



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2025 – 12:44 PM JST

PDB ID : 5ZJI / pdb_00005zji
EMDB ID : EMD-6932
Title : Structure of photosystem I supercomplex with light-harvesting complexes I and II
Authors : Pan, X.W.; Ma, J.; Su, X.D.; Cao, P.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2018-03-20
Resolution : 3.30 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

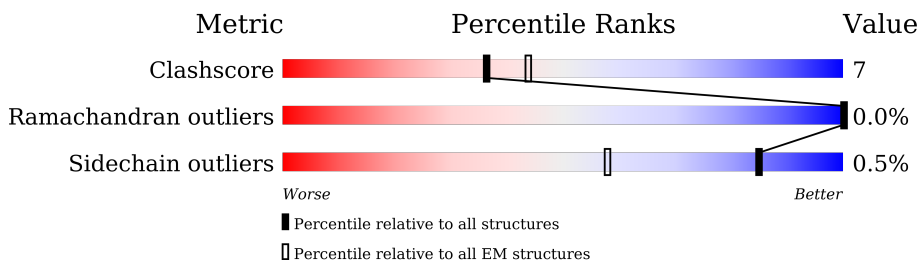
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	245	
2	2	270	
3	3	267	
4	4	252	
5	A	750	
6	B	734	
7	C	81	
8	D	199	

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Mol	Chain	Length	Quality of chain
9	E	136	
10	F	225	
11	G	145	
12	H	142	
13	I	36	
14	J	42	
15	K	134	
16	L	211	
17	O	127	
18	N	145	
19	X	232	
19	Z	232	
20	Y	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	1	601	X	-	-	-
21	CHL	1	607	X	-	-	-
21	CHL	2	601	X	-	-	-
21	CHL	2	606	X	-	-	-
21	CHL	2	607	X	-	-	-
21	CHL	2	608	X	-	-	-
21	CHL	2	618	X	-	-	-
21	CHL	3	608	X	-	-	-
21	CHL	4	606	X	-	-	-
21	CHL	4	607	X	-	-	-
21	CHL	4	608	X	-	-	-
21	CHL	4	618	X	-	-	-
21	CHL	X	601	X	-	-	-
21	CHL	X	605	X	-	-	-
21	CHL	X	606	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	617	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	302	X	-	-	-
22	CLA	L	303	X	-	-	-
22	CLA	L	304	X	-	-	-
22	CLA	N	1002	X	-	-	-
22	CLA	O	2001	X	-	-	-
22	CLA	O	2002	X	-	-	-
22	CLA	X	602	X	-	-	-
22	CLA	X	603	X	-	-	-
22	CLA	X	604	X	-	-	-
22	CLA	X	610	X	-	-	-
22	CLA	X	611	X	-	-	-
22	CLA	X	612	X	-	-	-
22	CLA	X	613	X	-	-	-
22	CLA	X	614	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
28	CL0	A	801	X	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 44708 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	196	Total	C	N	O	S	0	0
			1522	991	253	272	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	207	Total	C	N	O	S	0	0
			1624	1064	263	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1720	1130	276	307	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	199	Total	C	N	O	S	0	0
			1566	1020	257	285	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5836	3824	992	1002	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P04966

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5866	3849	997	1007	13		

- Molecule 7 is a protein called photosystem I subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	81	Total	C	N	O	S	0	0
			612	377	105	118	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1115	717	193	202	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	68	Total	C	N	O	0	0
			540	344	97	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	158	Total	C	N	O	S	0	0
			1238	805	212	218	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	97	Total	C	N	O	0	0
			752	489	125	138		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	95	Total	C	N	O	0	0
			729	477	116	136		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	33	Total	C	N	O	S	0	0
			260	178	38	43	1		

- 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	220	50	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			589	372	102	112	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	166	Total	C	N	O	S	0	0
			1246	820	198	226	2		

- Molecule 17 is a protein called 16kDa membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	76	Total	C	N	O	S	0	0
			621	418	101	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	84	Total	C	N	O	S	0	0
			685	439	112	129	5		

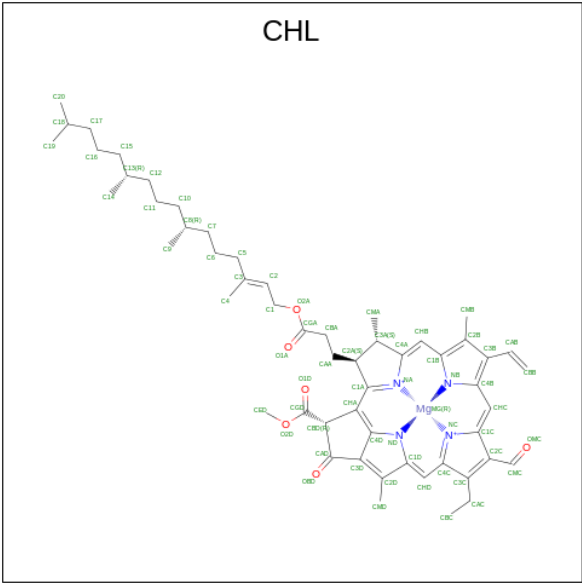
- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		
19	Z	218	Total	C	N	O	S	0	0
			1661	1080	269	306	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Y	228	Total	C	N	O	P	S	0	0
			1751	1132	290	322	1	6		

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



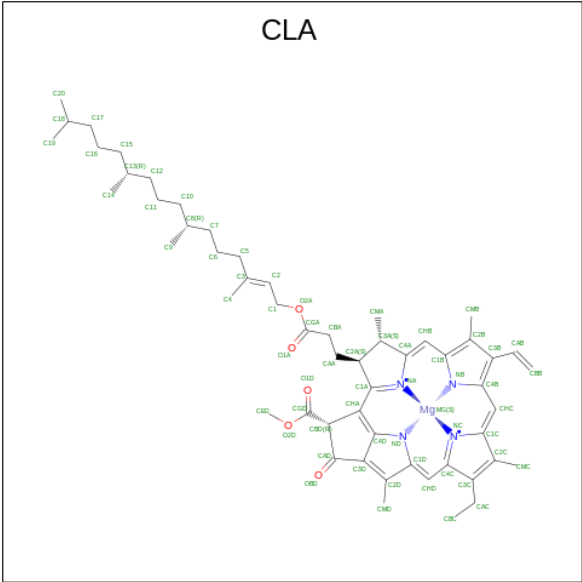
Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	X	1	Total 38	C 31	Mg 1	N 4	O 2	0
21	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	X	1	Total 39	C 30	Mg 1	N 4	O 4	0
21	X	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	X	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	X	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	Y	1	Total 63	C 53	Mg 1	N 4	O 5	0
21	Y	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	Y	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	Y	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	Y	1	Total 40	C 31	Mg 1	N 4	O 4	0
21	Y	1	Total 40	C 33	Mg 1	N 4	O 2	0
21	Z	1	Total 42	C 33	Mg 1	N 4	O 4	0
21	Z	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	Z	1	Total 39	C 32	Mg 1	N 4	O 2	0
21	Z	1	Total 44	C 33	Mg 1	N 4	O 6	0
21	Z	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	Z	1	Total 42	C 33	Mg 1	N 4	O 4	0

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



Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	2	1	Total 38	C 30	Mg 1	N 4	O 3	0
22	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
22	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	3	1	Total 36	C 30	Mg 1	N 4	O 1	0
22	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
22	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 37	C 31	Mg 1	N 4	O 1	0
22	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 39	C 31	Mg 1	N 4	O 3	0

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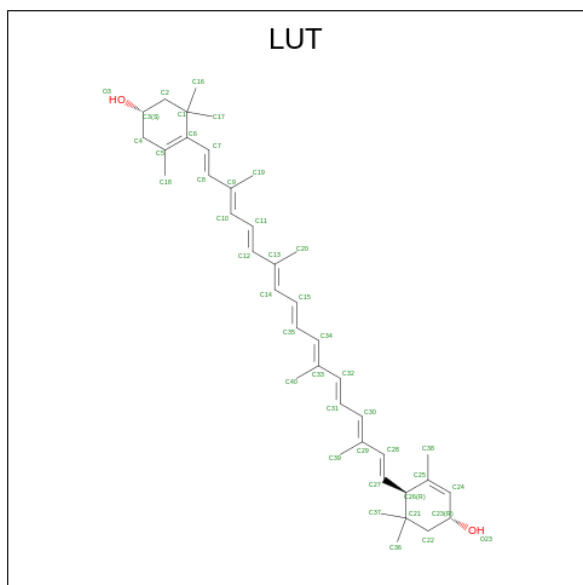
Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
22	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	X	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	X	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	X	1	Total 35	C 29	Mg 1	N 4	O 1	0
22	X	1	Total 39	C 32	Mg 1	N 4	O 2	0
22	X	1	Total 39	C 31	Mg 1	N 4	O 3	0
22	X	1	Total 36	C 30	Mg 1	N 4	O 1	0
22	X	1	Total 36	C 30	Mg 1	N 4	O 1	0
22	X	1	Total 39	C 31	Mg 1	N 4	O 3	0
22	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Y	1	Total 39	C 31	Mg 1	N 4	O 3	0
22	Y	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	Y	1	Total 39	C 31	Mg 1	N 4	O 3	0
22	Y	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	Y	1	Total 38	C 30	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
22	Y	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	Z	1	Total	C	Mg	N		0
			36	31	1	4		
22	Z	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
22	Z	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
22	Z	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	Z	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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



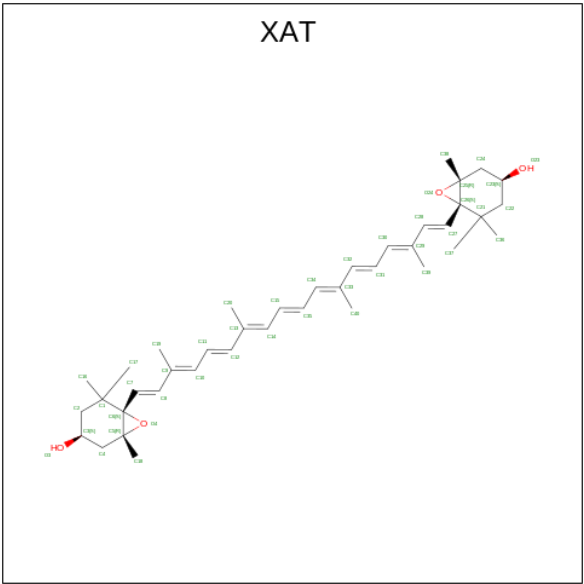
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	
23	3	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	X	1	Total	C	O	0
			42	40	2	
23	X	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	Z	1	Total	C	O	0
			42	40	2	
23	Z	1	Total	C	O	0
			42	40	2	

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



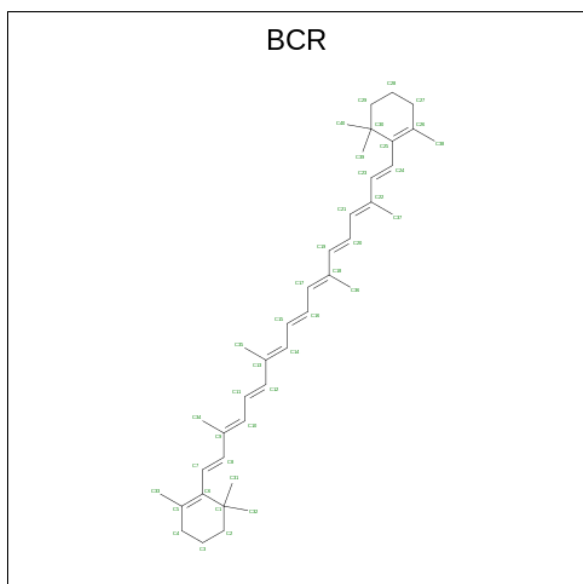
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	X	1	Total	C	O	0
			44	40	4	
24	Y	1	Total	C	O	0
			44	40	4	
24	Z	1	Total	C	O	0
			44	40	4	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



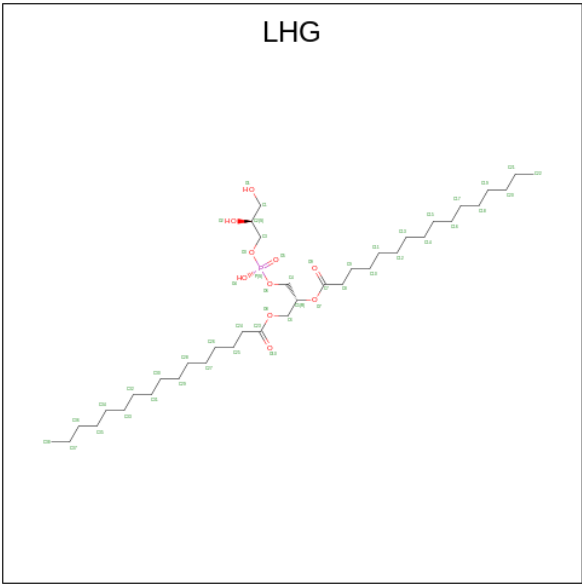
Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	2	1	Total	C	0
			40	40	
25	3	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	

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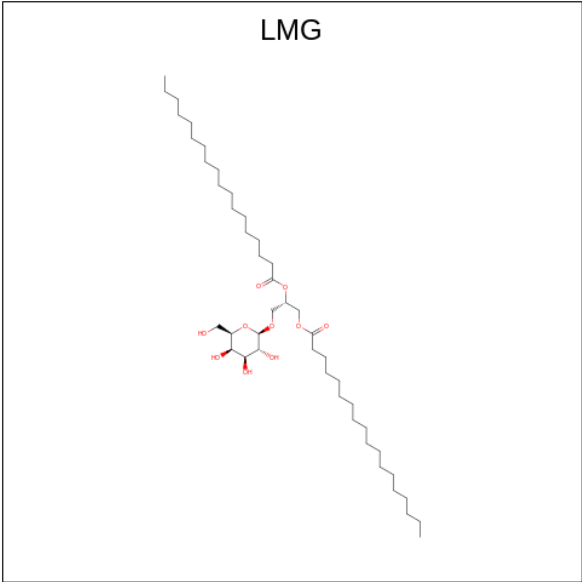
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C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

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



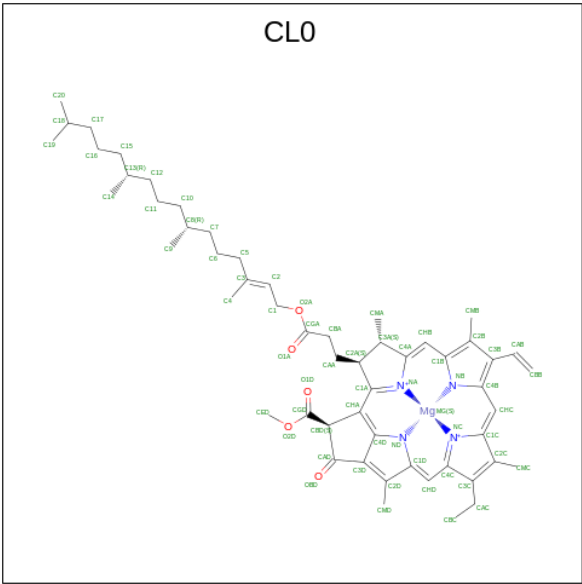
Mol	Chain	Residues	Atoms				AltConf
26	1	1	Total	C	O	P	0
			49	38	10	1	
26	2	1	Total	C	O	P	0
			37	26	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			30	19	10	1	
26	B	1	Total	C	O	P	0
			38	27	10	1	
26	X	1	Total	C	O	P	0
			22	11	10	1	
26	Y	1	Total	C	O	P	0
			45	34	10	1	
26	Z	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



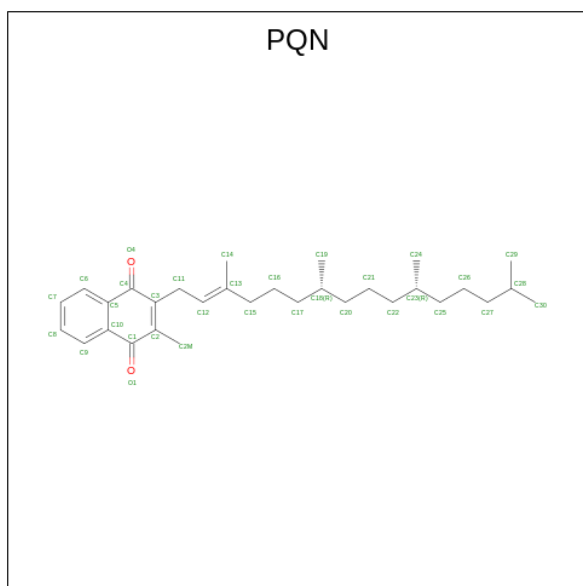
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			53	43	10	
27	2	1	Total	C	O	0
			36	26	10	
27	4	1	Total	C	O	0
			39	29	10	
27	4	1	Total	C	O	0
			33	23	10	
27	G	1	Total	C	O	0
			38	28	10	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



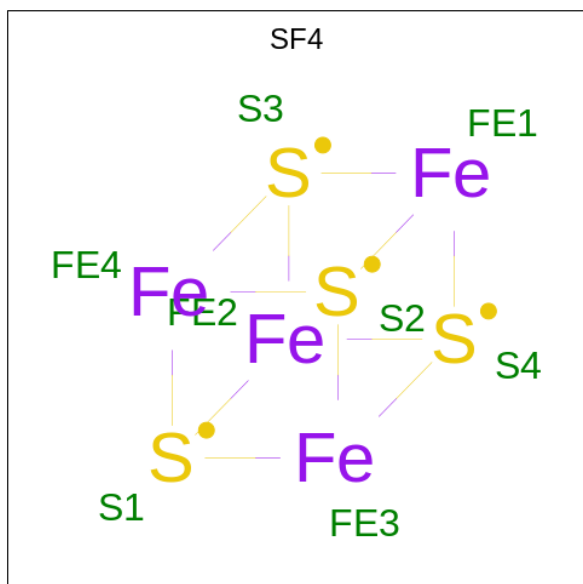
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



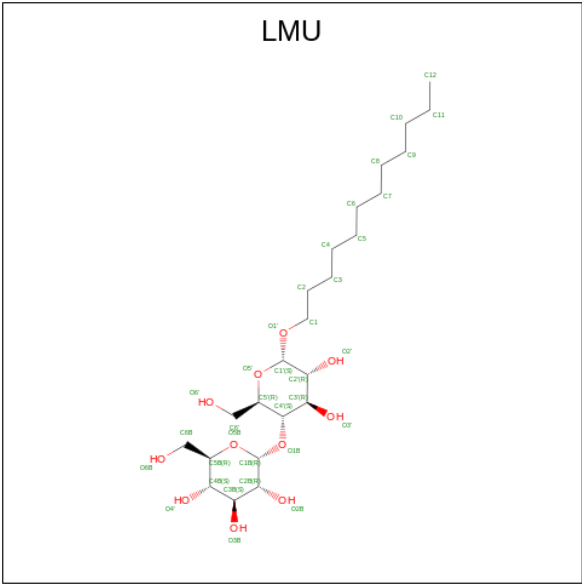
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



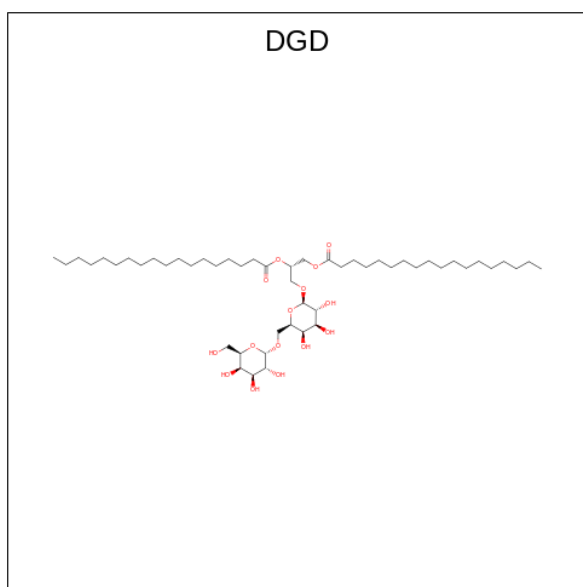
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



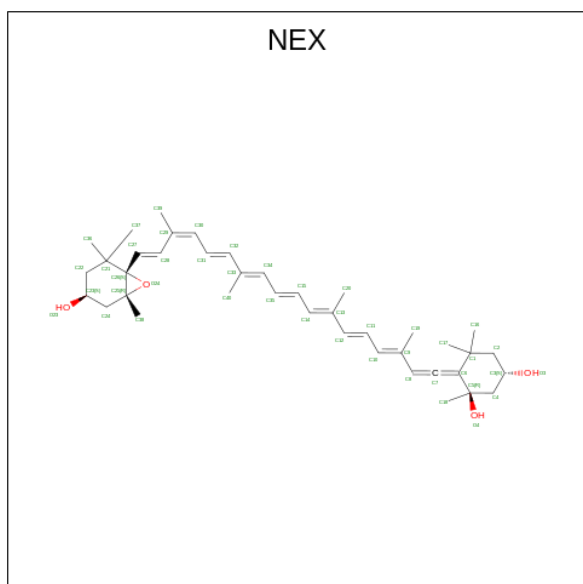
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			30	19	11	
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 33 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).

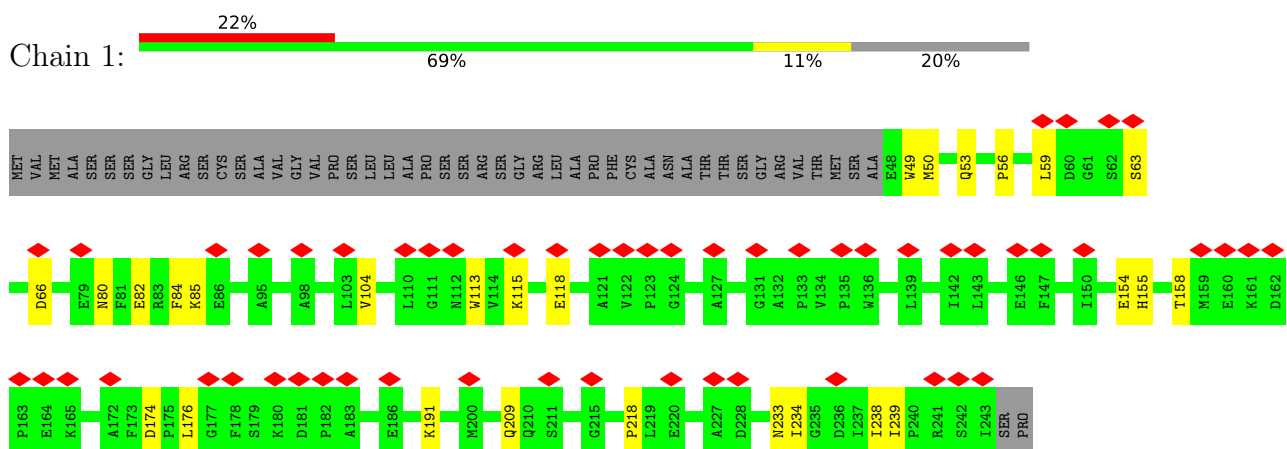


Mol	Chain	Residues	Atoms			AltConf
33	X	1	Total 44	C 40	O 4	0
33	Y	1	Total 44	C 40	O 4	0
33	Z	1	Total 44	C 40	O 4	0

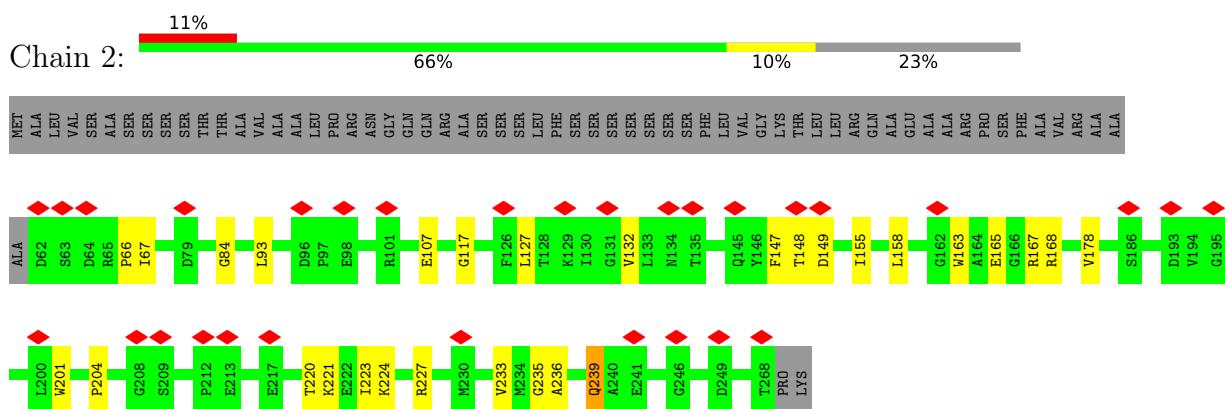
3 Residue-property plots

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.

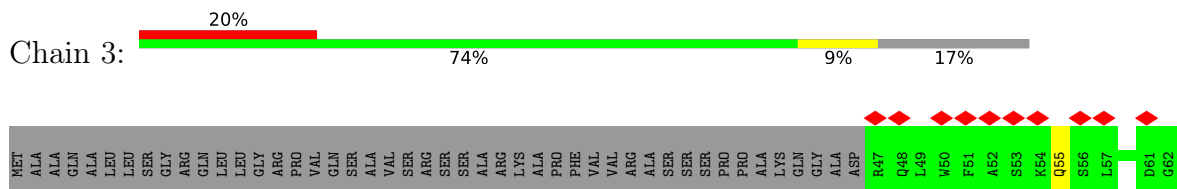
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

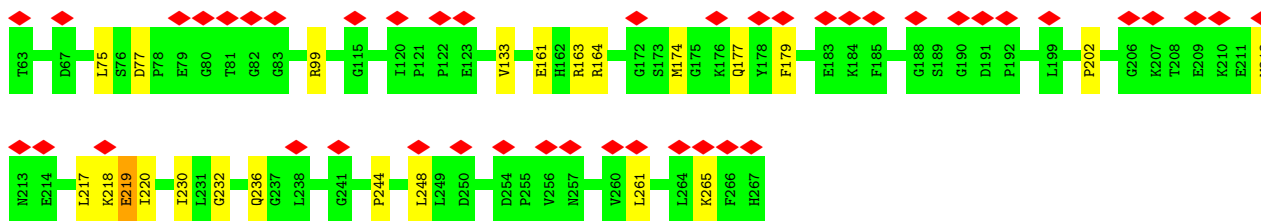


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

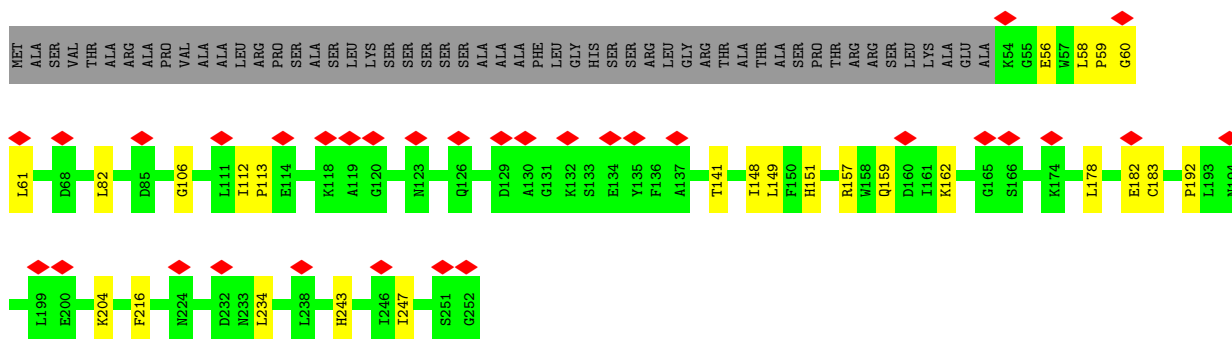


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

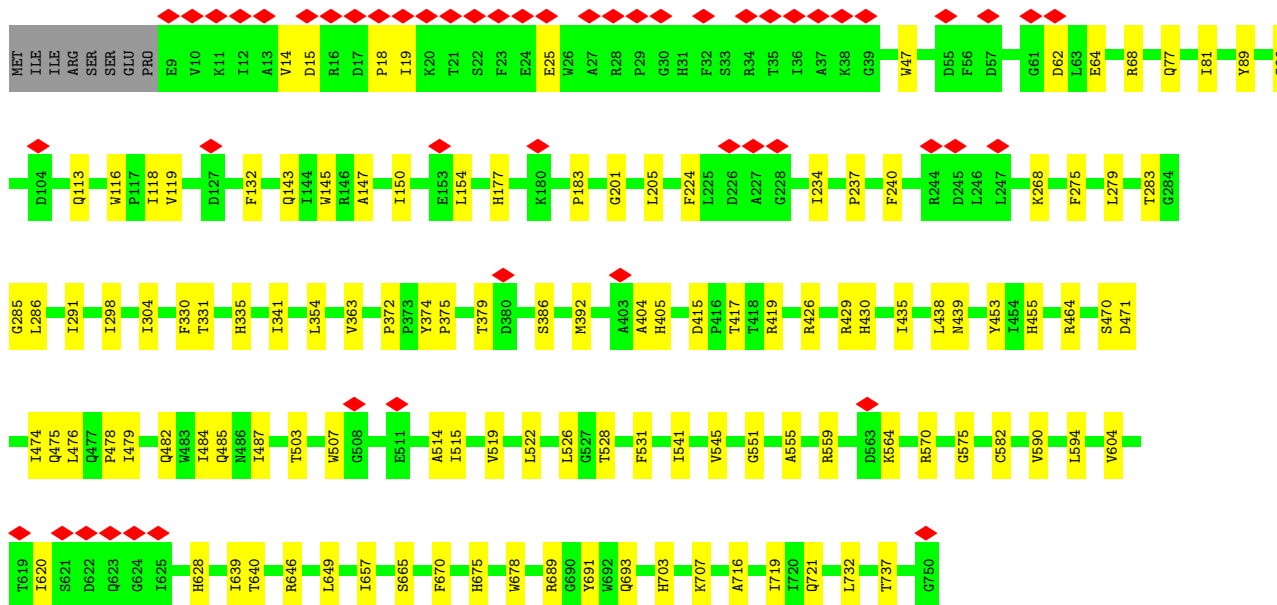
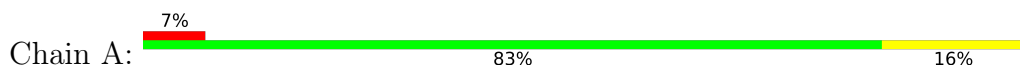




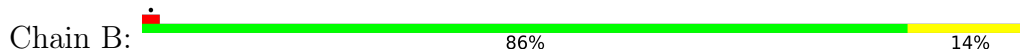
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

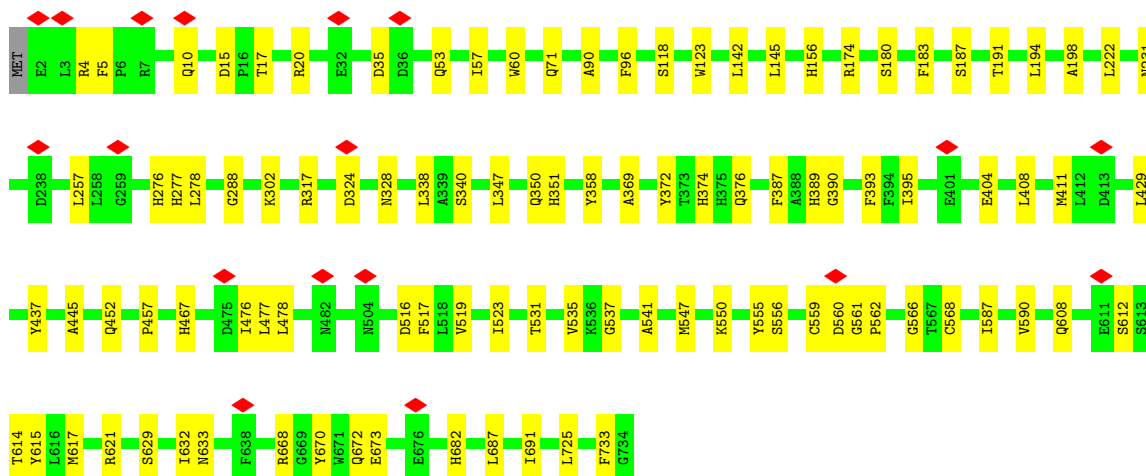


- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

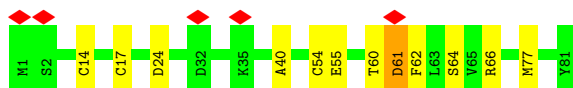
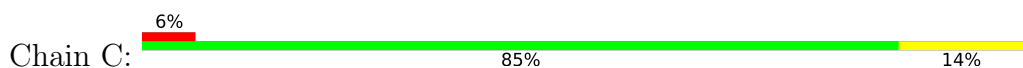


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

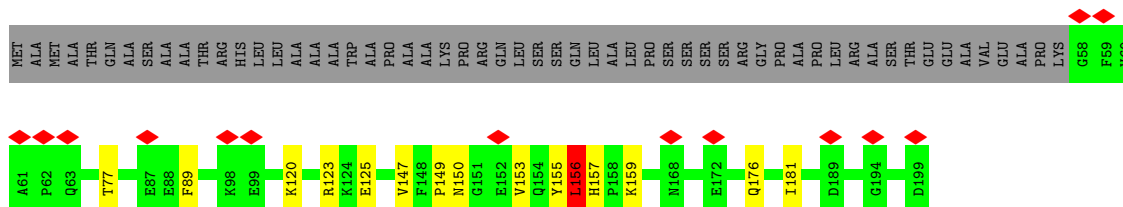




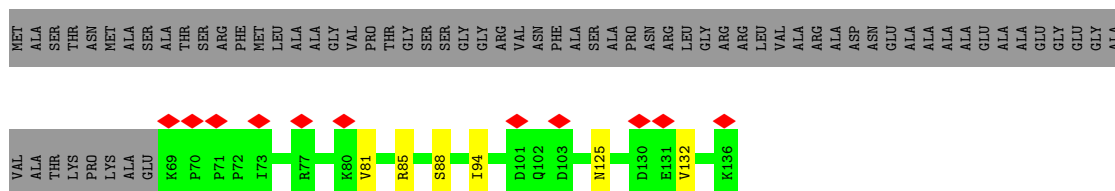
• Molecule 7: photosystem I subunit VII



• Molecule 8: Photosystem I reaction center subunit II

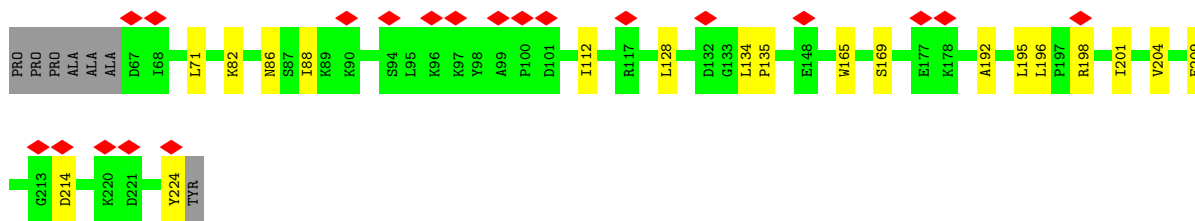


• Molecule 9: Photosystem I reaction center subunit IV A

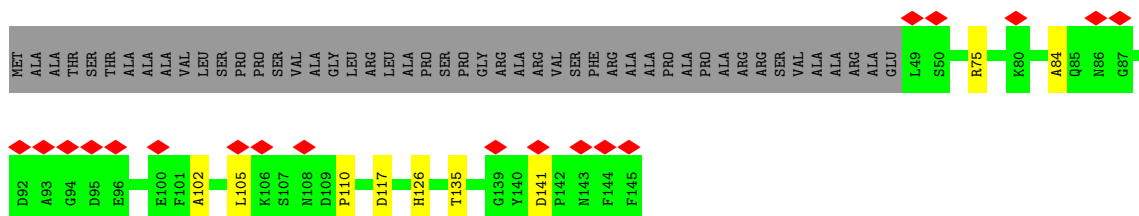


• Molecule 10: Photosystem I reaction center subunit III

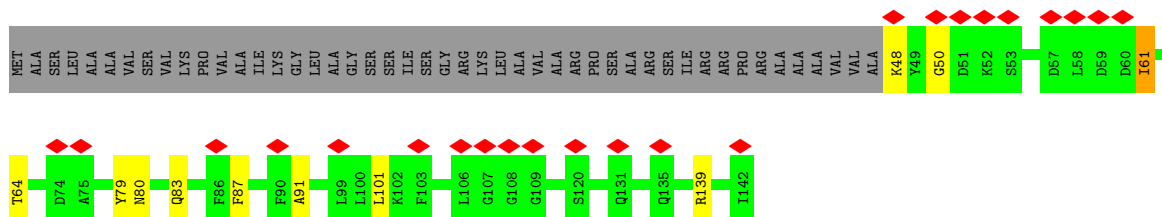




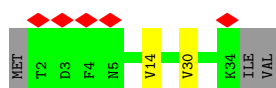
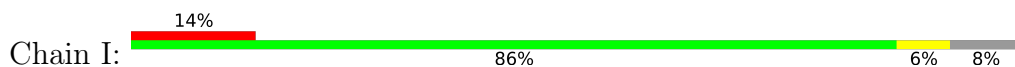
• Molecule 11: Photosystem I reaction center subunit V



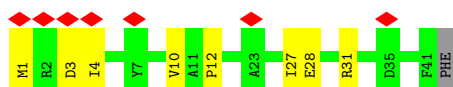
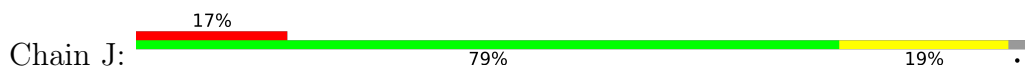
• Molecule 12: Photosystem I reaction center subunit VI, chloroplastic



• Molecule 13: Photosystem I reaction center subunit VIII



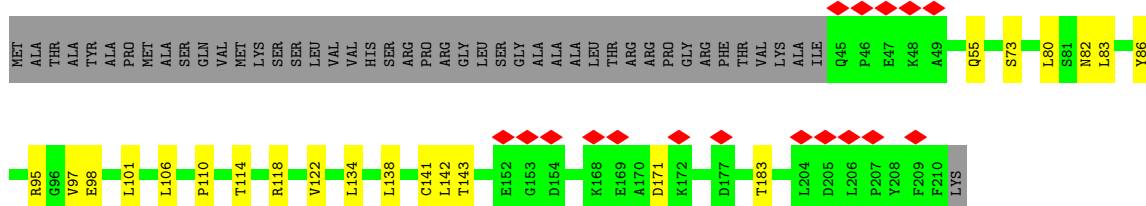
• Molecule 14: Photosystem I reaction center subunit IX



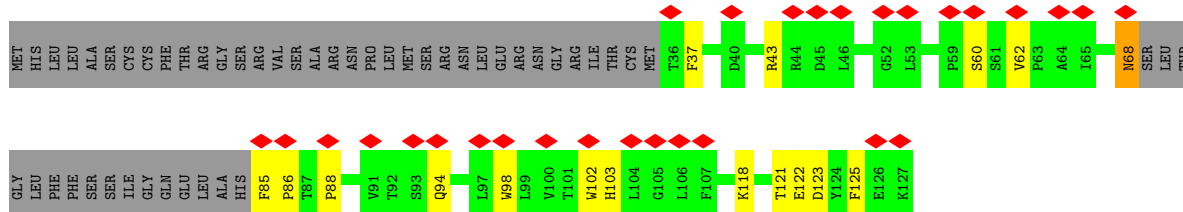
• Molecule 15: Photosystem I reaction center subunit psaK



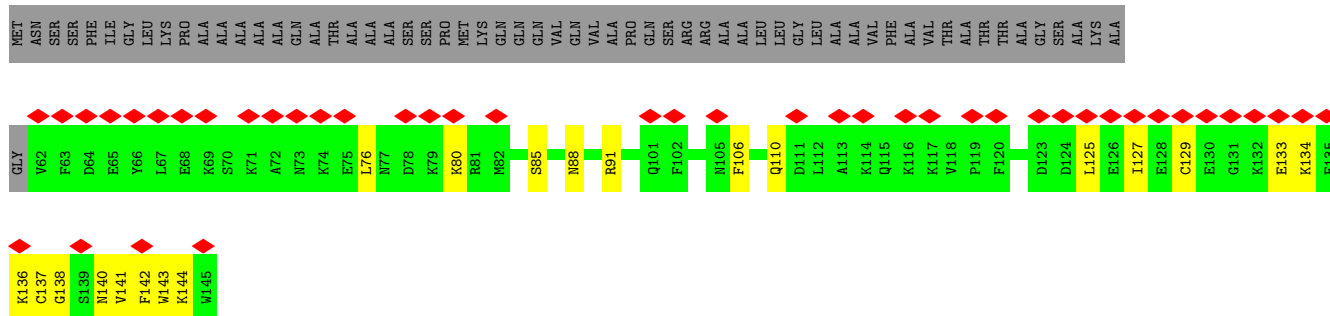
- Molecule 16: Photosystem I reaction center subunit XI



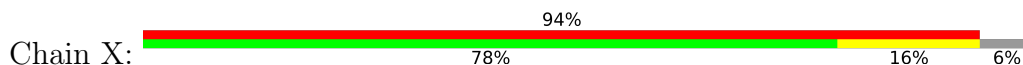
- Molecule 17: 16kDa membrane protein

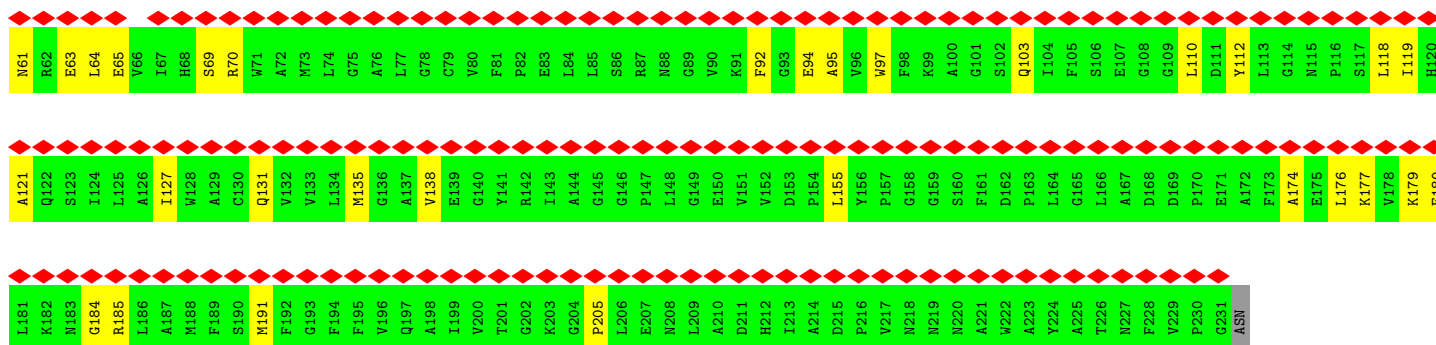


- Molecule 18: Photosystem I reaction center subunit N

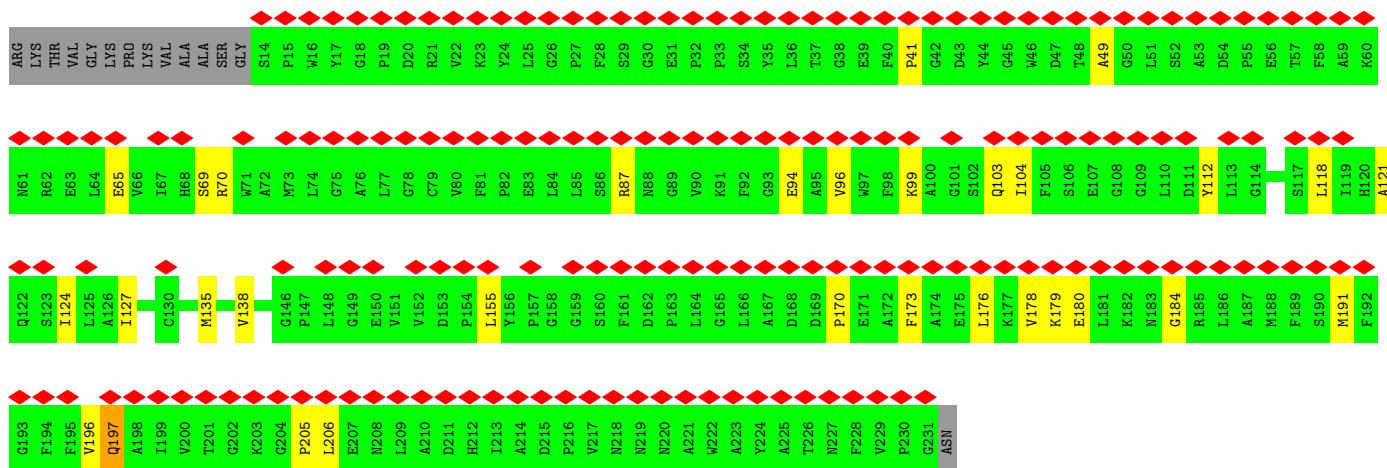
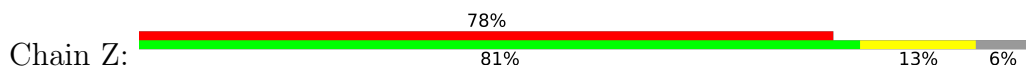


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

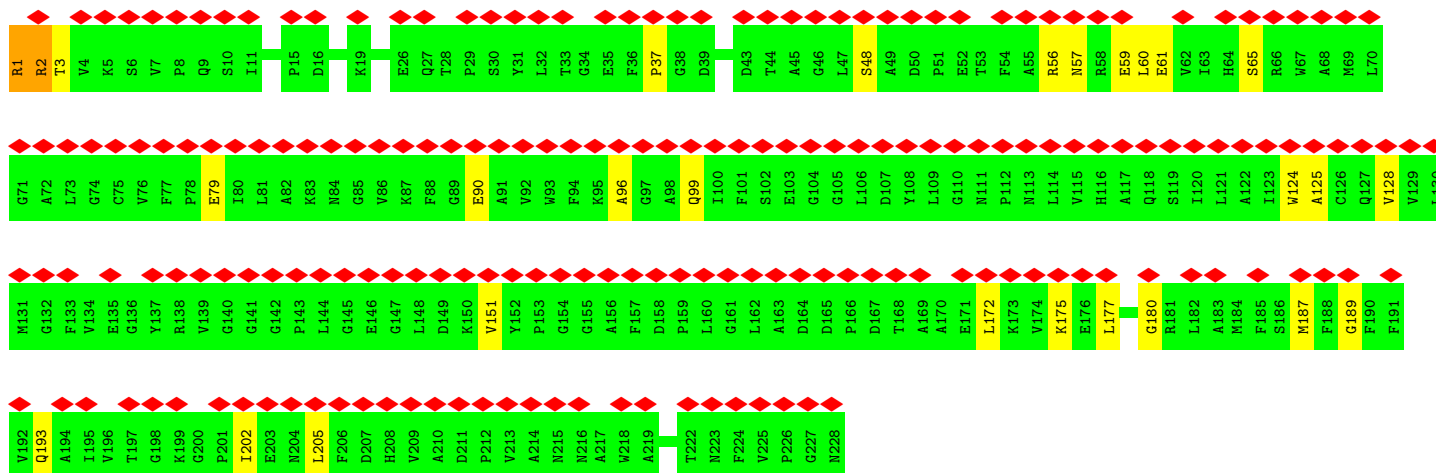
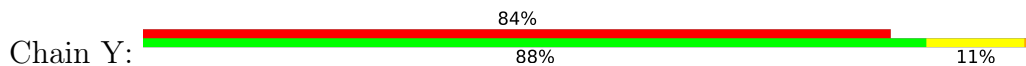




• Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	635845	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 ($e^-/\text{\AA}^2$)	50.0	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	0.292	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	296.8, 296.8, 296.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.35	1/1574 (0.1%)	0.61	0/2146
2	2	0.33	0/1684	0.63	1/2305 (0.0%)
3	3	0.34	0/1775	0.66	1/2410 (0.0%)
4	4	0.32	0/1617	0.61	0/2208
5	A	0.41	0/6034	0.63	0/8229
6	B	0.40	0/6077	0.63	2/8300 (0.0%)
7	C	0.43	0/623	0.75	0/844
8	D	0.37	0/1144	0.77	1/1547 (0.1%)
9	E	0.31	0/553	0.56	0/754
10	F	0.33	0/1267	0.62	0/1713
11	G	0.26	0/771	0.52	0/1046
12	H	0.30	0/752	0.60	0/1022
13	I	0.41	0/267	0.84	0/364
14	J	0.32	0/334	0.62	0/455
15	K	0.29	0/595	0.67	0/806
16	L	0.33	0/1284	0.66	1/1758 (0.1%)
17	O	0.36	0/646	0.84	2/882 (0.2%)
18	N	0.27	0/701	0.59	0/938
19	X	0.25	0/1714	0.52	0/2336
19	Z	0.25	0/1714	0.52	0/2336
20	Y	0.27	0/1792	0.60	0/2437
All	All	0.35	1/32918 (0.0%)	0.63	8/44836 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	104	VAL	C-N	6.39	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	156	LEU	N-CA-C	8.84	129.63	110.80
3	3	219	GLU	CA-CB-CG	6.73	127.56	114.10
17	O	94	GLN	CA-C-N	6.58	134.10	121.54
17	O	94	GLN	C-N-CA	6.58	134.10	121.54
16	L	73	SER	N-CA-C	-5.93	102.79	108.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	1522	0	1484	21	0
2	2	1624	0	1555	36	0
3	3	1720	0	1686	19	0
4	4	1566	0	1520	26	0
5	A	5836	0	5689	102	0
6	B	5866	0	5644	79	0
7	C	612	0	607	16	0
8	D	1115	0	1118	19	0
9	E	540	0	539	5	0
10	F	1238	0	1272	12	0
11	G	752	0	731	7	0
12	H	729	0	724	11	0
13	I	260	0	274	2	0
14	J	325	0	340	6	0
15	K	589	0	612	8	0
16	L	1246	0	1242	16	0
17	O	621	0	606	11	0
18	N	685	0	658	16	0
19	X	1661	0	1593	27	0
19	Z	1661	0	1593	24	0
20	Y	1751	0	1688	27	0
21	1	96	0	68	4	0
21	2	240	0	176	7	0
21	3	45	0	30	1	0
21	4	169	0	100	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	235	0	128	3	0
21	Y	259	0	156	1	0
21	Z	250	0	144	0	0
22	1	577	0	453	11	0
22	2	442	0	366	6	0
22	3	538	0	399	8	0
22	4	527	0	412	13	0
22	A	2533	0	2495	78	0
22	B	2261	0	2201	64	0
22	F	140	0	113	2	0
22	G	132	0	97	3	0
22	H	60	0	59	4	0
22	J	42	0	31	0	0
22	K	167	0	116	4	0
22	L	150	0	125	6	0
22	N	95	0	69	3	0
22	O	76	0	38	1	0
22	X	305	0	181	7	0
22	Y	325	0	194	3	0
22	Z	339	0	228	7	0
23	1	84	0	112	7	0
23	2	42	0	56	9	0
23	3	42	0	56	4	0
23	4	42	0	56	4	0
23	X	84	0	112	6	0
23	Y	84	0	112	5	0
23	Z	84	0	112	7	0
24	1	44	0	56	0	0
24	2	44	0	56	4	0
24	3	44	0	56	4	0
24	4	44	0	56	5	0
24	X	44	0	56	3	0
24	Y	44	0	56	2	0
24	Z	44	0	56	1	0
25	1	40	0	56	0	0
25	2	40	0	56	2	0
25	3	40	0	56	2	0
25	4	40	0	56	1	0
25	A	240	0	336	25	0
25	B	280	0	392	20	0
25	F	40	0	56	1	0
25	G	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	I	40	0	56	3	0
25	J	40	0	56	1	0
25	K	80	0	112	6	0
25	L	120	0	168	8	0
26	1	49	0	74	6	0
26	2	37	0	44	3	0
26	A	79	0	104	5	0
26	B	38	0	46	0	0
26	X	22	0	16	1	0
26	Y	45	0	60	4	0
26	Z	23	0	16	0	0
27	1	53	0	79	2	0
27	2	36	0	42	1	0
27	4	72	0	84	3	0
27	G	38	0	46	1	0
28	A	65	0	72	22	0
29	A	33	0	46	6	0
29	B	33	0	46	7	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	A	30	0	33	4	0
31	B	35	0	46	5	0
32	B	66	0	96	7	0
32	J	66	0	96	1	0
33	X	44	0	56	3	0
33	Y	44	0	56	2	0
33	Z	44	0	56	2	0
All	All	44708	0	43232	656	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 7.

The worst 5 of 656 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)
2:2:239:GLN:NE2	23:2:619:LUT:H42	1.53	1.21
2:2:235:GLY:O	2:2:239:GLN:HG2	1.62	0.97
2:2:236:ALA:HA	2:2:239:GLN:HG3	1.50	0.90
2:2:239:GLN:HE22	23:2:619:LUT:H42	1.38	0.89
20:Y:1:ARG:HG2	20:Y:1:ARG:HH11	1.39	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/245 (79%)	177 (91%)	17 (9%)	0	100	100
2	2	205/270 (76%)	199 (97%)	6 (3%)	0	100	100
3	3	219/267 (82%)	205 (94%)	14 (6%)	0	100	100
4	4	197/252 (78%)	182 (92%)	15 (8%)	0	100	100
5	A	740/750 (99%)	705 (95%)	35 (5%)	0	100	100
6	B	731/734 (100%)	699 (96%)	32 (4%)	0	100	100
7	C	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
8	D	140/199 (70%)	126 (90%)	14 (10%)	0	100	100
9	E	66/136 (48%)	61 (92%)	5 (8%)	0	100	100
10	F	156/225 (69%)	148 (95%)	8 (5%)	0	100	100
11	G	95/145 (66%)	91 (96%)	4 (4%)	0	100	100
12	H	93/142 (66%)	84 (90%)	9 (10%)	0	100	100
13	I	31/36 (86%)	26 (84%)	5 (16%)	0	100	100
14	J	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
15	K	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
16	L	164/211 (78%)	155 (94%)	9 (6%)	0	100	100
17	O	72/127 (57%)	60 (83%)	12 (17%)	0	100	100
18	N	82/145 (57%)	69 (84%)	13 (16%)	0	100	100
19	X	216/232 (93%)	202 (94%)	14 (6%)	0	100	100
19	Z	216/232 (93%)	205 (95%)	11 (5%)	0	100	100
20	Y	225/228 (99%)	202 (90%)	22 (10%)	1 (0%)	30	61
All	All	4042/4833 (84%)	3781 (94%)	260 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	Y	2	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	156/194 (80%)	156 (100%)	0	100	100
2	2	167/215 (78%)	166 (99%)	1 (1%)	84	90
3	3	176/210 (84%)	176 (100%)	0	100	100
4	4	166/204 (81%)	165 (99%)	1 (1%)	84	90
5	A	599/607 (99%)	598 (100%)	1 (0%)	92	95
6	B	599/600 (100%)	598 (100%)	1 (0%)	92	95
7	C	71/71 (100%)	70 (99%)	1 (1%)	62	78
8	D	119/159 (75%)	118 (99%)	1 (1%)	79	87
9	E	59/103 (57%)	57 (97%)	2 (3%)	32	59
10	F	127/171 (74%)	127 (100%)	0	100	100
11	G	79/110 (72%)	79 (100%)	0	100	100
12	H	78/110 (71%)	77 (99%)	1 (1%)	65	79
13	I	30/33 (91%)	30 (100%)	0	100	100
14	J	35/36 (97%)	34 (97%)	1 (3%)	37	63
15	K	59/96 (62%)	59 (100%)	0	100	100
16	L	130/164 (79%)	128 (98%)	2 (2%)	60	77
17	O	66/110 (60%)	65 (98%)	1 (2%)	60	77
18	N	73/111 (66%)	73 (100%)	0	100	100
19	X	168/178 (94%)	168 (100%)	0	100	100
19	Z	168/178 (94%)	167 (99%)	1 (1%)	84	90
20	Y	175/175 (100%)	174 (99%)	1 (1%)	84	90
All	All	3300/3835 (86%)	3285 (100%)	15 (0%)	85	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	E	132	VAL
20	Y	1	ARG
12	H	61	ILE
19	Z	197	GLN
16	L	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	114	ASN
6	B	633	ASN
20	Y	57	ASN
6	B	350	GLN
6	B	482	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	TPO	Y	3	20	8,10,11	1.06	0	10,14,16	1.63	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	TPO	Y	3	20	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	3	TPO	P-OG1-CB	-4.53	109.54	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

271 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	4	602	4	60,68,73	1.49	7 (11%)	70,107,113	1.60	10 (14%)
22	CLA	4	609	4	45,53,73	1.78	10 (22%)	52,89,113	1.84	9 (17%)
22	CLA	B	839	-	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
25	BCR	K	205	-	41,41,41	0.72	0	56,56,56	1.95	14 (25%)
25	BCR	B	801	-	41,41,41	0.78	0	56,56,56	2.09	12 (21%)
25	BCR	J	102	-	41,41,41	0.81	0	56,56,56	2.02	15 (26%)
22	CLA	X	604	-	36,43,73	2.01	8 (22%)	45,76,113	1.78	9 (20%)
22	CLA	B	826	-	62,70,73	1.50	9 (14%)	72,109,113	1.54	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	L	306	-	41,41,41	0.76	0	56,56,56	1.84	13 (23%)
21	CHL	Z	609	19	41,50,74	2.27	12 (29%)	42,85,114	3.00	17 (40%)
22	CLA	3	604	-	41,50,73	1.89	8 (19%)	51,86,113	1.73	8 (15%)
31	LMU	A	857	-	31,31,36	1.37	3 (9%)	42,42,47	1.55	8 (19%)
22	CLA	2	604	-	43,51,73	1.79	7 (16%)	48,86,113	1.70	6 (12%)
22	CLA	B	824	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
26	LHG	2	622	22	36,36,48	0.74	1 (2%)	39,42,54	1.29	5 (12%)
23	LUT	Y	4621	-	42,43,43	0.75	0	51,60,60	1.51	10 (19%)
22	CLA	B	822	-	42,50,73	1.79	8 (19%)	48,85,113	1.71	9 (18%)
22	CLA	A	833	-	56,64,73	1.52	8 (14%)	65,102,113	1.69	7 (10%)
22	CLA	Z	611	26	39,47,73	1.95	7 (17%)	49,82,113	1.81	11 (22%)
33	NEX	Y	4623	-	38,46,46	0.89	1 (2%)	50,70,70	2.37	19 (38%)
22	CLA	2	614	-	43,51,73	1.73	7 (16%)	49,86,113	1.93	11 (22%)
22	CLA	A	814	-	65,73,73	1.41	8 (12%)	76,113,113	1.44	9 (11%)
22	CLA	K	204	-	46,54,73	1.70	8 (17%)	53,90,113	1.63	7 (13%)
25	BCR	3	620	-	41,41,41	0.74	0	56,56,56	1.99	16 (28%)
26	LHG	Y	4630	22	44,44,48	0.60	0	47,50,54	1.23	4 (8%)
22	CLA	4	610	4	54,62,73	1.60	10 (18%)	62,99,113	1.62	6 (9%)
22	CLA	B	820	-	50,58,73	1.66	8 (16%)	58,95,113	1.65	6 (10%)
26	LHG	X	2630	22	21,21,48	0.85	1 (4%)	22,26,54	1.12	1 (4%)
23	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.71	15 (29%)
22	CLA	A	824	-	41,49,73	1.84	9 (21%)	47,84,113	1.79	11 (23%)
22	CLA	3	610	3	41,49,73	1.79	8 (19%)	47,84,113	1.80	8 (17%)
22	CLA	B	816	-	55,63,73	1.54	7 (12%)	64,101,113	1.73	6 (9%)
21	CHL	4	608	-	46,54,74	2.16	15 (32%)	49,90,114	2.83	18 (36%)
22	CLA	L	304	-	45,53,73	1.70	8 (17%)	52,89,113	1.88	9 (17%)
25	BCR	B	846	-	41,41,41	0.83	0	56,56,56	2.02	22 (39%)
22	CLA	B	805	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	11 (14%)
22	CLA	A	836	-	45,53,73	1.74	10 (22%)	52,89,113	1.70	6 (11%)
22	CLA	B	831	-	43,51,73	1.78	7 (16%)	49,86,113	1.77	7 (14%)
21	CHL	Z	605	19	37,46,74	2.37	14 (37%)	46,81,114	3.02	19 (41%)
22	CLA	F	303	-	42,50,73	1.81	7 (16%)	48,85,113	1.71	8 (16%)
22	CLA	O	2002	-	37,46,73	1.96	7 (18%)	46,81,113	2.02	11 (23%)
22	CLA	Z	604	-	46,54,73	1.78	8 (17%)	57,90,113	1.68	9 (15%)
23	LUT	2	619	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	614	-	45,53,73	1.79	7 (15%)	52,89,113	1.65	10 (19%)
22	CLA	A	854	-	65,73,73	1.46	8 (12%)	76,113,113	1.47	8 (10%)
21	CHL	2	607	-	43,51,74	2.14	12 (27%)	45,86,114	3.00	17 (37%)
22	CLA	N	1002	-	50,58,73	1.66	7 (14%)	58,95,113	1.71	7 (12%)
22	CLA	B	802	-	65,73,73	1.49	10 (15%)	76,113,113	1.33	5 (6%)
22	CLA	G	204	11	45,53,73	1.78	9 (20%)	52,89,113	1.64	7 (13%)
22	CLA	4	604	-	43,51,73	1.82	8 (18%)	54,87,113	1.69	8 (14%)
25	BCR	A	850	-	41,41,41	0.89	2 (4%)	56,56,56	2.25	19 (33%)
22	CLA	A	816	-	42,50,73	1.74	7 (16%)	48,85,113	1.84	8 (16%)
24	XAT	3	619	-	39,47,47	0.92	2 (5%)	54,74,74	2.51	19 (35%)
22	CLA	A	818	-	60,68,73	1.44	7 (11%)	70,107,113	1.83	12 (17%)
22	CLA	B	829	-	56,64,73	1.76	10 (17%)	65,102,113	1.89	10 (15%)
22	CLA	3	602	3	60,68,73	1.57	8 (13%)	70,107,113	1.47	8 (11%)
22	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	8 (12%)
25	BCR	A	856	-	41,41,41	0.73	0	56,56,56	1.88	14 (25%)
22	CLA	H	201	-	60,68,73	1.51	8 (13%)	70,107,113	1.48	8 (11%)
21	CHL	X	609	19	37,44,74	2.23	13 (35%)	46,77,114	2.91	24 (52%)
25	BCR	G	205	-	41,41,41	0.75	0	56,56,56	1.90	16 (28%)
22	CLA	B	804	-	41,49,73	1.76	7 (17%)	47,84,113	1.96	8 (17%)
22	CLA	L	303	-	60,68,73	1.51	9 (15%)	70,107,113	1.50	10 (14%)
27	LMG	2	623	-	36,36,55	1.01	2 (5%)	44,44,63	1.15	3 (6%)
25	BCR	B	843	-	41,41,41	0.84	1 (2%)	56,56,56	2.01	16 (28%)
21	CHL	Y	601	20	62,71,74	1.85	13 (20%)	76,111,114	2.32	21 (27%)
22	CLA	X	611	26	38,47,73	1.94	6 (15%)	44,81,113	1.64	7 (15%)
33	NEX	X	2623	-	38,46,46	0.86	1 (2%)	50,70,70	2.27	15 (30%)
22	CLA	A	827	-	59,67,73	1.51	9 (15%)	68,105,113	1.43	9 (13%)
25	BCR	2	621	-	41,41,41	0.71	0	56,56,56	1.87	11 (19%)
25	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.02	18 (32%)
22	CLA	Y	614	-	38,47,73	1.93	7 (18%)	47,82,113	1.84	10 (21%)
22	CLA	A	822	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	6 (7%)
21	CHL	X	607	-	41,49,74	2.39	15 (36%)	48,84,114	2.91	20 (41%)
22	CLA	A	828	-	65,73,73	1.44	9 (13%)	76,113,113	1.42	6 (7%)
30	SF4	A	853	-	0,12,12	-	-	-	-	-
22	CLA	3	614	-	39,48,73	1.85	7 (17%)	44,83,113	1.78	7 (15%)
27	LMG	4	622	-	39,39,55	0.90	1 (2%)	47,47,63	1.24	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	821	-	45,53,73	1.76	9 (20%)	52,89,113	1.71	7 (13%)
22	CLA	A	842	-	65,73,73	1.45	8 (12%)	76,113,113	1.54	9 (11%)
21	CHL	2	618	2	43,51,74	2.22	15 (34%)	45,86,114	3.04	20 (44%)
25	BCR	A	848	-	41,41,41	0.81	0	56,56,56	1.84	13 (23%)
22	CLA	B	828	-	65,73,73	1.44	11 (16%)	76,113,113	1.55	13 (17%)
23	LUT	Y	4620	-	42,43,43	0.75	0	51,60,60	1.63	13 (25%)
25	BCR	1	619	-	41,41,41	0.67	0	56,56,56	1.80	13 (23%)
22	CLA	Z	602	19	52,60,73	1.72	8 (15%)	64,97,113	1.59	8 (12%)
21	CHL	1	607	1	40,49,74	2.42	16 (40%)	41,84,114	2.85	20 (48%)
27	LMG	4	623	-	33,33,55	1.15	3 (9%)	41,41,63	1.20	6 (14%)
21	CHL	X	605	19	41,50,74	2.25	13 (31%)	49,85,114	2.68	16 (32%)
26	LHG	B	851	22	37,37,48	0.67	1 (2%)	40,43,54	1.23	4 (10%)
22	CLA	1	604	-	49,57,73	1.69	8 (16%)	55,93,113	1.66	7 (12%)
22	CLA	3	617	-	39,48,73	1.84	8 (20%)	44,83,113	1.76	8 (18%)
22	CLA	X	612	19	37,44,73	1.98	7 (18%)	46,77,113	1.84	10 (21%)
22	CLA	A	831	-	65,73,73	1.55	11 (16%)	76,113,113	1.65	8 (10%)
22	CLA	Z	613	19	43,51,73	1.78	6 (13%)	49,86,113	1.77	8 (16%)
21	CHL	4	618	4	40,49,74	2.16	12 (30%)	45,84,114	3.04	20 (44%)
22	CLA	3	607	3	41,49,73	1.87	7 (17%)	51,84,113	1.76	10 (19%)
22	CLA	A	845	26	50,58,73	1.66	8 (16%)	58,95,113	1.63	10 (17%)
22	CLA	B	807	6	52,60,73	1.61	9 (17%)	60,97,113	1.63	8 (13%)
22	CLA	B	838	-	47,55,73	1.71	8 (17%)	54,91,113	1.69	8 (14%)
22	CLA	3	603	3	55,63,73	1.61	10 (18%)	64,101,113	1.63	13 (20%)
23	LUT	X	2621	-	42,43,43	0.76	0	51,60,60	1.57	8 (15%)
22	CLA	B	810	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	11 (14%)
21	CHL	Z	601	19	41,50,74	2.38	16 (39%)	42,85,114	2.84	18 (42%)
22	CLA	2	612	2	44,52,73	1.79	8 (18%)	51,88,113	1.69	7 (13%)
22	CLA	B	834	-	60,68,73	1.50	8 (13%)	70,107,113	1.56	9 (12%)
22	CLA	B	809	6	65,73,73	1.49	10 (15%)	76,113,113	1.41	7 (9%)
23	LUT	Z	7621	-	42,43,43	0.80	1 (2%)	51,60,60	1.59	11 (21%)
21	CHL	Y	609	20	39,48,74	2.28	14 (35%)	42,82,114	2.95	17 (40%)
22	CLA	A	829	-	65,73,73	1.42	7 (10%)	76,113,113	1.67	10 (13%)
22	CLA	X	602	19	40,49,73	1.91	8 (20%)	45,84,113	1.62	6 (13%)
21	CHL	Z	607	-	43,52,74	5.32	15 (34%)	49,88,114	3.07	19 (38%)
22	CLA	F	301	-	57,65,73	1.60	9 (15%)	66,103,113	1.53	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	610	1	59,67,73	1.50	7 (11%)	69,106,113	1.55	7 (10%)
22	CLA	A	805	-	52,60,73	1.64	8 (15%)	60,97,113	1.68	8 (13%)
22	CLA	Y	610	20	39,47,73	1.93	7 (17%)	49,82,113	1.89	11 (22%)
22	CLA	Z	610	19	37,44,73	2.02	8 (21%)	41,77,113	1.85	8 (19%)
21	CHL	Y	605	20	37,46,74	2.46	14 (37%)	46,81,114	2.92	20 (43%)
22	CLA	2	602	2	65,73,73	1.49	10 (15%)	76,113,113	1.36	7 (9%)
22	CLA	A	810	5	50,58,73	1.68	10 (20%)	58,95,113	1.52	9 (15%)
30	SF4	C	102	-	0,12,12	-	-	-		
22	CLA	A	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	1	616	1	43,51,73	1.86	8 (18%)	54,87,113	1.70	10 (18%)
22	CLA	A	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.76	15 (19%)
24	XAT	1	618	-	39,47,47	0.99	2 (5%)	54,74,74	2.58	18 (33%)
22	CLA	4	612	4	40,49,73	1.83	7 (17%)	45,84,113	1.72	8 (17%)
22	CLA	Y	603	-	38,47,73	1.91	7 (18%)	43,82,113	1.74	7 (16%)
28	CL0	A	801	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	31 (40%)
22	CLA	A	804	-	65,73,73	1.42	8 (12%)	76,113,113	1.62	9 (11%)
26	LHG	1	620	22	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
22	CLA	1	612	1	45,53,73	1.79	7 (15%)	52,89,113	1.69	8 (15%)
22	CLA	4	601	4	46,54,73	1.74	10 (21%)	53,90,113	1.61	9 (16%)
22	CLA	B	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.91	12 (15%)
24	XAT	Z	4622	-	39,47,47	0.98	0	54,74,74	2.88	18 (33%)
22	CLA	B	830	-	43,51,73	1.77	10 (23%)	49,86,113	1.66	7 (14%)
25	BCR	K	202	-	41,41,41	0.78	0	56,56,56	2.25	14 (25%)
22	CLA	X	610	19	39,47,73	1.86	6 (15%)	42,81,113	1.87	7 (16%)
22	CLA	2	613	2	65,73,73	1.48	9 (13%)	76,113,113	1.52	7 (9%)
22	CLA	X	613	19	37,44,73	1.94	6 (16%)	42,77,113	1.91	8 (19%)
26	LHG	A	847	22	29,29,48	0.87	1 (3%)	32,35,54	1.26	3 (9%)
22	CLA	B	821	-	47,55,73	1.64	9 (19%)	54,91,113	1.77	9 (16%)
25	BCR	B	848	-	41,41,41	0.79	0	56,56,56	2.01	16 (28%)
22	CLA	A	807	5	65,73,73	1.47	10 (15%)	76,113,113	1.41	7 (9%)
21	CHL	X	606	-	38,47,74	2.31	14 (36%)	45,81,114	3.14	23 (51%)
22	CLA	A	825	-	55,63,73	1.59	10 (18%)	64,101,113	1.65	11 (17%)
22	CLA	B	835	-	42,50,73	1.86	9 (21%)	48,85,113	1.64	7 (14%)
24	XAT	2	620	-	39,47,47	0.98	1 (2%)	54,74,74	2.75	23 (42%)
22	CLA	A	834	-	65,73,73	1.46	8 (12%)	76,113,113	1.50	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	806	6	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
26	LHG	A	846	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	5 (9%)
21	CHL	Z	608	-	44,53,74	2.20	13 (29%)	46,89,114	2.93	17 (36%)
22	CLA	K	206	15	37,47,73	1.92	6 (16%)	42,81,113	1.81	10 (23%)
22	CLA	F	304	-	41,49,73	1.79	9 (21%)	47,84,113	1.76	7 (14%)
22	CLA	A	808	-	50,58,73	1.61	8 (16%)	58,95,113	1.68	8 (13%)
22	CLA	K	201	15	38,45,73	1.92	10 (26%)	43,78,113	1.86	9 (20%)
22	CLA	A	838	-	51,59,73	1.55	7 (13%)	59,96,113	1.91	14 (23%)
22	CLA	B	823	-	45,53,73	1.74	9 (20%)	52,89,113	1.73	7 (13%)
22	CLA	B	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.52	6 (7%)
22	CLA	Y	613	20	42,51,73	1.92	7 (16%)	52,87,113	1.77	8 (15%)
22	CLA	A	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.66	9 (11%)
22	CLA	3	606	3	40,49,73	1.82	10 (25%)	45,84,113	1.78	11 (24%)
22	CLA	A	826	-	65,73,73	1.43	8 (12%)	76,113,113	1.54	9 (11%)
22	CLA	G	203	-	42,50,73	1.77	7 (16%)	48,85,113	1.68	9 (18%)
22	CLA	3	613	3	53,62,73	1.61	8 (15%)	61,100,113	1.53	6 (9%)
22	CLA	N	1001	18	44,53,73	1.77	8 (18%)	50,89,113	1.65	7 (14%)
22	CLA	B	819	-	55,63,73	1.63	11 (20%)	64,101,113	1.60	7 (10%)
22	CLA	4	603	4	44,52,73	1.87	9 (20%)	55,88,113	1.65	11 (20%)
22	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.82	11 (18%)
22	CLA	A	823	-	42,50,73	1.75	7 (16%)	48,85,113	1.82	7 (14%)
22	CLA	Z	614	-	44,52,73	1.81	6 (13%)	51,88,113	1.60	6 (11%)
22	CLA	A	813	-	54,62,73	1.59	8 (14%)	62,99,113	1.66	6 (9%)
21	CHL	2	608	-	51,59,74	2.03	14 (27%)	55,96,114	2.80	20 (36%)
24	XAT	Y	2622	-	39,47,47	0.84	0	54,74,74	2.61	18 (33%)
21	CHL	Z	606	-	38,47,74	2.30	14 (36%)	41,81,114	2.97	20 (48%)
21	CHL	X	601	19	37,46,74	2.29	13 (35%)	44,80,114	3.06	20 (45%)
23	LUT	1	621	-	42,43,43	0.74	0	51,60,60	1.57	10 (19%)
22	CLA	1	611	26	37,46,73	1.94	9 (24%)	46,81,113	1.80	9 (19%)
22	CLA	1	608	-	43,52,73	1.80	6 (13%)	49,88,113	1.54	7 (14%)
21	CHL	4	606	-	40,49,74	2.22	13 (32%)	42,84,114	2.89	18 (42%)
21	CHL	2	601	2	61,69,74	1.88	14 (22%)	67,108,114	2.67	23 (34%)
22	CLA	B	841	26	65,73,73	1.43	9 (13%)	76,113,113	1.46	8 (10%)
22	CLA	O	2001	-	36,46,73	1.93	6 (16%)	41,80,113	1.67	7 (17%)
22	CLA	1	609	1	40,48,73	1.90	8 (20%)	50,83,113	1.86	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LUT	X	2620	-	42,43,43	0.70	0	51,60,60	1.65	9 (17%)
22	CLA	3	615	-	37,44,73	1.89	7 (18%)	42,77,113	1.83	7 (16%)
22	CLA	B	814	-	65,73,73	1.45	9 (13%)	76,113,113	1.58	8 (10%)
22	CLA	B	832	-	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
22	CLA	A	830	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
27	LMG	G	202	-	38,38,55	1.00	1 (2%)	46,46,63	1.22	6 (13%)
22	CLA	1	614	-	37,46,73	1.99	8 (21%)	46,81,113	1.81	10 (21%)
22	CLA	B	817	-	59,67,73	1.52	10 (16%)	68,105,113	1.50	7 (10%)
22	CLA	B	837	-	65,73,73	1.43	7 (10%)	76,113,113	1.64	11 (14%)
22	CLA	B	818	-	60,68,73	1.47	10 (16%)	70,107,113	1.59	9 (12%)
22	CLA	A	835	-	65,73,73	1.43	11 (16%)	76,113,113	1.67	13 (17%)
22	CLA	3	609	3	45,53,73	1.81	11 (24%)	52,89,113	1.83	11 (21%)
22	CLA	B	827	-	65,73,73	1.39	8 (12%)	76,113,113	1.55	8 (10%)
22	CLA	B	811	-	54,62,73	1.63	9 (16%)	67,100,113	1.57	9 (13%)
25	BCR	A	852	-	41,41,41	0.74	0	56,56,56	1.98	11 (19%)
22	CLA	G	201	-	45,53,73	1.76	9 (20%)	52,89,113	1.70	8 (15%)
22	CLA	A	812	-	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
22	CLA	J	101	14	42,50,73	1.80	6 (14%)	48,85,113	1.73	8 (16%)
25	BCR	I	101	-	41,41,41	0.83	0	56,56,56	2.14	18 (32%)
30	SF4	C	101	-	0,12,12	-	-	-	-	-
31	LMU	B	849	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
23	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	12 (23%)
22	CLA	2	603	-	43,52,73	1.78	10 (23%)	49,88,113	1.74	9 (18%)
22	CLA	A	840	-	52,60,73	1.63	8 (15%)	60,97,113	1.73	8 (13%)
22	CLA	A	815	-	45,53,73	1.70	9 (20%)	52,89,113	1.83	10 (19%)
25	BCR	B	847	-	41,41,41	1.03	3 (7%)	56,56,56	2.52	25 (44%)
24	XAT	X	7622	-	39,47,47	0.93	0	54,74,74	2.95	19 (35%)
27	LMG	1	622	-	53,53,55	0.84	2 (3%)	61,61,63	1.28	5 (8%)
22	CLA	A	820	-	65,73,73	1.50	10 (15%)	76,113,113	1.64	8 (10%)
22	CLA	B	808	-	65,73,73	1.46	11 (16%)	76,113,113	1.75	10 (13%)
29	PQN	A	844	-	34,34,34	2.88	11 (32%)	42,45,45	2.13	6 (14%)
22	CLA	A	819	-	59,67,73	1.63	10 (16%)	68,105,113	1.42	8 (11%)
22	CLA	B	813	-	65,73,73	1.42	11 (16%)	76,113,113	1.54	13 (17%)
32	DGD	J	103	-	67,67,67	0.95	4 (5%)	81,81,81	1.45	8 (9%)
21	CHL	2	606	-	42,50,74	2.21	13 (30%)	45,85,114	2.94	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	815	-	43,51,73	1.69	9 (20%)	49,86,113	1.86	7 (14%)
21	CHL	Y	608	-	39,48,74	2.24	15 (38%)	45,83,114	3.02	16 (35%)
21	CHL	X	608	-	38,47,74	2.40	15 (39%)	41,81,114	2.97	19 (46%)
22	CLA	Z	603	-	41,49,73	1.87	8 (19%)	51,84,113	1.82	11 (21%)
25	BCR	A	851	-	41,41,41	0.78	0	56,56,56	1.97	12 (21%)
22	CLA	1	606	-	39,48,73	1.82	7 (17%)	45,82,113	1.77	9 (20%)
21	CHL	3	608	-	45,53,74	2.13	14 (31%)	52,89,114	2.78	21 (40%)
29	PQN	B	842	-	34,34,34	2.89	11 (32%)	42,45,45	2.08	5 (11%)
22	CLA	4	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.50	9 (15%)
25	BCR	B	844	-	41,41,41	0.74	0	56,56,56	1.97	16 (28%)
33	NEX	Z	7623	-	38,46,46	0.90	1 (2%)	50,70,70	2.34	17 (34%)
22	CLA	2	611	26	38,45,73	2.94	10 (26%)	41,76,113	1.52	9 (21%)
22	CLA	4	611	-	42,50,73	1.78	7 (16%)	48,85,113	1.71	9 (18%)
22	CLA	Y	604	-	42,50,73	1.80	7 (16%)	48,85,113	1.90	8 (16%)
22	CLA	Y	612	20	37,46,73	2.03	8 (21%)	46,81,113	1.93	12 (26%)
22	CLA	Z	612	19	37,46,73	1.98	8 (21%)	48,80,113	1.78	12 (25%)
23	LUT	Z	7620	-	42,43,43	0.75	0	51,60,60	1.56	12 (23%)
22	CLA	A	841	-	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
22	CLA	3	612	3	43,51,73	1.82	6 (13%)	49,86,113	1.80	9 (18%)
22	CLA	B	833	-	45,53,73	1.76	10 (22%)	52,89,113	1.67	11 (21%)
21	CHL	4	607	-	41,49,74	2.23	14 (34%)	51,84,114	2.82	18 (35%)
22	CLA	1	602	1	61,69,73	1.51	6 (9%)	71,108,113	1.46	9 (12%)
22	CLA	2	610	2	55,63,73	1.54	10 (18%)	64,101,113	1.54	8 (12%)
22	CLA	A	832	-	50,58,73	1.65	9 (18%)	58,95,113	1.76	11 (18%)
25	BCR	A	849	-	41,41,41	0.89	2 (4%)	56,56,56	2.04	19 (33%)
22	CLA	A	817	-	45,53,73	1.75	9 (20%)	52,89,113	1.75	9 (17%)
22	CLA	A	837	5	45,53,73	1.78	7 (15%)	52,89,113	1.69	7 (13%)
22	CLA	1	603	-	55,63,73	1.65	8 (14%)	64,101,113	1.54	9 (14%)
22	CLA	4	613	-	57,65,73	1.55	7 (12%)	66,103,113	1.58	9 (13%)
25	BCR	L	301	-	41,41,41	0.80	0	56,56,56	1.88	18 (32%)
25	BCR	L	305	-	41,41,41	0.74	0	56,56,56	1.92	12 (21%)
25	BCR	B	845	-	41,41,41	0.74	0	56,56,56	1.96	13 (23%)
32	DGD	B	850	-	67,67,67	1.07	5 (7%)	81,81,81	1.44	13 (16%)
22	CLA	K	203	-	45,53,73	1.74	9 (20%)	52,89,113	1.64	10 (19%)
22	CLA	A	809	5	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	1	613	-	65,73,73	1.45	10 (15%)	76,113,113	1.46	7 (9%)
22	CLA	X	614	-	38,47,73	1.98	7 (18%)	48,81,113	1.70	10 (20%)
22	CLA	2	609	2	45,53,73	1.71	7 (15%)	52,89,113	1.80	10 (19%)
24	XAT	4	620	-	39,47,47	0.95	2 (5%)	54,74,74	2.59	19 (35%)
22	CLA	A	811	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
26	LHG	Z	7630	22	22,22,48	0.90	1 (4%)	25,28,54	1.18	1 (4%)
21	CHL	1	601	1	54,63,74	2.09	16 (29%)	58,101,114	2.43	19 (32%)
22	CLA	L	302	16	45,53,73	1.76	9 (20%)	52,89,113	1.76	9 (17%)
22	CLA	Y	611	26	39,48,73	1.94	7 (17%)	48,83,113	1.74	9 (18%)
22	CLA	B	825	-	62,70,73	1.45	8 (12%)	72,109,113	1.46	11 (15%)
22	CLA	Y	602	20	45,53,73	1.81	9 (20%)	52,89,113	1.57	8 (15%)
22	CLA	B	812	-	43,51,73	1.69	7 (16%)	49,86,113	1.95	7 (14%)
21	CHL	Y	607	-	40,48,74	2.28	12 (30%)	47,83,114	3.09	21 (44%)
21	CHL	Y	606	-	37,46,74	2.42	13 (35%)	46,81,114	3.02	18 (39%)
23	LUT	3	618	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
22	CLA	X	603	-	39,48,73	1.89	6 (15%)	44,83,113	1.83	9 (20%)
22	CLA	A	843	-	65,73,73	1.49	10 (15%)	76,113,113	1.44	7 (9%)
25	BCR	F	305	-	41,41,41	0.78	0	56,56,56	1.84	13 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	602	4	1/1/14/20	12/31/109/115	-
22	CLA	4	609	4	1/1/11/20	6/13/91/115	-
22	CLA	B	839	-	1/1/15/20	13/37/115/115	-
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
25	BCR	J	102	-	-	7/29/63/63	0/2/2/2
22	CLA	X	604	-	1/1/8/20	-	-
22	CLA	B	826	-	1/1/14/20	14/34/112/115	-
25	BCR	L	306	-	-	6/29/63/63	0/2/2/2
21	CHL	Z	609	19	3/3/15/26	5/10/108/137	-
22	CLA	3	604	-	1/1/11/20	0/9/85/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMU	A	857	-	-	8/16/56/61	0/2/2/2
22	CLA	2	604	-	1/1/10/20	5/9/88/115	-
22	CLA	B	824	-	1/1/15/20	12/37/115/115	-
26	LHG	2	622	22	-	21/41/41/53	-
23	LUT	Y	4621	-	-	3/29/67/67	0/2/2/2
22	CLA	B	822	-	1/1/10/20	4/10/88/115	-
22	CLA	A	833	-	1/1/13/20	8/27/105/115	-
22	CLA	Z	611	26	1/1/10/20	2/6/82/115	-
33	NEX	Y	4623	-	-	5/27/83/83	0/3/3/3
22	CLA	2	614	-	1/1/10/20	3/11/89/115	-
22	CLA	A	814	-	1/1/15/20	18/37/115/115	-
22	CLA	K	204	-	1/1/11/20	11/15/93/115	-
25	BCR	3	620	-	-	5/29/63/63	0/2/2/2
26	LHG	Y	4630	22	-	13/49/49/53	-
22	CLA	4	610	4	1/1/12/20	6/24/102/115	-
22	CLA	B	820	-	1/1/12/20	6/19/97/115	-
26	LHG	X	2630	22	-	8/25/25/53	-
23	LUT	1	617	-	-	4/29/67/67	0/2/2/2
22	CLA	A	824	-	1/1/10/20	2/8/86/115	-
22	CLA	3	610	3	1/1/10/20	3/8/86/115	-
22	CLA	B	816	-	1/1/13/20	6/25/103/115	-
21	CHL	4	608	-	3/3/16/26	5/15/113/137	-
22	CLA	L	304	-	1/1/11/20	3/13/91/115	-
25	BCR	B	846	-	-	1/29/63/63	0/2/2/2
22	CLA	B	805	-	1/1/15/20	15/37/115/115	-
22	CLA	A	836	-	1/1/11/20	1/13/91/115	-
22	CLA	B	831	-	1/1/10/20	3/11/89/115	-
21	CHL	Z	605	19	3/3/15/26	1/4/100/137	-
22	CLA	F	303	-	1/1/10/20	4/10/88/115	-
22	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
22	CLA	Z	604	-	1/1/11/20	3/16/92/115	-
23	LUT	2	619	-	-	2/29/67/67	0/2/2/2
22	CLA	4	614	-	1/1/11/20	3/13/91/115	-
22	CLA	A	854	-	1/1/15/20	16/37/115/115	-
21	CHL	2	607	-	3/3/15/26	4/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	N	1002	-	1/1/12/20	9/19/97/115	-
22	CLA	B	802	-	1/1/15/20	18/37/115/115	-
22	CLA	G	204	11	1/1/11/20	8/13/91/115	-
22	CLA	4	604	-	1/1/11/20	5/11/87/115	-
25	BCR	A	850	-	-	3/29/63/63	0/2/2/2
22	CLA	A	816	-	1/1/10/20	3/10/88/115	-
24	XAT	3	619	-	-	2/31/93/93	0/4/4/4
22	CLA	A	818	-	1/1/14/20	12/31/109/115	-
22	CLA	B	829	-	1/1/13/20	10/27/105/115	-
22	CLA	3	602	3	1/1/14/20	10/31/109/115	-
22	CLA	A	839	-	1/1/13/20	7/25/103/115	-
25	BCR	A	856	-	-	6/29/63/63	0/2/2/2
22	CLA	H	201	-	1/1/14/20	14/31/109/115	-
21	CHL	X	609	19	3/3/13/26	0/2/94/137	-
25	BCR	G	205	-	-	0/29/63/63	0/2/2/2
22	CLA	B	804	-	1/1/10/20	2/8/86/115	-
22	CLA	L	303	-	1/1/14/20	16/31/109/115	-
27	LMG	2	623	-	-	16/31/51/70	0/1/1/1
25	BCR	B	843	-	-	5/29/63/63	0/2/2/2
21	CHL	Y	601	20	4/4/20/26	18/35/131/137	-
22	CLA	X	611	26	1/1/9/20	1/6/80/115	-
33	NEX	X	2623	-	-	5/27/83/83	0/3/3/3
22	CLA	A	827	-	1/1/13/20	11/30/108/115	-
25	BCR	2	621	-	-	4/29/63/63	0/2/2/2
25	BCR	4	621	-	-	10/29/63/63	0/2/2/2
22	CLA	Y	614	-	1/1/10/20	4/6/82/115	-
22	CLA	A	822	-	1/1/15/20	13/37/115/115	-
21	CHL	X	607	-	3/3/15/26	4/10/106/137	-
22	CLA	A	828	-	1/1/15/20	14/37/115/115	-
30	SF4	A	853	-	-	-	0/6/5/5
22	CLA	3	614	-	1/1/10/20	1/6/84/115	-
27	LMG	4	622	-	-	12/34/54/70	0/1/1/1
22	CLA	A	821	-	1/1/11/20	0/13/91/115	-
22	CLA	A	842	-	1/1/15/20	9/37/115/115	-
21	CHL	2	618	2	3/3/15/26	4/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	A	848	-	-	4/29/63/63	0/2/2/2
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
23	LUT	Y	4620	-	-	7/29/67/67	0/2/2/2
25	BCR	1	619	-	-	6/29/63/63	0/2/2/2
22	CLA	Z	602	19	1/1/12/20	7/22/98/115	-
21	CHL	1	607	1	3/3/15/26	2/8/106/137	-
27	LMG	4	623	-	-	11/28/48/70	0/1/1/1
21	CHL	X	605	19	3/3/15/26	5/7/105/137	-
26	LHG	B	851	22	-	19/42/42/53	-
22	CLA	1	604	-	1/1/11/20	10/18/96/115	-
22	CLA	3	617	-	1/1/10/20	0/6/84/115	-
22	CLA	X	612	19	1/1/8/20	2/2/74/115	-
22	CLA	A	831	-	1/1/15/20	12/37/115/115	-
22	CLA	Z	613	19	1/1/10/20	1/11/89/115	-
21	CHL	4	618	4	3/3/15/26	2/10/106/137	-
22	CLA	3	607	3	1/1/10/20	2/10/86/115	-
22	CLA	A	845	26	1/1/12/20	8/19/97/115	-
22	CLA	B	838	-	1/1/11/20	7/16/94/115	-
22	CLA	B	807	6	-	4/22/100/115	-
22	CLA	3	603	3	1/1/13/20	8/25/103/115	-
23	LUT	X	2621	-	-	5/29/67/67	0/2/2/2
22	CLA	B	810	-	1/1/15/20	13/37/115/115	-
21	CHL	Z	601	19	3/3/15/26	4/10/108/137	-
22	CLA	2	612	2	1/1/11/20	7/11/89/115	-
22	CLA	B	834	-	1/1/14/20	8/31/109/115	-
22	CLA	B	809	6	1/1/15/20	16/37/115/115	-
23	LUT	Z	7621	-	-	3/29/67/67	0/2/2/2
21	CHL	Y	609	20	3/3/14/26	0/6/104/137	-
22	CLA	A	829	-	1/1/15/20	13/37/115/115	-
22	CLA	X	602	19	1/1/10/20	3/8/86/115	-
21	CHL	Z	607	-	3/3/16/26	5/13/109/137	-
22	CLA	F	301	-	1/1/13/20	11/28/106/115	-
22	CLA	1	610	1	1/1/14/20	2/29/107/115	-
22	CLA	A	805	-	1/1/12/20	7/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Y	610	20	1/1/10/20	3/6/82/115	-
22	CLA	Z	610	19	1/1/8/20	0/0/74/115	-
21	CHL	Y	605	20	3/3/15/26	2/4/100/137	-
22	CLA	2	602	2	1/1/15/20	13/37/115/115	-
22	CLA	A	810	5	1/1/12/20	8/19/97/115	-
30	SF4	C	102	-	-	-	0/6/5/5
22	CLA	A	803	-	1/1/15/20	5/37/115/115	-
22	CLA	1	616	1	-	6/11/87/115	-
22	CLA	A	802	-	1/1/15/20	13/37/115/115	-
24	XAT	1	618	-	-	3/31/93/93	0/4/4/4
22	CLA	4	612	4	1/1/10/20	2/8/86/115	-
22	CLA	Y	603	-	1/1/10/20	1/4/82/115	-
28	CL0	A	801	-	3/3/20/25	7/37/135/135	-
22	CLA	A	804	-	1/1/15/20	12/37/115/115	-
26	LHG	1	620	22	-	23/53/53/53	-
22	CLA	1	612	1	1/1/11/20	3/13/91/115	-
22	CLA	4	601	4	1/1/11/20	7/15/93/115	-
22	CLA	B	803	-	1/1/15/20	15/37/115/115	-
24	XAT	Z	4622	-	-	3/31/93/93	0/4/4/4
22	CLA	B	830	-	1/1/10/20	3/11/89/115	-
25	BCR	K	202	-	-	6/29/63/63	0/2/2/2
22	CLA	X	610	19	1/1/9/20	0/2/82/115	-
22	CLA	2	613	2	1/1/15/20	10/37/115/115	-
22	CLA	X	613	19	1/1/8/20	0/0/74/115	-
26	LHG	A	847	22	-	14/34/34/53	-
22	CLA	B	821	-	1/1/11/20	6/16/94/115	-
25	BCR	B	848	-	-	3/29/63/63	0/2/2/2
22	CLA	A	807	5	1/1/15/20	19/37/115/115	-
21	CHL	X	606	-	3/3/14/26	0/8/100/137	-
22	CLA	A	825	-	1/1/13/20	16/25/103/115	-
22	CLA	B	835	-	1/1/10/20	4/10/88/115	-
24	XAT	2	620	-	-	3/31/93/93	0/4/4/4
22	CLA	A	834	-	1/1/15/20	15/37/115/115	-
22	CLA	B	806	6	1/1/15/20	12/37/115/115	-
26	LHG	A	846	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	Z	608	-	3/3/16/26	7/13/111/137	-
22	CLA	K	206	15	1/1/9/20	0/6/80/115	-
22	CLA	F	304	-	1/1/10/20	2/8/86/115	-
22	CLA	A	808	-	1/1/12/20	2/19/97/115	-
22	CLA	K	201	15	1/1/8/20	0/2/76/115	-
22	CLA	A	838	-	1/1/12/20	7/21/99/115	-
22	CLA	B	823	-	1/1/11/20	4/13/91/115	-
22	CLA	B	840	-	1/1/15/20	13/37/115/115	-
22	CLA	Y	613	20	1/1/11/20	4/11/87/115	-
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-
22	CLA	3	606	3	1/1/10/20	5/8/86/115	-
22	CLA	A	826	-	1/1/15/20	17/37/115/115	-
22	CLA	G	203	-	1/1/10/20	3/10/88/115	-
22	CLA	3	613	3	1/1/13/20	8/23/101/115	-
22	CLA	N	1001	18	-	5/13/91/115	-
22	CLA	B	819	-	1/1/13/20	8/25/103/115	-
22	CLA	4	603	4	1/1/11/20	2/13/89/115	-
22	CLA	B	836	-	1/1/12/20	3/19/97/115	-
22	CLA	A	823	-	1/1/10/20	6/10/88/115	-
22	CLA	Z	614	-	1/1/11/20	5/11/89/115	-
22	CLA	A	813	-	1/1/12/20	3/24/102/115	-
21	CHL	2	608	-	3/3/17/26	7/21/119/137	-
24	XAT	Y	2622	-	-	4/31/93/93	0/4/4/4
21	CHL	Z	606	-	3/3/14/26	2/4/102/137	-
21	CHL	X	601	19	3/3/14/26	2/4/100/137	-
23	LUT	1	621	-	-	2/29/67/67	0/2/2/2
22	CLA	1	611	26	1/1/10/20	1/4/80/115	-
22	CLA	1	608	-	1/1/11/20	4/11/89/115	-
21	CHL	4	606	-	3/3/15/26	4/8/106/137	-
21	CHL	2	601	2	4/4/19/26	16/33/131/137	-
22	CLA	B	841	26	1/1/15/20	14/37/115/115	-
22	CLA	O	2001	-	1/1/9/20	2/4/78/115	-
22	CLA	1	609	1	1/1/10/20	2/8/84/115	-
23	LUT	X	2620	-	-	4/29/67/67	0/2/2/2
22	CLA	3	615	-	1/1/8/20	0/0/74/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	814	-	1/1/15/20	7/37/115/115	-
22	CLA	B	832	-	1/1/15/20	9/37/115/115	-
22	CLA	A	830	-	1/1/15/20	14/37/115/115	-
27	LMG	G	202	-	-	20/33/53/70	0/1/1/1
22	CLA	1	614	-	1/1/10/20	0/4/80/115	-
22	CLA	B	817	-	1/1/13/20	10/30/108/115	-
22	CLA	B	837	-	1/1/15/20	8/37/115/115	-
22	CLA	B	818	-	1/1/14/20	18/31/109/115	-
22	CLA	A	835	-	1/1/15/20	19/37/115/115	-
22	CLA	3	609	3	1/1/11/20	5/13/91/115	-
22	CLA	B	827	-	1/1/15/20	20/37/115/115	-
22	CLA	B	811	-	1/1/13/20	10/25/101/115	-
25	BCR	A	852	-	-	8/29/63/63	0/2/2/2
22	CLA	G	201	-	1/1/11/20	4/13/91/115	-
22	CLA	A	812	-	1/1/15/20	14/37/115/115	-
22	CLA	J	101	14	1/1/10/20	5/10/88/115	-
25	BCR	I	101	-	-	3/29/63/63	0/2/2/2
31	LMU	B	849	-	-	11/21/61/61	0/2/2/2
30	SF4	C	101	-	-	-	0/6/5/5
23	LUT	4	619	-	-	2/29/67/67	0/2/2/2
22	CLA	2	603	-	1/1/11/20	2/11/89/115	-
22	CLA	A	840	-	1/1/12/20	3/22/100/115	-
22	CLA	A	815	-	1/1/11/20	6/13/91/115	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
24	XAT	X	7622	-	-	1/31/93/93	0/4/4/4
27	LMG	1	622	-	-	26/48/68/70	0/1/1/1
22	CLA	A	820	-	1/1/15/20	12/37/115/115	-
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
29	PQN	A	844	-	-	11/23/43/43	0/2/2/2
22	CLA	A	819	-	1/1/13/20	9/30/108/115	-
22	CLA	B	813	-	1/1/15/20	18/37/115/115	-
32	DGD	J	103	-	-	29/55/95/95	0/2/2/2
21	CHL	2	606	-	3/3/15/26	0/10/108/137	-
22	CLA	B	815	-	1/1/10/20	1/11/89/115	-
21	CHL	Y	608	-	3/3/15/26	2/8/104/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	X	608	-	3/3/14/26	1/4/102/137	-
22	CLA	Z	603	-	1/1/10/20	4/10/86/115	-
25	BCR	A	851	-	-	6/29/63/63	0/2/2/2
22	CLA	1	606	-	1/1/9/20	4/8/82/115	-
21	CHL	3	608	-	3/3/16/26	7/13/111/137	-
29	PQN	B	842	-	-	9/23/43/43	0/2/2/2
22	CLA	4	617	-	1/1/12/20	8/19/97/115	-
25	BCR	B	844	-	-	8/29/63/63	0/2/2/2
33	NEX	Z	7623	-	-	2/27/83/83	0/3/3/3
22	CLA	2	611	26	1/1/7/20	3/10/70/115	-
22	CLA	4	611	-	1/1/10/20	6/10/88/115	-
22	CLA	Y	604	-	1/1/10/20	7/10/88/115	-
22	CLA	Y	612	20	1/1/10/20	0/4/80/115	-
22	CLA	Z	612	19	1/1/9/20	2/4/80/115	-
23	LUT	Z	7620	-	-	2/29/67/67	0/2/2/2
22	CLA	A	841	-	1/1/15/20	13/37/115/115	-
22	CLA	3	612	3	-	4/11/89/115	-
22	CLA	B	833	-	1/1/11/20	6/13/91/115	-
21	CHL	4	607	-	3/3/15/26	0/10/106/137	-
22	CLA	1	602	1	1/1/14/20	5/33/111/115	-
22	CLA	2	610	2	1/1/13/20	8/25/103/115	-
22	CLA	A	832	-	1/1/12/20	8/19/97/115	-
25	BCR	A	849	-	-	3/29/63/63	0/2/2/2
22	CLA	A	817	-	1/1/11/20	6/13/91/115	-
22	CLA	A	837	5	1/1/11/20	7/13/91/115	-
22	CLA	1	603	-	1/1/13/20	11/25/103/115	-
22	CLA	4	613	-	1/1/13/20	9/28/106/115	-
25	BCR	L	301	-	-	4/29/63/63	0/2/2/2
25	BCR	L	305	-	-	10/29/63/63	0/2/2/2
25	BCR	B	845	-	-	6/29/63/63	0/2/2/2
32	DGD	B	850	-	-	22/55/95/95	0/2/2/2
22	CLA	K	203	-	1/1/11/20	4/13/91/115	-
22	CLA	A	809	5	1/1/15/20	12/37/115/115	-
22	CLA	1	613	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	X	614	-	1/1/9/20	5/8/80/115	-
22	CLA	2	609	2	1/1/11/20	6/13/91/115	-
24	XAT	4	620	-	-	2/31/93/93	0/4/4/4
22	CLA	A	811	-	1/1/15/20	16/37/115/115	-
26	LHG	Z	7630	22	-	13/26/26/53	-
21	CHL	1	601	1	4/4/18/26	14/25/123/137	-
22	CLA	L	302	16	1/1/11/20	5/13/91/115	-
22	CLA	Y	611	26	1/1/10/20	1/8/84/115	-
22	CLA	B	825	-	1/1/14/20	9/34/112/115	-
22	CLA	Y	602	20	1/1/11/20	7/13/91/115	-
22	CLA	B	812	-	1/1/10/20	4/11/89/115	-
21	CHL	Y	607	-	3/3/15/26	4/8/104/137	-
21	CHL	Y	606	-	3/3/15/26	1/4/100/137	-
23	LUT	3	618	-	-	4/29/67/67	0/2/2/2
22	CLA	X	603	-	1/1/10/20	2/6/84/115	-
22	CLA	A	843	-	1/1/15/20	16/37/115/115	-
25	BCR	F	305	-	-	2/29/63/63	0/2/2/2

The worst 5 of 1925 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	607	CHL	C4B-NB	29.20	1.61	1.35
22	2	611	CLA	C1A-NA	12.62	1.40	1.29
21	Z	607	CHL	C1B-NB	12.55	1.46	1.35
29	A	844	PQN	C12-C13	8.56	1.53	1.33
29	B	842	PQN	C12-C13	8.52	1.53	1.33

The worst 5 of 2886 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	7622	XAT	O24-C25-C24	10.93	121.59	113.38
22	B	808	CLA	C4A-NA-C1A	9.49	110.97	106.71
24	Z	4622	XAT	O24-C25-C24	9.46	120.49	113.38
33	Y	4623	NEX	O24-C25-C24	9.16	120.26	113.38
21	X	601	CHL	CMD-C2D-C1D	9.10	140.76	124.71

5 of 263 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	601	CHL	C8
21	1	601	CHL	NC
21	1	601	CHL	NA
21	1	601	CHL	ND
21	1	607	CHL	NC

5 of 1886 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	601	CHL	C1A-C2A-CAA-CBA
21	1	601	CHL	C3A-C2A-CAA-CBA
21	2	601	CHL	C1A-C2A-CAA-CBA
21	2	601	CHL	C1C-C2C-CMC-OMC
21	2	601	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

181 monomers are involved in 384 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	602	CLA	4	0
22	4	609	CLA	3	0
22	B	839	CLA	2	0
25	K	205	BCR	2	0
25	B	801	BCR	1	0
25	J	102	BCR	1	0
22	B	826	CLA	4	0
25	L	306	BCR	2	0
31	A	857	LMU	4	0
22	B	824	CLA	1	0
26	2	622	LHG	3	0
23	Y	4621	LUT	3	0
22	A	833	CLA	1	0
33	Y	4623	NEX	2	0
22	A	814	CLA	2	0
22	K	204	CLA	2	0
25	3	620	BCR	2	0
26	Y	4630	LHG	4	0
22	4	610	CLA	2	0
26	X	2630	LHG	1	0
23	1	617	LUT	6	0
22	3	610	CLA	2	0
22	B	816	CLA	2	0
22	L	304	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	846	BCR	3	0
22	B	805	CLA	2	0
22	B	831	CLA	1	0
22	F	303	CLA	1	0
23	2	619	LUT	9	0
22	A	854	CLA	5	0
22	N	1002	CLA	2	0
22	B	802	CLA	3	0
22	G	204	CLA	1	0
25	A	850	BCR	2	0
24	3	619	XAT	4	0
22	A	818	CLA	1	0
22	B	829	CLA	3	0
22	3	602	CLA	2	0
22	A	839	CLA	2	0
25	A	856	BCR	5	0
22	H	201	CLA	4	0
25	G	205	BCR	2	0
22	L	303	CLA	1	0
27	2	623	LMG	1	0
25	B	843	BCR	1	0
21	Y	601	CHL	1	0
33	X	2623	NEX	3	0
22	A	827	CLA	1	0
25	2	621	BCR	2	0
25	4	621	BCR	1	0
22	A	822	CLA	4	0
22	A	828	CLA	4	0
27	4	622	LMG	2	0
22	A	842	CLA	4	0
21	2	618	CHL	1	0
25	A	848	BCR	6	0
22	B	828	CLA	4	0
23	Y	4620	LUT	2	0
22	Z	602	CLA	2	0
27	4	623	LMG	1	0
21	X	605	CHL	1	0
22	X	612	CLA	1	0
22	A	831	CLA	6	0
22	Z	613	CLA	1	0
21	4	618	CHL	1	0
22	B	807	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	838	CLA	1	0
23	X	2621	LUT	4	0
22	B	810	CLA	2	0
22	2	612	CLA	1	0
22	B	809	CLA	4	0
23	Z	7621	LUT	3	0
22	A	829	CLA	5	0
22	X	602	CLA	4	0
22	F	301	CLA	1	0
22	1	610	CLA	2	0
22	Z	610	CLA	2	0
22	A	810	CLA	1	0
30	C	102	SF4	1	0
22	A	803	CLA	6	0
22	A	802	CLA	2	0
22	4	612	CLA	2	0
28	A	801	CL0	22	0
26	1	620	LHG	6	0
22	1	612	CLA	1	0
22	B	803	CLA	2	0
24	Z	4622	XAT	1	0
22	B	830	CLA	2	0
25	K	202	BCR	4	0
22	X	610	CLA	2	0
26	A	847	LHG	2	0
25	B	848	BCR	3	0
22	A	807	CLA	2	0
22	A	825	CLA	3	0
24	2	620	XAT	4	0
22	A	834	CLA	1	0
26	A	846	LHG	3	0
22	K	206	CLA	1	0
22	A	808	CLA	1	0
22	K	201	CLA	1	0
22	A	838	CLA	1	0
22	B	823	CLA	2	0
22	B	840	CLA	3	0
22	Y	613	CLA	1	0
22	A	806	CLA	3	0
22	3	606	CLA	1	0
22	A	826	CLA	1	0
22	G	203	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	1001	CLA	1	0
22	Z	614	CLA	1	0
21	2	608	CHL	1	0
24	Y	2622	XAT	2	0
21	X	601	CHL	2	0
23	1	621	LUT	1	0
21	2	601	CHL	3	0
22	B	841	CLA	1	0
22	O	2001	CLA	1	0
22	1	609	CLA	1	0
23	X	2620	LUT	2	0
22	B	814	CLA	1	0
22	B	832	CLA	4	0
22	A	830	CLA	3	0
27	G	202	LMG	1	0
22	B	817	CLA	3	0
22	B	837	CLA	4	0
22	B	818	CLA	6	0
22	A	835	CLA	2	0
22	3	609	CLA	3	0
22	B	827	CLA	5	0
22	B	811	CLA	2	0
25	A	852	BCR	4	0
22	A	812	CLA	3	0
25	I	101	BCR	3	0
31	B	849	LMU	5	0
23	4	619	LUT	4	0
22	A	840	CLA	2	0
22	A	815	CLA	1	0
25	B	847	BCR	6	0
24	X	7622	XAT	3	0
27	1	622	LMG	2	0
22	A	820	CLA	5	0
22	B	808	CLA	1	0
29	A	844	PQN	6	0
22	A	819	CLA	1	0
22	B	813	CLA	4	0
32	J	103	DGD	1	0
21	2	606	CHL	2	0
25	A	851	BCR	2	0
21	3	608	CHL	1	0
29	B	842	PQN	7	0

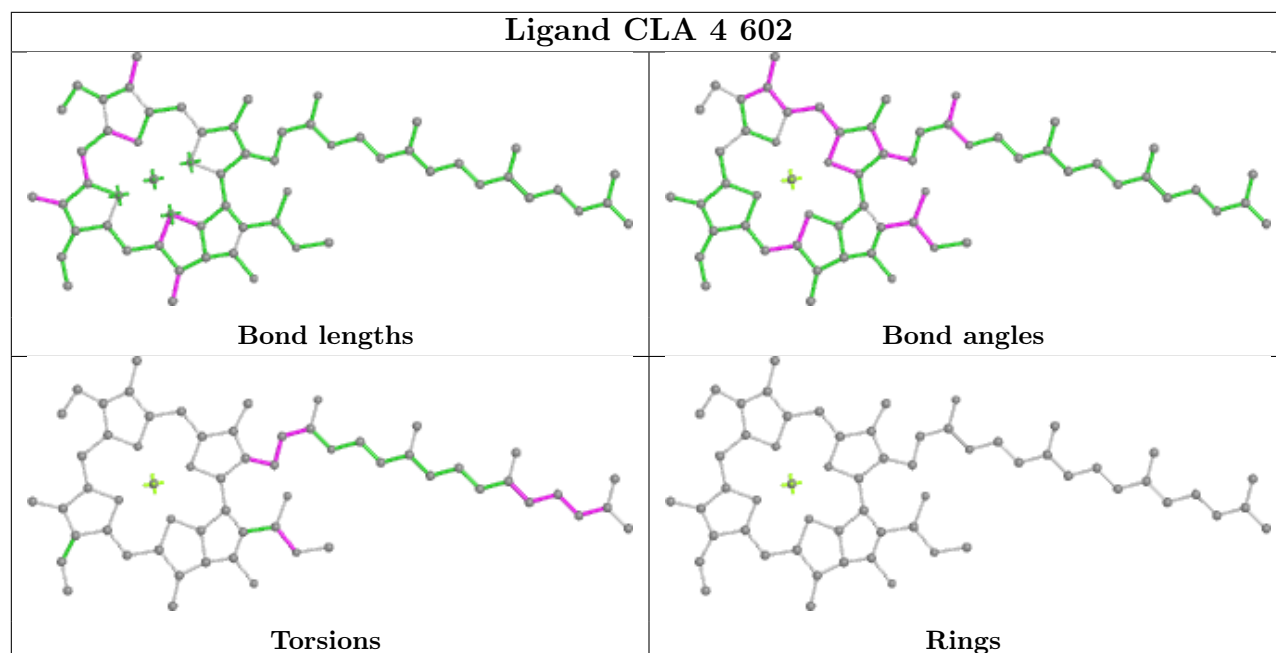
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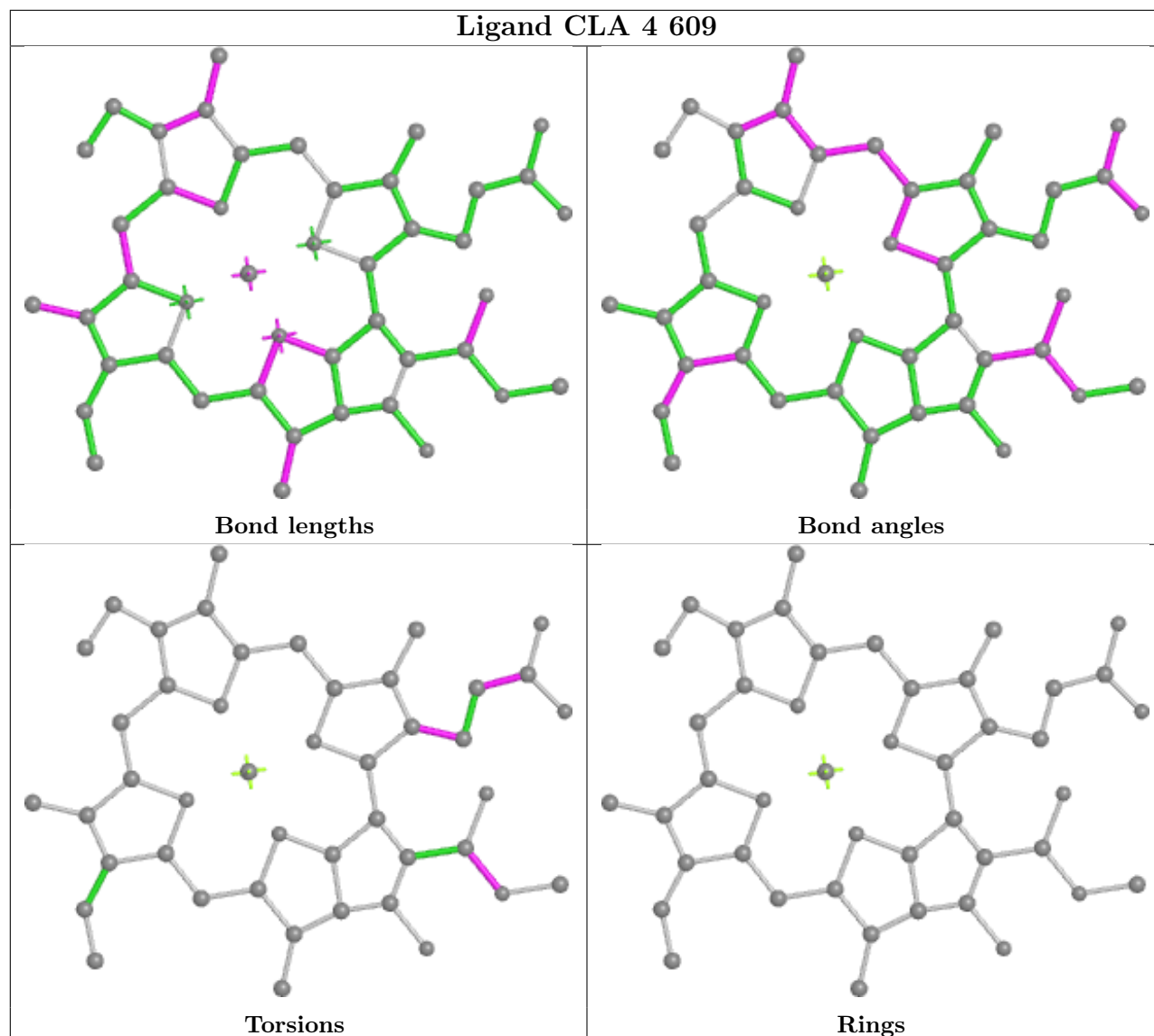
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	617	CLA	3	0
25	B	844	BCR	1	0
33	Z	7623	NEX	2	0
22	2	611	CLA	1	0
22	4	611	CLA	1	0
22	Y	604	CLA	1	0
22	Z	612	CLA	1	0
23	Z	7620	LUT	4	0
22	A	841	CLA	4	0
22	3	612	CLA	1	0
22	1	602	CLA	3	0
22	2	610	CLA	3	0
25	A	849	BCR	7	0
22	A	837	CLA	1	0
22	1	603	CLA	2	0
25	L	305	BCR	6	0
25	B	845	BCR	5	0
32	B	850	DGD	7	0
22	A	809	CLA	3	0
22	1	613	CLA	2	0
22	2	609	CLA	1	0
24	4	620	XAT	5	0
22	A	811	CLA	2	0
21	1	601	CHL	4	0
22	L	302	CLA	2	0
22	B	825	CLA	3	0
22	Y	602	CLA	1	0
23	3	618	LUT	4	0
22	X	603	CLA	1	0
22	A	843	CLA	2	0
25	F	305	BCR	1	0

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

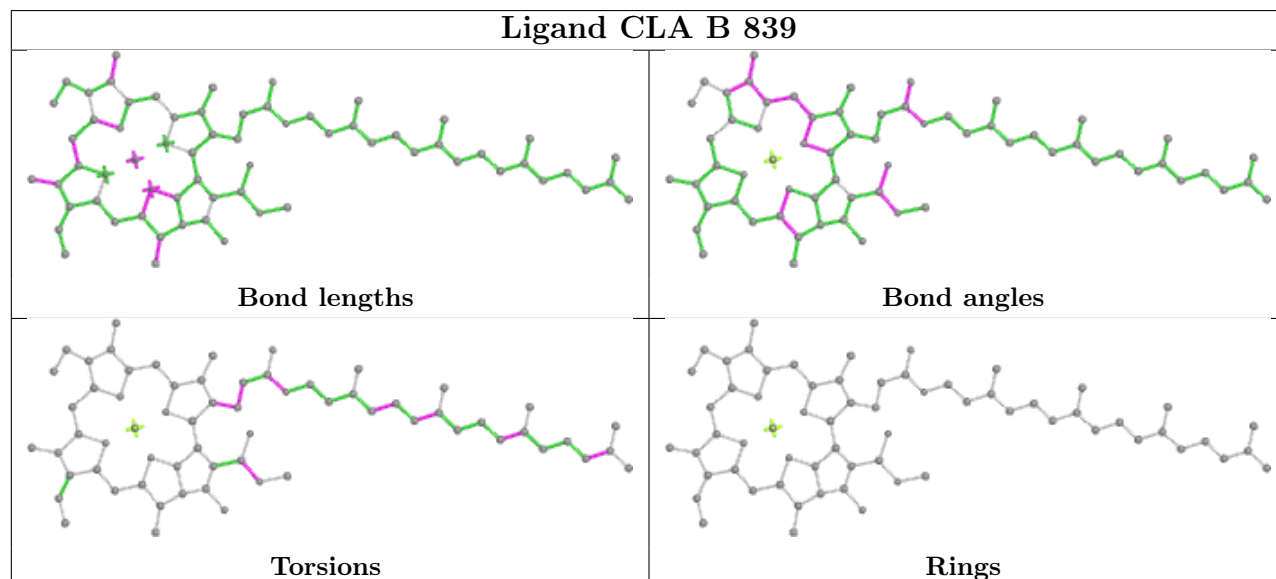
equivalents in the CSD to analyse the geometry.

