



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:53 PM UTC

PDB ID : 8J7B / pdb_00008j7b
EMDB ID : EMD-36037
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 2 (PSI-ST2)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

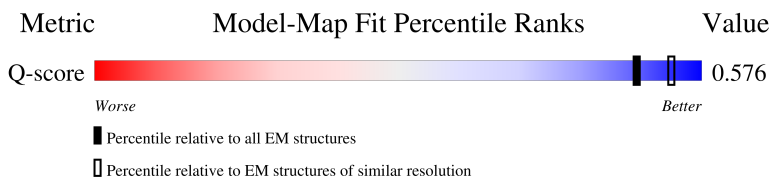
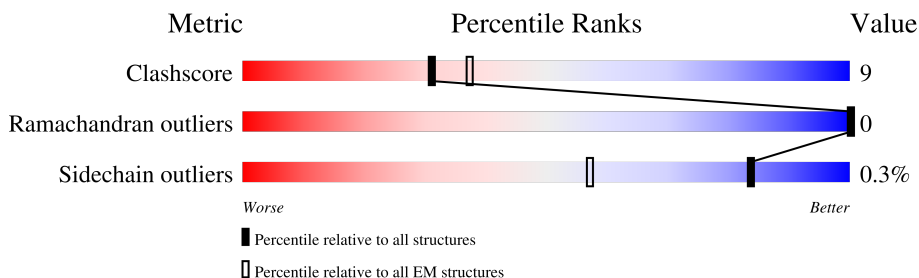
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.72 - 3.72)

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	
2	2	257	
3	3	273	
4	4	251	

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	204	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	A	845	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	G	203	X	-	-	-
18	CLA	H	201	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
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 35077 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	193	Total	C	N	O	S	0	0
			1496	975	248	268	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	218	Total	C	N	O	S	0	0
			1666	1088	270	303	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	737	Total	C	N	O	S	0	0
			5807	3807	986	996	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	S	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	152	Total	C	N	O	S	0	0
			1208	789	207	209	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	S	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	90	Total	C	N	O	S	0	0
			693	451	112	130			

- 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		

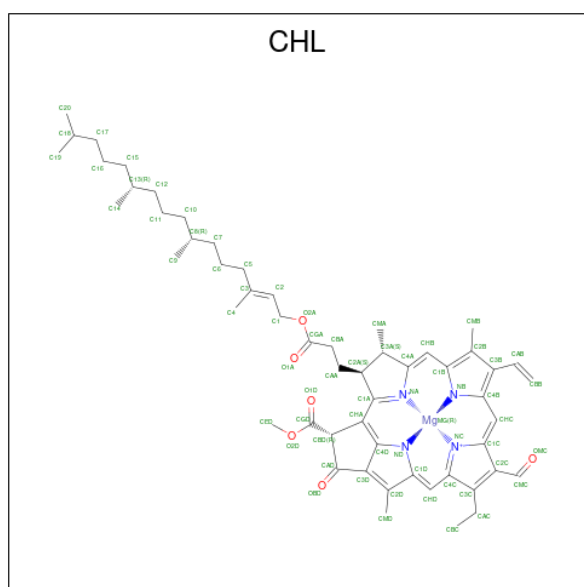
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	84	Total	C	N	O	S	0	0
			593	373	104	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	160	Total	C	N	O	S	0	0
			1207	799	191	215	2		

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



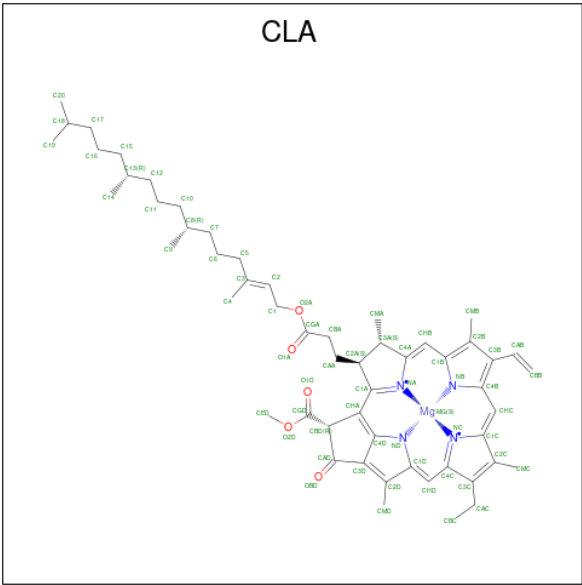
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
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 (CCD ID: 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 44	C 34	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 47	C 37	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 34	Mg 1	N 4	O 4	0
18	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	2	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	2	1	Total 44	C 34	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 36	C 30	Mg 1	N 4	O 1	0
18	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	3	1	Total 54	C 44	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 60	C 50	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 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	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 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 54	C 44	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	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	4	1	Total 42	C 34	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 50	C 40	Mg 1	N 4	O 5	0
18	4	1	Total 44	C 34	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 52	C 42	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 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	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
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 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 50	C 40	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 41	C 33	Mg 1	N 4	O 3	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 52	C 42	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

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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 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 55	C 45	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
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 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 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 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 51	C 41	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 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 43	C 35	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
18	B	1	Total 65	C 55	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 42	C 34	Mg 1	N 4	O 3	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 45	C 35	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 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 54	C 44	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 65	C 55	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 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

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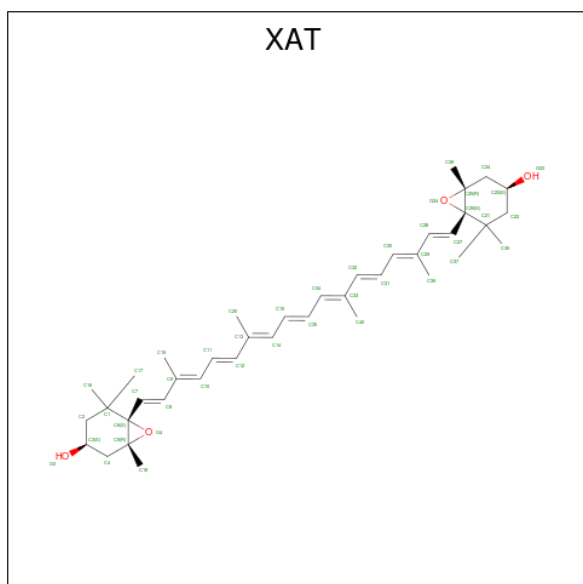
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 52	C 42	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 43	C 35	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 56	C 46	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 59	C 49	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 47	C 37	Mg 1	N 4	O 5	0
18	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	F	1	Total 51	C 41	Mg 1	N 4	O 5	0

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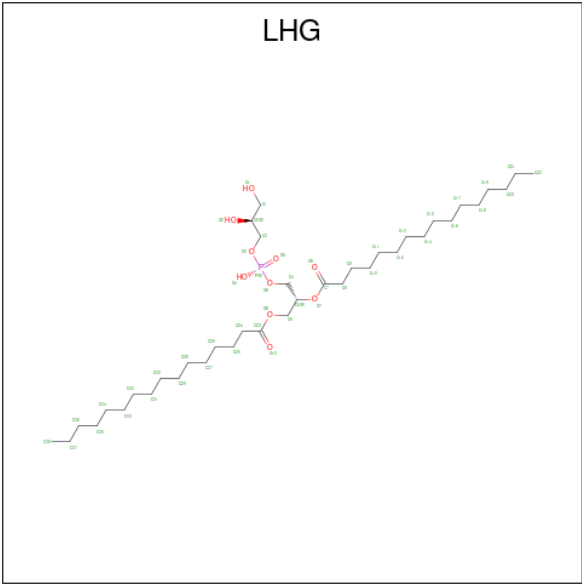
Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
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	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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



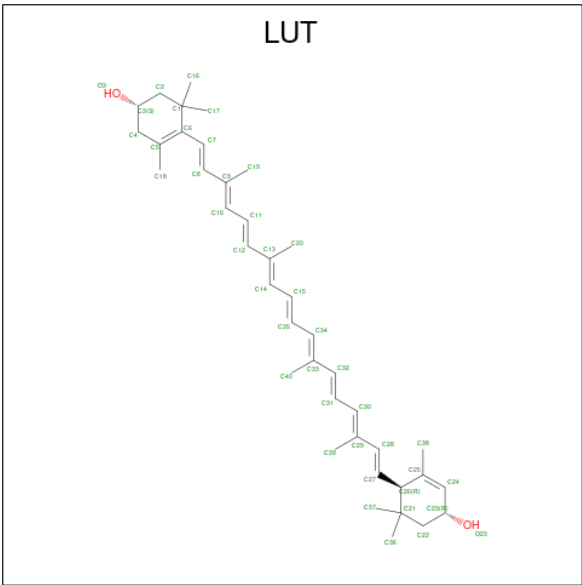
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	
19	4	1	Total	C	O	0
			44	40	4	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



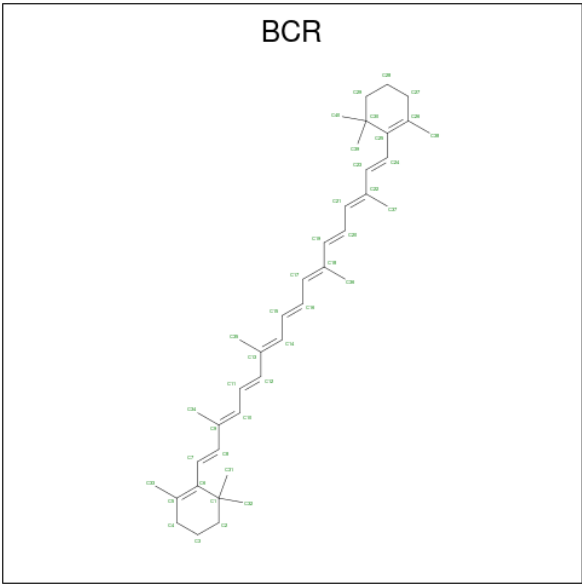
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: 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 (CCD ID: BCR) (formula: C₄₀H₅₆).



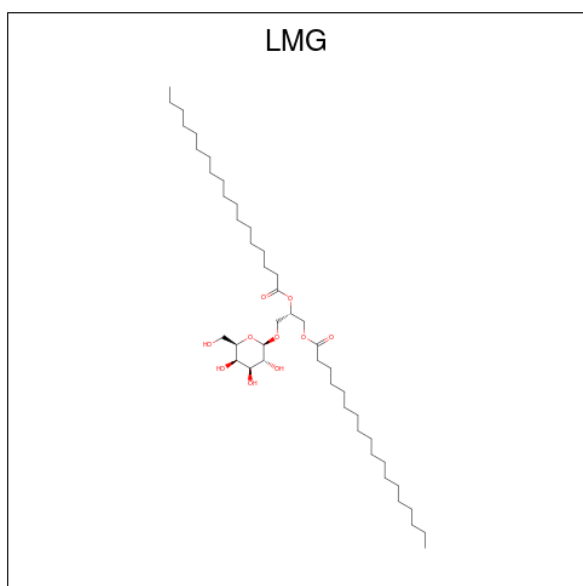
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 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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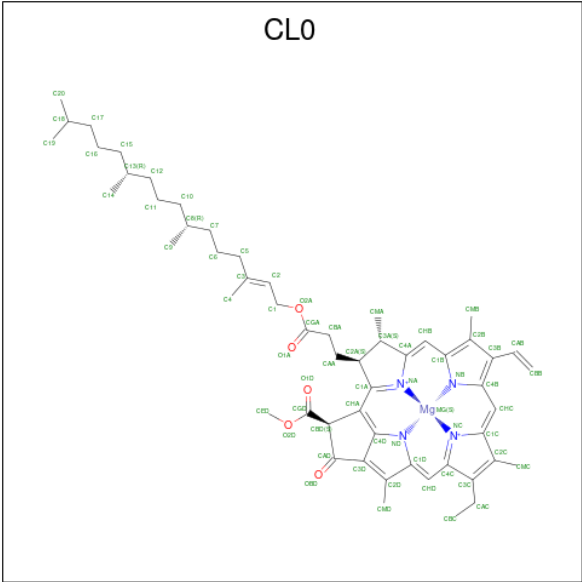
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	

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



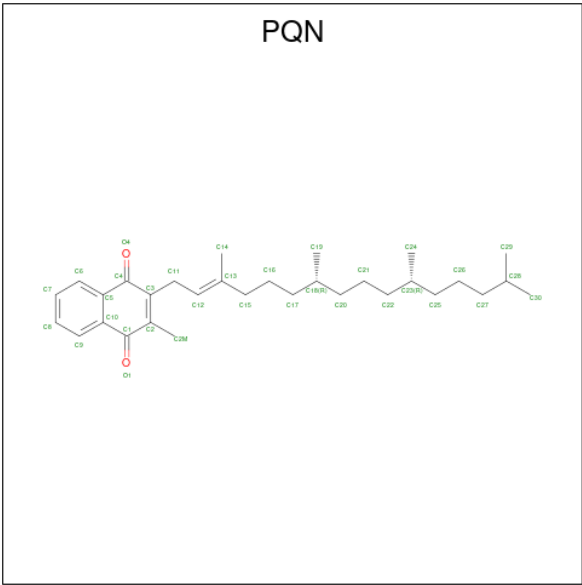
Mol	Chain	Residues	Atoms			AltConf
23	4	1	Total	C	O	0
			39	29	10	
23	4	1	Total	C	O	0
			33	23	10	

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



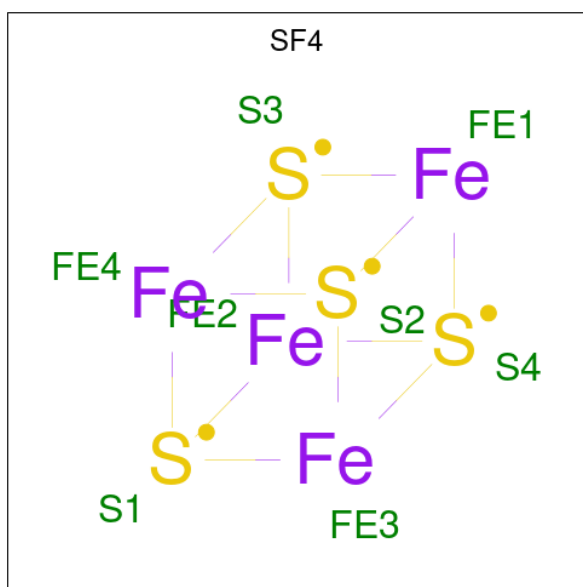
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	52	1	4	3	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



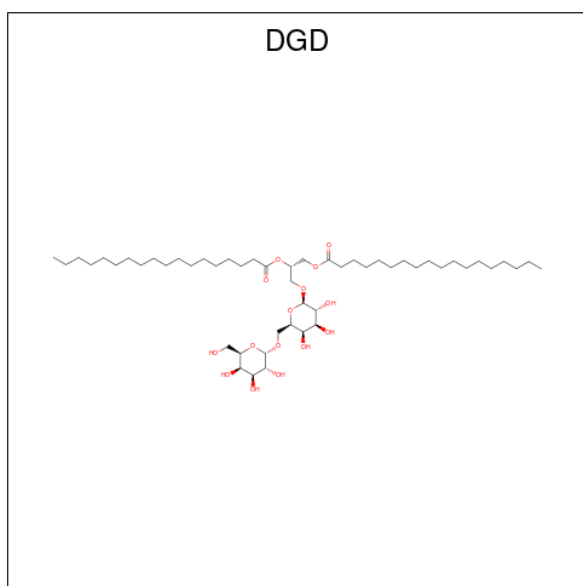
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

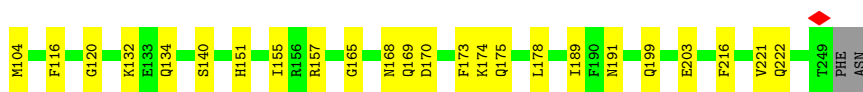


Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

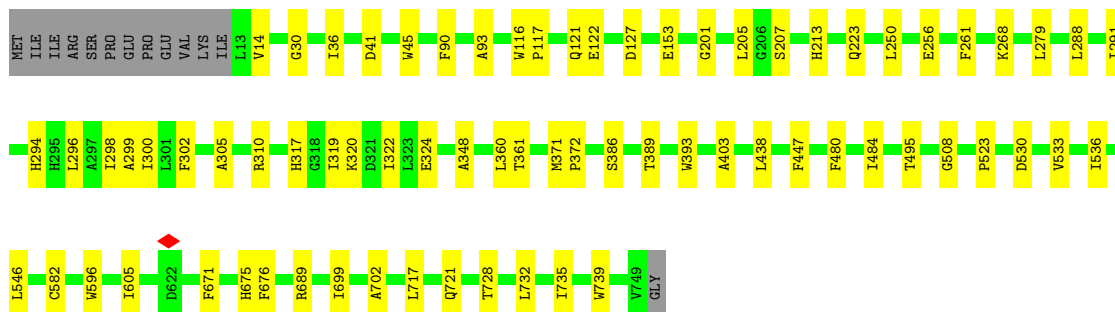
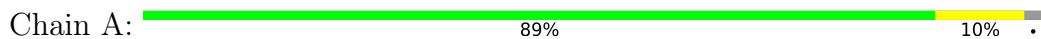
- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



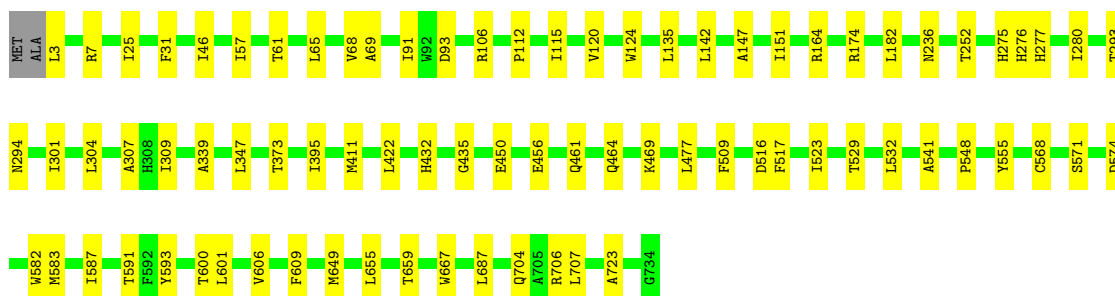
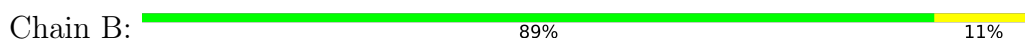
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			66	51	15	



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



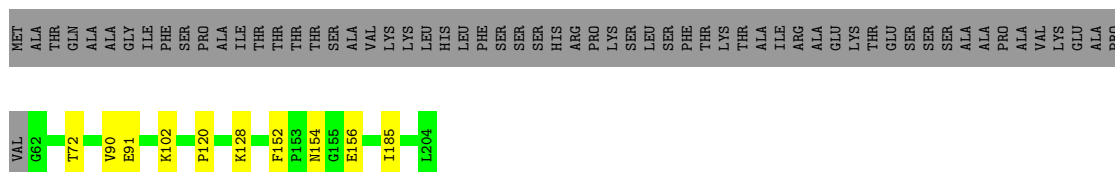
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 7: Photosystem I iron-sulfur center

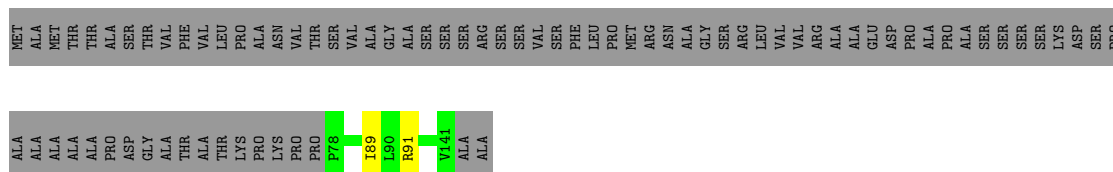


- Molecule 8: Photosystem I reaction center subunit II-2, chloroplatic



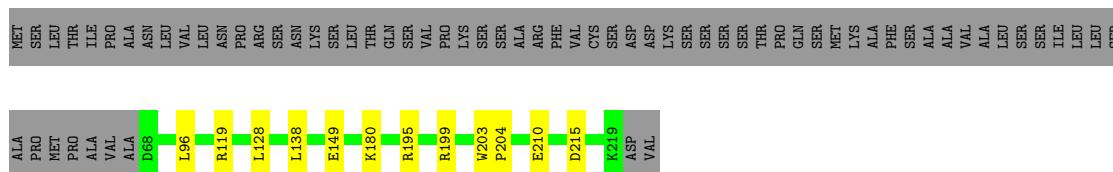
- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

Chain E:  43% 55%



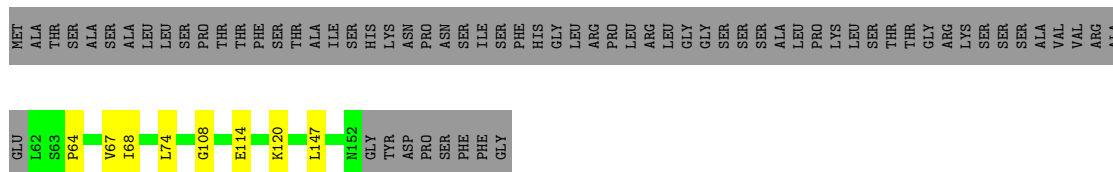
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:  63% 5% 31%



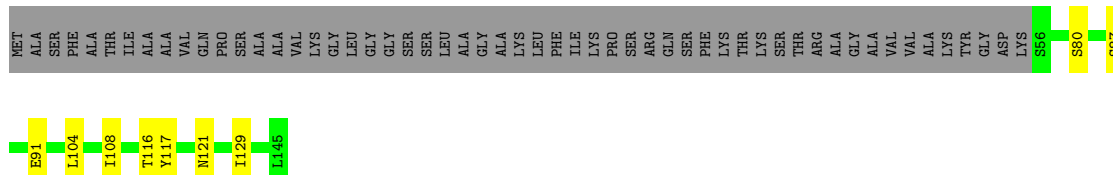
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G:  52% 5% 43%



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

Chain H:  56% 6% 38%



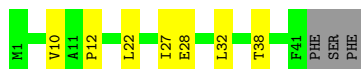
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  76% 8% 16%

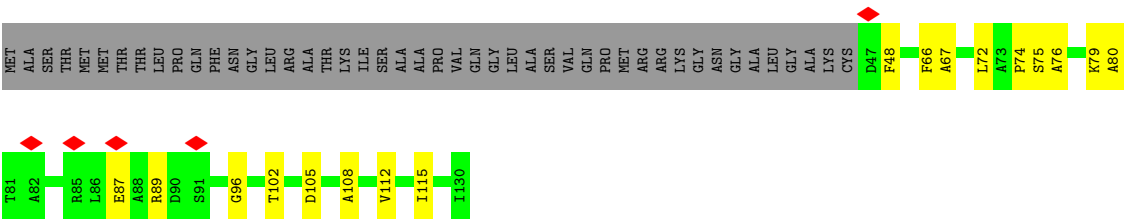


- Molecule 14: Photosystem I reaction center subunit IX

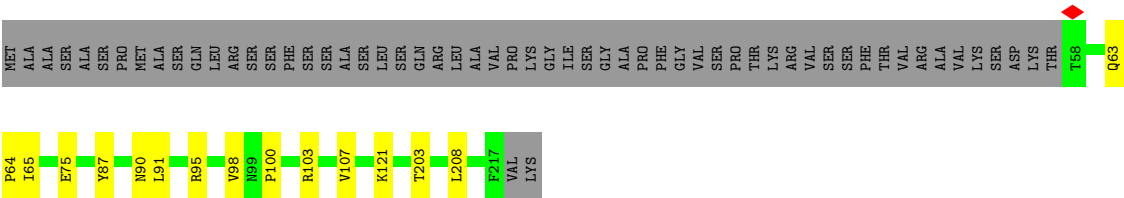
Chain J:  77% 16% 7%



● 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	137602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	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	35.714	Depositor
Minimum map value	-22.642	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	3.21	Depositor
Map size ($\text{\AA}$)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.12	0/1546	0.32	0/2110
2	2	0.12	0/1622	0.28	0/2219
3	3	0.13	0/1717	0.30	0/2336
4	4	0.12	0/1599	0.29	0/2178
5	A	0.10	0/6005	0.25	0/8194
6	B	0.11	0/6065	0.28	1/8279 (0.0%)
7	C	0.12	0/629	0.38	0/852
8	D	0.10	0/1157	0.30	0/1563
9	E	0.08	0/528	0.23	0/715
10	F	0.11	0/1238	0.26	0/1670
11	G	0.08	0/724	0.25	0/981
12	H	0.10	0/713	0.27	0/968
13	I	0.12	0/245	0.29	0/333
14	J	0.10	0/336	0.25	0/458
15	K	0.16	0/599	0.50	3/809 (0.4%)
16	L	0.10	0/1244	0.27	0/1700
All	All	0.11	0/25967	0.28	4/35365 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	74	PRO	CA-N-CD	-7.69	101.24	112.00
15	K	74	PRO	N-CD-CG	-5.20	95.41	103.20
6	B	477	LEU	CB-CA-C	-5.12	110.26	117.23
15	K	74	PRO	CB-CG-CD	-5.12	89.72	106.10

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	1496	0	1471	30	0
2	2	1566	0	1519	22	0
3	3	1666	0	1627	19	0
4	4	1551	0	1508	24	0
5	A	5807	0	5659	55	0
6	B	5854	0	5646	63	0
7	C	616	0	600	5	0
8	D	1128	0	1134	8	0
9	E	517	0	526	1	0
10	F	1208	0	1243	9	0
11	G	708	0	700	6	0
12	H	693	0	690	6	0
13	I	239	0	258	3	0
14	J	327	0	342	7	0
15	K	593	0	614	13	0
16	L	1207	0	1209	13	0
17	1	93	0	62	10	0
17	2	226	0	150	12	0
17	3	45	0	30	1	0
17	4	169	0	100	3	0
18	1	496	0	354	24	0
18	2	434	0	352	25	0
18	3	498	0	377	13	0
18	4	527	0	412	18	0
18	A	2533	0	2495	104	0
18	B	2284	0	2242	93	0
18	F	149	0	123	6	0
18	G	132	0	97	1	0
18	H	60	0	59	2	0
18	J	51	0	41	2	0
18	K	167	0	116	2	0
18	L	155	0	138	7	0
19	1	44	0	56	18	0
19	2	44	0	56	7	0
19	4	44	0	56	5	0
20	1	49	0	74	13	0
20	2	37	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	79	0	104	6	0
20	B	87	0	120	5	0
21	1	42	0	56	3	0
21	2	84	0	112	10	0
21	3	42	0	56	6	0
21	4	42	0	56	4	0
22	3	40	0	56	4	0
22	4	40	0	56	4	0
22	A	240	0	336	27	0
22	B	320	0	448	44	0
22	F	40	0	56	2	0
22	G	40	0	56	2	0
22	I	40	0	56	1	0
22	J	40	0	56	6	0
22	K	80	0	112	7	0
22	L	120	0	168	18	0
23	4	72	0	84	1	0
24	A	60	0	68	5	0
25	A	33	0	46	3	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	66	0	96	5	0
All	All	35077	0	34424	610	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 9.

The worst 5 of 610 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)
18:B:814:CLA:H3A	22:B:845:BCR:H393	1.51	0.91
17:1:601:CHL:HBB1	20:1:615:LHG:H252	1.57	0.84
21:2:619:LUT:H8	21:2:619:LUT:H181	1.60	0.82
22:B:801:BCR:H12C	22:B:801:BCR:H341	1.63	0.81
3:3:79:LEU:HD13	18:A:813:CLA:H2	1.63	0.81

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	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	198 (100%)	1 (0%)	0	100	100
3	3	216/273 (79%)	213 (99%)	3 (1%)	0	100	100
4	4	194/251 (77%)	191 (98%)	3 (2%)	0	100	100
5	A	735/750 (98%)	725 (99%)	10 (1%)	0	100	100
6	B	730/734 (100%)	716 (98%)	14 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	149 (99%)	1 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	28 (97%)	1 (3%)	0	100	100
14	J	39/44 (89%)	38 (97%)	1 (3%)	0	100	100
15	K	82/130 (63%)	82 (100%)	0	0	100	100
16	L	158/219 (72%)	155 (98%)	3 (2%)	0	100	100
All	All	3181/3890 (82%)	3133 (98%)	48 (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	153/190 (80%)	151 (99%)	2 (1%)	61	75
2	2	163/205 (80%)	163 (100%)	0	100	100
3	3	167/211 (79%)	166 (99%)	1 (1%)	78	83
4	4	163/210 (78%)	162 (99%)	1 (1%)	78	83
5	A	598/610 (98%)	597 (100%)	1 (0%)	87	88
6	B	599/600 (100%)	598 (100%)	1 (0%)	87	88
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	121/170 (71%)	121 (100%)	0	100	100
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	125/185 (68%)	124 (99%)	1 (1%)	73	80
11	G	77/133 (58%)	77 (100%)	0	100	100
12	H	75/113 (66%)	75 (100%)	0	100	100
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	126 (100%)	0	100	100
All	All	2618/3153 (83%)	2611 (100%)	7 (0%)	84	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	132	LYS
5	A	127	ASP
10	F	96	LEU
6	B	309	ILE
3	3	136	GLN

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

Mol	Chain	Res	Type
5	A	349	GLN
11	G	140	HIS
6	B	178	HIS
8	D	67	GLN
6	B	114	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

201 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	806	6	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	1	603	-	58,62,73	1.28	8 (13%)	68,99,113	1.37	5 (7%)
18	CLA	B	836	-	54,58,73	1.32	8 (14%)	64,95,113	3.34	9 (14%)
18	CLA	A	829	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
18	CLA	B	823	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	A	844	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	B	840	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	4 (4%)
18	CLA	B	833	-	49,53,73	1.39	7 (14%)	58,89,113	1.49	6 (10%)
18	CLA	3	604	-	44,49,73	1.44	8 (18%)	50,84,113	1.41	4 (8%)
22	BCR	A	849	-	41,41,41	1.38	8 (19%)	56,56,56	1.93	15 (26%)
18	CLA	4	613	-	49,53,73	1.39	7 (14%)	58,89,113	1.58	5 (8%)
22	BCR	3	614	-	41,41,41	1.39	8 (19%)	56,56,56	1.49	11 (19%)
18	CLA	B	834	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	6 (7%)
18	CLA	B	838	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	821	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
18	CLA	3	612	-	43,48,73	1.44	7 (16%)	51,83,113	1.51	5 (9%)
18	CLA	A	826	-	69,73,73	1.18	6 (8%)	82,113,113	1.27	5 (6%)
20	LHG	B	852	-	48,48,48	0.28	0	51,54,54	0.34	0
18	CLA	A	845	20	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
22	BCR	A	851	-	41,41,41	1.43	7 (17%)	56,56,56	2.41	19 (33%)
23	LMG	4	620	-	33,33,55	0.24	0	41,41,63	0.34	0
18	CLA	J	101	-	55,59,73	1.33	7 (12%)	64,96,113	1.38	5 (7%)
18	CLA	B	825	-	66,70,73	1.19	6 (9%)	78,109,113	1.34	9 (11%)
25	PQN	B	842	-	34,34,34	0.44	0	43,45,45	0.54	1 (2%)
18	CLA	A	814	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	3	601	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	6 (7%)
21	LUT	2	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.99	13 (25%)
18	CLA	A	810	5	54,58,73	1.33	8 (14%)	64,95,113	1.51	9 (14%)
18	CLA	B	821	-	51,55,73	1.34	7 (13%)	60,91,113	1.55	7 (11%)
18	CLA	A	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	7 (8%)
21	LUT	1	616	-	42,43,43	1.28	7 (16%)	51,60,60	2.11	15 (29%)
18	CLA	4	604	-	47,51,73	1.52	9 (19%)	58,87,113	1.46	6 (10%)
18	CLA	4	610	-	46,50,73	1.40	8 (17%)	53,85,113	1.43	4 (7%)
18	CLA	A	813	-	58,62,73	1.28	7 (12%)	68,99,113	1.40	6 (8%)
18	CLA	B	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	8 (9%)
18	CLA	A	817	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
18	CLA	A	838	-	55,59,73	1.32	8 (14%)	64,96,113	1.40	6 (9%)
18	CLA	4	601	4	50,54,73	1.36	8 (16%)	59,90,113	1.42	4 (6%)
21	LUT	2	619	-	42,43,43	1.29	8 (19%)	51,60,60	1.82	13 (25%)
17	CHL	1	606	-	35,49,74	4.56	17 (48%)	28,84,114	1.67	9 (32%)
18	CLA	B	818	-	64,68,73	1.22	6 (9%)	76,107,113	1.33	8 (10%)
18	CLA	A	827	-	63,67,73	1.23	7 (11%)	74,105,113	1.35	6 (8%)
20	LHG	A	847	18	29,29,48	0.33	0	32,35,54	0.44	0
18	CLA	2	604	-	46,51,73	1.41	8 (17%)	54,86,113	1.46	4 (7%)
18	CLA	A	811	-	69,73,73	1.17	7 (10%)	82,113,113	1.27	6 (7%)
22	BCR	B	843	-	41,41,41	1.39	8 (19%)	56,56,56	1.86	14 (25%)
18	CLA	A	819	-	63,67,73	1.23	8 (12%)	74,105,113	1.34	6 (8%)
27	DGD	B	850	-	67,67,67	0.85	2 (2%)	81,81,81	0.94	4 (4%)
17	CHL	2	601	2	41,55,74	4.16	18 (43%)	35,91,114	2.39	11 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	608	-	45,49,73	1.40	7 (15%)	54,84,113	1.55	6 (11%)
18	CLA	1	613	-	41,46,73	1.60	9 (21%)	51,81,113	1.55	7 (13%)
18	CLA	4	608	4	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
18	CLA	A	824	-	45,49,73	1.43	7 (15%)	54,84,113	1.48	5 (9%)
19	XAT	2	617	-	41,47,47	1.30	7 (17%)	54,74,74	2.00	14 (25%)
18	CLA	B	832	-	69,73,73	1.17	6 (8%)	82,113,113	1.24	4 (4%)
18	CLA	1	608	1	44,48,73	1.53	9 (20%)	55,83,113	1.53	8 (14%)
18	CLA	2	602	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	G	202	-	46,50,73	1.41	7 (15%)	53,85,113	1.43	4 (7%)
18	CLA	B	812	-	47,51,73	1.40	7 (14%)	55,86,113	1.41	4 (7%)
17	CHL	4	606	-	35,49,74	3.97	15 (42%)	33,84,114	2.38	11 (33%)
18	CLA	A	804	-	69,73,73	1.18	8 (11%)	82,113,113	1.37	7 (8%)
22	BCR	J	102	-	41,41,41	1.38	8 (19%)	56,56,56	1.69	14 (25%)
22	BCR	A	848	-	41,41,41	1.38	8 (19%)	56,56,56	1.52	11 (19%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
22	BCR	A	853	-	41,41,41	1.41	8 (19%)	56,56,56	1.71	15 (26%)
18	CLA	1	612	-	50,54,73	1.36	8 (16%)	59,90,113	1.48	5 (8%)
18	CLA	A	830	-	69,73,73	1.17	6 (8%)	82,113,113	1.38	7 (8%)
18	CLA	B	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)
18	CLA	A	807	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	6 (7%)
22	BCR	A	850	-	41,41,41	1.41	8 (19%)	56,56,56	1.85	13 (23%)
18	CLA	4	603	-	48,52,73	1.50	9 (18%)	59,88,113	1.46	6 (10%)
17	CHL	4	615	4	36,49,74	4.28	16 (44%)	30,84,114	2.06	9 (30%)
18	CLA	F	301	-	61,65,73	1.25	8 (13%)	72,103,113	1.30	5 (6%)
18	CLA	2	612	2	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
18	CLA	3	607	-	49,53,73	1.40	7 (14%)	58,89,113	1.43	4 (6%)
18	CLA	A	835	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
18	CLA	B	804	-	45,49,73	1.41	7 (15%)	54,84,113	1.54	6 (11%)
22	BCR	B	801	-	41,41,41	1.42	8 (19%)	56,56,56	1.71	13 (23%)
18	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
18	CLA	A	822	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	2	610	20	40,45,73	2.62	10 (25%)	46,76,113	1.33	6 (13%)
22	BCR	B	846	-	41,41,41	1.38	8 (19%)	56,56,56	1.62	11 (19%)
18	CLA	B	830	-	47,51,73	1.39	8 (17%)	55,86,113	1.44	4 (7%)
19	XAT	1	614	-	41,47,47	0.89	2 (4%)	54,74,74	3.01	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	K	201	15	41,45,73	1.47	8 (19%)	50,78,113	1.46	4 (8%)
22	BCR	B	844	-	41,41,41	1.37	8 (19%)	56,56,56	1.72	12 (21%)
18	CLA	1	604	-	53,57,73	1.33	8 (15%)	61,93,113	1.46	5 (8%)
18	CLA	A	815	-	49,53,73	1.38	7 (14%)	58,89,113	1.44	4 (6%)
18	CLA	2	611	-	48,52,73	1.41	7 (14%)	57,88,113	1.48	5 (8%)
17	CHL	4	605	-	35,49,74	4.11	17 (48%)	30,84,114	2.09	12 (40%)
18	CLA	B	829	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
18	CLA	B	835	-	46,50,73	1.41	8 (17%)	53,85,113	1.43	4 (7%)
22	BCR	B	849	-	41,41,41	1.38	8 (19%)	56,56,56	1.73	13 (23%)
18	CLA	A	820	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
22	BCR	F	304	-	41,41,41	1.39	7 (17%)	56,56,56	2.11	16 (28%)
18	CLA	A	831	-	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
18	CLA	4	609	-	58,62,73	1.27	9 (15%)	68,99,113	1.37	6 (8%)
18	CLA	A	808	-	54,58,73	1.33	8 (14%)	64,95,113	1.41	6 (9%)
18	CLA	4	602	4	64,68,73	1.21	7 (10%)	76,107,113	1.32	7 (9%)
18	CLA	A	837	5	49,53,73	1.40	7 (14%)	58,89,113	1.42	4 (6%)
21	LUT	3	613	-	42,43,43	1.30	8 (19%)	51,60,60	1.92	17 (33%)
17	CHL	2	607	-	45,59,74	3.93	19 (42%)	40,96,114	2.28	15 (37%)
18	CLA	B	826	-	66,70,73	1.20	7 (10%)	78,109,113	1.31	6 (7%)
18	CLA	A	840	-	56,60,73	1.31	7 (12%)	65,97,113	1.39	6 (9%)
18	CLA	1	609	-	46,50,73	1.40	8 (17%)	54,85,113	1.50	4 (7%)
18	CLA	F	303	10	45,49,73	1.43	6 (13%)	54,84,113	1.50	5 (9%)
23	LMG	4	619	-	39,39,55	0.22	0	47,47,63	0.25	0
18	CLA	A	833	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	4 (5%)
22	BCR	L	306	-	41,41,41	1.37	8 (19%)	56,56,56	1.83	16 (28%)
26	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	A	803	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
18	CLA	3	611	-	40,44,73	1.51	9 (22%)	49,77,113	1.47	4 (8%)
18	CLA	B	814	-	69,73,73	1.16	6 (8%)	82,113,113	1.28	6 (7%)
18	CLA	K	203	-	49,53,73	1.39	7 (14%)	58,89,113	1.46	5 (8%)
18	CLA	B	820	-	54,58,73	1.32	7 (12%)	64,95,113	1.42	6 (9%)
18	CLA	L	304	-	49,53,73	1.40	7 (14%)	58,89,113	1.45	4 (6%)
18	CLA	4	611	-	44,49,73	1.45	8 (18%)	50,84,113	1.42	4 (8%)
18	CLA	L	303	-	69,73,73	1.16	6 (8%)	82,113,113	1.30	6 (7%)
22	BCR	I	101	-	41,41,41	1.38	8 (19%)	56,56,56	1.42	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CHL	3	606	-	38,53,74	3.94	18 (47%)	36,89,114	2.34	11 (30%)
18	CLA	B	808	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
18	CLA	A	825	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
18	CLA	2	609	-	51,55,73	1.34	8 (15%)	60,91,113	1.43	6 (10%)
18	CLA	B	837	-	69,73,73	1.17	6 (8%)	82,113,113	1.30	6 (7%)
18	CLA	B	810	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
19	XAT	4	617	-	41,47,47	1.28	8 (19%)	54,74,74	1.66	12 (22%)
22	BCR	B	845	-	41,41,41	1.41	8 (19%)	56,56,56	1.74	14 (25%)
18	CLA	4	612	-	61,65,73	1.24	7 (11%)	72,103,113	1.35	6 (8%)
25	PQN	A	855	-	34,34,34	0.42	0	43,45,45	0.57	1 (2%)
18	CLA	A	809	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	B	817	-	63,67,73	1.23	9 (14%)	74,105,113	1.32	6 (8%)
18	CLA	K	206	15	42,47,73	1.50	7 (16%)	48,81,113	1.48	5 (10%)
18	CLA	A	841	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
17	CHL	1	601	1	46,60,74	3.94	18 (39%)	40,97,114	1.86	13 (32%)
18	CLA	B	803	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
18	CLA	A	843	-	69,73,73	1.17	6 (8%)	82,113,113	1.29	4 (4%)
18	CLA	A	816	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
22	BCR	B	847	-	41,41,41	1.39	8 (19%)	56,56,56	1.49	11 (19%)
18	CLA	3	610	-	43,48,73	1.46	7 (16%)	51,83,113	1.48	5 (9%)
18	CLA	B	827	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
18	CLA	1	605	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)
18	CLA	G	201	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
18	CLA	B	811	-	58,62,73	1.36	9 (15%)	71,100,113	1.41	7 (9%)
18	CLA	B	802	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	BCR	K	205	-	41,41,41	1.38	8 (19%)	56,56,56	1.90	17 (30%)
18	CLA	3	602	-	59,63,73	1.28	8 (13%)	70,101,113	1.32	5 (7%)
18	CLA	B	809	6	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
18	CLA	3	605	-	45,49,73	1.51	9 (20%)	54,84,113	1.52	6 (11%)
18	CLA	A	818	-	64,68,73	1.21	7 (10%)	76,107,113	5.01	7 (9%)
18	CLA	2	603	-	47,52,73	1.42	8 (17%)	55,88,113	1.42	4 (7%)
18	CLA	G	203	11	49,53,73	1.39	7 (14%)	58,89,113	1.44	5 (8%)
18	CLA	H	201	-	64,68,73	1.22	8 (12%)	76,107,113	1.30	4 (5%)
18	CLA	B	841	20	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
17	CHL	2	605	-	36,50,74	4.10	17 (47%)	31,85,114	2.30	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	824	-	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
18	CLA	A	805	-	56,60,73	1.30	6 (10%)	65,97,113	1.39	5 (7%)
22	BCR	L	305	-	41,41,41	1.40	8 (19%)	56,56,56	1.68	15 (26%)
18	CLA	B	816	-	59,63,73	1.26	7 (11%)	70,101,113	1.36	6 (8%)
17	CHL	4	607	-	40,54,74	4.13	19 (47%)	34,90,114	2.49	12 (35%)
20	LHG	B	851	18	37,37,48	0.30	0	40,43,54	0.49	0
18	CLA	3	609	-	57,62,73	1.30	8 (14%)	67,100,113	1.32	5 (7%)
26	SF4	C	102	-	0,12,12	-	-	-	-	-
22	BCR	B	848	-	41,41,41	1.39	8 (19%)	56,56,56	1.51	12 (21%)
18	CLA	1	602	1	58,62,73	1.28	7 (12%)	68,99,113	1.35	5 (7%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.54	1 (2%)
24	CL0	A	801	-	53,67,73	3.01	17 (32%)	47,102,113	2.28	12 (25%)
22	BCR	G	204	-	41,41,41	1.38	8 (19%)	56,56,56	1.57	12 (21%)
18	CLA	A	832	-	54,58,73	1.31	7 (12%)	64,95,113	1.42	6 (9%)
20	LHG	A	846	-	48,48,48	0.27	0	51,54,54	0.34	0
17	CHL	2	606	-	37,51,74	4.35	17 (45%)	30,86,114	2.45	12 (40%)
18	CLA	B	807	-	56,60,73	1.30	6 (10%)	65,97,113	1.39	5 (7%)
22	BCR	A	852	-	41,41,41	1.38	8 (19%)	56,56,56	1.83	15 (26%)
18	CLA	2	608	-	49,53,73	1.38	6 (12%)	58,89,113	1.44	4 (6%)
18	CLA	A	812	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
18	CLA	B	805	-	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
22	BCR	4	618	-	41,41,41	1.38	8 (19%)	56,56,56	1.63	10 (17%)
22	BCR	K	202	-	41,41,41	1.38	8 (19%)	56,56,56	1.85	14 (25%)
18	CLA	2	613	-	47,51,73	1.40	8 (17%)	55,86,113	1.42	4 (7%)
18	CLA	F	302	-	55,59,73	1.32	8 (14%)	64,96,113	1.43	6 (9%)
18	CLA	1	610	20	41,46,73	1.60	9 (21%)	51,81,113	1.54	7 (13%)
18	CLA	A	823	-	46,50,73	1.40	6 (13%)	53,85,113	1.45	5 (9%)
18	CLA	B	828	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
17	CHL	2	615	2	37,51,74	4.37	17 (45%)	30,86,114	2.30	10 (33%)
18	CLA	1	611	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	1	607	-	47,52,73	1.42	7 (14%)	55,88,113	1.42	4 (7%)
22	BCR	L	301	-	41,41,41	1.39	8 (19%)	56,56,56	2.10	12 (21%)
18	CLA	3	603	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
18	CLA	A	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
18	CLA	A	802	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	836	-	49,53,73	1.41	8 (16%)	58,89,113	1.43	4 (6%)
18	CLA	B	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	L	302	-	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
18	CLA	B	813	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	8 (9%)
18	CLA	B	815	-	47,51,73	1.38	7 (14%)	55,86,113	1.44	4 (7%)
18	CLA	K	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.43	4 (6%)
18	CLA	A	839	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	6 (8%)
18	CLA	A	834	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
18	CLA	4	614	-	54,58,73	1.32	8 (14%)	64,95,113	1.44	6 (9%)
26	SF4	C	101	-	0,12,12	-	-	-	-	-
21	LUT	4	616	-	42,43,43	1.28	8 (19%)	51,60,60	1.49	11 (21%)
18	CLA	B	831	-	47,51,73	1.39	7 (14%)	55,86,113	1.45	4 (7%)

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	806	6	1/1/15/20	11/39/115/115	-
18	CLA	1	603	-	1/1/12/20	8/26/102/115	-
18	CLA	B	836	-	1/1/12/20	7/21/97/115	-
18	CLA	A	829	-	1/1/15/20	15/39/115/115	-
18	CLA	B	823	-	1/1/11/20	6/15/91/115	-
18	CLA	A	844	-	1/1/15/20	12/39/115/115	-
18	CLA	B	840	-	1/1/15/20	18/39/115/115	-
18	CLA	B	833	-	1/1/11/20	4/15/91/115	-
18	CLA	3	604	-	1/1/10/20	2/10/86/115	-
22	BCR	A	849	-	-	6/29/63/63	0/2/2/2
18	CLA	4	613	-	1/1/11/20	2/15/91/115	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	B	834	-	1/1/14/20	9/33/109/115	-
18	CLA	B	838	-	1/1/11/20	0/18/94/115	-
18	CLA	A	821	-	1/1/11/20	1/15/91/115	-
18	CLA	3	612	-	1/1/10/20	2/8/84/115	-
18	CLA	A	826	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	B	852	-	-	13/53/53/53	-
18	CLA	A	845	20	1/1/12/20	6/21/97/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
23	LMG	4	620	-	-	7/28/48/70	0/1/1/1
18	CLA	J	101	-	1/1/12/20	7/23/99/115	-
18	CLA	B	825	-	1/1/14/20	10/36/112/115	-
25	PQN	B	842	-	-	6/23/43/43	0/2/2/2
18	CLA	A	814	-	1/1/15/20	11/39/115/115	-
18	CLA	3	601	-	1/1/14/20	13/33/109/115	-
21	LUT	2	616	-	-	4/29/67/67	0/2/2/2
18	CLA	A	810	5	1/1/12/20	4/21/97/115	-
18	CLA	B	821	-	1/1/11/20	3/18/94/115	-
18	CLA	A	842	-	1/1/15/20	16/39/115/115	-
21	LUT	1	616	-	-	2/29/67/67	0/2/2/2
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	4	610	-	1/1/10/20	2/12/88/115	-
18	CLA	A	813	-	1/1/12/20	11/26/102/115	-
18	CLA	B	822	-	1/1/15/20	15/39/115/115	-
18	CLA	A	817	-	1/1/11/20	4/15/91/115	-
18	CLA	A	838	-	1/1/12/20	7/23/99/115	-
18	CLA	4	601	4	1/1/11/20	5/17/93/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
18	CLA	B	818	-	1/1/14/20	8/33/109/115	-
18	CLA	A	827	-	1/1/13/20	2/32/108/115	-
20	LHG	A	847	18	-	1/34/34/53	-
18	CLA	2	604	-	1/1/10/20	9/12/88/115	-
18	CLA	A	811	-	1/1/15/20	9/39/115/115	-
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	A	819	-	1/1/13/20	17/32/108/115	-
27	DGD	B	850	-	-	11/55/95/95	0/2/2/2
17	CHL	2	601	2	3/3/16/26	6/17/115/137	-
18	CLA	3	608	-	1/1/10/20	2/10/86/115	-
18	CLA	1	613	-	1/1/10/20	0/4/80/115	-
18	CLA	4	608	4	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	824	-	1/1/10/20	4/10/86/115	-
19	XAT	2	617	-	-	17/31/93/93	0/4/4/4
18	CLA	B	832	-	1/1/15/20	13/39/115/115	-
18	CLA	1	608	1	1/1/10/20	2/8/84/115	-
18	CLA	2	602	2	1/1/15/20	16/39/115/115	-
18	CLA	G	202	-	1/1/10/20	4/12/88/115	-
18	CLA	B	812	-	1/1/10/20	0/13/89/115	-
17	CHL	4	606	-	3/3/15/26	4/10/106/137	-
18	CLA	A	804	-	1/1/15/20	17/39/115/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	LHG	1	615	18	-	34/53/53/53	-
22	BCR	A	853	-	-	3/29/63/63	0/2/2/2
18	CLA	1	612	-	1/1/11/20	8/17/93/115	-
18	CLA	A	830	-	1/1/15/20	13/39/115/115	-
18	CLA	B	819	-	1/1/13/20	11/27/103/115	-
18	CLA	A	807	-	1/1/15/20	12/39/115/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
18	CLA	4	603	-	1/1/11/20	5/13/89/115	-
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
18	CLA	F	301	-	1/1/13/20	14/30/106/115	-
18	CLA	2	612	2	1/1/15/20	14/39/115/115	-
18	CLA	3	607	-	1/1/11/20	3/15/91/115	-
18	CLA	A	835	-	1/1/15/20	18/39/115/115	-
18	CLA	B	804	-	1/1/10/20	2/10/86/115	-
22	BCR	B	801	-	-	4/29/63/63	0/2/2/2
18	CLA	A	828	-	1/1/15/20	7/39/115/115	-
18	CLA	A	822	-	1/1/15/20	11/39/115/115	-
18	CLA	2	610	20	1/1/7/20	5/10/70/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	B	830	-	1/1/10/20	2/13/89/115	-
19	XAT	1	614	-	-	8/31/93/93	0/4/4/4
18	CLA	K	201	15	1/1/8/20	2/4/76/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	604	-	1/1/11/20	6/20/96/115	-
18	CLA	A	815	-	1/1/11/20	5/15/91/115	-
18	CLA	2	611	-	1/1/11/20	5/13/89/115	-
17	CHL	4	605	-	3/3/15/26	3/8/106/137	-
18	CLA	B	829	-	1/1/13/20	3/29/105/115	-
18	CLA	B	835	-	1/1/10/20	6/12/88/115	-
22	BCR	B	849	-	-	7/29/63/63	0/2/2/2
18	CLA	A	820	-	1/1/15/20	12/39/115/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	A	831	-	1/1/15/20	11/39/115/115	-
18	CLA	4	609	-	1/1/12/20	7/26/102/115	-
18	CLA	A	808	-	1/1/12/20	4/21/97/115	-
18	CLA	4	602	4	1/1/14/20	5/33/109/115	-
18	CLA	A	837	5	1/1/11/20	3/15/91/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
17	CHL	2	607	-	3/3/17/26	8/21/119/137	-
18	CLA	B	826	-	1/1/14/20	6/36/112/115	-
18	CLA	A	840	-	1/1/12/20	6/24/100/115	-
18	CLA	1	609	-	1/1/10/20	4/11/87/115	-
18	CLA	F	303	10	1/1/10/20	4/10/86/115	-
23	LMG	4	619	-	-	5/34/54/70	0/1/1/1
18	CLA	A	833	-	1/1/13/20	7/29/105/115	-
22	BCR	L	306	-	-	5/29/63/63	0/2/2/2
26	SF4	A	854	-	-	-	0/6/5/5
18	CLA	A	803	-	1/1/15/20	19/39/115/115	-
18	CLA	3	611	-	1/1/8/20	2/2/74/115	-
18	CLA	B	814	-	1/1/15/20	14/39/115/115	-
18	CLA	K	203	-	1/1/11/20	6/15/91/115	-
18	CLA	B	820	-	1/1/12/20	5/21/97/115	-
18	CLA	L	304	-	1/1/11/20	3/15/91/115	-
18	CLA	4	611	-	1/1/10/20	6/10/86/115	-
18	CLA	L	303	-	1/1/15/20	10/39/115/115	-
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
17	CHL	3	606	-	3/3/16/26	5/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	808	-	1/1/15/20	16/39/115/115	-
18	CLA	A	825	-	1/1/13/20	7/27/103/115	-
18	CLA	2	609	-	1/1/11/20	7/18/94/115	-
18	CLA	B	837	-	1/1/15/20	10/39/115/115	-
18	CLA	B	810	-	1/1/15/20	10/39/115/115	-
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	4	612	-	1/1/13/20	11/30/106/115	-
25	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	A	809	-	1/1/15/20	14/39/115/115	-
18	CLA	B	817	-	1/1/13/20	11/32/108/115	-
18	CLA	K	206	15	1/1/9/20	1/8/80/115	-
18	CLA	A	841	-	1/1/15/20	13/39/115/115	-
17	CHL	1	601	1	3/3/17/26	9/22/120/137	-
18	CLA	B	803	-	1/1/15/20	9/39/115/115	-
18	CLA	A	843	-	1/1/15/20	11/39/115/115	-
18	CLA	A	816	-	1/1/10/20	4/12/88/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	3	610	-	1/1/10/20	3/8/84/115	-
18	CLA	B	827	-	1/1/15/20	21/39/115/115	-
18	CLA	1	605	-	1/1/11/20	7/17/93/115	-
18	CLA	G	201	-	1/1/11/20	9/15/91/115	-
18	CLA	B	811	-	1/1/13/20	11/25/101/115	-
18	CLA	B	802	-	1/1/15/20	14/39/115/115	-
22	BCR	K	205	-	-	9/29/63/63	0/2/2/2
18	CLA	3	602	-	1/1/13/20	11/27/103/115	-
18	CLA	B	809	6	1/1/15/20	18/39/115/115	-
18	CLA	3	605	-	1/1/10/20	6/10/86/115	-
18	CLA	A	818	-	1/1/14/20	13/33/109/115	-
18	CLA	2	603	-	1/1/11/20	3/13/89/115	-
18	CLA	G	203	11	1/1/11/20	3/15/91/115	-
18	CLA	H	201	-	1/1/14/20	14/33/109/115	-
18	CLA	B	841	20	1/1/15/20	20/39/115/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	824	-	1/1/15/20	12/39/115/115	-
18	CLA	A	805	-	1/1/12/20	5/24/100/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	B	816	-	1/1/13/20	6/27/103/115	-
17	CHL	4	607	-	3/3/16/26	4/15/113/137	-
20	LHG	B	851	18	-	5/42/42/53	-
18	CLA	3	609	-	1/1/13/20	8/25/101/115	-
26	SF4	C	102	-	-	-	0/6/5/5
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
18	CLA	1	602	1	1/1/12/20	5/26/102/115	-
24	CL0	A	801	-	2/2/16/25	8/31/115/135	-
20	LHG	2	618	18	-	9/41/41/53	-
22	BCR	G	204	-	-	2/29/63/63	0/2/2/2
18	CLA	A	832	-	1/1/12/20	4/21/97/115	-
20	LHG	A	846	-	-	4/53/53/53	-
17	CHL	2	606	-	3/3/15/26	4/12/110/137	-
18	CLA	B	807	-	1/1/12/20	5/24/100/115	-
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
18	CLA	2	608	-	1/1/11/20	7/15/91/115	-
18	CLA	A	812	-	1/1/15/20	19/39/115/115	-
18	CLA	B	805	-	1/1/15/20	16/39/115/115	-
22	BCR	4	618	-	-	6/29/63/63	0/2/2/2
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	2	613	-	1/1/10/20	5/13/89/115	-
18	CLA	F	302	-	1/1/12/20	6/23/99/115	-
18	CLA	1	610	20	1/1/10/20	1/4/80/115	-
18	CLA	A	823	-	1/1/10/20	4/12/88/115	-
18	CLA	B	828	-	1/1/15/20	17/39/115/115	-
17	CHL	2	615	2	3/3/15/26	2/12/110/137	-
18	CLA	1	611	-	1/1/11/20	6/15/91/115	-
18	CLA	1	607	-	1/1/11/20	8/13/89/115	-
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	3	603	-	1/1/11/20	9/15/91/115	-
18	CLA	A	806	-	1/1/15/20	18/39/115/115	-
18	CLA	A	802	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	836	-	1/1/11/20	9/15/91/115	-
18	CLA	B	839	-	1/1/15/20	9/39/115/115	-
18	CLA	L	302	-	1/1/11/20	2/15/91/115	-
18	CLA	B	813	-	1/1/15/20	15/39/115/115	-
18	CLA	B	815	-	1/1/10/20	2/13/89/115	-
18	CLA	K	204	-	1/1/11/20	12/17/93/115	-
18	CLA	A	839	-	1/1/13/20	9/27/103/115	-
18	CLA	A	834	-	1/1/15/20	9/39/115/115	-
18	CLA	4	614	-	1/1/12/20	10/21/97/115	-
26	SF4	C	101	-	-	-	0/6/5/5
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	B	831	-	1/1/10/20	0/13/89/115	-

The worst 5 of 1538 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	610	CLA	C1A-NA	13.18	1.40	1.29
17	1	606	CHL	C2C-C3C	11.26	1.47	1.36
17	1	601	CHL	C2C-C3C	10.85	1.46	1.36
17	2	615	CHL	C2C-C3C	10.85	1.46	1.36
17	2	606	CHL	C2C-C3C	10.85	1.46	1.36

The worst 5 of 1364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.49	157.54	111.23
18	A	818	CLA	O2D-CGD-O1D	-25.34	74.53	123.85
18	A	818	CLA	O1D-CGD-CBD	-21.04	83.01	124.52
18	B	836	CLA	C5-C3-C4	-15.99	77.79	114.59
18	B	836	CLA	C4-C3-C2	-13.38	82.51	122.66

5 of 179 chirality outliers are listed below:

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

5 of 1473 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	2	605	CHL	C1C-C2C-CMC-OMC
17	2	605	CHL	C3C-C2C-CMC-OMC
17	2	601	CHL	C3A-C2A-CAA-CBA
17	2	607	CHL	CHA-CBD-CGD-O1D
17	3	606	CHL	CHA-CBD-CGD-O2D

There are no ring outliers.

164 monomers are involved in 464 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	806	CLA	3	0
18	1	603	CLA	1	0
18	B	836	CLA	2	0
18	A	829	CLA	6	0
18	B	823	CLA	2	0
18	A	844	CLA	4	0
18	B	840	CLA	6	0
18	B	833	CLA	1	0
22	A	849	BCR	2	0
18	4	613	CLA	2	0
22	3	614	BCR	4	0
18	B	834	CLA	1	0
18	B	838	CLA	2	0
18	A	821	CLA	2	0
18	3	612	CLA	1	0
18	A	826	CLA	2	0
20	B	852	LHG	3	0
18	A	845	CLA	1	0
22	A	851	BCR	8	0
23	4	620	LMG	1	0
18	J	101	CLA	2	0
18	B	825	CLA	2	0
25	B	842	PQN	2	0
18	A	814	CLA	2	0
18	3	601	CLA	4	0
21	2	616	LUT	4	0
18	A	810	CLA	1	0
18	B	821	CLA	1	0
18	A	842	CLA	5	0
21	1	616	LUT	3	0
18	4	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	813	CLA	4	0
18	B	822	CLA	8	0
18	A	817	CLA	1	0
21	2	619	LUT	6	0
18	B	818	CLA	4	0
18	A	827	CLA	1	0
18	2	604	CLA	5	0
18	A	811	CLA	3	0
22	B	843	BCR	4	0
18	A	819	CLA	4	0
27	B	850	DGD	5	0
17	2	601	CHL	1	0
18	4	608	CLA	2	0
19	2	617	XAT	7	0
18	B	832	CLA	6	0
18	1	608	CLA	1	0
18	2	602	CLA	8	0
18	B	812	CLA	1	0
18	A	804	CLA	6	0
22	J	102	BCR	6	0
22	A	848	BCR	3	0
20	1	615	LHG	13	0
22	A	853	BCR	7	0
18	1	612	CLA	1	0
18	A	830	CLA	4	0
18	B	819	CLA	1	0
18	A	807	CLA	3	0
22	A	850	BCR	5	0
18	4	603	CLA	1	0
17	4	615	CHL	1	0
18	F	301	CLA	1	0
18	2	612	CLA	4	0
18	3	607	CLA	3	0
18	A	835	CLA	5	0
18	B	804	CLA	1	0
22	B	801	BCR	10	0
18	A	828	CLA	1	0
18	A	822	CLA	4	0
22	B	846	BCR	7	0
18	B	830	CLA	1	0
19	1	614	XAT	18	0
18	K	201	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	844	BCR	2	0
18	1	604	CLA	3	0
18	A	815	CLA	1	0
17	4	605	CHL	1	0
22	B	849	BCR	4	0
18	A	820	CLA	4	0
22	F	304	BCR	2	0
18	A	831	CLA	1	0
18	4	609	CLA	4	0
18	A	808	CLA	2	0
18	4	602	CLA	5	0
21	3	613	LUT	6	0
17	2	607	CHL	2	0
18	B	826	CLA	3	0
18	A	840	CLA	1	0
18	1	609	CLA	7	0
18	A	833	CLA	3	0
22	L	306	BCR	5	0
18	A	803	CLA	3	0
18	B	814	CLA	3	0
18	B	820	CLA	2	0
18	L	303	CLA	5	0
22	I	101	BCR	1	0
17	3	606	CHL	1	0
18	B	808	CLA	5	0
18	A	825	CLA	3	0
18	2	609	CLA	5	0
18	B	837	CLA	2	0
19	4	617	XAT	5	0
22	B	845	BCR	8	0
18	4	612	CLA	2	0
25	A	855	PQN	3	0
18	A	809	CLA	9	0
18	B	817	CLA	3	0
18	A	841	CLA	6	0
17	1	601	CHL	10	0
18	B	803	CLA	4	0
18	A	843	CLA	2	0
22	B	847	BCR	4	0
18	B	827	CLA	5	0
18	1	605	CLA	1	0
18	G	201	CLA	1	0

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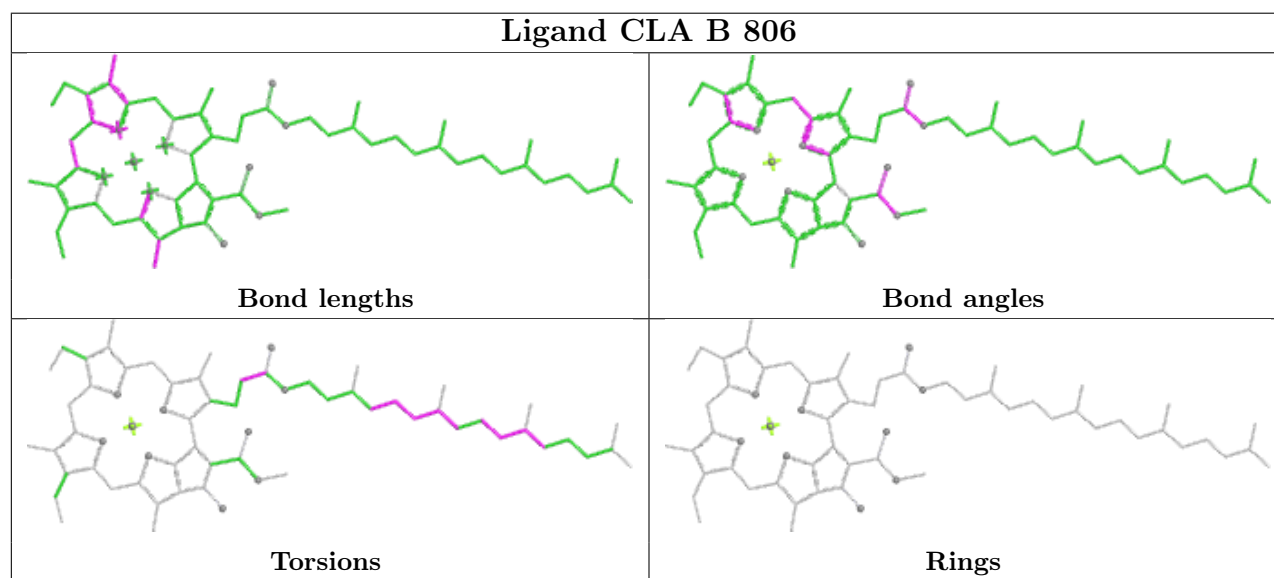
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	K	205	BCR	4	0
18	3	602	CLA	2	0
18	B	809	CLA	4	0
18	3	605	CLA	1	0
18	A	818	CLA	1	0
18	H	201	CLA	2	0
18	B	841	CLA	2	0
17	2	605	CHL	3	0
18	B	824	CLA	6	0
18	A	805	CLA	3	0
22	L	305	BCR	9	0
17	4	607	CHL	2	0
20	B	851	LHG	2	0
18	3	609	CLA	1	0
22	B	848	BCR	5	0
18	1	602	CLA	8	0
20	2	618	LHG	3	0
24	A	801	CL0	5	0
22	G	204	BCR	2	0
18	A	832	CLA	1	0
20	A	846	LHG	6	0
17	2	606	CHL	1	0
22	A	852	BCR	2	0
18	2	608	CLA	2	0
18	A	812	CLA	6	0
18	B	805	CLA	6	0
22	4	618	BCR	4	0
22	K	202	BCR	3	0
18	2	613	CLA	1	0
18	F	302	CLA	5	0
18	A	823	CLA	1	0
18	B	828	CLA	6	0
17	2	615	CHL	5	0
18	1	611	CLA	1	0
18	1	607	CLA	1	0
22	L	301	BCR	4	0
18	3	603	CLA	2	0
18	A	806	CLA	3	0
18	A	802	CLA	3	0
18	A	836	CLA	1	0
18	L	302	CLA	2	0

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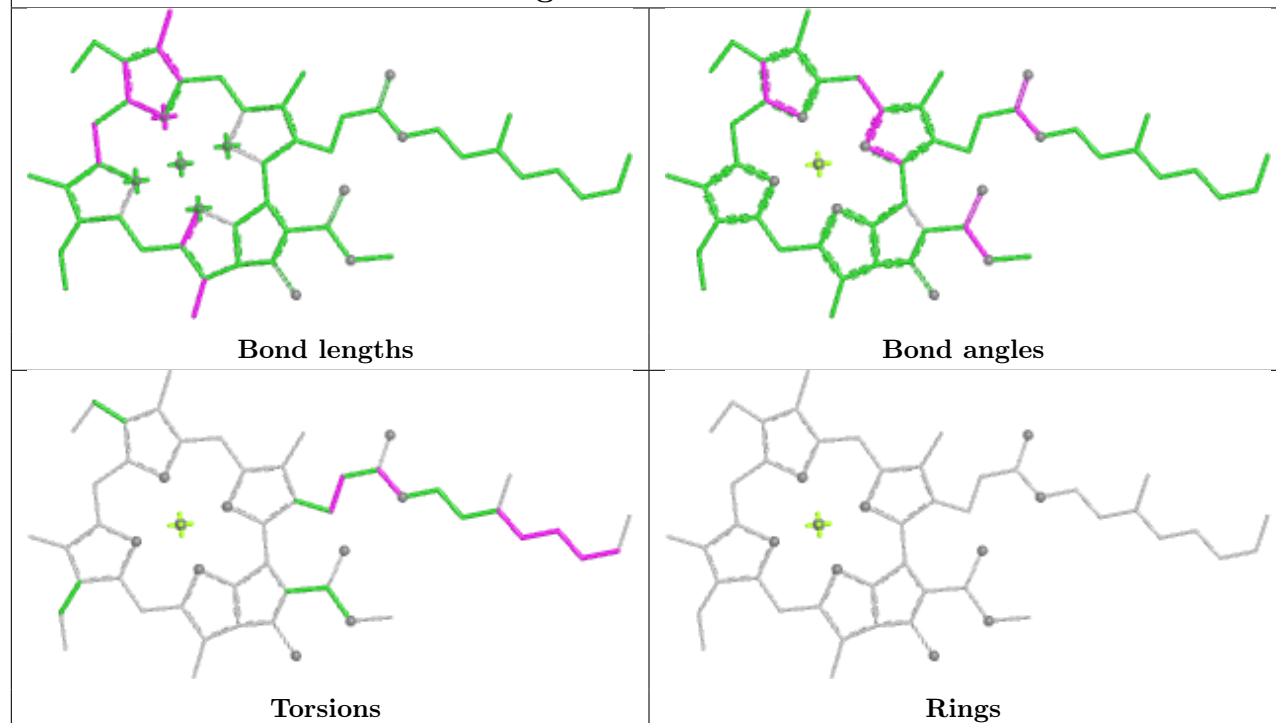
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	813	CLA	4	0
18	K	204	CLA	1	0
18	A	839	CLA	1	0
18	A	834	CLA	3	0
18	4	614	CLA	2	0
21	4	616	LUT	4	0
18	B	831	CLA	1	0

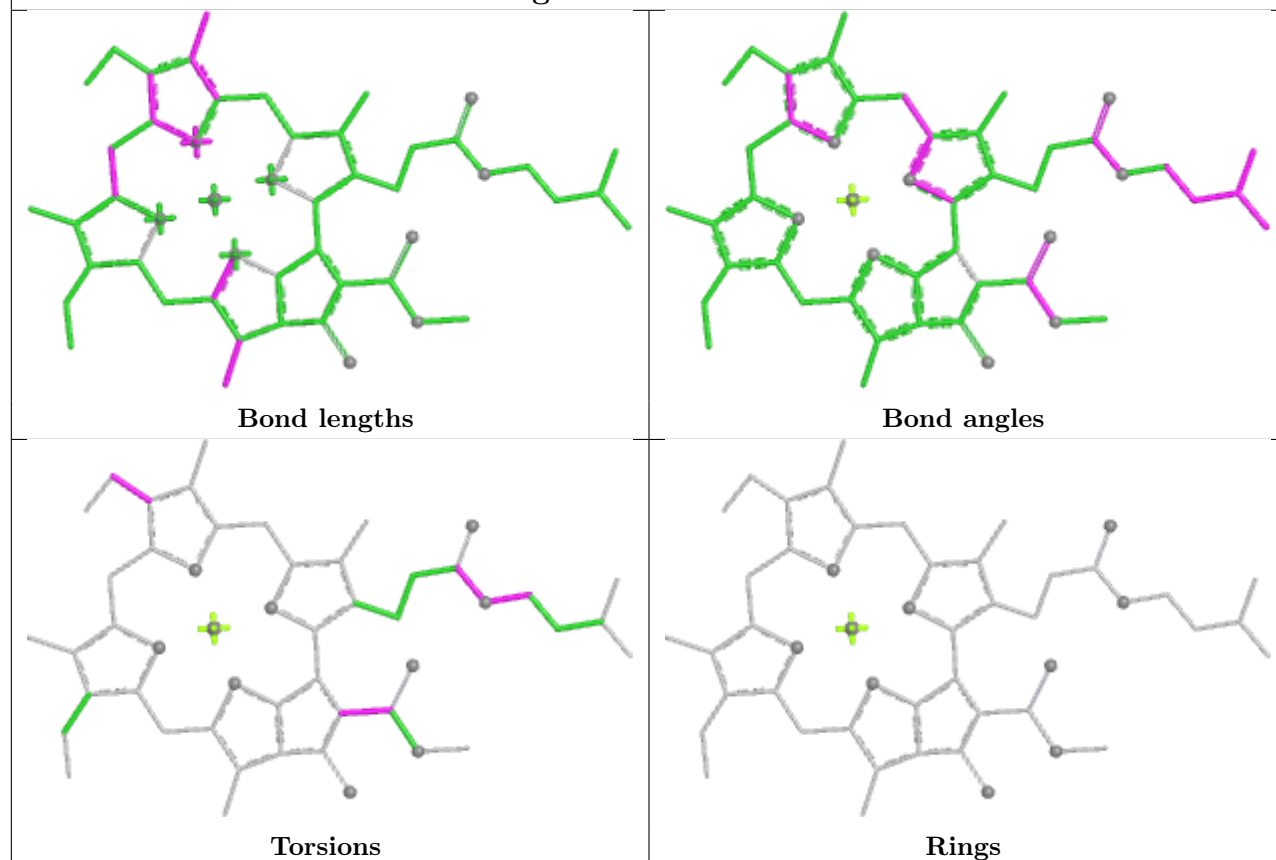
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

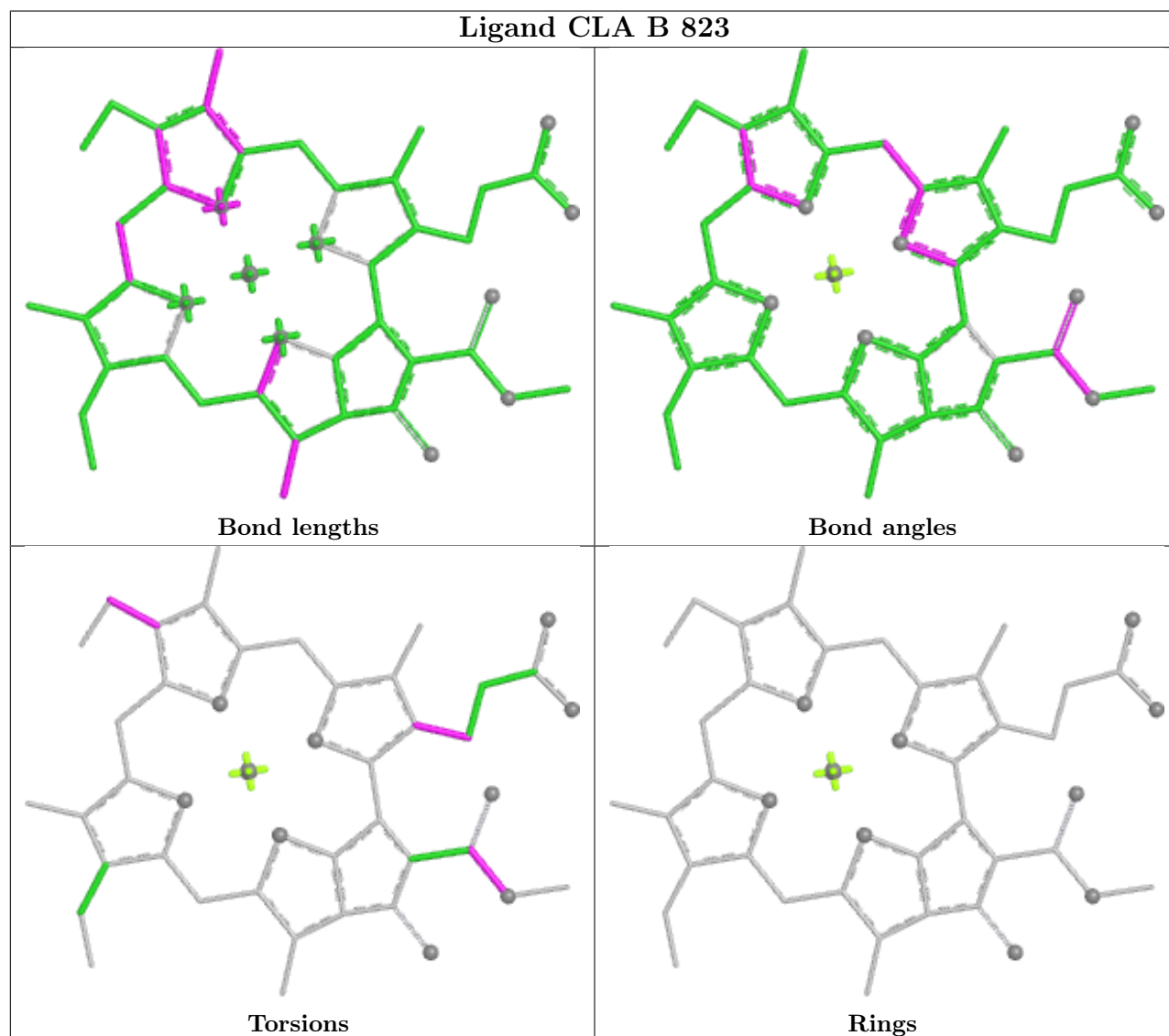
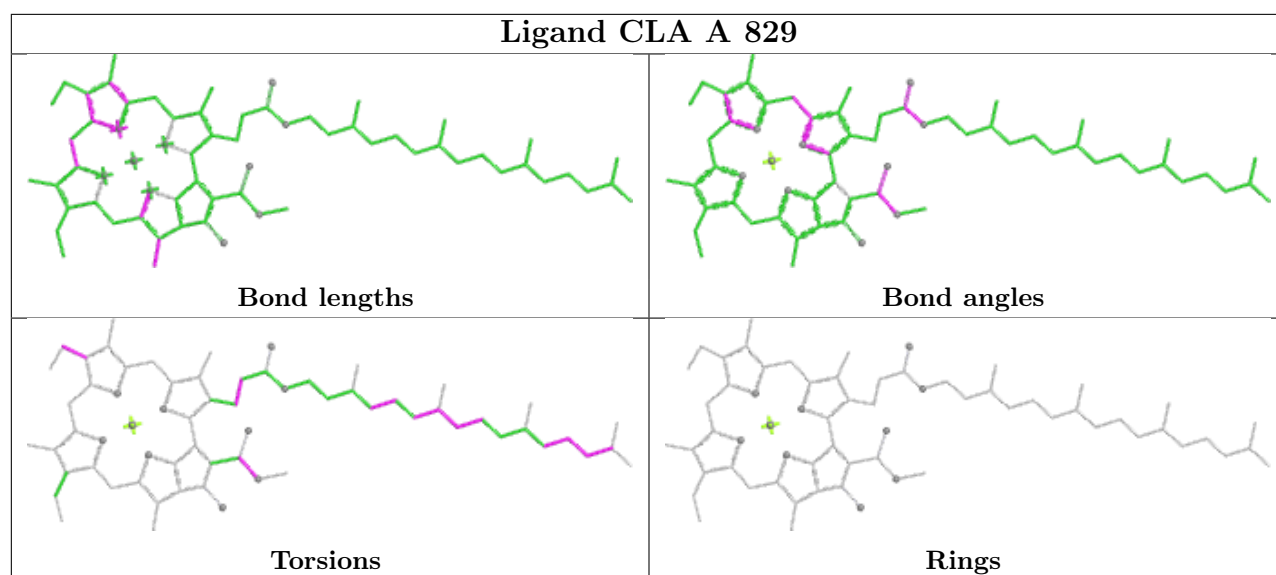


