



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:11 PM UTC

PDB ID : 8J7A / pdb_00008j7a
EMDB ID : EMD-36036
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 1 (PSI-ST1)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-27
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

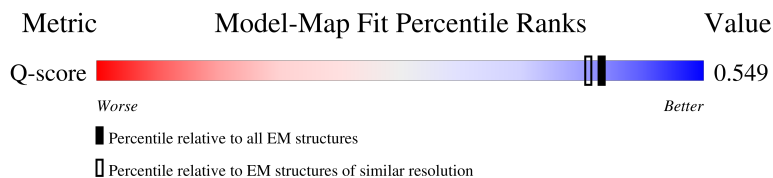
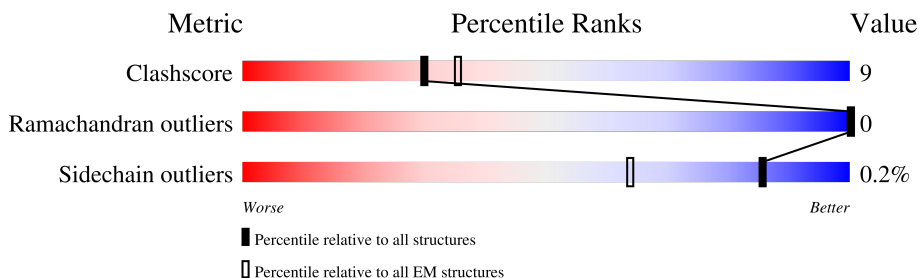
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
18	CLA	G	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	H	201	X	-	-	-
18	CLA	K	201	X	-	-	-
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
24	CL0	A	801	X	-	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O	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	149	Total	C	N	O	S	0	0
			1183	773	203	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	91	Total	C	N	O	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	86	Total	C	N	O	S	0	0
			660	431	104	125			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	41	Total	C	N	O	S	0	0
			327	221	50	55	1		

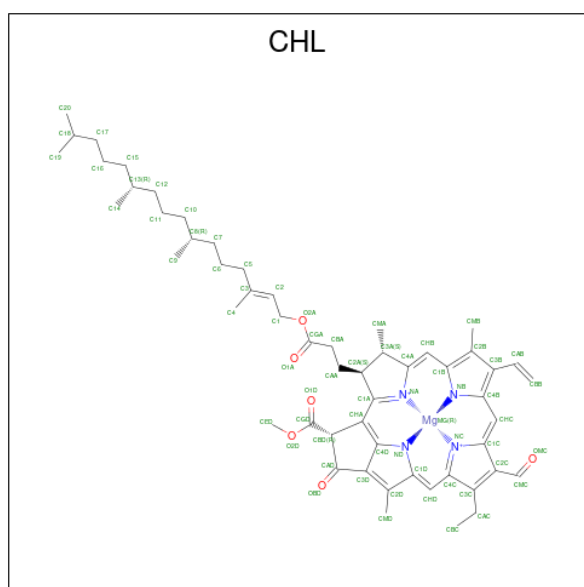
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

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

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

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

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



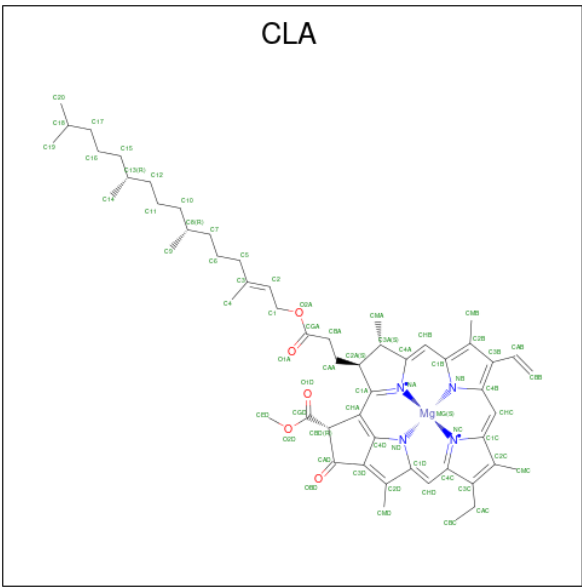
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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

- Molecule 18 is CHLOROPHYLL A (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 43	C 34	Mg 1	N 4	O 4	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	2	1	Total 38	C 30	Mg 1	N 4	O 3	0
18	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
18	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
18	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
18	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	3	1	Total 55	C 45	Mg 1	N 4	O 5	0

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

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

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

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

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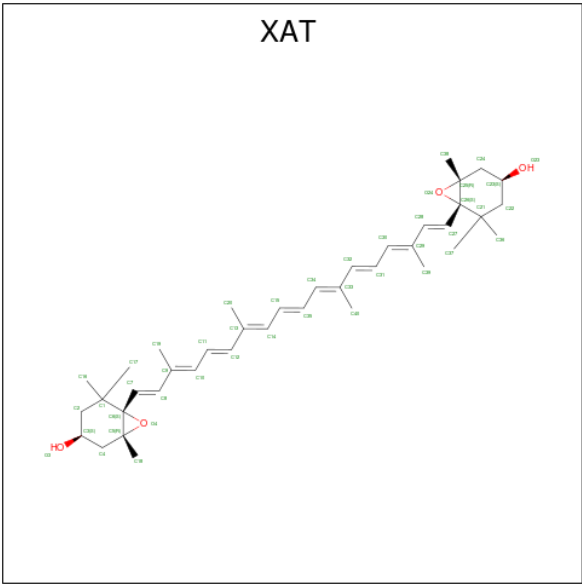
Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0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

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

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



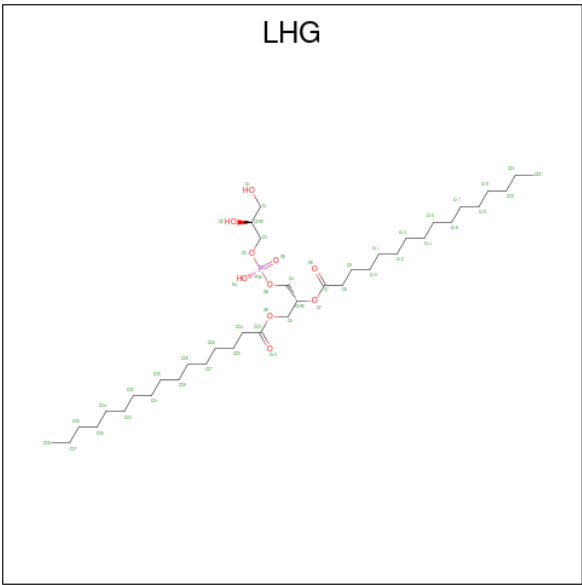
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	2	1	Total	C	O	0
			44	40	4	

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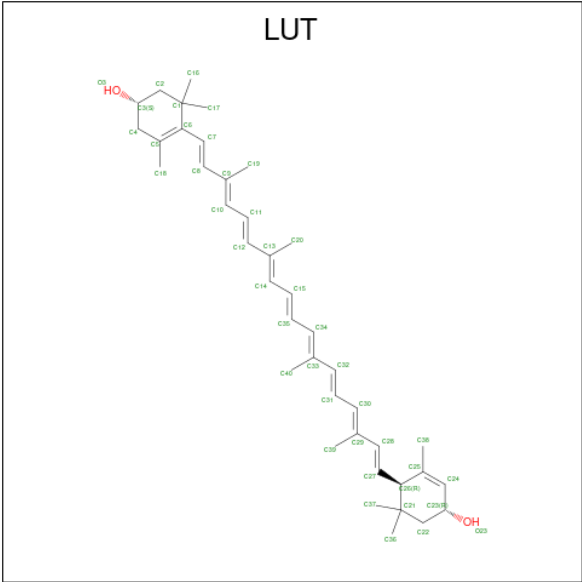
Mol	Chain	Residues	Atoms			AltConf
19	4	1	Total	C	O	0
			44	40	4	

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



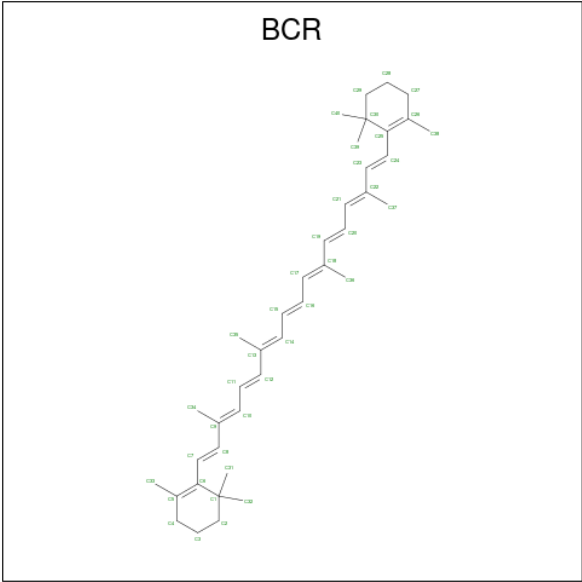
Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			37	26	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			38	27	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	

- 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).



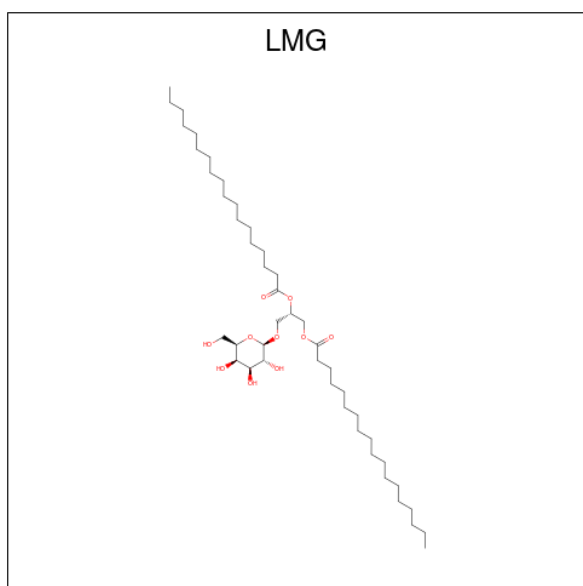
Mol	Chain	Residues	Atoms	AltConf
22	3	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C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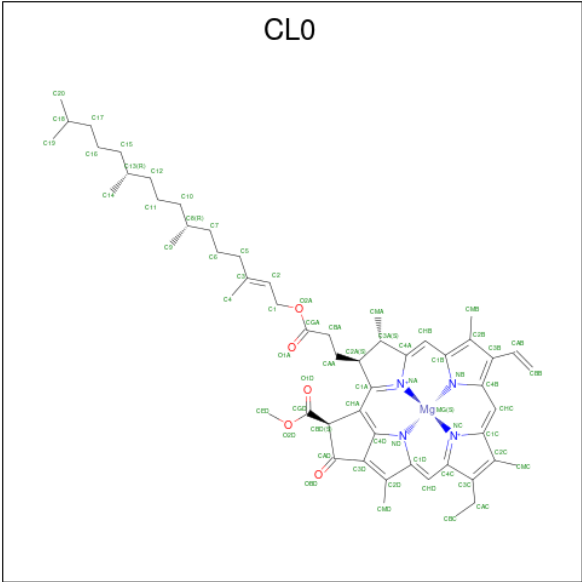
Mol	Chain	Residues	Atoms		AltConf
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	

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



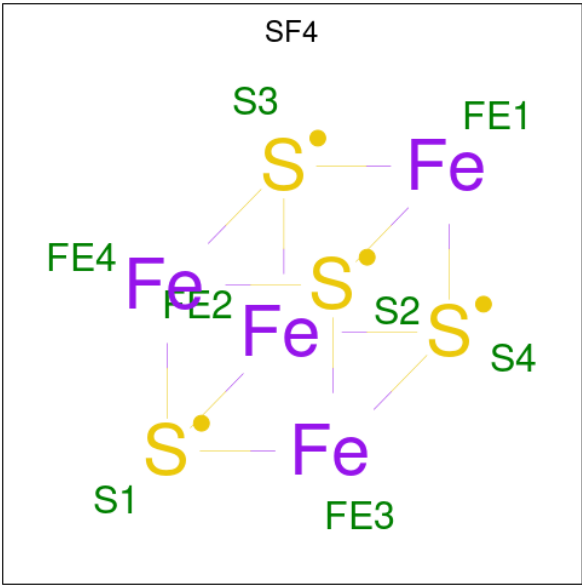
Mol	Chain	Residues	Atoms			AltConf
23	4	1	Total	C	O	0
			33	23	10	
23	4	1	Total	C	O	0
			39	29	10	

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



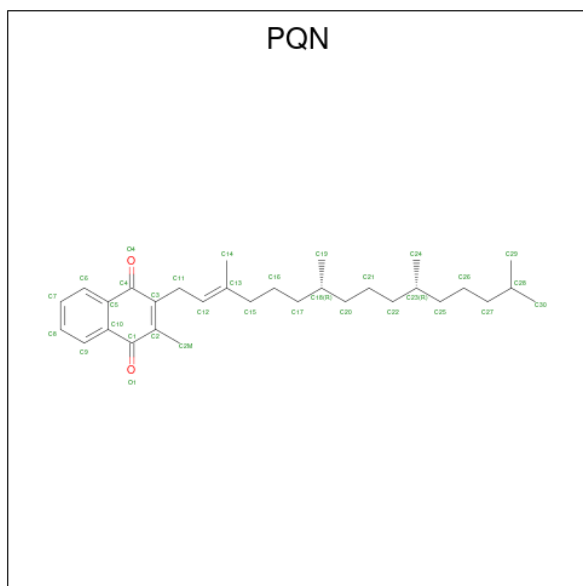
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			60	52	1	4	3	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



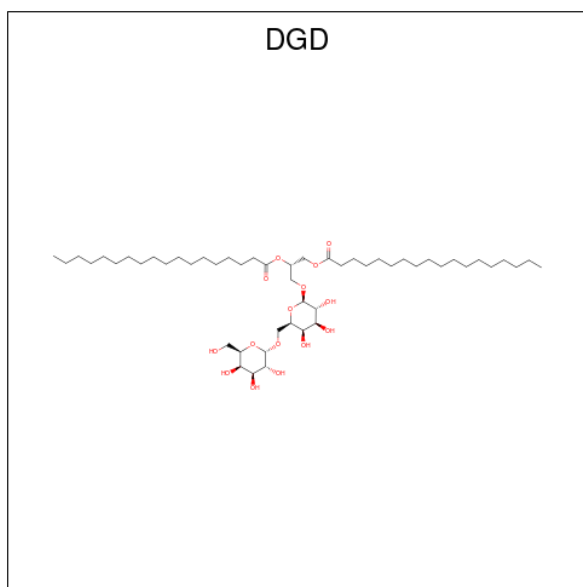
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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

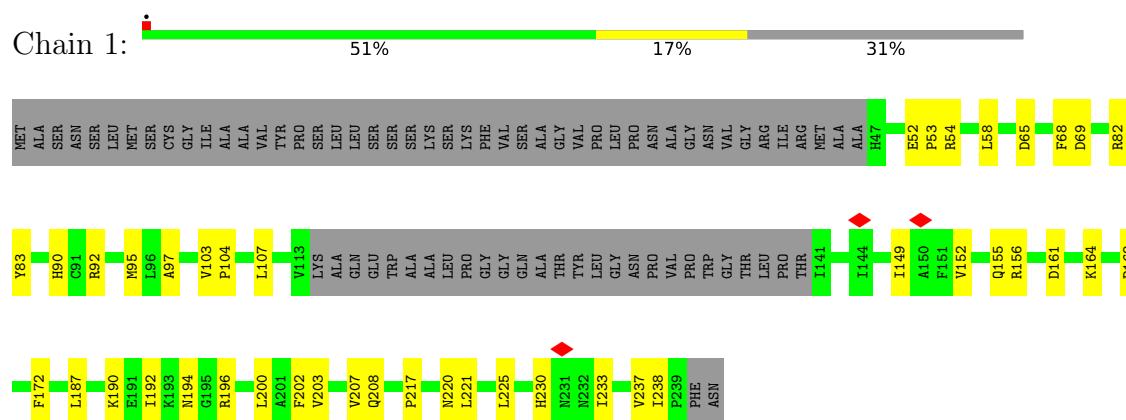


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	66	51	15	0

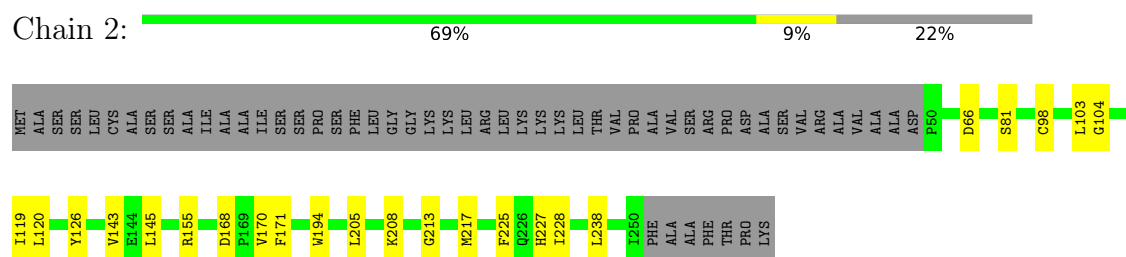
3 Residue-property plots [i](#)

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

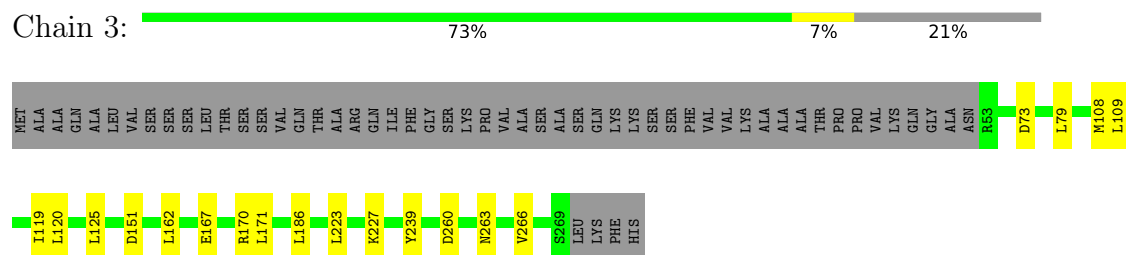
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

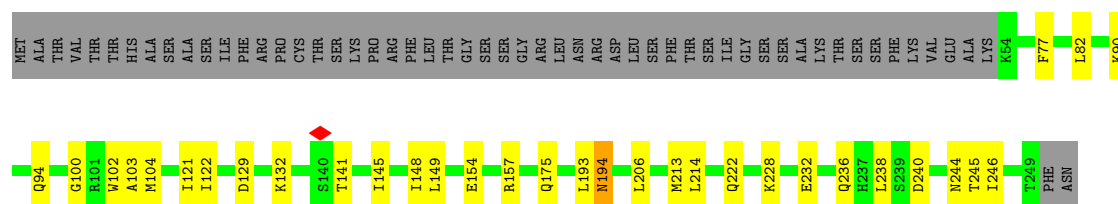


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



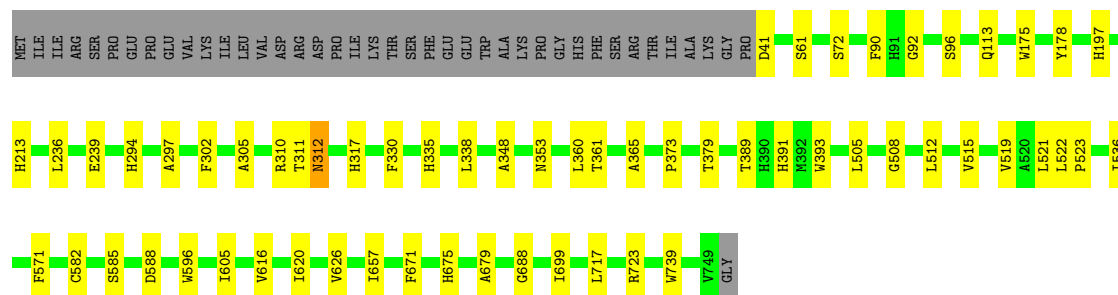
- Molecule 4: Chlorophyll a-b binding protein 4, chloroplastic

Chain 4:  65% 13% 22%



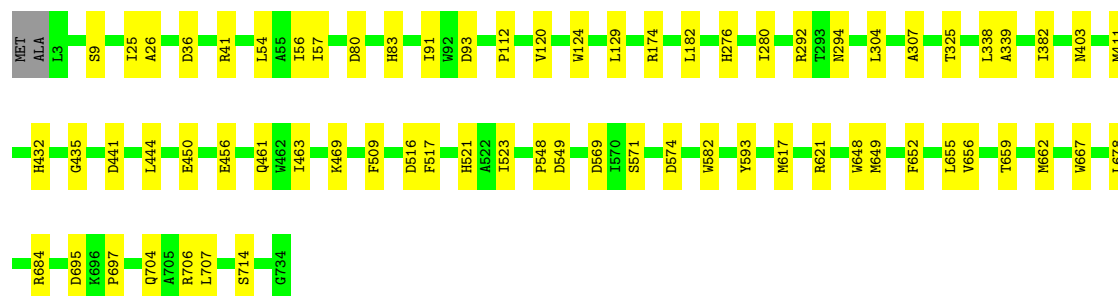
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  86% 8% 5%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  90% 9%



- Molecule 7: Photosystem I iron-sulfur center

Chain C:  83% 16%



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

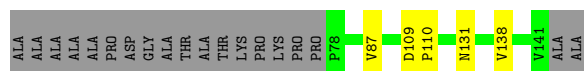
Chain D:  66% 30%





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

Chain E: 41% 55%



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

Chain F: 62% 6% 33%



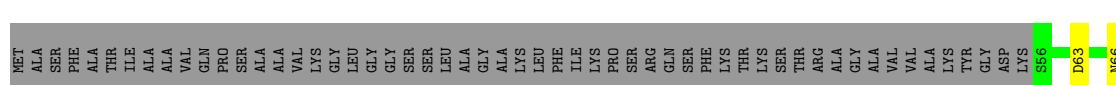
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G: 51% 6% 43%



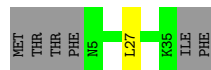
- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic

Chain H: 54% 6% 41%



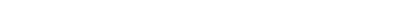
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I: 81% 16%



- Molecule 14: Photosystem I reaction center subunit IX

M1	R2	V10	A11	P12	L22	L25	L26	I29	F33	A36	L37	T38	F41	PHE	SER	PHE
----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain K:  37% 6% 57%

[illegible]

- Chain L:  67% 6% 27%

I65	ALA	MET
E75	ALA	ALA
N90	SER	ALA
V98	SER	SER
V107	MET	PRO
L137	SER	ALA
V144	GLN	GLN
I152	LEU	ARG
Y153	SER	SER
S168	SER	SER
L169	ALA	ALA
T170	SER	SER
L171	LEU	LEU
T172	SER	GLN
L209	GLN	ARG
F217	LEU	LEU
V218	VAL	ALA
LYS	PRO	LYS
	LYS	LYS
	GLY	GLY
	GLY	GLY
	ALA	ALA
	PRO	PRO
	PHE	PHE
	GLY	GLY
	VAL	VAL
	SER	SER
	PRO	PRO
	THR	THR
	LYS	LYS
	ARG	ARG
	VAL	VAL
	SER	SER
	SER	SER
	PHE	PHE
	THR	THR
	VAL	VAL
	ARG	ARG
	ALA	ALA
	VAL	VAL
	LYS	LYS
	SER	SER
	ASP	ASP
	LYS	LYS
	THR	THR
	THR	THR
	F69	F69

4 Experimental information

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/1336	0.38	1/1816 (0.1%)
2	2	0.14	0/1622	0.28	0/2219
3	3	0.14	0/1712	0.28	0/2329
4	4	0.14	0/1599	0.27	0/2178
5	A	0.15	0/5772	0.26	0/7878
6	B	0.16	0/6065	0.27	0/8279
7	C	0.16	0/629	0.32	0/852
8	D	0.13	0/1157	0.27	0/1563
9	E	0.12	0/528	0.21	0/715
10	F	0.12	0/1213	0.24	0/1637
11	G	0.19	0/724	0.48	1/981 (0.1%)
12	H	0.12	0/680	0.24	0/927
13	I	0.14	0/245	0.28	0/333
14	J	0.19	0/336	0.40	0/458
15	K	0.14	0/401	0.30	0/542
16	L	0.13	0/1237	0.28	0/1690
All	All	0.15	0/25256	0.29	2/34397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	64	PRO	CA-N-CD	-11.01	96.59	112.00
1	1	104	PRO	CA-N-CD	-9.12	99.23	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1296	0	1277	38	0
2	2	1566	0	1519	20	0
3	3	1661	0	1625	18	0
4	4	1551	0	1508	41	0
5	A	5582	0	5436	52	0
6	B	5854	0	5646	64	0
7	C	616	0	600	13	0
8	D	1128	0	1134	6	0
9	E	517	0	526	3	0
10	F	1183	0	1215	8	0
11	G	708	0	700	9	0
12	H	660	0	650	5	0
13	I	239	0	258	1	0
14	J	327	0	342	12	0
15	K	397	0	409	5	0
16	L	1200	0	1202	12	0
17	1	93	0	62	7	0
17	2	226	0	150	5	0
17	3	45	0	30	0	0
17	4	169	0	100	4	0
18	1	496	0	354	26	0
18	2	434	0	352	22	0
18	3	498	0	377	10	0
18	4	527	0	412	22	0
18	A	2483	0	2456	114	0
18	B	2284	0	2242	79	0
18	F	149	0	123	8	0
18	G	132	0	97	1	0
18	H	60	0	59	1	0
18	K	128	0	91	1	0
18	L	155	0	138	6	0
19	1	44	0	56	9	0
19	2	44	0	56	6	0
19	4	44	0	52	18	0
20	1	49	0	74	20	0
20	2	37	0	44	0	0
20	A	79	0	104	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	87	0	120	1	0
21	1	42	0	56	9	0
21	2	84	0	112	12	0
21	3	42	0	56	7	0
21	4	42	0	56	3	0
22	3	40	0	56	2	0
22	4	40	0	56	8	0
22	A	240	0	336	31	0
22	B	320	0	448	49	0
22	F	40	0	56	1	0
22	G	40	0	56	3	0
22	I	40	0	56	2	0
22	J	40	0	56	4	0
22	K	80	0	112	9	0
22	L	120	0	168	14	0
23	4	72	0	84	1	0
24	A	60	0	68	7	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	A	33	0	46	5	0
26	B	33	0	46	1	0
27	B	66	0	96	8	0
All	All	34246	0	33616	620	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 620 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	134/190 (70%)	134 (100%)	0	100	100
2	2	163/205 (80%)	163 (100%)	0	100	100
3	3	167/211 (79%)	167 (100%)	0	100	100
4	4	163/210 (78%)	161 (99%)	2 (1%)	63	75
5	A	574/610 (94%)	573 (100%)	1 (0%)	87	87
6	B	599/600 (100%)	599 (100%)	0	100	100
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	122/185 (66%)	122 (100%)	0	100	100
11	G	77/133 (58%)	77 (100%)	0	100	100
12	H	72/113 (64%)	70 (97%)	2 (3%)	38	63
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	43/95 (45%)	43 (100%)	0	100	100
16	L	125/174 (72%)	125 (100%)	0	100	100
All	All	2550/3153 (81%)	2545 (100%)	5 (0%)	85	87

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

Mol	Chain	Res	Type
4	4	194	ASN
4	4	222	GLN
5	A	312	ASN
12	H	121	ASN
12	H	125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	289	HIS
11	G	99	GLN
13	I	30	HIS
11	G	122	ASN
4	4	244	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

198 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	BCR	B	849	-	41,41,41	1.40	8 (19%)	56,56,56	1.82	13 (23%)
18	CLA	B	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
18	CLA	B	836	-	54,58,73	1.31	9 (16%)	64,95,113	3.37	10 (15%)
18	CLA	1	612	-	50,54,73	1.36	8 (16%)	59,90,113	1.44	4 (6%)
18	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
22	BCR	A	852	-	41,41,41	1.38	7 (17%)	56,56,56	1.96	16 (28%)
18	CLA	1	610	20	41,46,73	1.58	8 (19%)	51,81,113	1.53	7 (13%)
20	LHG	B	851	18	37,37,48	0.31	0	40,43,54	0.49	0
18	CLA	1	602	1	58,62,73	1.27	9 (15%)	68,99,113	1.36	5 (7%)
18	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
18	CLA	L	304	-	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
22	BCR	K	202	-	41,41,41	1.40	8 (19%)	56,56,56	1.87	14 (25%)
18	CLA	A	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	6 (7%)
22	BCR	A	853	-	41,41,41	1.42	8 (19%)	56,56,56	1.77	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PQN	B	842	-	34,34,34	0.41	0	43,45,45	0.55	1 (2%)
18	CLA	B	816	-	59,63,73	1.25	9 (15%)	70,101,113	1.39	6 (8%)
18	CLA	2	604	-	46,51,73	1.41	9 (19%)	54,86,113	1.49	4 (7%)
18	CLA	B	840	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
22	BCR	B	801	-	41,41,41	1.43	8 (19%)	56,56,56	1.77	12 (21%)
18	CLA	A	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
18	CLA	3	609	-	57,62,73	1.30	9 (15%)	67,100,113	1.35	6 (8%)
18	CLA	A	803	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
18	CLA	A	820	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
18	CLA	B	813	-	69,73,73	1.16	9 (13%)	82,113,113	1.39	8 (9%)
18	CLA	L	302	16	49,53,73	1.38	8 (16%)	58,89,113	1.46	5 (8%)
18	CLA	A	832	-	54,58,73	1.31	8 (14%)	64,95,113	1.42	7 (10%)
21	LUT	2	616	-	42,43,43	1.29	8 (19%)	51,60,60	1.96	13 (25%)
22	BCR	B	843	-	41,41,41	1.39	8 (19%)	56,56,56	1.86	14 (25%)
18	CLA	A	837	5	49,53,73	1.40	8 (16%)	58,89,113	1.43	5 (8%)
18	CLA	2	609	-	51,55,73	1.33	9 (17%)	60,91,113	1.45	6 (10%)
18	CLA	4	614	-	54,58,73	1.31	9 (16%)	64,95,113	1.46	6 (9%)
18	CLA	A	811	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
20	LHG	1	615	18	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
18	CLA	A	823	-	46,50,73	1.41	7 (15%)	53,85,113	1.43	5 (9%)
21	LUT	3	613	-	42,43,43	1.30	8 (19%)	51,60,60	2.00	17 (33%)
18	CLA	4	601	4	50,54,73	1.35	9 (18%)	59,90,113	1.44	5 (8%)
18	CLA	A	808	-	54,58,73	1.30	8 (14%)	64,95,113	1.45	6 (9%)
18	CLA	K	204	-	50,54,73	1.37	9 (18%)	59,90,113	1.41	4 (6%)
18	CLA	3	611	-	40,44,73	1.49	9 (22%)	49,77,113	1.46	4 (8%)
18	CLA	A	807	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	B	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
22	BCR	B	845	-	41,41,41	1.43	8 (19%)	56,56,56	1.88	15 (26%)
24	CL0	A	801	-	53,67,73	2.95	15 (28%)	47,102,113	2.19	12 (25%)
18	CLA	B	834	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	5 (6%)
22	BCR	J	102	-	41,41,41	1.39	8 (19%)	56,56,56	1.73	14 (25%)
18	CLA	A	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
18	CLA	4	604	-	47,51,73	1.51	9 (19%)	58,87,113	1.47	6 (10%)
18	CLA	F	303	10	45,49,73	1.42	9 (20%)	54,84,113	1.48	5 (9%)
18	CLA	A	821	-	49,53,73	1.38	8 (16%)	58,89,113	1.46	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LUT	4	616	-	42,43,43	1.29	8 (19%)	51,60,60	1.54	10 (19%)
19	XAT	4	617	-	41,47,47	6.09	28 (68%)	54,74,74	5.81	32 (59%)
17	CHL	1	601	1	46,60,74	3.87	18 (39%)	40,97,114	1.89	15 (37%)
18	CLA	A	819	-	63,67,73	1.21	9 (14%)	74,105,113	1.33	5 (6%)
18	CLA	4	611	-	44,49,73	1.44	8 (18%)	50,84,113	1.43	4 (8%)
18	CLA	4	612	-	61,65,73	1.23	9 (14%)	72,103,113	1.38	6 (8%)
18	CLA	B	832	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	4 (4%)
18	CLA	2	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
18	CLA	2	613	-	47,51,73	1.40	9 (19%)	55,86,113	1.47	5 (9%)
18	CLA	B	830	-	47,51,73	1.36	8 (17%)	55,86,113	1.46	5 (9%)
18	CLA	B	809	6	69,73,73	1.16	9 (13%)	82,113,113	1.31	9 (10%)
18	CLA	B	835	-	46,50,73	1.42	9 (19%)	53,85,113	1.42	4 (7%)
22	BCR	B	847	-	41,41,41	1.40	8 (19%)	56,56,56	1.48	10 (17%)
18	CLA	B	841	20	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
18	CLA	3	601	3	64,68,73	1.22	9 (14%)	76,107,113	1.33	6 (7%)
18	CLA	A	817	-	49,53,73	1.40	7 (14%)	58,89,113	1.44	4 (6%)
18	CLA	A	815	-	49,53,73	1.36	9 (18%)	58,89,113	1.54	7 (12%)
18	CLA	B	839	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
23	LMG	4	619	-	39,39,55	0.22	0	47,47,63	0.23	0
18	CLA	B	824	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
17	CHL	3	606	-	38,53,74	3.93	18 (47%)	36,89,114	2.33	12 (33%)
18	CLA	B	838	-	51,55,73	1.34	9 (17%)	60,91,113	1.44	5 (8%)
17	CHL	4	606	-	35,49,74	4.10	15 (42%)	33,84,114	2.21	9 (27%)
18	CLA	B	831	-	47,51,73	1.37	8 (17%)	55,86,113	1.46	4 (7%)
20	LHG	A	847	-	29,29,48	0.35	0	32,35,54	0.44	0
18	CLA	4	609	-	58,62,73	1.27	9 (15%)	68,99,113	1.39	7 (10%)
22	BCR	A	848	-	41,41,41	1.40	8 (19%)	56,56,56	1.59	11 (19%)
22	BCR	L	301	-	41,41,41	1.41	9 (21%)	56,56,56	2.14	13 (23%)
18	CLA	3	605	-	45,49,73	1.52	10 (22%)	54,84,113	1.50	6 (11%)
18	CLA	B	810	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
22	BCR	A	849	-	41,41,41	1.38	8 (19%)	56,56,56	1.97	14 (25%)
18	CLA	A	825	-	59,63,73	1.26	9 (15%)	70,101,113	1.38	7 (10%)
18	CLA	A	836	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
18	CLA	A	818	-	64,68,73	1.21	9 (14%)	76,107,113	5.01	7 (9%)
18	CLA	2	610	20	40,45,73	2.62	11 (27%)	46,76,113	1.32	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CHL	2	601	2	41,55,74	4.12	19 (46%)	35,91,114	2.33	13 (37%)
18	CLA	B	826	-	66,70,73	1.19	9 (13%)	78,109,113	1.31	7 (8%)
18	CLA	B	833	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	5 (8%)
18	CLA	A	813	-	58,62,73	1.27	7 (12%)	68,99,113	1.41	6 (8%)
18	CLA	A	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.37	7 (8%)
18	CLA	1	611	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
18	CLA	A	843	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	4 (4%)
18	CLA	A	831	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
21	LUT	2	619	-	42,43,43	1.30	8 (19%)	51,60,60	1.75	12 (23%)
20	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.33	0
18	CLA	H	201	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)
18	CLA	2	612	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	4 (4%)
19	XAT	2	617	-	41,47,47	1.32	8 (19%)	54,74,74	2.05	14 (25%)
18	CLA	1	607	-	47,52,73	1.42	9 (19%)	55,88,113	1.43	4 (7%)
18	CLA	B	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
18	CLA	A	809	5	69,73,73	1.16	8 (11%)	82,113,113	1.34	8 (9%)
27	DGD	B	850	-	67,67,67	0.84	2 (2%)	81,81,81	0.98	4 (4%)
18	CLA	B	804	-	45,49,73	1.40	9 (20%)	54,84,113	1.54	8 (14%)
18	CLA	3	604	-	44,49,73	1.43	9 (20%)	50,84,113	1.42	4 (8%)
18	CLA	L	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
18	CLA	K	203	-	49,53,73	1.38	8 (16%)	58,89,113	1.48	5 (8%)
18	CLA	G	201	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
18	CLA	4	608	4	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
18	CLA	A	814	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
18	CLA	3	612	-	43,48,73	1.43	8 (18%)	51,83,113	1.53	5 (9%)
22	BCR	L	305	-	41,41,41	1.42	8 (19%)	56,56,56	1.71	14 (25%)
18	CLA	A	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
18	CLA	3	603	-	49,53,73	1.41	8 (16%)	58,89,113	1.43	4 (6%)
20	LHG	2	618	18	36,36,48	0.31	0	39,42,54	0.49	0
22	BCR	4	618	-	41,41,41	1.39	8 (19%)	56,56,56	1.59	9 (16%)
21	LUT	1	616	-	42,43,43	1.28	7 (16%)	51,60,60	2.19	16 (31%)
25	SF4	A	854	-	0,12,12	-	-	-	-	-
18	CLA	A	805	-	56,60,73	1.29	9 (16%)	65,97,113	1.41	8 (12%)
17	CHL	1	606	-	35,49,74	4.60	17 (48%)	28,84,114	1.68	8 (28%)
18	CLA	B	823	-	49,53,73	1.38	9 (18%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	802	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
18	CLA	A	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	7 (8%)
20	LHG	B	852	-	48,48,48	0.28	0	51,54,54	0.32	0
18	CLA	1	613	-	41,46,73	1.60	9 (21%)	51,81,113	1.55	7 (13%)
18	CLA	A	827	-	63,67,73	1.22	9 (14%)	74,105,113	1.32	7 (9%)
18	CLA	G	202	-	46,50,73	1.41	8 (17%)	53,85,113	1.42	4 (7%)
18	CLA	4	603	-	48,52,73	1.48	9 (18%)	59,88,113	1.48	6 (10%)
18	CLA	B	807	-	56,60,73	1.28	8 (14%)	65,97,113	1.40	5 (7%)
18	CLA	3	610	-	43,48,73	1.46	7 (16%)	51,83,113	1.49	5 (9%)
18	CLA	3	607	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
18	CLA	4	610	-	46,50,73	1.39	9 (19%)	53,85,113	1.44	4 (7%)
18	CLA	A	844	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
17	CHL	2	605	-	36,50,74	4.07	18 (50%)	31,85,114	2.35	10 (32%)
18	CLA	B	811	-	58,62,73	1.35	10 (17%)	71,100,113	1.39	8 (11%)
22	BCR	B	844	-	41,41,41	1.40	8 (19%)	56,56,56	1.83	13 (23%)
18	CLA	B	821	-	51,55,73	1.33	9 (17%)	60,91,113	1.53	6 (10%)
18	CLA	1	604	-	53,57,73	1.32	8 (15%)	61,93,113	1.57	7 (11%)
17	CHL	2	615	2	37,51,74	4.35	18 (48%)	30,86,114	2.31	10 (33%)
17	CHL	4	607	-	40,54,74	4.03	19 (47%)	34,90,114	2.77	13 (38%)
18	CLA	G	203	11	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)
18	CLA	A	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	5 (6%)
18	CLA	B	812	-	47,51,73	1.38	9 (19%)	55,86,113	1.45	4 (7%)
18	CLA	A	824	-	45,49,73	1.43	8 (17%)	54,84,113	1.50	5 (9%)
18	CLA	A	810	5	54,58,73	1.32	8 (14%)	64,95,113	1.45	7 (10%)
22	BCR	A	851	-	41,41,41	1.43	8 (19%)	56,56,56	2.40	20 (35%)
18	CLA	A	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	9 (10%)
18	CLA	2	603	-	47,52,73	1.41	9 (19%)	55,88,113	1.43	4 (7%)
18	CLA	4	613	-	49,53,73	1.38	9 (18%)	58,89,113	1.60	6 (10%)
17	CHL	4	615	4	36,49,74	4.23	16 (44%)	30,84,114	1.93	8 (26%)
18	CLA	B	837	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
22	BCR	F	304	-	41,41,41	1.41	7 (17%)	56,56,56	2.12	16 (28%)
18	CLA	1	603	-	58,62,73	1.28	9 (15%)	68,99,113	1.36	5 (7%)
18	CLA	1	605	-	50,54,73	1.38	7 (14%)	59,90,113	1.47	4 (6%)
18	CLA	B	818	-	64,68,73	1.21	9 (14%)	76,107,113	1.42	9 (11%)
18	CLA	4	602	4	64,68,73	1.21	9 (14%)	76,107,113	1.31	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CHL	4	605	-	35,49,74	4.11	17 (48%)	30,84,114	1.77	10 (33%)
18	CLA	B	827	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	5 (6%)
19	XAT	1	614	-	41,47,47	0.87	1 (2%)	54,74,74	3.03	21 (38%)
22	BCR	G	204	-	41,41,41	1.39	8 (19%)	56,56,56	1.59	13 (23%)
22	BCR	L	306	-	41,41,41	1.37	8 (19%)	56,56,56	1.95	16 (28%)
18	CLA	B	817	-	63,67,73	1.22	9 (14%)	74,105,113	1.37	6 (8%)
18	CLA	F	301	-	61,65,73	1.25	8 (13%)	72,103,113	1.33	4 (5%)
22	BCR	A	850	-	41,41,41	1.42	8 (19%)	56,56,56	1.84	13 (23%)
18	CLA	2	608	2	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
18	CLA	A	839	-	59,63,73	1.26	9 (15%)	70,101,113	1.40	7 (10%)
17	CHL	2	606	-	37,51,74	4.37	18 (48%)	30,86,114	2.42	10 (33%)
22	BCR	K	205	-	41,41,41	1.38	7 (17%)	56,56,56	1.83	16 (28%)
18	CLA	B	822	-	69,73,73	1.17	8 (11%)	82,113,113	1.33	7 (8%)
18	CLA	A	828	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	9 (10%)
18	CLA	3	602	-	59,63,73	1.29	8 (13%)	70,101,113	1.32	5 (7%)
22	BCR	B	848	-	41,41,41	1.40	8 (19%)	56,56,56	1.47	11 (19%)
18	CLA	B	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.38	7 (10%)
18	CLA	1	609	-	46,50,73	1.40	7 (15%)	54,85,113	1.52	4 (7%)
22	BCR	I	101	-	41,41,41	1.40	8 (19%)	56,56,56	1.41	9 (16%)
25	SF4	C	101	-	0,12,12	-	-	-	-	-
18	CLA	A	842	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
22	BCR	B	846	-	41,41,41	1.40	8 (19%)	56,56,56	1.61	11 (19%)
18	CLA	3	608	-	45,49,73	1.41	9 (20%)	54,84,113	1.54	6 (11%)
18	CLA	B	815	-	47,51,73	1.38	9 (19%)	55,86,113	1.45	4 (7%)
18	CLA	A	826	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
22	BCR	3	614	-	41,41,41	1.39	8 (19%)	56,56,56	1.55	13 (23%)
18	CLA	F	302	-	55,59,73	1.31	8 (14%)	64,96,113	1.49	5 (7%)
18	CLA	A	833	-	60,64,73	1.24	9 (15%)	71,102,113	1.36	5 (7%)
18	CLA	B	825	-	66,70,73	1.18	9 (13%)	78,109,113	1.36	7 (8%)
18	CLA	A	840	-	56,60,73	1.29	8 (14%)	65,97,113	1.43	7 (10%)
23	LMG	4	620	-	33,33,55	0.23	0	41,41,63	0.27	0
25	SF4	C	102	-	0,12,12	-	-	-	-	-
18	CLA	K	201	15	41,45,73	1.47	9 (21%)	50,78,113	1.46	4 (8%)
17	CHL	2	607	-	45,59,74	3.87	19 (42%)	40,96,114	2.31	15 (37%)
18	CLA	1	608	-	44,48,73	1.51	9 (20%)	55,83,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PQN	A	855	-	34,34,34	0.40	0	43,45,45	0.57	1 (2%)
18	CLA	B	829	-	60,64,73	1.25	8 (13%)	71,102,113	1.37	6 (8%)
18	CLA	2	611	-	48,52,73	1.42	8 (16%)	57,88,113	1.46	5 (8%)
18	CLA	A	804	-	69,73,73	1.17	8 (11%)	82,113,113	1.45	9 (10%)
18	CLA	A	838	-	55,59,73	1.31	9 (16%)	64,96,113	1.39	6 (9%)
18	CLA	B	820	-	54,58,73	1.31	9 (16%)	64,95,113	1.45	9 (14%)
18	CLA	A	816	-	46,50,73	1.40	9 (19%)	53,85,113	1.45	4 (7%)
18	CLA	B	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
18	CLA	A	841	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (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
22	BCR	B	849	-	-	6/29/63/63	0/2/2/2
18	CLA	B	814	-	1/1/15/20	16/39/115/115	-
18	CLA	B	836	-	1/1/12/20	6/21/97/115	-
18	CLA	1	612	-	1/1/11/20	9/17/93/115	-
18	CLA	B	808	-	1/1/15/20	12/39/115/115	-
22	BCR	A	852	-	-	14/29/63/63	0/2/2/2
18	CLA	1	610	20	1/1/10/20	0/4/80/115	-
20	LHG	B	851	18	-	5/42/42/53	-
18	CLA	1	602	1	1/1/12/20	8/26/102/115	-
18	CLA	B	803	-	1/1/15/20	9/39/115/115	-
18	CLA	L	304	-	1/1/11/20	4/15/91/115	-
22	BCR	K	202	-	-	2/29/63/63	0/2/2/2
18	CLA	A	834	-	1/1/15/20	9/39/115/115	-
22	BCR	A	853	-	-	4/29/63/63	0/2/2/2
26	PQN	B	842	-	-	7/23/43/43	0/2/2/2
18	CLA	B	816	-	1/1/13/20	9/27/103/115	-
18	CLA	2	604	-	1/1/10/20	10/12/88/115	-
18	CLA	B	840	-	1/1/15/20	9/39/115/115	-
22	BCR	B	801	-	-	6/29/63/63	0/2/2/2
18	CLA	A	802	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	609	-	1/1/13/20	7/25/101/115	-
18	CLA	A	803	-	1/1/15/20	20/39/115/115	-
18	CLA	A	820	-	1/1/15/20	16/39/115/115	-
18	CLA	B	813	-	1/1/15/20	9/39/115/115	-
18	CLA	L	302	16	1/1/11/20	2/15/91/115	-
18	CLA	A	832	-	1/1/12/20	9/21/97/115	-
21	LUT	2	616	-	-	6/29/67/67	0/2/2/2
22	BCR	B	843	-	-	1/29/63/63	0/2/2/2
18	CLA	A	837	5	1/1/11/20	3/15/91/115	-
18	CLA	2	609	-	1/1/11/20	6/18/94/115	-
18	CLA	4	614	-	1/1/12/20	5/21/97/115	-
18	CLA	A	811	-	1/1/15/20	13/39/115/115	-
20	LHG	1	615	18	-	31/53/53/53	-
18	CLA	A	823	-	1/1/10/20	4/12/88/115	-
21	LUT	3	613	-	-	6/29/67/67	0/2/2/2
18	CLA	4	601	4	1/1/11/20	8/17/93/115	-
18	CLA	A	808	-	1/1/12/20	1/21/97/115	-
18	CLA	K	204	-	1/1/11/20	12/17/93/115	-
18	CLA	3	611	-	1/1/8/20	2/2/74/115	-
18	CLA	A	807	-	1/1/15/20	17/39/115/115	-
18	CLA	B	805	-	1/1/15/20	23/39/115/115	-
24	CL0	A	801	-	2/2/16/25	13/31/115/135	-
22	BCR	B	845	-	-	9/29/63/63	0/2/2/2
18	CLA	B	834	-	1/1/14/20	5/33/109/115	-
22	BCR	J	102	-	-	2/29/63/63	0/2/2/2
18	CLA	A	829	-	1/1/15/20	16/39/115/115	-
18	CLA	4	604	-	1/1/11/20	6/11/87/115	-
18	CLA	F	303	10	1/1/10/20	4/10/86/115	-
18	CLA	A	821	-	1/1/11/20	5/15/91/115	-
21	LUT	4	616	-	-	2/29/67/67	0/2/2/2
19	XAT	4	617	-	-	3/31/93/93	0/4/4/4
17	CHL	1	601	1	3/3/17/26	9/22/120/137	-
18	CLA	A	819	-	1/1/13/20	18/32/108/115	-
18	CLA	4	611	-	1/1/10/20	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	612	-	1/1/13/20	9/30/106/115	-
18	CLA	B	832	-	1/1/15/20	11/39/115/115	-
18	CLA	2	602	-	1/1/15/20	16/39/115/115	-
18	CLA	2	613	-	1/1/10/20	5/13/89/115	-
18	CLA	B	830	-	1/1/10/20	4/13/89/115	-
18	CLA	B	809	6	1/1/15/20	16/39/115/115	-
18	CLA	B	835	-	1/1/10/20	5/12/88/115	-
22	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	B	841	20	1/1/15/20	19/39/115/115	-
18	CLA	3	601	3	1/1/14/20	9/33/109/115	-
18	CLA	A	817	-	1/1/11/20	3/15/91/115	-
18	CLA	A	815	-	1/1/11/20	5/15/91/115	-
18	CLA	B	839	-	1/1/15/20	7/39/115/115	-
23	LMG	4	619	-	-	4/34/54/70	0/1/1/1
18	CLA	B	824	-	1/1/15/20	16/39/115/115	-
17	CHL	3	606	-	3/3/16/26	7/13/111/137	-
18	CLA	B	838	-	1/1/11/20	3/18/94/115	-
17	CHL	4	606	-	3/3/15/26	4/10/106/137	-
18	CLA	B	831	-	1/1/10/20	1/13/89/115	-
20	LHG	A	847	-	-	2/34/34/53	-
18	CLA	4	609	-	1/1/12/20	3/26/102/115	-
22	BCR	A	848	-	-	2/29/63/63	0/2/2/2
22	BCR	L	301	-	-	3/29/63/63	0/2/2/2
18	CLA	3	605	-	1/1/10/20	0/10/86/115	-
18	CLA	B	810	-	1/1/15/20	12/39/115/115	-
22	BCR	A	849	-	-	5/29/63/63	0/2/2/2
18	CLA	A	825	-	1/1/13/20	10/27/103/115	-
18	CLA	A	836	-	1/1/11/20	5/15/91/115	-
18	CLA	A	818	-	1/1/14/20	12/33/109/115	-
18	CLA	2	610	20	1/1/7/20	4/10/70/115	-
17	CHL	2	601	2	3/3/16/26	5/17/115/137	-
18	CLA	B	826	-	1/1/14/20	7/36/112/115	-
18	CLA	B	833	-	1/1/11/20	3/15/91/115	-
18	CLA	A	813	-	1/1/12/20	9/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	835	-	1/1/15/20	16/39/115/115	-
18	CLA	1	611	-	1/1/11/20	8/15/91/115	-
18	CLA	A	843	-	1/1/15/20	16/39/115/115	-
18	CLA	A	831	-	1/1/15/20	7/39/115/115	-
21	LUT	2	619	-	-	5/29/67/67	0/2/2/2
20	LHG	A	846	-	-	4/53/53/53	-
18	CLA	H	201	-	1/1/14/20	16/33/109/115	-
18	CLA	2	612	-	1/1/15/20	15/39/115/115	-
19	XAT	2	617	-	-	16/31/93/93	0/4/4/4
18	CLA	1	607	-	1/1/11/20	8/13/89/115	-
18	CLA	B	828	-	1/1/15/20	14/39/115/115	-
18	CLA	A	809	5	1/1/15/20	12/39/115/115	-
27	DGD	B	850	-	-	14/55/95/95	0/2/2/2
18	CLA	B	804	-	1/1/10/20	2/10/86/115	-
18	CLA	3	604	-	1/1/10/20	2/10/86/115	-
18	CLA	L	303	-	1/1/15/20	11/39/115/115	-
18	CLA	K	203	-	1/1/11/20	6/15/91/115	-
18	CLA	G	201	-	1/1/11/20	5/15/91/115	-
18	CLA	4	608	4	1/1/11/20	7/15/91/115	-
18	CLA	A	814	-	1/1/15/20	13/39/115/115	-
18	CLA	3	612	-	1/1/10/20	2/8/84/115	-
22	BCR	L	305	-	-	2/29/63/63	0/2/2/2
18	CLA	A	822	-	1/1/15/20	7/39/115/115	-
18	CLA	3	603	-	1/1/11/20	6/15/91/115	-
20	LHG	2	618	18	-	10/41/41/53	-
22	BCR	4	618	-	-	9/29/63/63	0/2/2/2
21	LUT	1	616	-	-	4/29/67/67	0/2/2/2
25	SF4	A	854	-	-	-	0/6/5/5
18	CLA	A	805	-	1/1/12/20	4/24/100/115	-
17	CHL	1	606	-	3/3/15/26	0/8/106/137	-
18	CLA	B	823	-	1/1/11/20	6/15/91/115	-
18	CLA	B	802	-	1/1/15/20	16/39/115/115	-
18	CLA	A	806	-	1/1/15/20	18/39/115/115	-
20	LHG	B	852	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	613	-	1/1/10/20	2/4/80/115	-
18	CLA	A	827	-	1/1/13/20	6/32/108/115	-
18	CLA	G	202	-	1/1/10/20	4/12/88/115	-
18	CLA	4	603	-	1/1/11/20	3/13/89/115	-
18	CLA	B	807	-	1/1/12/20	3/24/100/115	-
18	CLA	3	610	-	1/1/10/20	2/8/84/115	-
18	CLA	3	607	-	1/1/11/20	3/15/91/115	-
18	CLA	4	610	-	1/1/10/20	2/12/88/115	-
18	CLA	A	844	-	1/1/15/20	13/39/115/115	-
17	CHL	2	605	-	3/3/15/26	4/10/108/137	-
18	CLA	B	811	-	1/1/13/20	10/25/101/115	-
22	BCR	B	844	-	-	11/29/63/63	0/2/2/2
18	CLA	B	821	-	1/1/11/20	6/18/94/115	-
18	CLA	1	604	-	1/1/11/20	7/20/96/115	-
17	CHL	2	615	2	3/3/15/26	4/12/110/137	-
17	CHL	4	607	-	3/3/16/26	8/15/113/137	-
18	CLA	G	203	11	1/1/11/20	3/15/91/115	-
18	CLA	A	812	-	1/1/15/20	19/39/115/115	-
18	CLA	B	812	-	1/1/10/20	0/13/89/115	-
18	CLA	A	824	-	1/1/10/20	4/10/86/115	-
18	CLA	A	810	5	1/1/12/20	4/21/97/115	-
22	BCR	A	851	-	-	8/29/63/63	0/2/2/2
18	CLA	A	830	-	1/1/15/20	11/39/115/115	-
18	CLA	2	603	-	1/1/11/20	3/13/89/115	-
18	CLA	4	613	-	1/1/11/20	9/15/91/115	-
17	CHL	4	615	4	3/3/15/26	0/10/106/137	-
18	CLA	B	837	-	1/1/15/20	10/39/115/115	-
22	BCR	F	304	-	-	12/29/63/63	0/2/2/2
18	CLA	1	603	-	1/1/12/20	8/26/102/115	-
18	CLA	1	605	-	1/1/11/20	8/17/93/115	-
18	CLA	B	818	-	1/1/14/20	6/33/109/115	-
18	CLA	4	602	4	1/1/14/20	9/33/109/115	-
17	CHL	4	605	-	3/3/15/26	5/8/106/137	-
18	CLA	B	827	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	XAT	1	614	-	-	5/31/93/93	0/4/4/4
22	BCR	G	204	-	-	3/29/63/63	0/2/2/2
22	BCR	L	306	-	-	4/29/63/63	0/2/2/2
18	CLA	B	817	-	1/1/13/20	12/32/108/115	-
18	CLA	F	301	-	1/1/13/20	11/30/106/115	-
22	BCR	A	850	-	-	4/29/63/63	0/2/2/2
18	CLA	2	608	2	1/1/11/20	7/15/91/115	-
18	CLA	A	839	-	1/1/13/20	7/27/103/115	-
17	CHL	2	606	-	3/3/15/26	2/12/110/137	-
22	BCR	K	205	-	-	5/29/63/63	0/2/2/2
18	CLA	B	822	-	1/1/15/20	14/39/115/115	-
18	CLA	A	828	-	1/1/15/20	7/39/115/115	-
18	CLA	3	602	-	1/1/13/20	11/27/103/115	-
22	BCR	B	848	-	-	0/29/63/63	0/2/2/2
18	CLA	B	819	-	1/1/13/20	11/27/103/115	-
18	CLA	1	609	-	1/1/10/20	4/11/87/115	-
22	BCR	I	101	-	-	0/29/63/63	0/2/2/2
25	SF4	C	101	-	-	-	0/6/5/5
18	CLA	A	842	-	1/1/15/20	9/39/115/115	-
22	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	3	608	-	1/1/10/20	2/10/86/115	-
18	CLA	B	815	-	1/1/10/20	4/13/89/115	-
18	CLA	A	826	-	1/1/15/20	10/39/115/115	-
22	BCR	3	614	-	-	3/29/63/63	0/2/2/2
18	CLA	F	302	-	1/1/12/20	10/23/99/115	-
18	CLA	A	833	-	1/1/13/20	4/29/105/115	-
18	CLA	B	825	-	1/1/14/20	13/36/112/115	-
18	CLA	A	840	-	1/1/12/20	3/24/100/115	-
23	LMG	4	620	-	-	5/28/48/70	0/1/1/1
25	SF4	C	102	-	-	-	0/6/5/5
18	CLA	K	201	15	1/1/8/20	2/4/76/115	-
17	CHL	2	607	-	3/3/17/26	6/21/119/137	-
18	CLA	1	608	-	1/1/10/20	2/8/84/115	-
26	PQN	A	855	-	-	1/23/43/43	0/2/2/2
18	CLA	B	829	-	1/1/13/20	5/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	2	611	-	1/1/11/20	6/13/89/115	-
18	CLA	A	804	-	1/1/15/20	15/39/115/115	-
18	CLA	A	838	-	1/1/12/20	7/23/99/115	-
18	CLA	B	820	-	1/1/12/20	5/21/97/115	-
18	CLA	A	816	-	1/1/10/20	1/12/88/115	-
18	CLA	B	806	-	1/1/15/20	12/39/115/115	-
18	CLA	A	841	-	1/1/15/20	12/39/115/115	-

