



wwPDB EM Validation Summary Report ⓘ

May 22, 2024 – 04:35 PM JST

PDB ID : 8J7A
EMDB ID : EMD-36036
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 1 (PSI-ST1)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.06 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.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

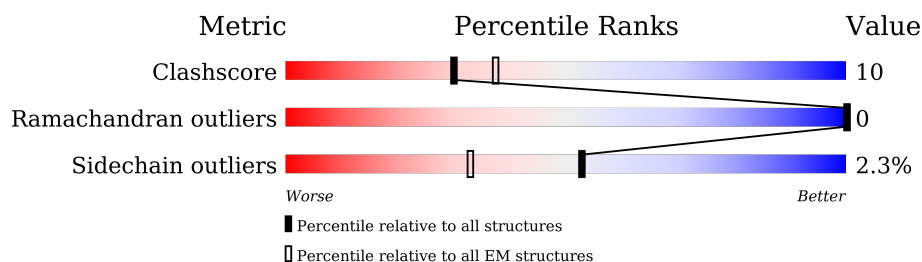
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	241	 51% 16% 31%
2	2	257	 68% 10% 22%
3	3	273	 70% 10% 21%
4	4	251	 65% 13% 22%
5	A	750	 85% 10% 5%
6	B	734	 88% 12%
7	C	81	 84% 15%
8	D	204	 64% 6% 30%

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Mol	Chain	Length	Quality of chain
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	

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
17	CHL	1	601	X	-	-	-
17	CHL	1	606	X	-	-	-
17	CHL	2	601	X	-	-	-
17	CHL	2	605	X	-	-	-
17	CHL	2	606	X	-	-	-
17	CHL	2	607	X	-	-	-
17	CHL	2	615	X	-	-	-
17	CHL	3	606	X	-	-	-
17	CHL	4	605	X	-	-	-
17	CHL	4	606	X	-	-	-
17	CHL	4	607	X	-	-	-
17	CHL	4	615	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	602	X	-	-	-
18	CLA	2	603	X	-	-	-
18	CLA	2	604	X	-	-	-
18	CLA	2	608	X	-	-	-
18	CLA	2	609	X	-	-	-
18	CLA	2	610	X	-	-	-
18	CLA	2	611	X	-	-	-
18	CLA	2	612	X	-	-	-
18	CLA	2	613	X	-	-	-
18	CLA	3	601	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	605	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	201	X	-	-	-
18	CLA	G	202	X	-	-	-
18	CLA	G	203	X	-	-	-
18	CLA	H	201	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	L	304	X	-	-	-
24	CL0	A	801	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34246 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 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	166	Total	C	N	O	S	0	0
			1296	844	215	232	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	201	Total	C	N	O	S	0	0
			1566	1024	256	282	4		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	217	Total	C	N	O	S	0	0
			1661	1085	269	302	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	196	Total	C	N	O	S	0	0
			1551	1013	253	282	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	709	Total	C	N	O	S	0	0
			5582	3662	946	956	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	732	Total	C	N	O	S	0	0
			5854	3842	997	1001	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			616	381	107	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1128	723	195	206	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O		0	0
			517	331	92	94			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	149	Total	C	N	O	S	0	0
			1183	773	203	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	91	Total	C	N	O		0	0
			708	458	118	132			

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	86	Total	C	N	O		0	0
			660	431	104	125			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	31	Total	C	N	O	S	0	0
			239	162	39	37	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
			327	221	50	55	1		

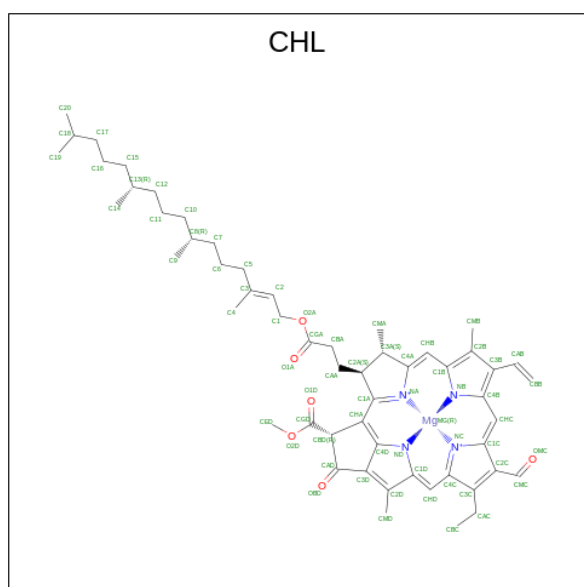
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	56	Total	C	N	O	S	0	0
			397	256	64	74	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	159	Total	C	N	O	S	0	0
			1200	795	190	213	2		

- Molecule 17 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



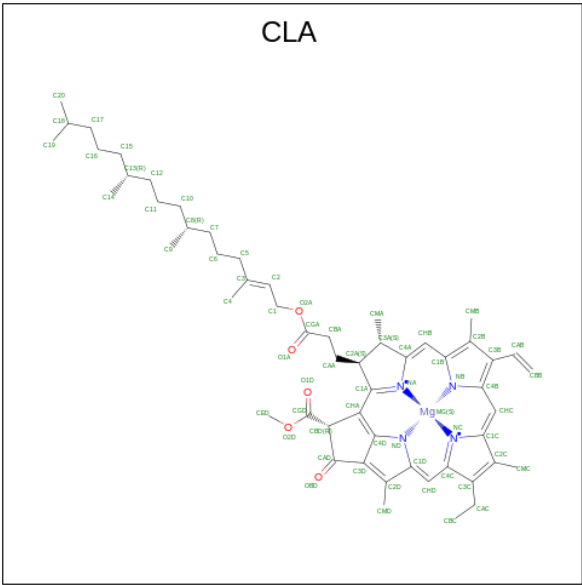
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	2	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 36	C 30	Mg 1	N 4	O 1	0
18	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0

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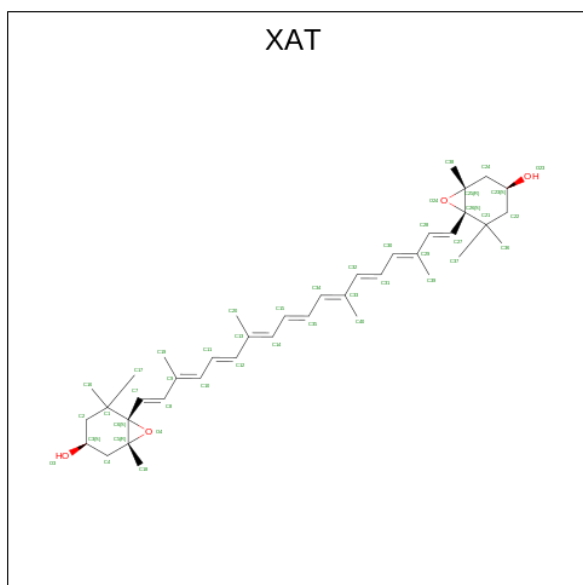
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



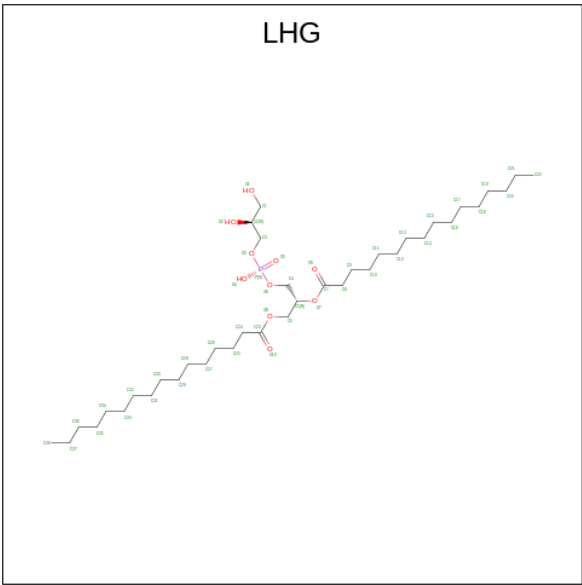
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	

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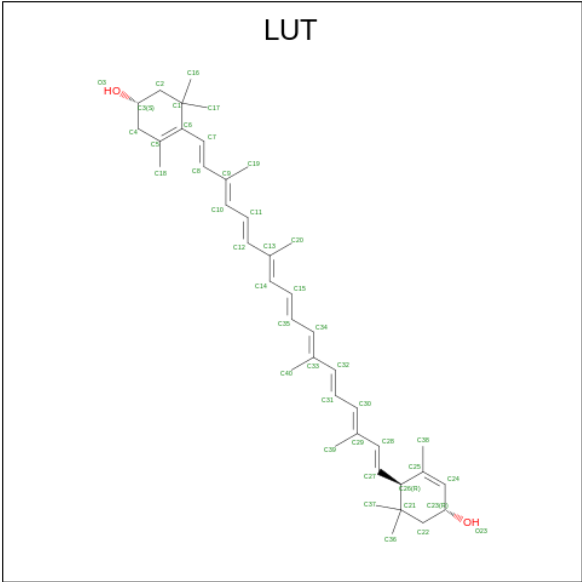
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			44	40	4	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



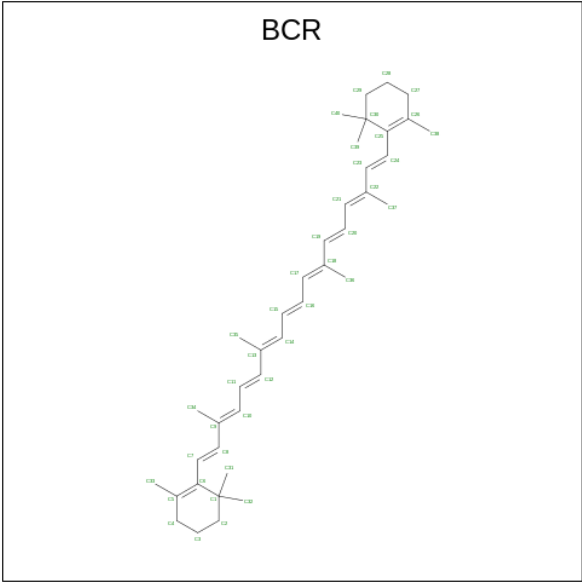
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



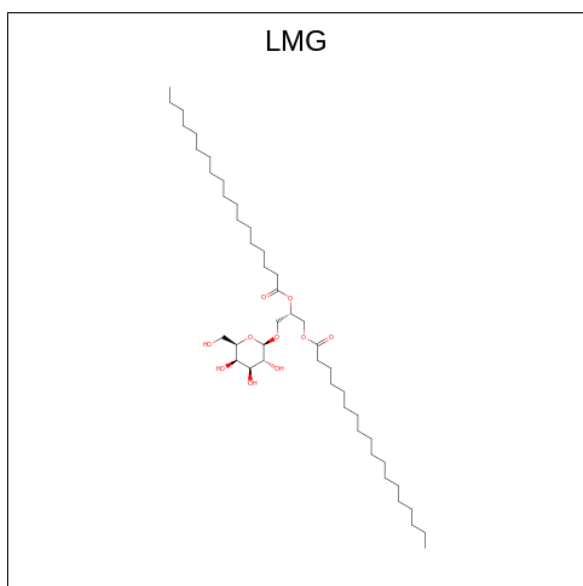
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0

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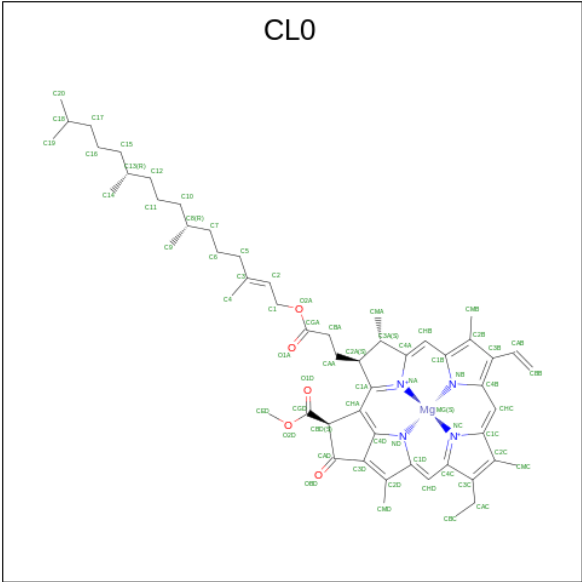
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



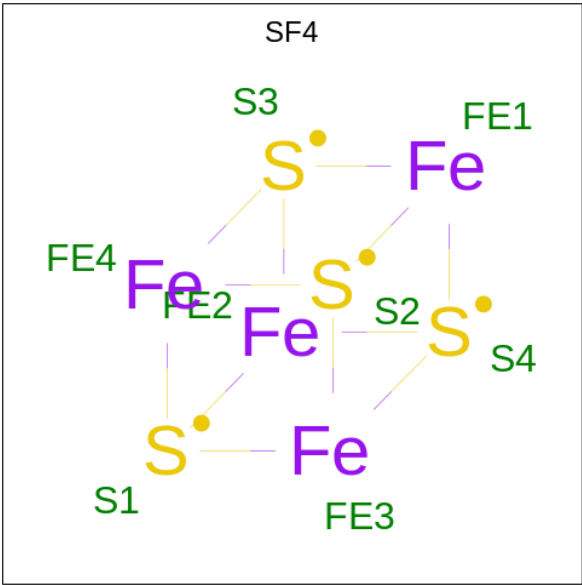
Mol	Chain	Residues	Atoms			AltConf
23	4	1	Total	C	O	0
			33	23	10	
23	4	1	Total	C	O	0
			39	29	10	

- Molecule 24 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



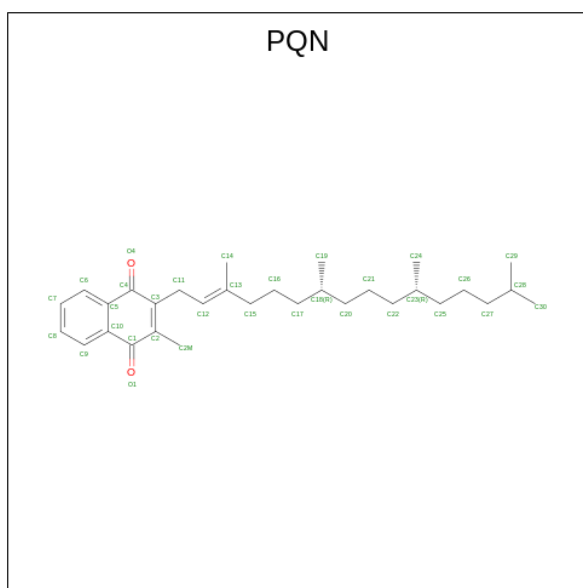
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	52	1	4	3	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



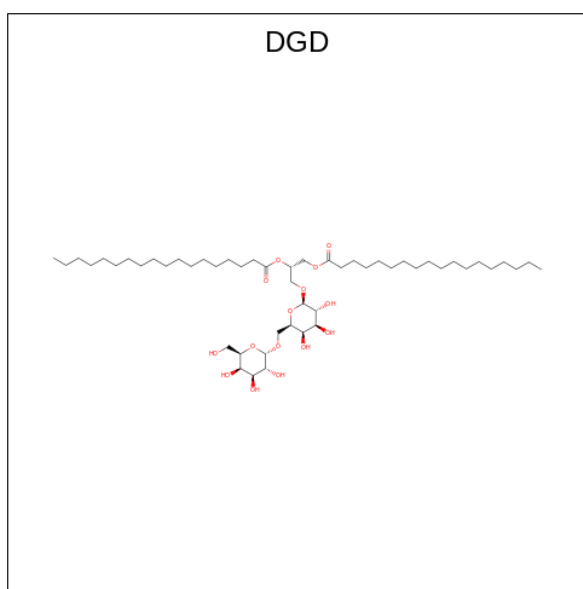
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



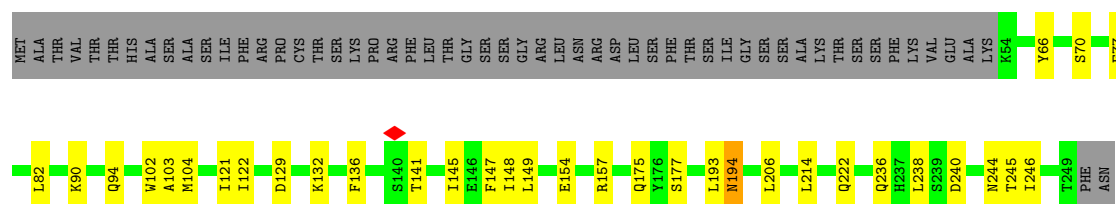
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	
26	B	1	Total	C	O	0
			33	31	2	

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




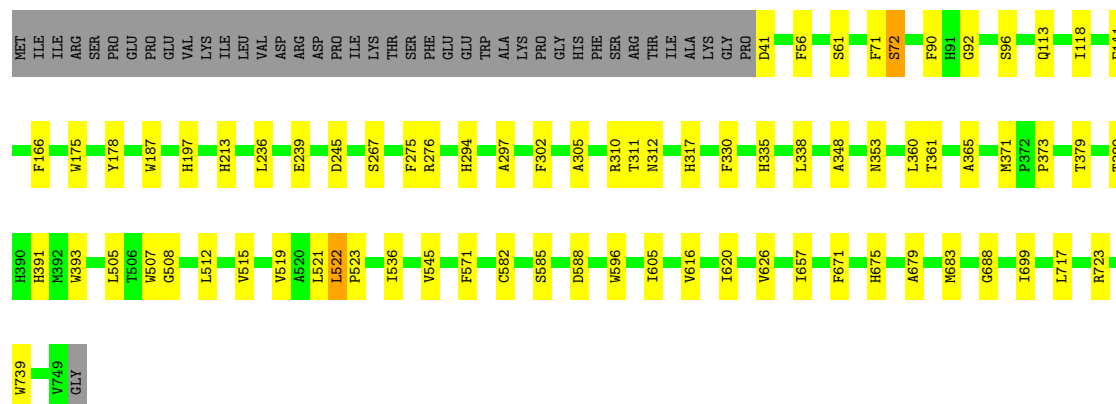
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			66	51	15	

Chain 4:  65% 13% 22%



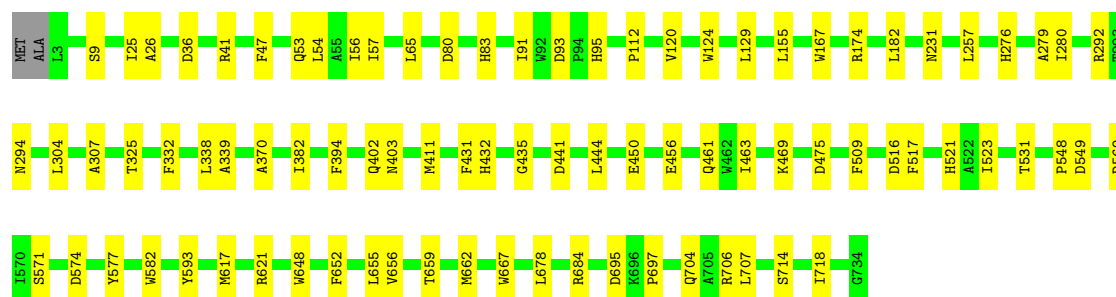
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  85% 10% 5%




- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  88% 12%



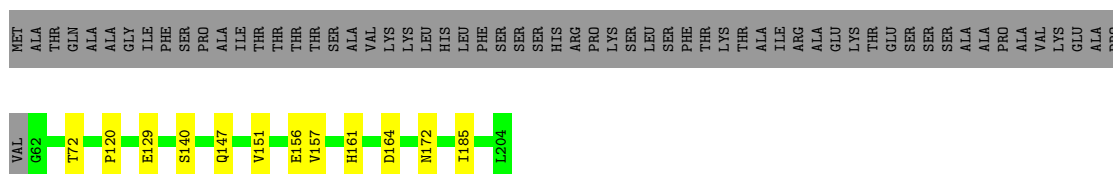
- Molecule 7: Photosystem I iron-sulfur center

Chain C:  84% 15%



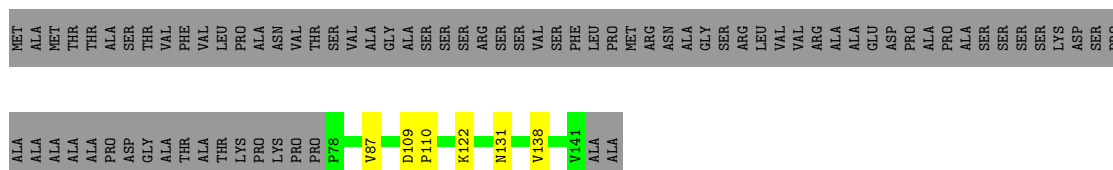
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D:  64% 6% 30%



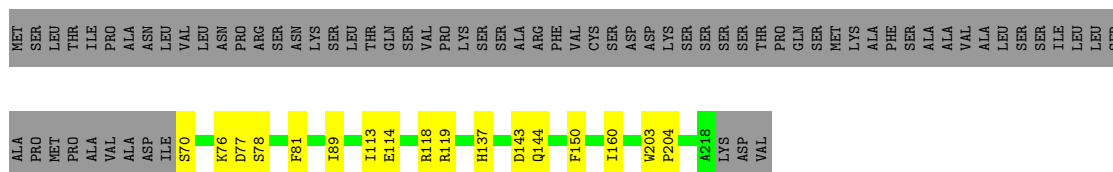
- Molecule 9: Photosystem I reaction center subunit IV A, chloroplactic

Chain E: 41% 55%



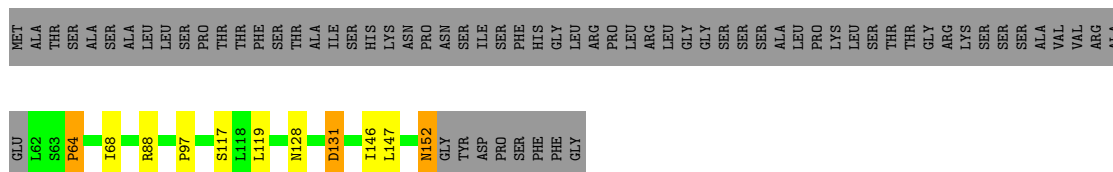
- Molecule 10: Photosystem I reaction center subunit III, chloroplactic

Chain F: 60% 8% 33%



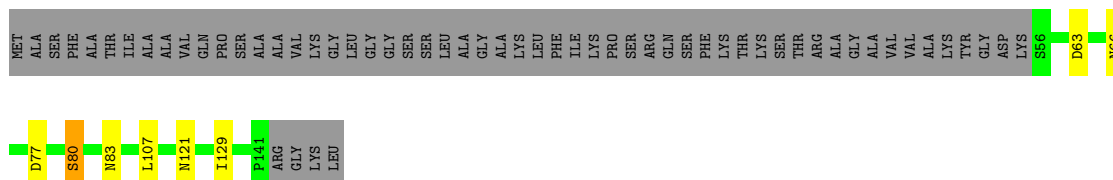
- Molecule 11: Photosystem I reaction center subunit V, chloroplactic

Chain G: 50% 5% 43%



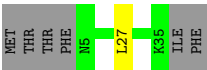
- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplactic

Chain H: 54% 5% 41%

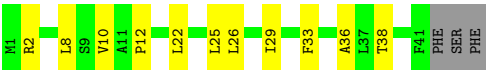


- Molecule 13: Photosystem I reaction center subunit VIII

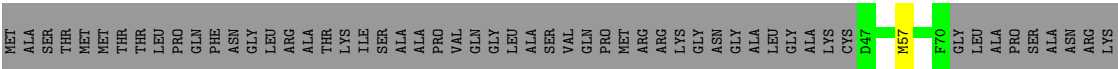
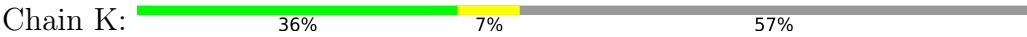
Chain I: 81% 16%



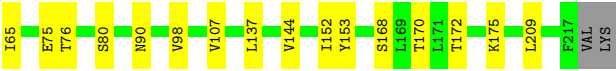
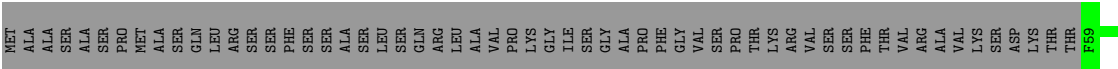
• Molecule 14: Photosystem I reaction center subunit IX



• Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic



• Molecule 16: Photosystem I reaction center subunit XI, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	48.607	Depositor
Minimum map value	-26.329	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.028	Depositor
Recommended contour level	2.57	Depositor
Map size (\AA)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/1336	0.50	1/1816 (0.1%)
2	2	0.26	0/1622	0.47	0/2219
3	3	0.27	0/1712	0.46	0/2329
4	4	0.27	0/1599	0.43	0/2178
5	A	0.27	0/5772	0.44	0/7878
6	B	0.27	0/6065	0.45	0/8279
7	C	0.28	0/629	0.55	0/852
8	D	0.26	0/1157	0.49	0/1563
9	E	0.28	0/528	0.48	0/715
10	F	0.26	0/1213	0.46	0/1637
11	G	0.29	0/724	0.58	1/981 (0.1%)
12	H	0.26	0/680	0.43	0/927
13	I	0.26	0/245	0.39	0/333
14	J	0.26	0/336	0.50	0/458
15	K	0.25	0/401	0.43	0/542
16	L	0.27	0/1237	0.44	0/1690
All	All	0.27	0/25256	0.46	2/34397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	64	PRO	CA-N-CD	-10.65	96.59	111.50
1	1	104	PRO	CA-N-CD	-8.76	99.23	111.50

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	1296	0	1277	38	0
2	2	1566	0	1519	23	0
3	3	1661	0	1625	27	0
4	4	1551	0	1508	39	0
5	A	5582	0	5436	56	0
6	B	5854	0	5646	70	0
7	C	616	0	600	10	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0
10	F	1183	0	1215	9	0
11	G	708	0	700	9	0
12	H	660	0	650	5	0
13	I	239	0	258	1	0
14	J	327	0	342	12	0
15	K	397	0	409	5	0
16	L	1200	0	1202	13	0
17	1	93	0	62	7	0
17	2	226	0	150	5	0
17	3	45	0	30	1	0
17	4	169	0	100	5	0
18	1	496	0	354	28	0
18	2	434	0	352	27	0
18	3	498	0	377	19	0
18	4	527	0	412	28	0
18	A	2483	0	2456	130	0
18	B	2284	0	2242	100	0
18	F	149	0	123	10	0
18	G	132	0	97	1	0
18	H	60	0	59	2	0
18	K	128	0	91	1	0
18	L	155	0	138	8	0
19	1	44	0	56	9	0
19	2	44	0	56	6	0
19	4	44	0	52	20	0
20	1	49	0	74	20	0
20	2	37	0	44	0	0
20	A	79	0	104	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	87	0	120	1	0
21	1	42	0	56	9	0
21	2	84	0	112	13	0
21	3	42	0	56	7	0
21	4	42	0	56	3	0
22	3	40	0	56	2	0
22	4	40	0	56	8	0
22	A	240	0	336	31	0
22	B	320	0	448	51	0
22	F	40	0	56	2	0
22	G	40	0	56	3	0
22	I	40	0	56	3	0
22	J	40	0	56	4	0
22	K	80	0	112	9	0
22	L	120	0	168	14	0
23	4	72	0	84	1	0
24	A	60	0	68	7	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	33	0	46	6	0
26	B	33	0	46	2	0
27	B	66	0	96	8	0
All	All	34246	0	33616	675	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 10.

The worst 5 of 675 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:619:LUT:H8	21:2:619:LUT:H181	1.55	0.88
18:1:604:CLA:HMB3	19:1:614:XAT:H162	1.55	0.86
4:4:77:PHE:HE2	19:4:617:XAT:C38	1.88	0.85
6:B:54:LEU:HD12	18:B:813:CLA:HED1	1.65	0.79
2:2:143:VAL:HG22	18:4:613:CLA:HBA2	1.64	0.78

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	162/241 (67%)	157 (97%)	5 (3%)	0	100	100
2	2	199/257 (77%)	195 (98%)	4 (2%)	0	100	100
3	3	215/273 (79%)	210 (98%)	5 (2%)	0	100	100
4	4	194/251 (77%)	189 (97%)	5 (3%)	0	100	100
5	A	707/750 (94%)	690 (98%)	17 (2%)	0	100	100
6	B	730/734 (100%)	712 (98%)	18 (2%)	0	100	100
7	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
8	D	141/204 (69%)	135 (96%)	6 (4%)	0	100	100
9	E	62/143 (43%)	60 (97%)	2 (3%)	0	100	100
10	F	147/221 (66%)	146 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	87 (98%)	2 (2%)	0	100	100
12	H	84/145 (58%)	84 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	39 (100%)	0	0	100	100
15	K	52/130 (40%)	51 (98%)	1 (2%)	0	100	100
16	L	157/219 (72%)	153 (98%)	4 (2%)	0	100	100
All	All	3085/3890 (79%)	3009 (98%)	76 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	134/190 (70%)	130 (97%)	4 (3%)	41	69
2	2	163/205 (80%)	158 (97%)	5 (3%)	40	68
3	3	167/211 (79%)	165 (99%)	2 (1%)	71	87
4	4	163/210 (78%)	158 (97%)	5 (3%)	40	68
5	A	574/610 (94%)	562 (98%)	12 (2%)	53	77
6	B	599/600 (100%)	588 (98%)	11 (2%)	59	80
7	C	70/71 (99%)	68 (97%)	2 (3%)	42	70
8	D	121/170 (71%)	118 (98%)	3 (2%)	47	74
9	E	57/114 (50%)	56 (98%)	1 (2%)	59	80
10	F	122/185 (66%)	119 (98%)	3 (2%)	47	74
11	G	77/133 (58%)	74 (96%)	3 (4%)	32	63
12	H	72/113 (64%)	69 (96%)	3 (4%)	30	60
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	35 (97%)	1 (3%)	43	71
15	K	43/95 (45%)	42 (98%)	1 (2%)	50	75
16	L	125/174 (72%)	123 (98%)	2 (2%)	62	83
All	All	2550/3153 (81%)	2492 (98%)	58 (2%)	53	75

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	47	PHE
15	K	105	ASP
6	B	431	PHE
14	J	8	LEU
11	G	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

198 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	$\# Z > 2$
18	CLA	B	802	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	8 (10%)
18	CLA	G	202	-	42,50,73	1.83	6 (14%)	48,85,113	1.58	7 (14%)
18	CLA	B	836	-	50,58,73	1.68	7 (14%)	58,95,113	3.68	12 (20%)
18	CLA	A	806	-	65,73,73	1.48	7 (10%)	76,113,113	1.43	8 (10%)
17	CHL	1	606	-	40,49,74	2.59	16 (40%)	41,84,114	2.92	17 (41%)
18	CLA	B	813	-	65,73,73	1.45	7 (10%)	76,113,113	1.51	9 (11%)
18	CLA	B	821	-	47,55,73	1.71	6 (12%)	54,91,113	1.69	8 (14%)
22	BCR	B	801	-	41,41,41	1.81	8 (19%)	56,56,56	1.83	12 (21%)
18	CLA	B	810	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	8 (10%)
18	CLA	4	603	-	44,52,73	1.83	7 (15%)	55,88,113	1.65	8 (14%)
20	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.32	0
18	CLA	2	602	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
18	CLA	3	610	-	39,48,73	1.90	5 (12%)	44,83,113	1.66	7 (15%)
18	CLA	A	827	-	59,67,73	1.54	7 (11%)	68,105,113	1.45	8 (11%)
18	CLA	B	827	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	7 (9%)
18	CLA	2	603	-	43,52,73	1.81	7 (16%)	49,88,113	1.59	6 (12%)
18	CLA	A	843	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	6 (7%)
18	CLA	2	613	-	43,51,73	1.82	6 (13%)	49,86,113	1.62	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	833	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	8 (15%)
22	BCR	4	618	-	41,41,41	1.74	8 (19%)	56,56,56	1.66	9 (16%)
18	CLA	4	608	4	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	A	814	-	65,73,73	1.48	8 (12%)	76,113,113	1.37	7 (9%)
18	CLA	F	303	10	41,49,73	1.84	6 (14%)	47,84,113	1.64	7 (14%)
18	CLA	B	822	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	9 (11%)
18	CLA	1	603	-	54,62,73	1.63	6 (11%)	62,99,113	1.49	7 (11%)
22	BCR	B	847	-	41,41,41	1.71	8 (19%)	56,56,56	1.56	9 (16%)
18	CLA	4	602	4	60,68,73	1.53	7 (11%)	70,107,113	1.45	8 (11%)
18	CLA	B	826	-	62,70,73	1.51	7 (11%)	72,109,113	1.43	7 (9%)
18	CLA	K	204	-	46,54,73	1.78	6 (13%)	53,90,113	1.54	7 (13%)
18	CLA	H	201	-	60,68,73	1.53	6 (10%)	70,107,113	1.39	8 (11%)
18	CLA	A	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	7 (9%)
18	CLA	A	839	-	55,63,73	1.58	6 (10%)	64,101,113	1.55	8 (12%)
18	CLA	B	837	-	65,73,73	1.46	7 (10%)	76,113,113	1.45	8 (10%)
17	CHL	1	601	1	51,60,74	2.19	16 (31%)	54,97,114	2.66	23 (42%)
18	CLA	2	611	-	44,52,73	1.82	6 (13%)	51,88,113	1.64	8 (15%)
18	CLA	F	301	-	57,65,73	1.59	6 (10%)	66,103,113	1.45	7 (10%)
18	CLA	A	813	-	54,62,73	1.63	6 (11%)	62,99,113	1.53	8 (12%)
22	BCR	L	301	-	41,41,41	1.76	9 (21%)	56,56,56	2.22	12 (21%)
22	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.66	11 (19%)
18	CLA	A	810	5	50,58,73	1.70	6 (12%)	58,95,113	1.59	10 (17%)
22	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.98	3 (3%)
18	CLA	3	609	-	53,62,73	1.65	6 (11%)	61,100,113	1.47	9 (14%)
18	CLA	A	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	3	601	3	60,68,73	1.55	7 (11%)	70,107,113	1.44	8 (11%)
18	CLA	A	838	-	51,59,73	1.67	6 (11%)	59,96,113	1.50	7 (11%)
18	CLA	4	601	4	46,54,73	1.76	7 (15%)	53,90,113	1.58	7 (13%)
22	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.15	16 (28%)
18	CLA	A	818	-	60,68,73	1.54	6 (10%)	70,107,113	5.15	10 (14%)
18	CLA	B	805	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	A	836	-	45,53,73	1.82	5 (11%)	52,89,113	1.59	7 (13%)
22	BCR	A	852	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	15 (26%)
22	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	832	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	6 (7%)
22	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.81	14 (25%)
18	CLA	4	609	-	54,62,73	1.61	6 (11%)	62,99,113	1.52	8 (12%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.26	0
24	CL0	A	801	-	60,67,73	2.06	15 (25%)	68,102,113	3.72	29 (42%)
18	CLA	A	819	-	59,67,73	1.55	7 (11%)	68,105,113	1.44	8 (11%)
17	CHL	2	601	2	47,55,74	2.31	16 (34%)	50,91,114	2.76	19 (38%)
22	BCR	B	843	-	41,41,41	1.77	8 (19%)	56,56,56	1.92	13 (23%)
18	CLA	1	611	-	45,53,73	1.80	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	B	830	-	43,51,73	1.77	6 (13%)	49,86,113	1.62	7 (14%)
18	CLA	B	818	-	60,68,73	1.51	7 (11%)	70,107,113	1.55	9 (12%)
21	LUT	3	613	-	42,43,43	1.70	8 (19%)	51,60,60	1.99	14 (27%)
18	CLA	A	825	-	55,63,73	1.58	5 (9%)	64,101,113	1.52	9 (14%)
18	CLA	F	302	-	51,59,73	1.68	5 (9%)	59,96,113	1.62	6 (10%)
20	LHG	A	847	-	29,29,48	0.35	0	32,35,54	0.43	0
21	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.98	12 (23%)
18	CLA	A	841	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)
22	BCR	L	306	-	41,41,41	1.71	8 (19%)	56,56,56	2.03	16 (28%)
18	CLA	1	609	-	42,50,73	1.82	6 (14%)	48,85,113	1.70	6 (12%)
18	CLA	K	201	15	38,45,73	1.91	6 (15%)	43,78,113	1.64	6 (13%)
18	CLA	1	602	1	54,62,73	1.60	6 (11%)	62,99,113	1.48	8 (12%)
21	LUT	1	616	-	42,43,43	1.68	7 (16%)	51,60,60	2.10	14 (27%)
17	CHL	4	615	4	40,49,74	2.24	13 (32%)	45,84,114	2.92	18 (40%)
18	CLA	B	814	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	B	819	-	55,63,73	1.62	8 (14%)	64,101,113	1.49	7 (10%)
18	CLA	B	840	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	6 (7%)
22	BCR	B	849	-	41,41,41	1.77	8 (19%)	56,56,56	1.87	12 (21%)
25	SF4	C	101	-	0,12,12	-	-	-	-	-
22	BCR	I	101	-	41,41,41	1.71	8 (19%)	56,56,56	1.50	8 (14%)
18	CLA	A	834	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	B	803	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
18	CLA	2	612	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	6 (7%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
18	CLA	A	832	-	50,58,73	1.68	6 (12%)	58,95,113	1.55	9 (15%)
18	CLA	B	812	-	43,51,73	1.80	6 (13%)	49,86,113	1.59	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	823	-	45,53,73	1.78	7 (15%)	52,89,113	1.54	7 (13%)
18	CLA	B	809	6	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
18	CLA	1	607	-	43,52,73	1.83	7 (16%)	49,88,113	1.58	6 (12%)
18	CLA	1	605	-	46,54,73	1.77	5 (10%)	53,90,113	1.62	6 (11%)
18	CLA	1	613	-	37,46,73	2.01	7 (18%)	46,81,113	1.74	9 (19%)
18	CLA	A	816	-	42,50,73	1.82	6 (14%)	48,85,113	1.62	6 (12%)
22	BCR	B	846	-	41,41,41	1.74	8 (19%)	56,56,56	1.69	10 (17%)
18	CLA	K	203	-	45,53,73	1.78	5 (11%)	52,89,113	1.63	8 (15%)
18	CLA	B	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
18	CLA	G	201	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	7 (13%)
18	CLA	3	611	-	37,44,73	1.93	7 (18%)	42,77,113	1.64	7 (16%)
18	CLA	B	820	-	50,58,73	1.66	6 (12%)	58,95,113	1.63	9 (15%)
19	XAT	1	614	-	39,47,47	0.85	1 (2%)	54,74,74	3.17	23 (42%)
18	CLA	3	604	-	40,49,73	1.87	6 (15%)	45,84,113	1.59	6 (13%)
18	CLA	B	817	-	59,67,73	1.56	7 (11%)	68,105,113	1.47	9 (13%)
18	CLA	L	304	-	45,53,73	1.79	7 (15%)	52,89,113	1.59	6 (11%)
18	CLA	4	614	-	50,58,73	1.68	6 (12%)	58,95,113	1.58	8 (13%)
18	CLA	A	821	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	A	844	-	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
18	CLA	4	611	-	40,49,73	1.89	6 (15%)	45,84,113	1.61	6 (13%)
22	BCR	B	845	-	41,41,41	1.83	8 (19%)	56,56,56	1.94	14 (25%)
18	CLA	G	203	11	45,53,73	1.76	6 (13%)	52,89,113	1.60	6 (11%)
18	CLA	A	842	-	65,73,73	1.45	6 (9%)	76,113,113	1.53	7 (9%)
18	CLA	4	610	-	42,50,73	1.80	6 (14%)	48,85,113	1.59	6 (12%)
18	CLA	2	604	-	43,51,73	1.81	9 (20%)	48,86,113	1.63	6 (12%)
18	CLA	2	610	20	38,45,73	2.95	9 (23%)	41,76,113	1.48	7 (17%)
18	CLA	B	825	-	62,70,73	1.48	6 (9%)	72,109,113	1.49	9 (12%)
17	CHL	2	615	2	43,51,74	2.36	15 (34%)	45,86,114	2.88	19 (42%)
18	CLA	B	835	-	42,50,73	1.85	5 (11%)	48,85,113	1.57	7 (14%)
18	CLA	3	612	-	39,48,73	1.84	6 (15%)	44,83,113	1.72	7 (15%)
22	BCR	L	305	-	41,41,41	1.76	8 (19%)	56,56,56	1.78	13 (23%)
18	CLA	1	604	-	49,57,73	1.70	6 (12%)	55,93,113	1.72	8 (14%)
21	LUT	2	619	-	42,43,43	1.68	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	A	829	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
18	CLA	B	807	-	52,60,73	1.64	6 (11%)	60,97,113	1.52	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	602	-	55,63,73	1.63	6 (10%)	64,101,113	1.42	7 (10%)
18	CLA	A	804	-	65,73,73	1.48	6 (9%)	76,113,113	1.55	10 (13%)
18	CLA	3	605	-	41,49,73	1.89	7 (17%)	51,84,113	1.69	9 (17%)
18	CLA	A	803	-	65,73,73	1.48	8 (12%)	76,113,113	1.32	7 (9%)
18	CLA	B	816	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	9 (14%)
18	CLA	B	824	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
17	CHL	3	606	-	45,53,74	2.34	15 (33%)	52,89,114	2.62	17 (32%)
18	CLA	A	820	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	6 (7%)
18	CLA	A	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.60	8 (13%)
18	CLA	A	833	-	56,64,73	1.57	6 (10%)	65,102,113	1.51	7 (10%)
18	CLA	1	608	-	40,48,73	1.88	7 (17%)	50,83,113	1.72	9 (18%)
18	CLA	B	806	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
18	CLA	B	829	-	56,64,73	1.59	6 (10%)	65,102,113	1.49	7 (10%)
17	CHL	2	607	-	51,59,74	2.19	16 (31%)	55,96,114	2.70	20 (36%)
18	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
18	CLA	A	809	5	65,73,73	1.47	6 (9%)	76,113,113	1.47	8 (10%)
25	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	B	834	-	60,68,73	1.56	6 (10%)	70,107,113	1.42	8 (11%)
17	CHL	2	605	-	42,50,74	2.35	15 (35%)	45,85,114	2.85	18 (40%)
18	CLA	1	612	-	46,54,73	1.74	5 (10%)	53,90,113	1.58	6 (11%)
18	CLA	2	609	-	47,55,73	1.69	7 (14%)	54,91,113	1.63	6 (11%)
20	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.33	0
22	BCR	G	204	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
23	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.23	0
18	CLA	1	610	20	37,46,73	1.98	7 (18%)	46,81,113	1.74	9 (19%)
18	CLA	4	613	-	45,53,73	1.78	6 (13%)	52,89,113	1.75	8 (15%)
18	CLA	3	608	-	41,49,73	1.82	7 (17%)	47,84,113	1.72	9 (19%)
18	CLA	L	302	16	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
18	CLA	A	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.46	9 (11%)
18	CLA	B	831	-	43,51,73	1.78	6 (13%)	49,86,113	1.63	7 (14%)
26	PQN	B	842	-	34,34,34	0.40	0	42,45,45	0.41	0
18	CLA	A	823	-	42,50,73	1.82	5 (11%)	48,85,113	1.63	7 (14%)
22	BCR	B	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)
22	BCR	3	614	-	41,41,41	1.72	8 (19%)	56,56,56	1.63	13 (23%)
18	CLA	B	808	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	830	-	65,73,73	1.45	6 (9%)	76,113,113	1.57	9 (11%)
18	CLA	B	838	-	47,55,73	1.74	6 (12%)	54,91,113	1.57	8 (14%)
18	CLA	B	815	-	43,51,73	1.79	7 (16%)	49,86,113	1.63	7 (14%)
22	BCR	B	844	-	41,41,41	1.76	8 (19%)	56,56,56	1.90	13 (23%)
26	PQN	A	855	-	34,34,34	0.38	0	42,45,45	0.42	0
17	CHL	4	606	-	41,49,74	2.43	14 (34%)	51,84,114	2.76	18 (35%)
22	BCR	A	853	-	41,41,41	1.82	8 (19%)	56,56,56	1.82	14 (25%)
18	CLA	A	811	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.48	0
18	CLA	A	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	7 (9%)
18	CLA	A	840	-	52,60,73	1.66	6 (11%)	60,97,113	1.54	8 (13%)
18	CLA	4	604	-	43,51,73	1.88	6 (13%)	54,87,113	1.64	9 (16%)
18	CLA	B	841	20	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
18	CLA	A	831	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
18	CLA	B	804	-	41,49,73	1.81	6 (14%)	47,84,113	1.76	8 (17%)
22	BCR	A	850	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
21	LUT	4	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.60	10 (19%)
18	CLA	A	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
25	SF4	C	102	-	0,12,12	-	-	-	-	-
18	CLA	A	807	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	8 (10%)
18	CLA	3	607	-	45,53,73	1.80	7 (15%)	52,89,113	1.55	6 (11%)
18	CLA	L	303	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
18	CLA	4	612	-	57,65,73	1.56	6 (10%)	66,103,113	1.50	8 (12%)
19	XAT	4	617	-	39,47,47	6.04	29 (74%)	54,74,74	5.93	34 (62%)
20	LHG	B	851	18	37,37,48	0.31	0	40,43,54	0.48	0
22	BCR	A	851	-	41,41,41	1.83	8 (19%)	56,56,56	2.47	20 (35%)
19	XAT	2	617	-	39,47,47	1.81	7 (17%)	54,74,74	2.10	15 (27%)
18	CLA	A	815	-	45,53,73	1.74	7 (15%)	52,89,113	1.72	9 (17%)
17	CHL	4	605	-	40,49,74	2.39	15 (37%)	42,84,114	2.78	18 (42%)
18	CLA	B	828	-	65,73,73	1.50	7 (10%)	76,113,113	1.37	7 (9%)
18	CLA	B	811	-	54,62,73	1.66	7 (12%)	67,100,113	1.53	10 (14%)
18	CLA	A	837	5	45,53,73	1.80	6 (13%)	52,89,113	1.58	7 (13%)
18	CLA	A	812	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
17	CHL	4	607	-	46,54,74	2.22	16 (34%)	49,90,114	2.84	20 (40%)
22	BCR	K	202	-	41,41,41	1.80	7 (17%)	56,56,56	1.95	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	608	2	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)
18	CLA	A	824	-	41,49,73	1.87	5 (12%)	47,84,113	1.67	8 (17%)
18	CLA	A	805	-	52,60,73	1.64	6 (11%)	60,97,113	1.57	8 (13%)
17	CHL	2	606	-	43,51,74	2.39	15 (34%)	45,86,114	2.86	21 (46%)
18	CLA	3	603	-	45,53,73	1.80	5 (11%)	52,89,113	1.60	8 (15%)

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
18	CLA	B	802	-	1/1/15/20	17/37/115/115	-
18	CLA	G	202	-	1/1/10/20	2/10/88/115	-
18	CLA	B	836	-	1/1/12/20	4/19/97/115	-
18	CLA	A	806	-	1/1/15/20	21/37/115/115	-
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
18	CLA	B	813	-	1/1/15/20	12/37/115/115	-
18	CLA	B	821	-	1/1/11/20	6/16/94/115	-
22	BCR	B	801	-	-	7/29/63/63	0/2/2/2
18	CLA	B	810	-	1/1/15/20	12/37/115/115	-
18	CLA	4	603	-	1/1/11/20	4/13/89/115	-
20	LHG	B	852	-	-	11/53/53/53	-
18	CLA	2	602	-	1/1/15/20	15/37/115/115	-
18	CLA	3	610	-	1/1/10/20	0/6/84/115	-
18	CLA	A	827	-	1/1/13/20	7/30/108/115	-
18	CLA	B	827	-	1/1/15/20	20/37/115/115	-
18	CLA	2	603	-	1/1/11/20	3/11/89/115	-
18	CLA	A	843	-	1/1/15/20	16/37/115/115	-
18	CLA	2	613	-	1/1/10/20	3/11/89/115	-
18	CLA	B	833	-	1/1/11/20	4/13/91/115	-
22	BCR	4	618	-	-	9/29/63/63	0/2/2/2
18	CLA	4	608	4	1/1/11/20	5/13/91/115	-
18	CLA	A	814	-	1/1/15/20	15/37/115/115	-
18	CLA	F	303	10	1/1/10/20	2/8/86/115	-
18	CLA	B	822	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	603	-	1/1/12/20	8/24/102/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	4	602	4	1/1/14/20	9/31/109/115	-
18	CLA	B	826	-	1/1/14/20	6/34/112/115	-
18	CLA	K	204	-	1/1/11/20	10/15/93/115	-
18	CLA	H	201	-	1/1/14/20	16/31/109/115	-
18	CLA	A	802	-	1/1/15/20	11/37/115/115	-
18	CLA	A	839	-	1/1/13/20	7/25/103/115	-
18	CLA	B	837	-	1/1/15/20	13/37/115/115	-
17	CHL	1	601	1	3/3/17/26	8/22/120/137	-
18	CLA	2	611	-	1/1/11/20	8/11/89/115	-
18	CLA	F	301	-	1/1/13/20	11/28/106/115	-
18	CLA	A	813	-	1/1/12/20	9/24/102/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
22	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	A	810	5	1/1/12/20	4/19/97/115	-
22	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	DGD	B	850	-	-	14/55/95/95	0/2/2/2
18	CLA	3	609	-	1/1/13/20	9/23/101/115	-
18	CLA	A	817	-	1/1/11/20	3/13/91/115	-
18	CLA	3	601	3	1/1/14/20	11/31/109/115	-
18	CLA	A	838	-	1/1/12/20	6/21/99/115	-
18	CLA	4	601	4	1/1/11/20	8/15/93/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	A	818	-	1/1/14/20	12/31/109/115	-
18	CLA	B	805	-	1/1/15/20	24/37/115/115	-
18	CLA	A	836	-	1/1/11/20	3/13/91/115	-
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
22	BCR	K	205	-	-	6/29/63/63	0/2/2/2
18	CLA	B	832	-	1/1/15/20	14/37/115/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
18	CLA	4	609	-	1/1/12/20	4/24/102/115	-
23	LMG	4	620	-	-	5/28/48/70	0/1/1/1
24	CL0	A	801	-	2/2/16/25	15/33/115/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	819	-	1/1/13/20	15/30/108/115	-
17	CHL	2	601	2	3/3/16/26	5/17/115/137	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	1	611	-	1/1/11/20	5/13/91/115	-
18	CLA	B	830	-	1/1/10/20	2/11/89/115	-
18	CLA	B	818	-	1/1/14/20	8/31/109/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
18	CLA	A	825	-	1/1/13/20	10/25/103/115	-
18	CLA	F	302	-	1/1/12/20	10/21/99/115	-
20	LHG	A	847	-	-	3/34/34/53	-
21	LUT	2	616	-	-	6/29/67/67	0/2/2/2
18	CLA	A	841	-	1/1/15/20	13/37/115/115	-
22	BCR	L	306	-	-	4/29/63/63	0/2/2/2
18	CLA	1	609	-	1/1/10/20	4/9/87/115	-
18	CLA	K	201	15	1/1/8/20	0/2/76/115	-
18	CLA	1	602	1	1/1/12/20	9/24/102/115	-
21	LUT	1	616	-	-	3/29/67/67	0/2/2/2
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
18	CLA	B	814	-	1/1/15/20	17/37/115/115	-
18	CLA	B	819	-	1/1/13/20	9/25/103/115	-
18	CLA	B	840	-	1/1/15/20	9/37/115/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
25	SF4	C	101	-	-	-	0/6/5/5
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	A	834	-	1/1/15/20	8/37/115/115	-
18	CLA	B	803	-	1/1/15/20	10/37/115/115	-
18	CLA	2	612	-	1/1/15/20	18/37/115/115	-
20	LHG	1	615	18	-	33/53/53/53	-
18	CLA	A	832	-	1/1/12/20	7/19/97/115	-
18	CLA	B	812	-	1/1/10/20	0/11/89/115	-
18	CLA	B	823	-	1/1/11/20	4/13/91/115	-
18	CLA	B	809	6	1/1/15/20	16/37/115/115	-
18	CLA	1	607	-	1/1/11/20	7/11/89/115	-
18	CLA	1	605	-	1/1/11/20	7/15/93/115	-
18	CLA	1	613	-	1/1/10/20	1/4/80/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	816	-	1/1/10/20	3/10/88/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	K	203	-	1/1/11/20	6/13/91/115	-
18	CLA	B	839	-	1/1/15/20	7/37/115/115	-
18	CLA	G	201	-	1/1/11/20	3/13/91/115	-
18	CLA	3	611	-	1/1/8/20	0/0/74/115	-
18	CLA	B	820	-	1/1/12/20	5/19/97/115	-
19	XAT	1	614	-	-	5/31/93/93	0/4/4/4
18	CLA	3	604	-	1/1/10/20	0/8/86/115	-
18	CLA	B	817	-	1/1/13/20	11/30/108/115	-
18	CLA	L	304	-	1/1/11/20	3/13/91/115	-
18	CLA	4	614	-	1/1/12/20	6/19/97/115	-
18	CLA	A	821	-	1/1/11/20	5/13/91/115	-
18	CLA	A	844	-	1/1/15/20	10/37/115/115	-
18	CLA	4	611	-	1/1/10/20	0/8/86/115	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	G	203	11	1/1/11/20	3/13/91/115	-
18	CLA	A	842	-	1/1/15/20	11/37/115/115	-
18	CLA	4	610	-	1/1/10/20	2/10/88/115	-
18	CLA	2	604	-	1/1/10/20	7/9/88/115	-
18	CLA	2	610	20	1/1/7/20	2/10/70/115	-
18	CLA	B	825	-	1/1/14/20	13/34/112/115	-
17	CHL	2	615	2	3/3/15/26	2/12/110/137	-
18	CLA	B	835	-	1/1/10/20	4/10/88/115	-
18	CLA	3	612	-	1/1/10/20	0/6/84/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	1	604	-	1/1/11/20	9/18/96/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
18	CLA	A	829	-	1/1/15/20	17/37/115/115	-
18	CLA	B	807	-	1/1/12/20	1/22/100/115	-
18	CLA	3	602	-	1/1/13/20	11/25/103/115	-
18	CLA	A	804	-	1/1/15/20	17/37/115/115	-
18	CLA	3	605	-	1/1/10/20	1/10/86/115	-
18	CLA	A	803	-	1/1/15/20	19/37/115/115	-
18	CLA	B	816	-	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	824	-	1/1/15/20	16/37/115/115	-
17	CHL	3	606	-	3/3/16/26	7/13/111/137	-
18	CLA	A	820	-	1/1/15/20	16/37/115/115	-
18	CLA	A	808	-	1/1/12/20	0/19/97/115	-
18	CLA	A	833	-	1/1/13/20	4/27/105/115	-
18	CLA	1	608	-	1/1/10/20	3/8/84/115	-
18	CLA	B	806	-	1/1/15/20	13/37/115/115	-
18	CLA	B	829	-	1/1/13/20	6/27/105/115	-
17	CHL	2	607	-	3/3/17/26	4/21/119/137	-
18	CLA	A	826	-	1/1/15/20	12/37/115/115	-
18	CLA	A	809	5	1/1/15/20	13/37/115/115	-
25	SF4	A	854	-	-	-	0/6/5/5
18	CLA	B	834	-	1/1/14/20	5/31/109/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	1	612	-	1/1/11/20	7/15/93/115	-
18	CLA	2	609	-	1/1/11/20	6/16/94/115	-
20	LHG	A	846	-	-	5/53/53/53	-
22	BCR	G	204	-	-	3/29/63/63	0/2/2/2
23	LMG	4	619	-	-	4/34/54/70	0/1/1/1
18	CLA	1	610	20	1/1/10/20	0/4/80/115	-
18	CLA	4	613	-	1/1/11/20	6/13/91/115	-
18	CLA	3	608	-	1/1/10/20	3/8/86/115	-
18	CLA	L	302	16	1/1/11/20	1/13/91/115	-
18	CLA	A	835	-	1/1/15/20	14/37/115/115	-
18	CLA	B	831	-	1/1/10/20	1/11/89/115	-
26	PQN	B	842	-	-	7/23/43/43	0/2/2/2
18	CLA	A	823	-	1/1/10/20	4/10/88/115	-
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	808	-	1/1/15/20	11/37/115/115	-
18	CLA	A	830	-	1/1/15/20	11/37/115/115	-
18	CLA	B	838	-	1/1/11/20	3/16/94/115	-
18	CLA	B	815	-	1/1/10/20	5/11/89/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
26	PQN	A	855	-	-	1/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CHL	4	606	-	3/3/15/26	2/10/106/137	-
22	BCR	A	853	-	-	4/29/63/63	0/2/2/2
18	CLA	A	811	-	1/1/15/20	13/37/115/115	-
20	LHG	2	618	18	-	11/41/41/53	-
18	CLA	A	828	-	1/1/15/20	9/37/115/115	-
18	CLA	A	840	-	1/1/12/20	5/22/100/115	-
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	B	841	20	1/1/15/20	20/37/115/115	-
18	CLA	A	831	-	1/1/15/20	8/37/115/115	-
18	CLA	B	804	-	1/1/10/20	2/8/86/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	A	822	-	1/1/15/20	11/37/115/115	-
25	SF4	C	102	-	-	-	0/6/5/5
18	CLA	A	807	-	1/1/15/20	14/37/115/115	-
18	CLA	3	607	-	1/1/11/20	2/13/91/115	-
18	CLA	L	303	-	1/1/15/20	11/37/115/115	-
18	CLA	4	612	-	1/1/13/20	11/28/106/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
20	LHG	B	851	18	-	5/42/42/53	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
19	XAT	2	617	-	-	15/31/93/93	0/4/4/4
18	CLA	A	815	-	1/1/11/20	5/13/91/115	-
17	CHL	4	605	-	3/3/15/26	5/8/106/137	-
18	CLA	B	828	-	1/1/15/20	17/37/115/115	-
18	CLA	B	811	-	1/1/13/20	11/25/101/115	-
18	CLA	A	837	5	1/1/11/20	3/13/91/115	-
18	CLA	A	812	-	1/1/15/20	21/37/115/115	-
17	CHL	4	607	-	3/3/16/26	6/15/113/137	-
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	2	608	2	1/1/11/20	7/13/91/115	-
18	CLA	A	824	-	1/1/10/20	2/8/86/115	-
18	CLA	A	805	-	1/1/12/20	4/22/100/115	-
17	CHL	2	606	-	3/3/15/26	2/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	603	-	1/1/11/20	3/13/91/115	-

The worst 5 of 1355 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	XAT	O24-C25	-13.10	1.27	1.46
18	2	610	CLA	C1A-NA	12.61	1.40	1.29
19	4	617	XAT	C2-C3	-11.35	1.36	1.52
19	4	617	XAT	C2-C1	-10.99	1.37	1.54
19	4	617	XAT	O4-C5	-10.50	1.31	1.46

The worst 5 of 1756 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.07	157.59	111.27
18	A	818	CLA	O2D-CGD-O1D	-25.32	74.34	123.84
18	A	818	CLA	O1D-CGD-CBD	-20.15	83.25	124.48
19	4	617	XAT	C4-C3-C2	-19.33	73.45	110.77
18	B	836	CLA	C5-C3-C4	-16.75	77.61	114.60

5 of 176 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	601	CHL	ND
17	1	601	CHL	NA
17	1	601	CHL	NC
17	1	606	CHL	ND
17	1	606	CHL	NA

5 of 1440 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	601	CHL	CAD-CBD-CGD-O1D
17	1	601	CHL	CAD-CBD-CGD-O2D
17	2	601	CHL	C1A-C2A-CAA-CBA
17	2	601	CHL	C3A-C2A-CAA-CBA
17	3	606	CHL	C2A-CAA-CBA-CGA

There are no ring outliers.

164 monomers are involved in 534 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	802	CLA	6	0
18	B	836	CLA	2	0
18	A	806	CLA	8	0
18	B	813	CLA	5	0
22	B	801	BCR	9	0
18	4	603	CLA	3	0
20	B	852	LHG	1	0
18	2	602	CLA	8	0
18	A	827	CLA	2	0
18	B	827	CLA	5	0
18	2	603	CLA	3	0
18	A	843	CLA	3	0
18	2	613	CLA	1	0
18	B	833	CLA	2	0
22	4	618	BCR	8	0
18	4	608	CLA	3	0
18	A	814	CLA	2	0
18	F	303	CLA	1	0
18	B	822	CLA	7	0
18	1	603	CLA	3	0
22	B	847	BCR	8	0
18	4	602	CLA	6	0
18	B	826	CLA	4	0
18	H	201	CLA	2	0
18	A	802	CLA	7	0
18	A	839	CLA	1	0
18	B	837	CLA	2	0
17	1	601	CHL	7	0
18	2	611	CLA	2	0
18	F	301	CLA	2	0
18	A	813	CLA	2	0
22	L	301	BCR	4	0
22	A	848	BCR	7	0
18	A	810	CLA	3	0
22	A	849	BCR	3	0
27	B	850	DGD	8	0
18	3	609	CLA	4	0
18	3	601	CLA	2	0
18	A	838	CLA	1	0
22	F	304	BCR	2	0
18	A	818	CLA	4	0
18	B	805	CLA	5	0
18	A	836	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	852	BCR	4	0
22	K	205	BCR	4	0
18	B	832	CLA	7	0
22	J	102	BCR	4	0
18	4	609	CLA	3	0
24	A	801	CL0	7	0
18	A	819	CLA	4	0
17	2	601	CHL	1	0
22	B	843	BCR	4	0
18	B	830	CLA	2	0
18	B	818	CLA	2	0
21	3	613	LUT	7	0
18	A	825	CLA	3	0
18	F	302	CLA	7	0
20	A	847	LHG	2	0
21	2	616	LUT	8	0
18	A	841	CLA	5	0
22	L	306	BCR	2	0
18	1	609	CLA	5	0
18	1	602	CLA	2	0
21	1	616	LUT	9	0
18	B	814	CLA	5	0
18	B	819	CLA	2	0
18	B	840	CLA	3	0
22	B	849	BCR	9	0
22	I	101	BCR	3	0
18	A	834	CLA	4	0
18	B	803	CLA	4	0
18	2	612	CLA	2	0
20	1	615	LHG	20	0
18	A	832	CLA	2	0
18	B	823	CLA	2	0
18	B	809	CLA	4	0
18	1	607	CLA	6	0
18	1	605	CLA	1	0
22	B	846	BCR	7	0
18	K	203	CLA	1	0
18	B	839	CLA	1	0
18	G	201	CLA	1	0
18	B	820	CLA	1	0
19	1	614	XAT	9	0
18	B	817	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	304	CLA	2	0
18	4	614	CLA	4	0
18	A	821	CLA	2	0
18	A	844	CLA	8	0
18	4	611	CLA	1	0
22	B	845	BCR	6	0
18	A	842	CLA	7	0
18	4	610	CLA	3	0
18	2	604	CLA	4	0
18	B	825	CLA	7	0
17	2	615	CHL	1	0
18	B	835	CLA	1	0
18	3	612	CLA	2	0
22	L	305	BCR	8	0
18	1	604	CLA	4	0
21	2	619	LUT	5	0
18	A	829	CLA	6	0
18	3	602	CLA	1	0
18	A	804	CLA	8	0
18	A	803	CLA	7	0
18	B	816	CLA	2	0
18	B	824	CLA	3	0
17	3	606	CHL	1	0
18	A	820	CLA	4	0
18	A	808	CLA	1	0
18	A	833	CLA	2	0
18	1	608	CLA	4	0
18	B	806	CLA	5	0
18	B	829	CLA	2	0
17	2	607	CHL	1	0
18	A	826	CLA	4	0
18	A	809	CLA	10	0
18	B	834	CLA	2	0
17	2	605	CHL	2	0
18	1	612	CLA	5	0
18	2	609	CLA	5	0
20	A	846	LHG	3	0
22	G	204	BCR	3	0
23	4	619	LMG	1	0
18	4	613	CLA	3	0
18	3	608	CLA	4	0
18	L	302	CLA	2	0

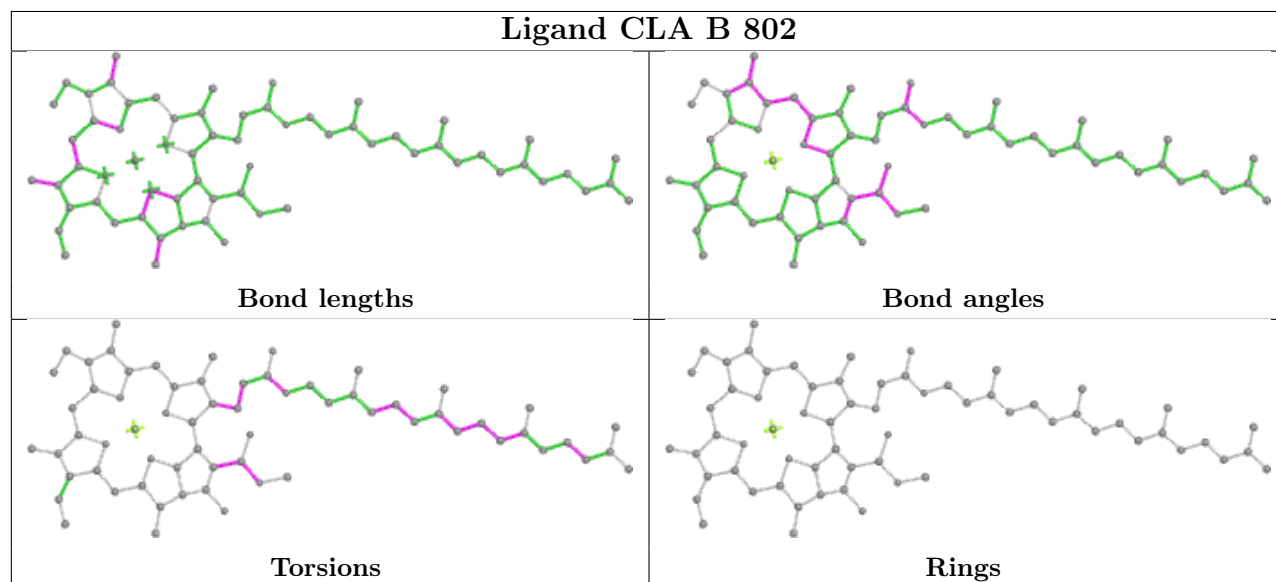
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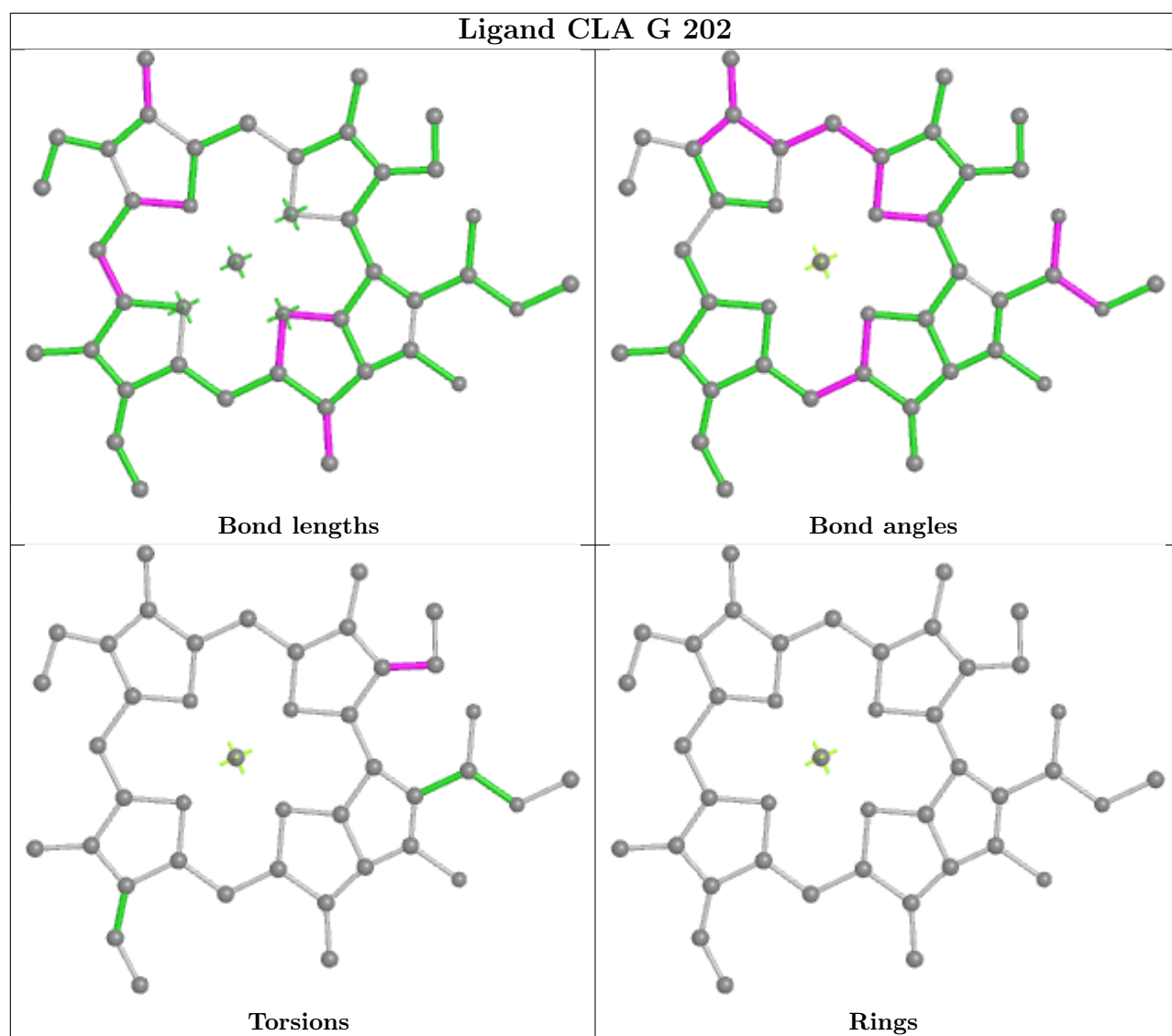
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	835	CLA	1	0
26	B	842	PQN	2	0
22	B	848	BCR	2	0
22	3	614	BCR	2	0
18	B	808	CLA	3	0
18	A	830	CLA	7	0
18	B	838	CLA	3	0
22	B	844	BCR	7	0
26	A	855	PQN	6	0
17	4	606	CHL	2	0
22	A	853	BCR	4	0
18	A	811	CLA	4	0
18	A	828	CLA	2	0
18	A	840	CLA	1	0
18	4	604	CLA	3	0
18	B	841	CLA	2	0
18	A	831	CLA	1	0
22	A	850	BCR	6	0
21	4	616	LUT	3	0
18	A	822	CLA	4	0
18	A	807	CLA	3	0
18	3	607	CLA	5	0
18	L	303	CLA	4	0
18	4	612	CLA	1	0
19	4	617	XAT	20	0
22	A	851	BCR	7	0
19	2	617	XAT	6	0
18	A	815	CLA	1	0
17	4	605	CHL	2	0
18	B	828	CLA	8	0
18	B	811	CLA	3	0
18	A	812	CLA	7	0
17	4	607	CHL	1	0
22	K	202	BCR	6	0
18	2	608	CLA	3	0
18	A	805	CLA	3	0
18	3	603	CLA	3	0

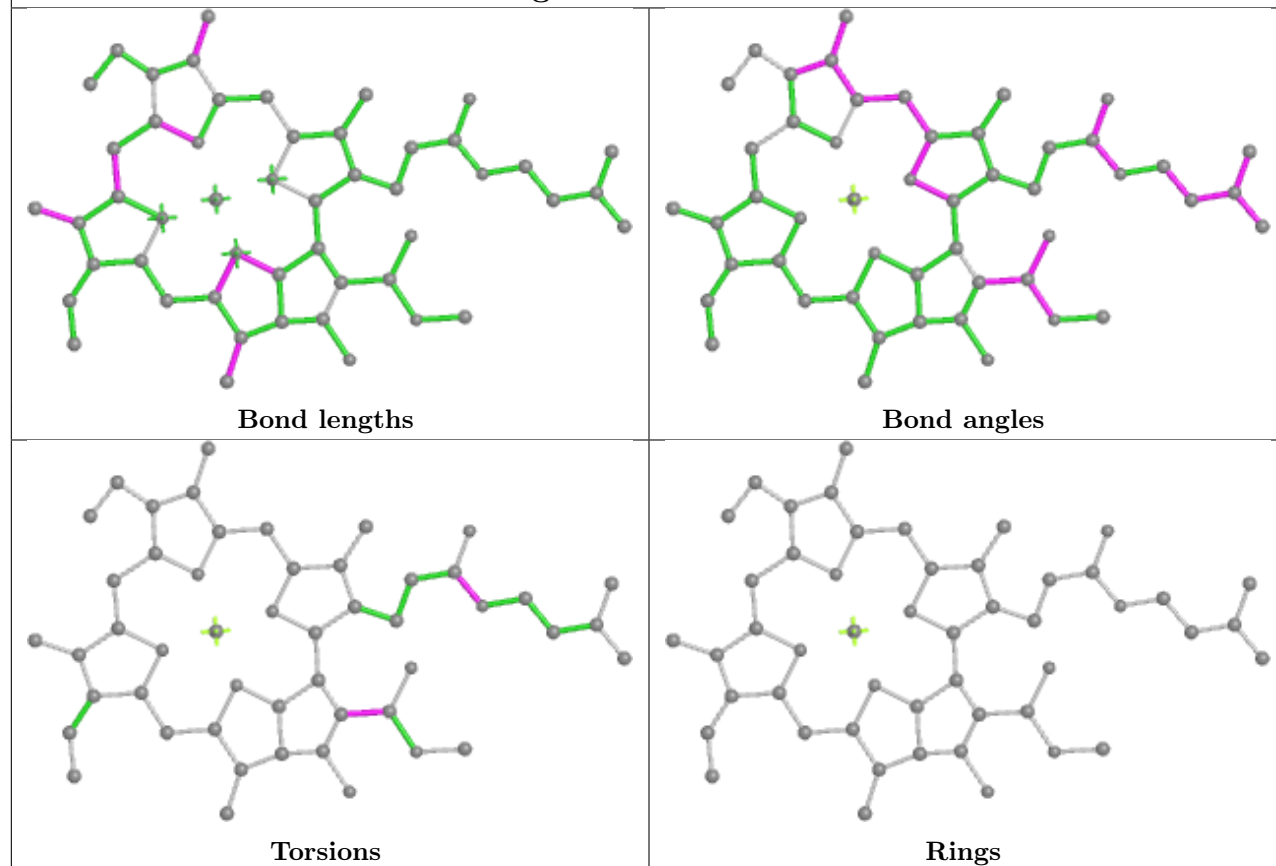
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

