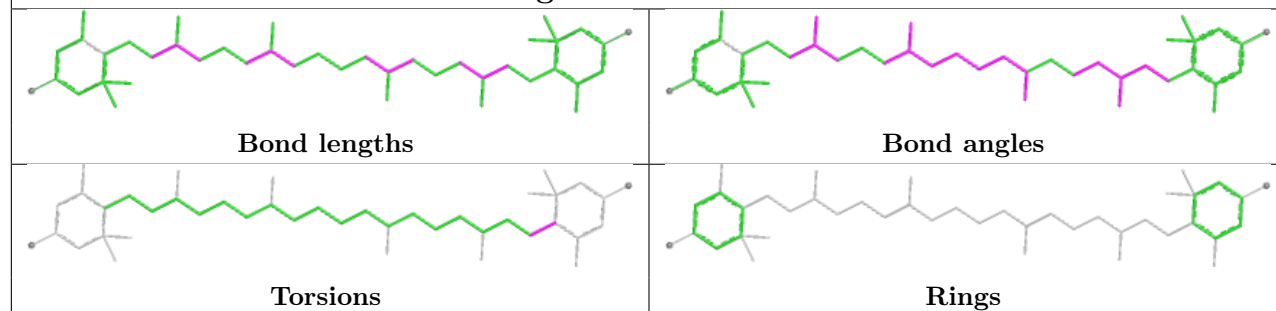
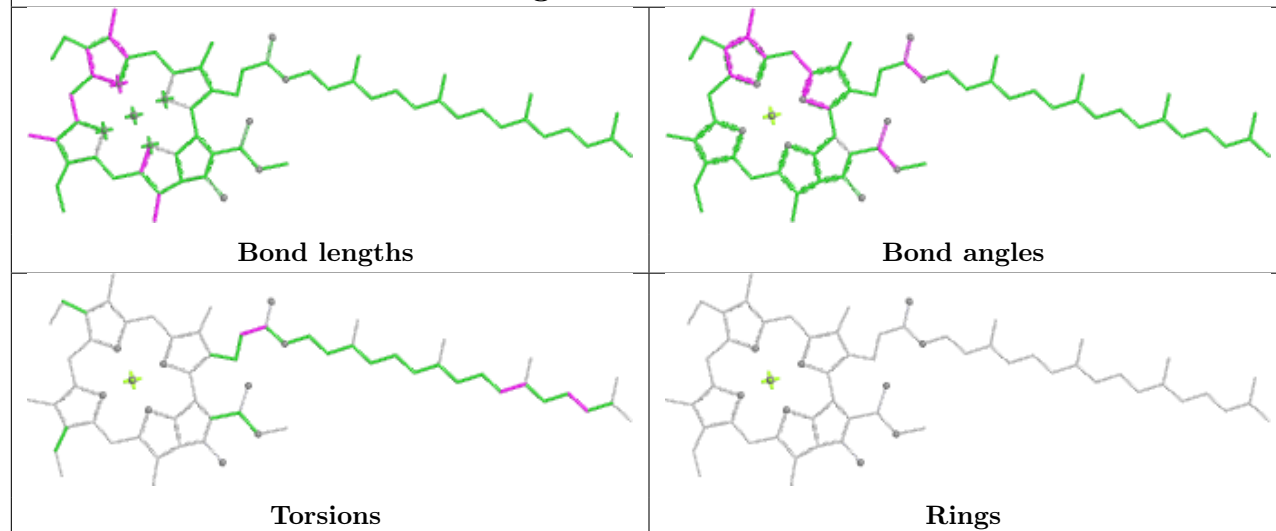
Ligand CLA 7 410



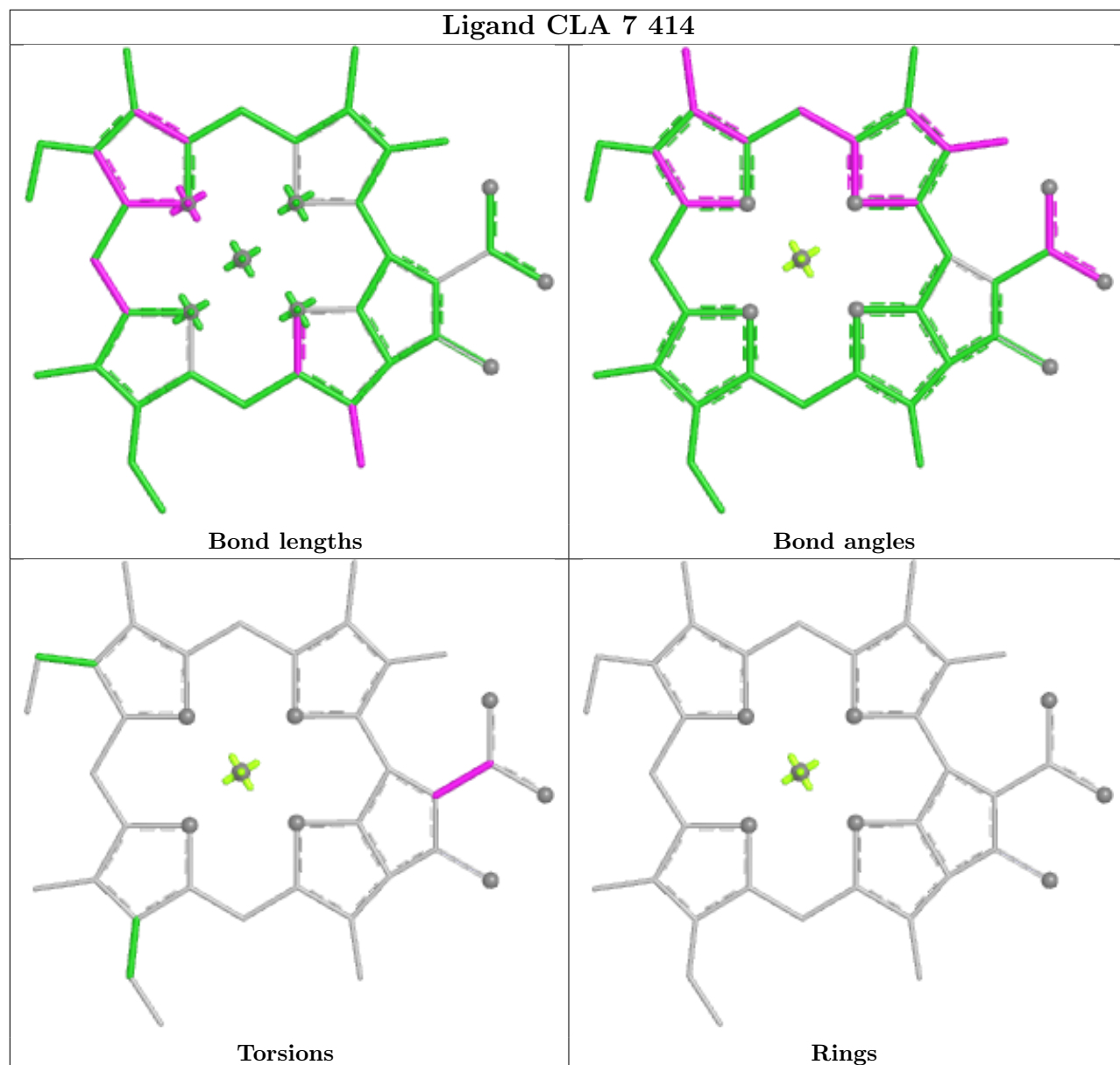
Ligand BCR 3 418

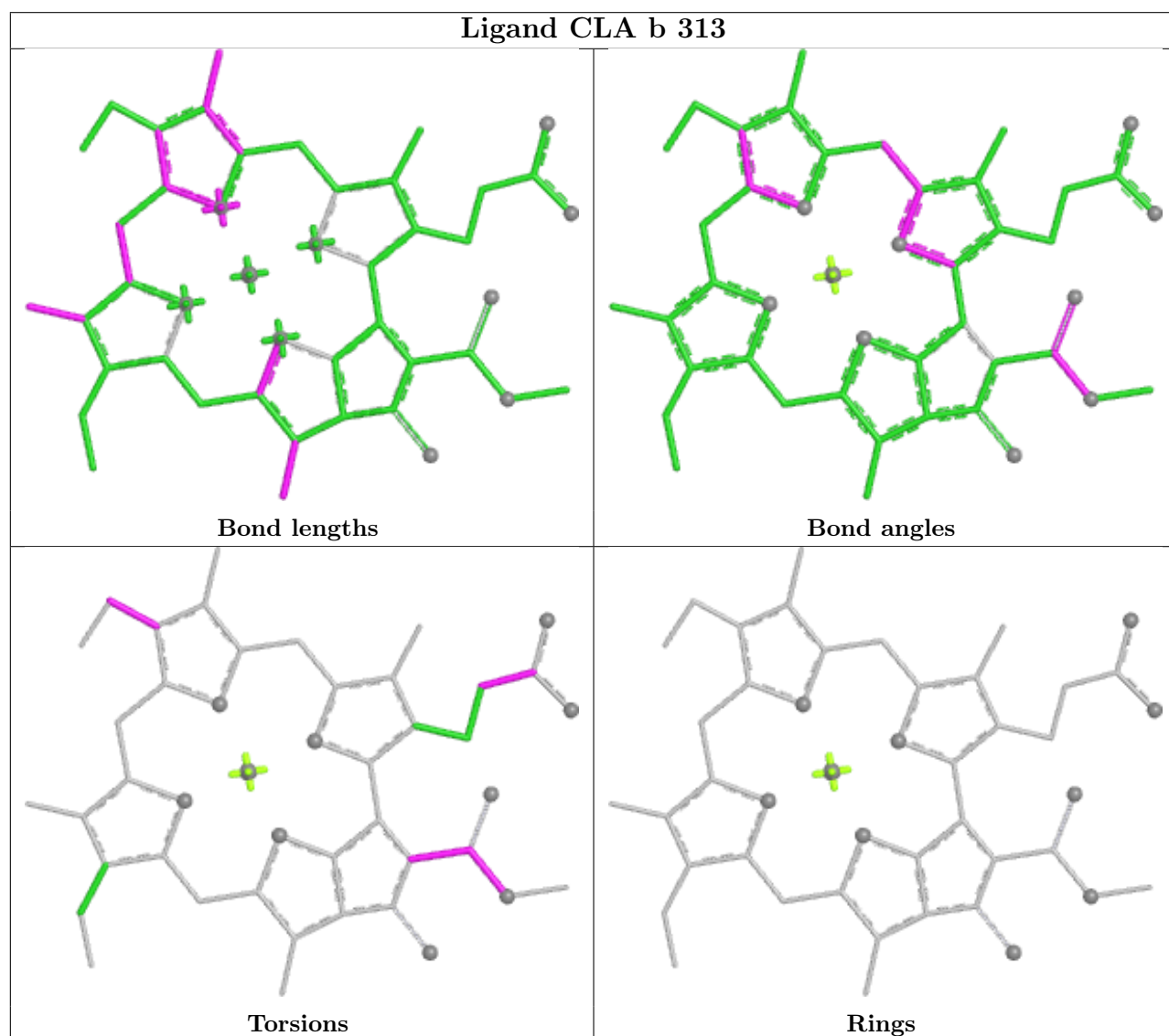
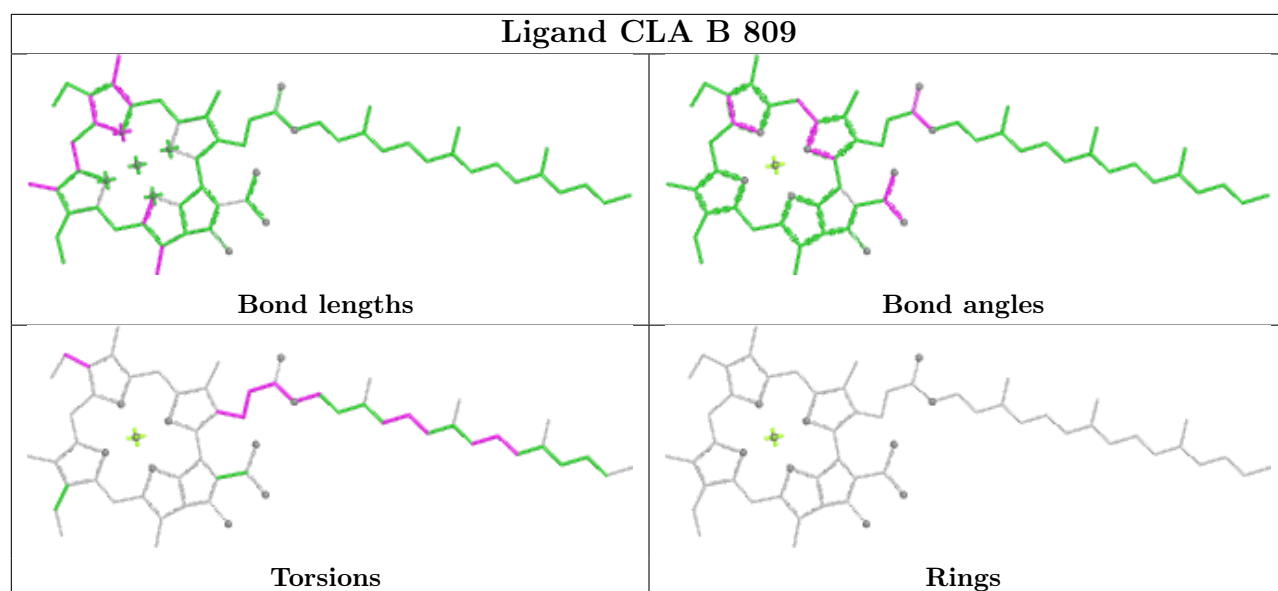




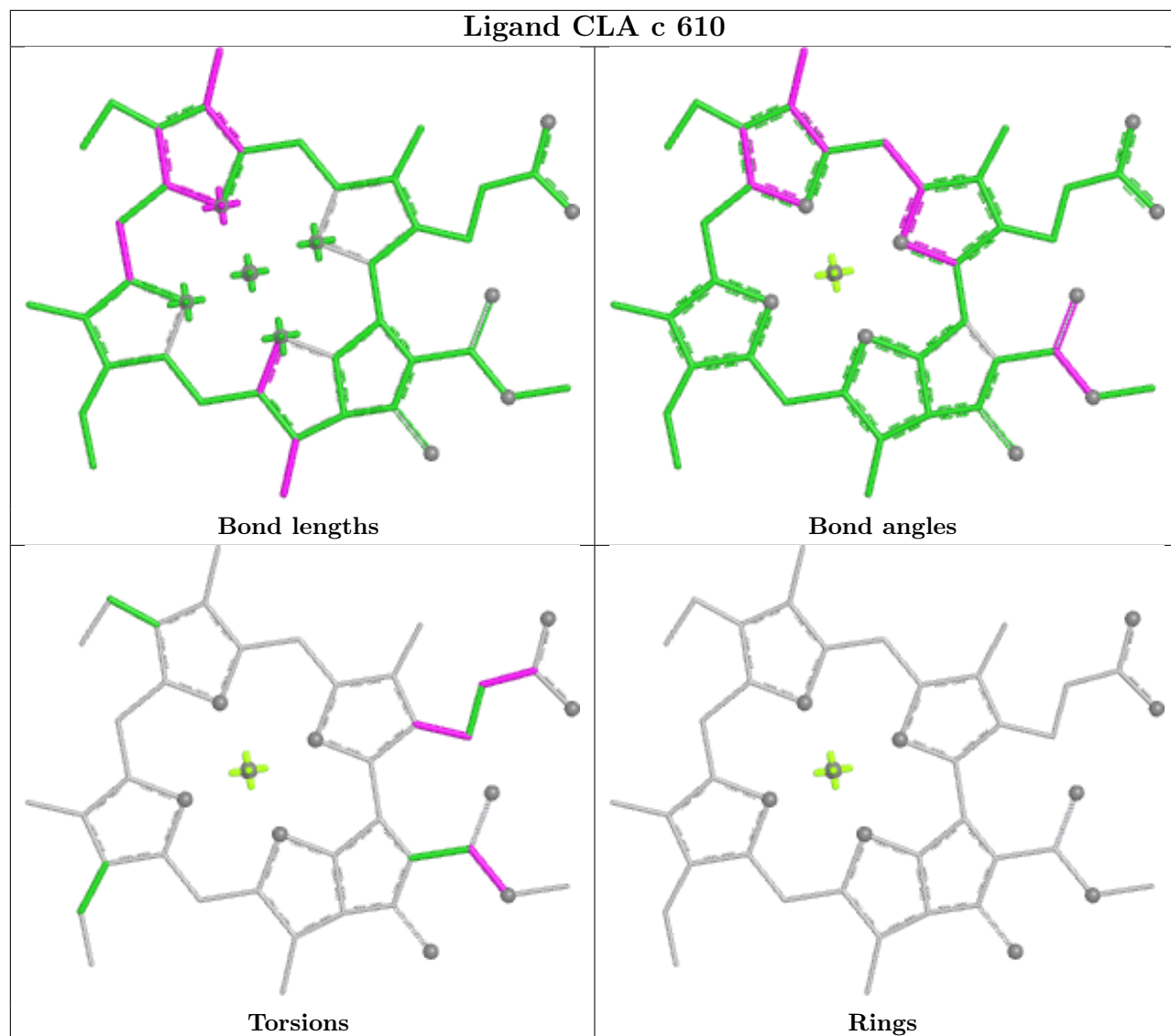
Ligand CLA 3 408**Ligand LUT 9 614****Ligand CLA B 840**