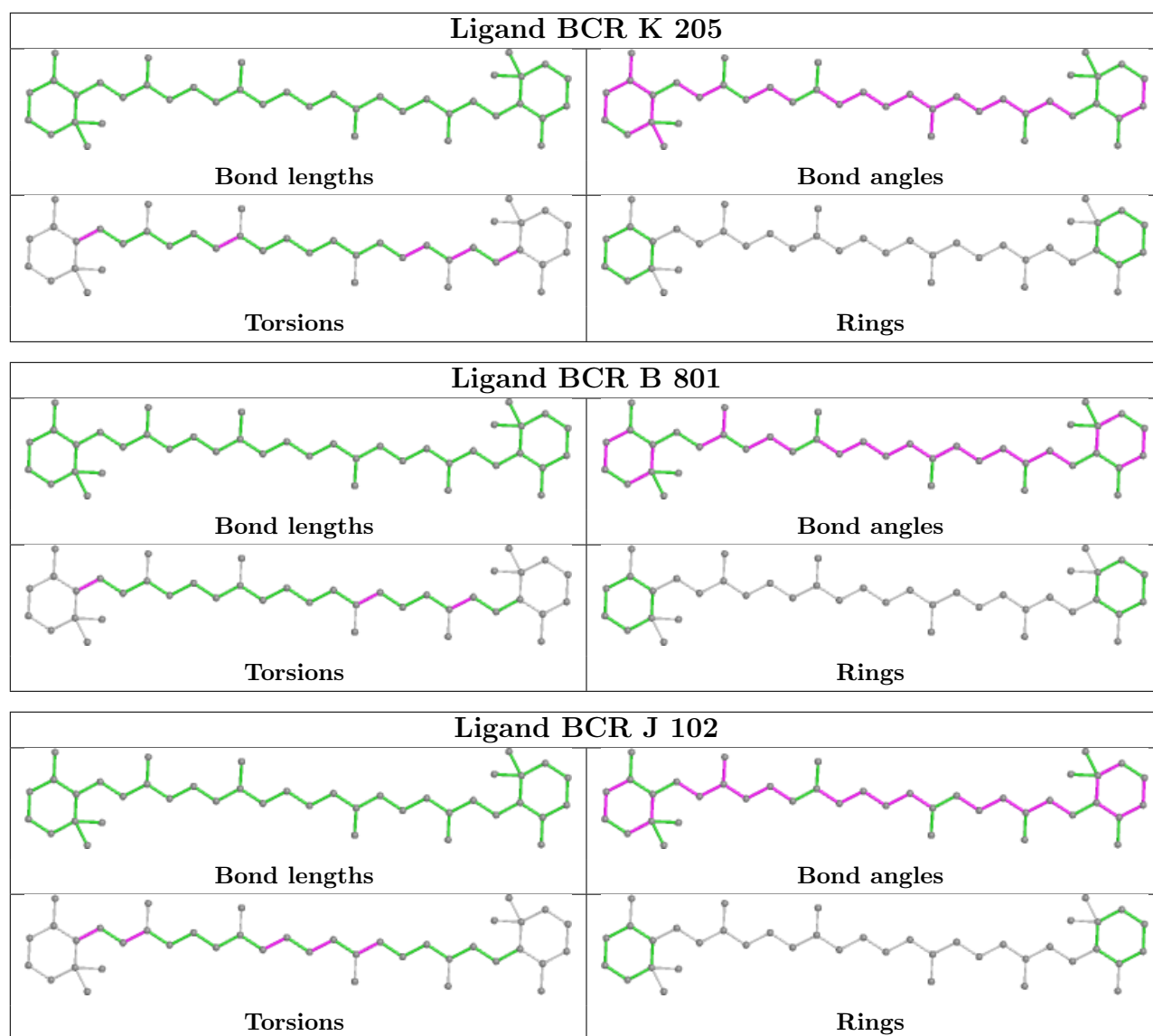


Ligand CLA 4 609

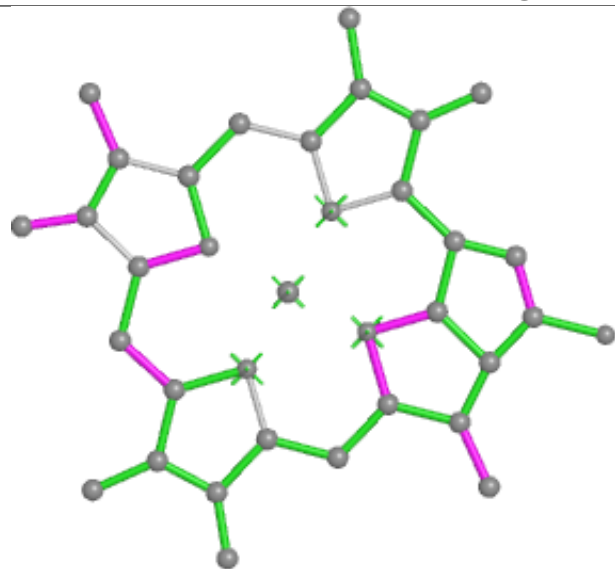


Ligand CLA B 839

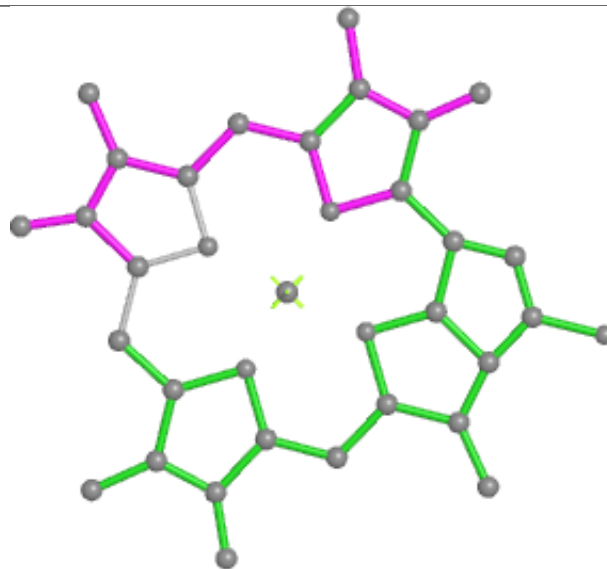




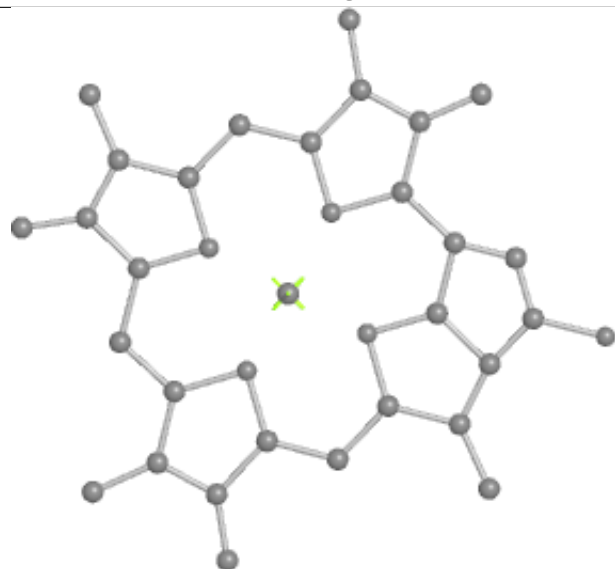
Ligand CLA X 604



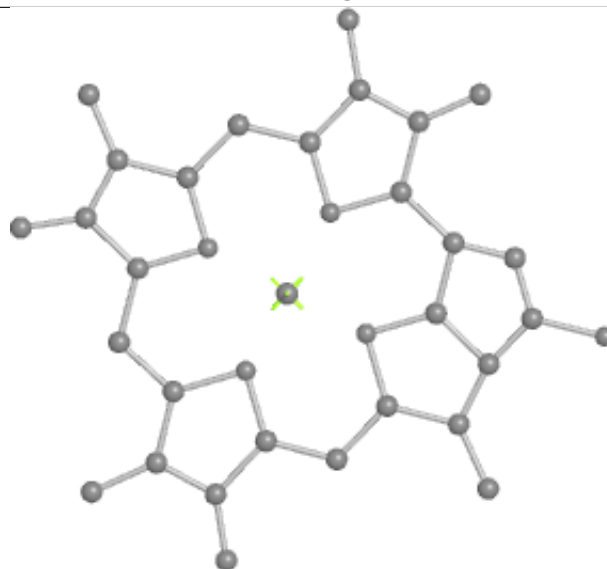
Bond lengths



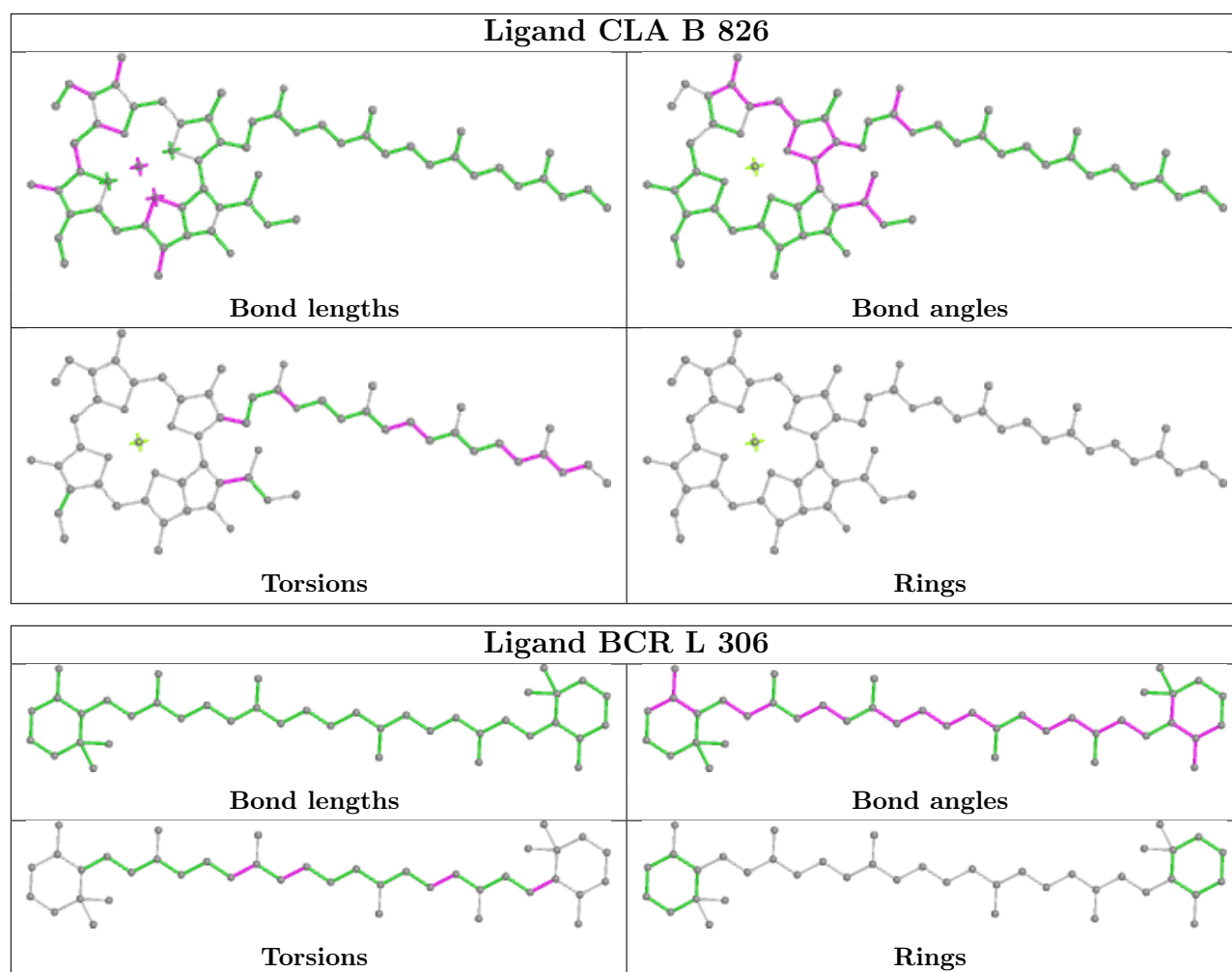
Bond angles



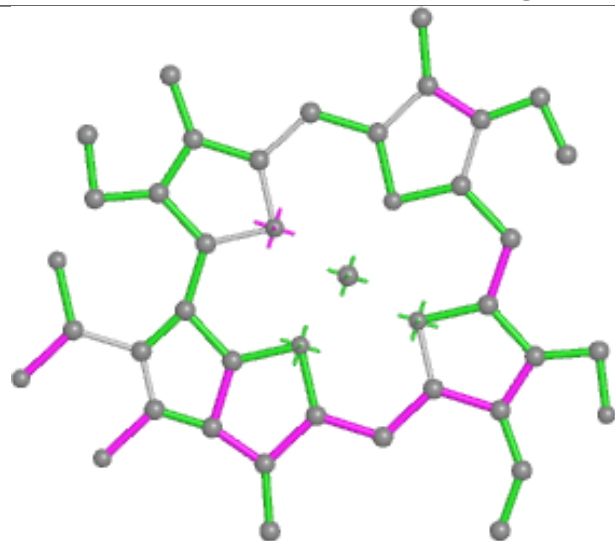
Torsions



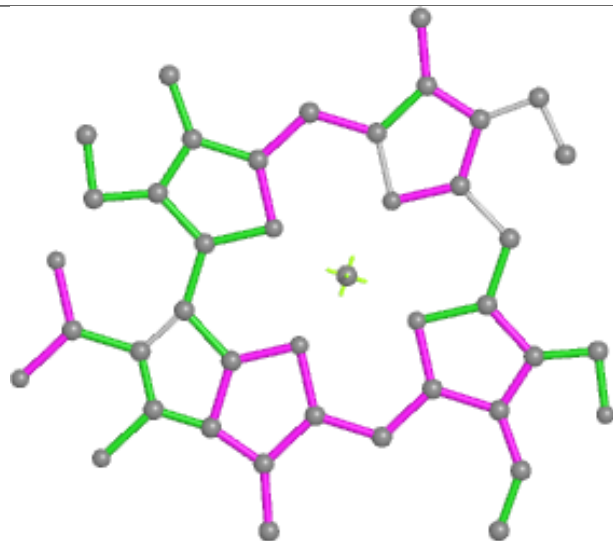
Rings



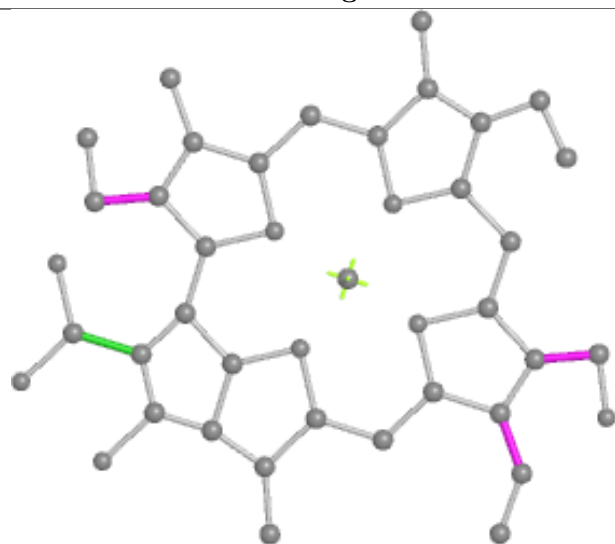
Ligand CHL Z 609



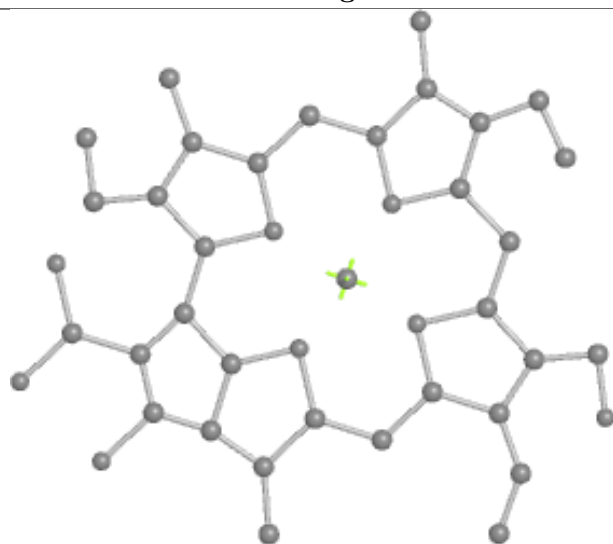
Bond lengths



Bond angles

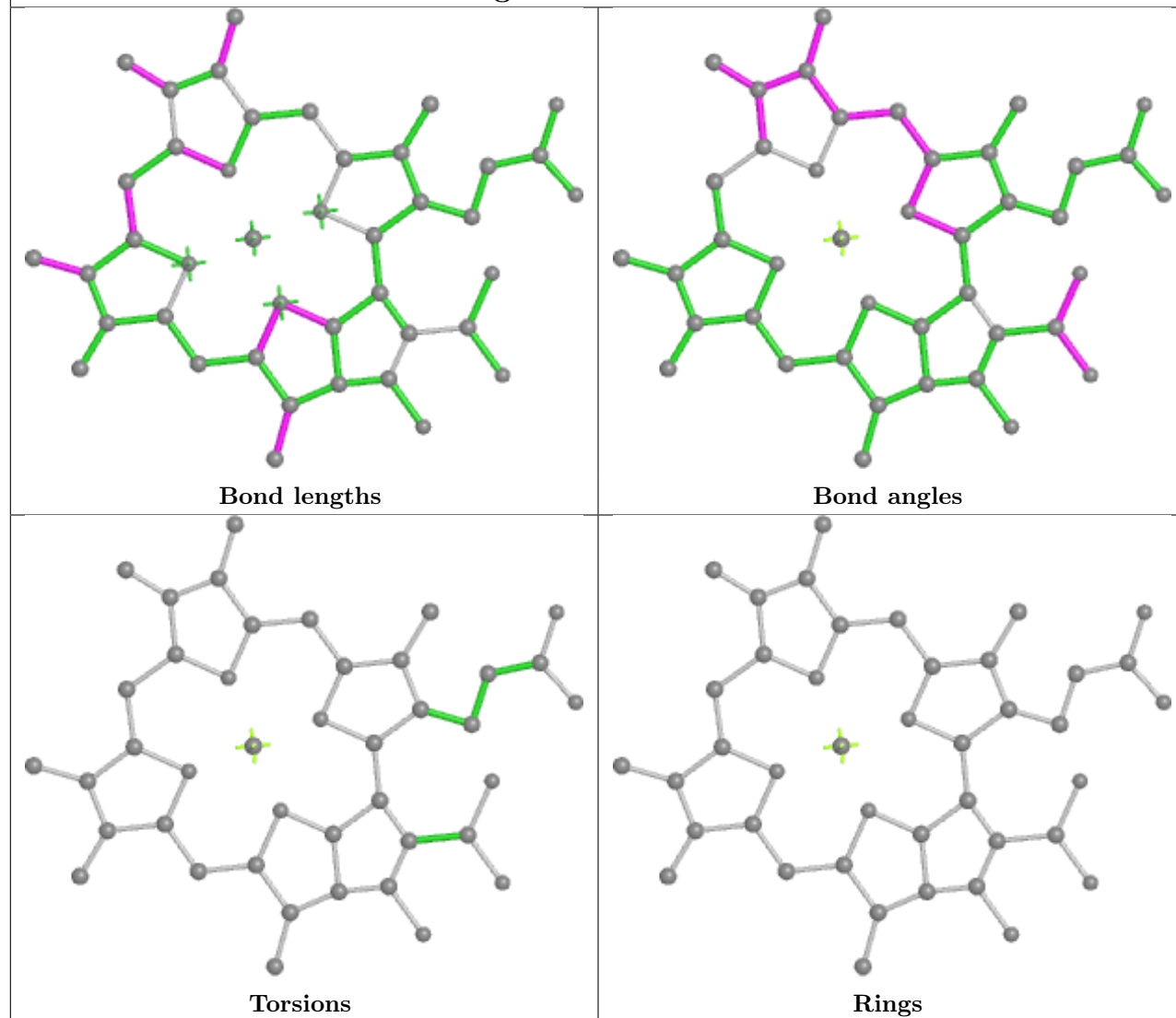


Torsions

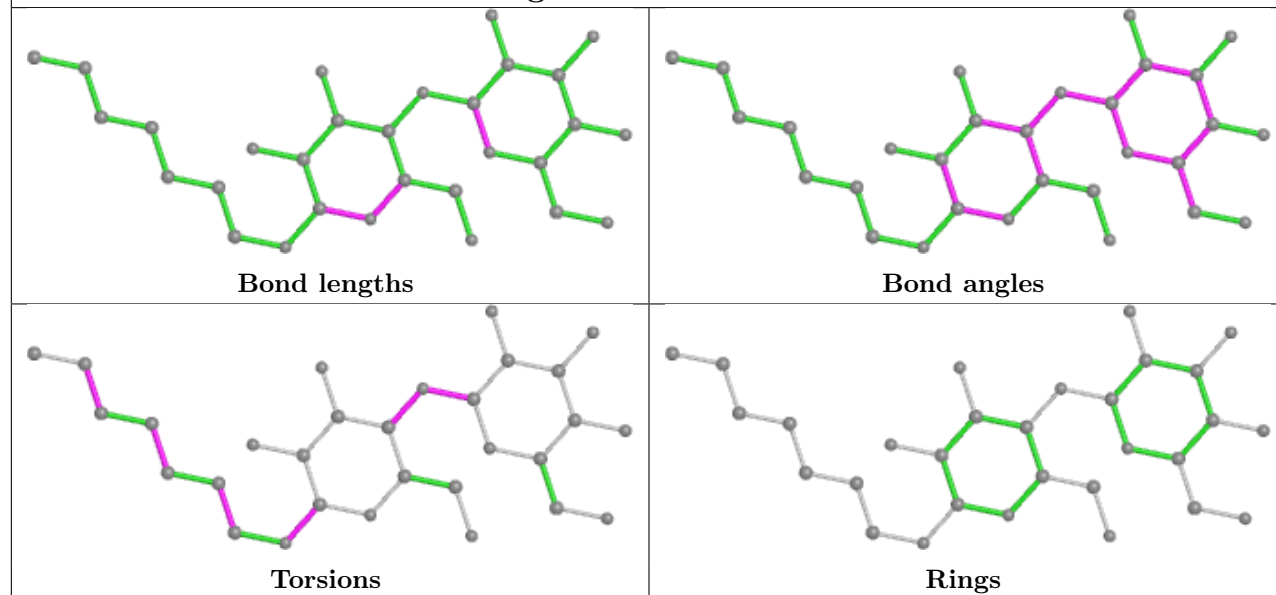


Rings

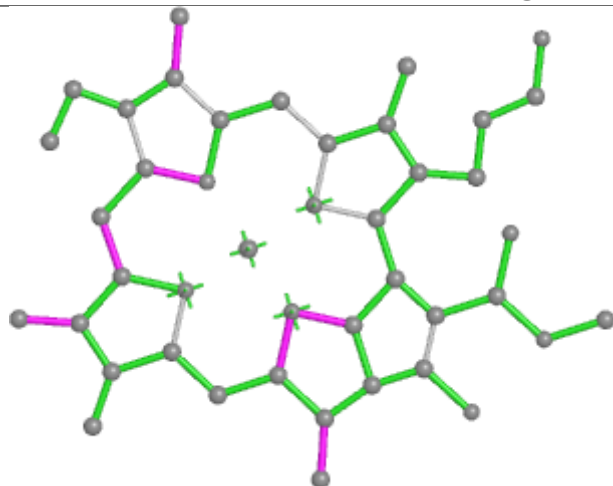
Ligand CLA 3 604



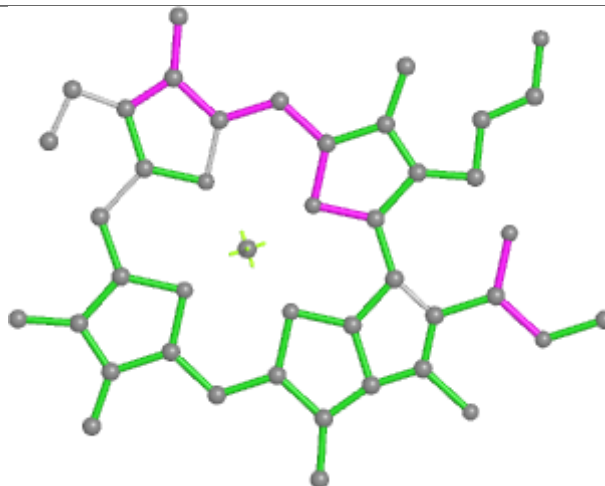
Ligand LMU A 857



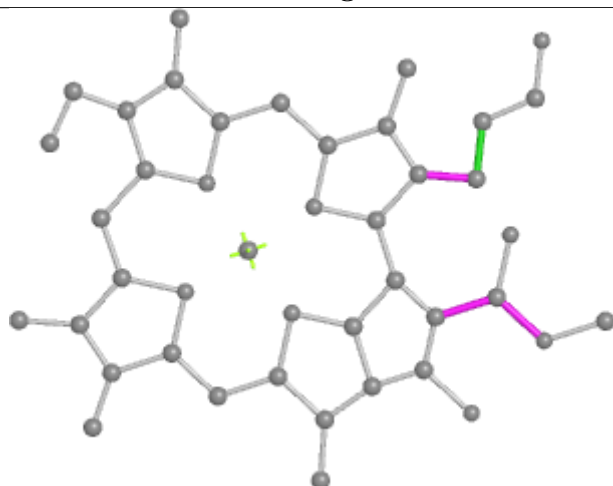
Ligand CLA 2 604



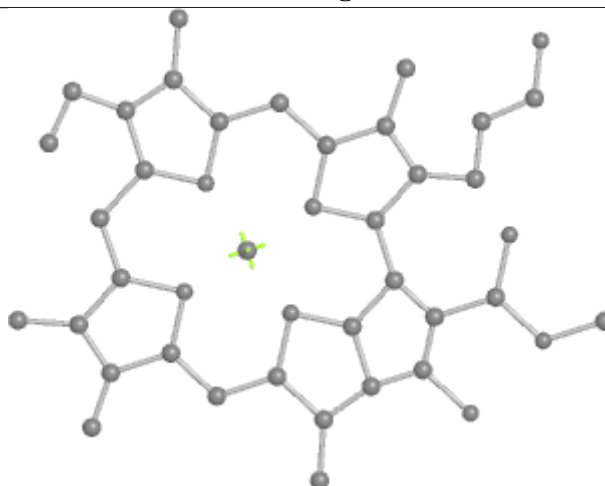
Bond lengths



Bond angles

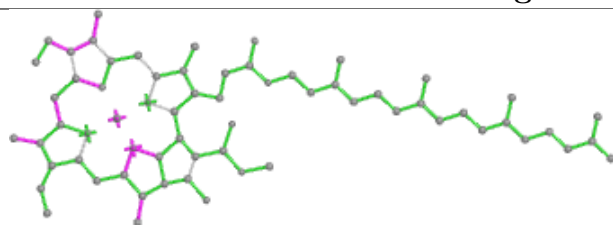


Torsions

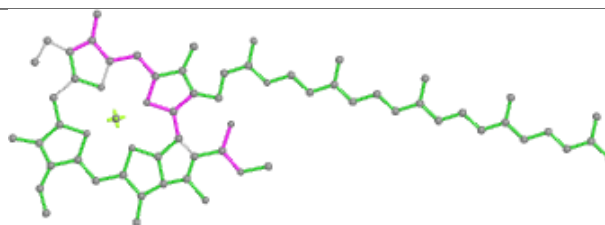


Rings

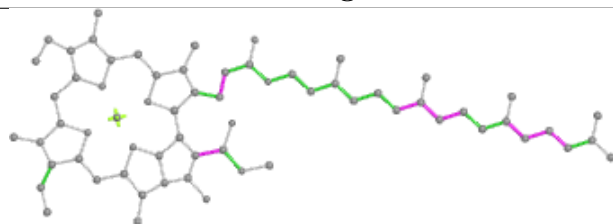
Ligand CLA B 824



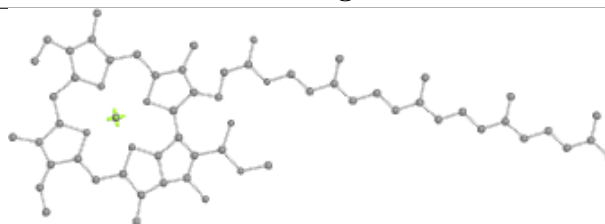
Bond lengths



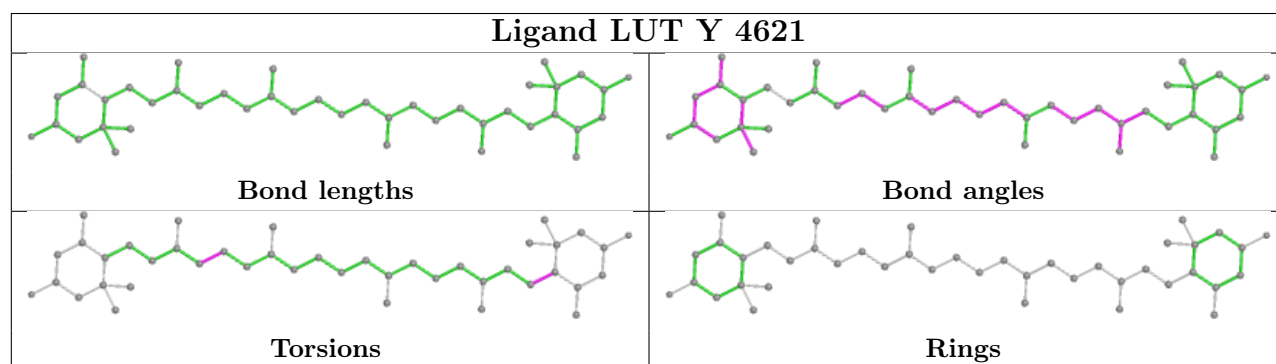
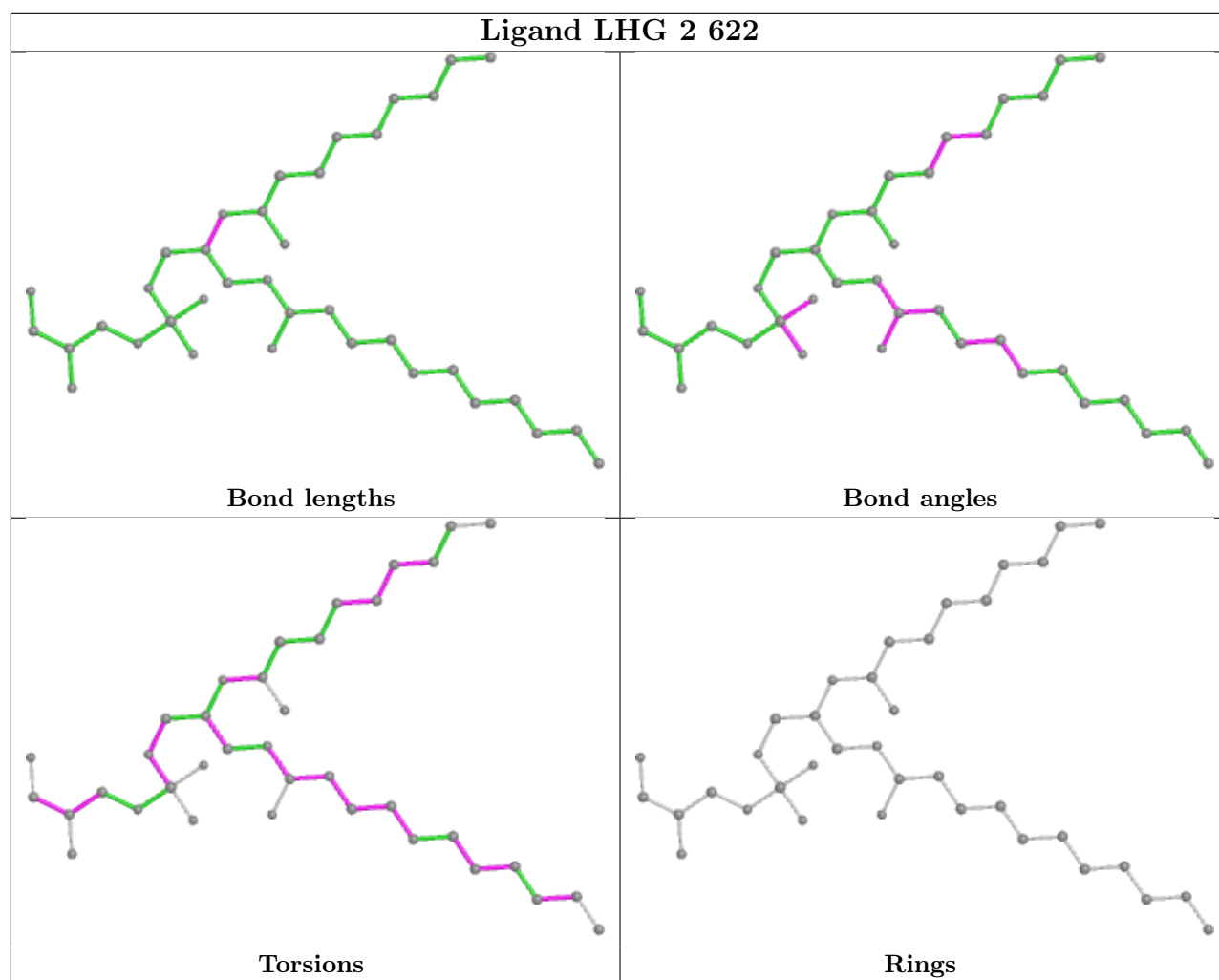
Bond angles



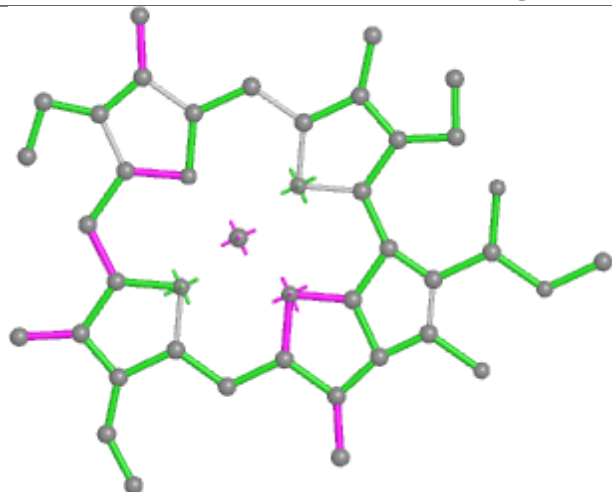
Torsions



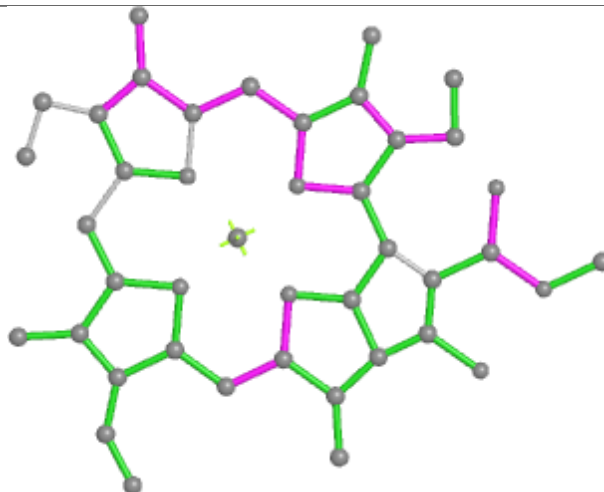
Rings



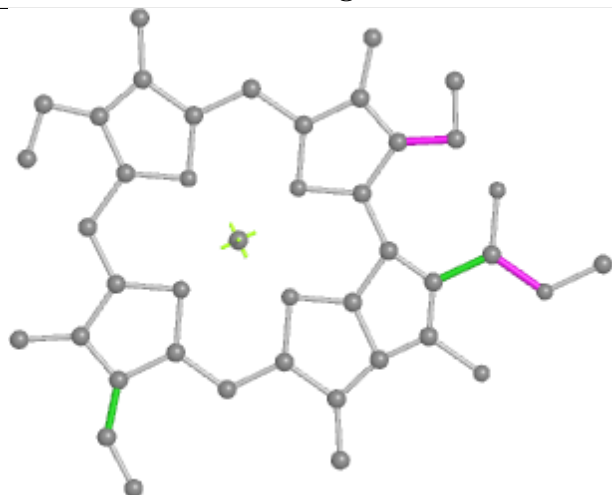
Ligand CLA B 822



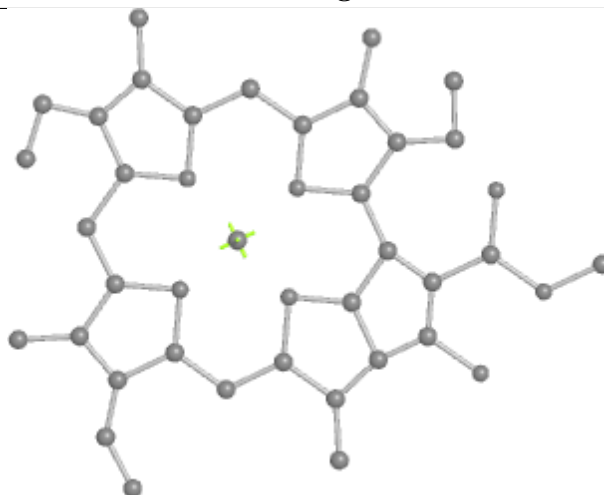
Bond lengths



Bond angles

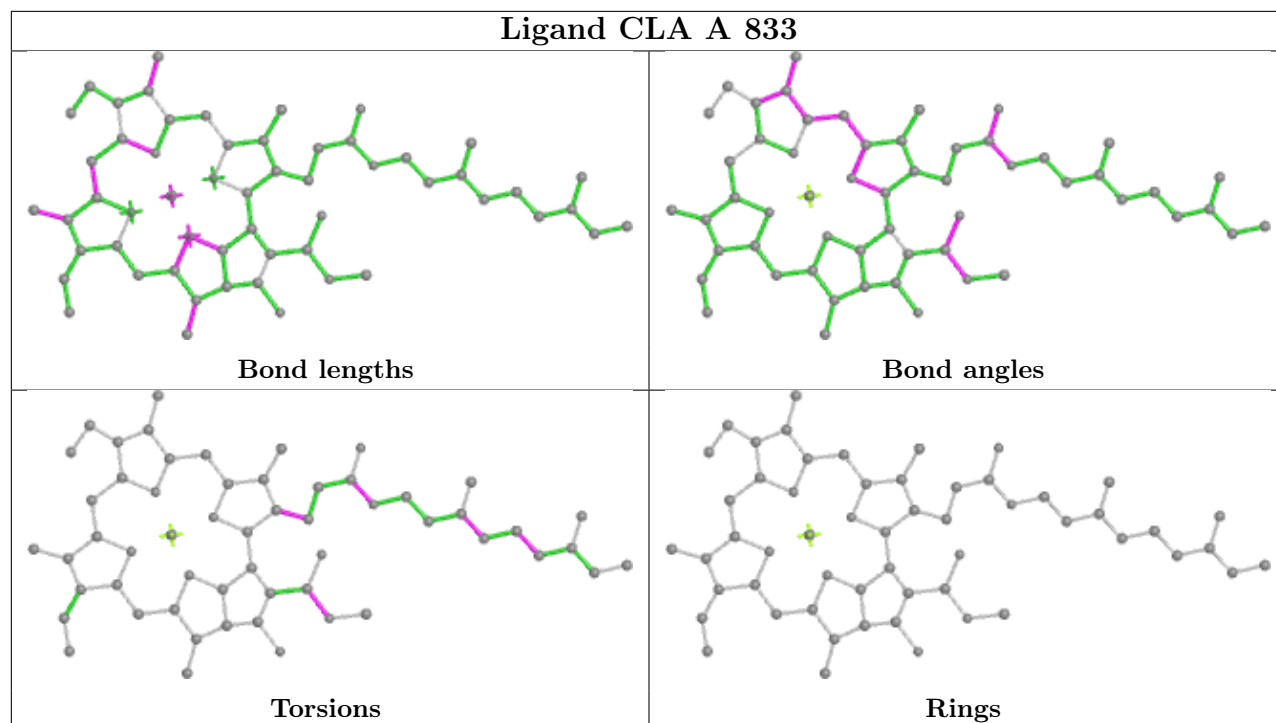


Torsions

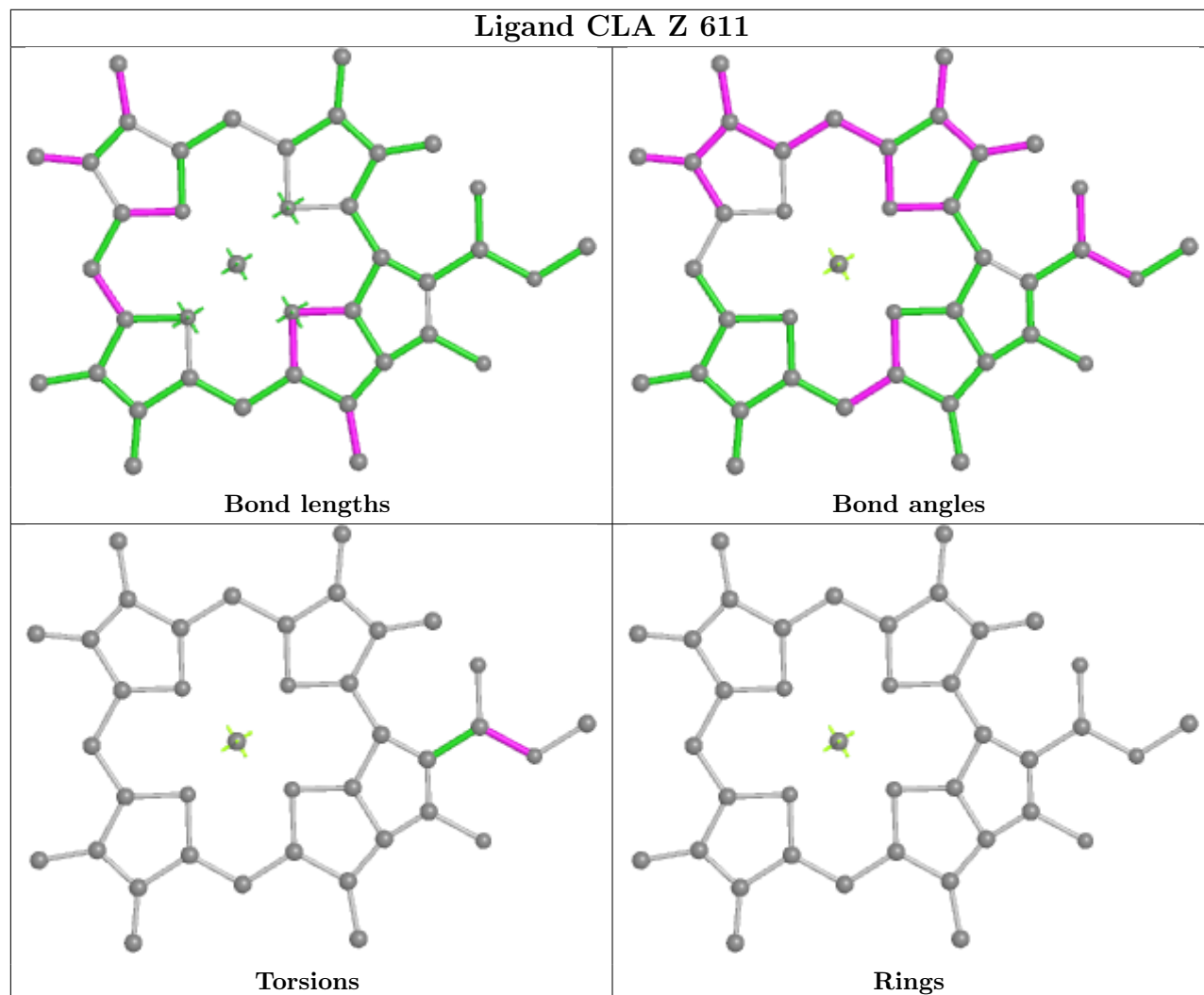


Rings

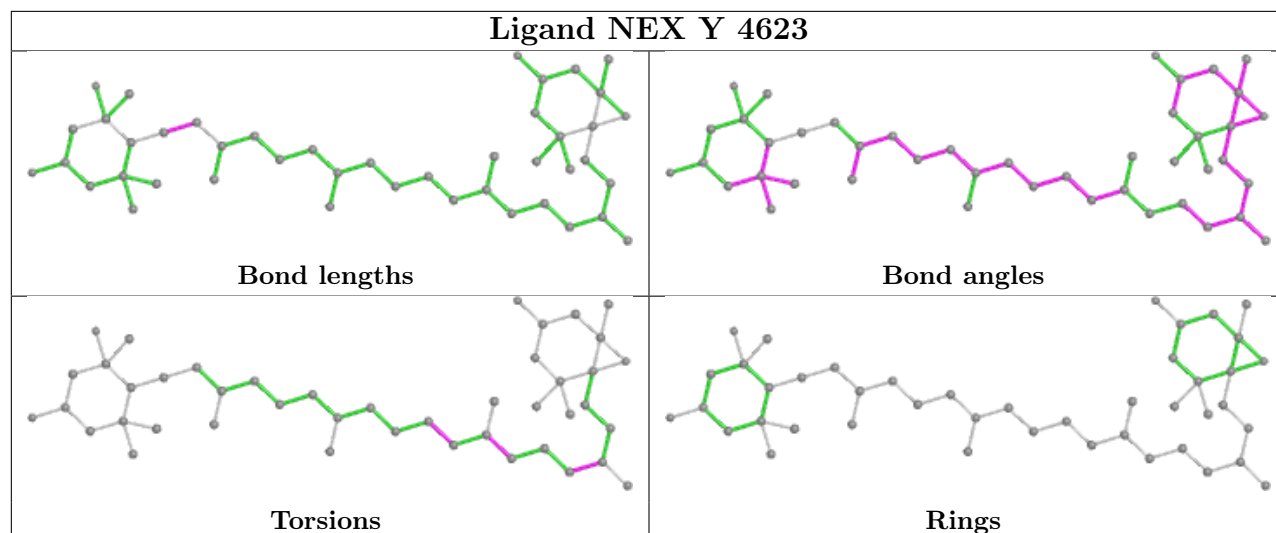
Ligand CLA A 833



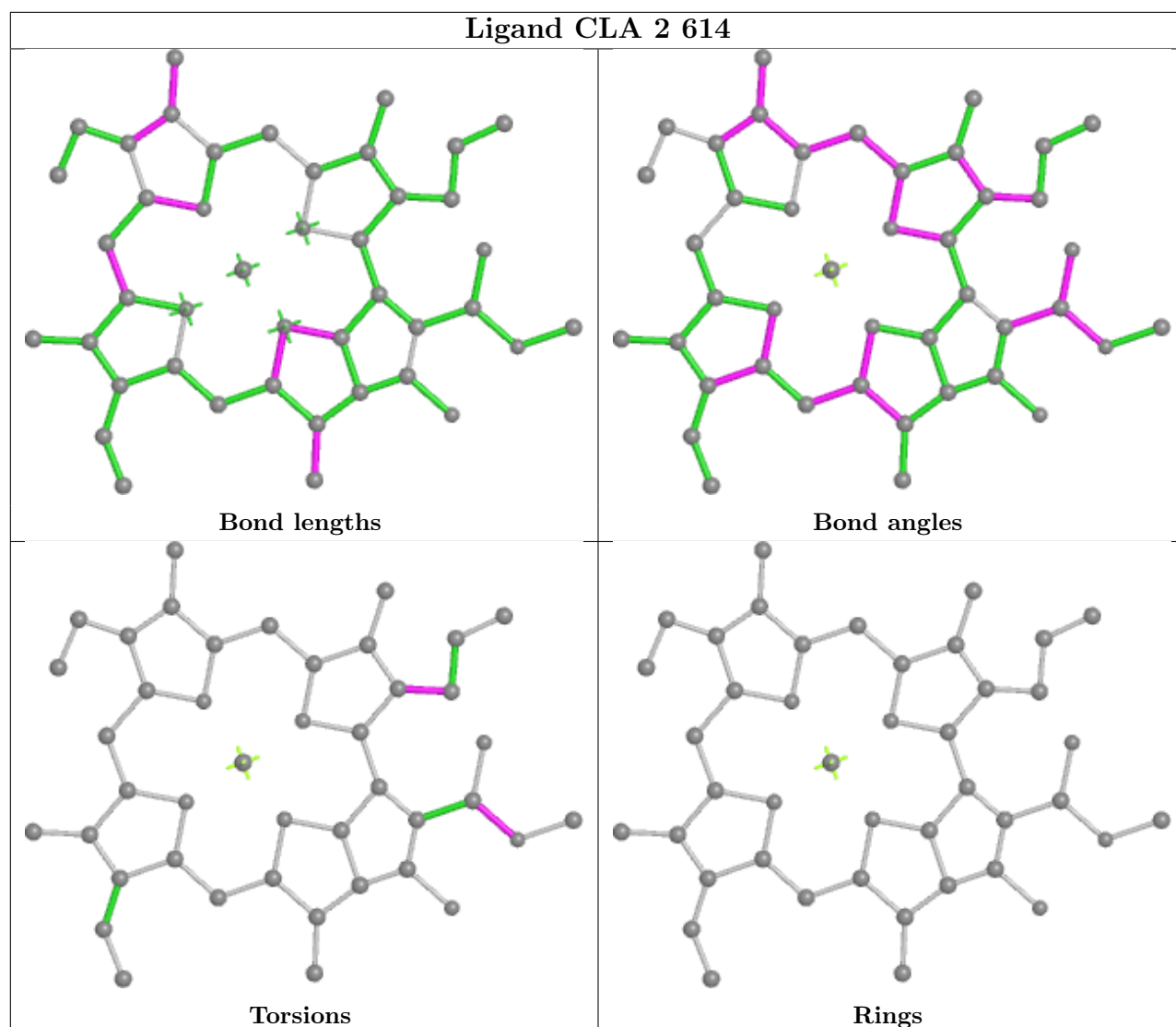
Ligand CLA Z 611



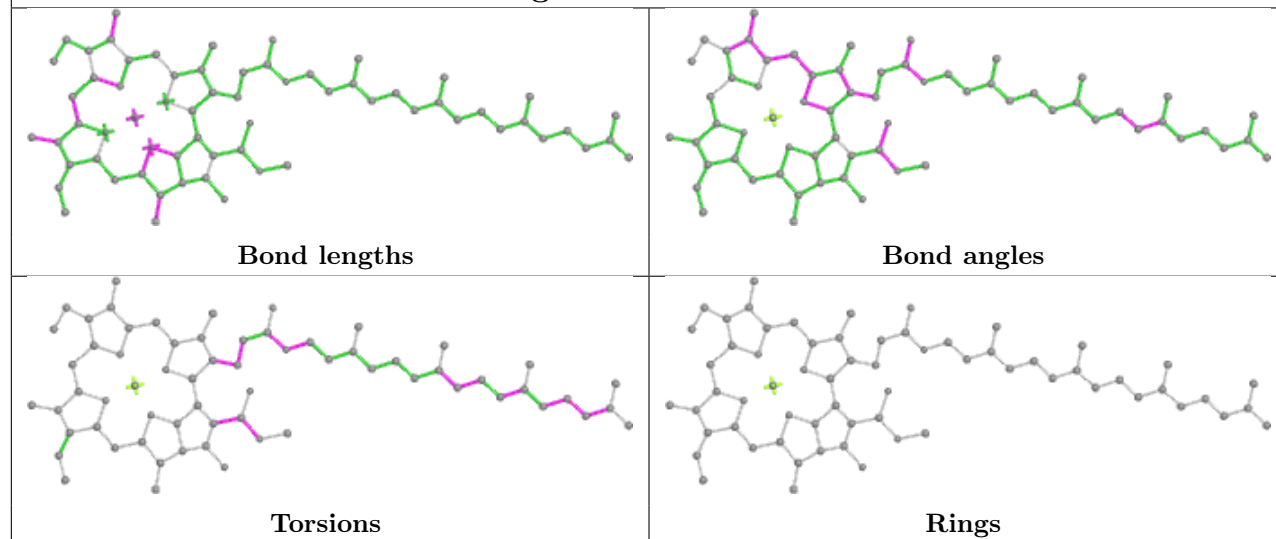
Ligand NEX Y 4623



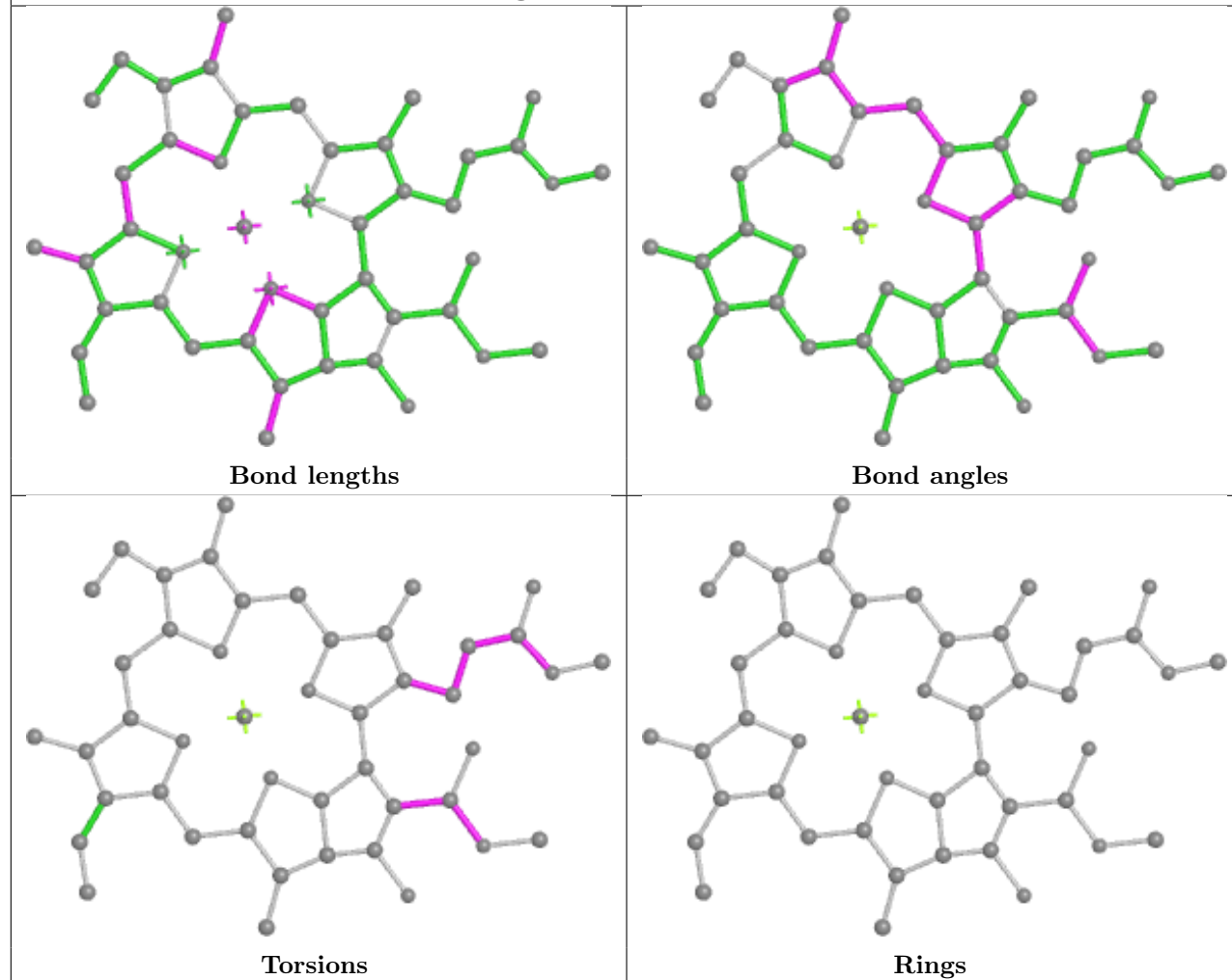
Ligand CLA 2 614

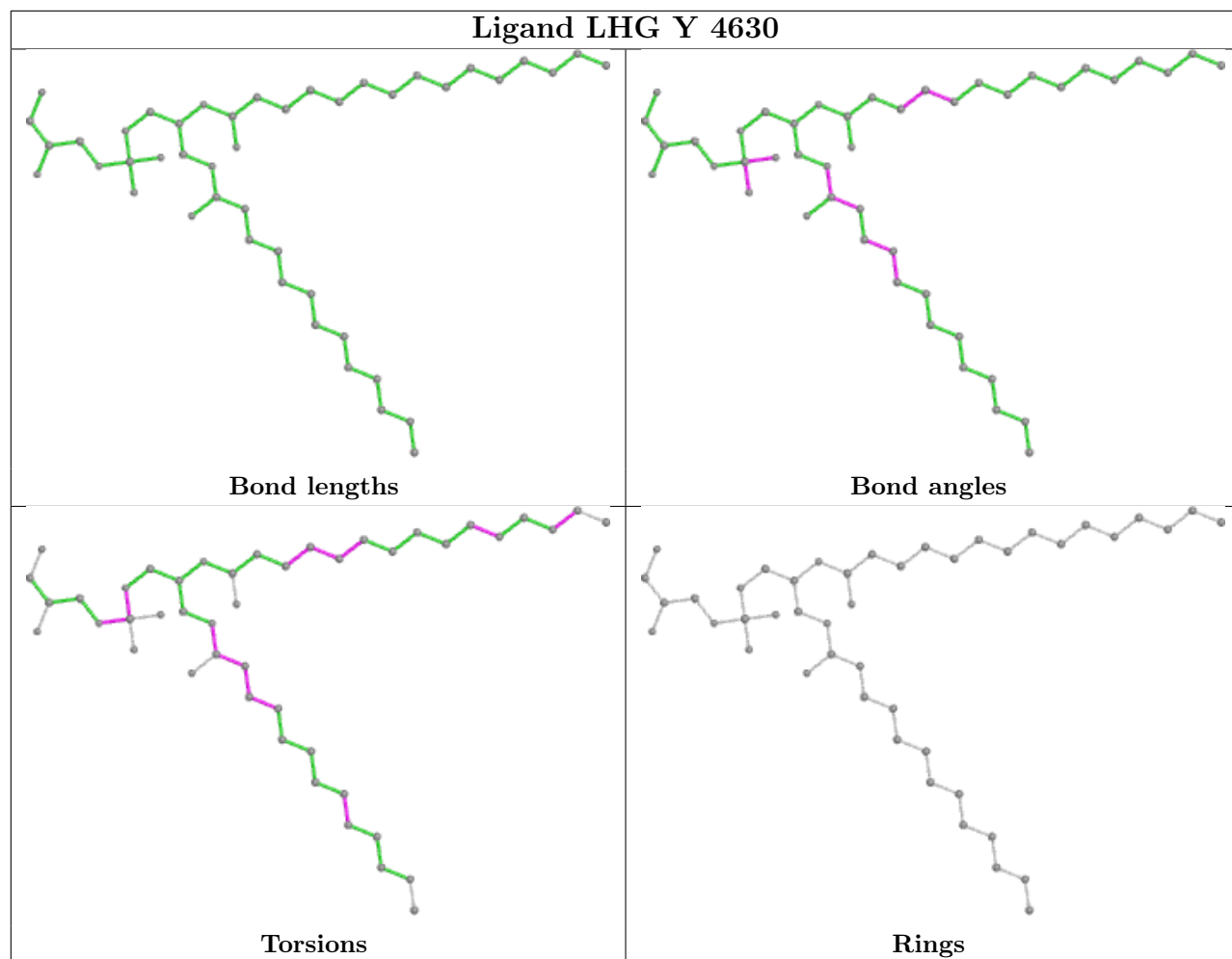
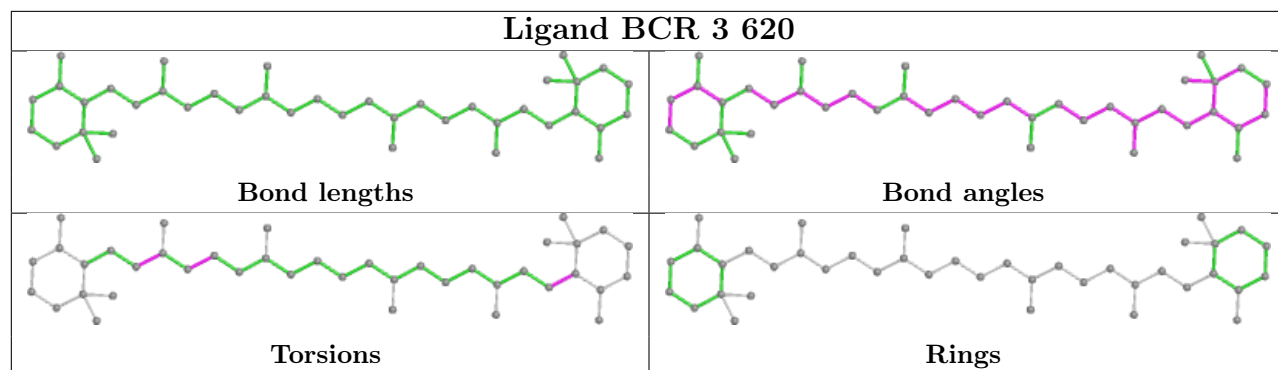


Ligand CLA A 814

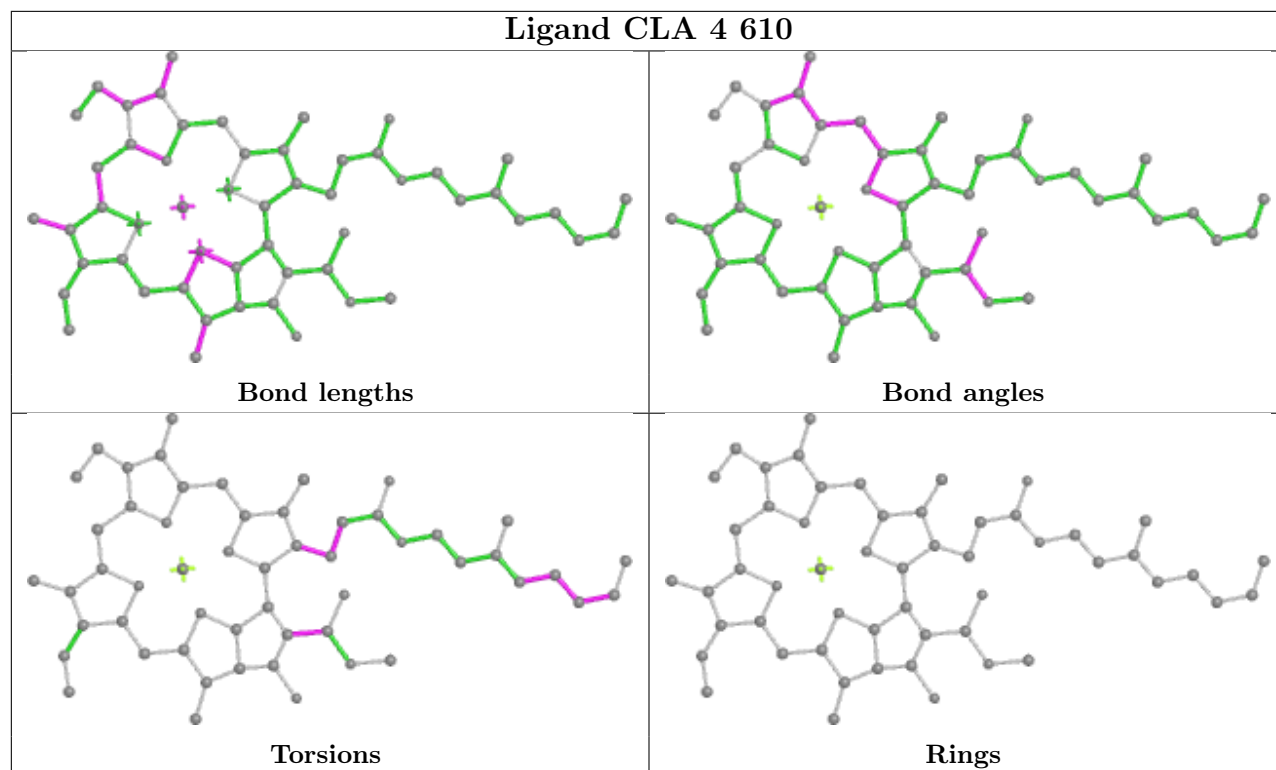


Ligand CLA K 204

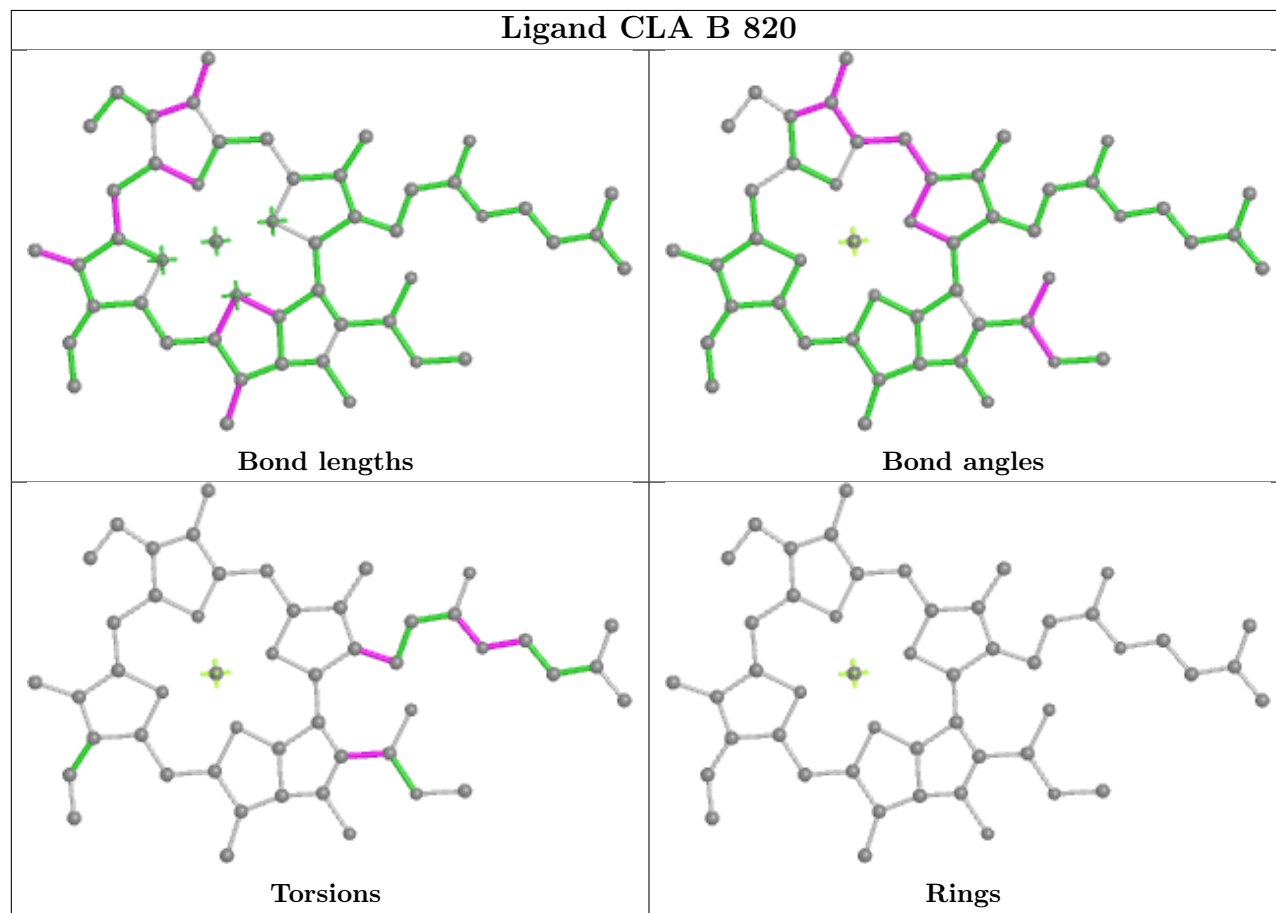


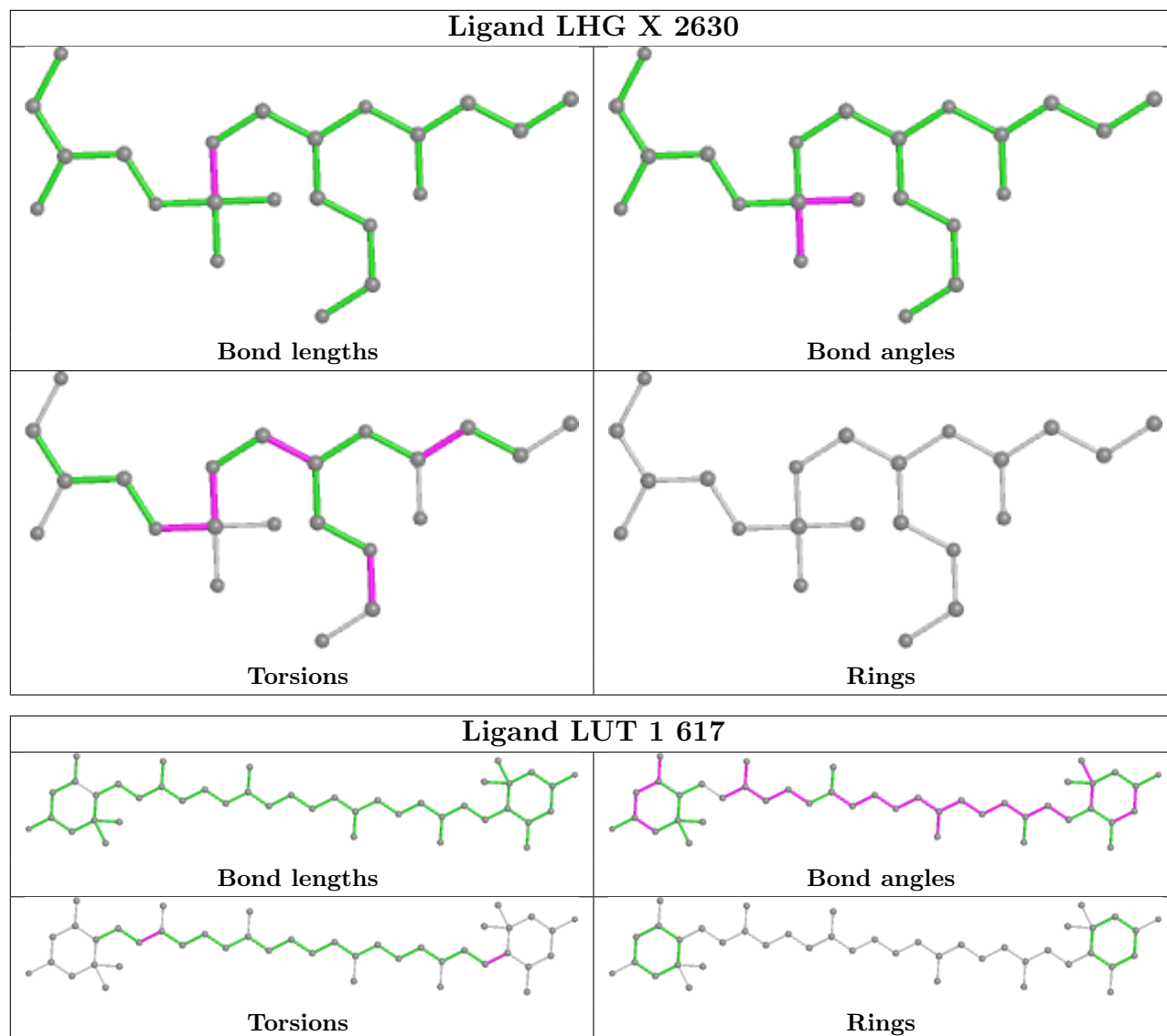


Ligand CLA 4 610

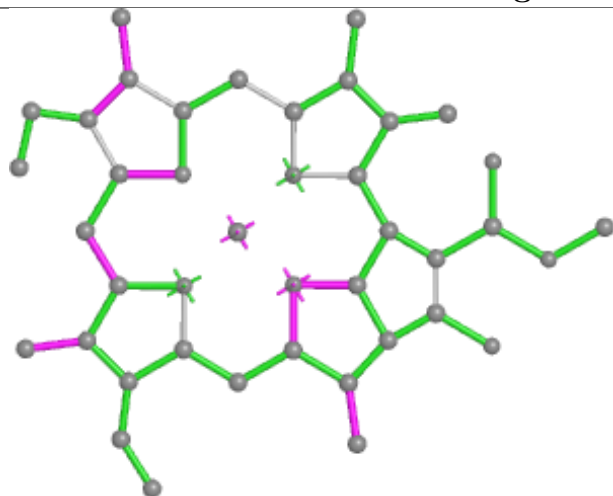


Ligand CLA B 820

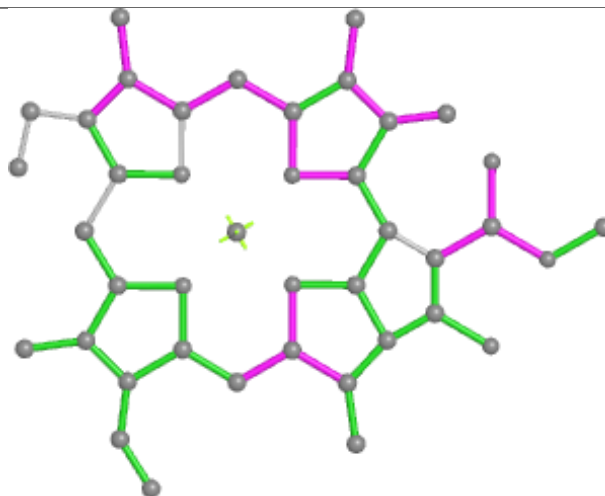




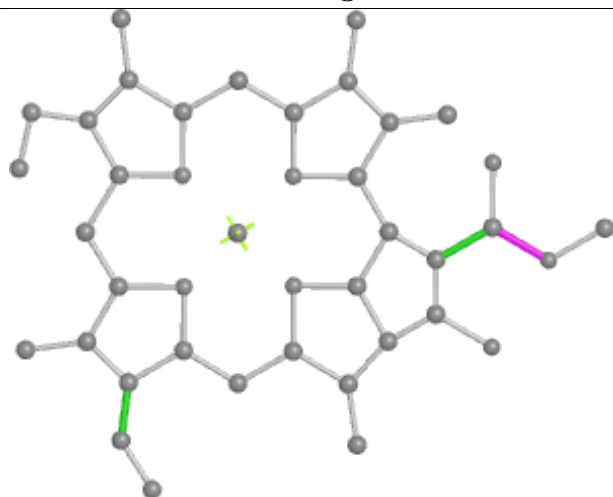
Ligand CLA A 824



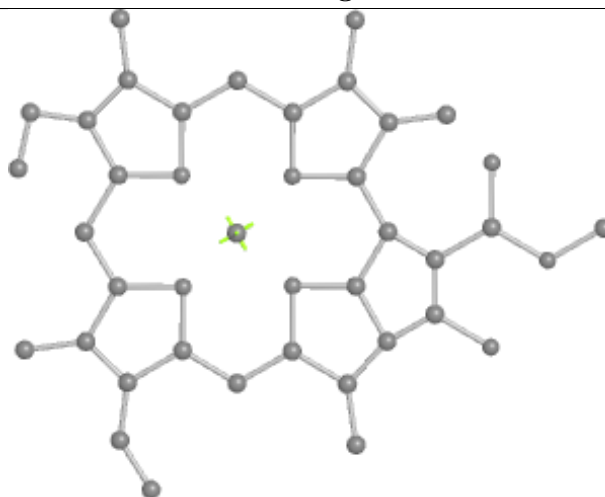
Bond lengths



Bond angles

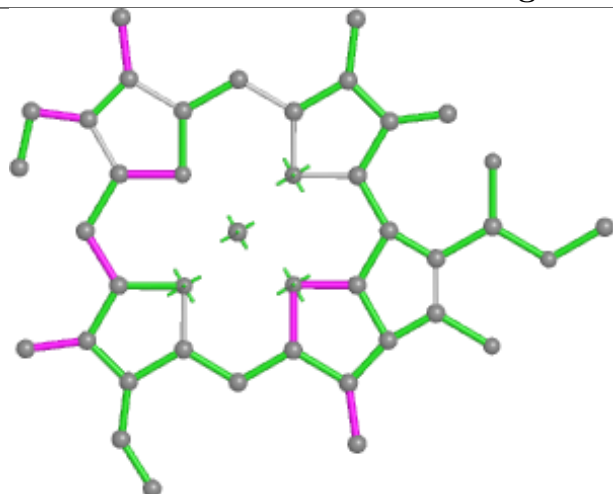


Torsions

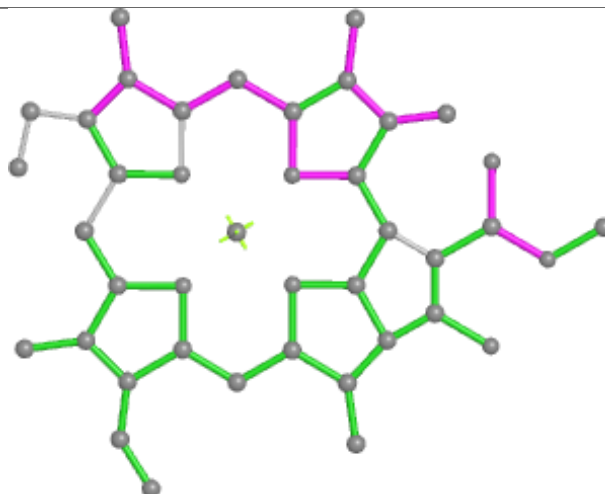


Rings

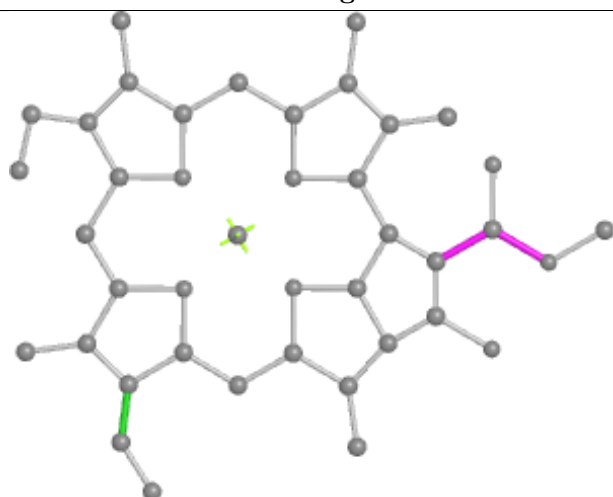
Ligand CLA 3 610



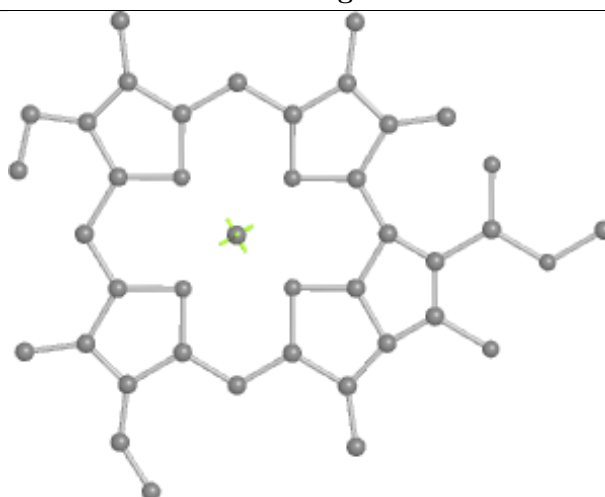
Bond lengths



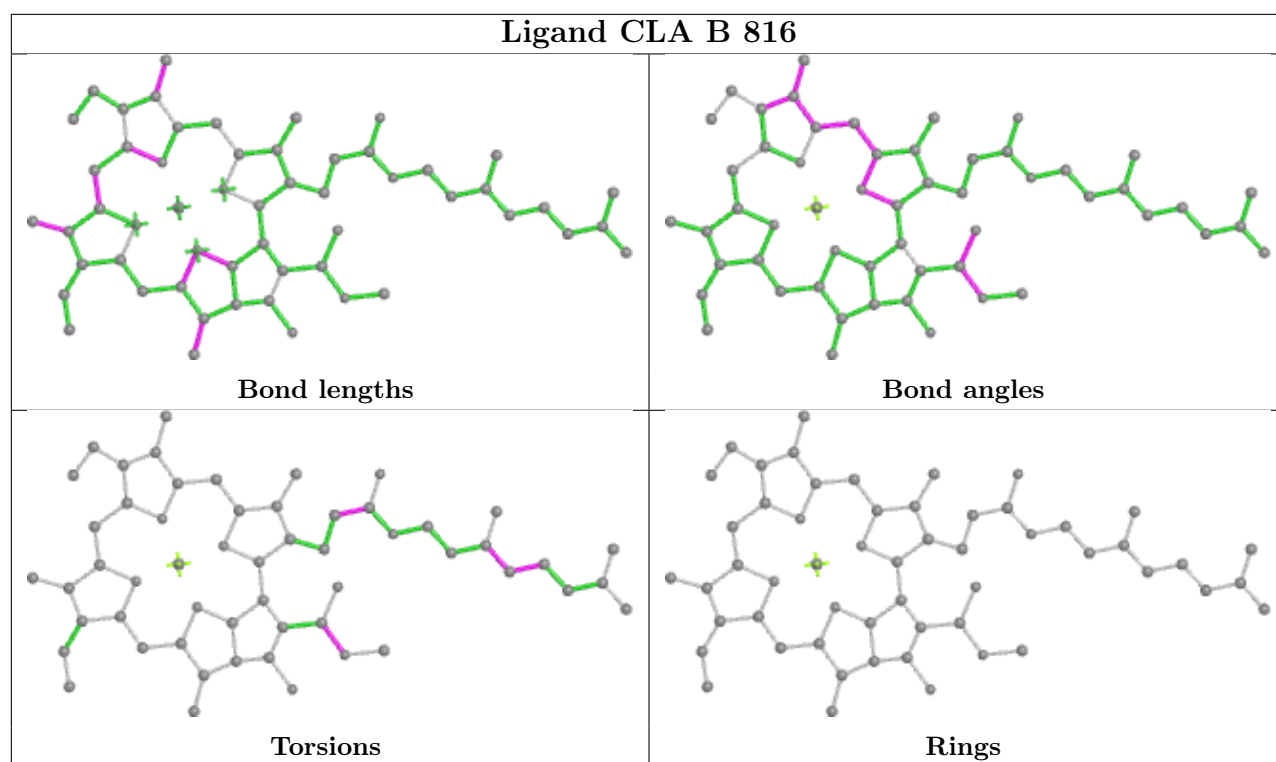
Bond angles



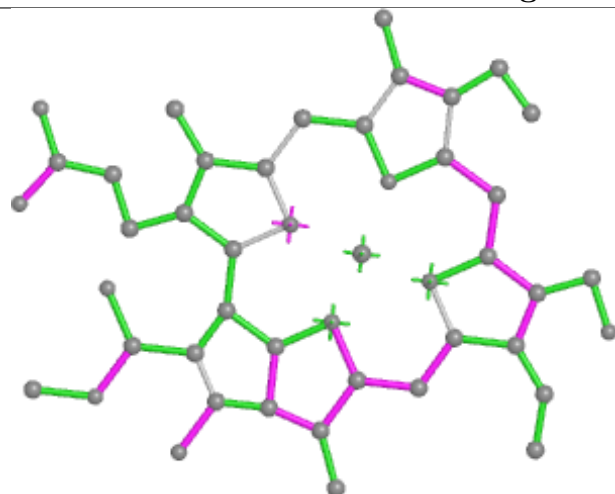
Torsions



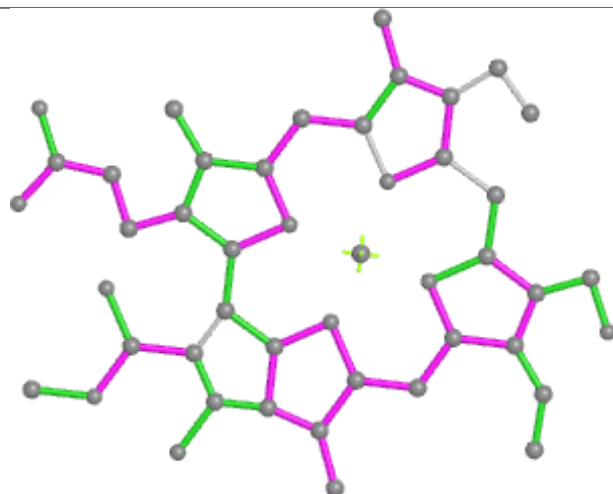
Rings



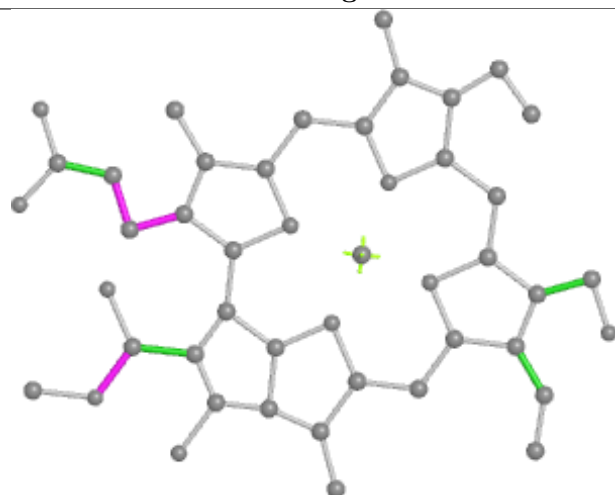
Ligand CHL 4 608



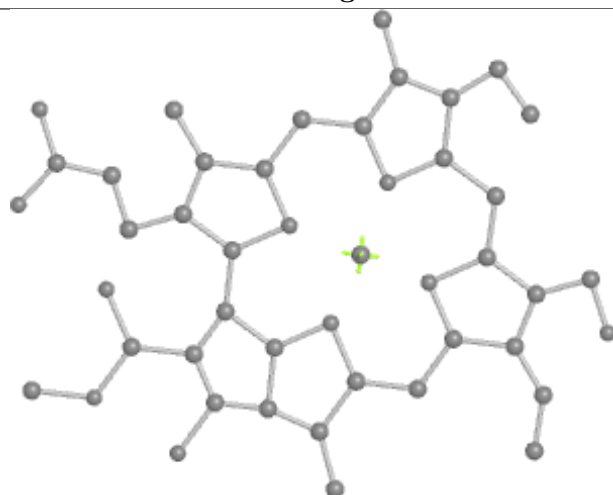
Bond lengths



Bond angles

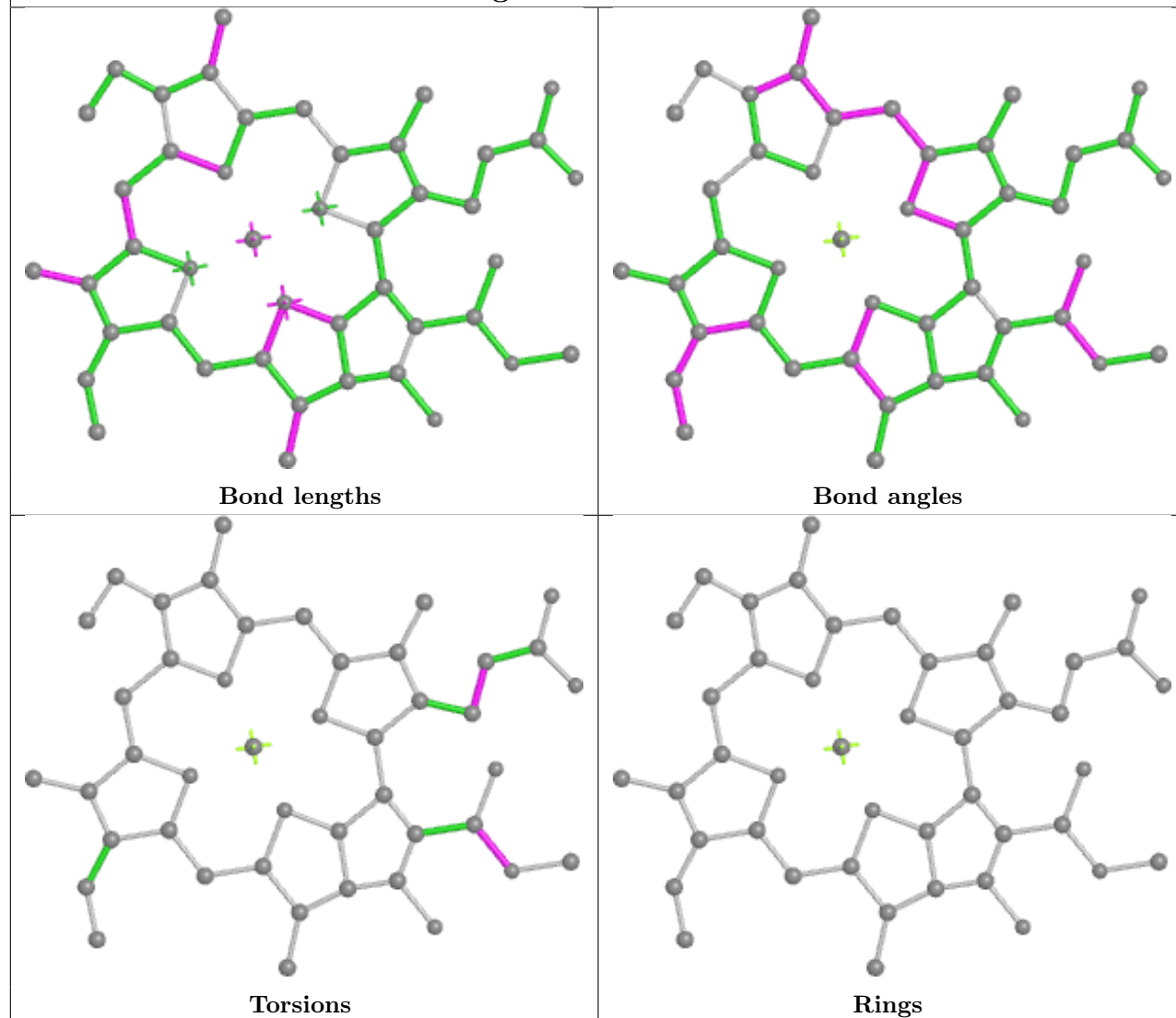


Torsions

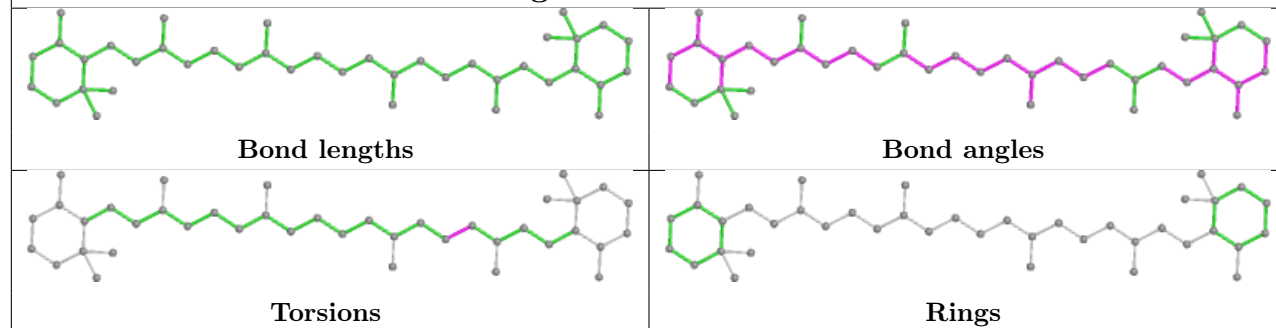


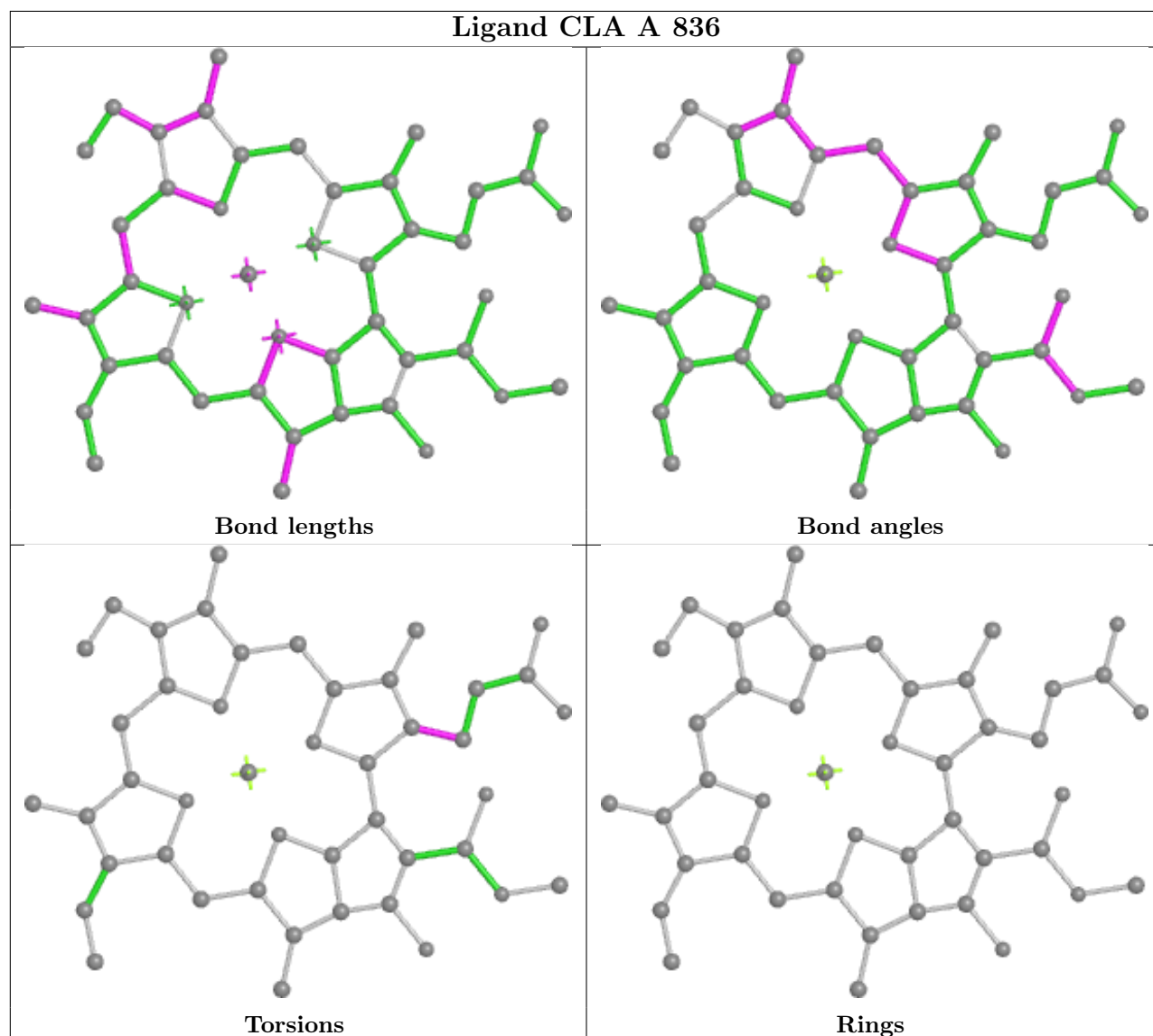
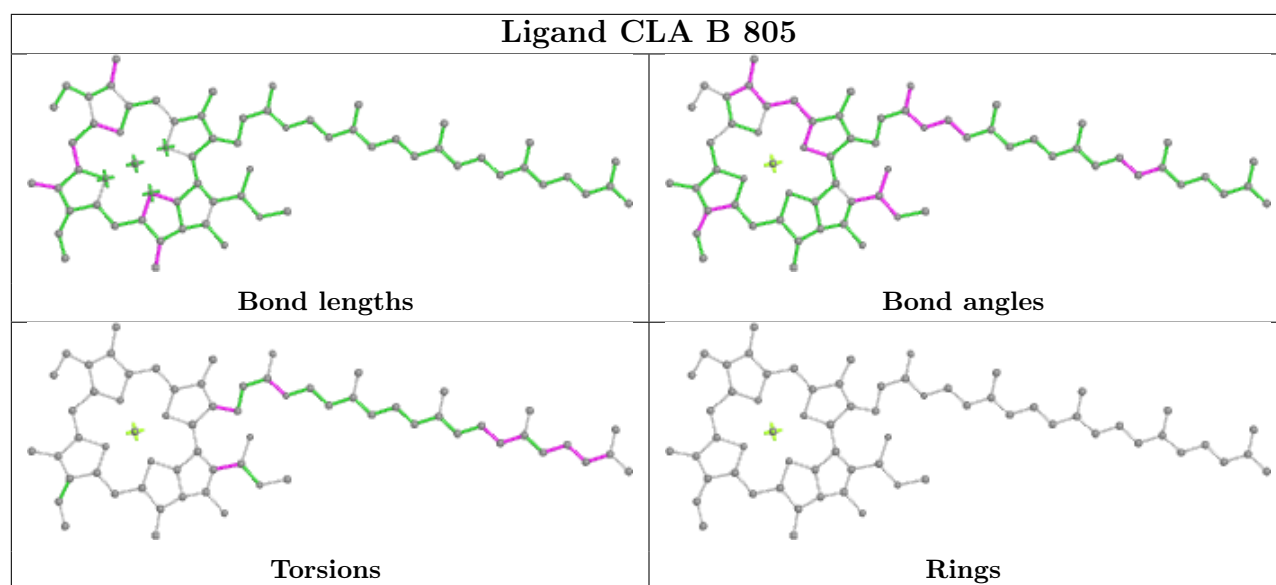
Rings