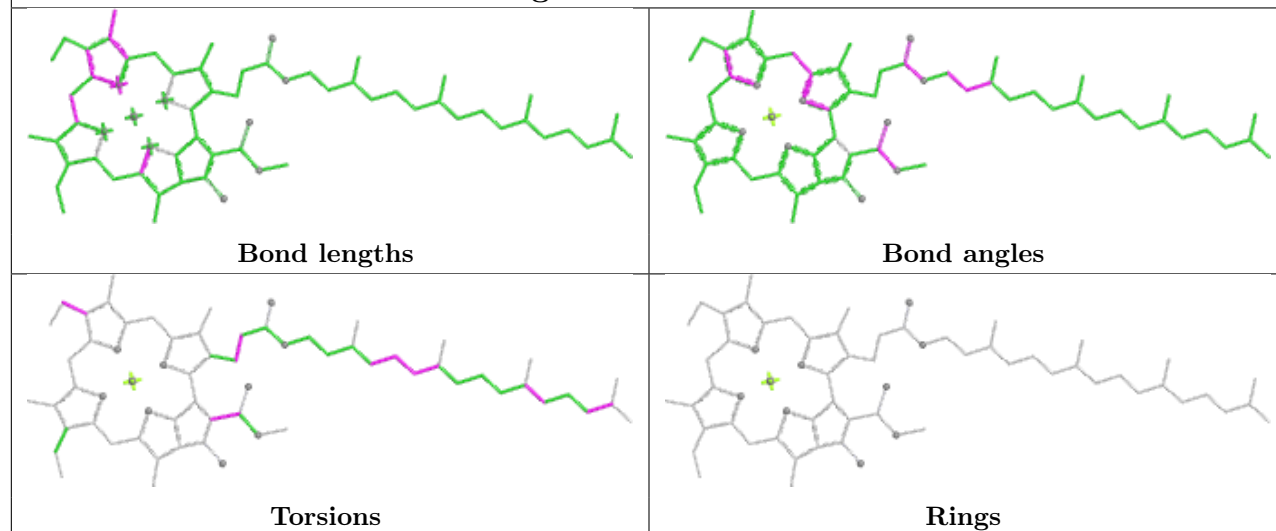
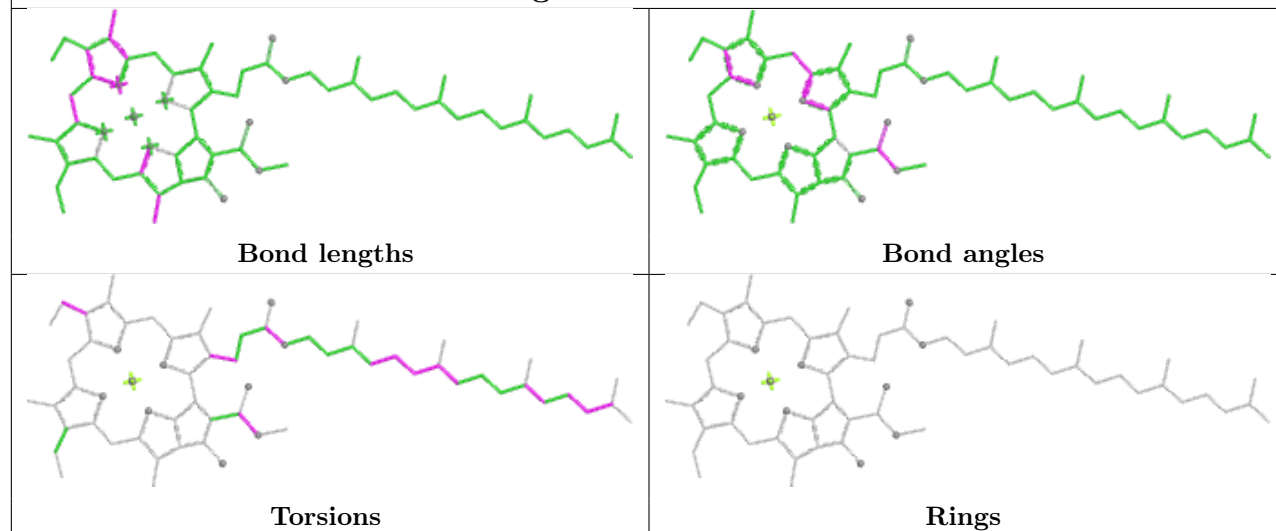
Ligand CLA 1 603



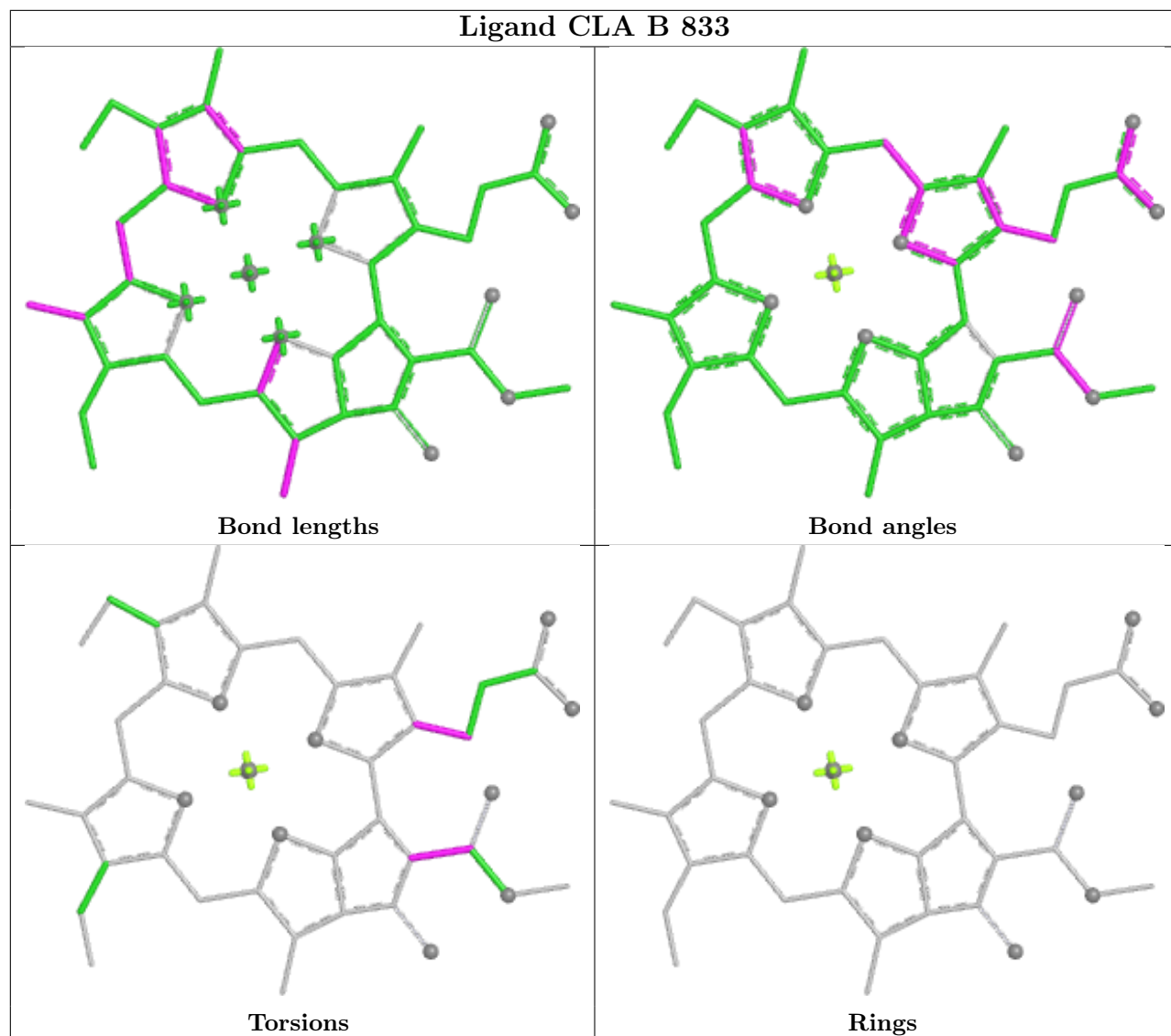
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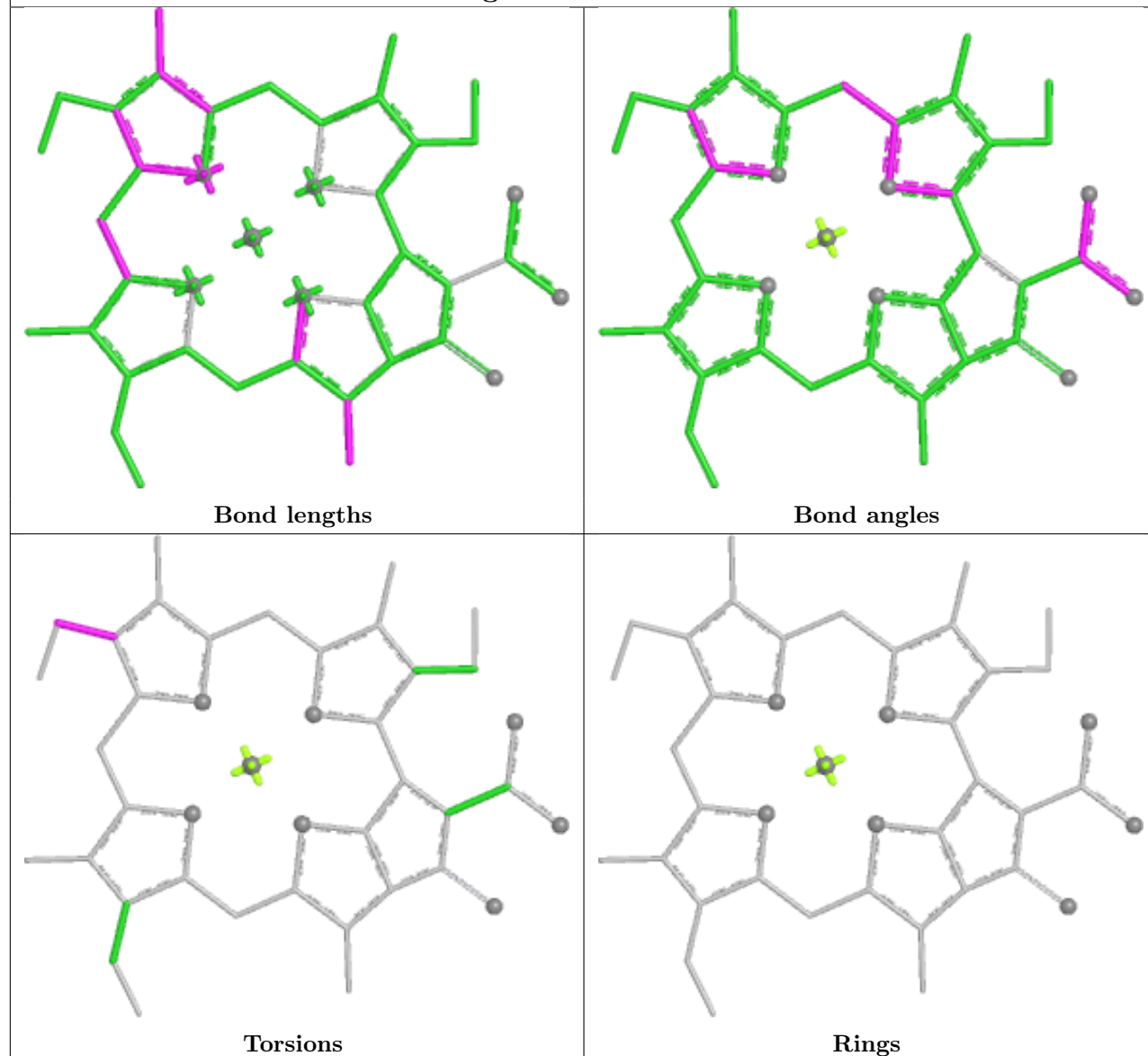


Ligand CLA A 844**Ligand CLA B 840**

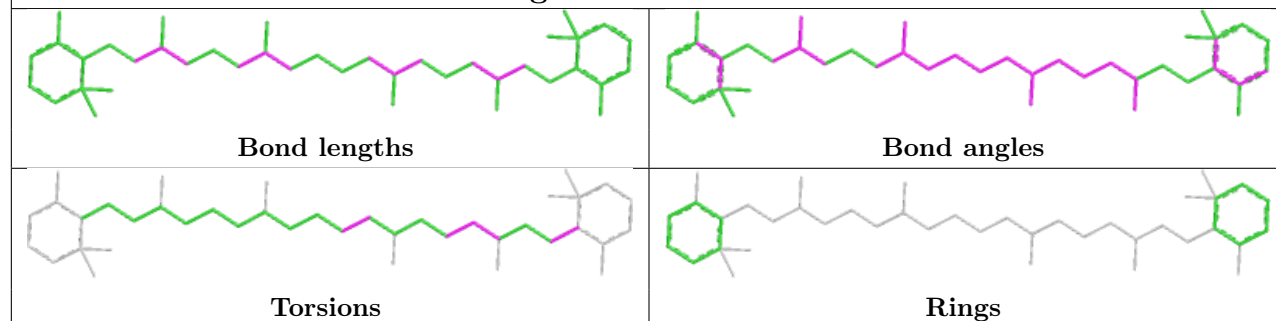
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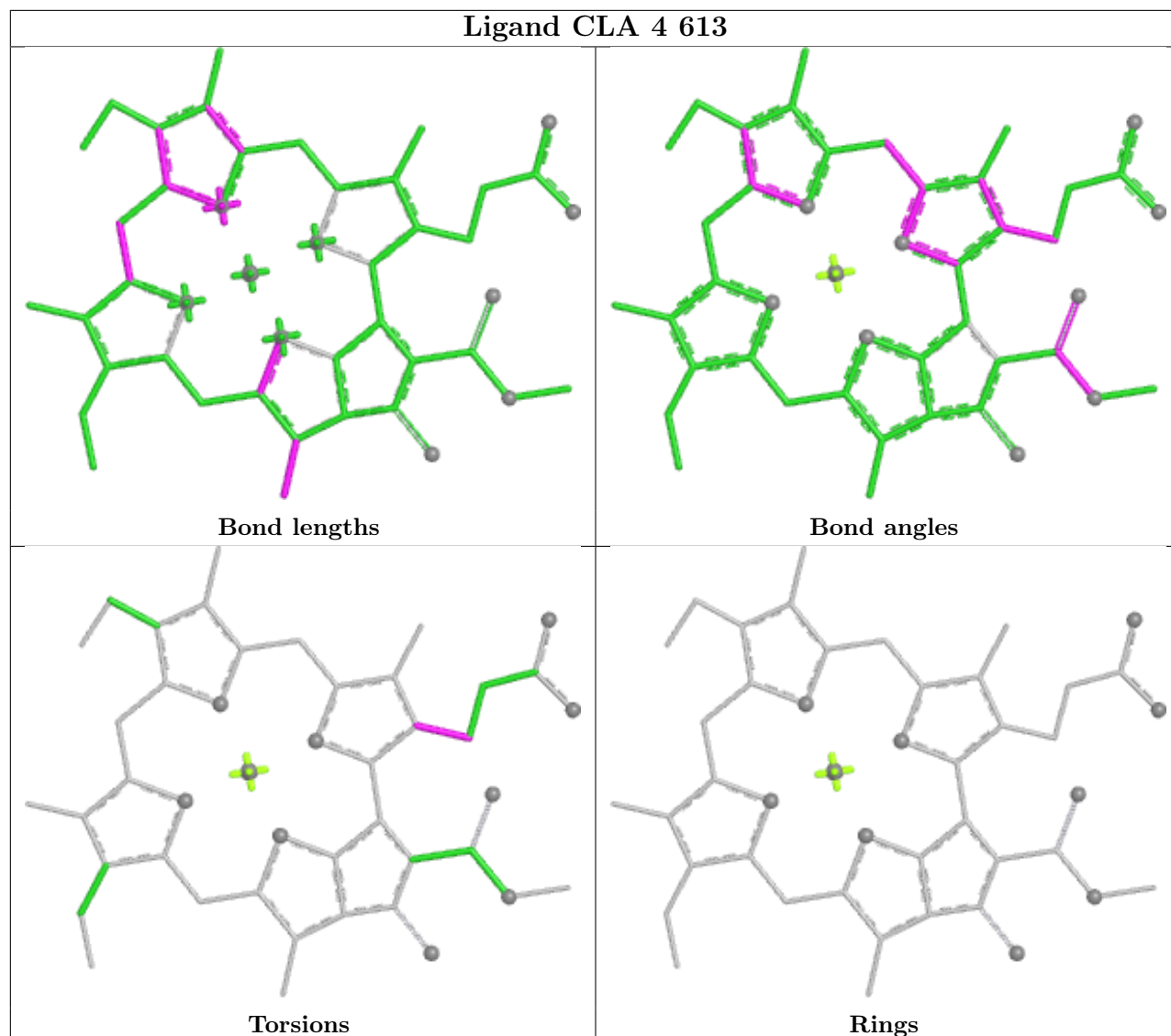
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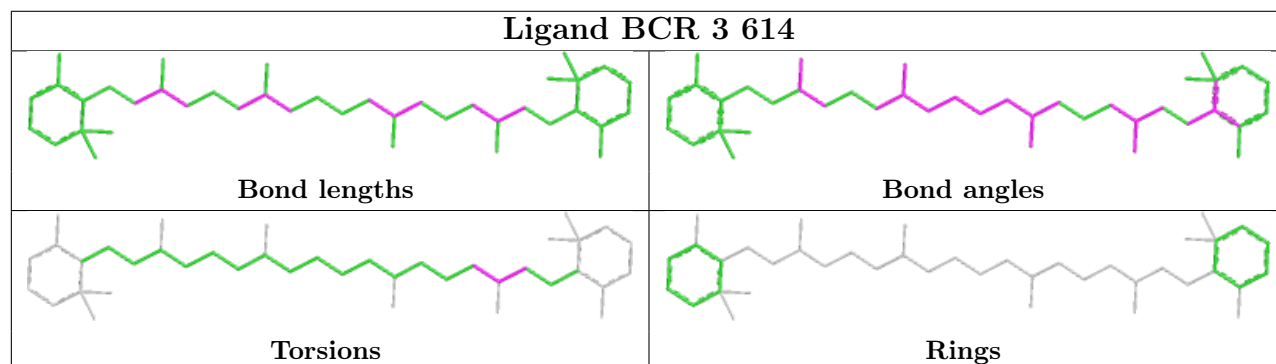
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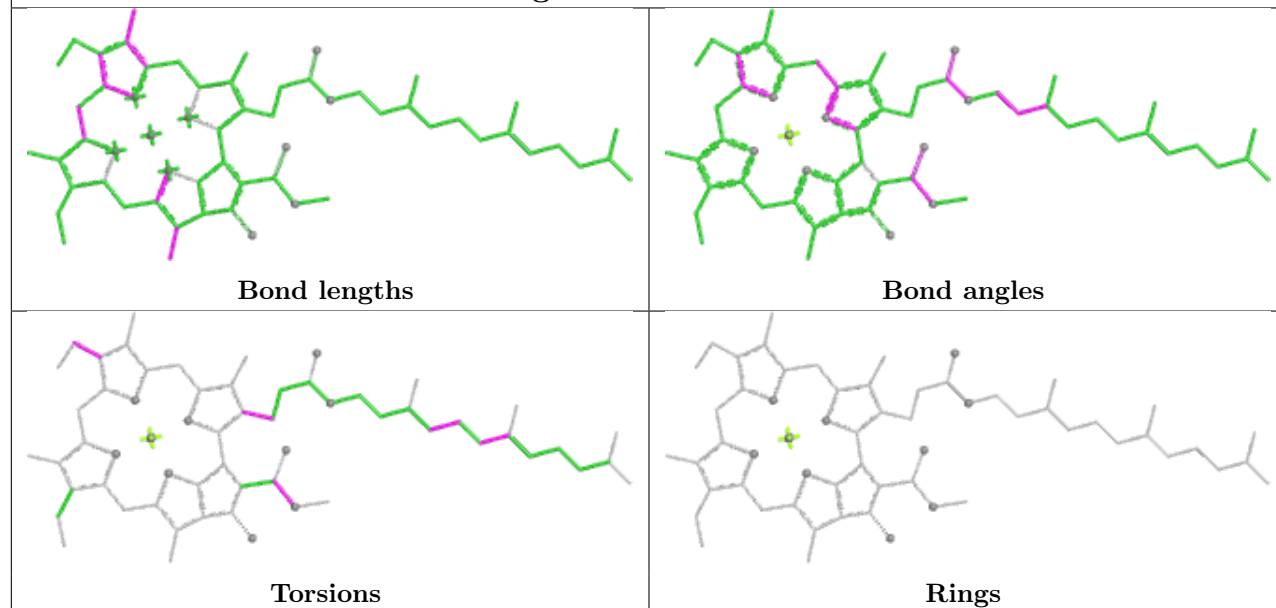
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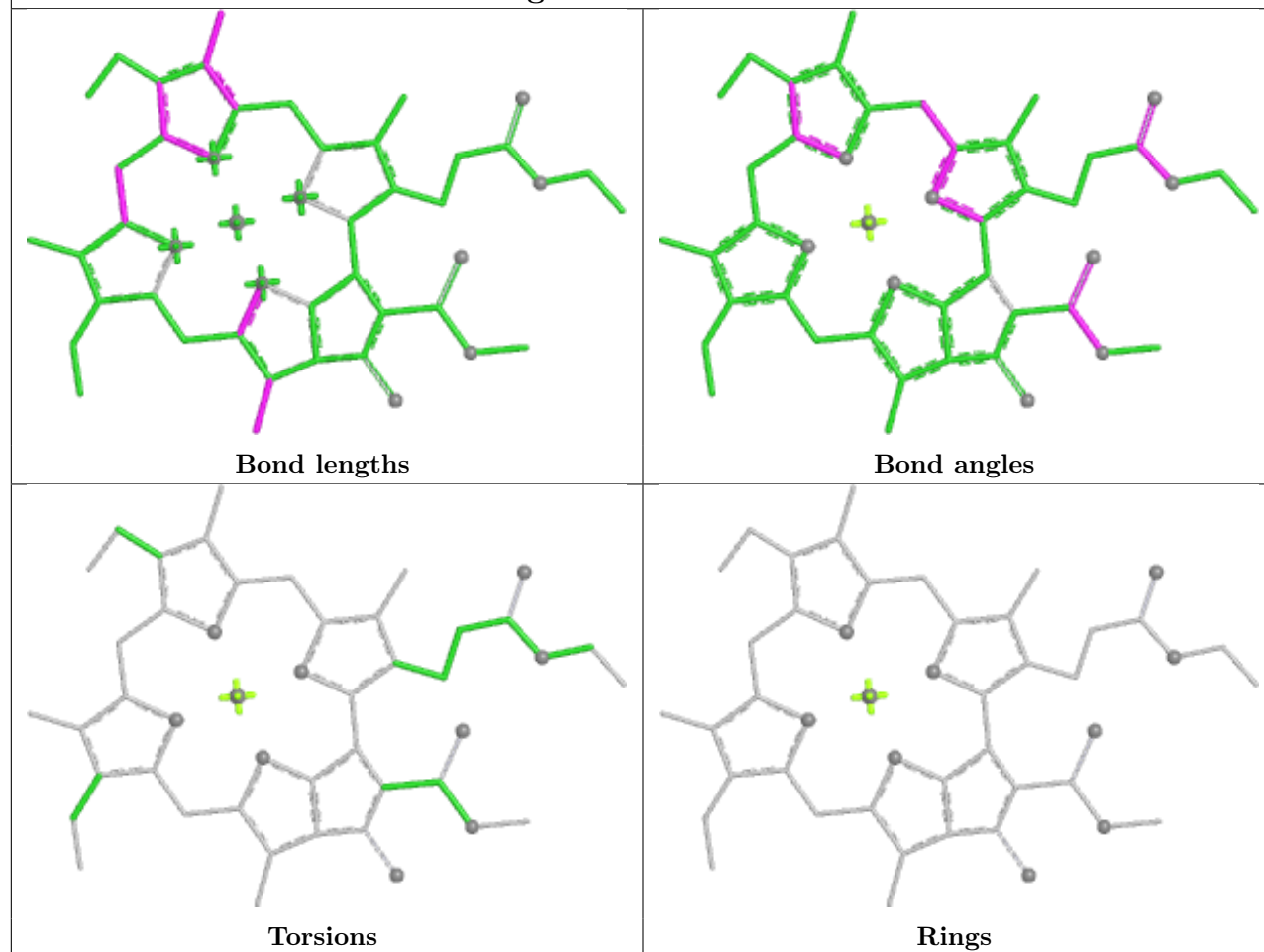
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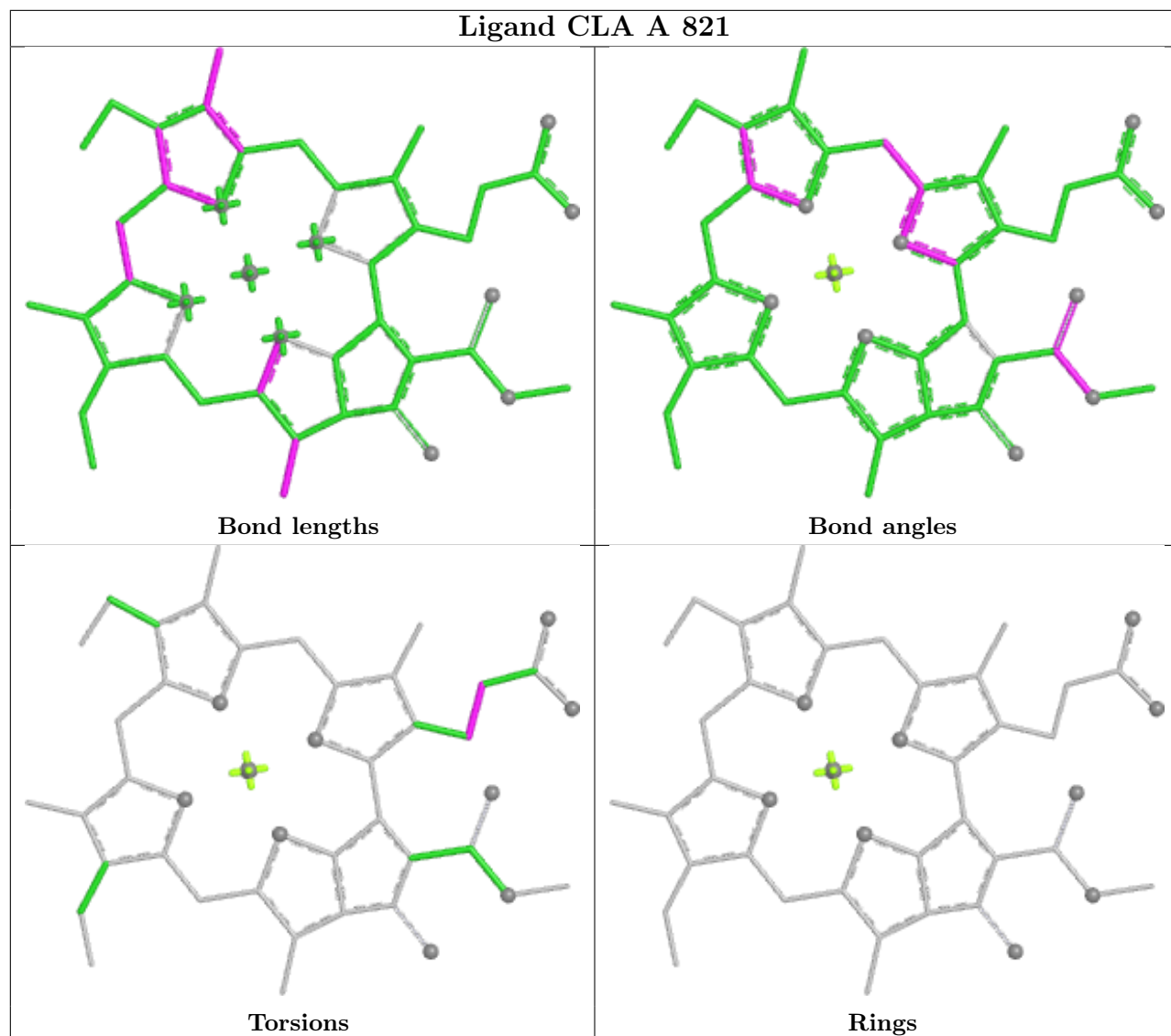
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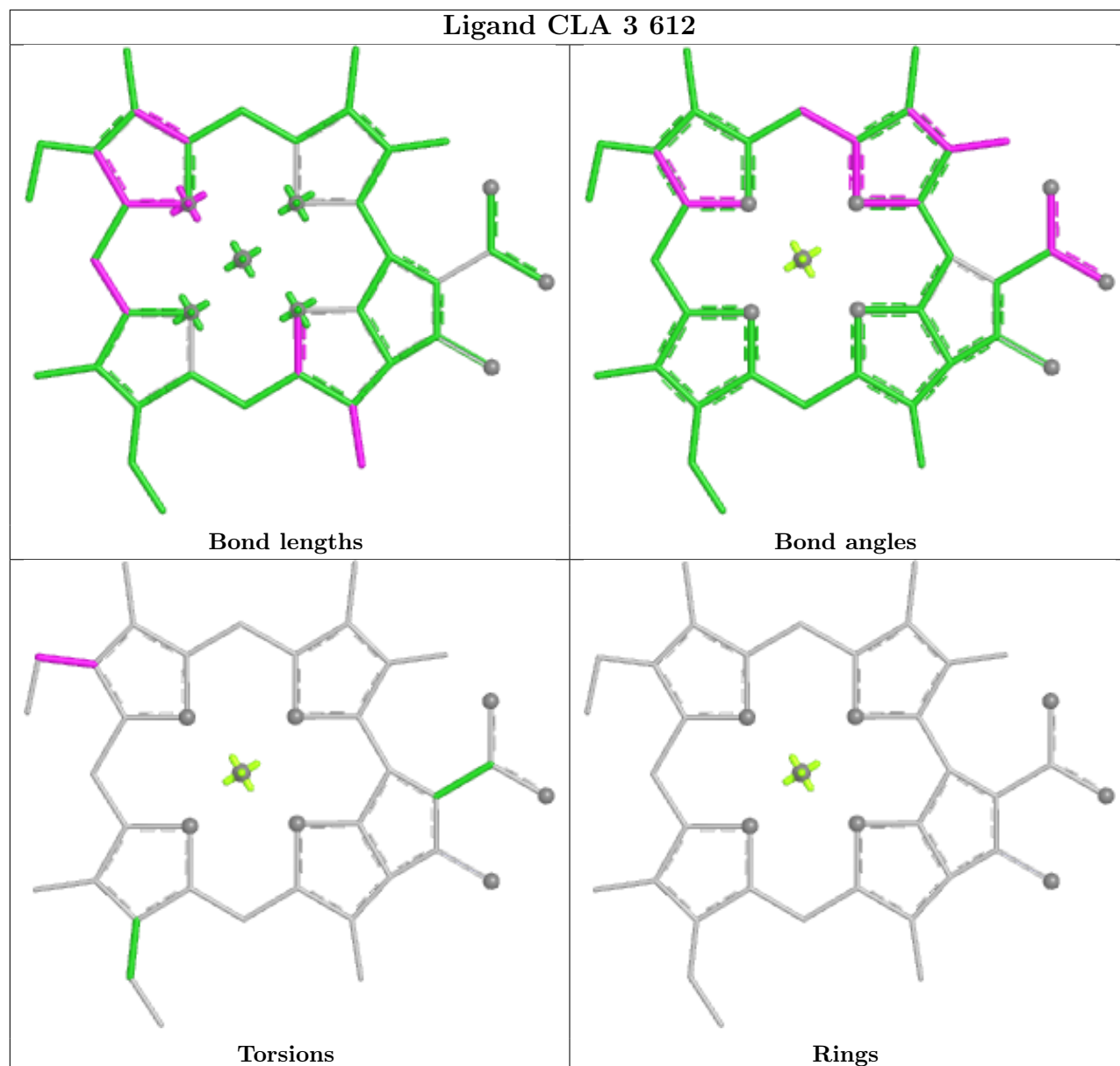
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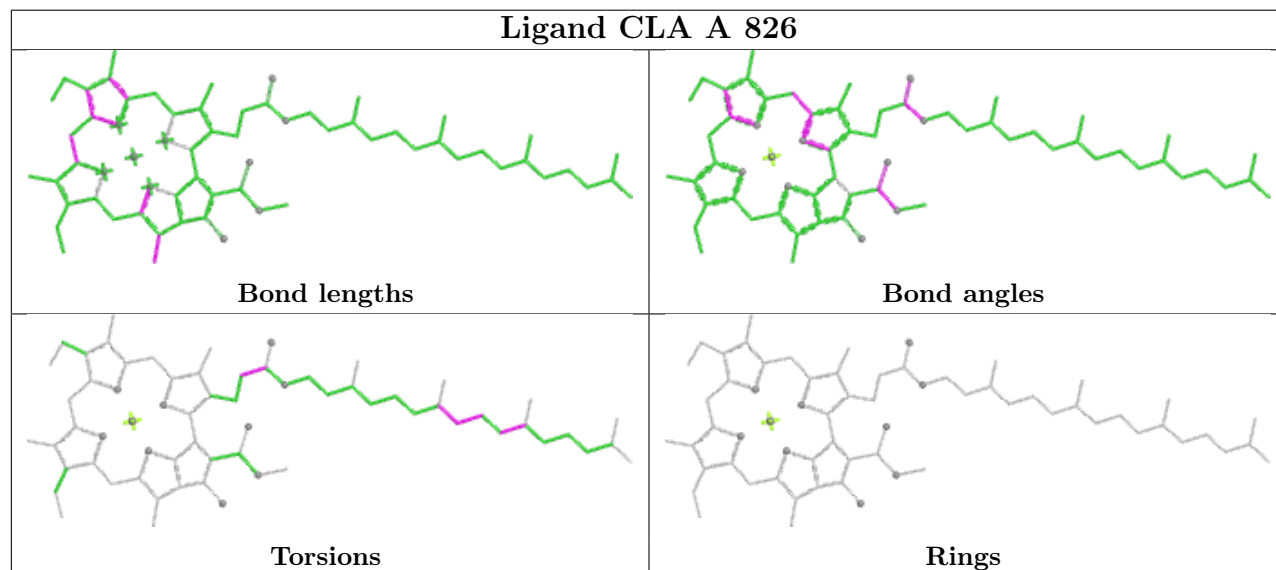
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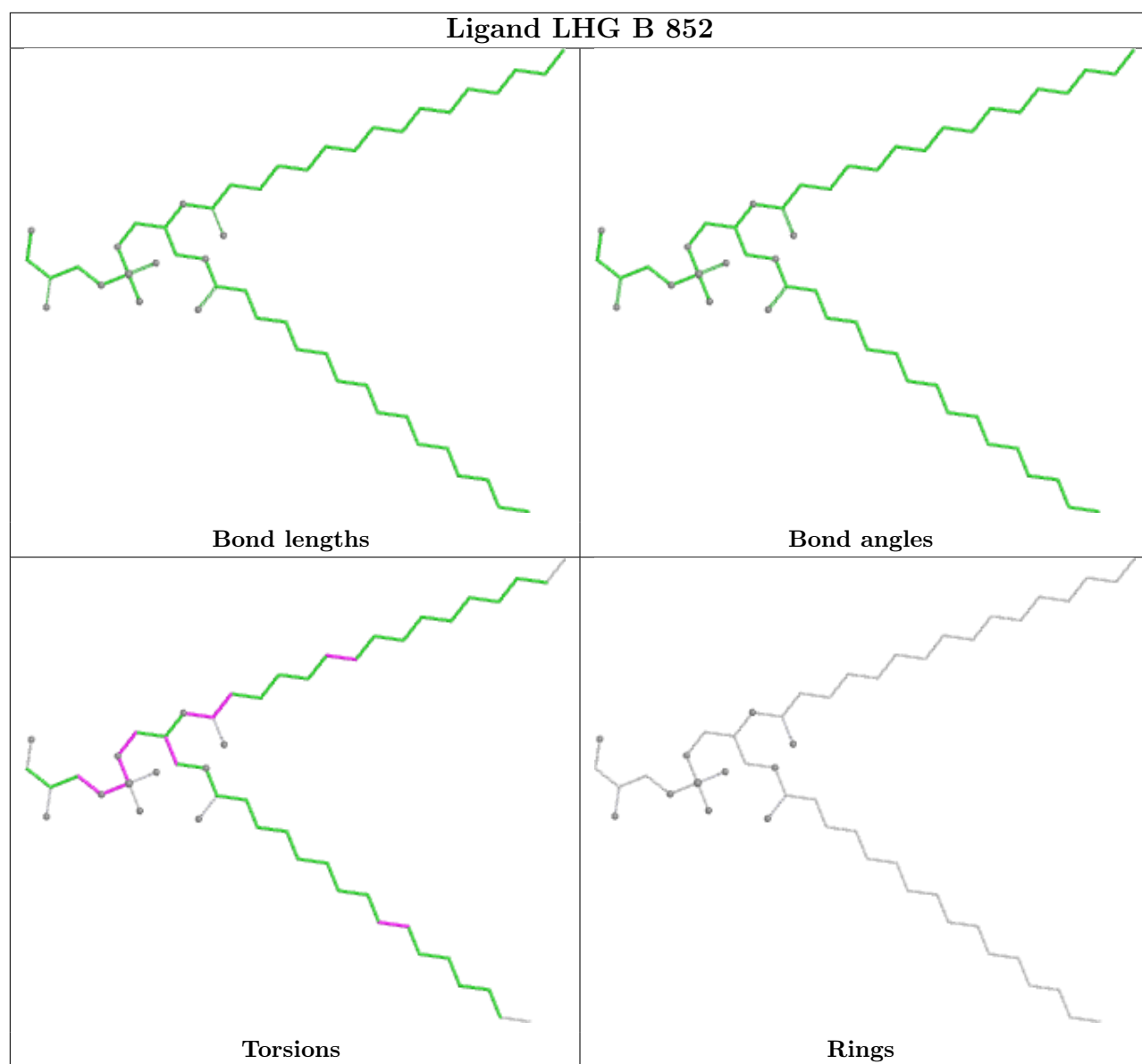


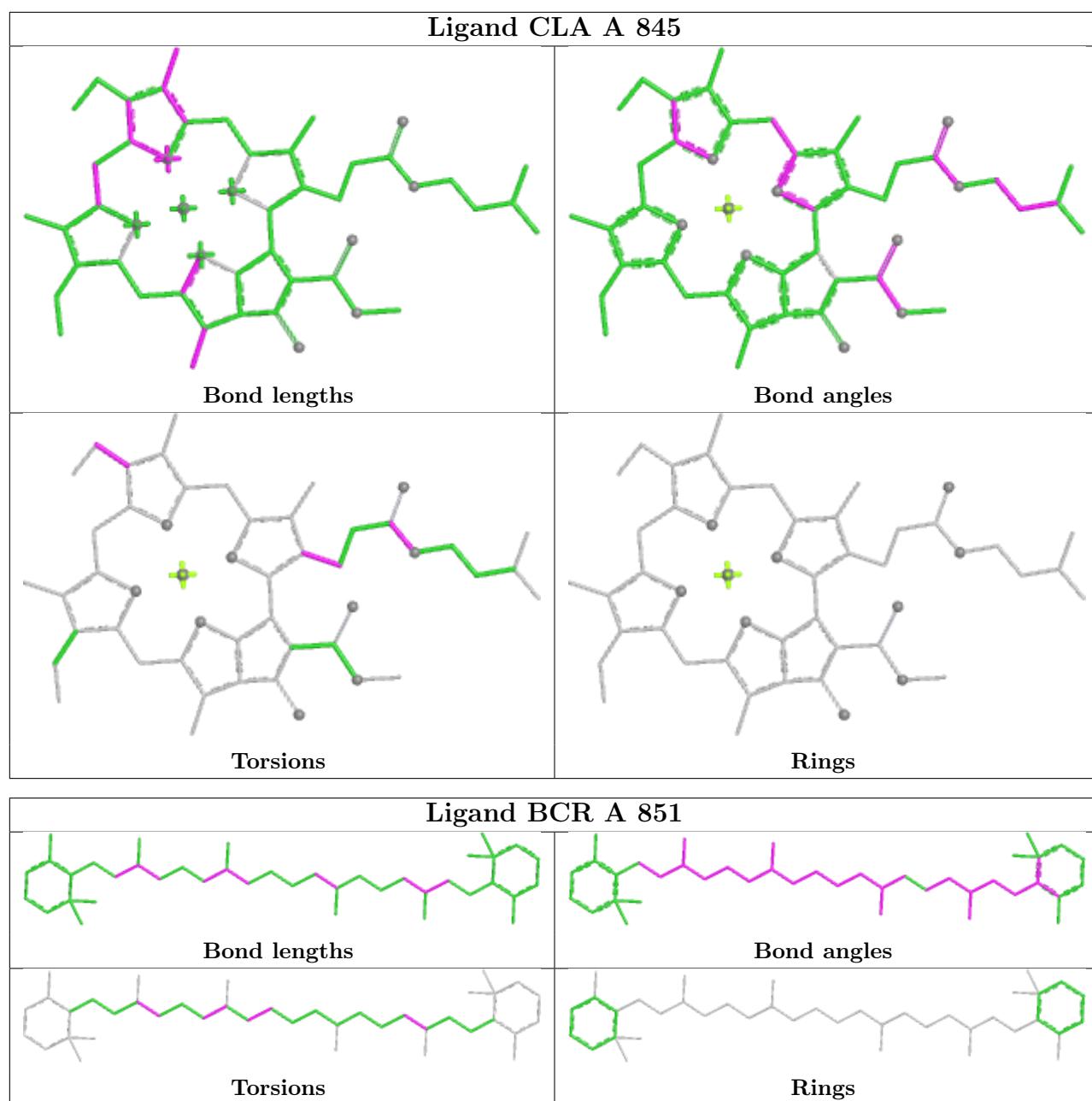
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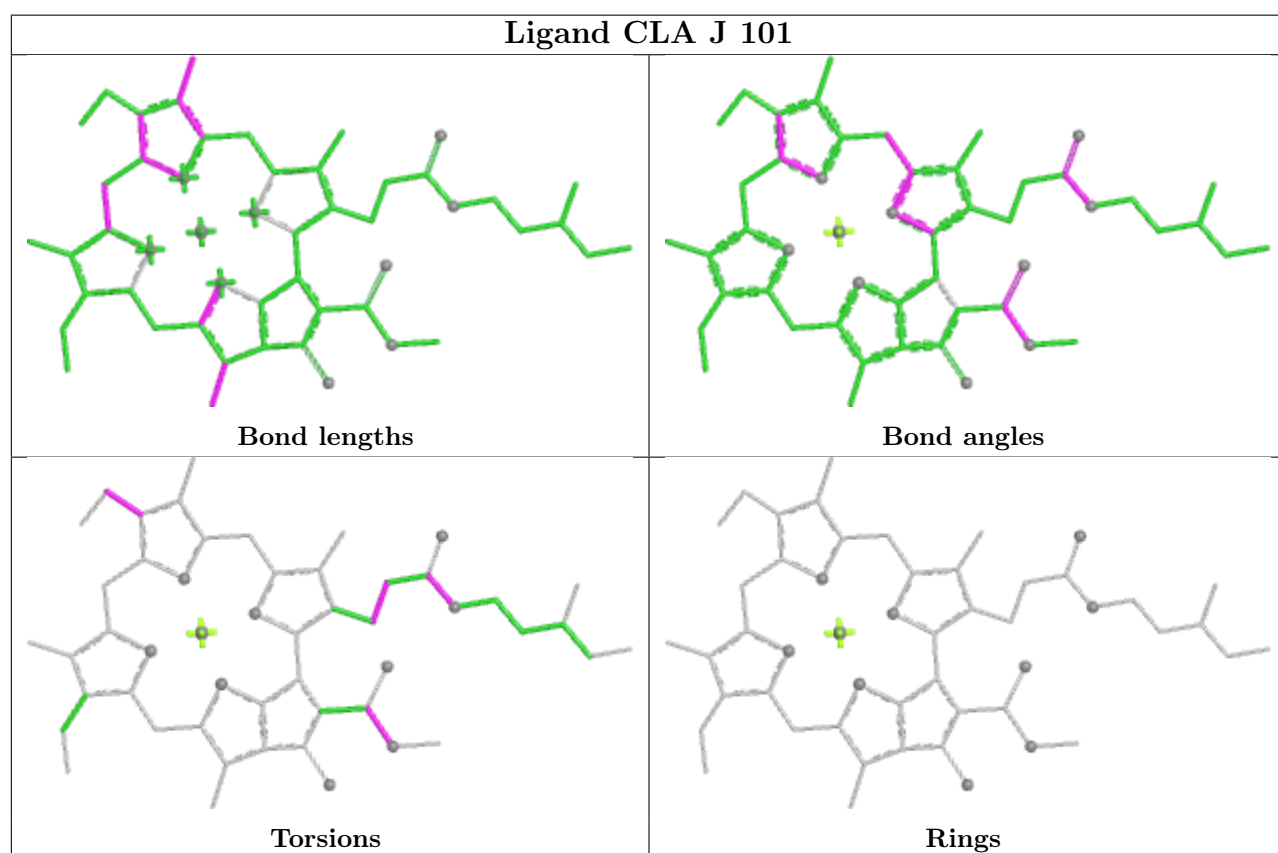
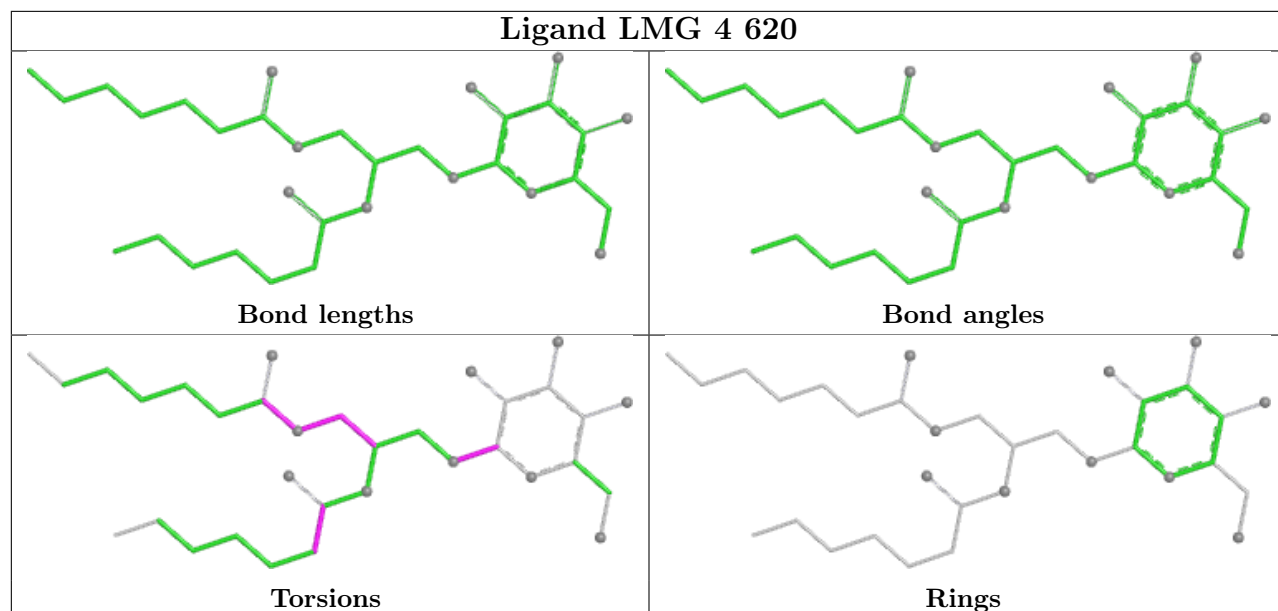


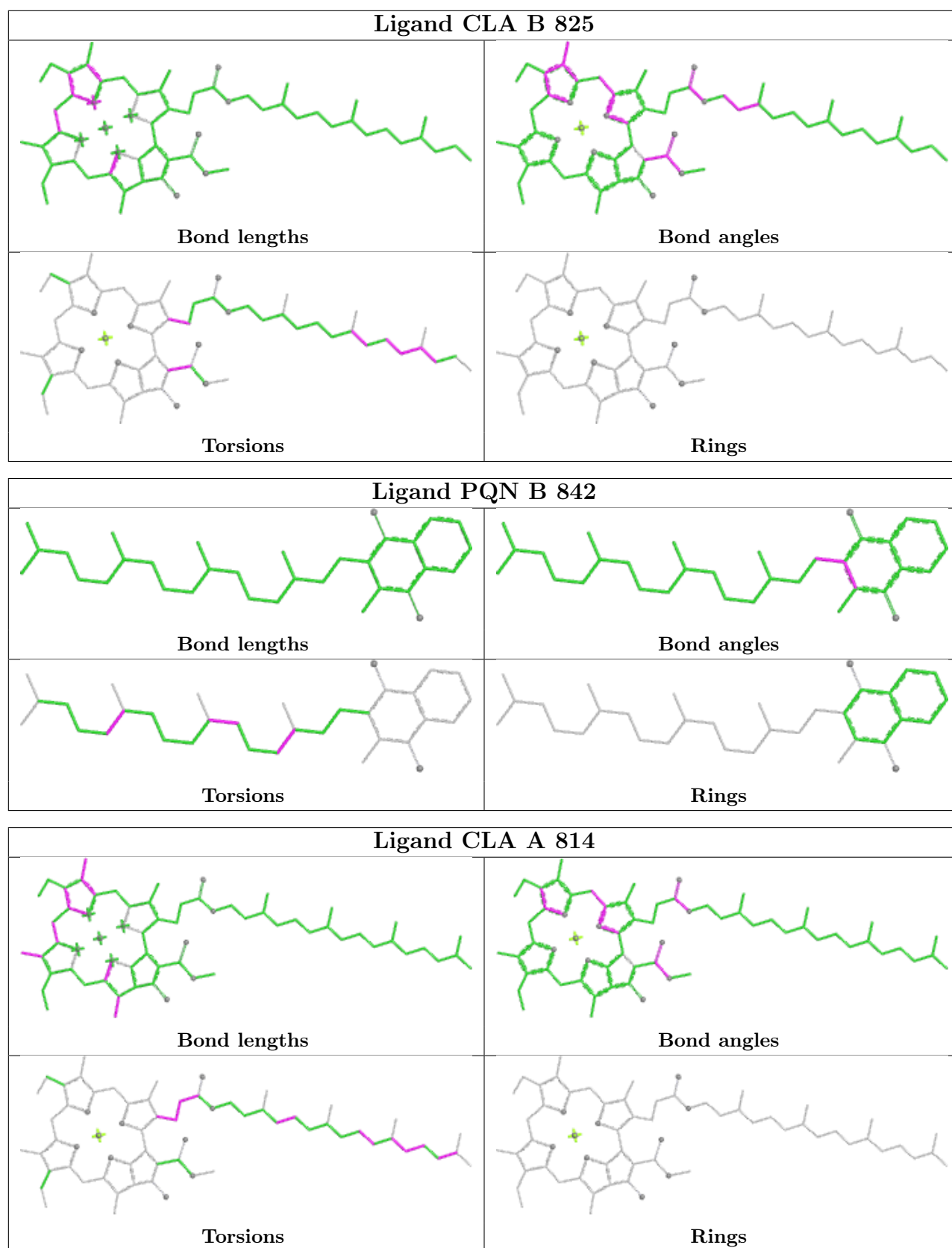
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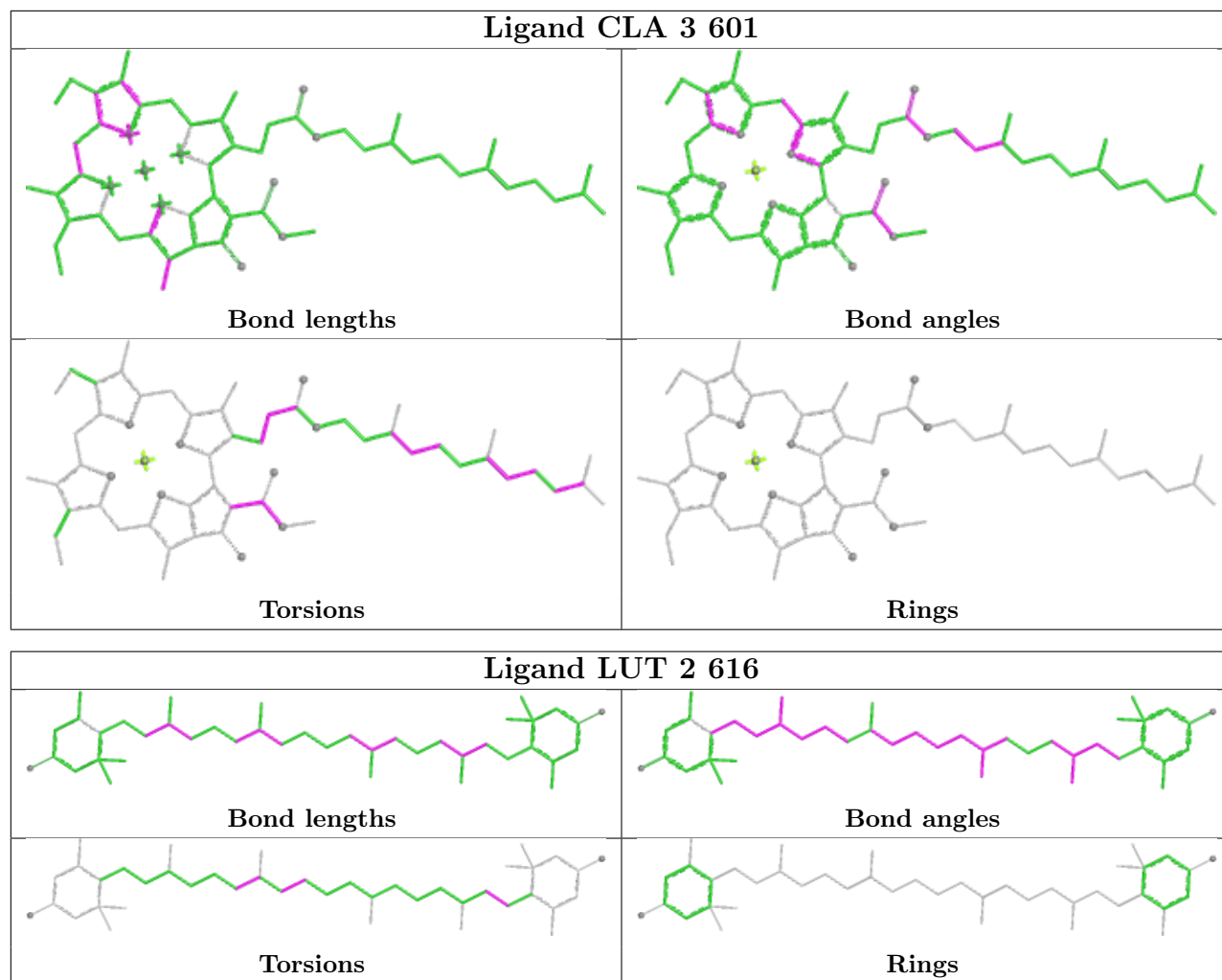


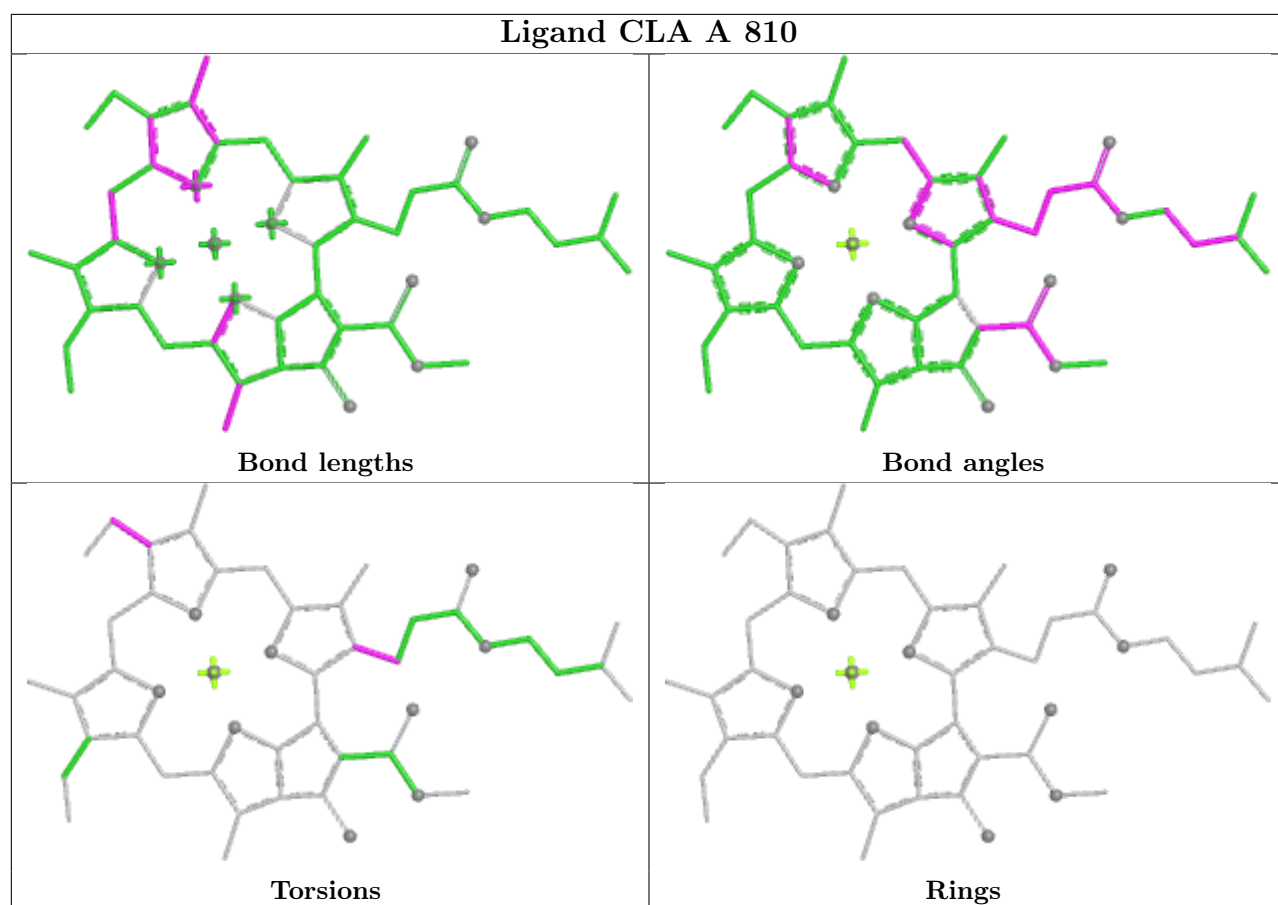




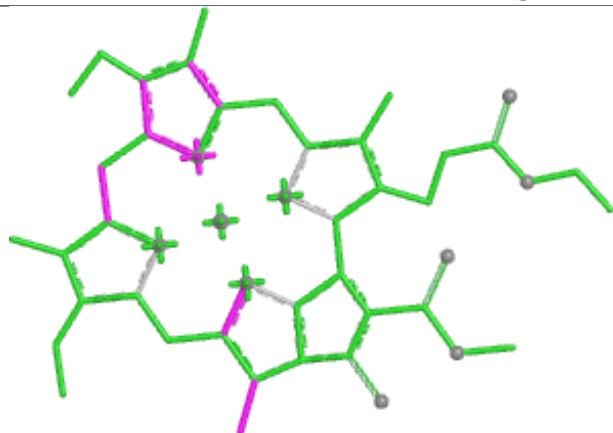




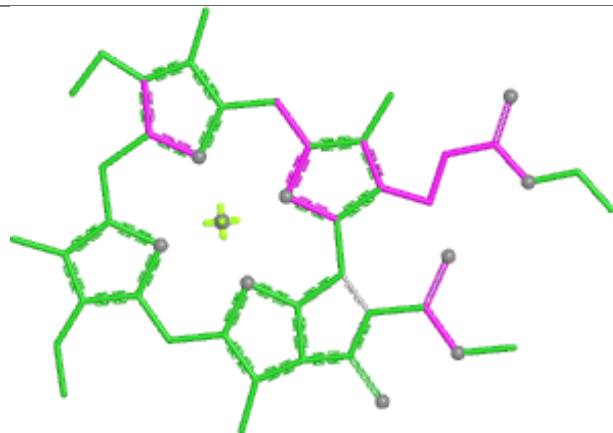




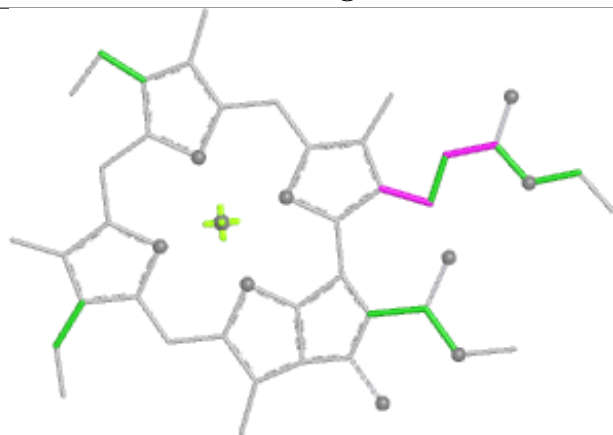
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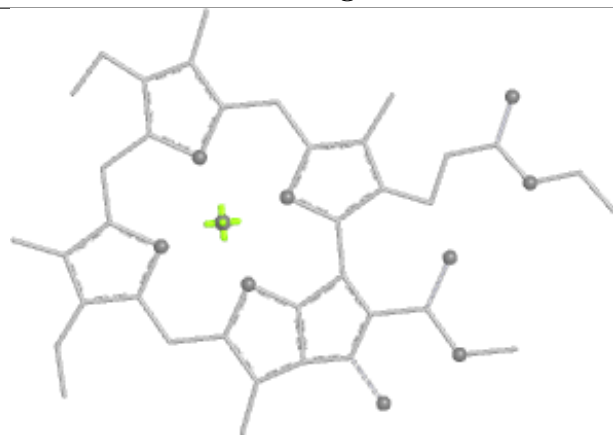
Bond lengths



Bond angles

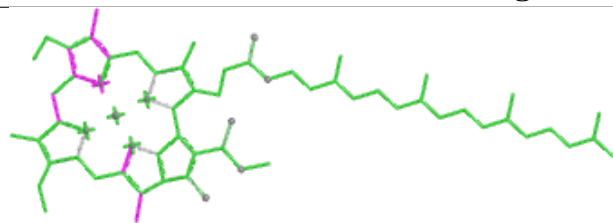


Torsions

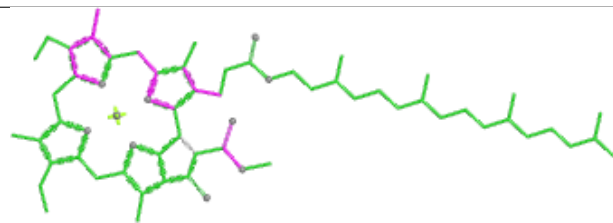


Rings

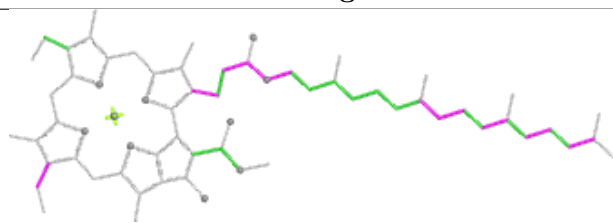
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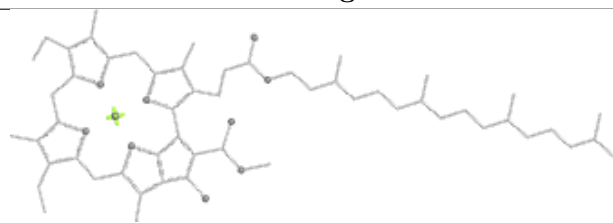
Bond lengths



Bond angles

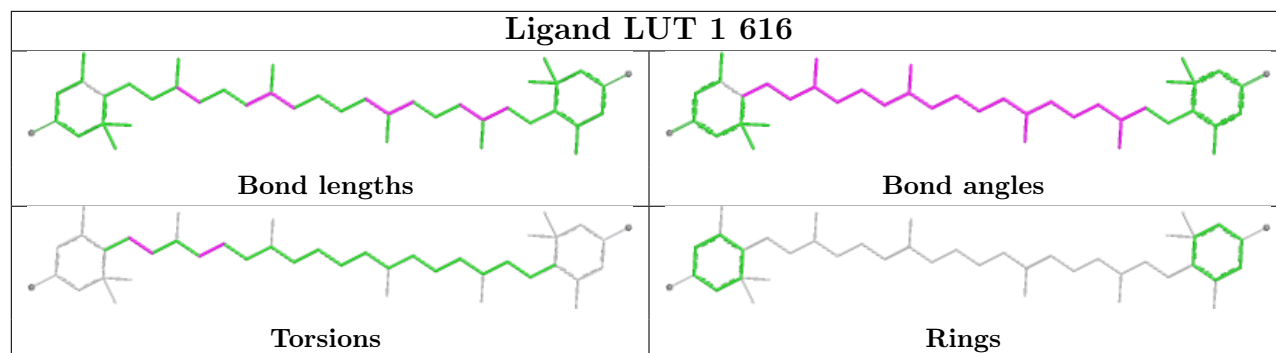


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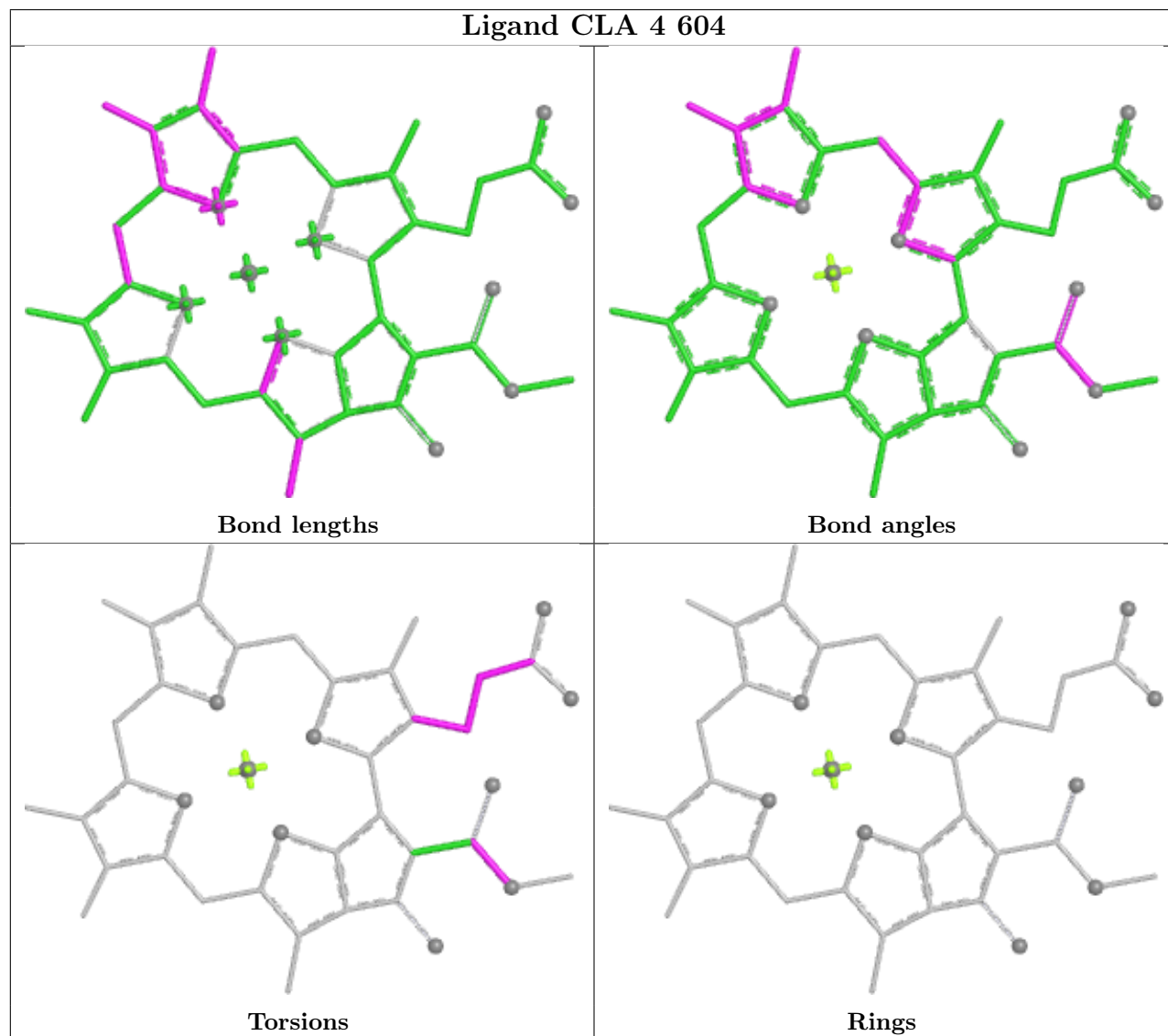


Rings

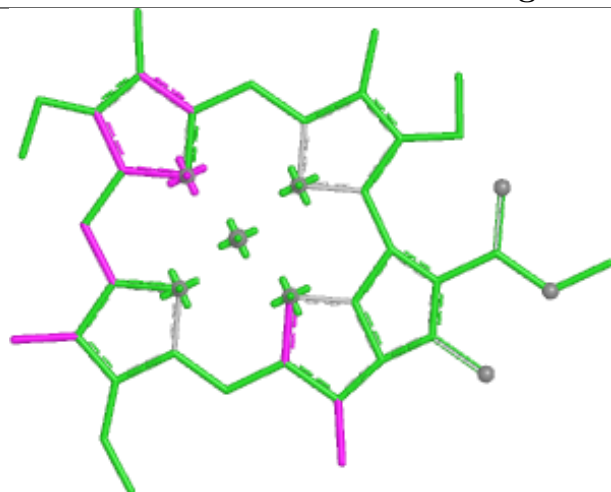
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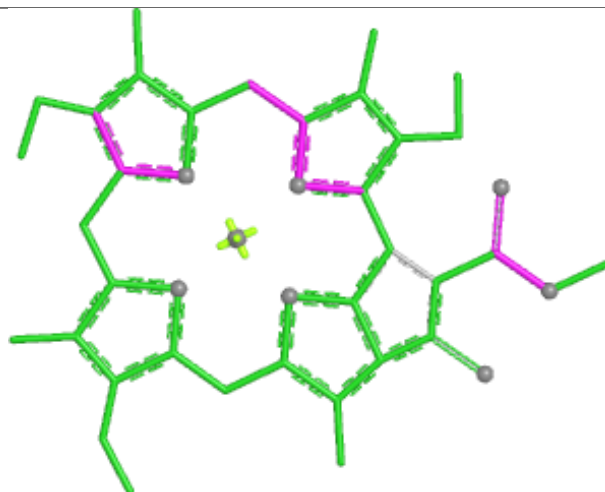
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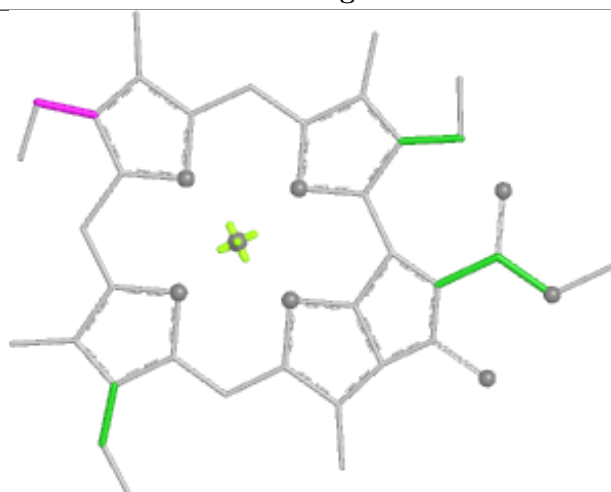
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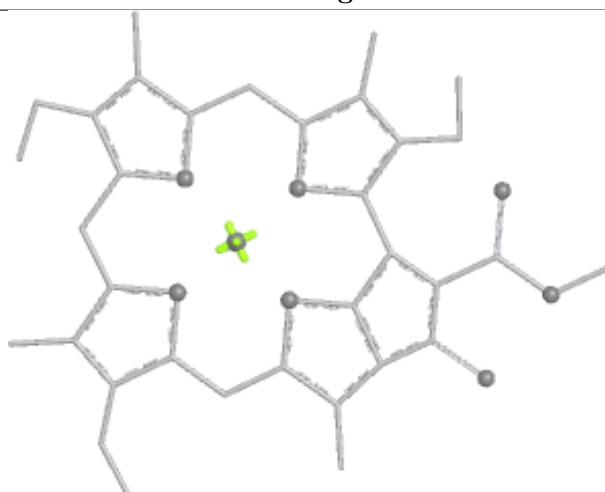
Bond lengths