Ligand CLA 7 414

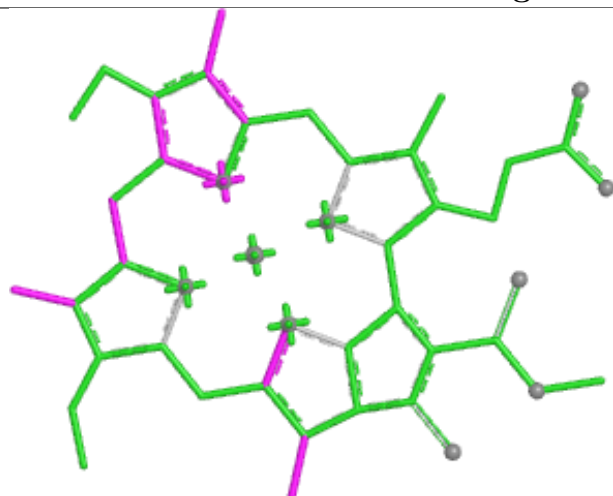




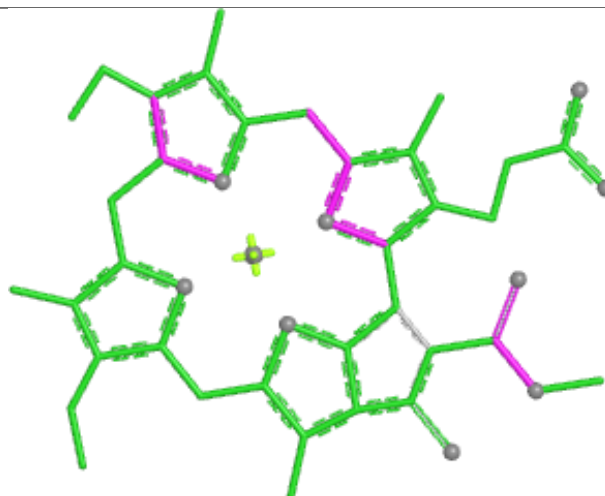
Ligand CLA c 610



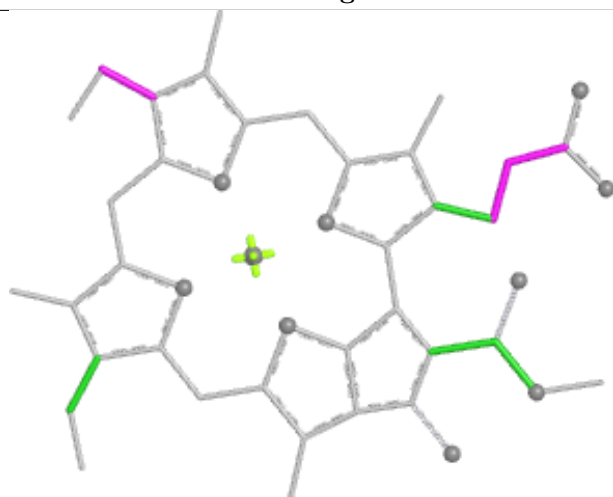
Ligand CLA K 204



Bond lengths



Bond angles

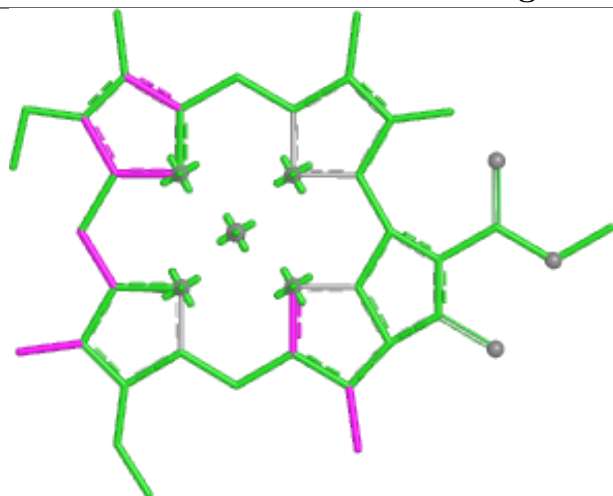


Torsions

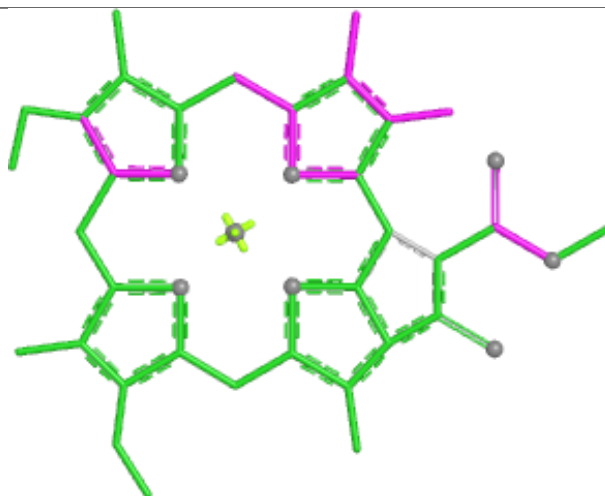


Rings

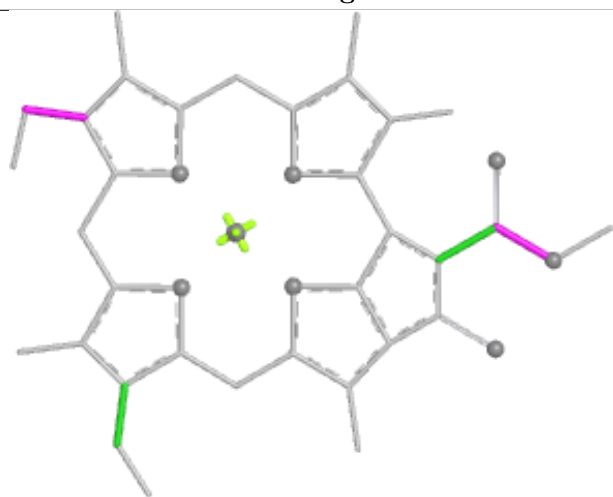
Ligand CLA 8 618



Bond lengths



Bond angles

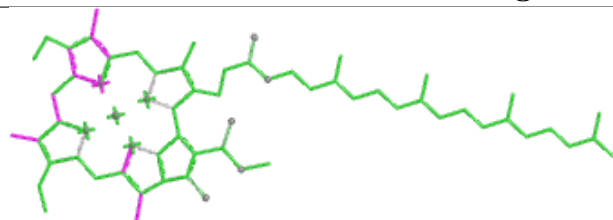


Torsions

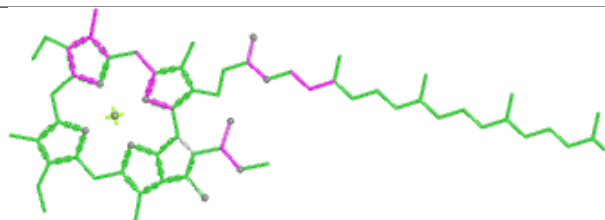


Rings

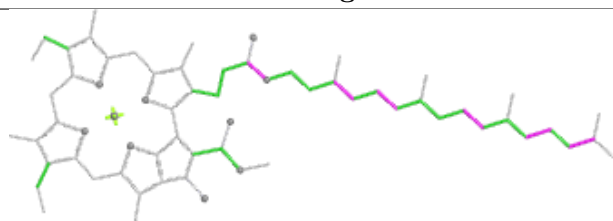
Ligand CLA B 825



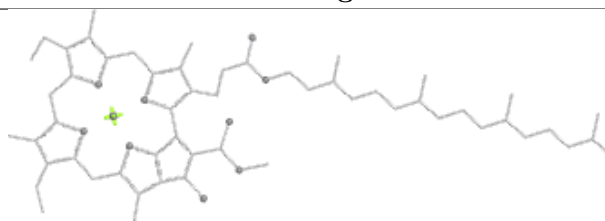
Bond lengths



Bond angles

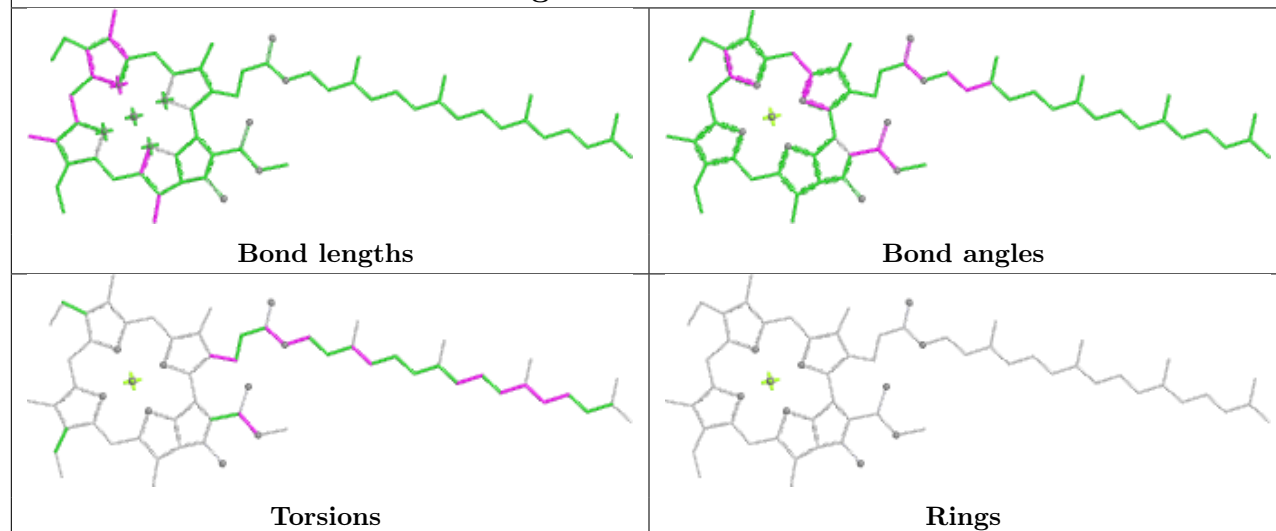


Torsions

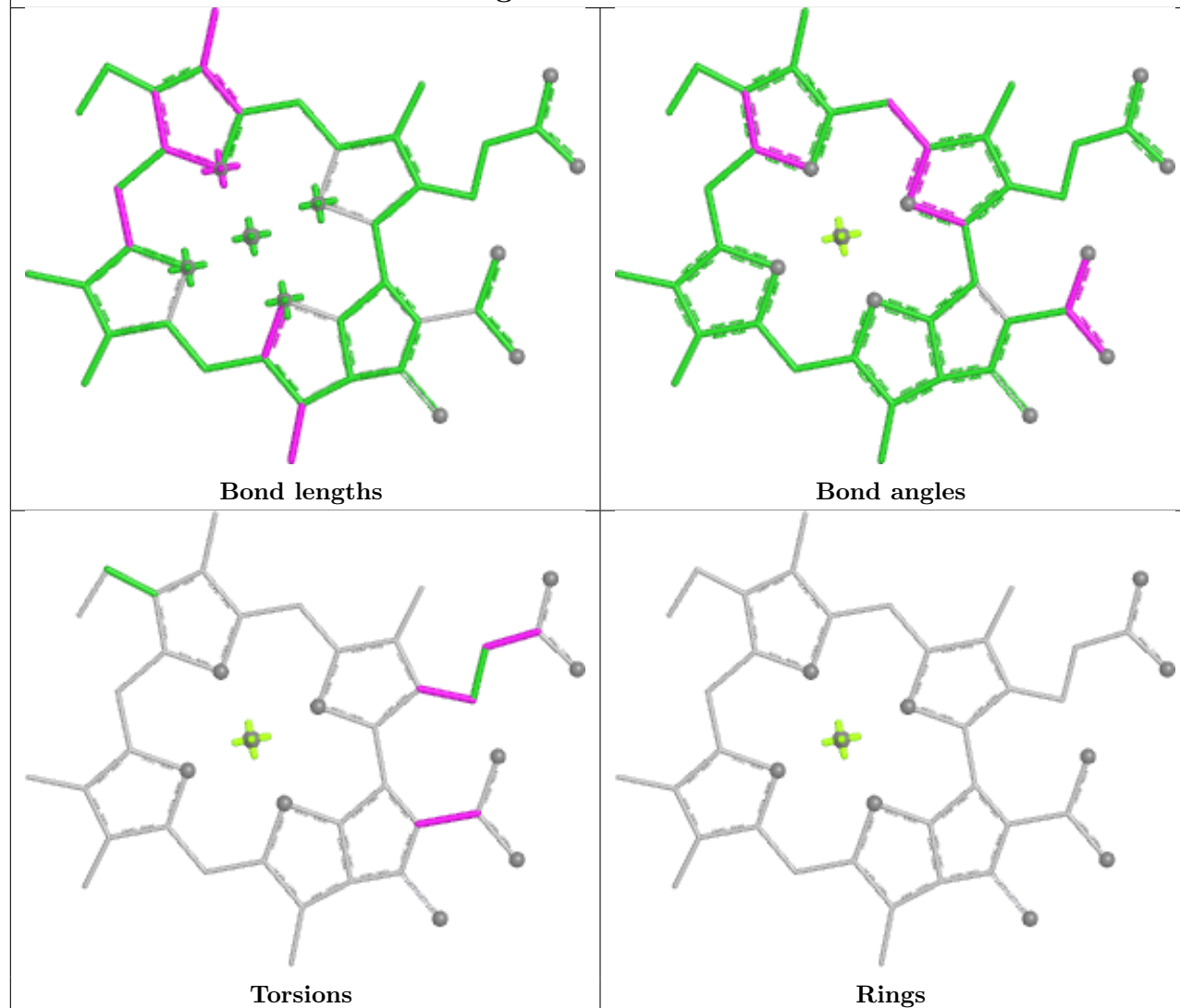


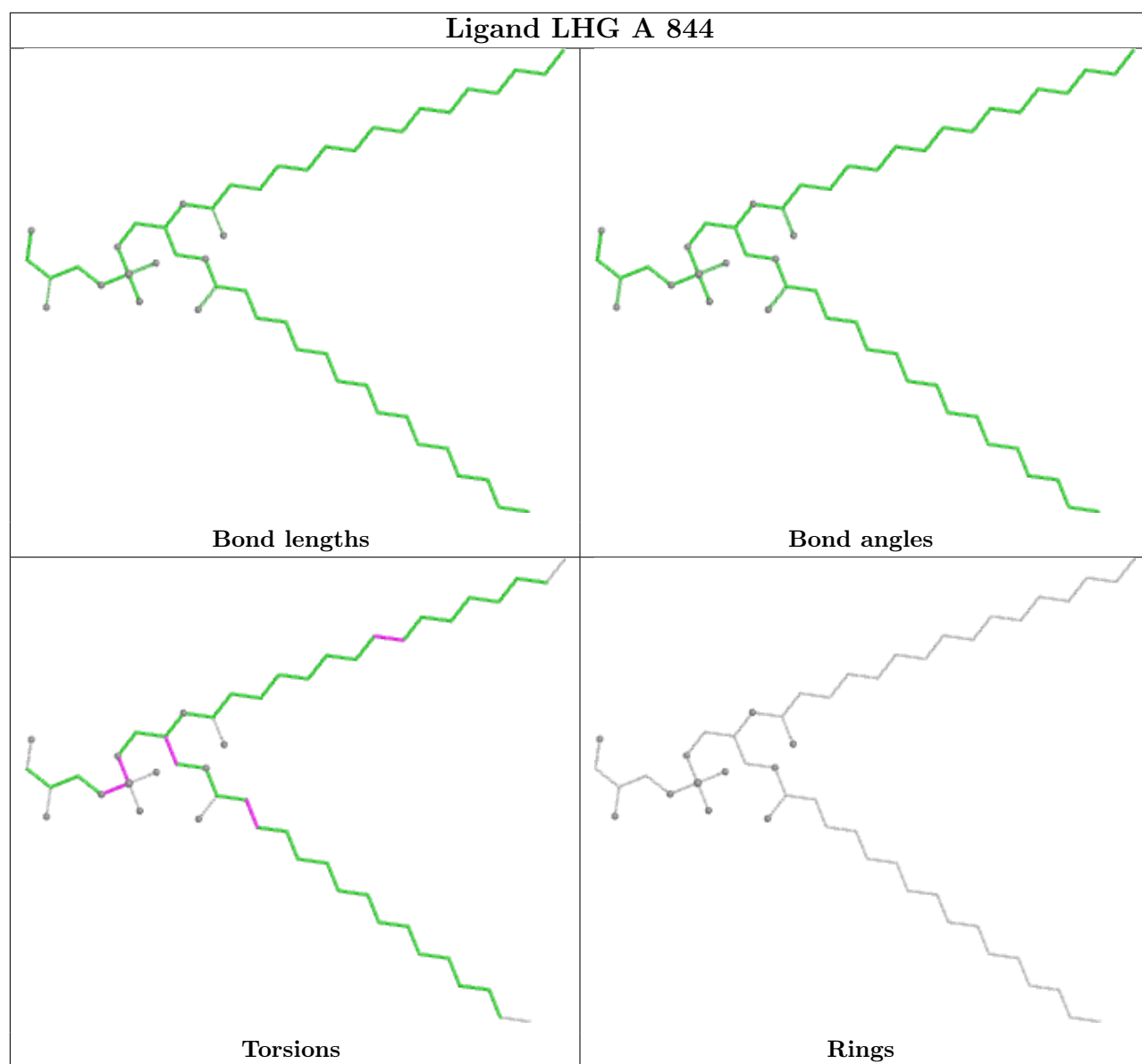
Rings

Ligand CLA A 819

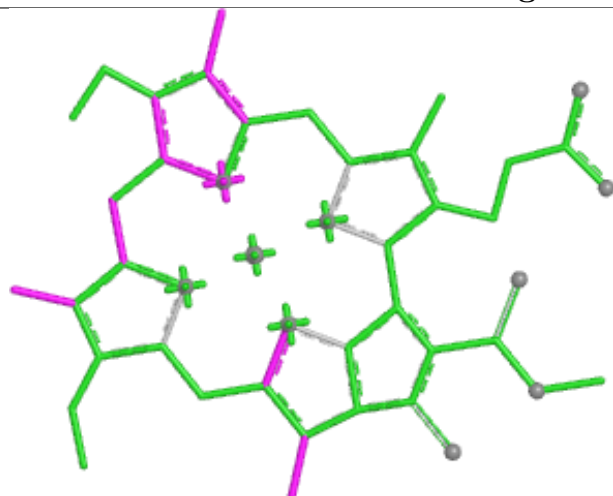


Ligand CLA 5 609

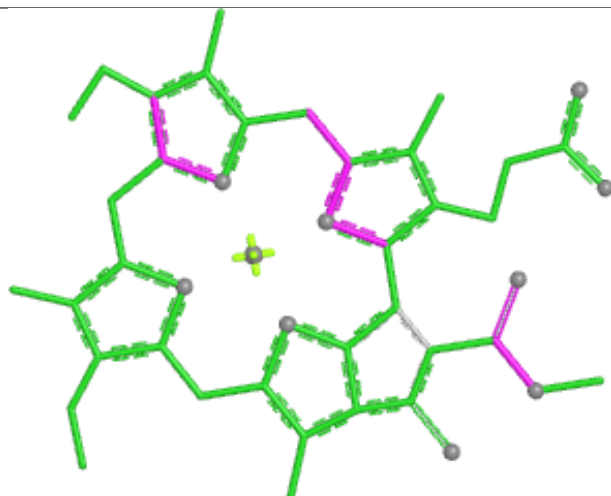




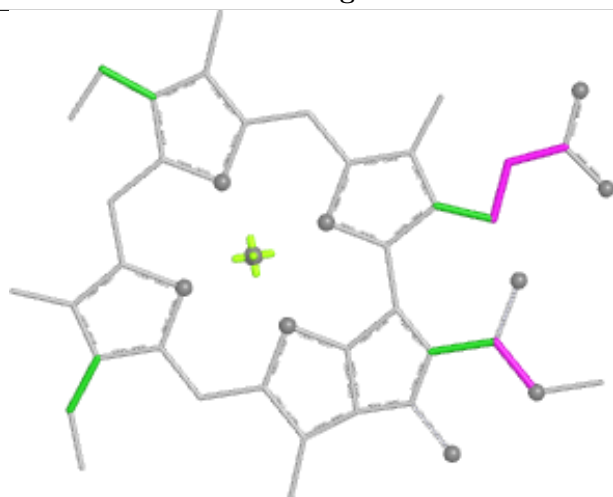
Ligand CLA 1 312



Bond lengths



Bond angles

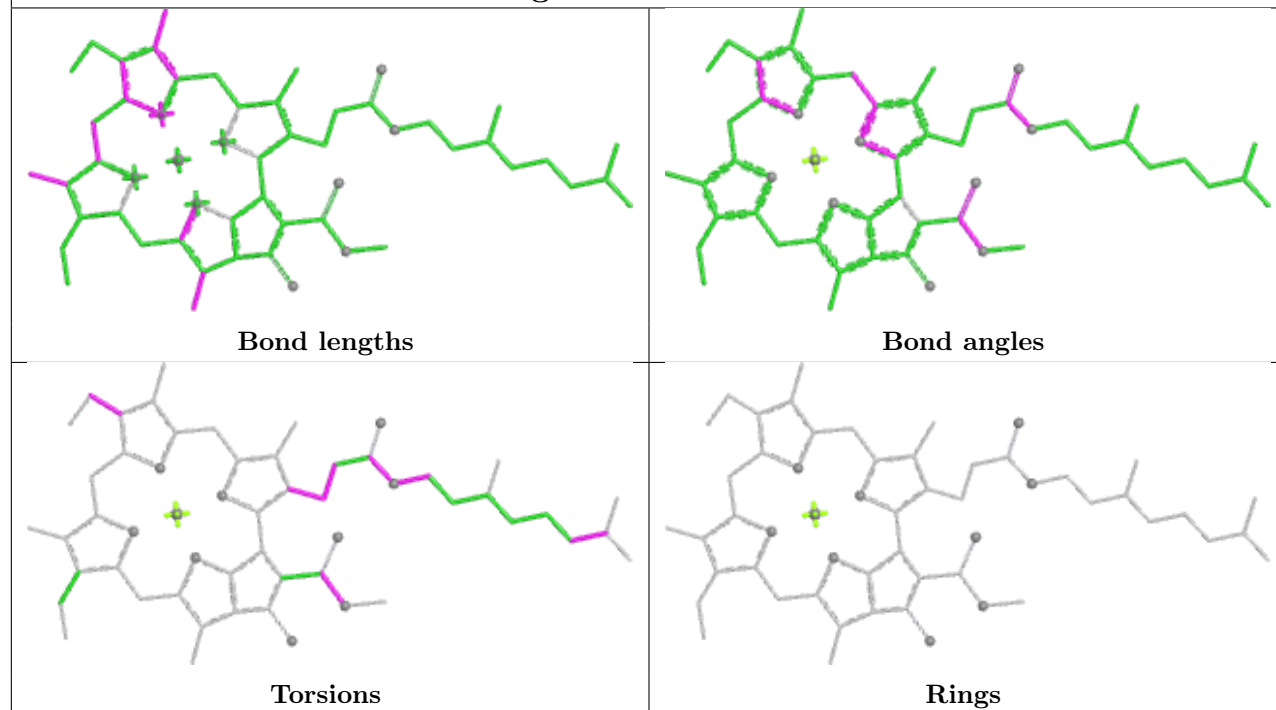


Torsions

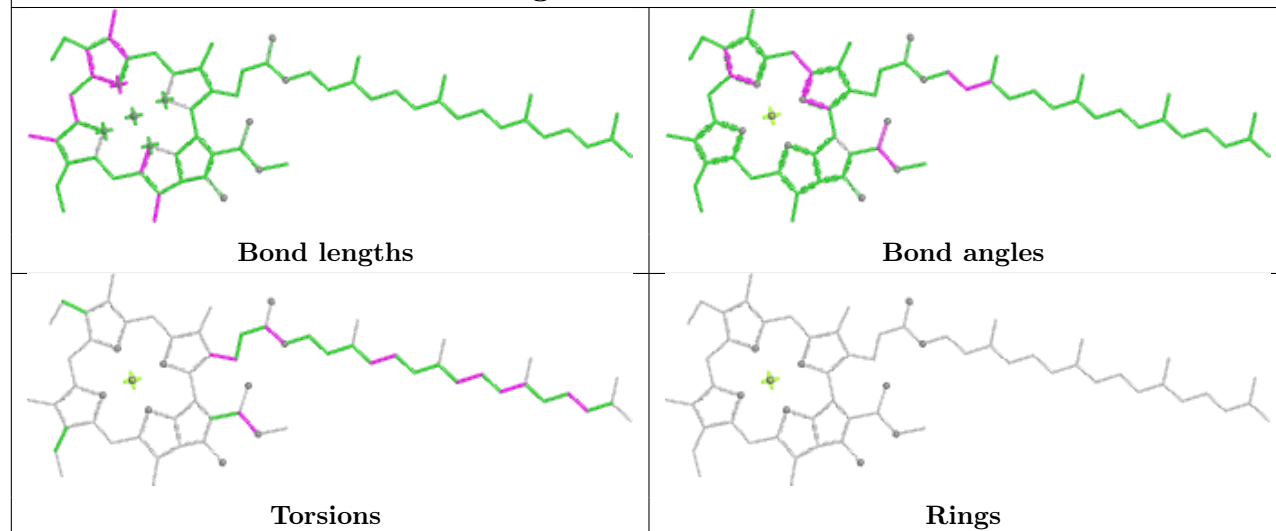


Rings

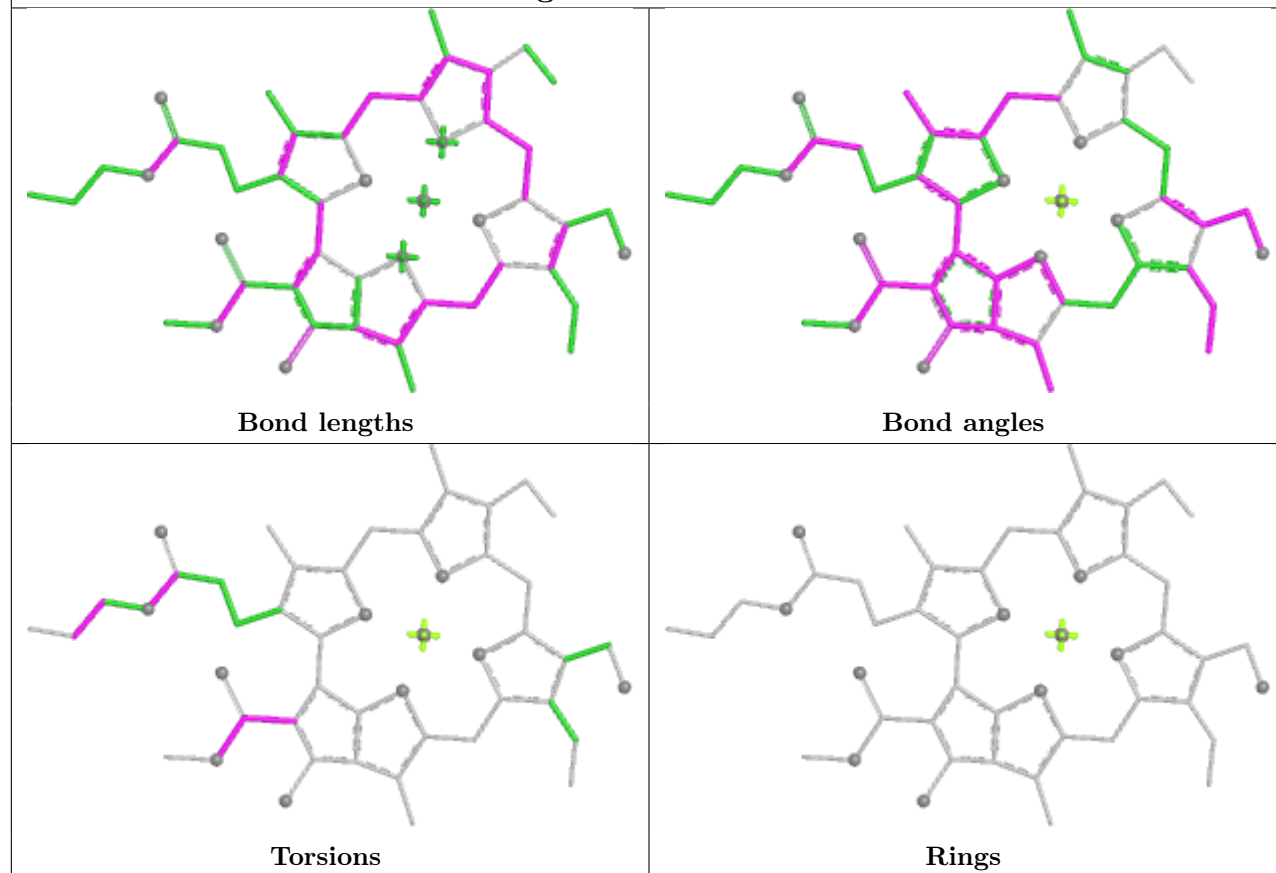
Ligand CLA A 824



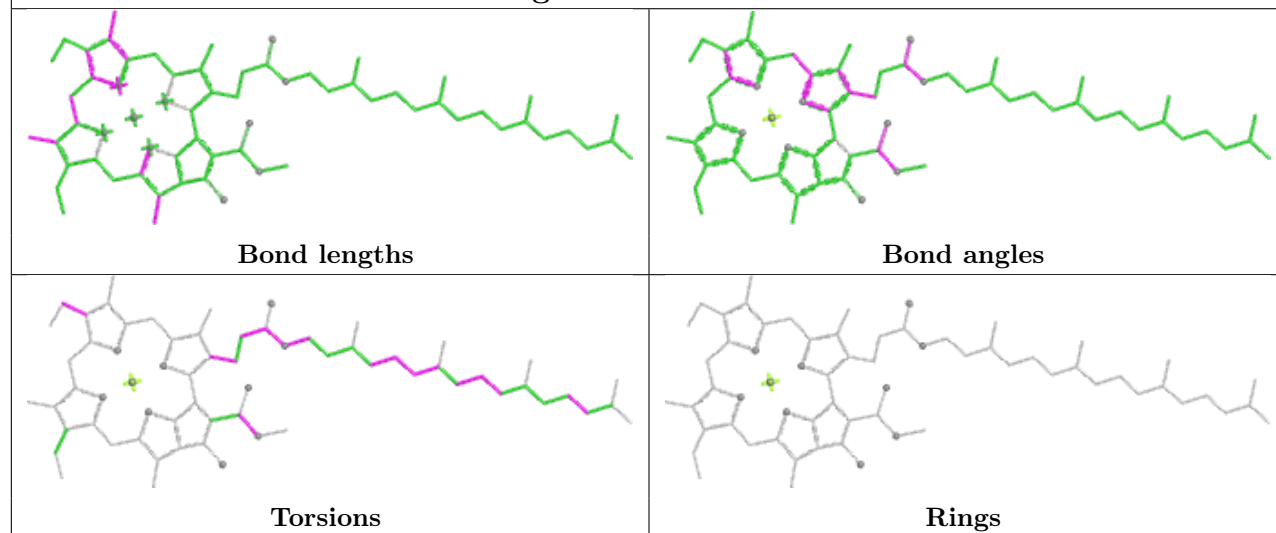
Ligand CLA A 807



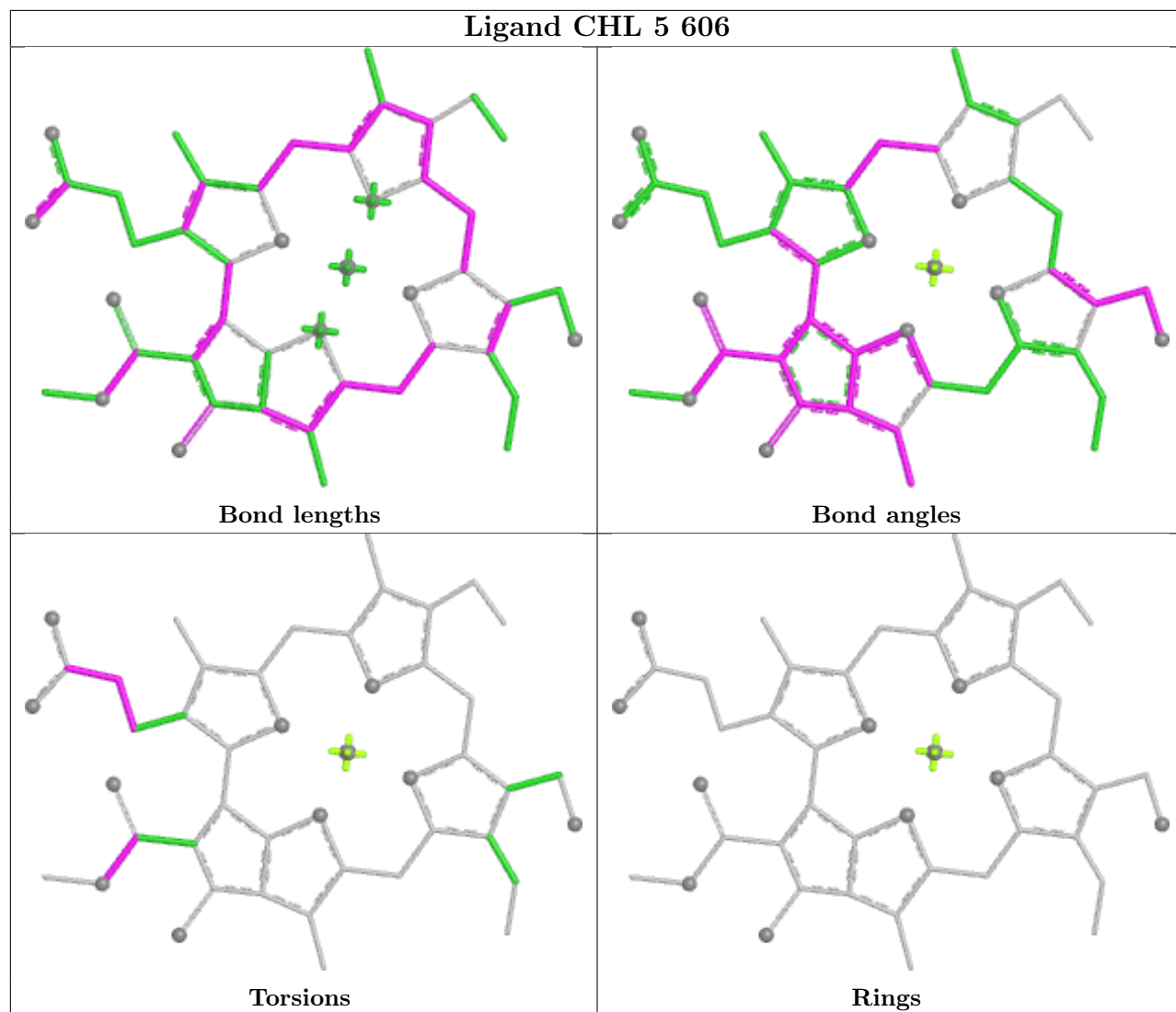
Ligand CHL c 601

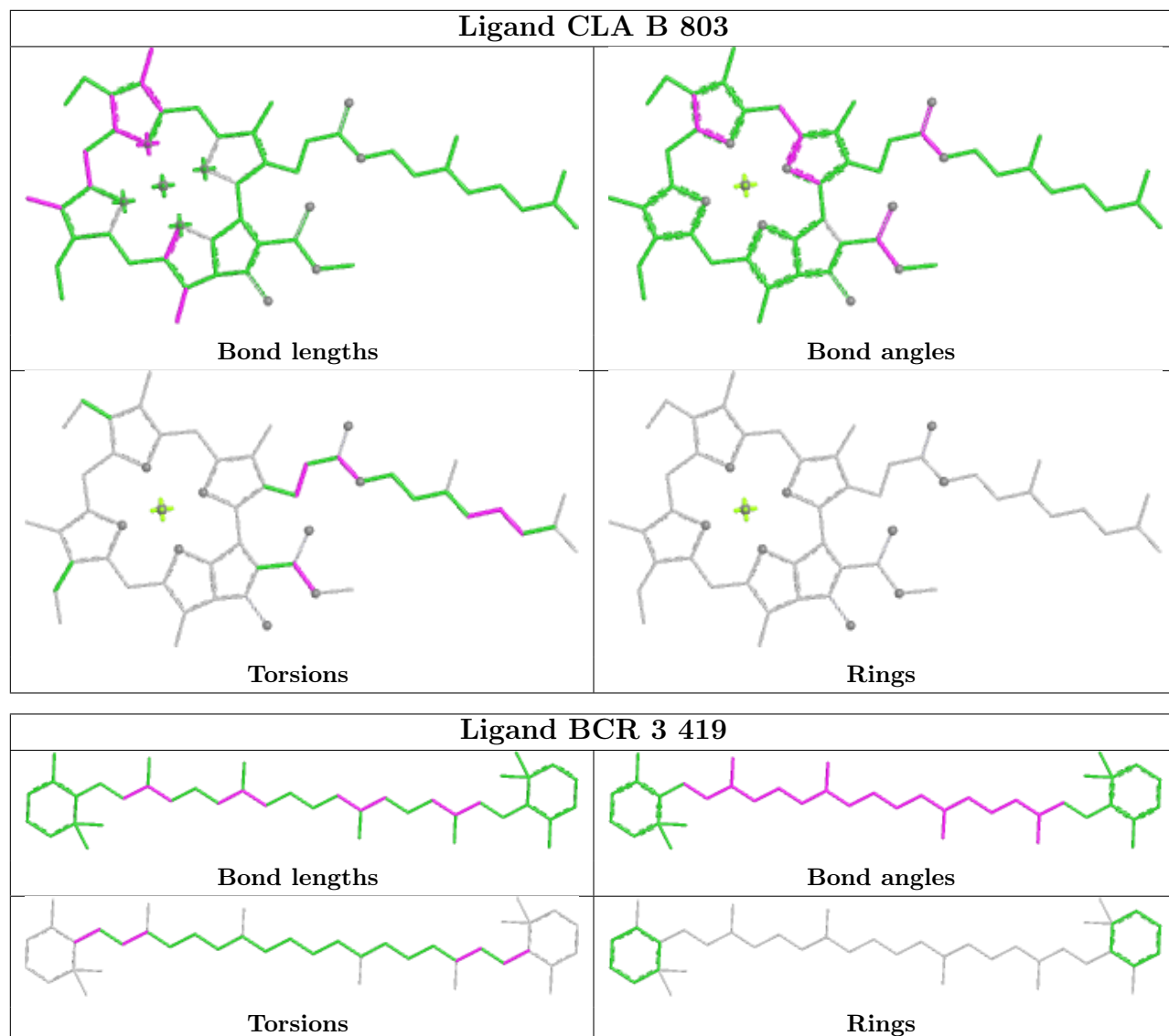


Ligand CLA B 807

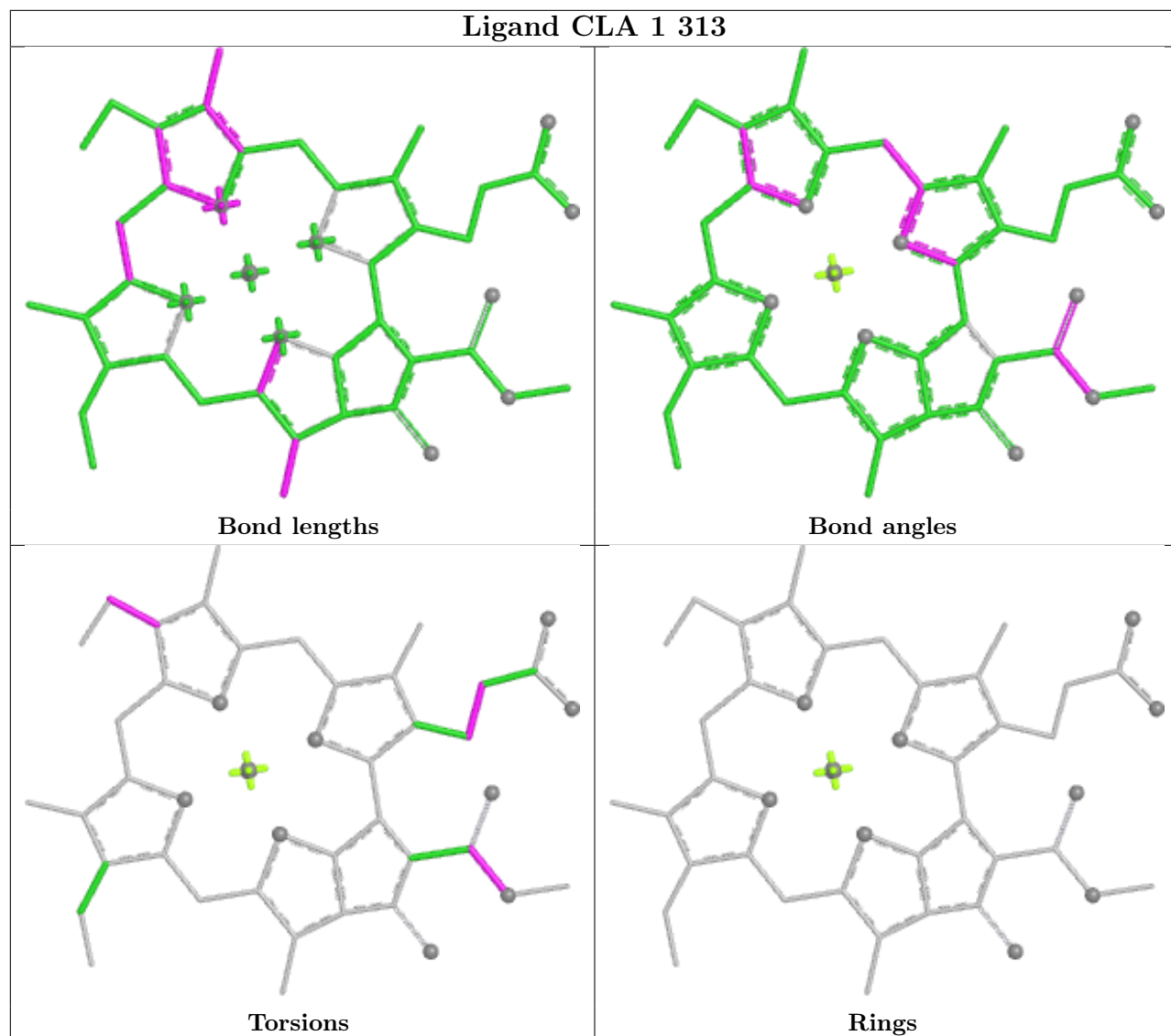


Ligand CHL 5 606

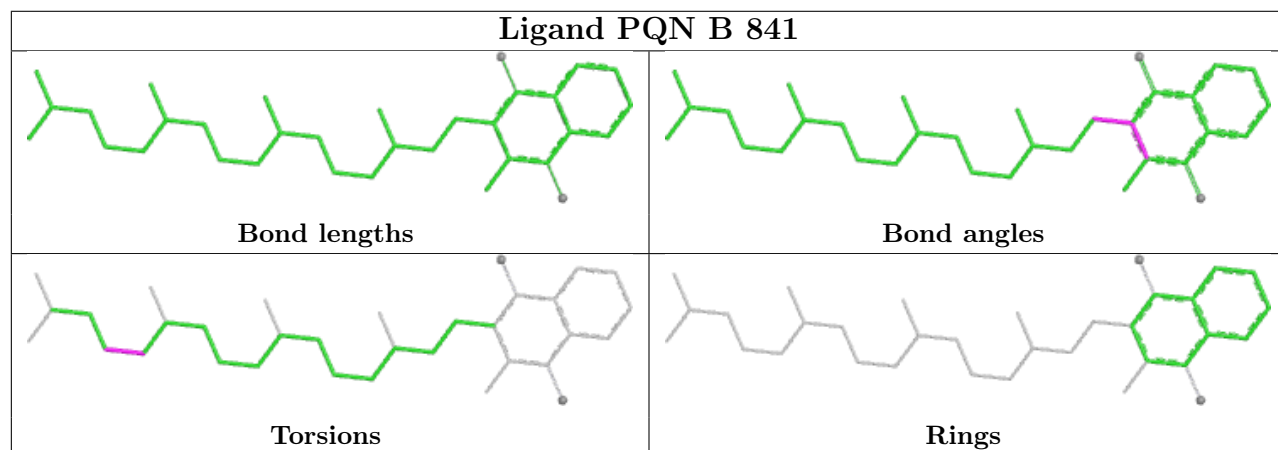


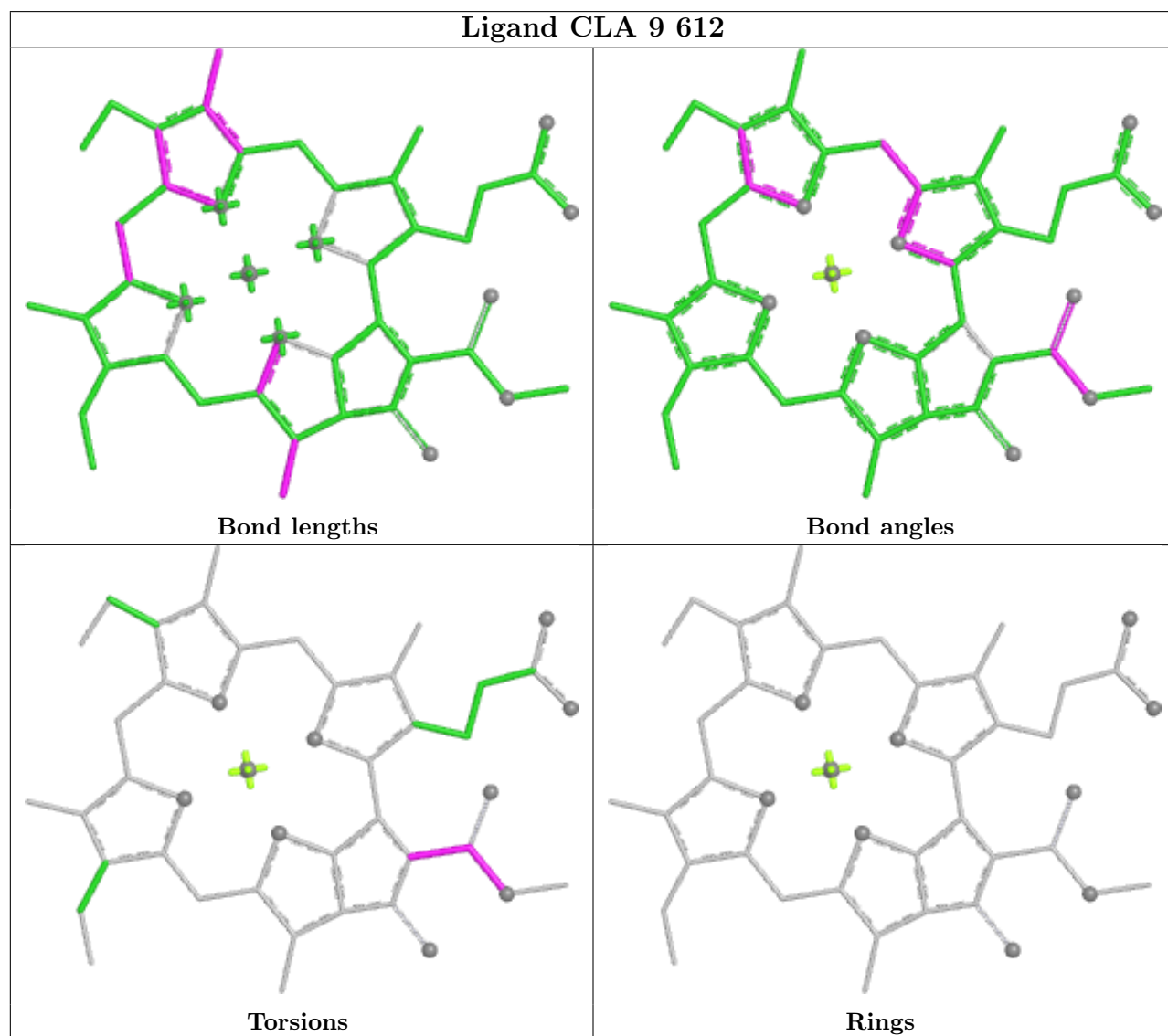
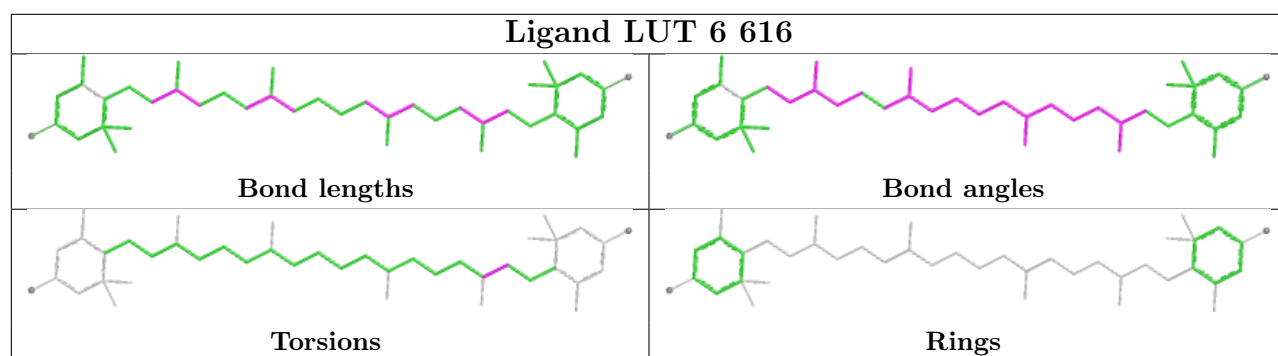


