



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:25 PM UTC

PDB ID : 7KUX / pdb_00007kux
EMDB ID : EMD-23040
Title : The Structure of the moss PSI-LHCI reveals the evolution of the LHCI antenna
Authors : Riddle, R.; Gorski, C.; Toporik, H.; Dobson, Z.; Da, Z.; Williams, D.; Mazor, Y.
Deposited on : 2020-11-25
Resolution : 2.80 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

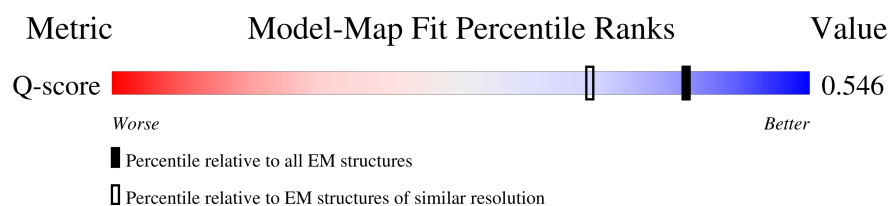
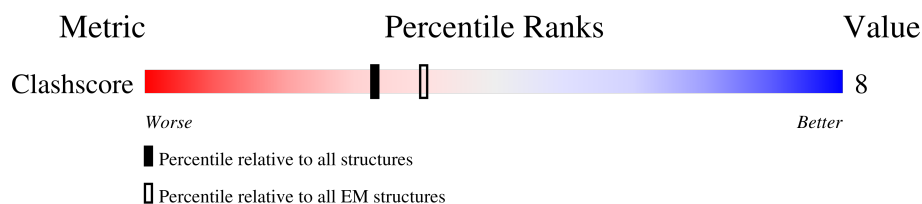
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

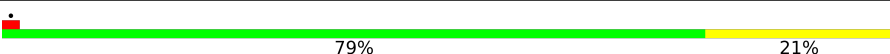
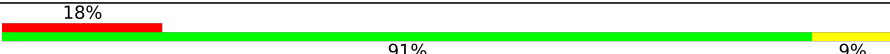
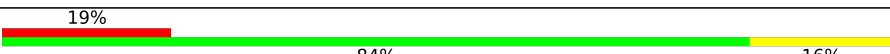
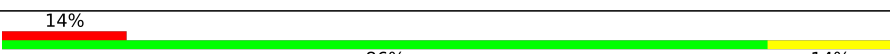
The reported resolution of this entry is 2.80 Å.

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.



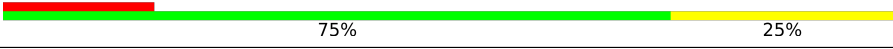
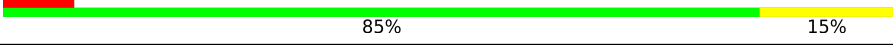
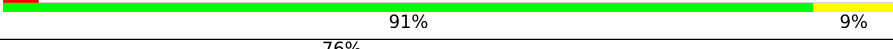
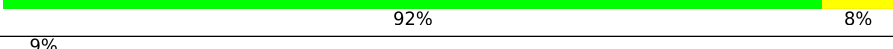
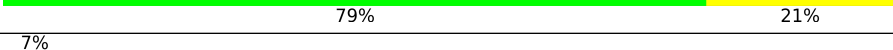
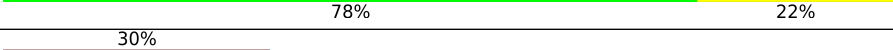
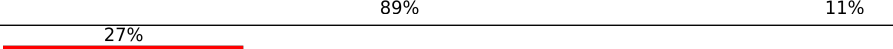
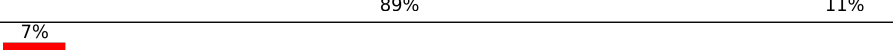
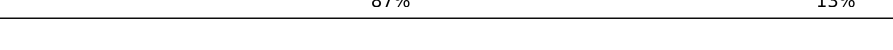
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	
2	B	732	
3	1	192	
4	2	203	
5	3	218	
6	4	203	

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Mol	Chain	Length	Quality of chain
7	C	80	
8	D	142	
9	E	63	
10	F	160	
11	G	91	
12	H	87	
13	I	34	
14	J	41	
15	K	81	
16	L	160	
17	M	30	

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
18	CL0	A	1011	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	604	X	-	-	-
19	CLA	1	606	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	609	X	-	-	-
19	CLA	1	610	X	-	-	-
19	CLA	1	612	X	-	-	-
19	CLA	1	613	X	-	-	-
19	CLA	1	614	X	-	-	-
19	CLA	1	615	X	-	-	-
19	CLA	2	603	X	-	-	-
19	CLA	2	604	X	-	-	-
19	CLA	2	609	X	-	-	-
19	CLA	2	610	X	-	-	-
19	CLA	2	612	X	-	-	-
19	CLA	2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	614	X	-	-	-
19	CLA	3	602	X	-	-	-
19	CLA	3	604	X	-	-	-
19	CLA	3	605	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	607	X	-	-	-
19	CLA	3	609	X	-	-	-
19	CLA	3	610	X	-	-	-
19	CLA	3	611	X	-	-	-
19	CLA	3	612	X	-	-	-
19	CLA	3	613	X	-	-	-
19	CLA	3	614	X	-	-	-
19	CLA	3	617	X	-	-	-
19	CLA	4	601	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	610	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	613	X	-	-	-
19	CLA	4	614	X	-	-	-
19	CLA	A	1022	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1105	X	-	-	-
19	CLA	A	1106	X	-	-	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1114	X	-	-	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1139	X	-	-	-
19	CLA	A	1801	X	-	-	-
19	CLA	B	1012	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1220	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	G	201	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	H	200	X	-	-	-
19	CLA	J	102	X	-	-	-
19	CLA	K	201	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	L	303	X	-	-	-
27	CHL	1	601	X	-	-	-
27	CHL	1	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	2	601	X	-	-	-
27	CHL	2	602	X	-	-	-
27	CHL	2	606	X	-	-	-
27	CHL	2	607	X	-	-	-
27	CHL	2	608	X	-	-	-
27	CHL	2	611	X	-	-	-
27	CHL	2	615	X	-	-	-
27	CHL	3	608	X	-	-	-
27	CHL	4	606	X	-	-	-
27	CHL	4	607	X	-	-	-
27	CHL	4	608	X	-	-	-
27	CHL	4	615	X	-	-	-
28	LUT	2	623	X	-	-	-
28	LUT	4	623	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35803 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
			5837	3827	993	998	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5845	3836	995	998	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	192	Total	C	N	O	S	0	0
			1473	961	247	264	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	203	Total	C	N	O	S	0	0
			1567	1021	262	280	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	218	Total	C	N	O	S	0	0
			1678	1099	272	300	7		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	203	Total	C	N	O	S	0	0
			1574	1024	264	281	5		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

- Molecule 8 is a protein called PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1109	711	195	200	3		

- Molecule 9 is a protein called PsuE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			500	317	89	94		

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	160	Total	C	N	O	S	0	0
			1239	801	215	220	3		

- Molecule 11 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	91	Total	C	N	O	0	0
			689	444	119	126		

- Molecule 12 is a protein called PsuH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	87	Total	C	N	O	S	0	0
			659	418	114	126	1		

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

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

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

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

- Molecule 15 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	81	Total	C	N	O	S	0	0
			561	352	97	108	4		

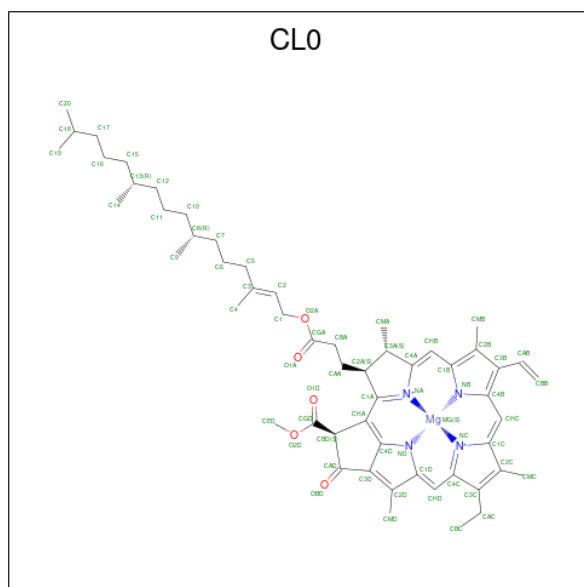
- Molecule 16 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1171	771	188	210	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

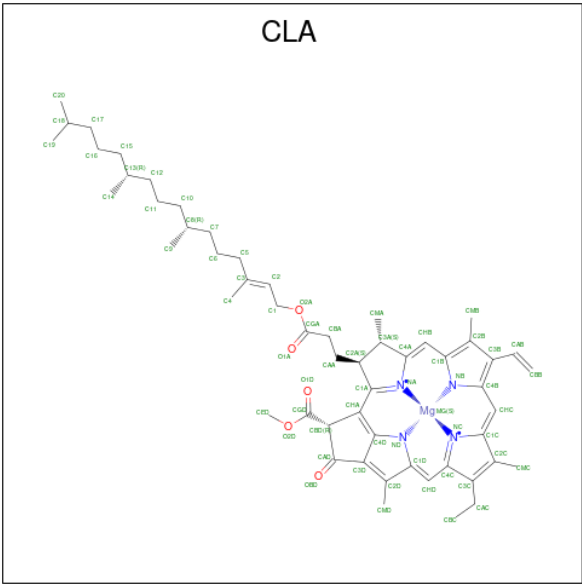
Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	30	Total	C	N	O		0	0
			223	146	36	41			

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N		0
			27	22	1	4		
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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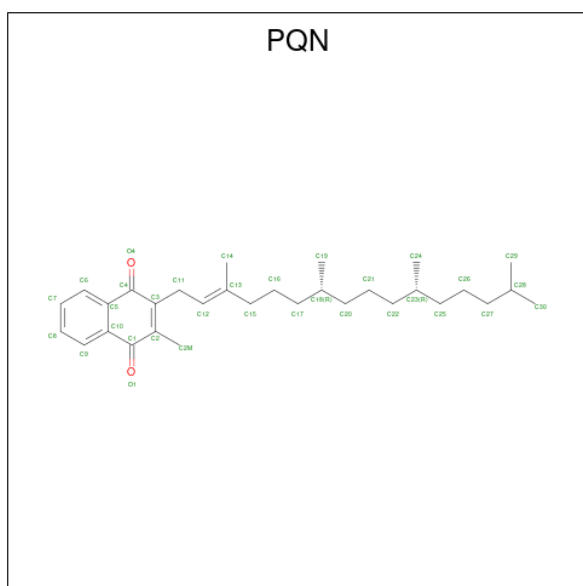
Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	F	1	Total 27	C 22	Mg 1	N 4		0
19	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	K	1	Total 27	C 22	Mg 1	N 4		0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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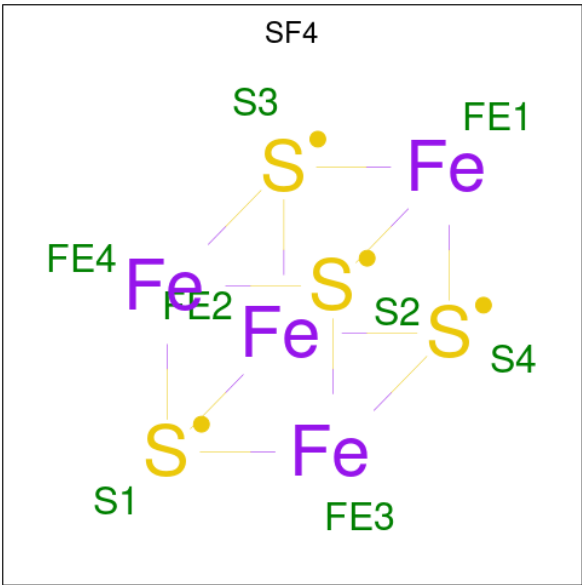
Mol	Chain	Residues	Atoms					AltConf
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



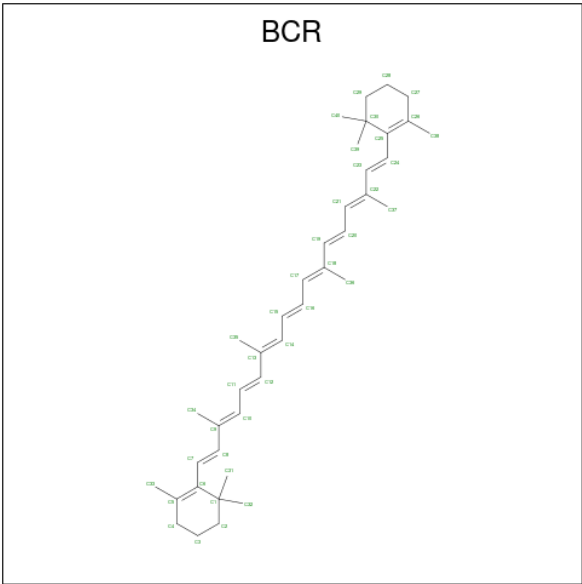
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



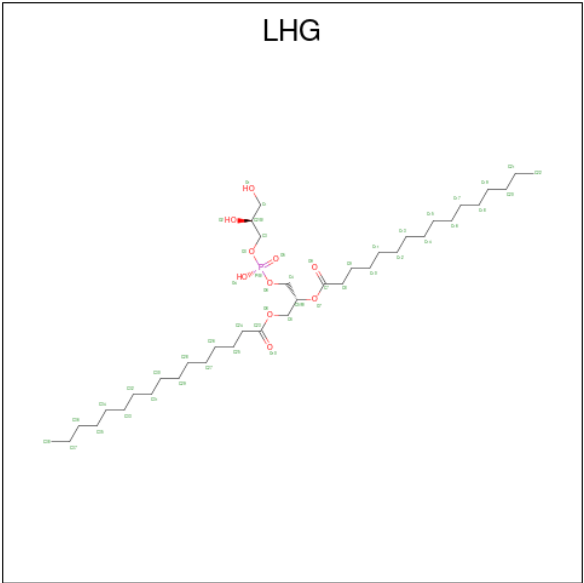
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	1	1	Total C 25 25	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	J	1	Total C 40 40	0

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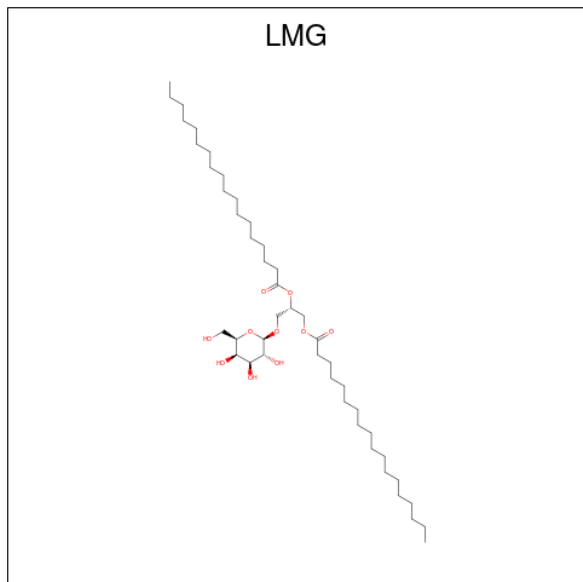
Mol	Chain	Residues	Atoms		AltConf
22	K	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	M	1	Total	C	0
			40	40	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



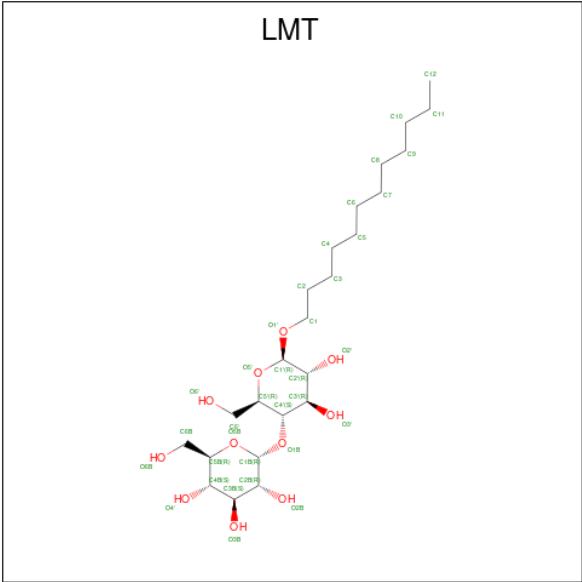
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			31	20	10	1	
23	B	1	Total	C	O	P	0
			35	24	10	1	
23	1	1	Total	C	O	P	0
			37	26	10	1	
23	2	1	Total	C	O	P	0
			32	21	10	1	
23	3	1	Total	C	O	P	0
			34	23	10	1	
23	4	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



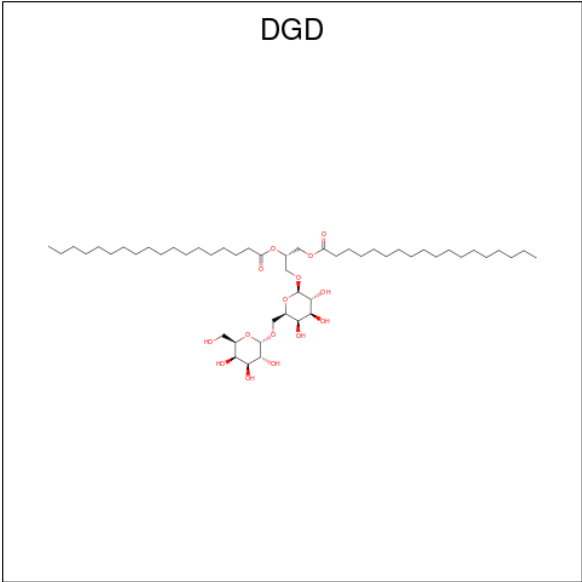
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			34	24	10	
24	2	1	Total	C	O	0
			36	26	10	
24	J	1	Total	C	O	0
			49	39	10	
24	J	1	Total	C	O	0
			26	16	10	

- Molecule 25 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



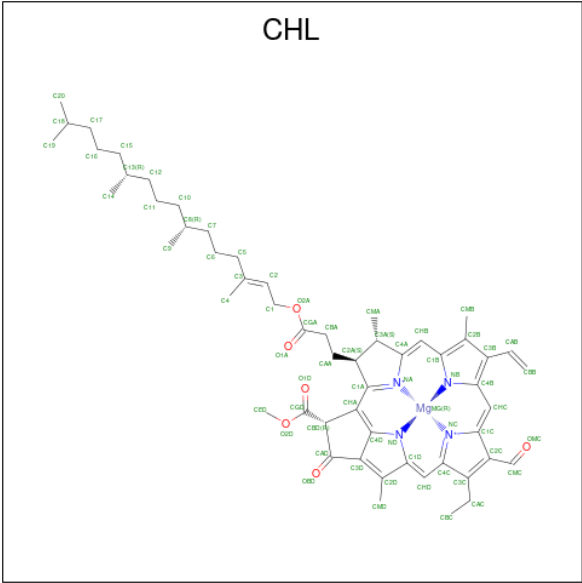
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	22	11	
25	B	1	Total	C	O	0
			31	20	11	
25	1	1	Total	C	O	0
			35	24	11	
25	4	1	Total	C	O	0
			35	24	11	
25	G	1	Total	C	O	0
			35	24	11	
25	G	1	Total	C	O	0
			31	20	11	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			61	46	15	

- Molecule 27 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



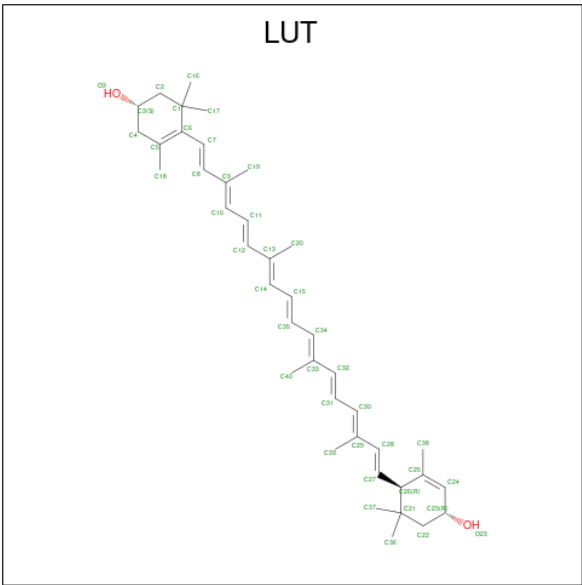
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		AltConf
29	A	15	Total	O	0
			15	15	
29	B	23	Total	O	0
			23	23	

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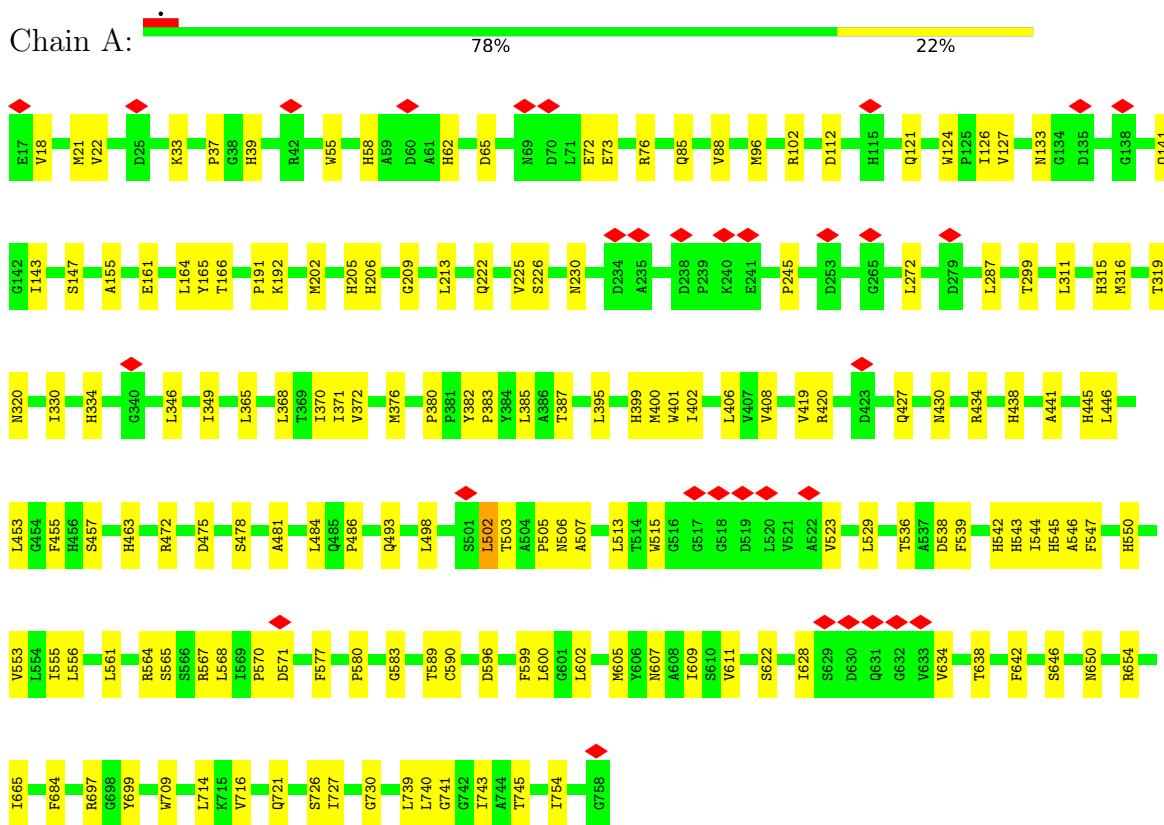
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Mol	Chain	Residues	Atoms		AltConf
29	3	1	Total 1	O 1	0
29	4	1	Total 1	O 1	0
29	C	2	Total 2	O 2	0
29	D	1	Total 1	O 1	0
29	F	1	Total 1	O 1	0
29	G	1	Total 1	O 1	0

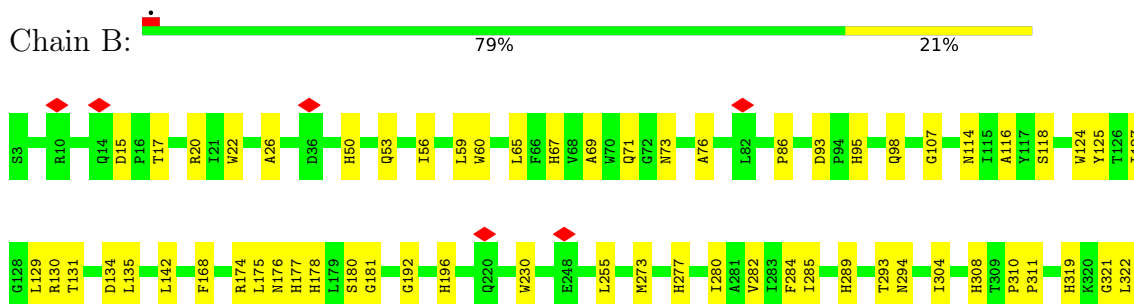
3 Residue-property plots

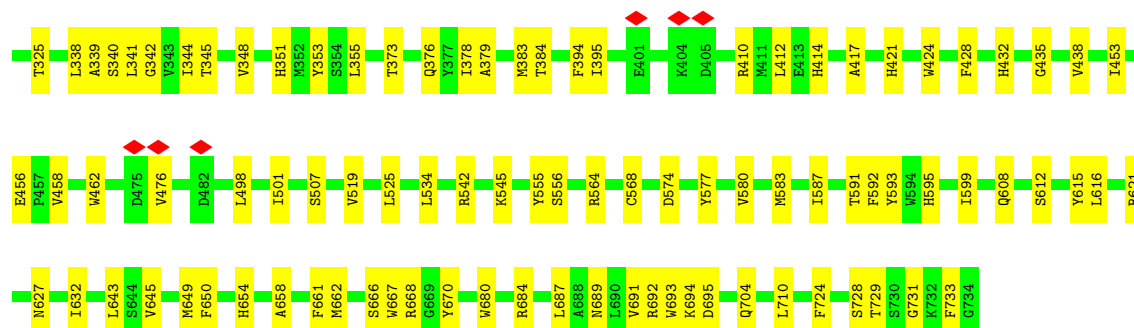
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

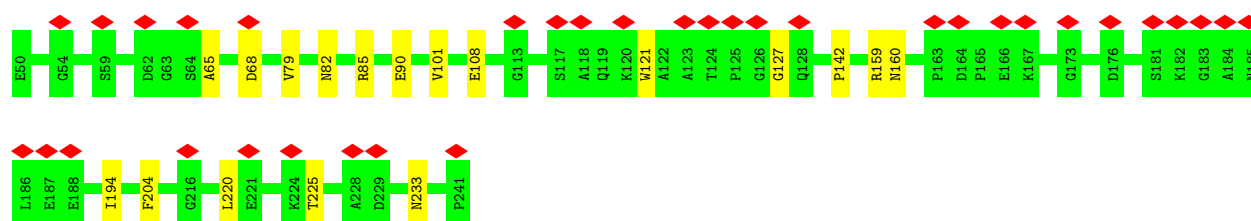


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

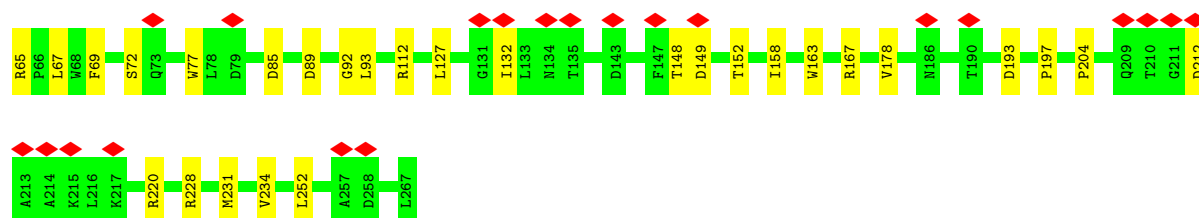
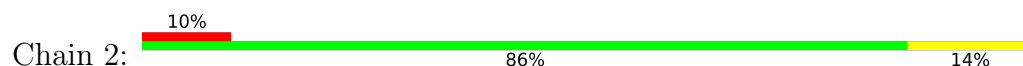




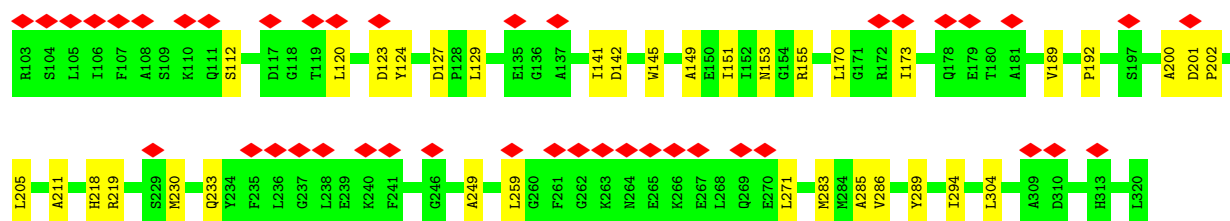
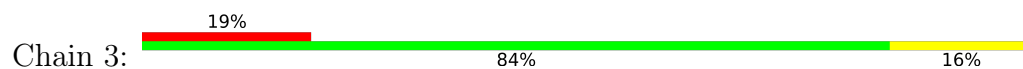
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic



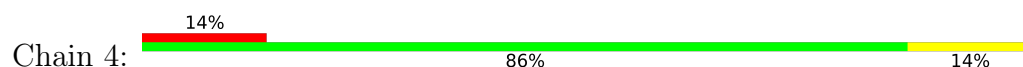
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

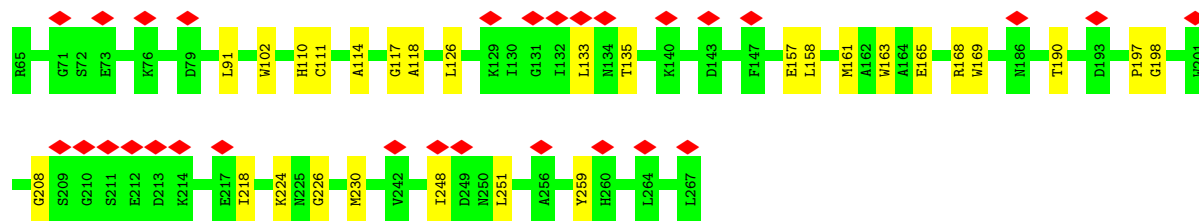


• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

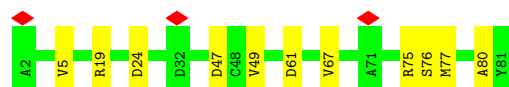
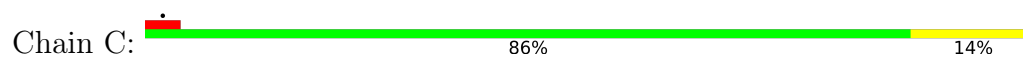


• Molecule 6: Chlorophyll a-b binding protein, chloroplastic

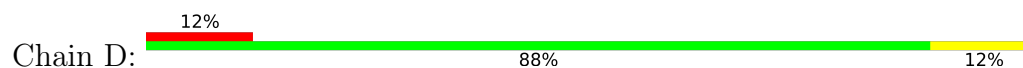




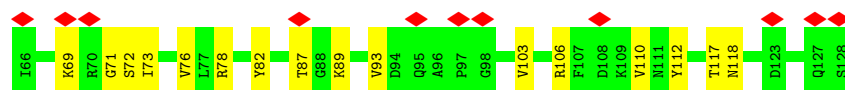
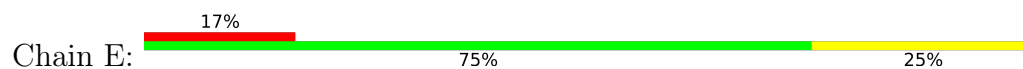
- Molecule 7: Photosystem I iron-sulfur center



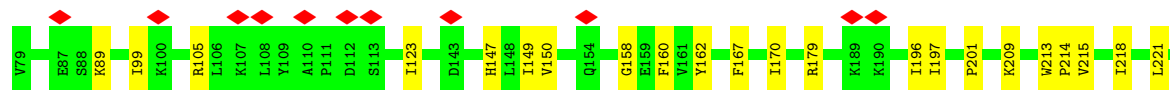
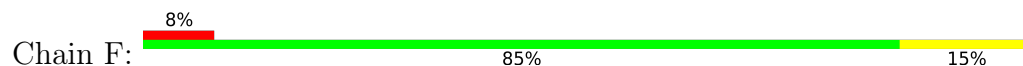
- Molecule 8: PsaD



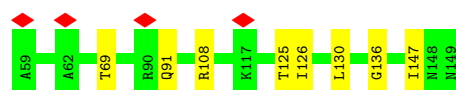
- Molecule 9: PsaE



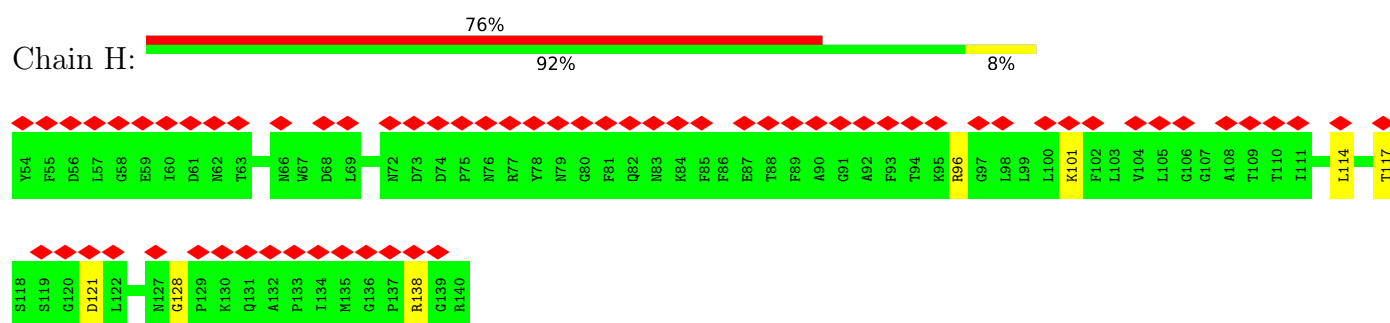
- Molecule 10: PSI-F



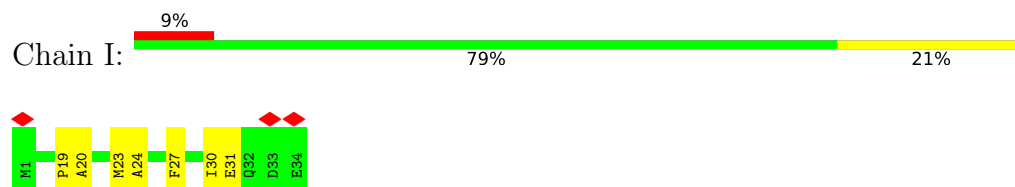
- Molecule 11: PSI-G



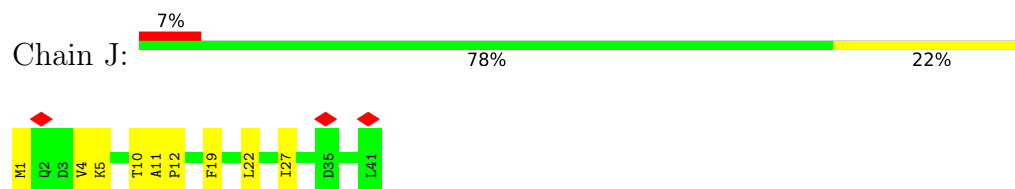
- Molecule 12: PsaH



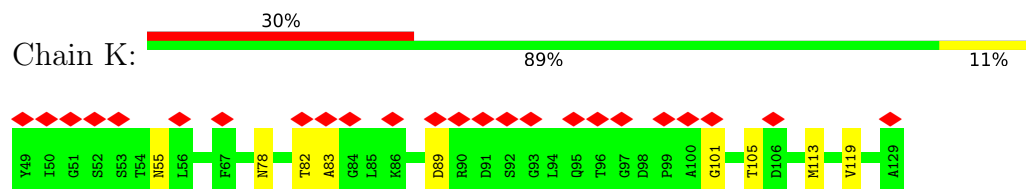
- Molecule 13: Photosystem I reaction center subunit VIII



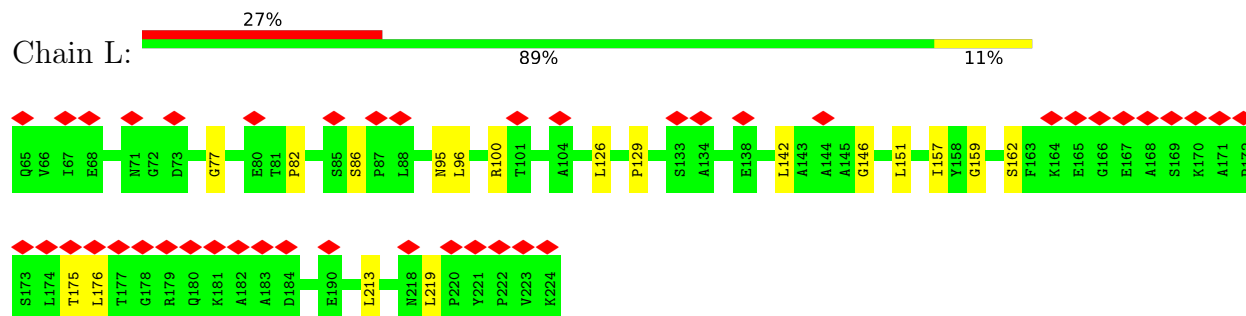
- Molecule 14: Photosystem I reaction center subunit IX



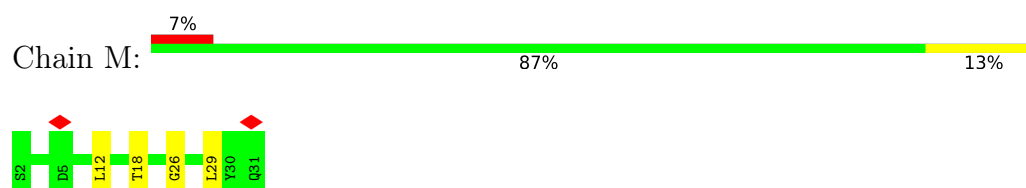
- Molecule 15: PsaK



- Molecule 16: PSI subunit V



- Molecule 17: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114608	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 ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.882	Depositor
Minimum map value	-3.405	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	291.2, 291.2, 291.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0400001, 1.0400001, 1.0400001	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/6032	0.61	3/8227 (0.0%)
2	B	0.30	0/6059	0.64	0/8267
3	1	0.22	0/1522	0.51	0/2081
4	2	0.18	0/1618	0.42	0/2218
5	3	0.20	0/1729	0.46	0/2349
6	4	0.24	0/1623	0.57	0/2219
7	C	0.23	0/606	0.57	0/821
8	D	0.17	0/1136	0.46	0/1538
9	E	0.15	0/511	0.37	0/694
10	F	0.30	1/1265 (0.1%)	0.54	0/1710
11	G	0.16	0/704	0.40	0/960
12	H	0.19	0/673	0.48	0/909
13	I	0.29	0/273	0.61	0/373
14	J	0.20	0/334	0.46	0/457
15	K	0.16	0/567	0.41	0/768
16	L	0.22	0/1202	0.57	0/1645
17	M	0.16	0/224	0.46	0/302
All	All	0.26	1/26078 (0.0%)	0.56	3/35538 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	213	TRP	C-N	6.98	1.42	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	LEU	CA-CB-CG	5.62	135.98	116.30
1	A	502	LEU	CA-CB-CG	5.19	134.46	116.30
1	A	506	ASN	N-CA-C	5.11	121.67	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5837	0	5725	125	0
2	B	5845	0	5618	120	0
3	1	1473	0	1448	15	0
4	2	1567	0	1527	22	0
5	3	1678	0	1638	31	0
6	4	1574	0	1549	22	0
7	C	596	0	573	9	0
8	D	1109	0	1111	14	0
9	E	500	0	494	10	0
10	F	1239	0	1288	21	0
11	G	689	0	681	6	0
12	H	659	0	636	6	0
13	I	266	0	274	7	0
14	J	325	0	341	9	0
15	K	561	0	574	7	0
16	L	1171	0	1186	15	0
17	M	223	0	244	4	0
18	A	65	0	72	5	0
19	1	614	0	508	9	0
19	2	378	0	334	4	0
19	3	648	0	530	14	0
19	4	527	0	448	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	2384	0	2226	104	0
19	B	2177	0	1998	104	0
19	F	118	0	69	4	0
19	G	151	0	121	0	0
19	H	45	0	33	2	0
19	I	65	0	72	7	0
19	J	45	0	33	0	0
19	K	173	0	118	3	0
19	L	155	0	131	9	0
20	A	33	0	46	2	0
20	B	33	0	46	5	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	25	0	33	0	0
22	3	80	0	112	4	0
22	A	240	0	336	8	0
22	B	280	0	392	29	0
22	F	40	0	56	2	0
22	G	40	0	56	3	0
22	I	80	0	112	5	0
22	J	80	0	112	4	0
22	K	40	0	56	1	0
22	L	80	0	112	7	0
22	M	40	0	56	5	0
23	1	37	0	44	1	0
23	2	32	0	34	2	0
23	3	34	0	38	1	0
23	4	38	0	46	2	0
23	A	80	0	106	4	0
23	B	35	0	40	0	0
24	2	36	0	42	0	0
24	A	34	0	38	2	0
24	J	75	0	90	4	0
25	1	35	0	46	2	0
25	4	35	0	45	3	0
25	A	33	0	39	1	0
25	B	31	0	35	0	0
25	G	66	0	80	3	0
26	B	61	0	83	5	0
27	1	103	0	78	2	0
27	2	366	0	290	11	0
27	3	47	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	188	0	128	1	0
28	1	84	0	112	8	0
28	2	126	0	165	9	0
28	3	84	0	110	9	0
28	4	126	0	166	7	0
29	3	1	0	0	0	0
29	4	1	0	0	0	0
29	A	15	0	0	0	0
29	B	23	0	0	0	0
29	C	2	0	0	0	0
29	D	1	0	0	0	0
29	F	1	0	0	0	0
29	G	1	0	0	0	0
All	All	35803	0	35011	595	0

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

The worst 5 of 595 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)
19:A:1134:CLA:H2A	19:A:1134:CLA:HED3	1.63	0.80
19:4:601:CLA:HBB2	19:4:602:CLA:HHD	1.64	0.79
19:3:610:CLA:HAB	28:3:620:LUT:H32	1.67	0.75
19:4:610:CLA:HAB	28:4:620:LUT:H32	1.69	0.75
1:A:209:GLY:HA3	19:A:1111:CLA:HBB1	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

215 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	$\# Z > 2$
28	LUT	3	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.58	5 (9%)
20	PQN	B	2002	-	34,34,34	0.42	0	43,45,45	1.07	1 (2%)
27	CHL	2	601	-	60,74,74	3.39	19 (31%)	58,114,114	2.45	17 (29%)
19	CLA	B	1202	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
27	CHL	2	608	-	42,56,74	3.92	18 (42%)	36,92,114	2.66	12 (33%)
19	CLA	1	610	-	59,63,73	1.24	7 (11%)	70,101,113	1.65	9 (12%)
19	CLA	A	1140	-	55,59,73	1.31	8 (14%)	64,96,113	1.39	9 (14%)
22	BCR	A	4007	-	41,41,41	1.11	3 (7%)	56,56,56	1.88	18 (32%)
19	CLA	2	613	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	B	1208	-	49,53,73	1.38	8 (16%)	58,89,113	1.56	7 (12%)
22	BCR	3	623	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	7 (12%)
19	CLA	B	1222	-	50,54,73	1.34	8 (16%)	59,90,113	1.57	9 (15%)
19	CLA	3	609	-	64,68,73	1.21	8 (12%)	76,107,113	1.31	8 (10%)
22	BCR	A	4002	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	605	-	27,35,73	1.85	7 (25%)	32,60,113	1.64	6 (18%)
22	BCR	A	4003	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
23	LHG	3	630	-	33,33,48	0.75	1 (3%)	36,39,54	1.30	4 (11%)
19	CLA	A	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
28	LUT	4	621	-	42,43,43	2.53	4 (9%)	51,60,60	3.06	14 (27%)
19	CLA	B	1229	-	59,63,73	1.28	8 (13%)	70,101,113	1.31	7 (10%)
19	CLA	4	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.35	5 (7%)
19	CLA	A	1022	-	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
19	CLA	B	1240	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	9 (10%)
19	CLA	A	5005	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	8 (12%)
19	CLA	1	603	-	59,63,73	1.26	8 (13%)	70,101,113	1.38	8 (11%)
27	CHL	2	615	-	41,55,74	4.11	19 (46%)	35,91,114	2.82	11 (31%)
19	CLA	B	1227	-	49,53,73	1.40	10 (20%)	58,89,113	1.71	10 (17%)
19	CLA	A	1125	-	64,68,73	1.22	9 (14%)	76,107,113	1.69	14 (18%)
19	CLA	A	1108	-	49,53,73	1.36	8 (16%)	58,89,113	1.66	6 (10%)
19	CLA	A	1132	-	69,73,73	1.14	8 (11%)	82,113,113	1.63	14 (17%)
19	CLA	3	610	-	59,63,73	1.25	8 (13%)	70,101,113	1.24	7 (10%)
19	CLA	H	200	-	49,53,73	1.39	6 (12%)	58,89,113	1.33	6 (10%)
19	CLA	1	615	-	50,54,73	1.38	8 (16%)	59,90,113	1.45	5 (8%)
19	CLA	B	1203	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	9 (10%)
19	CLA	B	1216	-	59,63,73	1.27	10 (16%)	70,101,113	1.72	11 (15%)
27	CHL	3	608	-	41,55,74	4.05	19 (46%)	35,91,114	2.75	13 (37%)
19	CLA	A	1110	-	59,63,73	1.28	9 (15%)	70,101,113	1.45	6 (8%)
19	CLA	B	1213	-	59,63,73	1.22	8 (13%)	70,101,113	1.48	9 (12%)
19	CLA	B	1012	-	59,63,73	1.30	8 (13%)	70,101,113	1.45	10 (14%)
19	CLA	3	603	-	59,63,73	1.28	9 (15%)	70,101,113	1.39	5 (7%)
22	BCR	3	624	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	2	610	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	5 (6%)
19	CLA	B	1204	-	65,69,73	1.19	8 (12%)	77,108,113	1.13	6 (7%)
19	CLA	4	601	-	54,58,73	1.32	7 (12%)	64,95,113	1.43	5 (7%)
19	CLA	3	613	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	3 (4%)
19	CLA	1	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	7 (11%)
22	BCR	F	416	-	41,41,41	1.02	2 (4%)	56,56,56	1.36	10 (17%)
28	LUT	1	621	-	42,43,43	2.66	2 (4%)	51,60,60	2.23	9 (17%)
19	CLA	A	1114	-	49,53,73	1.39	6 (12%)	58,89,113	1.70	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1221	-	58,62,73	1.30	10 (17%)	68,99,113	1.64	9 (13%)
25	LMT	B	5001	-	32,32,36	1.24	6 (18%)	43,43,47	0.96	0
19	CLA	B	1239	-	49,53,73	1.38	7 (14%)	58,89,113	1.58	9 (15%)
19	CLA	A	1013	-	60,64,73	1.23	10 (16%)	71,102,113	1.82	14 (19%)
19	CLA	K	202	-	50,54,73	1.37	8 (16%)	59,90,113	1.36	6 (10%)
19	CLA	B	1231	-	49,53,73	1.40	7 (14%)	58,89,113	1.46	6 (10%)
19	CLA	A	1139	-	54,58,73	1.31	9 (16%)	64,95,113	1.45	6 (9%)
19	CLA	B	1234	-	55,59,73	1.30	9 (16%)	64,96,113	1.49	8 (12%)
19	CLA	2	612	-	56,60,73	1.31	7 (12%)	65,97,113	1.42	6 (9%)
19	CLA	B	1236	-	51,55,73	1.33	8 (15%)	60,91,113	1.41	5 (8%)
21	SF4	C	1003	7	0,12,12	-	-	-	-	-
19	CLA	B	1219	-	49,53,73	1.40	9 (18%)	58,89,113	1.62	9 (15%)
28	LUT	2	623	-	42,43,43	2.55	1 (2%)	51,60,60	1.76	9 (17%)
27	CHL	2	607	-	41,55,74	4.10	19 (46%)	35,91,114	2.75	16 (45%)
19	CLA	K	203	-	27,35,73	1.85	6 (22%)	32,60,113	1.60	5 (15%)
22	BCR	1	623	-	25,25,41	1.04	2 (8%)	33,33,56	1.29	5 (15%)
19	CLA	4	603	-	59,63,73	1.25	8 (13%)	70,101,113	1.32	7 (10%)
19	CLA	A	1138	-	64,68,73	1.20	8 (12%)	76,107,113	1.42	7 (9%)
27	CHL	4	606	-	41,55,74	4.09	18 (43%)	35,91,114	2.85	14 (40%)
19	CLA	A	1104	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	9 (10%)
19	CLA	4	612	-	50,54,73	1.37	7 (14%)	59,90,113	1.28	4 (6%)
19	CLA	A	1134	-	49,53,73	1.38	8 (16%)	58,89,113	1.62	6 (10%)
19	CLA	3	612	-	49,53,73	1.39	7 (14%)	58,89,113	1.34	5 (8%)
19	CLA	F	302	-	50,54,73	1.36	8 (16%)	59,90,113	1.38	5 (8%)
19	CLA	B	1220	-	49,53,73	1.38	8 (16%)	58,89,113	1.39	6 (10%)
19	CLA	B	1223	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	10 (12%)
19	CLA	L	302	-	64,68,73	1.21	7 (10%)	76,107,113	1.21	7 (9%)
22	BCR	L	420	-	41,41,41	0.99	1 (2%)	56,56,56	1.50	10 (17%)
22	BCR	M	4021	-	41,41,41	0.99	2 (4%)	56,56,56	1.31	9 (16%)
19	CLA	B	1021	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	9 (10%)
19	CLA	3	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.53	9 (11%)
28	LUT	3	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.85	10 (19%)
19	CLA	B	1215	-	64,68,73	1.22	9 (14%)	76,107,113	1.70	11 (14%)
19	CLA	B	1238	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
19	CLA	I	121	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1137	-	49,53,73	1.40	7 (14%)	58,89,113	1.41	5 (8%)
19	CLA	A	1115	-	58,62,73	1.26	8 (13%)	68,99,113	1.41	10 (14%)
19	CLA	G	218	-	59,63,73	1.27	7 (11%)	70,101,113	1.28	4 (5%)
24	LMG	J	301	-	49,49,55	0.81	1 (2%)	57,57,63	1.27	5 (8%)
19	CLA	J	102	-	49,53,73	1.39	8 (16%)	58,89,113	1.51	4 (6%)
19	CLA	A	1118	-	59,63,73	1.28	6 (10%)	70,101,113	1.25	6 (8%)
19	CLA	K	204	-	49,53,73	1.40	9 (18%)	58,89,113	1.49	9 (15%)
19	CLA	4	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	7 (10%)
19	CLA	A	1122	-	64,68,73	1.22	9 (14%)	76,107,113	1.42	5 (6%)
19	CLA	A	1127	-	69,73,73	1.18	11 (15%)	82,113,113	1.56	11 (13%)
24	LMG	2	631	-	36,36,55	0.94	0	44,44,63	1.21	5 (11%)
19	CLA	A	1130	-	64,68,73	1.21	8 (12%)	76,107,113	1.29	9 (11%)
24	LMG	A	5002	-	34,34,55	0.95	0	42,42,63	1.23	3 (7%)
19	CLA	B	1230	-	49,53,73	1.39	8 (16%)	58,89,113	1.36	5 (8%)
19	CLA	B	1201	-	54,58,73	1.30	8 (14%)	64,95,113	1.40	10 (15%)
18	CL0	A	1011	-	58,73,73	2.21	11 (18%)	60,113,113	1.65	14 (23%)
19	CLA	F	301	-	49,53,73	1.38	8 (16%)	58,89,113	1.47	4 (6%)
27	CHL	1	601	-	50,64,74	3.63	18 (36%)	46,102,114	2.60	17 (36%)
19	CLA	A	1102	-	49,53,73	1.36	9 (18%)	58,89,113	1.35	7 (12%)
27	CHL	4	615	-	37,51,74	4.27	18 (48%)	30,86,114	2.92	12 (40%)
19	CLA	B	1232	-	49,53,73	1.44	8 (16%)	58,89,113	1.78	7 (12%)
19	CLA	1	613	-	59,63,73	1.27	9 (15%)	70,101,113	1.31	6 (8%)
22	BCR	B	4006	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	5 (8%)
25	LMT	4	631	-	36,36,36	1.18	5 (13%)	47,47,47	0.95	1 (2%)
27	CHL	4	607	-	41,55,74	4.10	18 (43%)	35,91,114	2.72	13 (37%)
19	CLA	1	606	-	49,53,73	1.39	9 (18%)	58,89,113	1.53	8 (13%)
19	CLA	A	8895	-	69,73,73	1.19	9 (13%)	82,113,113	1.46	5 (6%)
28	LUT	4	620	-	42,43,43	2.51	2 (4%)	51,60,60	2.04	12 (23%)
19	CLA	A	1116	-	58,62,73	1.27	10 (17%)	68,99,113	1.33	7 (10%)
19	CLA	2	614	-	54,58,73	1.31	8 (14%)	64,95,113	1.51	7 (10%)
19	CLA	F	303	-	27,35,73	1.85	6 (22%)	32,60,113	1.62	5 (15%)
19	CLA	A	1131	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
19	CLA	B	1217	-	49,53,73	1.38	7 (14%)	58,89,113	1.37	6 (10%)
23	LHG	A	5003	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
25	LMT	1	631	-	36,36,36	1.15	4 (11%)	47,47,47	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DGD	B	5002	-	62,62,67	0.97	4 (6%)	76,76,81	1.26	8 (10%)
19	CLA	B	1206	-	51,55,73	1.34	9 (17%)	60,91,113	1.49	6 (10%)
28	LUT	1	620	-	42,43,43	2.72	2 (4%)	51,60,60	2.30	14 (27%)
19	CLA	A	1113	-	49,53,73	1.38	8 (16%)	58,89,113	1.57	10 (17%)
19	CLA	L	303	-	49,53,73	1.37	8 (16%)	58,89,113	1.61	8 (13%)
24	LMG	J	302	-	26,26,55	1.12	2 (7%)	34,34,63	1.16	4 (11%)
19	CLA	A	1124	-	61,65,73	1.23	7 (11%)	72,103,113	1.27	5 (6%)
22	BCR	A	4001	-	41,41,41	1.04	2 (4%)	56,56,56	1.37	7 (12%)
19	CLA	G	201	-	54,58,73	1.33	8 (14%)	64,95,113	1.36	5 (7%)
19	CLA	G	202	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
22	BCR	B	4009	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
19	CLA	2	609	-	59,63,73	1.26	7 (11%)	70,101,113	1.63	6 (8%)
23	LHG	1	630	-	36,36,48	0.68	1 (2%)	39,42,54	1.26	4 (10%)
27	CHL	2	602	-	50,64,74	3.75	18 (36%)	46,102,114	2.47	17 (36%)
22	BCR	A	4011	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	2	604	-	54,58,73	1.32	8 (14%)	64,95,113	1.36	6 (9%)
19	CLA	3	617	-	50,54,73	1.36	8 (16%)	59,90,113	1.33	5 (8%)
19	CLA	B	1205	-	69,73,73	1.18	9 (13%)	82,113,113	1.47	10 (12%)
22	BCR	B	4017	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	5 (8%)
25	LMT	G	402	-	32,32,36	1.23	5 (15%)	43,43,47	0.91	0
19	CLA	A	1109	-	69,73,73	1.18	10 (14%)	82,113,113	1.31	7 (8%)
19	CLA	A	1136	-	69,73,73	1.18	8 (11%)	82,113,113	1.40	9 (10%)
27	CHL	2	611	-	50,64,74	3.66	18 (36%)	46,102,114	2.71	15 (32%)
19	CLA	A	1801	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	5 (7%)
25	LMT	A	5004	-	34,34,36	1.20	4 (11%)	45,45,47	1.05	1 (2%)
19	CLA	A	1126	-	64,68,73	1.19	9 (14%)	76,107,113	1.81	16 (21%)
22	BCR	I	118	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	8 (14%)
19	CLA	4	602	-	64,68,73	1.19	7 (10%)	76,107,113	1.37	8 (10%)
19	CLA	2	603	-	50,54,73	1.34	8 (16%)	59,90,113	1.38	4 (6%)
19	CLA	A	1120	-	49,53,73	1.37	8 (16%)	58,89,113	1.45	4 (6%)
19	CLA	1	604	-	54,58,73	1.30	8 (14%)	64,95,113	1.49	7 (10%)
19	CLA	4	611	-	59,63,73	1.26	9 (15%)	70,101,113	1.47	7 (10%)
22	BCR	J	212	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
19	CLA	A	1121	-	55,59,73	1.32	8 (14%)	64,96,113	1.54	8 (12%)
19	CLA	1	609	-	64,68,73	1.24	8 (12%)	76,107,113	1.59	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	611	-	45,49,73	1.43	8 (17%)	54,84,113	1.37	3 (5%)
19	CLA	A	1106	-	59,63,73	1.25	9 (15%)	70,101,113	1.60	6 (8%)
22	BCR	J	213	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	7 (12%)
19	CLA	B	1224	-	65,69,73	1.22	10 (15%)	77,108,113	1.46	10 (12%)
27	CHL	1	607	-	41,55,74	4.23	19 (46%)	35,91,114	2.90	14 (40%)
22	BCR	I	120	-	41,41,41	1.06	3 (7%)	56,56,56	1.77	15 (26%)
19	CLA	B	1211	-	60,64,73	1.25	7 (11%)	71,102,113	1.45	7 (9%)
19	CLA	B	1023	-	65,69,73	1.20	9 (13%)	77,108,113	1.52	12 (15%)
19	CLA	3	604	-	54,58,73	1.33	8 (14%)	64,95,113	1.45	8 (12%)
19	CLA	4	610	-	59,63,73	1.26	10 (16%)	70,101,113	1.55	8 (11%)
27	CHL	4	608	-	45,59,74	3.85	18 (40%)	40,96,114	2.49	12 (30%)
19	CLA	A	1105	-	54,58,73	1.31	8 (14%)	64,95,113	1.63	7 (10%)
19	CLA	A	1103	-	69,73,73	1.19	9 (13%)	82,113,113	1.22	6 (7%)
19	CLA	A	1119	-	69,73,73	1.16	9 (13%)	82,113,113	1.49	8 (9%)
19	CLA	B	1214	-	63,67,73	1.24	10 (15%)	74,105,113	1.51	11 (14%)
19	CLA	1	608	-	54,58,73	1.31	7 (12%)	64,95,113	1.44	7 (10%)
19	CLA	B	1212	-	49,53,73	1.37	9 (18%)	58,89,113	1.54	7 (12%)
22	BCR	B	4005	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)
23	LHG	A	5001	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
21	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
19	CLA	A	1117	-	69,73,73	1.17	9 (13%)	82,113,113	1.48	13 (15%)
28	LUT	2	620	-	42,43,43	2.47	1 (2%)	51,60,60	2.11	19 (37%)
25	LMT	G	401	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	1 (2%)
19	CLA	4	614	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	5 (8%)
21	SF4	C	1002	7	0,12,12	-	-	-	-	-
22	BCR	A	4008	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
19	CLA	3	614	-	52,56,73	1.35	7 (13%)	61,92,113	1.53	6 (9%)
19	CLA	B	1210	-	69,73,73	1.18	8 (11%)	82,113,113	1.50	9 (10%)
19	CLA	A	1112	-	49,53,73	1.38	9 (18%)	58,89,113	1.31	8 (13%)
19	CLA	3	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	4 (5%)
22	BCR	G	311	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	9 (16%)
22	BCR	B	4010	-	41,41,41	1.08	1 (2%)	56,56,56	1.70	13 (23%)
19	CLA	1	612	-	50,54,73	1.37	8 (16%)	59,90,113	1.30	7 (11%)
19	CLA	K	201	-	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
23	LHG	B	5101	-	34,34,48	0.75	1 (2%)	37,40,54	1.29	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	2	630	-	31,31,48	0.79	2 (6%)	34,37,54	1.24	3 (8%)
19	CLA	B	1226	-	59,63,73	1.31	9 (15%)	70,101,113	1.71	11 (15%)
19	CLA	1	602	-	64,68,73	1.22	8 (12%)	76,107,113	1.45	7 (9%)
19	CLA	B	1209	-	49,53,73	1.41	7 (14%)	58,89,113	1.54	6 (10%)
28	LUT	2	621	-	42,43,43	2.38	1 (2%)	51,60,60	1.58	6 (11%)
22	BCR	B	2004	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
19	CLA	1	611	-	50,54,73	1.36	7 (14%)	59,90,113	1.28	4 (6%)
19	CLA	A	1135	-	55,59,73	1.33	8 (14%)	64,96,113	1.44	7 (10%)
19	CLA	B	1237	-	69,73,73	1.21	8 (11%)	82,113,113	1.32	7 (8%)
20	PQN	A	2001	-	34,34,34	0.41	0	43,45,45	1.04	1 (2%)
19	CLA	A	1111	-	69,73,73	1.19	9 (13%)	82,113,113	1.34	6 (7%)
28	LUT	4	623	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	8 (15%)
19	CLA	B	1235	-	59,63,73	1.26	9 (15%)	70,101,113	1.32	5 (7%)
19	CLA	4	609	-	59,63,73	1.26	8 (13%)	70,101,113	1.69	9 (12%)
23	LHG	4	630	-	37,37,48	0.83	2 (5%)	40,43,54	1.26	3 (7%)
19	CLA	A	1107	-	49,53,73	1.39	8 (16%)	58,89,113	1.60	7 (12%)
19	CLA	B	1225	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	8 (9%)
22	BCR	K	301	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	6 (10%)
19	CLA	A	1128	-	69,73,73	1.21	9 (13%)	82,113,113	1.41	14 (17%)
19	CLA	3	606	-	50,54,73	1.38	9 (18%)	59,90,113	1.30	3 (5%)
19	CLA	L	301	-	54,58,73	1.35	8 (14%)	64,95,113	1.63	9 (14%)
22	BCR	B	4014	-	41,41,41	1.03	2 (4%)	56,56,56	1.41	9 (16%)
19	CLA	B	1228	-	53,57,73	1.31	9 (16%)	61,93,113	1.42	7 (11%)
27	CHL	2	606	-	40,54,74	4.13	18 (45%)	34,90,114	2.94	13 (38%)
19	CLA	A	1133	-	49,53,73	1.41	6 (12%)	58,89,113	1.18	4 (6%)
22	BCR	L	419	-	41,41,41	0.97	1 (2%)	56,56,56	1.59	12 (21%)

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
28	LUT	3	620	-	-	2/29/67/67	0/2/2/2
20	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
27	CHL	2	601	-	3/3/20/26	21/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1202	-	1/1/15/20	10/39/115/115	-
19	CLA	1	610	-	1/1/13/20	6/27/103/115	-
19	CLA	A	1140	-	-	8/23/99/115	-
22	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
19	CLA	2	613	-	1/1/15/20	13/39/115/115	-
19	CLA	B	1208	-	1/1/11/20	3/15/91/115	-
22	BCR	3	623	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1222	-	1/1/11/20	6/17/93/115	-
19	CLA	3	609	-	1/1/14/20	10/33/109/115	-
22	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
19	CLA	3	605	-	1/1/5/20	-	-
22	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
23	LHG	3	630	-	-	12/38/38/53	-
19	CLA	A	1101	-	1/1/12/20	10/21/97/115	-
28	LUT	4	621	-	-	4/29/67/67	0/2/2/2
19	CLA	B	1229	-	1/1/13/20	9/27/103/115	-
19	CLA	4	613	-	1/1/13/20	8/27/103/115	-
19	CLA	A	1022	-	1/1/15/20	9/39/115/115	-
19	CLA	B	1240	-	1/1/15/20	13/39/115/115	-
19	CLA	A	5005	-	-	6/21/97/115	-
19	CLA	1	603	-	1/1/13/20	14/27/103/115	-
27	CHL	2	615	-	3/3/16/26	11/17/115/137	-
19	CLA	B	1227	-	-	1/15/91/115	-
19	CLA	A	1125	-	1/1/14/20	13/33/109/115	-
19	CLA	A	1108	-	1/1/11/20	5/15/91/115	-
19	CLA	A	1132	-	1/1/15/20	8/39/115/115	-
19	CLA	3	610	-	1/1/13/20	9/27/103/115	-
19	CLA	H	200	-	1/1/11/20	5/15/91/115	-
19	CLA	1	615	-	1/1/11/20	8/17/93/115	-
19	CLA	B	1203	-	1/1/15/20	13/39/115/115	-
19	CLA	B	1216	-	1/1/13/20	9/27/103/115	-
27	CHL	3	608	-	3/3/16/26	5/17/115/137	-
19	CLA	A	1110	-	1/1/13/20	7/27/103/115	-
19	CLA	B	1213	-	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1012	-	1/1/13/20	14/27/103/115	-
19	CLA	3	603	-	-	12/27/103/115	-
22	BCR	3	624	-	-	16/29/63/63	0/2/2/2
19	CLA	2	610	-	1/1/14/20	10/33/109/115	-
19	CLA	B	1204	-	1/1/14/20	8/35/111/115	-
19	CLA	4	601	-	1/1/12/20	9/21/97/115	-
19	CLA	3	613	-	1/1/13/20	10/27/103/115	-
19	CLA	1	614	-	1/1/11/20	8/17/93/115	-
22	BCR	F	416	-	-	17/29/63/63	0/2/2/2
28	LUT	1	621	-	-	5/29/67/67	0/2/2/2
19	CLA	A	1114	-	1/1/11/20	6/15/91/115	-
19	CLA	B	1221	-	-	1/26/102/115	-
25	LMT	B	5001	-	-	4/17/57/61	0/2/2/2
19	CLA	B	1239	-	-	6/15/91/115	-
19	CLA	A	1013	-	-	3/29/105/115	-
19	CLA	K	202	-	1/1/11/20	8/17/93/115	-
19	CLA	B	1231	-	-	7/15/91/115	-
19	CLA	A	1139	-	1/1/12/20	6/21/97/115	-
19	CLA	B	1234	-	1/1/12/20	6/23/99/115	-
19	CLA	2	612	-	1/1/12/20	7/24/100/115	-
19	CLA	B	1236	-	-	6/18/94/115	-
21	SF4	C	1003	7	-	-	0/6/5/5
19	CLA	B	1219	-	-	3/15/91/115	-
28	LUT	2	623	-	1/1/12/27	9/29/67/67	0/2/2/2
27	CHL	2	607	-	3/3/16/26	10/17/115/137	-
19	CLA	K	203	-	1/1/5/20	-	-
22	BCR	1	623	-	-	5/18/35/63	0/1/1/2
19	CLA	4	603	-	1/1/13/20	12/27/103/115	-
19	CLA	A	1138	-	1/1/14/20	9/33/109/115	-
27	CHL	4	606	-	3/3/16/26	9/17/115/137	-
19	CLA	A	1104	-	-	19/39/115/115	-
19	CLA	4	612	-	1/1/11/20	10/17/93/115	-
19	CLA	A	1134	-	-	6/15/91/115	-
19	CLA	3	612	-	1/1/11/20	5/15/91/115	-
22	BCR	L	419	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	F	302	-	1/1/11/20	7/17/93/115	-
19	CLA	B	1220	-	1/1/11/20	4/15/91/115	-
19	CLA	B	1223	-	1/1/15/20	6/39/115/115	-
19	CLA	L	302	-	-	12/33/109/115	-
22	BCR	L	420	-	-	7/29/63/63	0/2/2/2
22	BCR	M	4021	-	-	5/29/63/63	0/2/2/2
19	CLA	B	1021	-	1/1/15/20	16/39/115/115	-
19	CLA	3	602	-	1/1/14/20	8/33/109/115	-
28	LUT	3	621	-	-	8/29/67/67	0/2/2/2
19	CLA	B	1215	-	1/1/14/20	11/33/109/115	-
19	CLA	B	1238	-	1/1/15/20	16/39/115/115	-
19	CLA	I	121	-	-	12/39/115/115	-
19	CLA	A	1137	-	1/1/11/20	5/15/91/115	-
19	CLA	A	1115	-	-	6/26/102/115	-
19	CLA	G	218	-	-	10/27/103/115	-
24	LMG	J	301	-	-	15/44/64/70	0/1/1/1
19	CLA	J	102	-	1/1/11/20	9/15/91/115	-
19	CLA	K	204	-	1/1/11/20	8/15/91/115	-
19	CLA	A	1118	-	-	13/27/103/115	-
19	CLA	4	604	-	1/1/12/20	6/21/97/115	-
19	CLA	A	1122	-	1/1/14/20	14/33/109/115	-
19	CLA	A	1127	-	-	18/39/115/115	-
24	LMG	2	631	-	-	6/31/51/70	0/1/1/1
19	CLA	A	1130	-	-	6/33/109/115	-
24	LMG	A	5002	-	-	13/29/49/70	0/1/1/1
19	CLA	B	1230	-	1/1/11/20	8/15/91/115	-
19	CLA	B	1201	-	1/1/12/20	10/21/97/115	-
18	CL0	A	1011	-	2/2/20/25	8/37/135/135	-
19	CLA	F	301	-	1/1/11/20	3/15/91/115	-
27	CHL	1	601	-	3/3/18/26	11/27/125/137	-
19	CLA	A	1102	-	-	8/15/91/115	-
27	CHL	4	615	-	3/3/15/26	2/12/110/137	-
19	CLA	B	1232	-	1/1/11/20	6/15/91/115	-
19	CLA	1	613	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
25	LMT	4	631	-	-	4/21/61/61	0/2/2/2
27	CHL	4	607	-	3/3/16/26	8/17/115/137	-
19	CLA	1	606	-	1/1/11/20	6/15/91/115	-
19	CLA	A	8895	-	-	9/39/115/115	-
28	LUT	4	620	-	-	9/29/67/67	0/2/2/2
19	CLA	A	1116	-	1/1/12/20	8/26/102/115	-
19	CLA	2	614	-	1/1/12/20	5/21/97/115	-
19	CLA	F	303	-	1/1/5/20	-	-
19	CLA	A	1131	-	1/1/15/20	6/39/115/115	-
19	CLA	B	1217	-	-	5/15/91/115	-
23	LHG	A	5003	-	-	11/35/35/53	-
25	LMT	1	631	-	-	6/21/61/61	0/2/2/2
26	DGD	B	5002	-	-	18/50/90/95	0/2/2/2
19	CLA	B	1206	-	-	7/18/94/115	-
28	LUT	1	620	-	-	5/29/67/67	0/2/2/2
19	CLA	L	303	-	1/1/11/20	7/15/91/115	-
19	CLA	A	1113	-	-	4/15/91/115	-
24	LMG	J	302	-	-	6/21/41/70	0/1/1/1
19	CLA	A	1124	-	-	11/30/106/115	-
22	BCR	A	4001	-	-	15/29/63/63	0/2/2/2
19	CLA	G	201	-	1/1/12/20	6/21/97/115	-
19	CLA	G	202	-	1/1/11/20	8/17/93/115	-
22	BCR	B	4009	-	-	3/29/63/63	0/2/2/2
19	CLA	2	609	-	1/1/13/20	3/27/103/115	-
23	LHG	1	630	-	-	14/41/41/53	-
27	CHL	2	602	-	3/3/18/26	12/27/125/137	-
22	BCR	A	4011	-	-	18/29/63/63	0/2/2/2
19	CLA	2	604	-	1/1/12/20	5/21/97/115	-
19	CLA	3	617	-	1/1/11/20	6/17/93/115	-
19	CLA	B	1205	-	1/1/15/20	9/39/115/115	-
22	BCR	B	4017	-	-	17/29/63/63	0/2/2/2
25	LMT	G	402	-	-	6/17/57/61	0/2/2/2
19	CLA	A	1109	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1136	-	1/1/15/20	10/39/115/115	-
27	CHL	2	611	-	3/3/18/26	6/27/125/137	-
19	CLA	A	1801	-	1/1/12/20	7/21/97/115	-
25	LMT	A	5004	-	-	7/19/59/61	0/2/2/2
19	CLA	A	1126	-	-	11/33/109/115	-
22	BCR	I	118	-	-	11/29/63/63	0/2/2/2
19	CLA	4	602	-	1/1/14/20	3/33/109/115	-
19	CLA	2	603	-	1/1/11/20	7/17/93/115	-
19	CLA	A	1120	-	-	3/15/91/115	-
19	CLA	1	604	-	1/1/12/20	4/21/97/115	-
19	CLA	4	611	-	-	6/27/103/115	-
22	BCR	J	212	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1121	-	1/1/12/20	9/23/99/115	-
19	CLA	1	609	-	1/1/14/20	6/33/109/115	-
19	CLA	3	611	-	1/1/10/20	4/10/86/115	-
19	CLA	A	1106	-	1/1/13/20	8/27/103/115	-
22	BCR	J	213	-	-	8/29/63/63	0/2/2/2
19	CLA	B	1224	-	1/1/14/20	11/35/111/115	-
27	CHL	1	607	-	3/3/16/26	11/17/115/137	-
22	BCR	I	120	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1211	-	1/1/13/20	9/29/105/115	-
19	CLA	B	1023	-	-	8/35/111/115	-
19	CLA	3	604	-	1/1/12/20	6/21/97/115	-
19	CLA	4	610	-	1/1/13/20	7/27/103/115	-
27	CHL	4	608	-	3/3/17/26	7/21/119/137	-
19	CLA	A	1105	-	1/1/12/20	0/21/97/115	-
19	CLA	A	1103	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1119	-	1/1/15/20	10/39/115/115	-
19	CLA	B	1214	-	-	8/32/108/115	-
19	CLA	1	608	-	1/1/12/20	3/21/97/115	-
19	CLA	B	1212	-	-	3/15/91/115	-
22	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
23	LHG	A	5001	-	-	20/53/53/53	-
21	SF4	A	3001	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1117	-	1/1/15/20	10/39/115/115	-
28	LUT	2	620	-	-	6/29/67/67	0/2/2/2
25	LMT	G	401	-	-	5/21/61/61	0/2/2/2
19	CLA	4	614	-	1/1/11/20	7/17/93/115	-
22	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
21	SF4	C	1002	7	-	-	0/6/5/5
19	CLA	3	614	-	1/1/11/20	9/19/95/115	-
19	CLA	B	1210	-	1/1/15/20	22/39/115/115	-
19	CLA	3	607	-	1/1/14/20	18/33/109/115	-
19	CLA	A	1112	-	-	6/15/91/115	-
22	BCR	G	311	-	-	7/29/63/63	0/2/2/2
22	BCR	B	4010	-	-	6/29/63/63	0/2/2/2
19	CLA	1	612	-	1/1/11/20	8/17/93/115	-
19	CLA	K	201	-	1/1/13/20	7/27/103/115	-
23	LHG	B	5101	-	-	9/39/39/53	-
23	LHG	2	630	-	-	10/36/36/53	-
19	CLA	B	1226	-	1/1/13/20	6/27/103/115	-
19	CLA	1	602	-	1/1/14/20	2/33/109/115	-
19	CLA	B	1209	-	-	2/15/91/115	-
28	LUT	2	621	-	-	2/29/67/67	0/2/2/2
22	BCR	B	2004	-	-	14/29/63/63	0/2/2/2
19	CLA	1	611	-	-	4/17/93/115	-
19	CLA	A	1135	-	-	8/23/99/115	-
19	CLA	B	1237	-	1/1/15/20	11/39/115/115	-
20	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
19	CLA	A	1111	-	-	15/39/115/115	-
28	LUT	4	623	-	1/1/12/27	12/29/67/67	0/2/2/2
19	CLA	B	1235	-	1/1/13/20	9/27/103/115	-
19	CLA	4	609	-	1/1/13/20	10/27/103/115	-
23	LHG	4	630	-	-	15/42/42/53	-
19	CLA	A	1107	-	-	9/15/91/115	-
19	CLA	B	1225	-	-	15/39/115/115	-
22	BCR	K	301	-	-	14/29/63/63	0/2/2/2
19	CLA	3	606	-	1/1/11/20	11/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1128	-	-	12/39/115/115	-
19	CLA	L	301	-	-	7/21/97/115	-
22	BCR	B	4014	-	-	19/29/63/63	0/2/2/2
19	CLA	B	1228	-	1/1/11/20	9/20/96/115	-
27	CHL	2	606	-	3/3/16/26	7/15/113/137	-
19	CLA	A	1133	-	-	7/15/91/115	-
27	CHL	2	608	-	3/3/16/26	9/18/116/137	-

The worst 5 of 1531 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	620	LUT	C24-C25	16.76	1.53	1.33
28	1	621	LUT	C24-C25	16.27	1.52	1.33
28	2	623	LUT	C24-C25	15.79	1.51	1.33
28	4	620	LUT	C24-C25	15.47	1.51	1.33
28	2	620	LUT	C24-C25	15.22	1.51	1.33

The worst 5 of 1618 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	621	LUT	O23-C23-C22	-11.92	88.94	110.06
27	2	611	CHL	O2D-CGD-CBD	10.45	122.43	110.95
27	2	601	CHL	O2D-CGD-CBD	10.20	122.15	110.95
19	2	609	CLA	C4A-NA-C1A	10.10	111.29	106.68
19	4	609	CLA	C4A-NA-C1A	9.85	111.17	106.68

5 of 145 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1011	CL0	NC
18	A	1011	CL0	NA
19	A	1022	CLA	ND
19	A	1101	CLA	ND
19	A	1103	CLA	ND

5 of 1810 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1013	CLA	CBD-CGD-O2D-CED
19	A	1022	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	1022	CLA	C3A-C2A-CAA-CBA
19	A	1101	CLA	CHA-CBD-CGD-O1D
19	A	1101	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

163 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	620	LUT	7	0
20	B	2002	PQN	5	0
27	2	601	CHL	7	0
19	B	1202	CLA	6	0
27	2	608	CHL	3	0
19	A	1140	CLA	4	0
22	A	4007	BCR	2	0
19	2	613	CLA	1	0
19	B	1208	CLA	4	0
22	3	623	BCR	1	0
19	3	609	CLA	2	0
22	A	4003	BCR	2	0
23	3	630	LHG	1	0
19	A	1101	CLA	2	0
28	4	621	LUT	2	0
19	B	1229	CLA	1	0
19	A	1022	CLA	8	0
19	B	1240	CLA	2	0
19	A	5005	CLA	4	0
19	1	603	CLA	4	0
19	B	1227	CLA	2	0
19	A	1125	CLA	2	0
19	A	1108	CLA	3	0
19	A	1132	CLA	4	0
19	3	610	CLA	4	0
19	H	200	CLA	2	0
19	B	1203	CLA	4	0
19	B	1216	CLA	2	0
27	3	608	CHL	2	0
19	A	1110	CLA	2	0
19	B	1213	CLA	3	0
19	B	1012	CLA	6	0
22	3	624	BCR	3	0
19	2	610	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1204	CLA	5	0
19	4	601	CLA	1	0
19	3	613	CLA	2	0
22	F	416	BCR	2	0
28	1	621	LUT	5	0
19	A	1114	CLA	2	0
19	B	1221	CLA	5	0
19	B	1239	CLA	2	0
19	A	1013	CLA	2	0
19	B	1231	CLA	1	0
19	A	1139	CLA	2	0
19	B	1236	CLA	1	0
19	B	1219	CLA	1	0
28	2	623	LUT	1	0
19	4	603	CLA	4	0
19	A	1138	CLA	5	0
19	A	1104	CLA	5	0
19	A	1134	CLA	1	0
19	3	612	CLA	1	0
19	B	1220	CLA	2	0
19	B	1223	CLA	6	0
19	L	302	CLA	5	0
22	L	420	BCR	4	0
22	M	4021	BCR	5	0
19	B	1021	CLA	2	0
19	3	602	CLA	3	0
28	3	621	LUT	2	0
19	B	1215	CLA	1	0
19	B	1238	CLA	7	0
19	I	121	CLA	7	0
19	A	1137	CLA	3	0
19	A	1115	CLA	1	0
24	J	301	LMG	3	0
19	A	1118	CLA	4	0
19	K	204	CLA	2	0
19	A	1122	CLA	3	0
19	A	1127	CLA	6	0
19	A	1130	CLA	3	0
24	A	5002	LMG	2	0
19	B	1230	CLA	3	0
19	B	1201	CLA	2	0
18	A	1011	CL0	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	301	CLA	4	0
27	1	601	CHL	1	0
19	A	1102	CLA	4	0
19	B	1232	CLA	1	0
22	B	4006	BCR	4	0
25	4	631	LMT	3	0
19	1	606	CLA	1	0
19	A	8895	CLA	4	0
28	4	620	LUT	4	0
19	A	1116	CLA	4	0
19	A	1131	CLA	2	0
19	B	1217	CLA	4	0
23	A	5003	LHG	1	0
25	1	631	LMT	2	0
26	B	5002	DGD	5	0
19	B	1206	CLA	4	0
28	1	620	LUT	3	0
19	A	1113	CLA	1	0
19	L	303	CLA	4	0
24	J	302	LMG	1	0
19	A	1124	CLA	3	0
22	A	4001	BCR	1	0
22	B	4009	BCR	2	0
19	2	609	CLA	1	0
23	1	630	LHG	1	0
27	2	602	CHL	2	0
22	A	4011	BCR	1	0
19	3	617	CLA	1	0
19	B	1205	CLA	5	0
22	B	4017	BCR	7	0
19	A	1109	CLA	2	0
19	A	1136	CLA	3	0
19	A	1801	CLA	1	0
25	A	5004	LMT	1	0
19	A	1126	CLA	5	0
22	I	118	BCR	1	0
19	4	602	CLA	2	0
19	A	1120	CLA	1	0
22	J	212	BCR	1	0
19	1	609	CLA	3	0
19	A	1106	CLA	3	0
22	J	213	BCR	3	0

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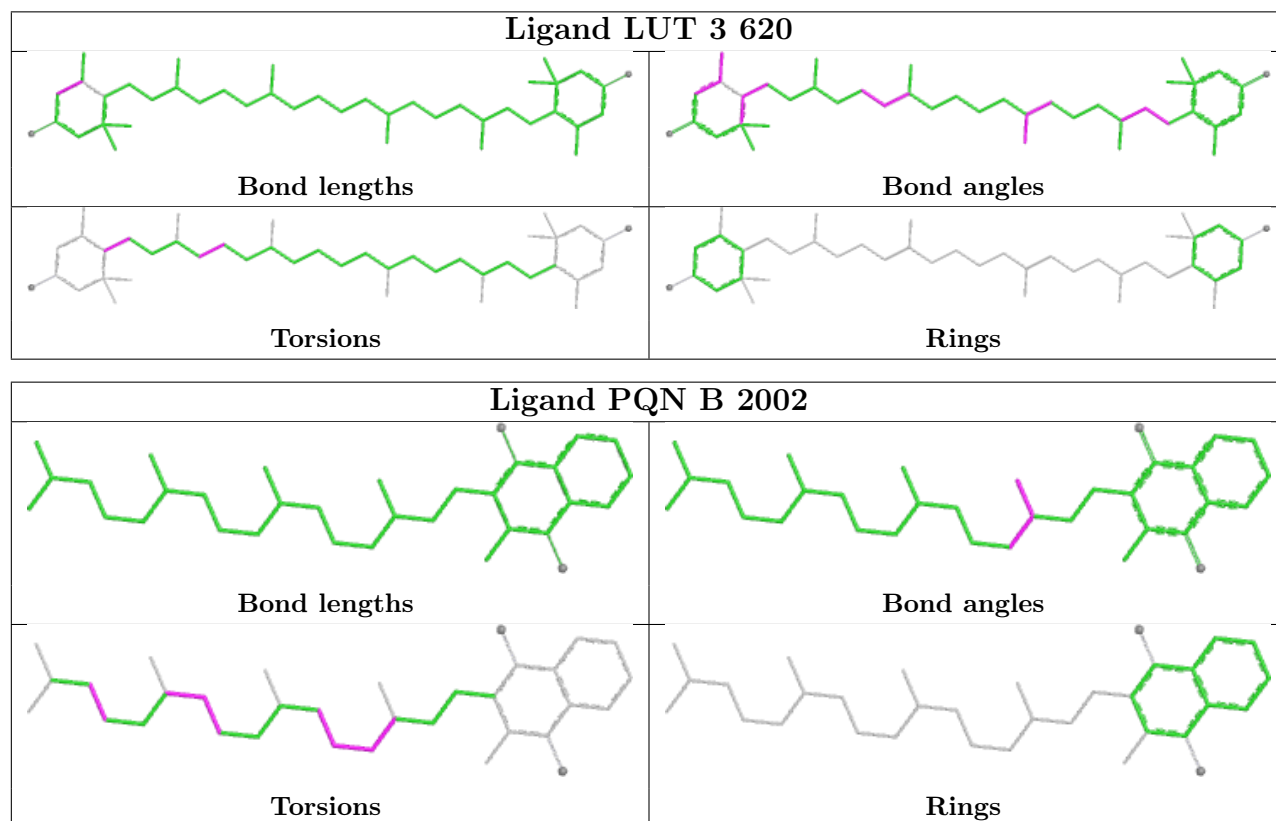
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1224	CLA	4	0
27	1	607	CHL	1	0
22	I	120	BCR	5	0
19	B	1023	CLA	5	0
19	3	604	CLA	1	0
19	4	610	CLA	3	0
27	4	608	CHL	1	0
19	A	1105	CLA	1	0
19	A	1103	CLA	4	0
19	A	1119	CLA	2	0
19	B	1214	CLA	3	0
19	B	1212	CLA	1	0
22	B	4005	BCR	3	0
23	A	5001	LHG	3	0
19	A	1117	CLA	7	0
28	2	620	LUT	6	0
25	G	401	LMT	3	0
22	A	4008	BCR	2	0
19	B	1210	CLA	6	0
19	3	607	CLA	1	0
22	G	311	BCR	3	0
22	B	4010	BCR	5	0
19	K	201	CLA	1	0
23	2	630	LHG	2	0
19	B	1226	CLA	3	0
19	1	602	CLA	2	0
19	B	1209	CLA	2	0
28	2	621	LUT	2	0
22	B	2004	BCR	1	0
19	A	1135	CLA	2	0
19	B	1237	CLA	8	0
20	A	2001	PQN	2	0
19	A	1111	CLA	6	0
28	4	623	LUT	1	0
19	B	1235	CLA	2	0
23	4	630	LHG	2	0
19	A	1107	CLA	1	0
19	B	1225	CLA	5	0
22	K	301	BCR	1	0
19	A	1128	CLA	5	0
19	L	301	CLA	1	0
22	B	4014	BCR	7	0