Ligand CLA L 304

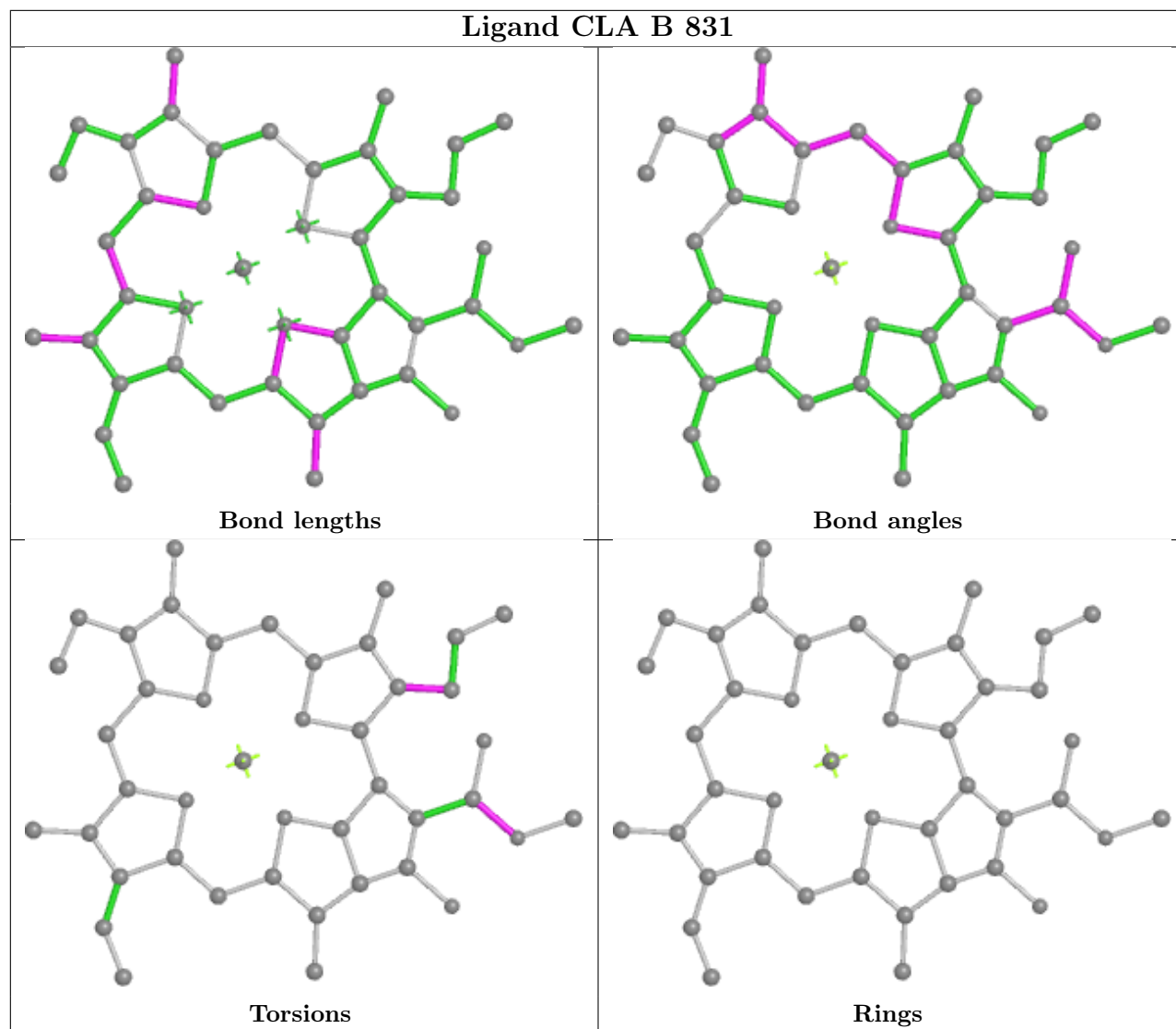


Ligand BCR B 846

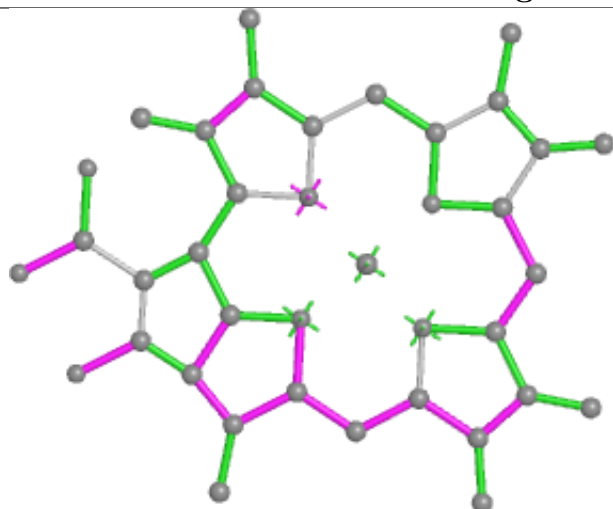




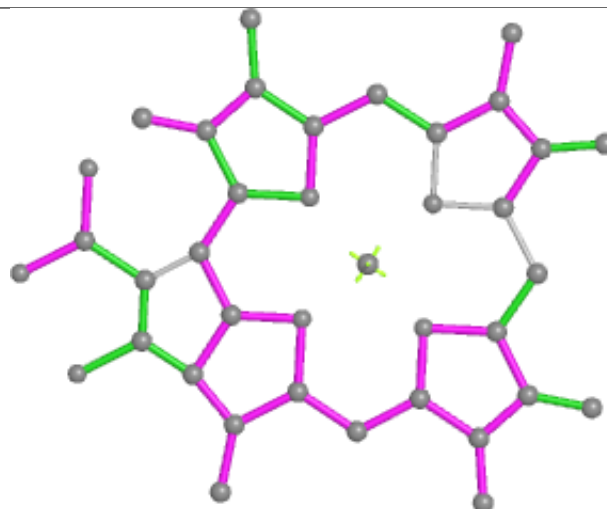
Ligand CLA B 831



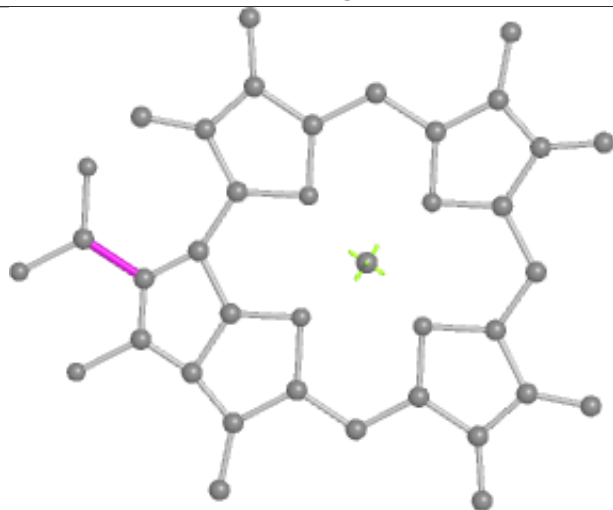
Ligand CHL Z 605



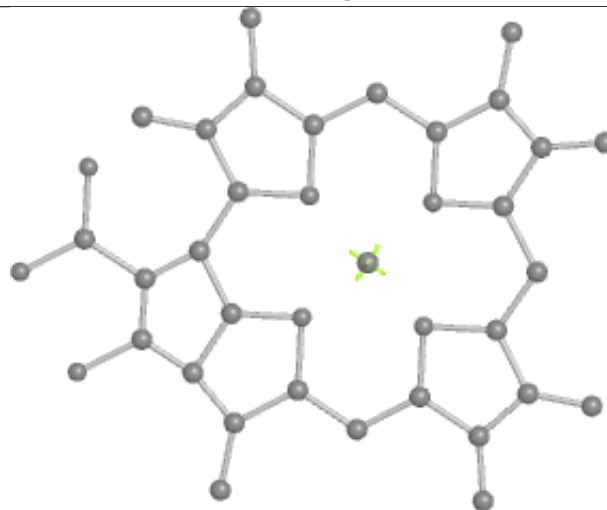
Bond lengths



Bond angles

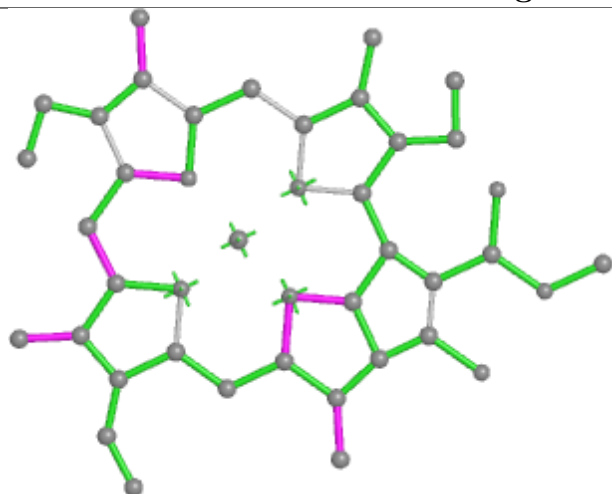


Torsions

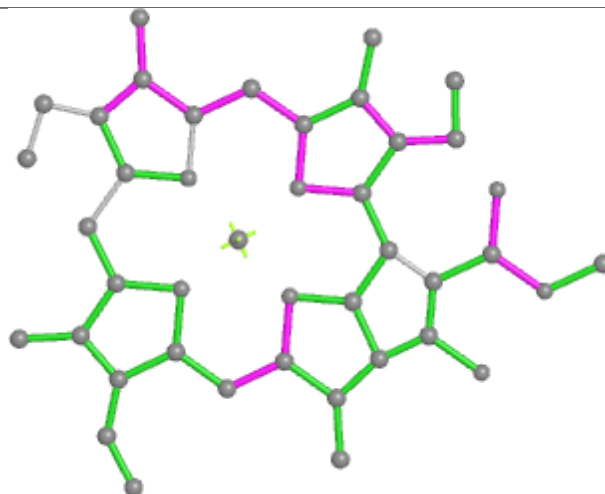


Rings

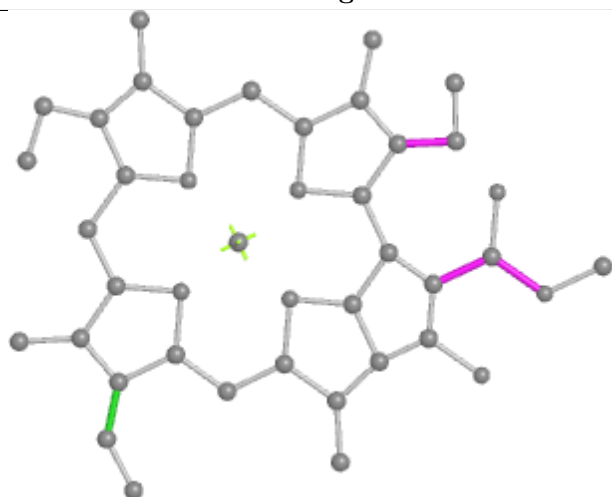
Ligand CLA F 303



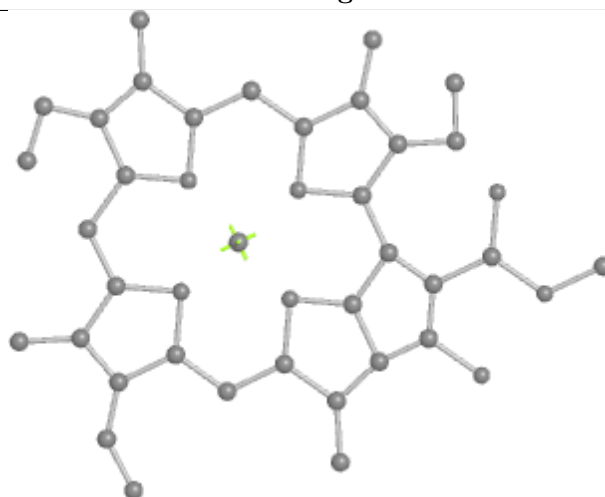
Bond lengths



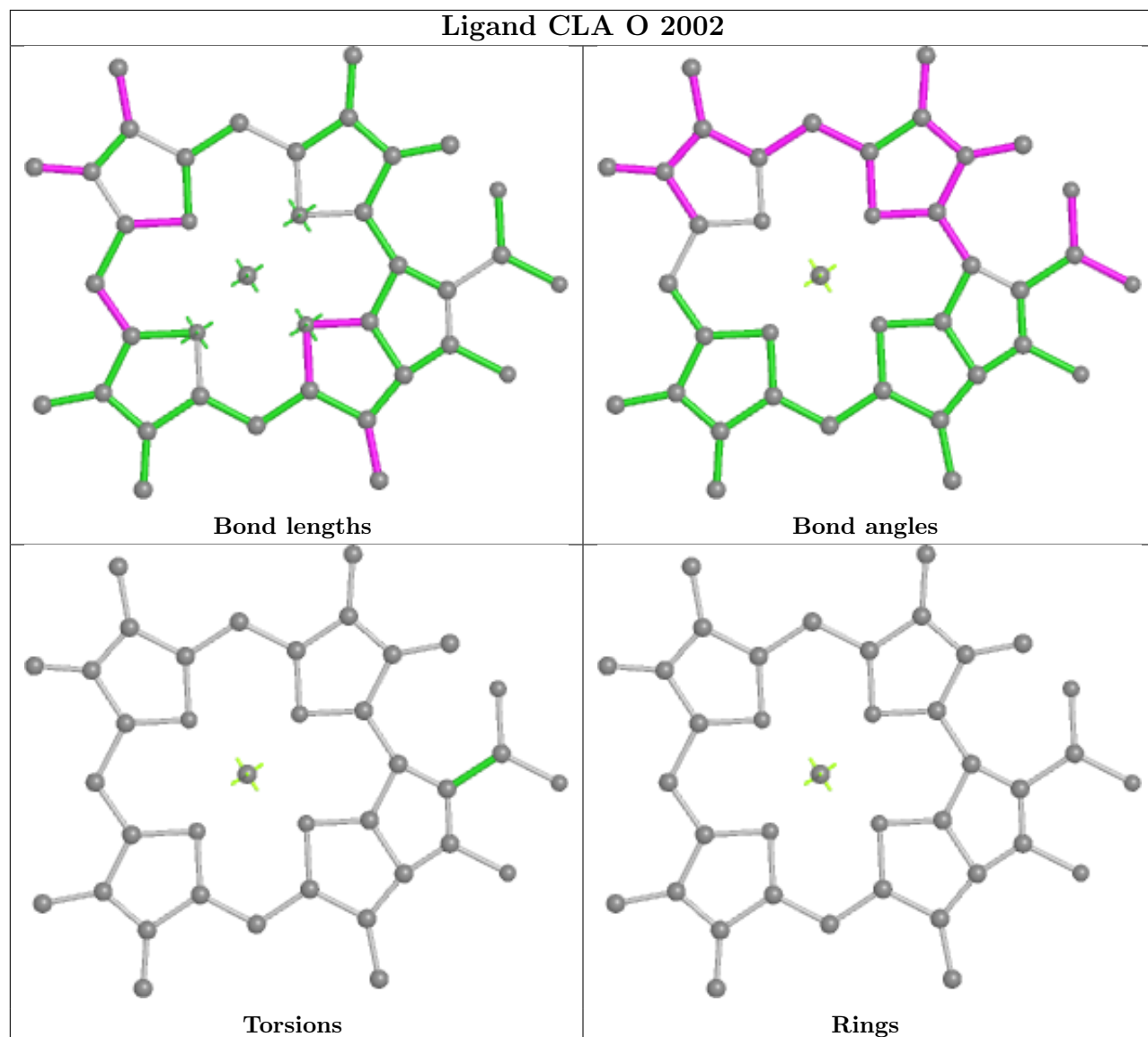
Bond angles



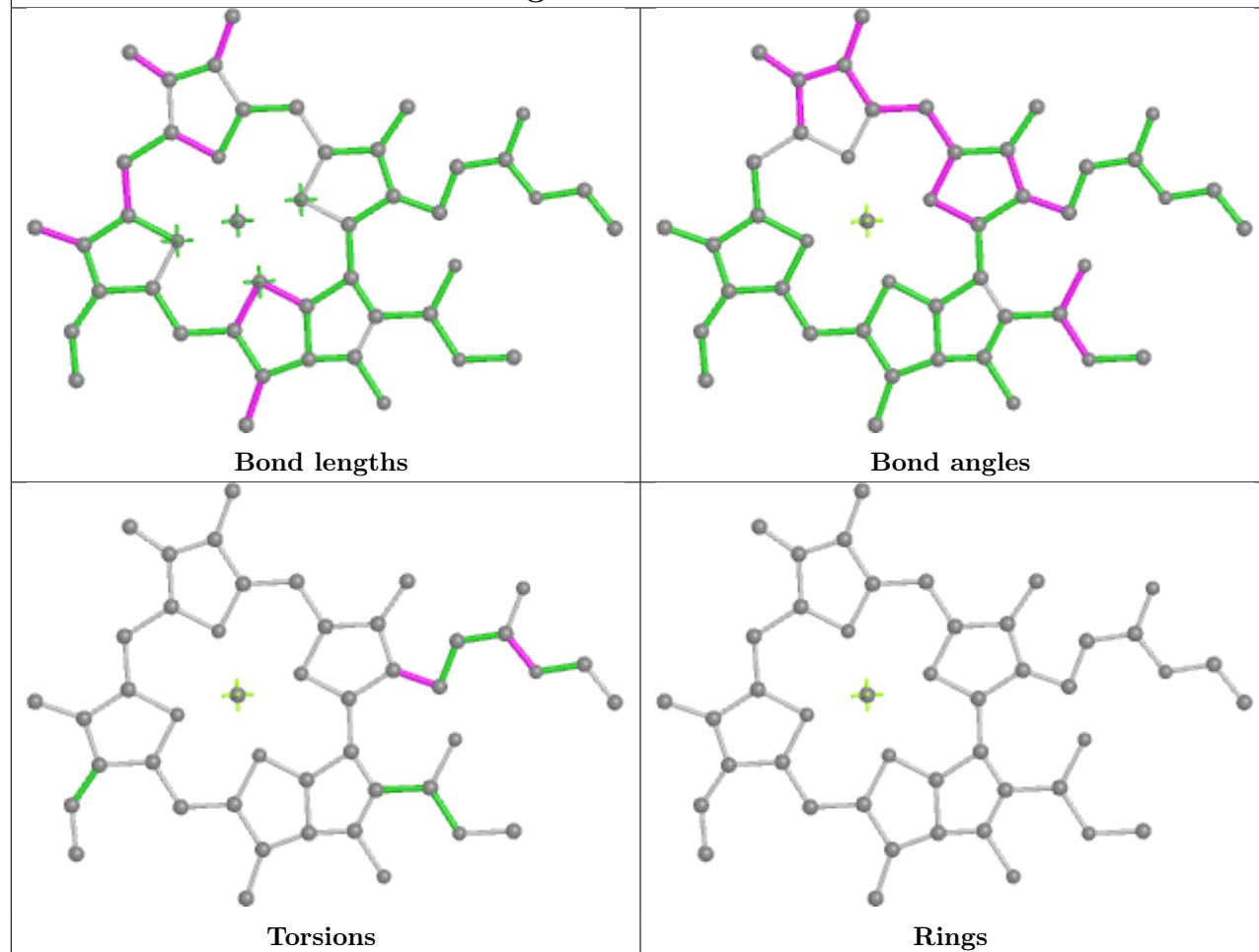
Torsions



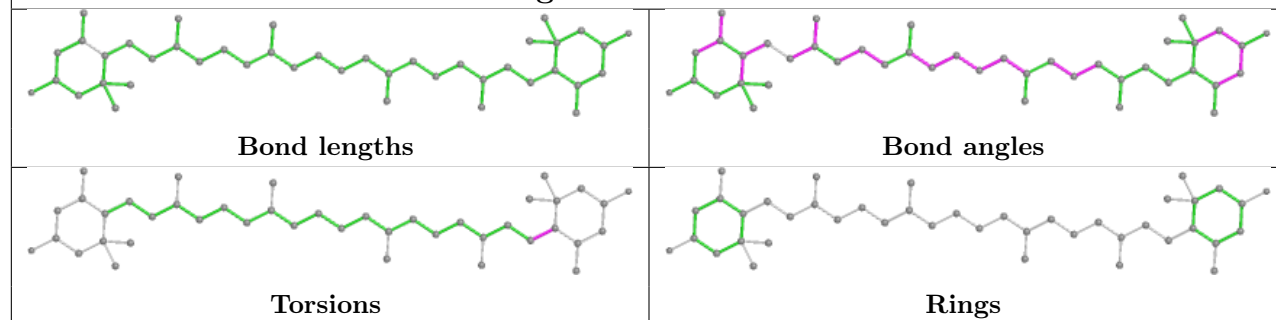
Rings



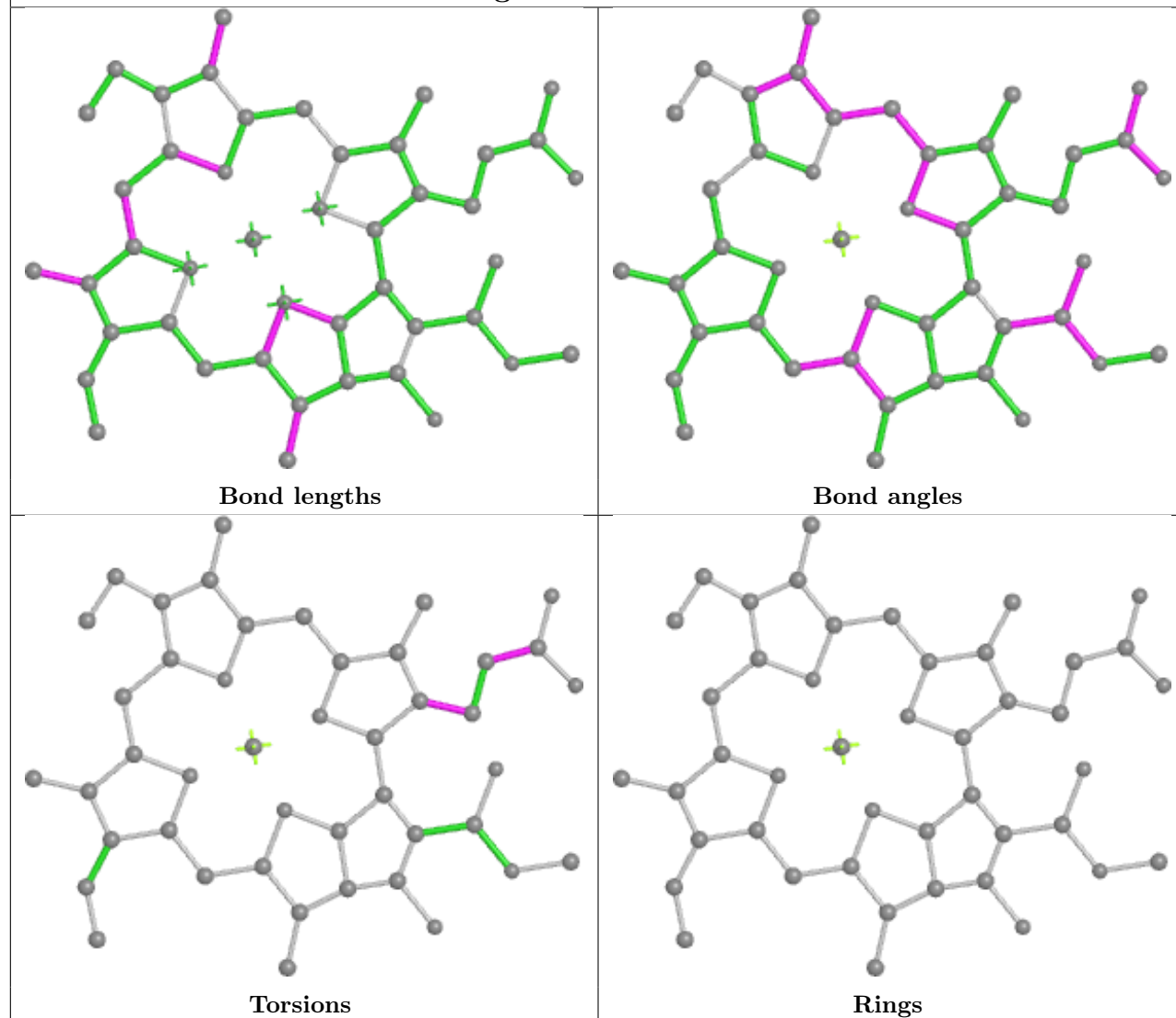
Ligand CLA Z 604



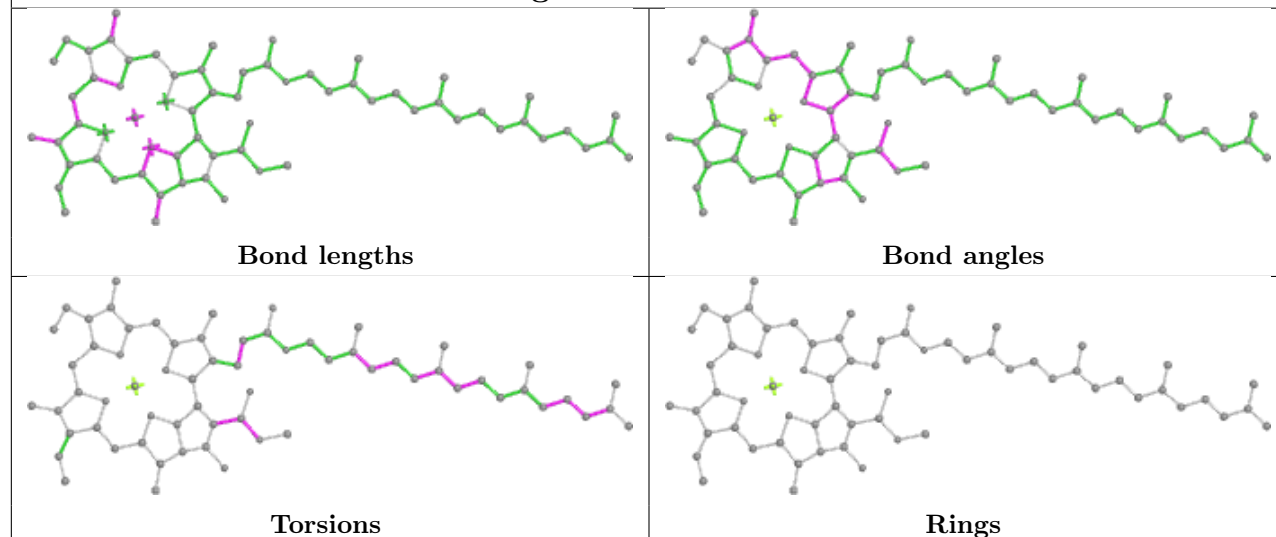
Ligand LUT 2 619



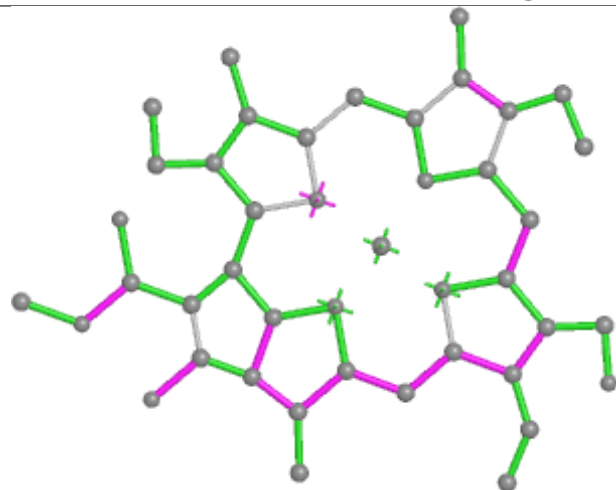
Ligand CLA 4 614



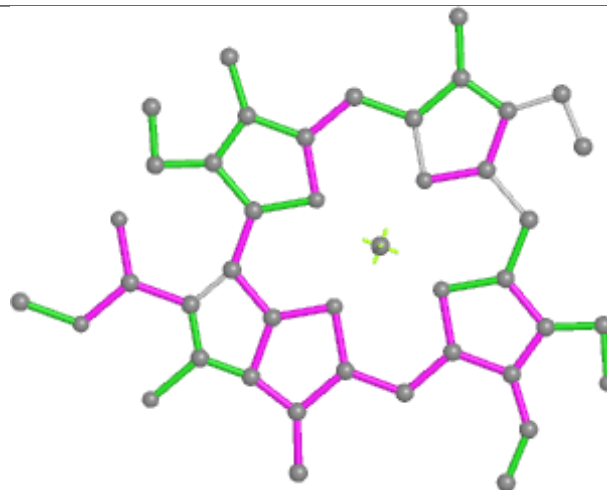
Ligand CLA A 854



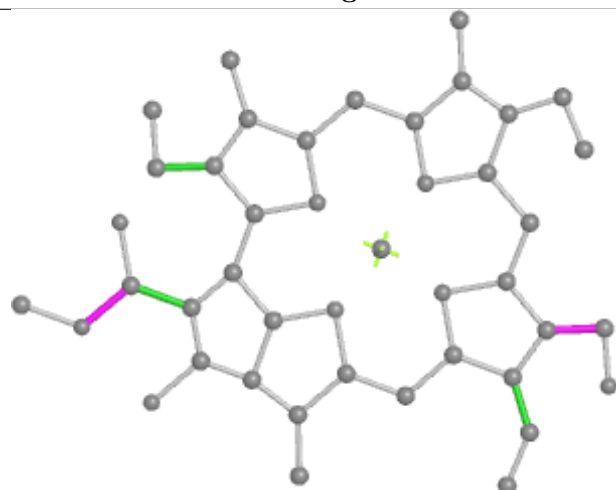
Ligand CHL 2 607



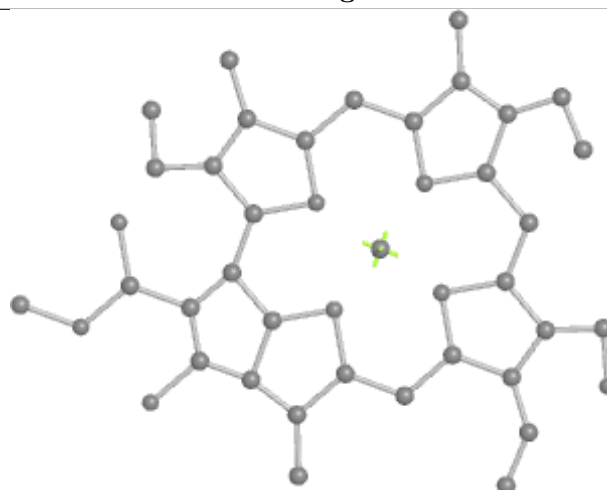
Bond lengths



Bond angles

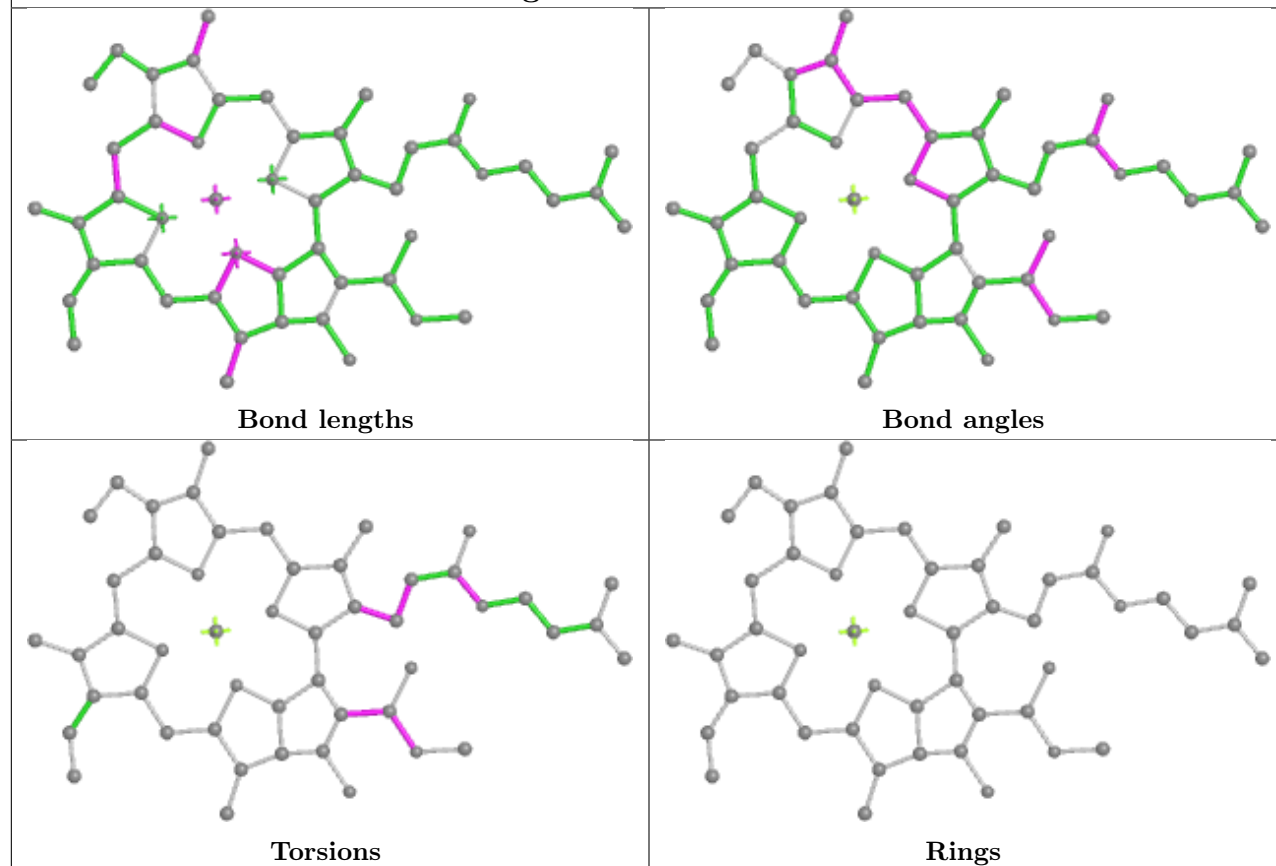


Torsions

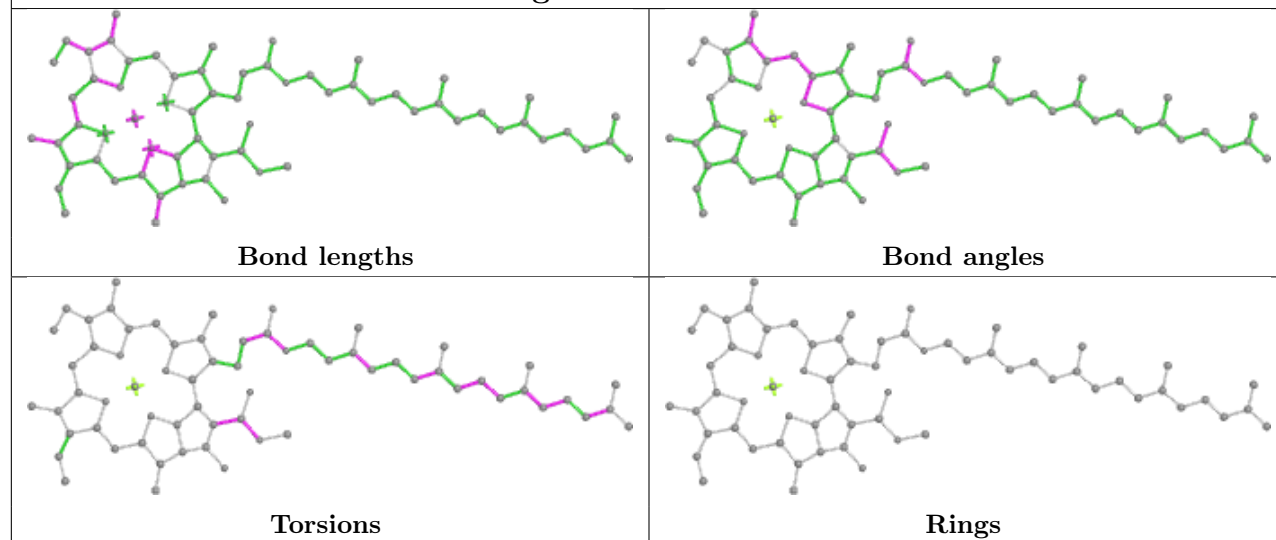


Rings

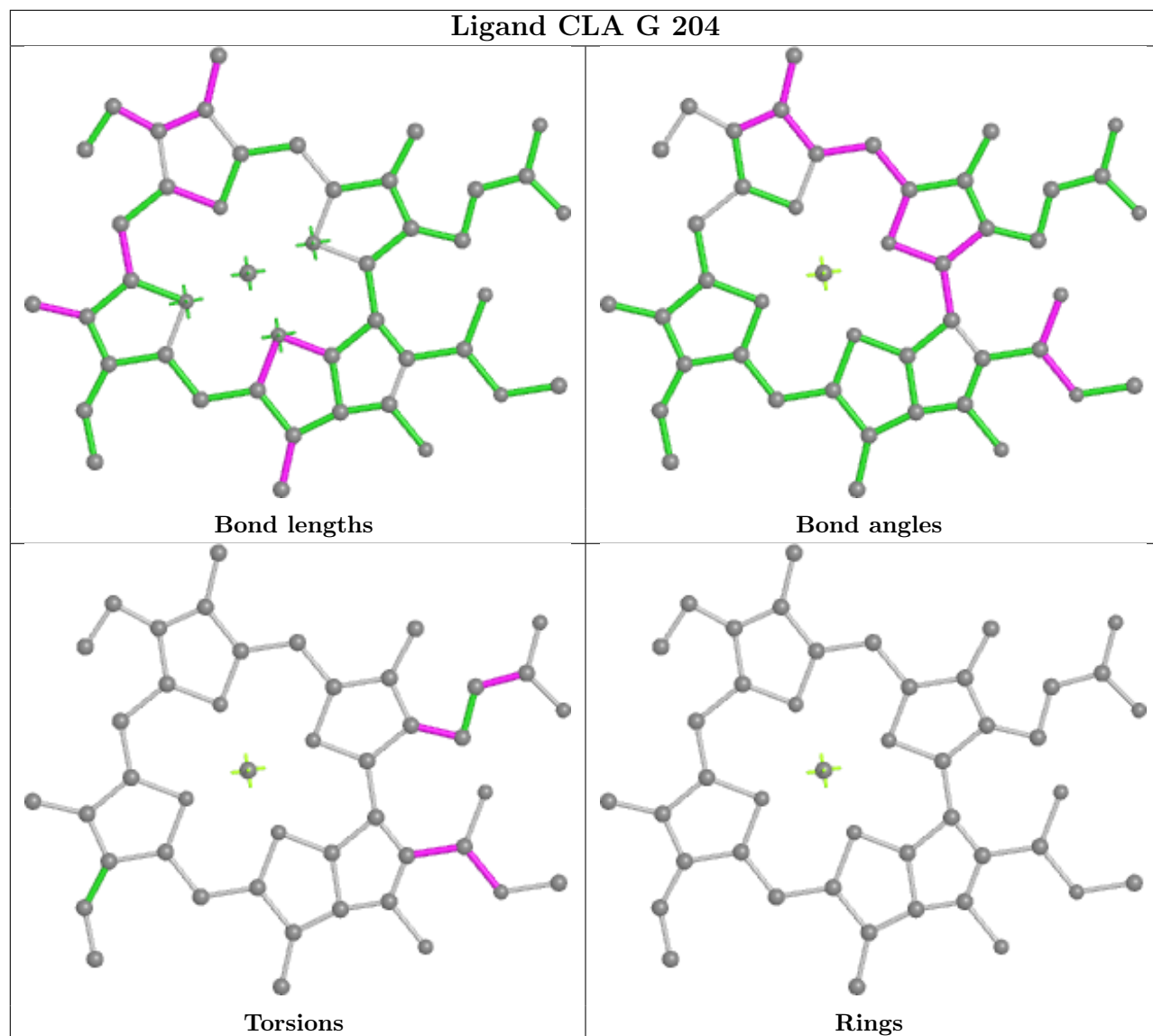
Ligand CLA N 1002



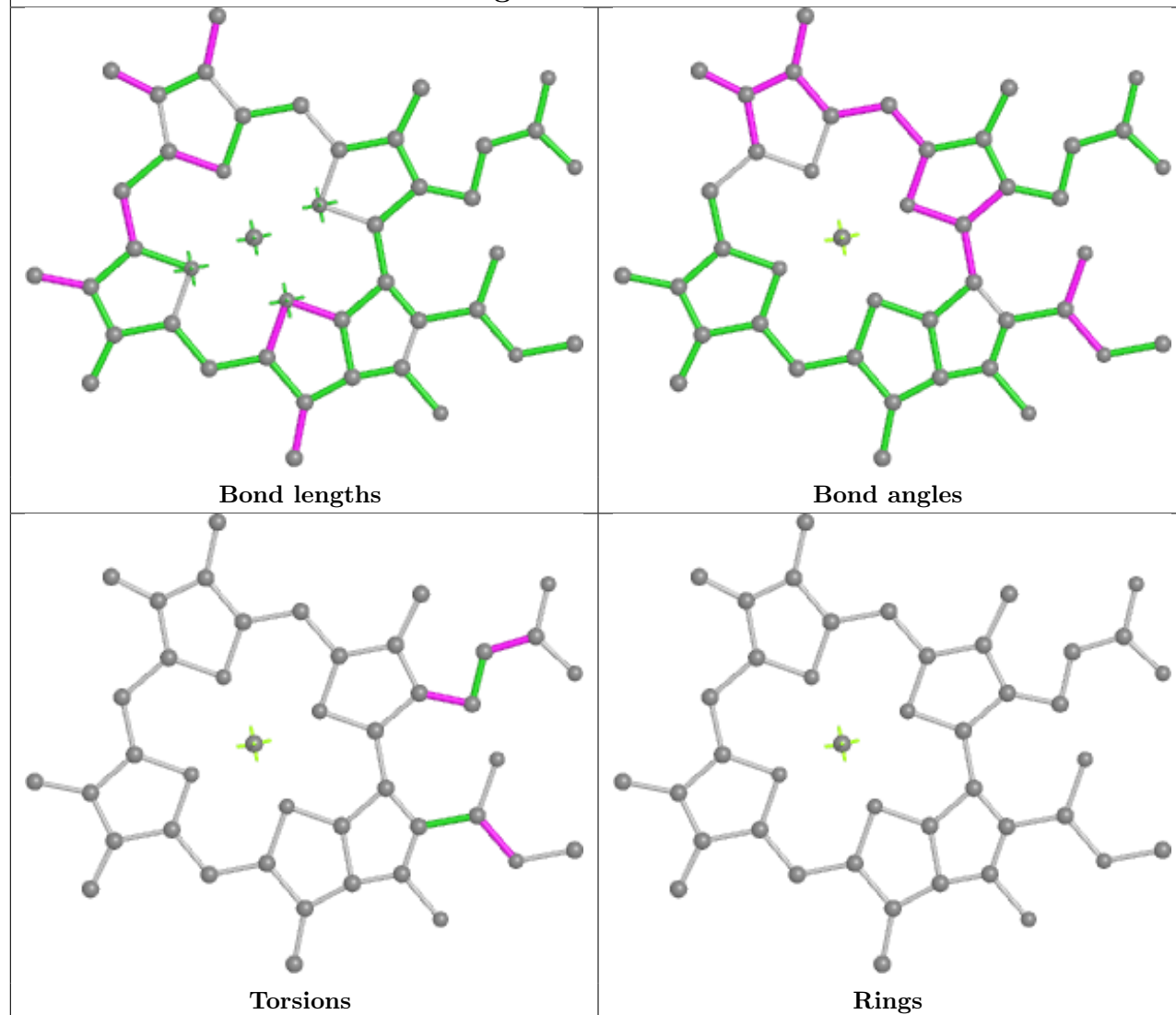
Ligand CLA B 802



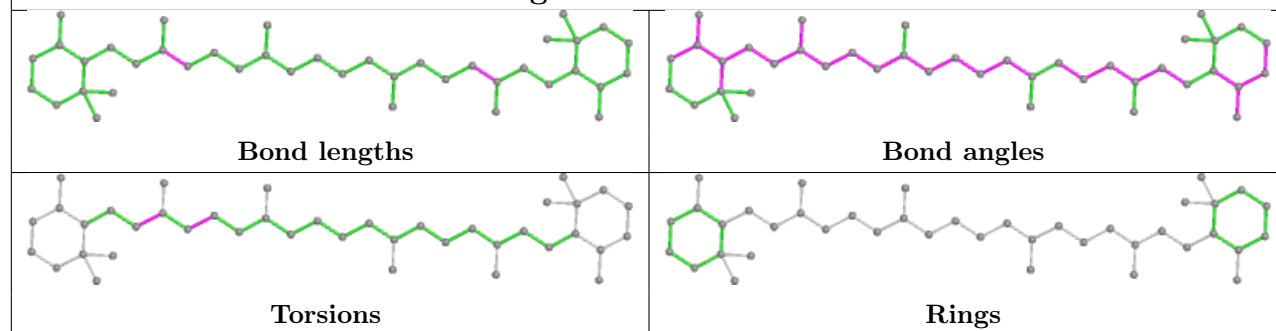
Ligand CLA G 204



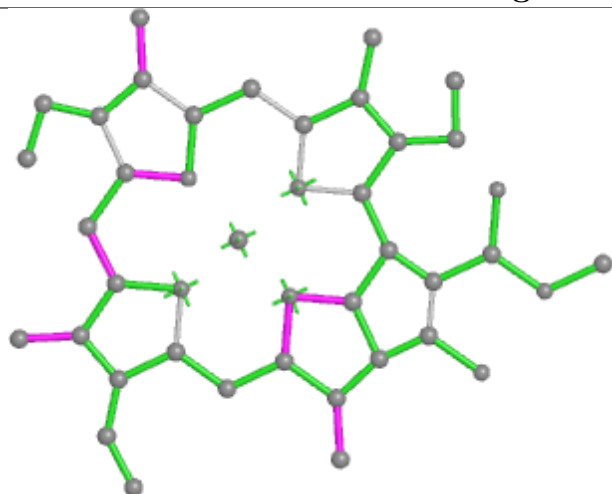
Ligand CLA 4 604



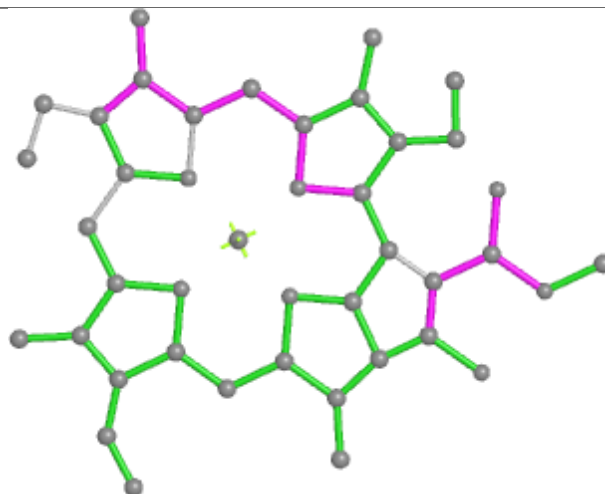
Ligand BCR A 850



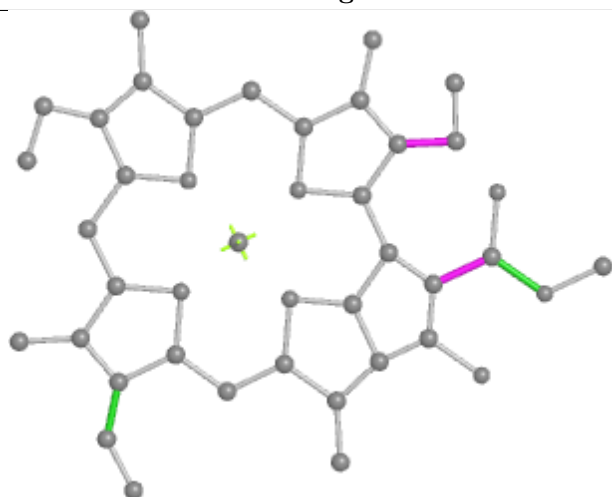
Ligand CLA A 816



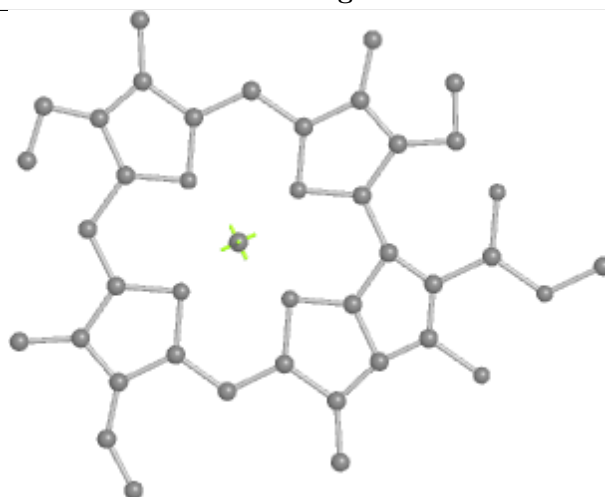
Bond lengths



Bond angles

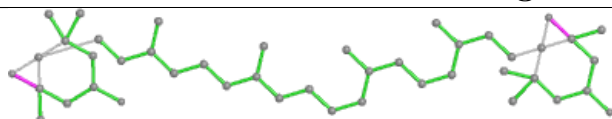


Torsions

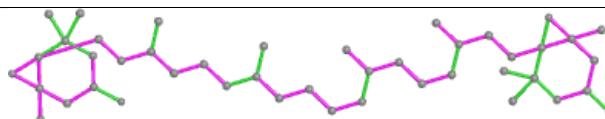


Rings

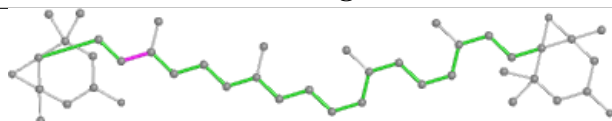
Ligand XAT 3 619



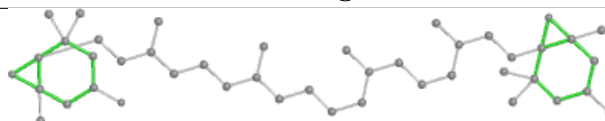
Bond lengths



Bond angles

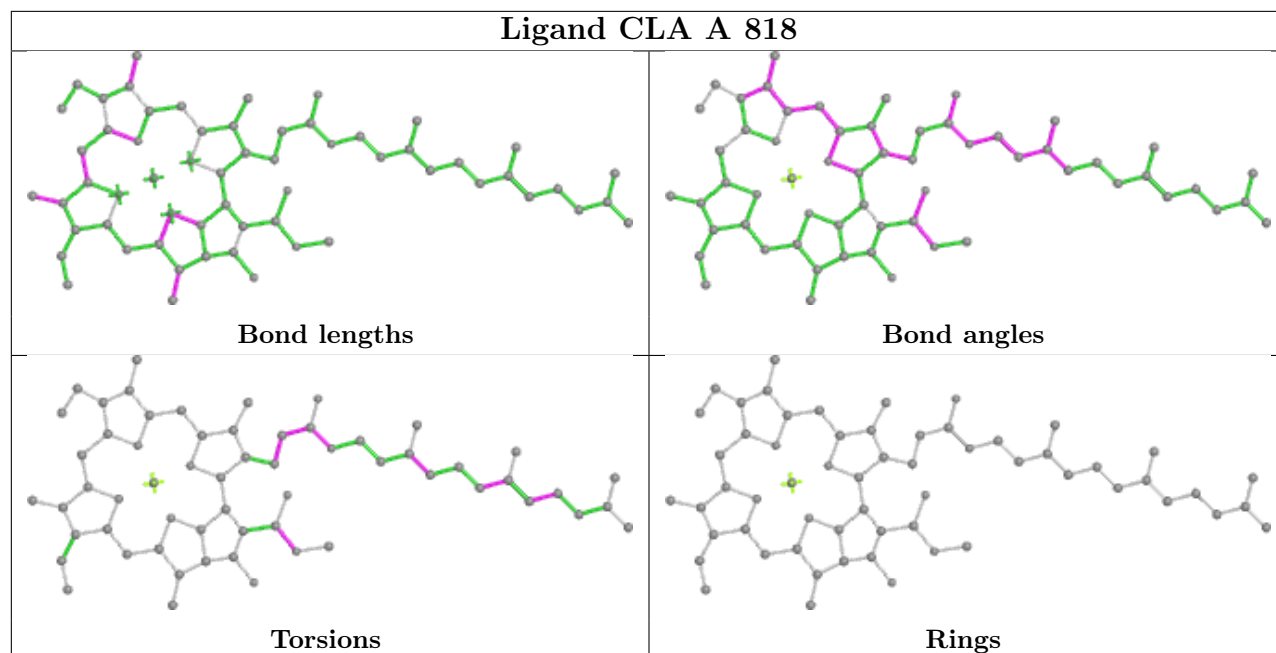


Torsions

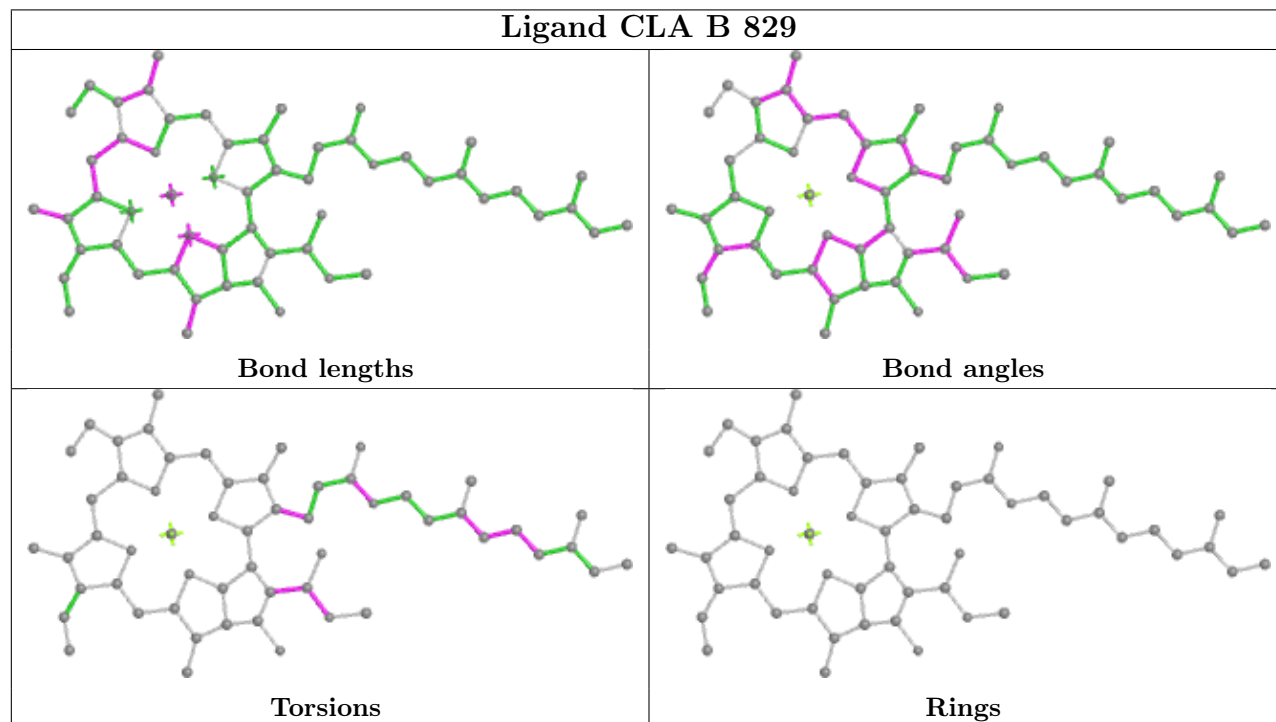


Rings

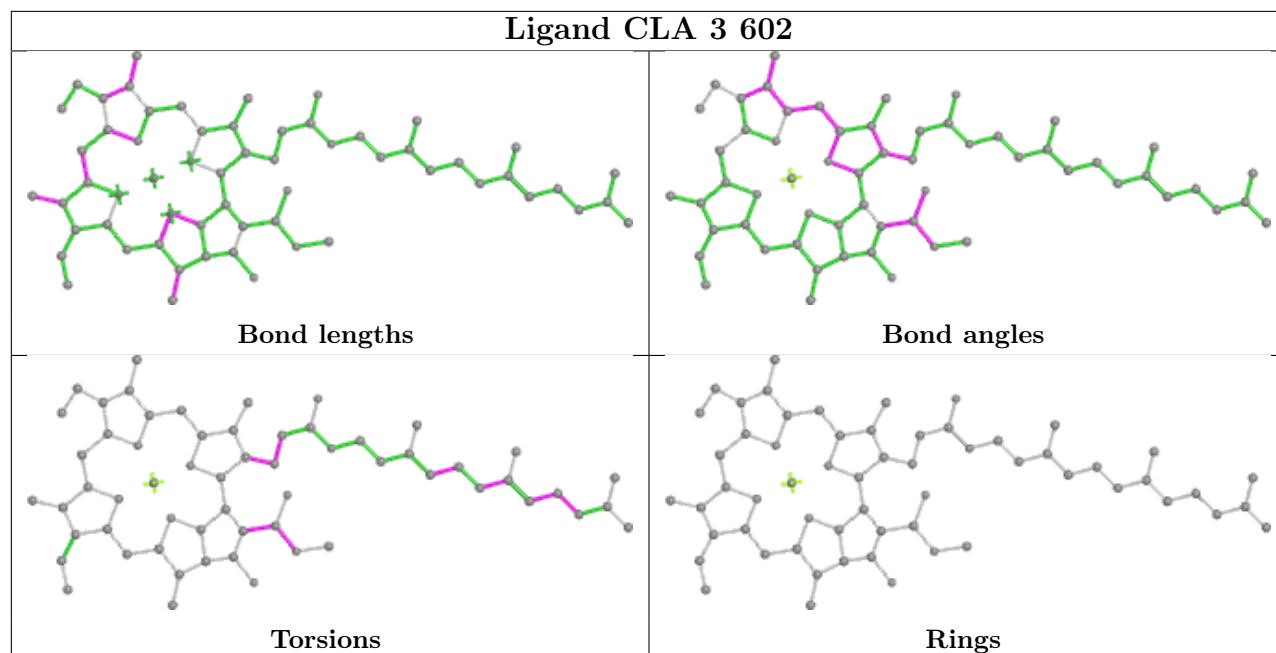
Ligand CLA A 818



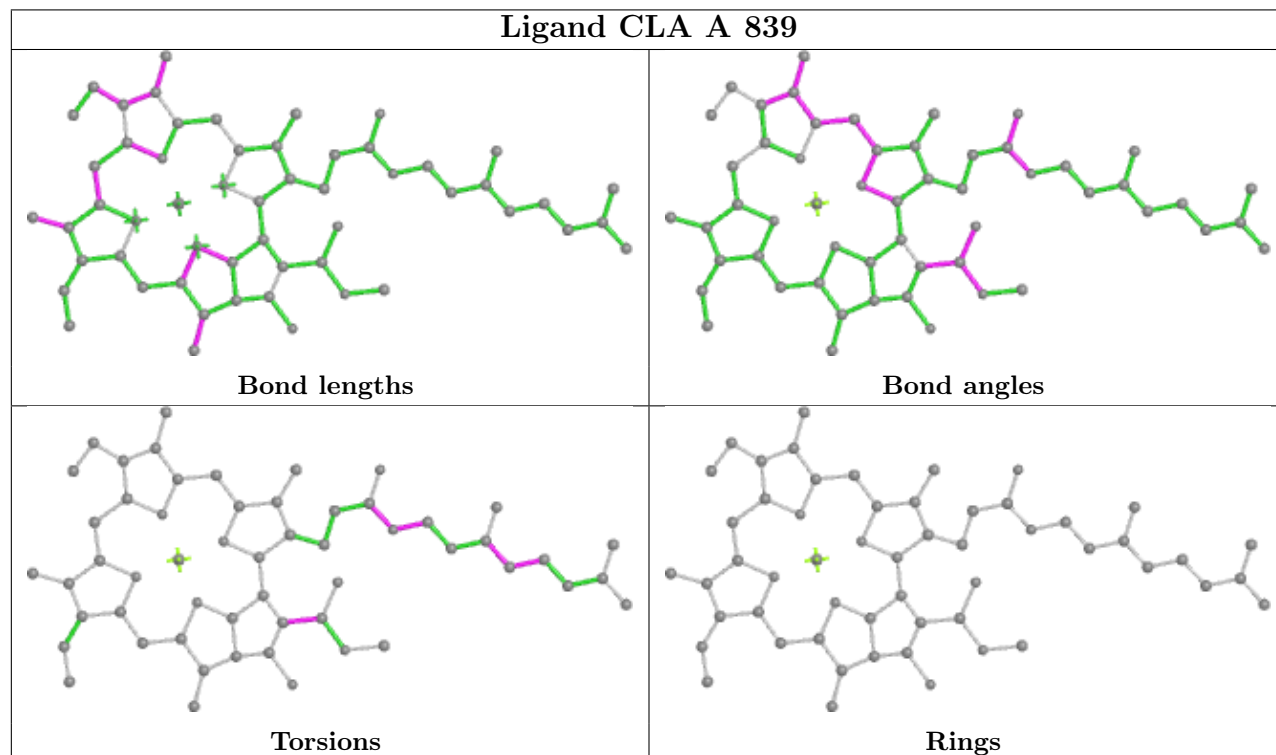
Ligand CLA B 829



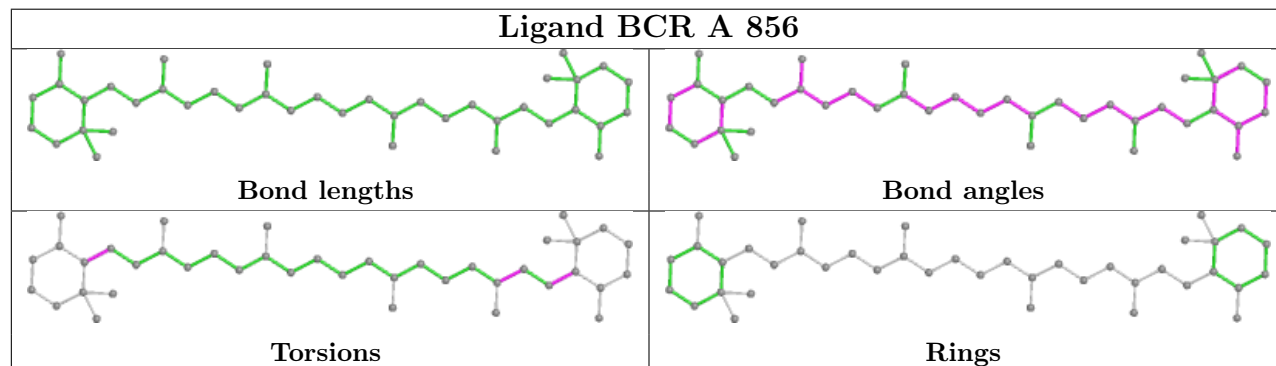
Ligand CLA 3 602

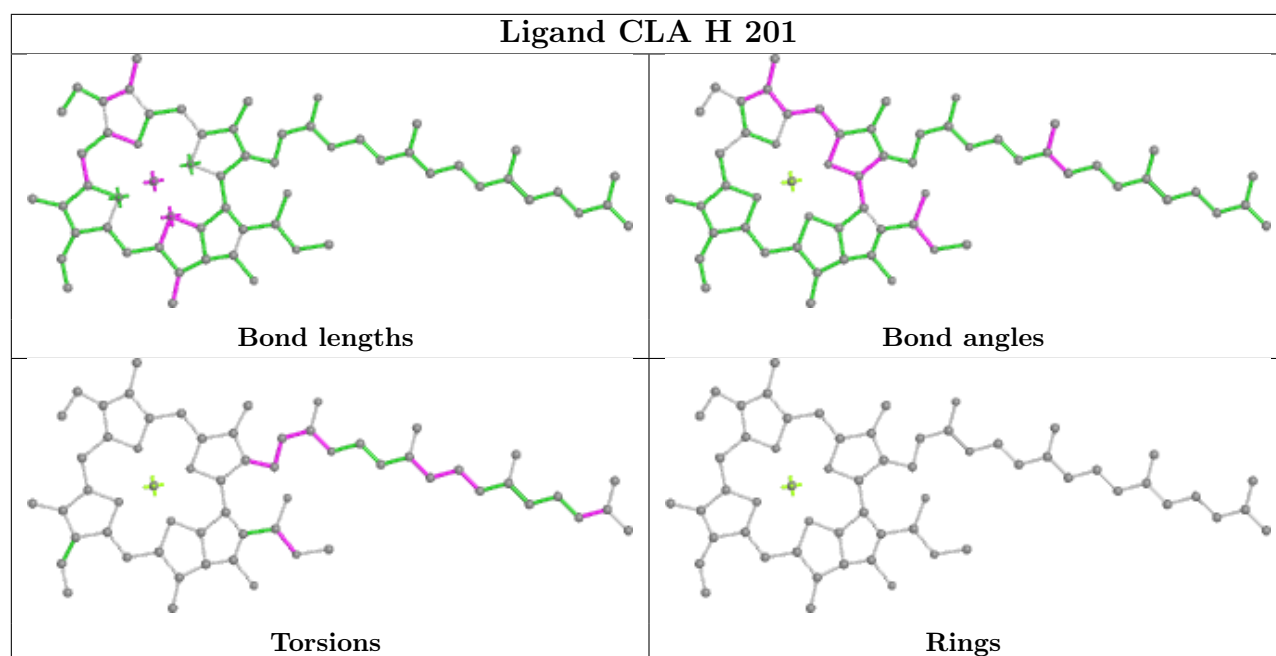


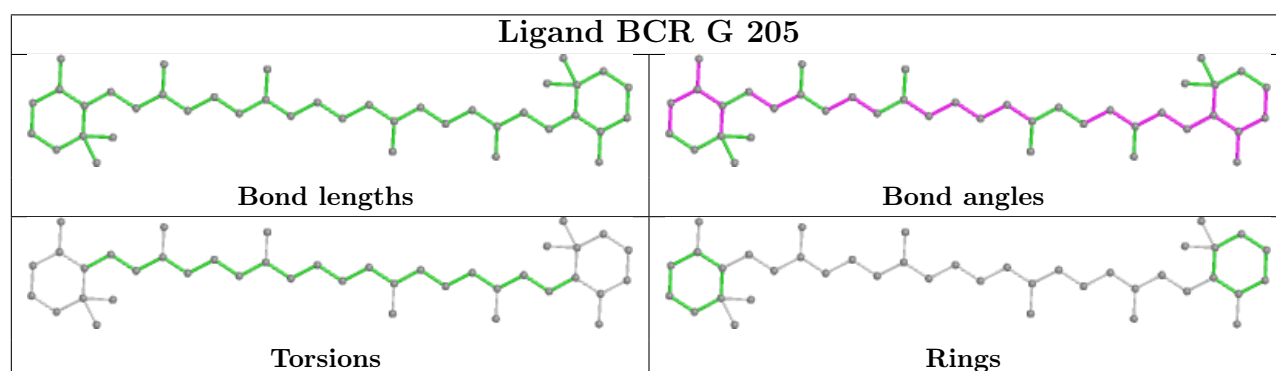
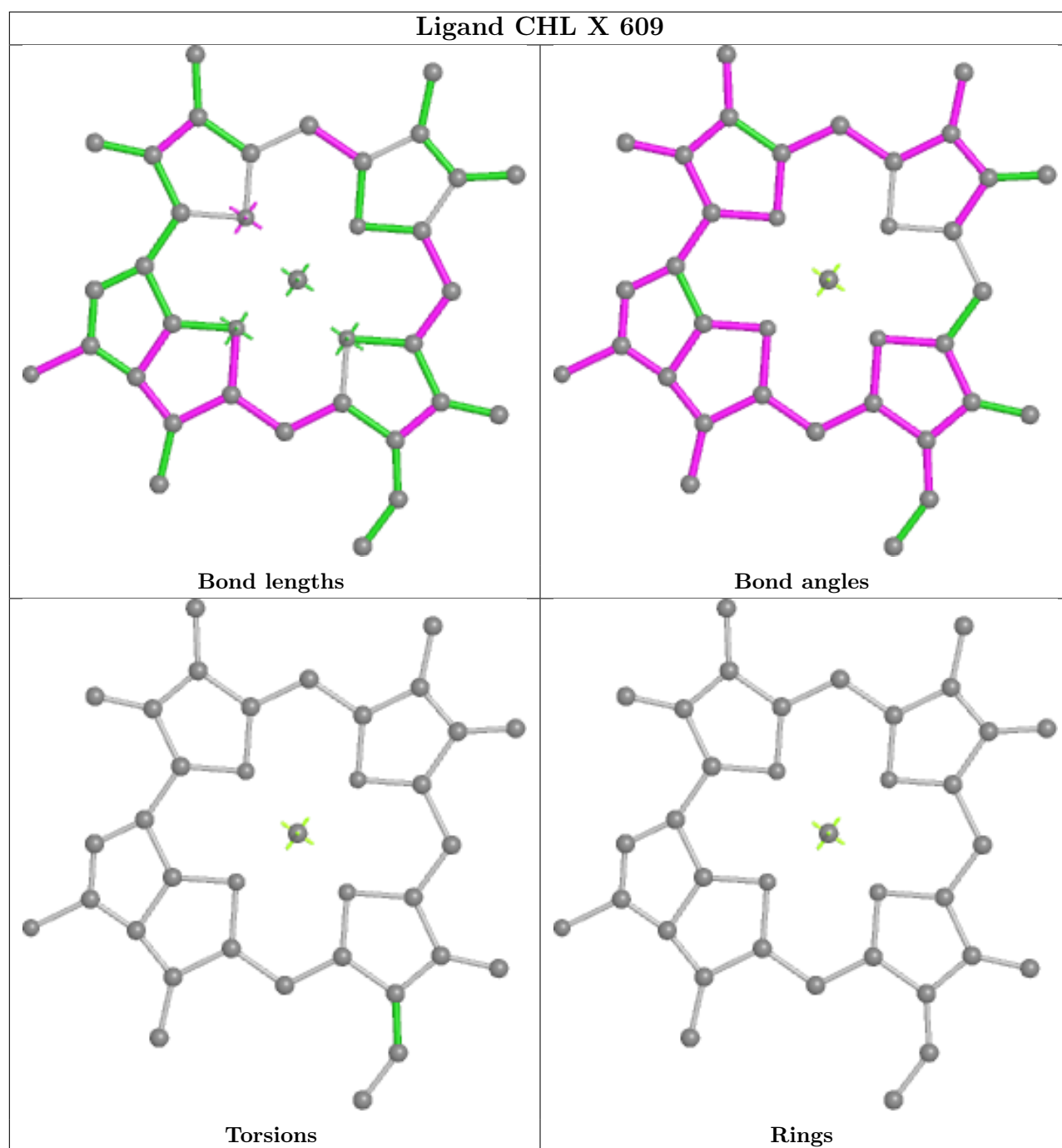
Ligand CLA A 839



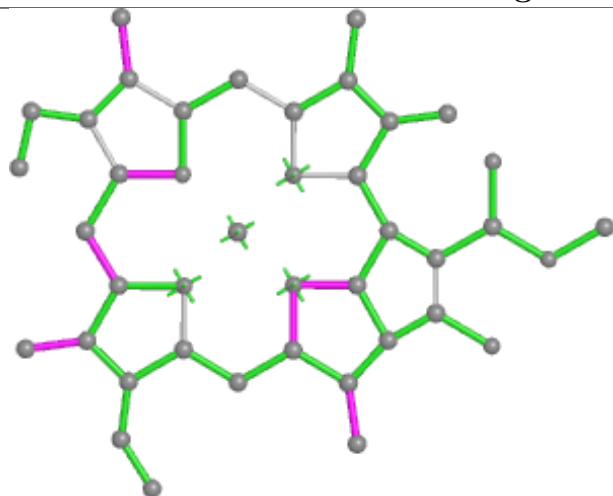
Ligand BCR A 856



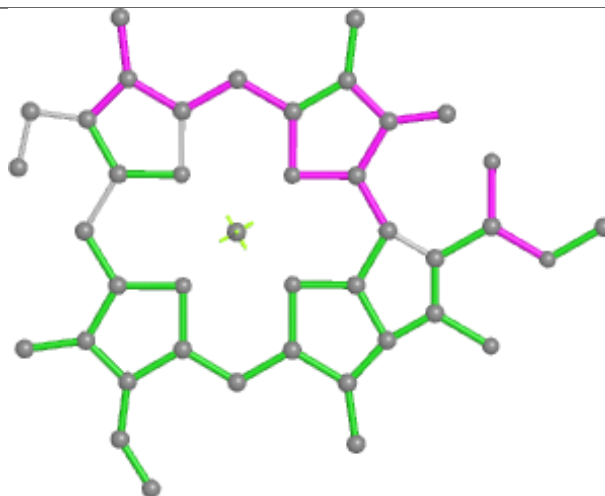




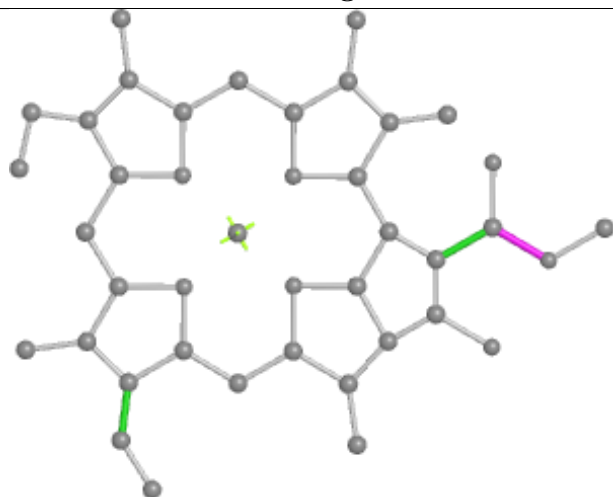
Ligand CLA B 804



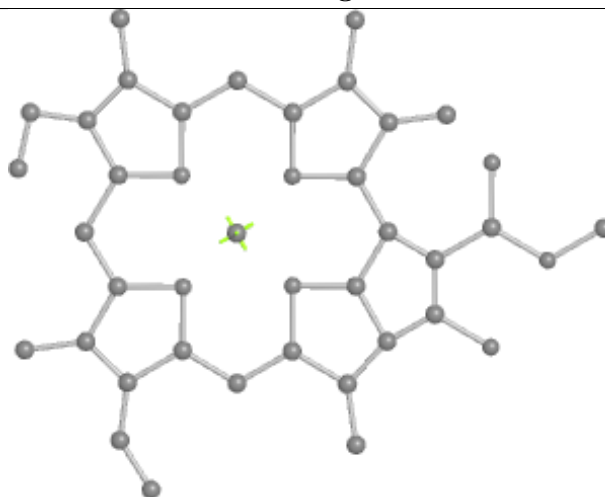
Bond lengths



Bond angles

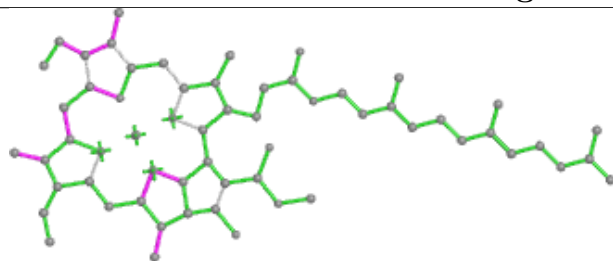


Torsions

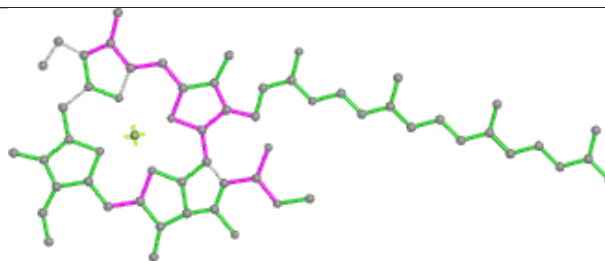


Rings

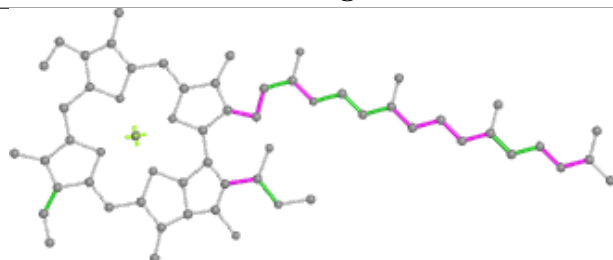
Ligand CLA L 303



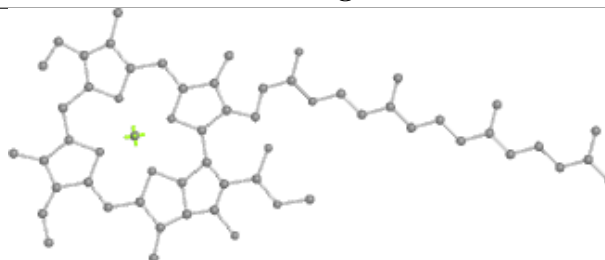
Bond lengths



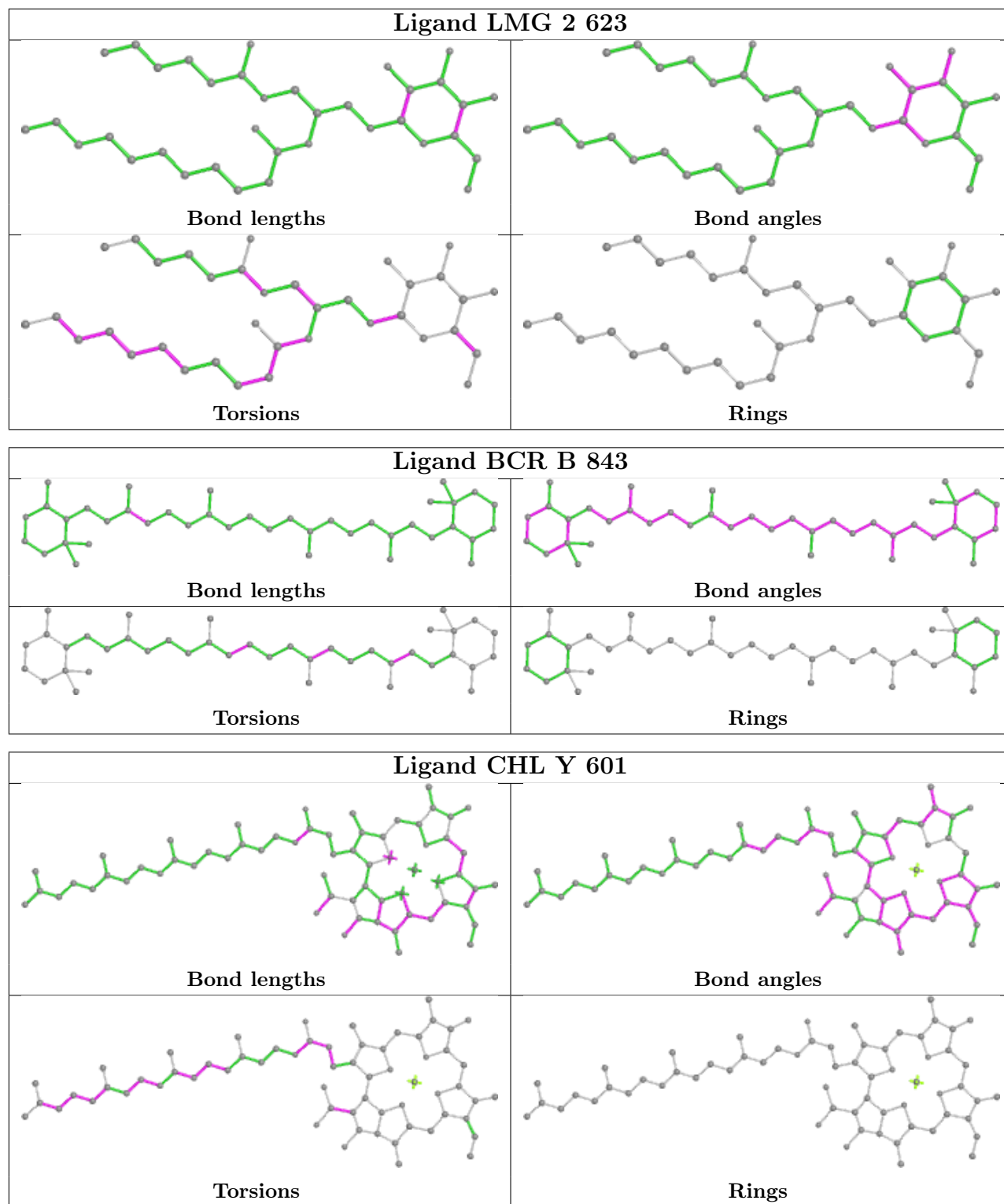
Bond angles



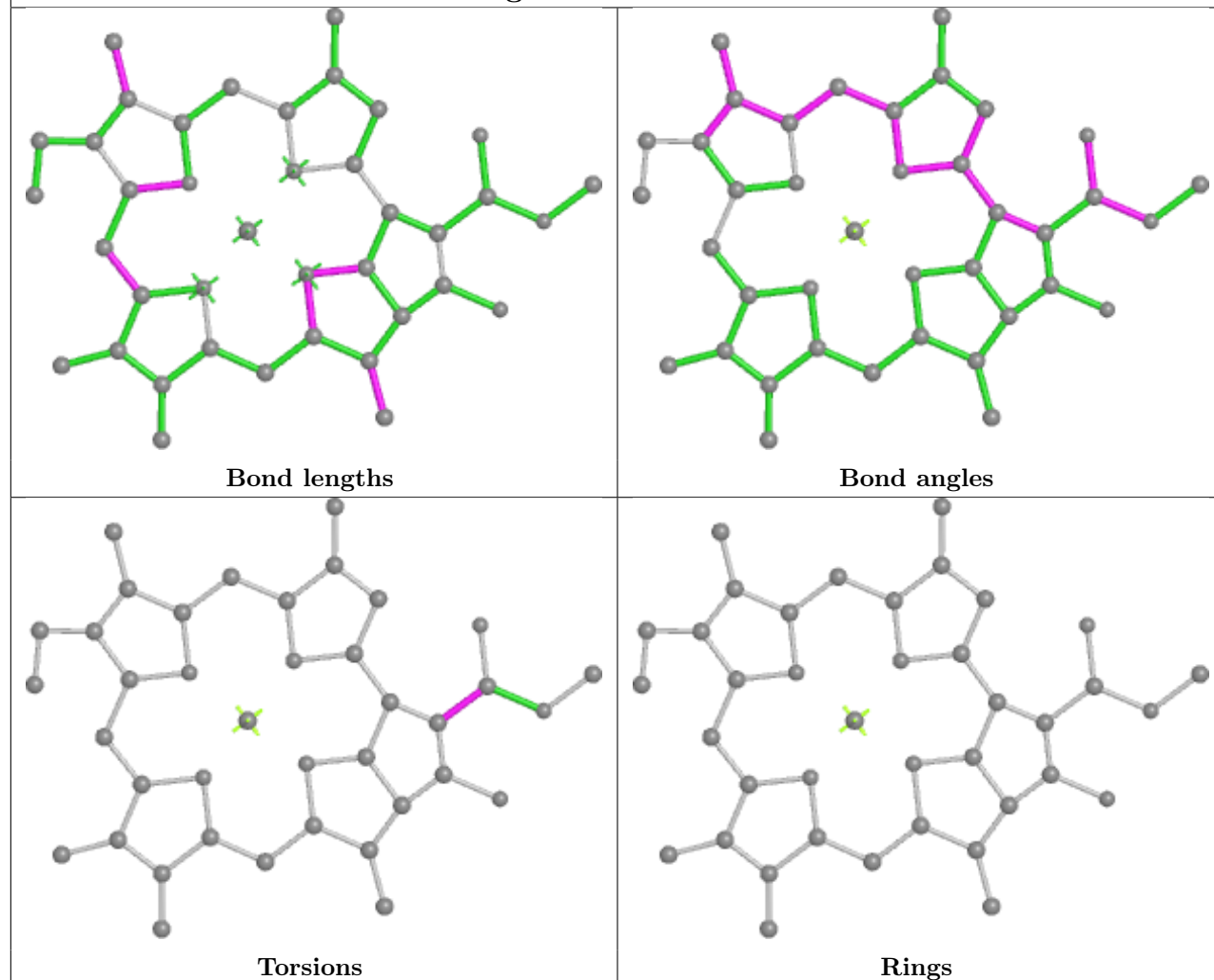
Torsions



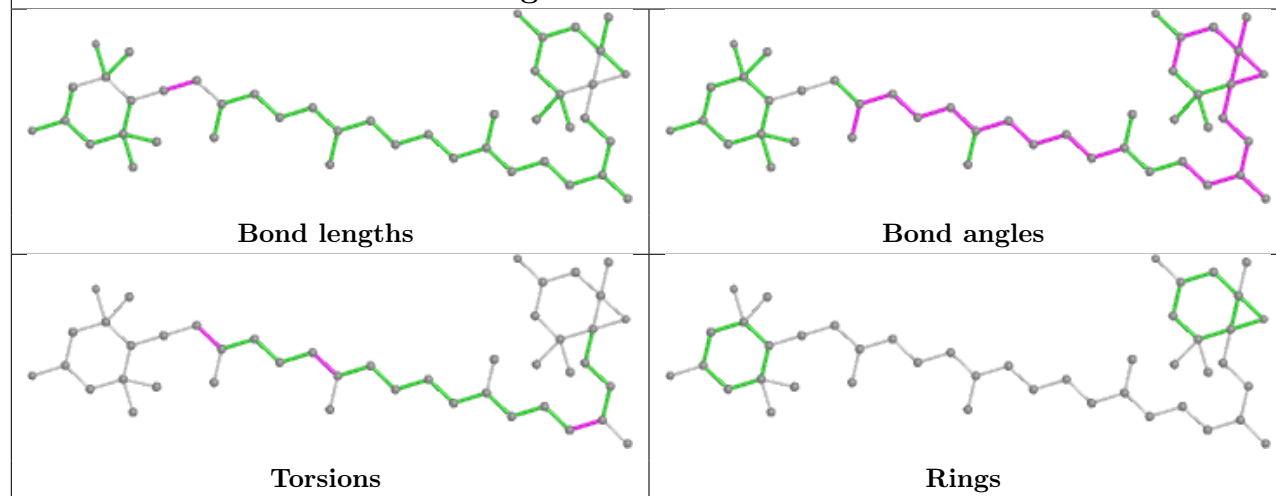
Rings

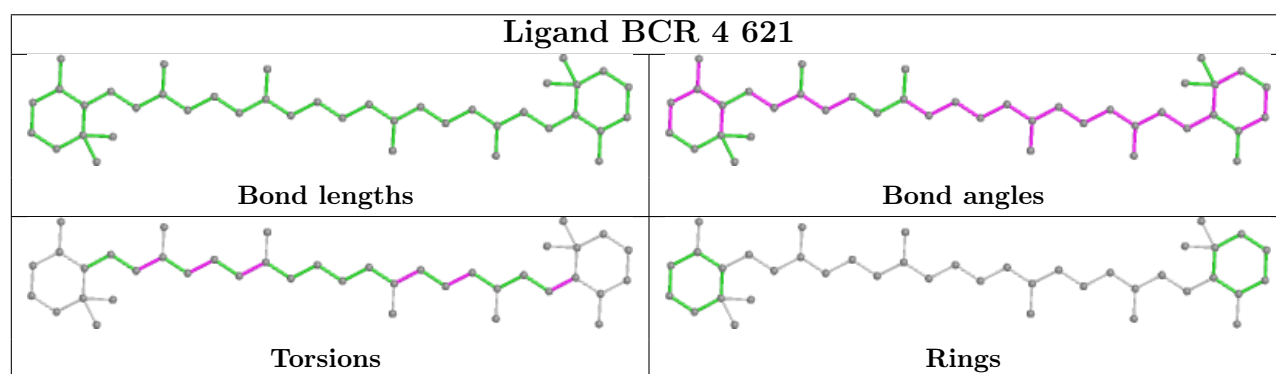
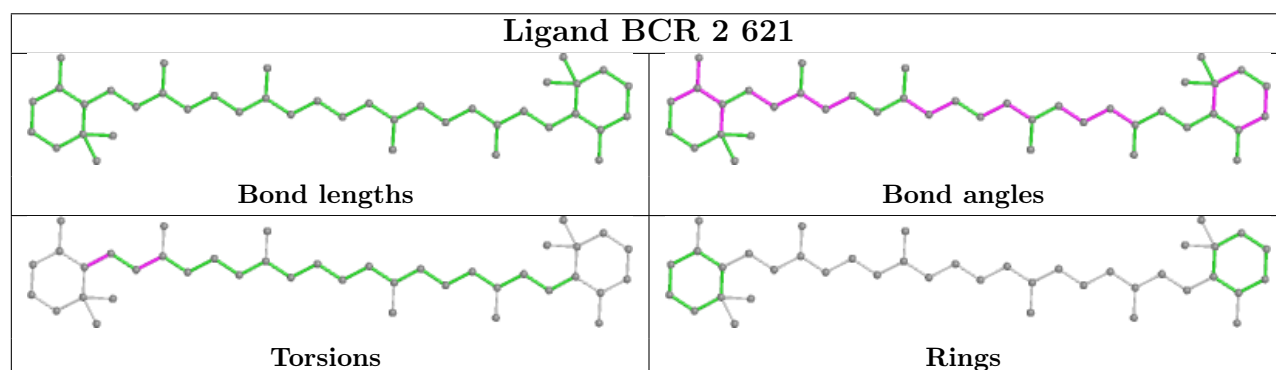
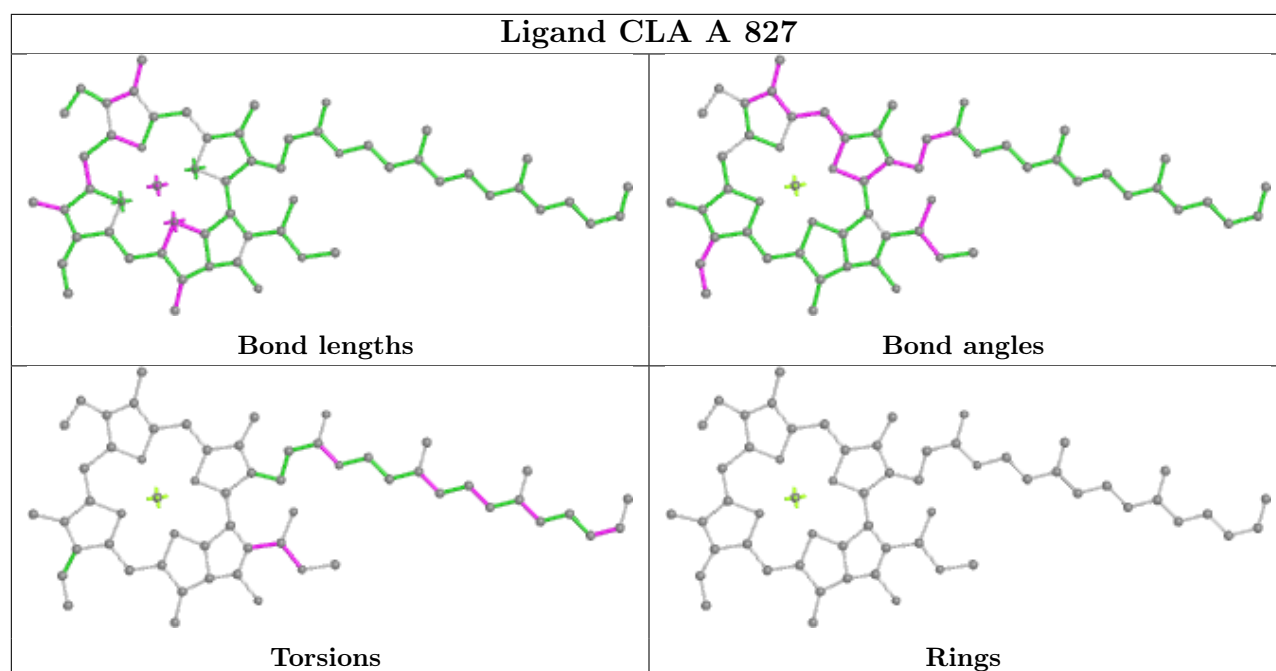


Ligand CLA X 611

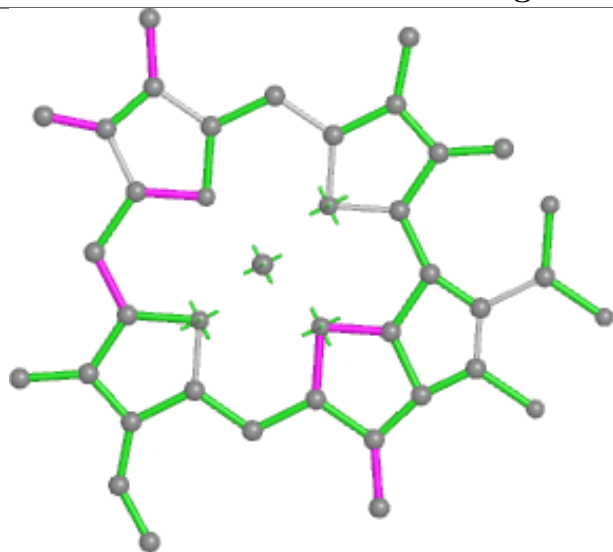


Ligand NEX X 2623

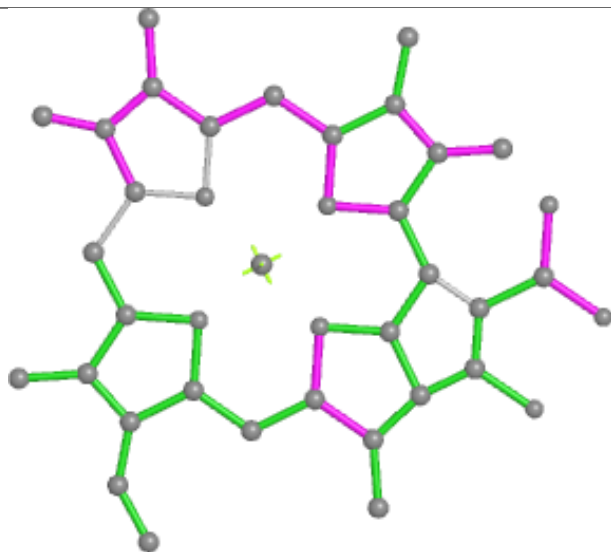




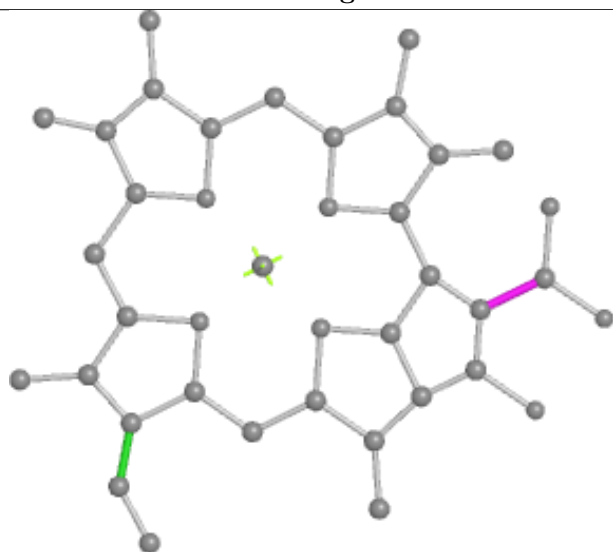
Ligand CLA Y 614



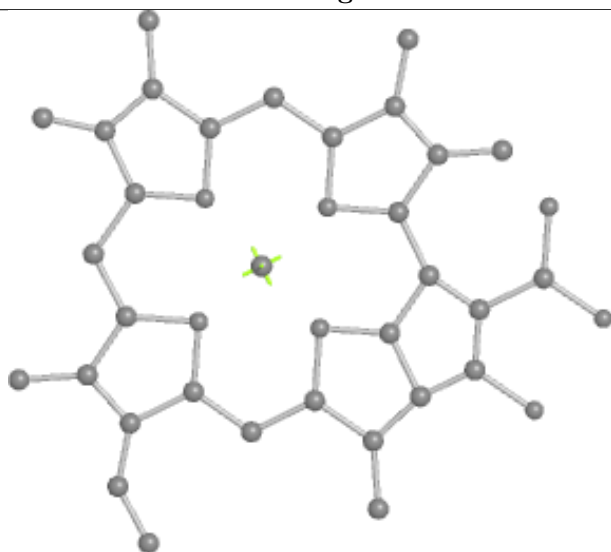
Bond lengths



Bond angles

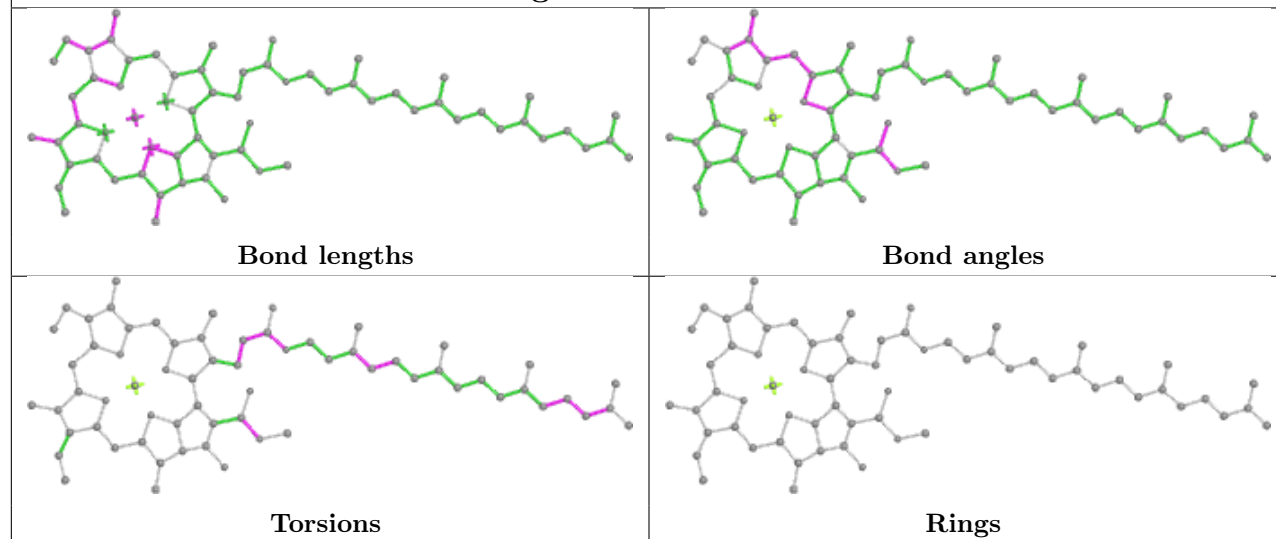


Torsions

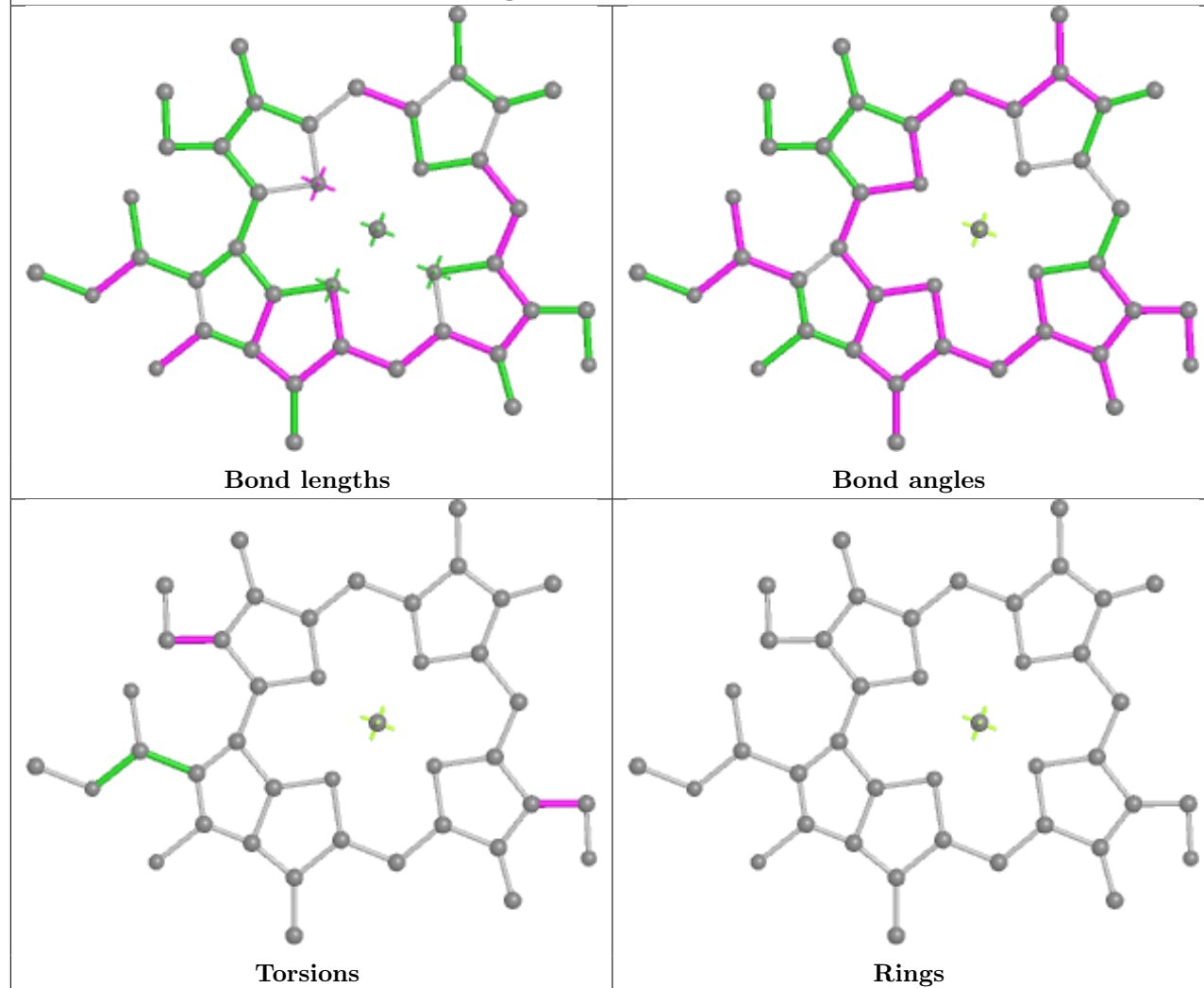


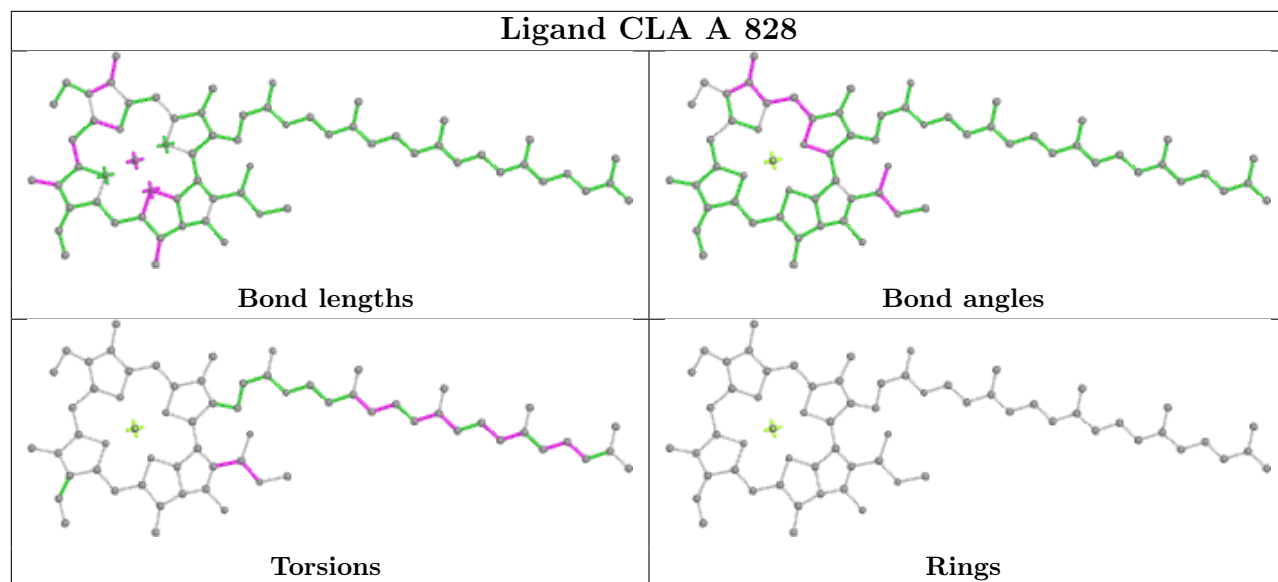
Rings

Ligand CLA A 822

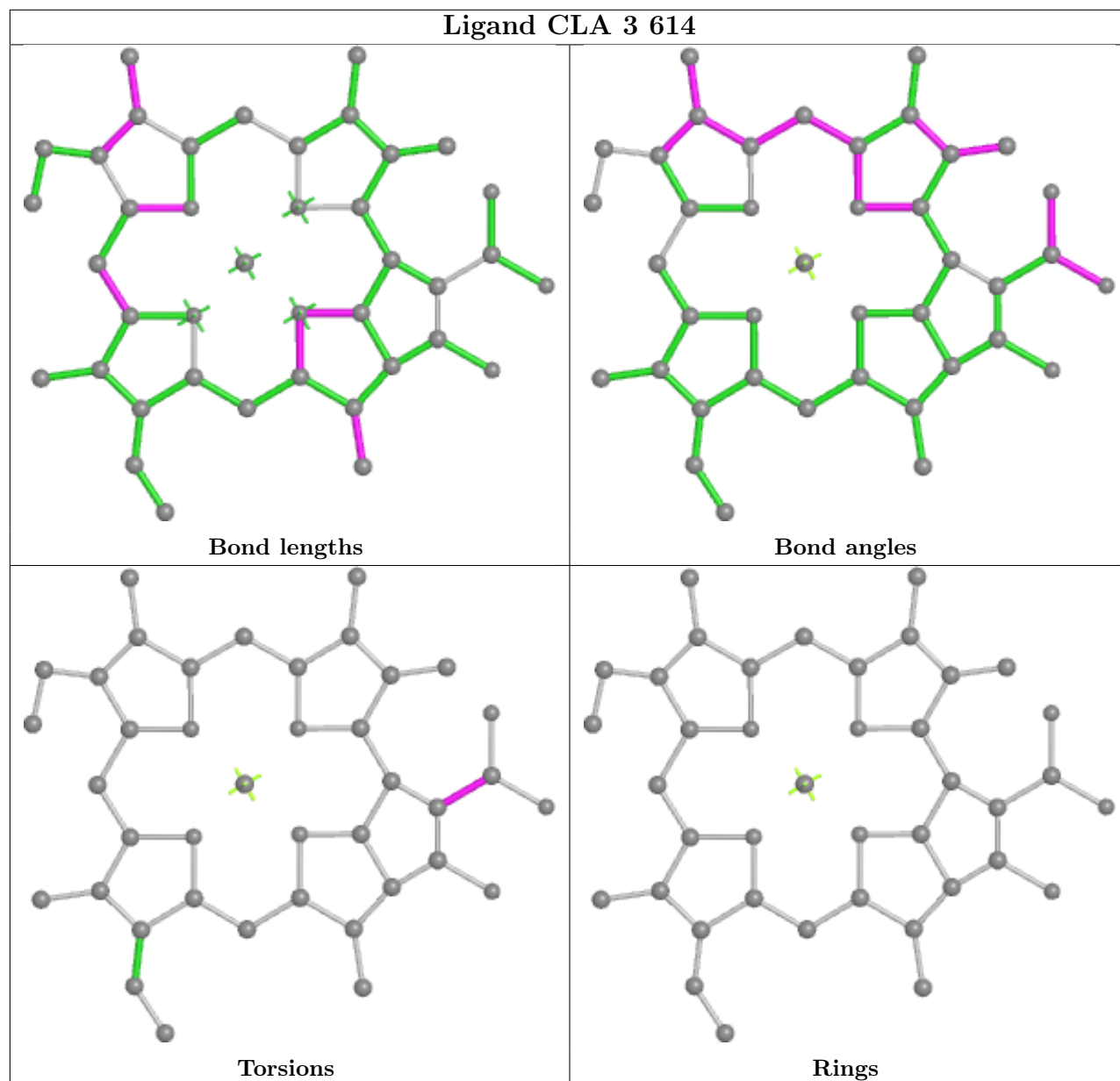


Ligand CHL X 607

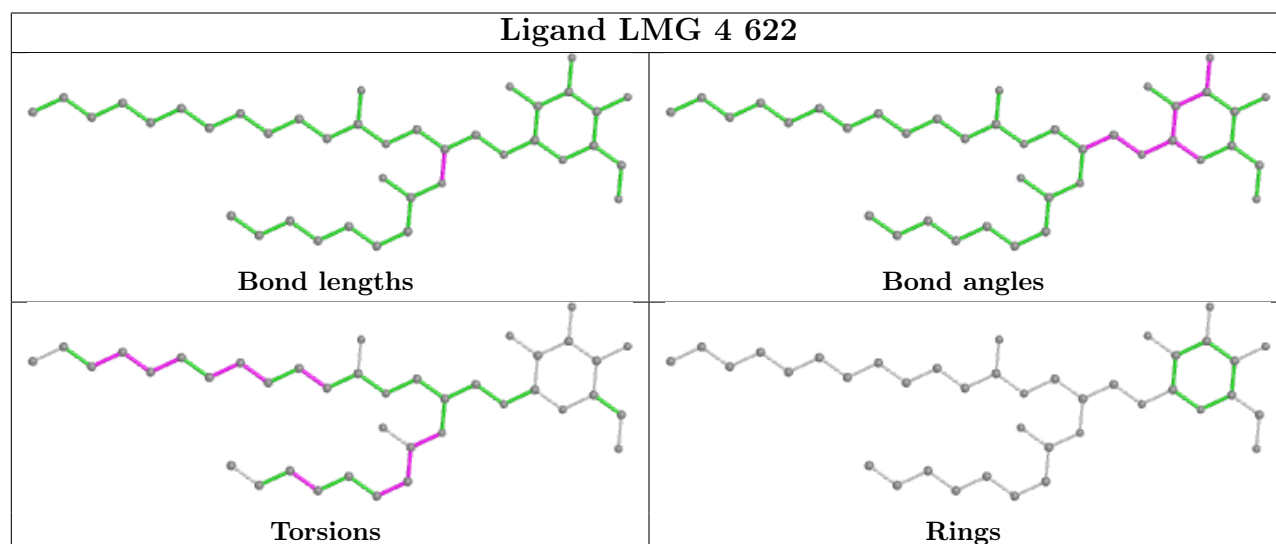




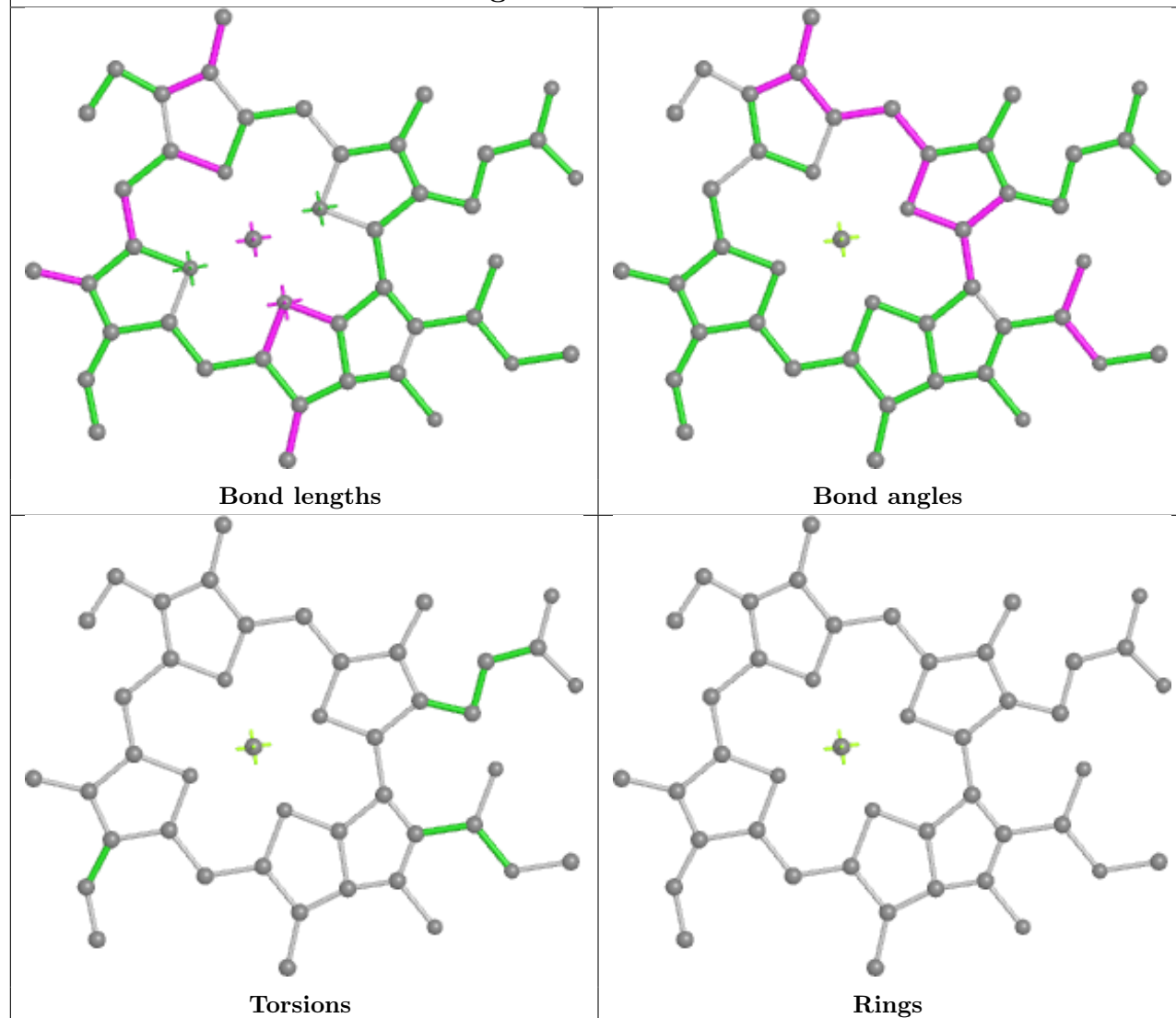
Ligand CLA 3 614



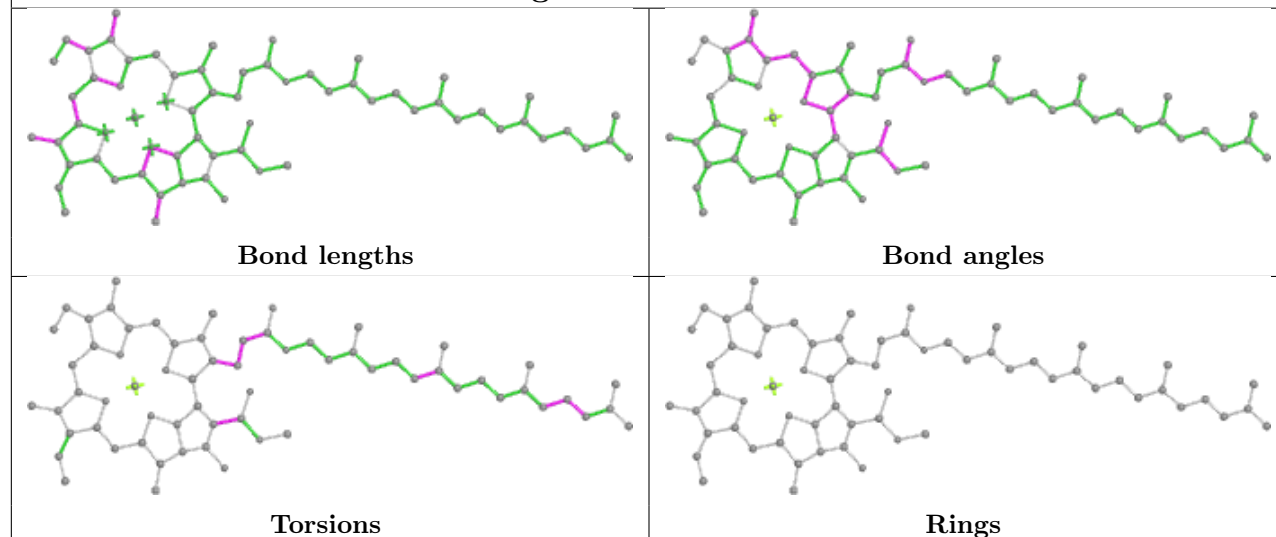
Ligand LMG 4 622



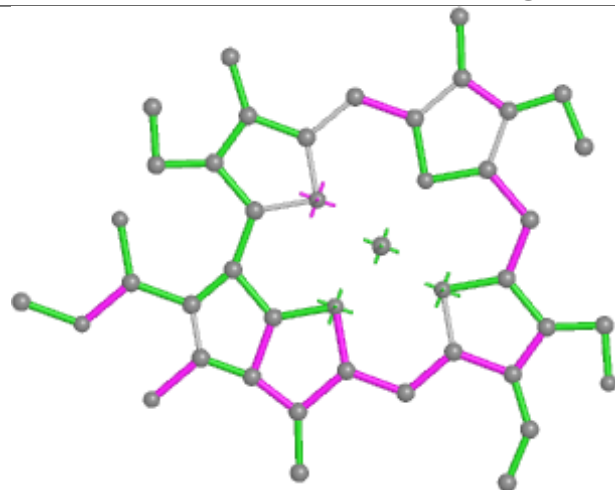
Ligand CLA A 821



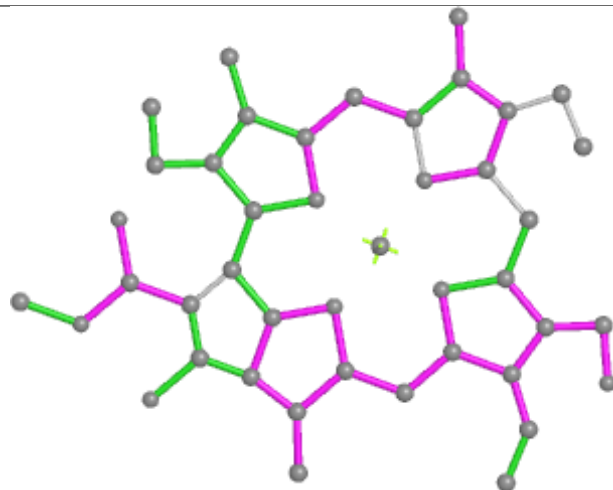
Ligand CLA A 842



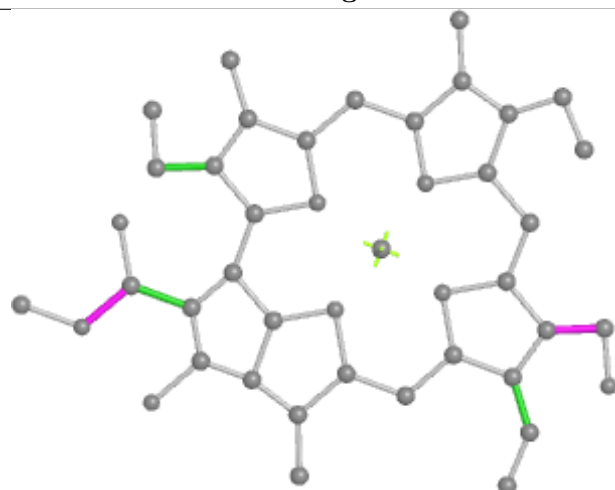
Ligand CHL 2 618



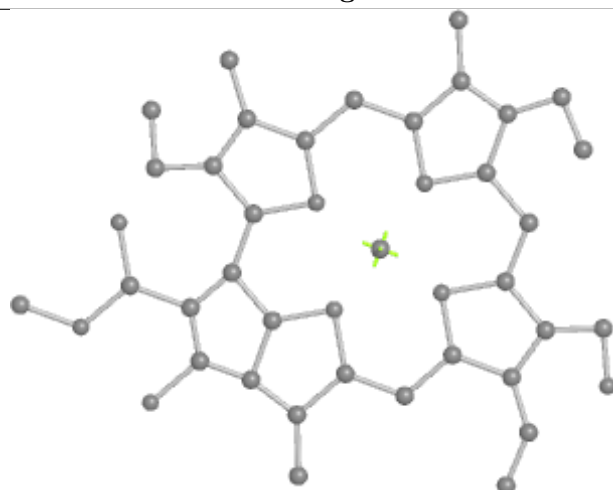
Bond lengths



Bond angles

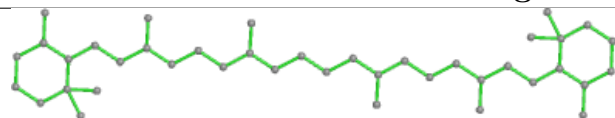


Torsions

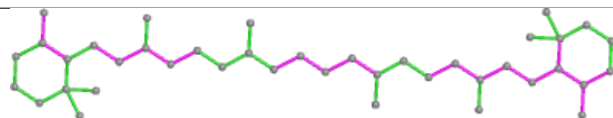


Rings

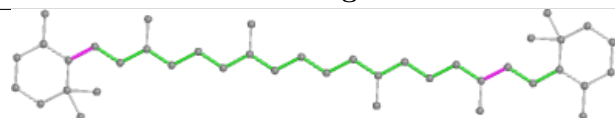
Ligand BCR A 848



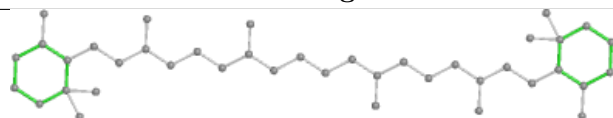
Bond lengths



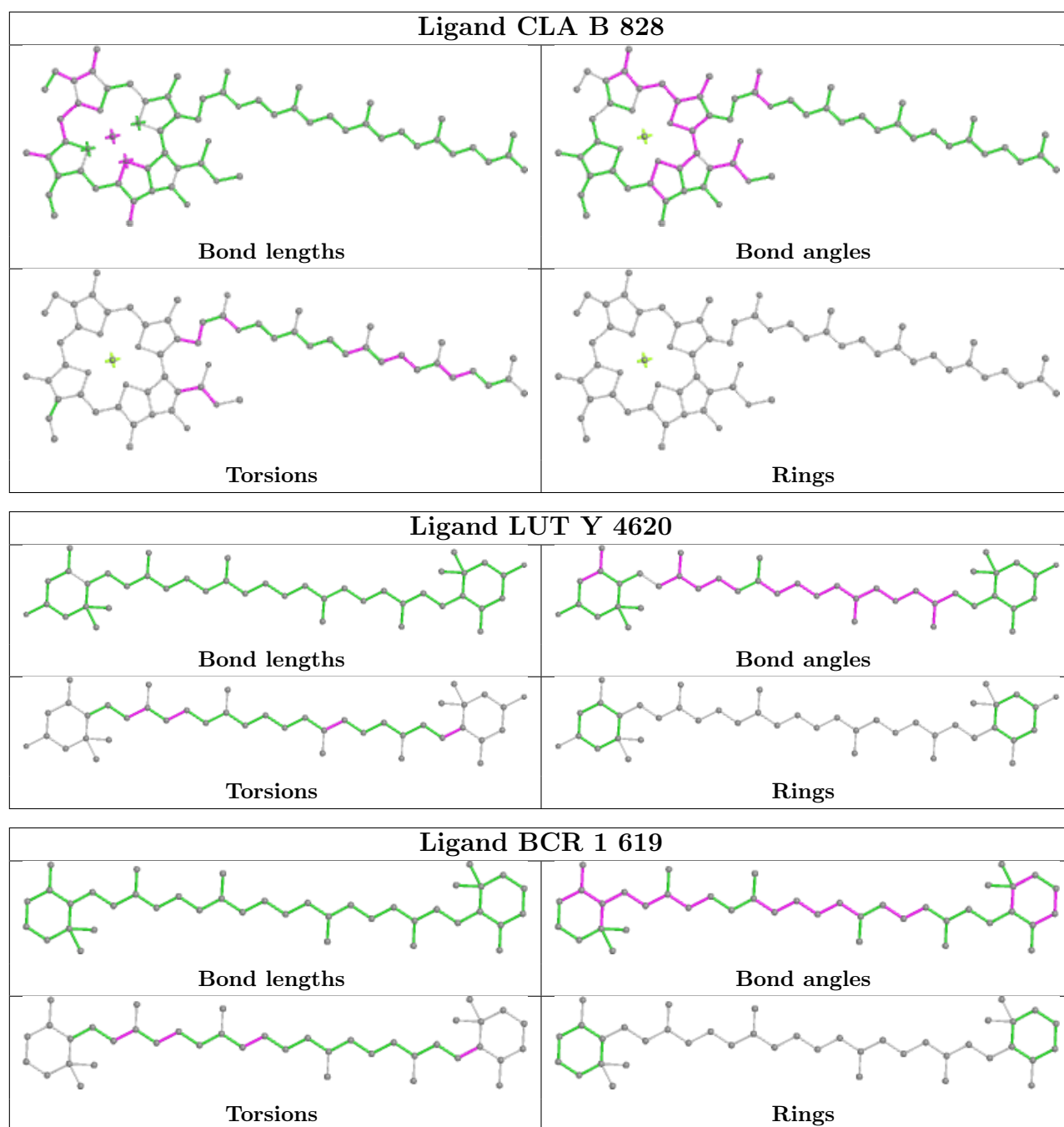
Bond angles

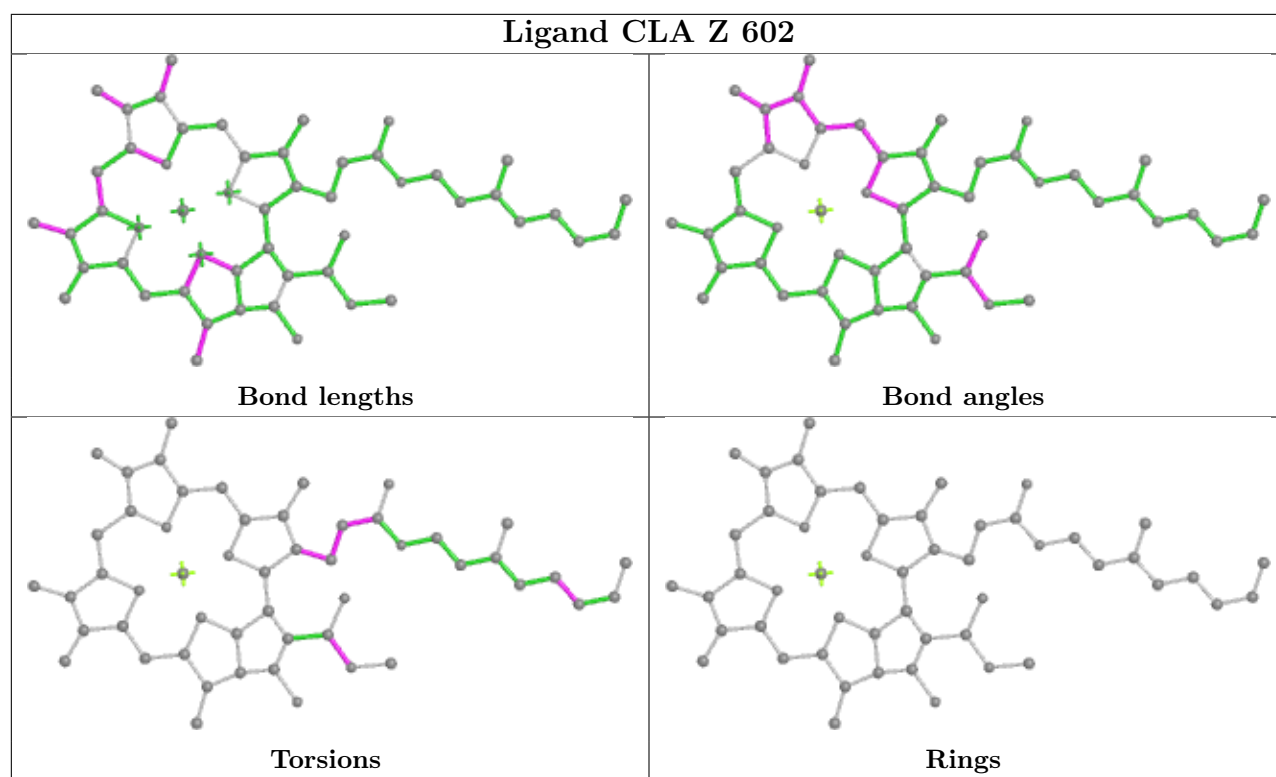


Torsions

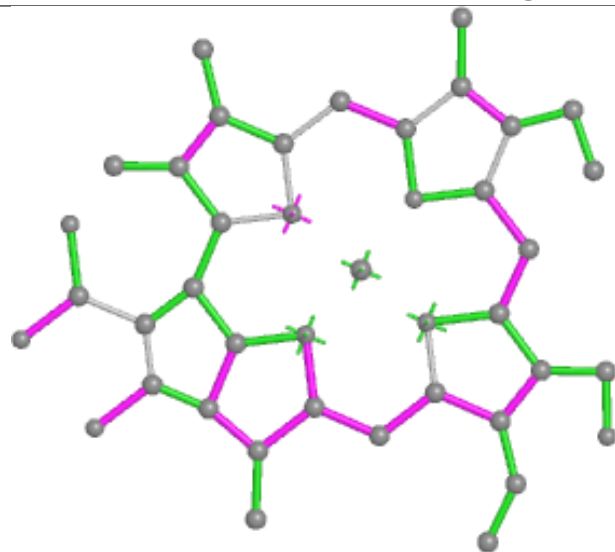


Rings

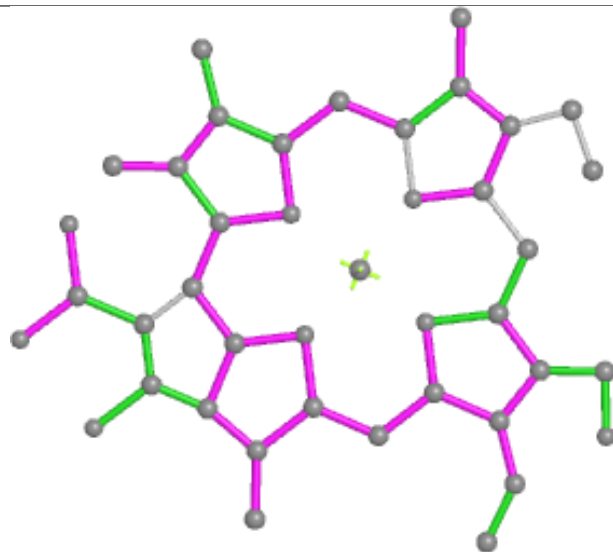




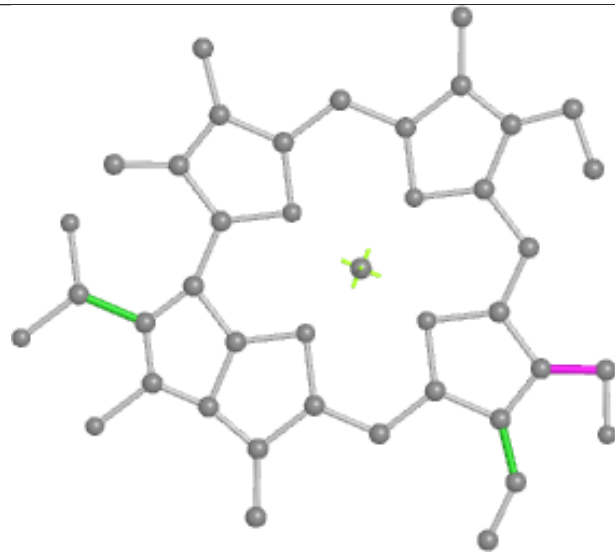
Ligand CHL 1 607



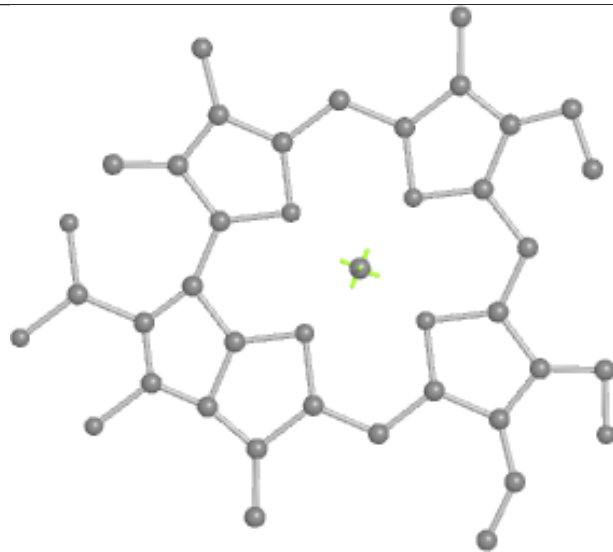
Bond lengths



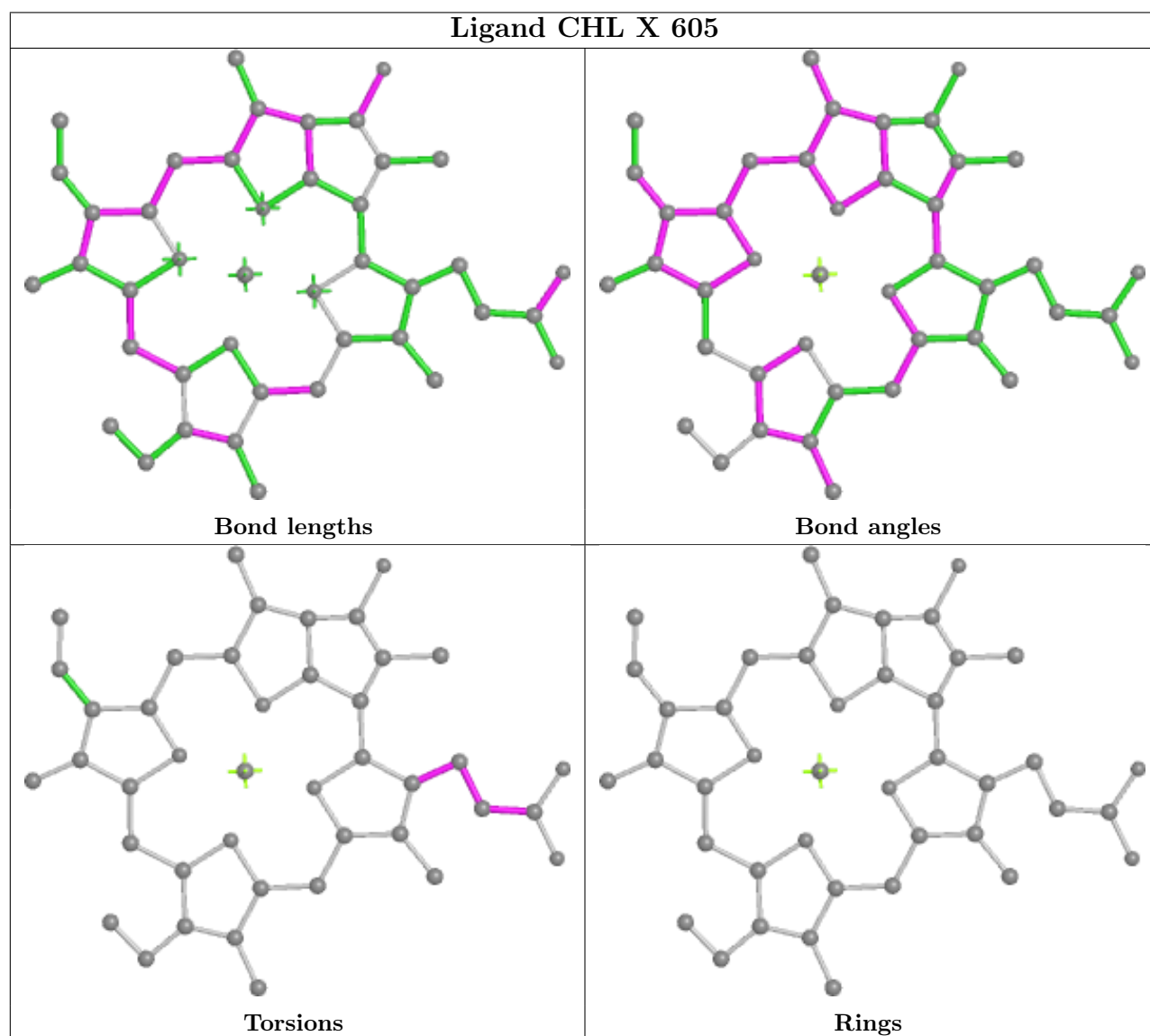
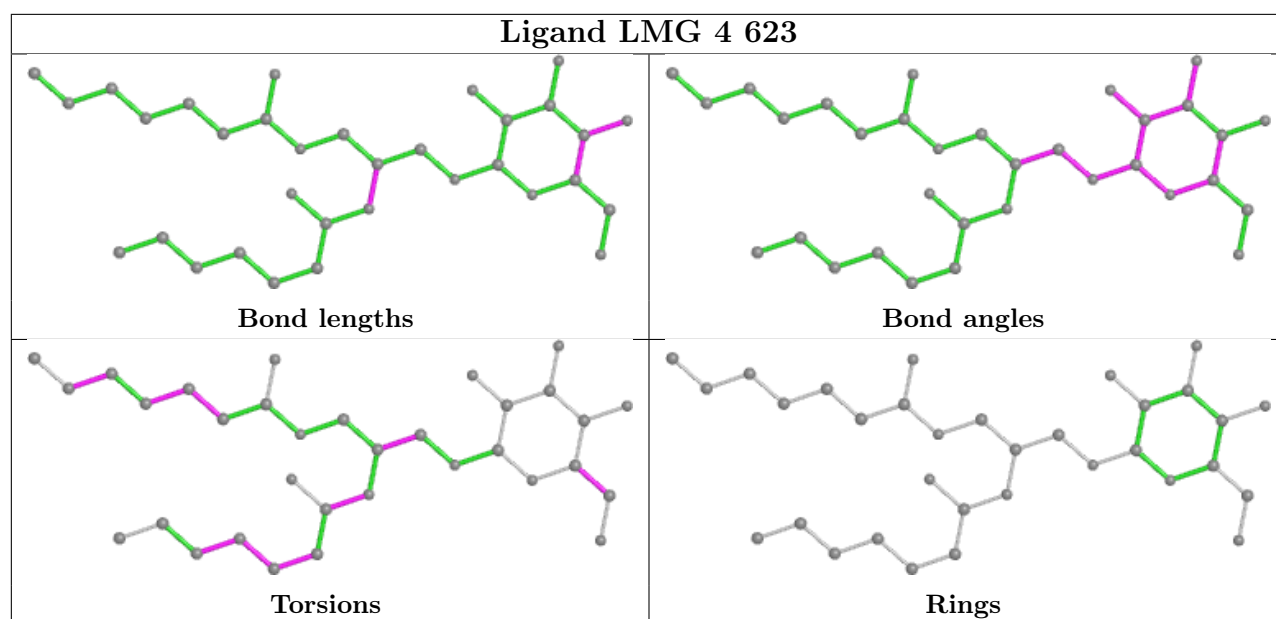
Bond angles