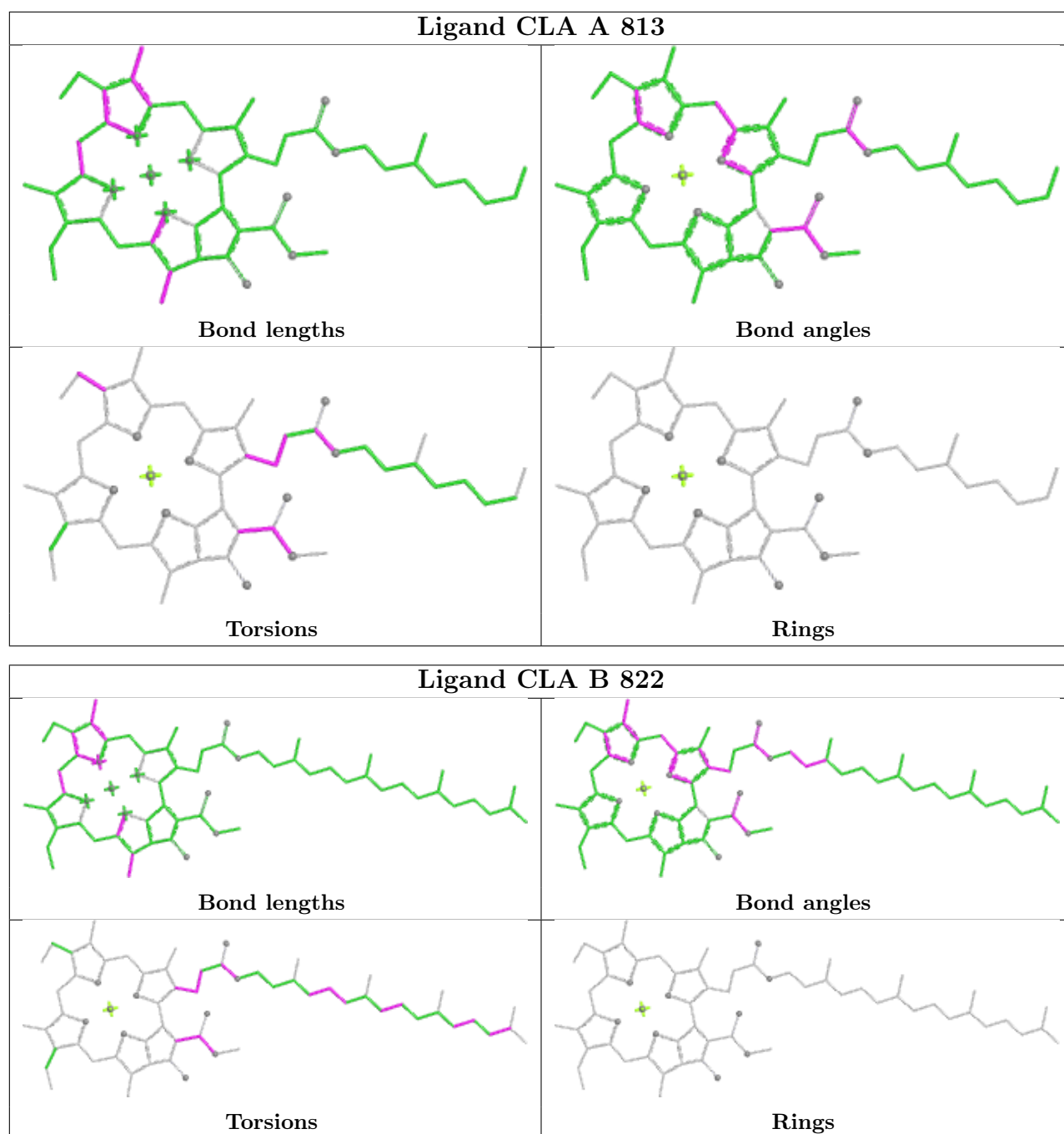
Bond angles

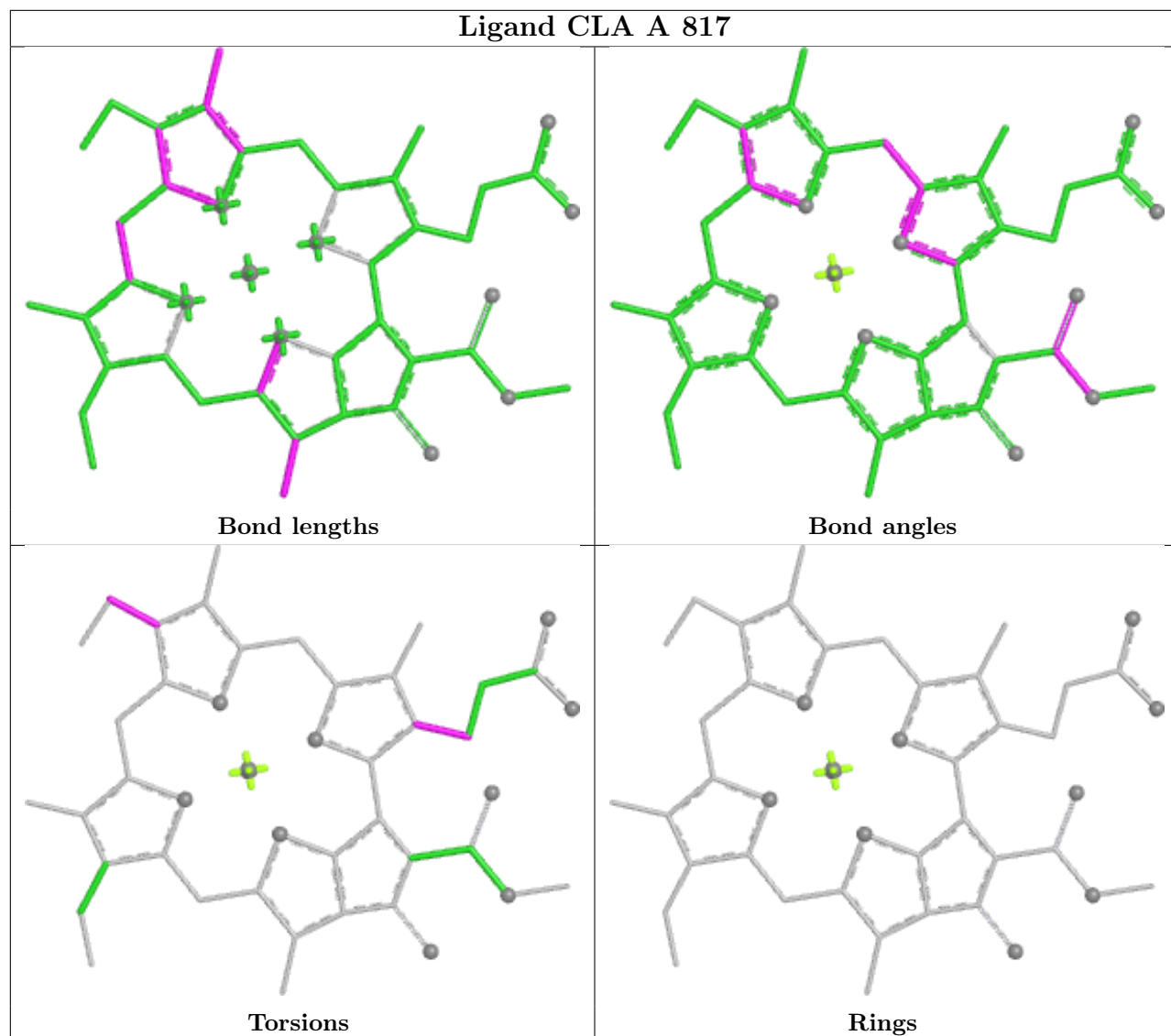


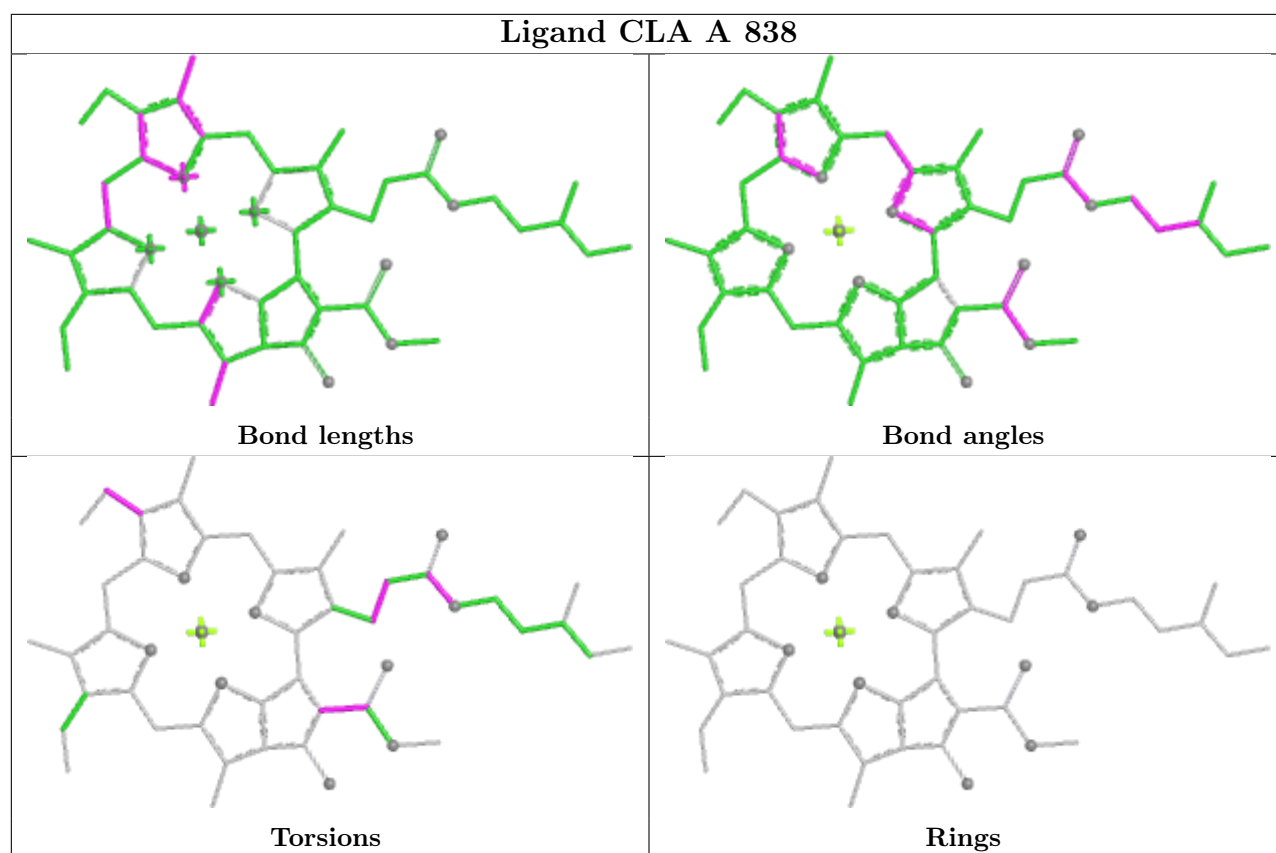
Torsions



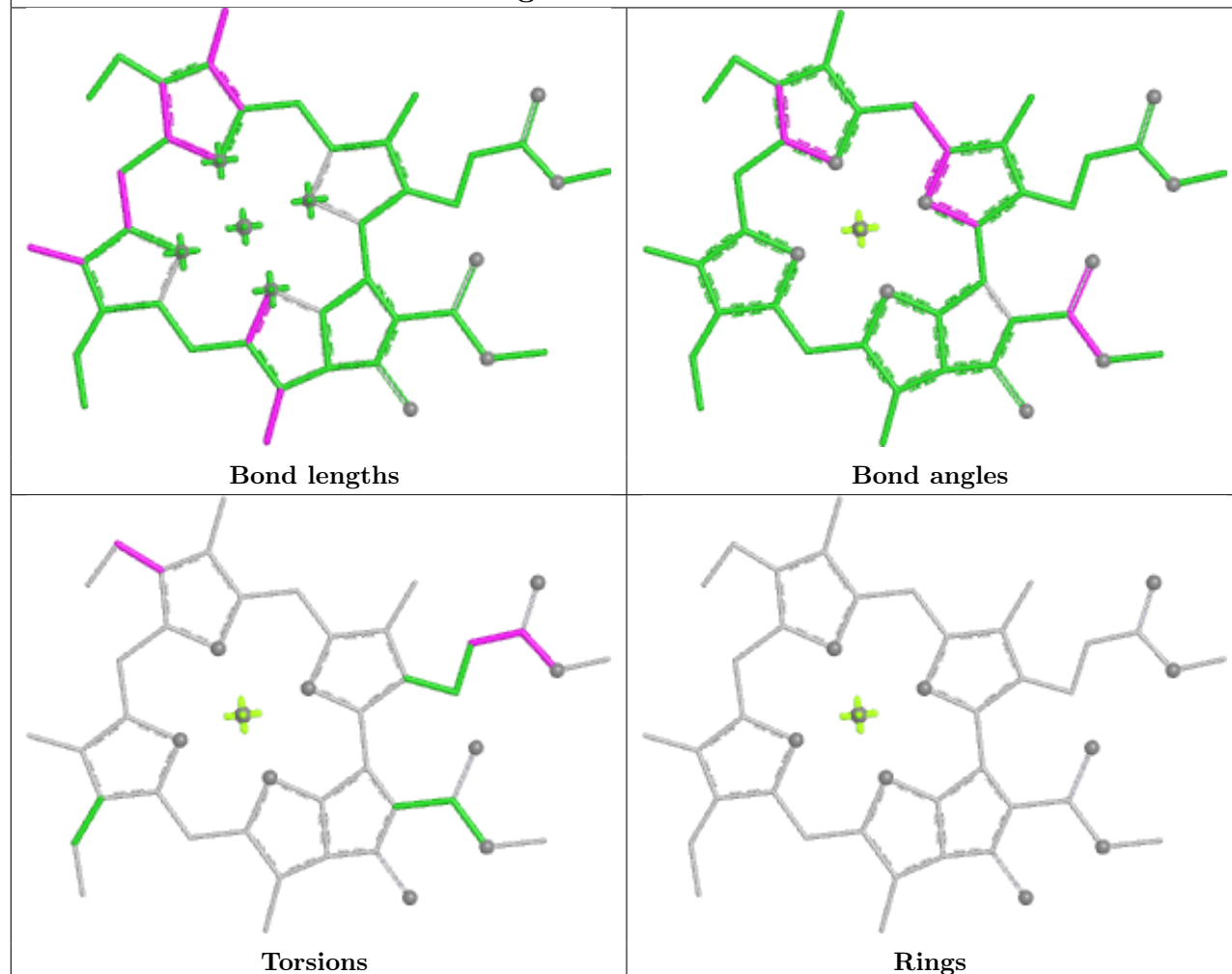
Rings



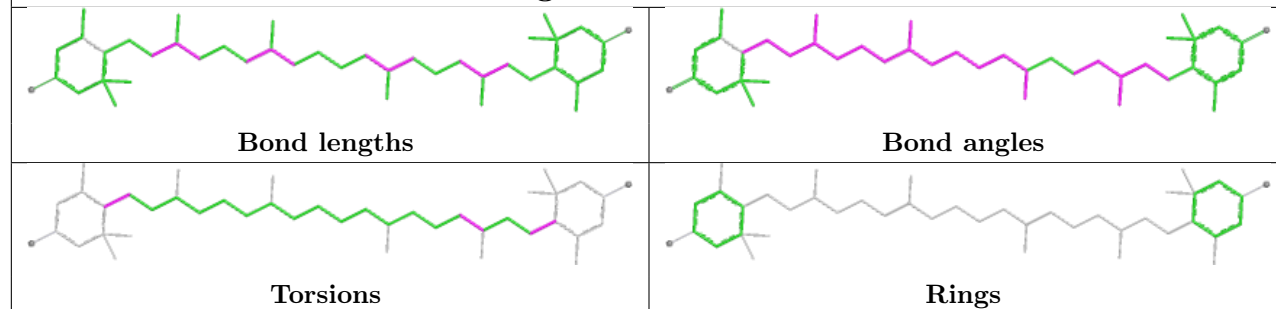


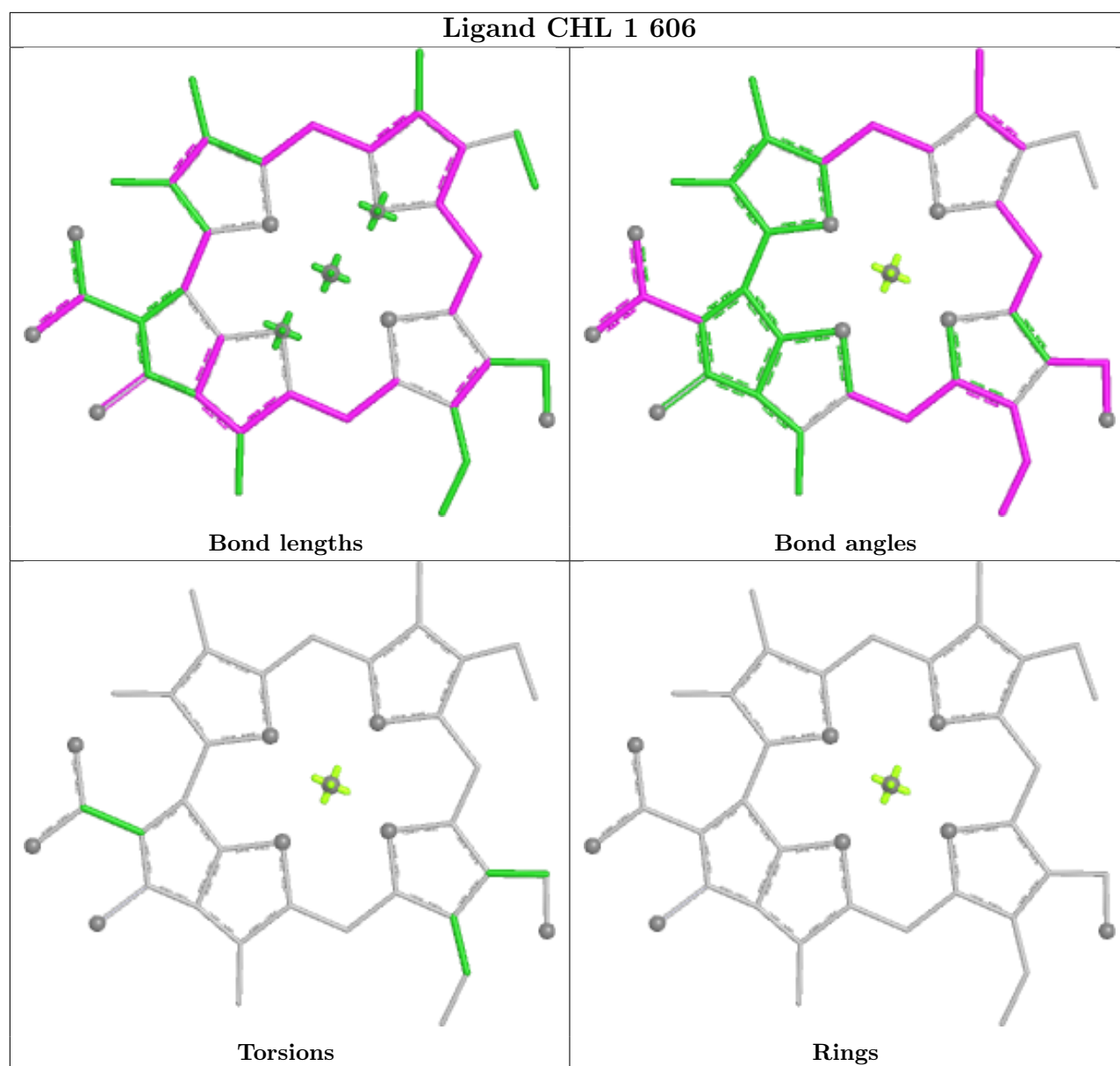


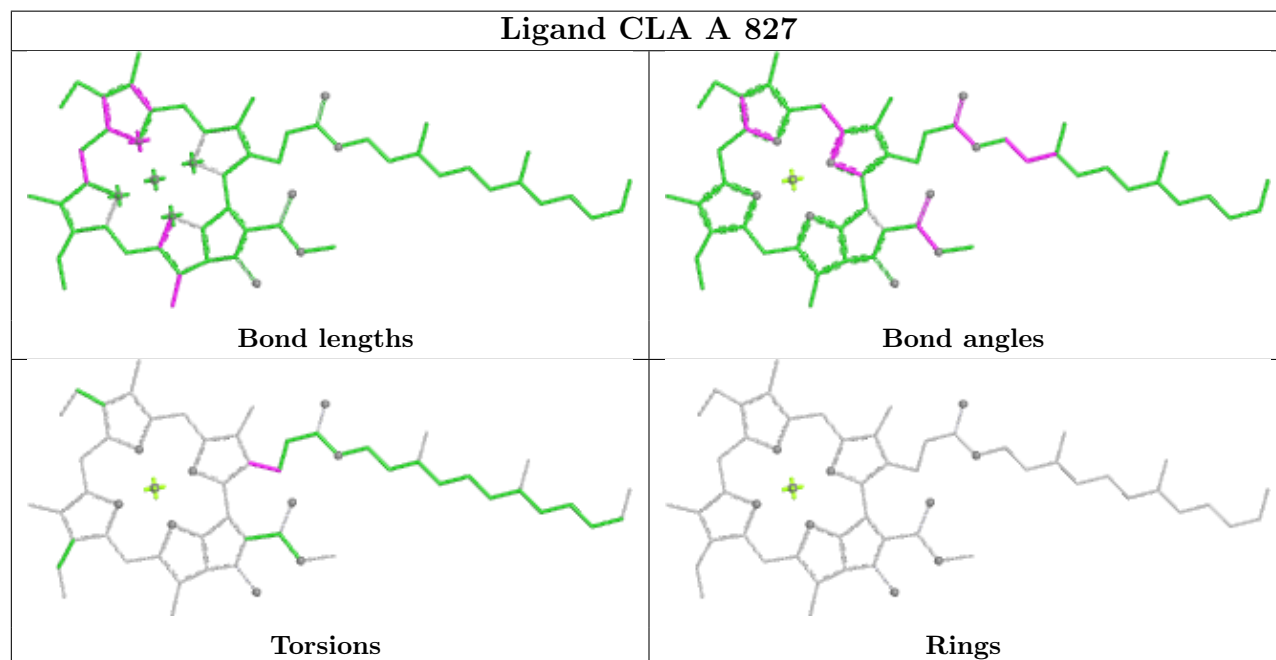
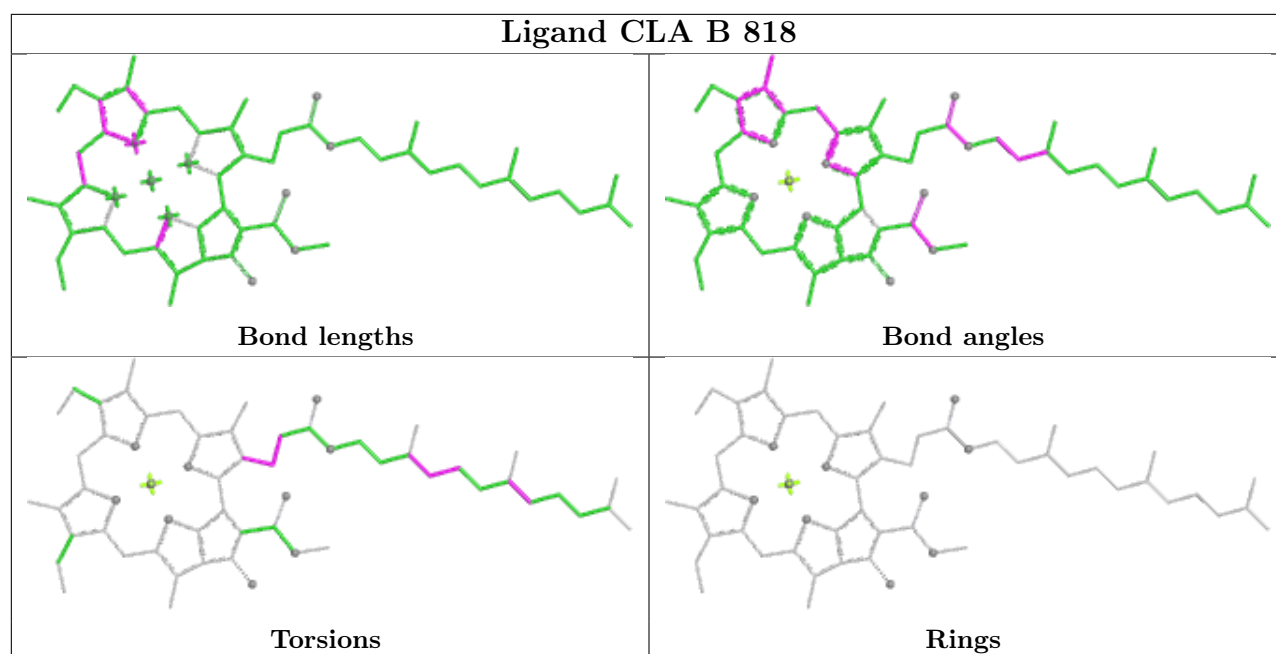
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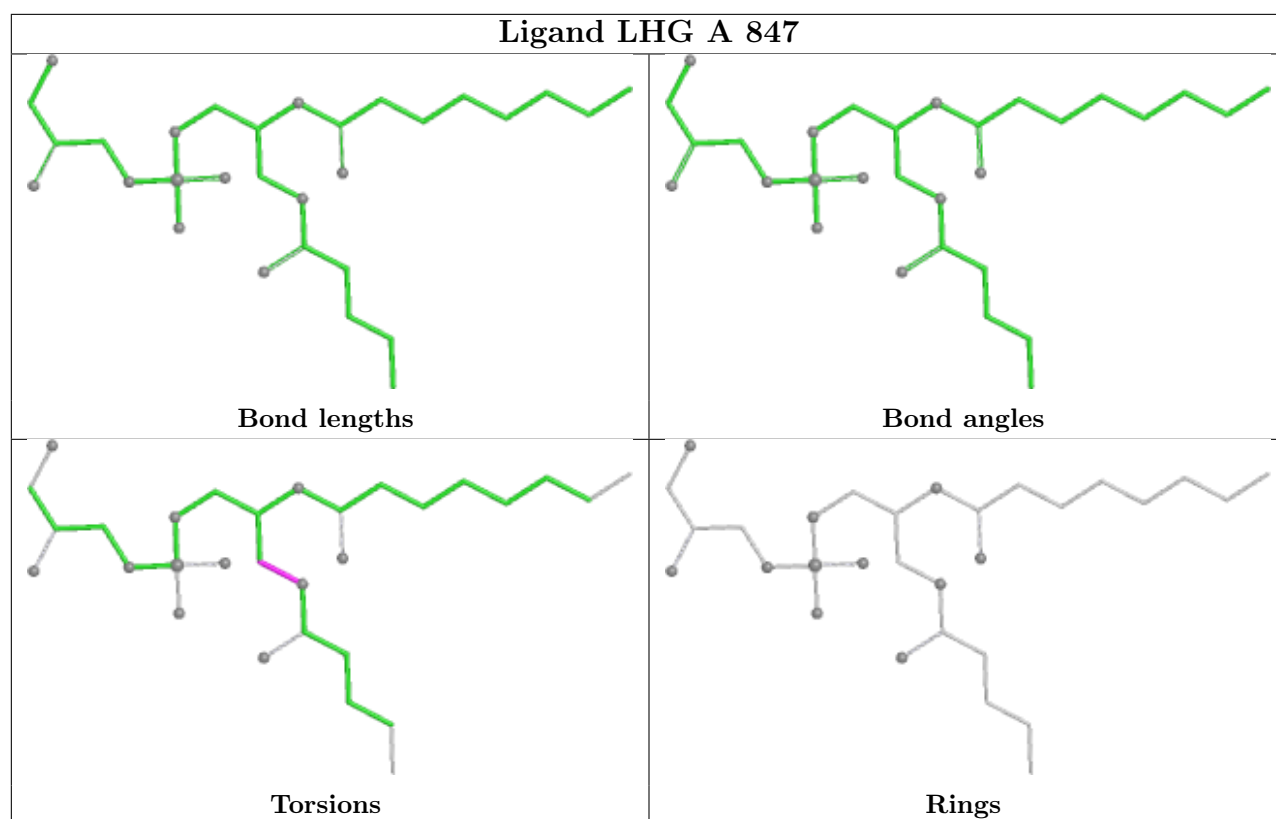


Ligand LUT 2 619

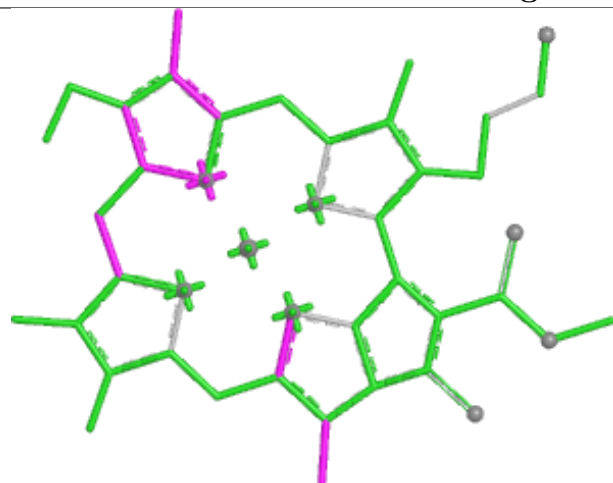




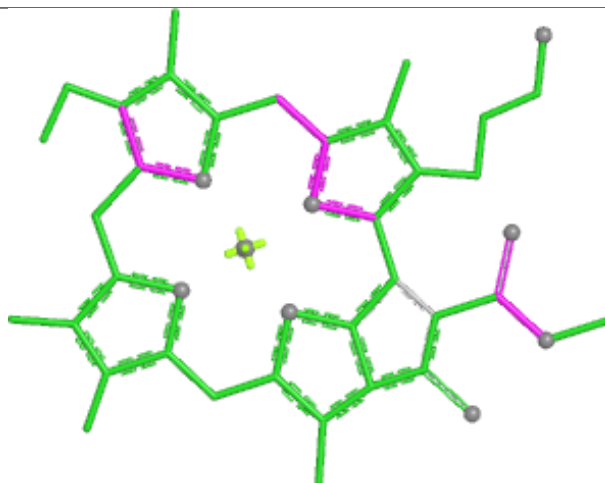




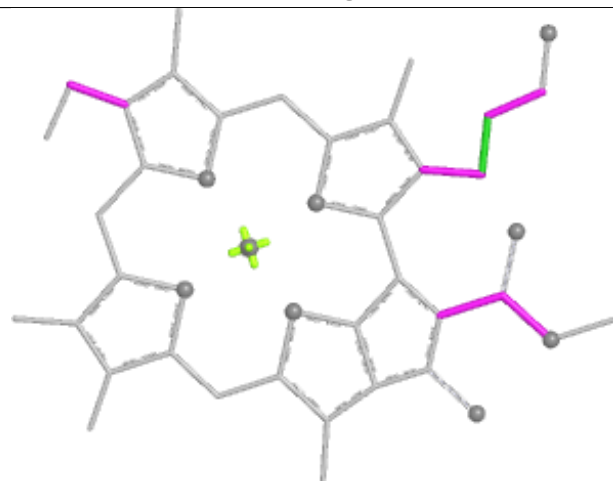
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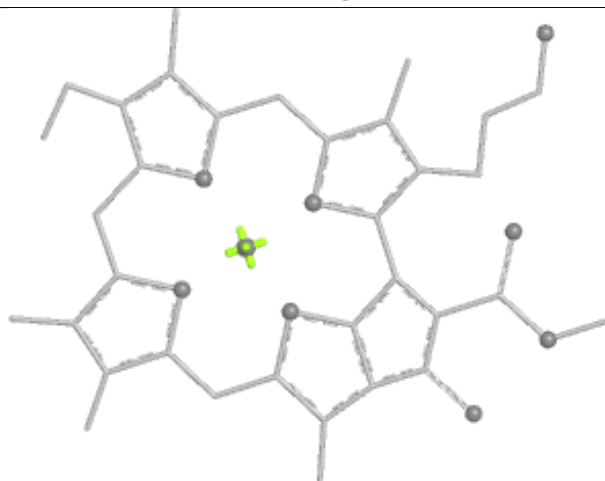
Bond lengths



Bond angles

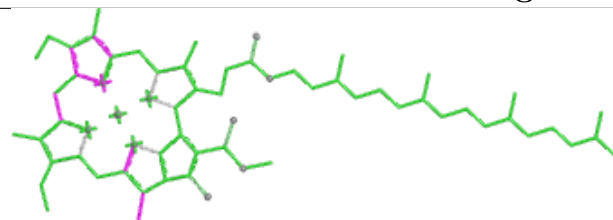


Torsions

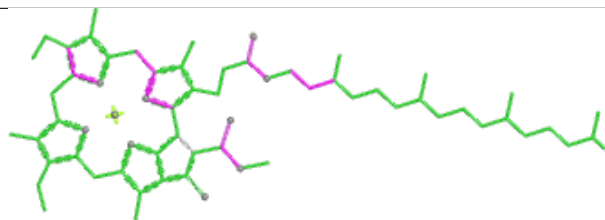


Rings

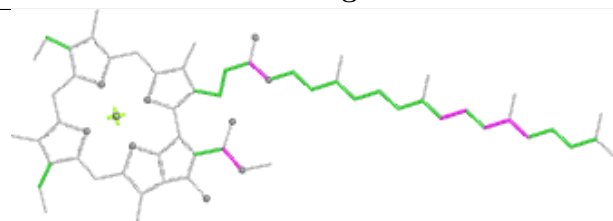
Ligand CLA A 811



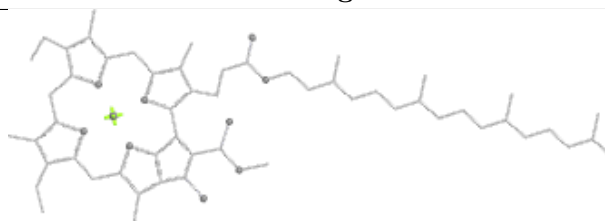
Bond lengths



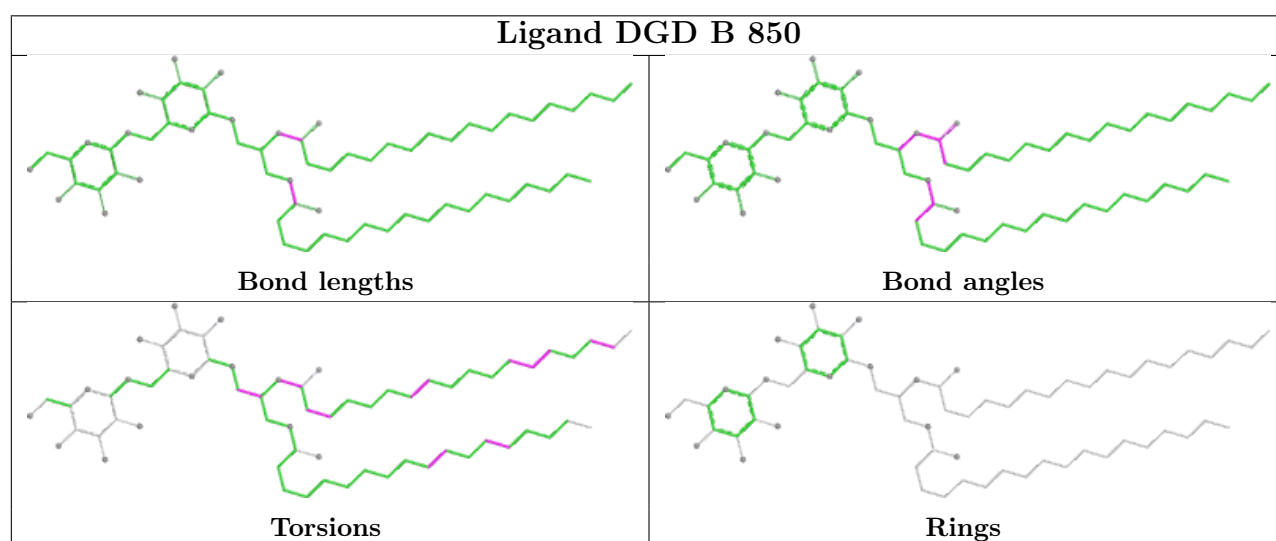
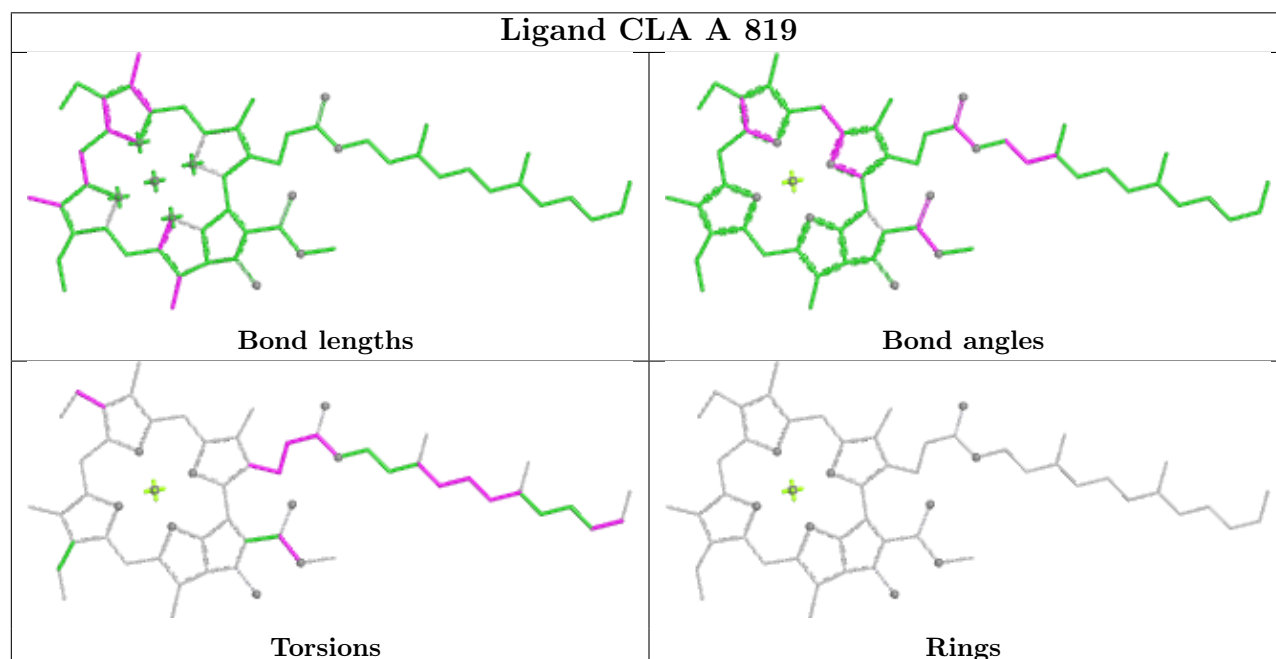
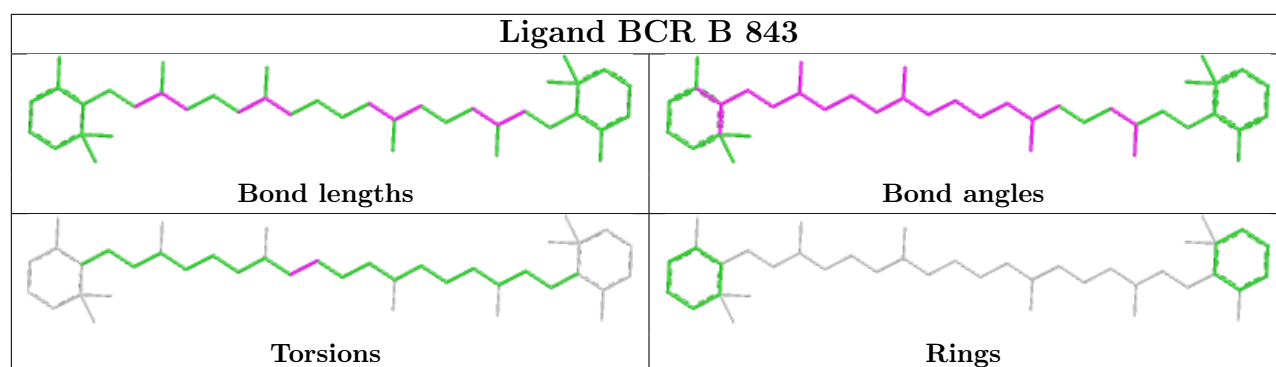
Bond angles



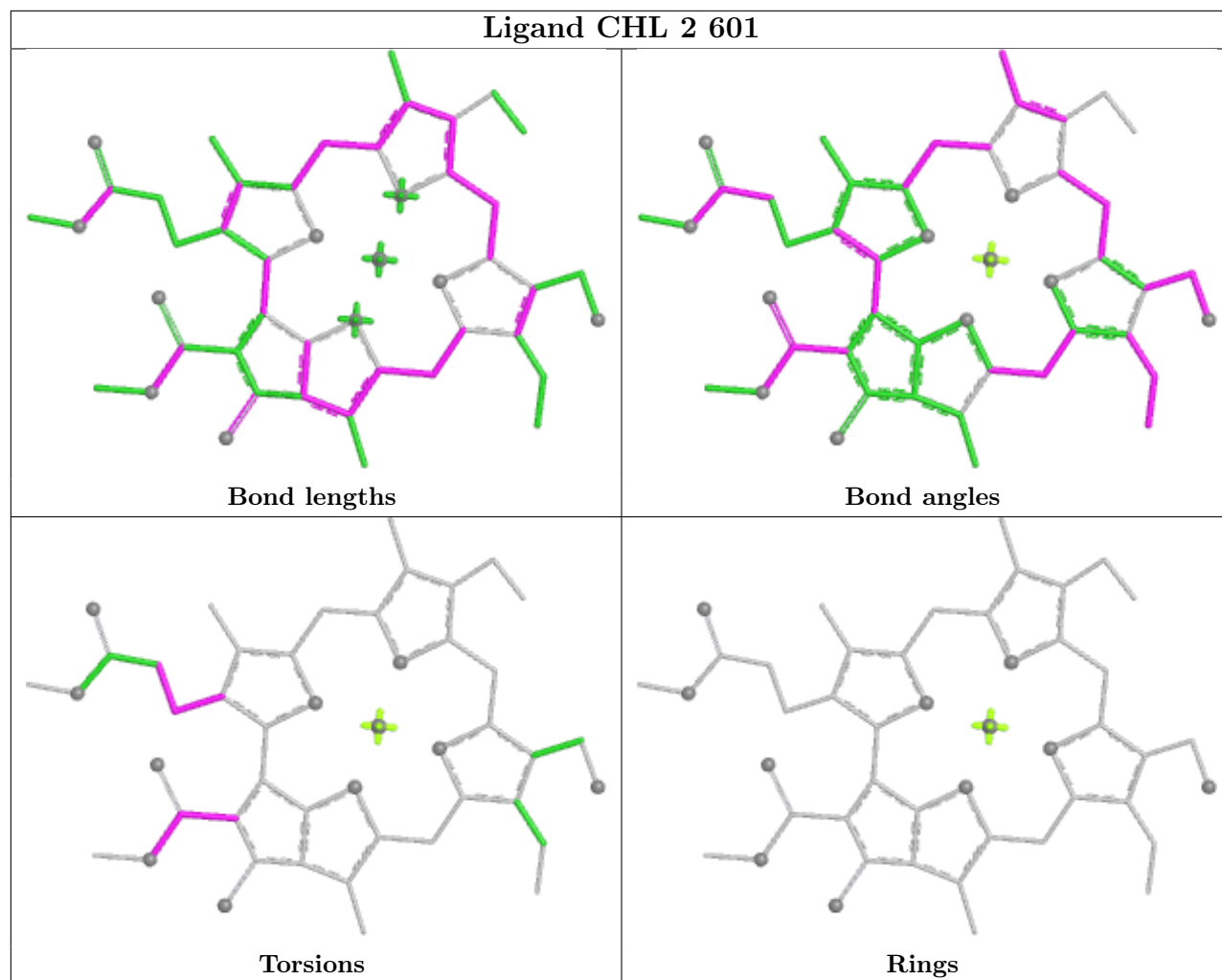
Torsions



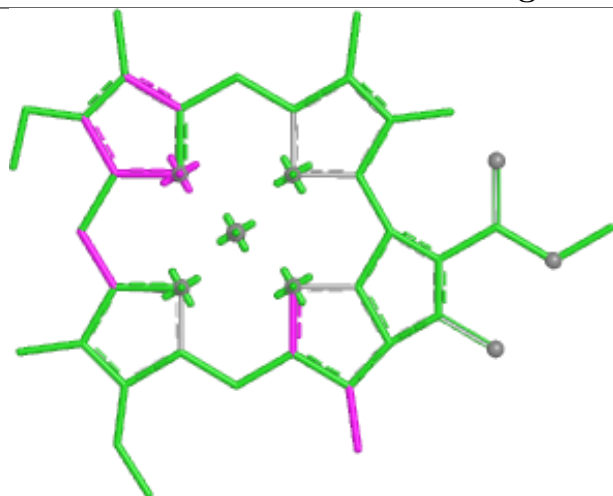
Rings



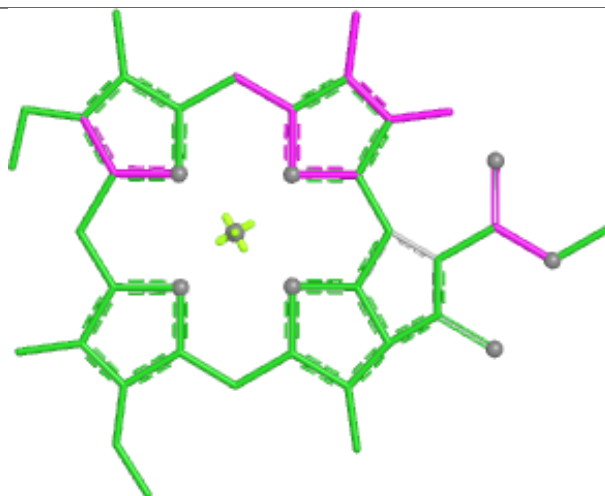
Ligand CHL 2 601



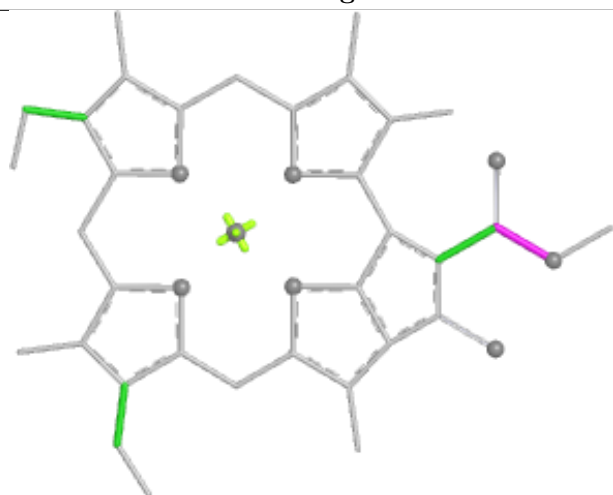
Ligand CLA 3 608



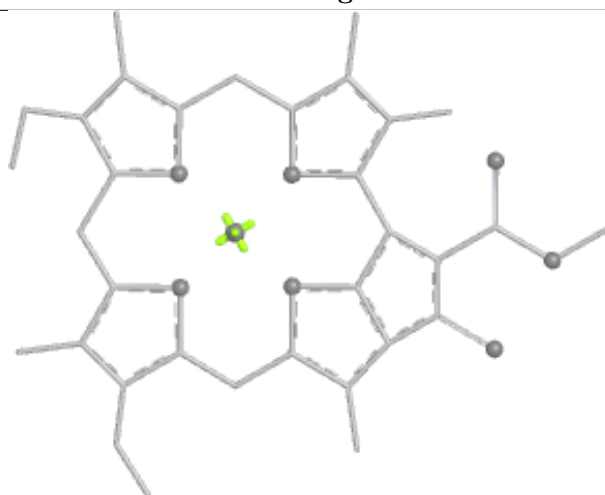
Bond lengths



Bond angles

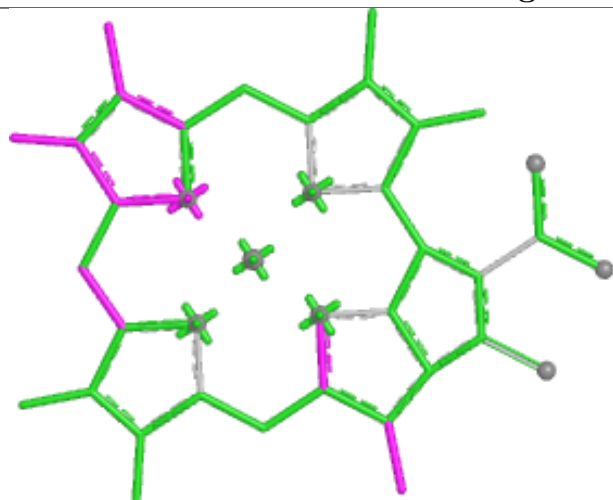


Torsions

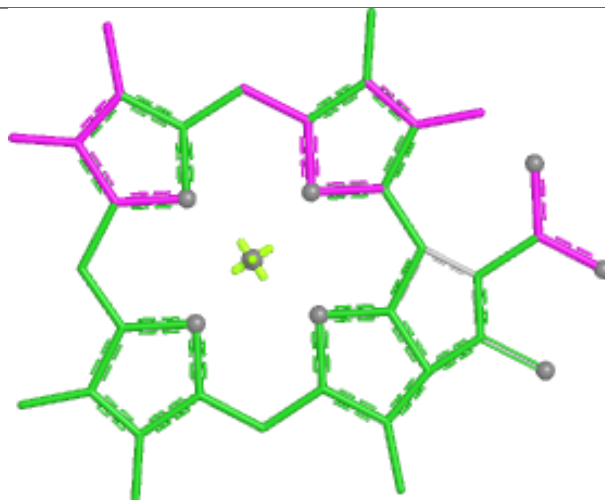


Rings

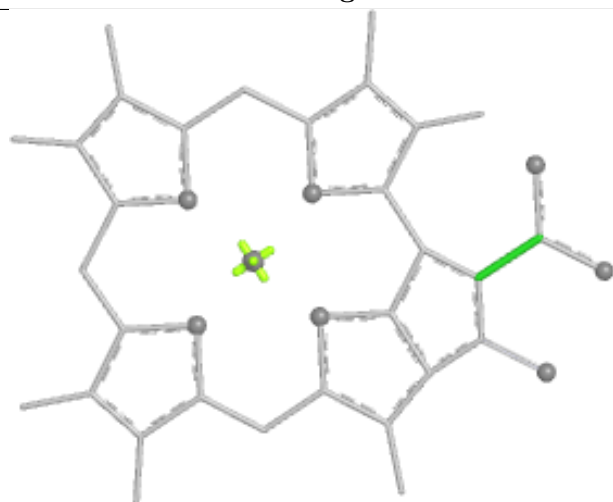
Ligand CLA 1 613



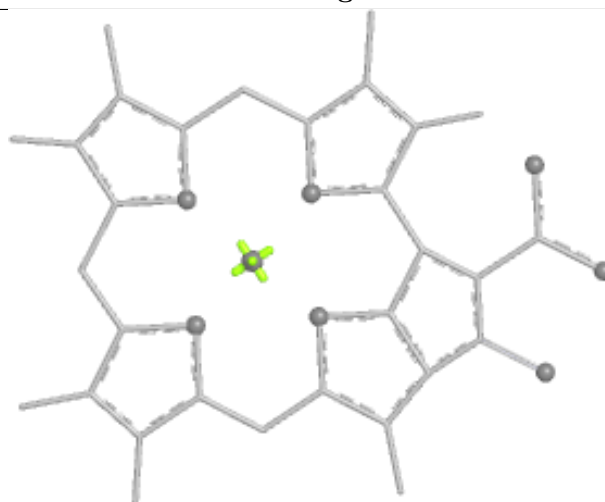
Bond lengths



Bond angles

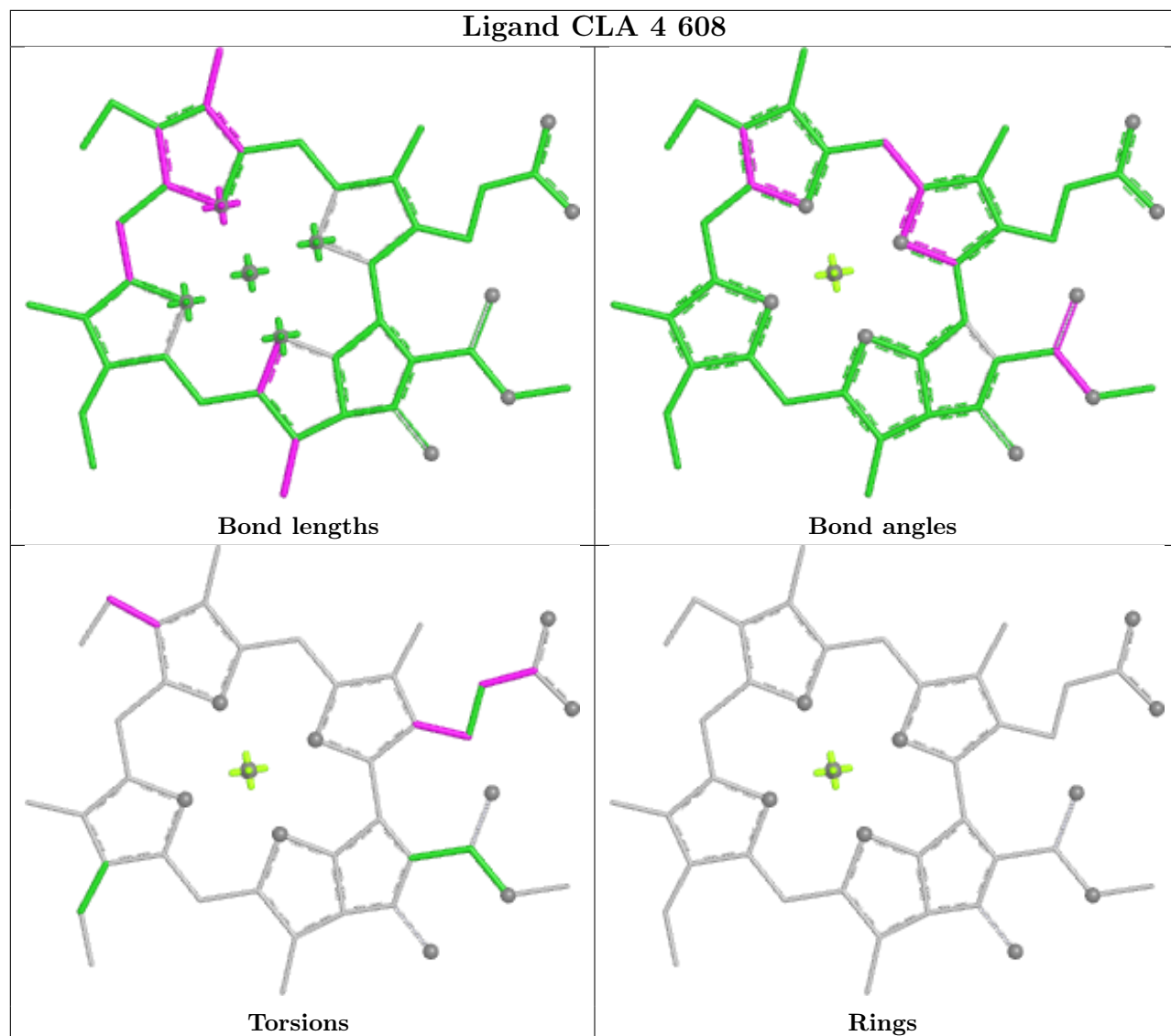


Torsions

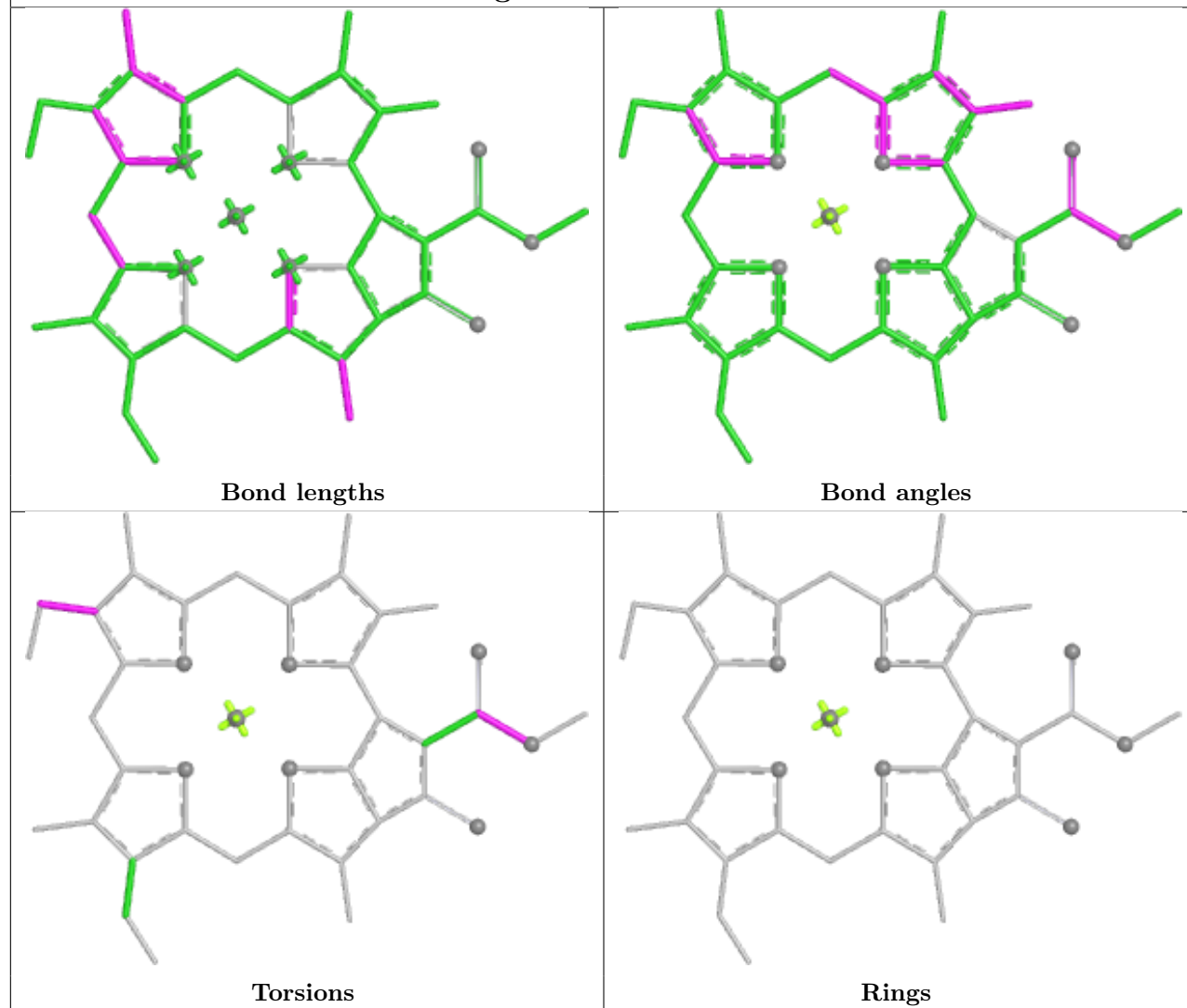


Rings

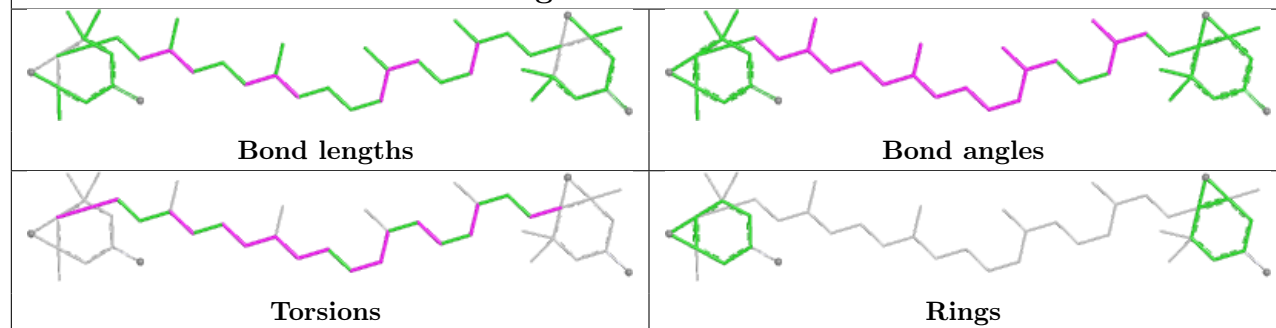
Ligand CLA 4 608

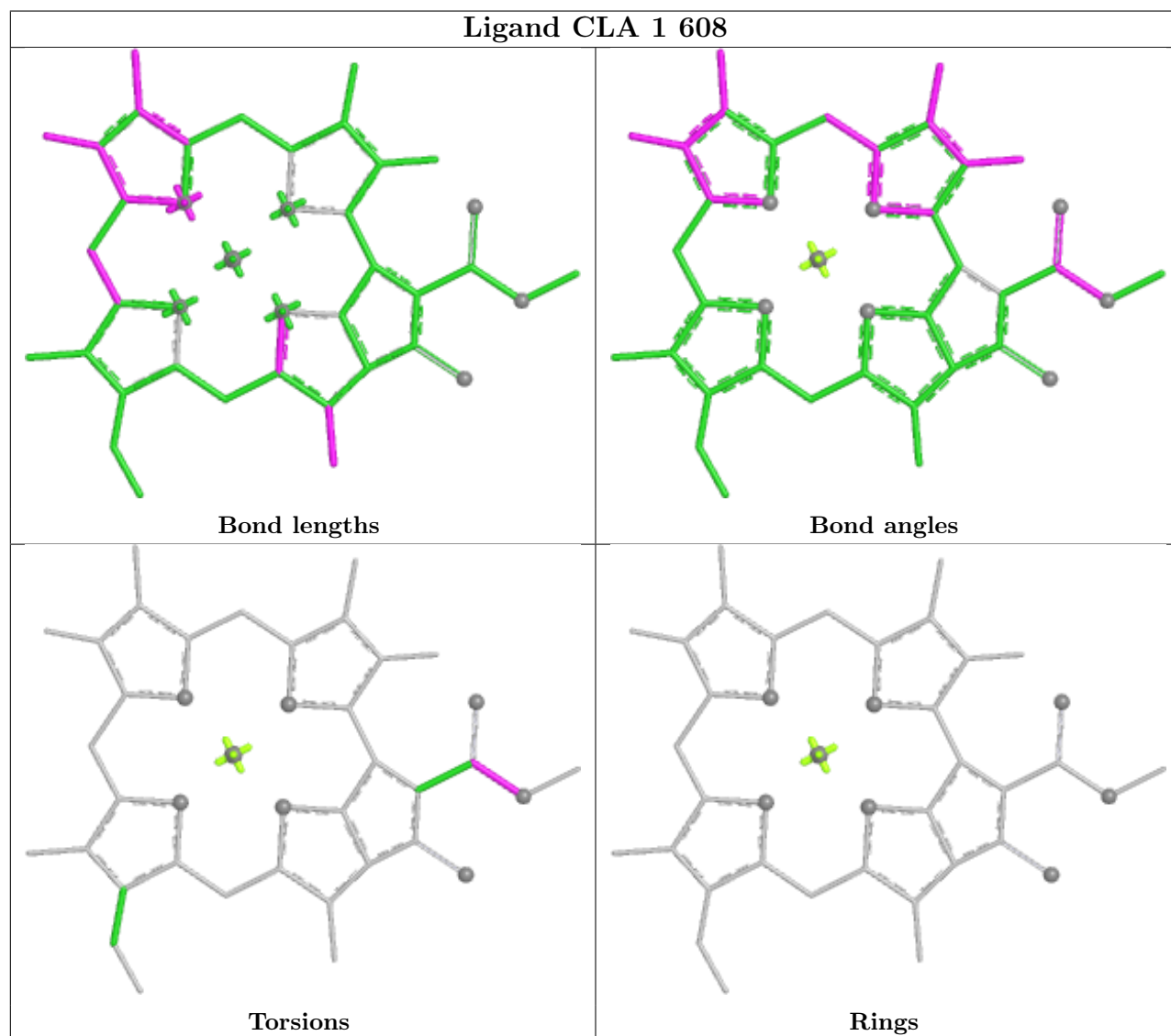
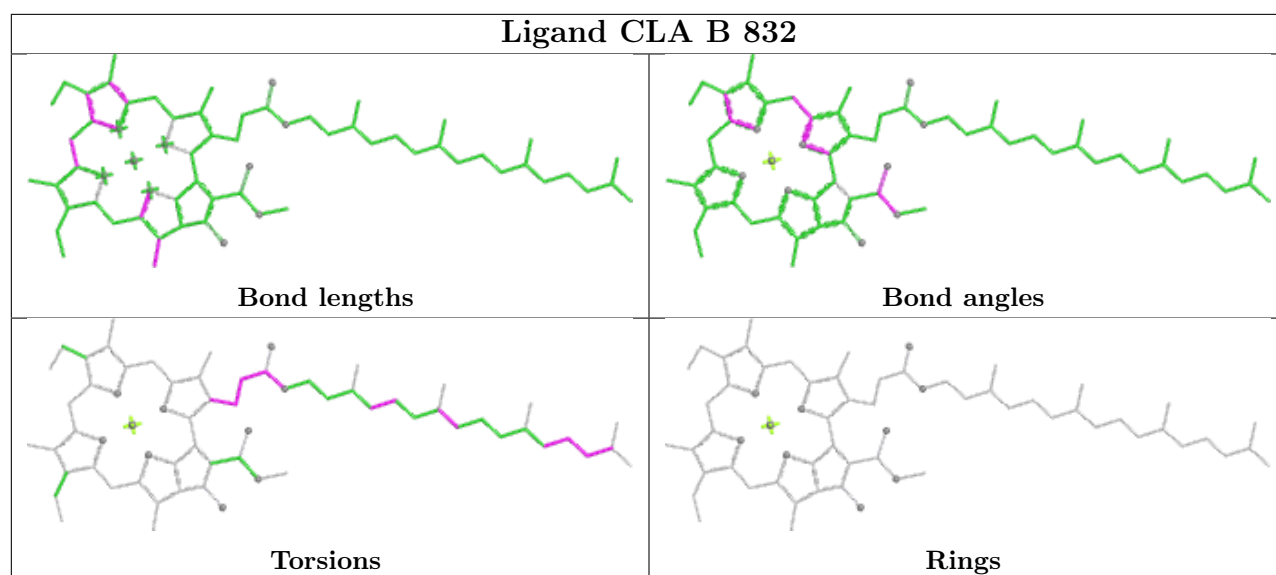


Ligand CLA A 824

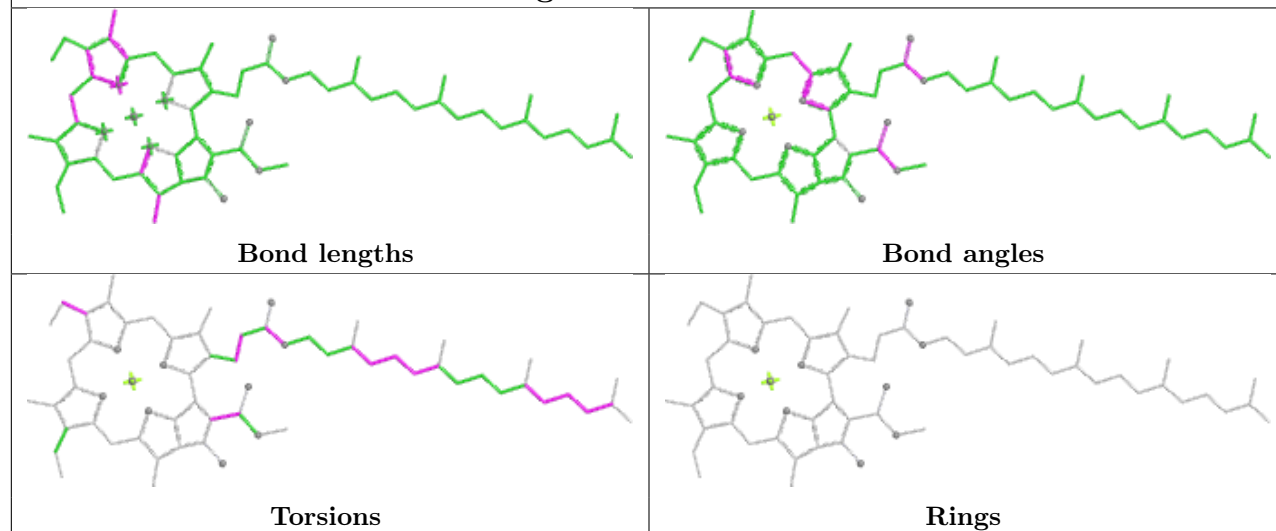


Ligand XAT 2 617

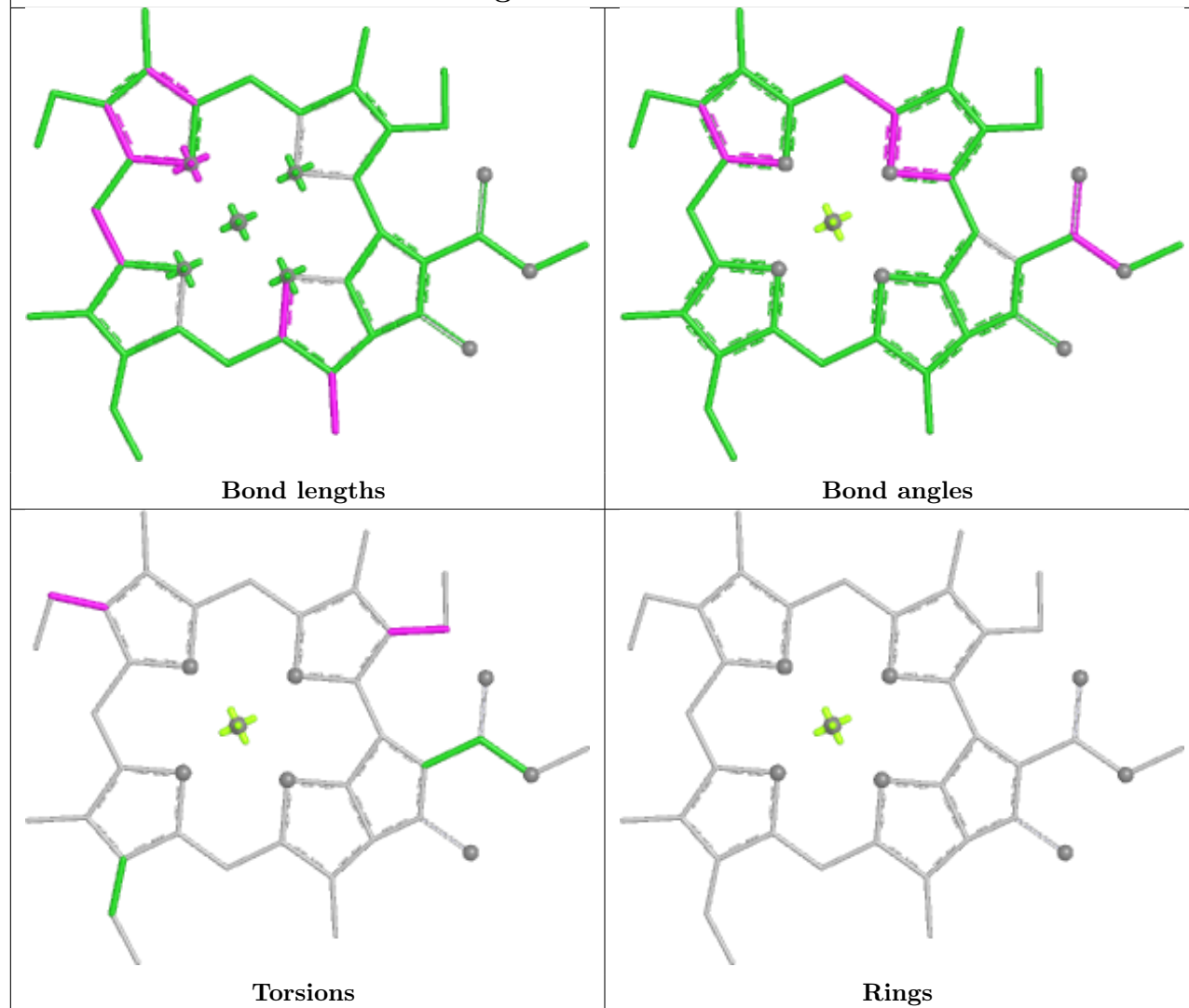




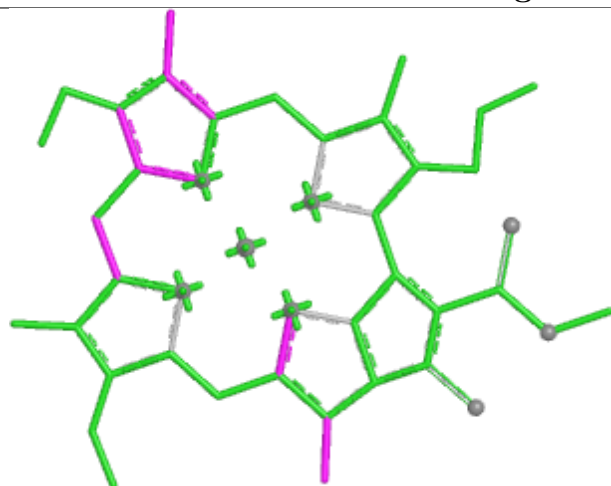
Ligand CLA 2 602



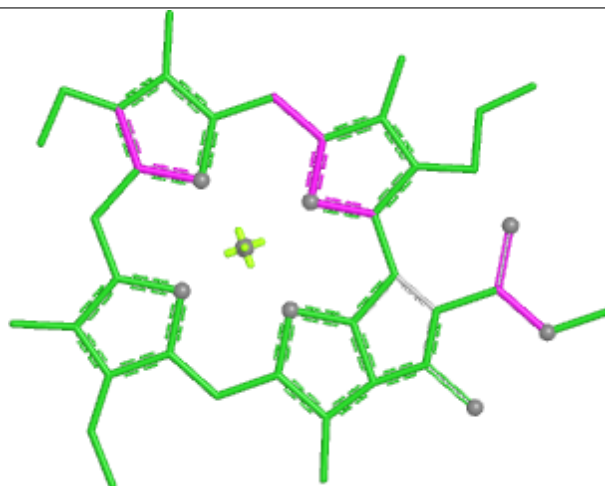
Ligand CLA G 202



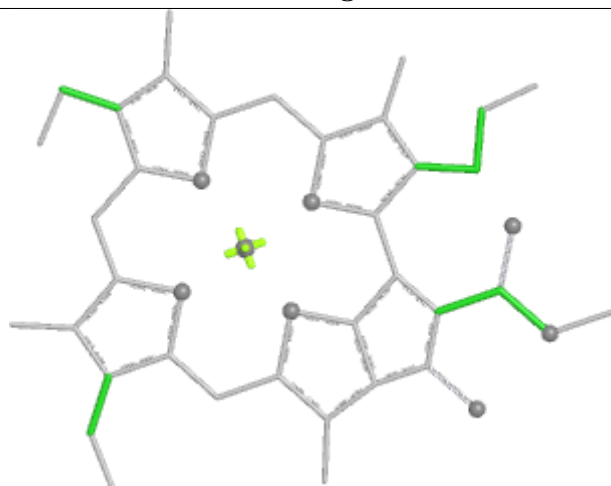
Ligand CLA B 812



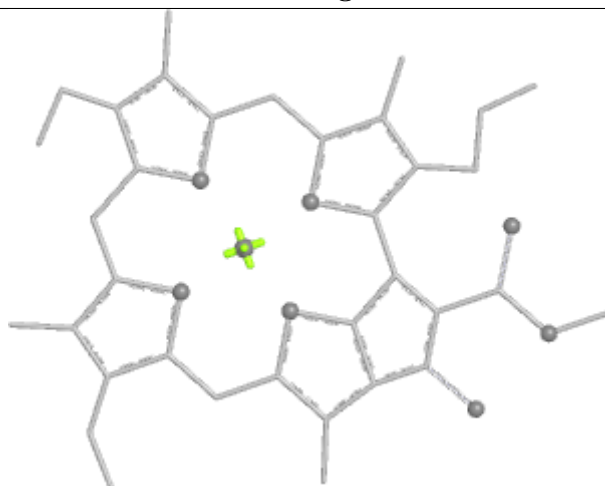
Bond lengths



Bond angles

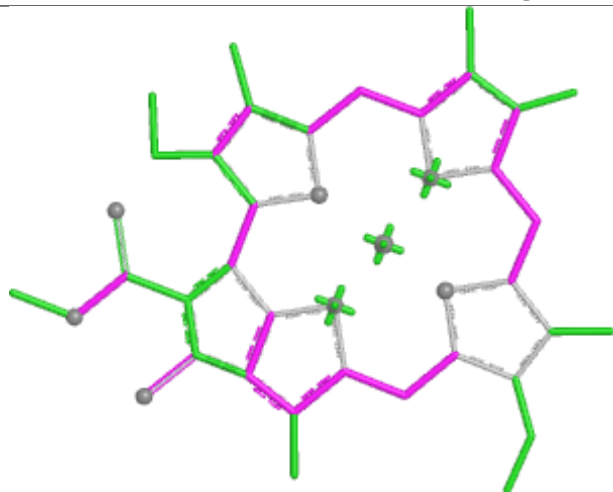


Torsions

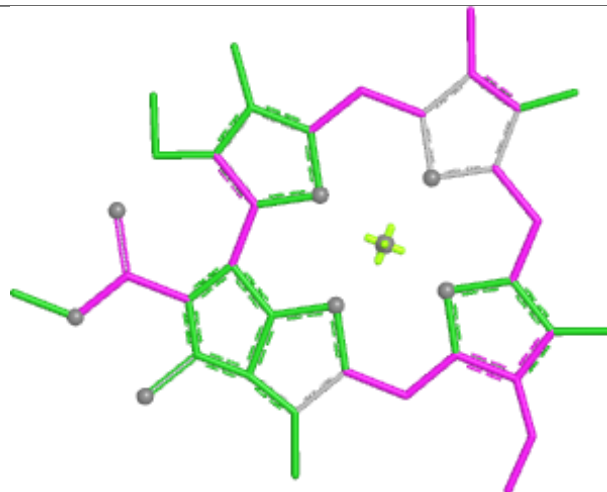


Rings

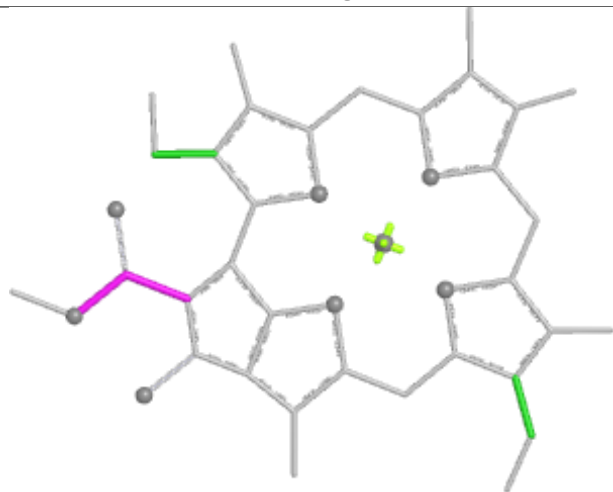
Ligand CHL 4 606



Bond lengths



Bond angles

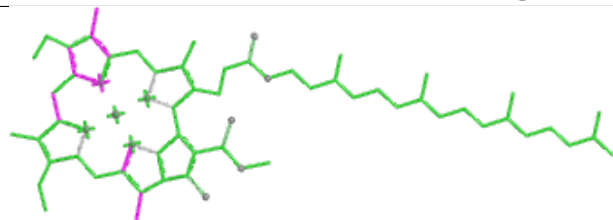


Torsions

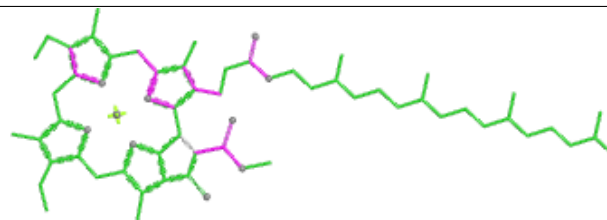


Rings

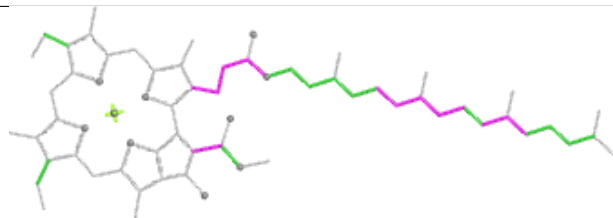
Ligand CLA A 804



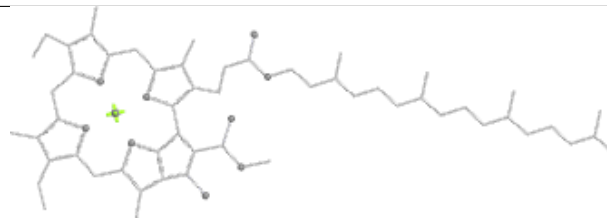
Bond lengths



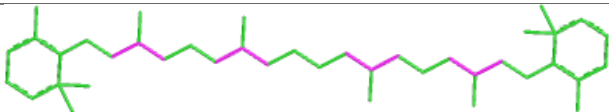
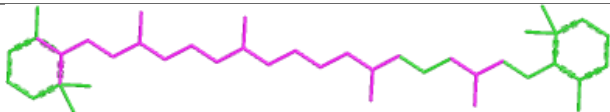
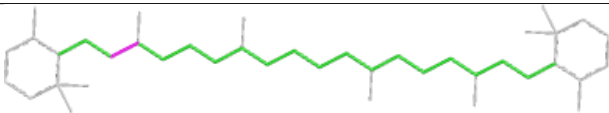
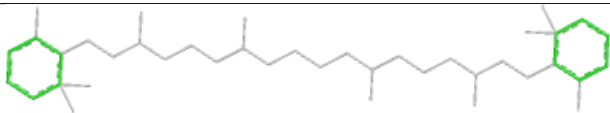
Bond angles