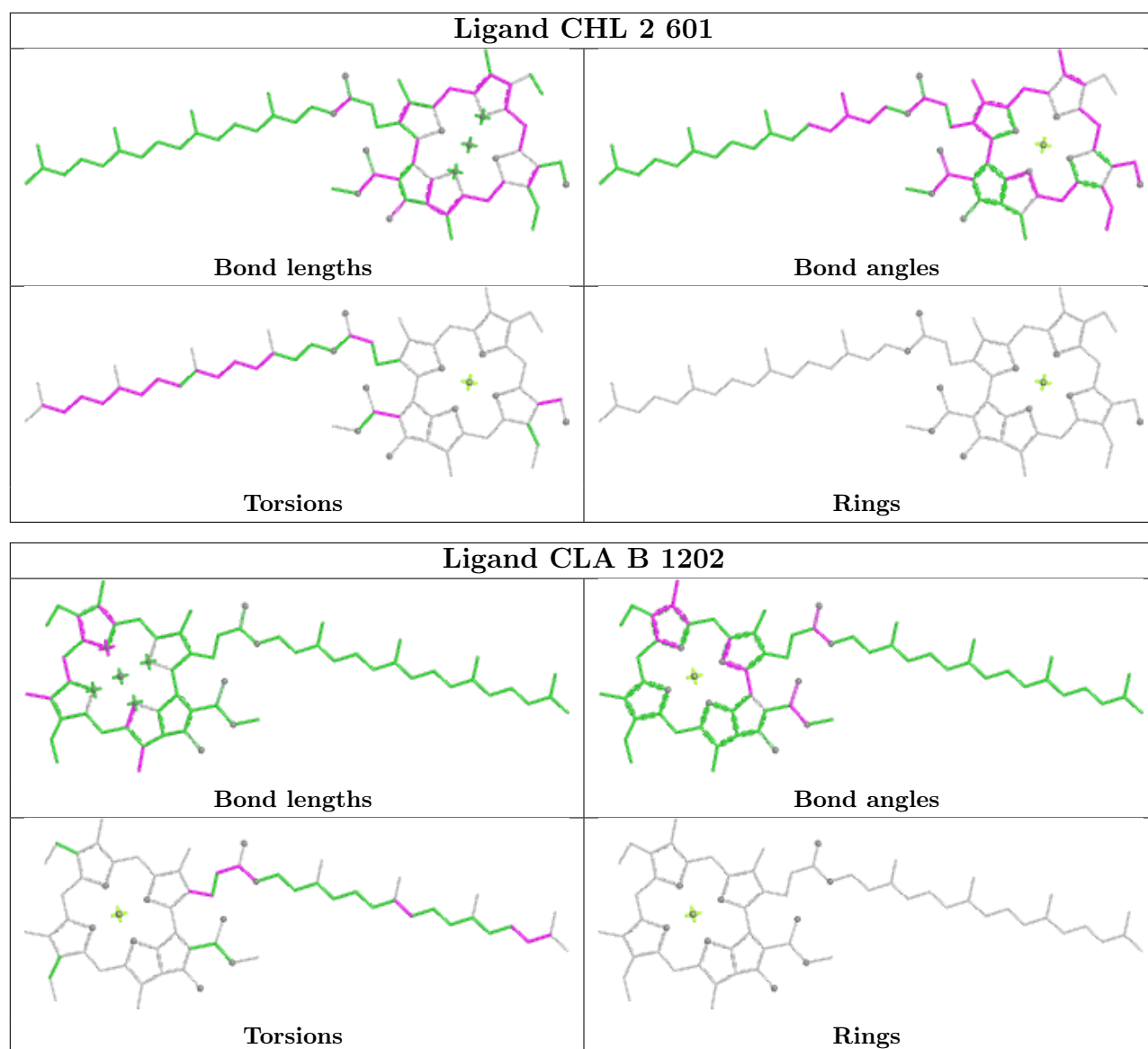
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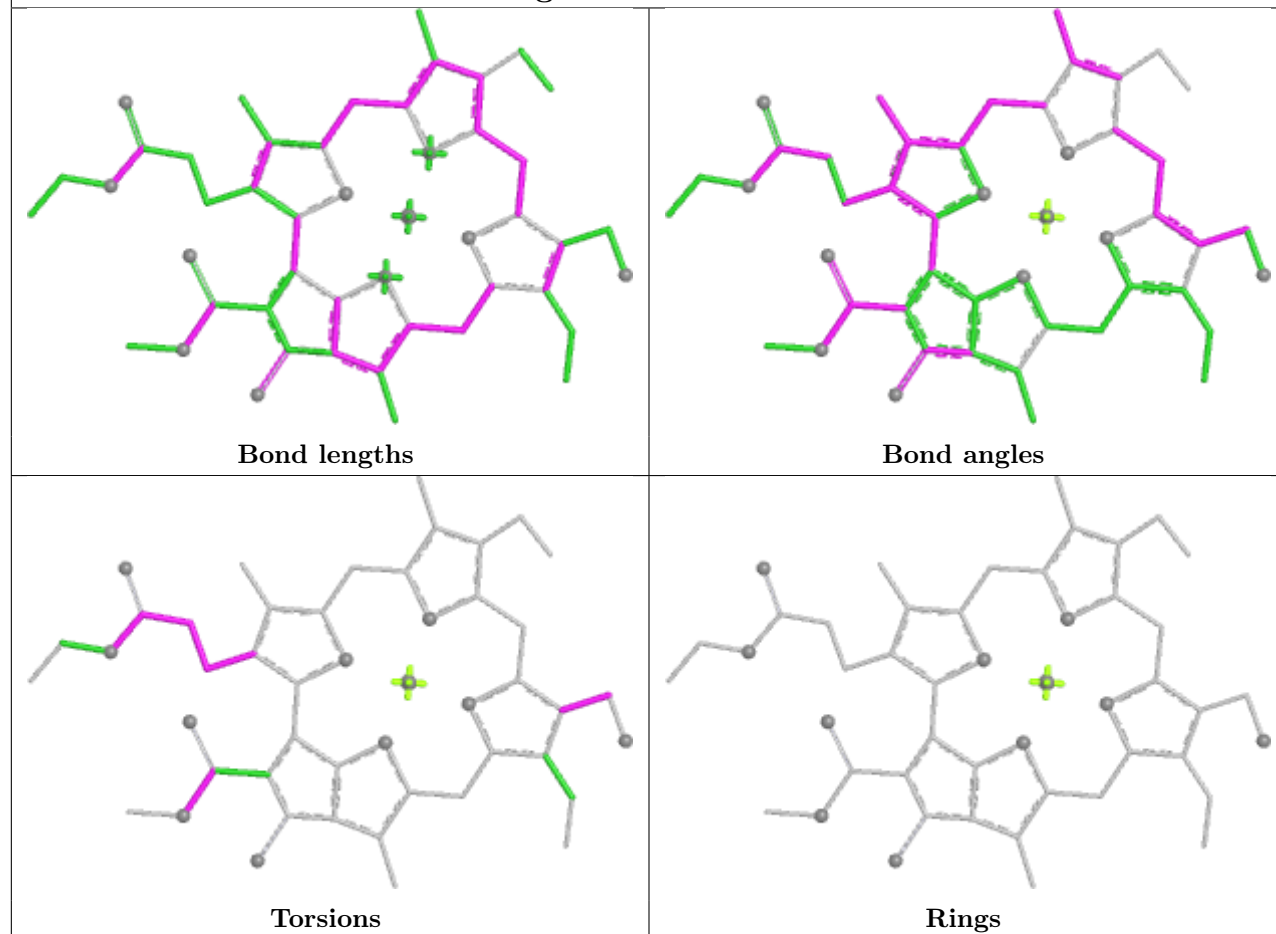
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1228	CLA	3	0
19	A	1133	CLA	2	0
22	L	419	BCR	3	0

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

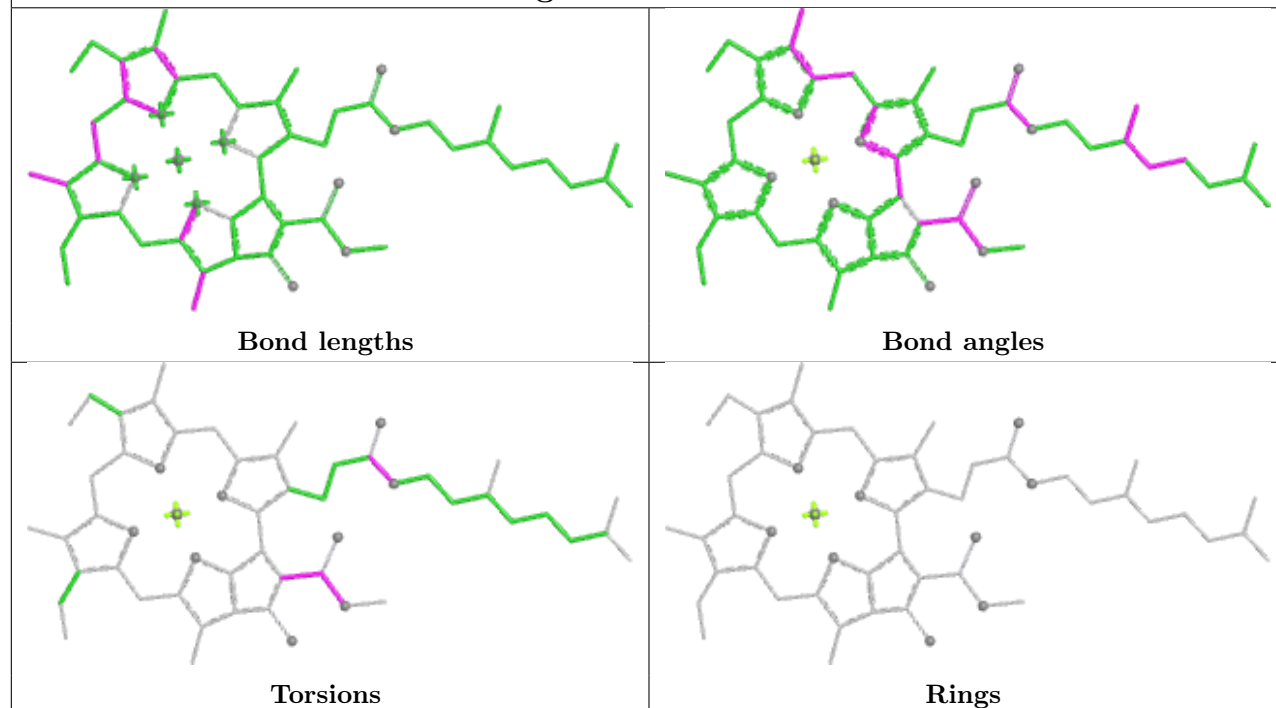




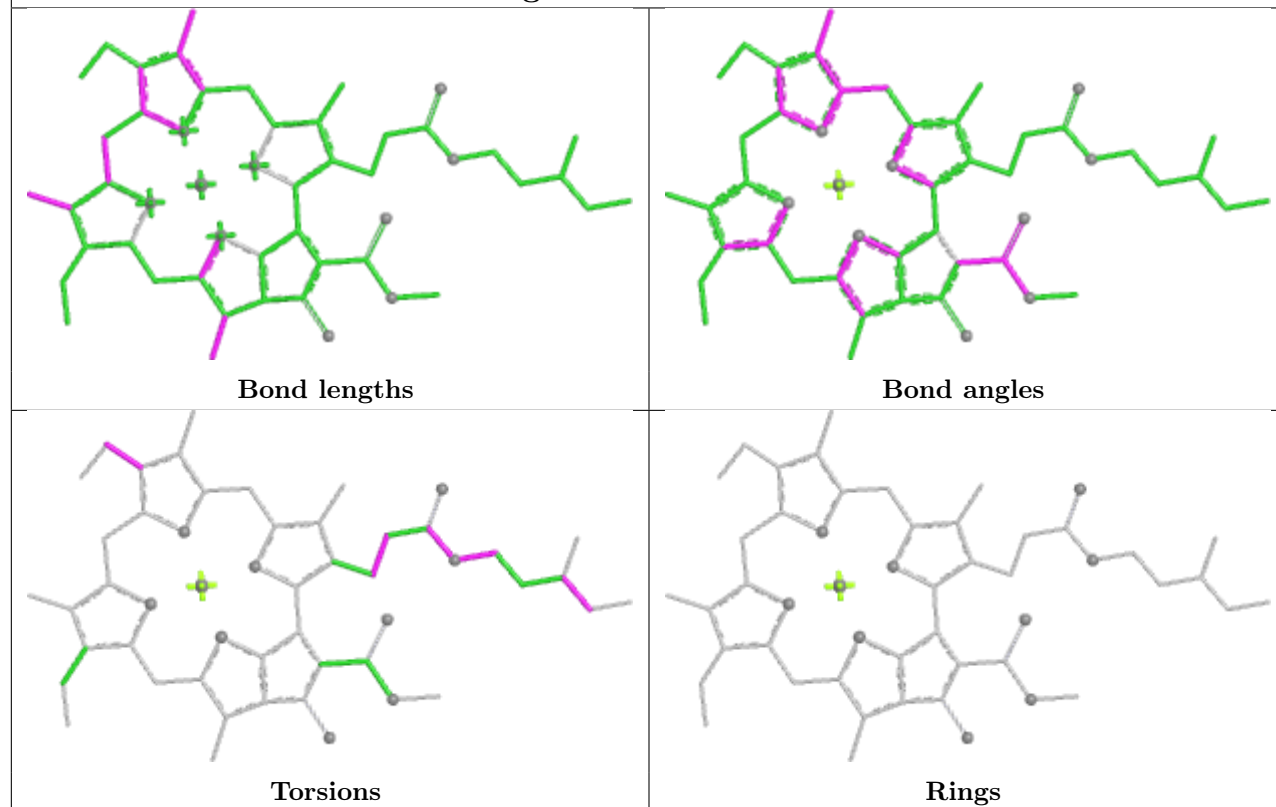
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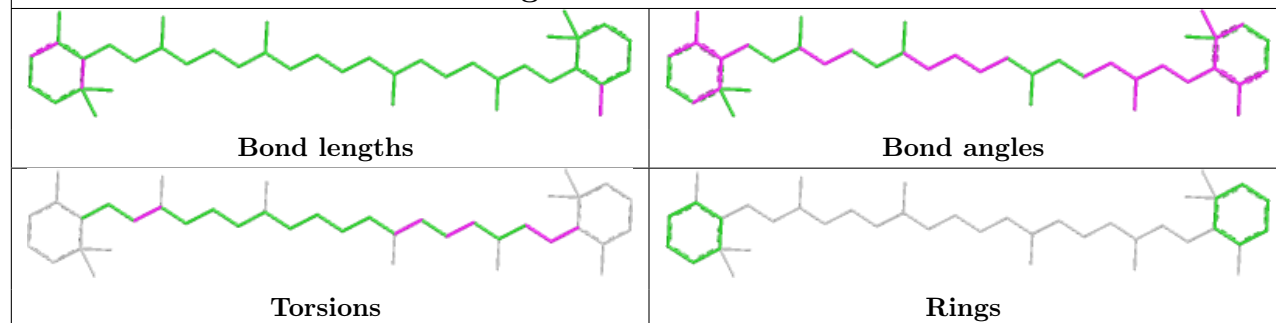
Ligand CLA 1 610



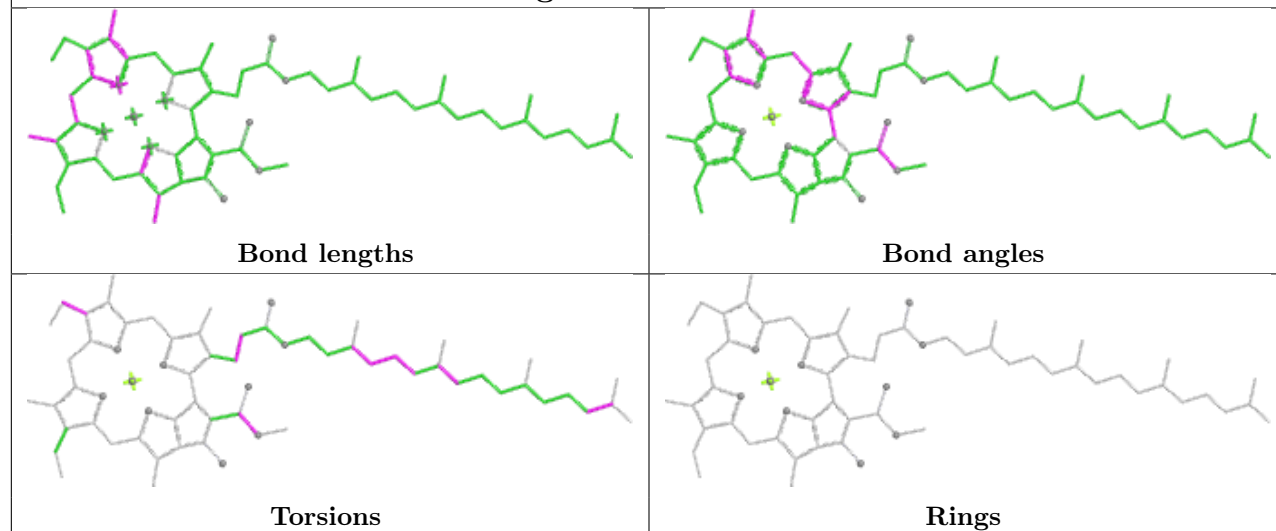
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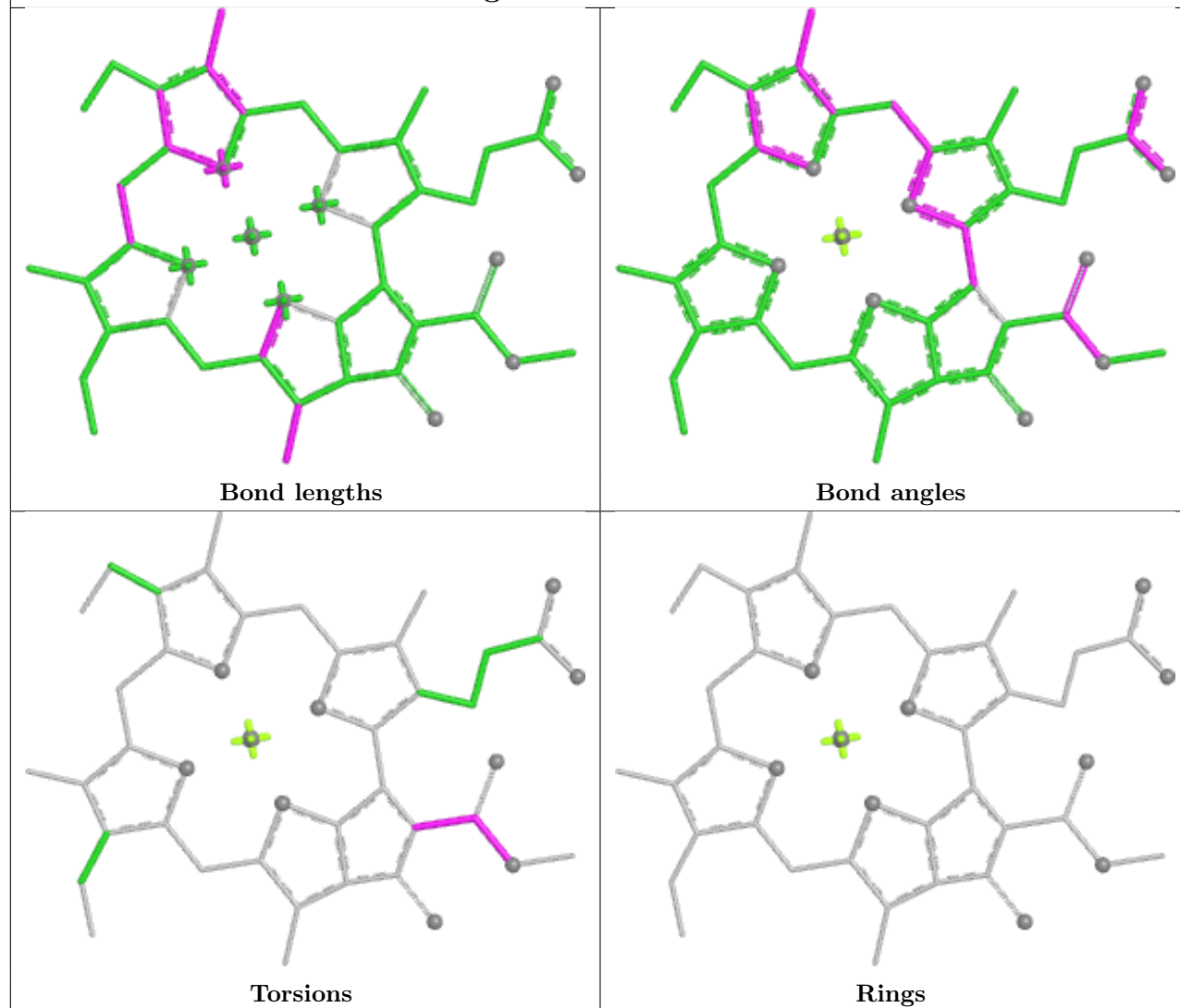
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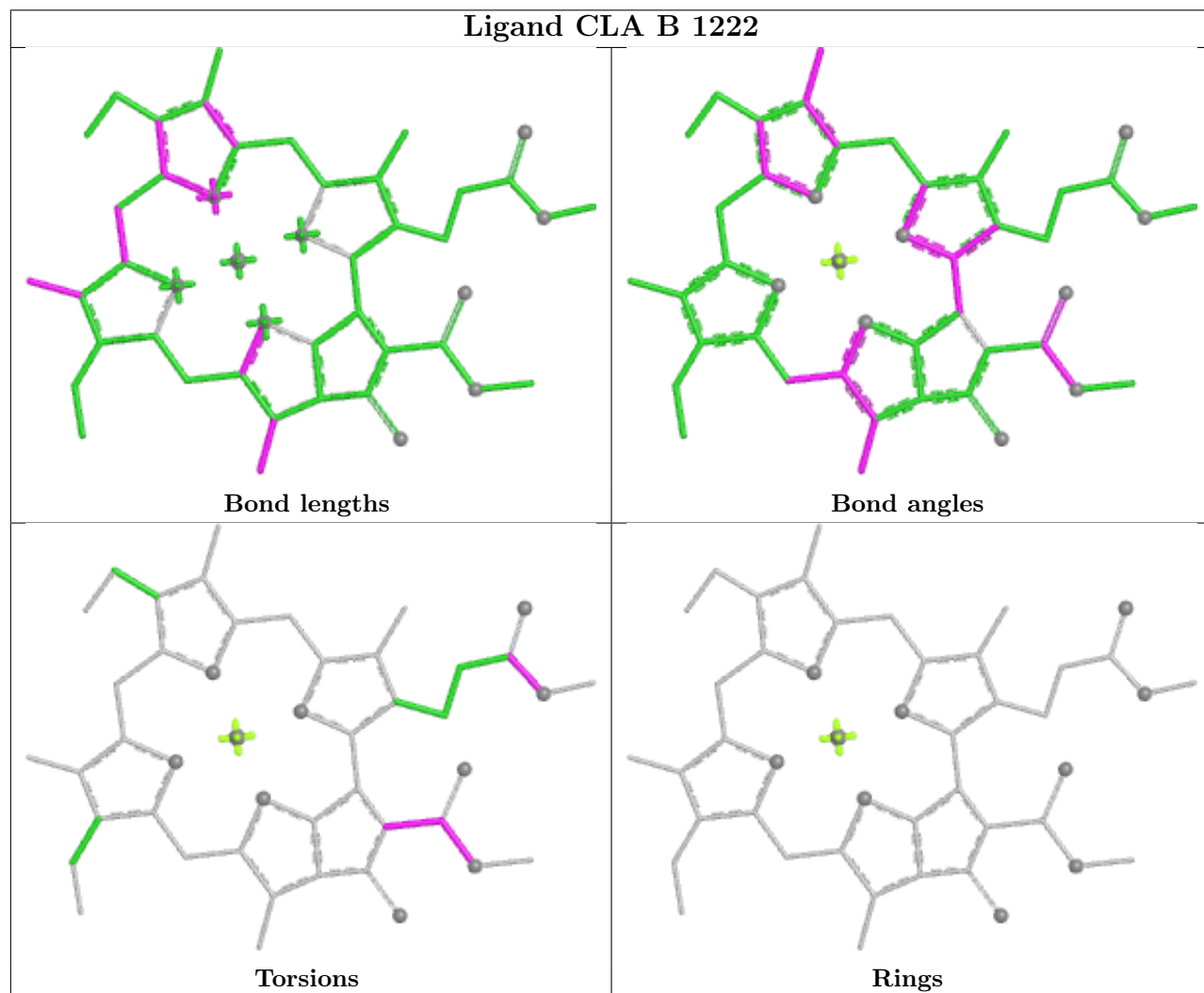
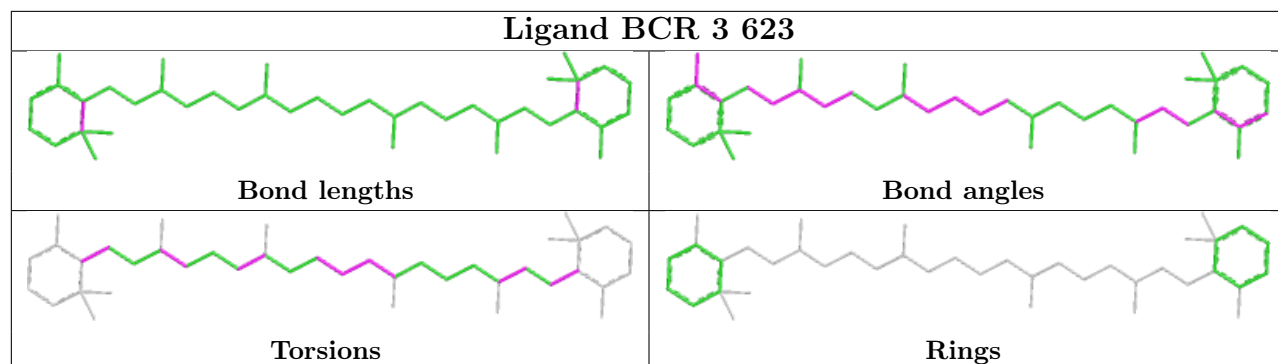


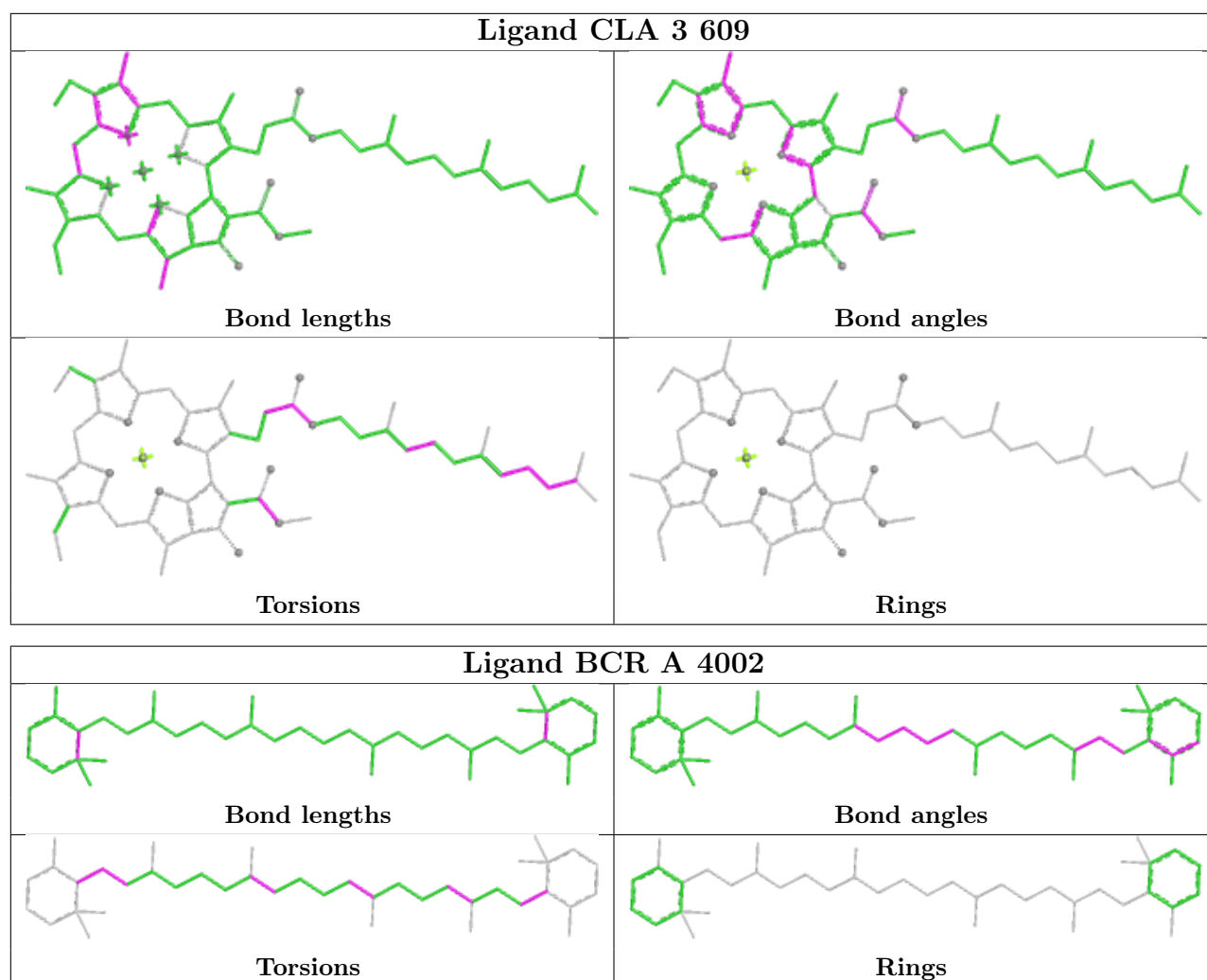
Ligand CLA 2 613

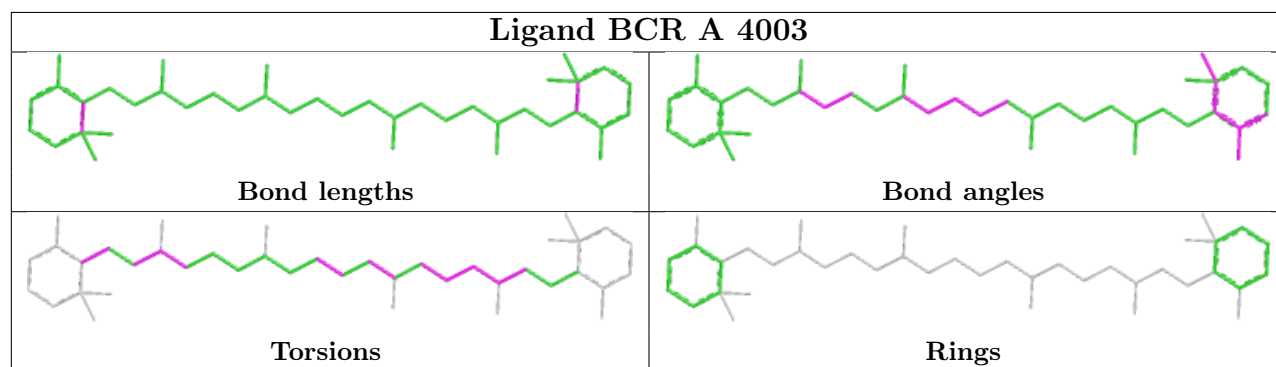
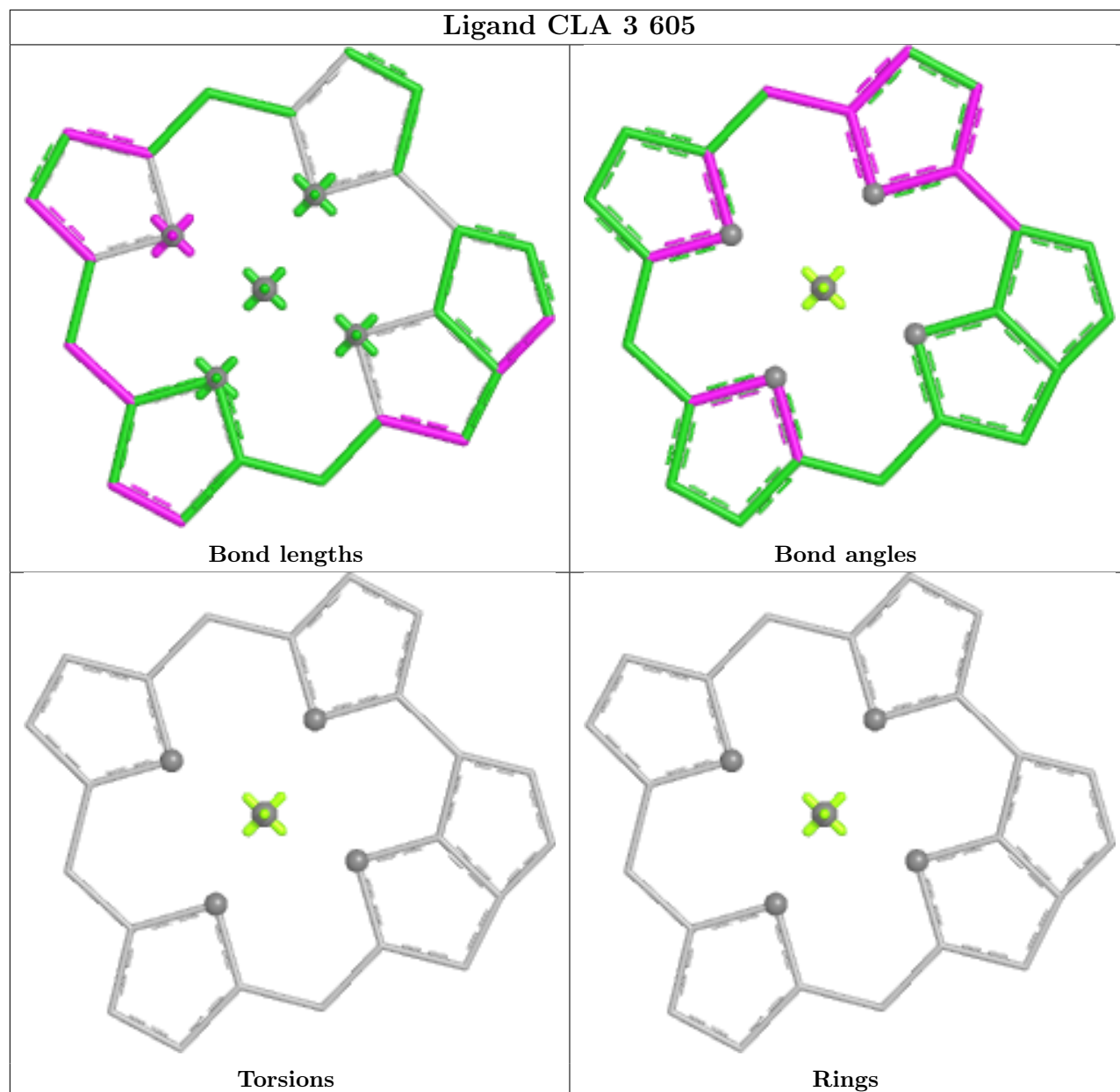


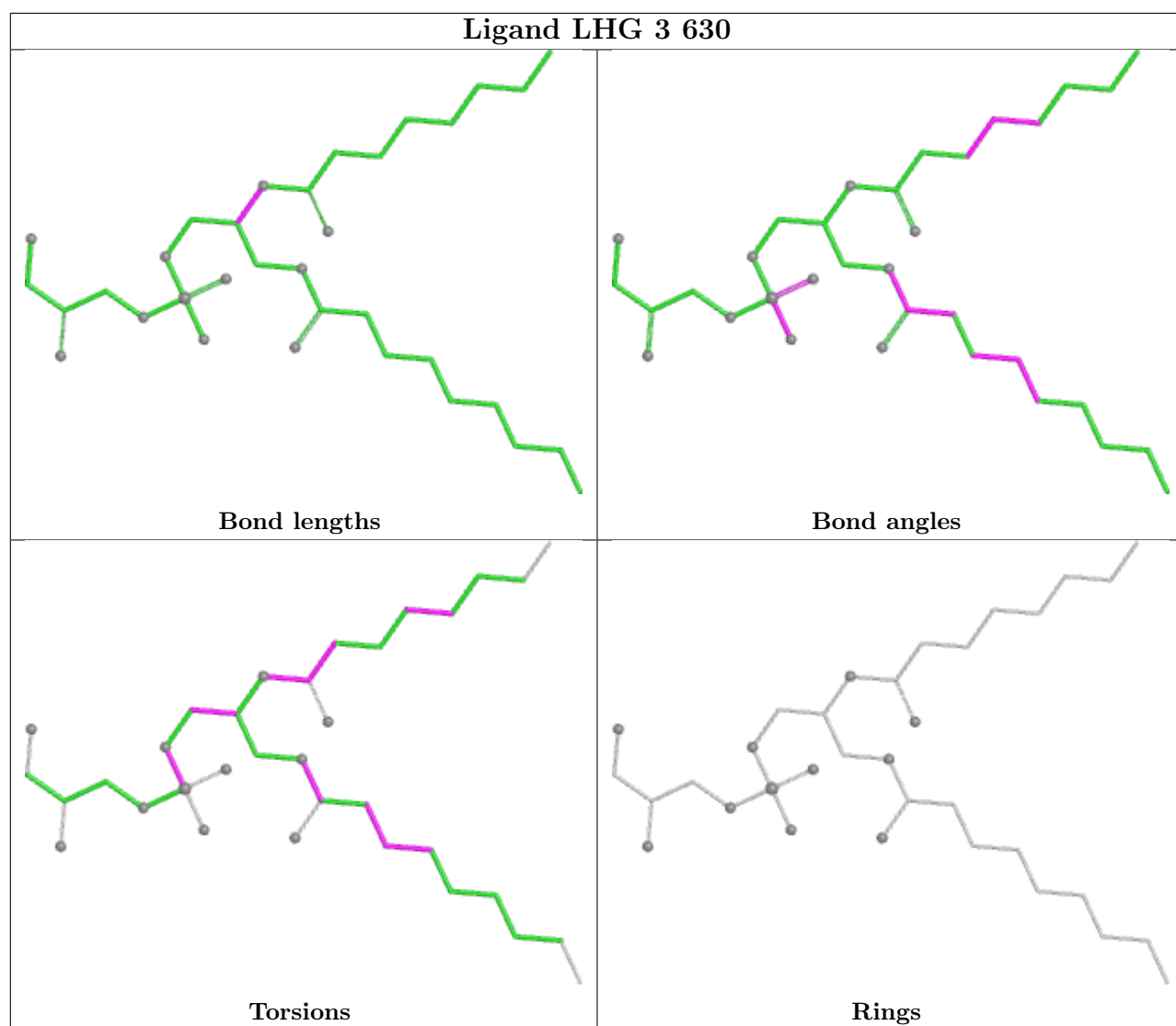
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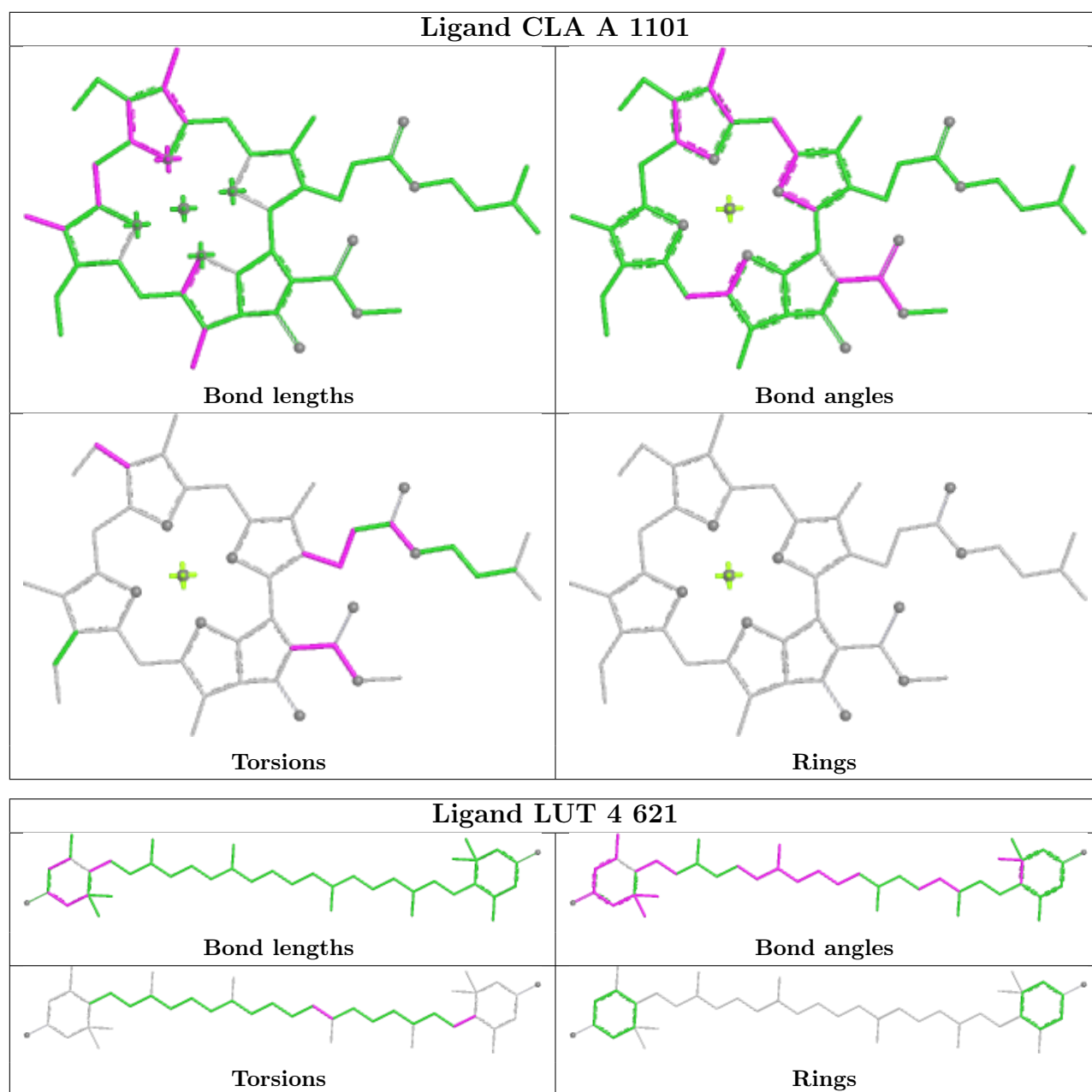




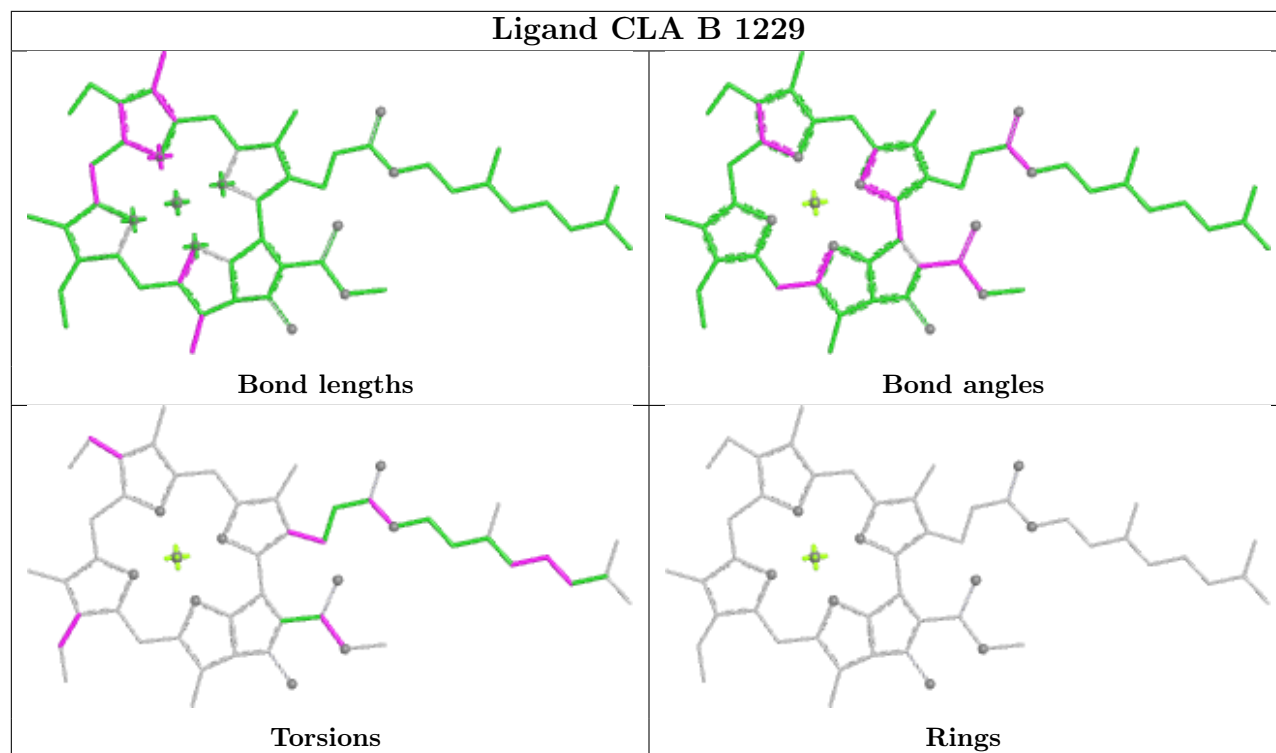




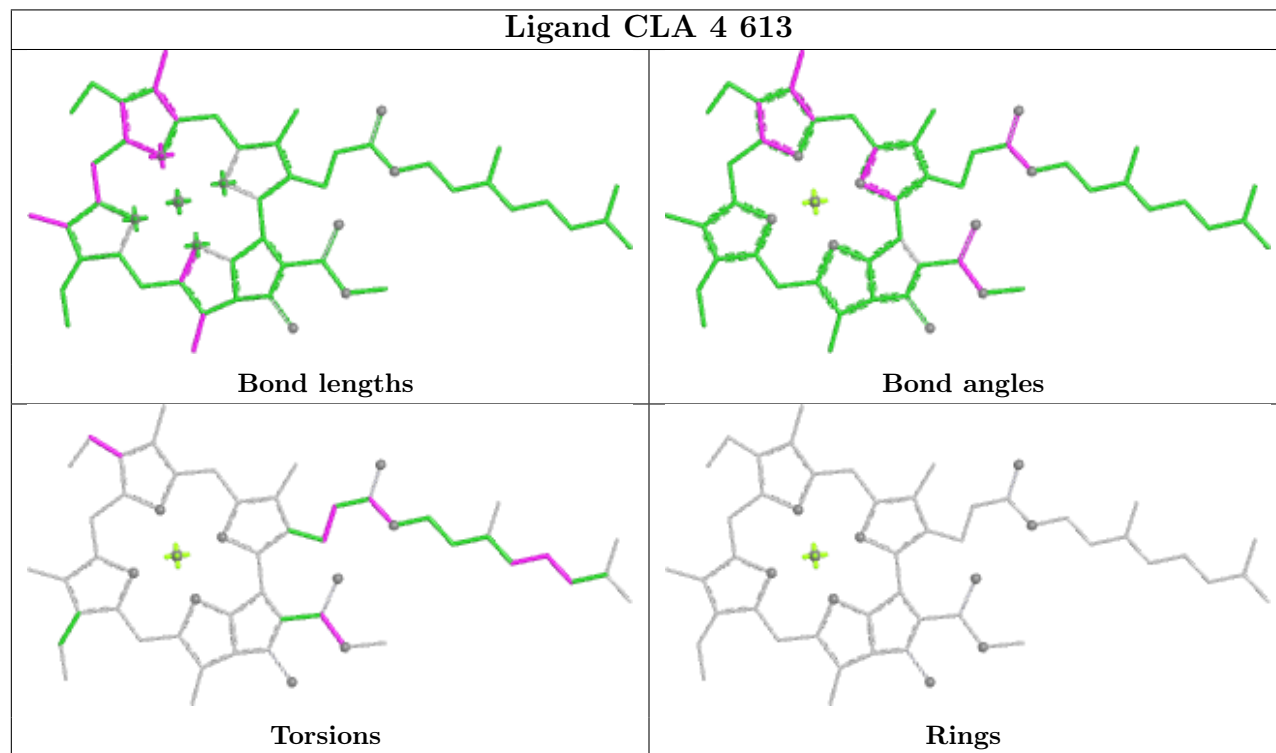


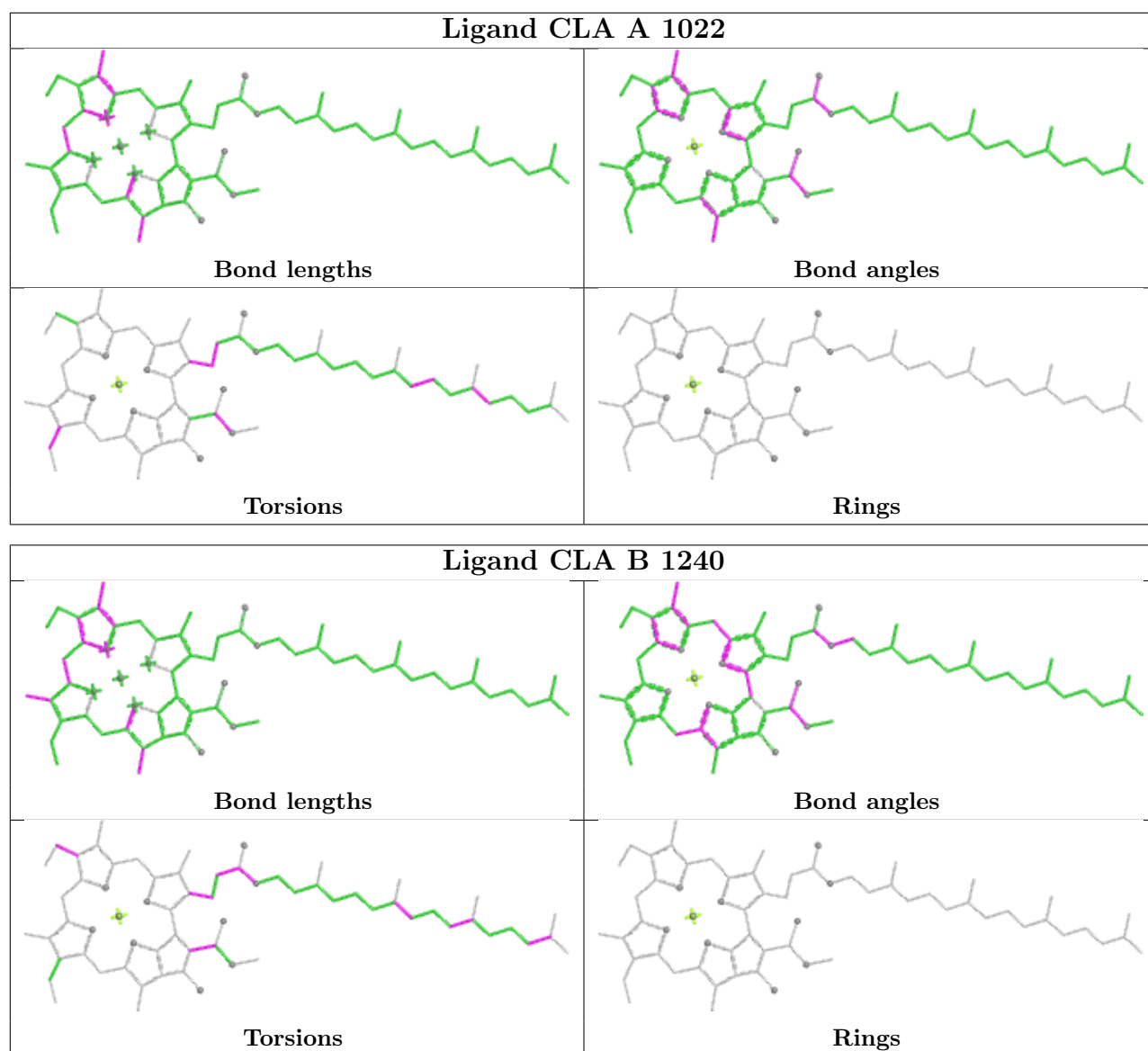


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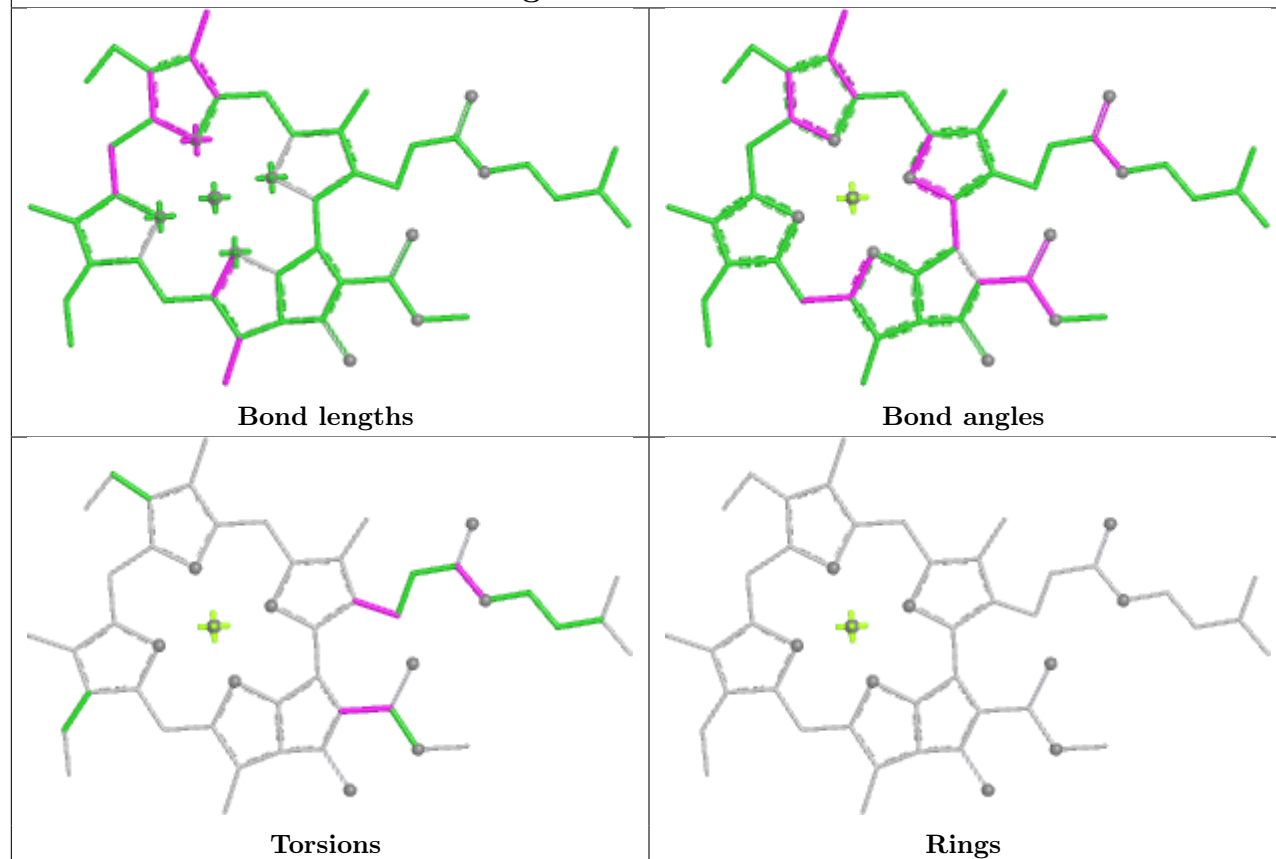


Ligand CLA 4 613

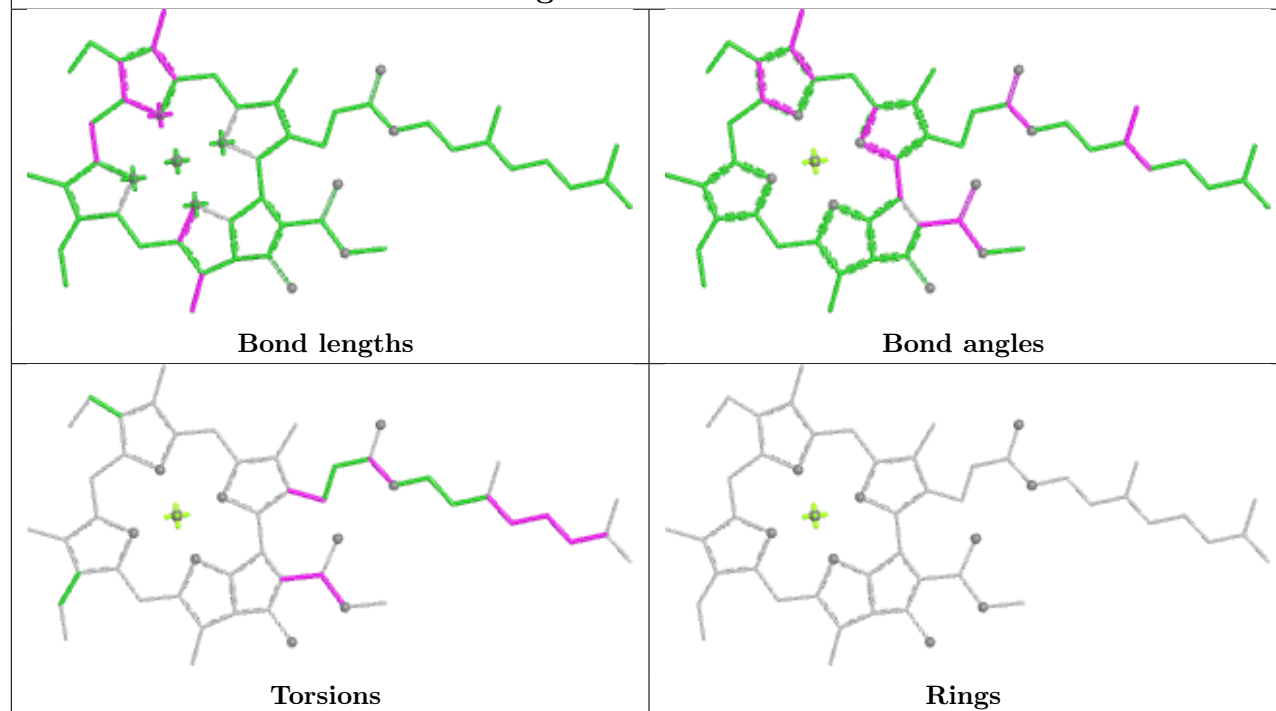




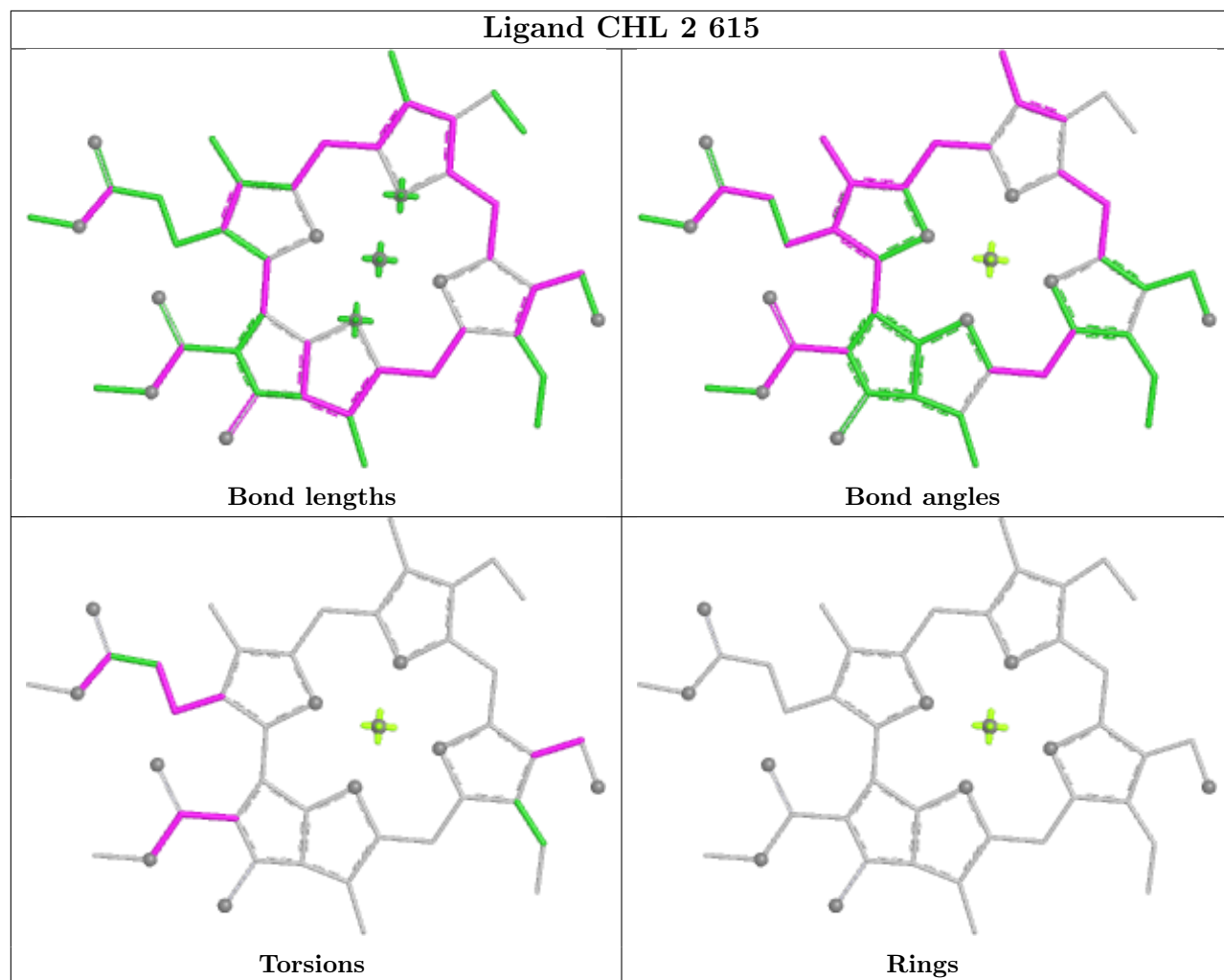
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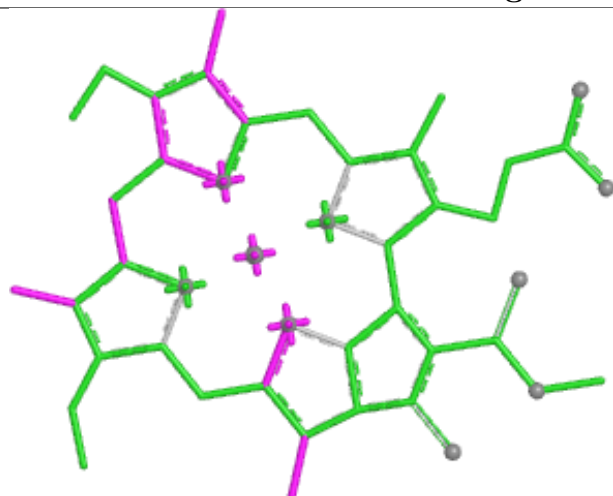
Ligand CLA 1 603



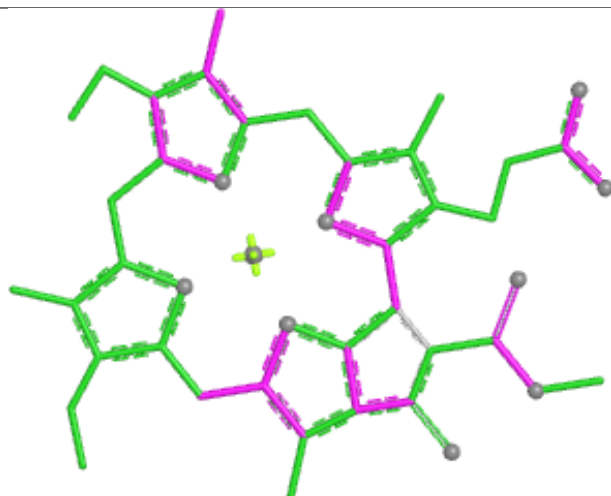
Ligand CHL 2 615



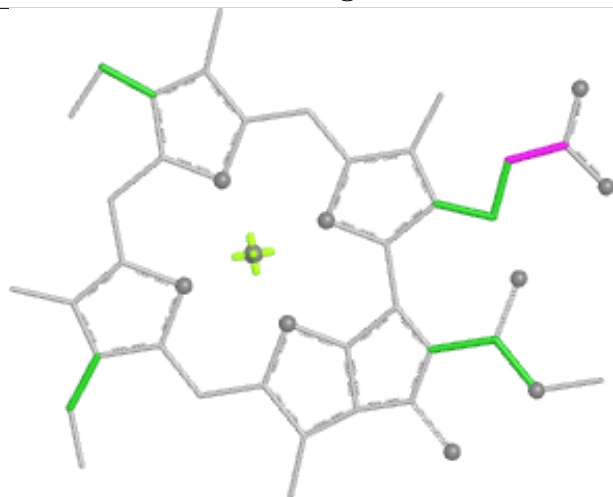
Ligand CLA B 1227



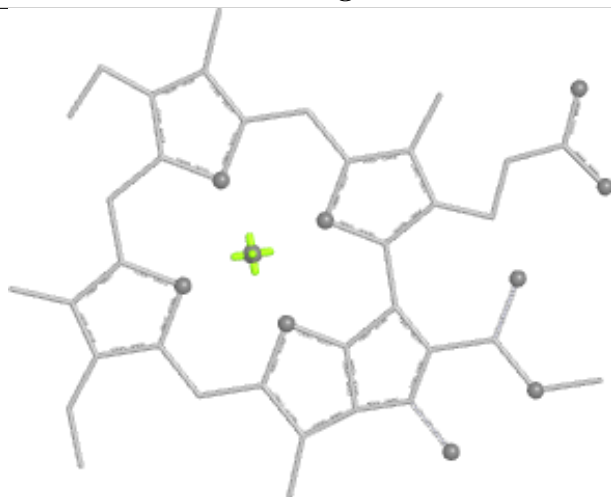
Bond lengths



Bond angles

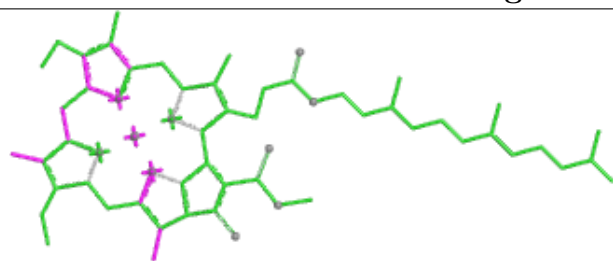


Torsions

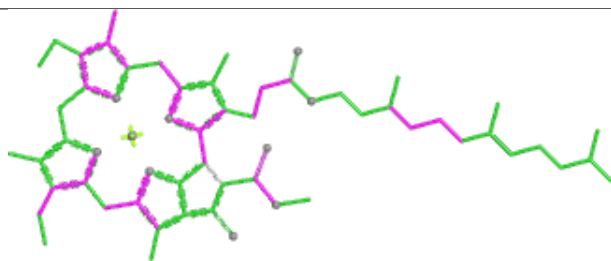


Rings

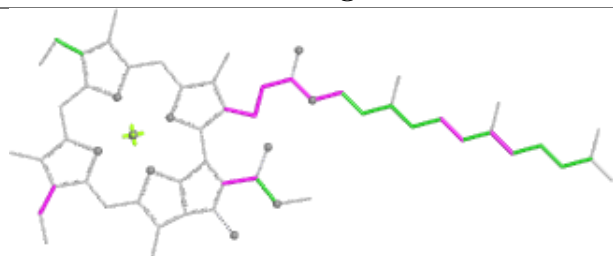
Ligand CLA A 1125



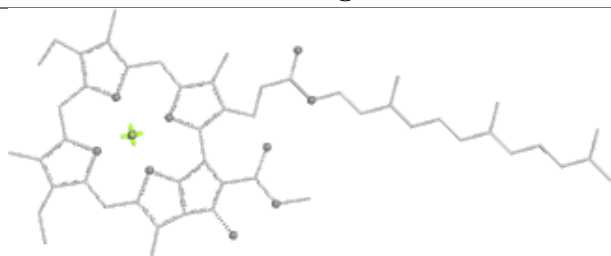
Bond lengths



Bond angles

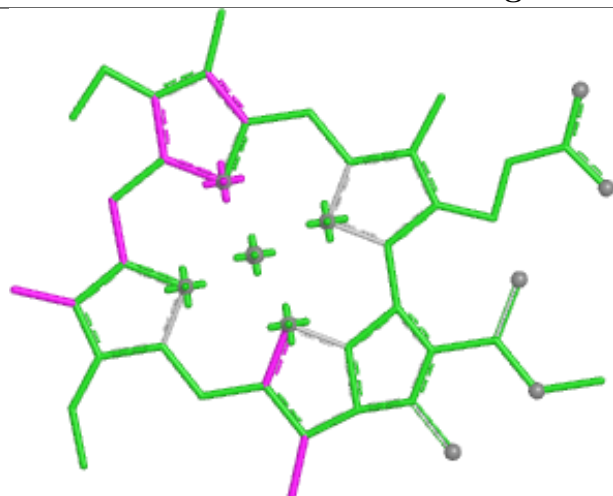


Torsions

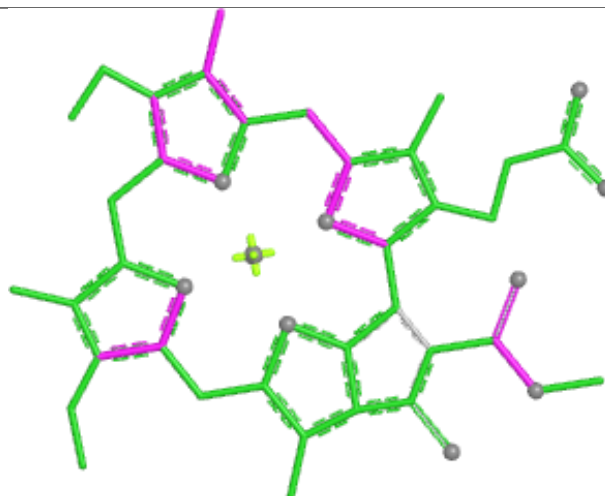


Rings

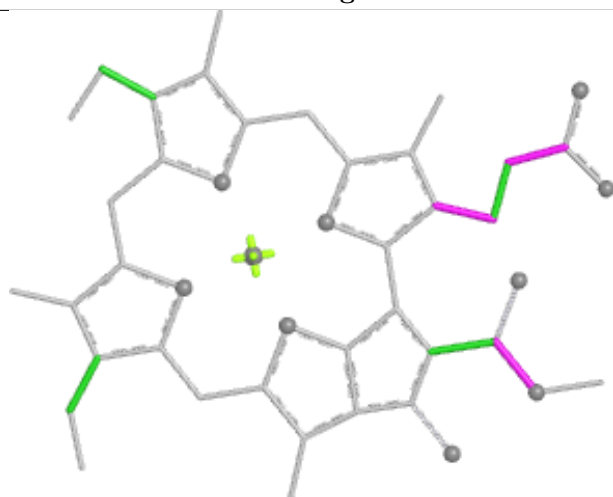
Ligand CLA A 1108



Bond lengths



Bond angles

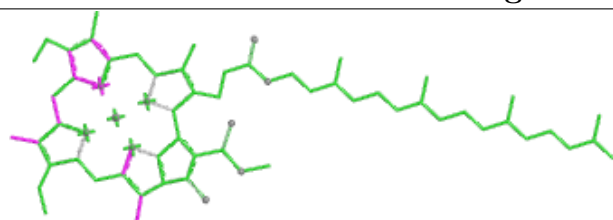


Torsions

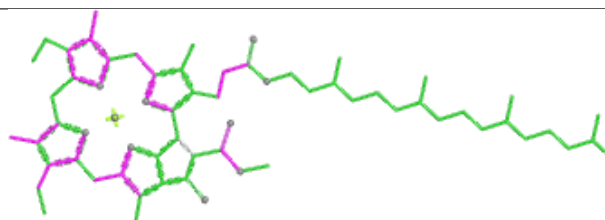


Rings

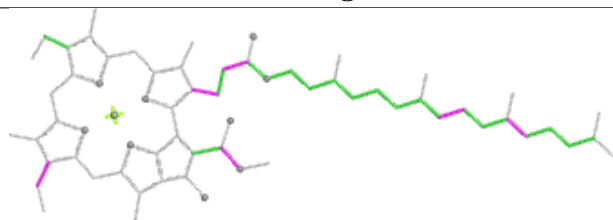
Ligand CLA A 1132



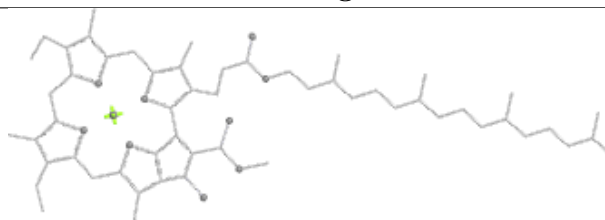
Bond lengths



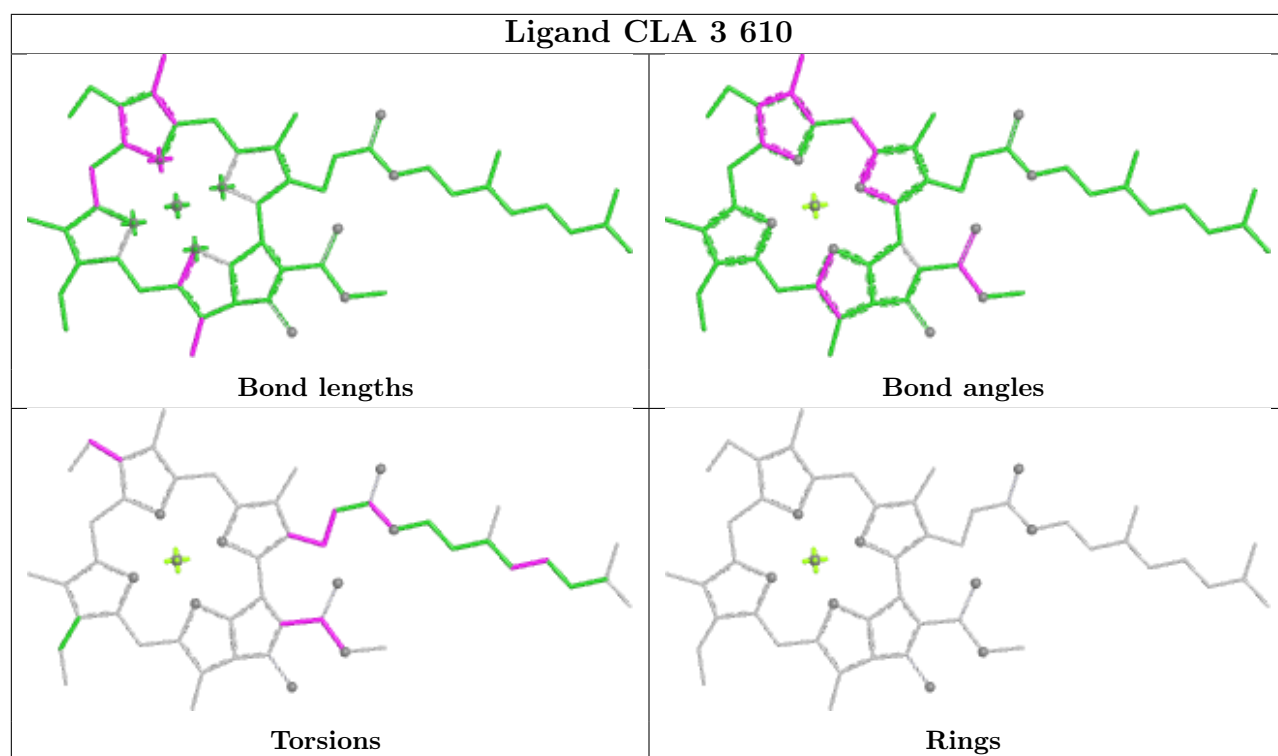
Bond angles

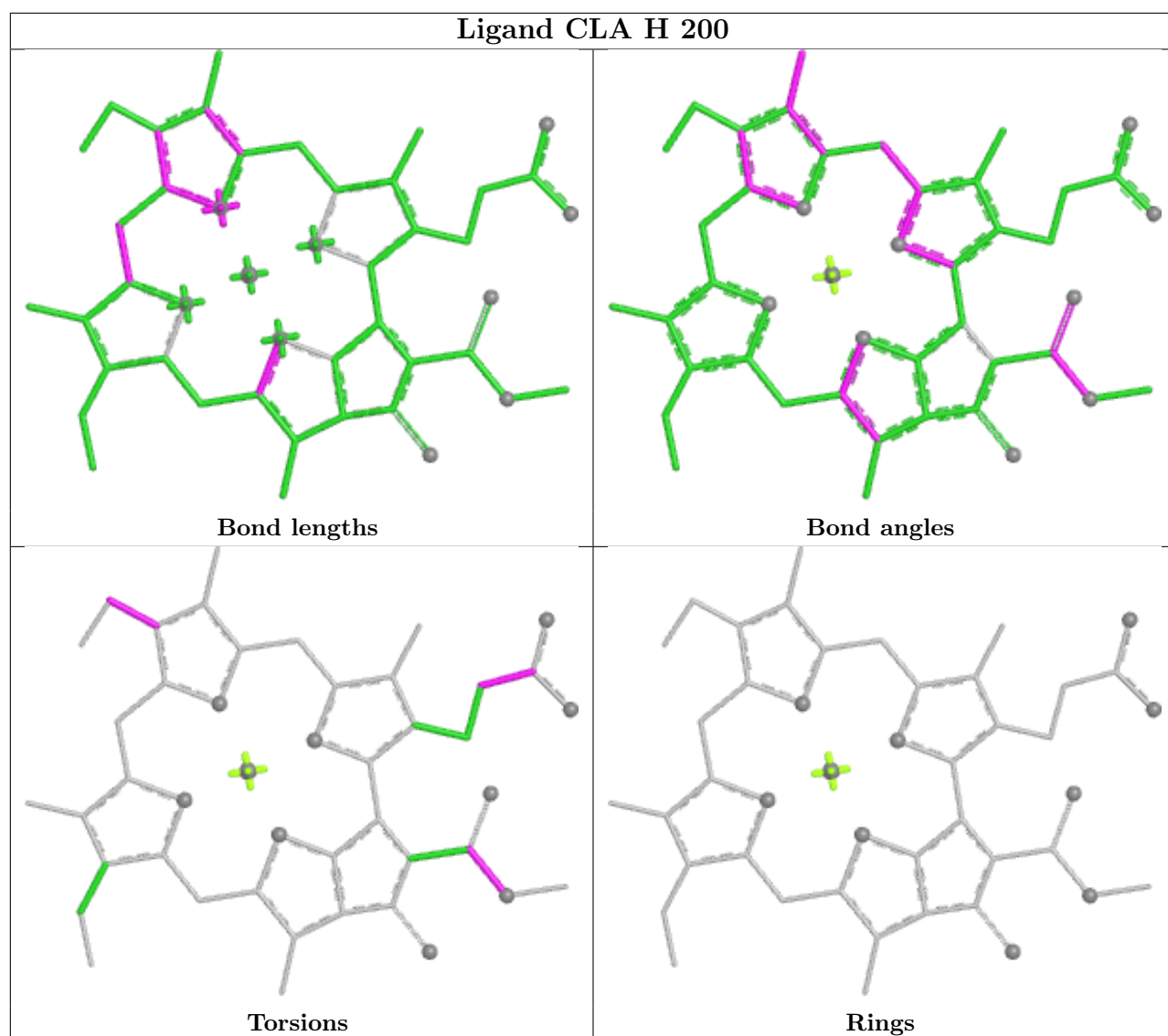


Torsions

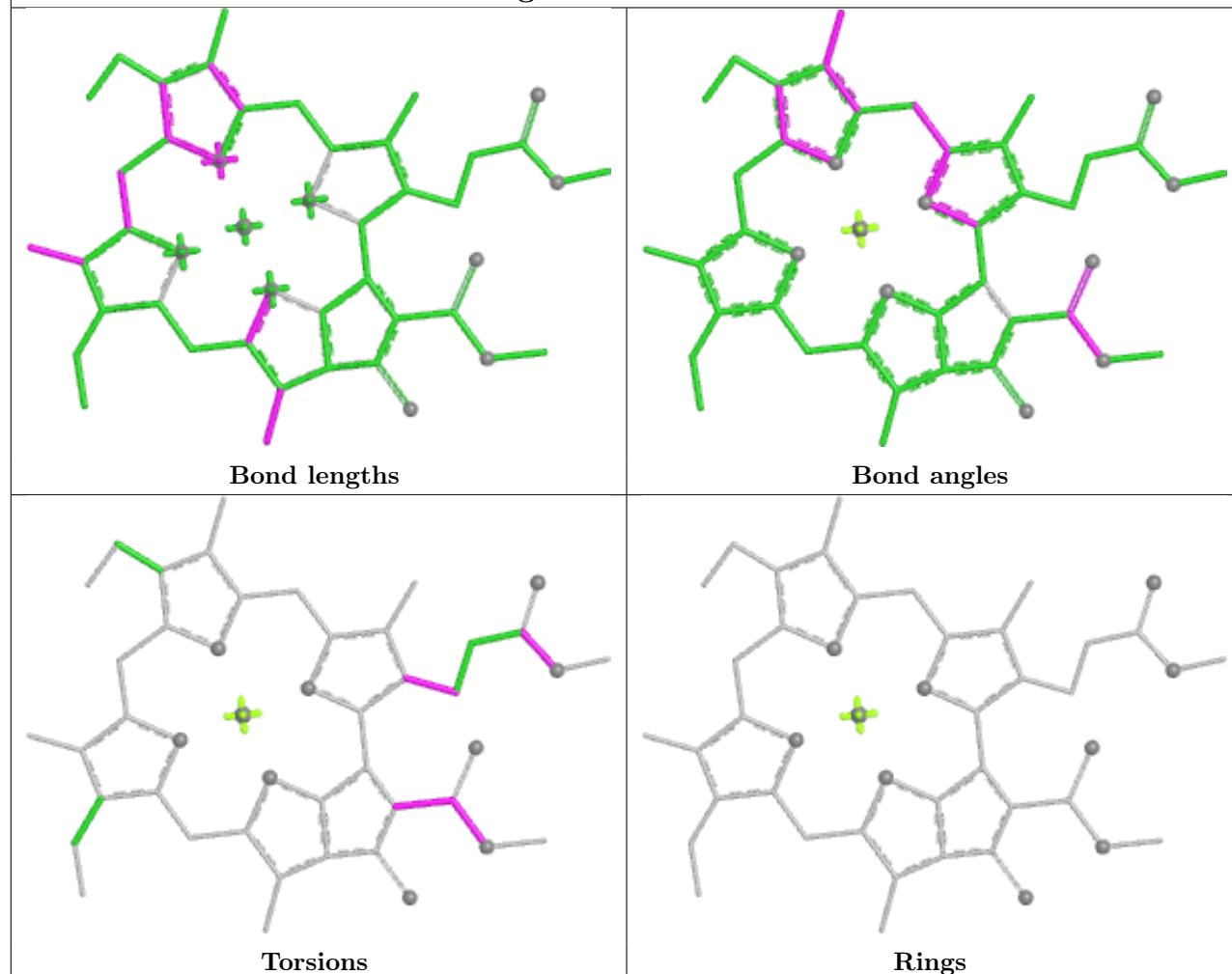


Rings

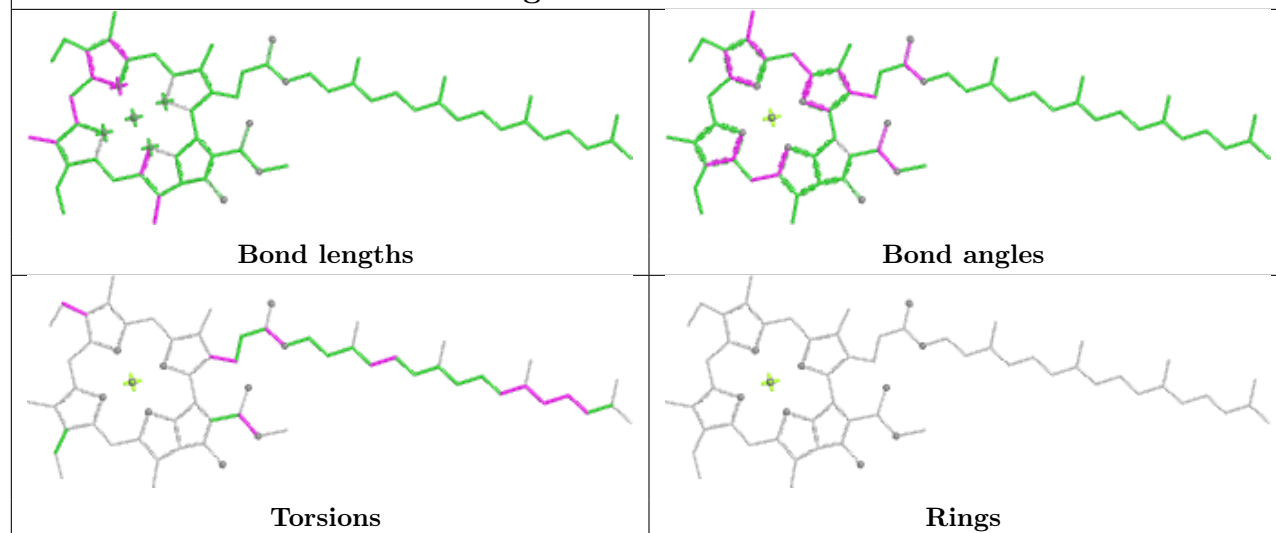


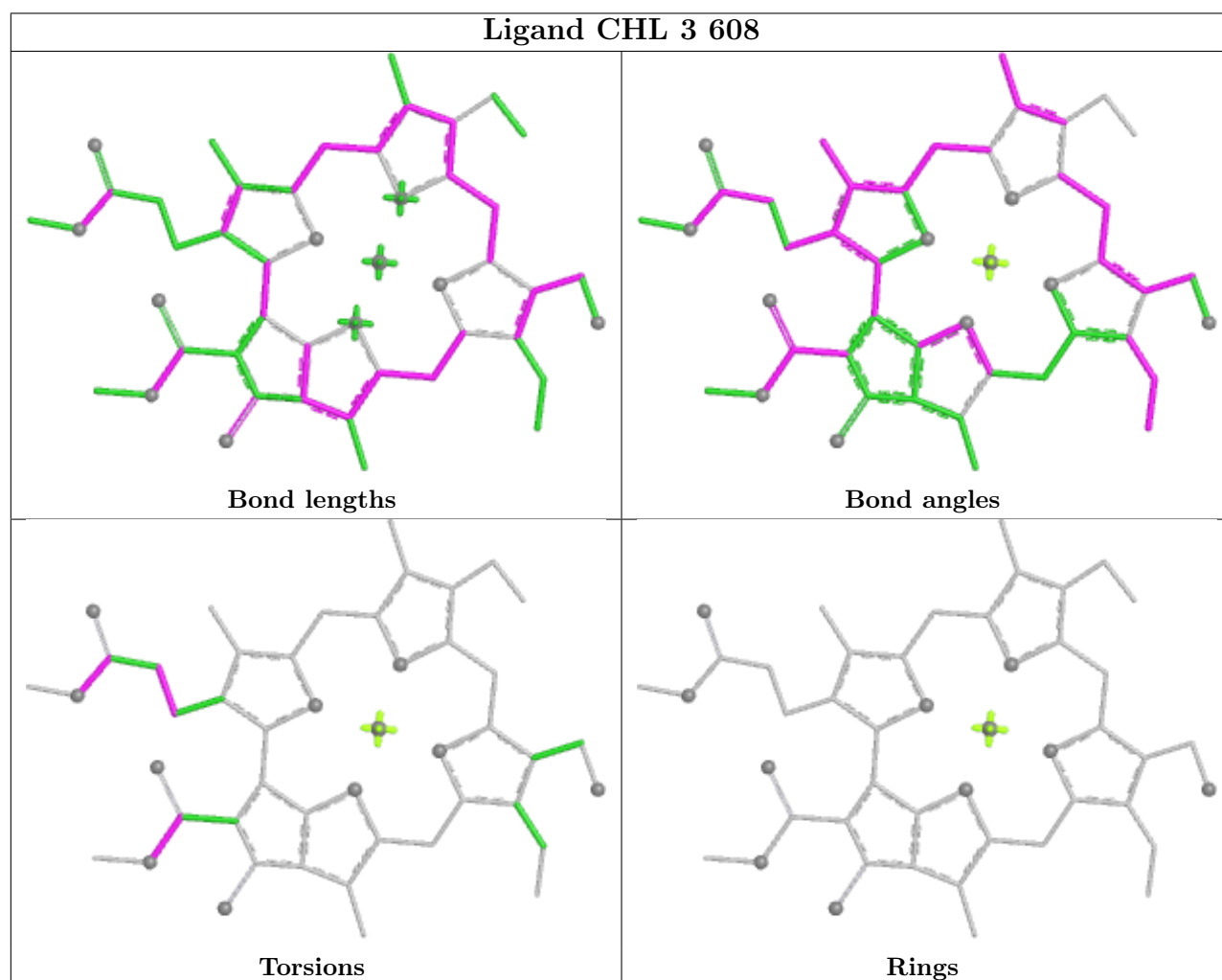
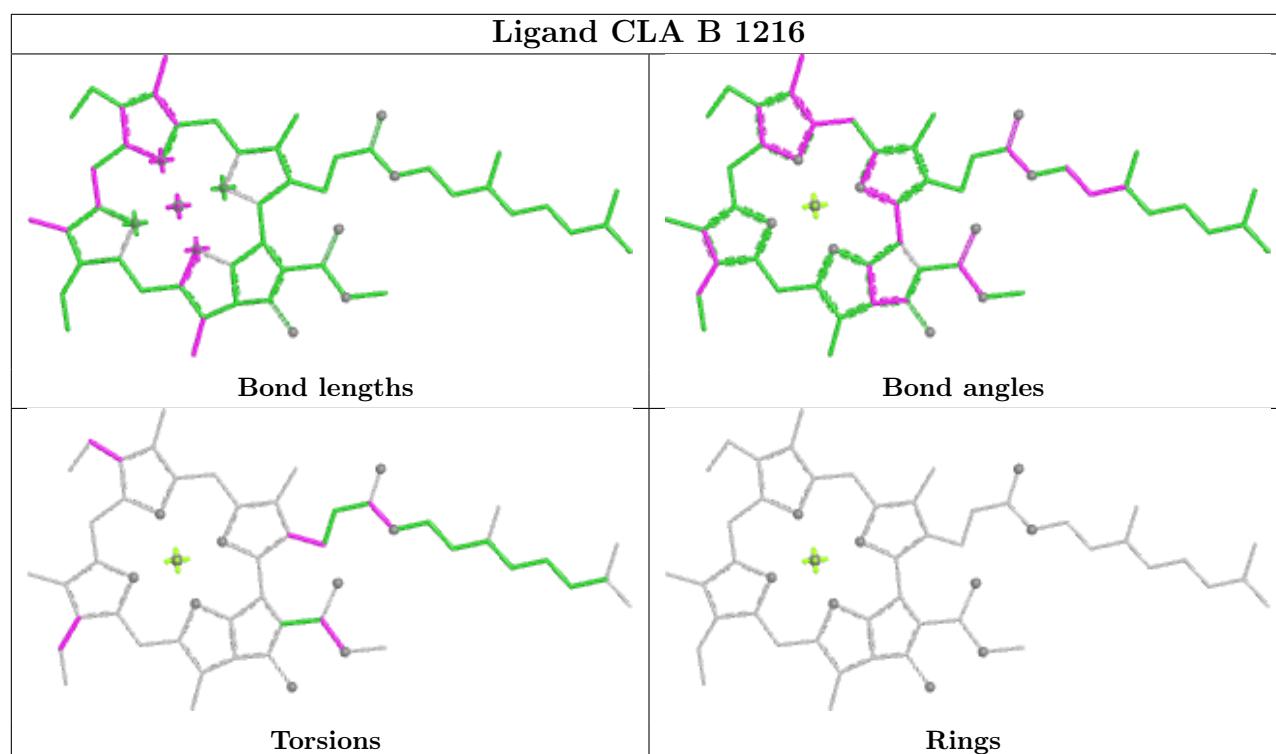