Ligand CLA 1 313

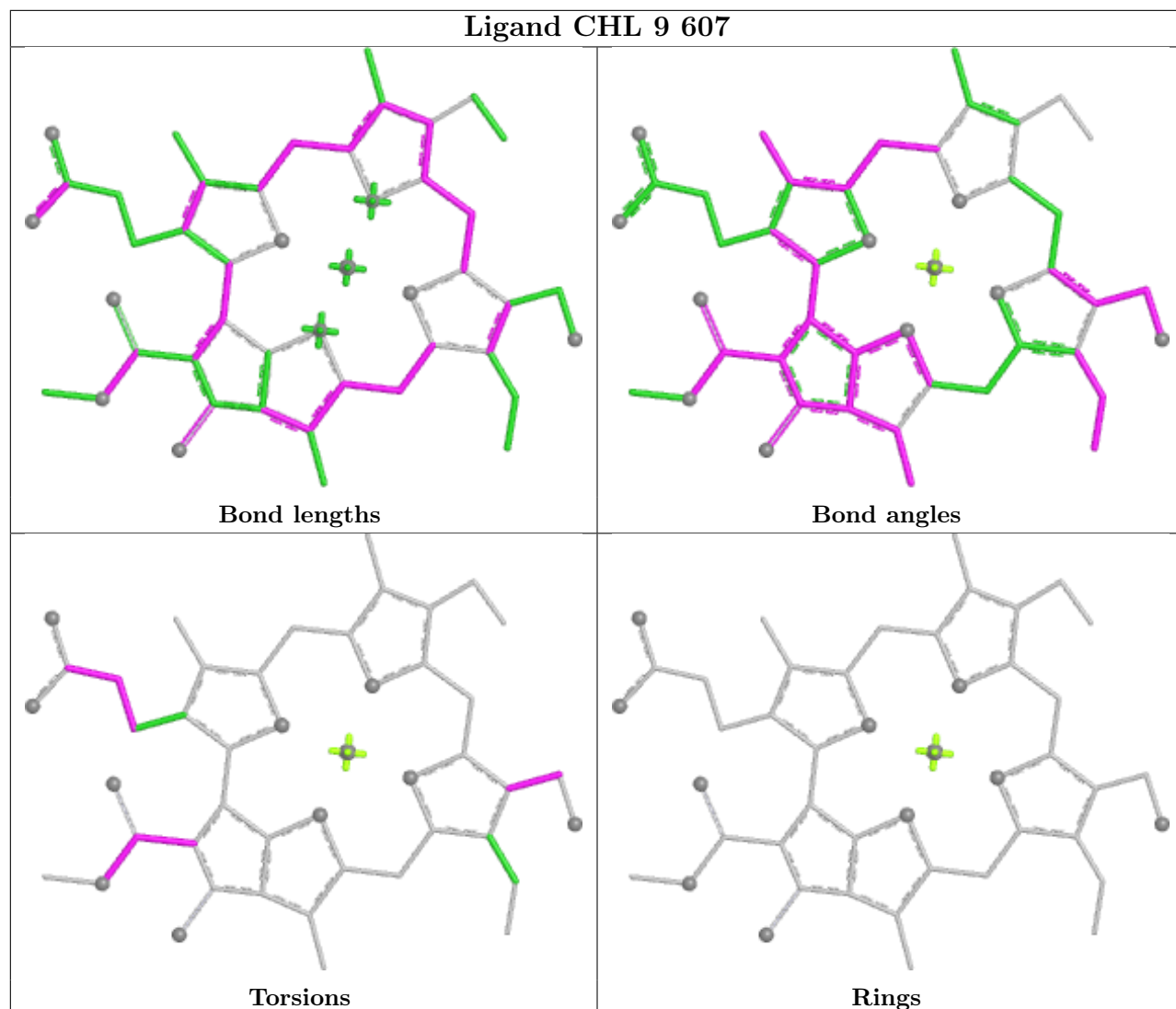


Ligand PQN B 841

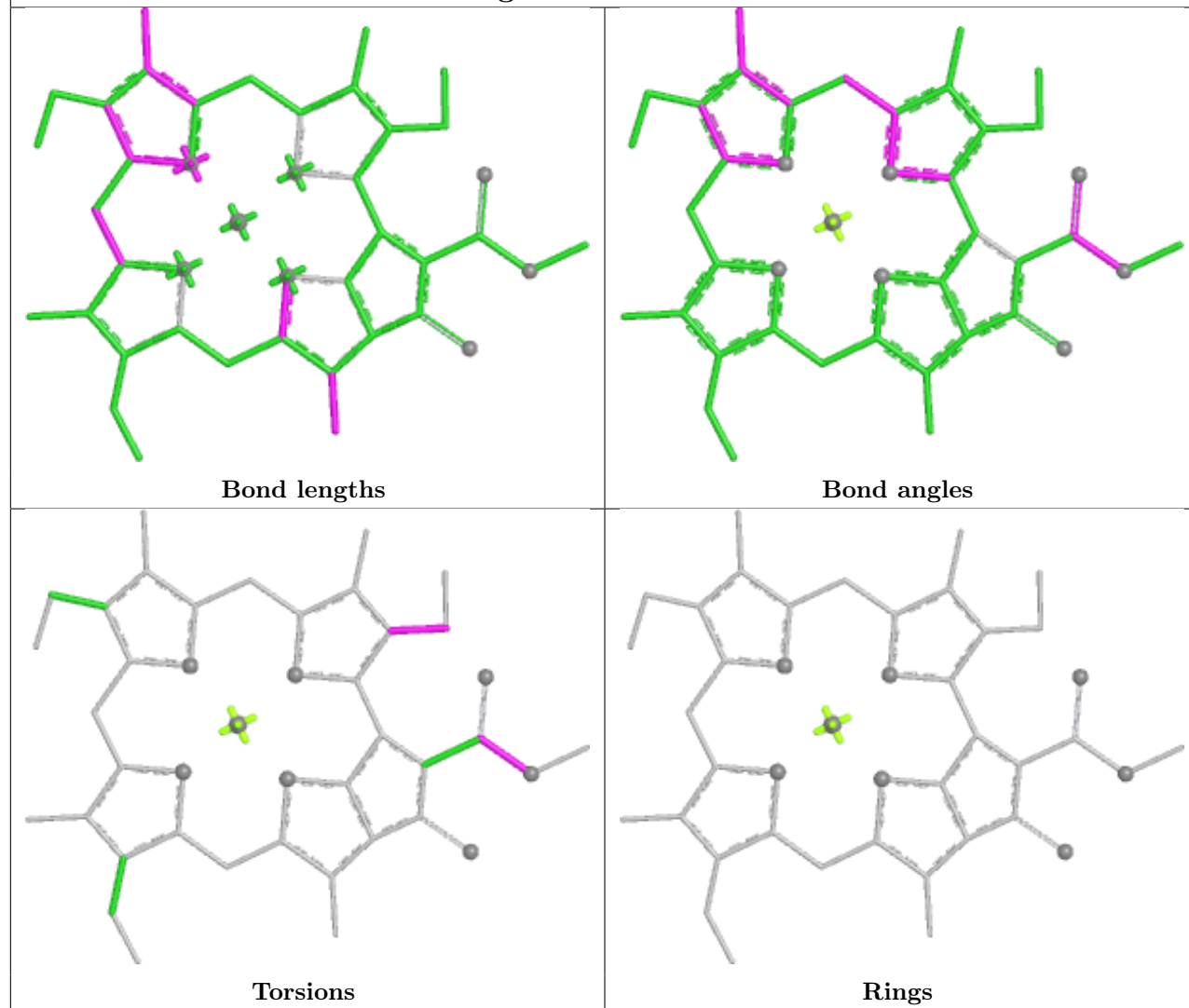




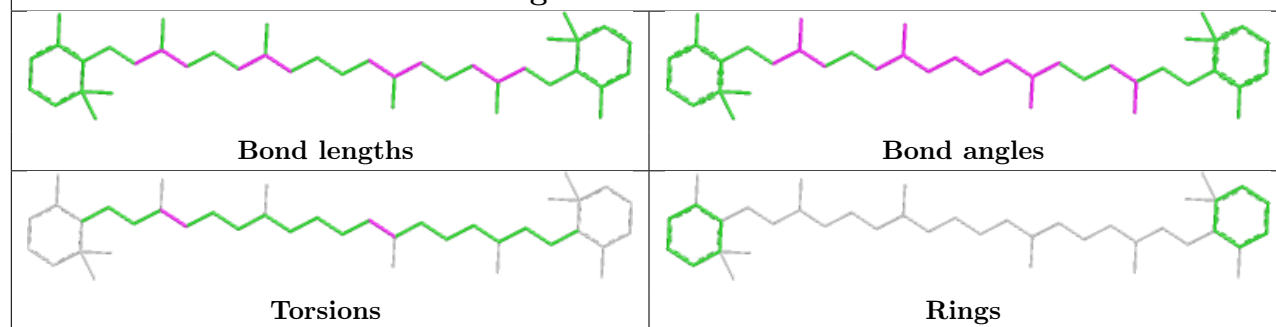
Ligand CHL 9 607



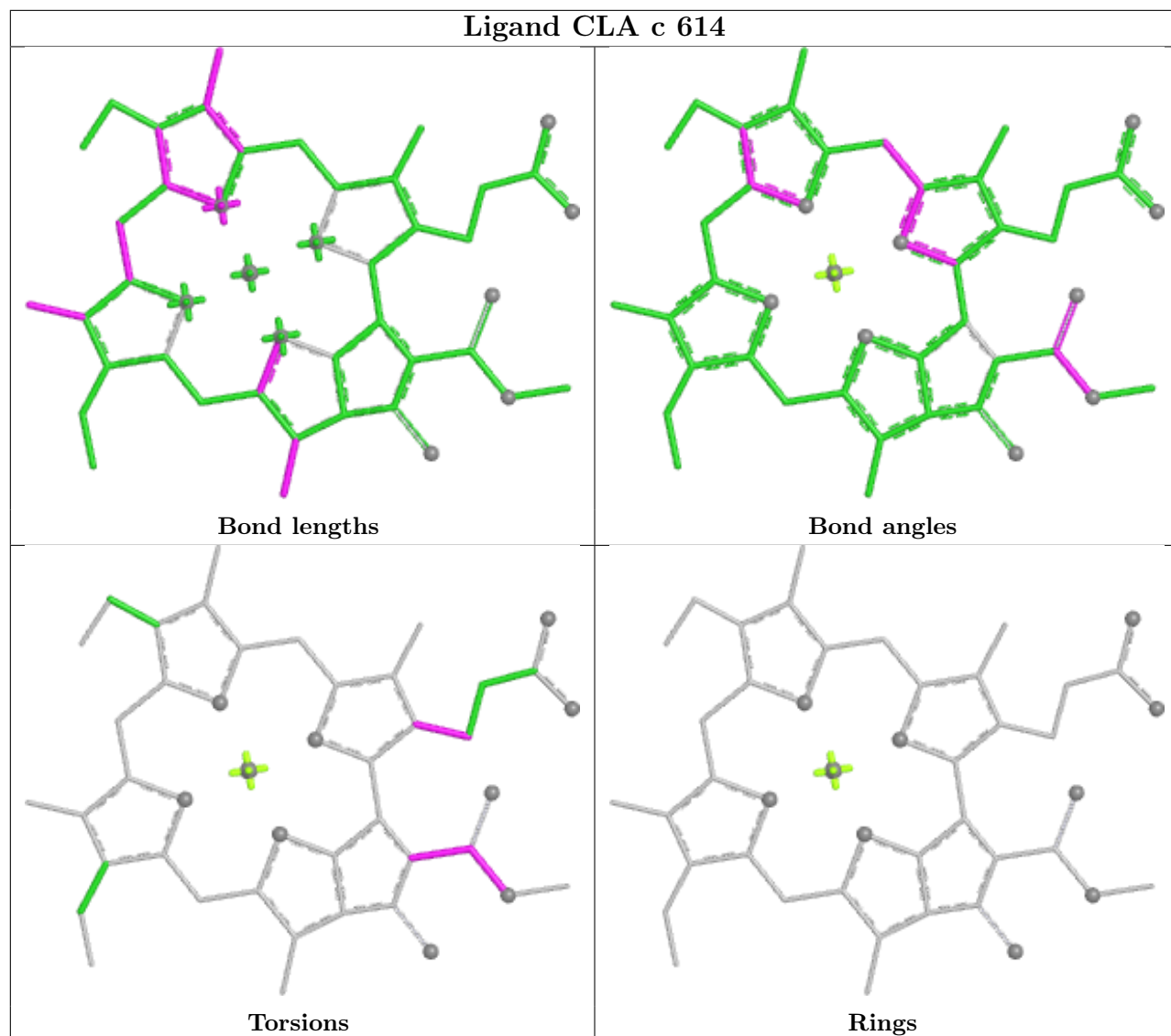
Ligand CLA L 304



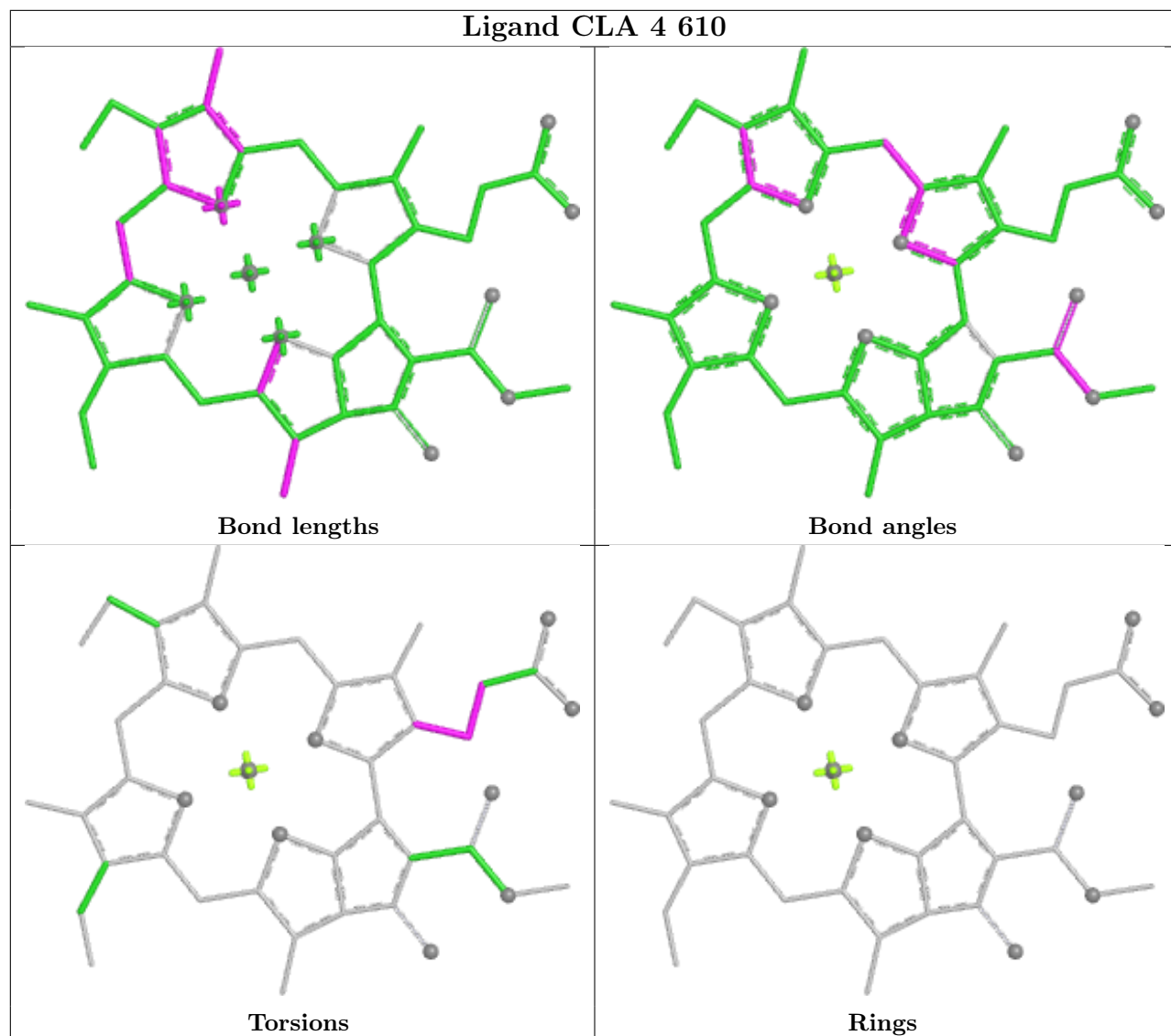
Ligand BCR A 850



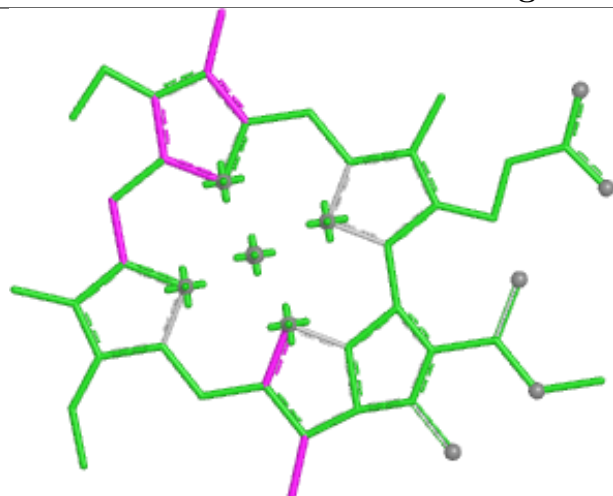
Ligand CLA c 614



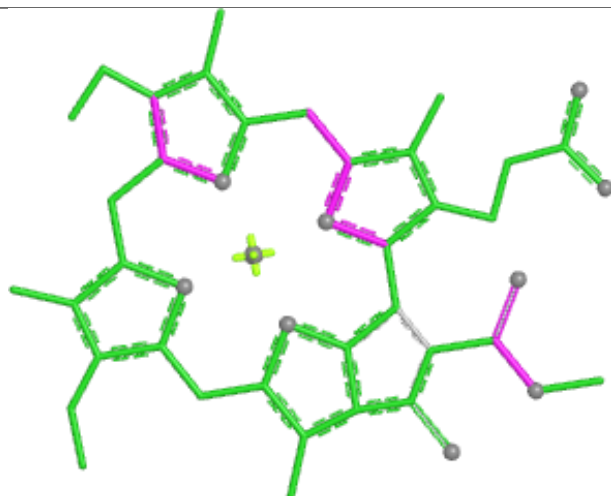
Ligand CLA 4 610



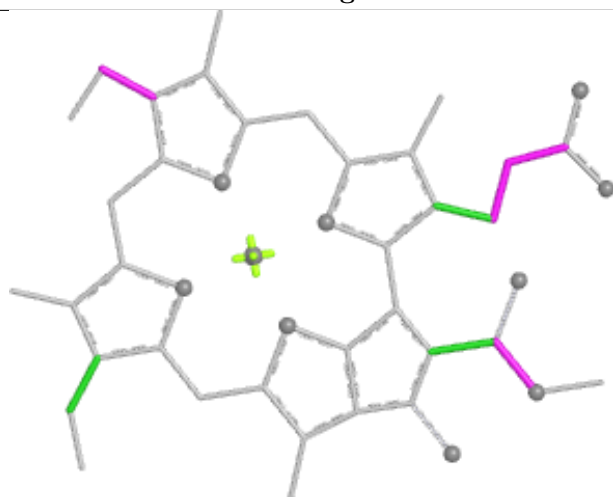
Ligand CLA 6 612



Bond lengths



Bond angles

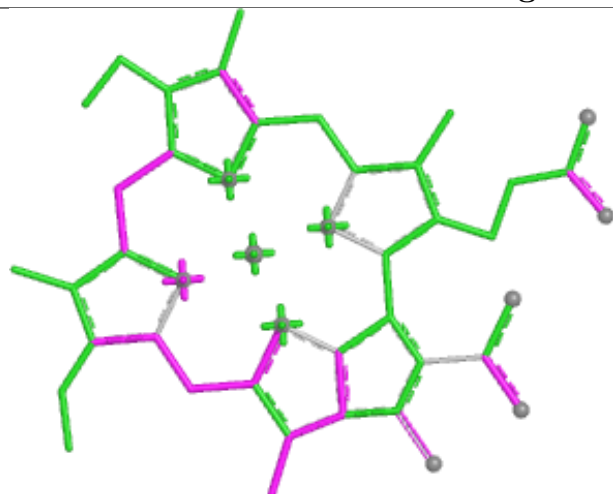


Torsions

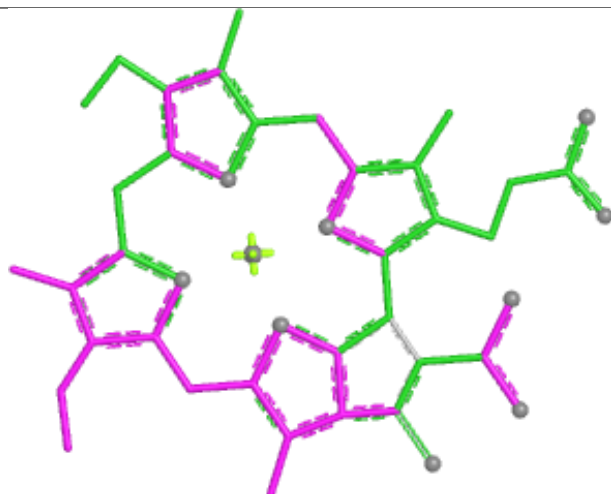


Rings

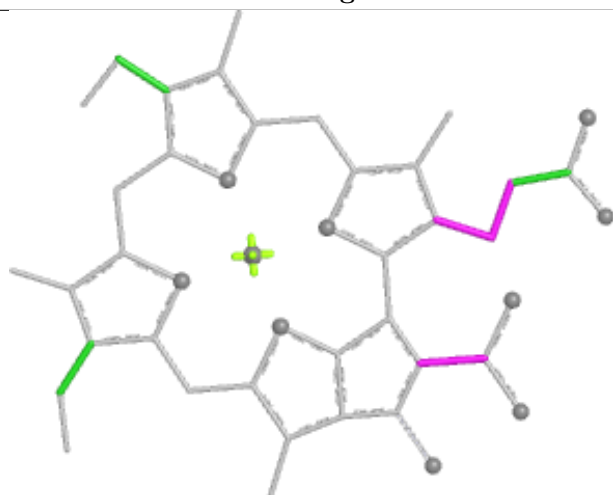
Ligand CLA 7 407



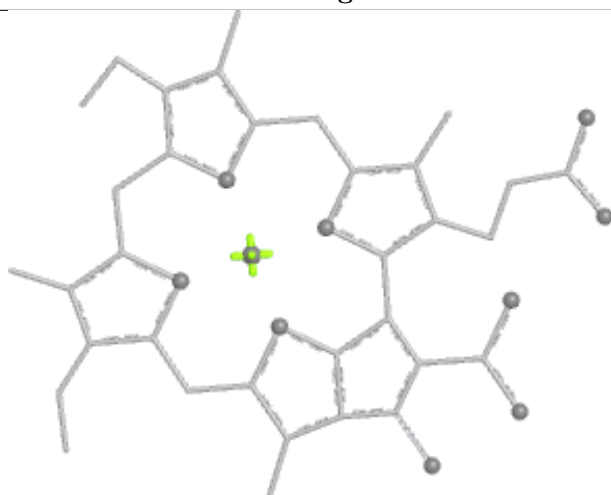
Bond lengths



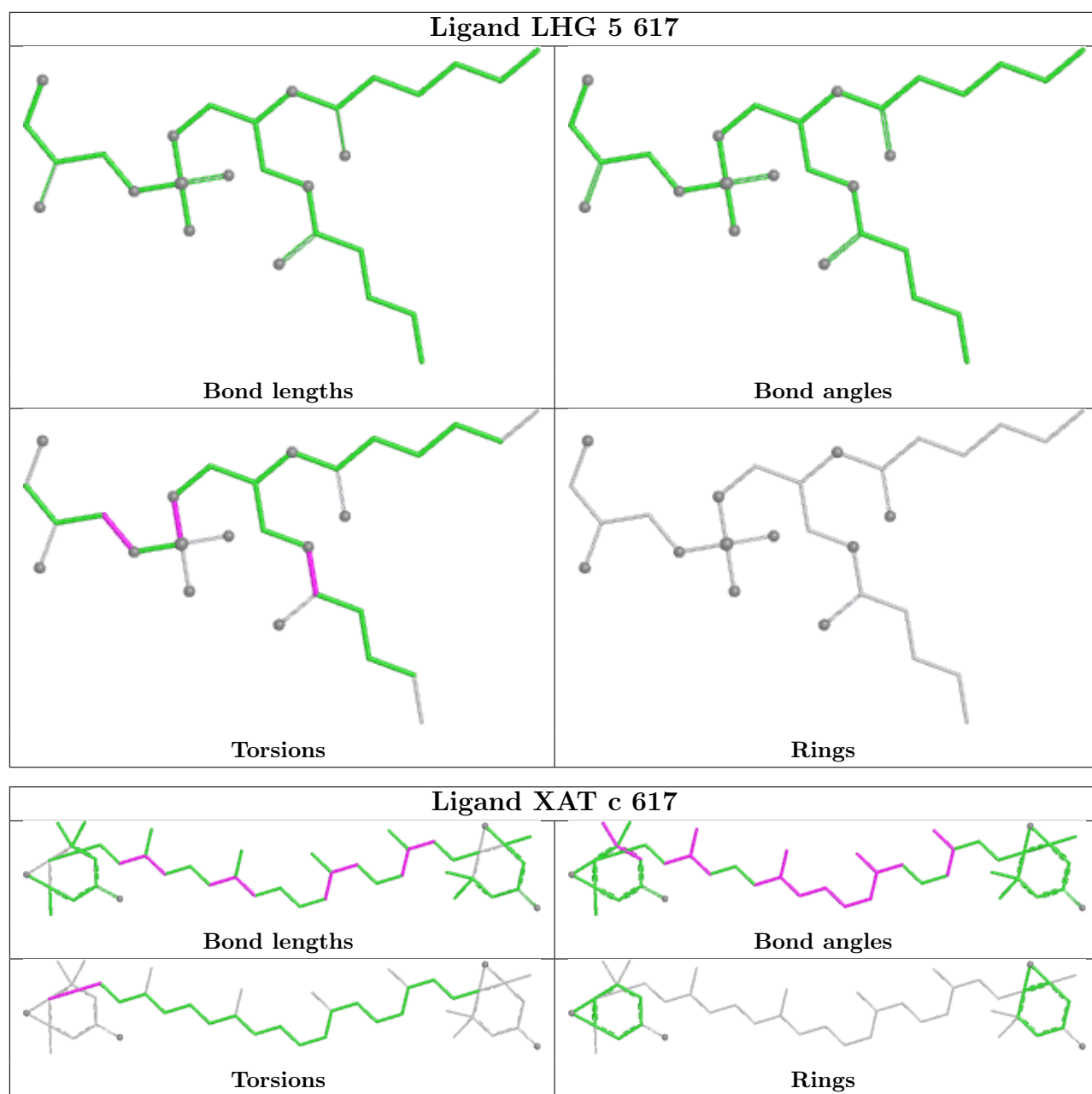
Bond angles



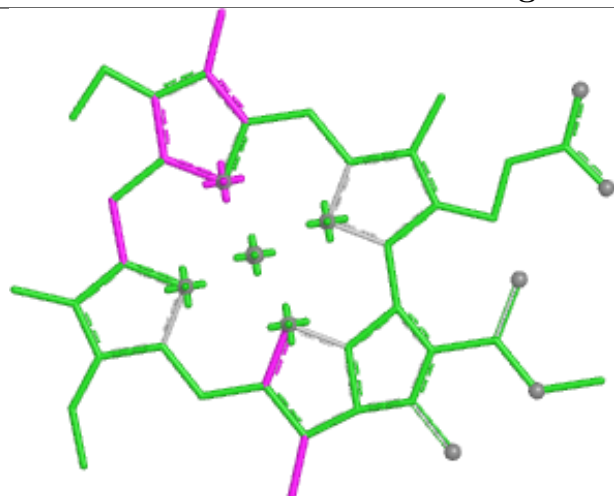
Torsions



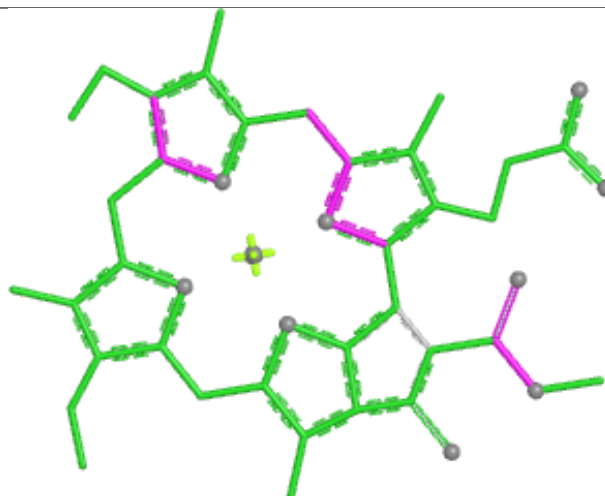
Rings



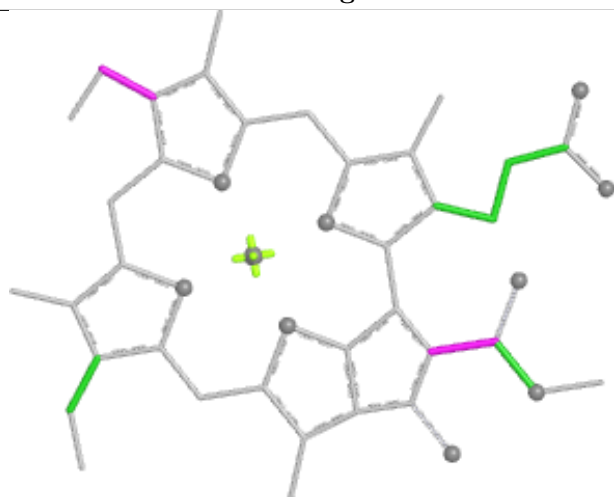
Ligand CLA 4 601



Bond lengths



Bond angles

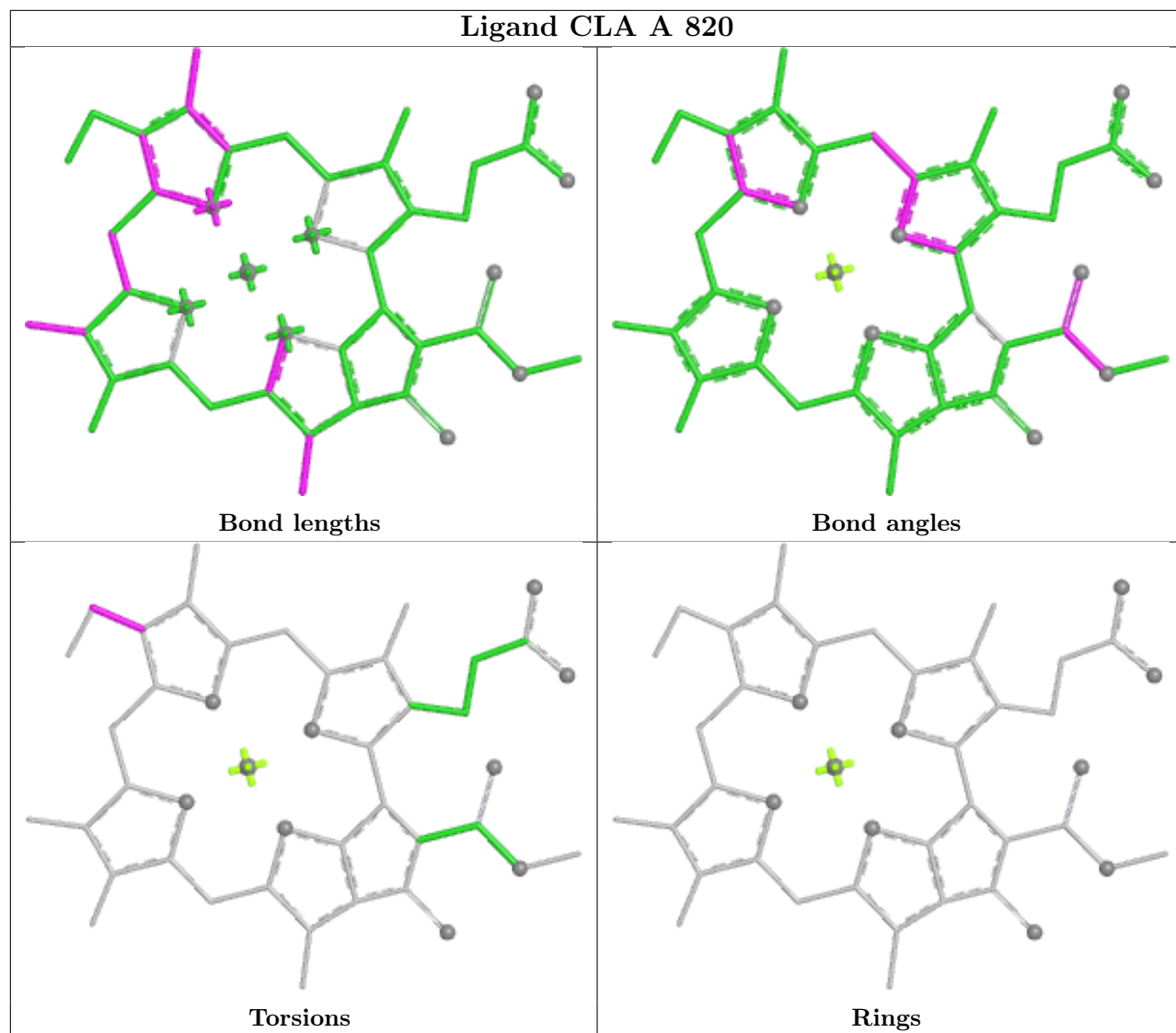


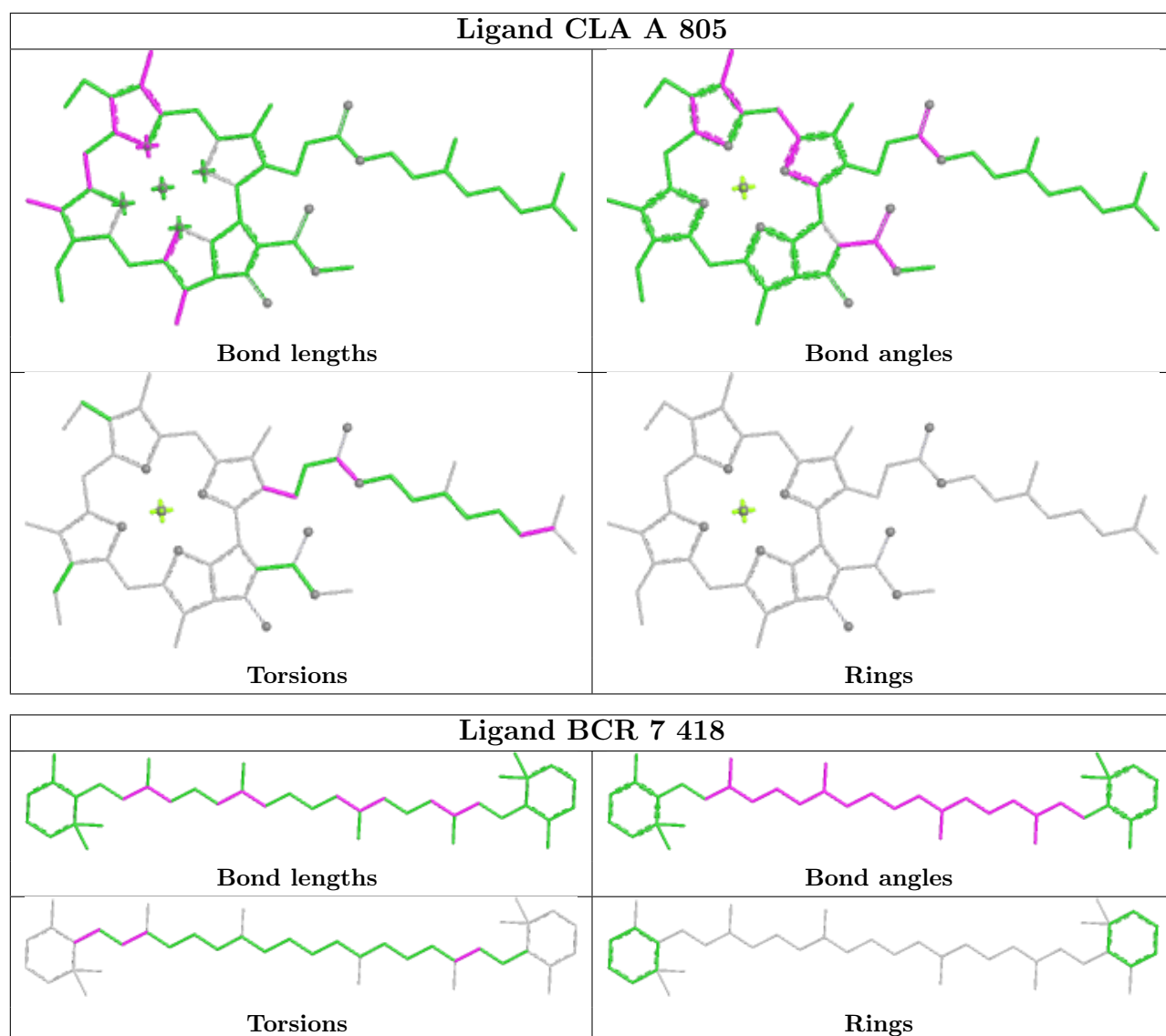
Torsions



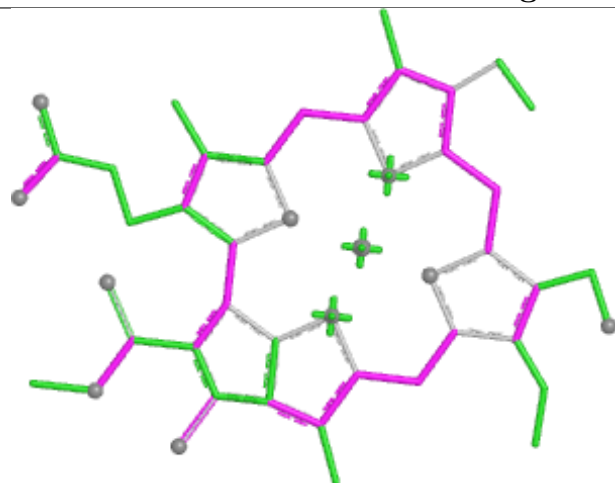
Rings

Ligand CLA A 820

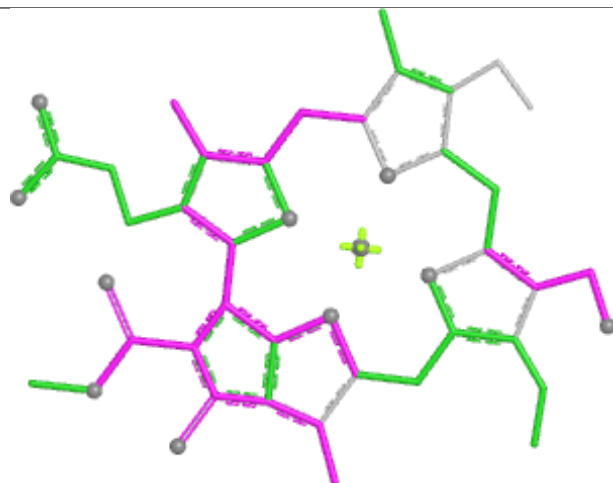




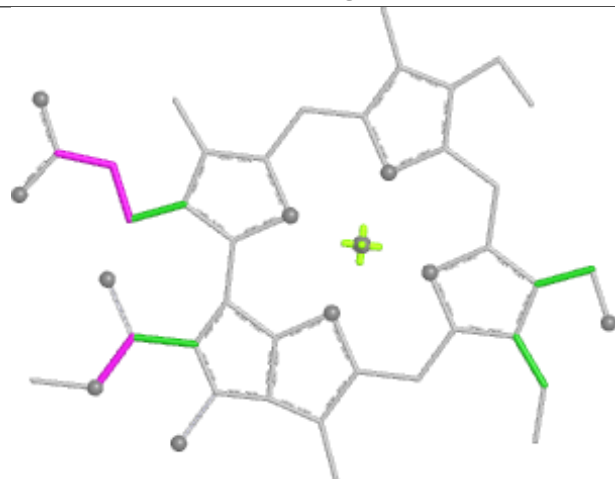
Ligand CHL 4 606



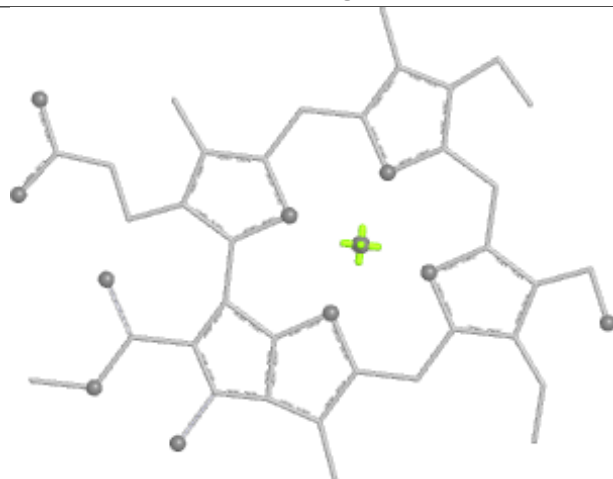
Bond lengths



Bond angles

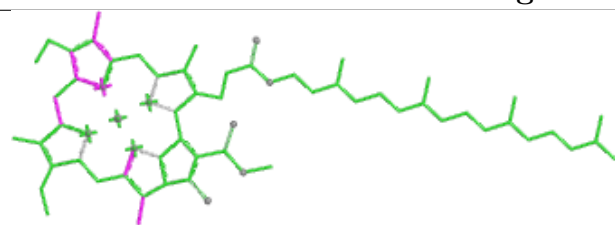


Torsions

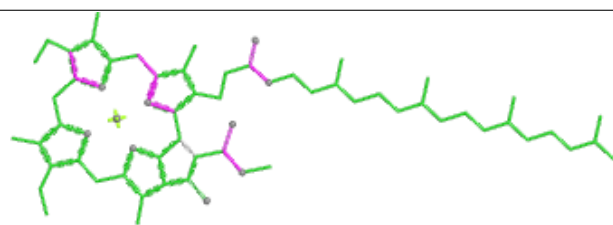


Rings

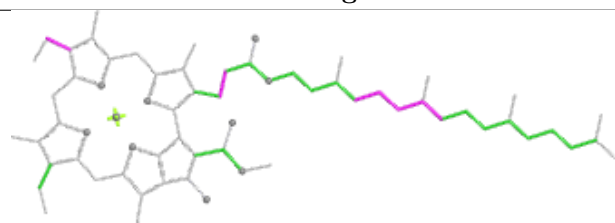
Ligand CLA B 838



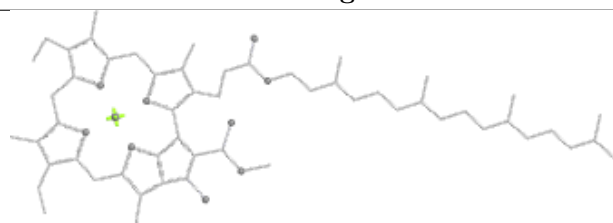
Bond lengths



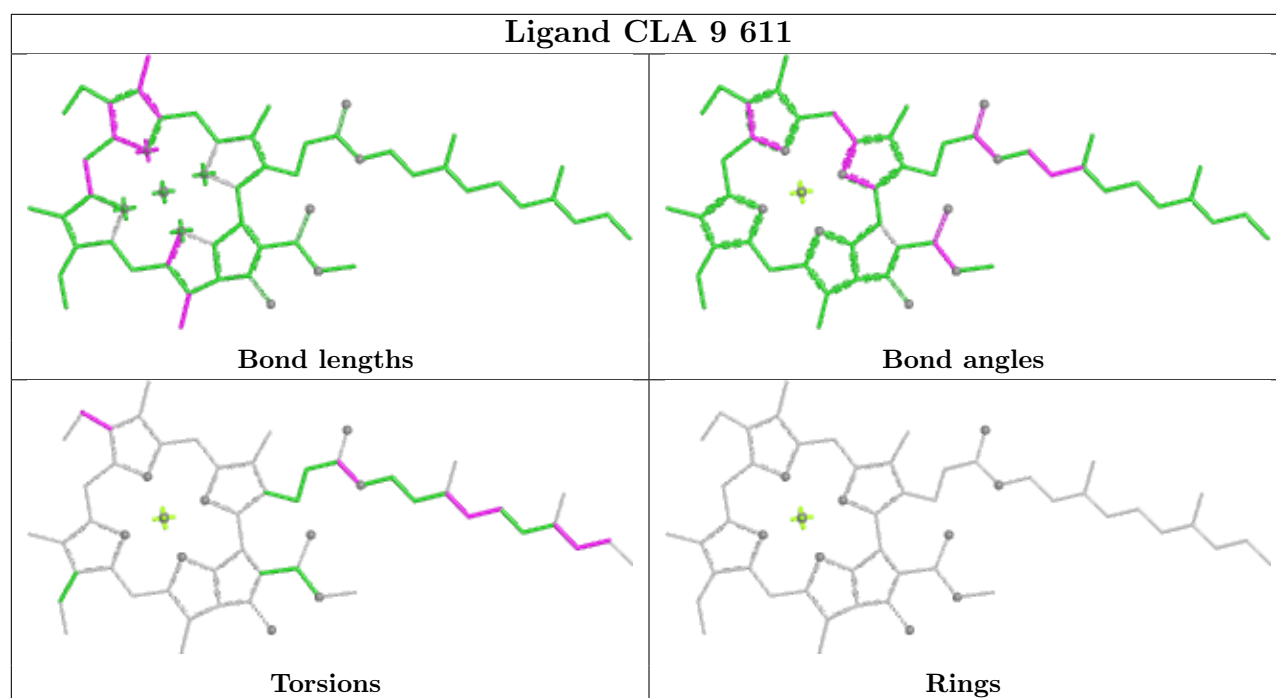
Bond angles



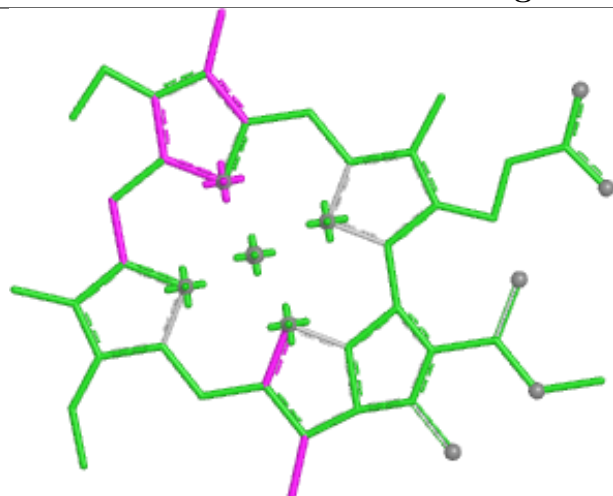
Torsions



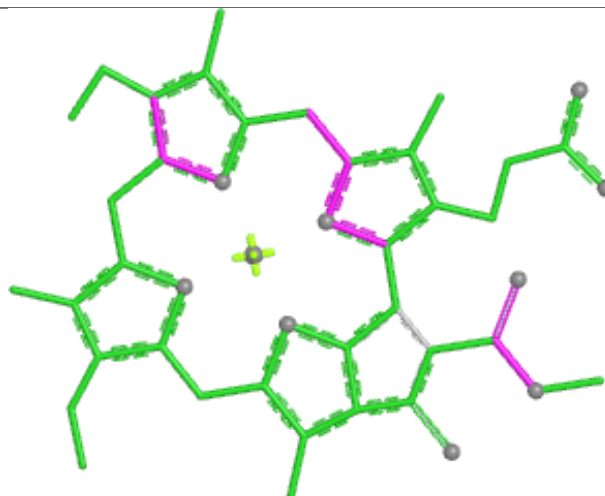
Rings