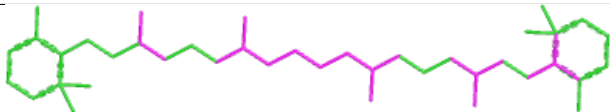
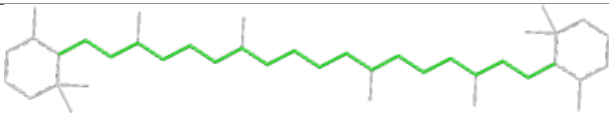
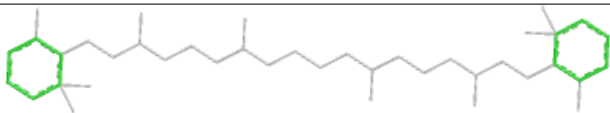


Torsions

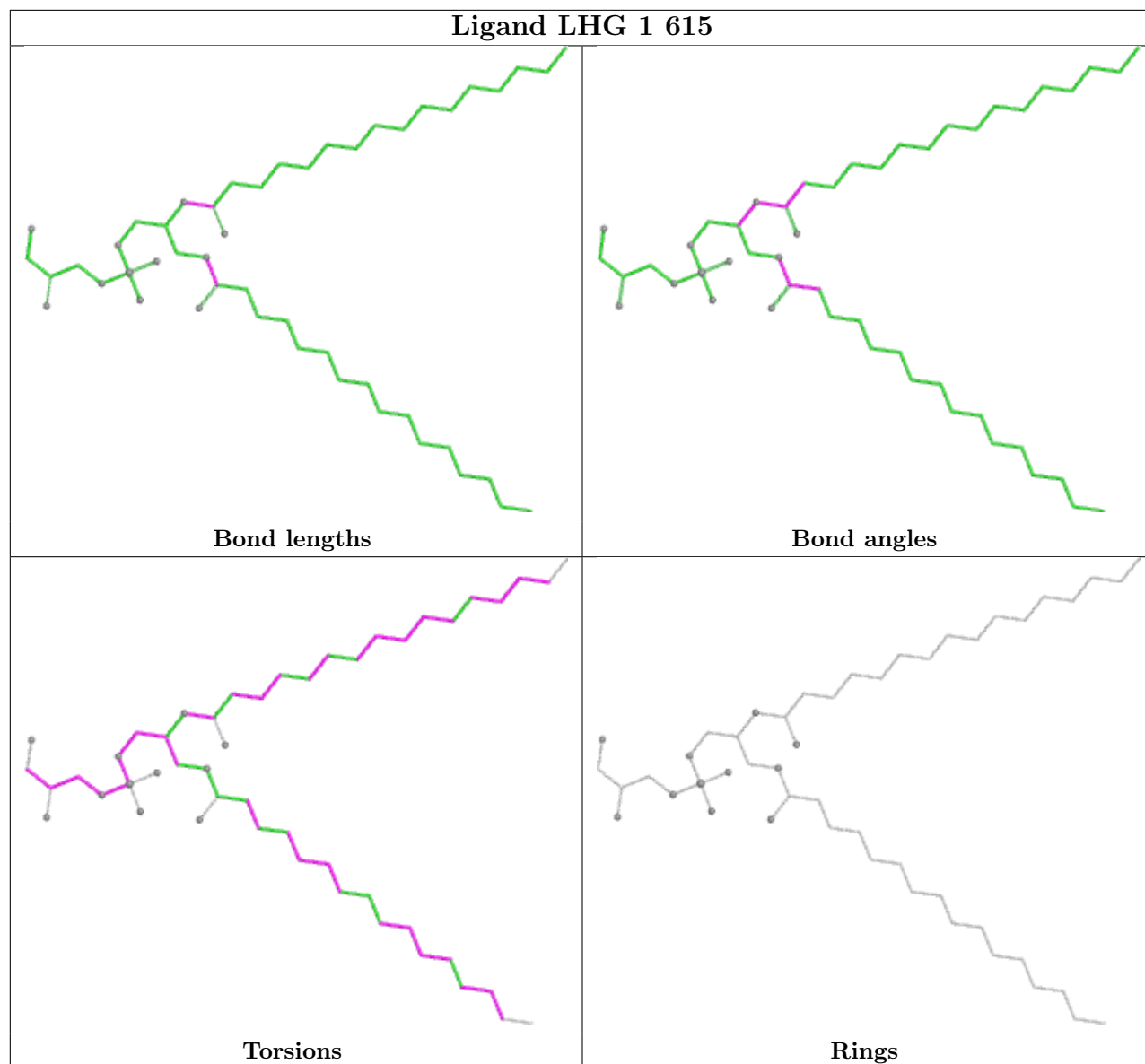


Rings

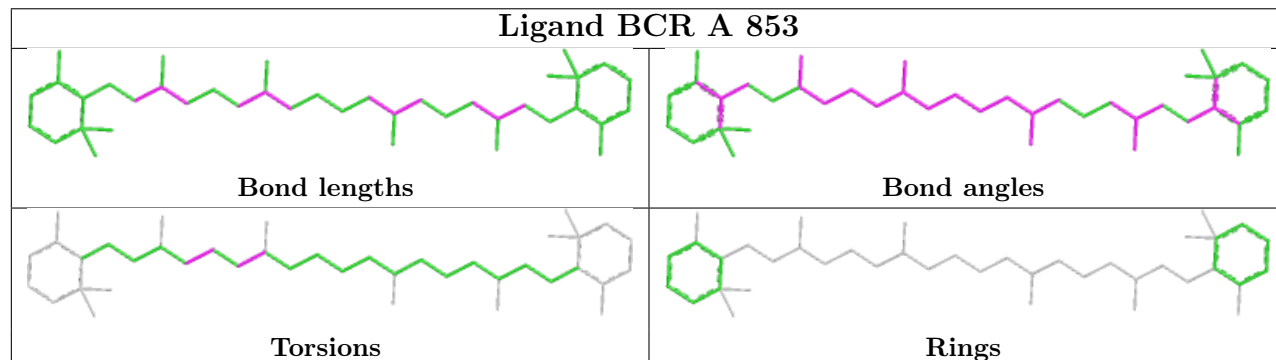
Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

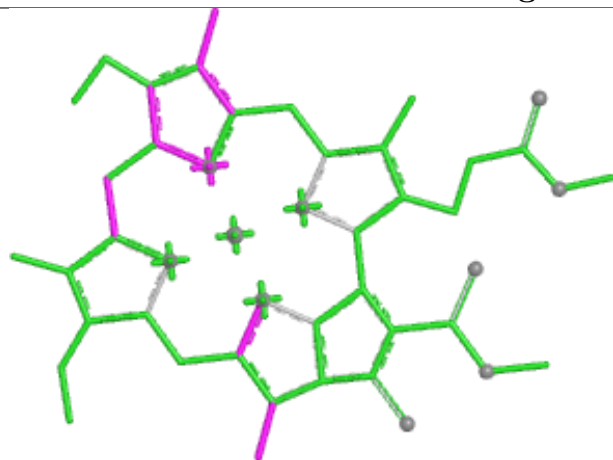
Ligand LHG 1 615



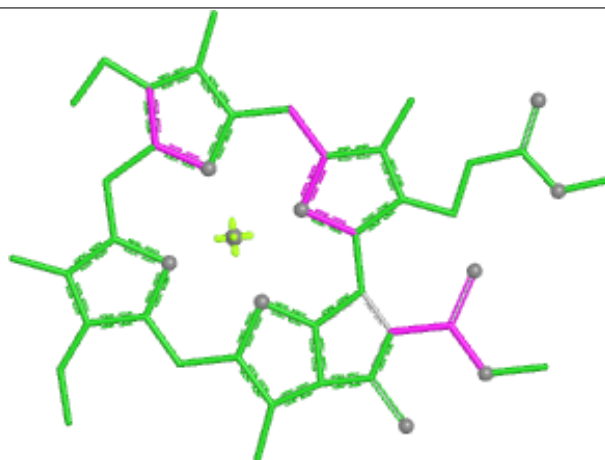
Ligand BCR A 853



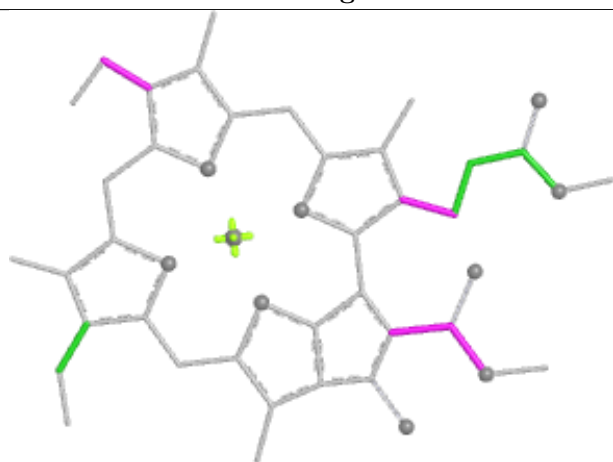
Ligand CLA 1 612



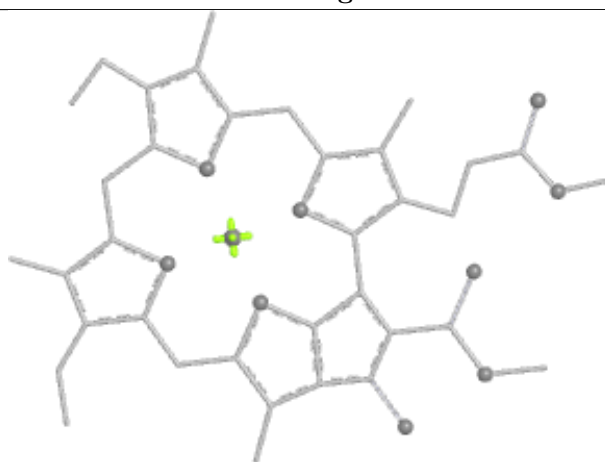
Bond lengths



Bond angles

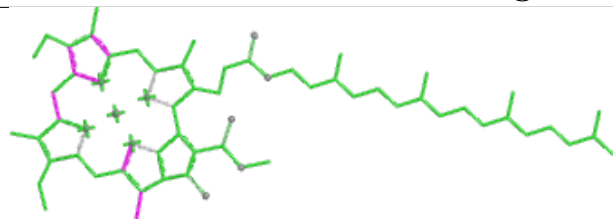


Torsions

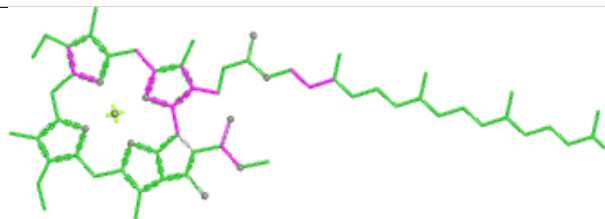


Rings

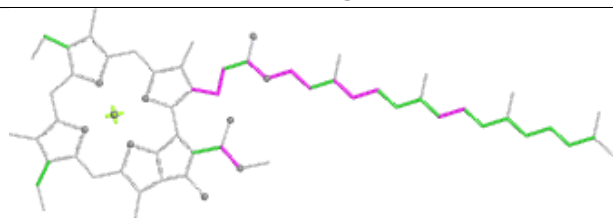
Ligand CLA A 830



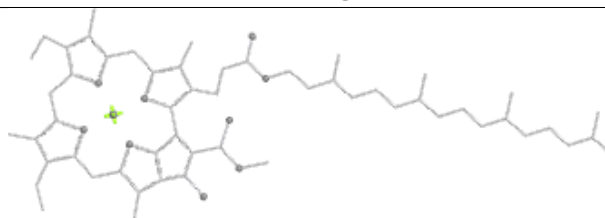
Bond lengths



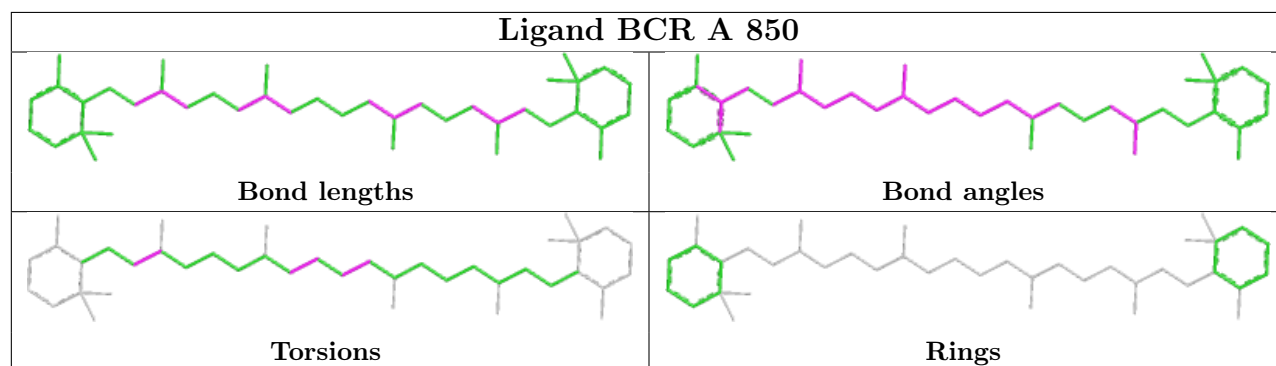
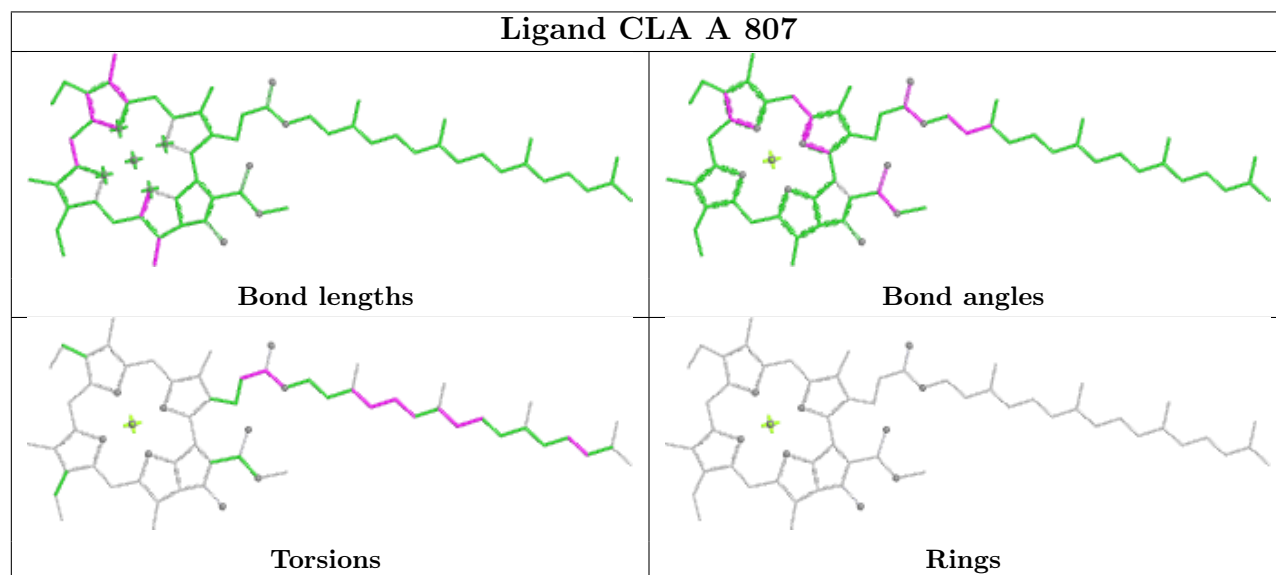
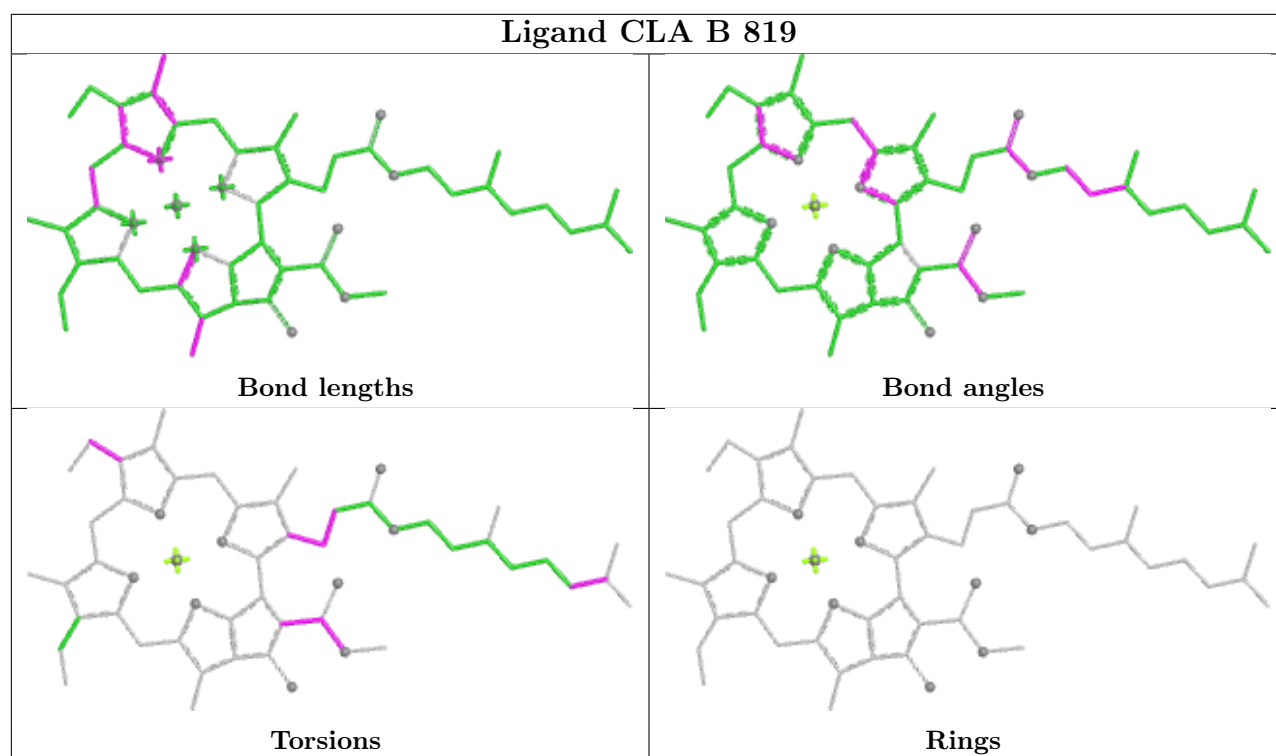
Bond angles



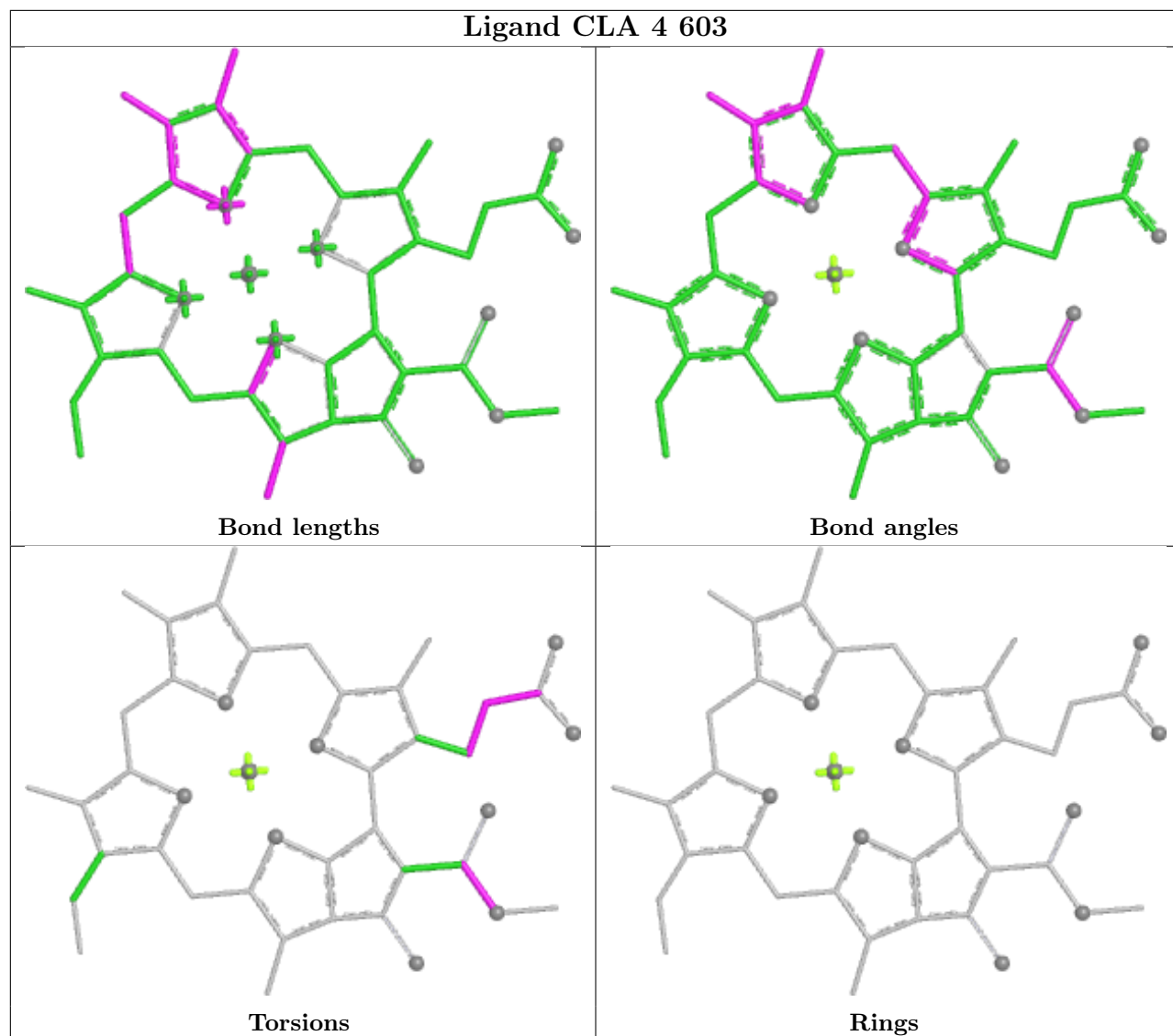
Torsions



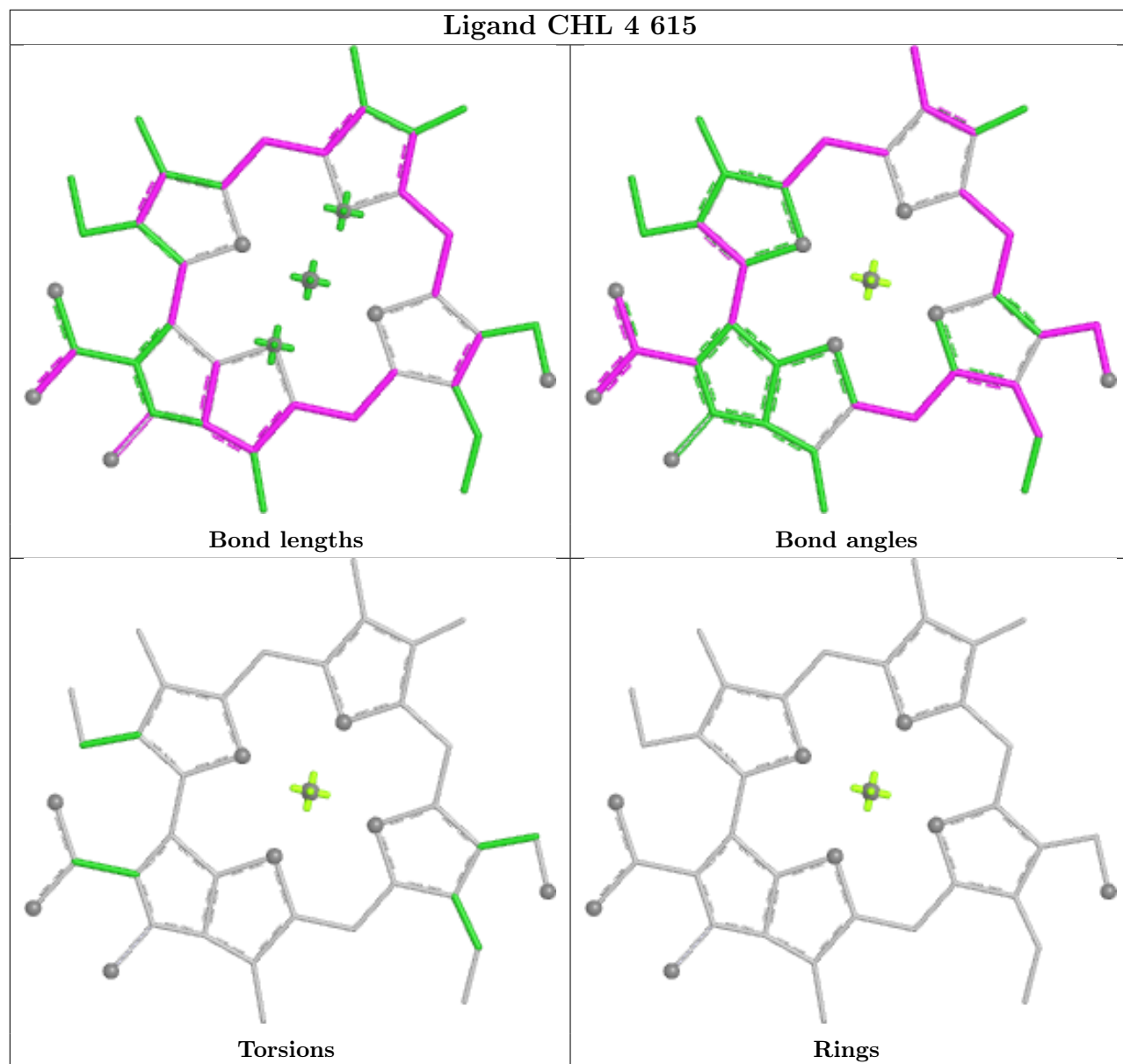
Rings



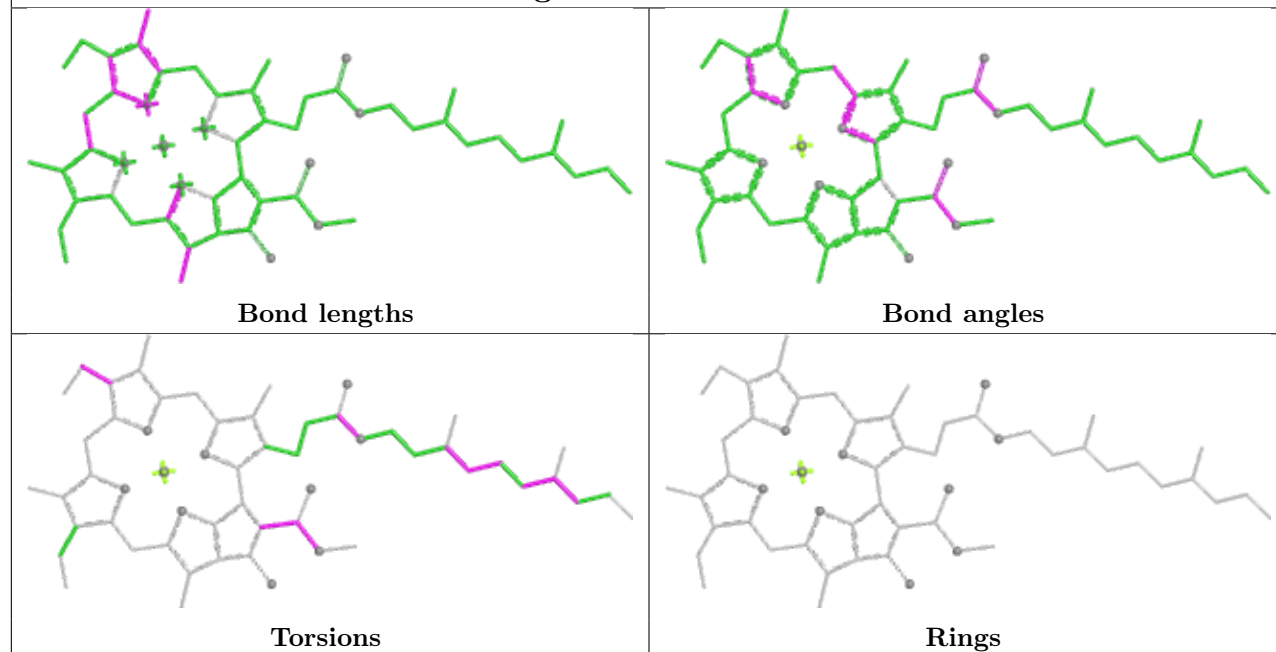
Ligand CLA 4 603



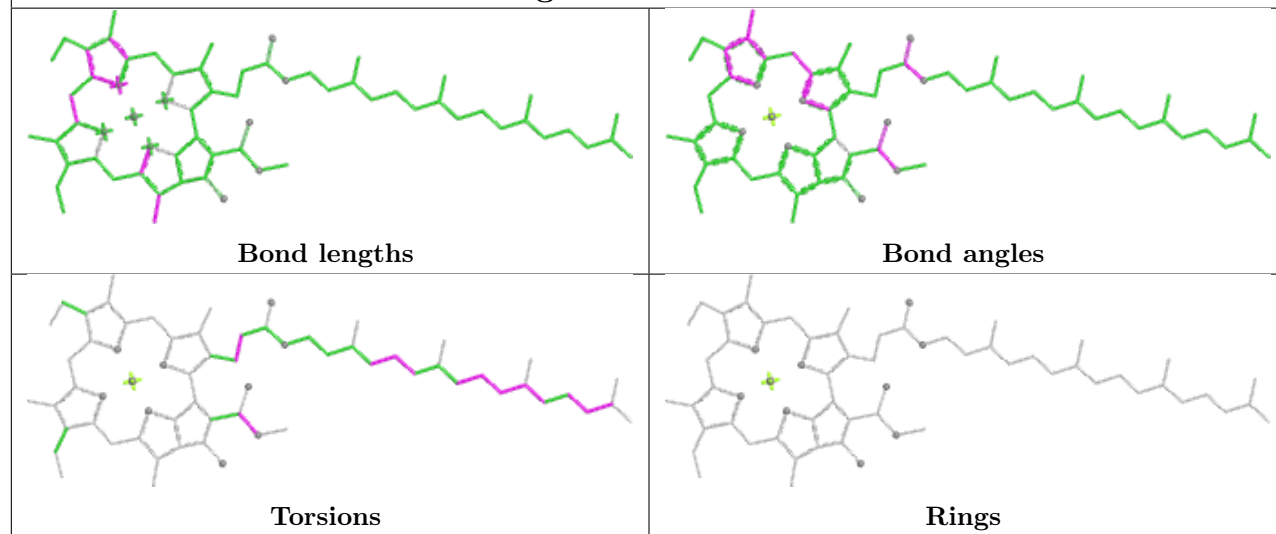
Ligand CHL 4 615



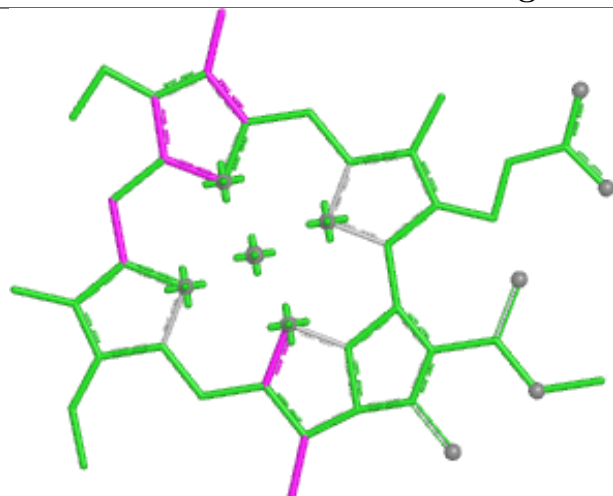
Ligand CLA F 301



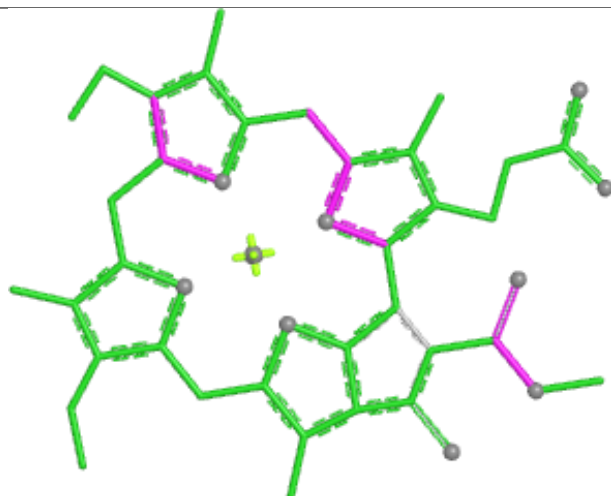
Ligand CLA 2 612



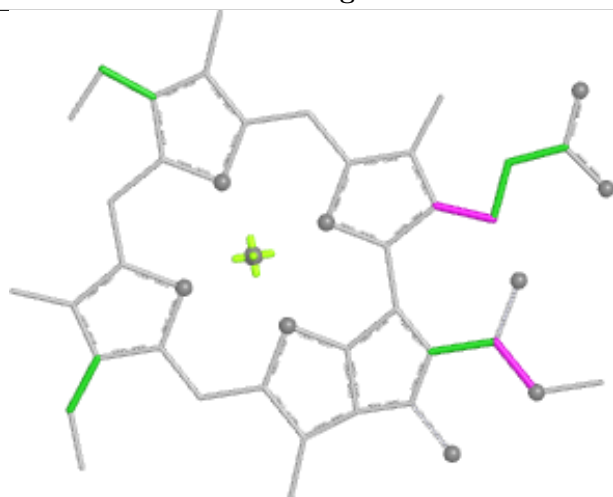
Ligand CLA 3 607



Bond lengths



Bond angles

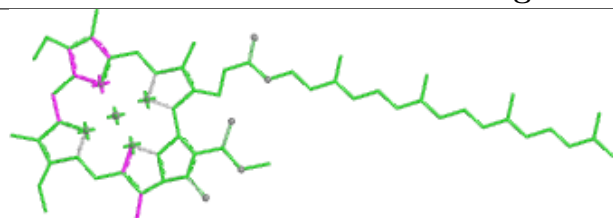


Torsions

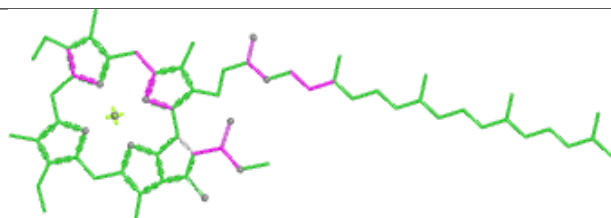


Rings

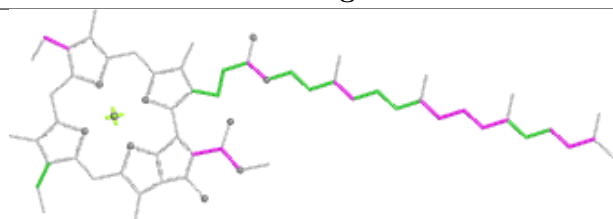
Ligand CLA A 835



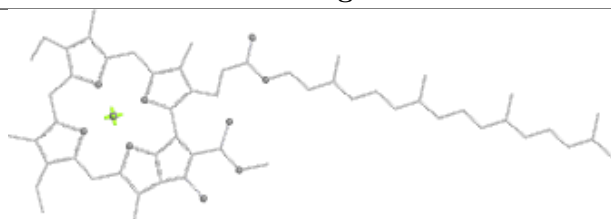
Bond lengths



Bond angles

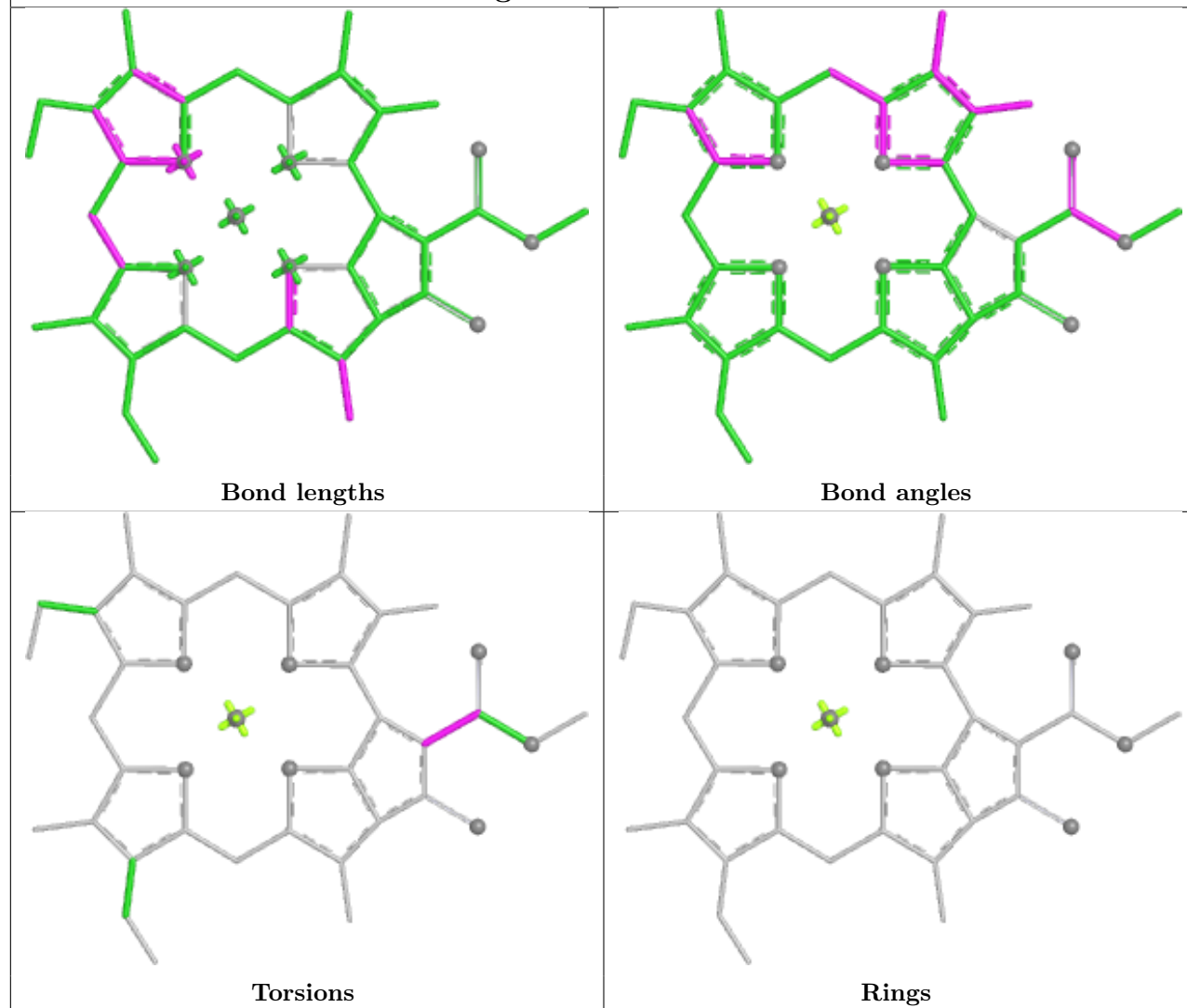


Torsions

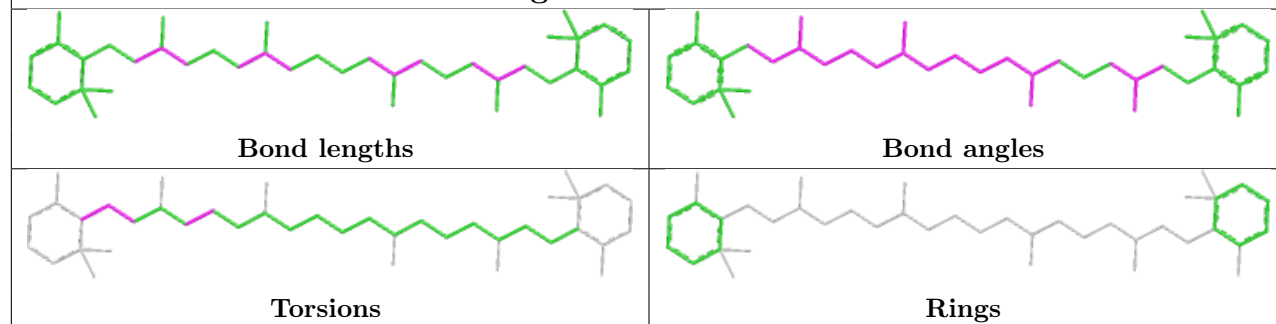


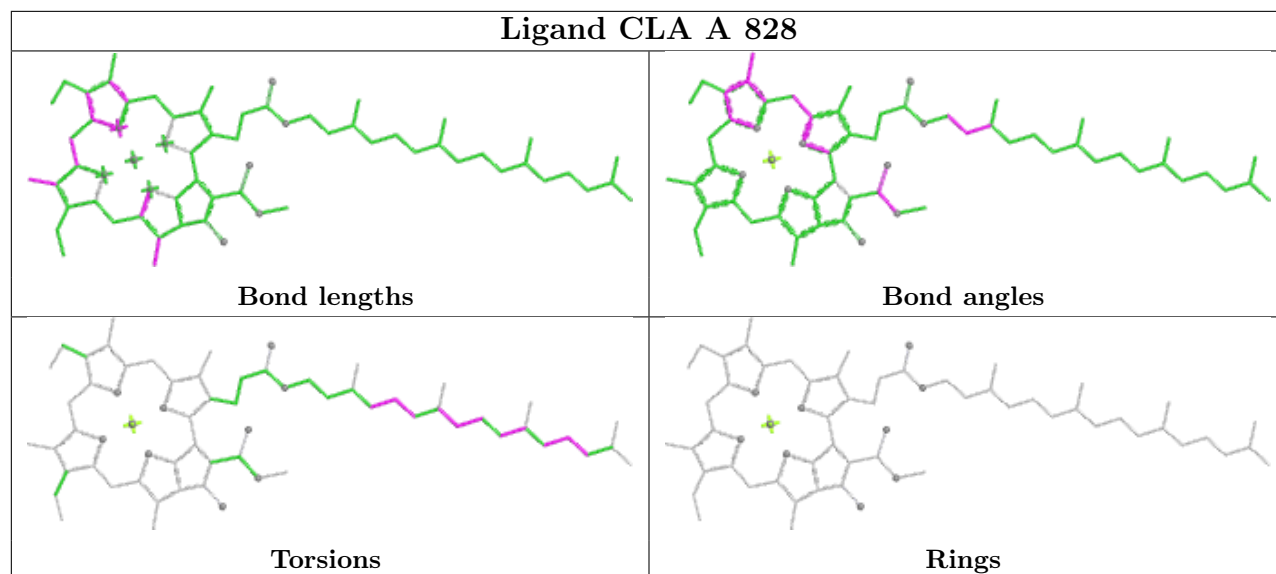
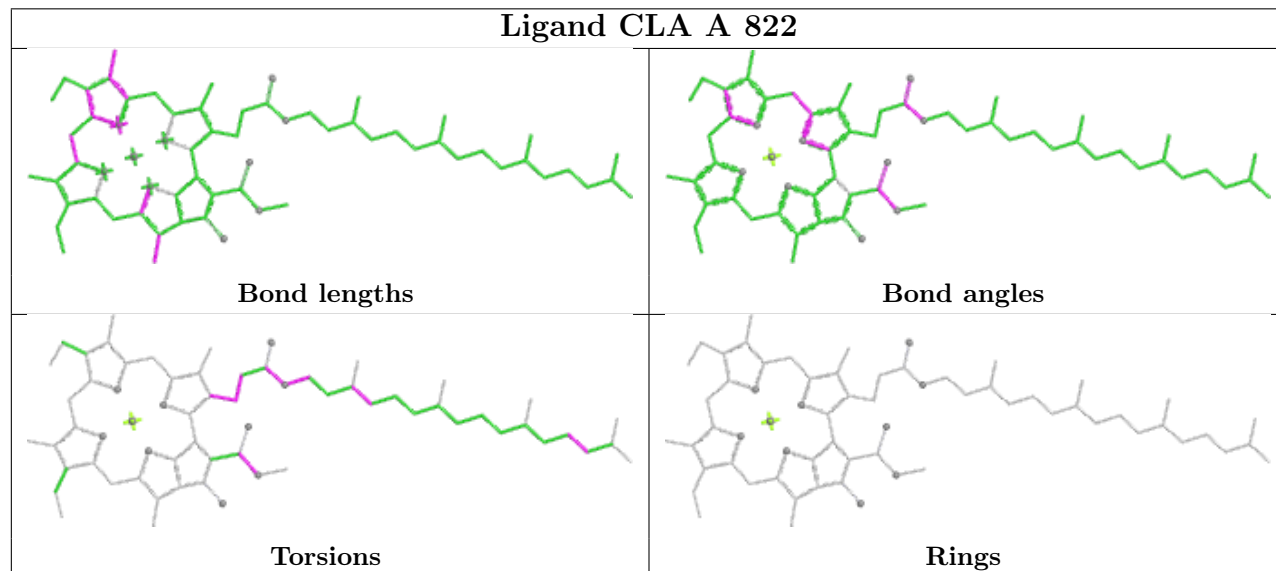
Rings