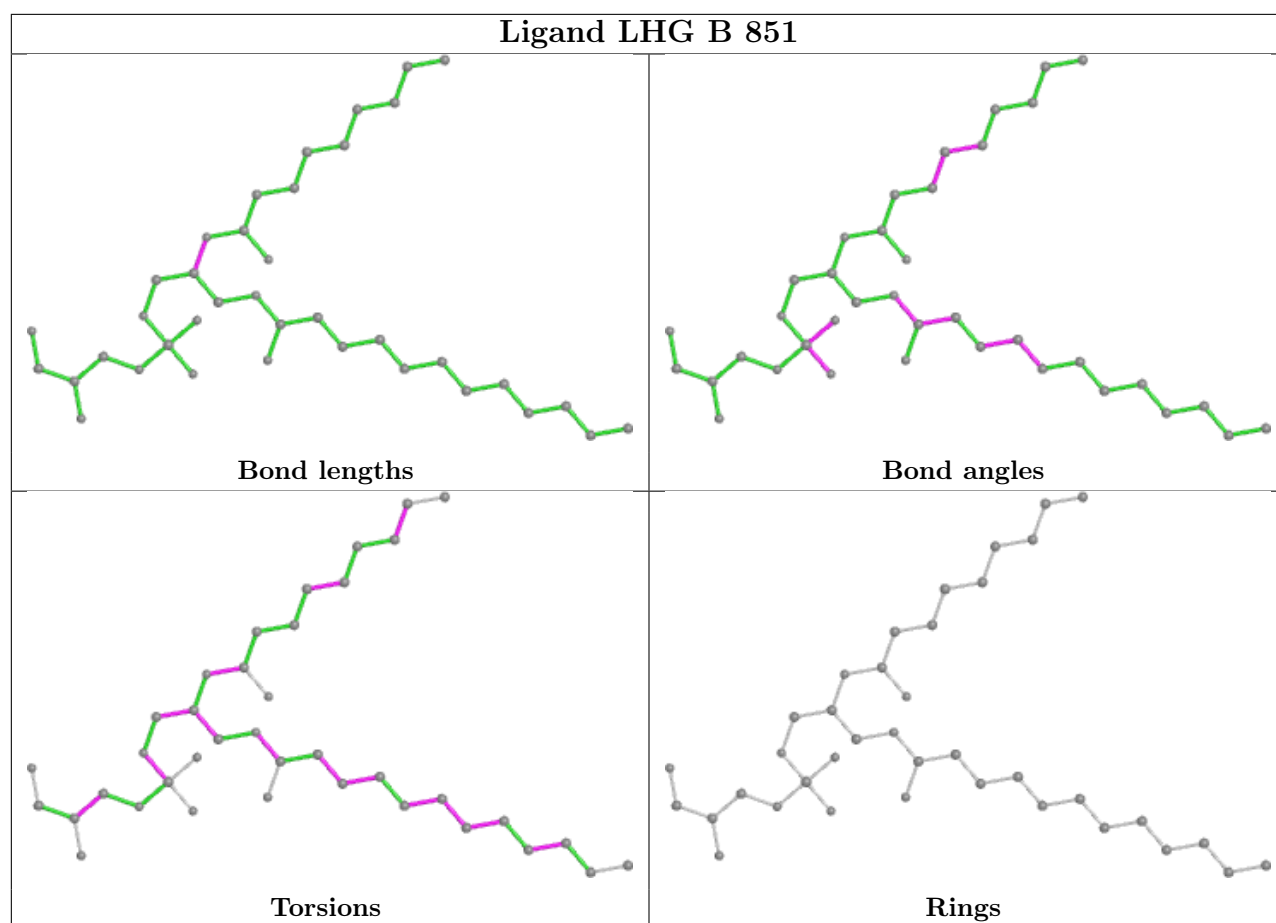


Torsions

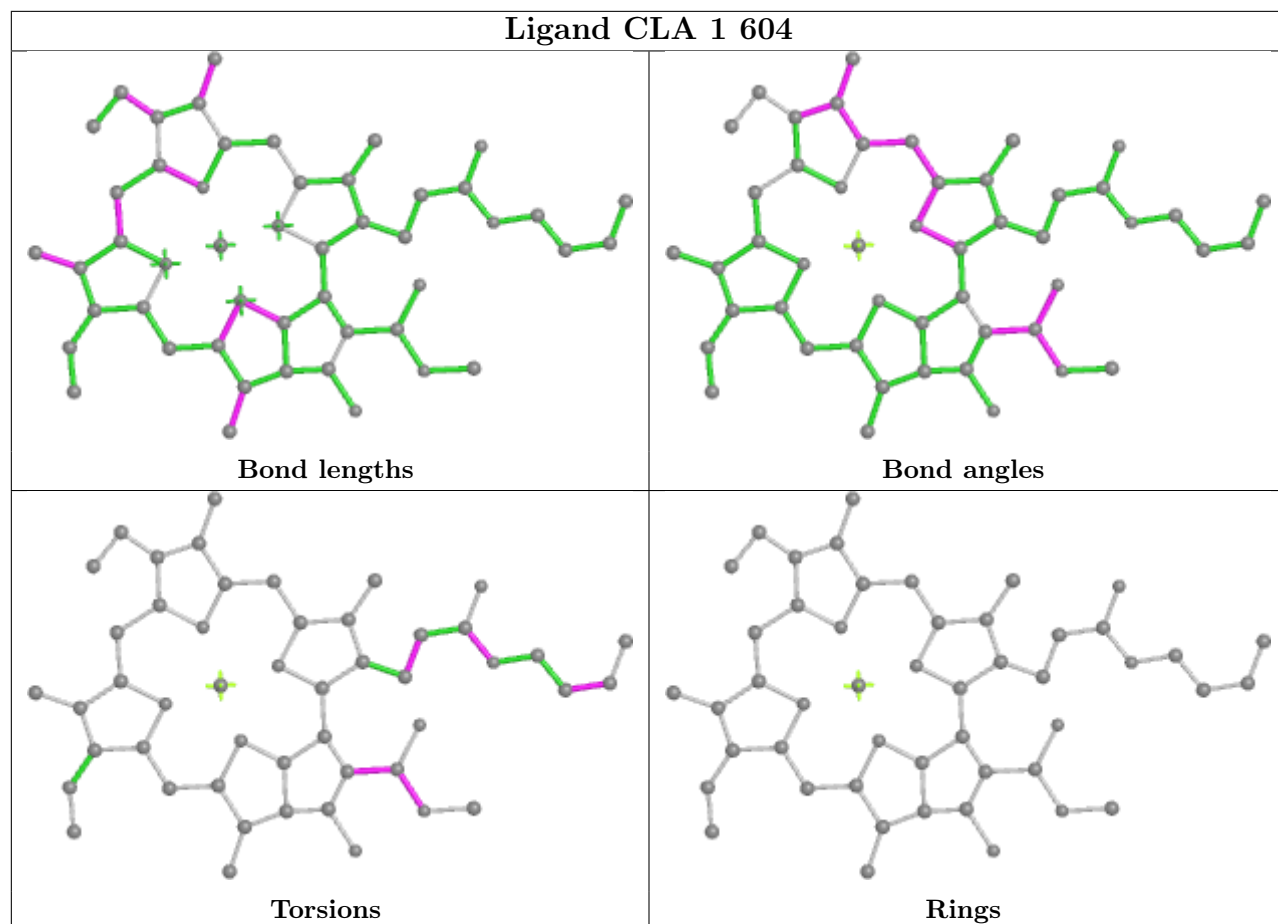


Rings

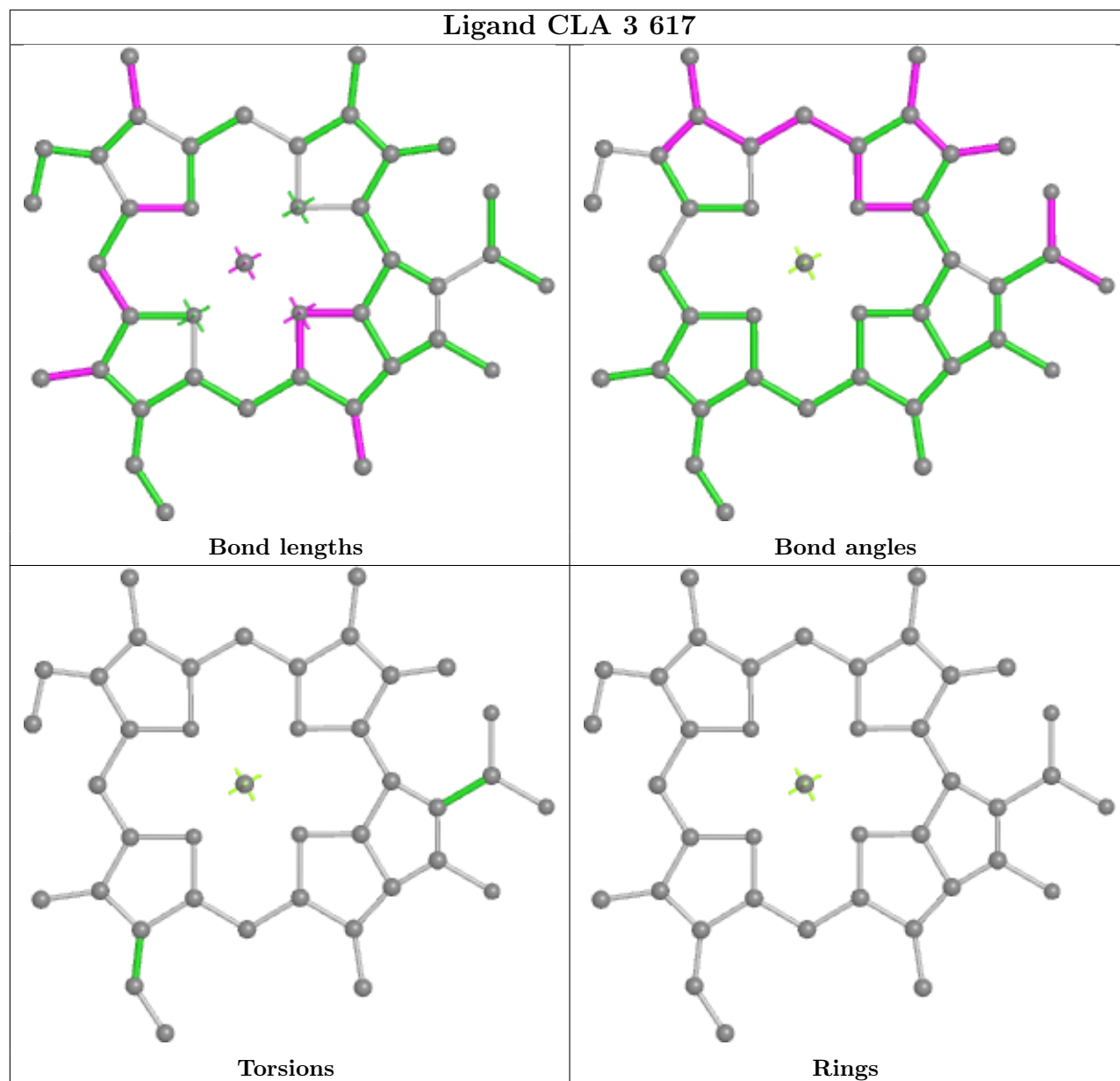




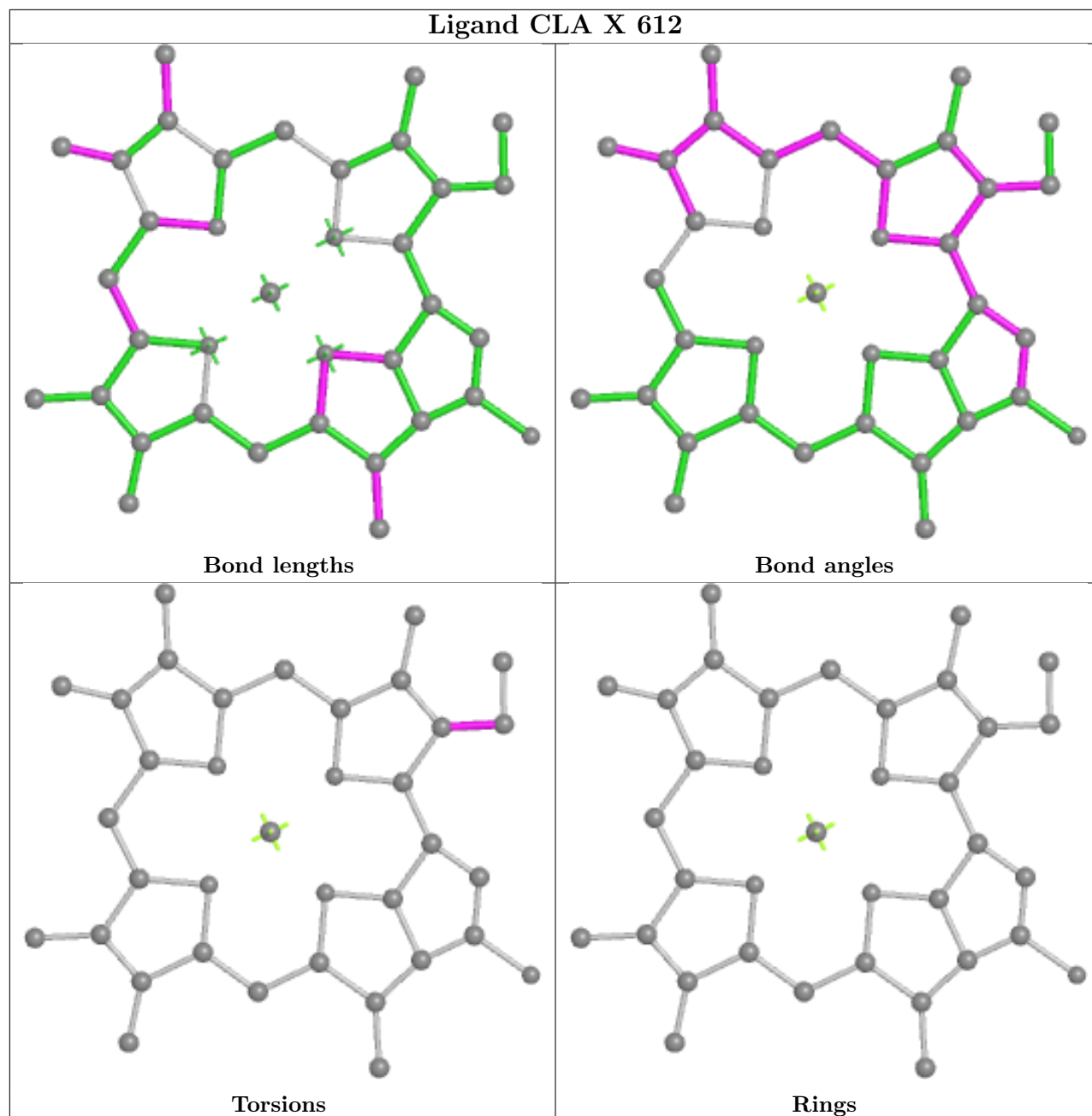
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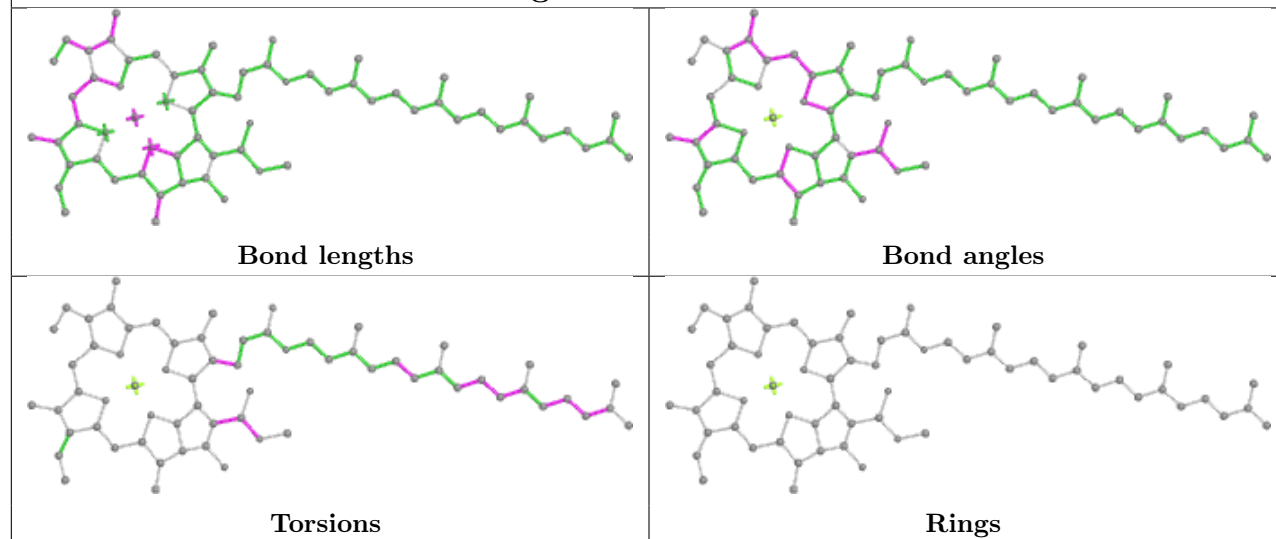
Ligand CLA 3 617



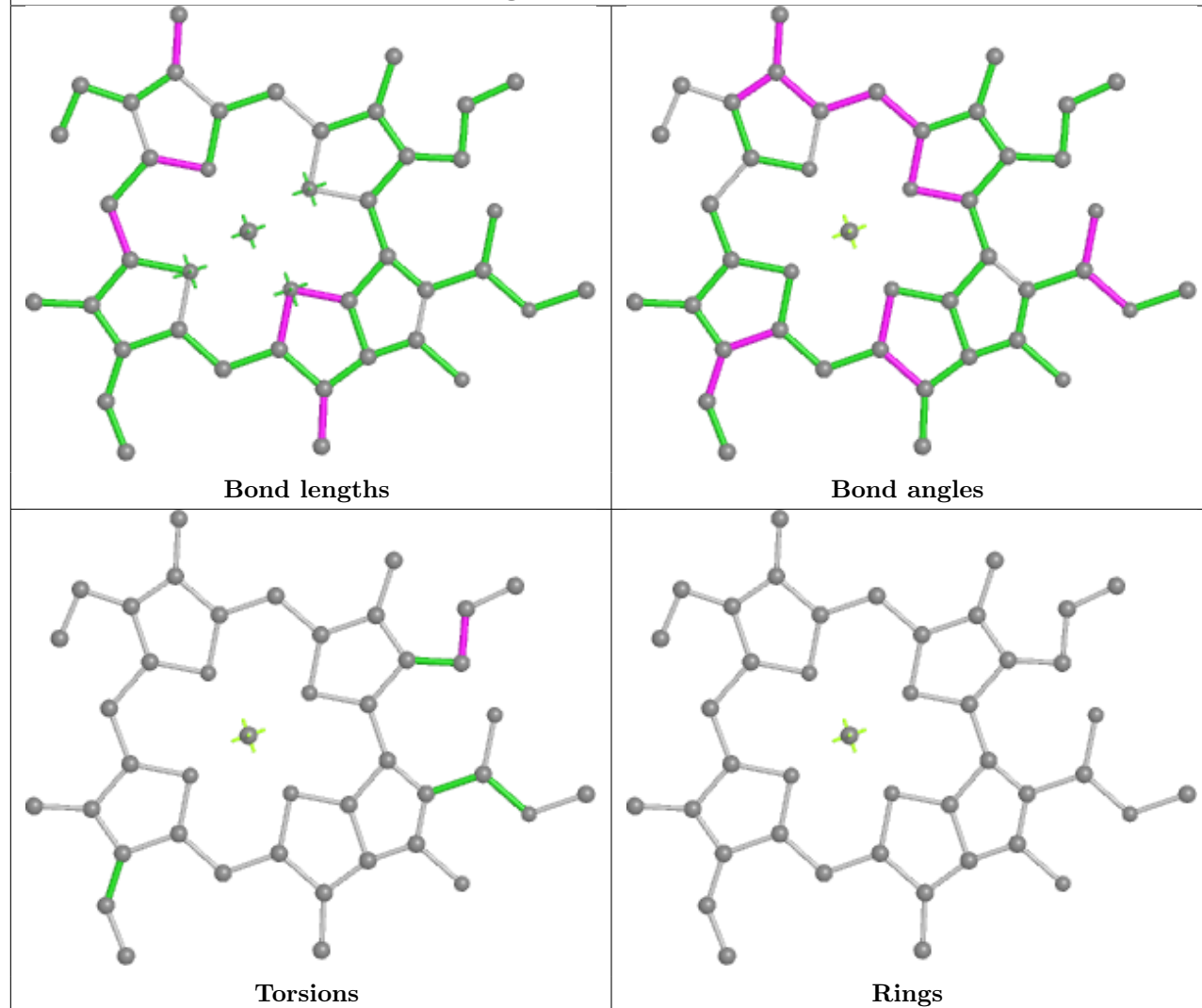
Ligand CLA X 612



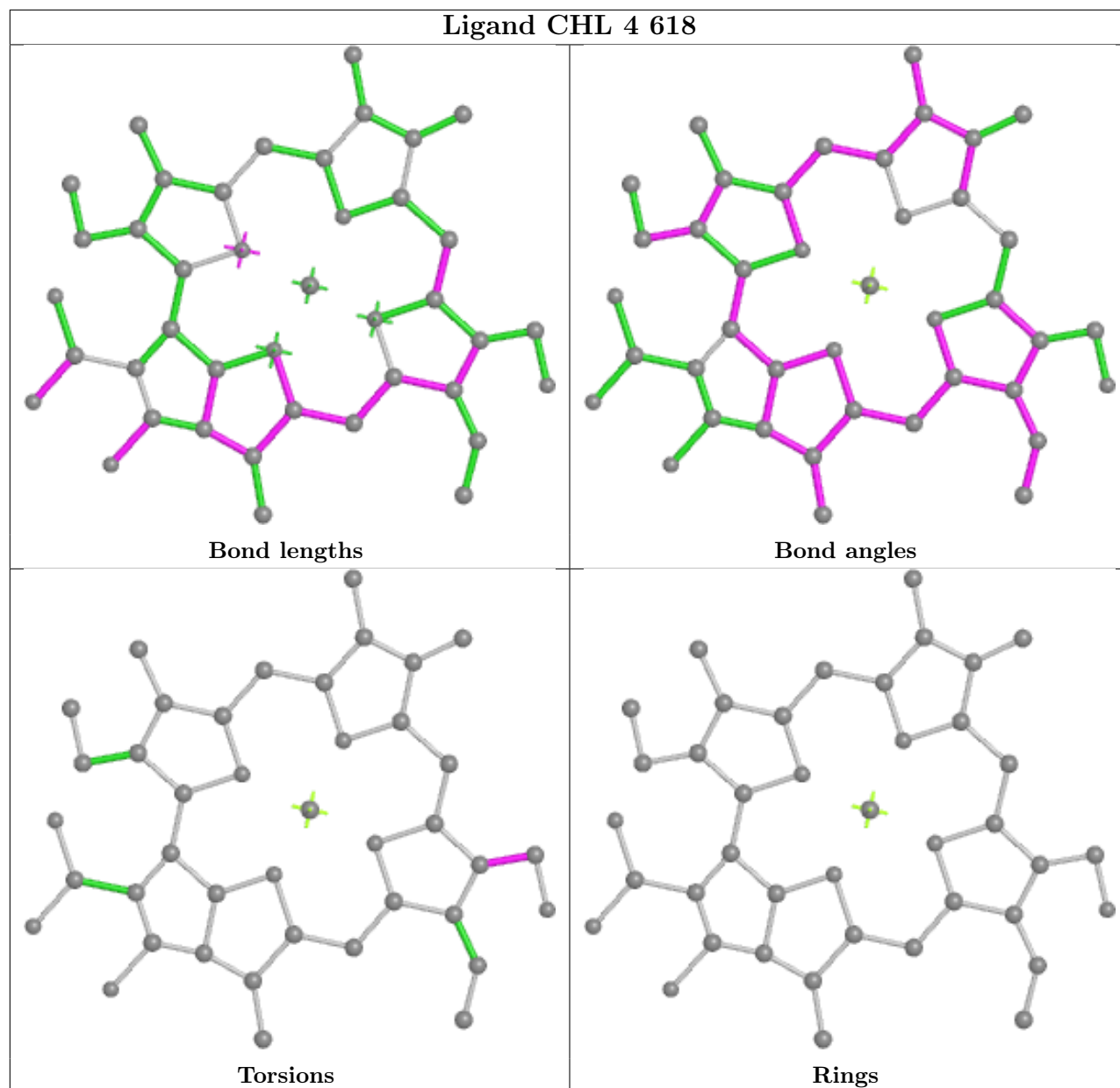
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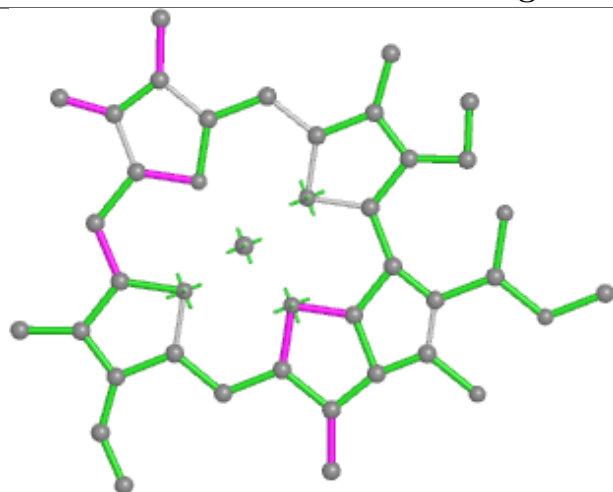
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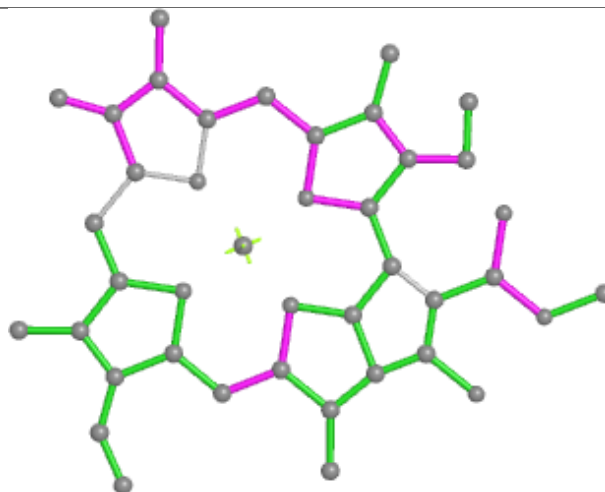
Ligand CHL 4 618



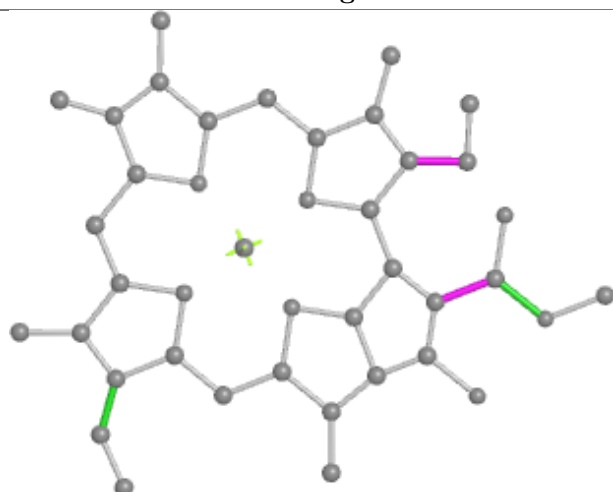
Ligand CLA 3 607



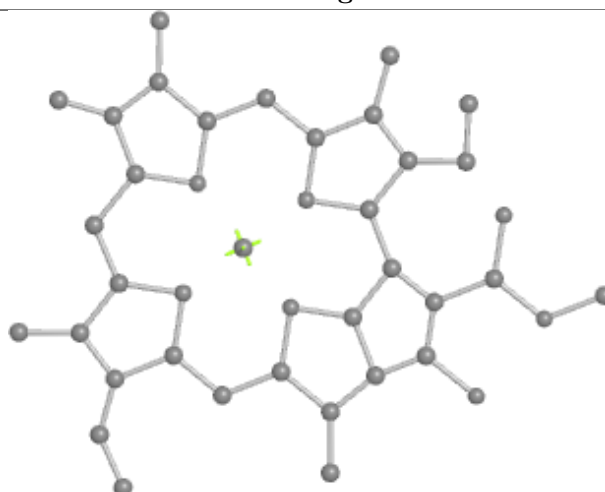
Bond lengths



Bond angles

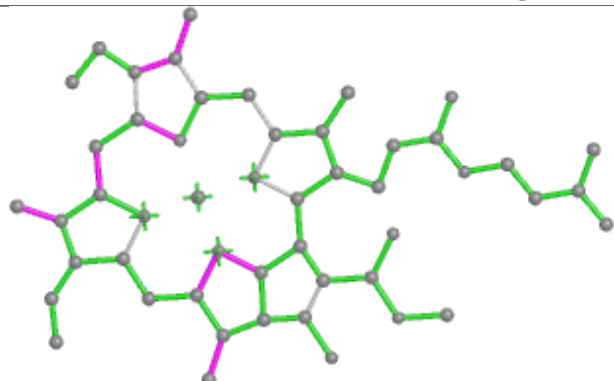


Torsions

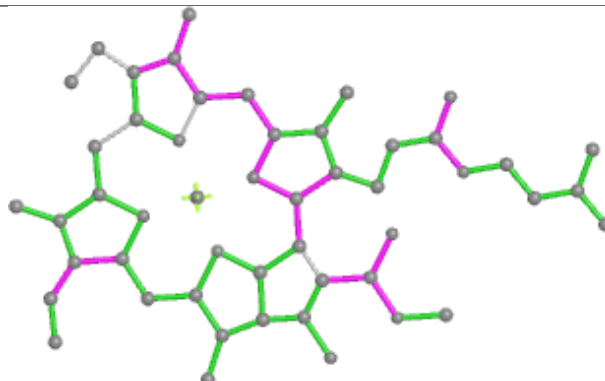


Rings

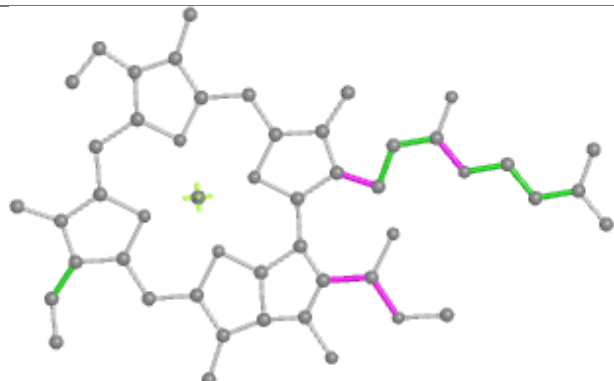
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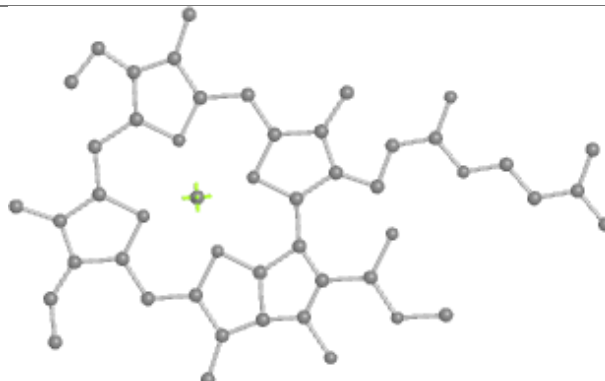
Bond lengths



Bond angles

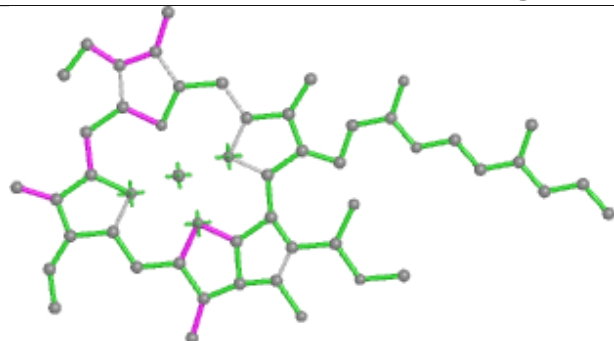


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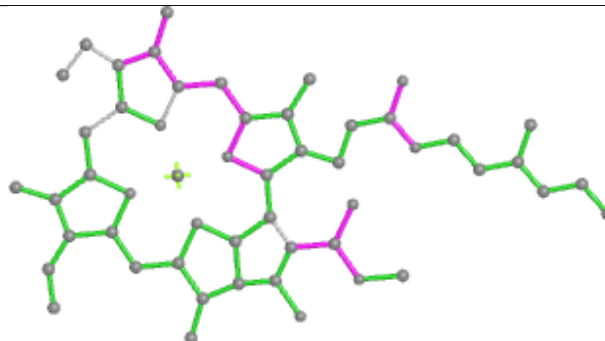


Rings

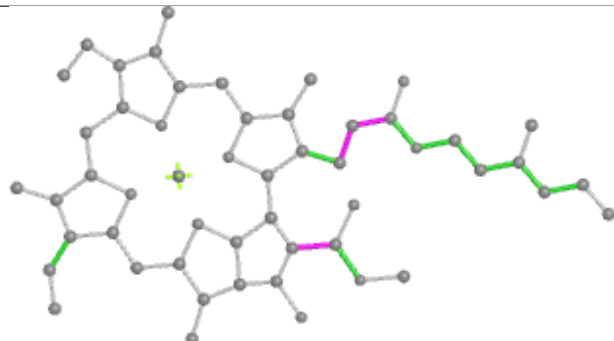
Ligand CLA B 807



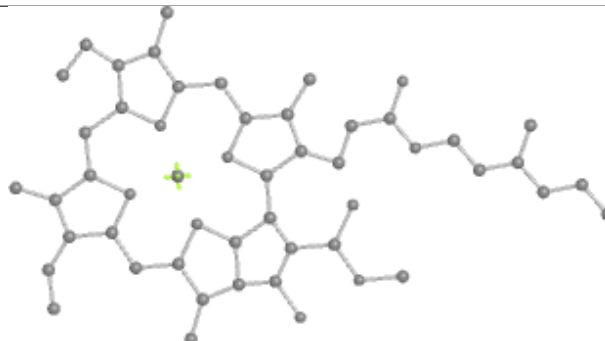
Bond lengths



Bond angles

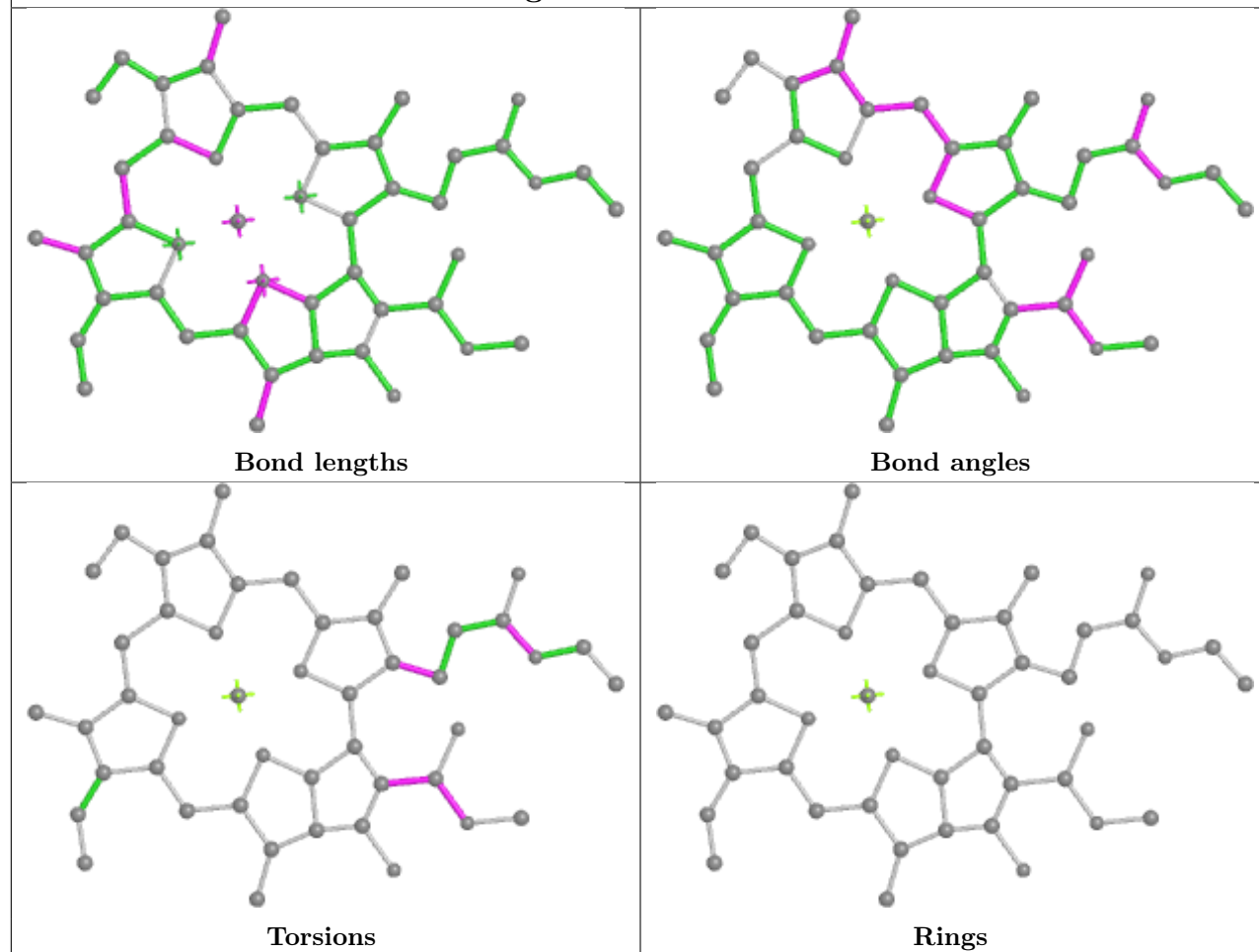


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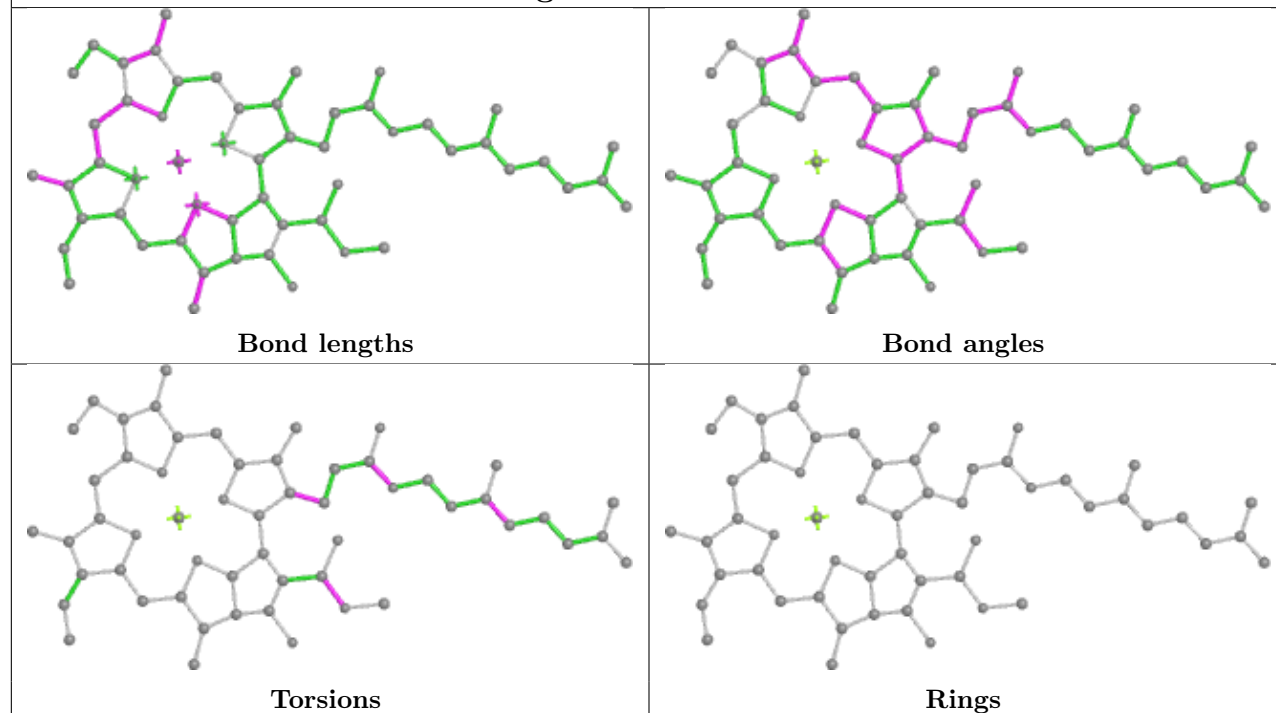


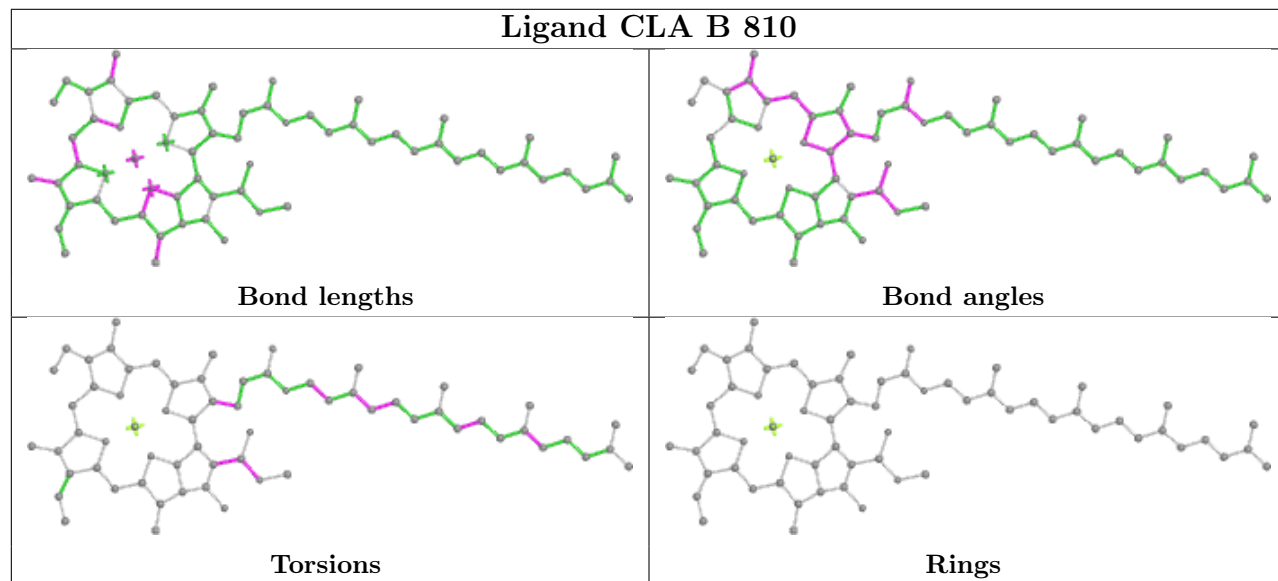
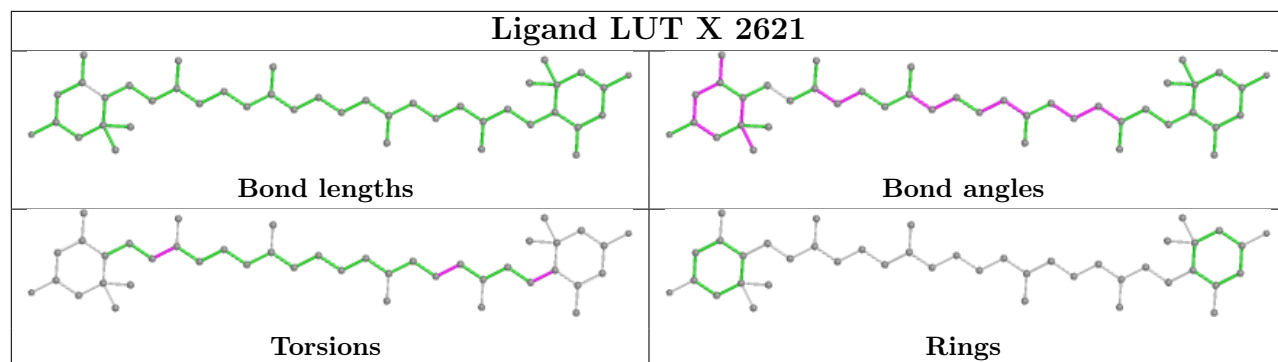
Rings

Ligand CLA B 838

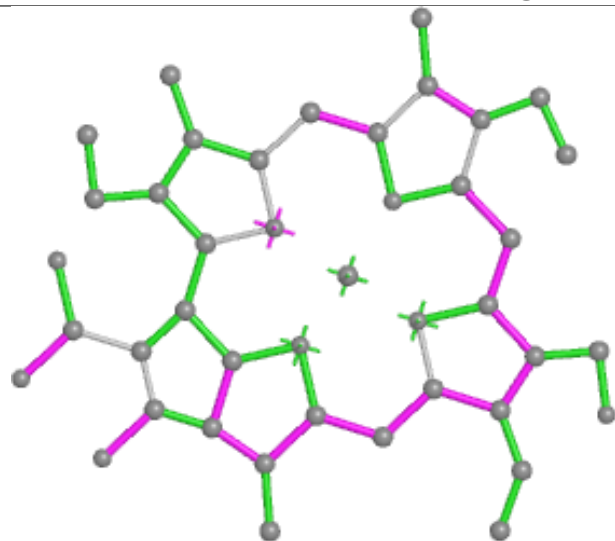


Ligand CLA 3 603

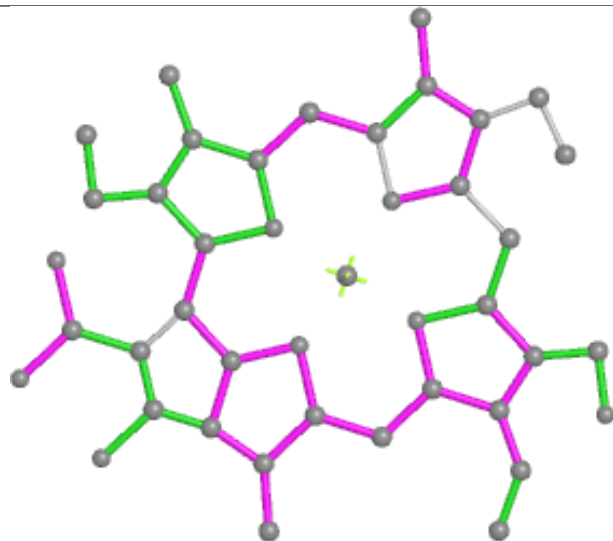




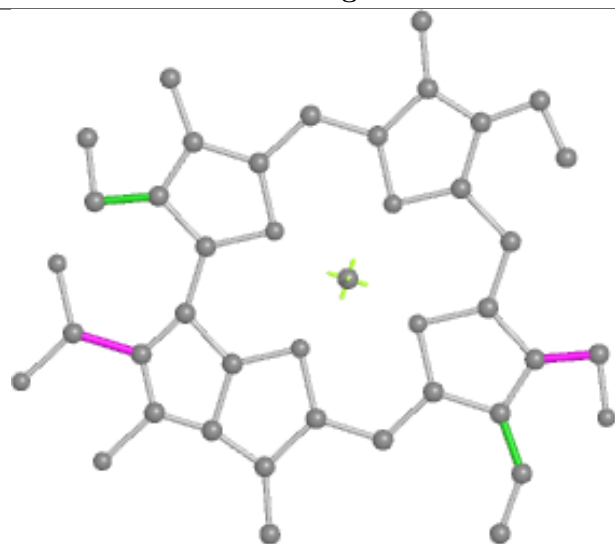
Ligand CHL Z 601



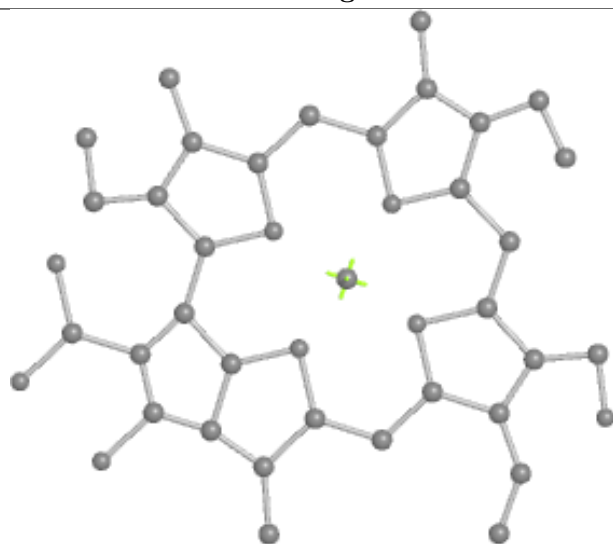
Bond lengths



Bond angles

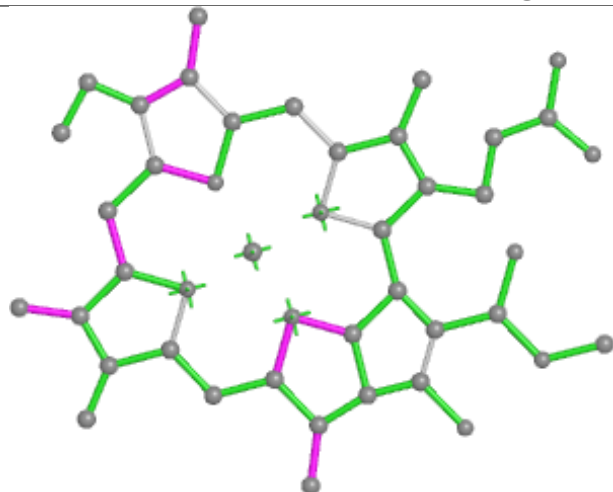


Torsions

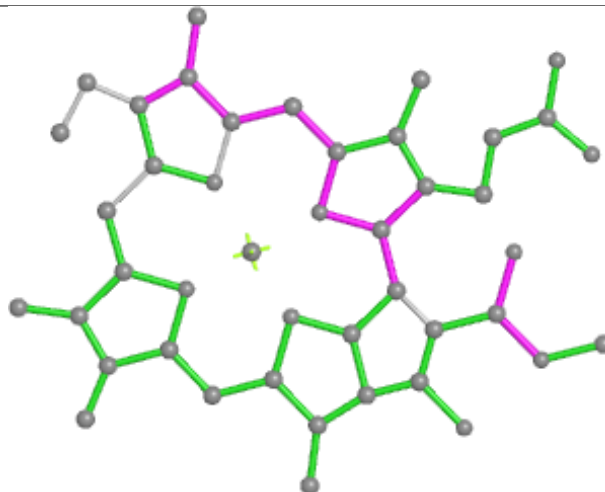


Rings

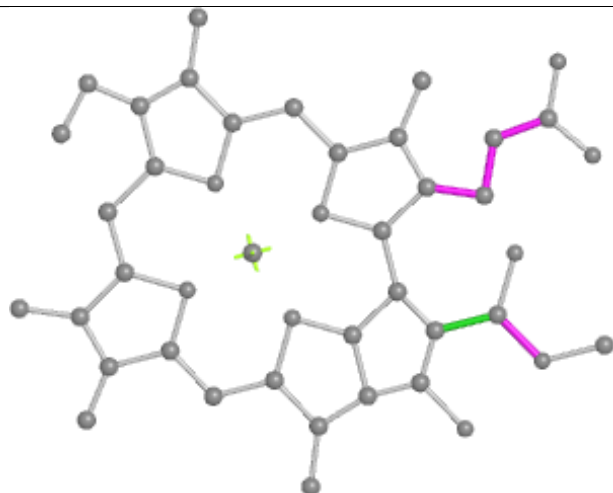
Ligand CLA 2 612



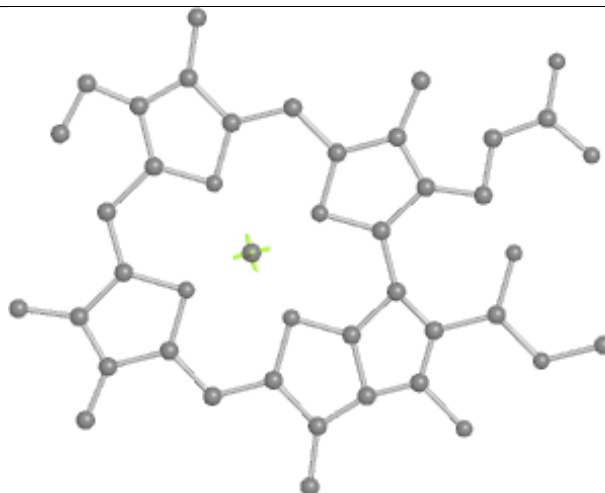
Bond lengths



Bond angles

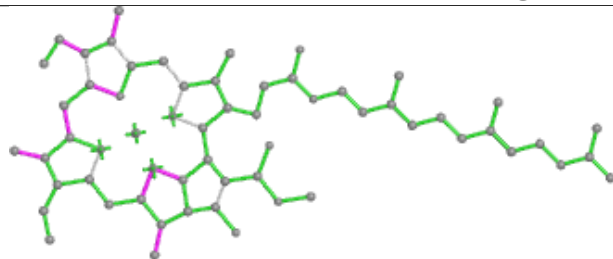


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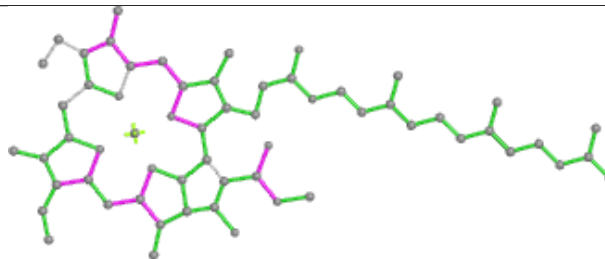


Rings

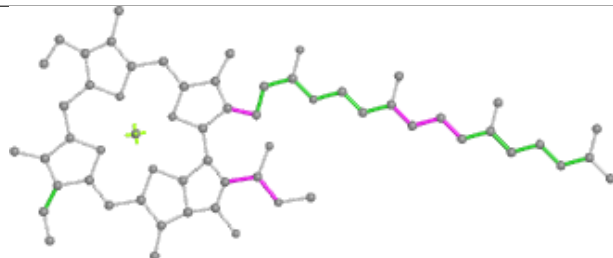
Ligand CLA B 834



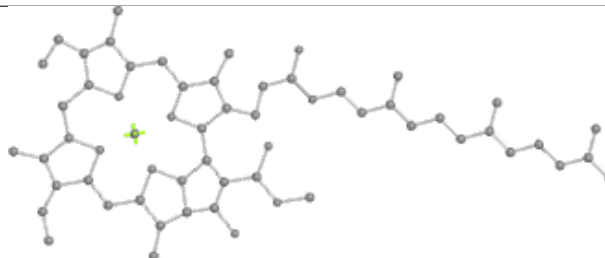
Bond lengths



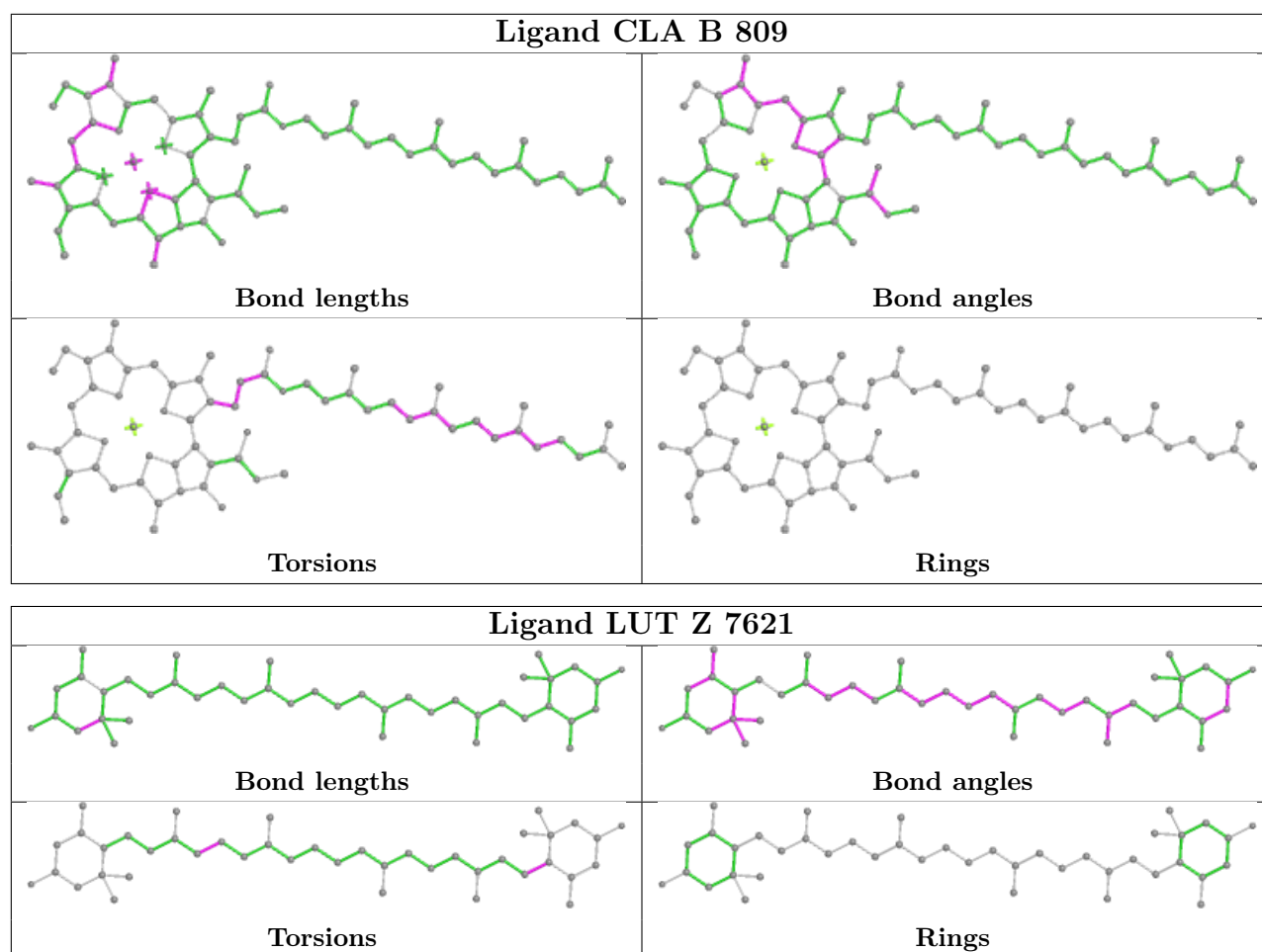
Bond angles

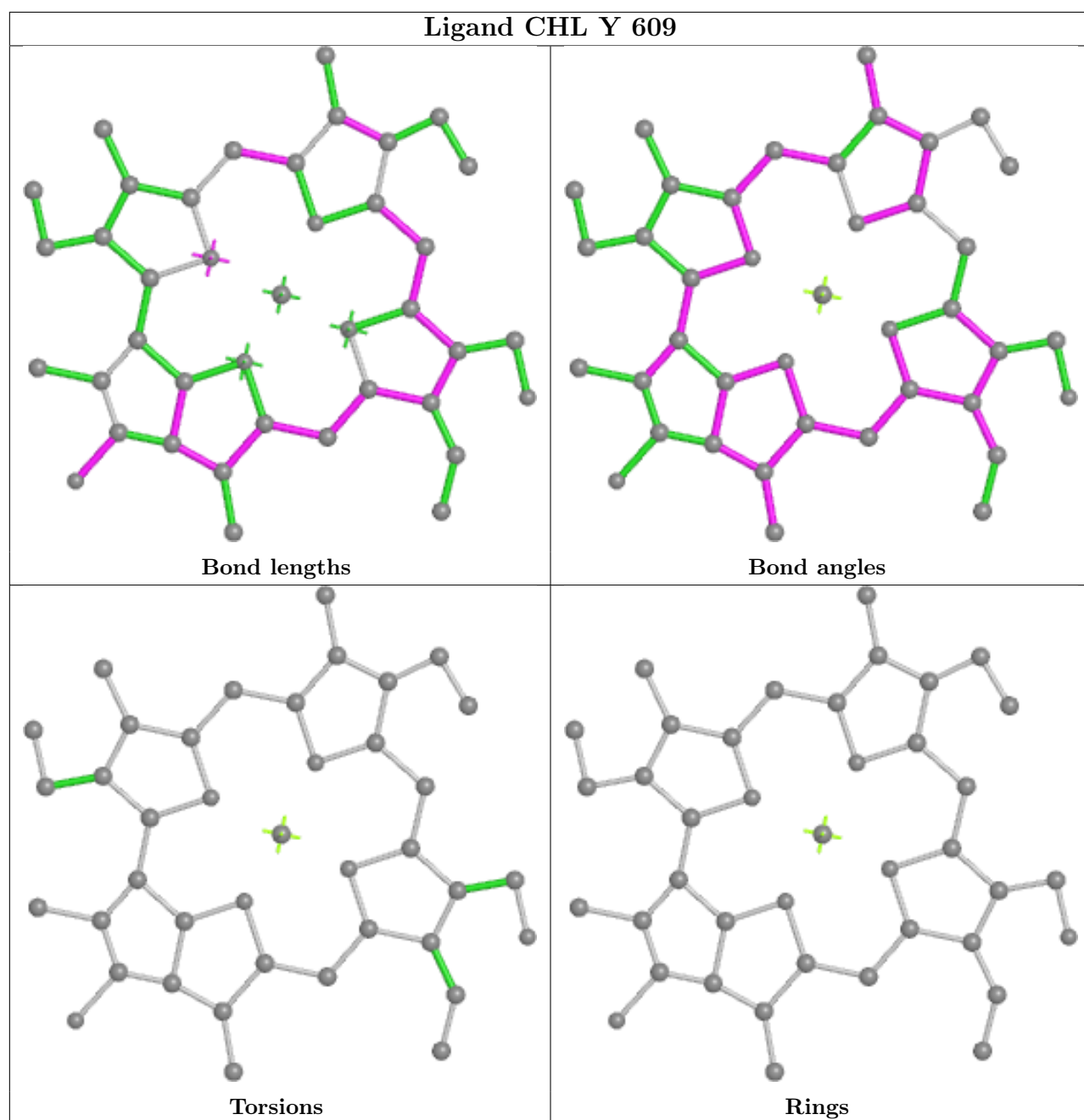


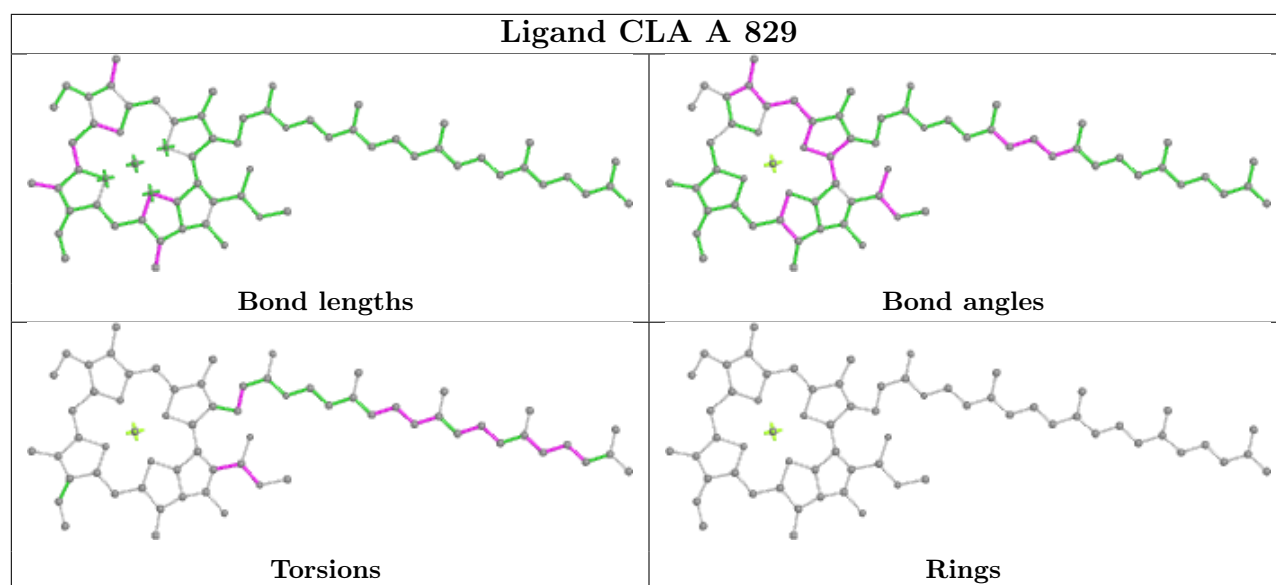
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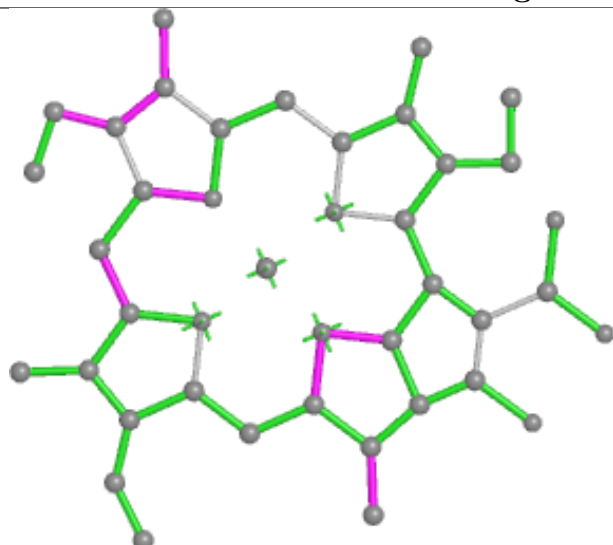
Rings



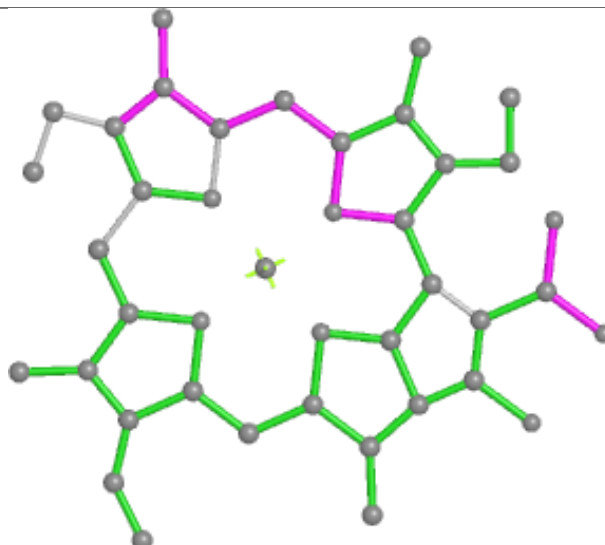




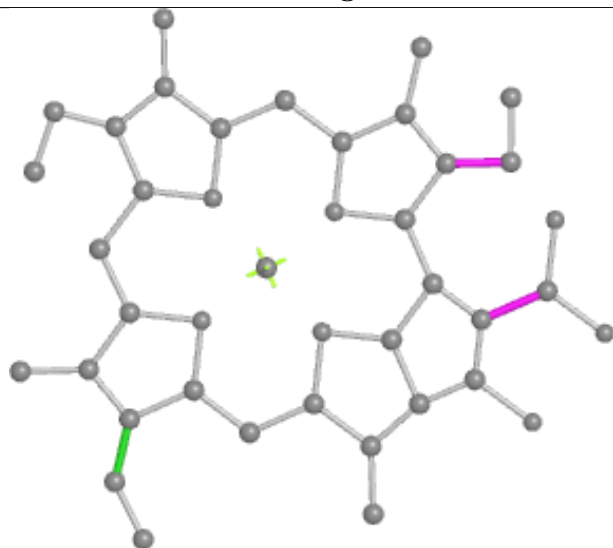
Ligand CLA X 602



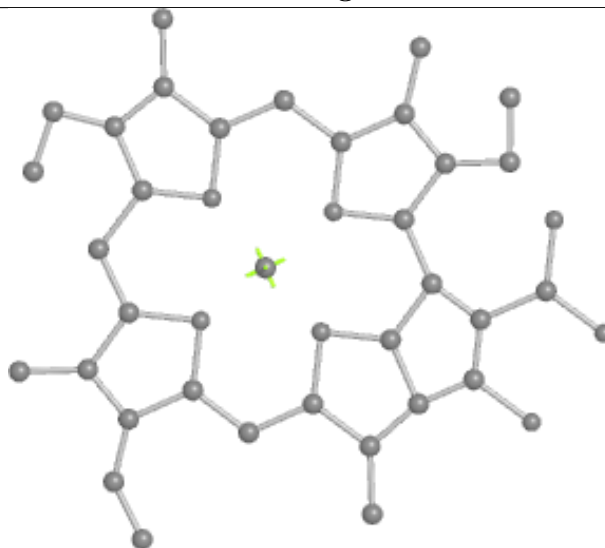
Bond lengths



Bond angles

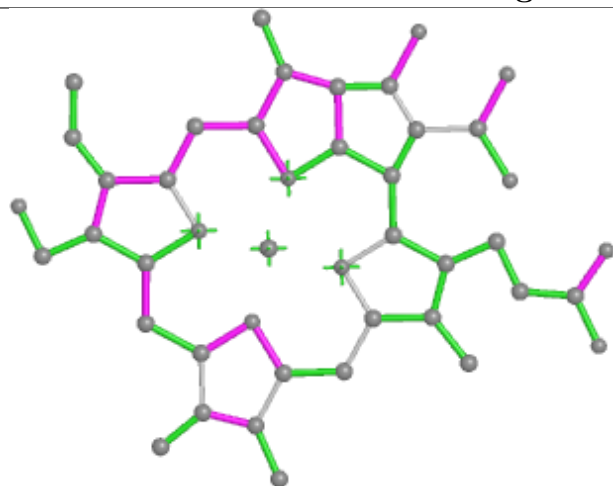


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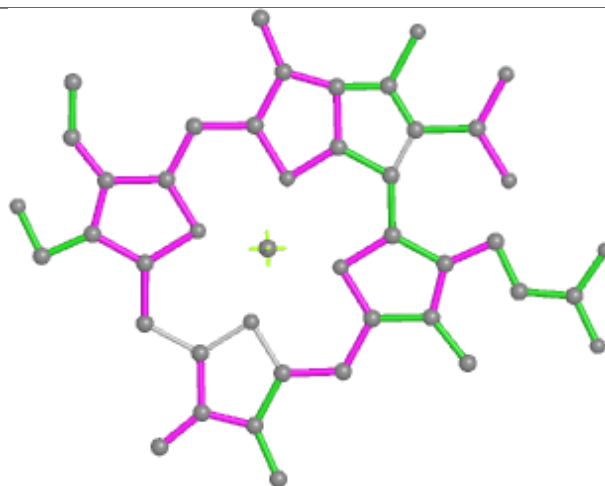


Rings

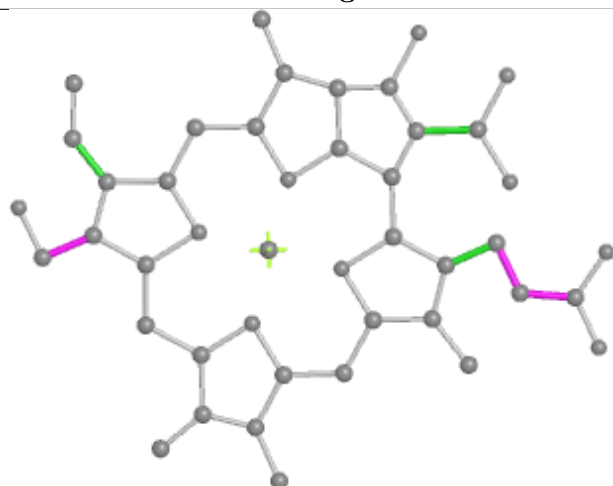
Ligand CHL Z 607



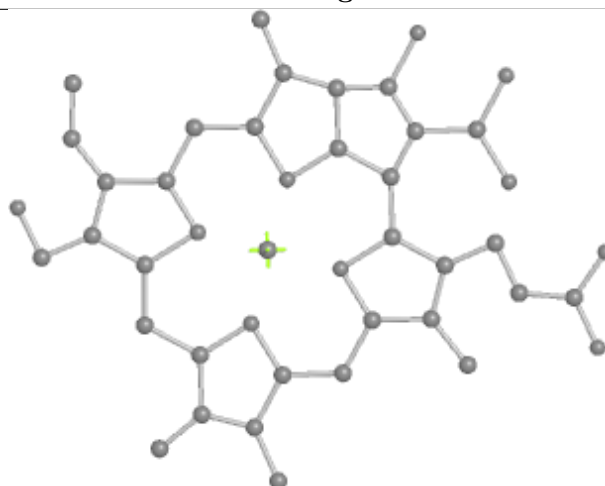
Bond lengths



Bond angles

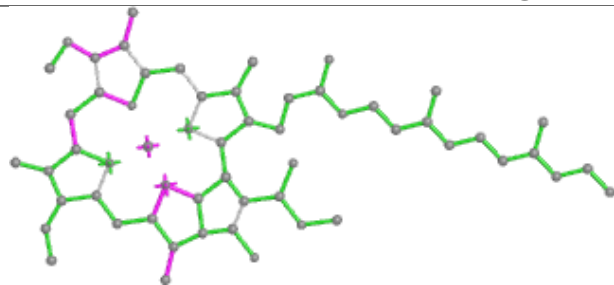


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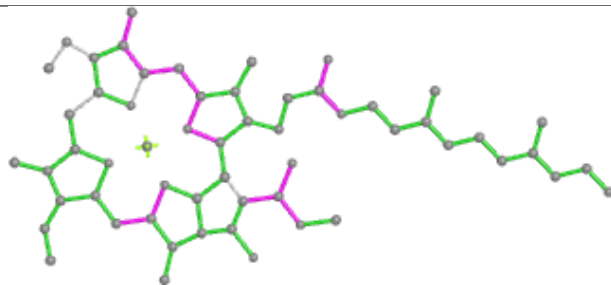


Rings

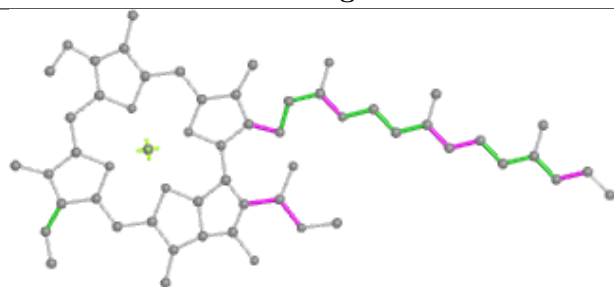
Ligand CLA F 301



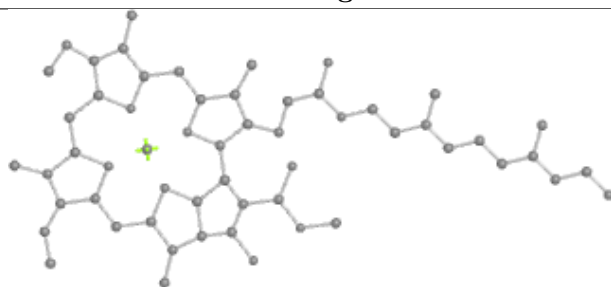
Bond lengths



Bond angles

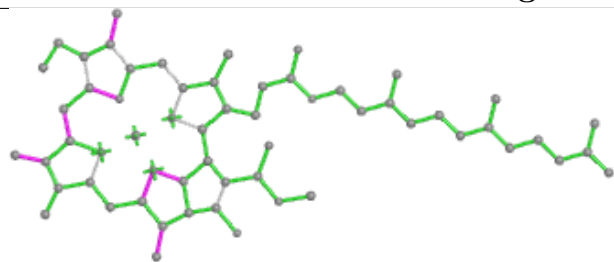


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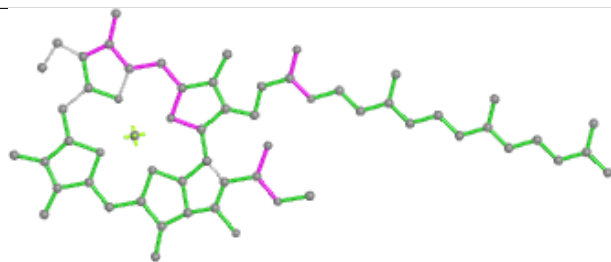


Rings

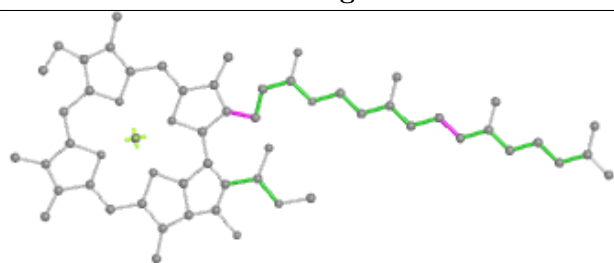
Ligand CLA 1 610



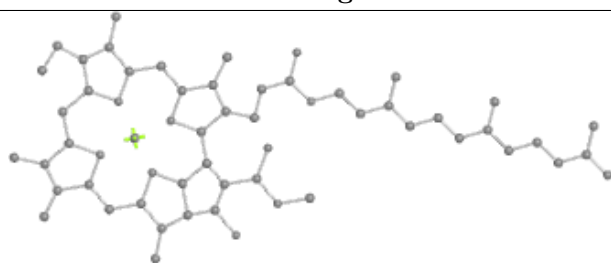
Bond lengths



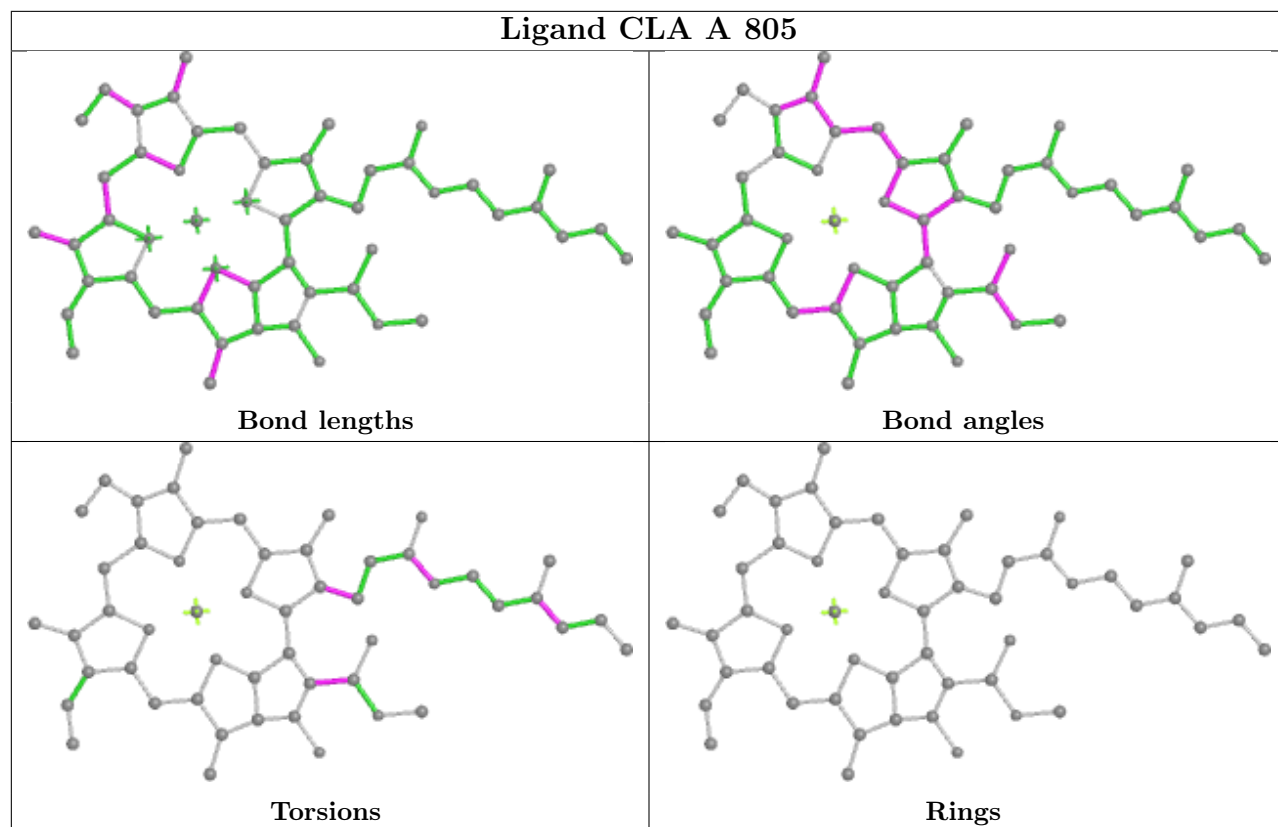
Bond angles



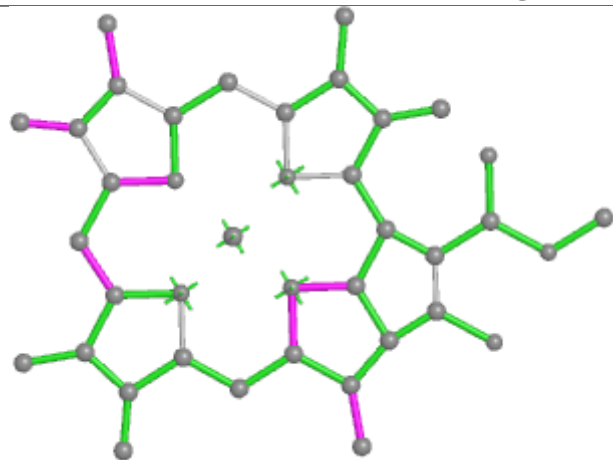
Torsions



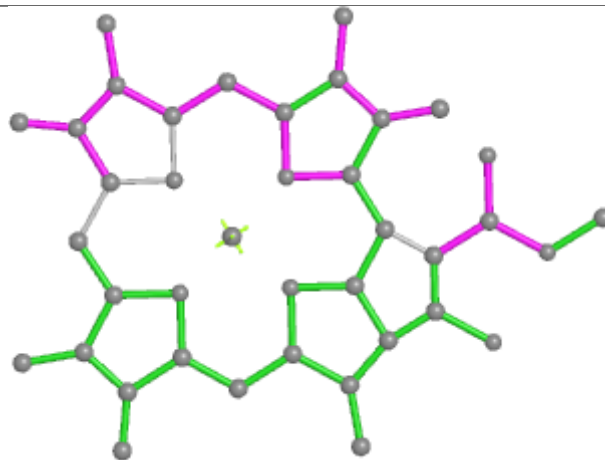
Rings



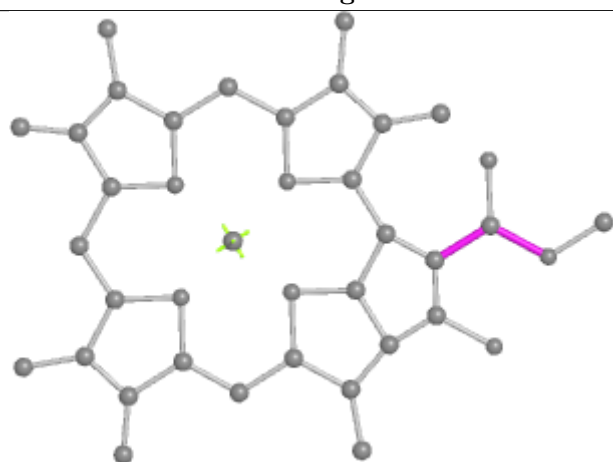
Ligand CLA Y 610



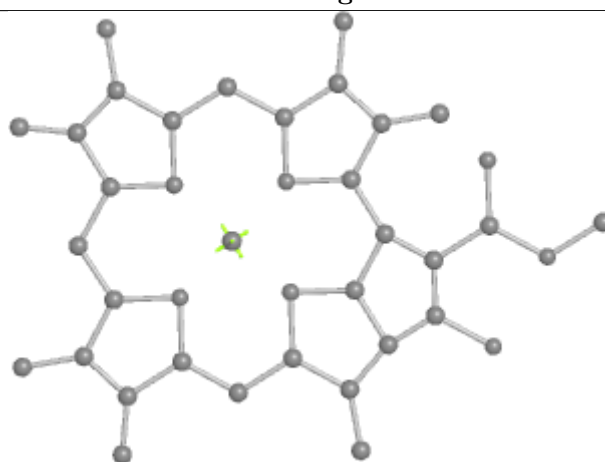
Bond lengths



Bond angles

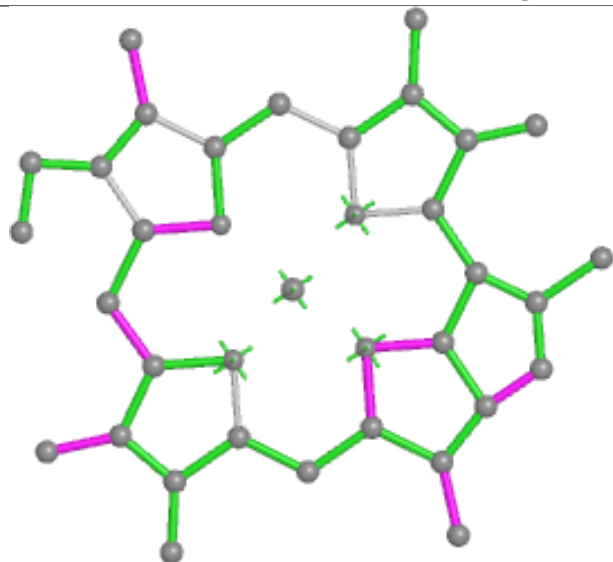


Torsions

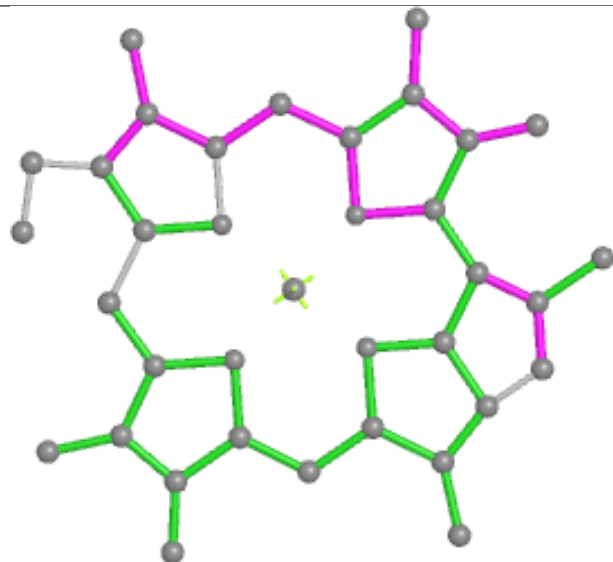


Rings

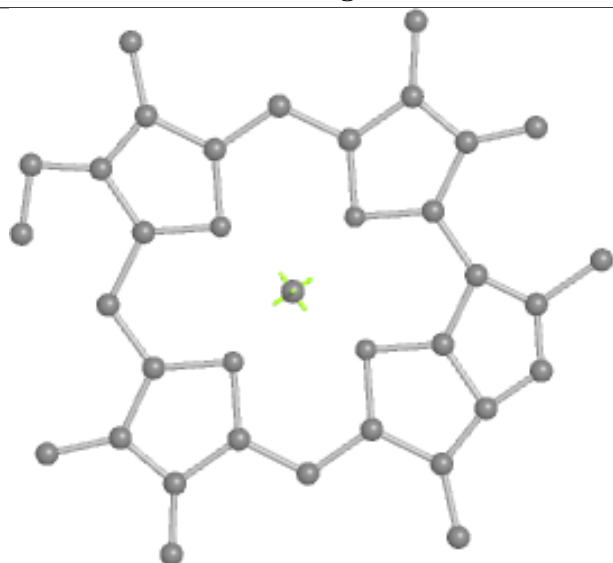
Ligand CLA Z 610



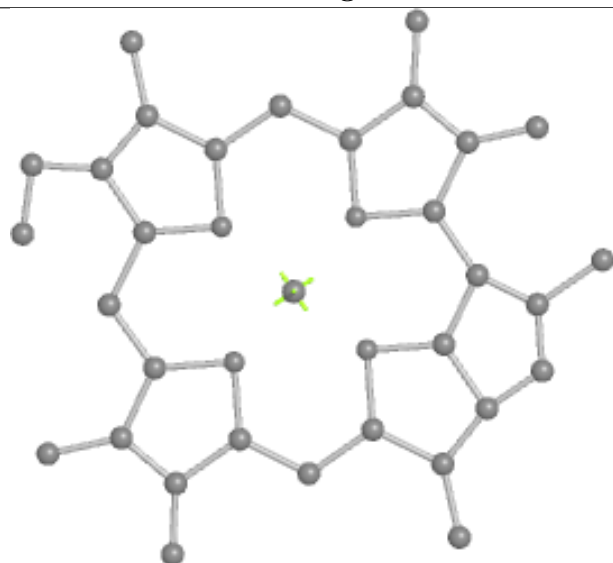
Bond lengths



Bond angles

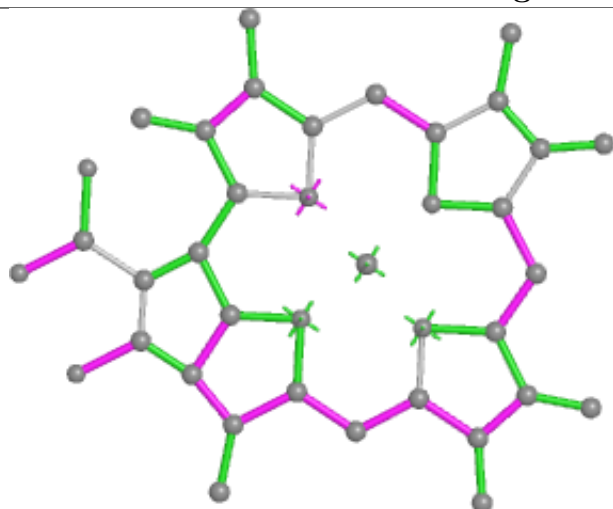


Torsions

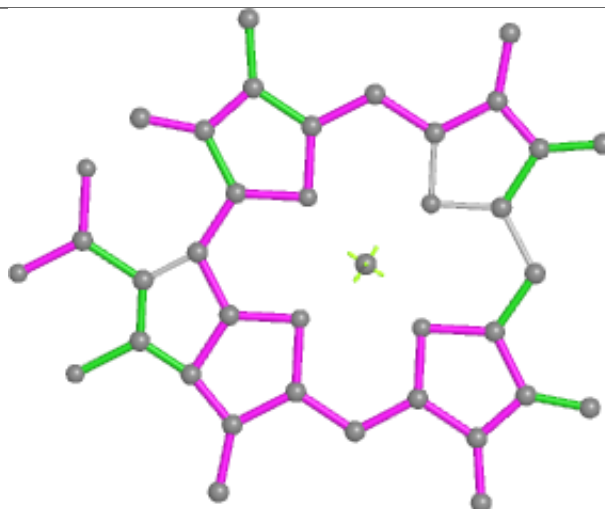


Rings

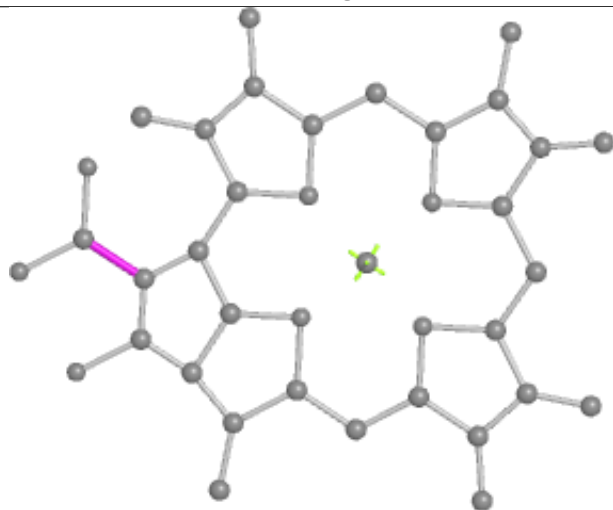
Ligand CHL Y 605



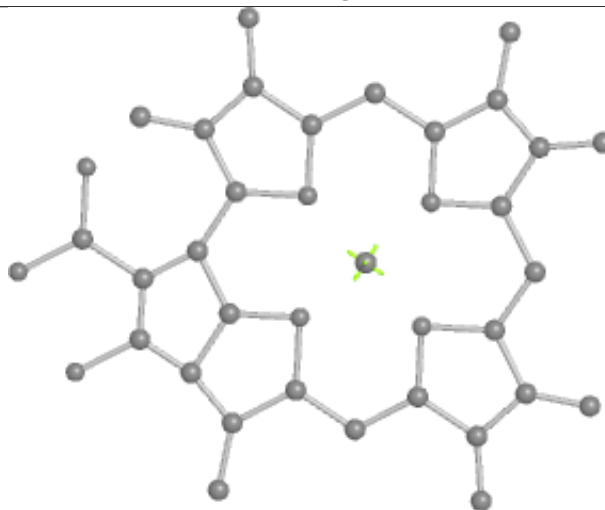
Bond lengths



Bond angles

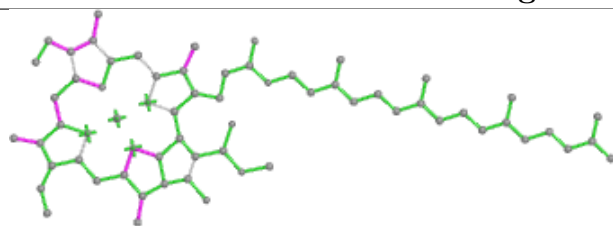


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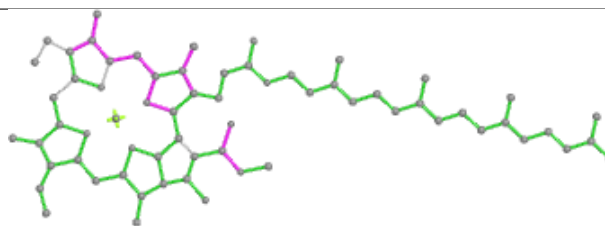