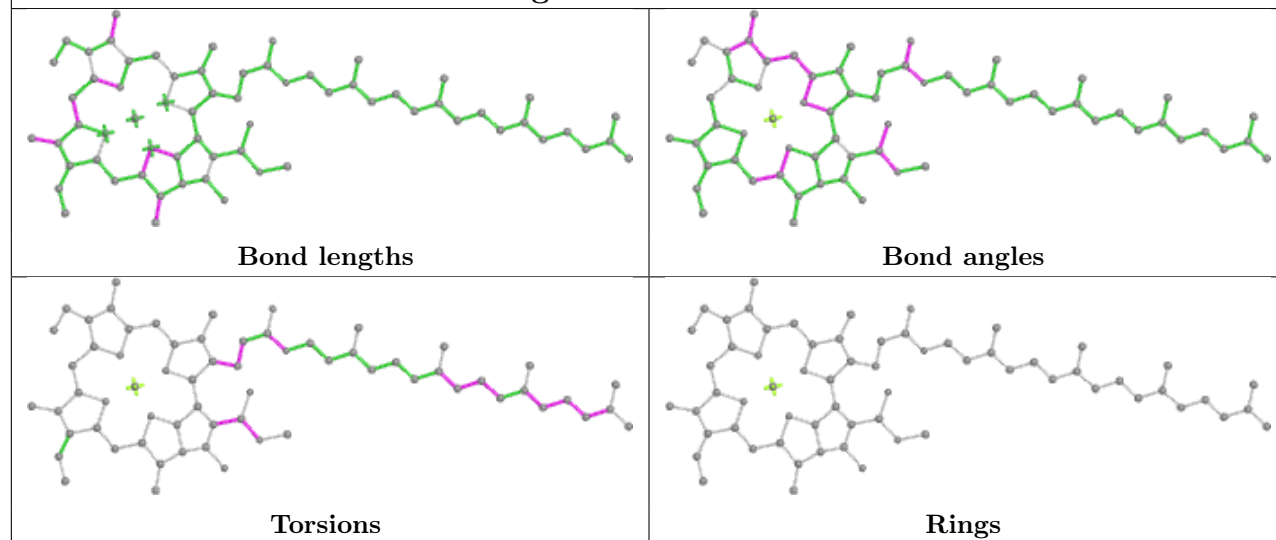




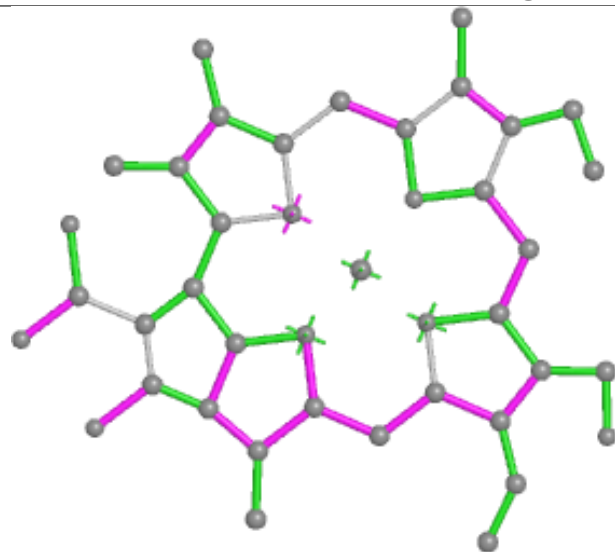
Ligand CLA B 836



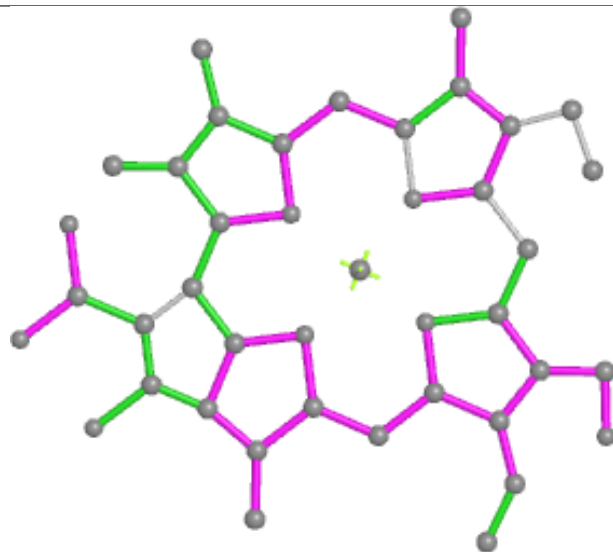
Ligand CLA A 806



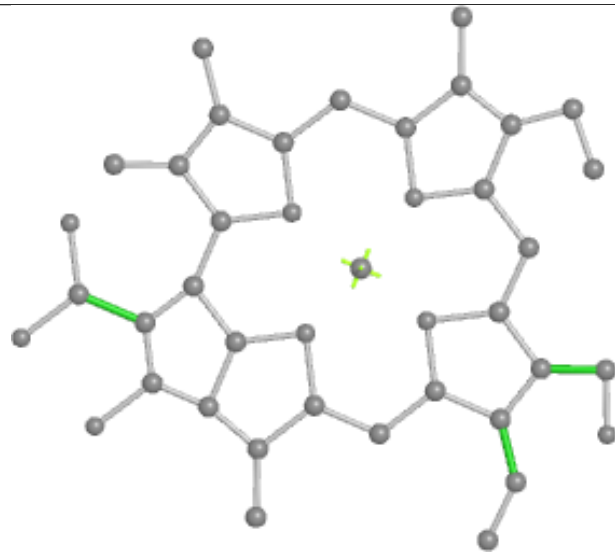
Ligand CHL 1 606



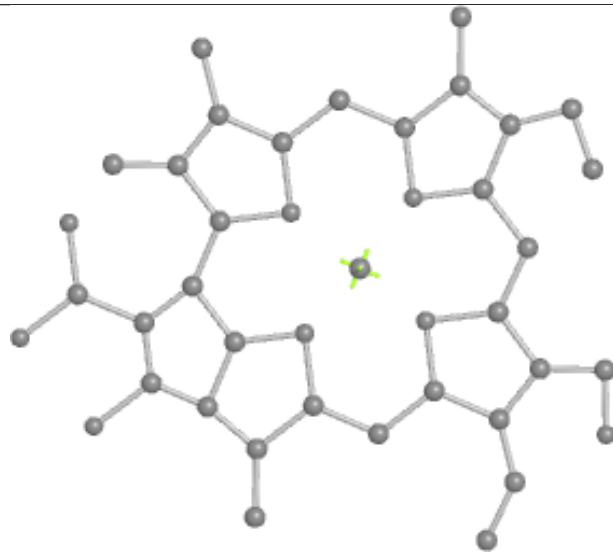
Bond lengths



Bond angles

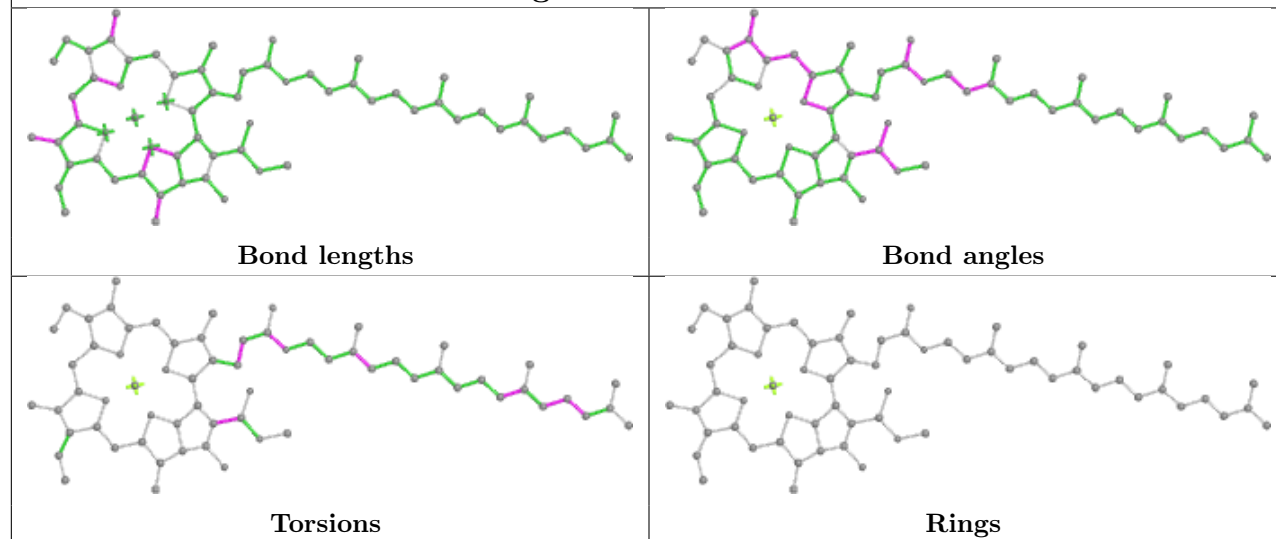


Torsions

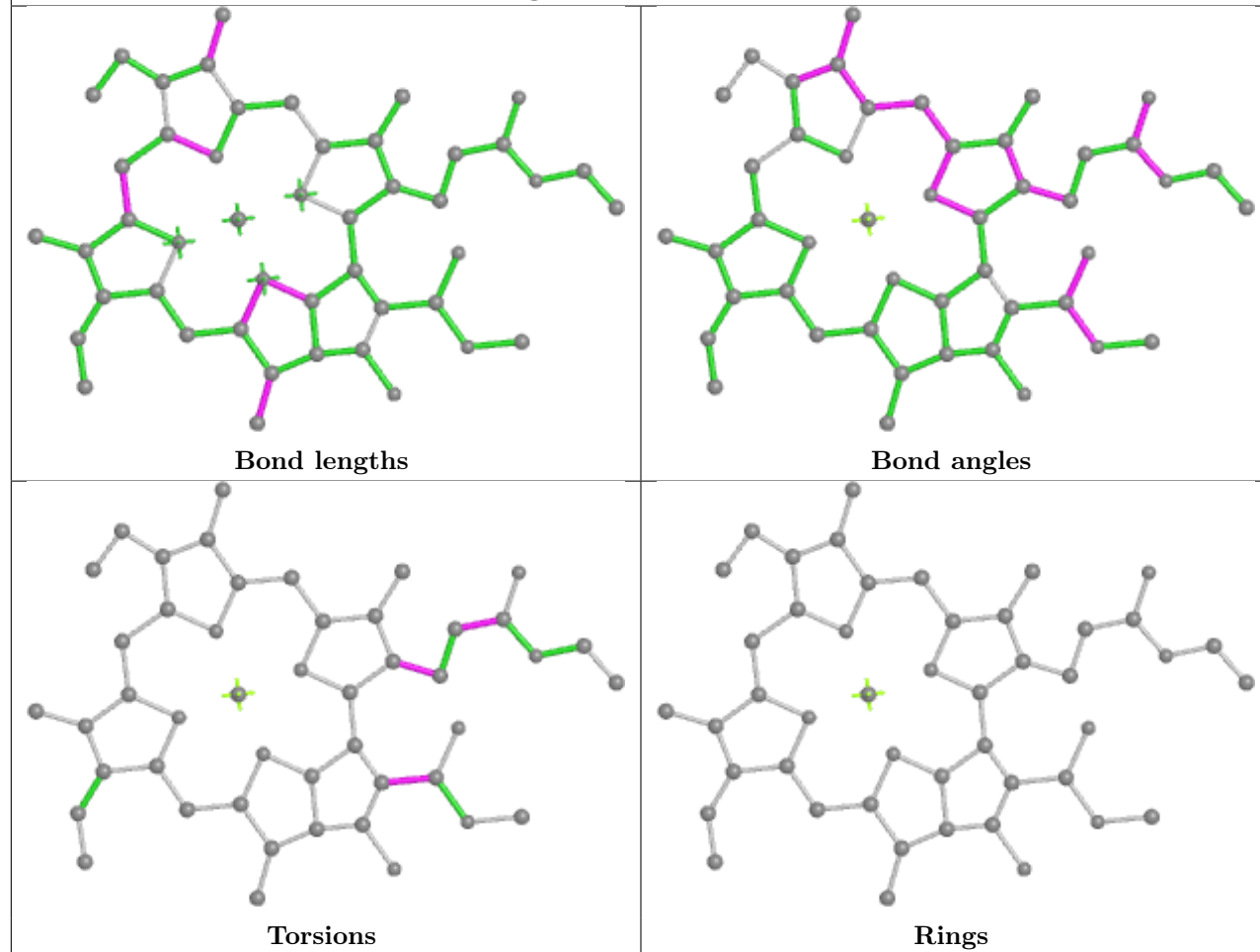


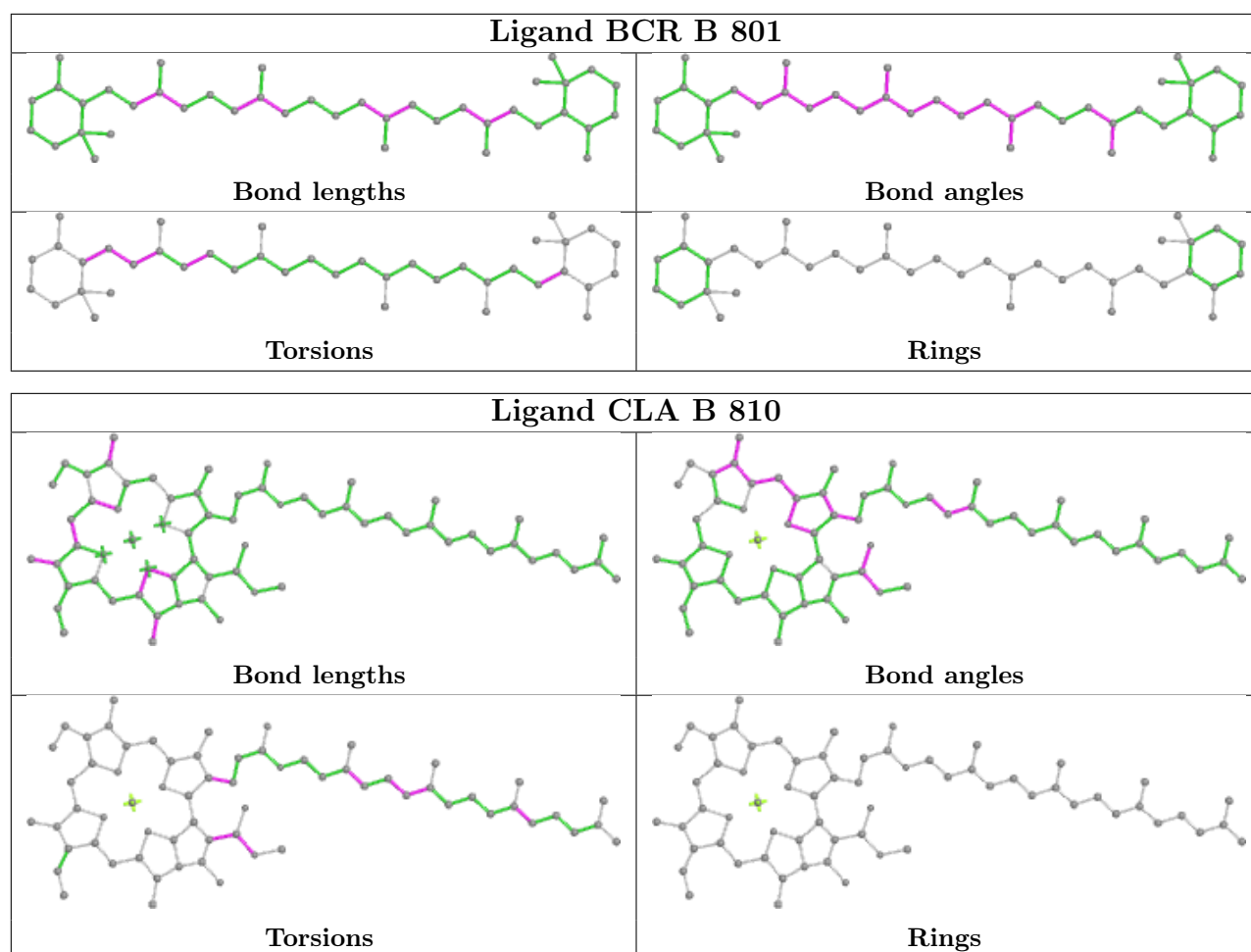
Rings

Ligand CLA B 813

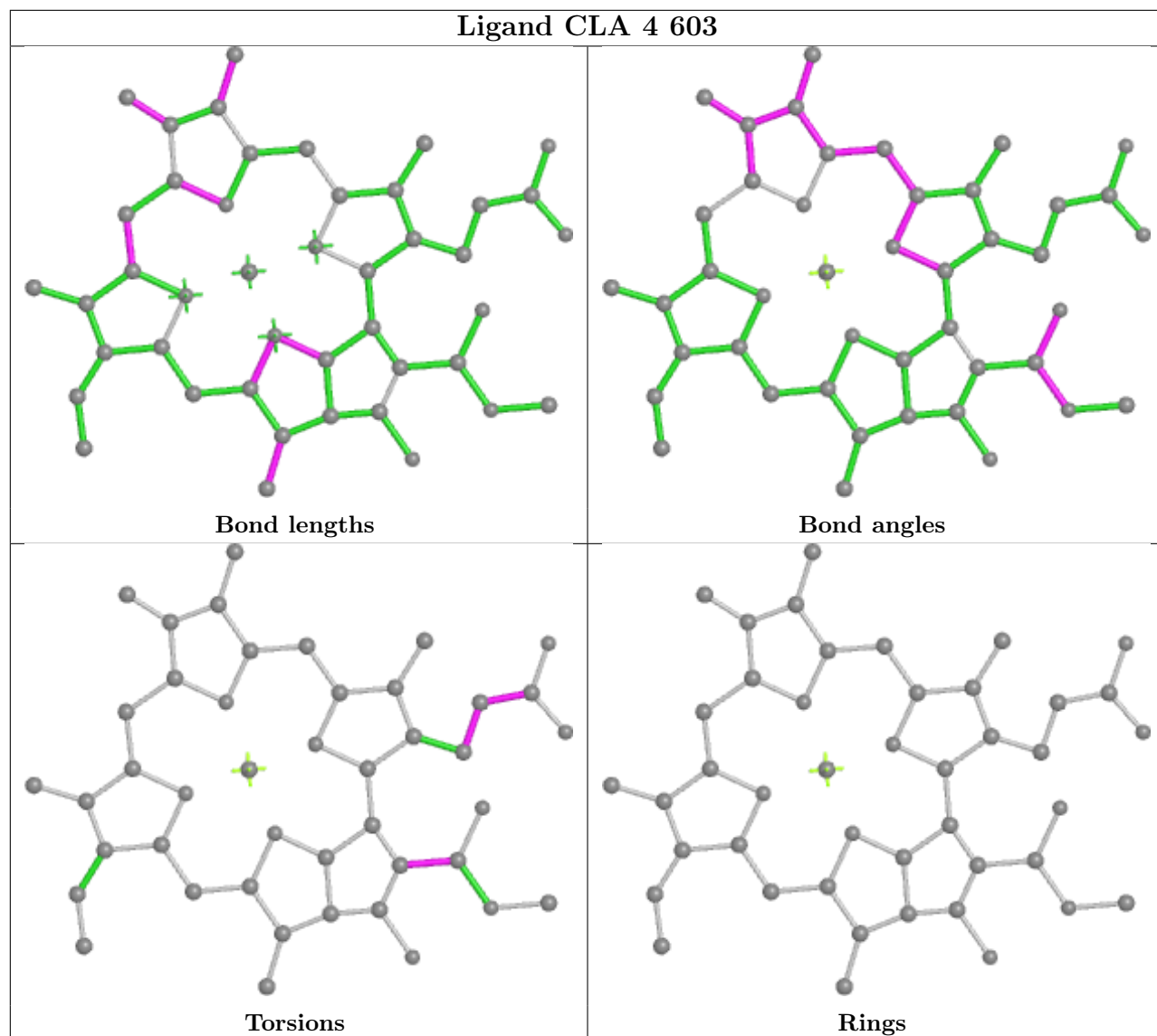


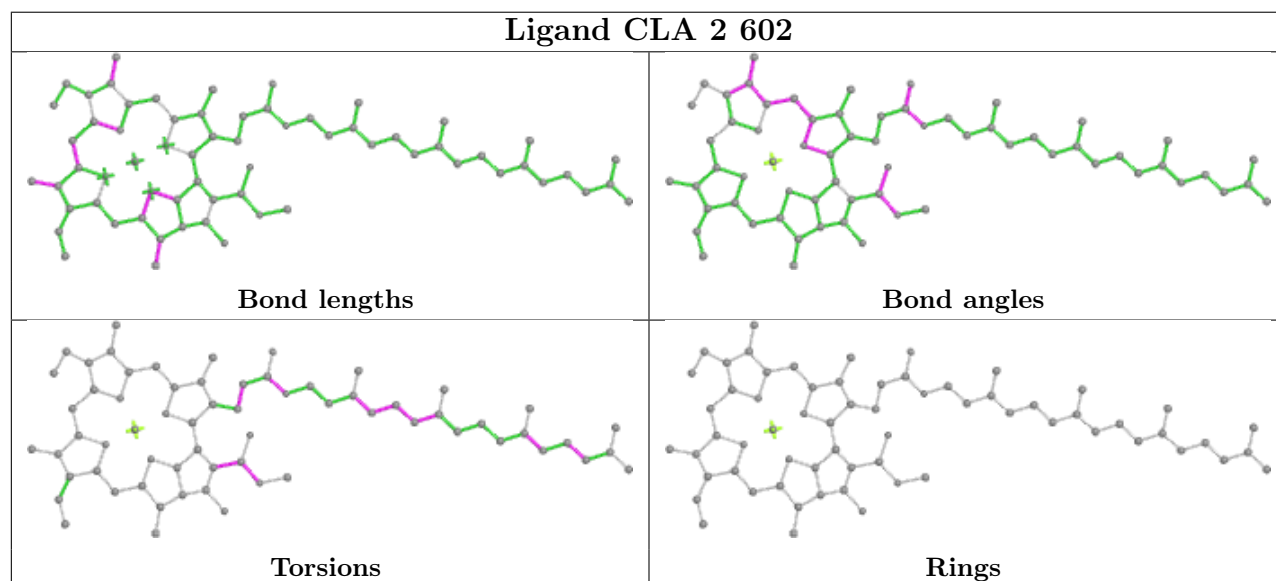
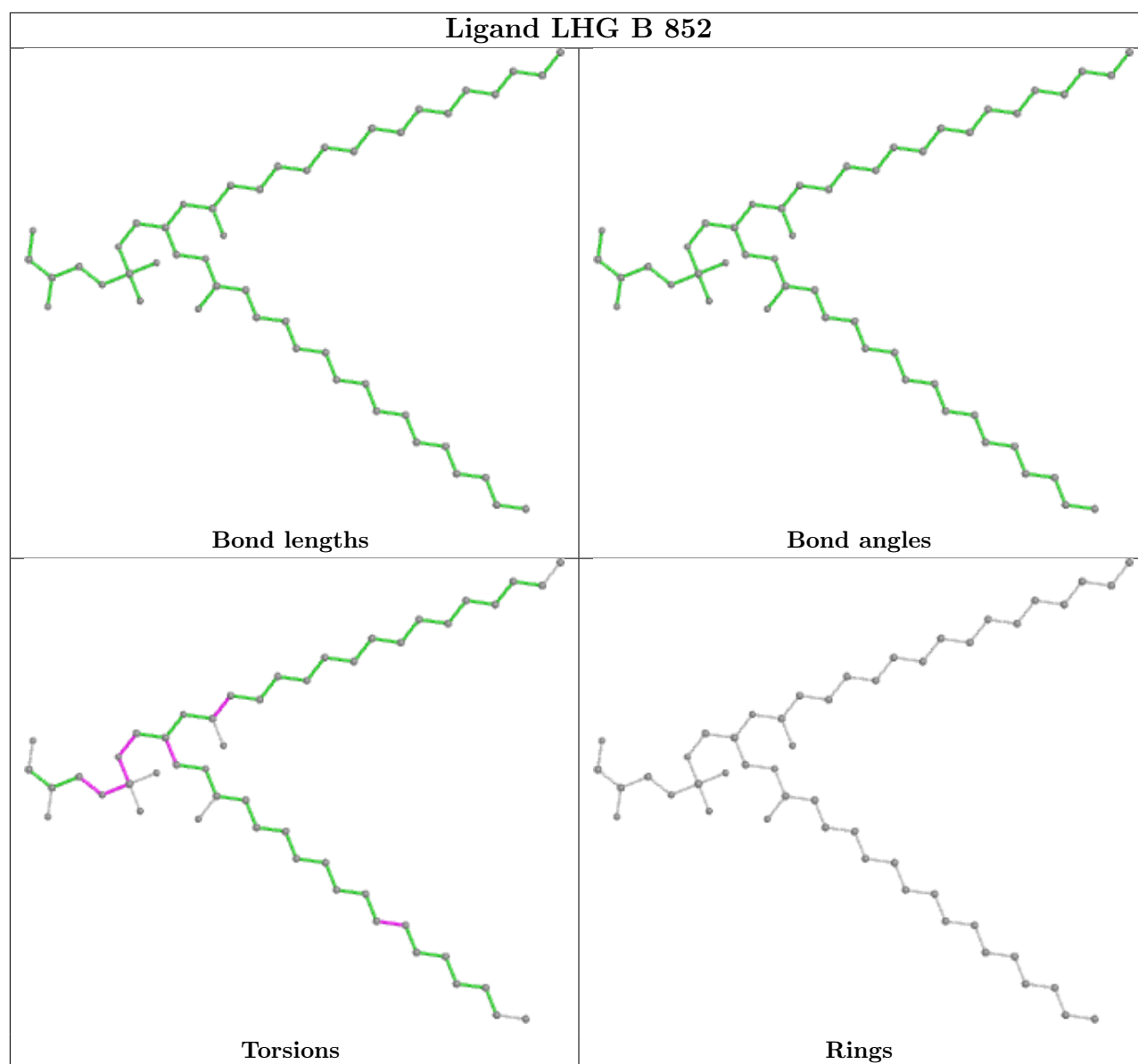
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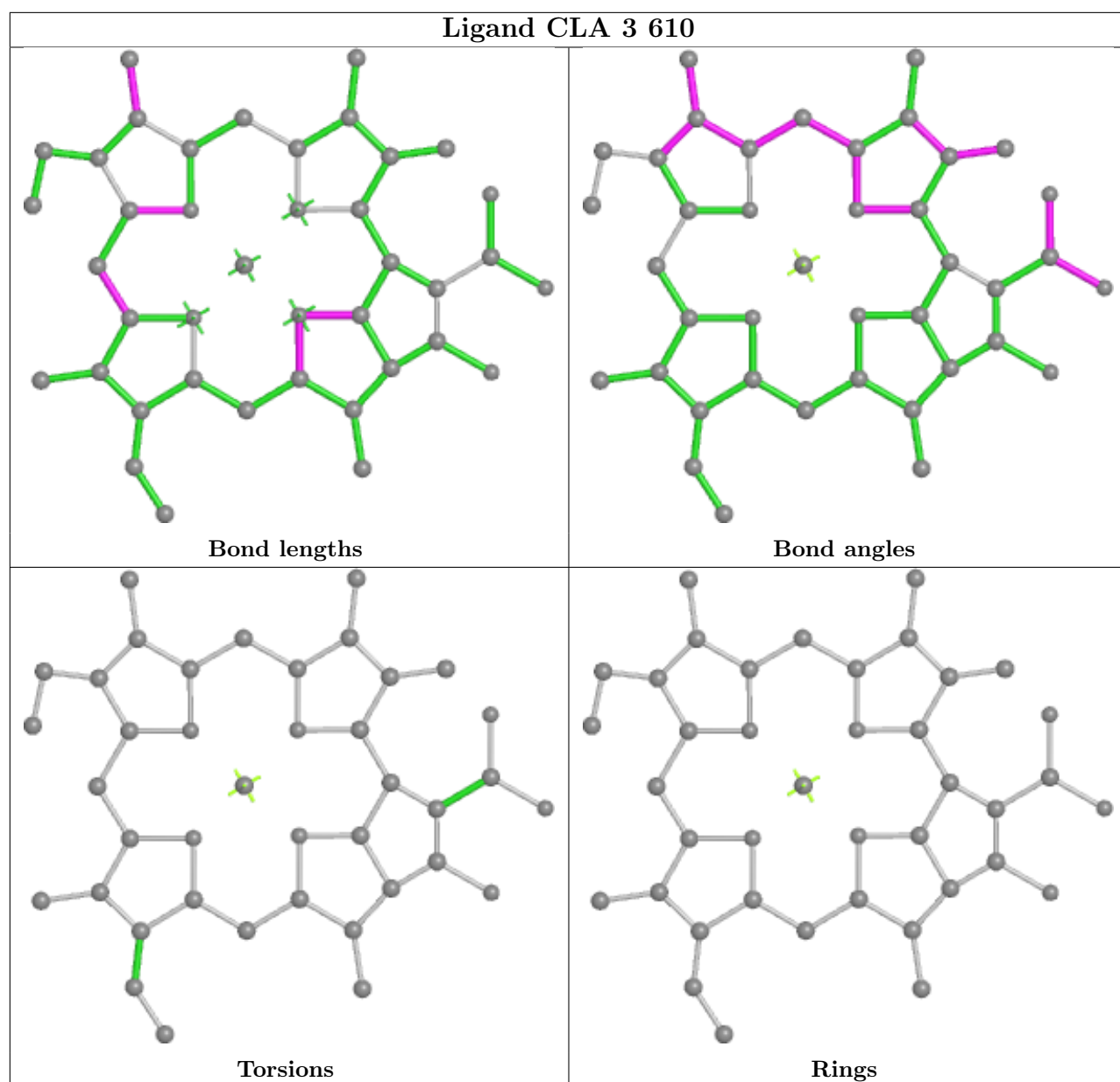


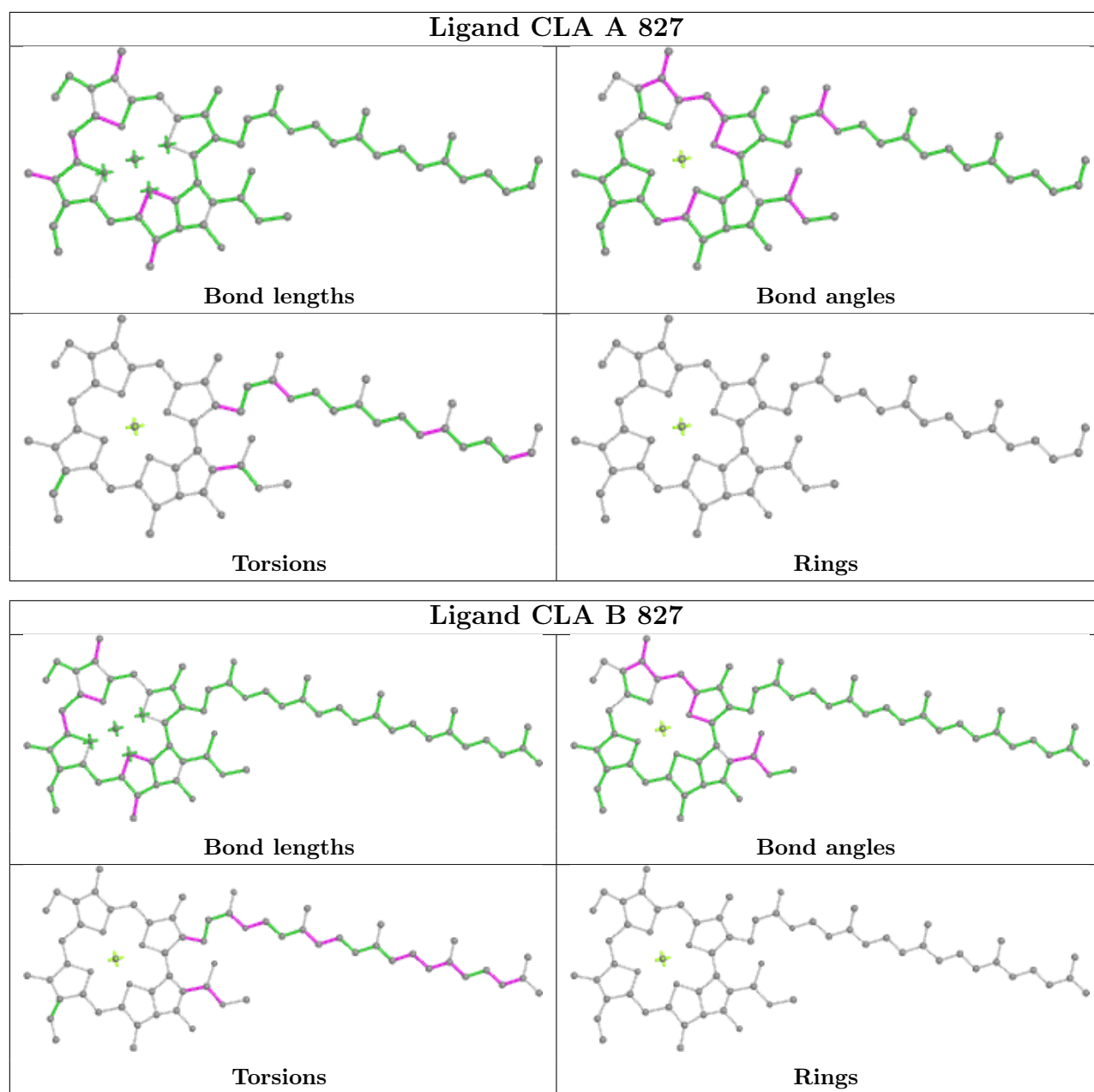


Ligand CLA 4 603

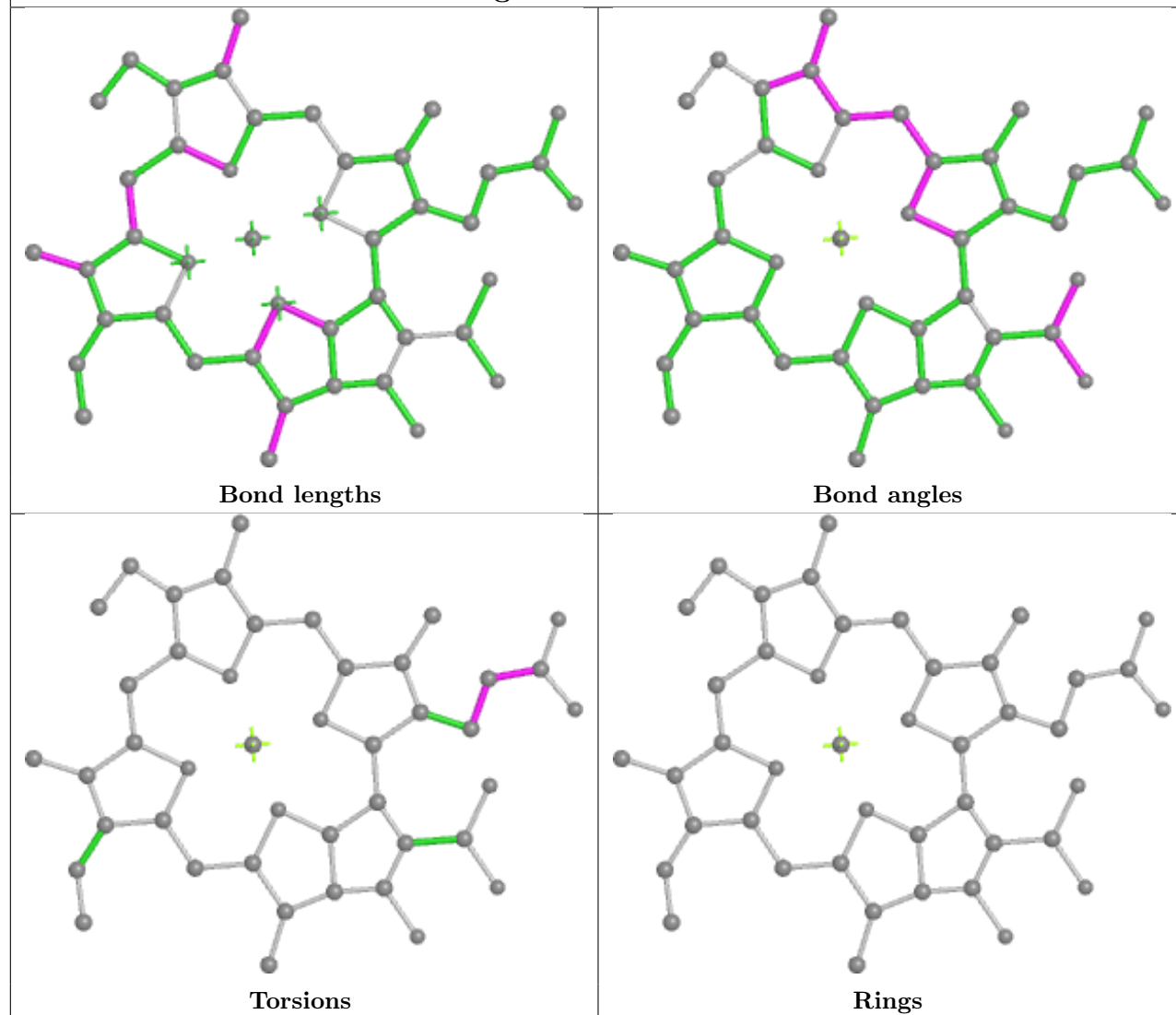




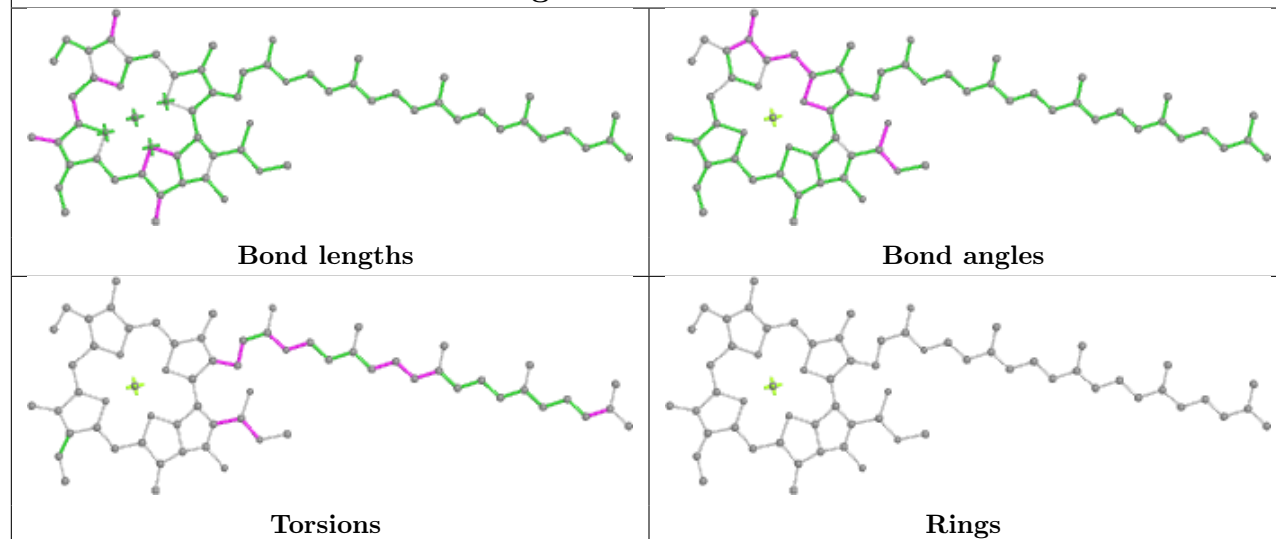




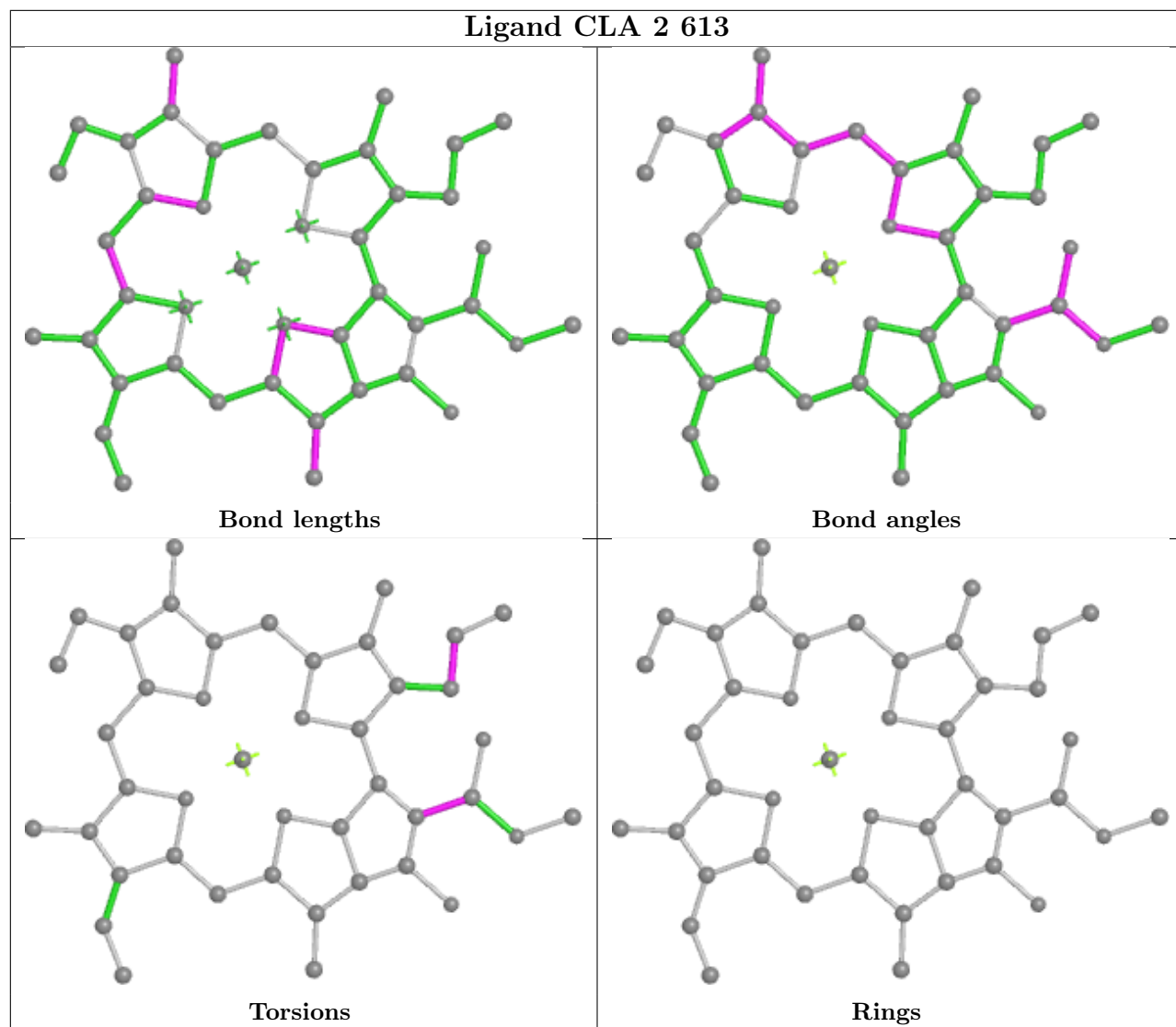
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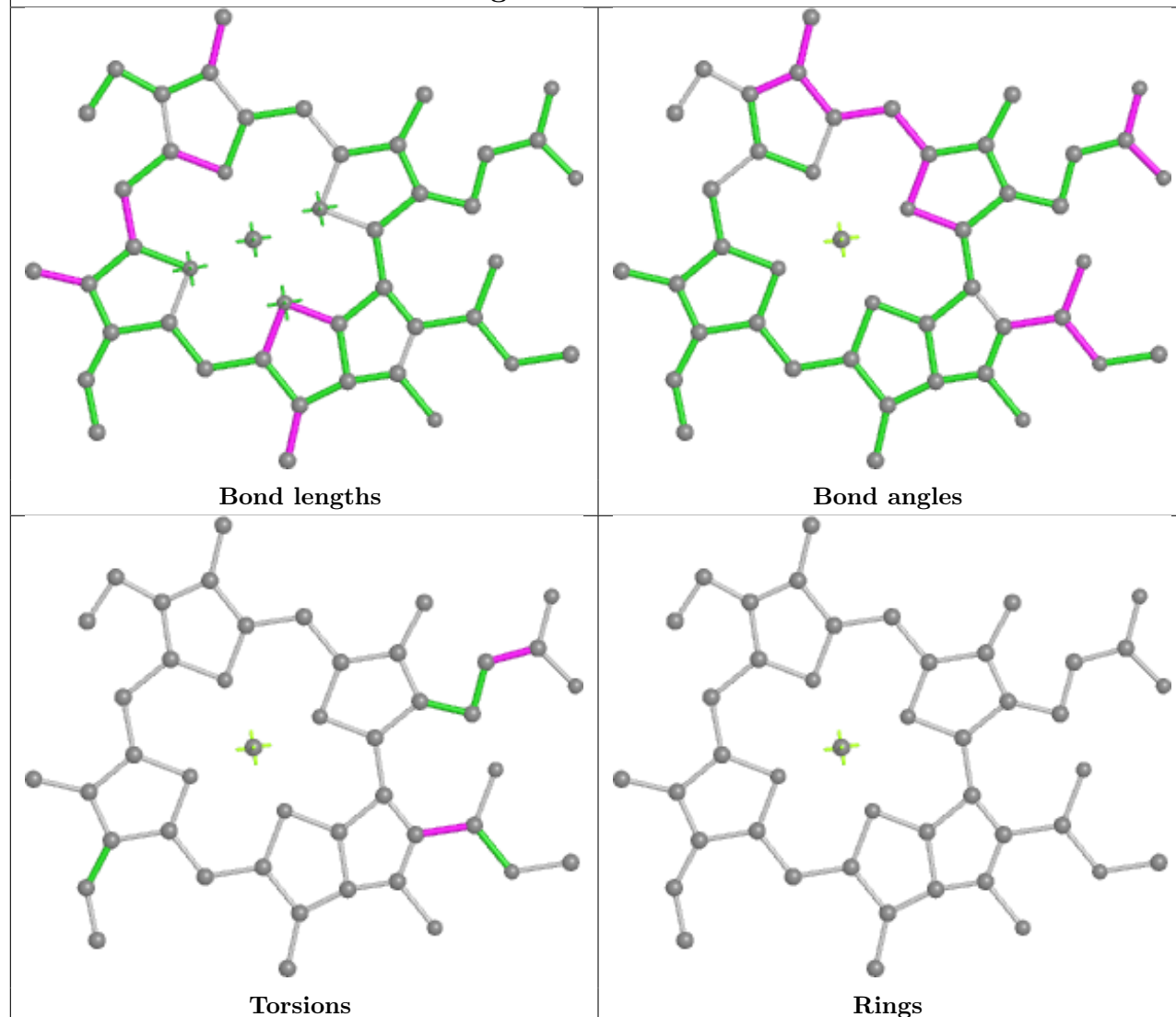
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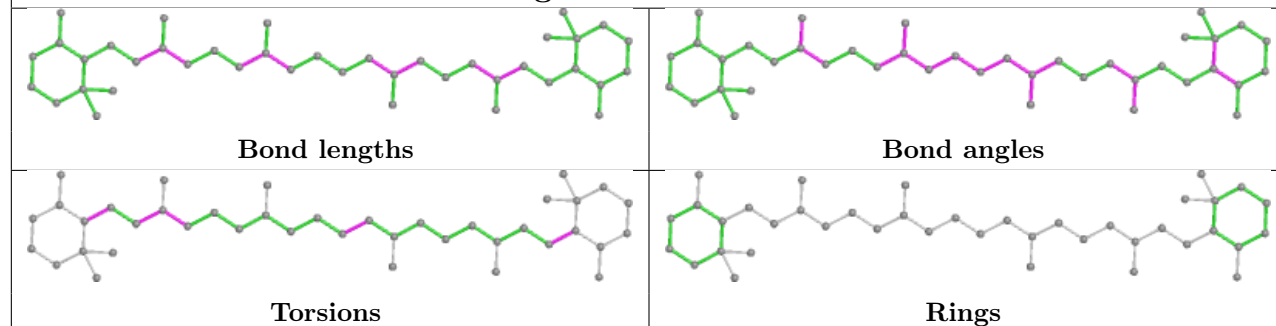
Ligand CLA 2 613



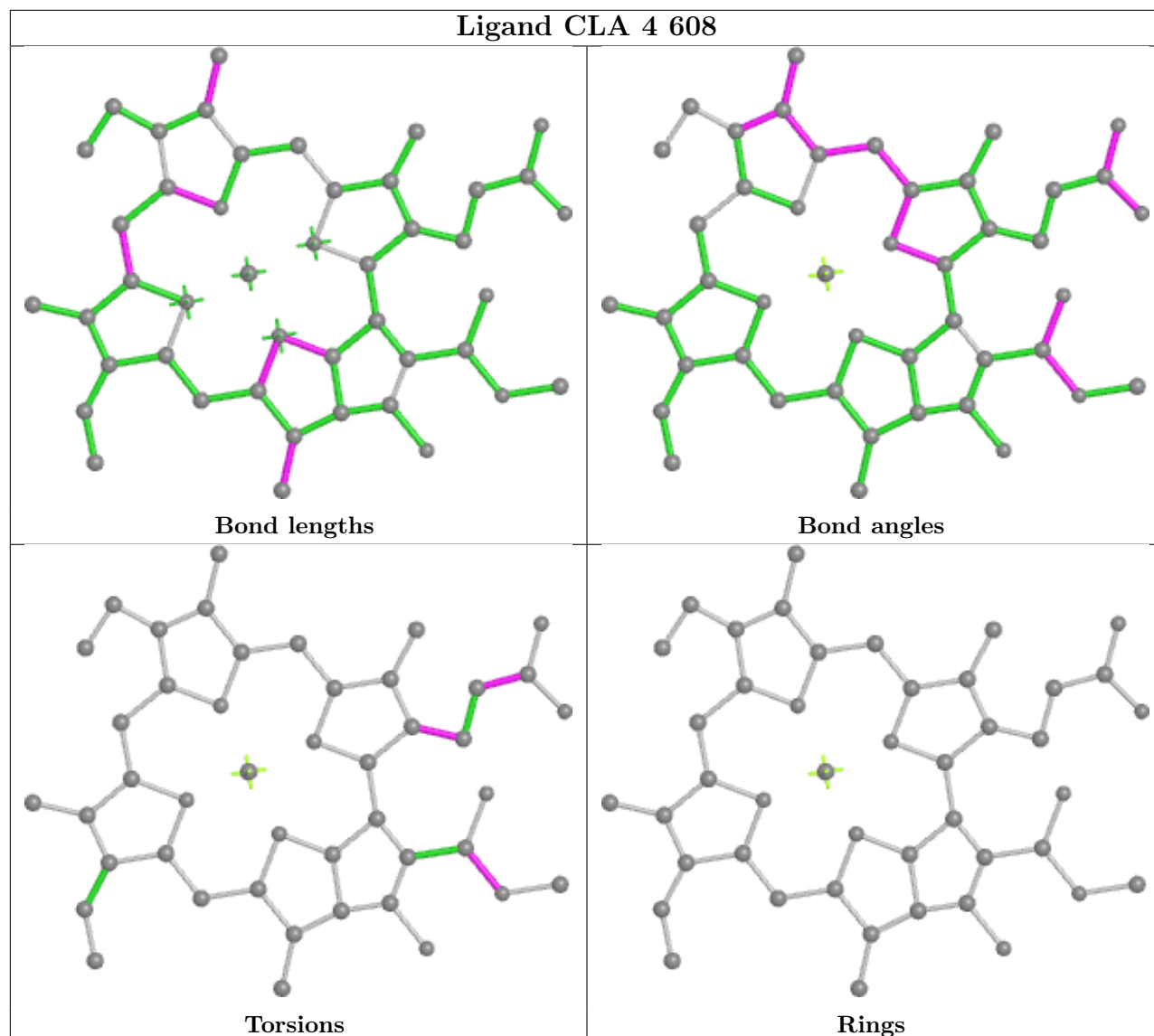
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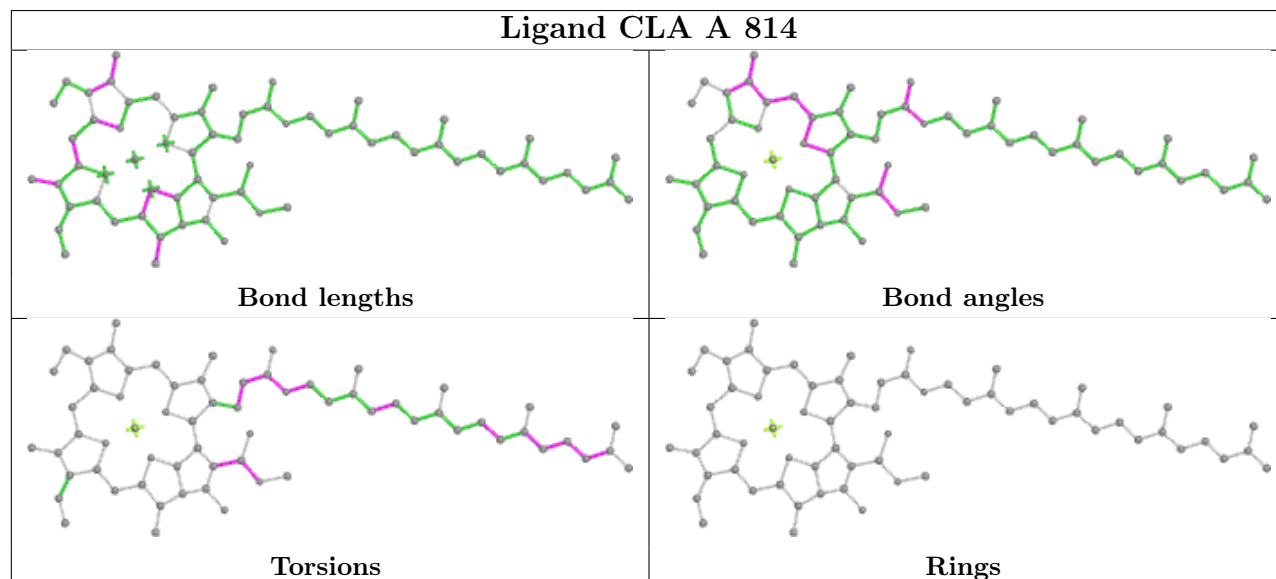
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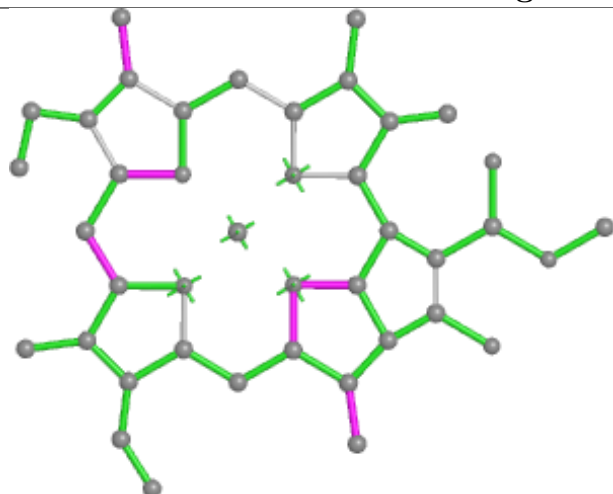
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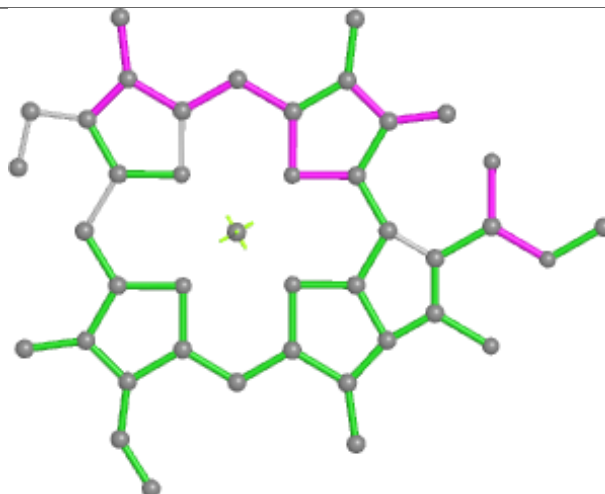
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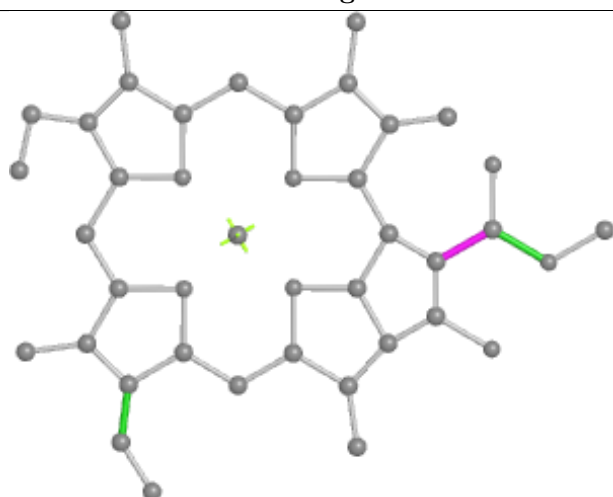
Ligand CLA F 303



Bond lengths



Bond angles

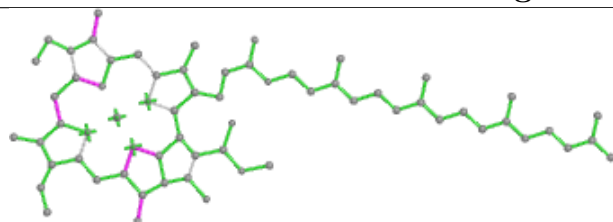


Torsions

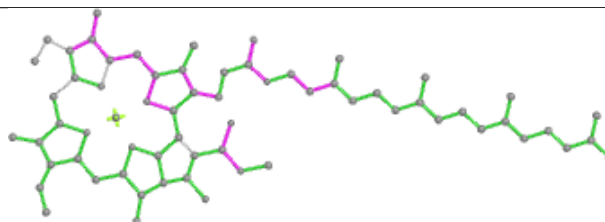


Rings

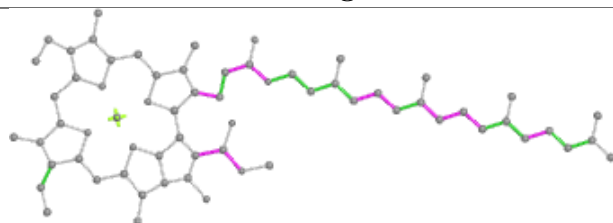
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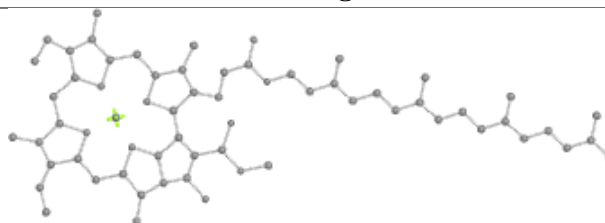
Bond lengths



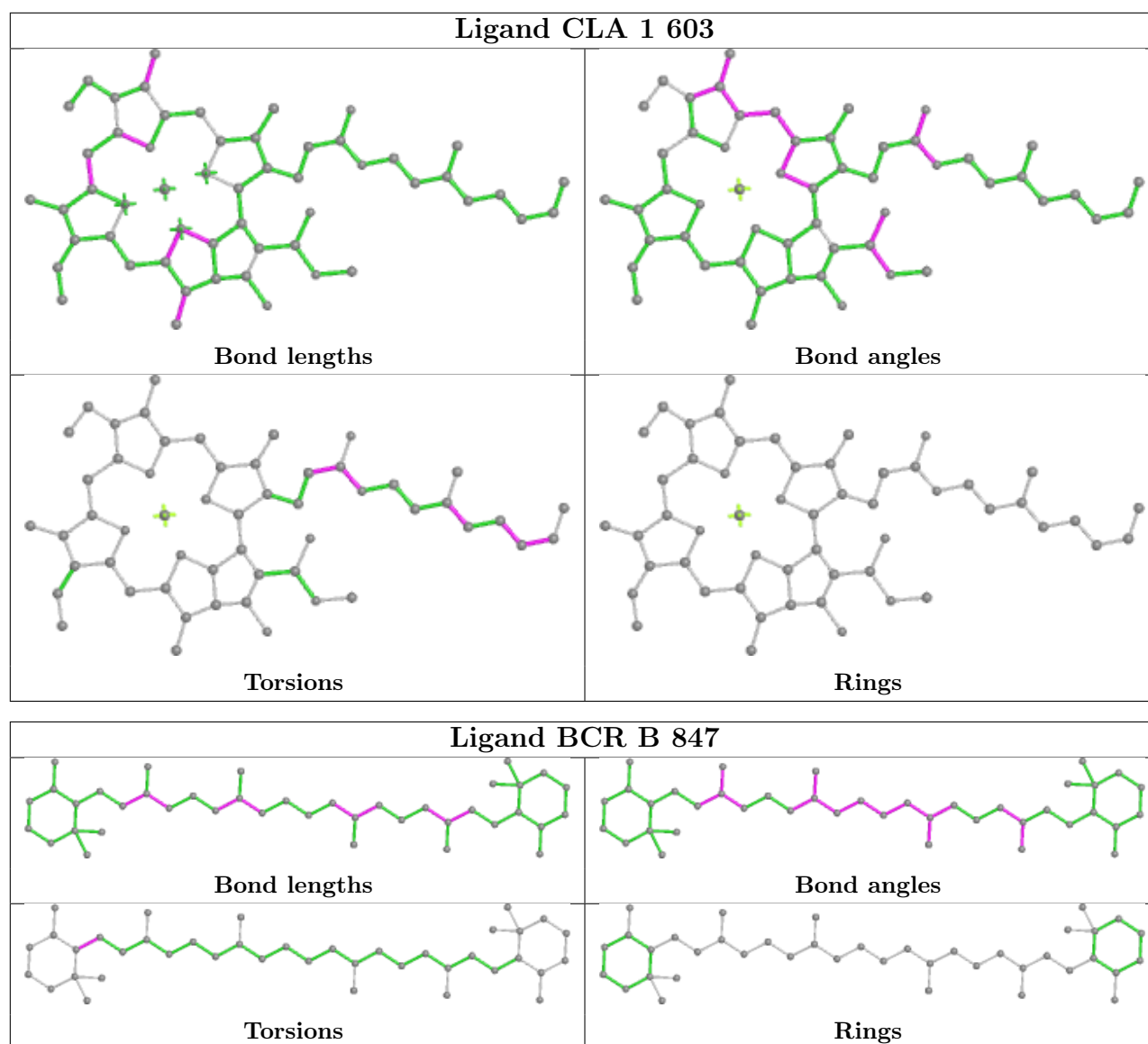
Bond angles

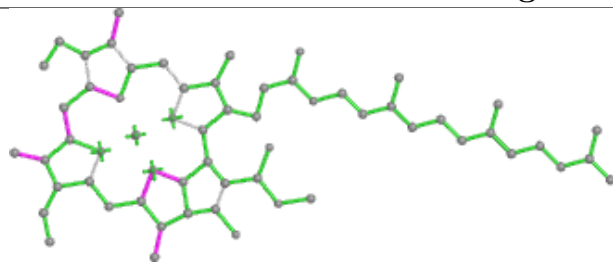


Torsions

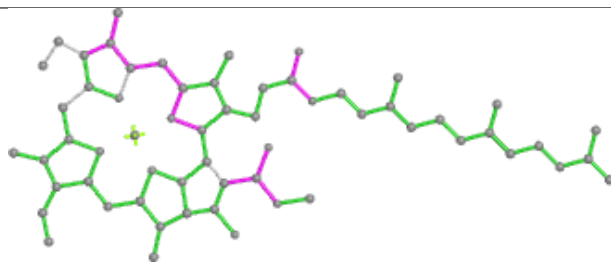


Rings

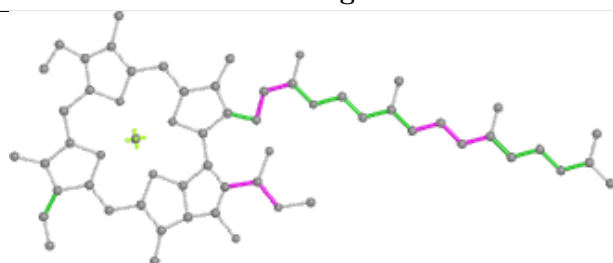


Ligand CLA 4 602

Bond lengths



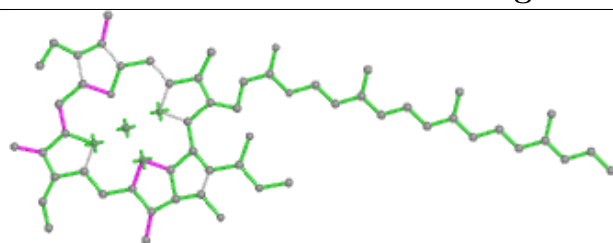
Bond angles



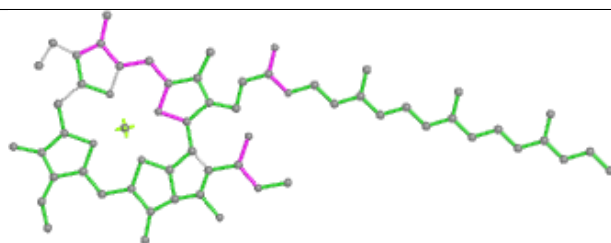
Torsions



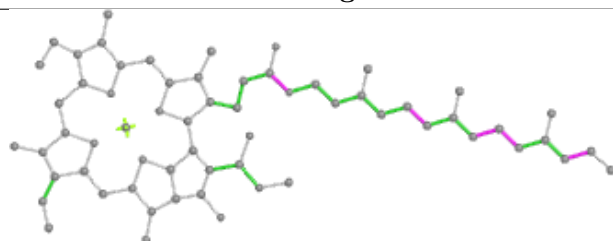
Rings

Ligand CLA B 826

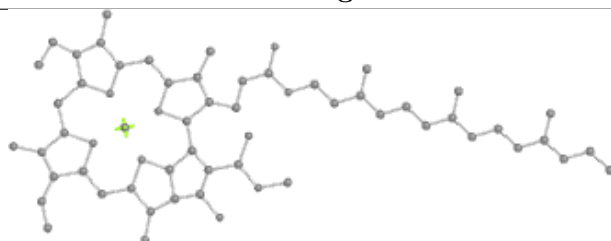
Bond lengths



Bond angles

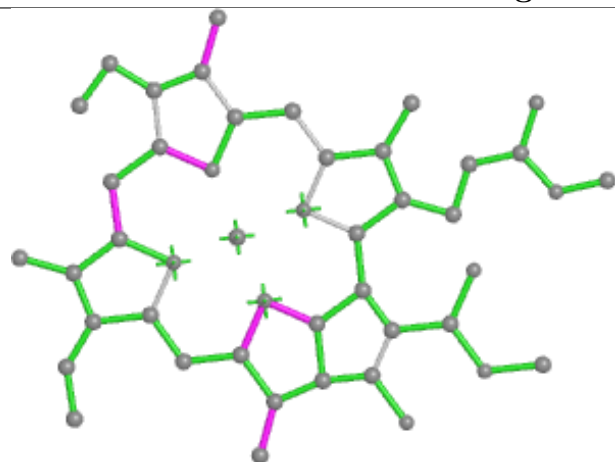


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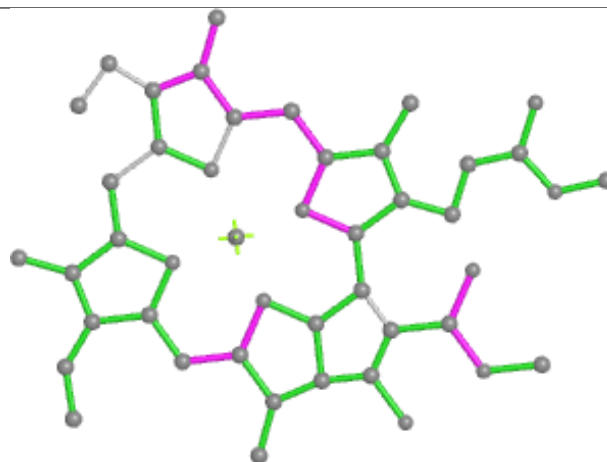


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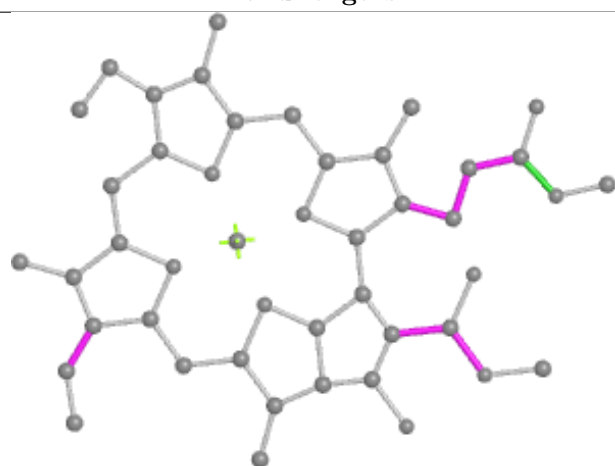
Ligand CLA K 204



Bond lengths



Bond angles

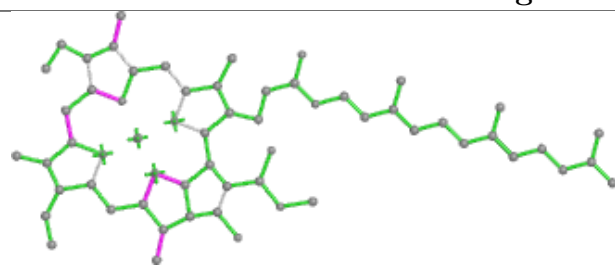


Torsions

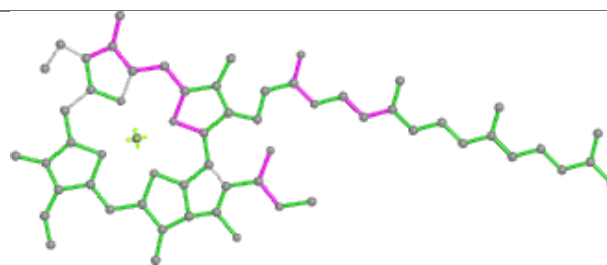


Rings

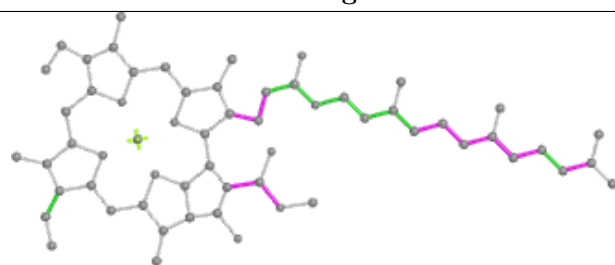
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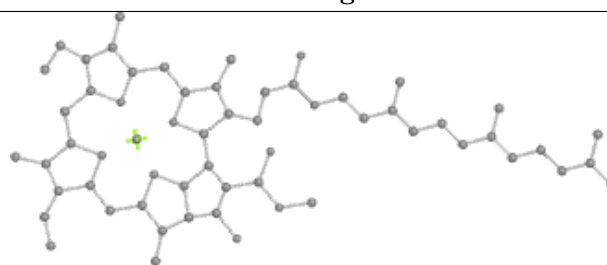
Bond lengths



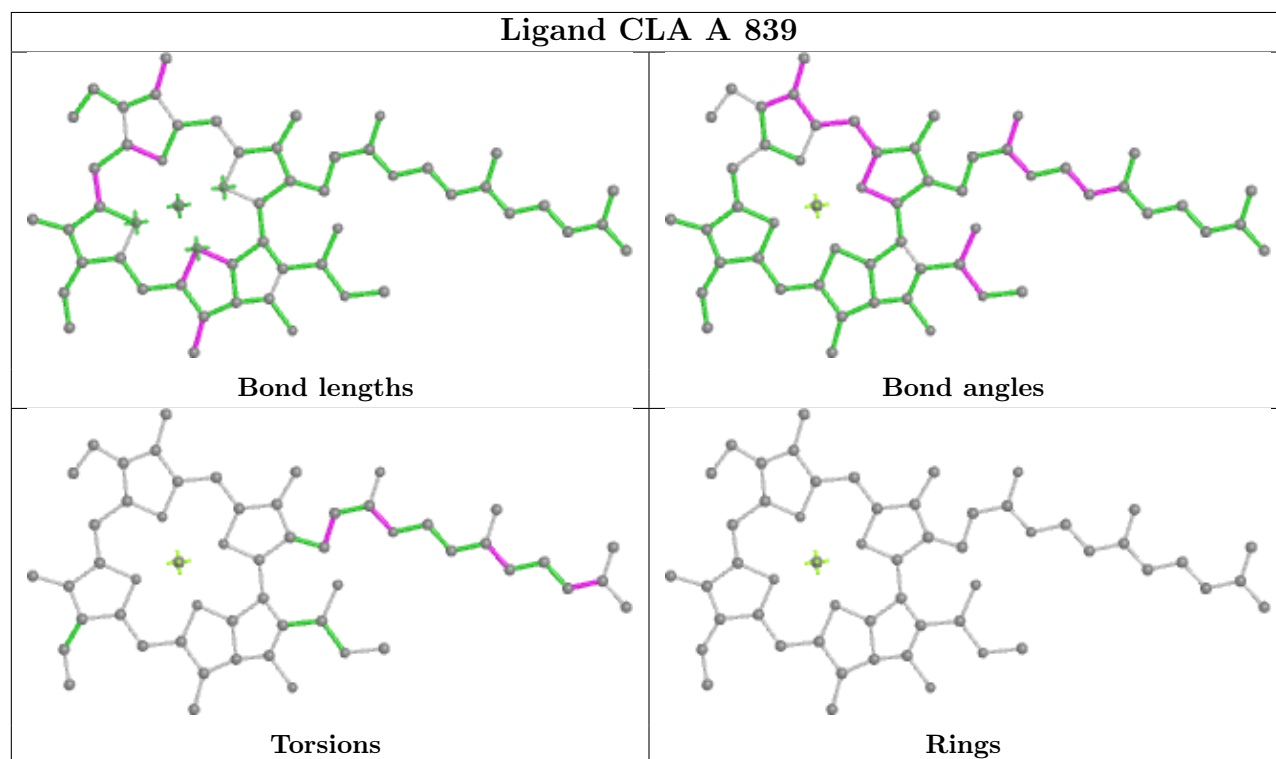
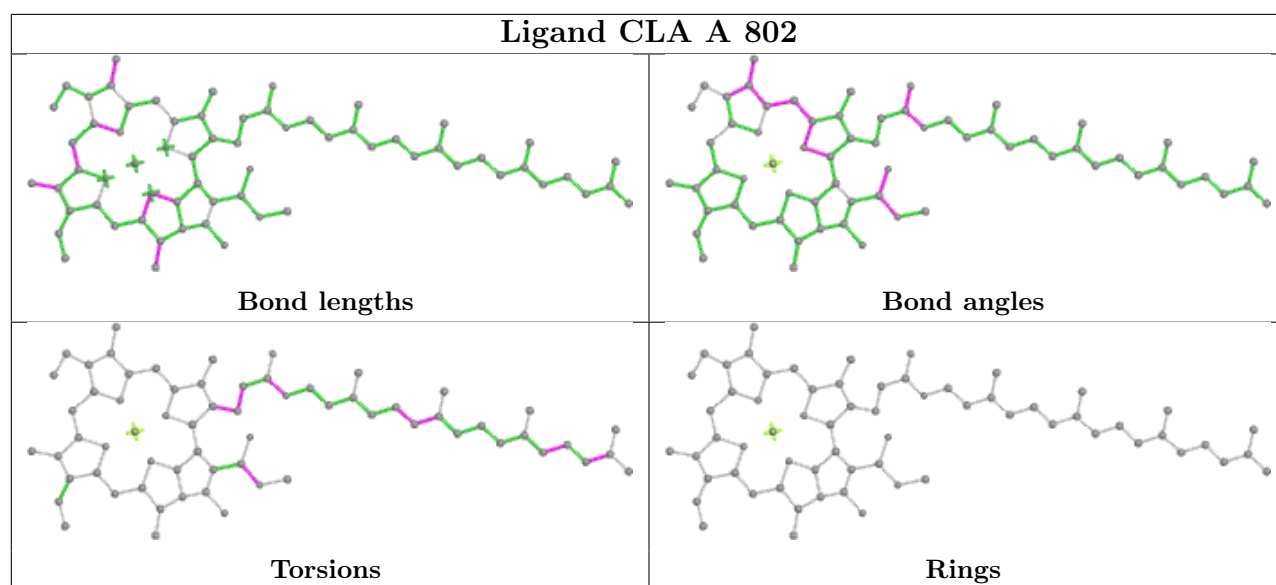
Bond angles



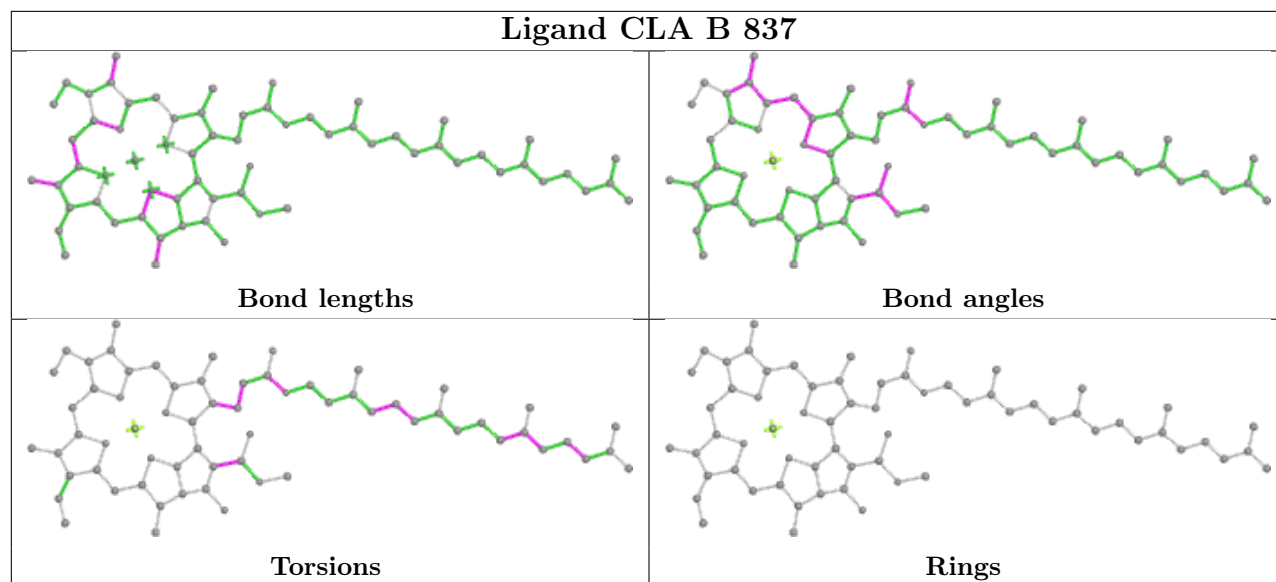
Torsions



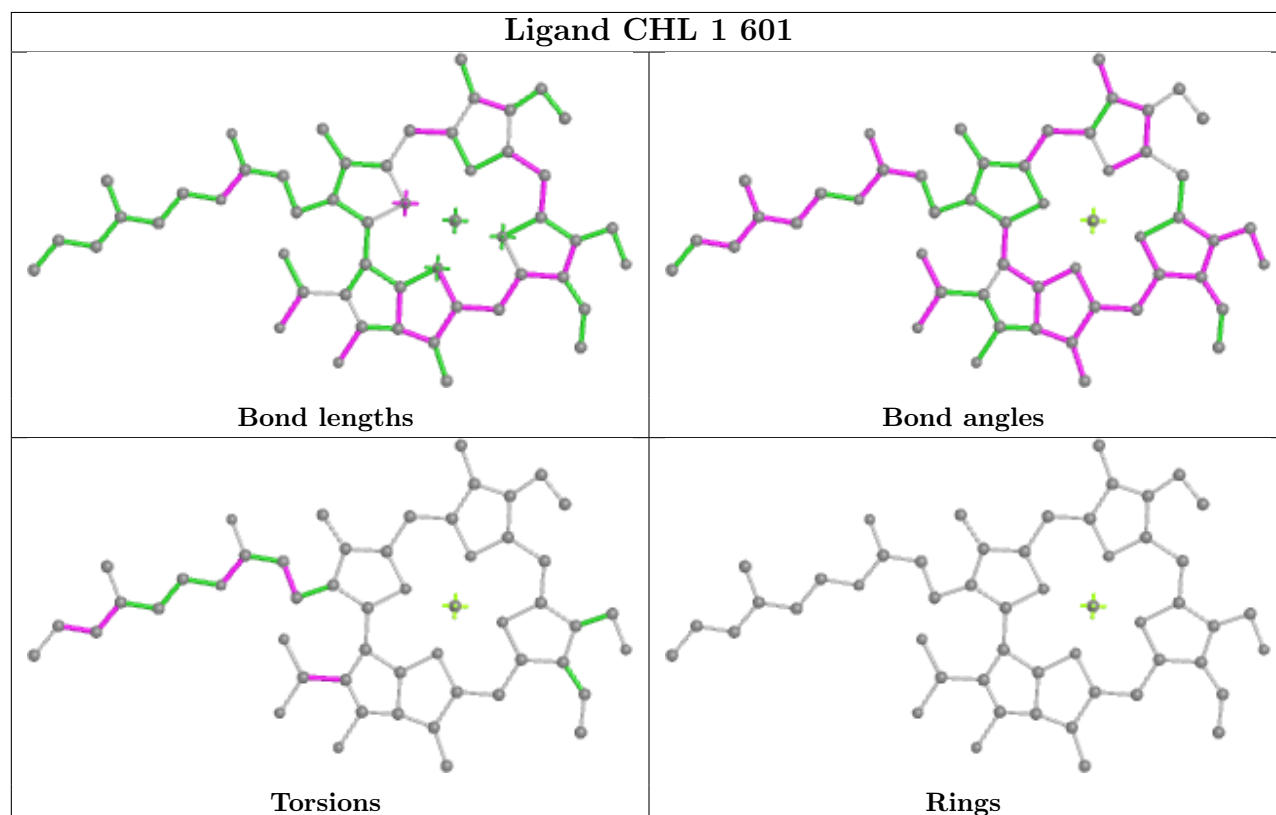
Rings



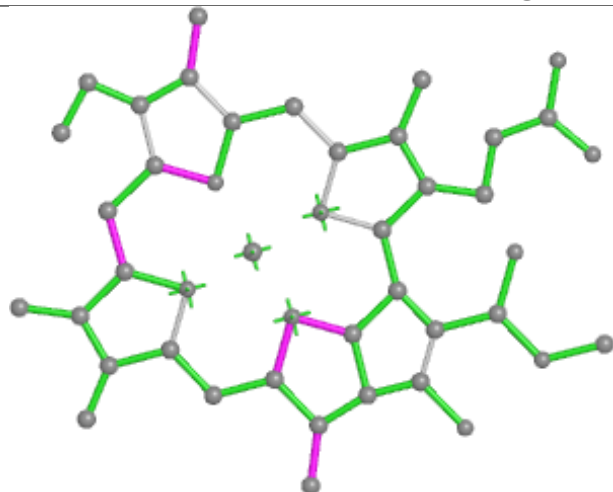
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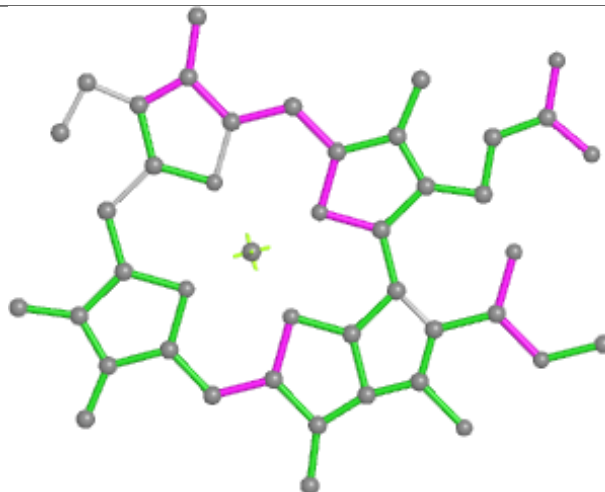
Ligand CHL 1 601