Ligand CLA B 804

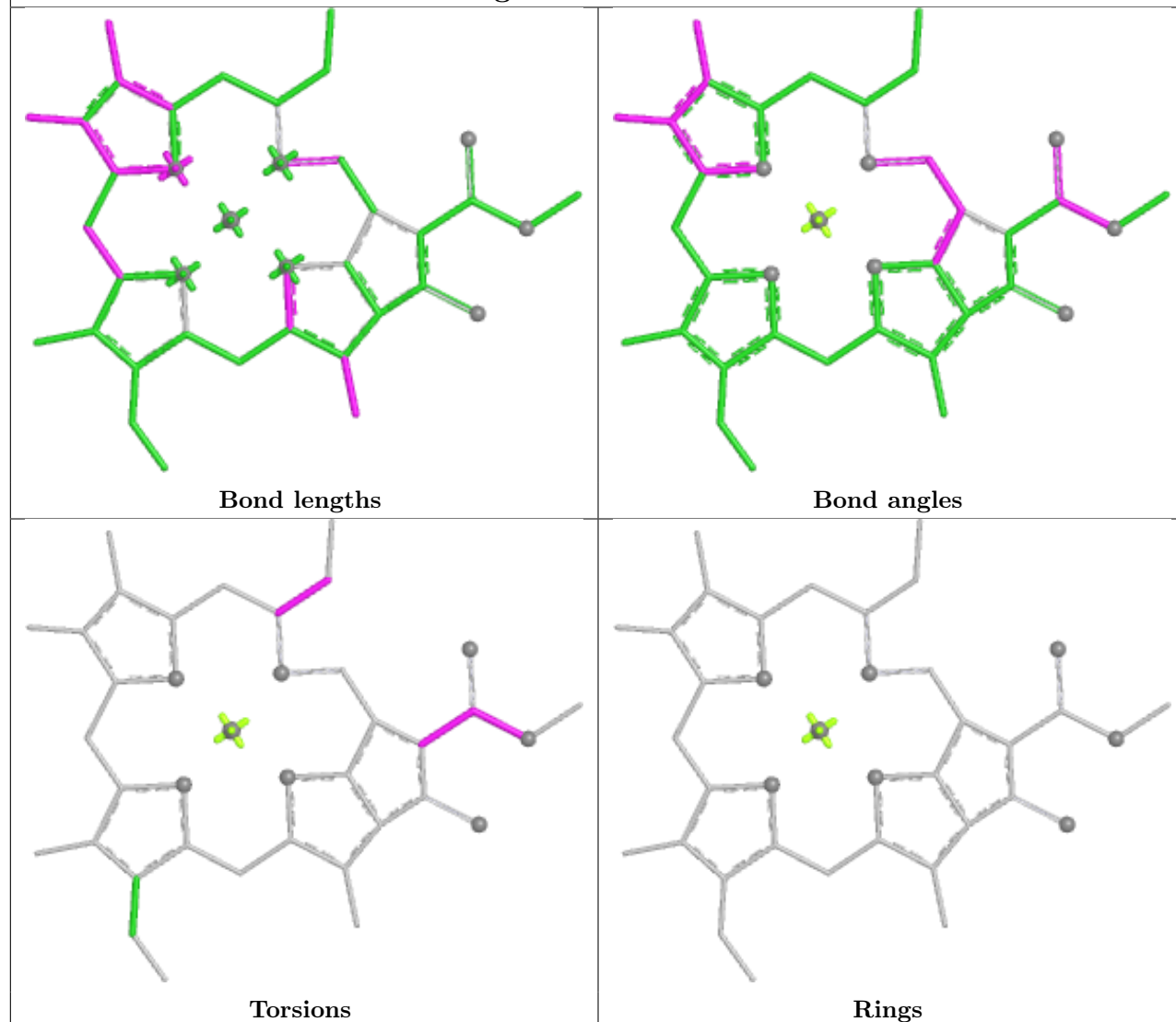


Ligand BCR B 801

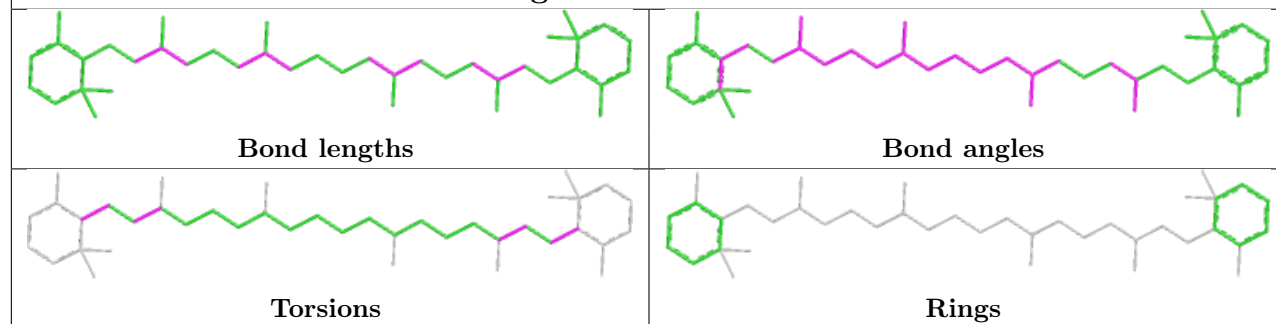


Ligand CLA A 828**Ligand CLA A 822**

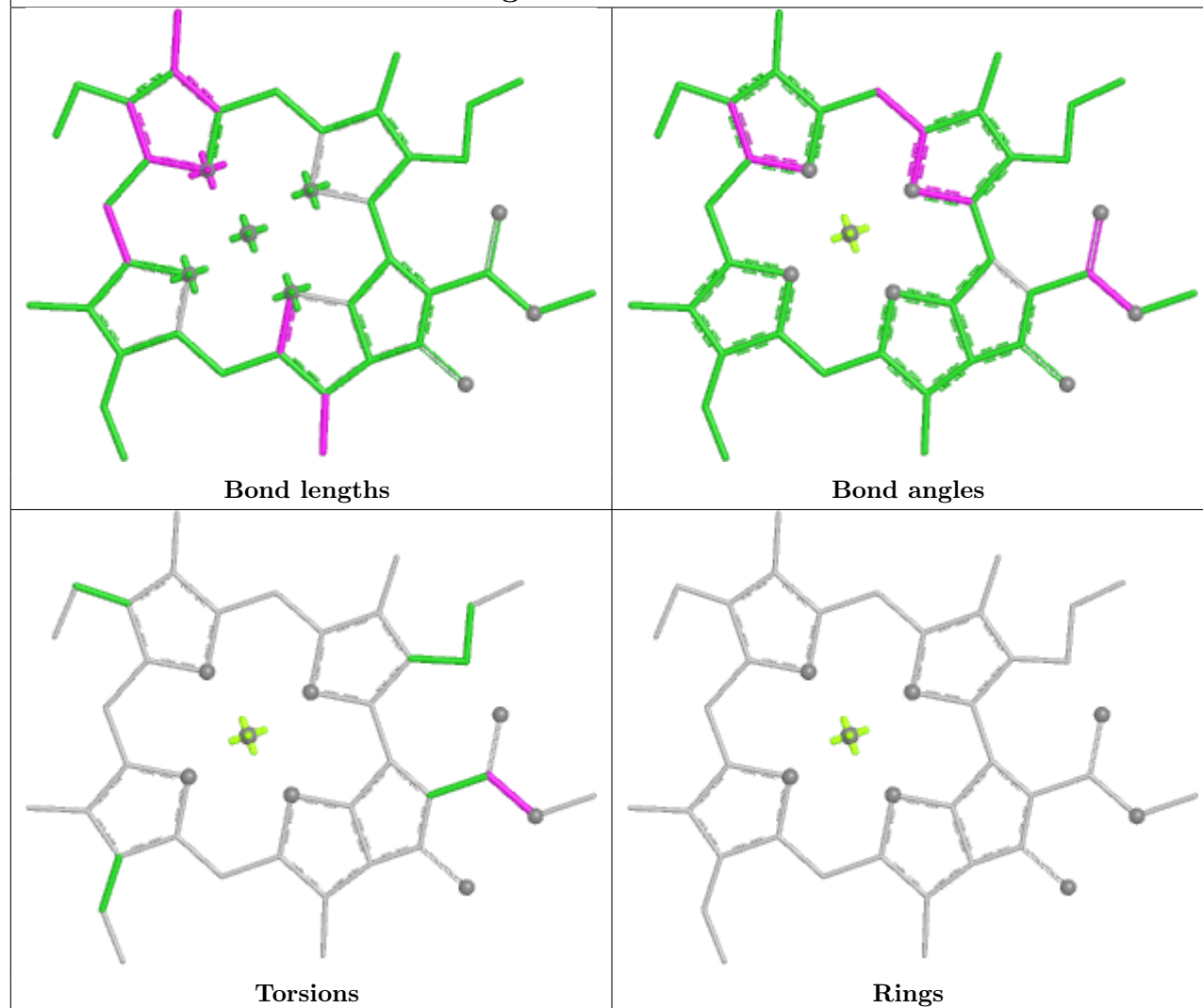
Ligand CLA 2 610



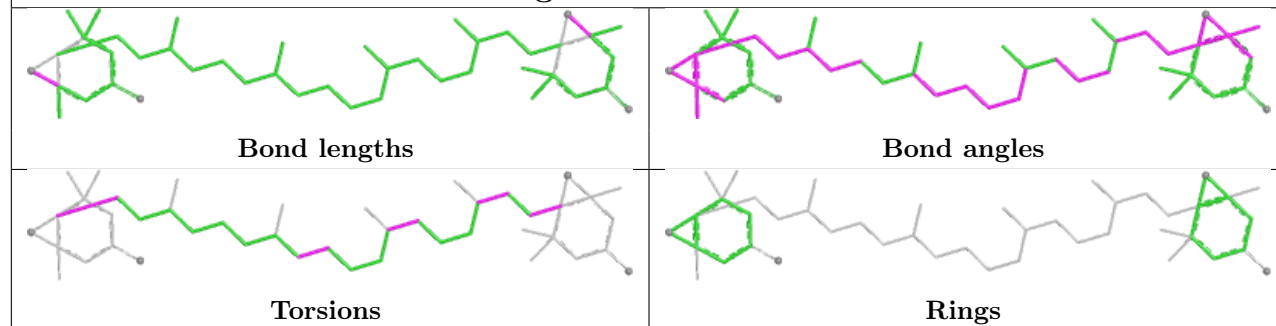
Ligand BCR B 846



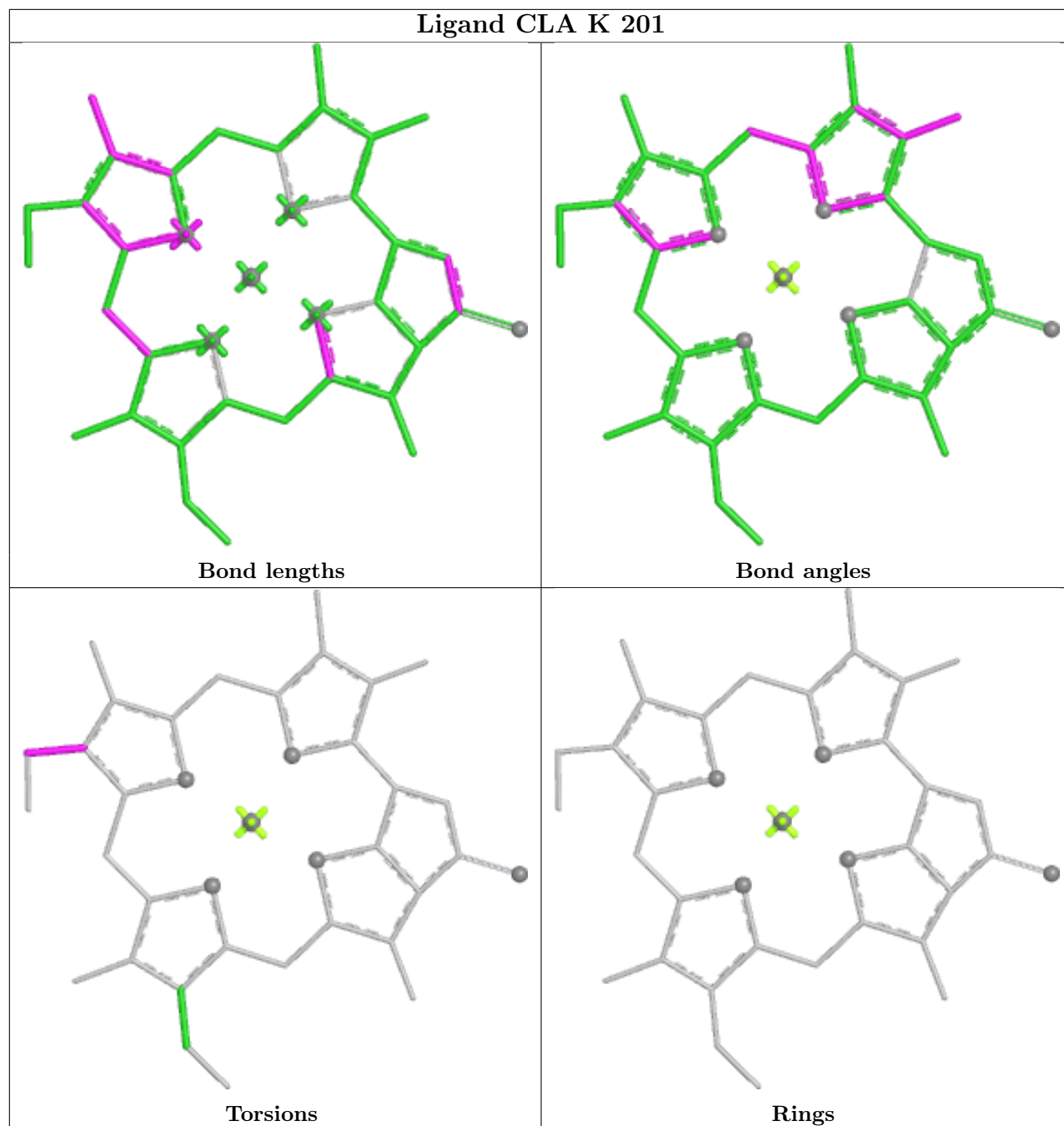
Ligand CLA B 830



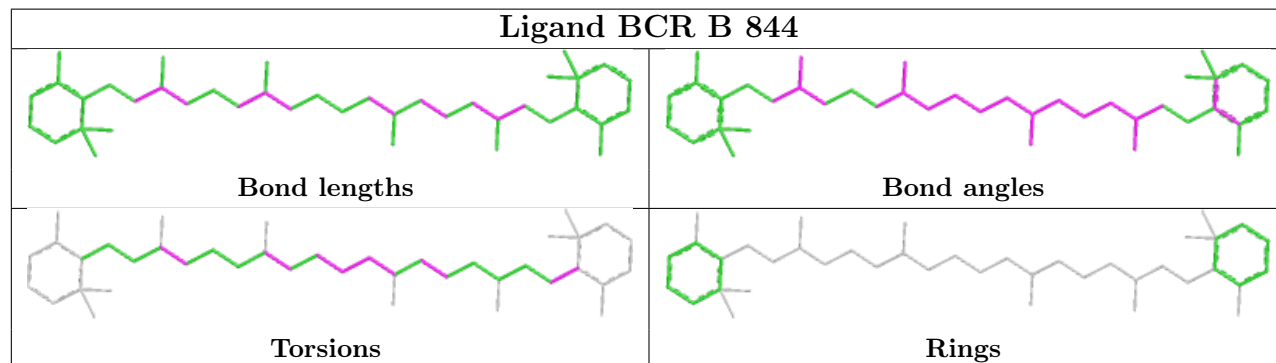
Ligand XAT 1 614



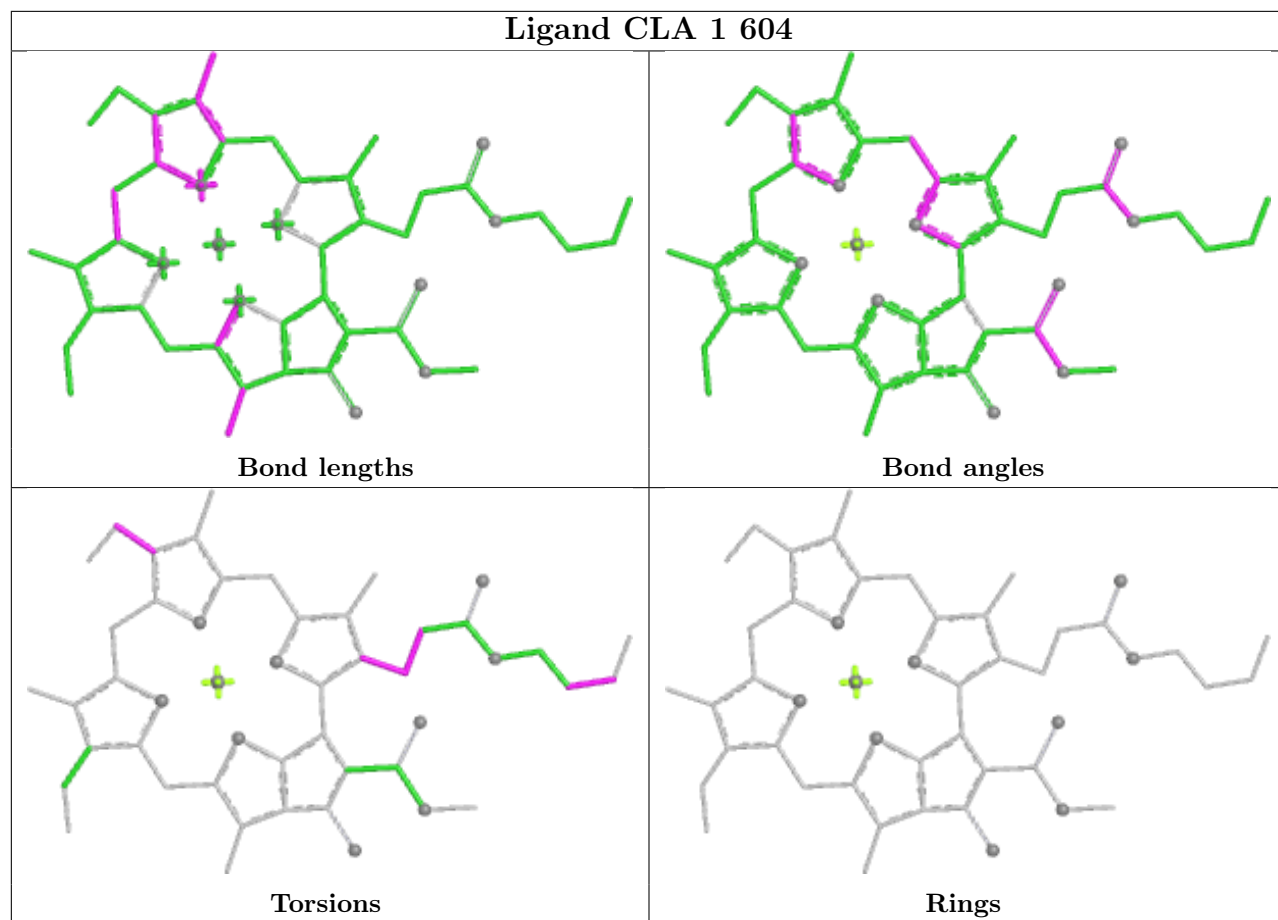
Ligand CLA K 201

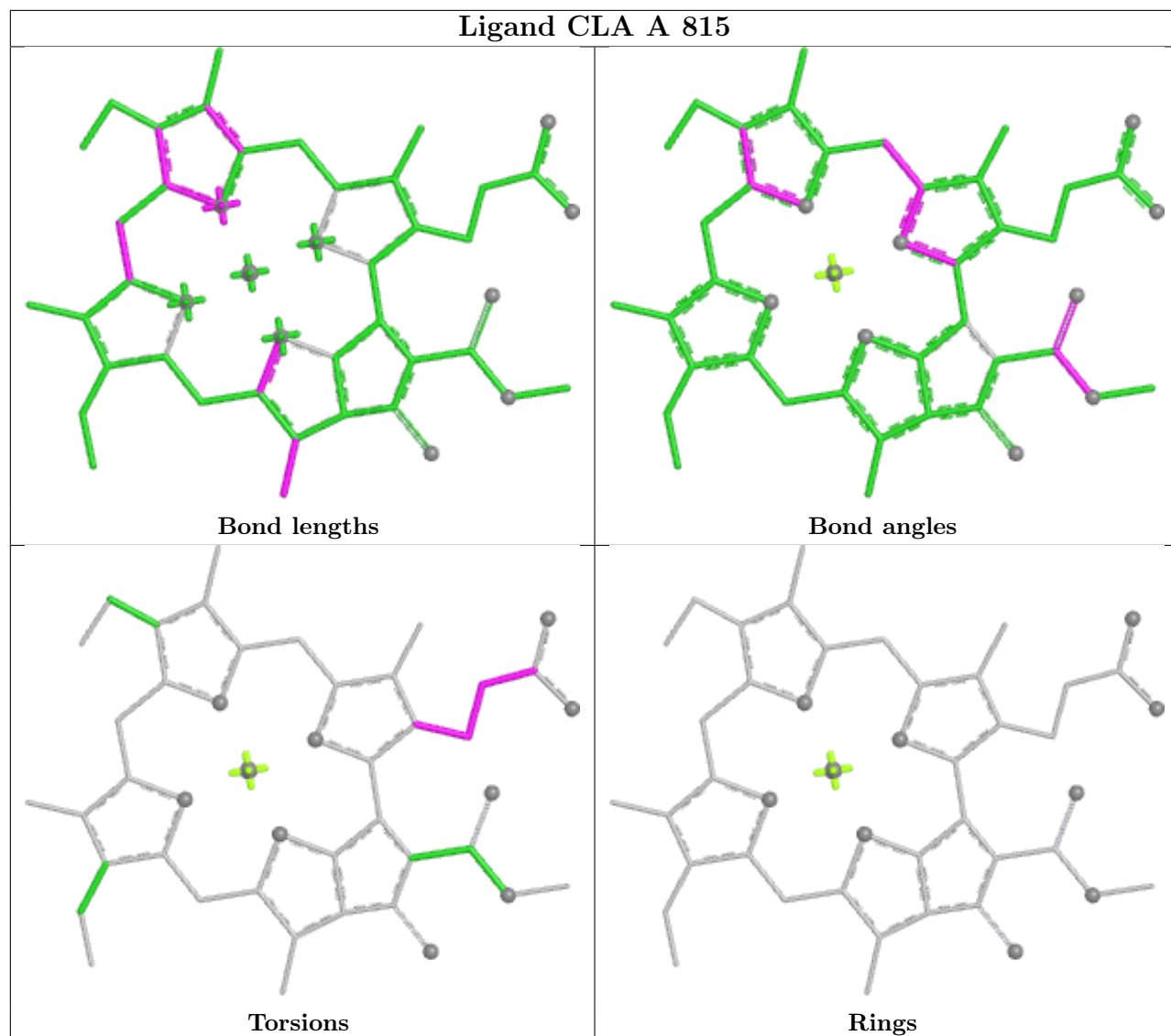


Ligand BCR B 844

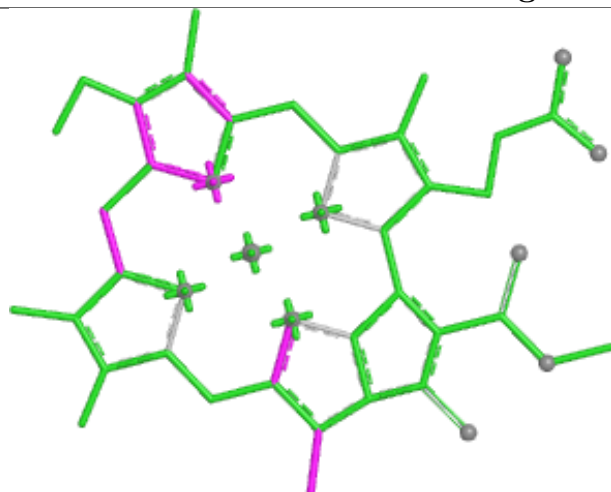


Ligand CLA 1 604

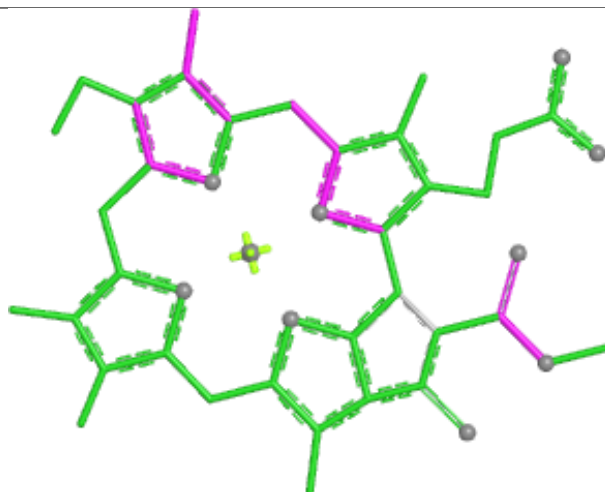




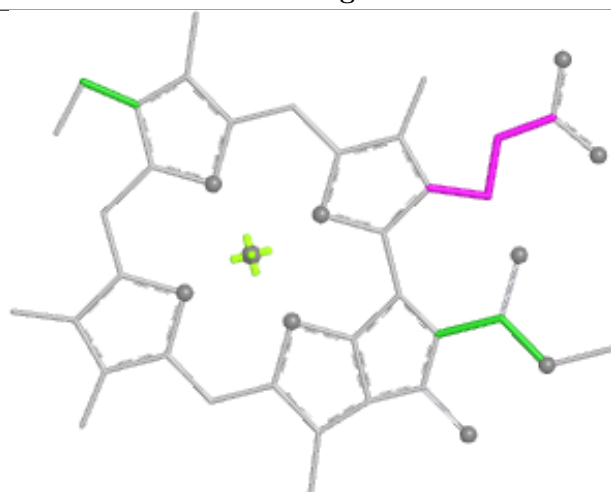
Ligand CLA 2 611



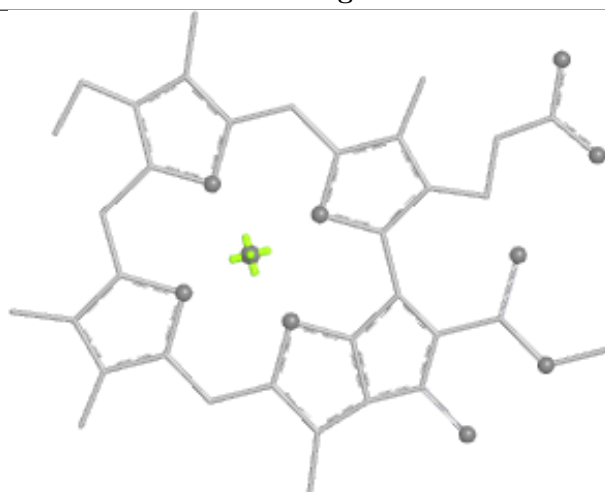
Bond lengths



Bond angles

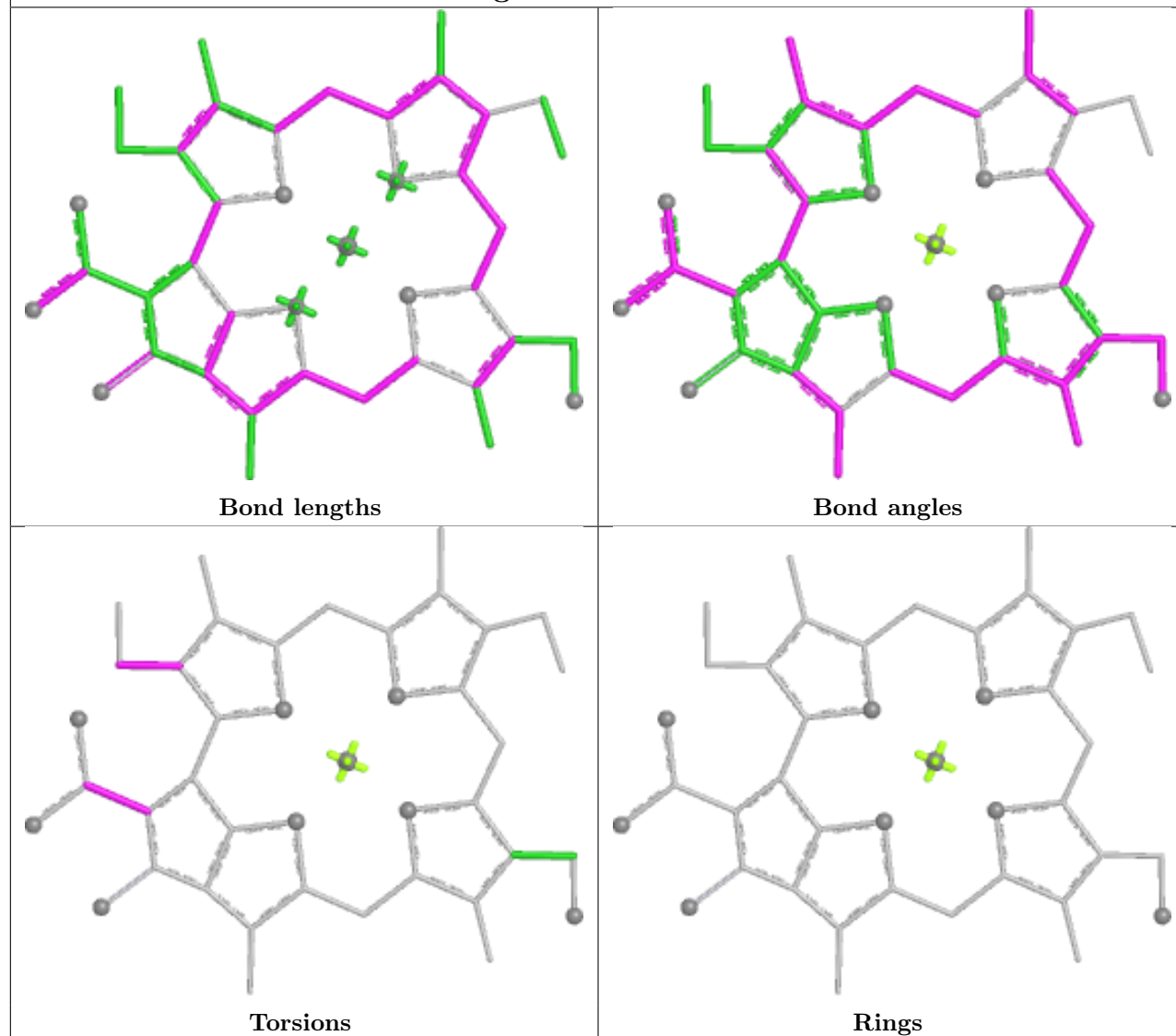


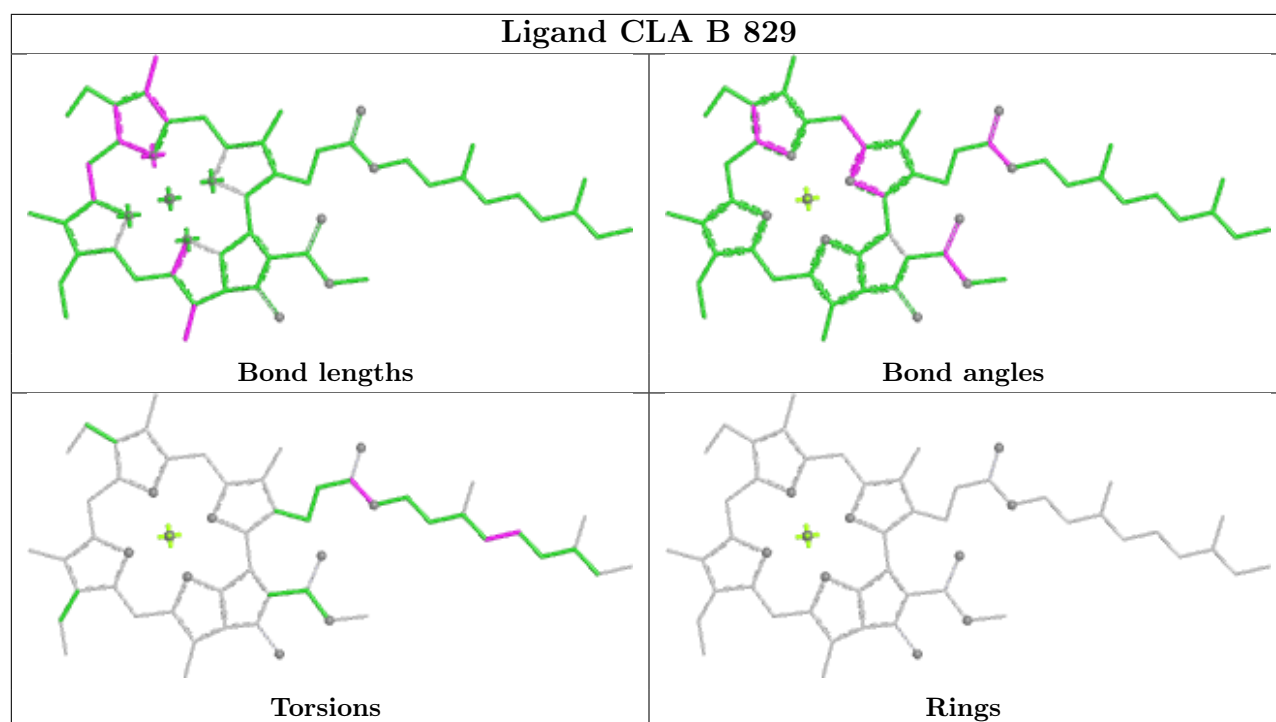
Torsions



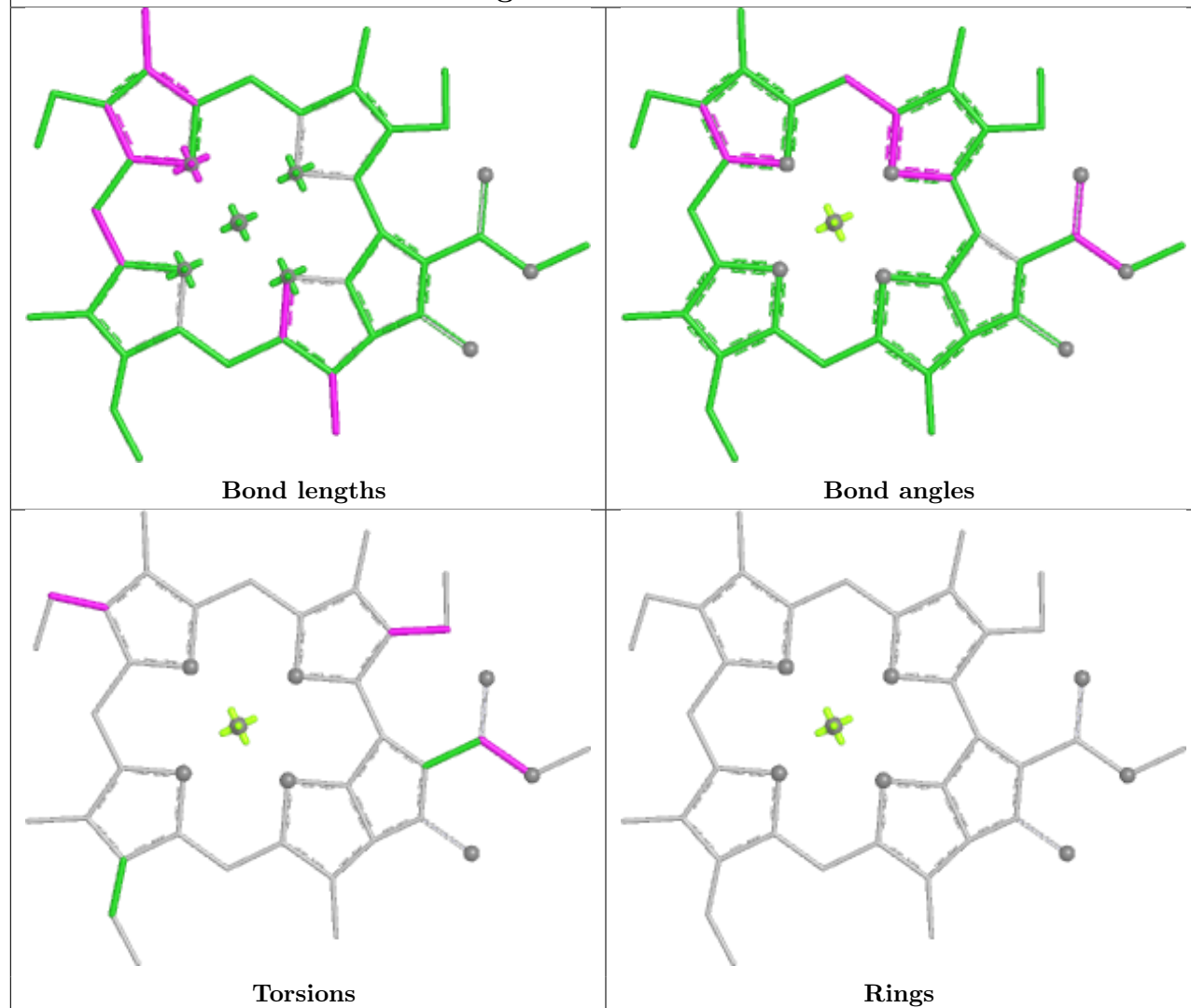
Rings

Ligand CHL 4 605

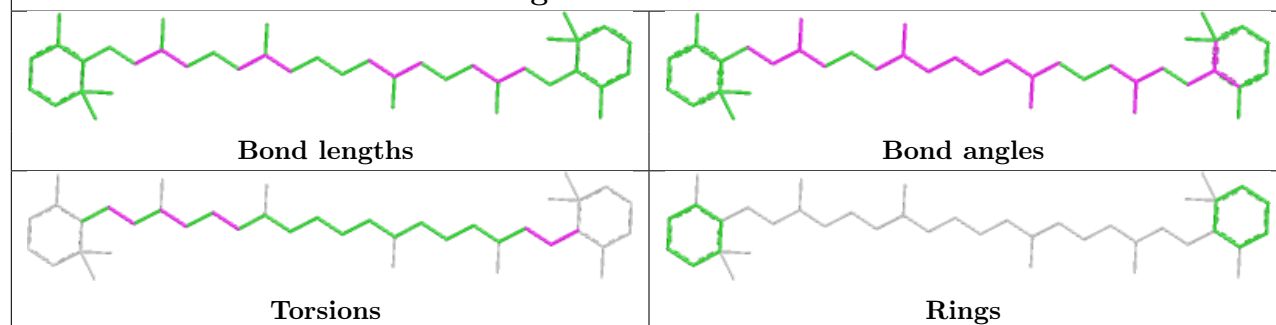


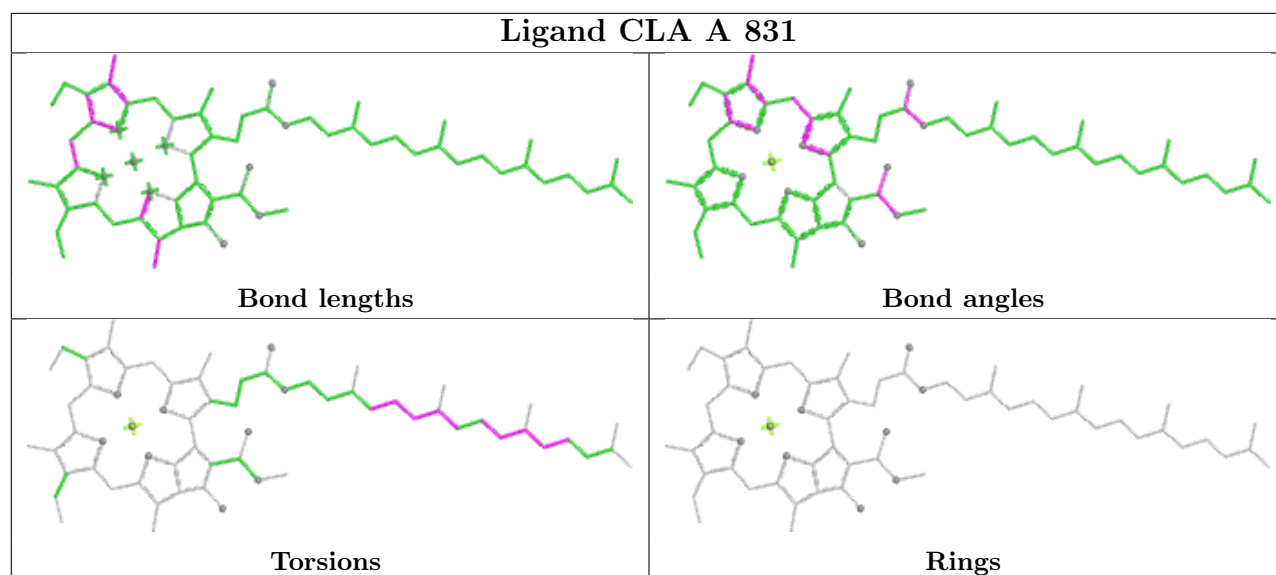
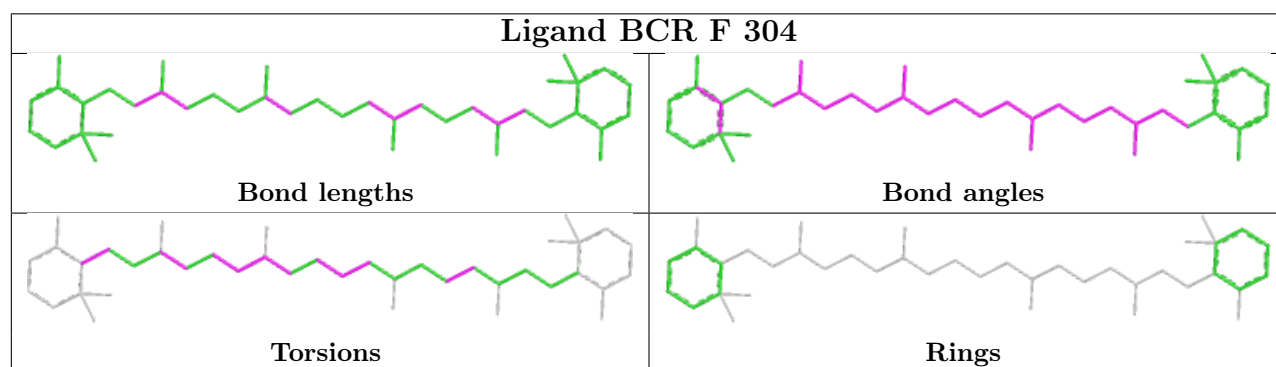
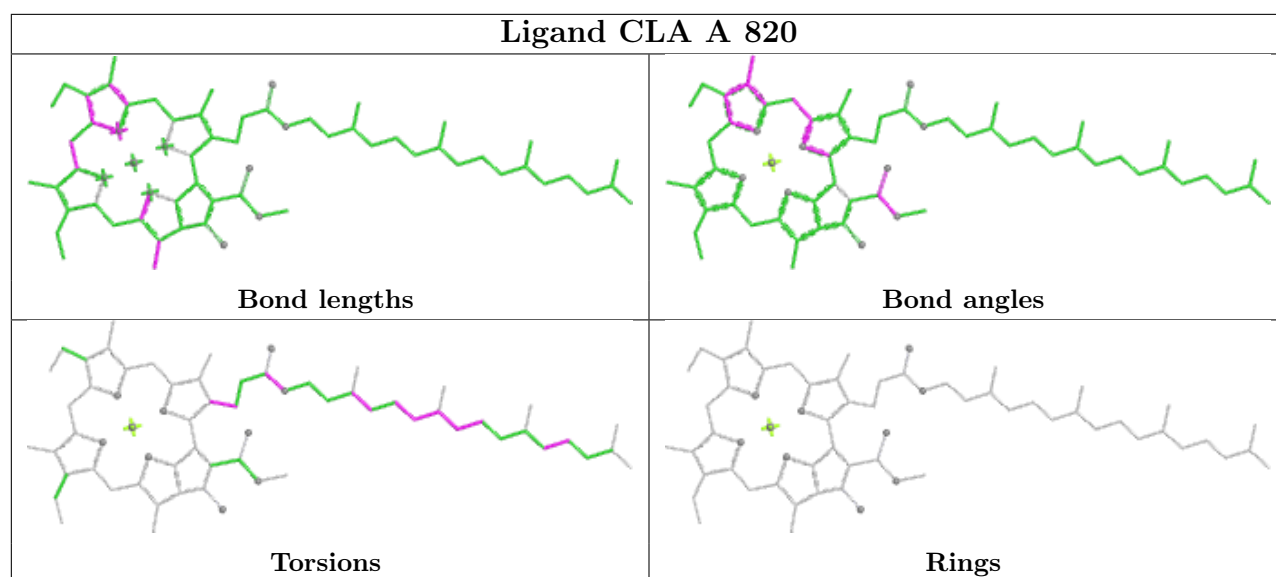


Ligand CLA B 835

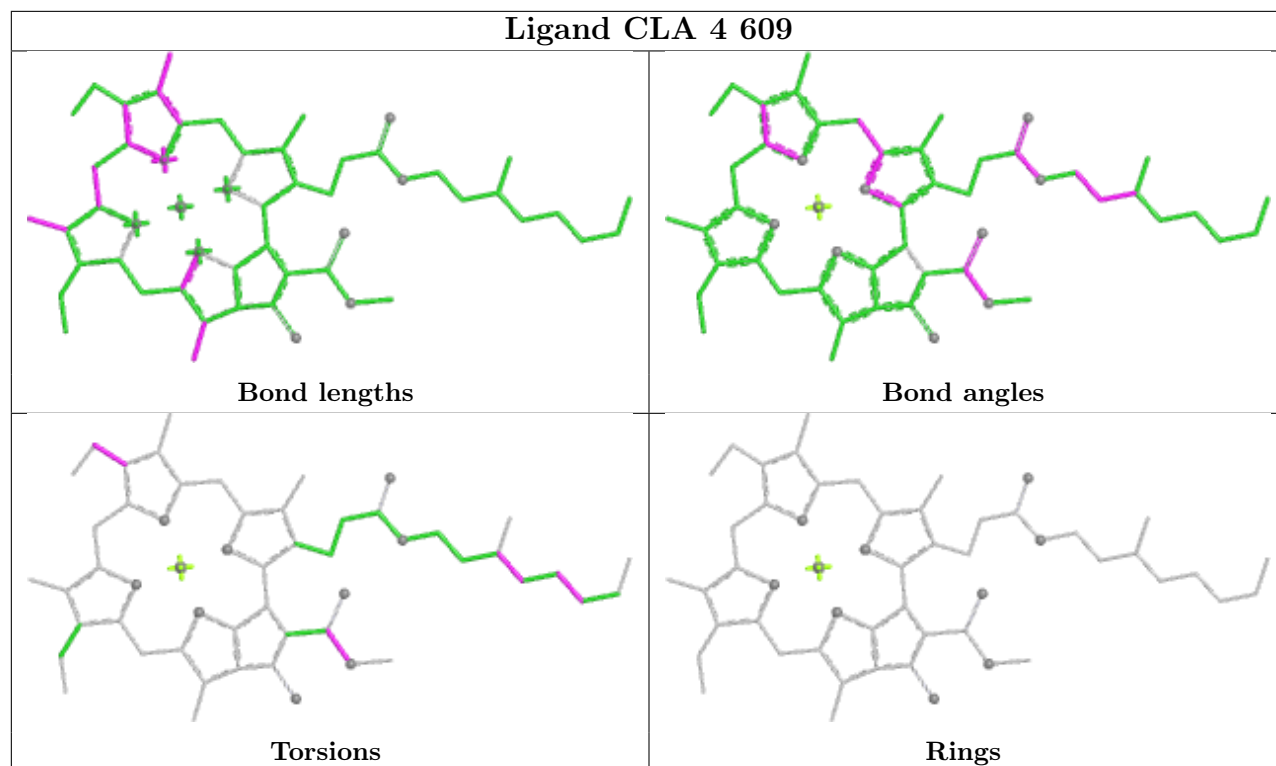


Ligand BCR B 849

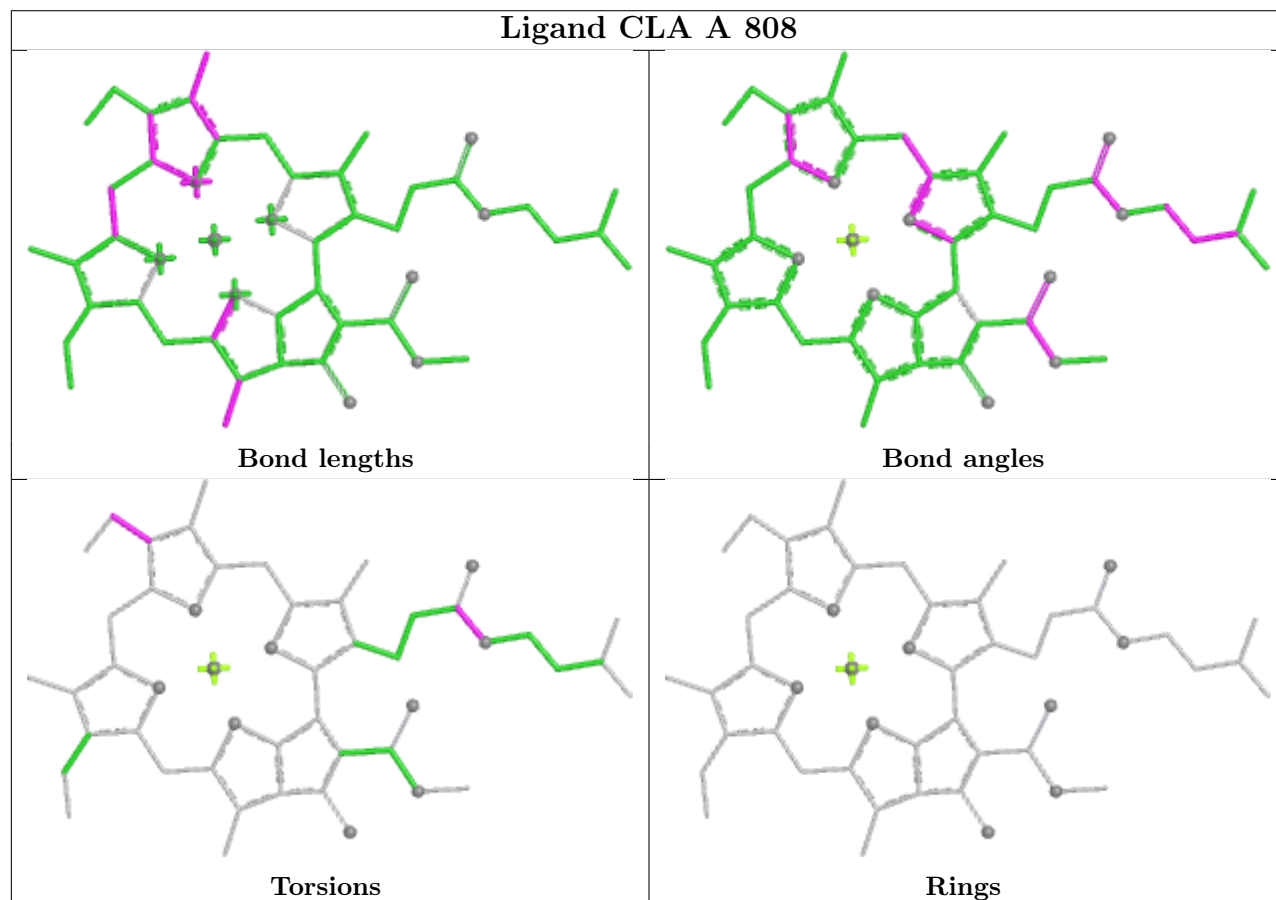




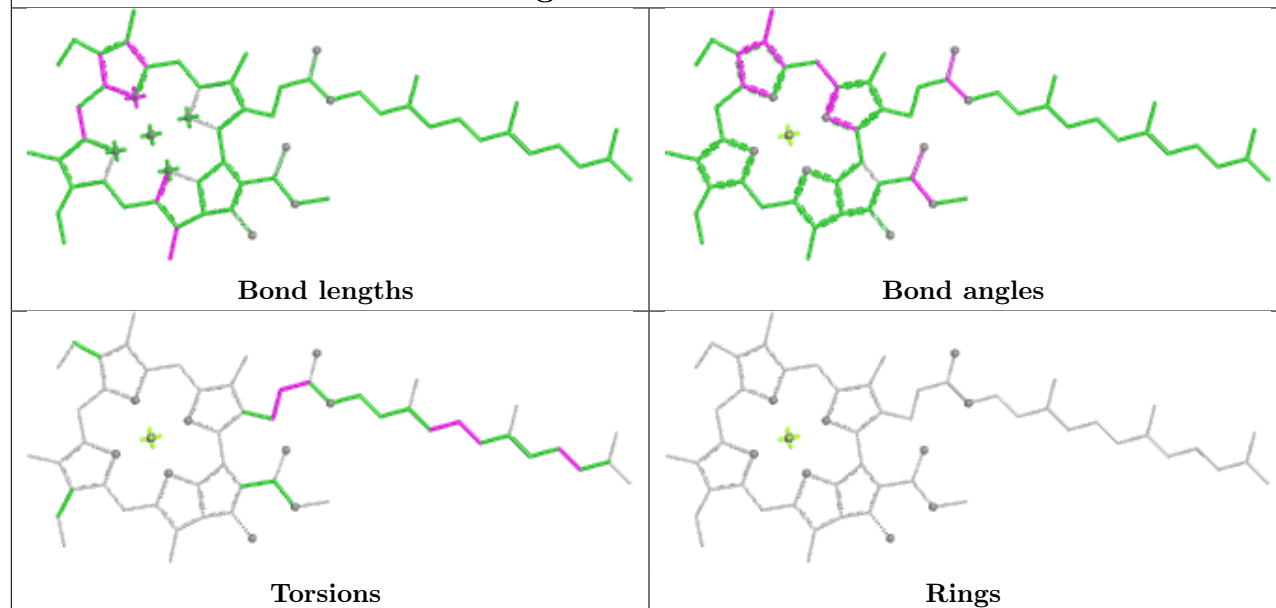
Ligand CLA 4 609



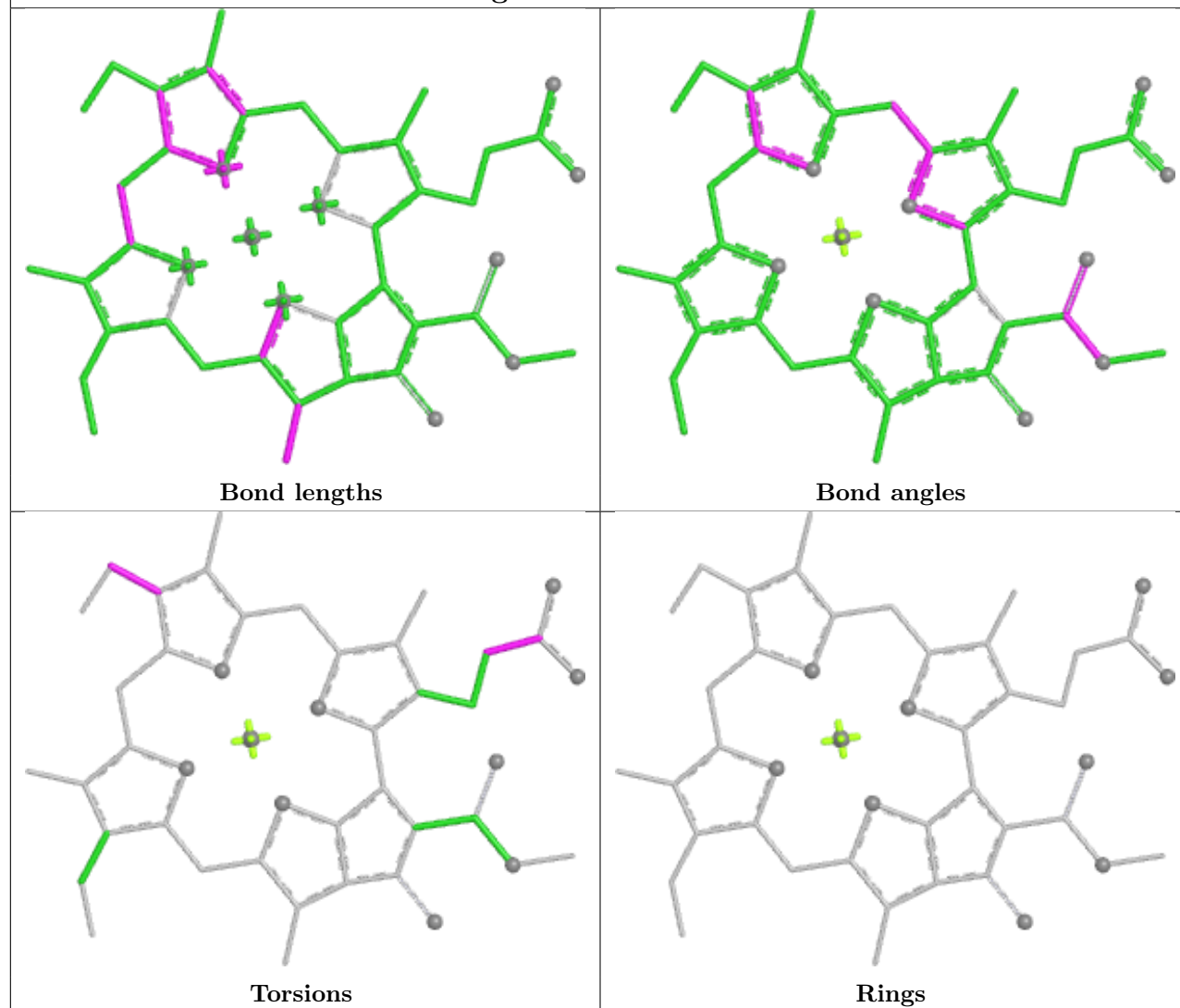
Ligand CLA A 808

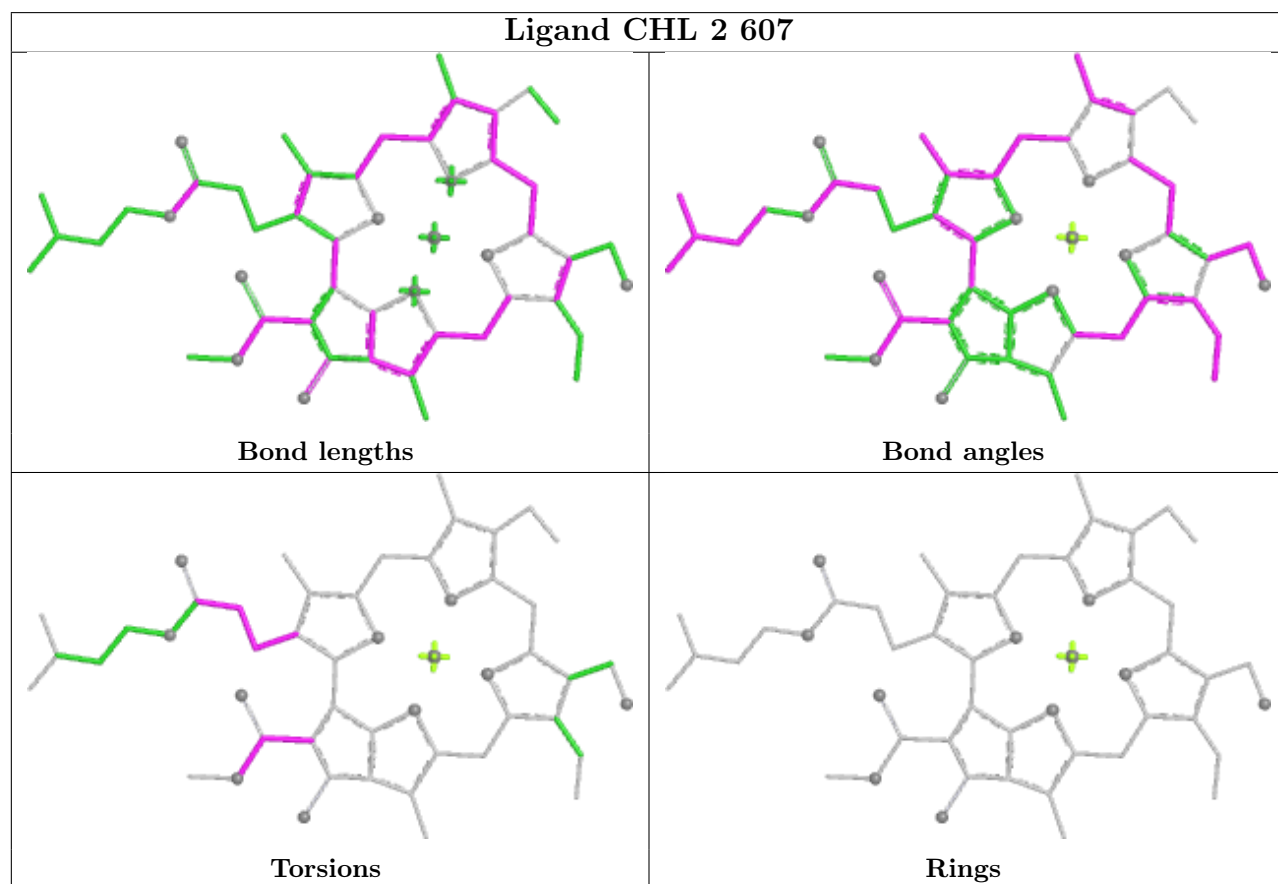
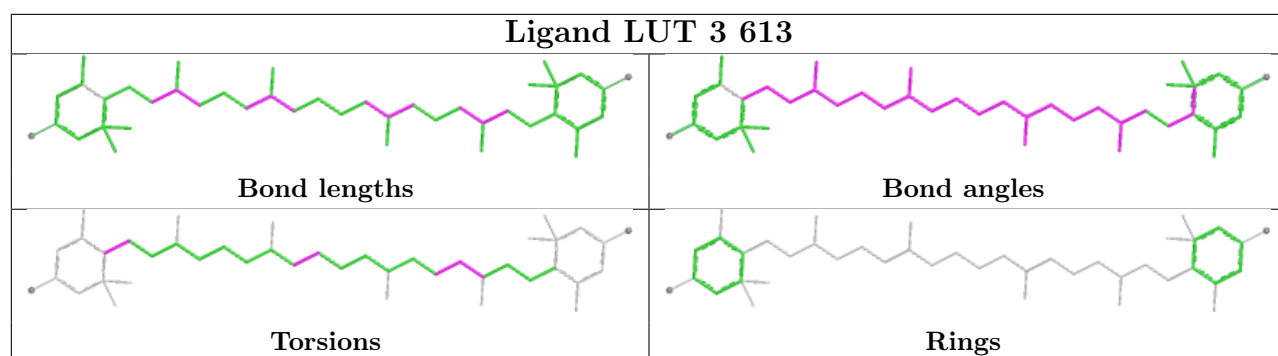


Ligand CLA 4 602

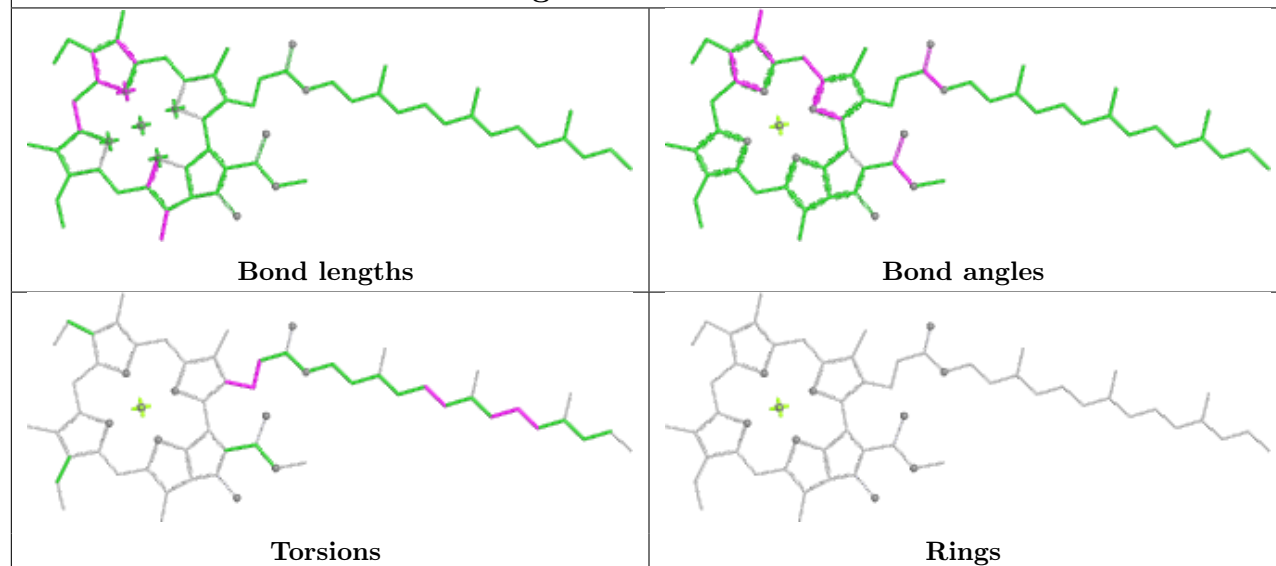


Ligand CLA A 837

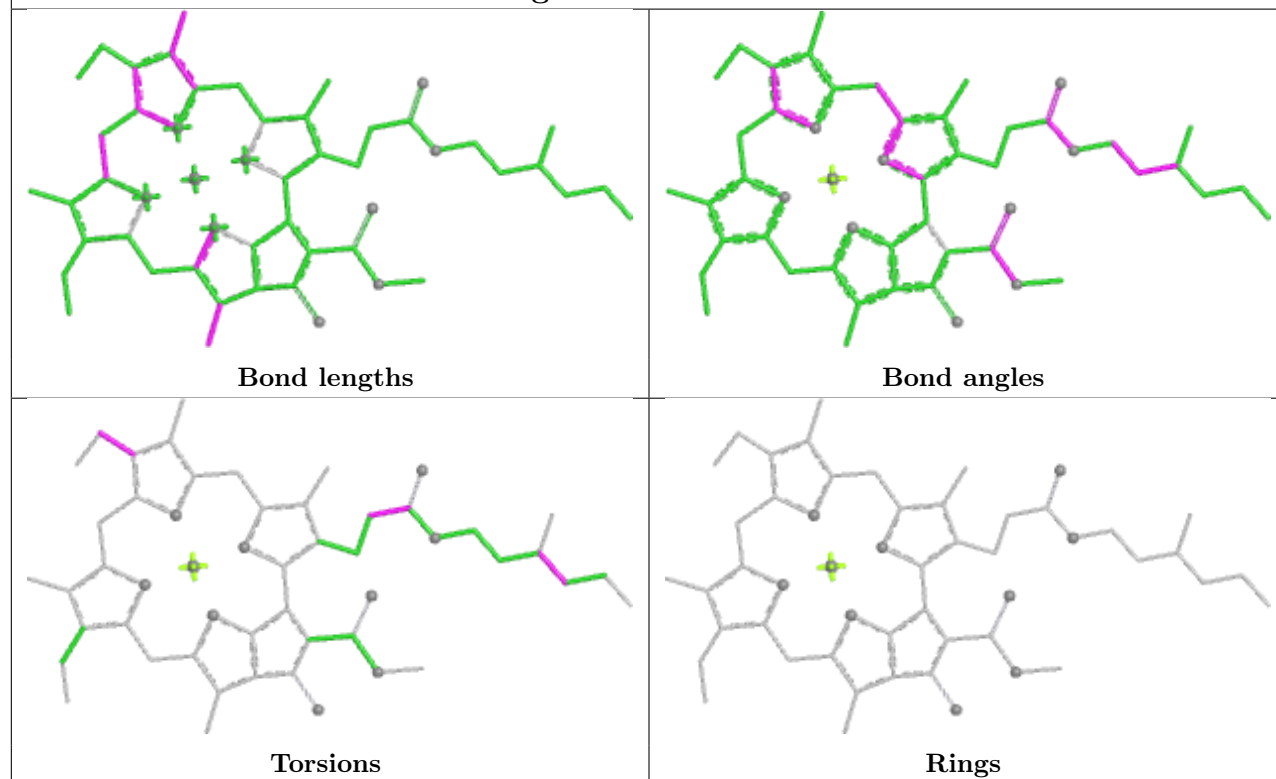




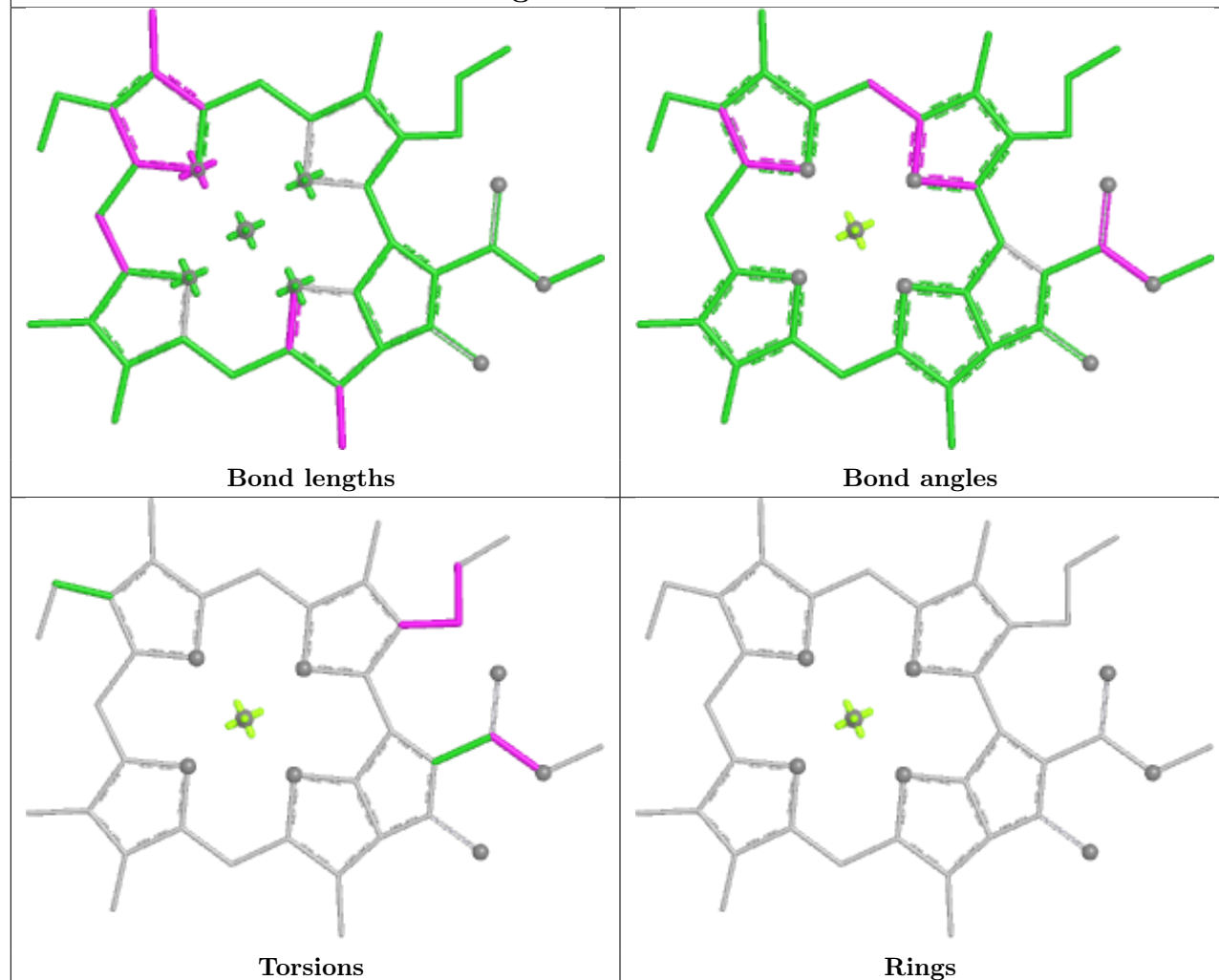
Ligand CLA B 826



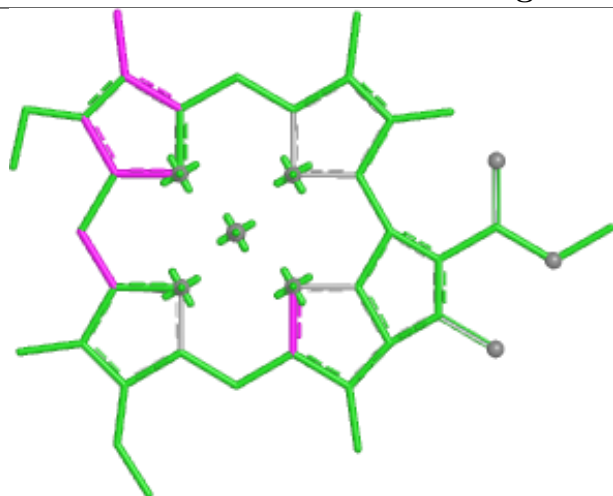
Ligand CLA A 840



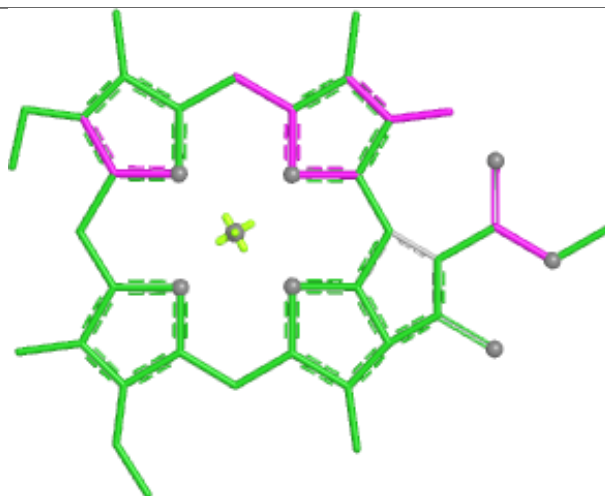
Ligand CLA 1 609



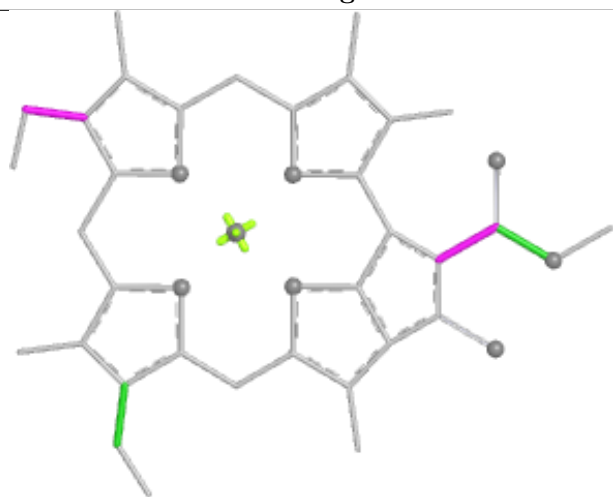
Ligand CLA F 303



Bond lengths



Bond angles

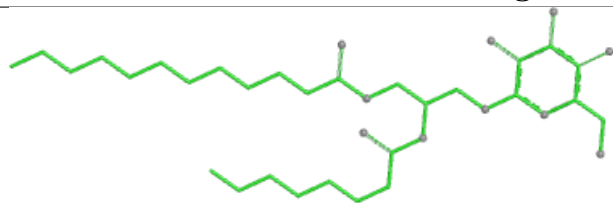


Torsions

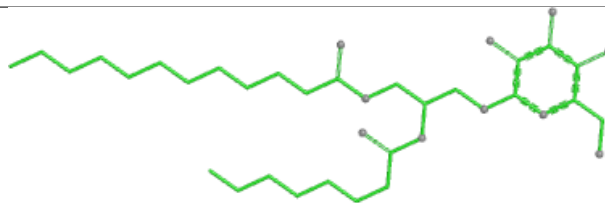


Rings

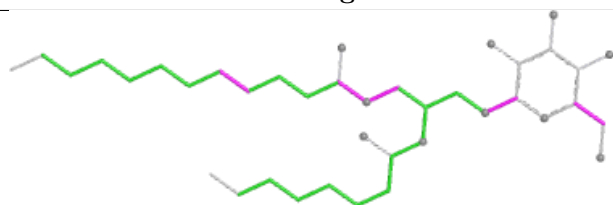
Ligand LMG 4 619



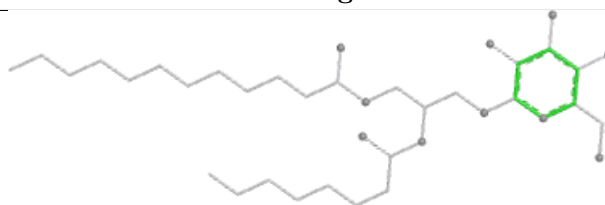
Bond lengths



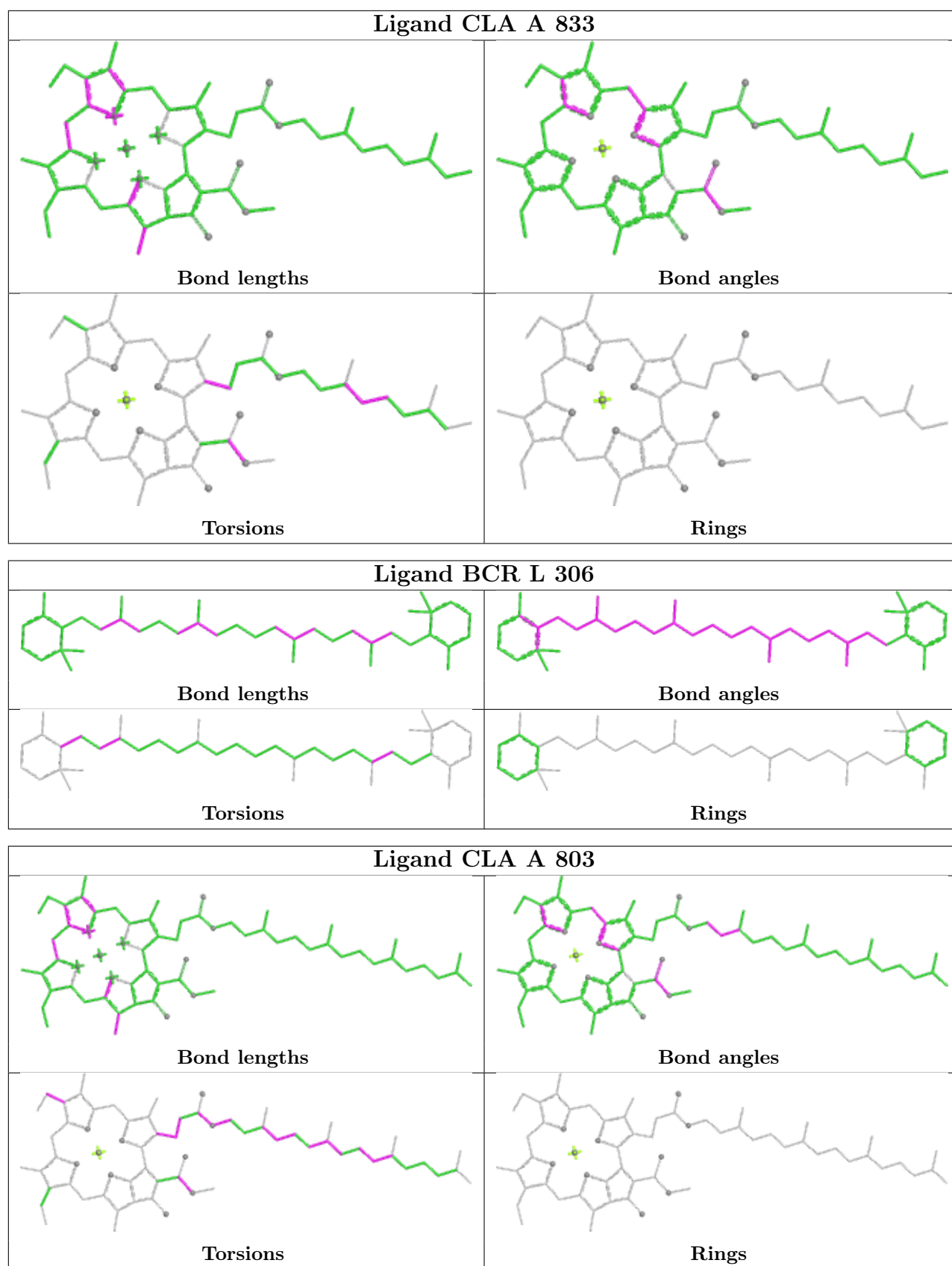
Bond angles



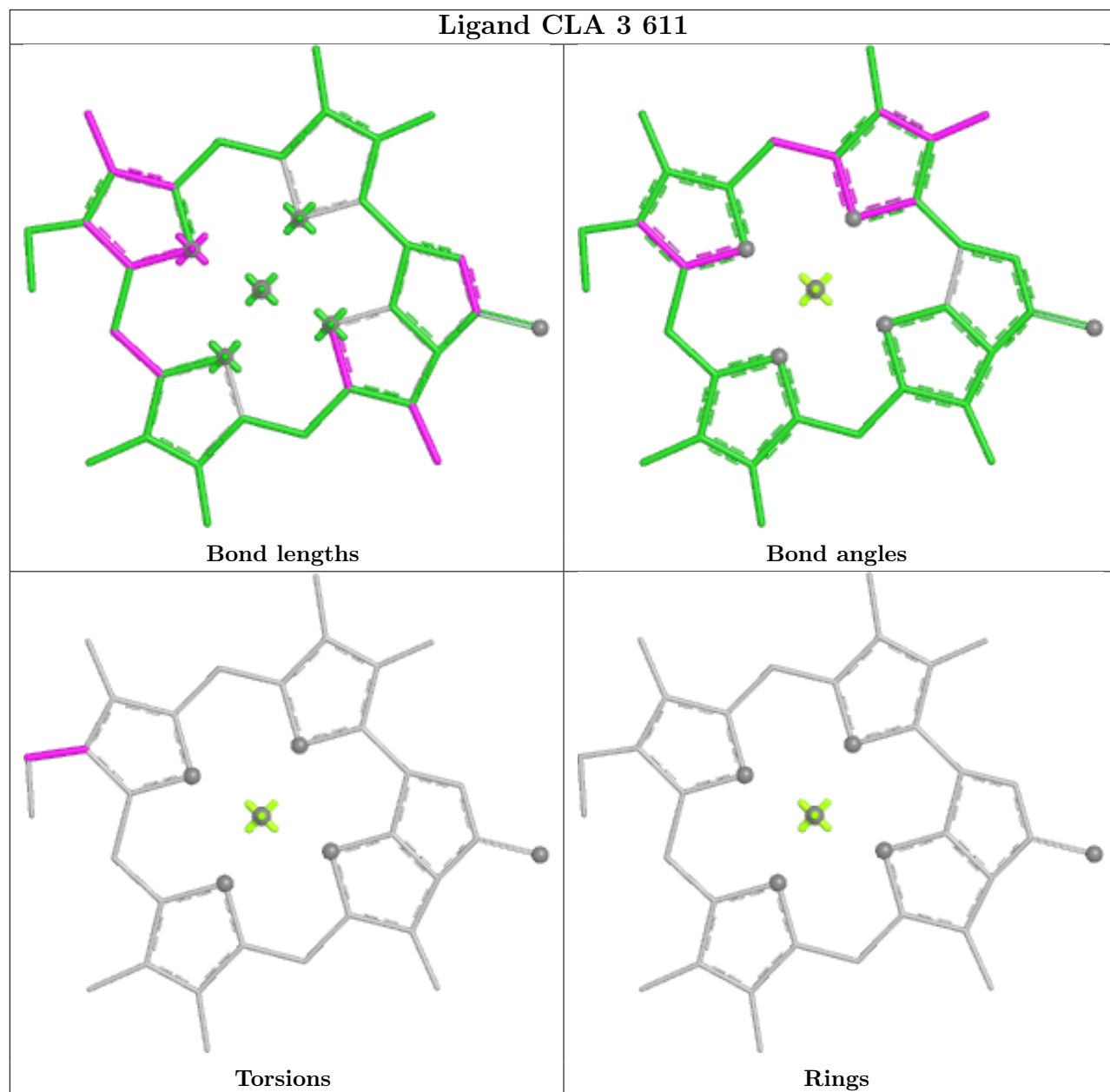
Torsions

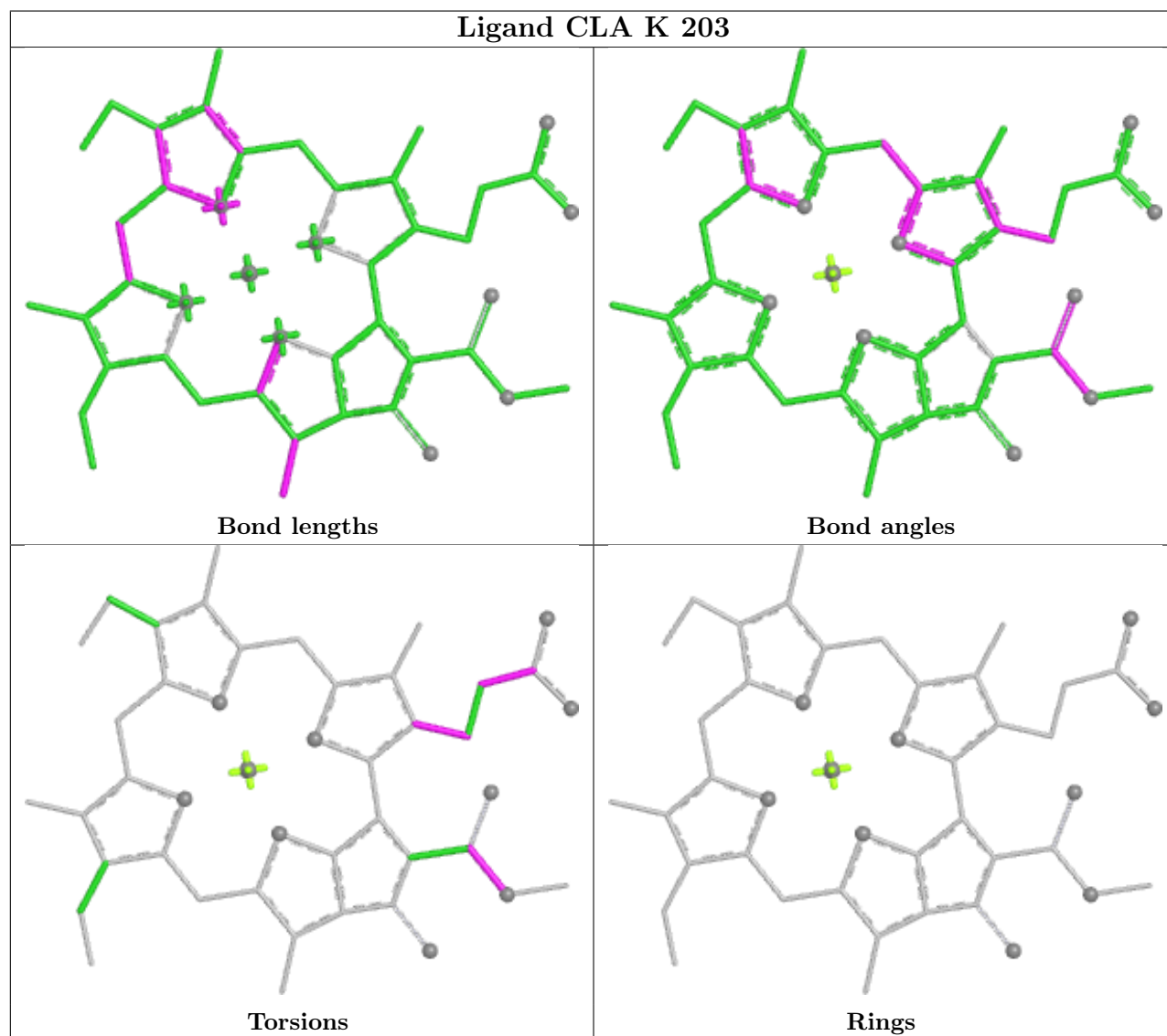
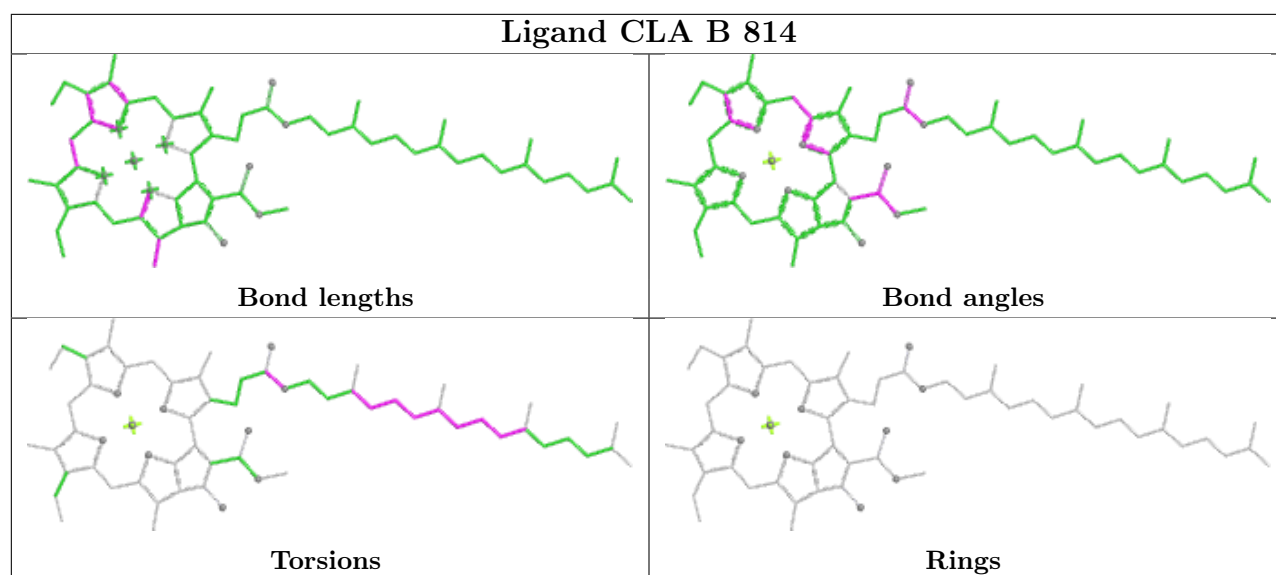


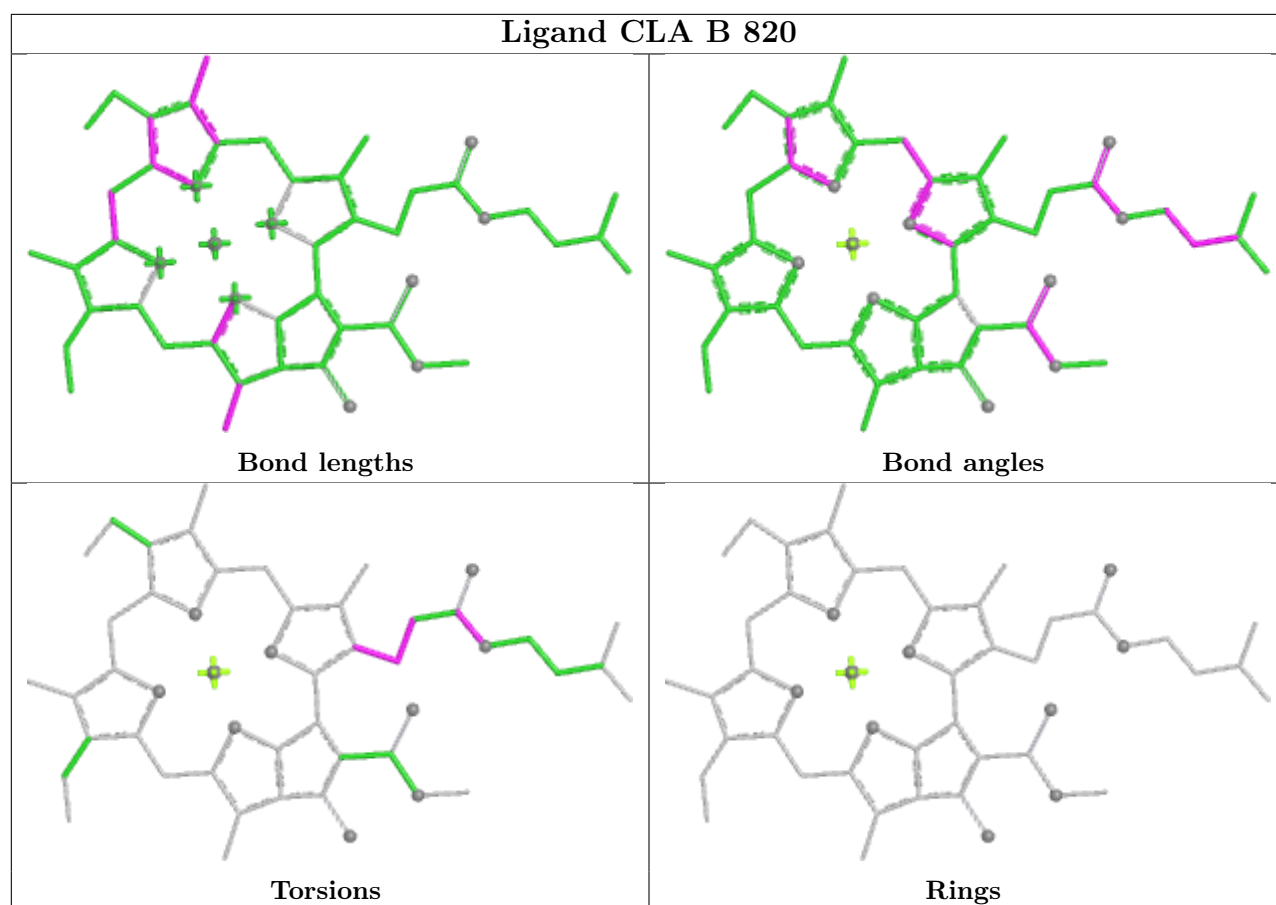
Rings



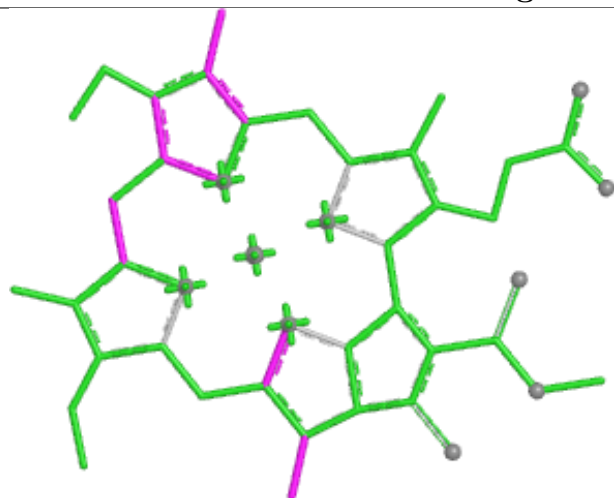
Ligand CLA 3 611



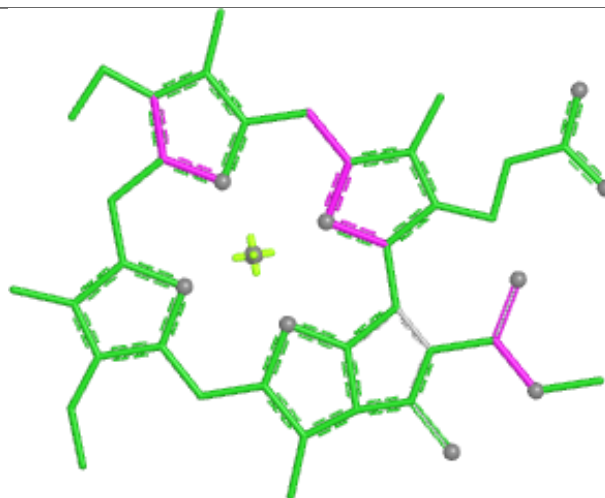




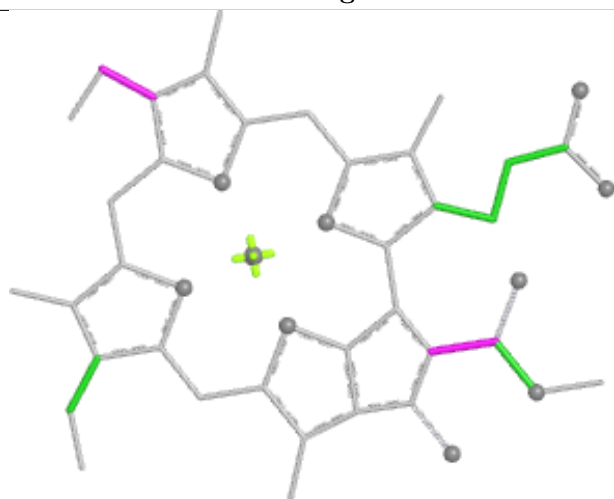
Ligand CLA L 304



Bond lengths



Bond angles

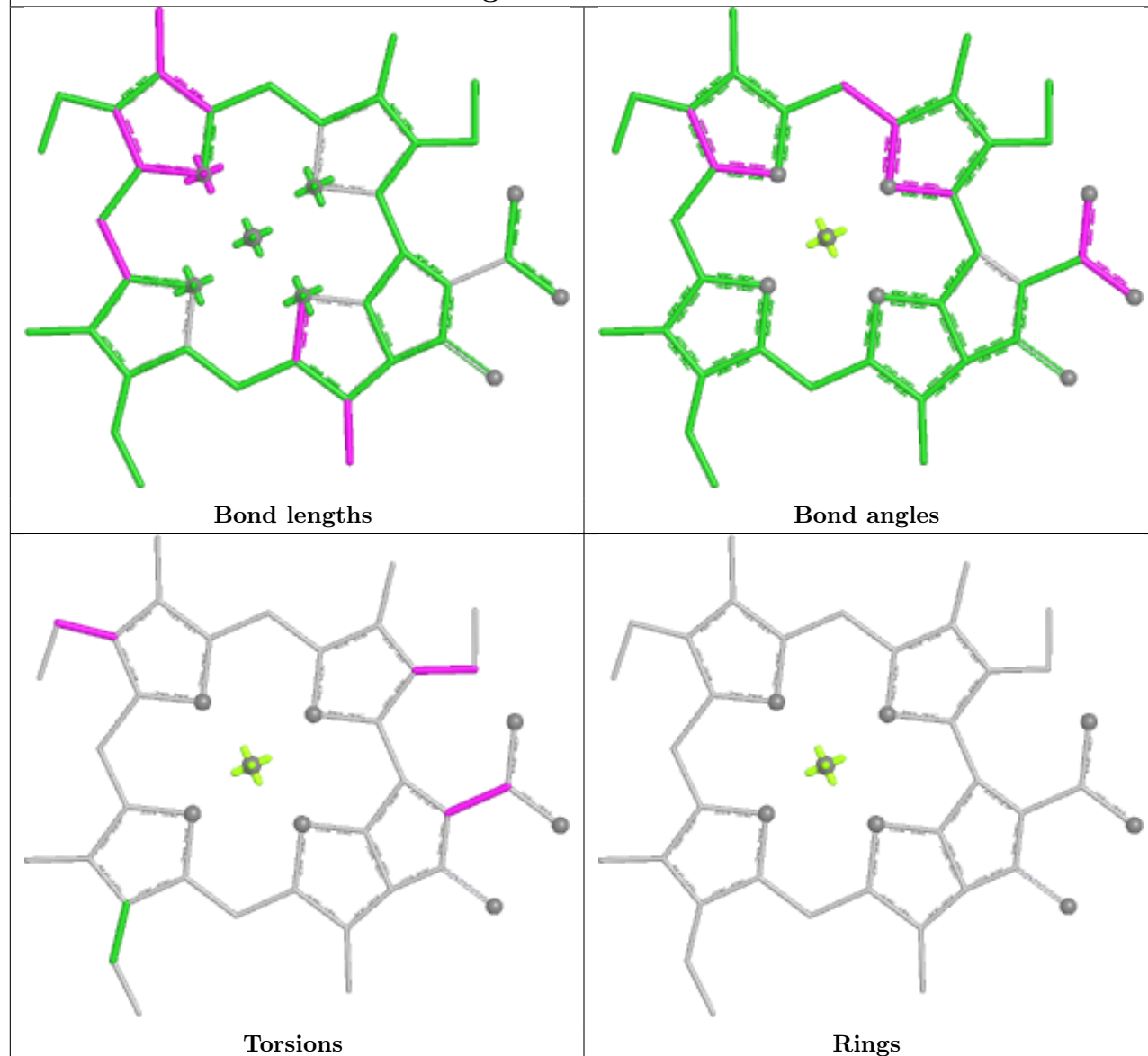


Torsions

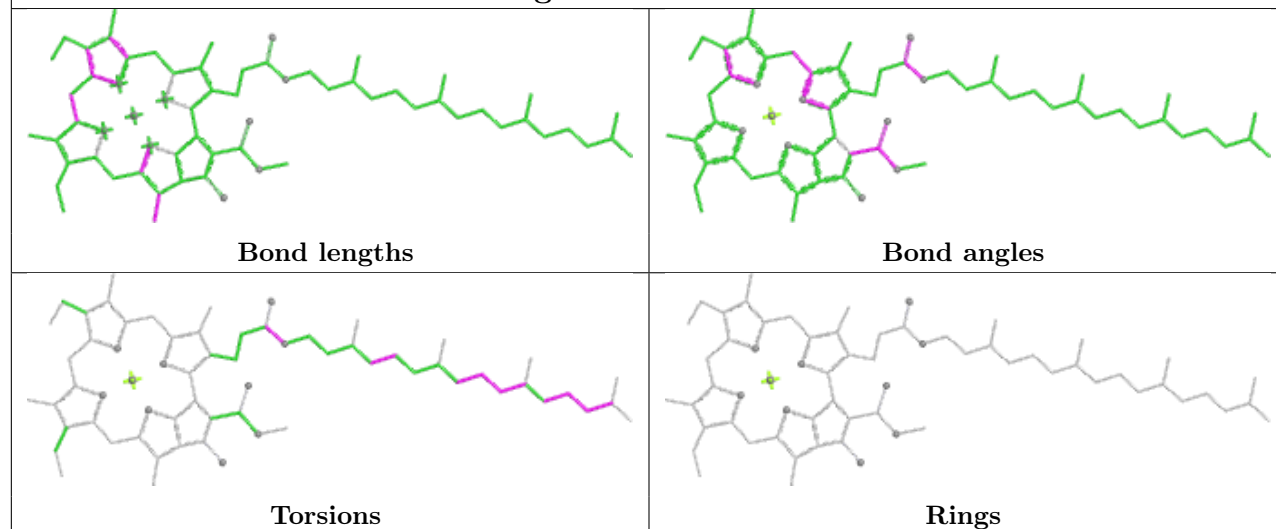


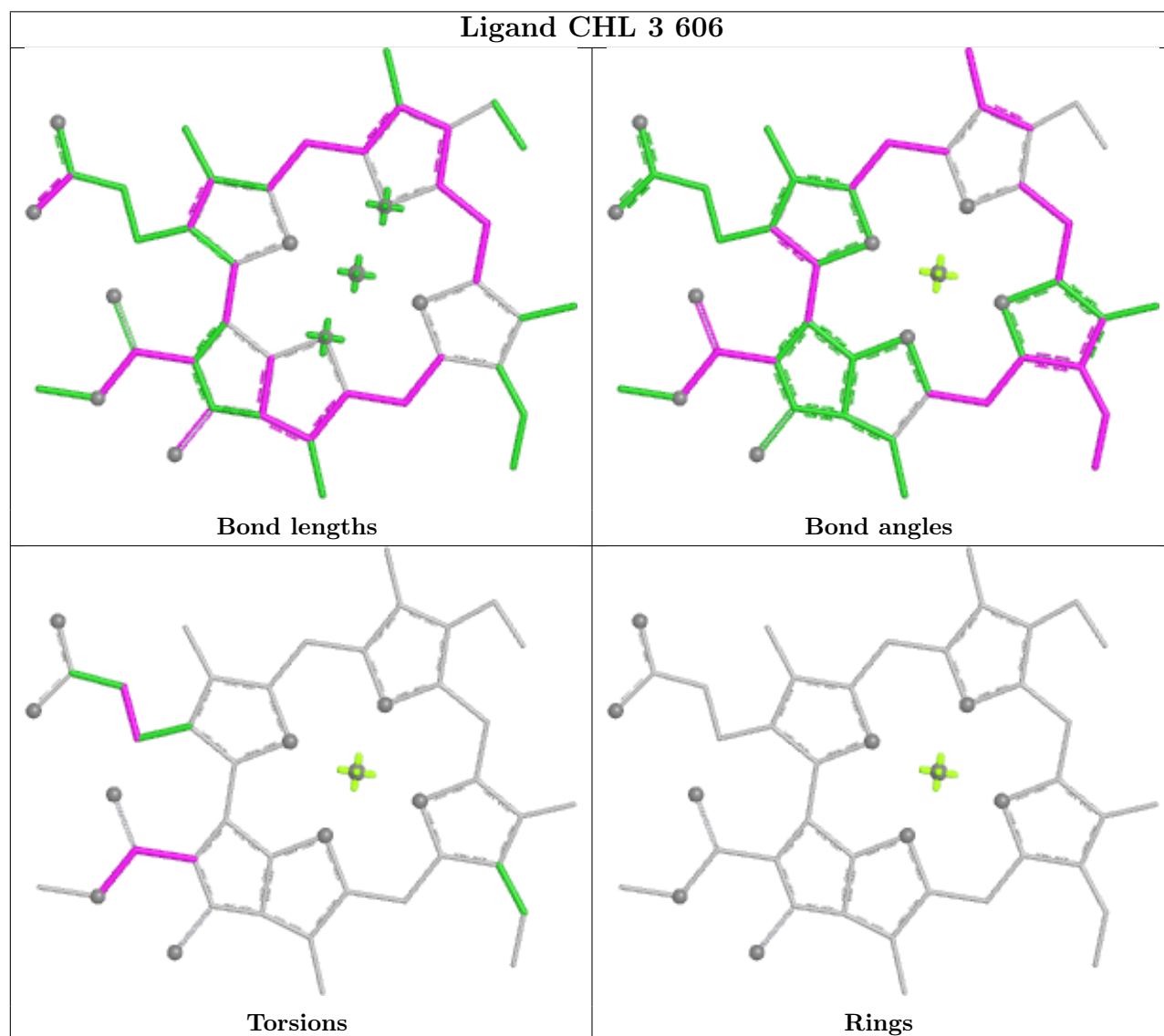
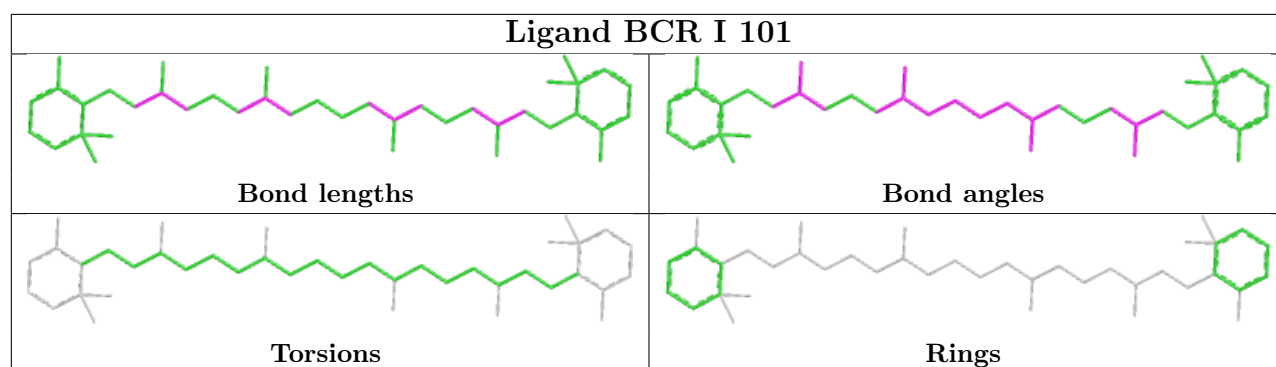
Rings