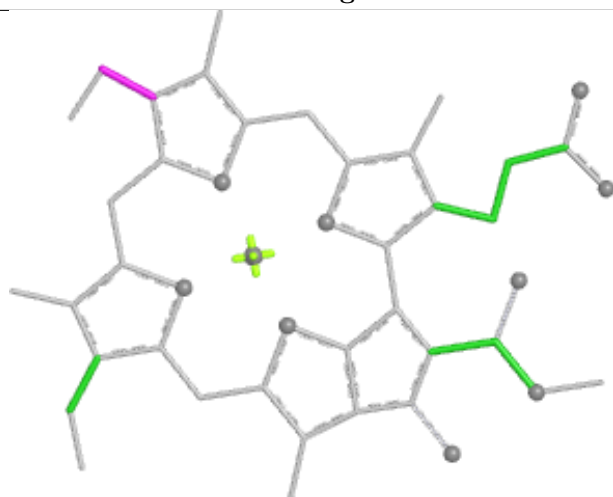
Ligand CLA B 833



Bond lengths



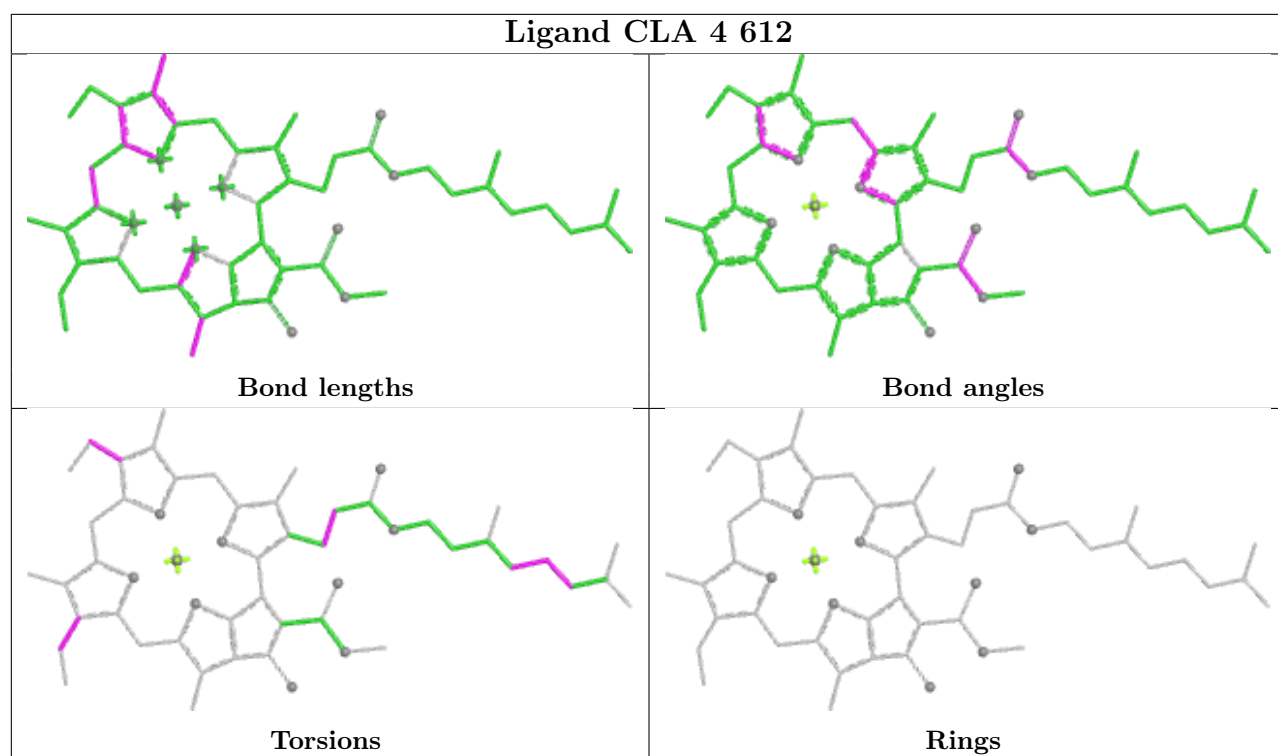
Bond angles



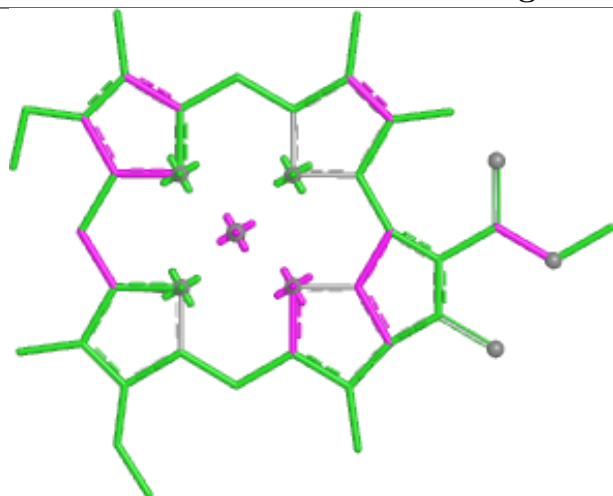
Torsions



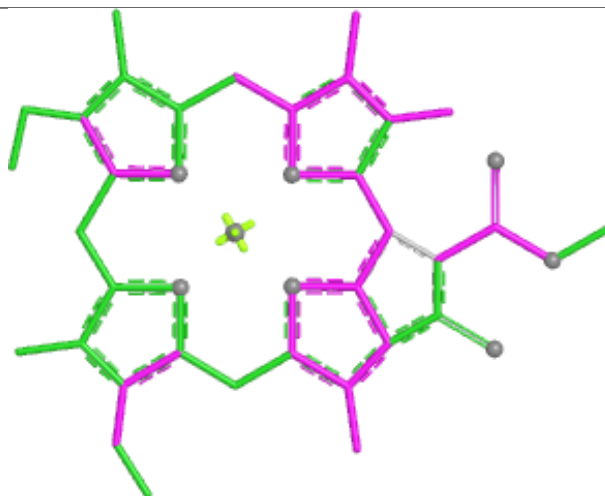
Rings



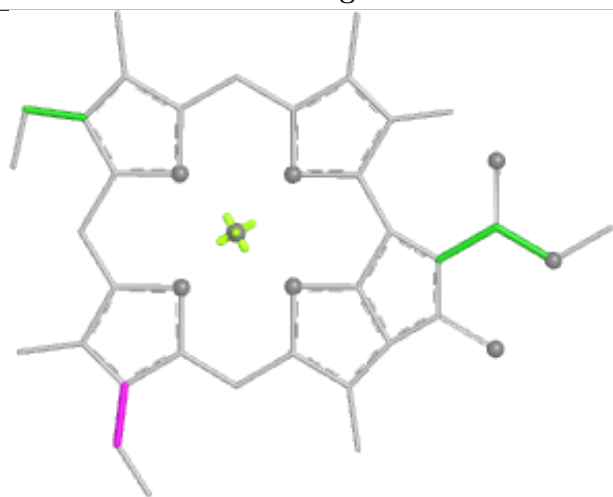
Ligand CLA 1 309



Bond lengths



Bond angles

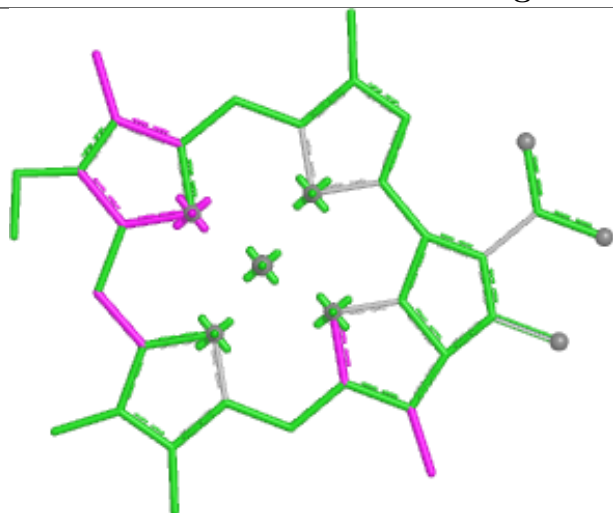


Torsions

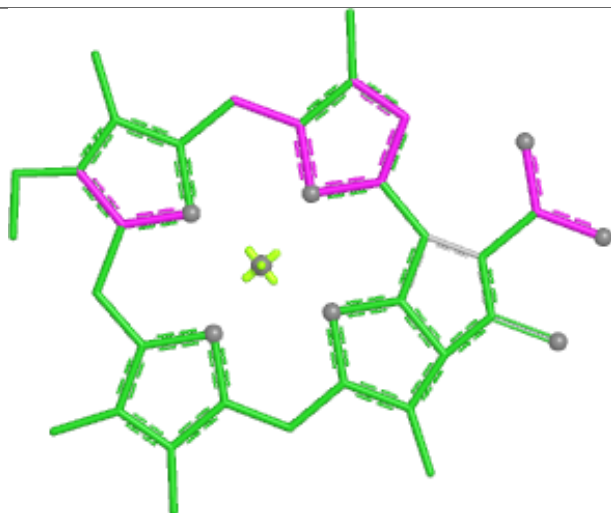


Rings

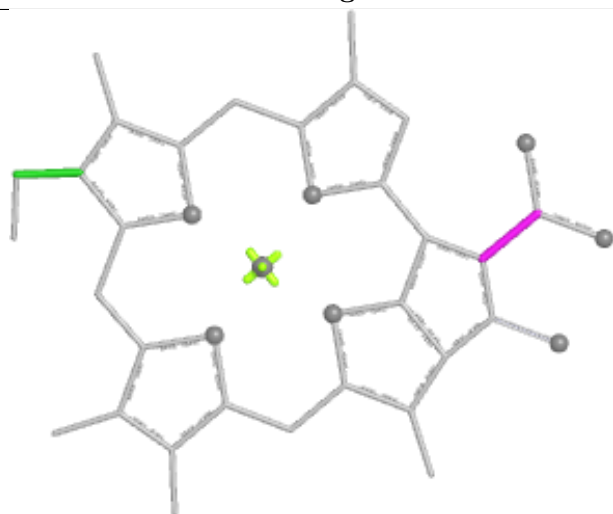
Ligand CLA O 202



Bond lengths



Bond angles

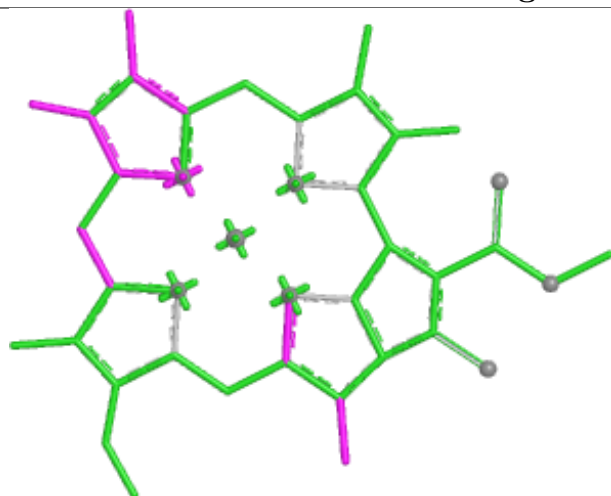


Torsions

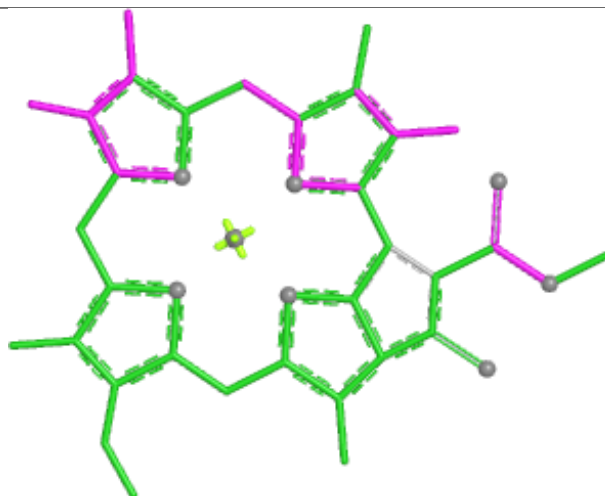


Rings

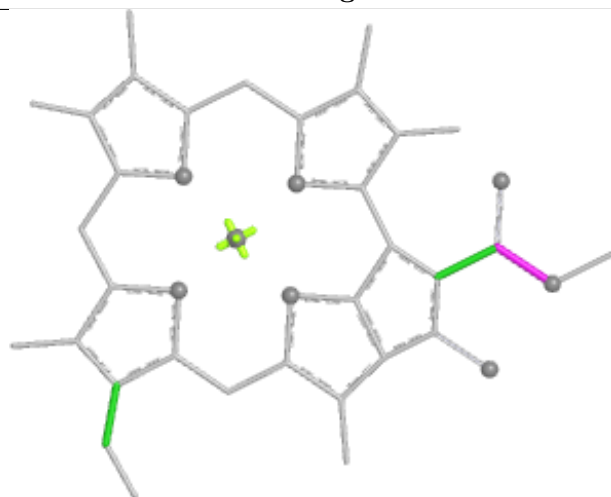
Ligand CLA 5 608



Bond lengths



Bond angles

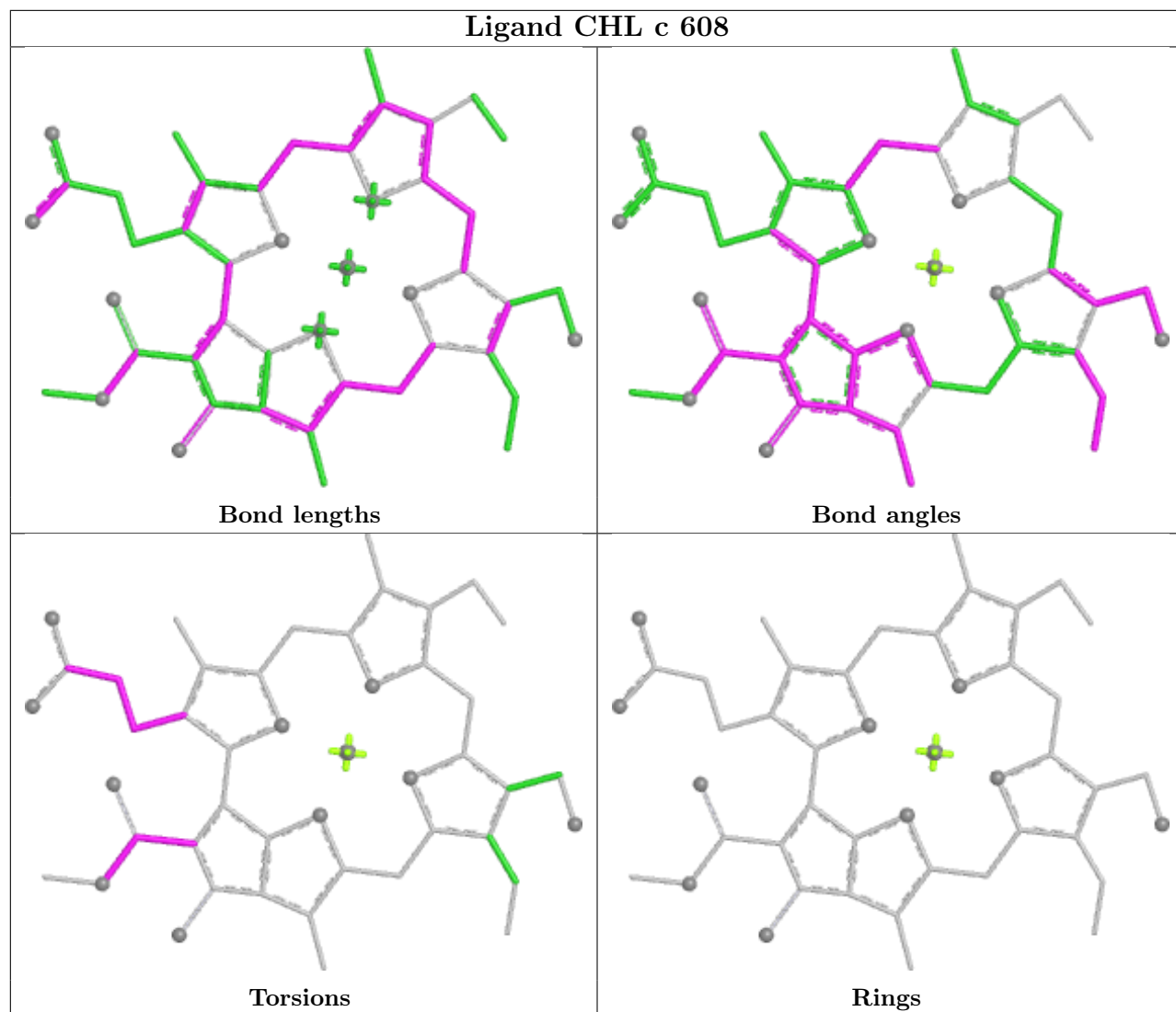


Torsions

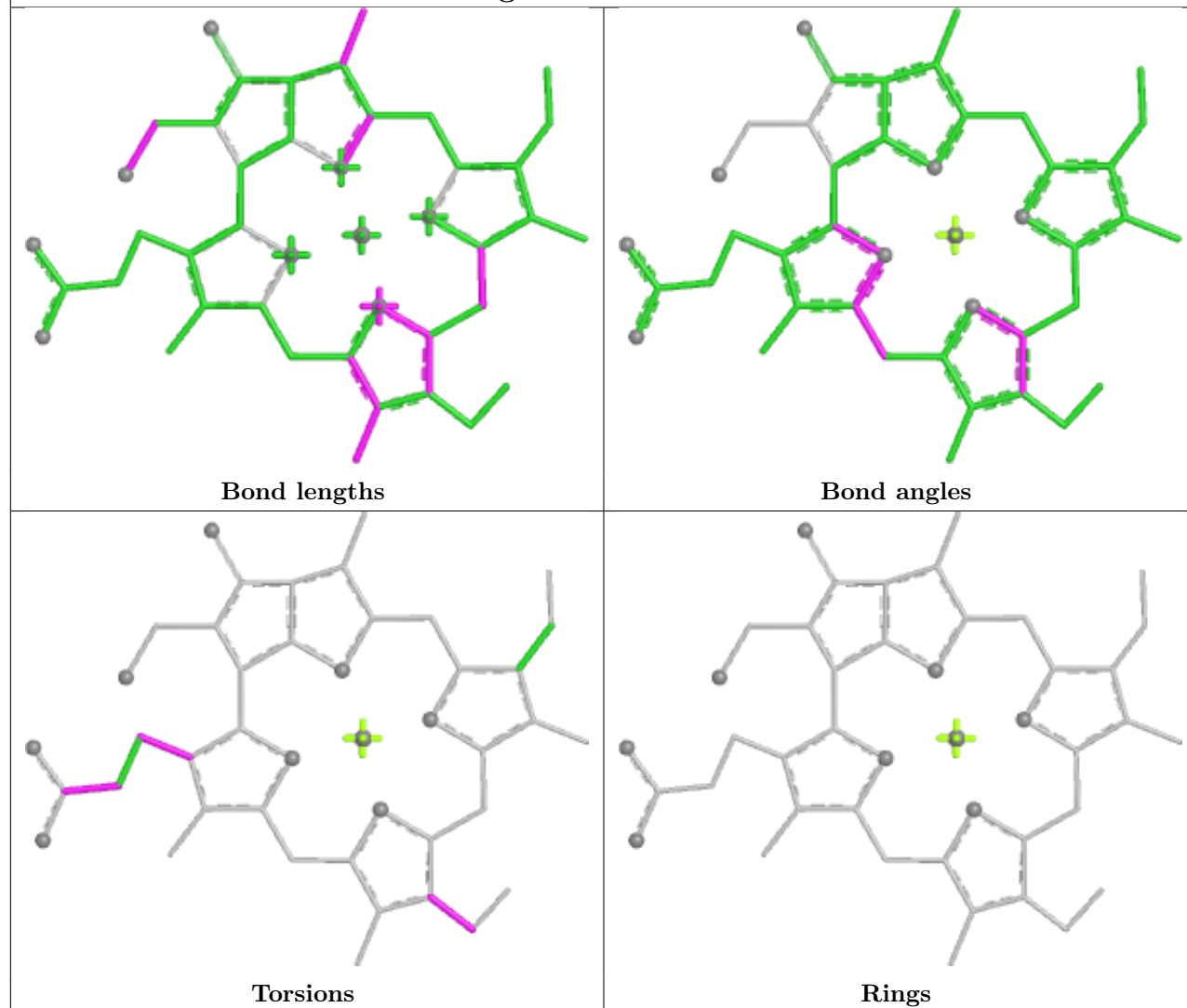


Rings

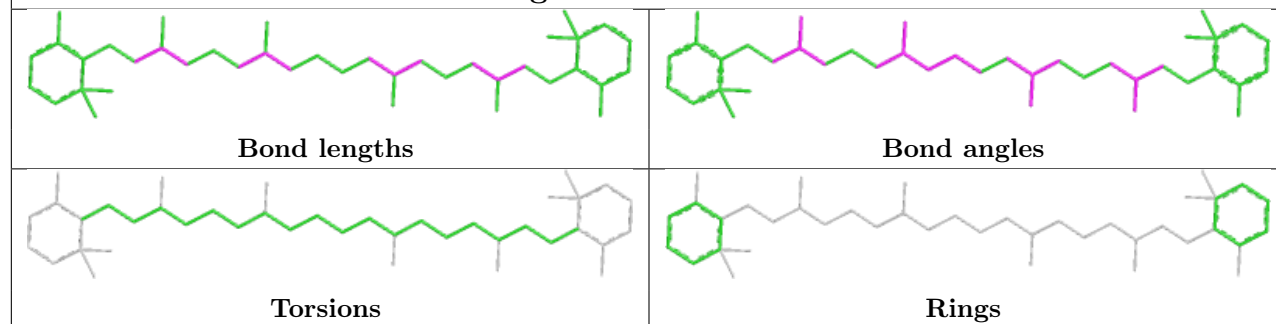
Ligand CHL c 608



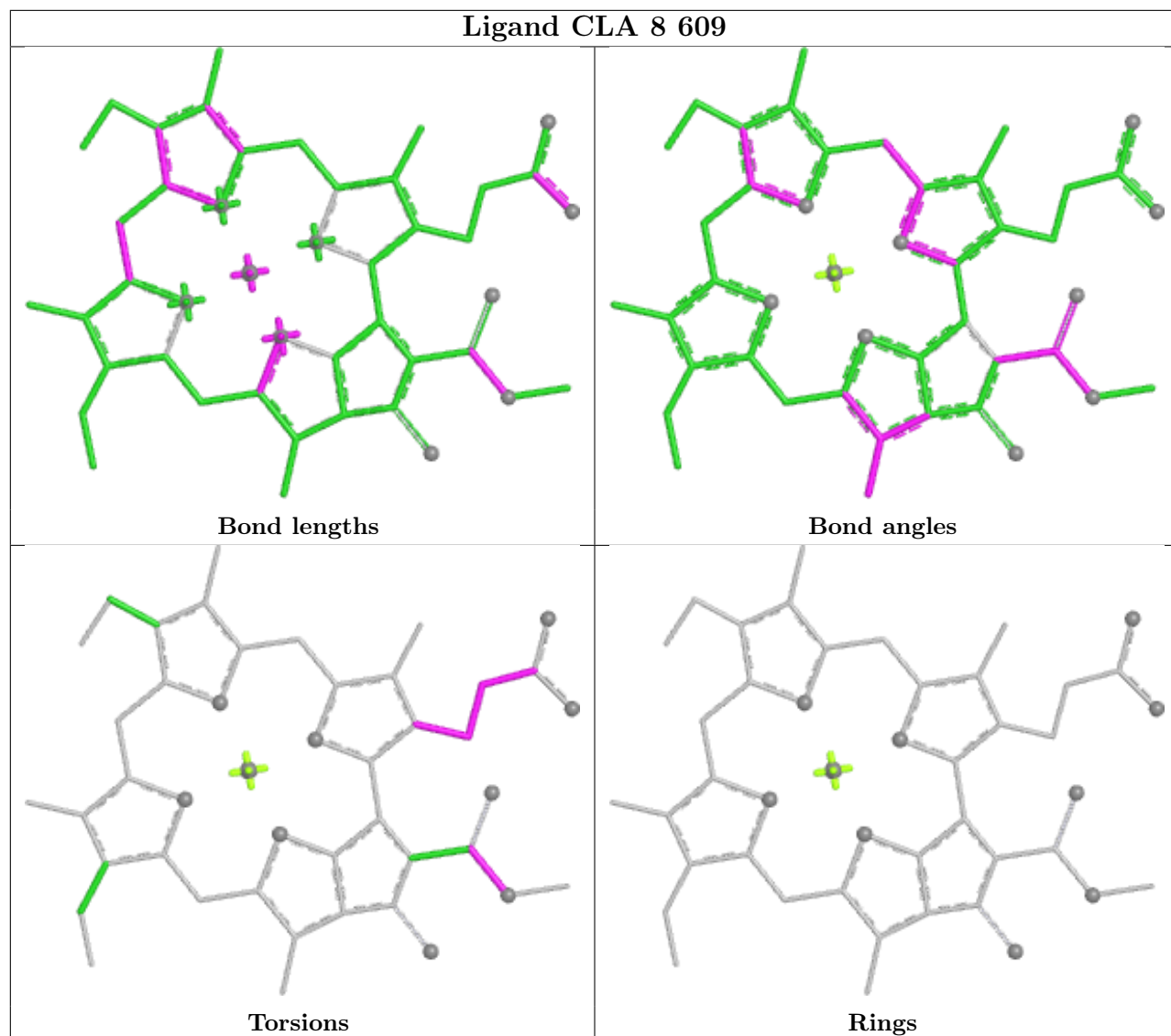
Ligand CLA 8 608

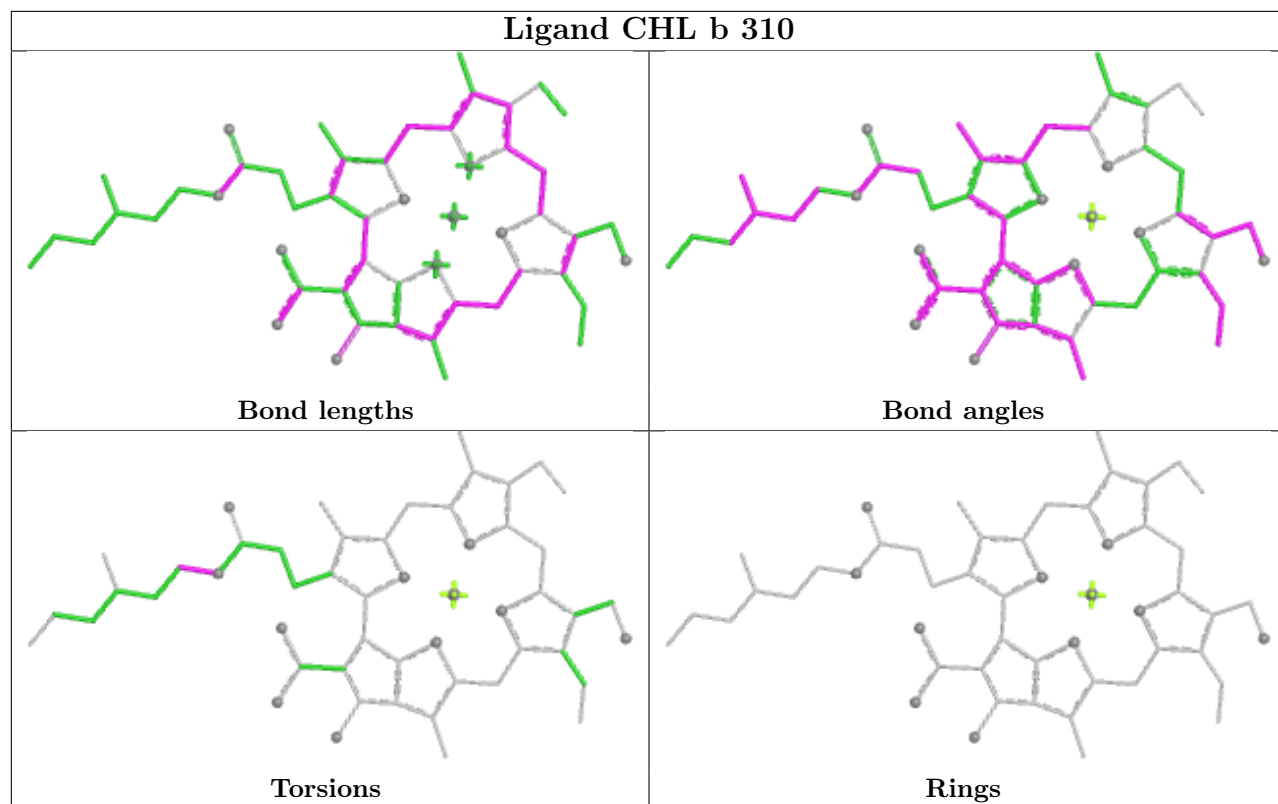


Ligand BCR A 847

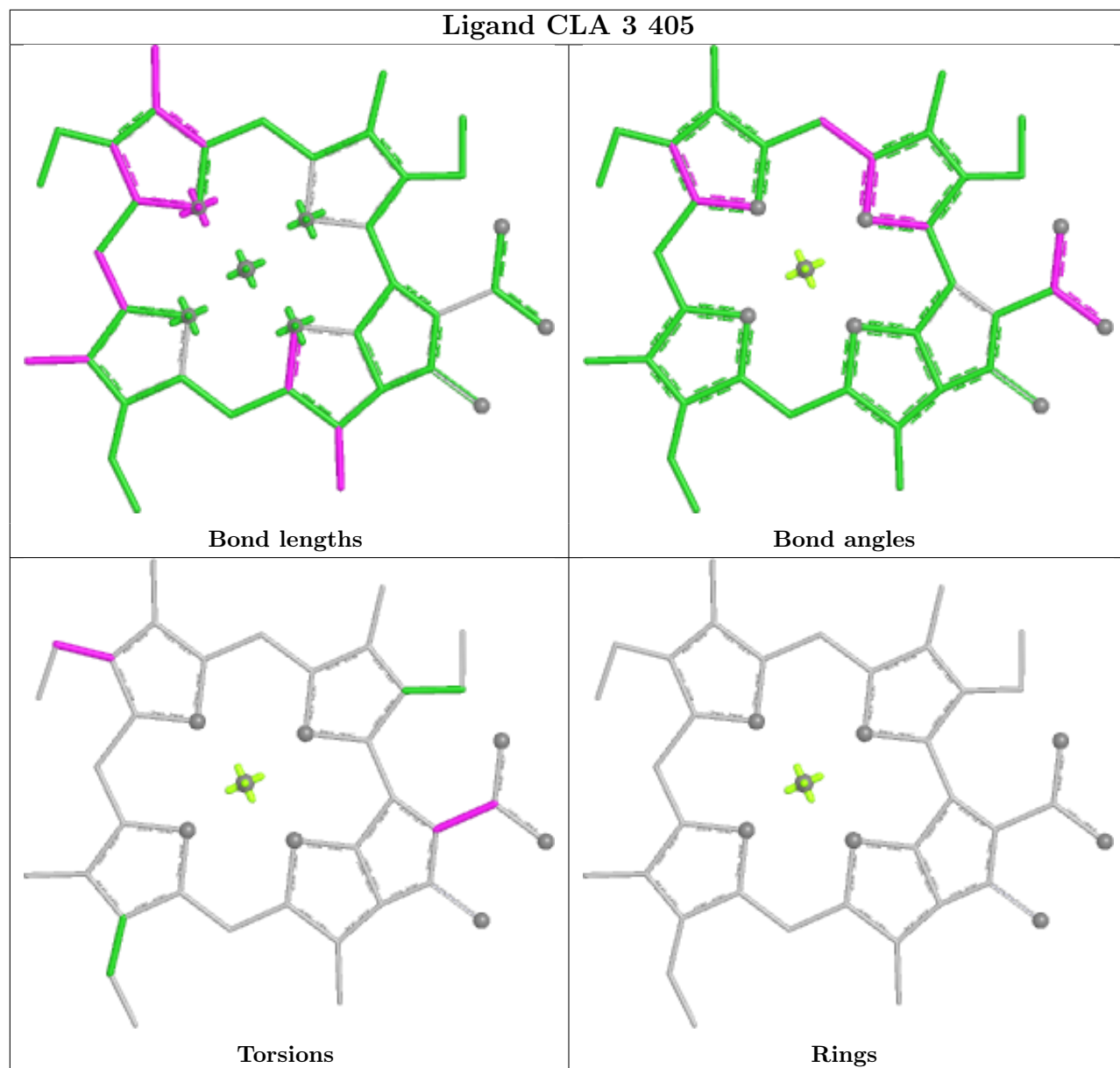


Ligand CLA 8 609

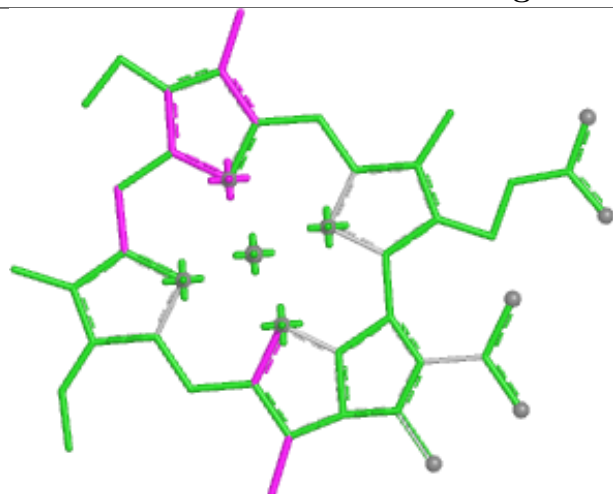




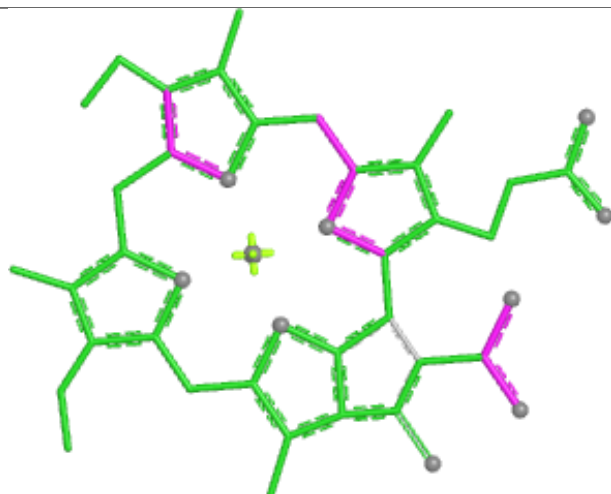
Ligand CLA 3 405



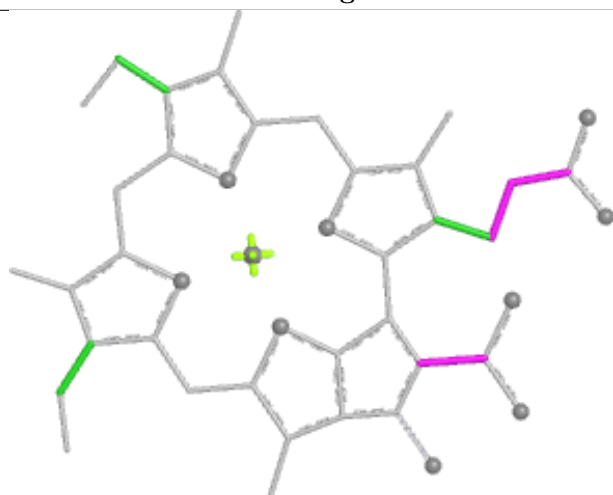
Ligand CLA G 204



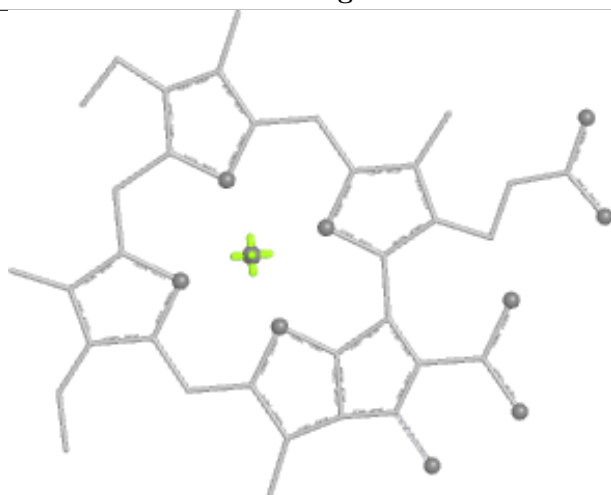
Bond lengths



Bond angles

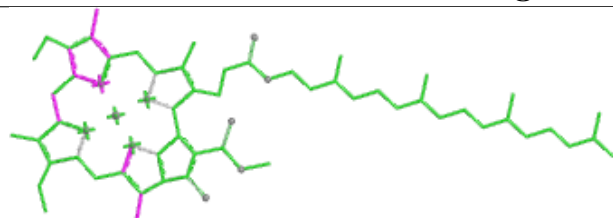


Torsions

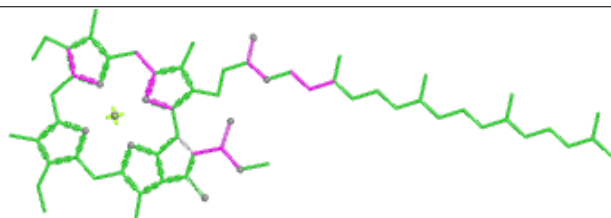


Rings

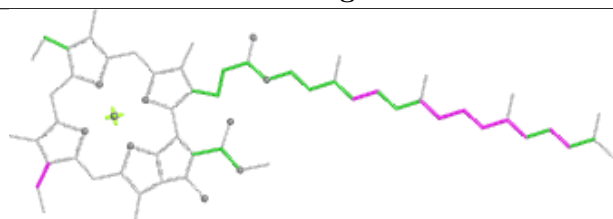
Ligand CLA B 823



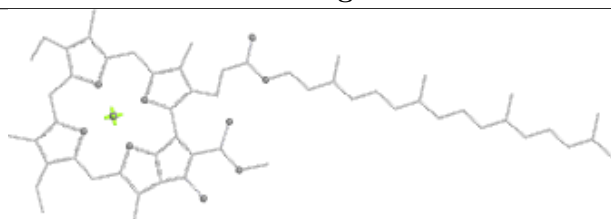
Bond lengths



Bond angles

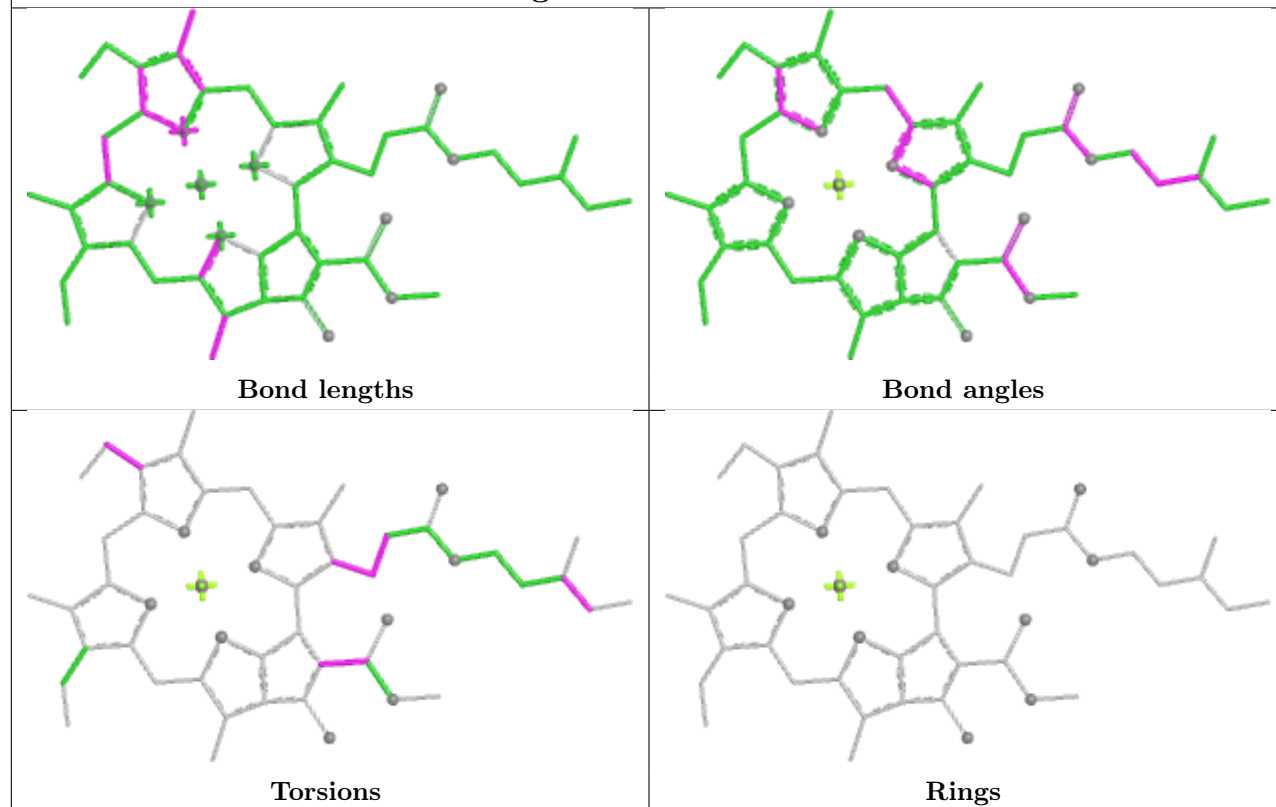


Torsions

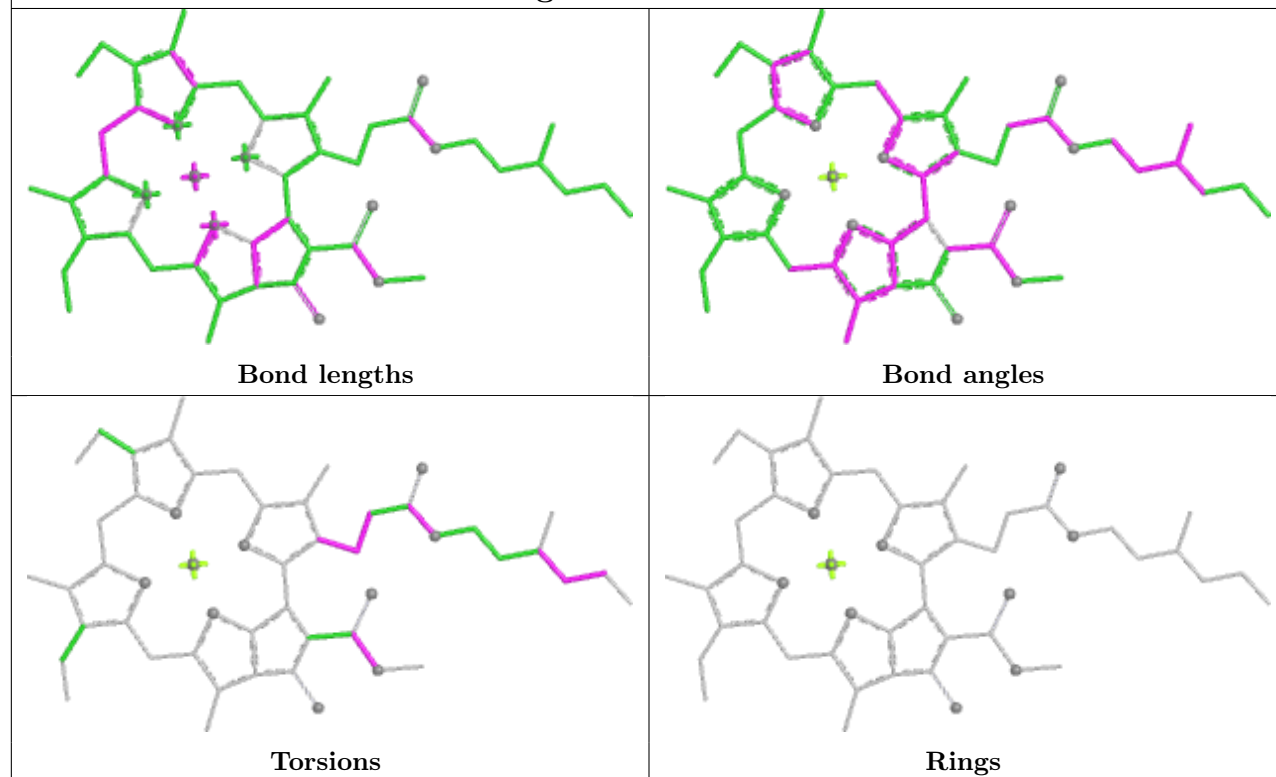


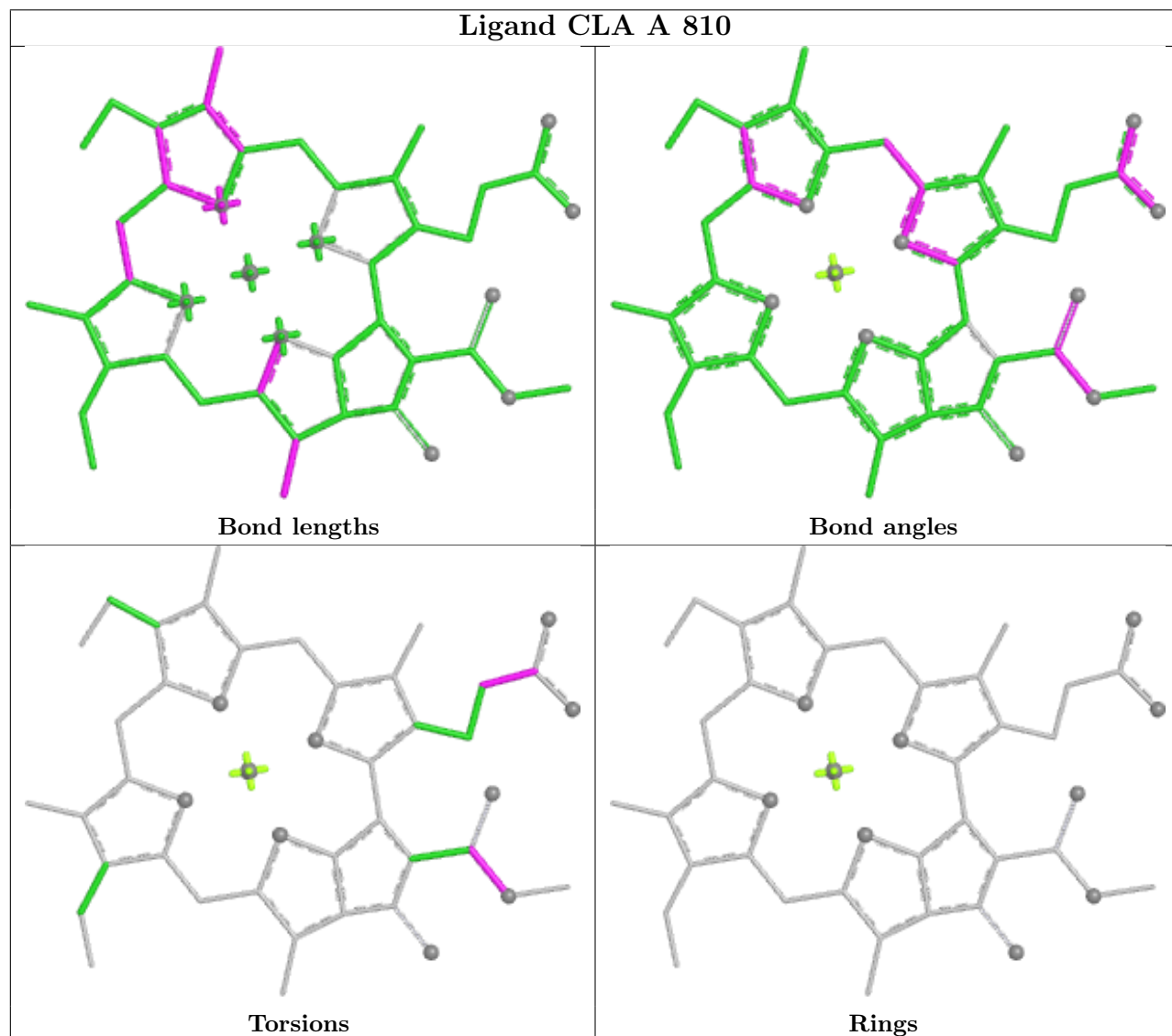
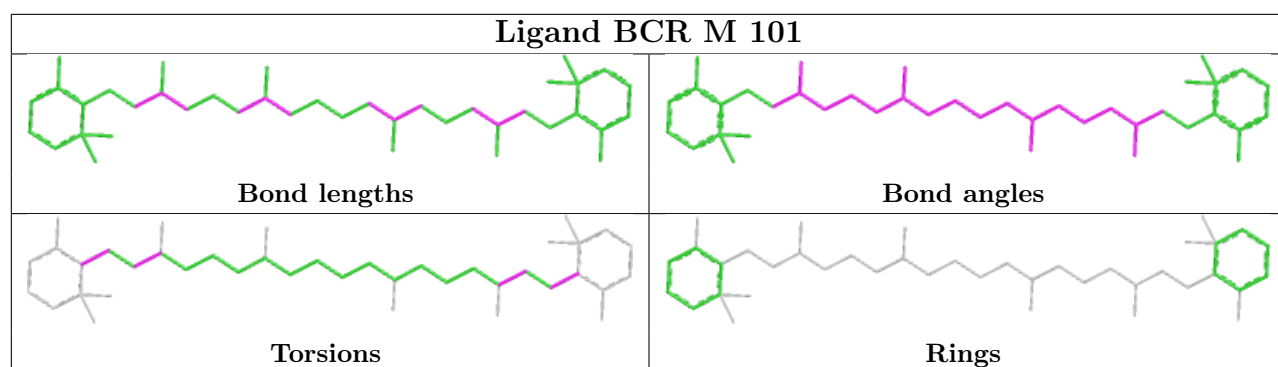
Rings