The worst 5 of 1696 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	617	XAT	O24-C25	-14.52	1.27	1.46
18	2	610	CLA	C1A-NA	13.12	1.40	1.29
19	4	617	XAT	O4-C5	-11.64	1.31	1.46
19	4	617	XAT	C2-C3	-11.52	1.36	1.52
17	1	606	CHL	C2C-C3C	11.38	1.47	1.36

The worst 5 of 1412 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	818	CLA	O2D-CGD-CBD	26.52	157.59	111.23
18	A	818	CLA	O2D-CGD-O1D	-25.43	74.34	123.85
18	A	818	CLA	O1D-CGD-CBD	-20.92	83.25	124.52
19	4	617	XAT	C4-C3-C2	-19.96	73.45	110.79
19	4	617	XAT	C38-C25-C26	-16.27	95.53	122.30

5 of 176 chirality outliers are listed below:

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

5 of 1451 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	601	CHL	CAD-CBD-CGD-O1D
17	1	601	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	2	615	CHL	CHA-CBD-CGD-O1D
17	2	601	CHL	C3A-C2A-CAA-CBA
17	4	605	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

156 monomers are involved in 471 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	849	BCR	9	0
18	B	814	CLA	5	0
18	B	836	CLA	2	0
18	1	612	CLA	5	0
18	B	808	CLA	4	0
22	A	852	BCR	4	0
18	1	602	CLA	2	0
18	B	803	CLA	4	0
18	L	304	CLA	1	0
22	K	202	BCR	6	0
18	A	834	CLA	2	0
22	A	853	BCR	4	0
26	B	842	PQN	1	0
18	B	816	CLA	1	0
18	2	604	CLA	4	0
18	B	840	CLA	1	0
22	B	801	BCR	9	0
18	A	802	CLA	7	0
18	3	609	CLA	3	0
18	A	803	CLA	6	0
18	A	820	CLA	4	0
18	B	813	CLA	3	0
18	L	302	CLA	1	0
18	A	832	CLA	1	0
21	2	616	LUT	8	0
22	B	843	BCR	4	0
18	2	609	CLA	3	0
18	4	614	CLA	3	0
18	A	811	CLA	2	0
20	1	615	LHG	20	0
21	3	613	LUT	7	0
18	A	808	CLA	1	0
18	A	807	CLA	3	0
18	B	805	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	845	BCR	6	0
24	A	801	CL0	7	0
18	B	834	CLA	1	0
22	J	102	BCR	4	0
18	A	829	CLA	6	0
18	4	604	CLA	2	0
18	A	821	CLA	2	0
21	4	616	LUT	3	0
19	4	617	XAT	18	0
17	1	601	CHL	7	0
18	A	819	CLA	4	0
18	4	612	CLA	2	0
18	B	832	CLA	6	0
18	2	602	CLA	7	0
18	B	830	CLA	3	0
18	B	809	CLA	2	0
22	B	847	BCR	6	0
18	B	841	CLA	2	0
18	3	601	CLA	1	0
18	A	815	CLA	1	0
18	B	839	CLA	1	0
23	4	619	LMG	1	0
18	B	824	CLA	2	0
18	B	838	CLA	2	0
17	4	606	CHL	2	0
18	B	831	CLA	1	0
20	A	847	LHG	3	0
18	4	609	CLA	3	0
22	A	848	BCR	7	0
22	L	301	BCR	4	0
22	A	849	BCR	3	0
18	A	825	CLA	4	0
18	A	836	CLA	1	0
18	A	818	CLA	3	0
17	2	601	CHL	1	0
18	B	826	CLA	3	0
18	B	833	CLA	1	0
18	A	813	CLA	2	0
18	A	835	CLA	1	0
18	A	843	CLA	3	0
18	A	831	CLA	1	0
21	2	619	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	846	LHG	3	0
18	H	201	CLA	1	0
18	2	612	CLA	2	0
19	2	617	XAT	6	0
18	1	607	CLA	5	0
18	B	828	CLA	7	0
18	A	809	CLA	9	0
27	B	850	DGD	8	0
18	L	303	CLA	4	0
18	K	203	CLA	1	0
18	G	201	CLA	1	0
18	4	608	CLA	2	0
18	A	814	CLA	2	0
18	3	612	CLA	2	0
22	L	305	BCR	8	0
18	A	822	CLA	3	0
18	3	603	CLA	2	0
22	4	618	BCR	8	0
21	1	616	LUT	9	0
18	A	805	CLA	1	0
18	B	823	CLA	2	0
18	B	802	CLA	4	0
18	A	806	CLA	7	0
20	B	852	LHG	1	0
18	A	827	CLA	2	0
18	4	603	CLA	1	0
18	3	607	CLA	1	0
18	4	610	CLA	1	0
18	A	844	CLA	7	0
17	2	605	CHL	2	0
18	B	811	CLA	1	0
22	B	844	BCR	6	0
18	1	604	CLA	4	0
17	2	615	CHL	1	0
17	4	607	CHL	1	0
18	A	812	CLA	6	0
18	A	810	CLA	1	0
22	A	851	BCR	7	0
18	A	830	CLA	6	0
18	2	603	CLA	2	0
18	4	613	CLA	3	0
18	B	837	CLA	2	0

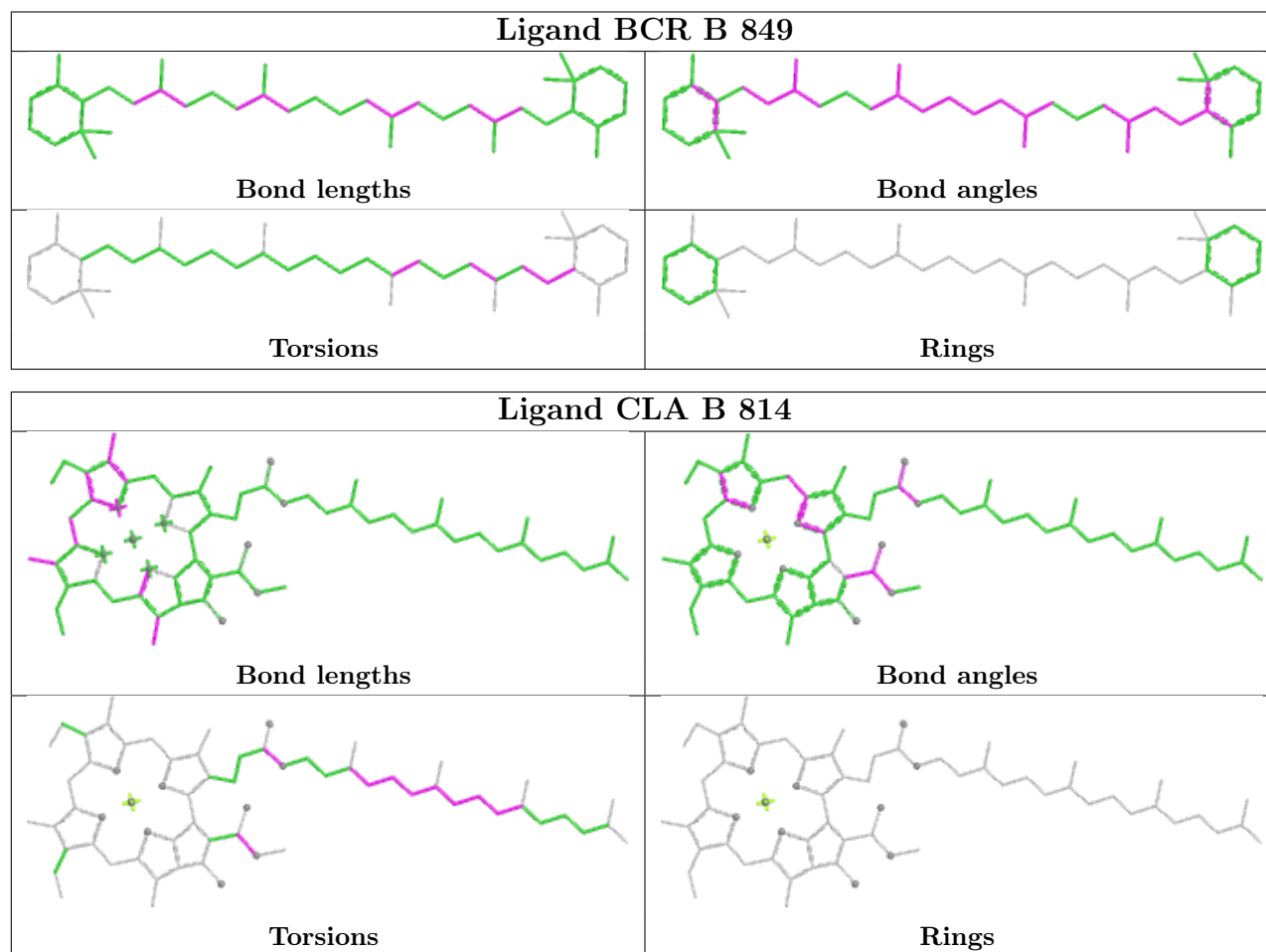
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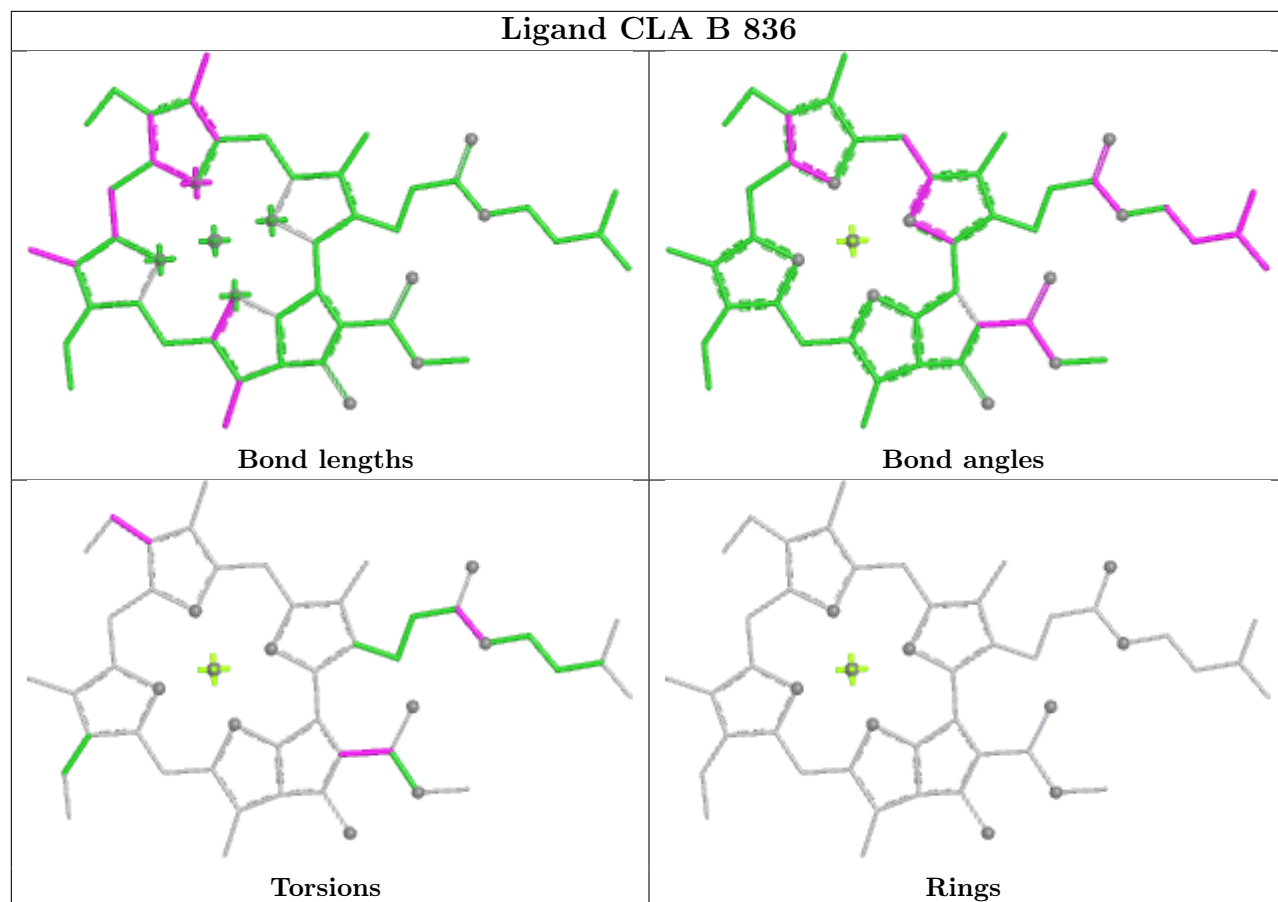
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	304	BCR	1	0
18	1	603	CLA	2	0
18	1	605	CLA	1	0
18	4	602	CLA	5	0
17	4	605	CHL	1	0
18	B	827	CLA	3	0
19	1	614	XAT	9	0
22	G	204	BCR	3	0
22	L	306	BCR	2	0
18	B	817	CLA	1	0
18	F	301	CLA	2	0
22	A	850	BCR	6	0
18	2	608	CLA	2	0
18	A	839	CLA	1	0
22	K	205	BCR	4	0
18	B	822	CLA	7	0
18	A	828	CLA	2	0
22	B	848	BCR	3	0
18	B	819	CLA	1	0
18	1	609	CLA	6	0
22	I	101	BCR	2	0
18	A	842	CLA	6	0
22	B	846	BCR	7	0
18	3	608	CLA	2	0
18	A	826	CLA	2	0
22	3	614	BCR	2	0
18	F	302	CLA	6	0
18	A	833	CLA	2	0
18	B	825	CLA	5	0
17	2	607	CHL	1	0
18	1	608	CLA	2	0
26	A	855	PQN	5	0
18	B	829	CLA	2	0
18	2	611	CLA	2	0
18	A	804	CLA	8	0
18	A	838	CLA	1	0
18	B	806	CLA	5	0
18	A	841	CLA	5	0

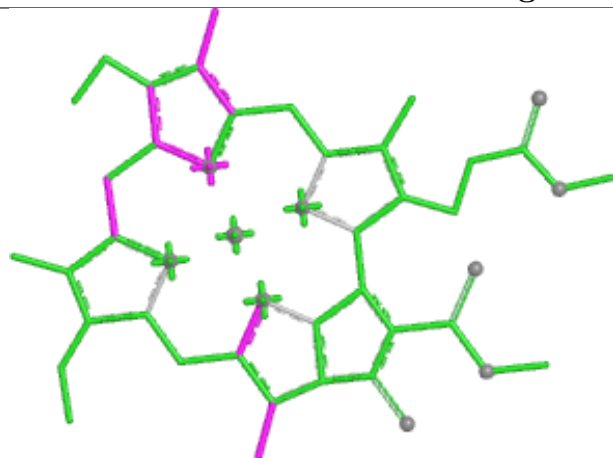
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

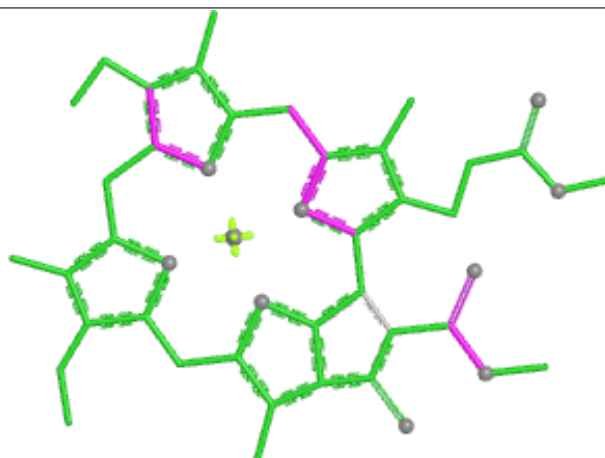




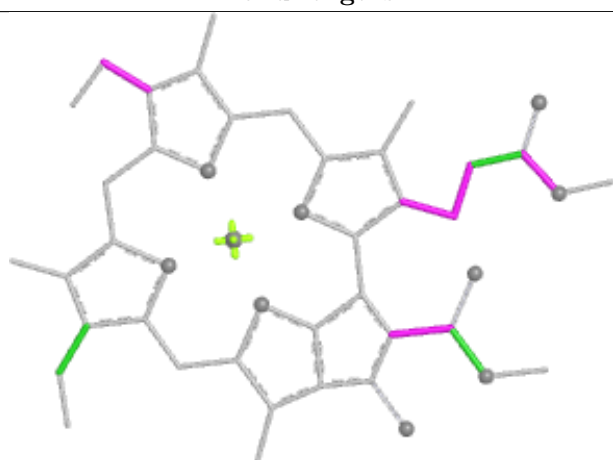
Ligand CLA 1 612



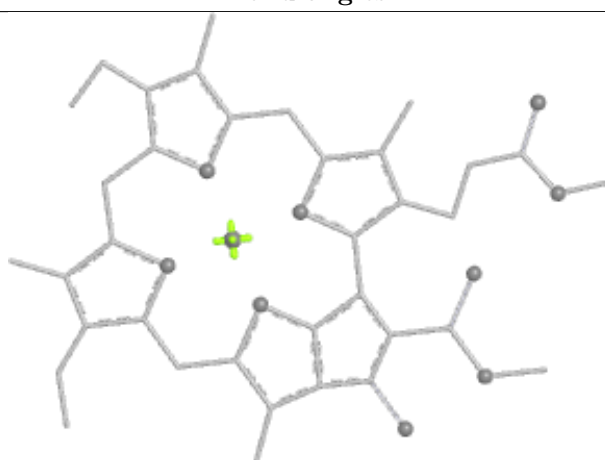
Bond lengths



Bond angles

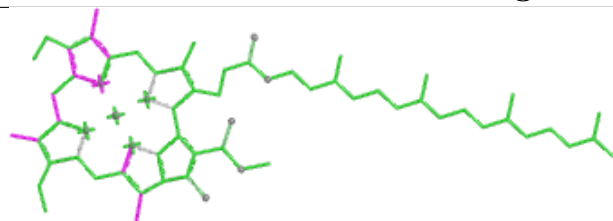


Torsions

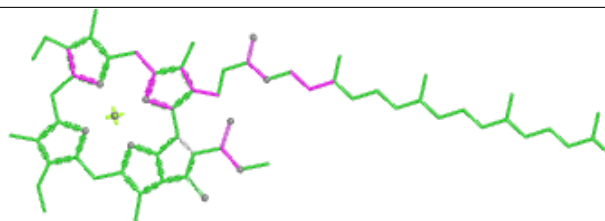


Rings

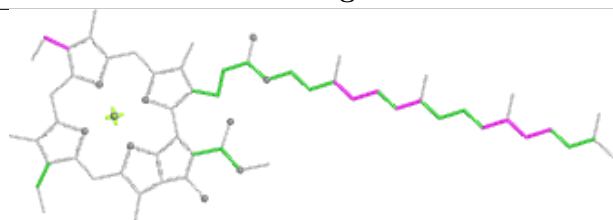
Ligand CLA B 808



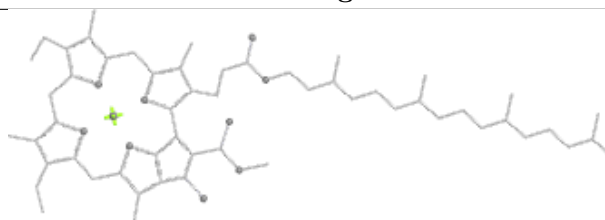
Bond lengths



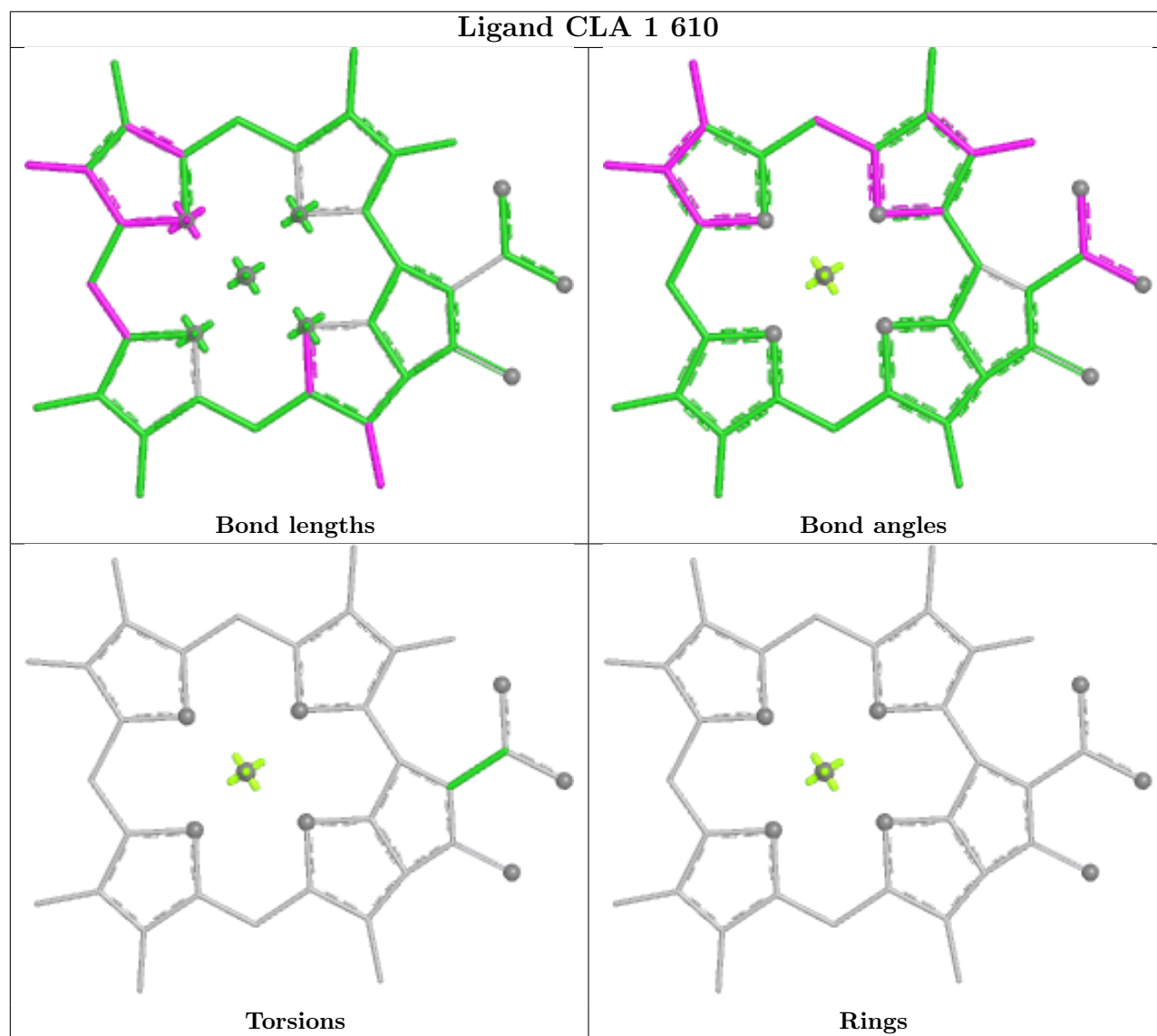
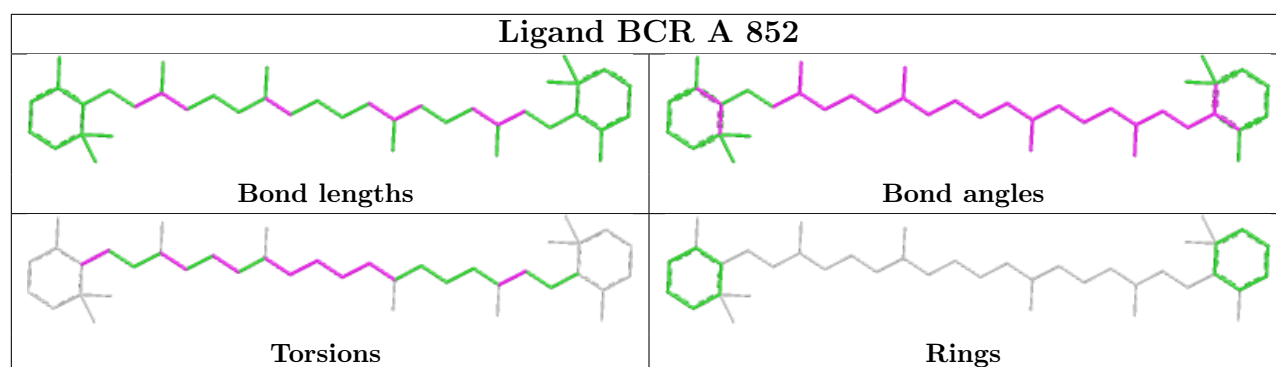
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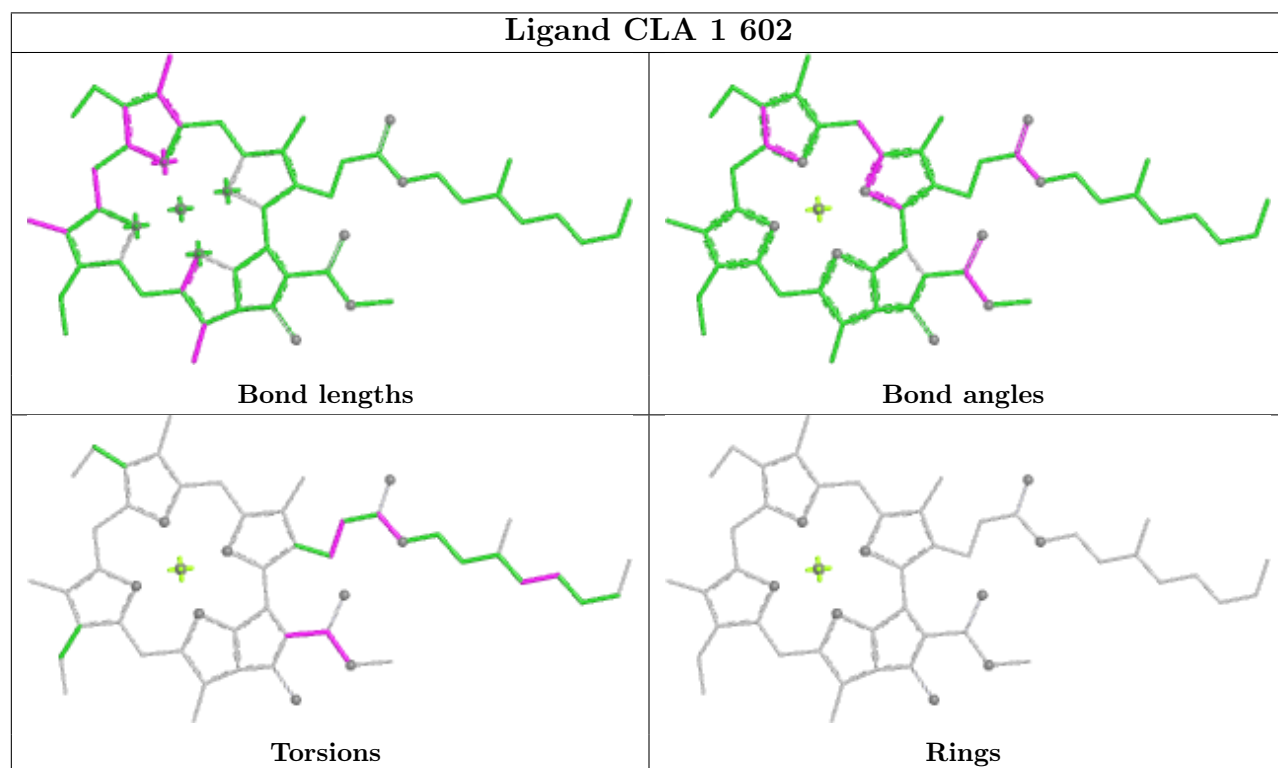
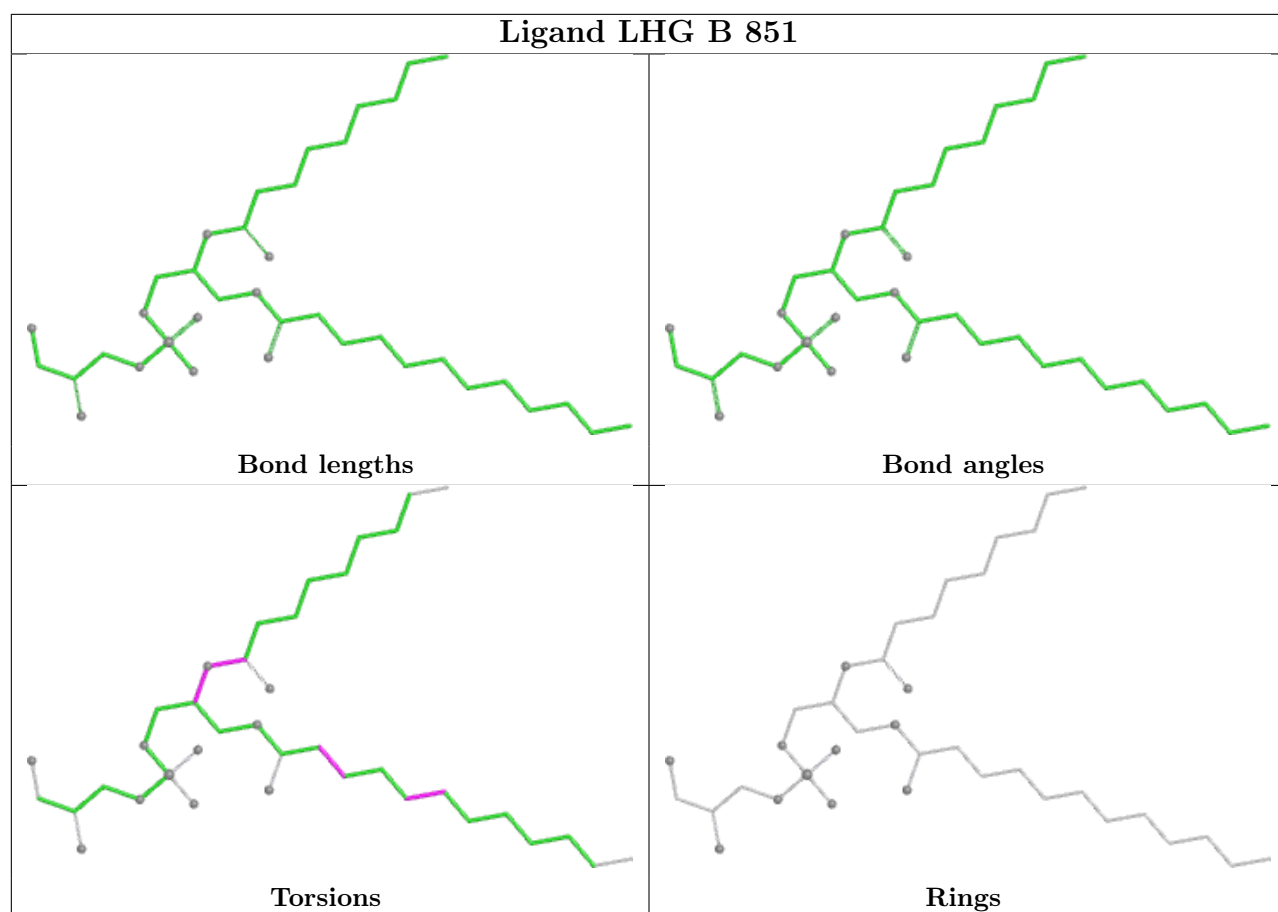