Ligand CLA 1 615

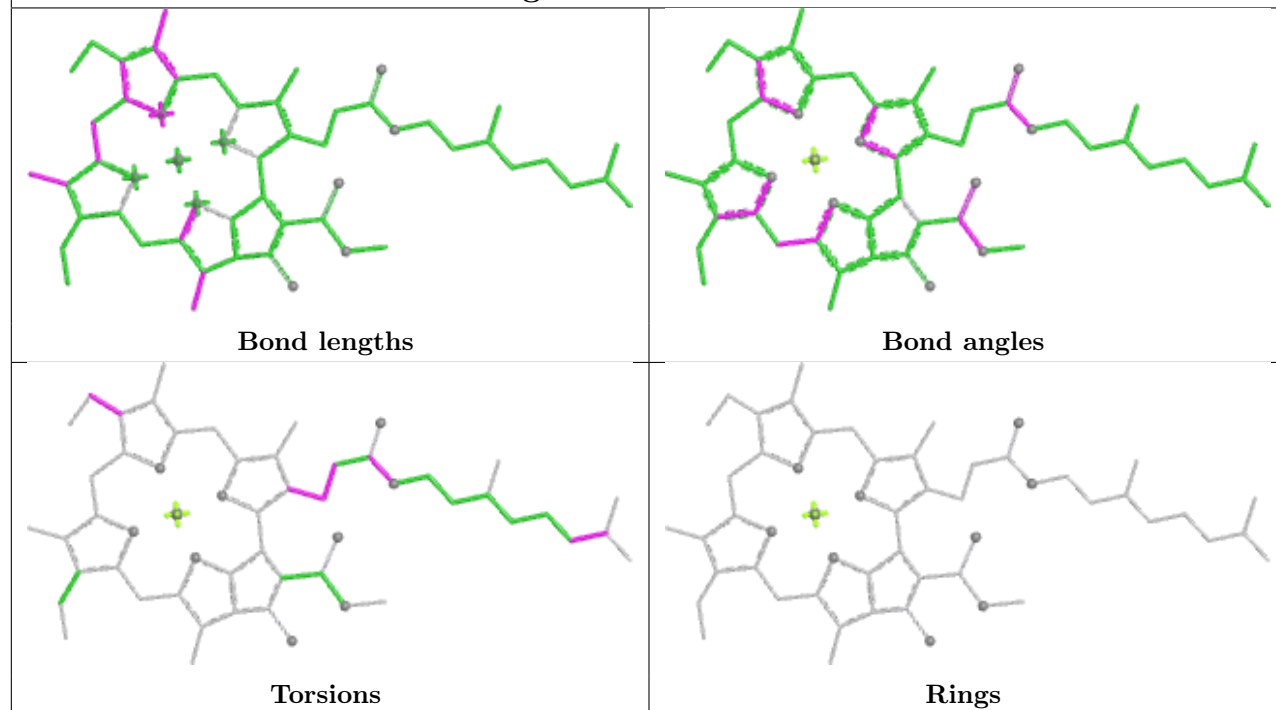


Ligand CLA B 1203

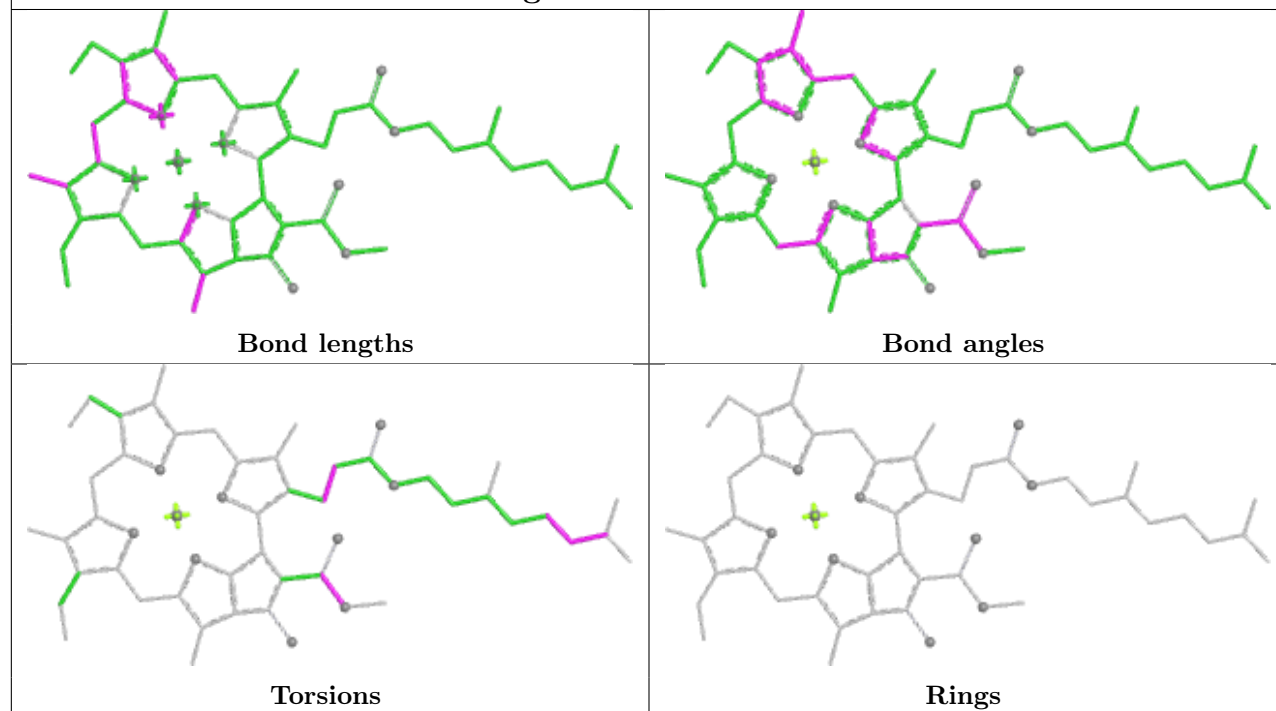




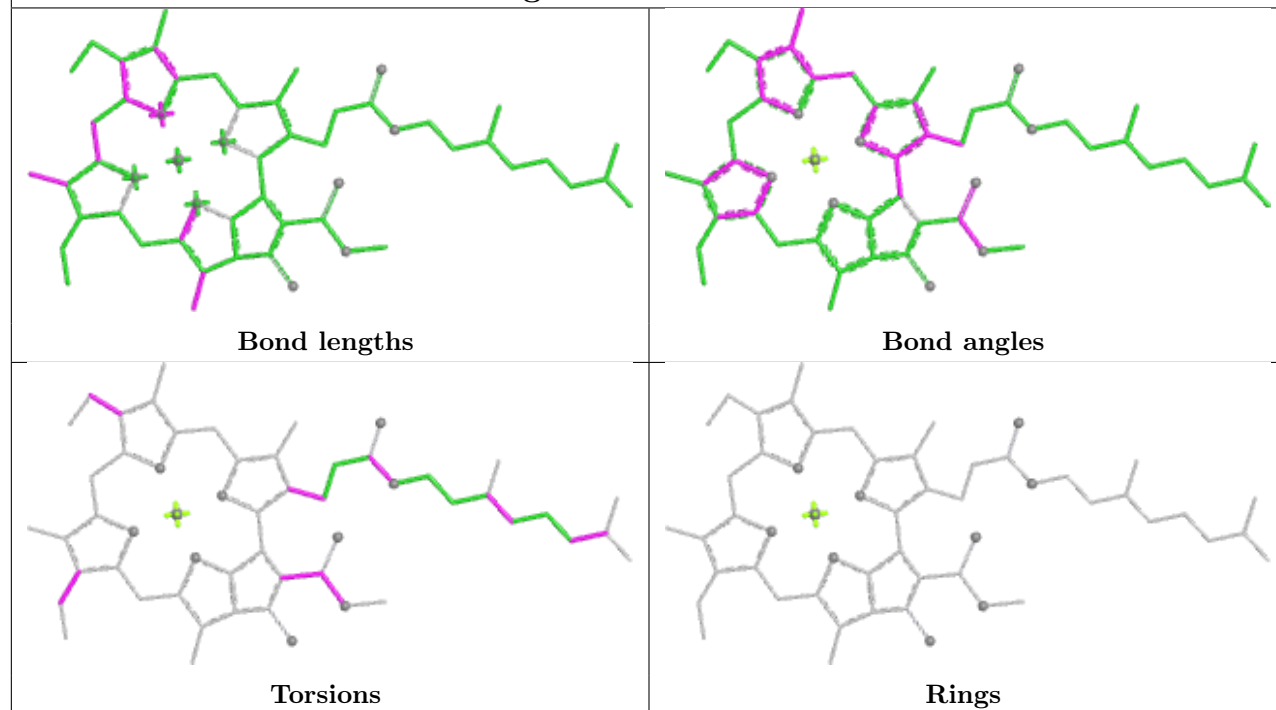
Ligand CLA A 1110



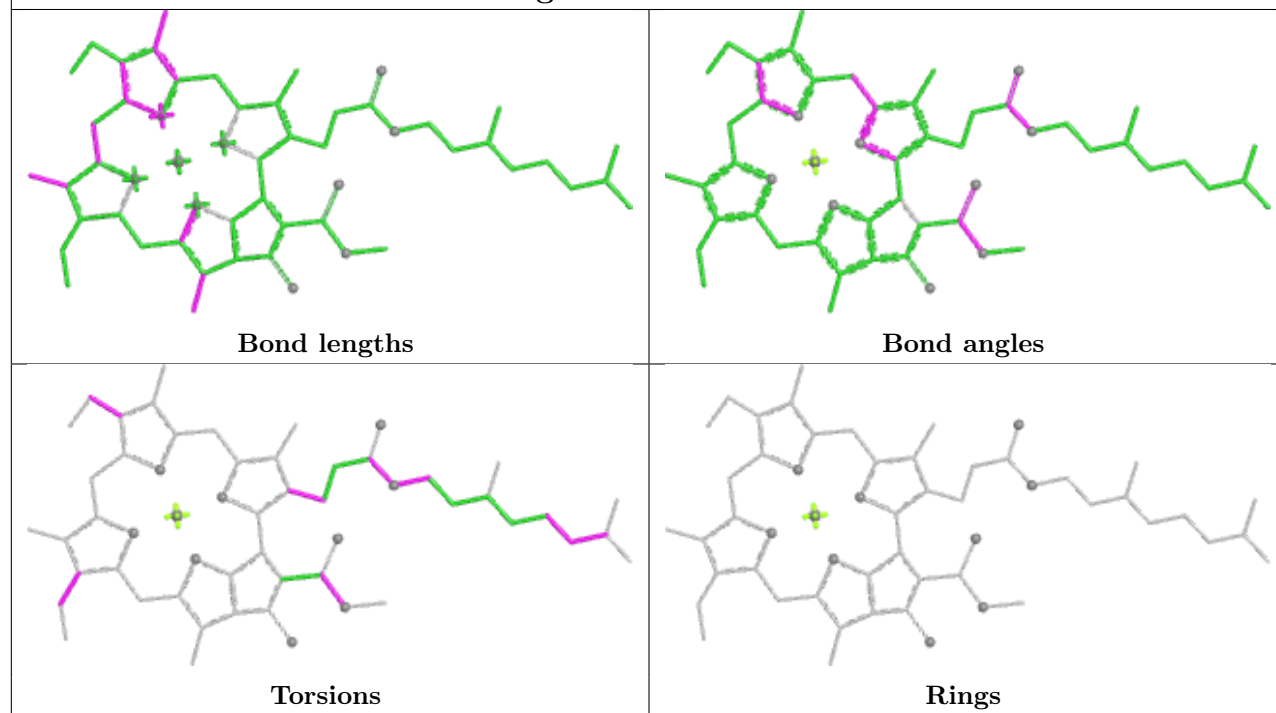
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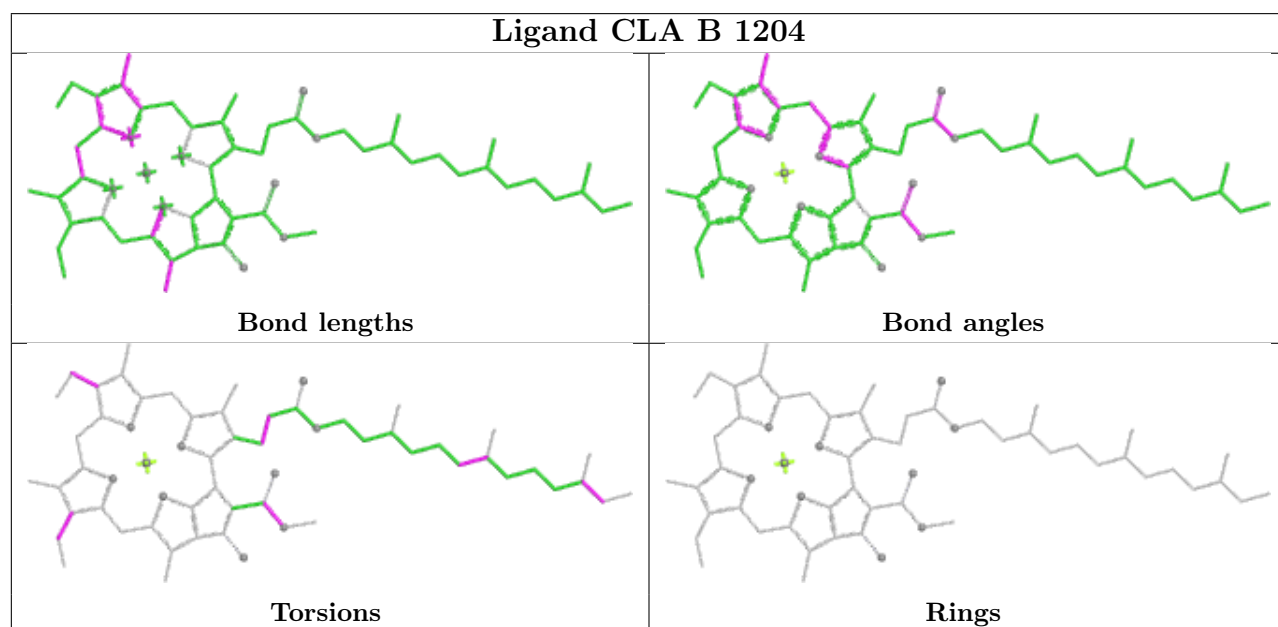
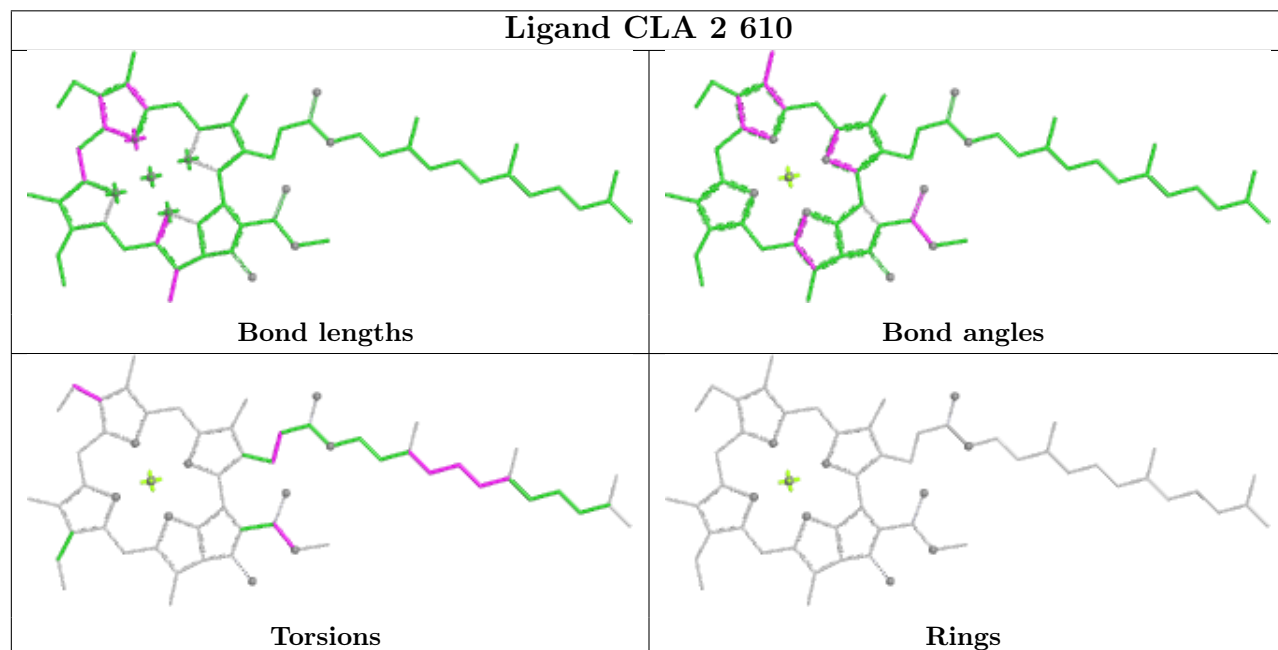
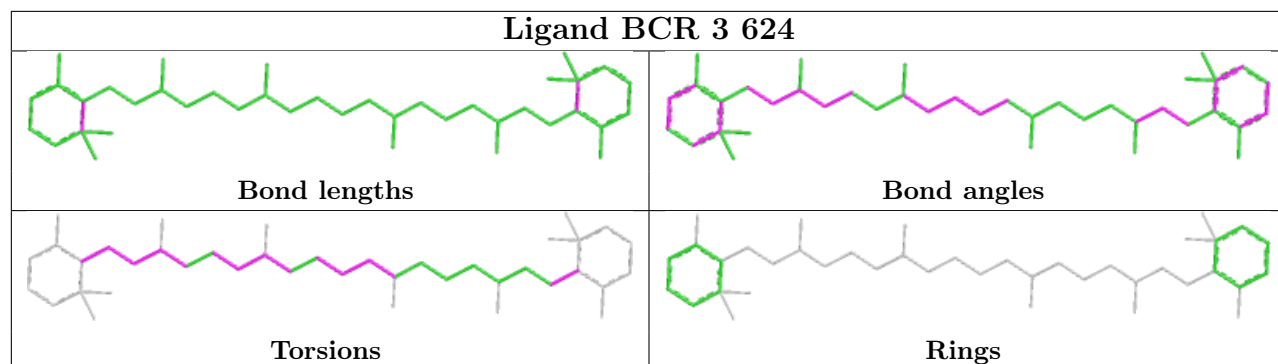


Ligand CLA B 1012

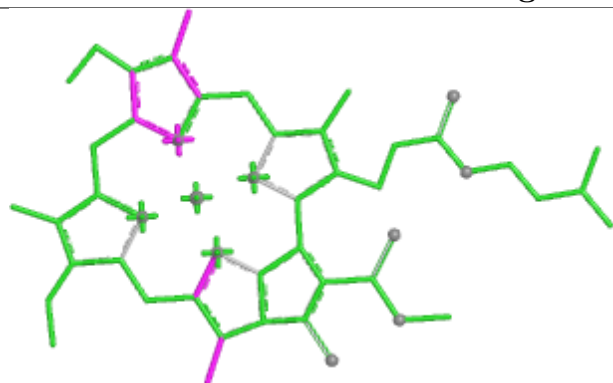


Ligand CLA 3 603

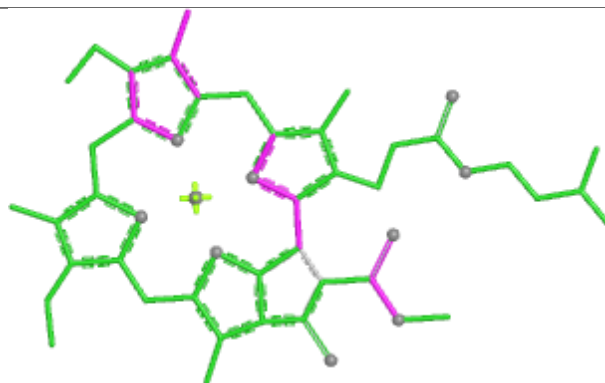




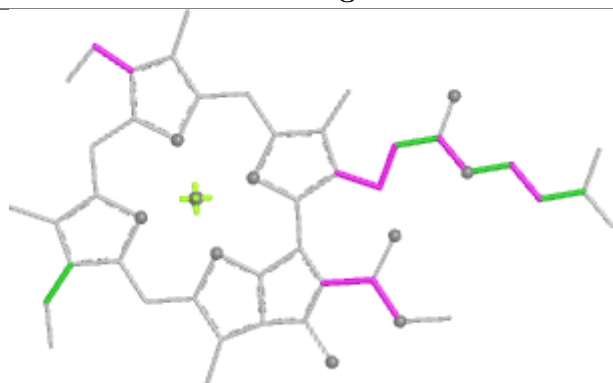
Ligand CLA 4 601



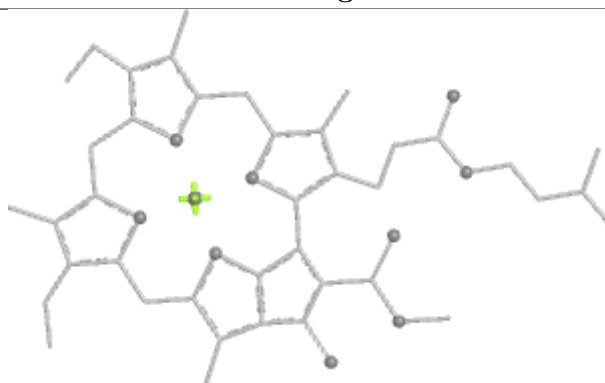
Bond lengths



Bond angles

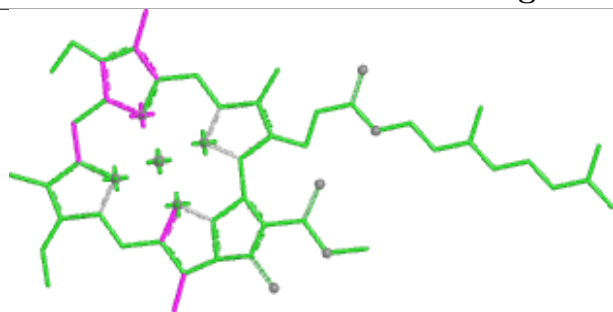


Torsions

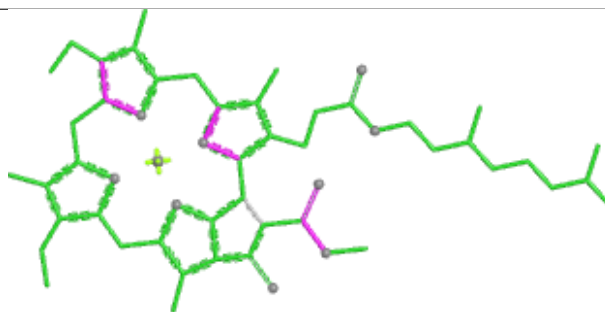


Rings

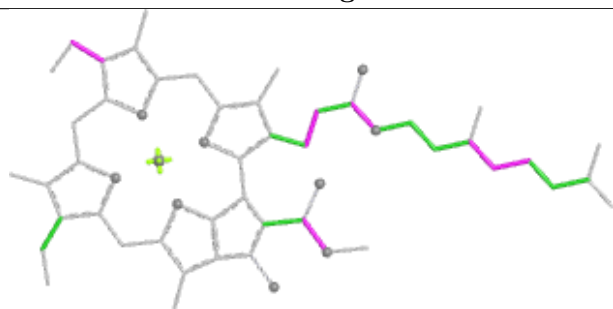
Ligand CLA 3 613



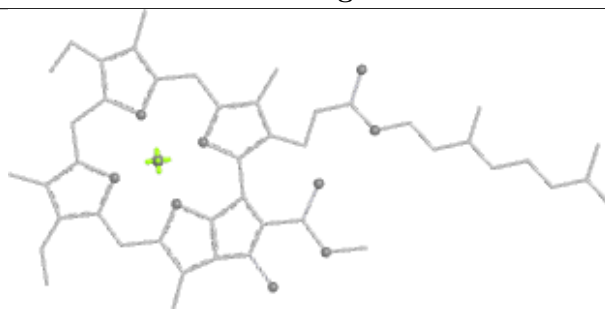
Bond lengths



Bond angles

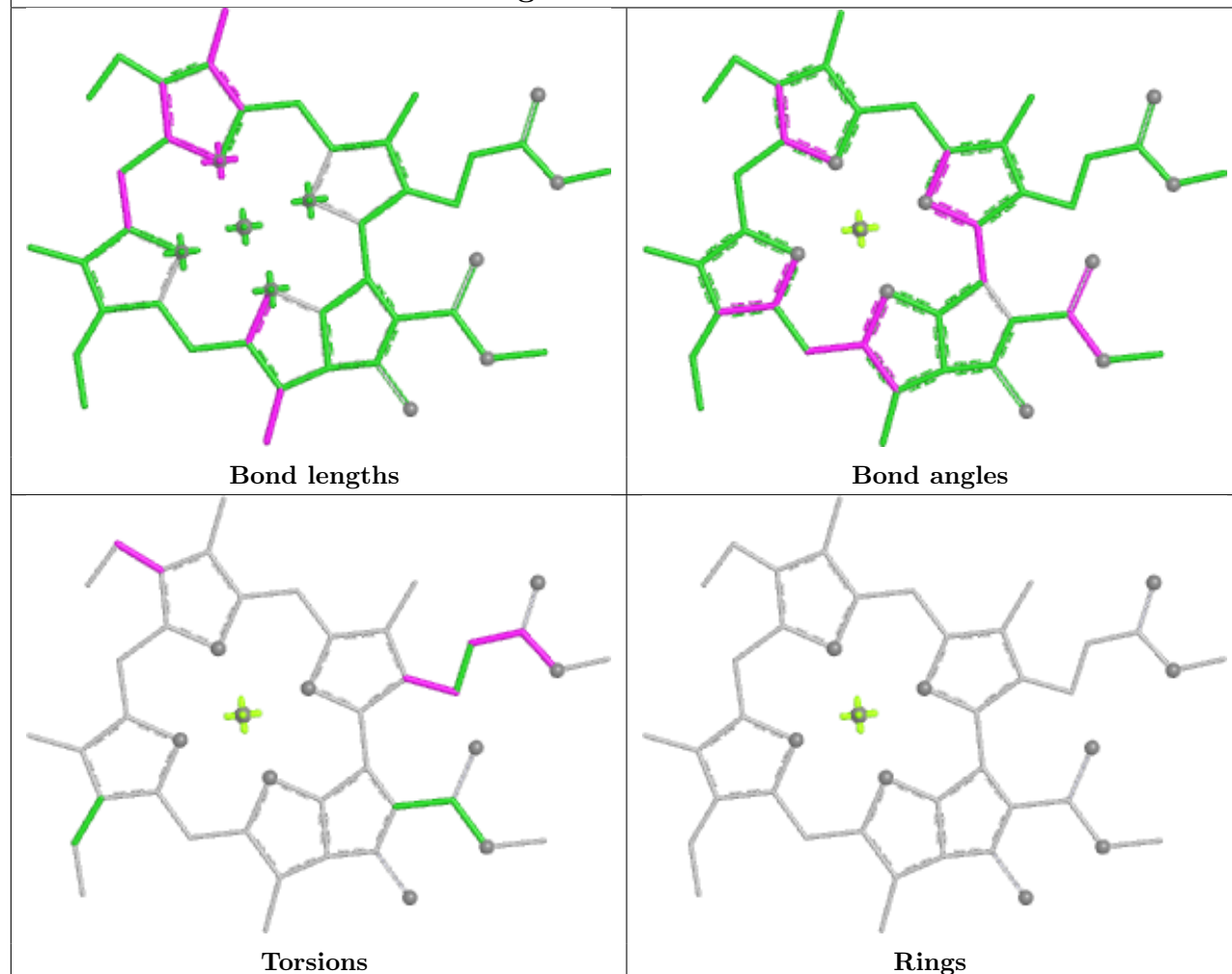


Torsions

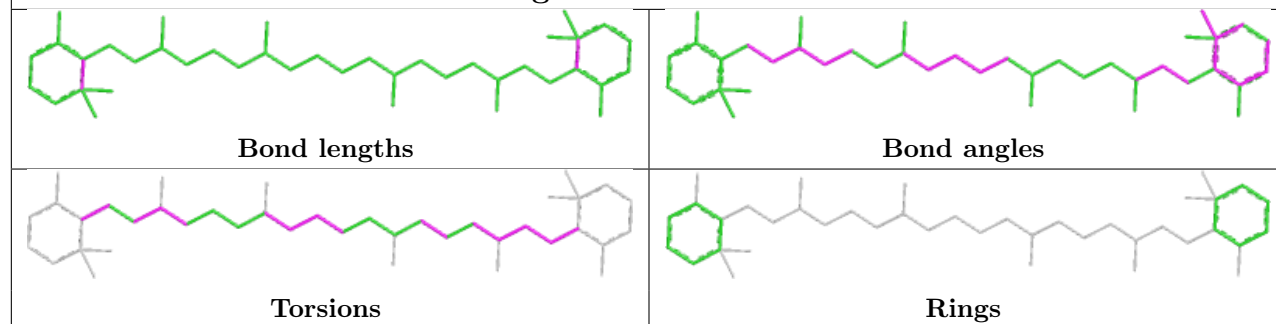


Rings

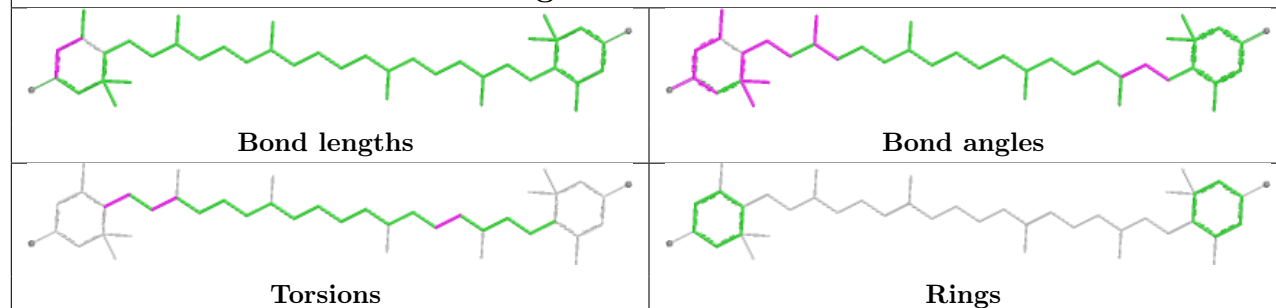
Ligand CLA 1 614



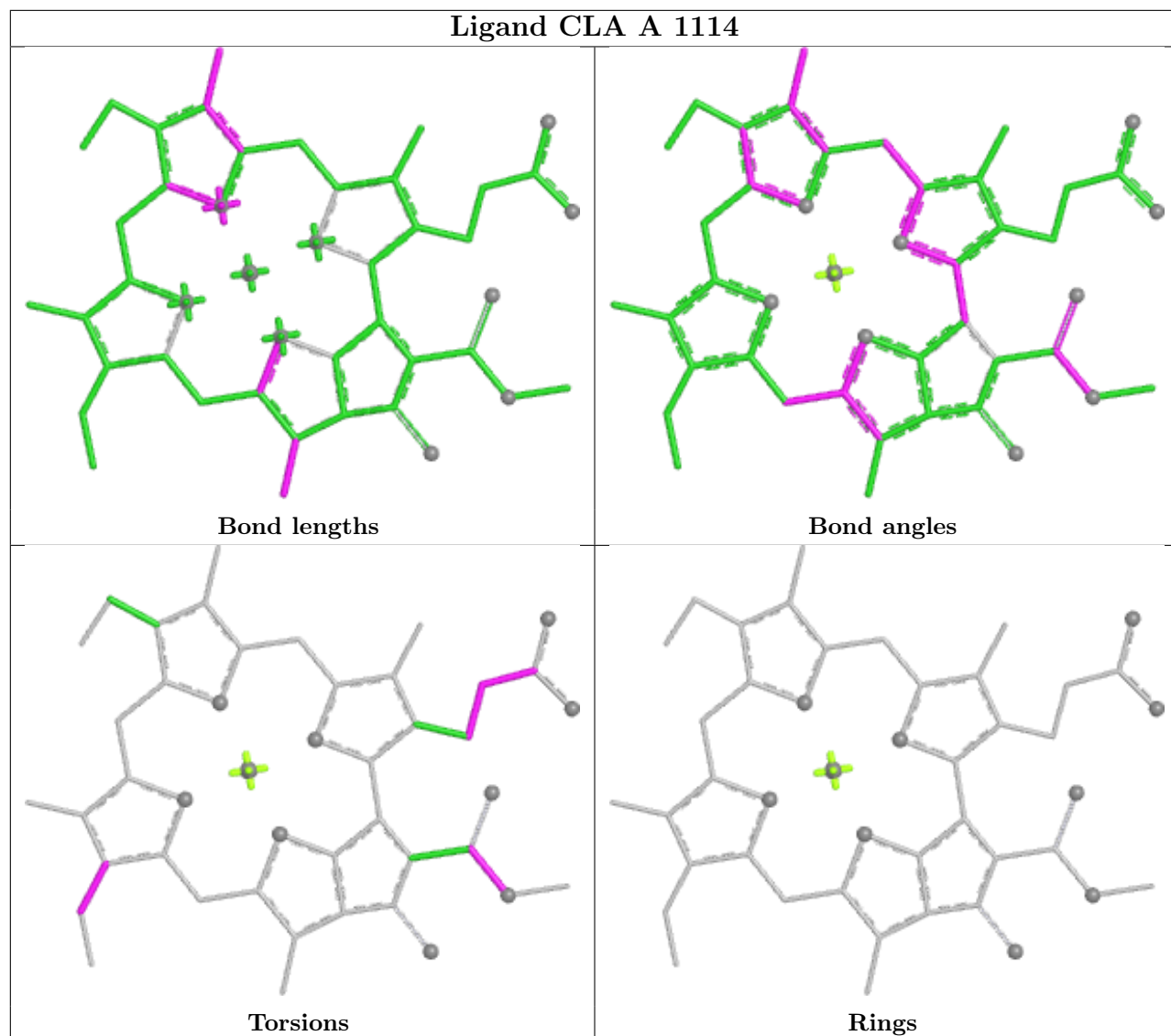
Ligand BCR F 416

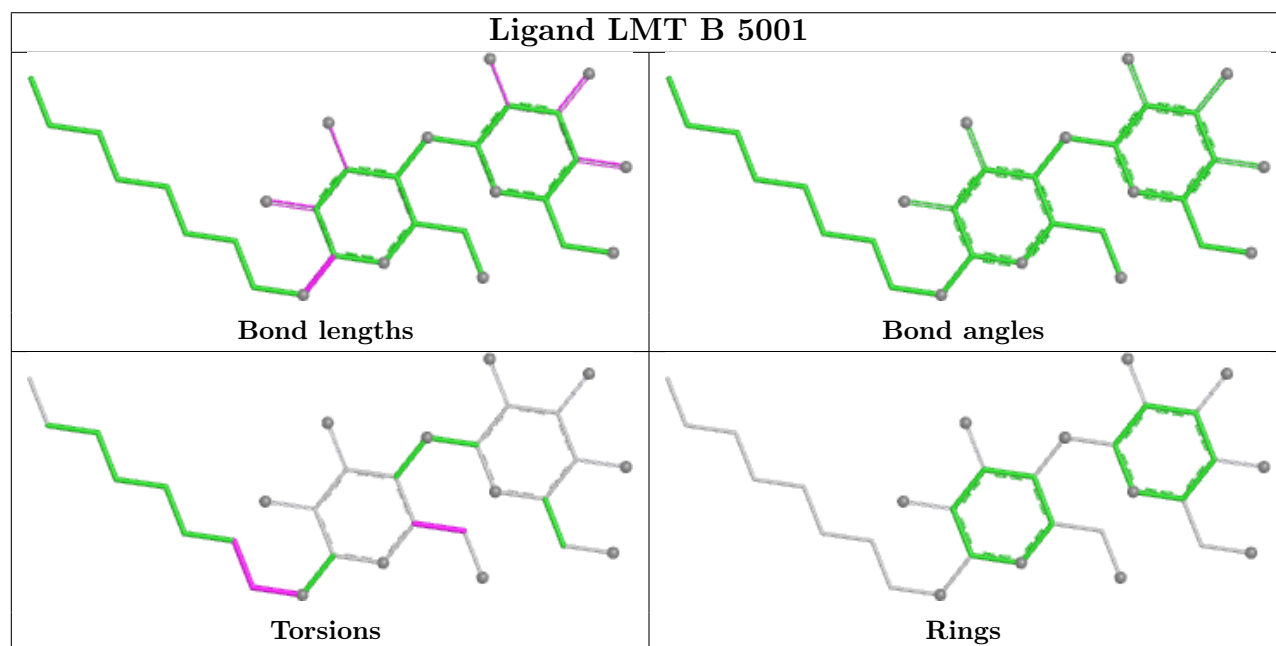
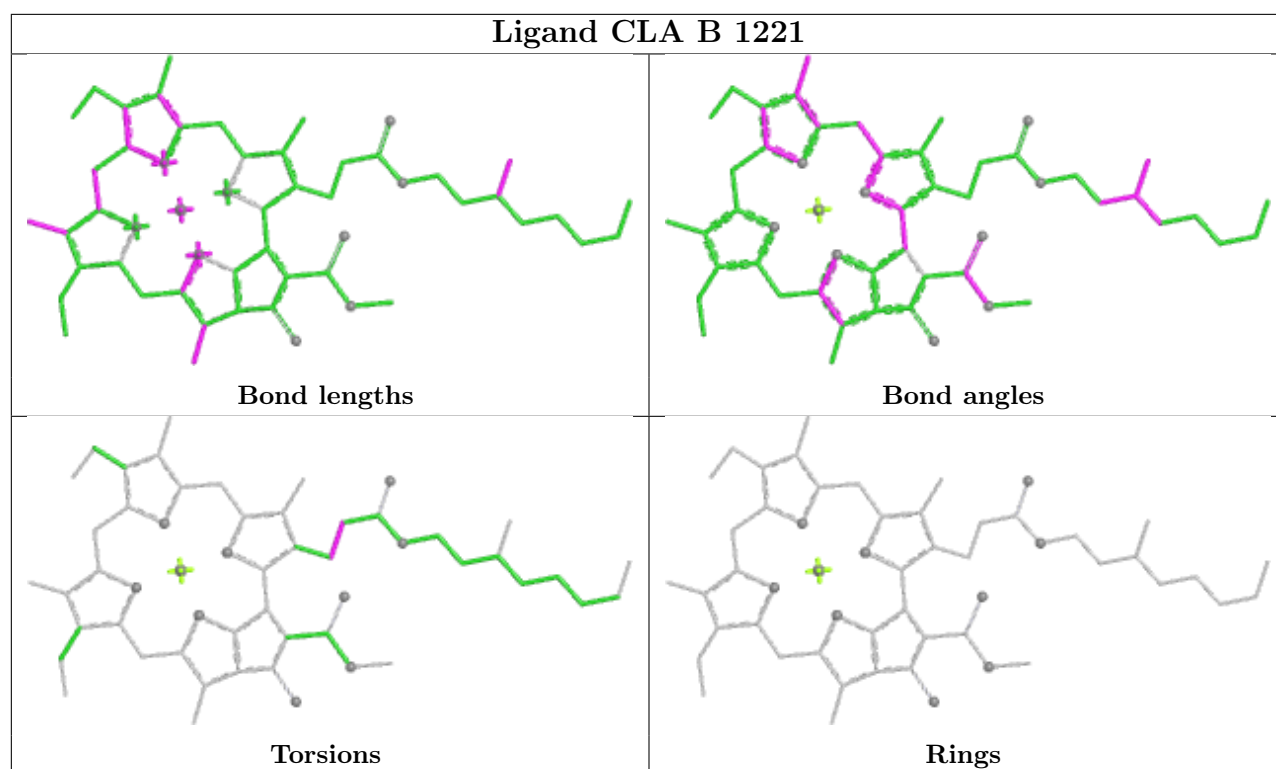


Ligand LUT 1 621

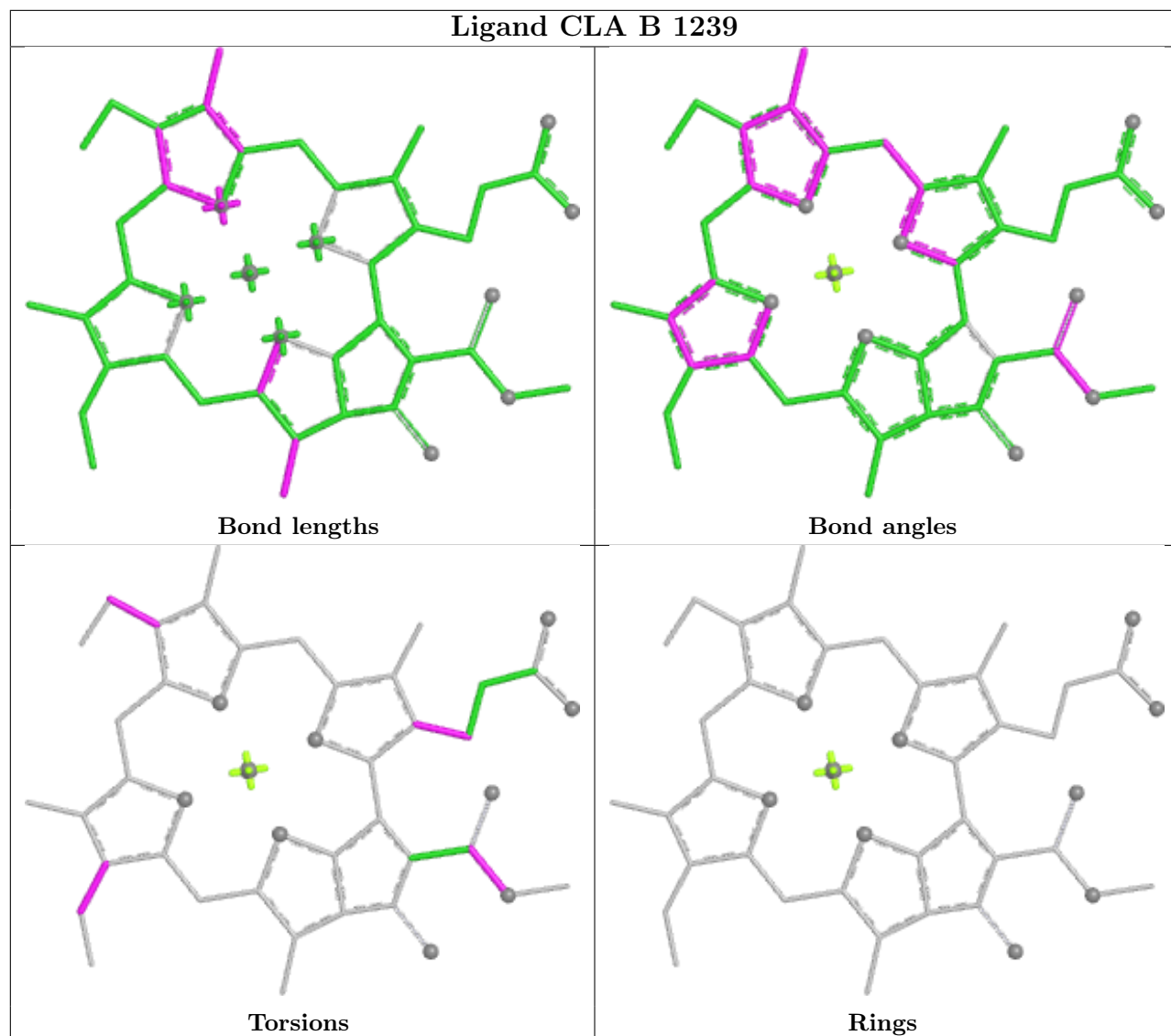


Ligand CLA A 1114

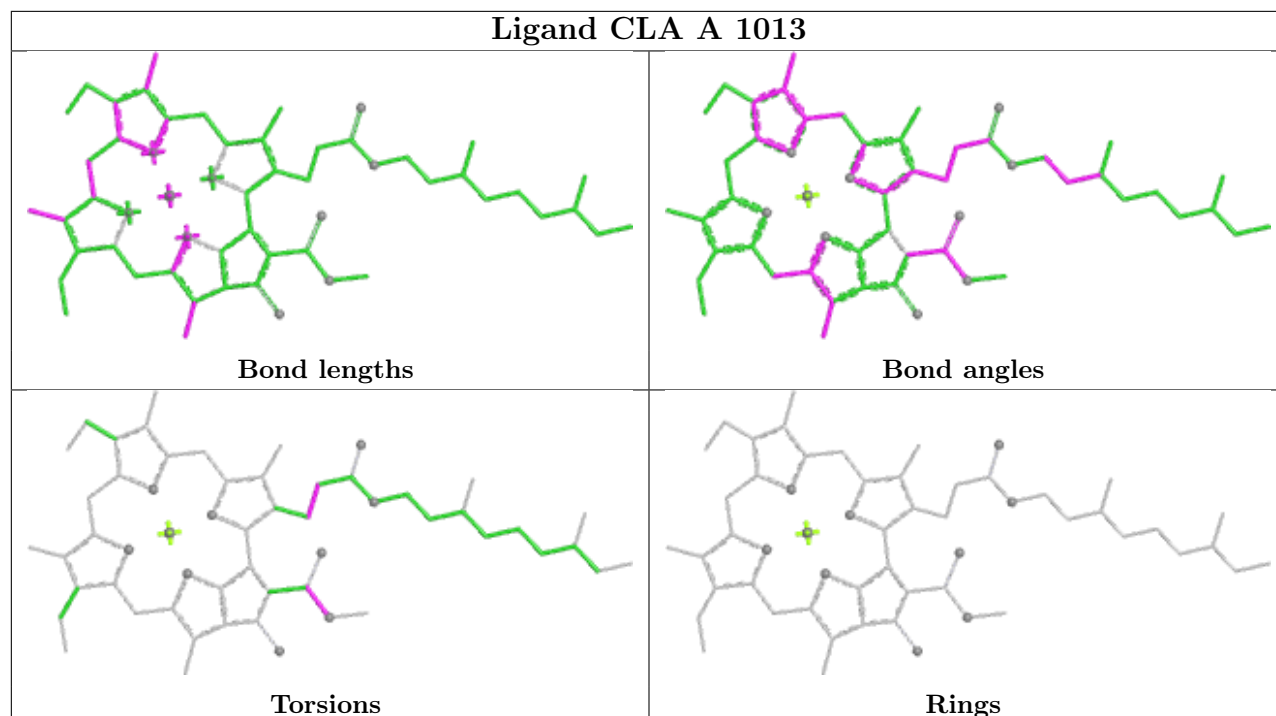




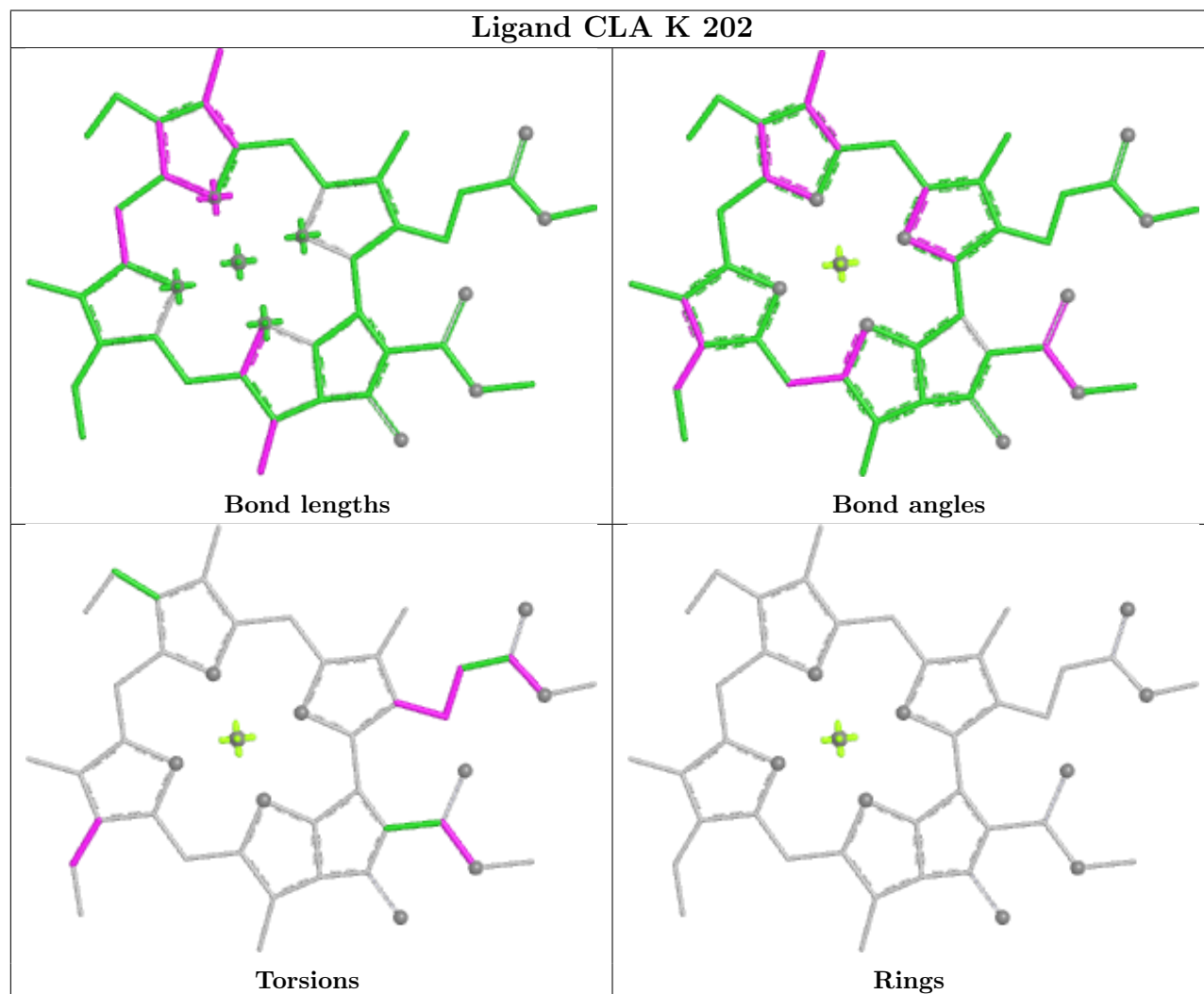
Ligand CLA B 1239

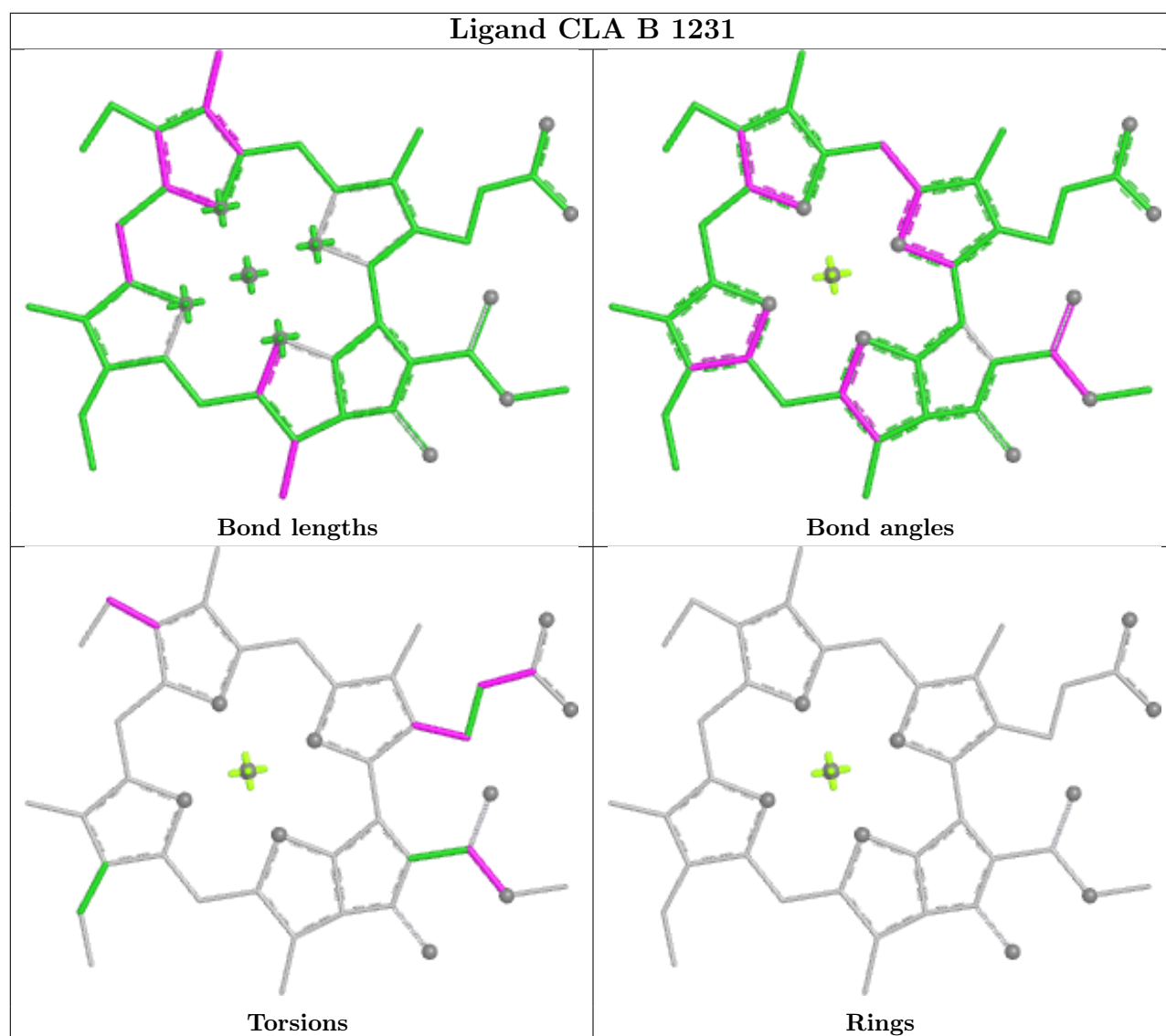


Ligand CLA A 1013

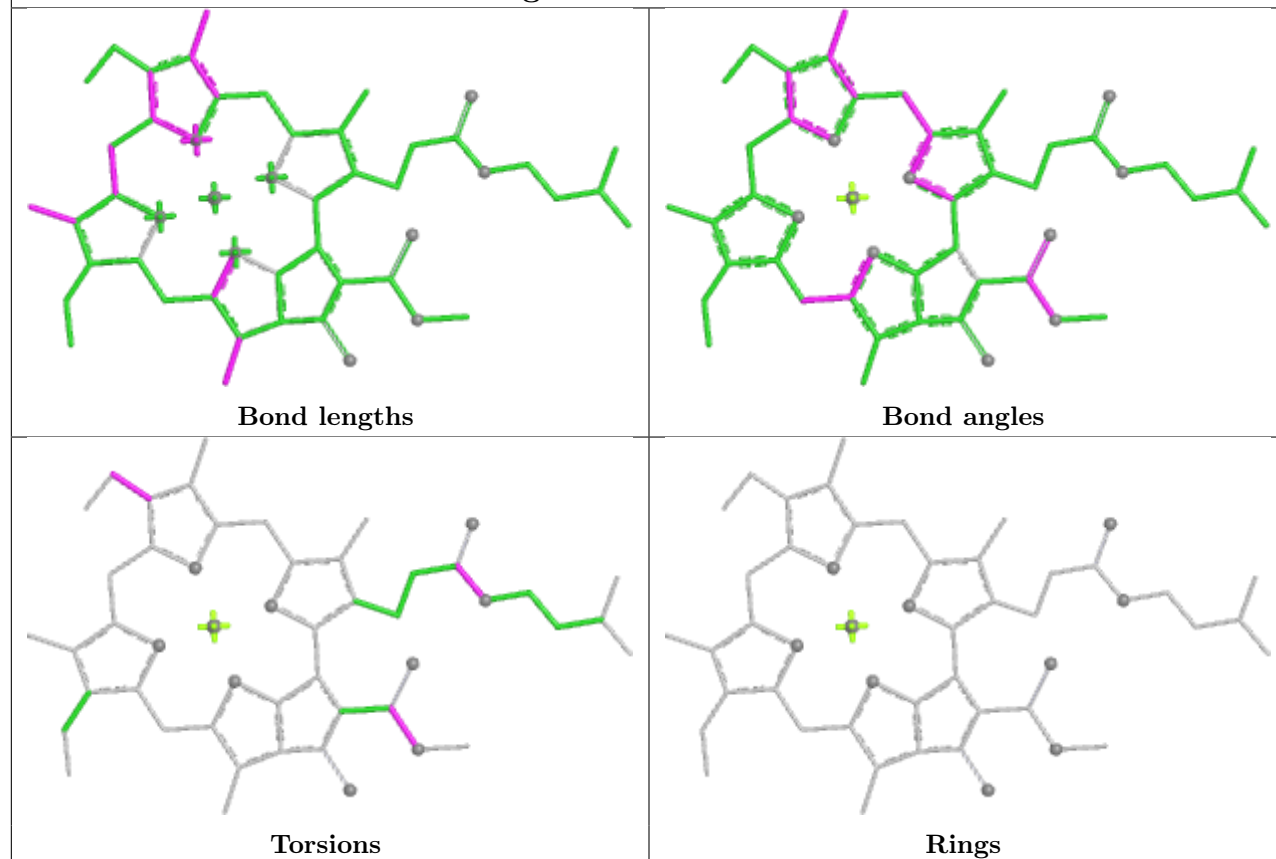


Ligand CLA K 202

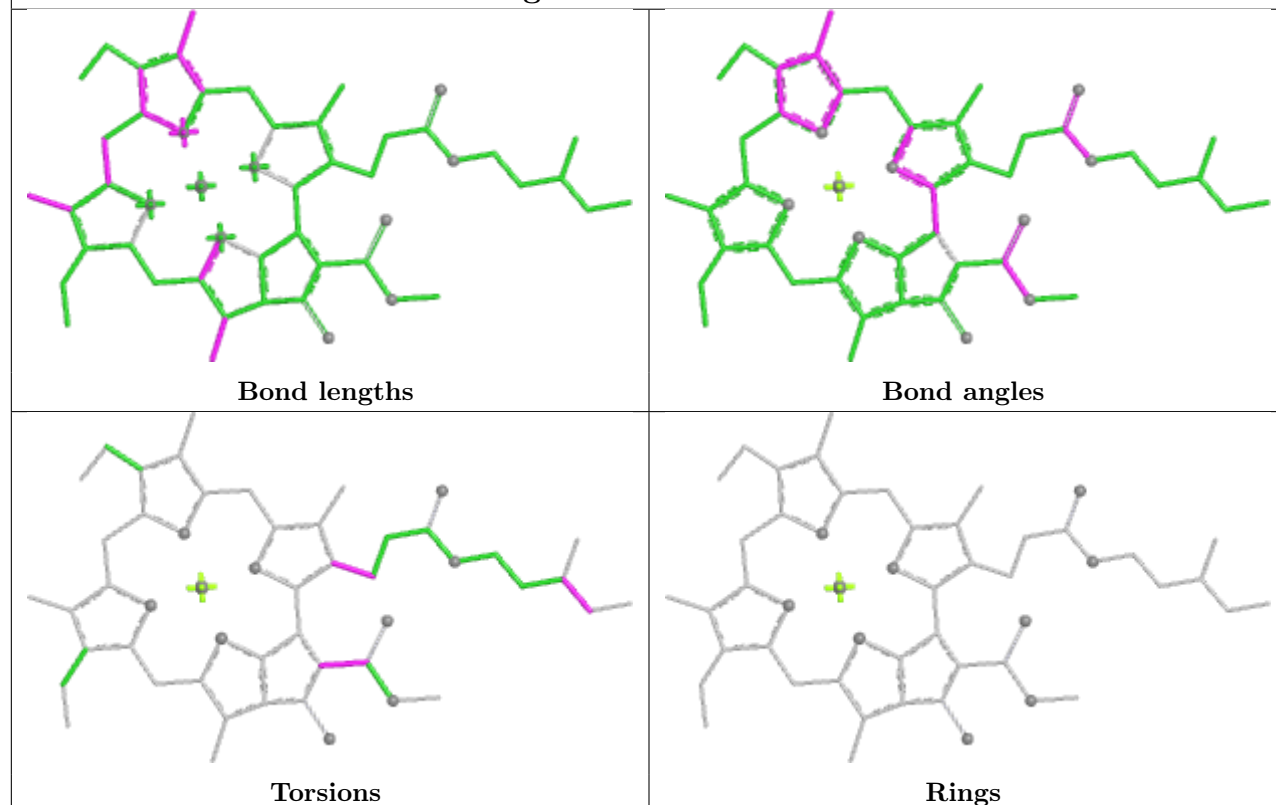


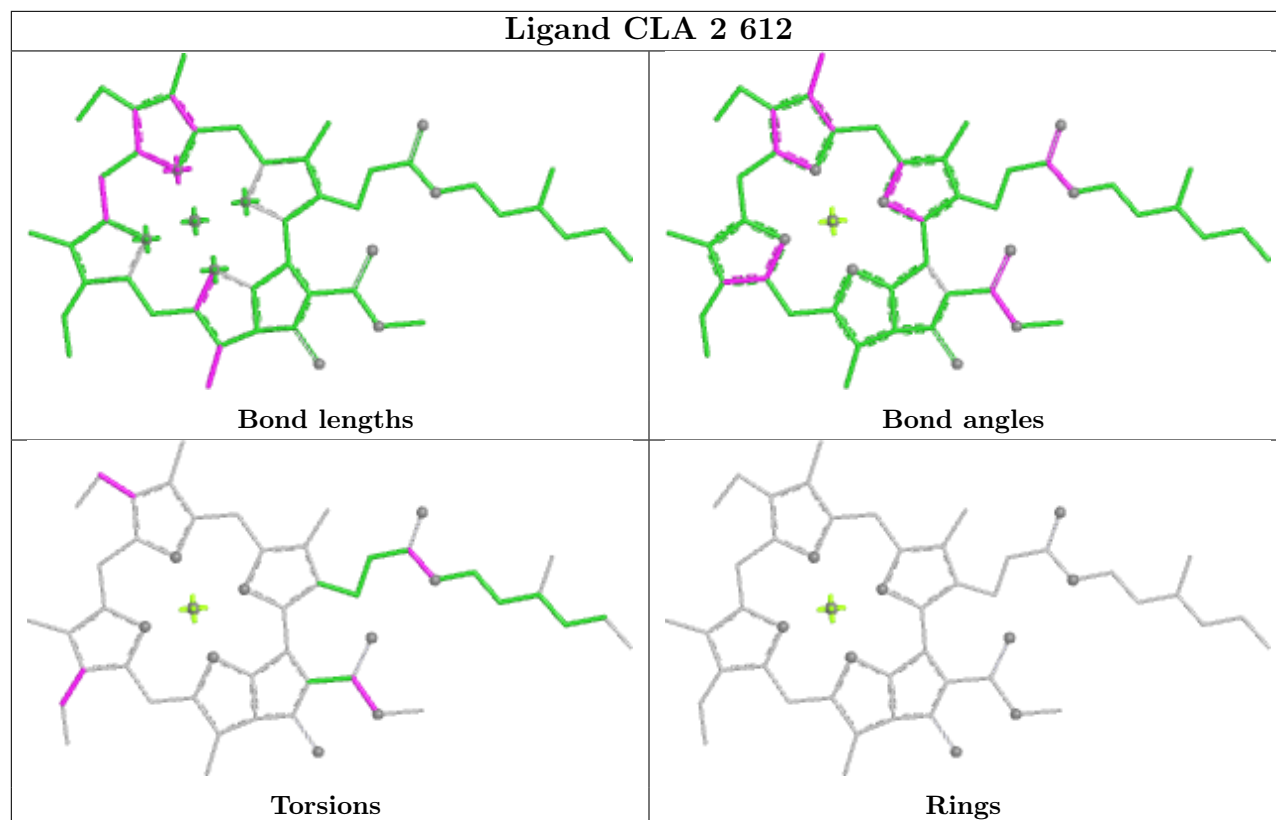


Ligand CLA A 1139

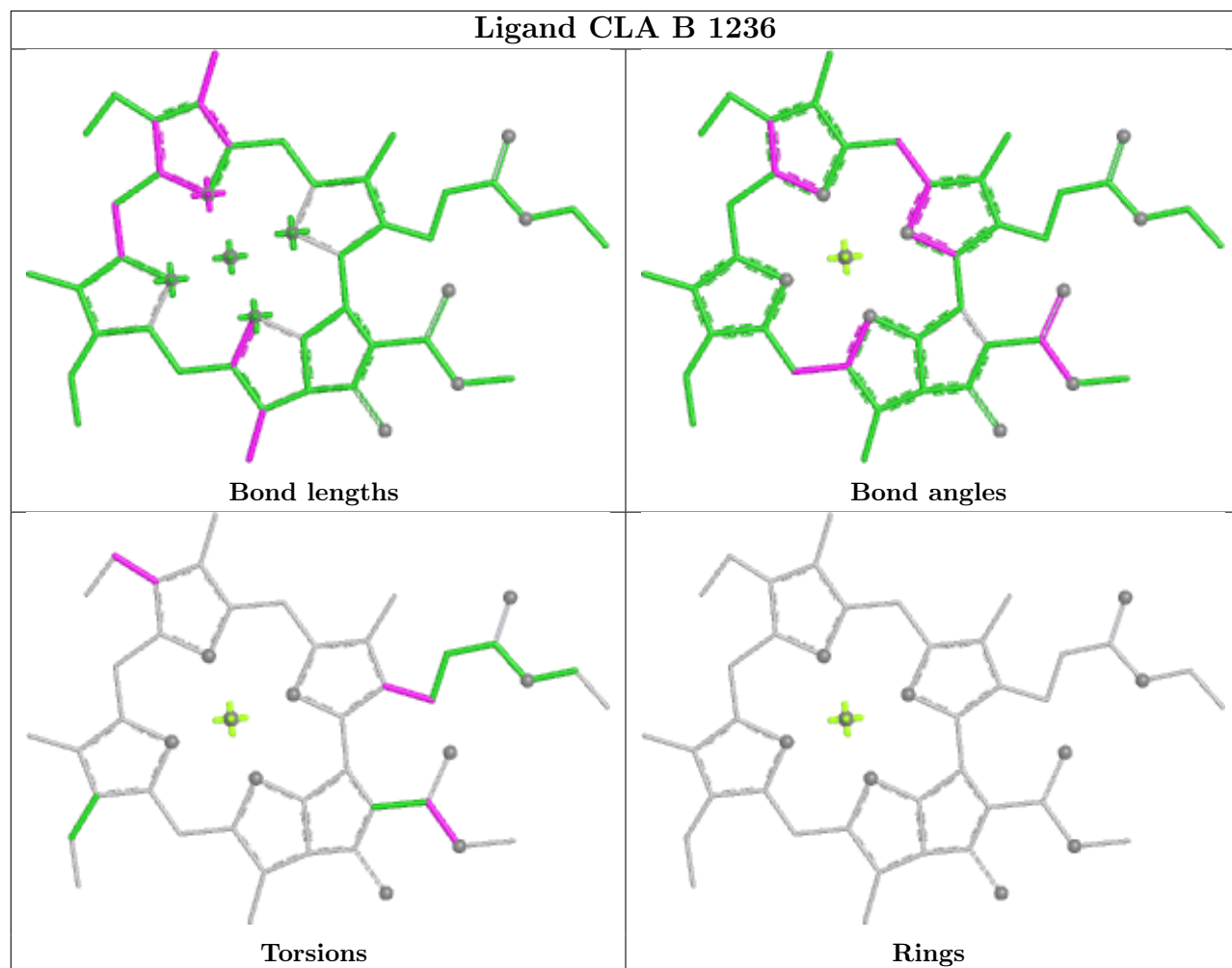


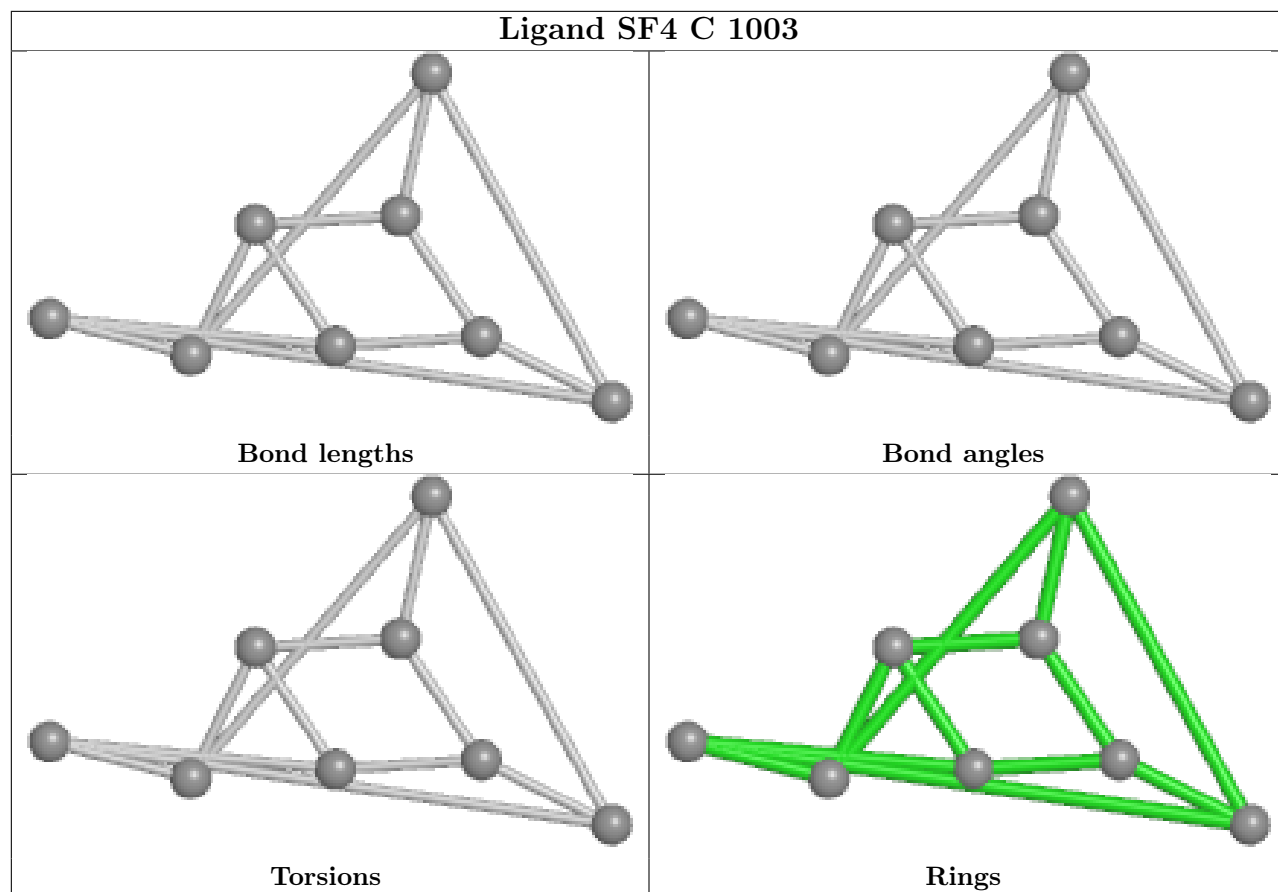
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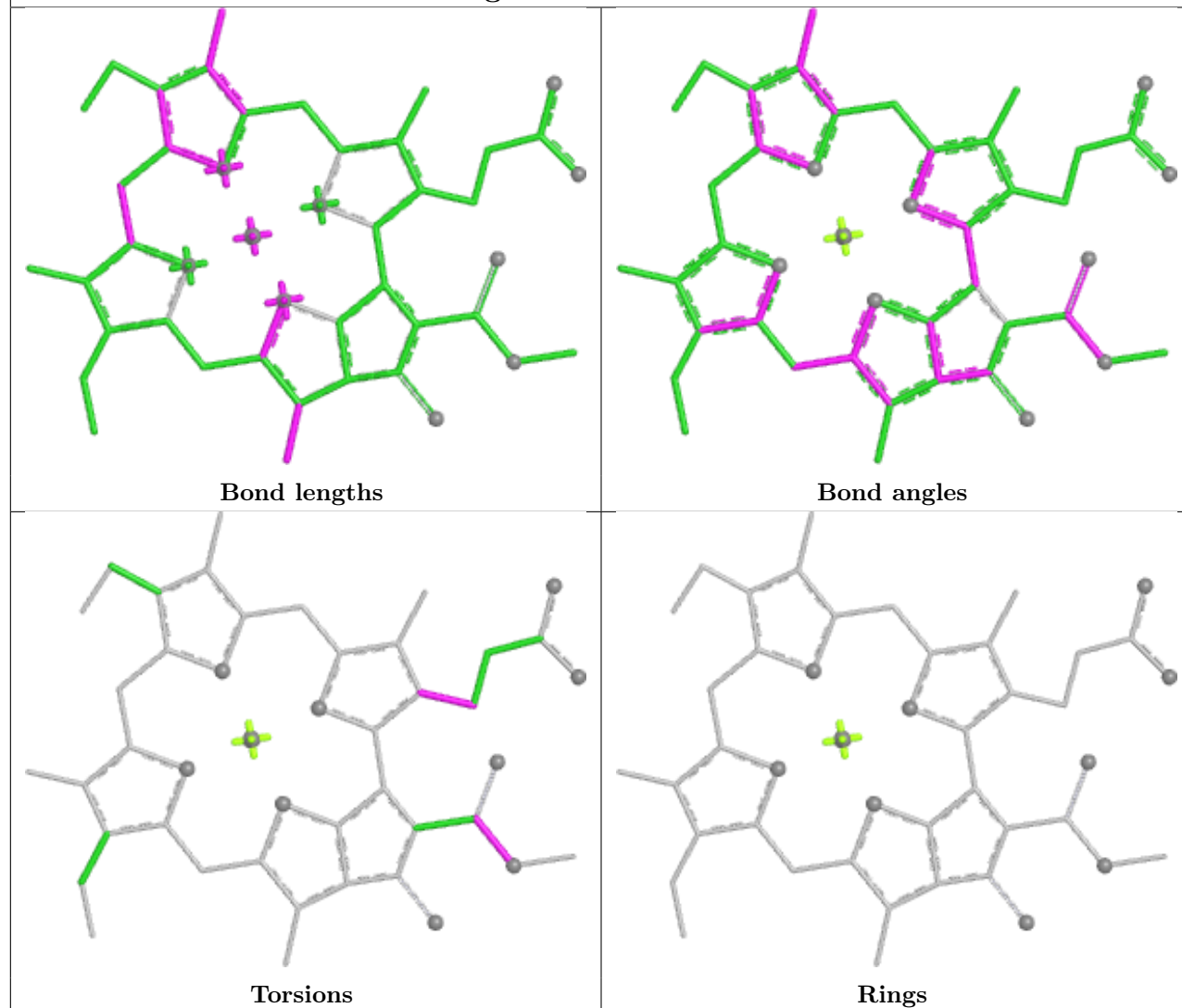