Ligand CLA A 837

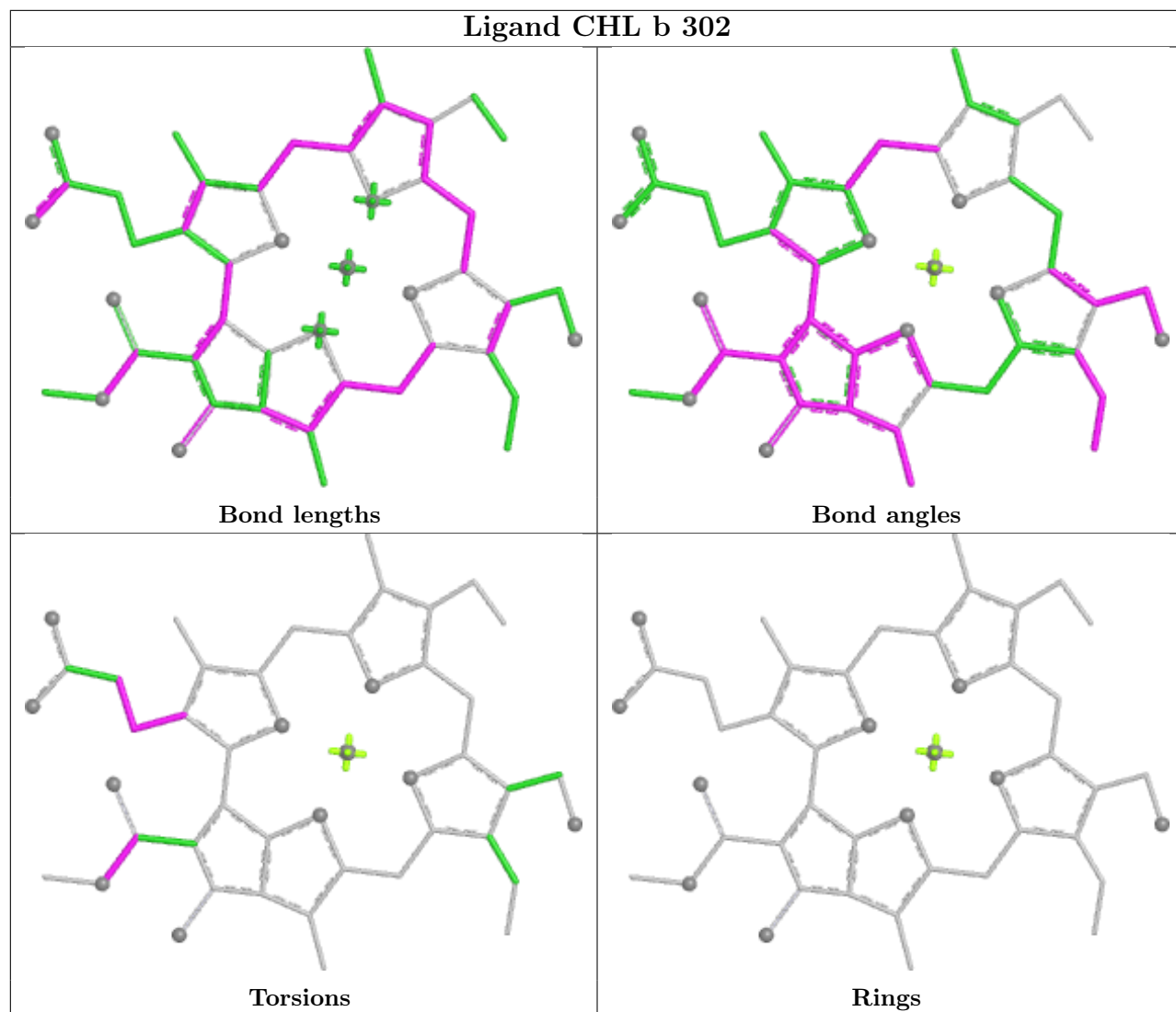


Ligand CLA 4 609

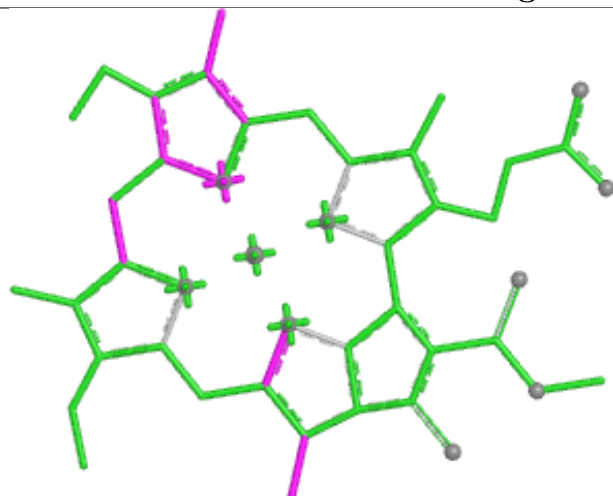




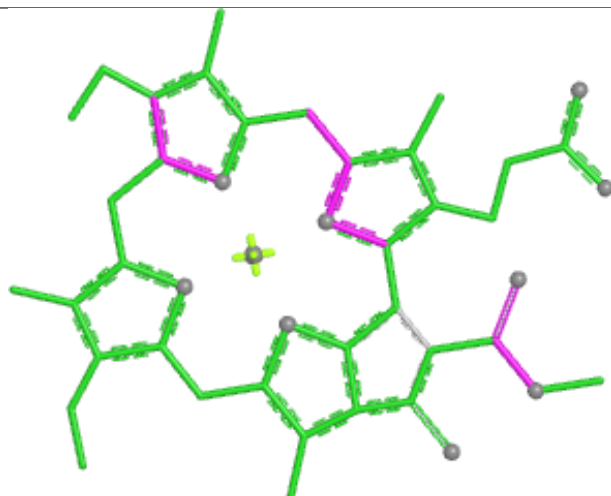
Ligand CHL b 302



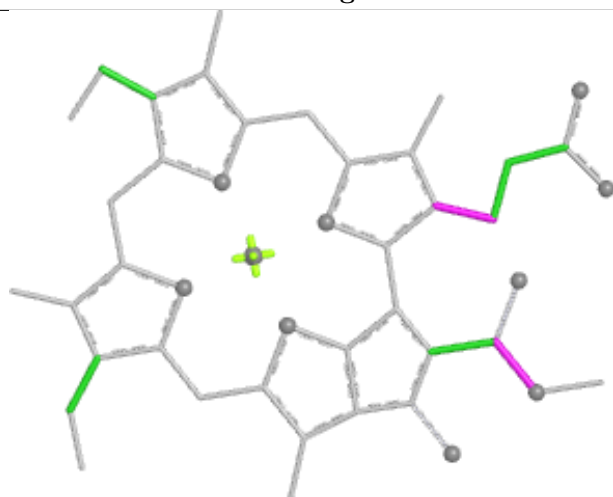
Ligand CLA 6 604



Bond lengths



Bond angles

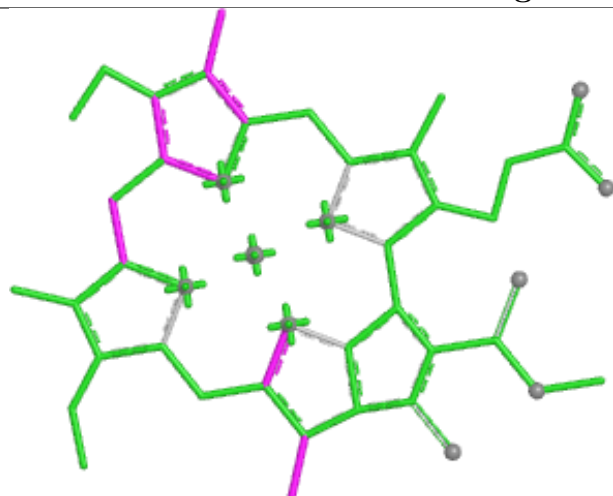


Torsions

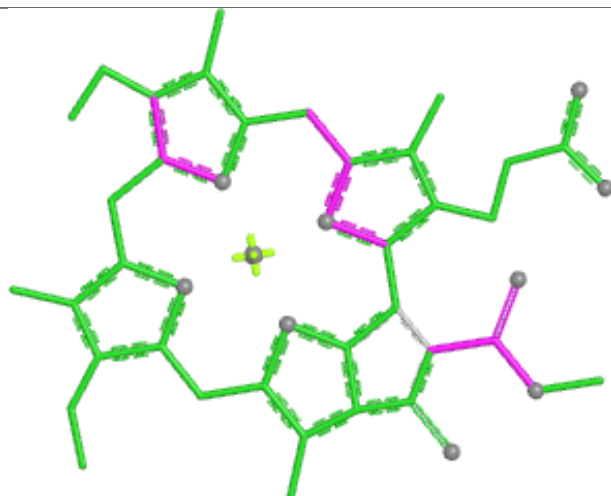


Rings

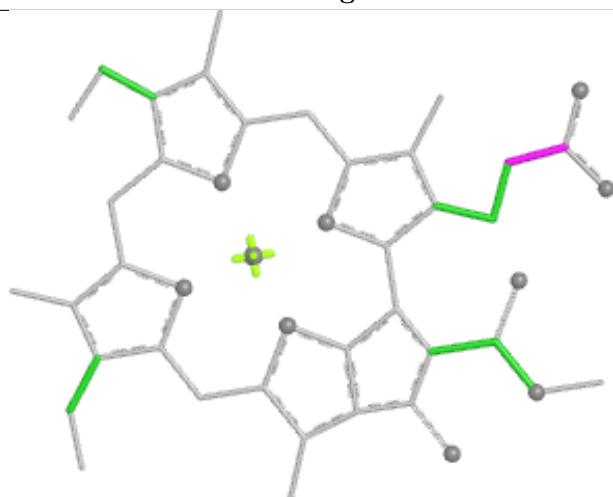
Ligand CLA B 829



Bond lengths



Bond angles

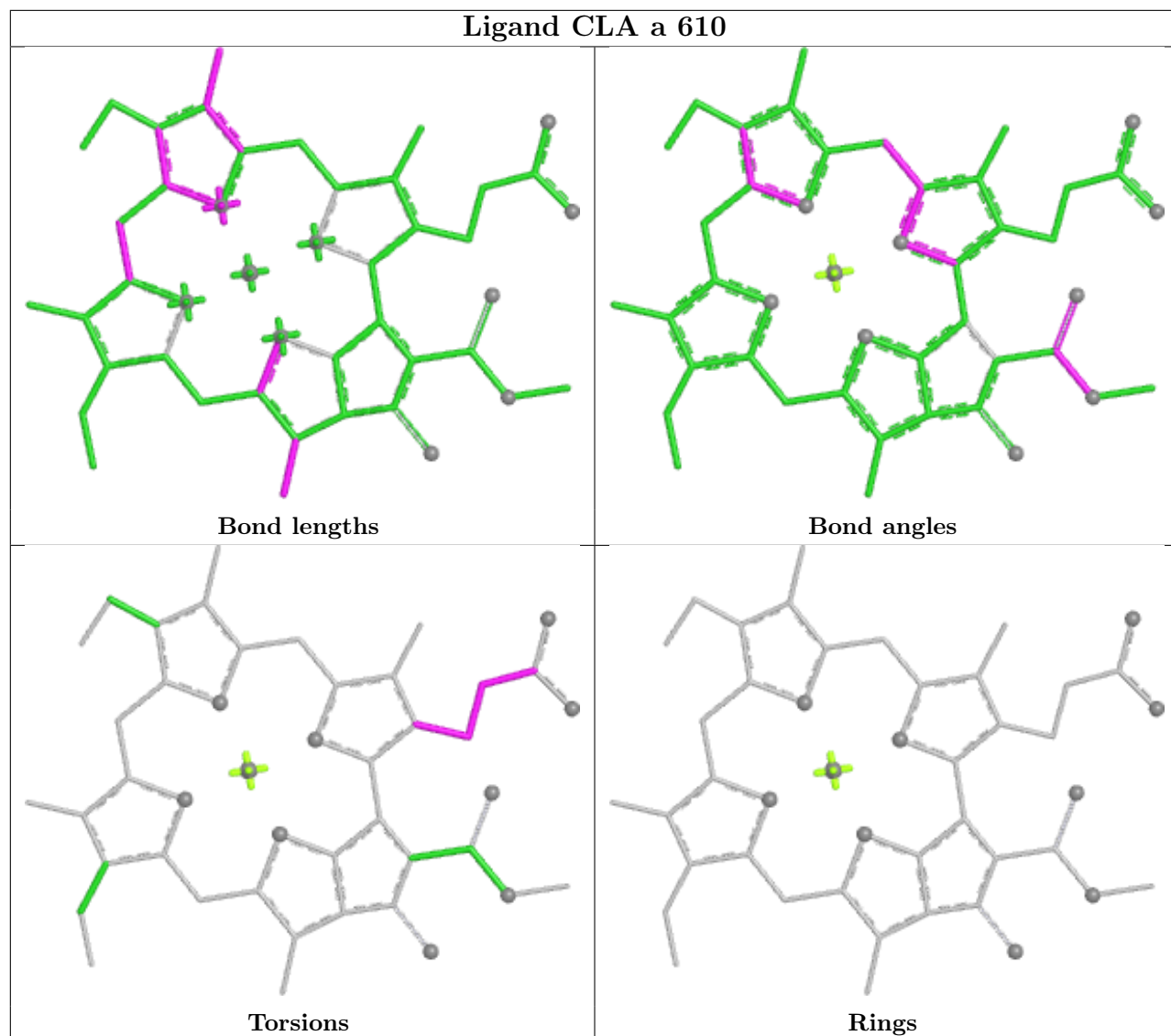


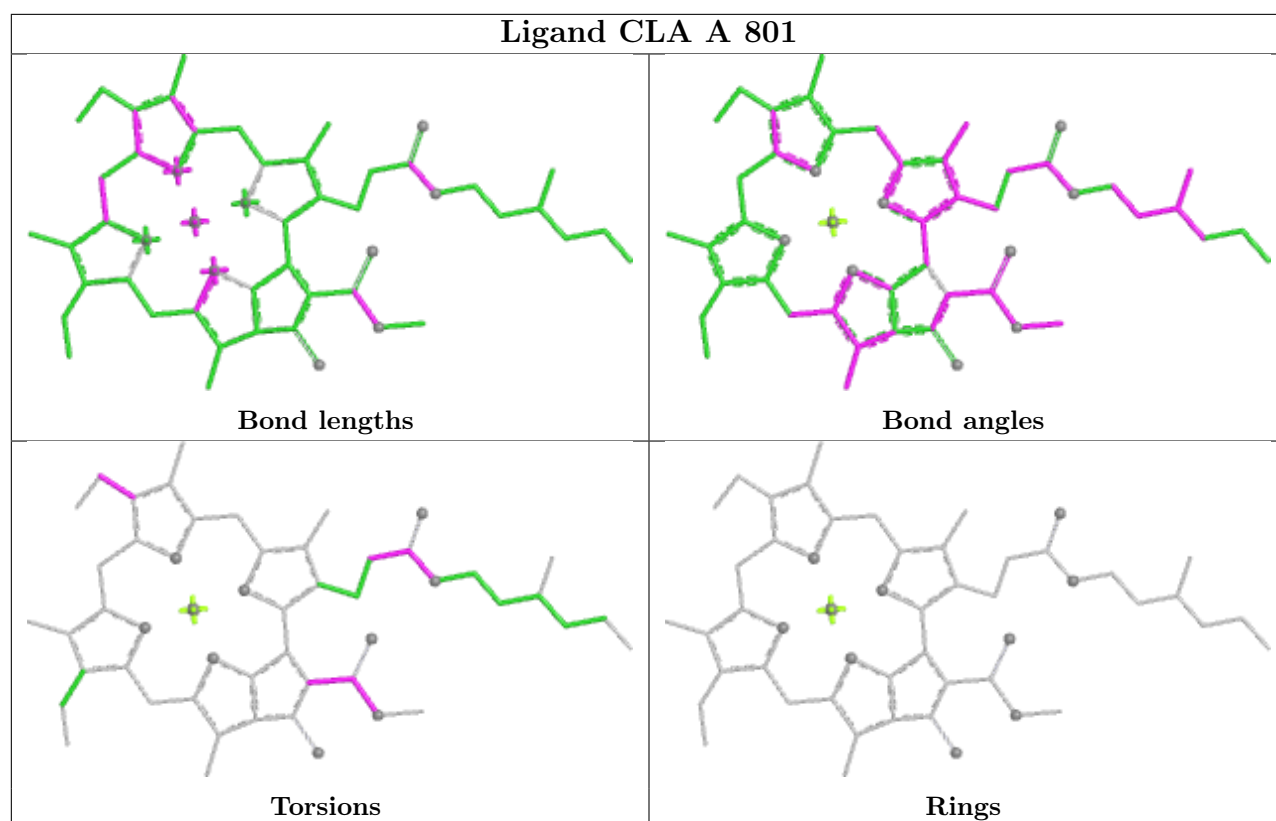
Torsions



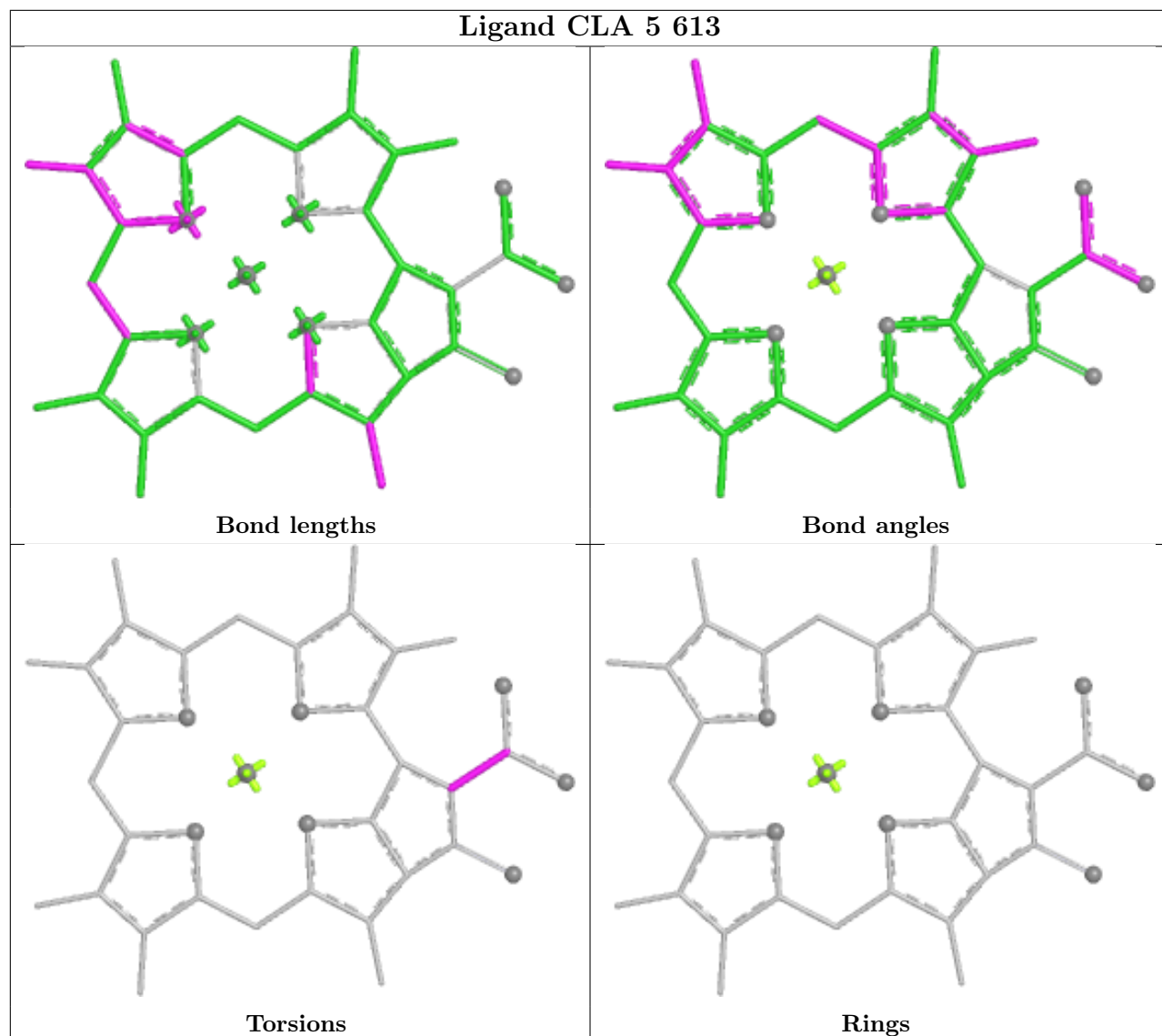
Rings

Ligand CLA a 610

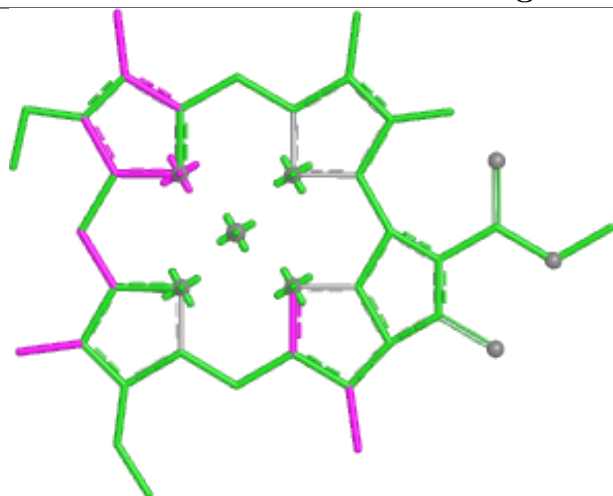




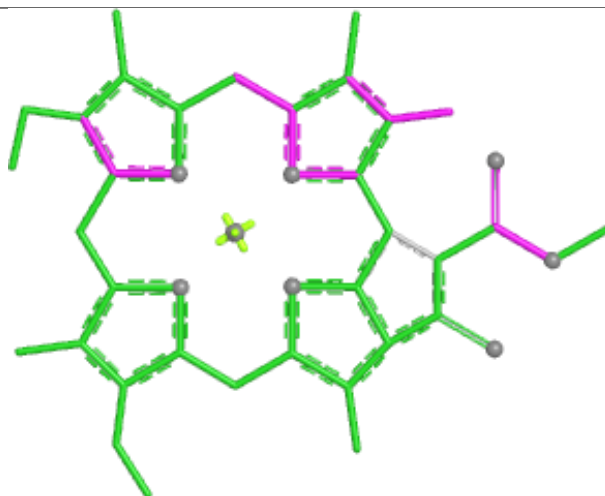
Ligand CLA 5 613



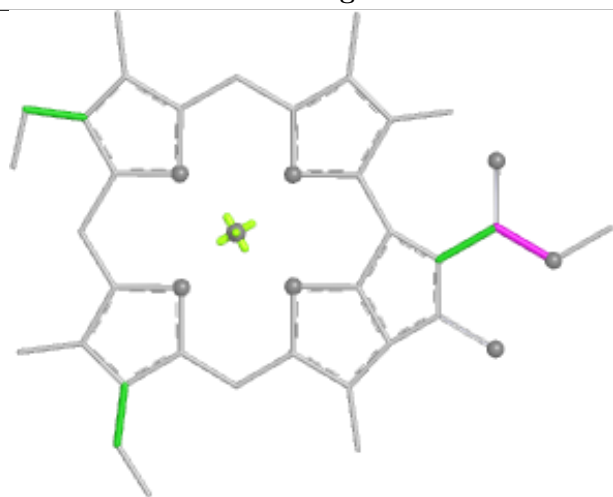
Ligand CLA F 305



Bond lengths



Bond angles

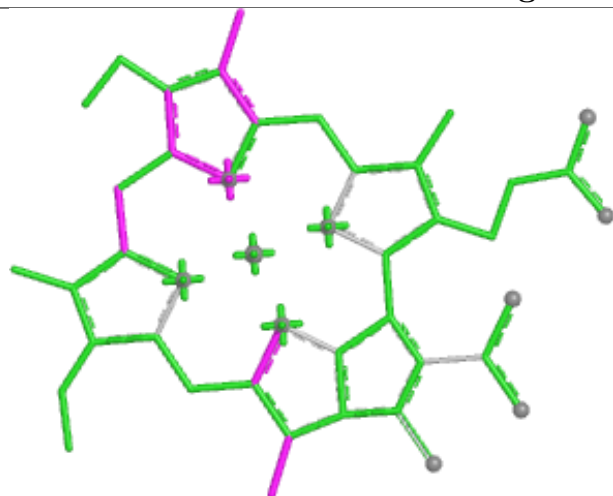


Torsions

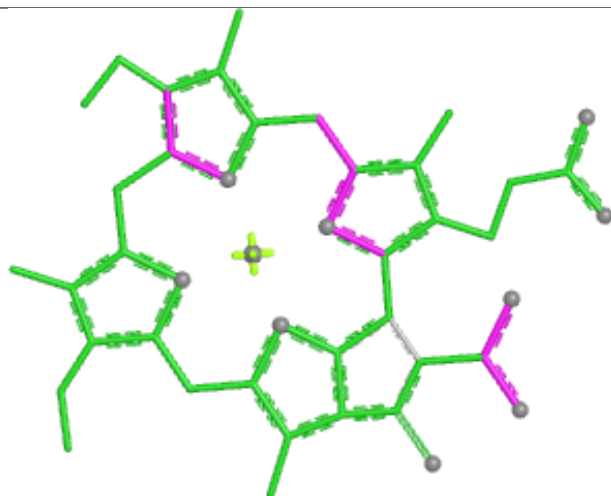


Rings

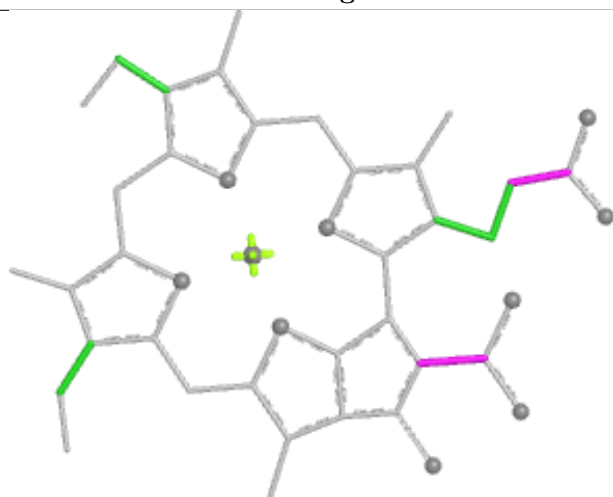
Ligand CLA 8 603



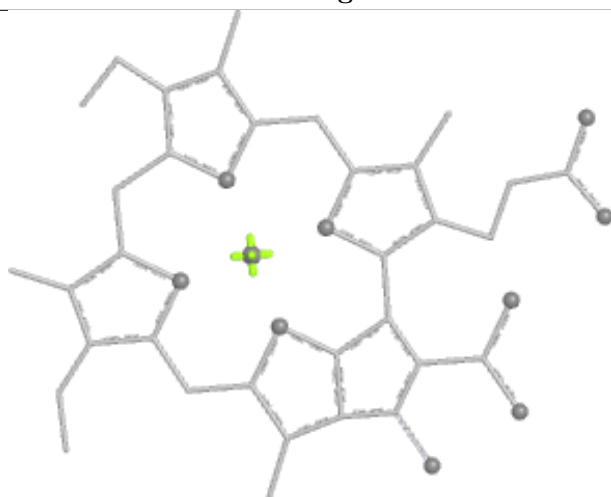
Bond lengths



Bond angles

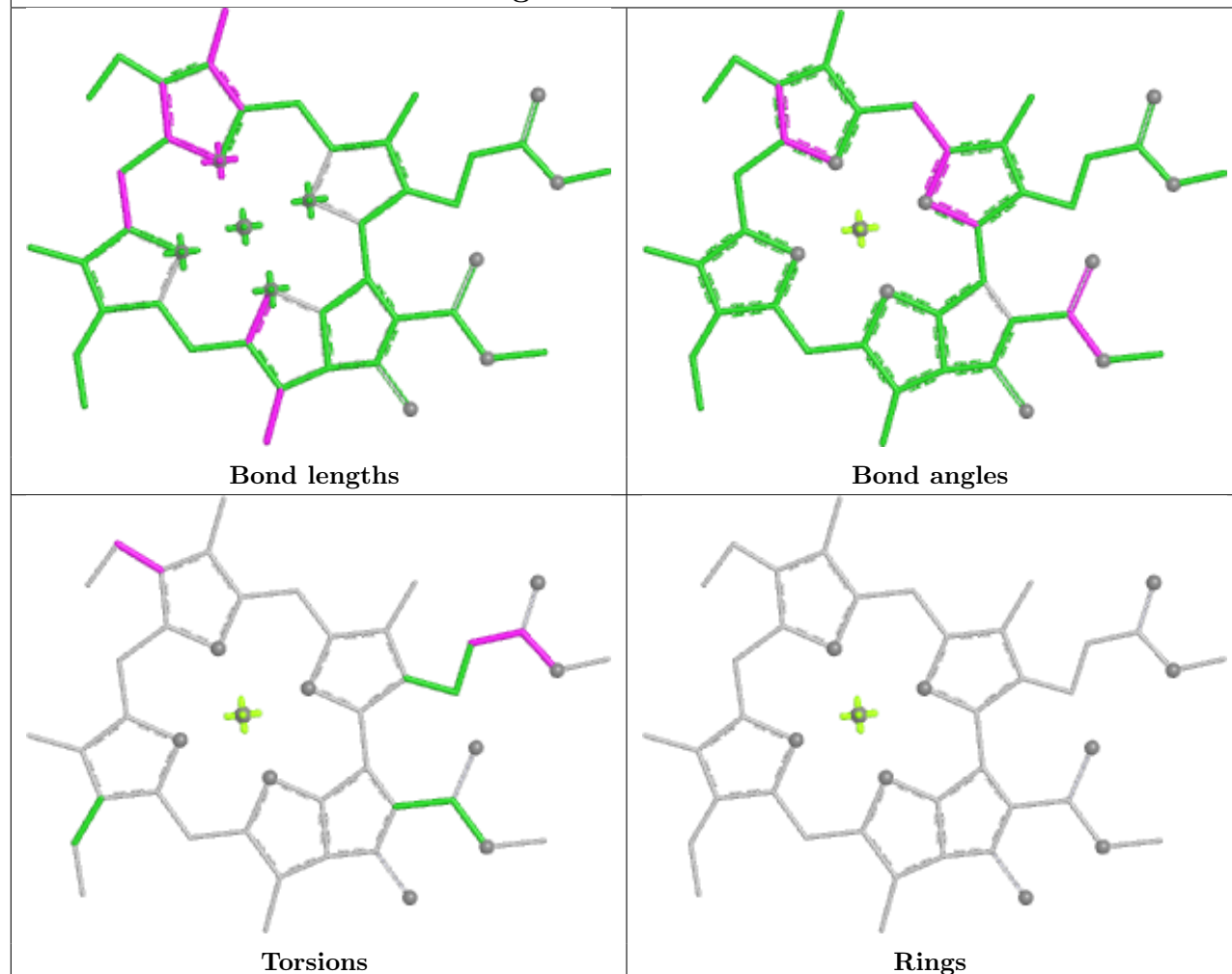


Torsions

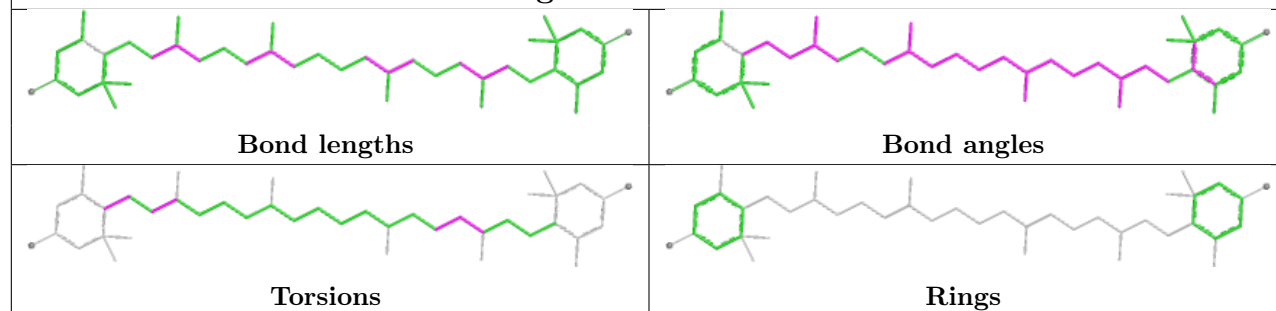


Rings

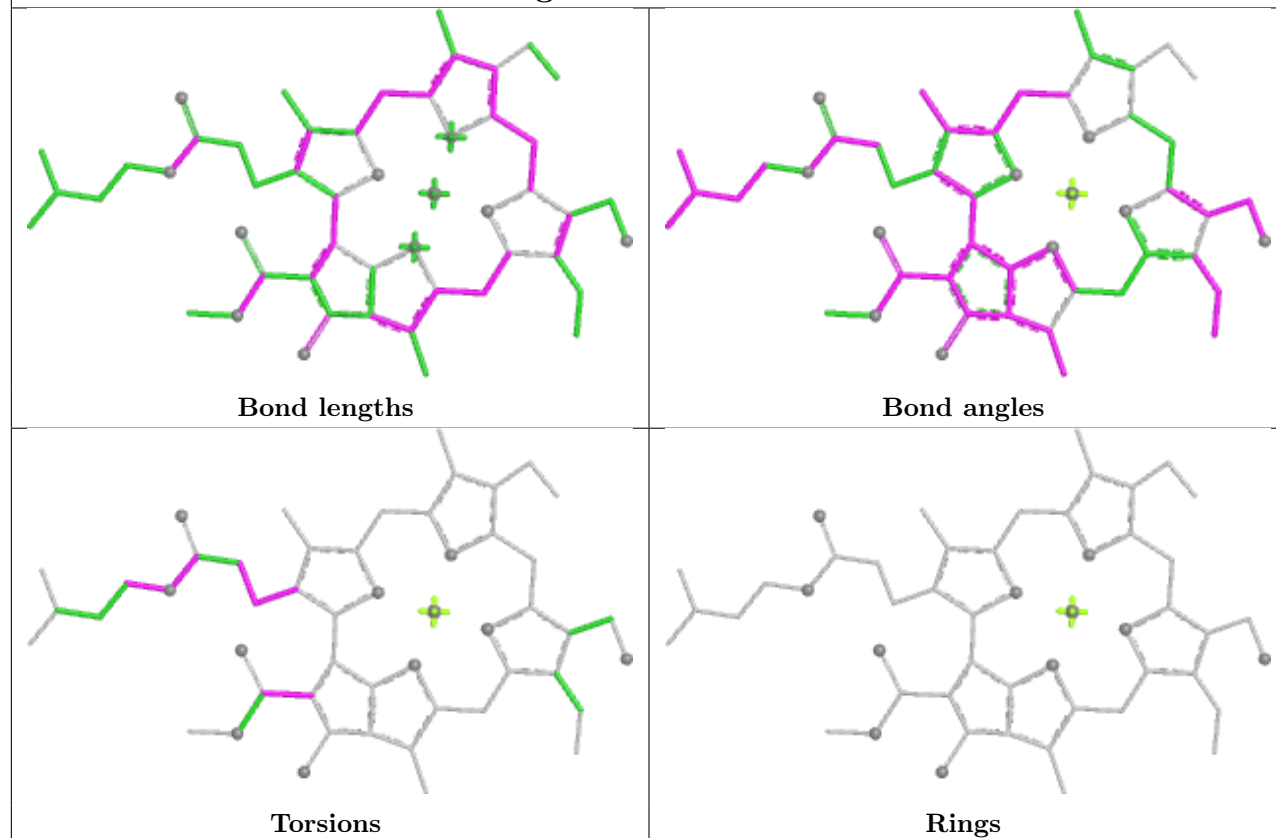
Ligand CLA K 201



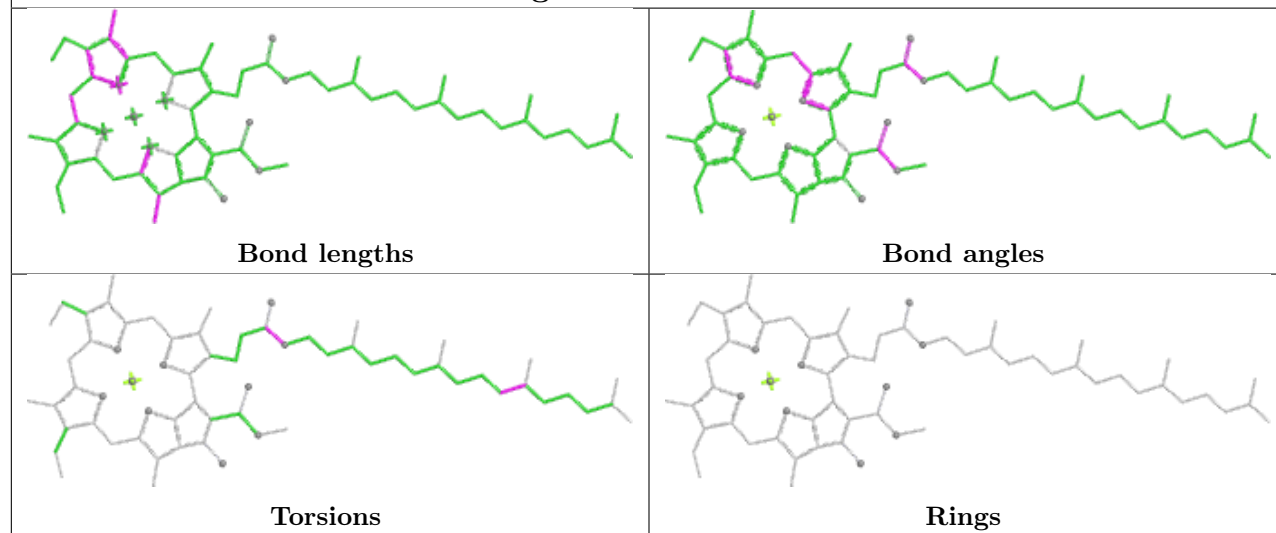
Ligand LUT 7 415

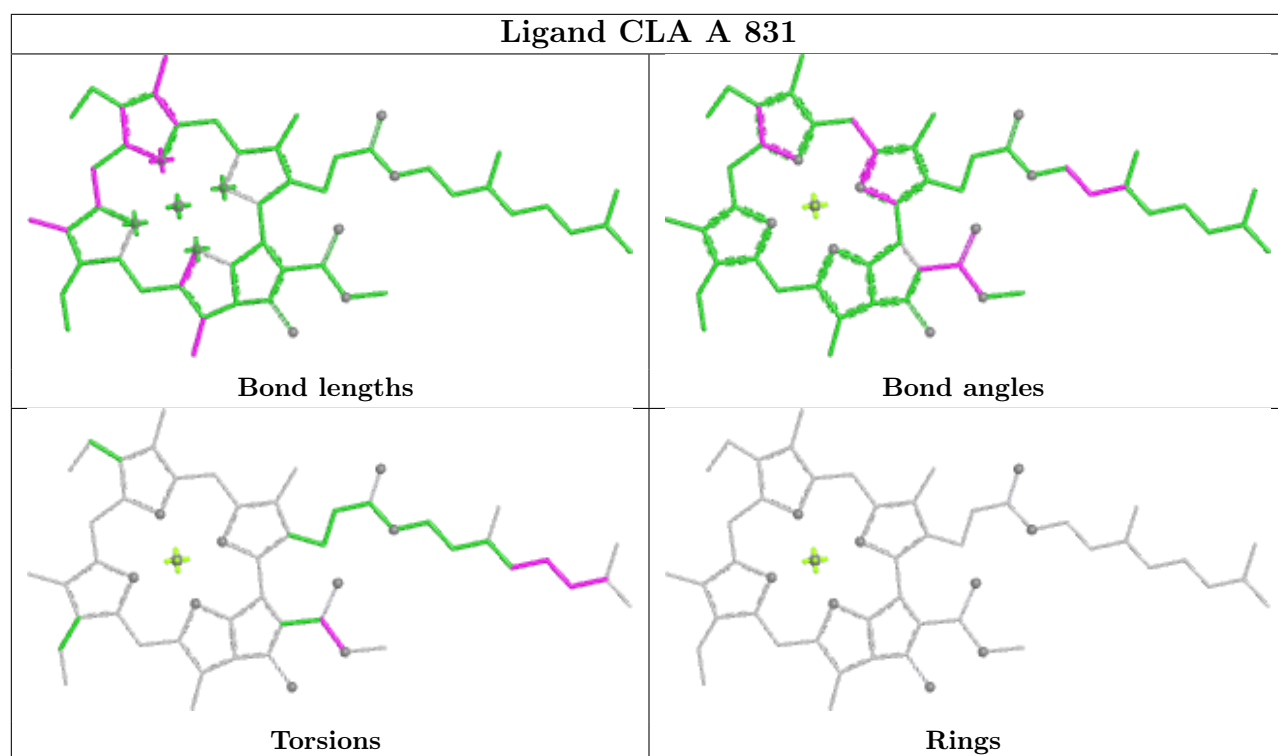


Ligand CHL 1 302

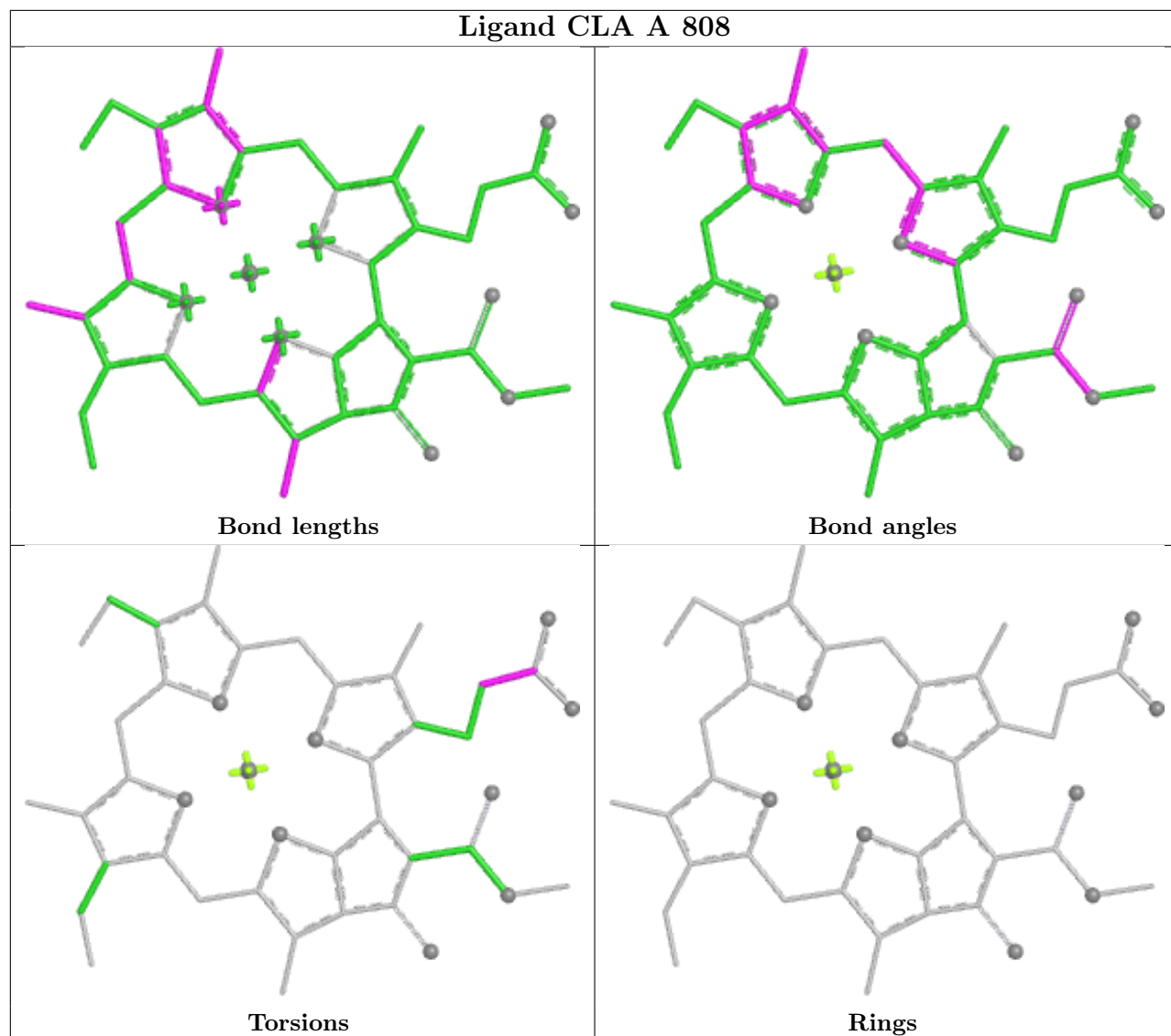


Ligand CLA A 812

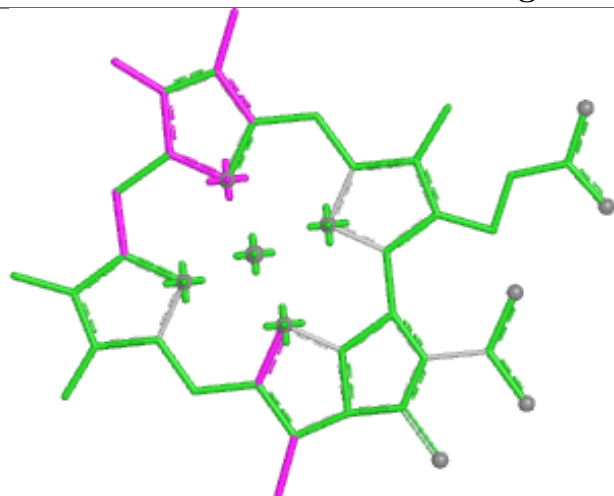




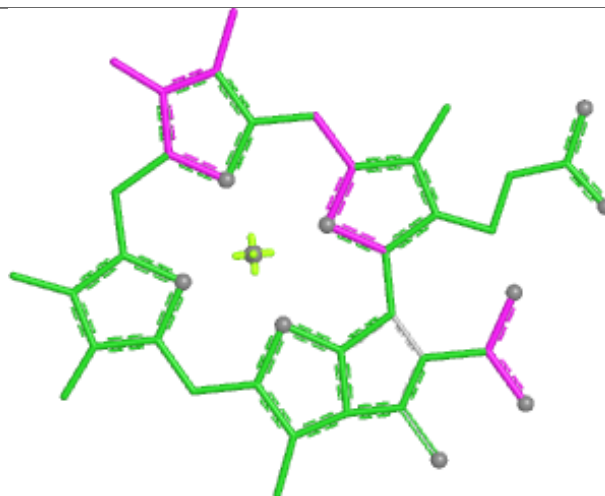
Ligand CLA A 808



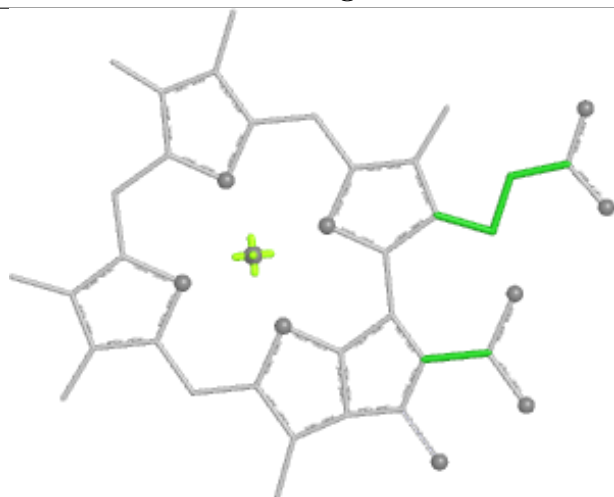
Ligand CLA 3 404



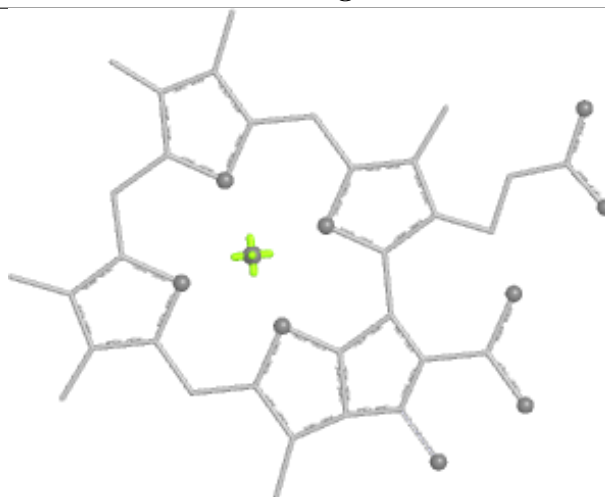
Bond lengths



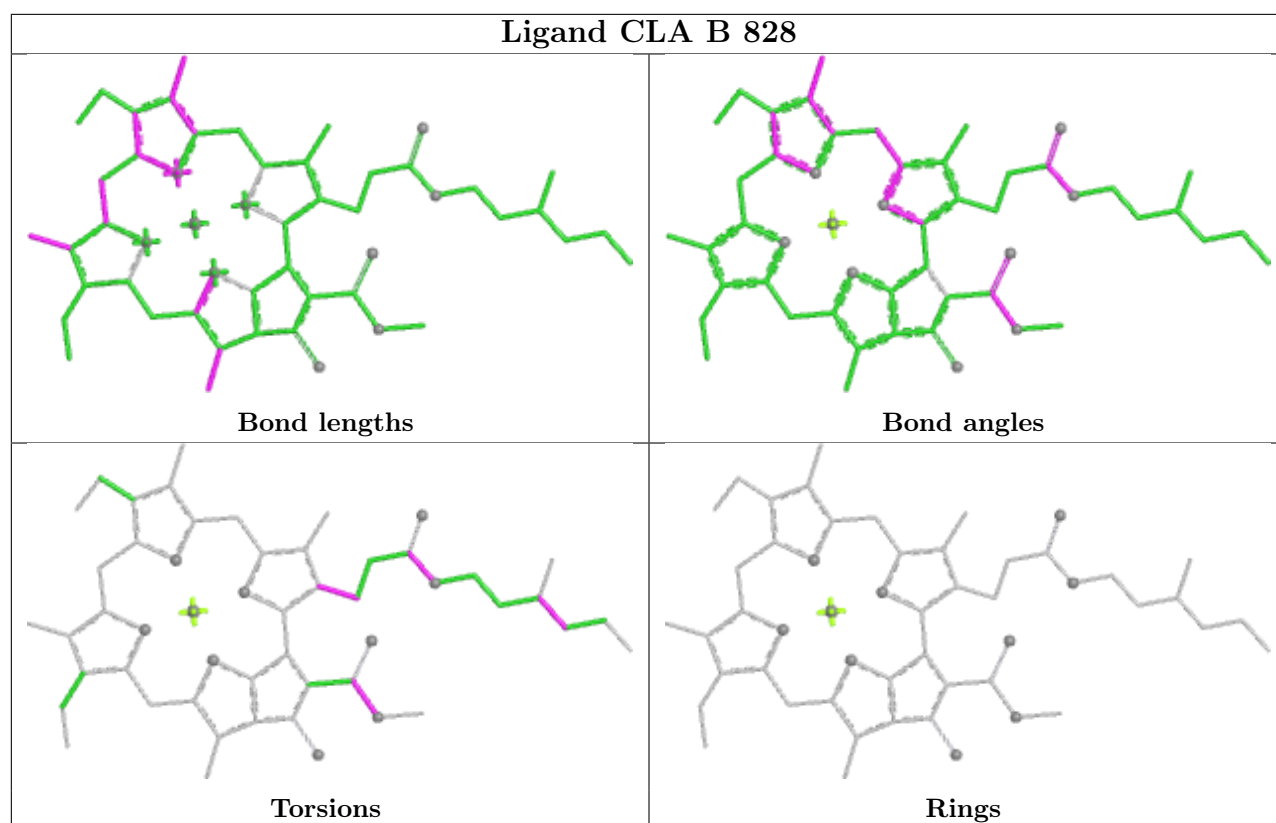
Bond angles

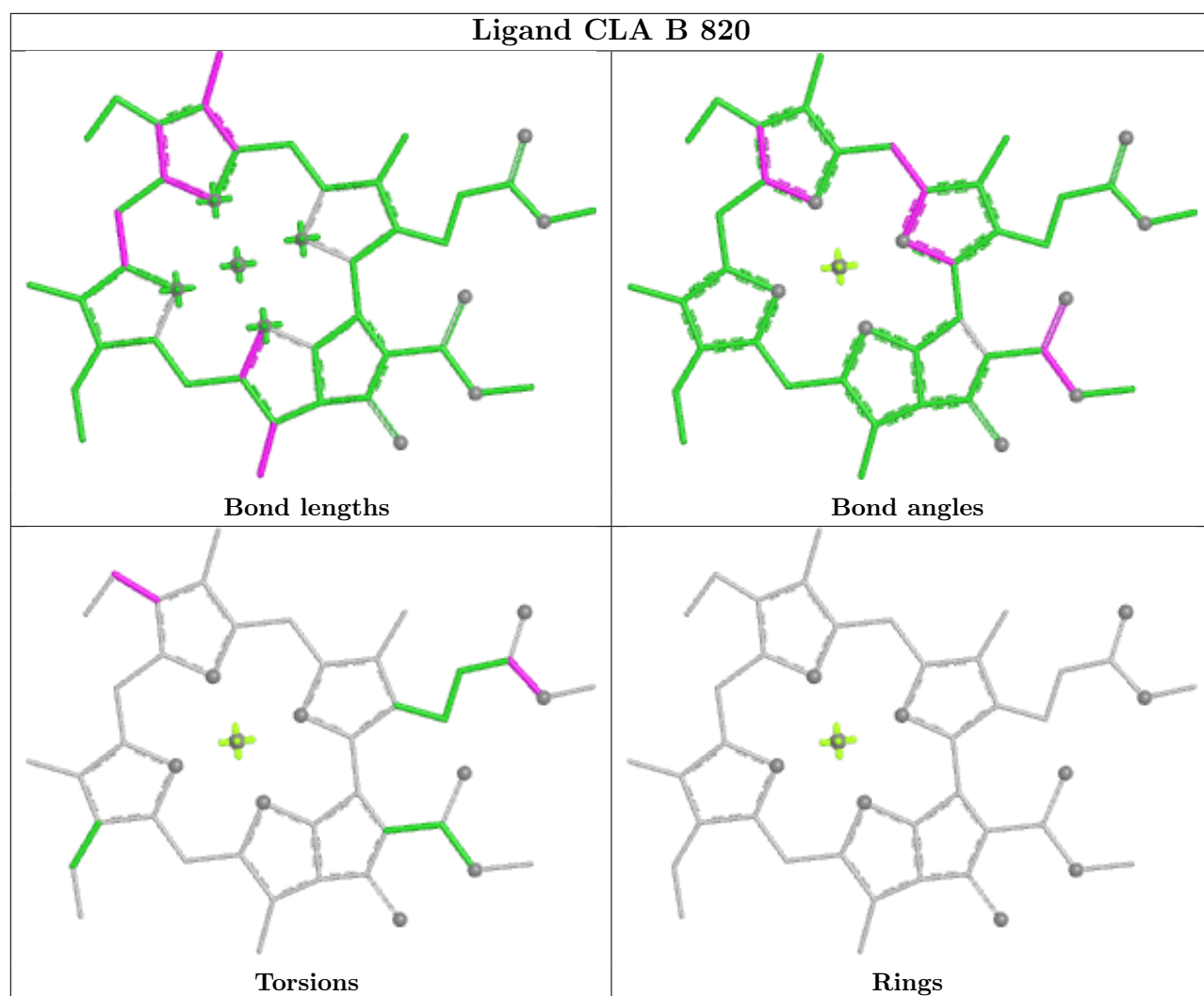


Torsions

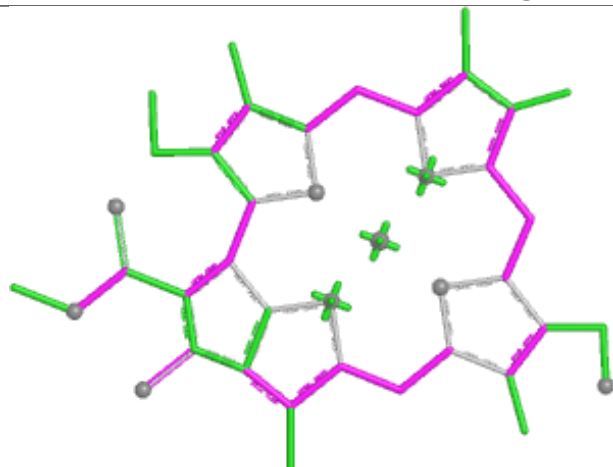


Rings

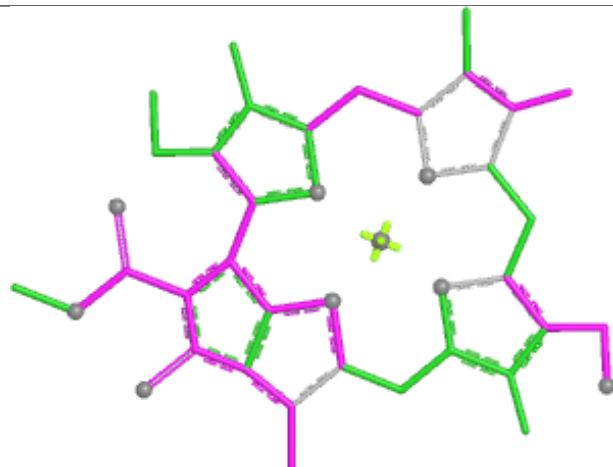




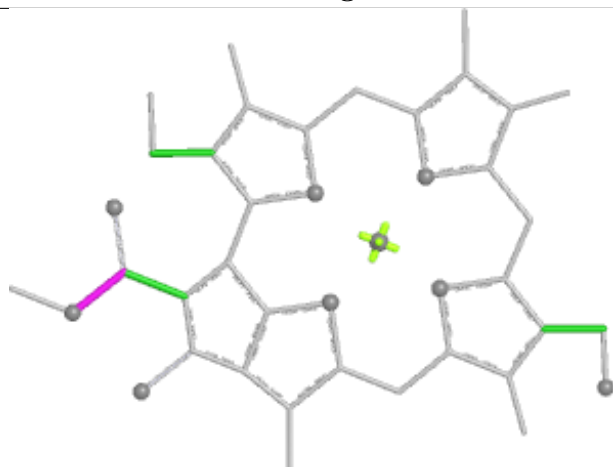
Ligand CHL 4 605



Bond lengths



Bond angles

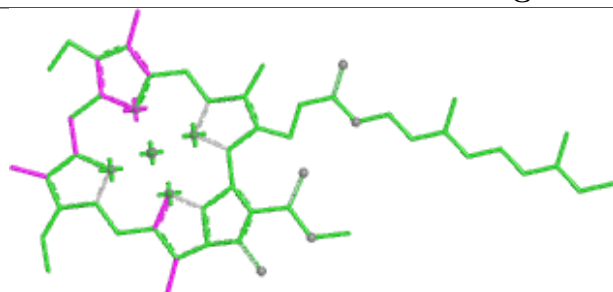


Torsions

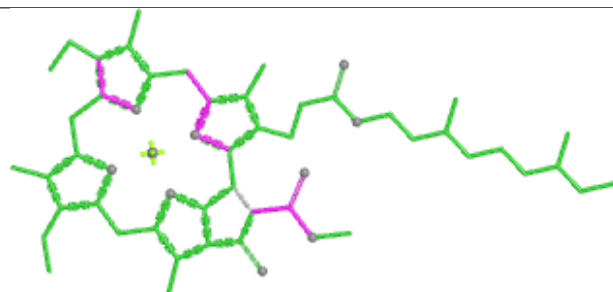


Rings

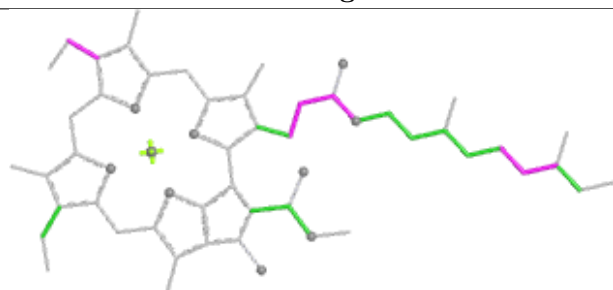
Ligand CLA A 823



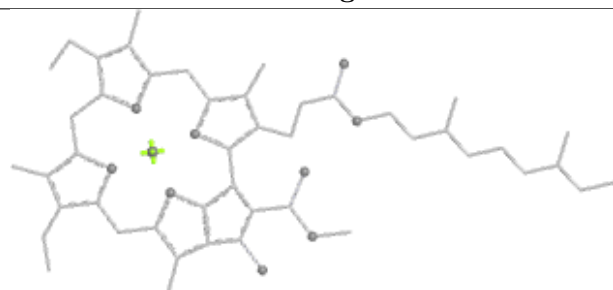
Bond lengths



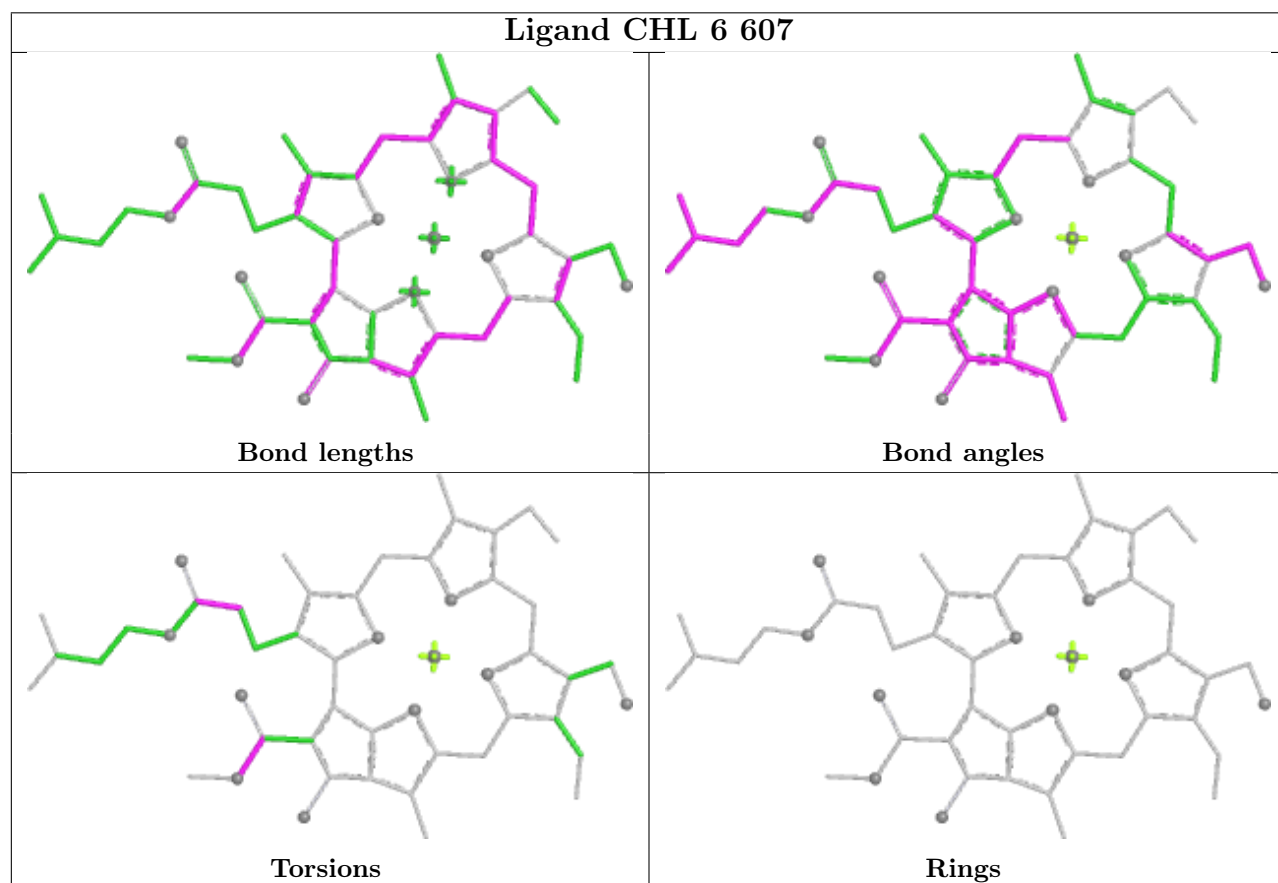
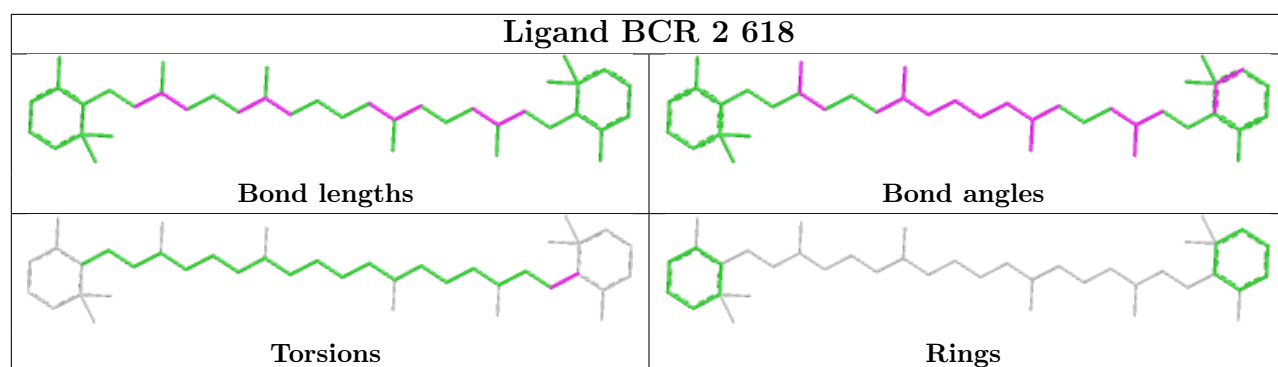
Bond angles

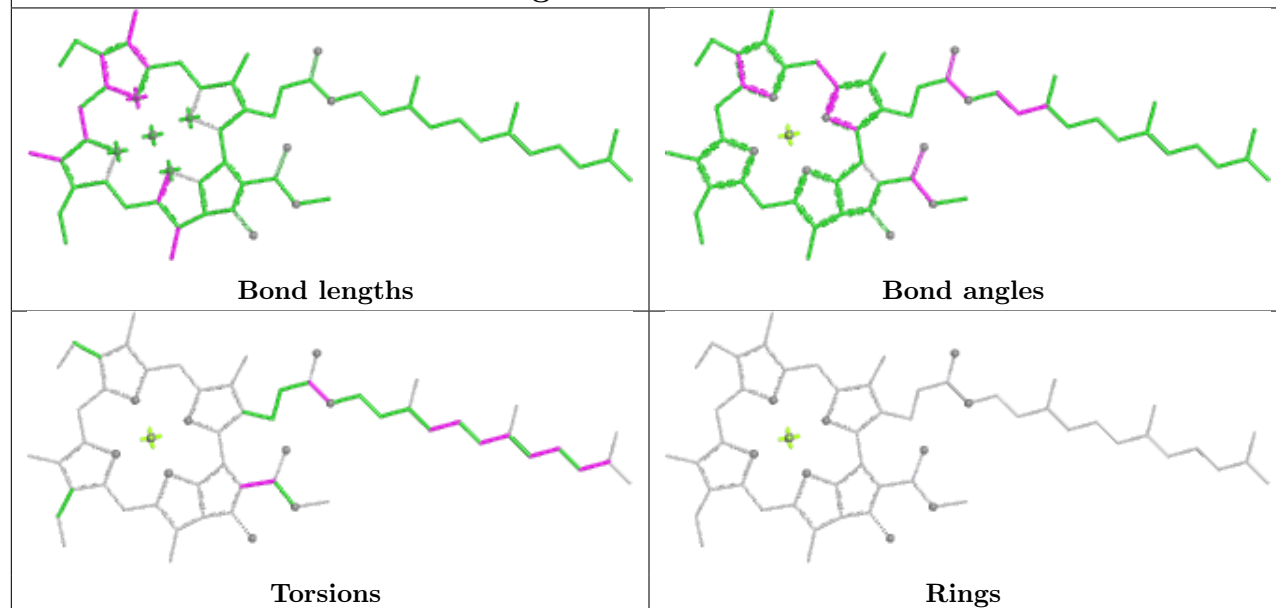
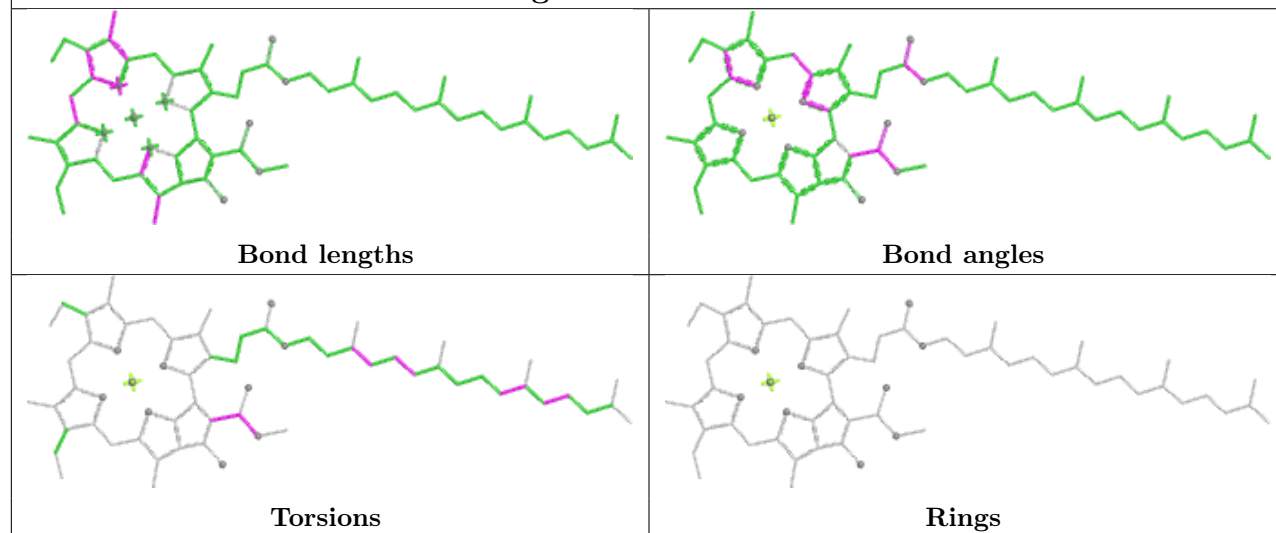