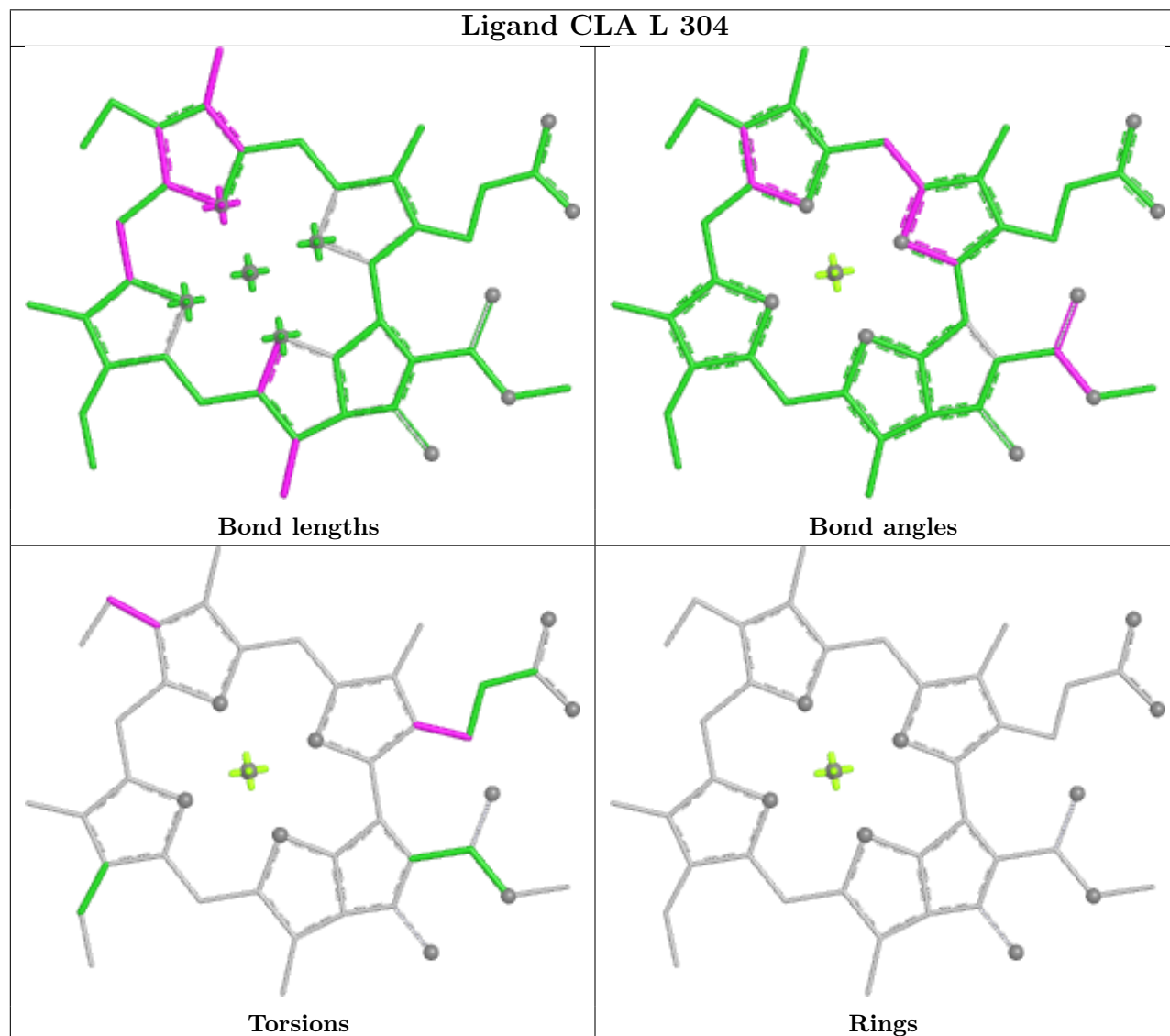
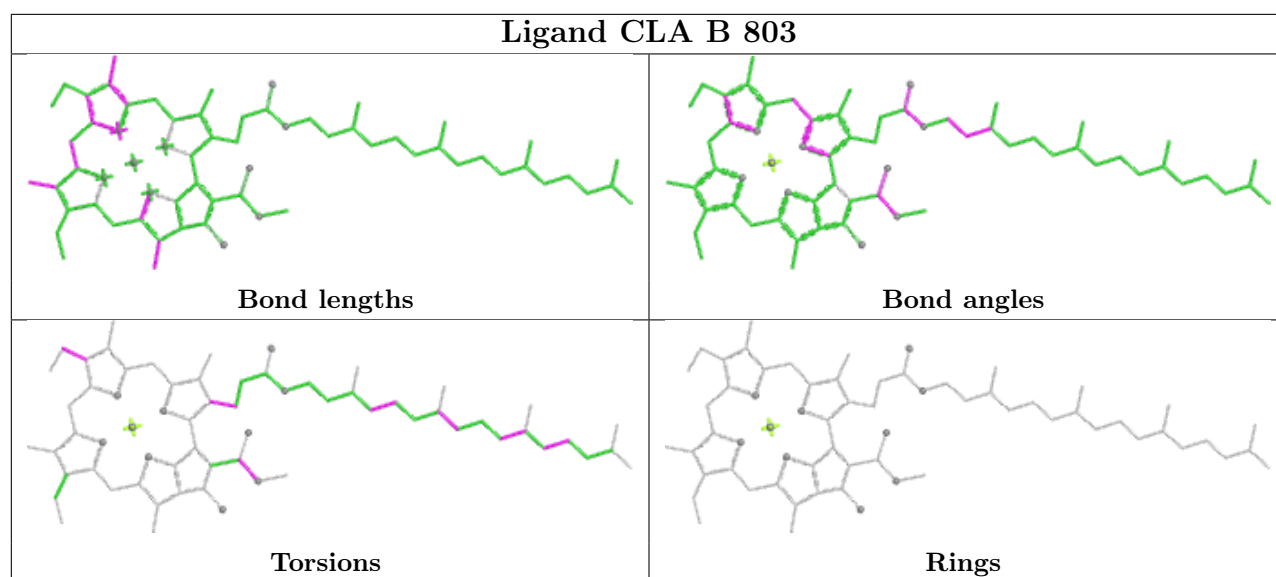
Torsions

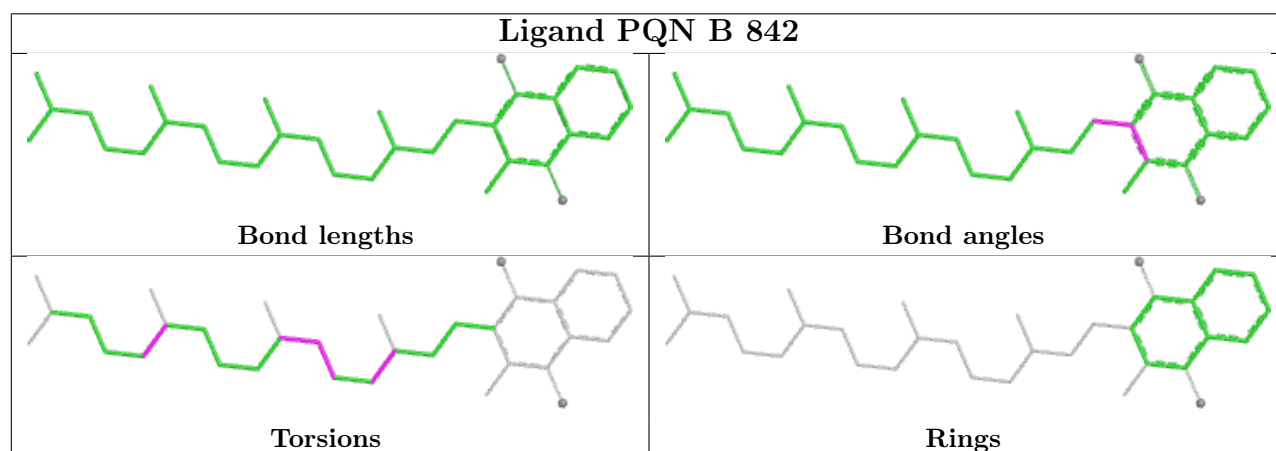
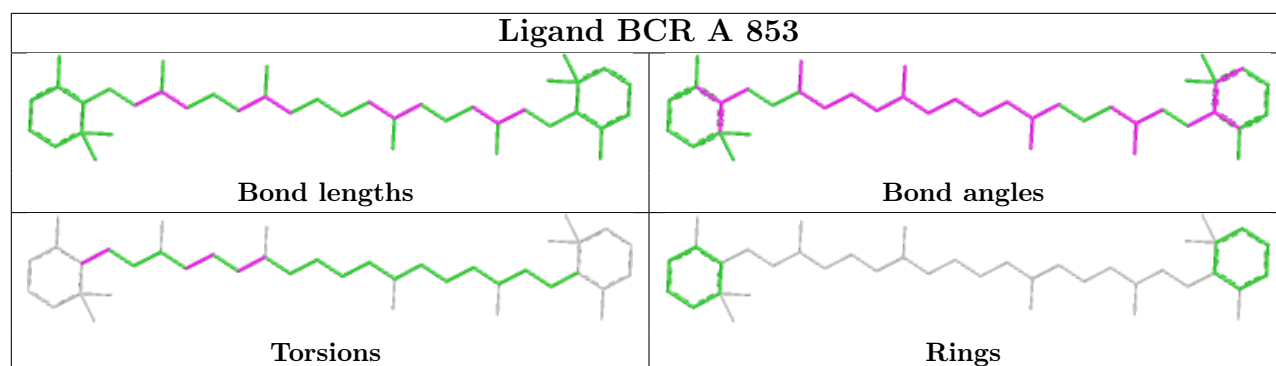
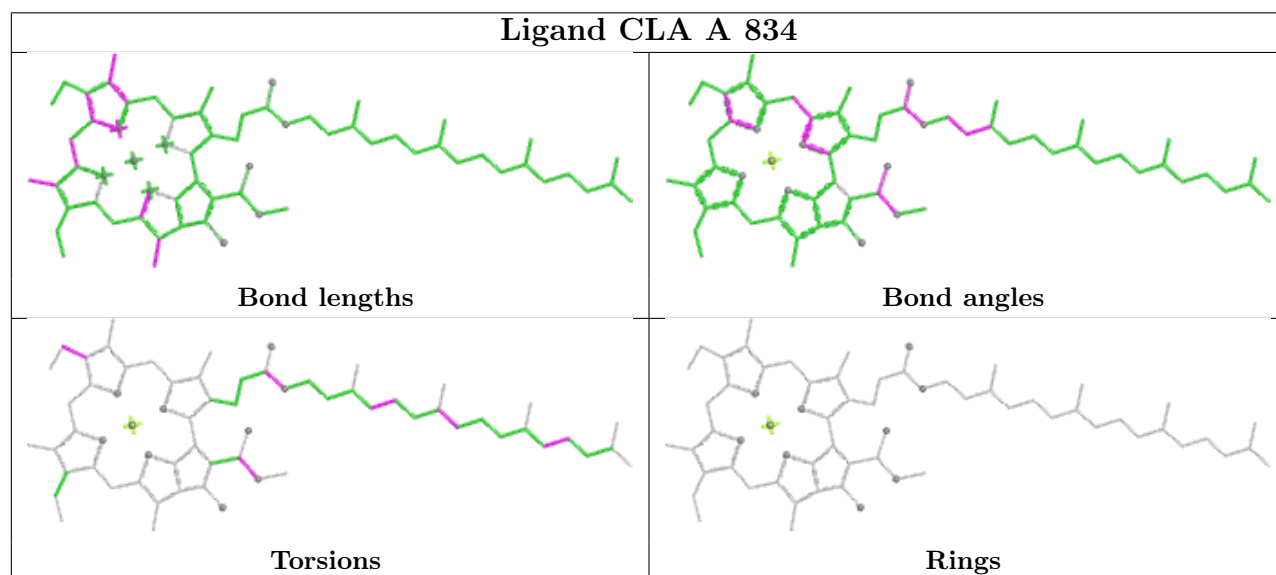
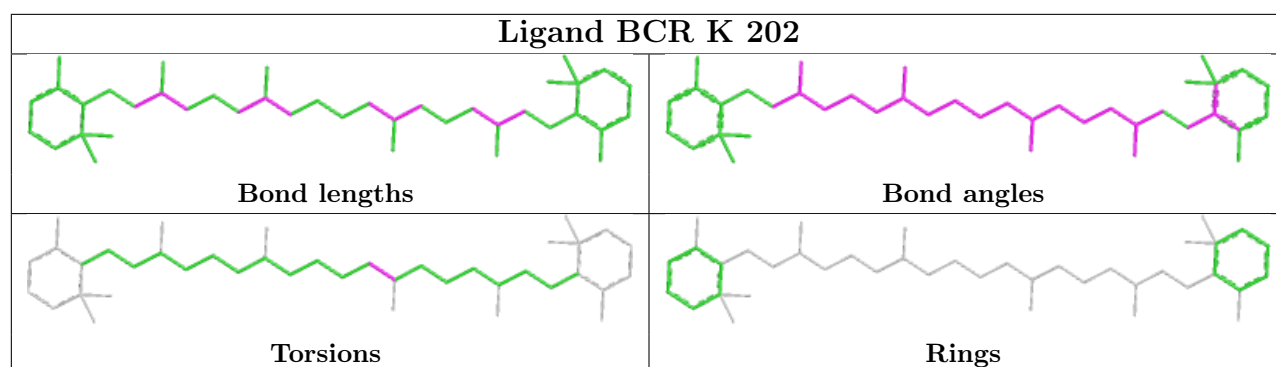


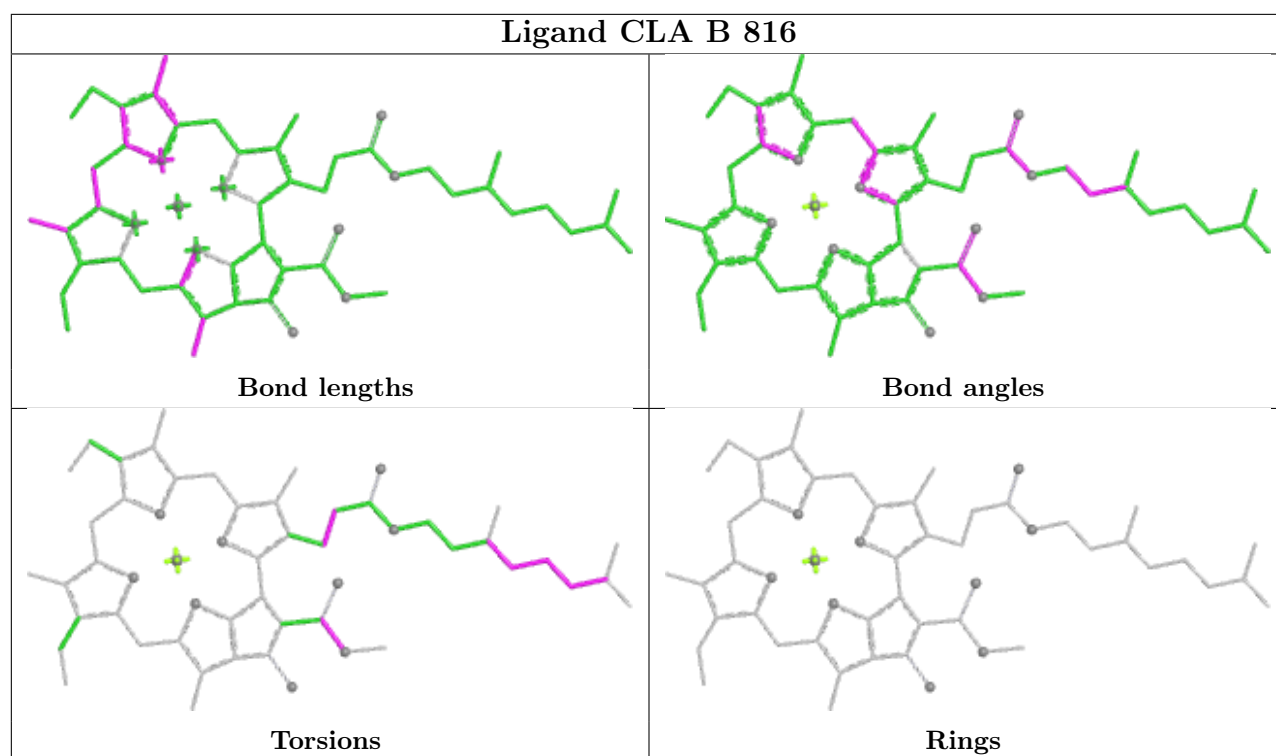
Rings

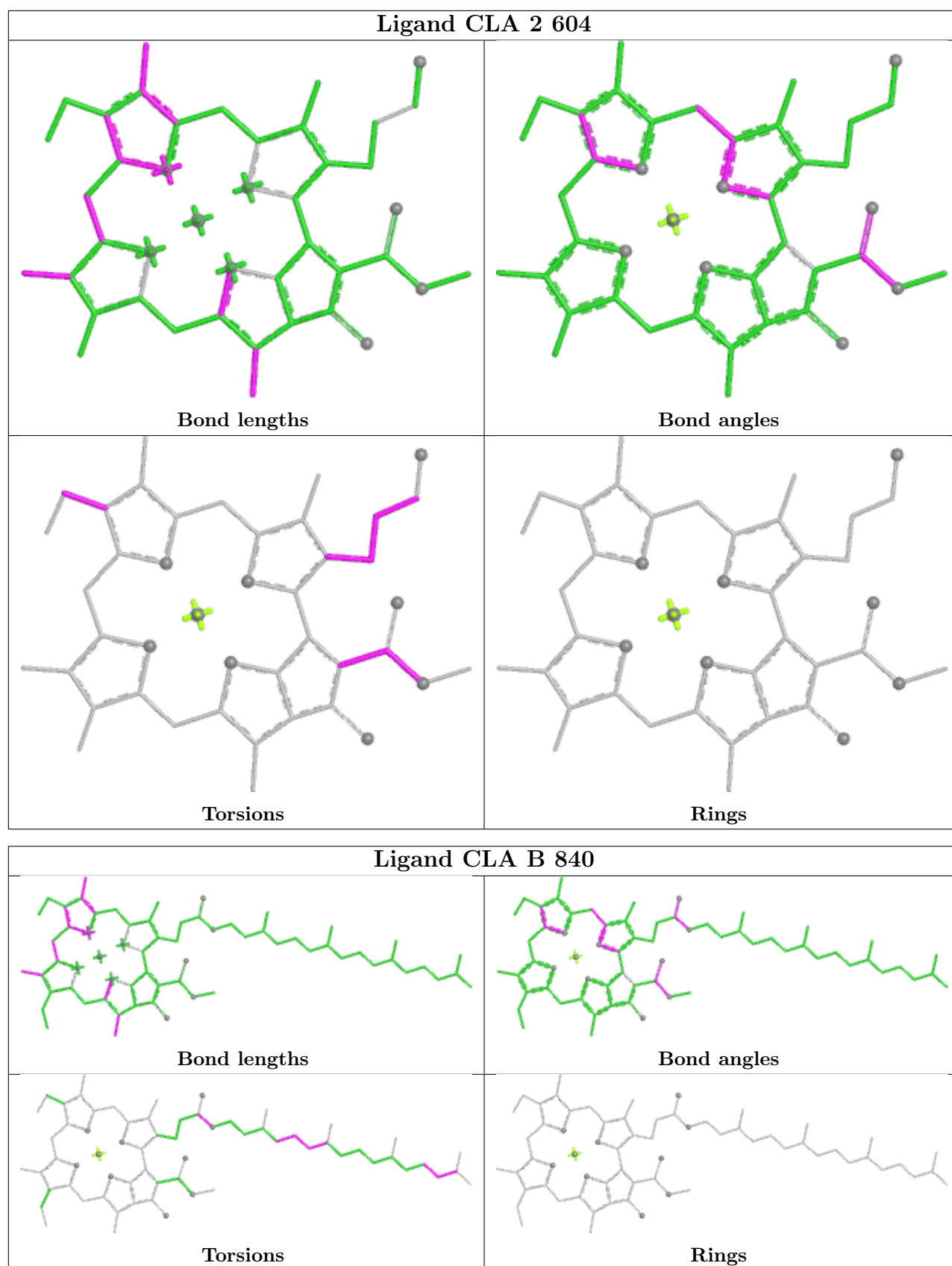


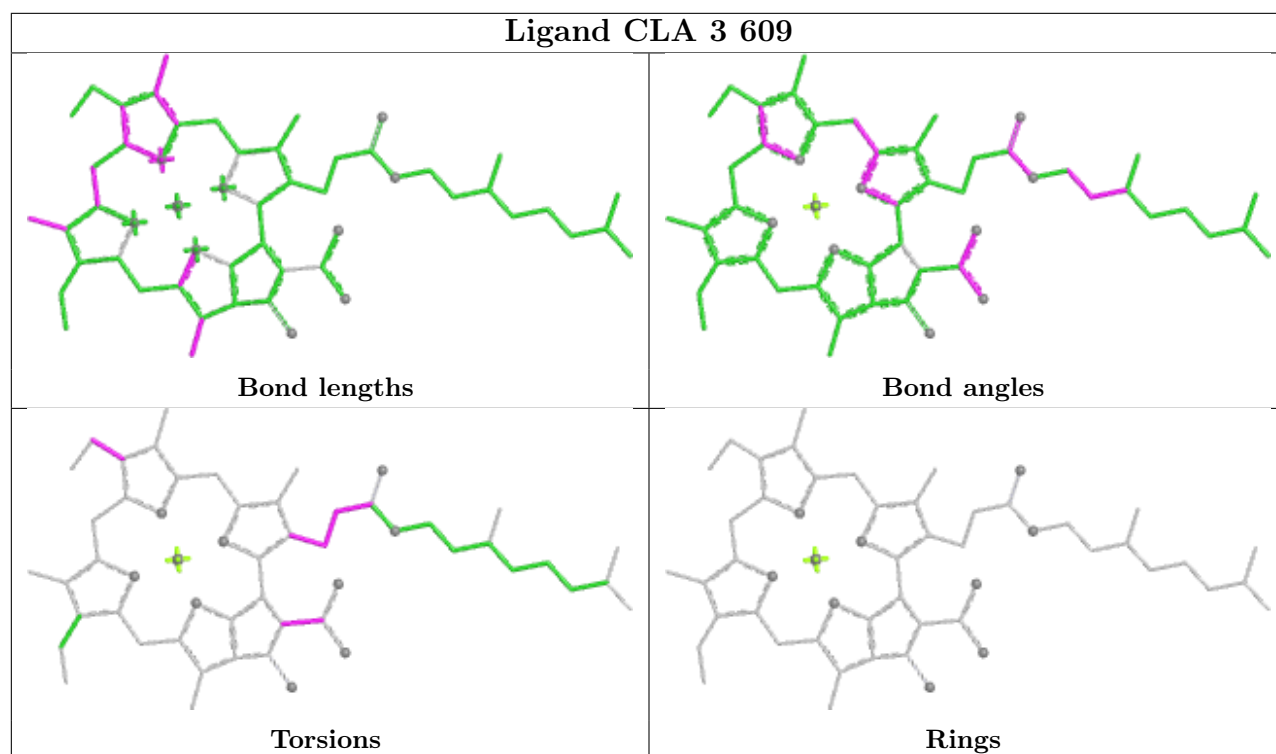
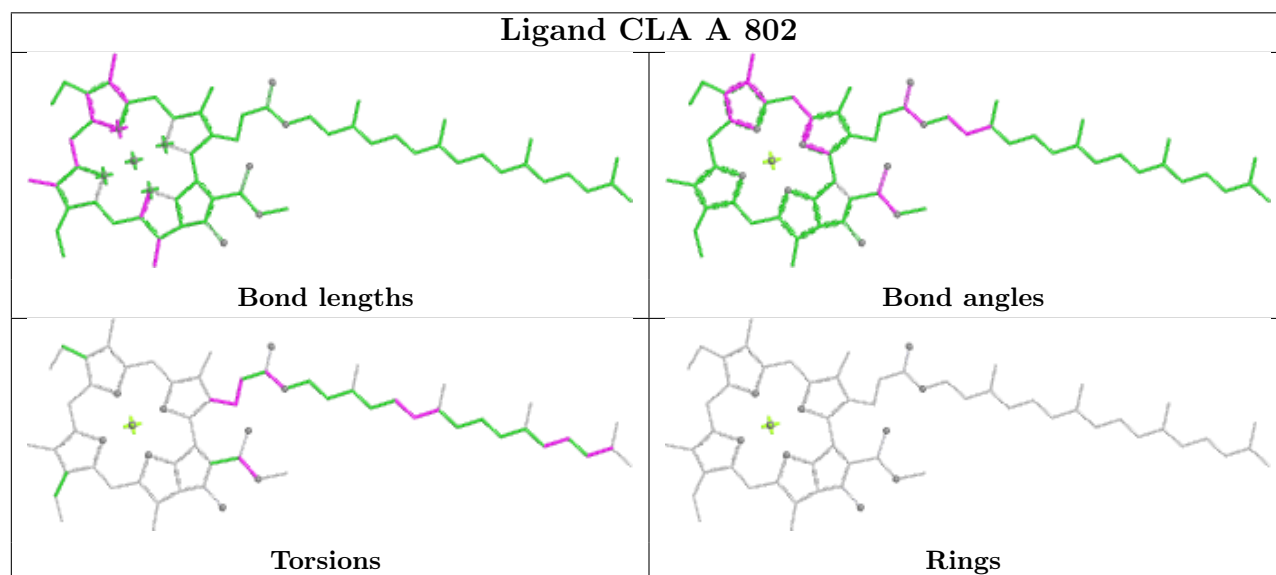
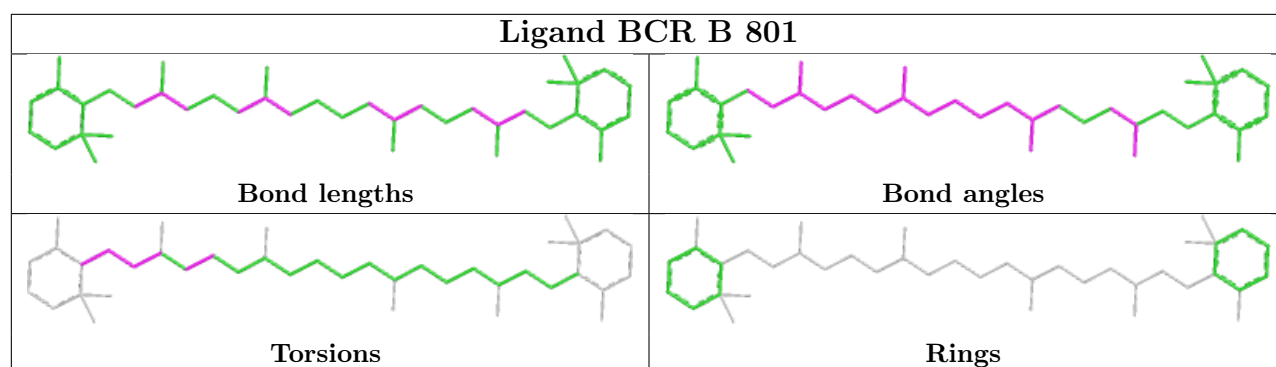


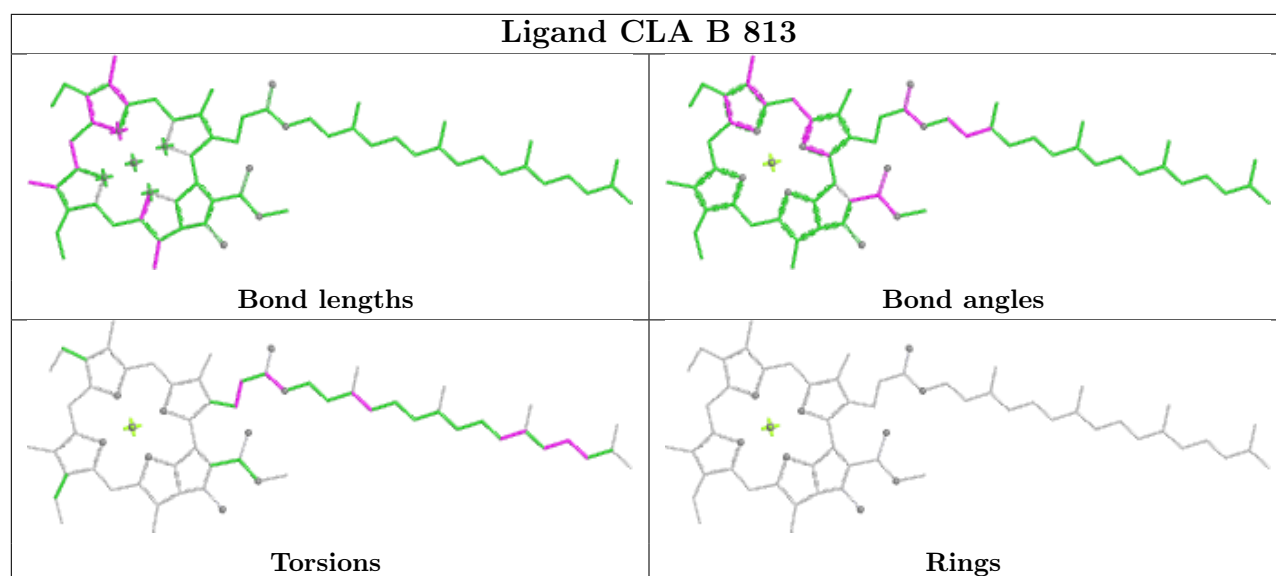
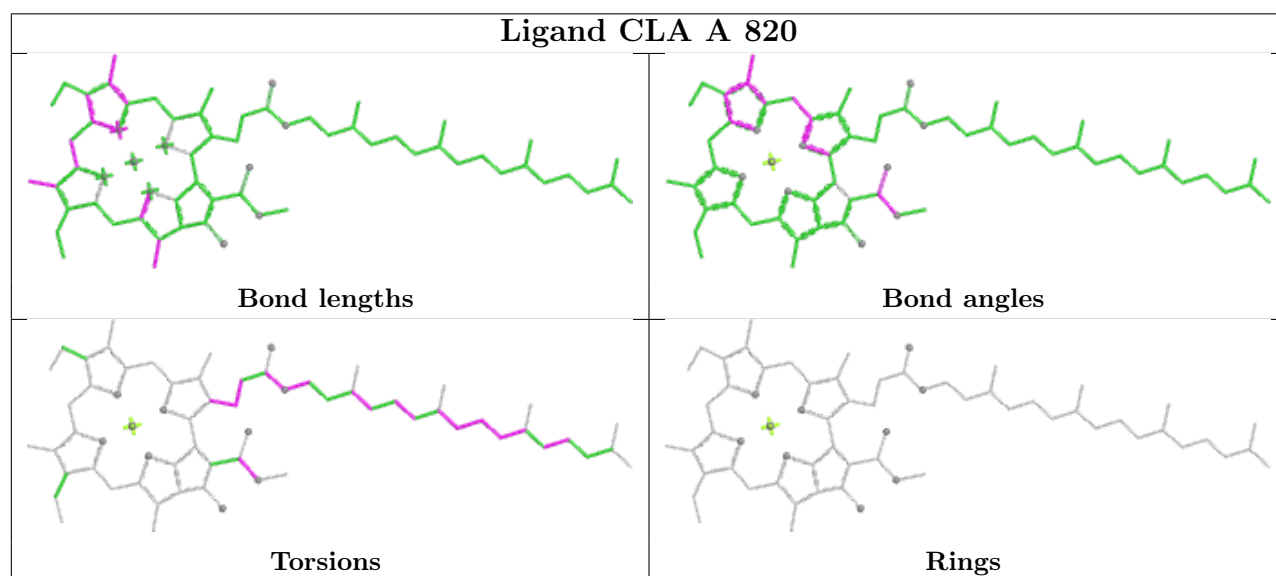
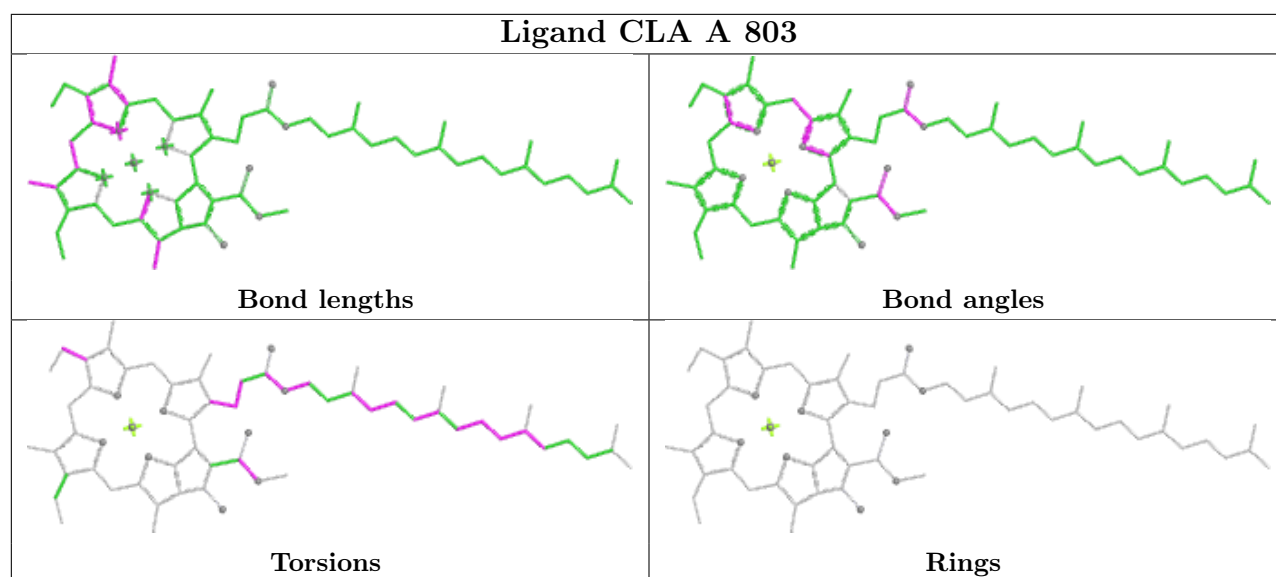