Ligand CLA 4 611

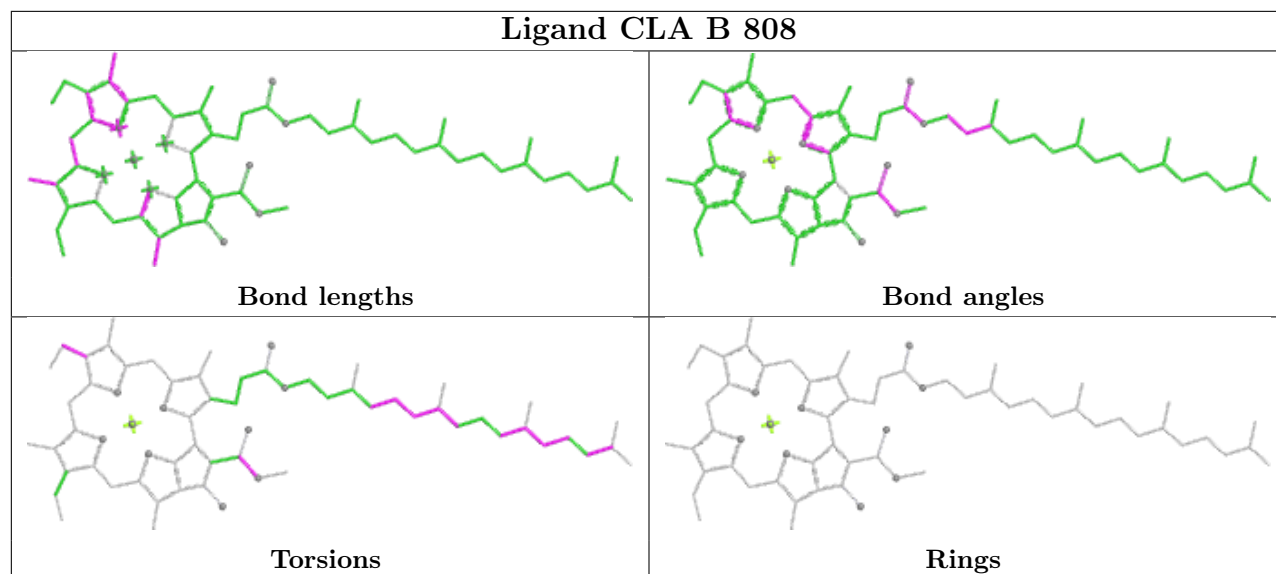


Ligand CLA L 303

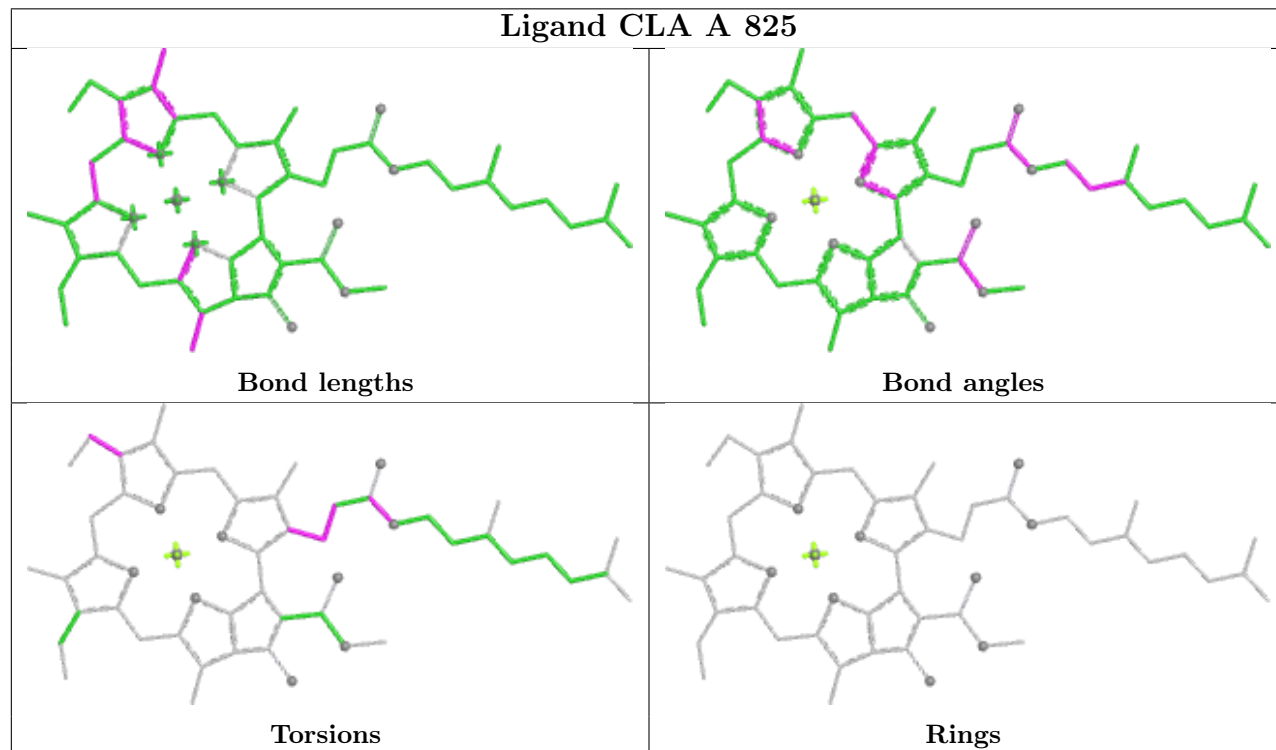




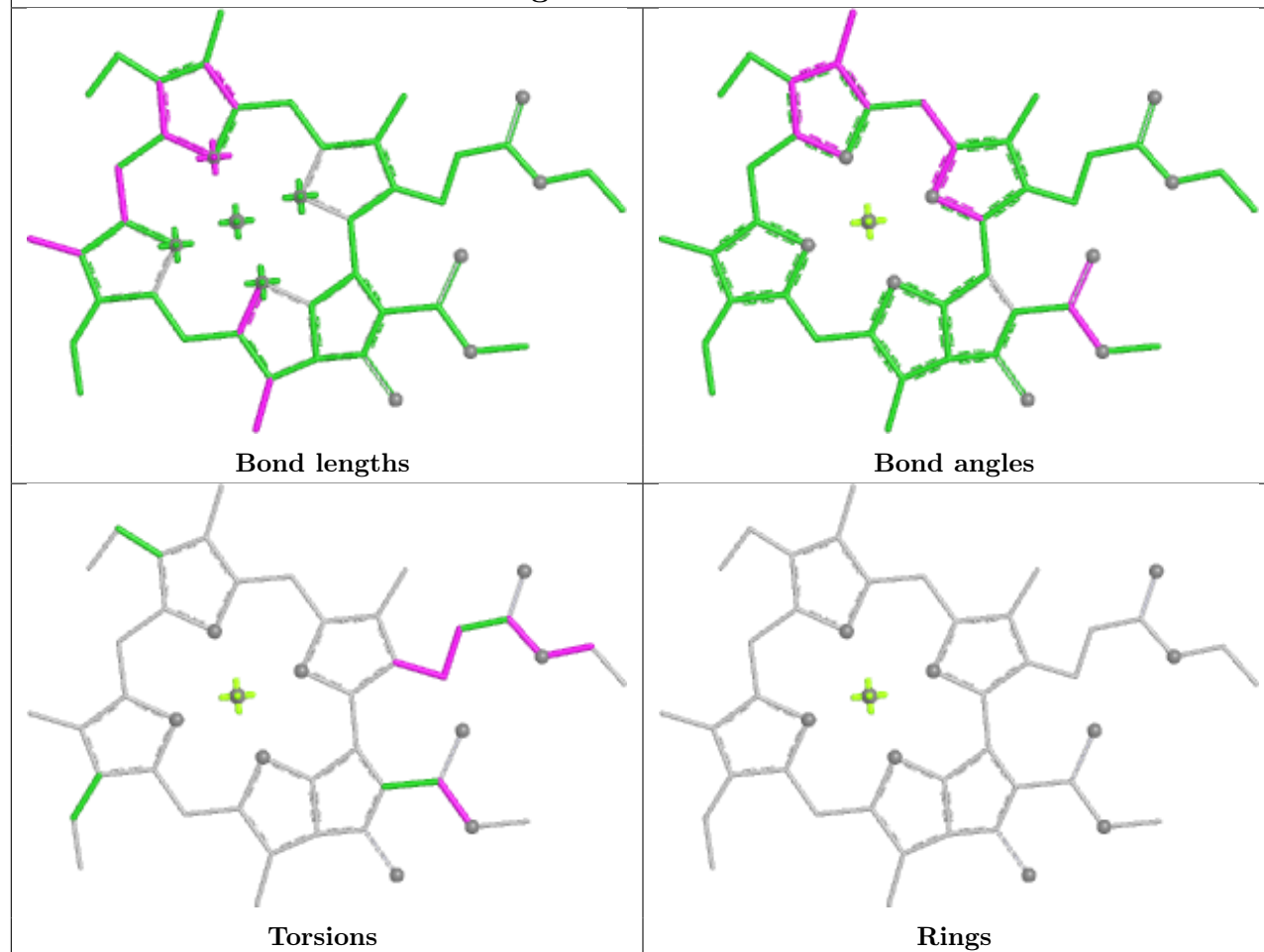
Ligand CLA B 808



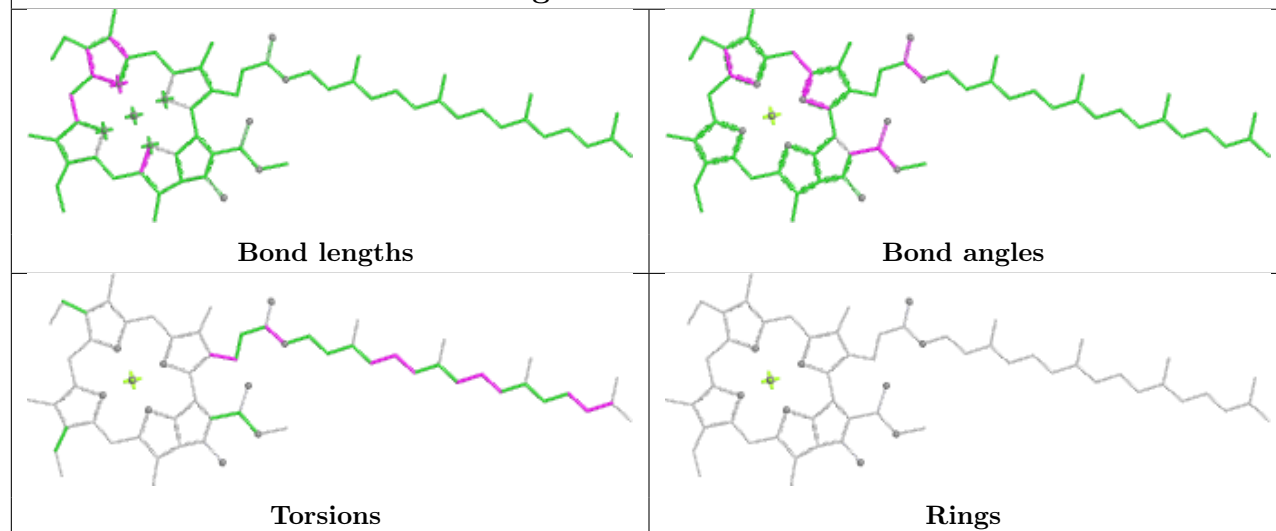
Ligand CLA A 825

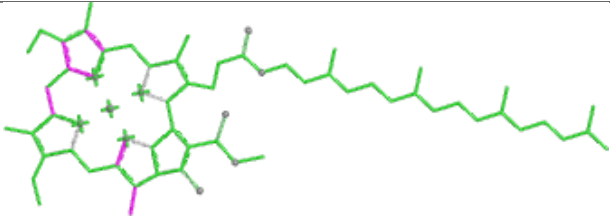
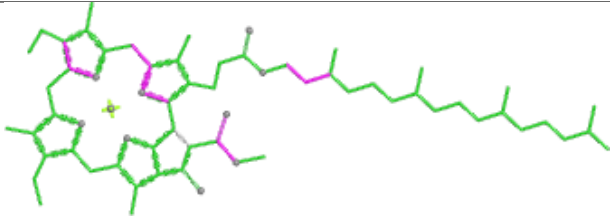
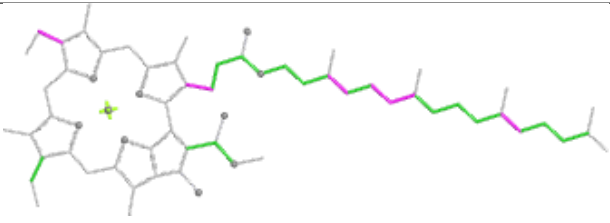
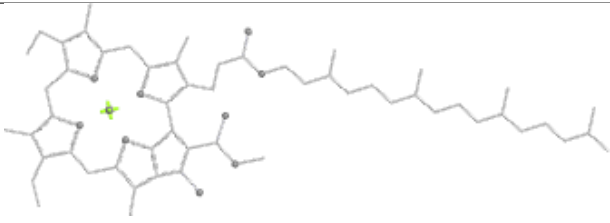
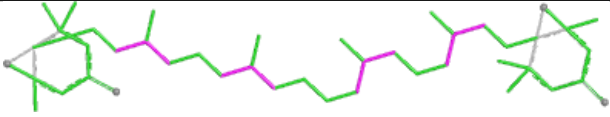
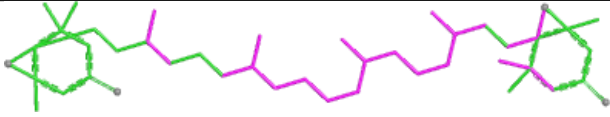
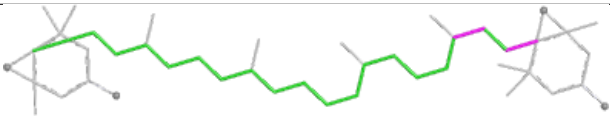
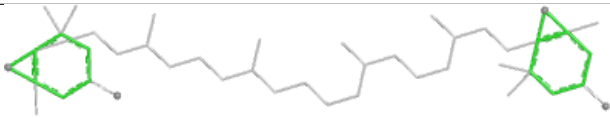
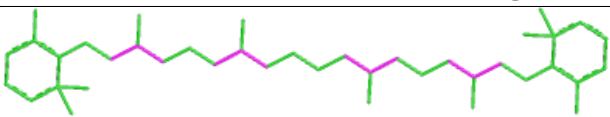
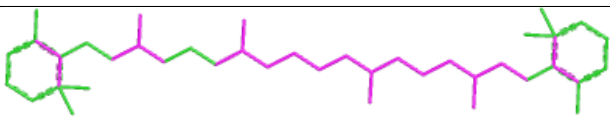
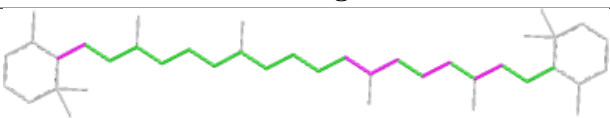
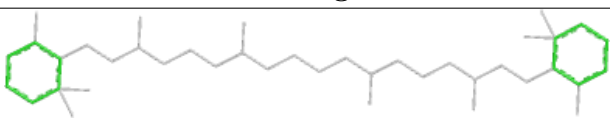


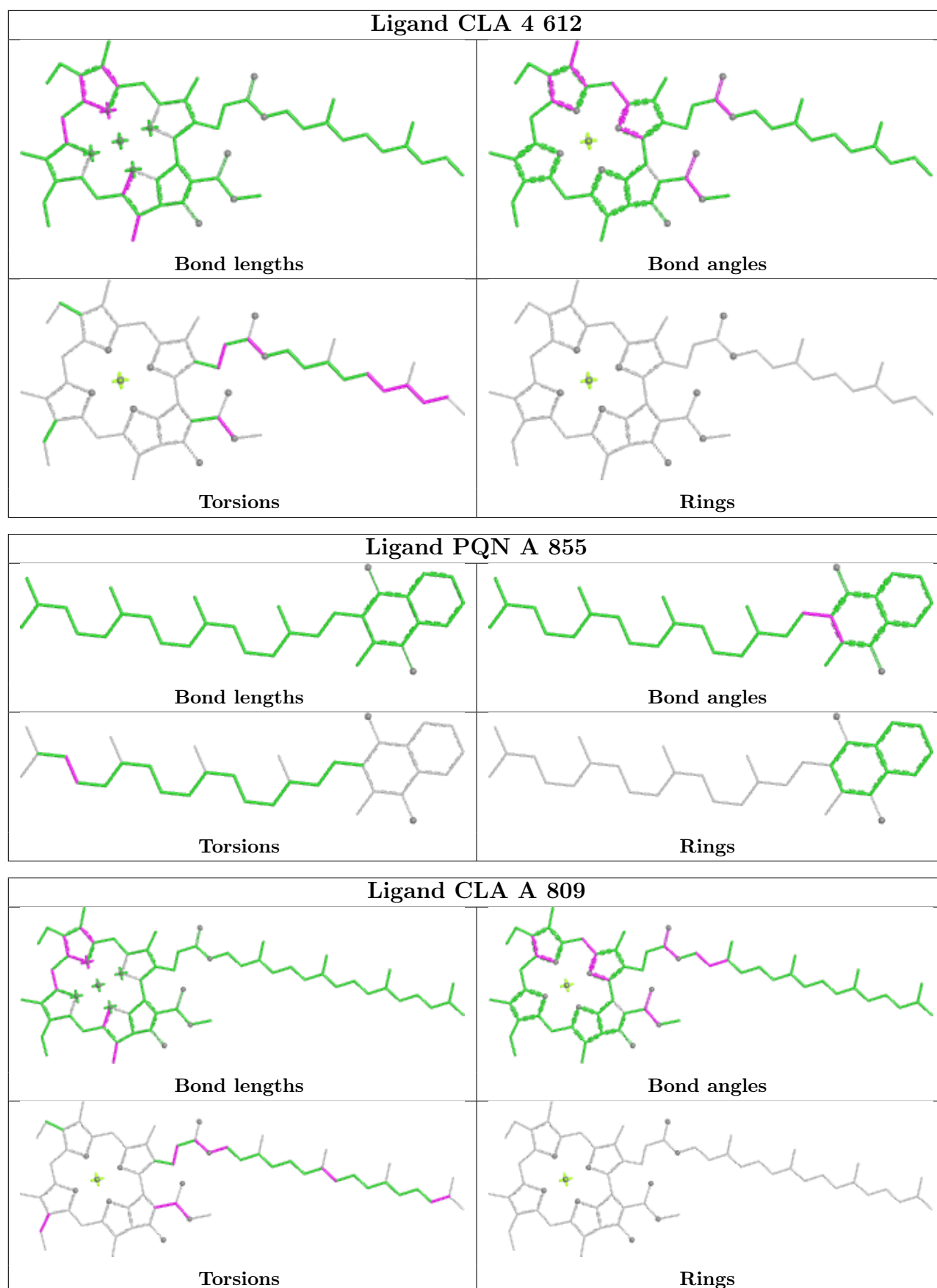
Ligand CLA 2 609

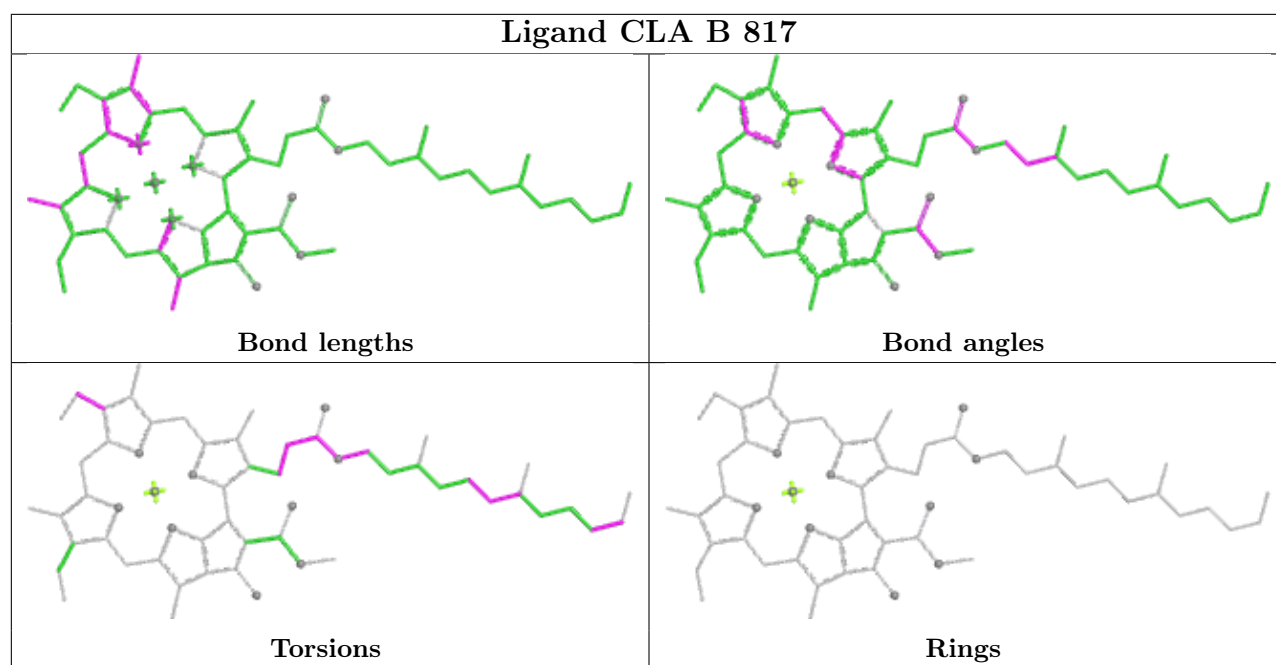


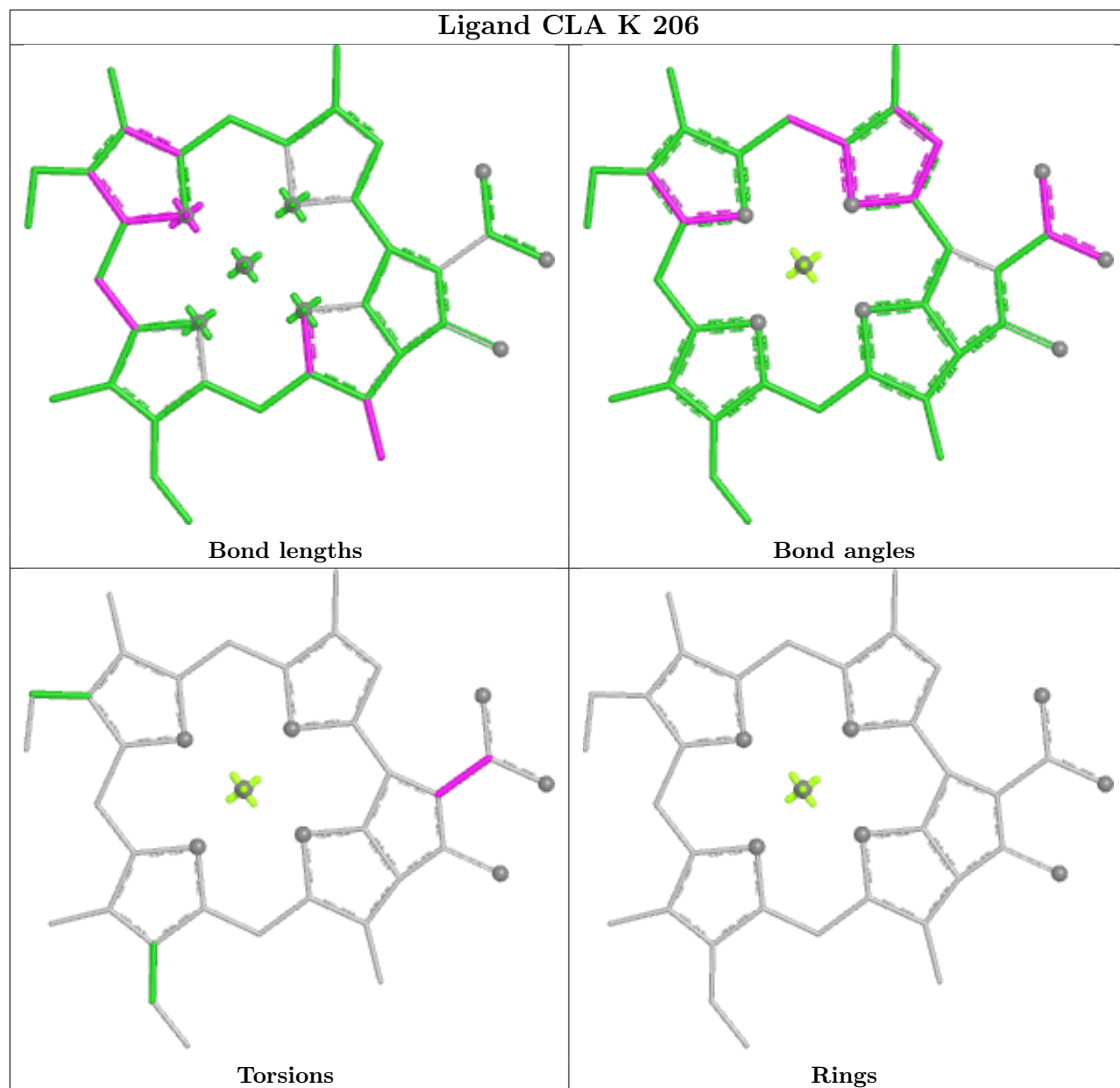
Ligand CLA B 837

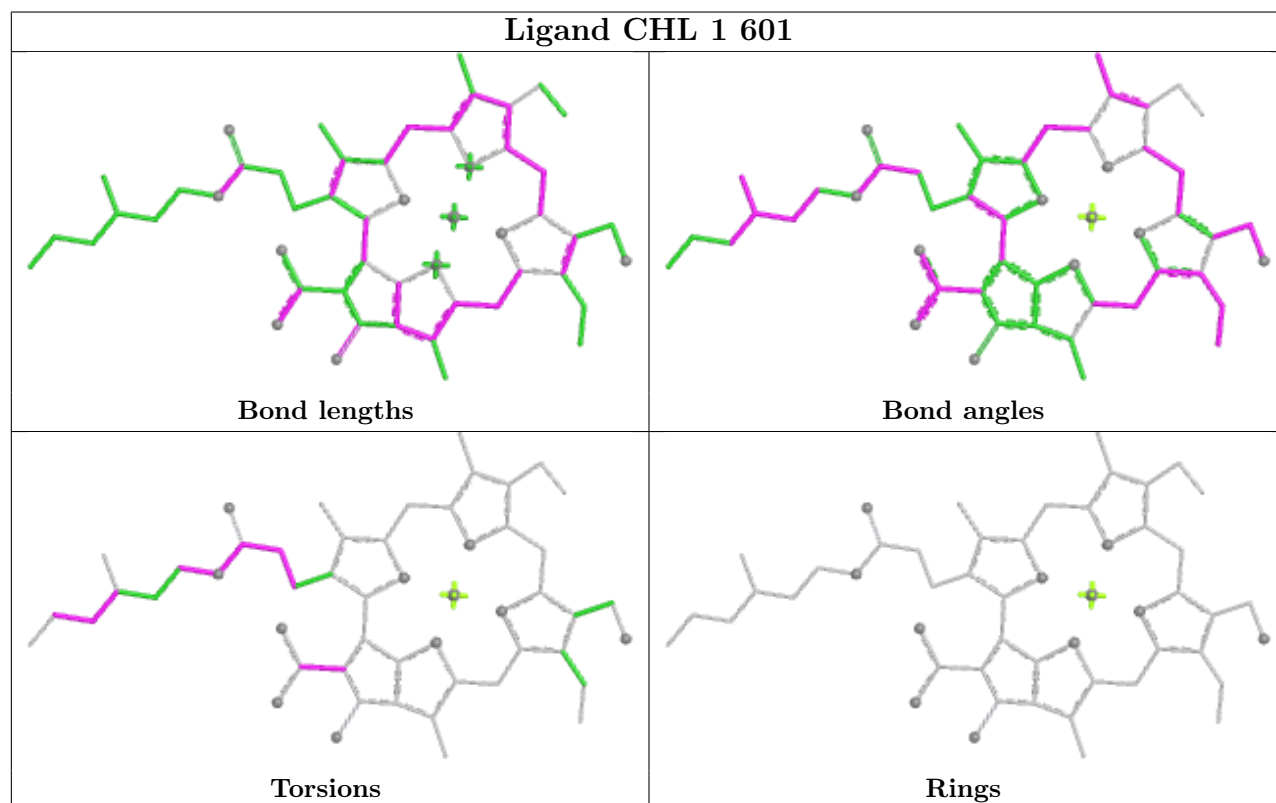
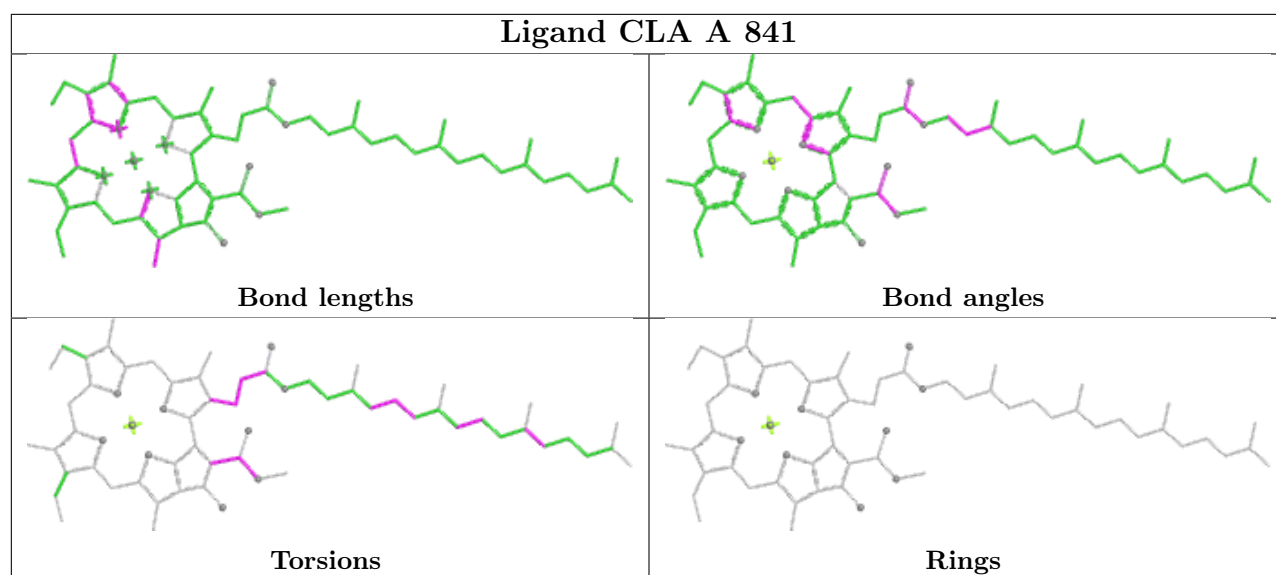


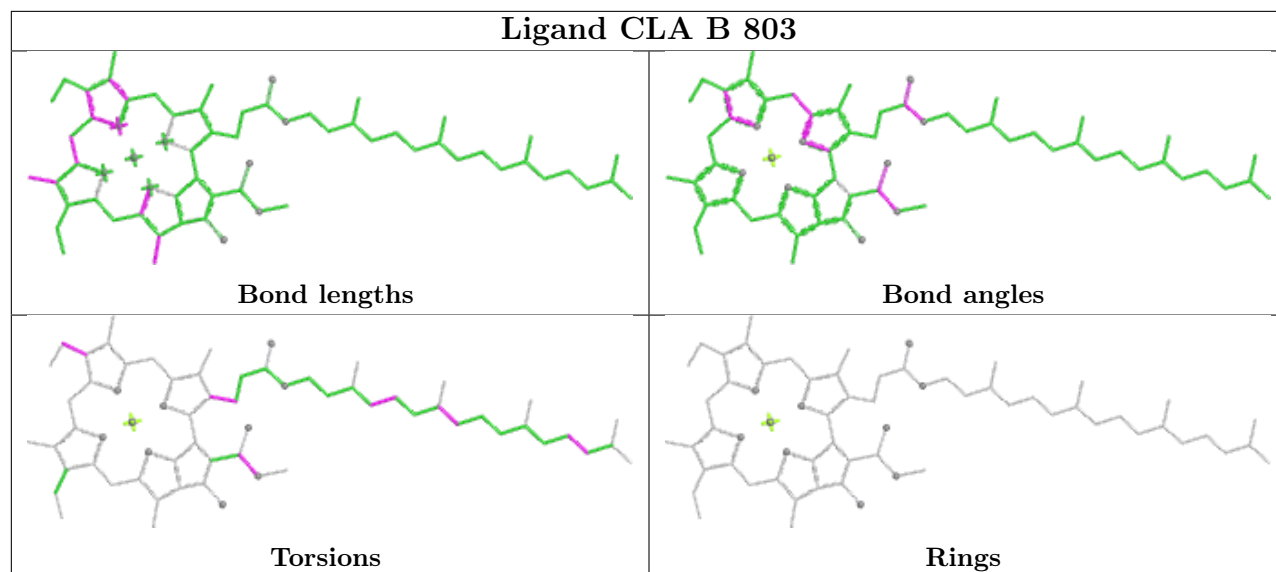
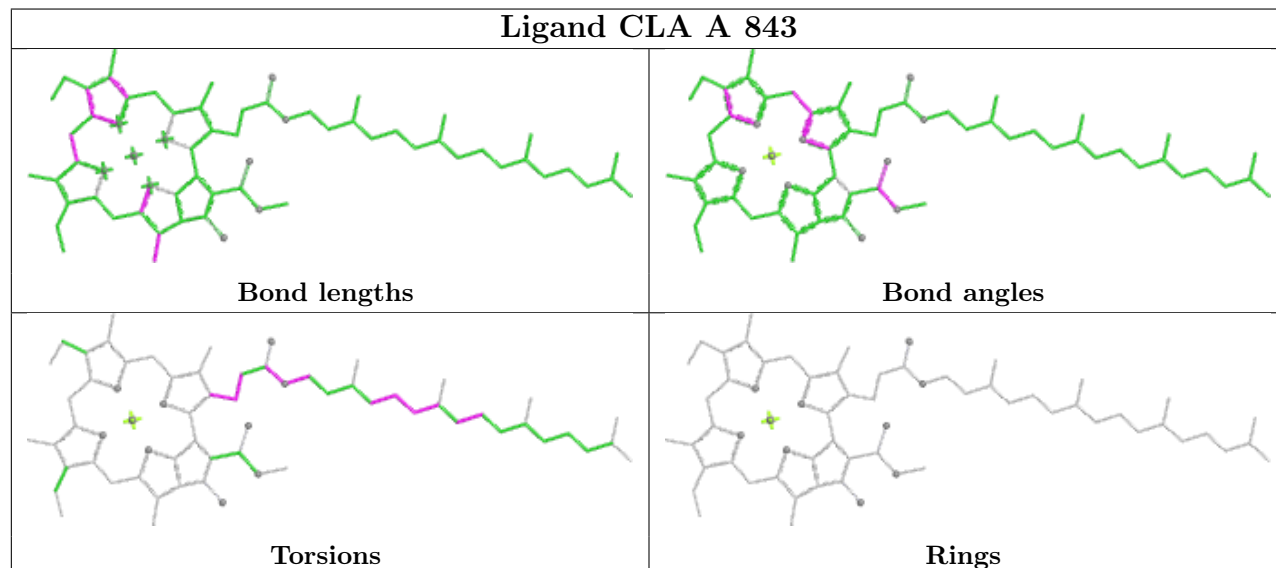
Ligand CLA B 810	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand XAT 4 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings



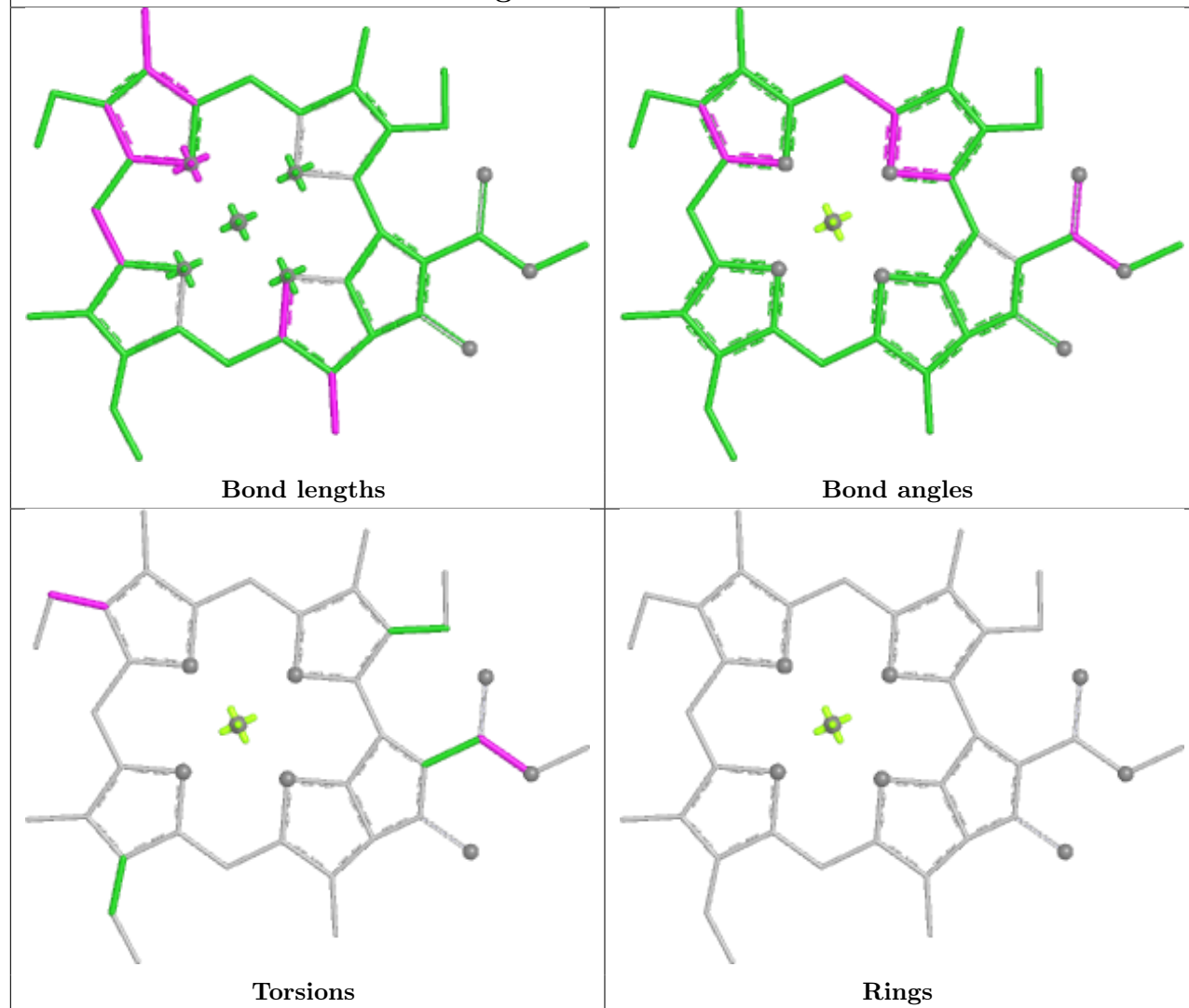




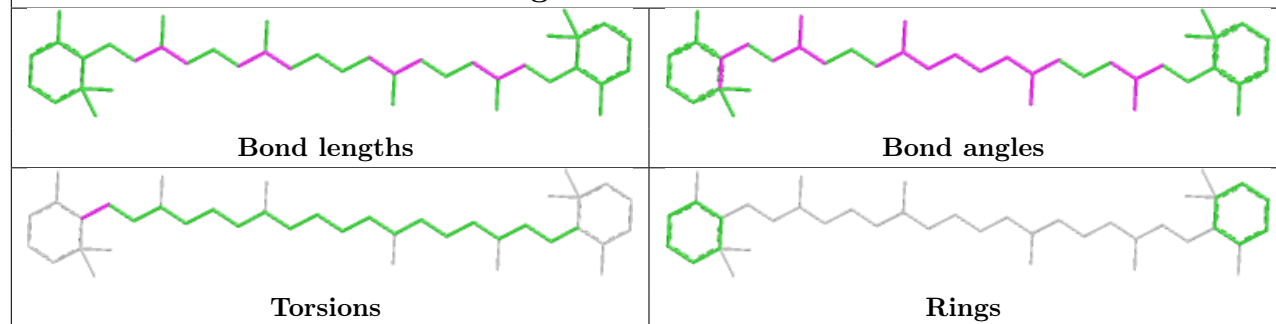


Ligand CLA B 803**Ligand CLA A 843**

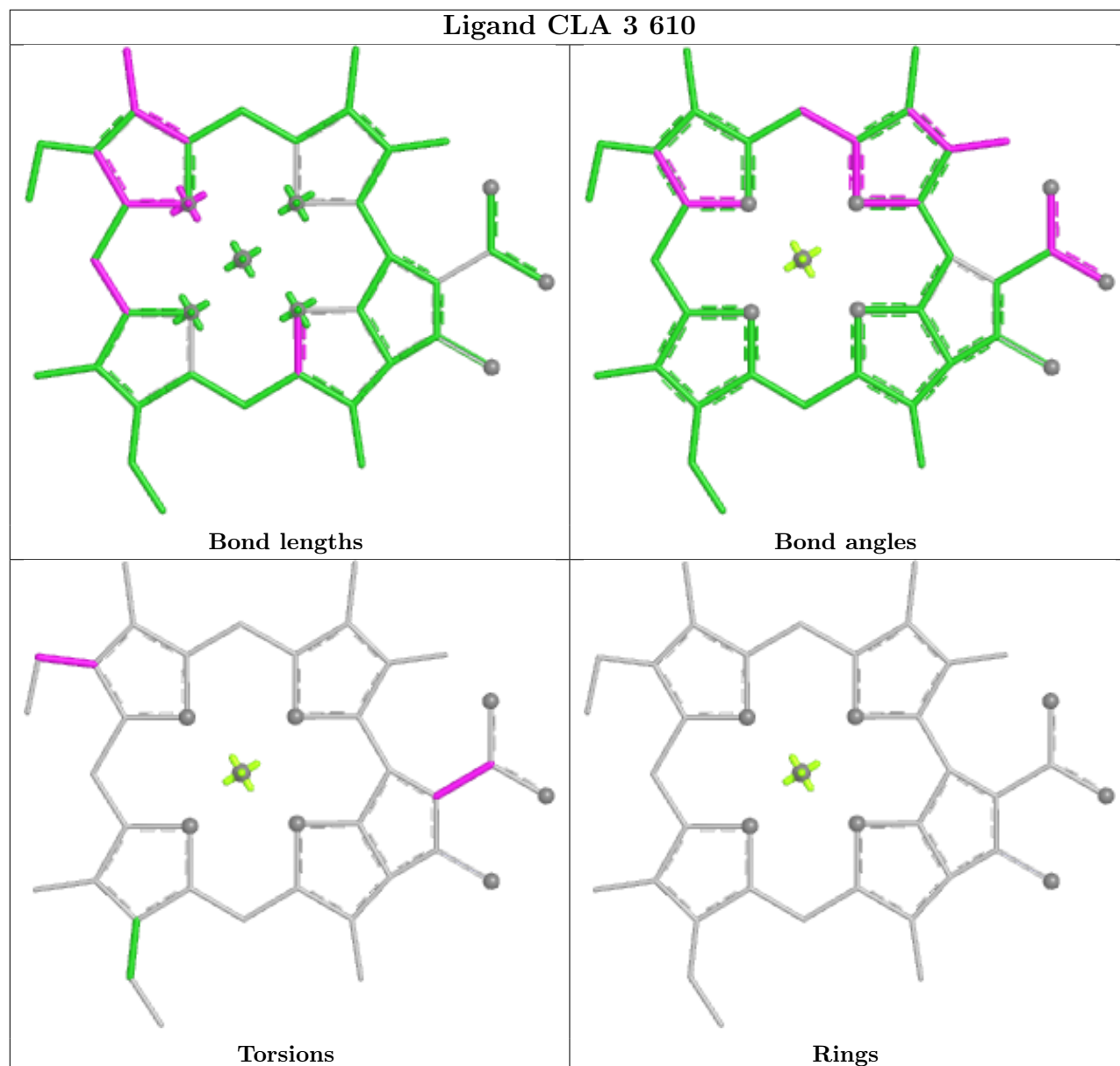
Ligand CLA A 816



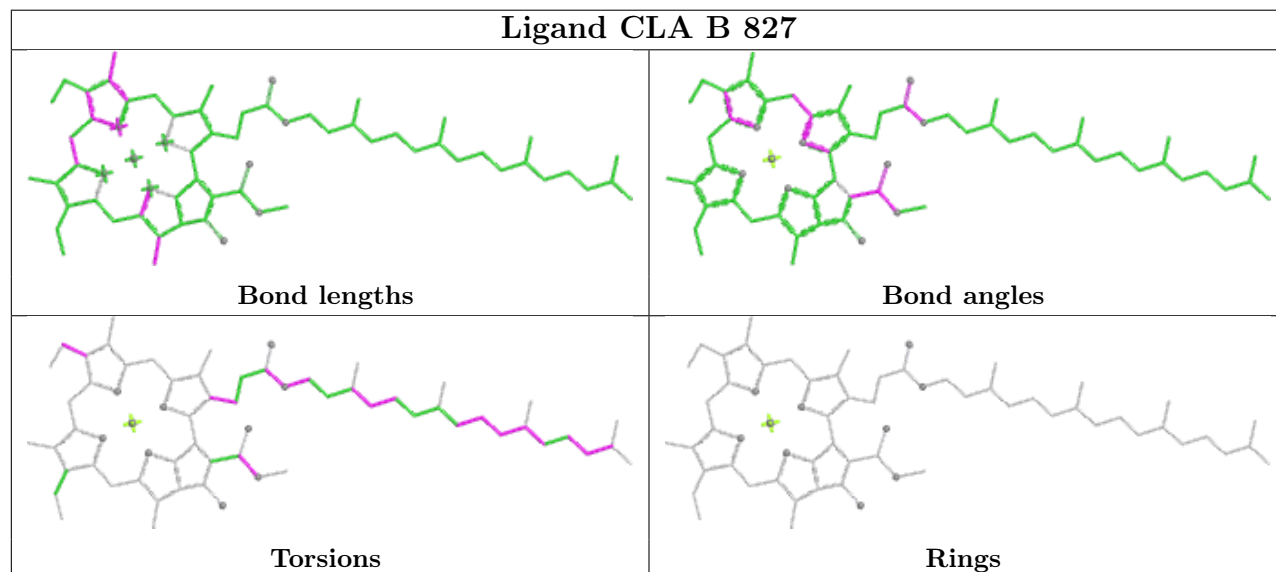
Ligand BCR B 847



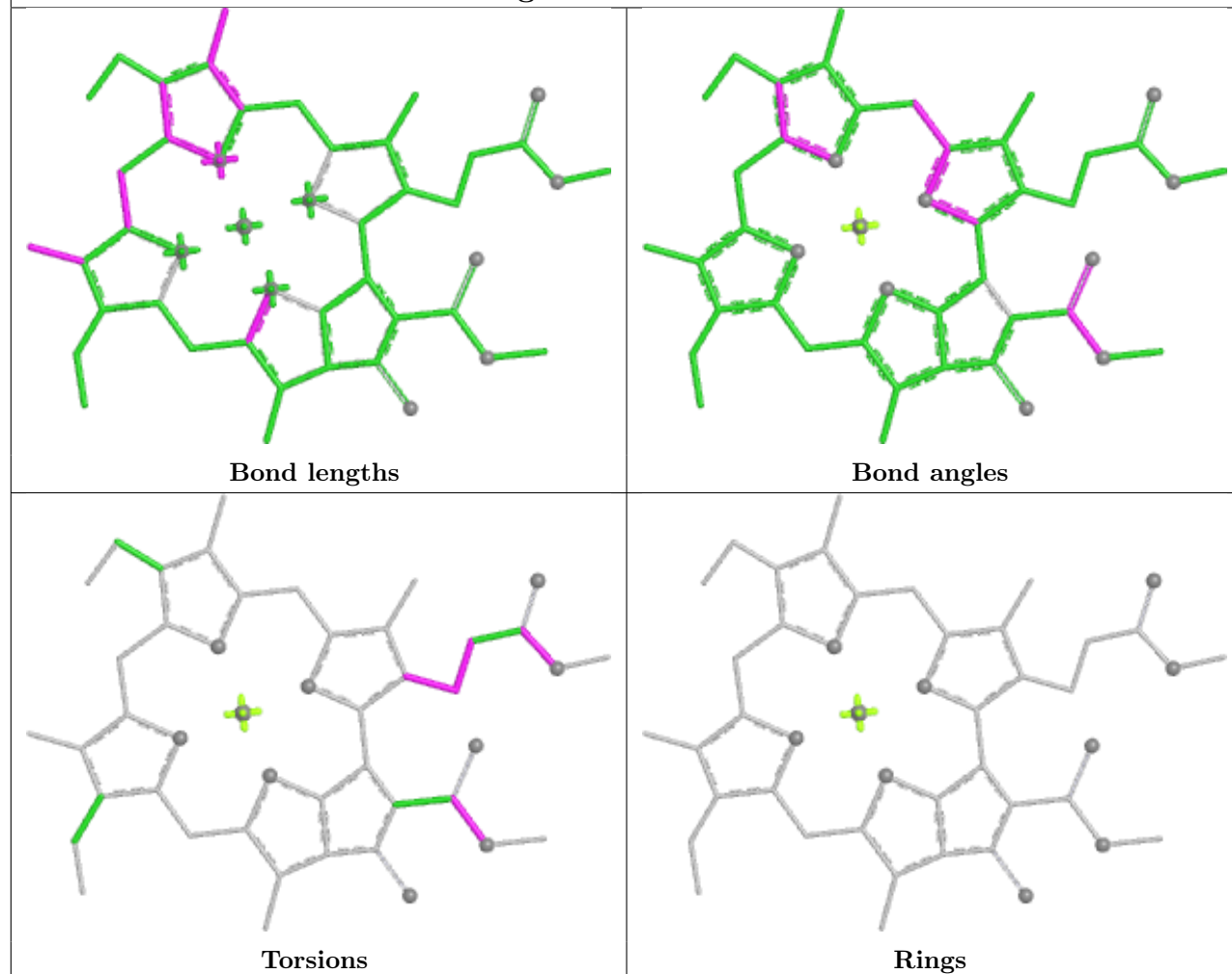
Ligand CLA 3 610

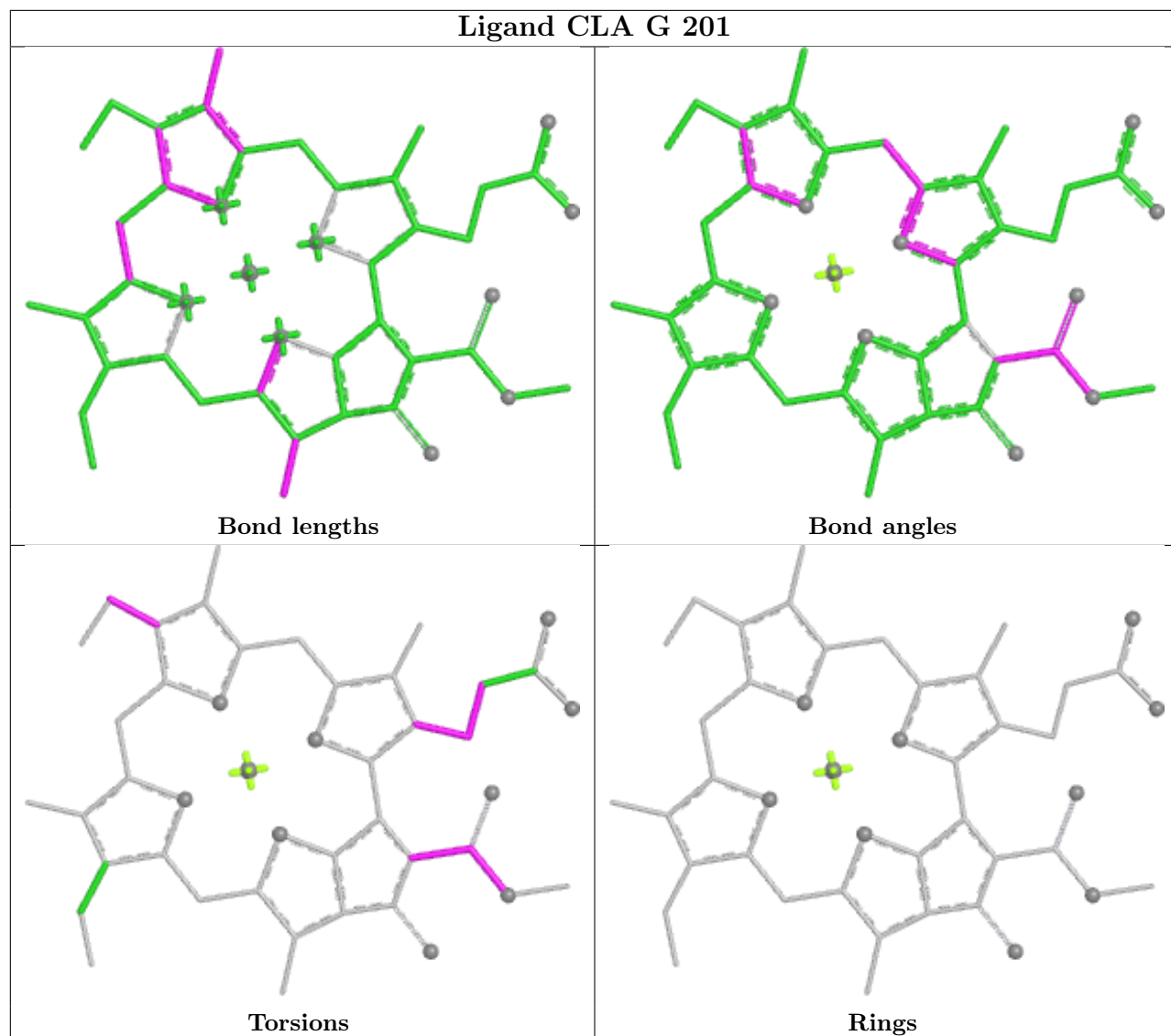


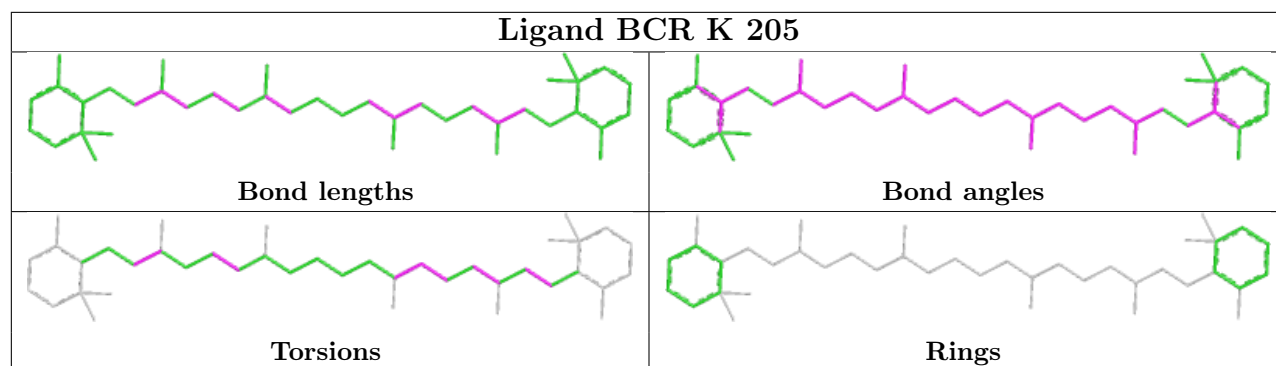
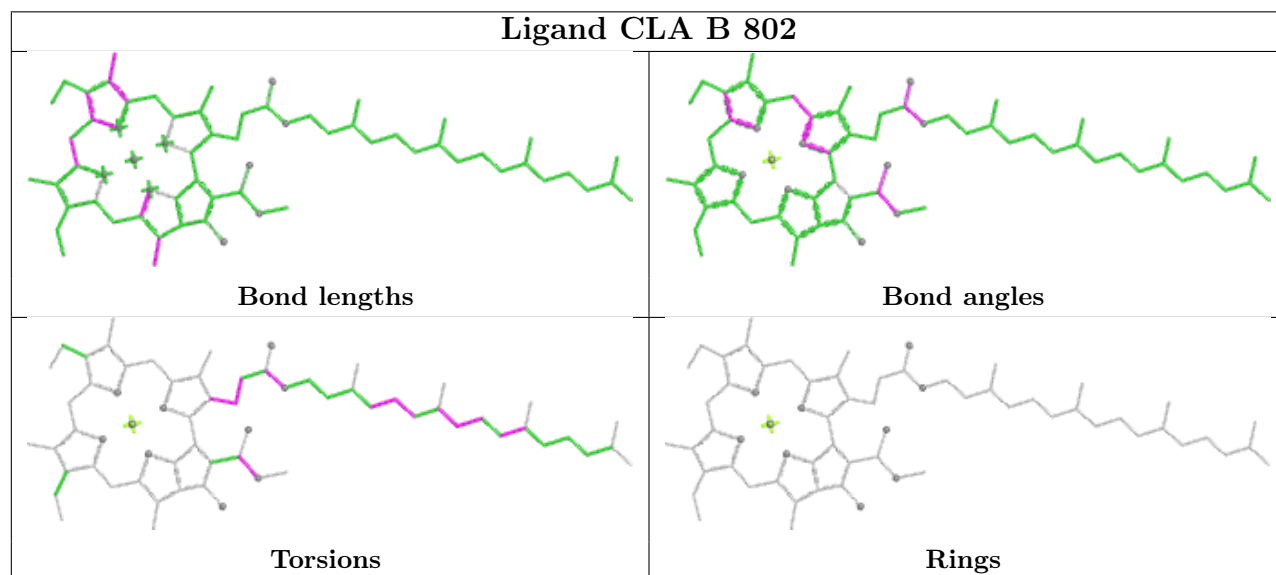
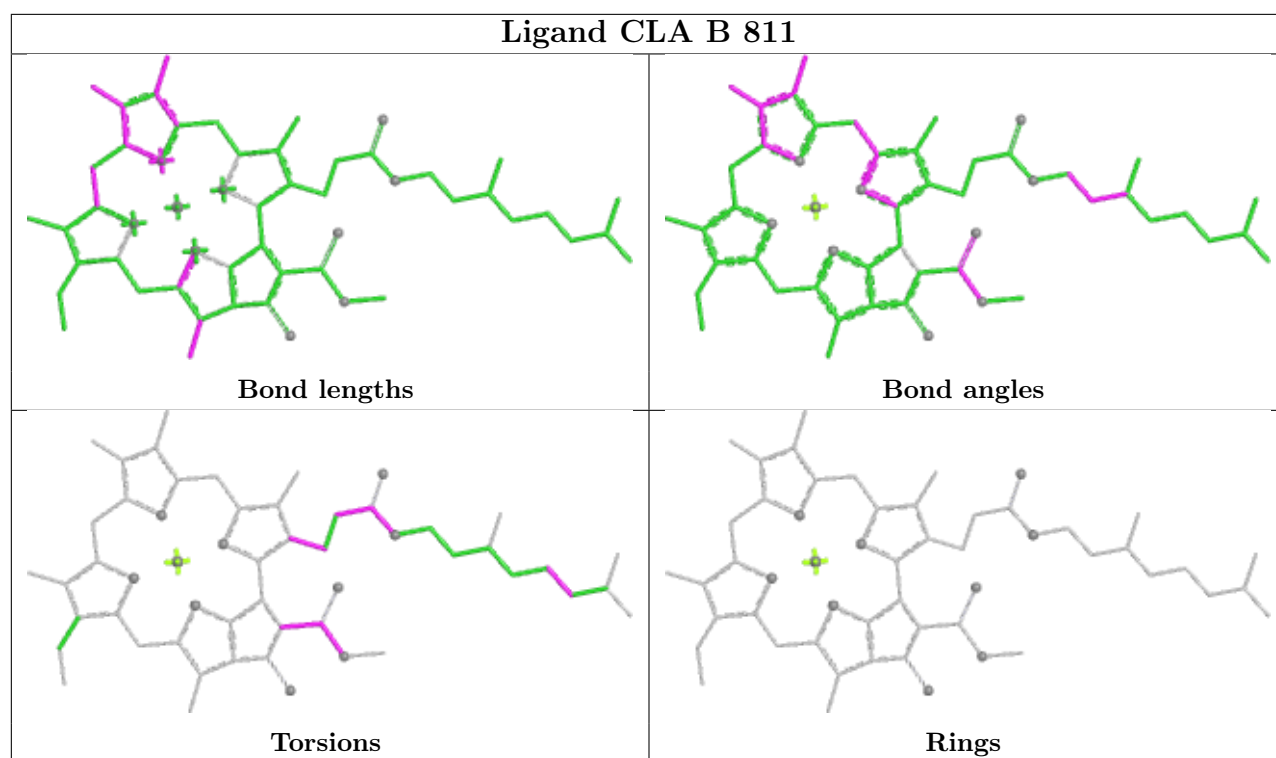
Ligand CLA B 827

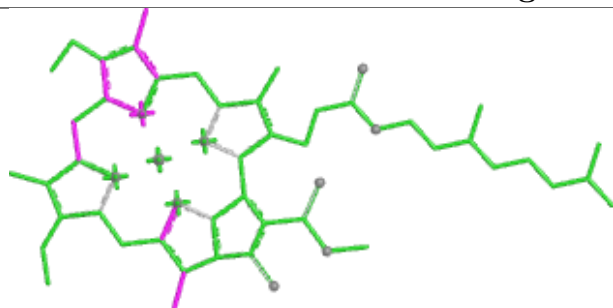


Ligand CLA 1 605

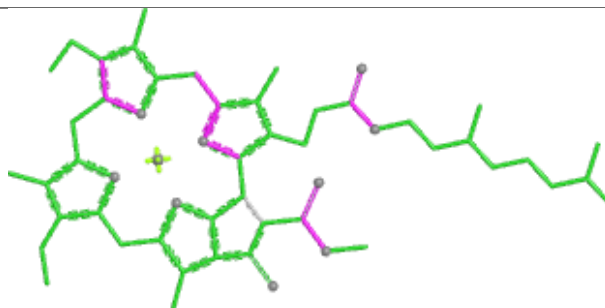




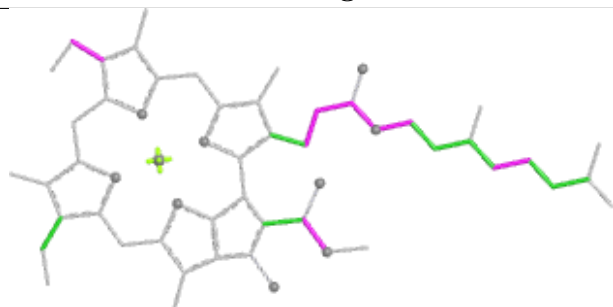


Ligand CLA 3 602

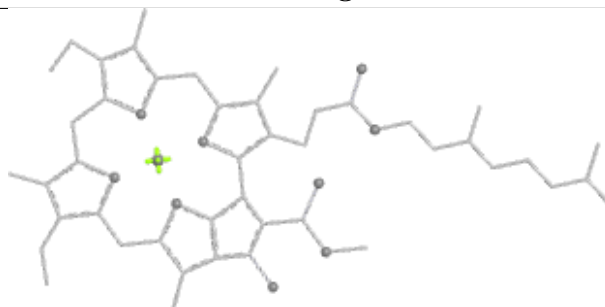
Bond lengths



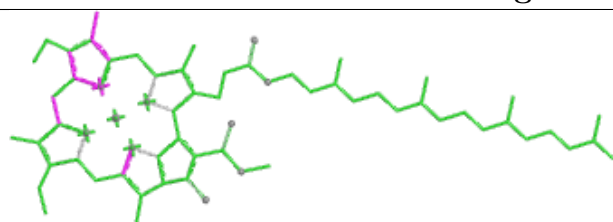
Bond angles



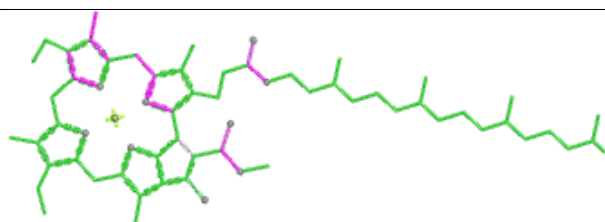
Torsions



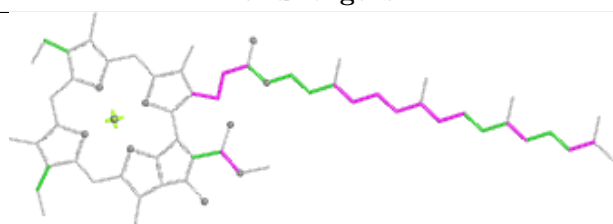
Rings

Ligand CLA B 809

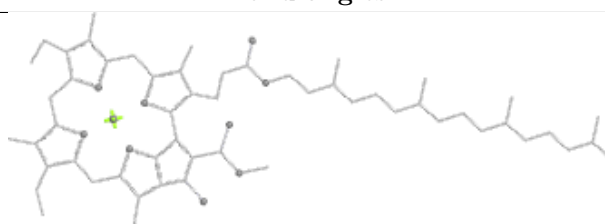
Bond lengths



Bond angles

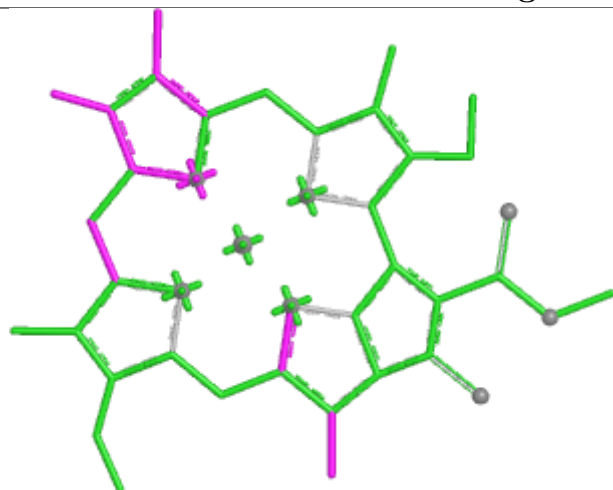


Torsions



Rings

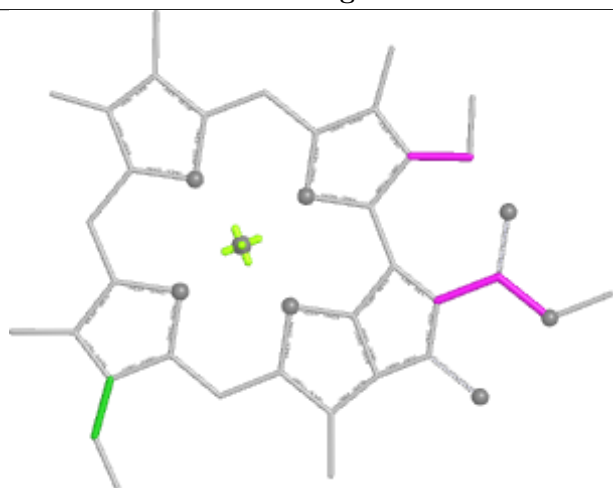
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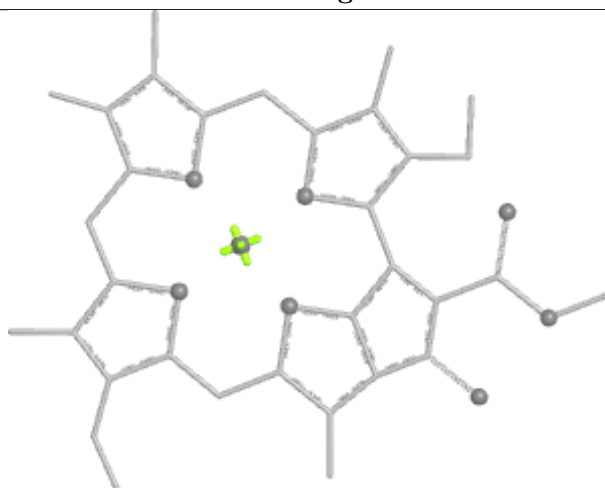
Bond lengths



Bond angles

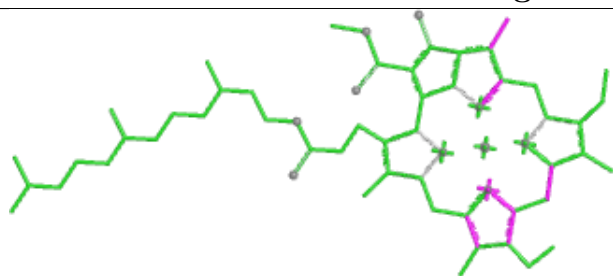


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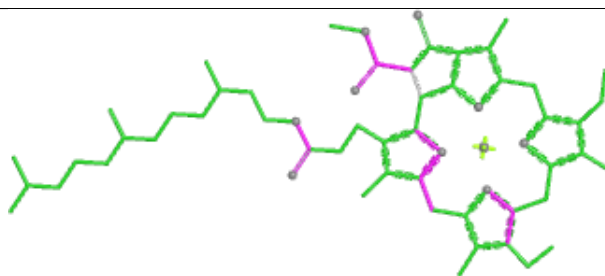