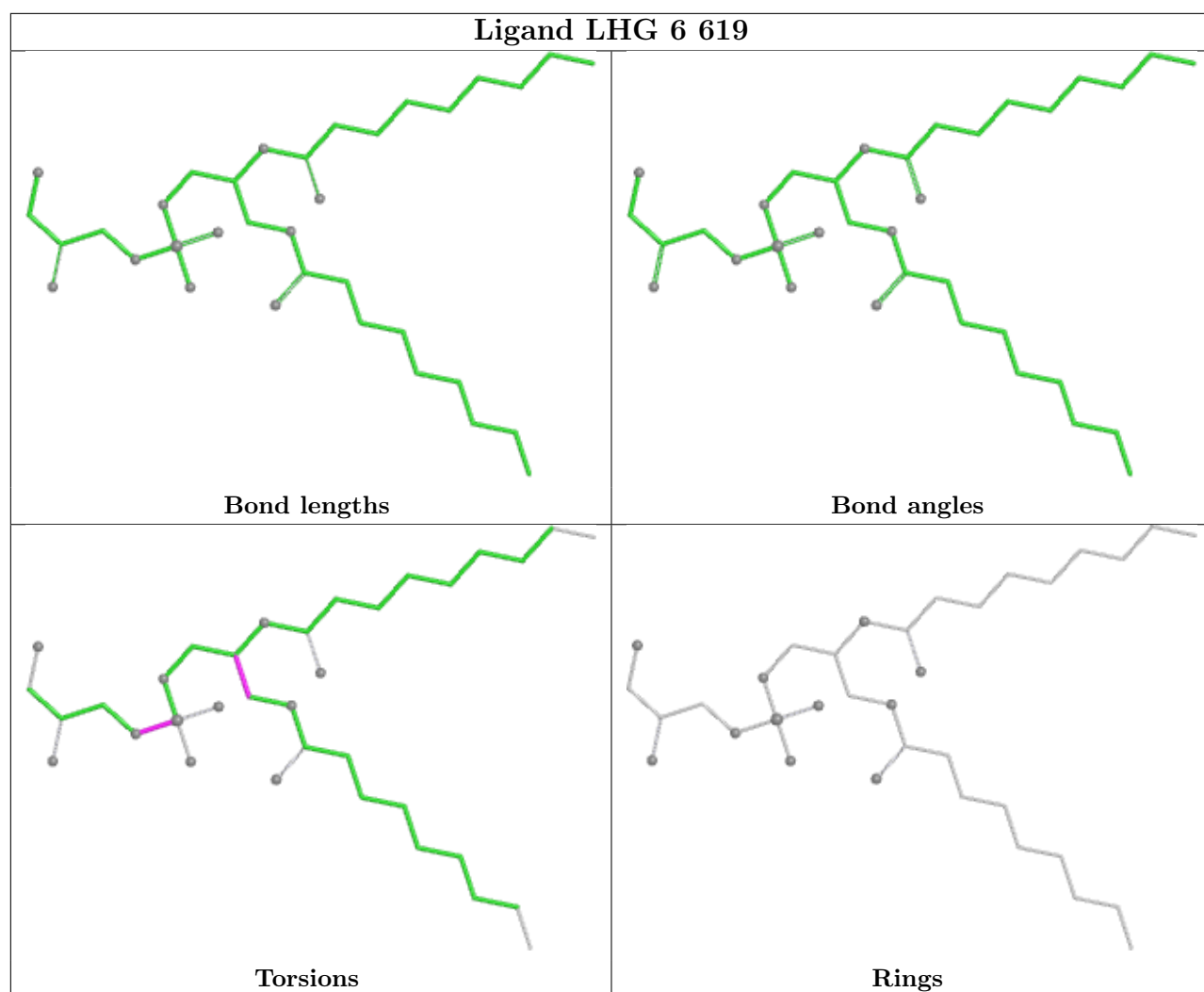
Torsions

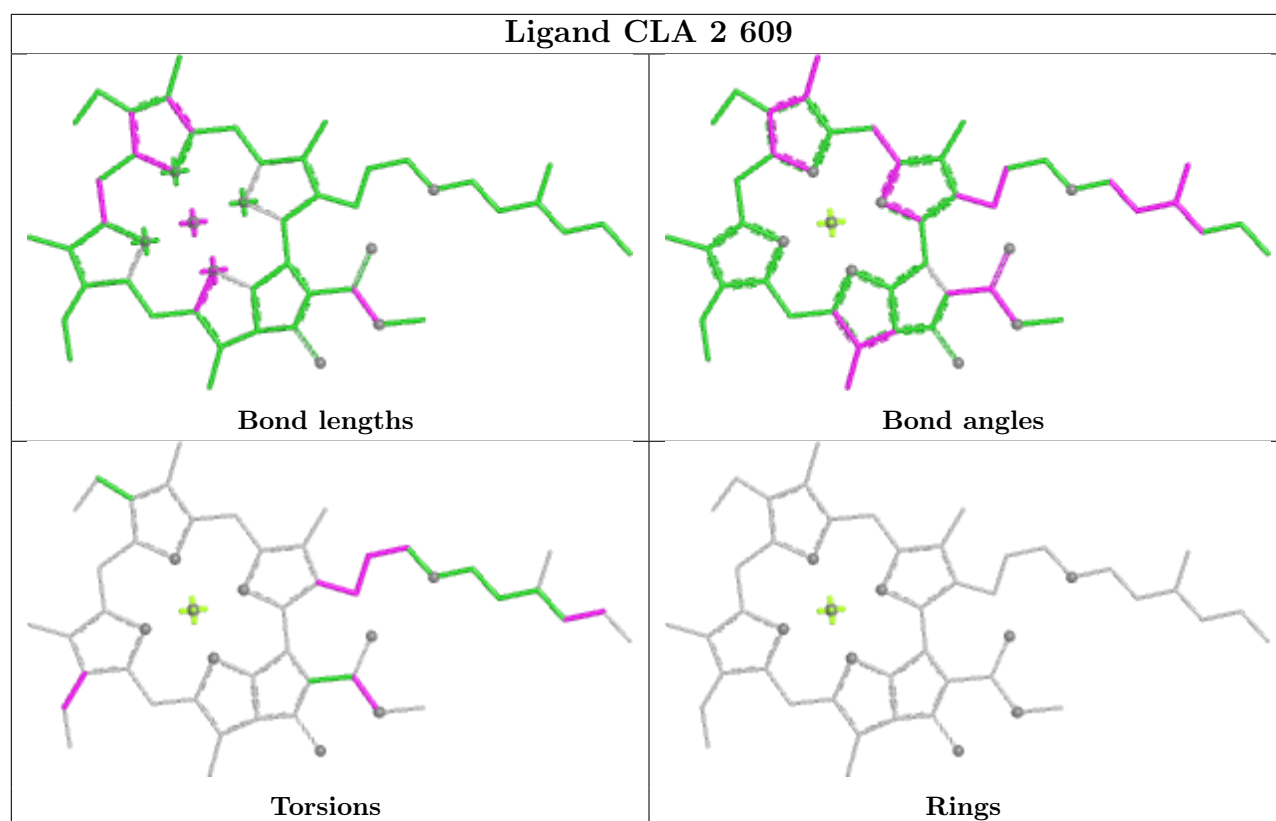


Rings

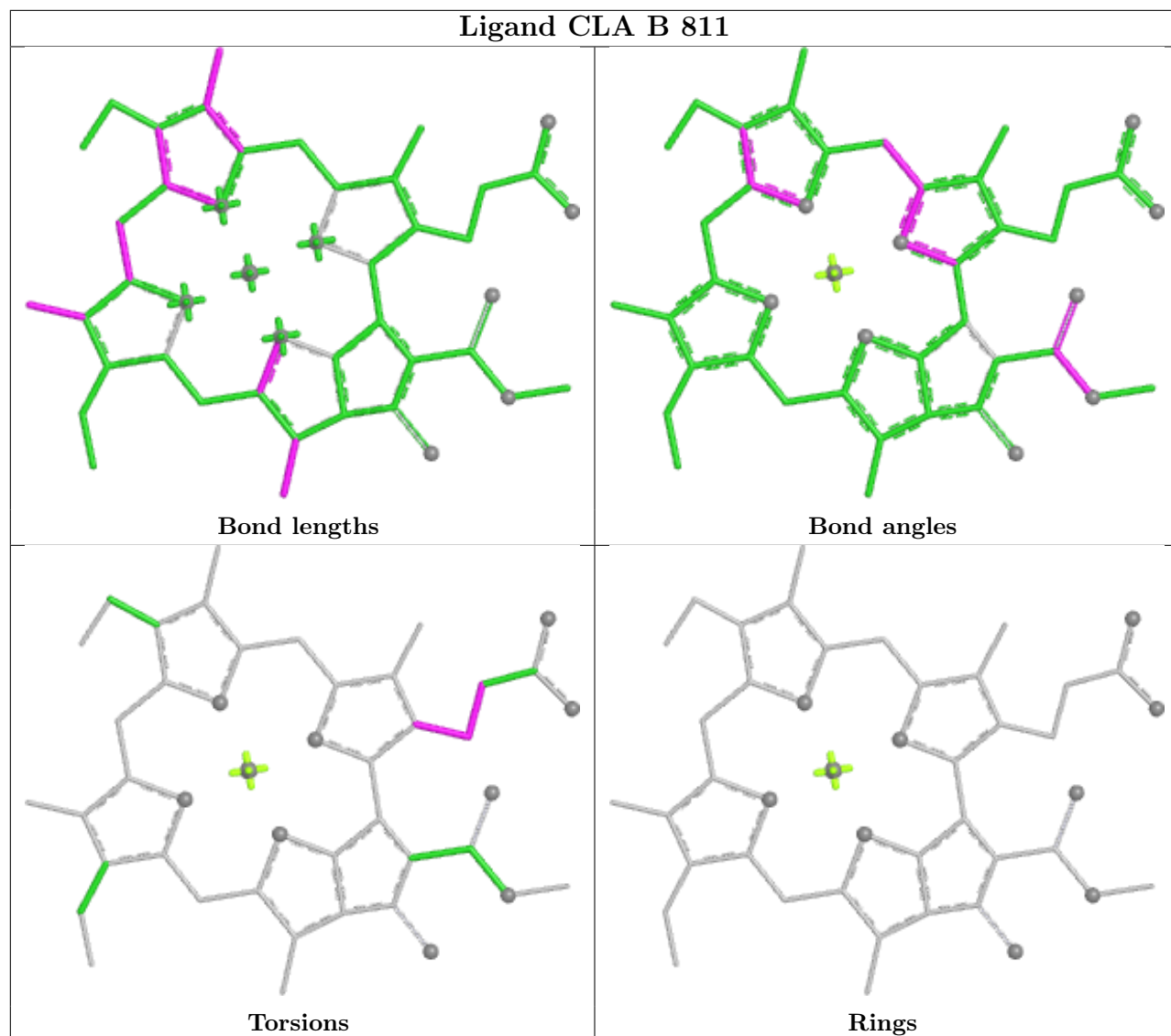


Ligand CLA B 814**Ligand CLA A 834**

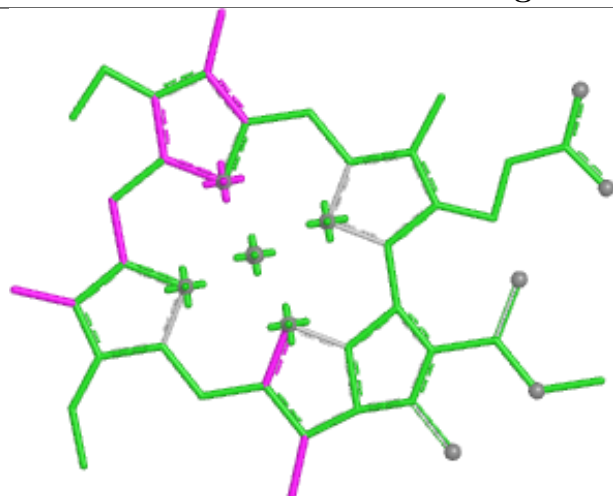




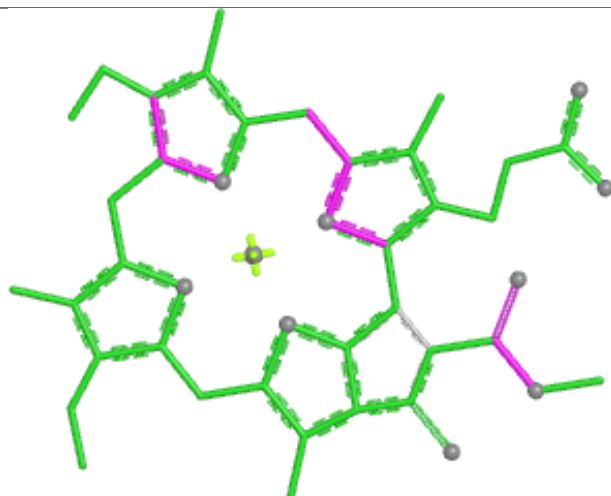
Ligand CLA B 811



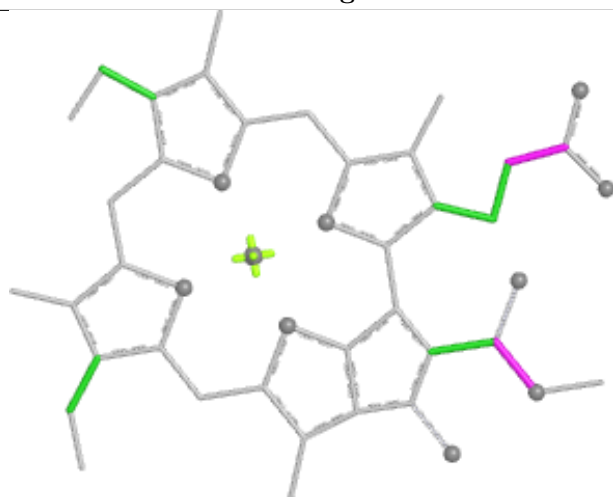
Ligand CLA B 822



Bond lengths



Bond angles

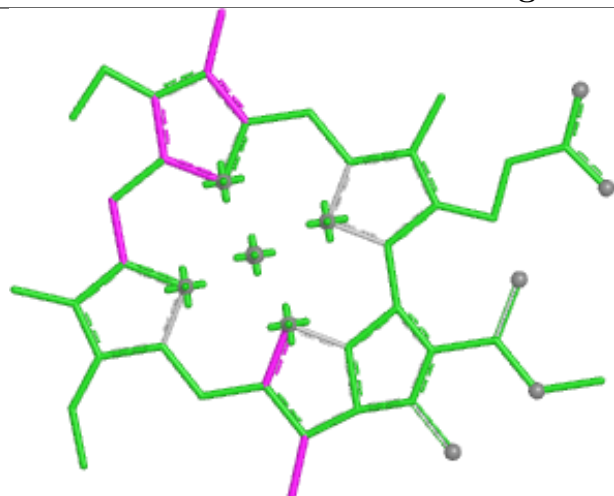


Torsions

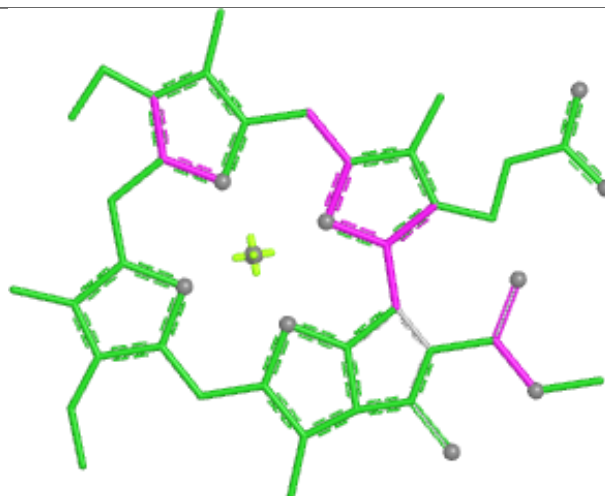


Rings

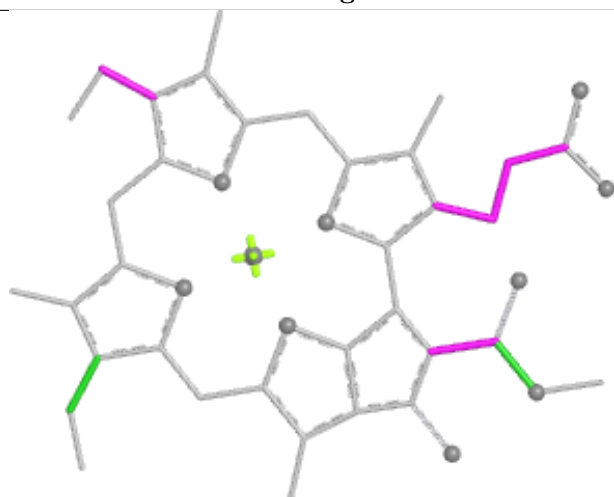
Ligand CLA 7 402



Bond lengths



Bond angles

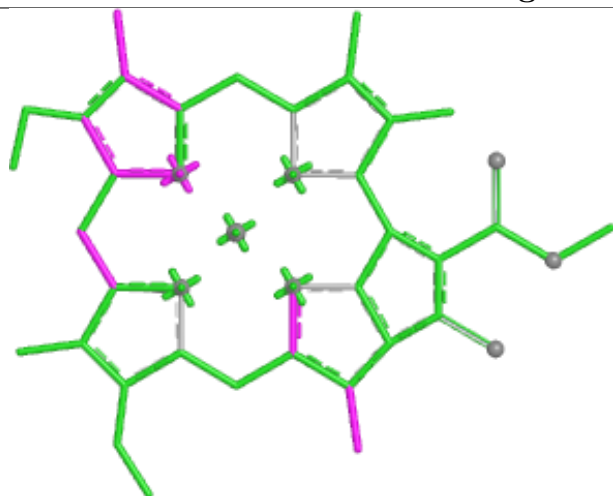


Torsions

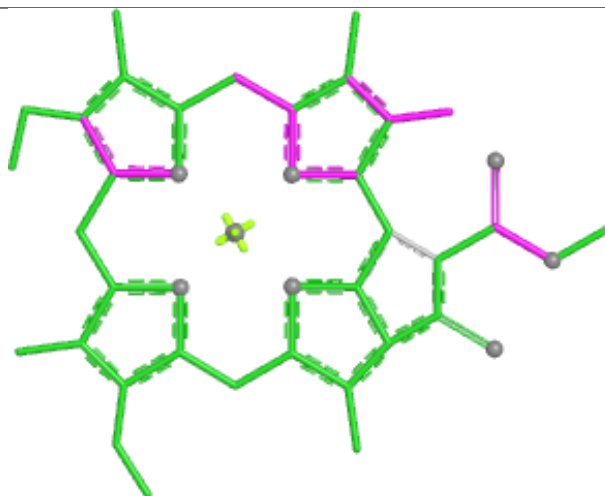


Rings

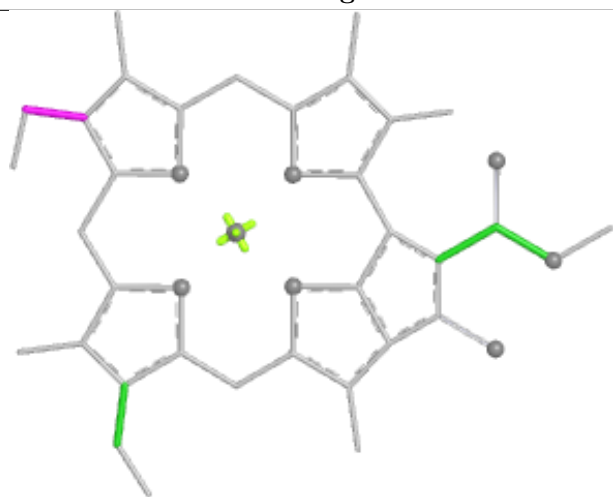
Ligand CLA a 614



Bond lengths



Bond angles

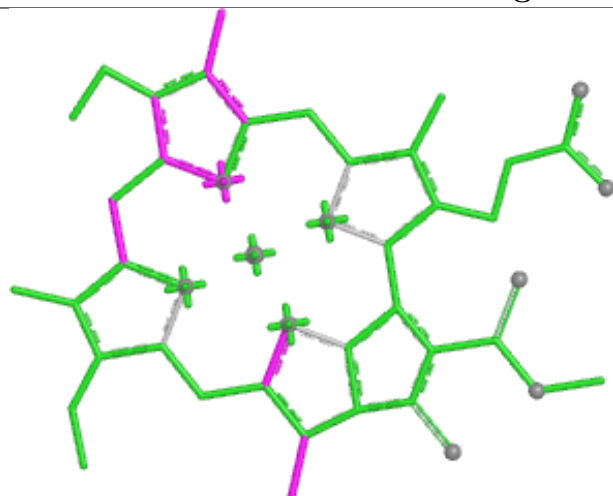


Torsions

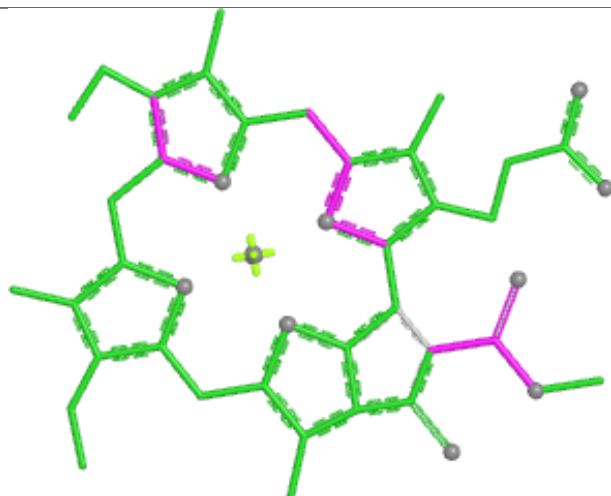


Rings

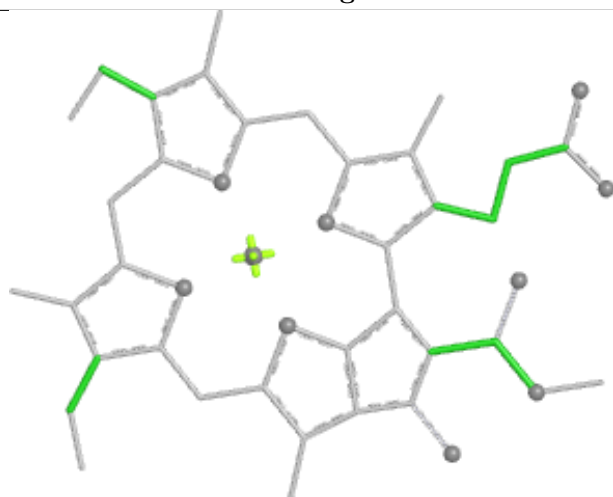
Ligand CLA A 839



Bond lengths



Bond angles

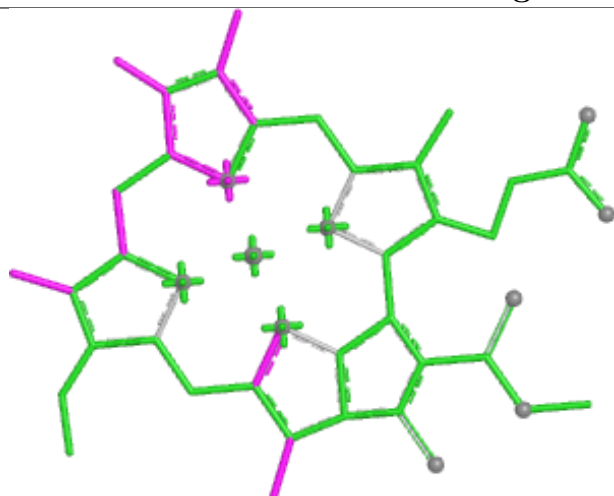


Torsions

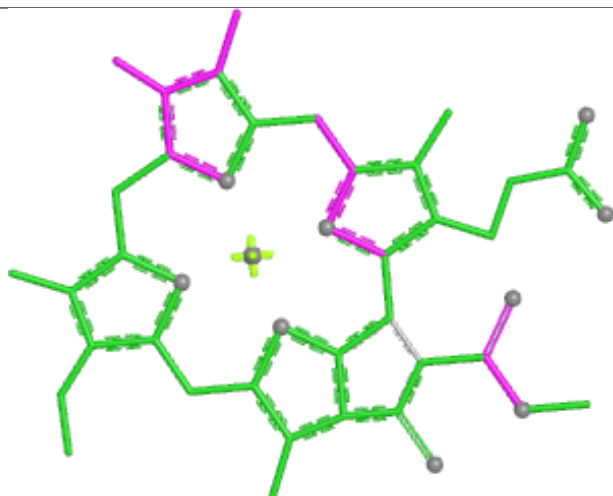


Rings

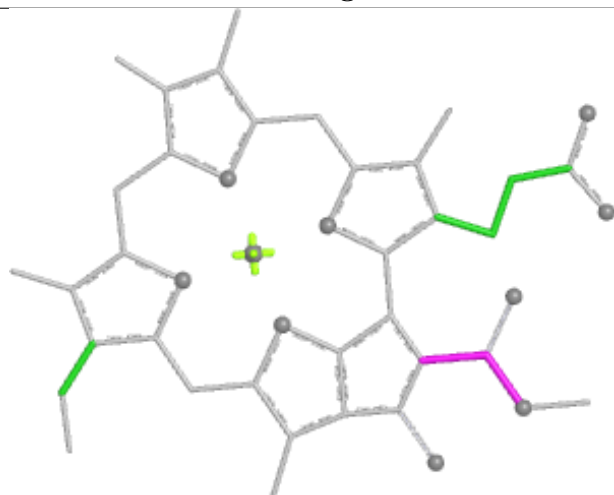
Ligand CLA K 203



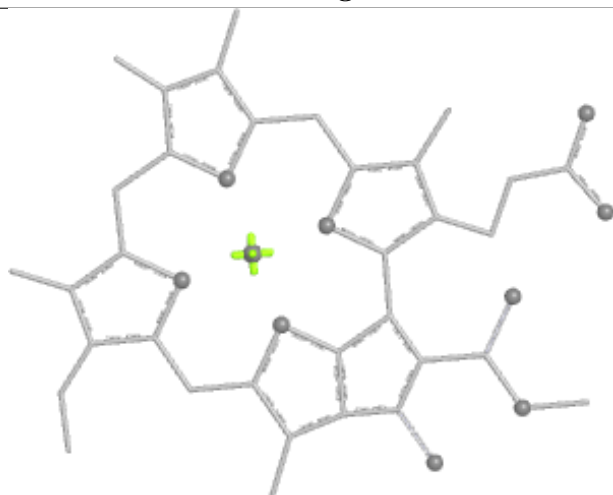
Bond lengths



Bond angles

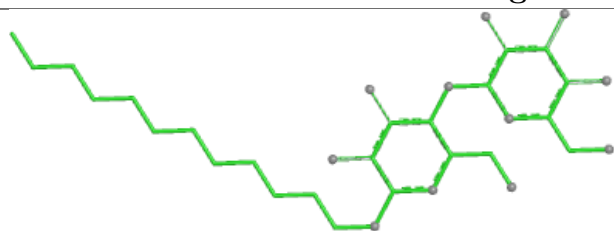


Torsions

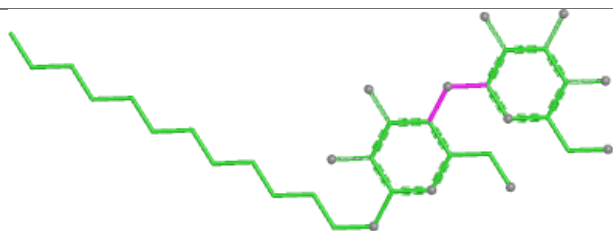


Rings

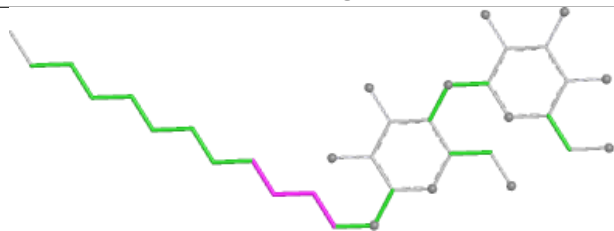
Ligand LMU A 856



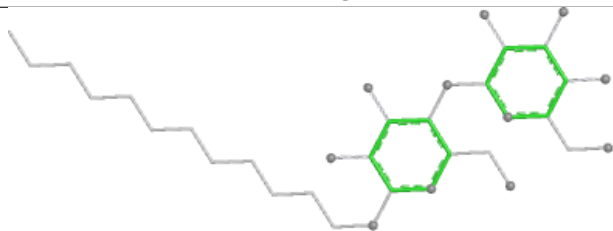
Bond lengths



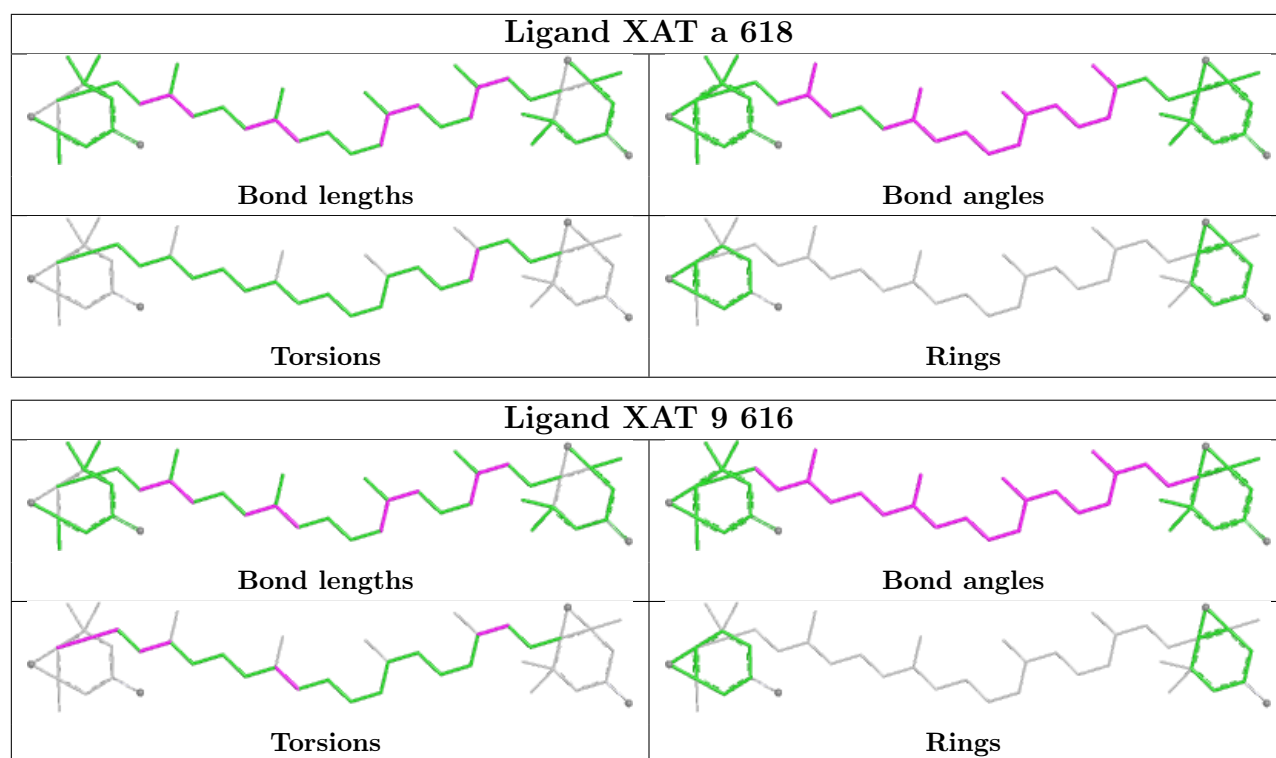
Bond angles



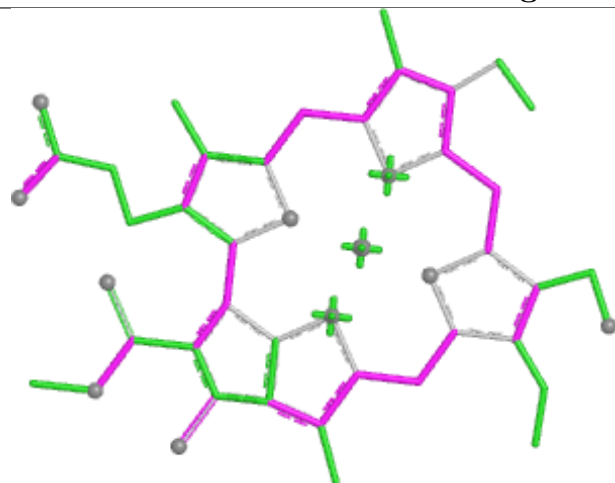
Torsions



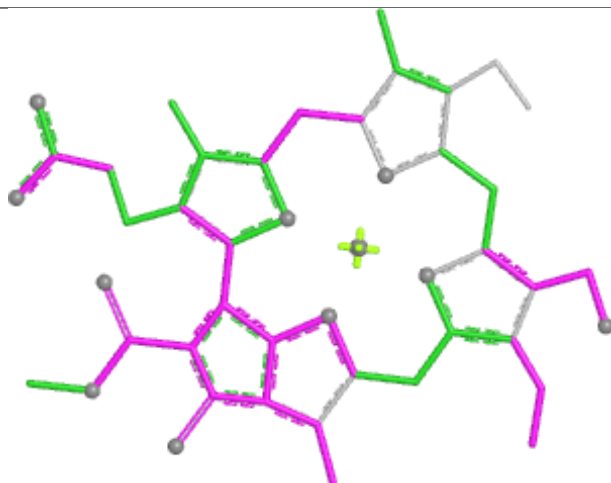
Rings



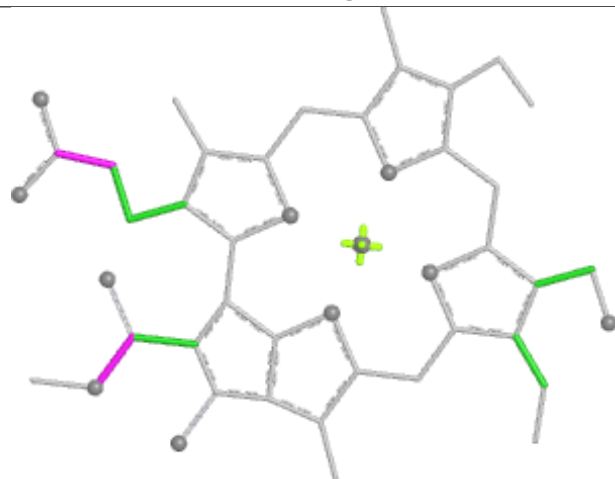
Ligand CHL a 606



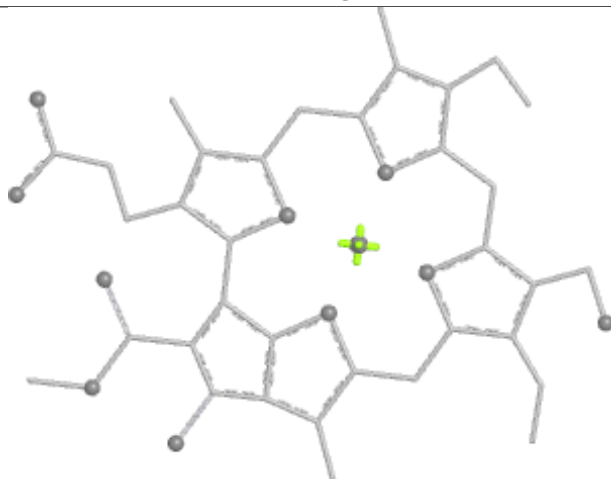
Bond lengths



Bond angles

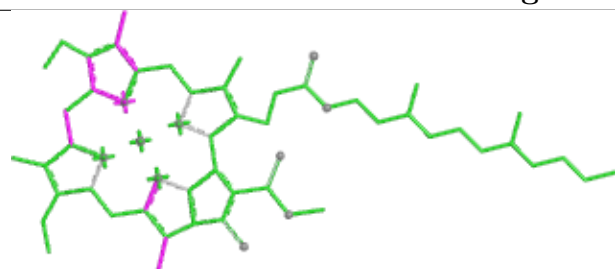


Torsions

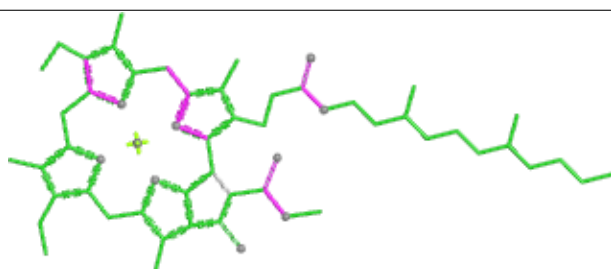


Rings

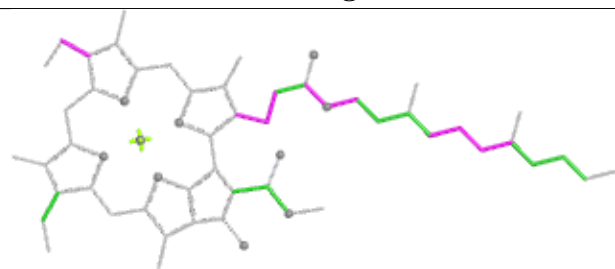
Ligand CLA c 611



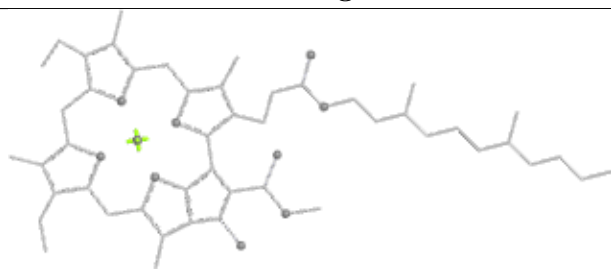
Bond lengths



Bond angles

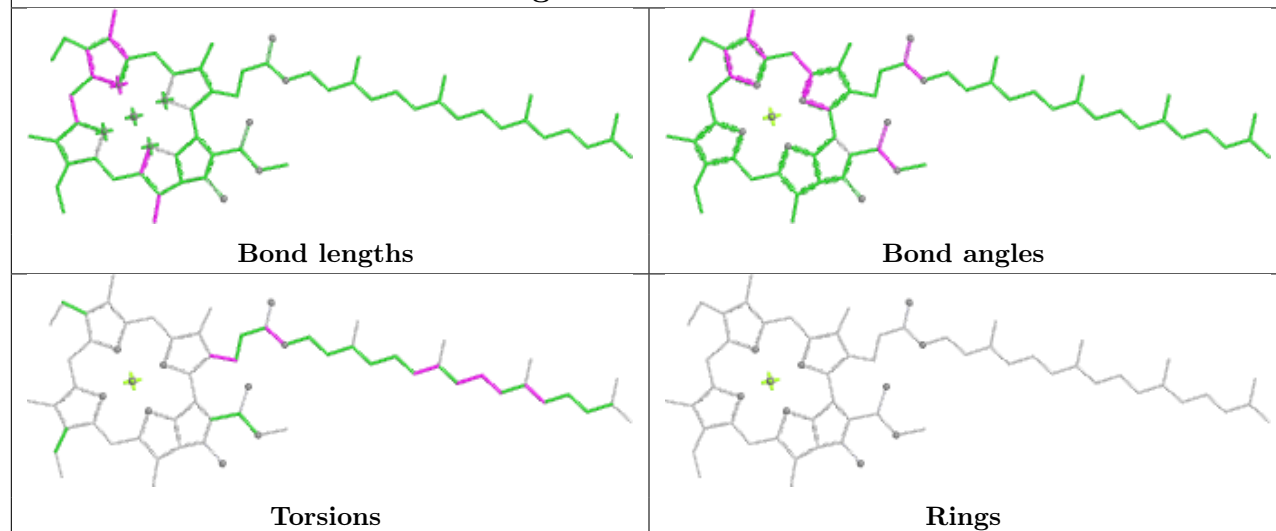


Torsions

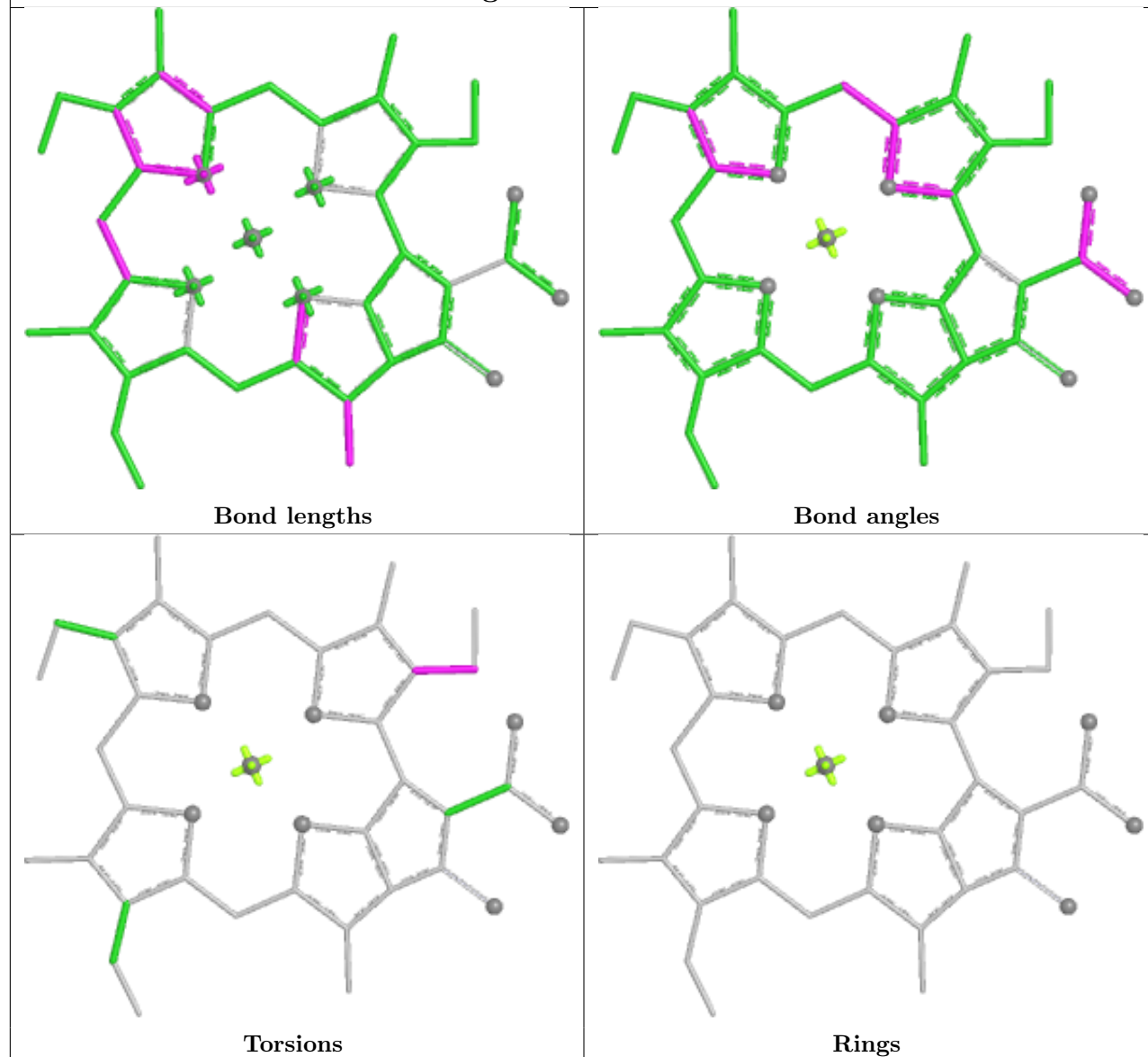


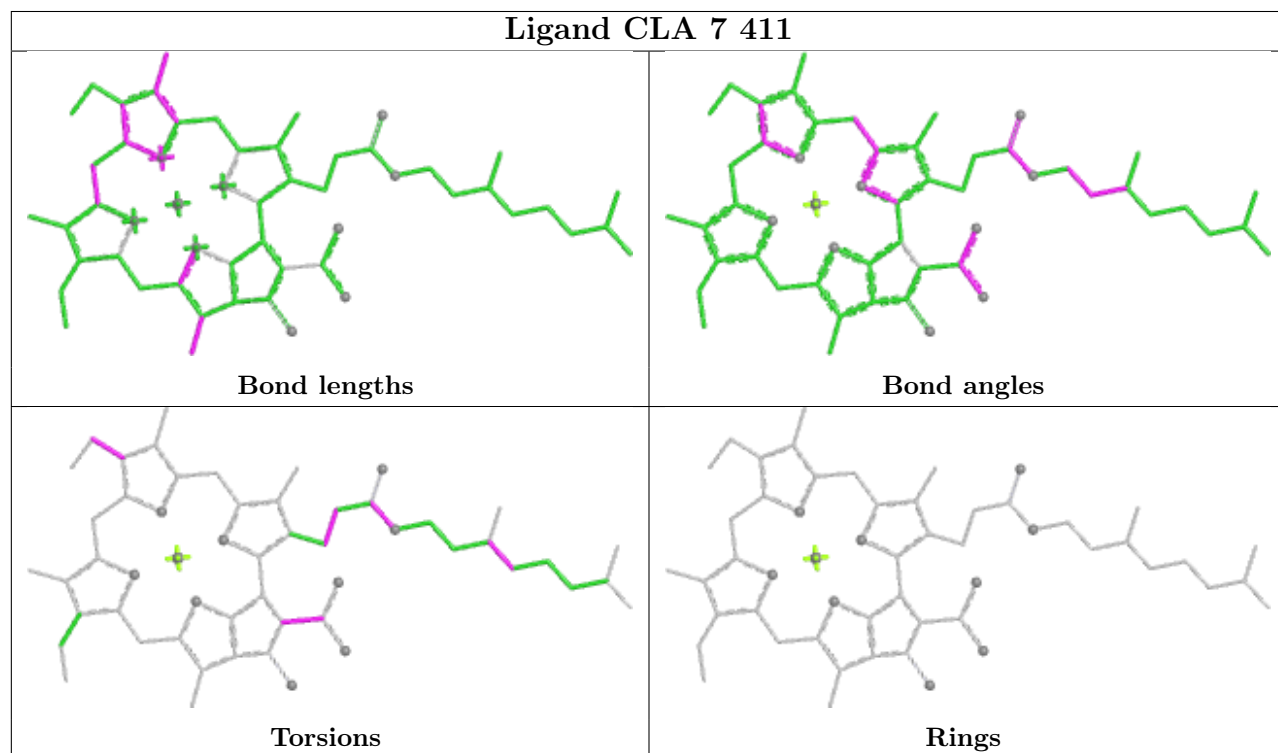
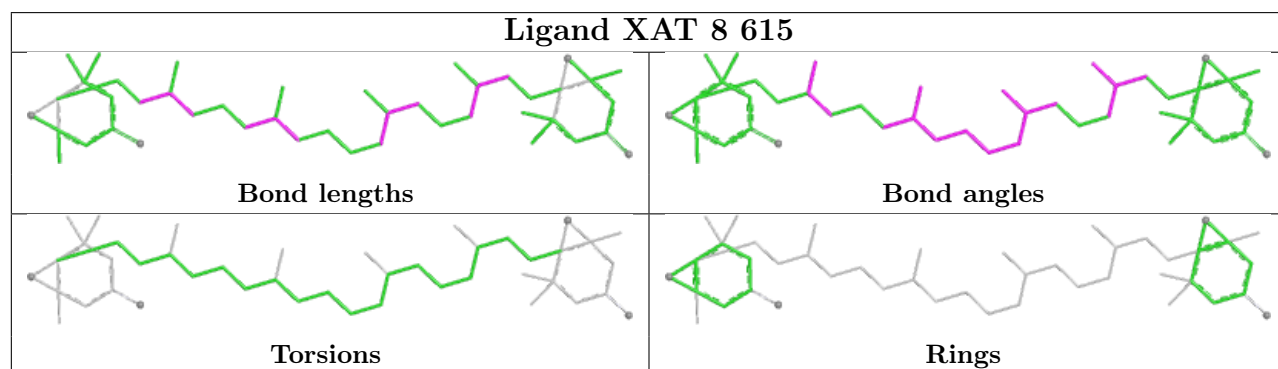
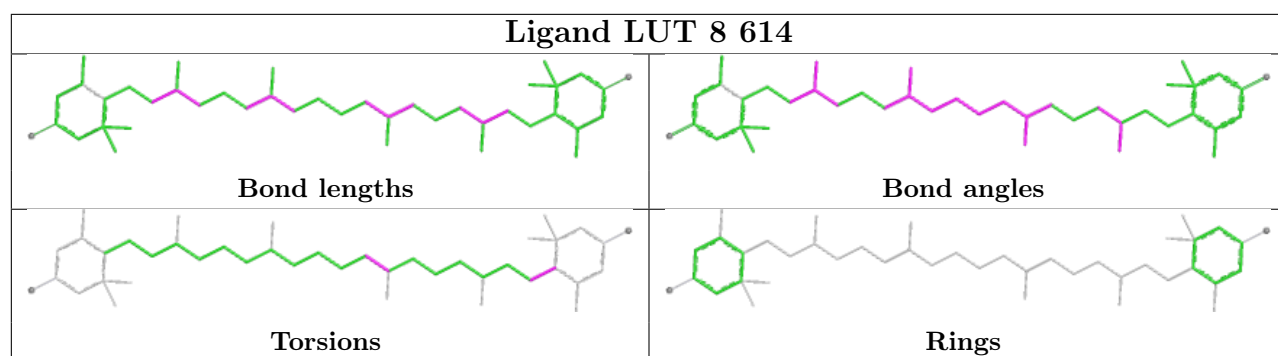
Rings