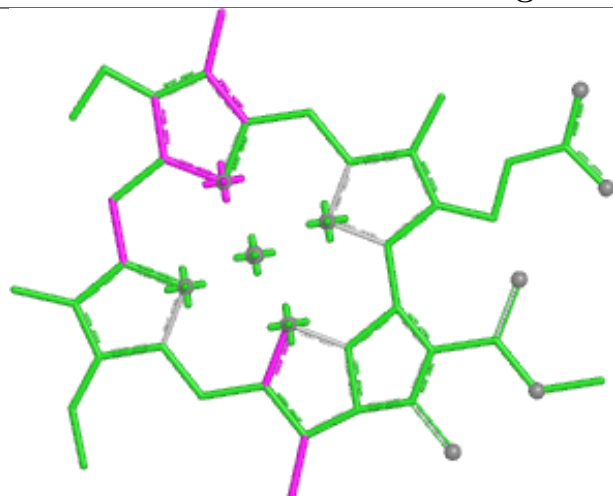




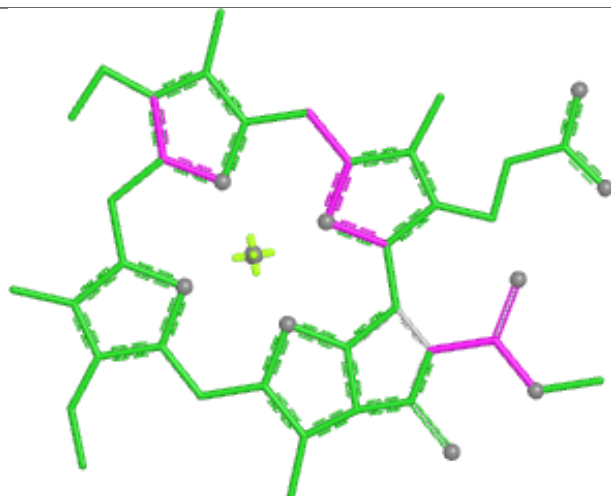




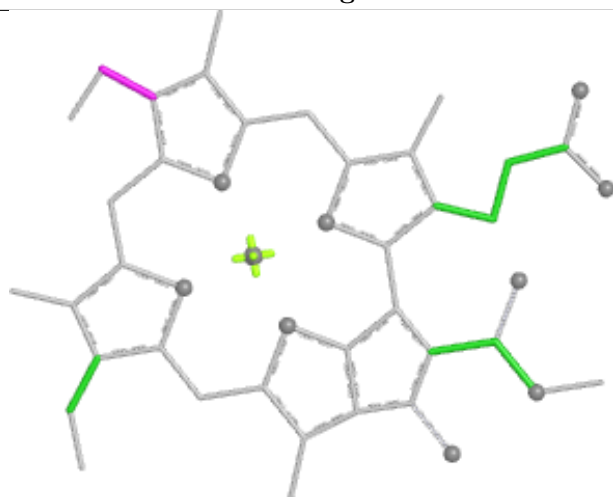
Ligand CLA L 302



Bond lengths



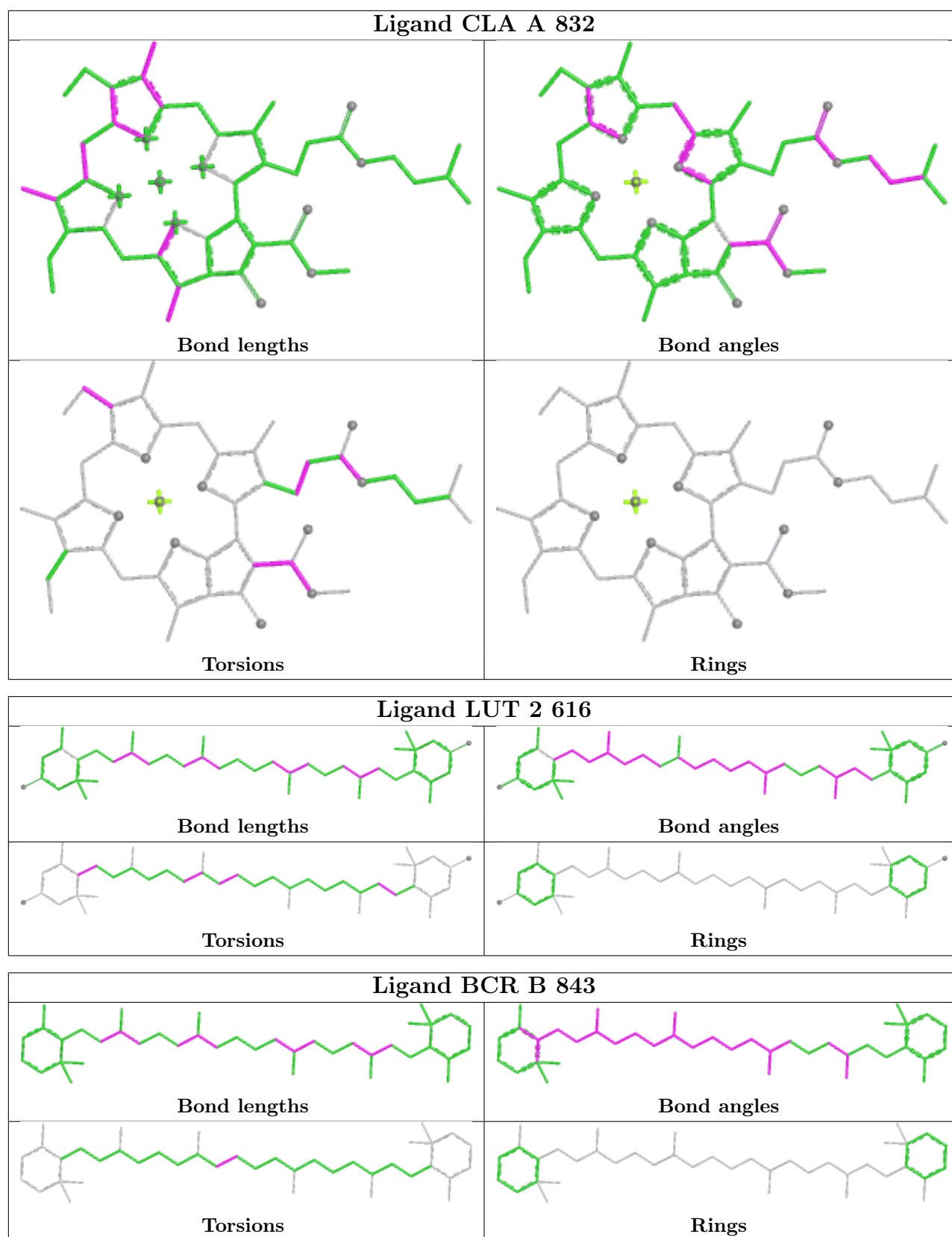
Bond angles



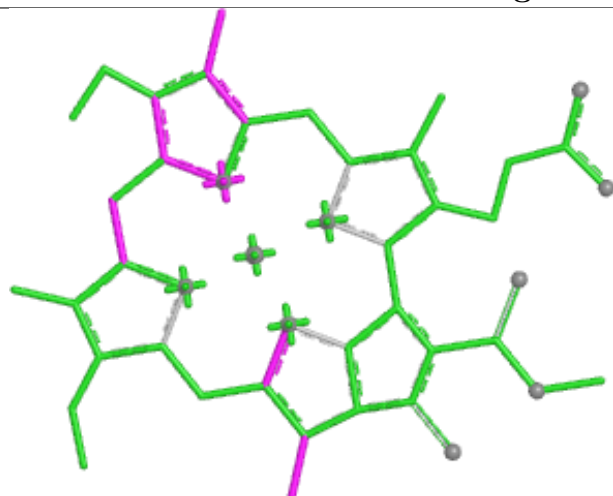
Torsions



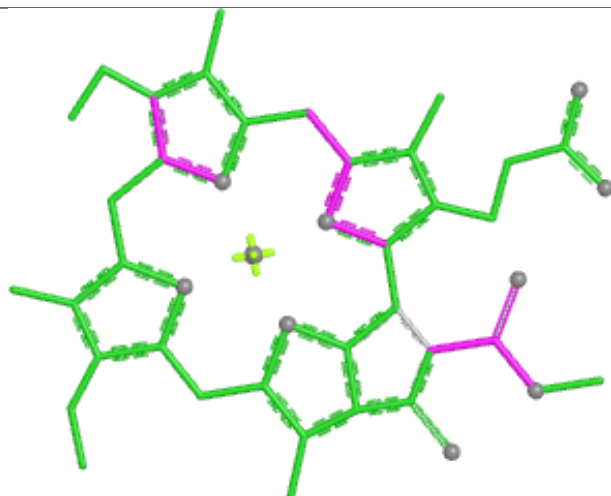
Rings



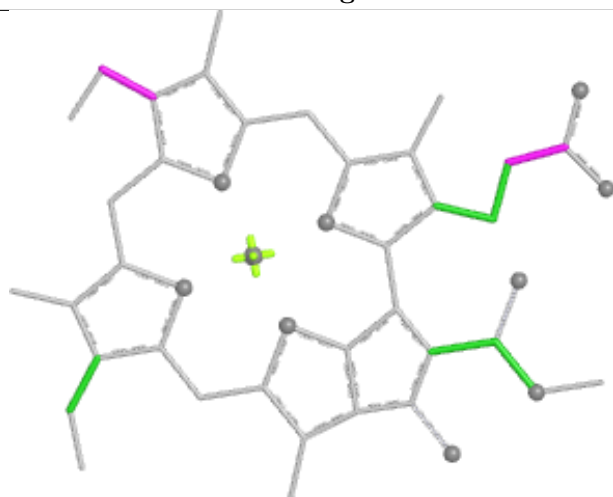
Ligand CLA A 837



Bond lengths



Bond angles

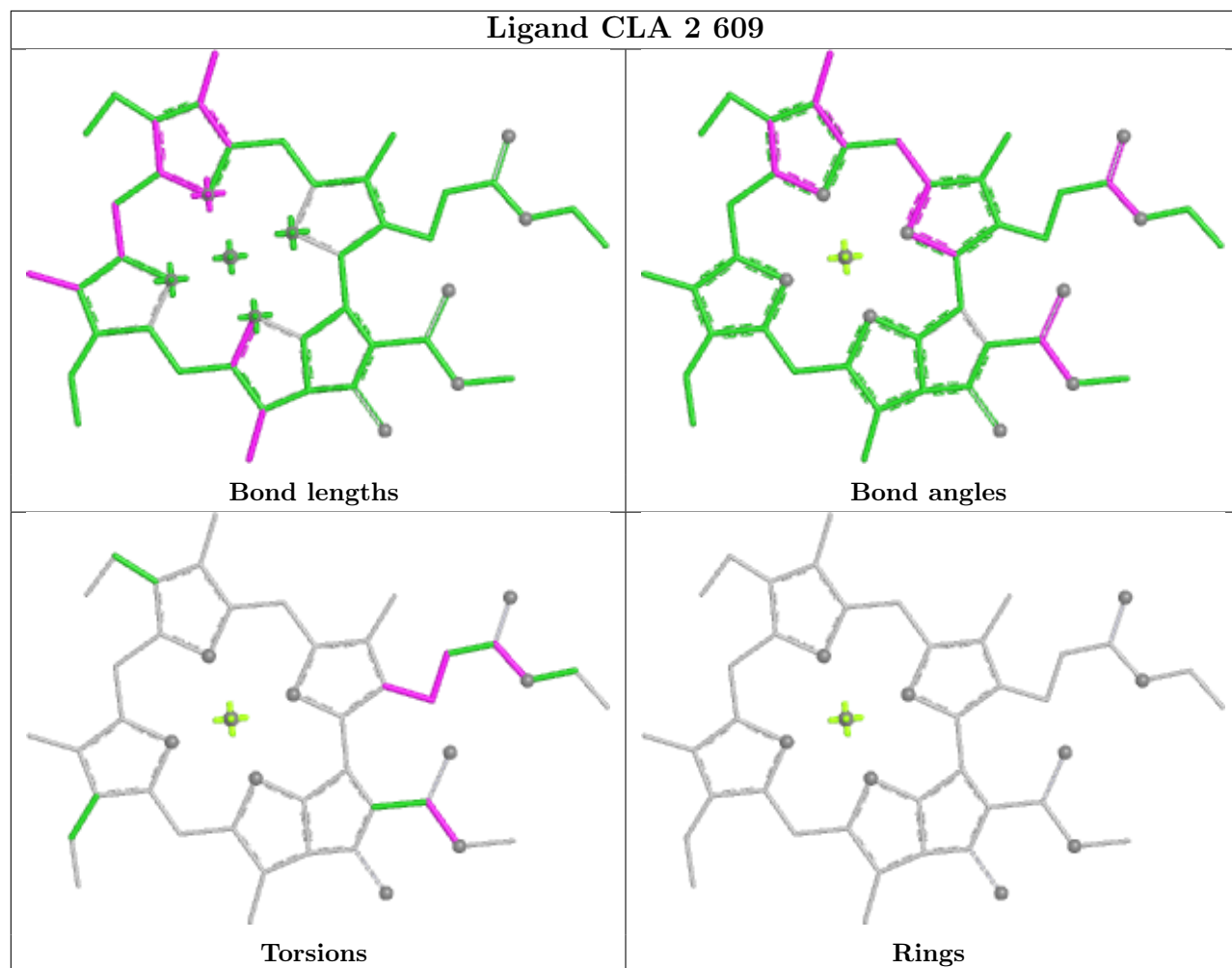


Torsions

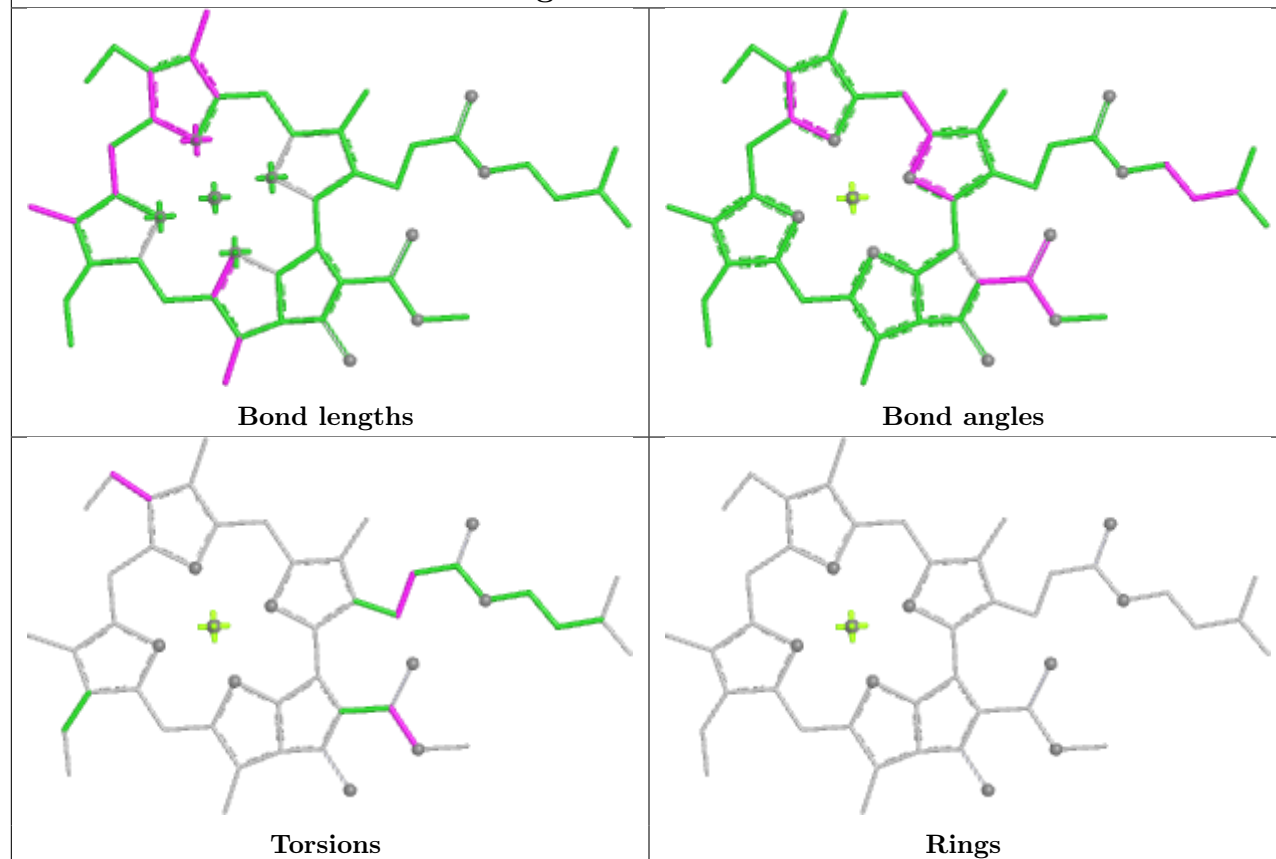


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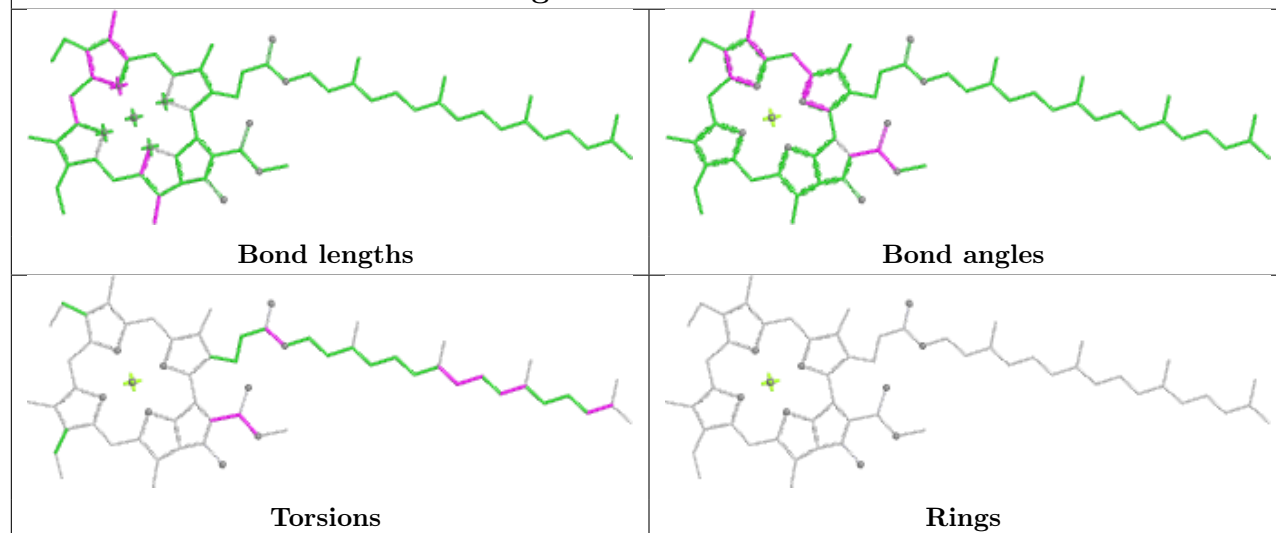
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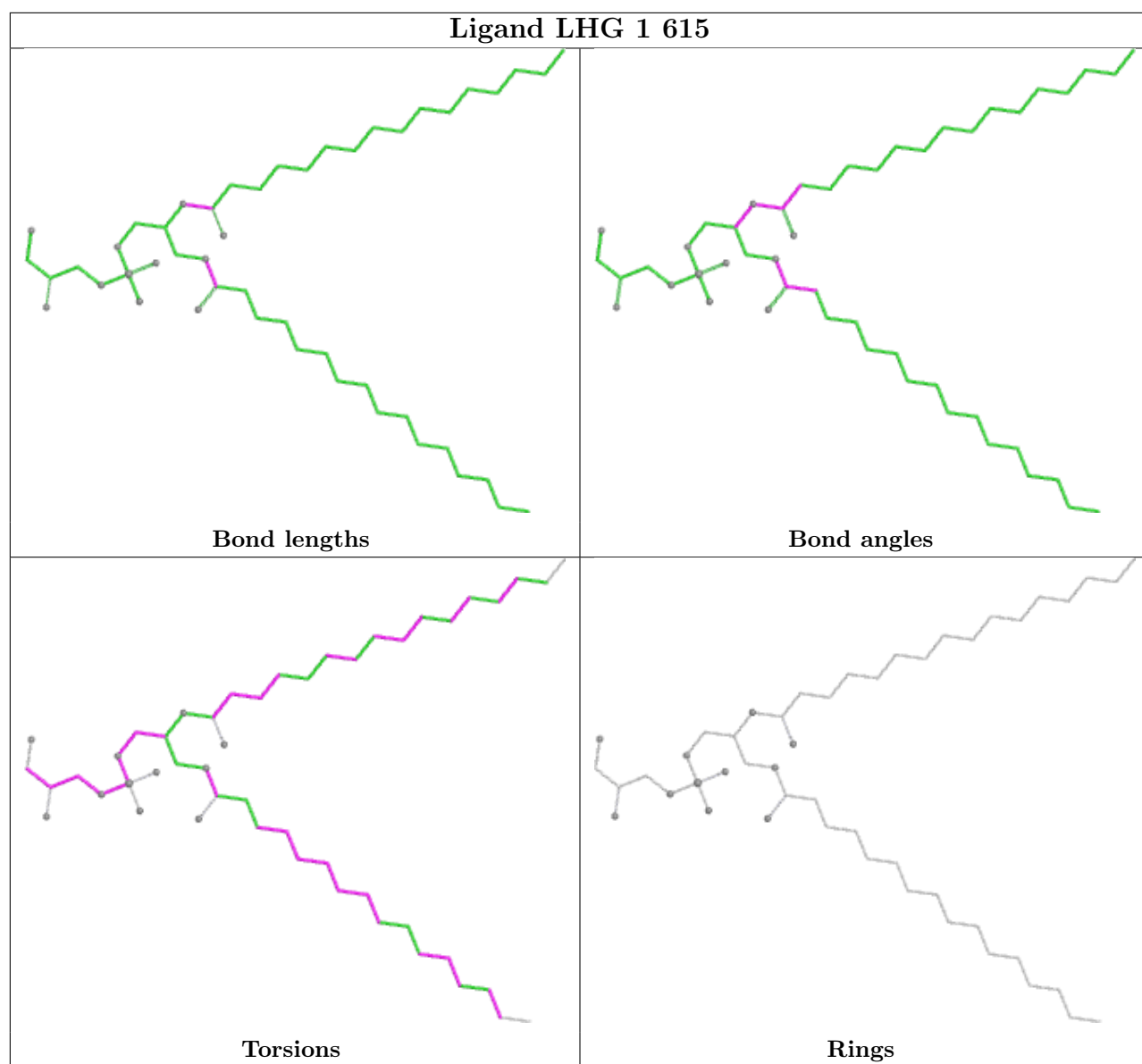


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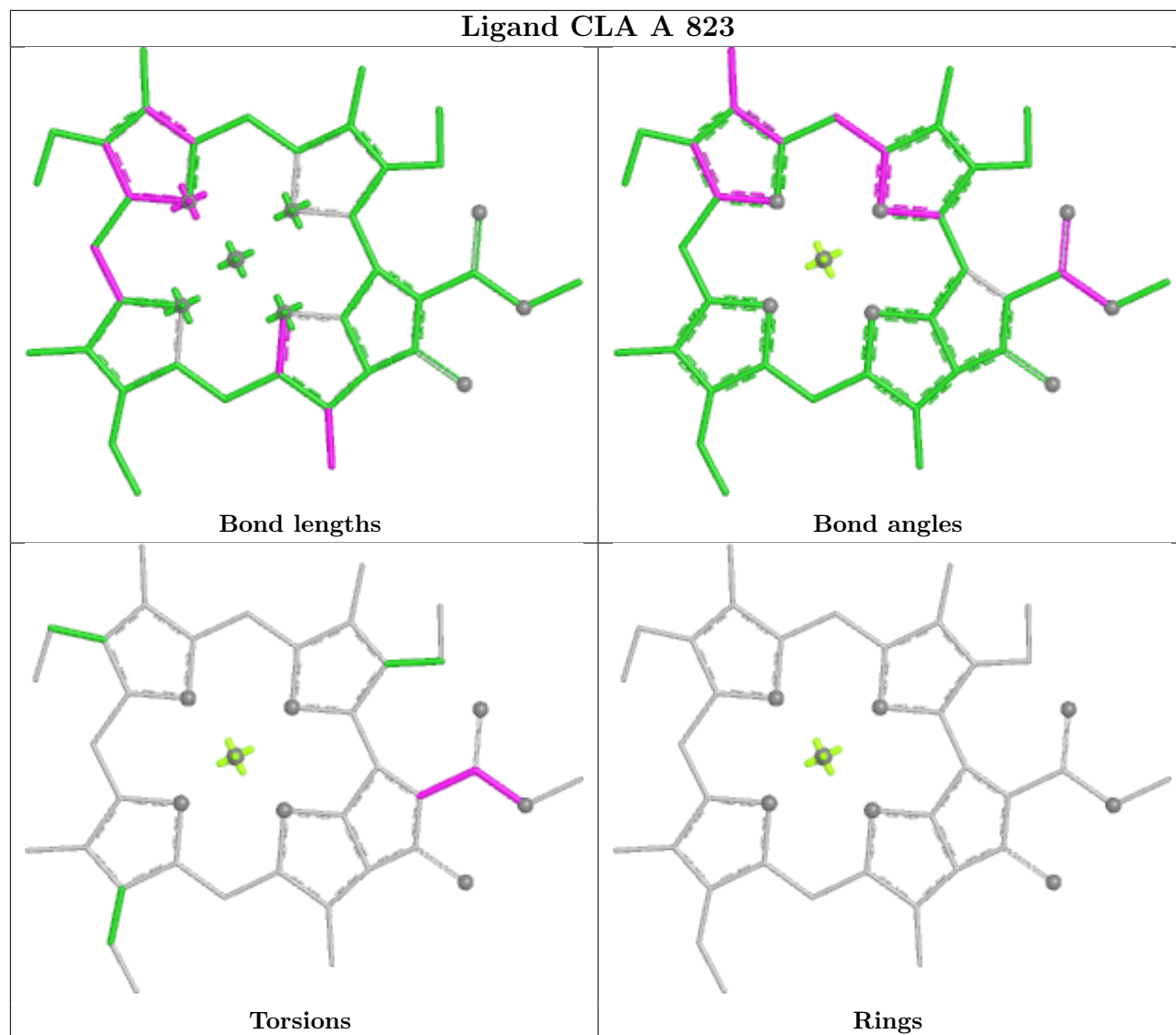


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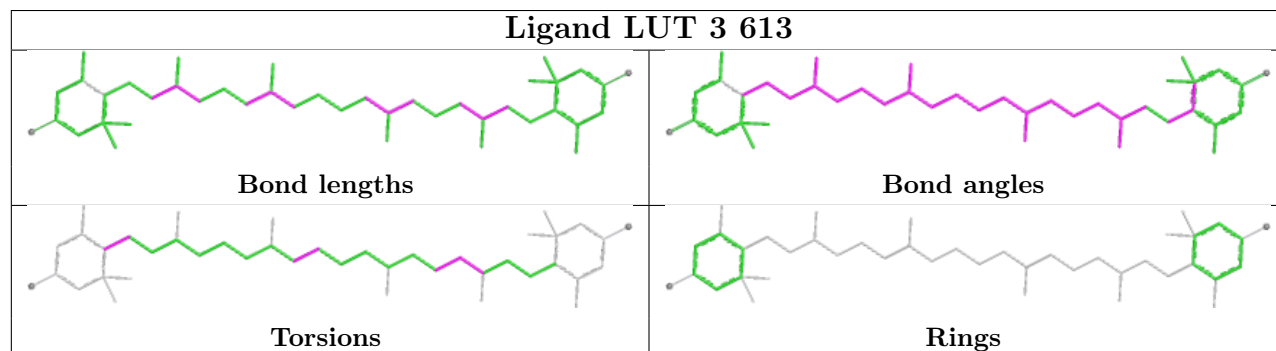




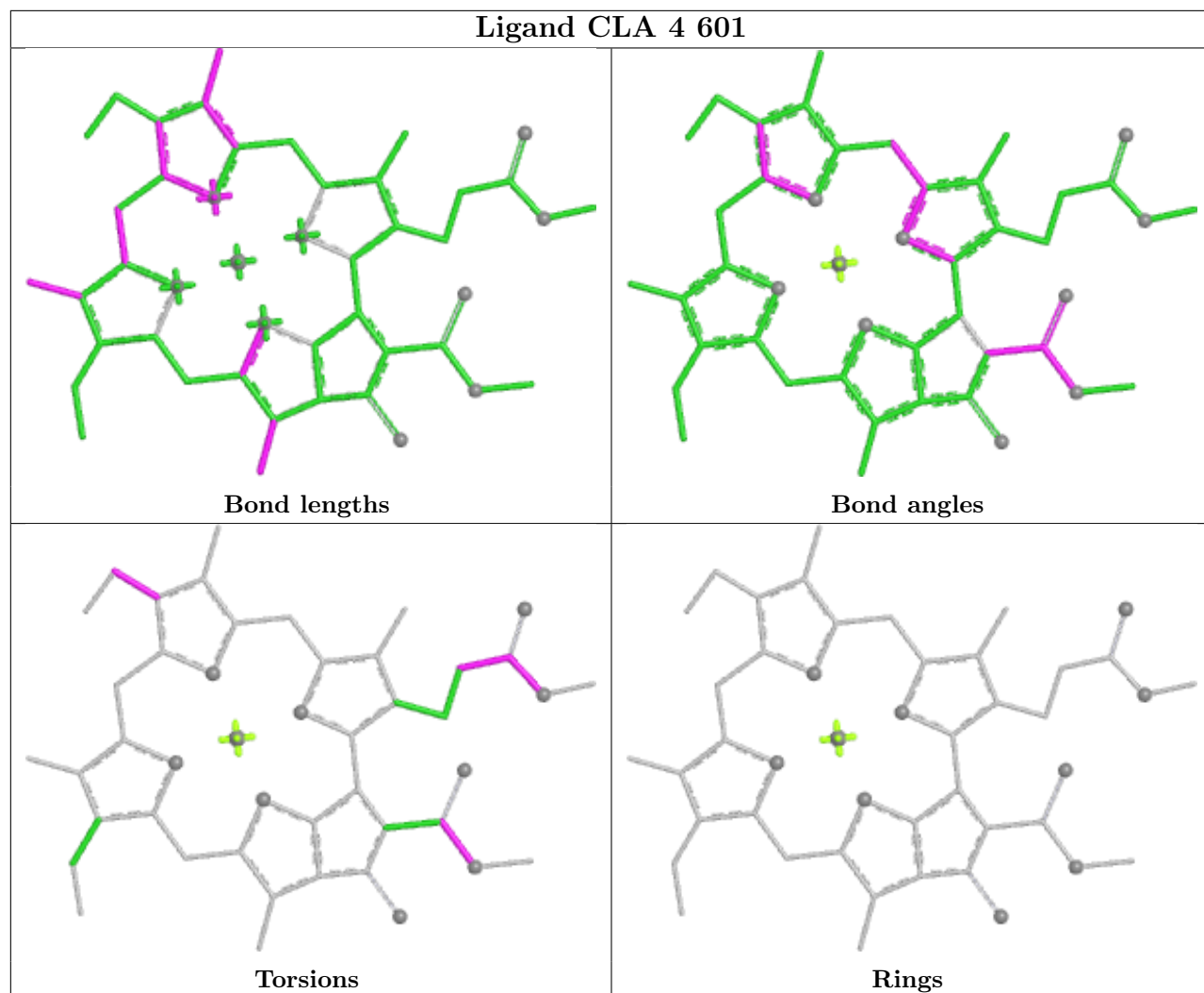
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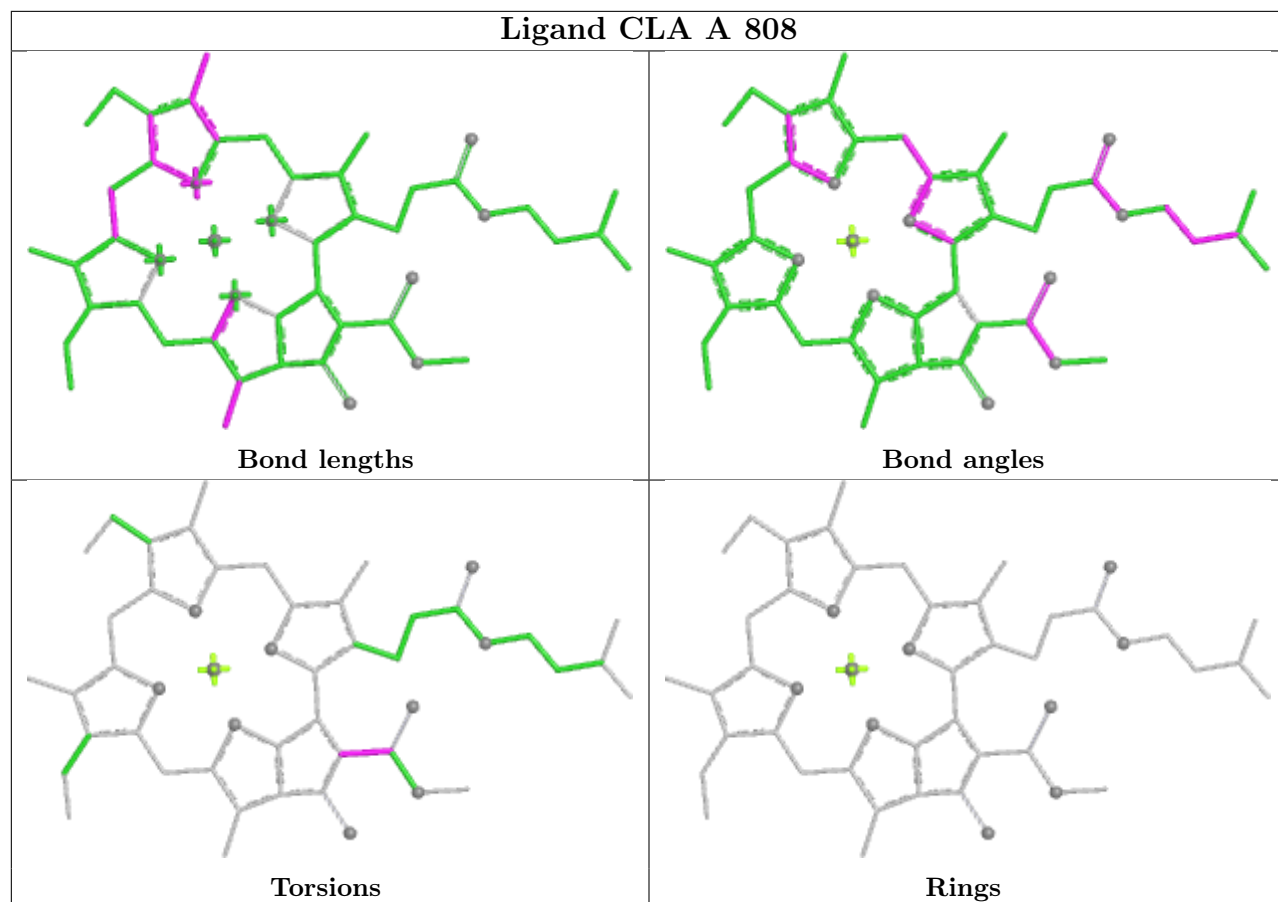


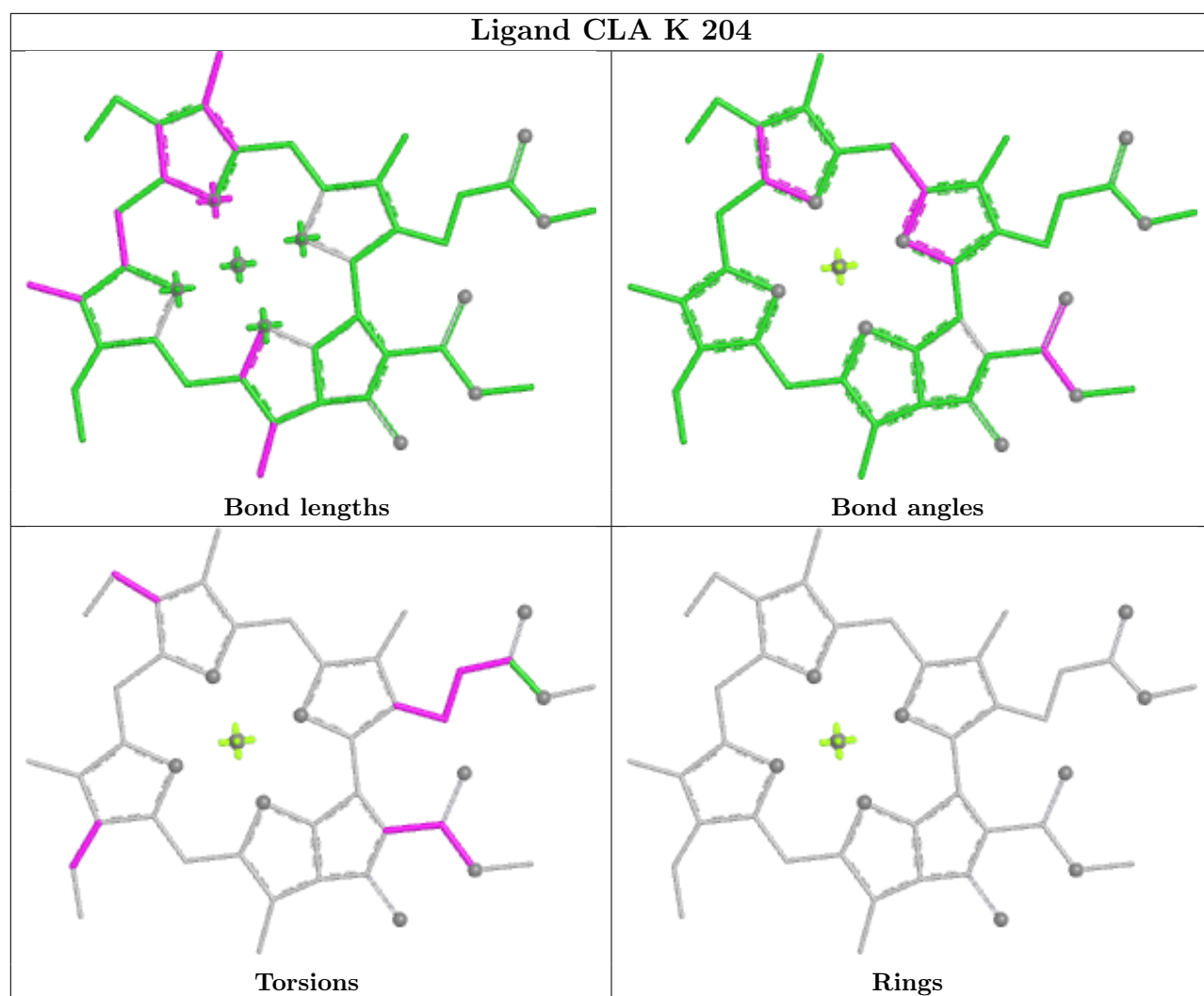
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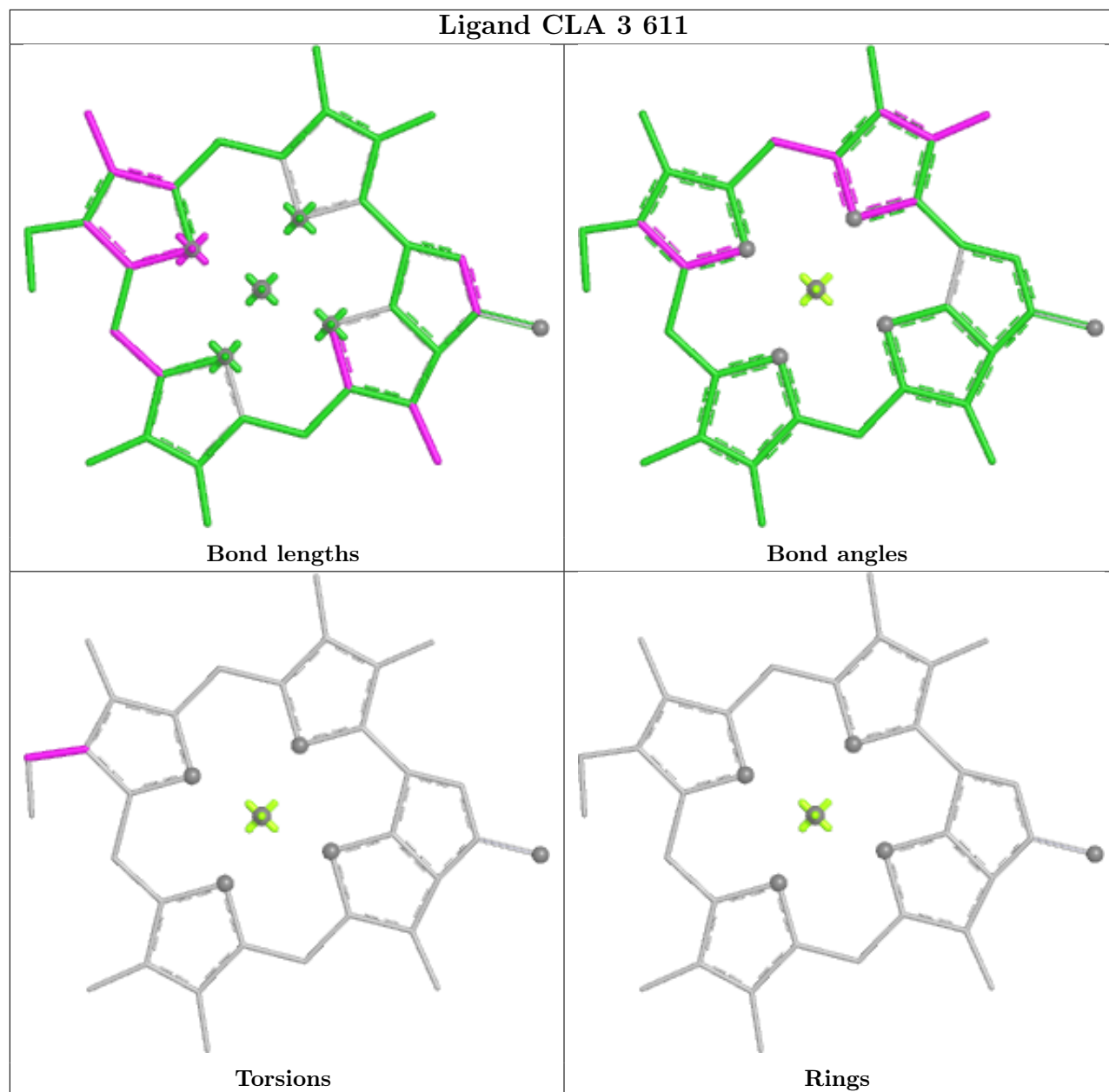


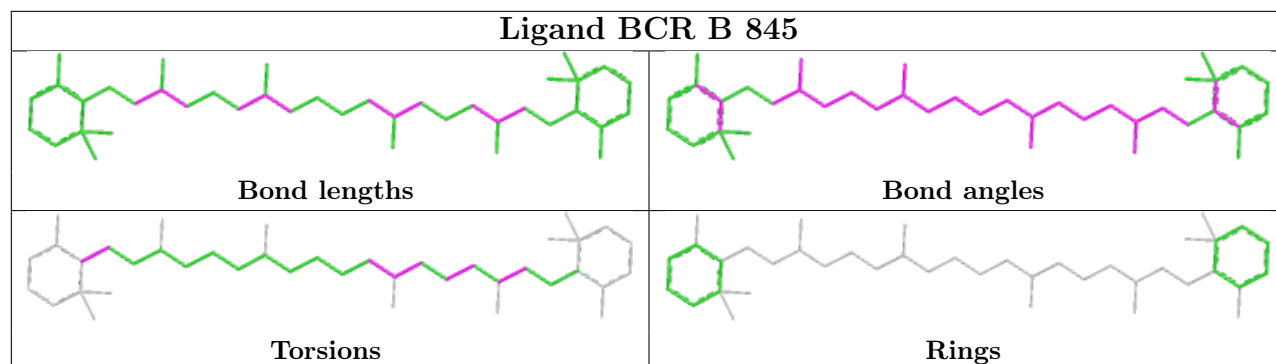
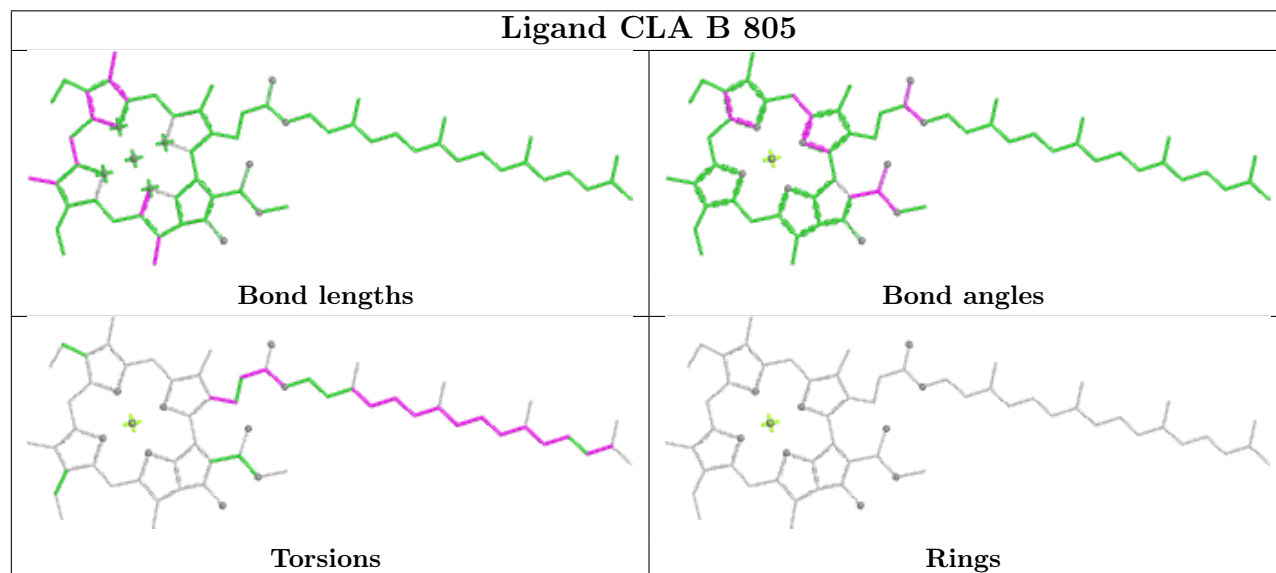
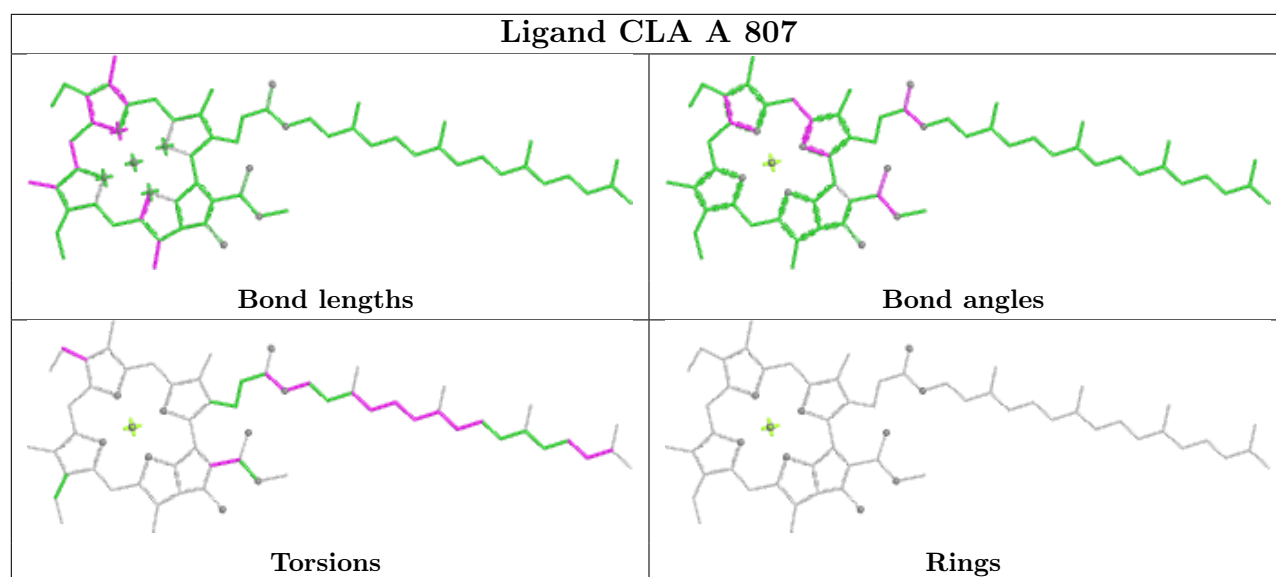
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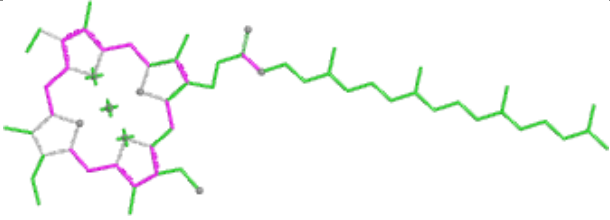
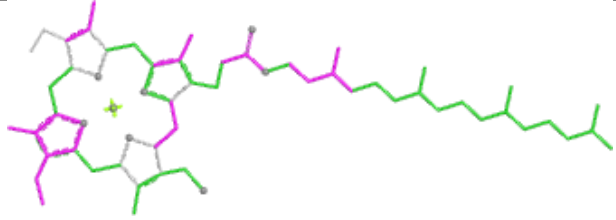
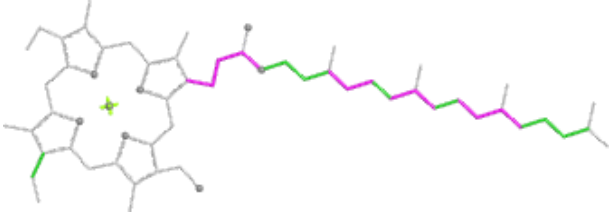
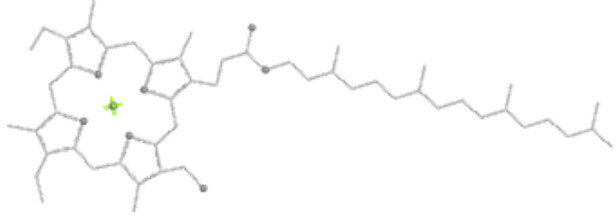
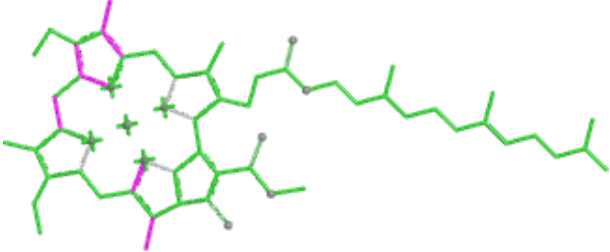
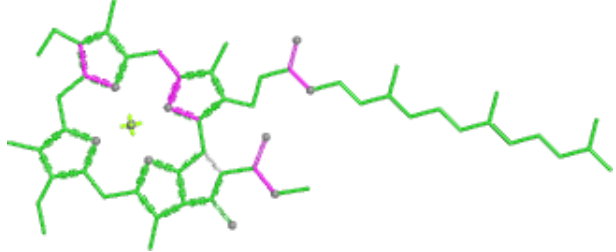
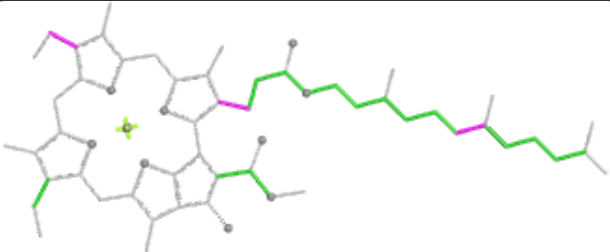
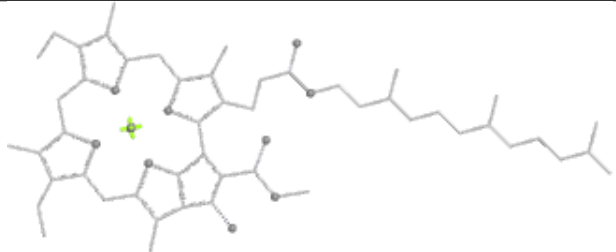
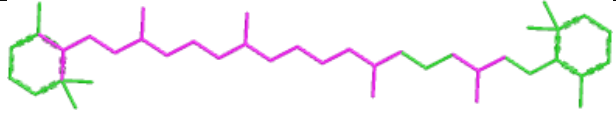
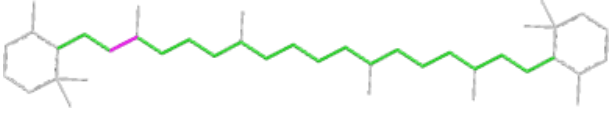
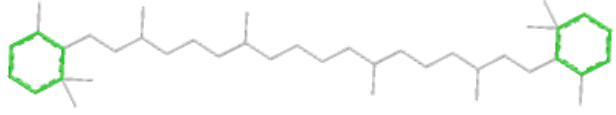




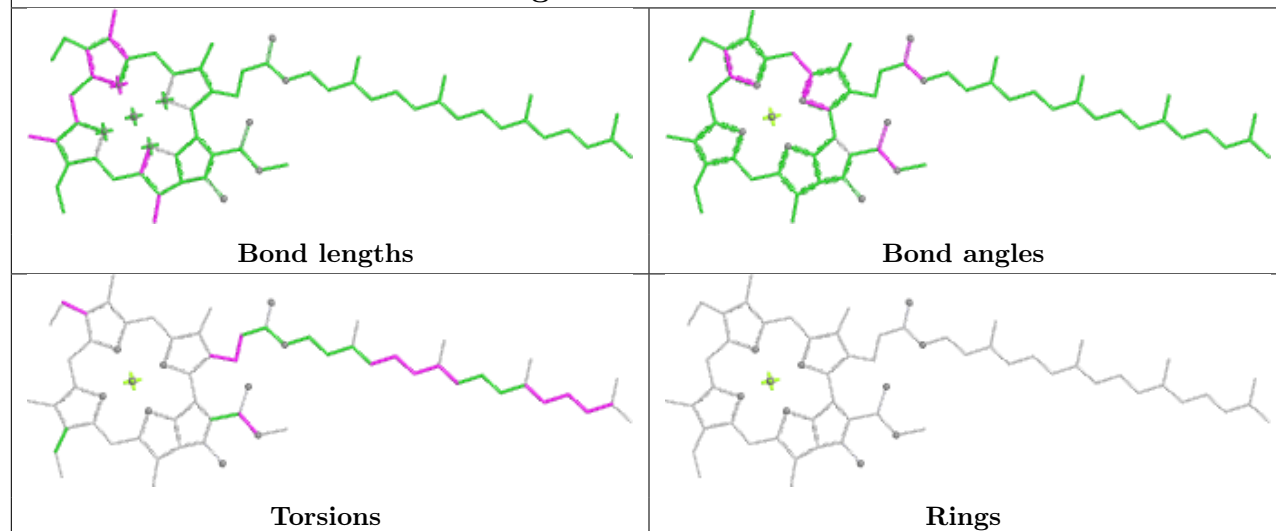




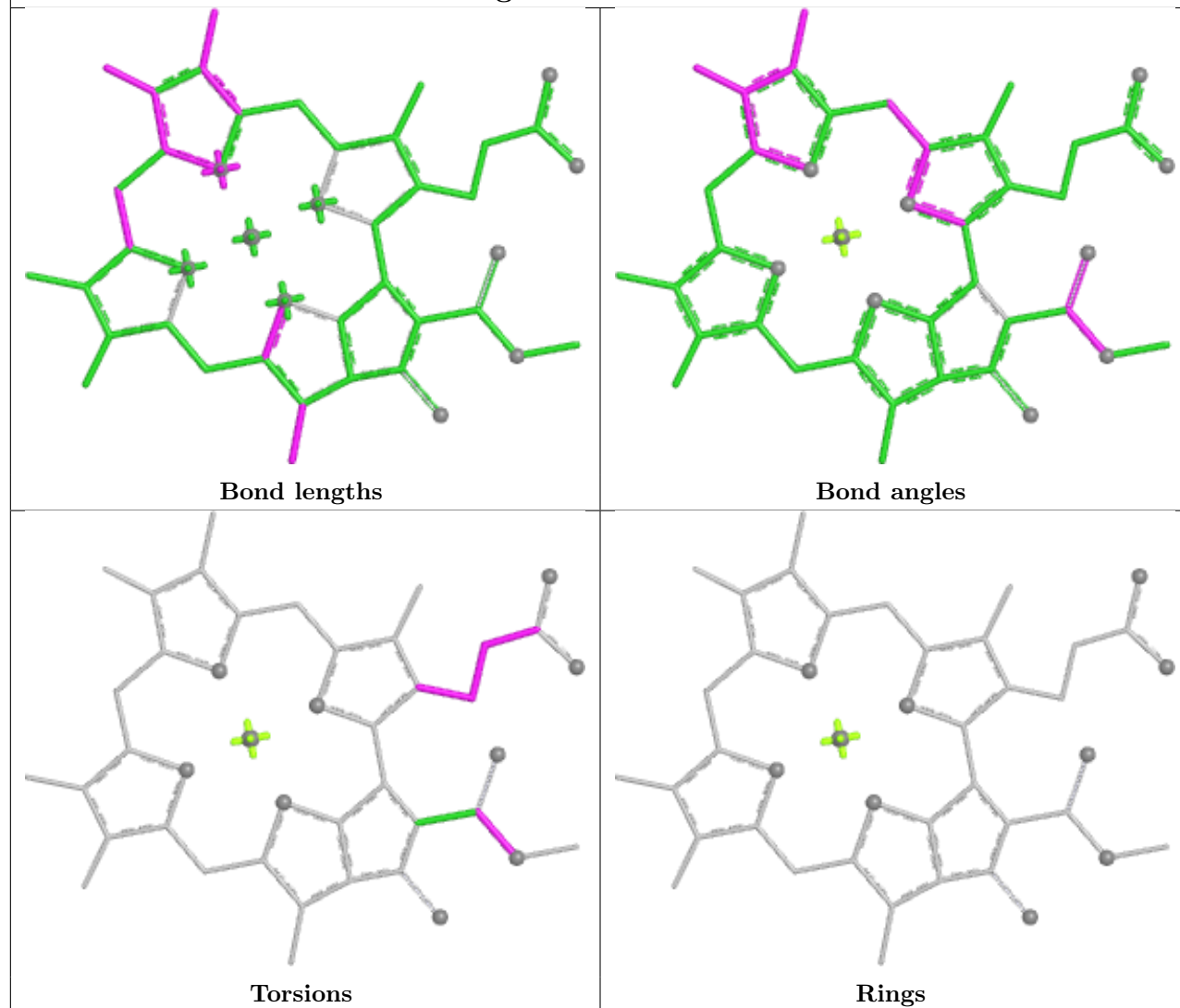


Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

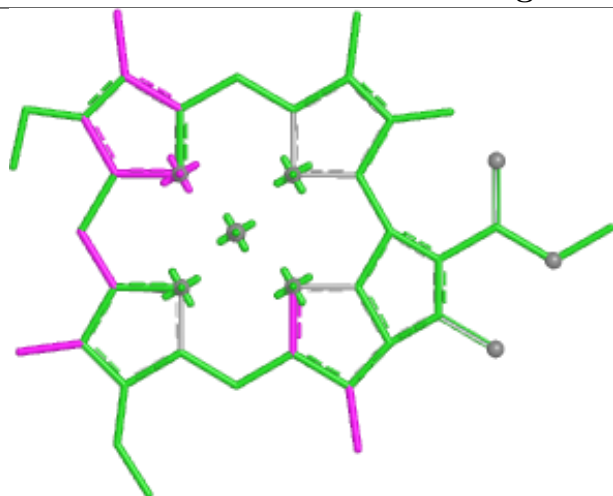
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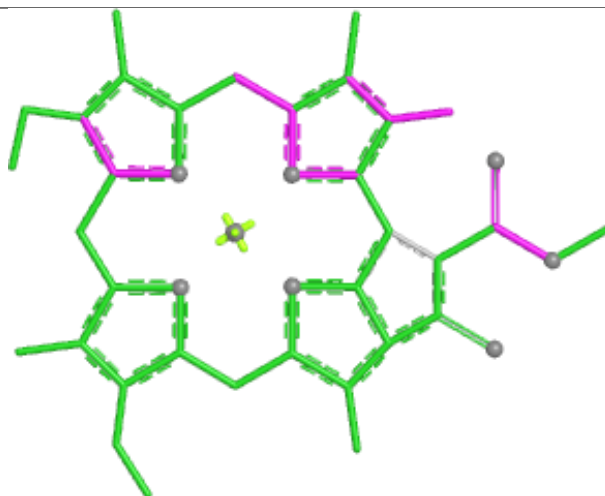
Ligand CLA 4 604