Ligand CLA B 1236

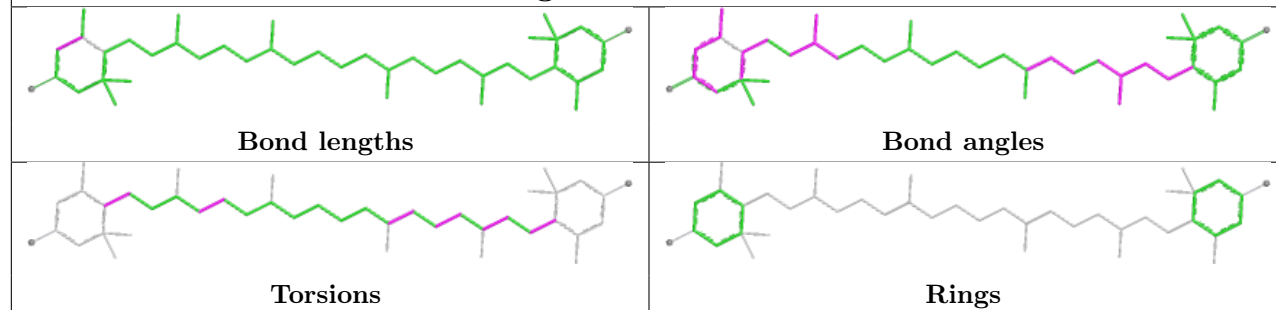


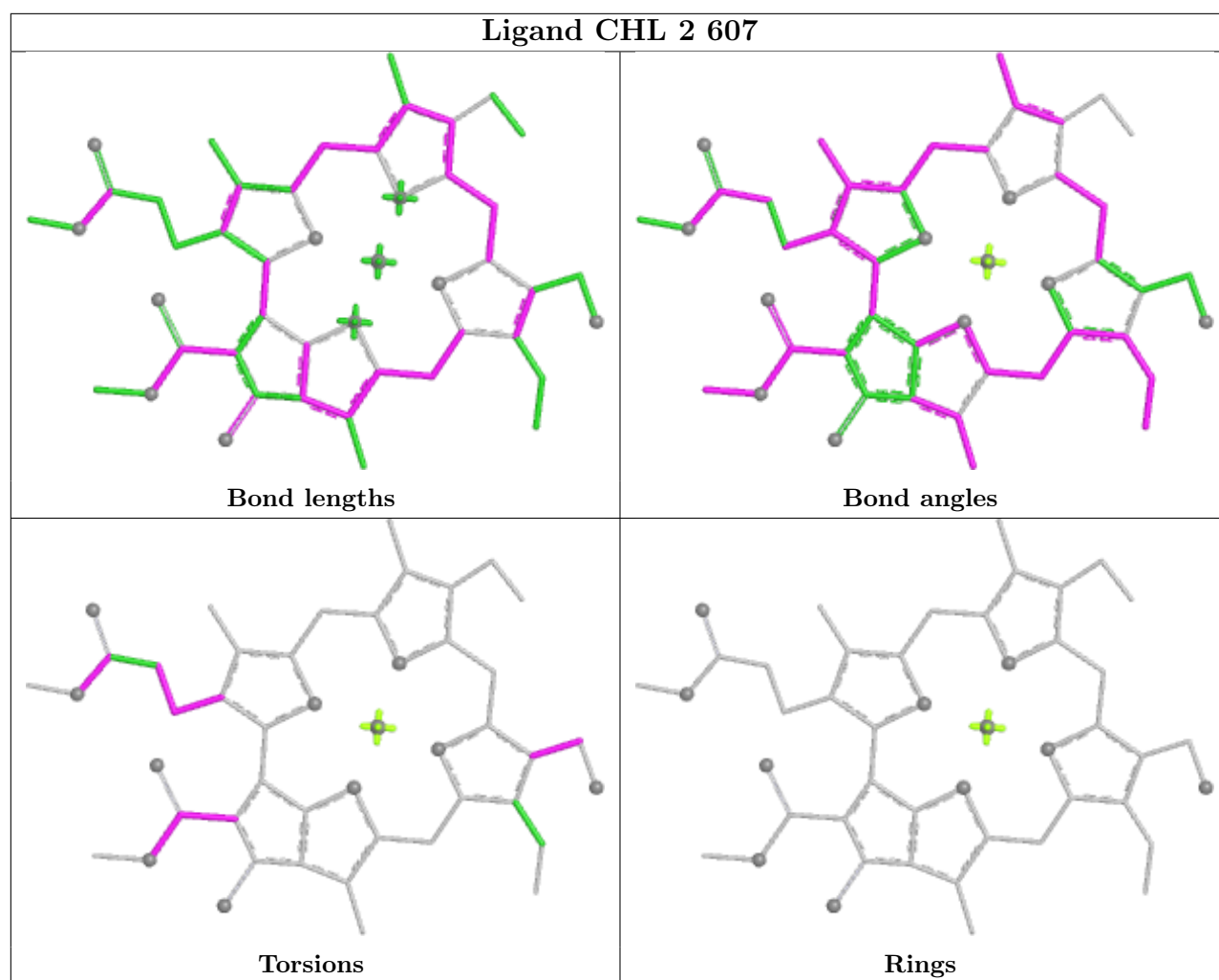


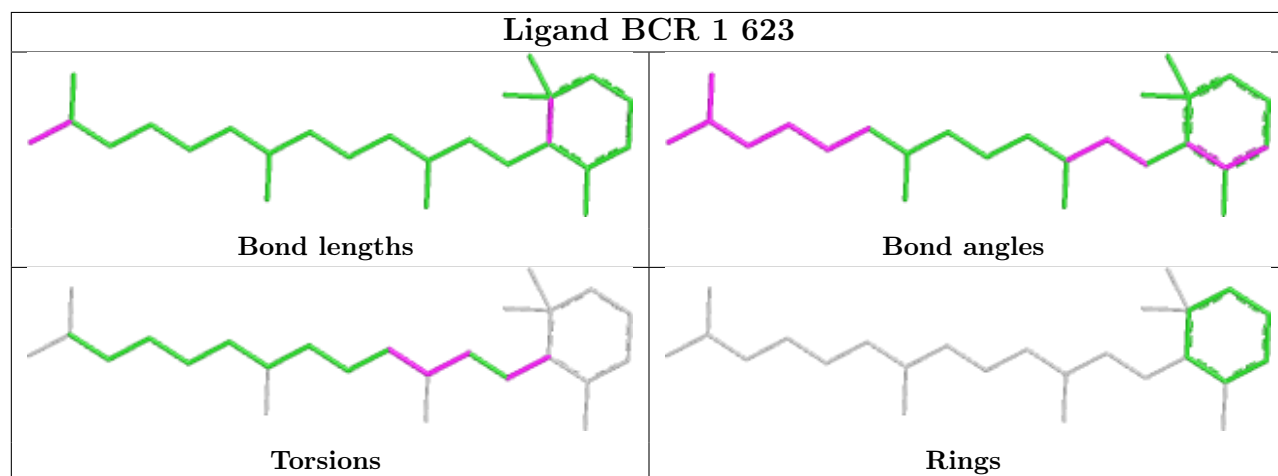
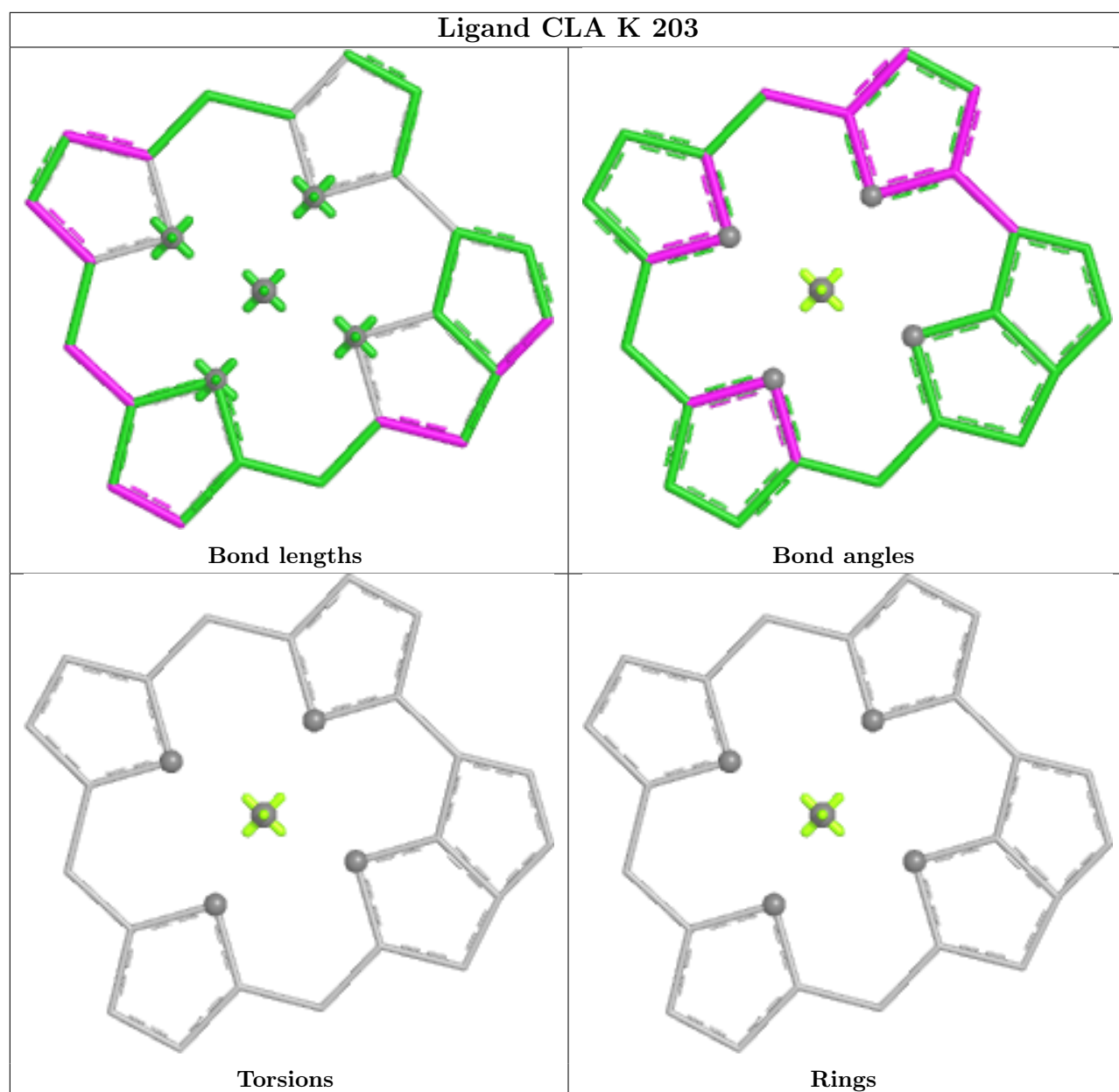
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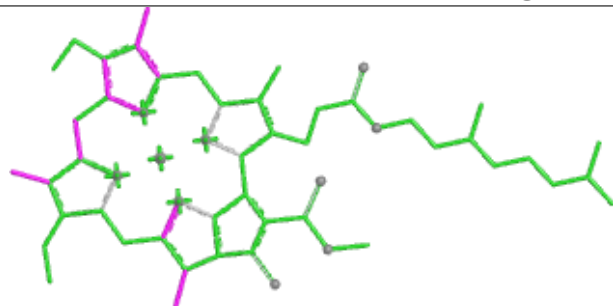


Ligand LUT 2 623

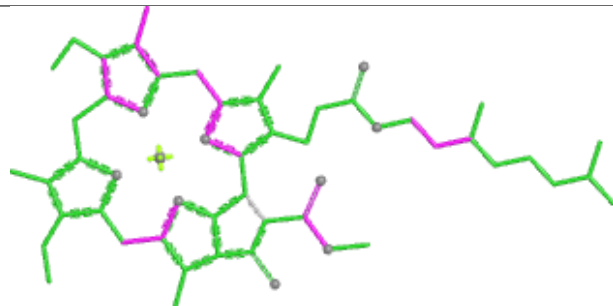




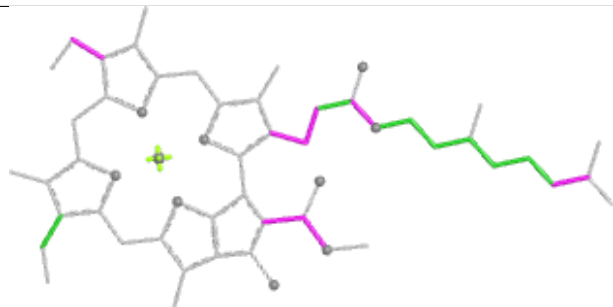


Ligand CLA 4 603

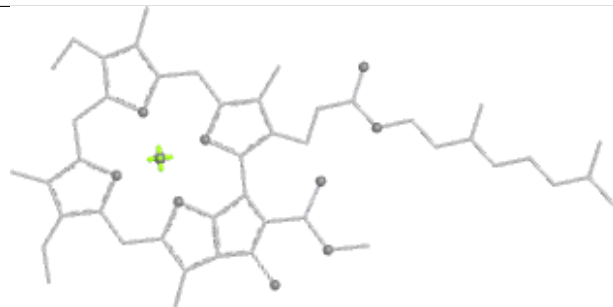
Bond lengths



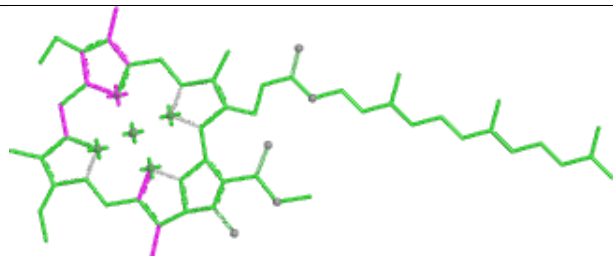
Bond angles



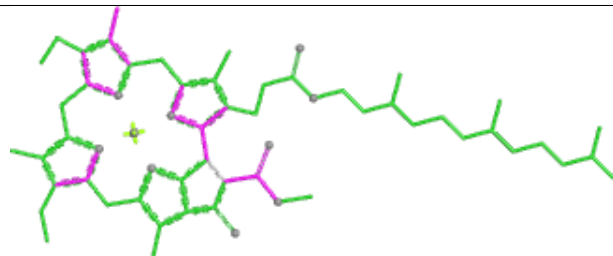
Torsions



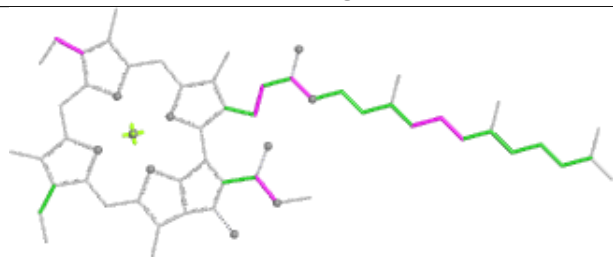
Rings

Ligand CLA A 1138

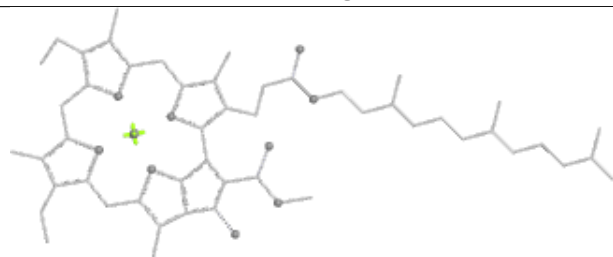
Bond lengths



Bond angles

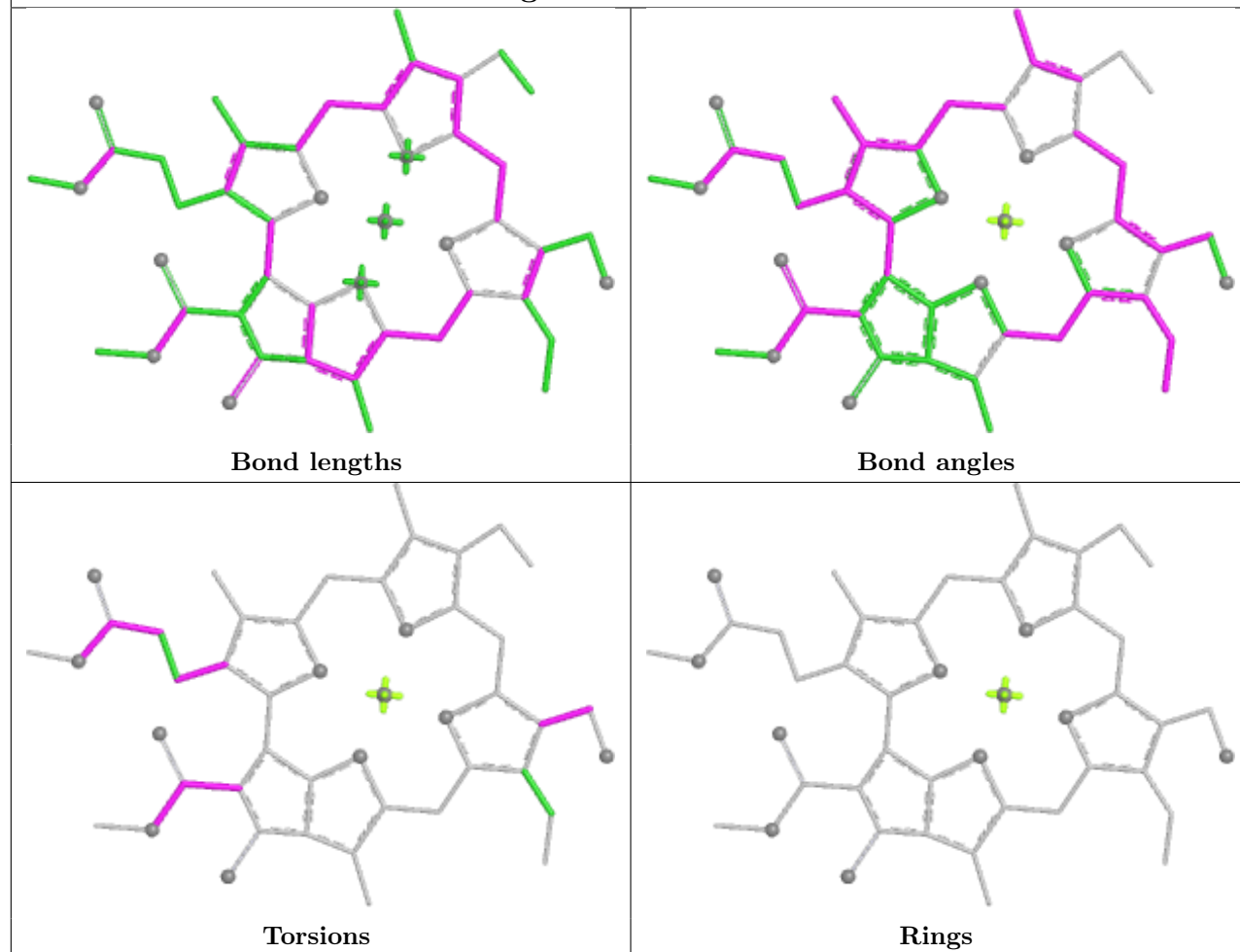


Torsions

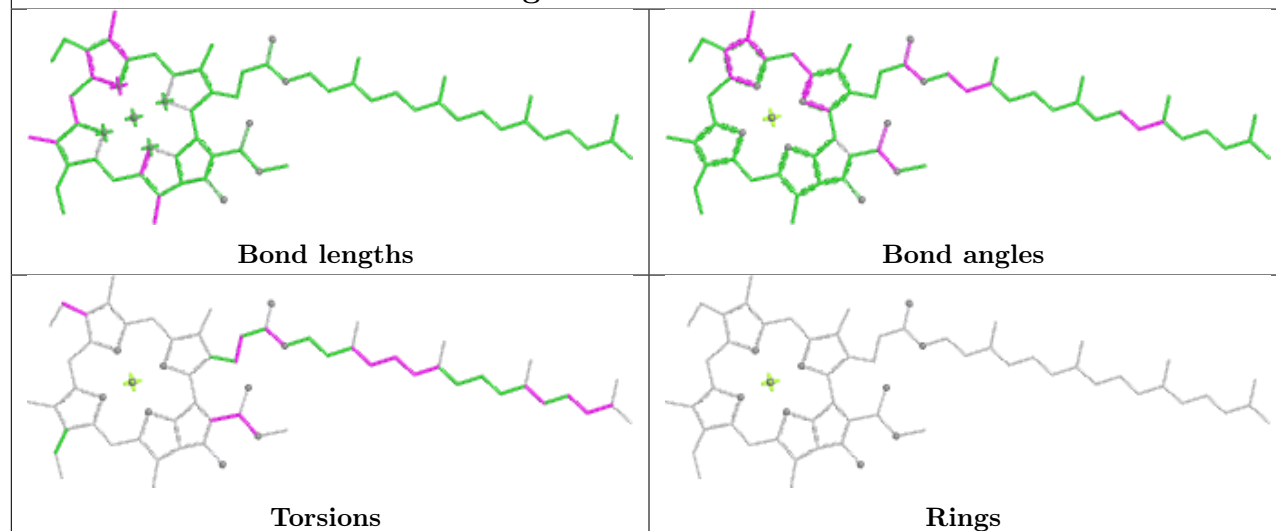


Rings

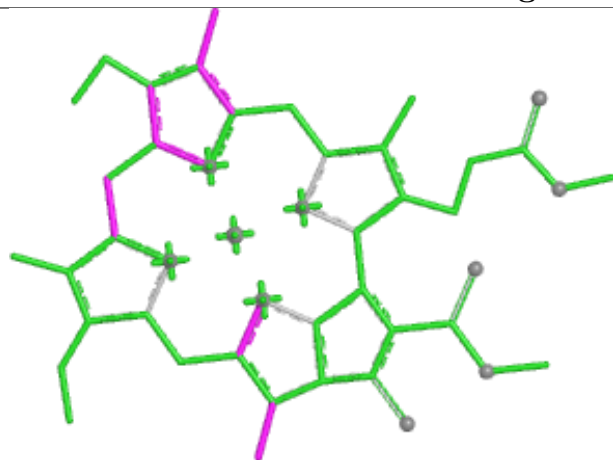
Ligand CHL 4 606



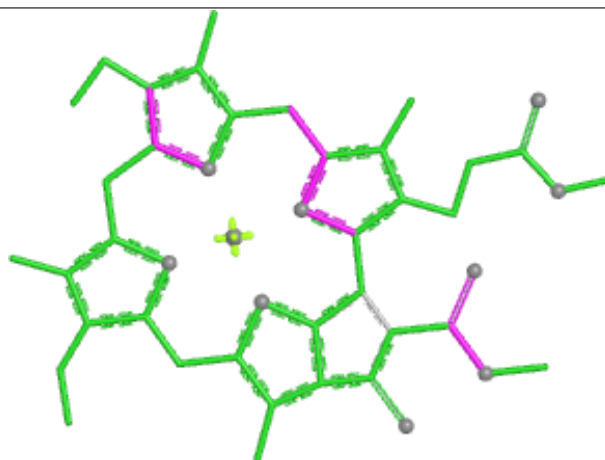
Ligand CLA A 1104



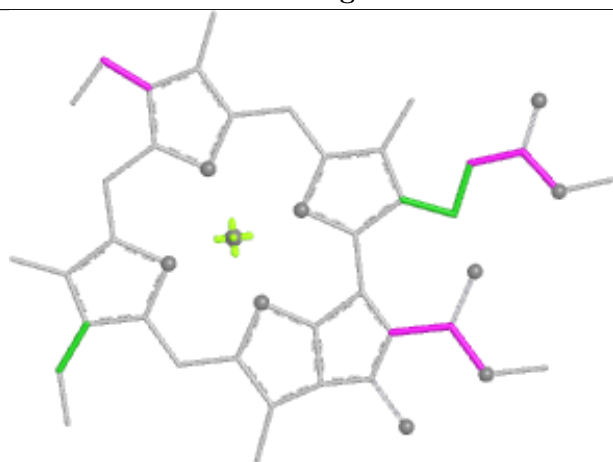
Ligand CLA 4 612



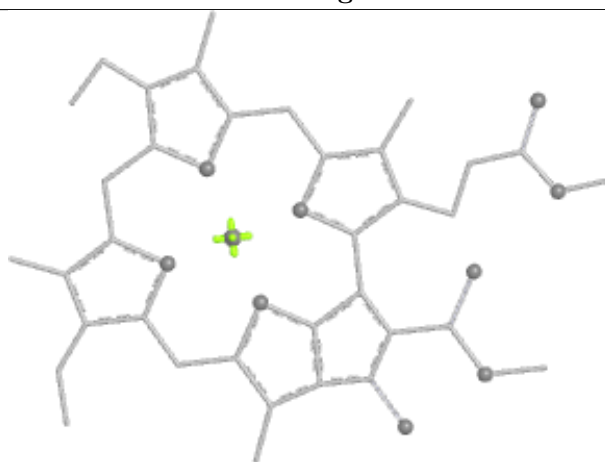
Bond lengths



Bond angles

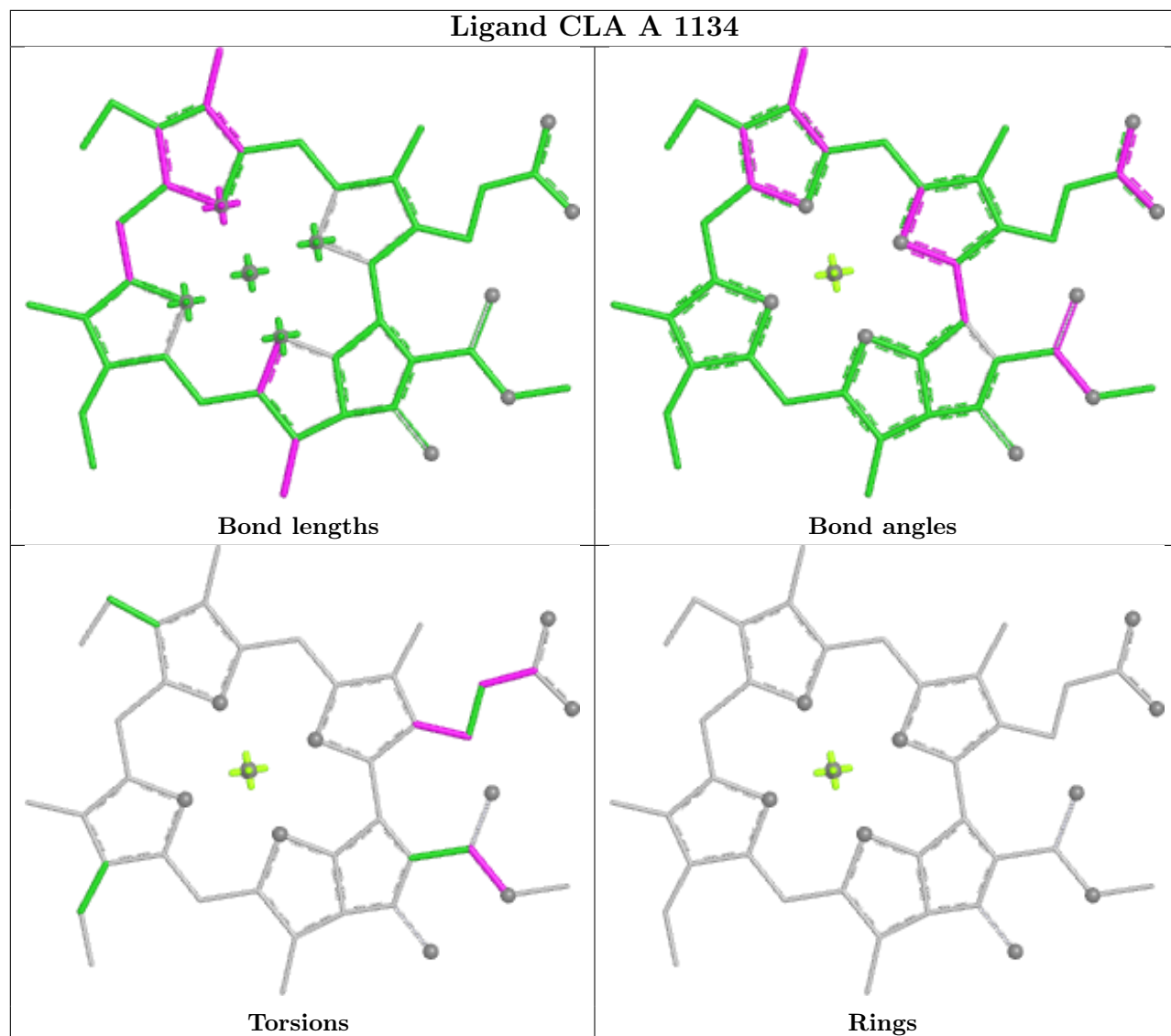


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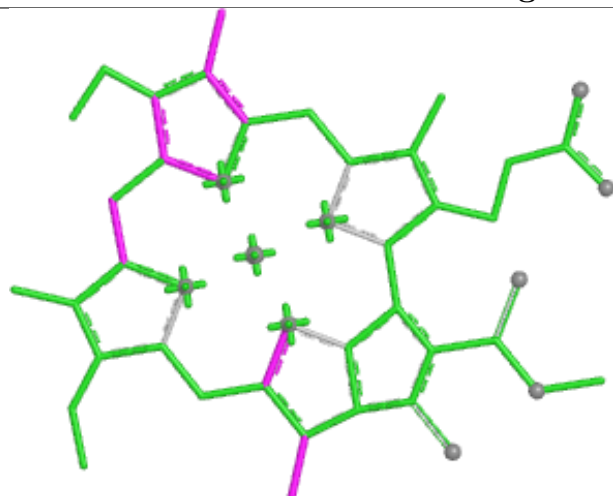


Rings

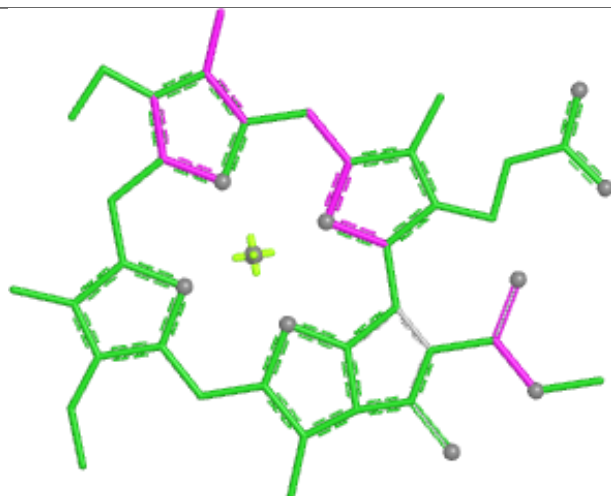
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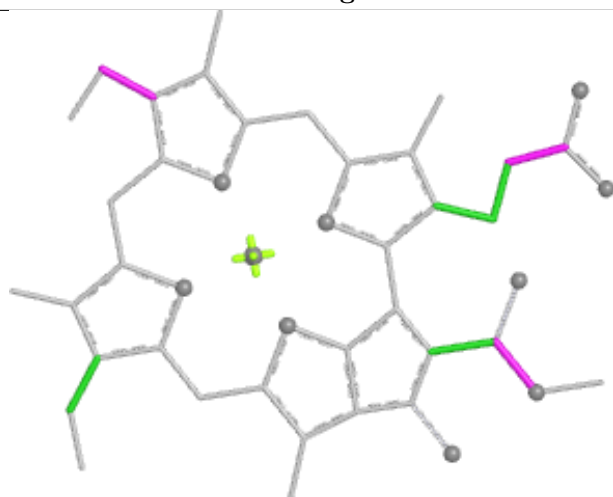
Ligand CLA 3 612



Bond lengths



Bond angles

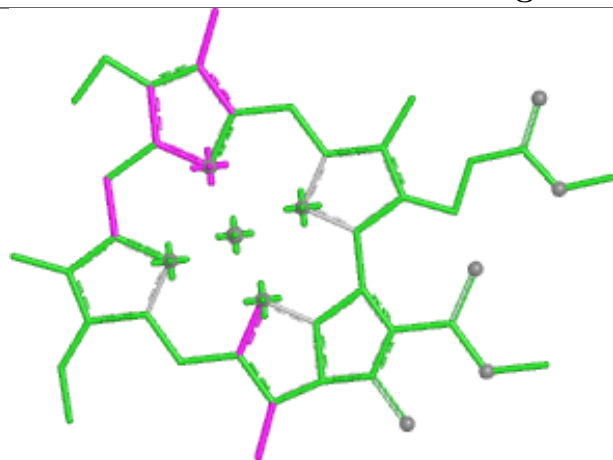


Torsions

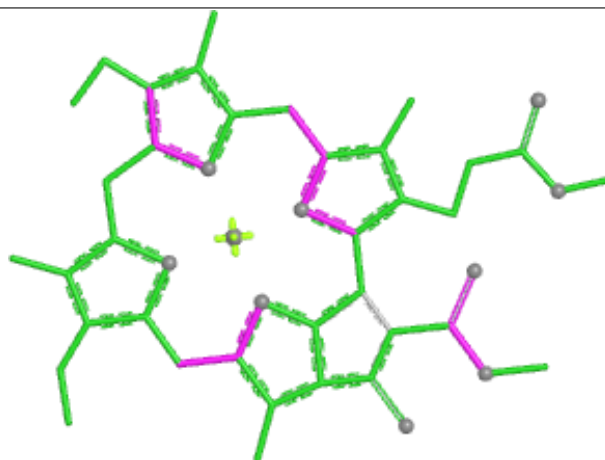


Rings

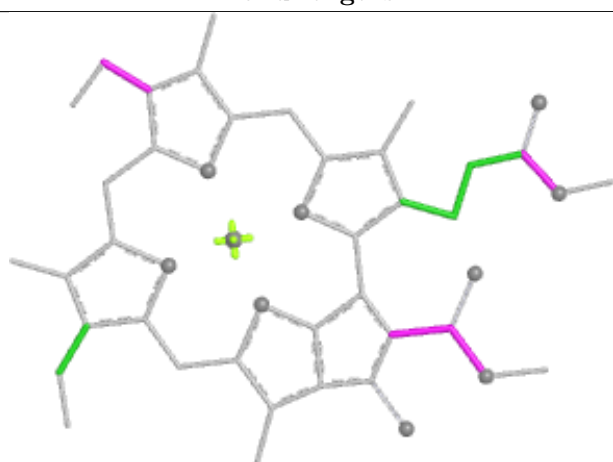
Ligand CLA F 302



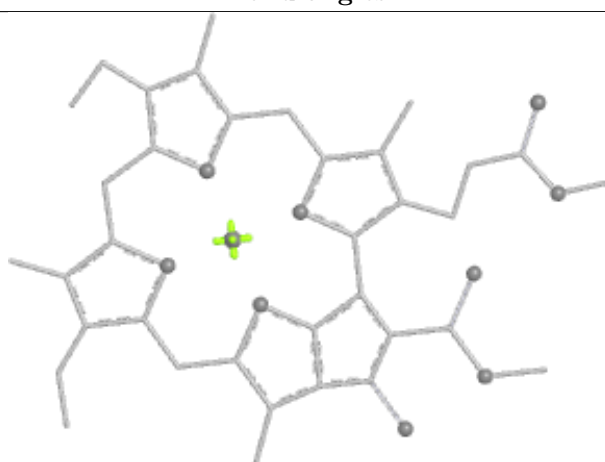
Bond lengths



Bond angles

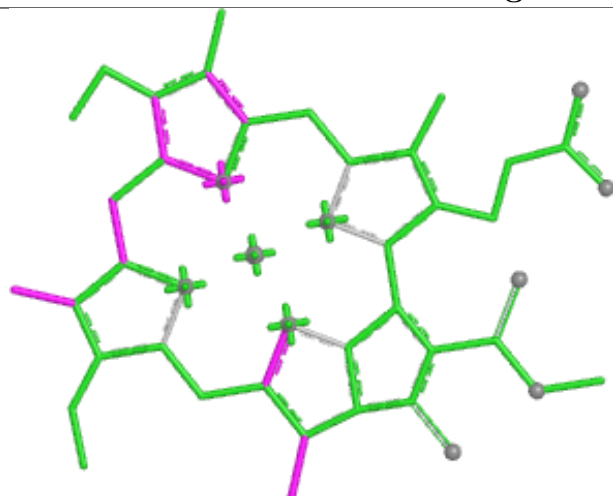


Torsions

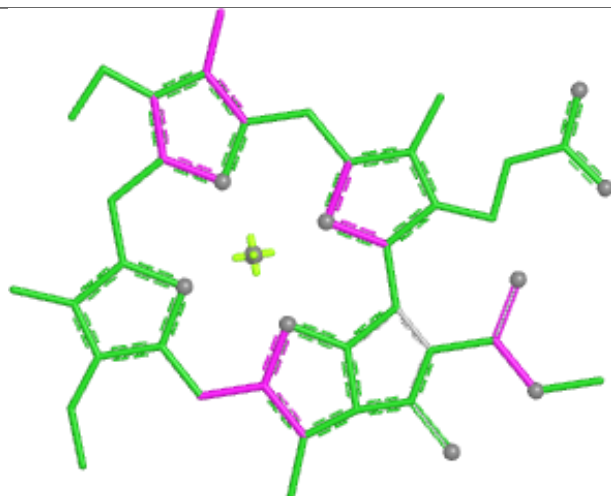


Rings

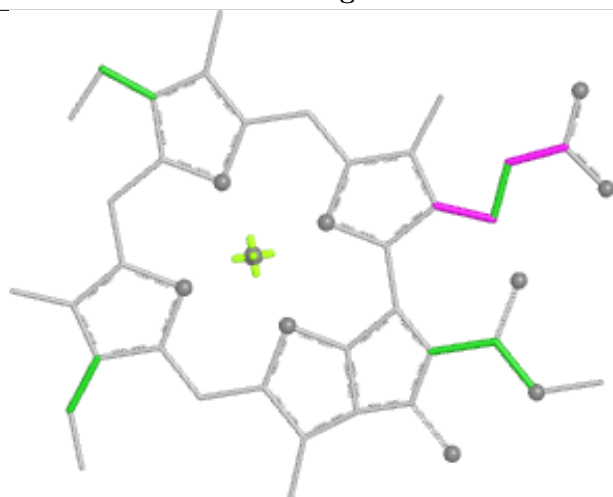
Ligand CLA B 1220



Bond lengths



Bond angles

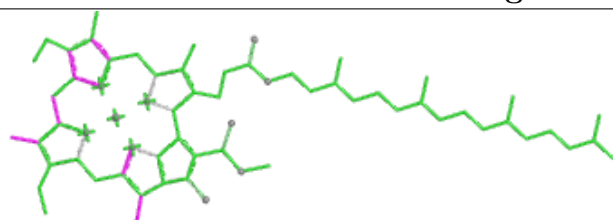


Torsions

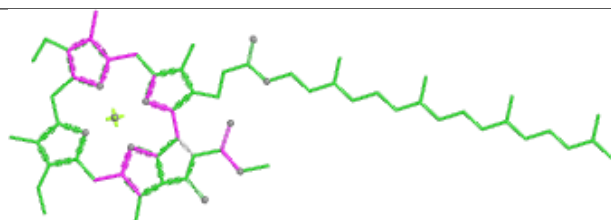


Rings

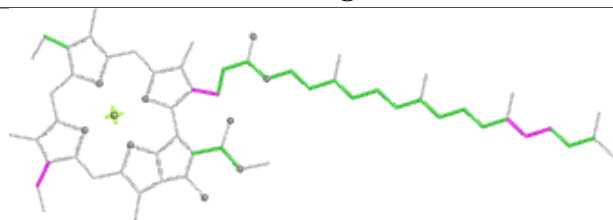
Ligand CLA B 1223



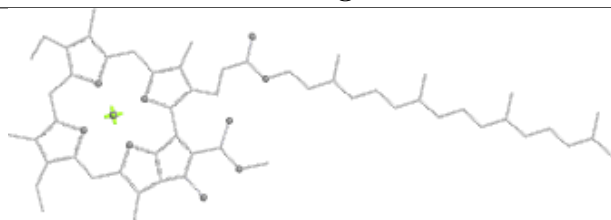
Bond lengths



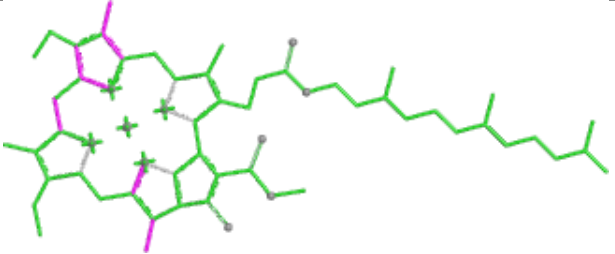
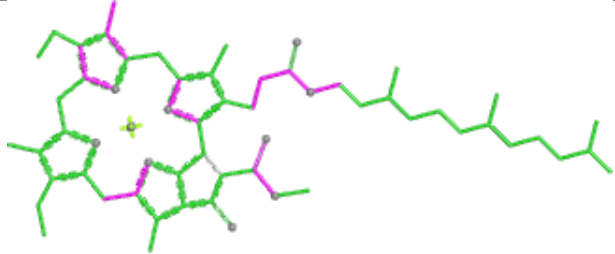
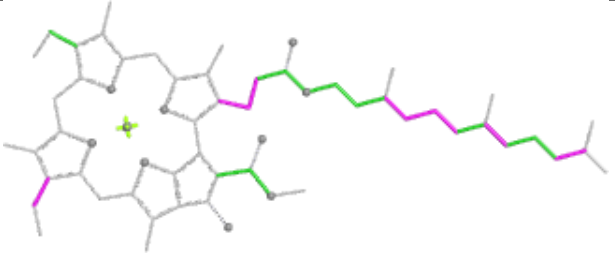
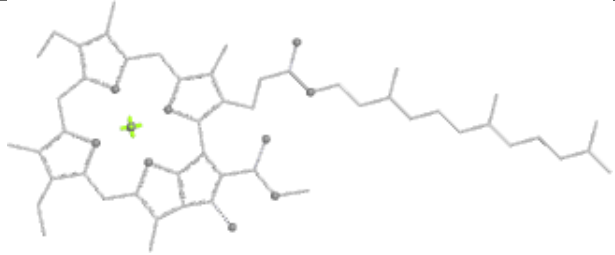
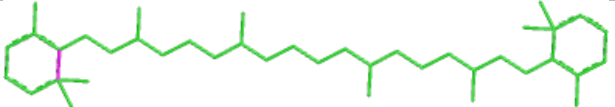
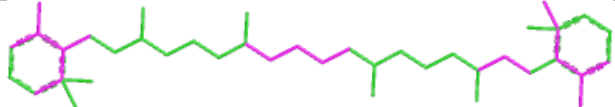
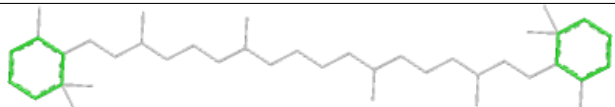
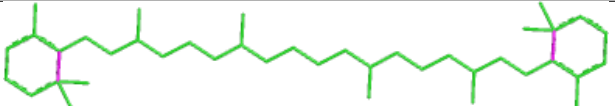
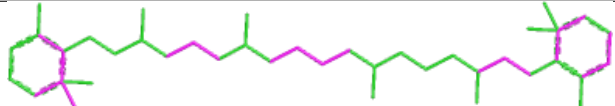
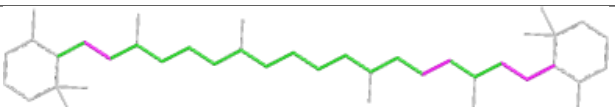
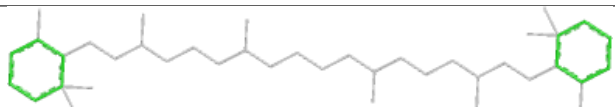
Bond angles

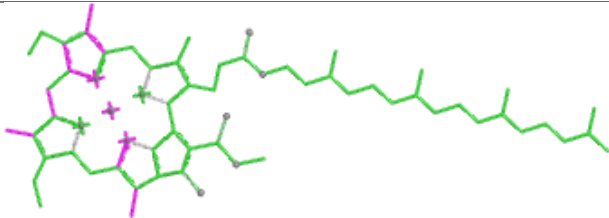
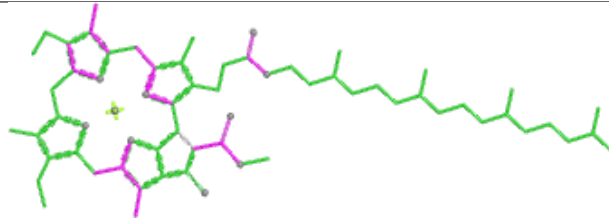
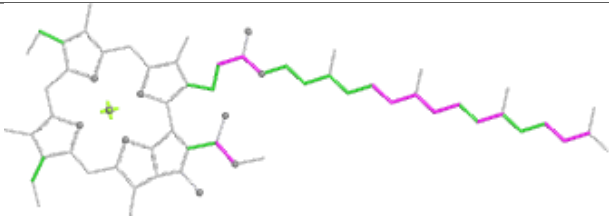
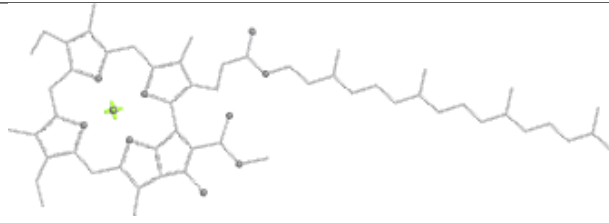


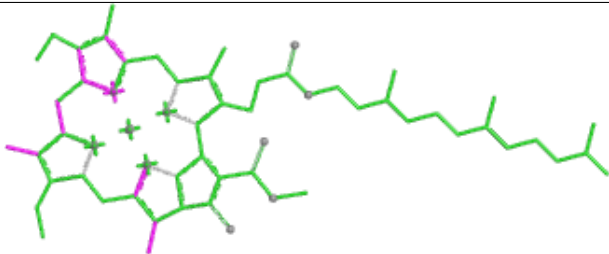
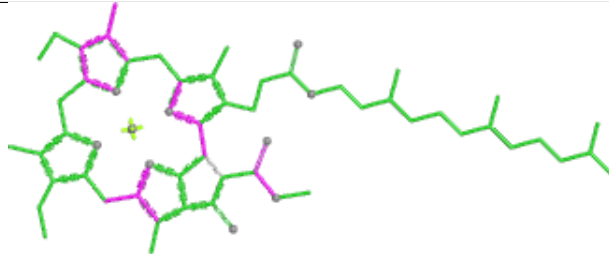
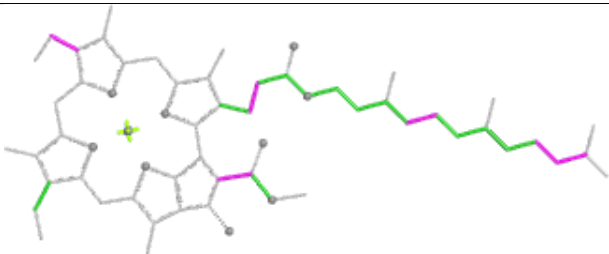
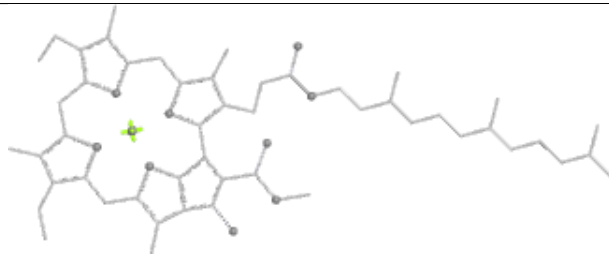
Torsions

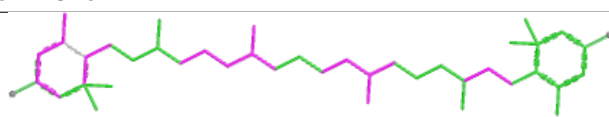
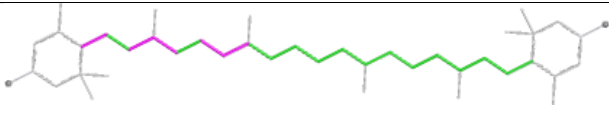
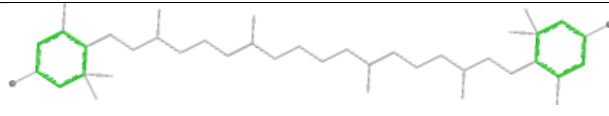


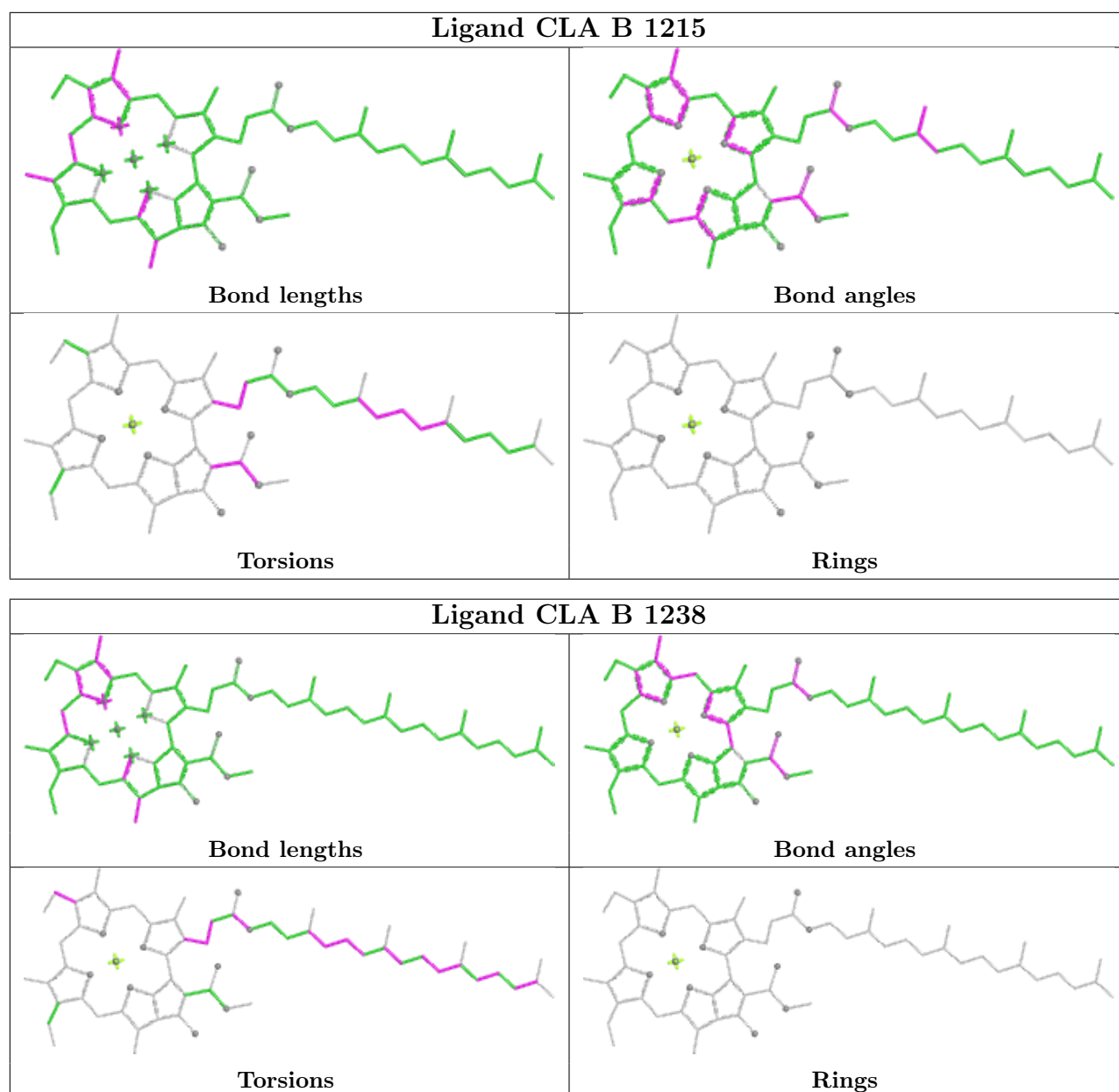
Rings

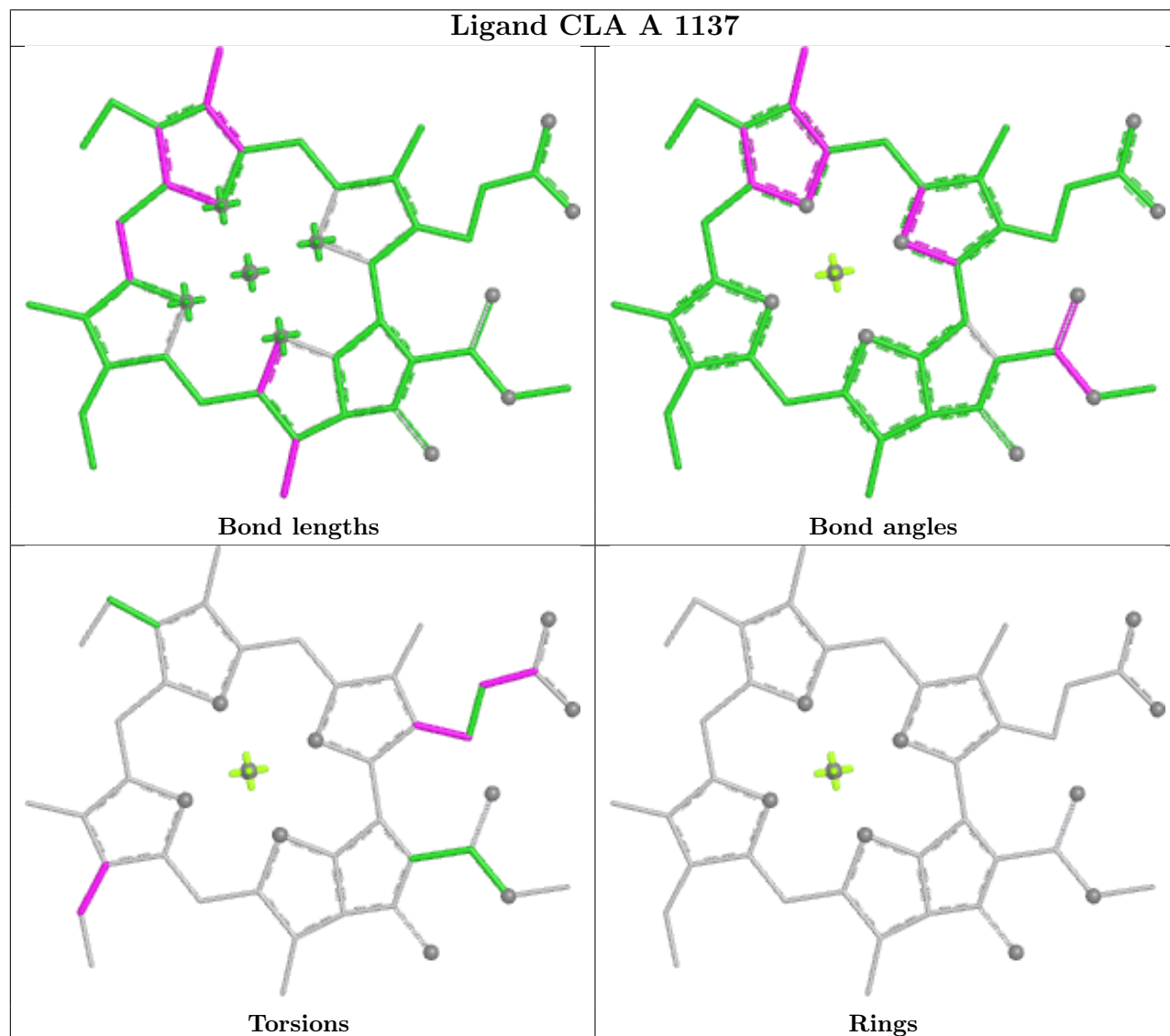
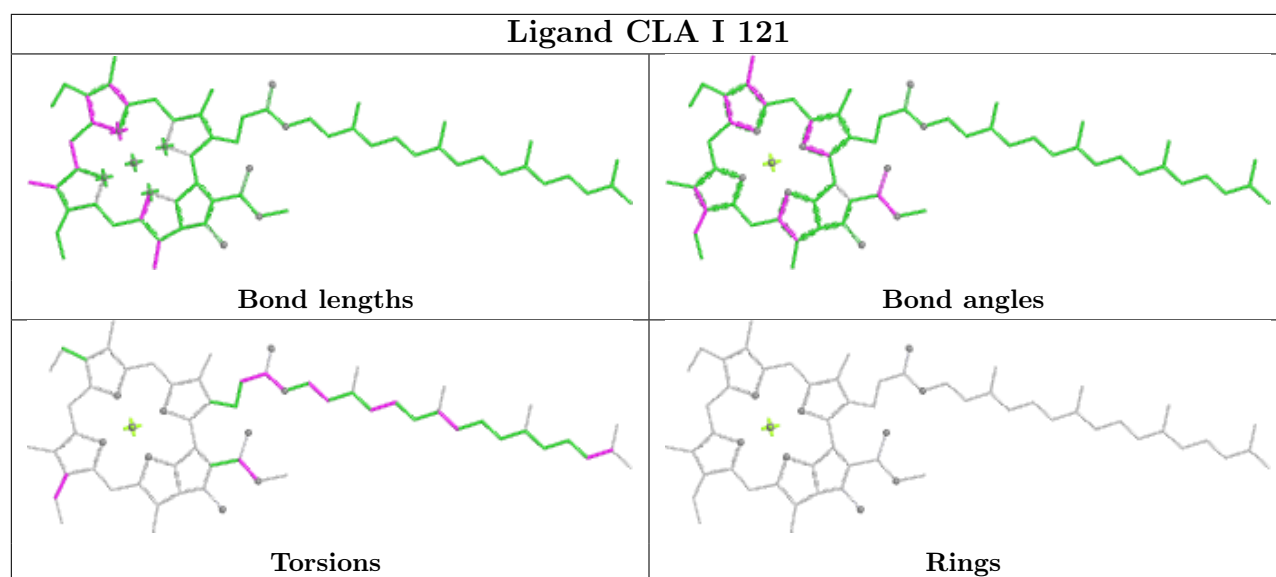
Ligand CLA L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 420	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR M 4021	
 Bond lengths	 Bond angles
 Torsions	 Rings

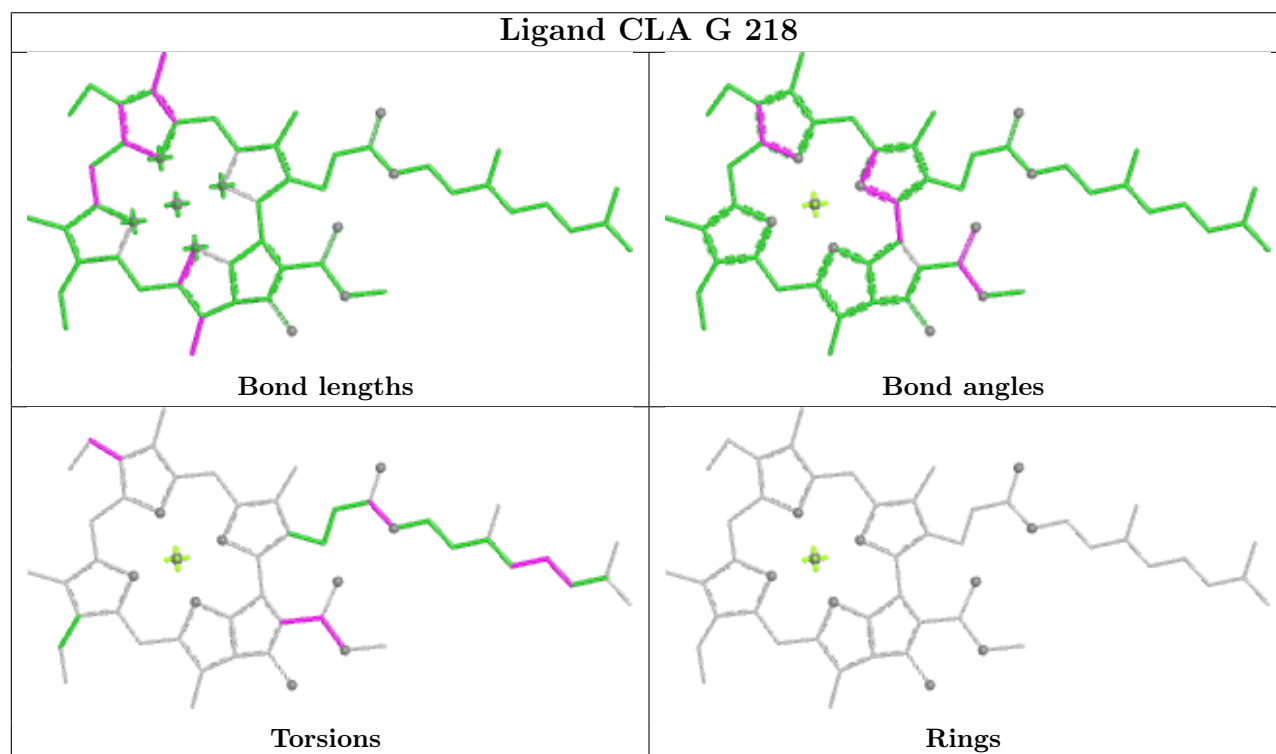
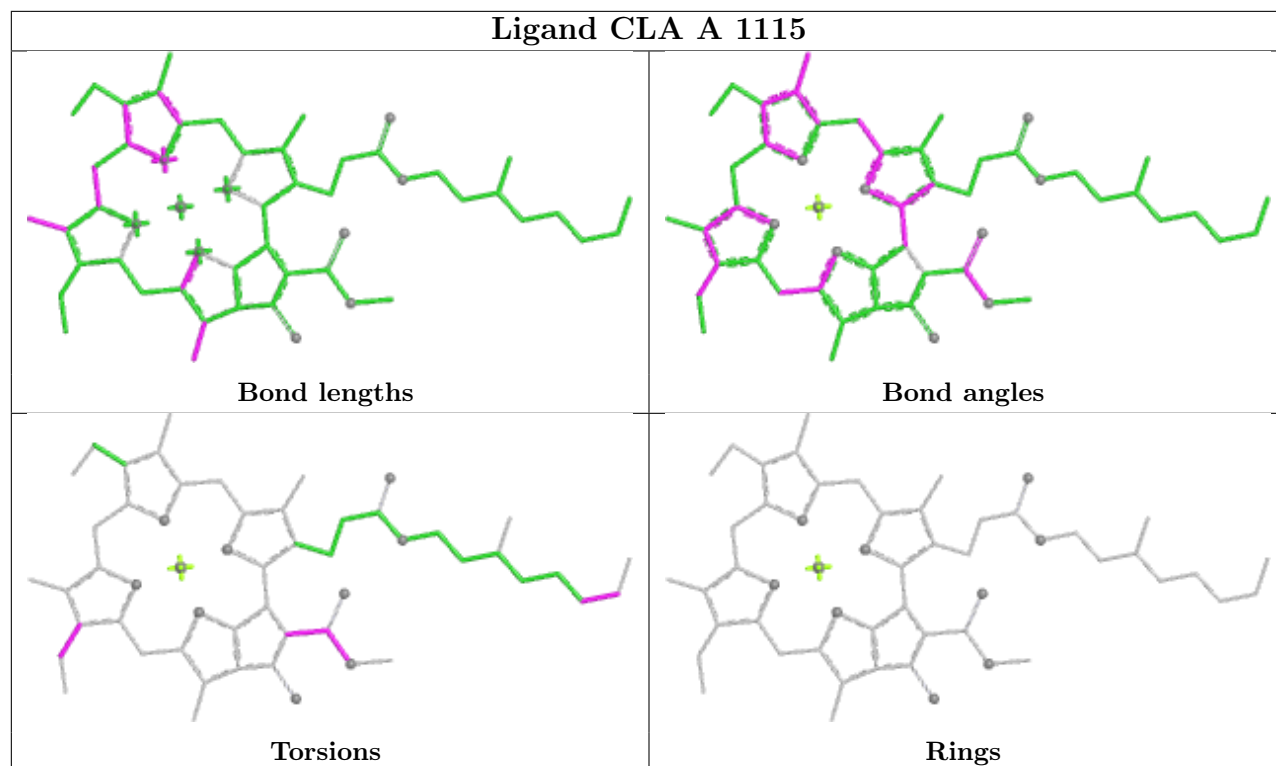
Ligand CLA B 1021	
	
Bond lengths	Bond angles
	
Torsions	Rings

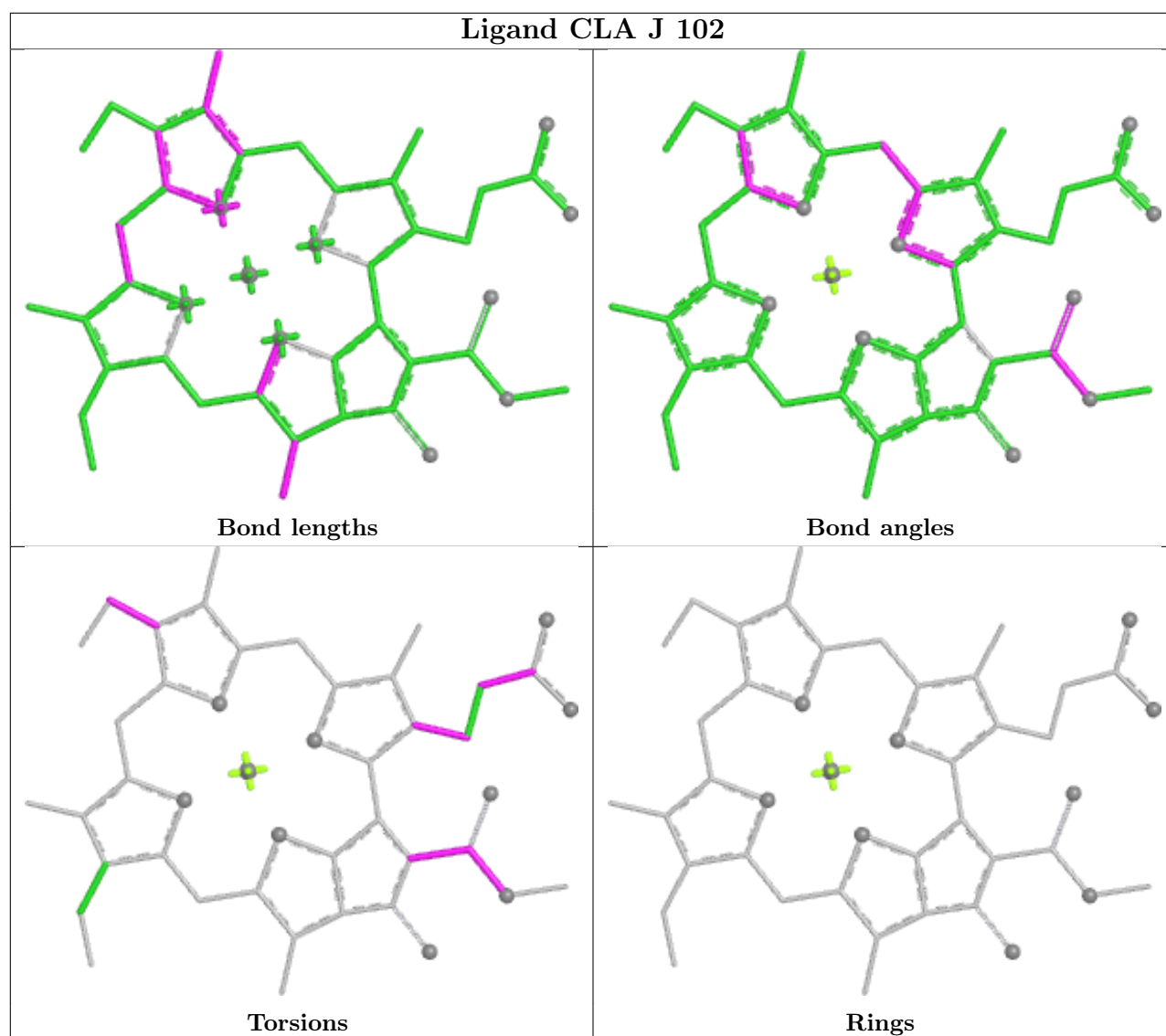
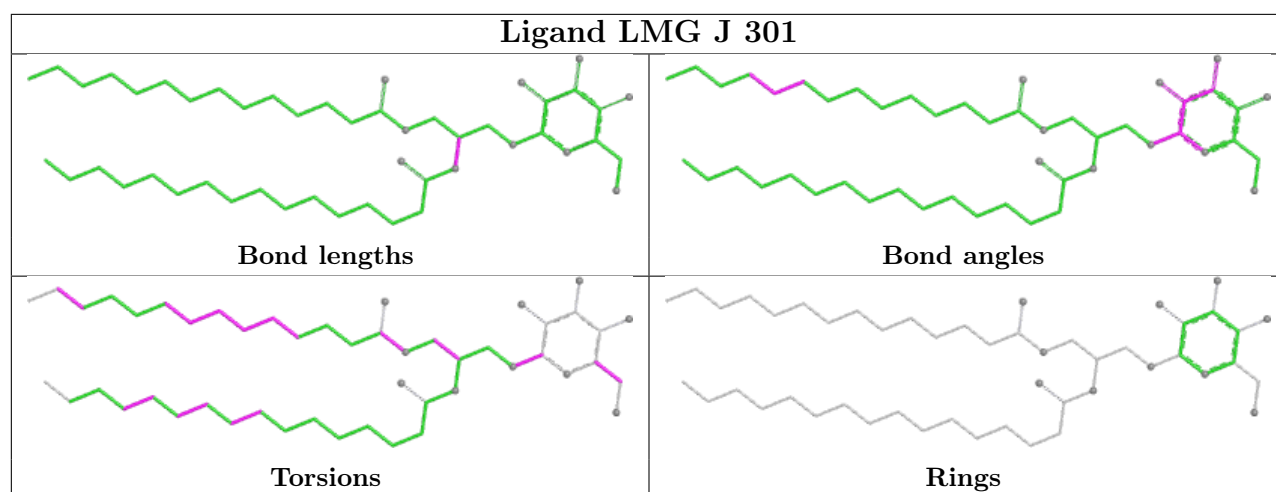
Ligand CLA 3 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

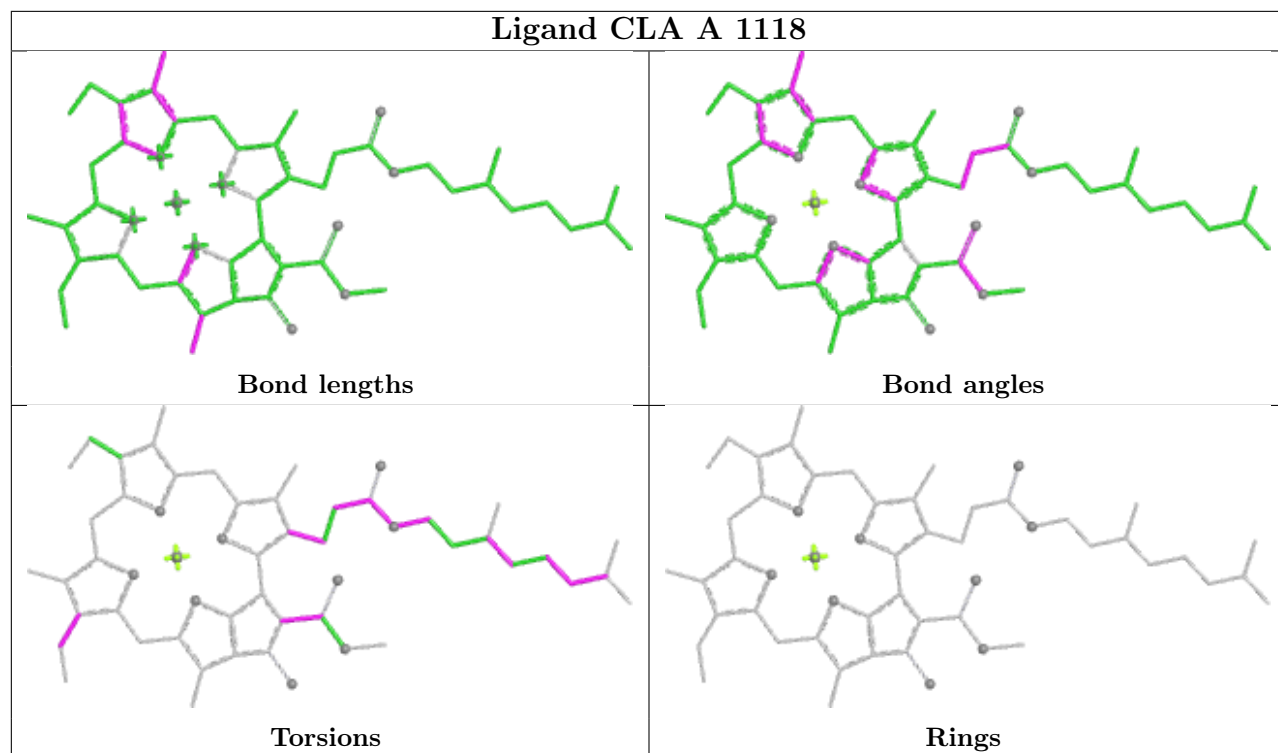
Ligand LUT 3 621	
	
Bond lengths	Bond angles
	
Torsions	Rings



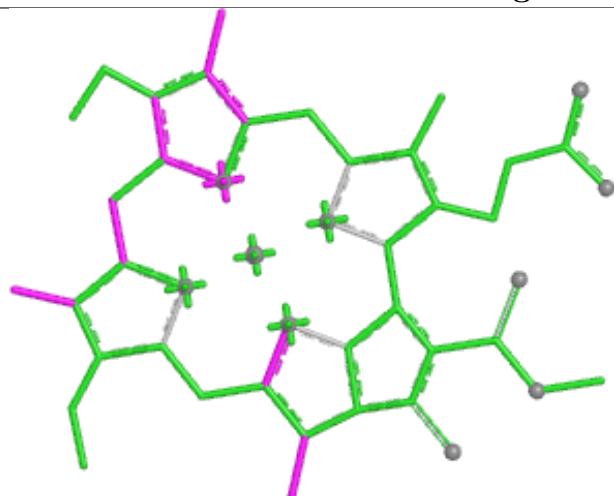




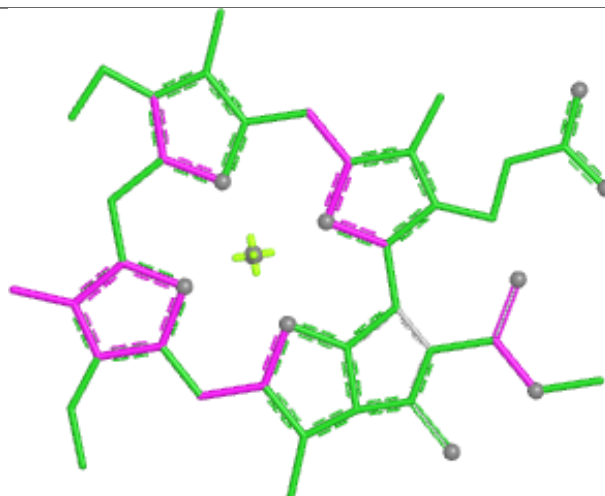




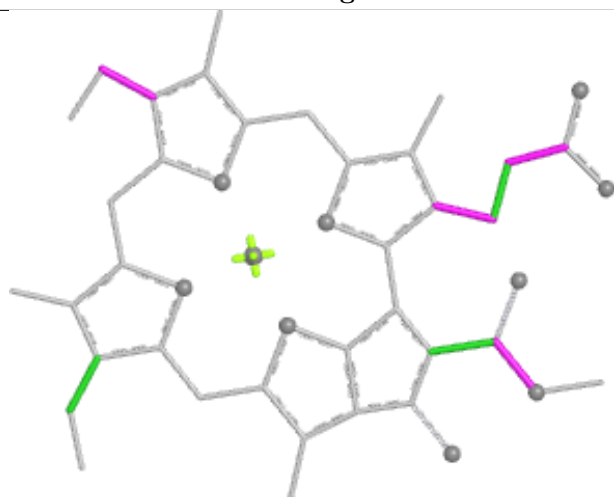
Ligand CLA K 204



Bond lengths



Bond angles

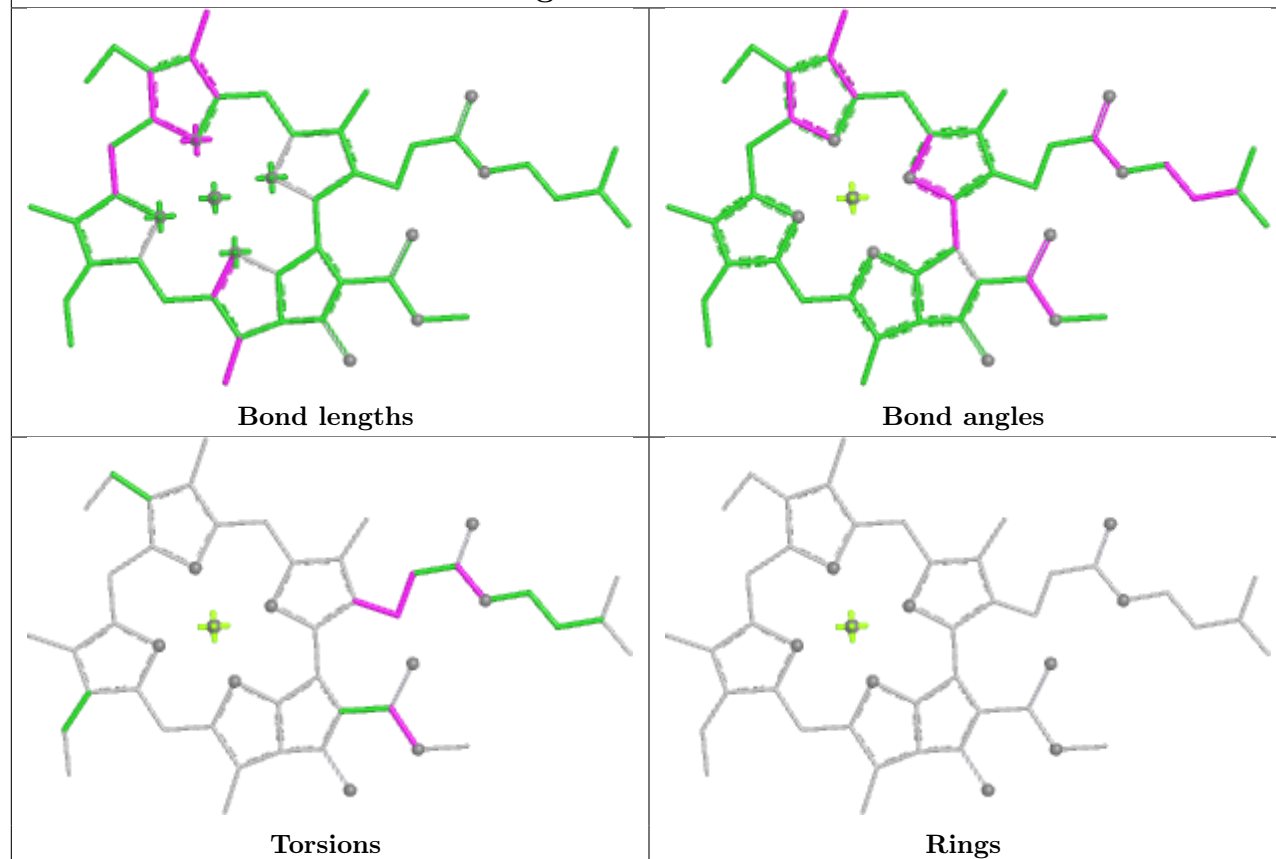


Torsions

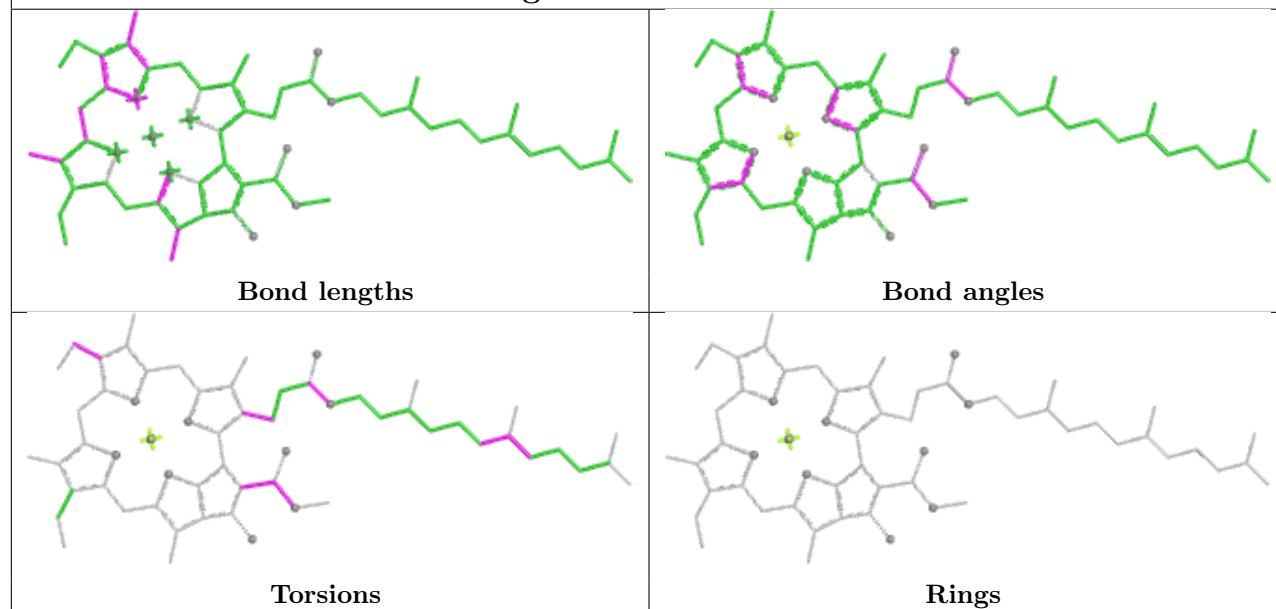


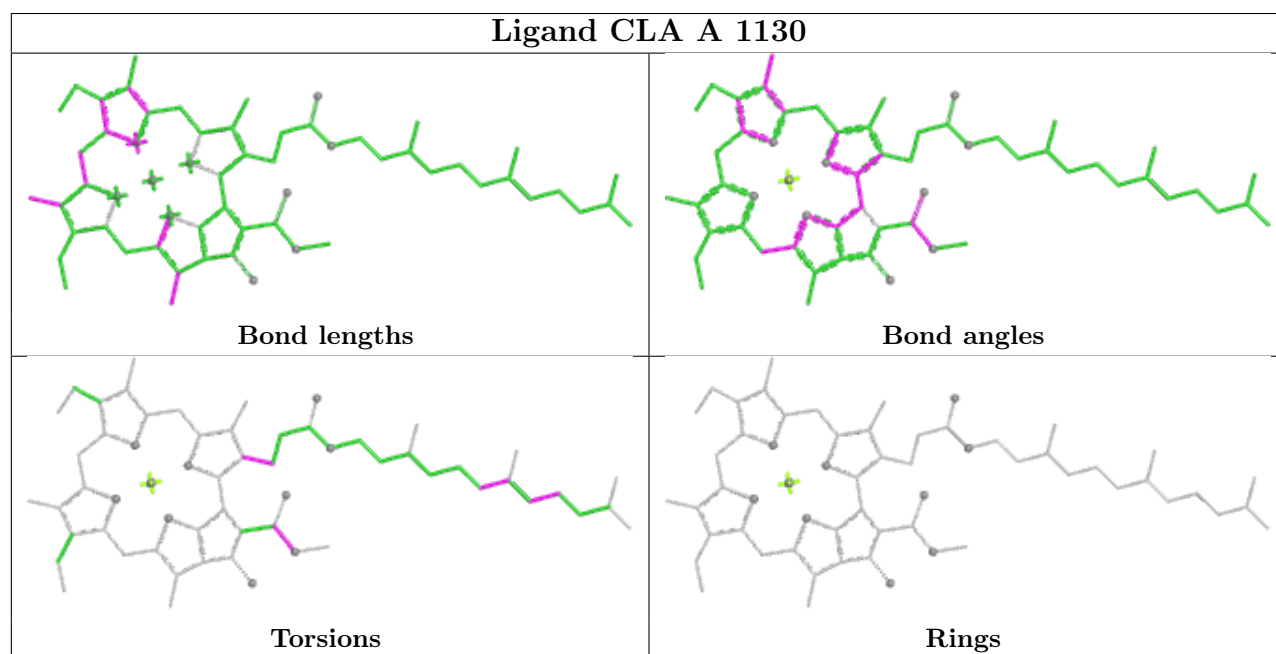
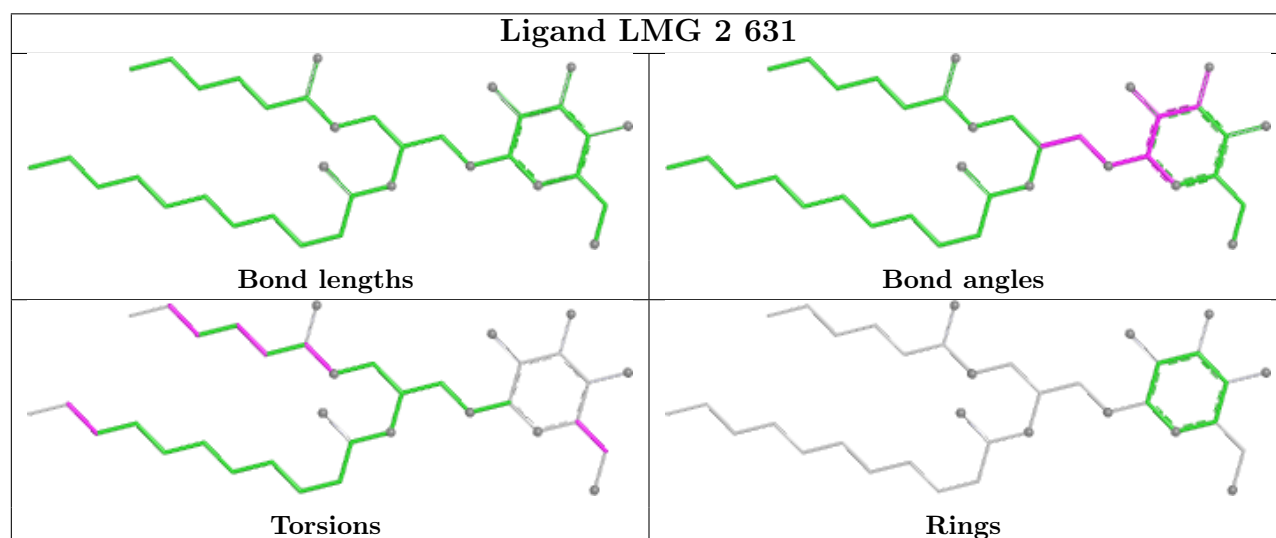
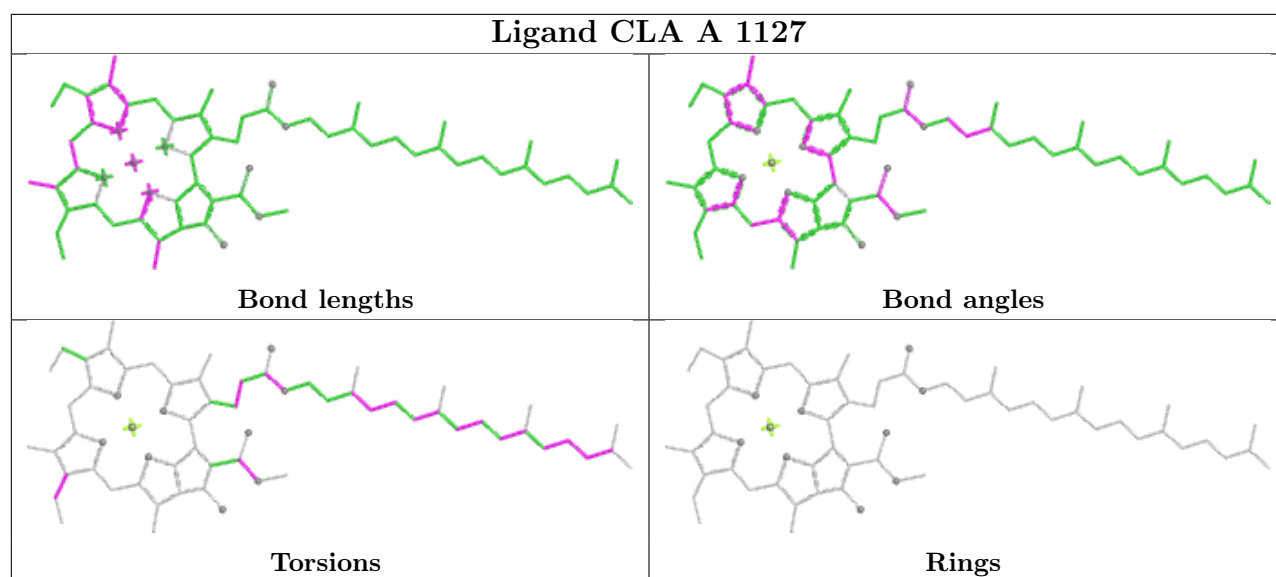
Rings