Rings

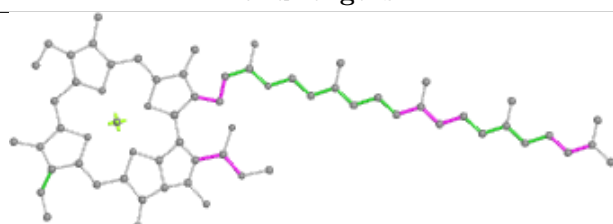
Ligand CLA 2 602



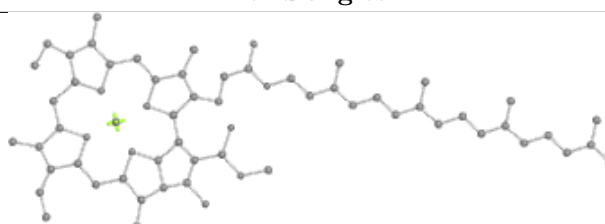
Bond lengths



Bond angles

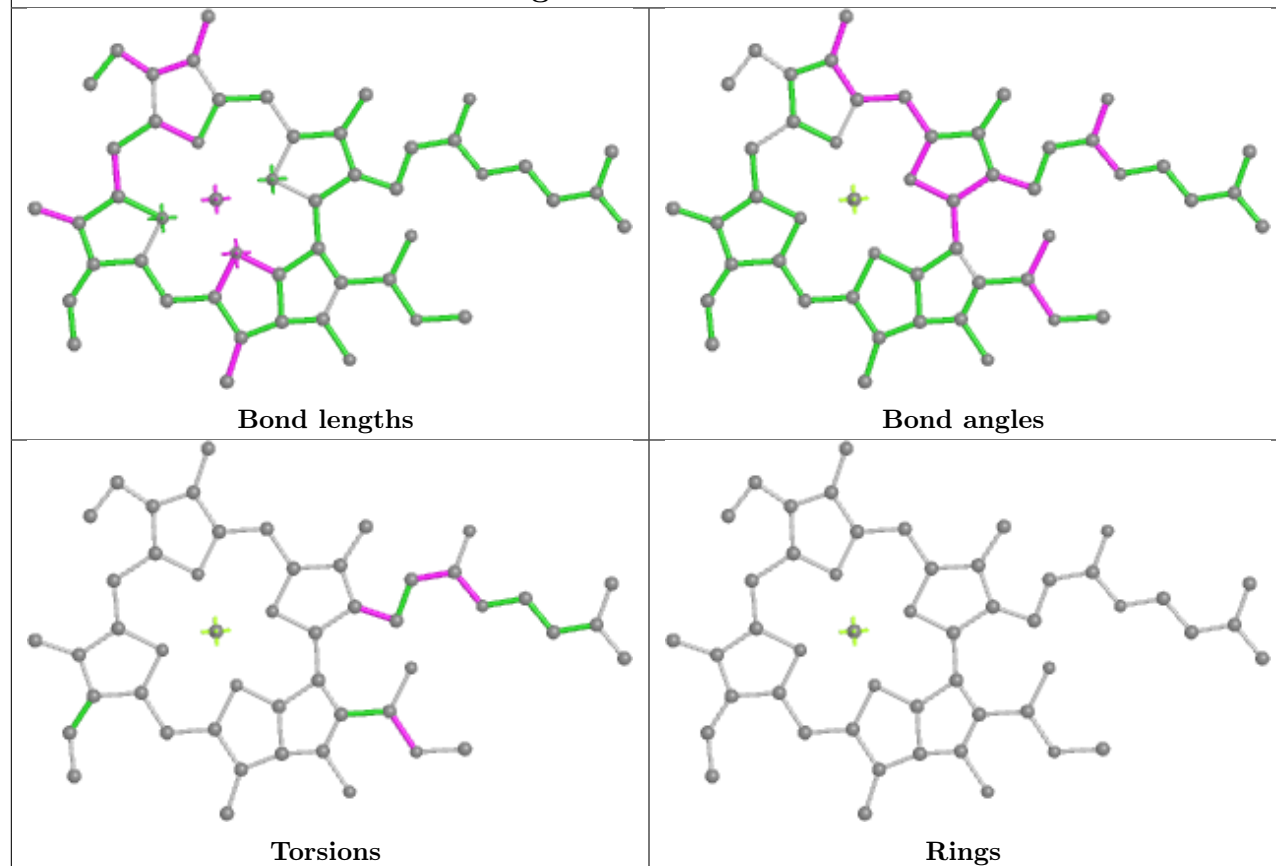


Torsions

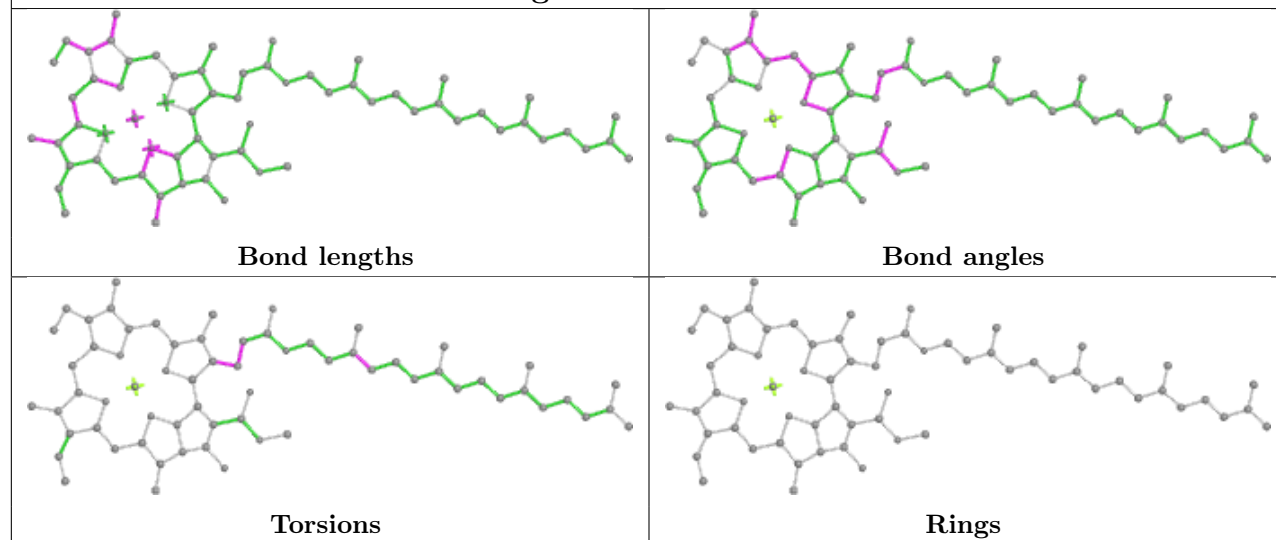


Rings

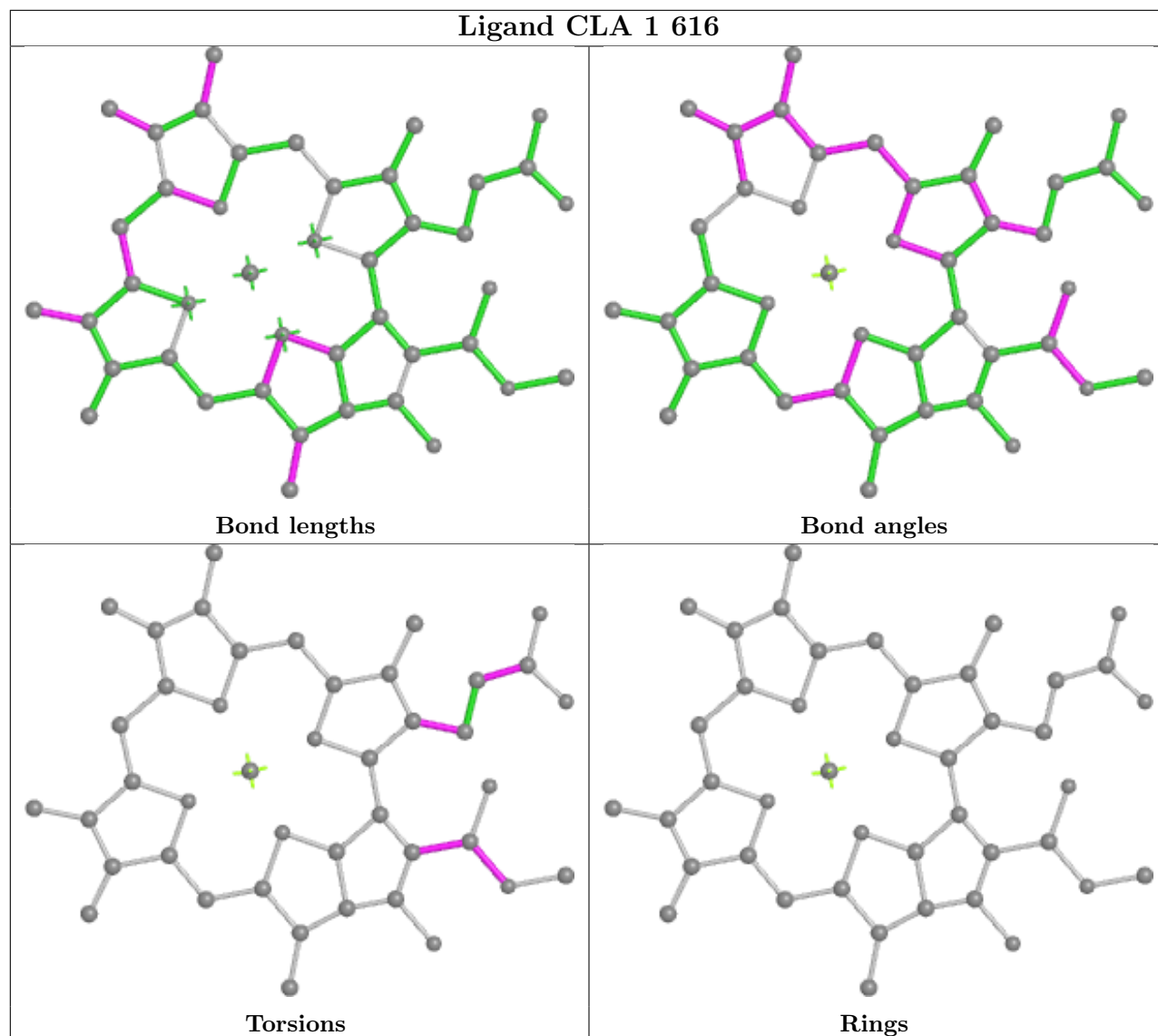
Ligand CLA A 810



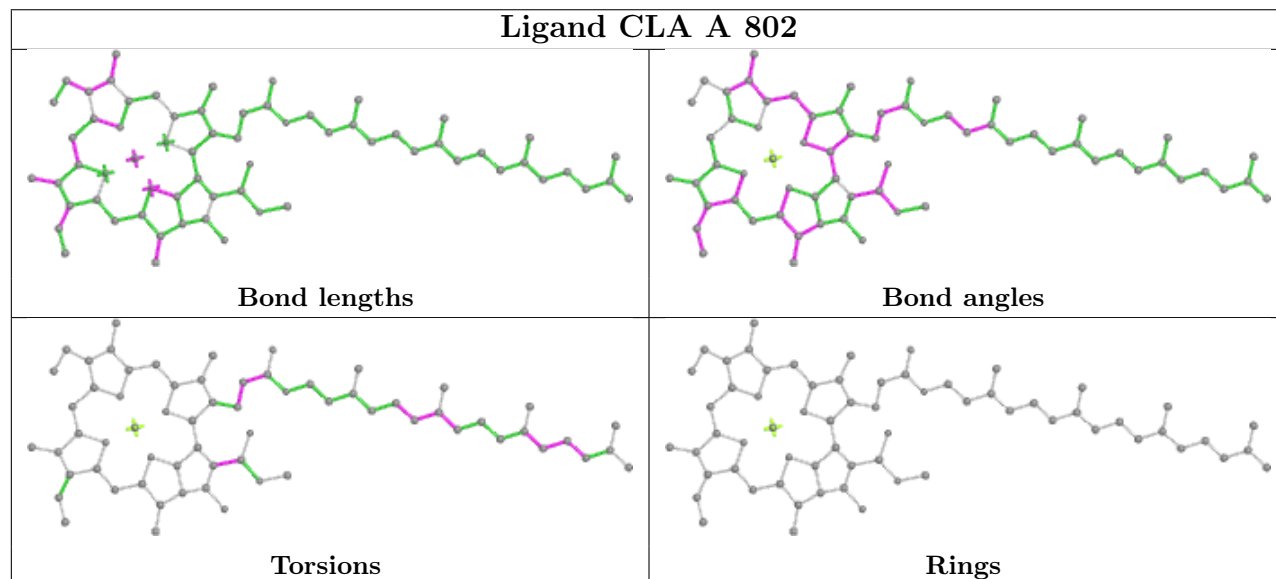
Ligand CLA A 803



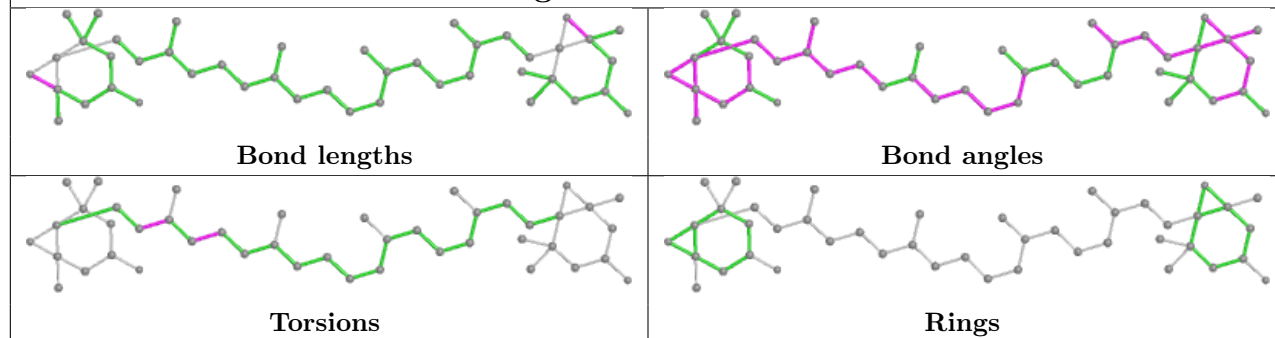
Ligand CLA 1 616



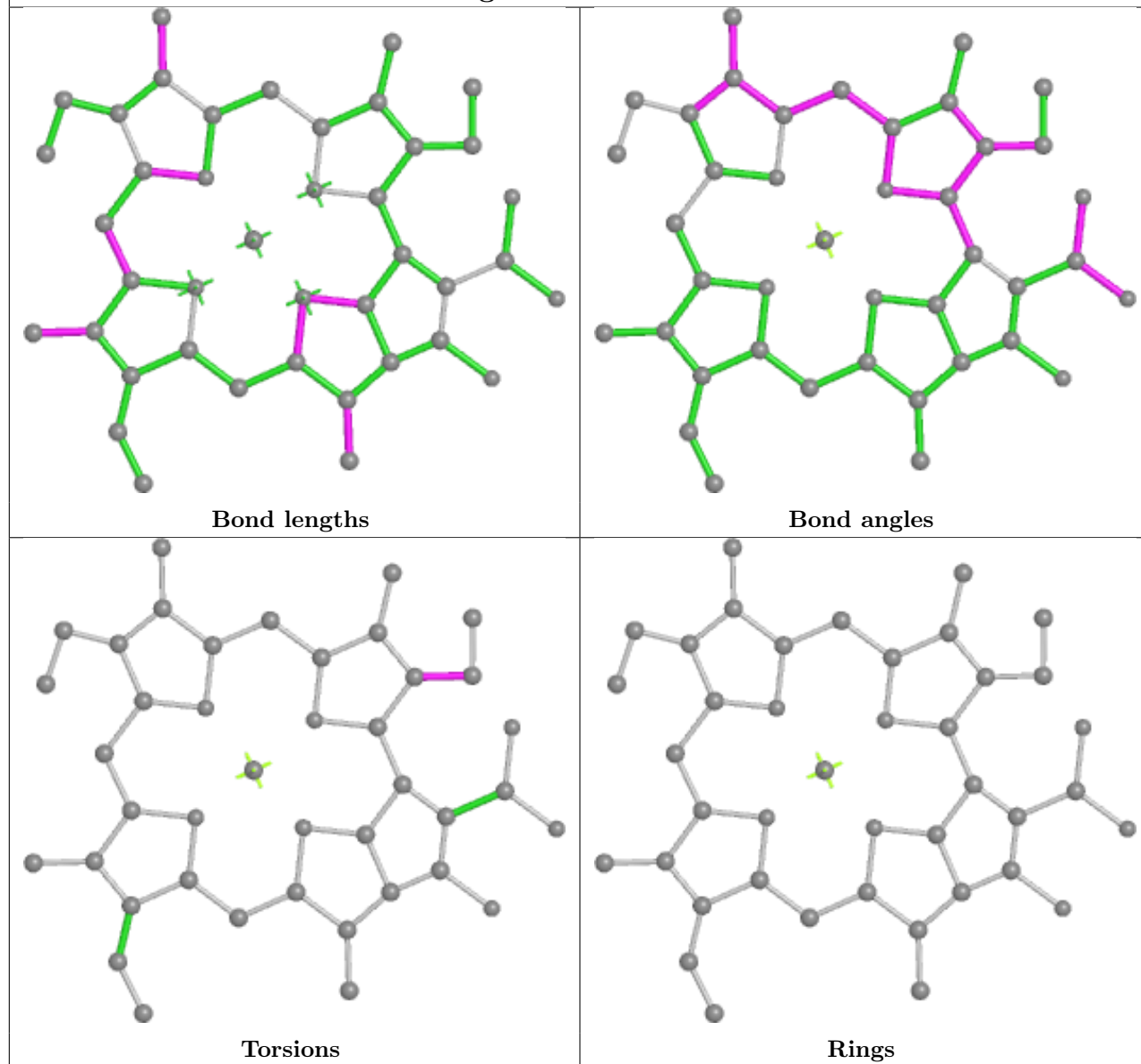
Ligand CLA A 802



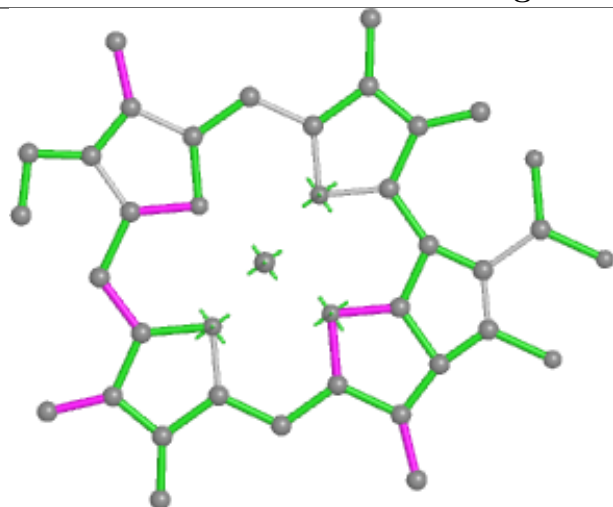
Ligand XAT 1 618



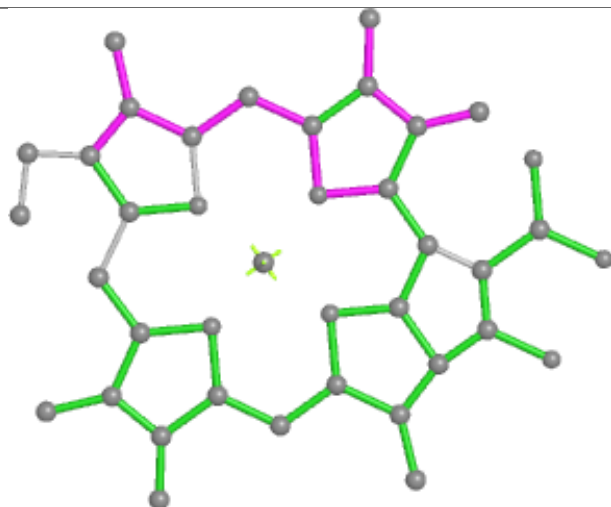
Ligand CLA 4 612



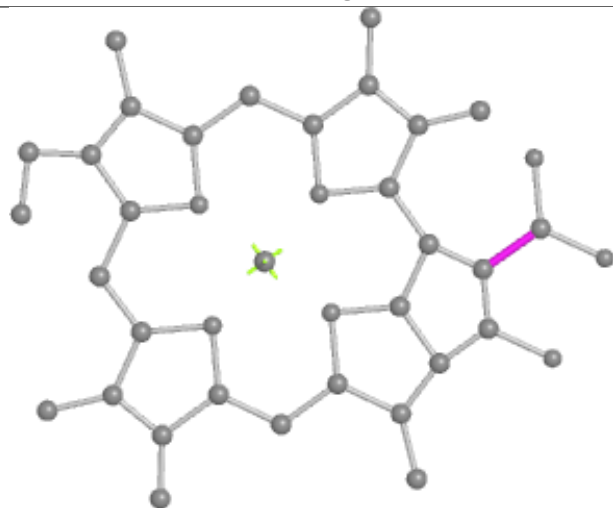
Ligand CLA Y 603



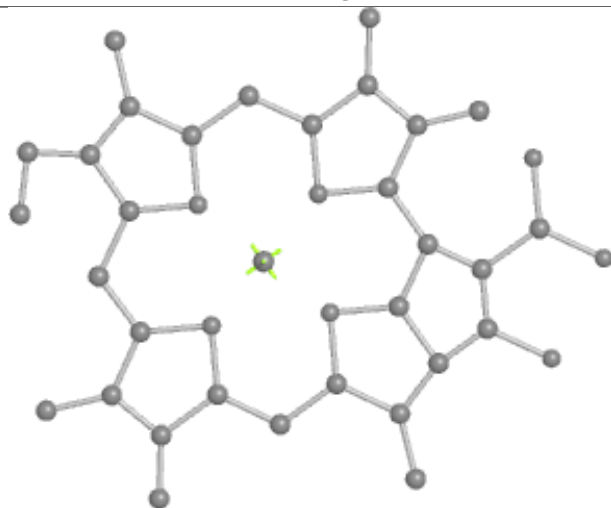
Bond lengths



Bond angles

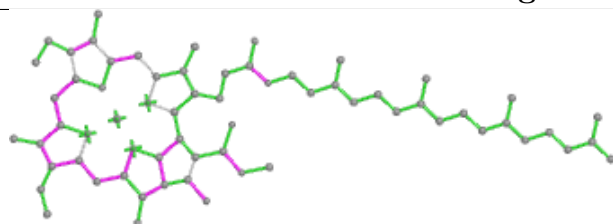


Torsions

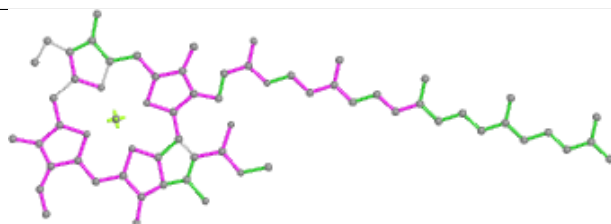


Rings

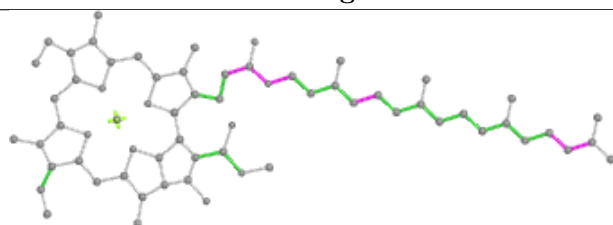
Ligand CL0 A 801



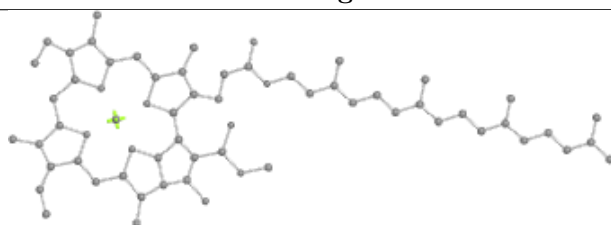
Bond lengths



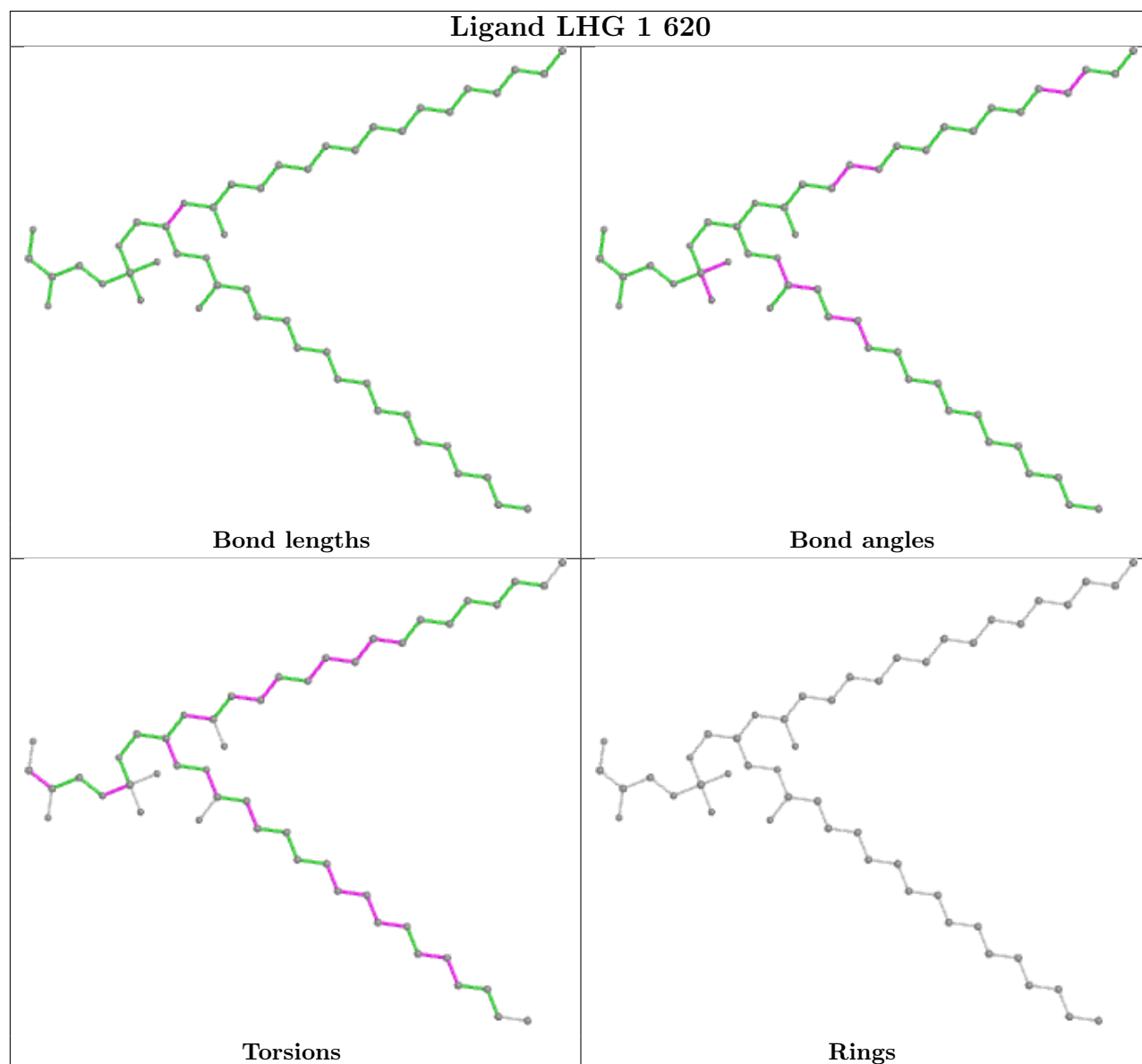
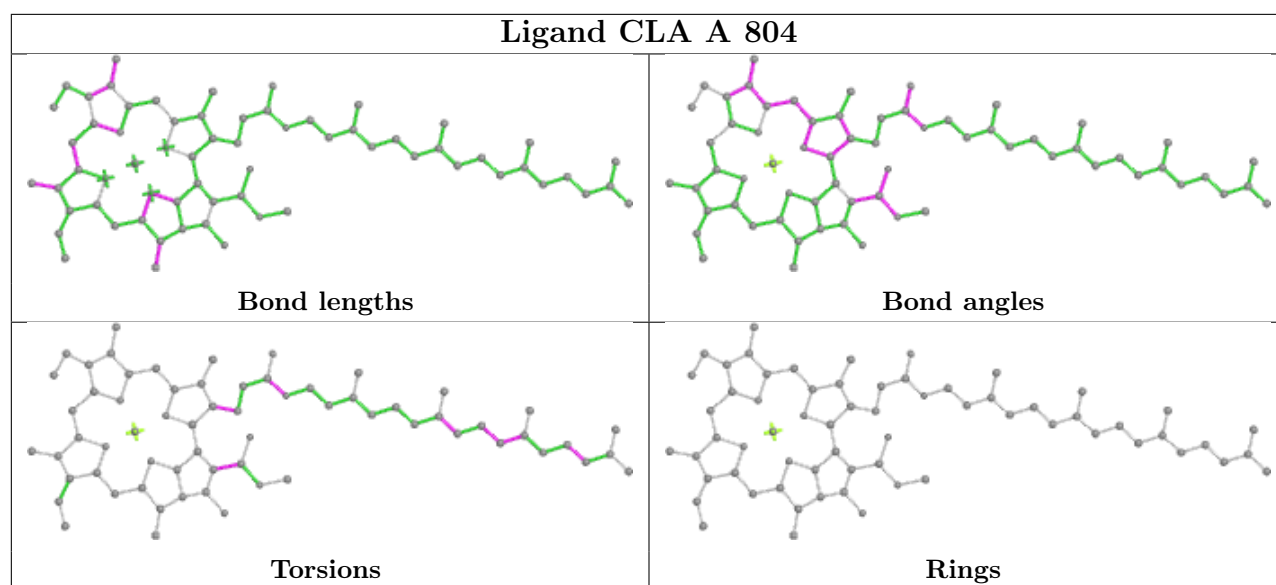
Bond angles



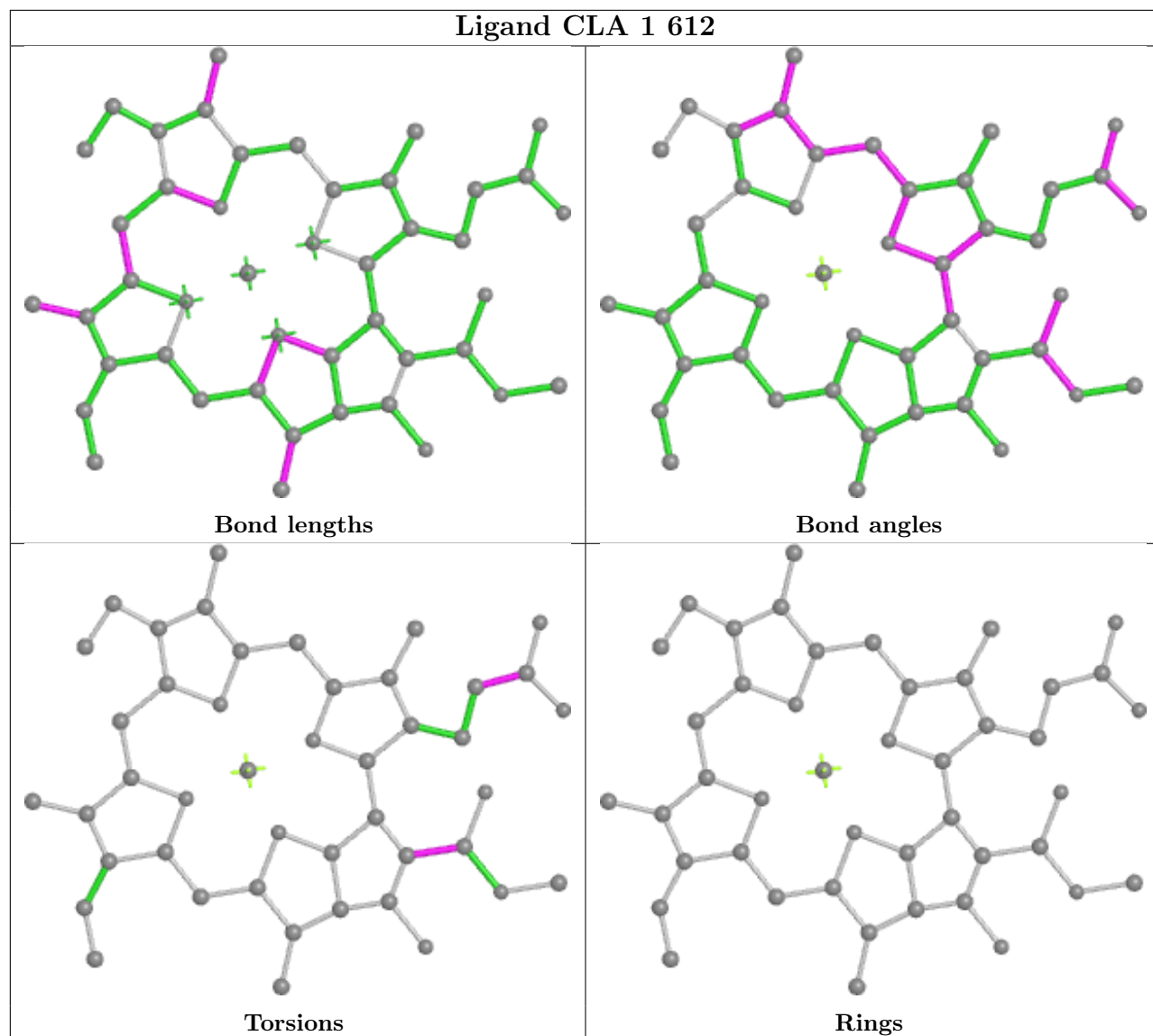
Torsions



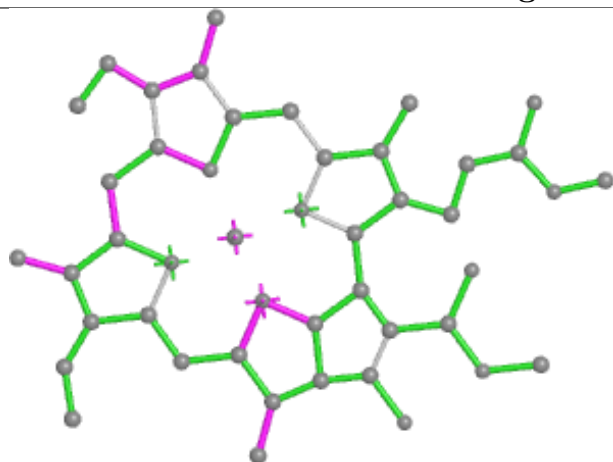
Rings



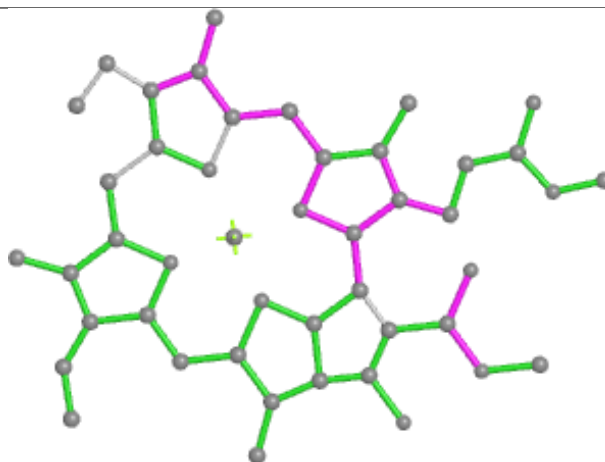
Ligand CLA 1 612



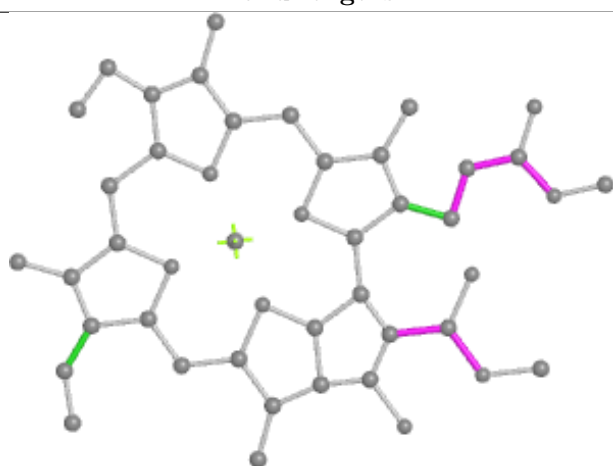
Ligand CLA 4 601



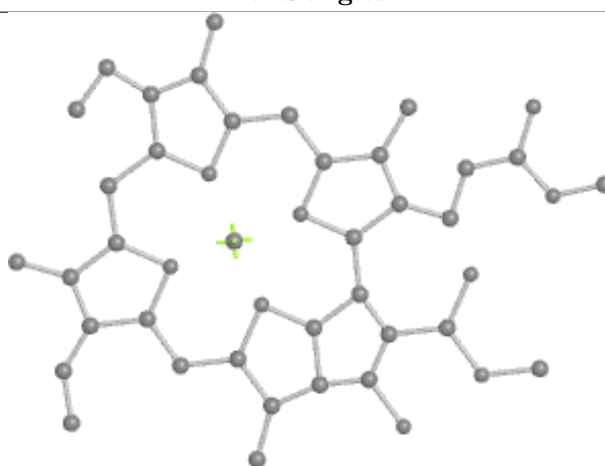
Bond lengths



Bond angles

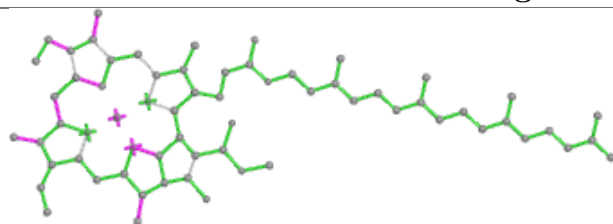


Torsions

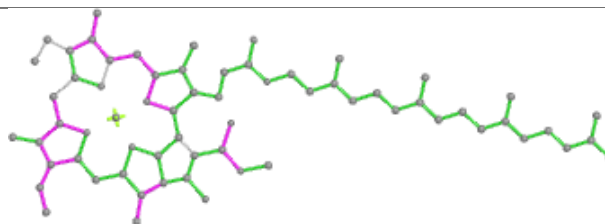


Rings

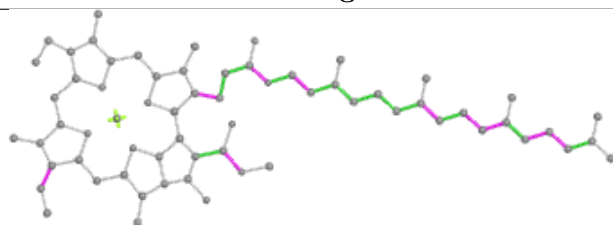
Ligand CLA B 803



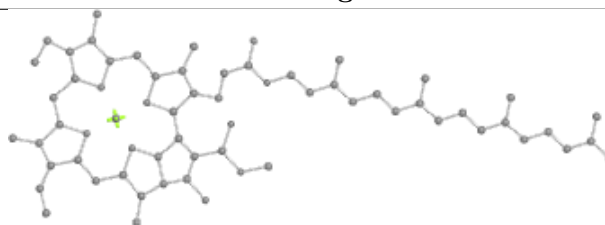
Bond lengths



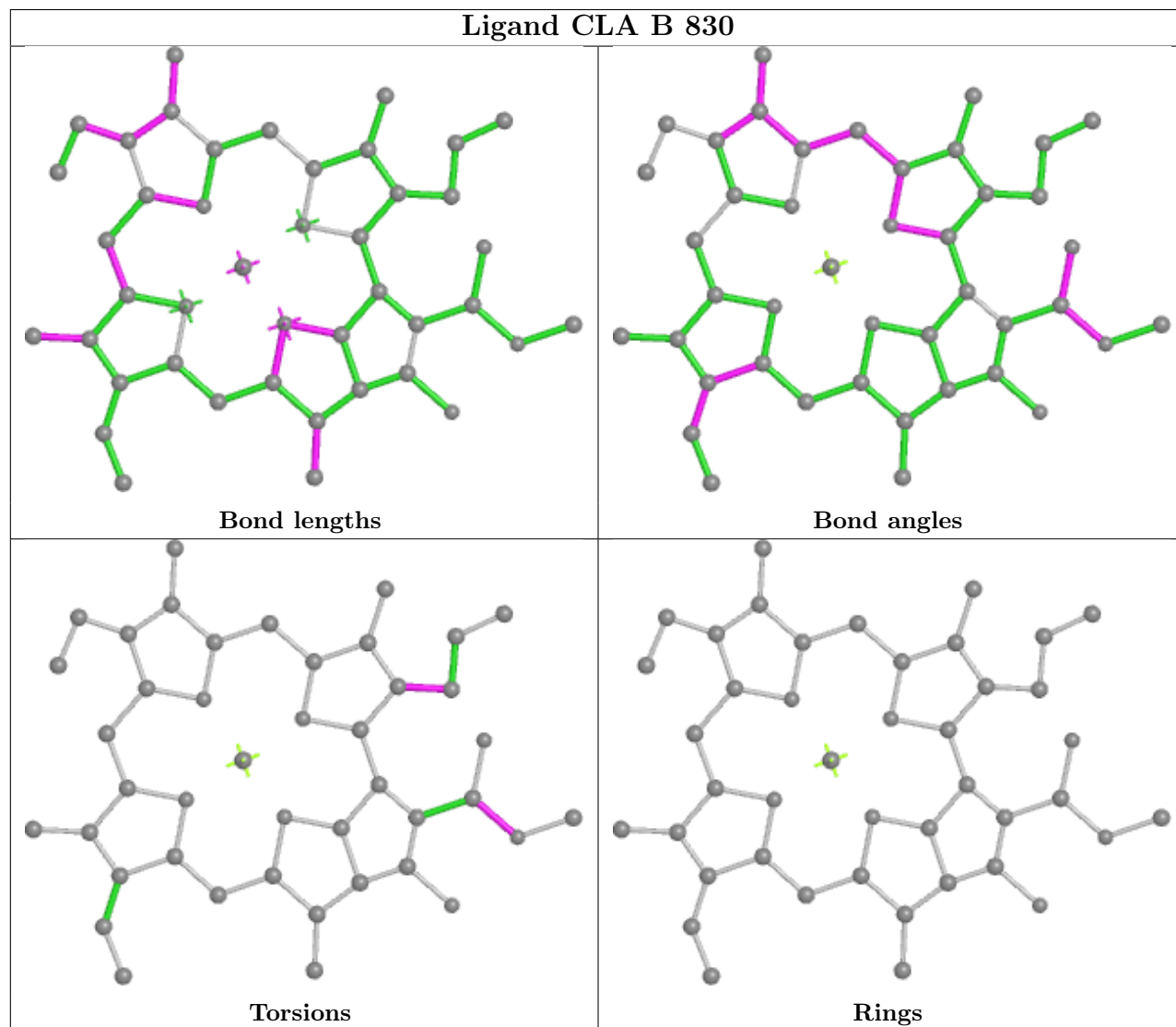
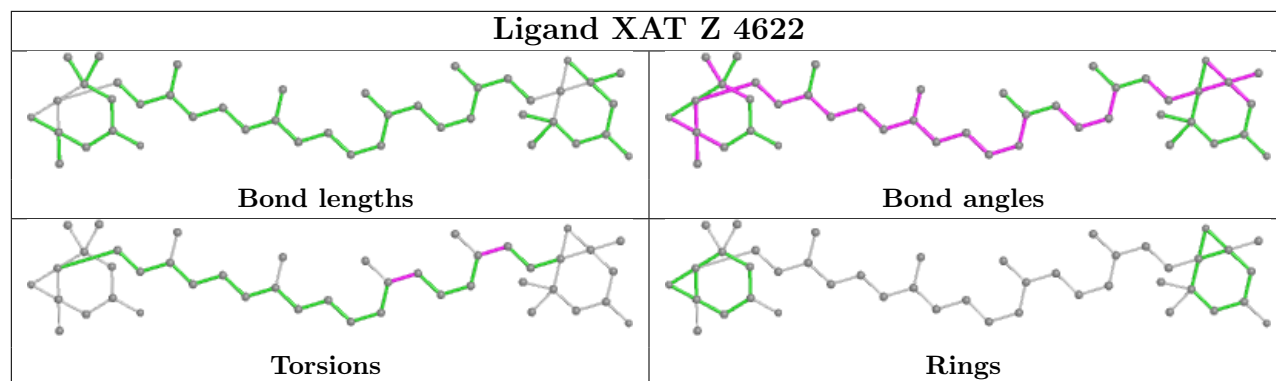
Bond angles

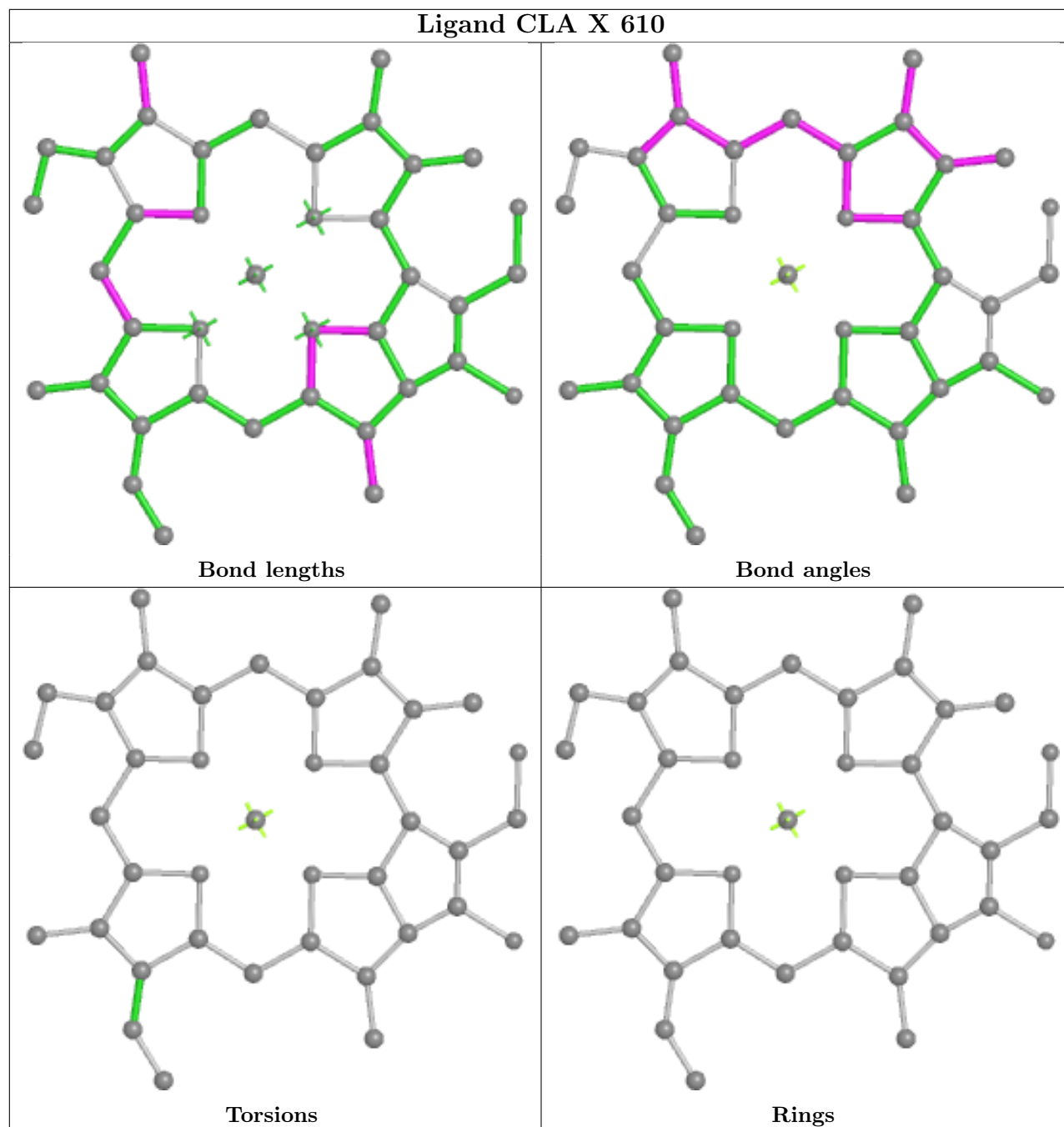
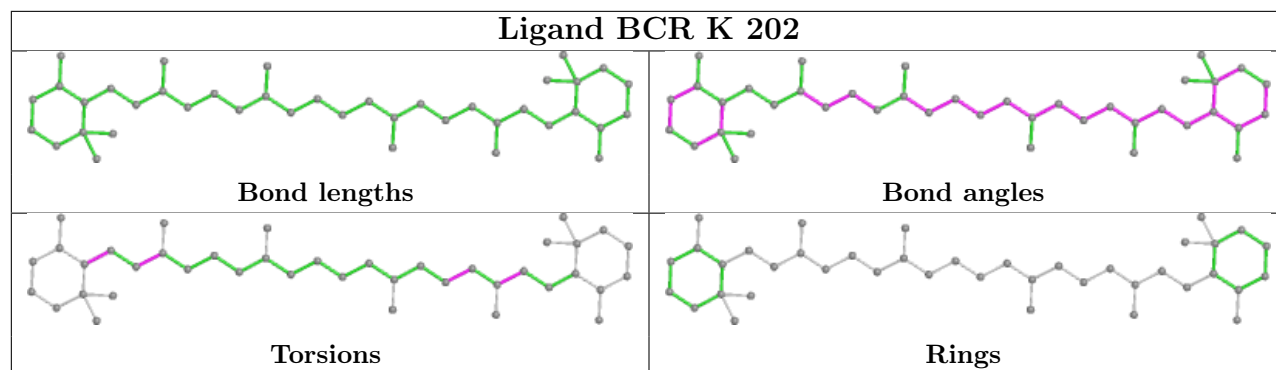


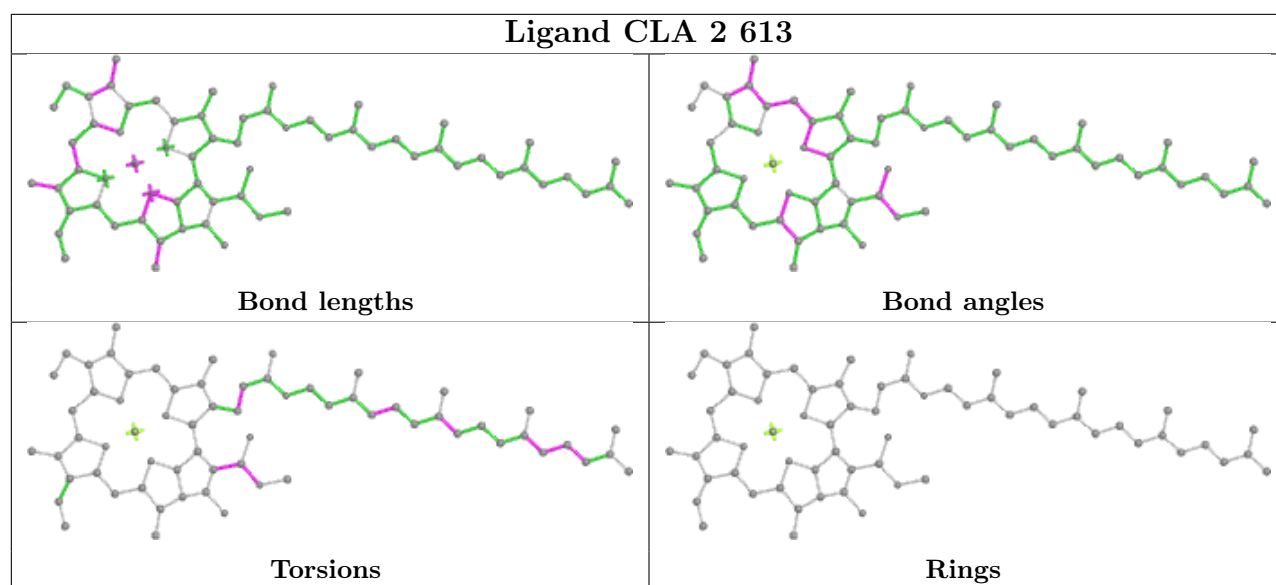
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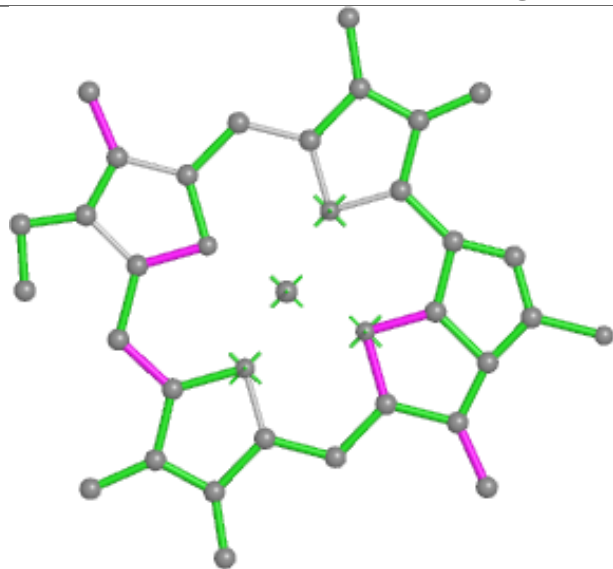
Rings



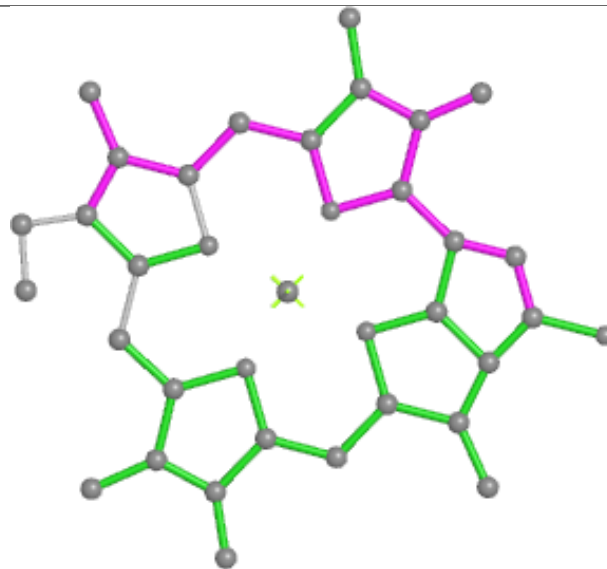




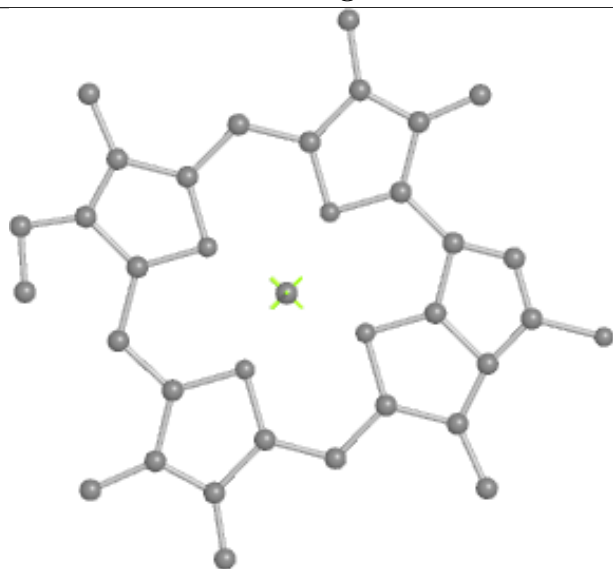
Ligand CLA X 613



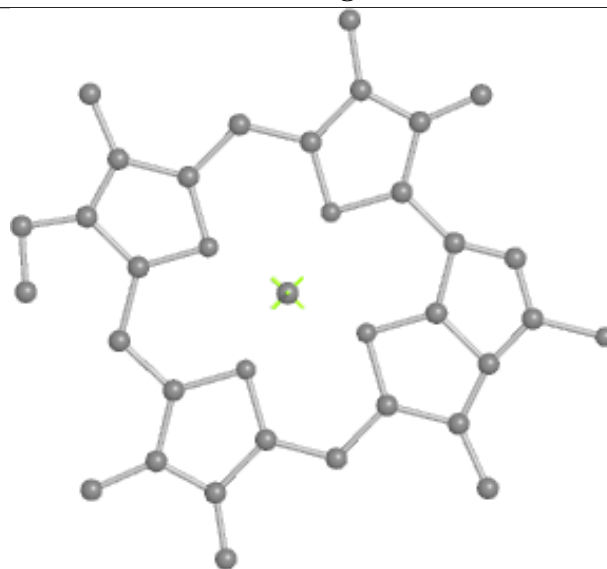
Bond lengths



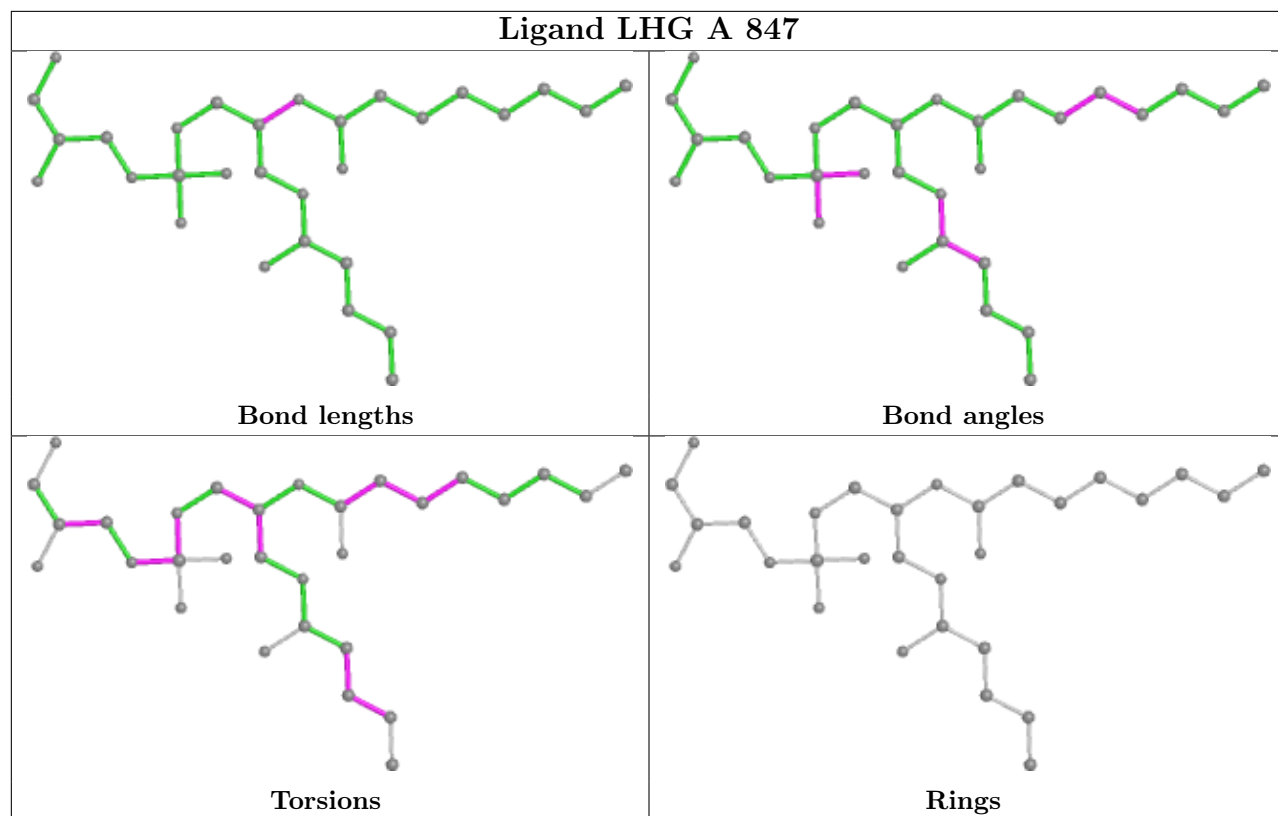
Bond angles



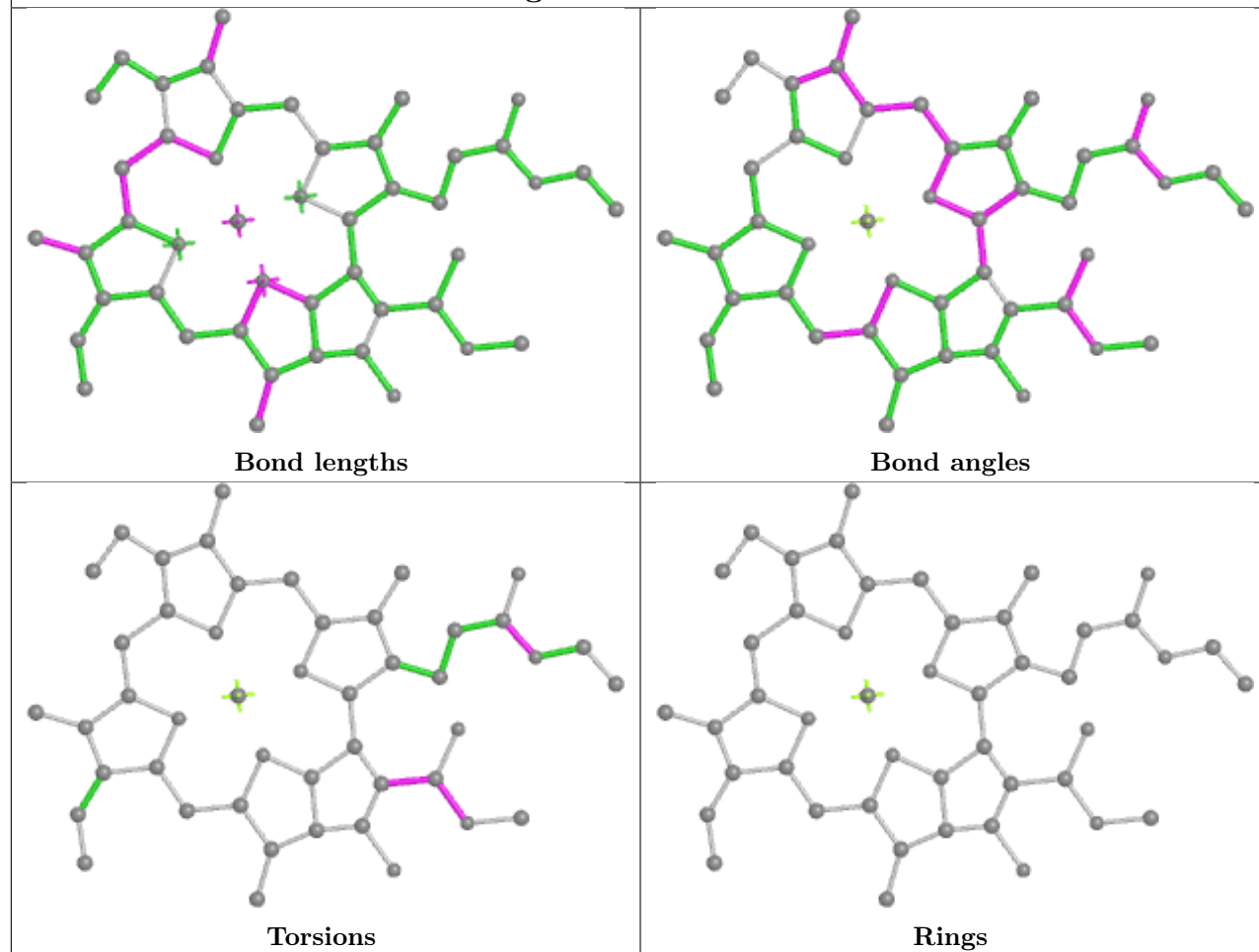
Torsions



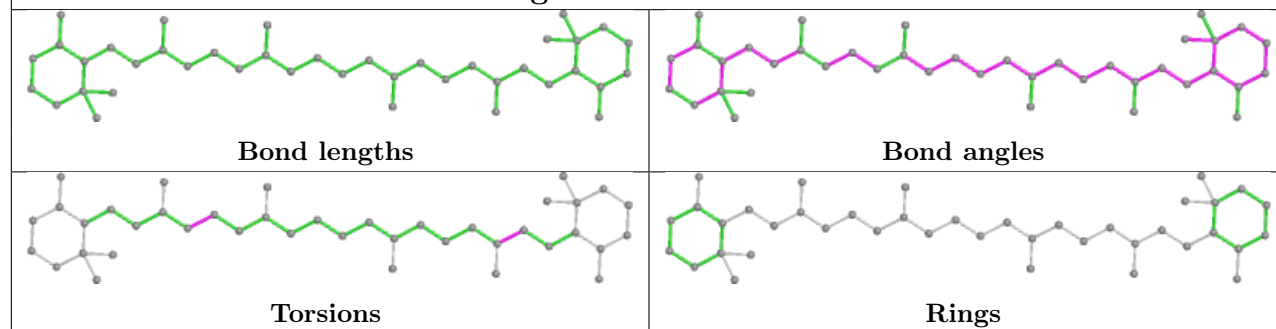
Rings



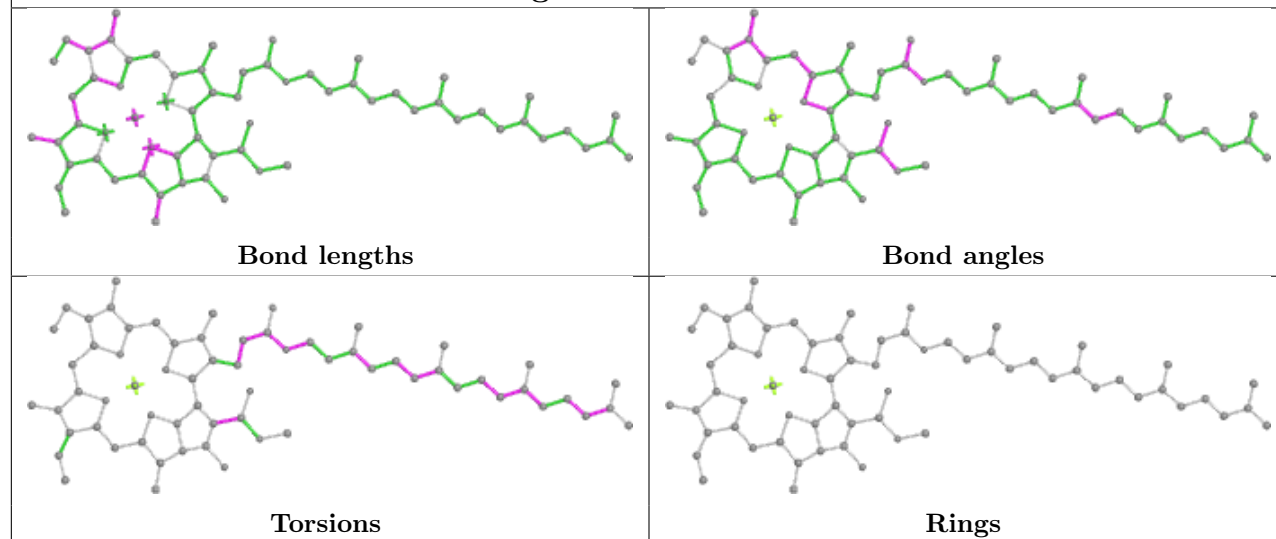
Ligand CLA B 821



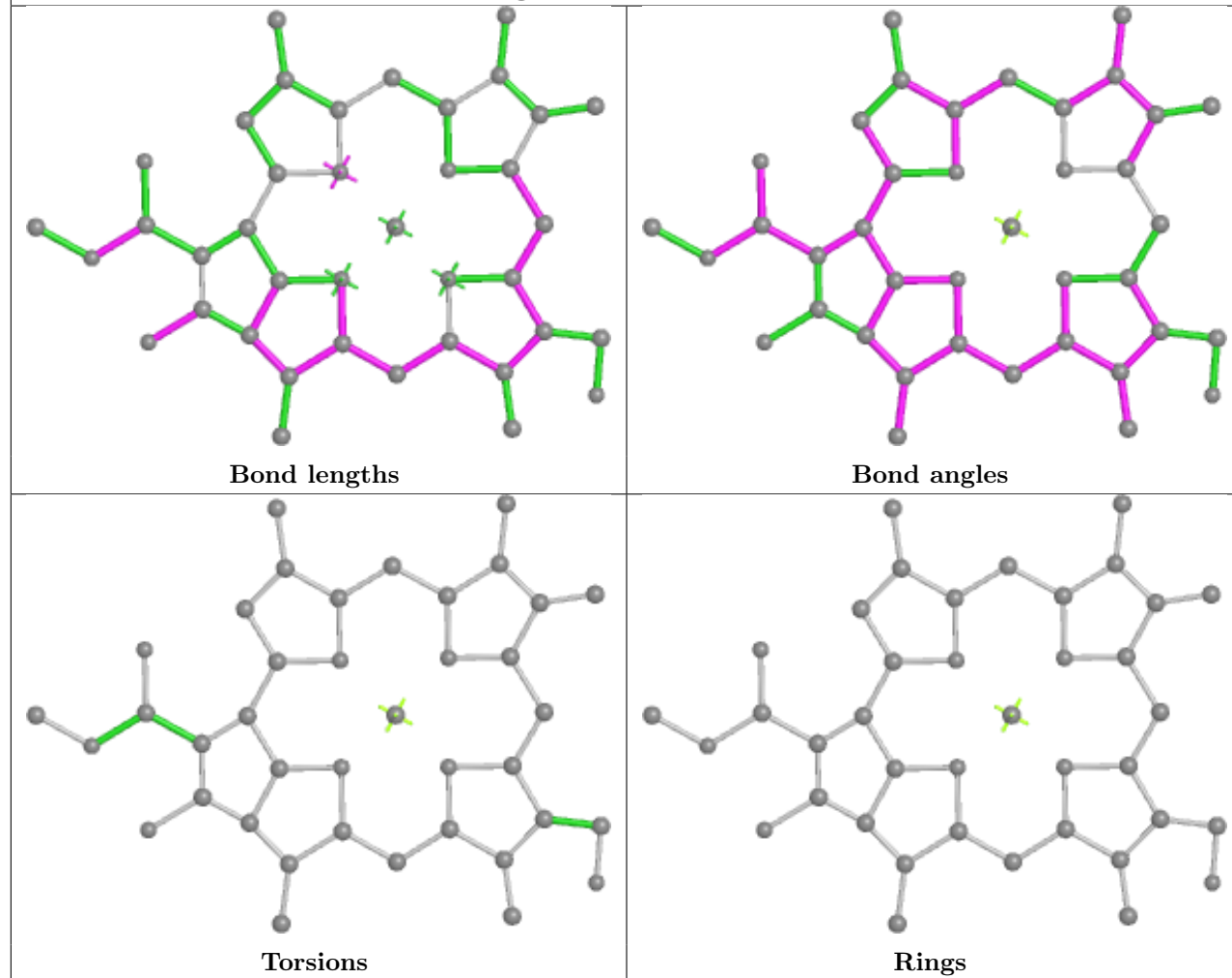
Ligand BCR B 848

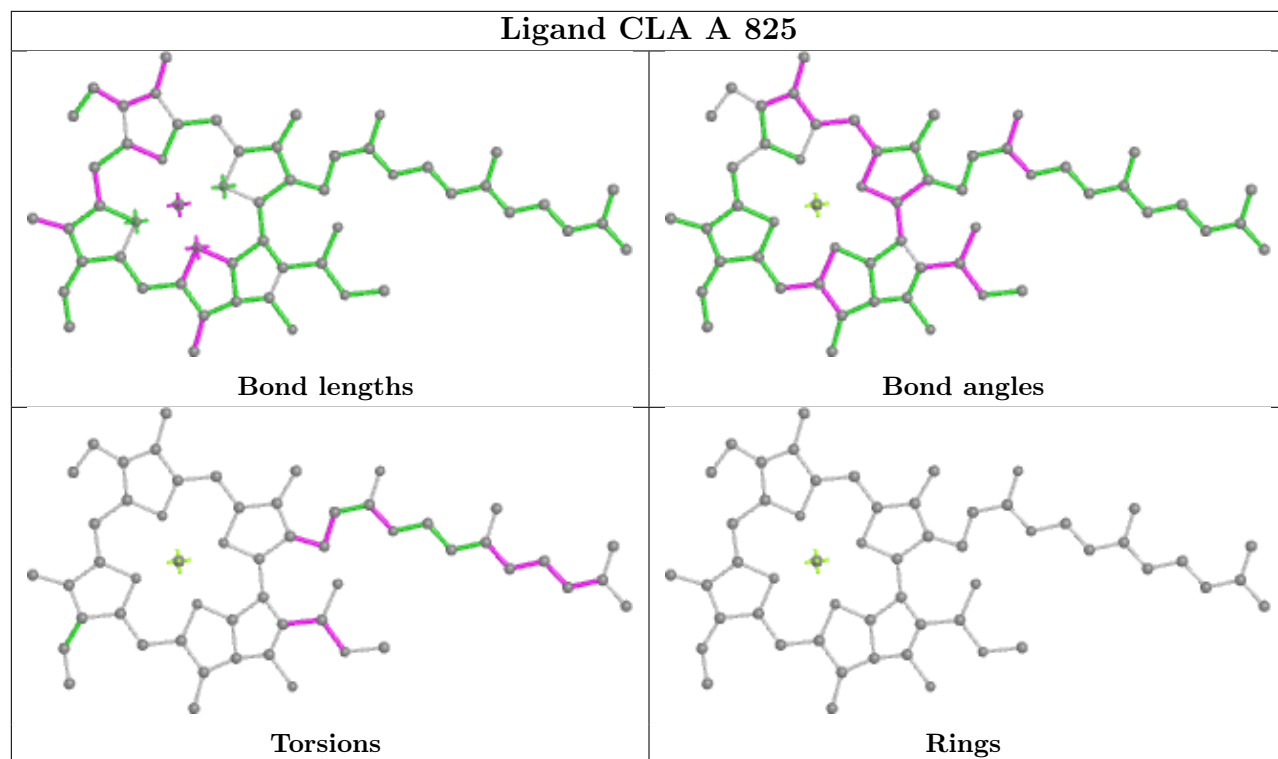


Ligand CLA A 807

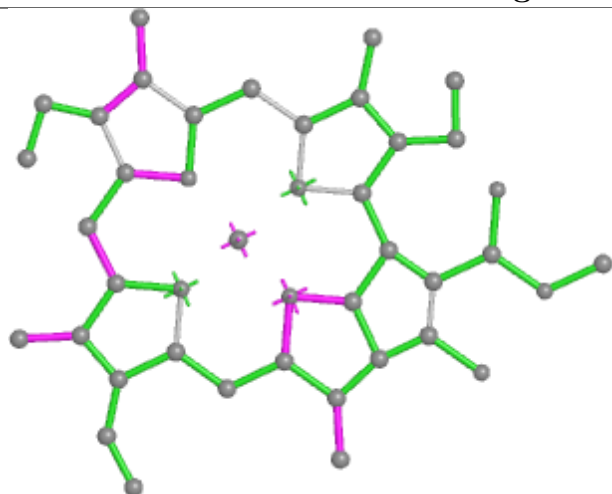


Ligand CHL X 606

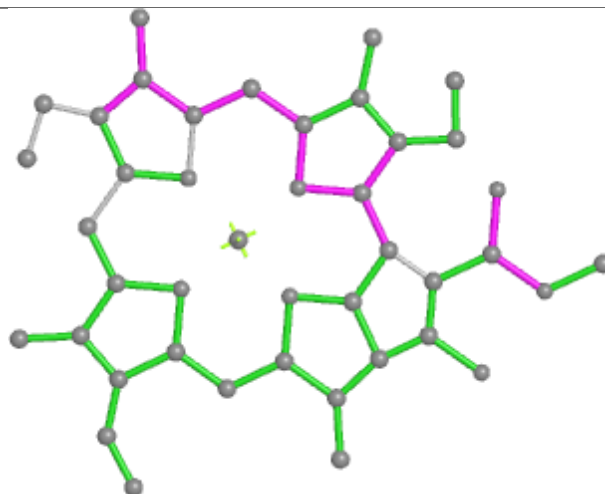




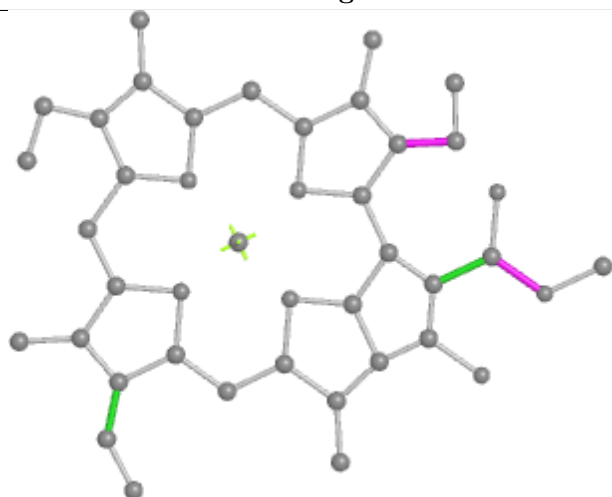
Ligand CLA B 835



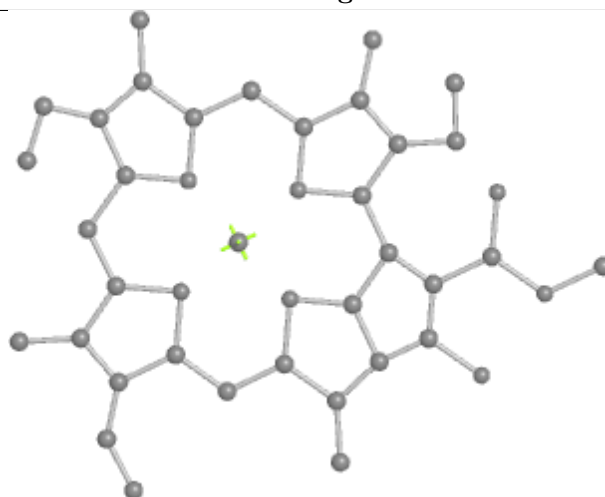
Bond lengths



Bond angles

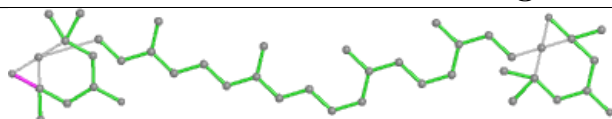


Torsions

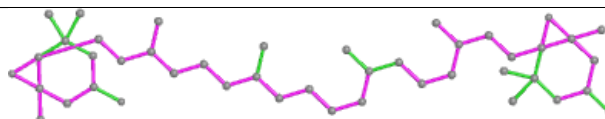


Rings

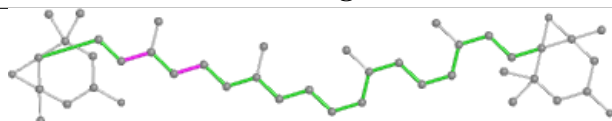
Ligand XAT 2 620



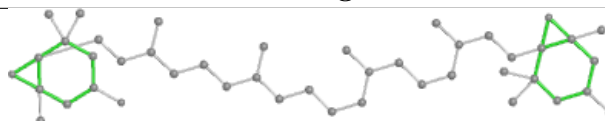
Bond lengths



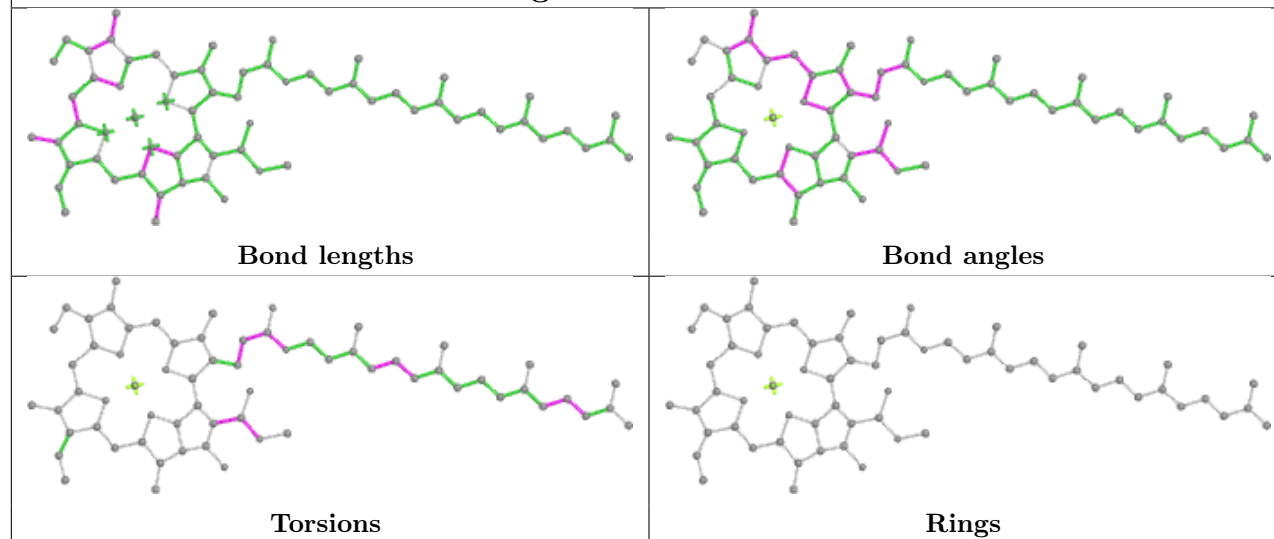
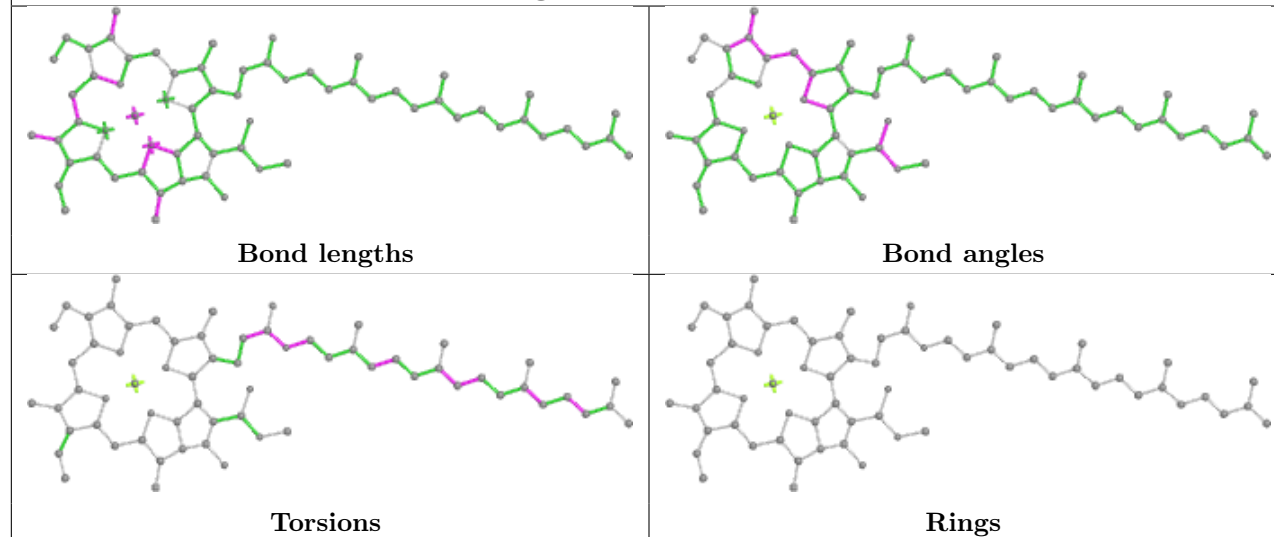
Bond angles

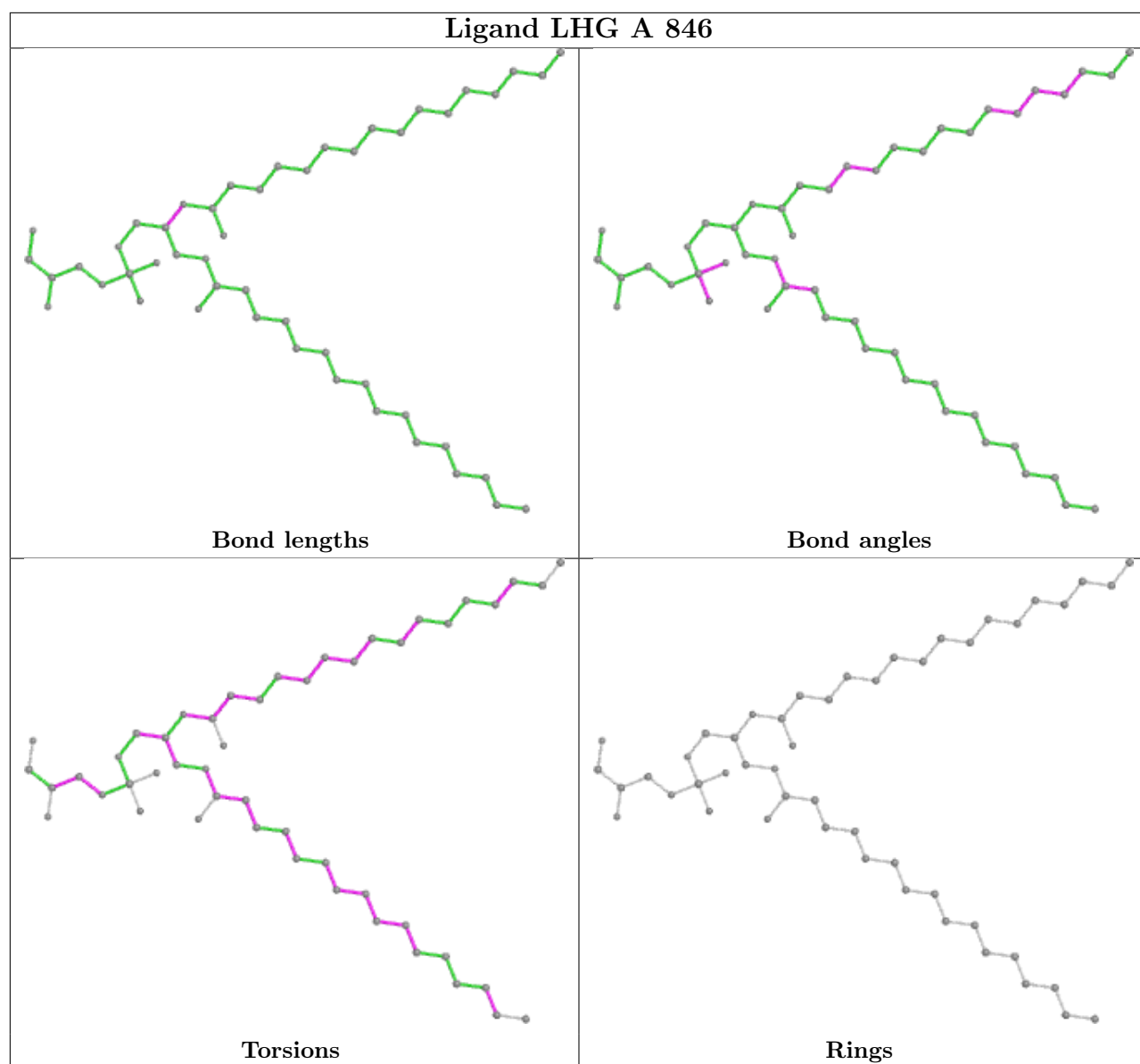


Torsions

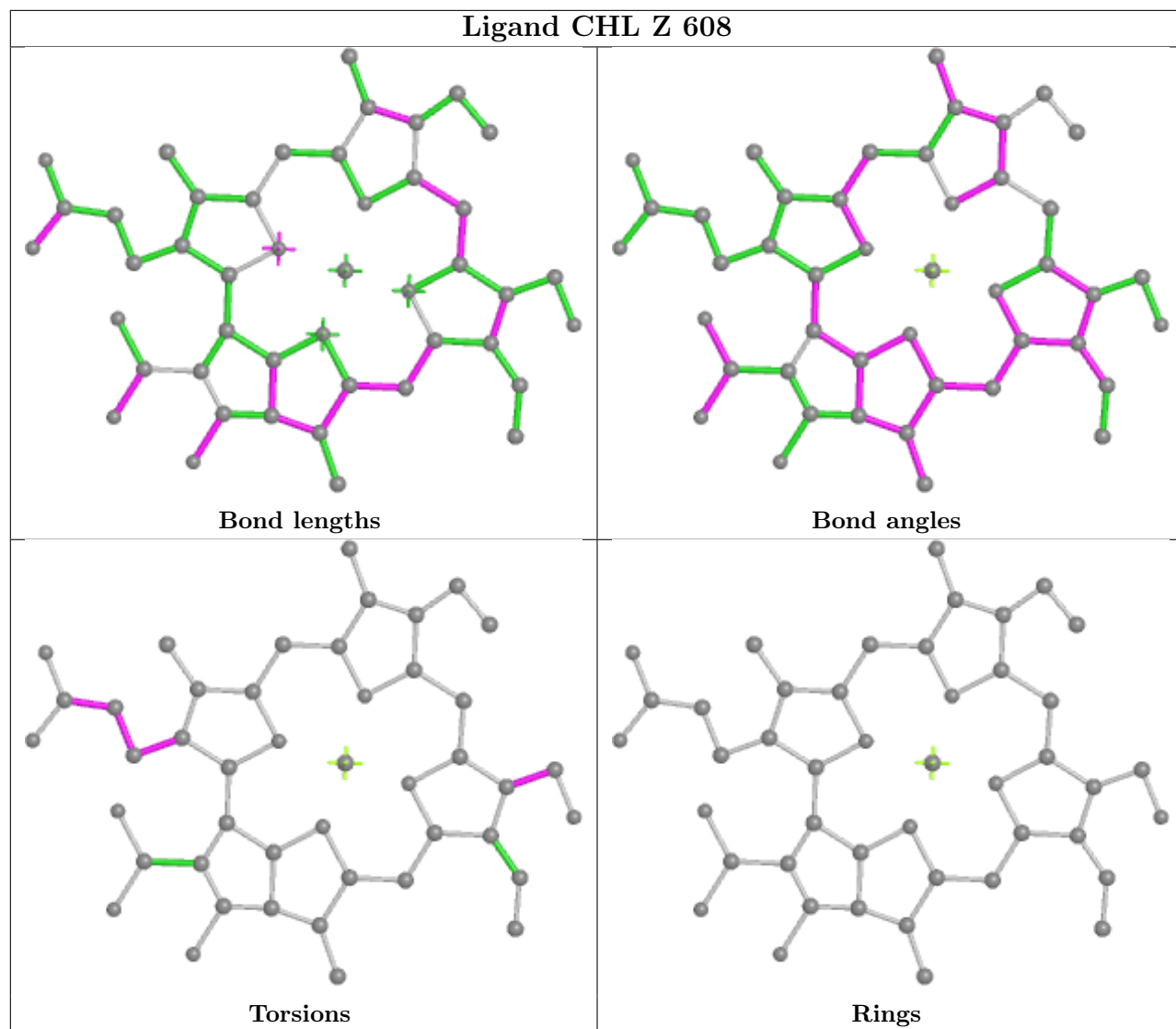


Rings

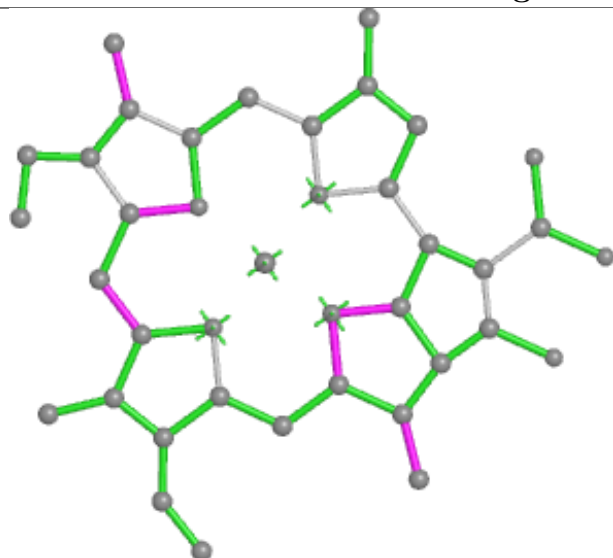
Ligand CLA A 834**Ligand CLA B 806**



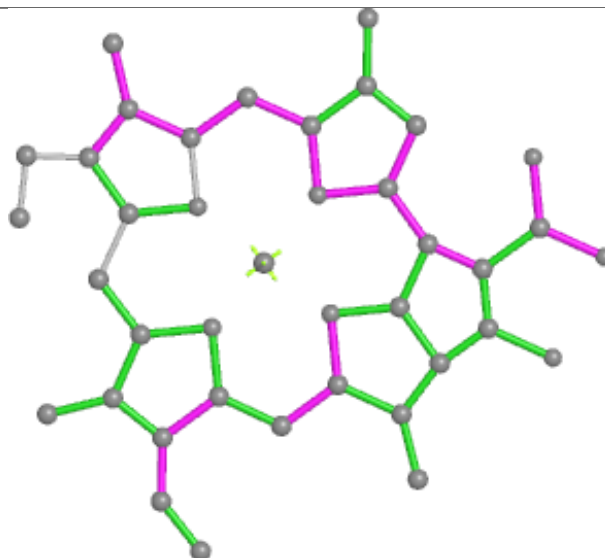
Ligand CHL Z 608



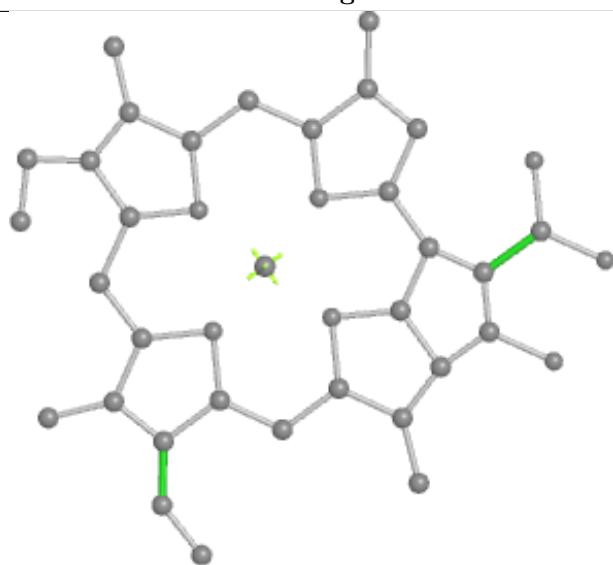
Ligand CLA K 206



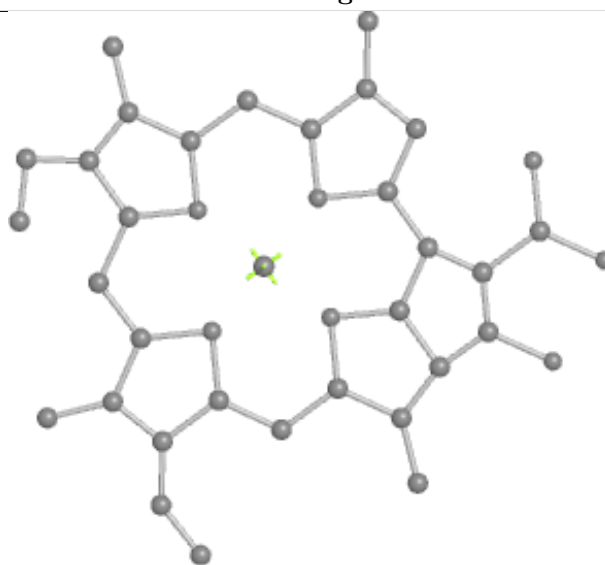
Bond lengths



Bond angles

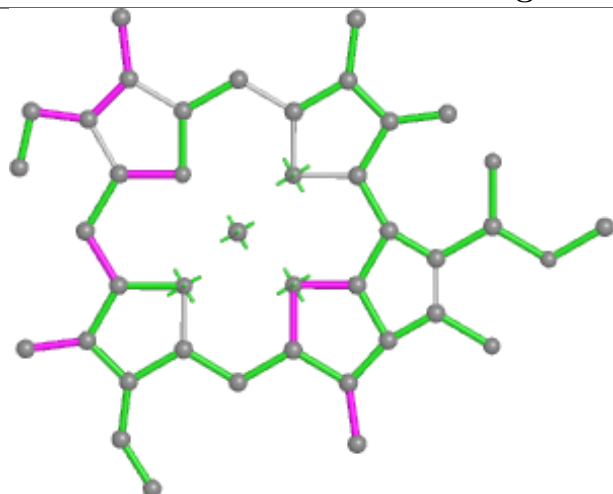


Torsions

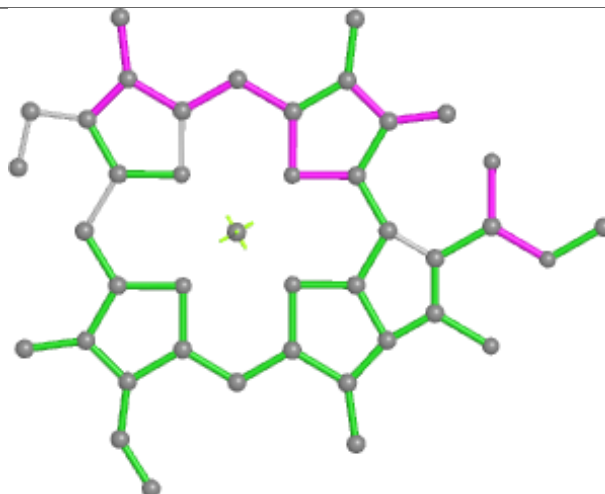


Rings

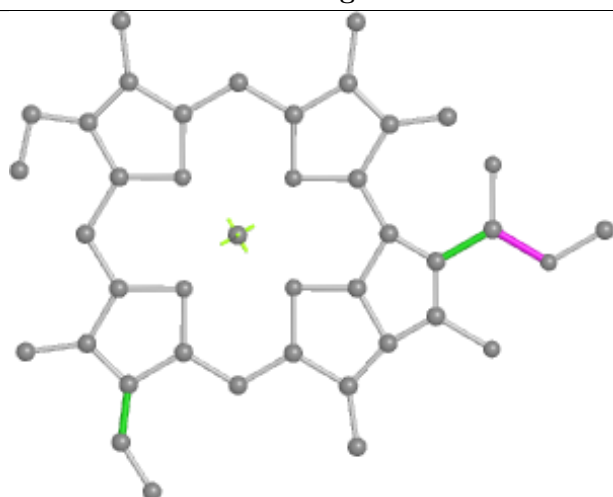
Ligand CLA F 304



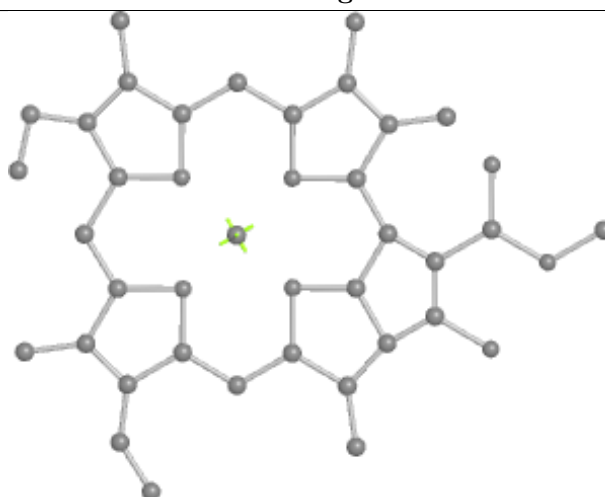
Bond lengths



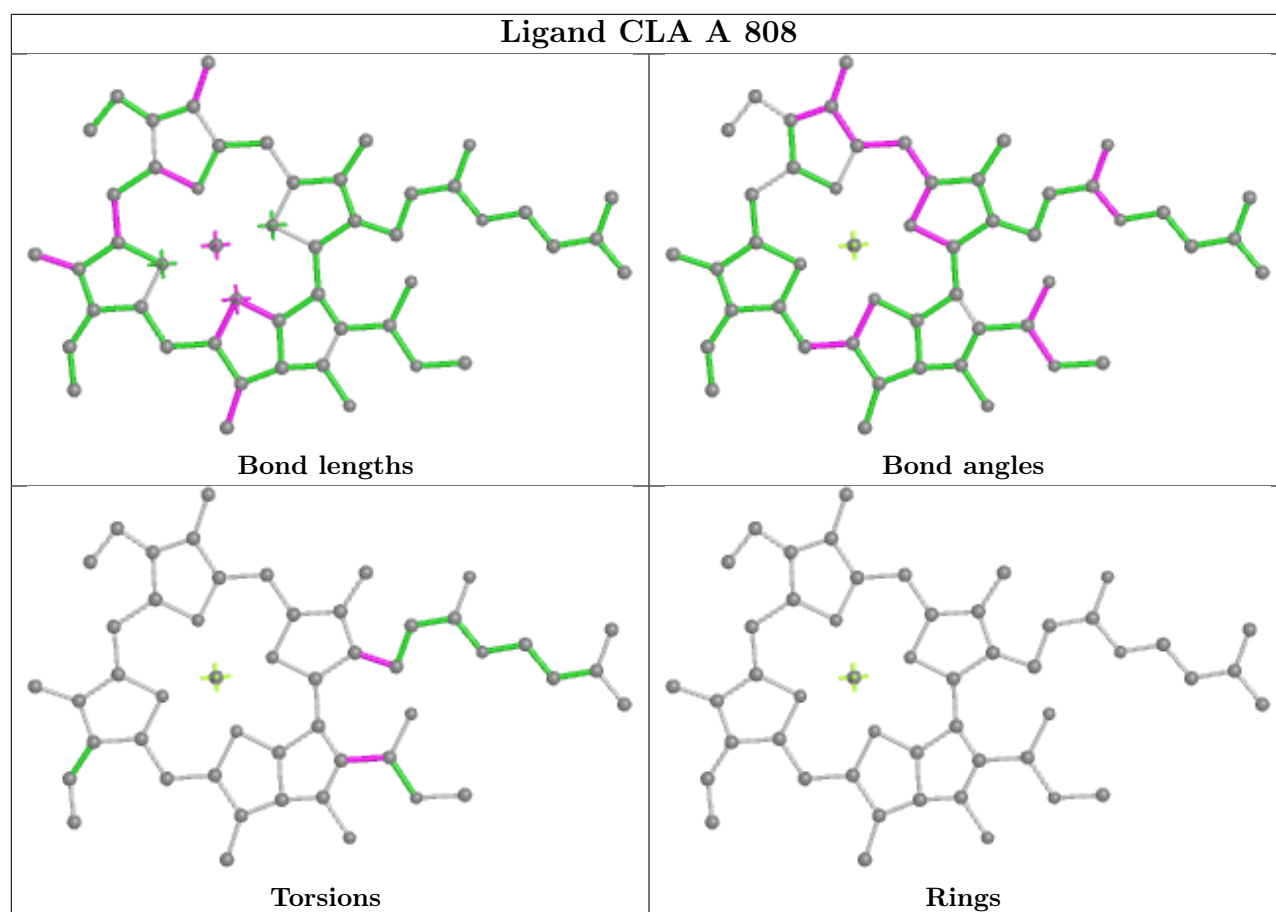
Bond angles



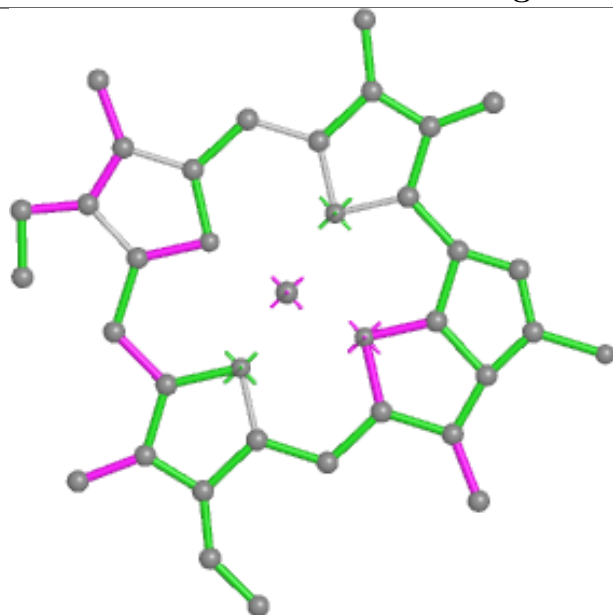
Torsions



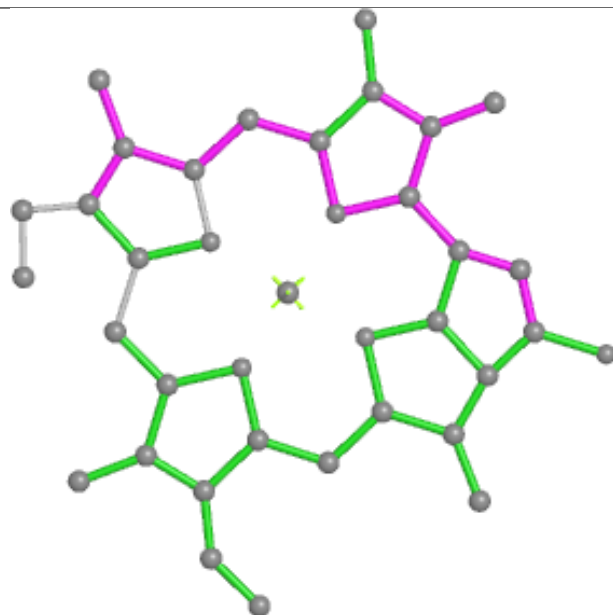
Rings



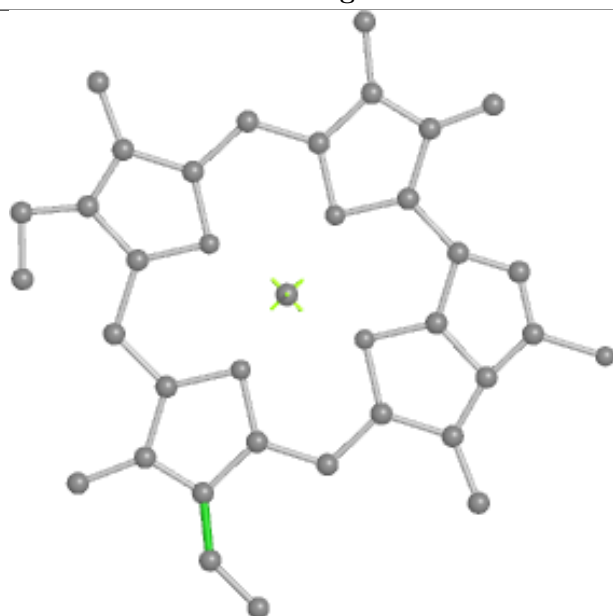
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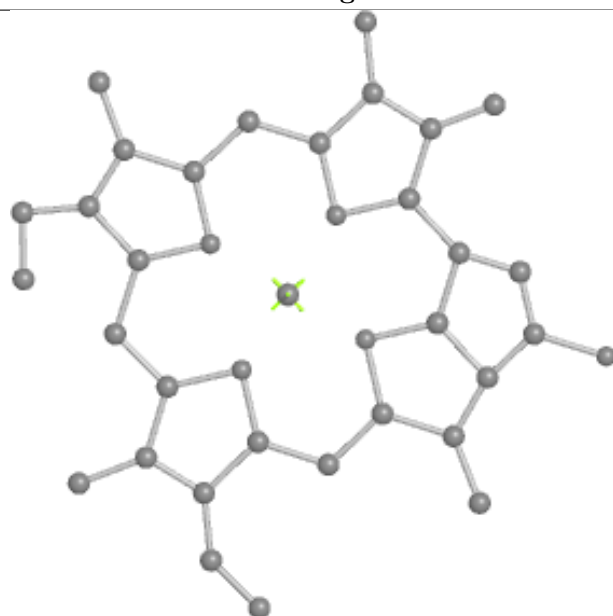
Bond lengths