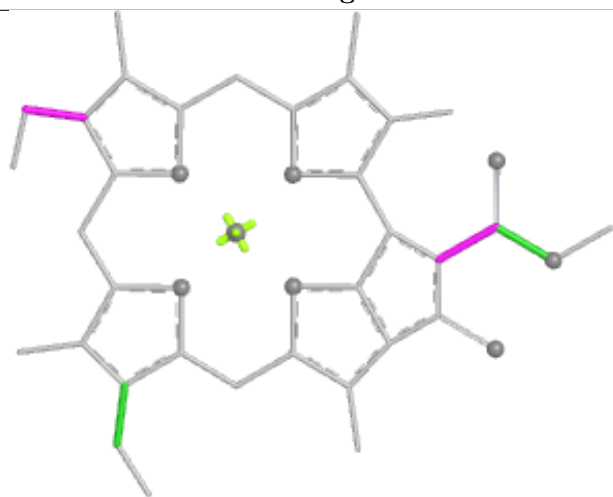
Ligand CLA F 303



Bond lengths



Bond angles

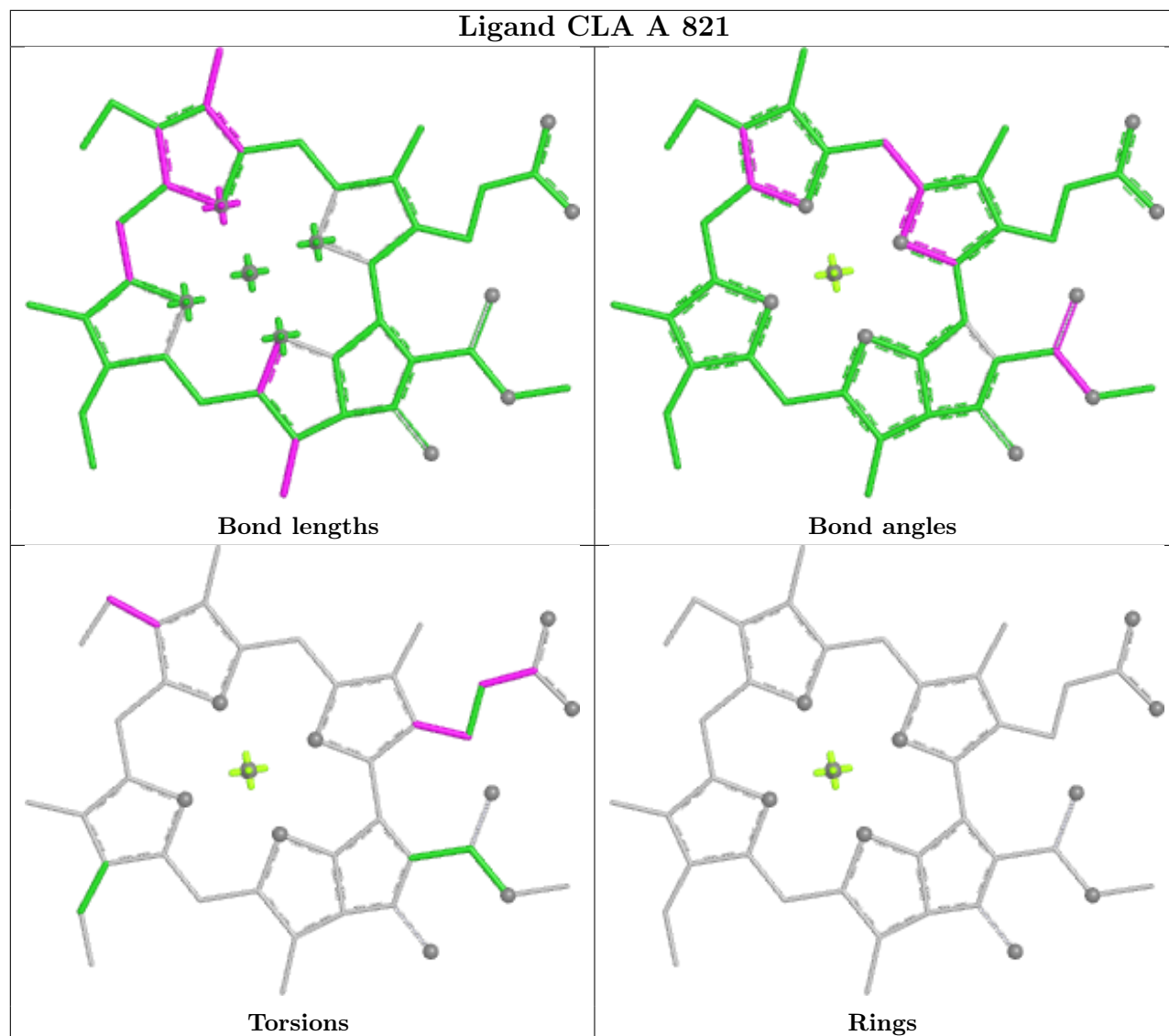


Torsions

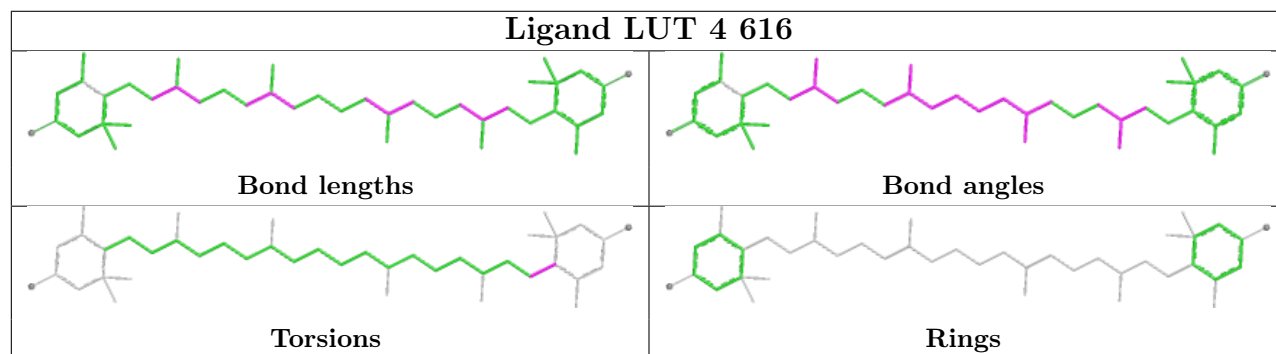


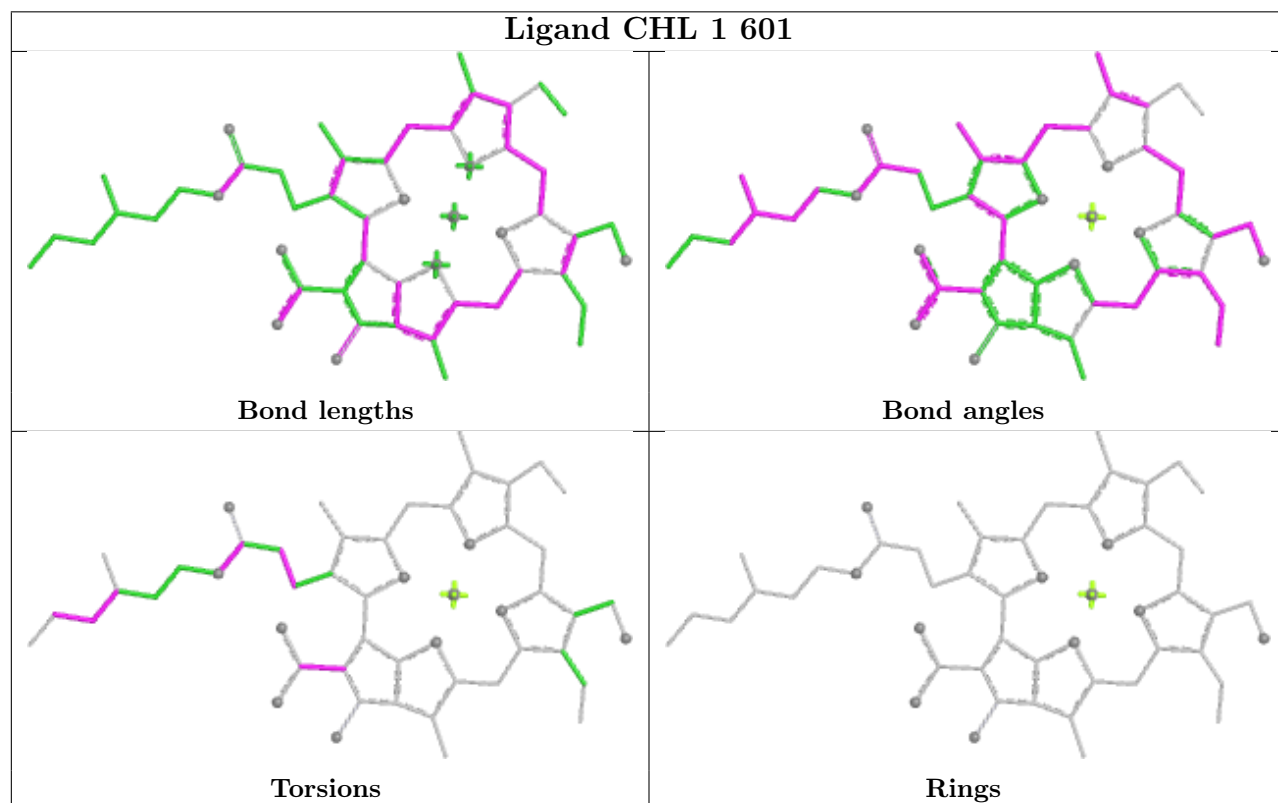
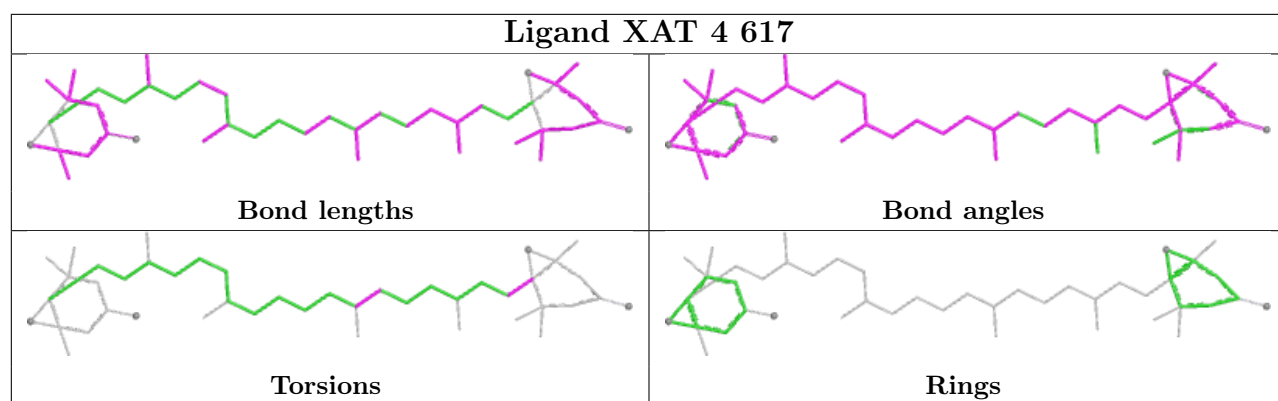
Rings

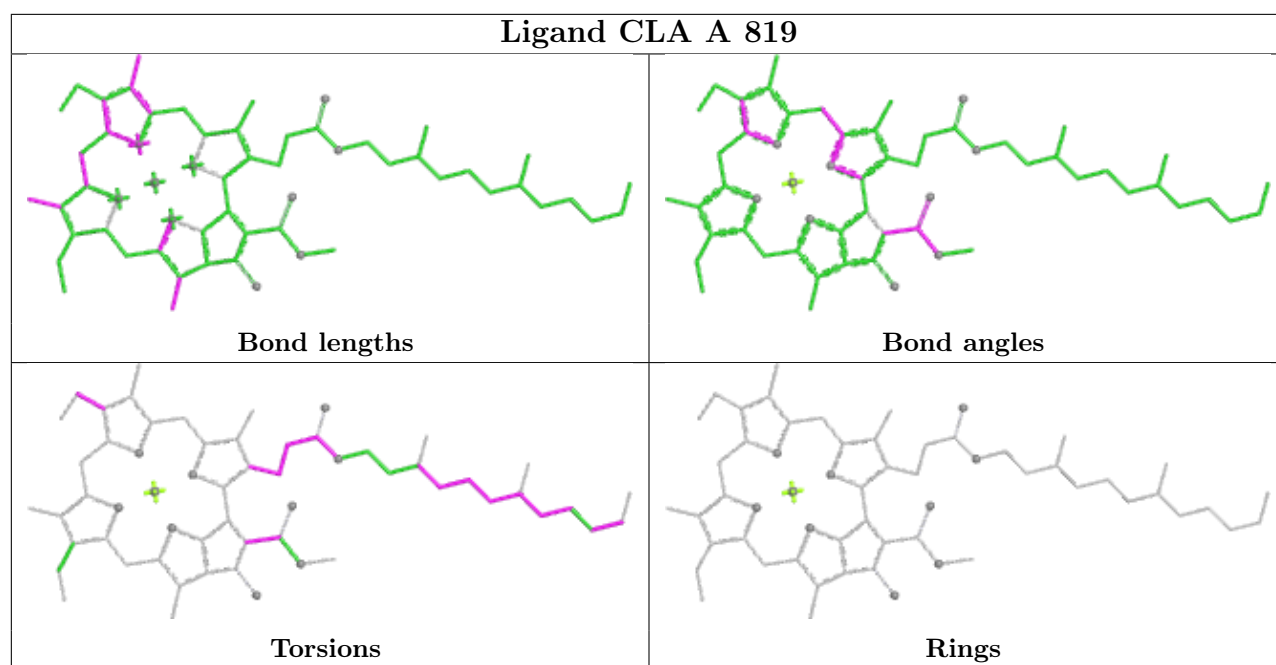
Ligand CLA A 821



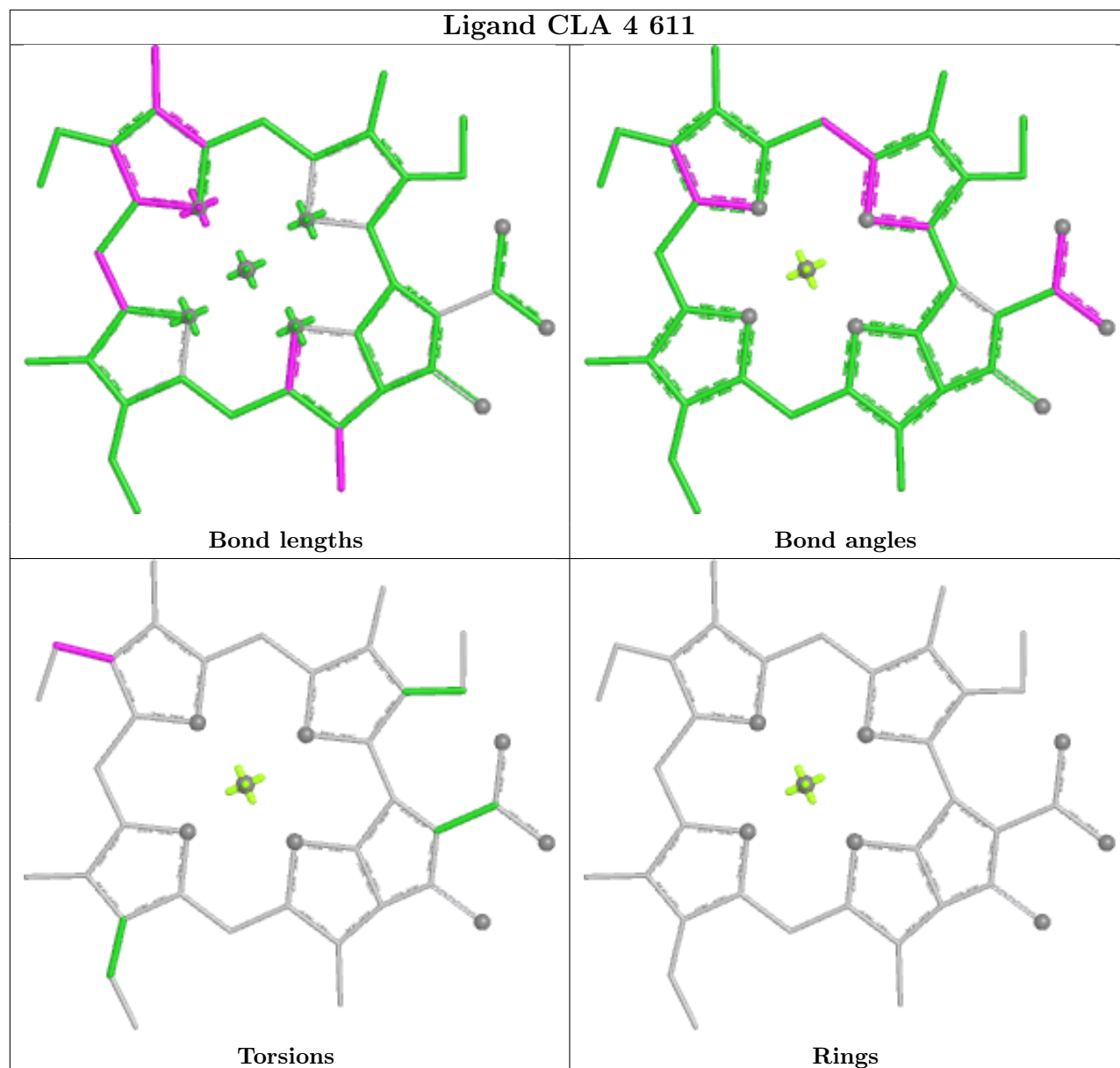
Ligand LUT 4 616

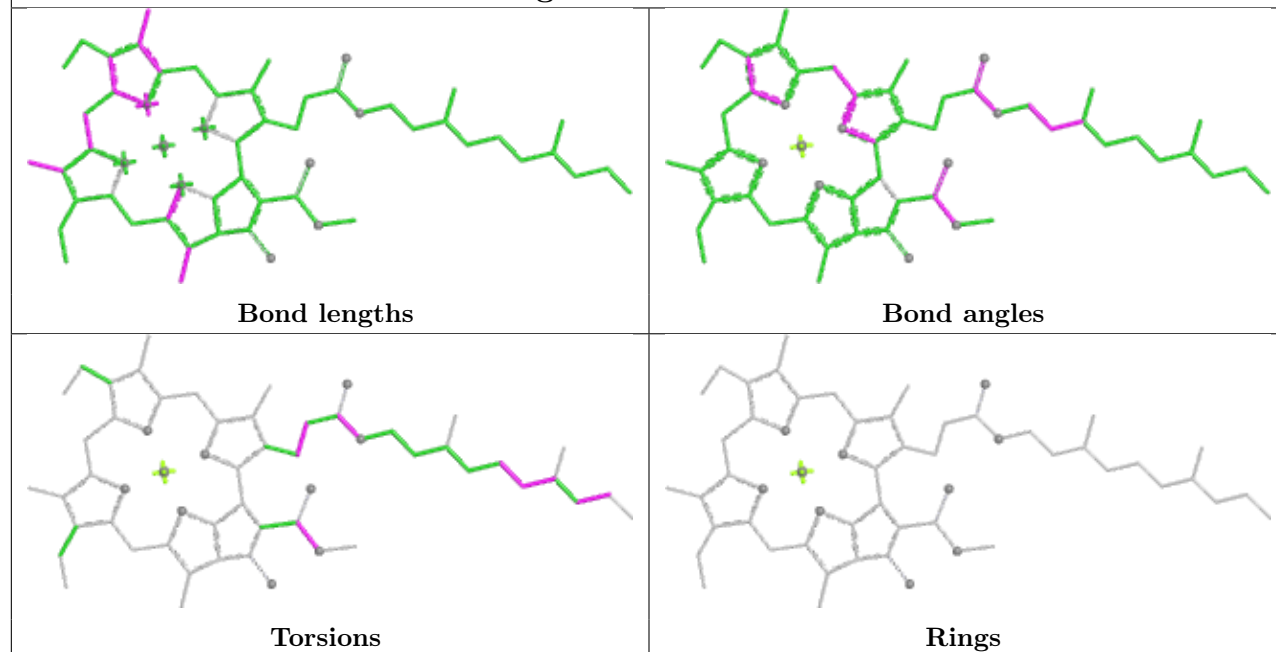
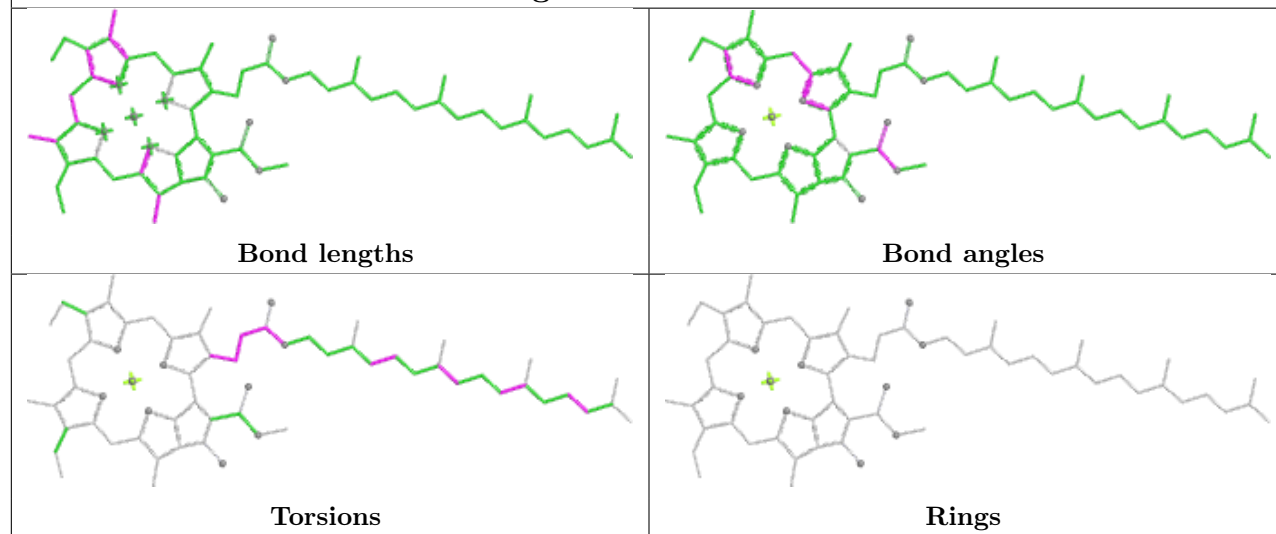




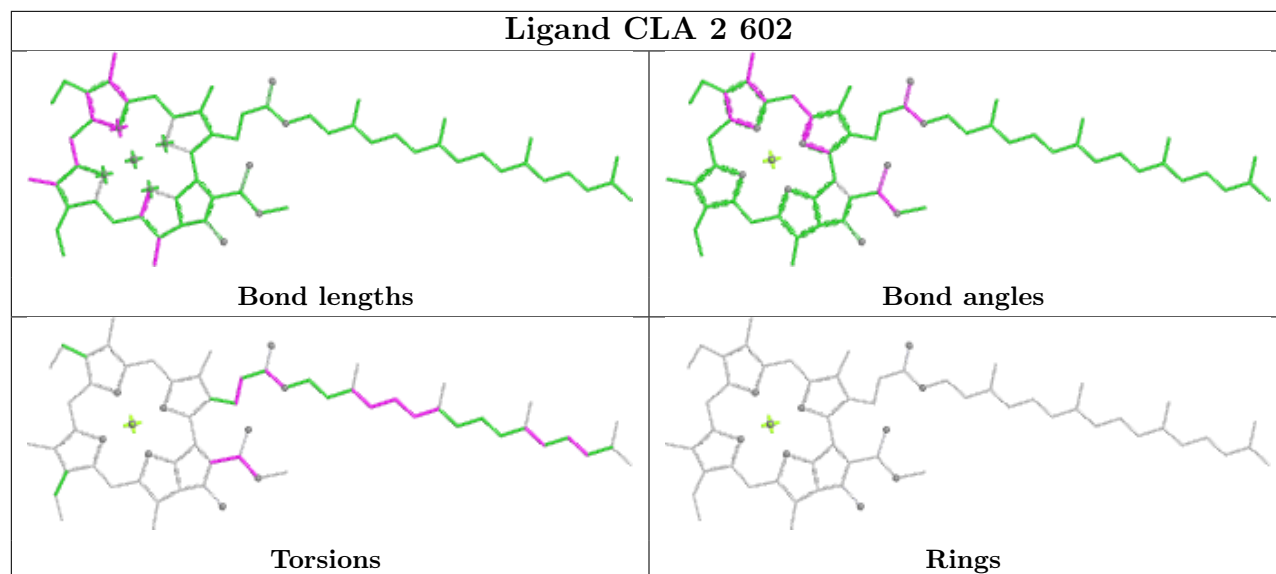


Ligand CLA 4 611

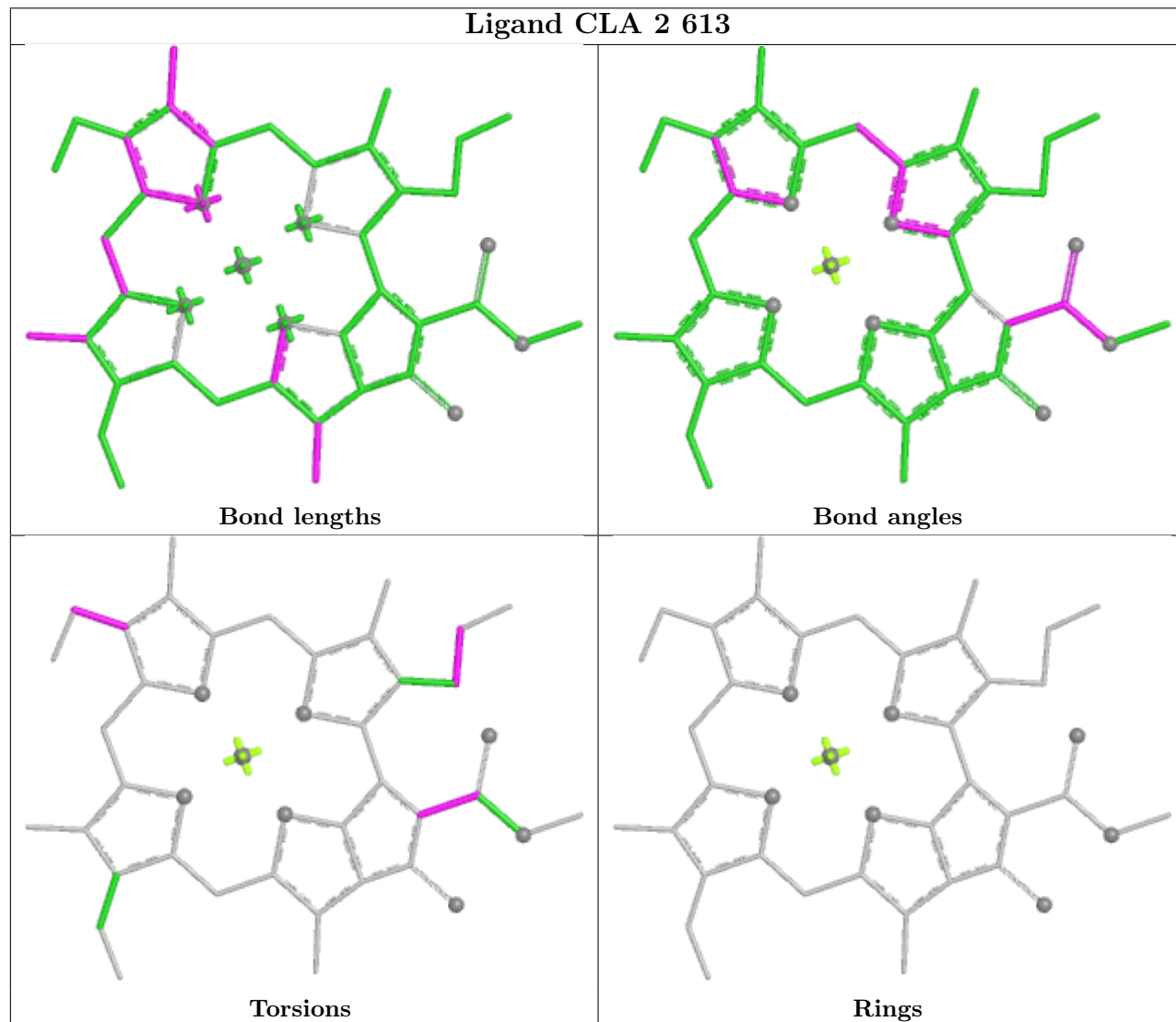


Ligand CLA 4 612**Ligand CLA B 832**

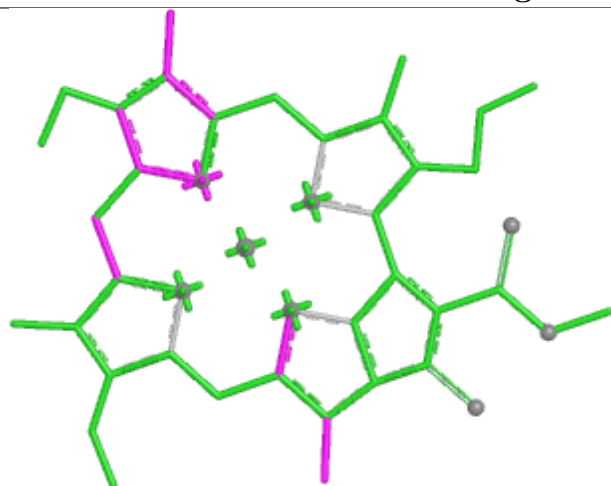
Ligand CLA 2 602



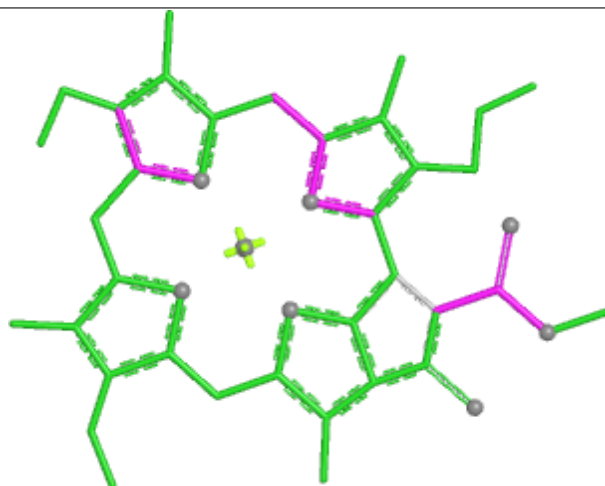
Ligand CLA 2 613



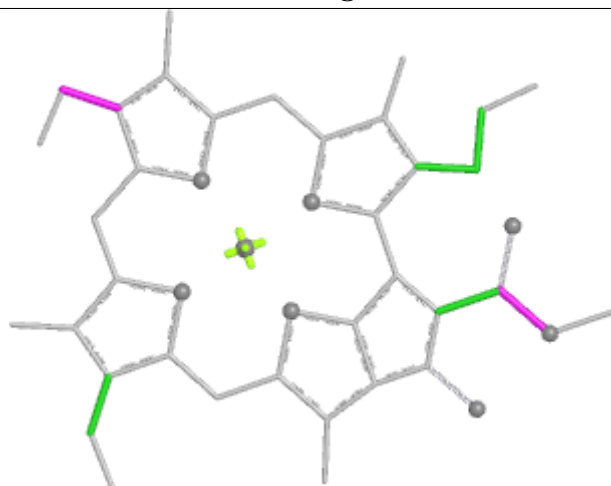
Ligand CLA B 830



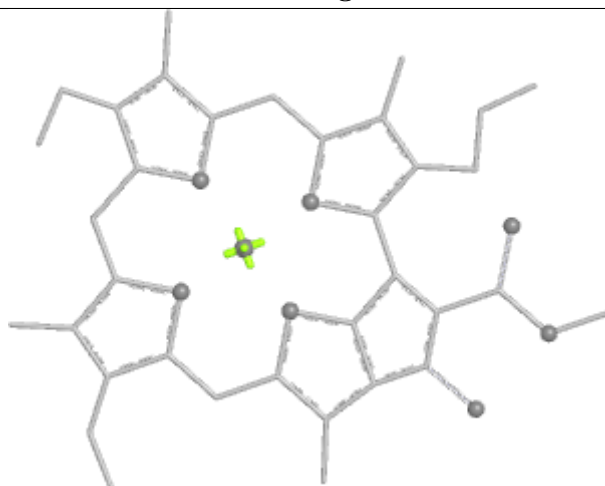
Bond lengths



Bond angles

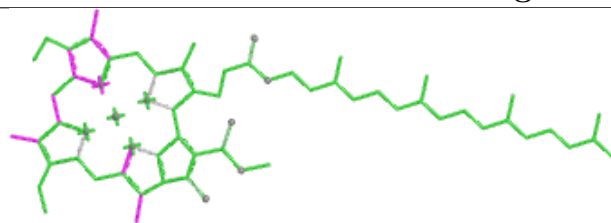


Torsions

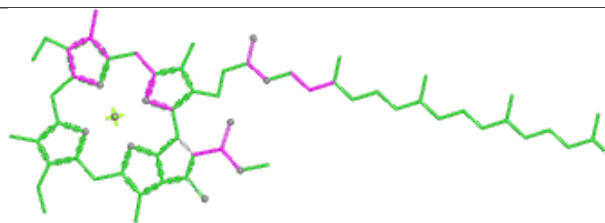


Rings

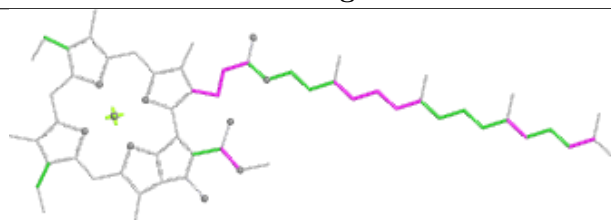
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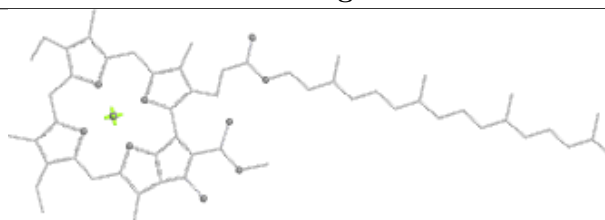
Bond lengths