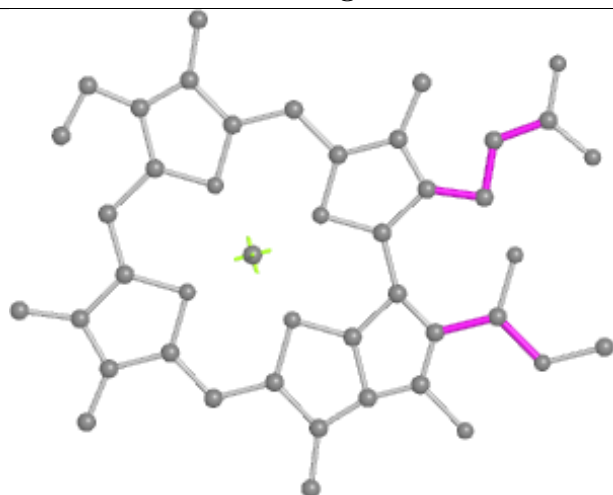
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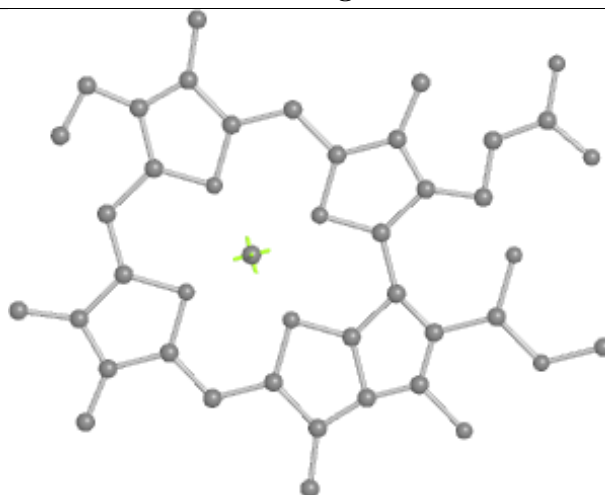
Bond lengths



Bond angles

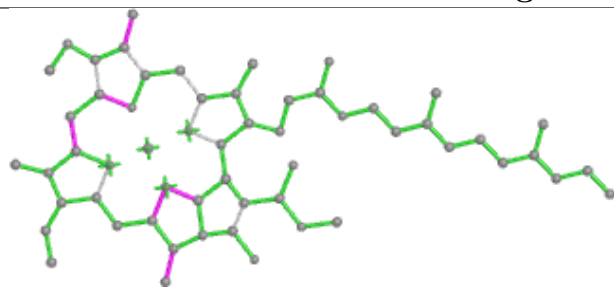


Torsions

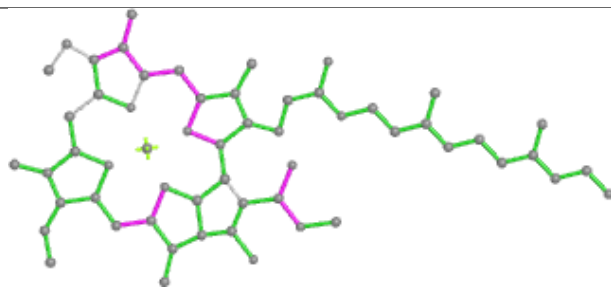


Rings

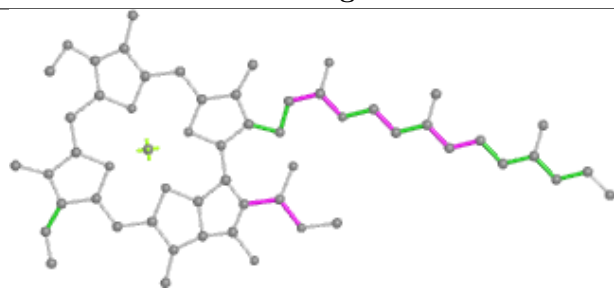
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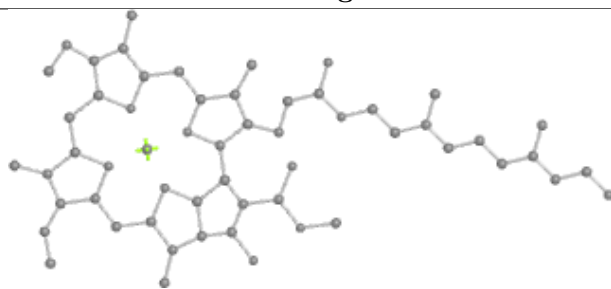
Bond lengths



Bond angles

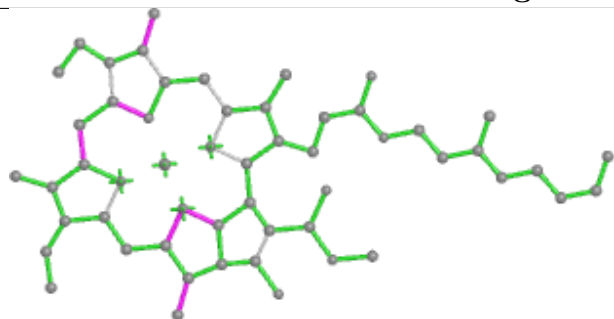


Torsions

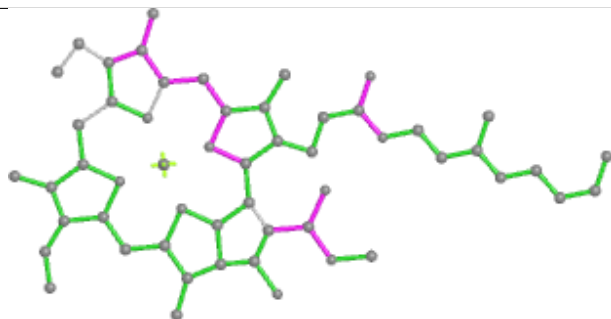


Rings

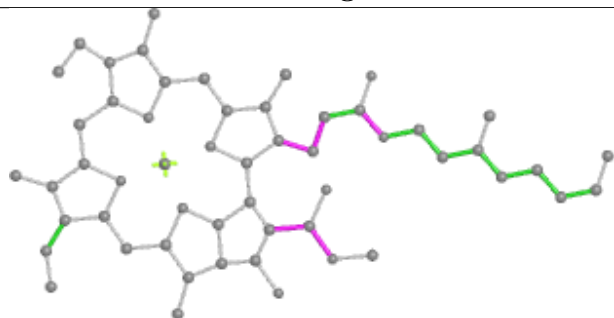
Ligand CLA A 813



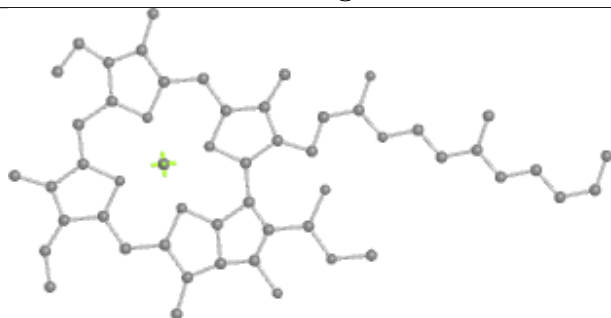
Bond lengths



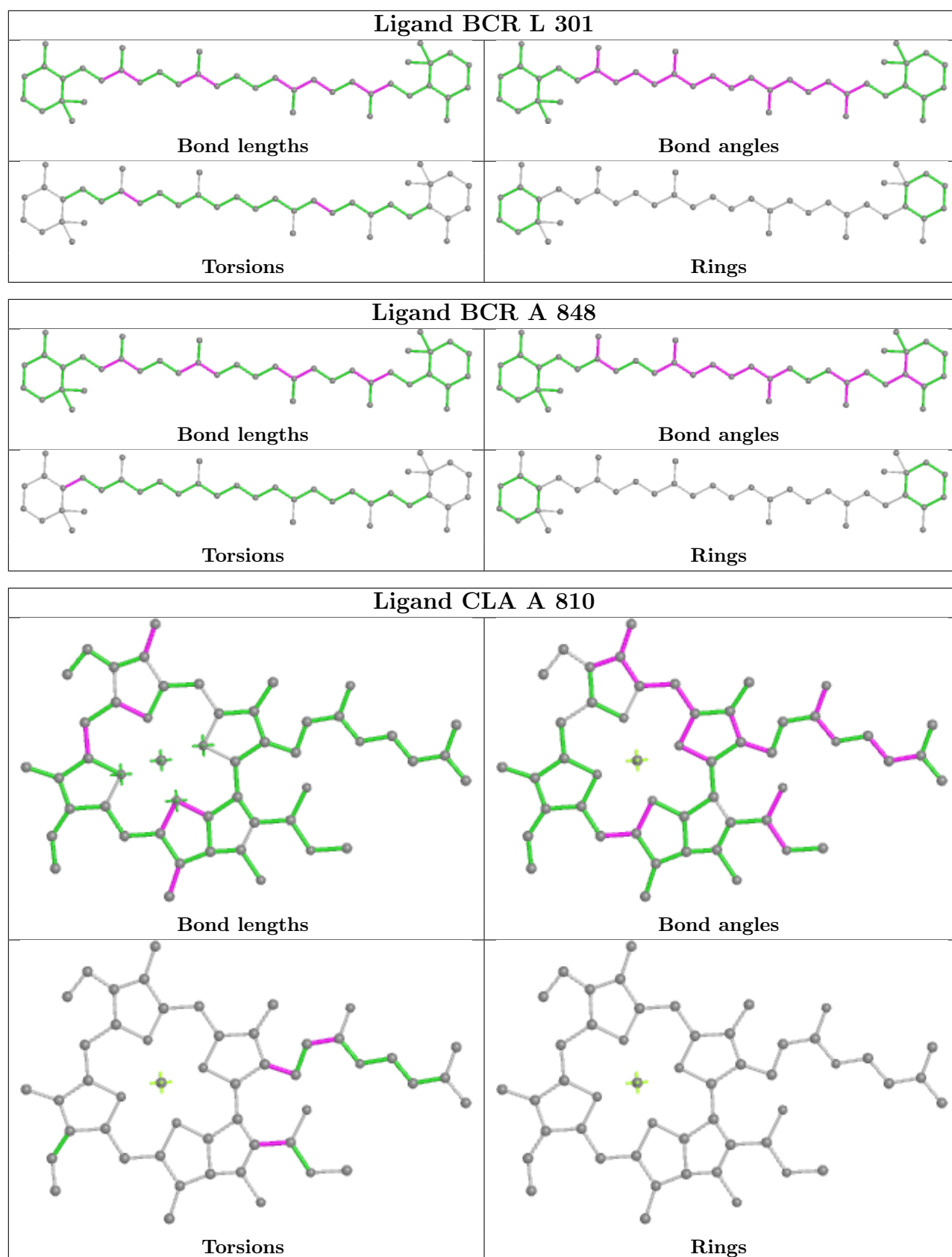
Bond angles

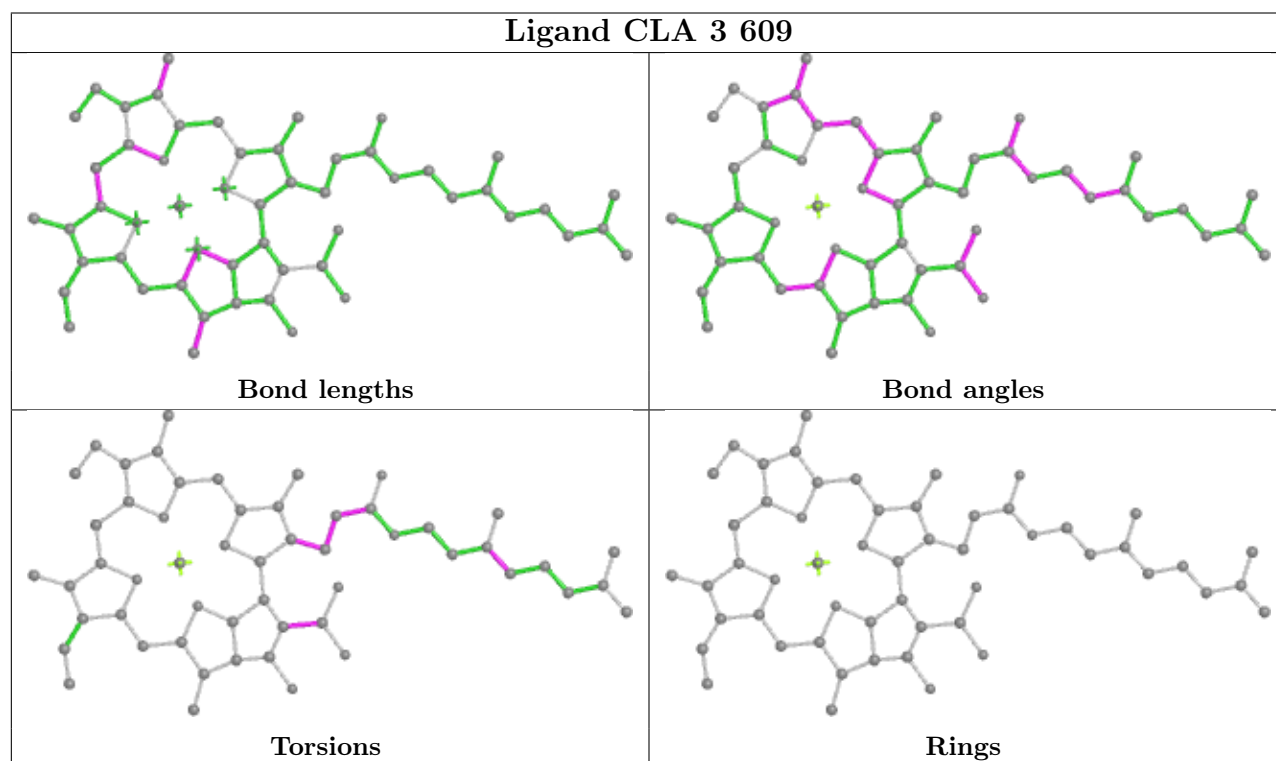
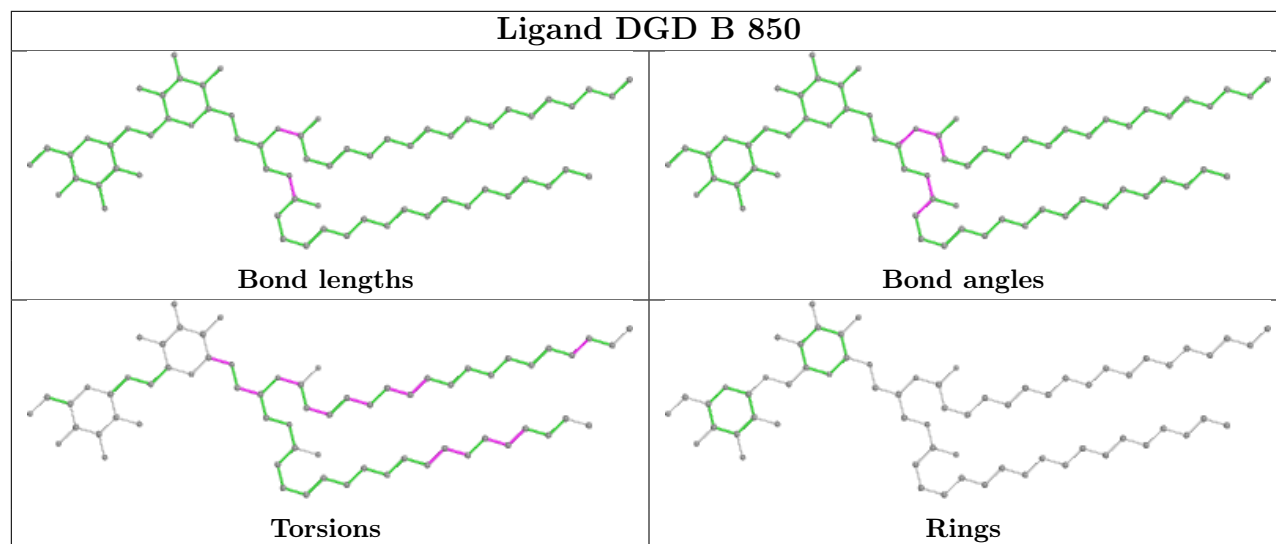
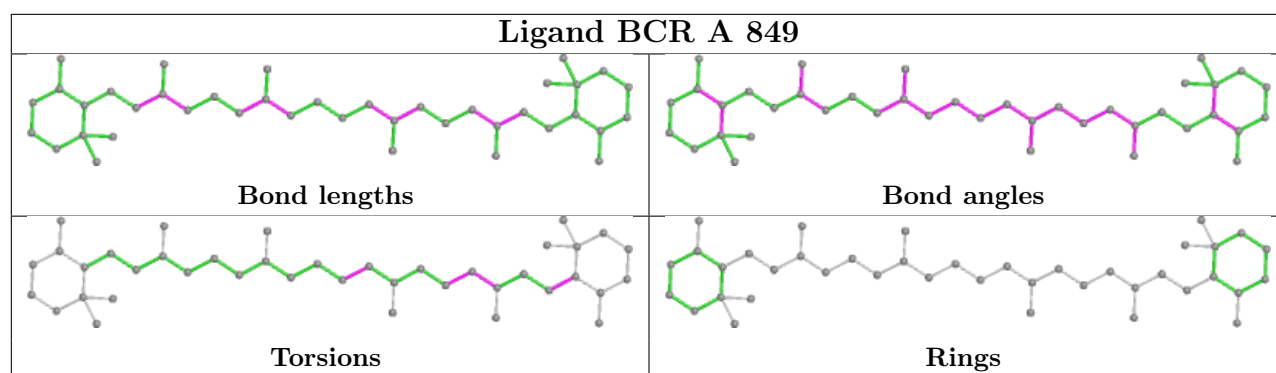


Torsions

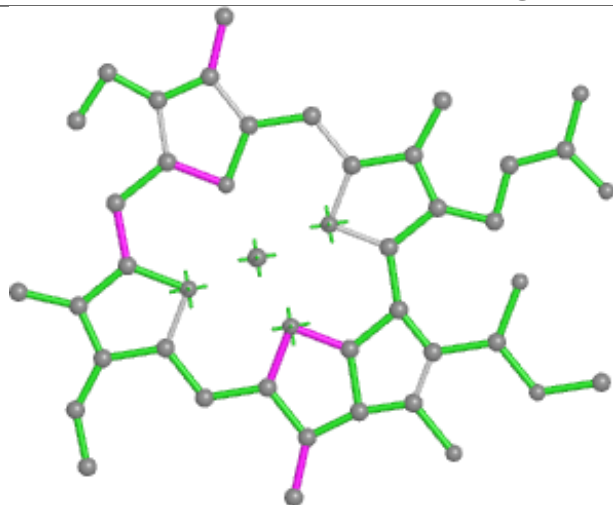


Rings

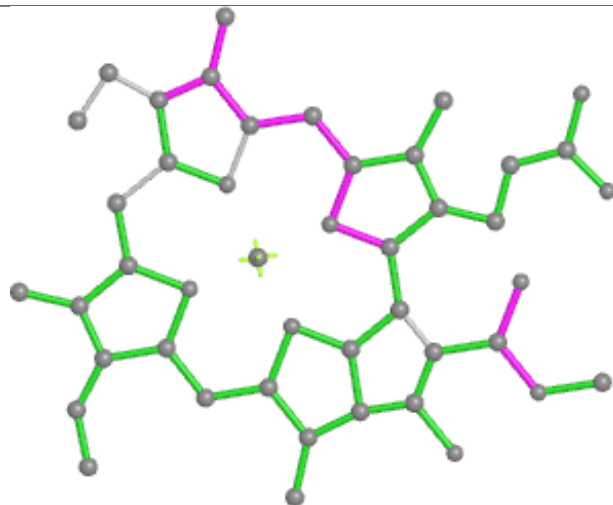




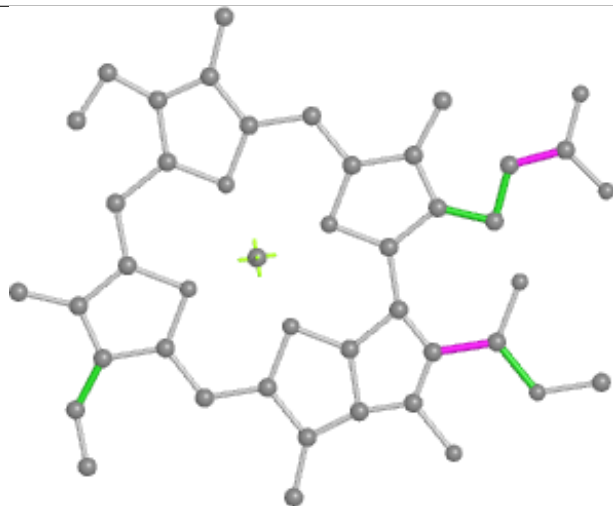
Ligand CLA A 817



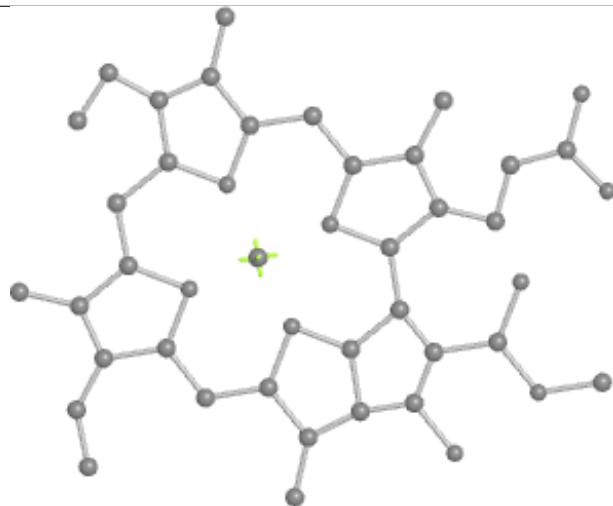
Bond lengths



Bond angles

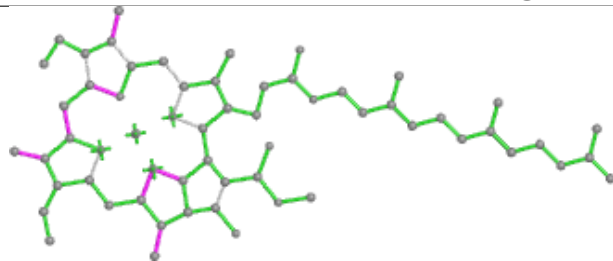


Torsions

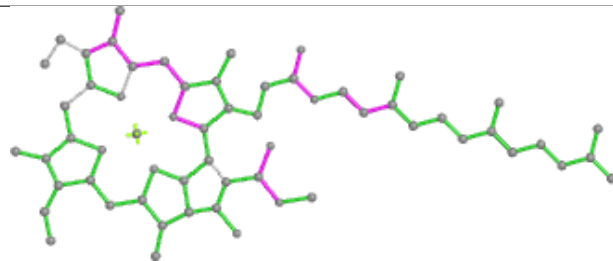


Rings

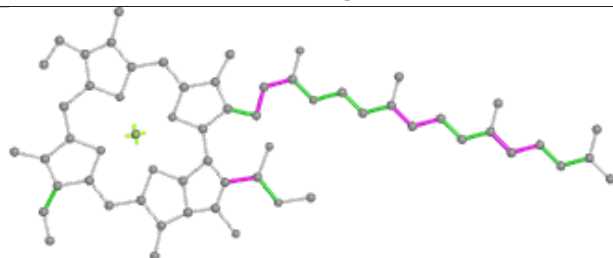
Ligand CLA 3 601



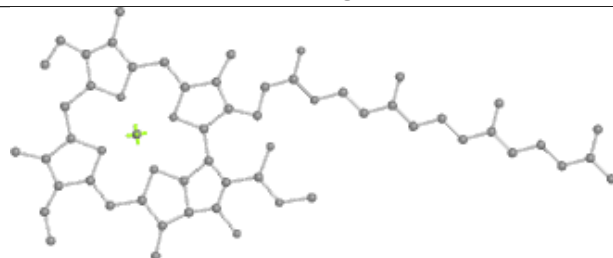
Bond lengths



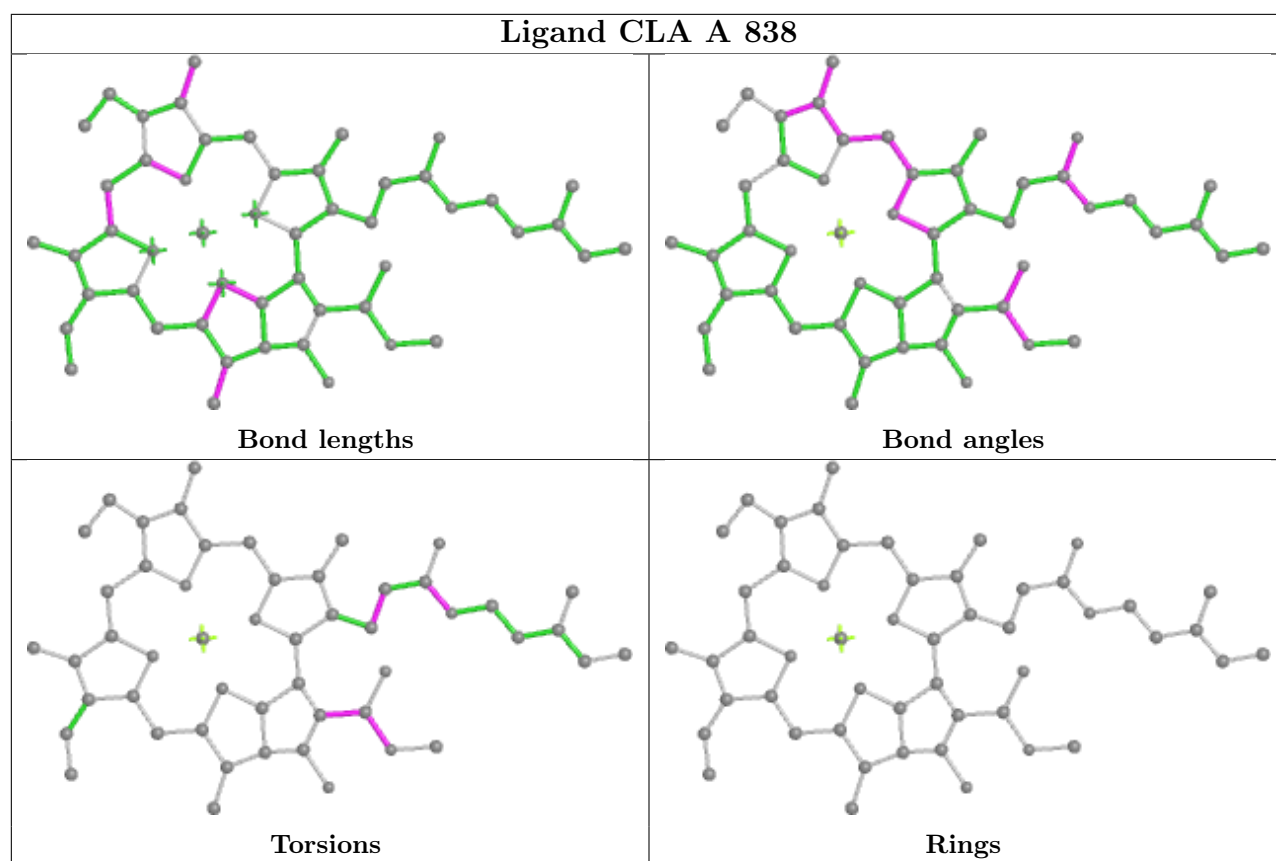
Bond angles



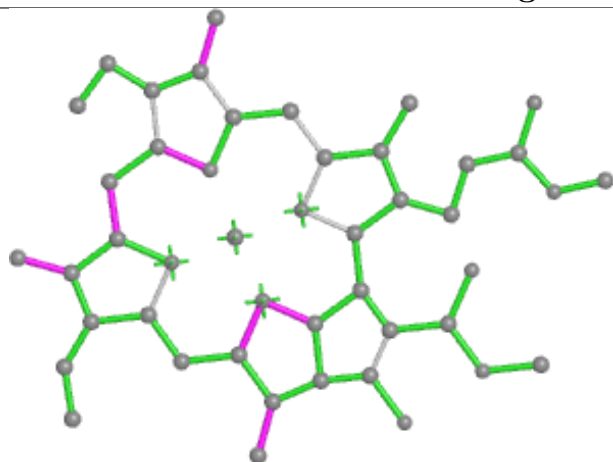
Torsions



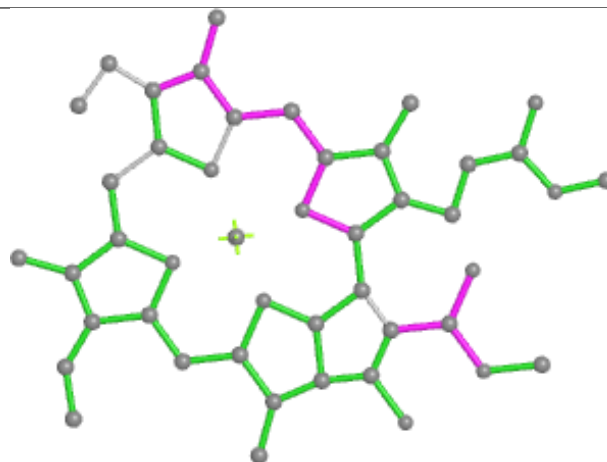
Rings



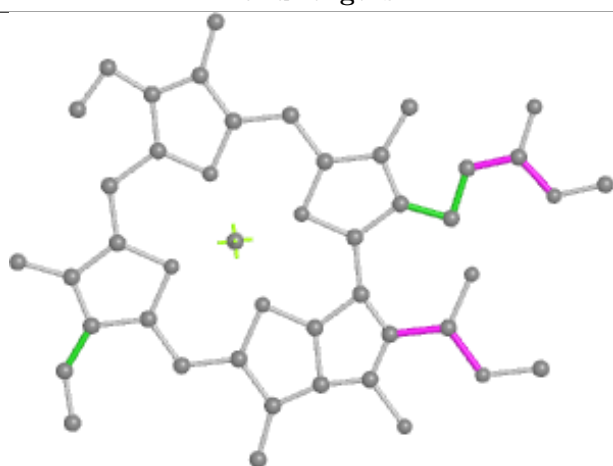
Ligand CLA 4 601



Bond lengths



Bond angles

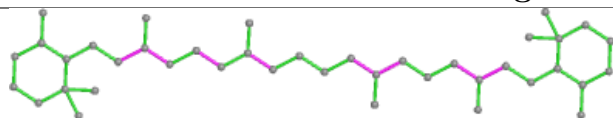


Torsions

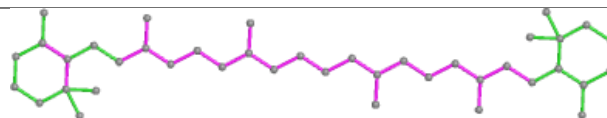


Rings

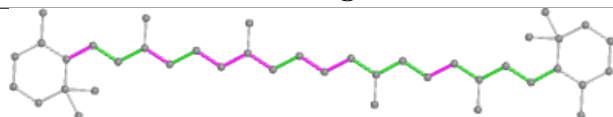
Ligand BCR F 304



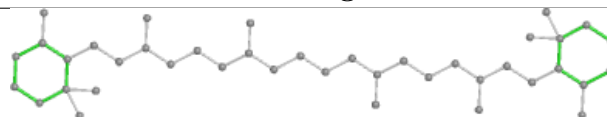
Bond lengths



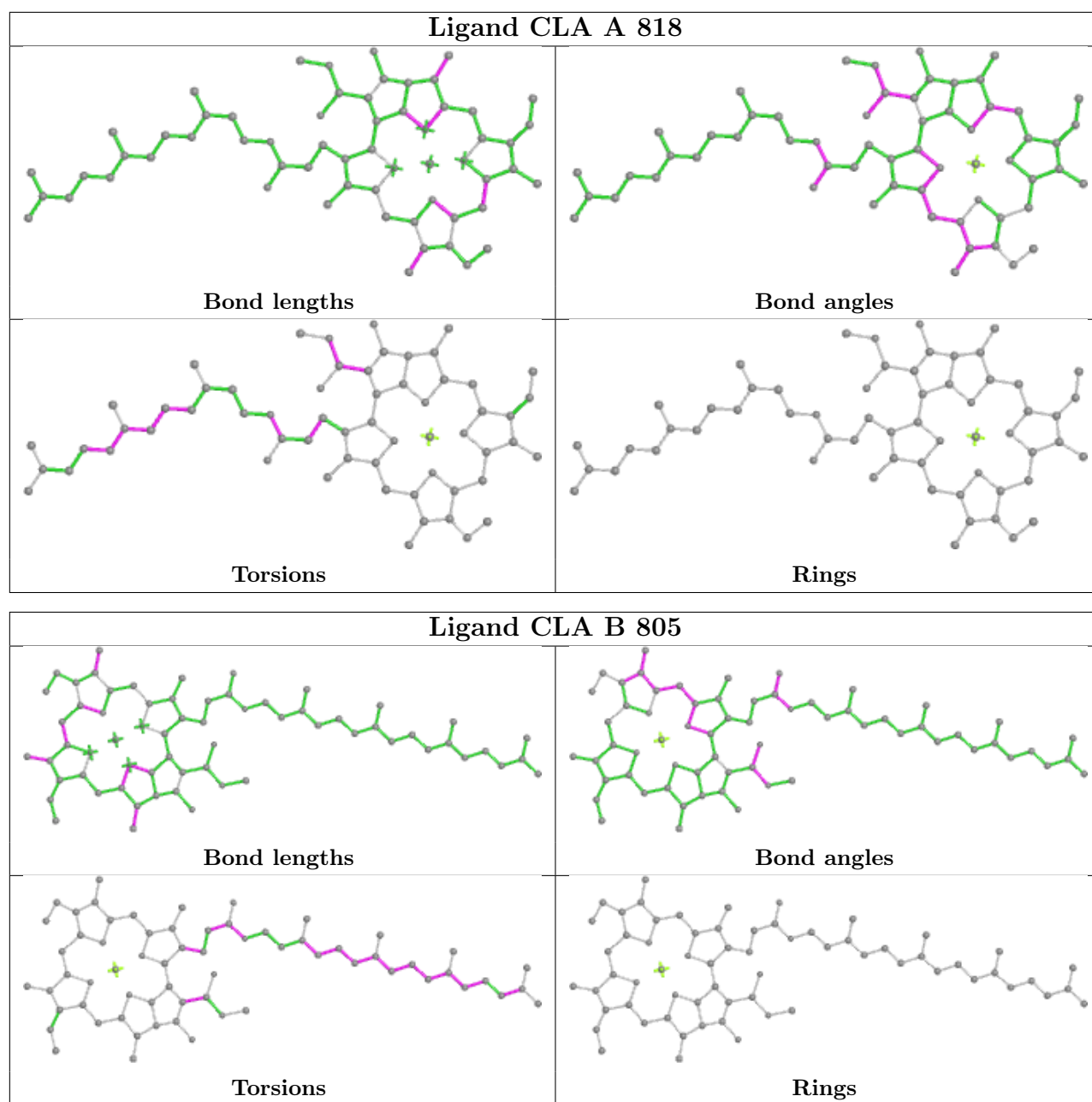
Bond angles



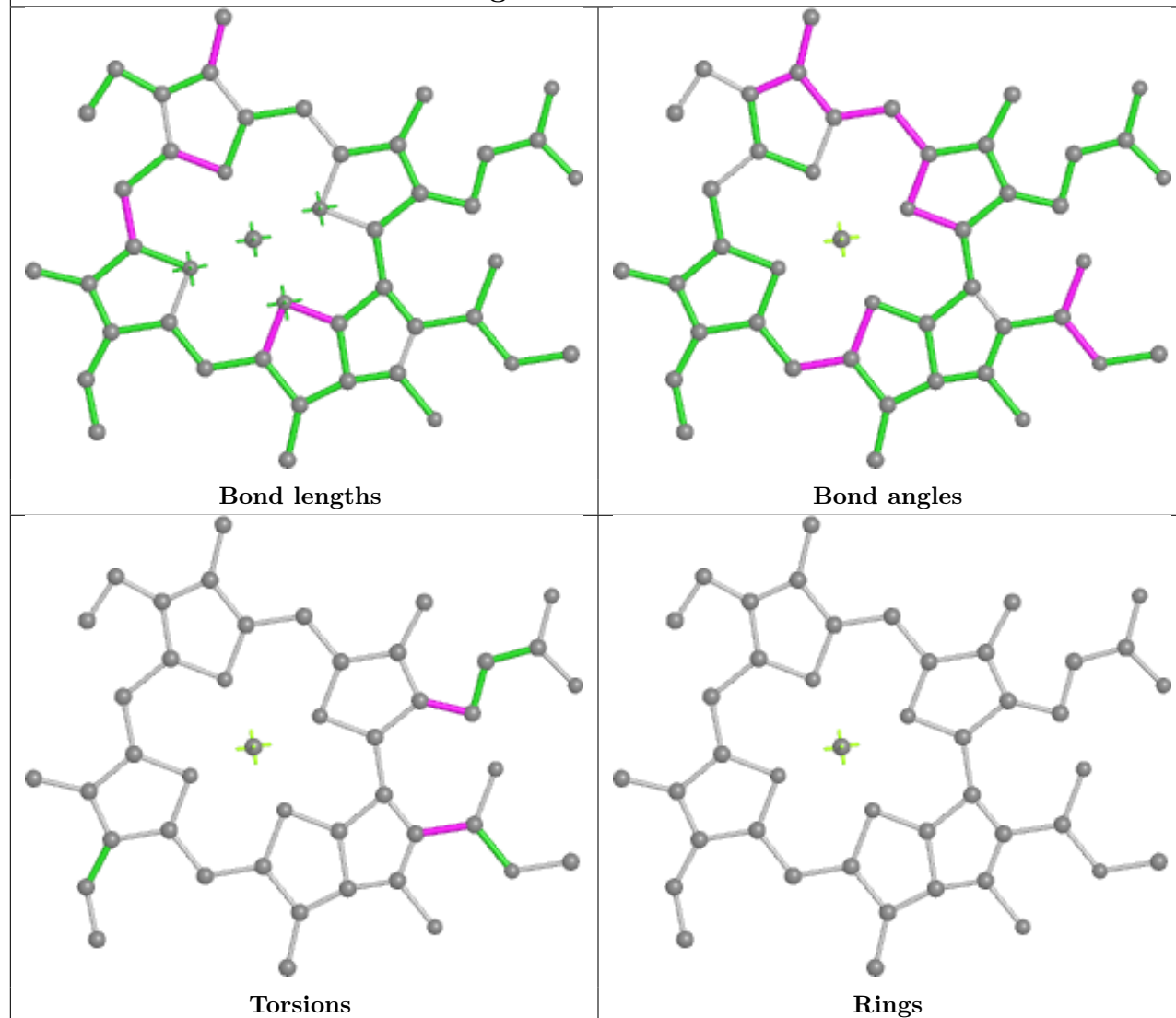
Torsions



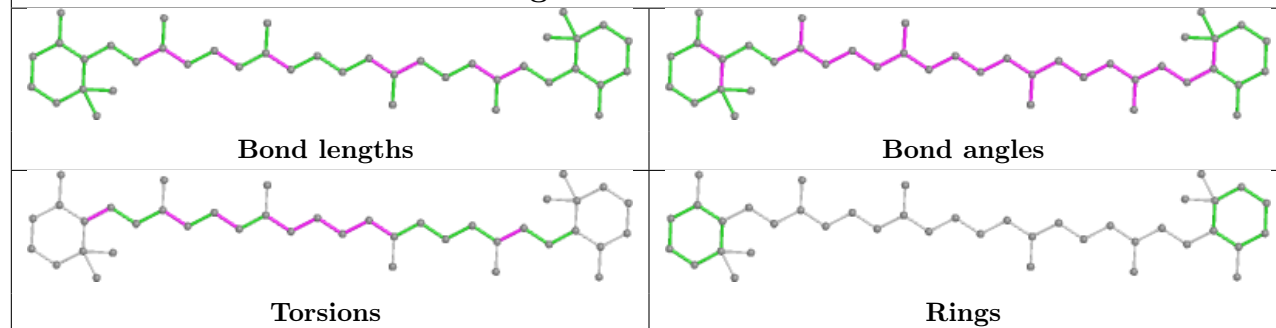
Rings

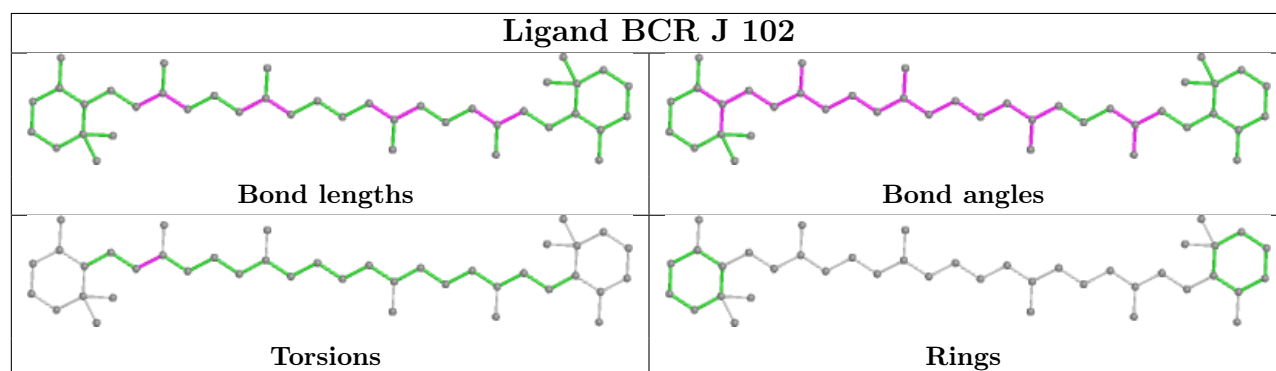
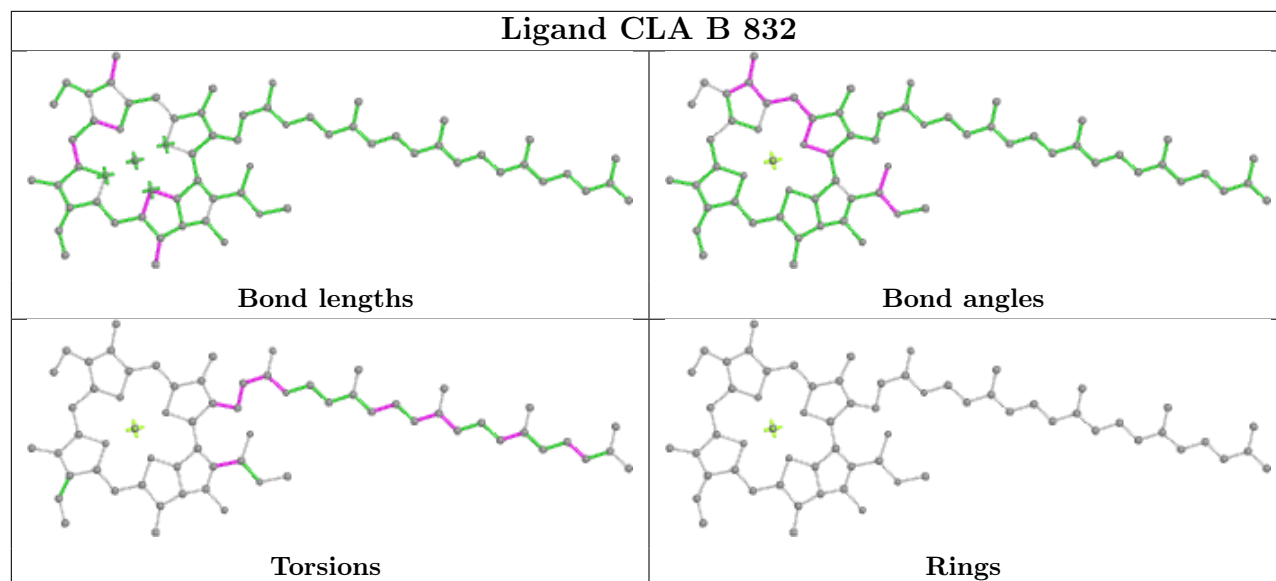
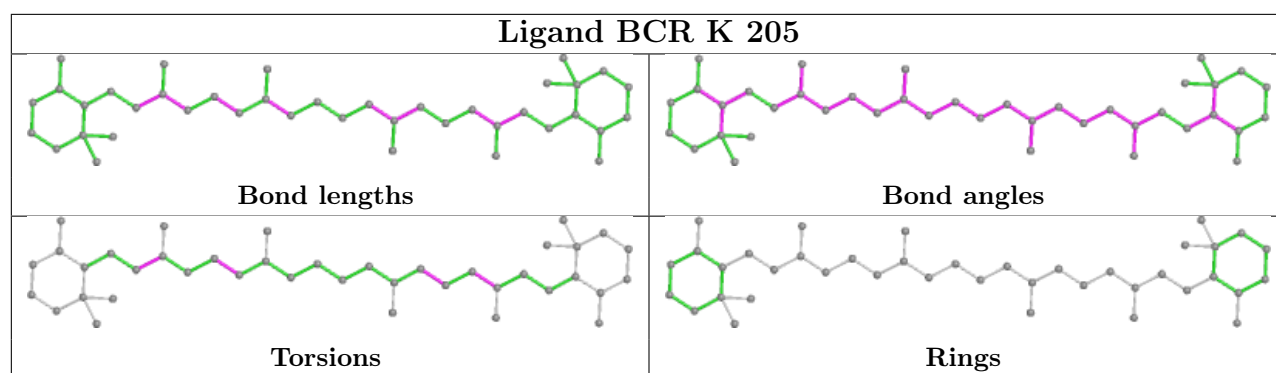


Ligand CLA A 836

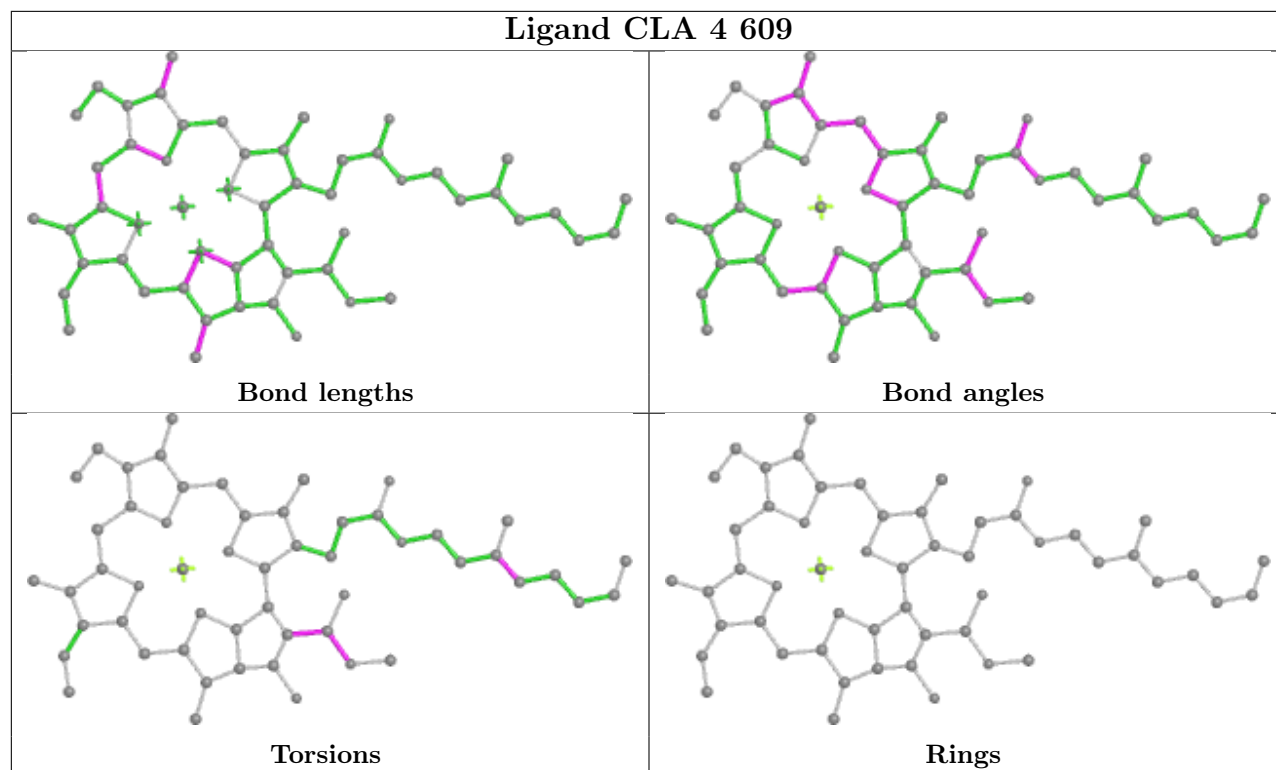


Ligand BCR A 852

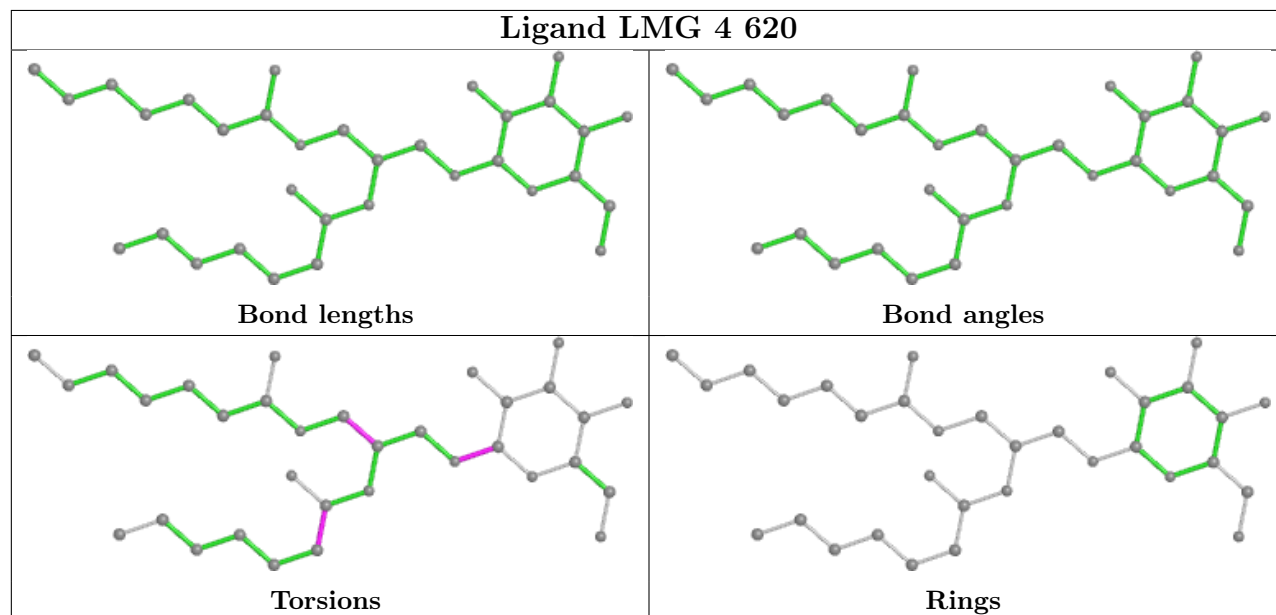




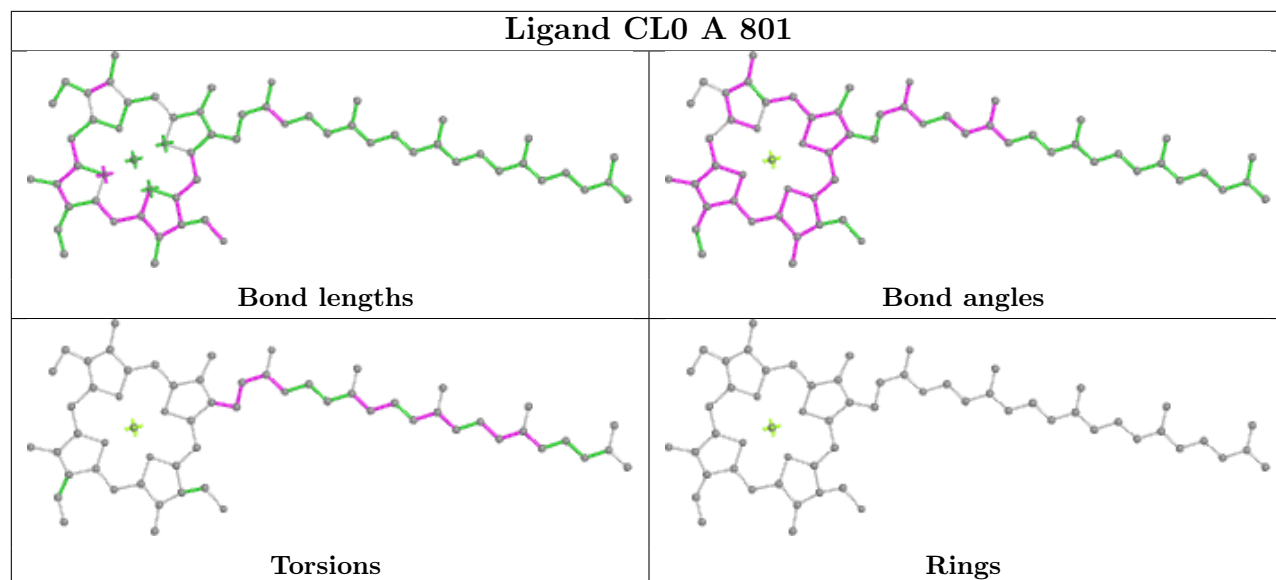
Ligand CLA 4 609



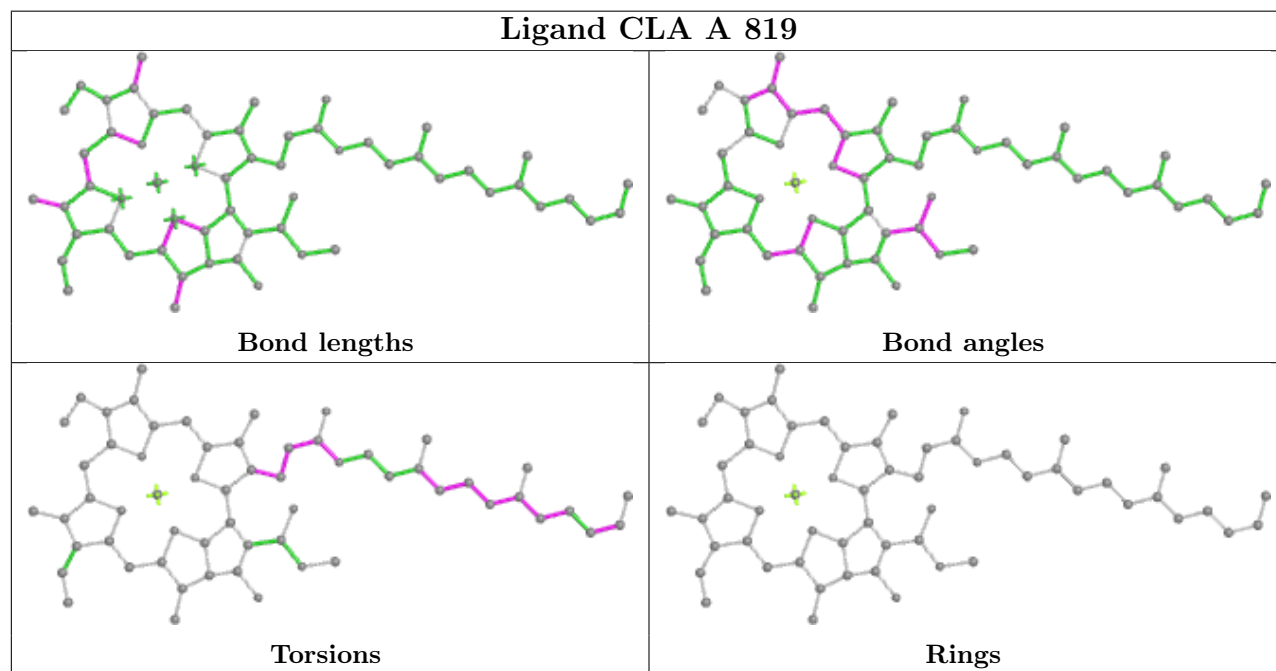
Ligand LMG 4 620



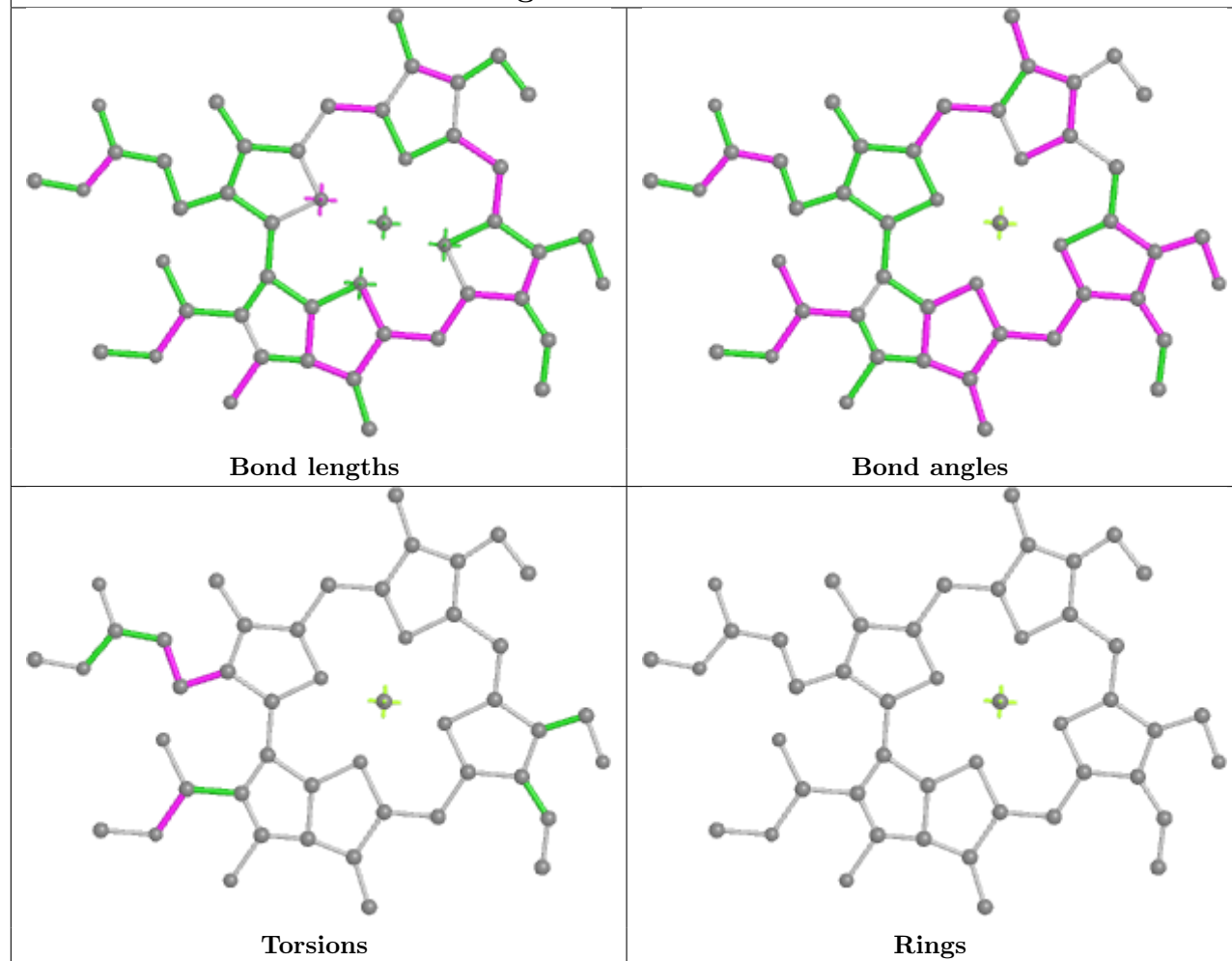
Ligand CL0 A 801



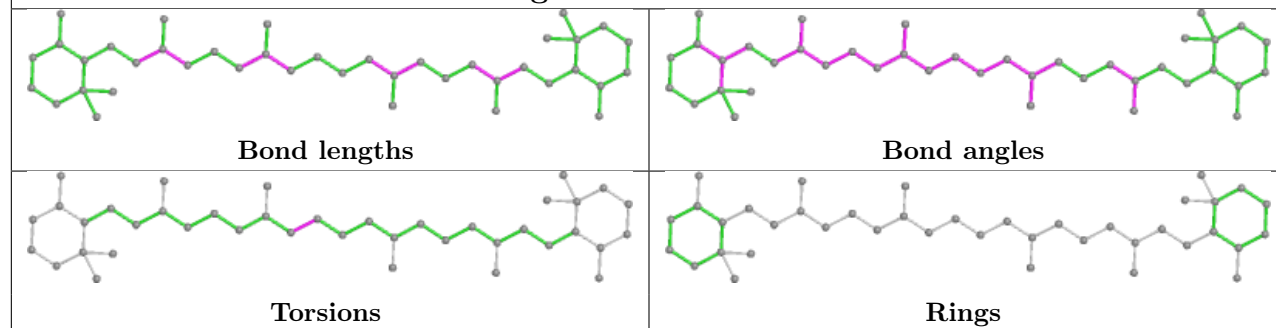
Ligand CLA A 819



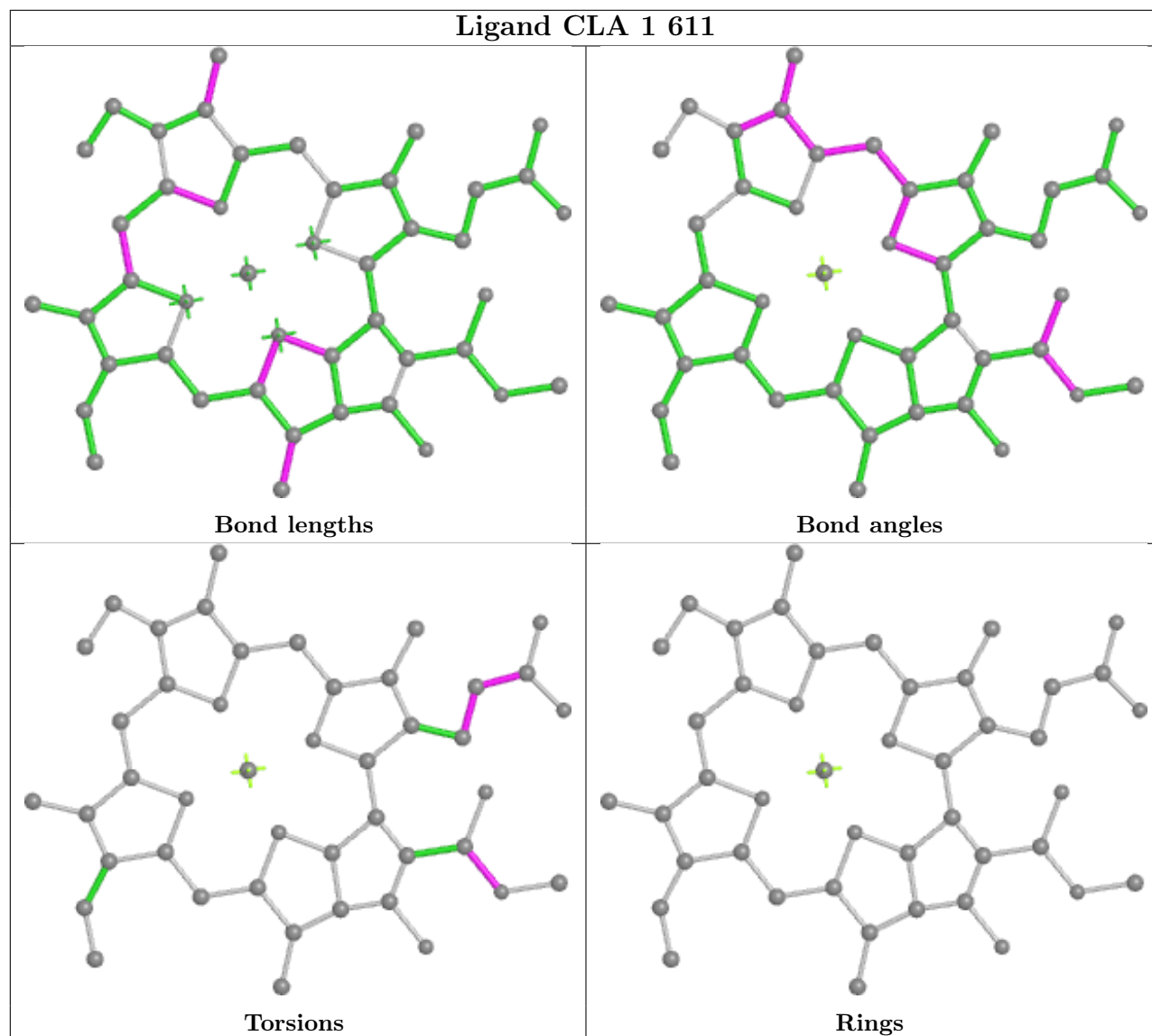
Ligand CHL 2 601



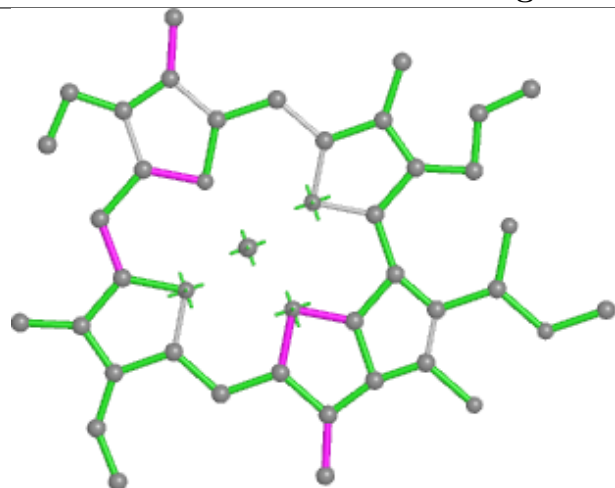
Ligand BCR B 843



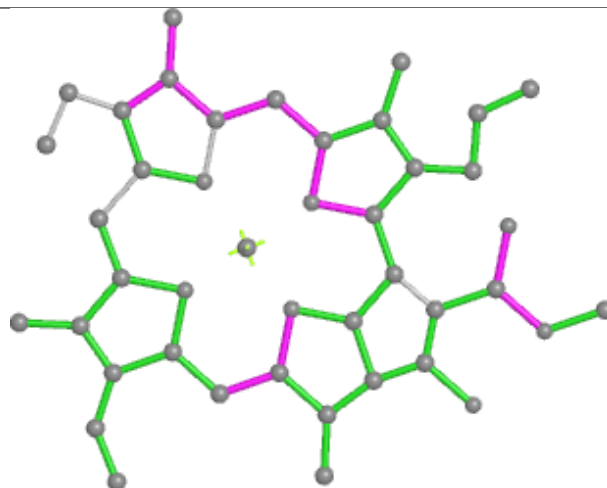
Ligand CLA 1 611



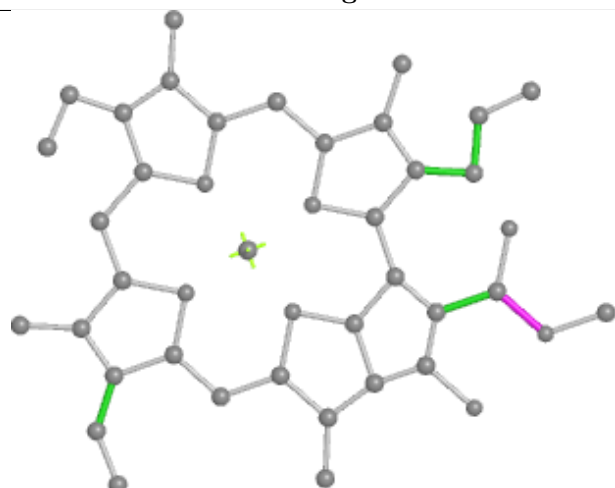
Ligand CLA B 830



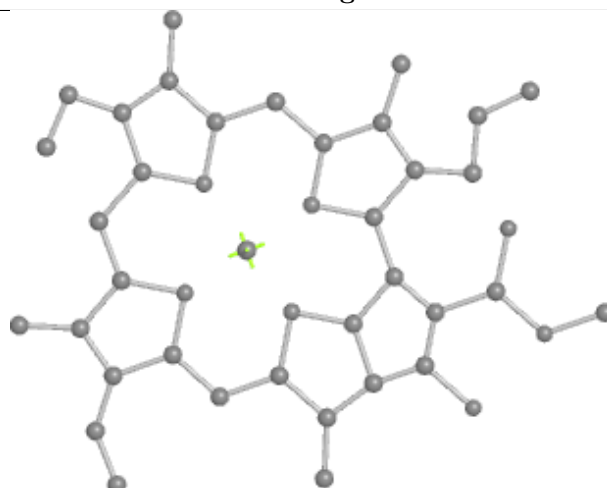
Bond lengths



Bond angles

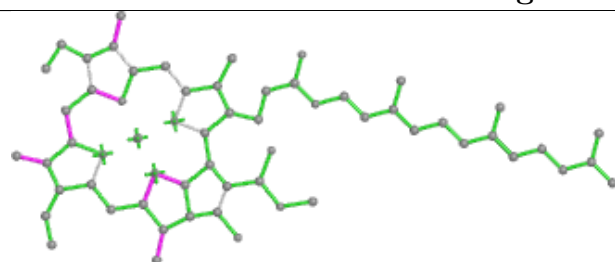


Torsions

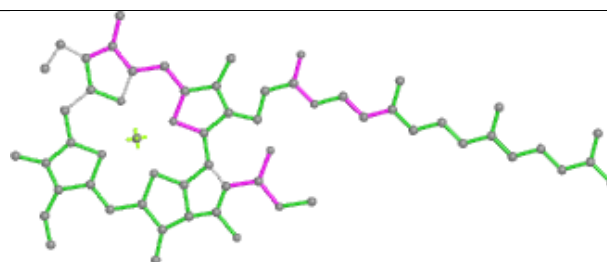


Rings

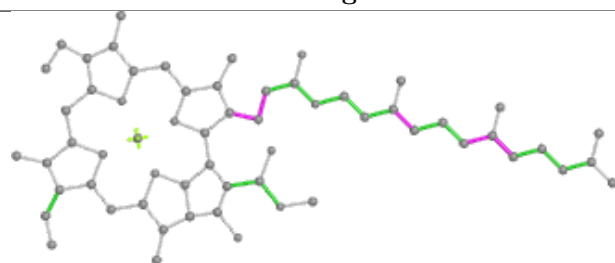
Ligand CLA B 818



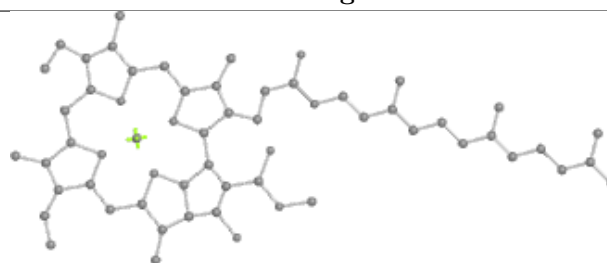
Bond lengths



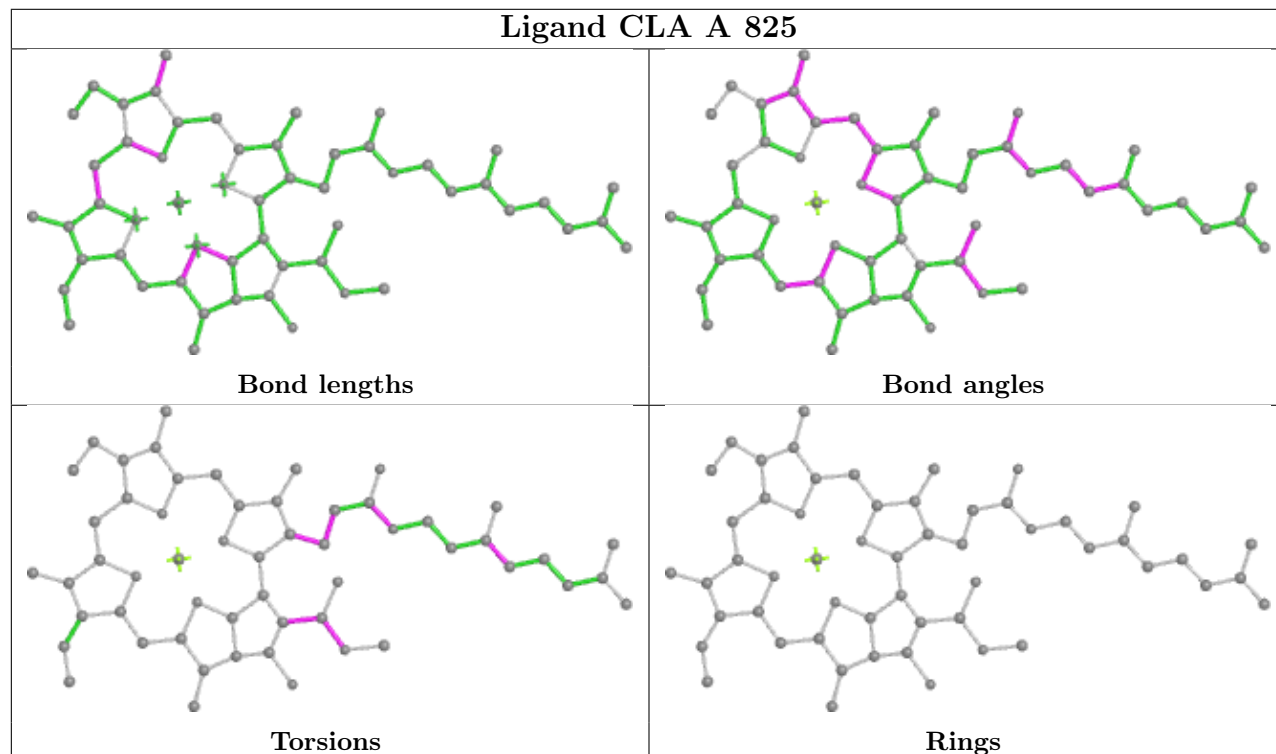
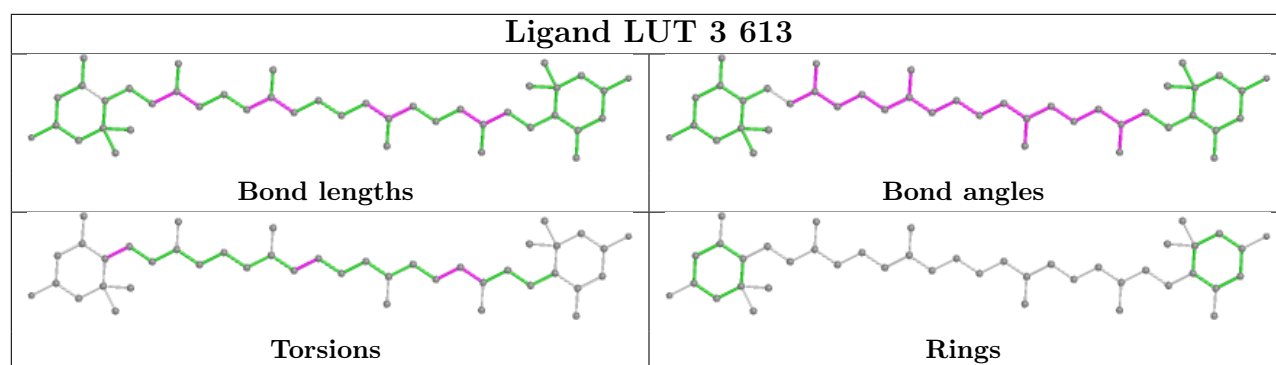
Bond angles