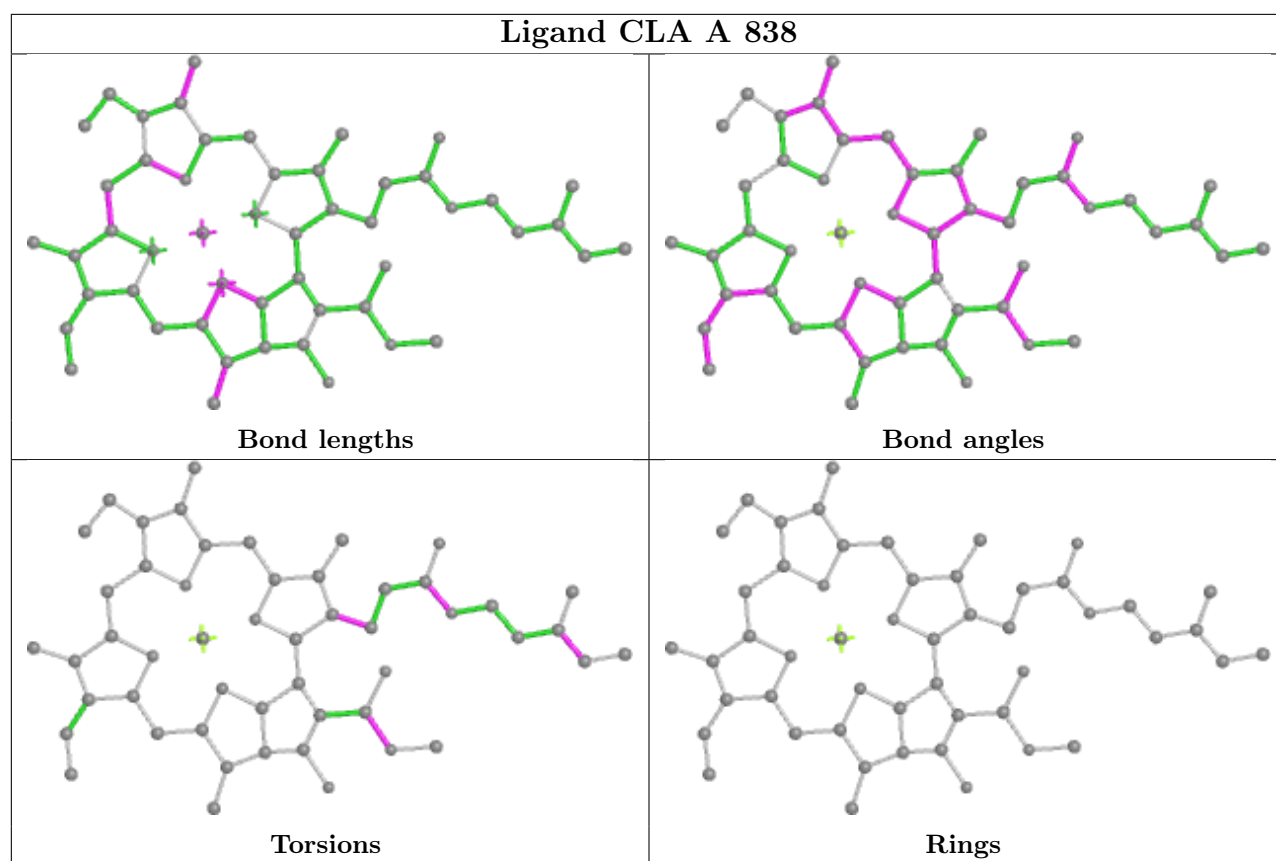
Bond angles



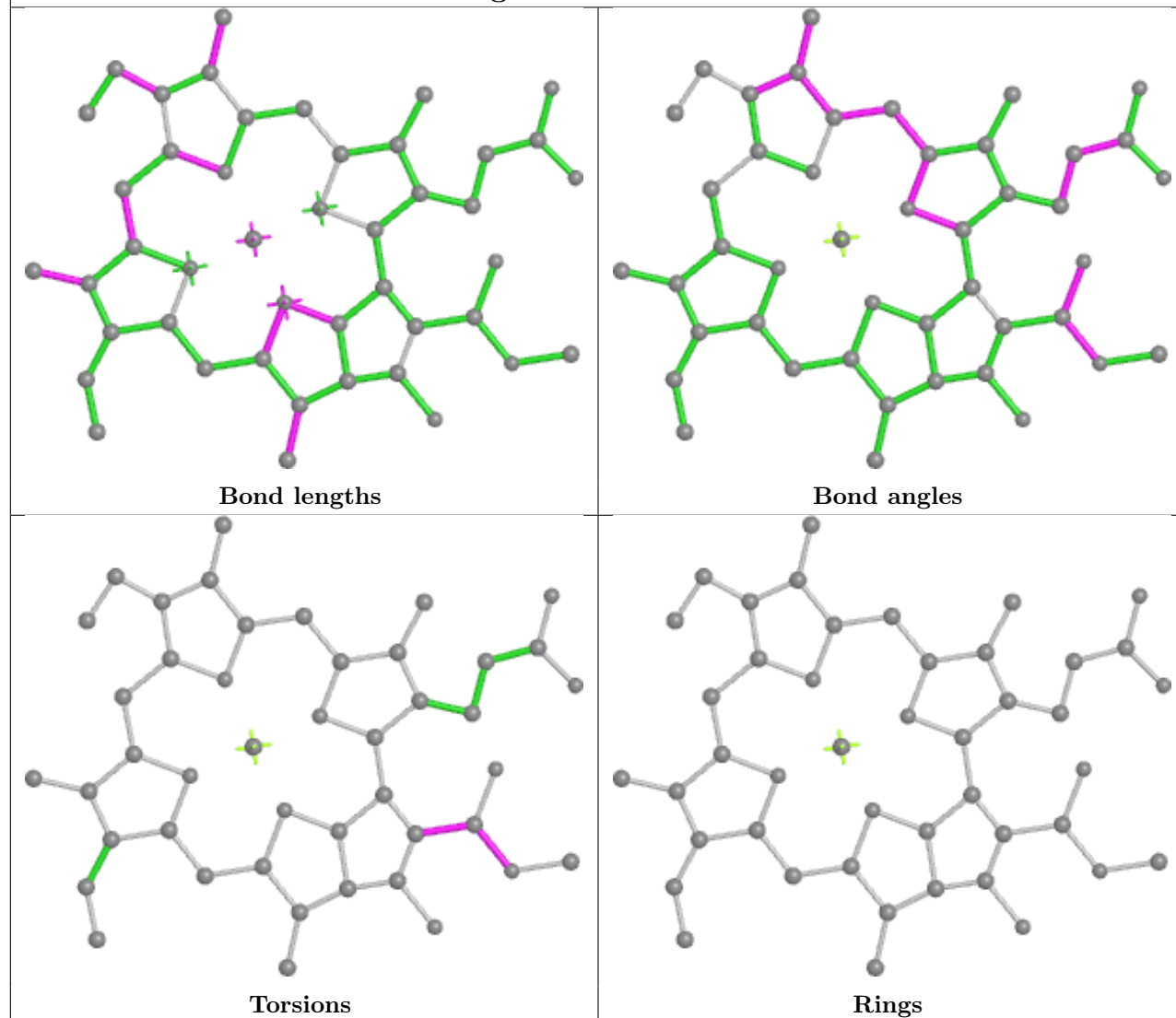
Torsions



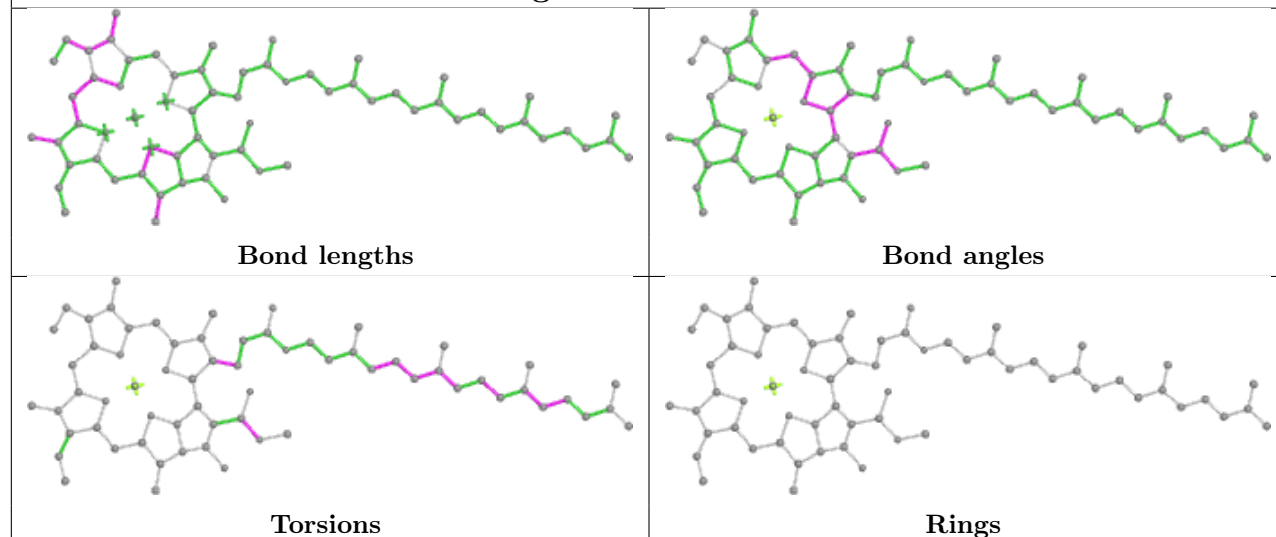
Rings



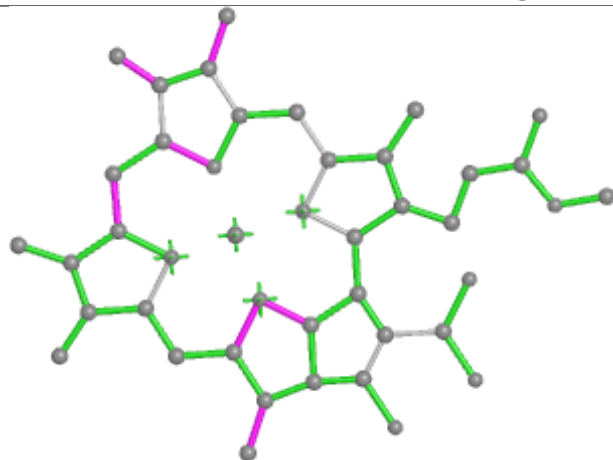
Ligand CLA B 823



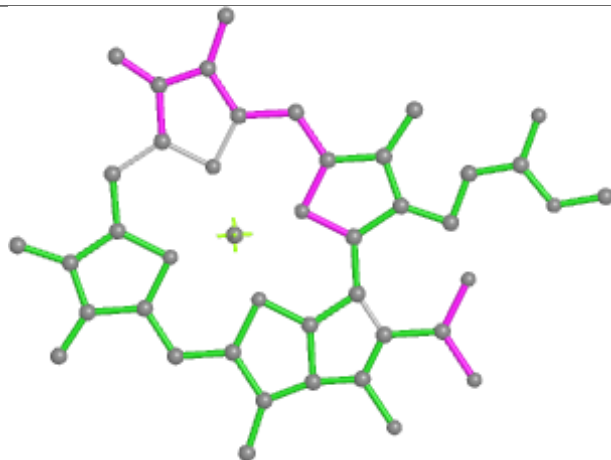
Ligand CLA B 840



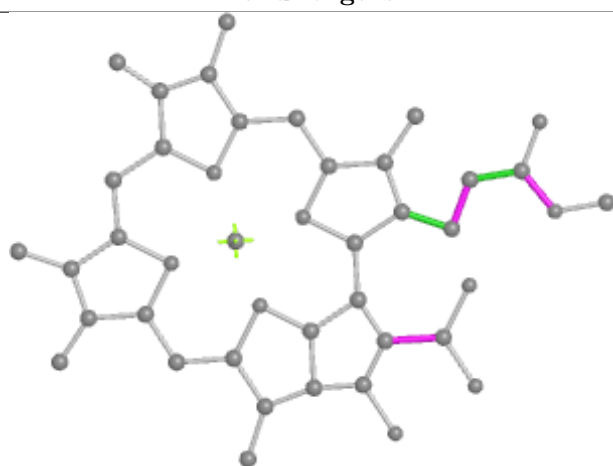
Ligand CLA Y 613



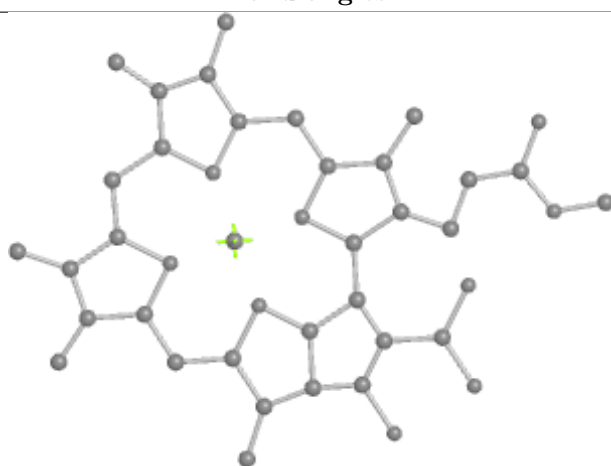
Bond lengths



Bond angles

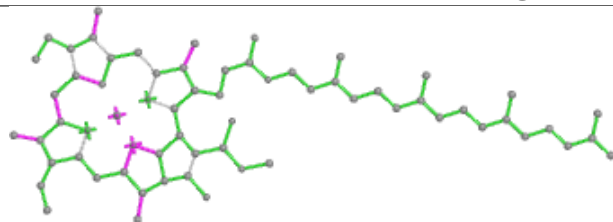


Torsions

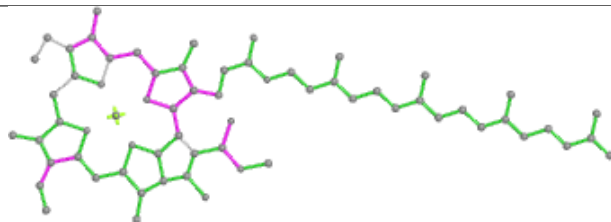


Rings

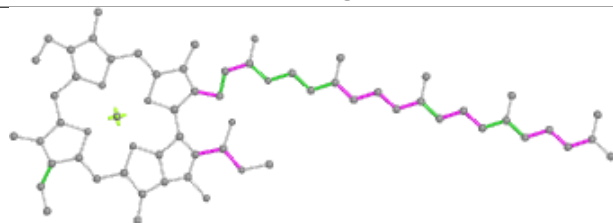
Ligand CLA A 806



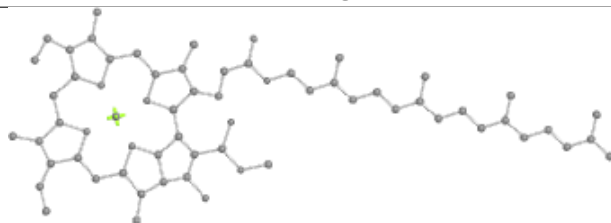
Bond lengths



Bond angles

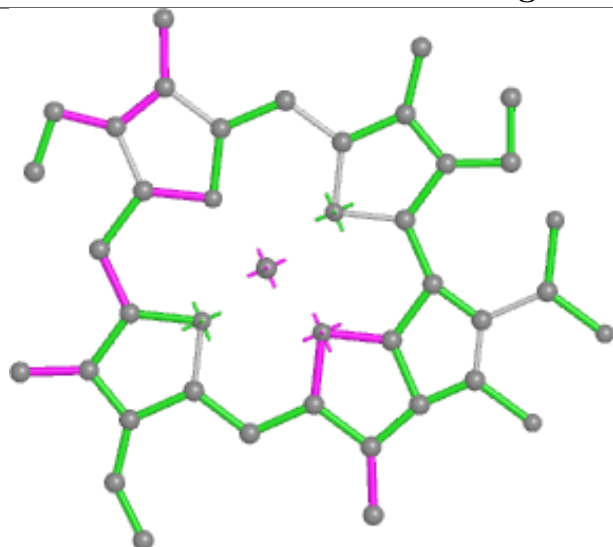


Torsions

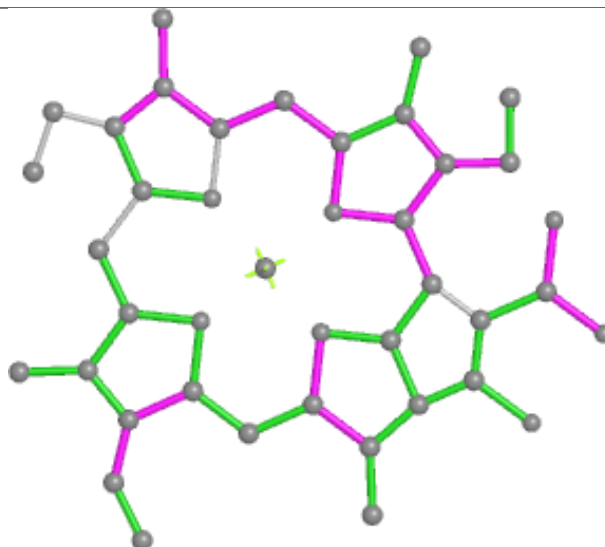


Rings

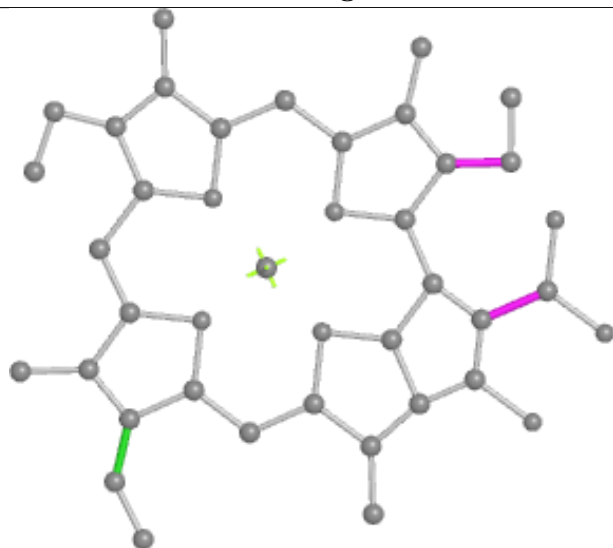
Ligand CLA 3 606



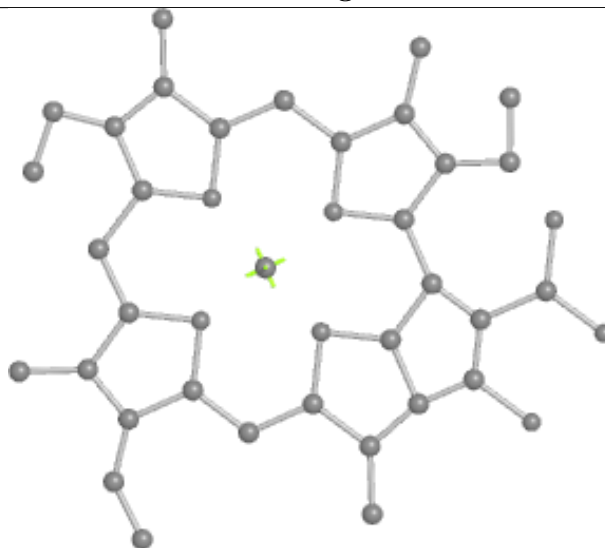
Bond lengths



Bond angles

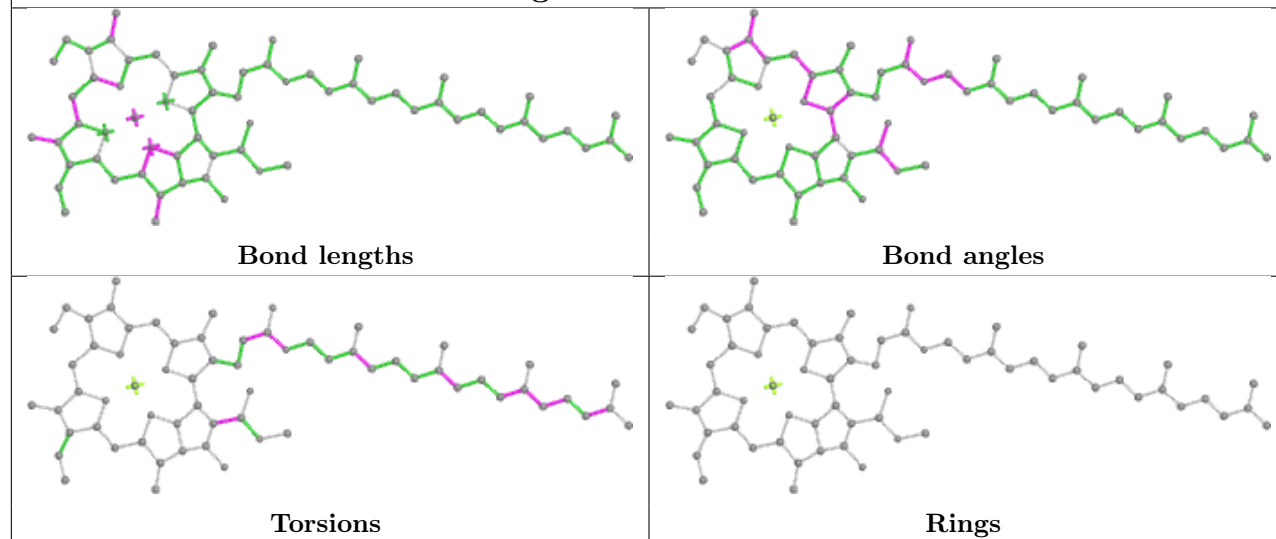


Torsions

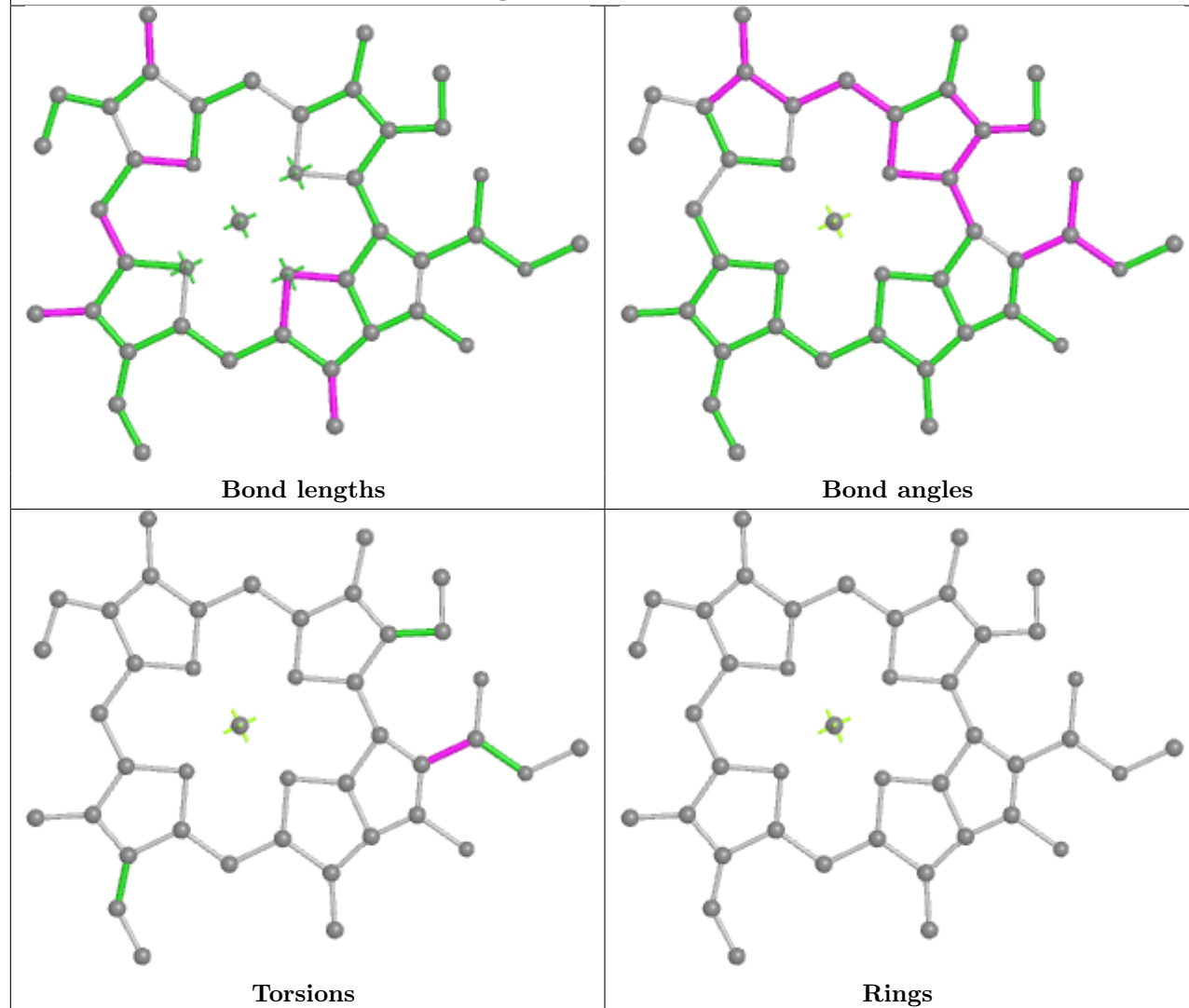


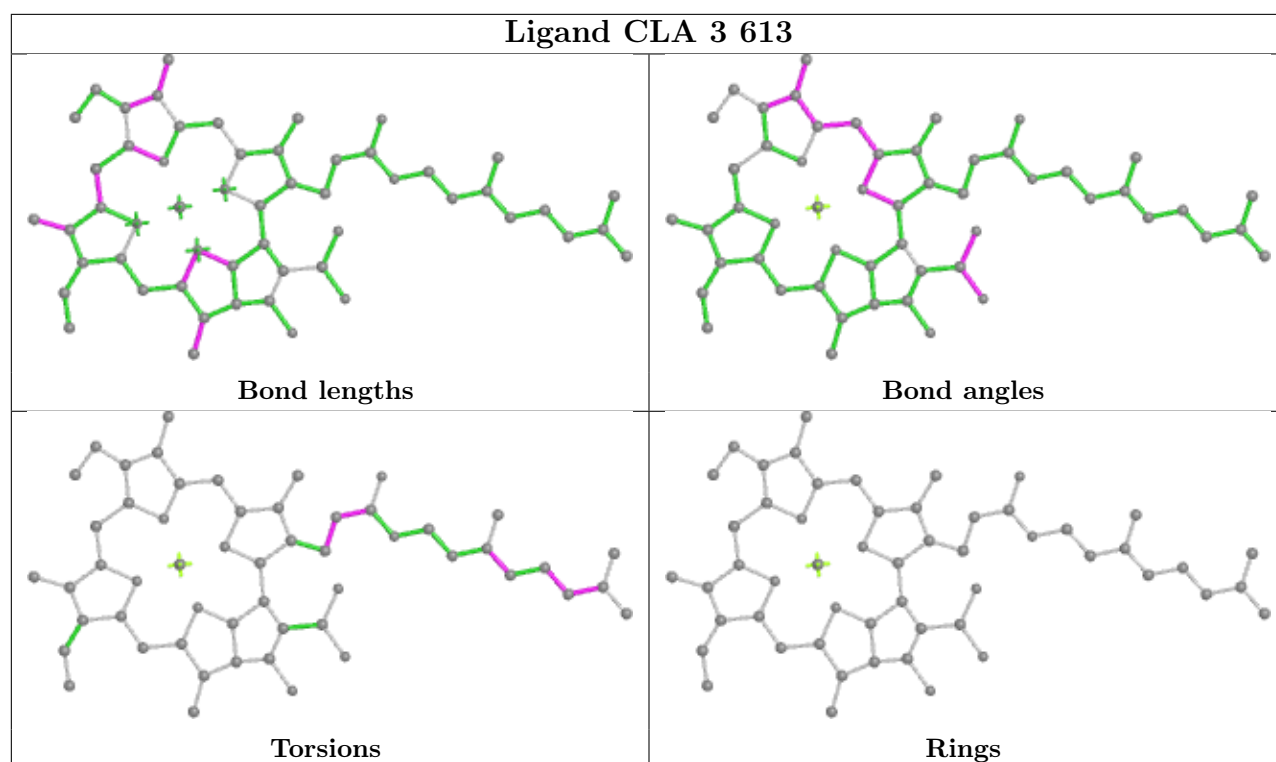
Rings

Ligand CLA A 826

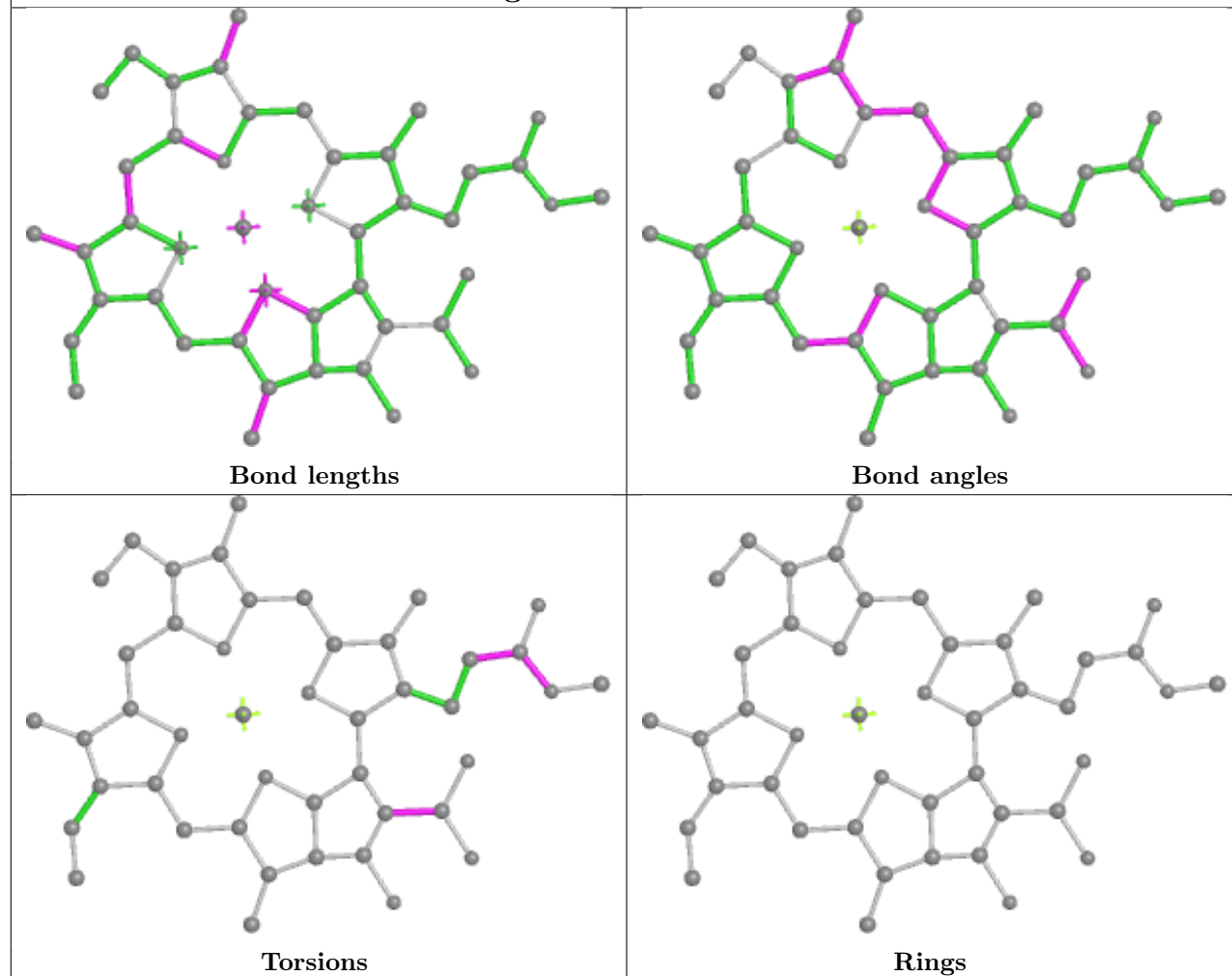


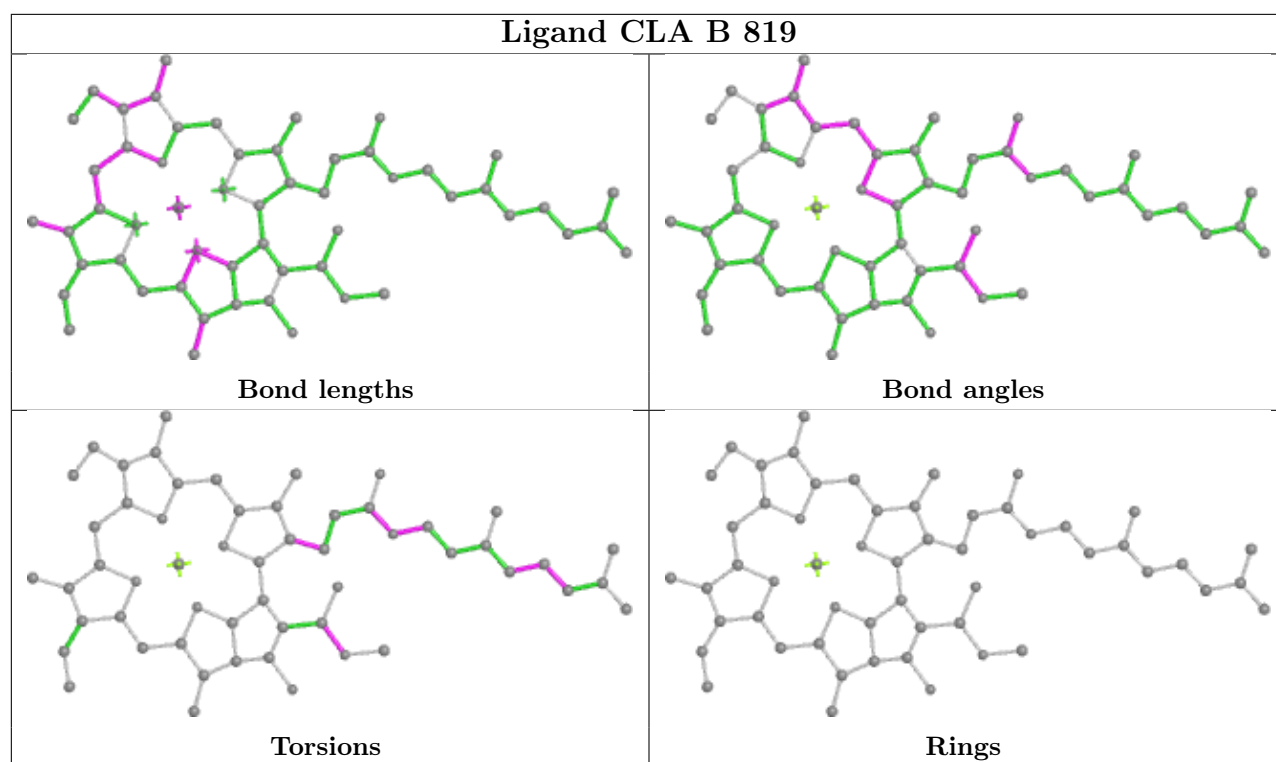
Ligand CLA G 203



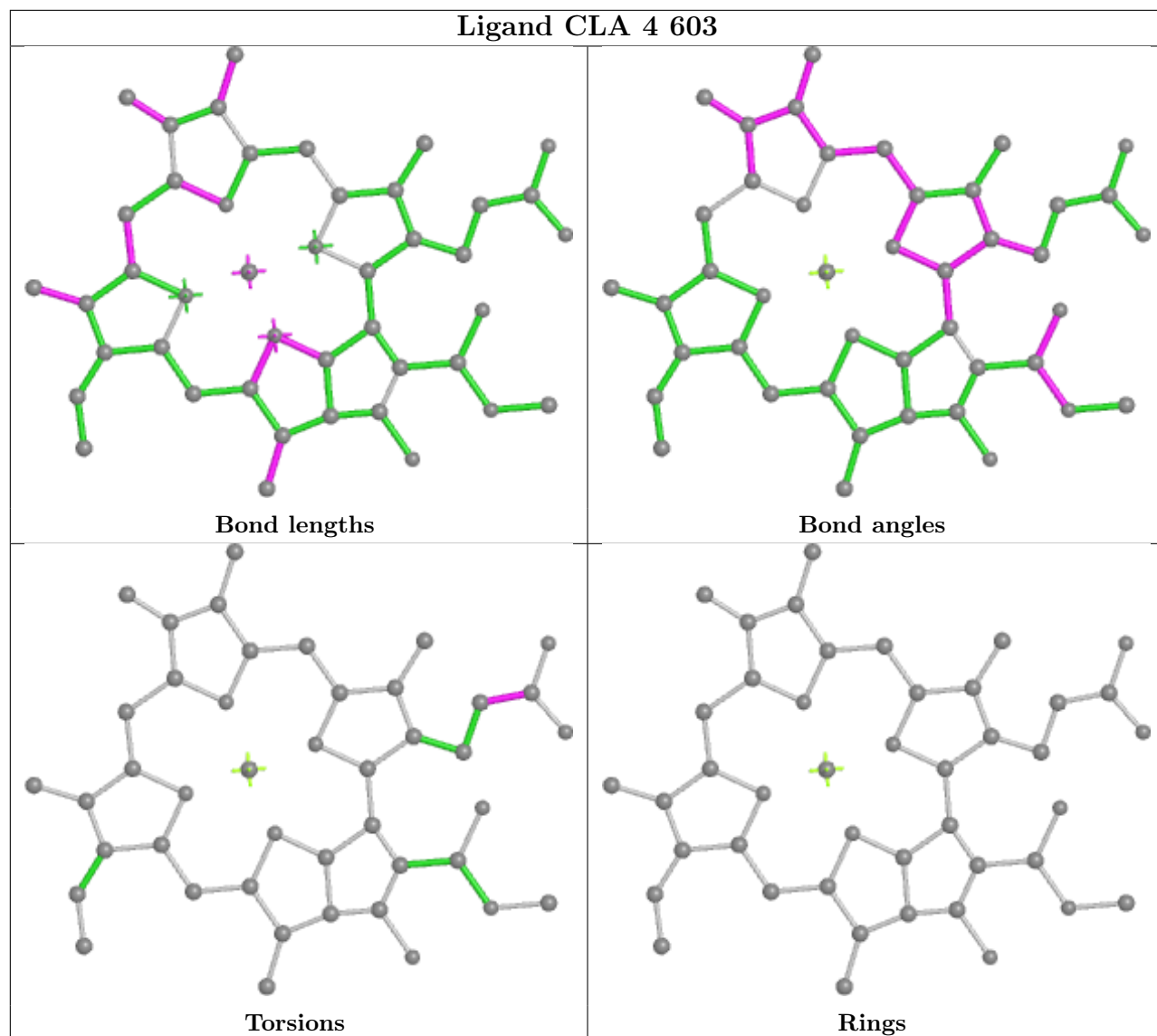


Ligand CLA N 1001

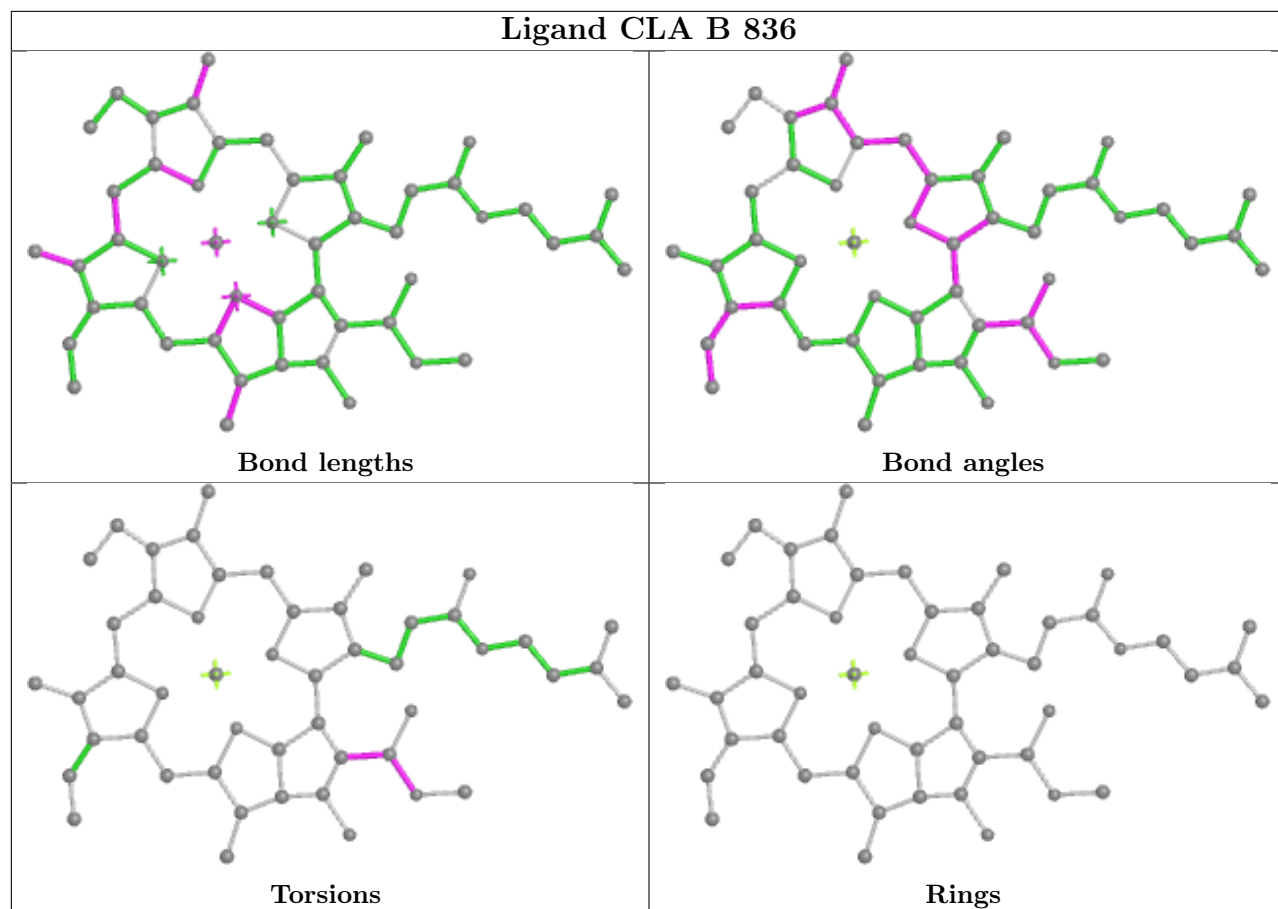




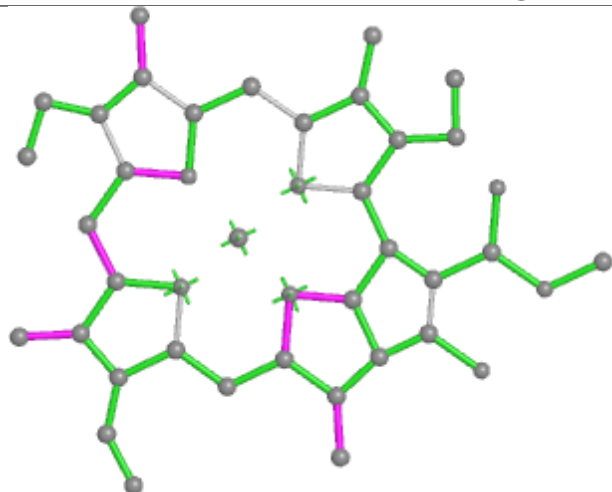
Ligand CLA 4 603



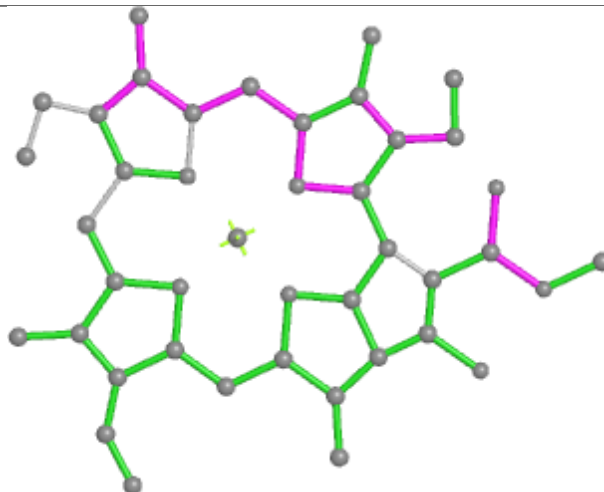
Ligand CLA B 836



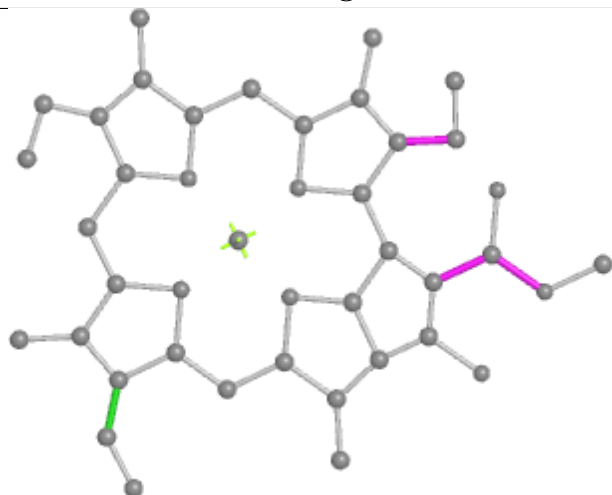
Ligand CLA A 823



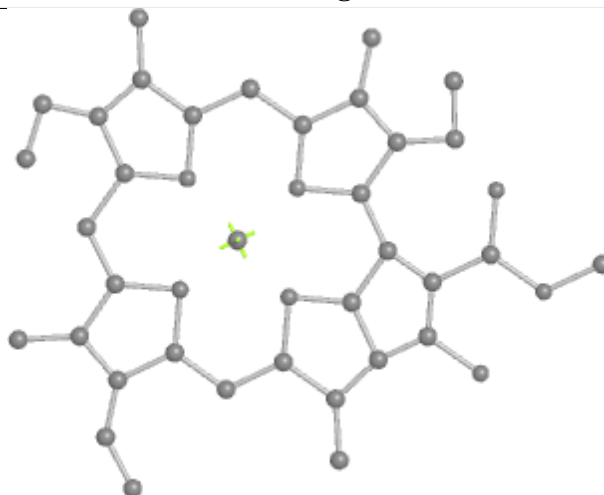
Bond lengths



Bond angles

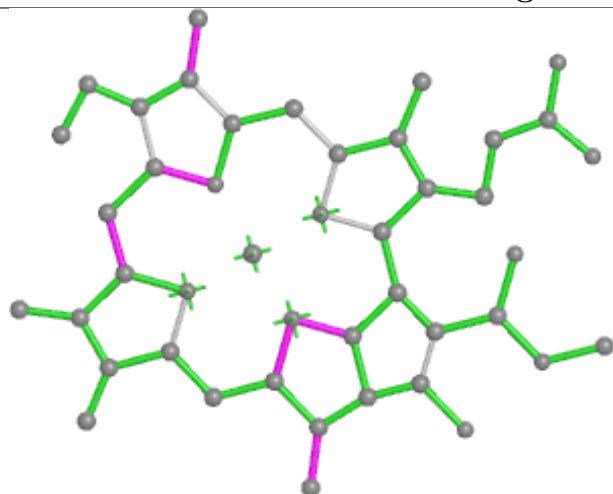


Torsions

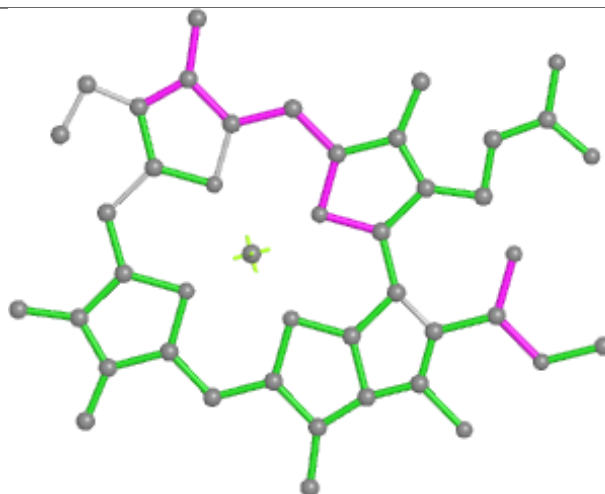


Rings

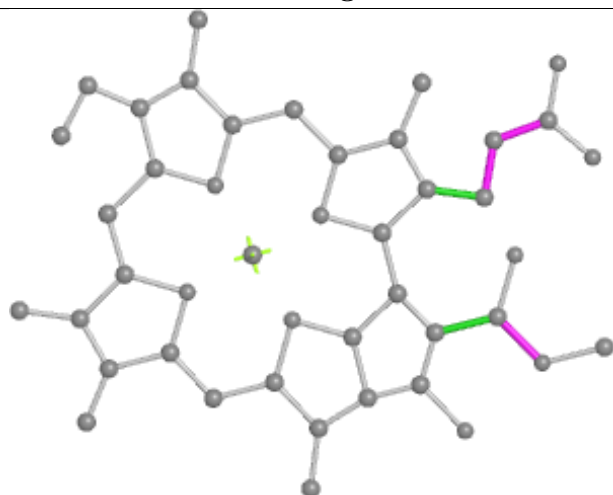
Ligand CLA Z 614



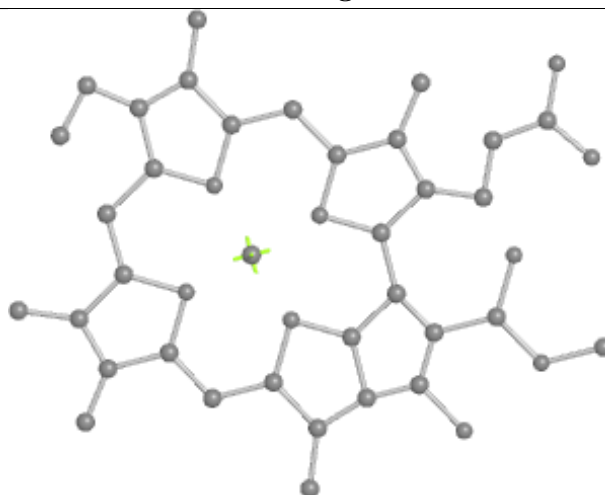
Bond lengths



Bond angles

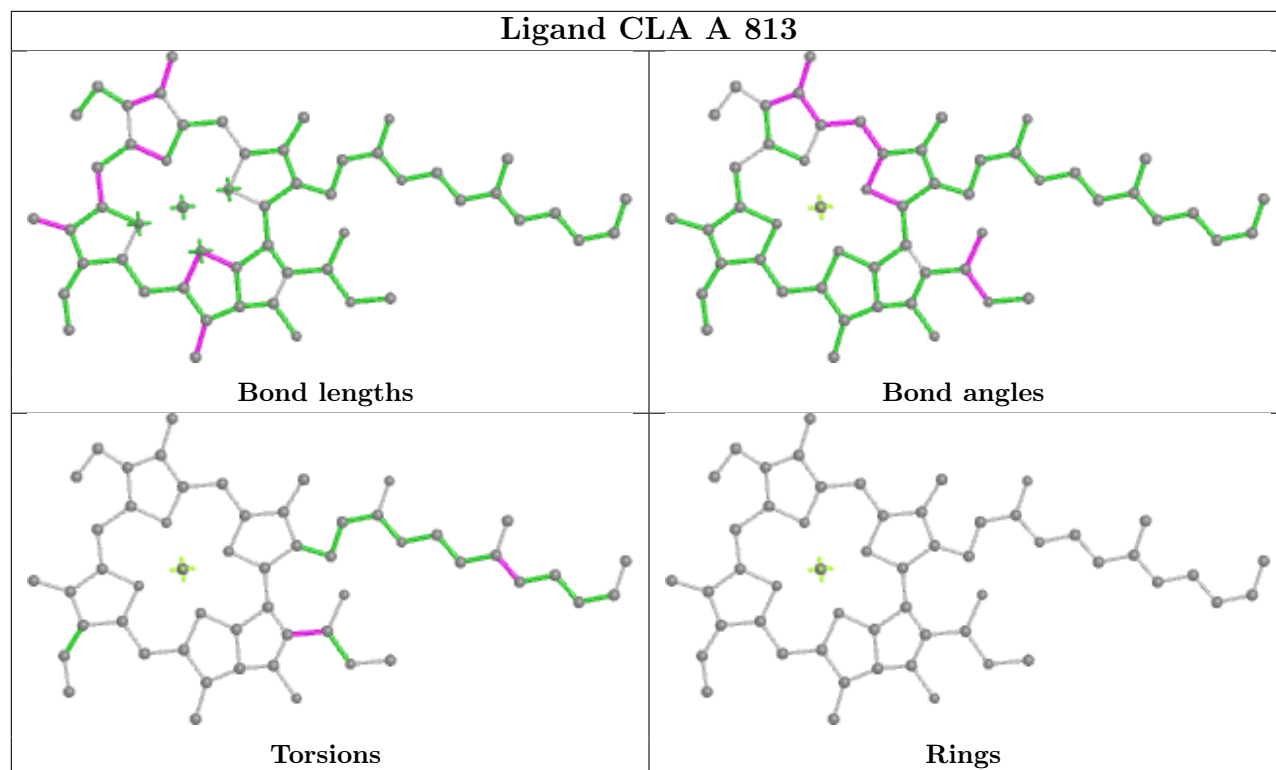


Torsions

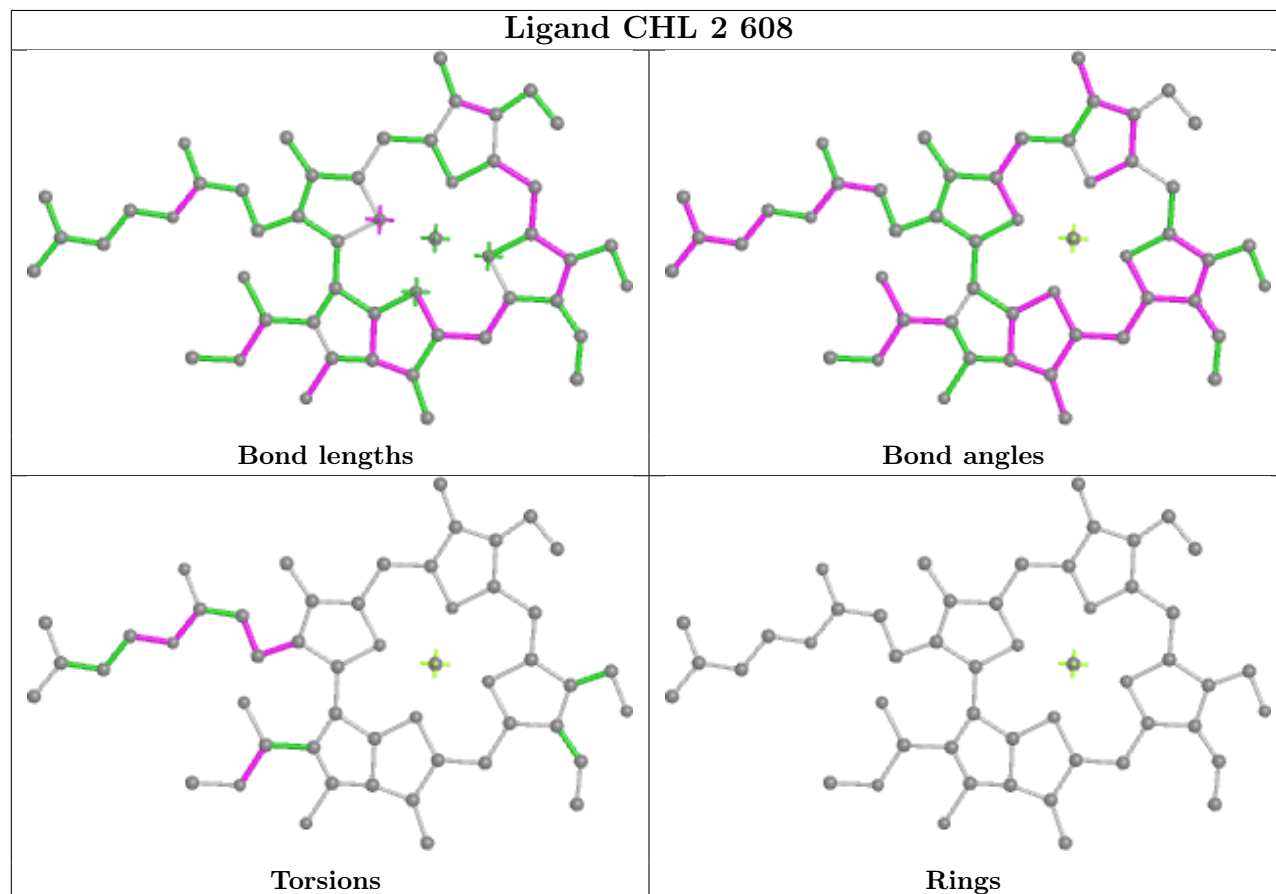


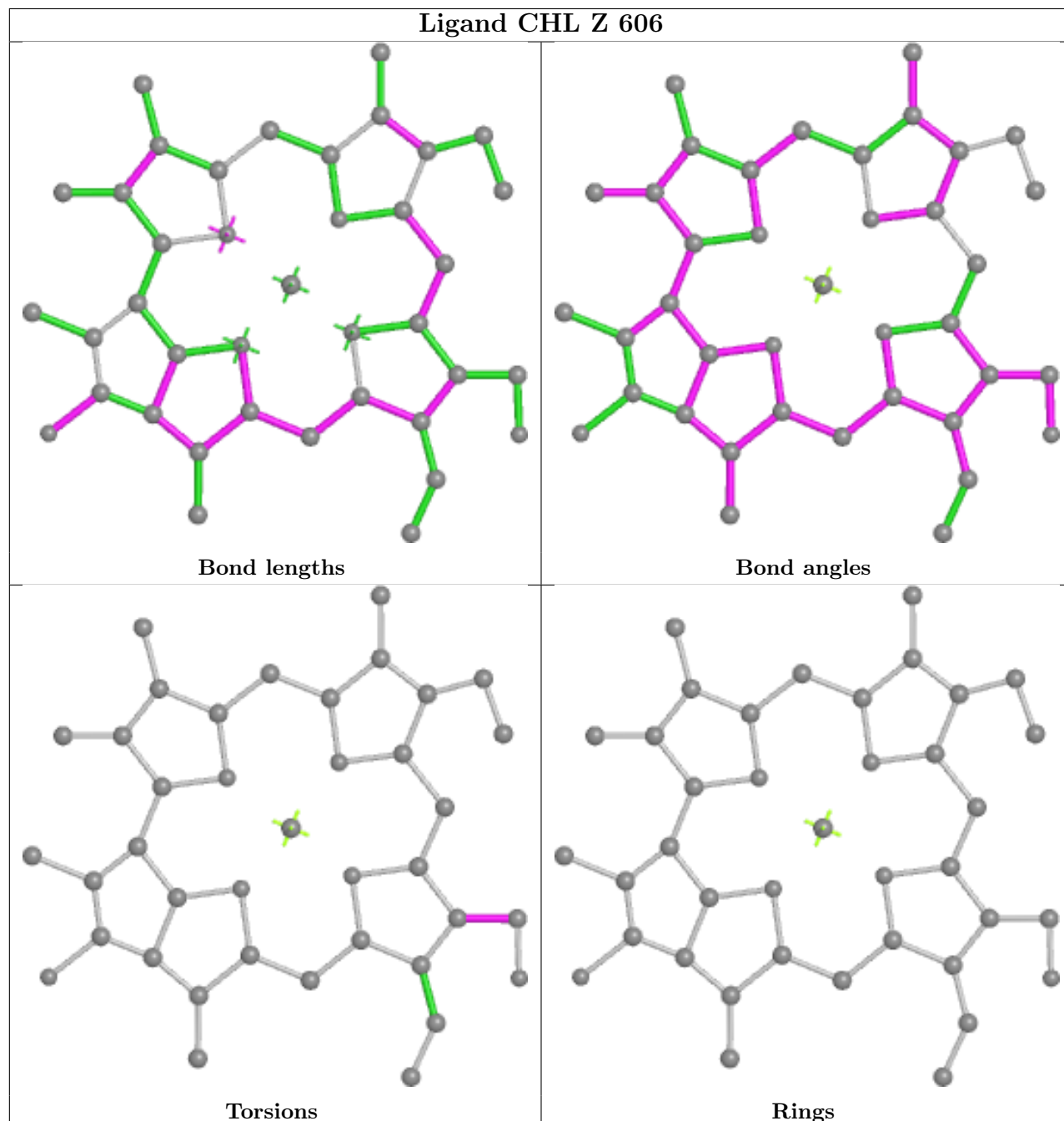
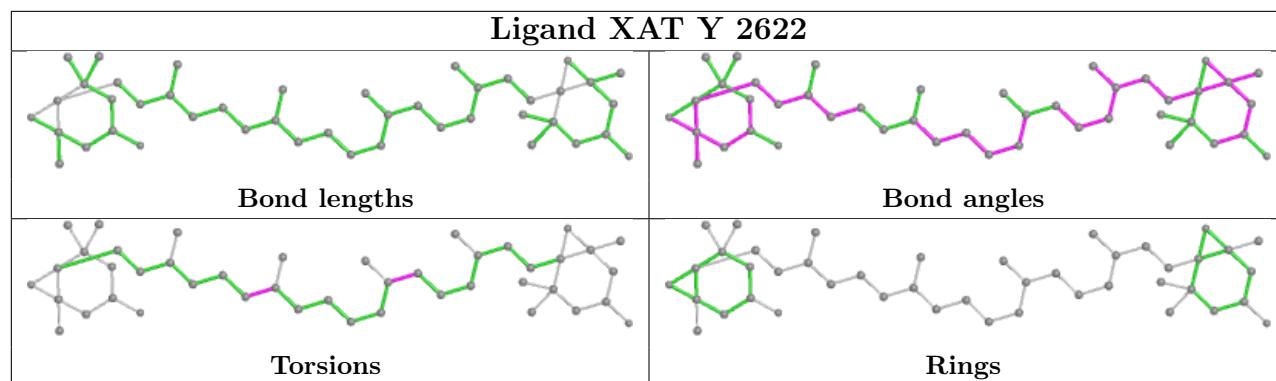
Rings

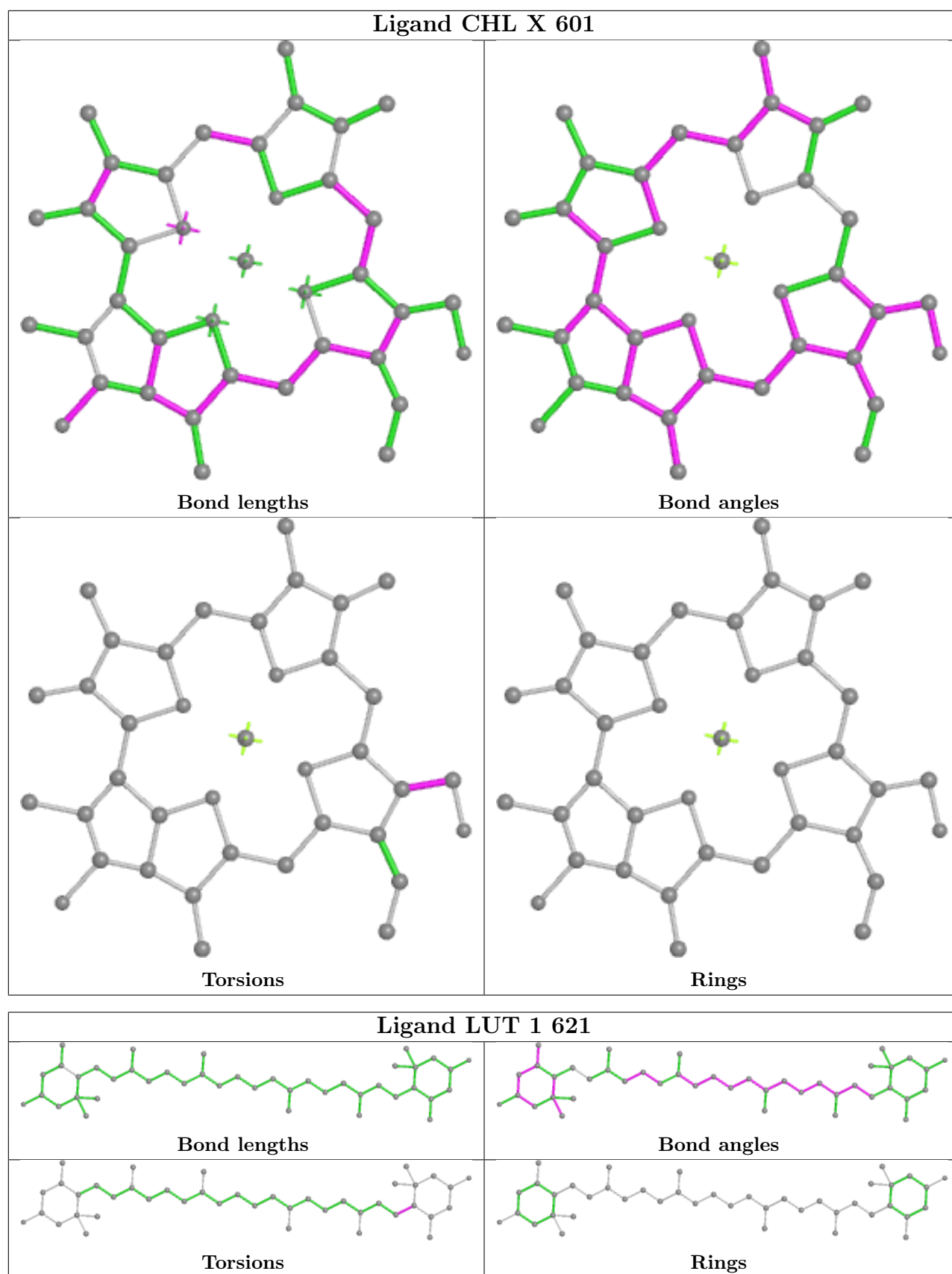
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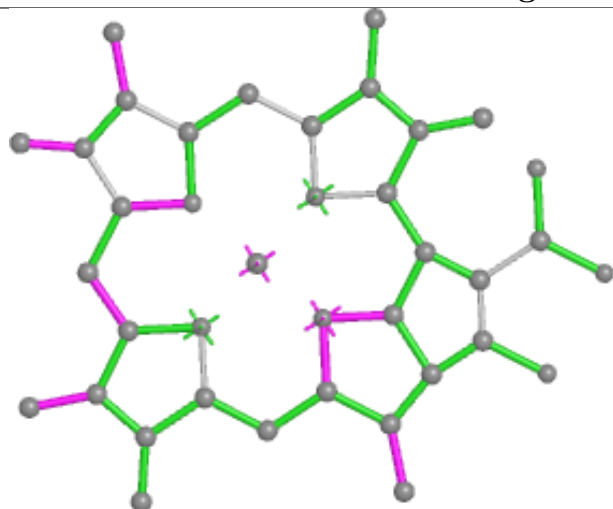
Ligand CHL 2 608



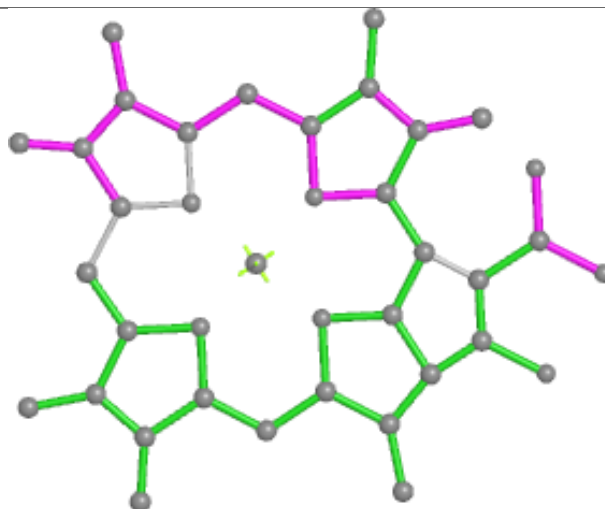




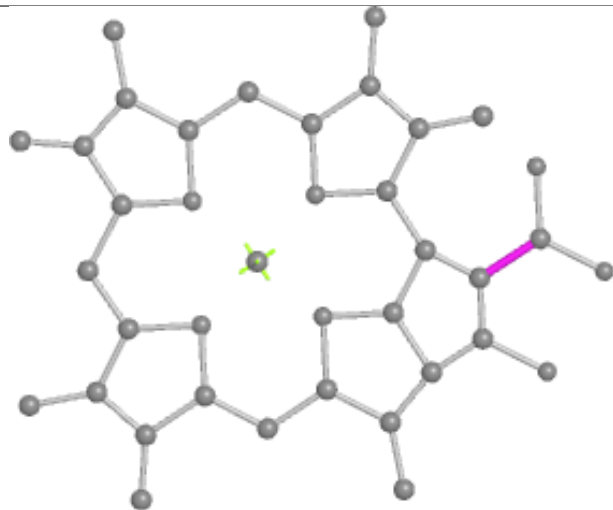
Ligand CLA 1 611



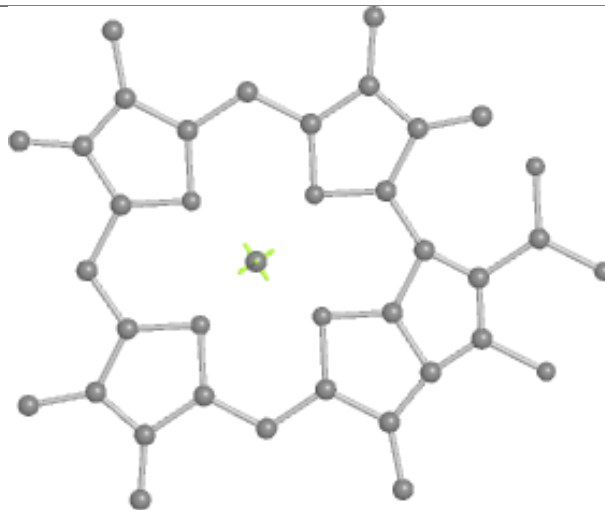
Bond lengths



Bond angles

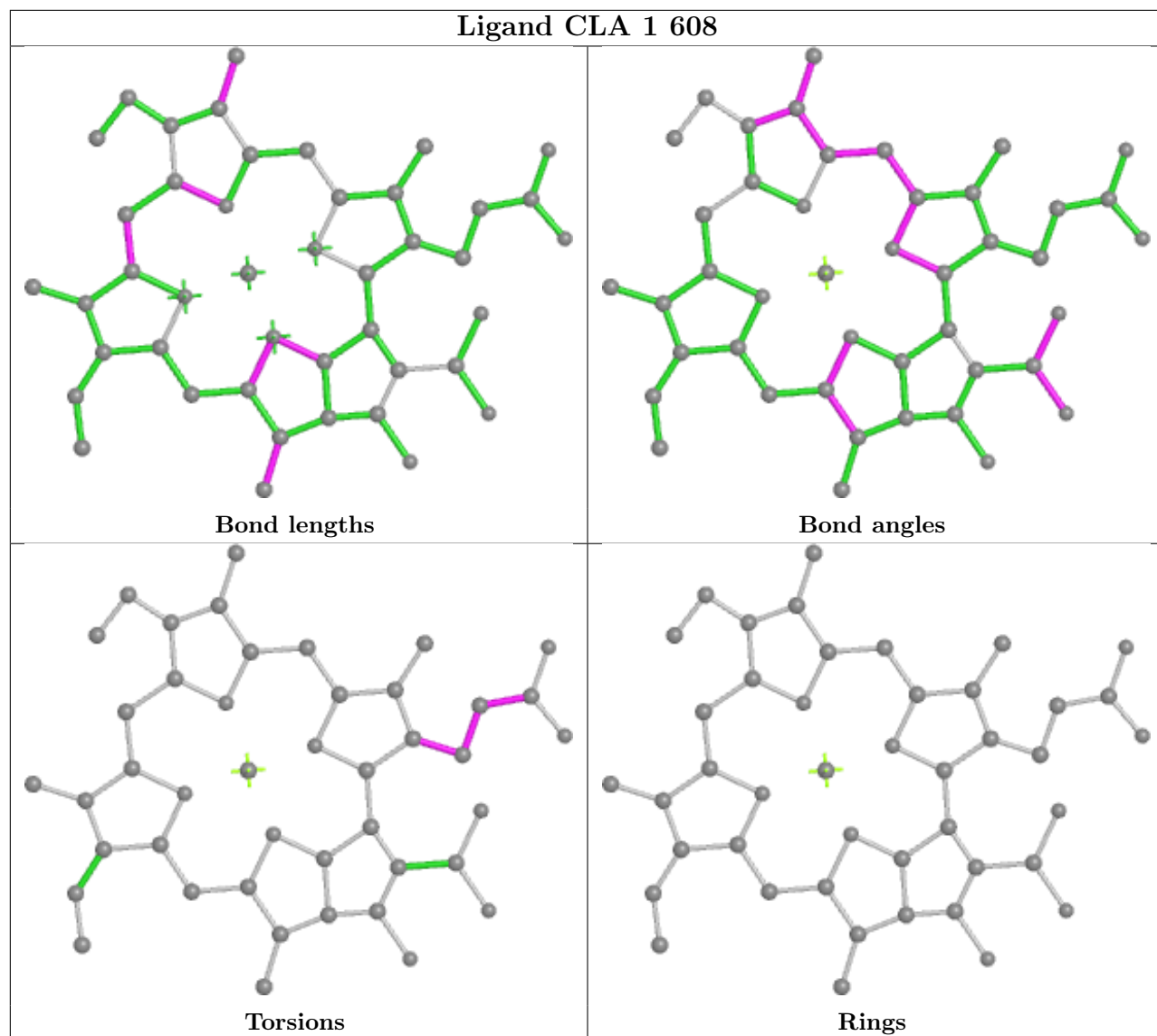


Torsions

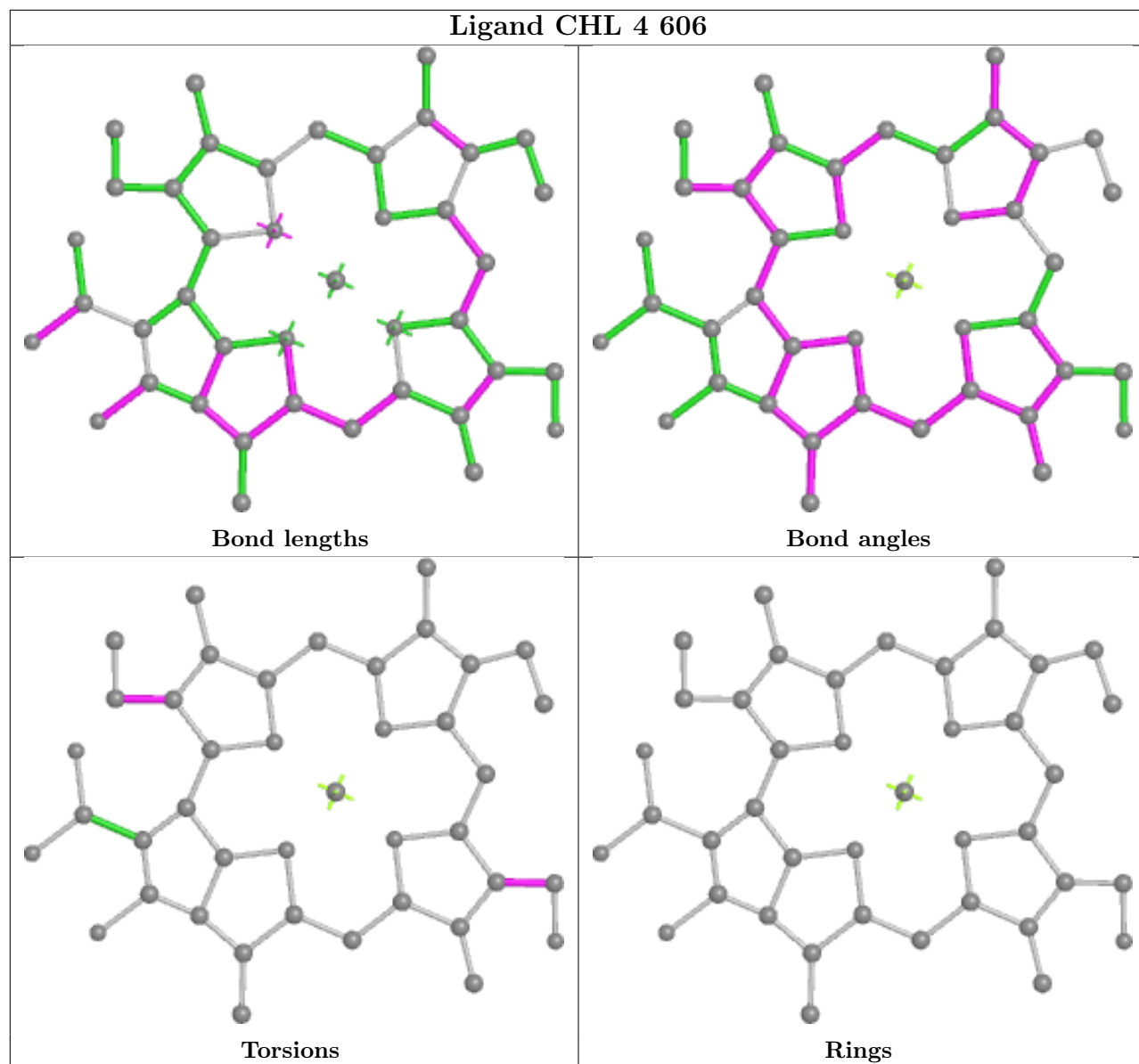


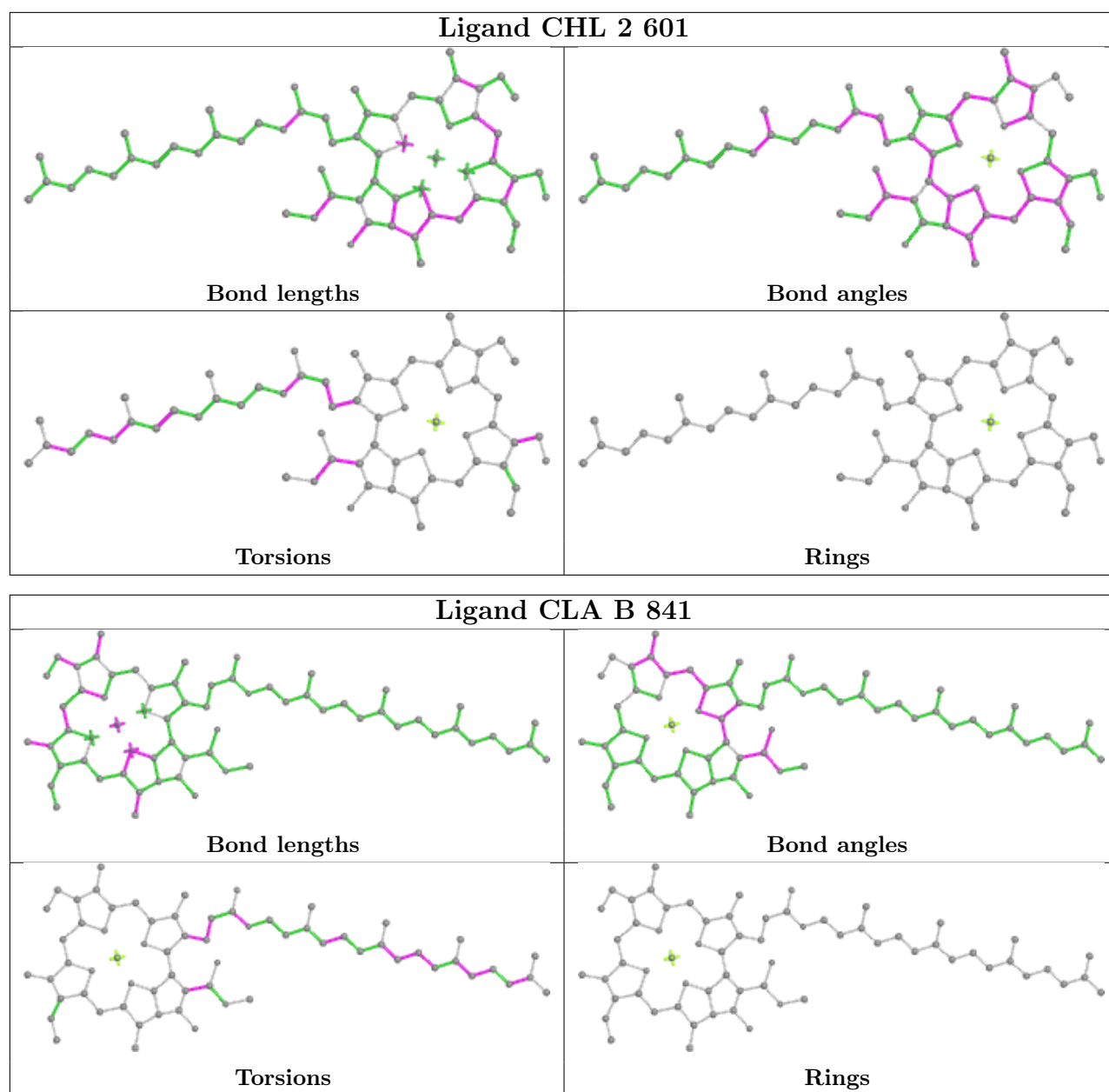
Rings

Ligand CLA 1 608

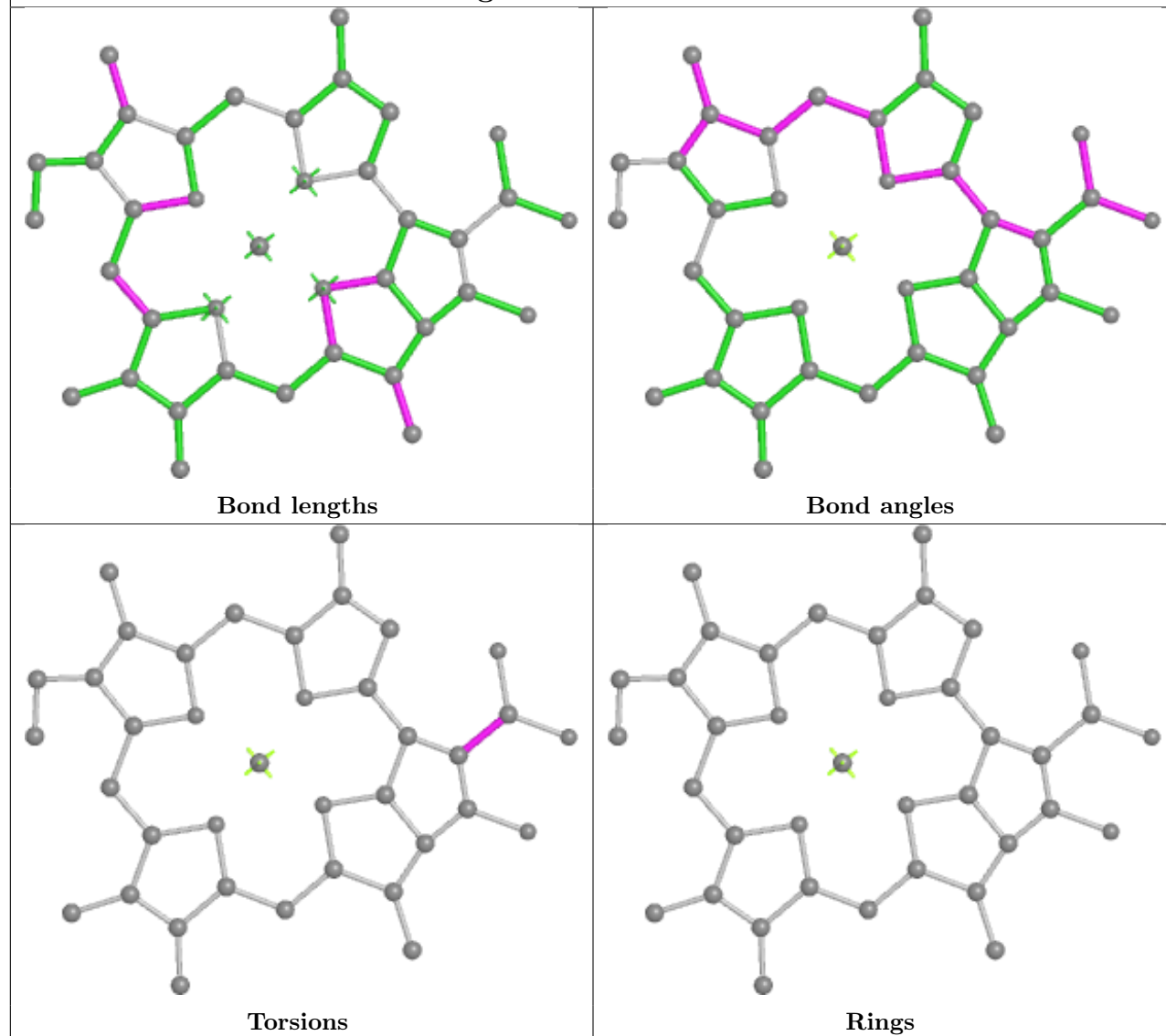


Ligand CHL 4 606

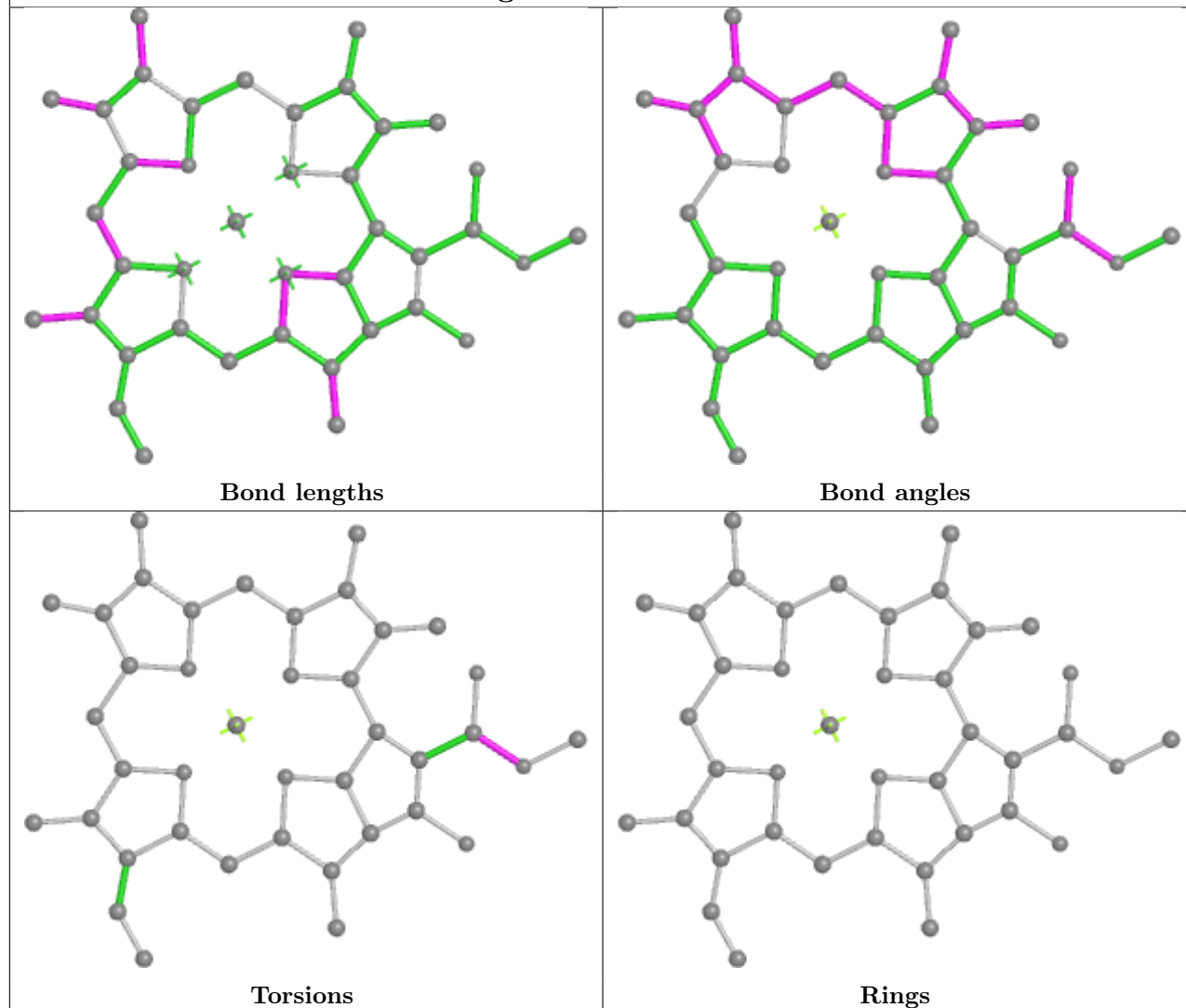




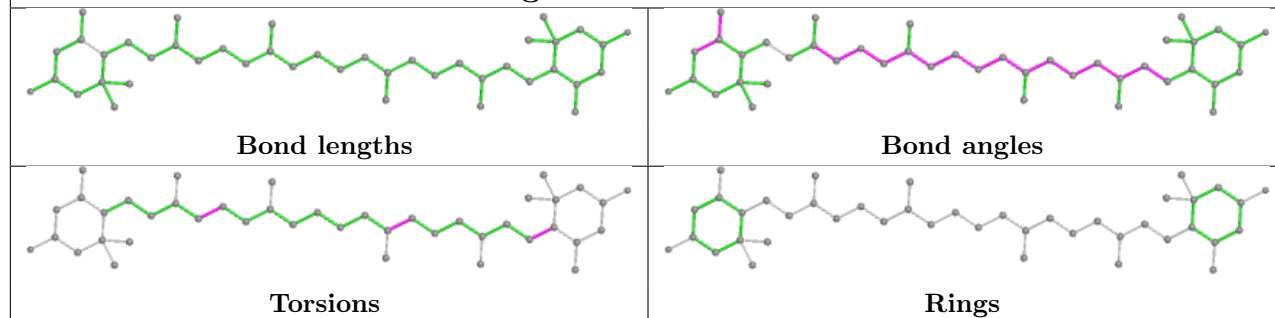
Ligand CLA O 2001



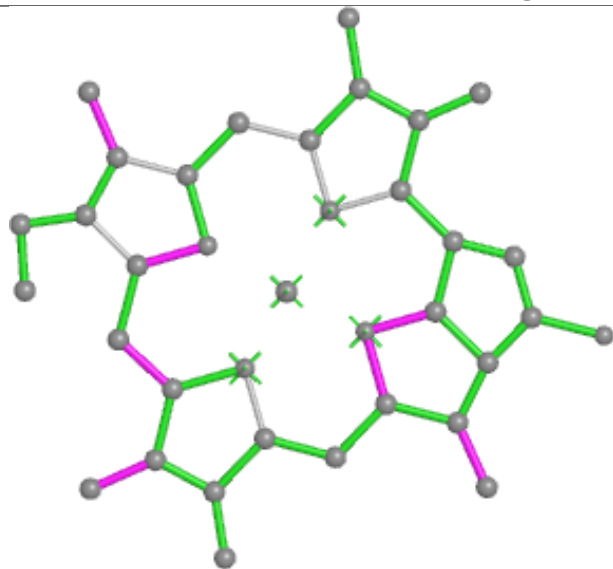
Ligand CLA 1 609



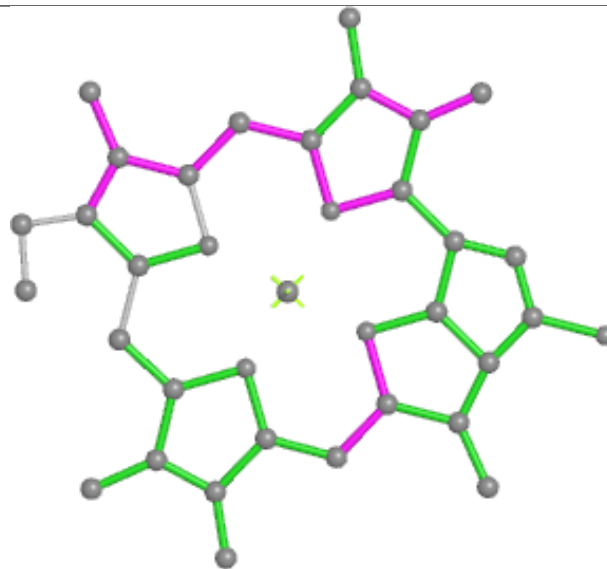
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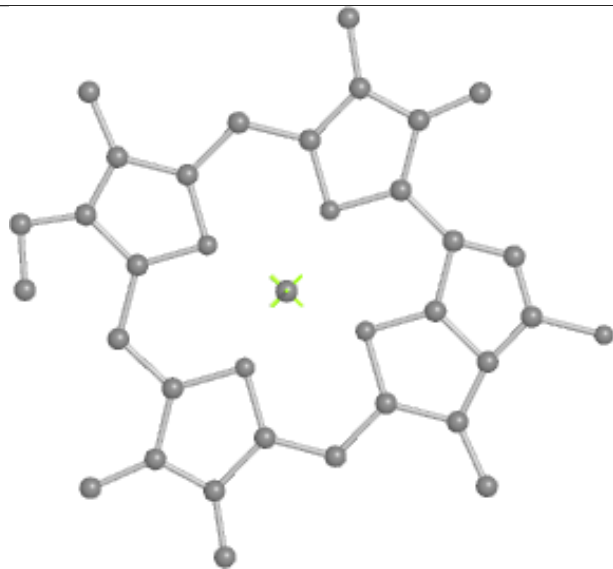
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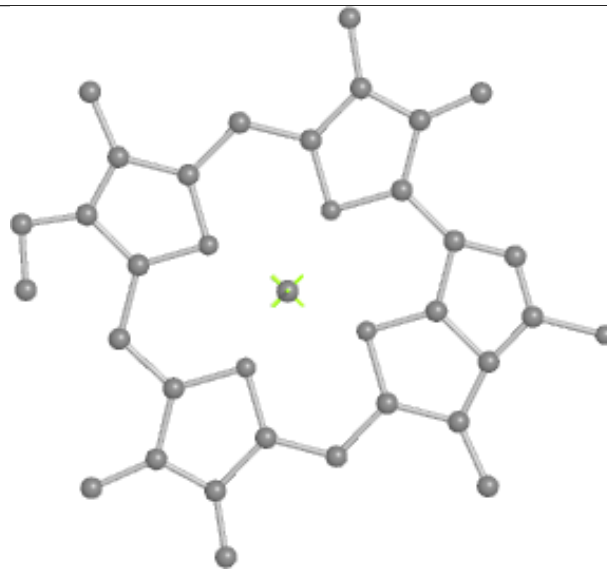
Bond lengths



Bond angles

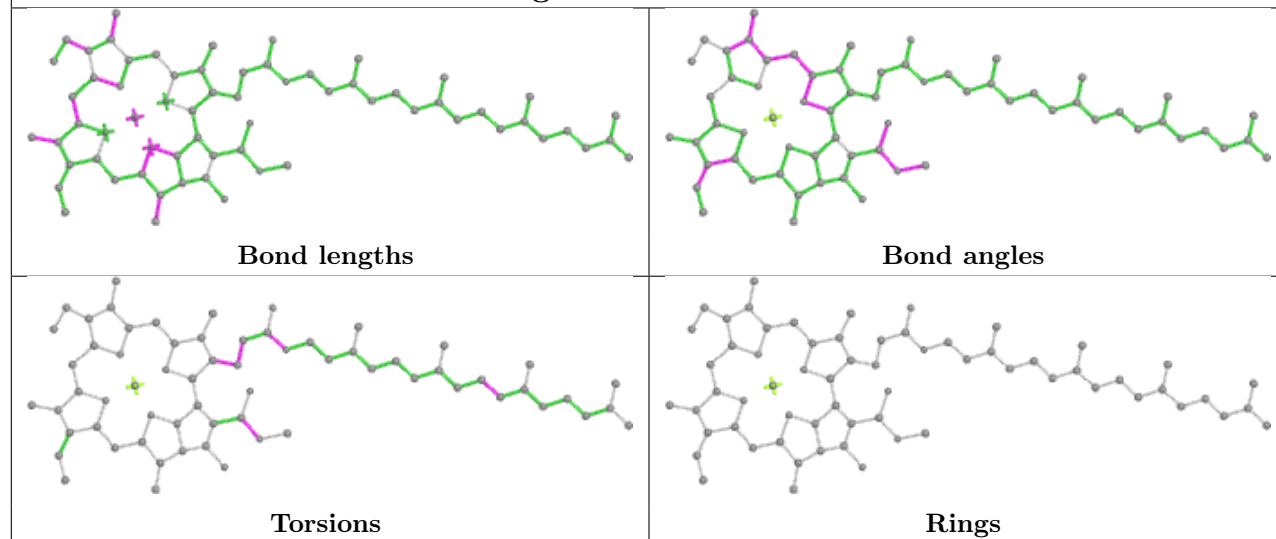


Torsions

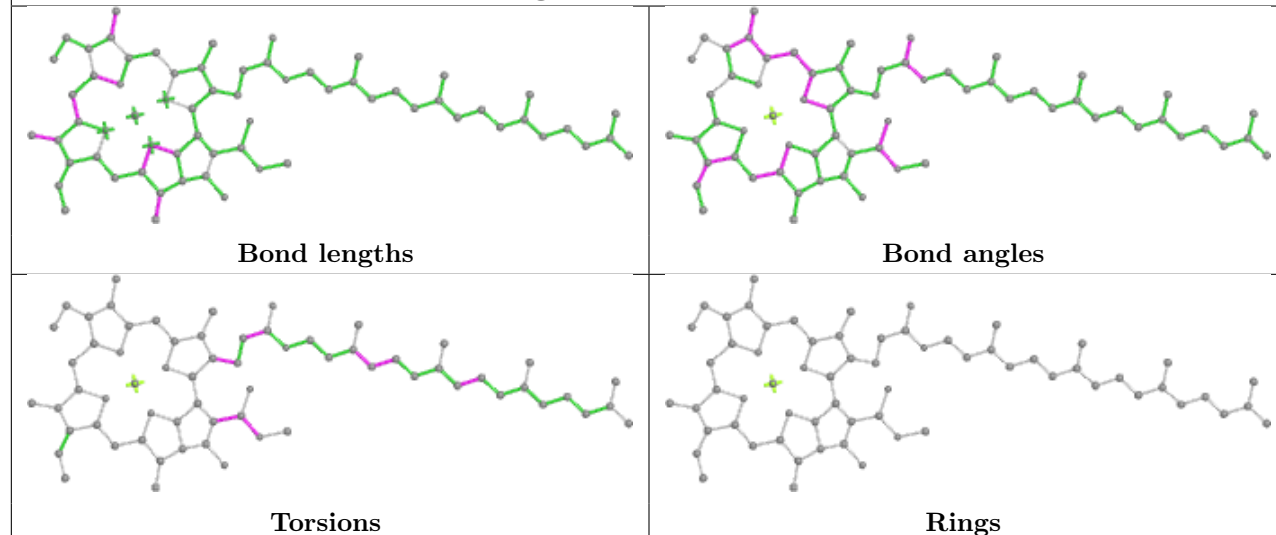


Rings

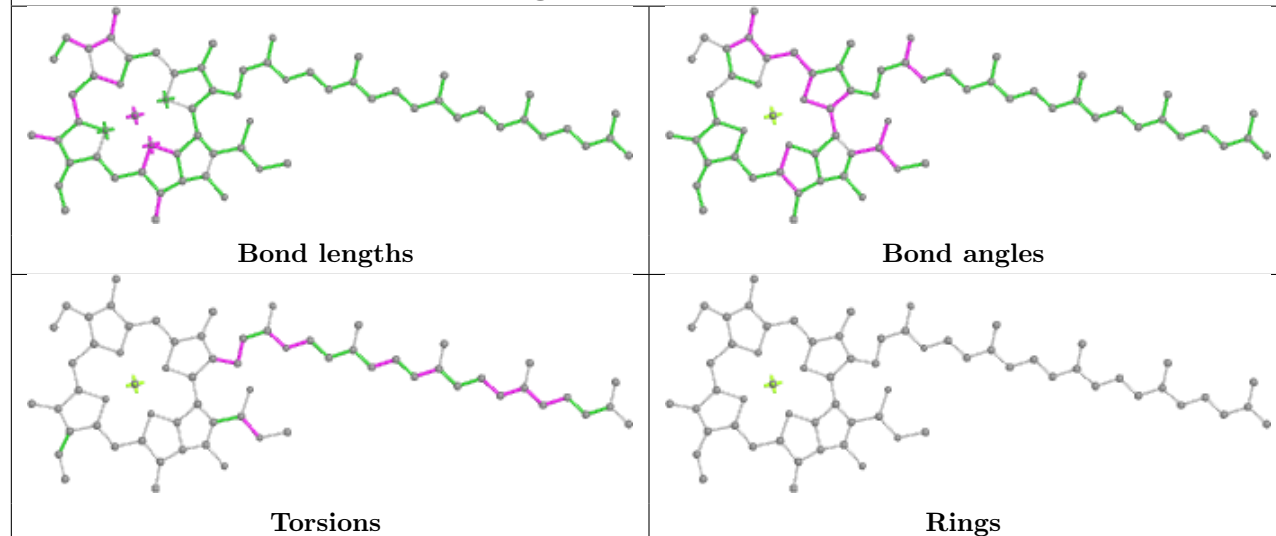
Ligand CLA B 814

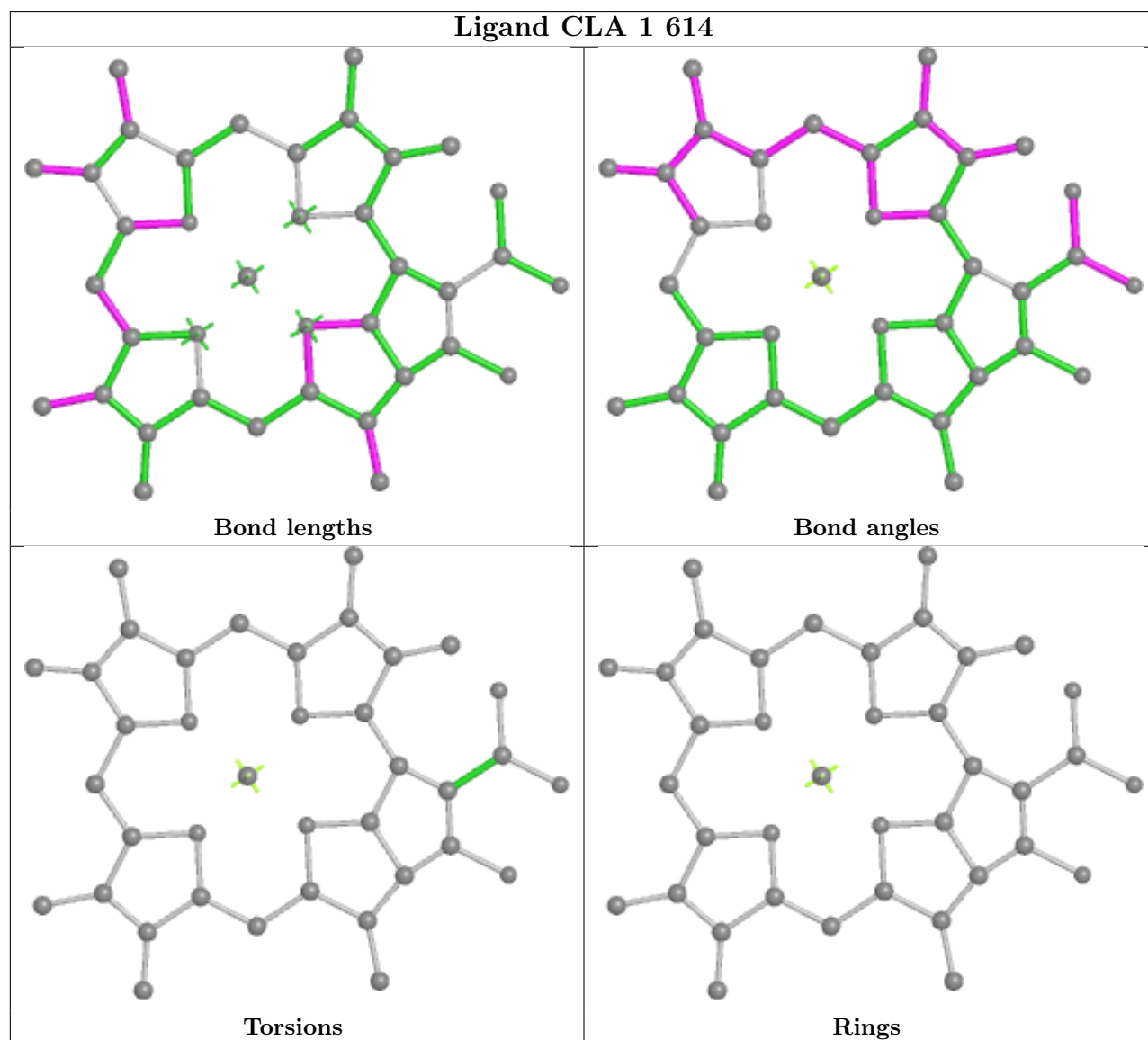
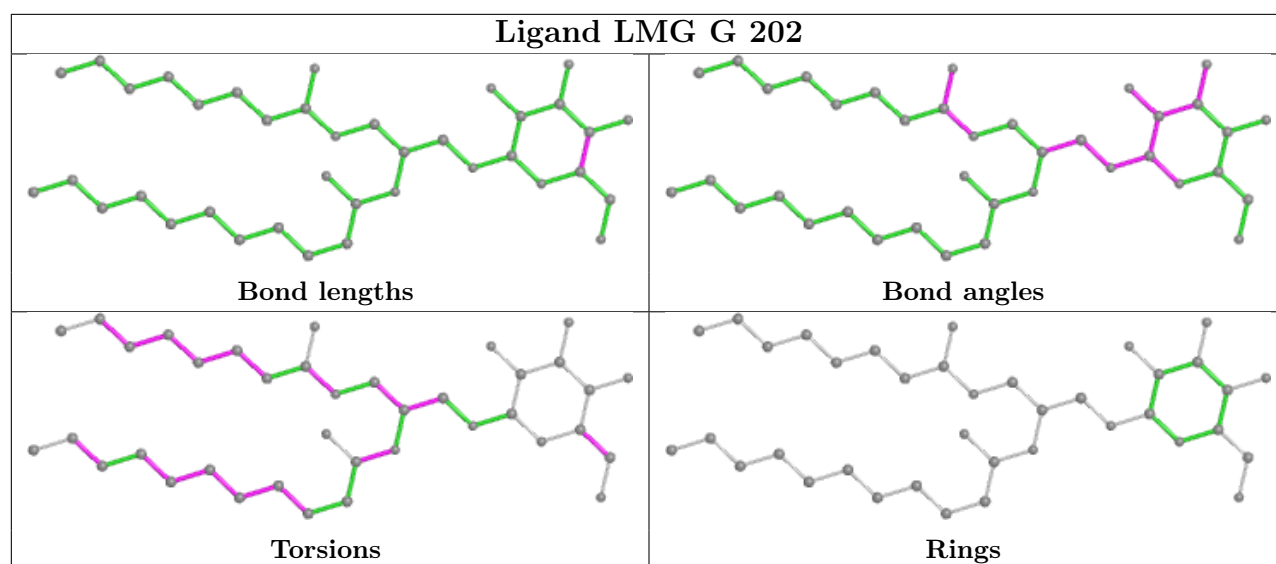


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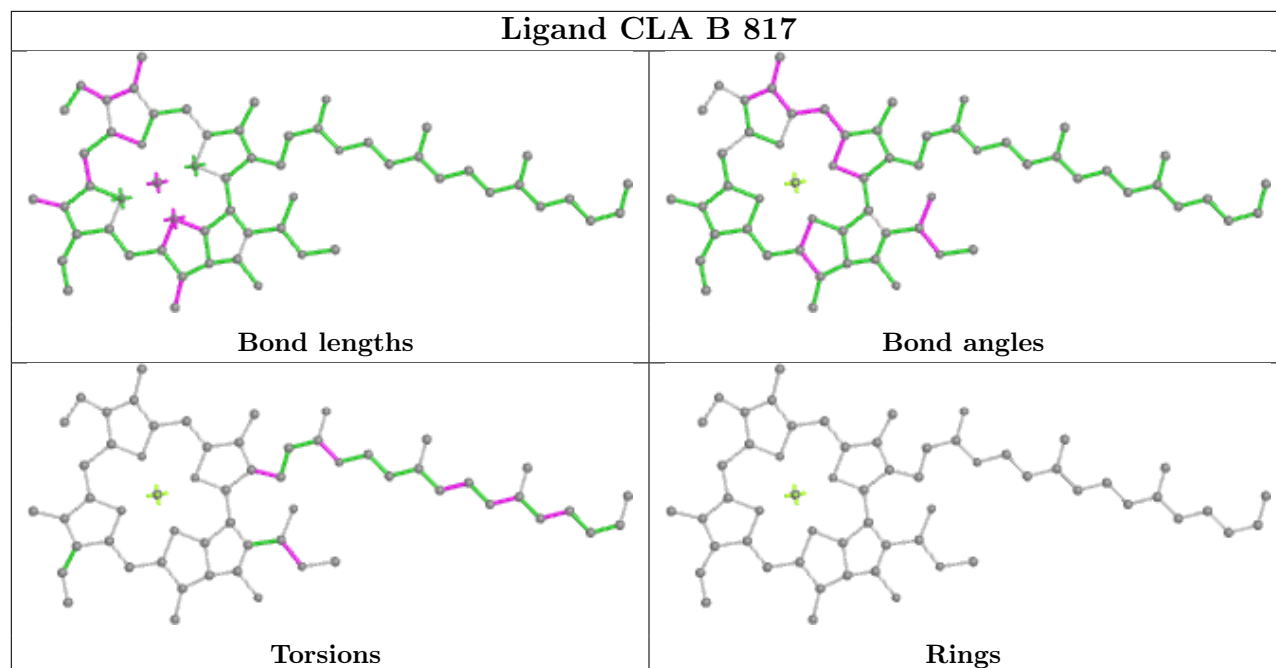


Ligand CLA A 830

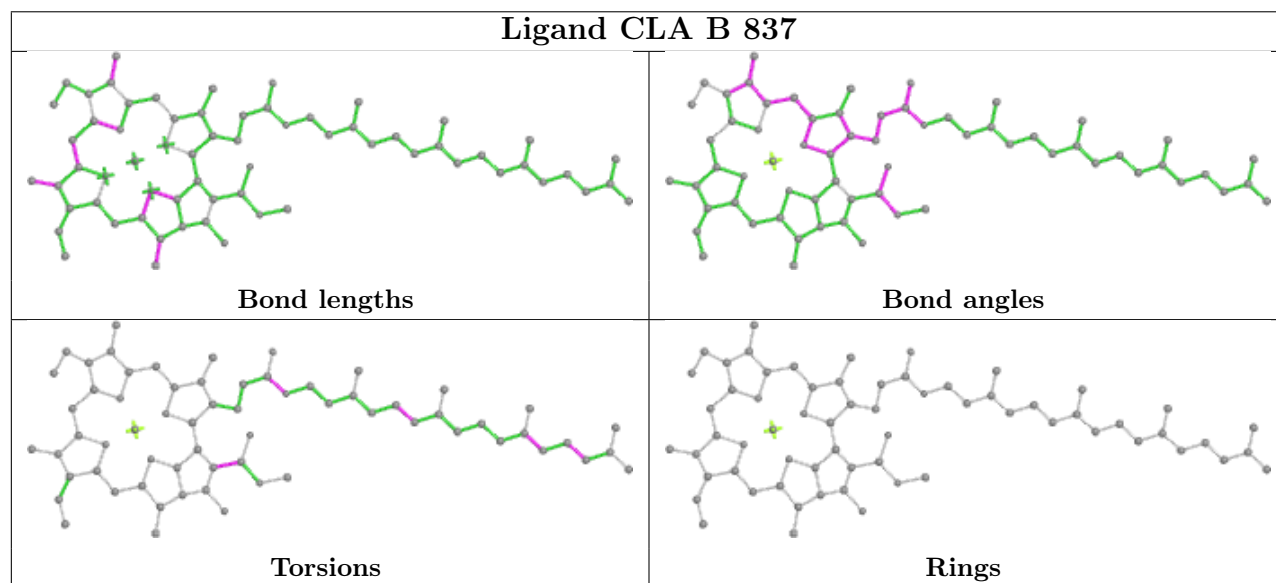


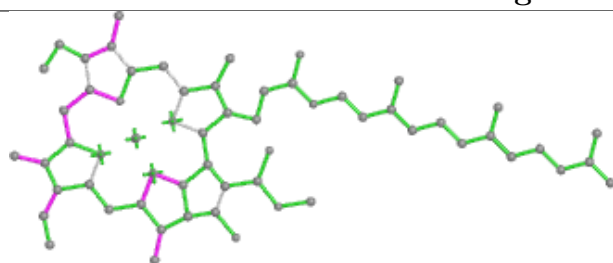


Ligand CLA B 817

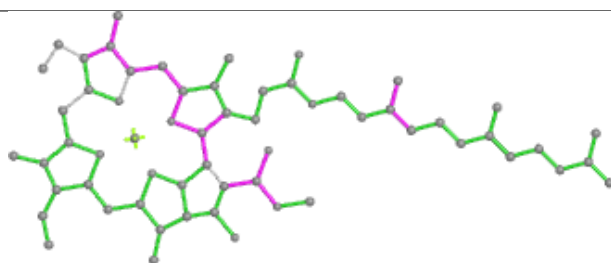


Ligand CLA B 837

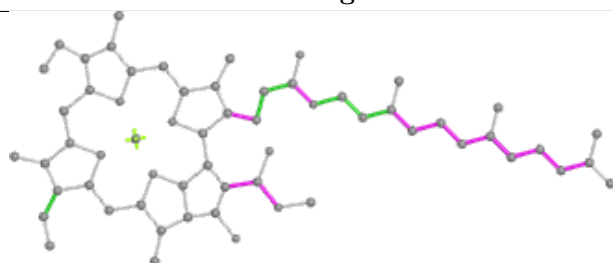


Ligand CLA B 818

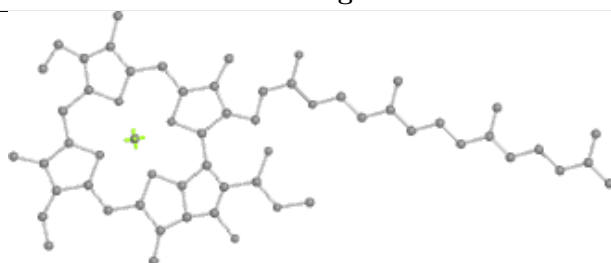
Bond lengths



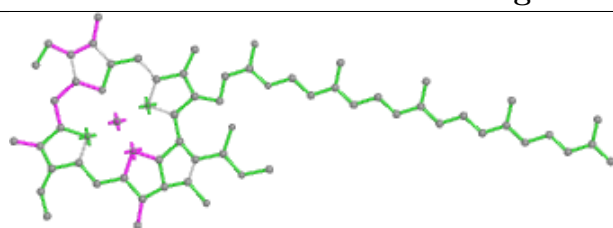
Bond angles



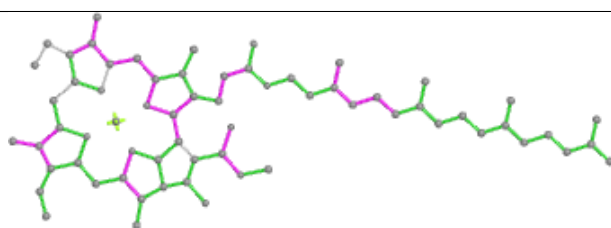
Torsions



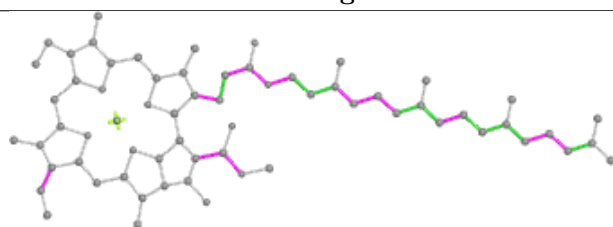
Rings

Ligand CLA A 835

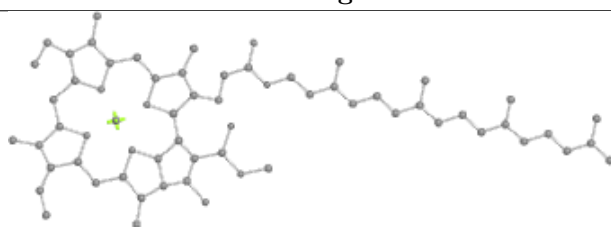
Bond lengths



Bond angles

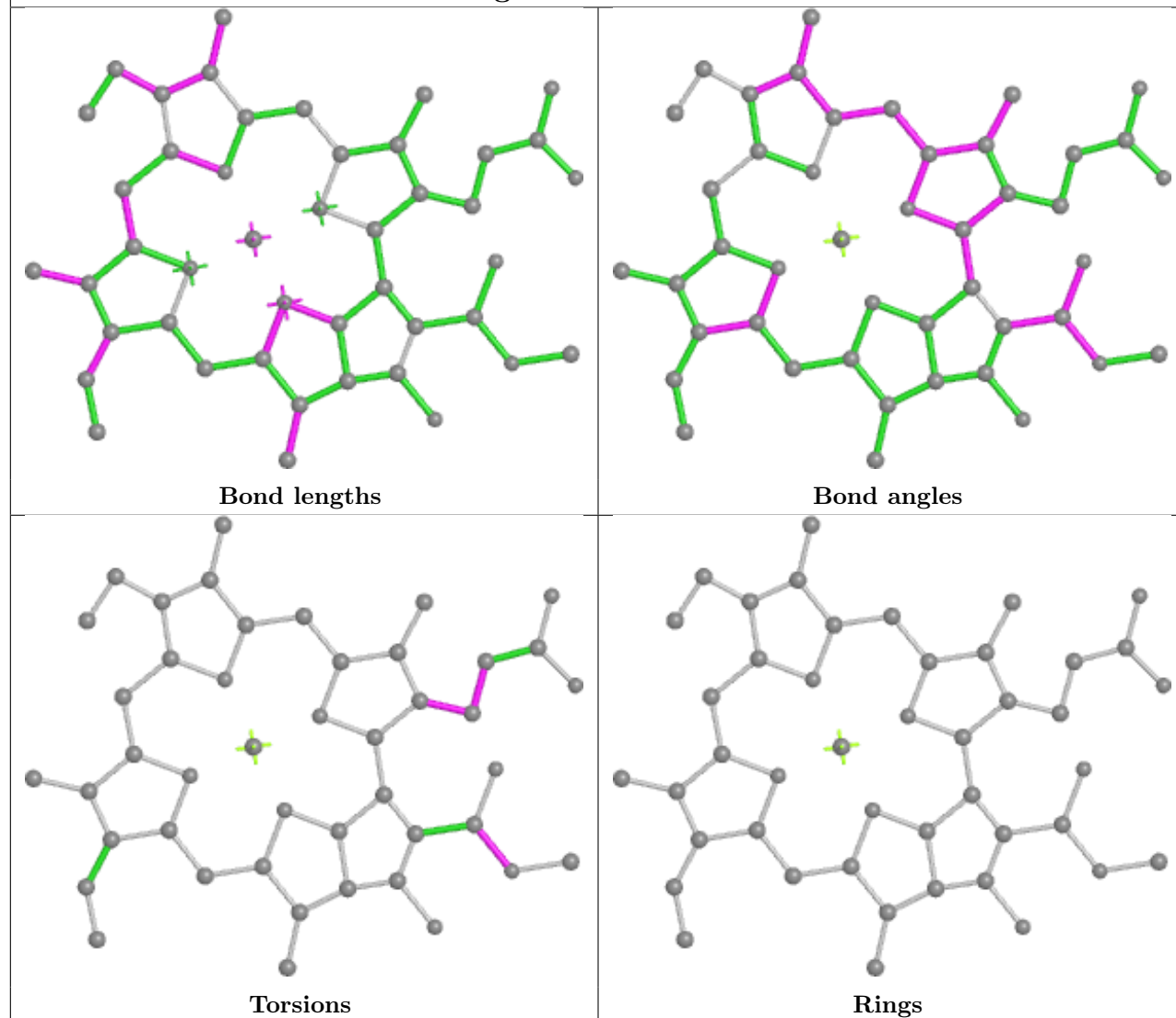


Torsions

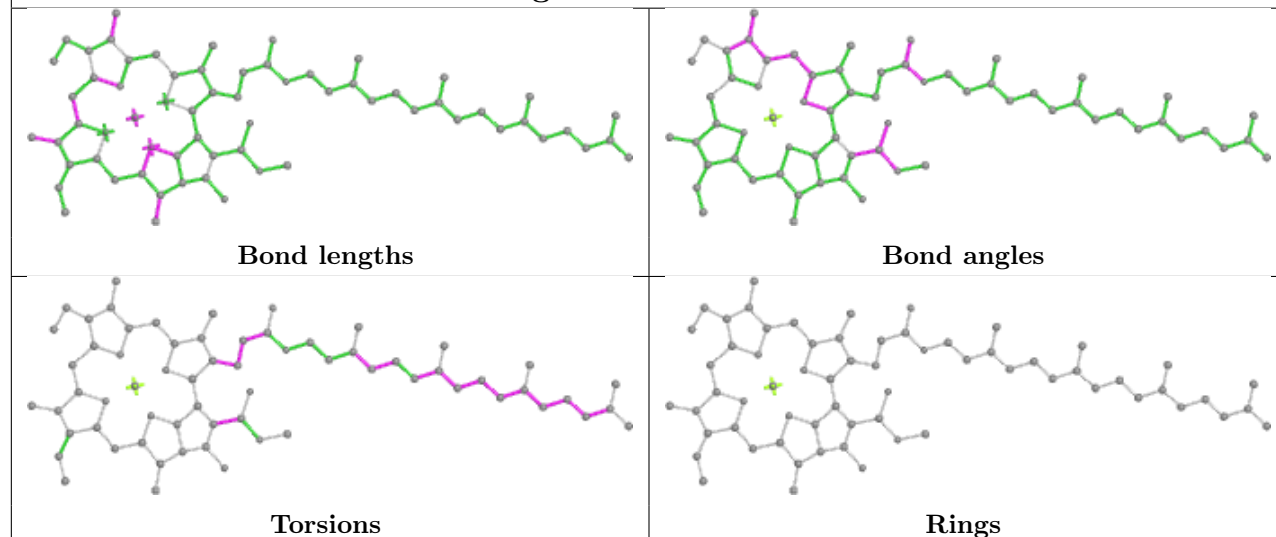


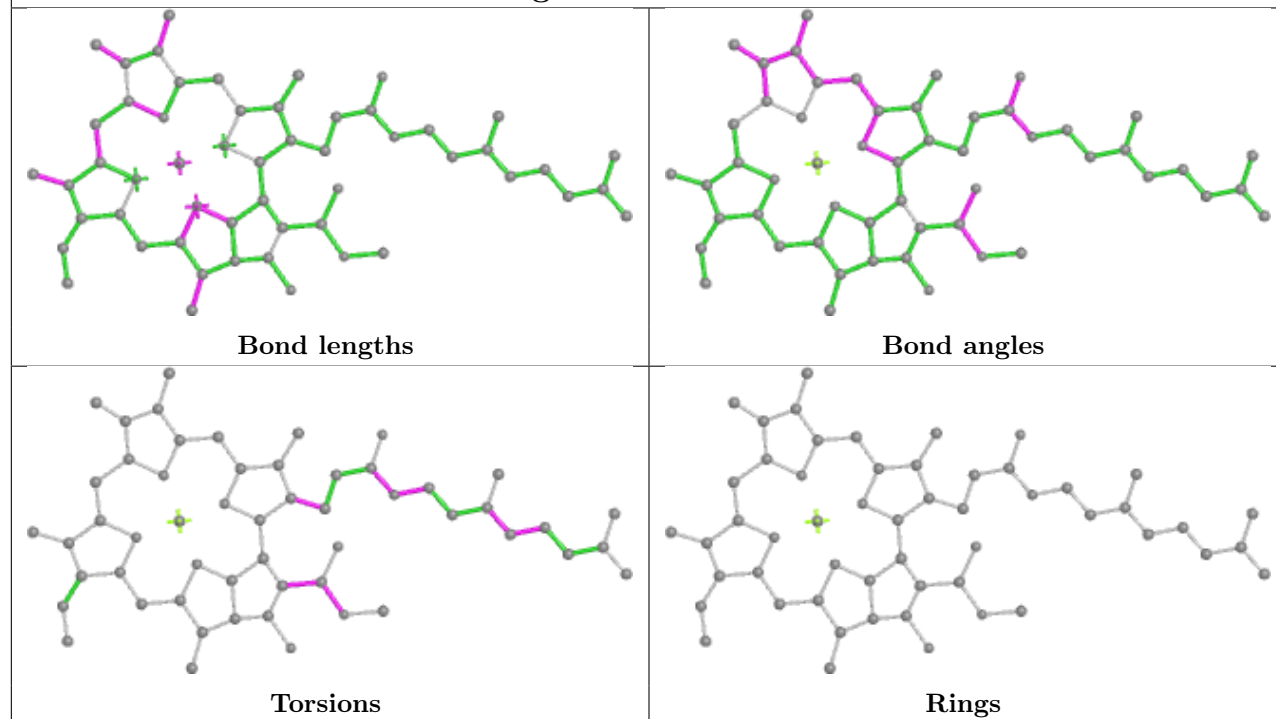
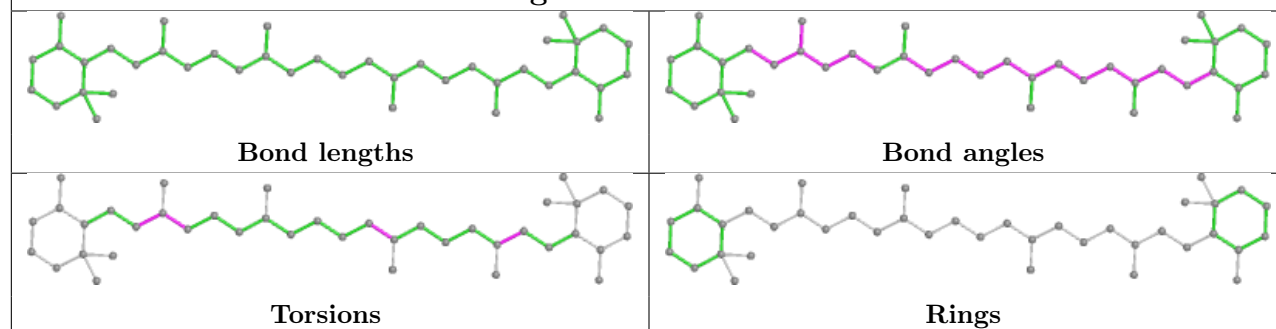
Rings