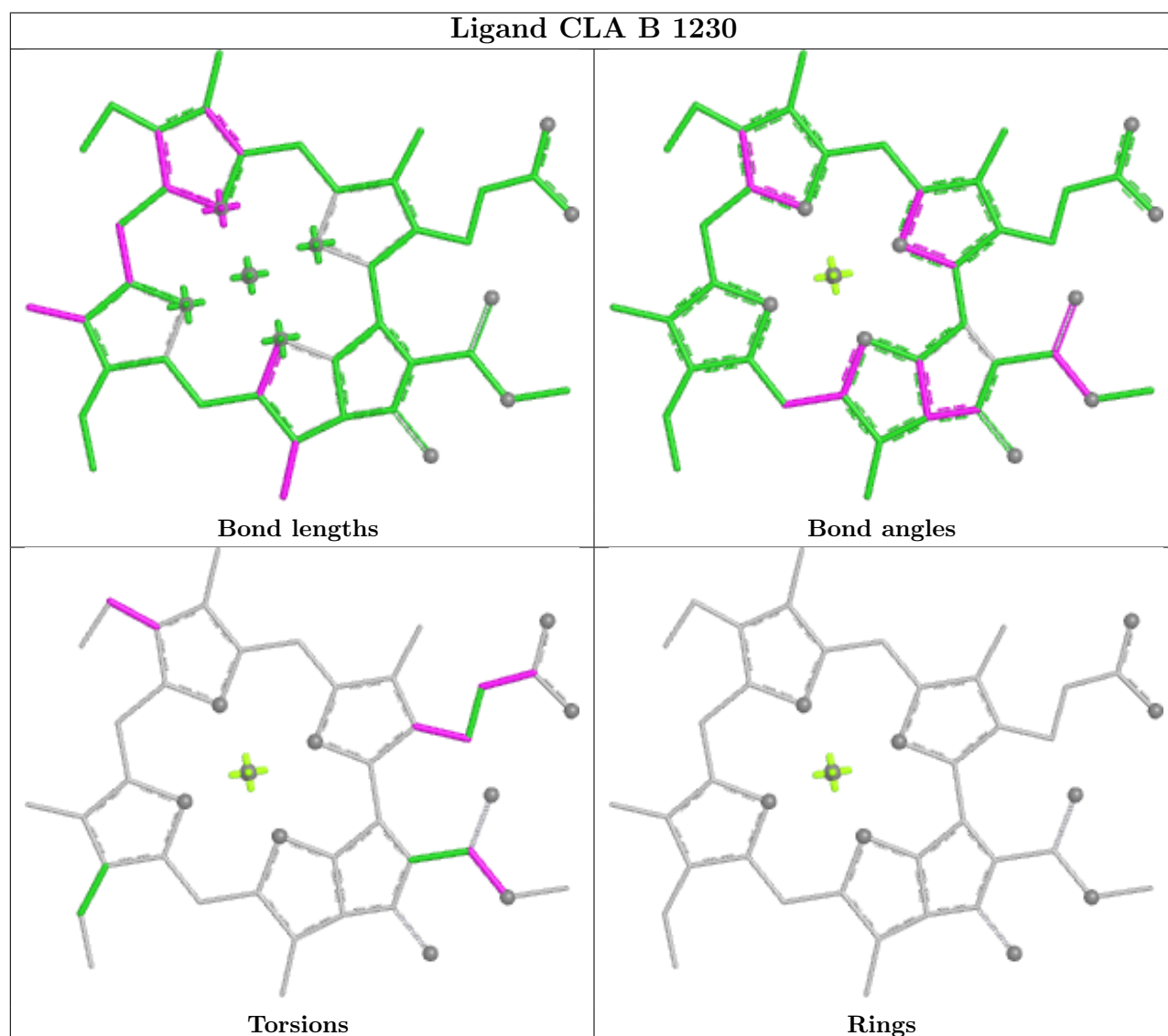
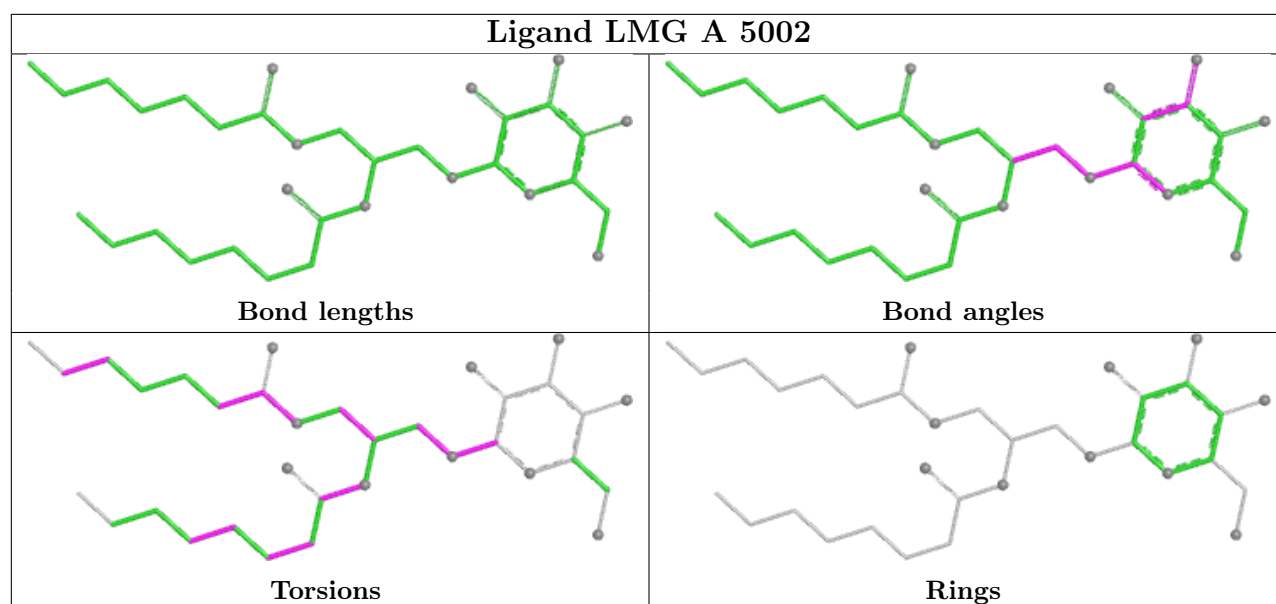
Ligand CLA 4 604

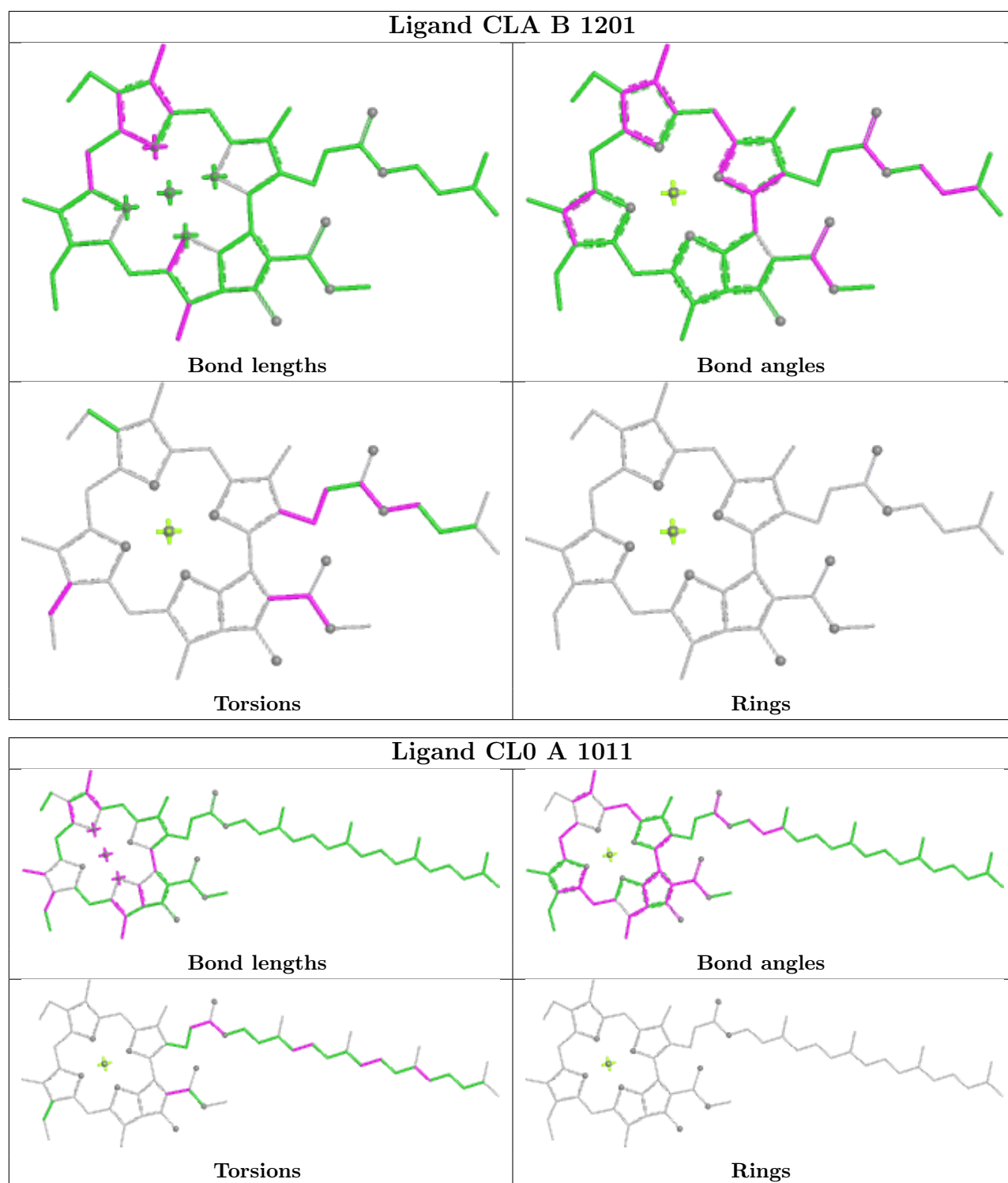


Ligand CLA A 1122

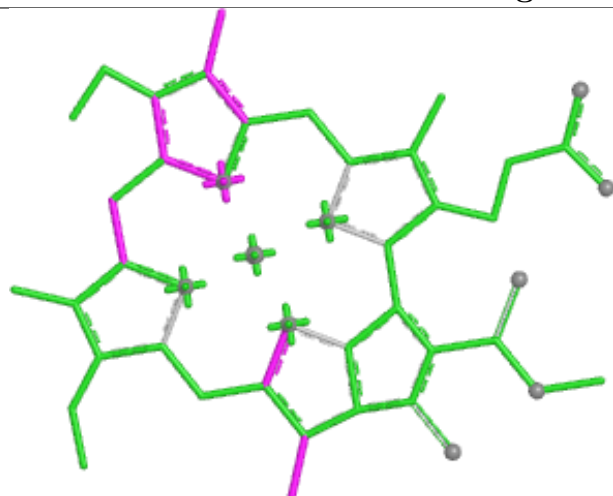




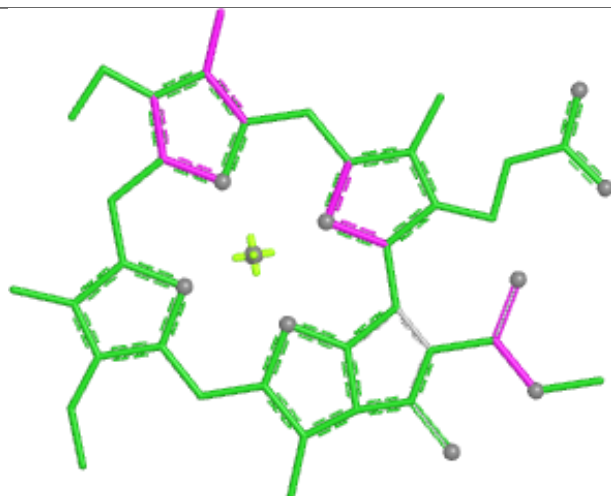




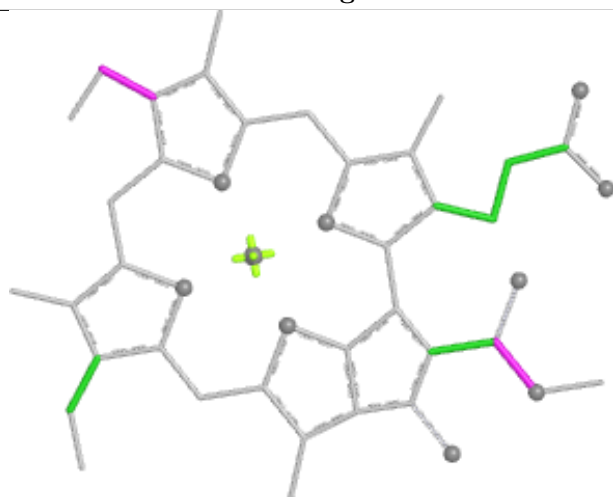
Ligand CLA F 301



Bond lengths



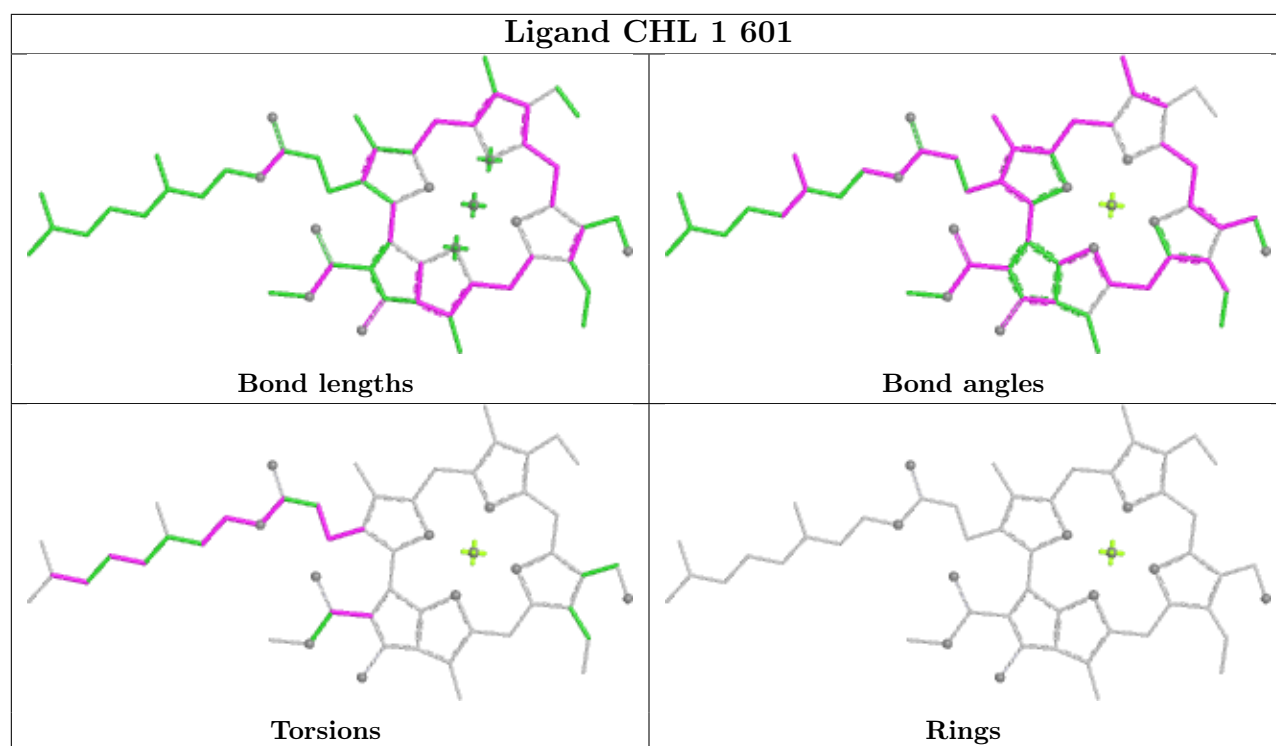
Bond angles



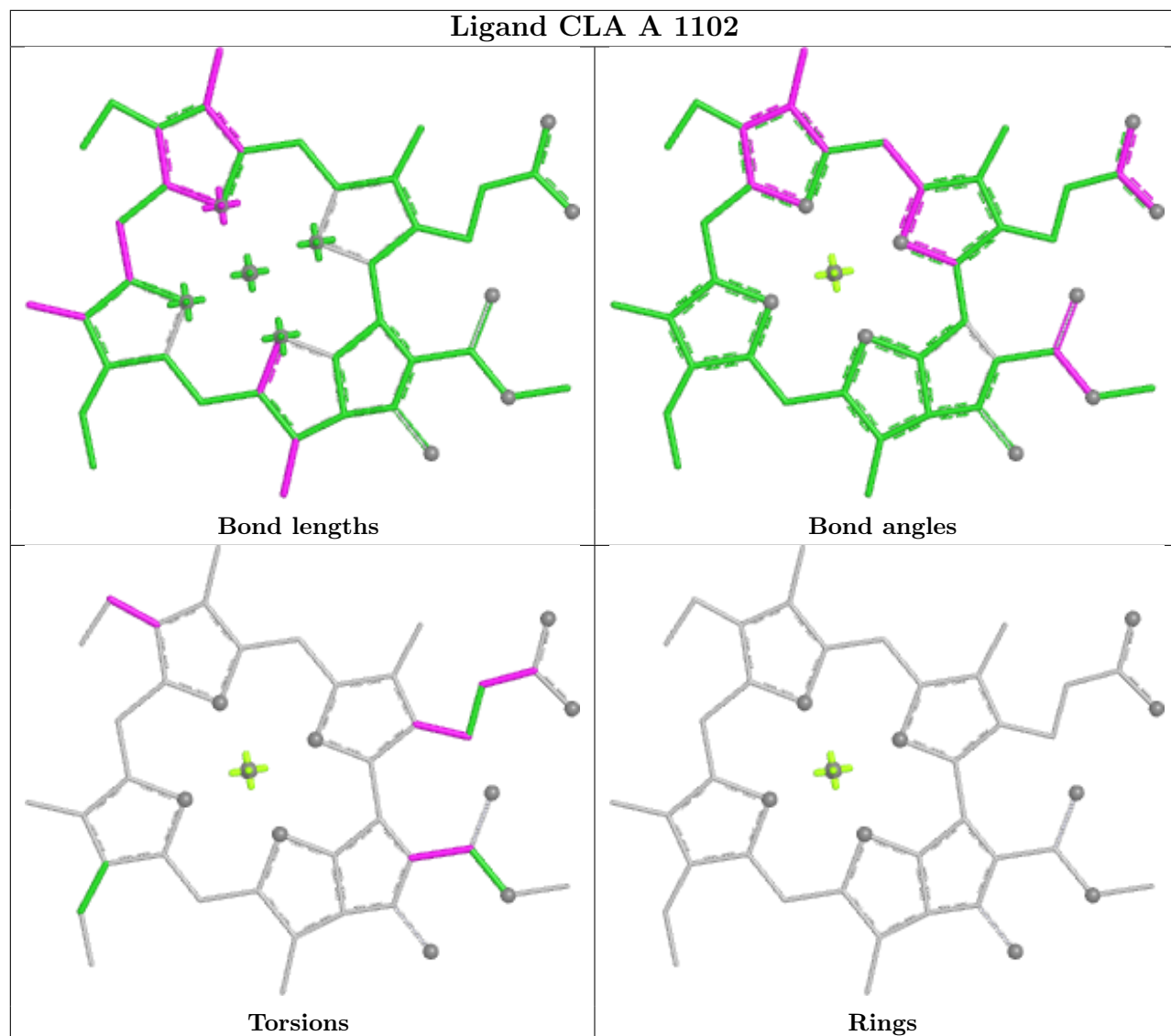
Torsions



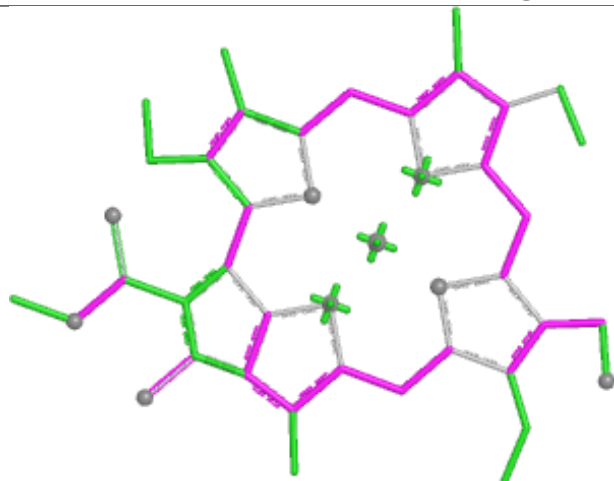
Rings



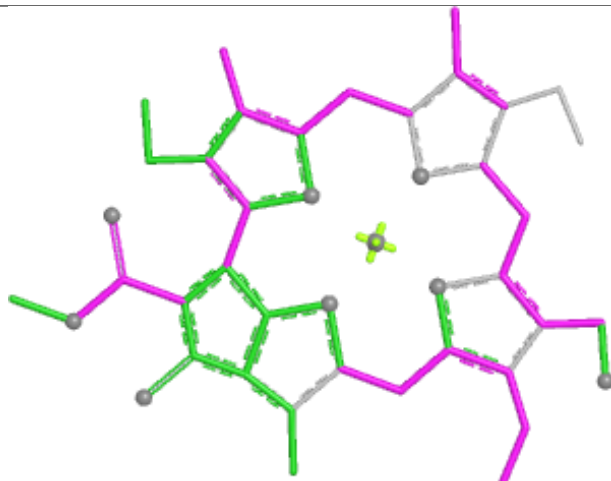
Ligand CLA A 1102



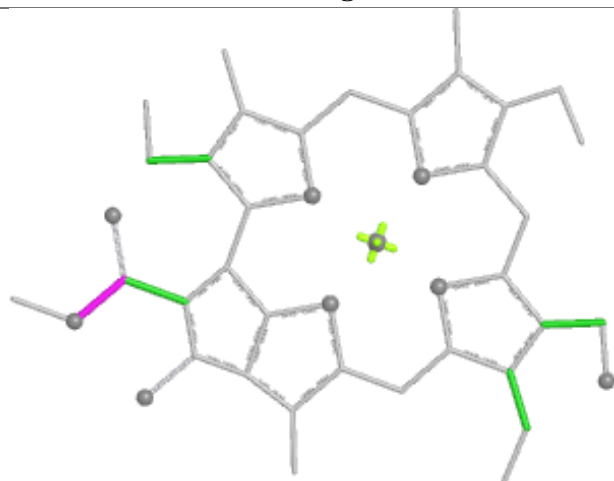
Ligand CHL 4 615



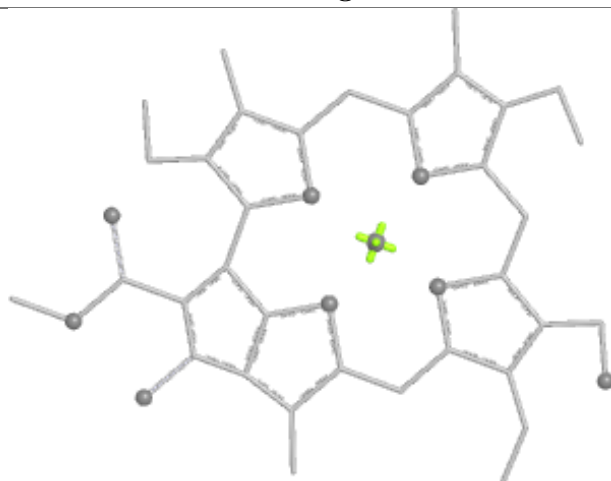
Bond lengths



Bond angles

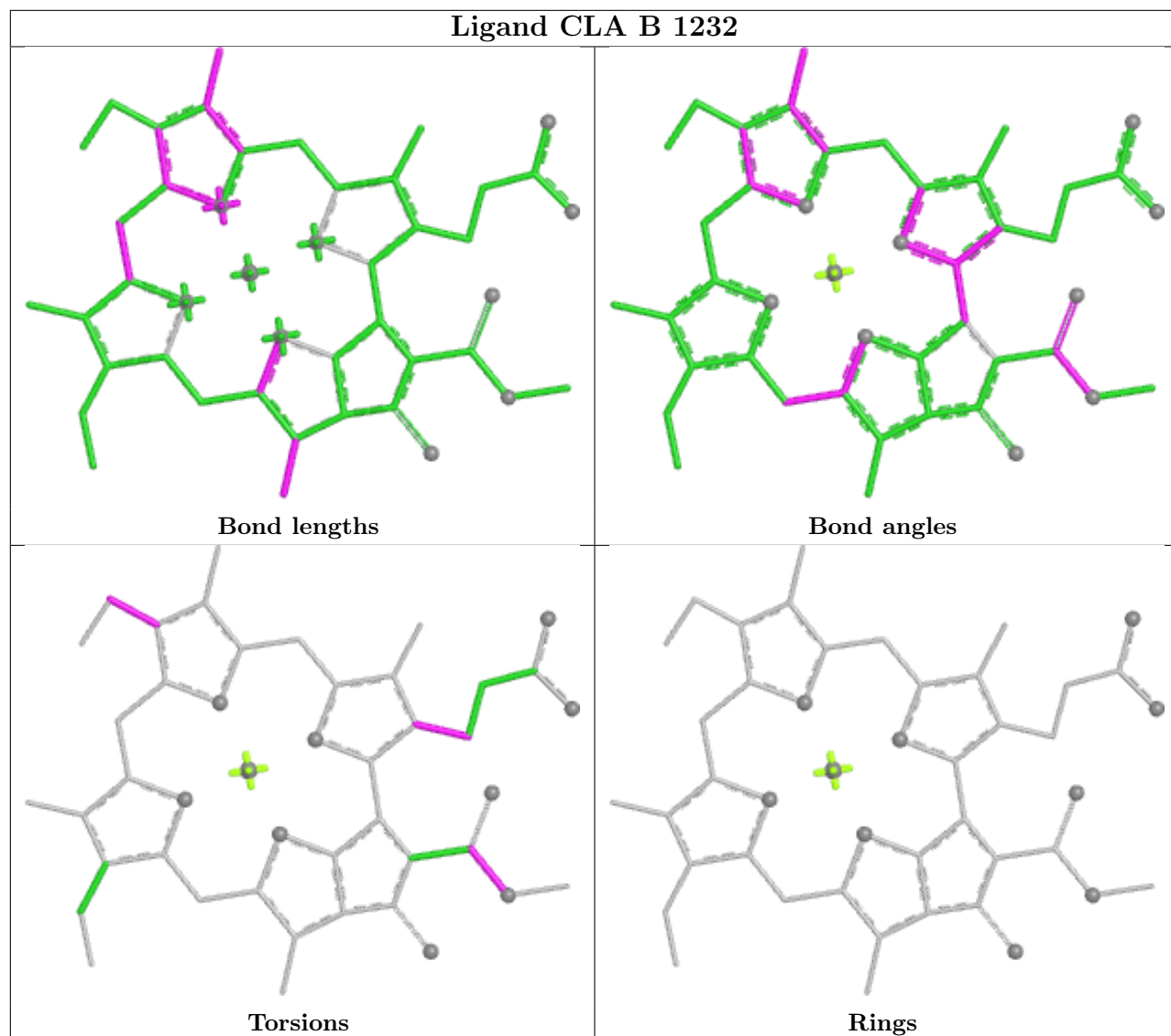


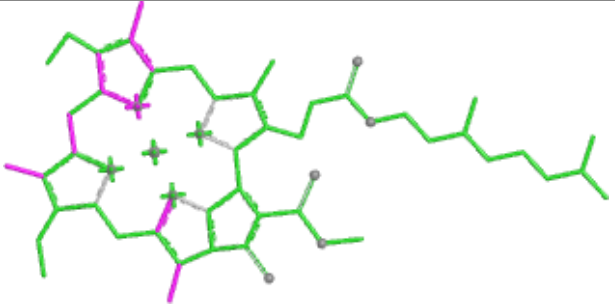
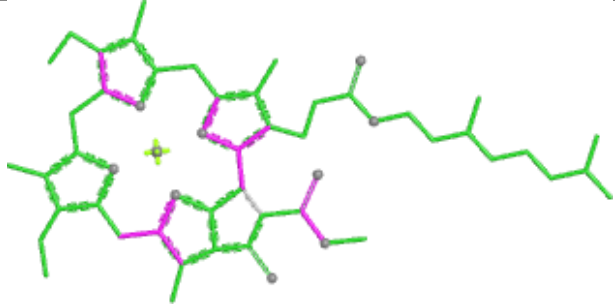
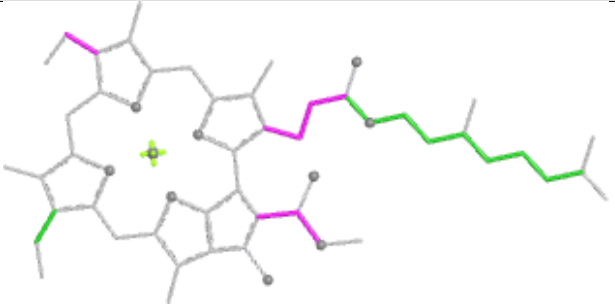
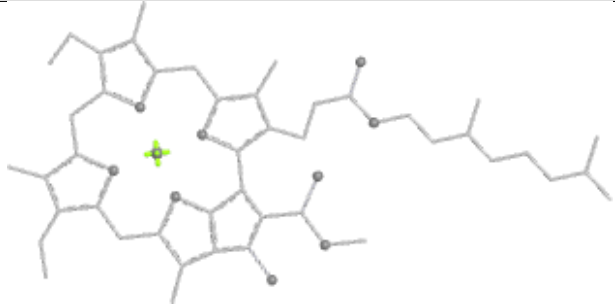
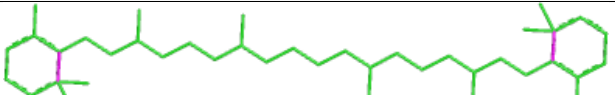
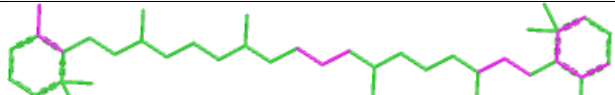
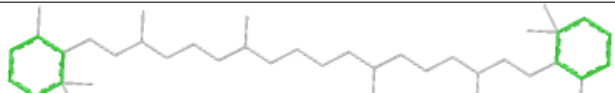
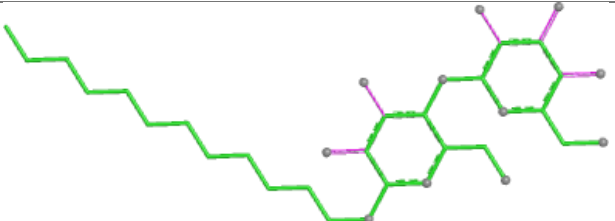
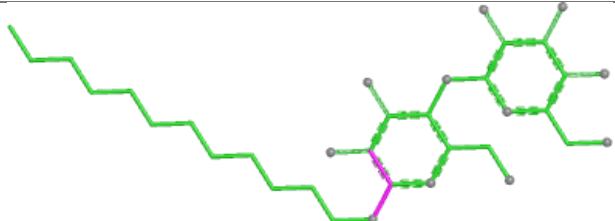
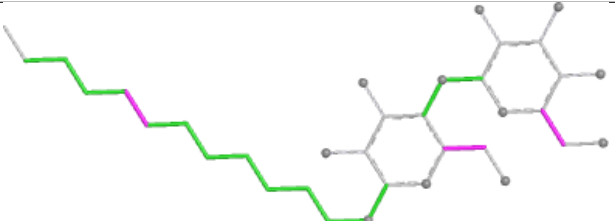
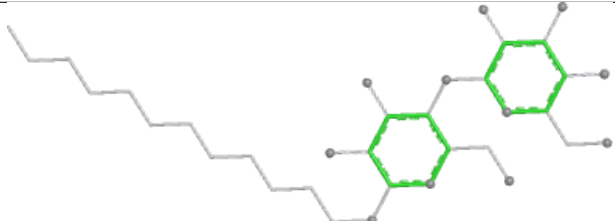
Torsions



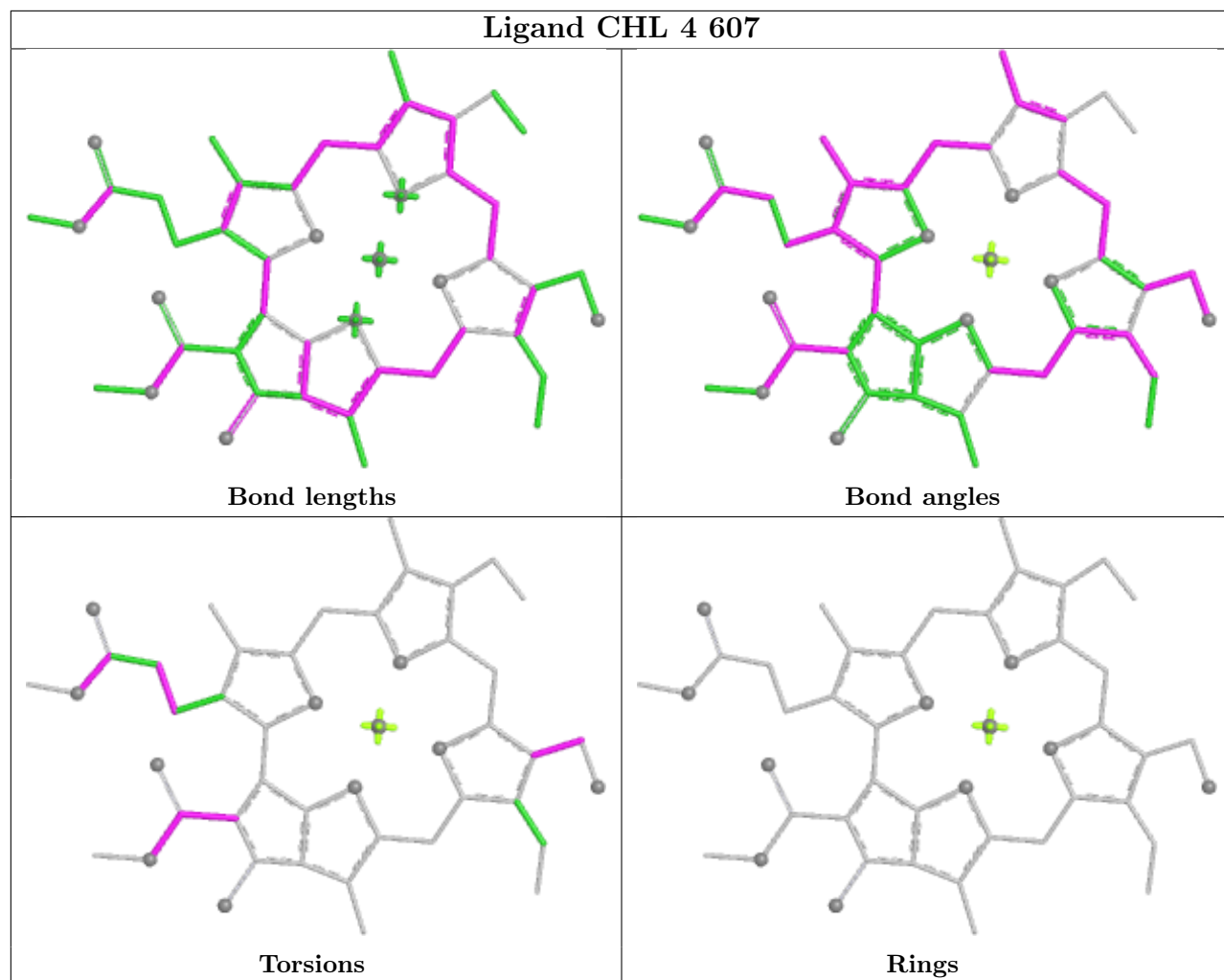
Rings

Ligand CLA B 1232

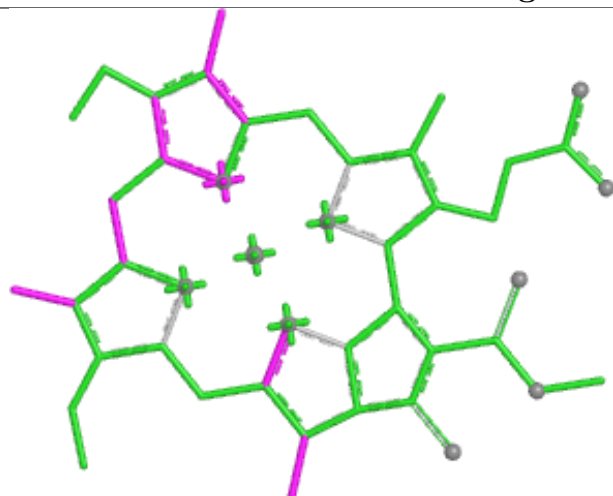


Ligand CLA 1 613	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 4006	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LMT 4 631	
	
Bond lengths	Bond angles
	
Torsions	Rings

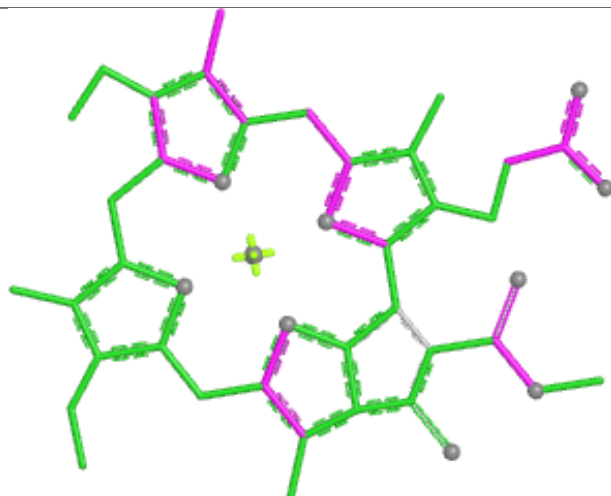
Ligand CHL 4 607



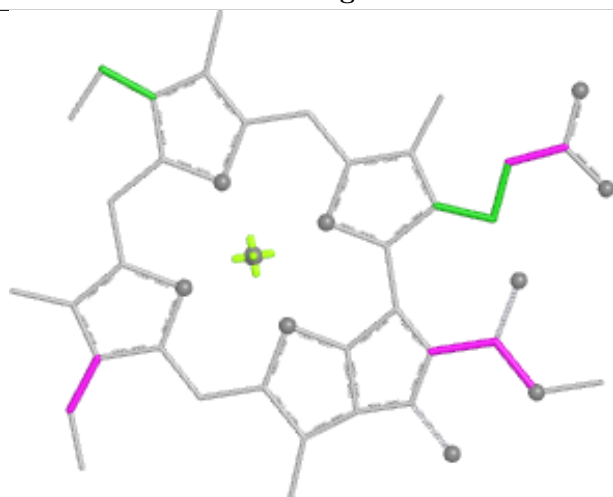
Ligand CLA 1 606



Bond lengths



Bond angles

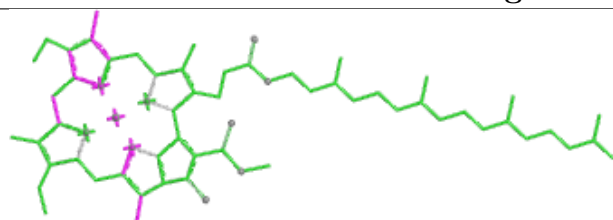


Torsions

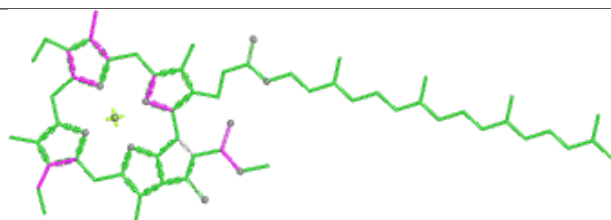


Rings

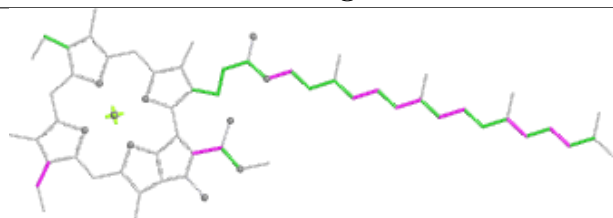
Ligand CLA A 8895



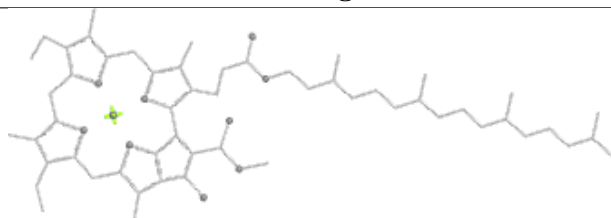
Bond lengths



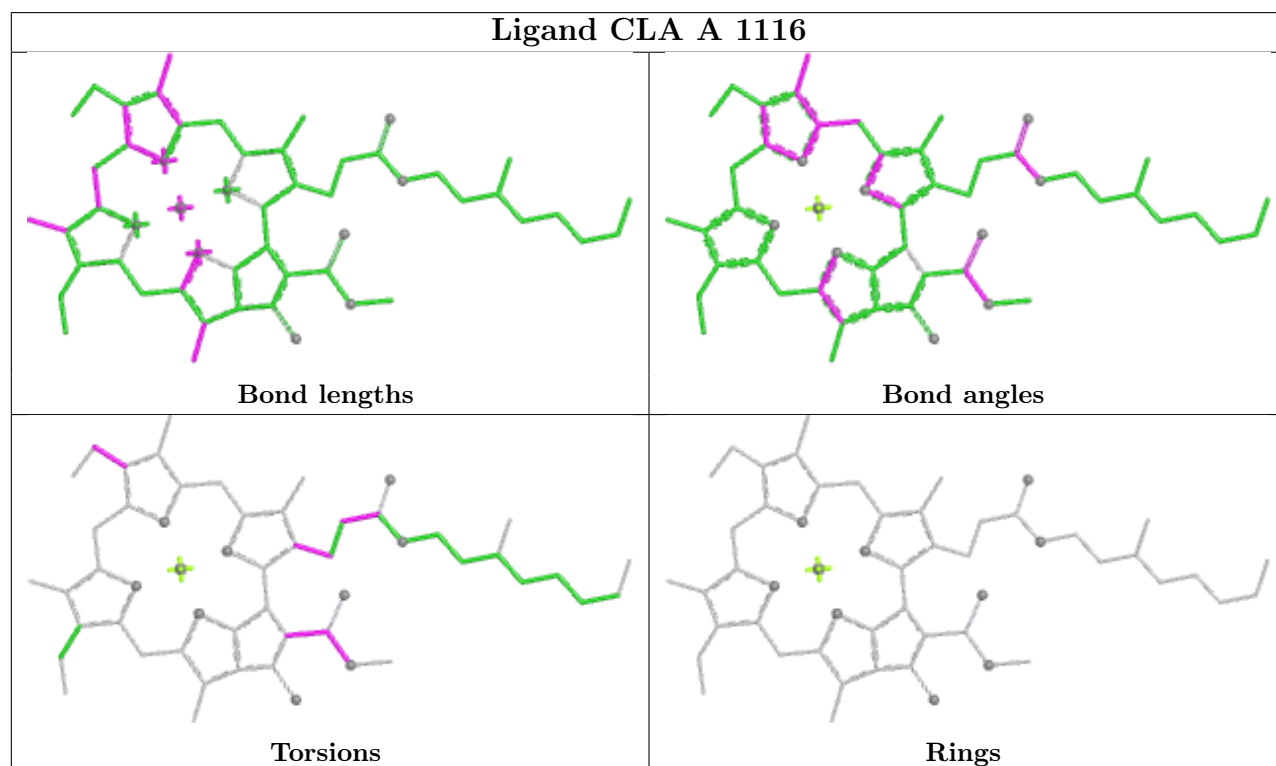
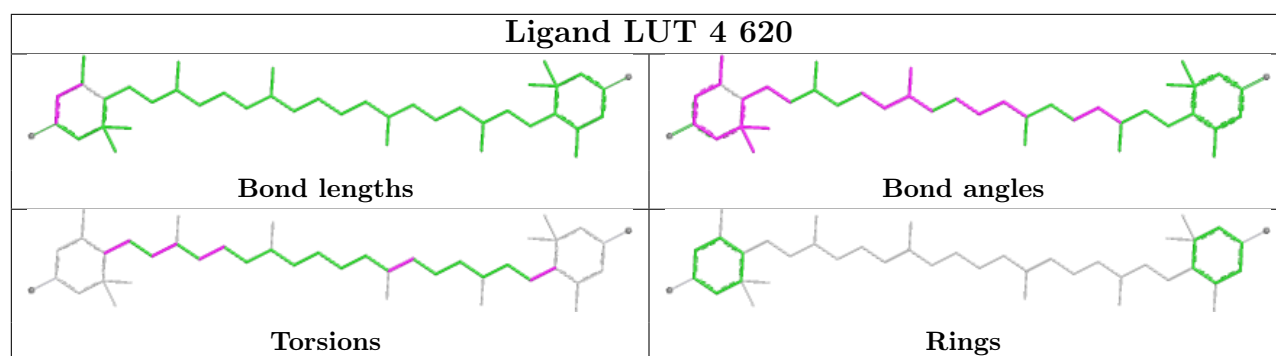
Bond angles



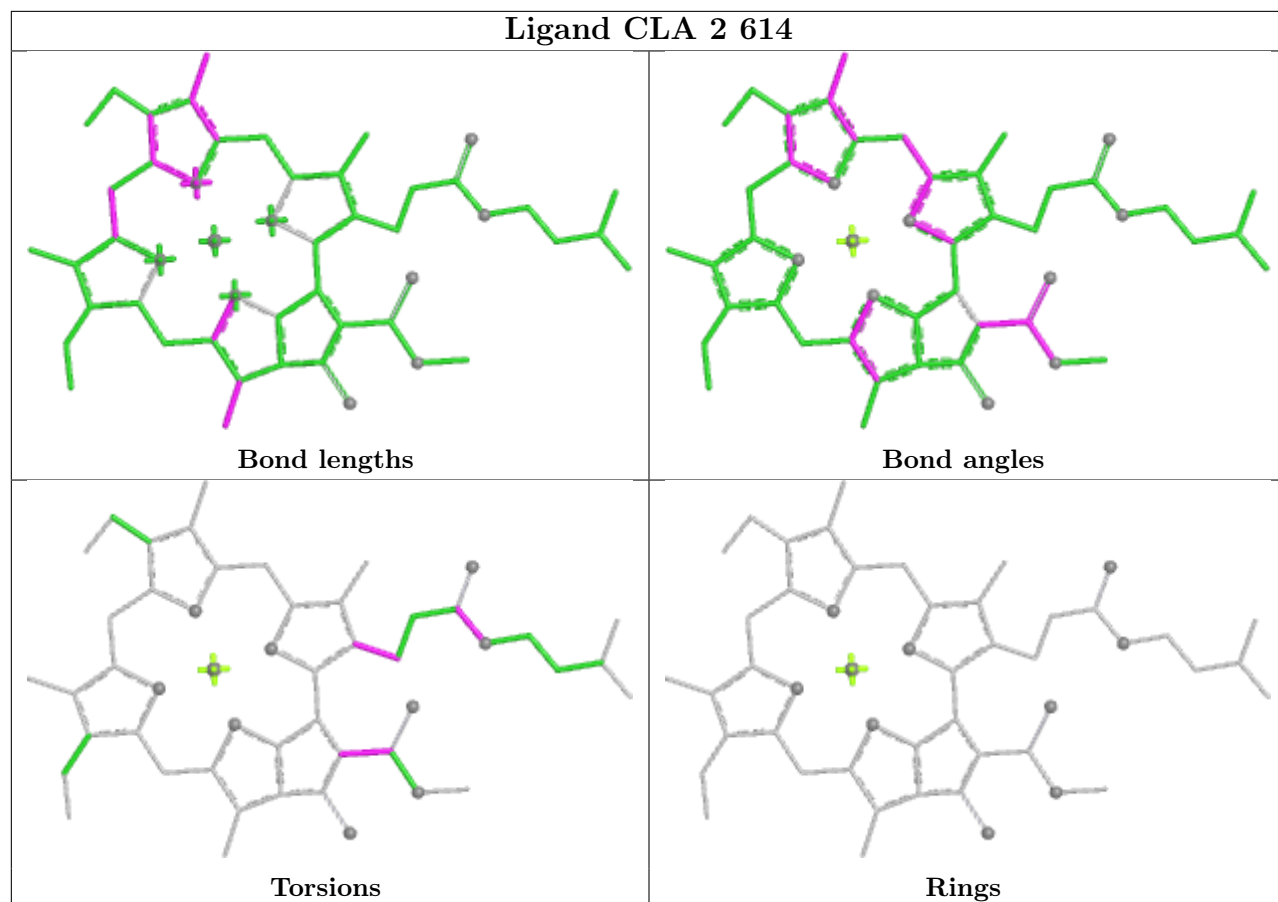
Torsions



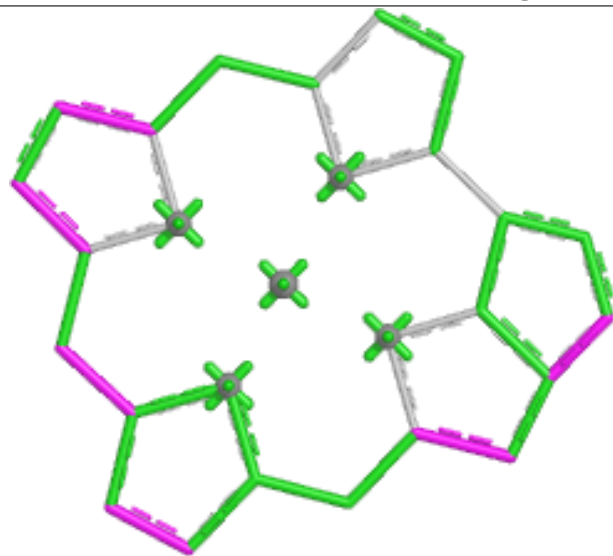
Rings



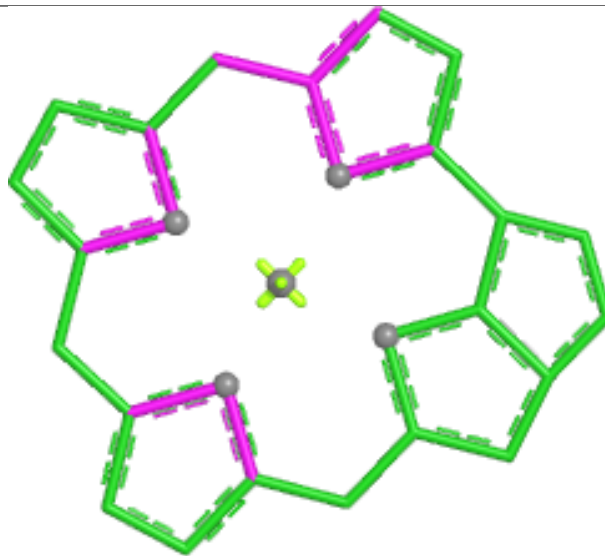
Ligand CLA 2 614



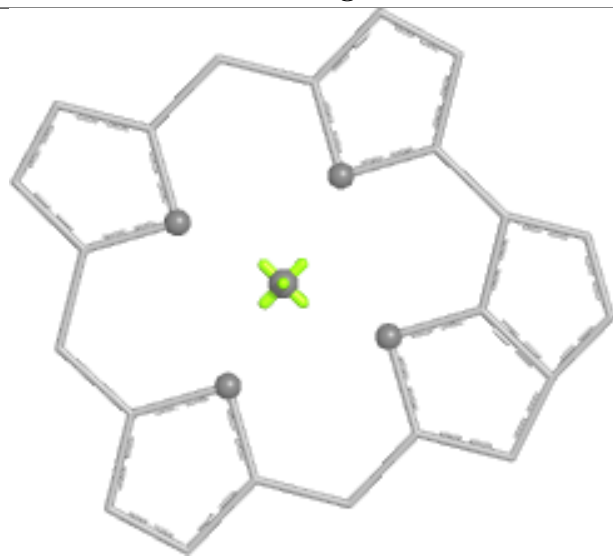
Ligand CLA F 303



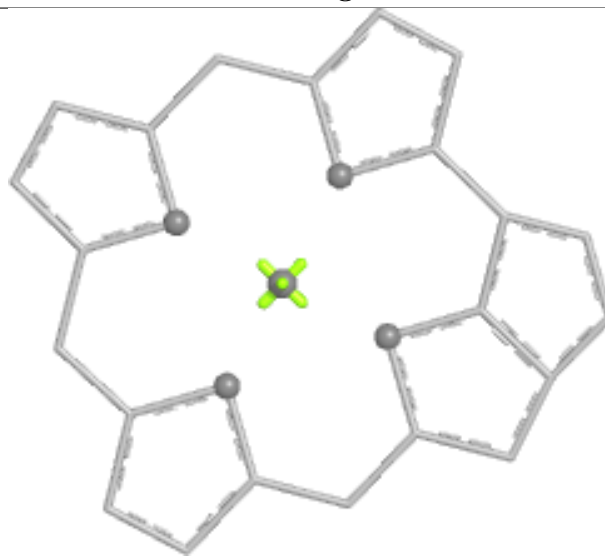
Bond lengths



Bond angles

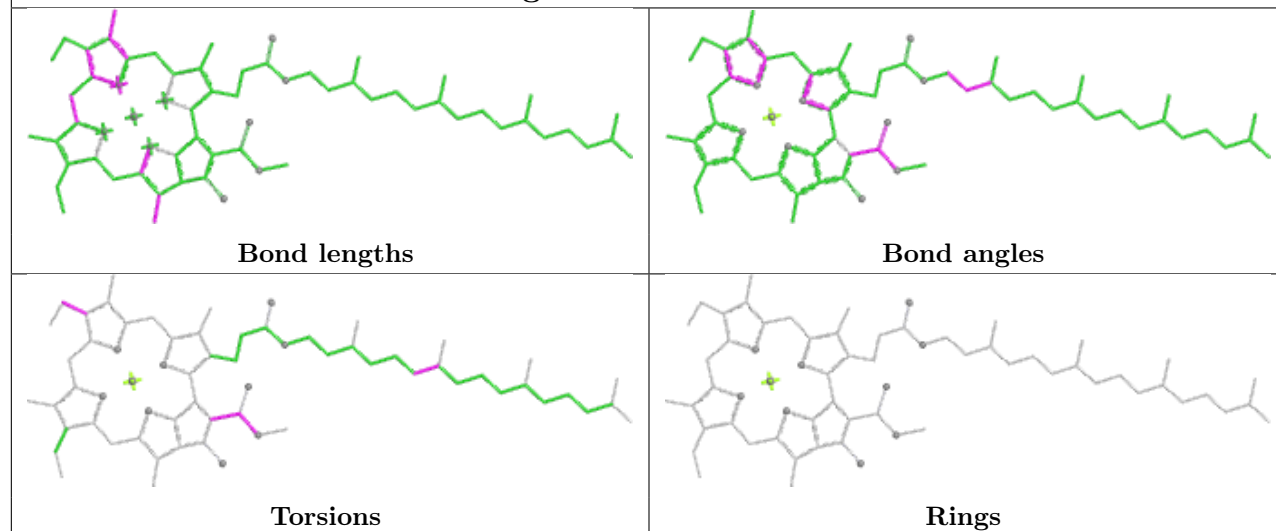


Torsions

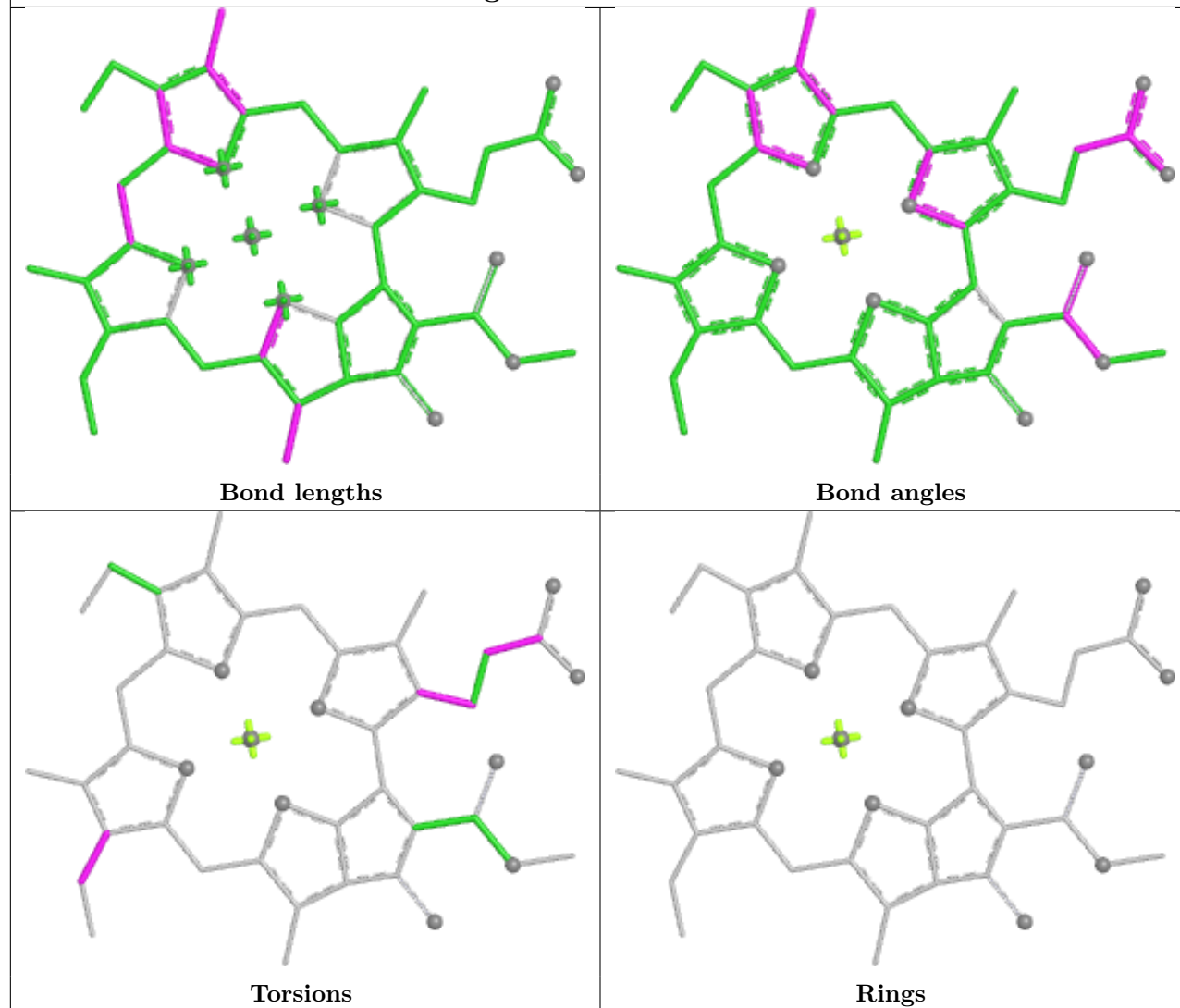


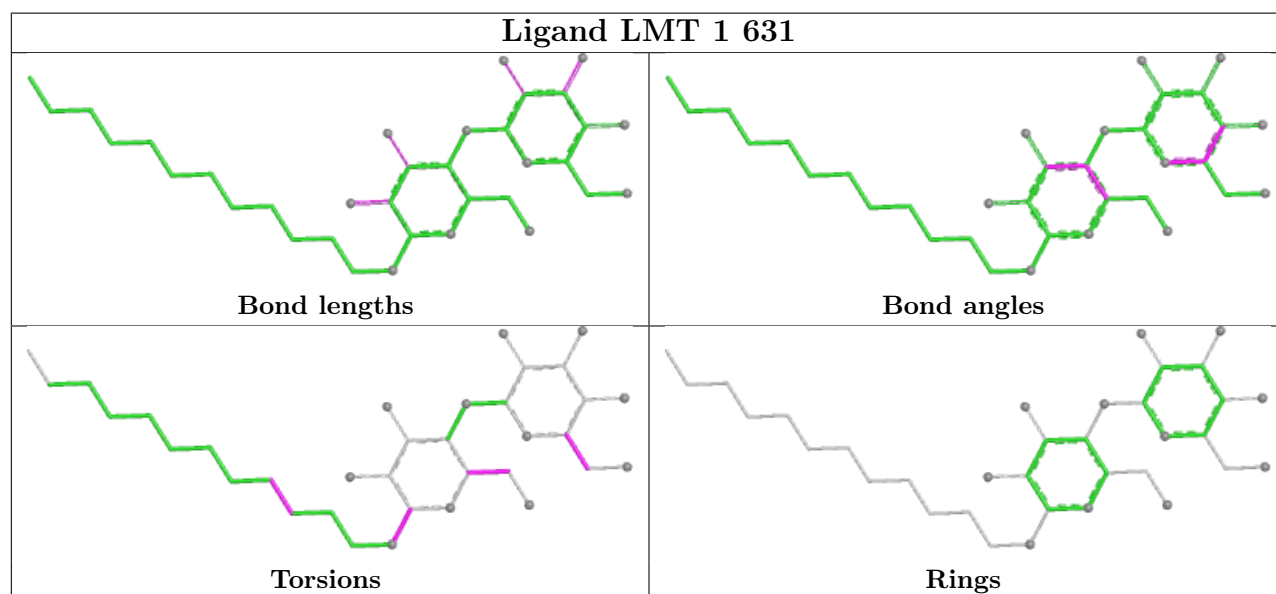
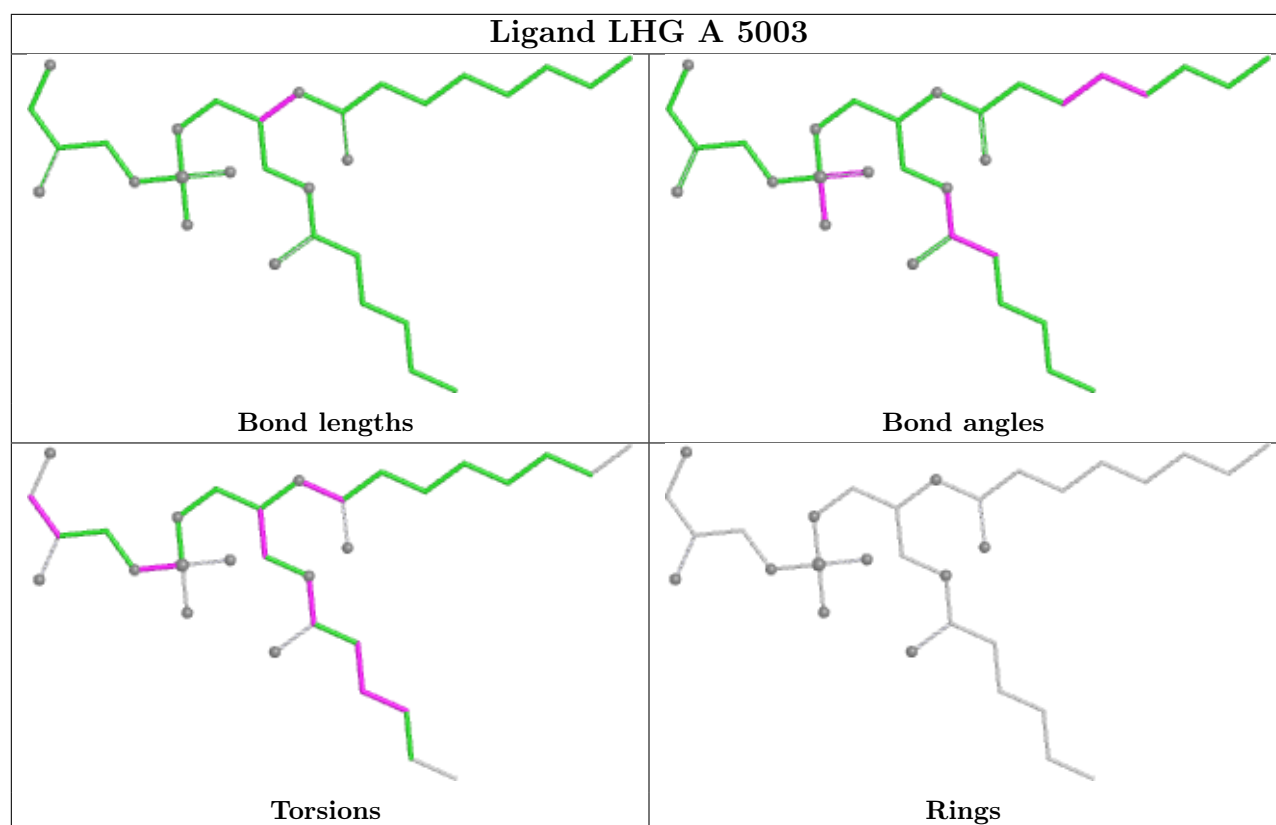
Rings

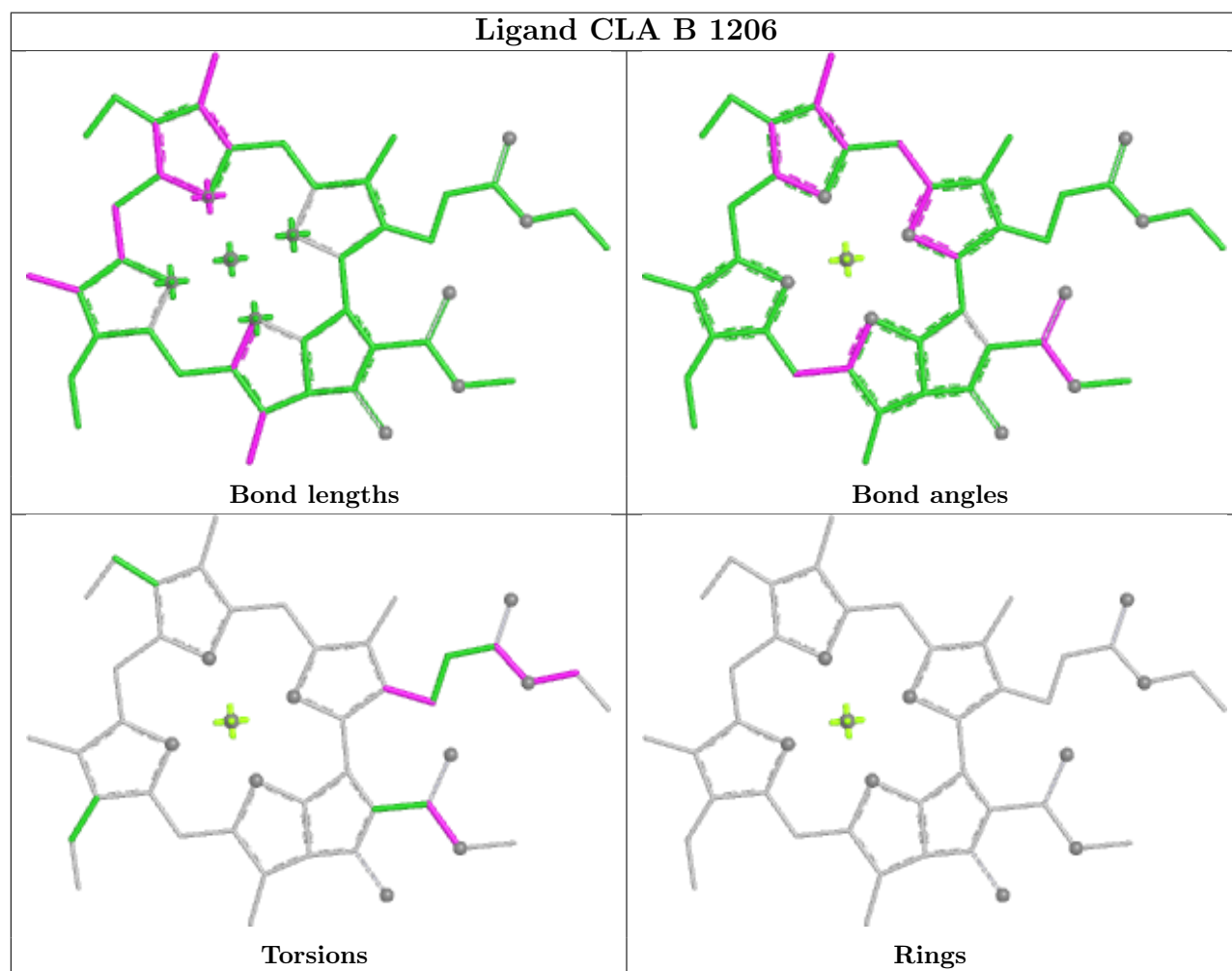
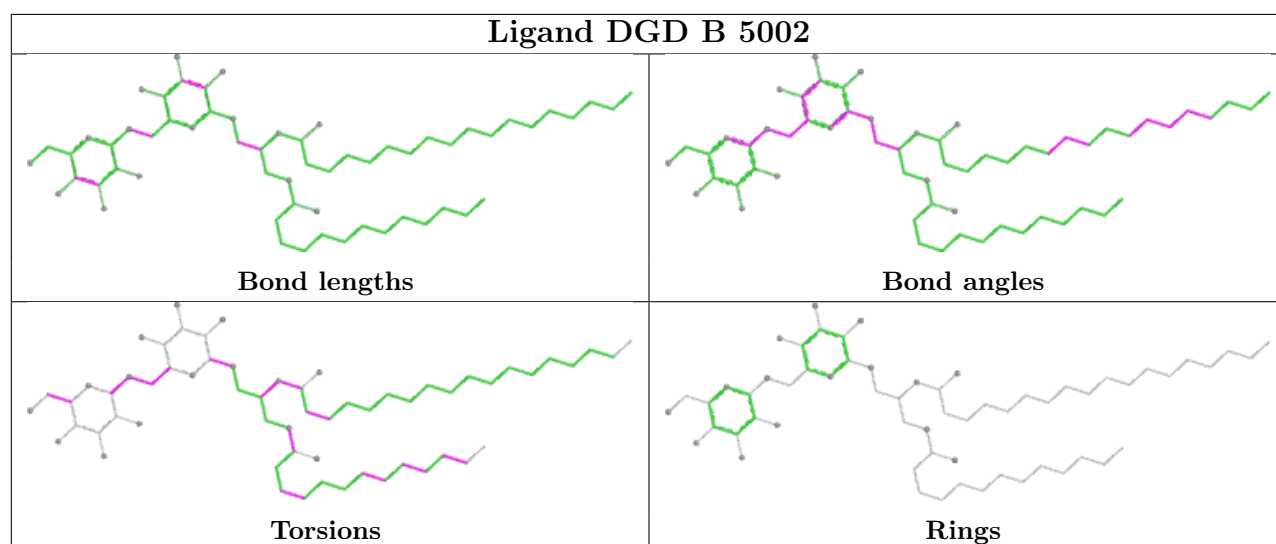
Ligand CLA A 1131

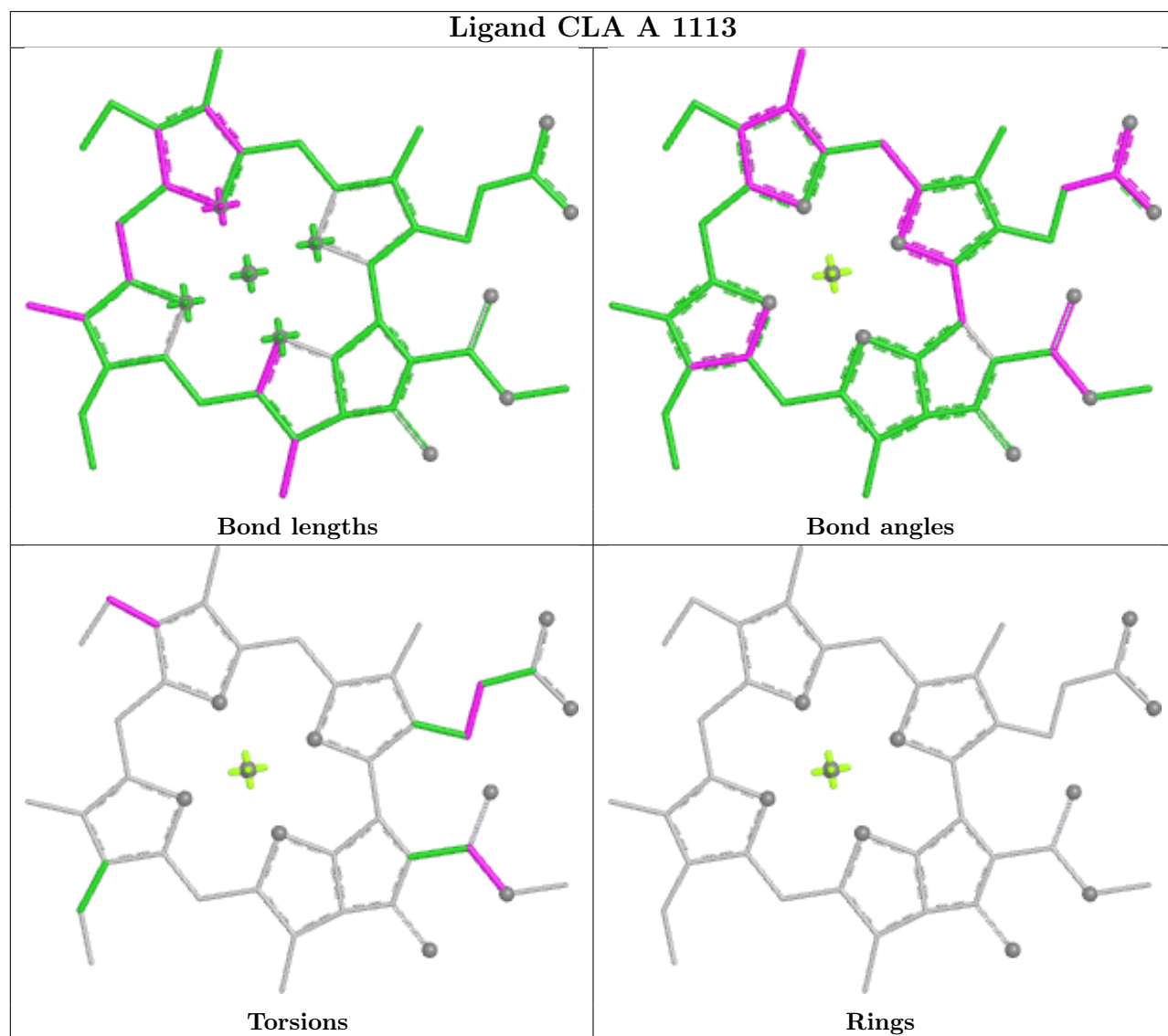
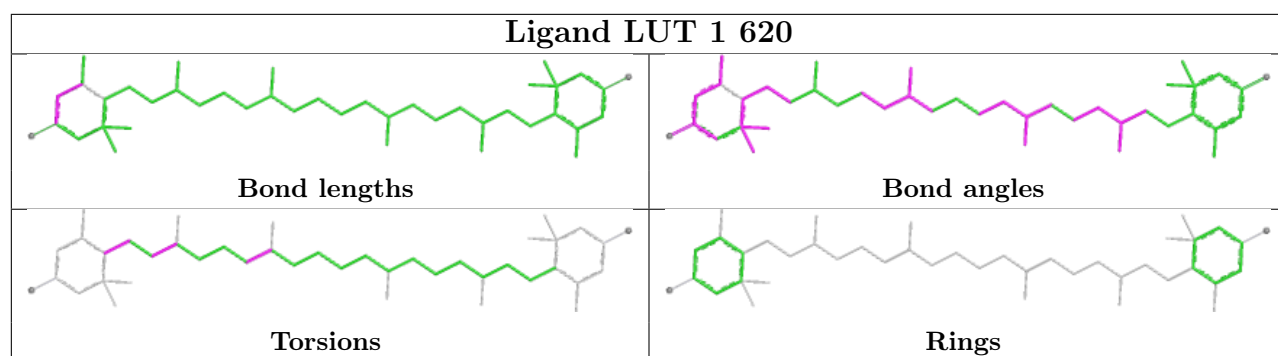


Ligand CLA B 1217

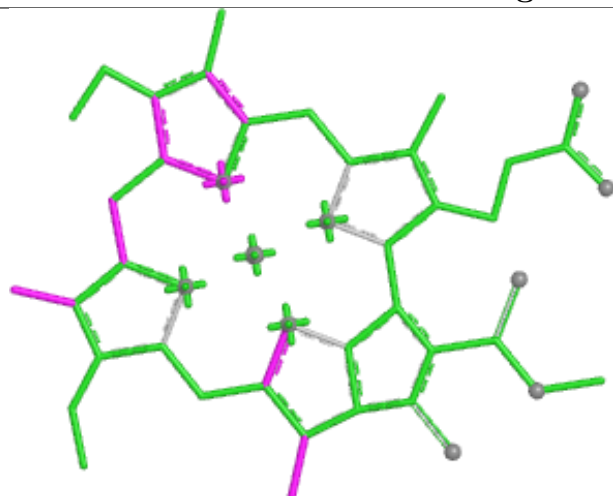




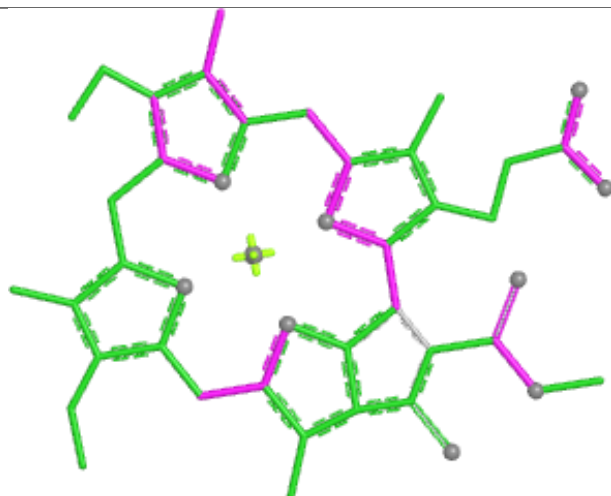




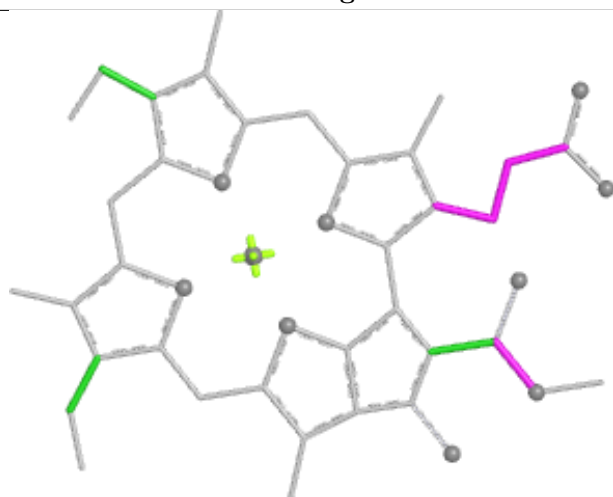
Ligand CLA L 303



Bond lengths



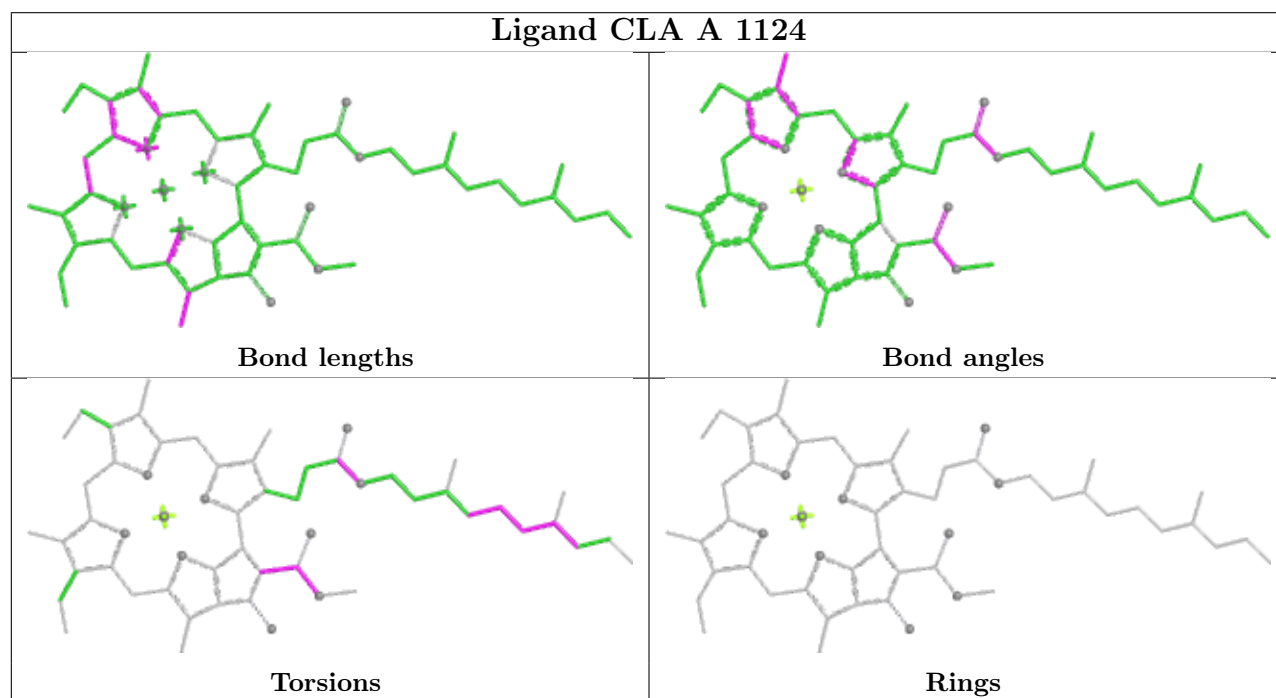
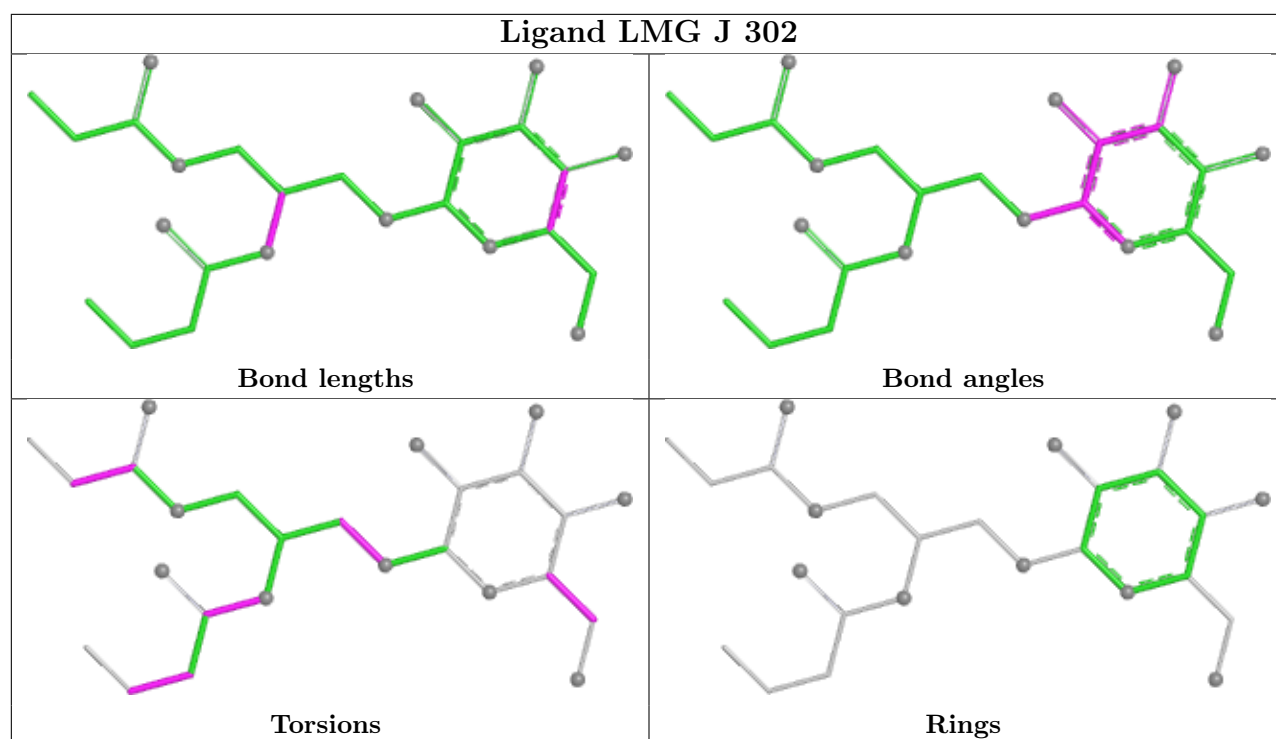
Bond angles