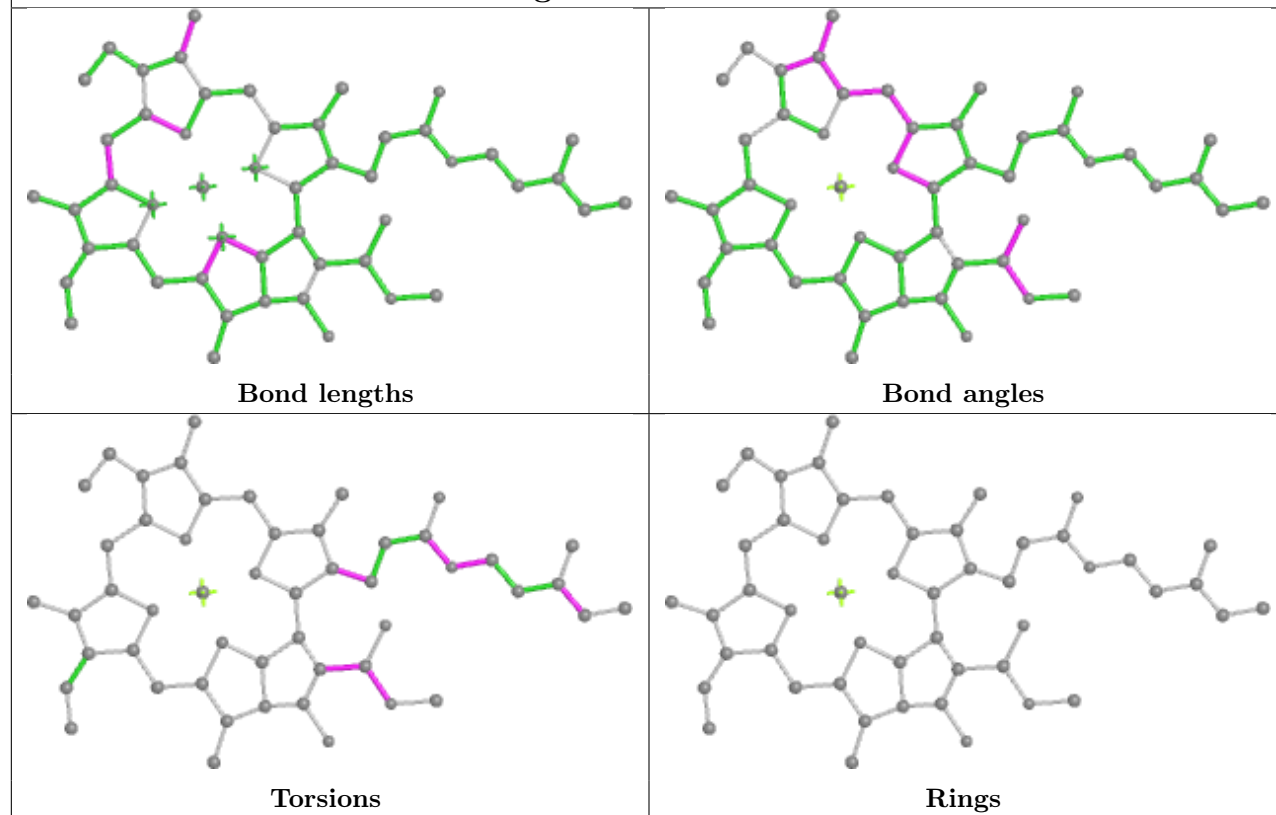
Torsions



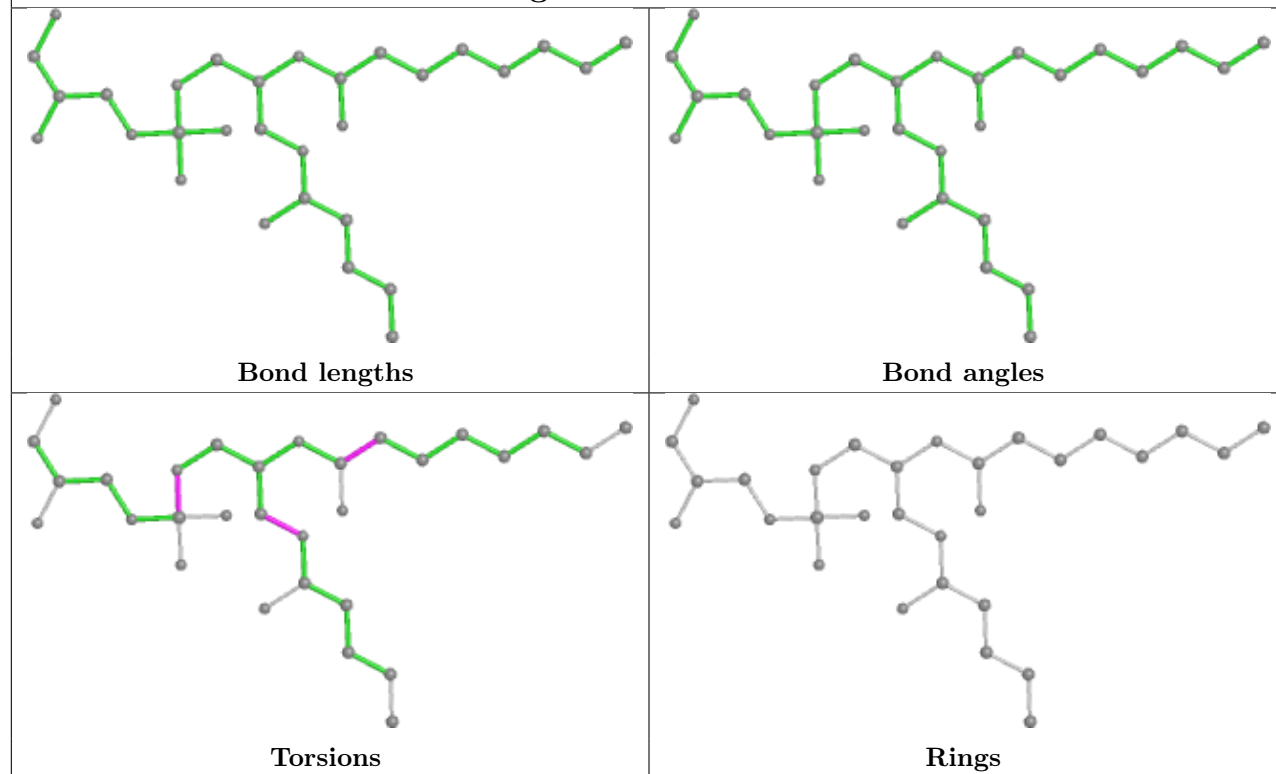
Rings

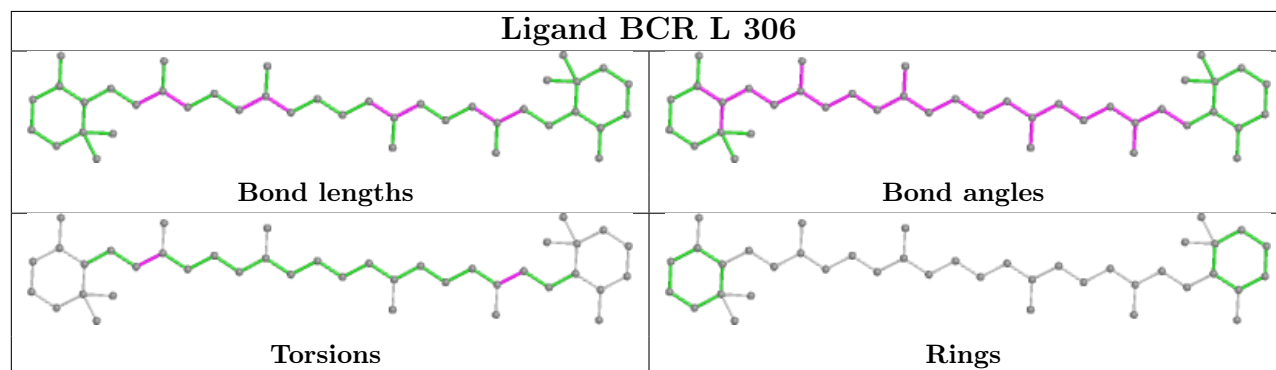
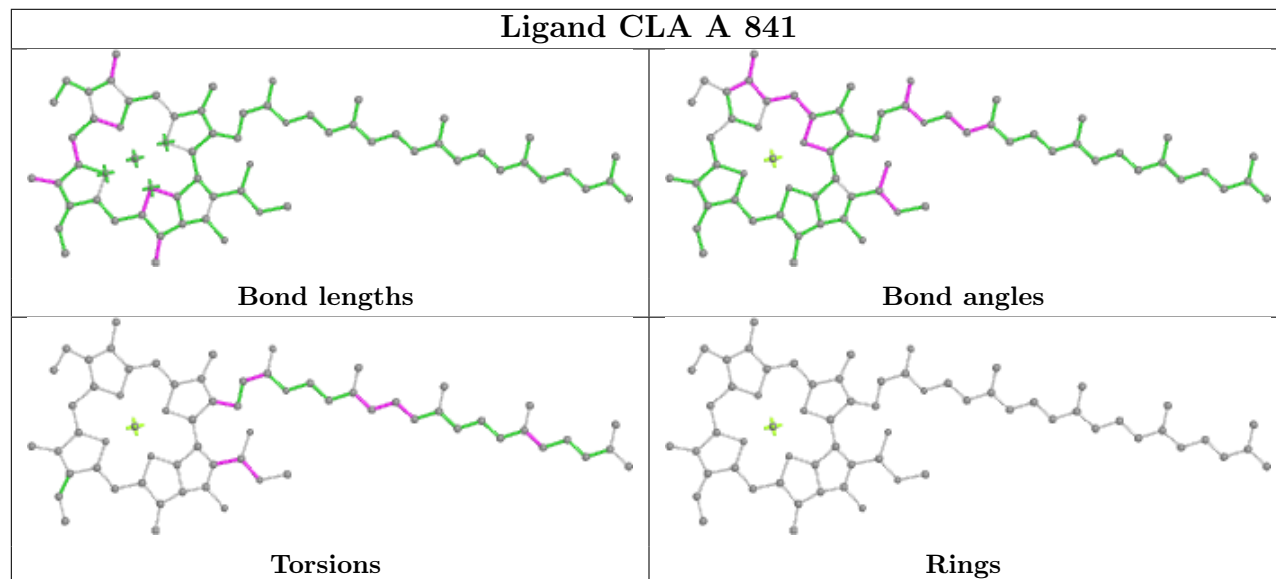
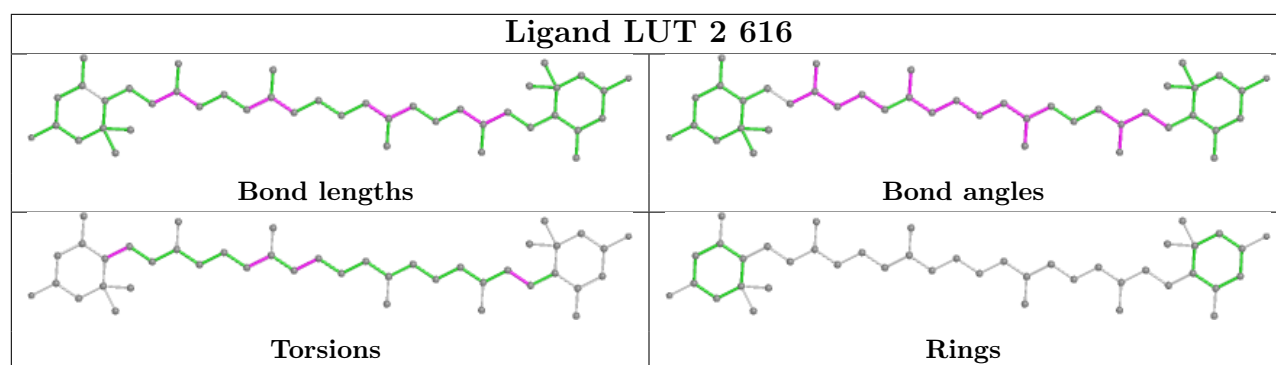


Ligand CLA F 302

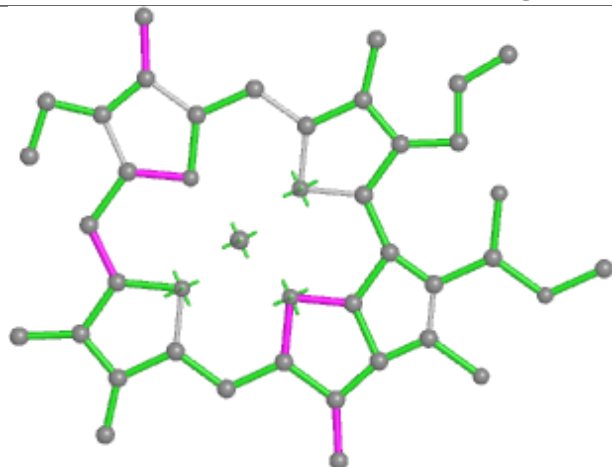


Ligand LHG A 847

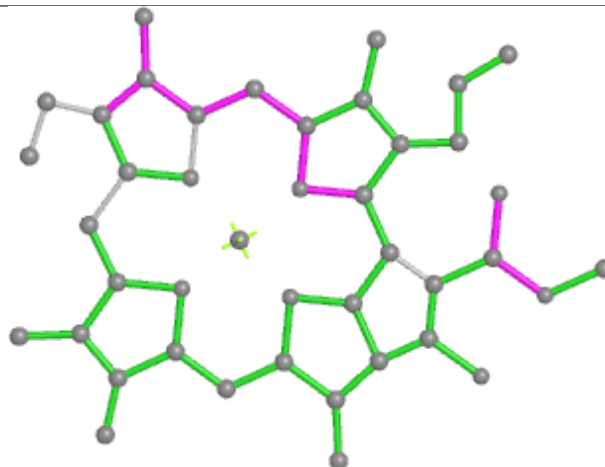




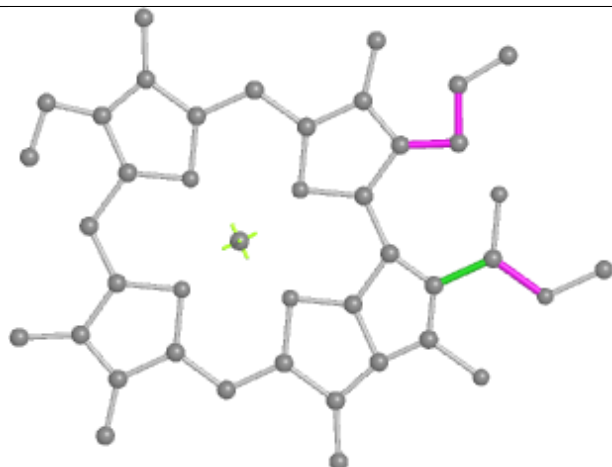
Ligand CLA 1 609



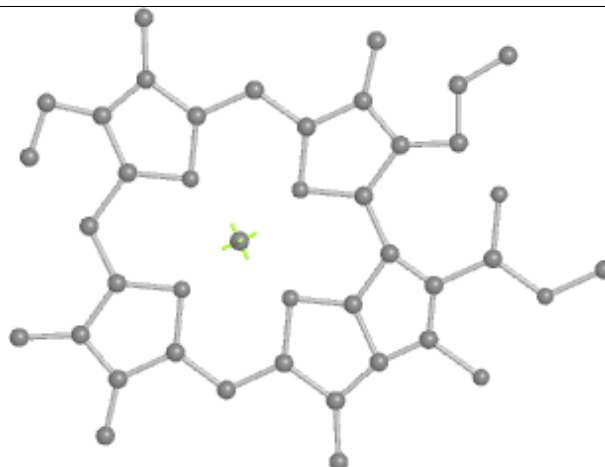
Bond lengths



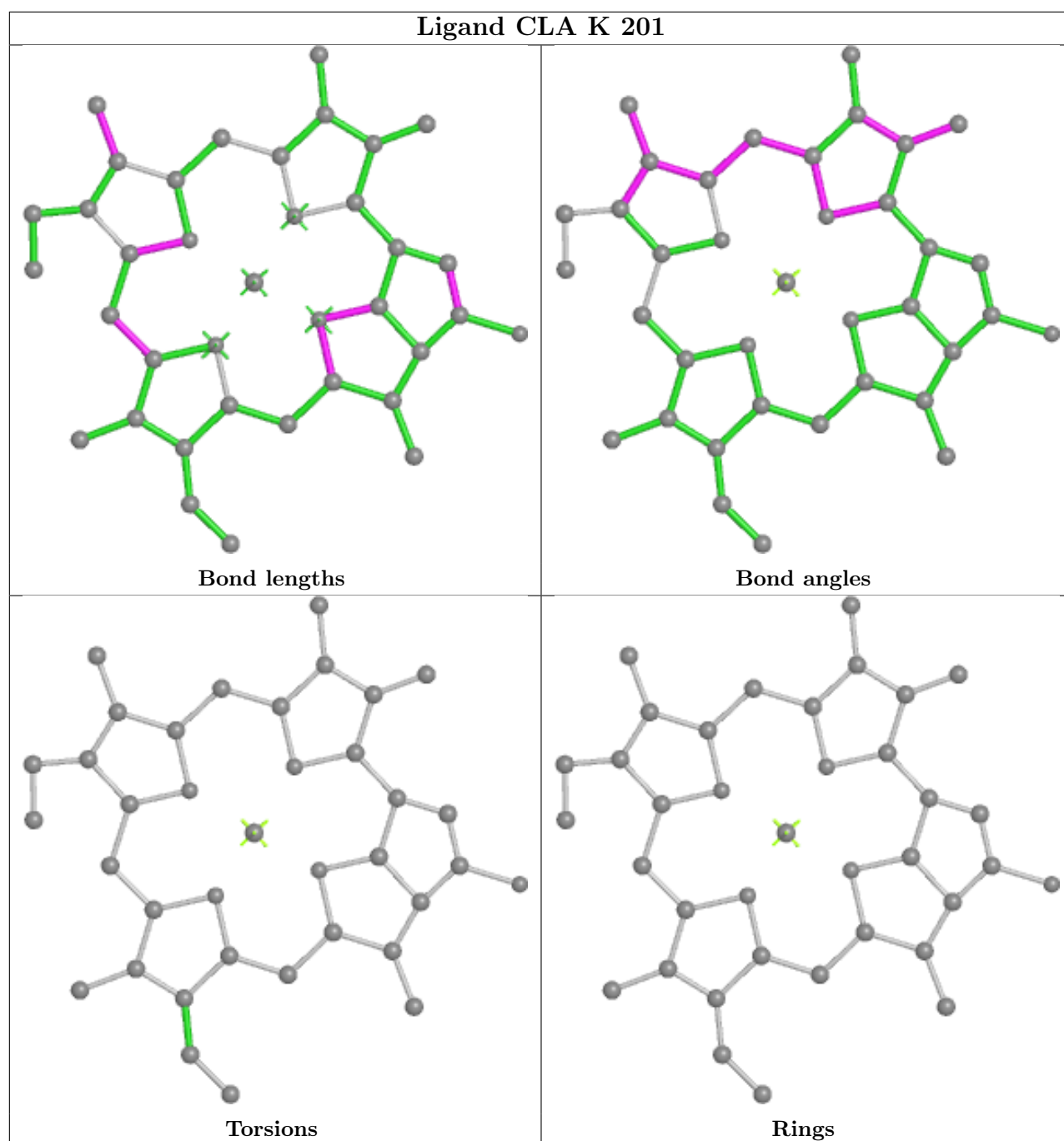
Bond angles

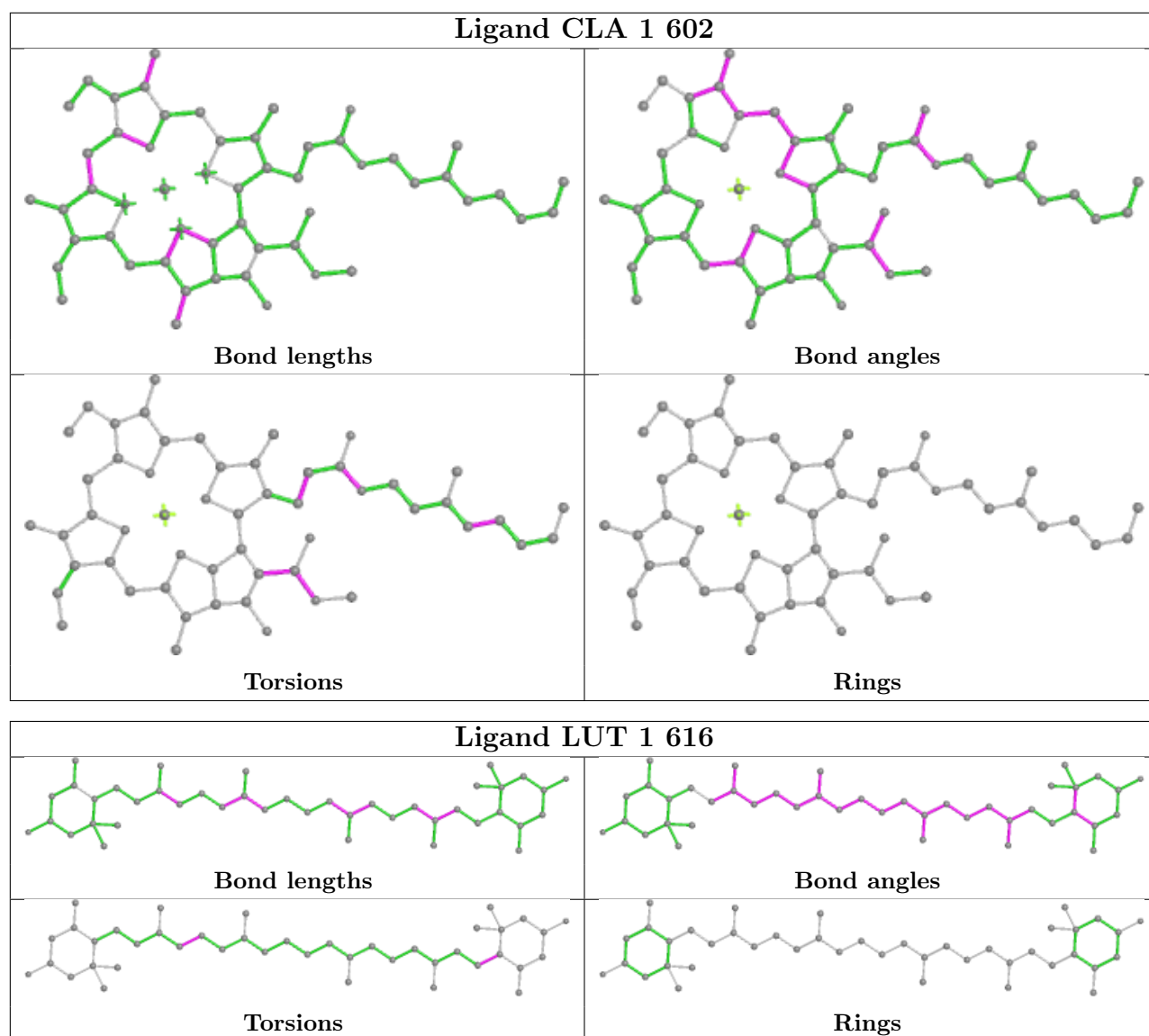


Torsions

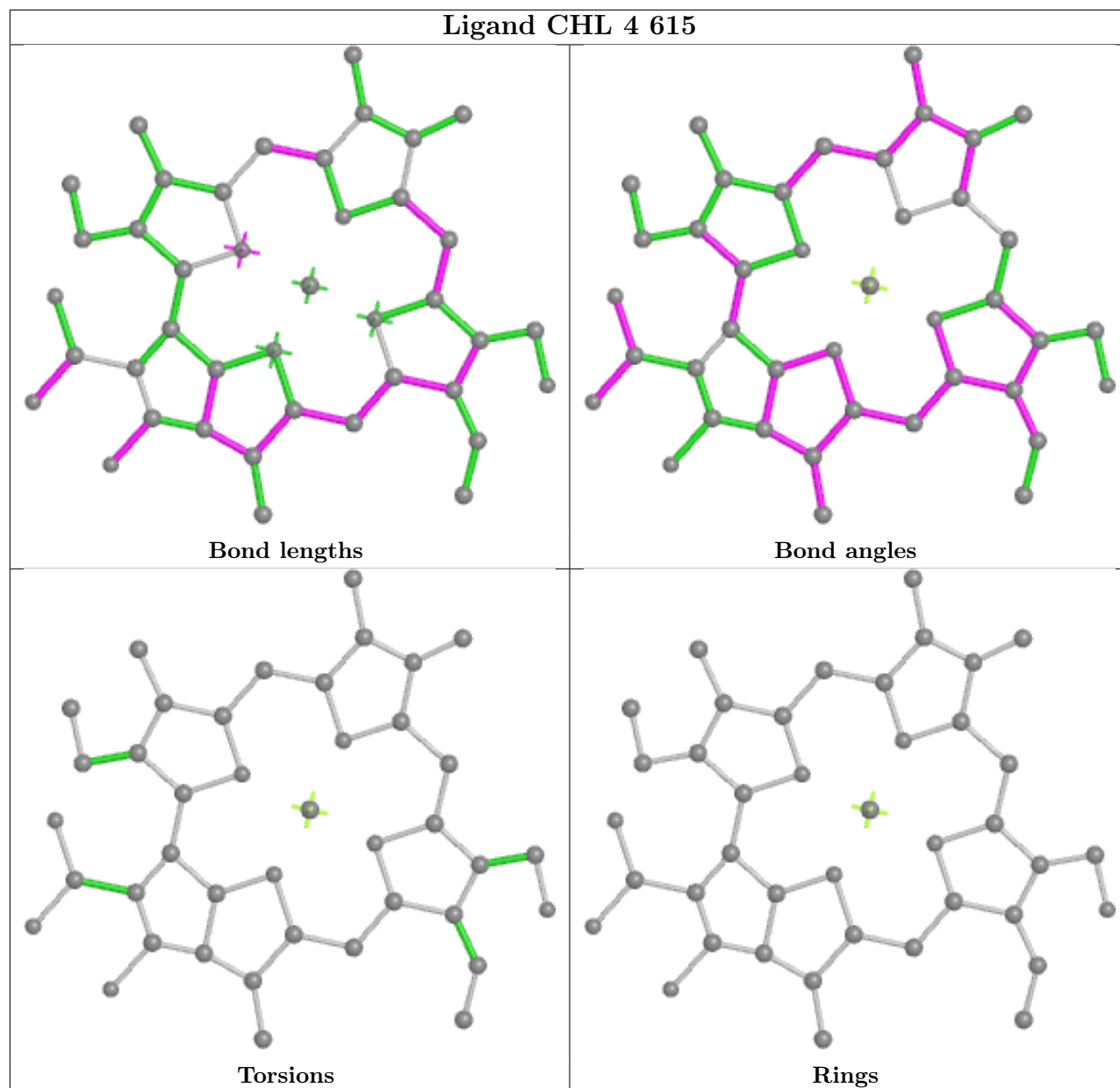


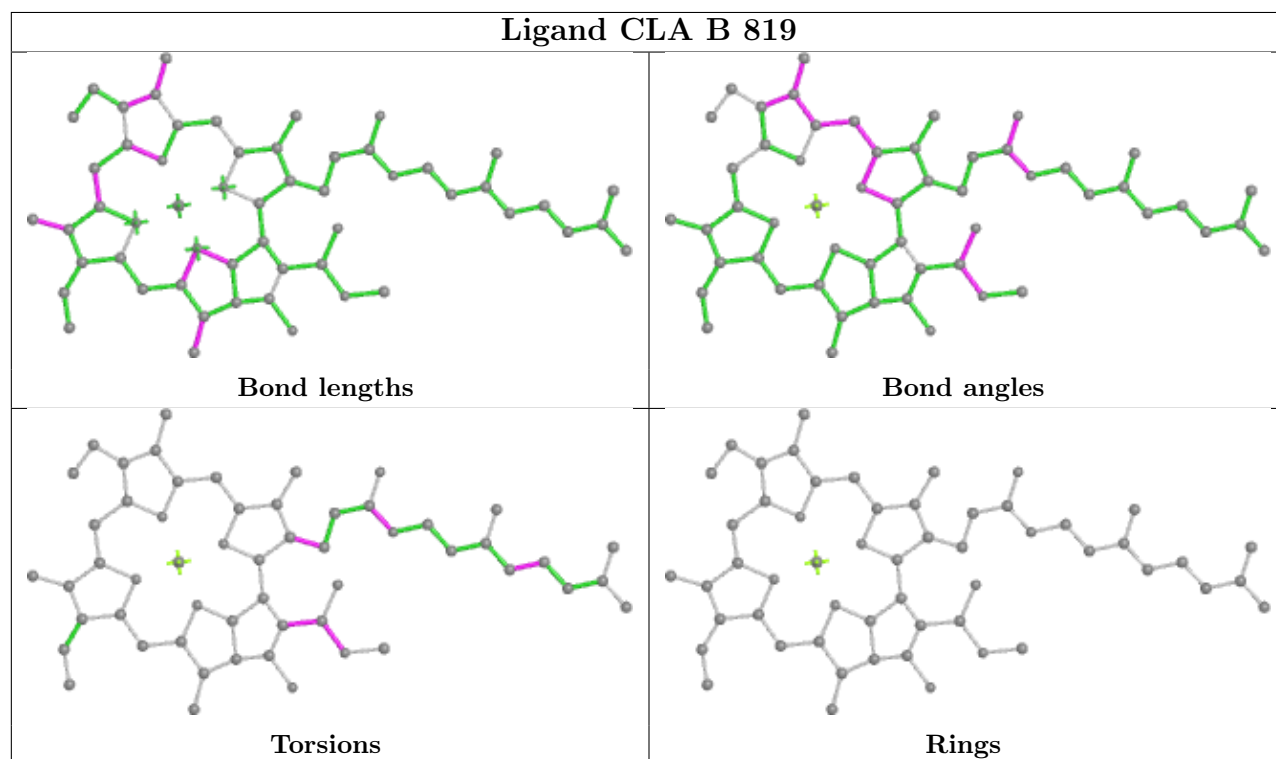
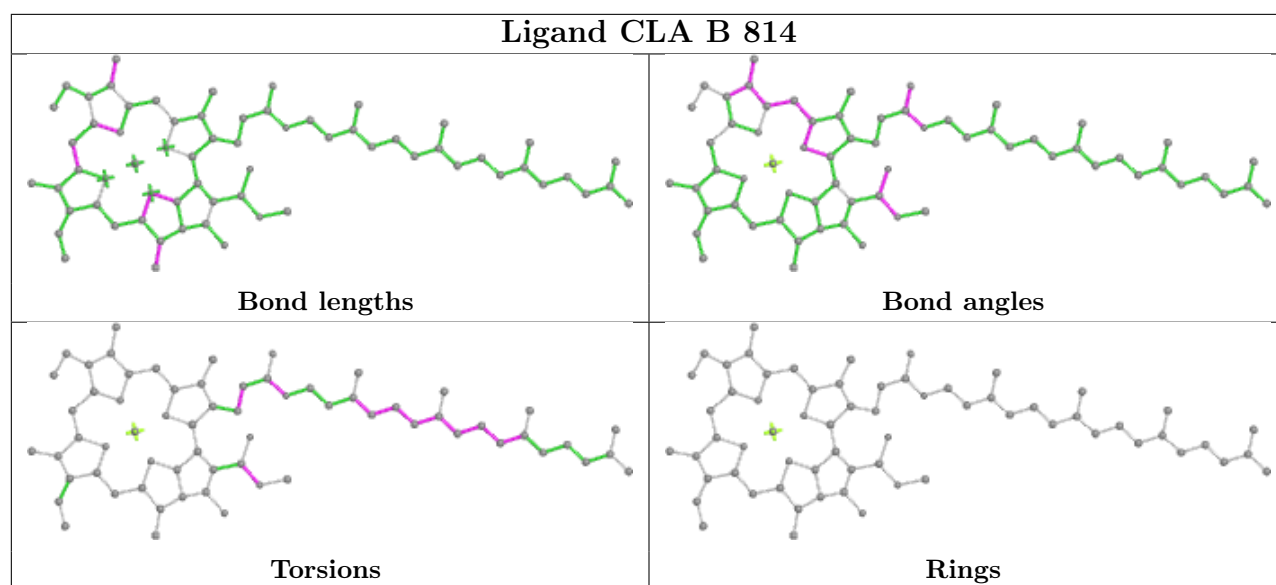
Rings

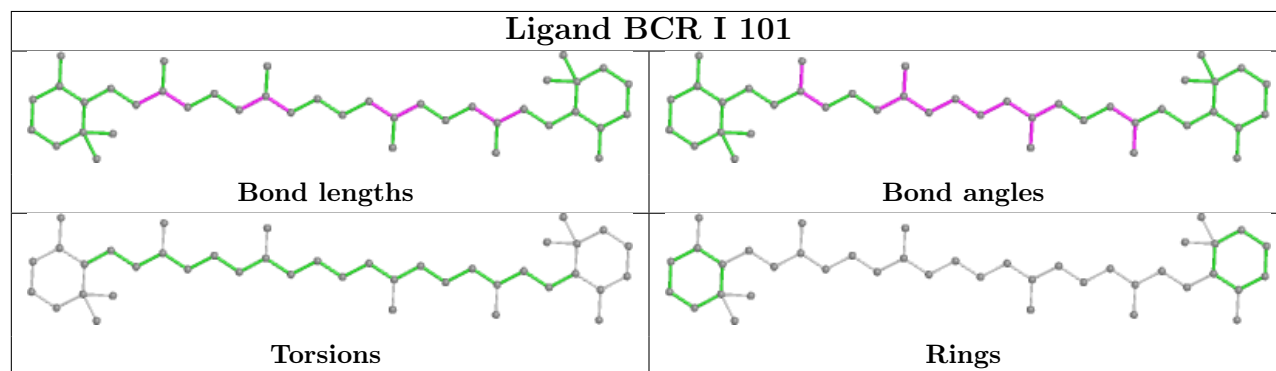
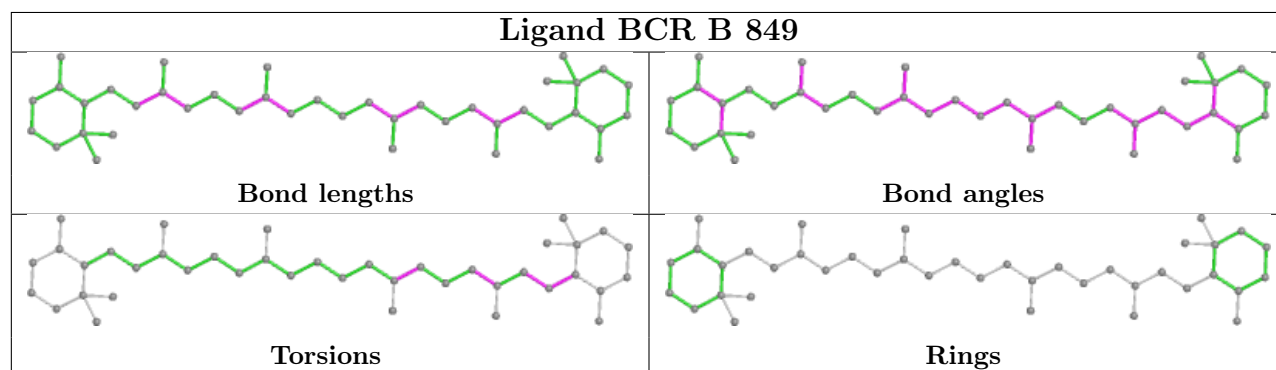
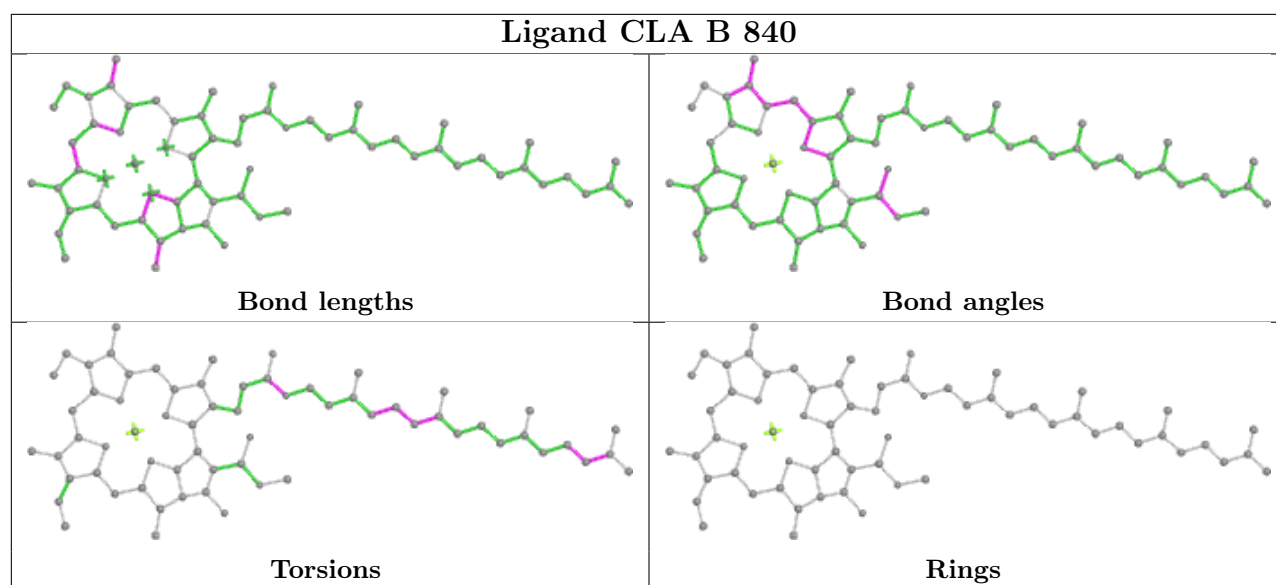


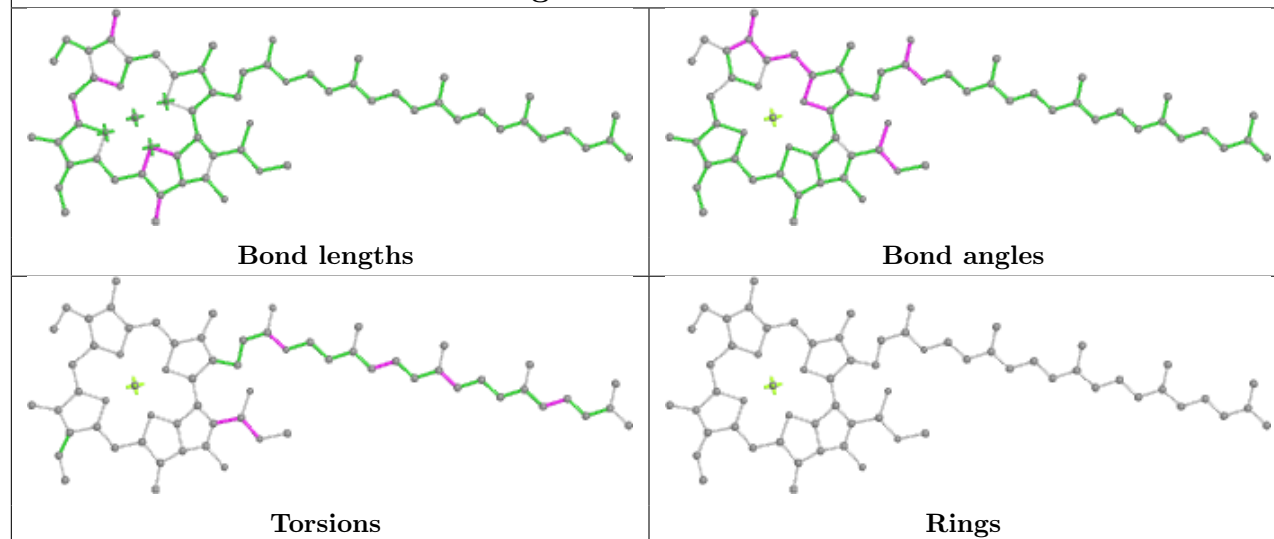
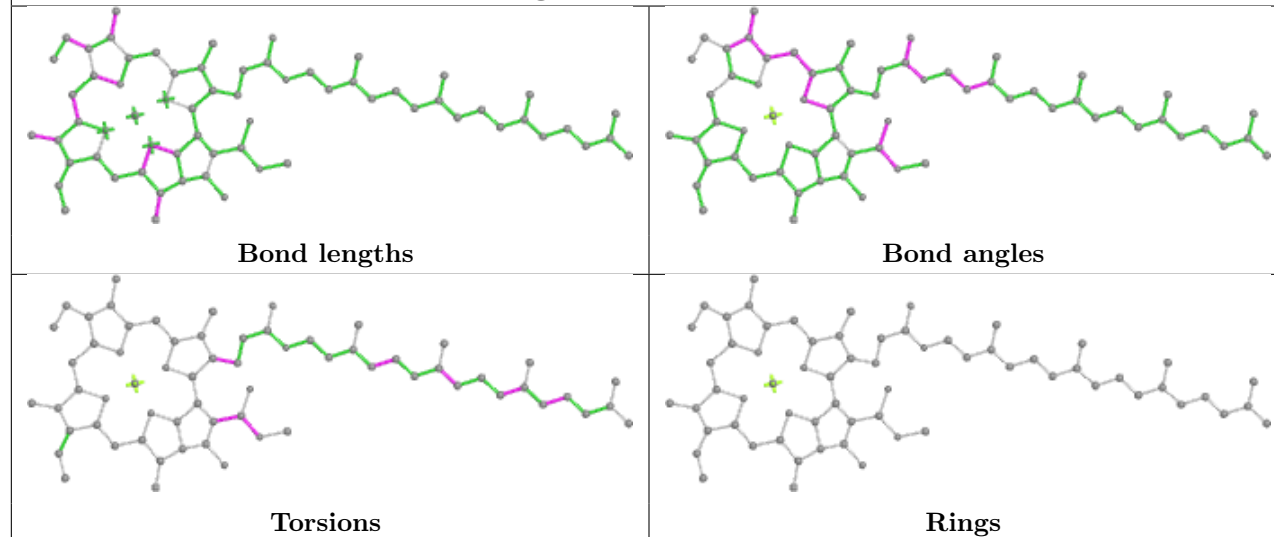
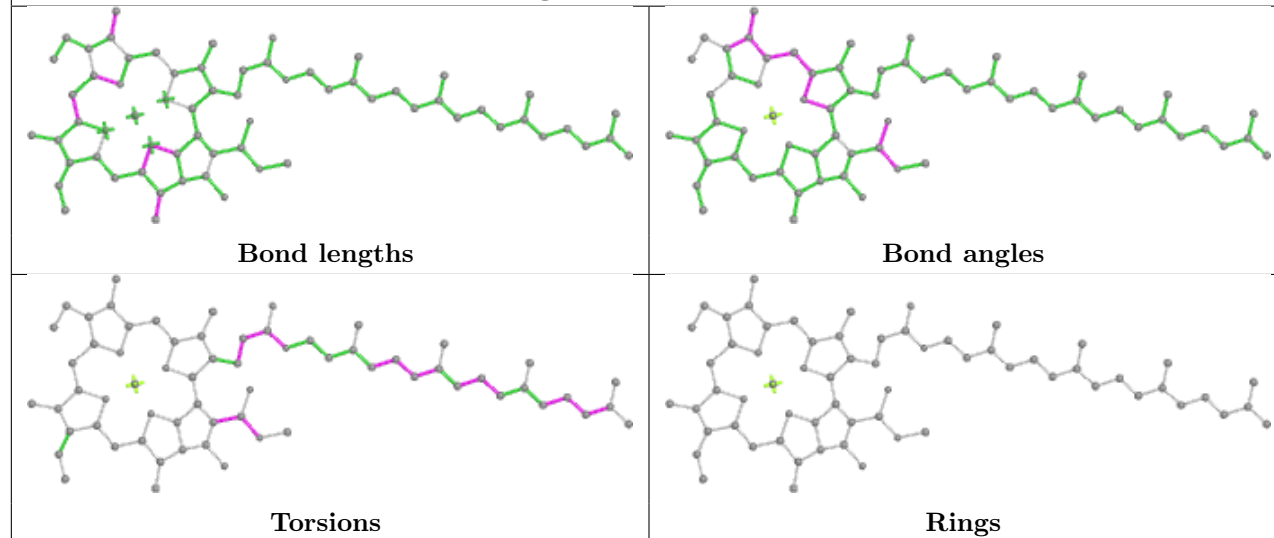