Ligand CLA 3 609

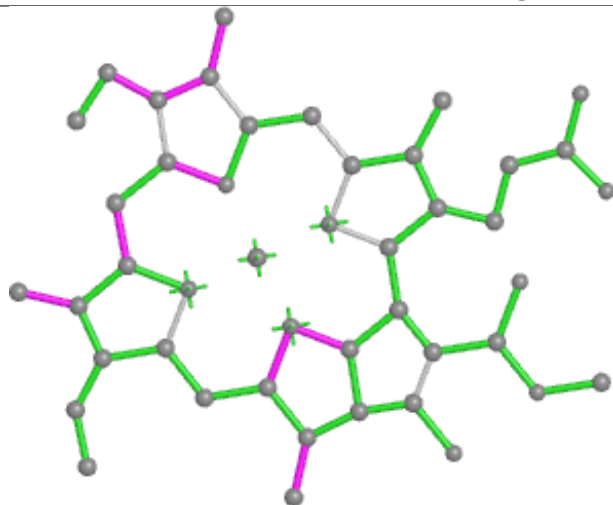


Ligand CLA B 827

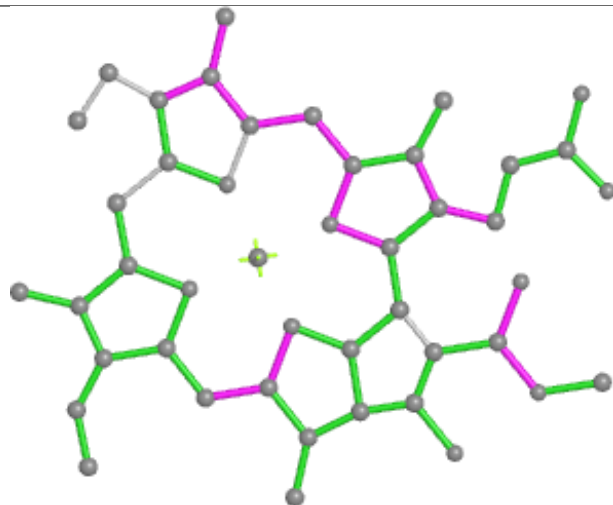


Ligand CLA B 811**Ligand BCR A 852**

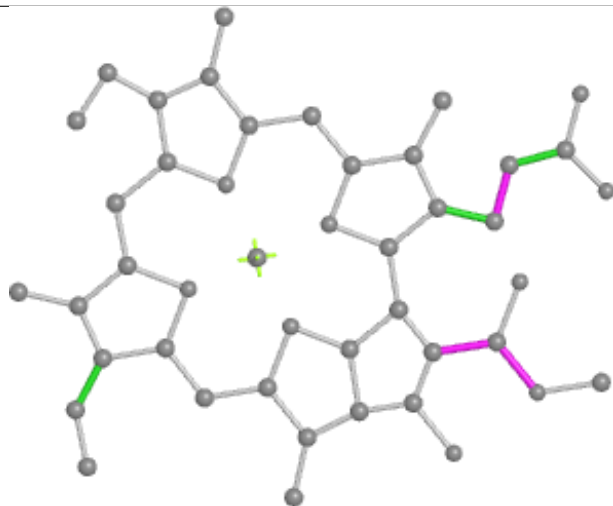
Ligand CLA G 201



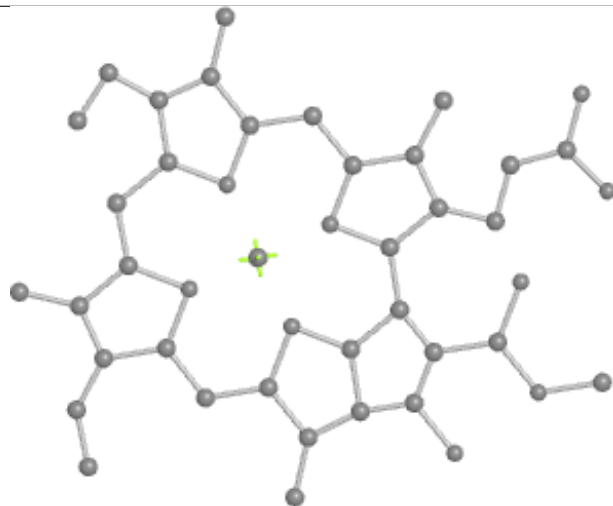
Bond lengths



Bond angles

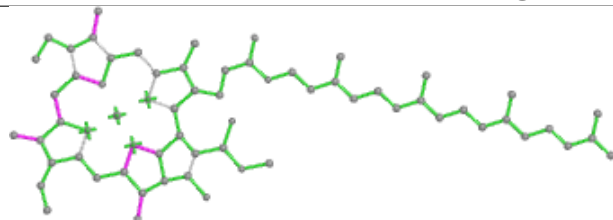


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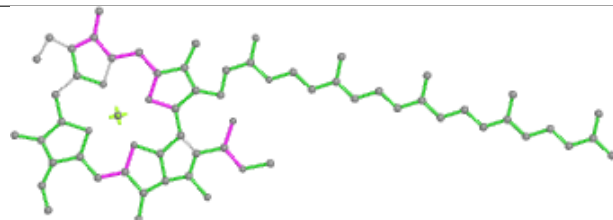


Rings

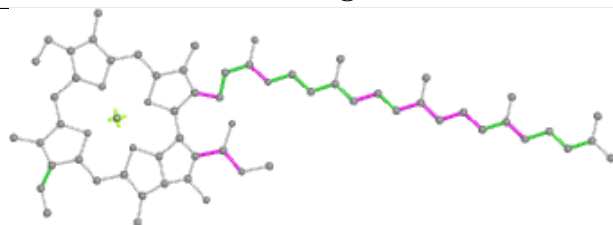
Ligand CLA A 812



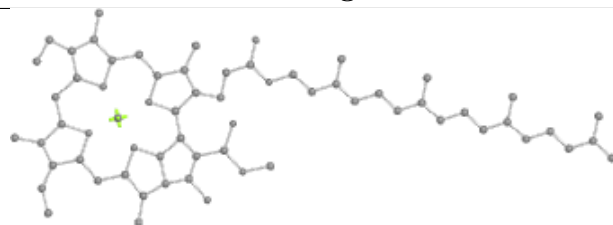
Bond lengths



Bond angles

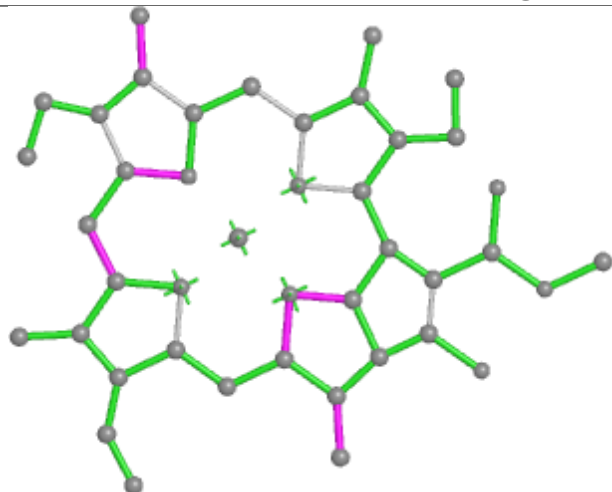


Torsions

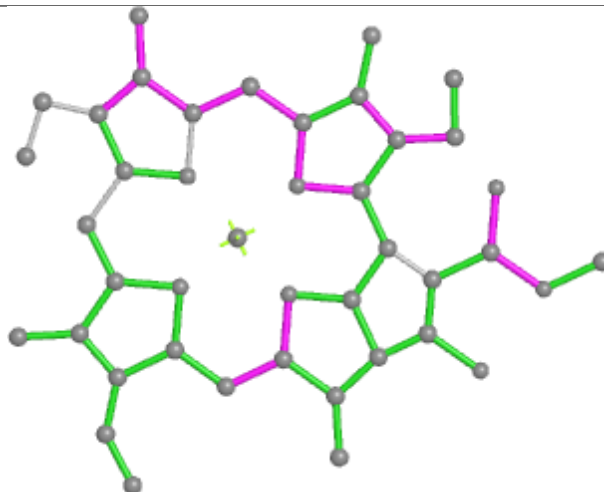


Rings

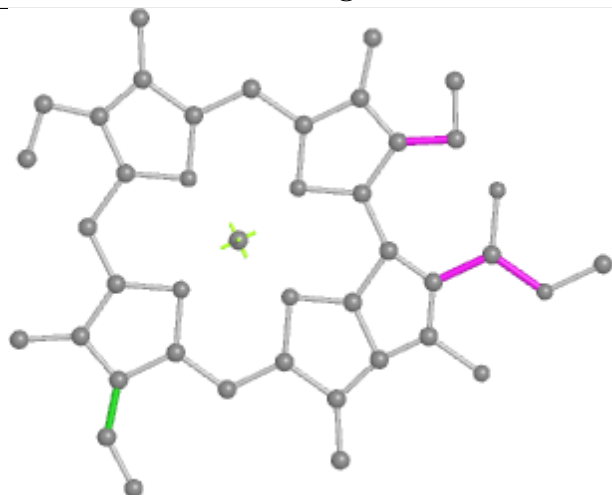
Ligand CLA J 101



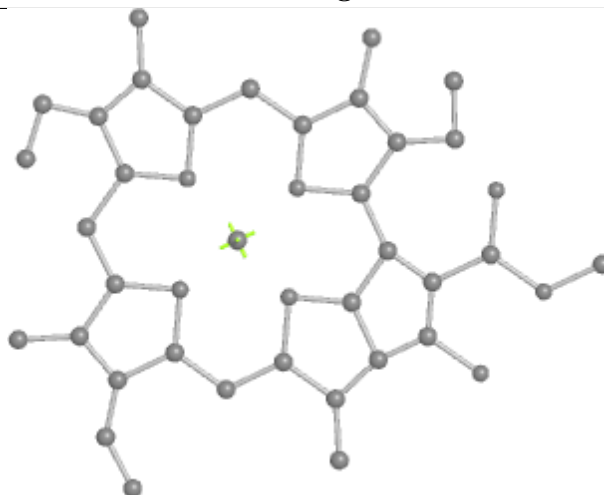
Bond lengths



Bond angles

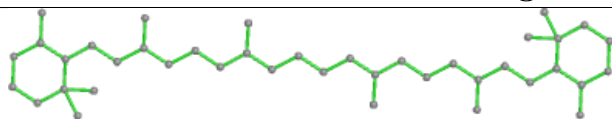


Torsions

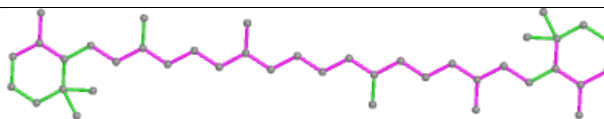


Rings

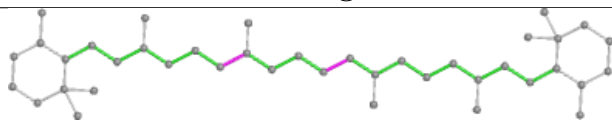
Ligand BCR I 101



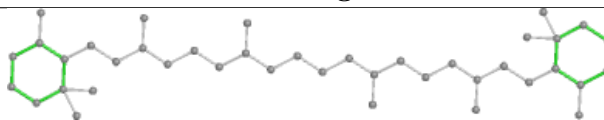
Bond lengths



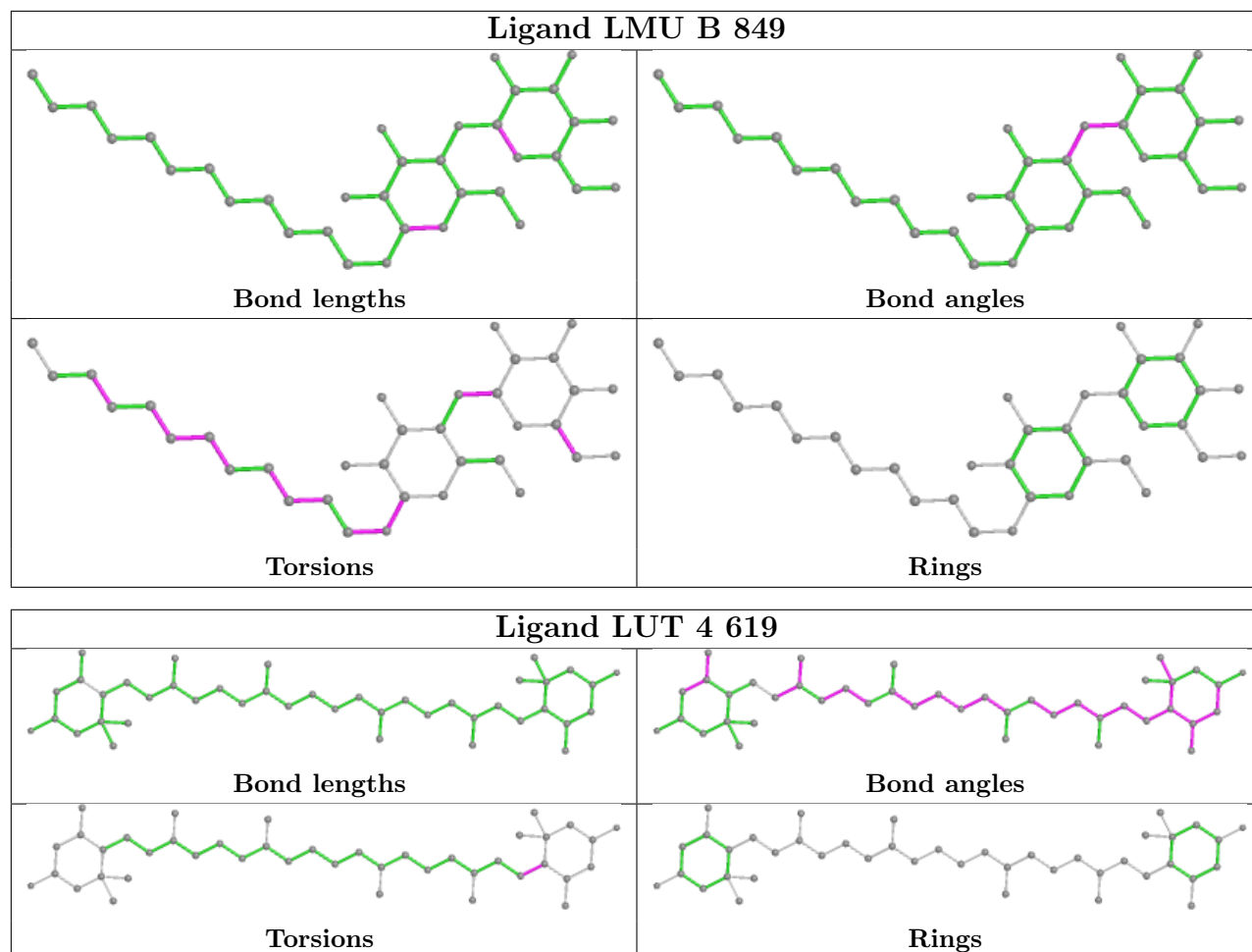
Bond angles



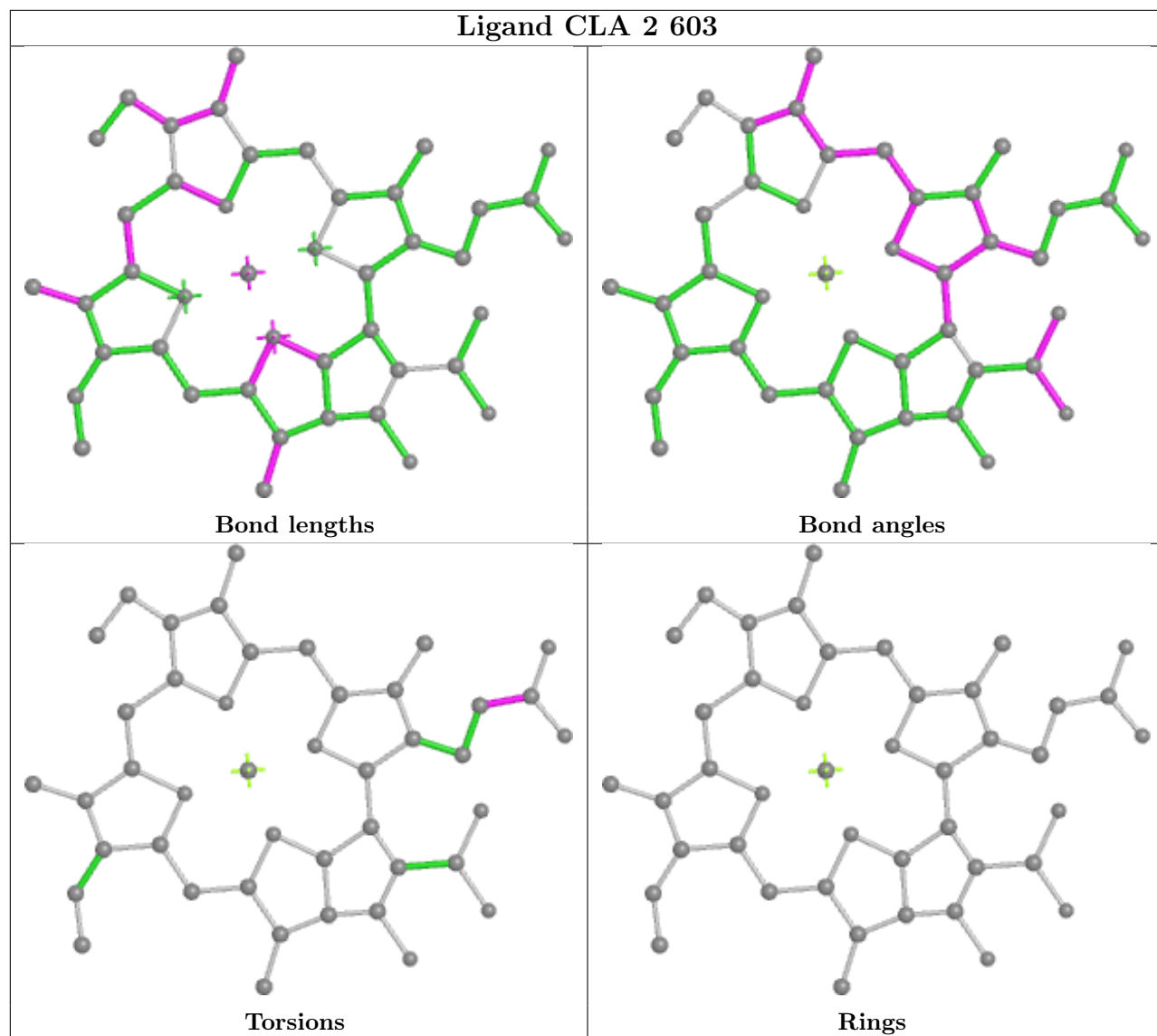
Torsions

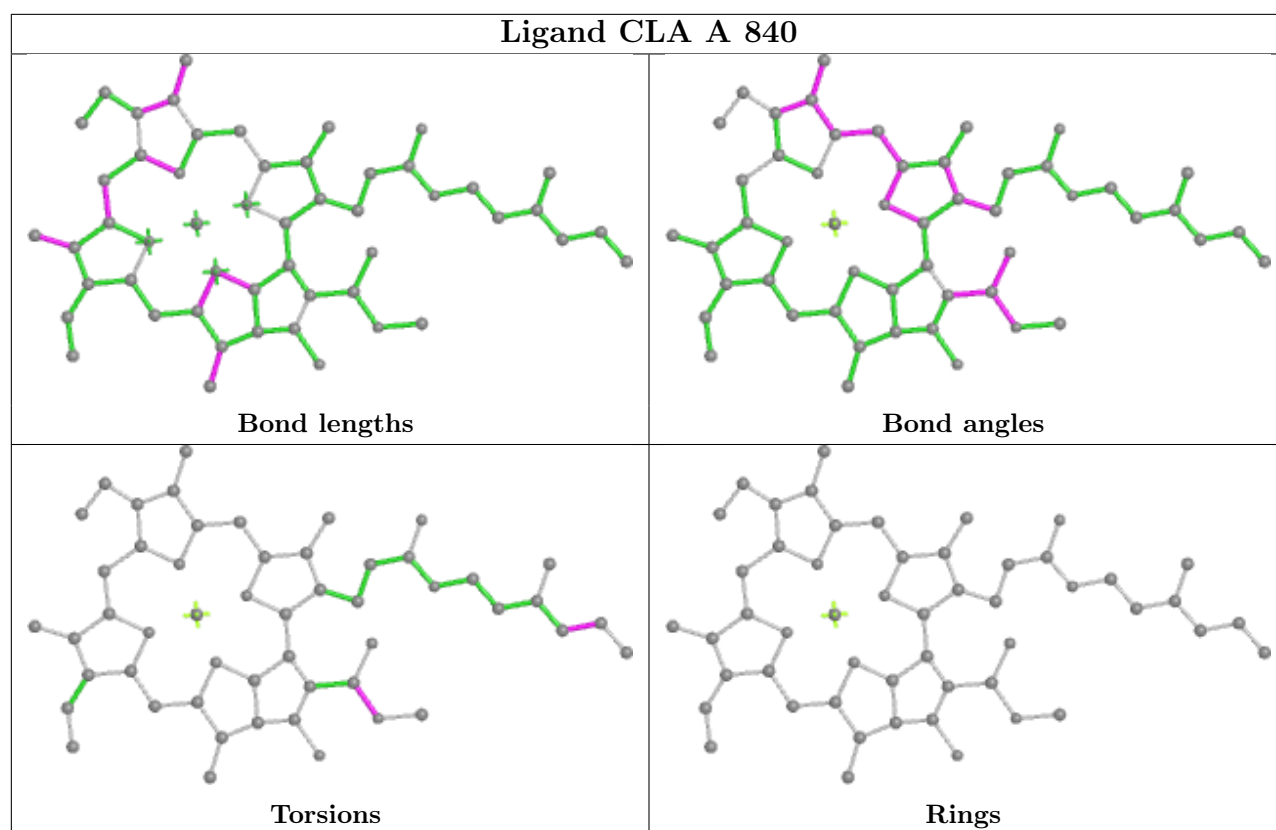


Rings

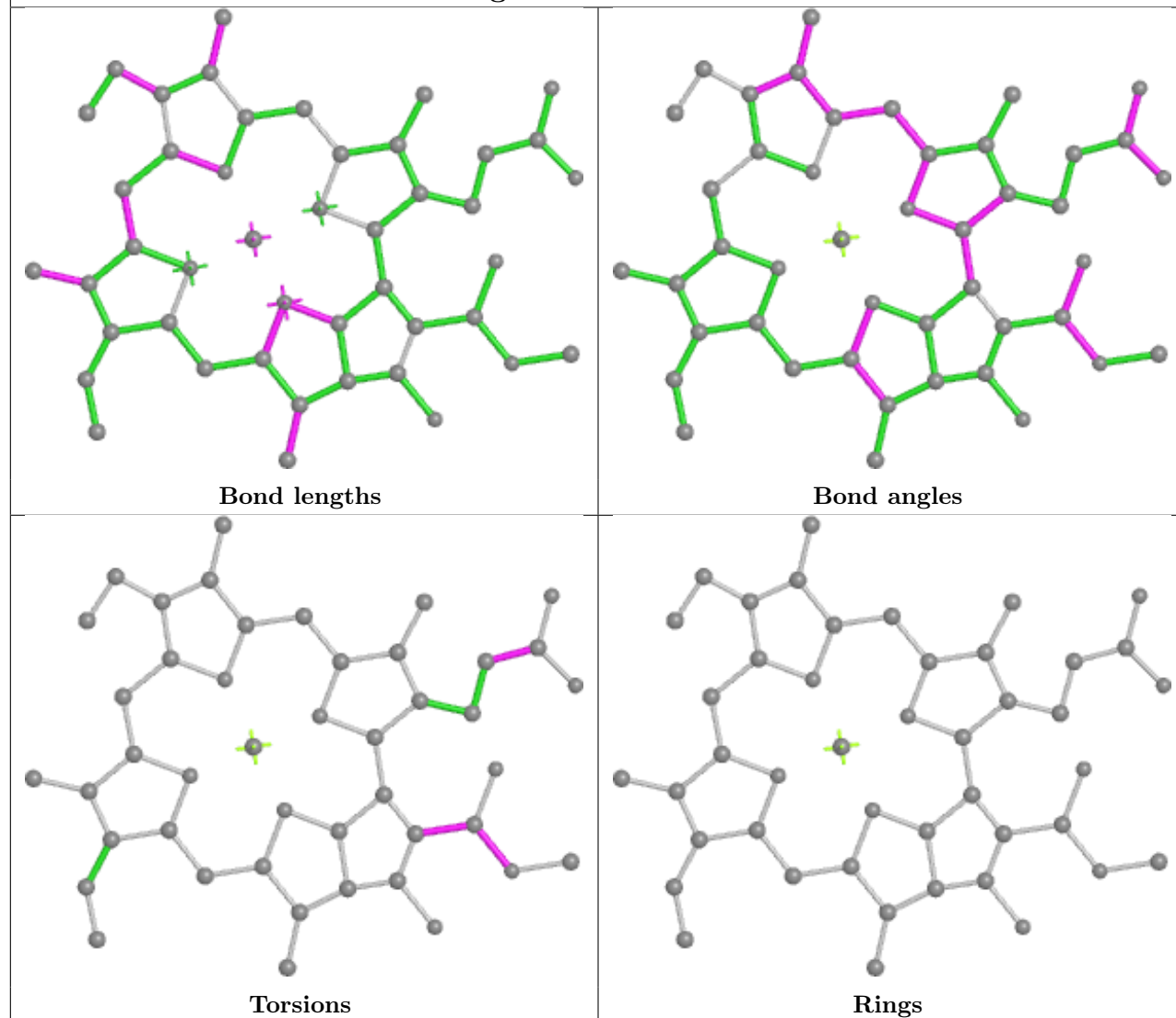


Ligand CLA 2 603

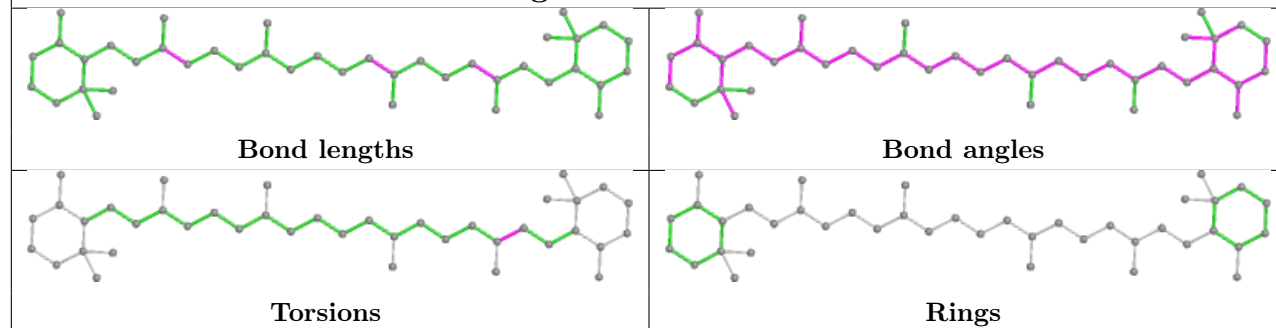


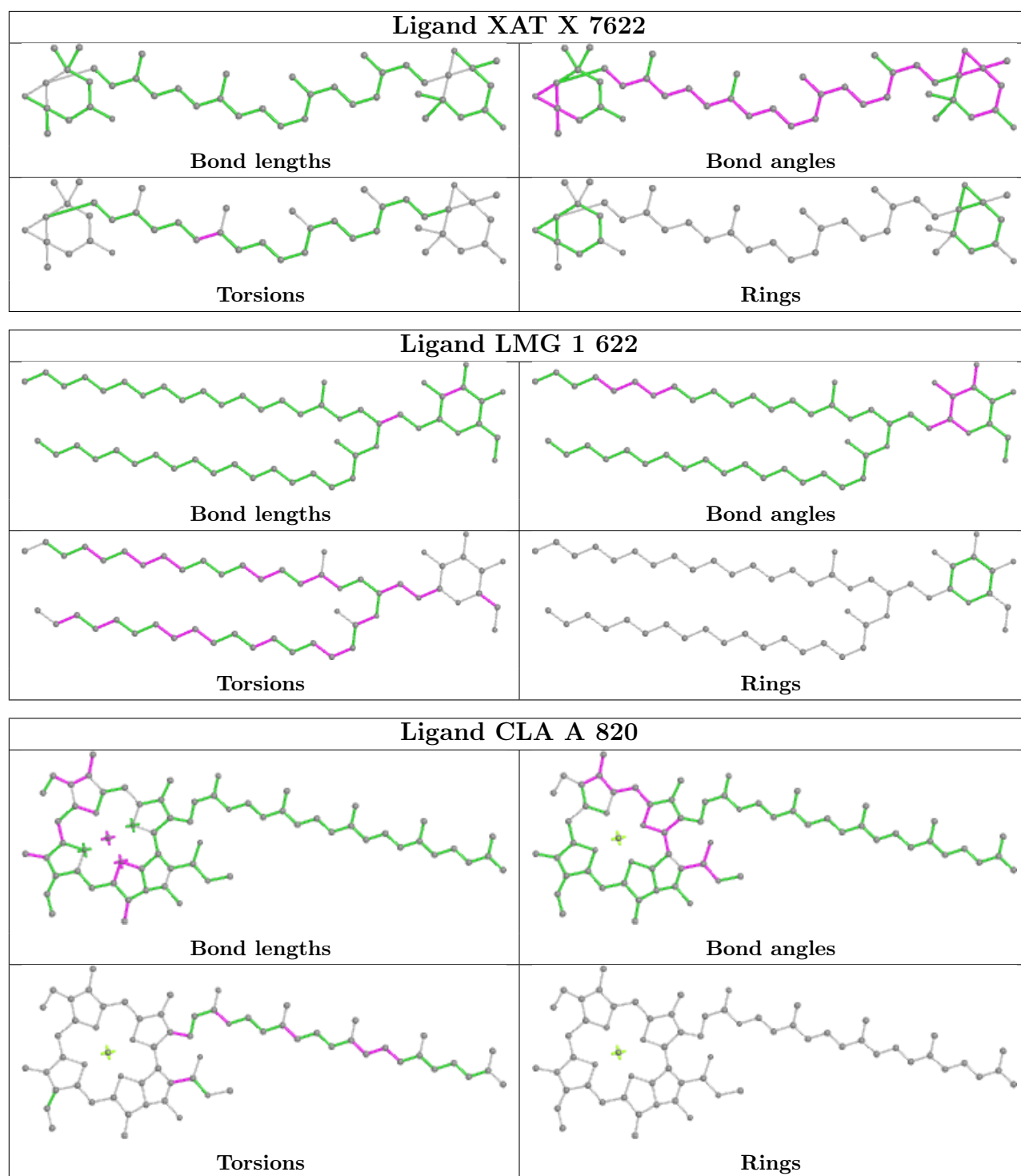


Ligand CLA A 815

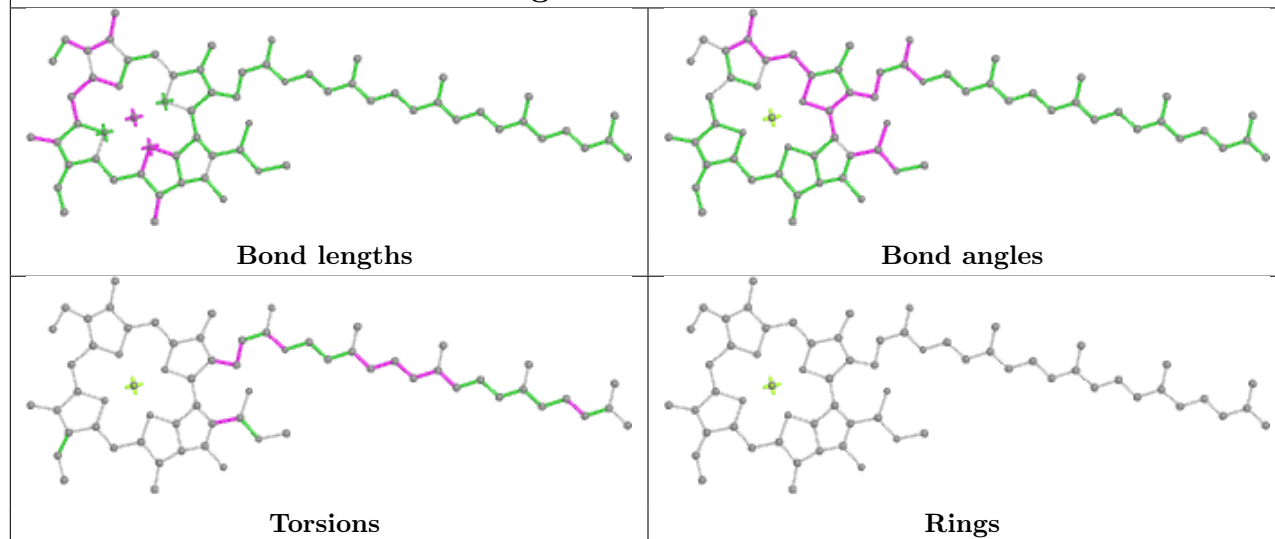


Ligand BCR B 847

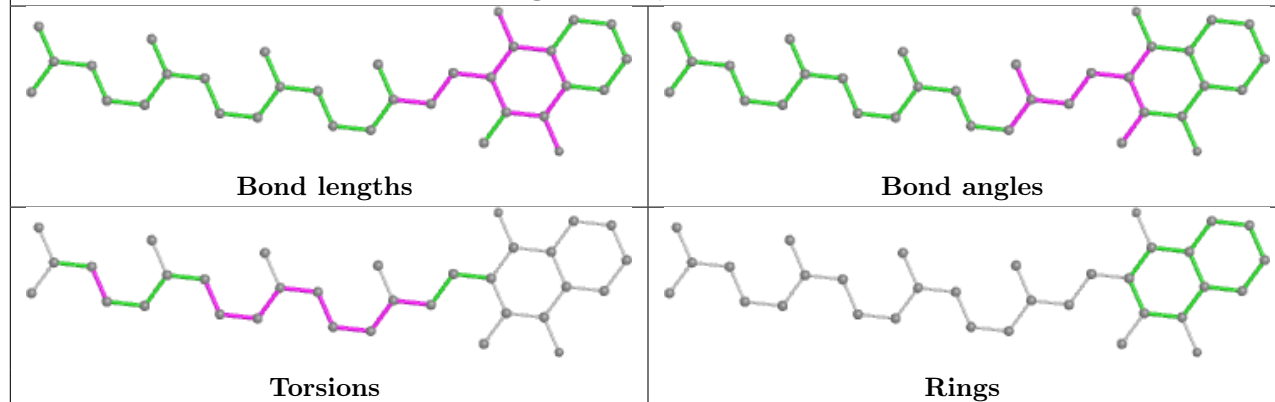




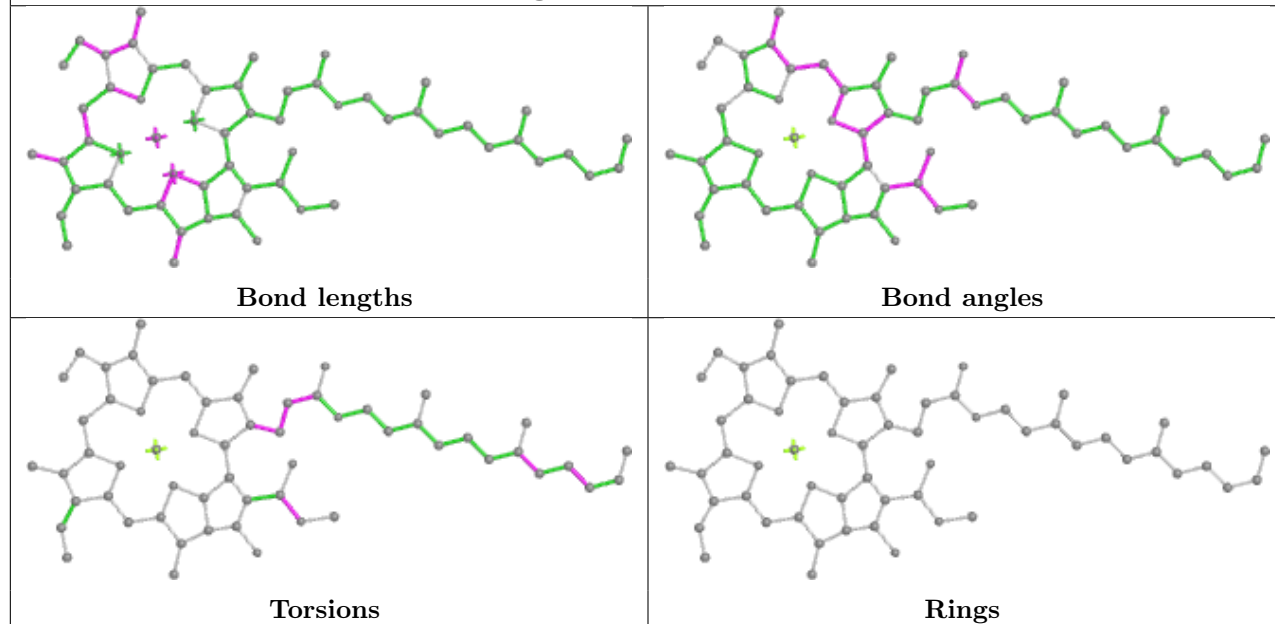
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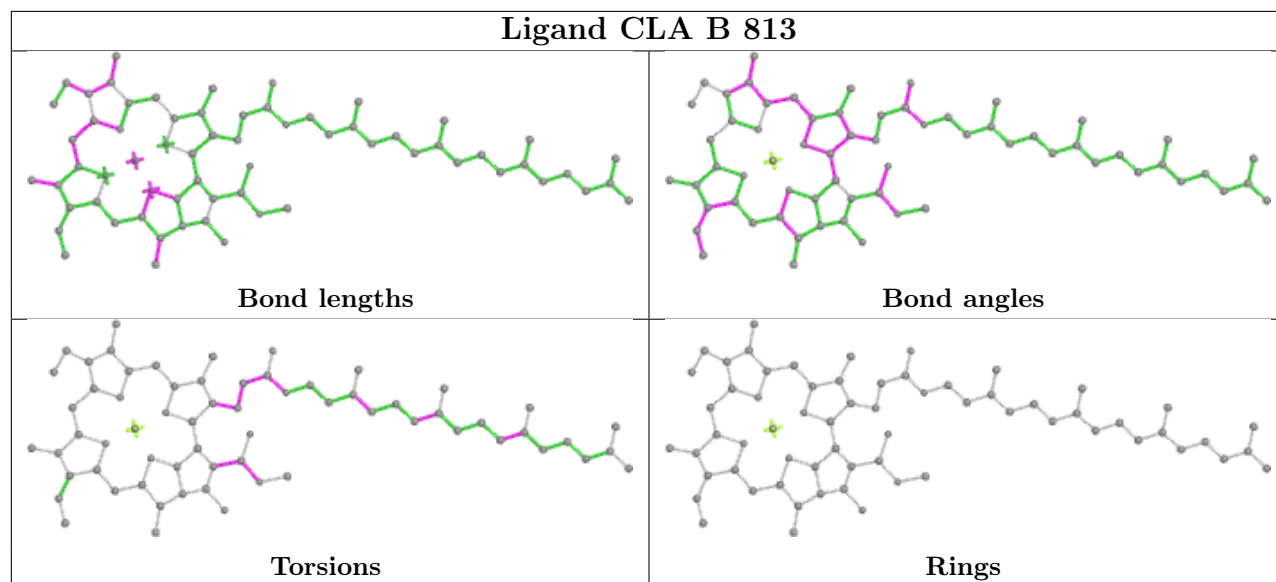
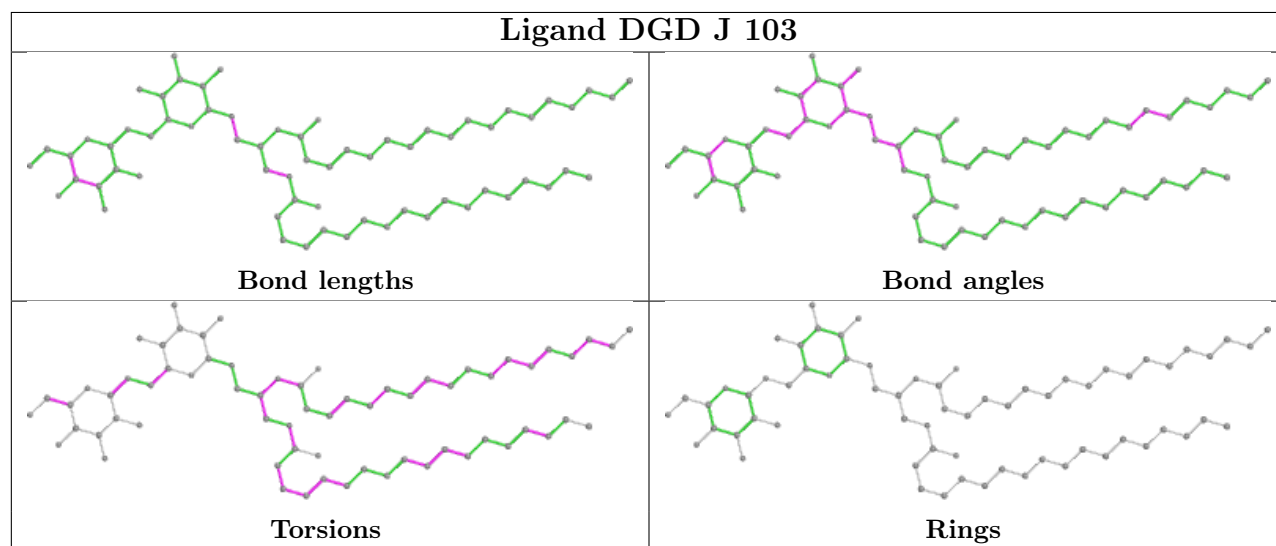


Ligand PQN A 844

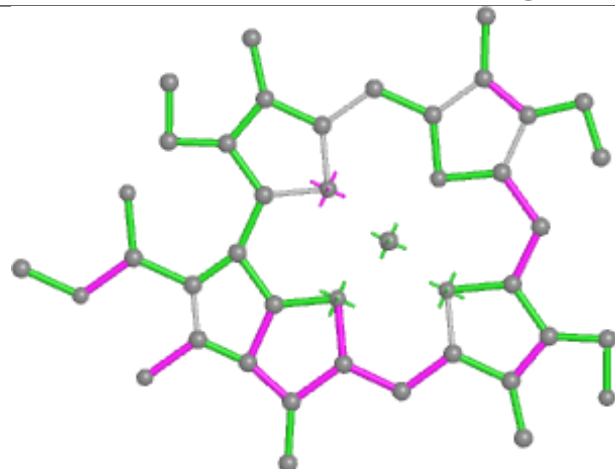


Ligand CLA A 819

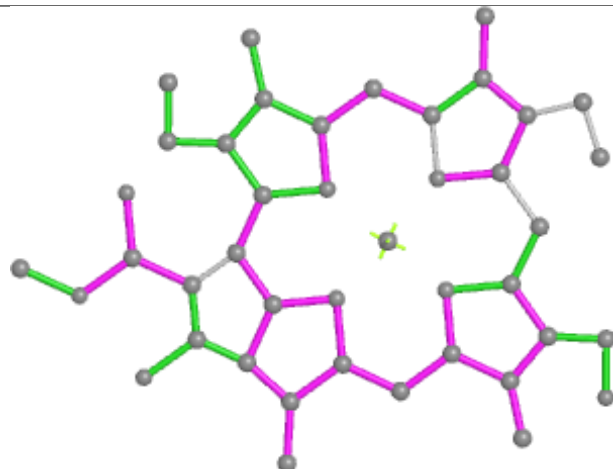


Ligand CLA B 813**Ligand DGD J 103**

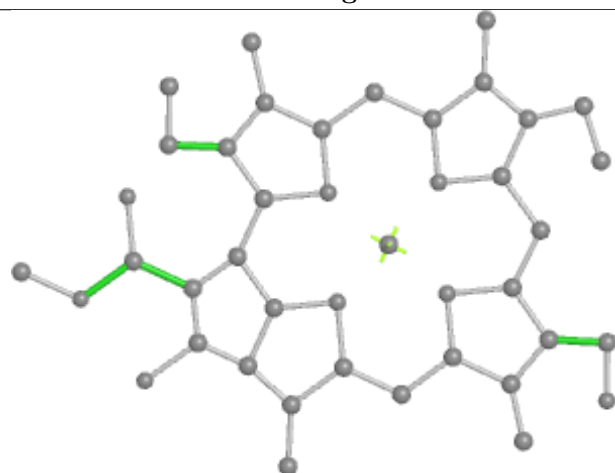
Ligand CHL 2 606



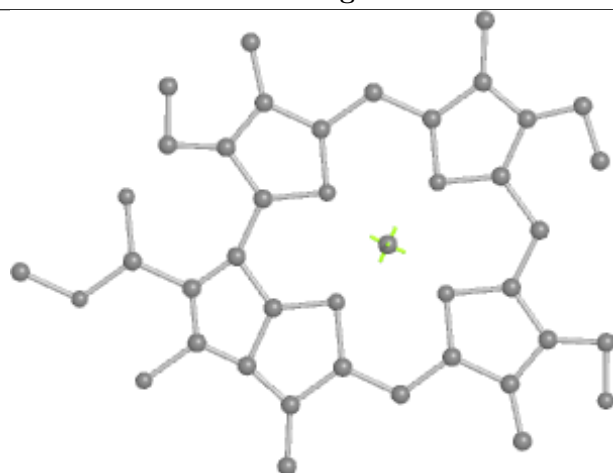
Bond lengths



Bond angles

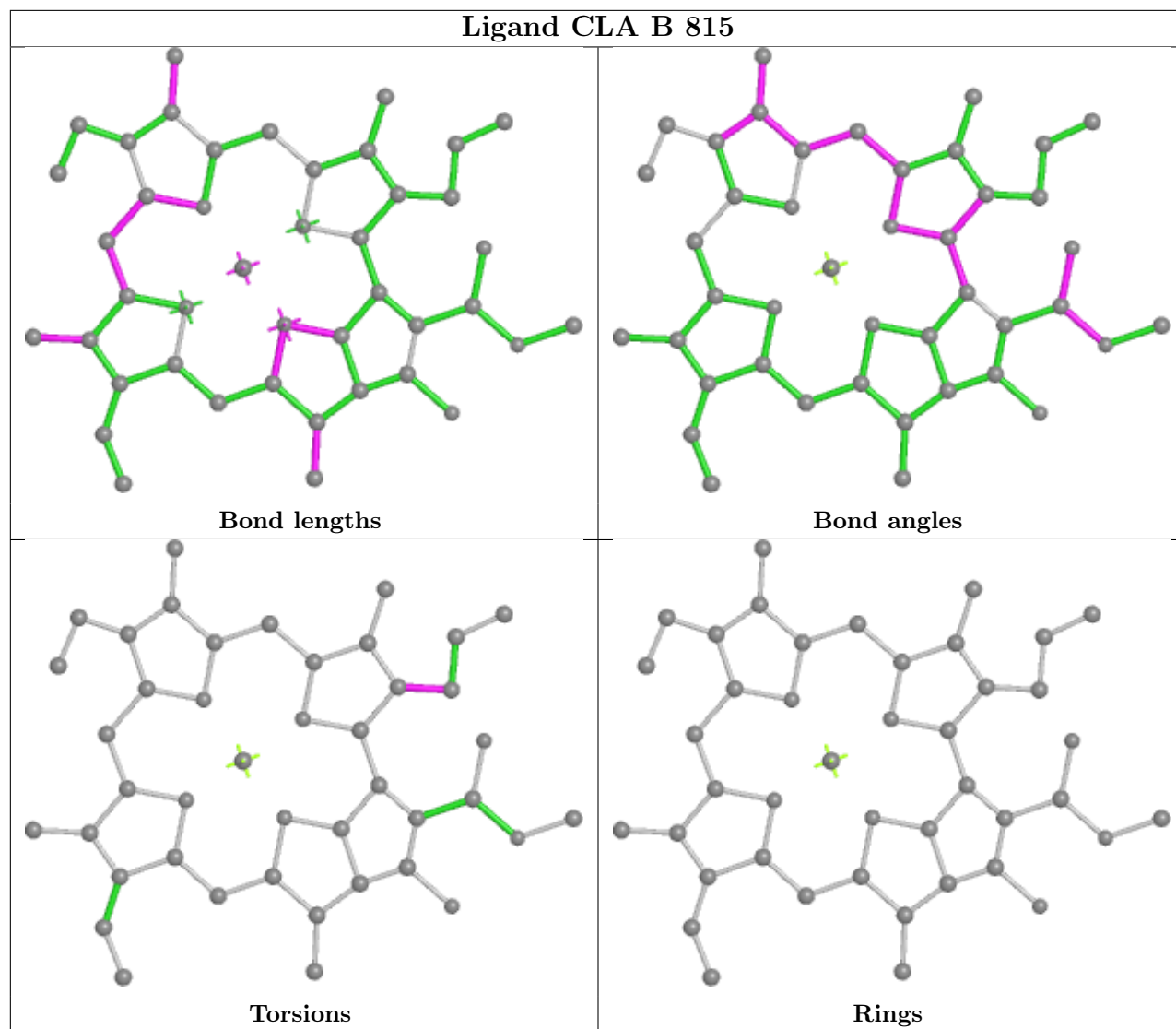


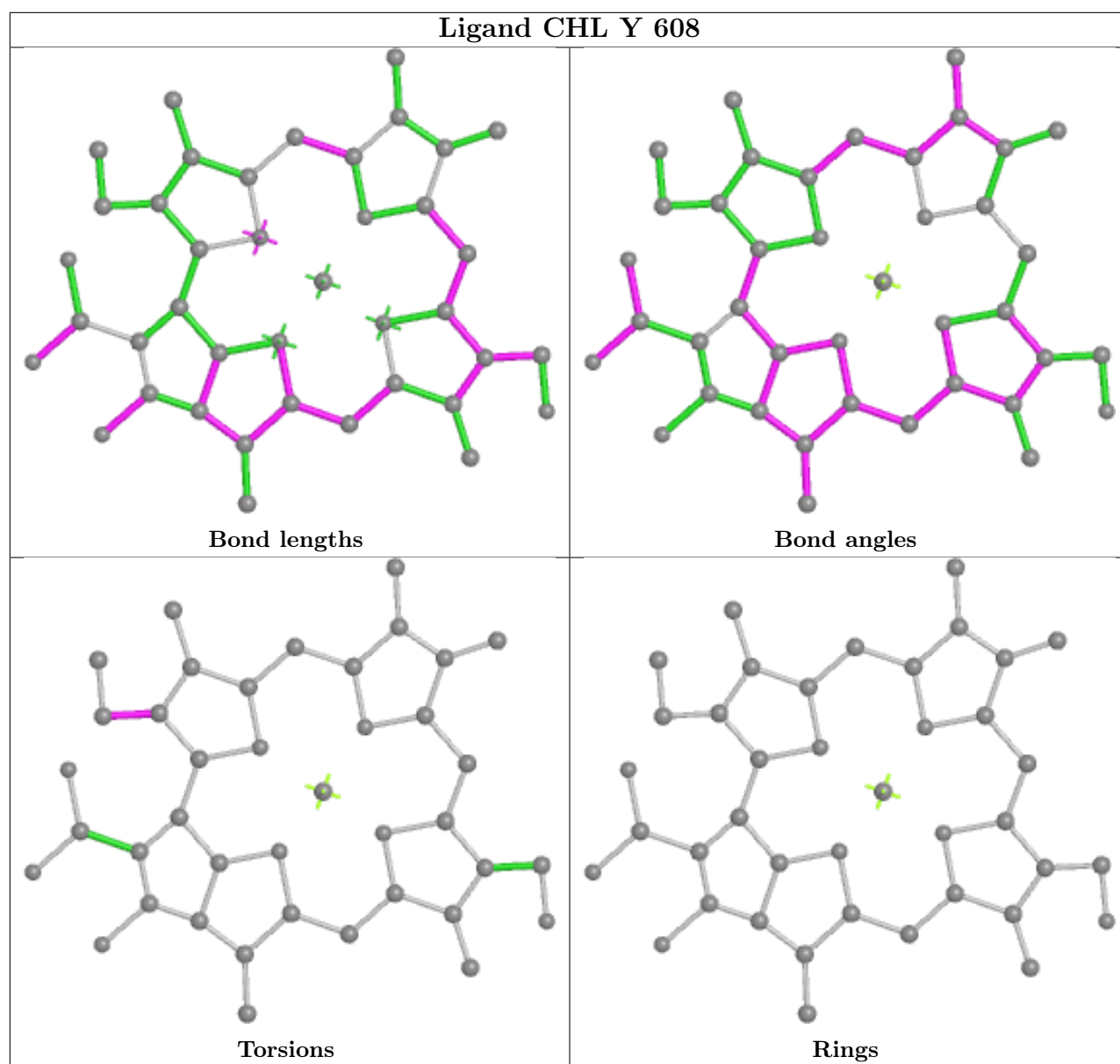
Torsions

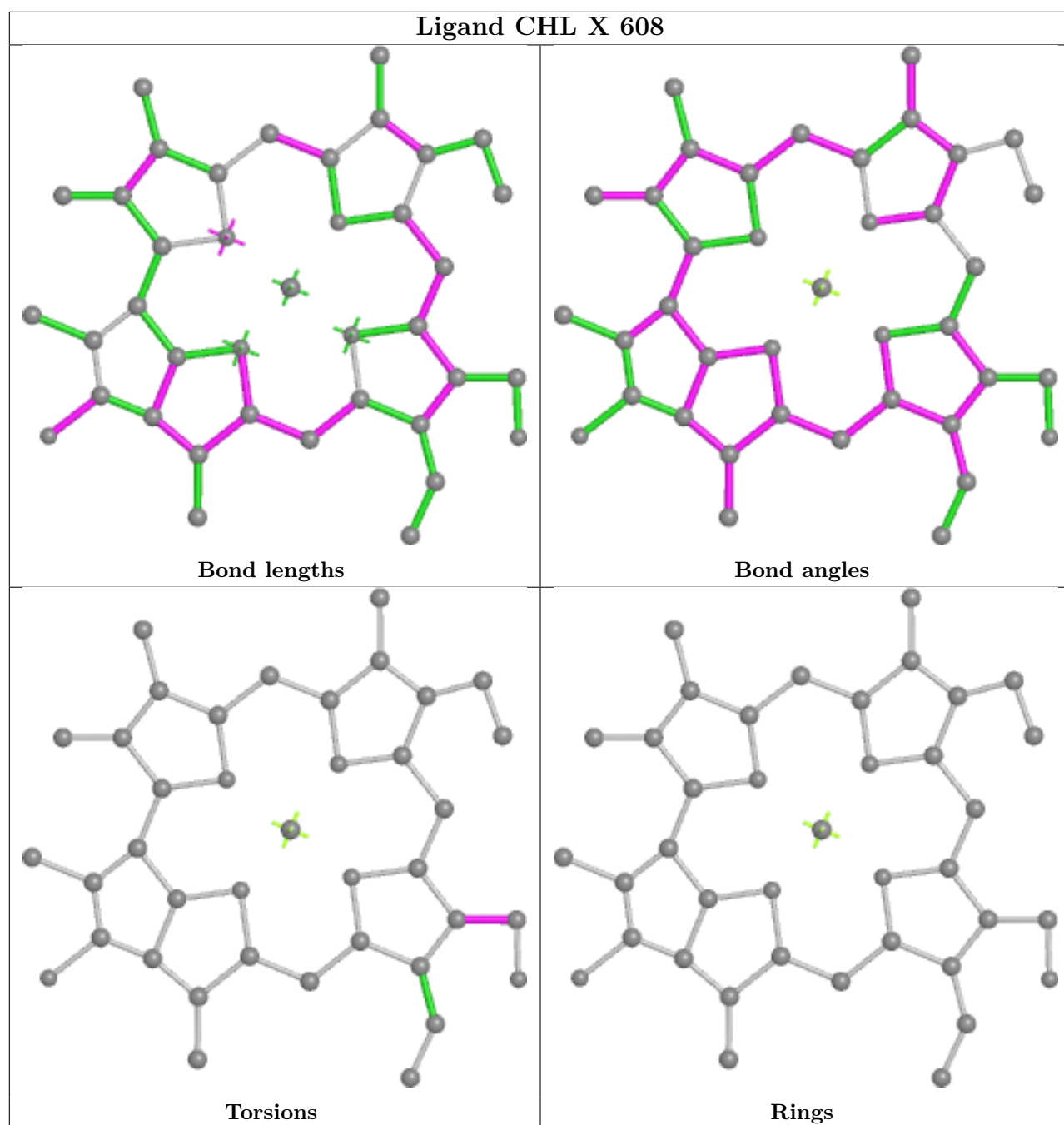


Rings

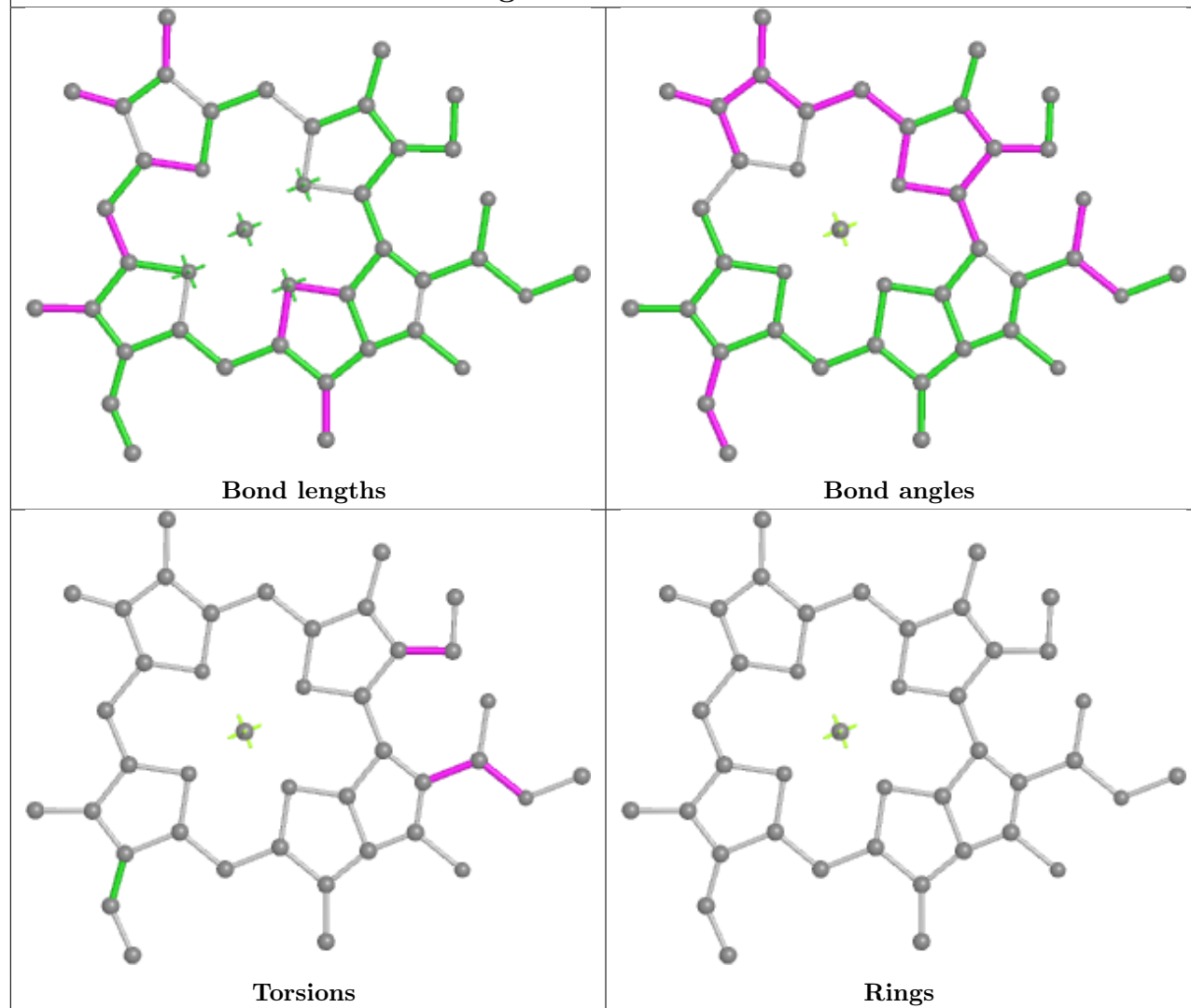
Ligand CLA B 815



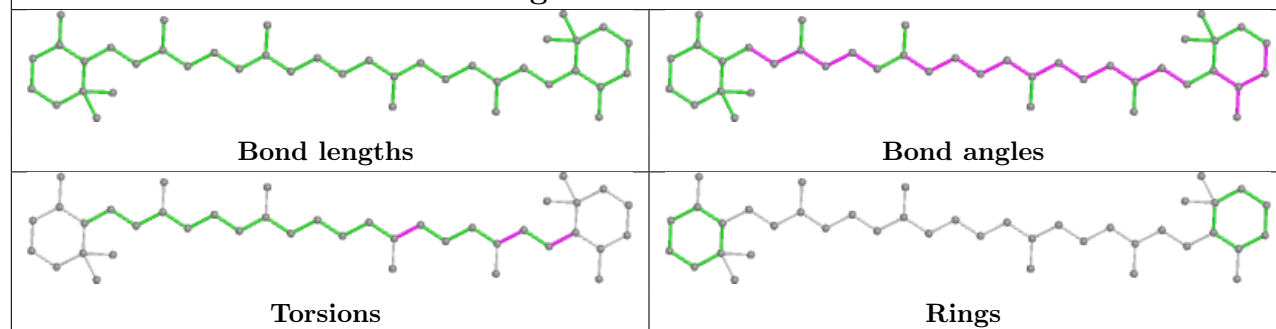




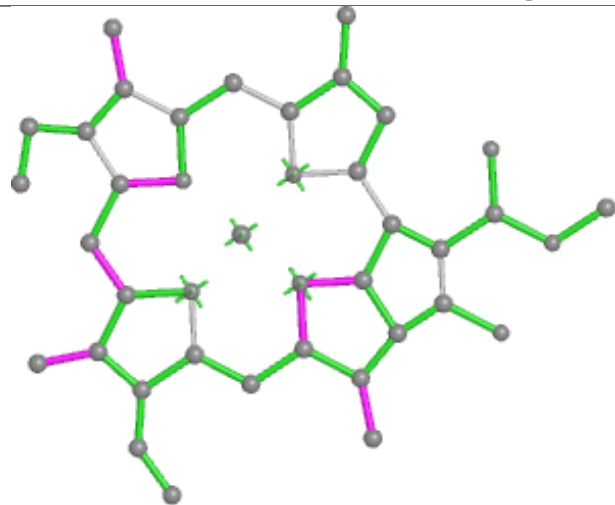
Ligand CLA Z 603



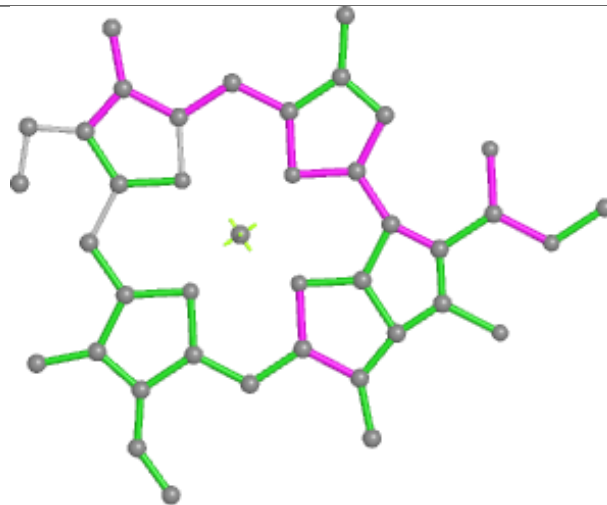
Ligand BCR A 851



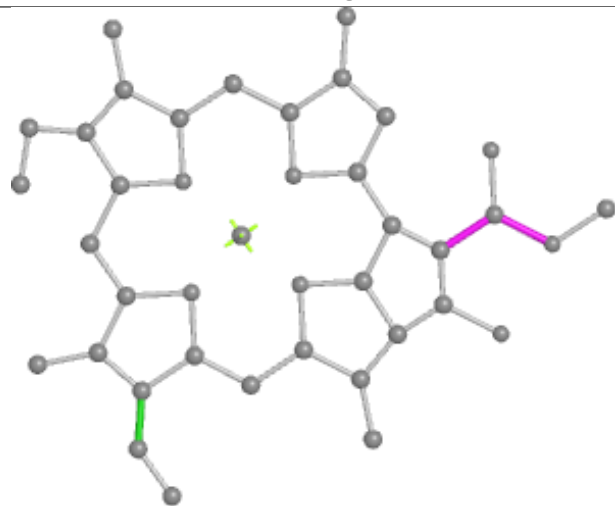
Ligand CLA 1 606



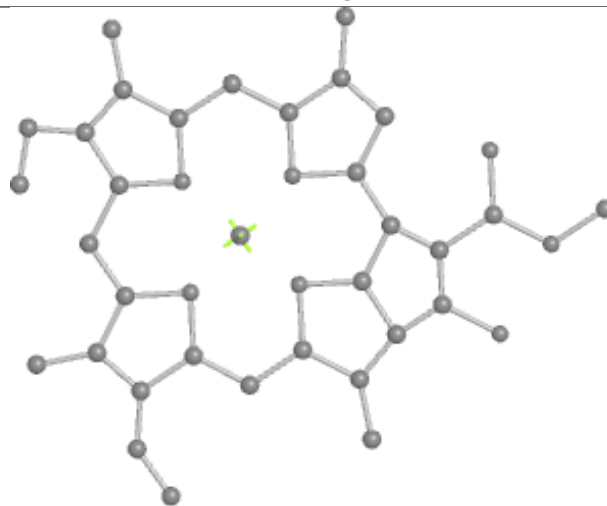
Bond lengths



Bond angles

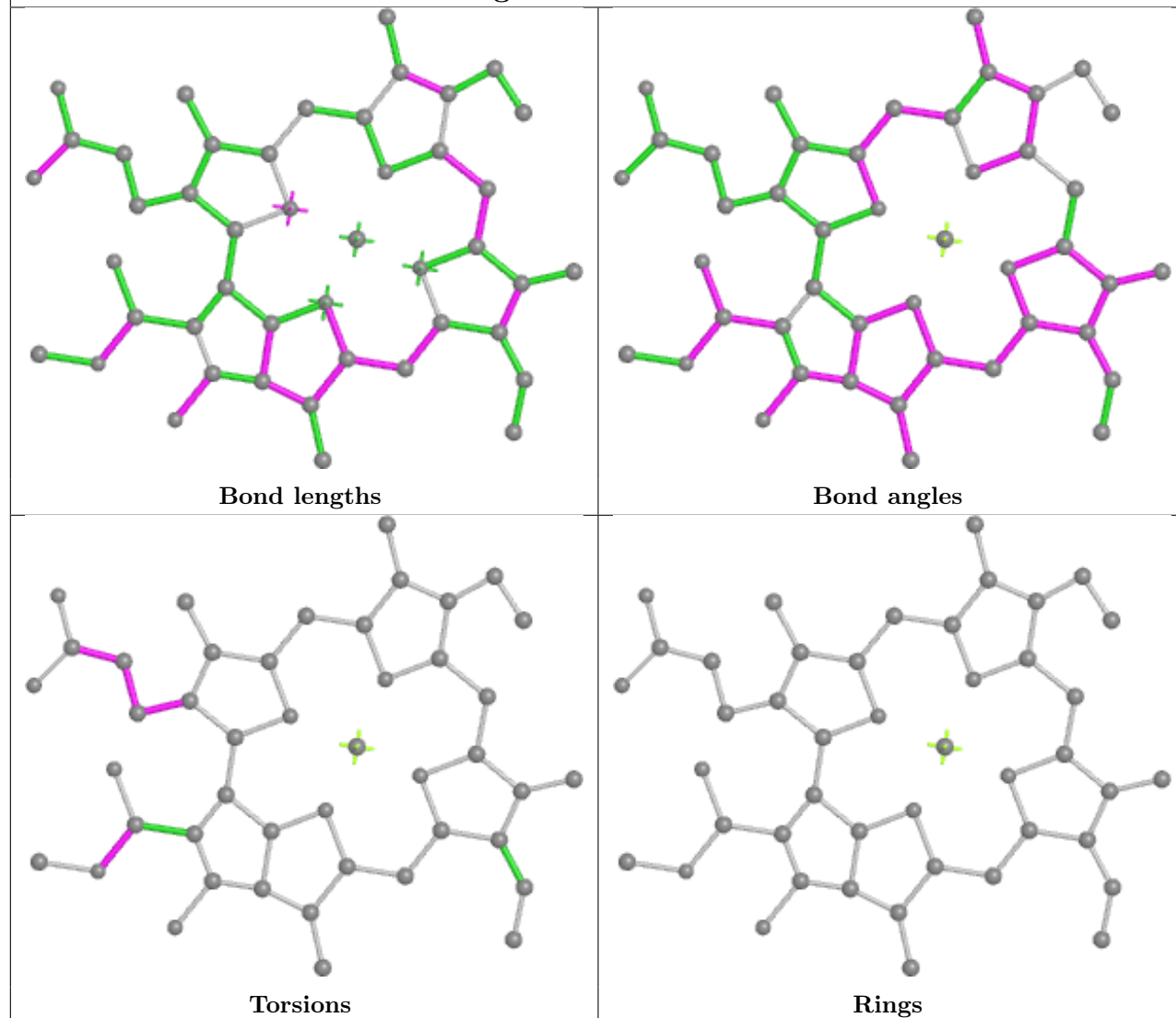


Torsions

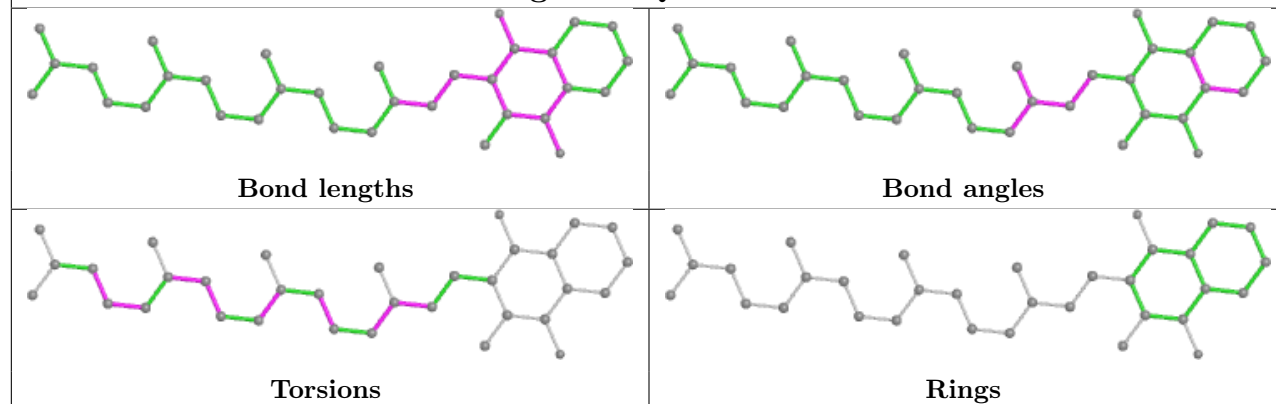


Rings

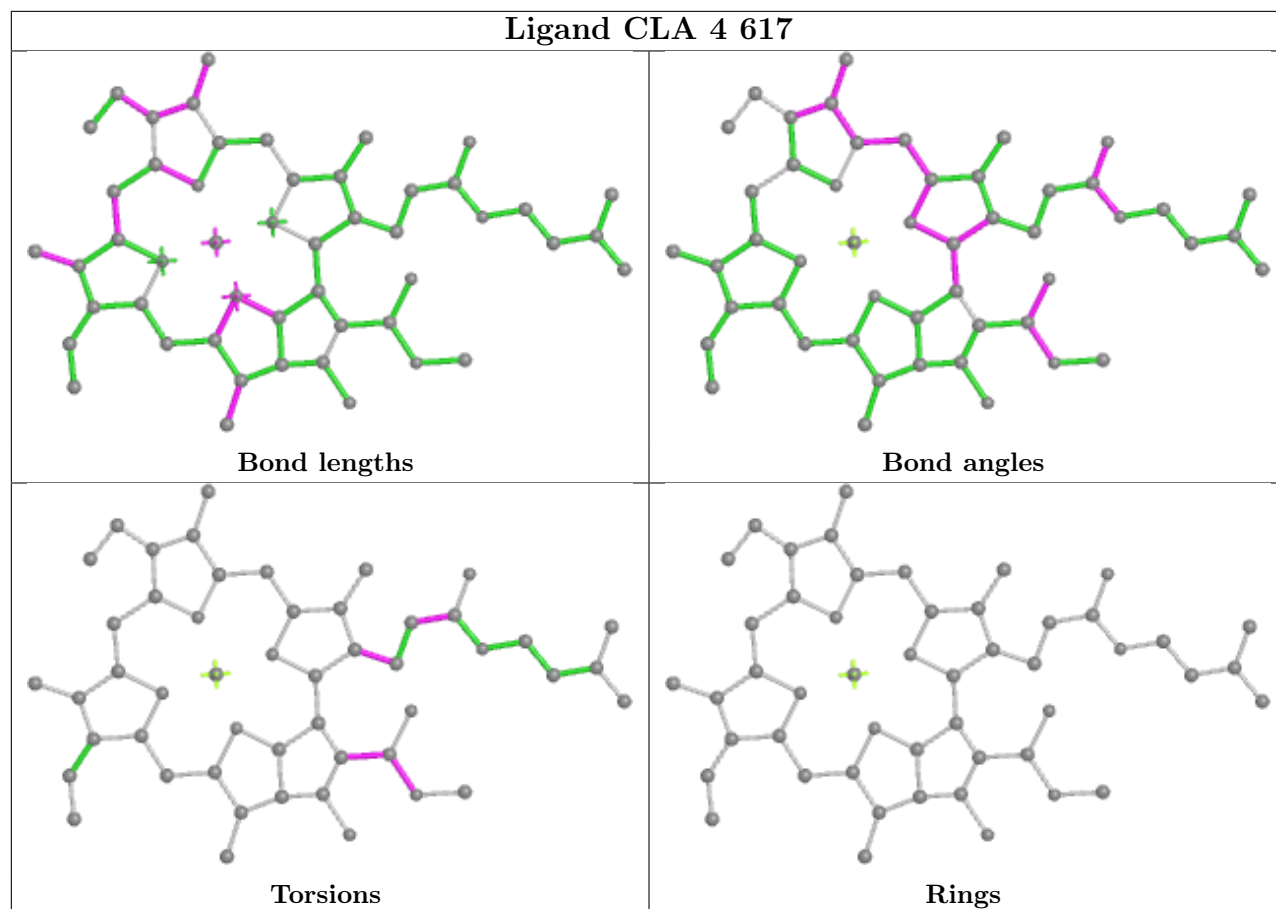
Ligand CHL 3 608



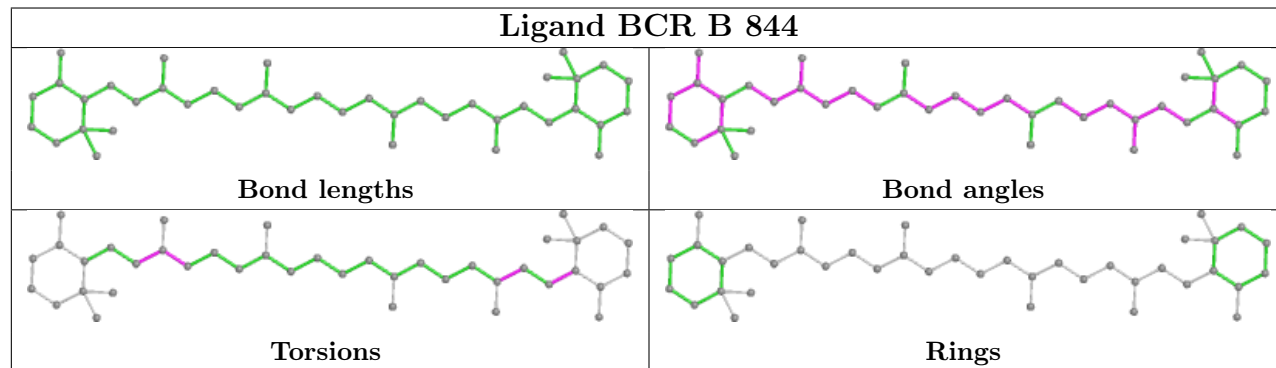
Ligand PQN B 842

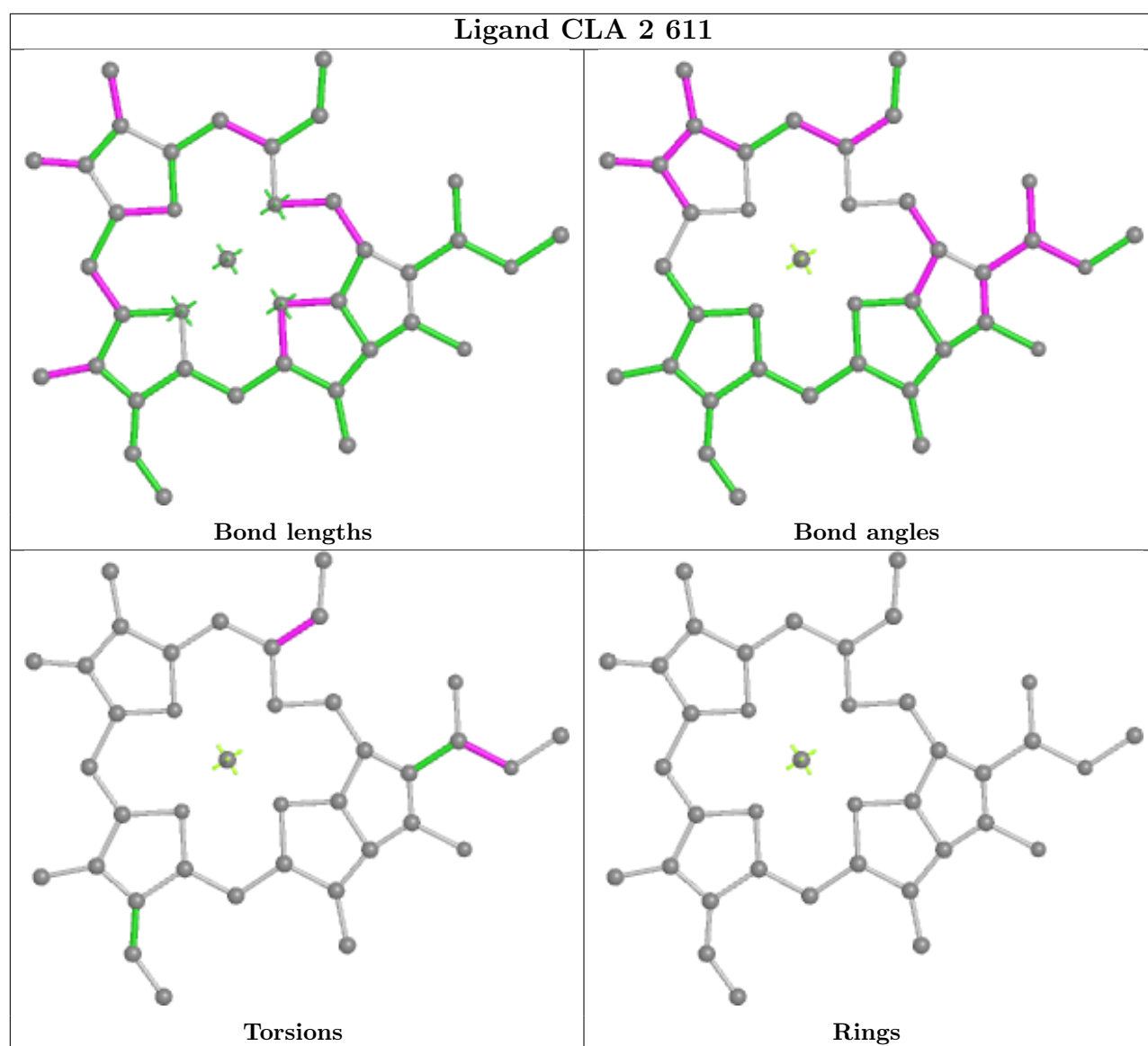
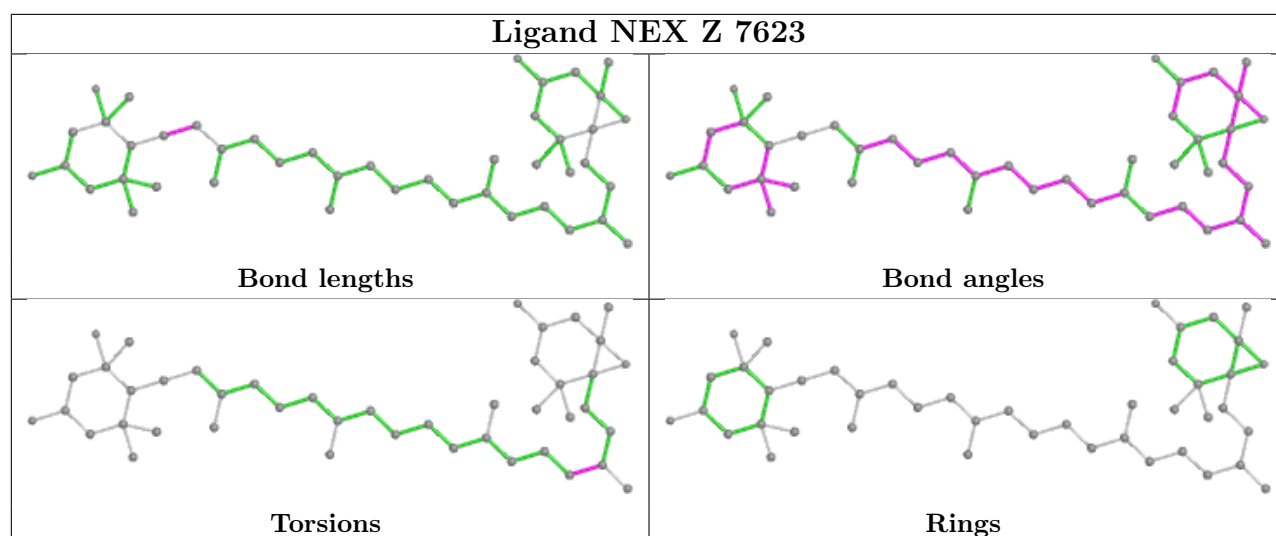


Ligand CLA 4 617

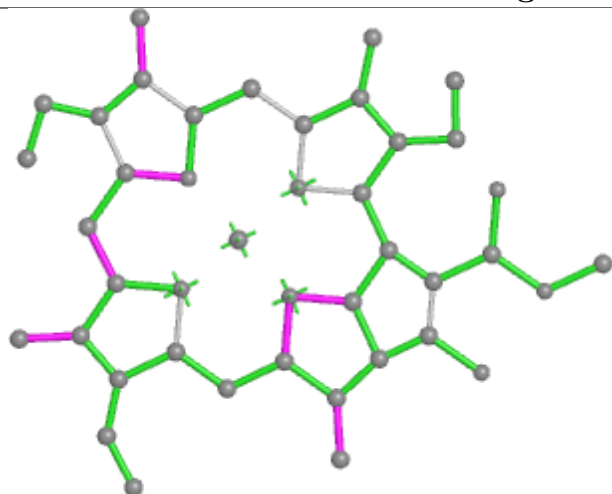


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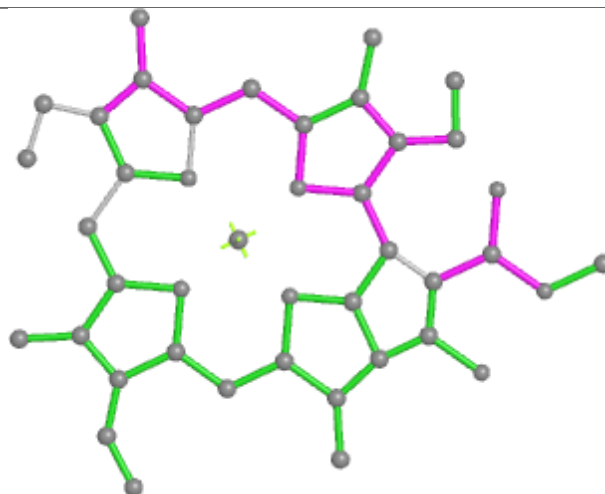




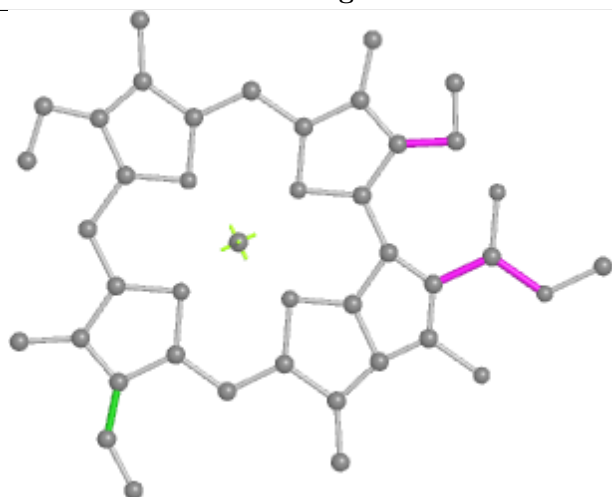
Ligand CLA 4 611



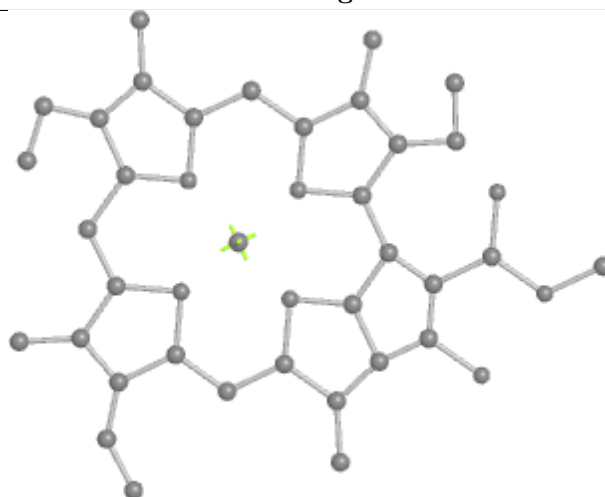
Bond lengths



Bond angles

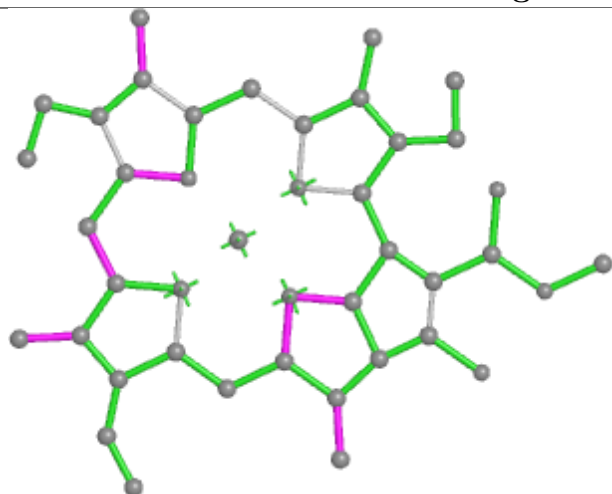


Torsions

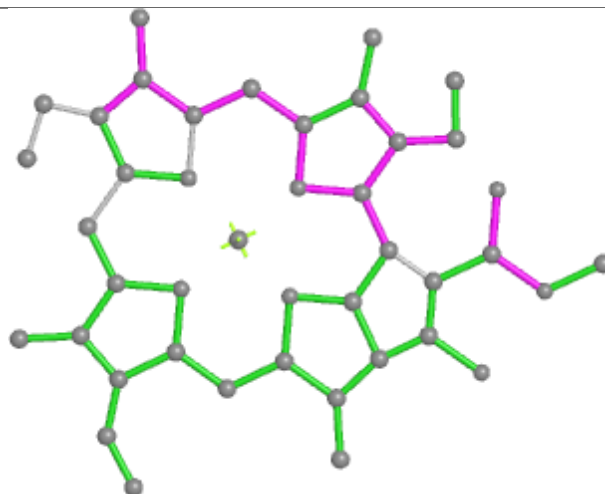


Rings

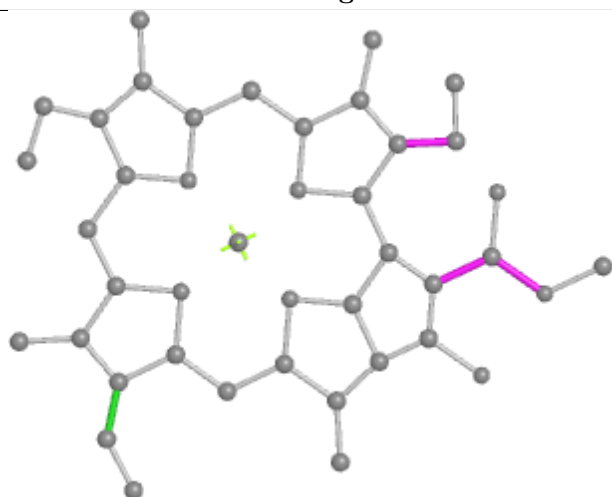
Ligand CLA Y 604



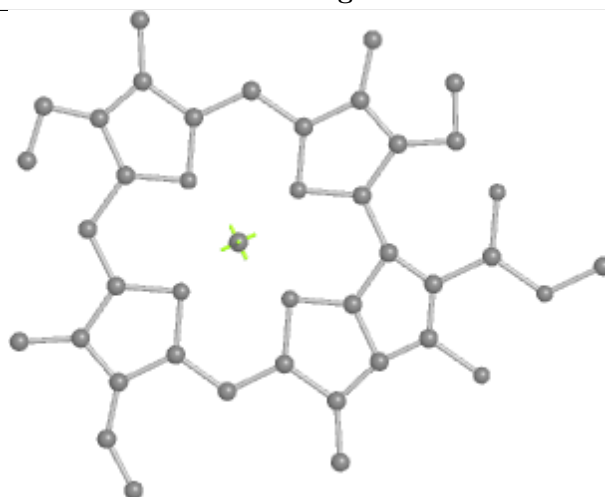
Bond lengths



Bond angles

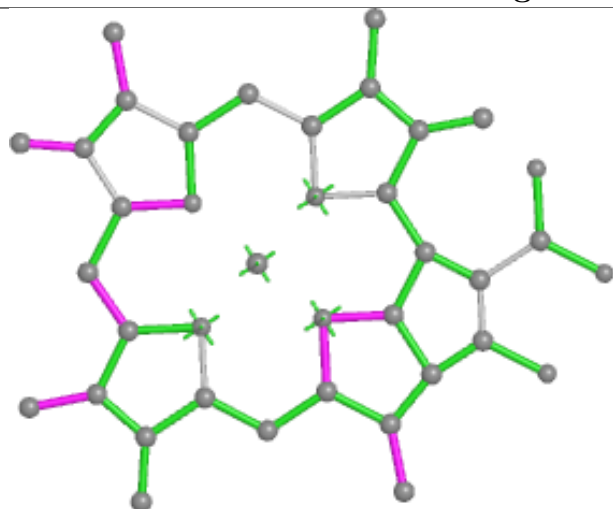


Torsions

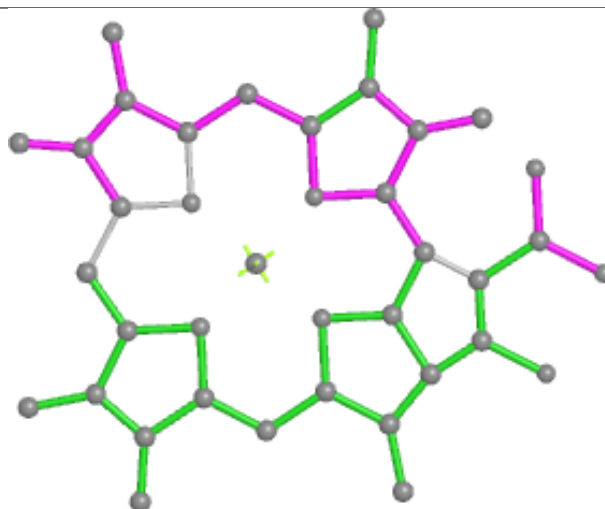


Rings

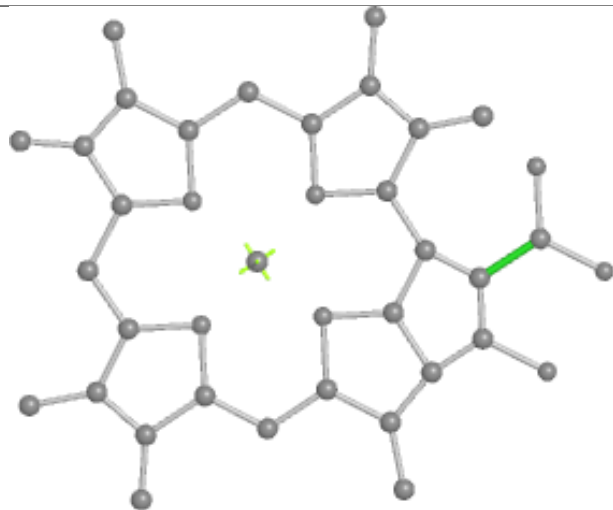
Ligand CLA Y 612



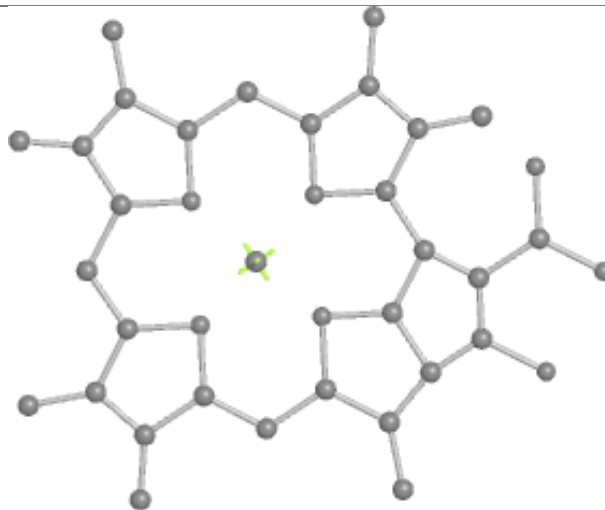
Bond lengths



Bond angles

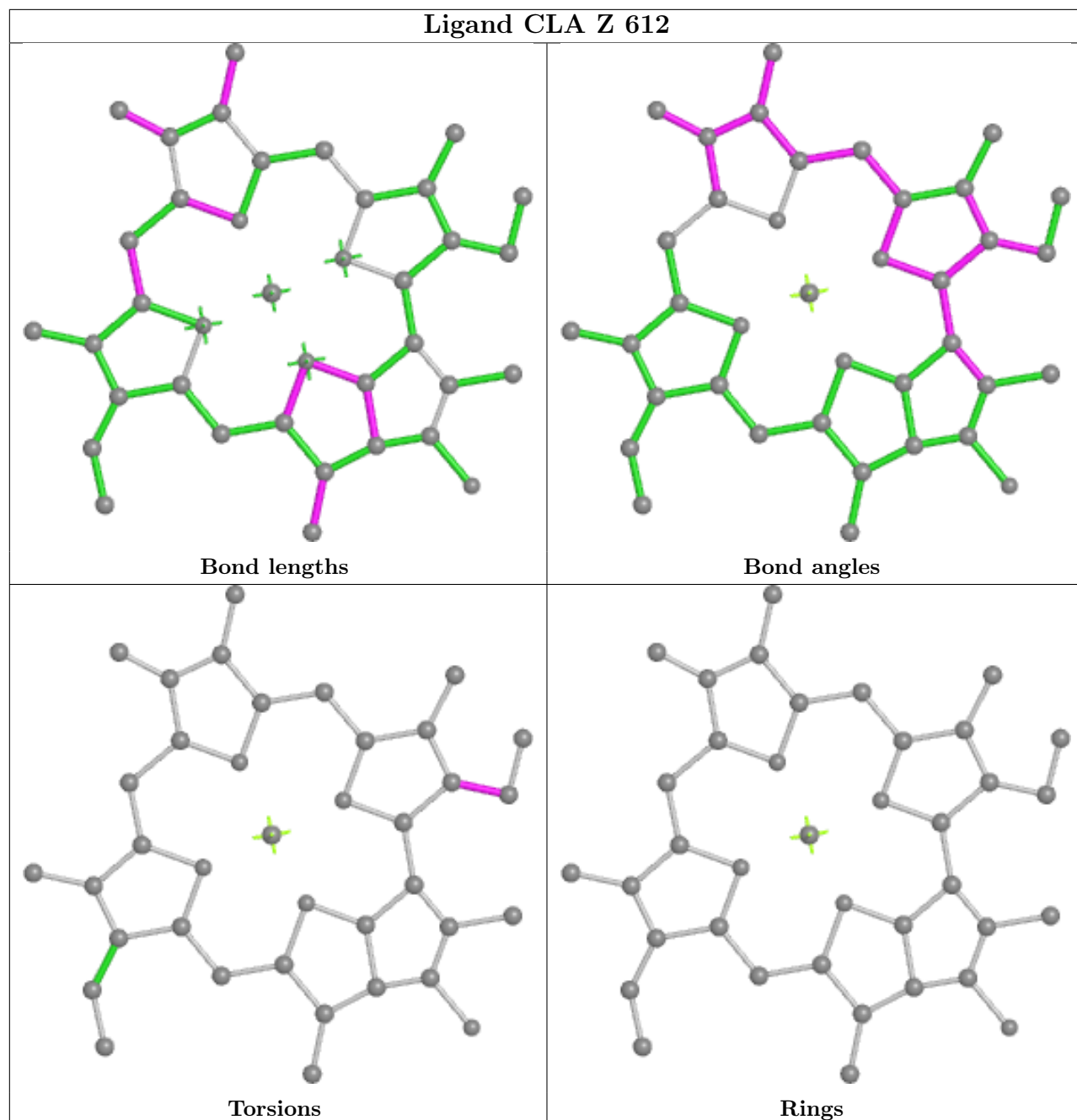


Torsions

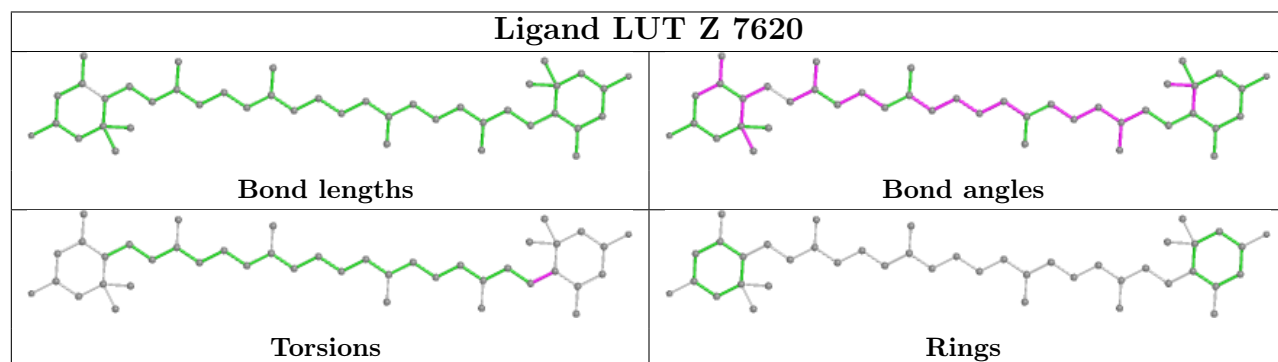


Rings

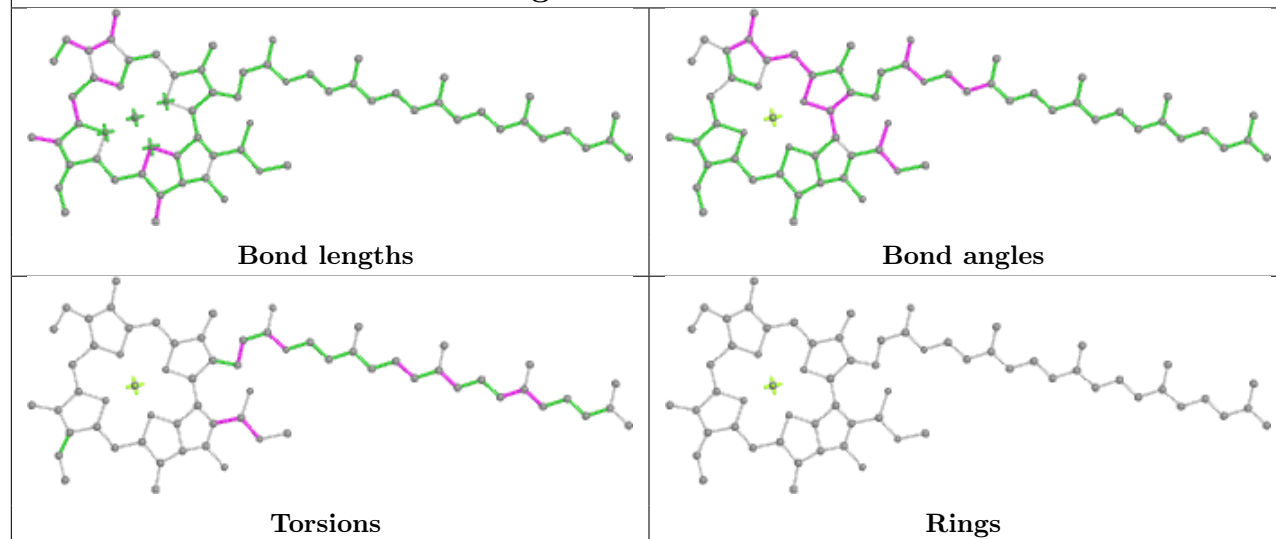
Ligand CLA Z 612



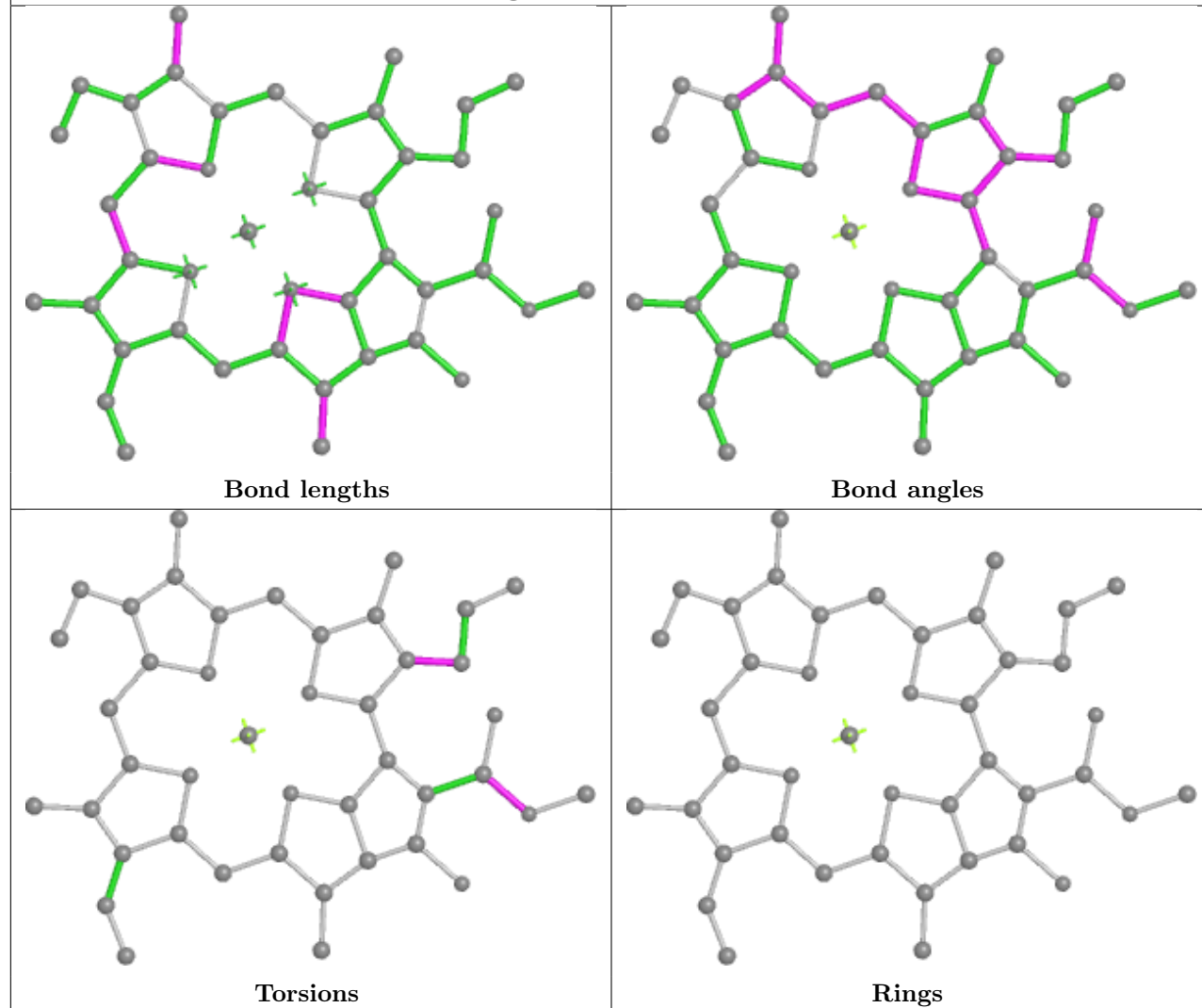
Ligand LUT Z 7620



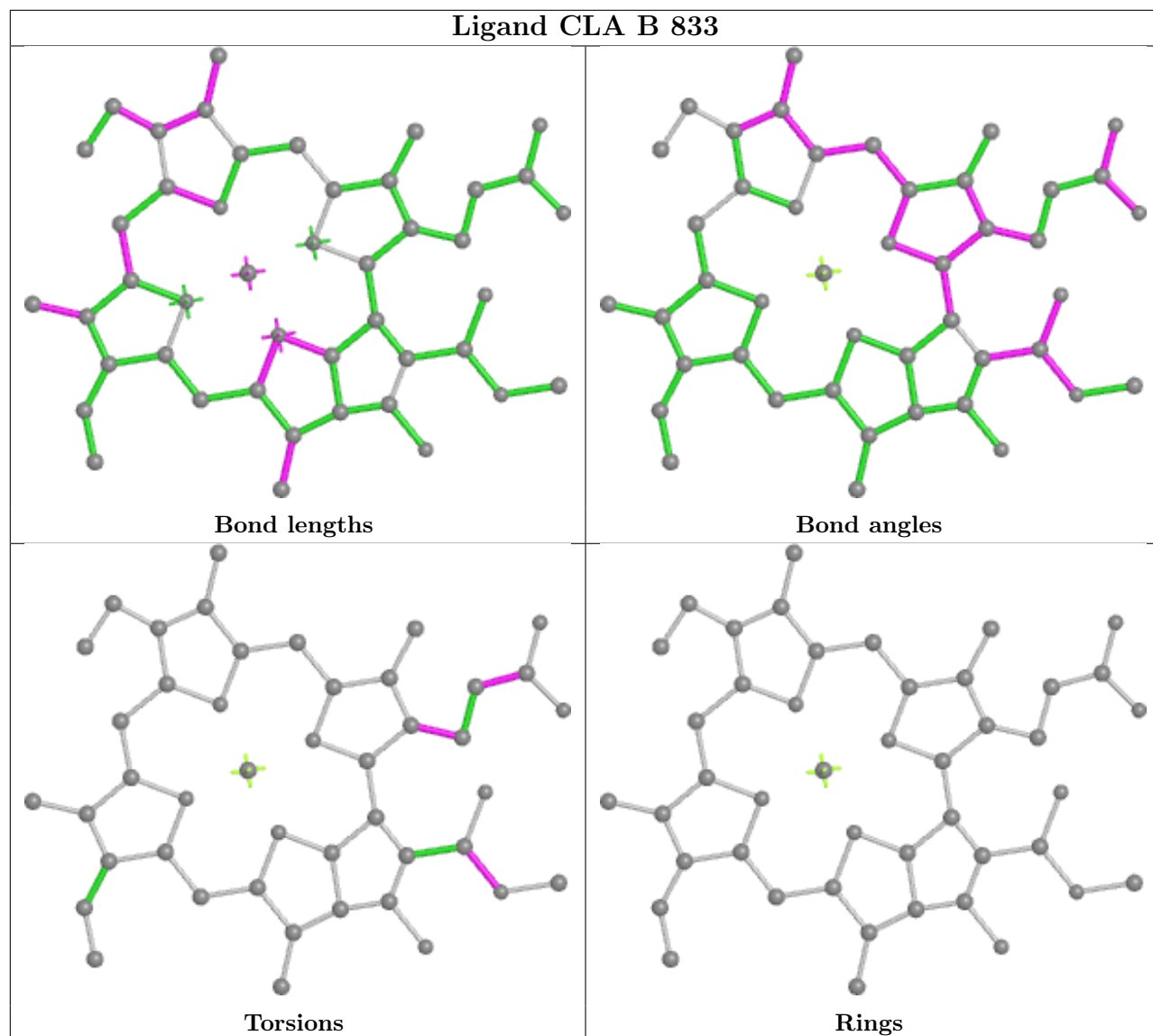
Ligand CLA A 841



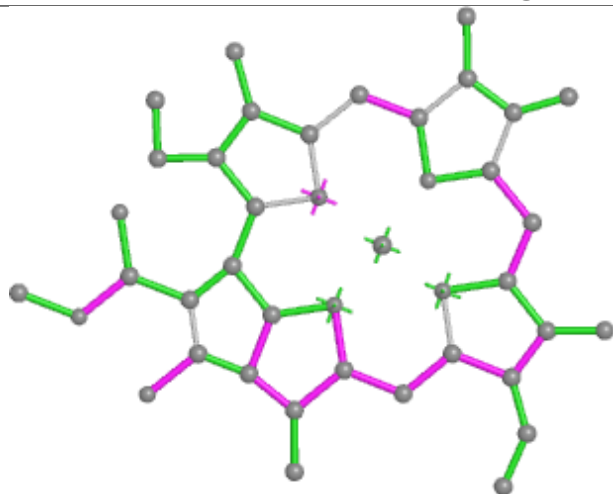
Ligand CLA 3 612



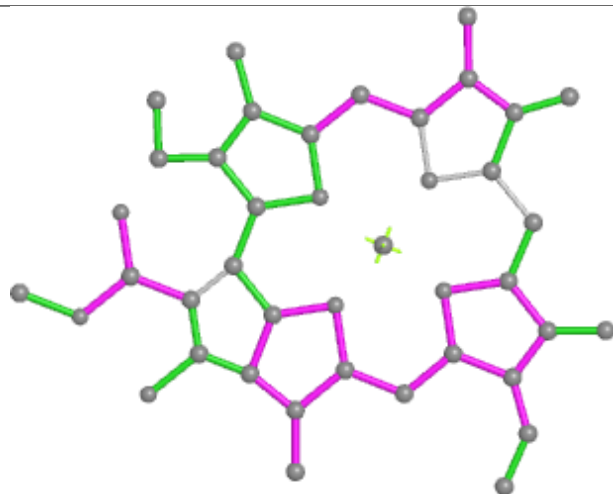
Ligand CLA B 833



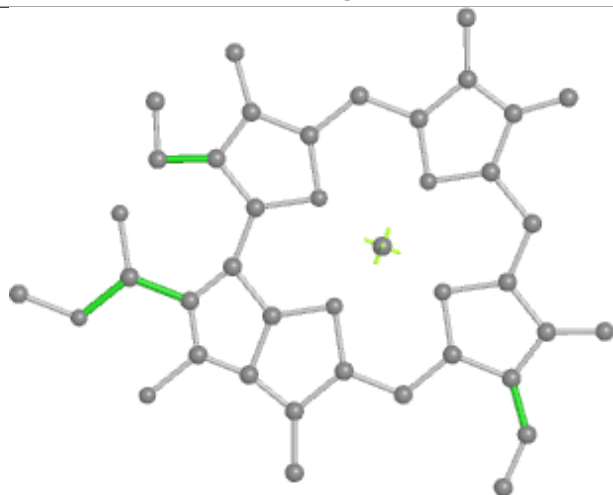
Ligand CHL 4 607



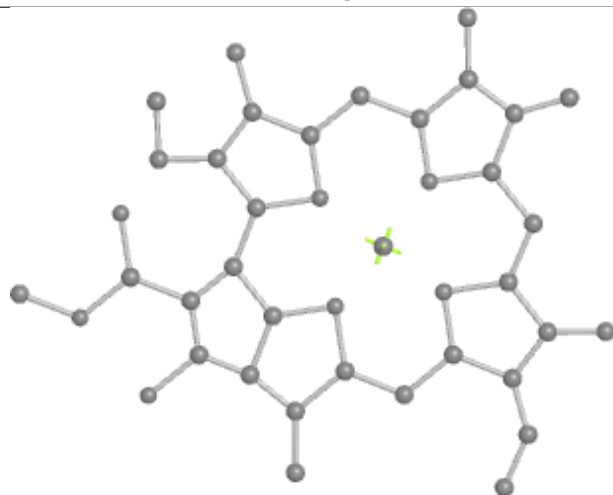
Bond lengths



Bond angles

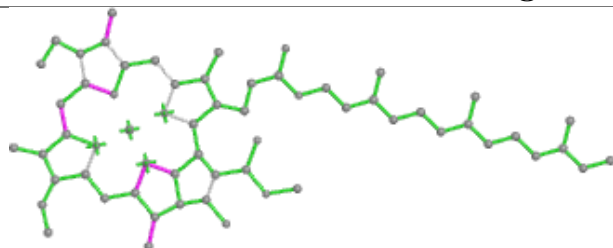


Torsions

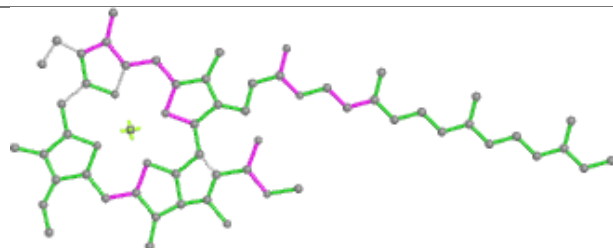


Rings

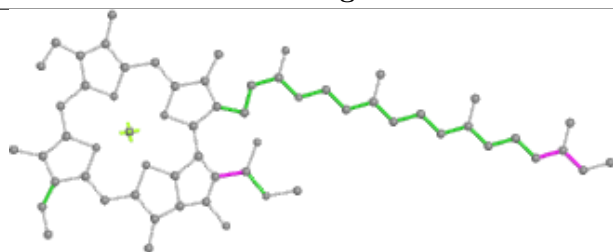
Ligand CLA 1 602



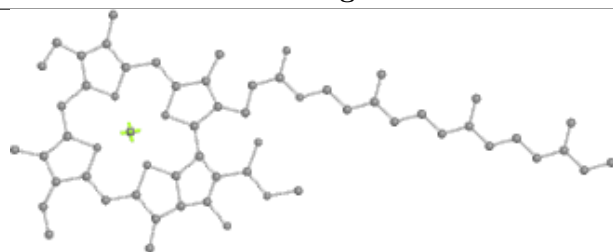
Bond lengths



Bond angles

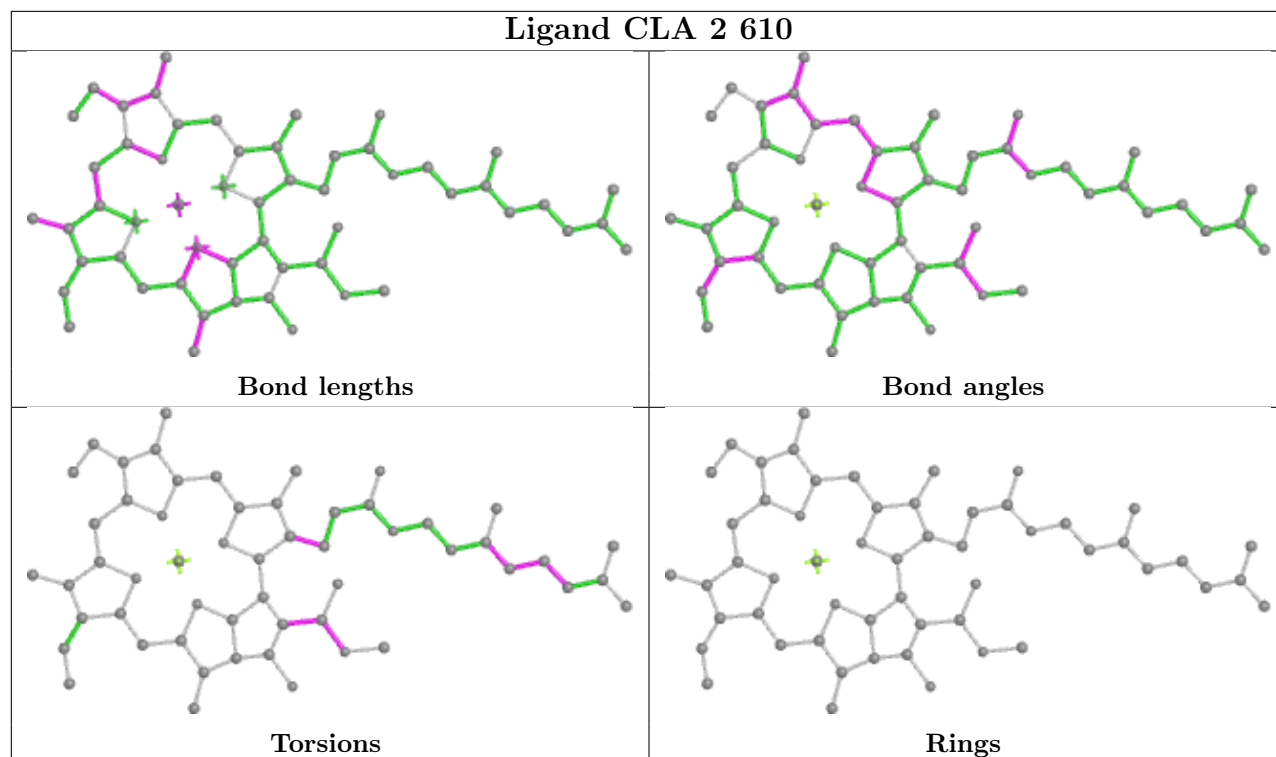


Torsions

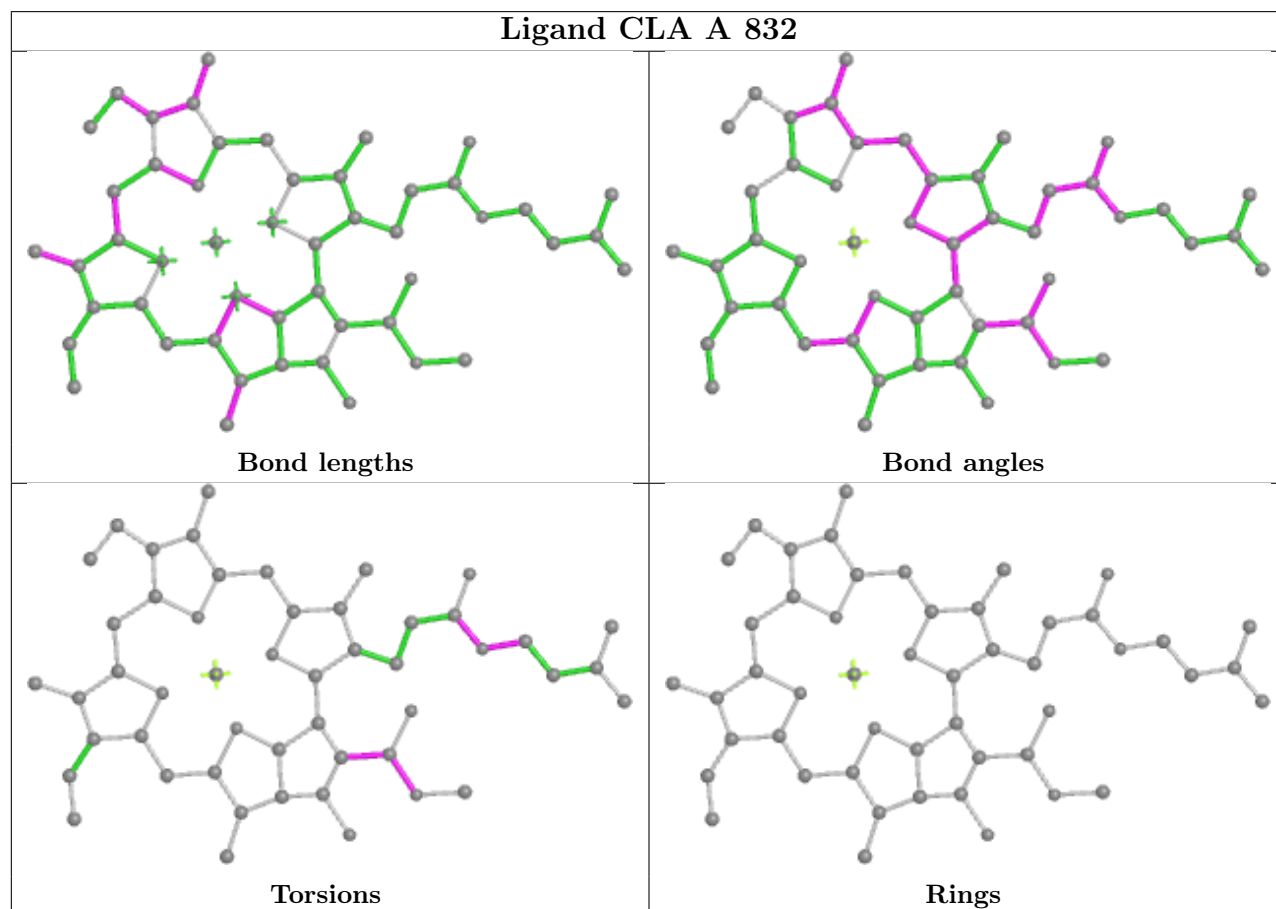


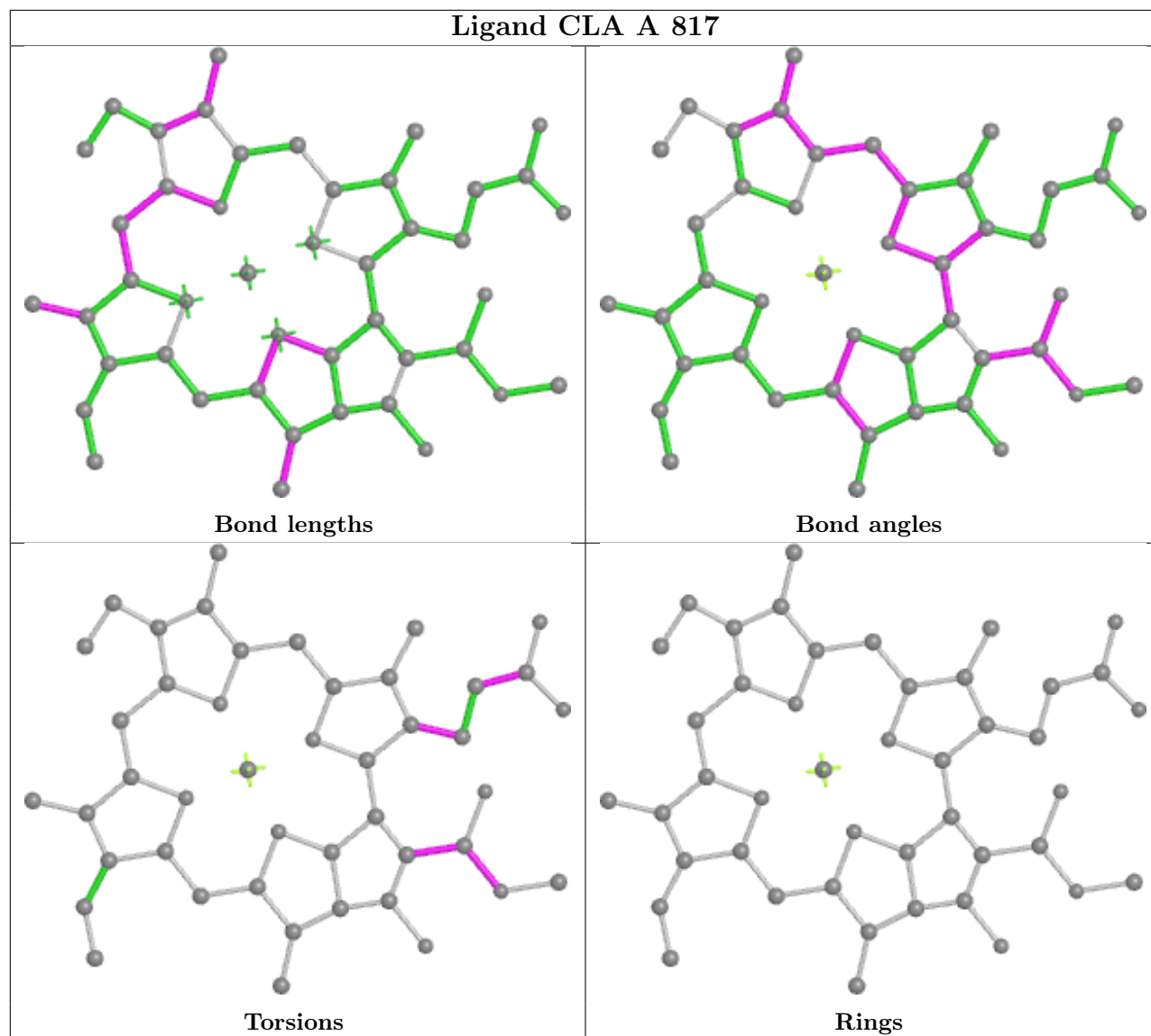
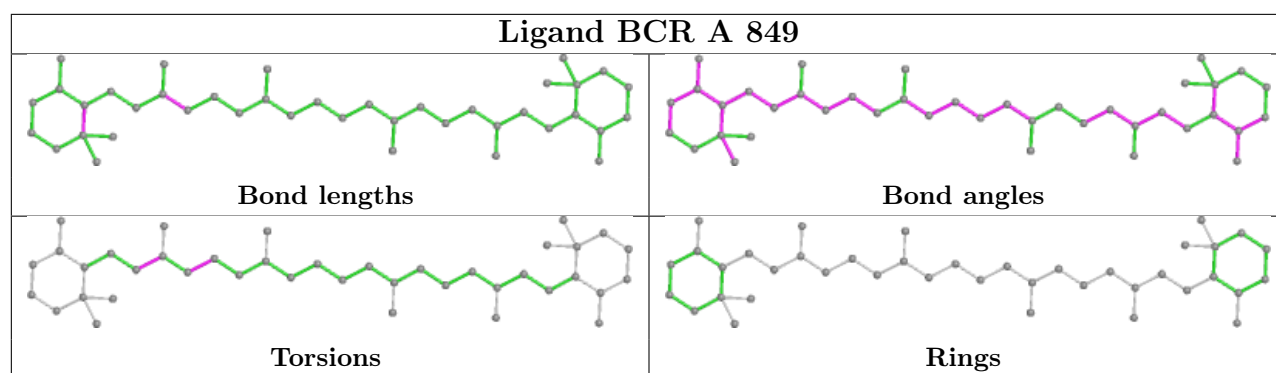
Rings