Bond angles

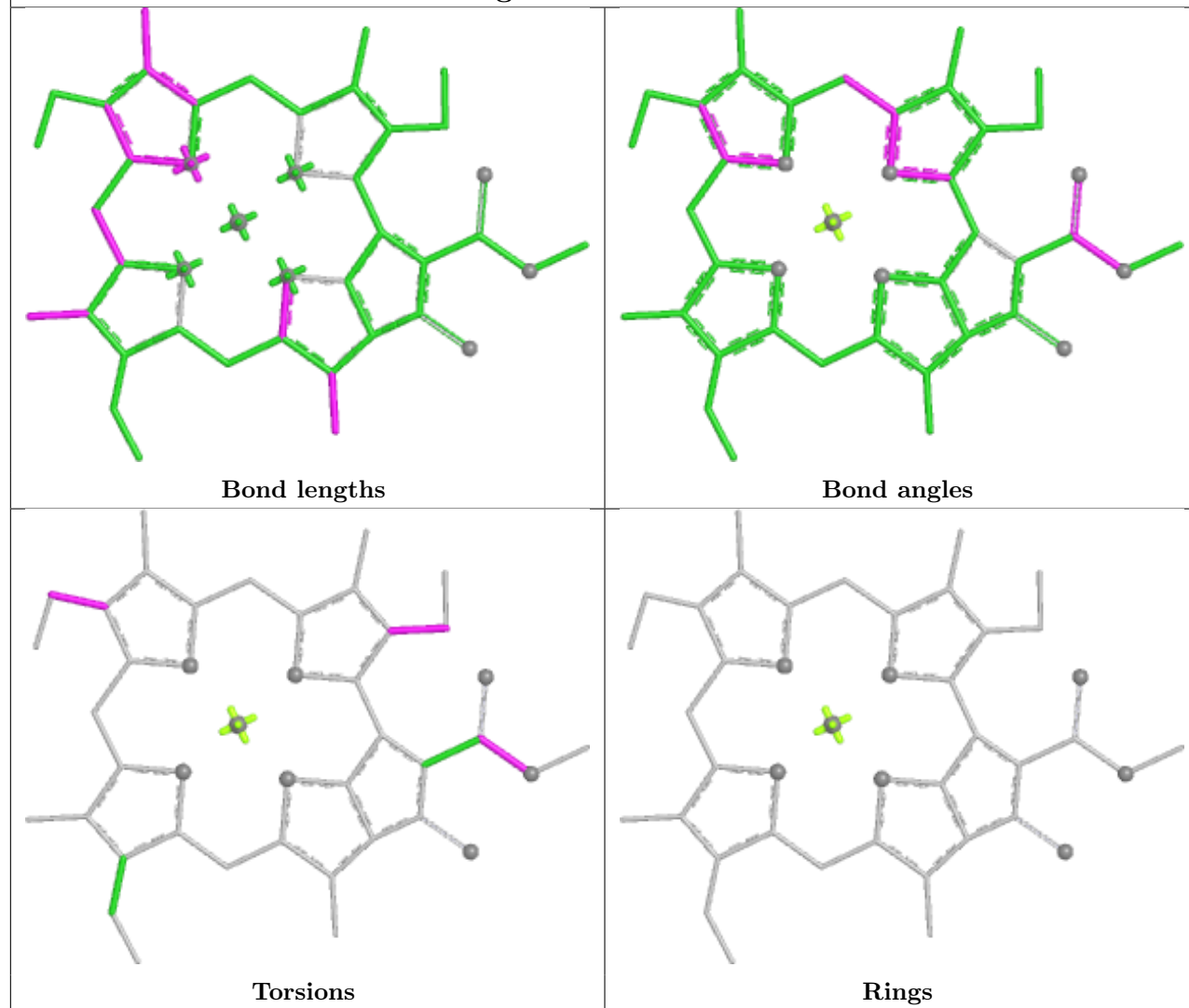


Torsions

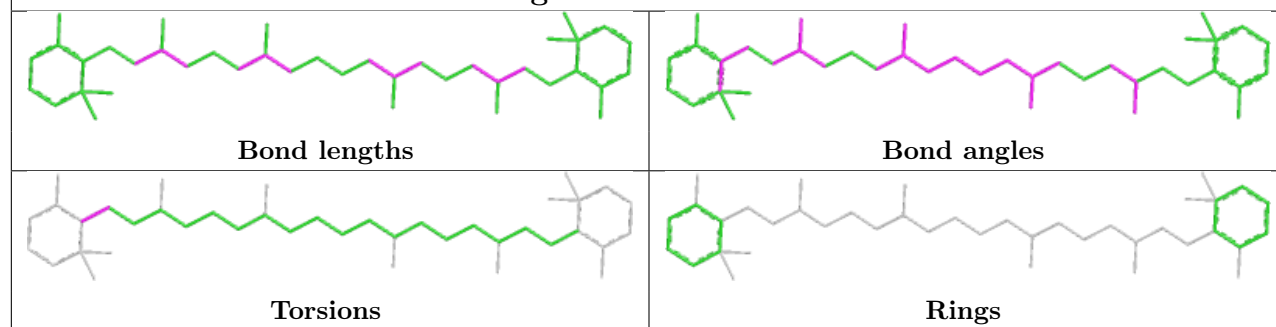


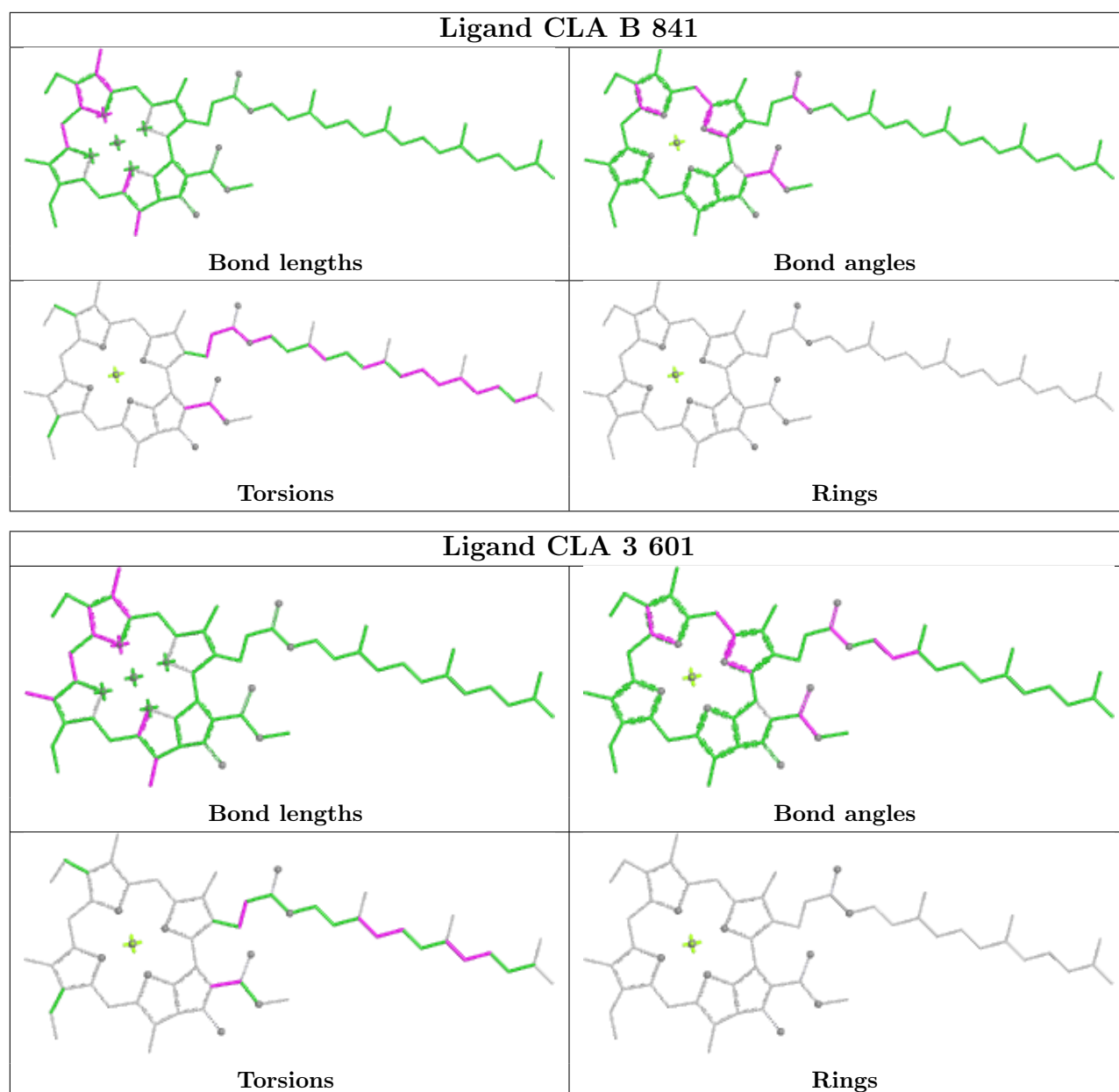
Rings

Ligand CLA B 835

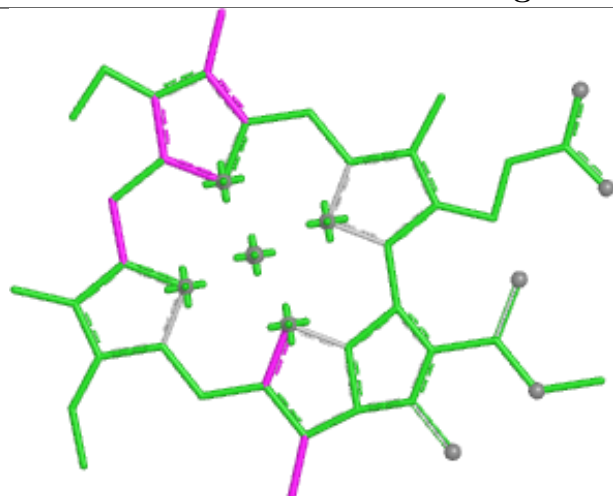


Ligand BCR B 847

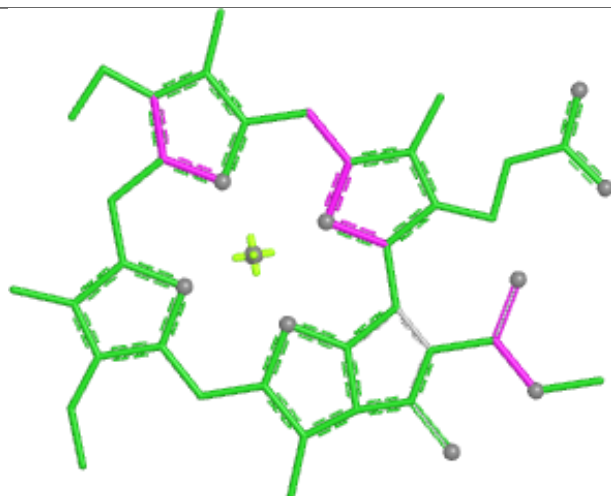




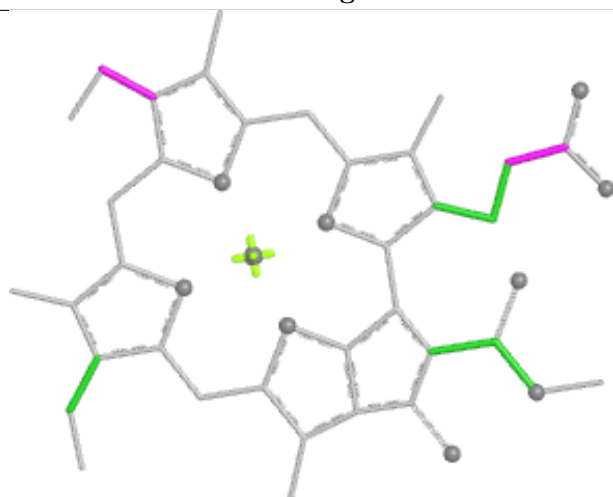
Ligand CLA A 817



Bond lengths



Bond angles

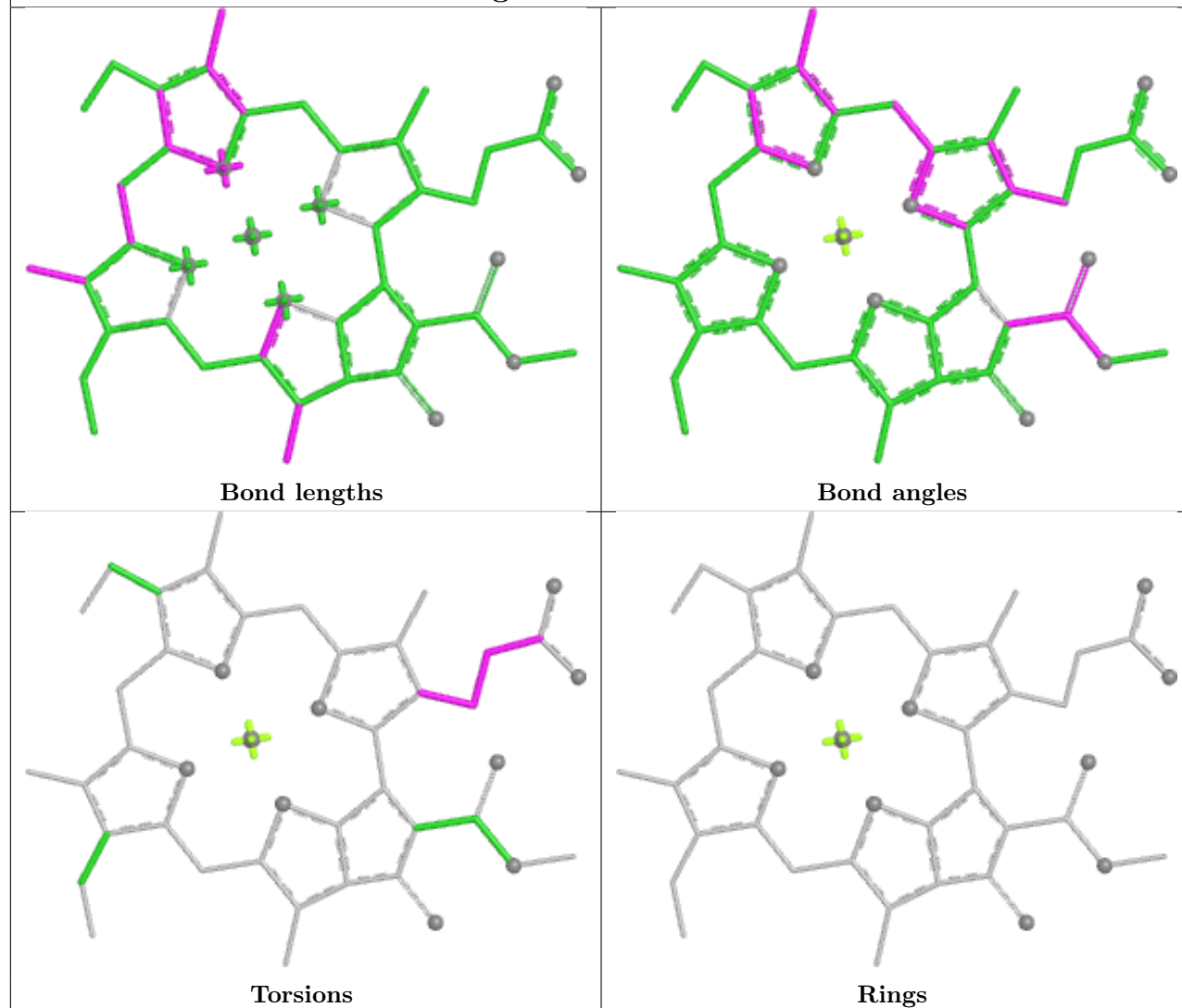


Torsions

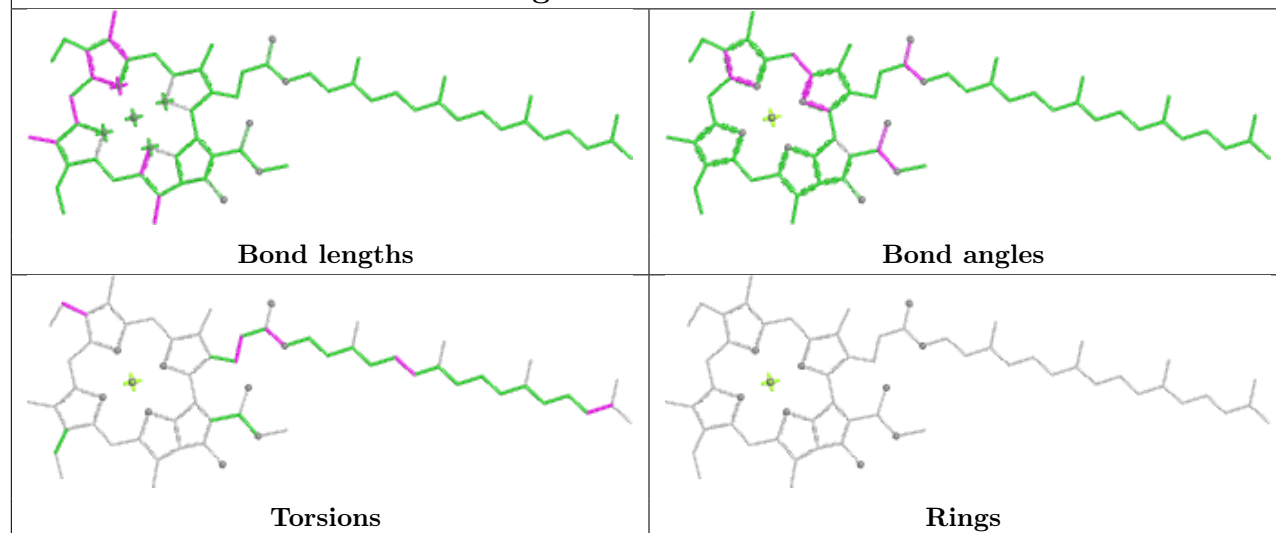


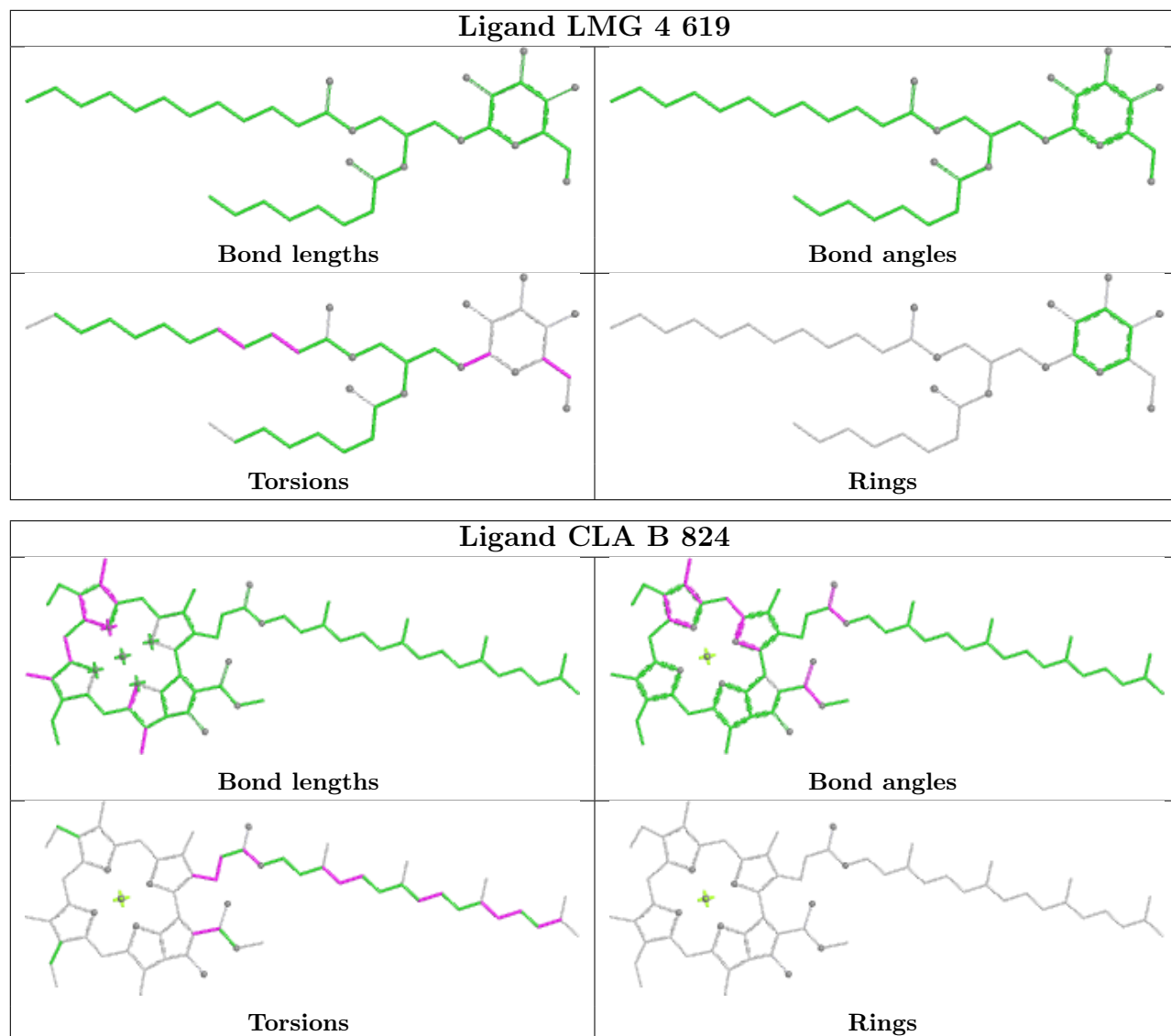
Rings

Ligand CLA A 815

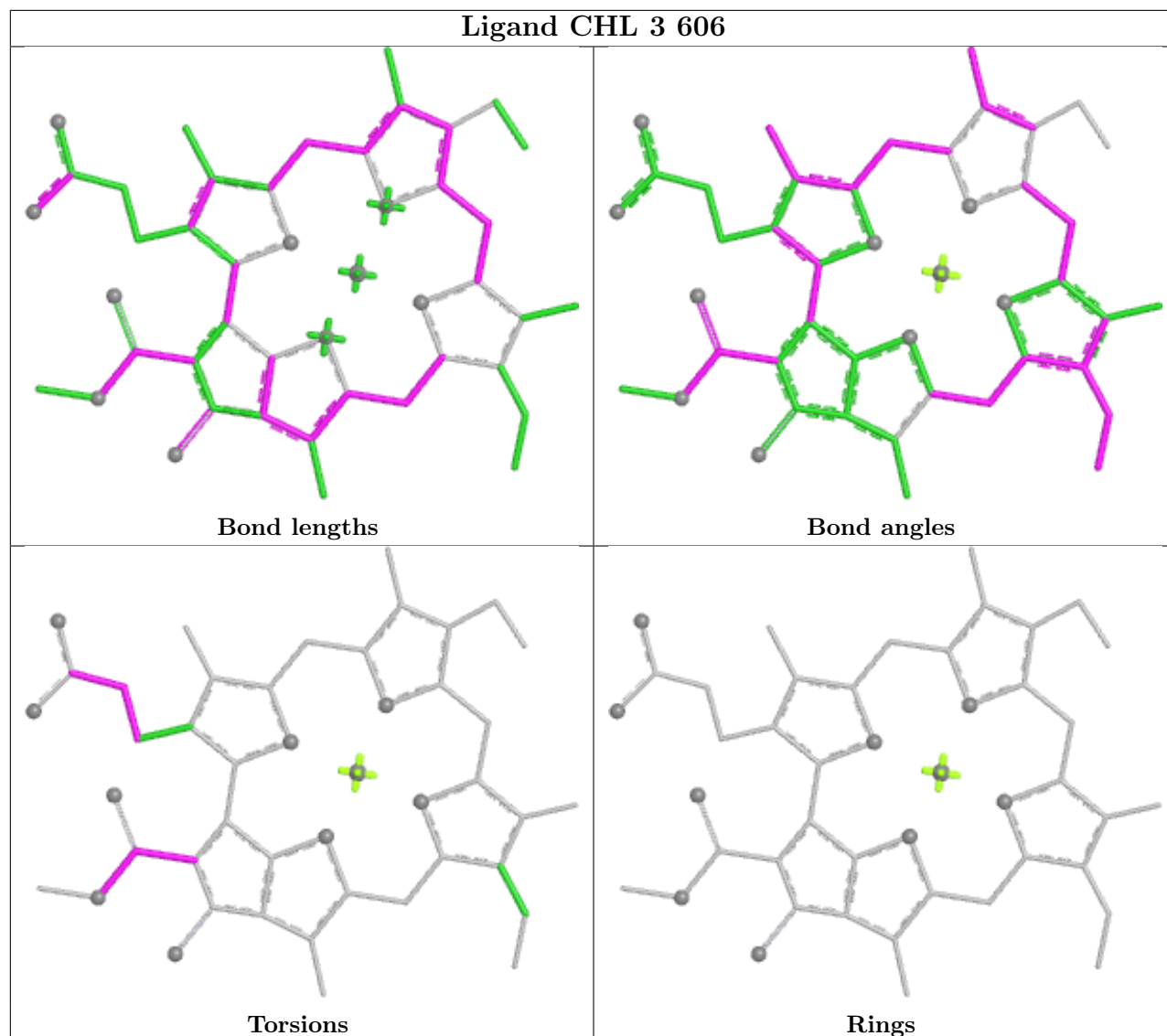


Ligand CLA B 839

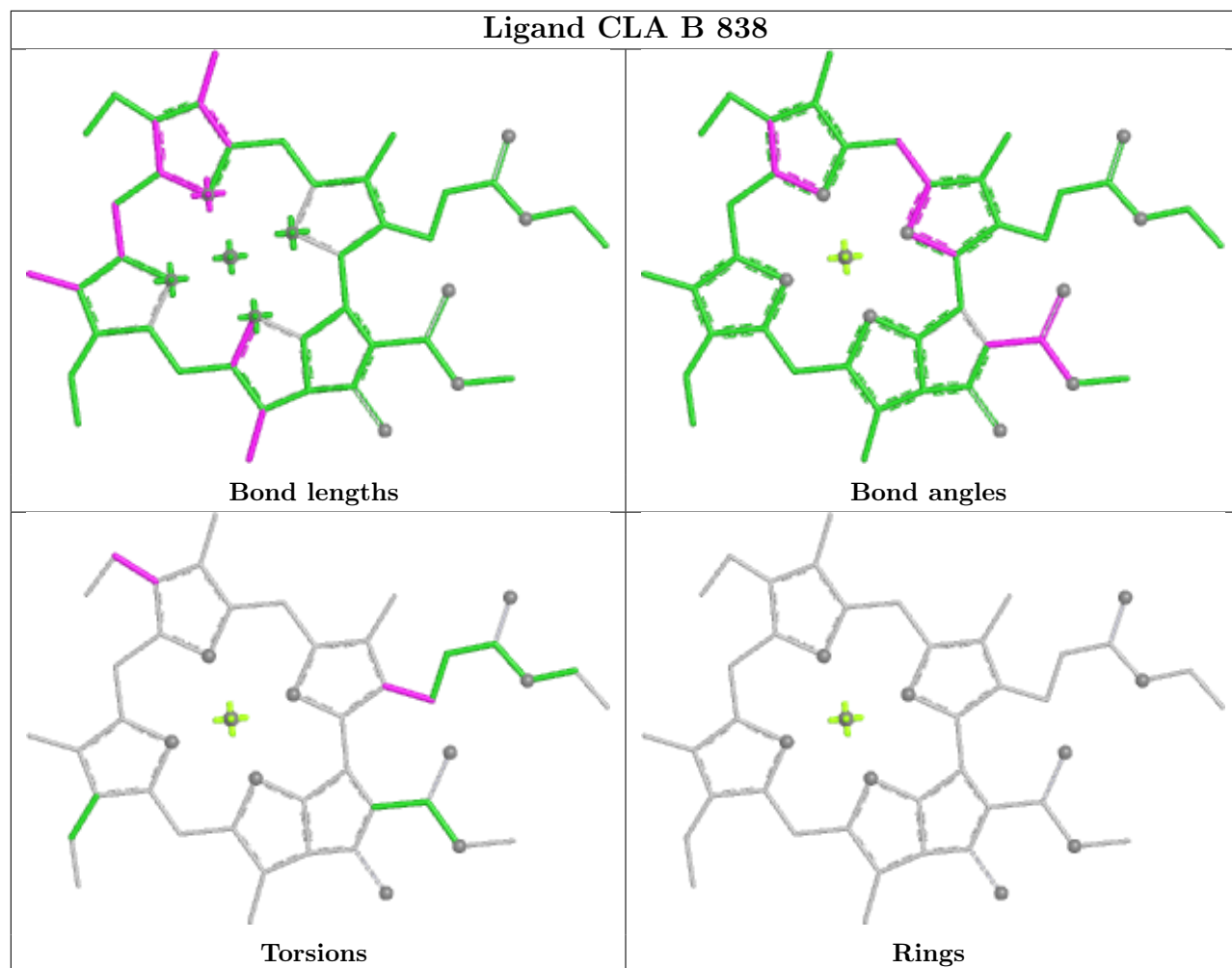




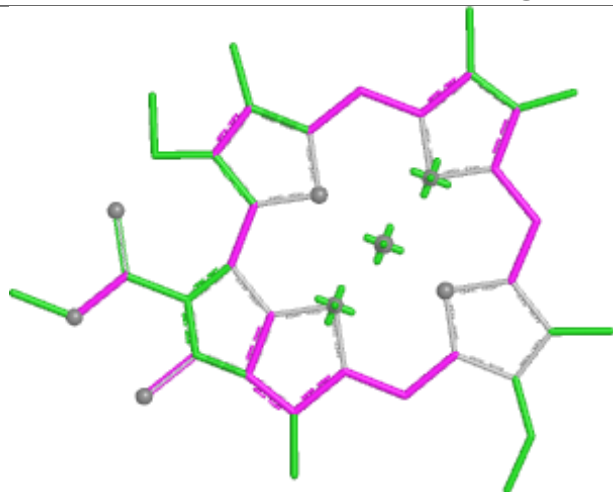
Ligand CHL 3 606



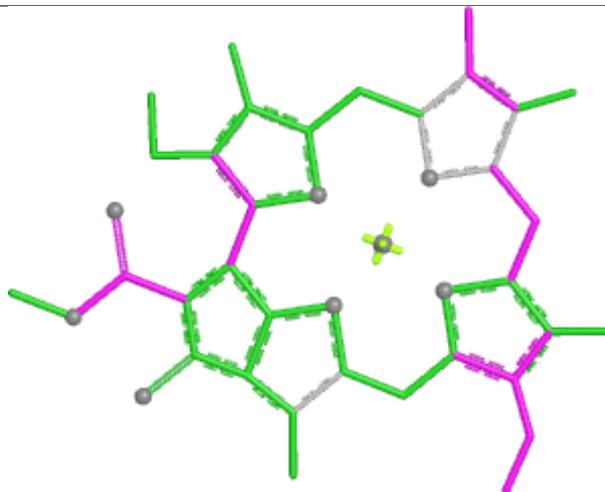
Ligand CLA B 838



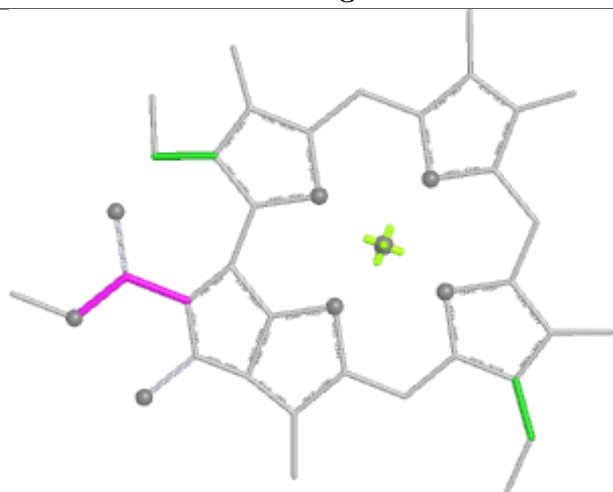
Ligand CHL 4 606



Bond lengths



Bond angles

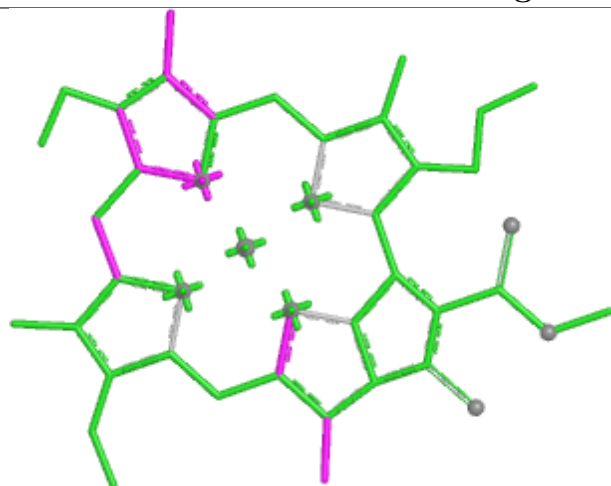


Torsions

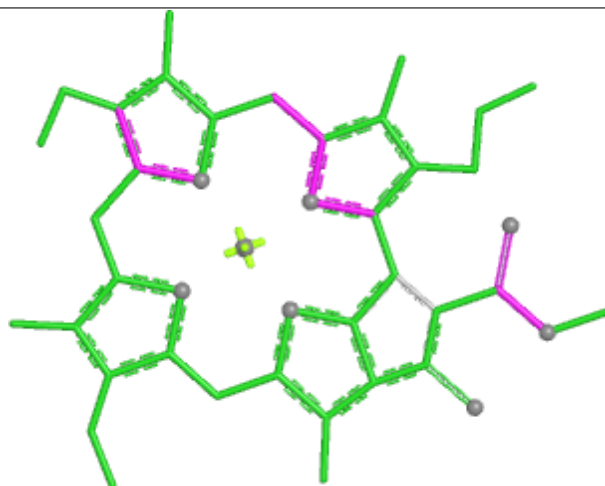


Rings

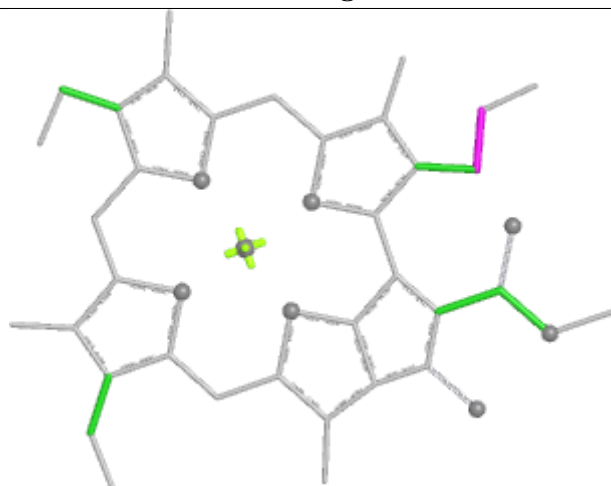
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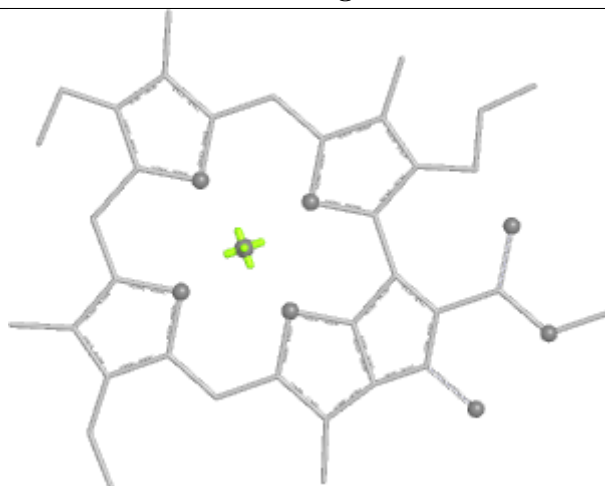
Bond lengths



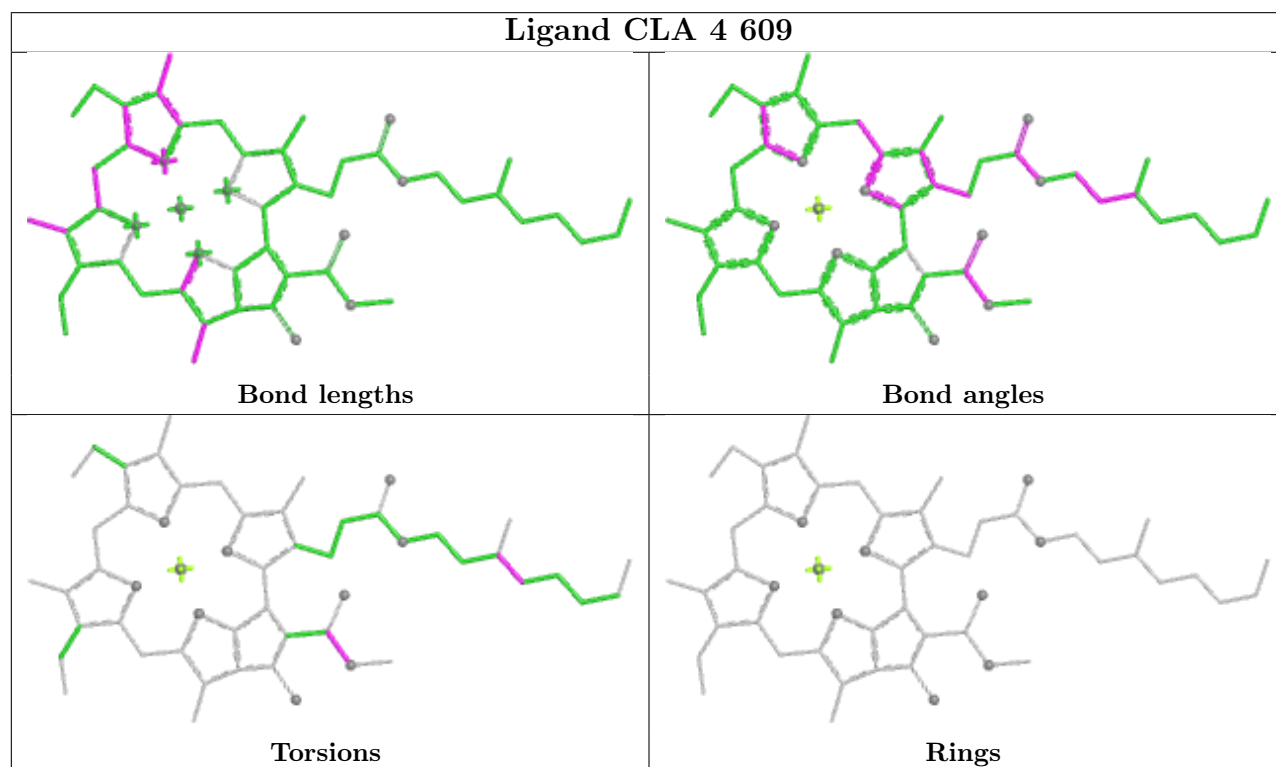
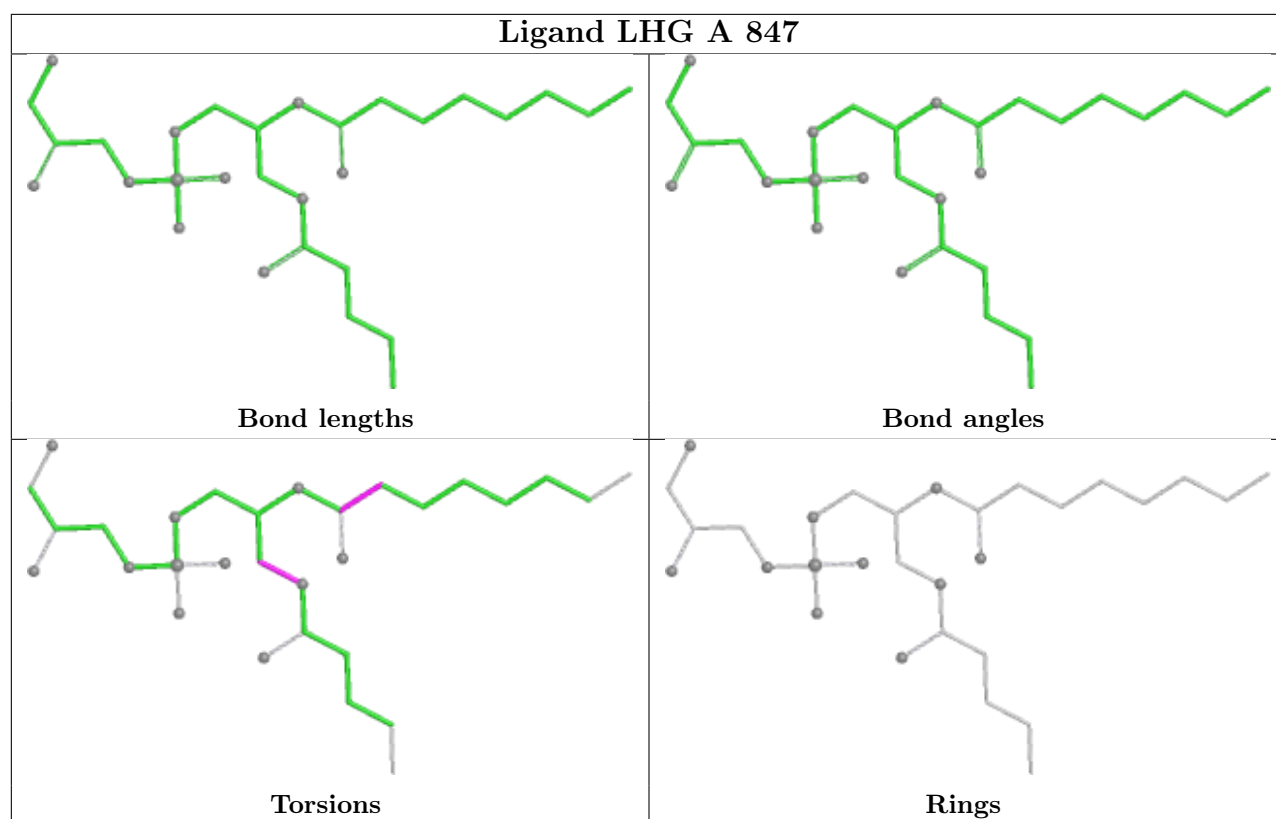
Bond angles

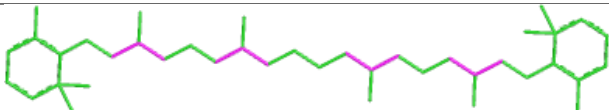
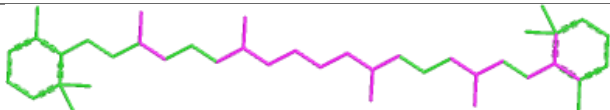
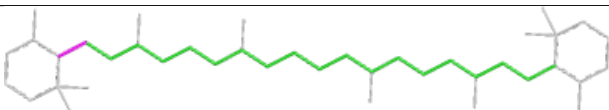
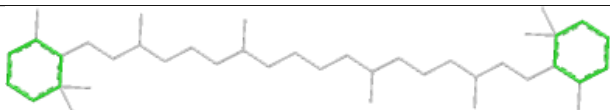


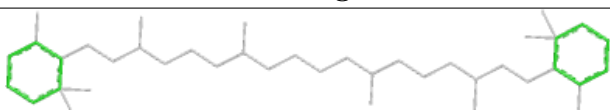
Torsions



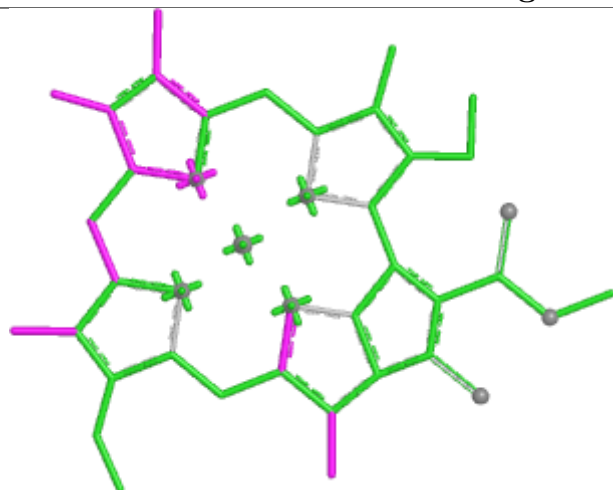
Rings



Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

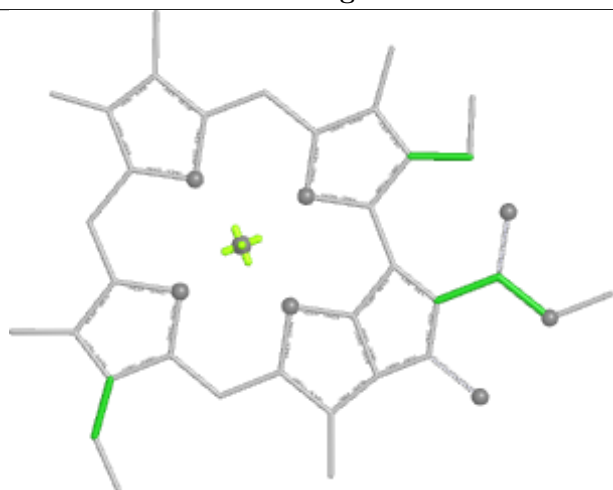
Ligand CLA 3 605



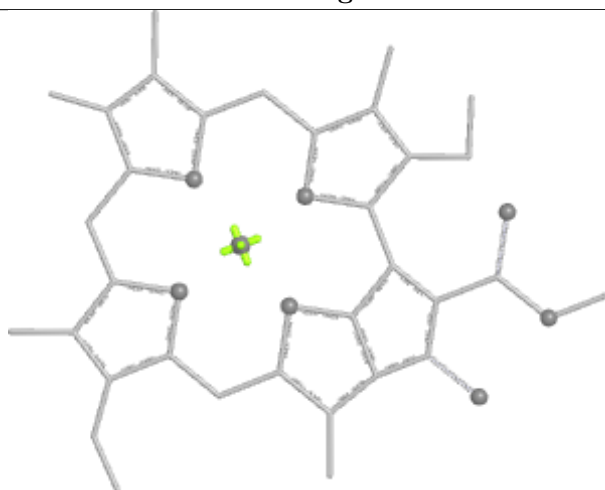
Bond lengths



Bond angles

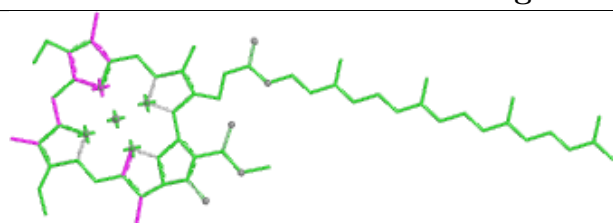


Torsions

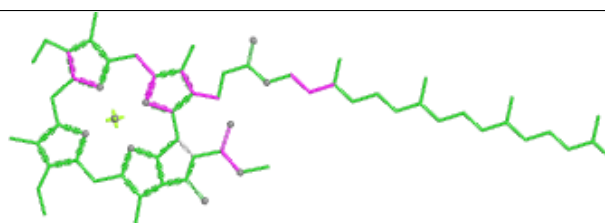


Rings

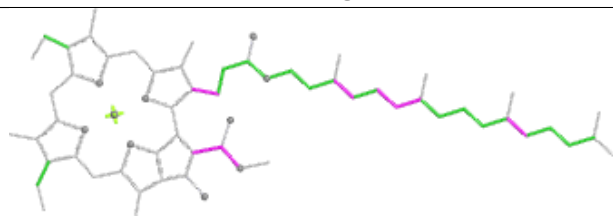
Ligand CLA B 810



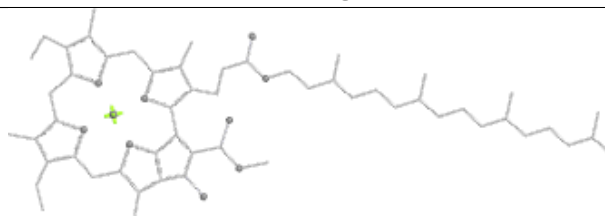
Bond lengths



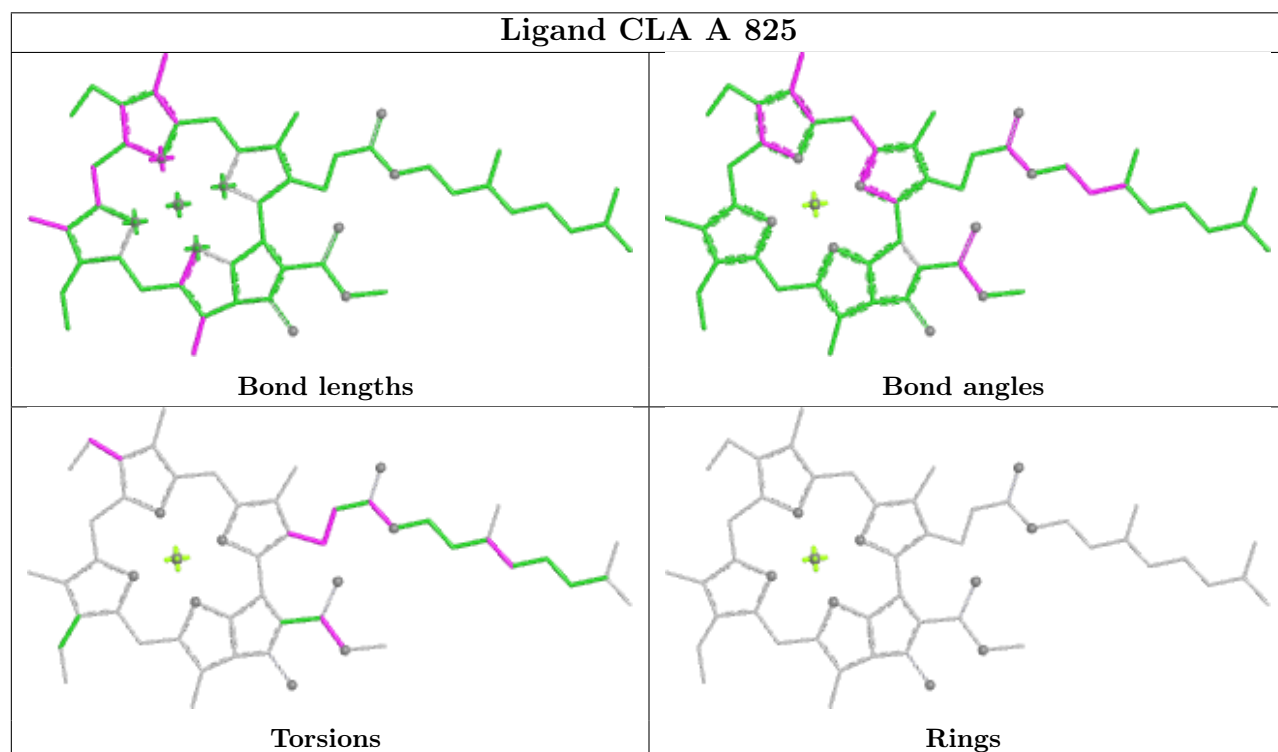
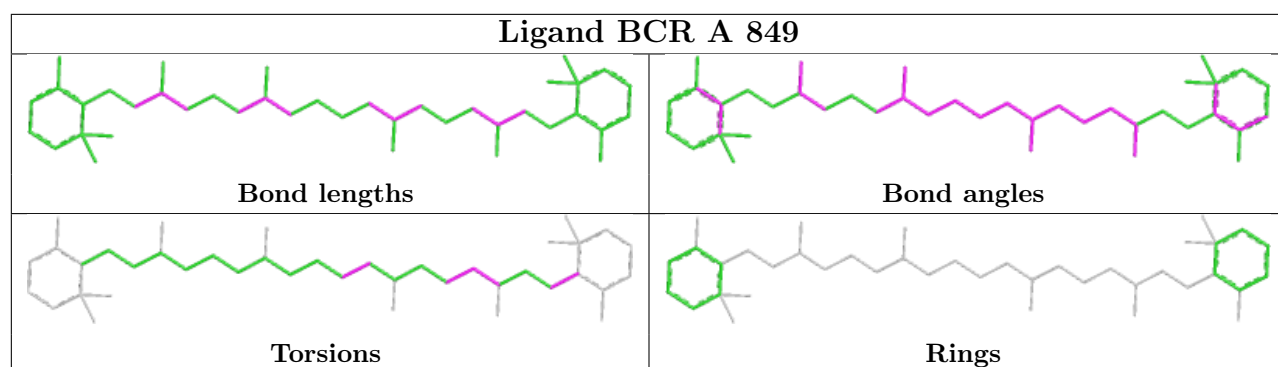
Bond angles