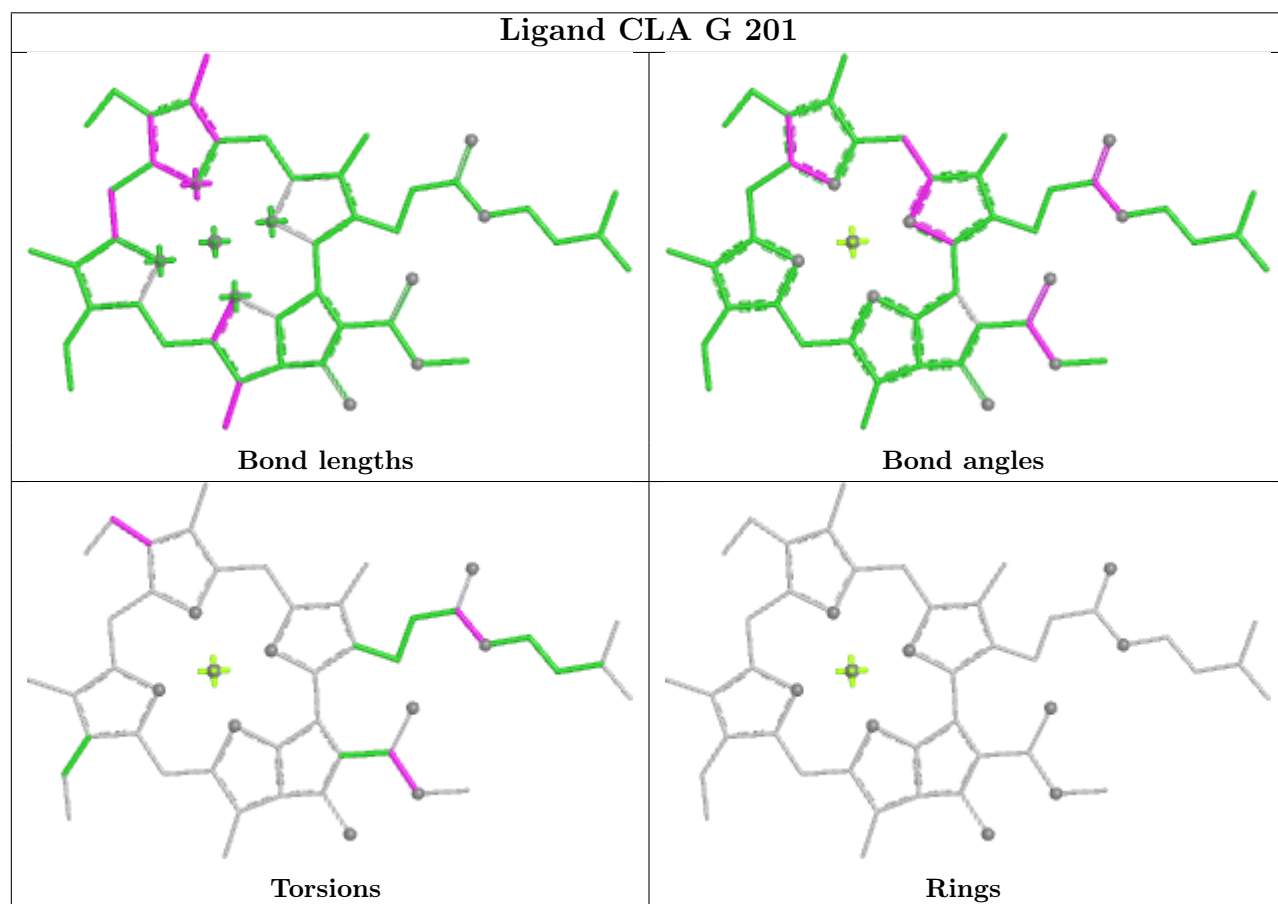
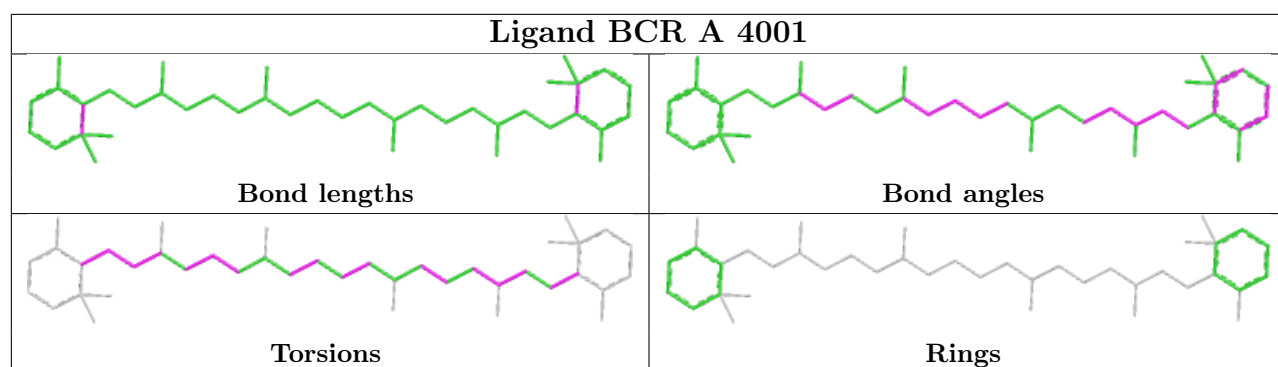


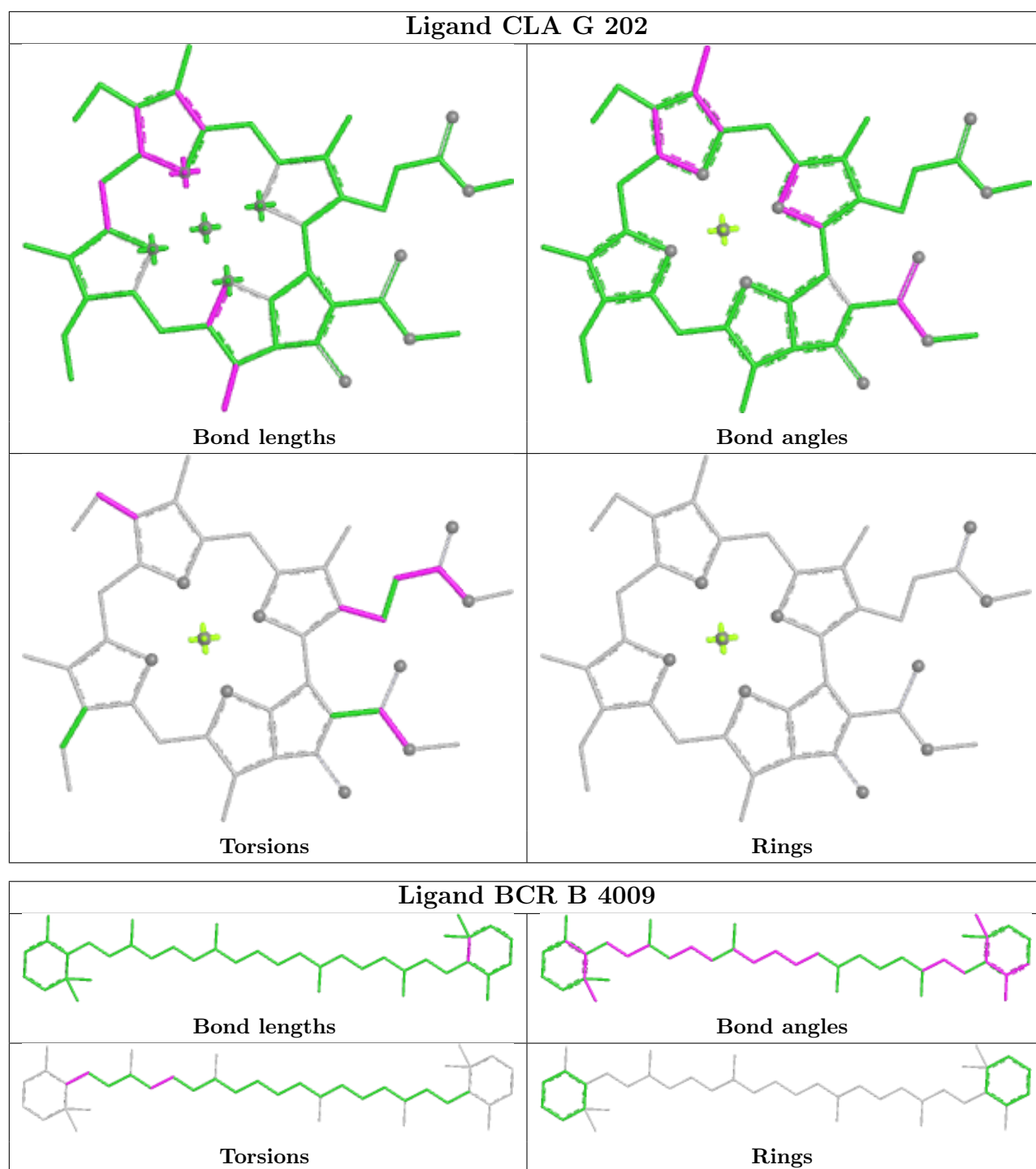
Torsions



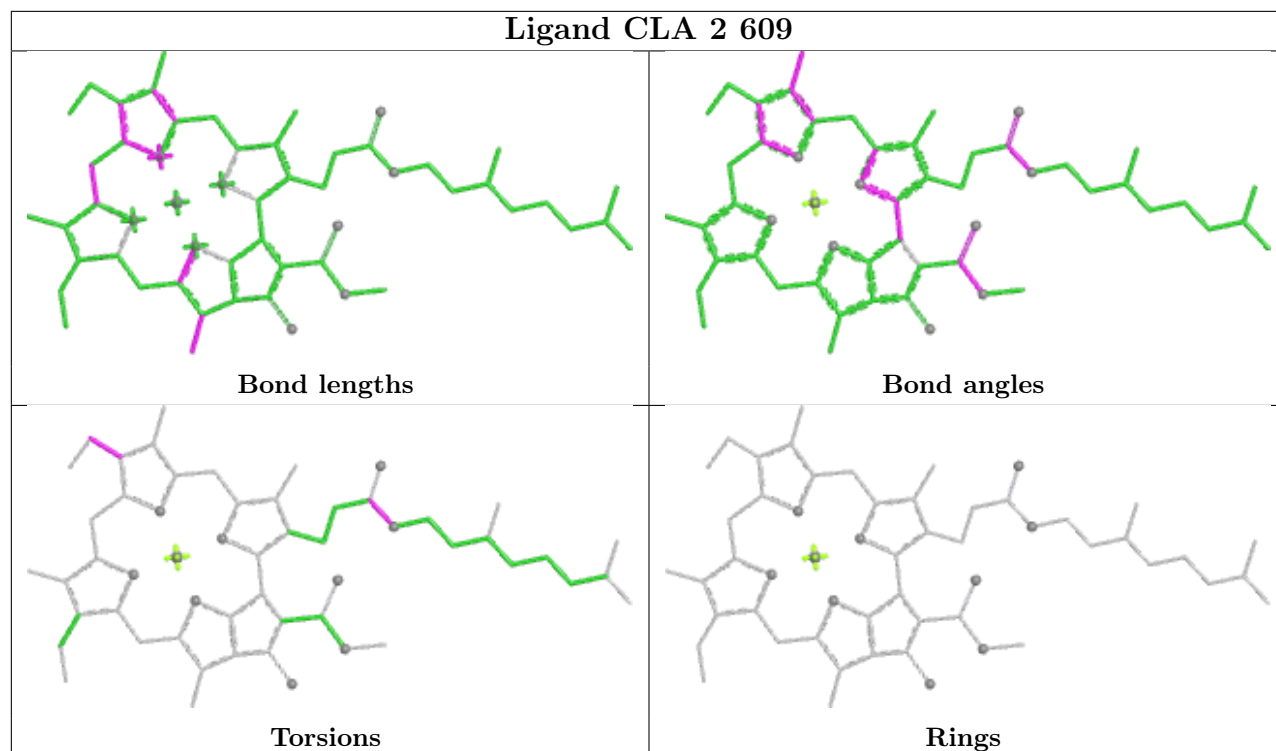
Rings



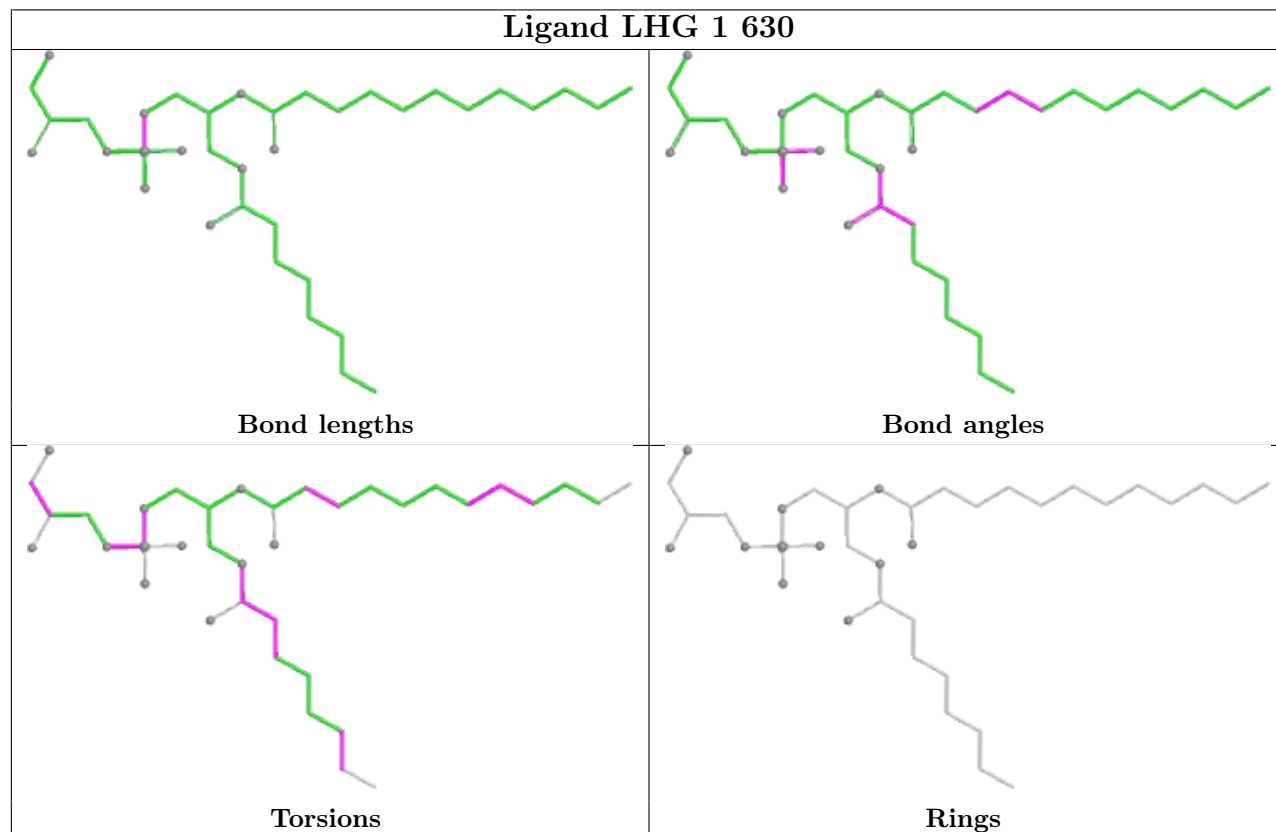


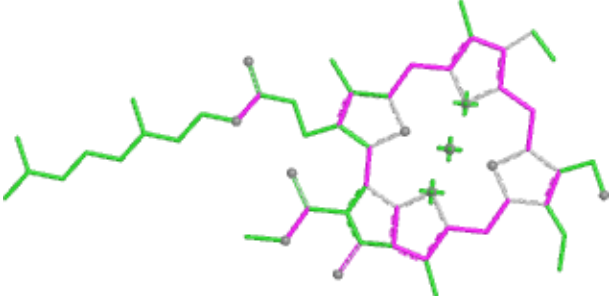
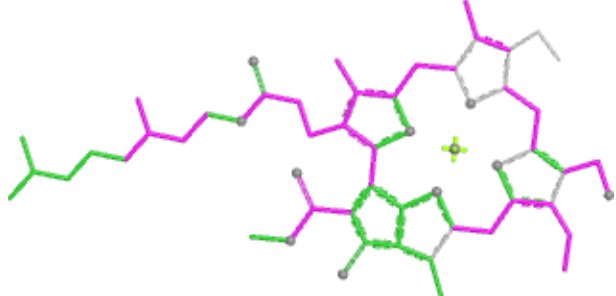
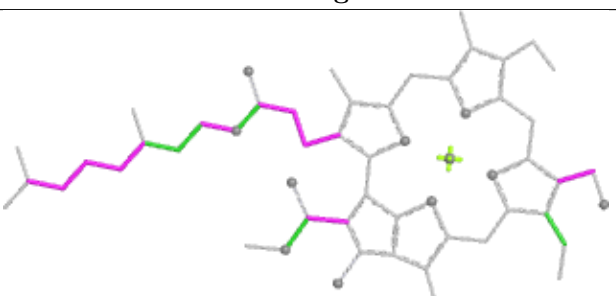
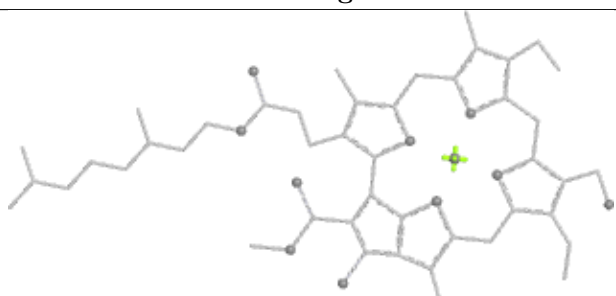
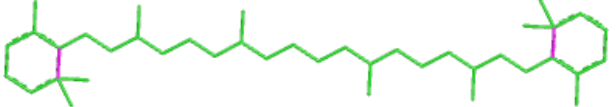
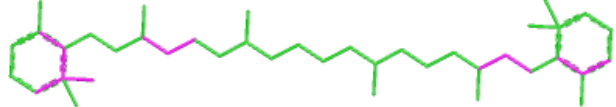
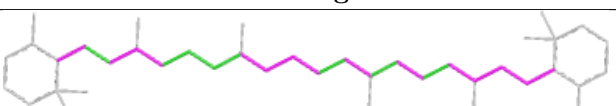
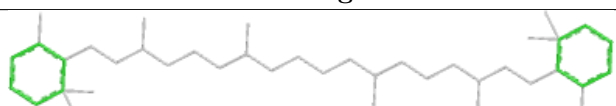


Ligand CLA 2 609

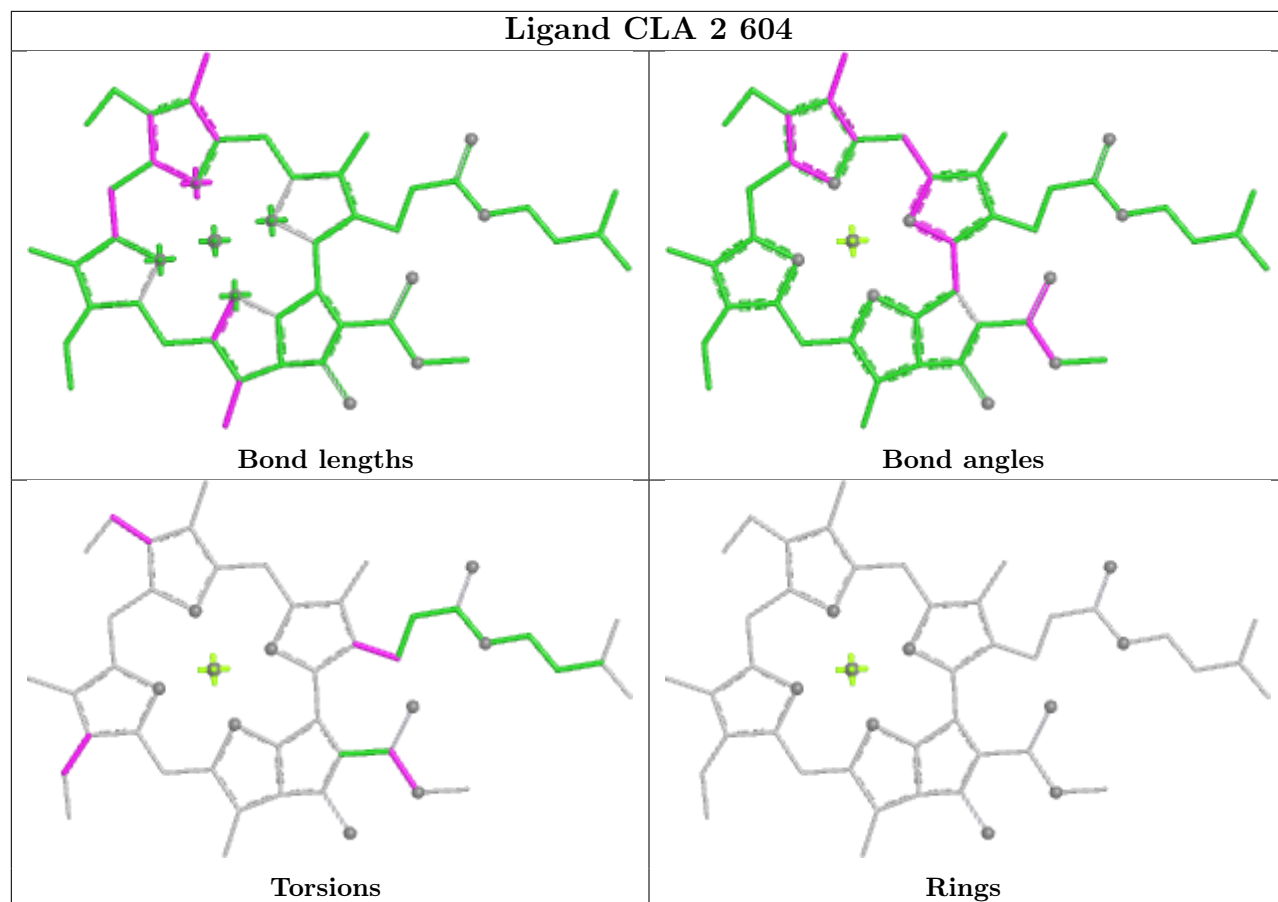


Ligand LHG 1 630

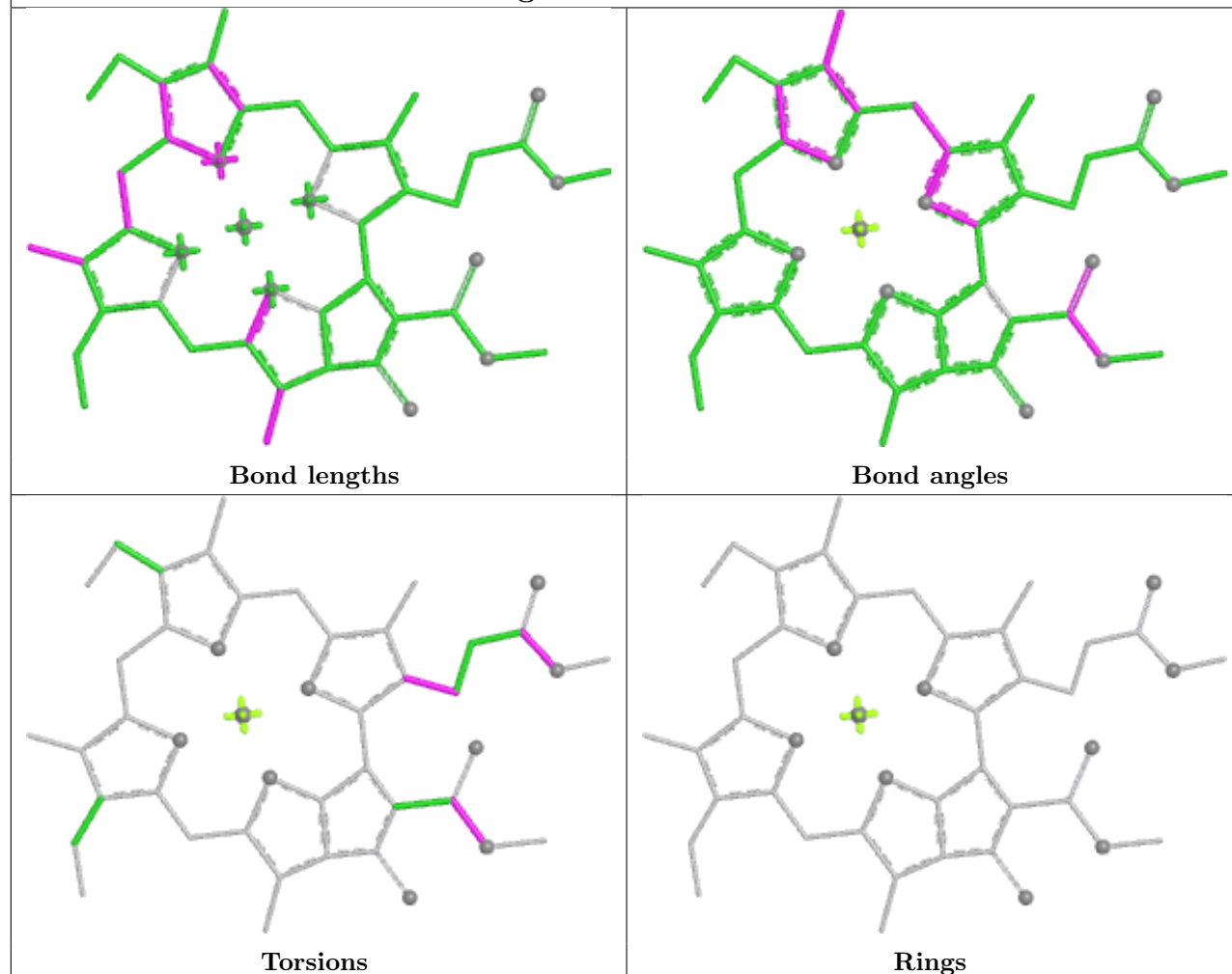


Ligand CHL 2 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4011	
 Bond lengths	 Bond angles
 Torsions	 Rings

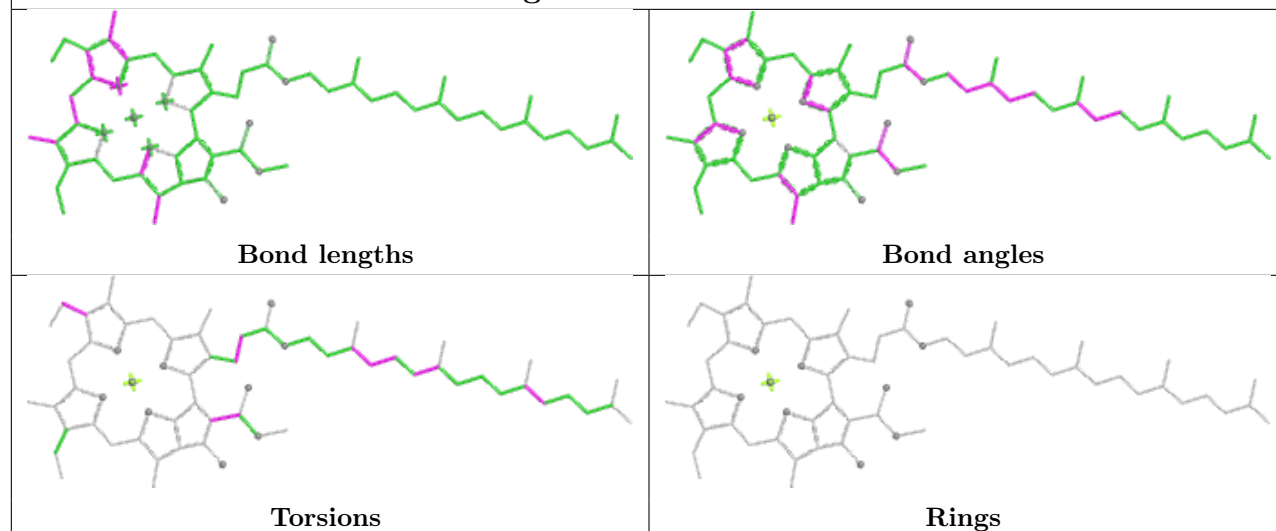
Ligand CLA 2 604

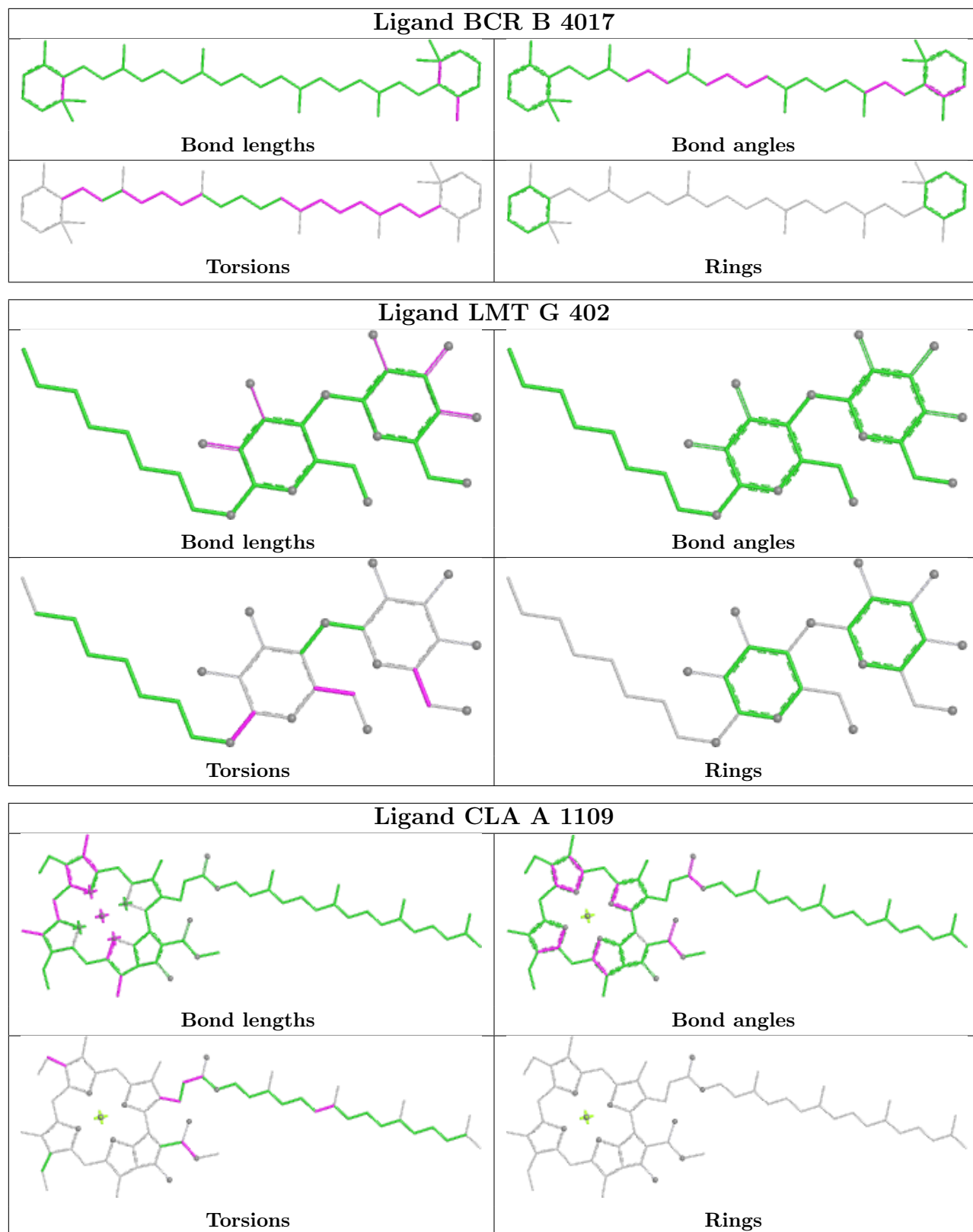


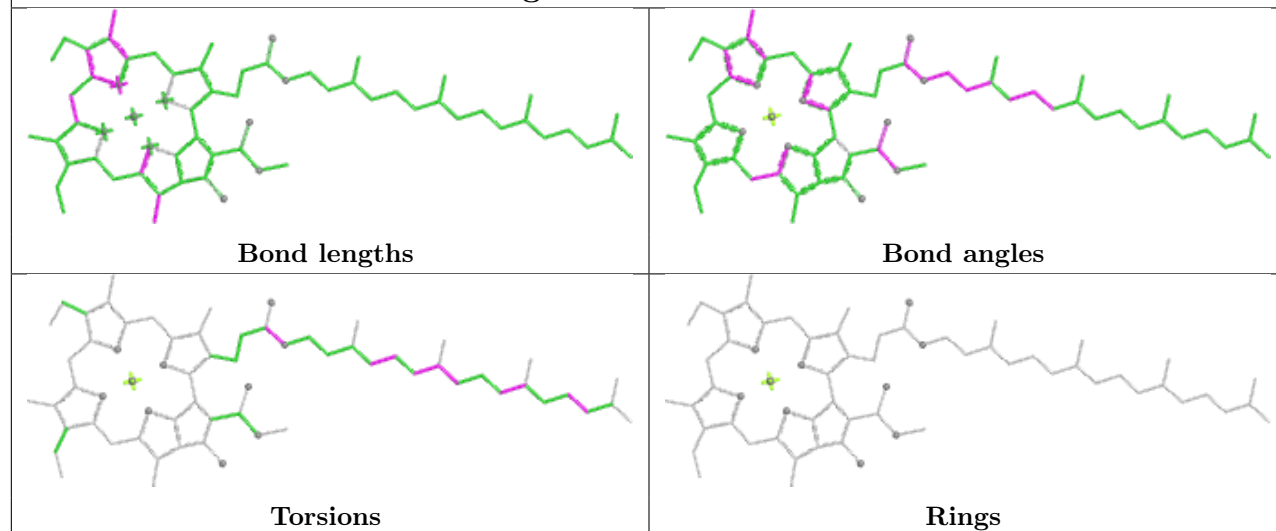
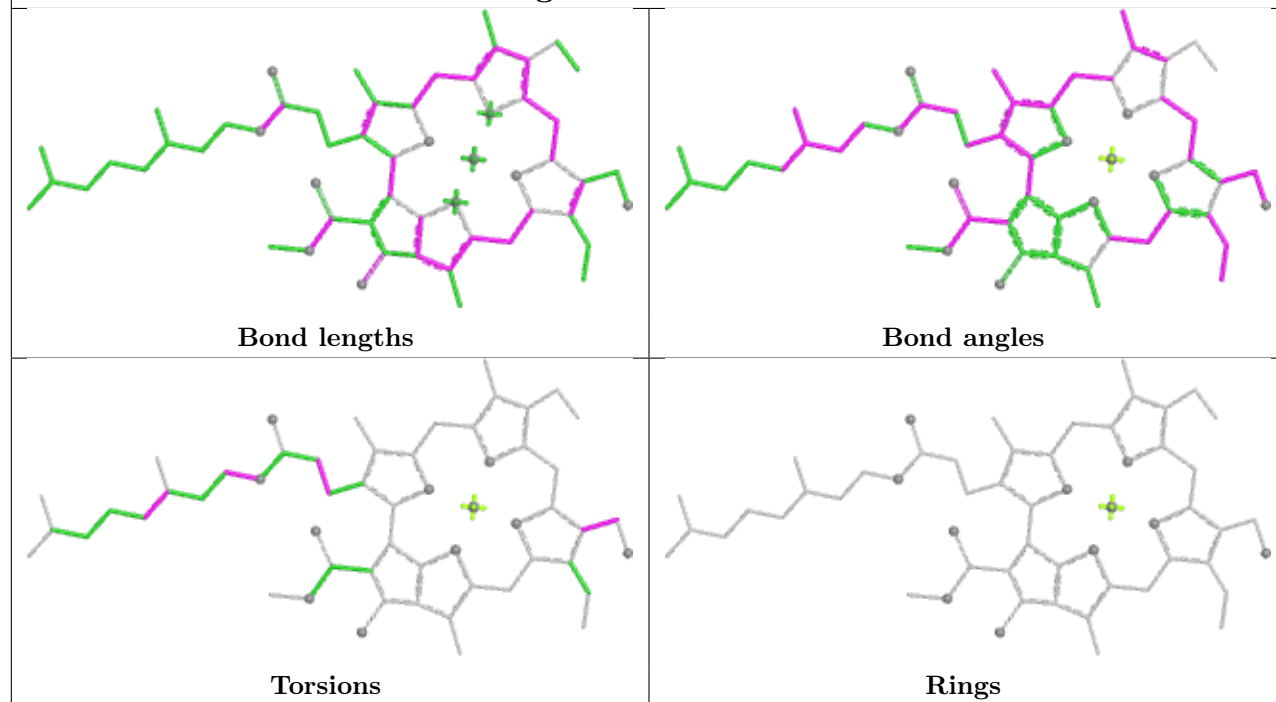
Ligand CLA 3 617



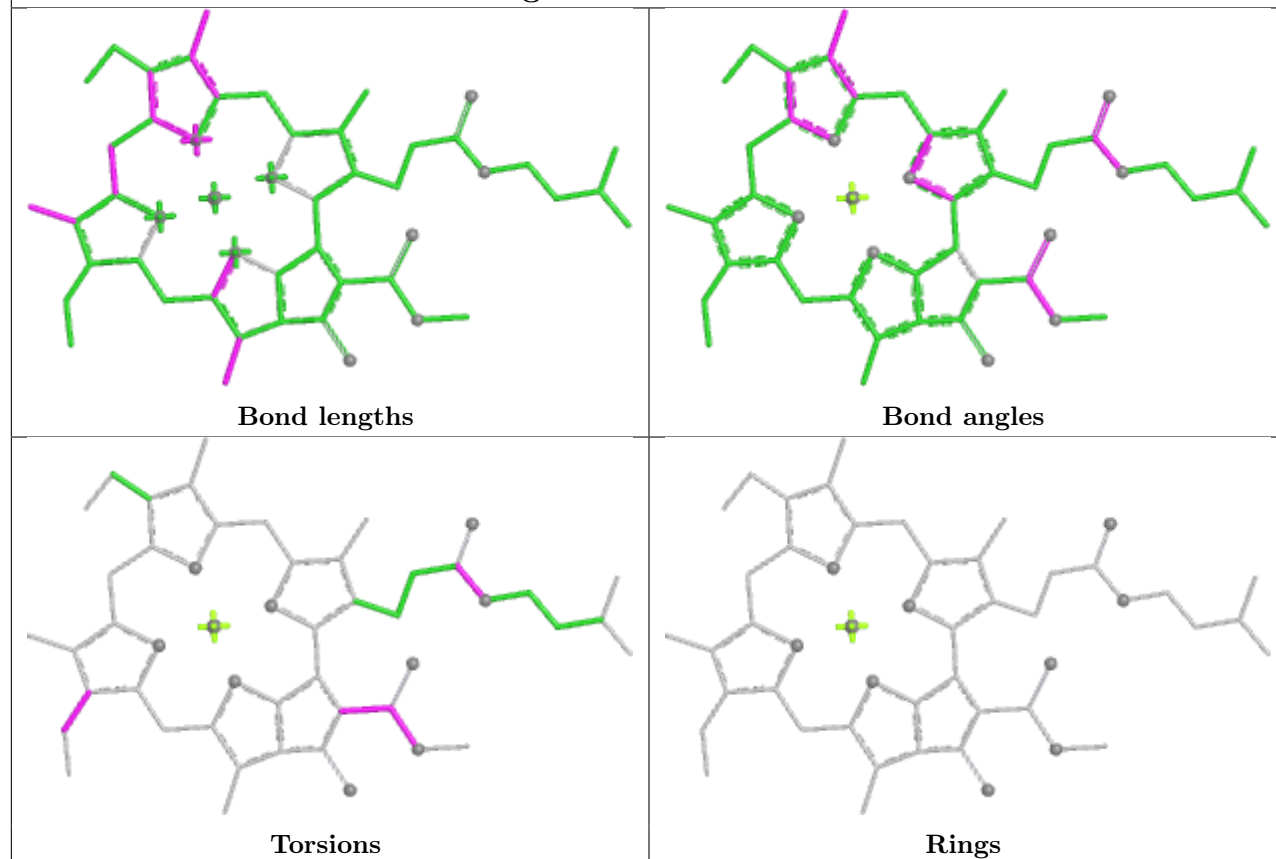
Ligand CLA B 1205



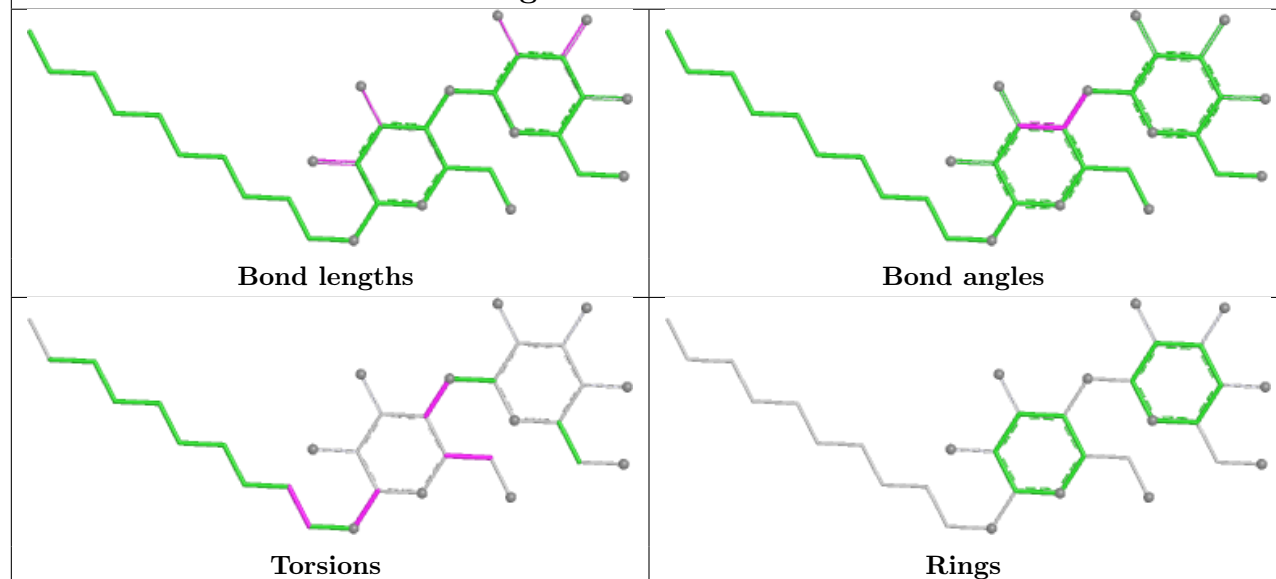


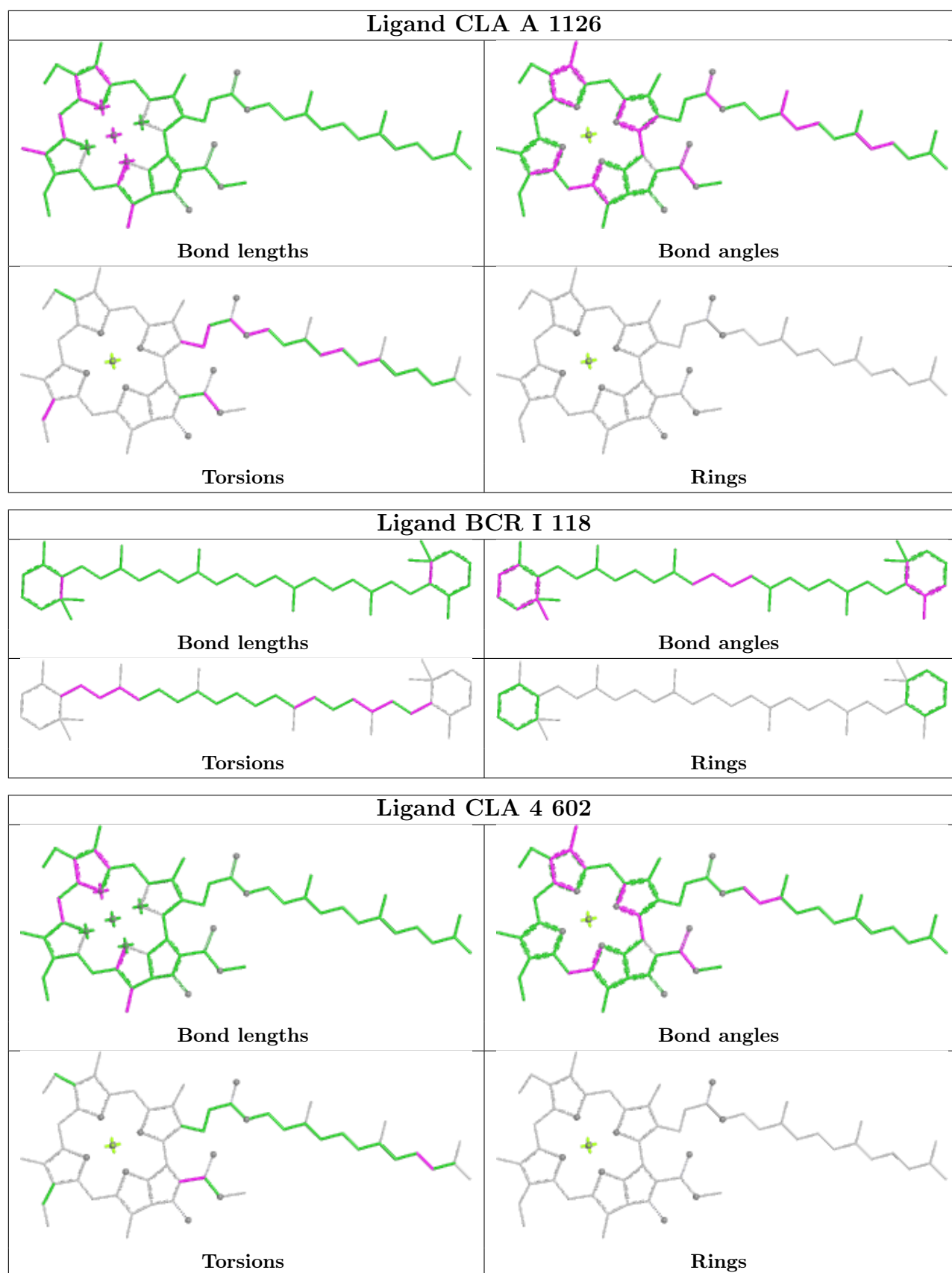
Ligand CLA A 1136**Ligand CHL 2 611**

Ligand CLA A 1801

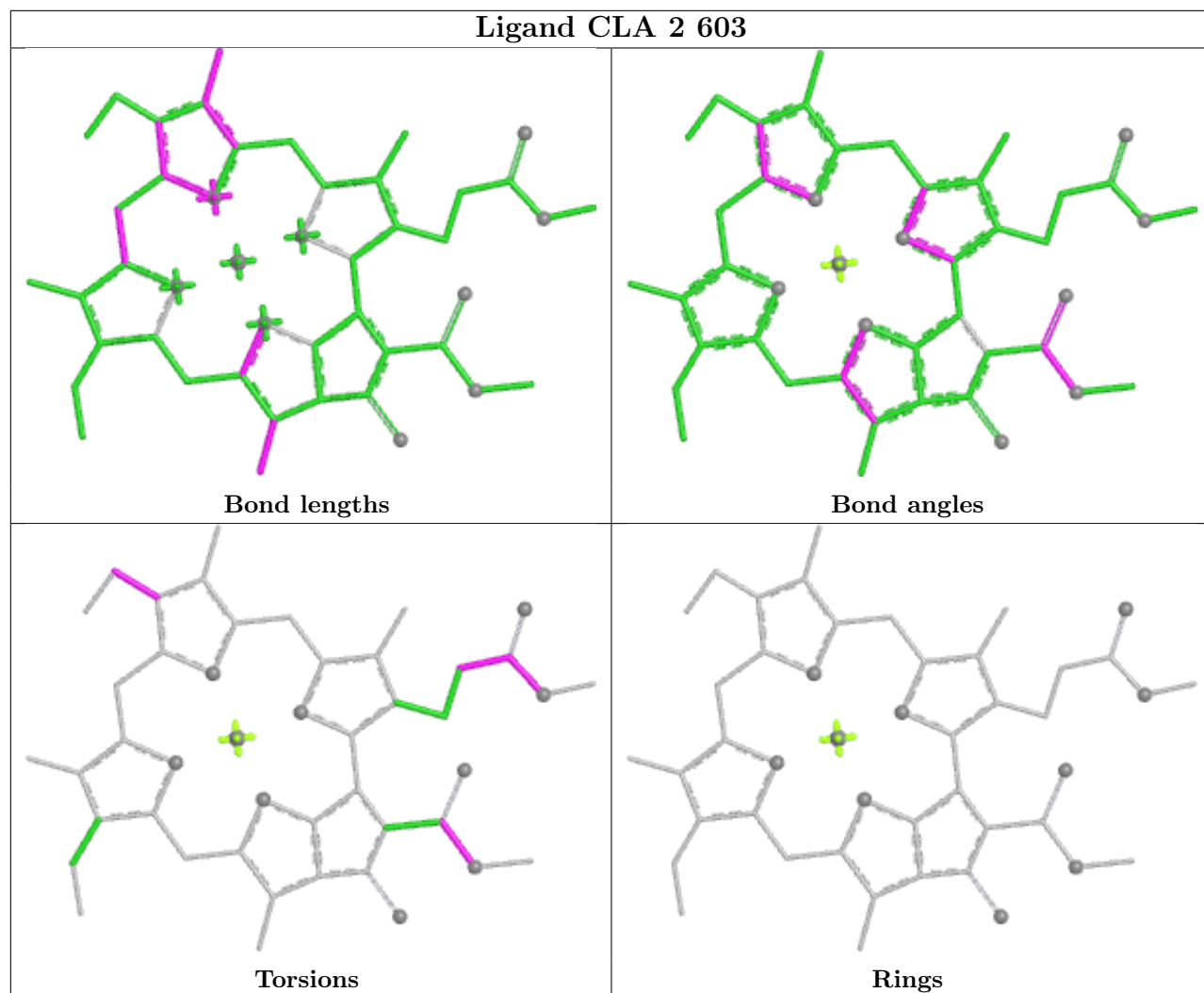


Ligand LMT A 5004

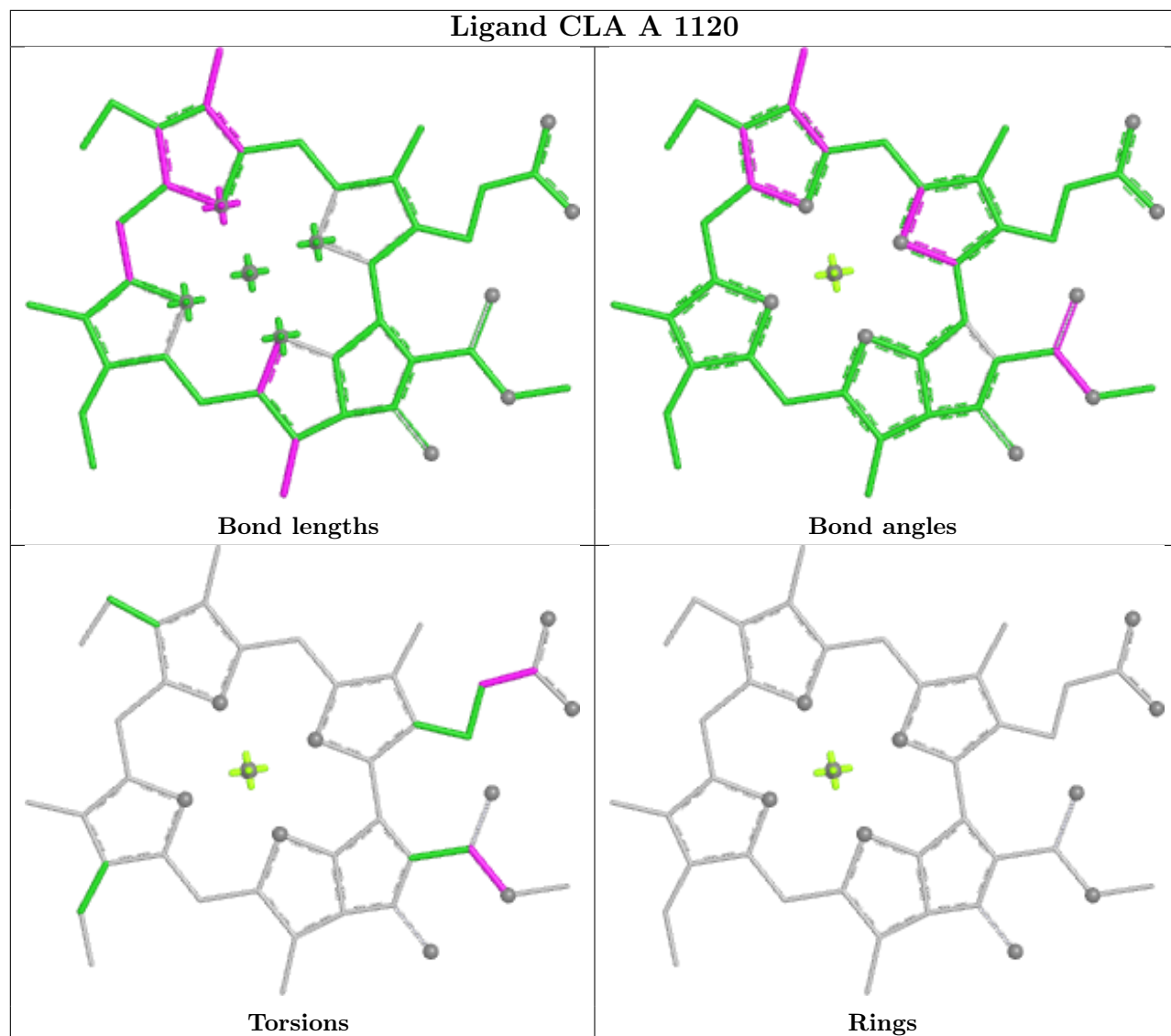




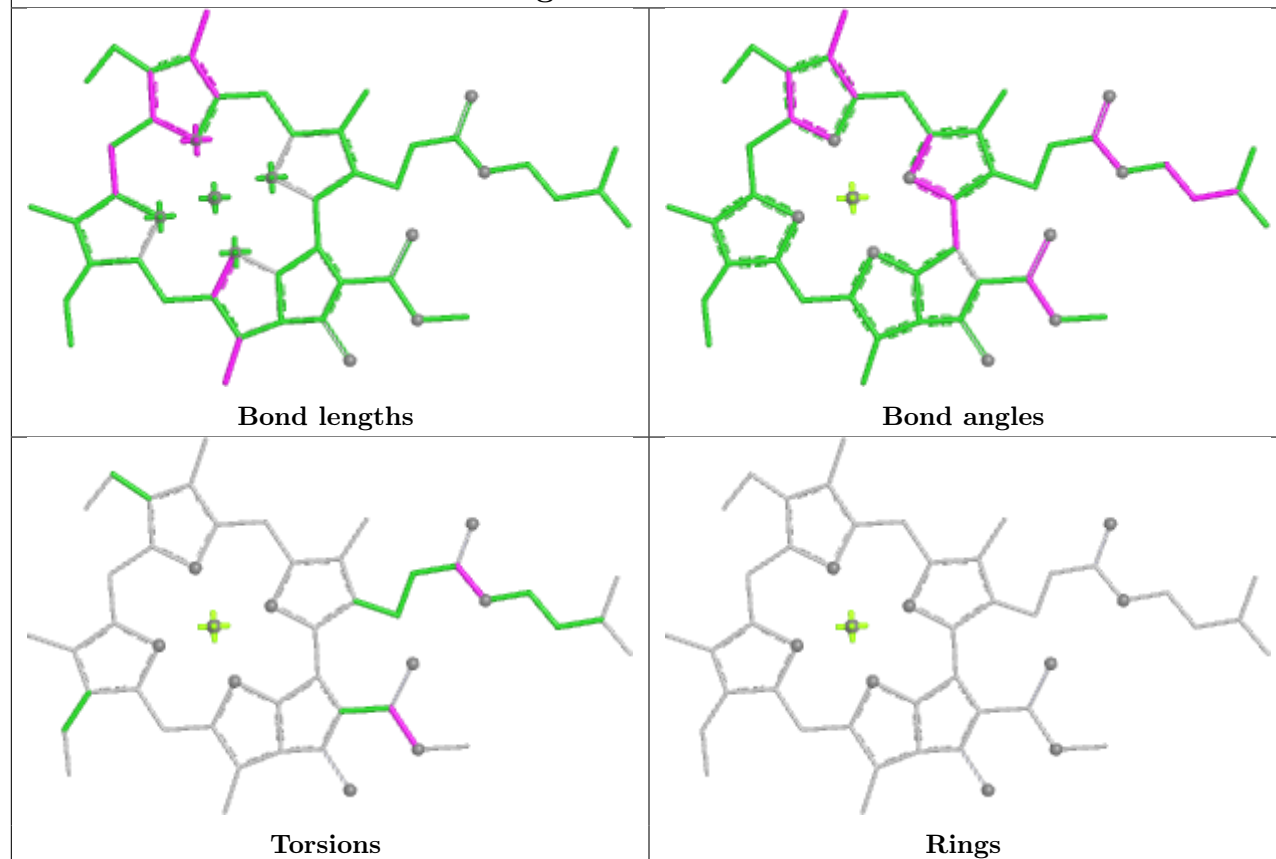
Ligand CLA 2 603



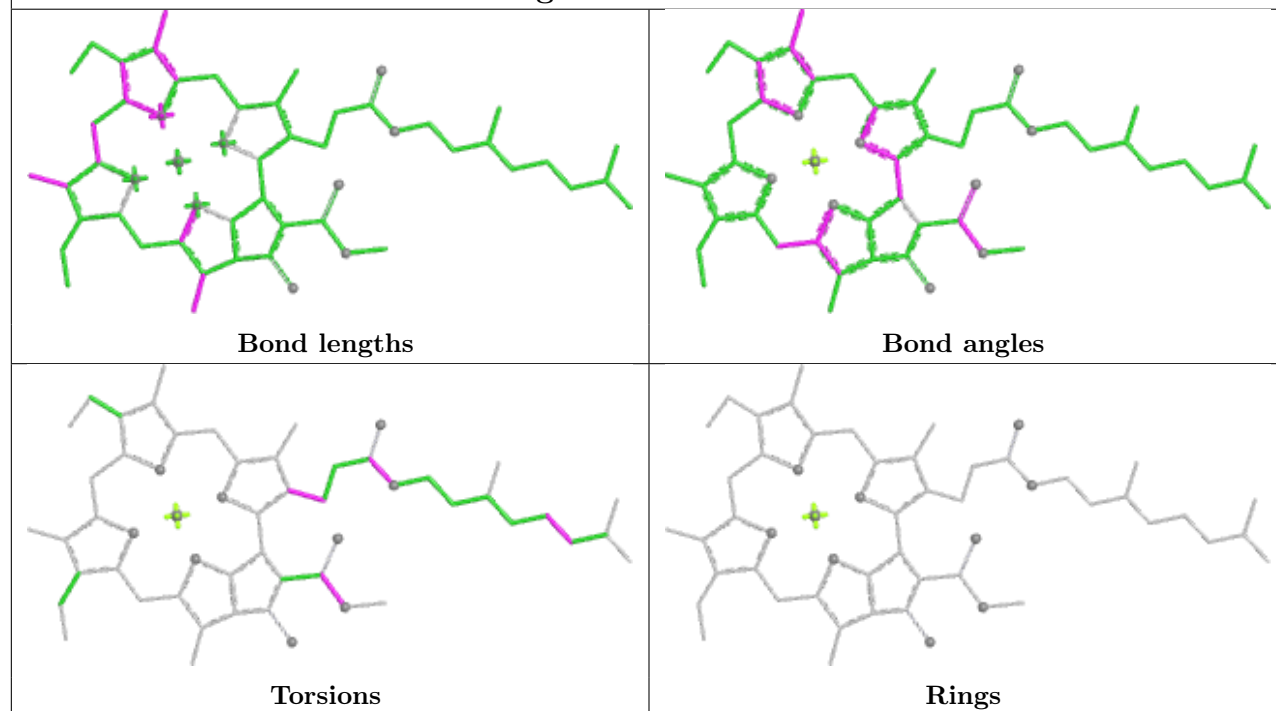
Ligand CLA A 1120

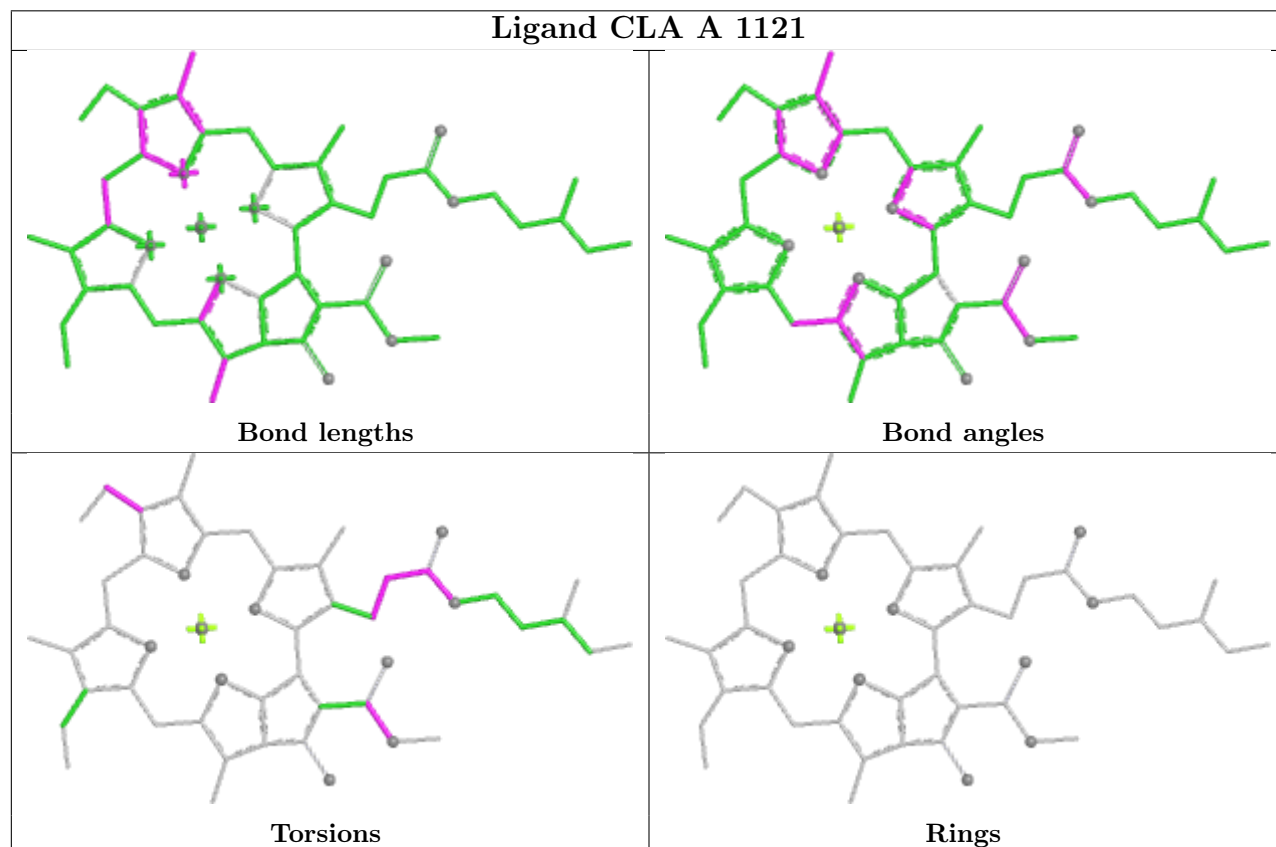
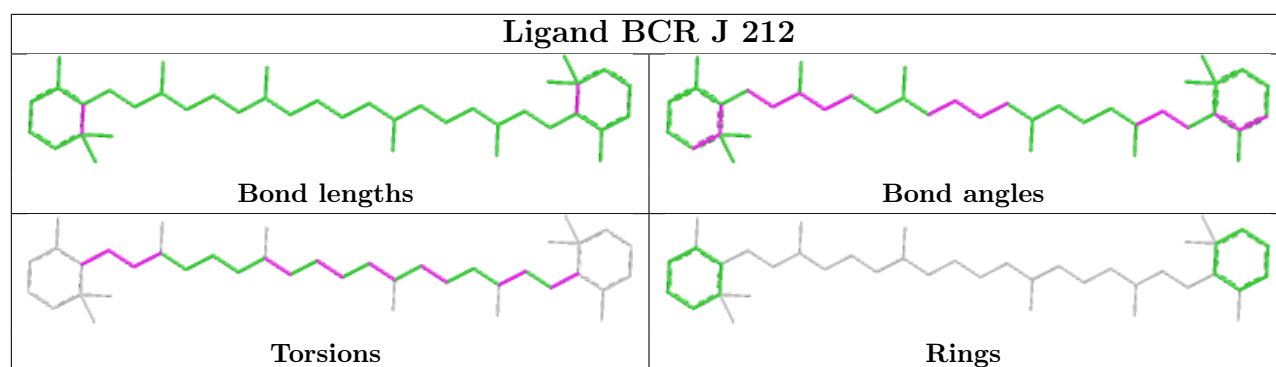