Ligand CLA 2 610

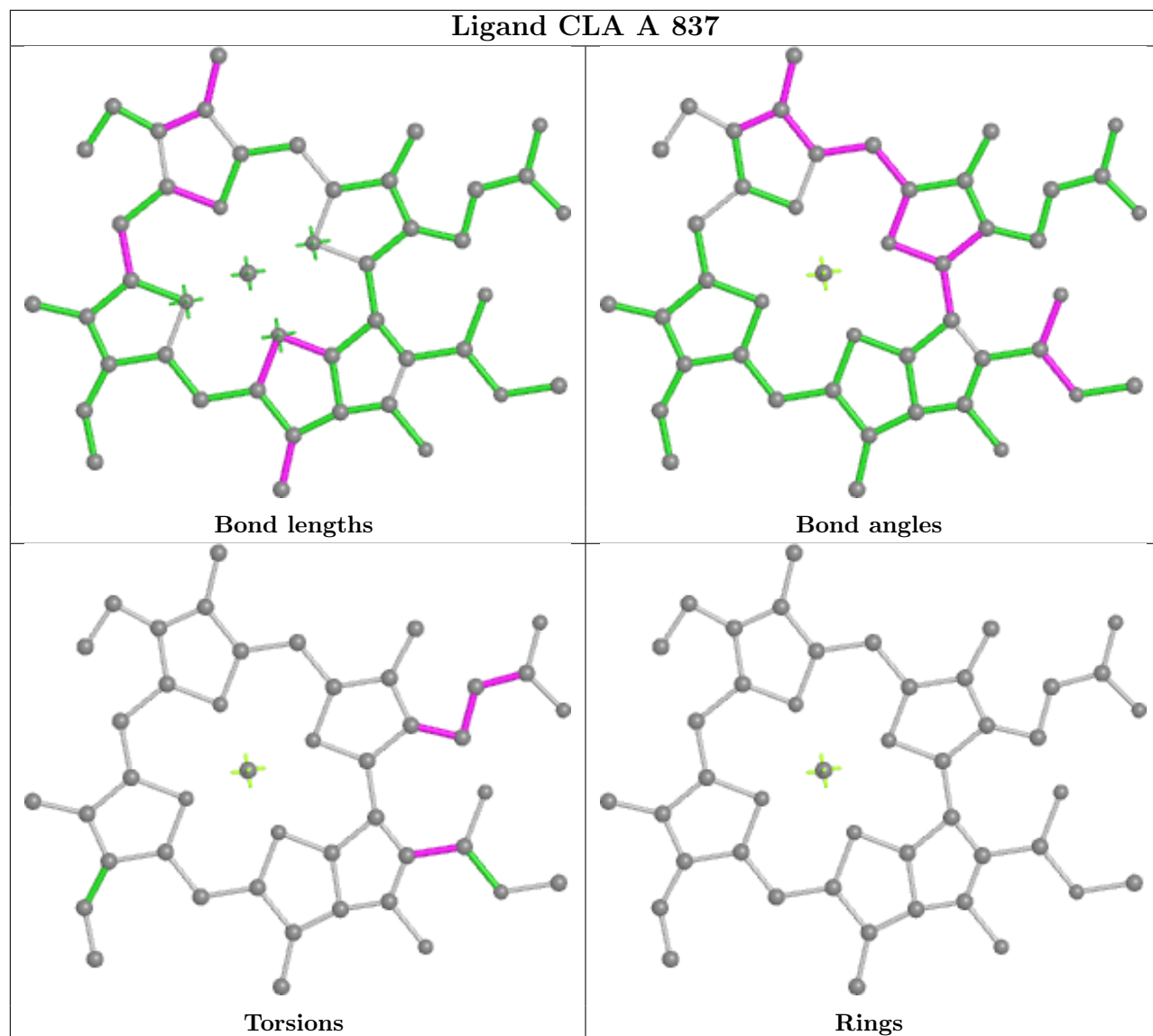


Ligand CLA A 832

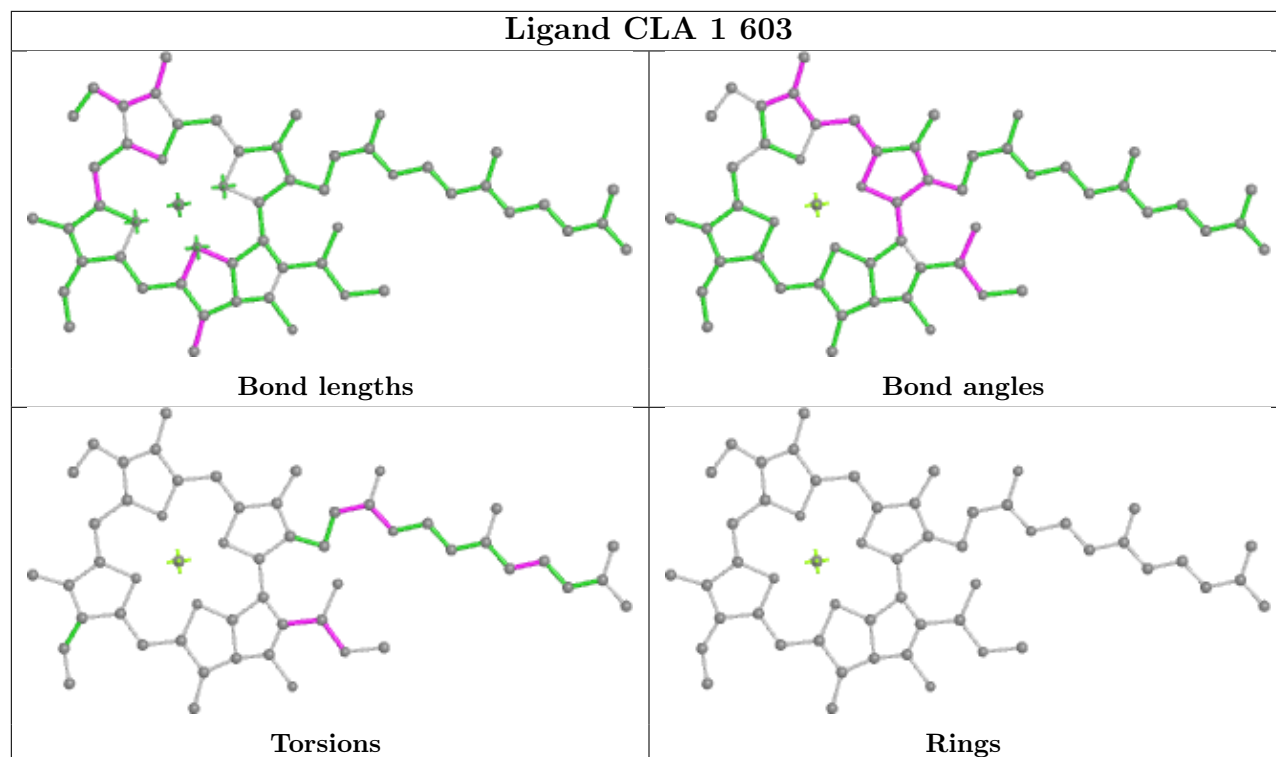




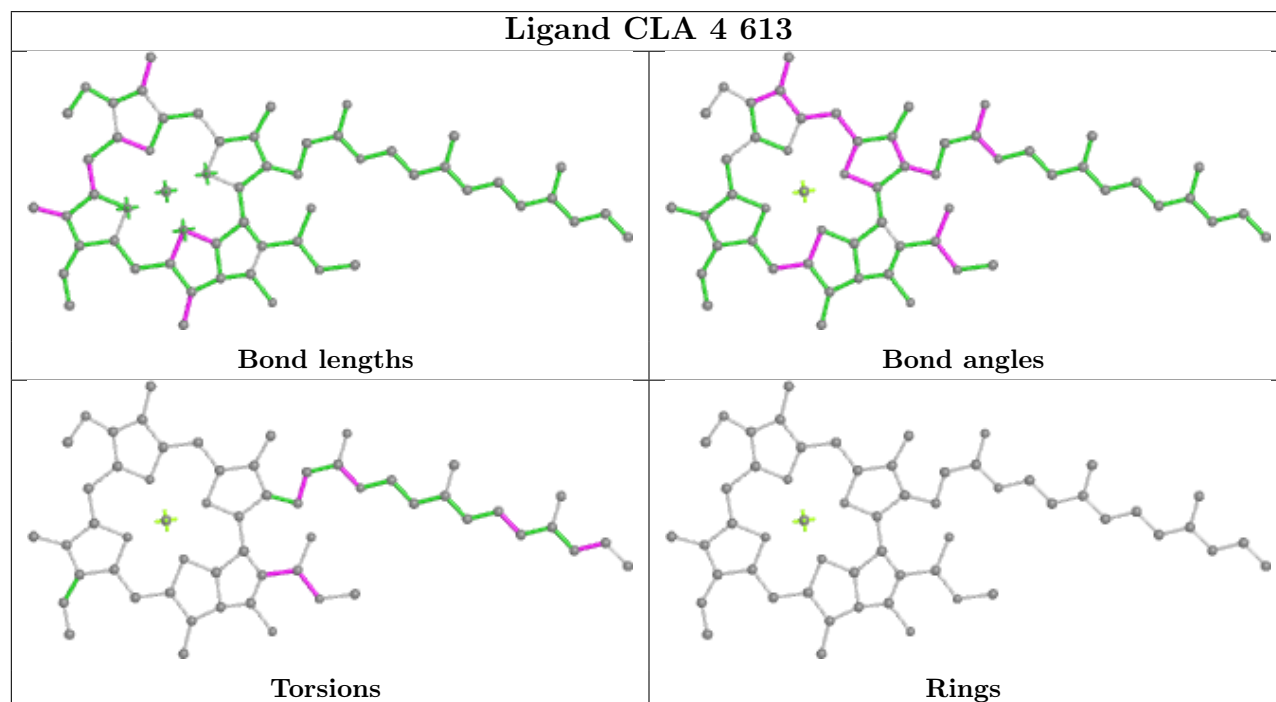
Ligand CLA A 837

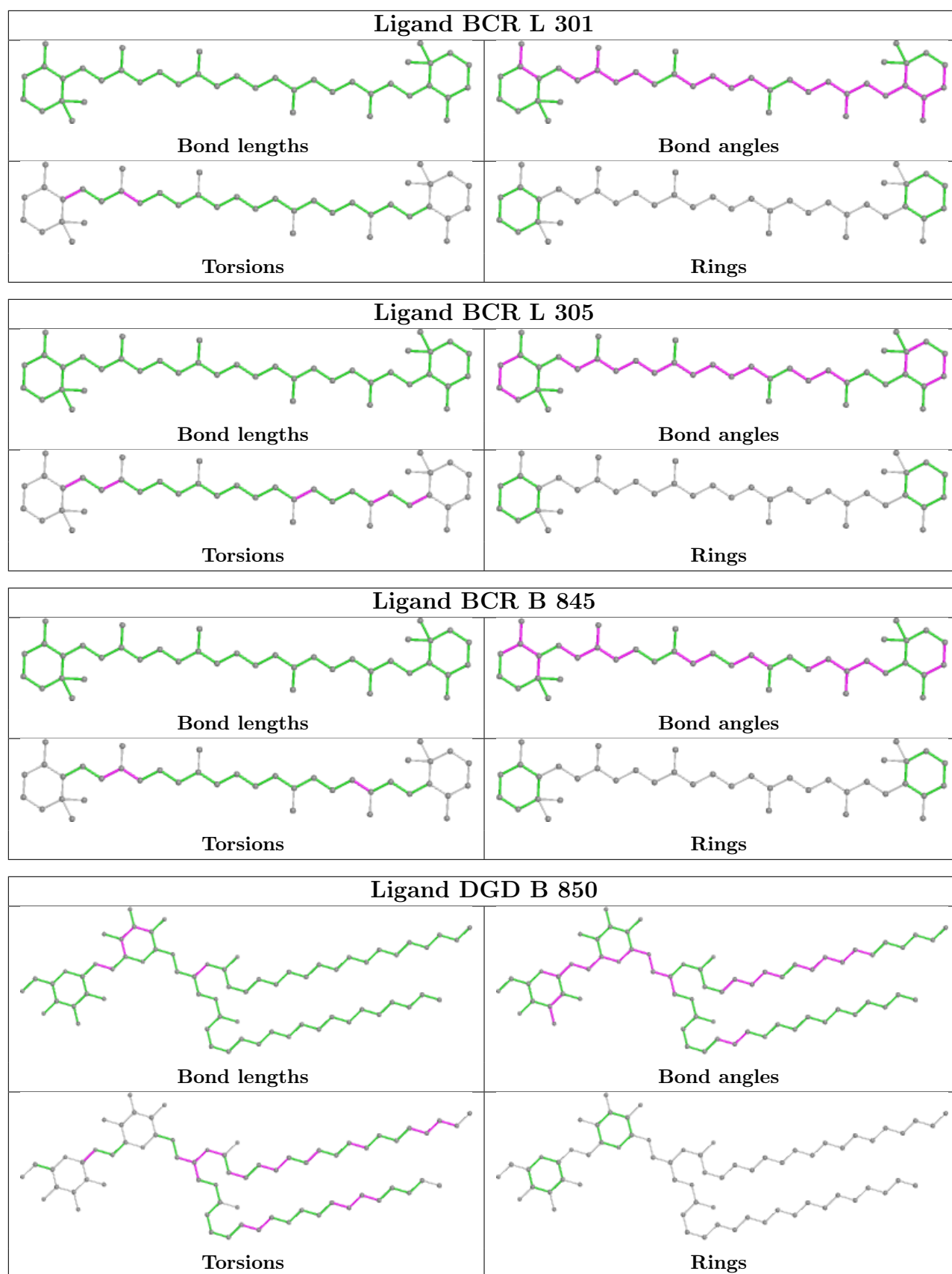


Ligand CLA 1 603

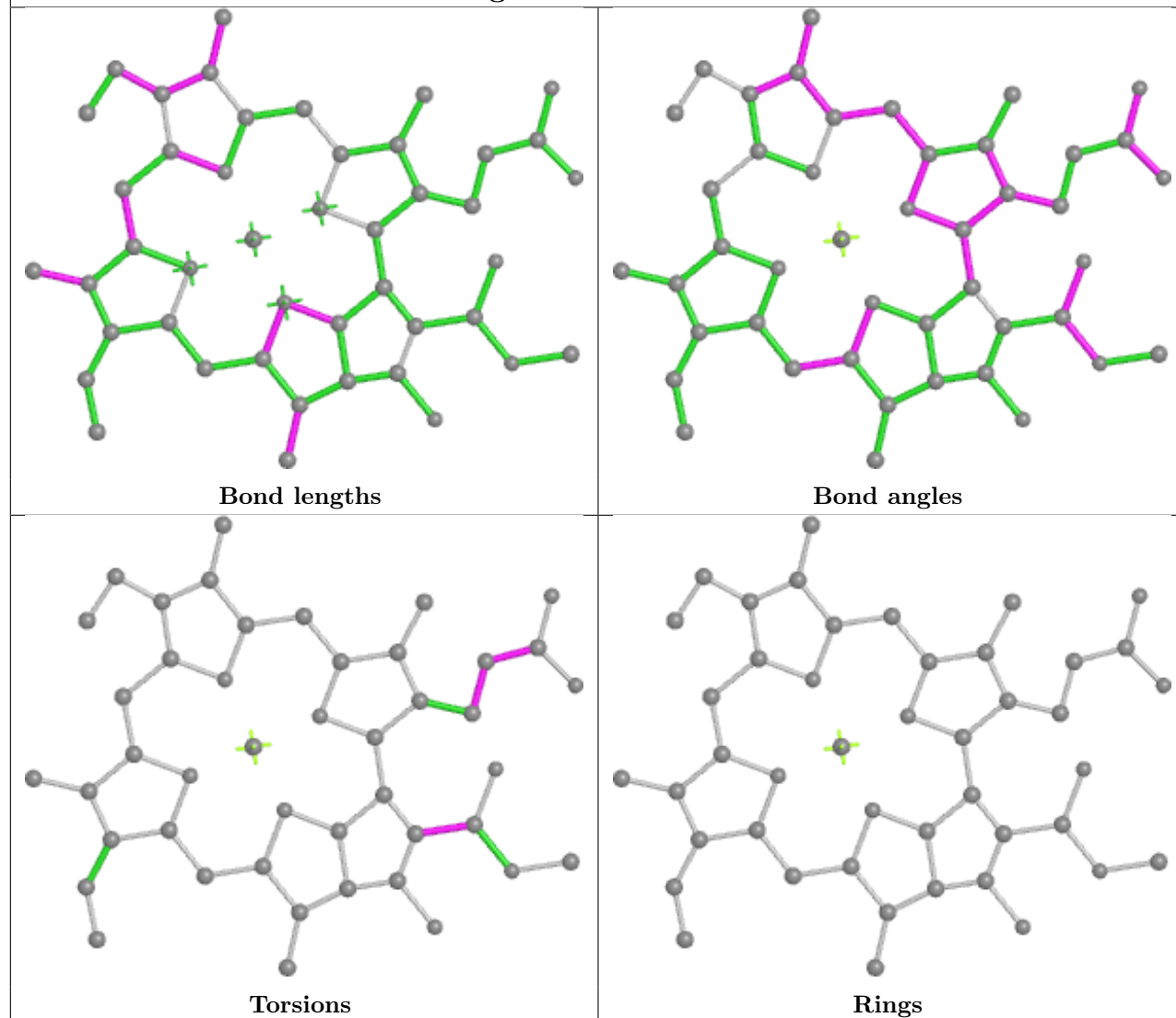


Ligand CLA 4 613

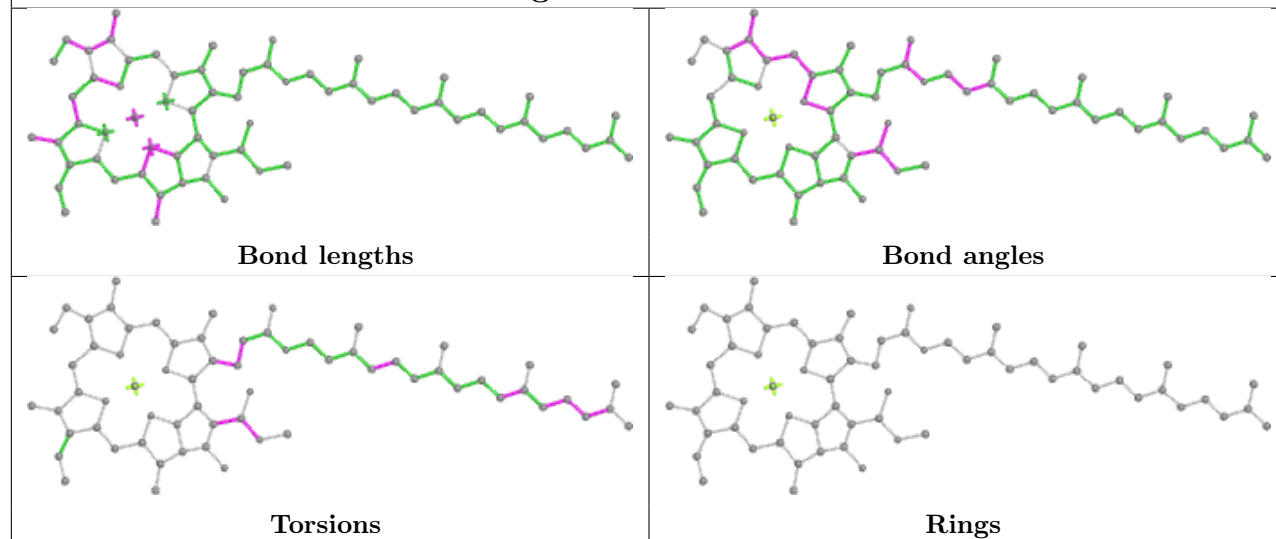




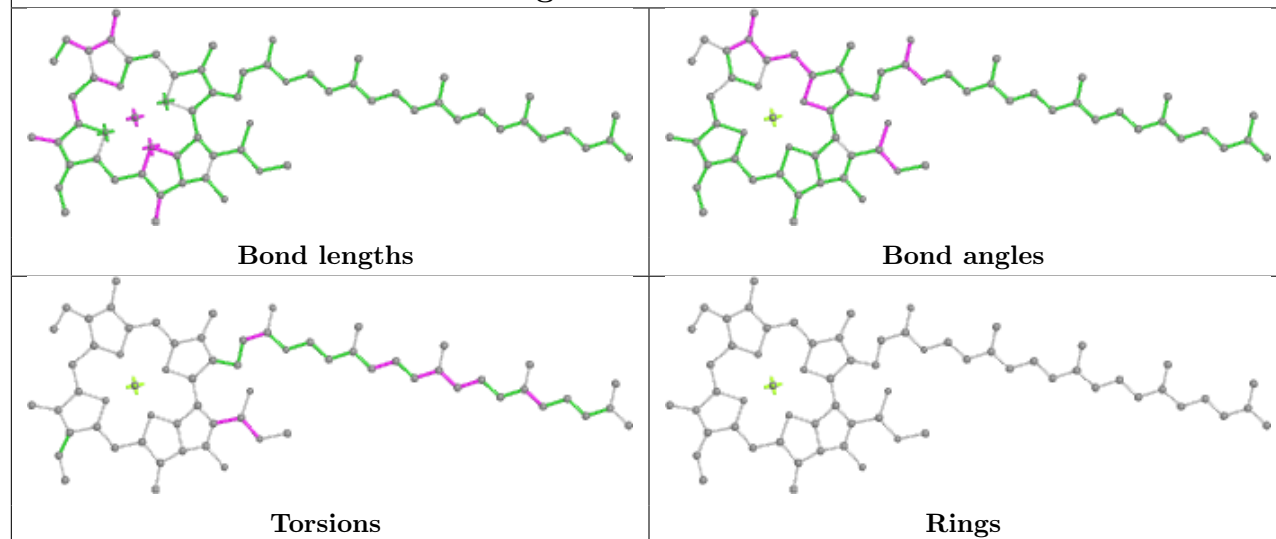
Ligand CLA K 203



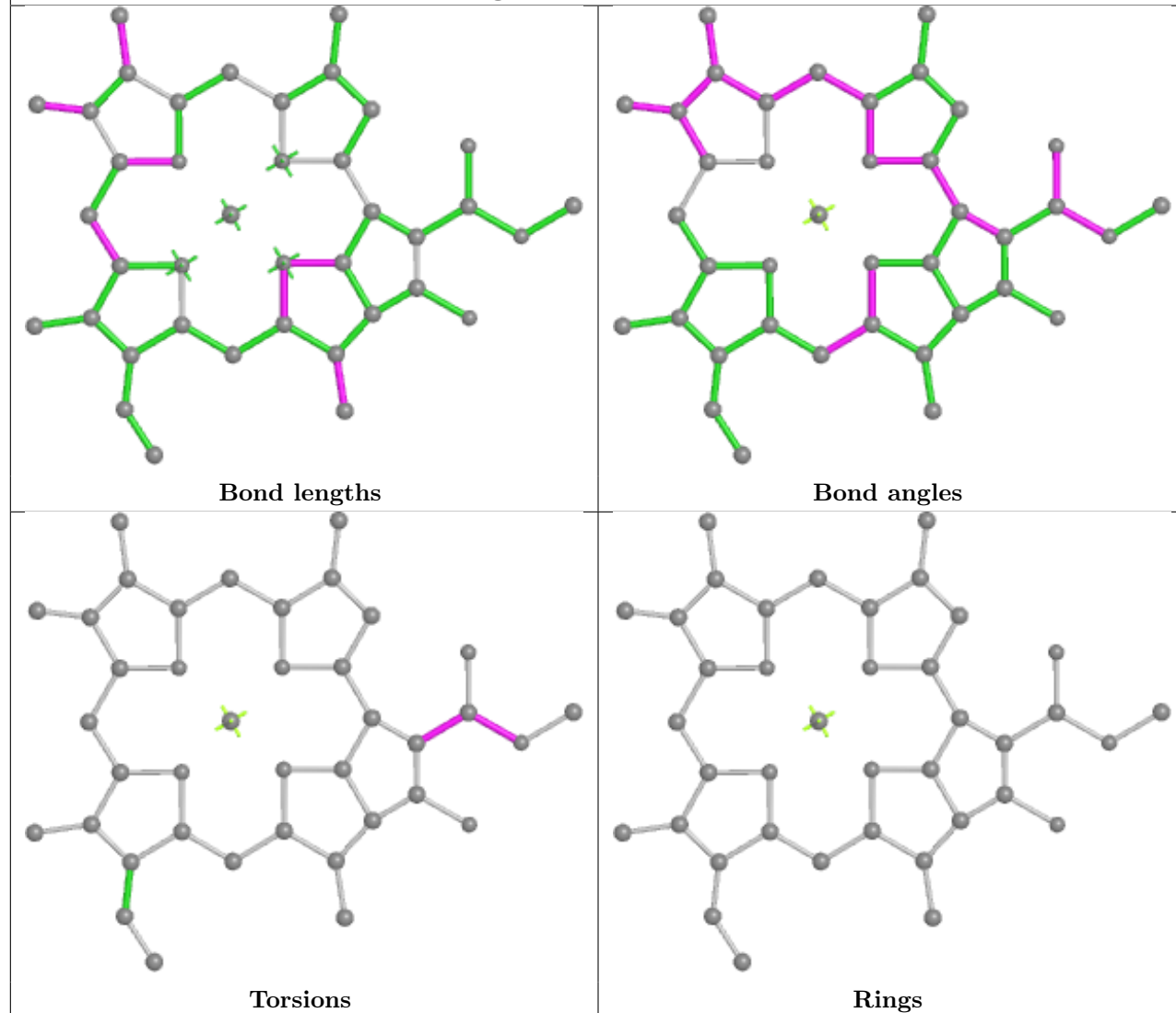
Ligand CLA A 809



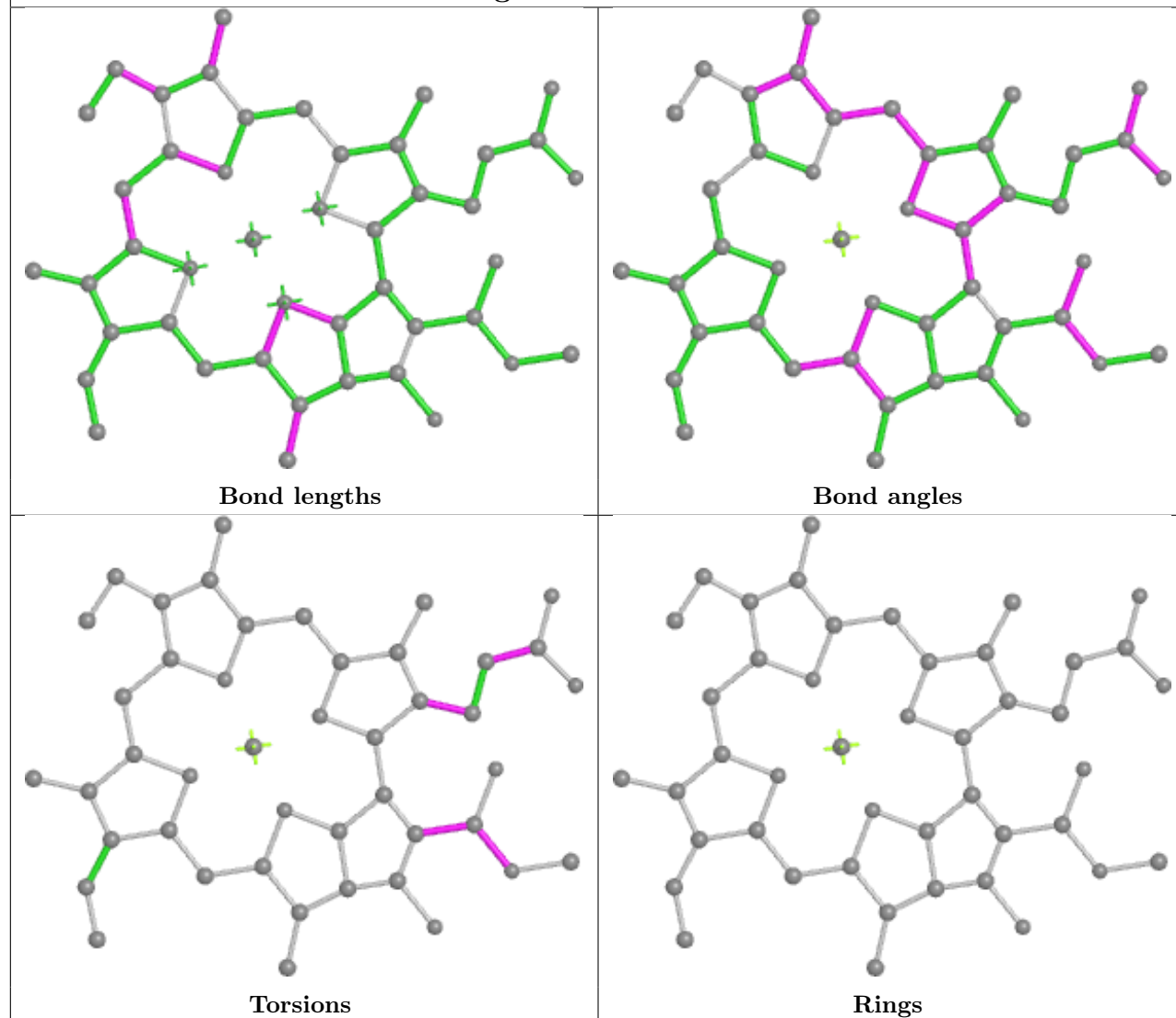
Ligand CLA 1 613



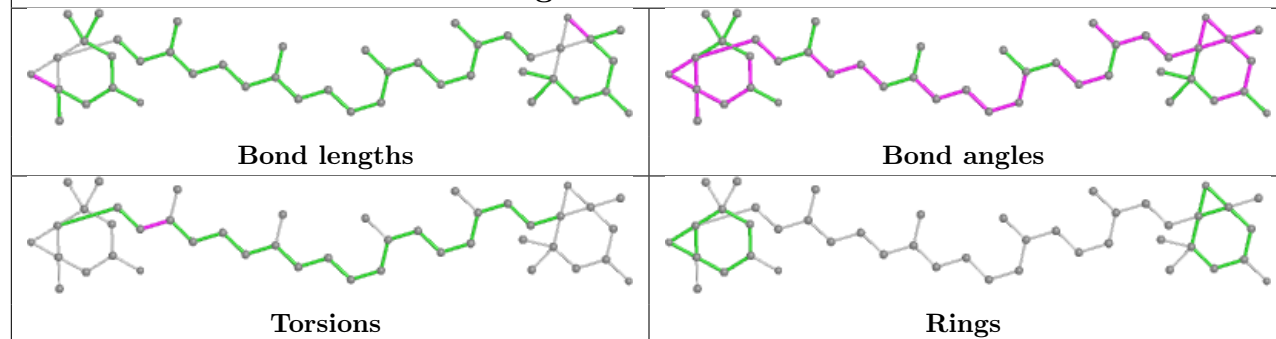
Ligand CLA X 614



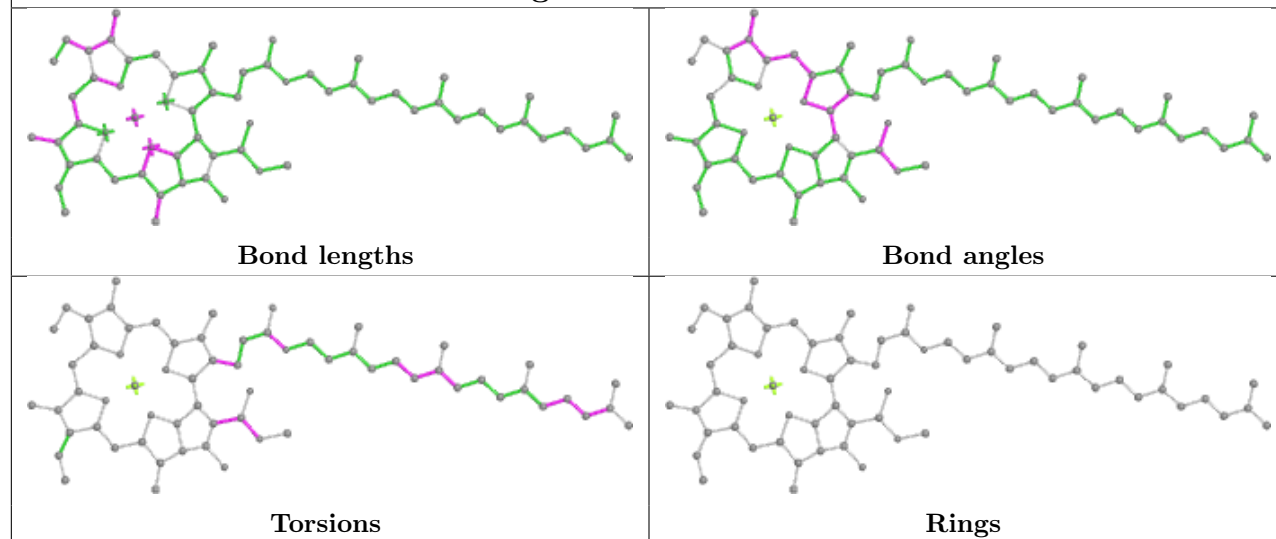
Ligand CLA 2 609



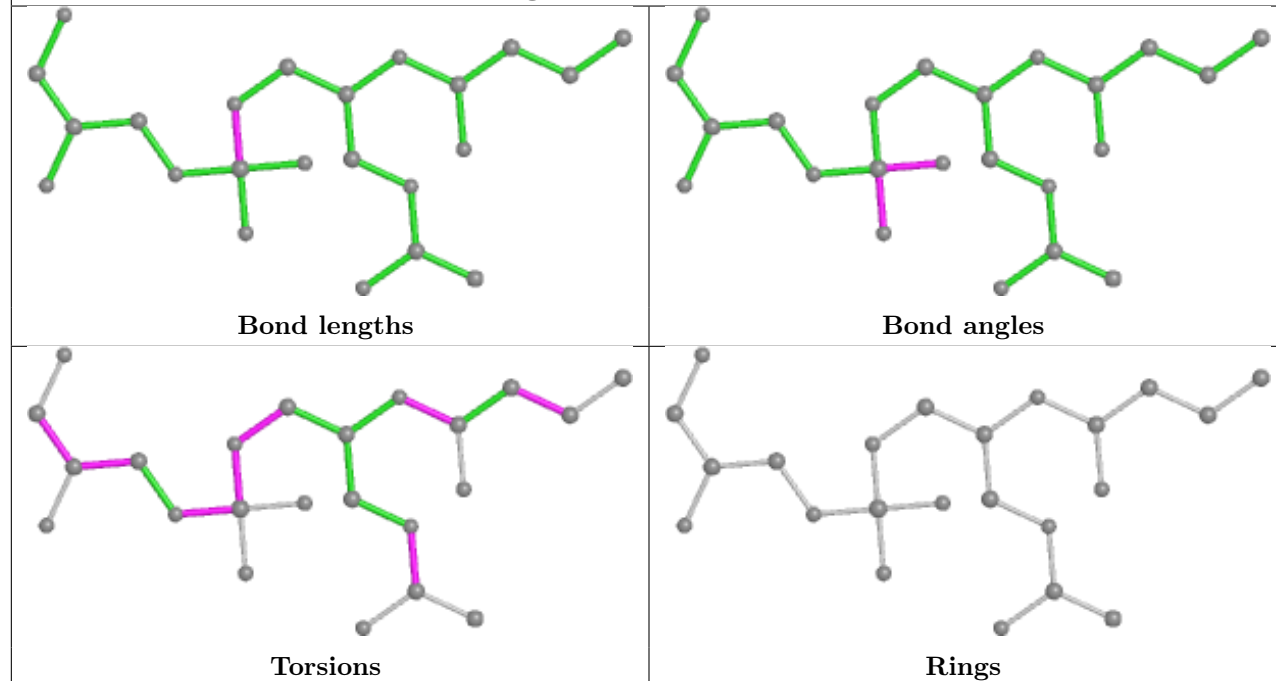
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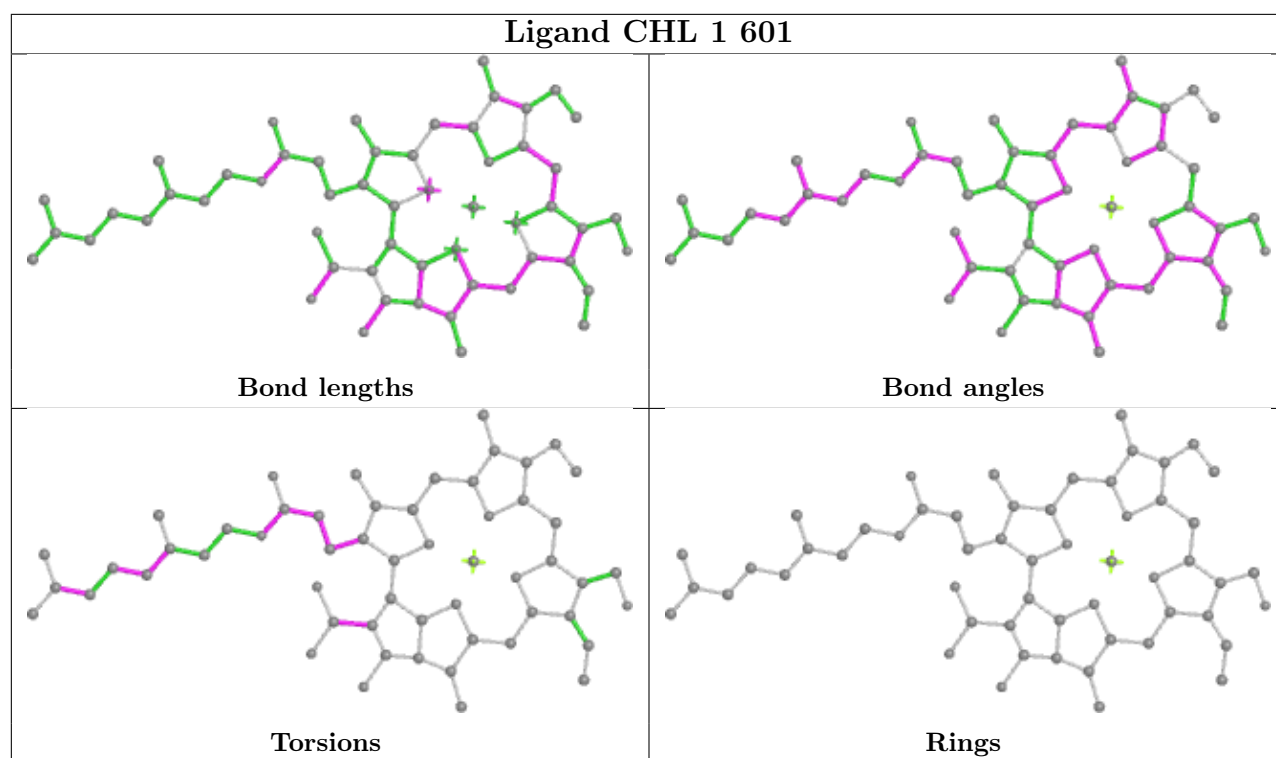


Ligand CLA A 811

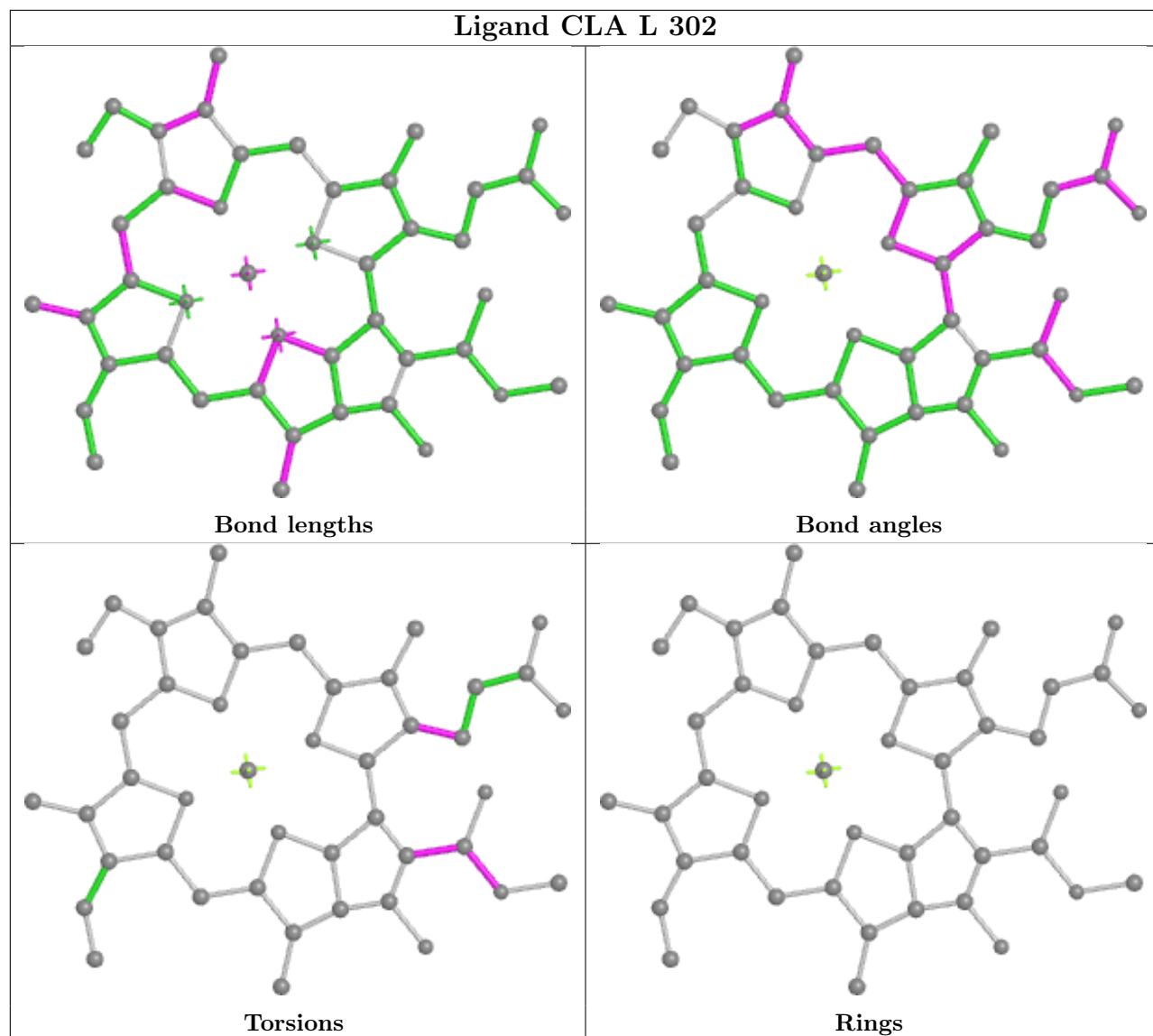


Ligand LHG Z 7630

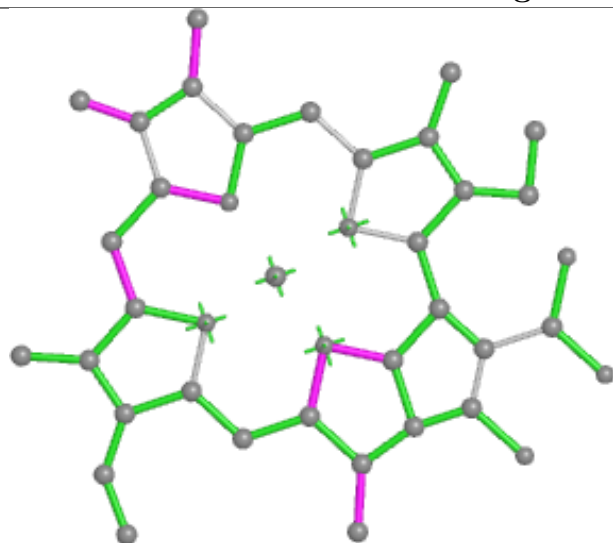




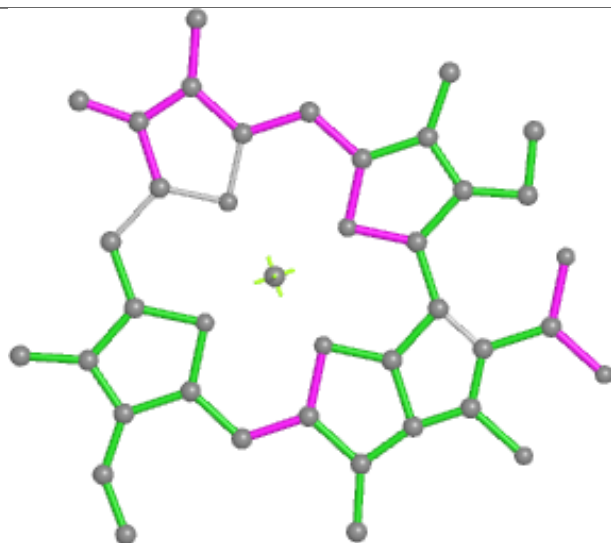
Ligand CLA L 302



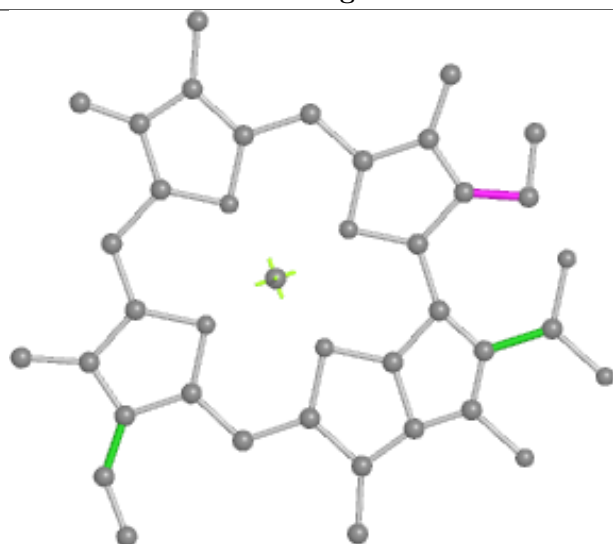
Ligand CLA Y 611



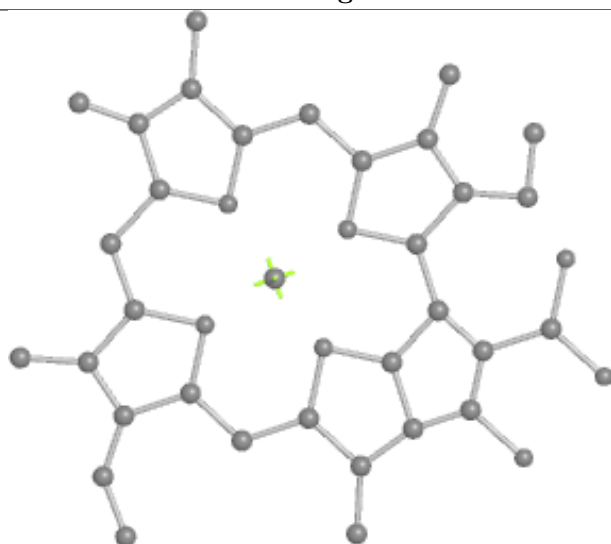
Bond lengths



Bond angles

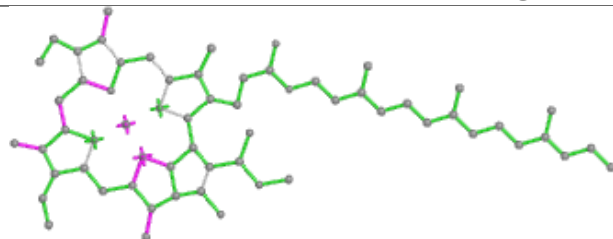


Torsions

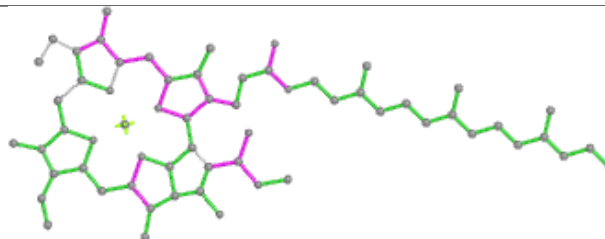


Rings

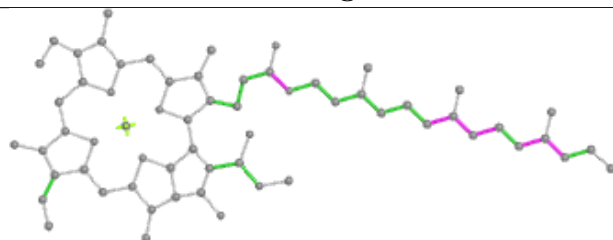
Ligand CLA B 825



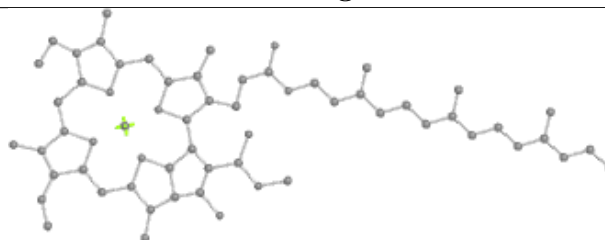
Bond lengths



Bond angles

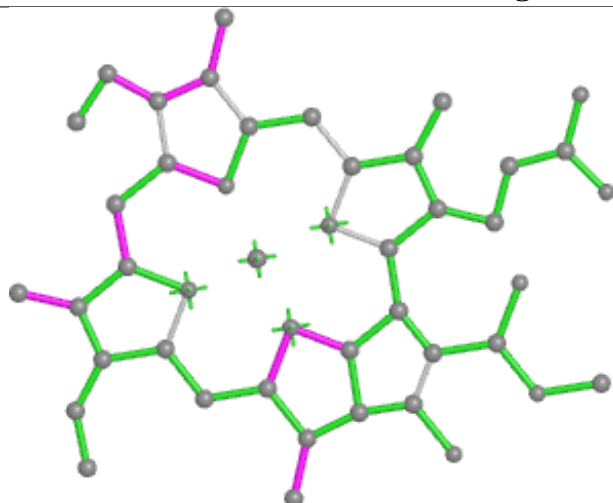


Torsions

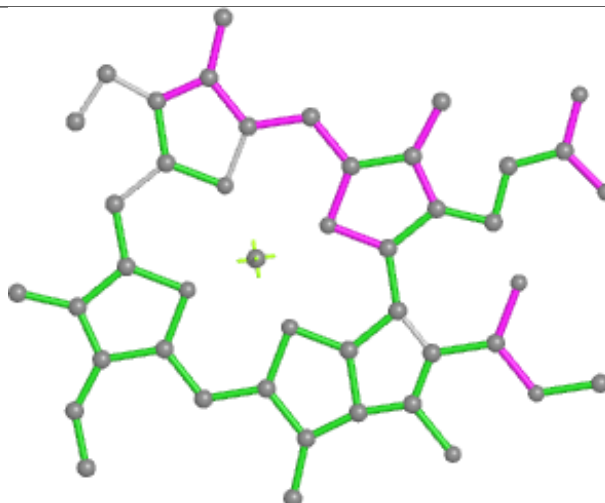


Rings

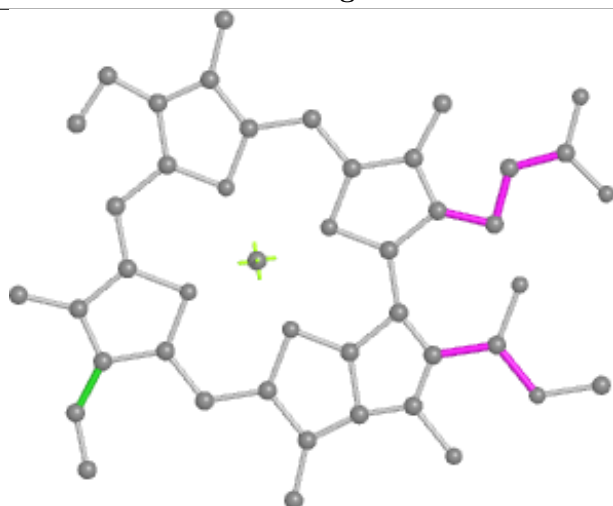
Ligand CLA Y 602



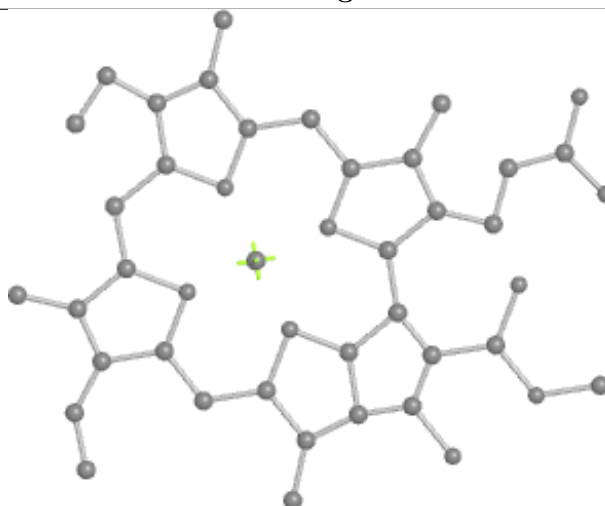
Bond lengths



Bond angles

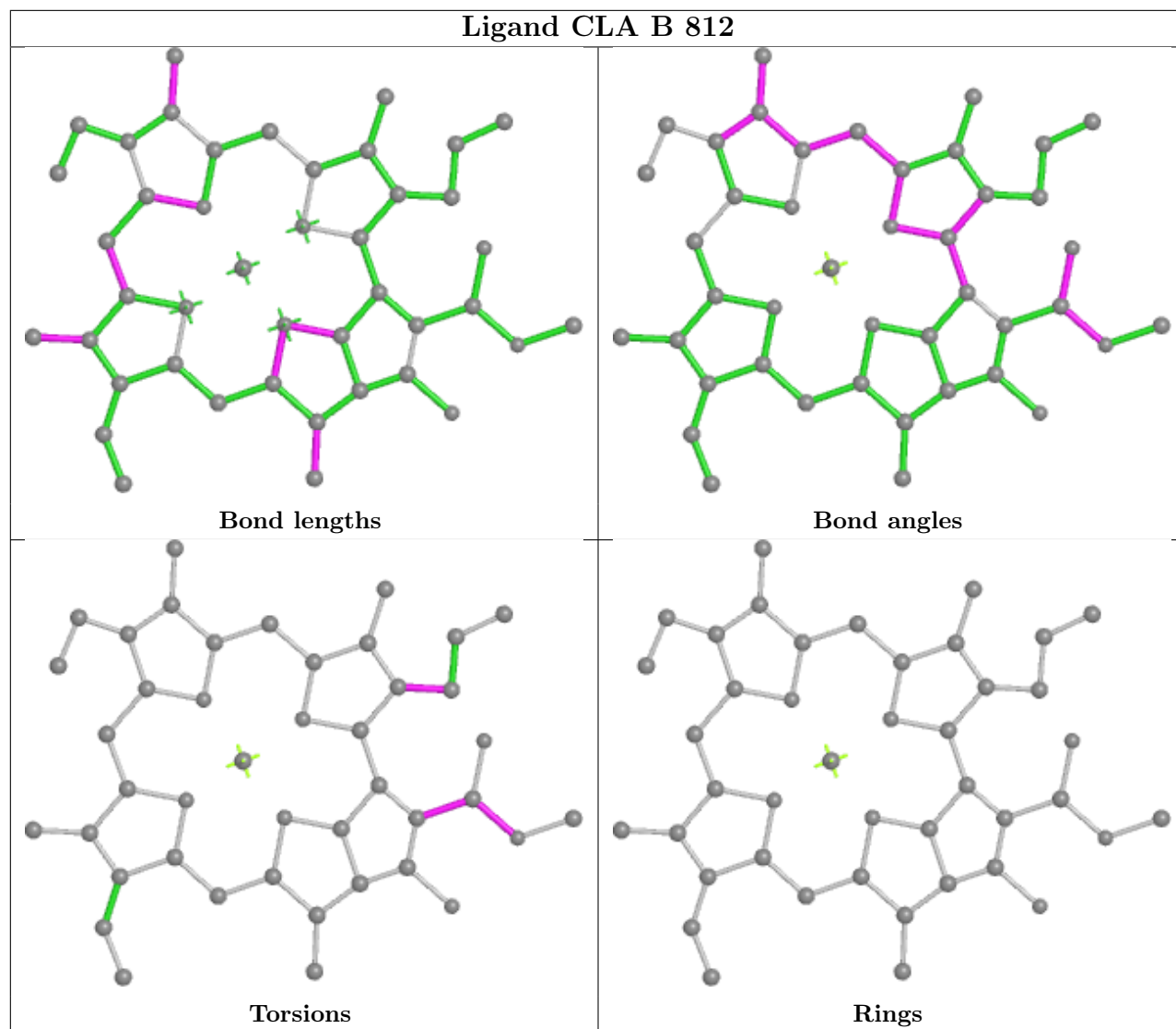


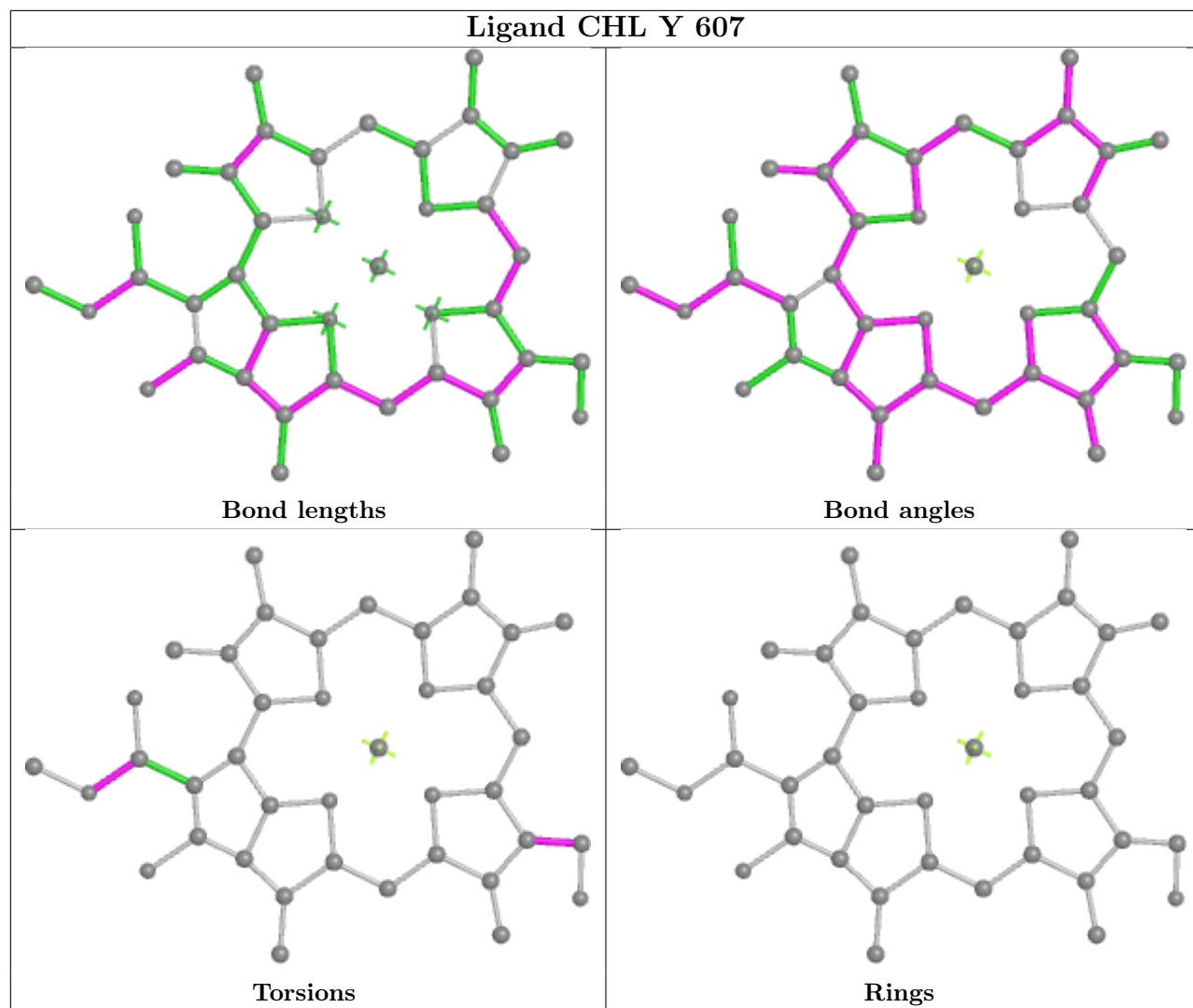
Torsions



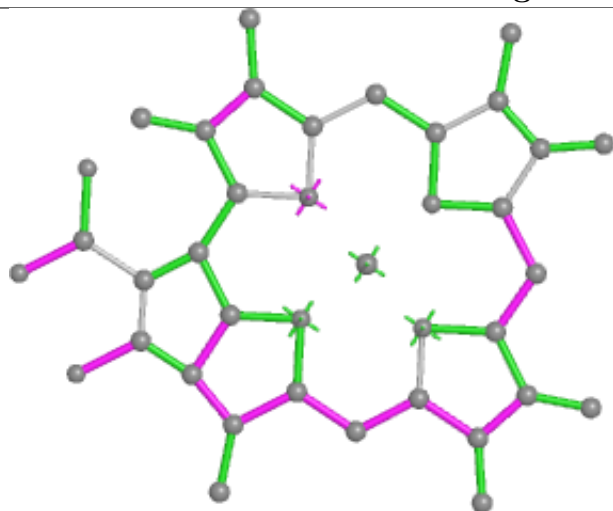
Rings

Ligand CLA B 812

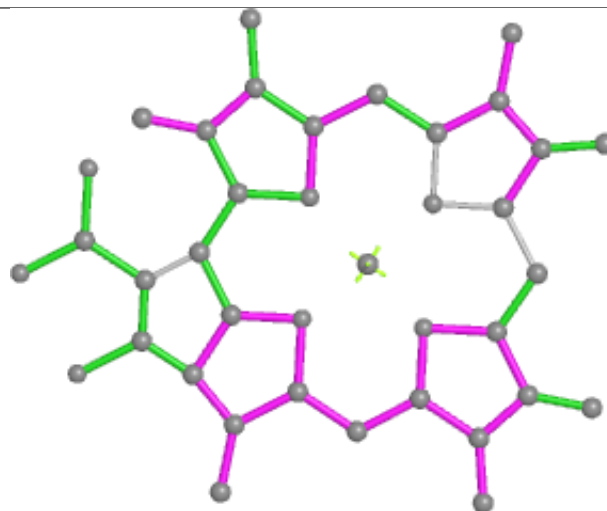




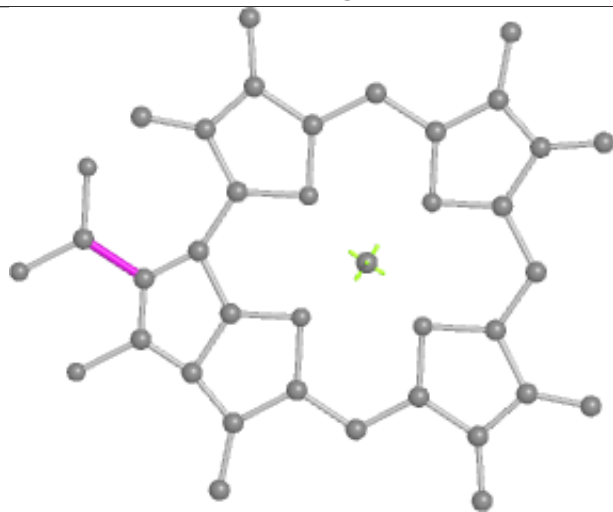
Ligand CHL Y 606



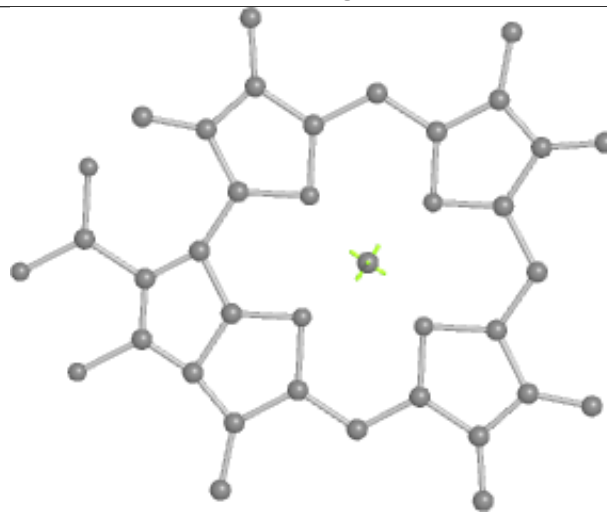
Bond lengths



Bond angles

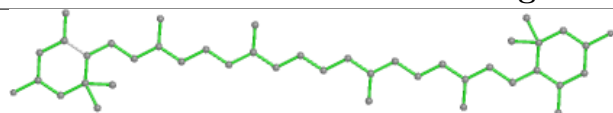


Torsions

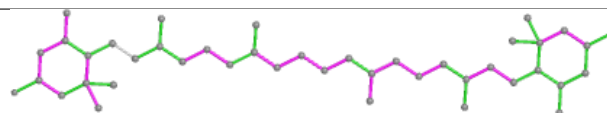


Rings

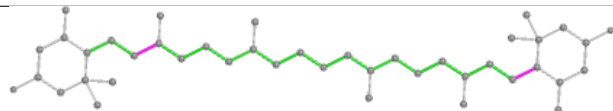
Ligand LUT 3 618



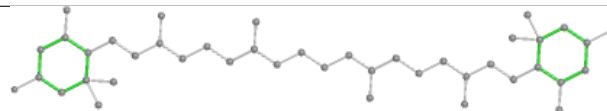
Bond lengths



Bond angles

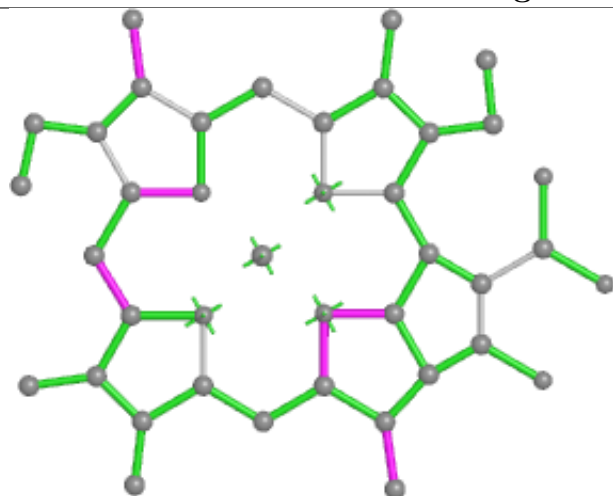


Torsions

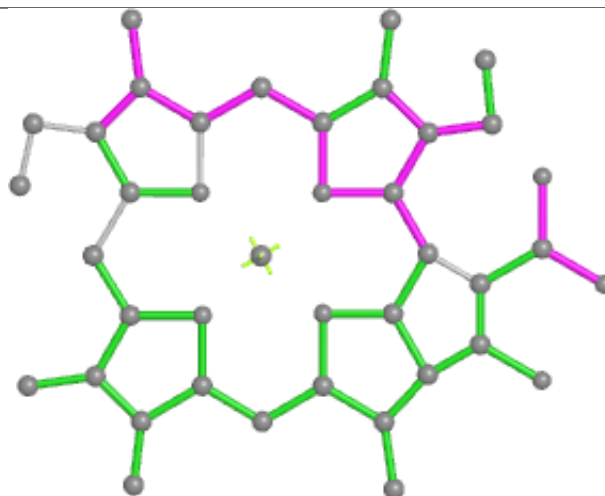


Rings

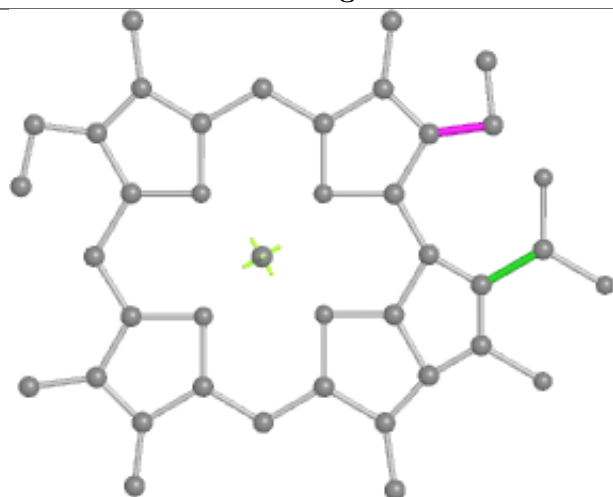
Ligand CLA X 603



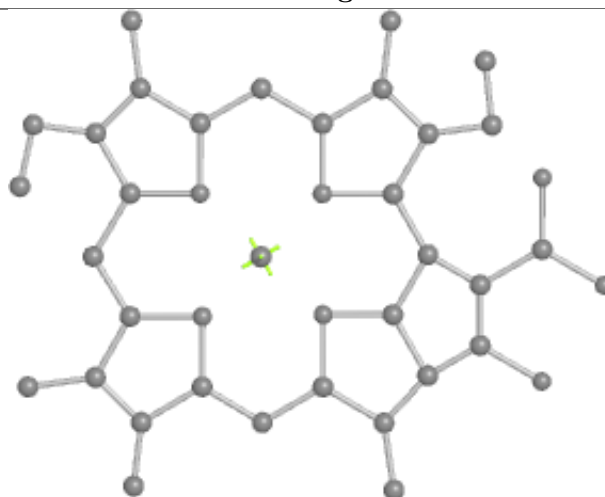
Bond lengths



Bond angles

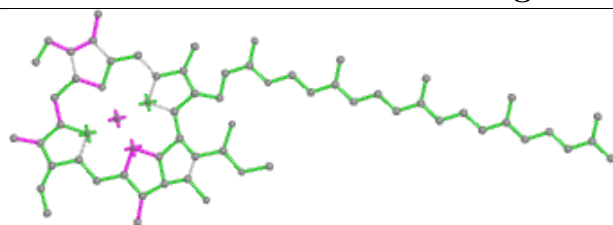


Torsions

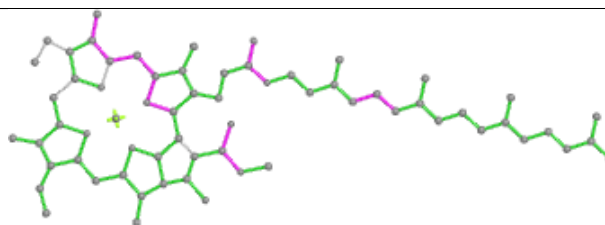


Rings

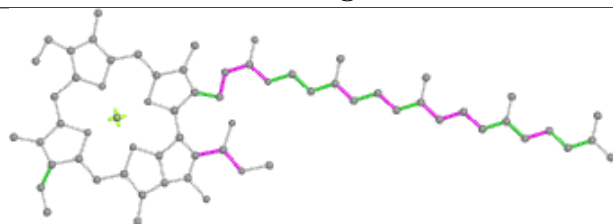
Ligand CLA A 843



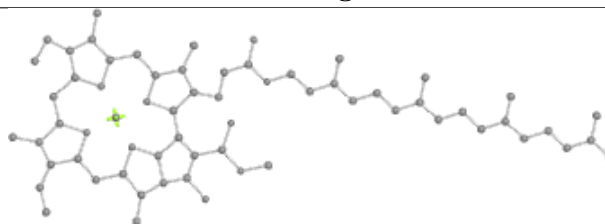
Bond lengths



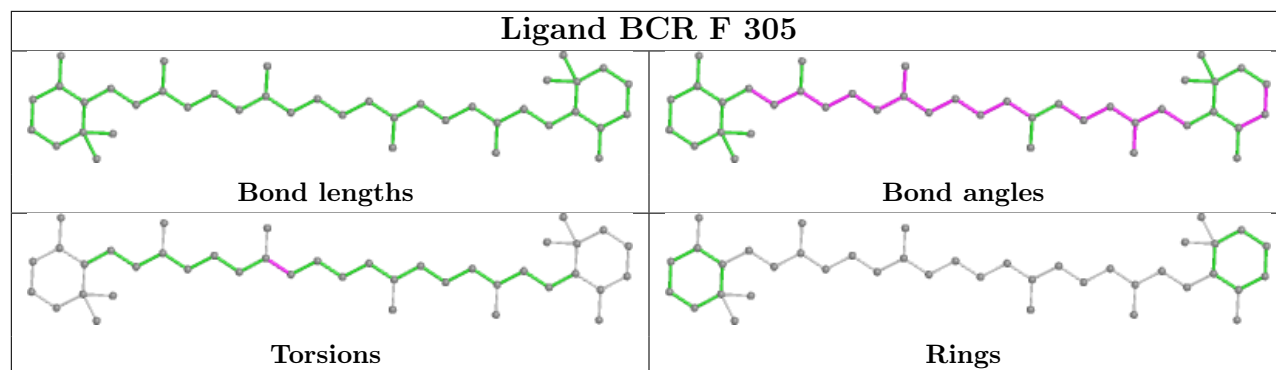
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

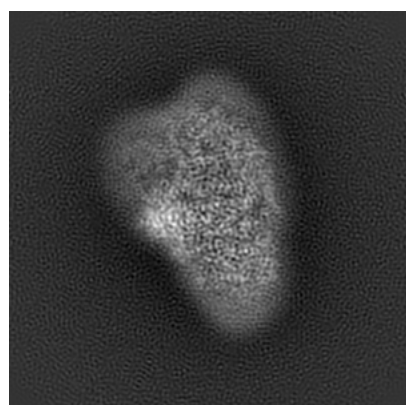
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6932. These allow visual inspection of the internal detail of the map and identification of artifacts.

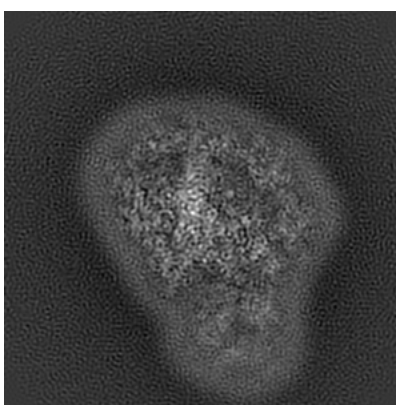
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

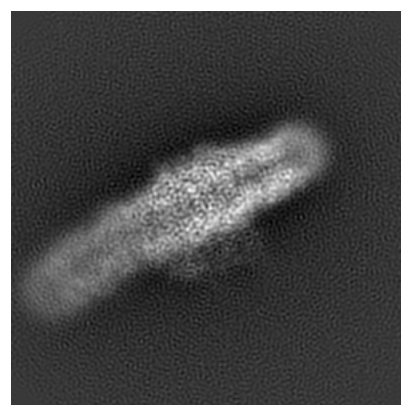
6.1.1 Primary map



X



Y

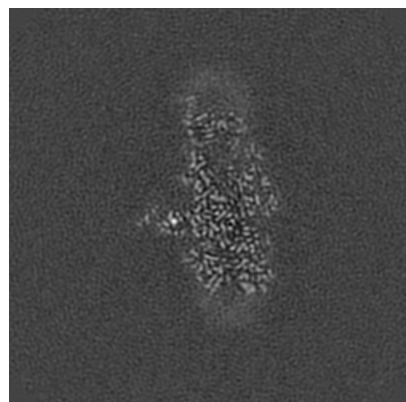


Z

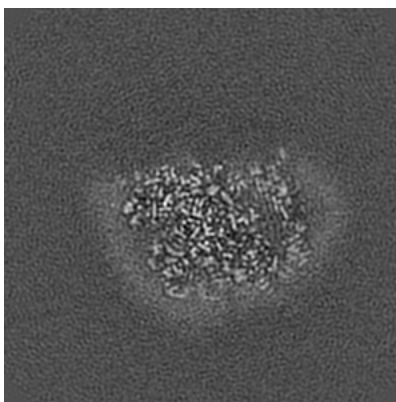
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

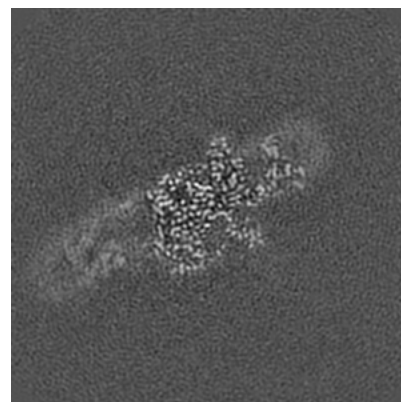
6.2.1 Primary map



X Index: 140



Y Index: 140

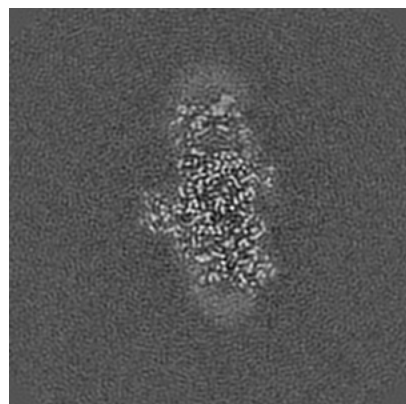


Z Index: 140

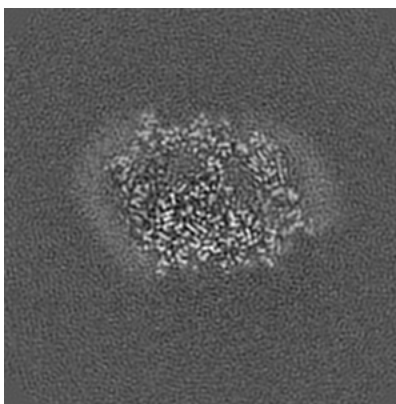
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

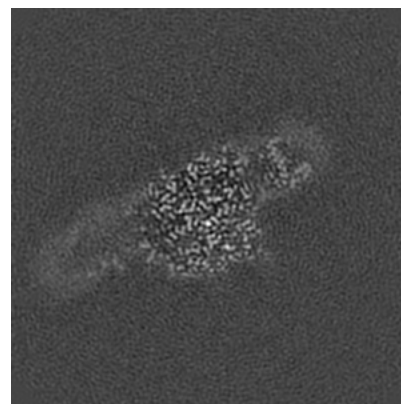
6.3.1 Primary map



X Index: 130



Y Index: 157

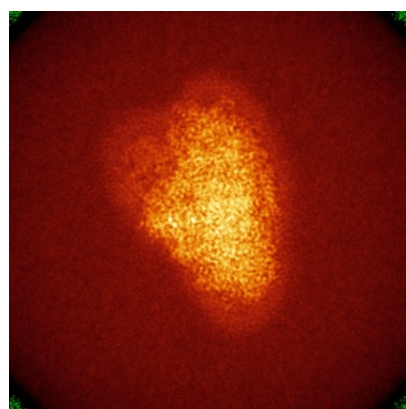


Z Index: 132

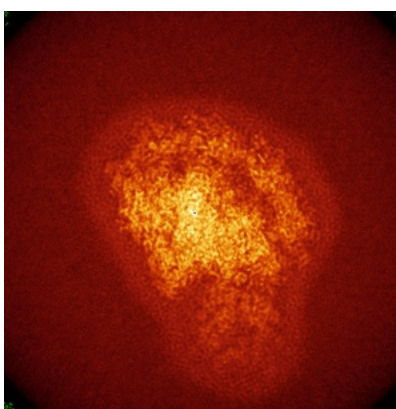
The images above show the largest variance slices of the map in three orthogonal directions.

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

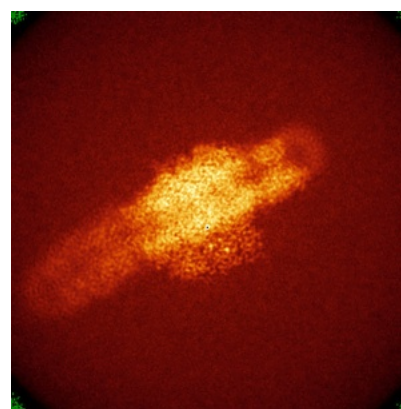
6.4.1 Primary map



X



Y

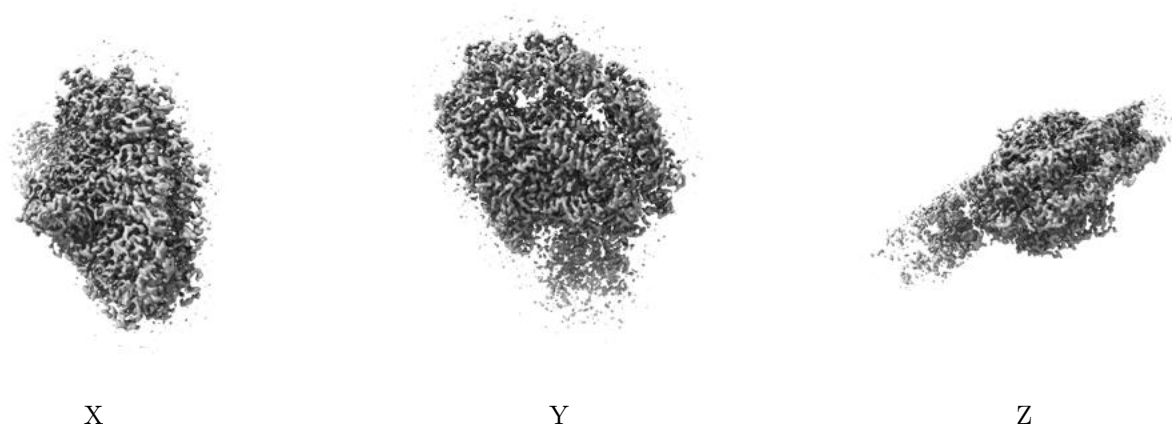


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

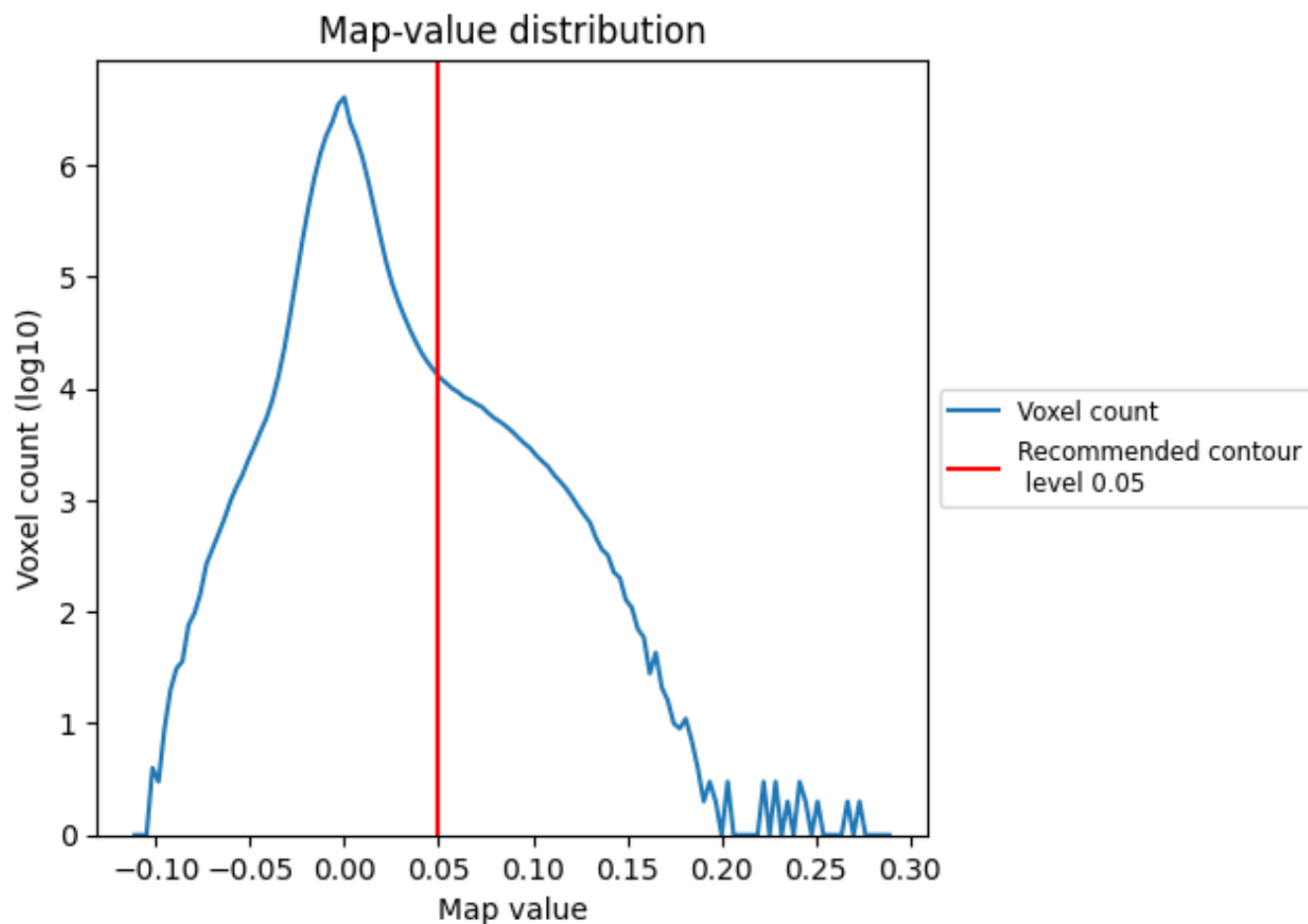
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

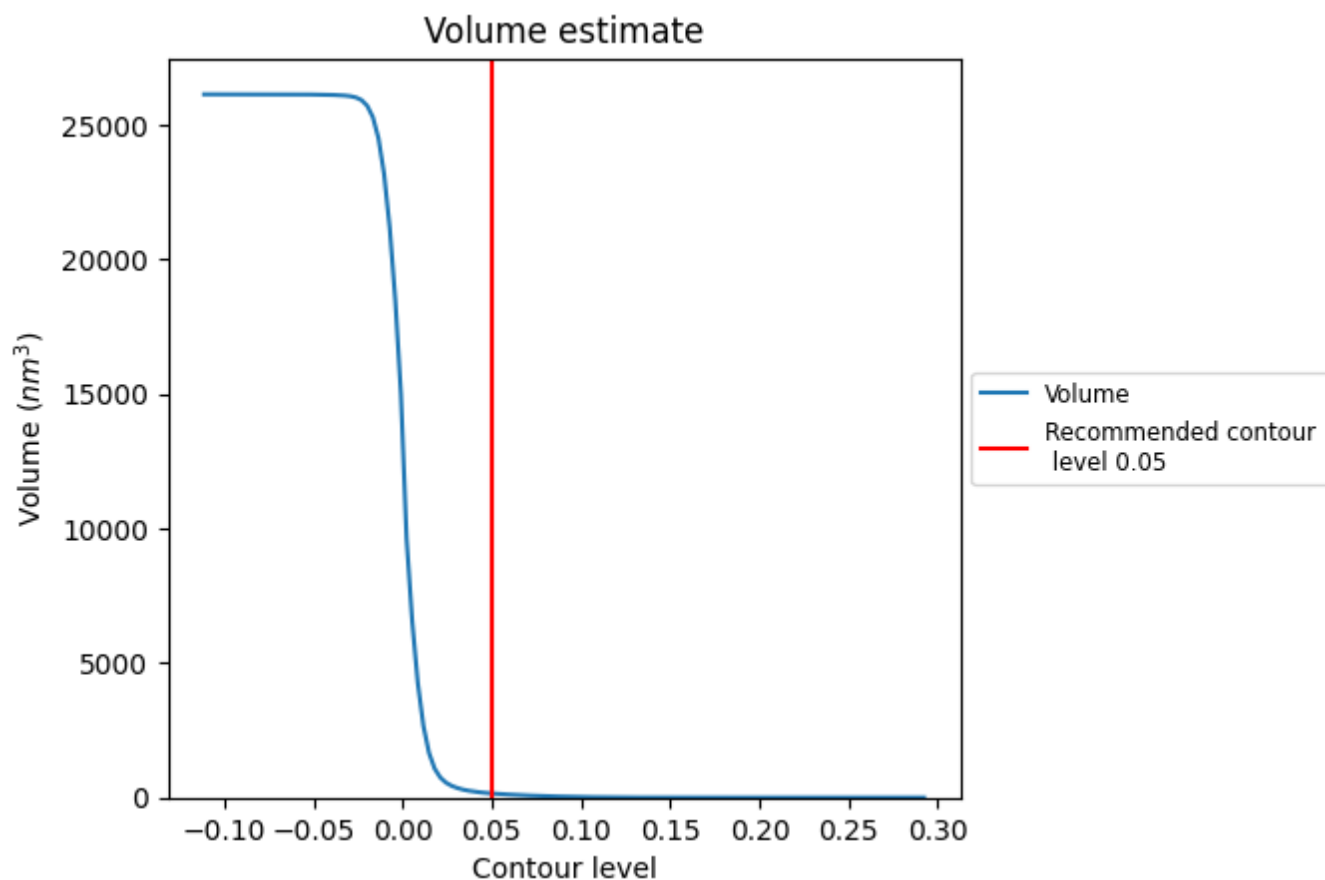
This section contains the results of statistical analysis of the map.

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.

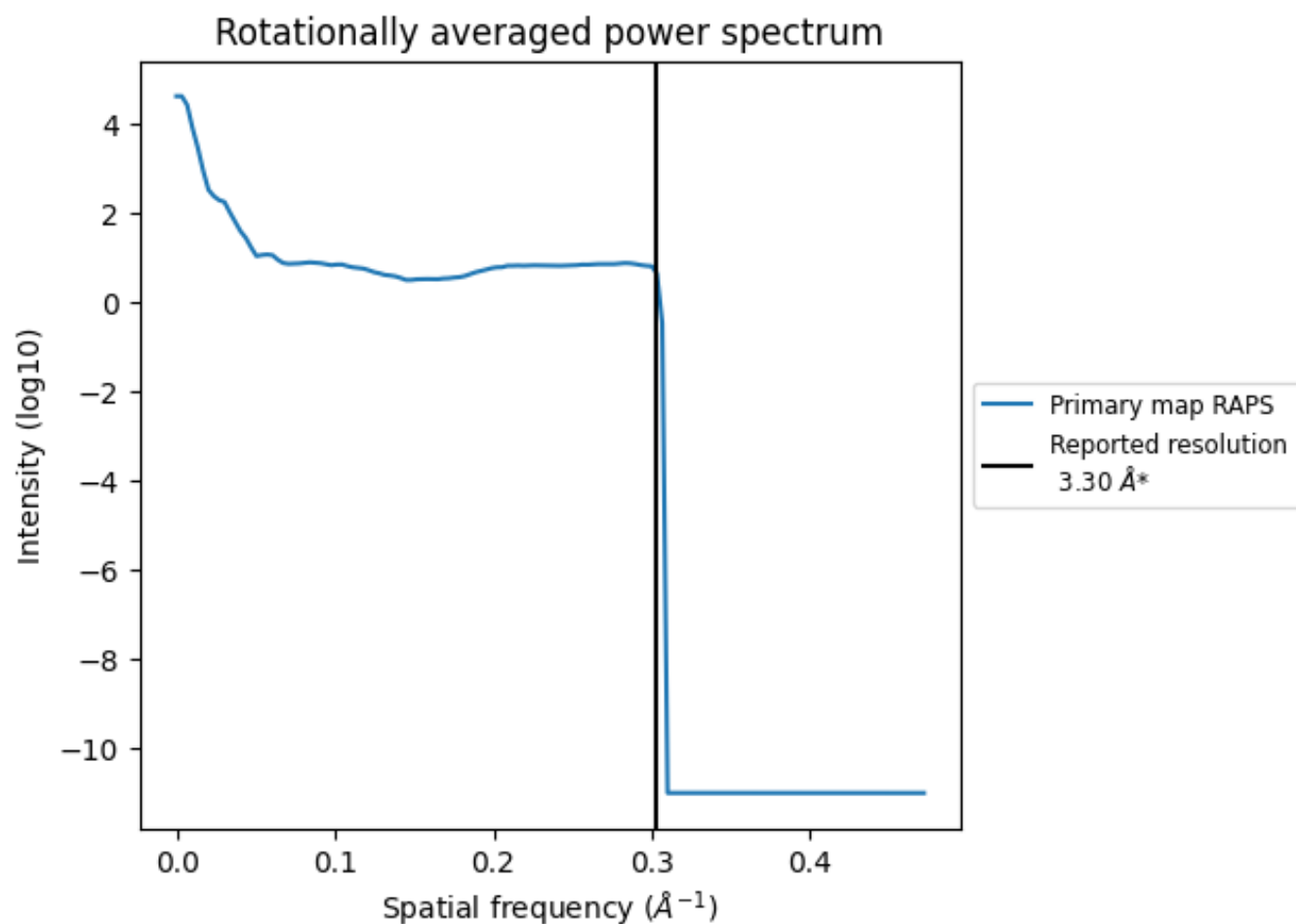
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; this corresponds to an approximate mass of 138 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 0.303 Å⁻¹

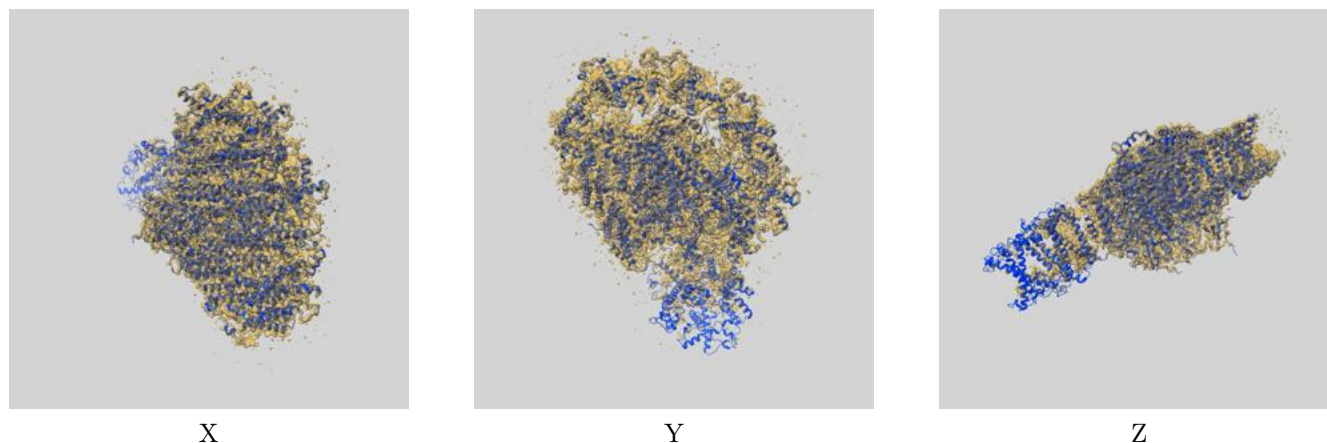
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

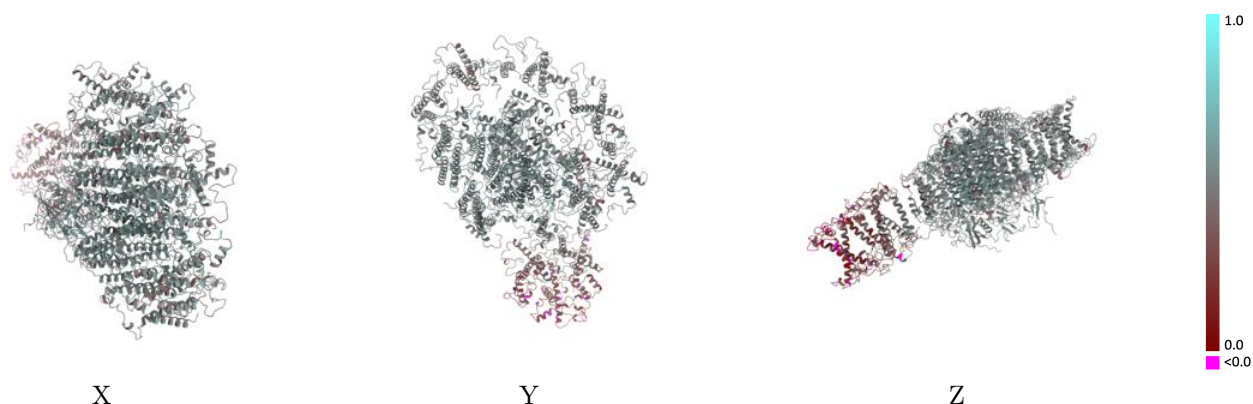
This section contains information regarding the fit between EMDB map EMD-6932 and PDB model 5ZJI. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



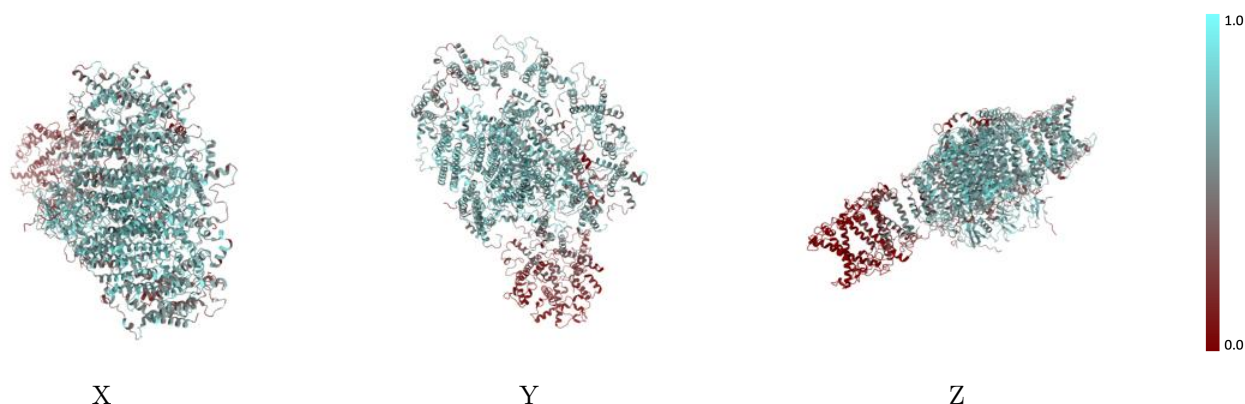
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



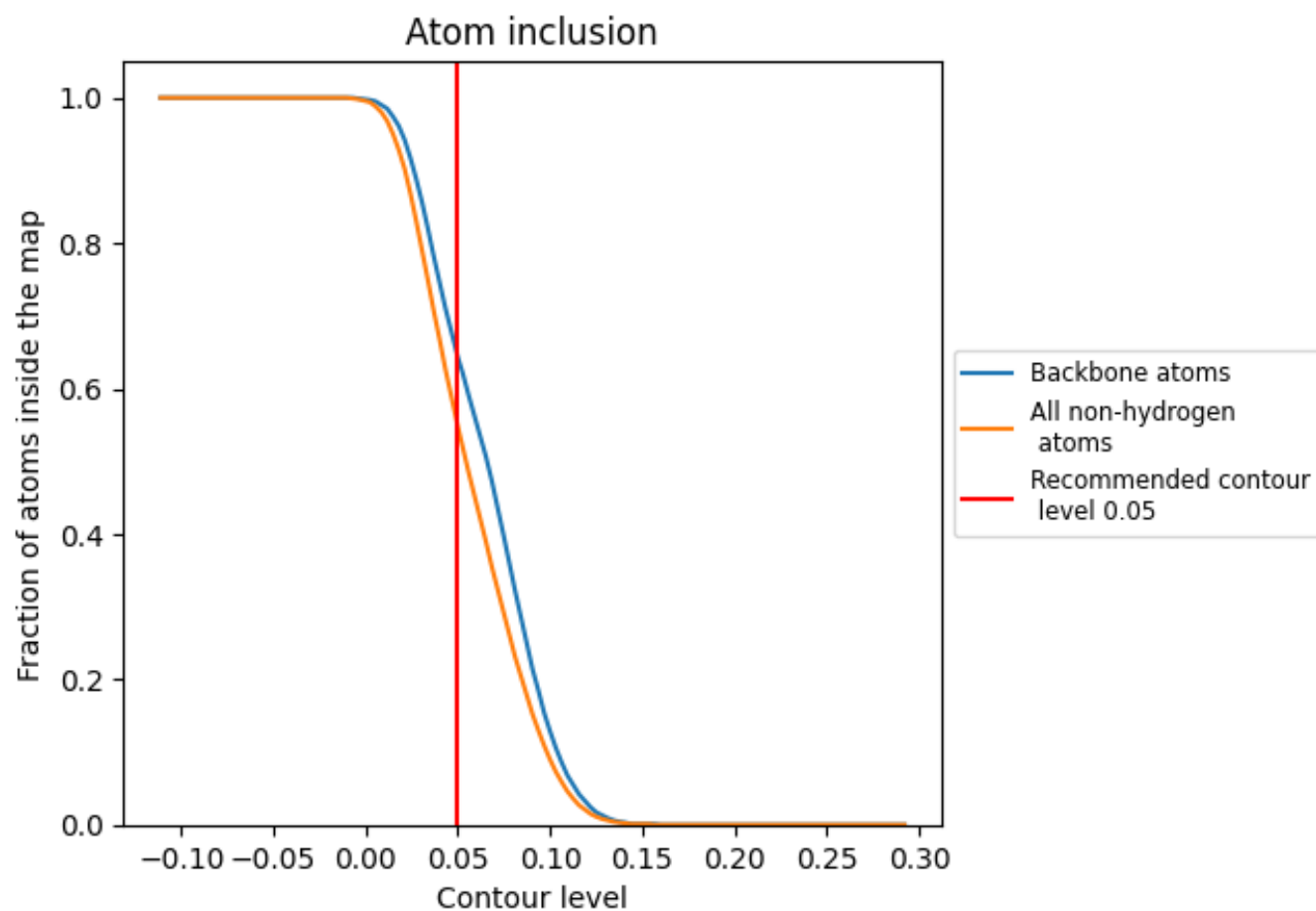
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 55% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5480	 0.4940
1	 0.5140	 0.4870
2	 0.5880	 0.5130
3	 0.5560	 0.4990
4	 0.5960	 0.5060
A	 0.6860	 0.5560
B	 0.6970	 0.5540
C	 0.7380	 0.5320
D	 0.6540	 0.5250
E	 0.6180	 0.5170
F	 0.6230	 0.5270
G	 0.5080	 0.4990
H	 0.5290	 0.4880
I	 0.5850	 0.5160
J	 0.5640	 0.5320
K	 0.5090	 0.4850
L	 0.6200	 0.5200
N	 0.3930	 0.4840
O	 0.4860	 0.4690
X	 0.0240	 0.2260
Y	 0.2200	 0.3500
Z	 0.2090	 0.3740