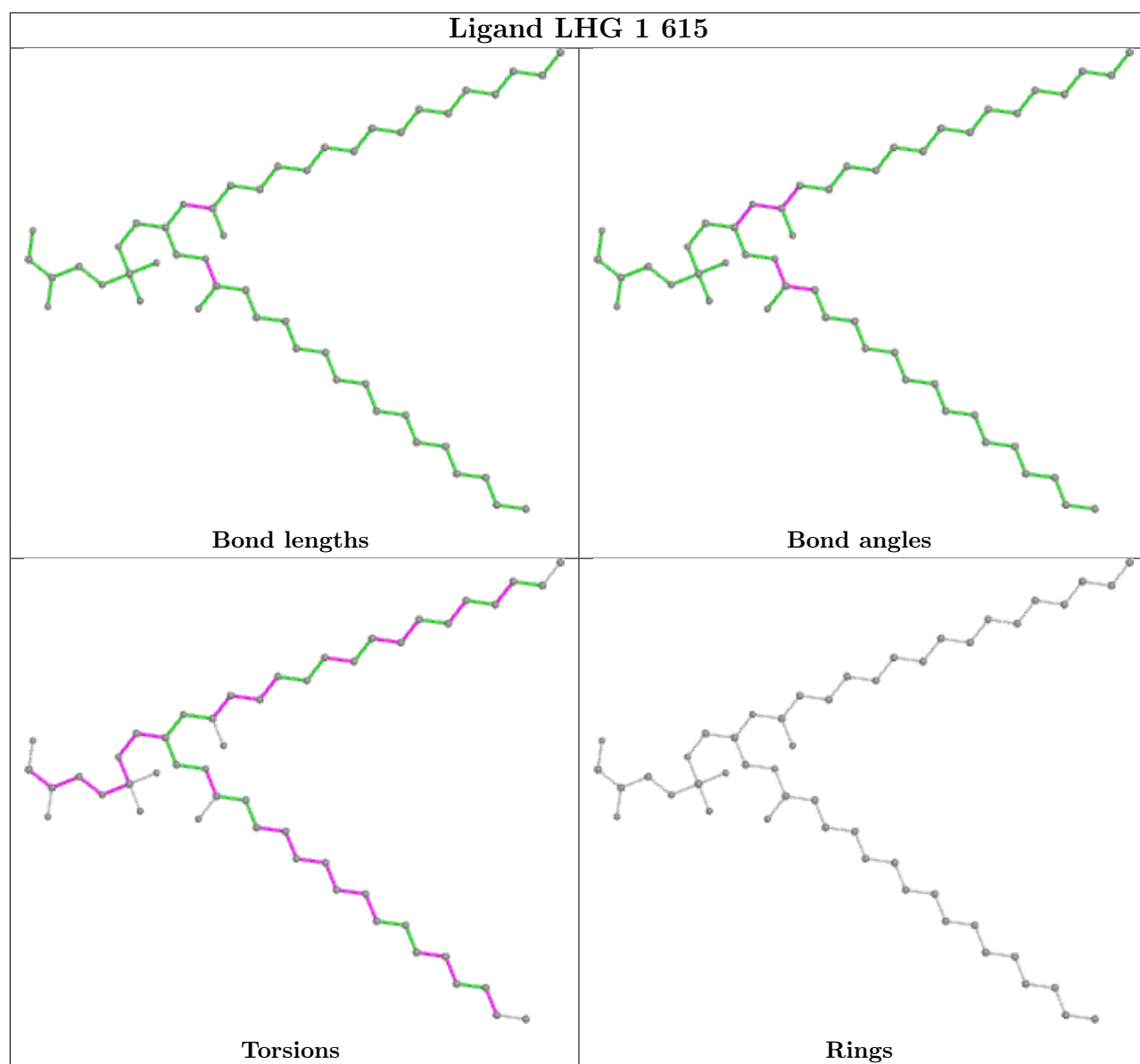
Ligand CHL 4 615

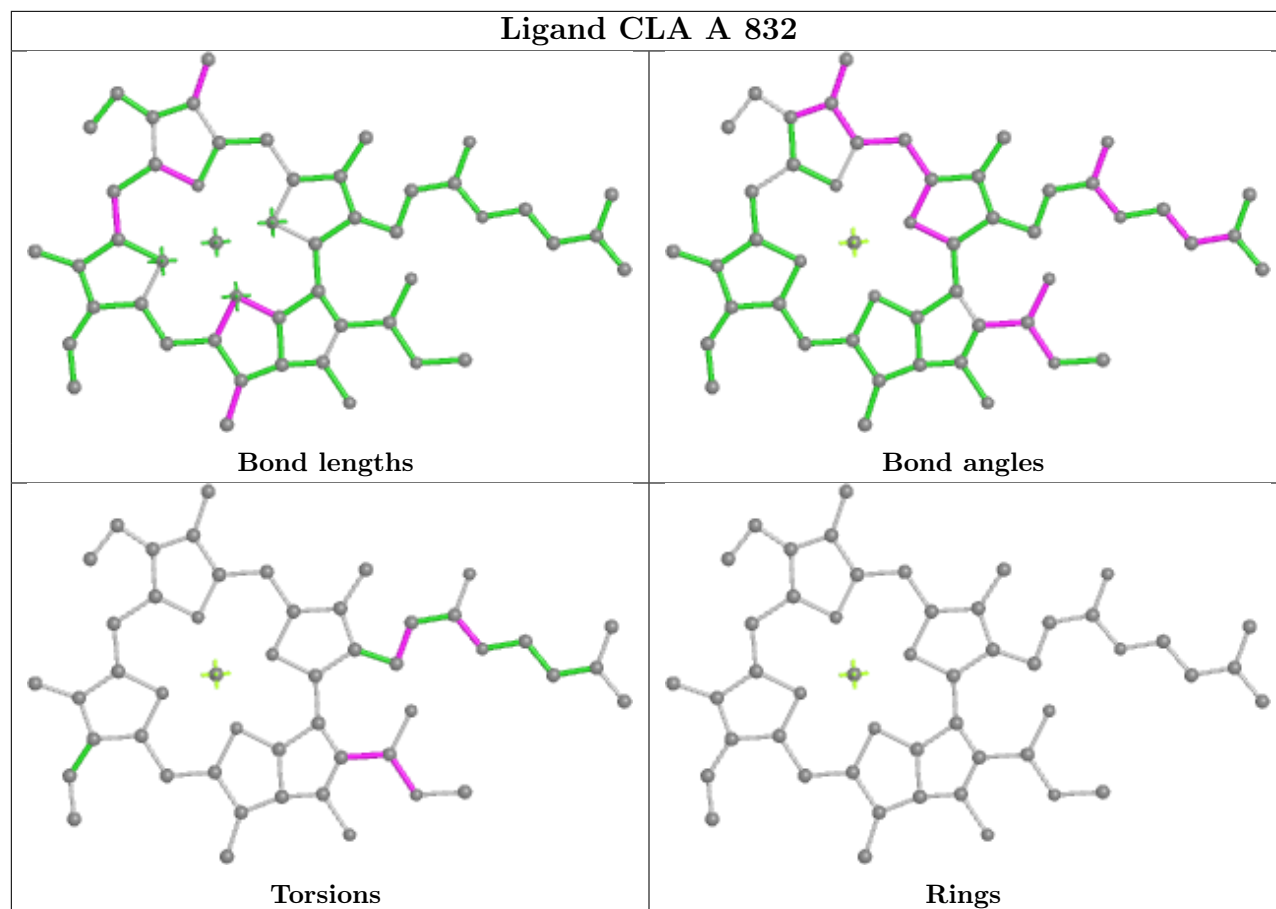




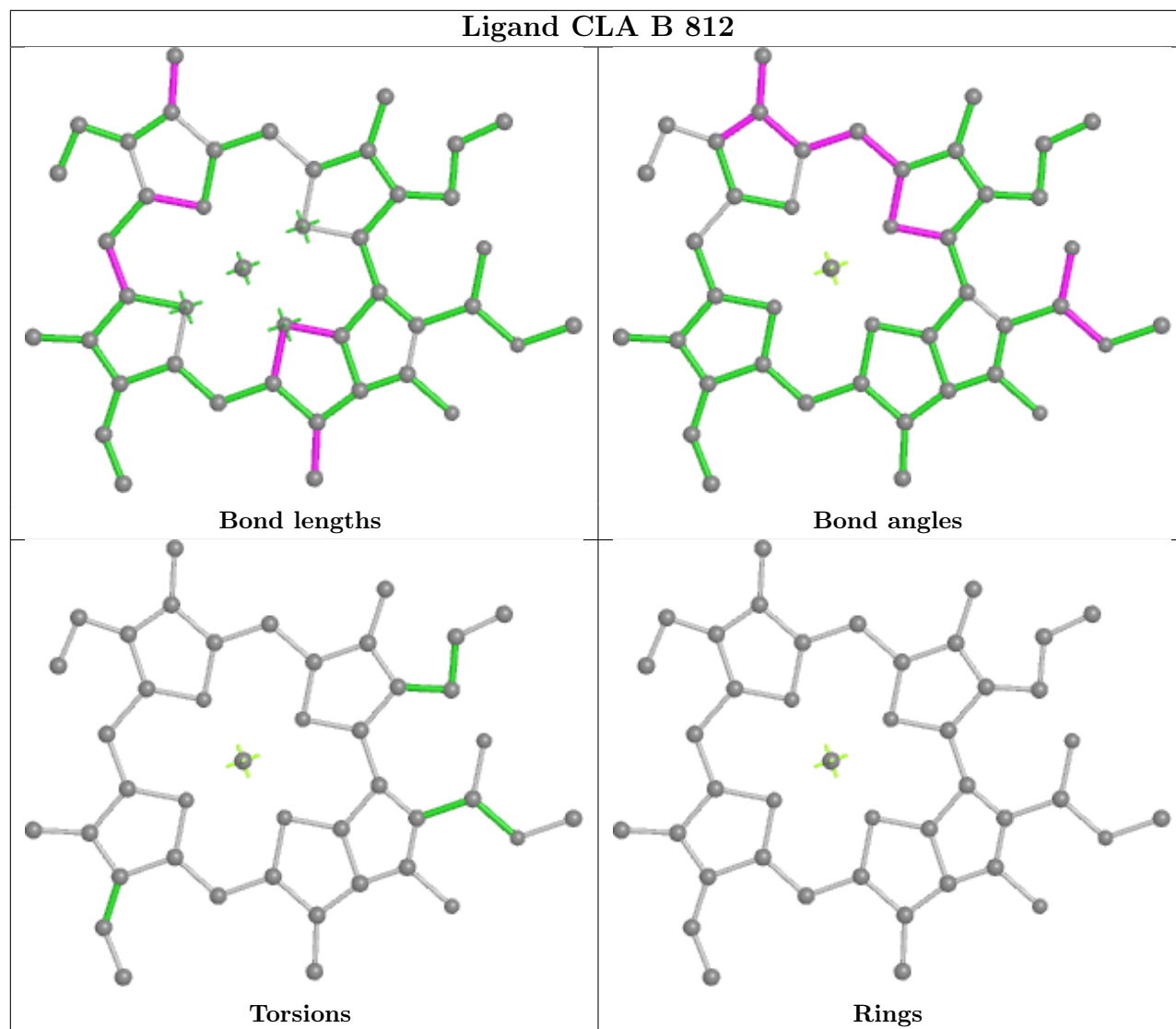


Ligand CLA A 834**Ligand CLA B 803****Ligand CLA 2 612**

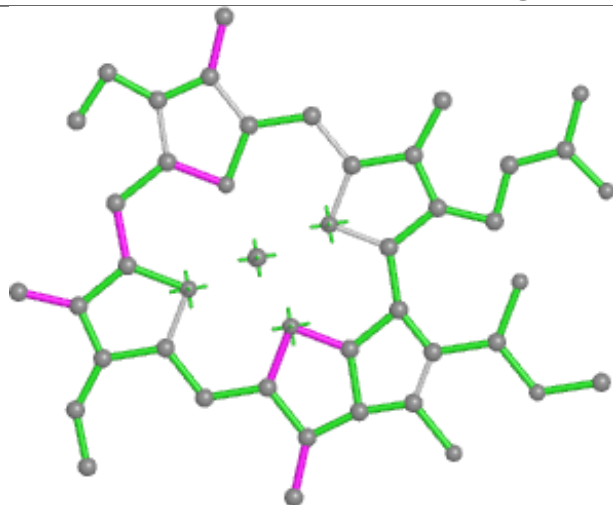




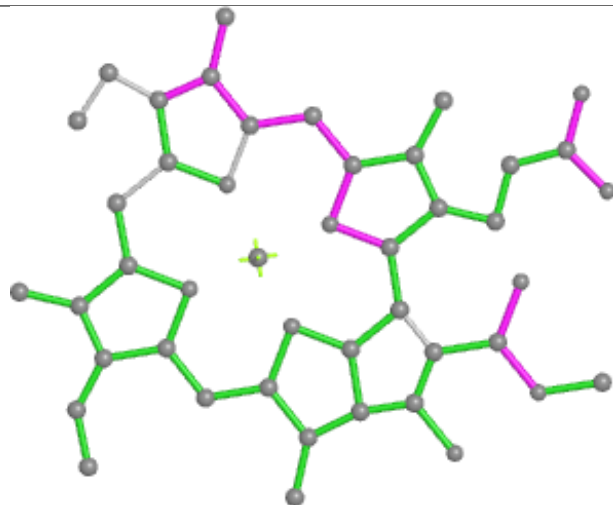
Ligand CLA B 812



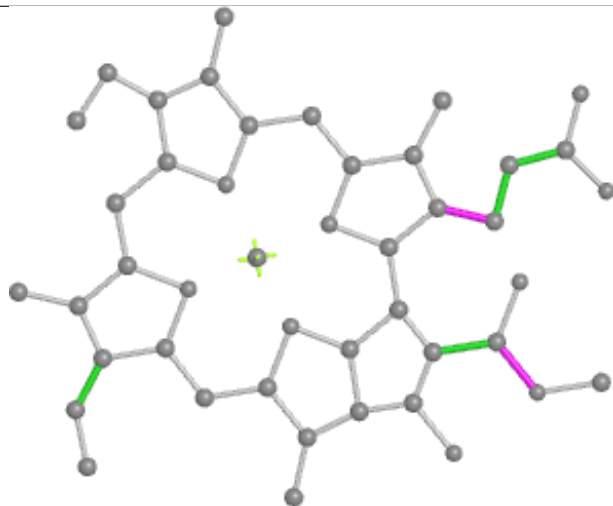
Ligand CLA B 823



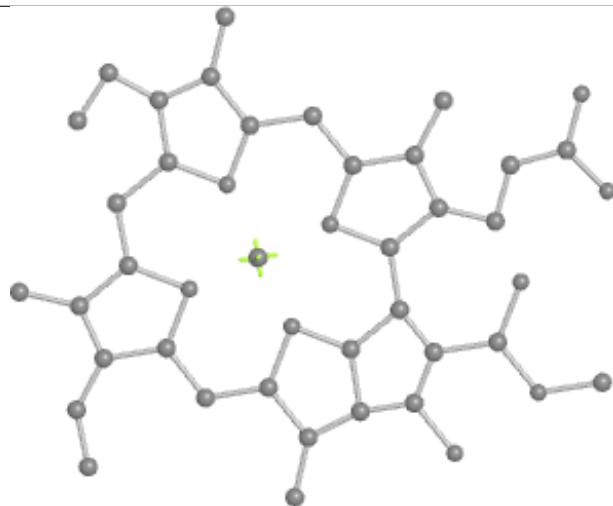
Bond lengths



Bond angles

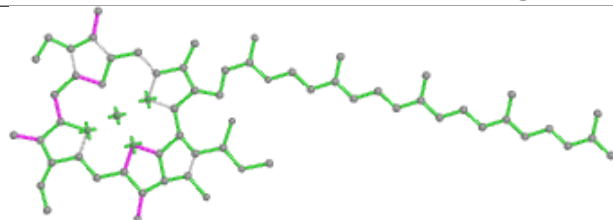


Torsions

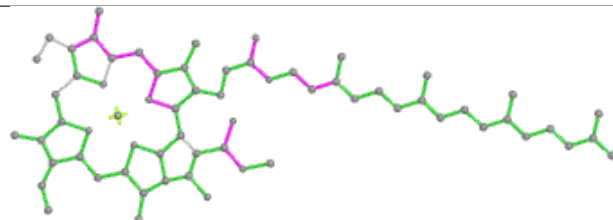


Rings

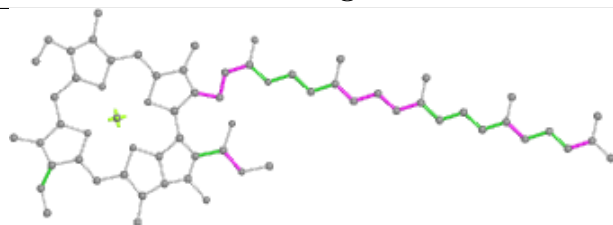
Ligand CLA B 809



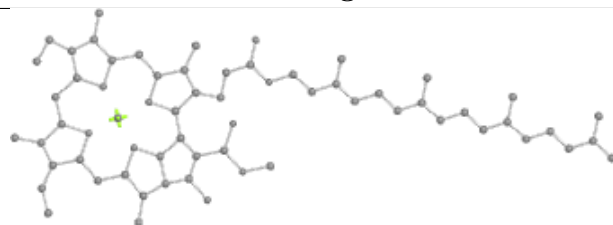
Bond lengths



Bond angles

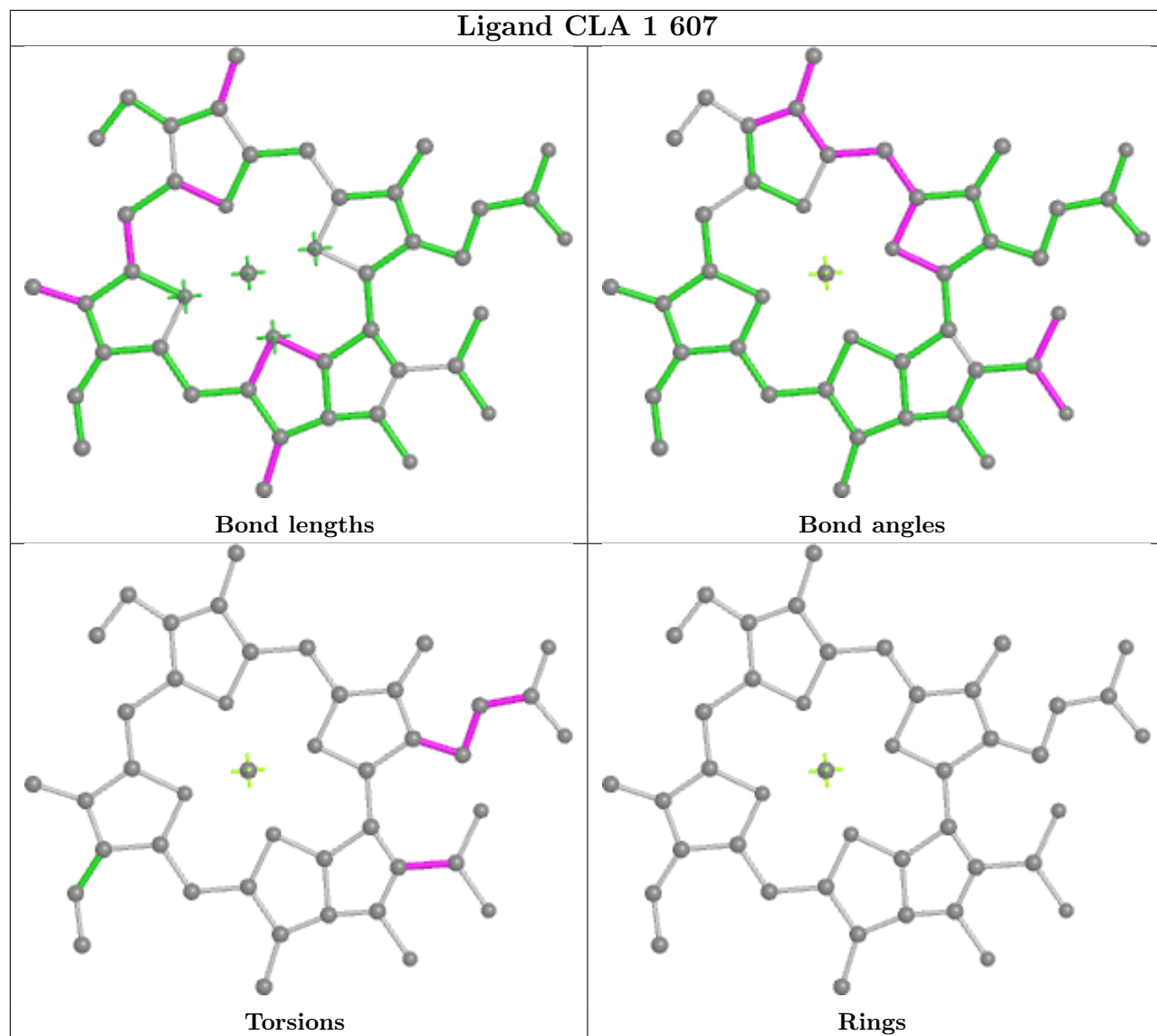


Torsions

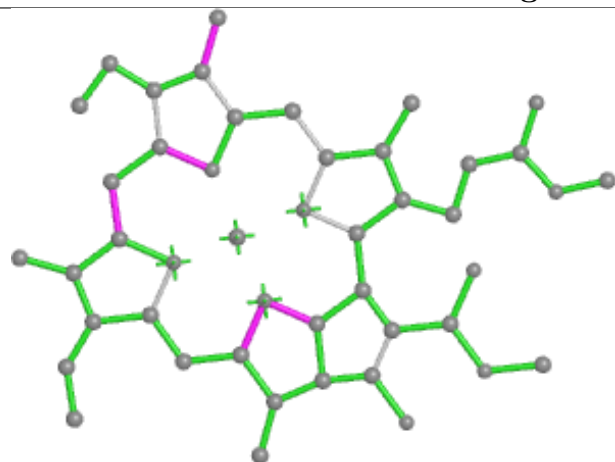


Rings

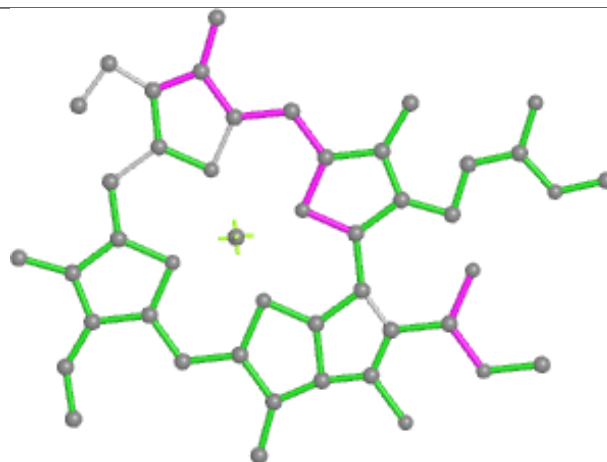
Ligand CLA 1 607



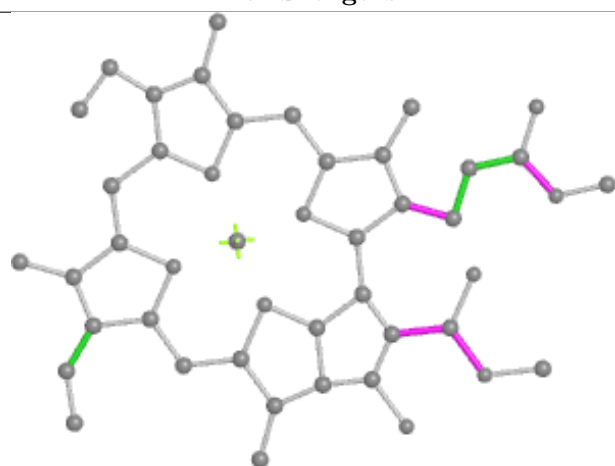
Ligand CLA 1 605



Bond lengths



Bond angles

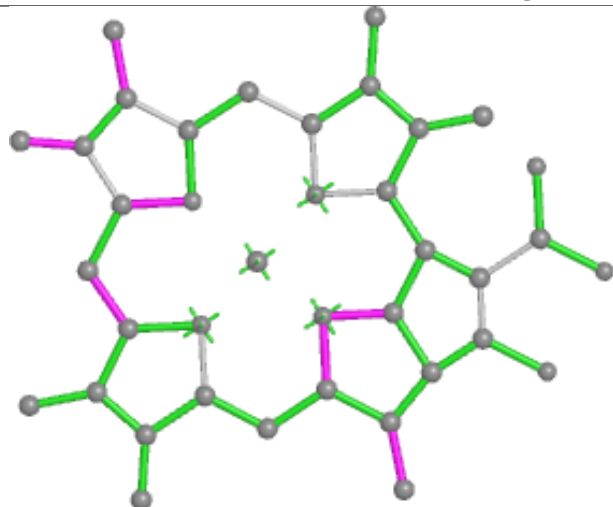


Torsions

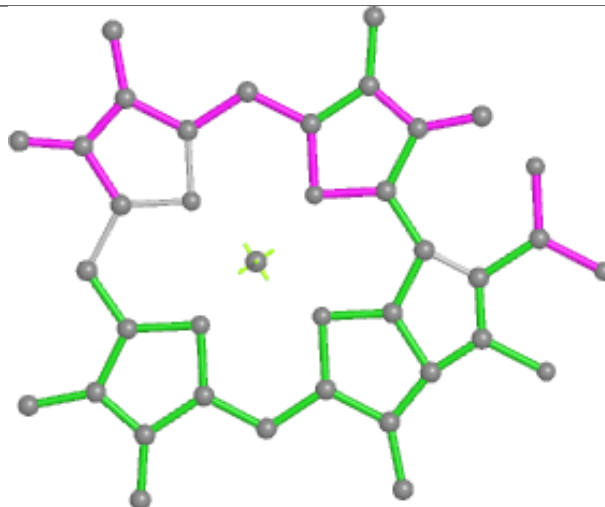


Rings

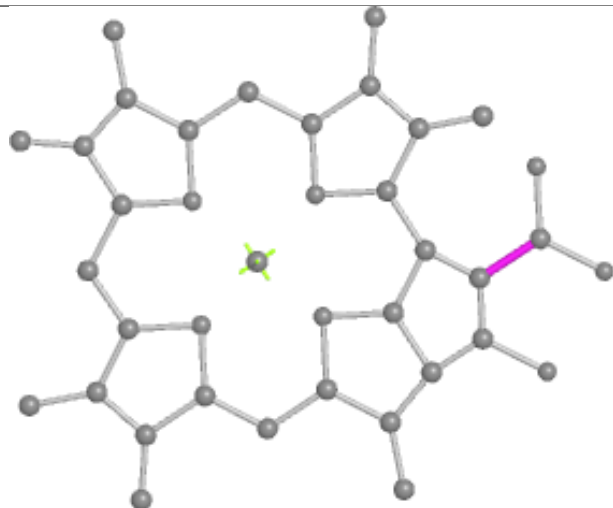
Ligand CLA 1 613



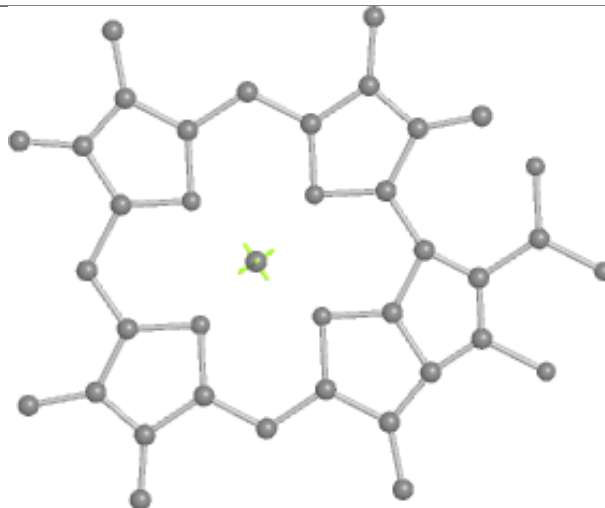
Bond lengths



Bond angles

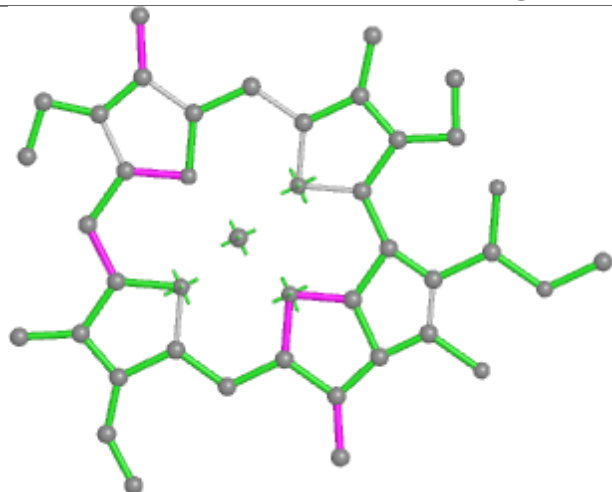


Torsions

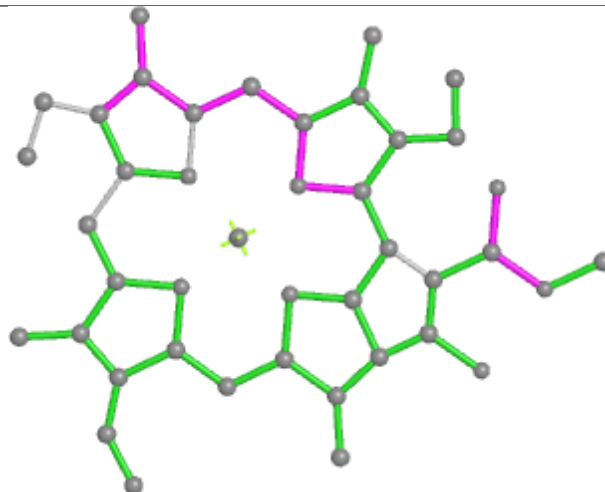


Rings

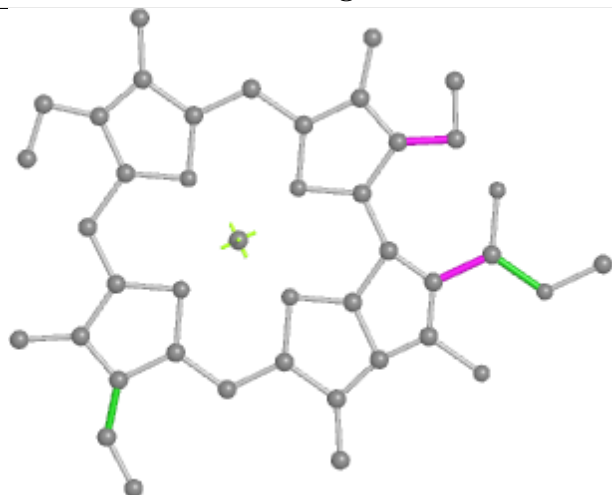
Ligand CLA A 816



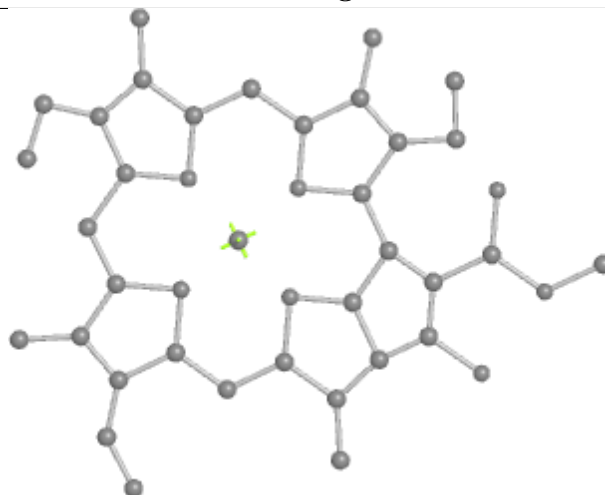
Bond lengths



Bond angles

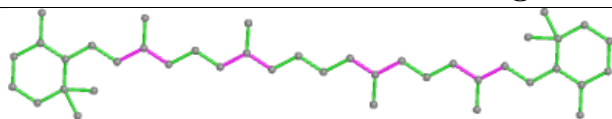


Torsions

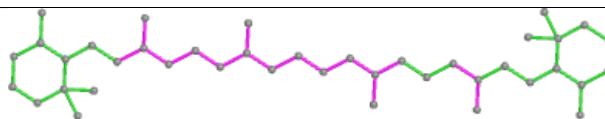


Rings

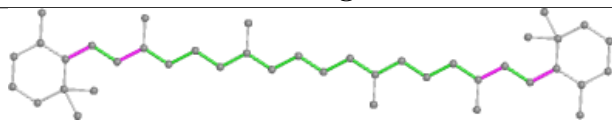
Ligand BCR B 846



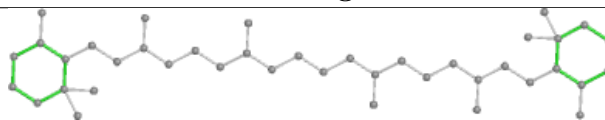
Bond lengths



Bond angles

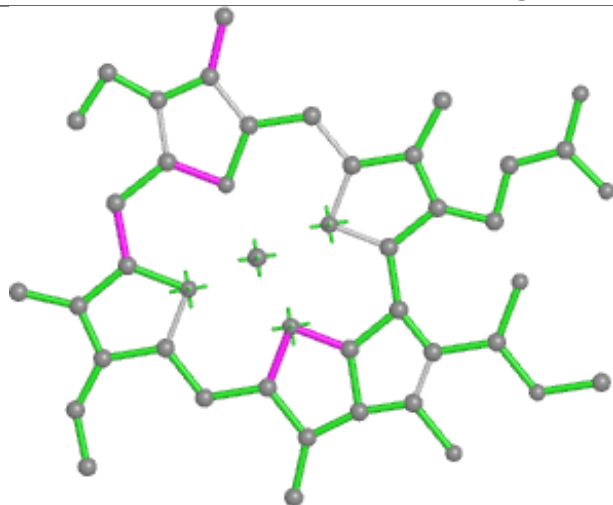


Torsions

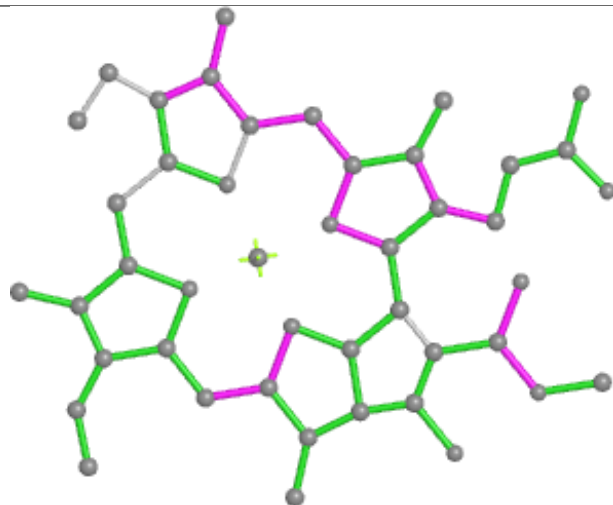


Rings

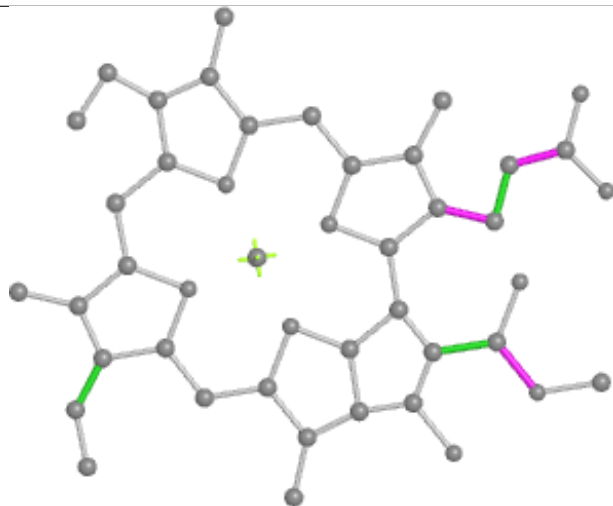
Ligand CLA K 203



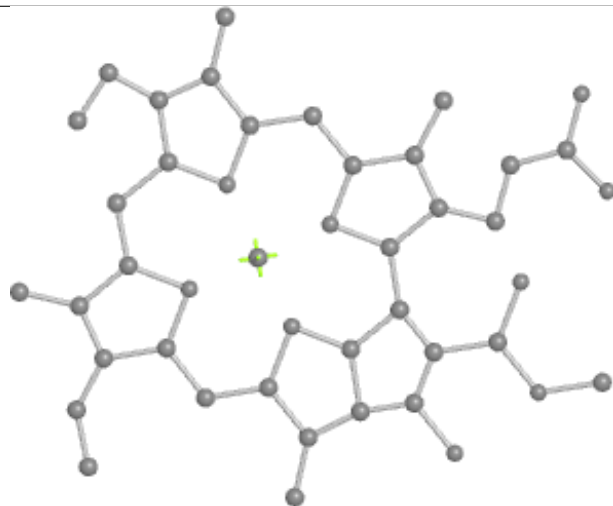
Bond lengths



Bond angles

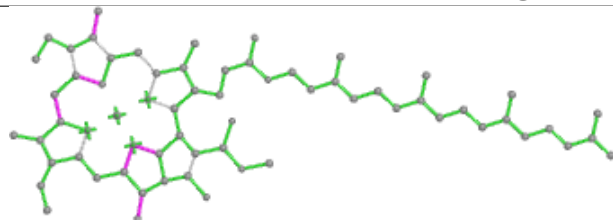


Torsions

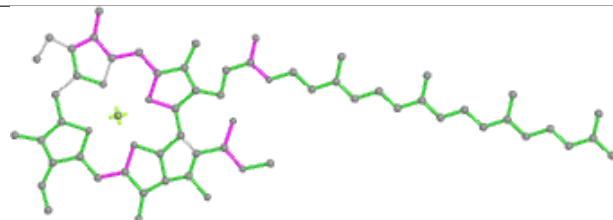


Rings

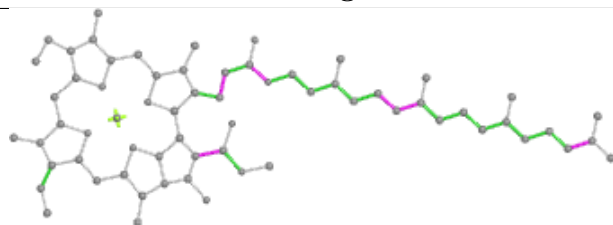
Ligand CLA B 839



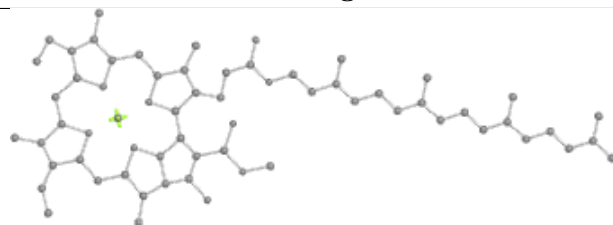
Bond lengths



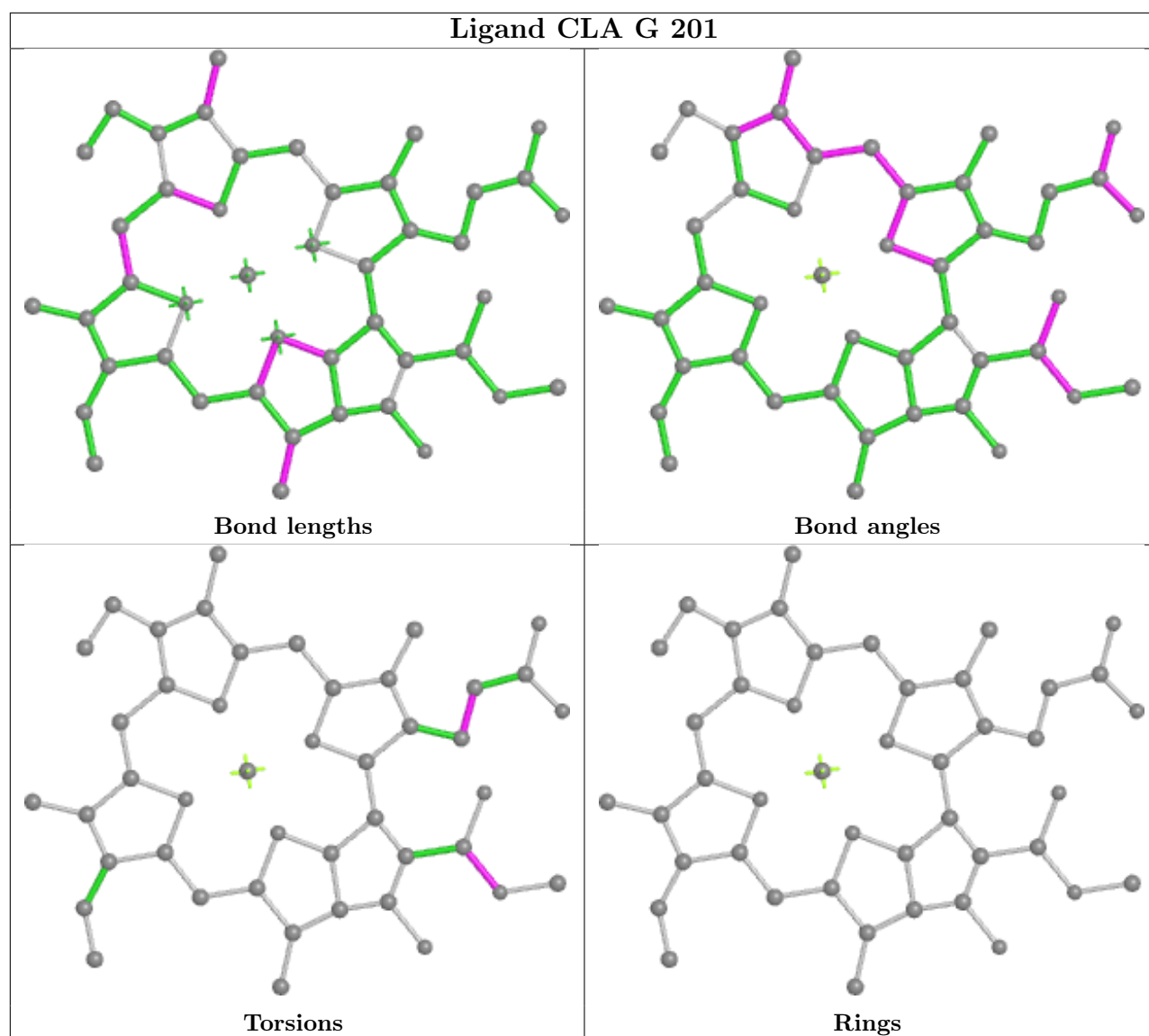
Bond angles



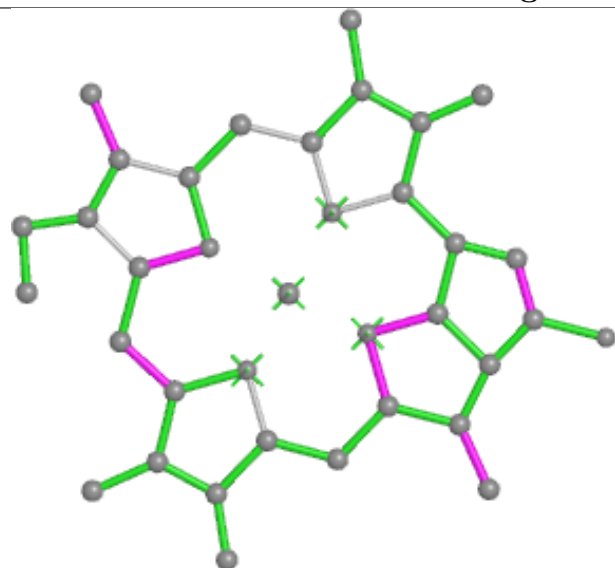
Torsions



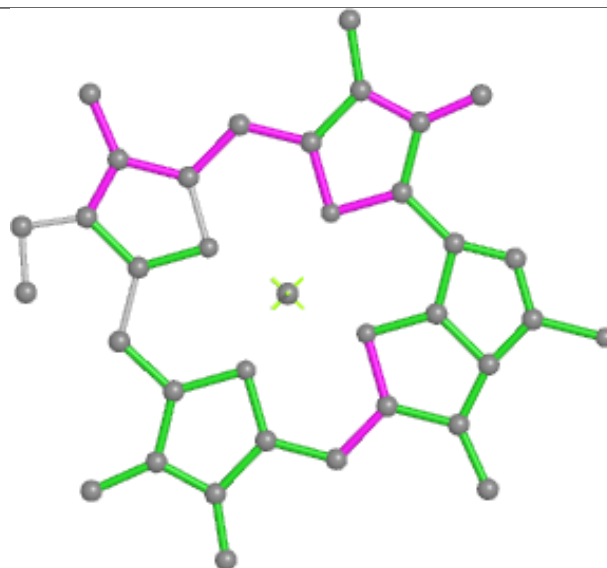
Rings



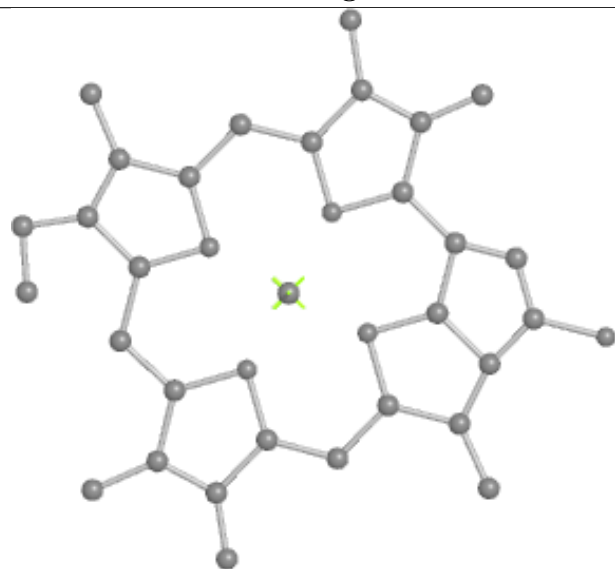
Ligand CLA 3 611



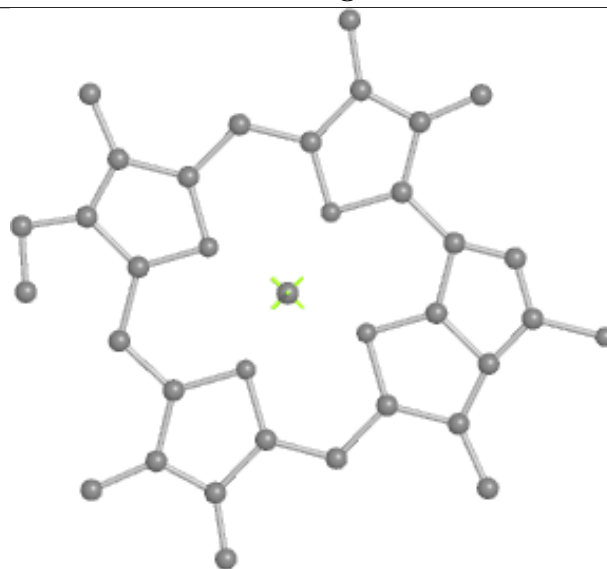
Bond lengths



Bond angles

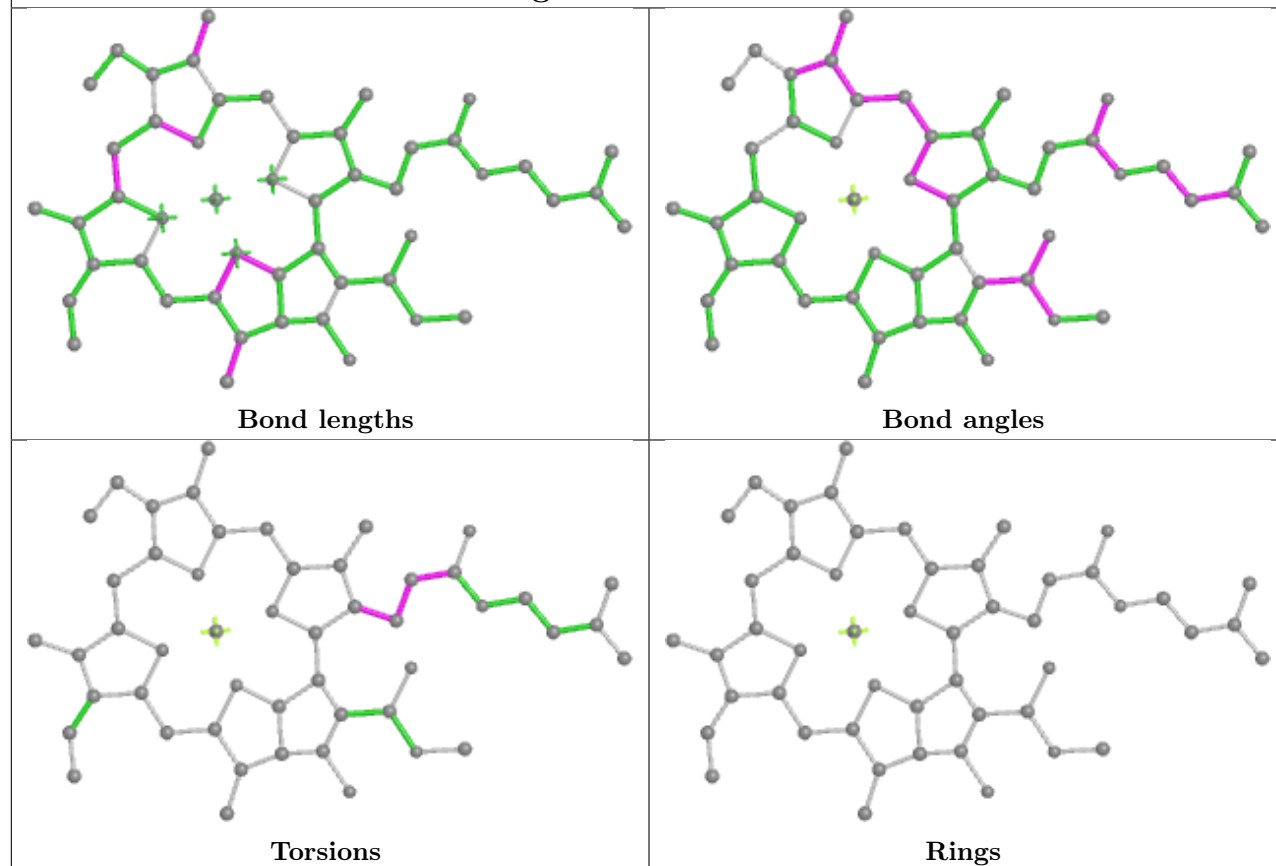


Torsions

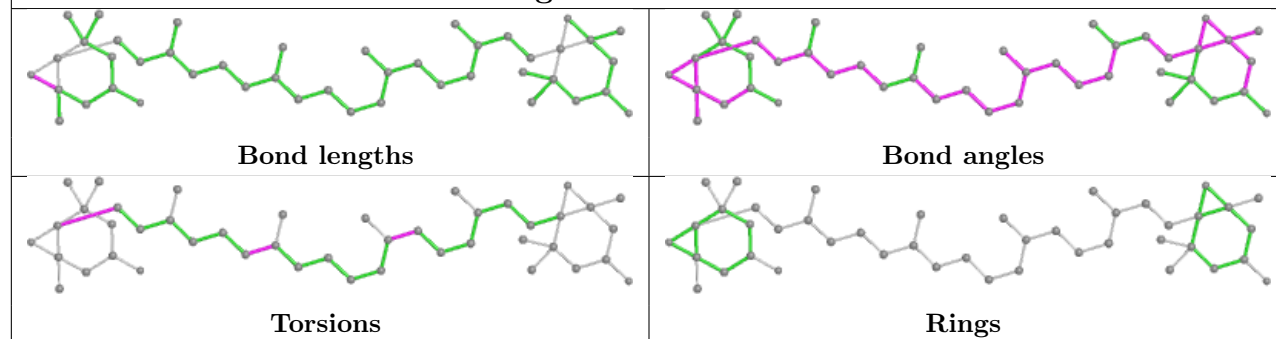


Rings

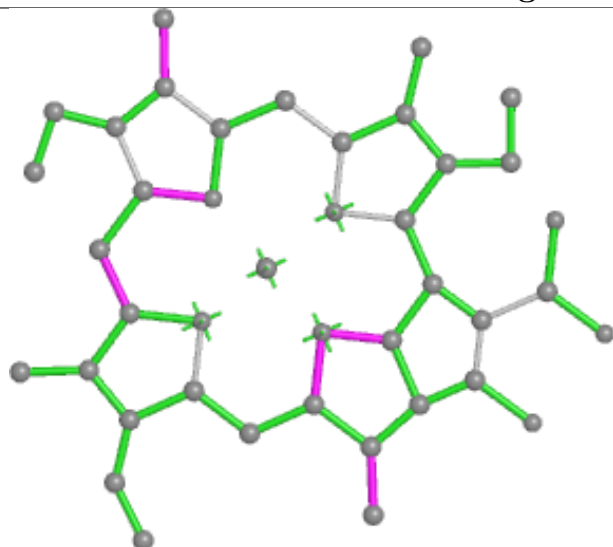
Ligand CLA B 820



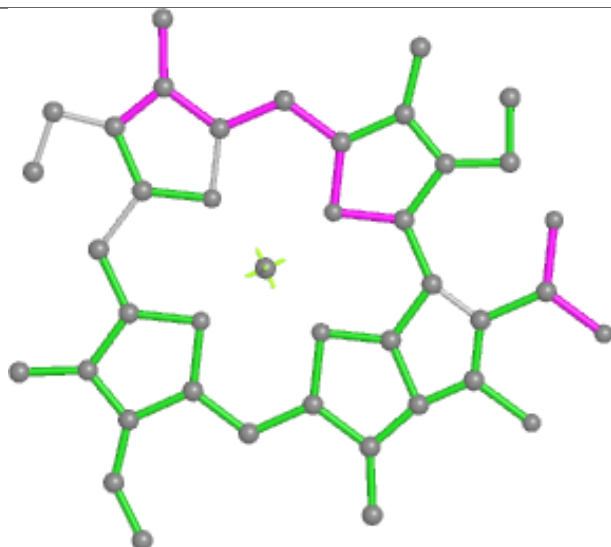
Ligand XAT 1 614



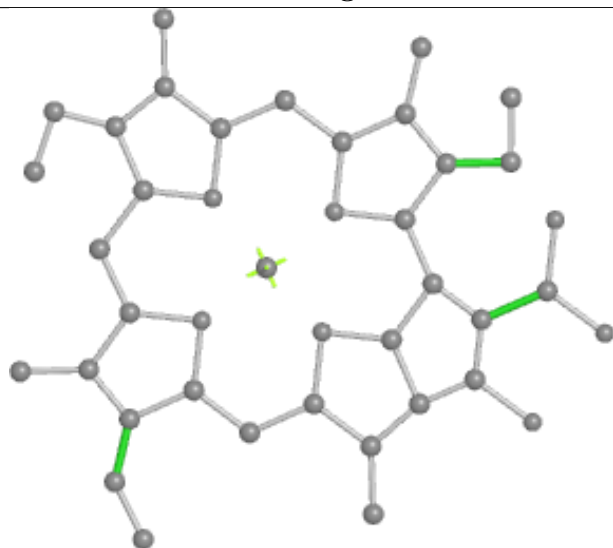
Ligand CLA 3 604



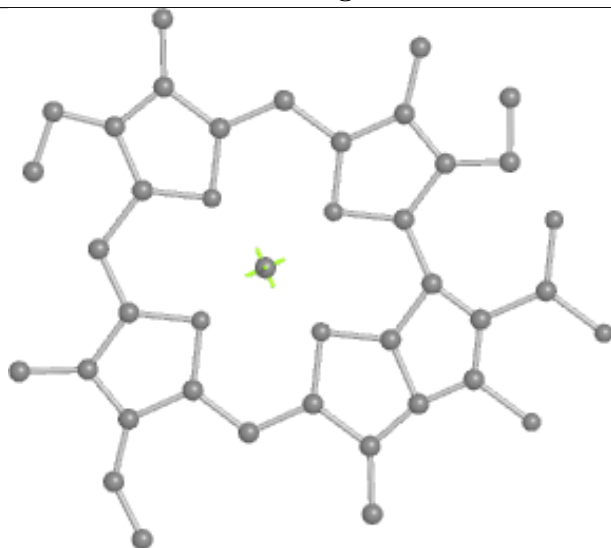
Bond lengths



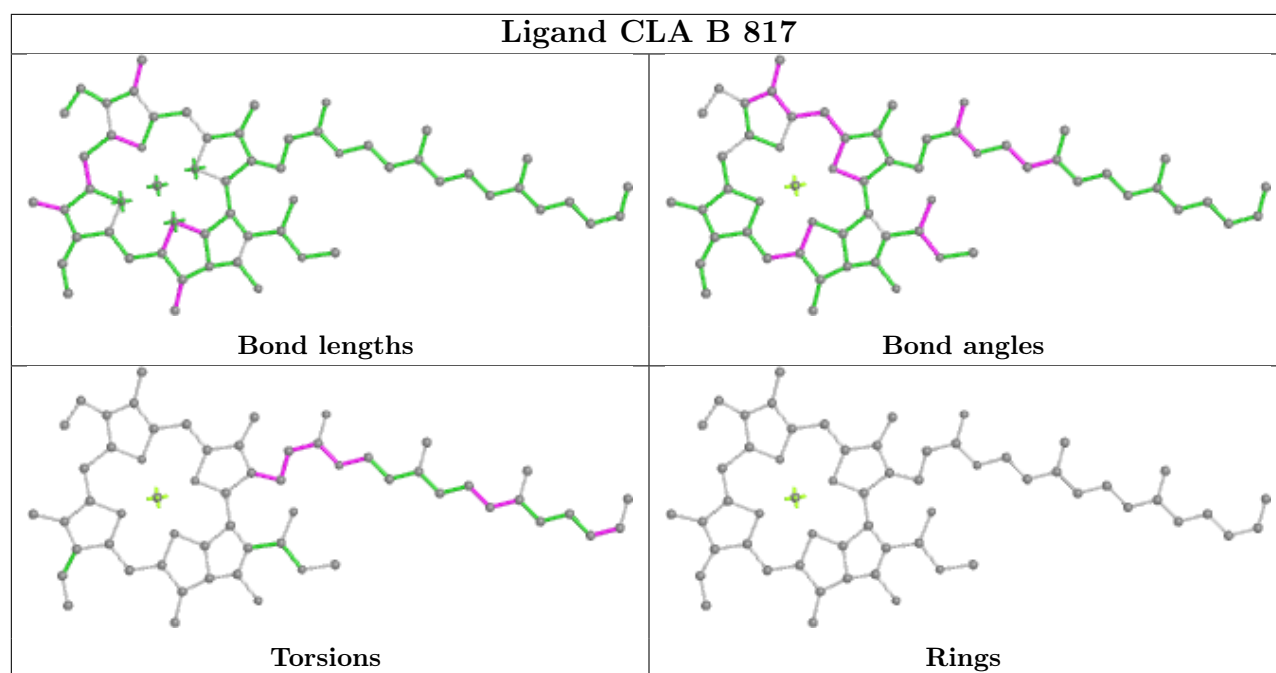
Bond angles



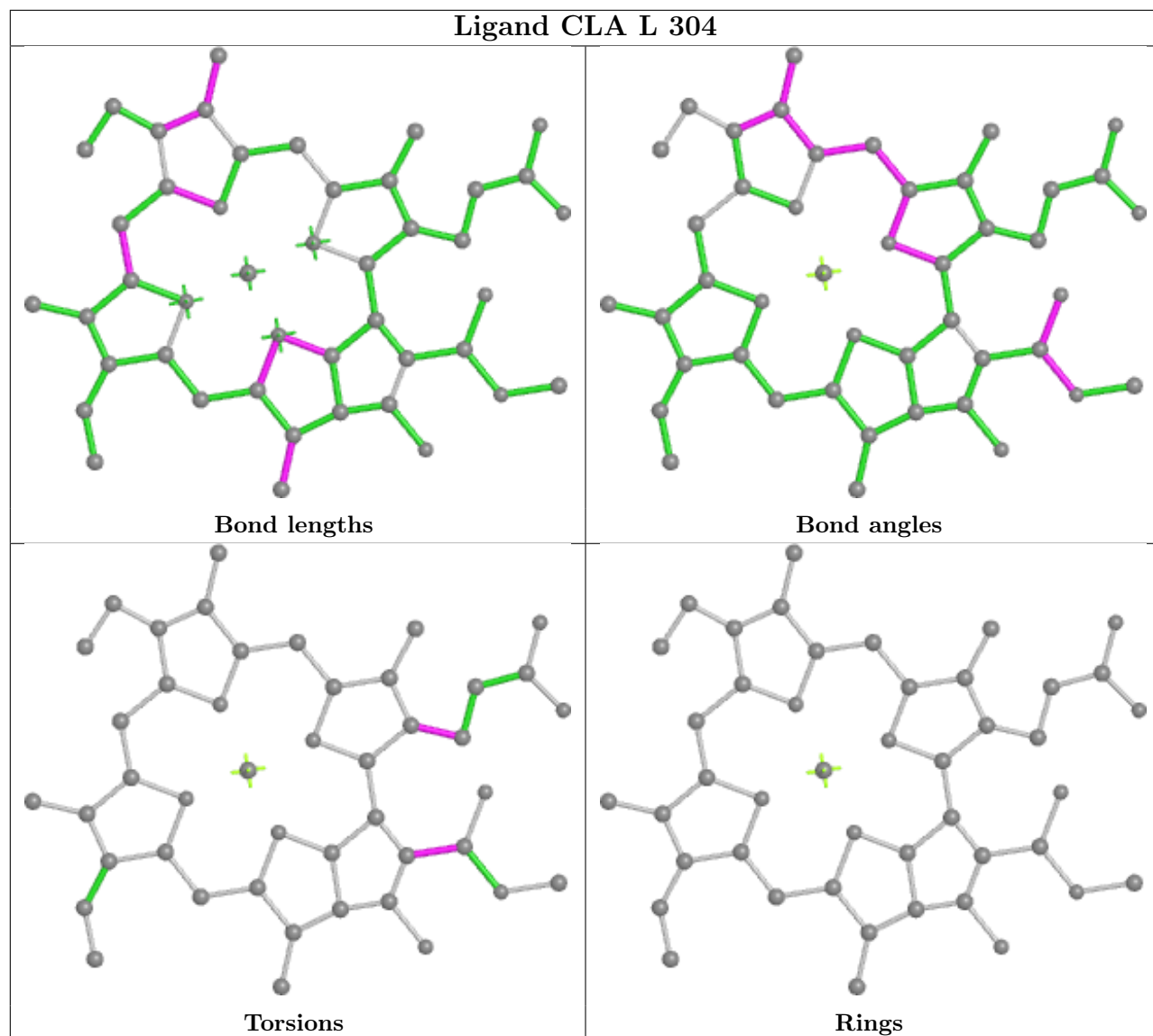
Torsions



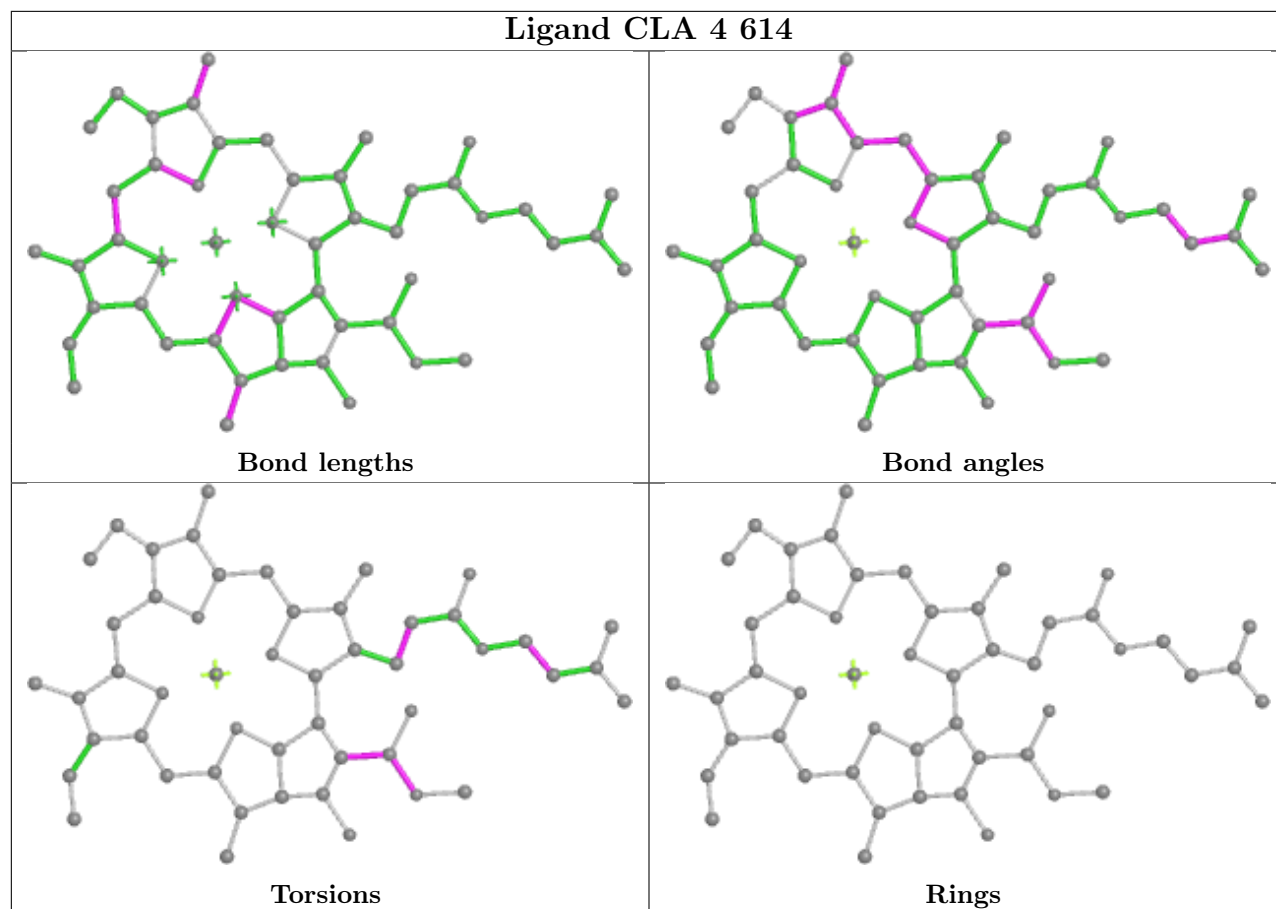
Rings



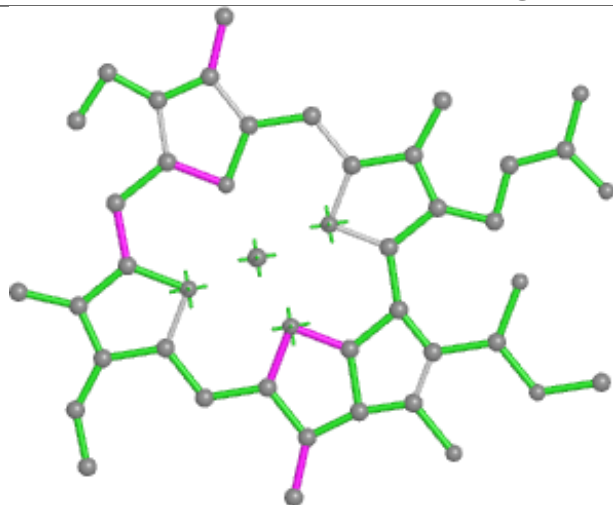
Ligand CLA L 304



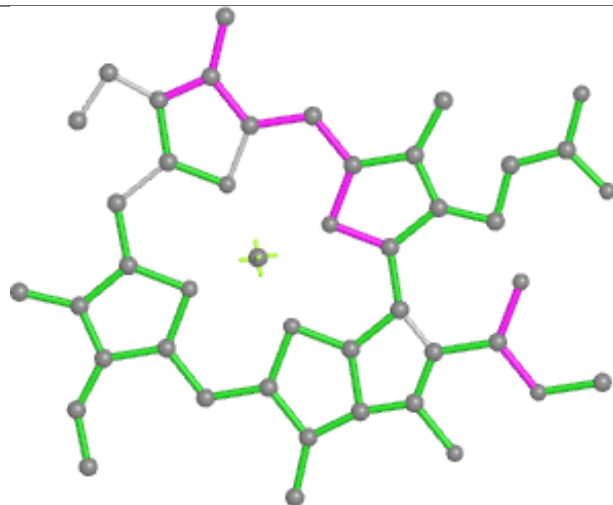
Ligand CLA 4 614



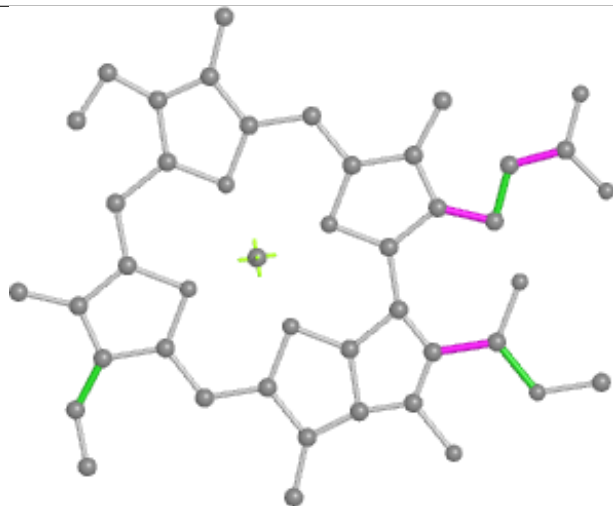
Ligand CLA A 821



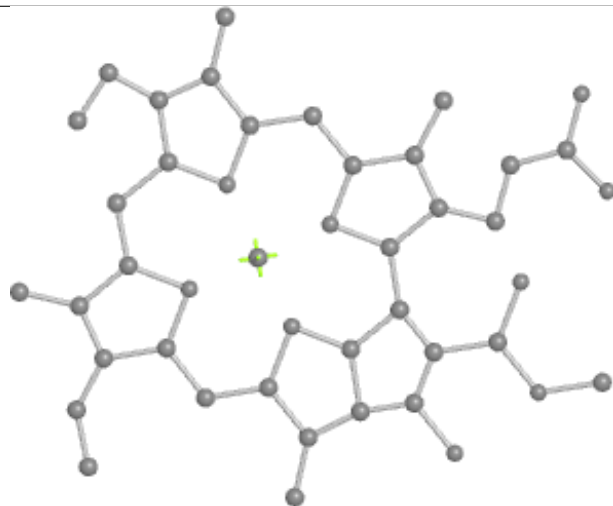
Bond lengths



Bond angles

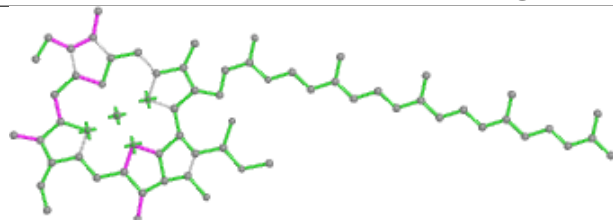


Torsions

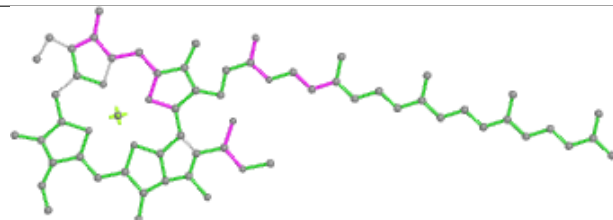


Rings

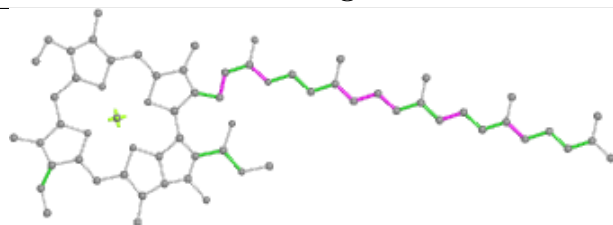
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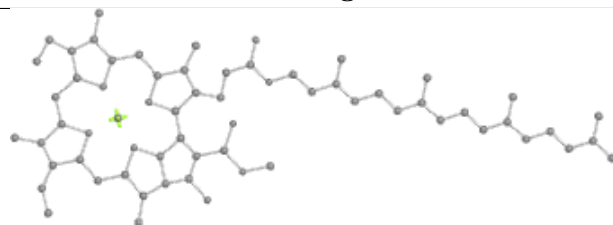
Bond lengths



Bond angles

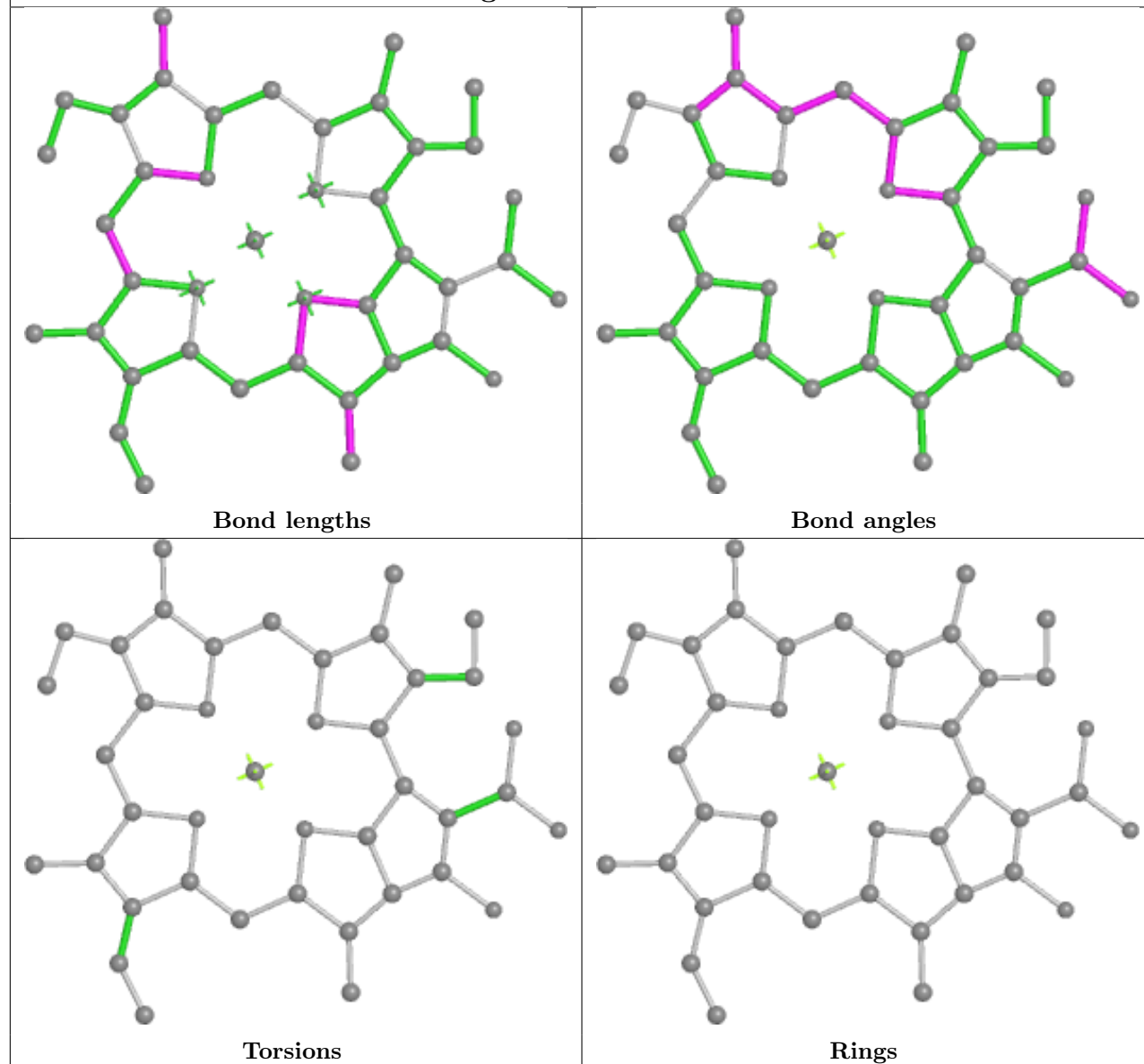


Torsions

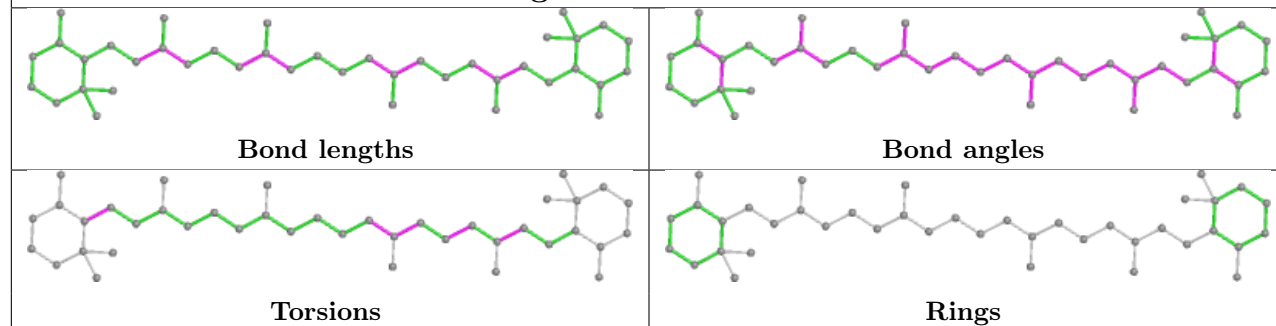


Rings

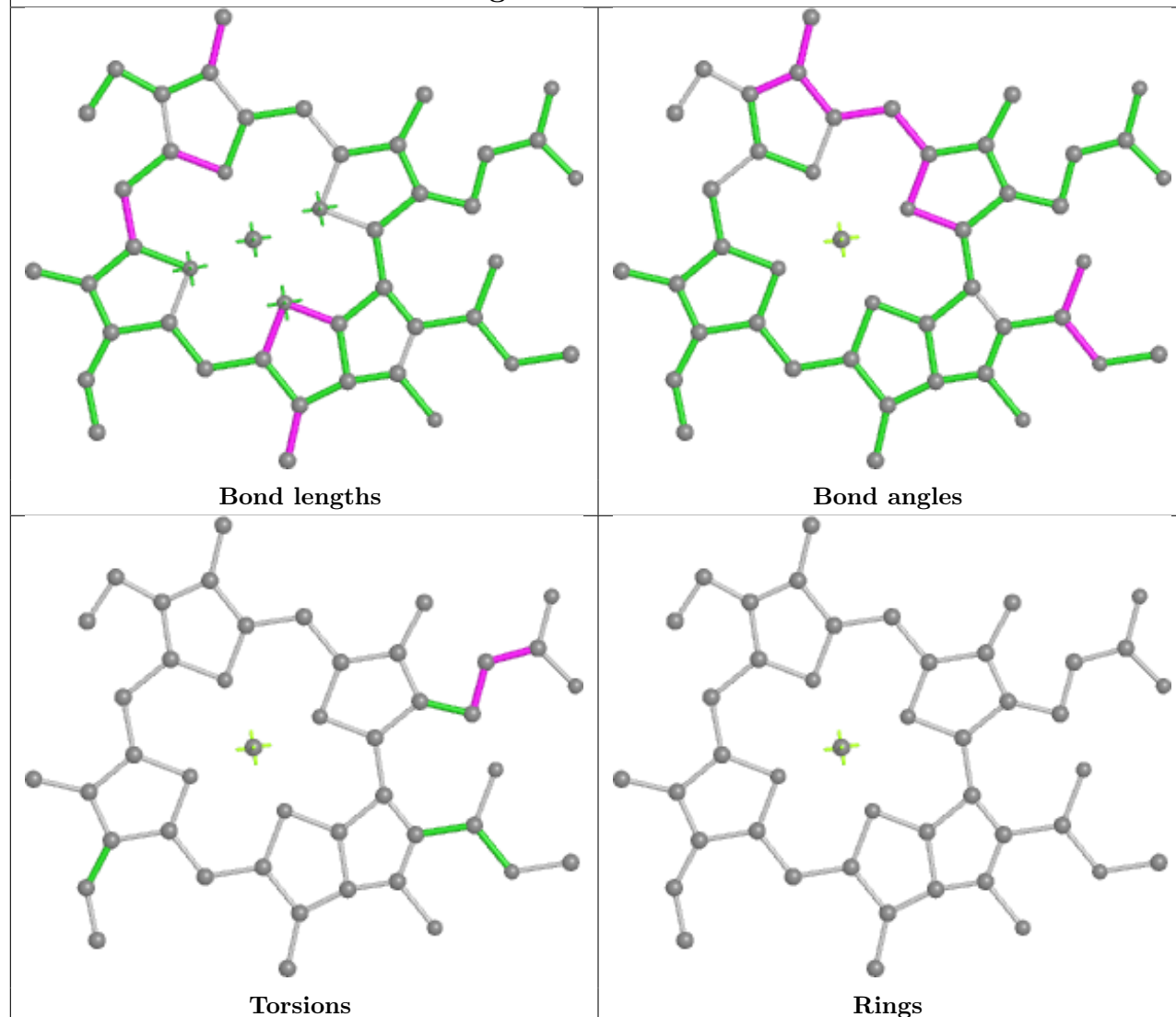
Ligand CLA 4 611



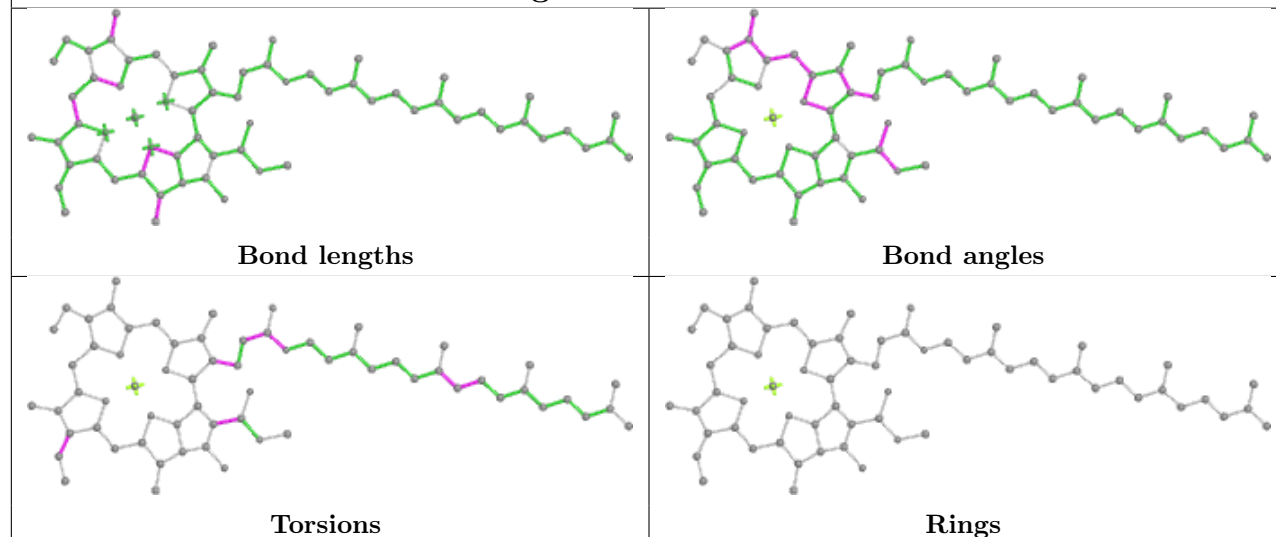
Ligand BCR B 845



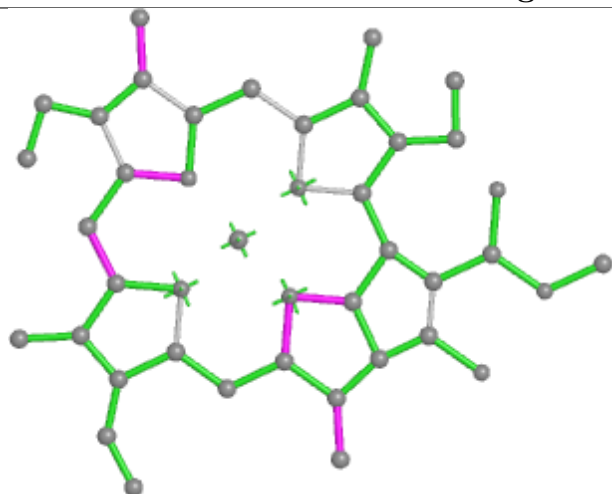
Ligand CLA G 203



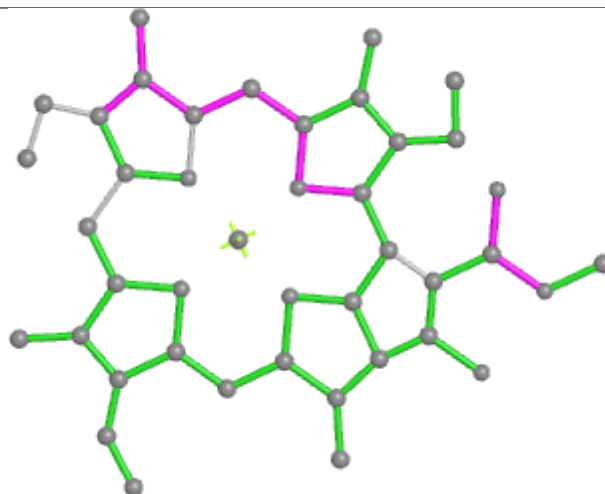
Ligand CLA A 842



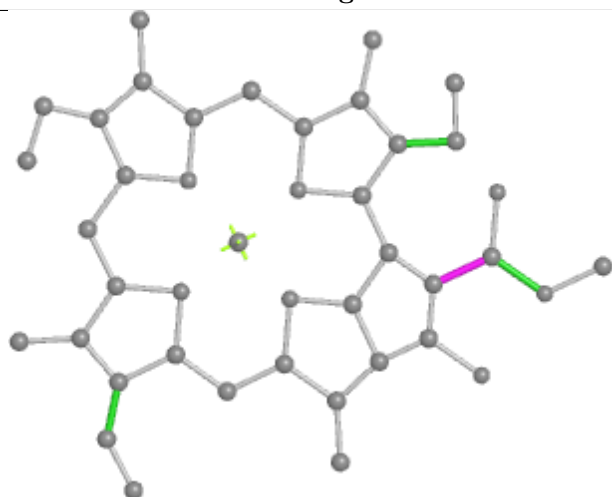
Ligand CLA 4 610



Bond lengths



Bond angles

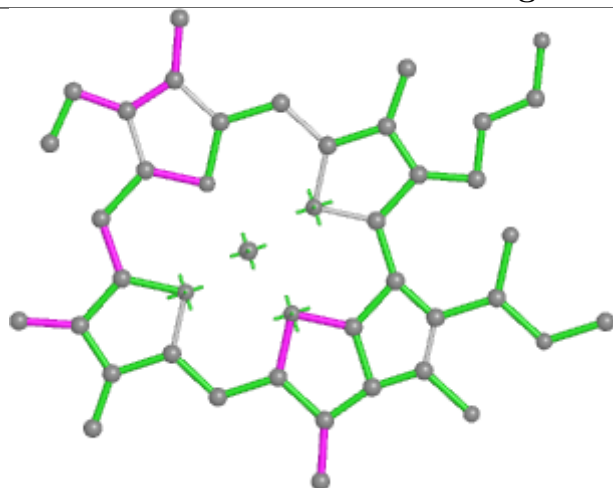


Torsions

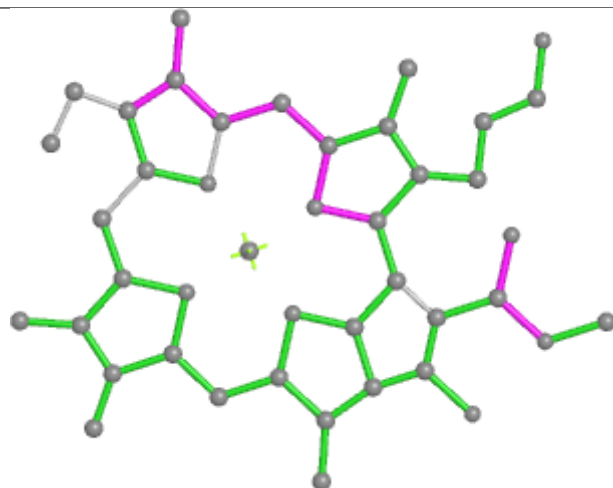


Rings

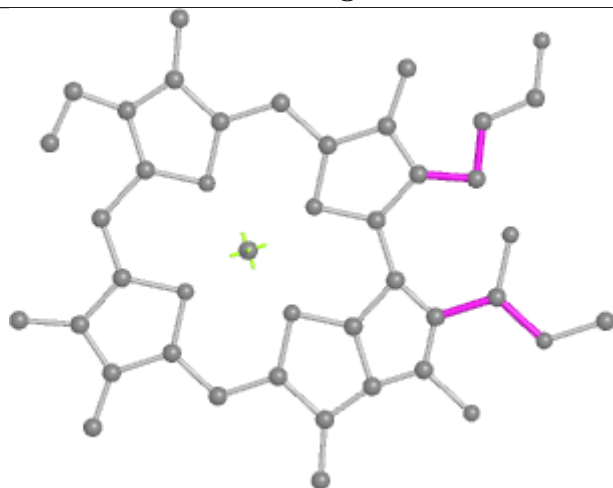
Ligand CLA 2 604



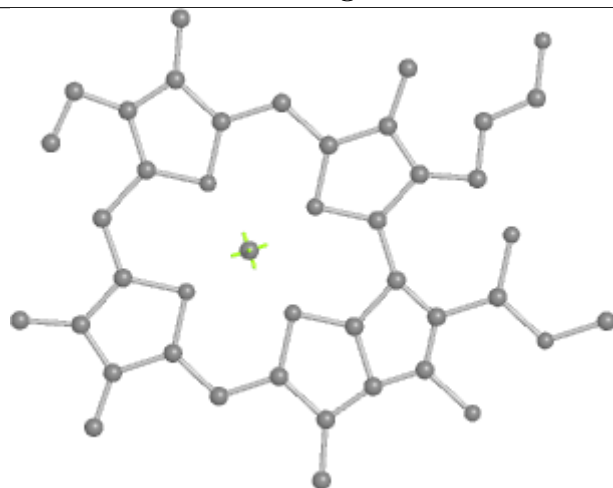
Bond lengths



Bond angles

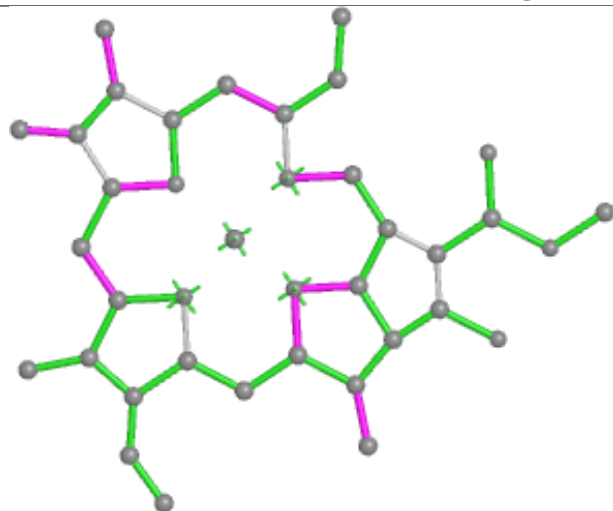


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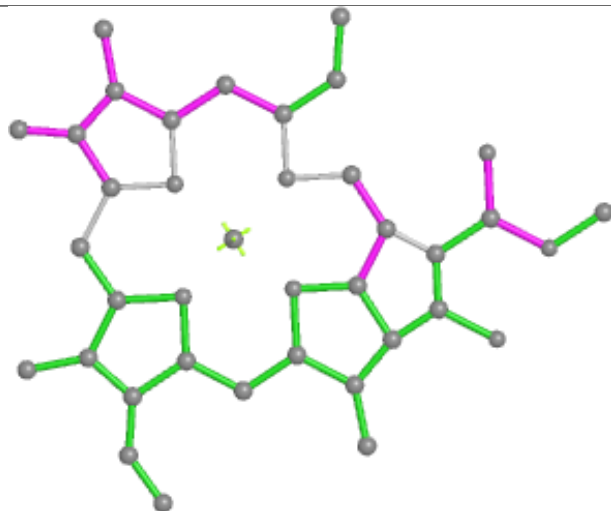


Rings

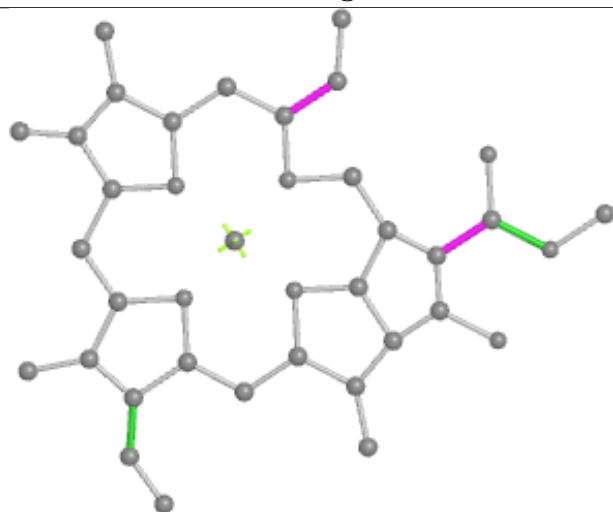
Ligand CLA 2 610



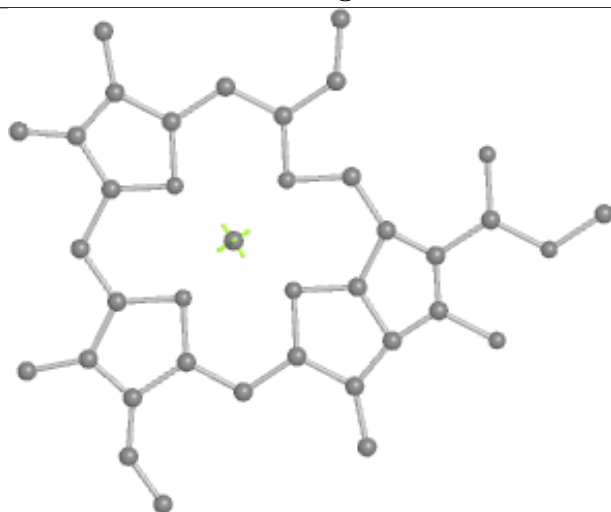
Bond lengths



Bond angles

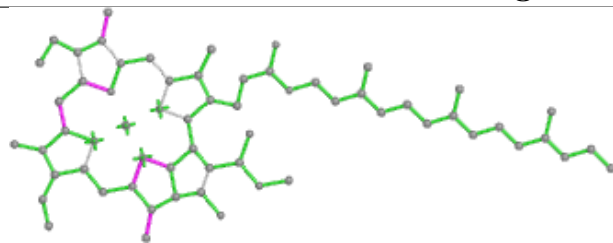


Torsions

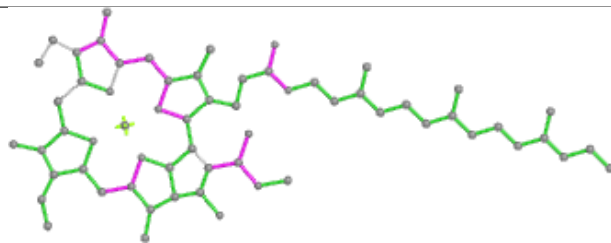


Rings

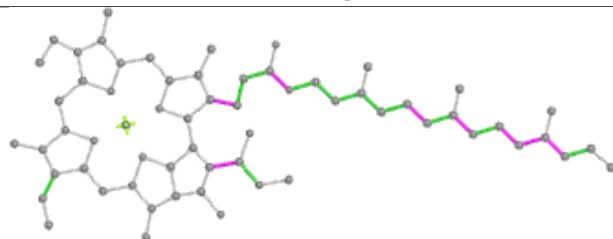
Ligand CLA B 825



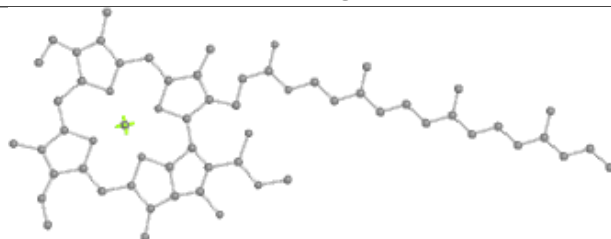
Bond lengths



Bond angles

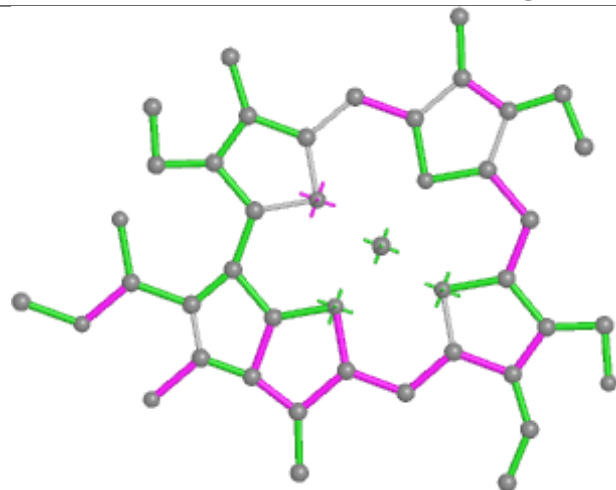


Torsions

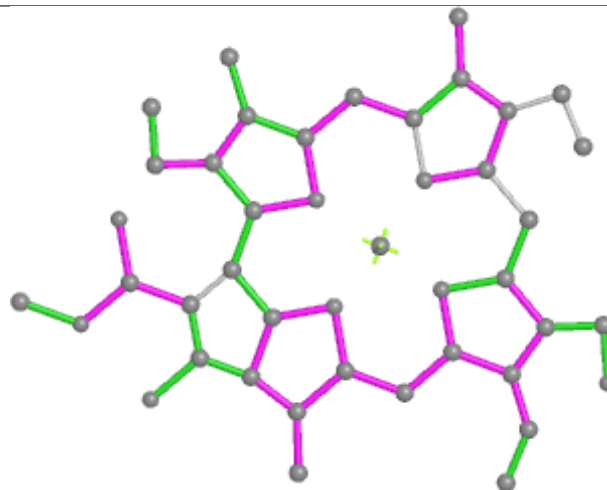


Rings

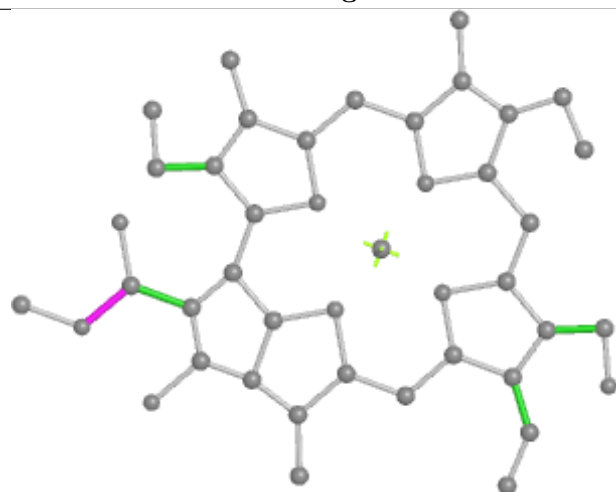
Ligand CHL 2 615



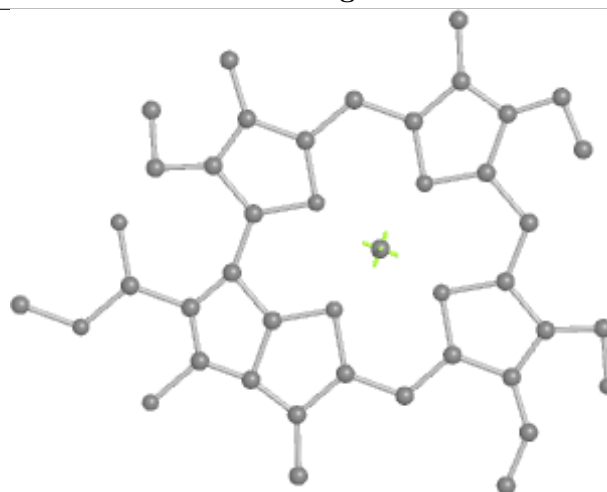
Bond lengths



Bond angles

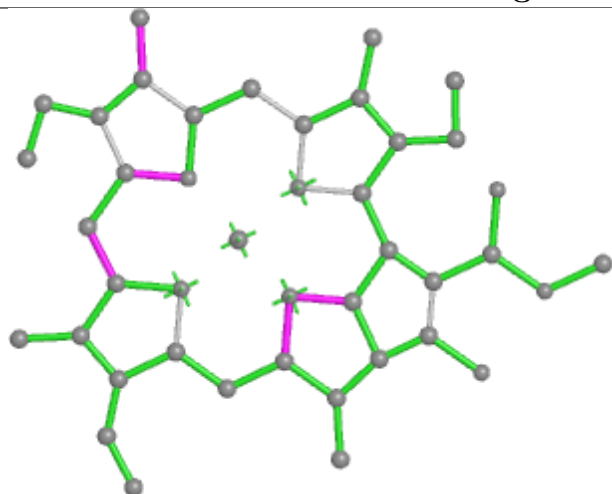


Torsions

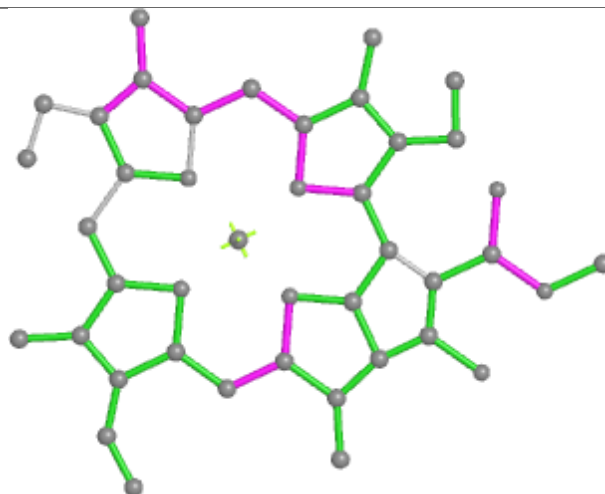


Rings

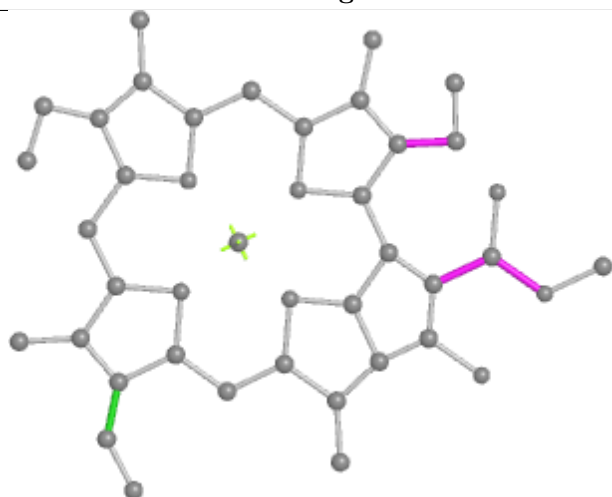
Ligand CLA B 835



Bond lengths



Bond angles

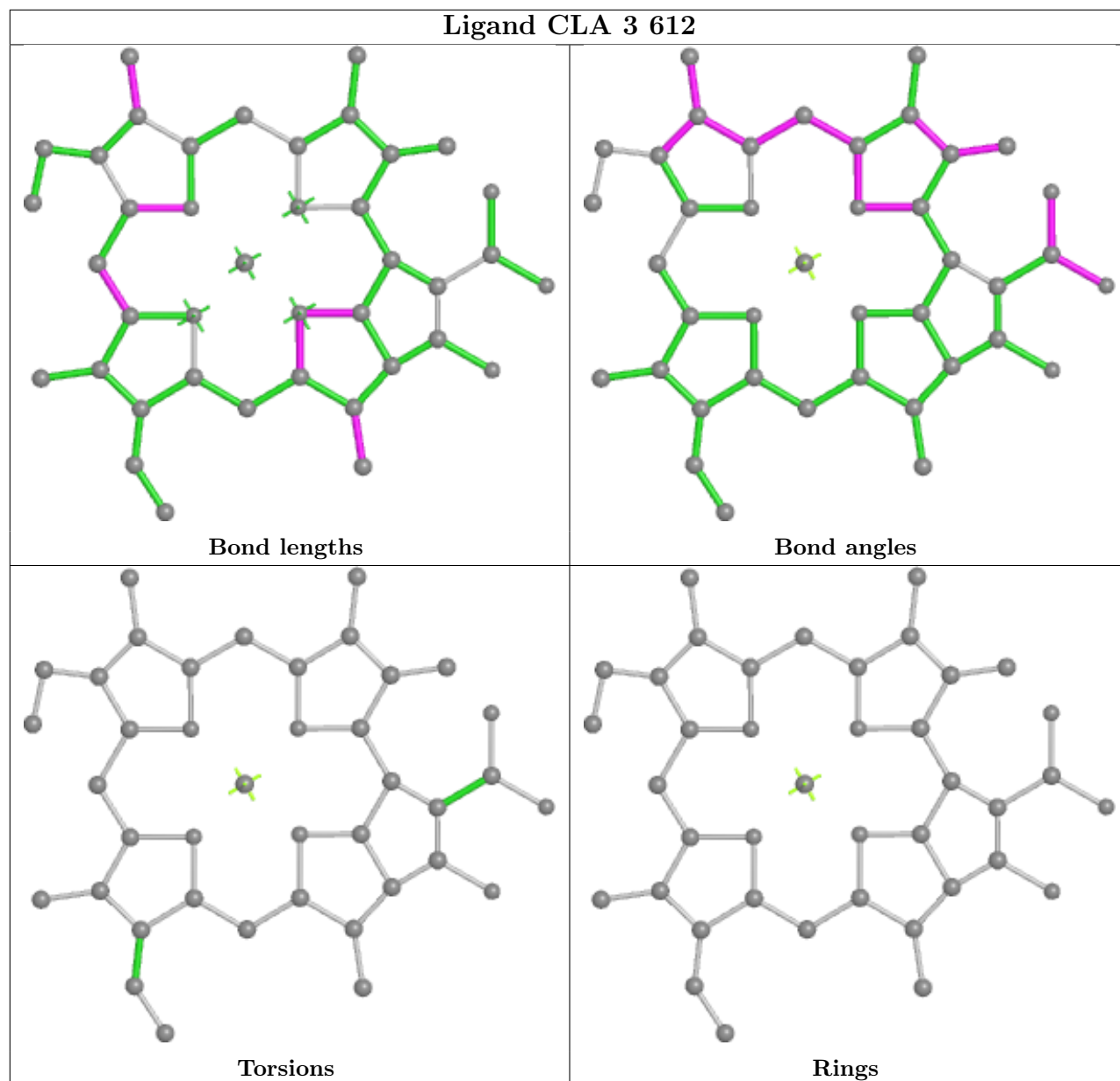


Torsions

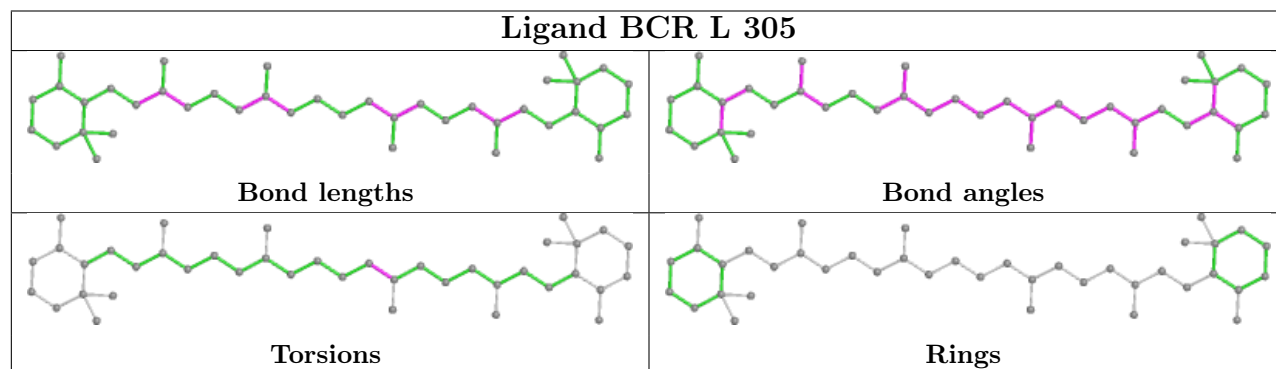


Rings

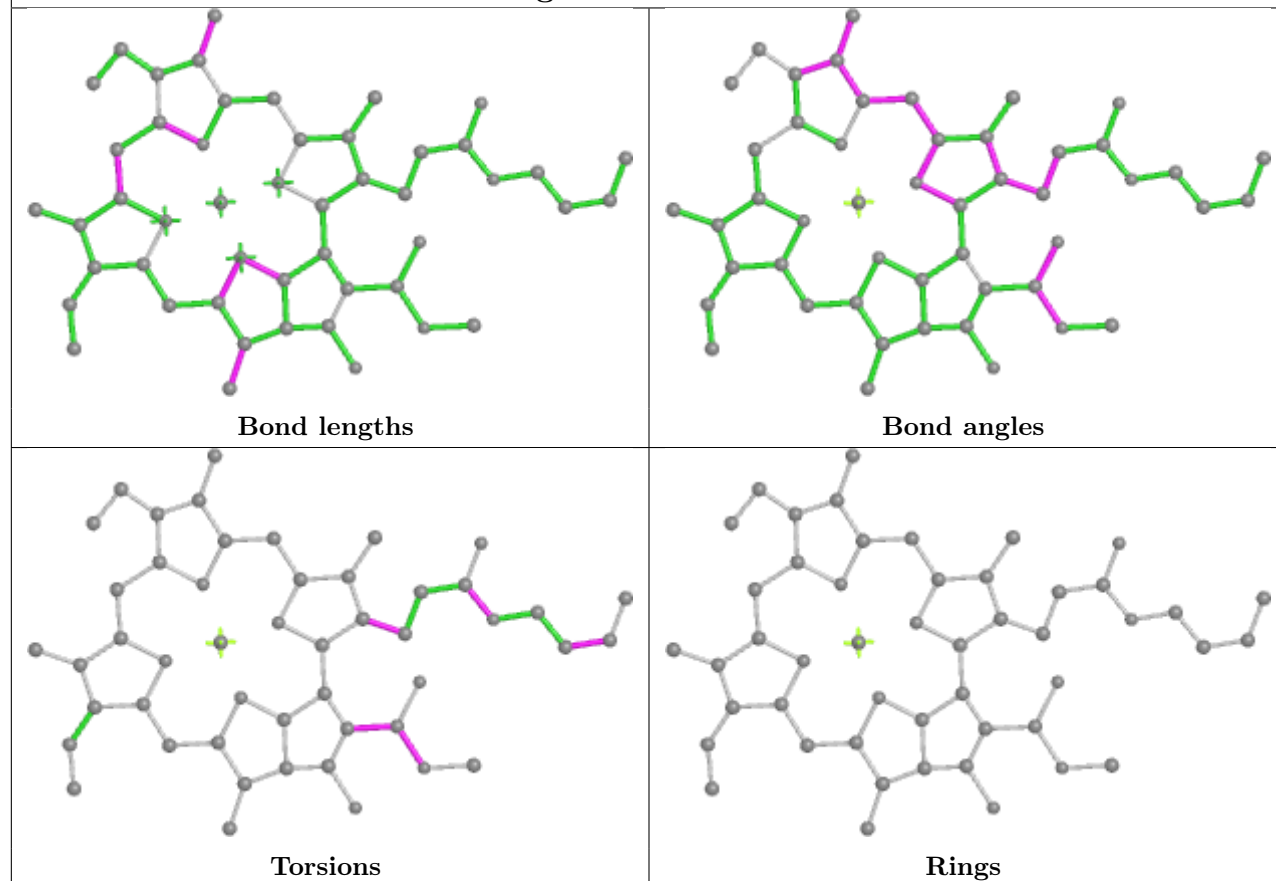
Ligand CLA 3 612



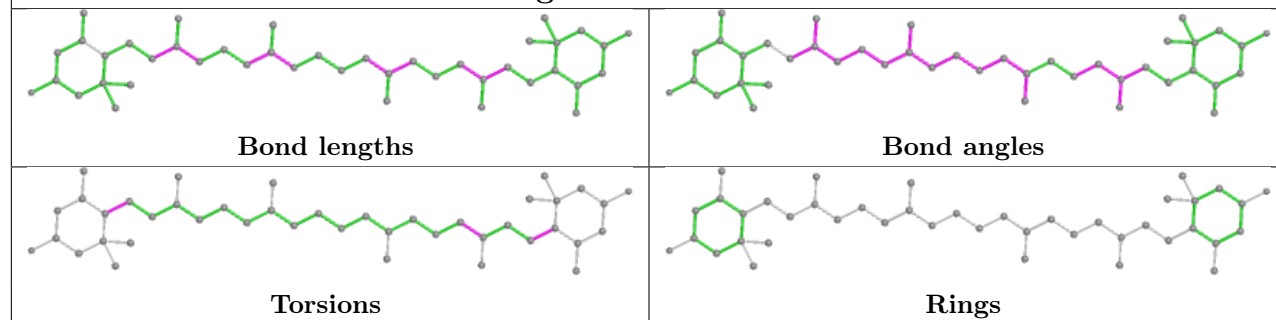
Ligand BCR L 305



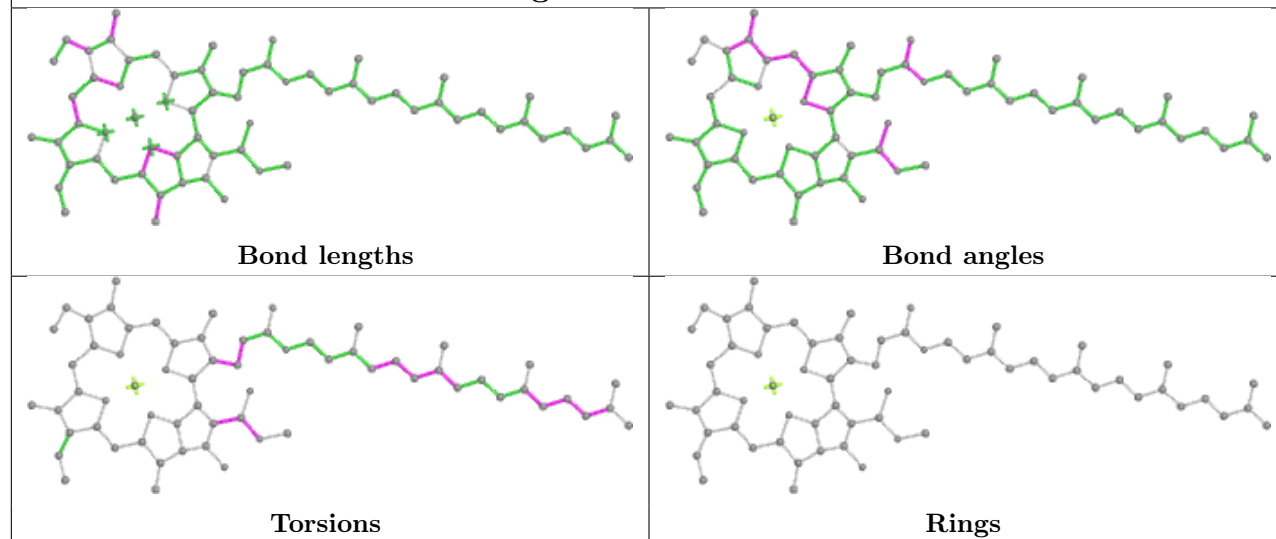
Ligand CLA 1 604



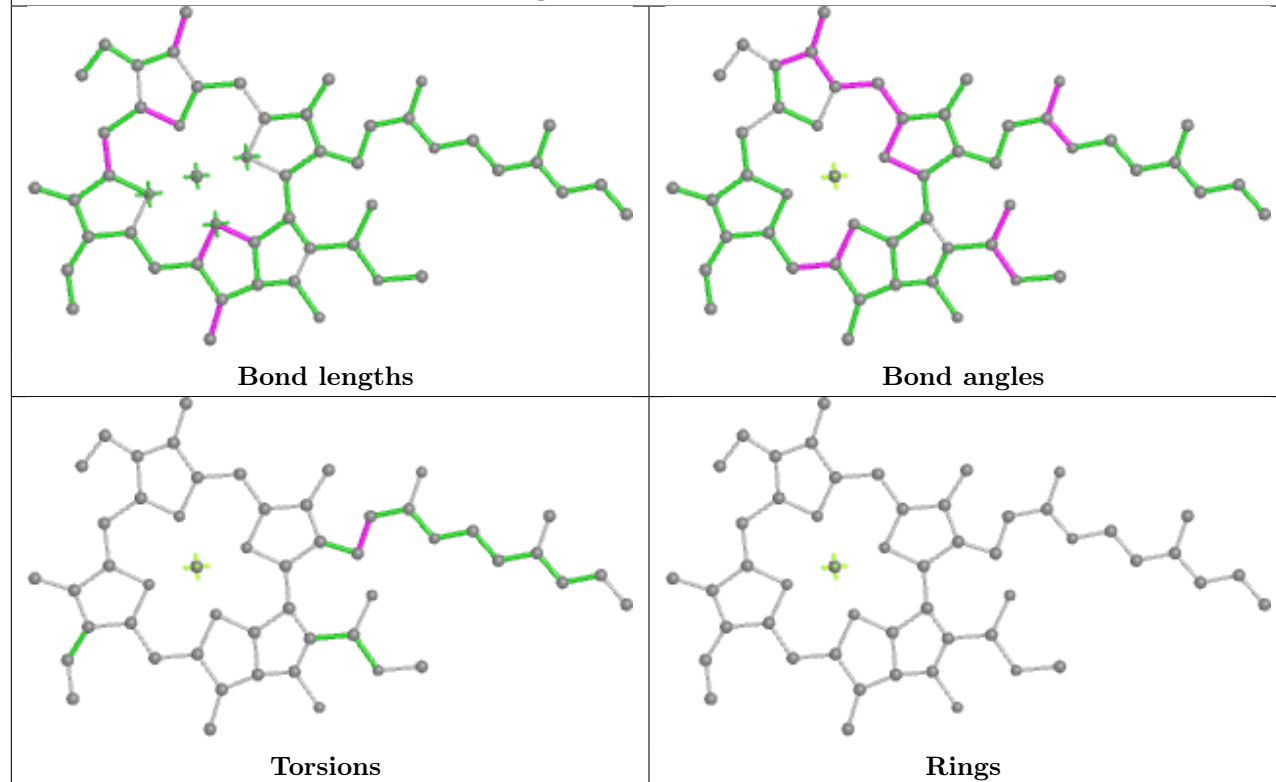
Ligand LUT 2 619

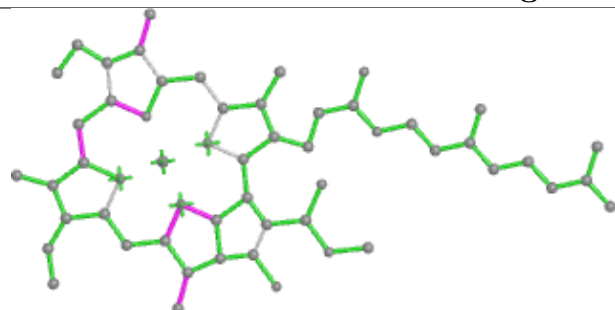
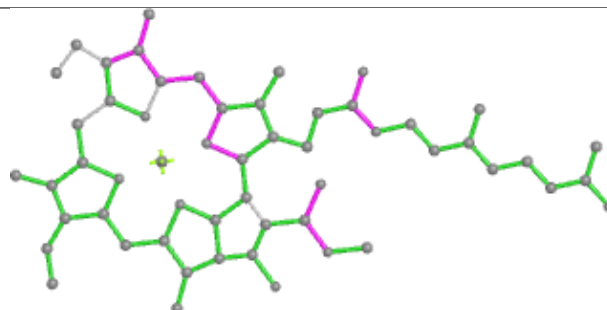
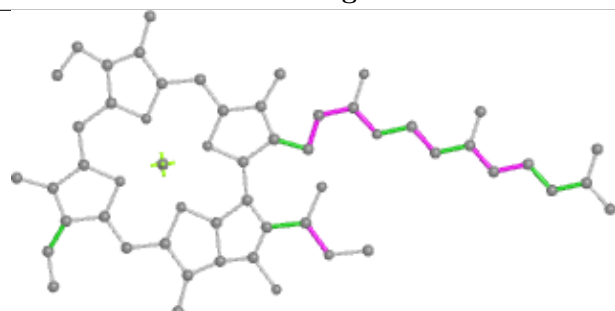
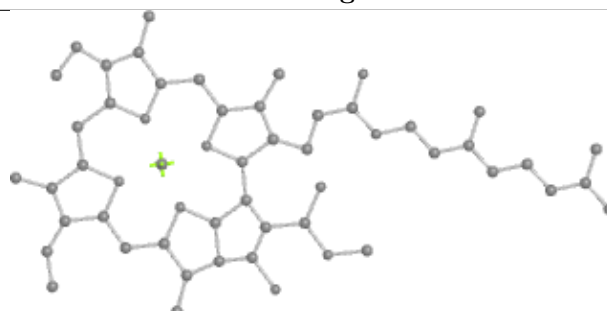
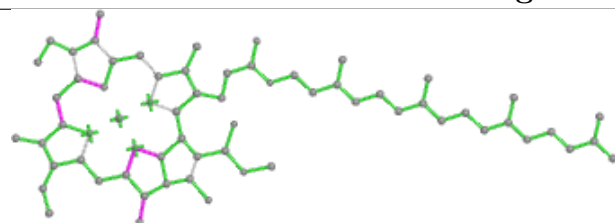
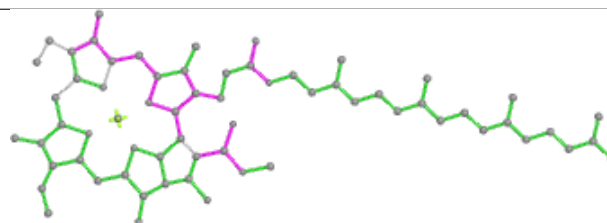
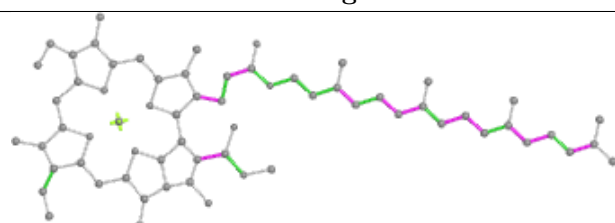
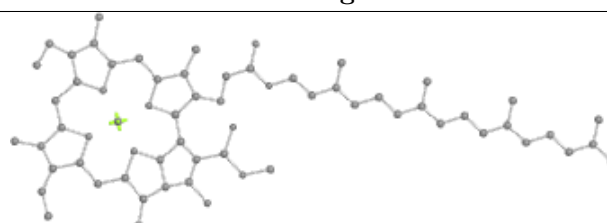