Ligand CLA 1 604

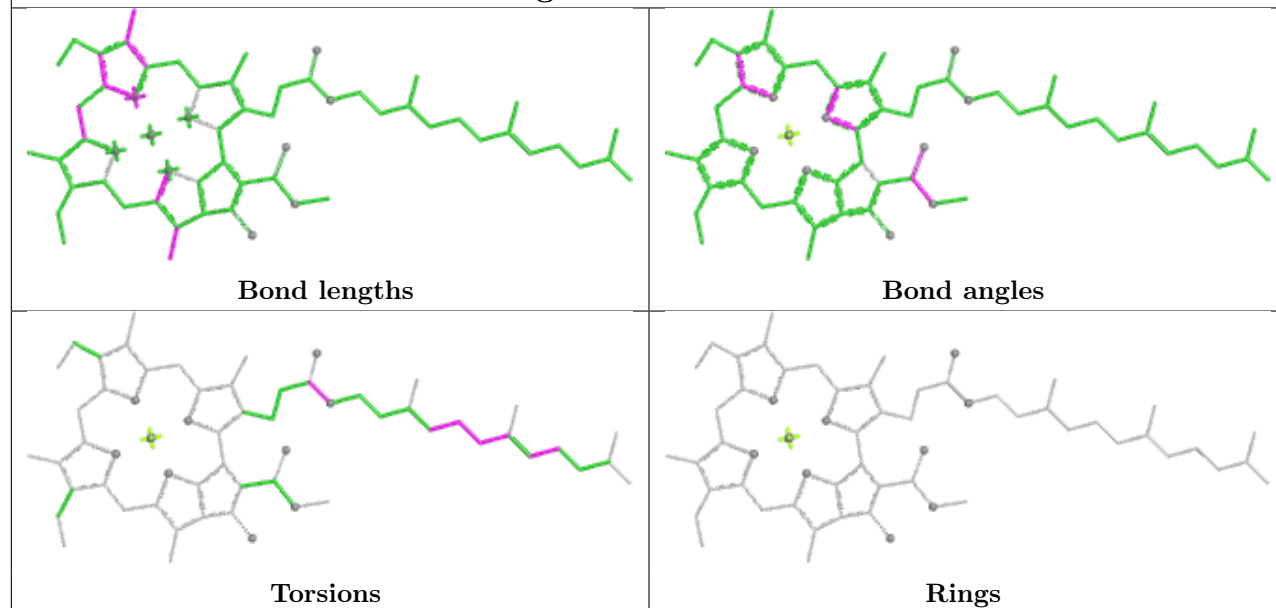


Ligand CLA 4 611

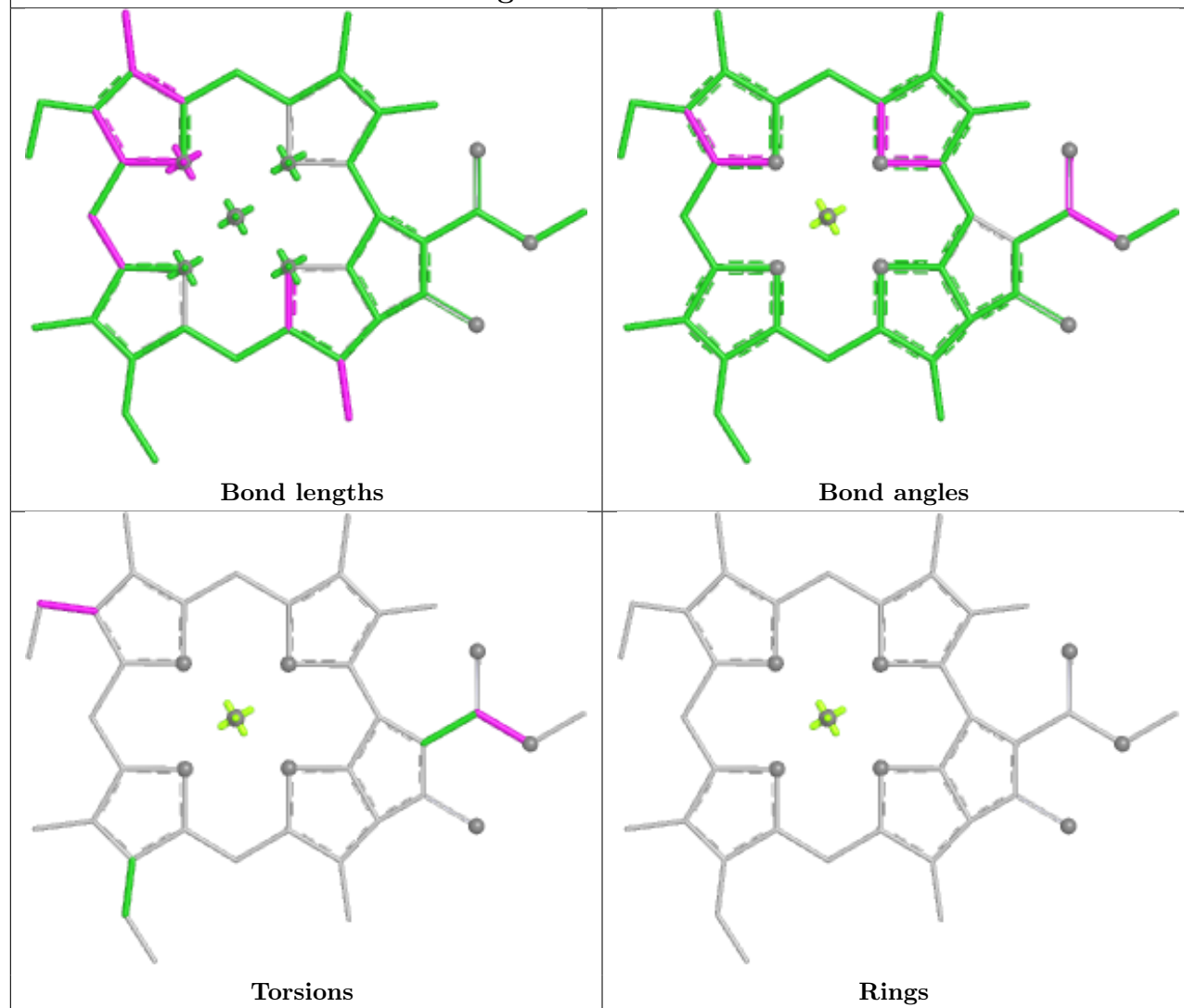


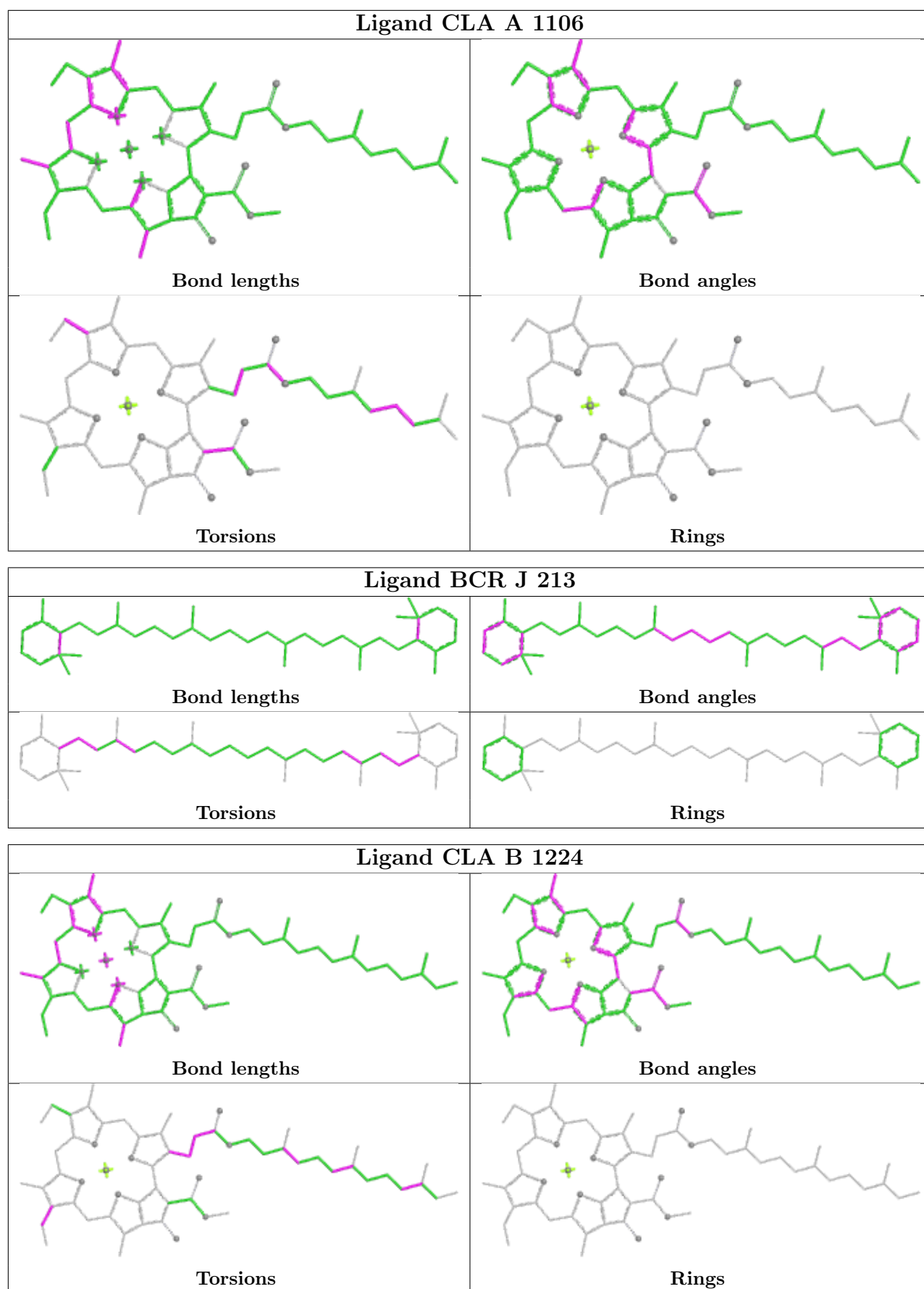


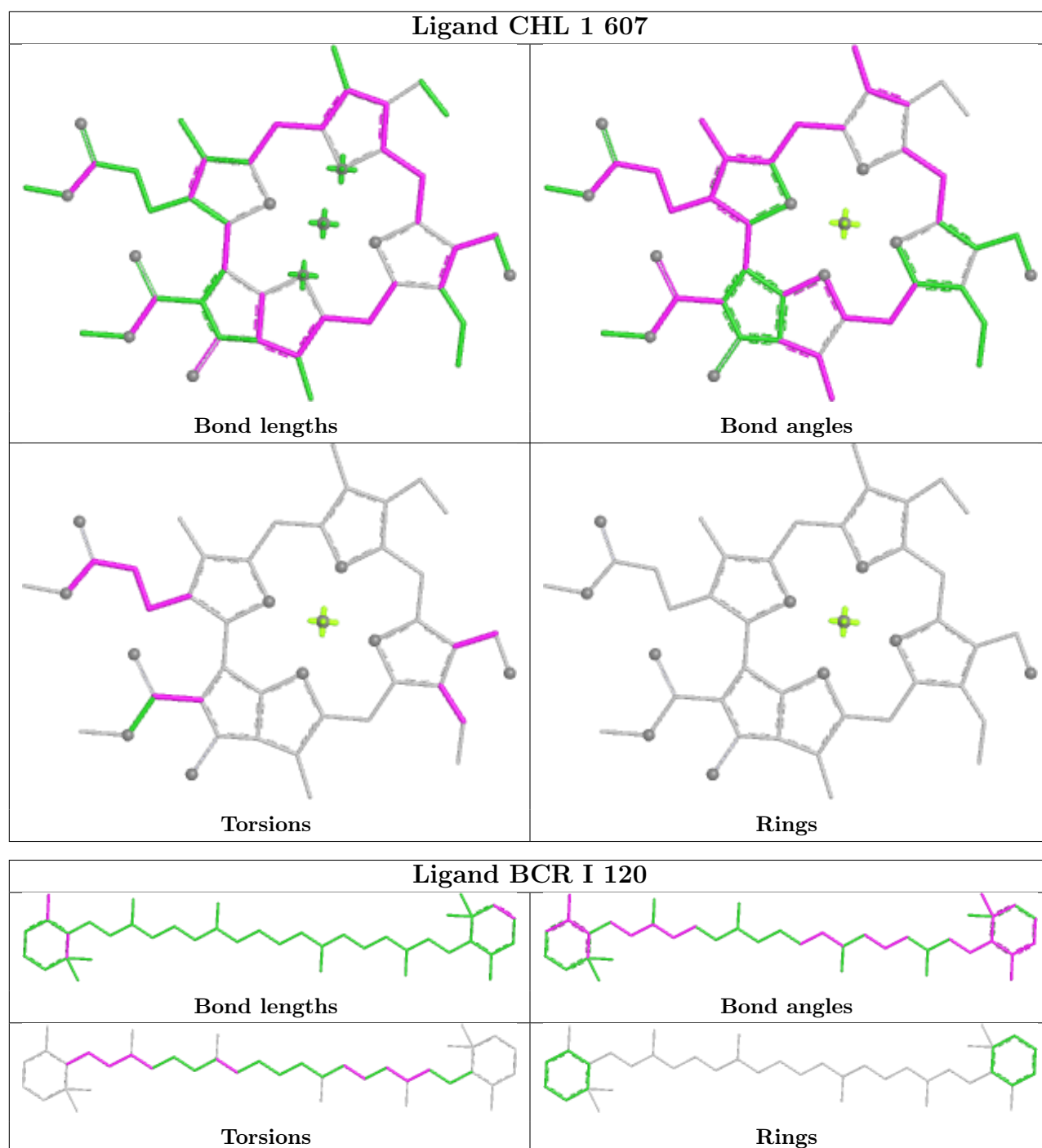
Ligand CLA 1 609

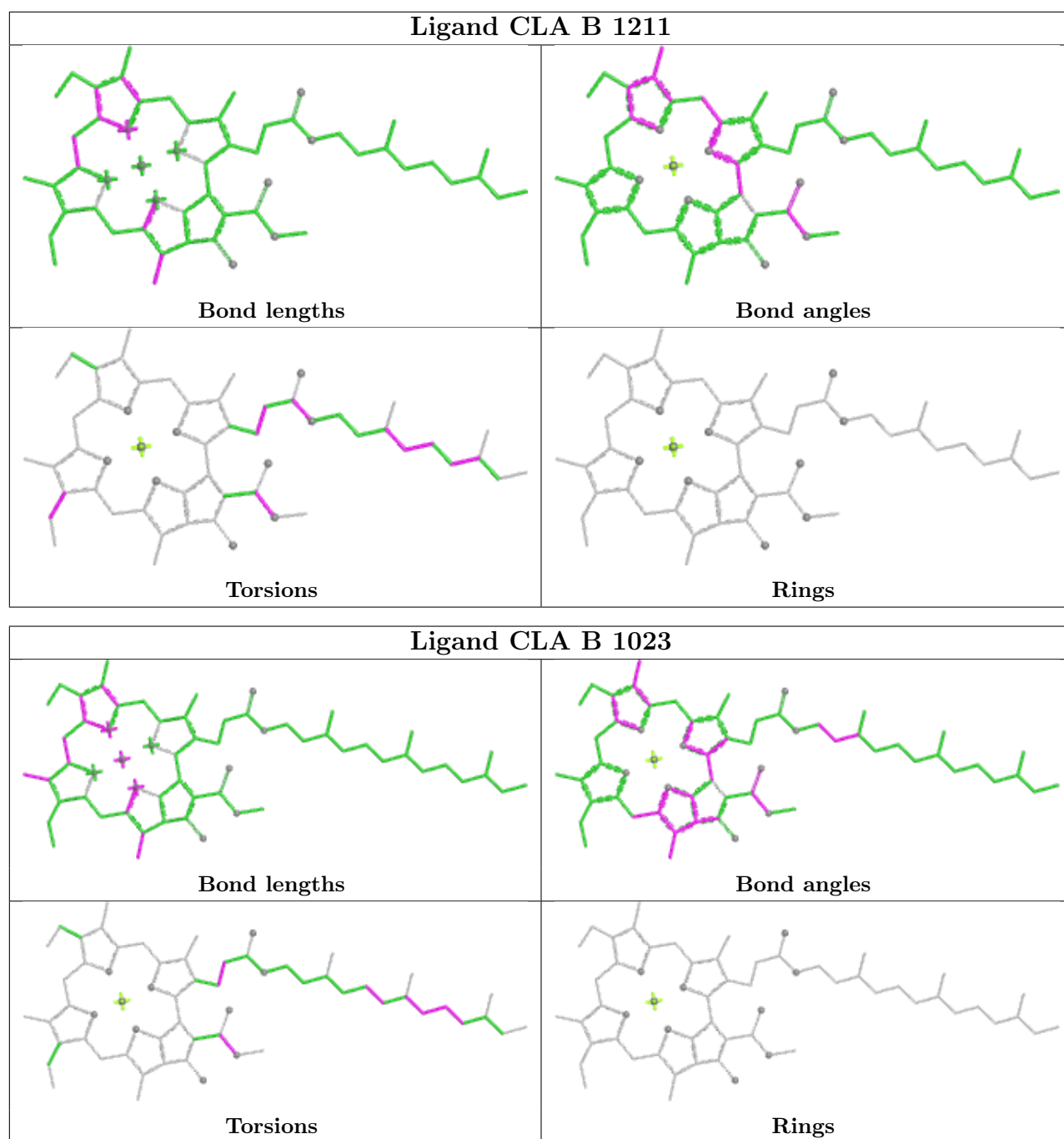


Ligand CLA 3 611

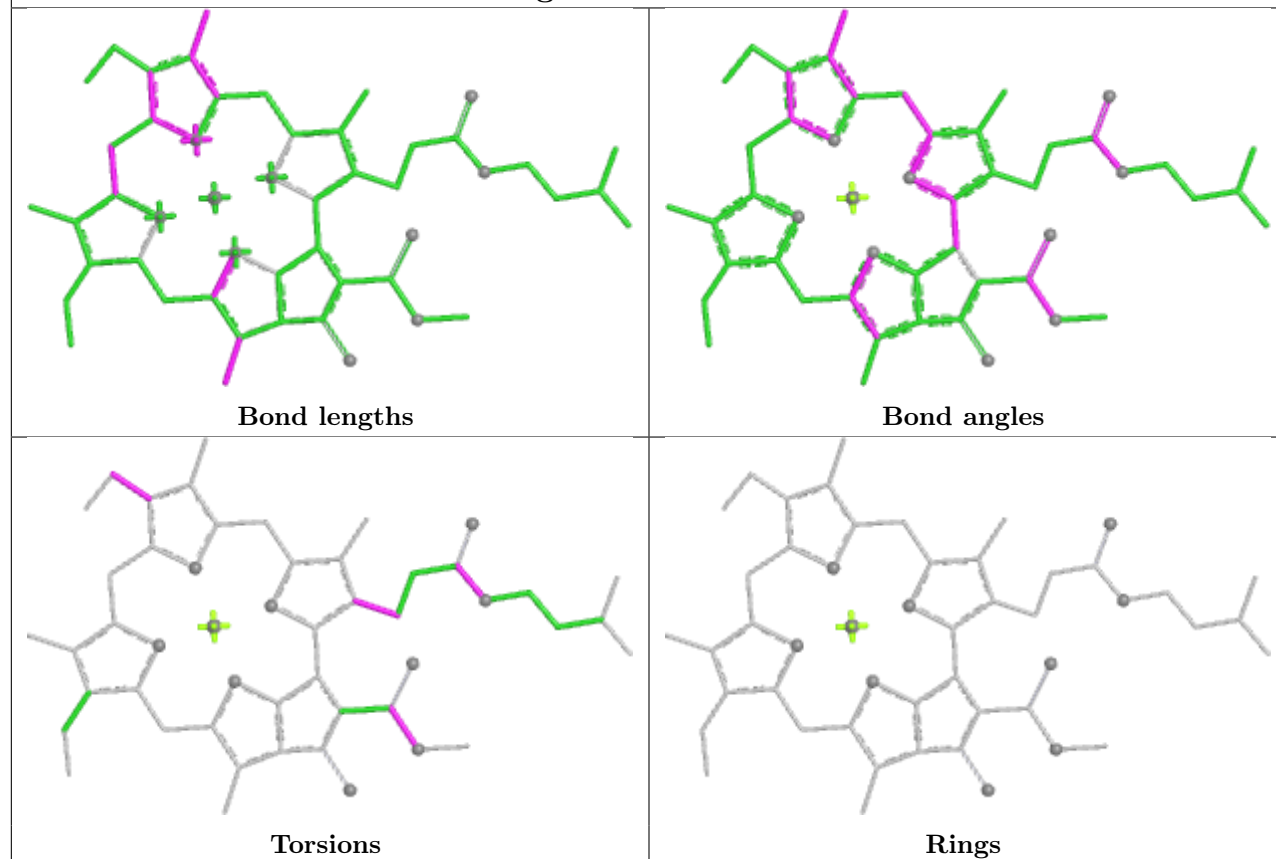




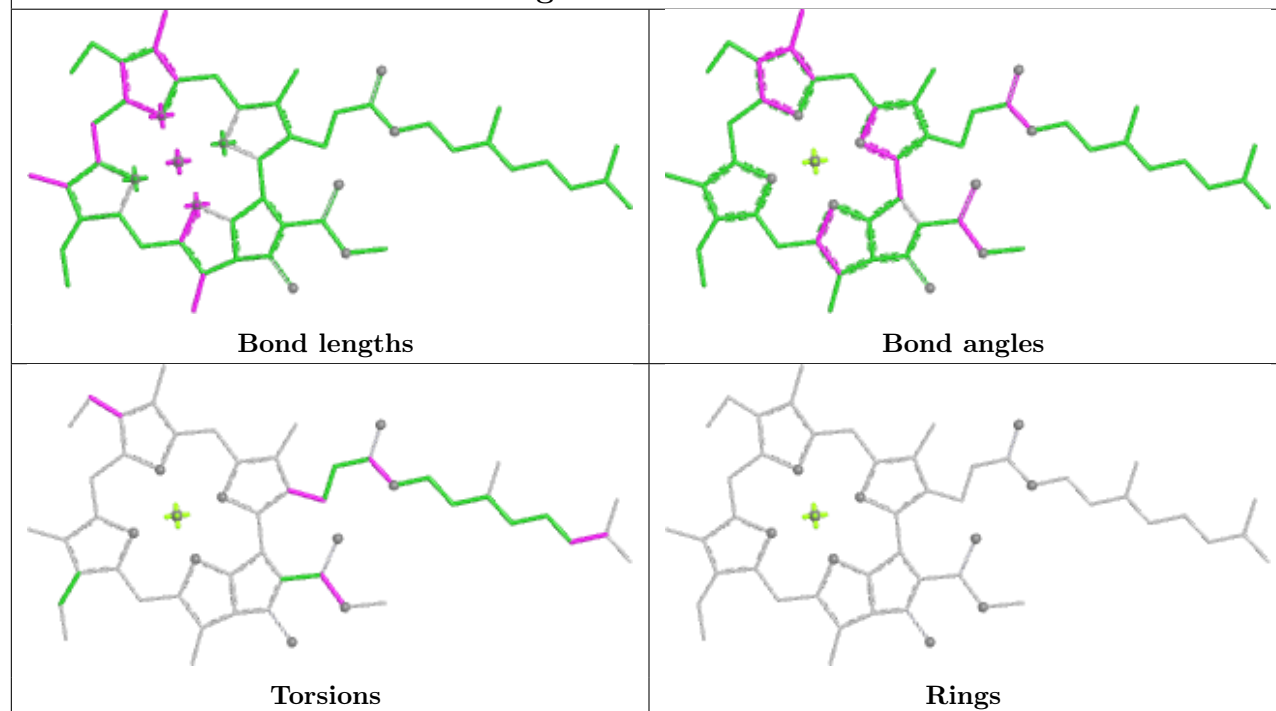




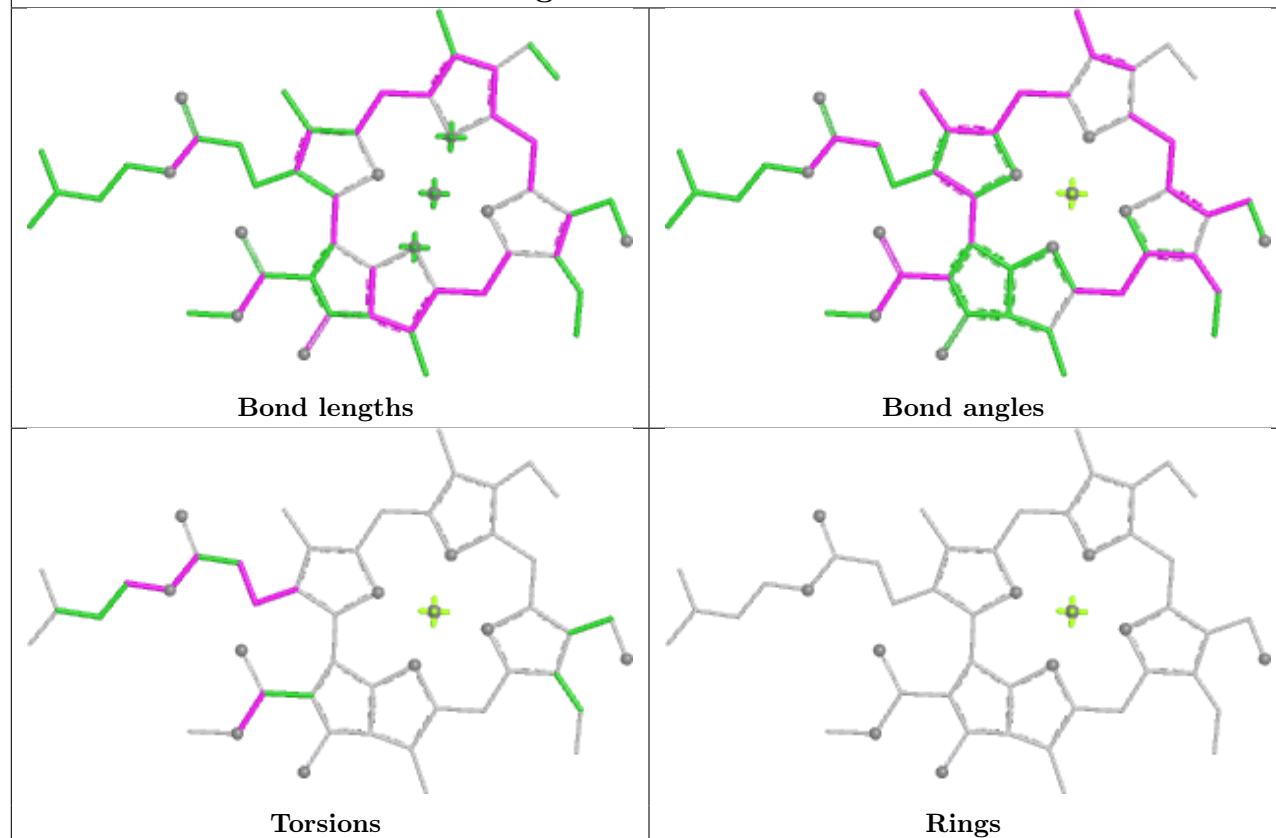
Ligand CLA 3 604



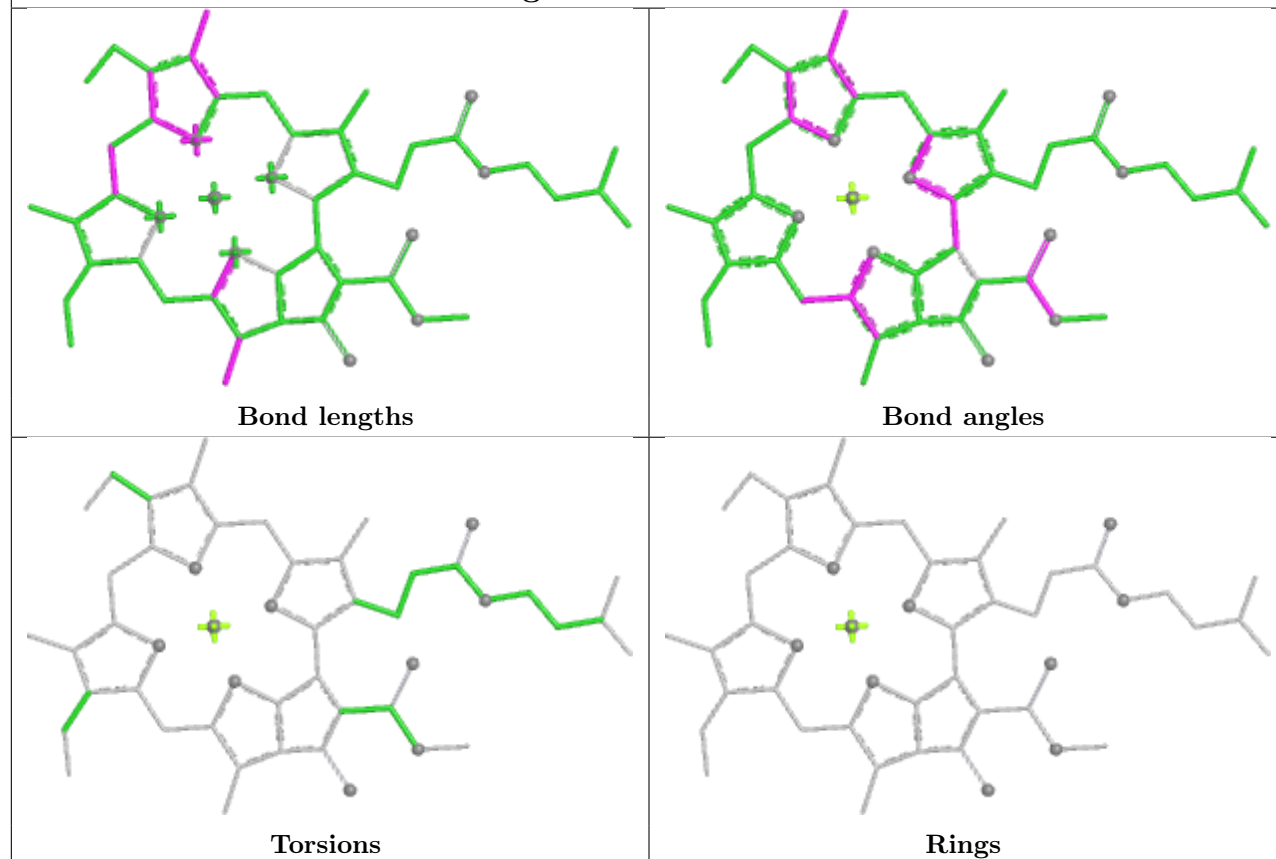
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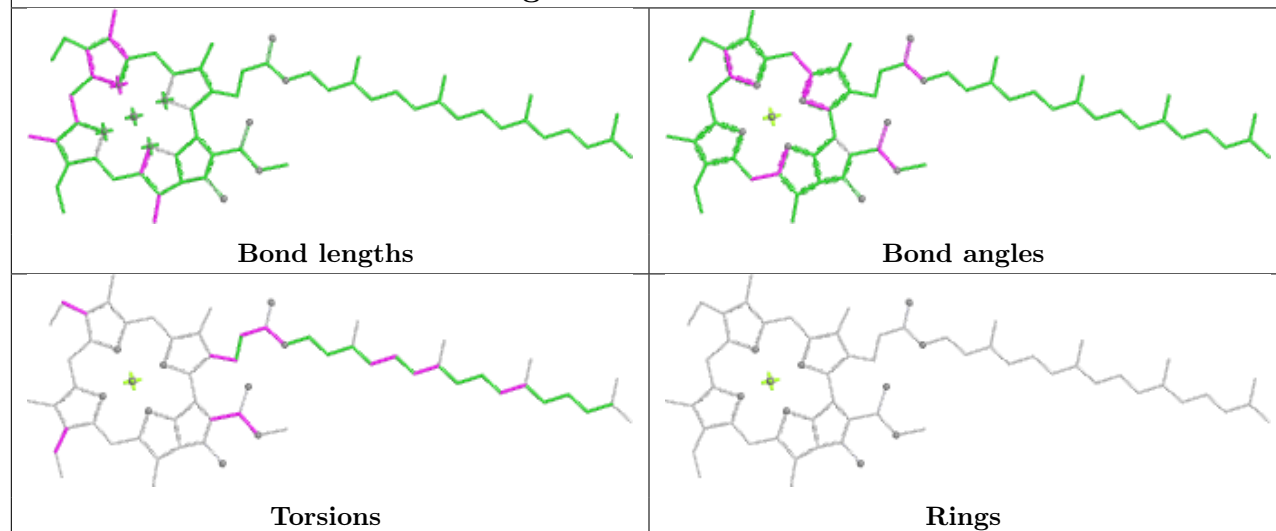
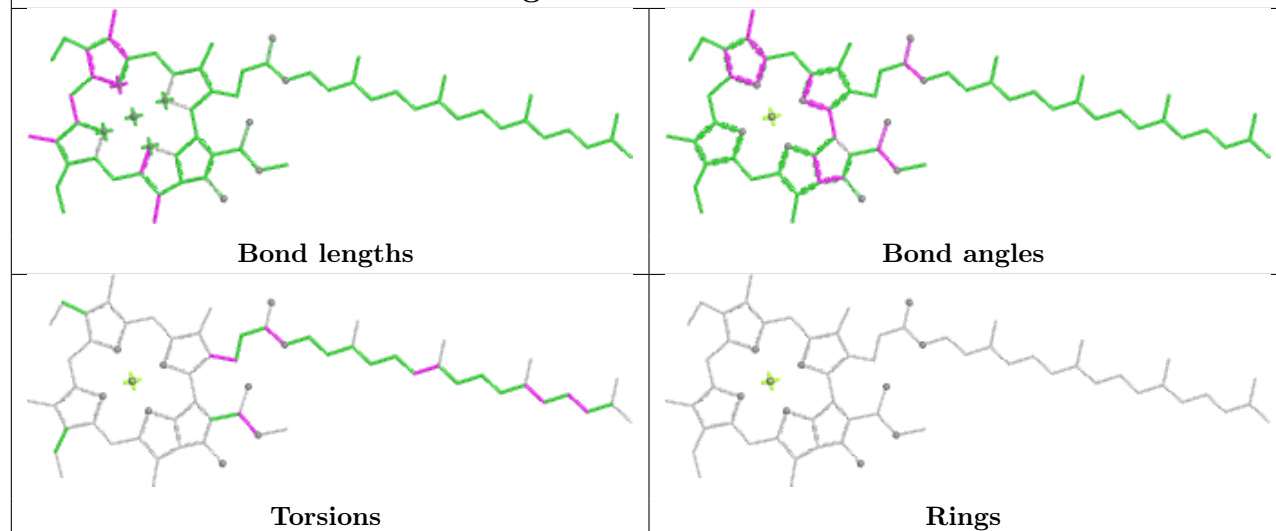


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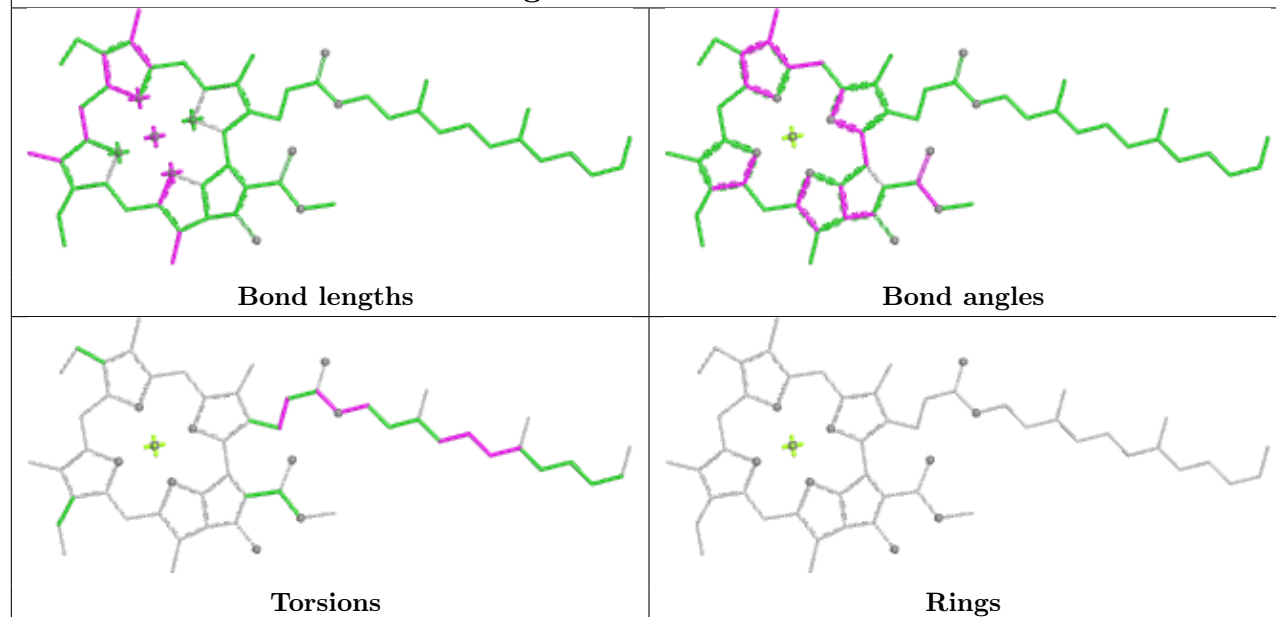


Ligand CLA A 1105

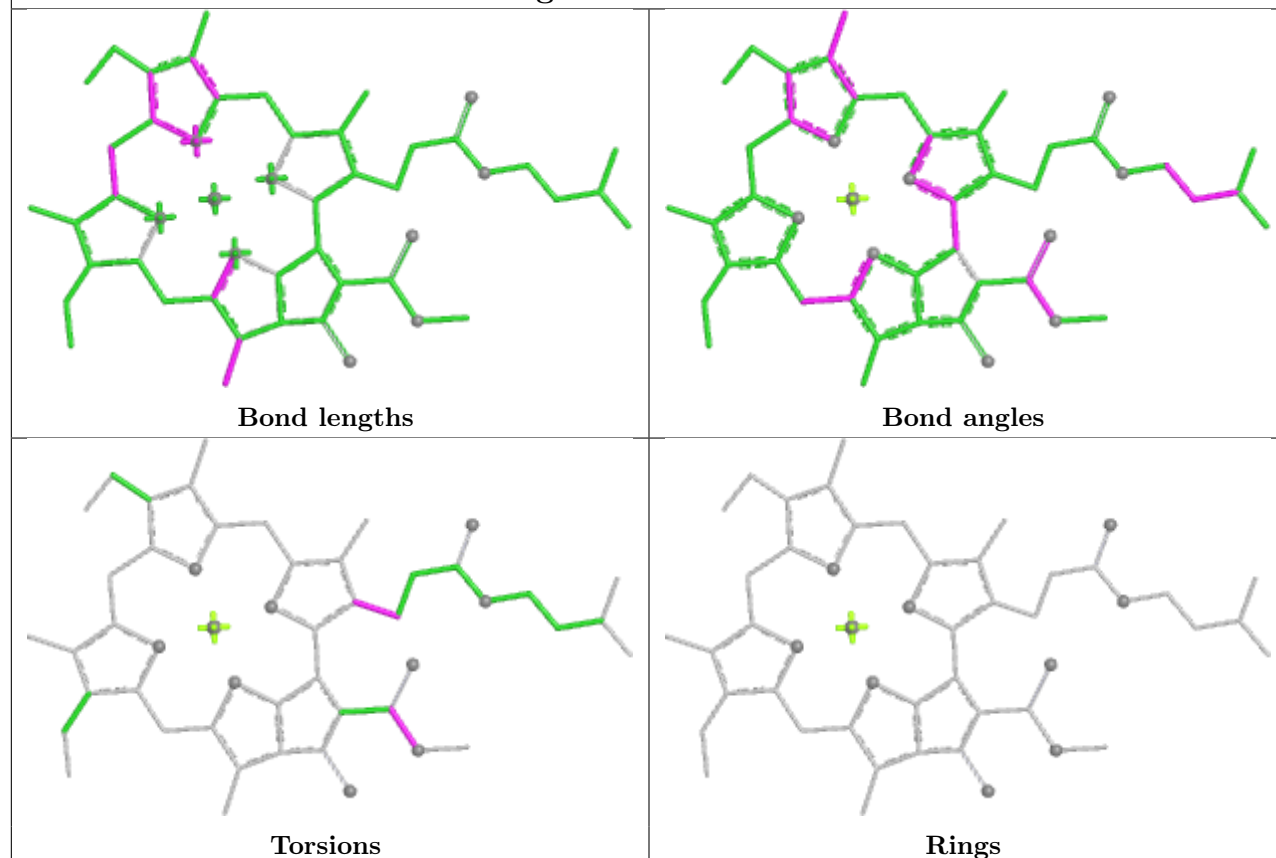


Ligand CLA A 1103**Ligand CLA A 1119**

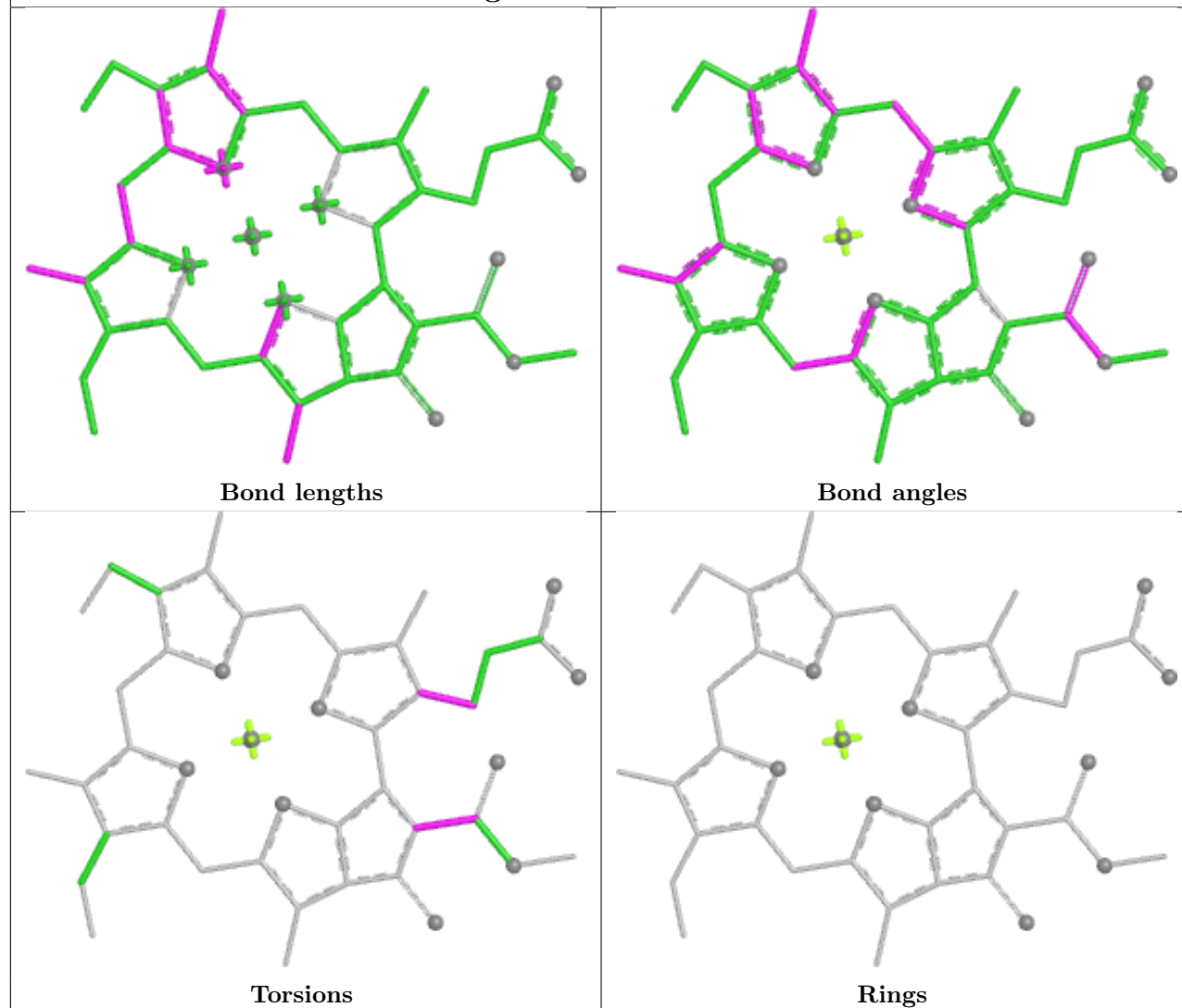
Ligand CLA B 1214



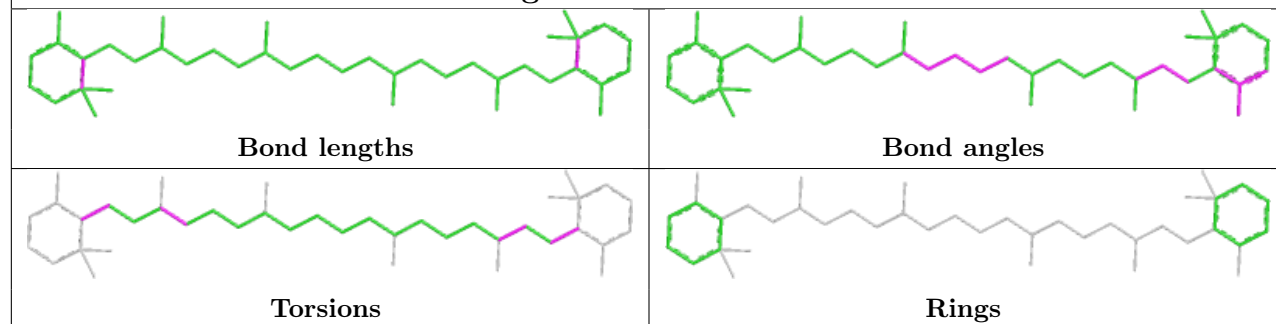
Ligand CLA 1 608

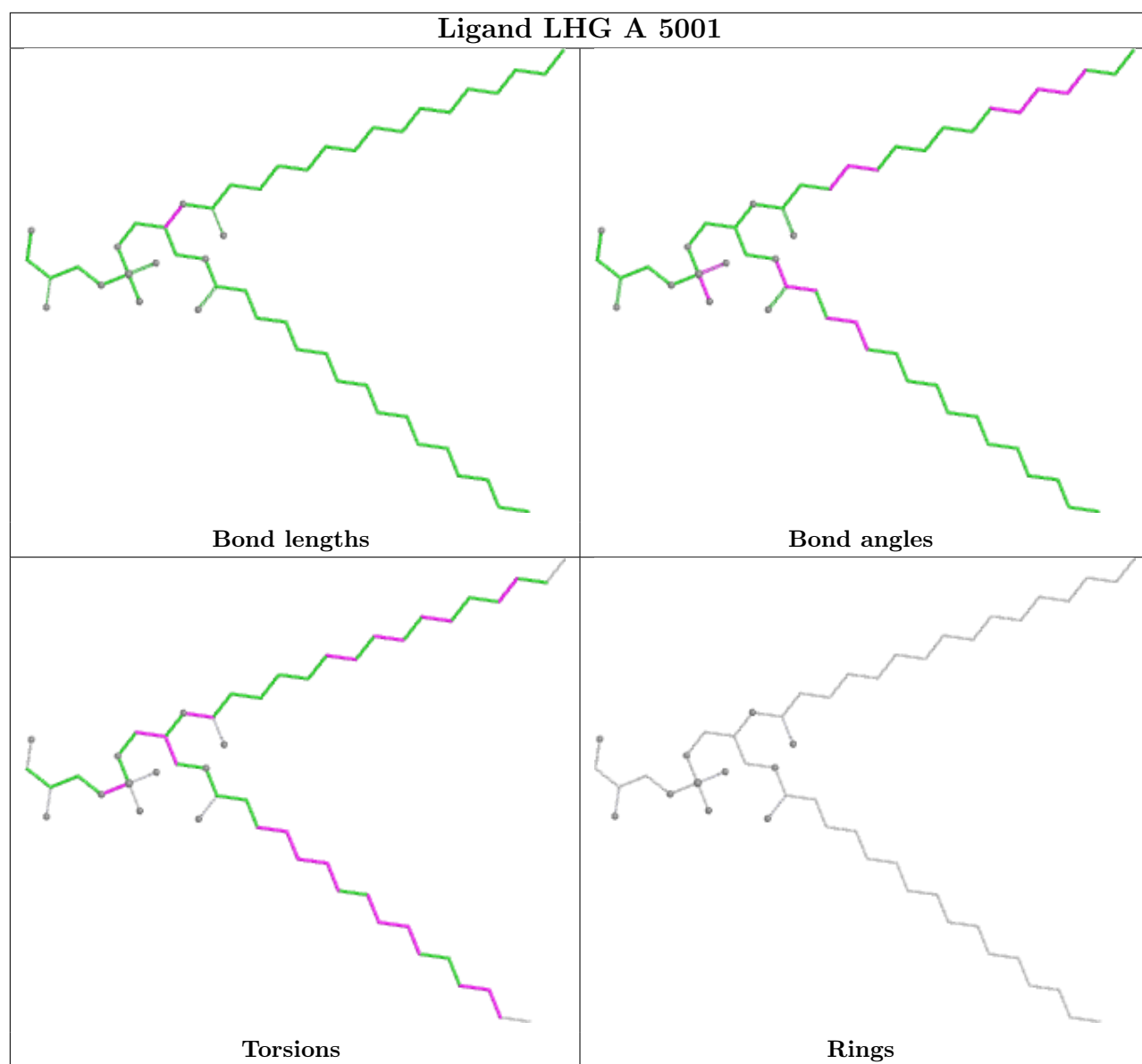


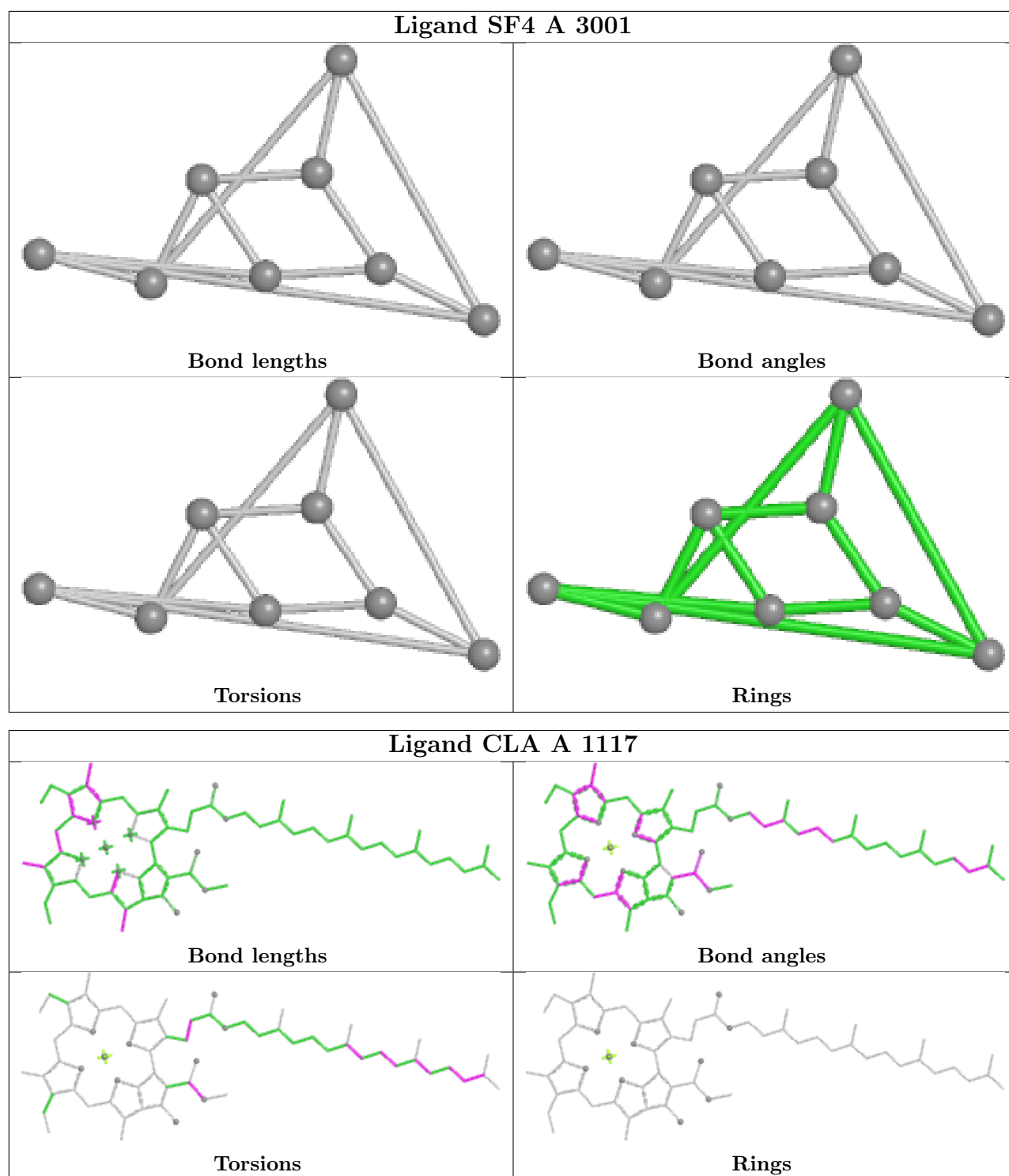
Ligand CLA B 1212

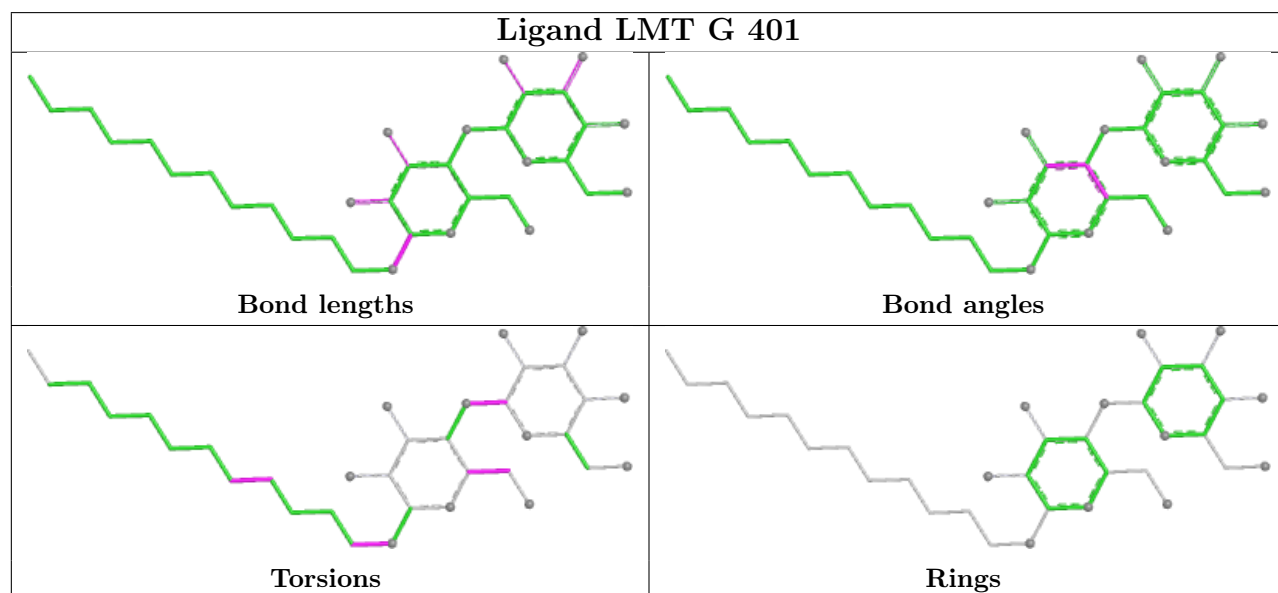
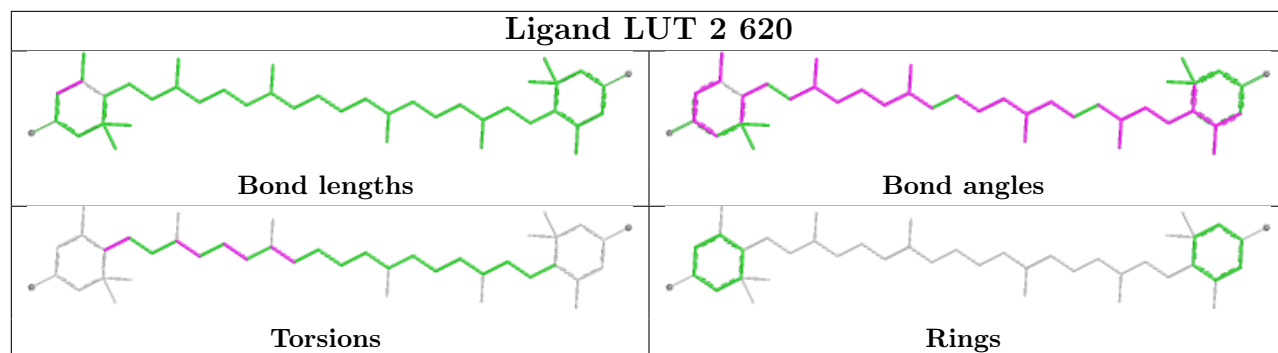


Ligand BCR B 4005

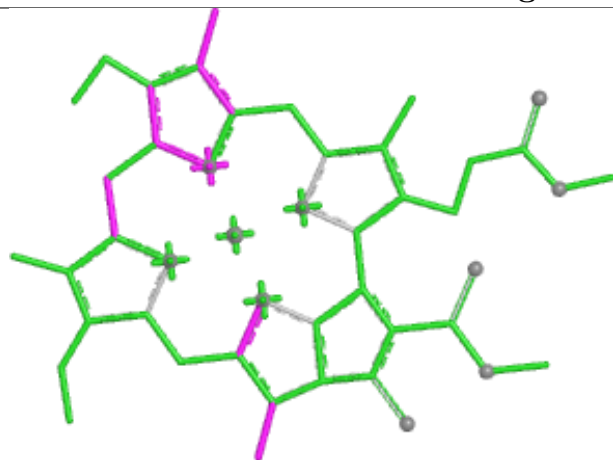




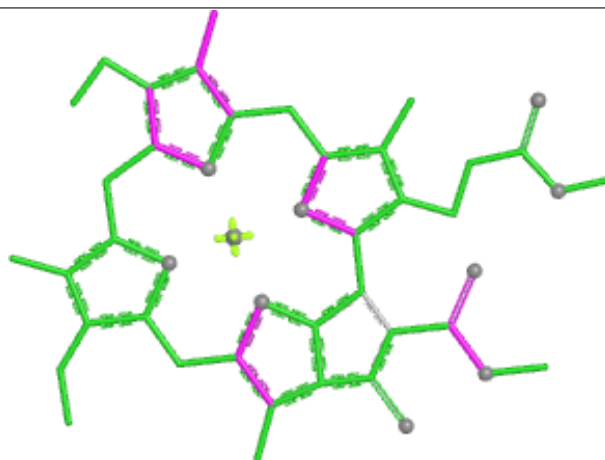




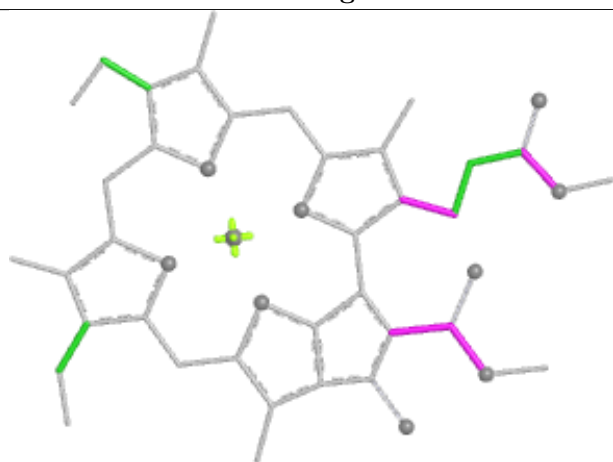
Ligand CLA 4 614



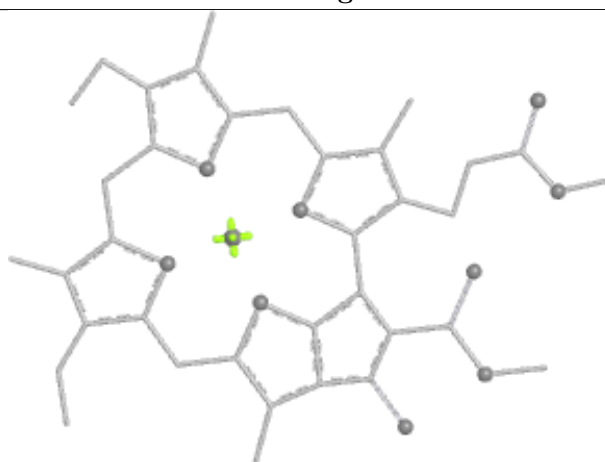
Bond lengths



Bond angles

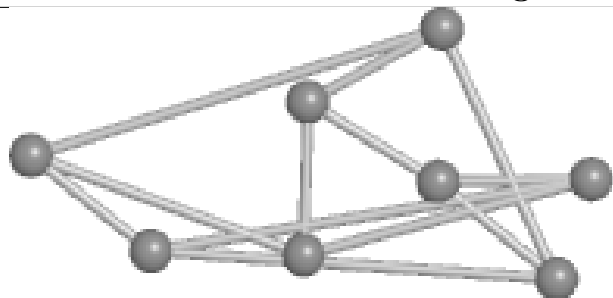


Torsions

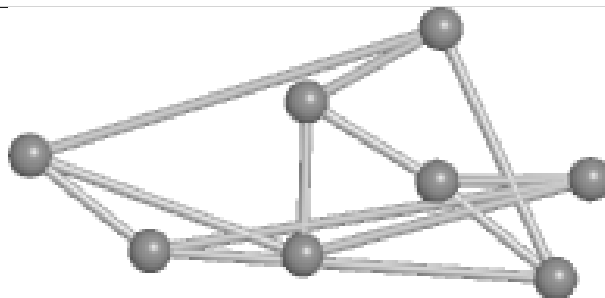


Rings

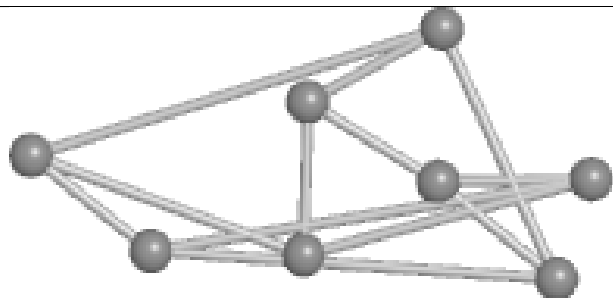
Ligand SF4 C 1002



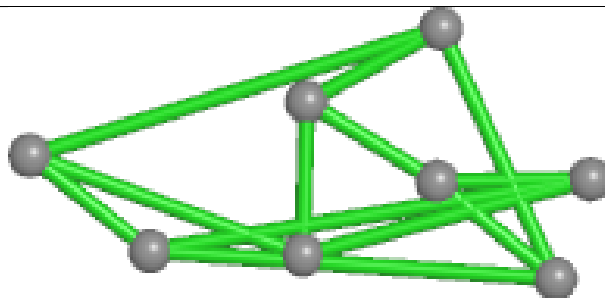
Bond lengths



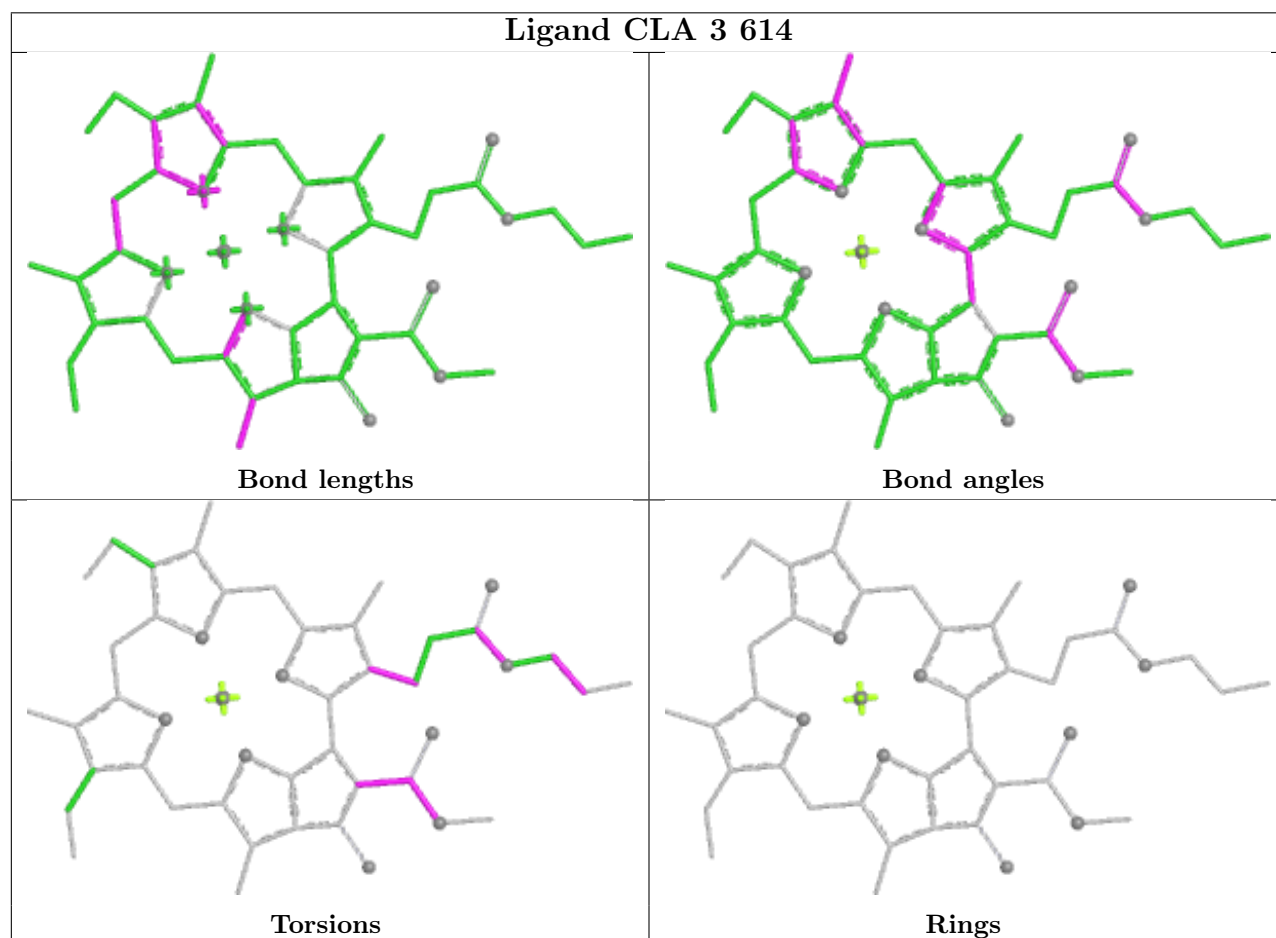
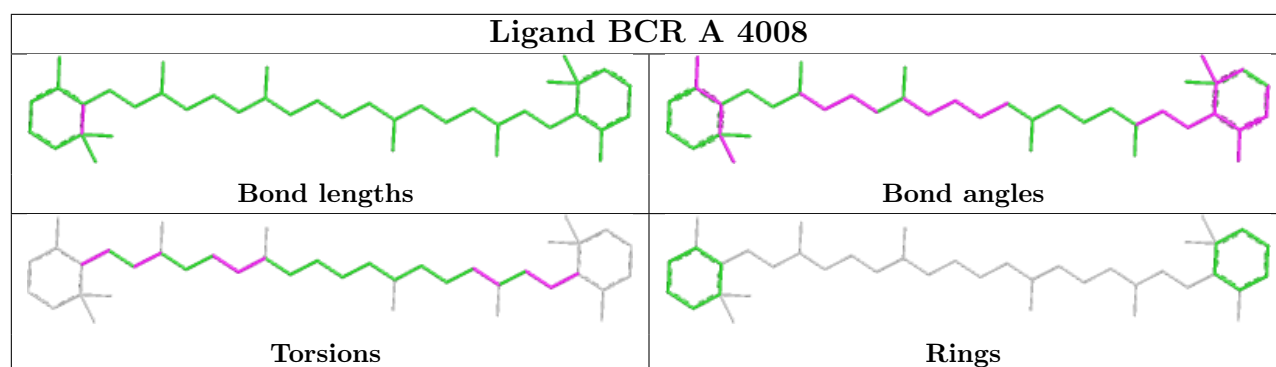
Bond angles

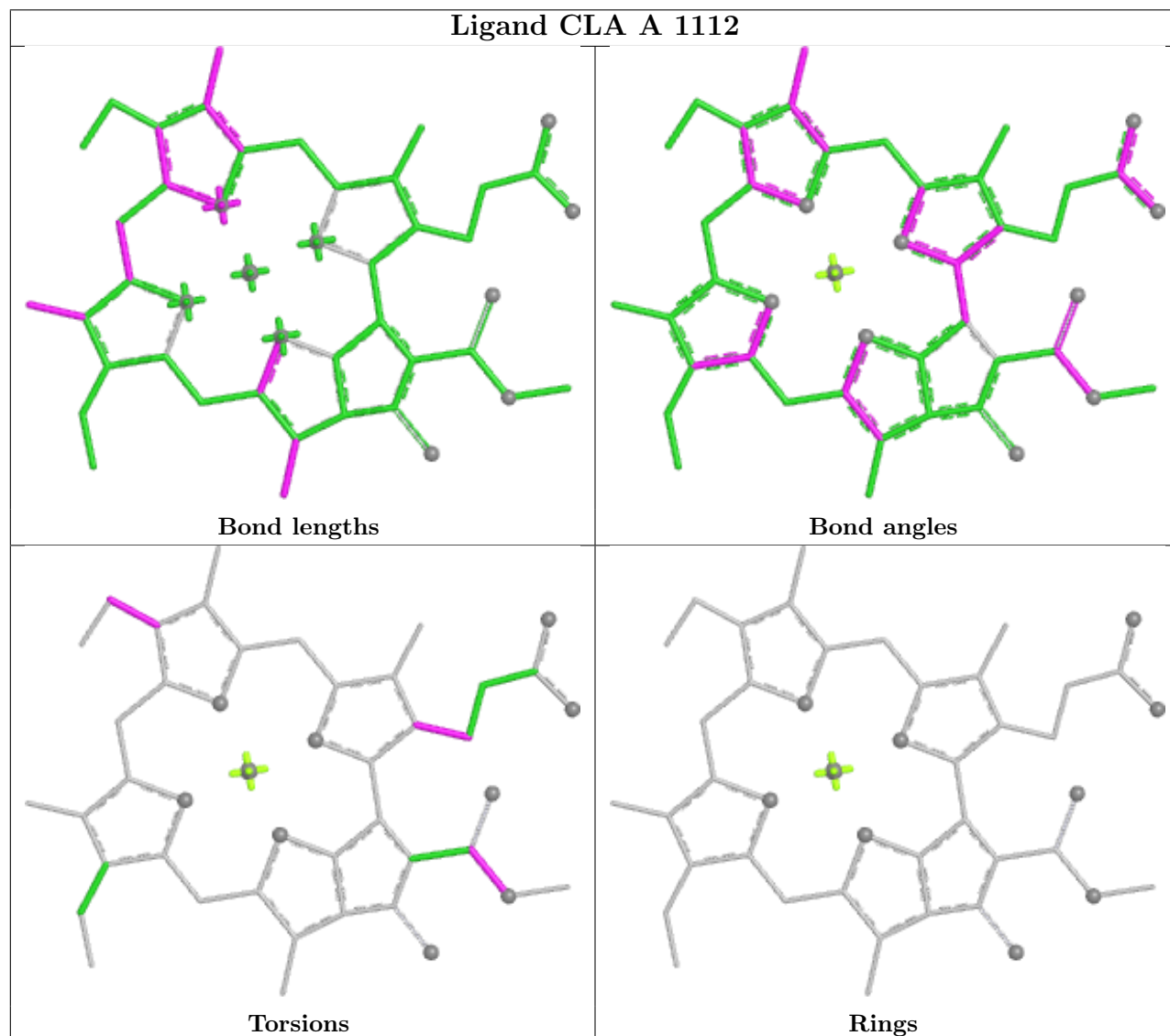
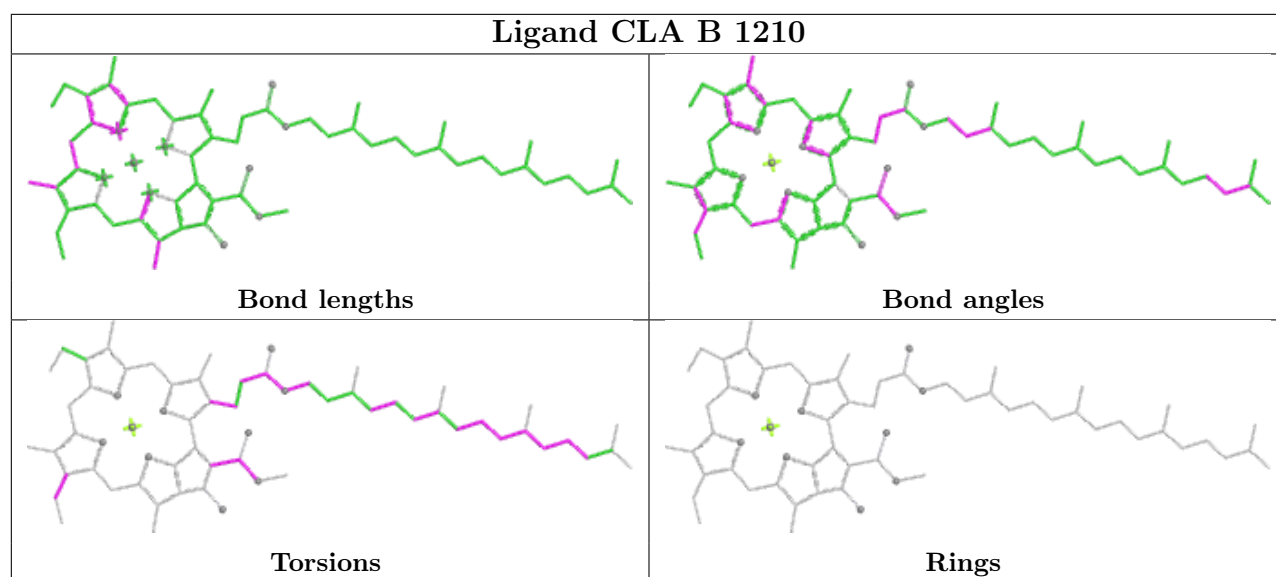


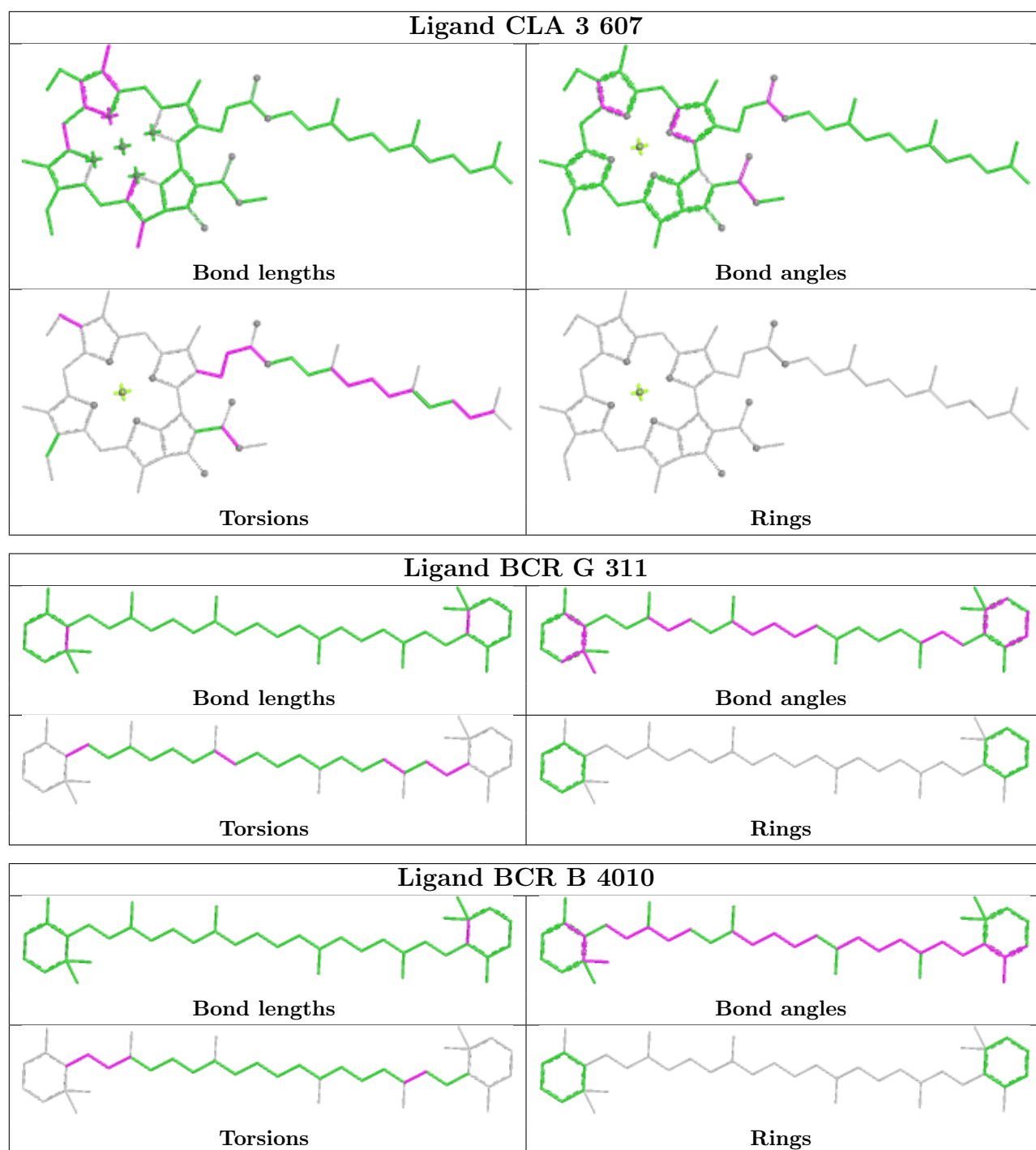
Torsions



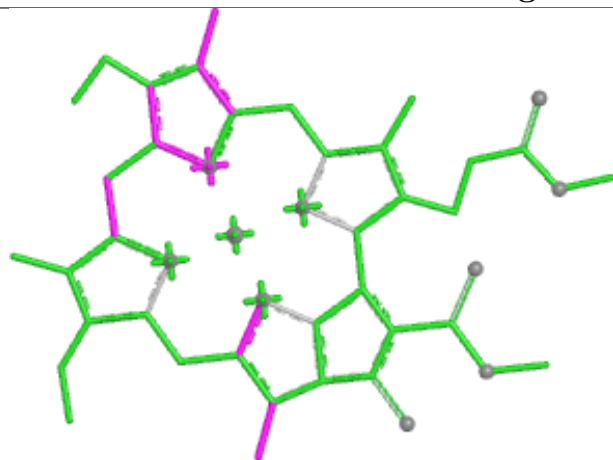
Rings



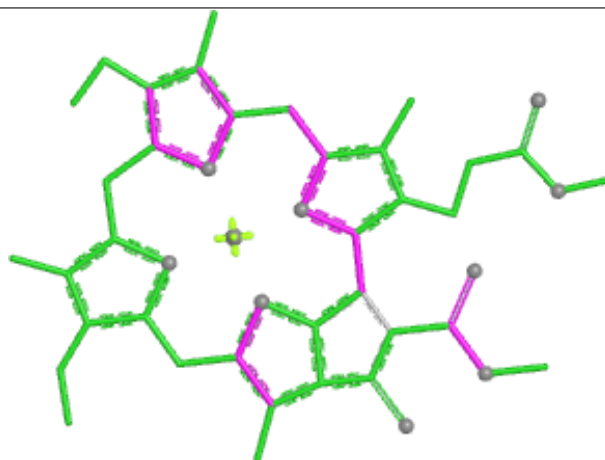




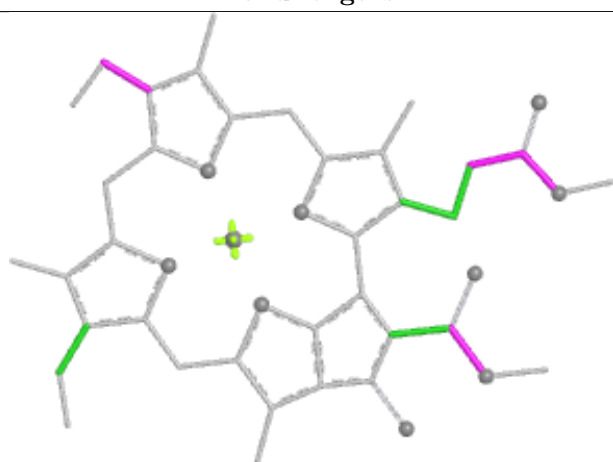
Ligand CLA 1 612



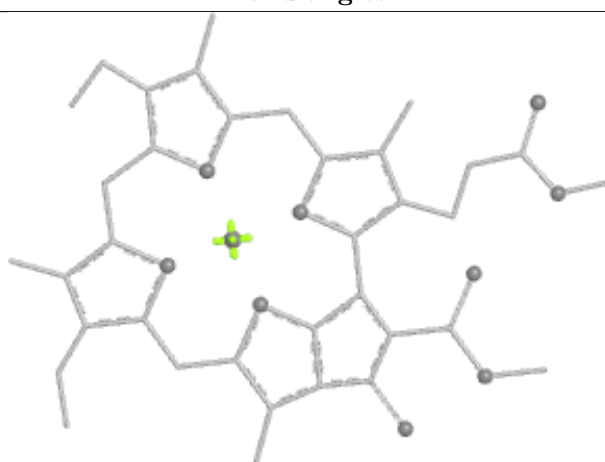
Bond lengths



Bond angles

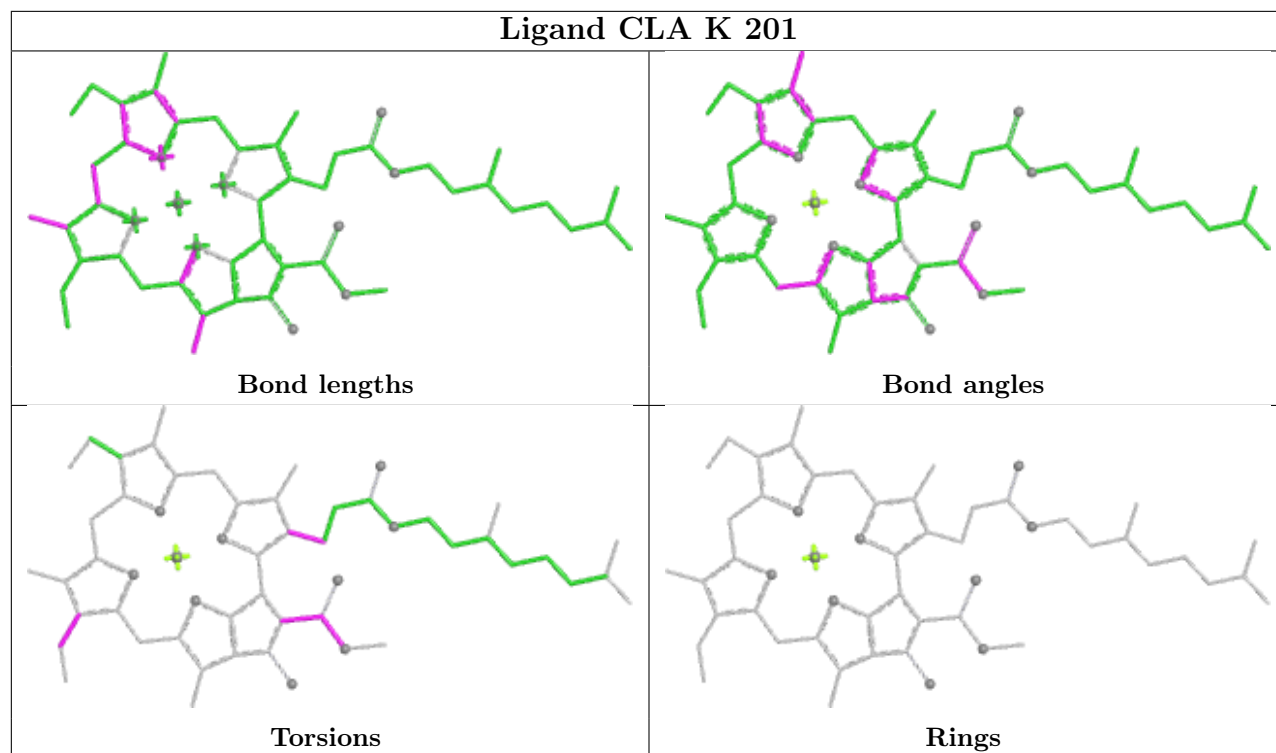


Torsions

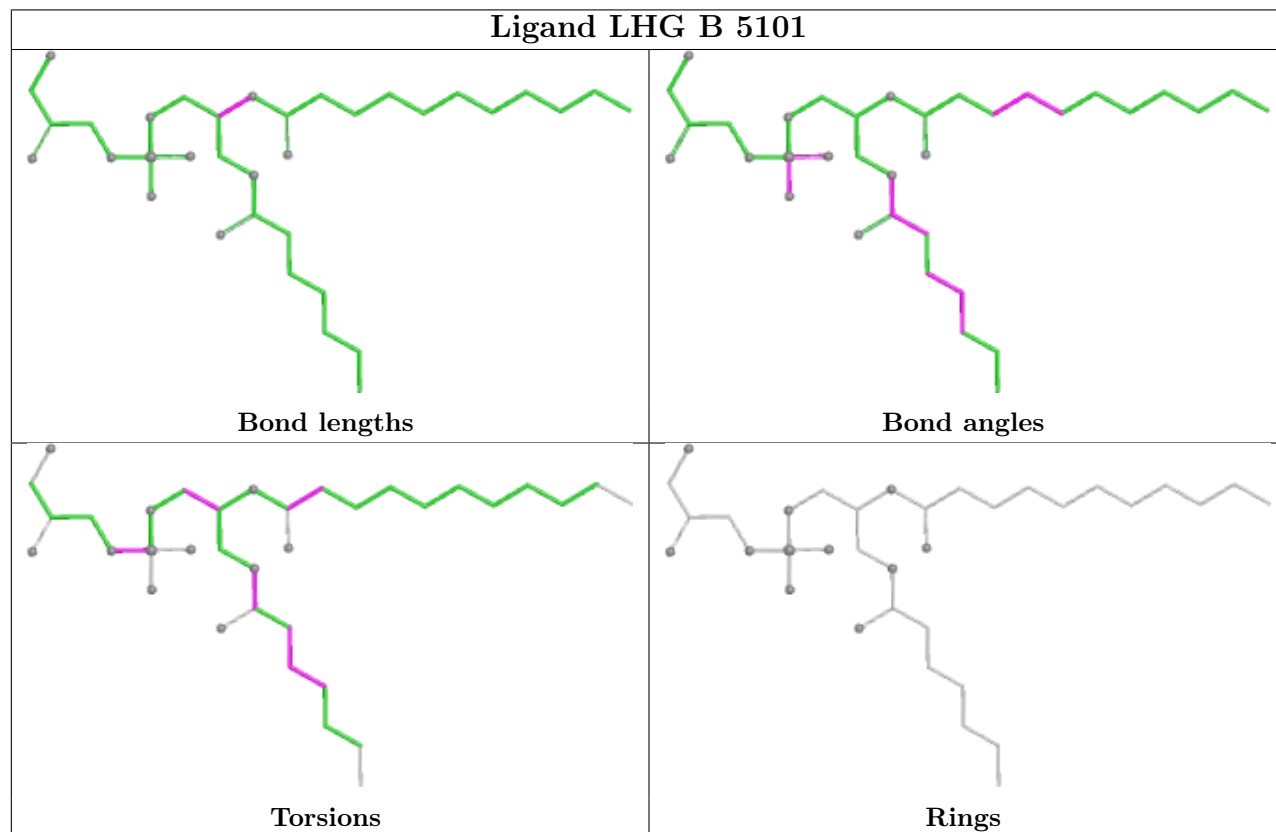


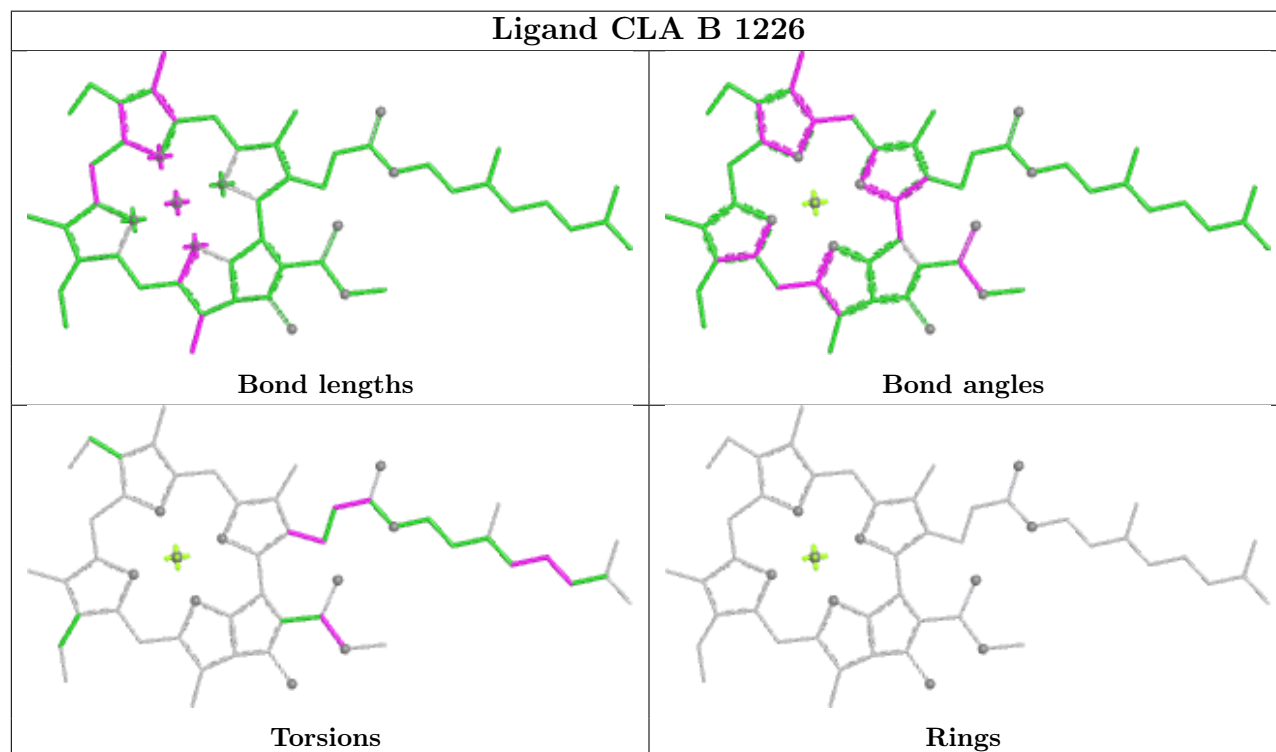
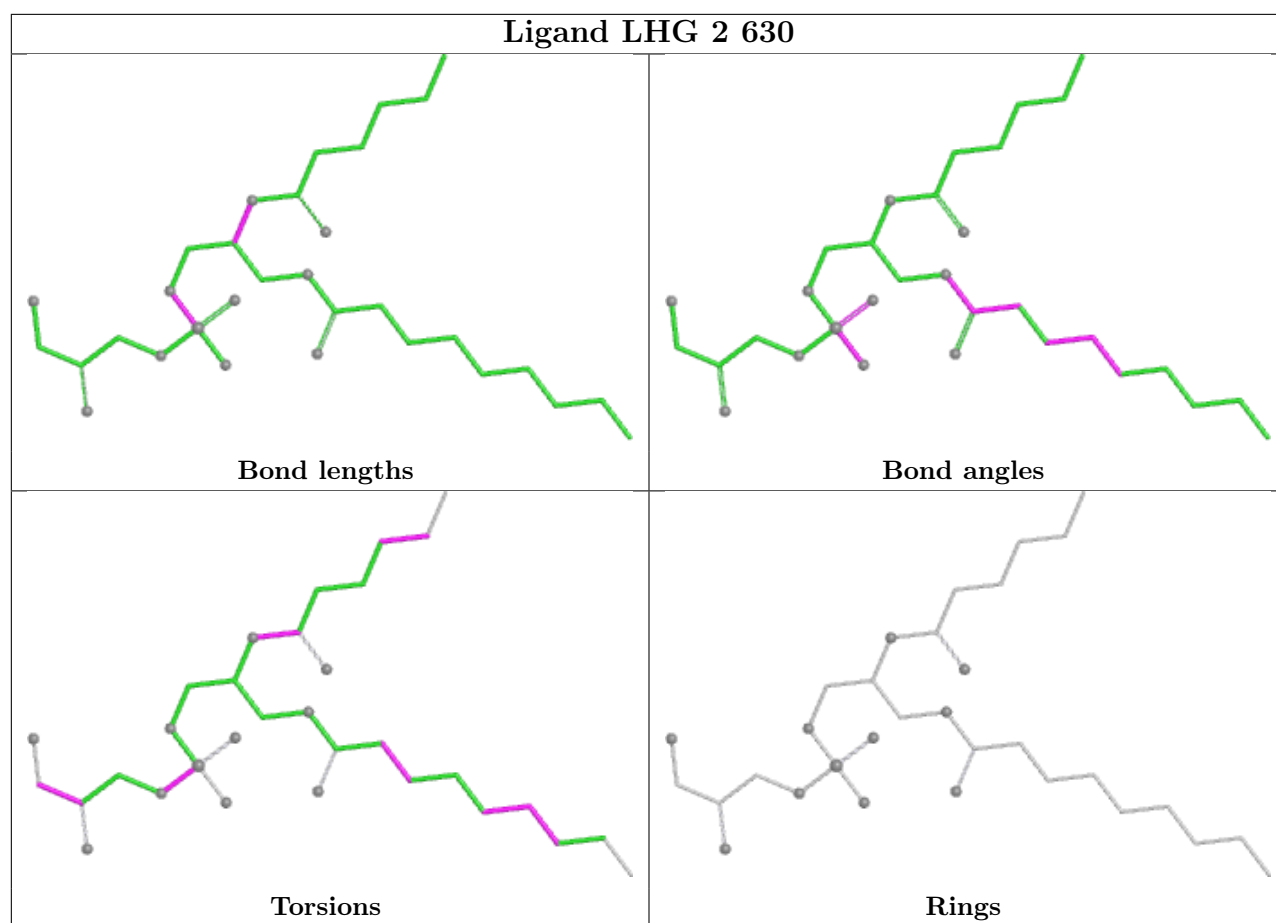
Rings