Ligand CLA B 824

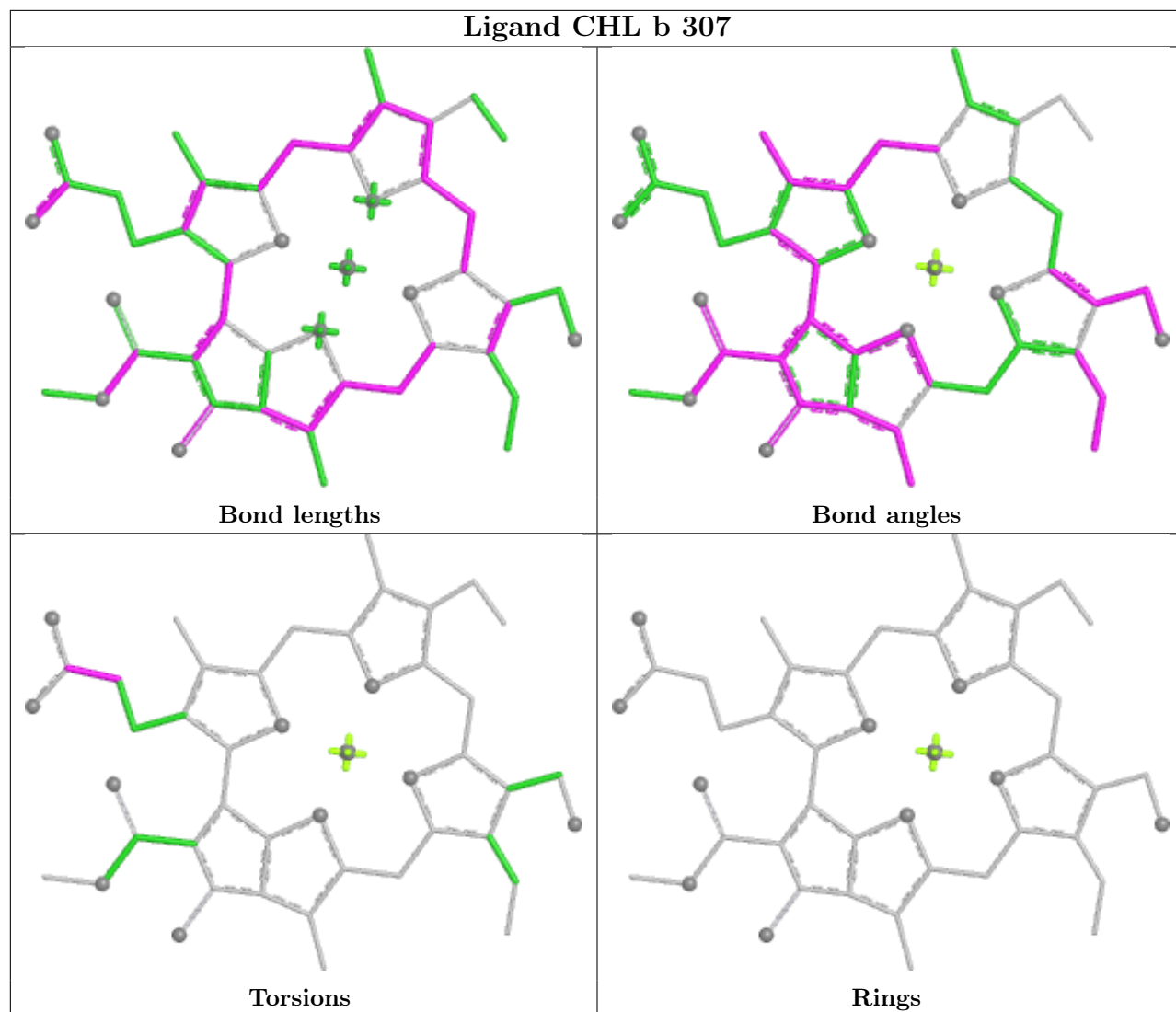


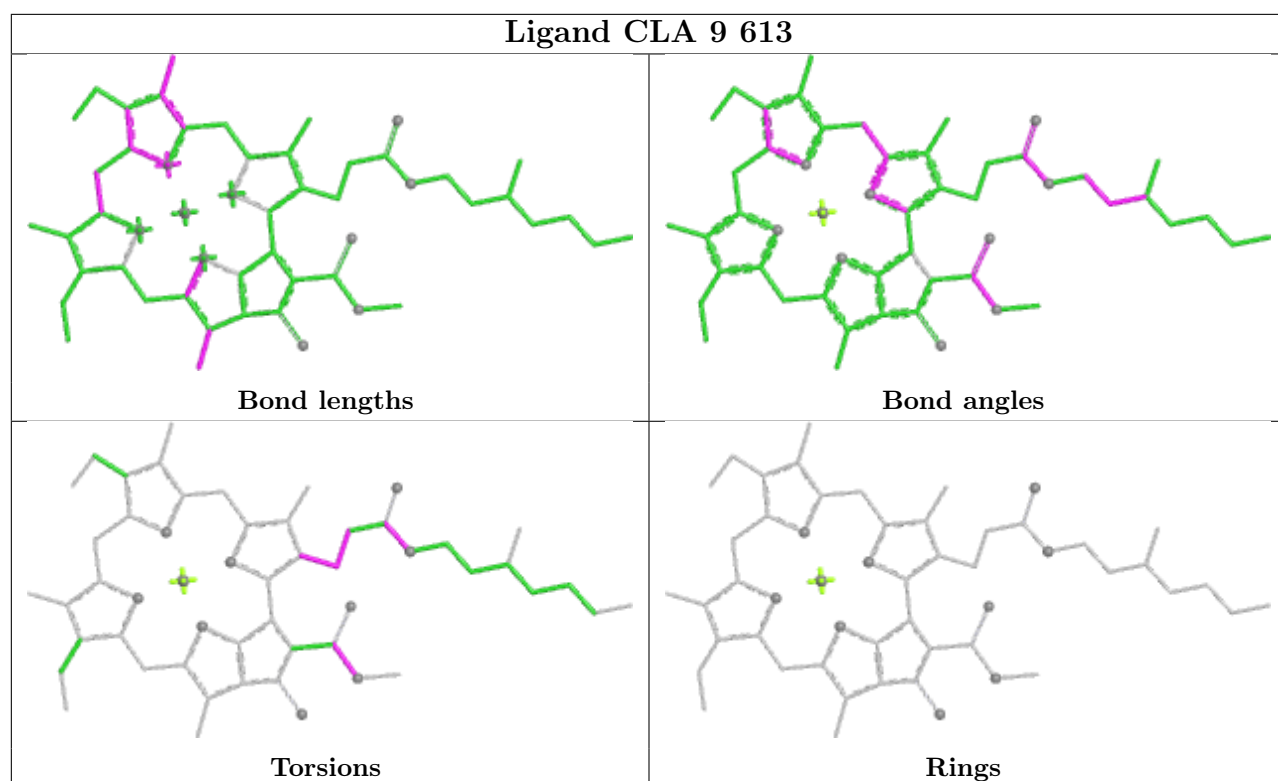
Ligand CLA 7 404



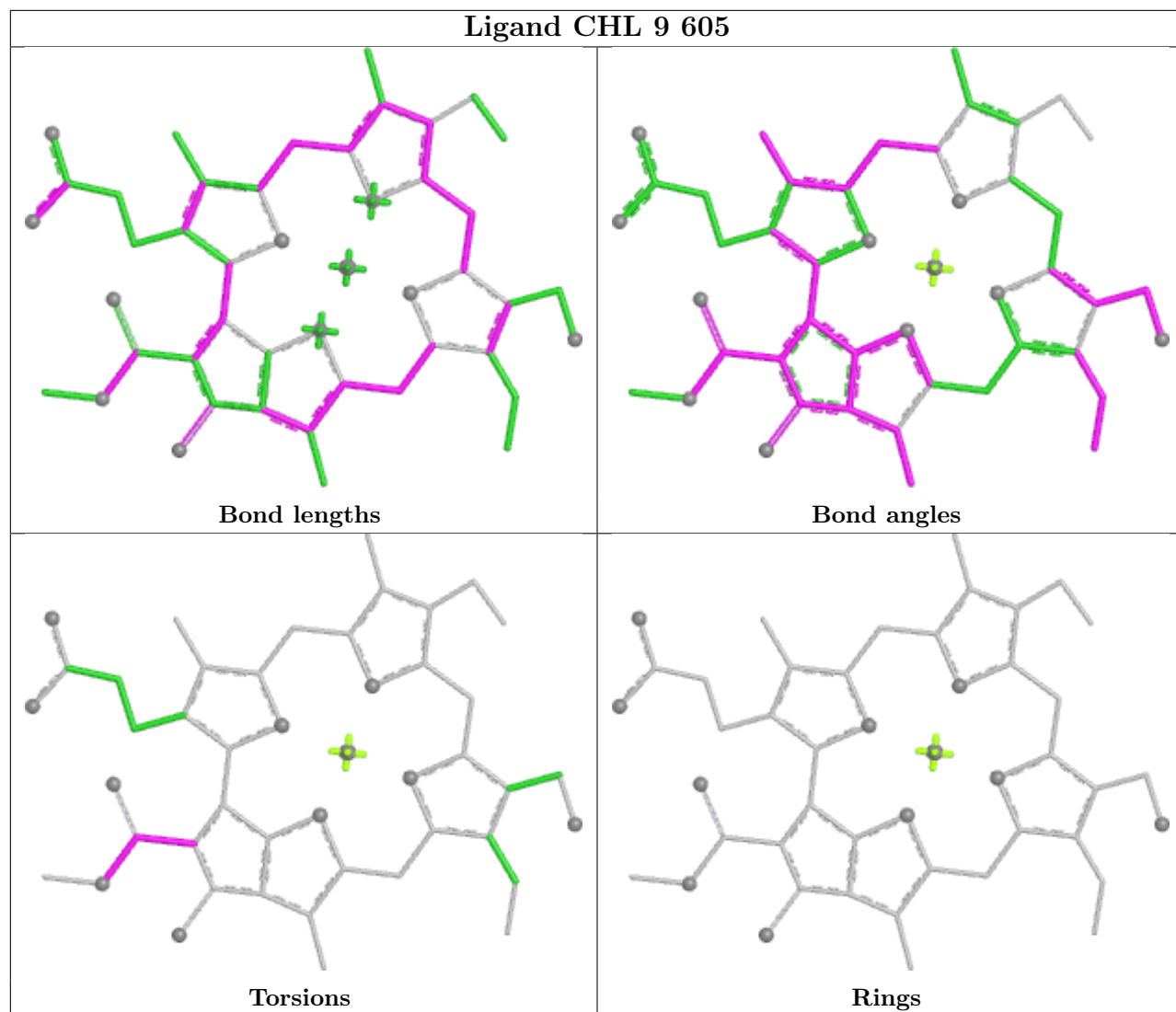


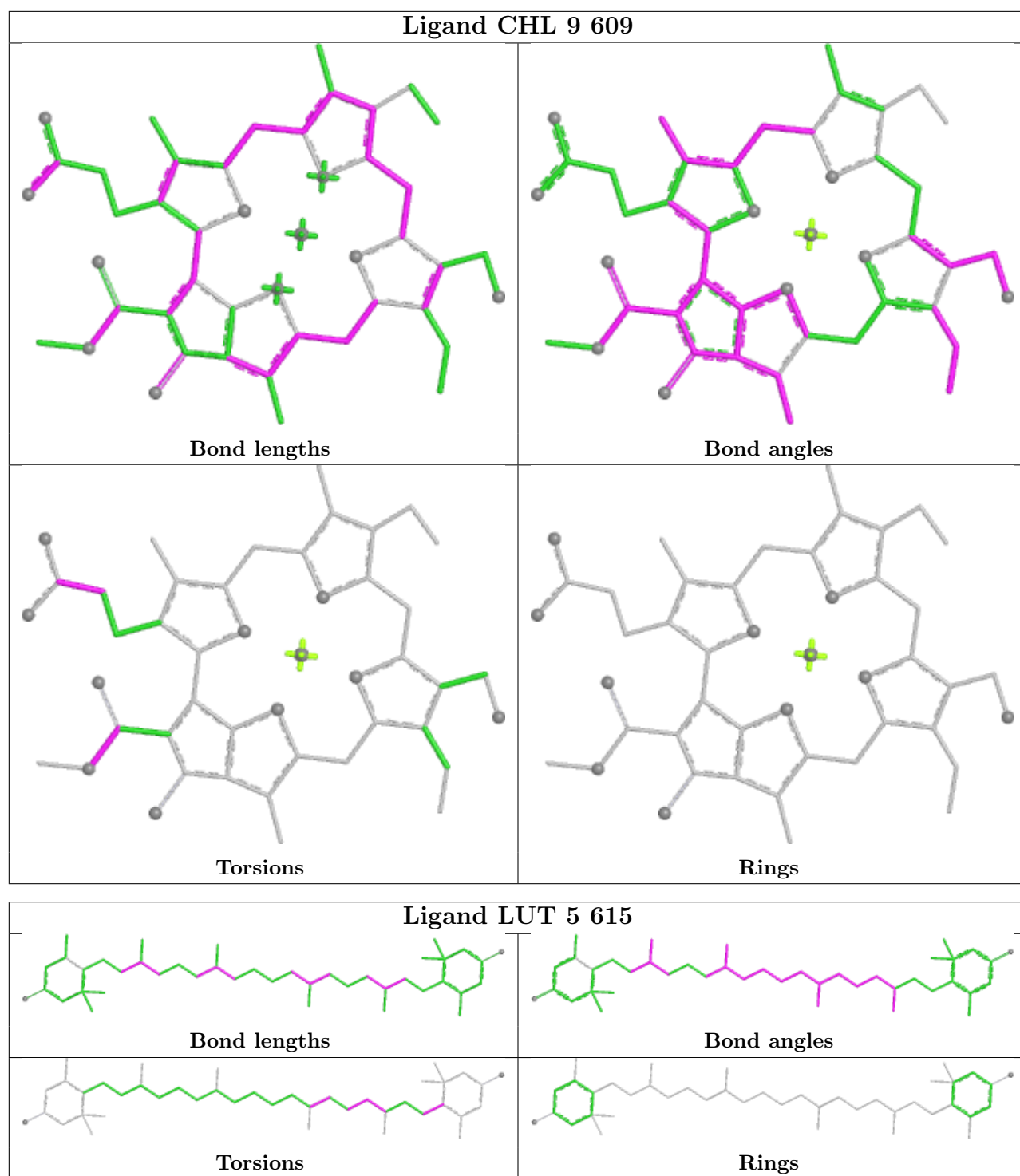
Ligand CHL b 307

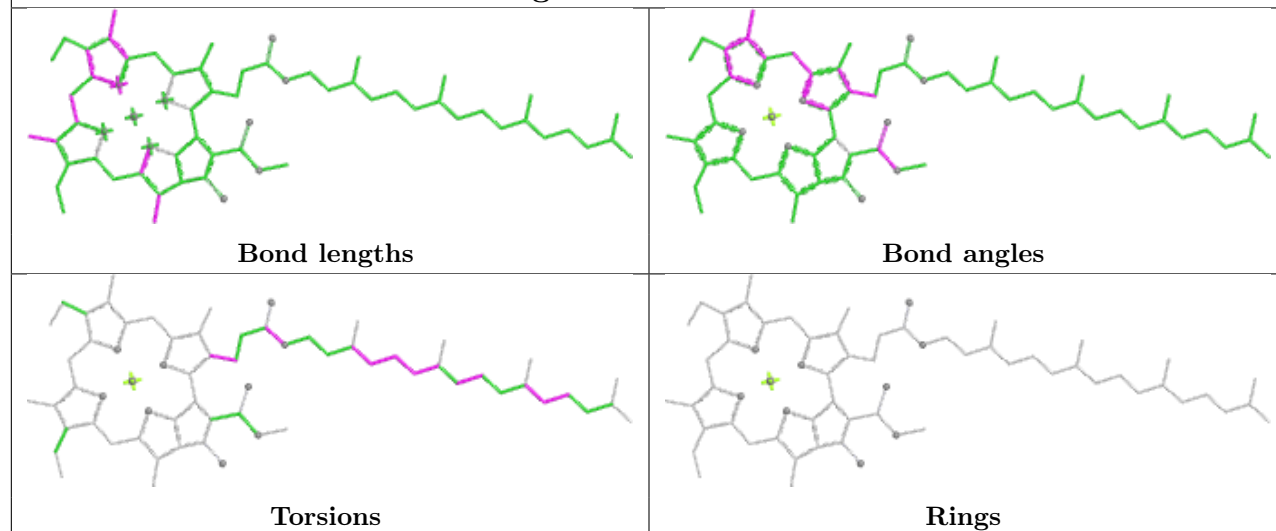
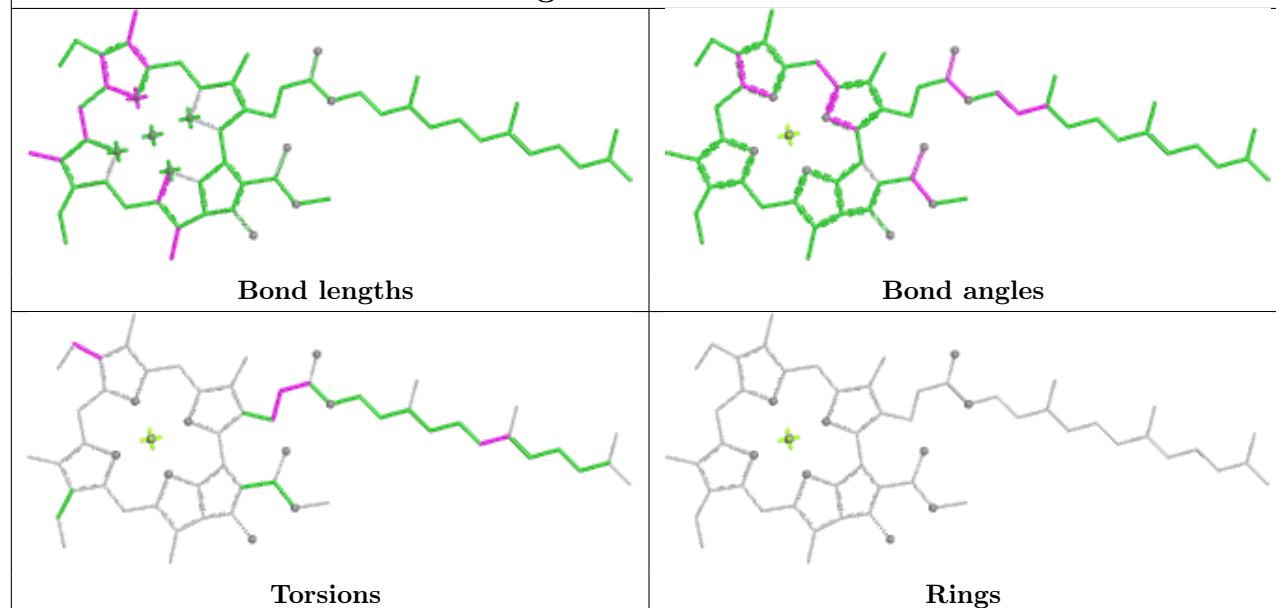


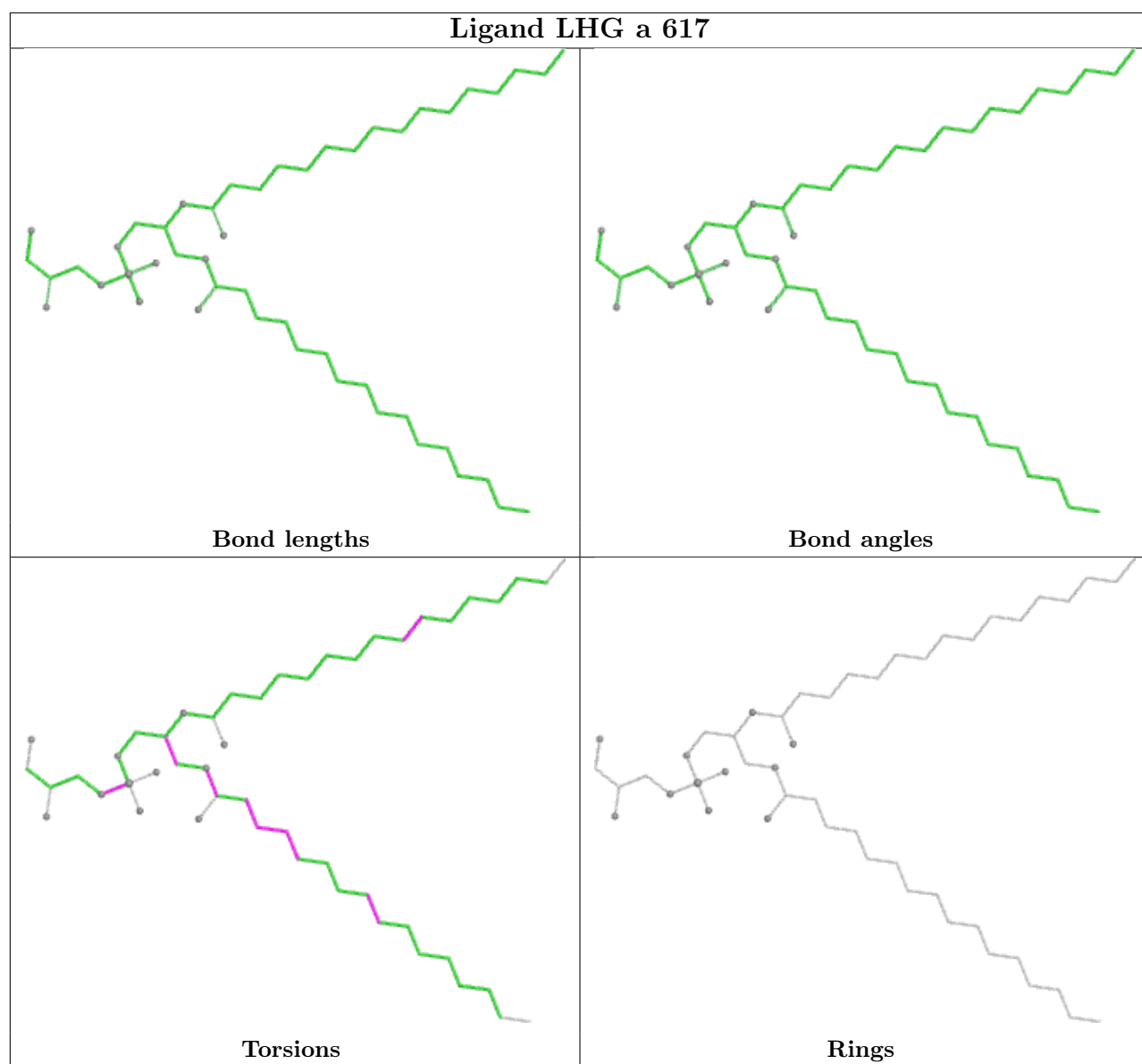


Ligand CHL 9 605

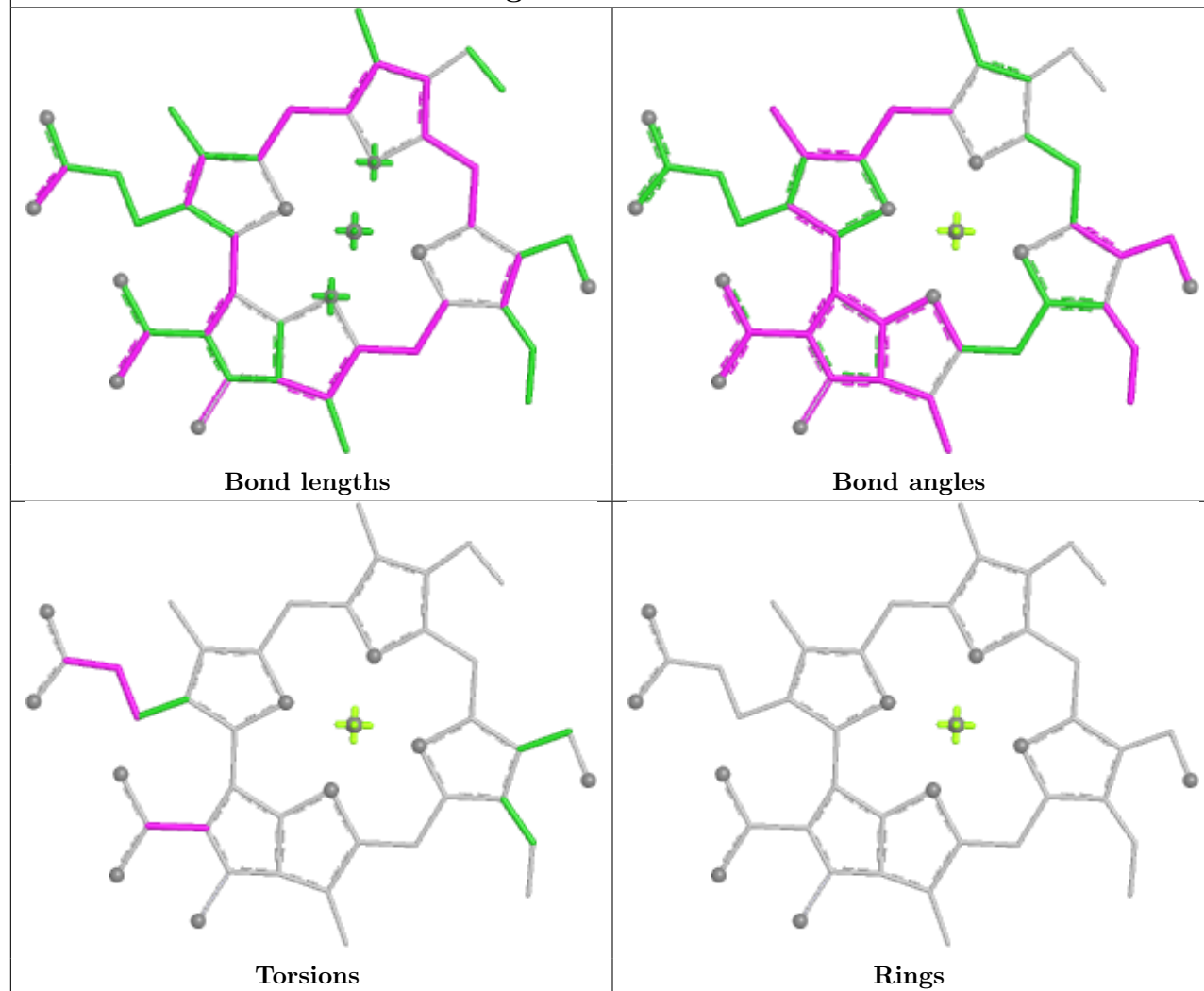




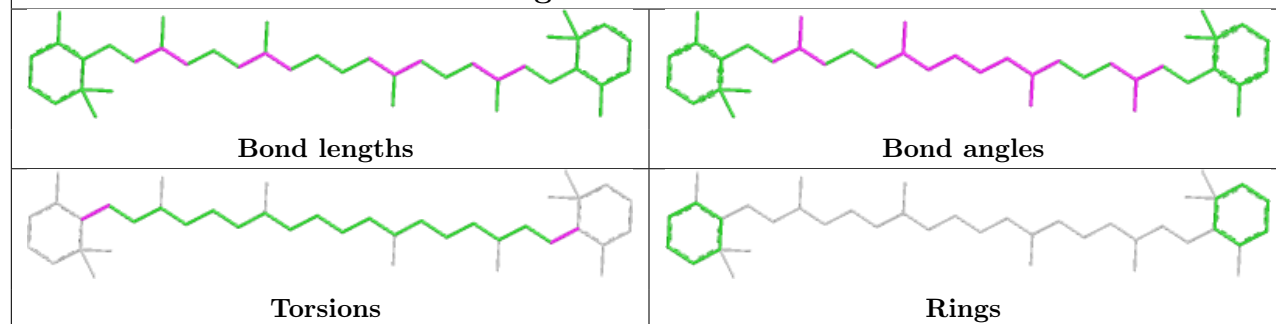
Ligand CLA B 836**Ligand CLA c 602**

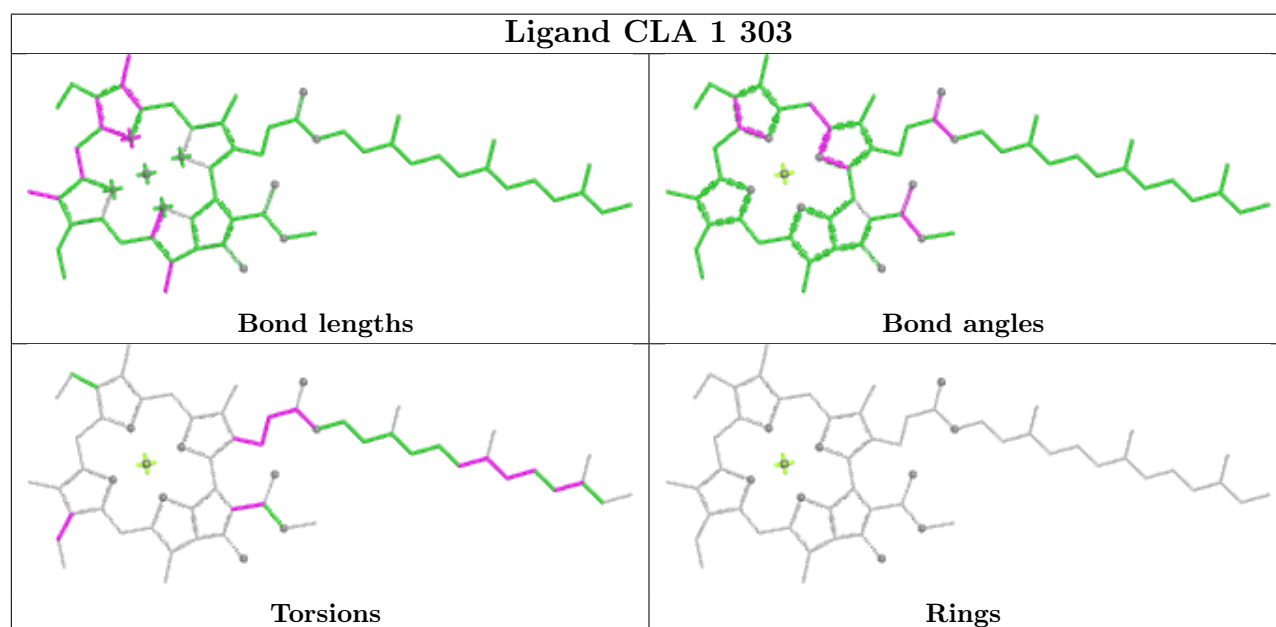
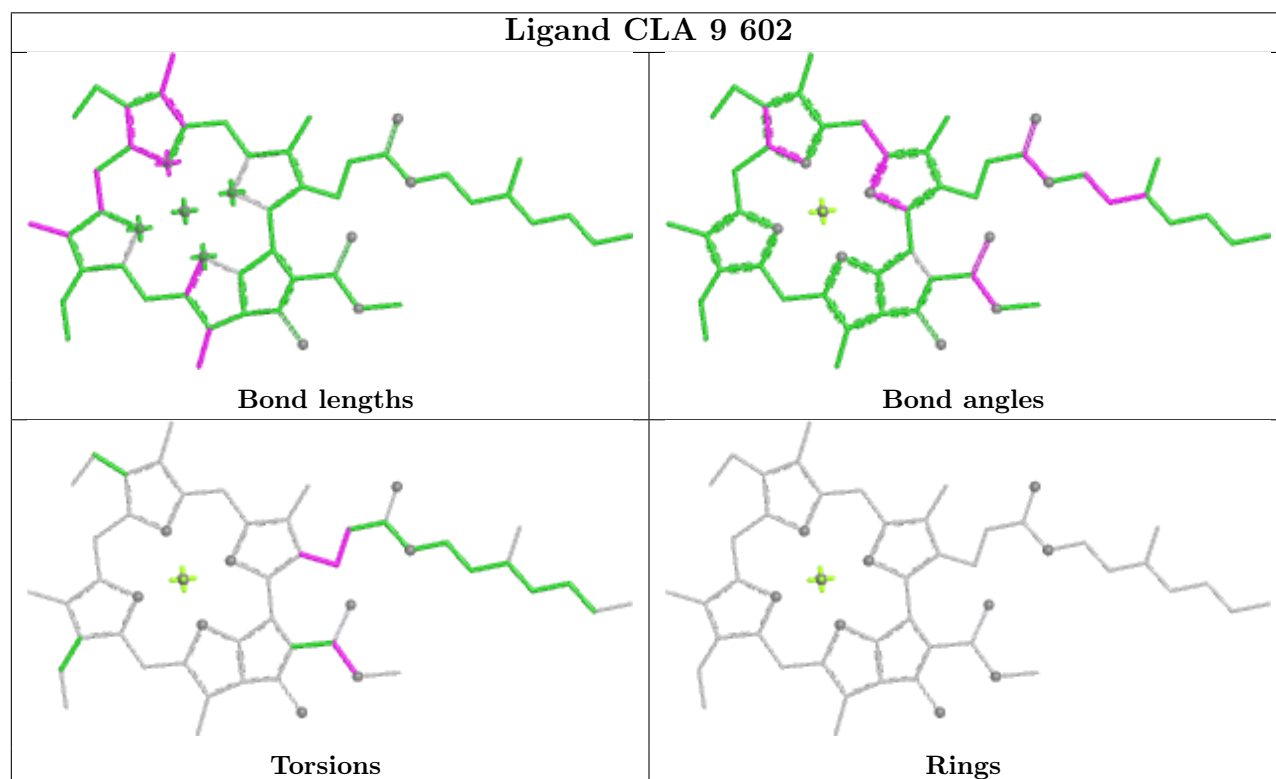
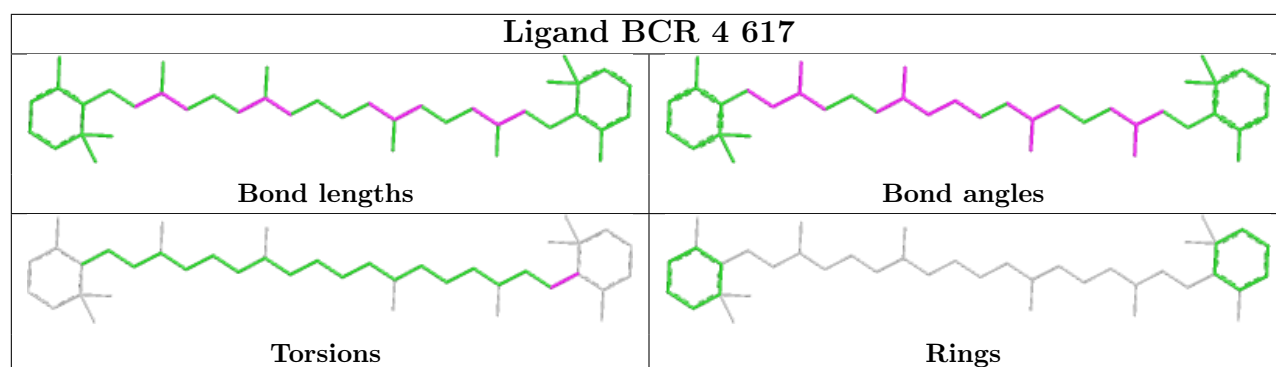


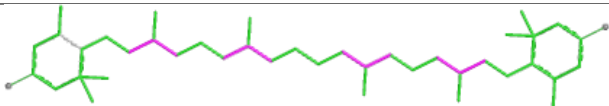
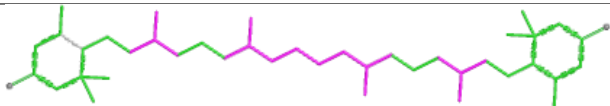
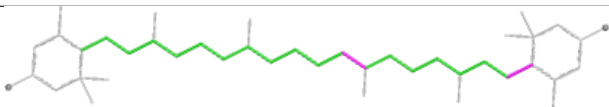
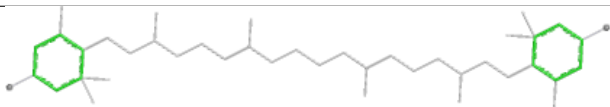
Ligand CHL a 605

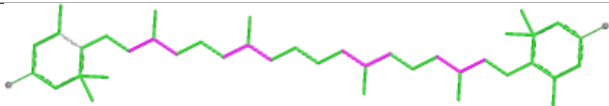
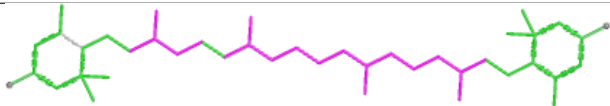
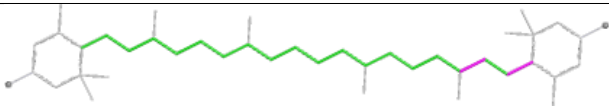
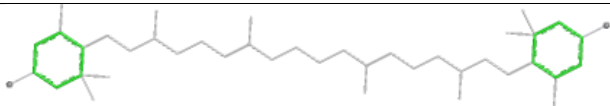


Ligand BCR 6 618

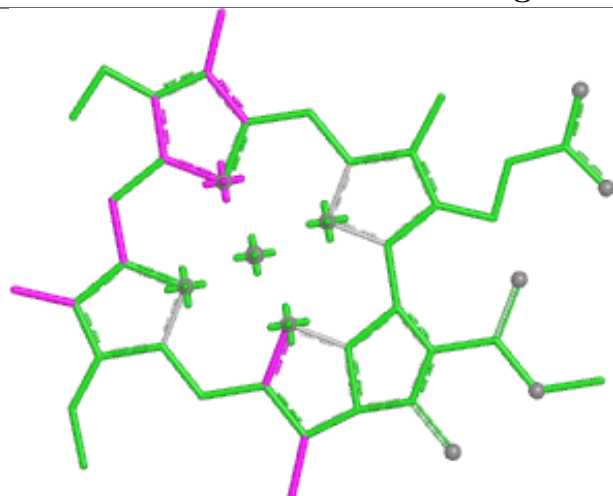




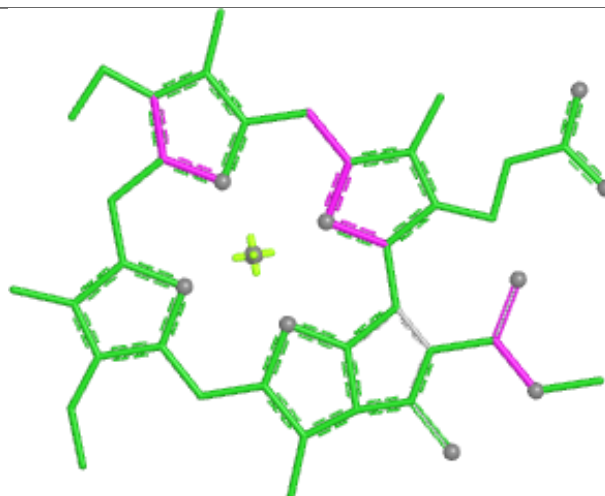
Ligand LUT 1 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