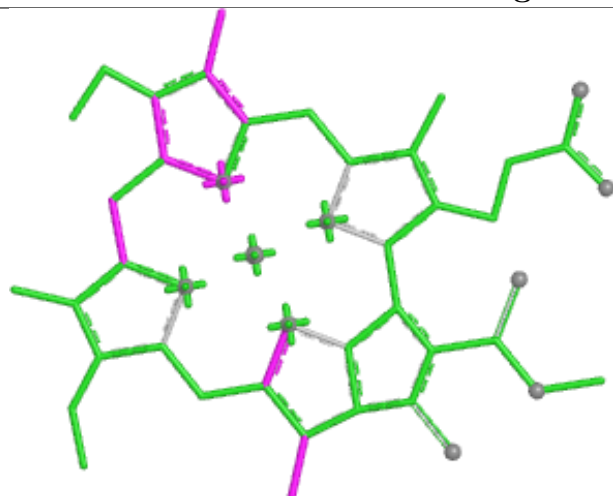
Torsions



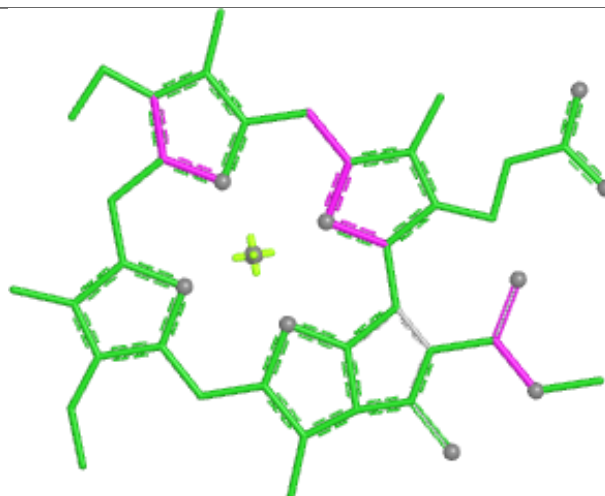
Rings



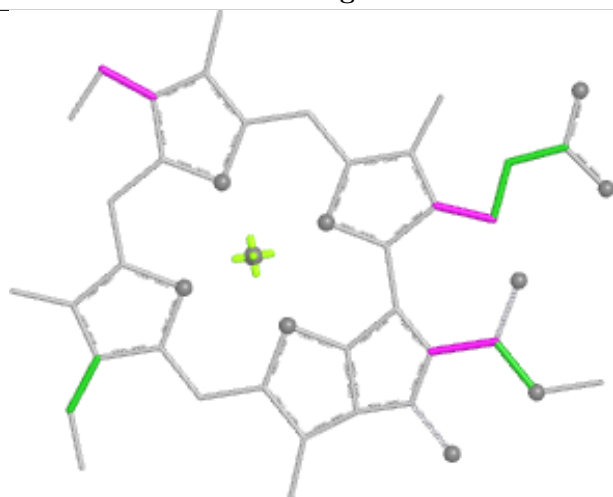
Ligand CLA A 836



Bond lengths



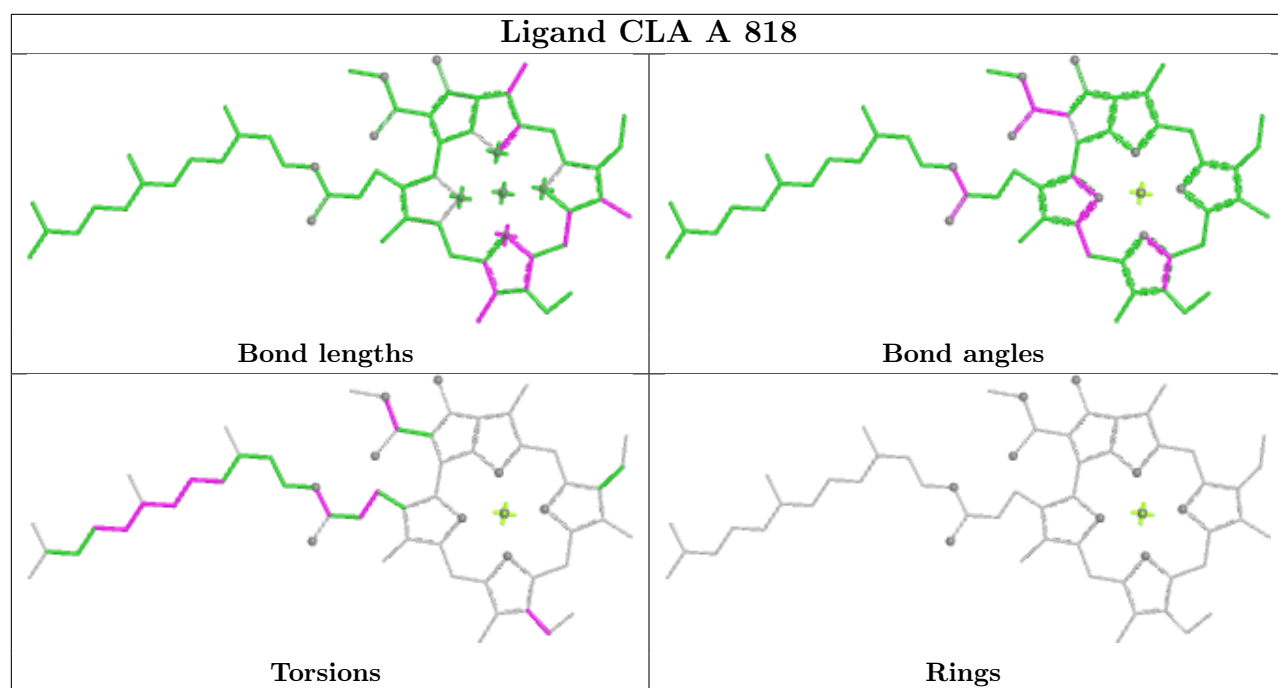
Bond angles



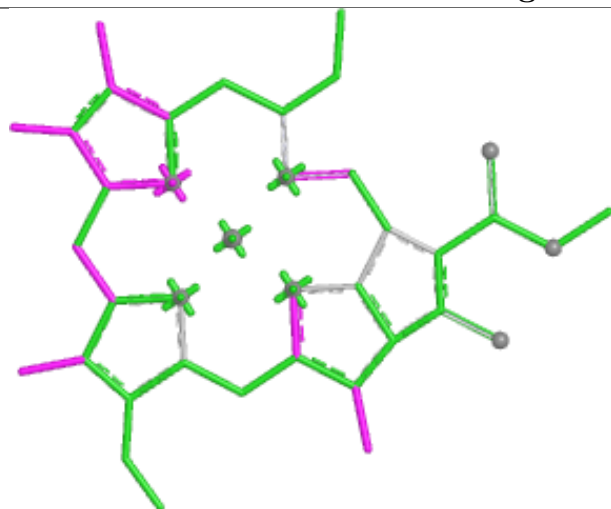
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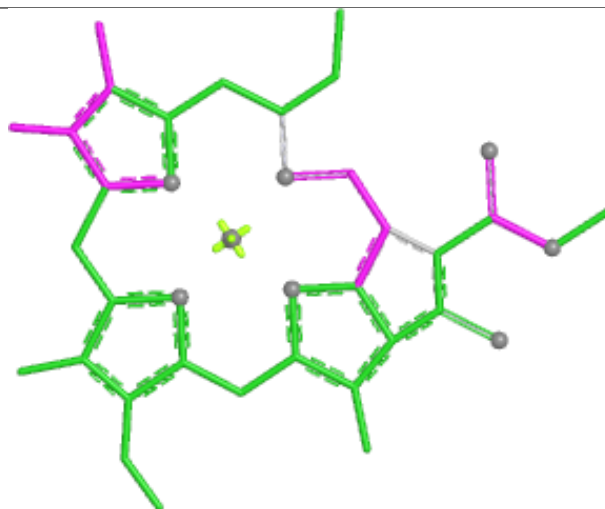
Rings



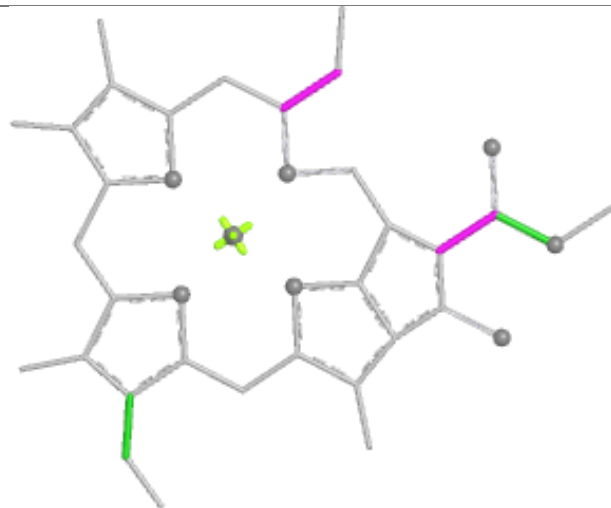
Ligand CLA 2 610



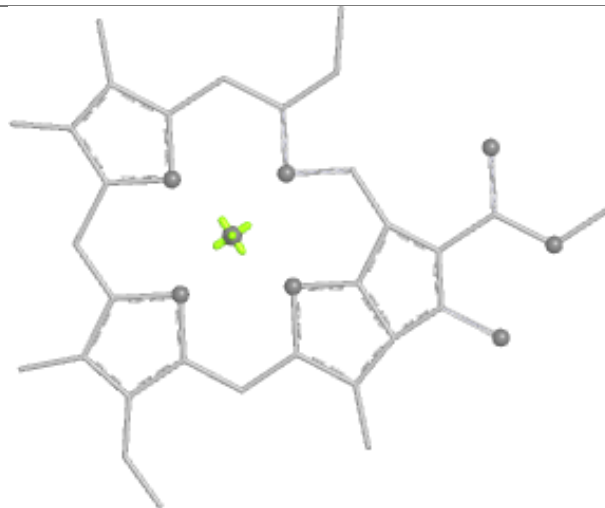
Bond lengths



Bond angles

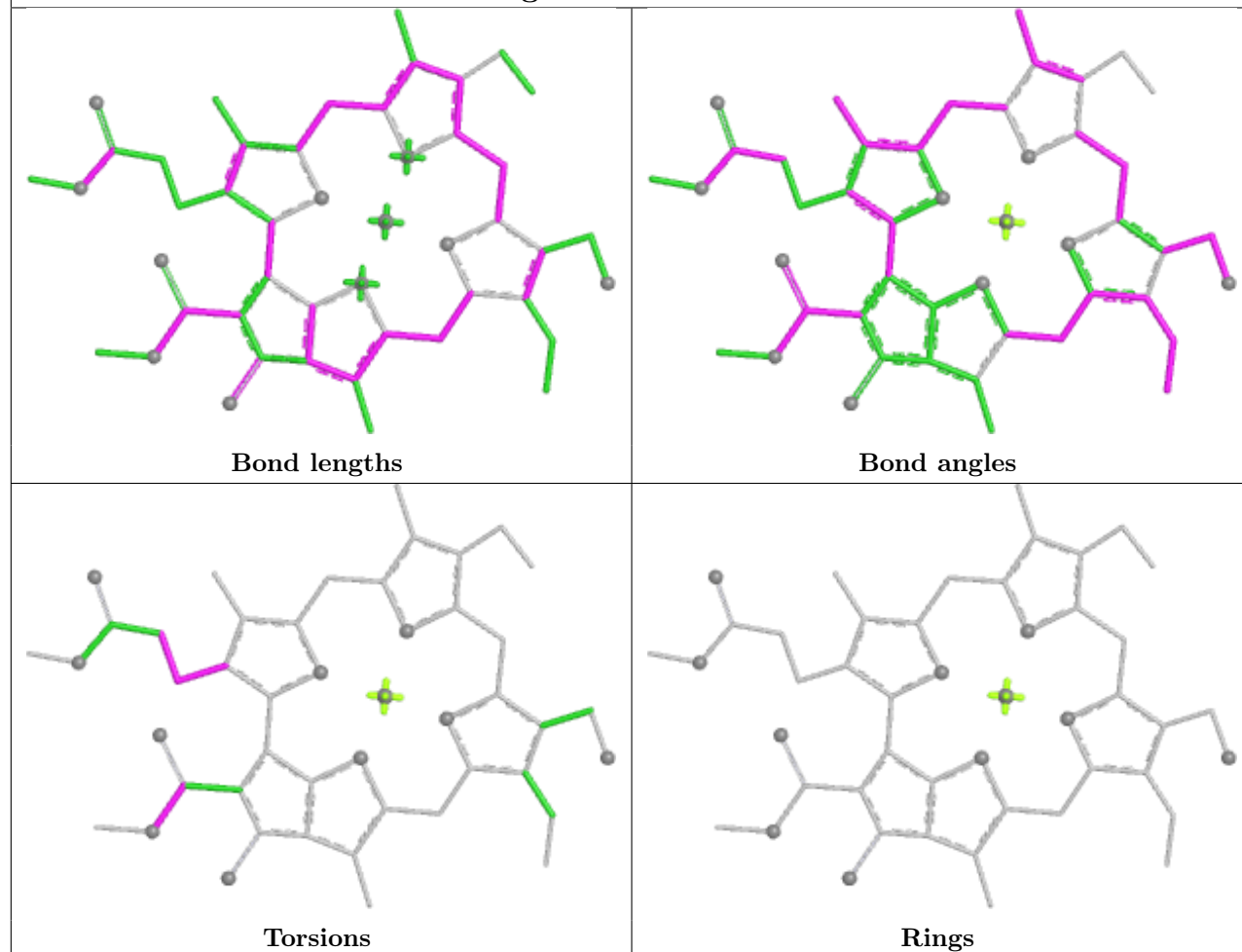


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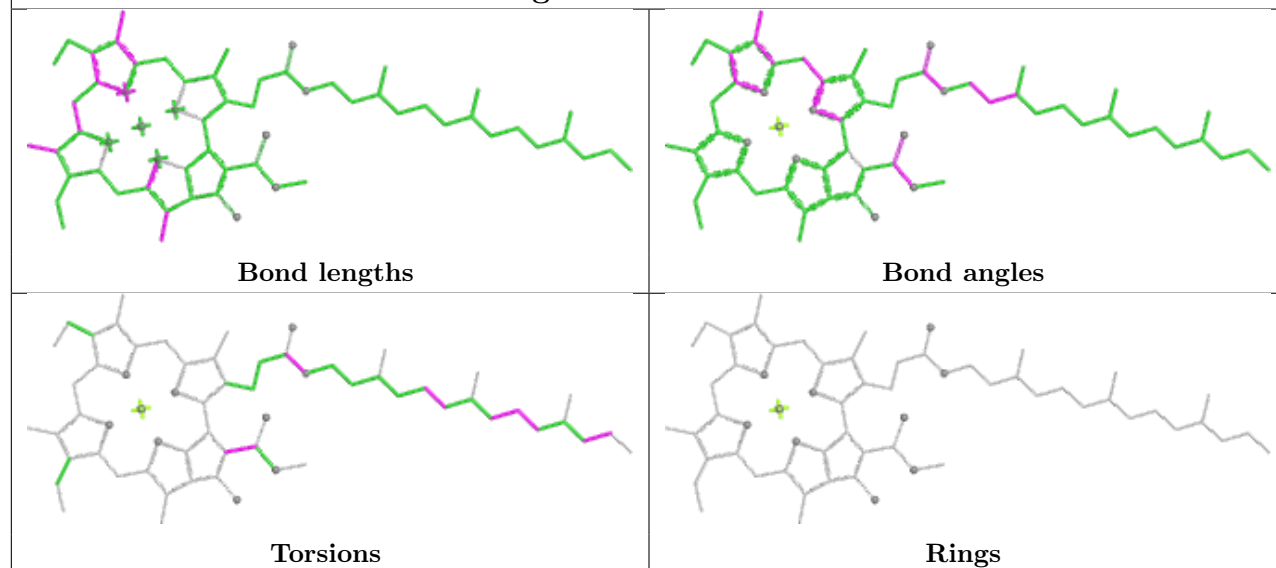


Rings

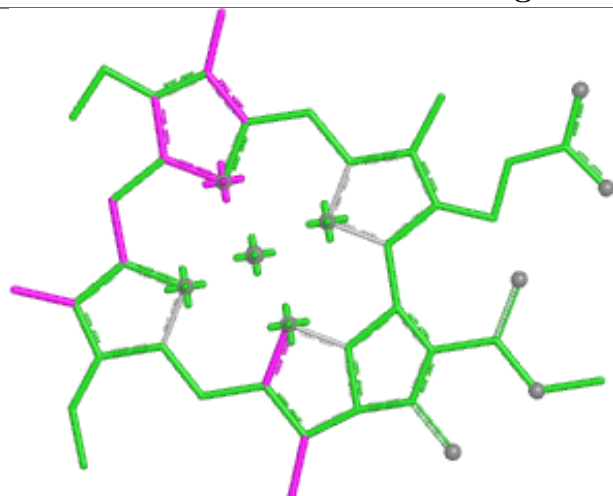
Ligand CHL 2 601



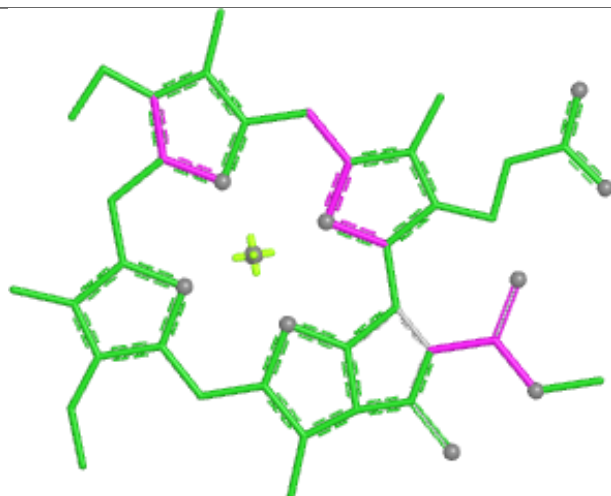
Ligand CLA B 826



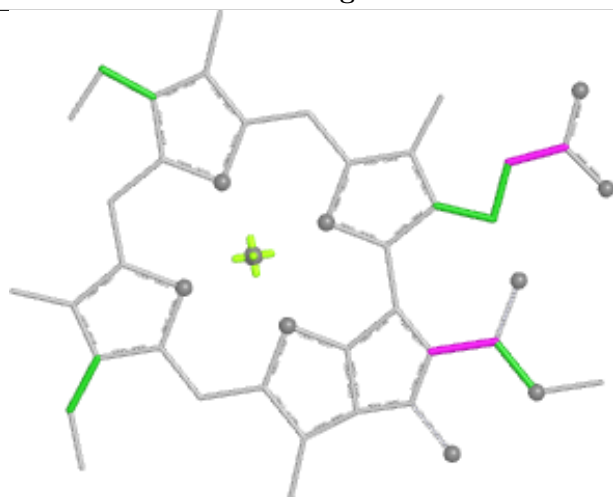
Ligand CLA B 833



Bond lengths



Bond angles

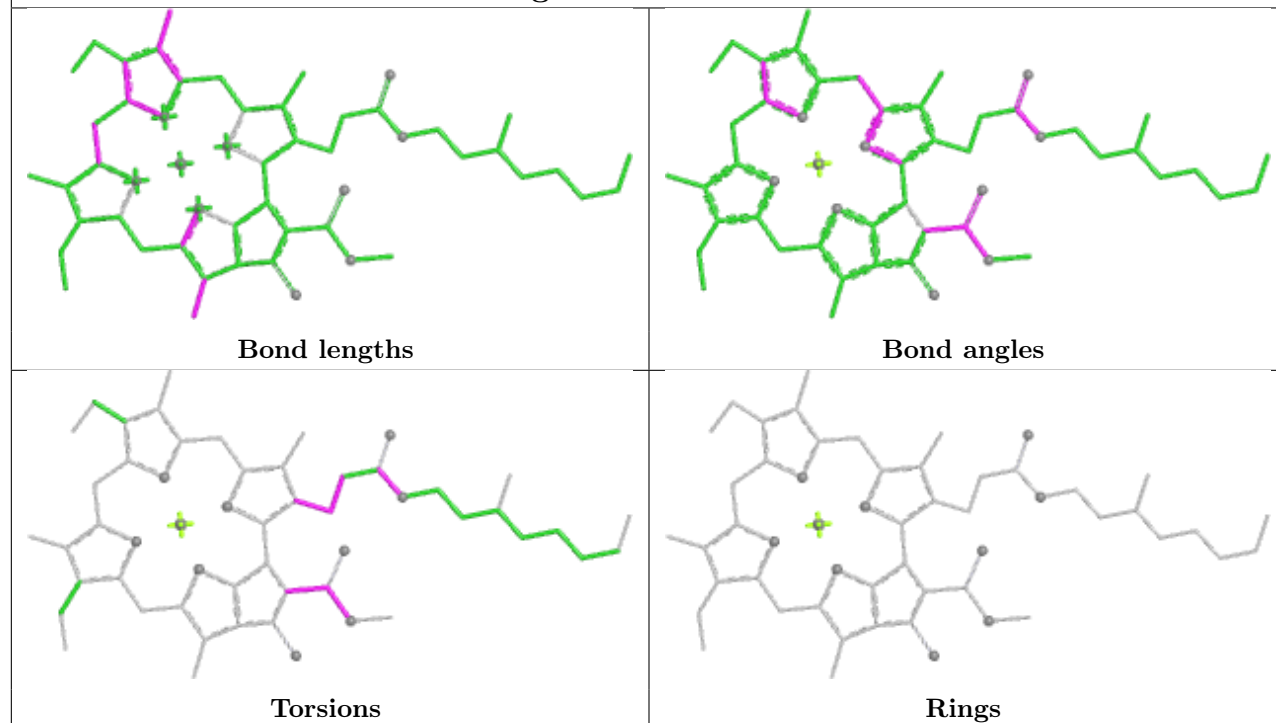


Torsions

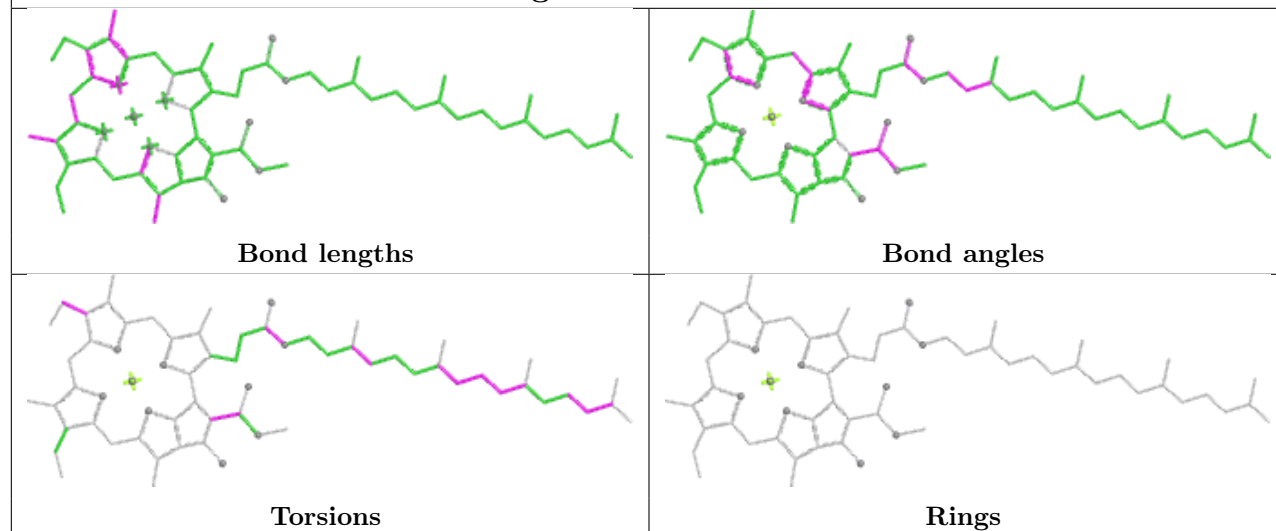


Rings

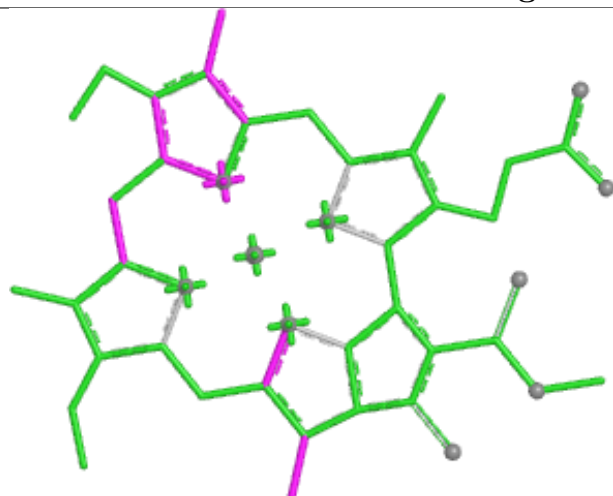
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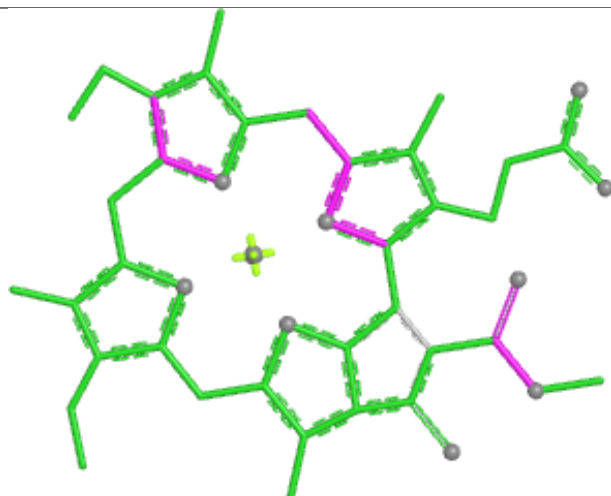
Ligand CLA A 835



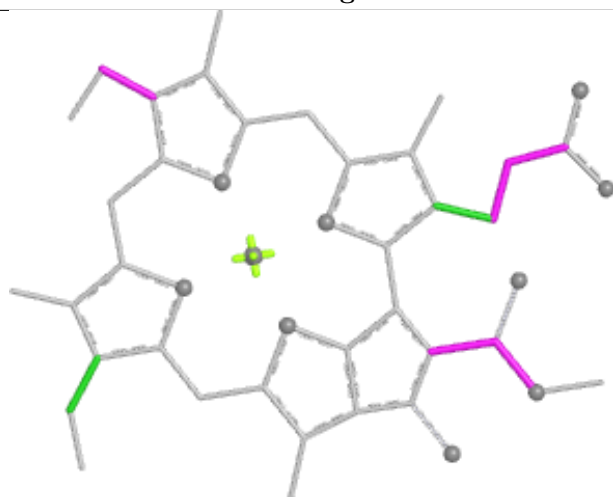
Ligand CLA 1 611



Bond lengths



Bond angles

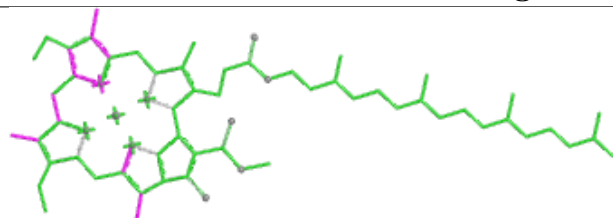


Torsions

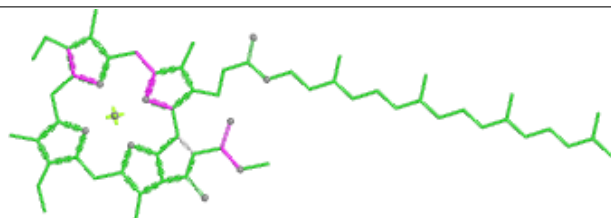


Rings

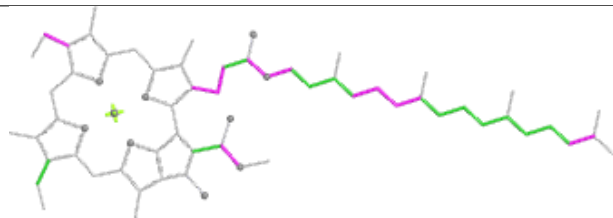
Ligand CLA A 843



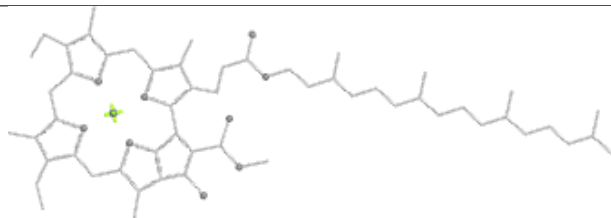
Bond lengths



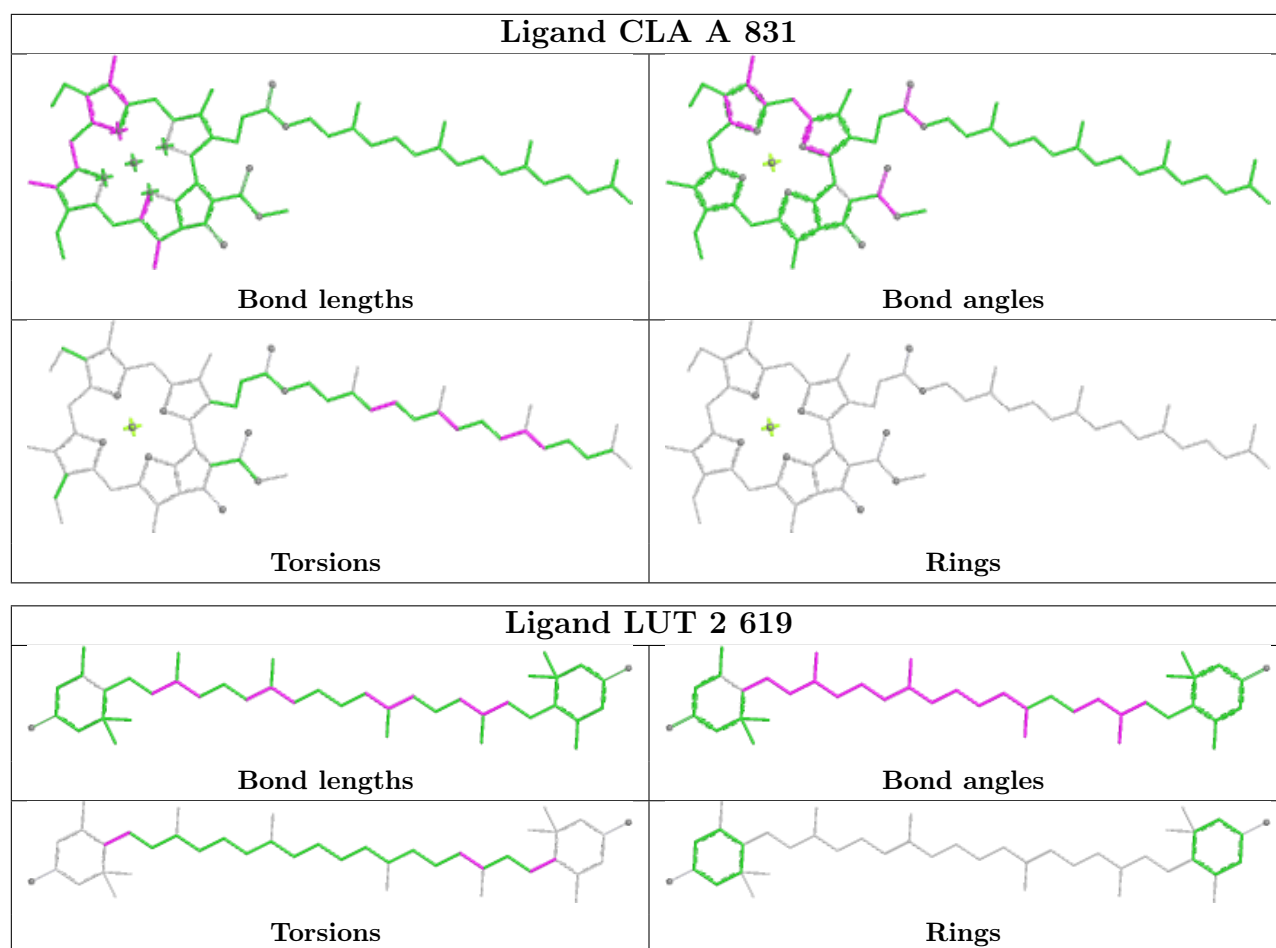
Bond angles

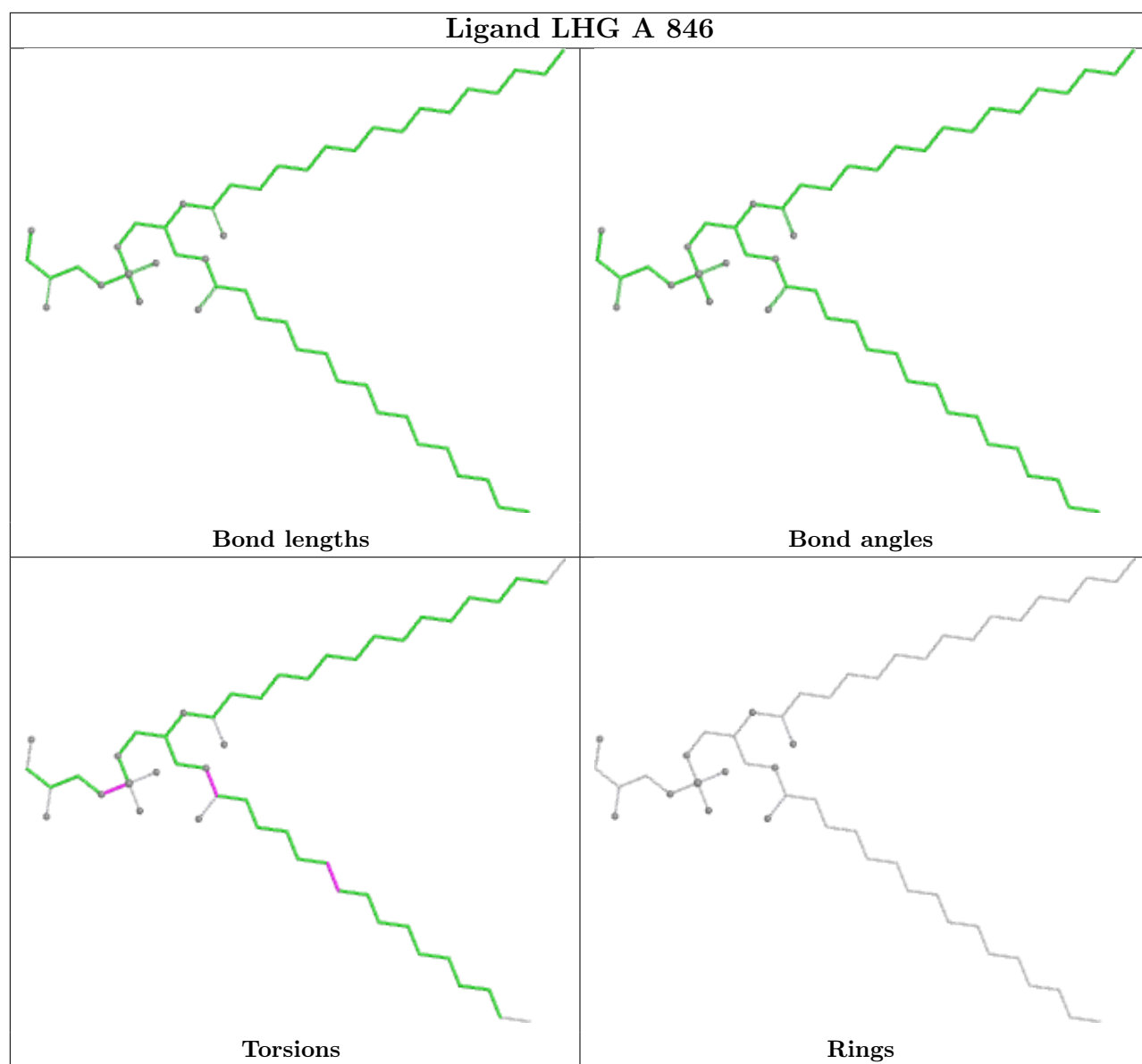


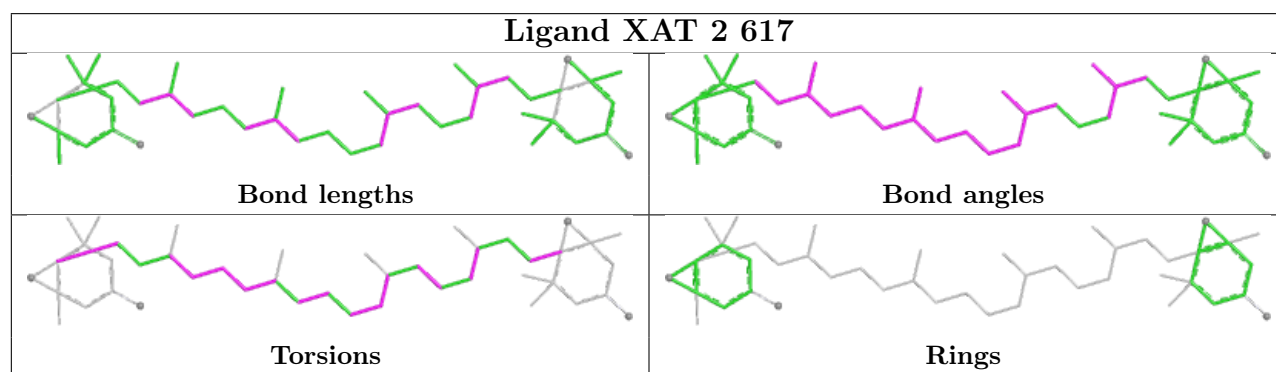
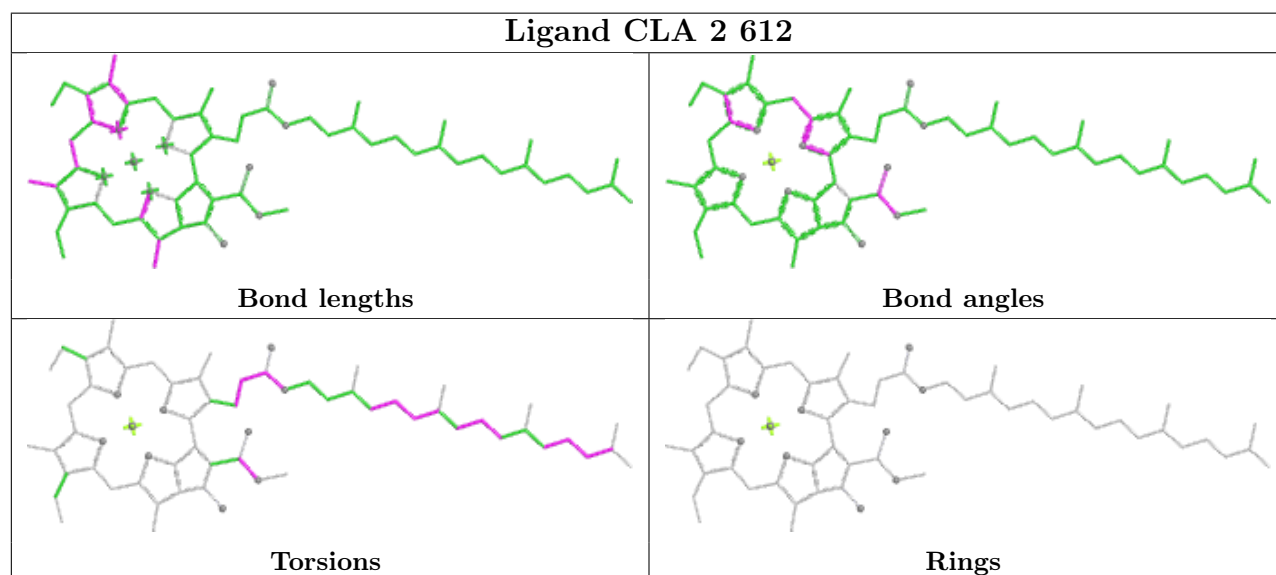
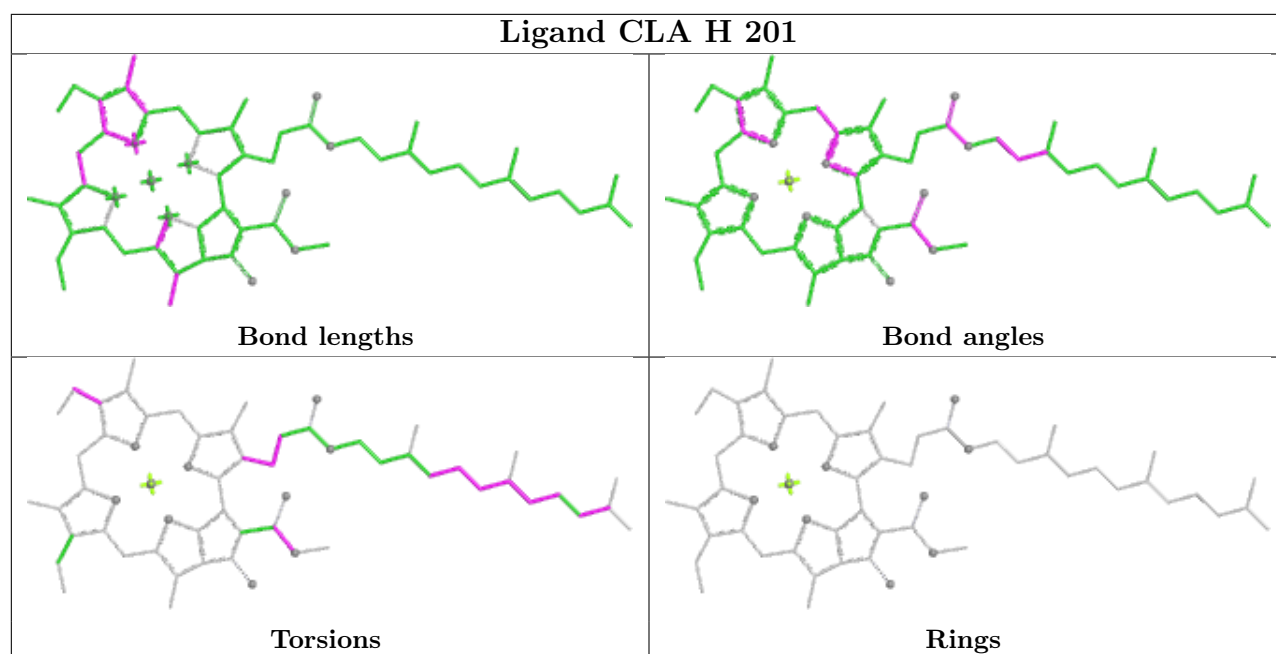
Torsions