Ligand CLA K 201

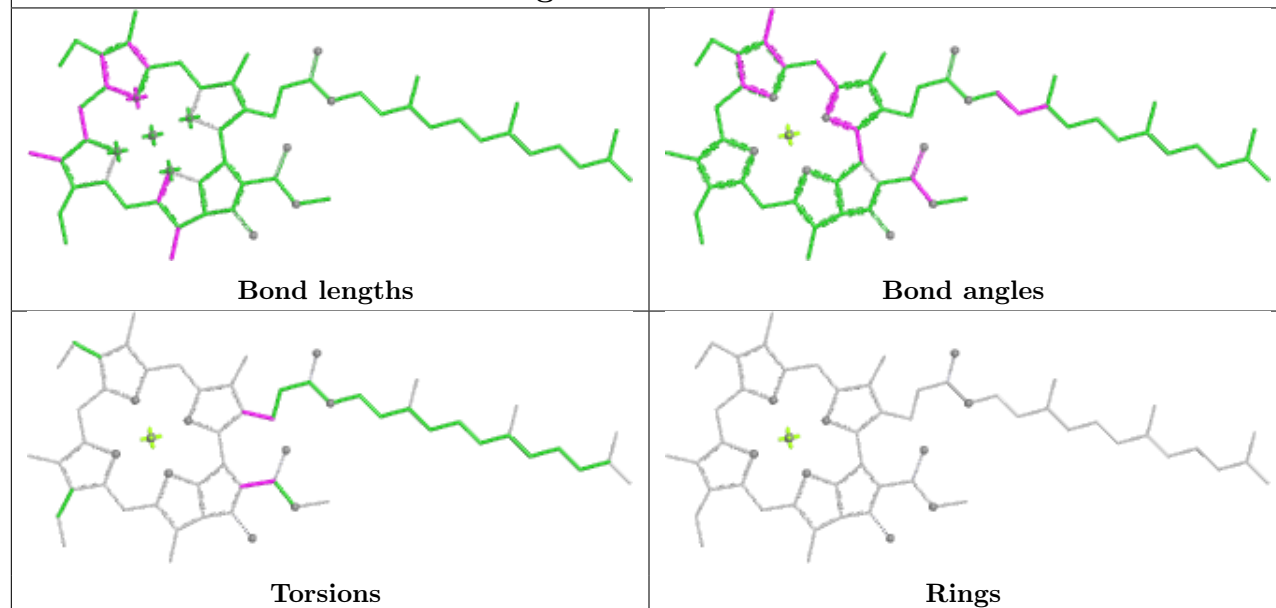


Ligand LHG B 5101

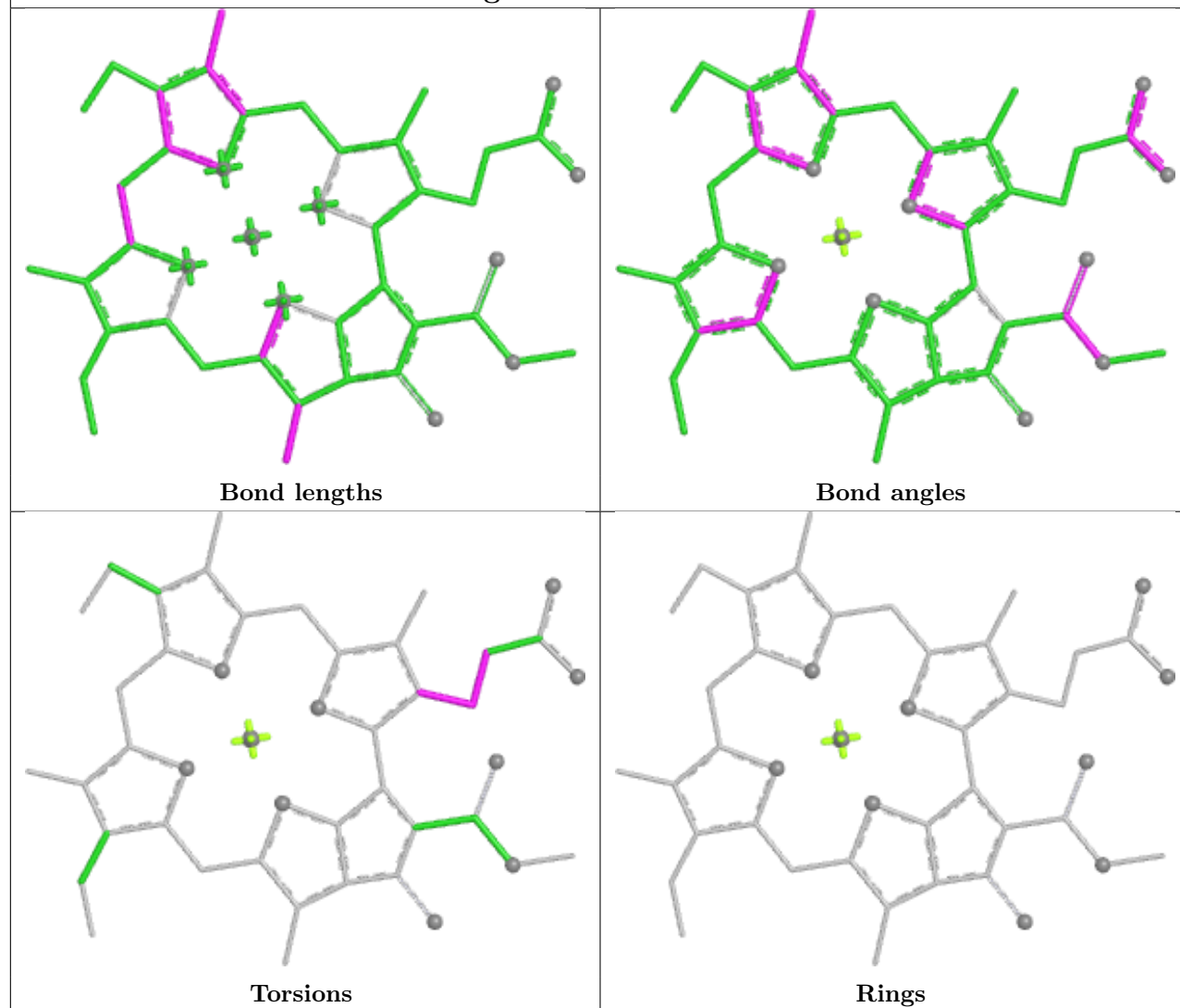


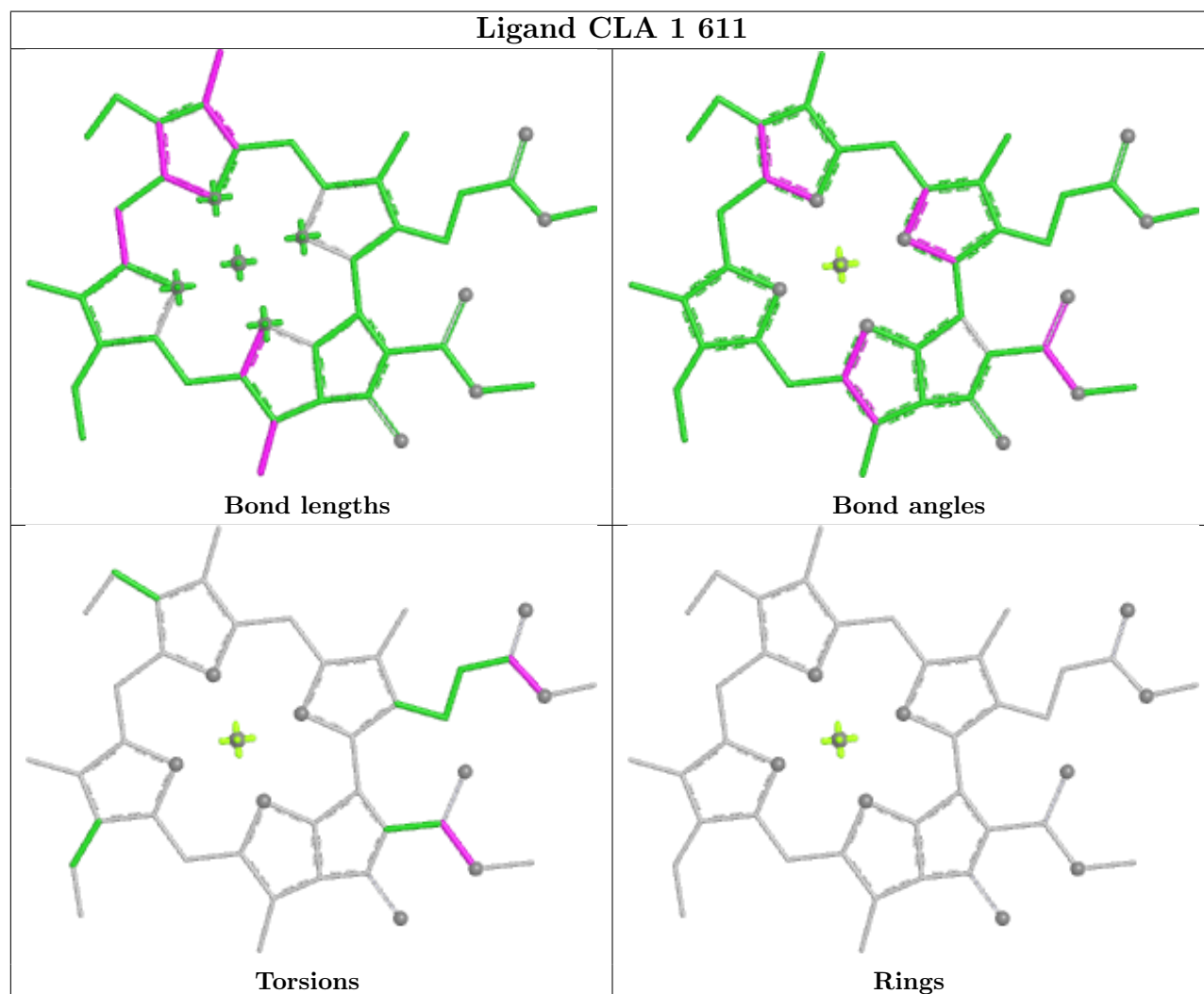
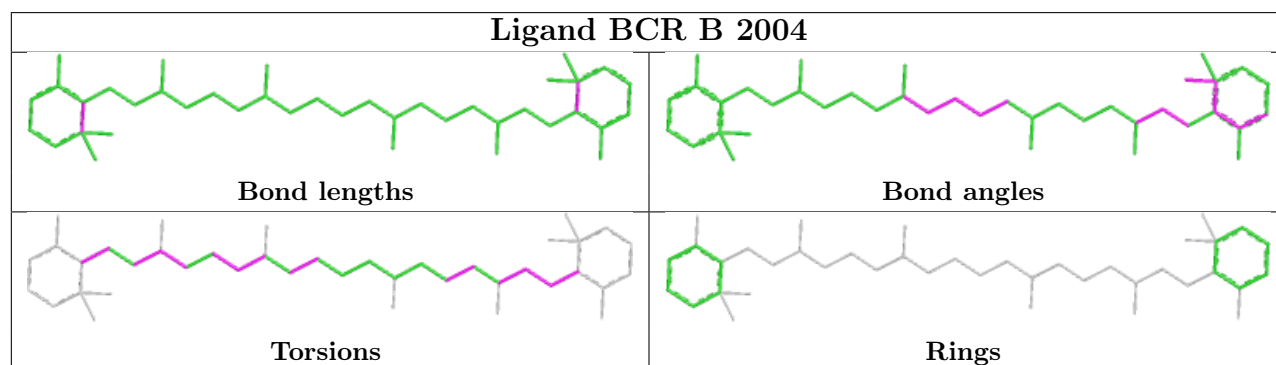
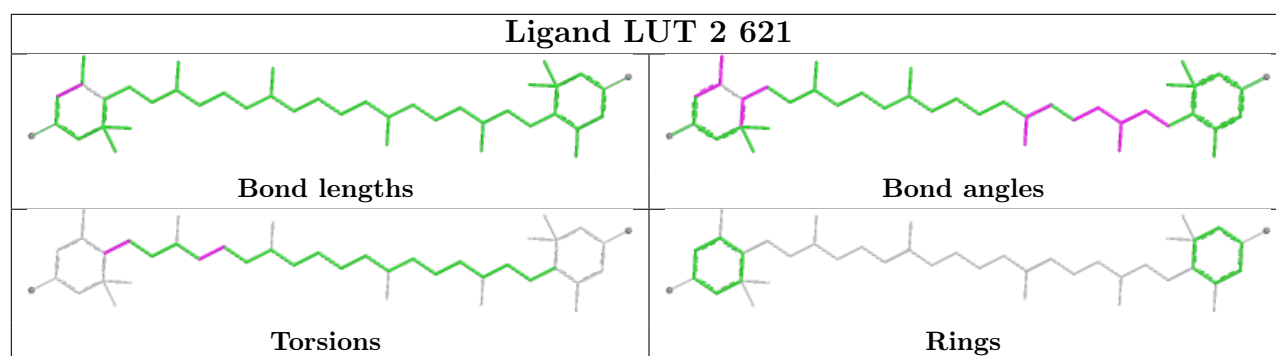


Ligand CLA 1 602

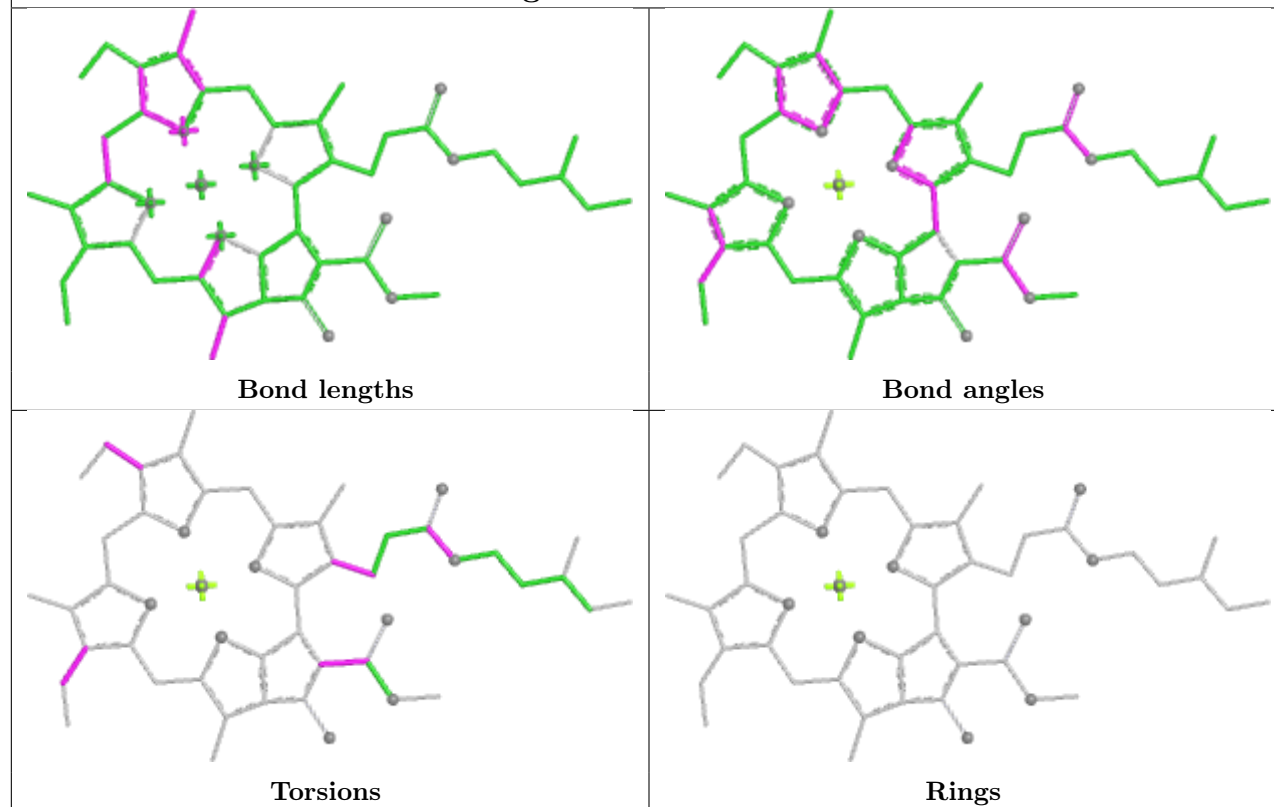


Ligand CLA B 1209

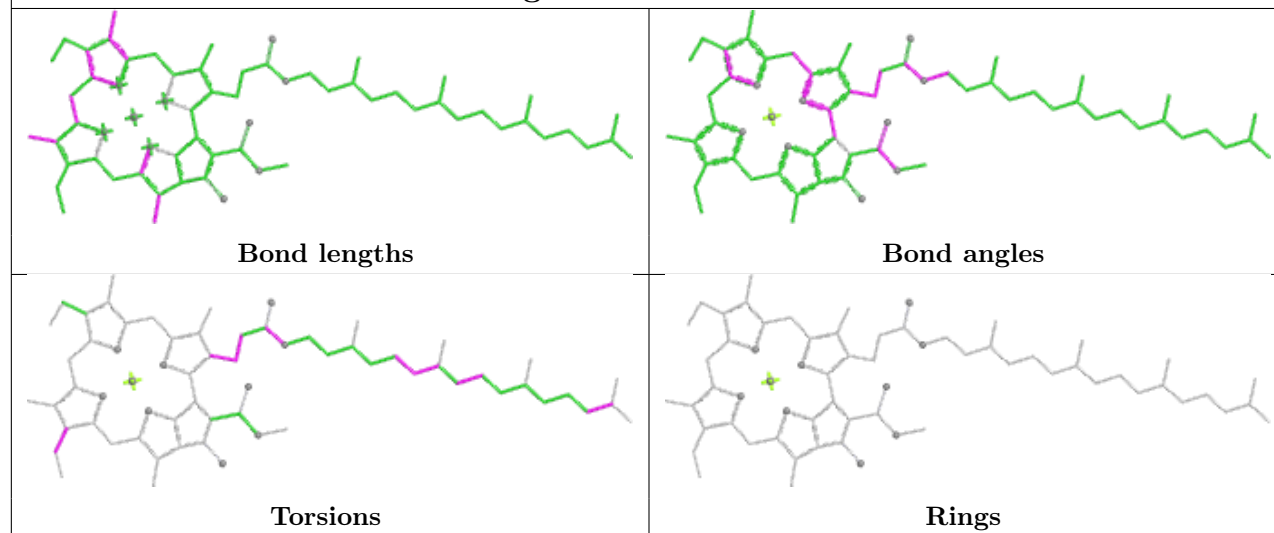


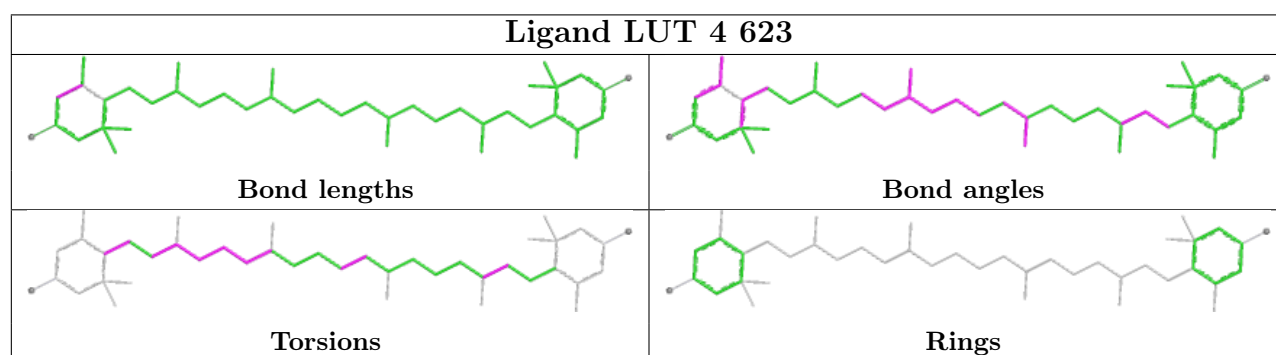
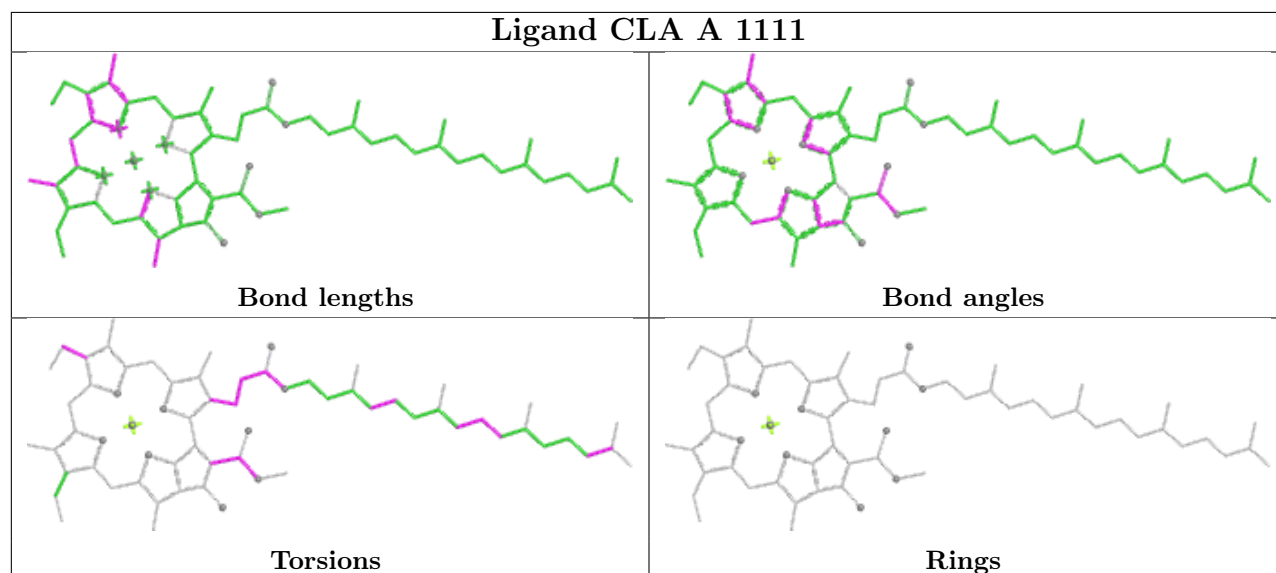
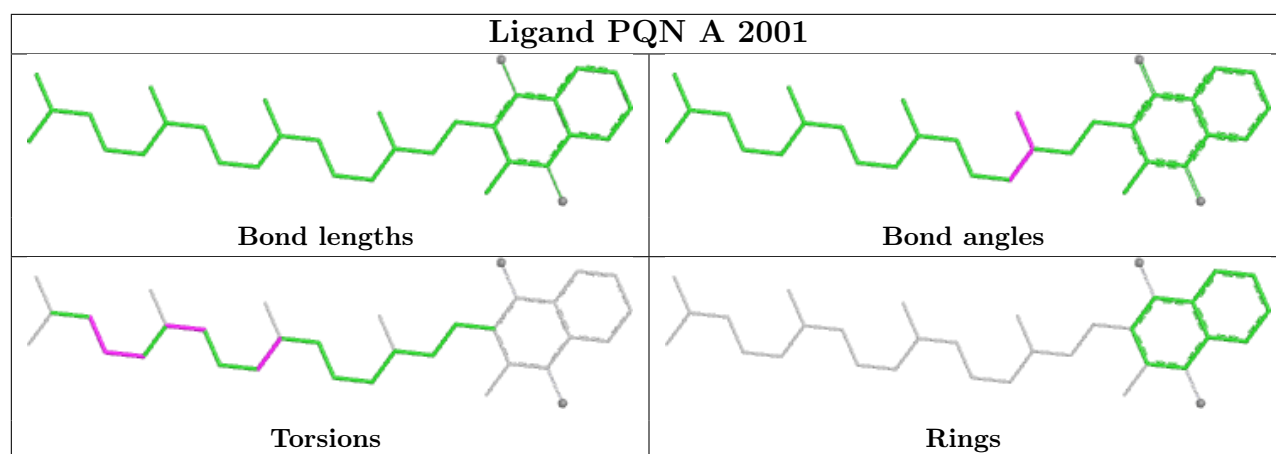


Ligand CLA A 1135

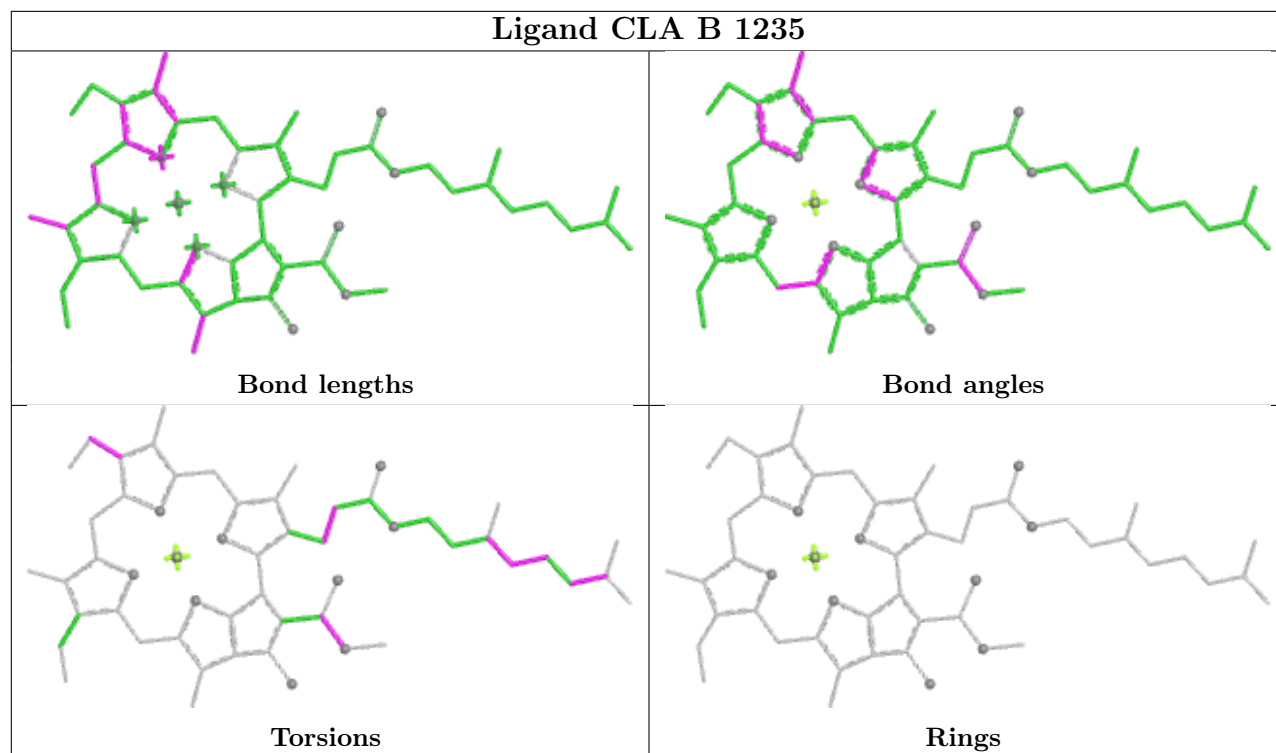


Ligand CLA B 1237

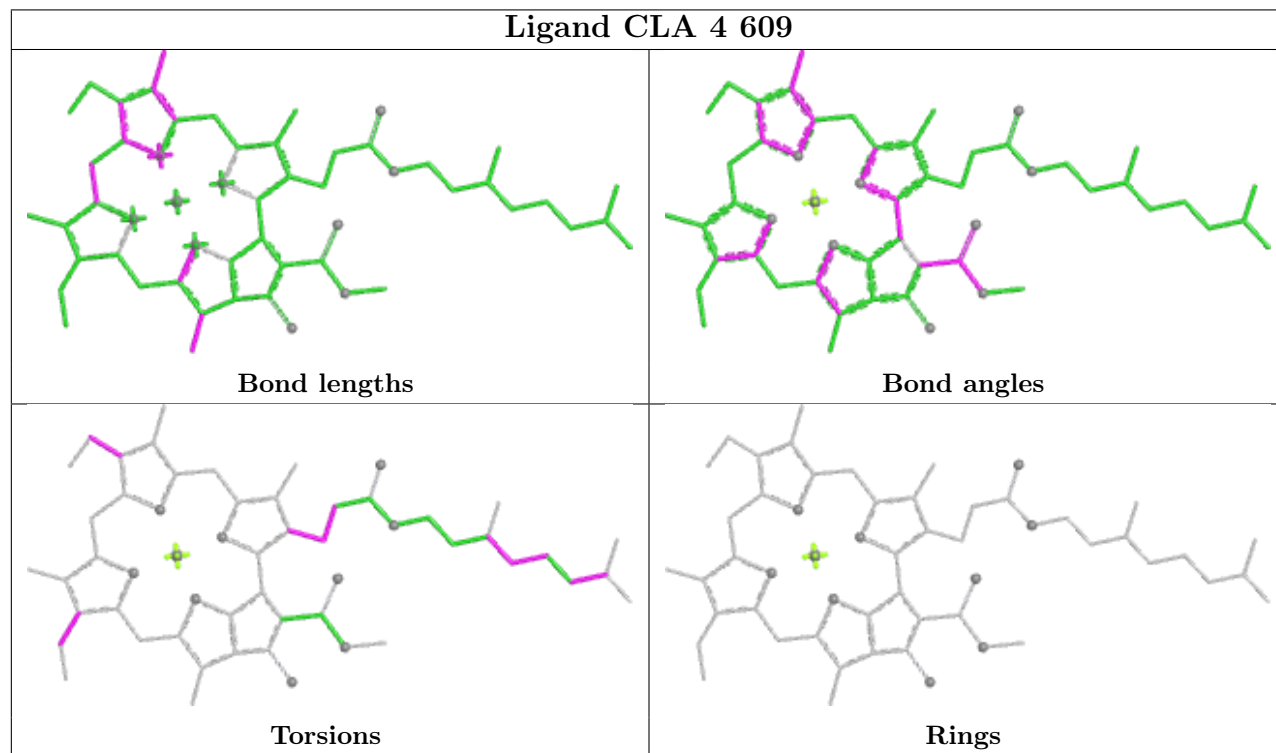


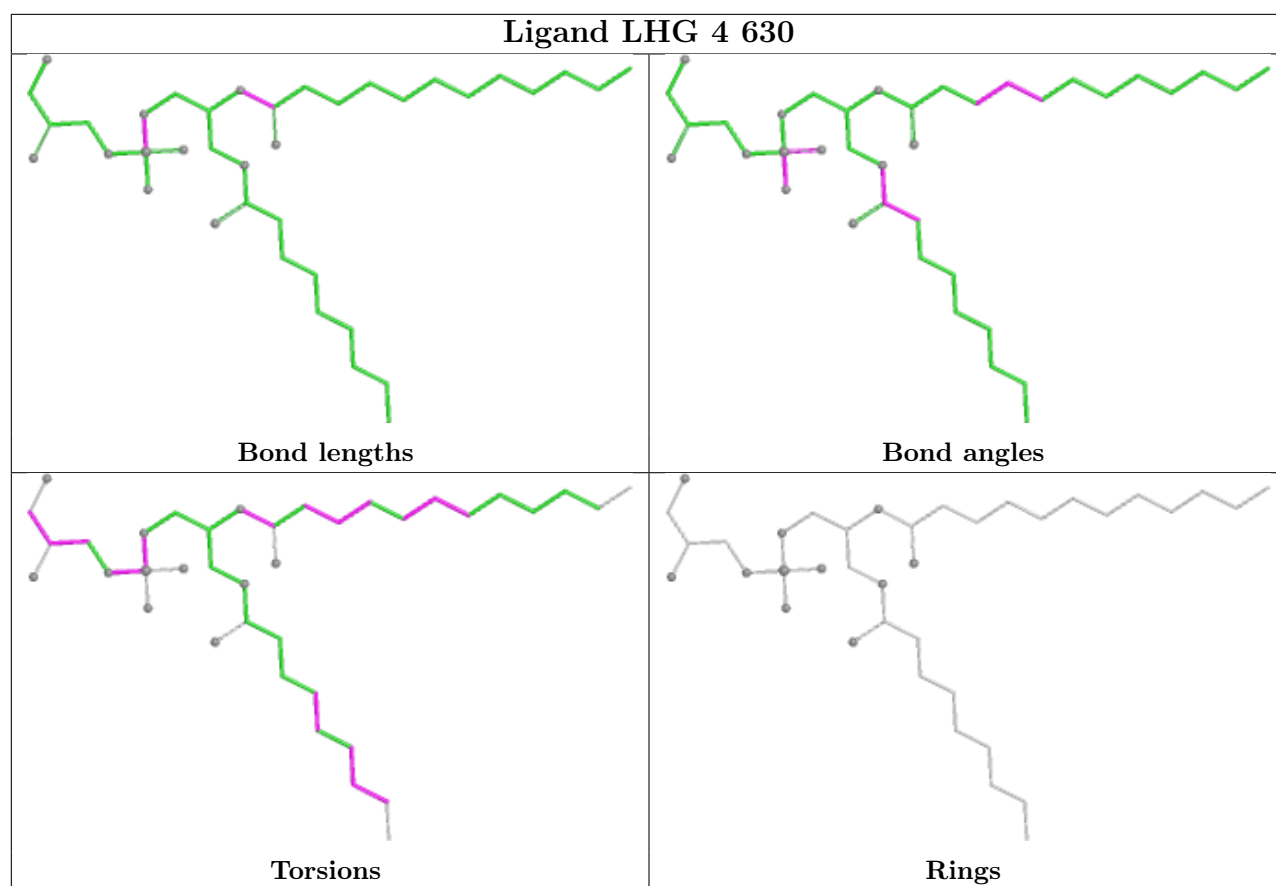


Ligand CLA B 1235

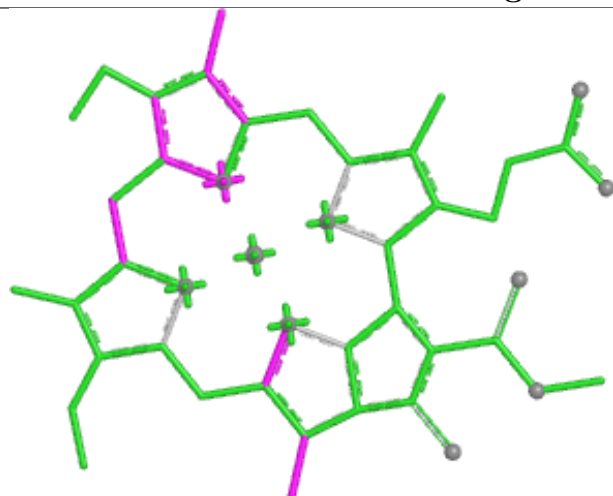


Ligand CLA 4 609

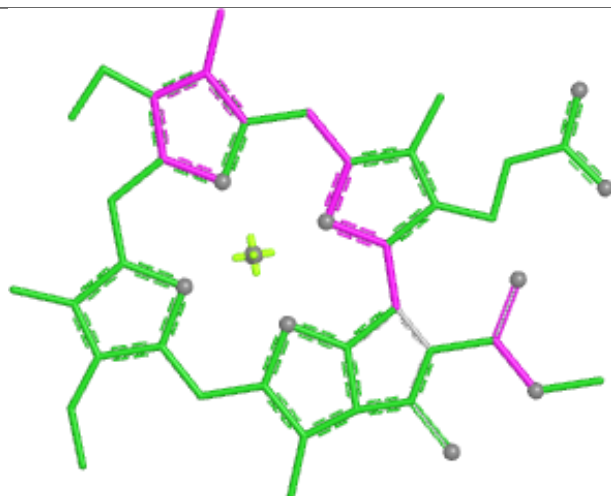




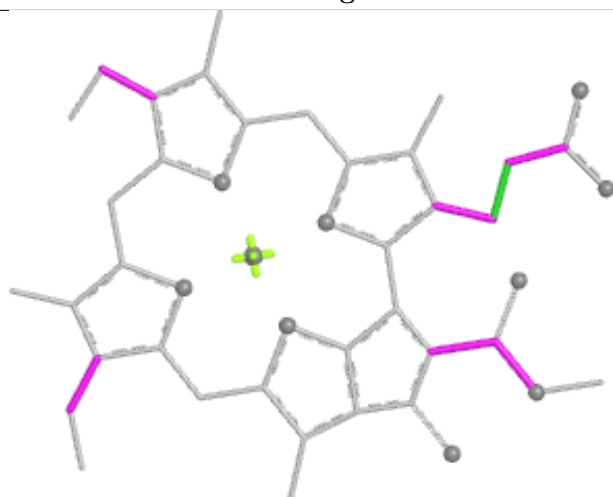
Ligand CLA A 1107



Bond lengths



Bond angles

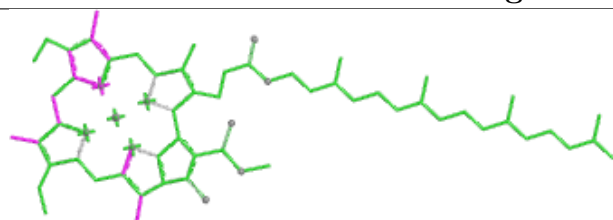


Torsions

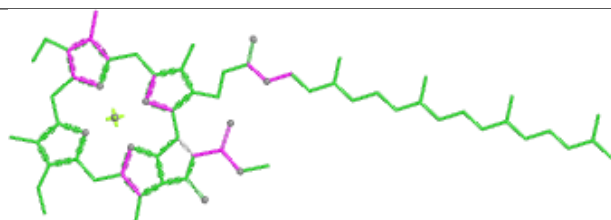


Rings

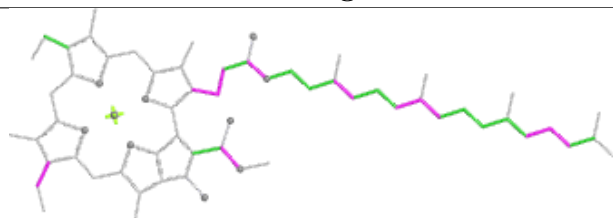
Ligand CLA B 1225



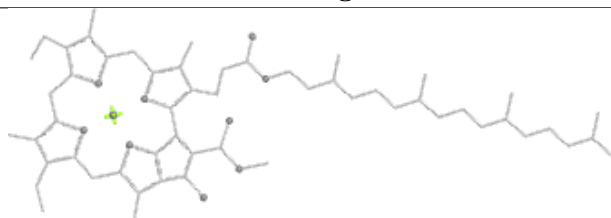
Bond lengths



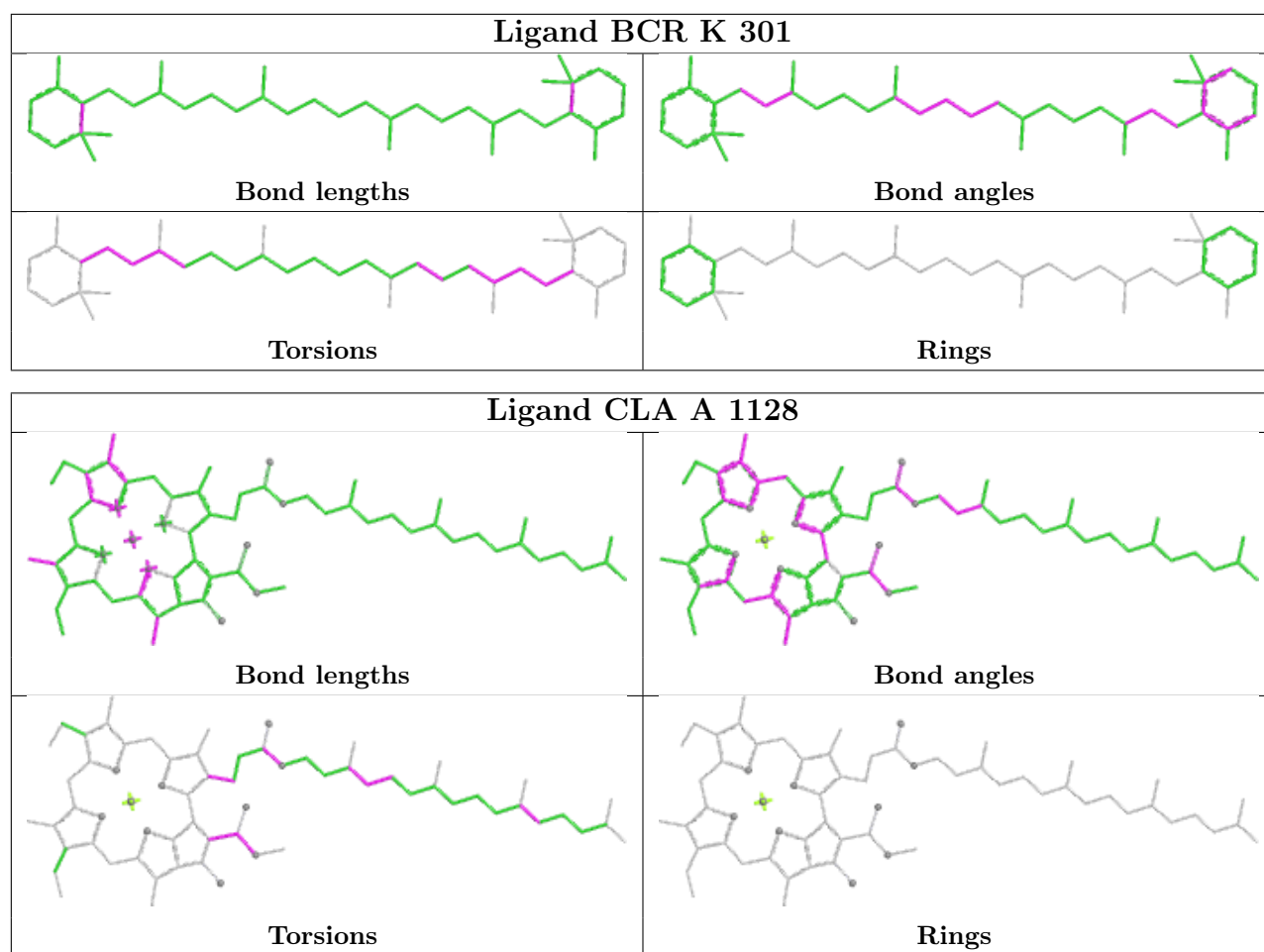
Bond angles



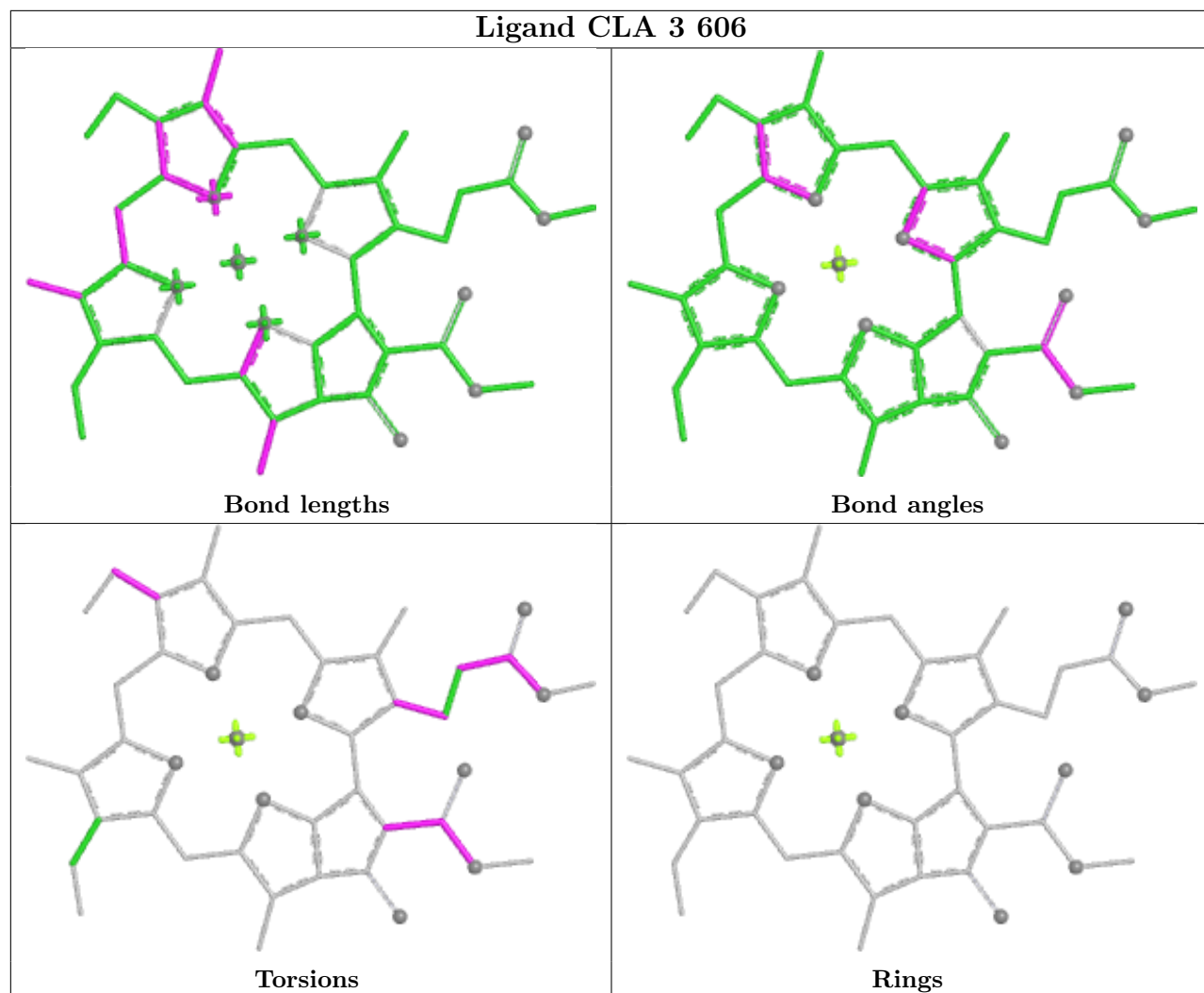
Torsions



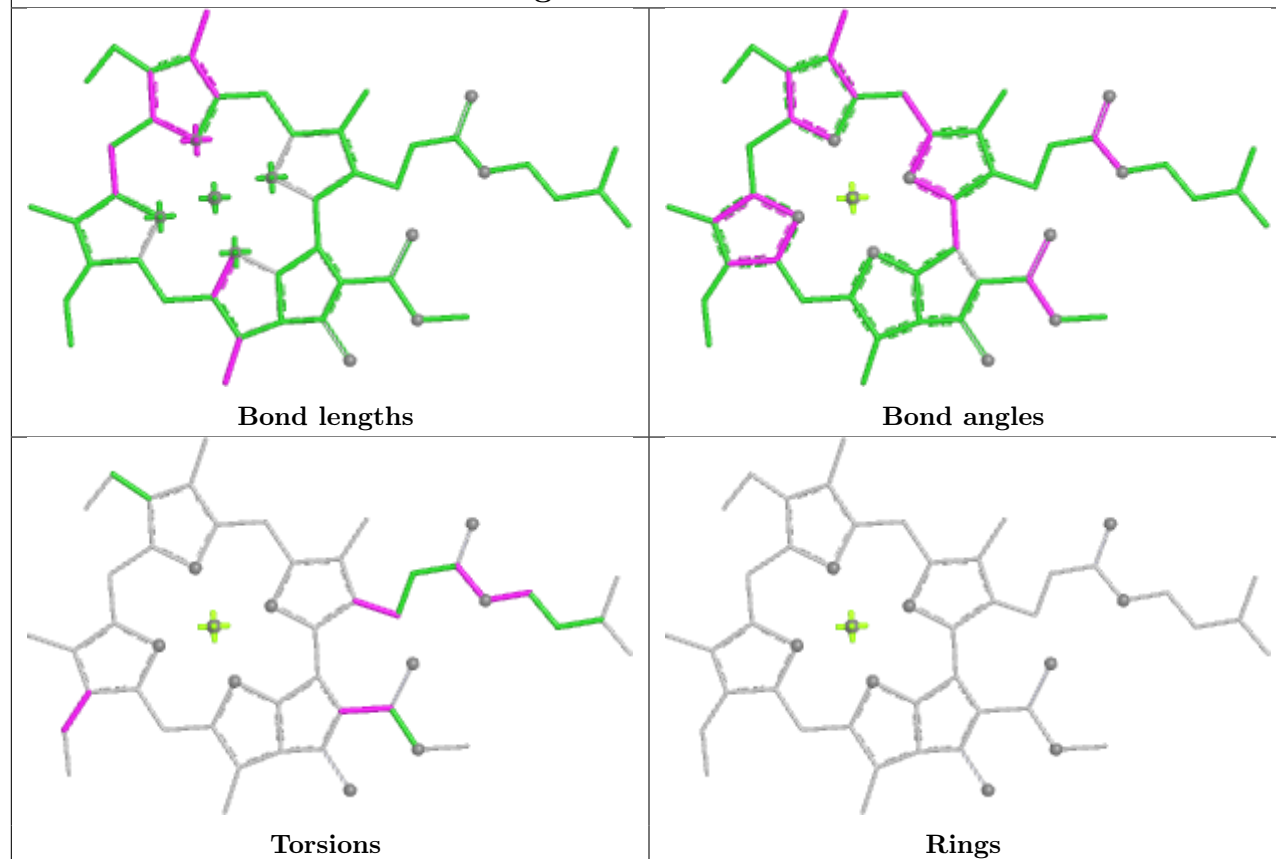
Rings



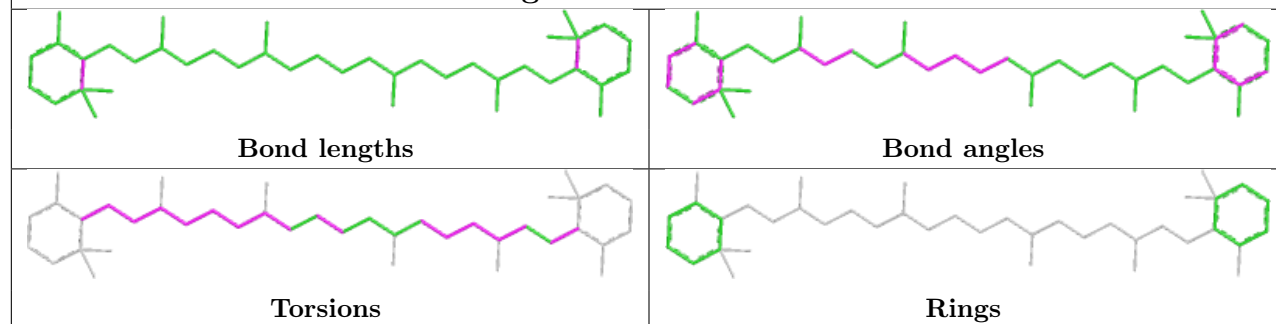
Ligand CLA 3 606

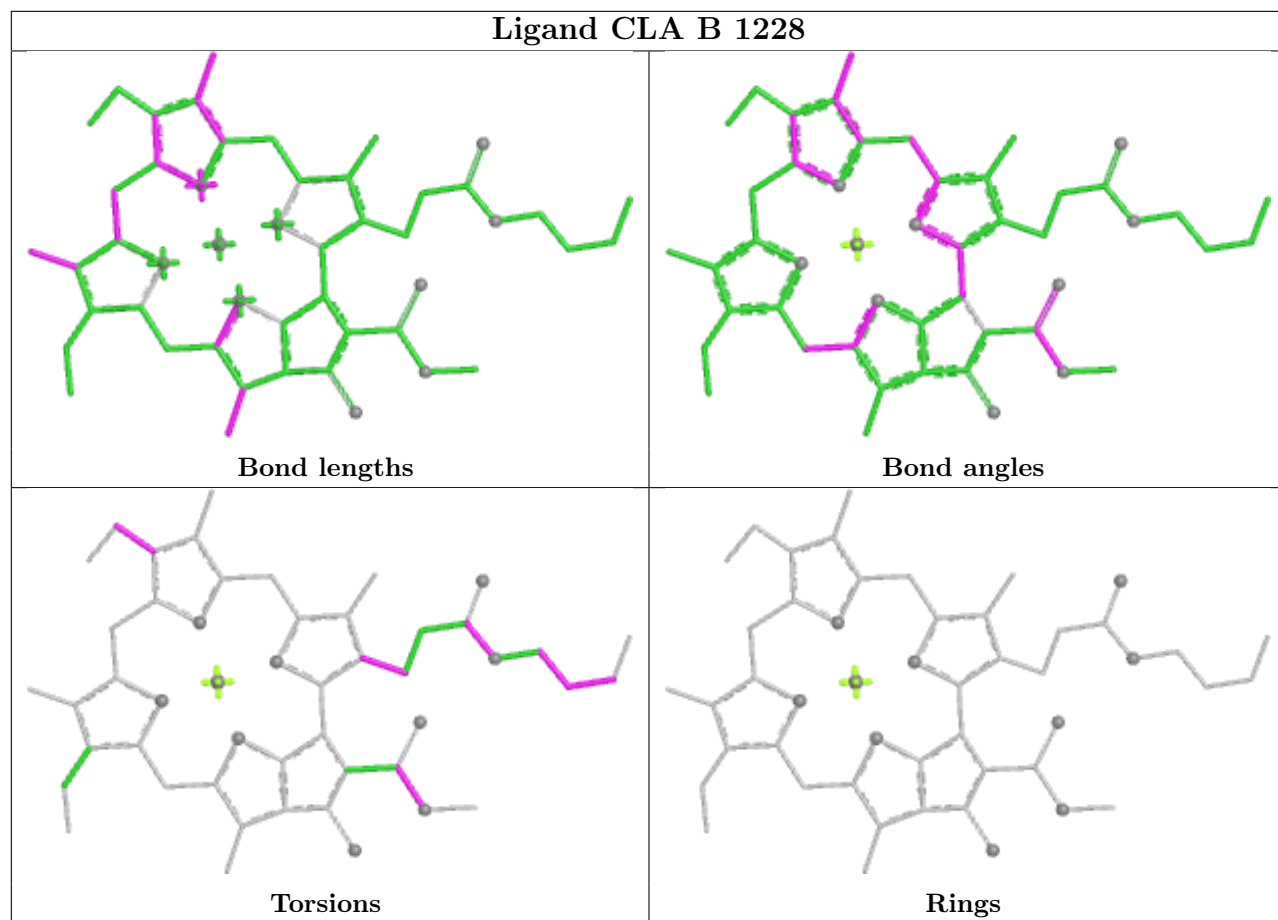


Ligand CLA L 301

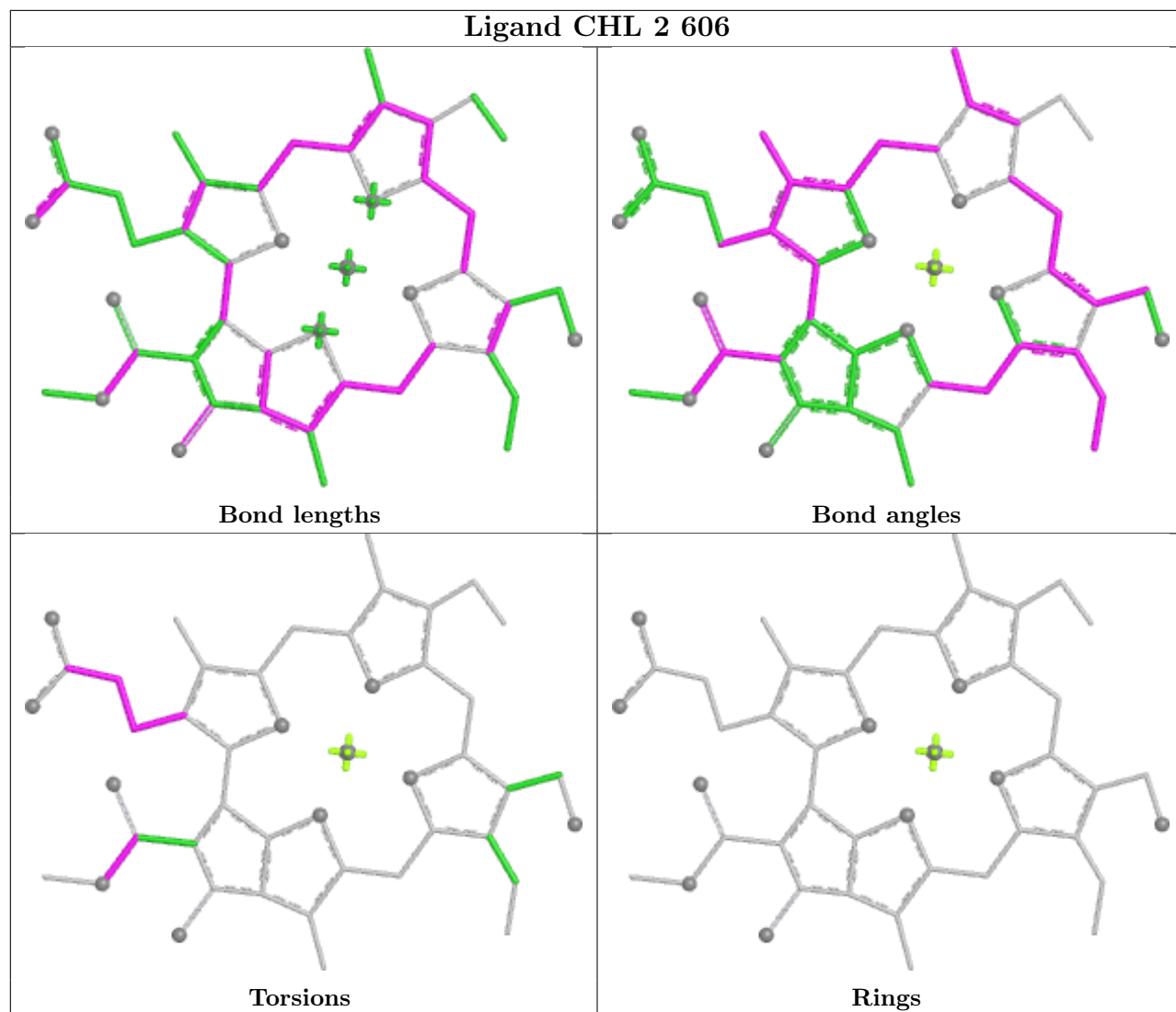


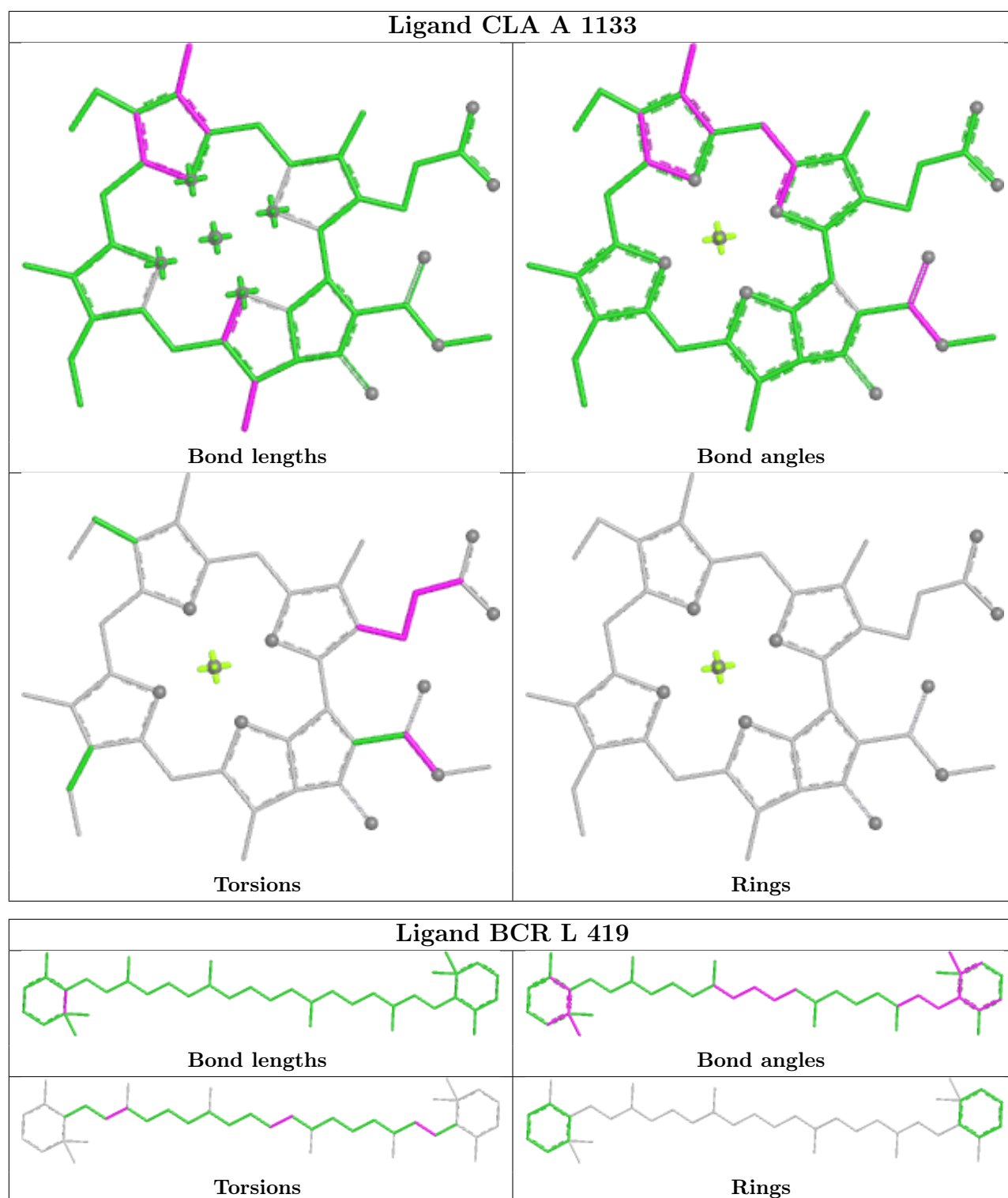
Ligand BCR B 4014





Ligand CHL 2 606





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

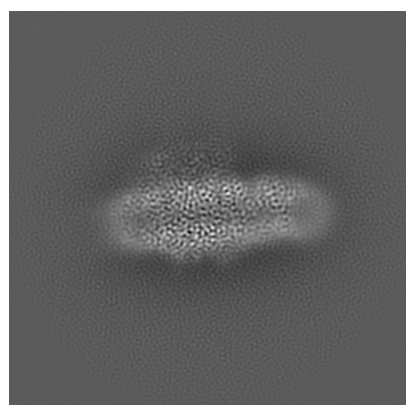
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23040. These allow visual inspection of the internal detail of the map and identification of artifacts.

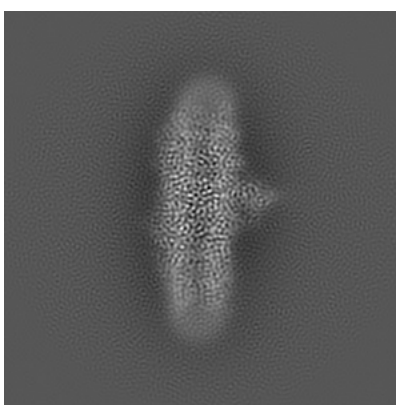
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

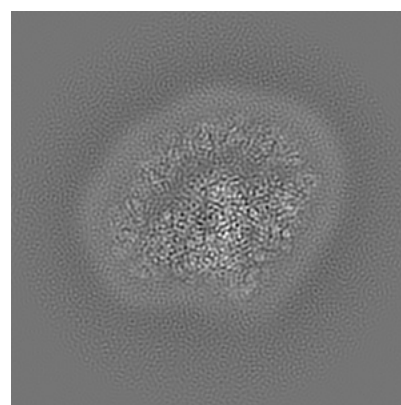
6.1.1 Primary map



X



Y

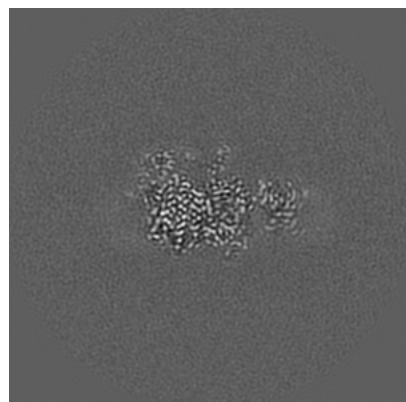


Z

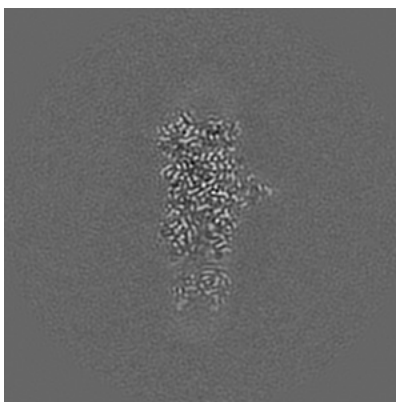
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

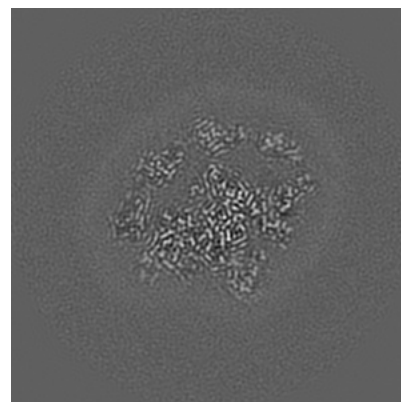
6.2.1 Primary map



X Index: 140



Y Index: 140

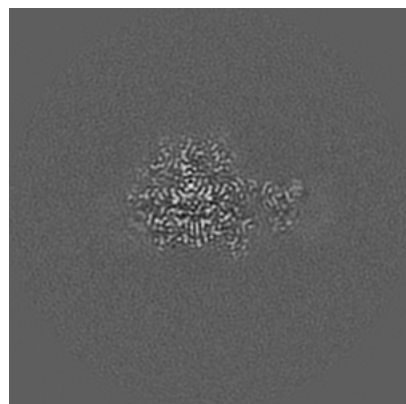


Z Index: 140

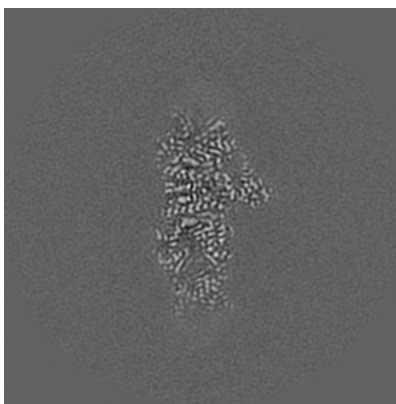
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

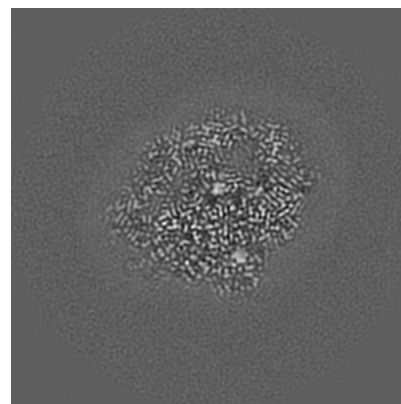
6.3.1 Primary map



X Index: 150



Y Index: 129

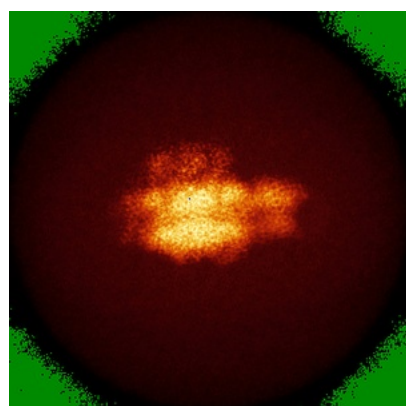


Z Index: 148

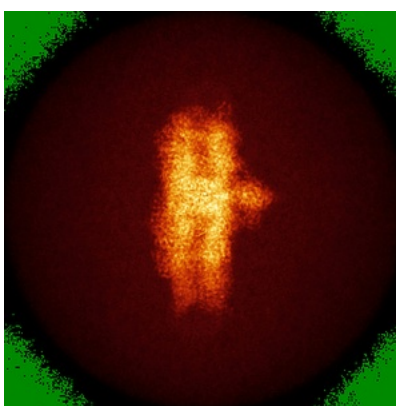
The images above show the largest variance slices of the map in three orthogonal directions.

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

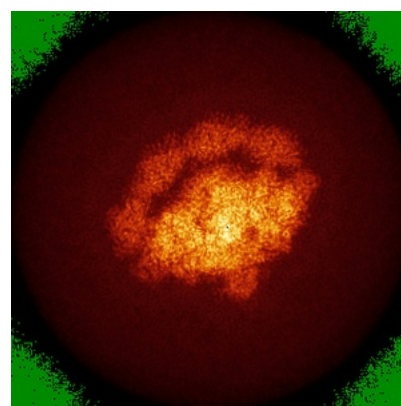
6.4.1 Primary map



X



Y

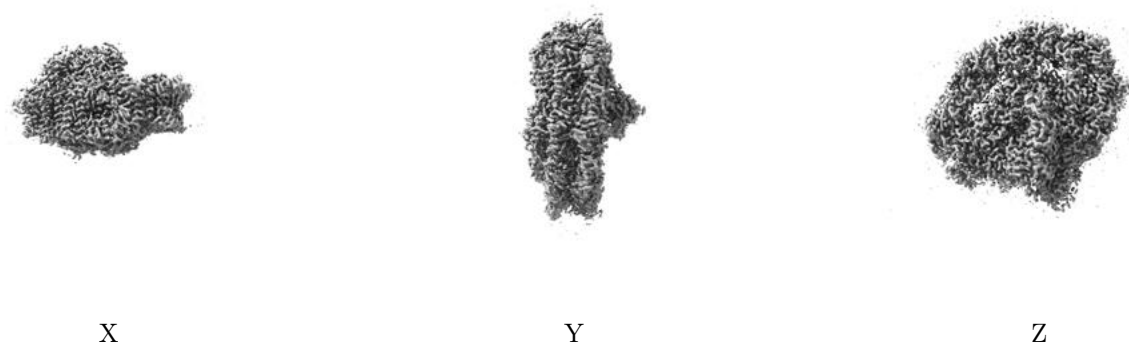


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

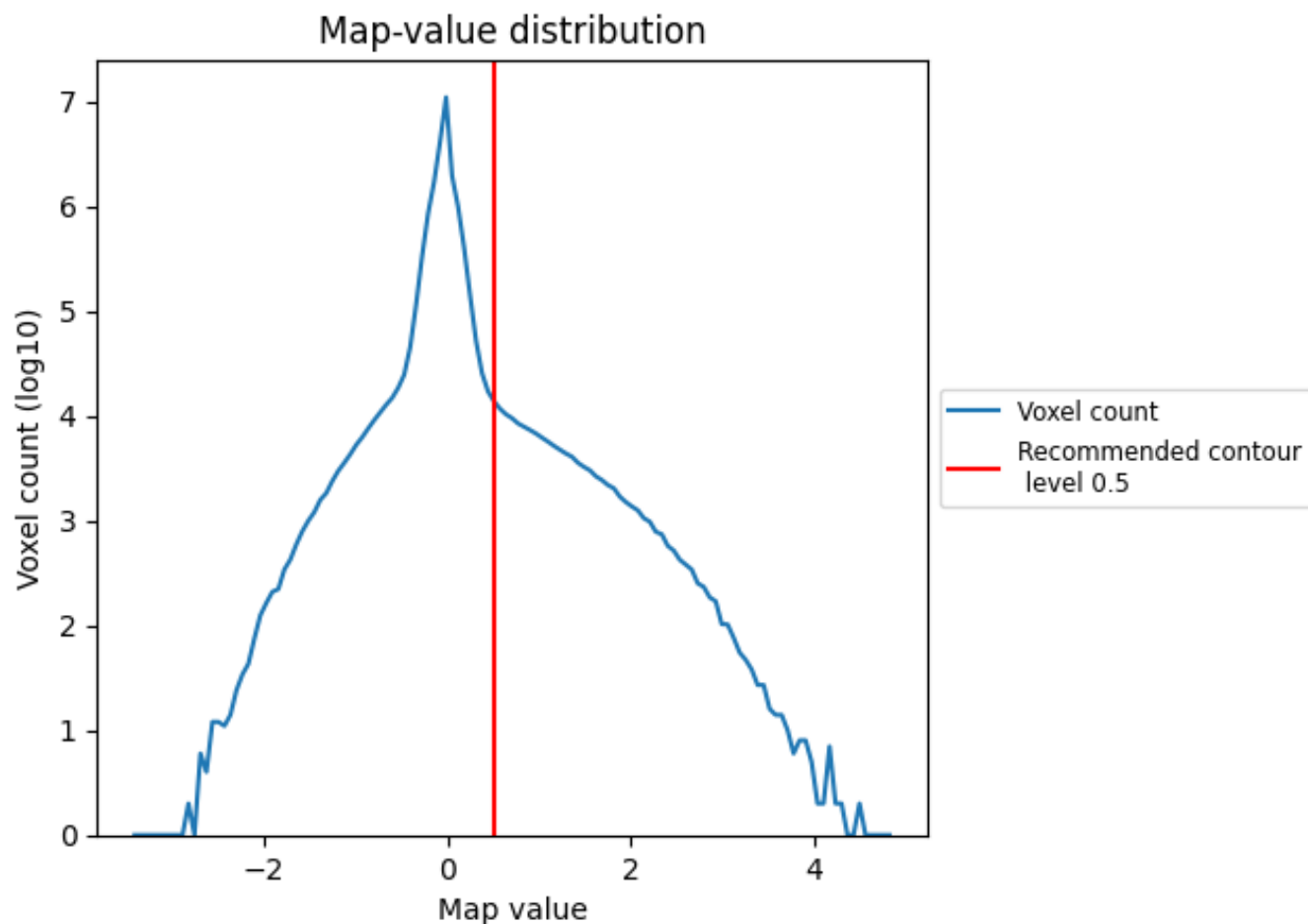
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

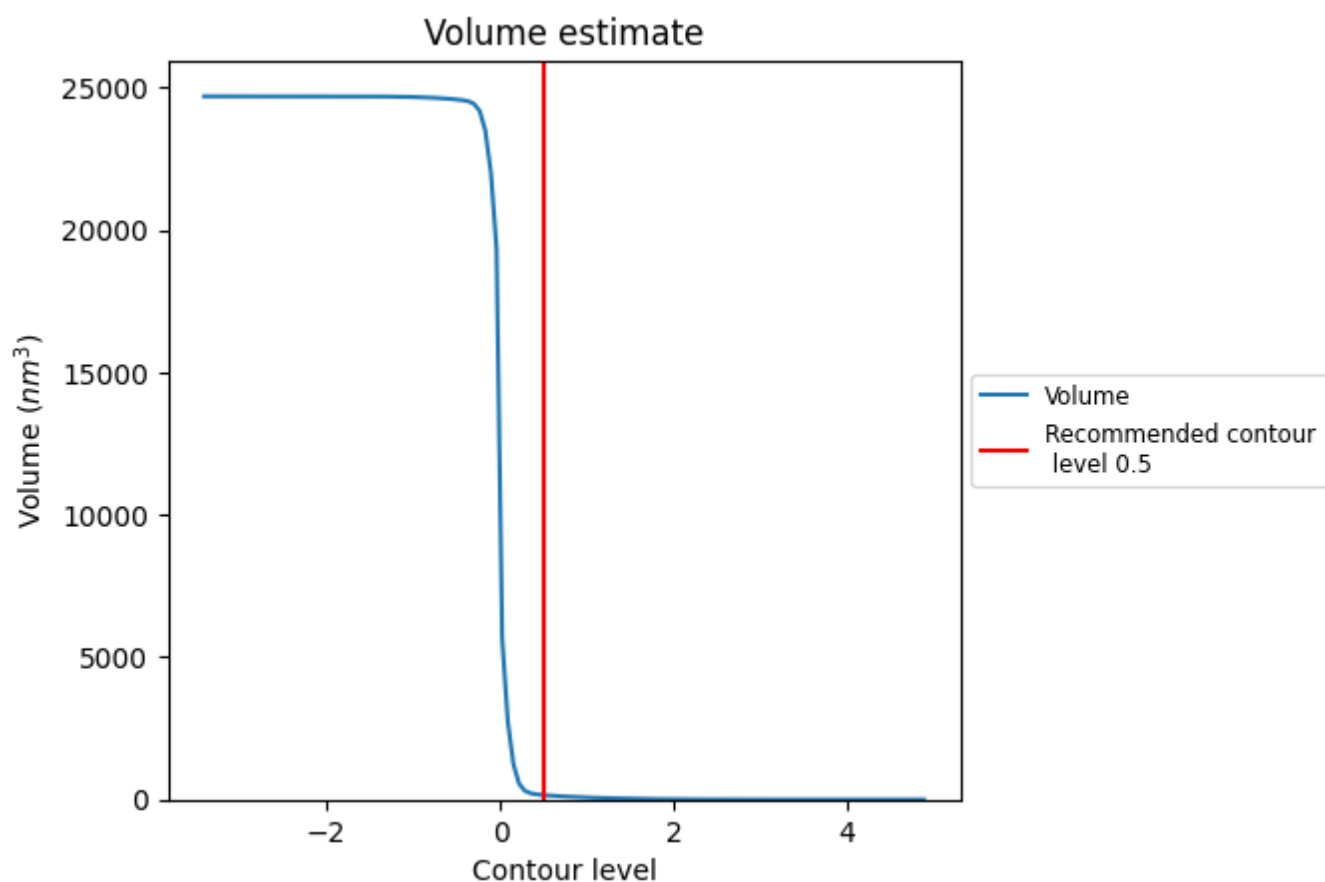
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

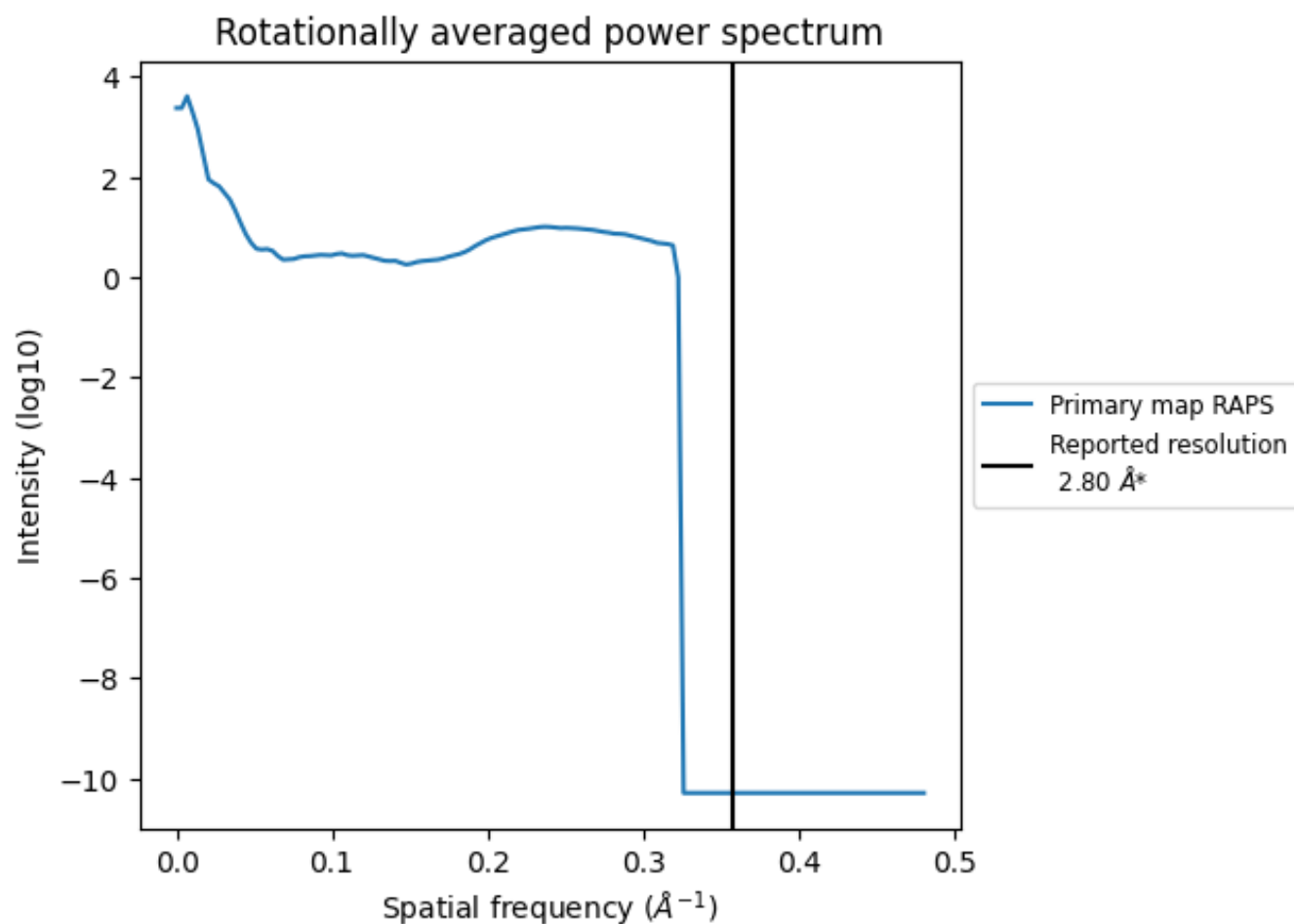
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm³; this corresponds to an approximate mass of 143 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 0.357 $\text{\AA}^{-1}$

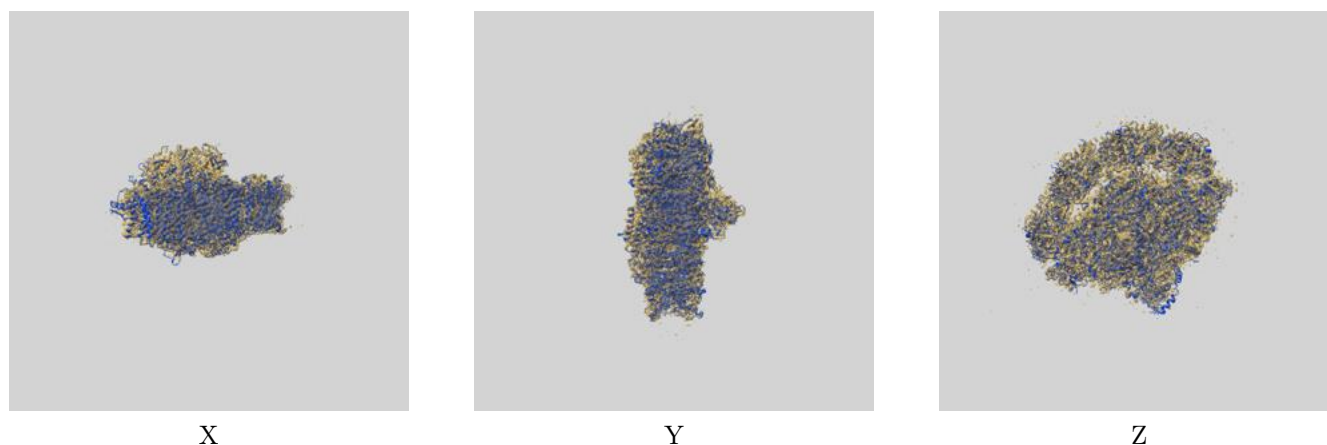
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

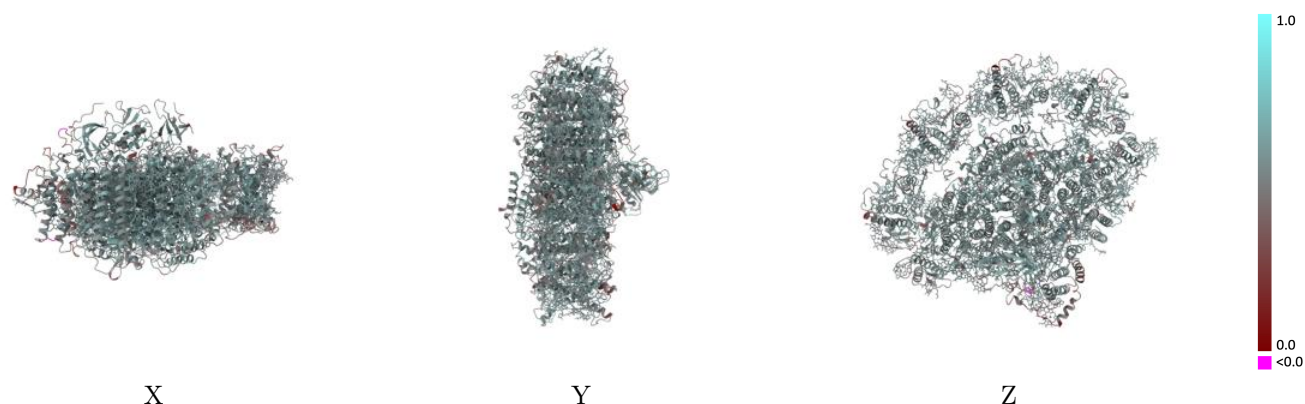
This section contains information regarding the fit between EMDB map EMD-23040 and PDB model 7KUX. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



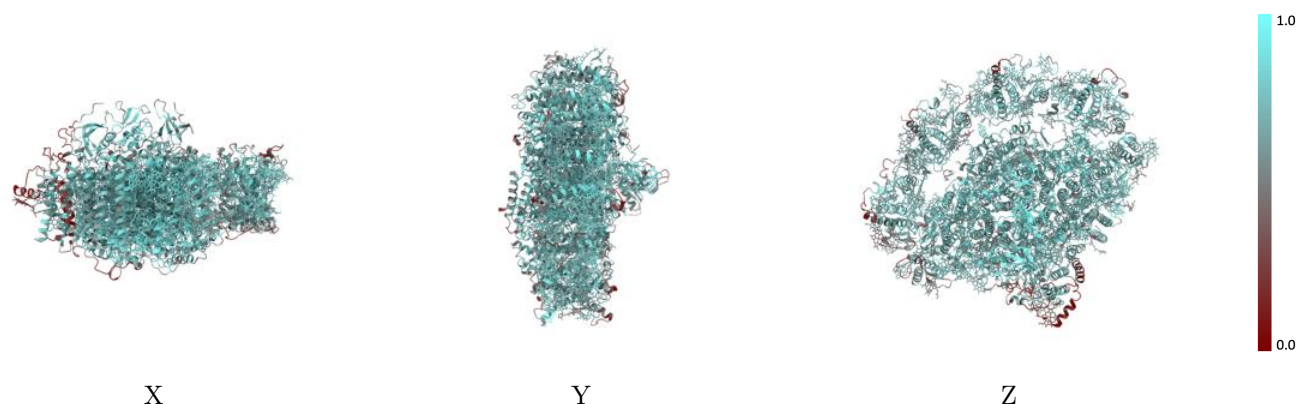
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



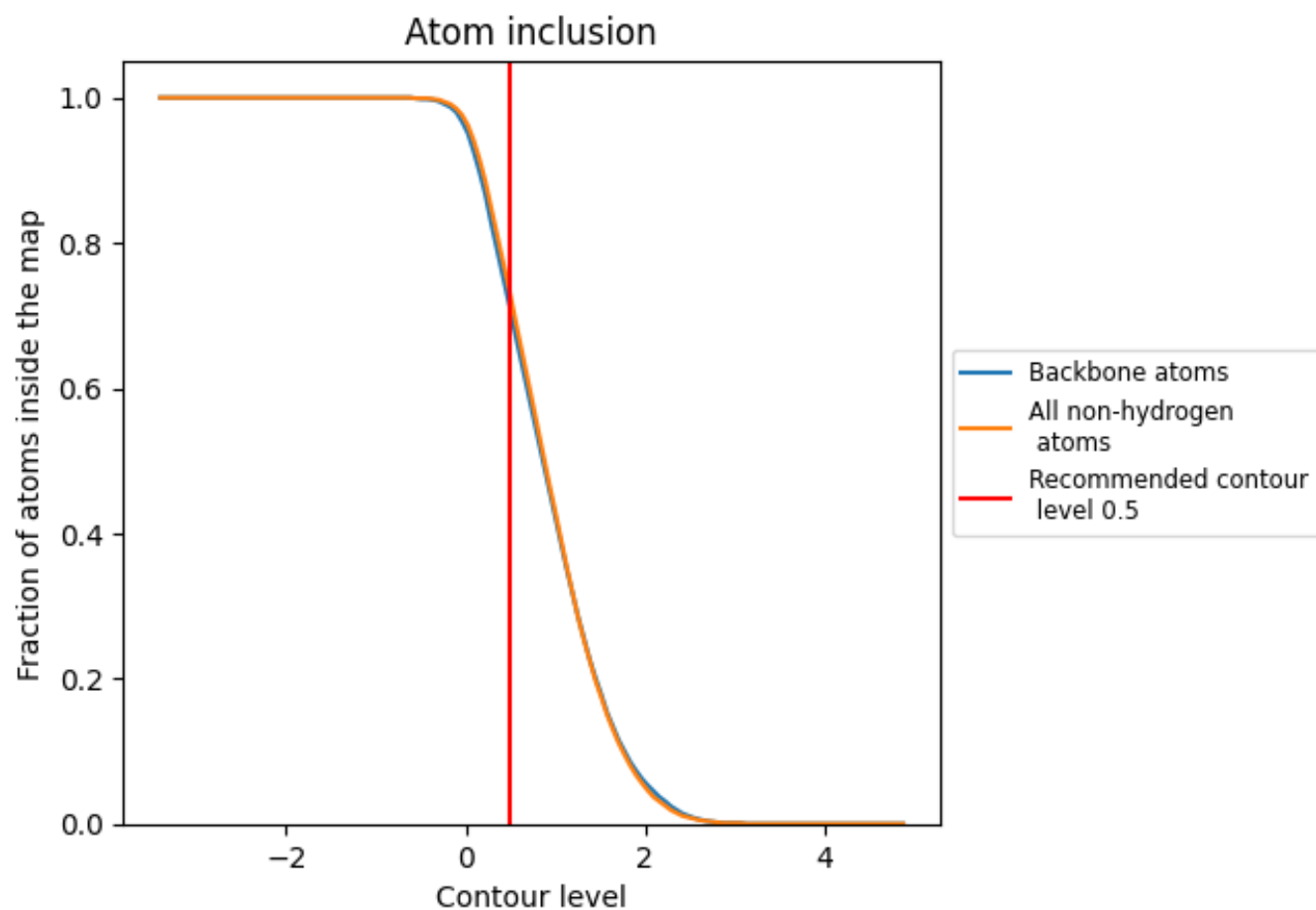
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 73% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.5460
1	0.6710	0.5260
2	0.6570	0.5240
3	0.6500	0.5290
4	0.6710	0.5180
A	0.8050	0.5680
B	0.8170	0.5730
C	0.8060	0.5680
D	0.6760	0.5320
E	0.6970	0.5370
F	0.7070	0.5490
G	0.6660	0.5370
H	0.2460	0.3980
I	0.7040	0.5450
J	0.7580	0.5580
K	0.5540	0.5000
L	0.5940	0.5040
M	0.6310	0.5120

1.0

0.0

<0.0