Rings

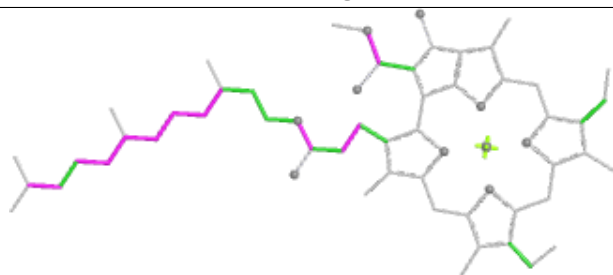
Ligand CLA A 818



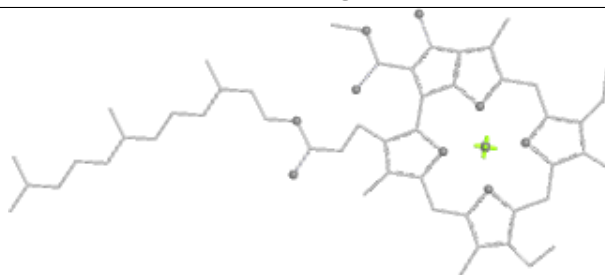
Bond lengths



Bond angles

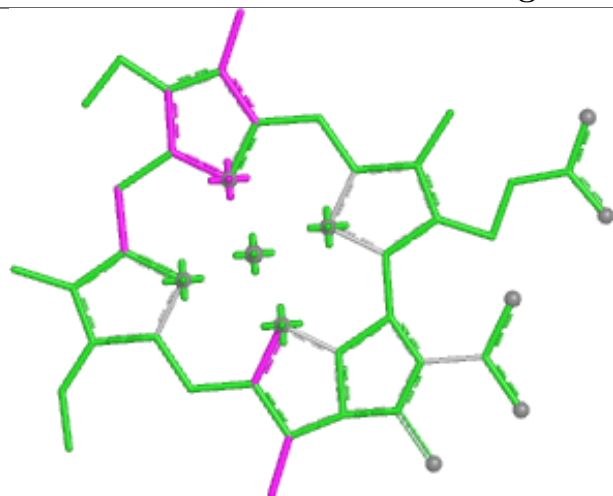


Torsions

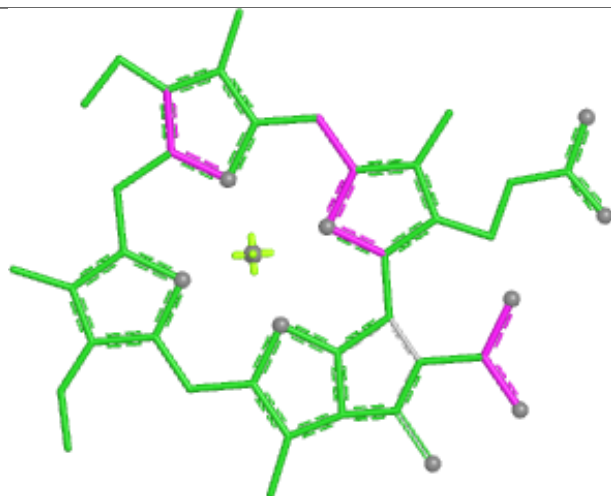


Rings

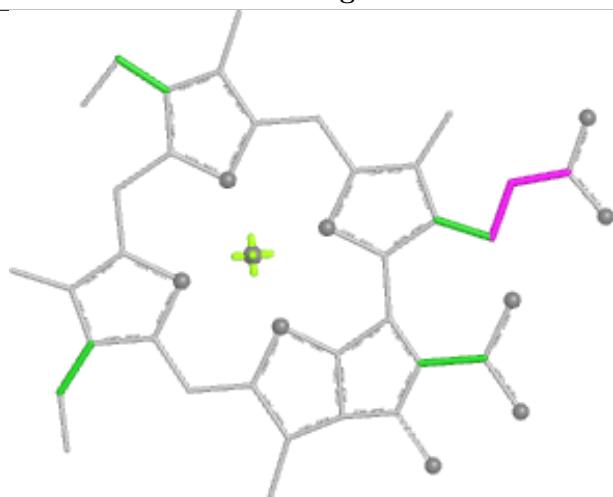
Ligand CLA 2 603



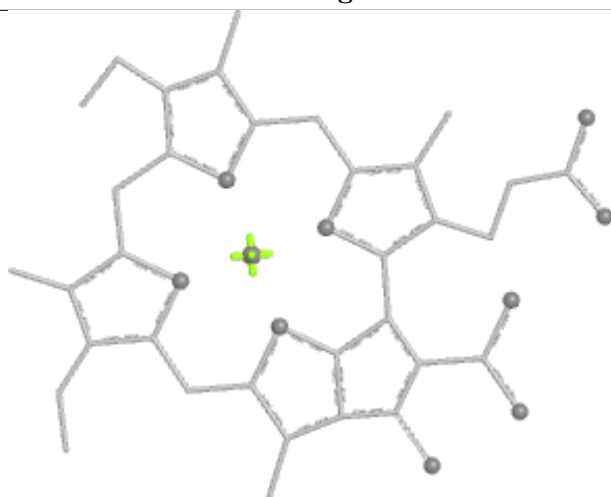
Bond lengths



Bond angles

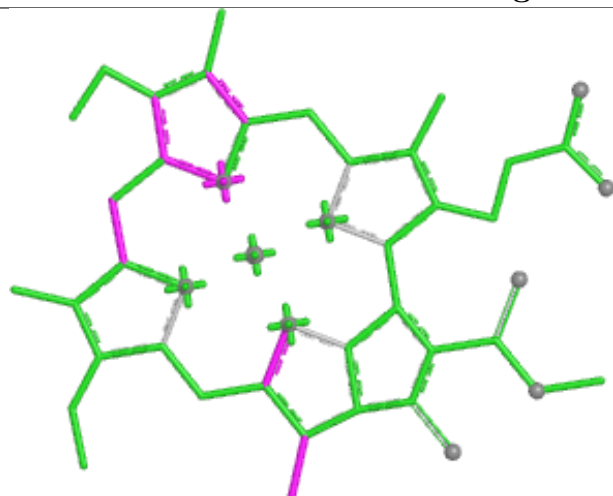


Torsions

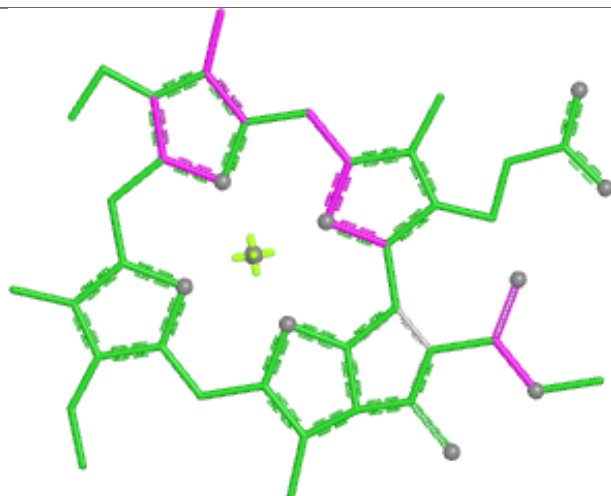


Rings

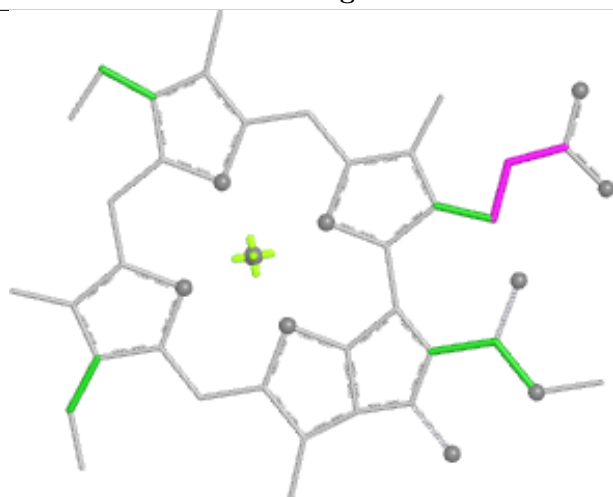
Ligand CLA G 203



Bond lengths



Bond angles

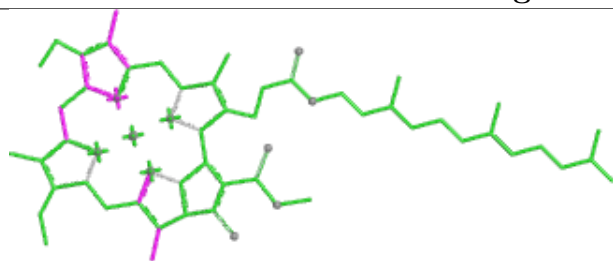


Torsions

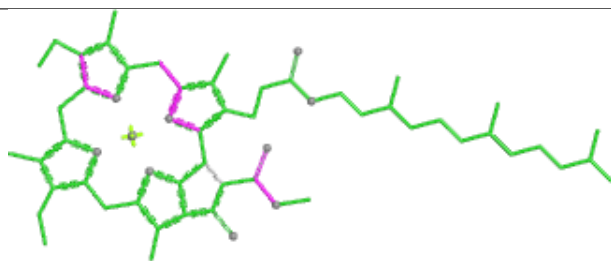


Rings

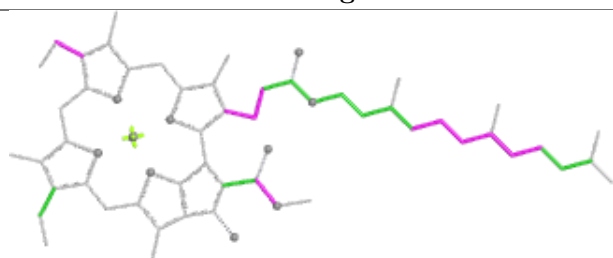
Ligand CLA H 201



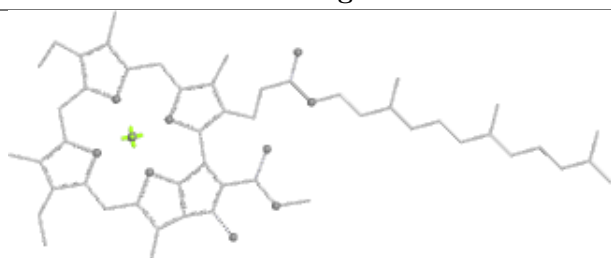
Bond lengths



Bond angles

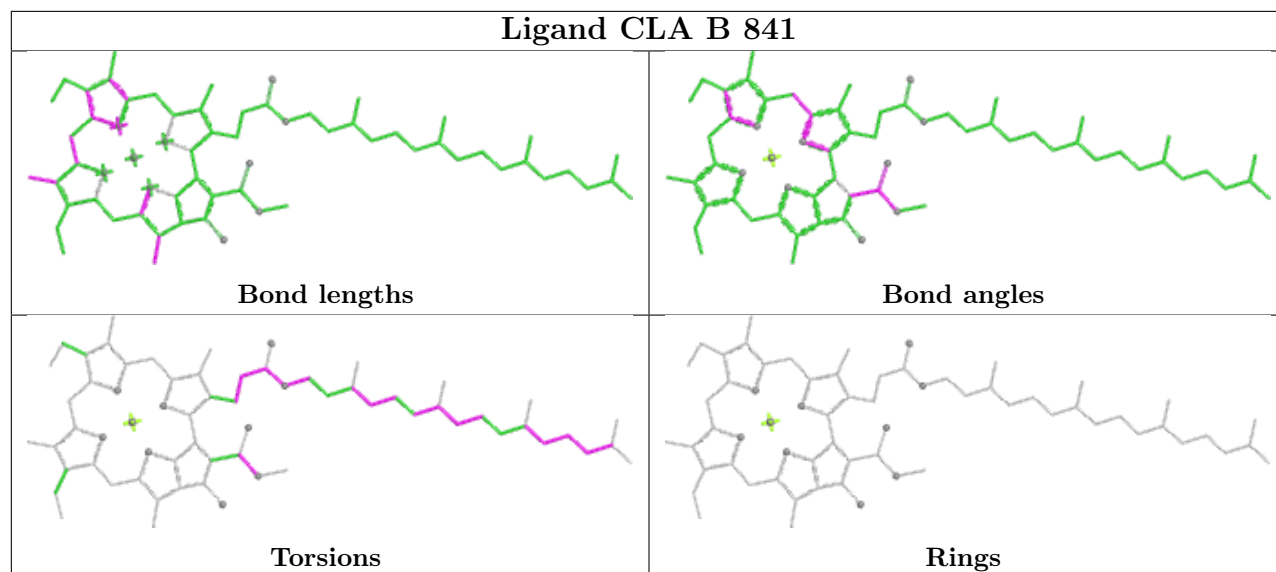


Torsions

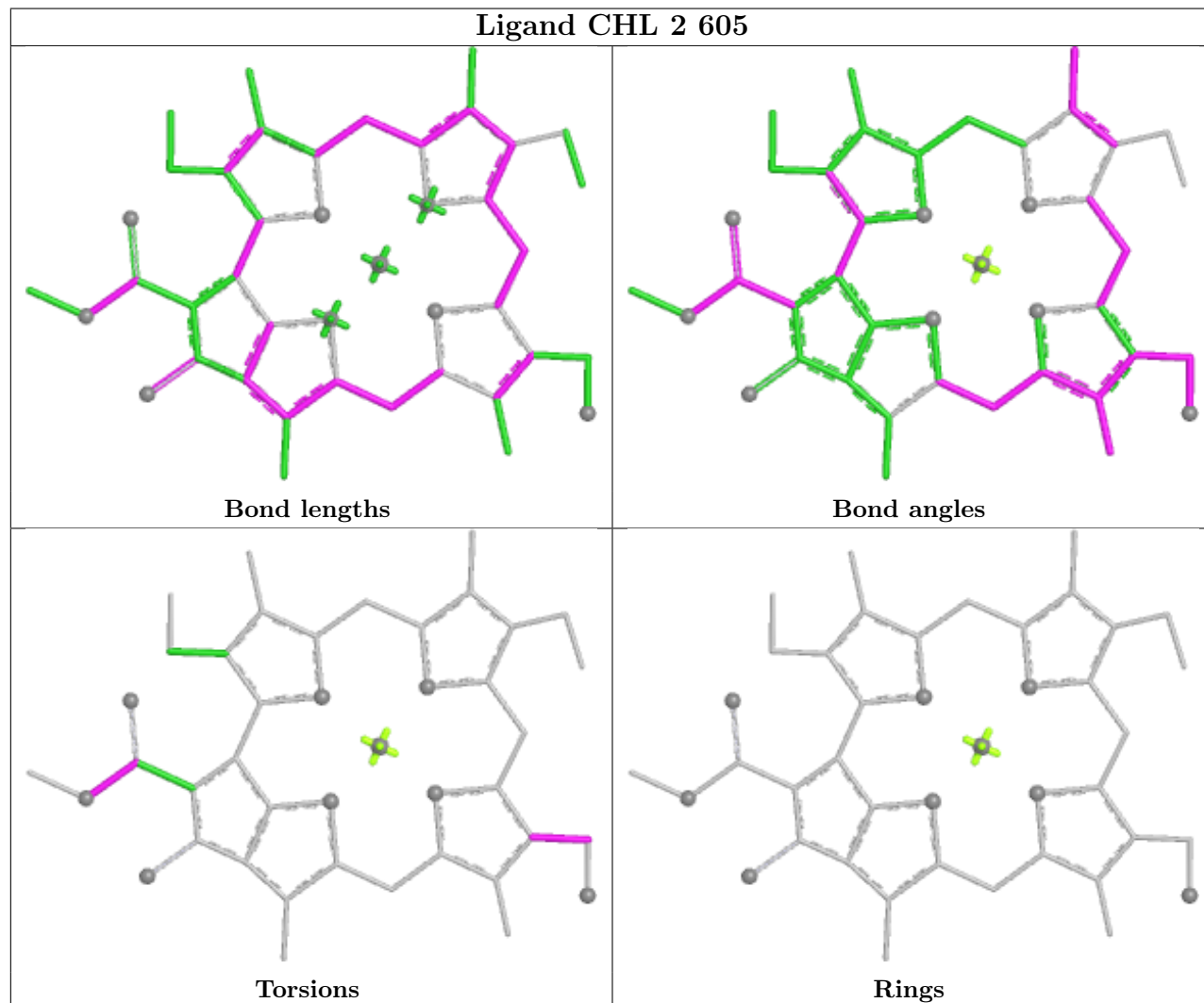


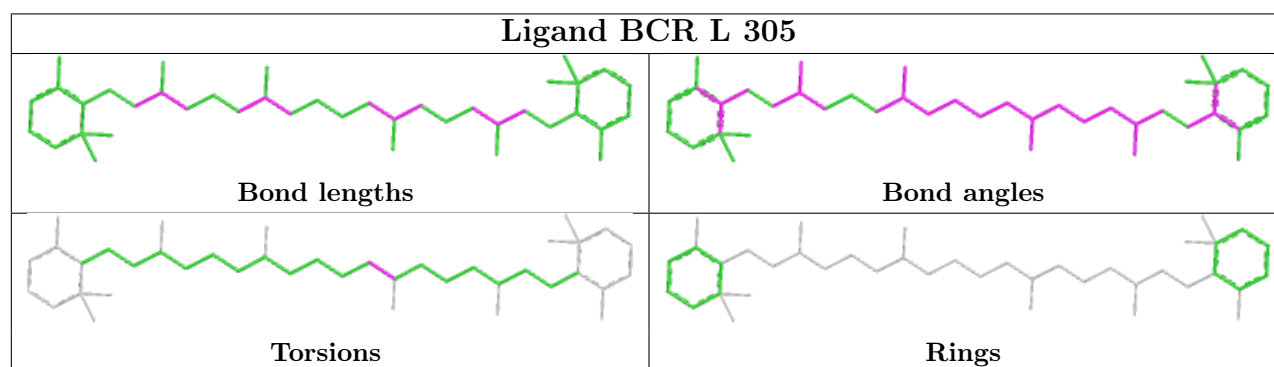
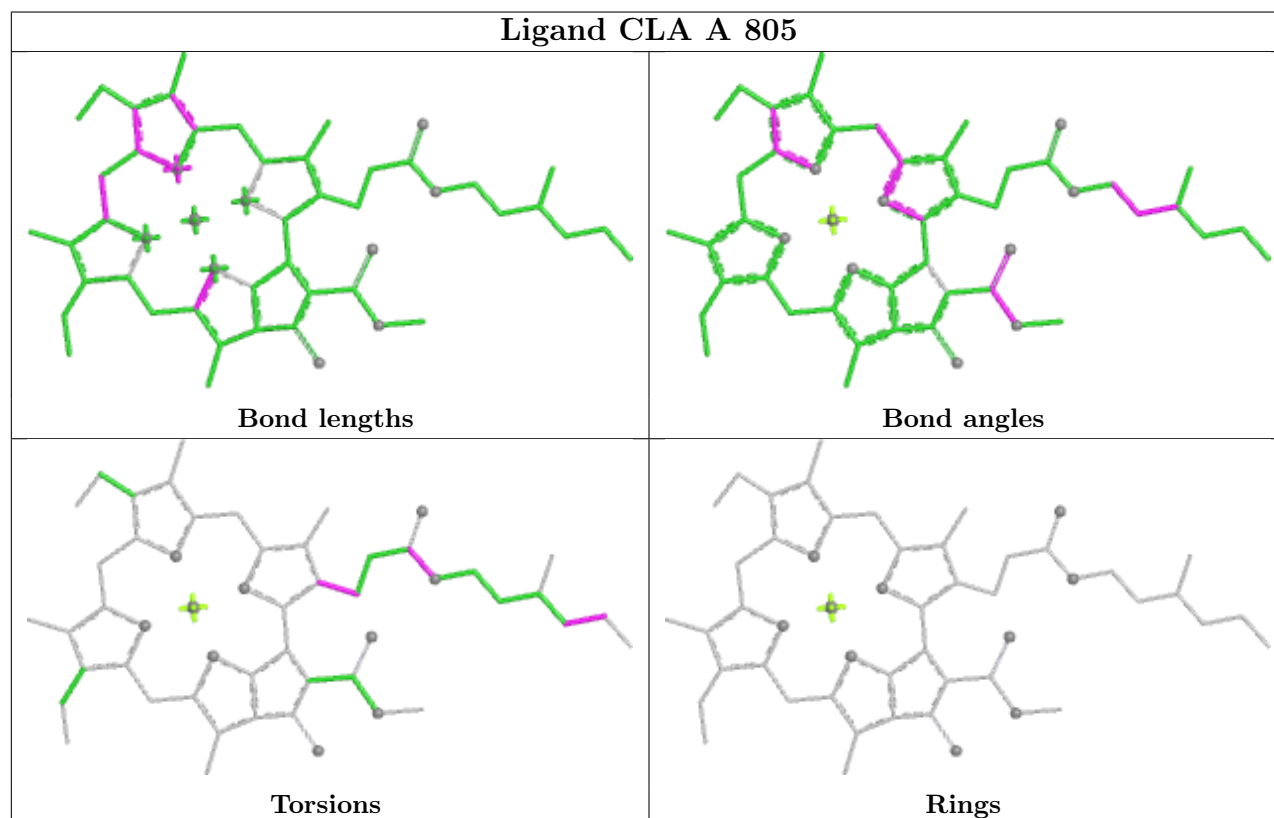
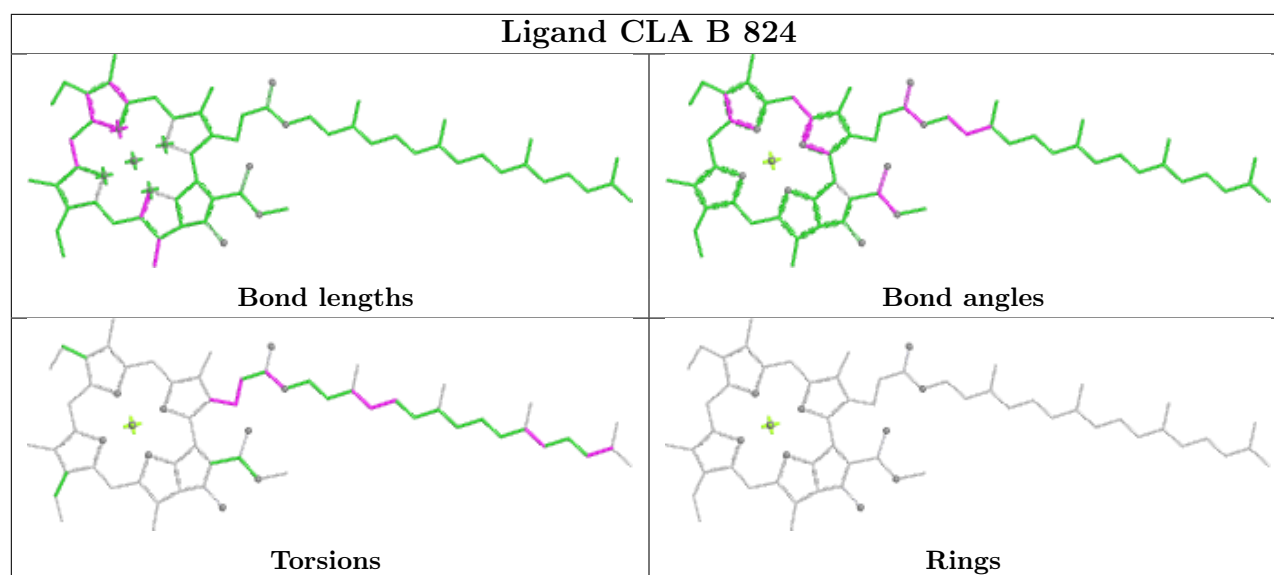
Rings

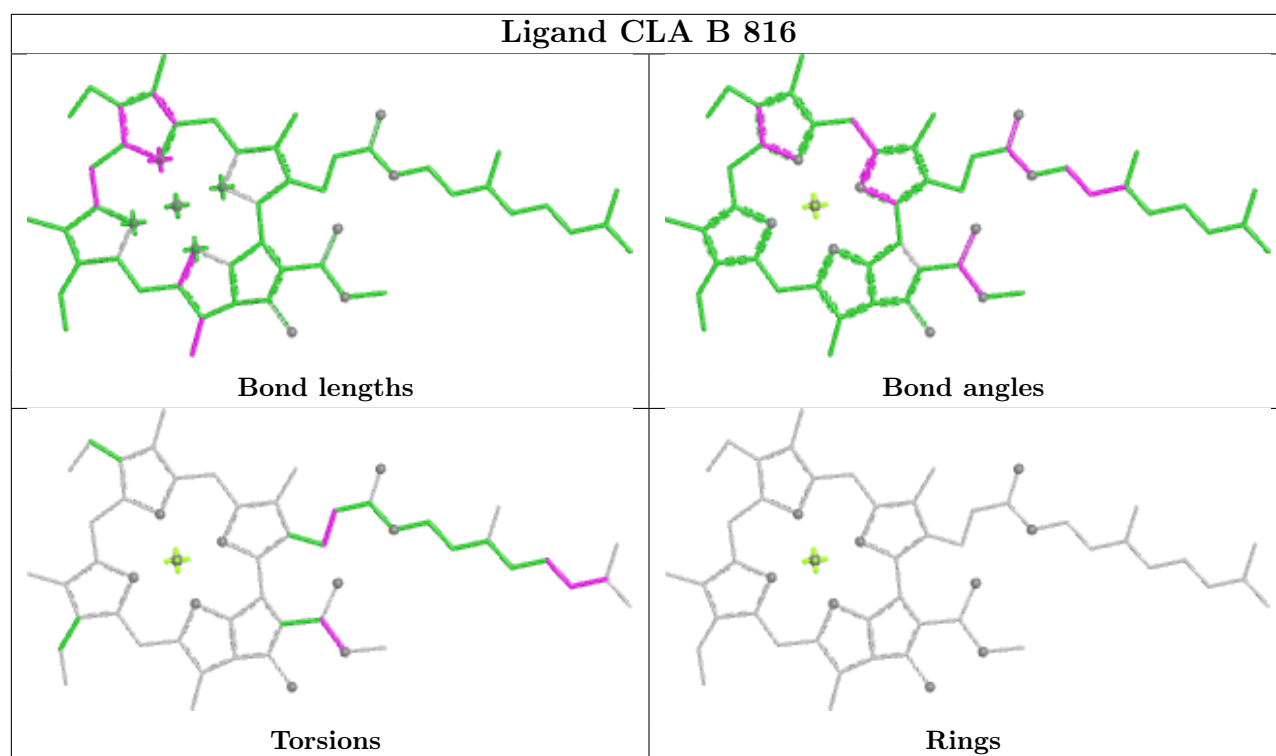
Ligand CLA B 841



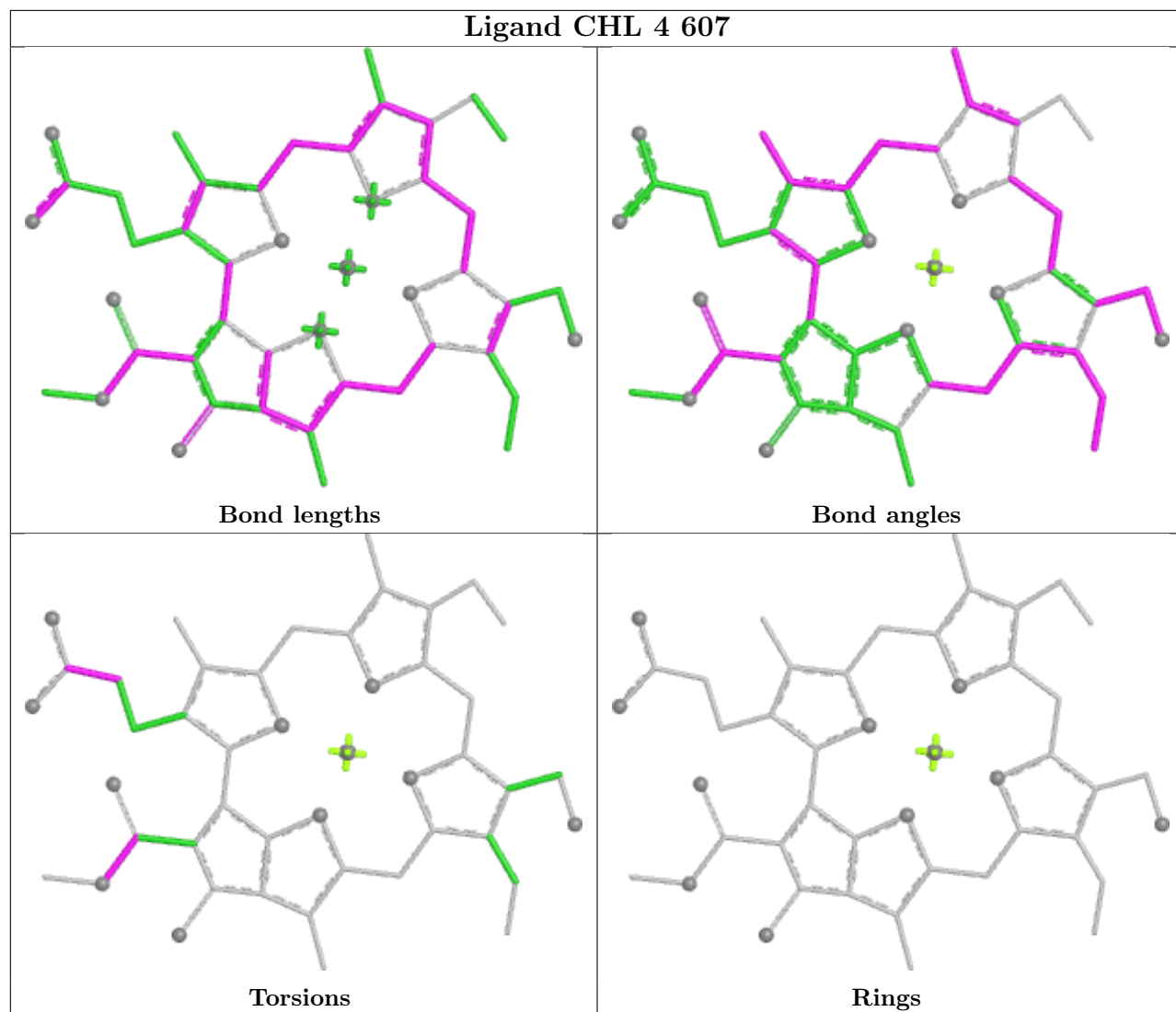
Ligand CHL 2 605

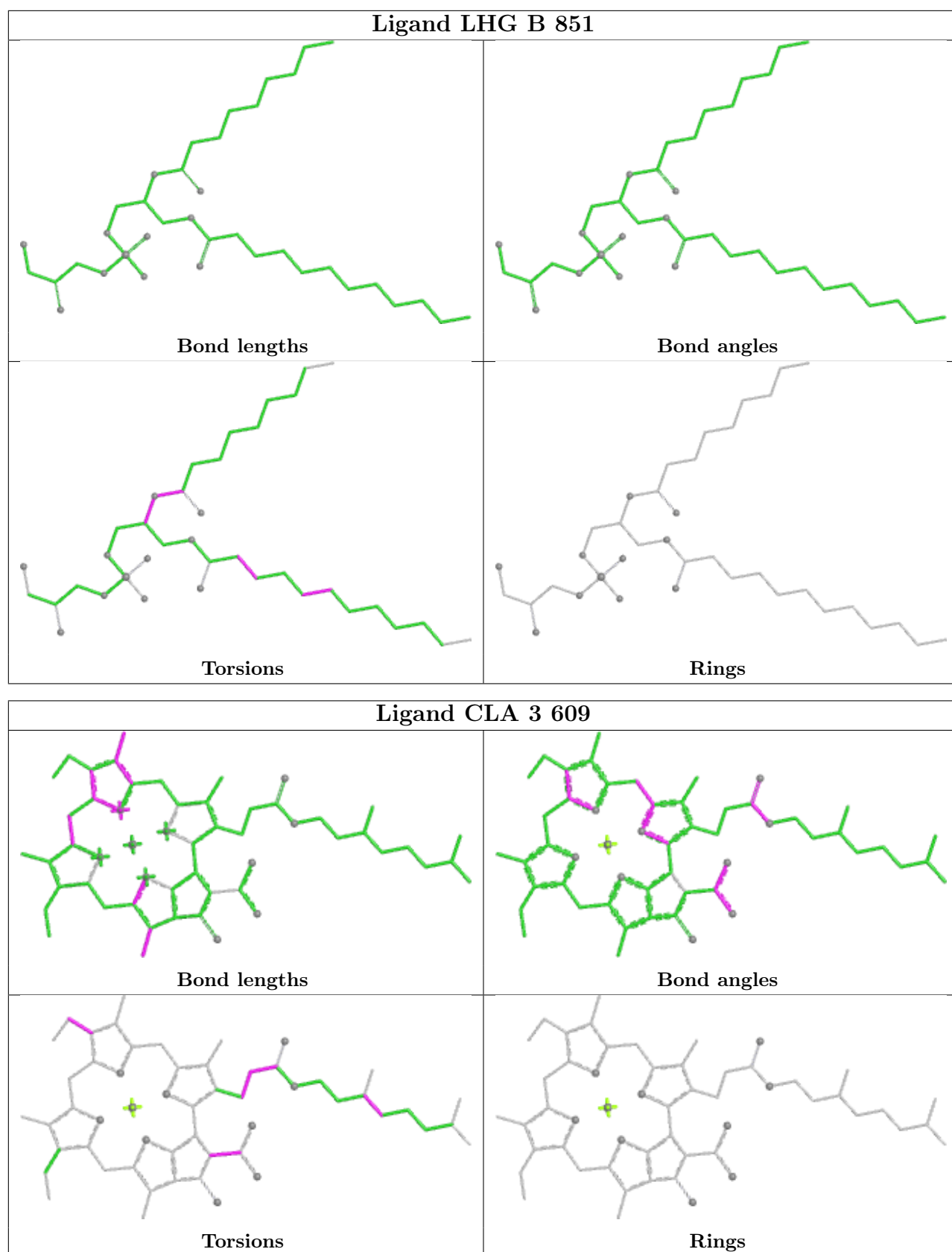


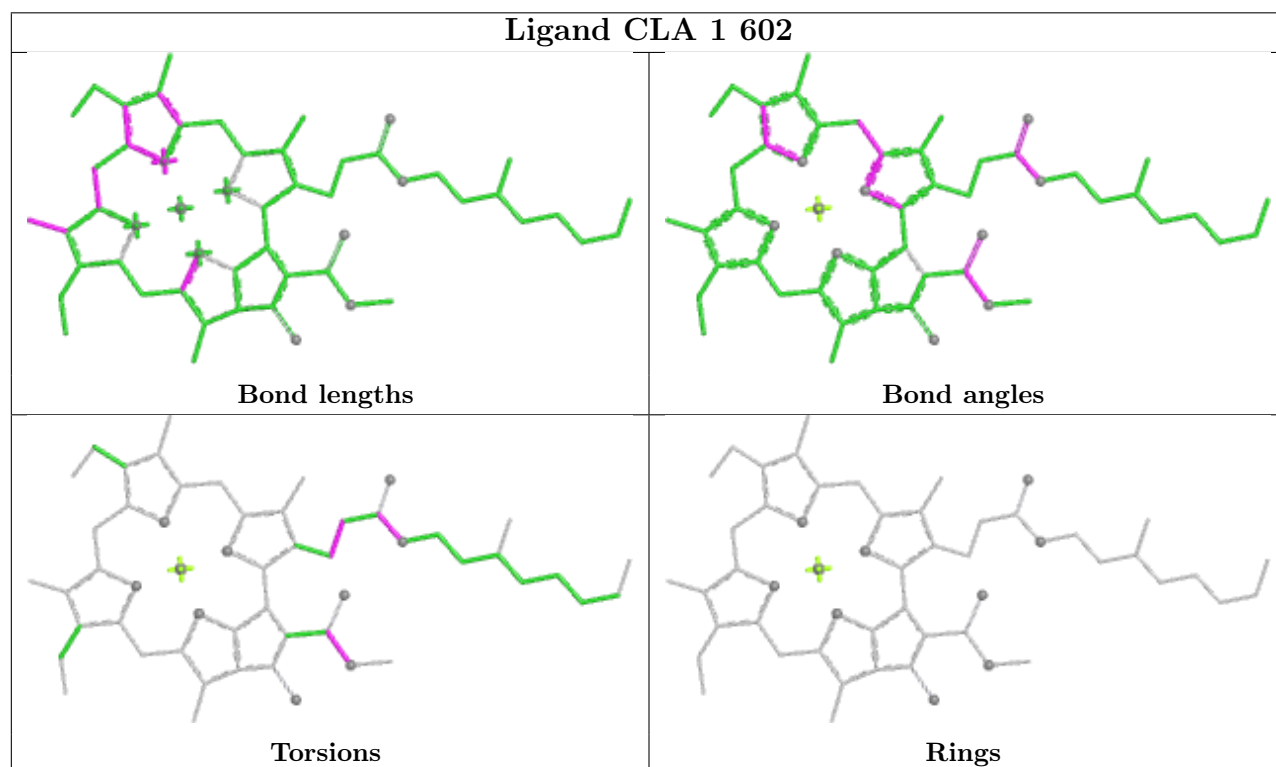
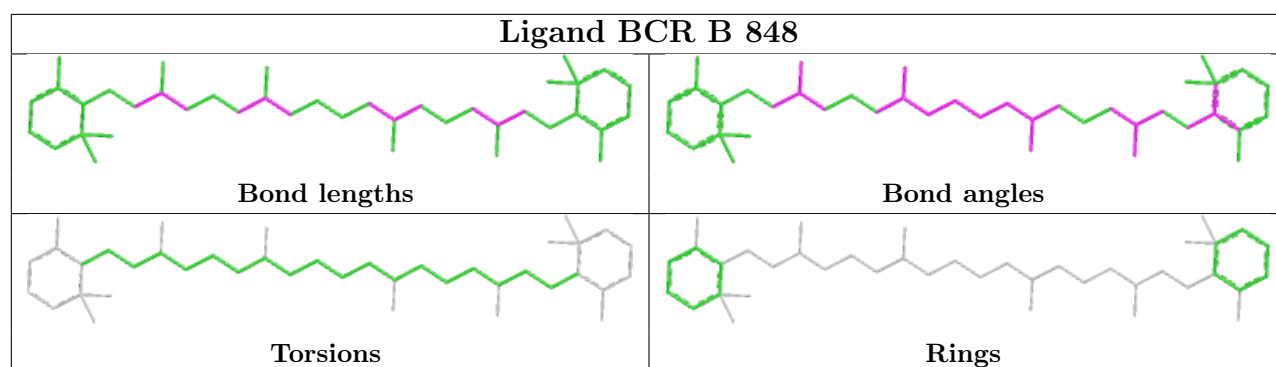




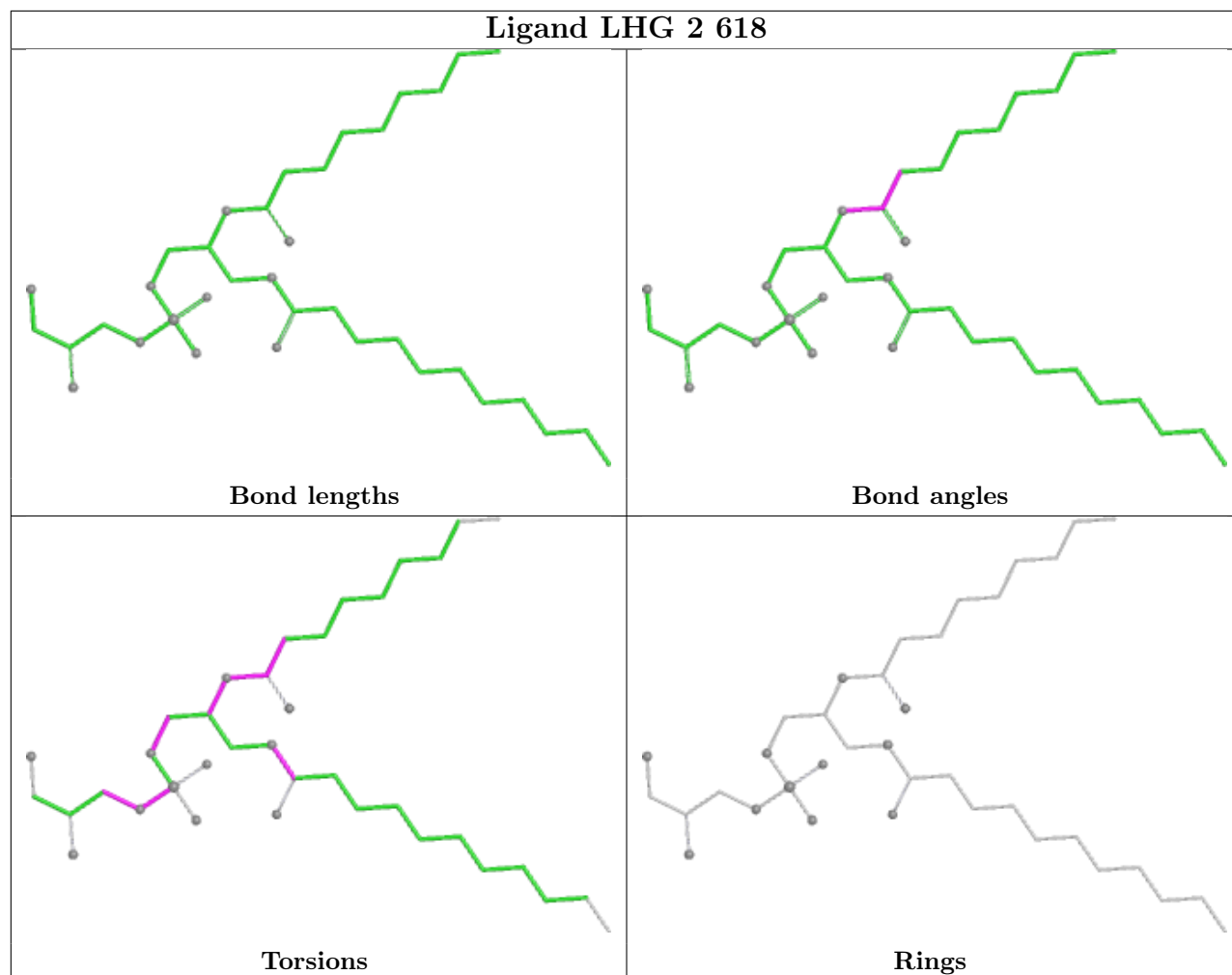
Ligand CHL 4 607



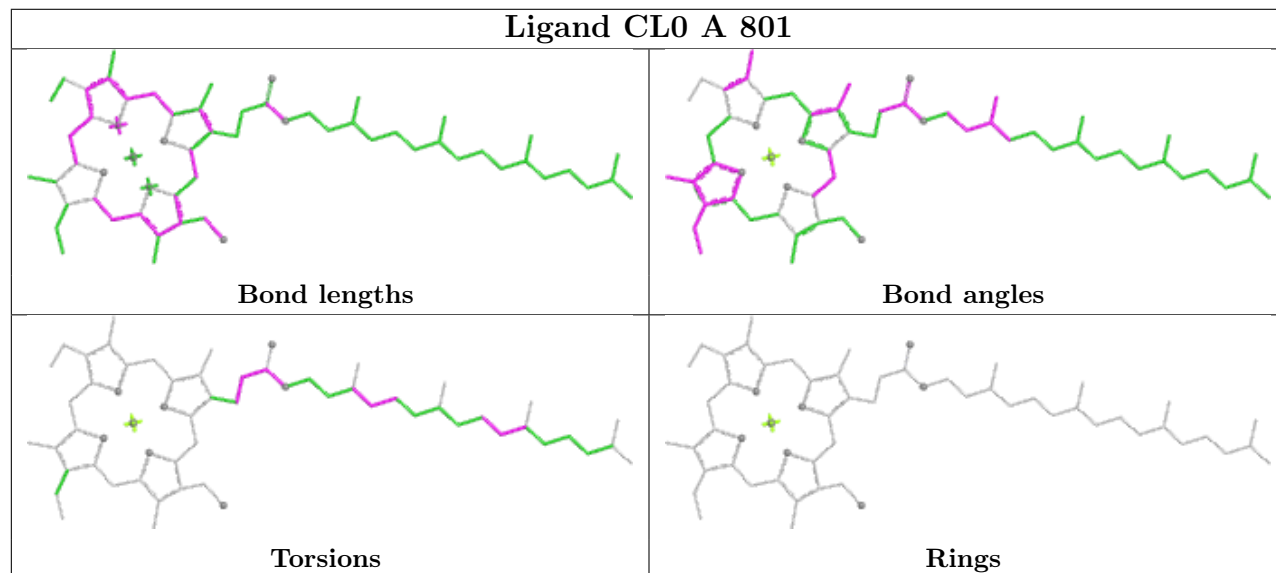


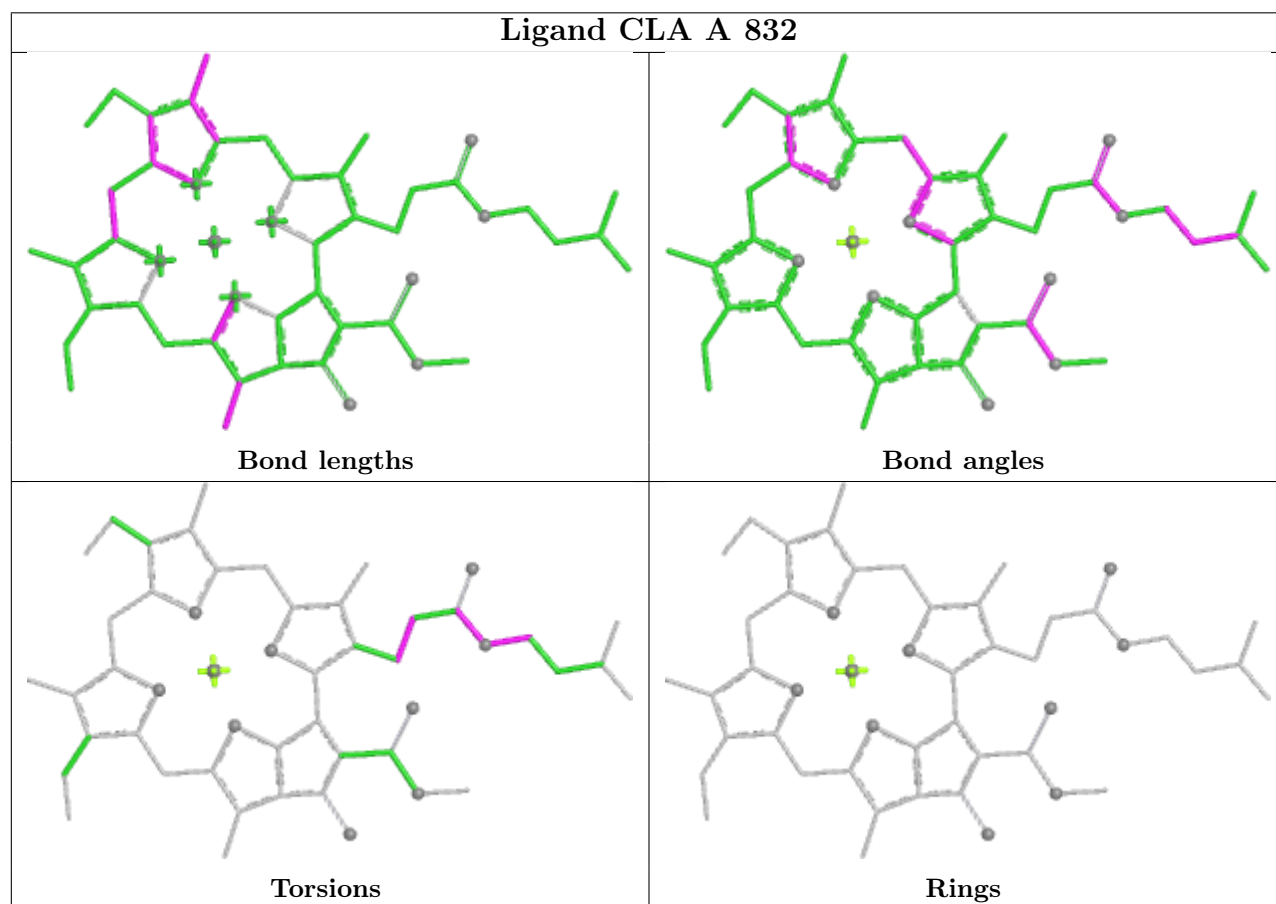
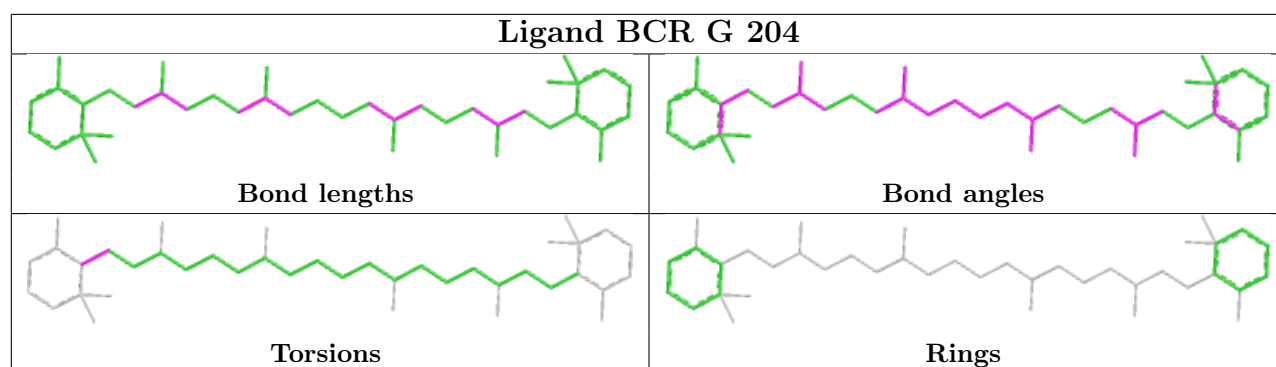


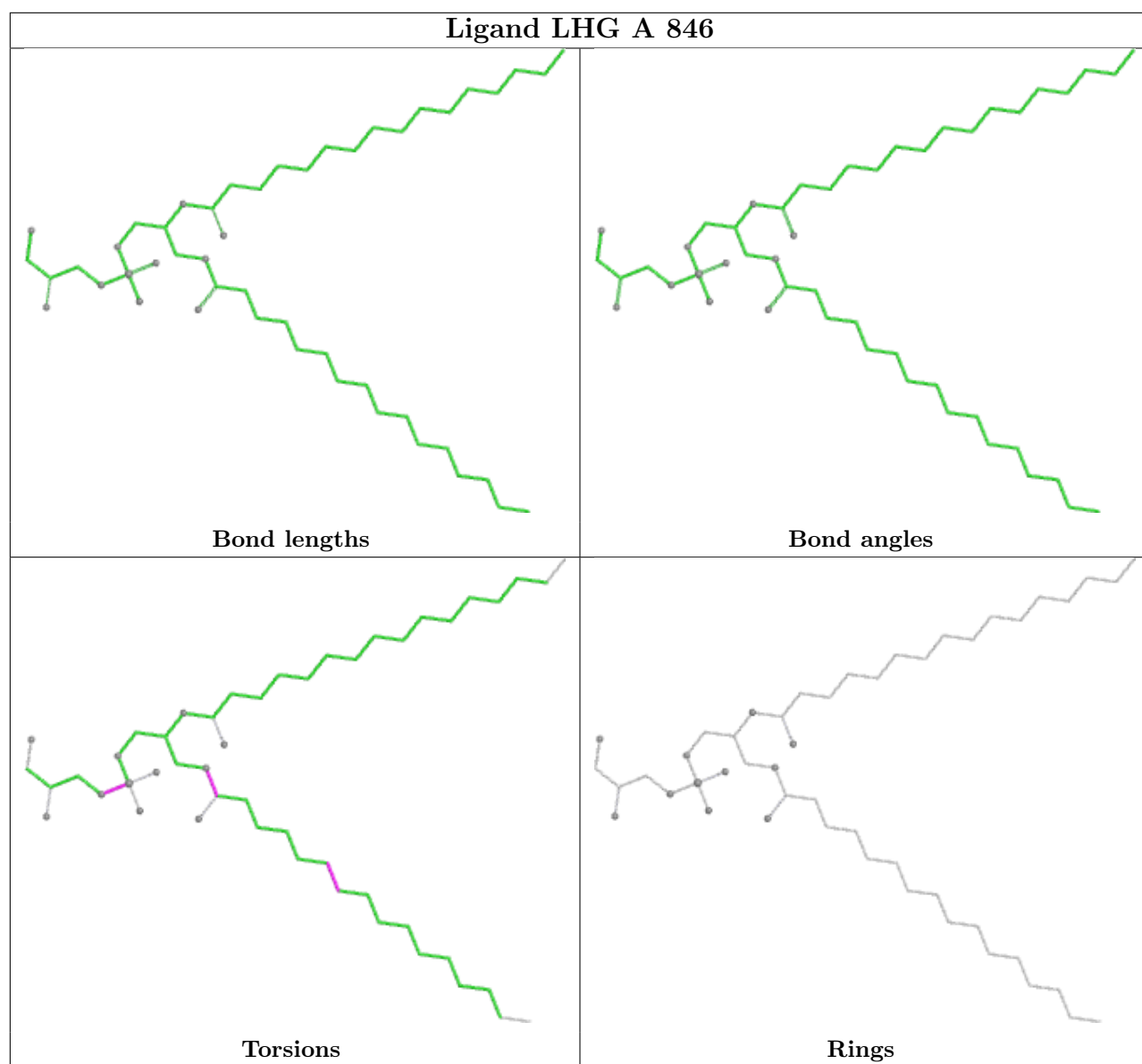
Ligand LHG 2 618



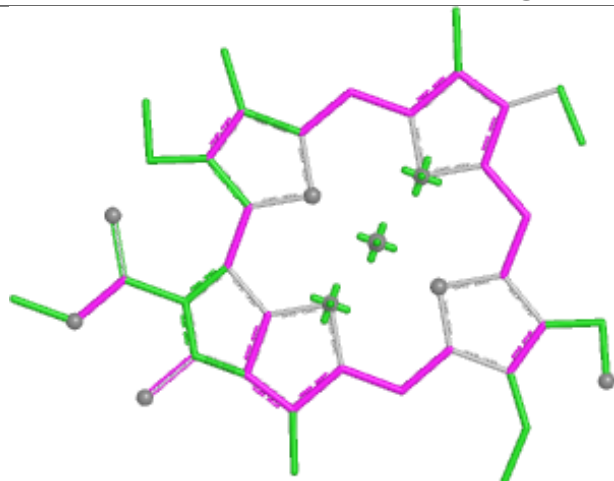
Ligand CL0 A 801



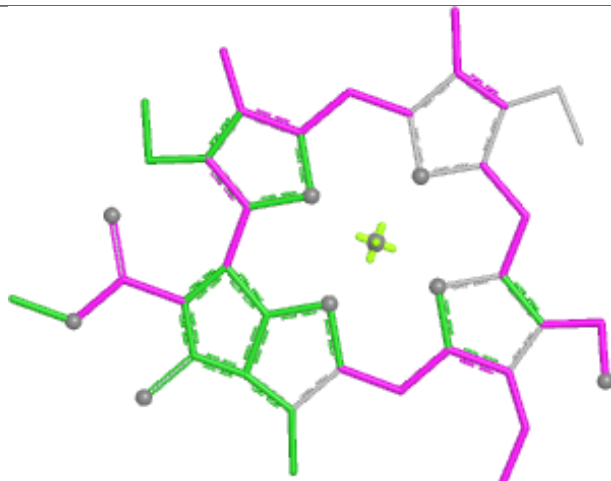




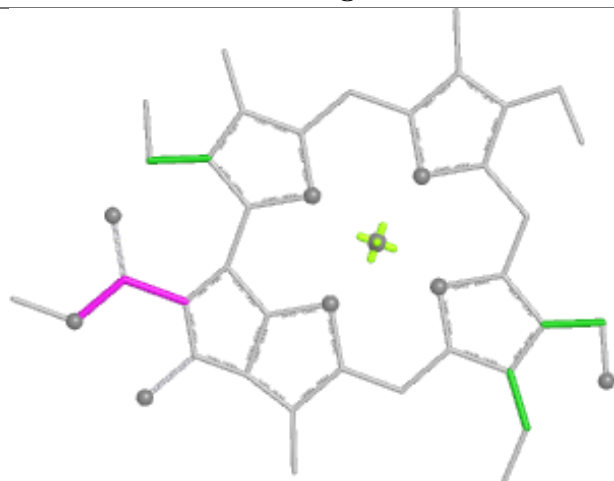
Ligand CHL 2 606



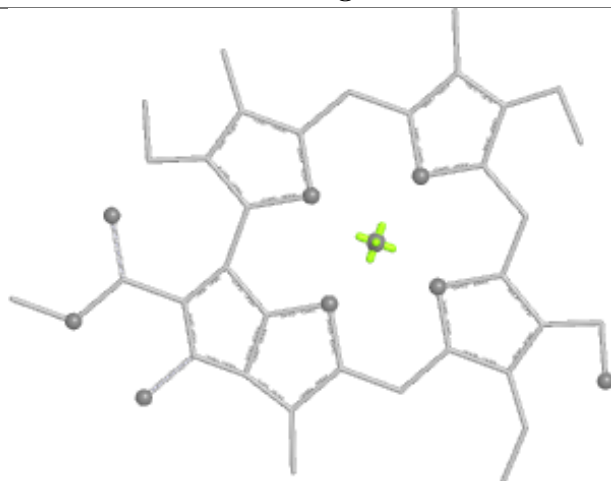
Bond lengths



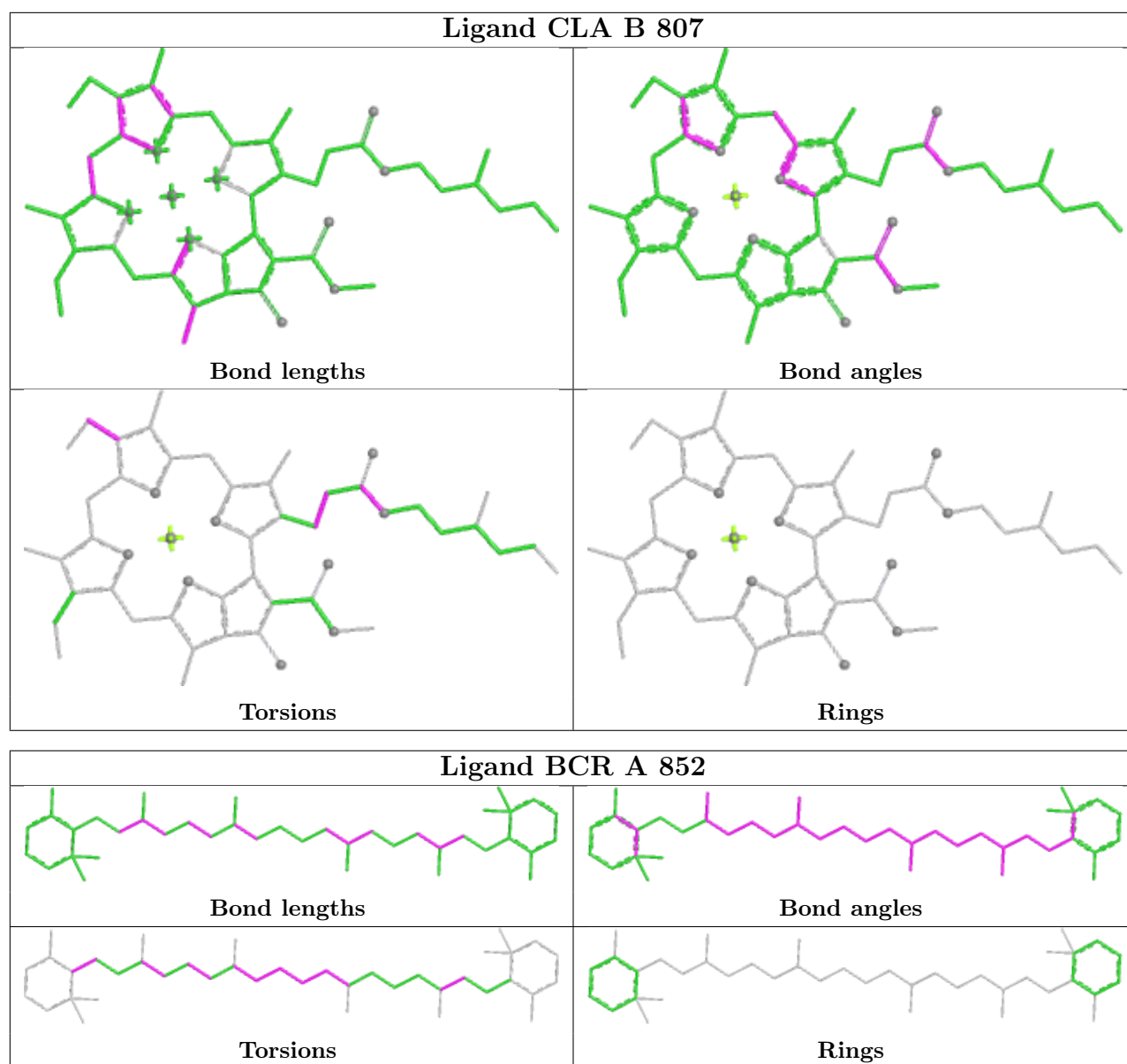
Bond angles



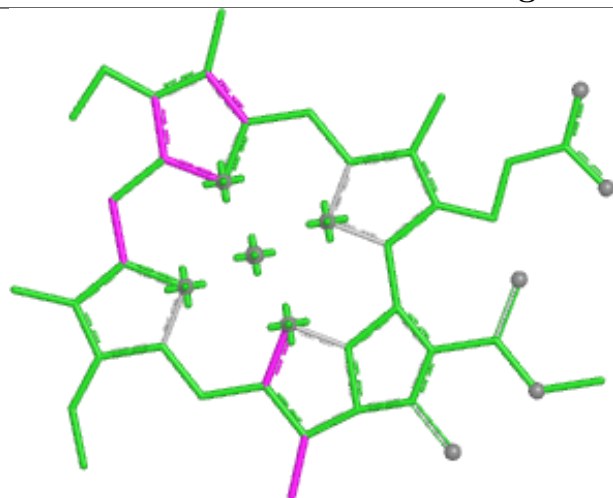
Torsions



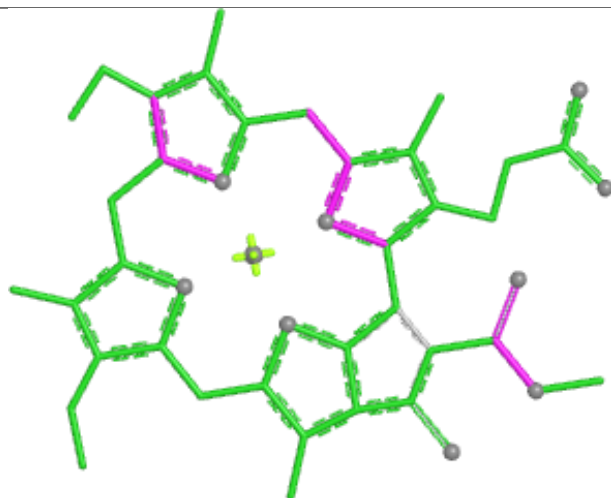
Rings



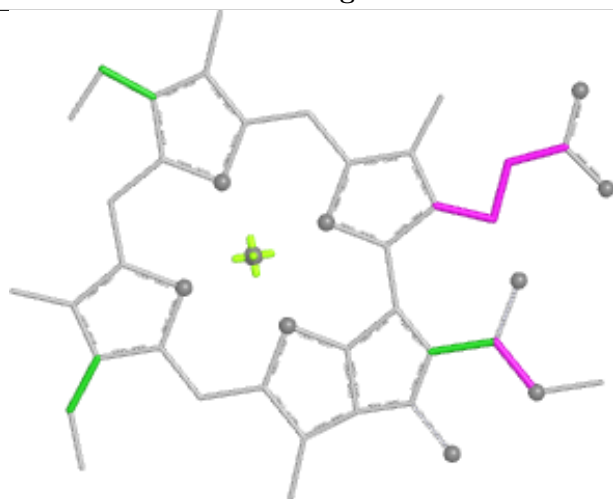
Ligand CLA 2 608



Bond lengths



Bond angles

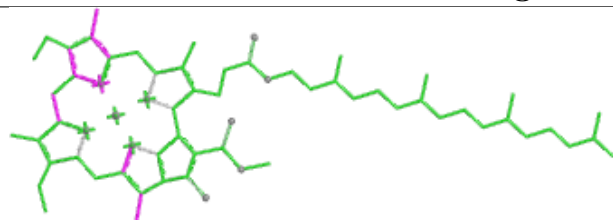


Torsions

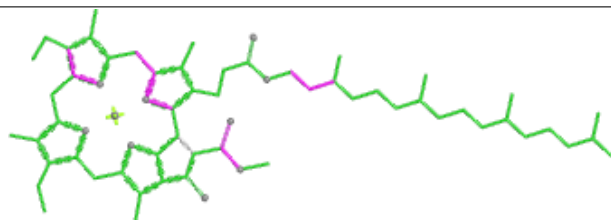


Rings

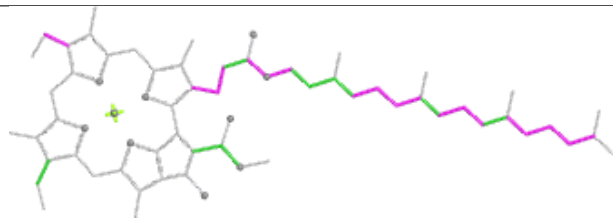
Ligand CLA A 812



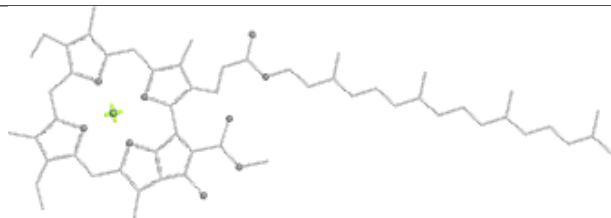
Bond lengths



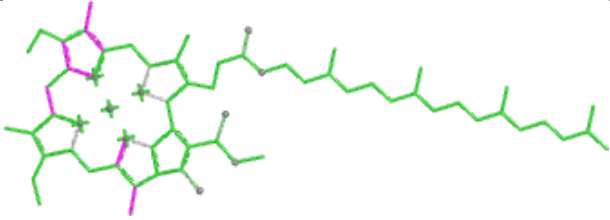
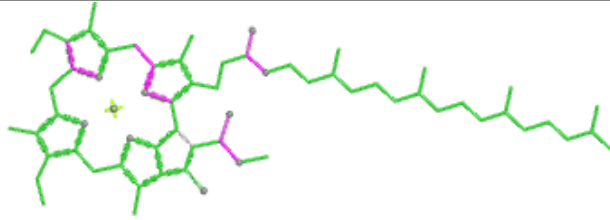
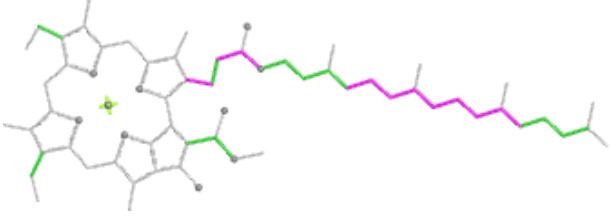
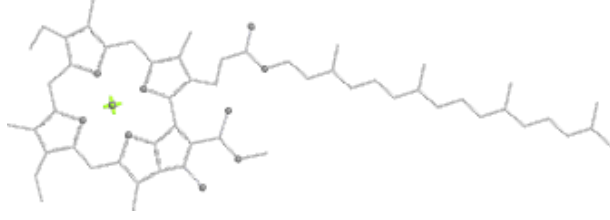
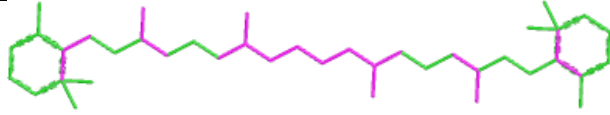
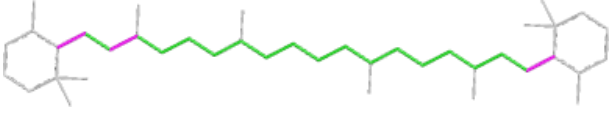
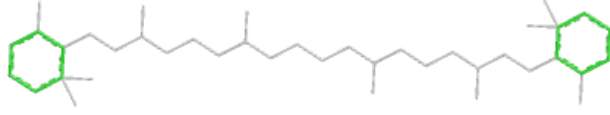
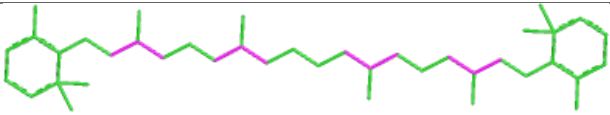
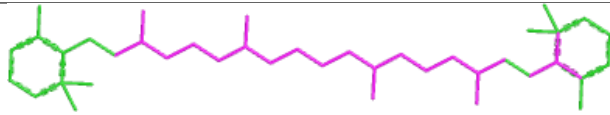
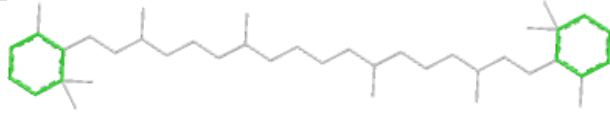
Bond angles



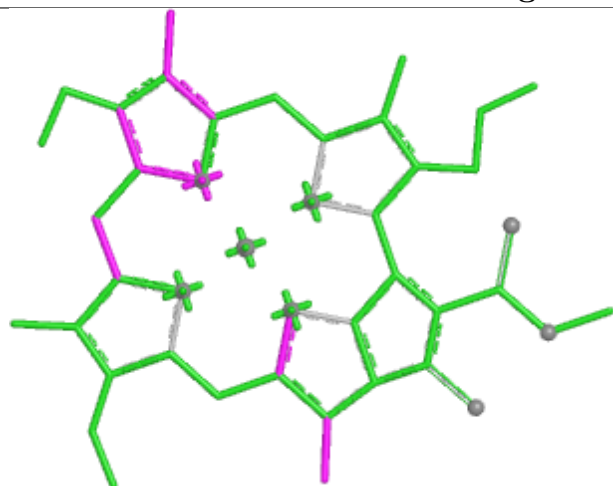
Torsions



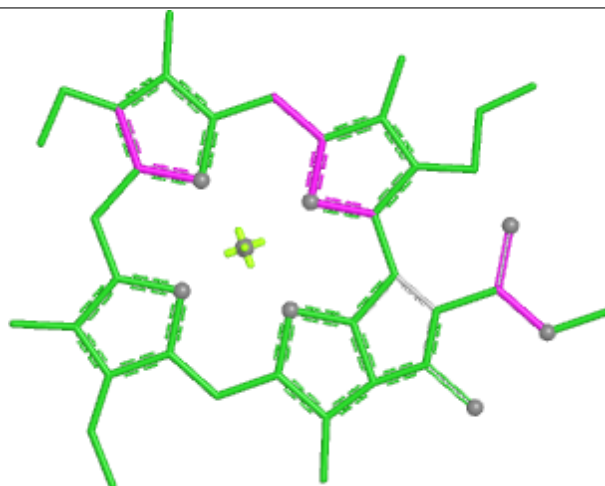
Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 4 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