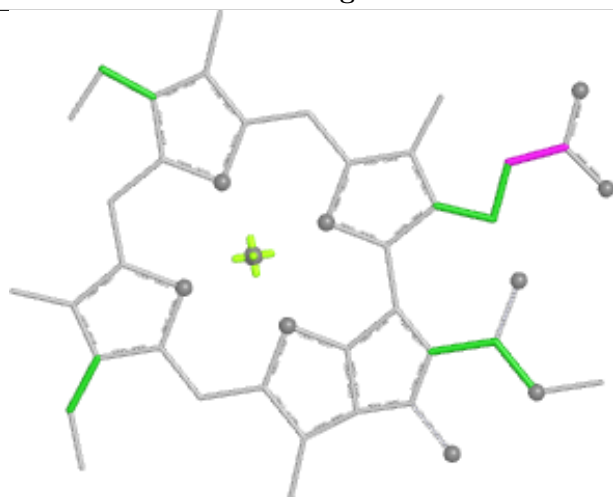
Ligand CLA A 836



Bond lengths



Bond angles

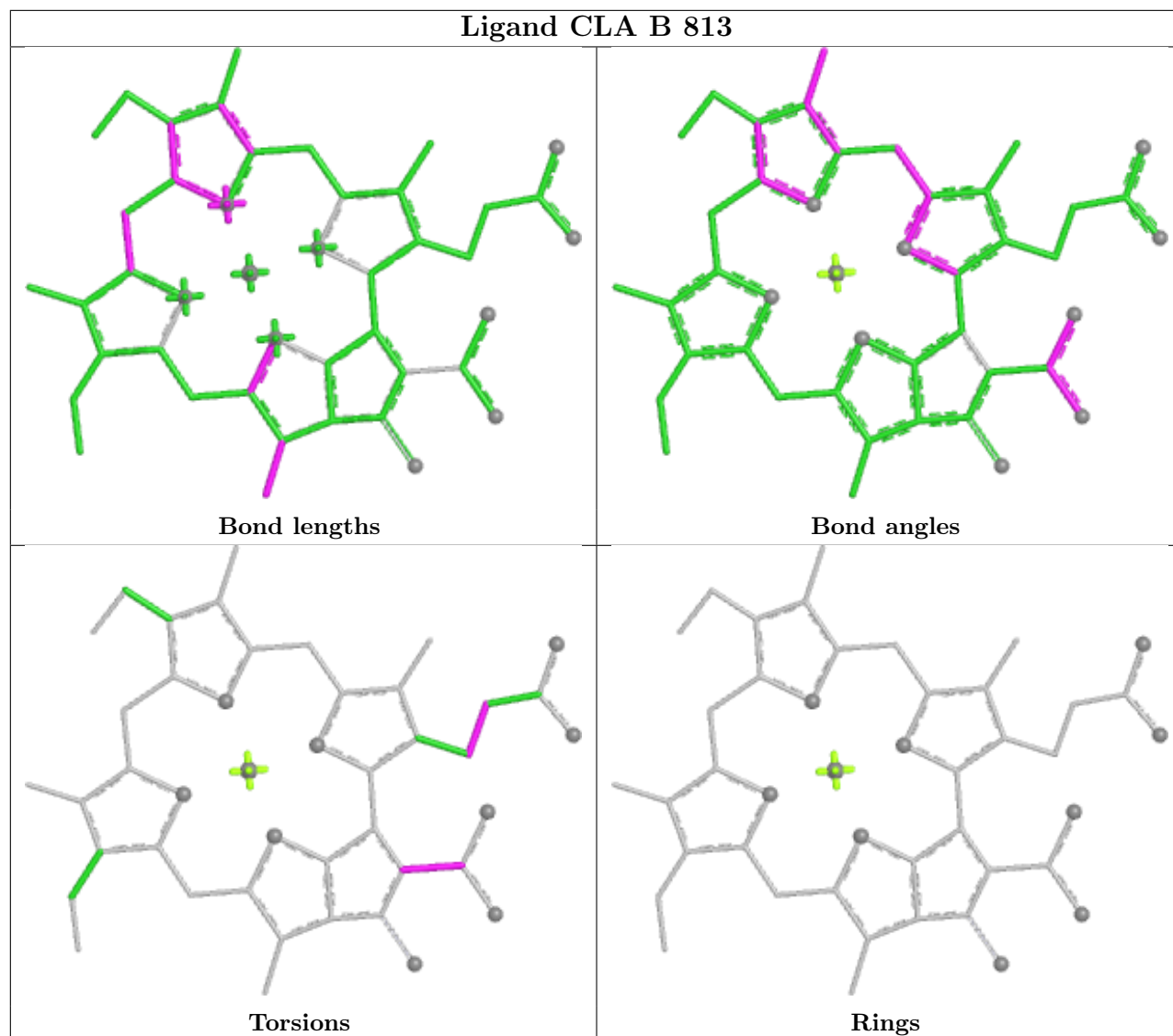


Torsions

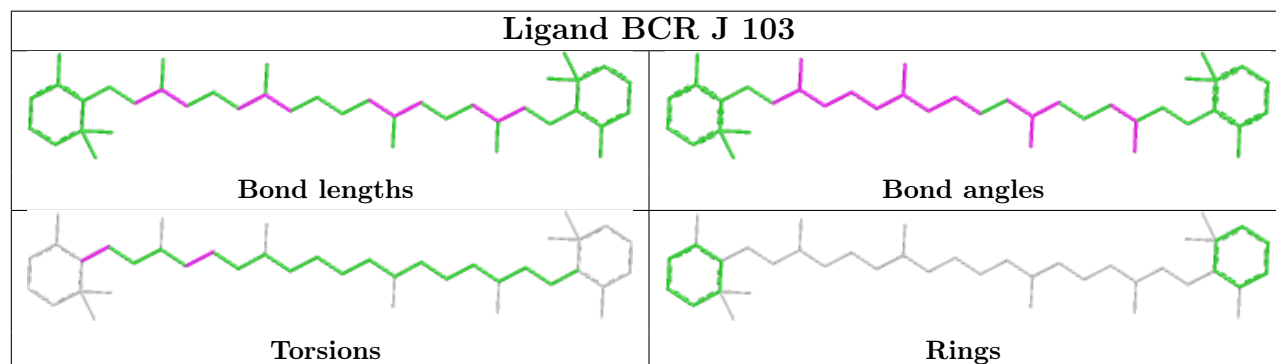


Rings

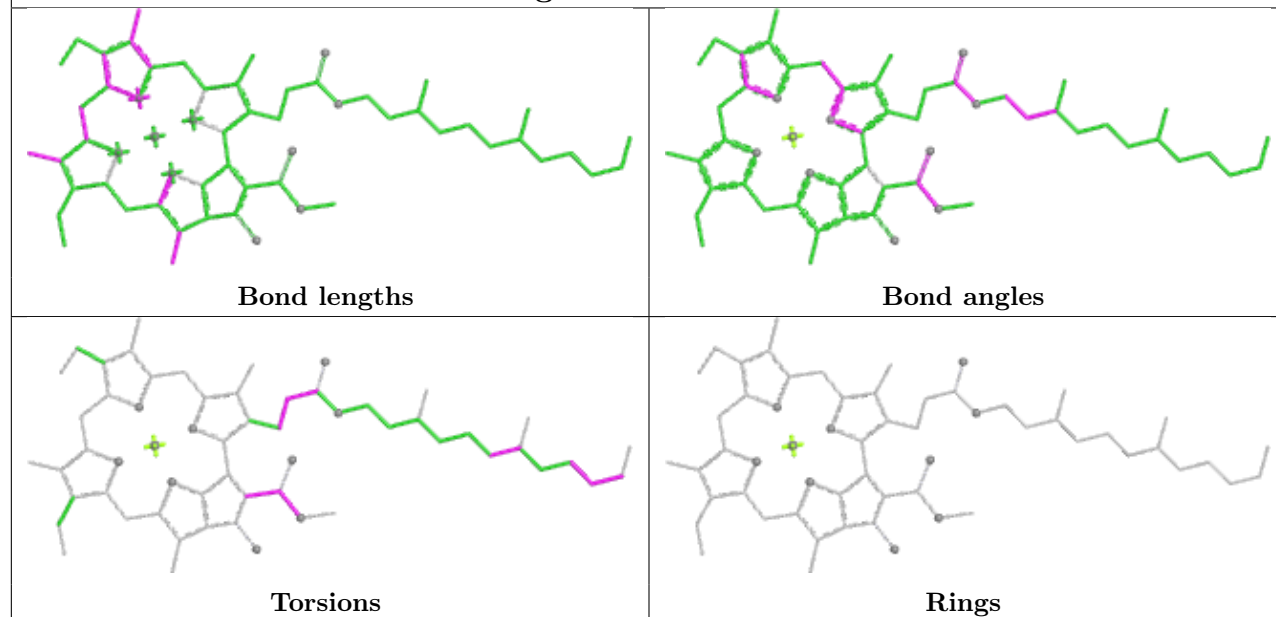
Ligand CLA B 813



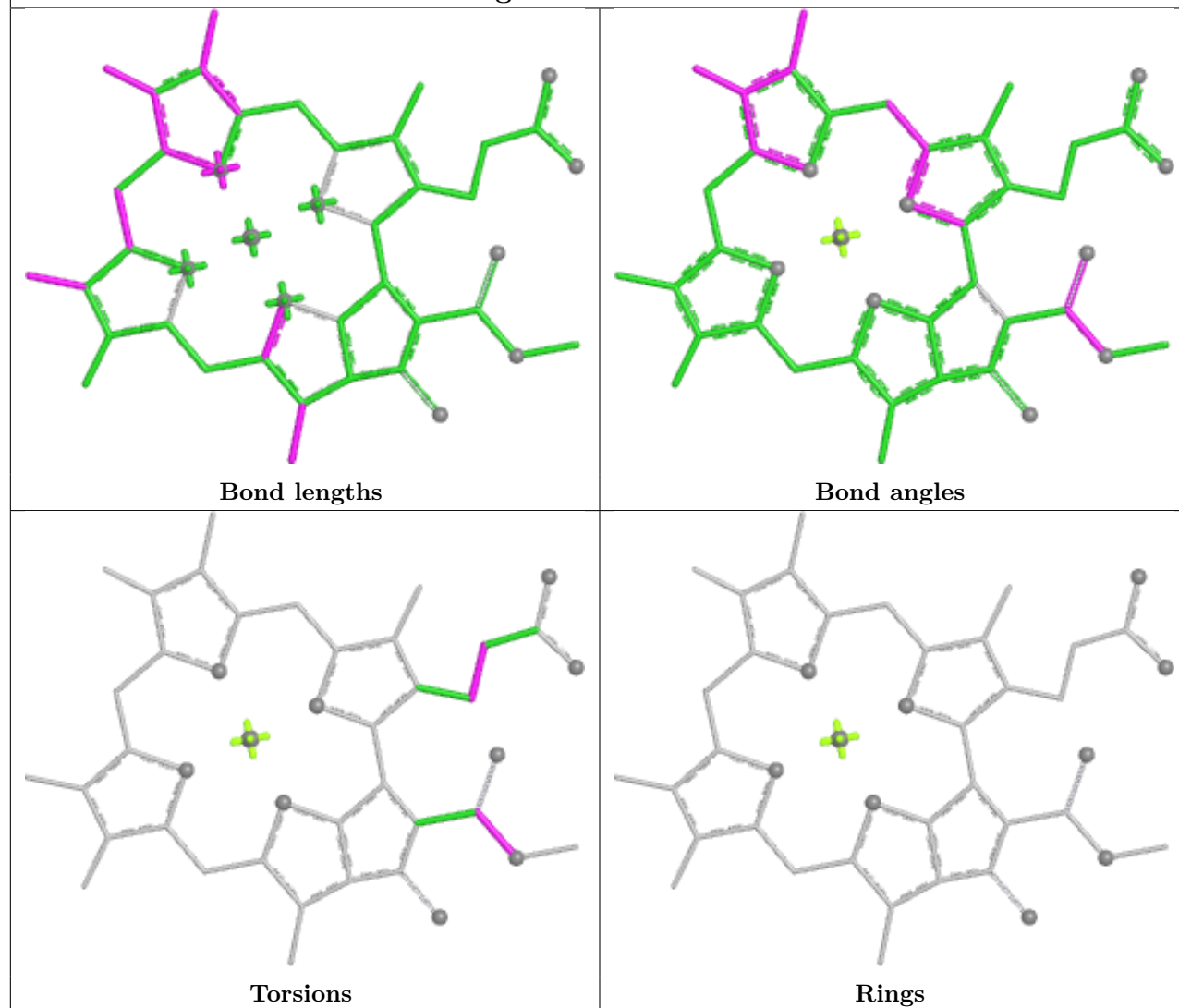
Ligand BCR J 103



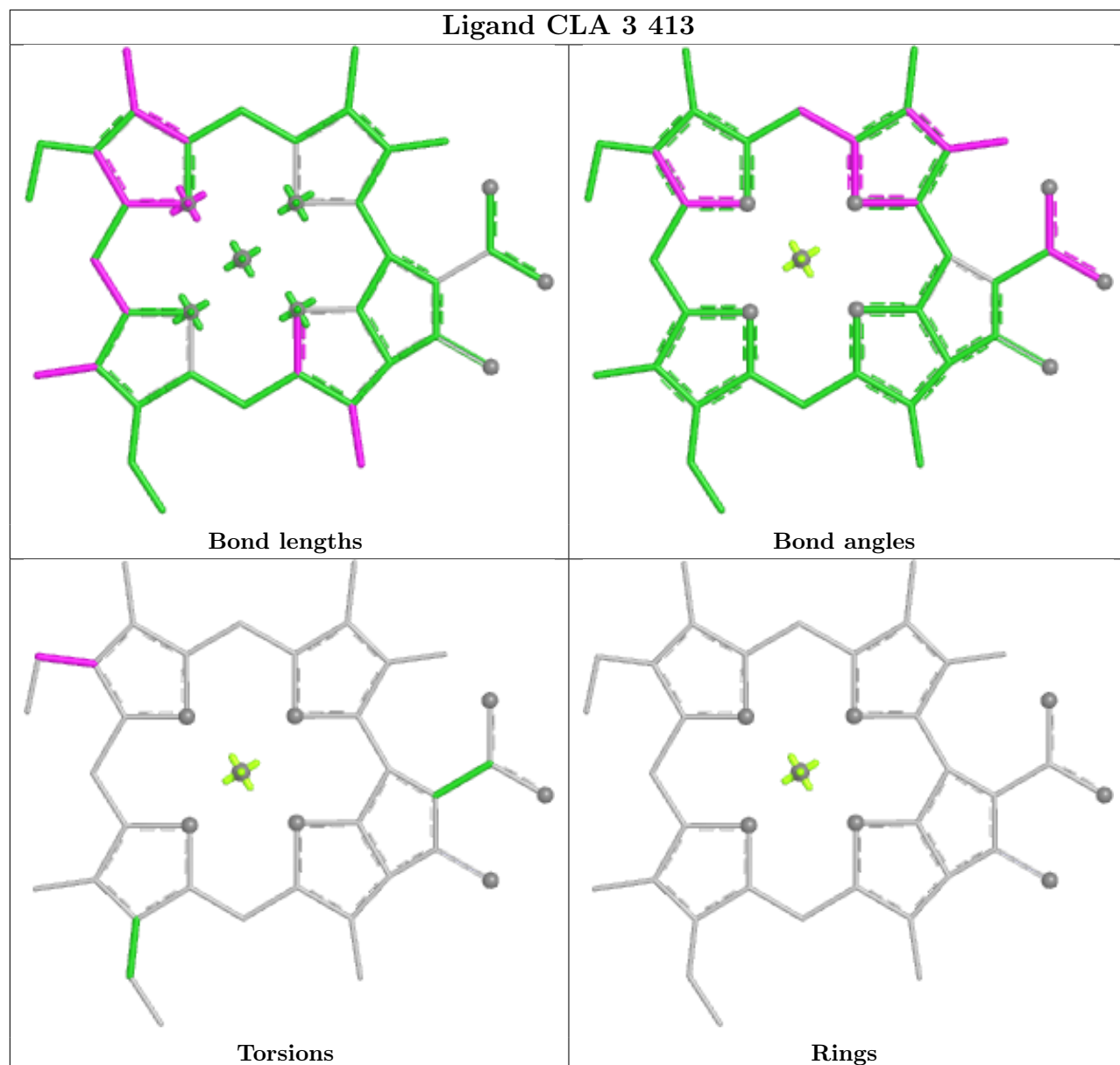
Ligand CLA b 303



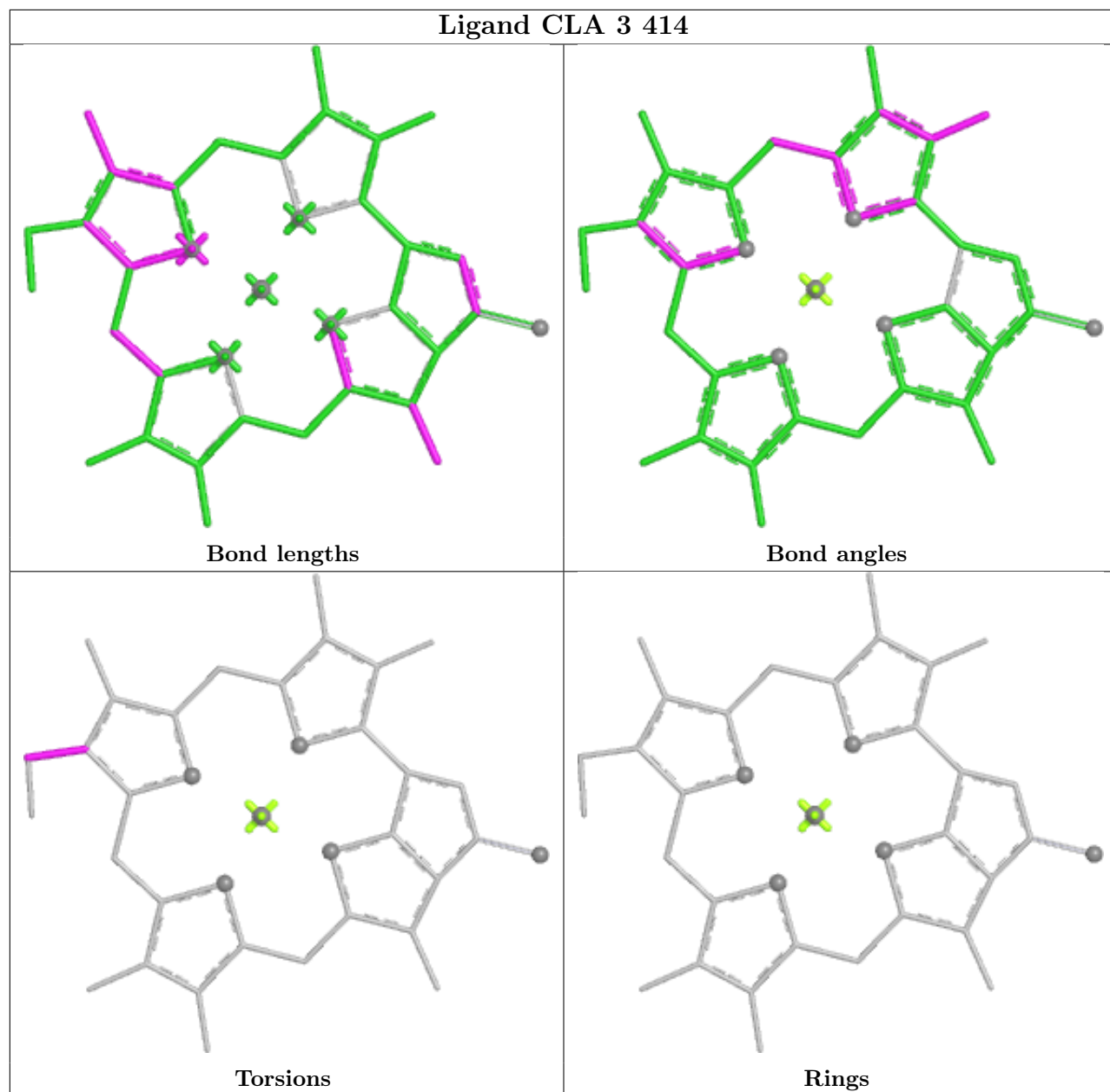
Ligand CLA 1 316



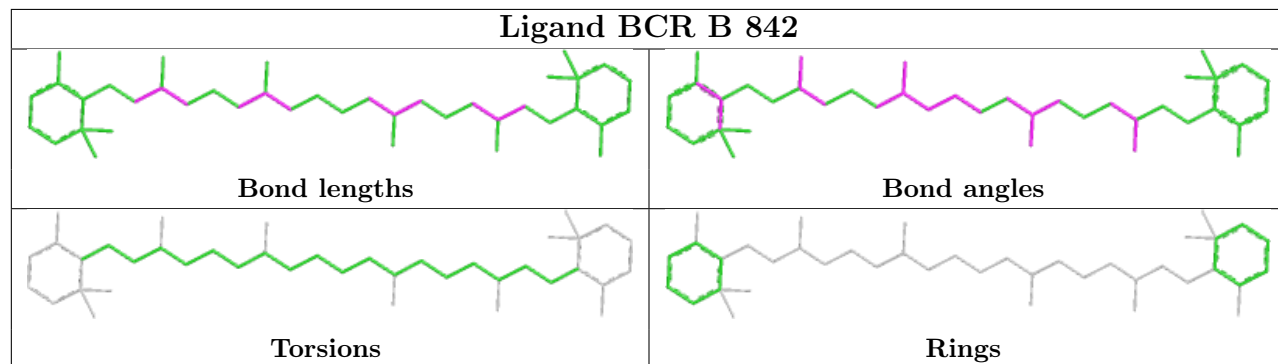
Ligand CLA 3 413

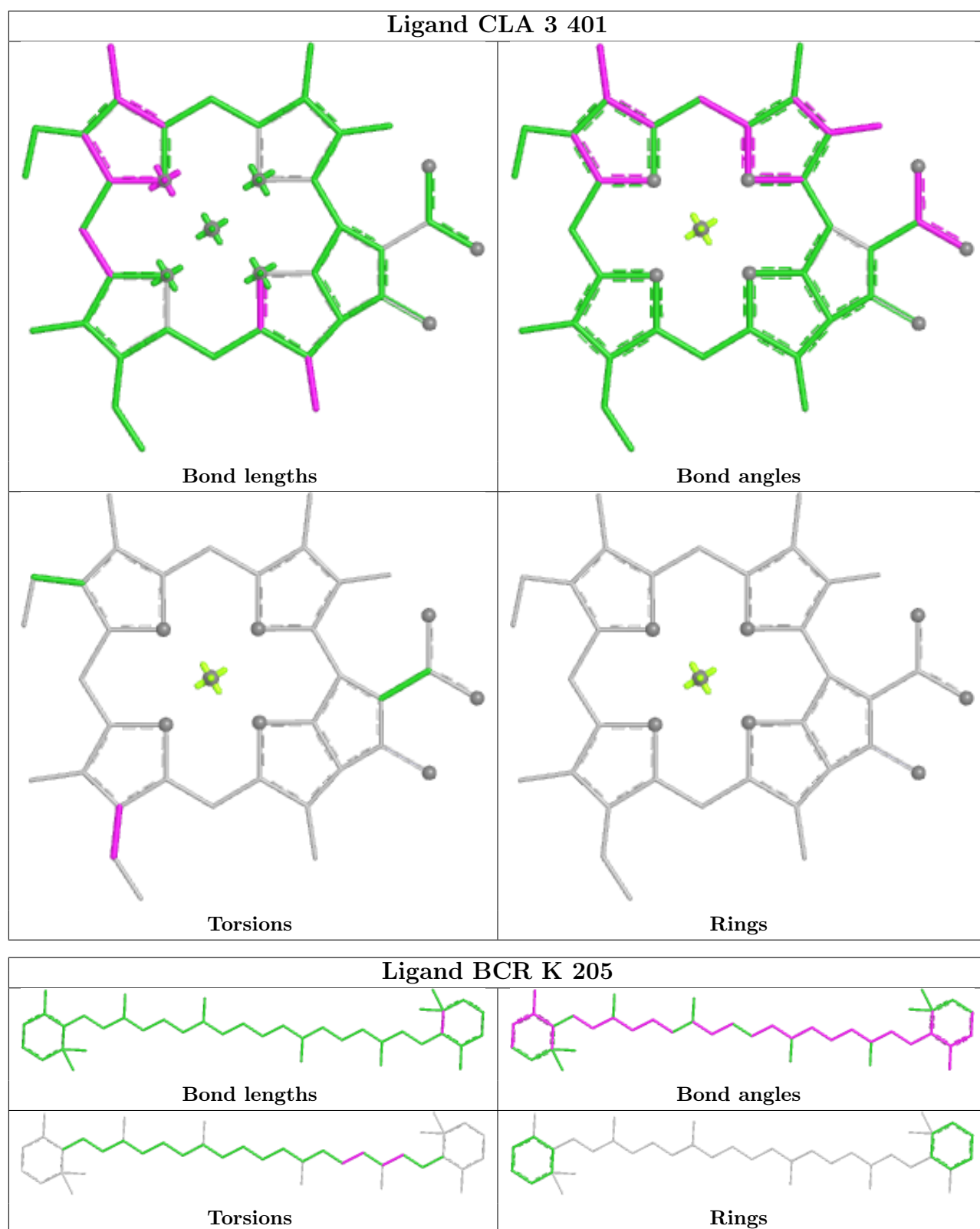


Ligand CLA 3 414



Ligand BCR B 842





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

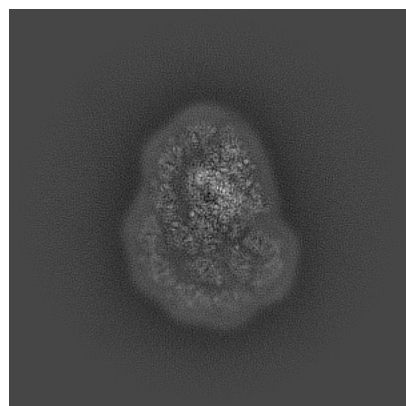
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33401. These allow visual inspection of the internal detail of the map and identification of artifacts.

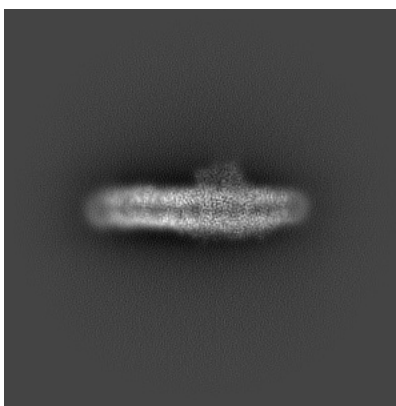
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

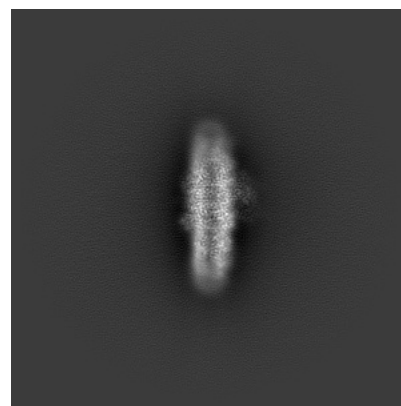
6.1.1 Primary map



X

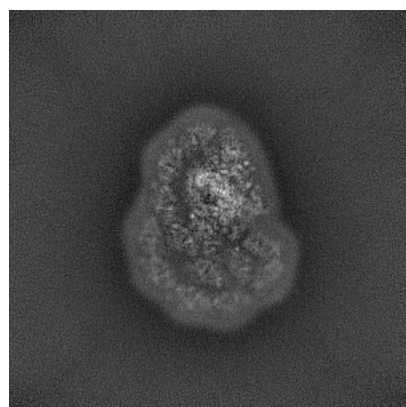


Y

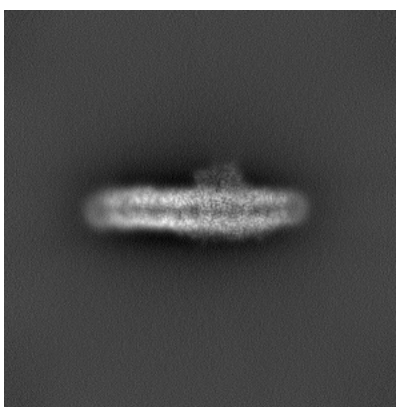


Z

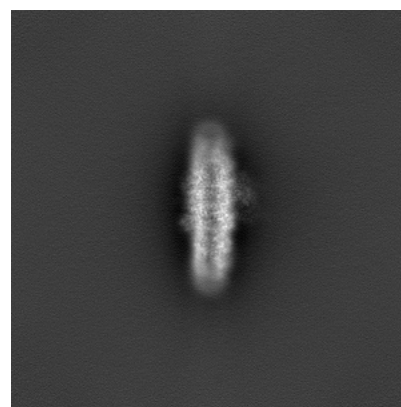
6.1.2 Raw map



X



Y

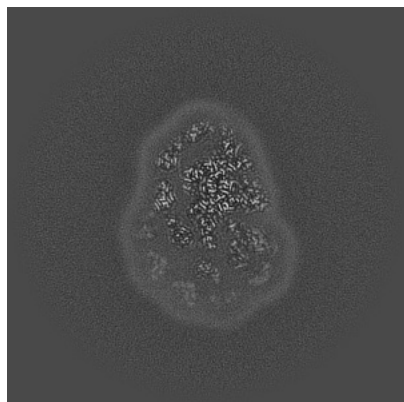


Z

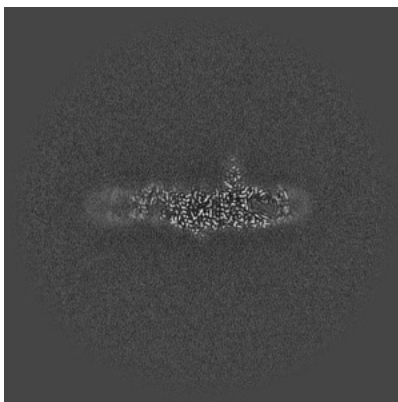
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

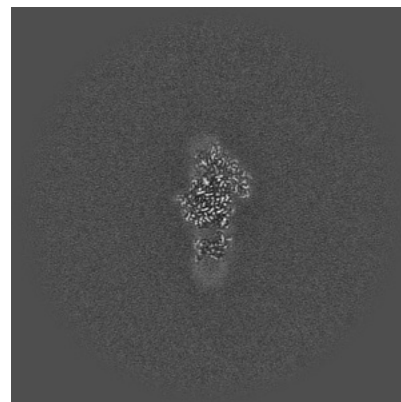
6.2.1 Primary map



X Index: 240

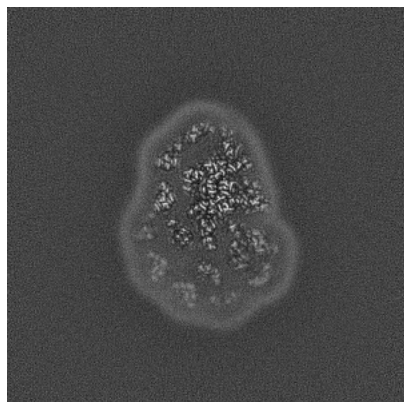


Y Index: 240

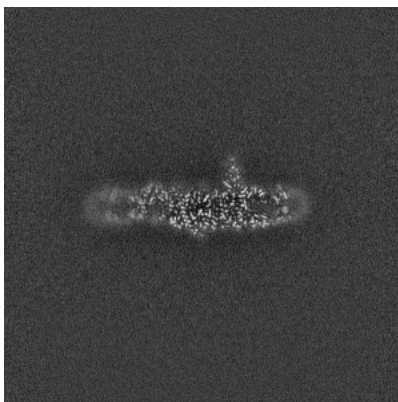


Z Index: 240

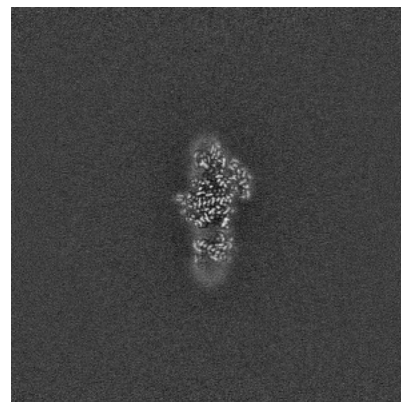
6.2.2 Raw map



X Index: 240



Y Index: 240

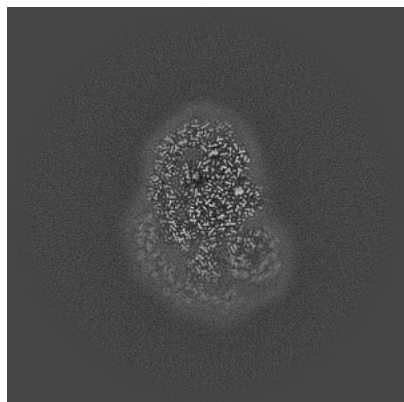


Z Index: 240

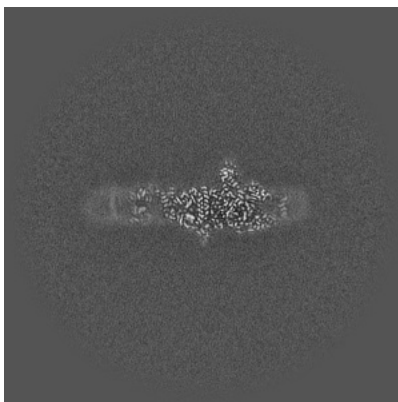
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

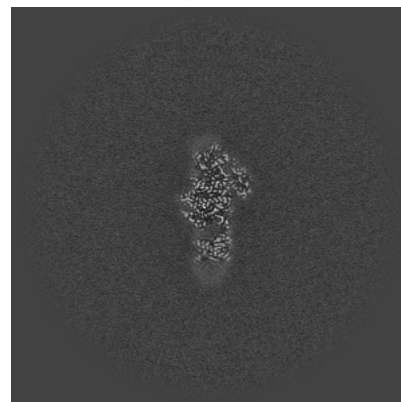
6.3.1 Primary map



X Index: 252

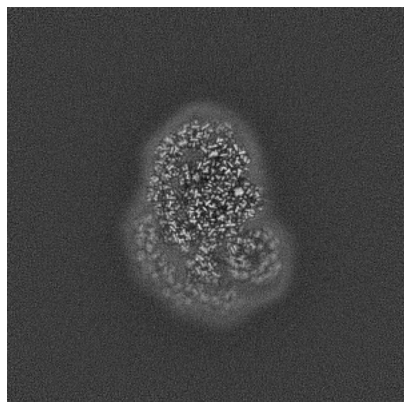


Y Index: 247

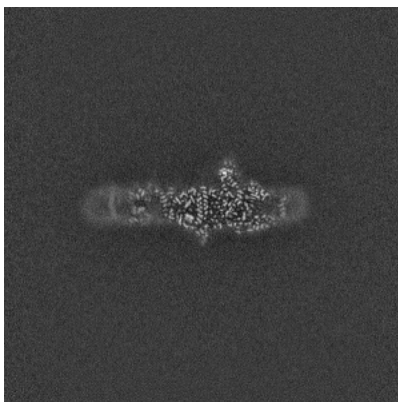


Z Index: 243

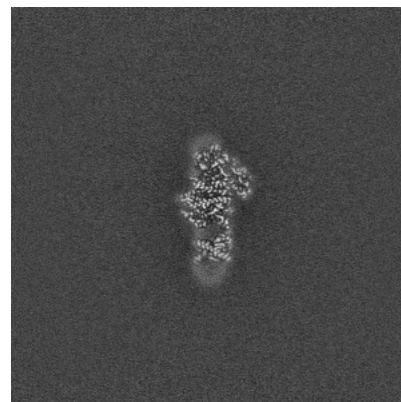
6.3.2 Raw map



X Index: 252



Y Index: 247

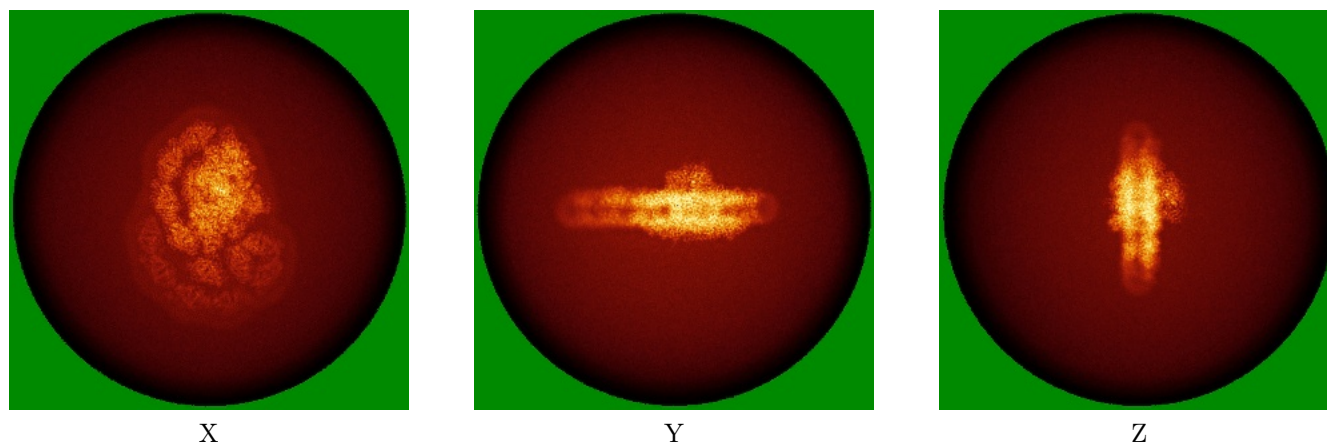


Z Index: 242

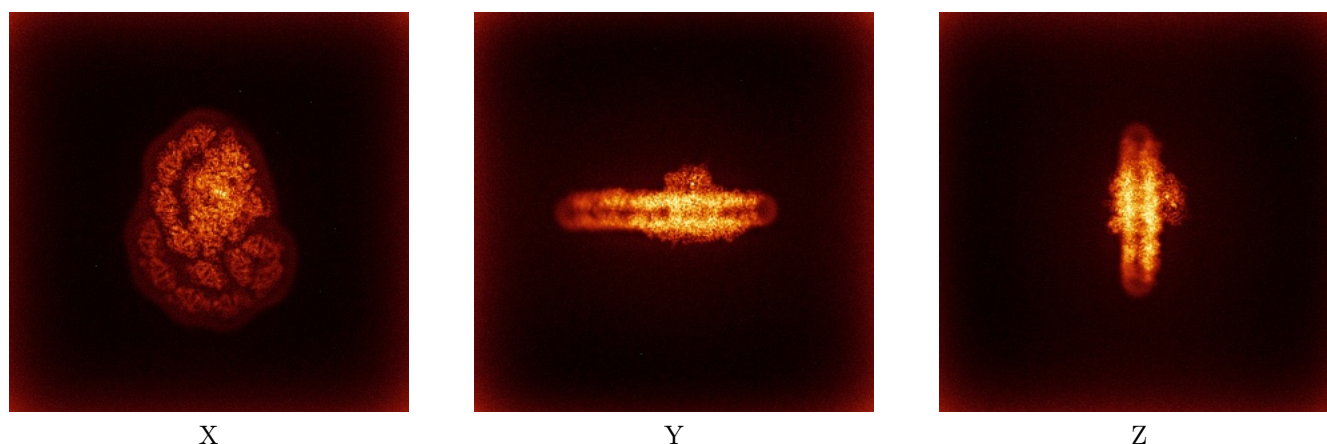
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

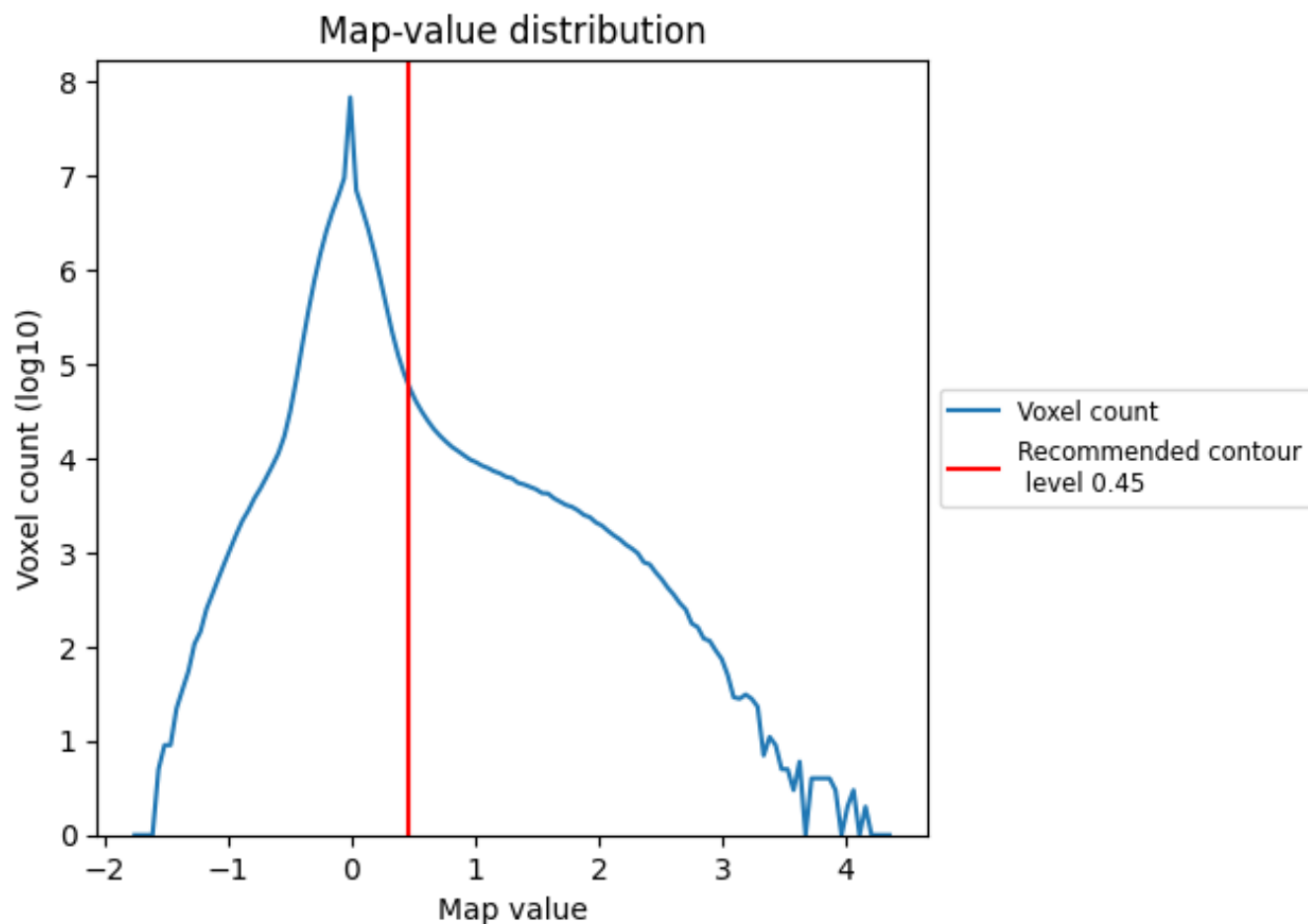
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

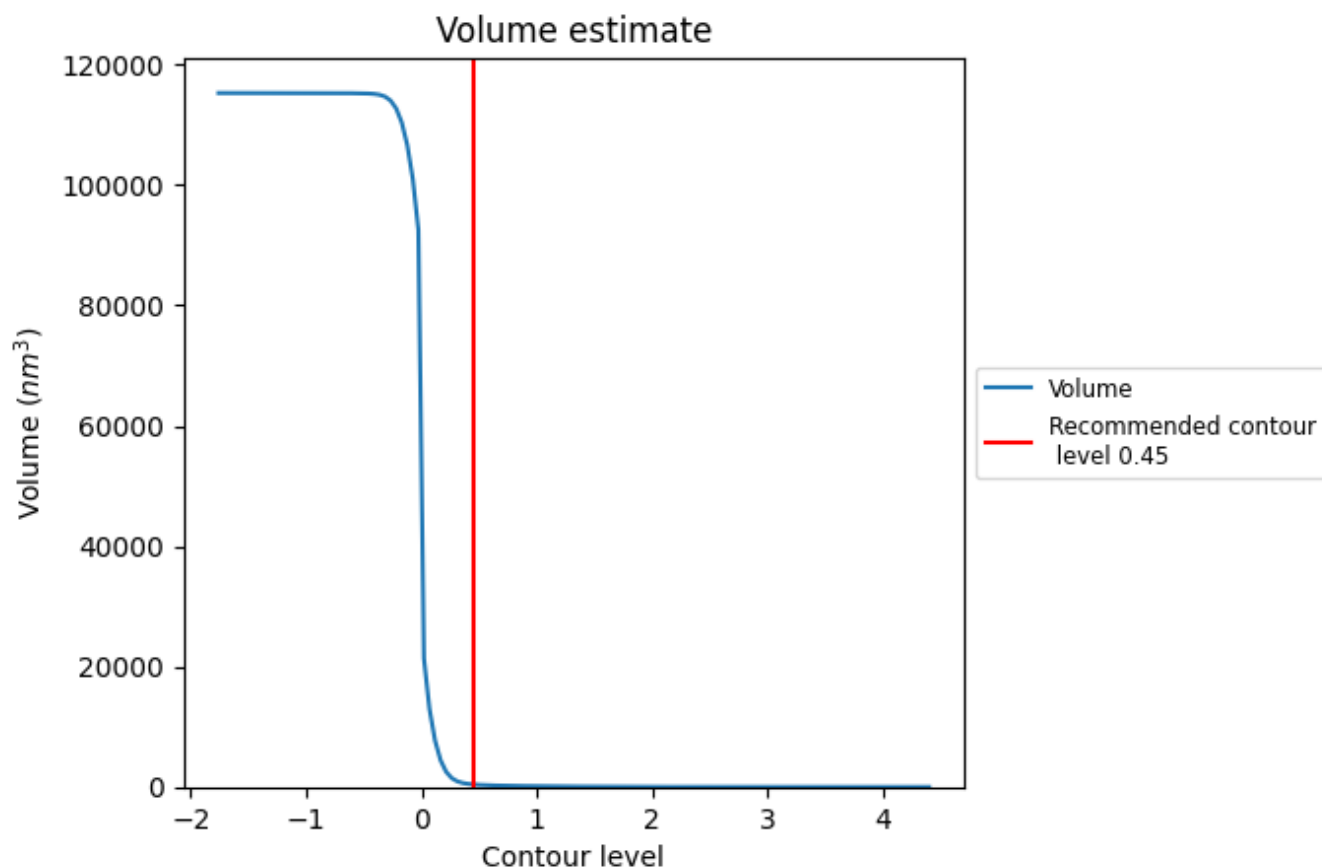
This section contains the results of statistical analysis of the map.

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.

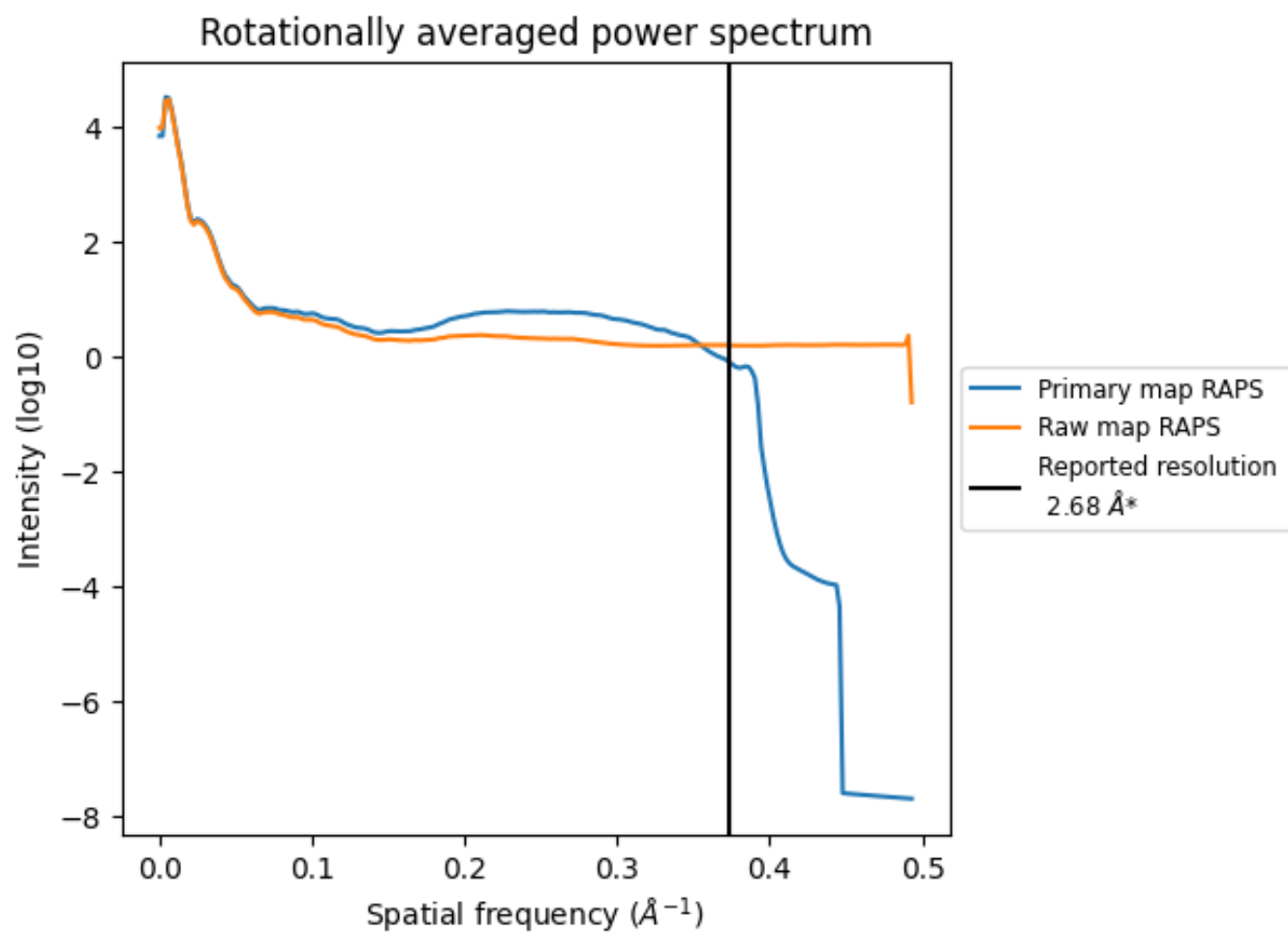
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 378 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 ⓘ

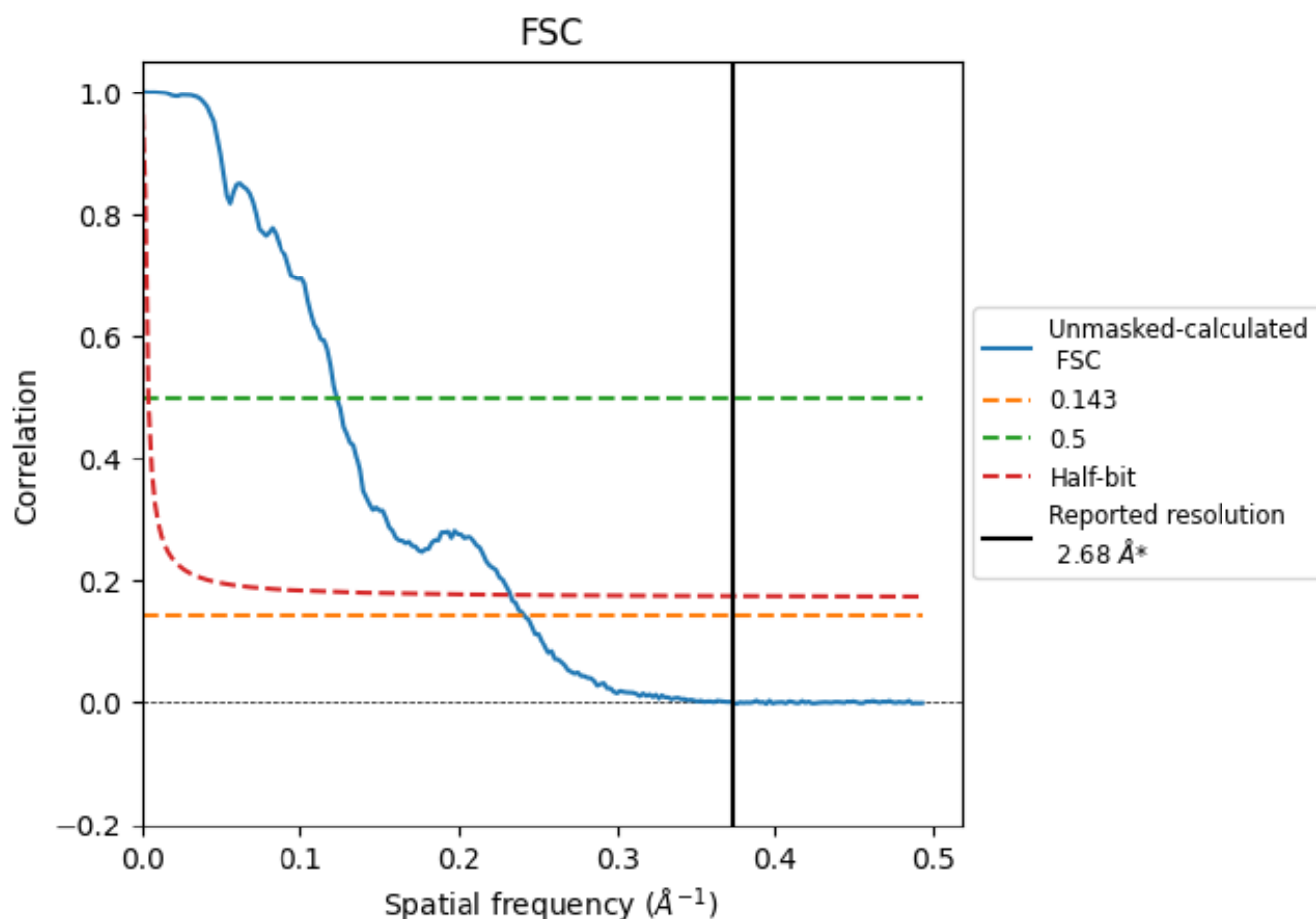


*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	8.13	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.68 by more than 10 %

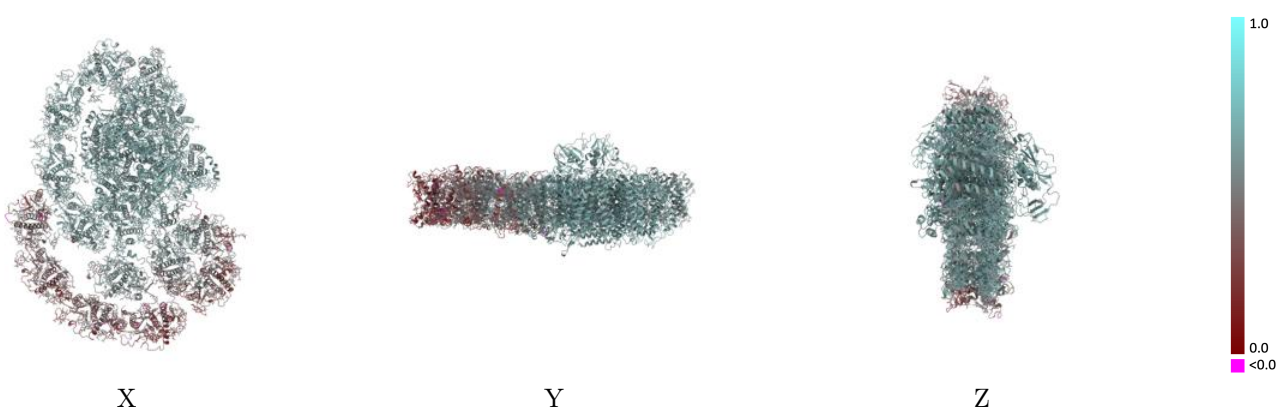
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33401 and PDB model 7XQP. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)

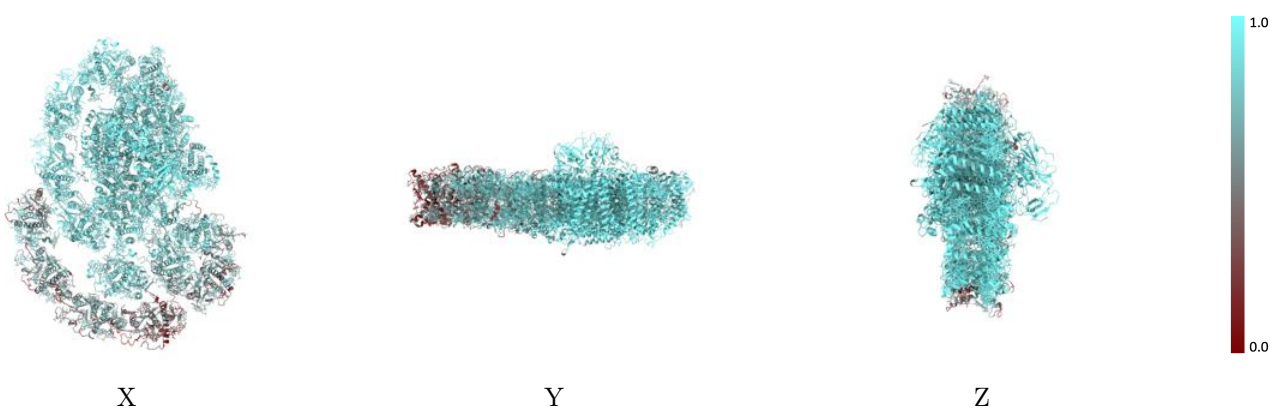
This section was not generated.

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



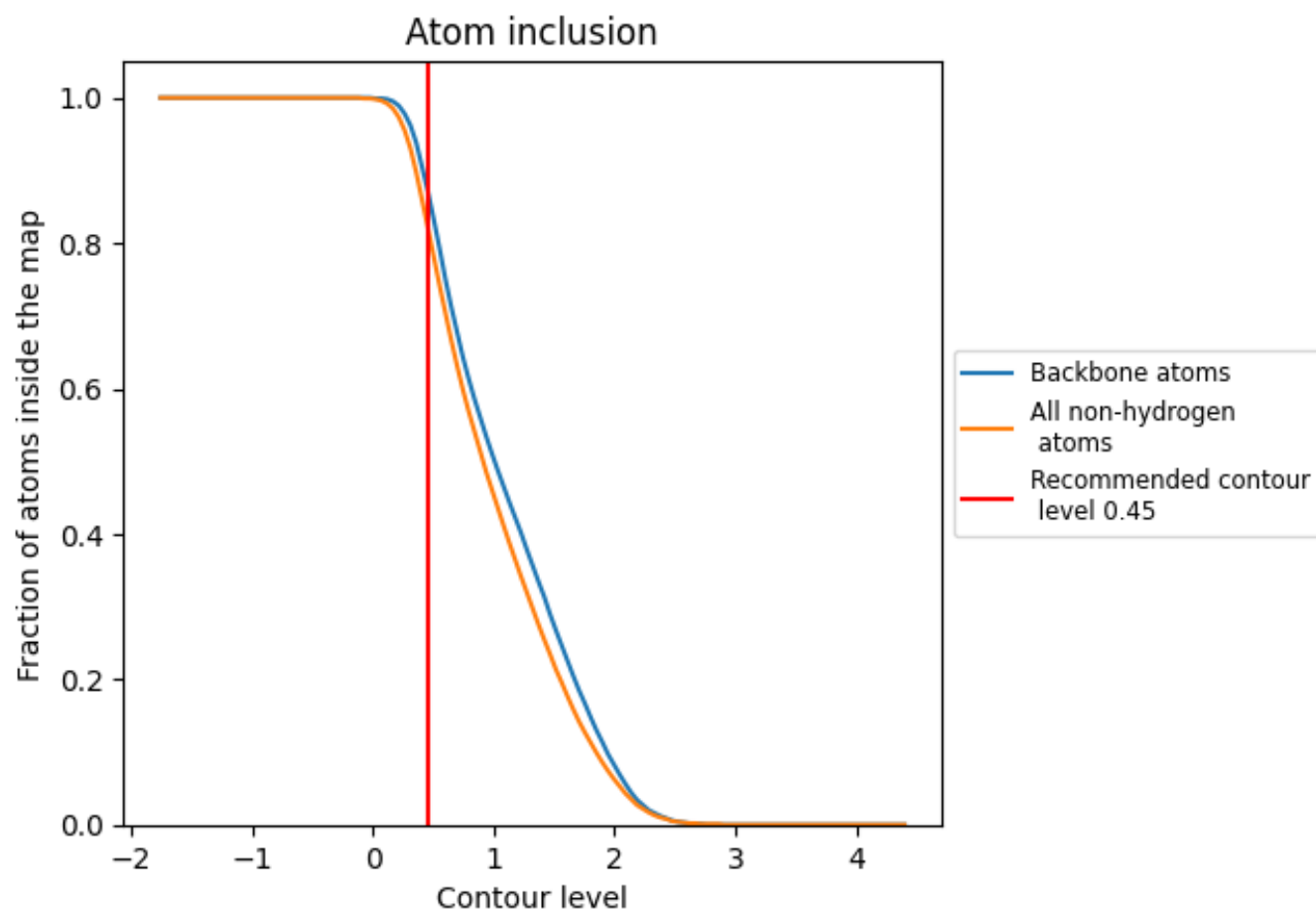
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5360
1	 0.9160	 0.5760
2	 0.9220	 0.5910
3	 0.9350	 0.6030
4	 0.9200	 0.5810
5	 0.5830	 0.3590
6	 0.5300	 0.3330
7	 0.3390	 0.2870
8	 0.5420	 0.3320
9	 0.8250	 0.5250
A	 0.9620	 0.6340
B	 0.9610	 0.6300
C	 0.9730	 0.6210
D	 0.9470	 0.6150
E	 0.9410	 0.6070
F	 0.9220	 0.6030
G	 0.7980	 0.5530
H	 0.8880	 0.5780
I	 0.9470	 0.6180
J	 0.9350	 0.6110
K	 0.9400	 0.6090
L	 0.9430	 0.6120
M	 0.8980	 0.5880
O	 0.8320	 0.5260
a	 0.5470	 0.3560
b	 0.7680	 0.4910
c	 0.7450	 0.4660