Ligand CLA A 829

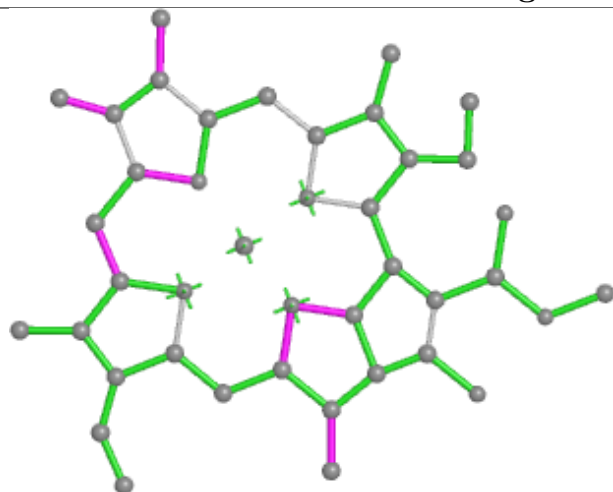


Ligand CLA B 807

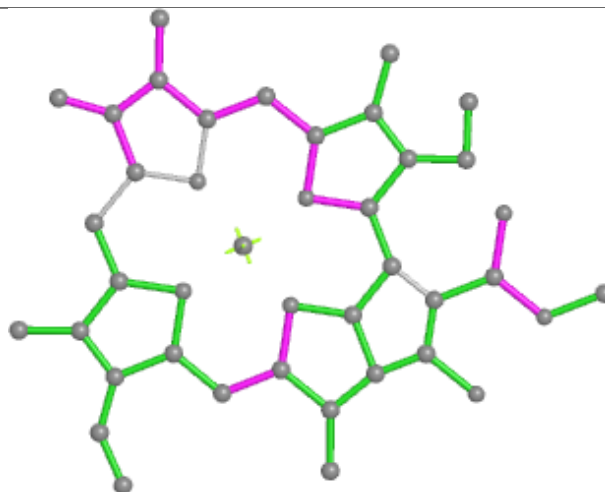


Ligand CLA 3 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 804****Bond lengths****Bond angles****Torsions****Rings**

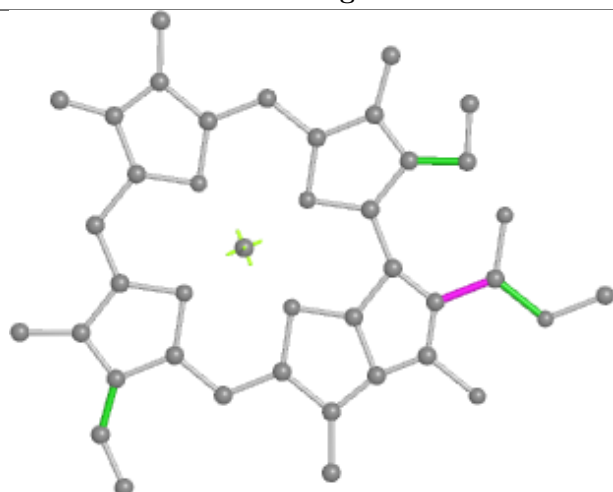
Ligand CLA 3 605



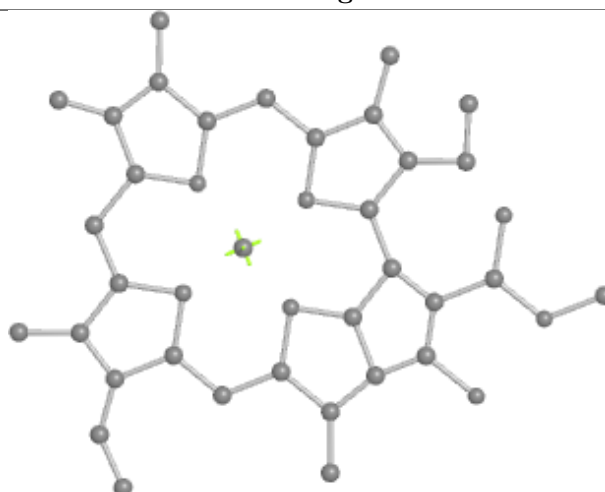
Bond lengths



Bond angles

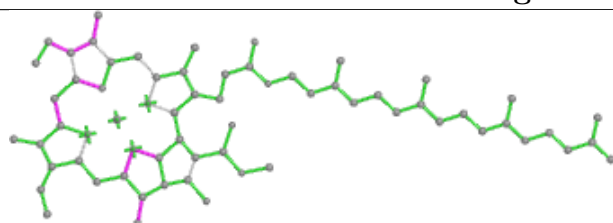


Torsions

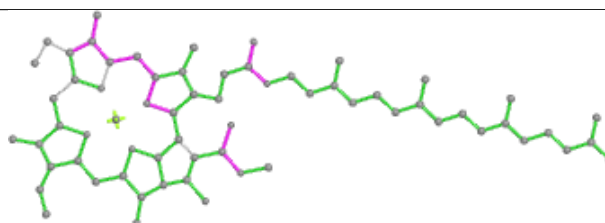


Rings

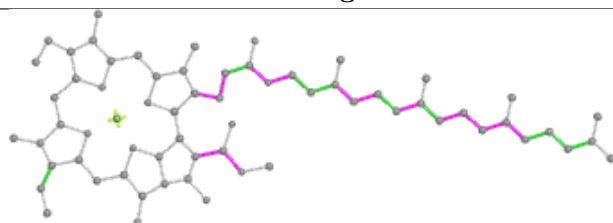
Ligand CLA A 803



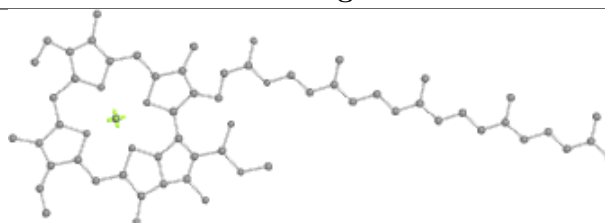
Bond lengths



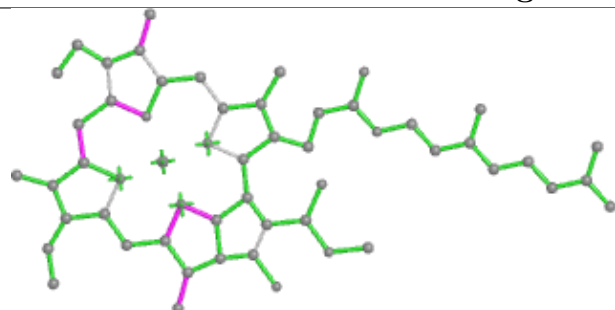
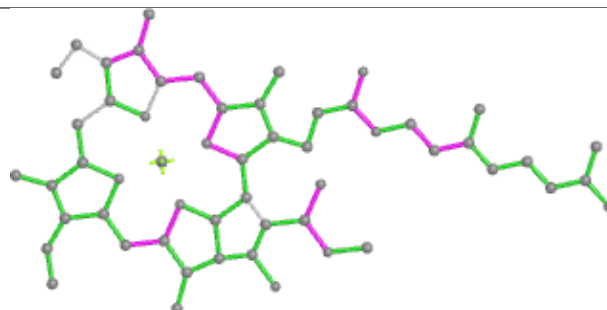
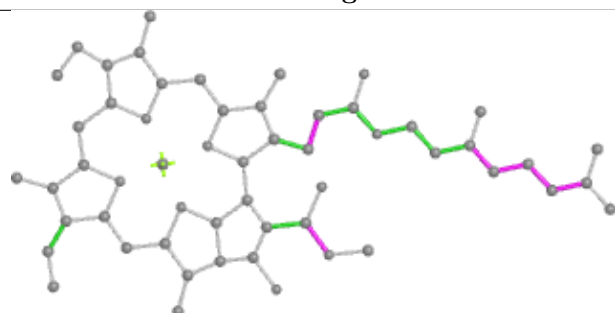
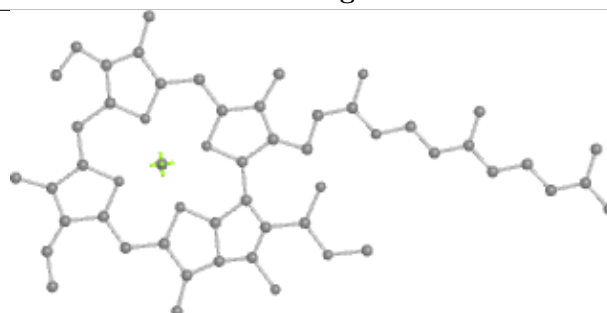
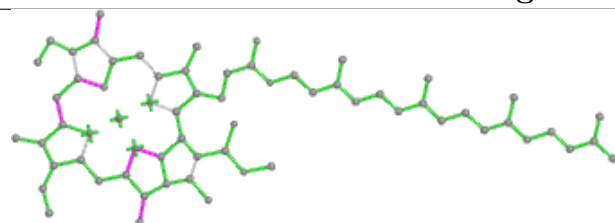
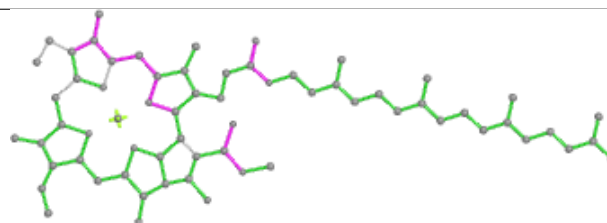
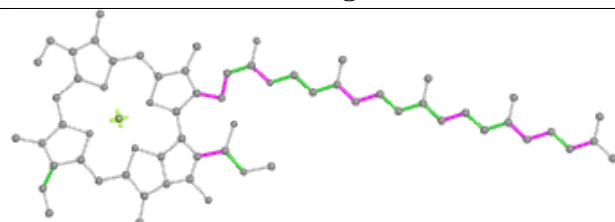
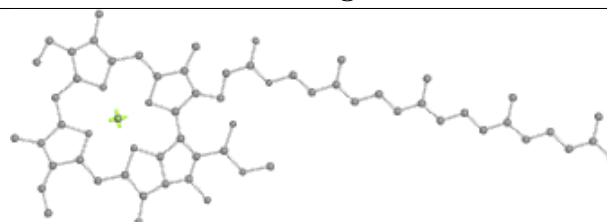
Bond angles



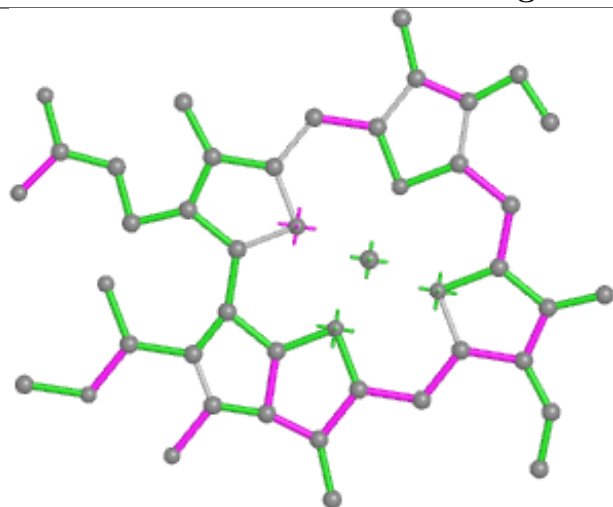
Torsions



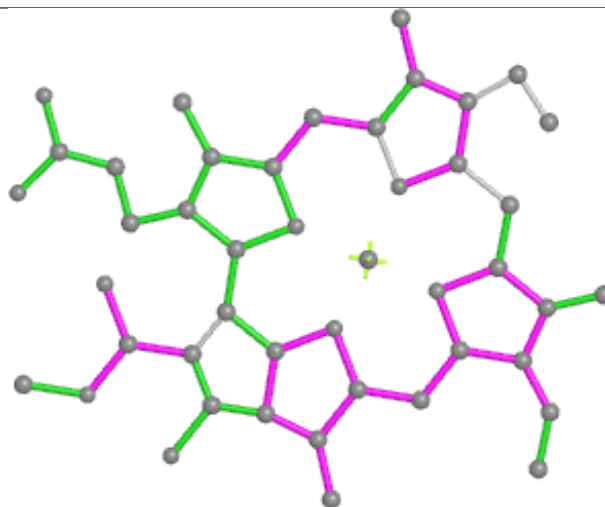
Rings

Ligand CLA B 816**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 824****Bond lengths****Bond angles****Torsions****Rings**

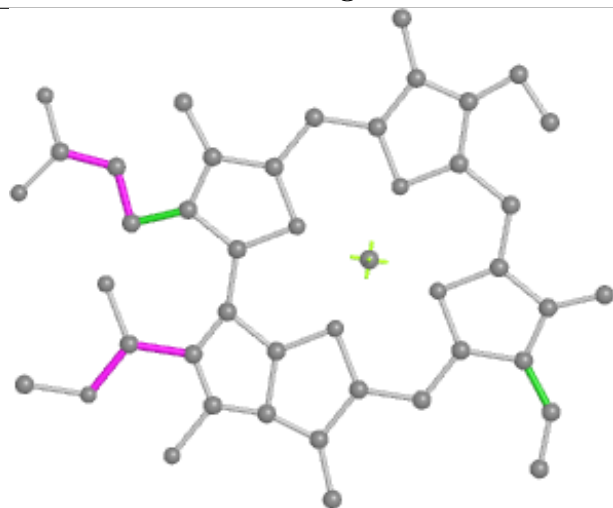
Ligand CHL 3 606



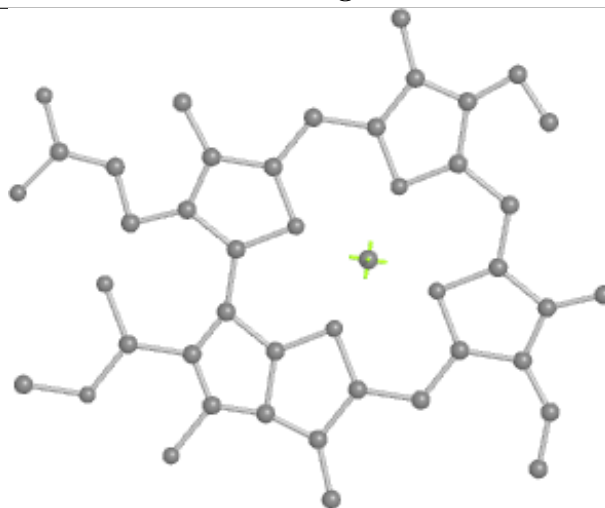
Bond lengths



Bond angles

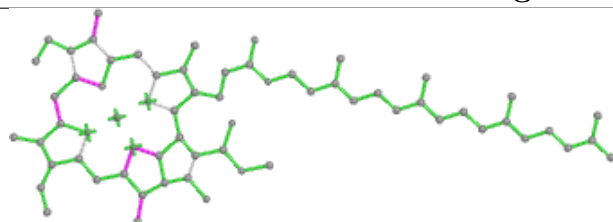


Torsions

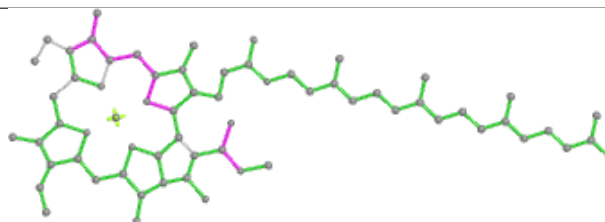


Rings

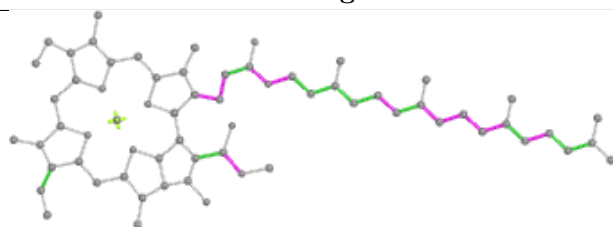
Ligand CLA A 820



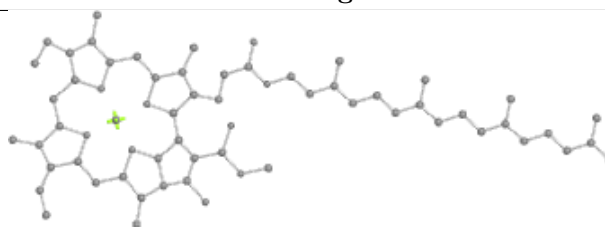
Bond lengths



Bond angles

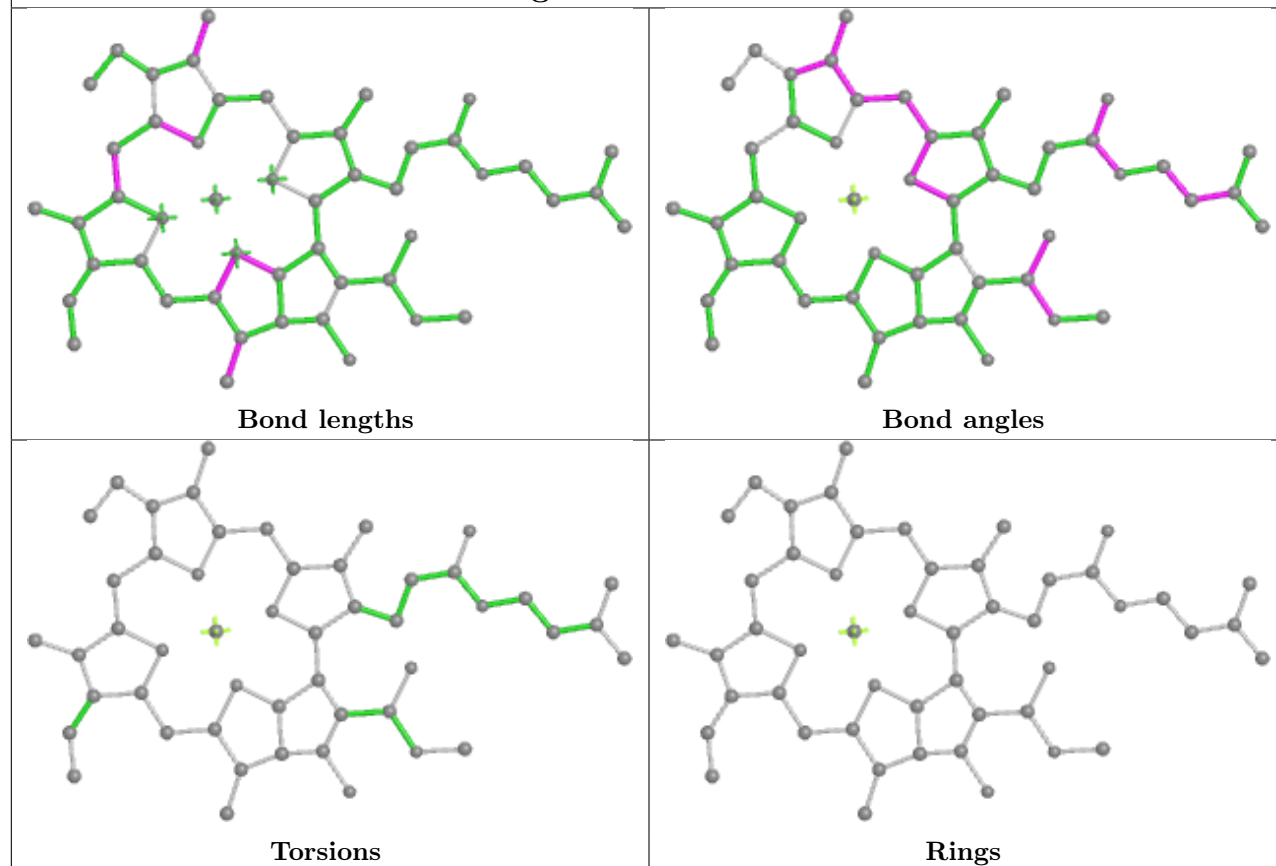


Torsions

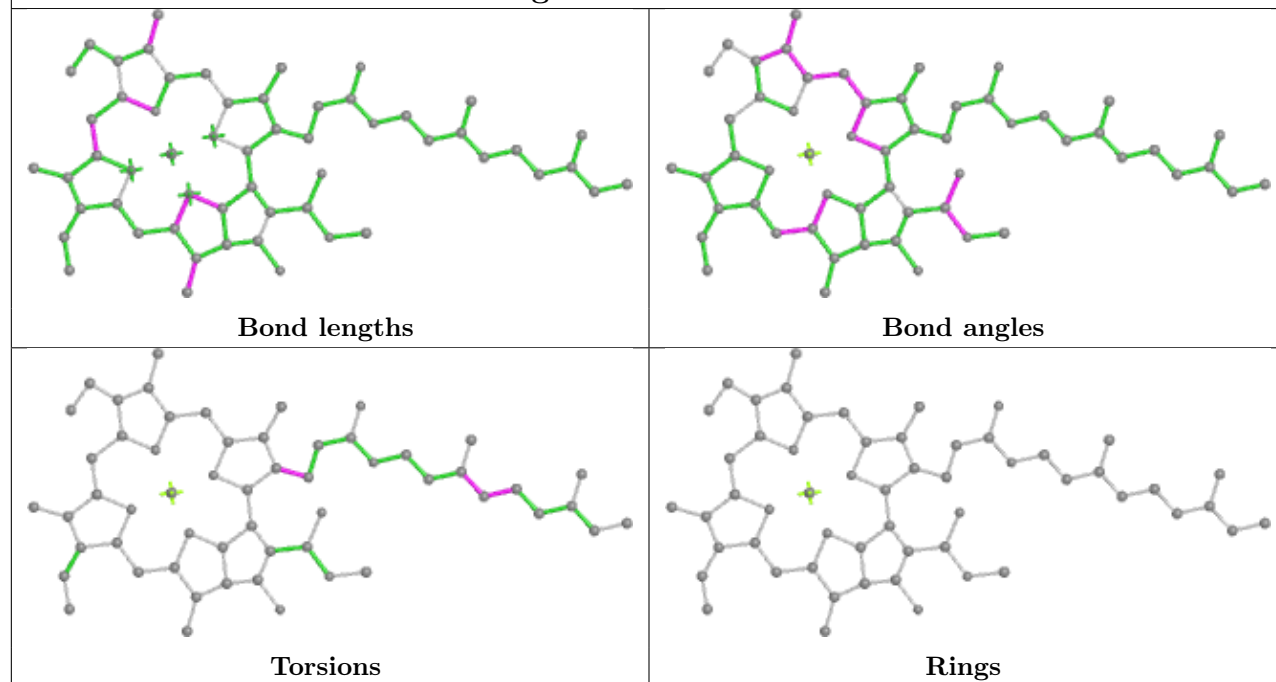


Rings

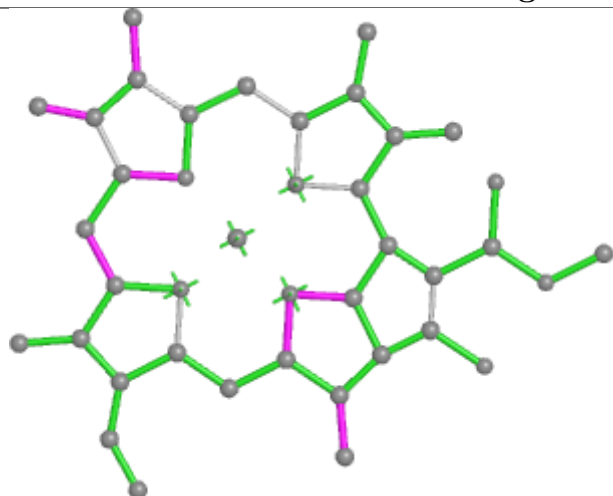
Ligand CLA A 808



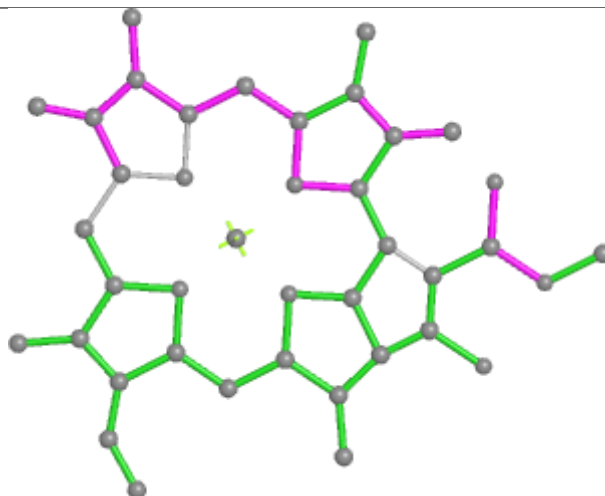
Ligand CLA A 833



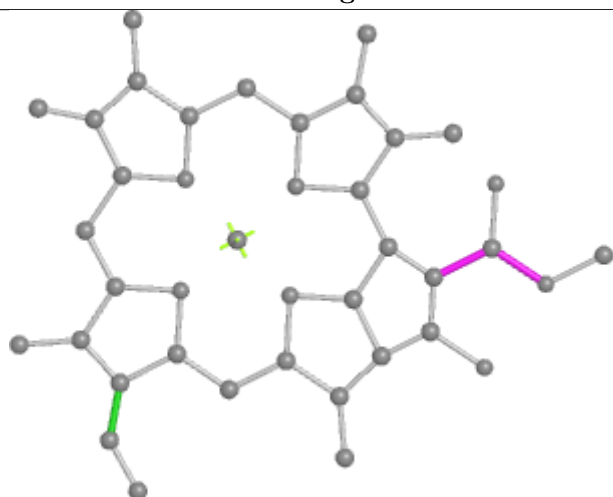
Ligand CLA 1 608



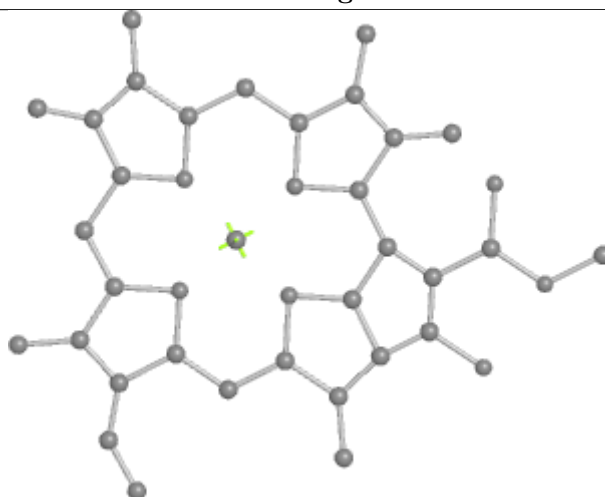
Bond lengths



Bond angles

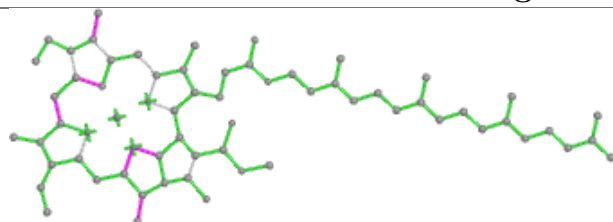


Torsions

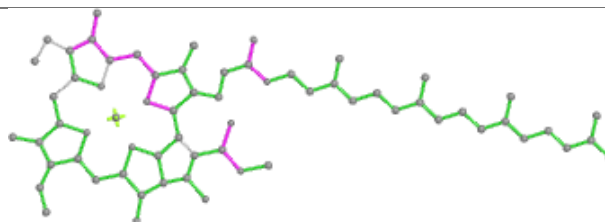


Rings

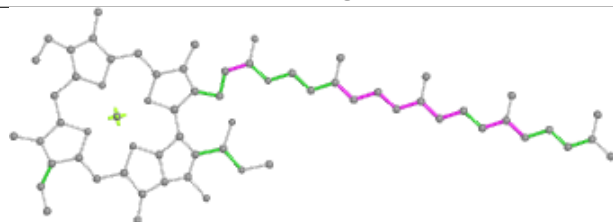
Ligand CLA B 806



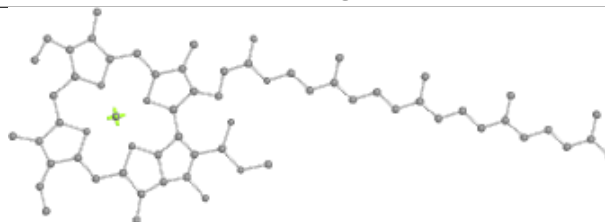
Bond lengths



Bond angles

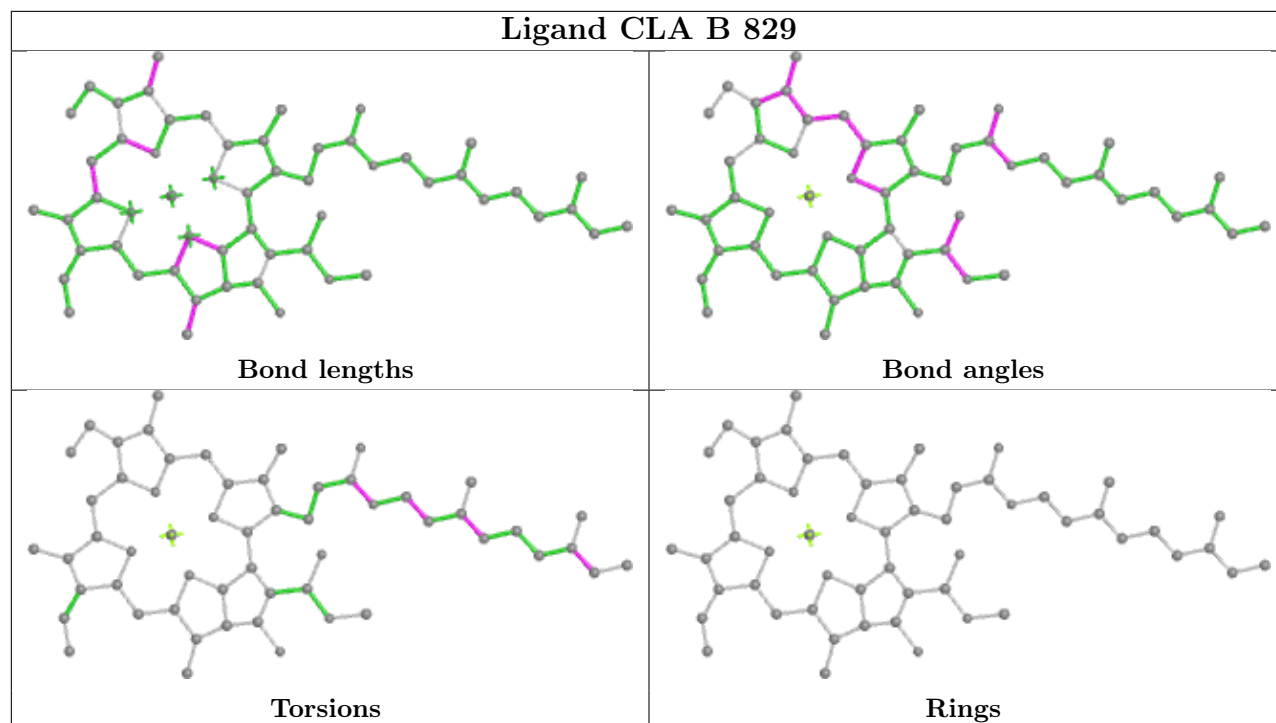


Torsions

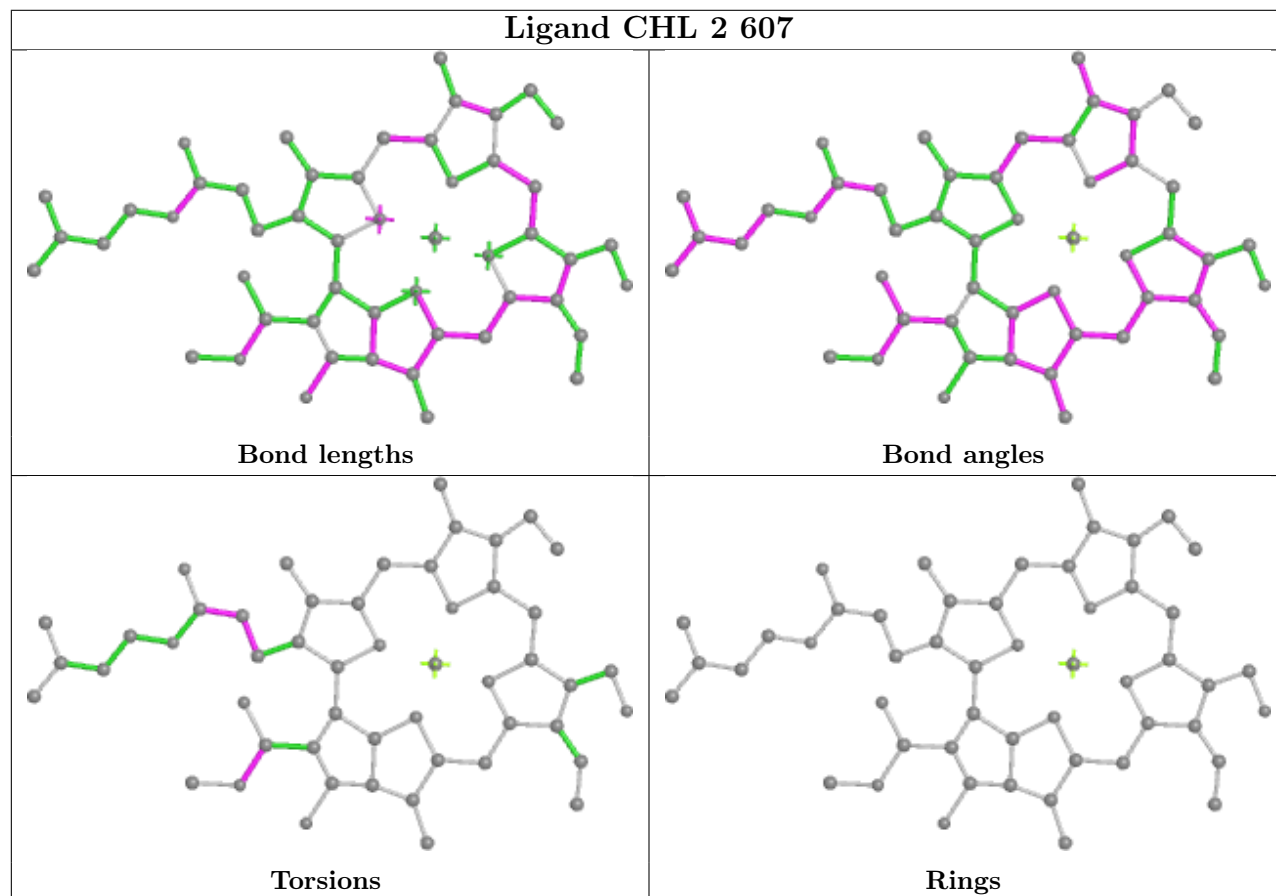


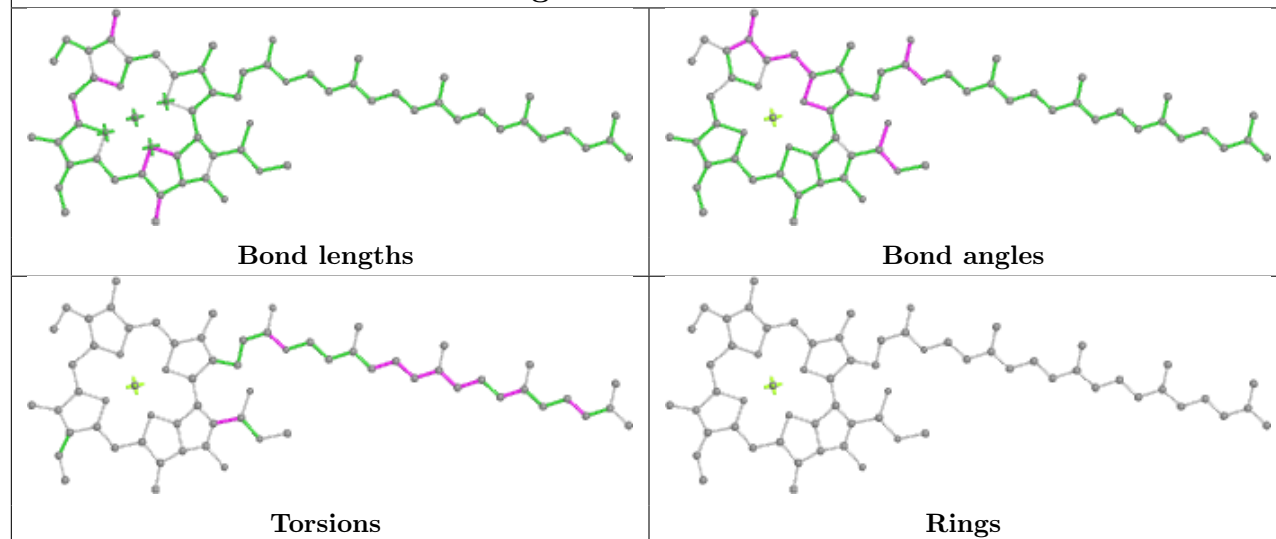
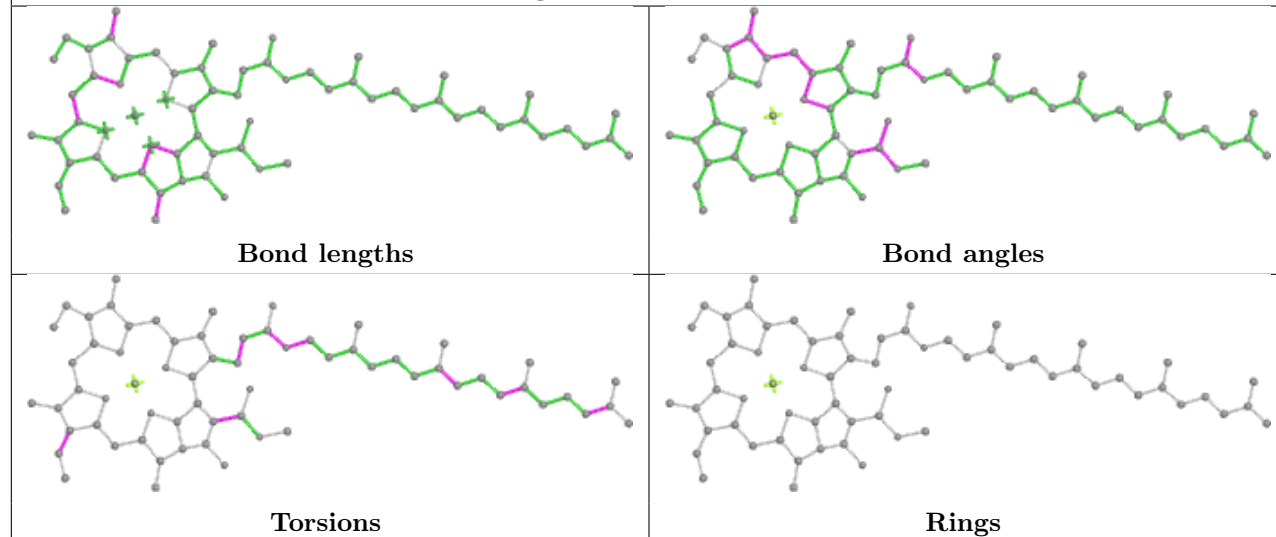
Rings

Ligand CLA B 829

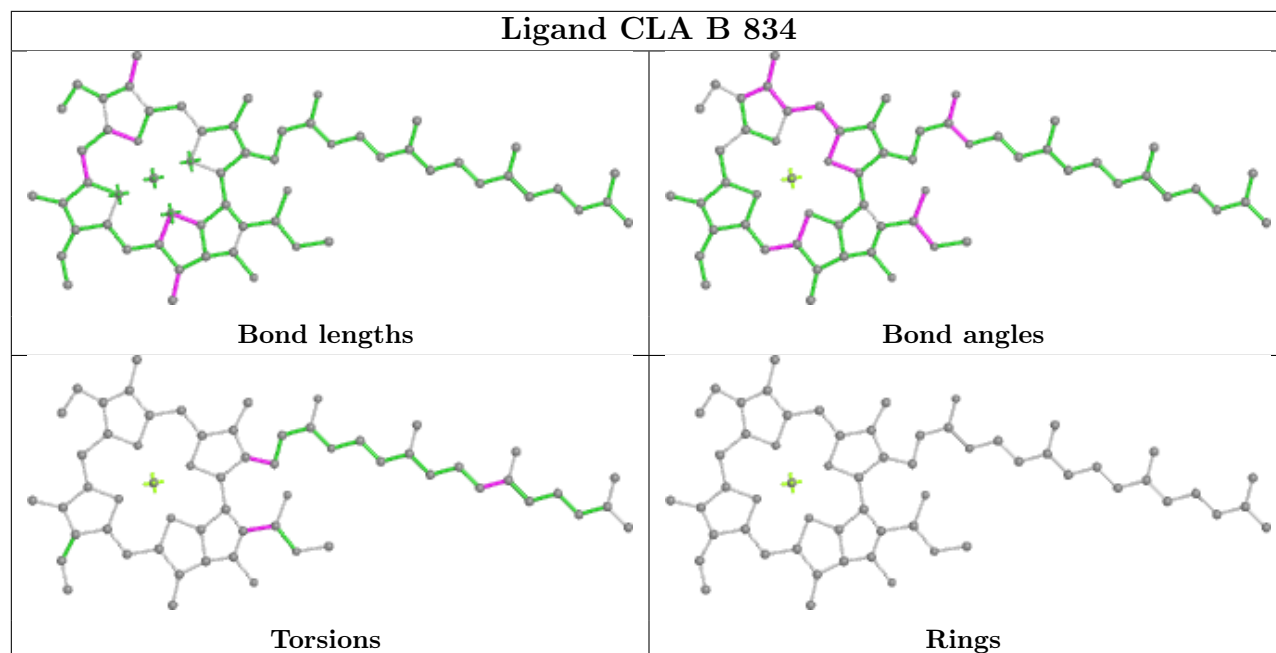


Ligand CHL 2 607

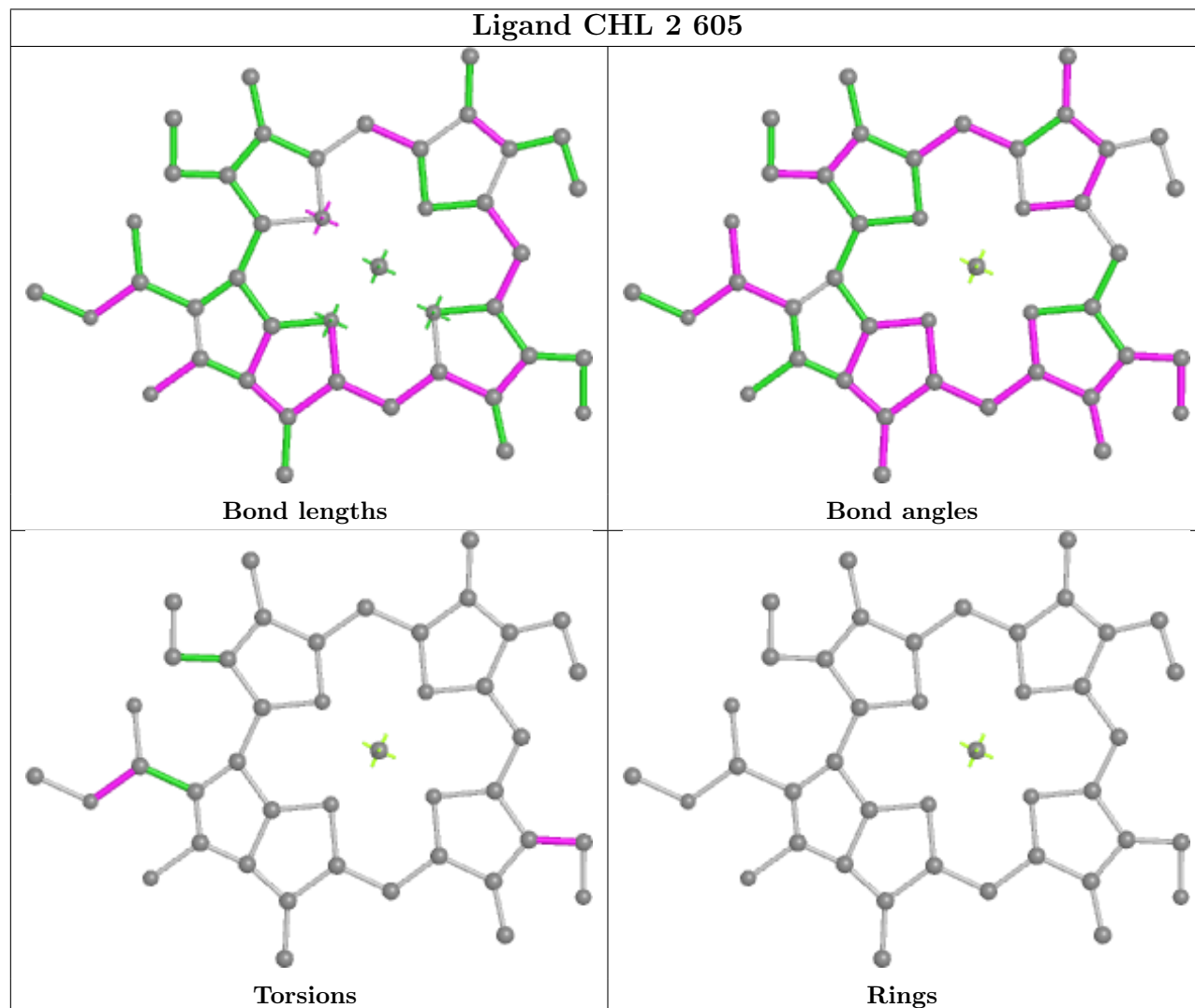


Ligand CLA A 826**Ligand CLA A 809**

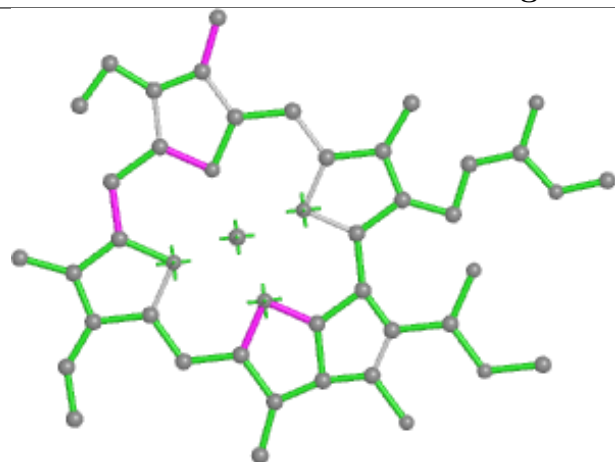
Ligand CLA B 834



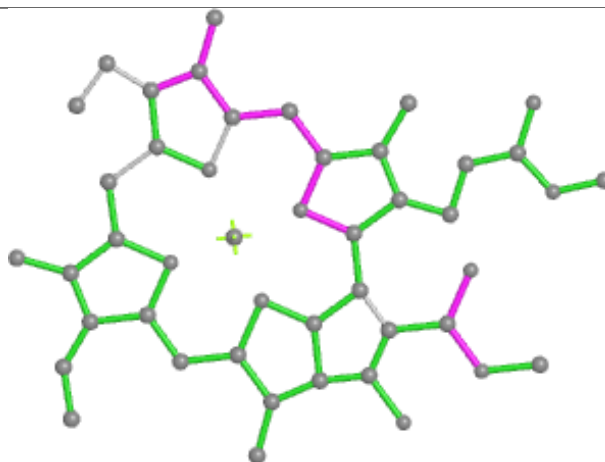
Ligand CHL 2 605



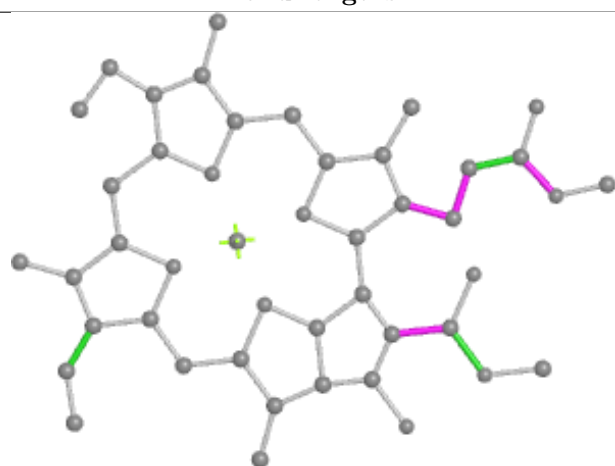
Ligand CLA 1 612



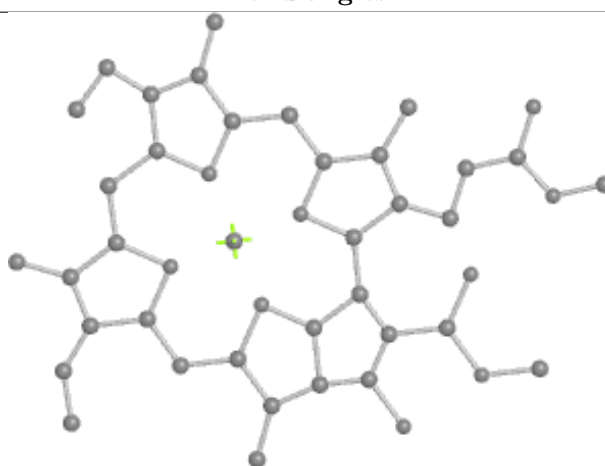
Bond lengths



Bond angles

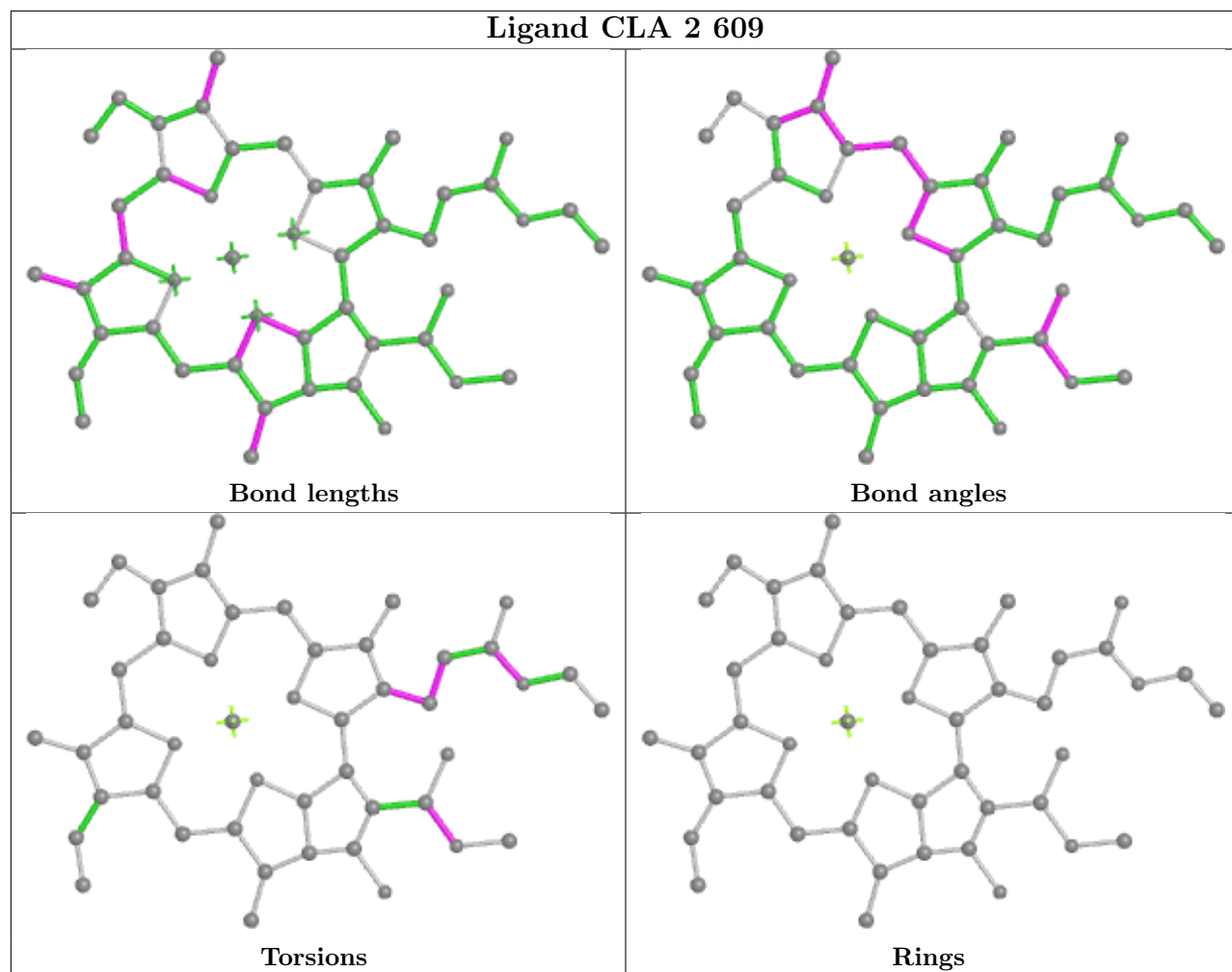


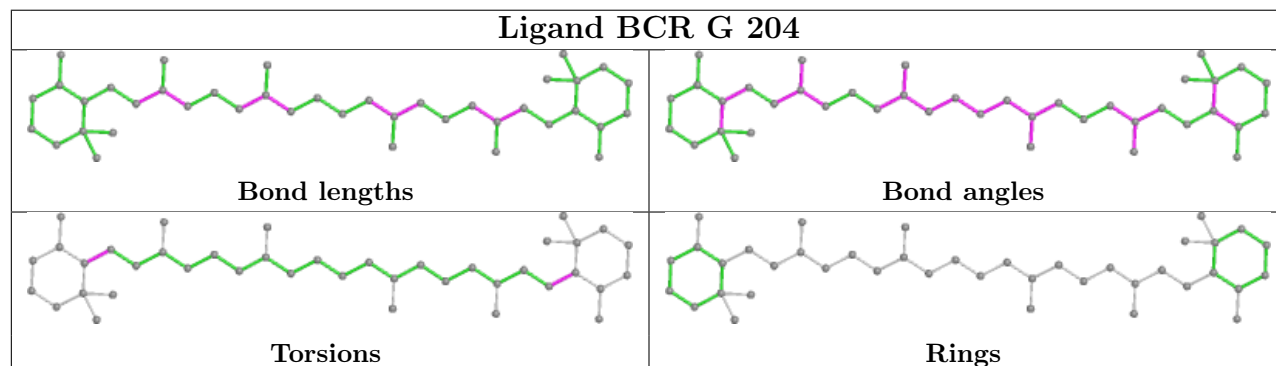
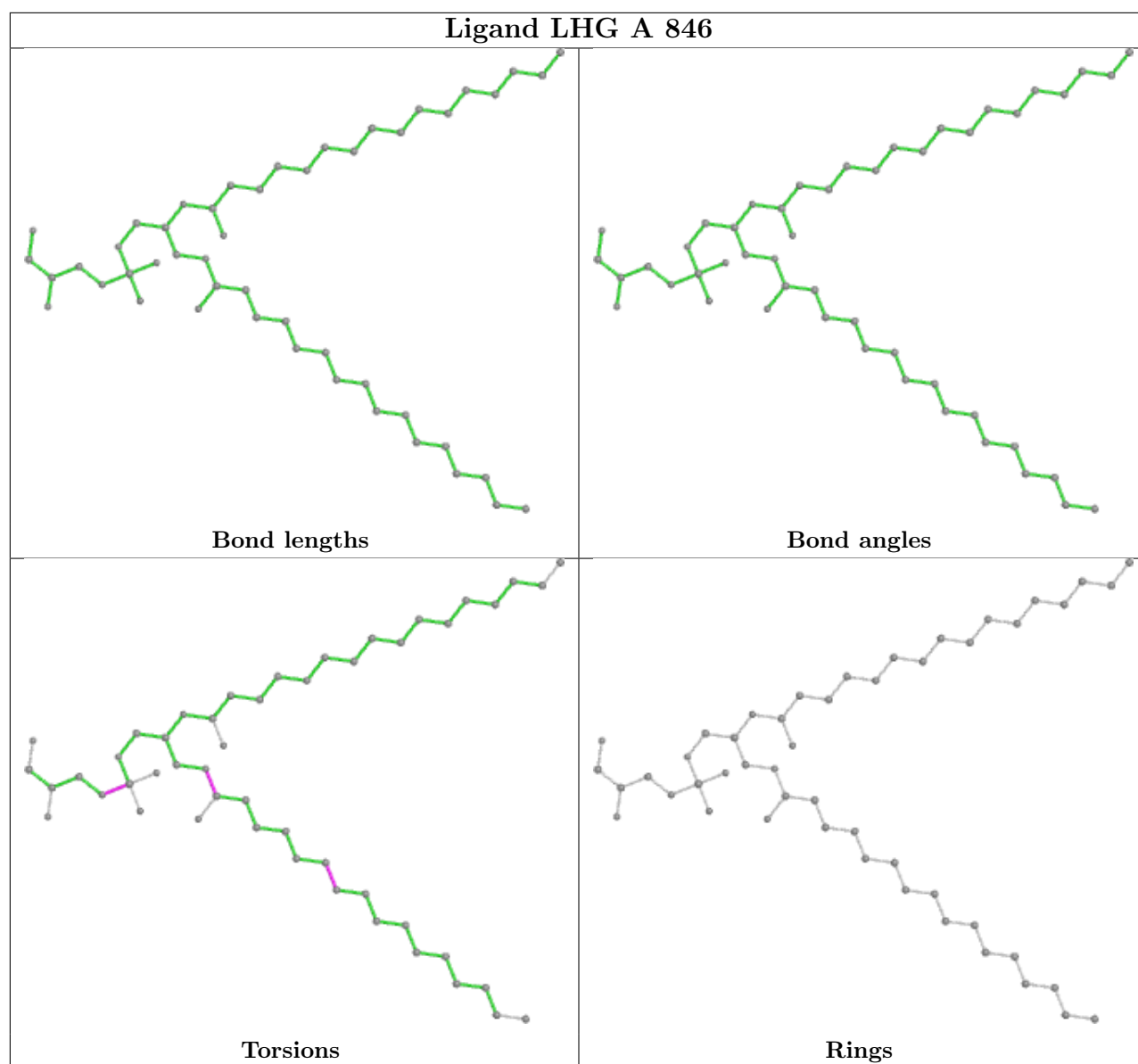
Torsions

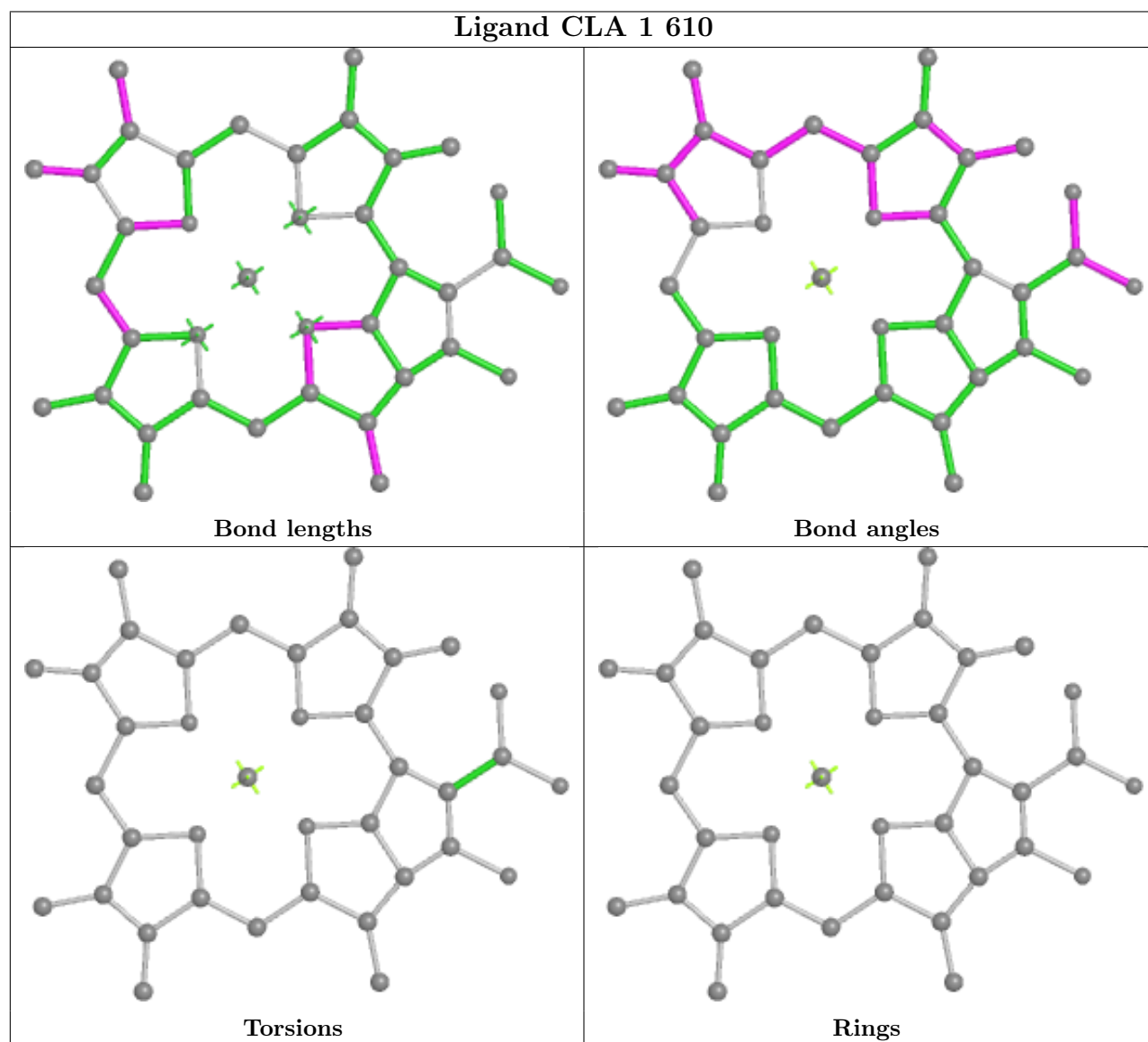
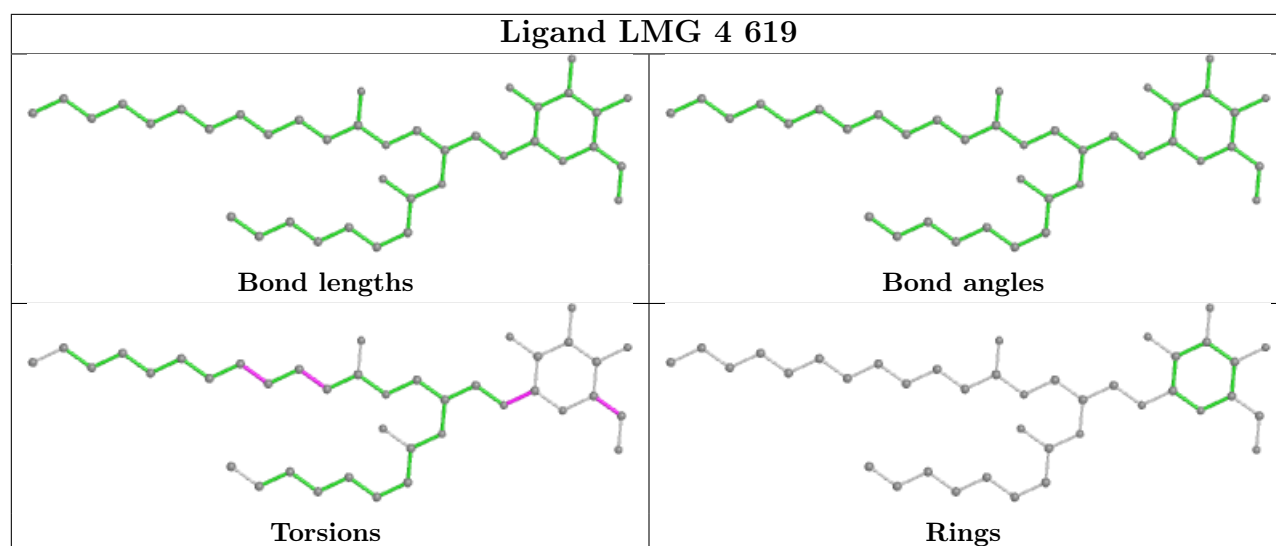