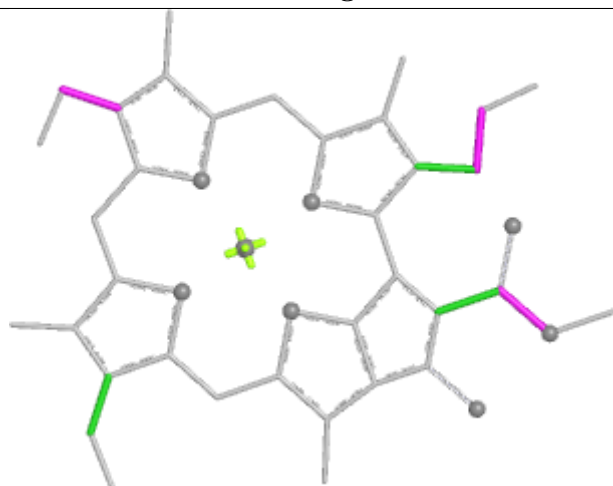
Ligand CLA 2 613



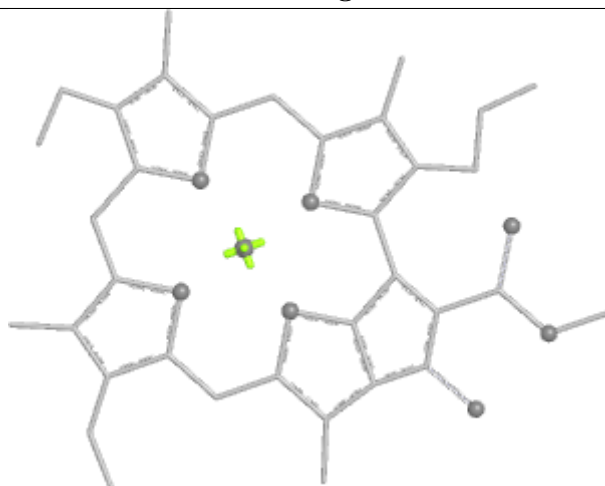
Bond lengths



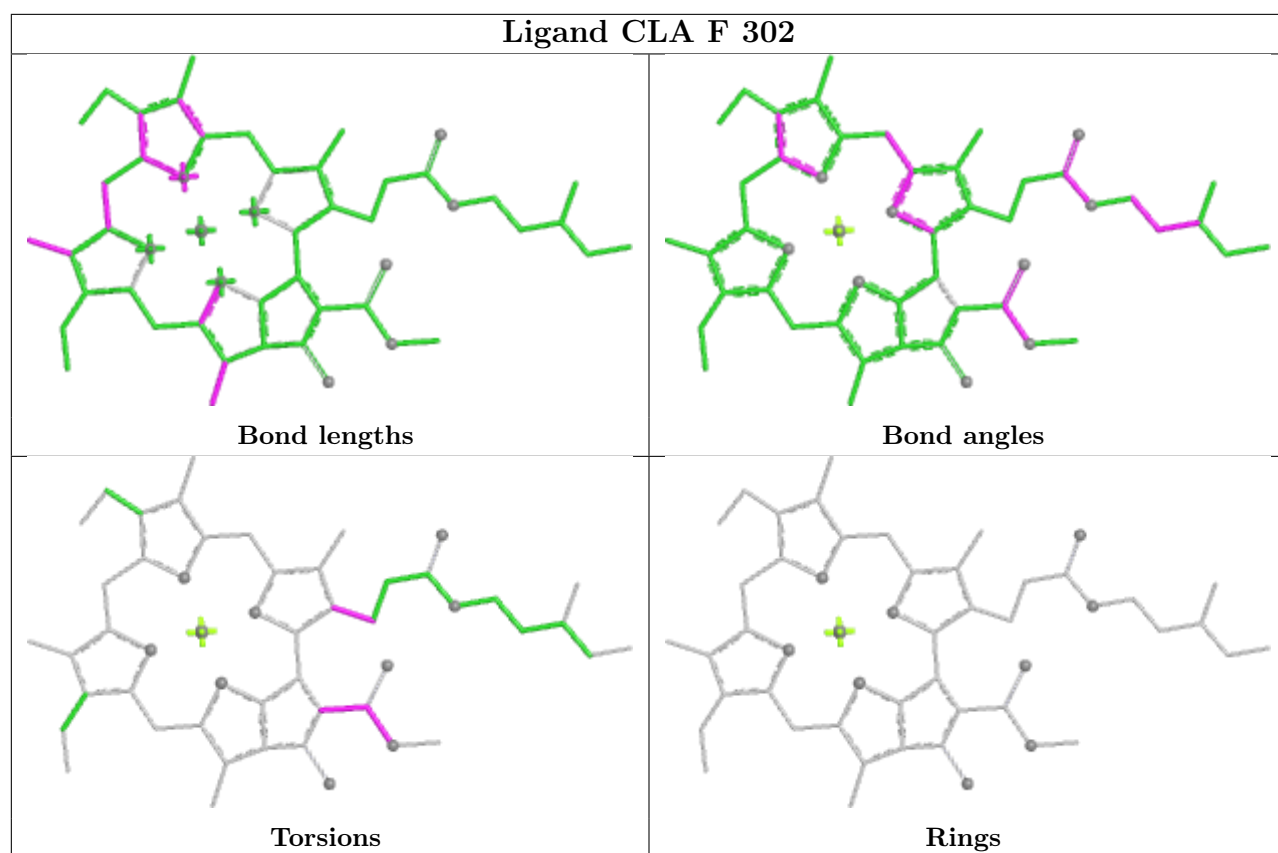
Bond angles



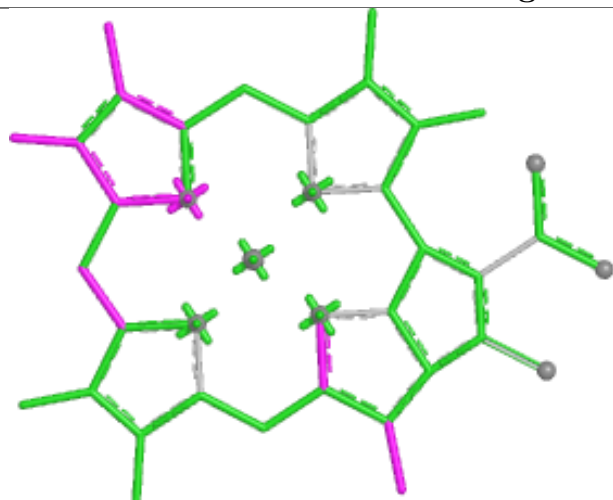
Torsions



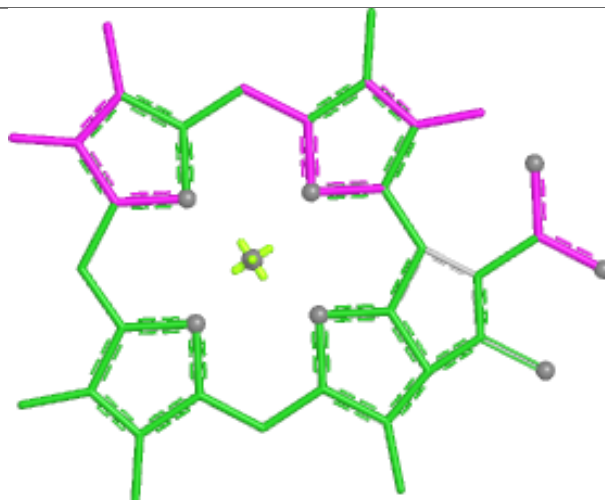
Rings



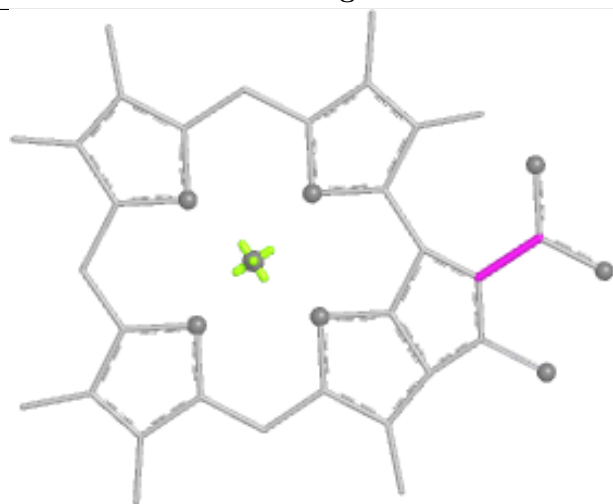
Ligand CLA 1 610



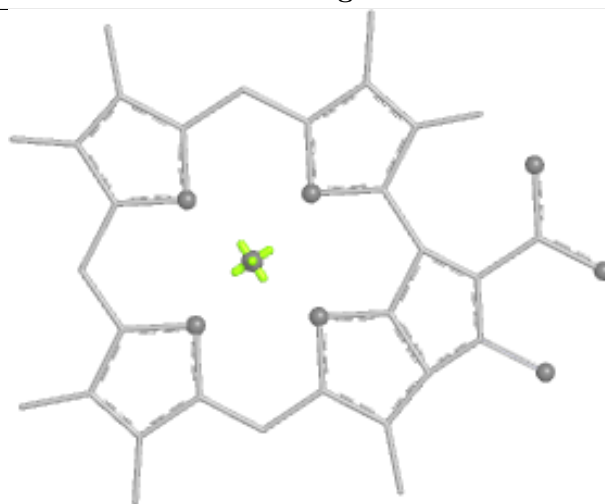
Bond lengths



Bond angles

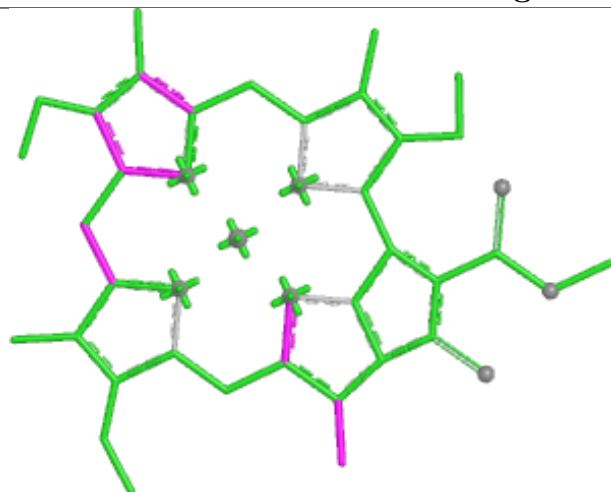


Torsions



Rings

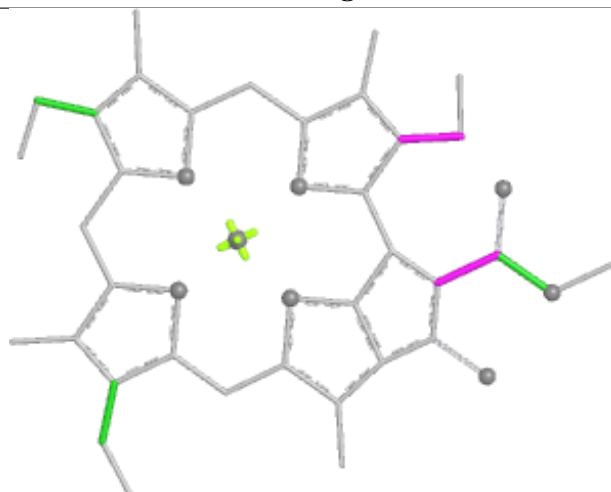
Ligand CLA A 823



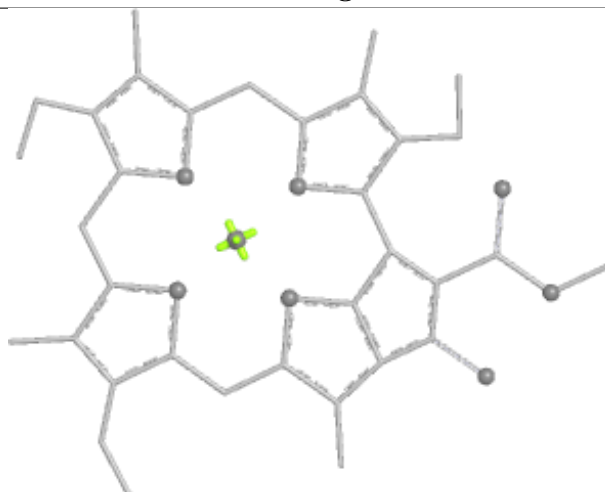
Bond lengths



Bond angles

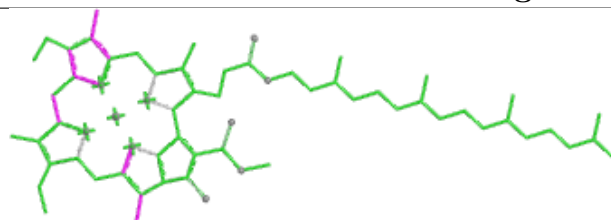


Torsions

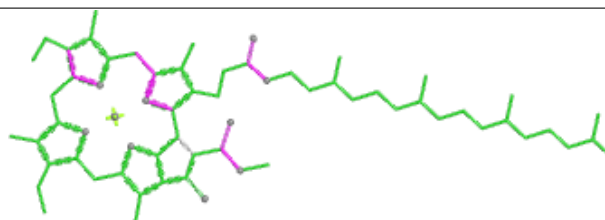


Rings

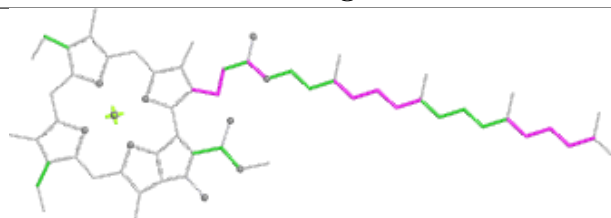
Ligand CLA B 828



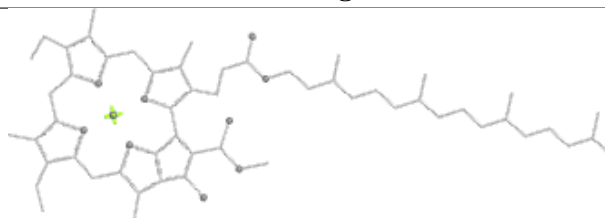
Bond lengths



Bond angles

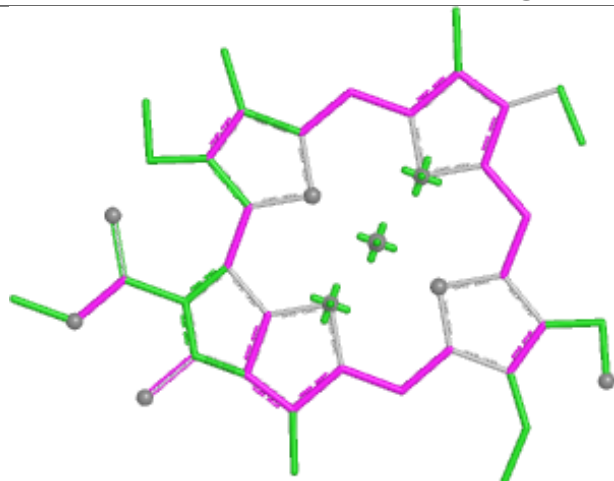


Torsions

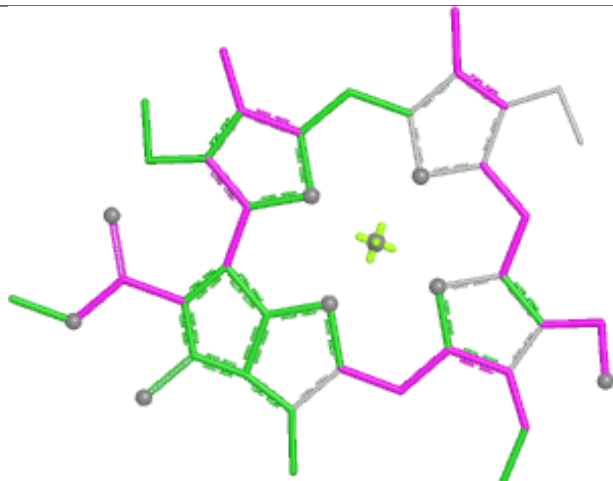


Rings

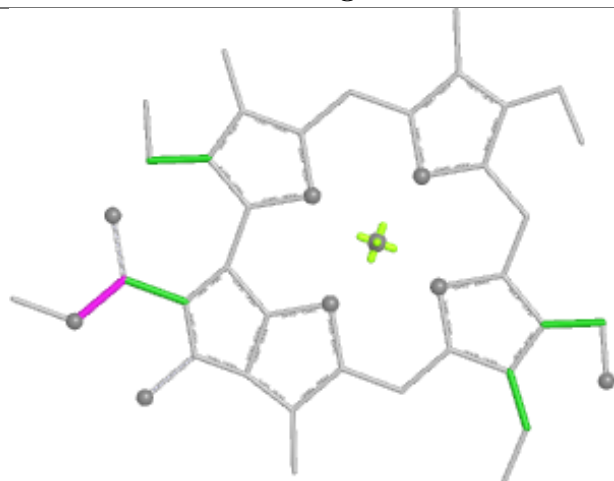
Ligand CHL 2 615



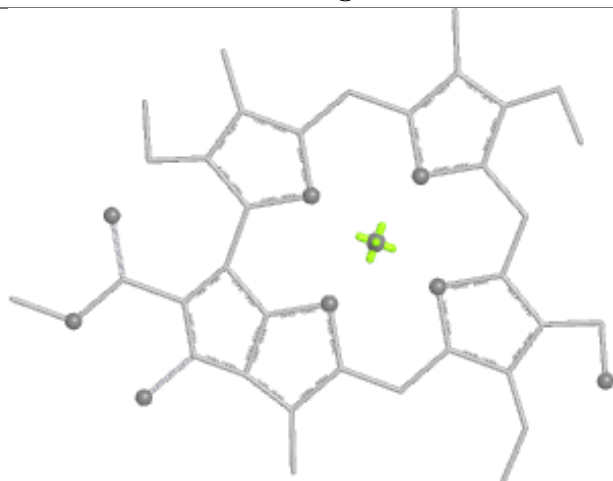
Bond lengths



Bond angles

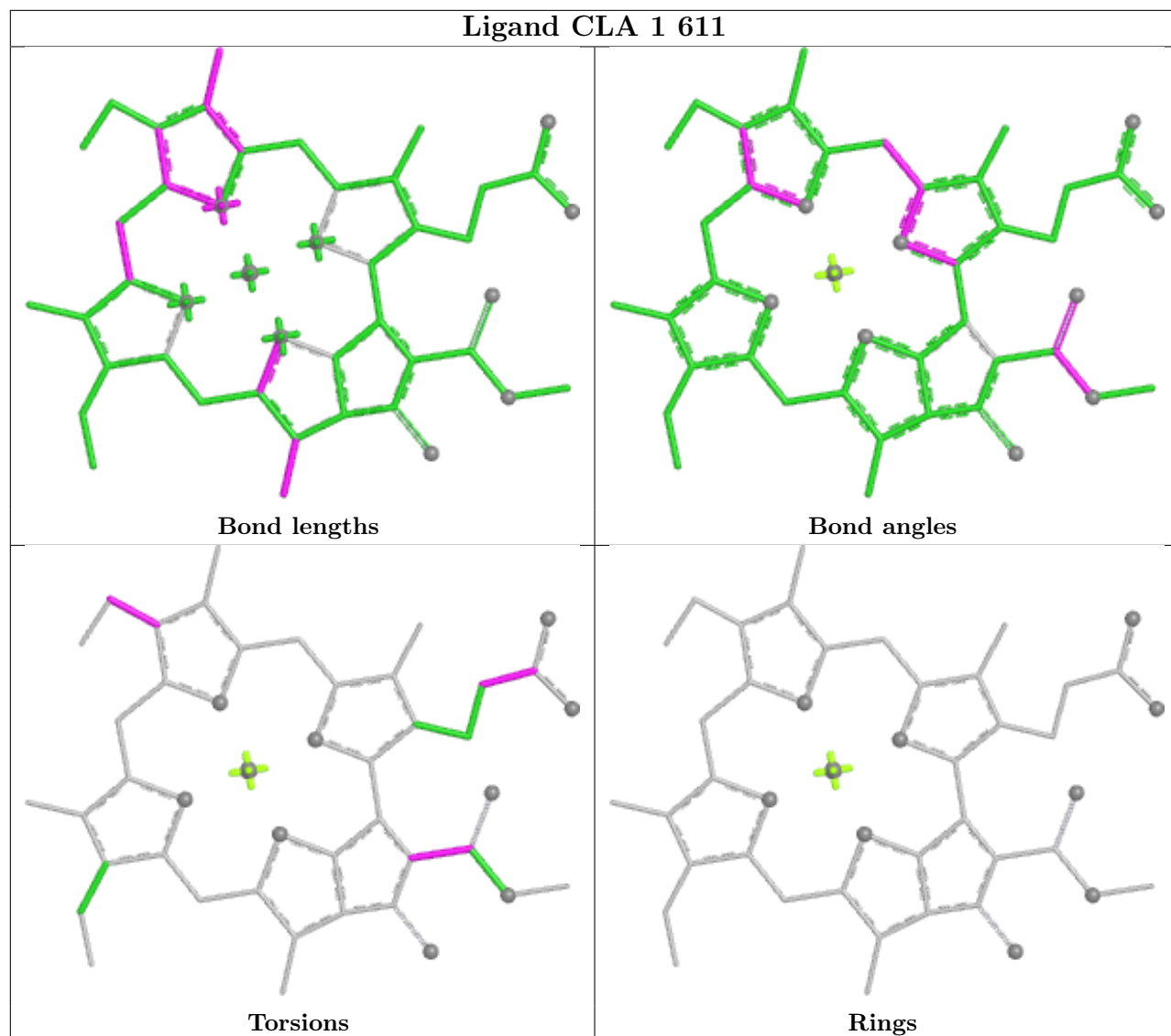


Torsions

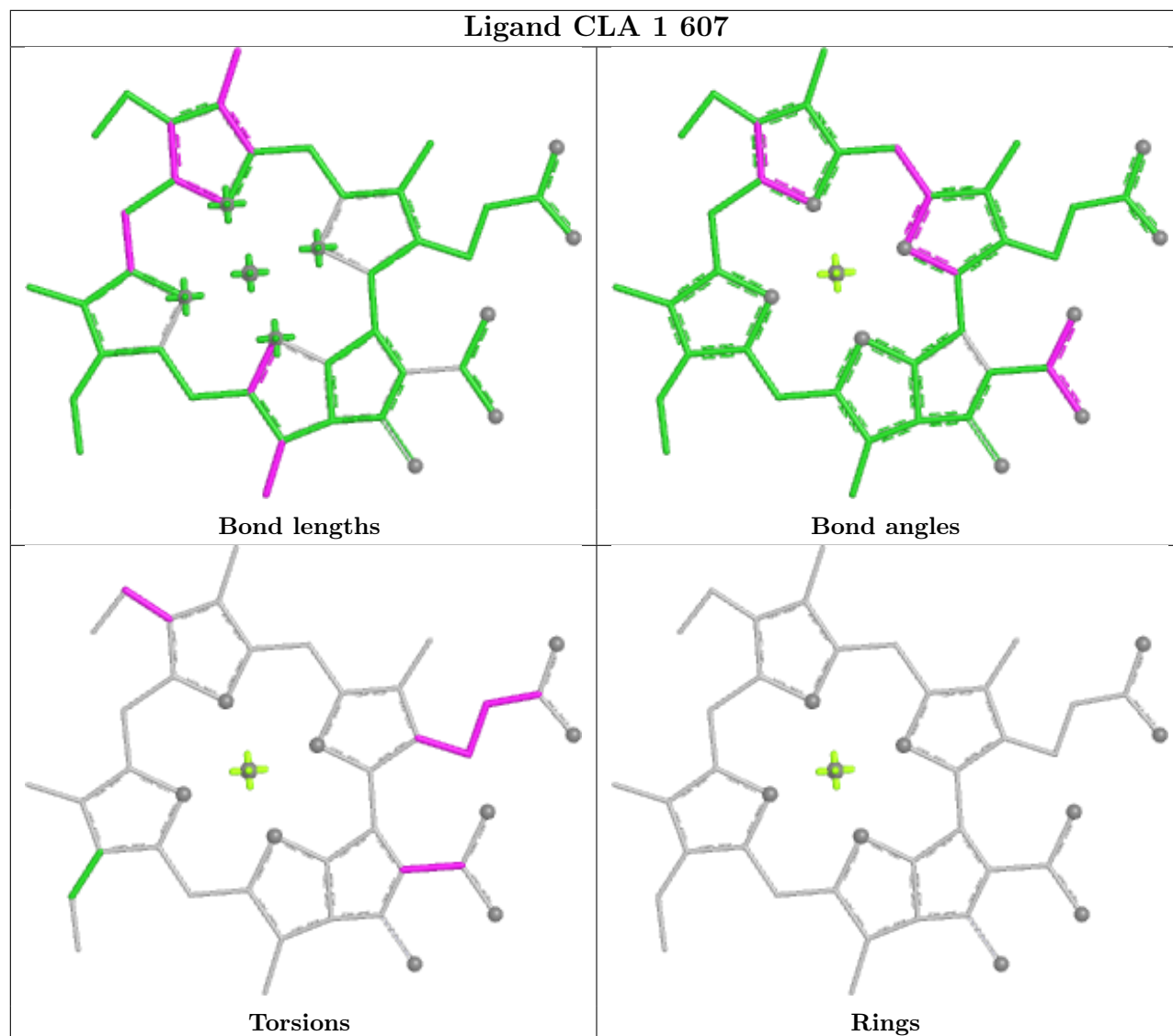


Rings

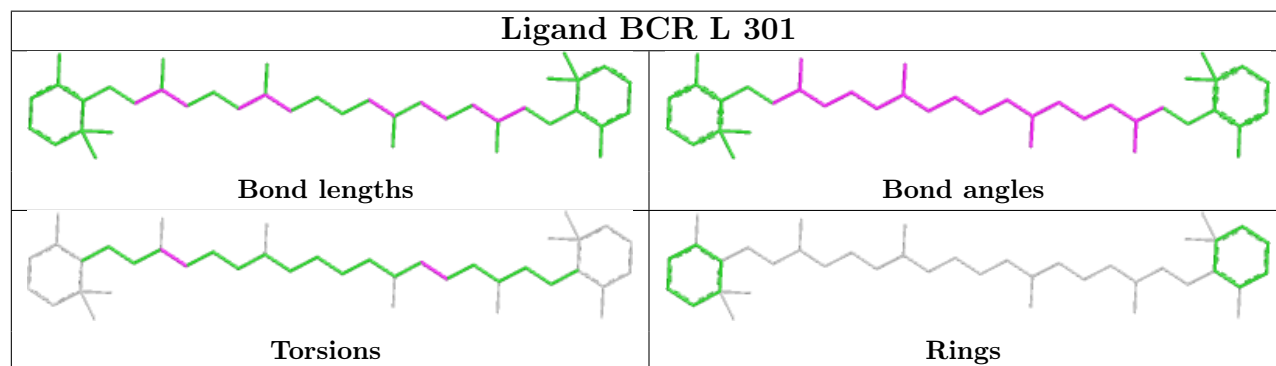
Ligand CLA 1 611



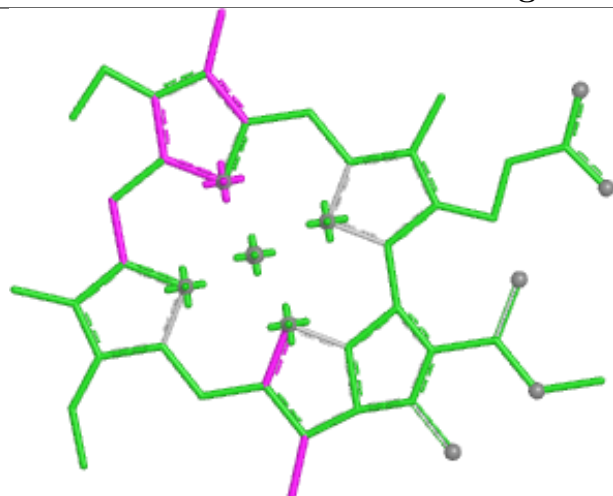
Ligand CLA 1 607



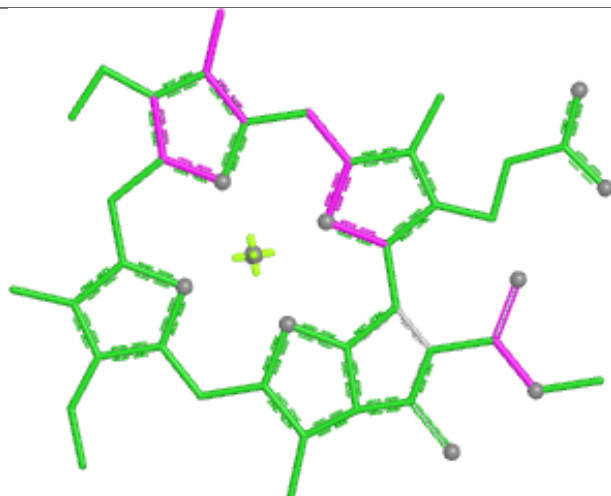
Ligand BCR L 301



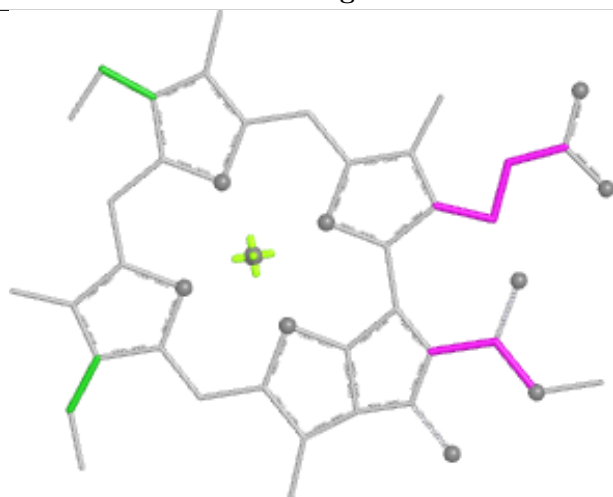
Ligand CLA 3 603



Bond lengths



Bond angles

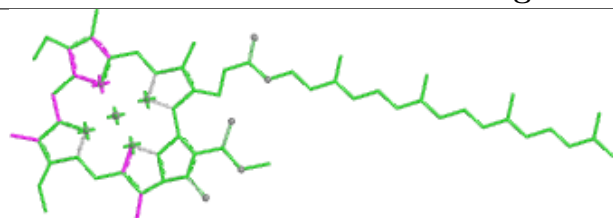


Torsions

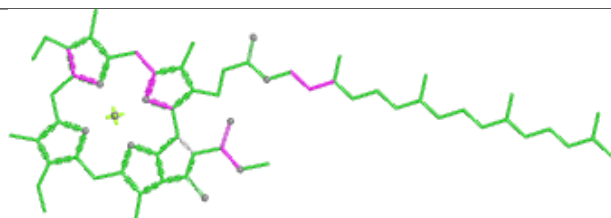


Rings

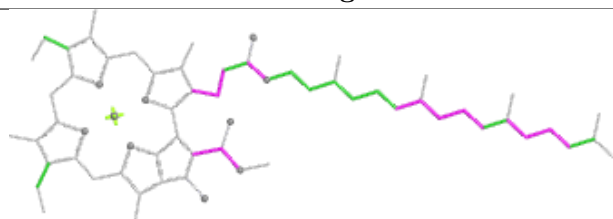
Ligand CLA A 806



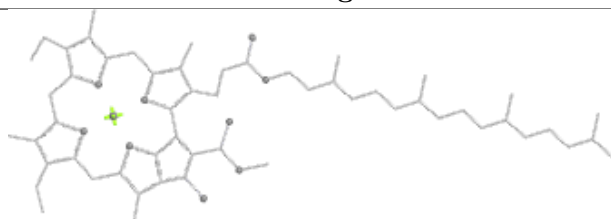
Bond lengths



Bond angles

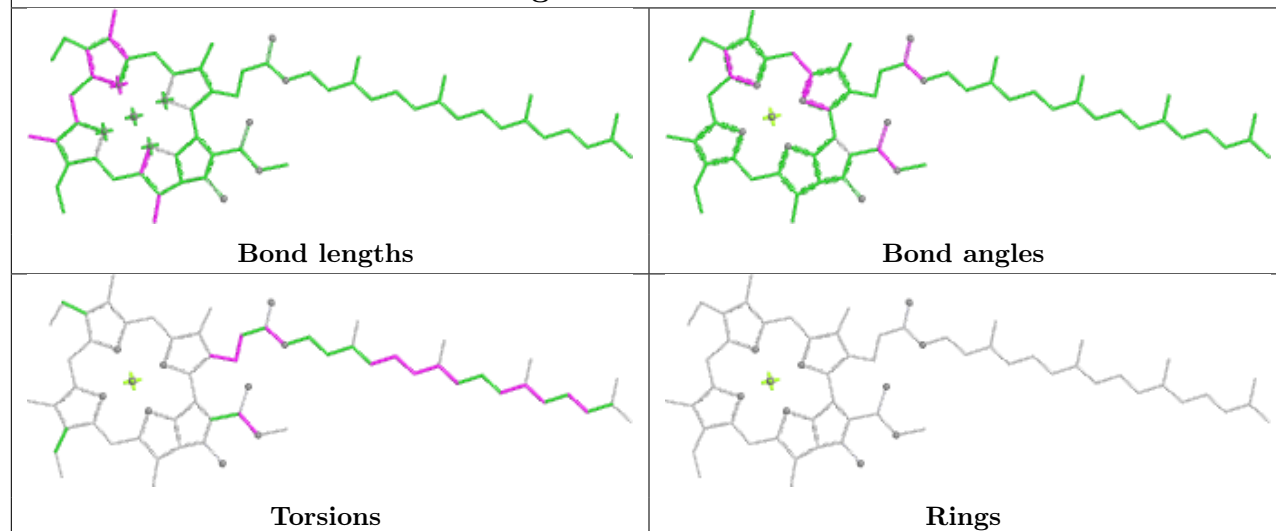


Torsions

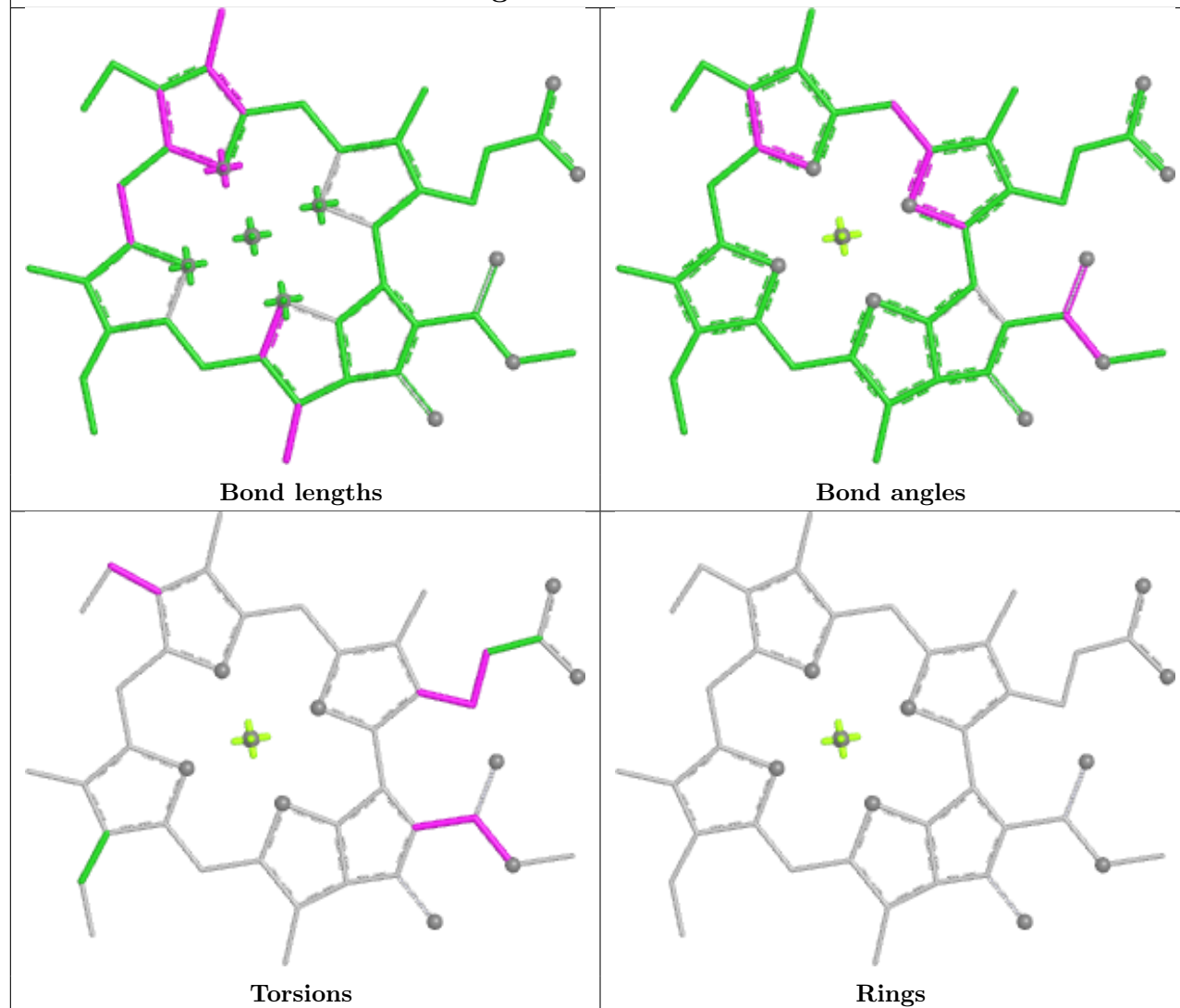


Rings

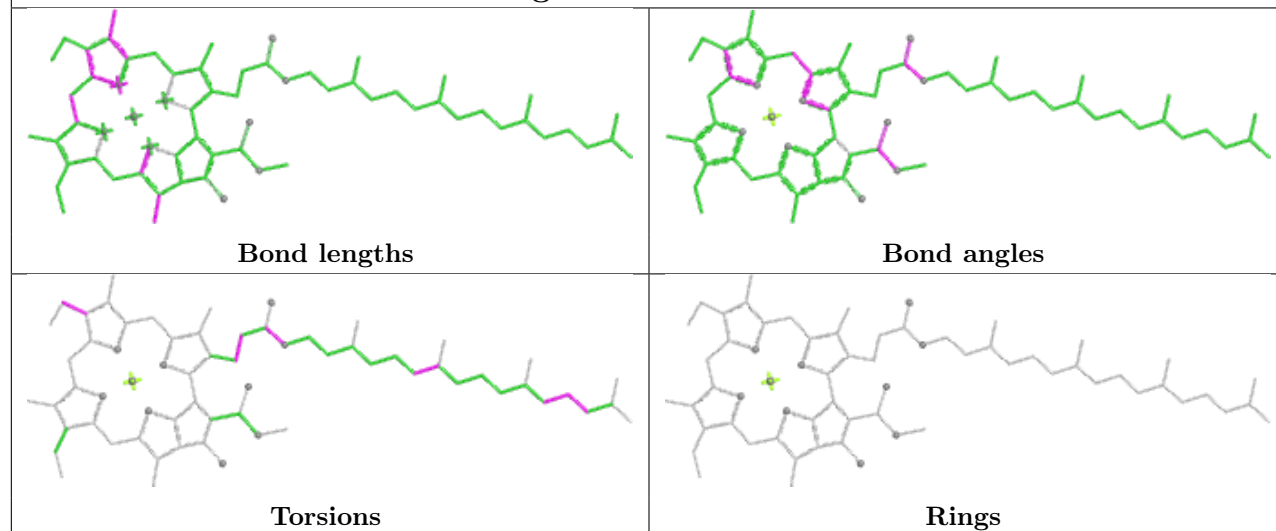
Ligand CLA A 802



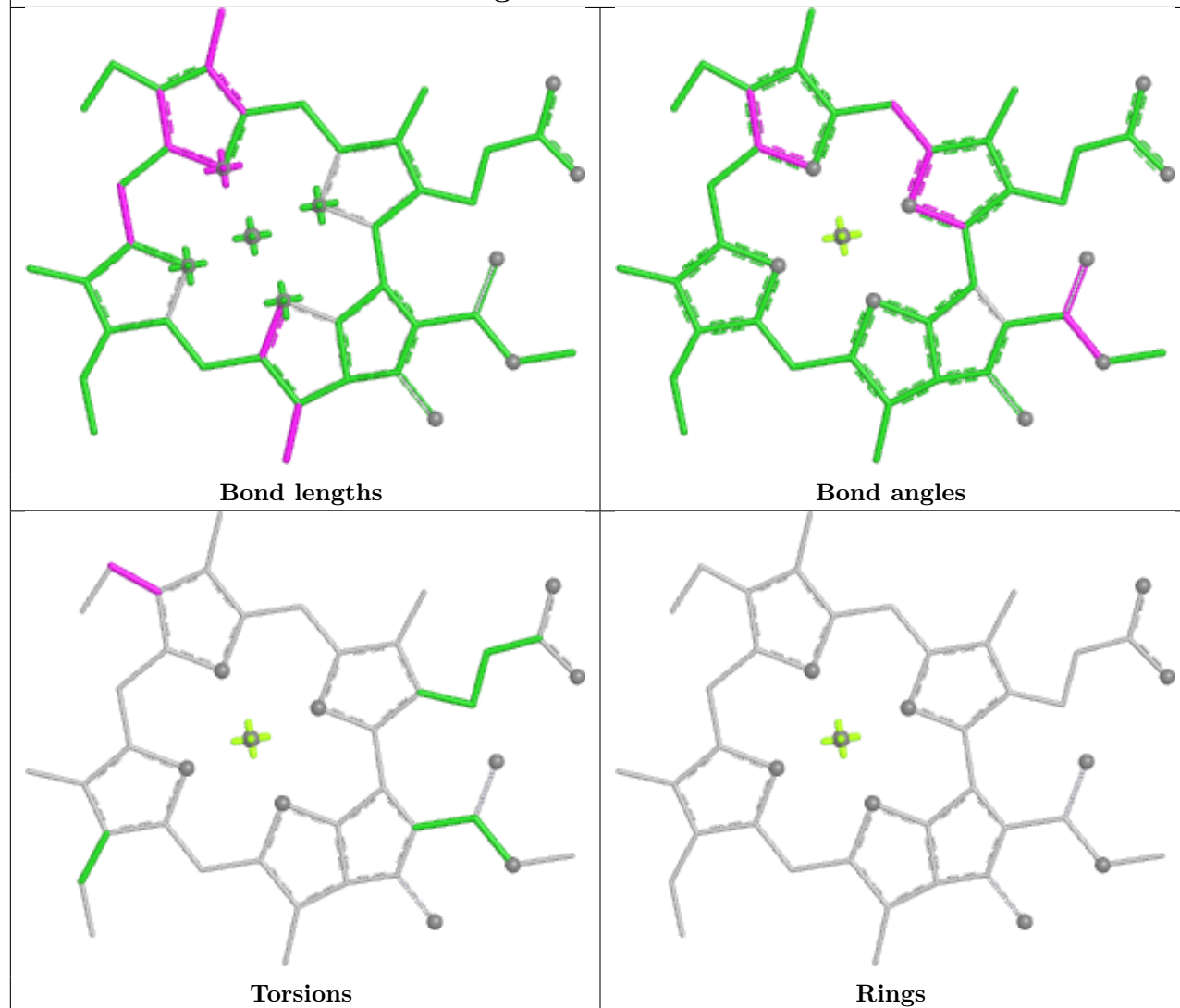
Ligand CLA A 836



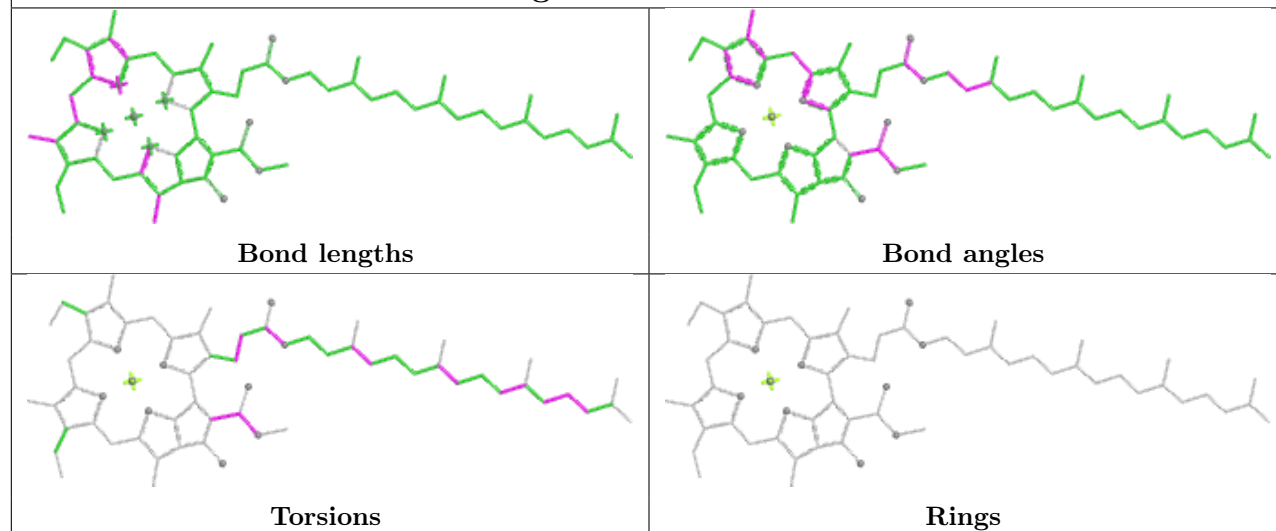
Ligand CLA B 839



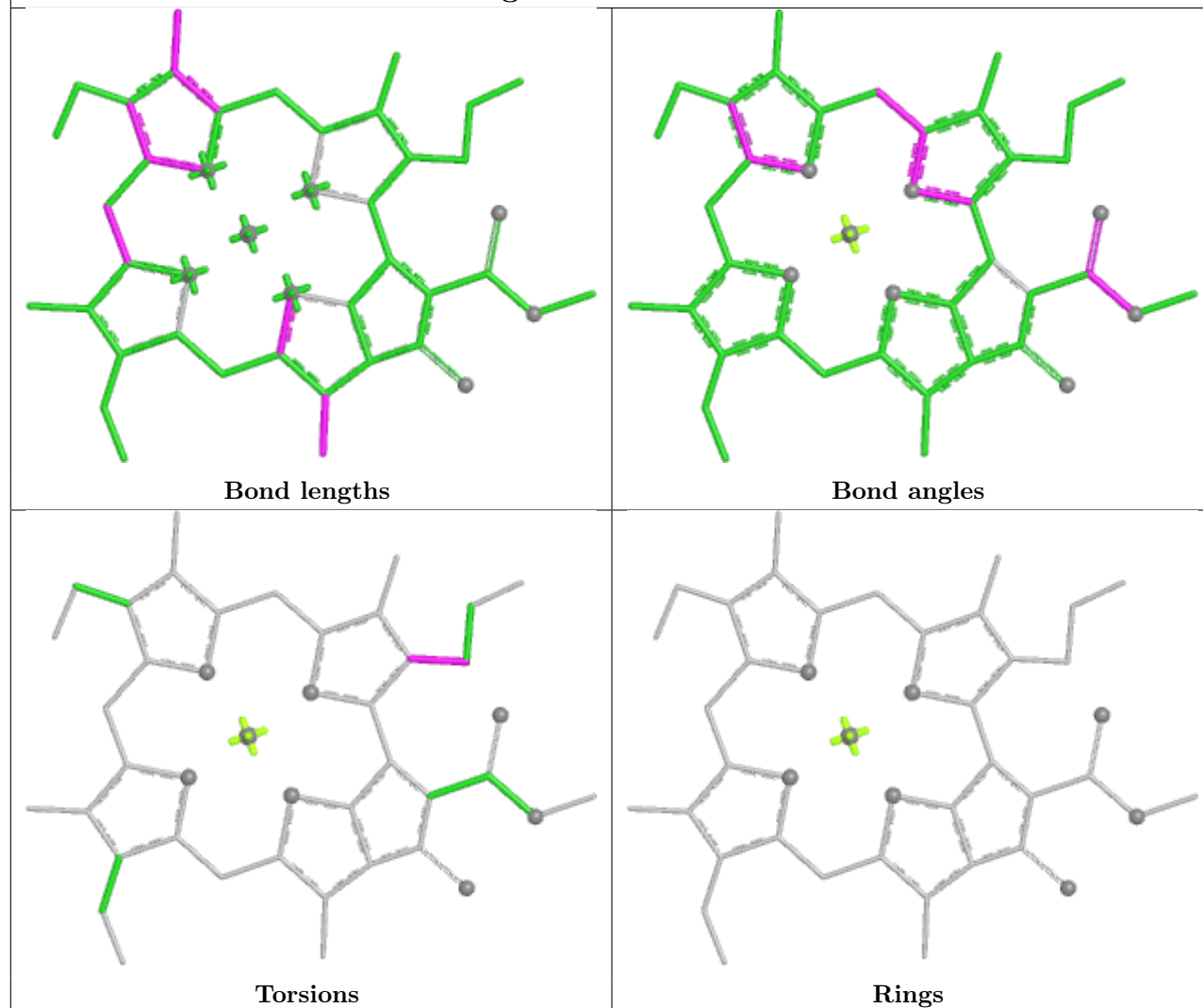
Ligand CLA L 302

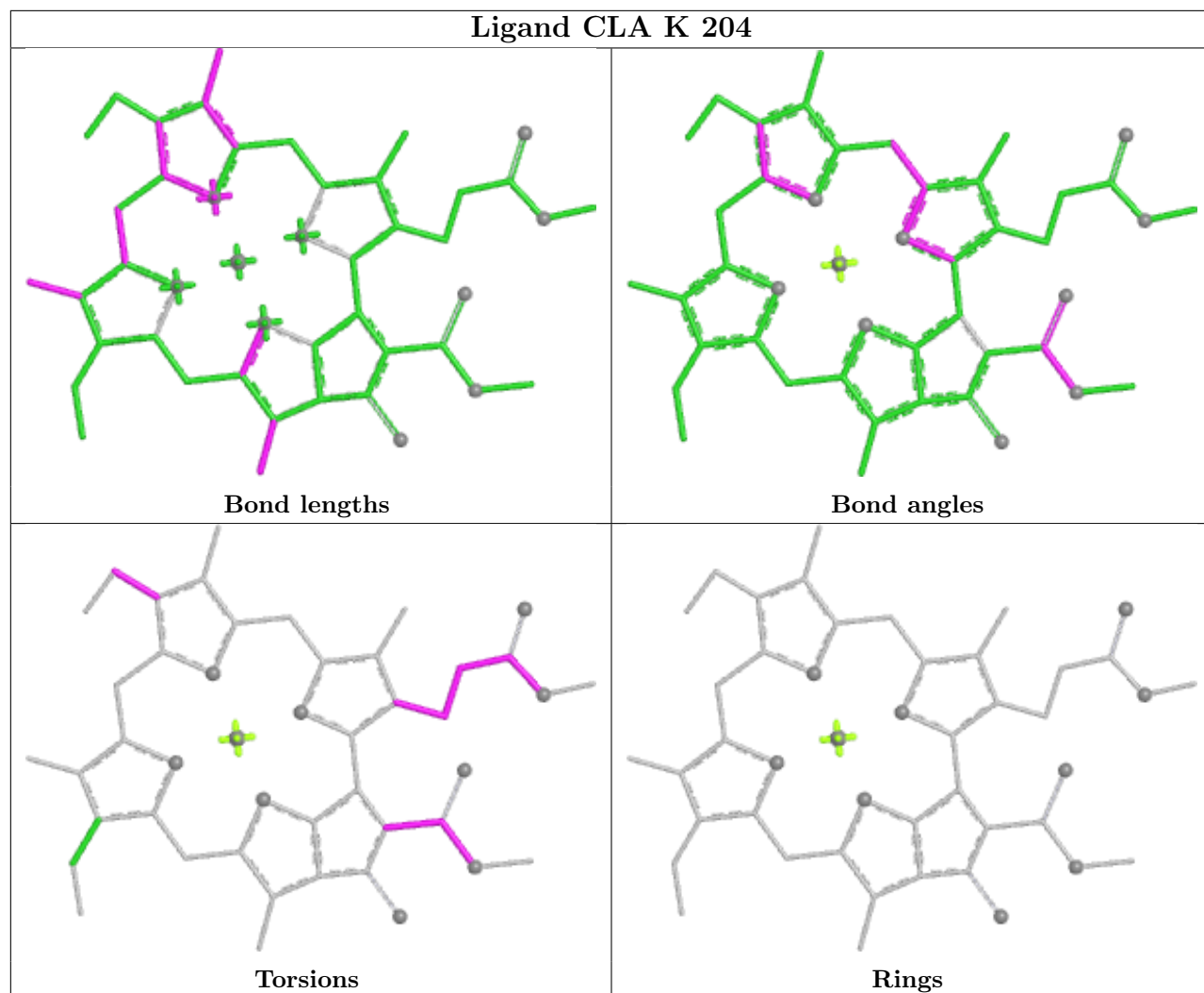


Ligand CLA B 813

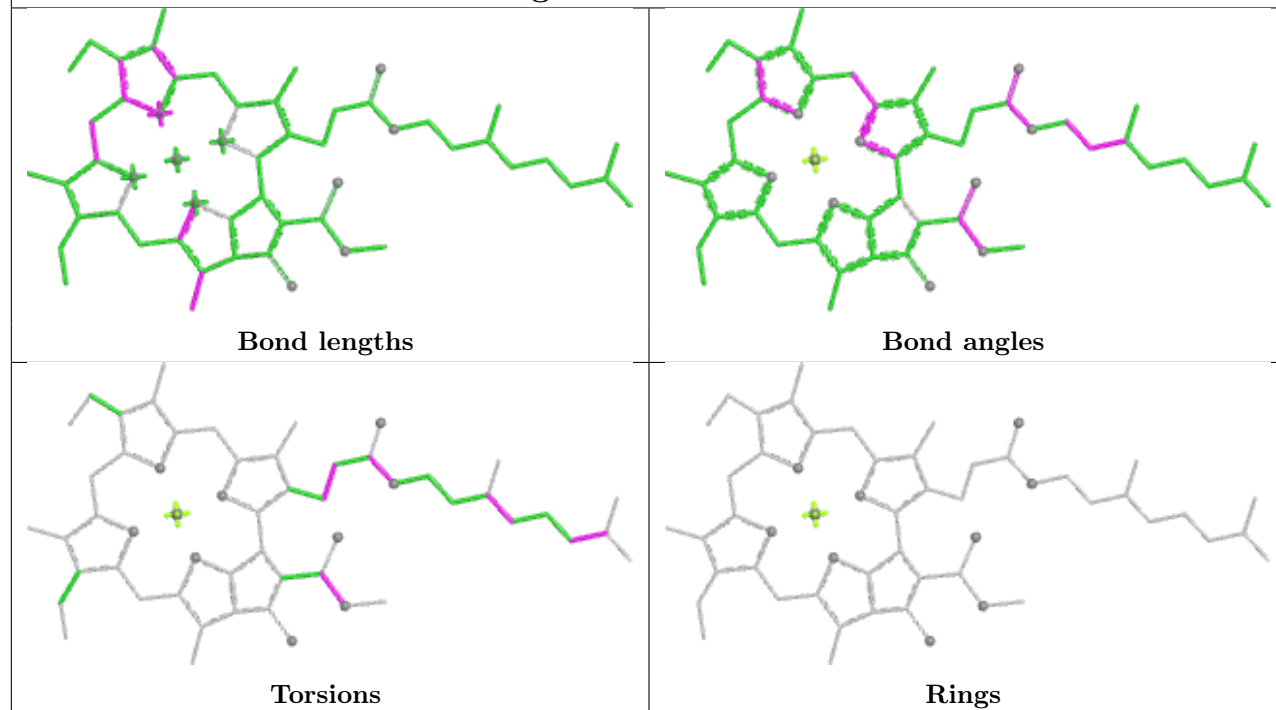


Ligand CLA B 815

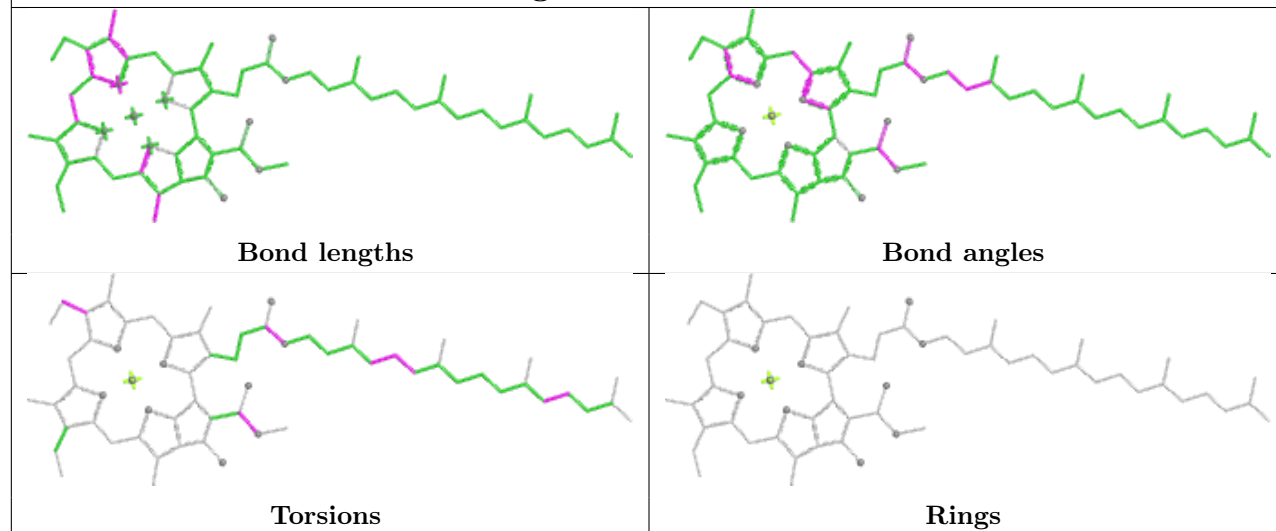




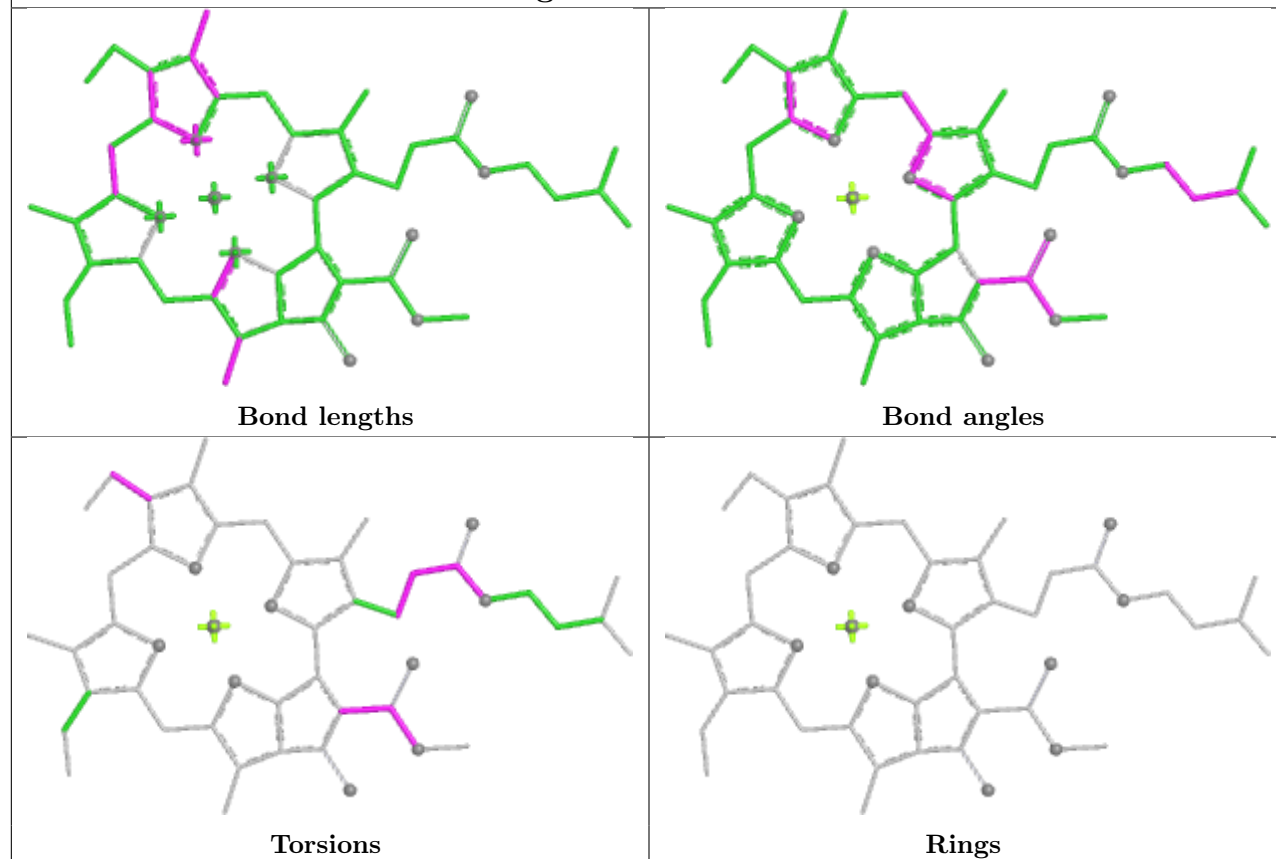
Ligand CLA A 839



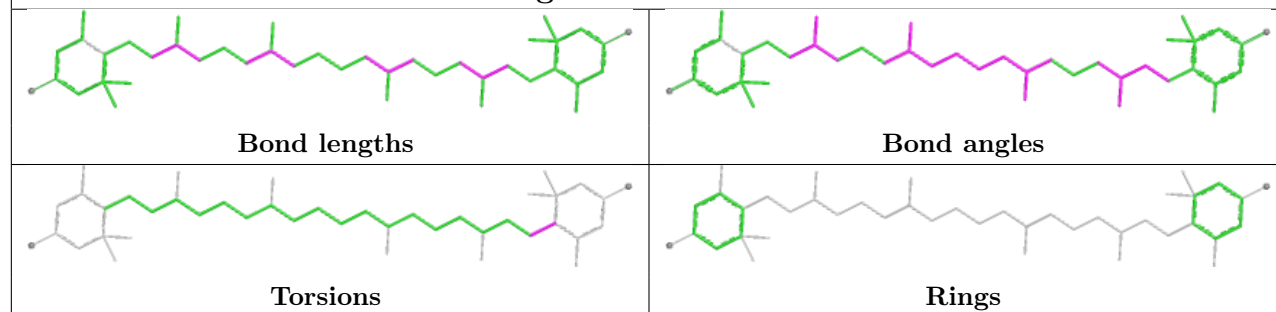
Ligand CLA A 834

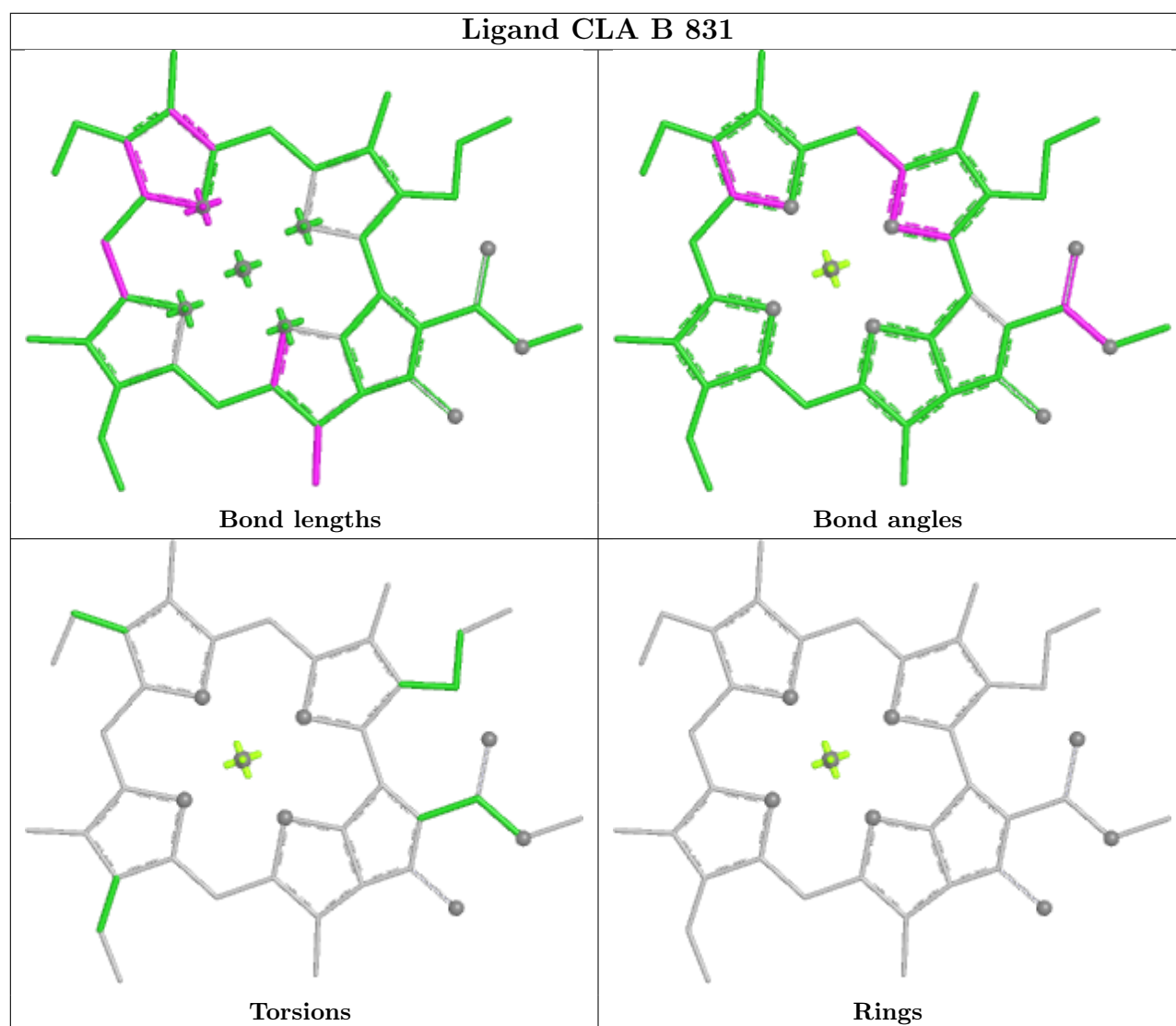


Ligand CLA 4 614



Ligand LUT 4 616





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.

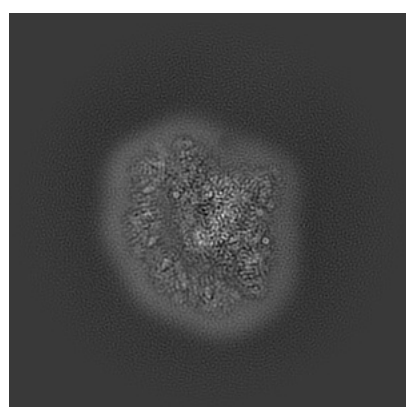
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36037. These allow visual inspection of the internal detail of the map and identification of artifacts.

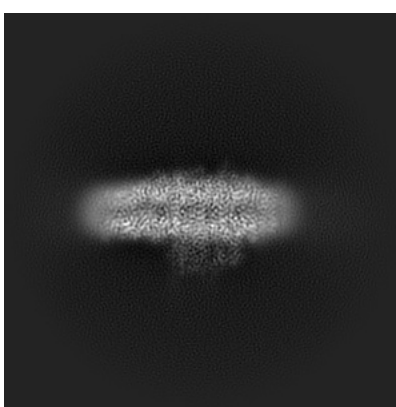
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

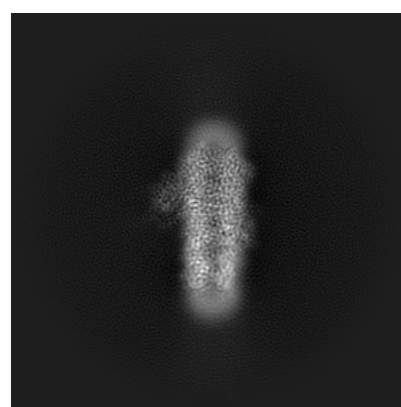
6.1.1 Primary map



X



Y

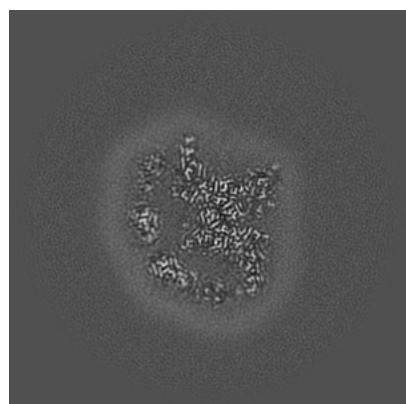


Z

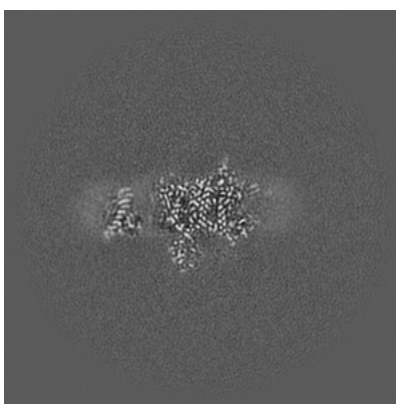
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

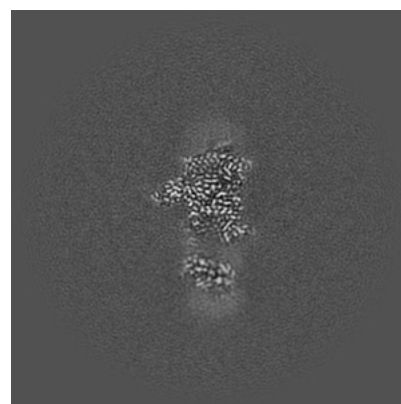
6.2.1 Primary map



X Index: 168



Y Index: 168

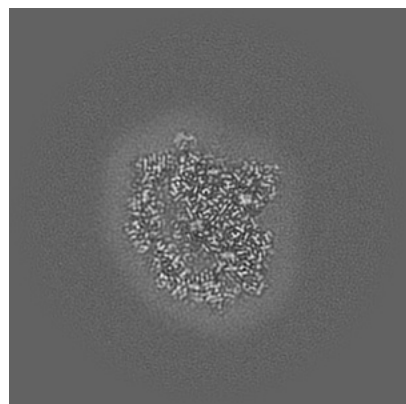


Z Index: 168

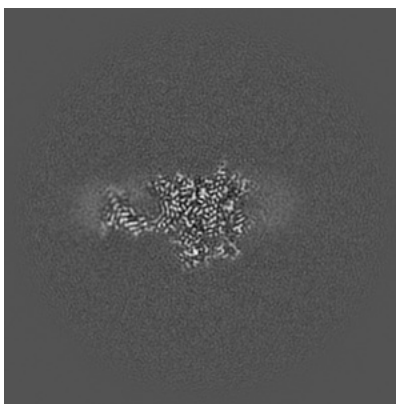
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

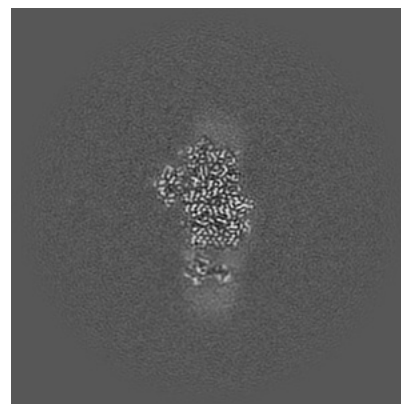
6.3.1 Primary map



X Index: 157



Y Index: 174

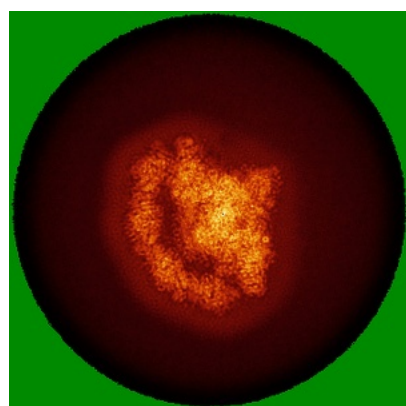


Z Index: 182

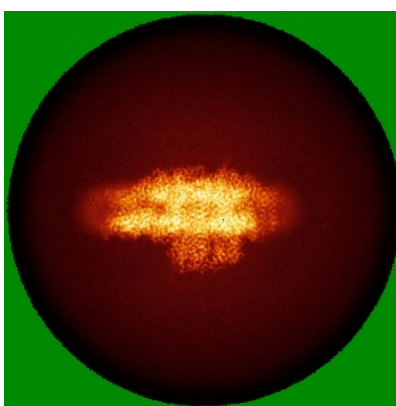
The images above show the largest variance slices of the map in three orthogonal directions.

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

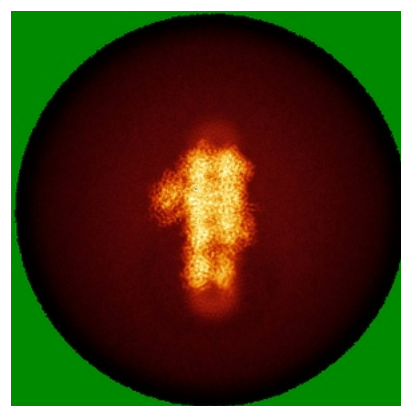
6.4.1 Primary map



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

This section was not generated.

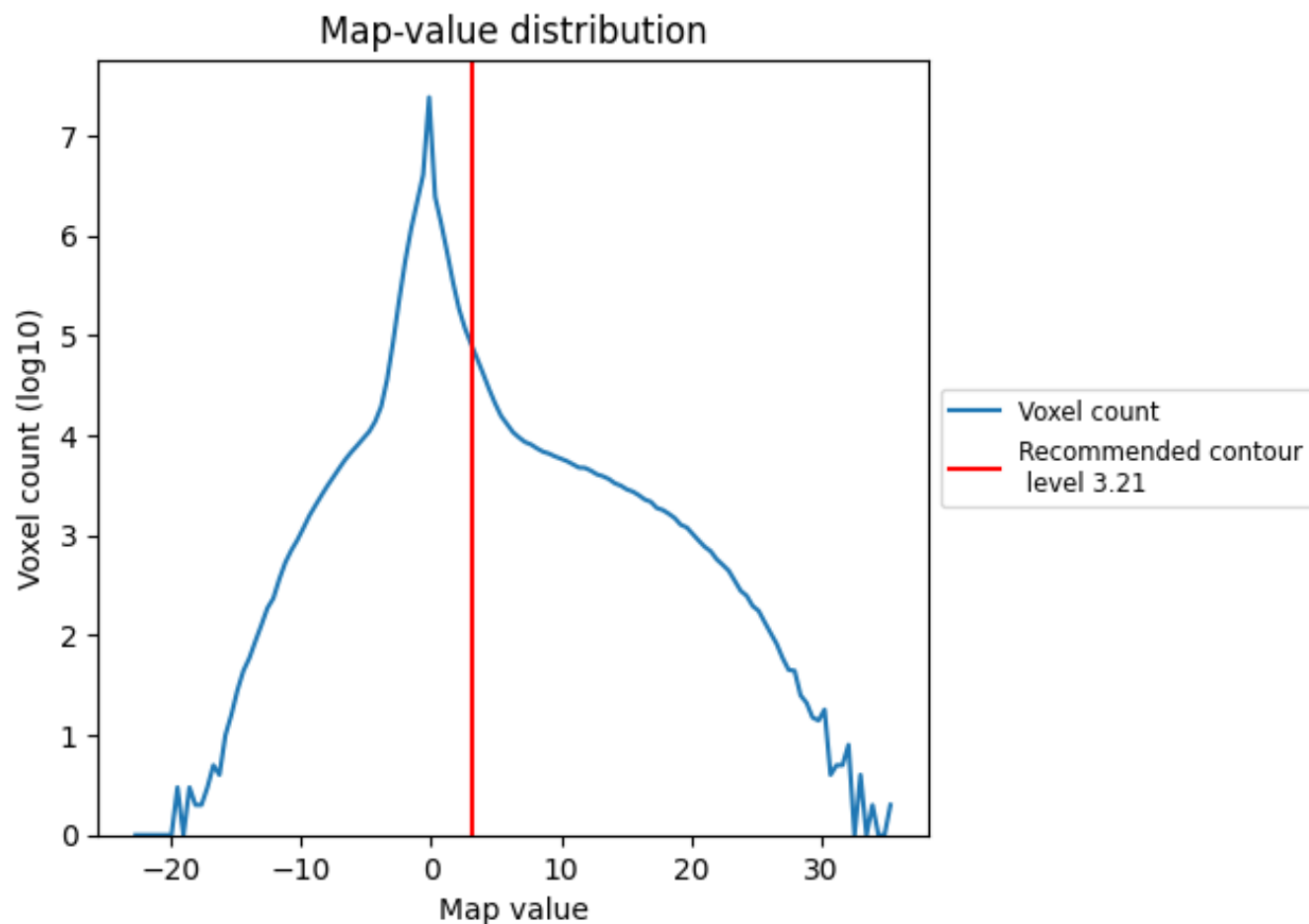
6.6 Mask visualisation

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

7 Map analysis [i](#)

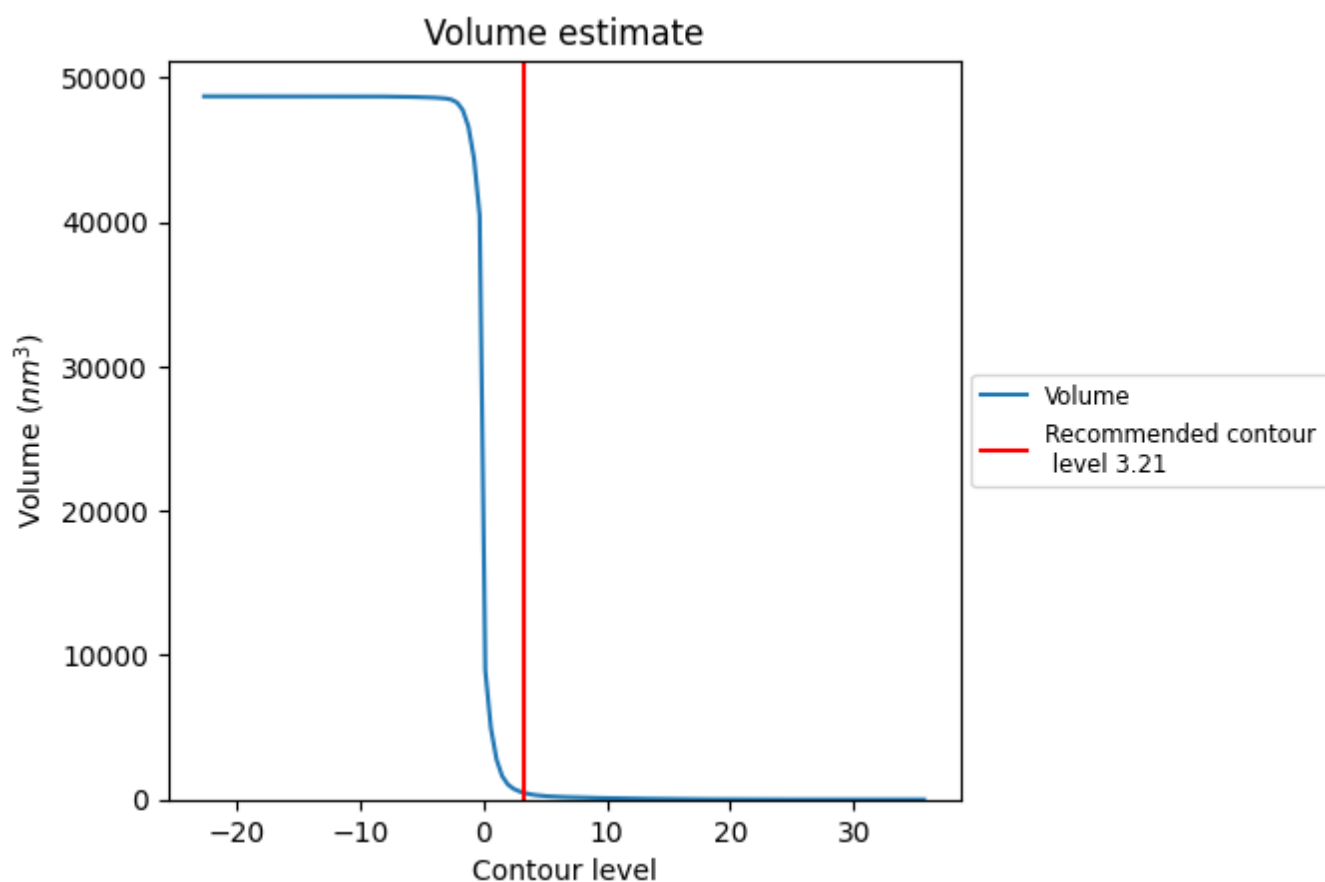
This section contains the results of statistical analysis of the map.

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.

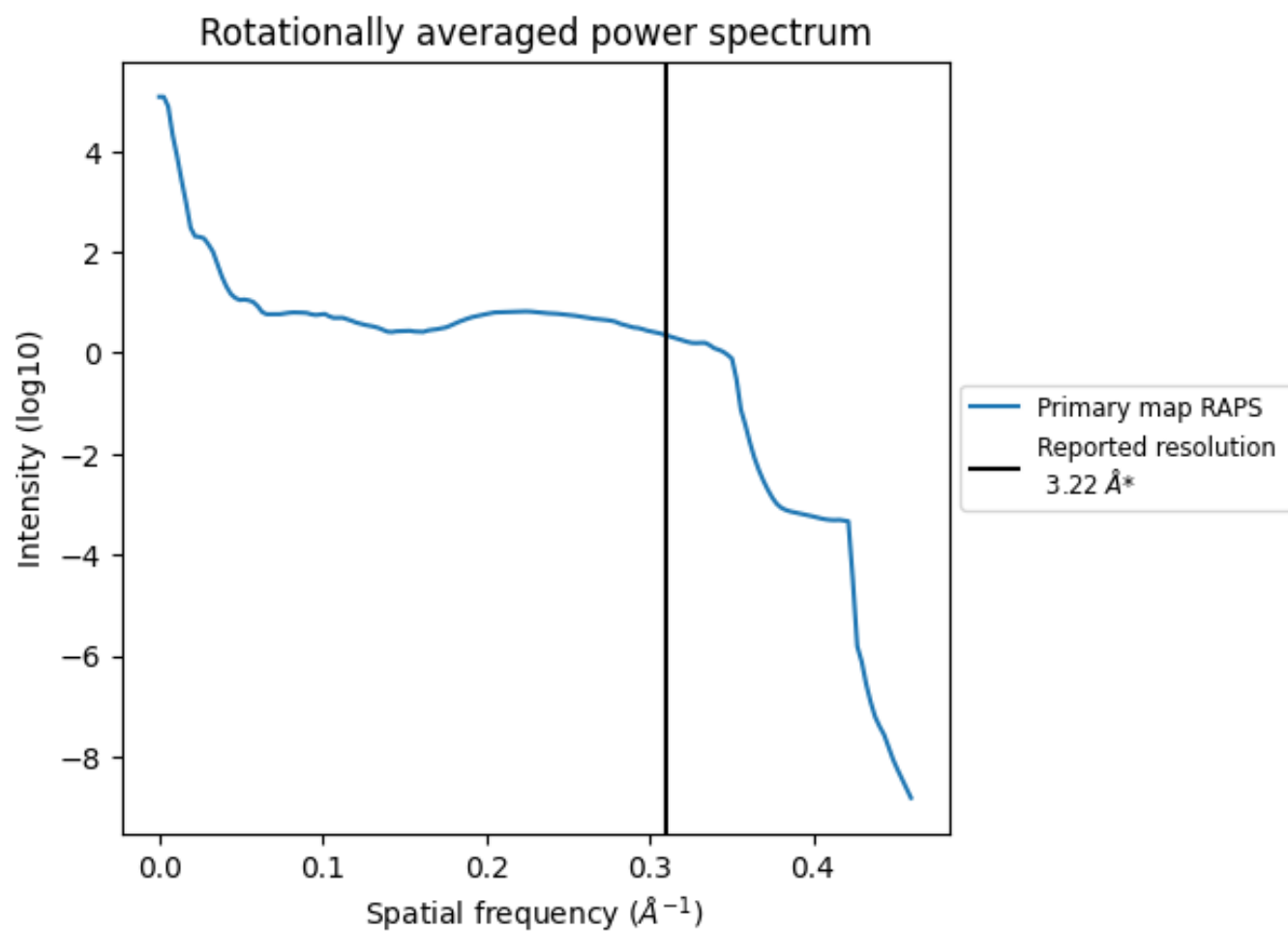
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 442 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 0.311 Å⁻¹

8 Fourier-Shell correlation

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

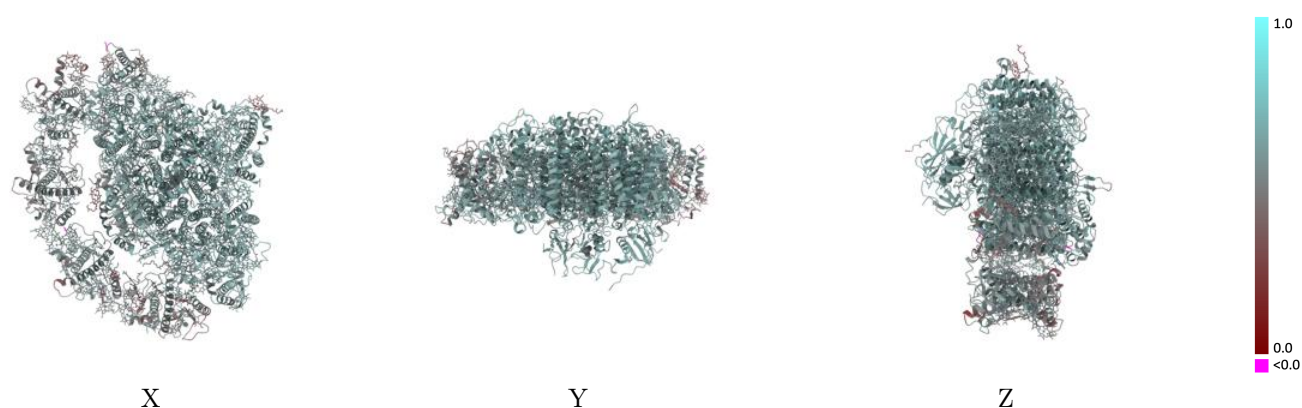
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36037 and PDB model 8J7B. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)

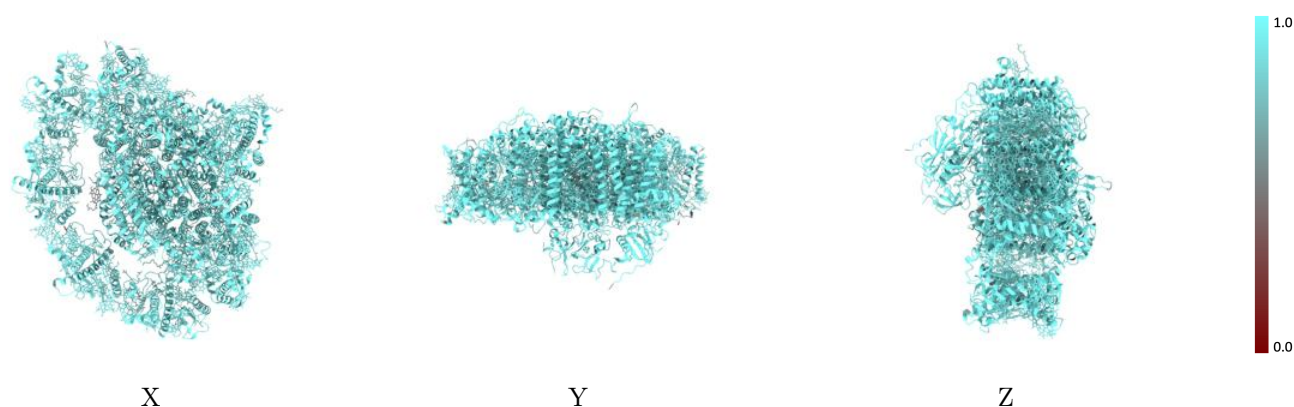
This section was not generated.

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



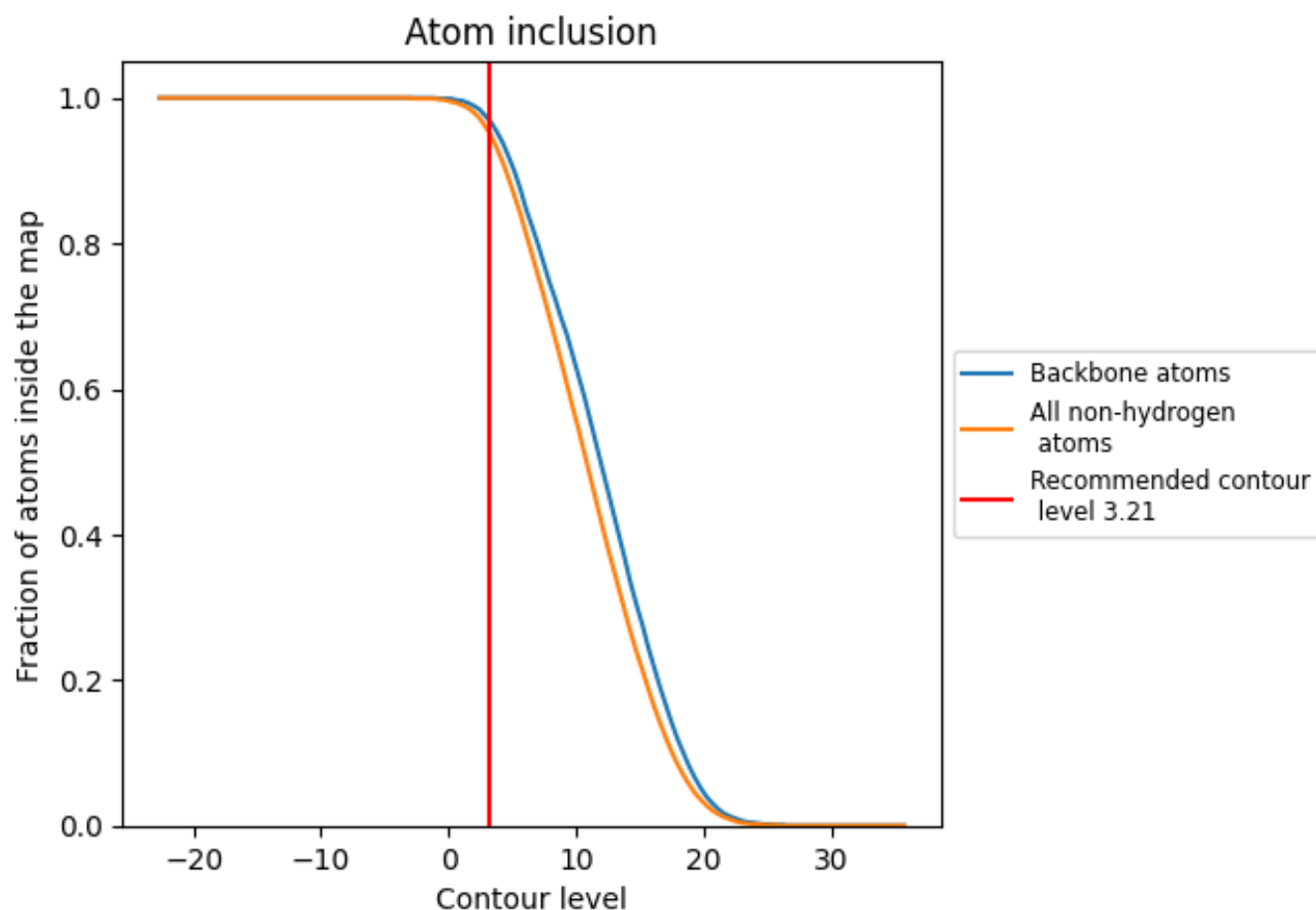
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (3.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.5760
1	0.9220	0.4980
2	0.9450	0.5180
3	0.9450	0.5120
4	0.9520	0.5350
A	0.9570	0.6050
B	0.9670	0.6150
C	0.9810	0.6130
D	0.9770	0.6080
E	0.9760	0.6050
F	0.9210	0.5690
G	0.9520	0.5730
H	0.9350	0.5650
I	0.9790	0.6000
J	0.8600	0.5340
K	0.8620	0.4680
L	0.9610	0.5960