Rings

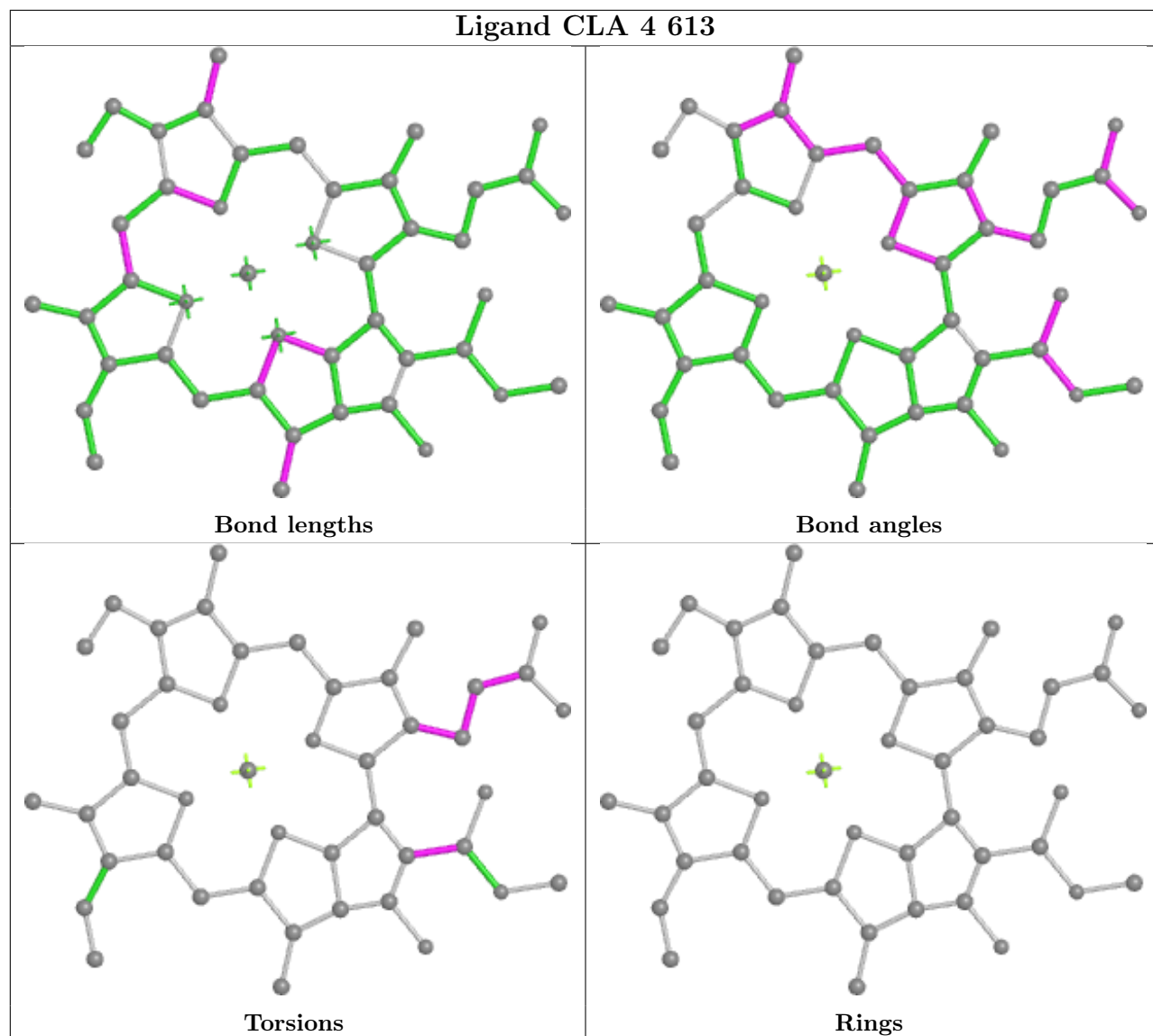
Ligand CLA 2 609



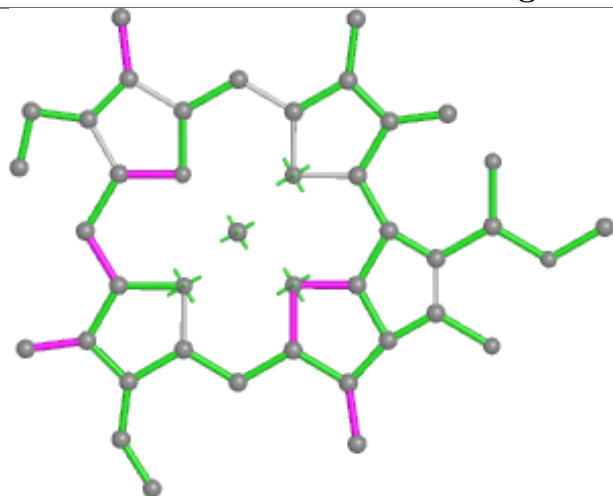




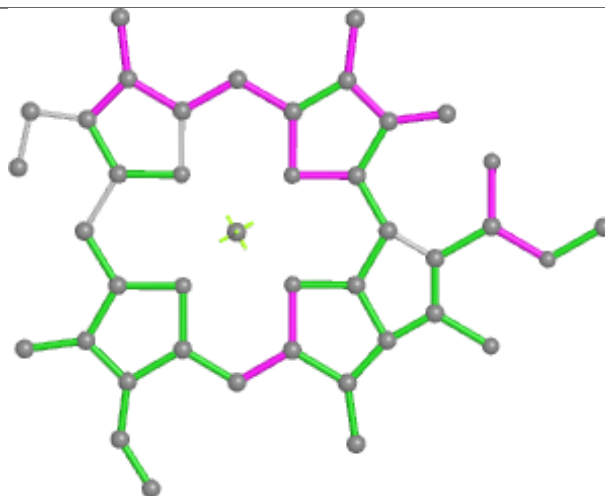
Ligand CLA 4 613



Ligand CLA 3 608



Bond lengths



Bond angles

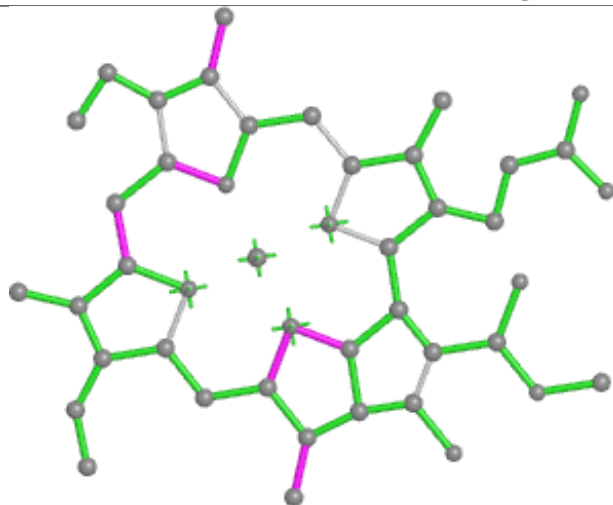


Torsions

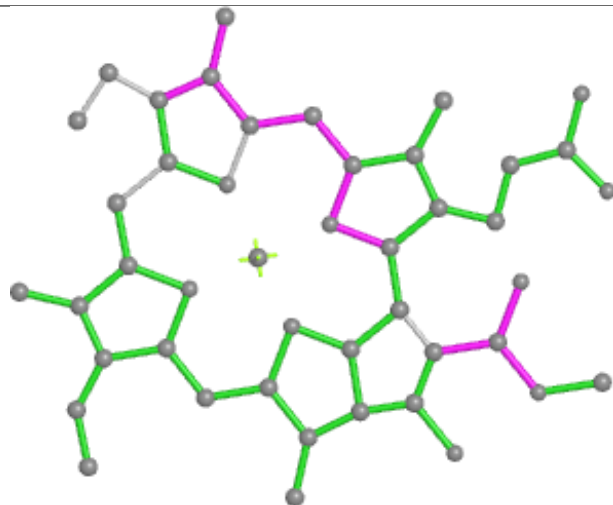


Rings

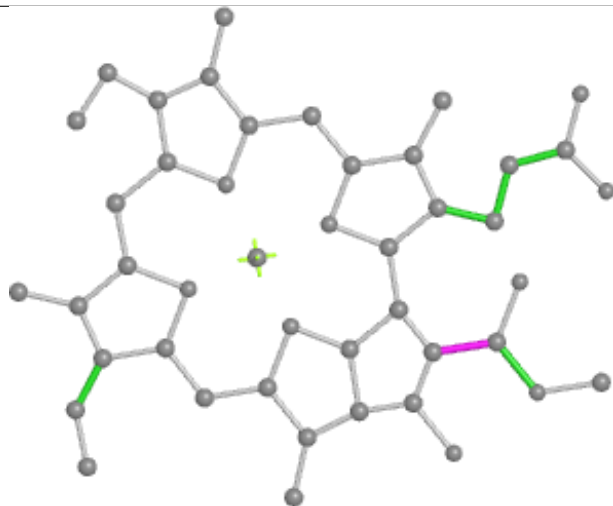
Ligand CLA L 302



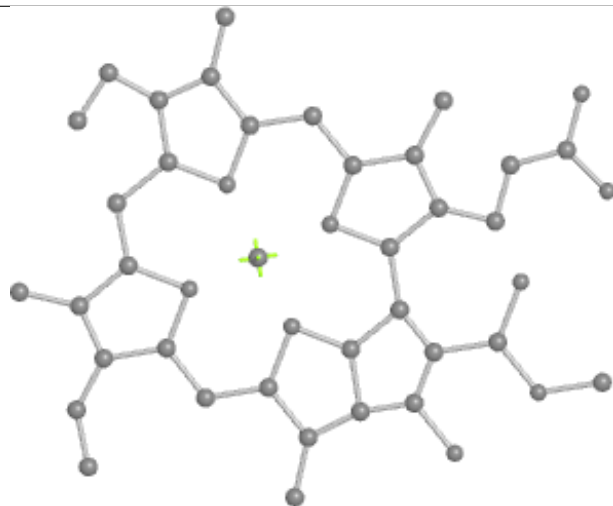
Bond lengths



Bond angles

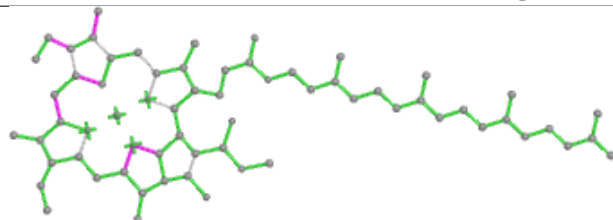


Torsions

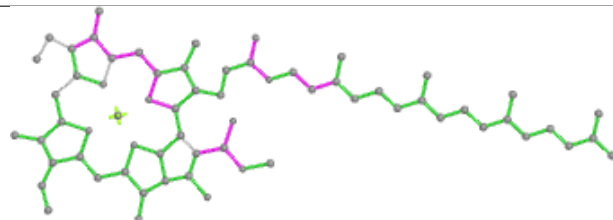


Rings

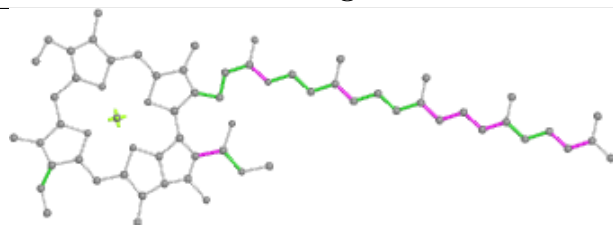
Ligand CLA A 835



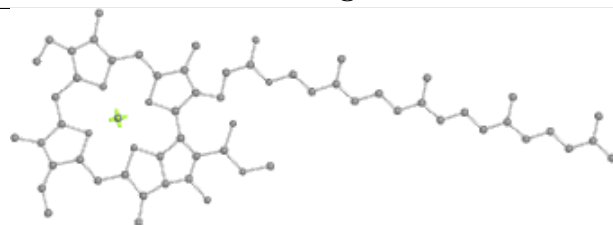
Bond lengths



Bond angles

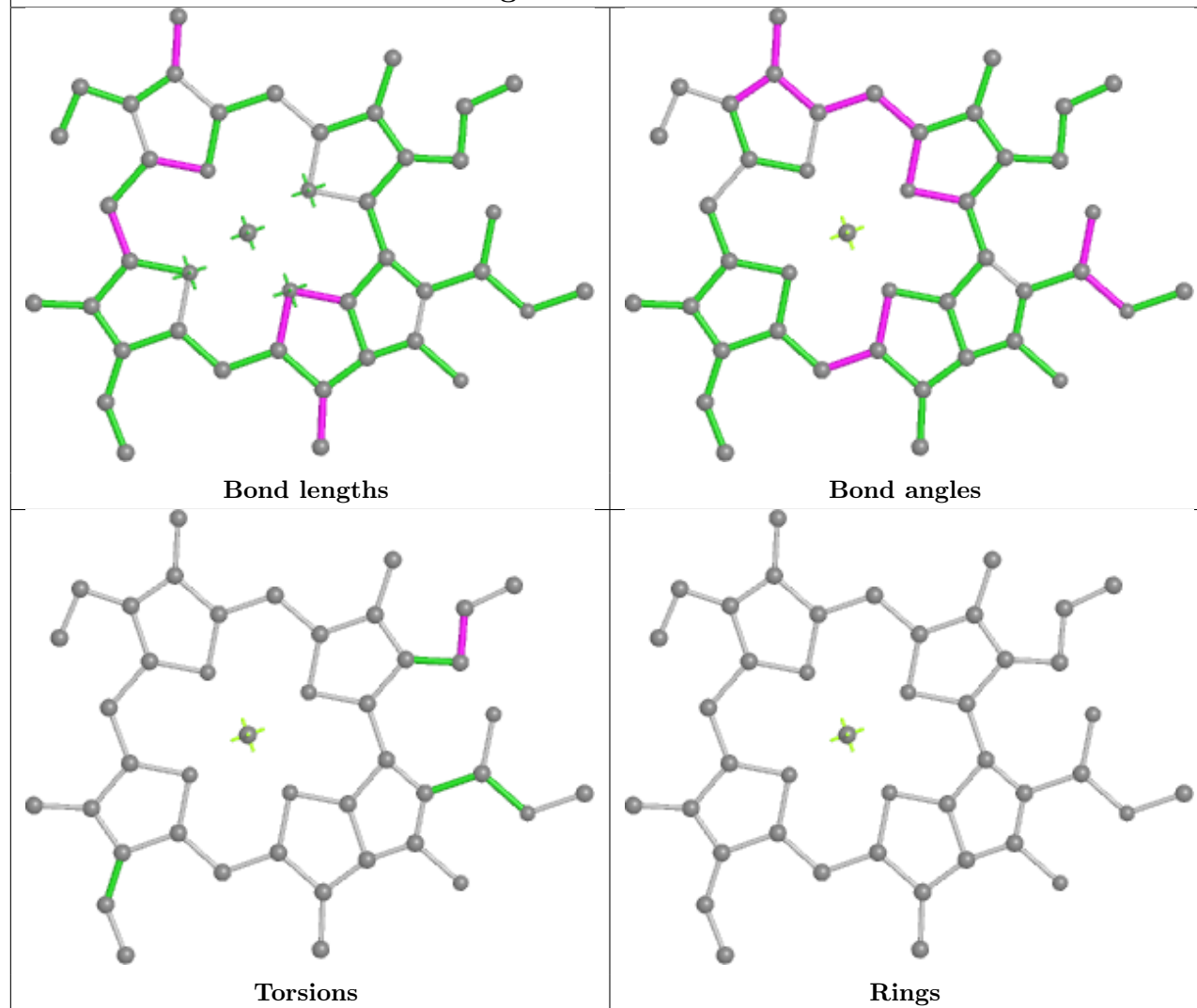


Torsions

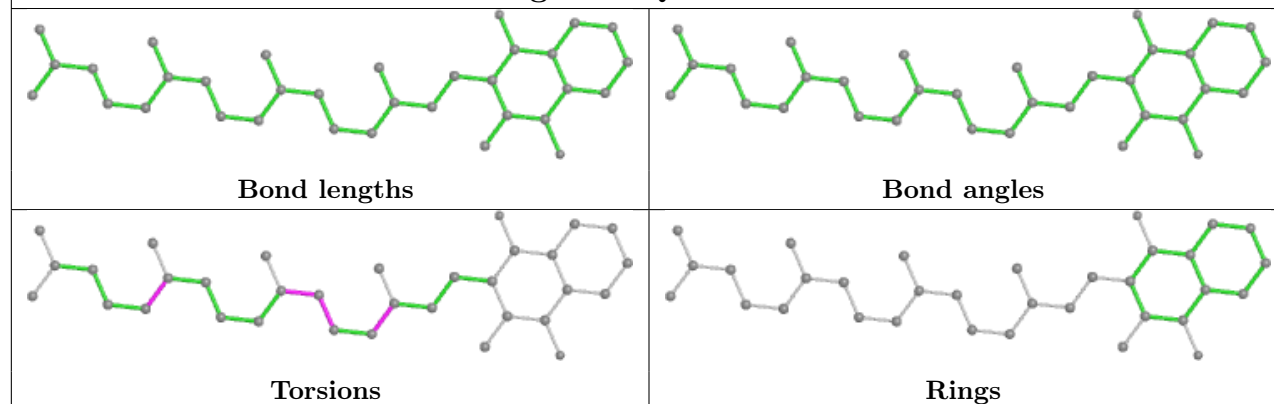


Rings

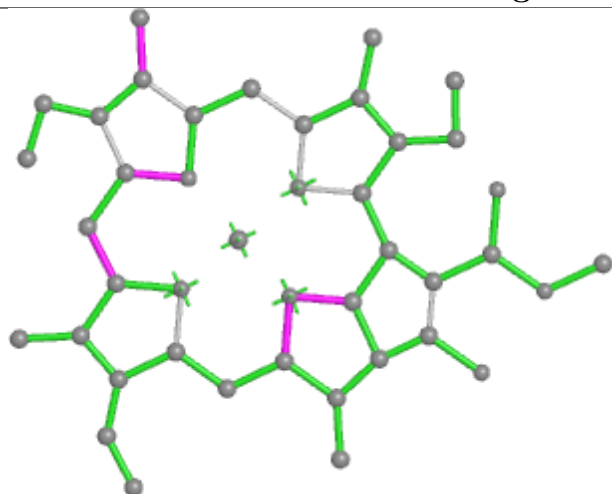
Ligand CLA B 831



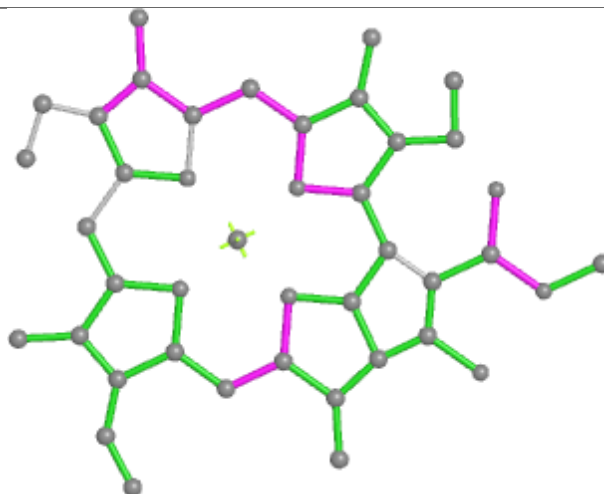
Ligand PQN B 842



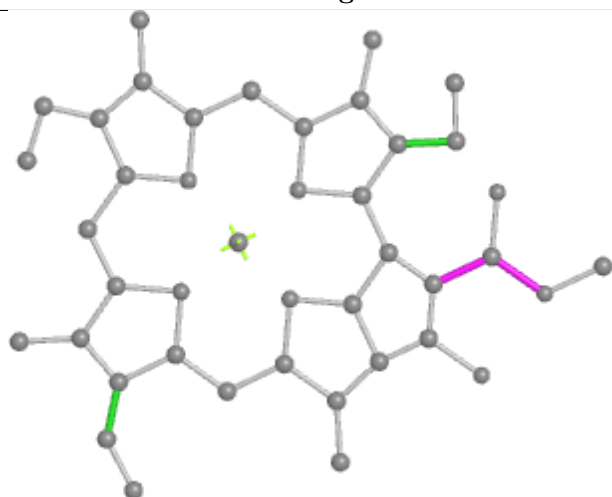
Ligand CLA A 823



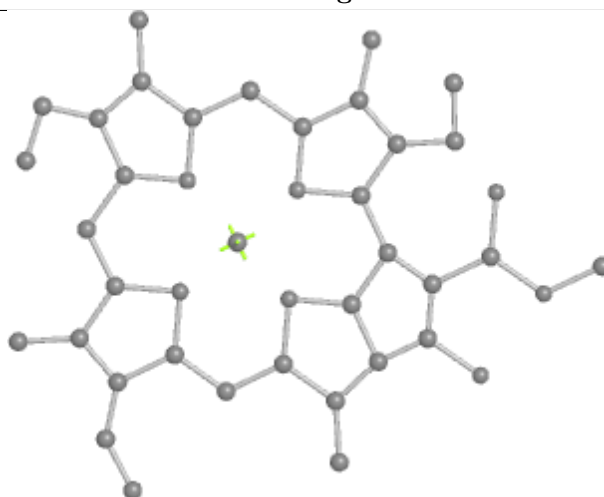
Bond lengths



Bond angles

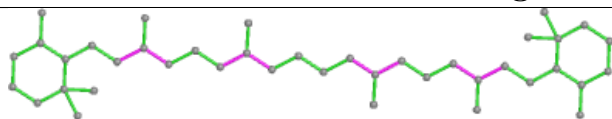


Torsions

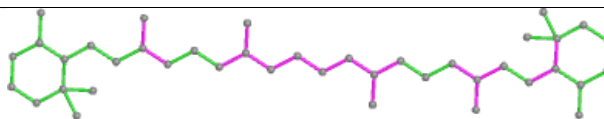


Rings

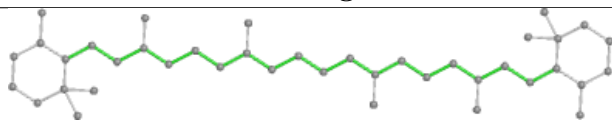
Ligand BCR B 848



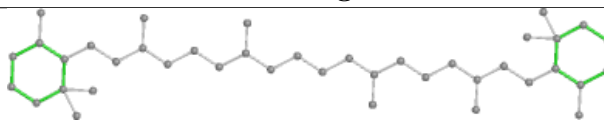
Bond lengths



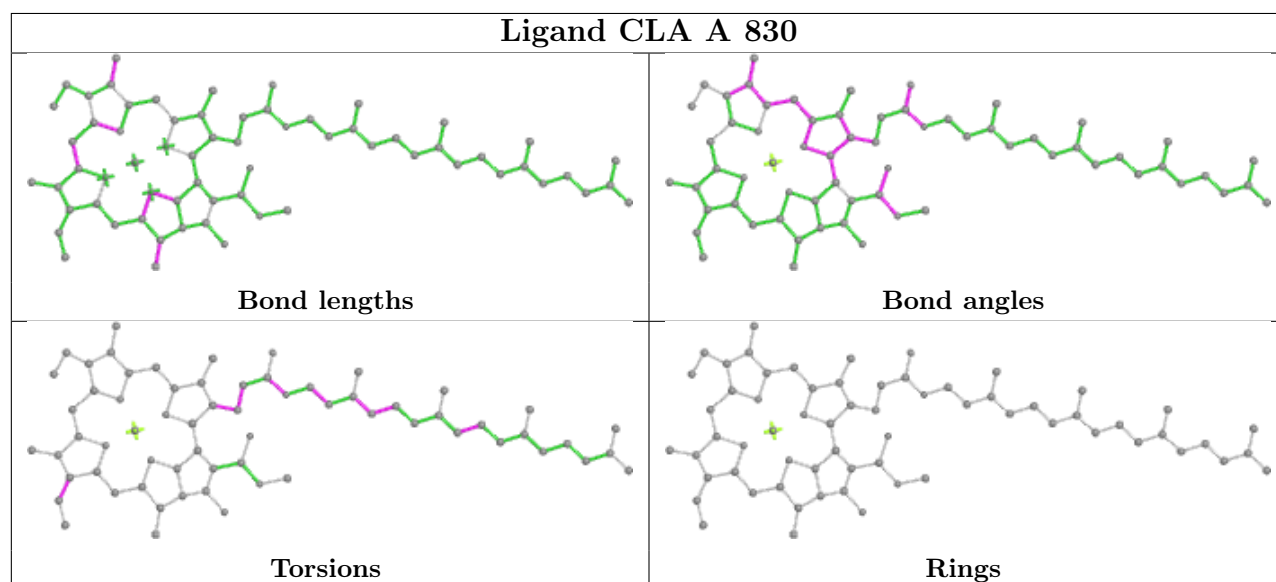
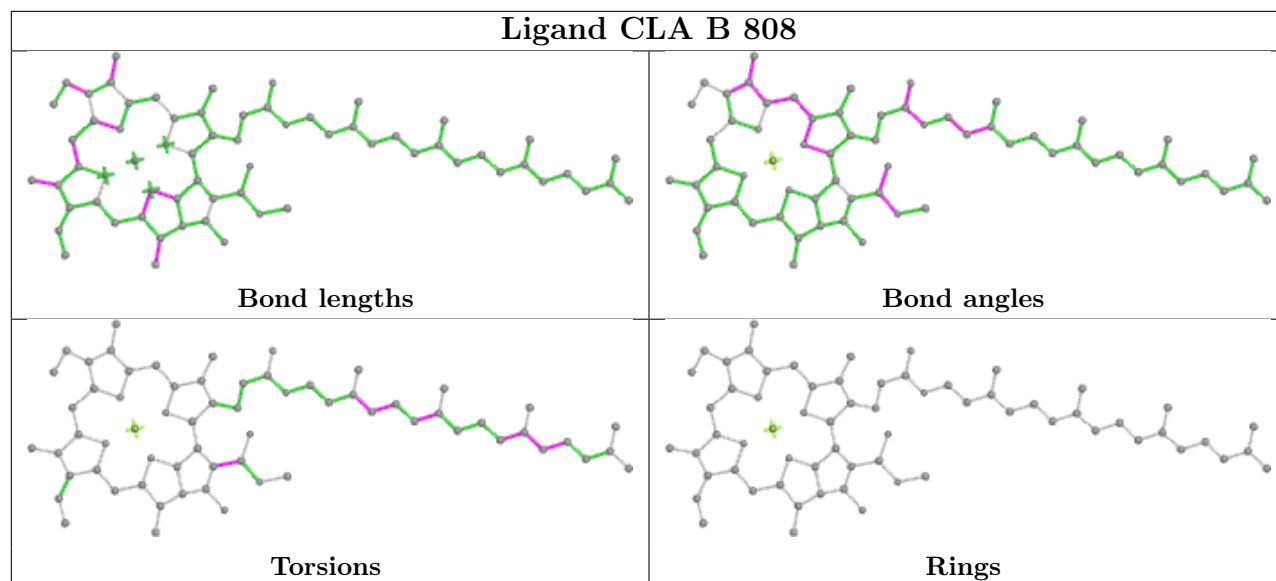
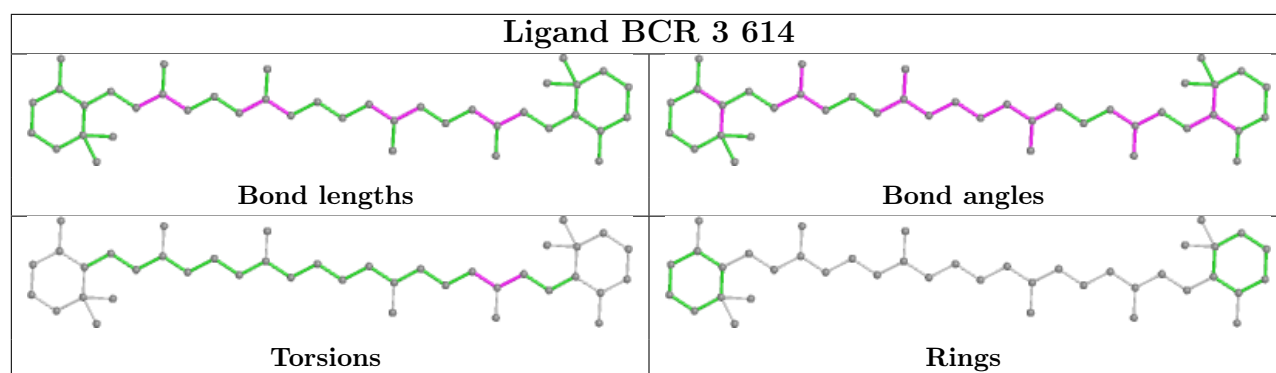
Bond angles



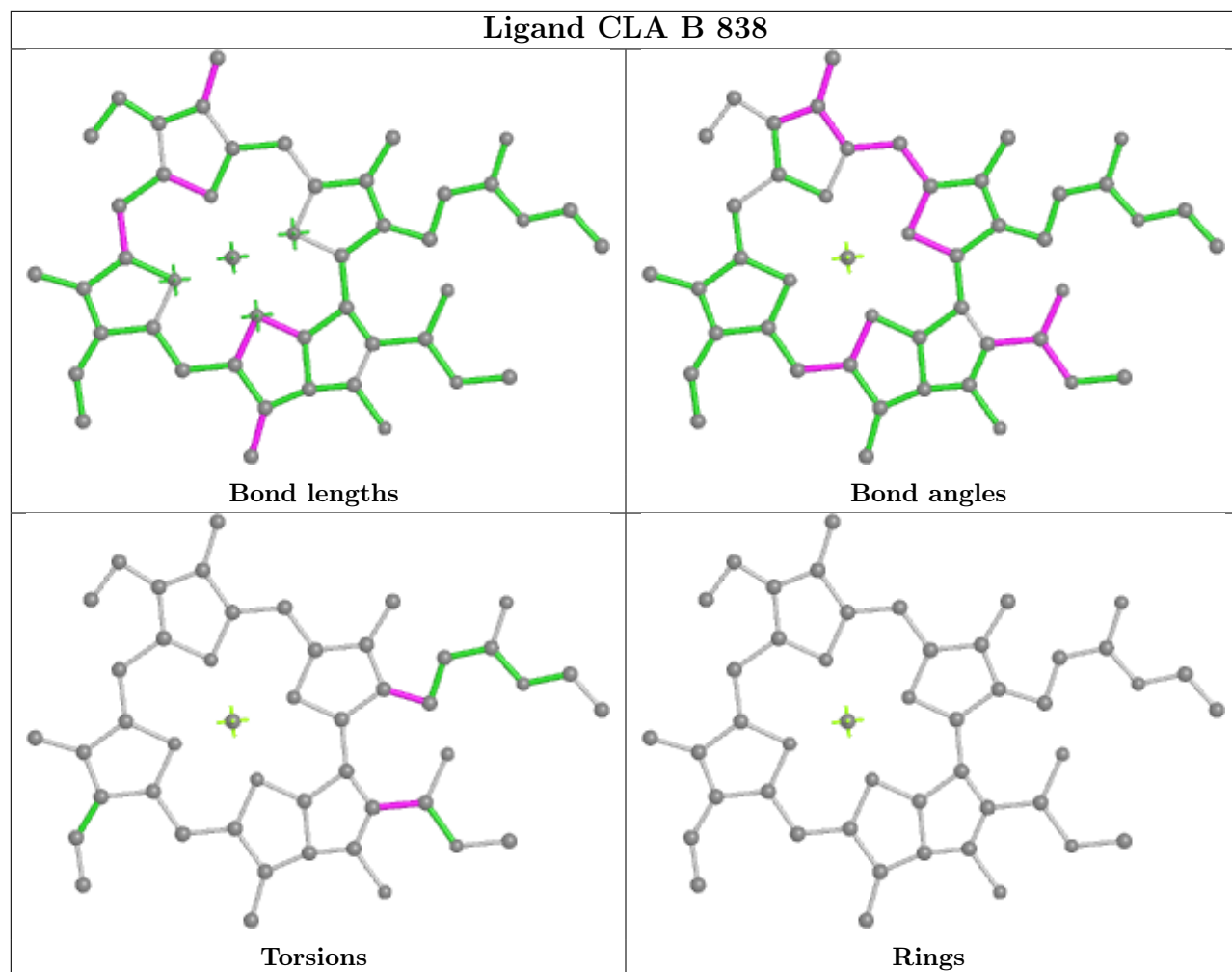
Torsions



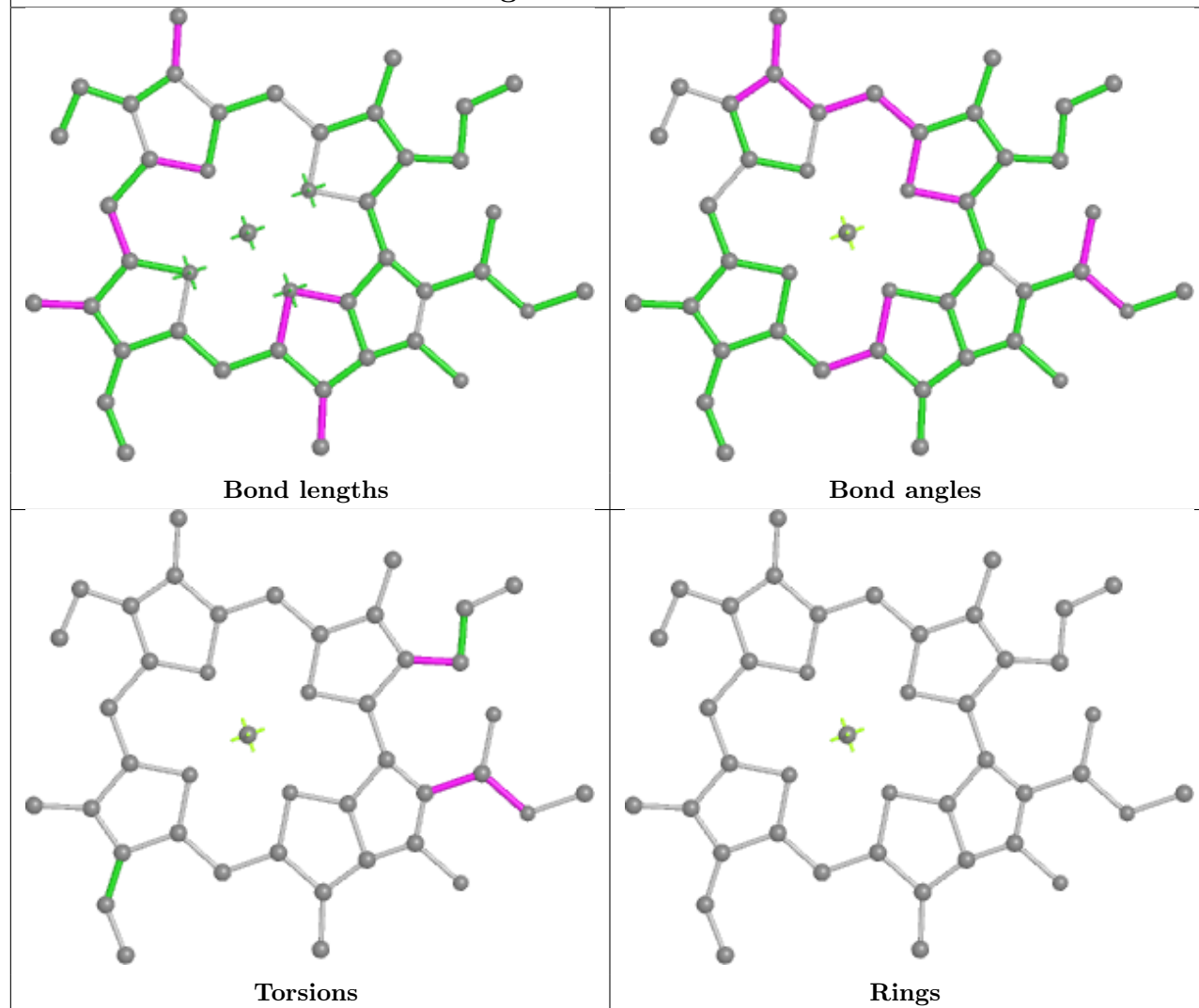
Rings



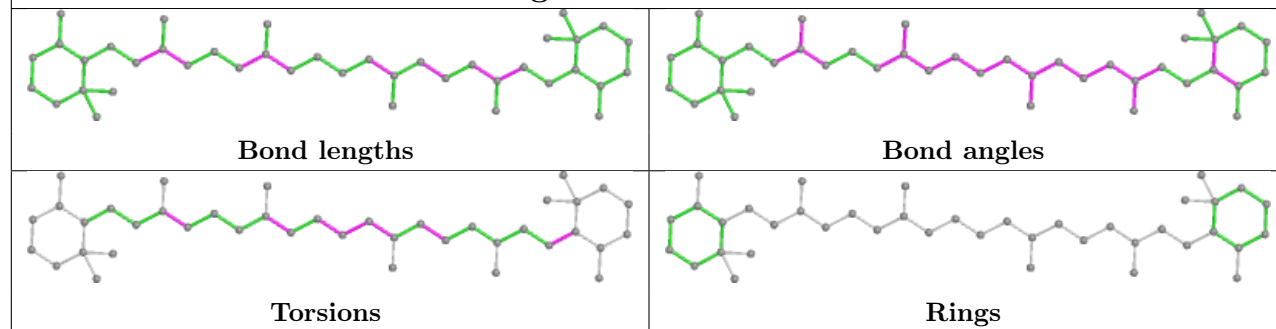
Ligand CLA B 838

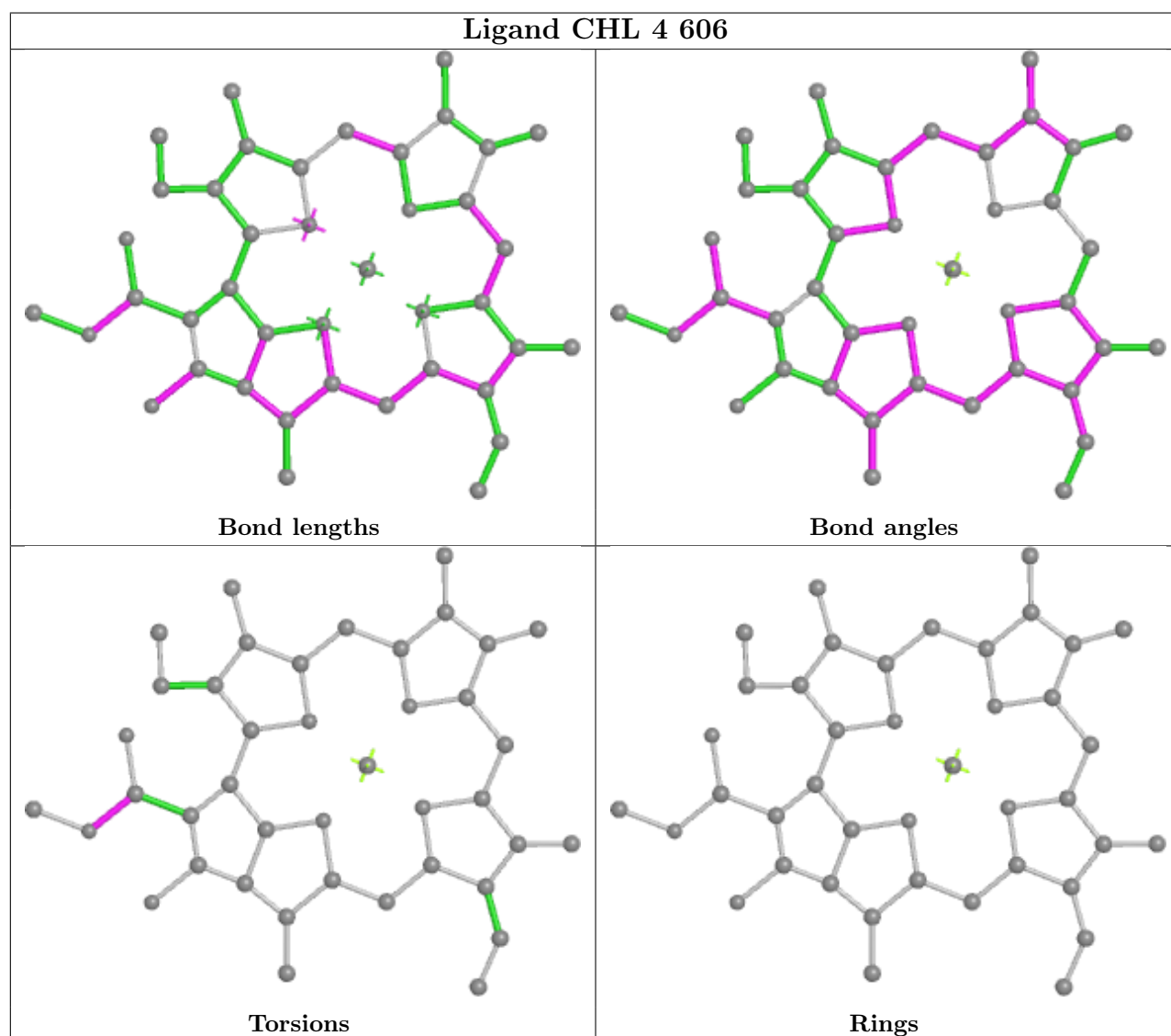
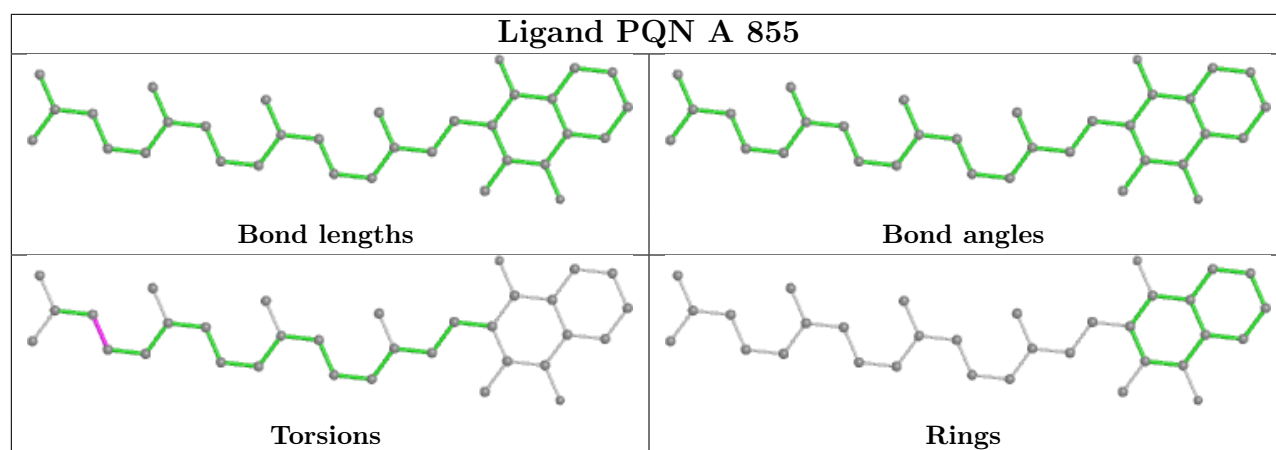


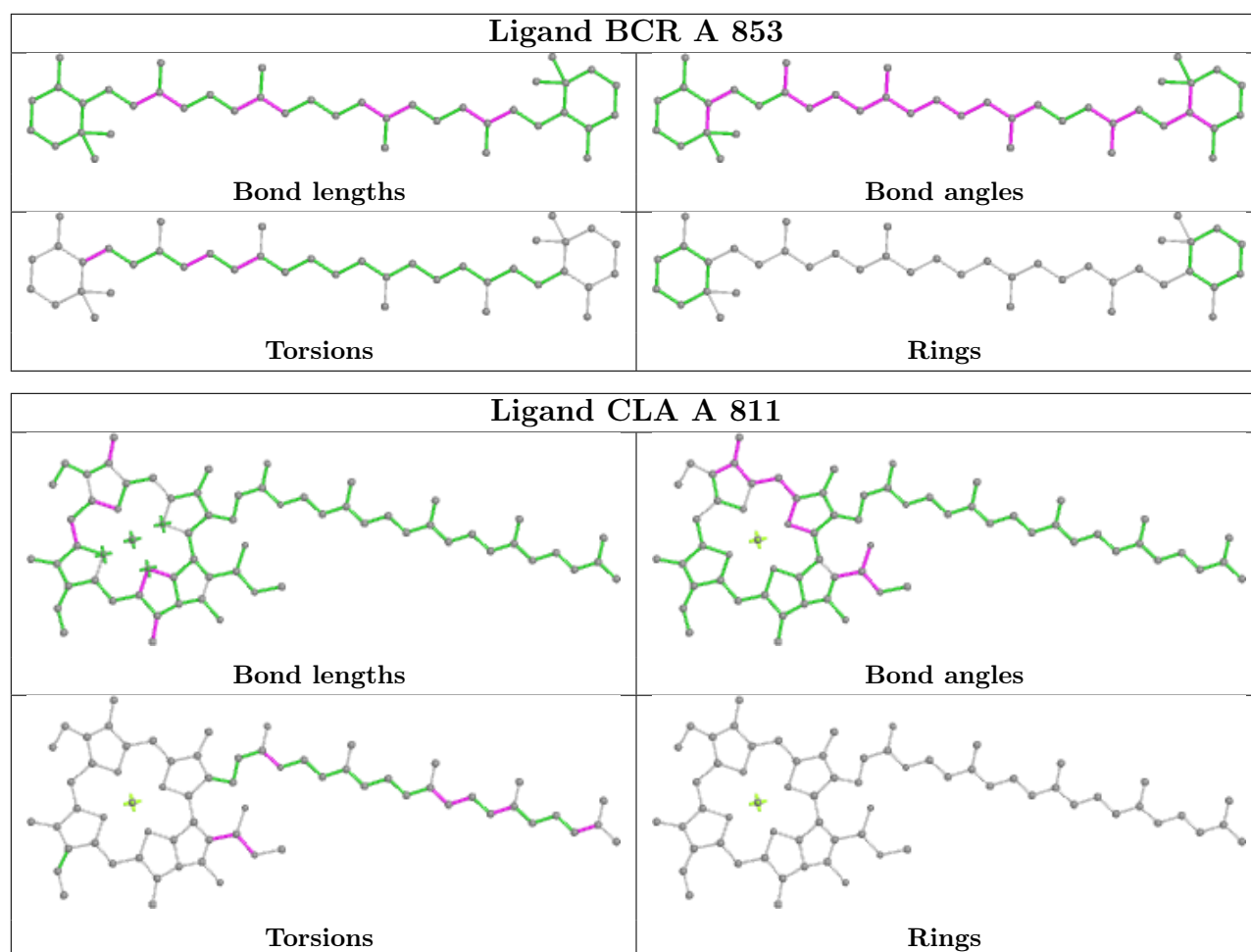
Ligand CLA B 815



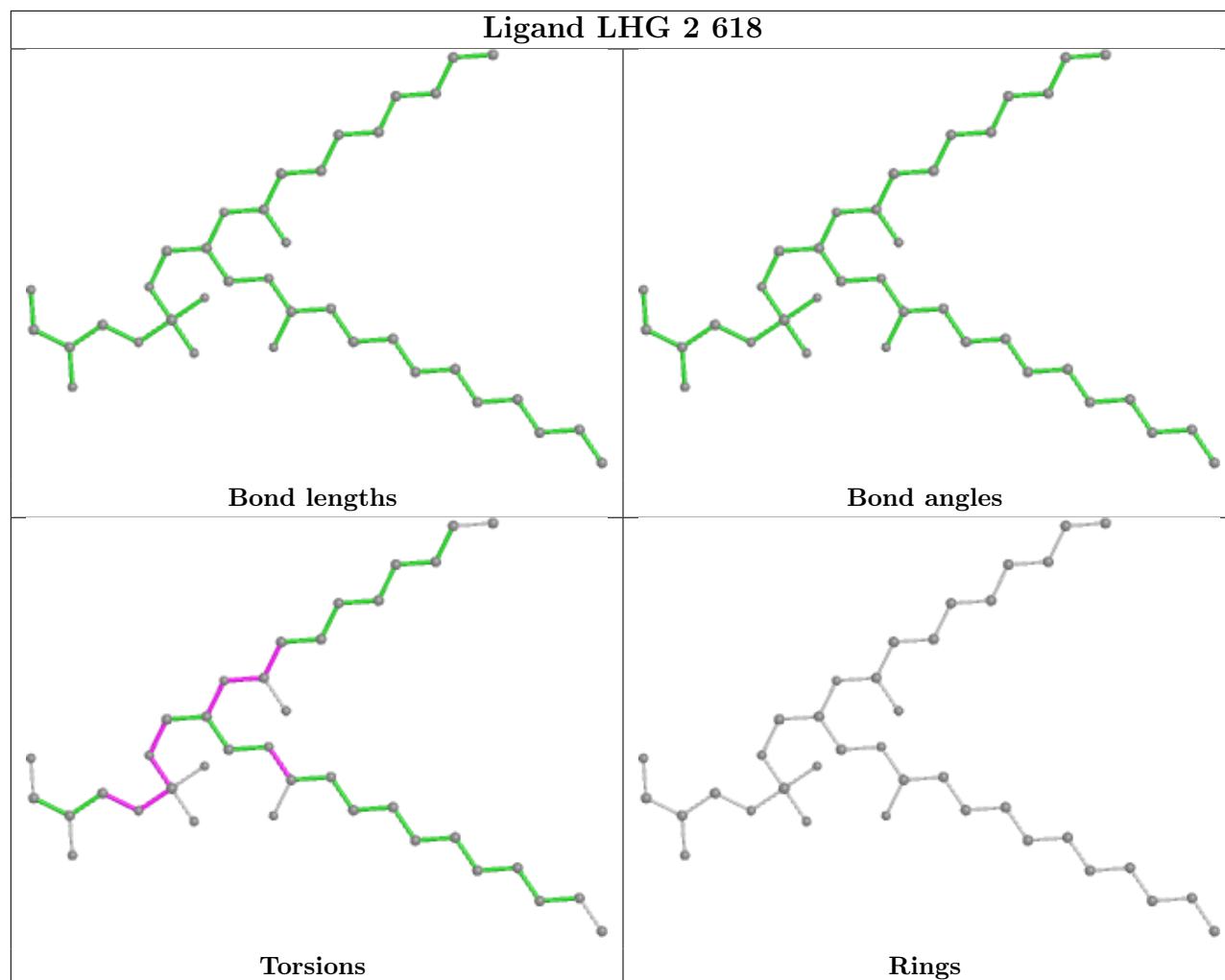
Ligand BCR B 844



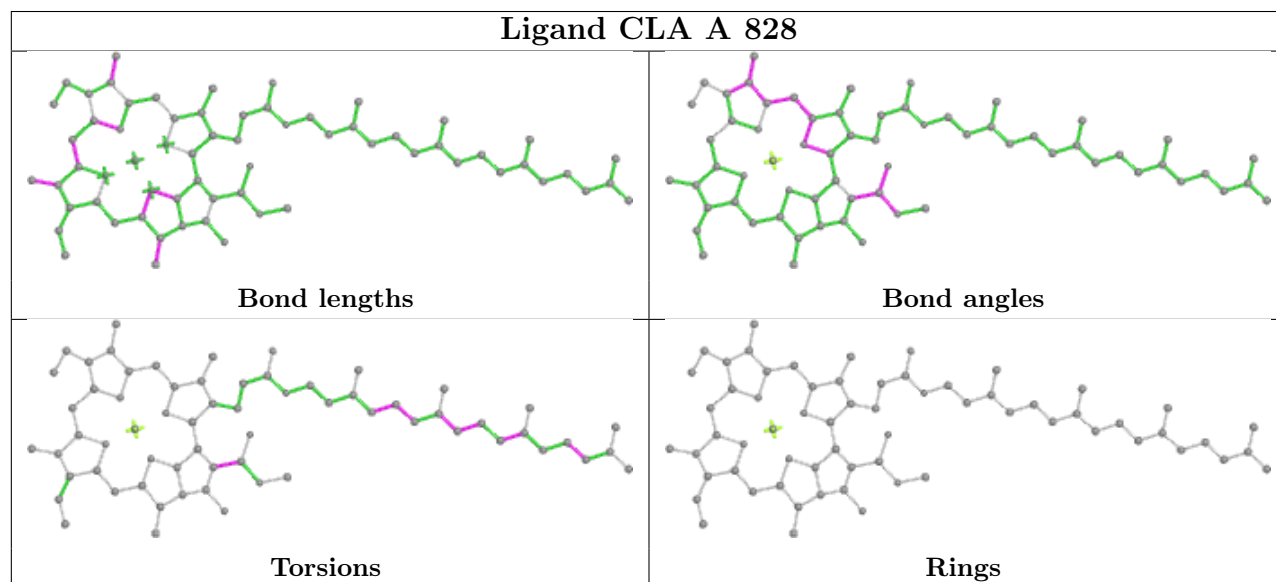


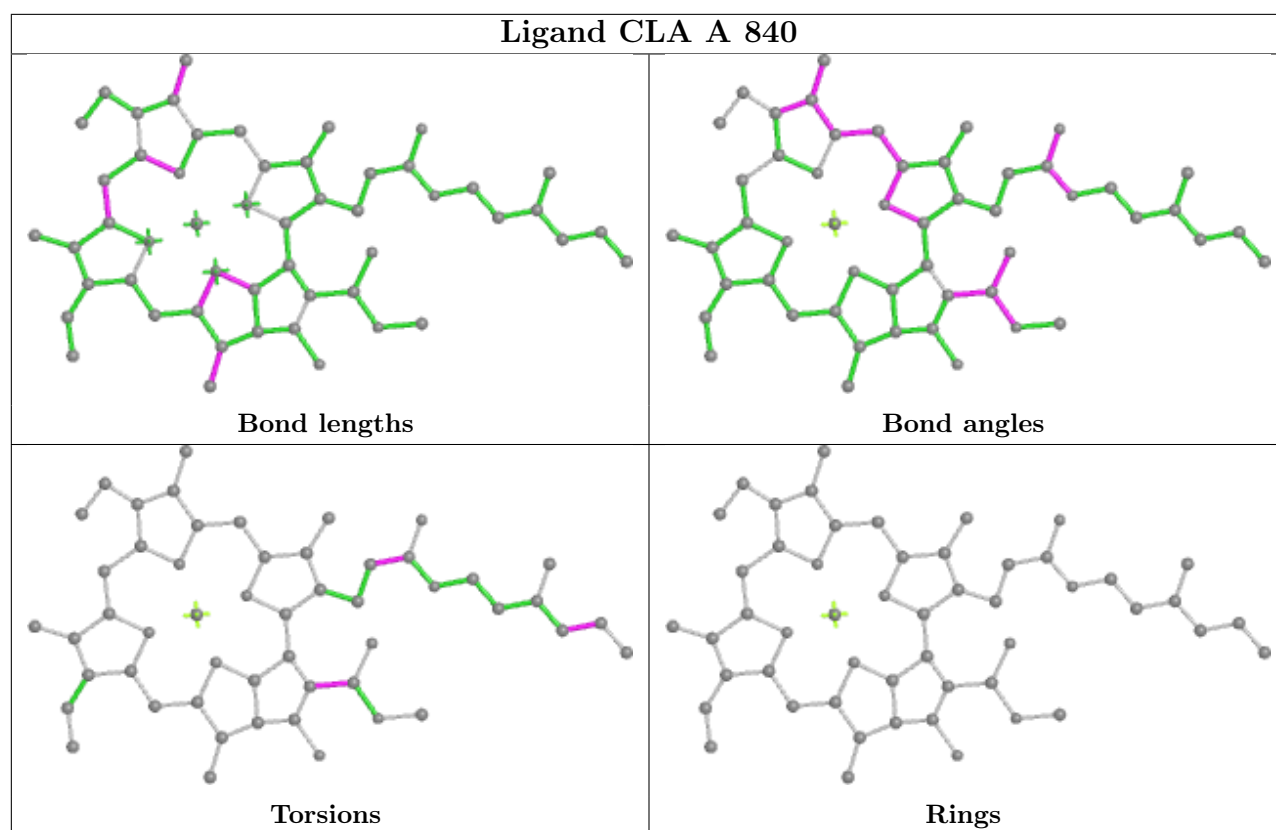


Ligand LHG 2 618

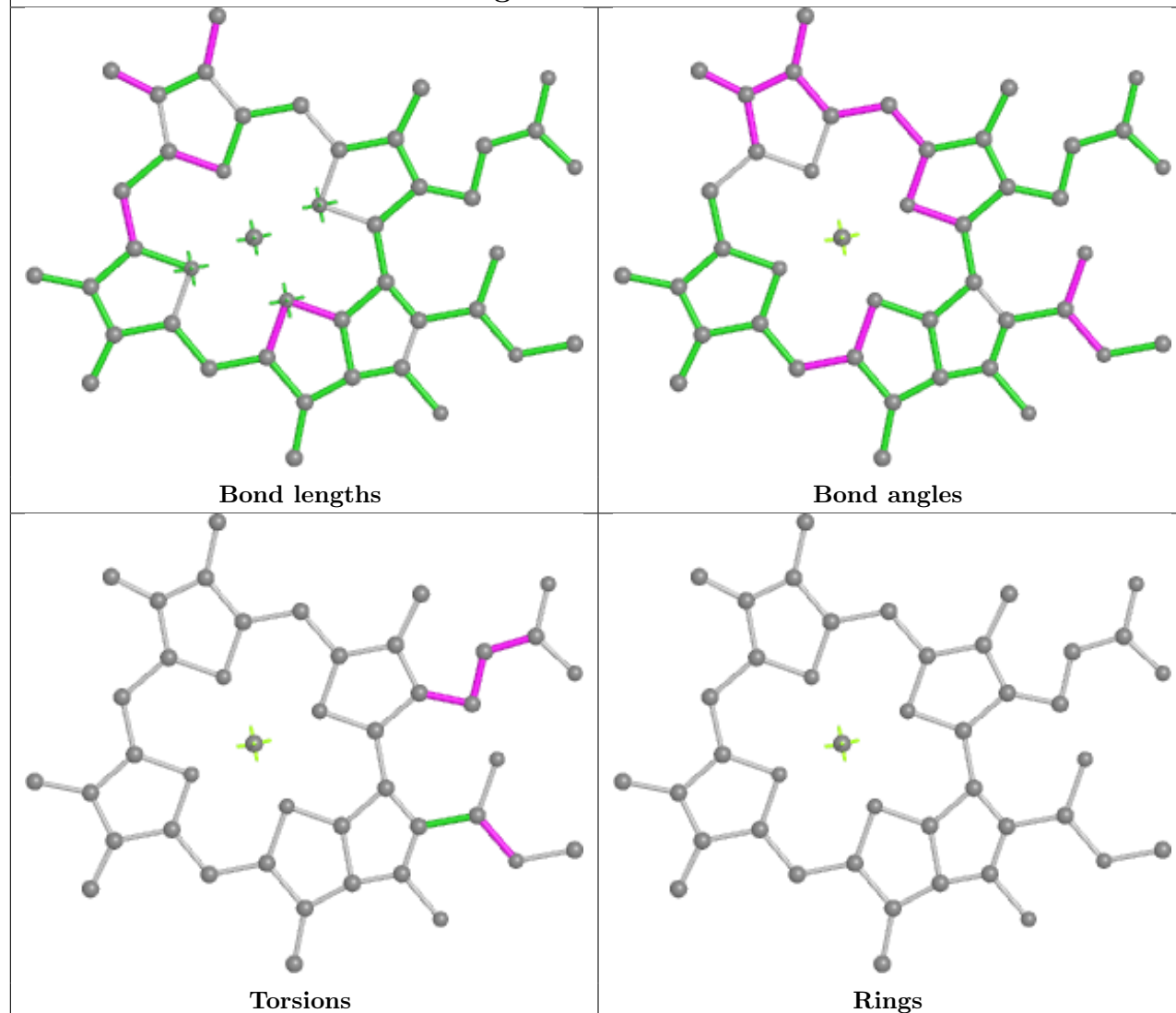


Ligand CLA A 828

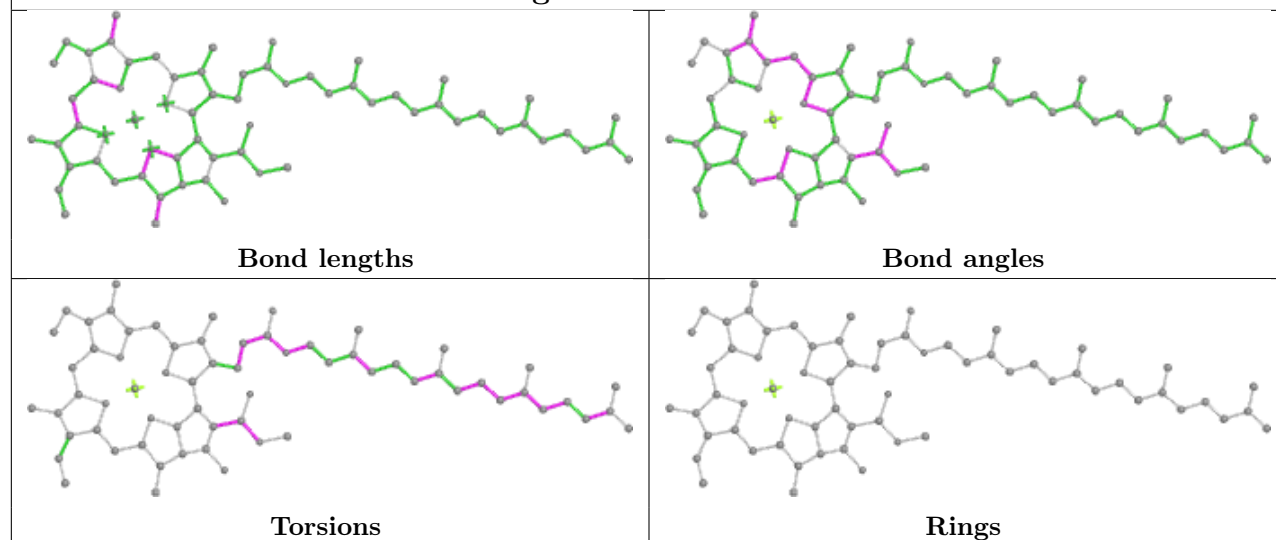




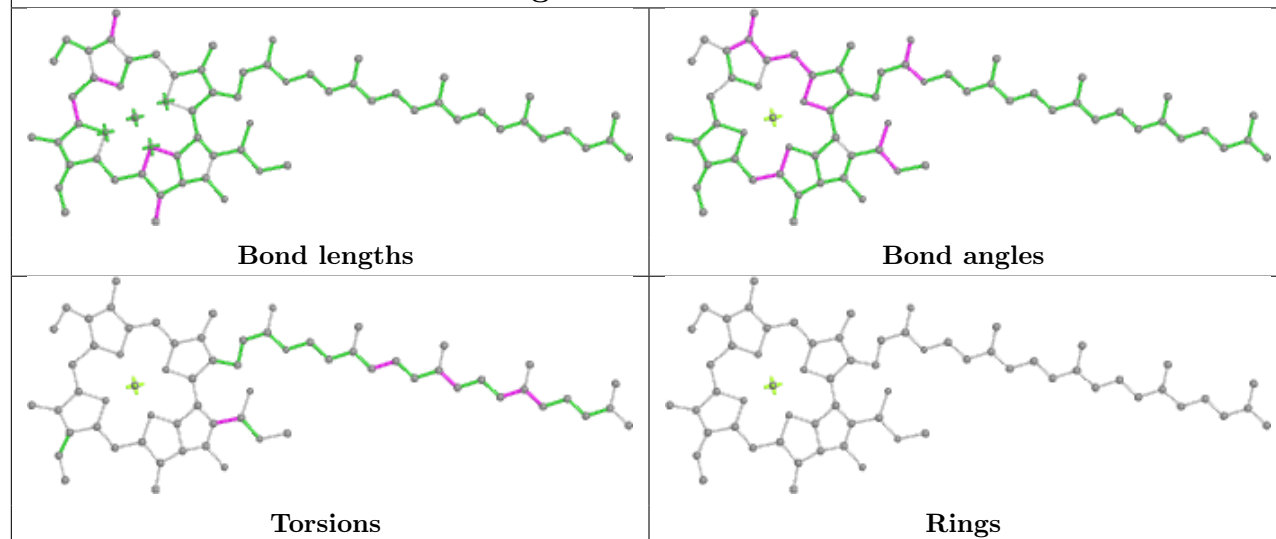
Ligand CLA 4 604



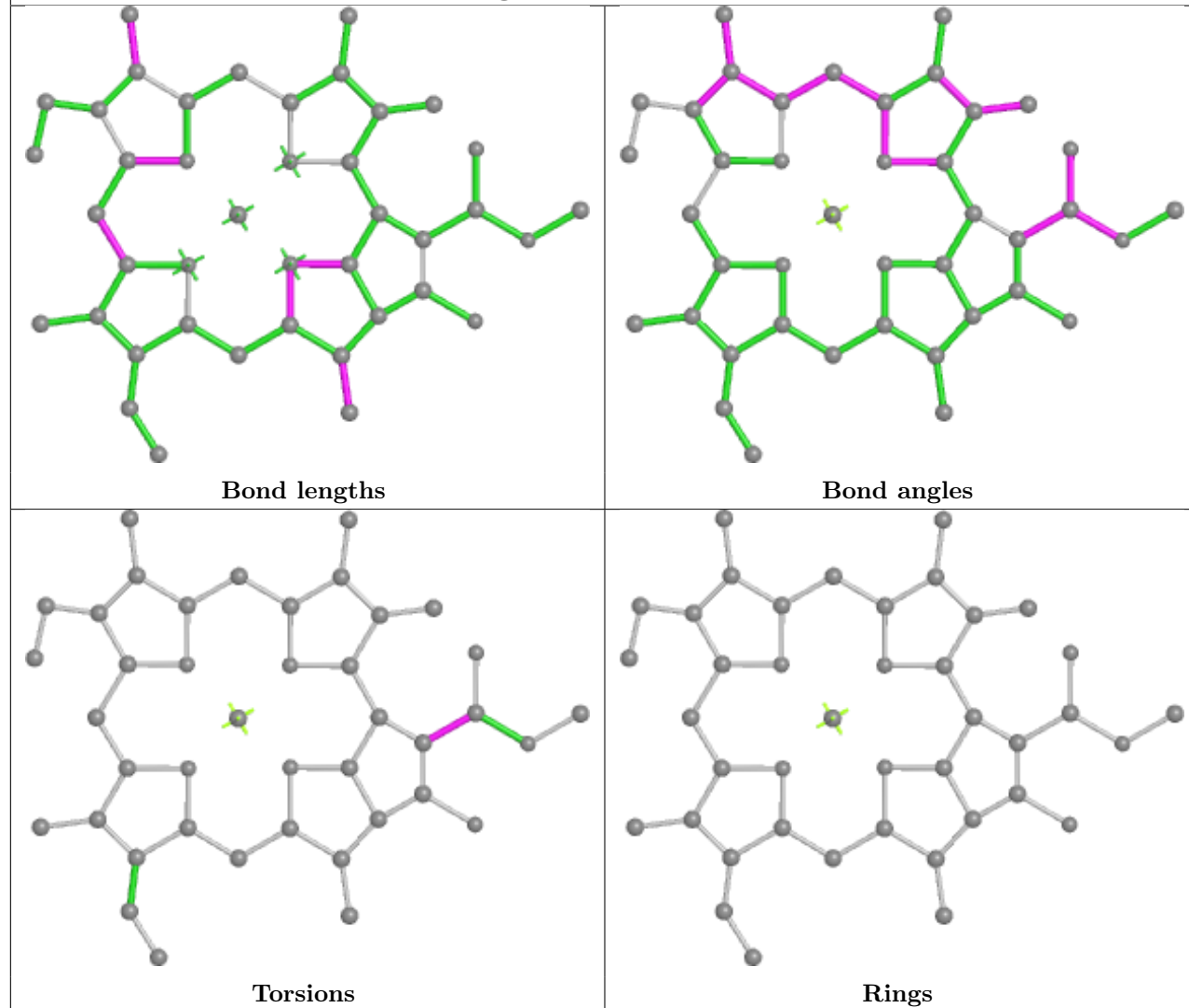
Ligand CLA B 841

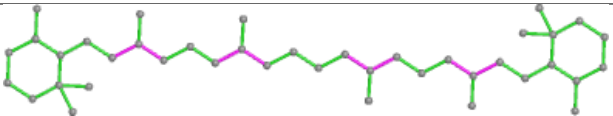
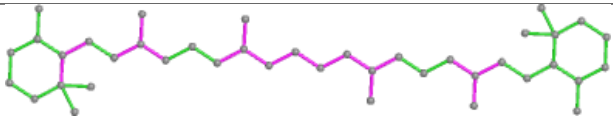
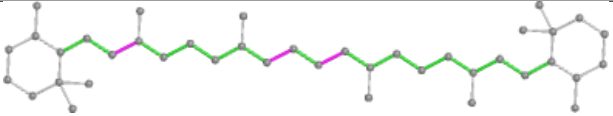
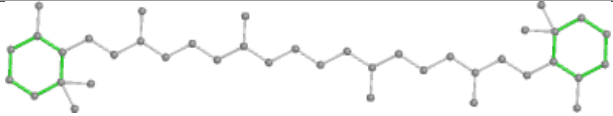


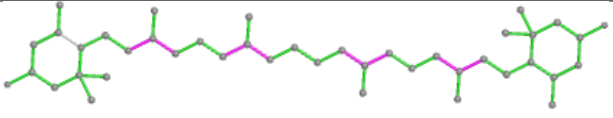
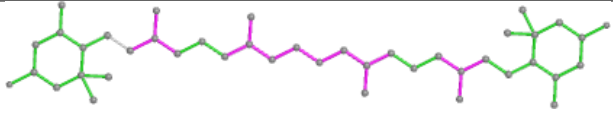
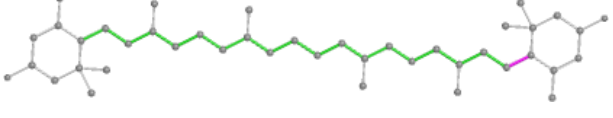
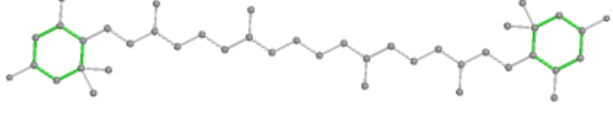
Ligand CLA A 831

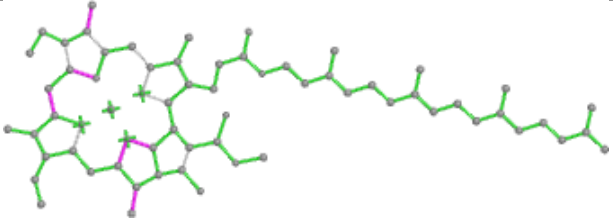
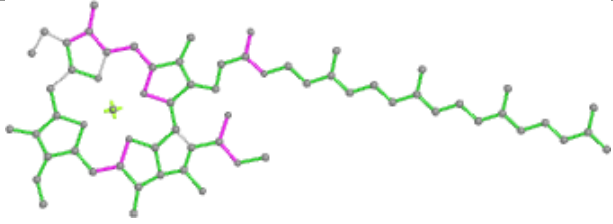
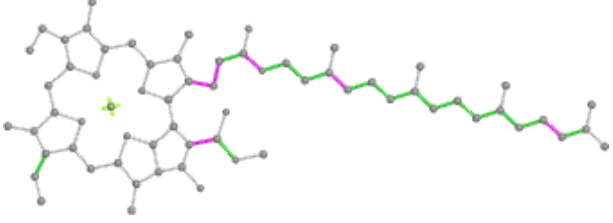
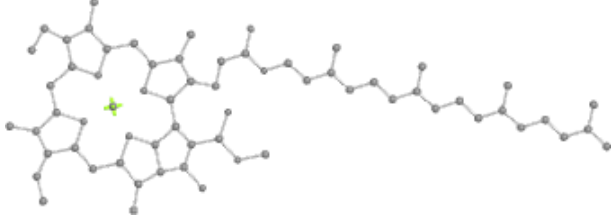


Ligand CLA B 804

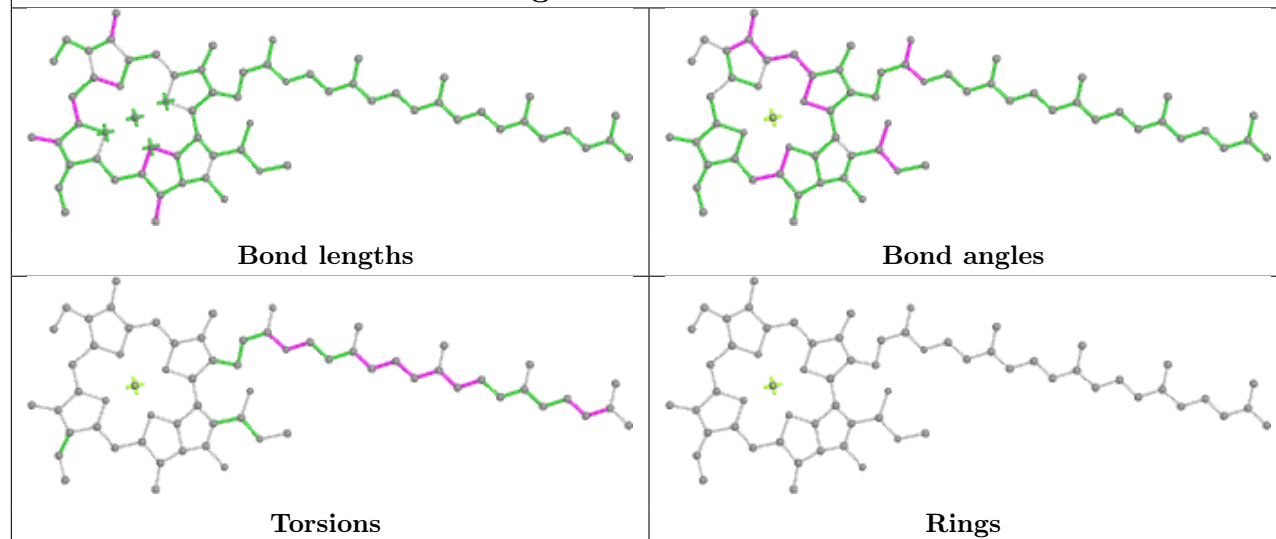


Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

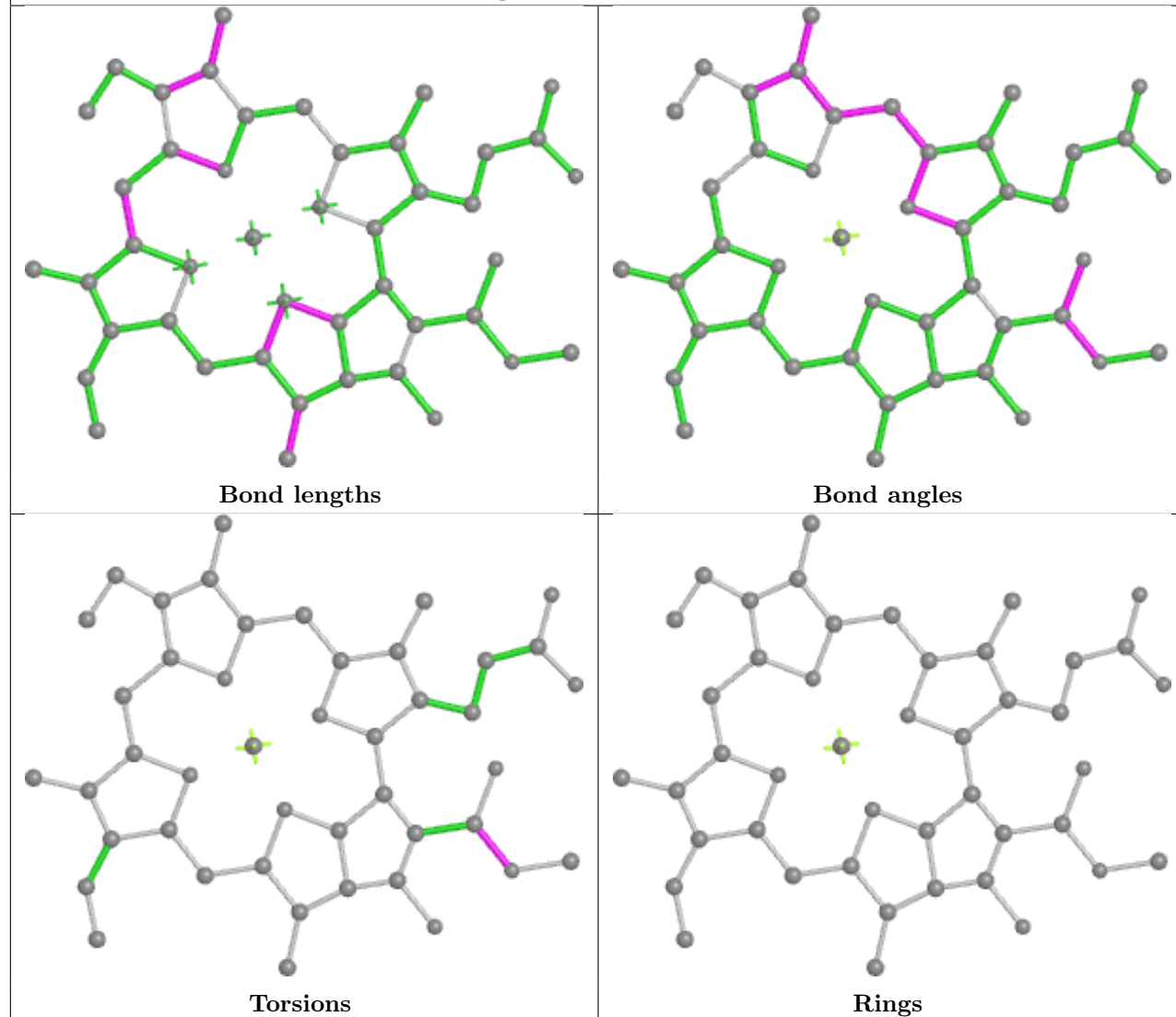
Ligand LUT 4 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

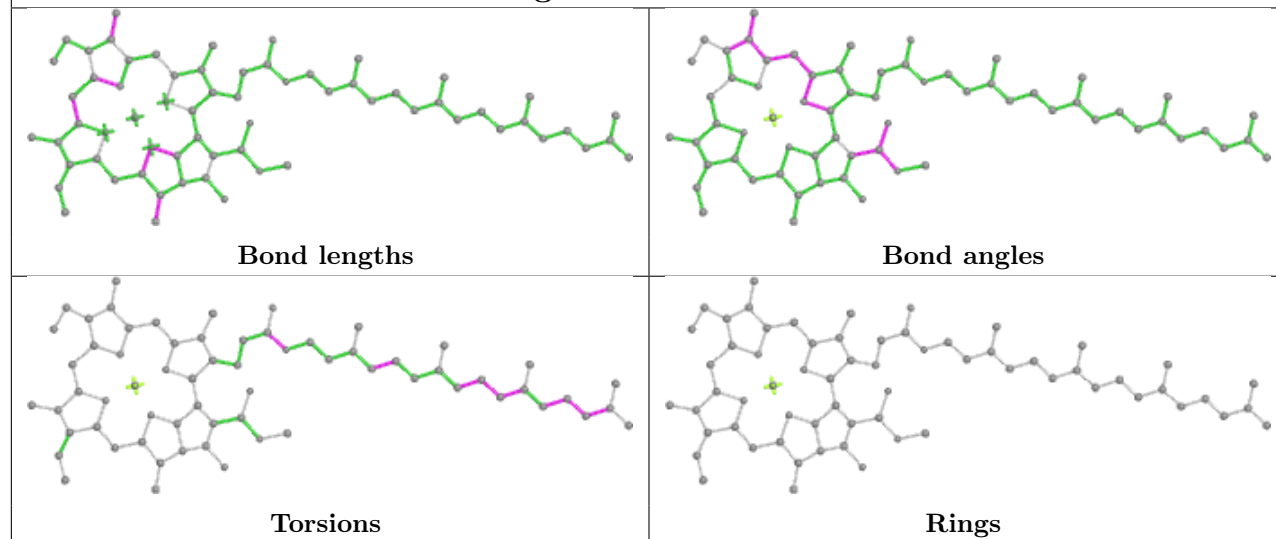
Ligand CLA A 807



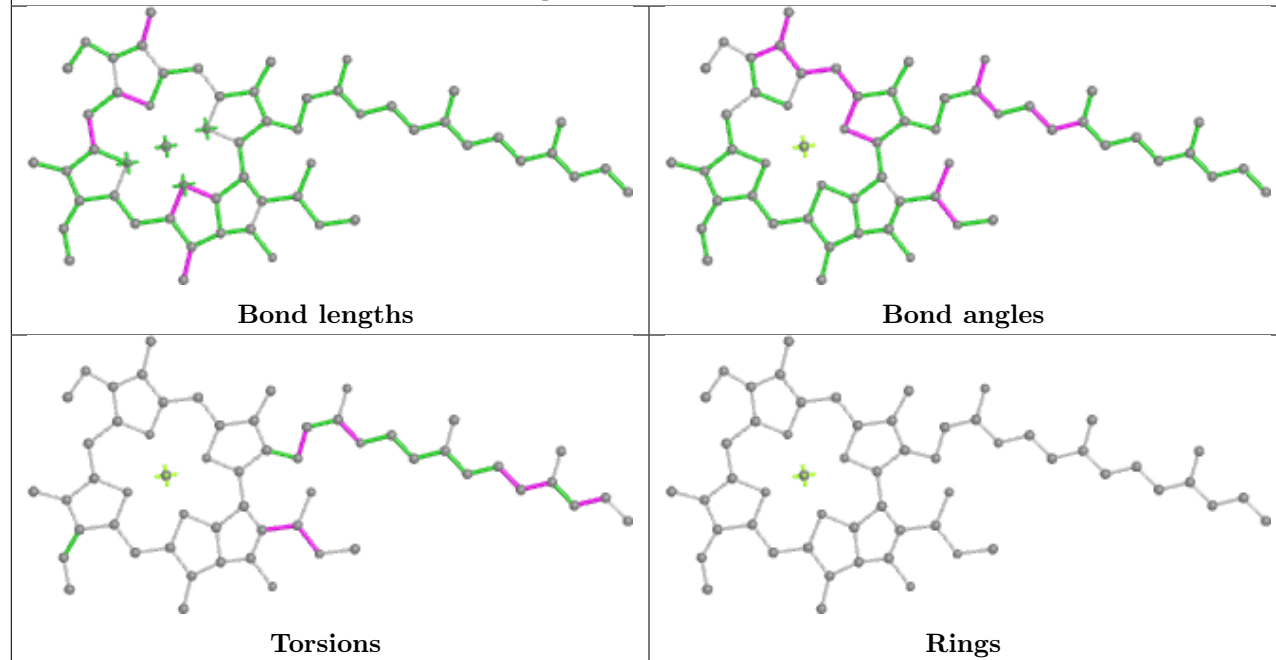
Ligand CLA 3 607



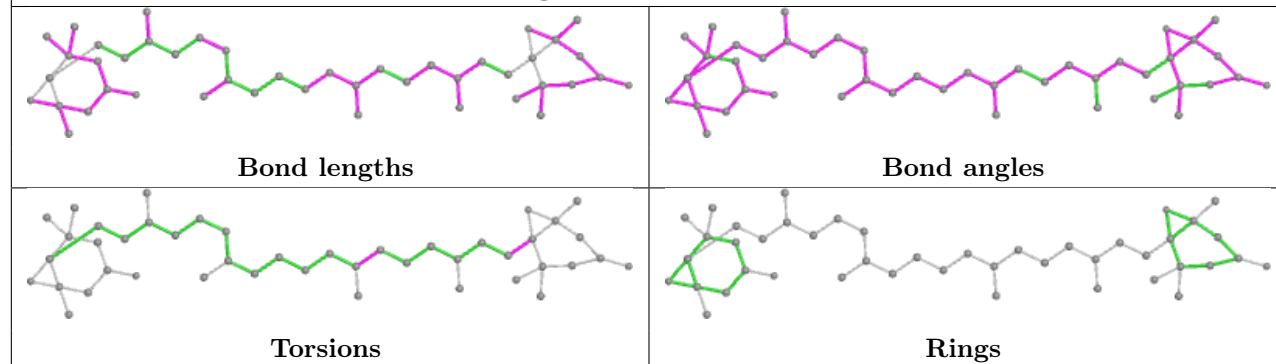
Ligand CLA L 303

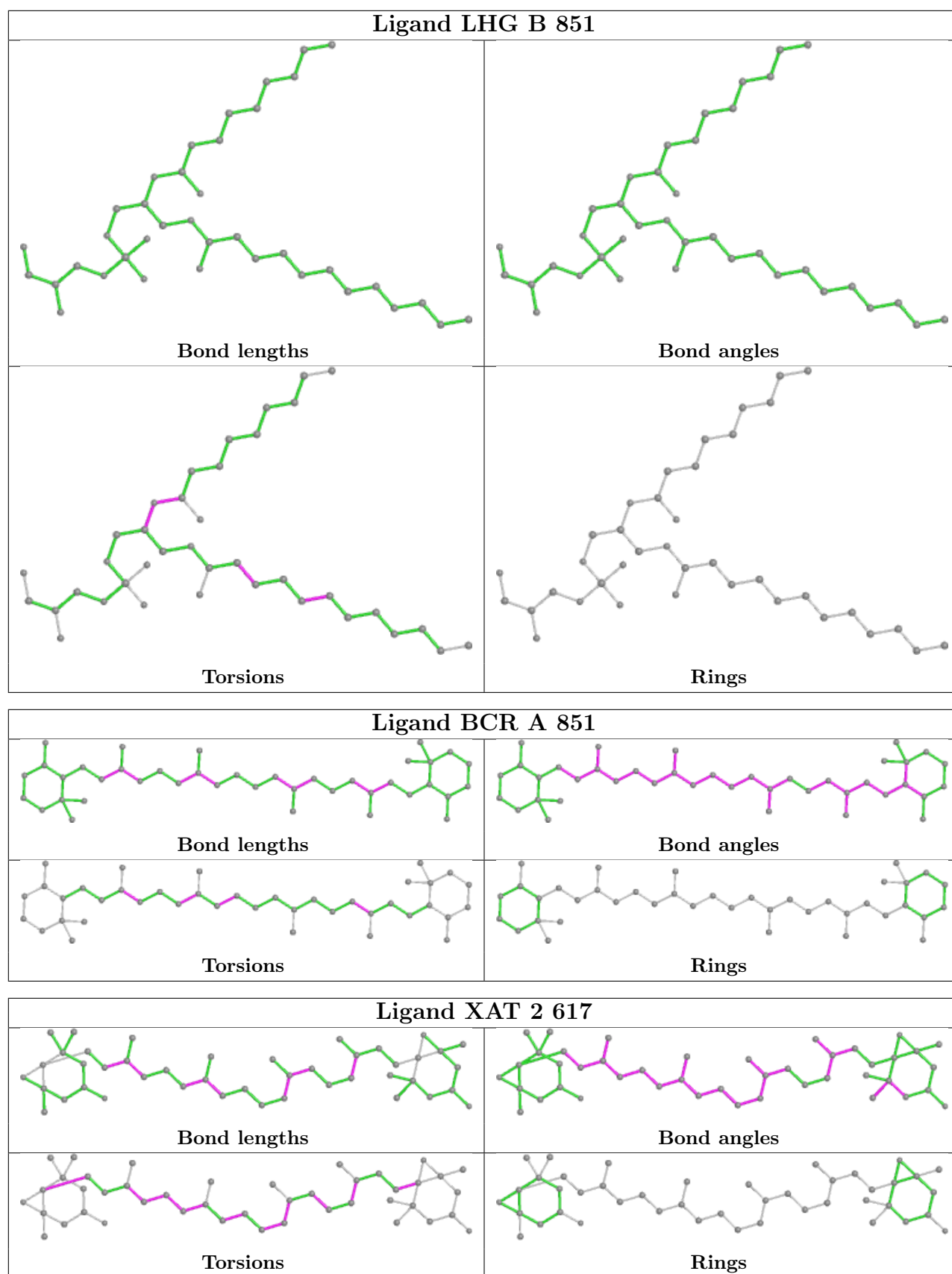


Ligand CLA 4 612

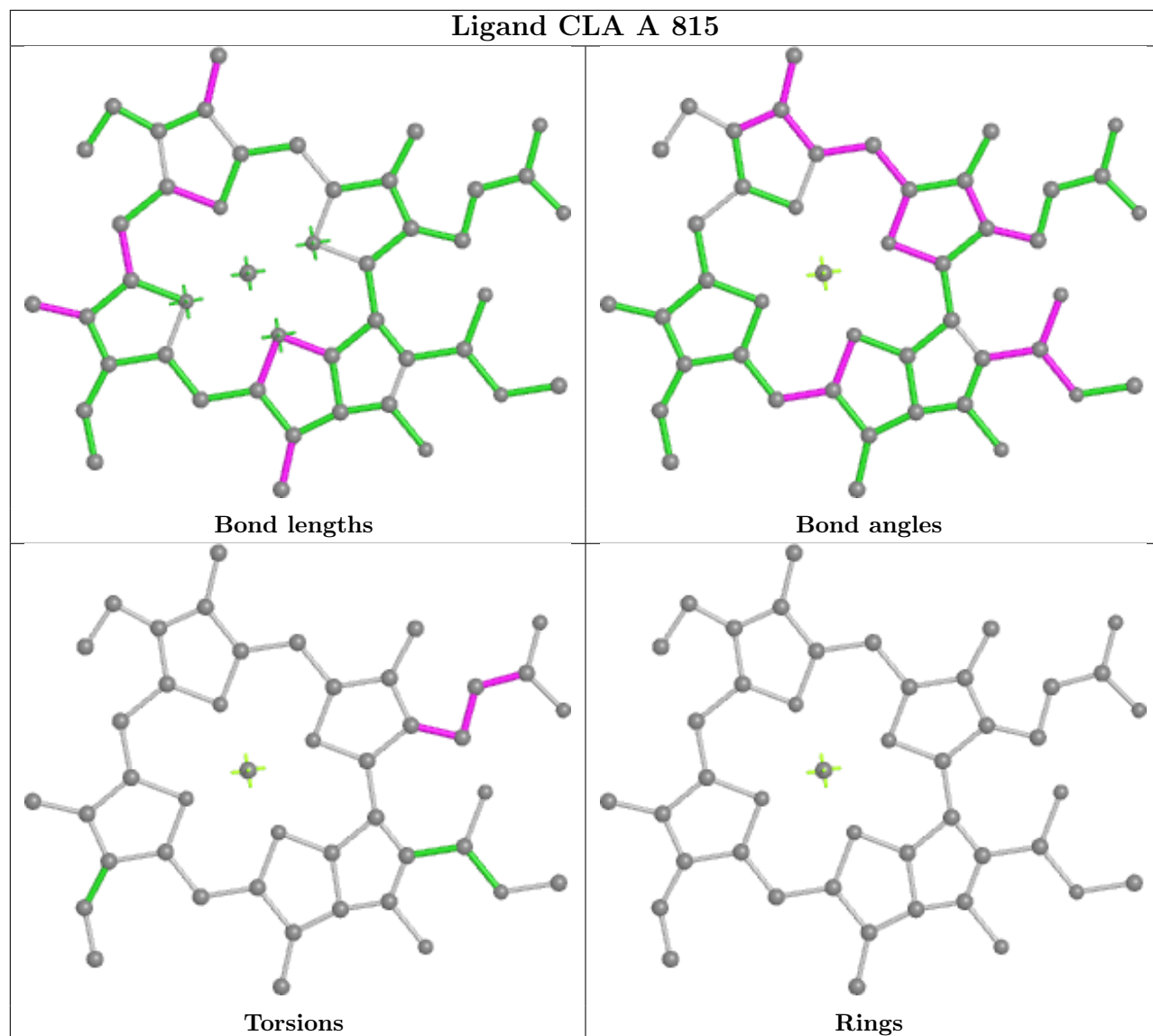


Ligand XAT 4 617

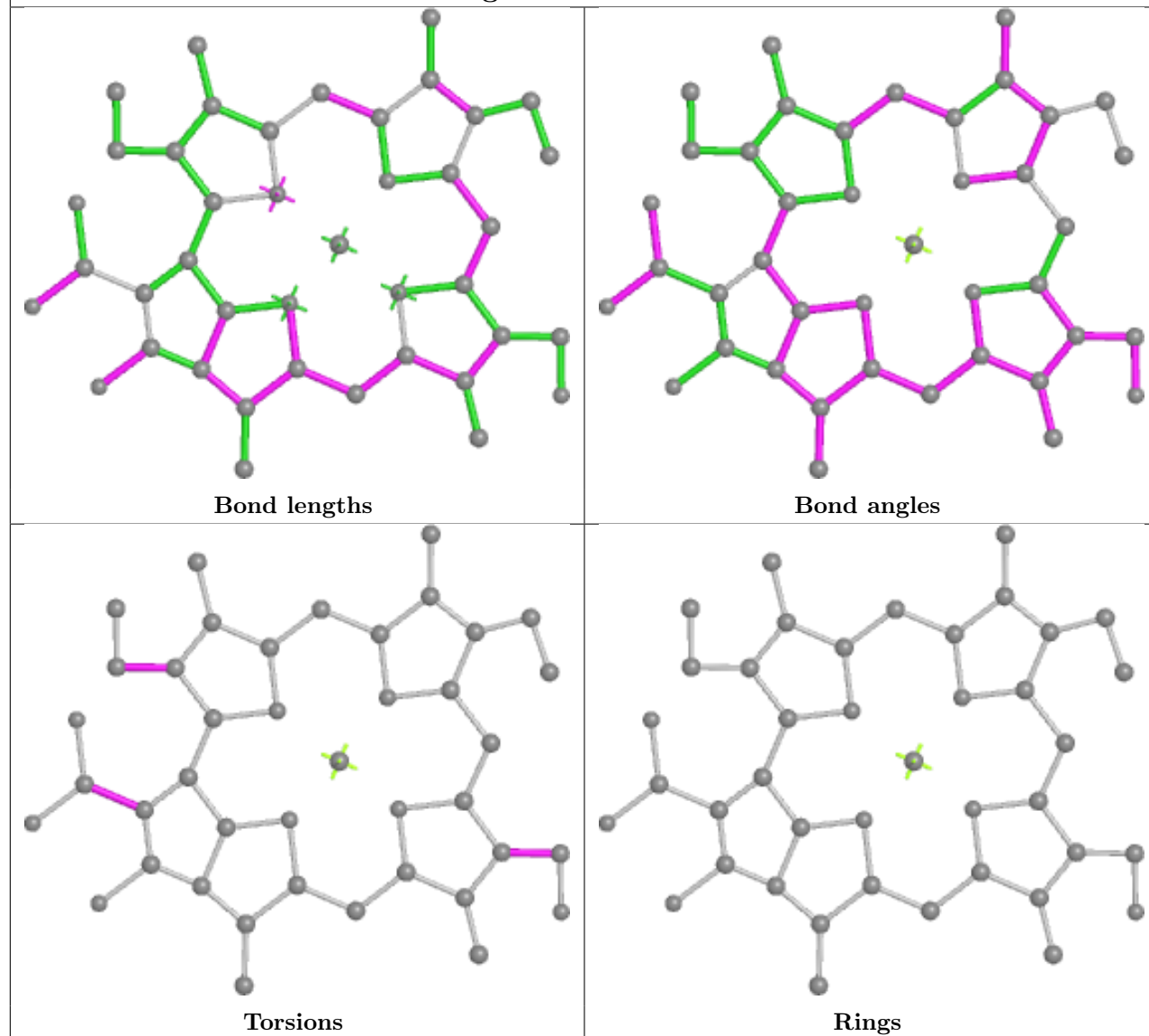




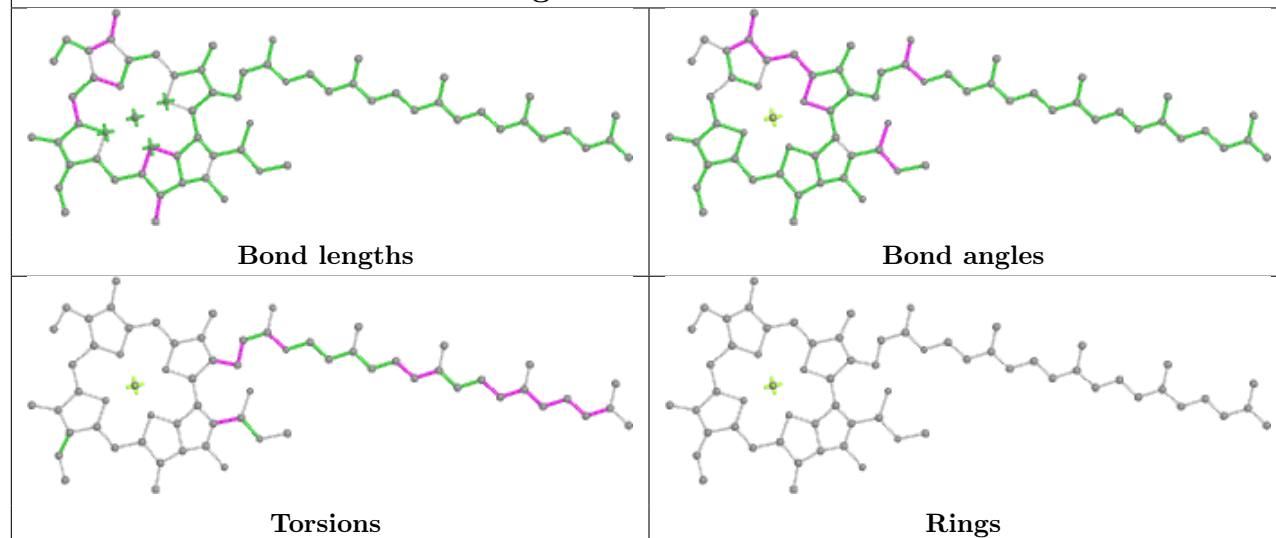
Ligand CLA A 815

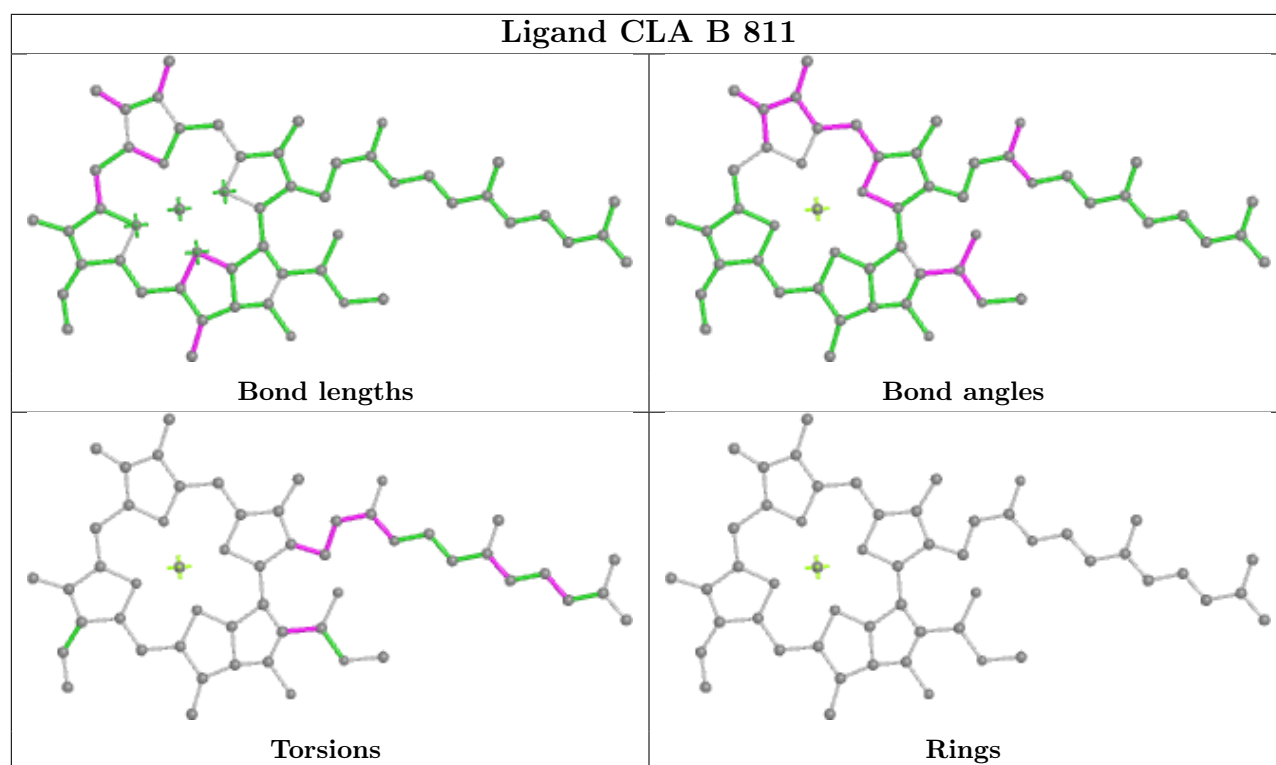


Ligand CHL 4 605

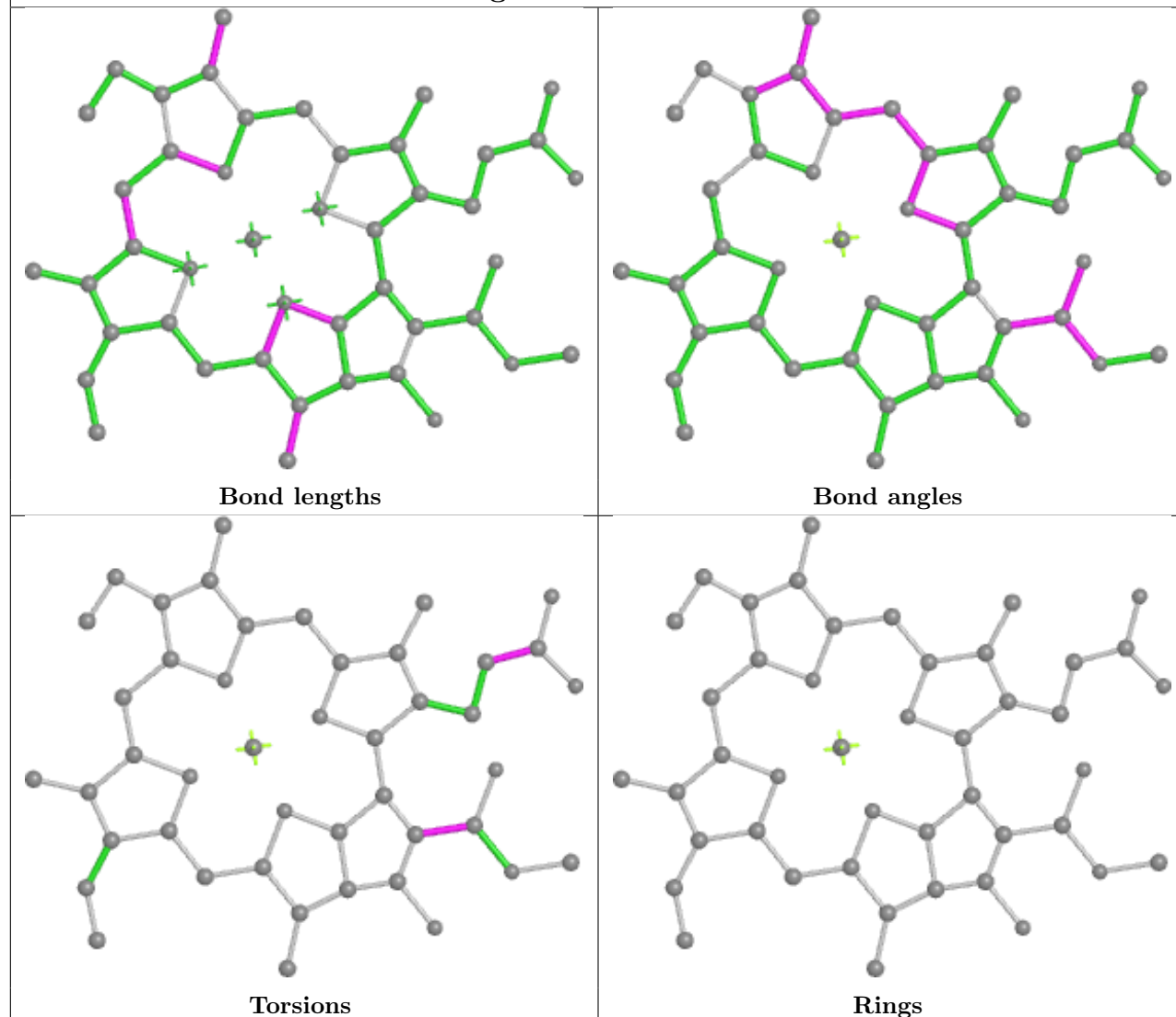


Ligand CLA B 828

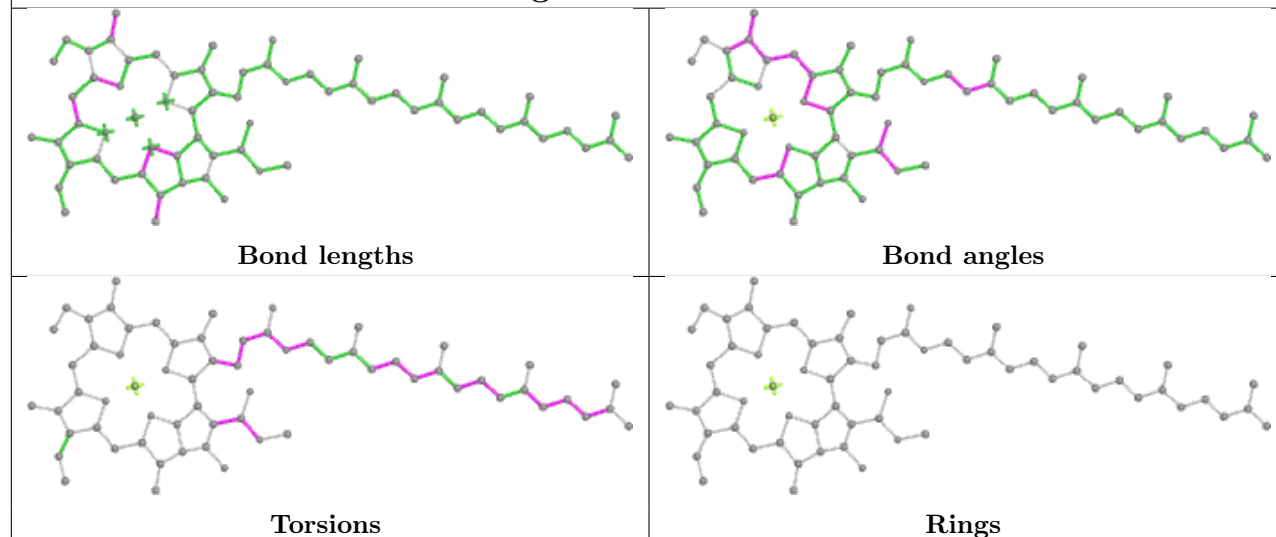




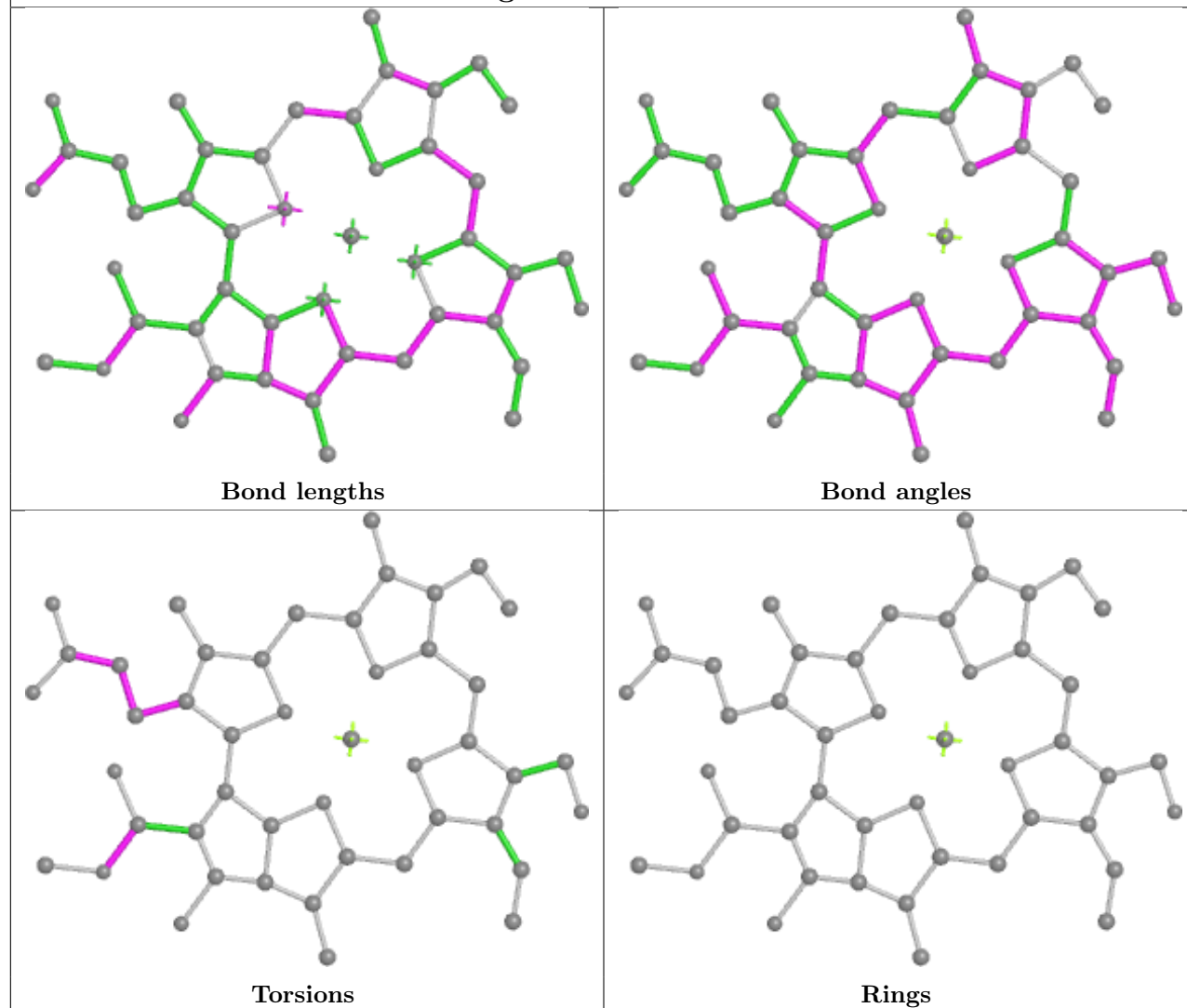
Ligand CLA A 837



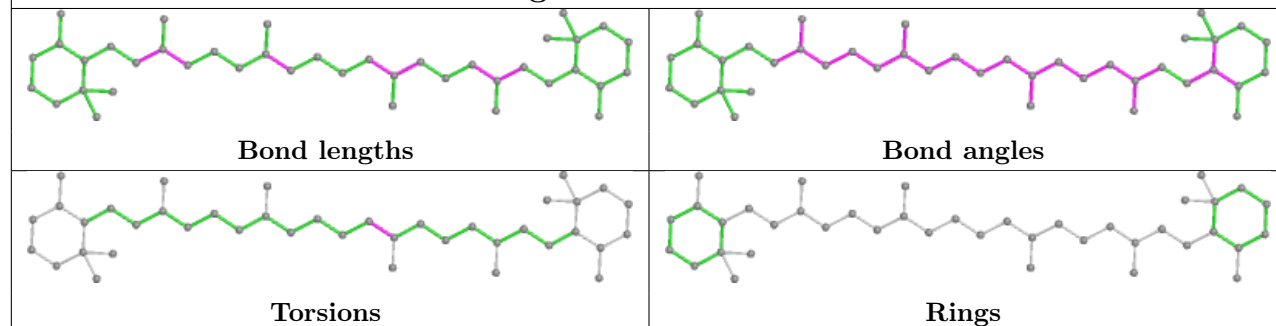
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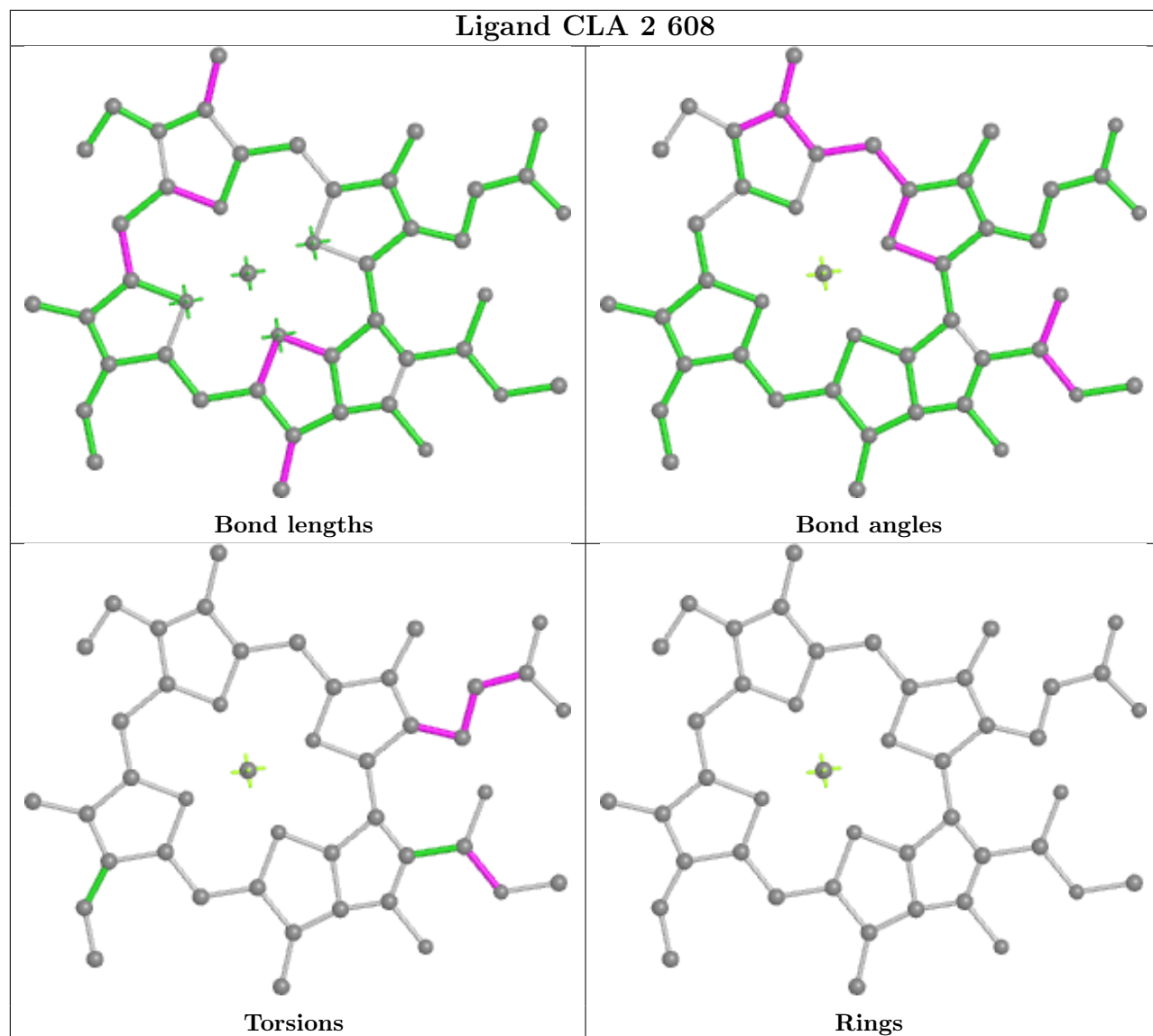
Ligand CHL 4 607

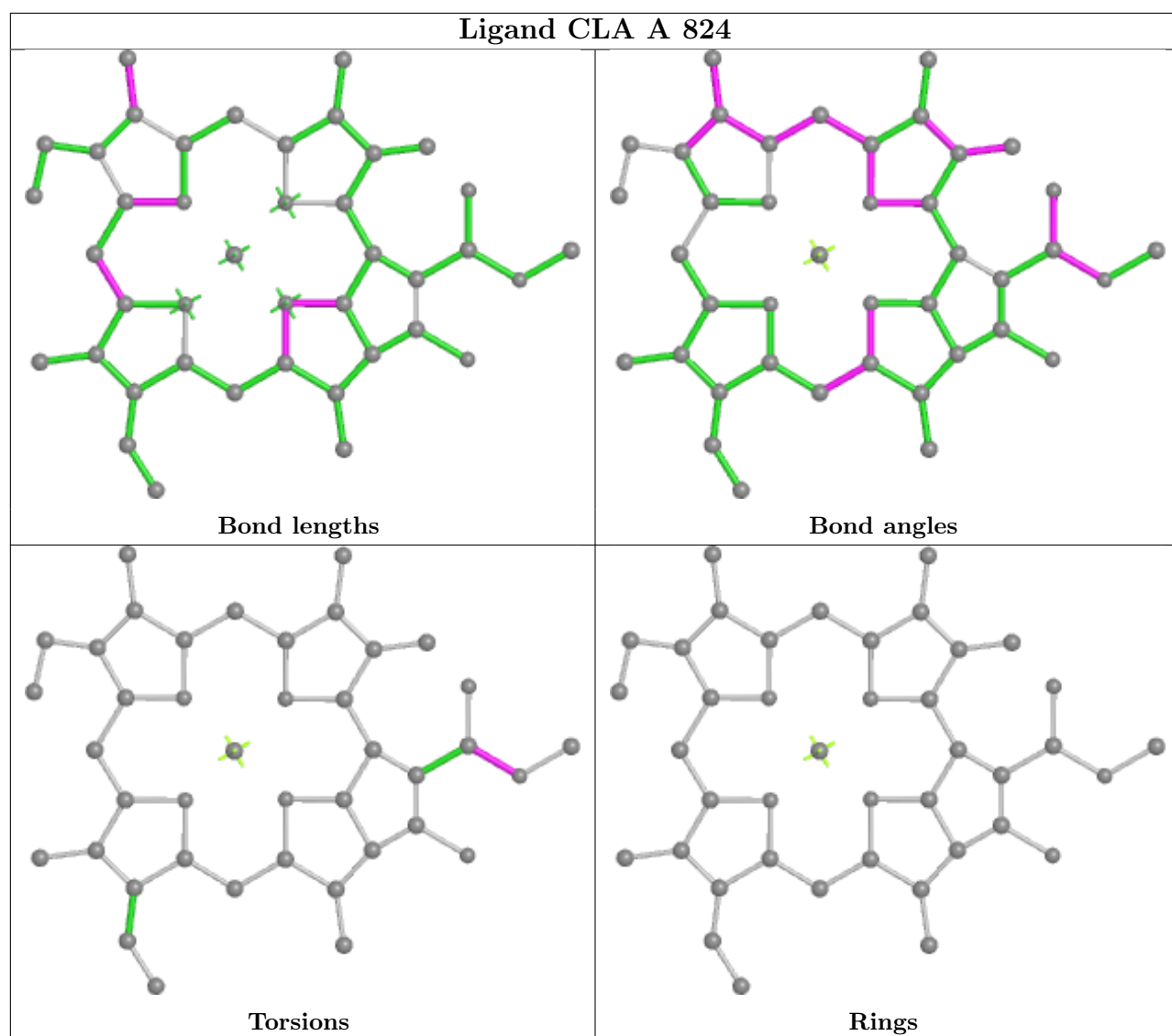


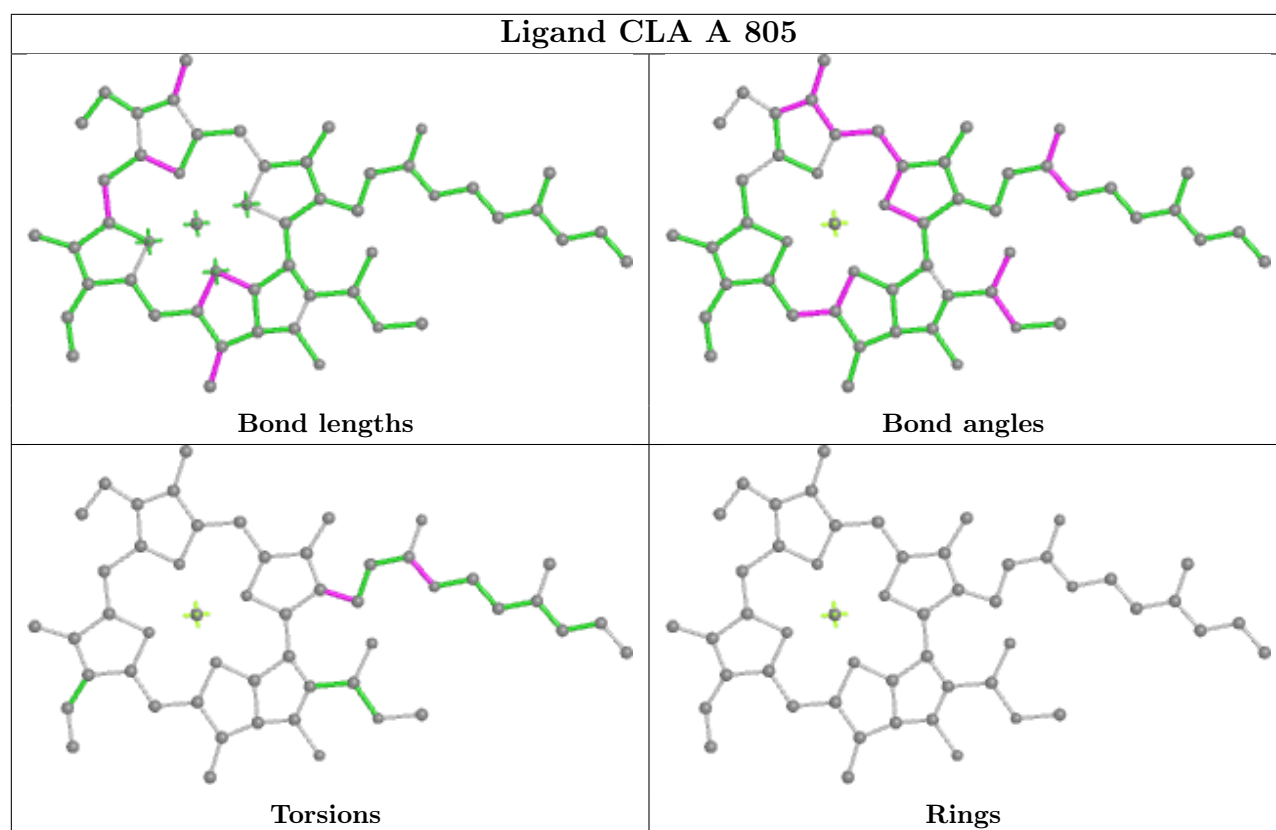
Ligand BCR K 202



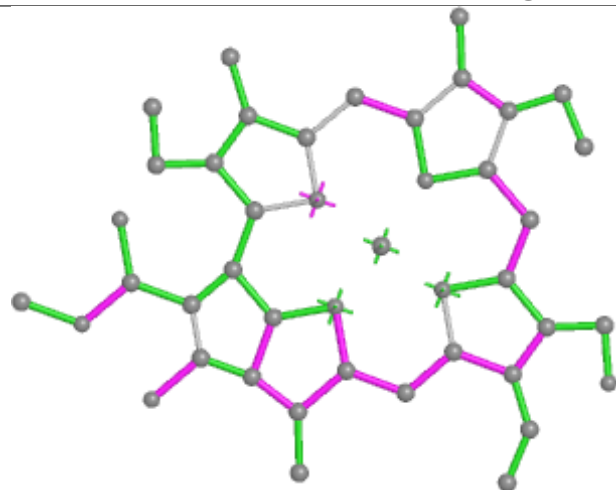
Ligand CLA 2 608



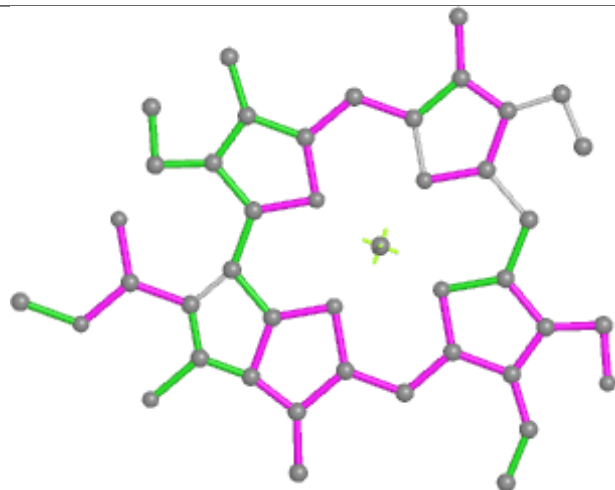




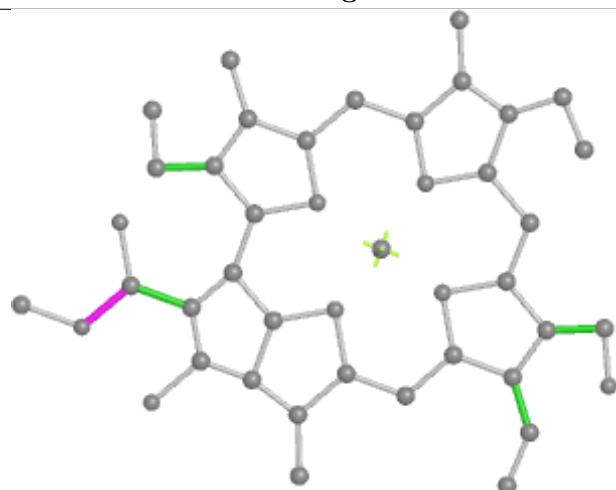
Ligand CHL 2 606



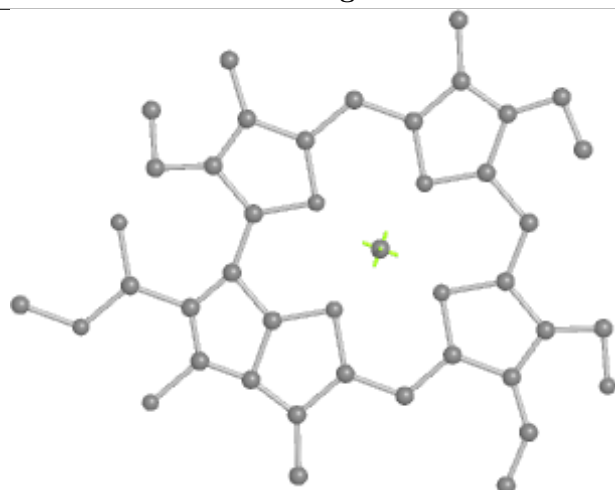
Bond lengths



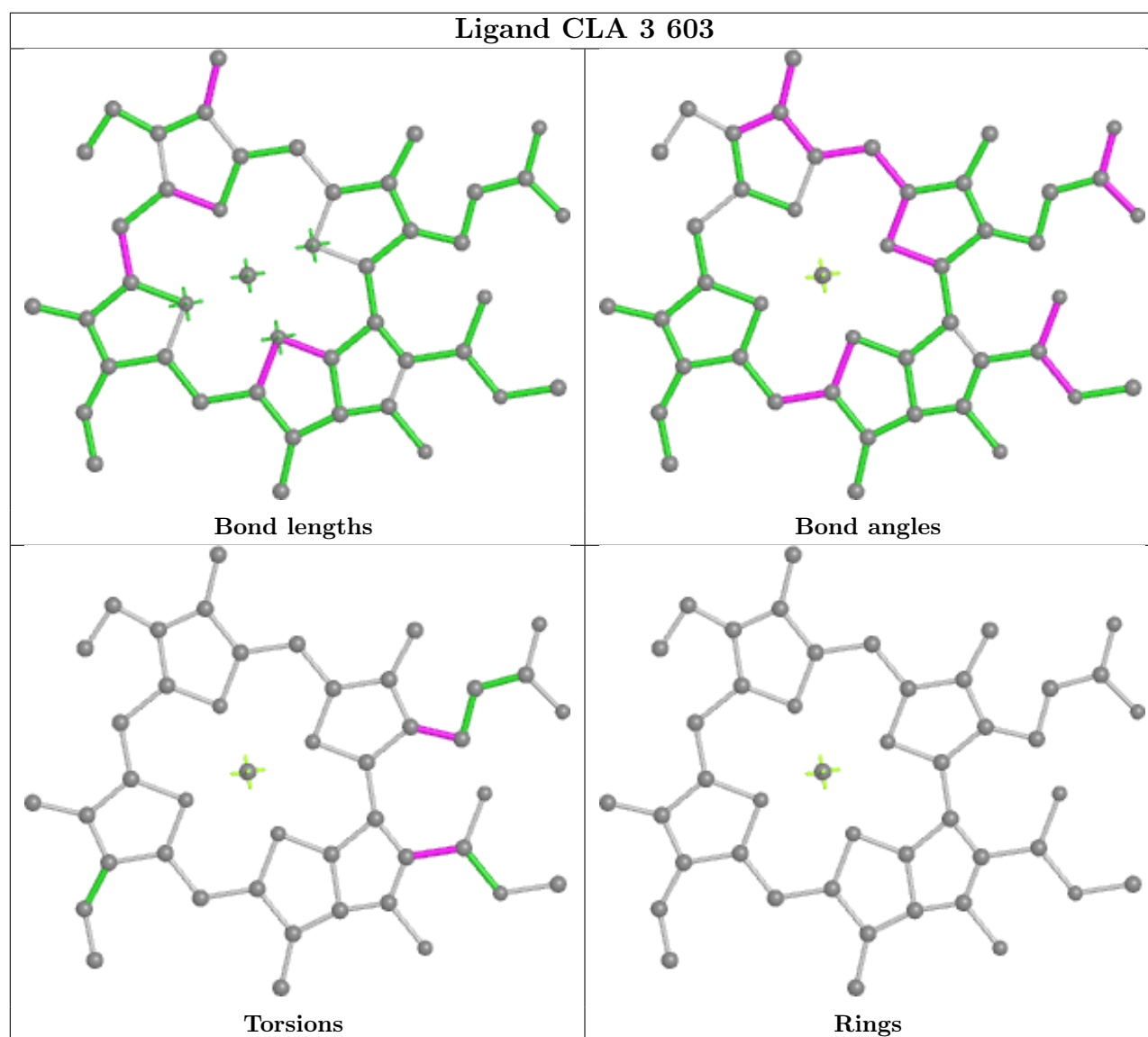
Bond angles



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.

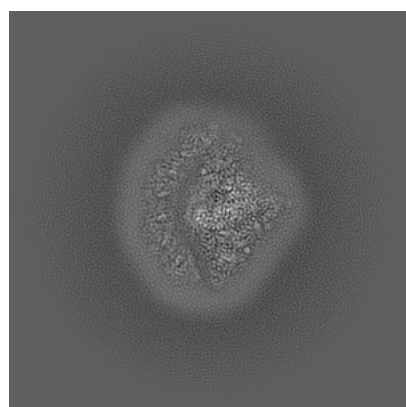
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36036. These allow visual inspection of the internal detail of the map and identification of artifacts.

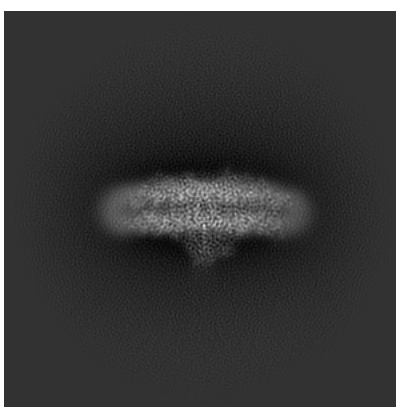
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

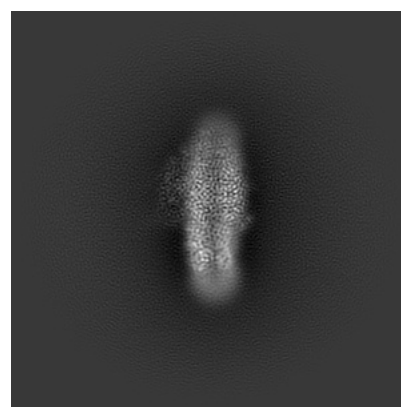
6.1.1 Primary map



X



Y

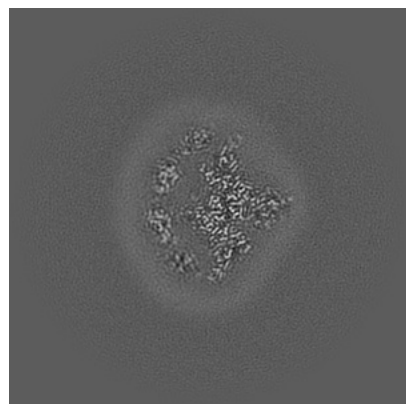


Z

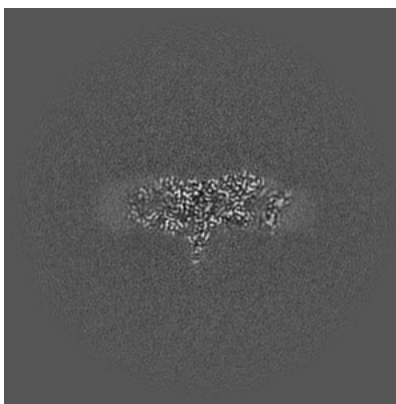
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

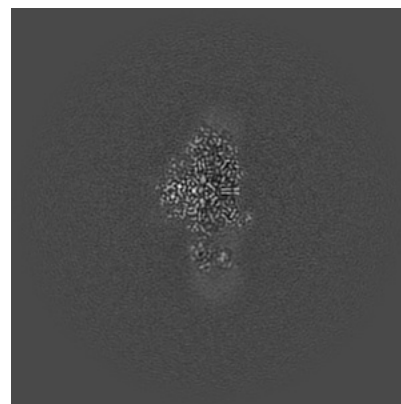
6.2.1 Primary map



X Index: 192



Y Index: 192

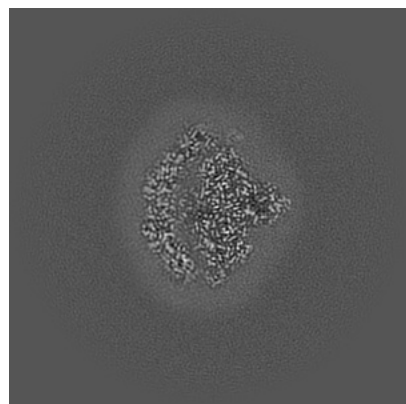


Z Index: 192

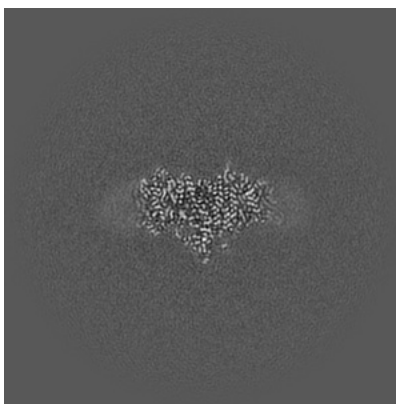
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

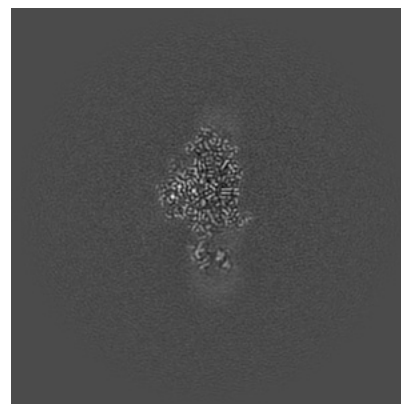
6.3.1 Primary map



X Index: 182



Y Index: 211

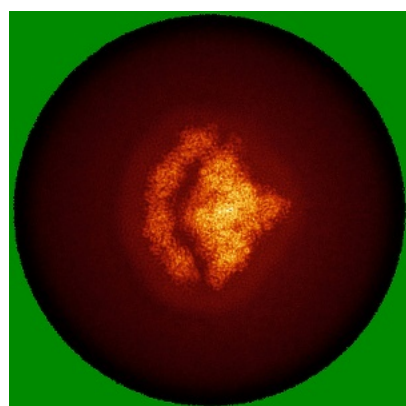


Z Index: 191

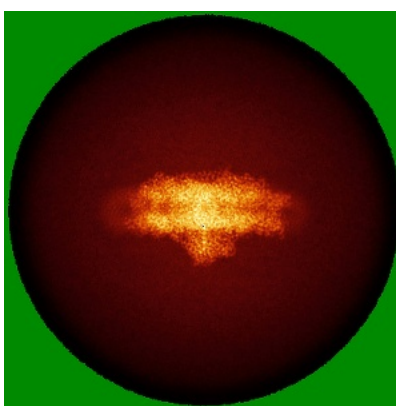
The images above show the largest variance slices of the map in three orthogonal directions.

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

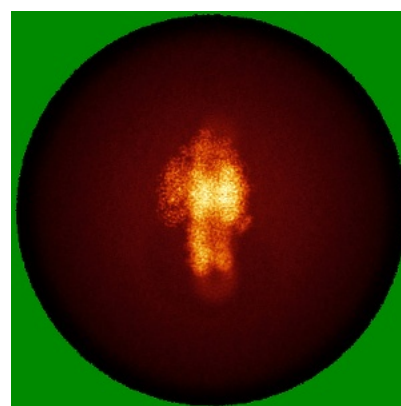
6.4.1 Primary map



X



Y

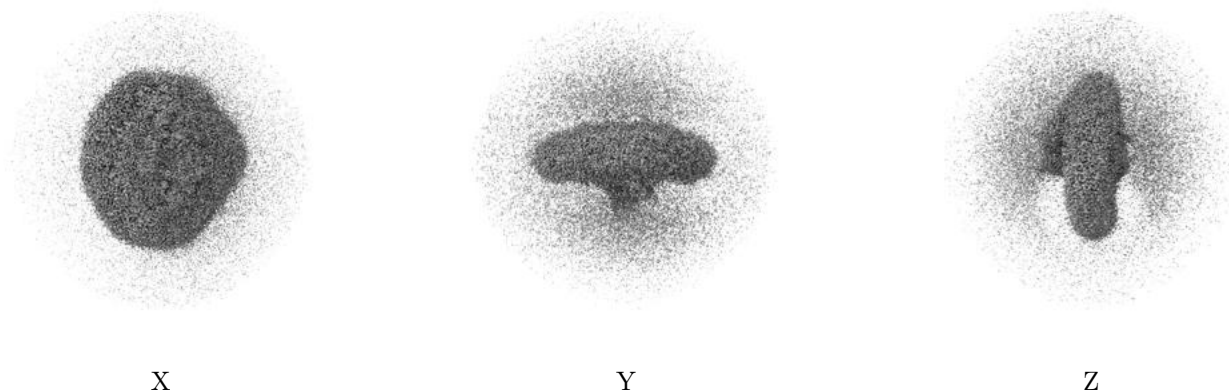


Z

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

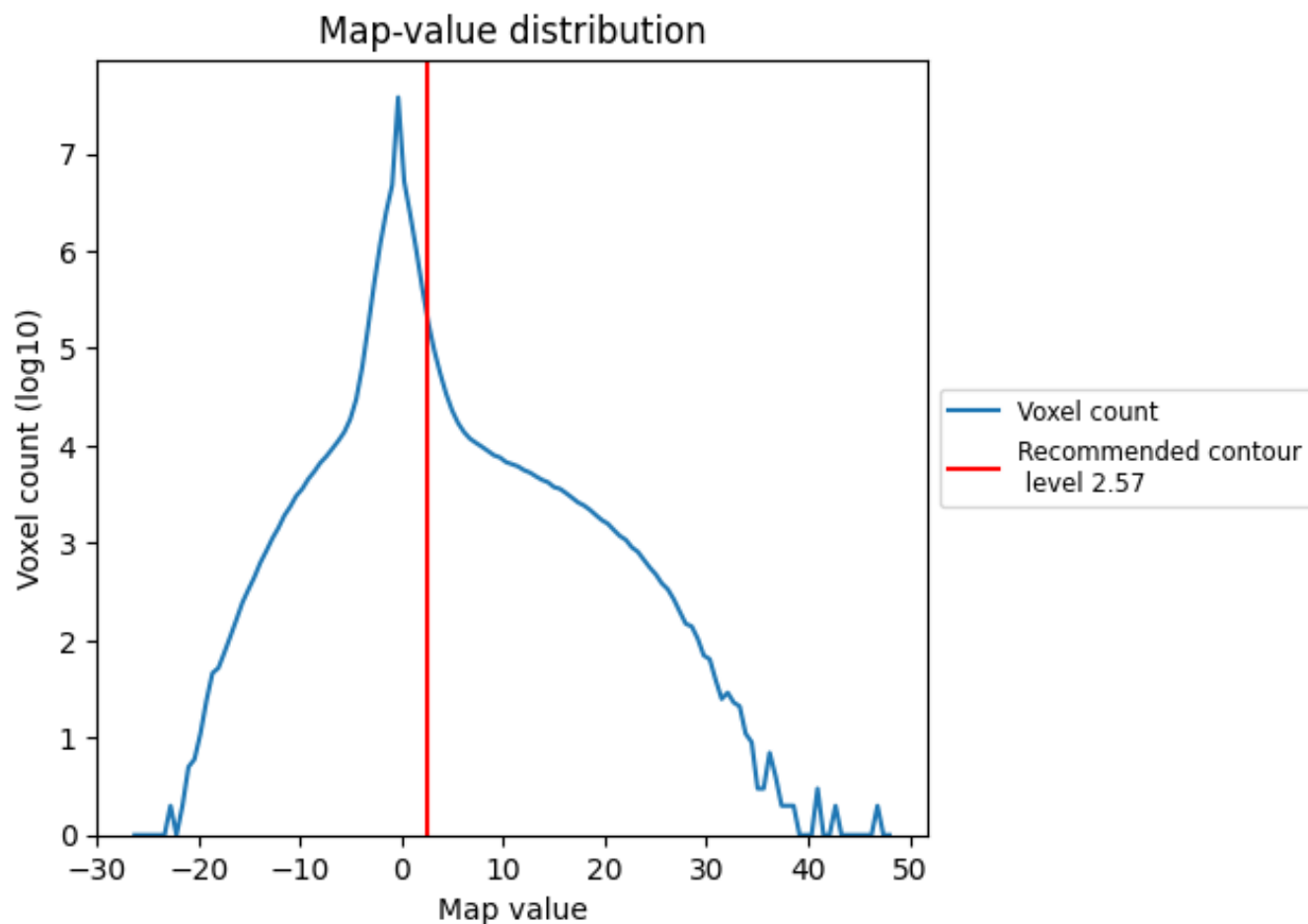
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

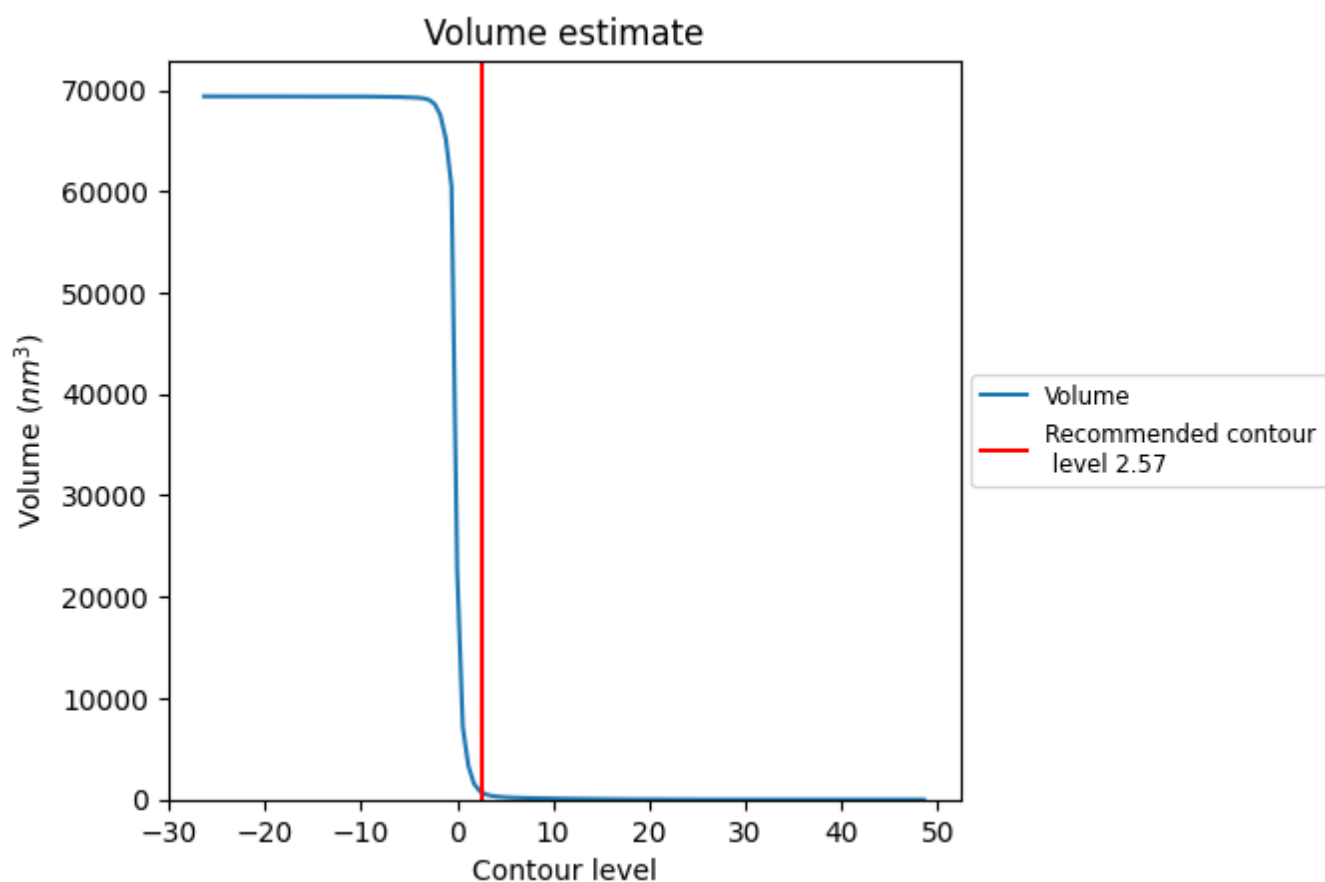
This section contains the results of statistical analysis of the map.

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.

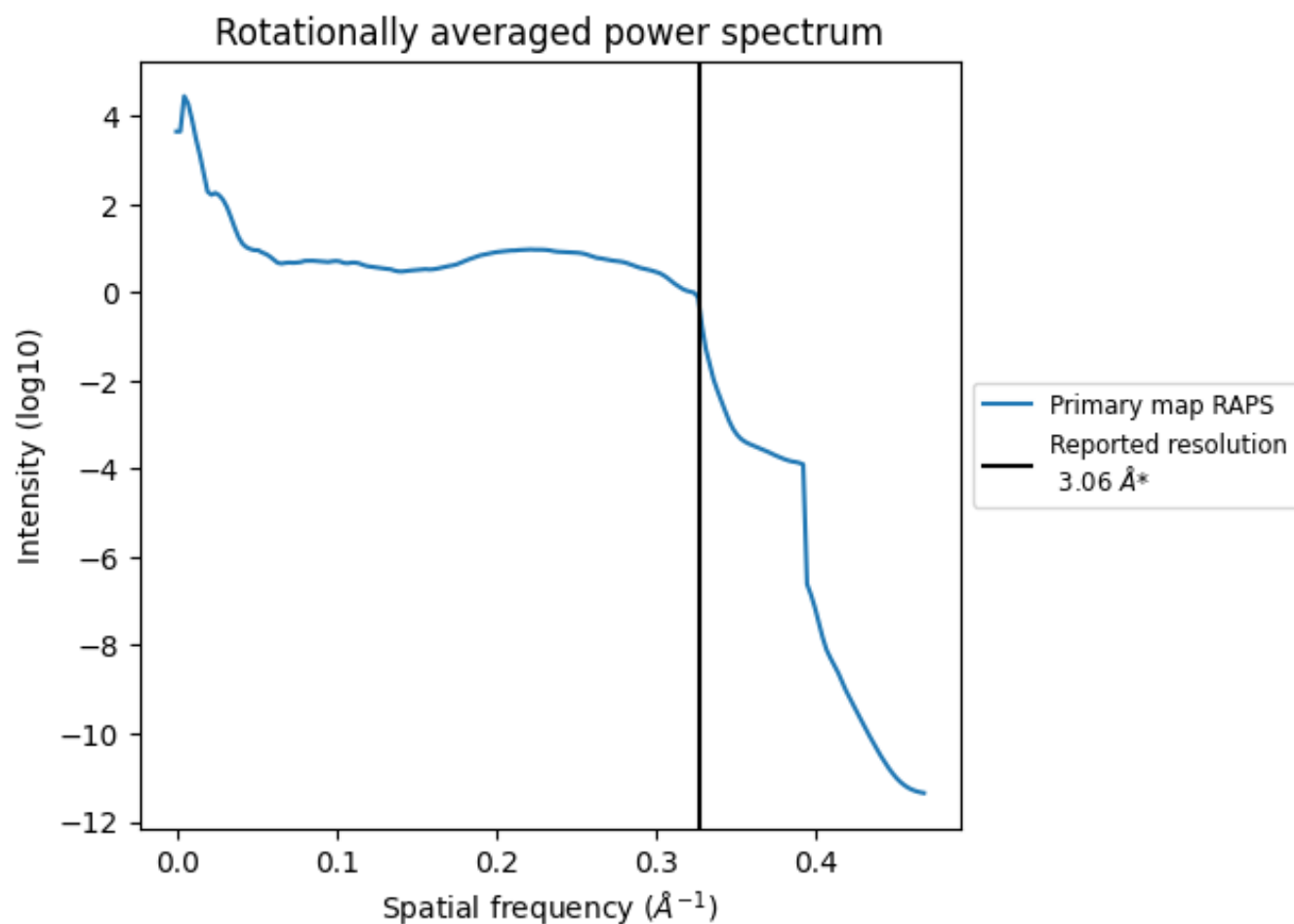
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm³; this corresponds to an approximate mass of 654 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 0.327 Å⁻¹

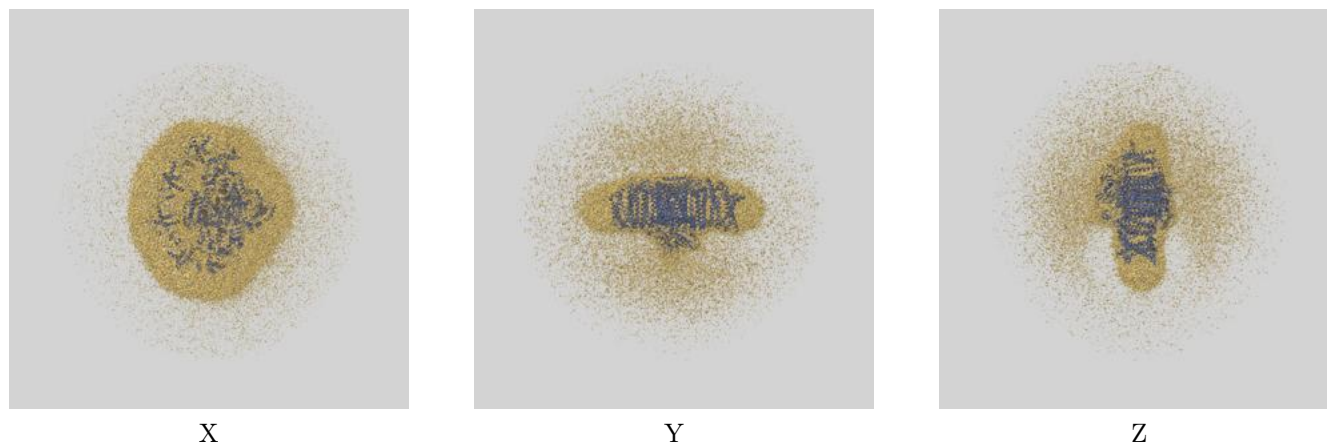
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

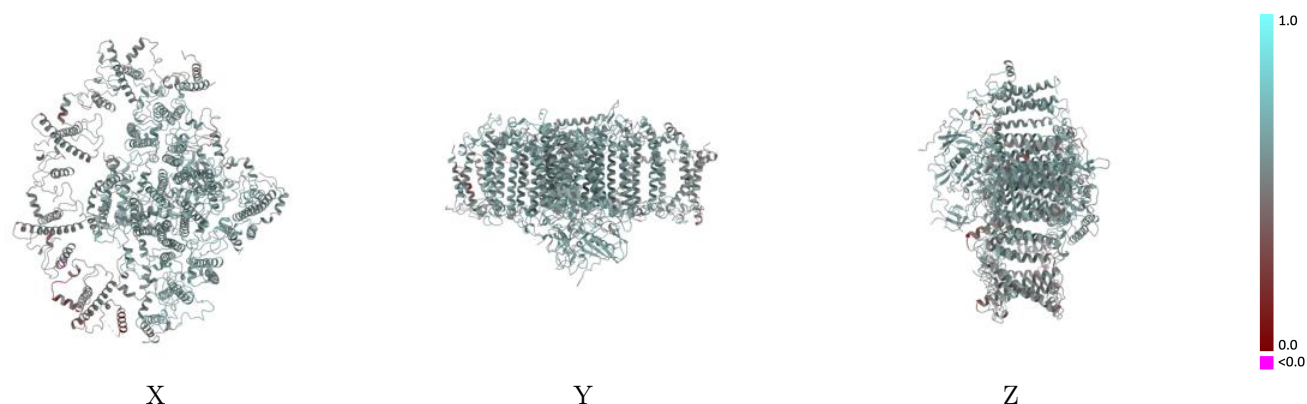
This section contains information regarding the fit between EMDB map EMD-36036 and PDB model 8J7A. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.57 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](#)



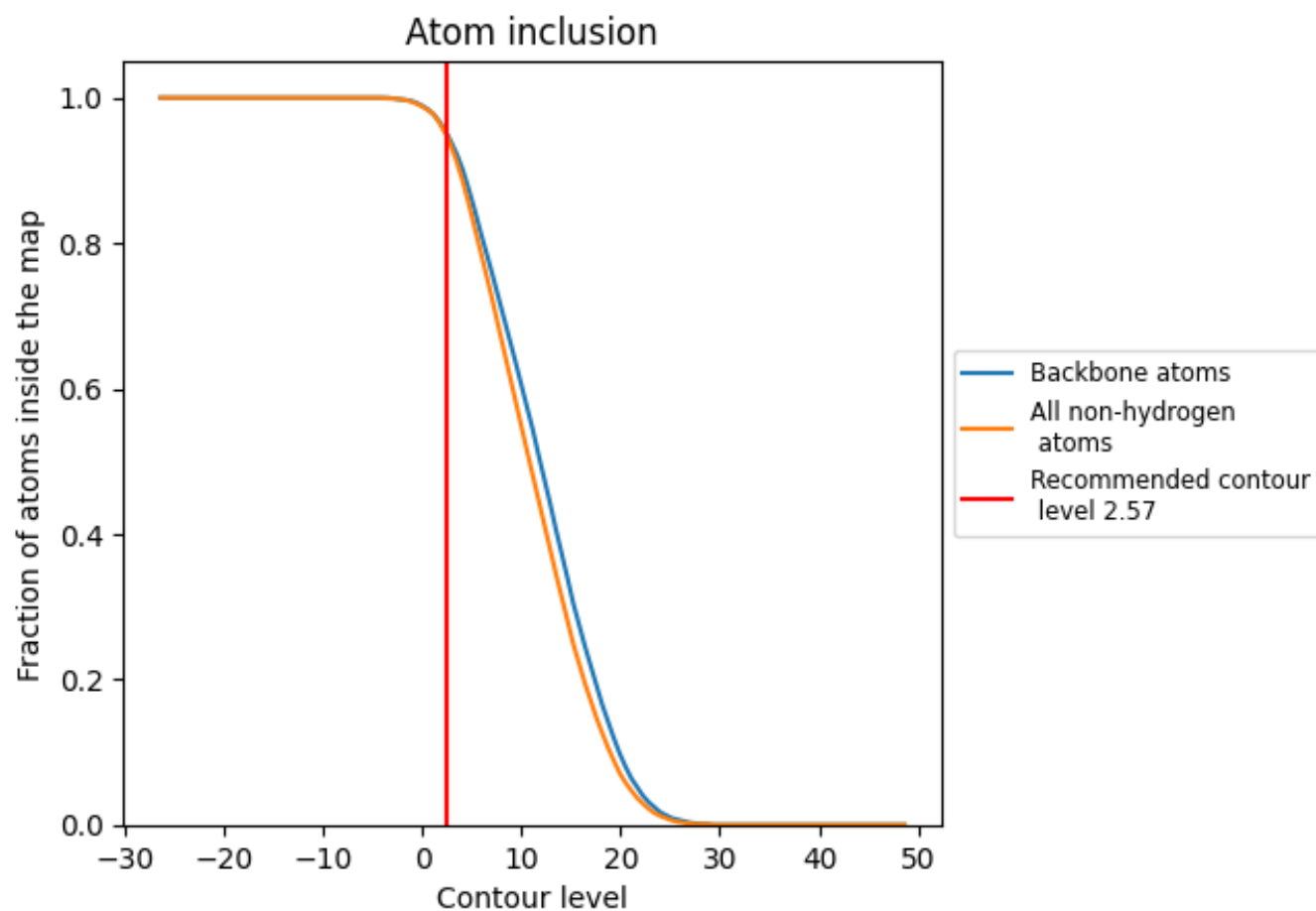
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.57).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (2.57) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9460	<div><div></div></div> 0.5490
1	<div><div></div></div> 0.8790	<div><div></div></div> 0.3980
2	<div><div></div></div> 0.9350	<div><div></div></div> 0.5010
3	<div><div></div></div> 0.9320	<div><div></div></div> 0.5130
4	<div><div></div></div> 0.9280	<div><div></div></div> 0.4910
A	<div><div></div></div> 0.9570	<div><div></div></div> 0.5800
B	<div><div></div></div> 0.9640	<div><div></div></div> 0.5900
C	<div><div></div></div> 0.9870	<div><div></div></div> 0.5880
D	<div><div></div></div> 0.9750	<div><div></div></div> 0.5830
E	<div><div></div></div> 0.9880	<div><div></div></div> 0.5750
F	<div><div></div></div> 0.9370	<div><div></div></div> 0.5560
G	<div><div></div></div> 0.9340	<div><div></div></div> 0.5440
H	<div><div></div></div> 0.9420	<div><div></div></div> 0.5440
I	<div><div></div></div> 0.9610	<div><div></div></div> 0.5630
J	<div><div></div></div> 0.8390	<div><div></div></div> 0.4940
K	<div><div></div></div> 0.8610	<div><div></div></div> 0.4450
L	<div><div></div></div> 0.9580	<div><div></div></div> 0.5700

1.0

0.0

<0.0