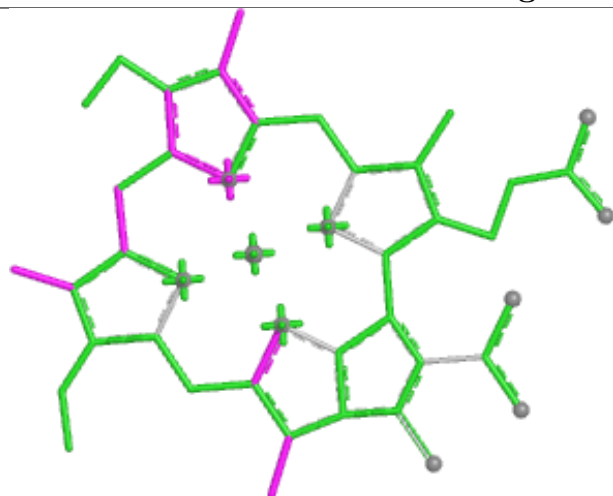
Rings



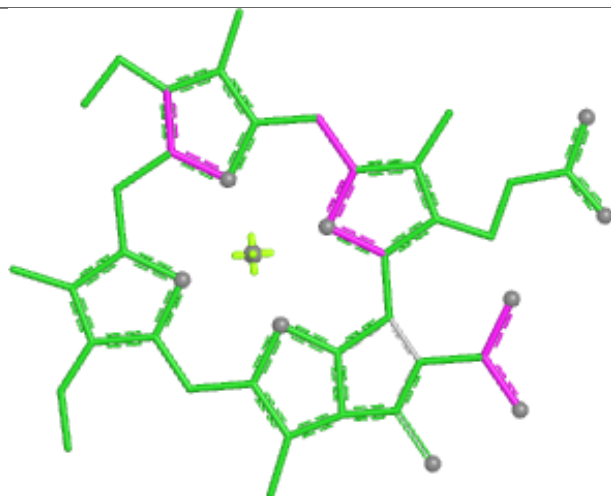




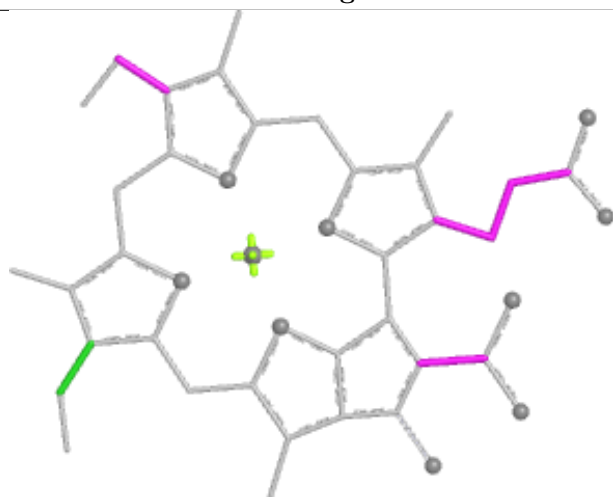
Ligand CLA 1 607



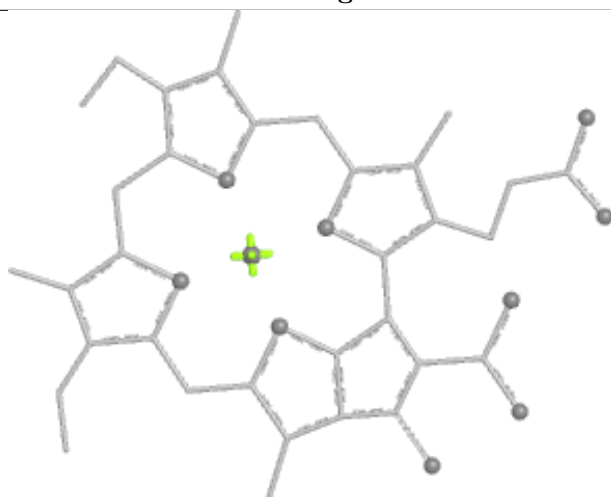
Bond lengths



Bond angles

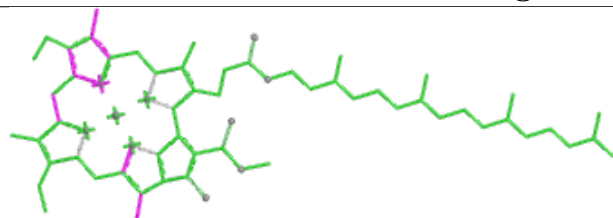


Torsions

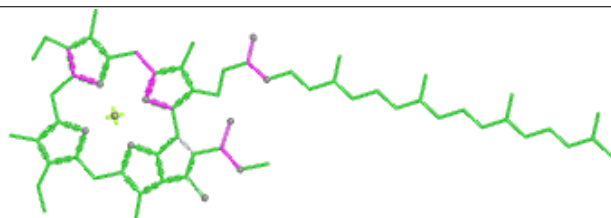


Rings

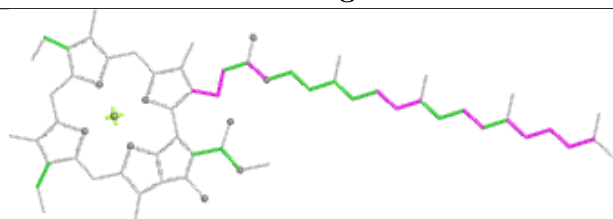
Ligand CLA B 828



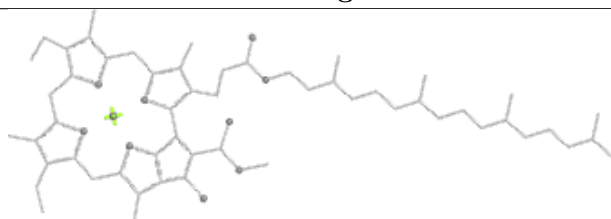
Bond lengths



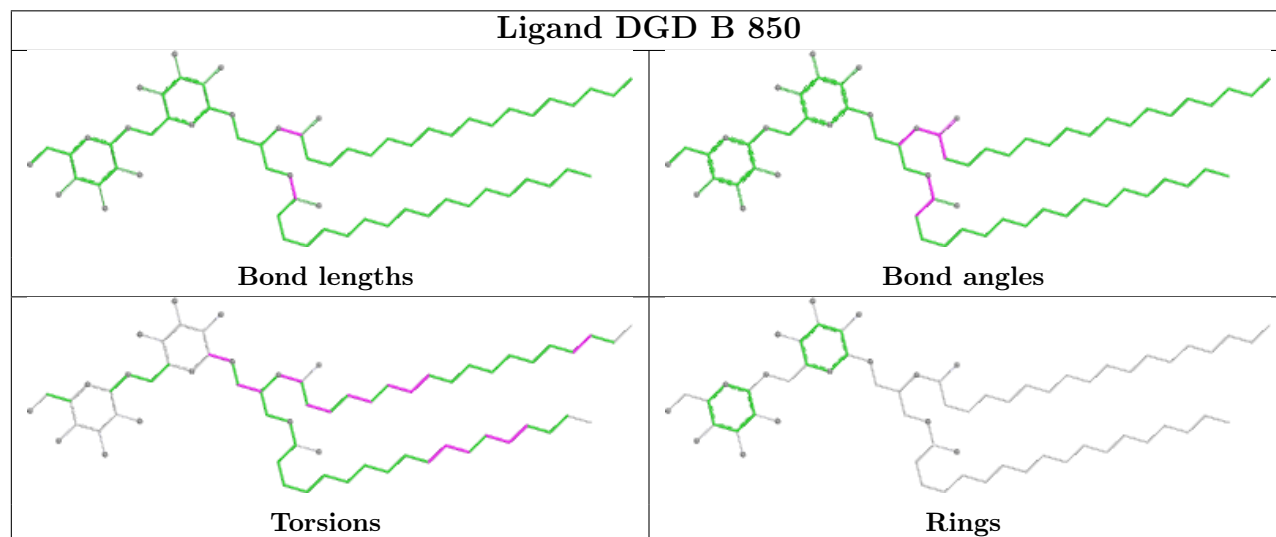
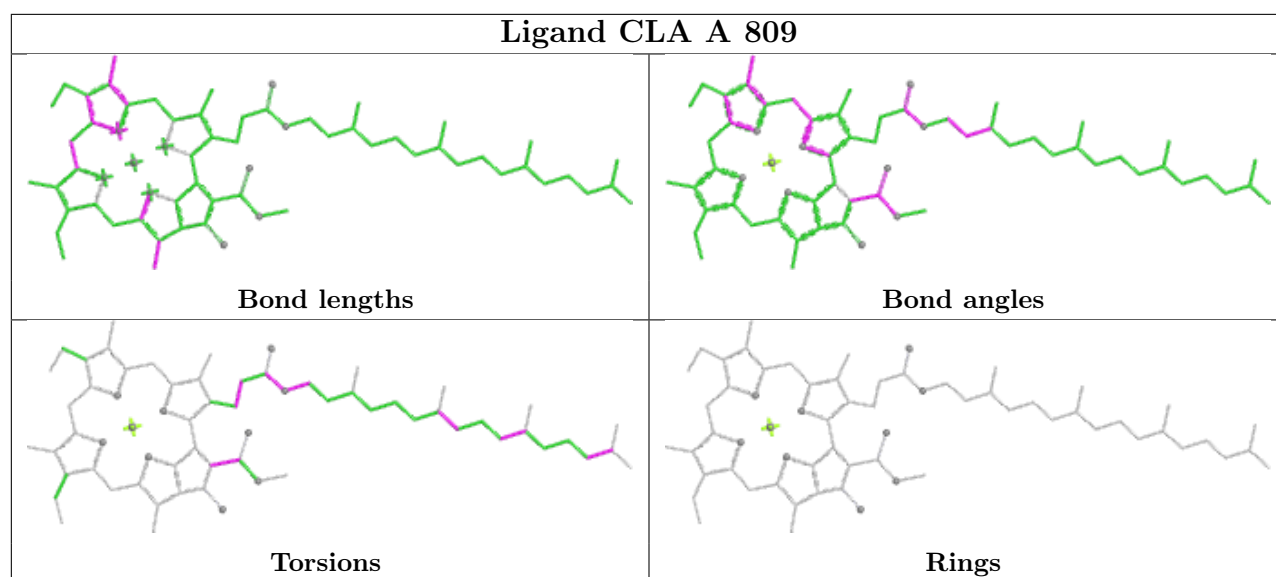
Bond angles



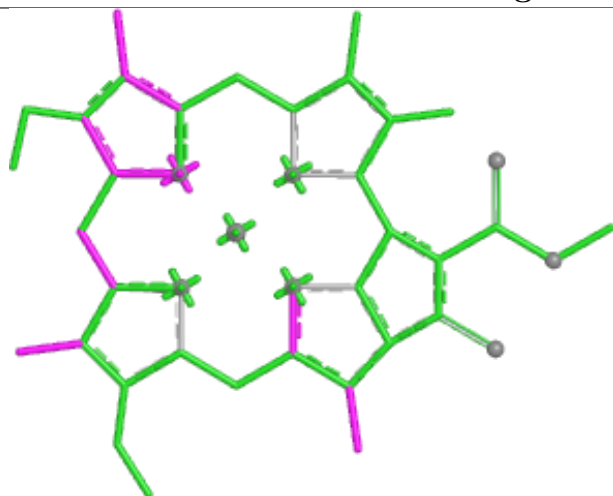
Torsions



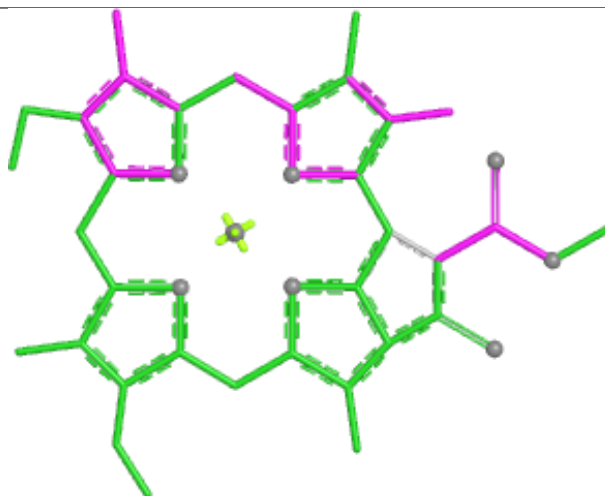
Rings



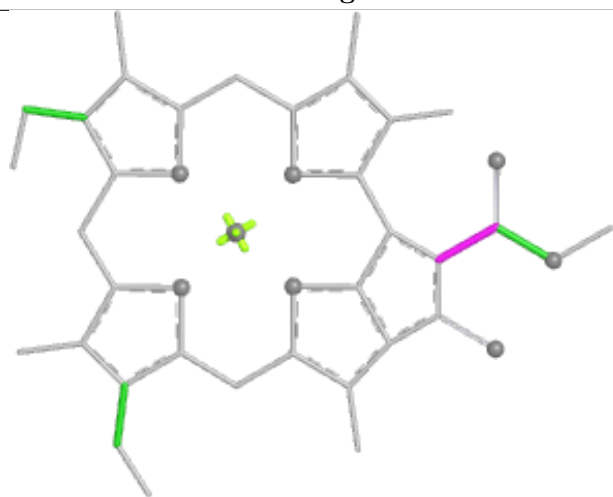
Ligand CLA B 804



Bond lengths



Bond angles

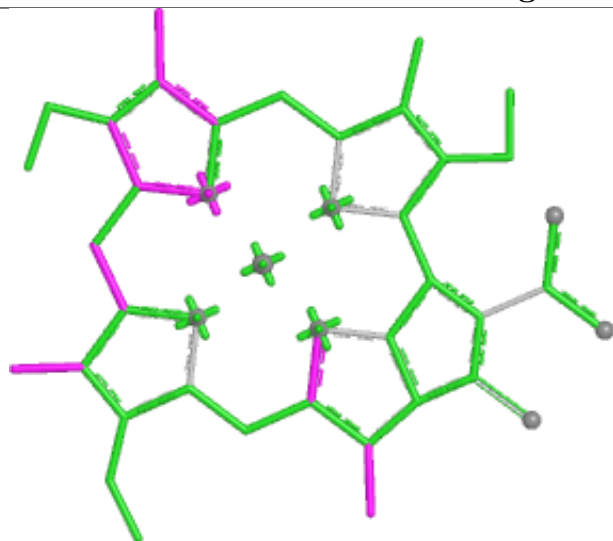


Torsions

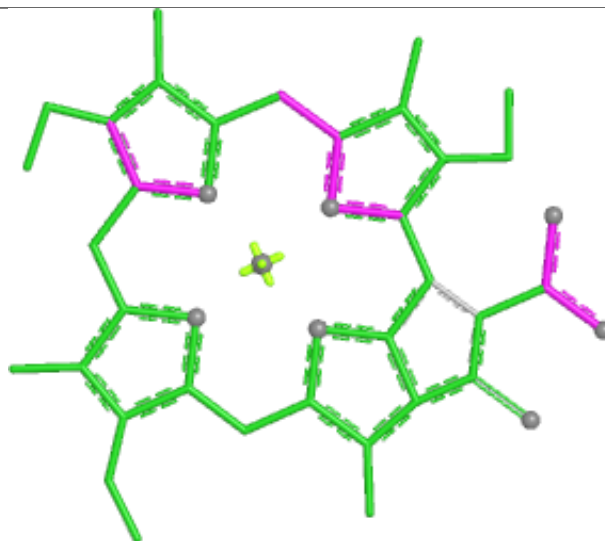


Rings

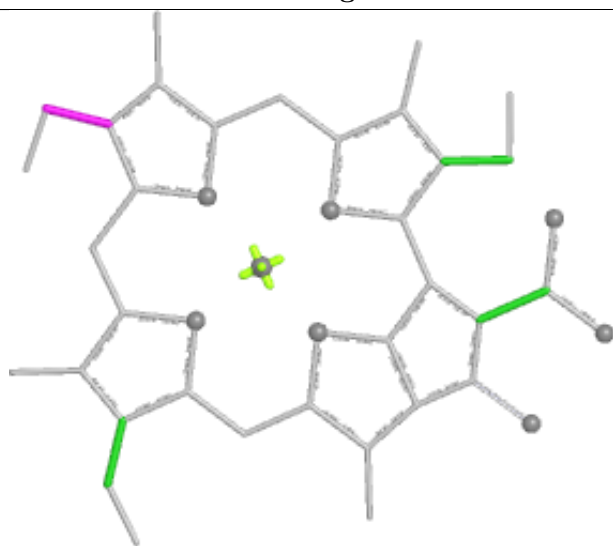
Ligand CLA 3 604



Bond lengths



Bond angles

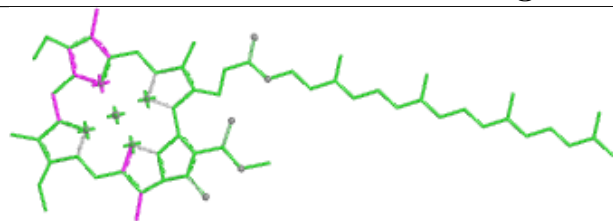


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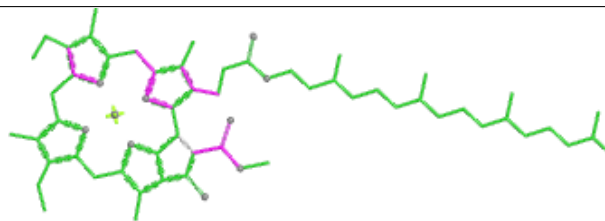


Rings

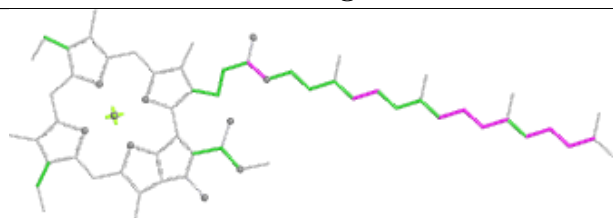
Ligand CLA L 303



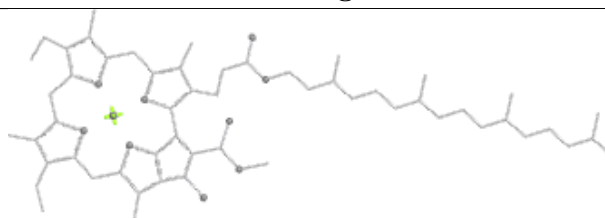
Bond lengths



Bond angles

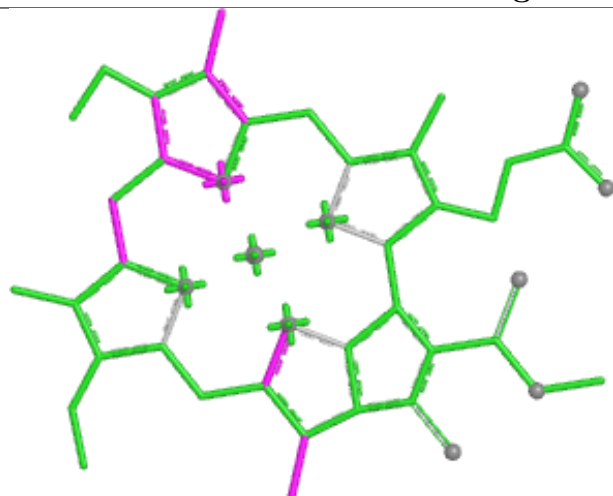


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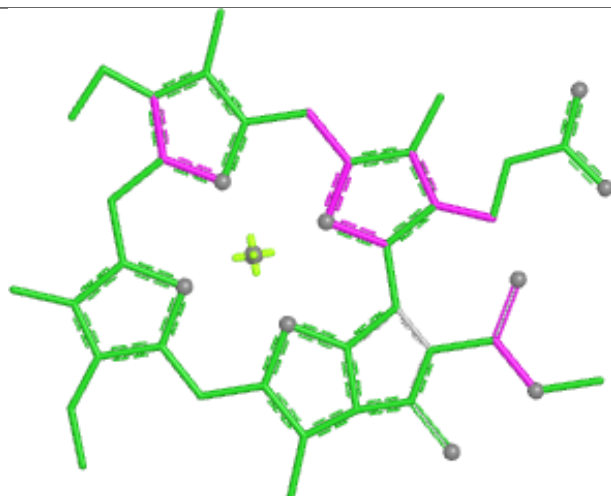


Rings

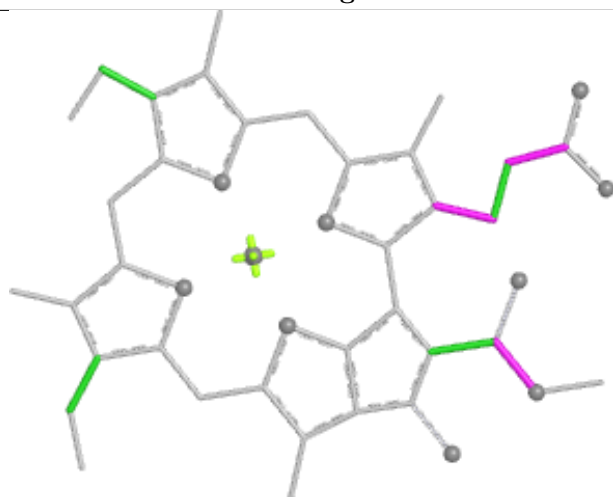
Ligand CLA K 203



Bond lengths



Bond angles

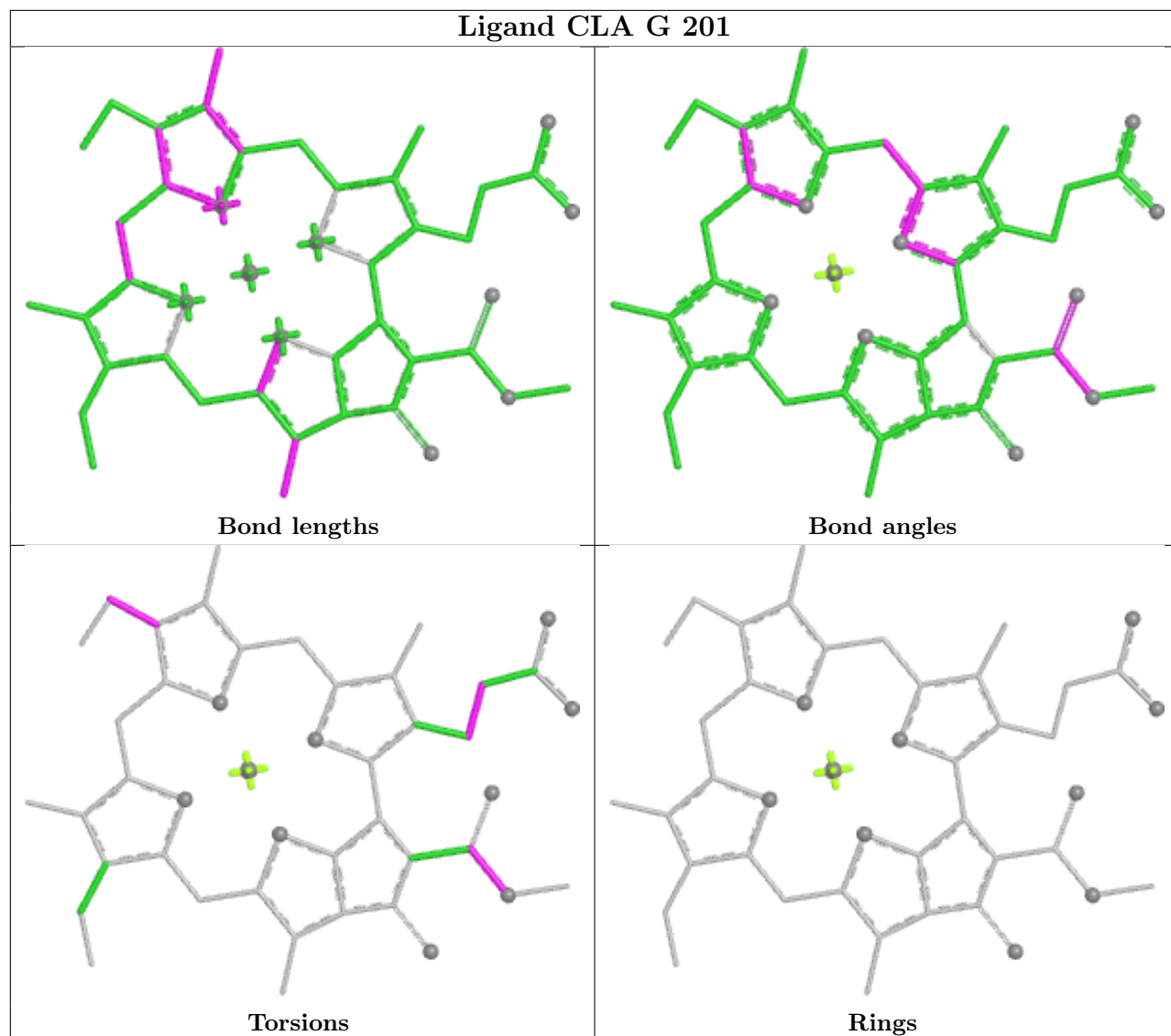


Torsions

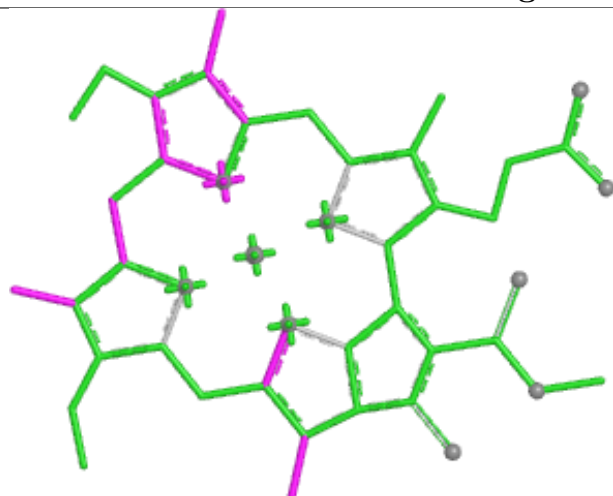


Rings

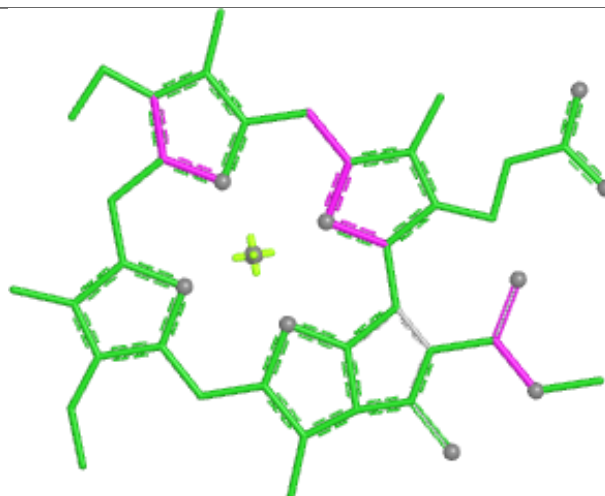
Ligand CLA G 201



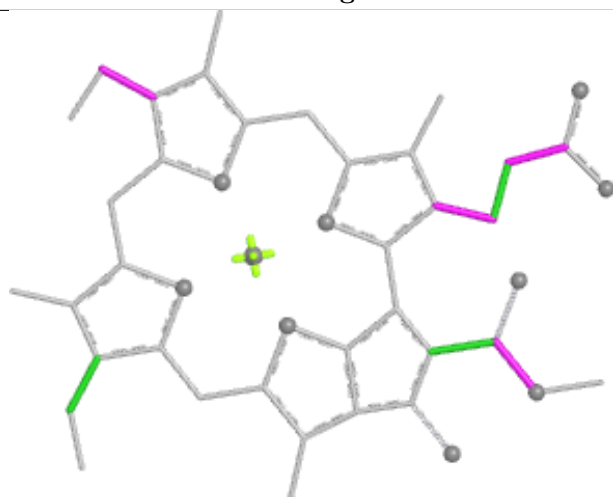
Ligand CLA 4 608



Bond lengths



Bond angles

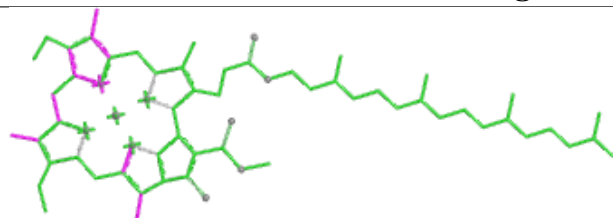


Torsions

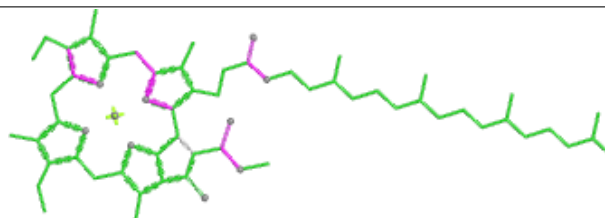


Rings

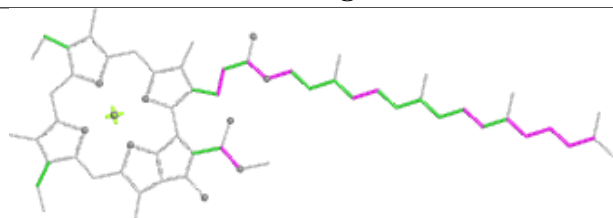
Ligand CLA A 814



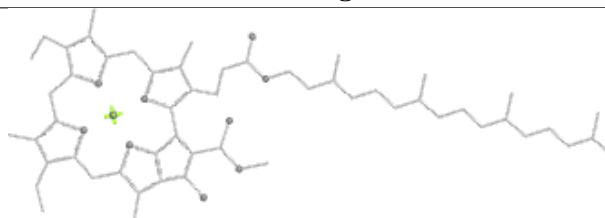
Bond lengths



Bond angles

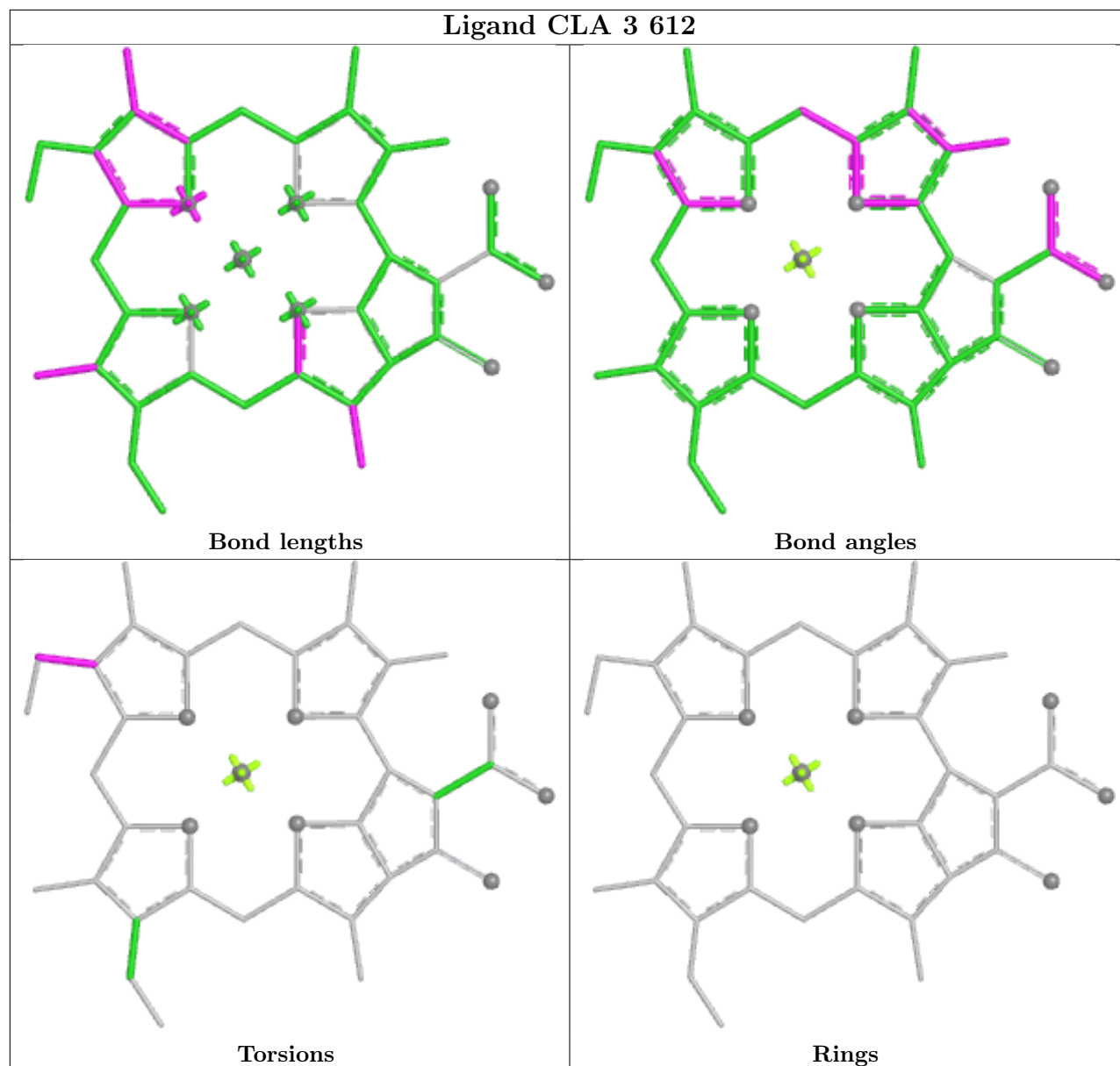


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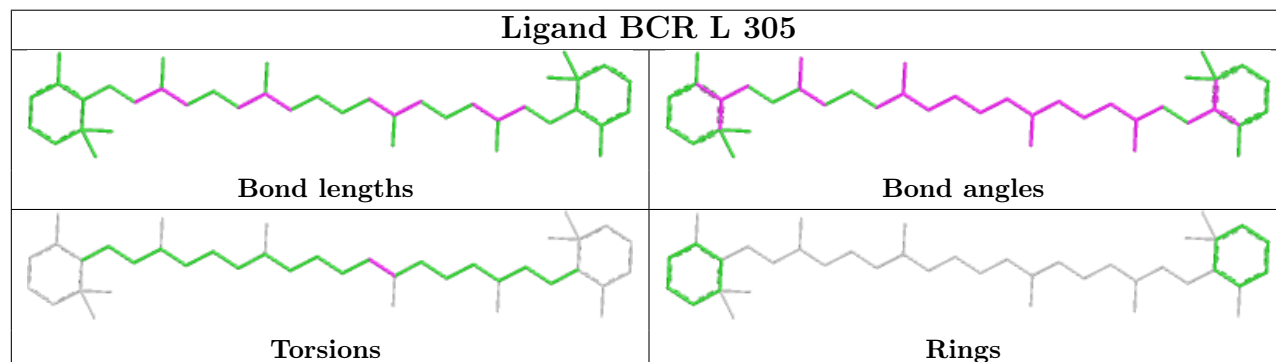


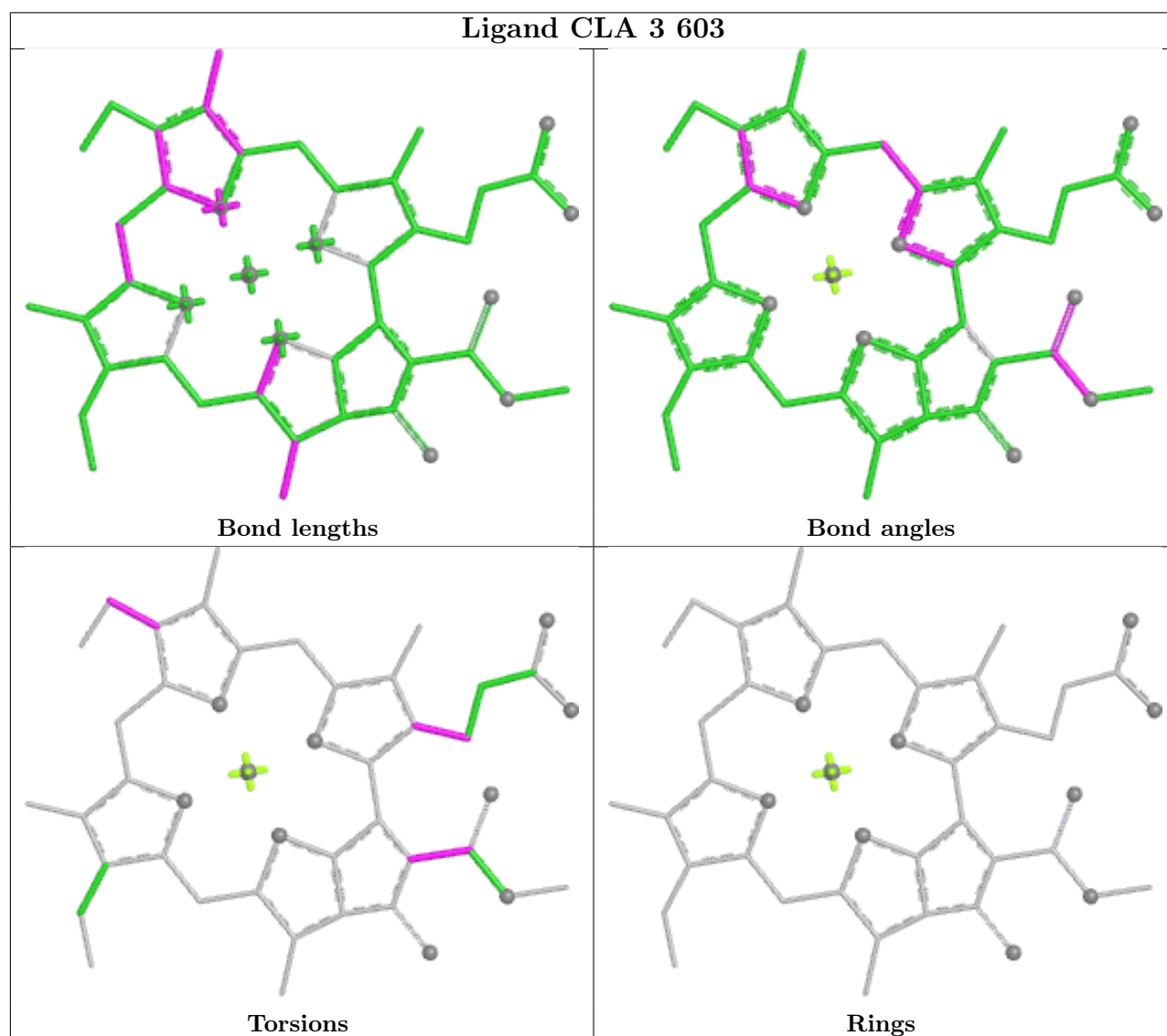
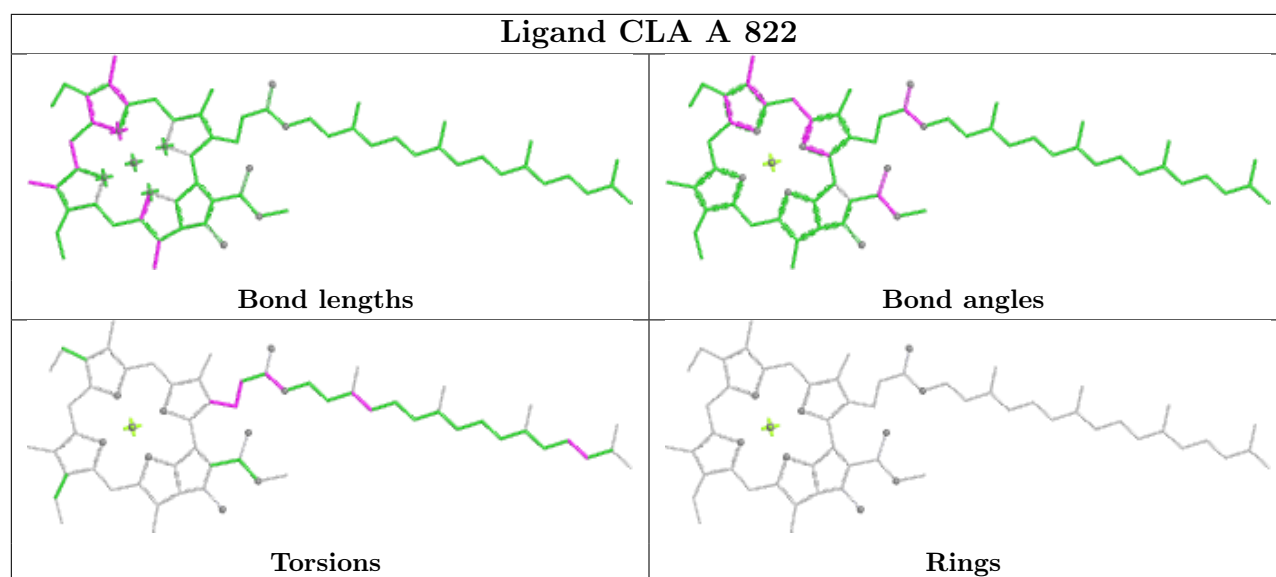
Rings

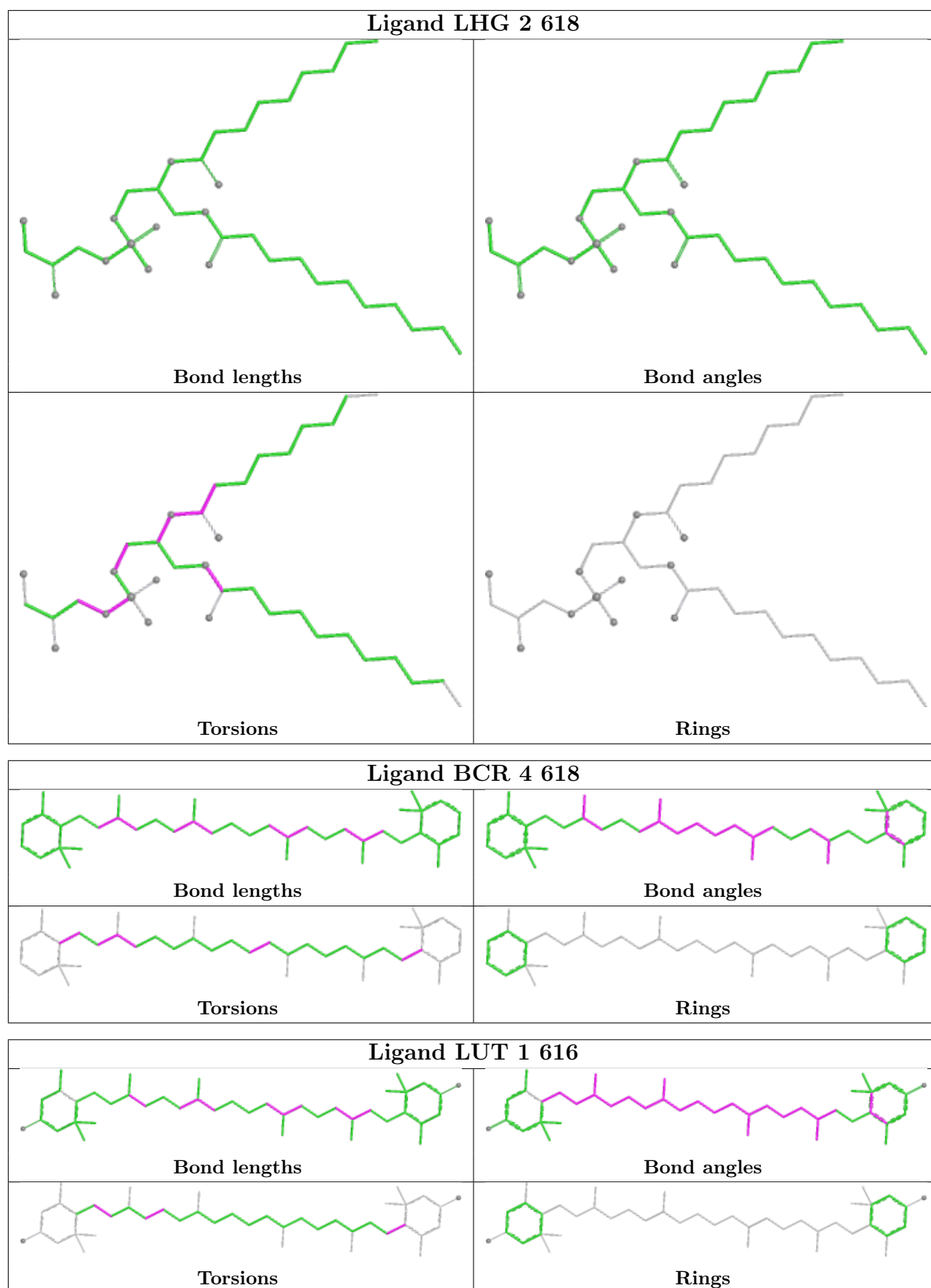
Ligand CLA 3 612

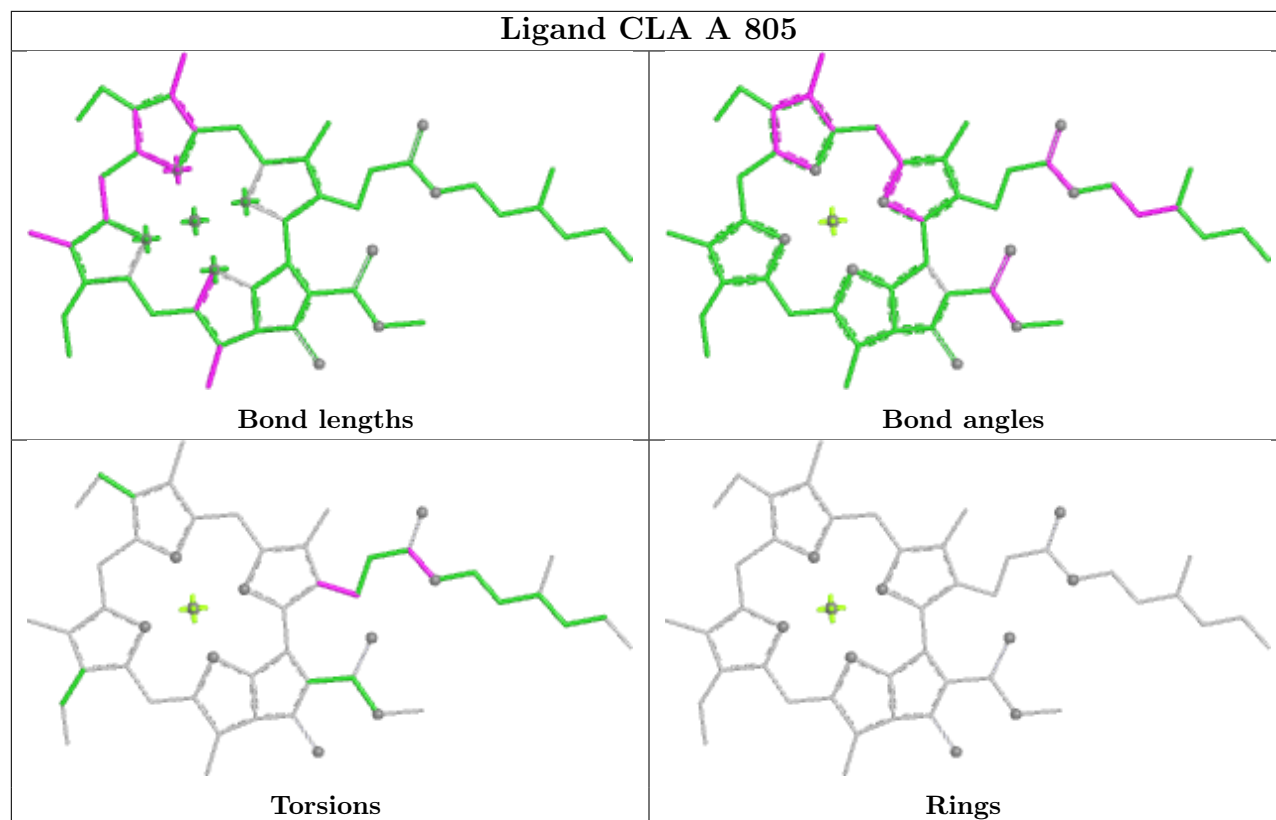


Ligand BCR L 305

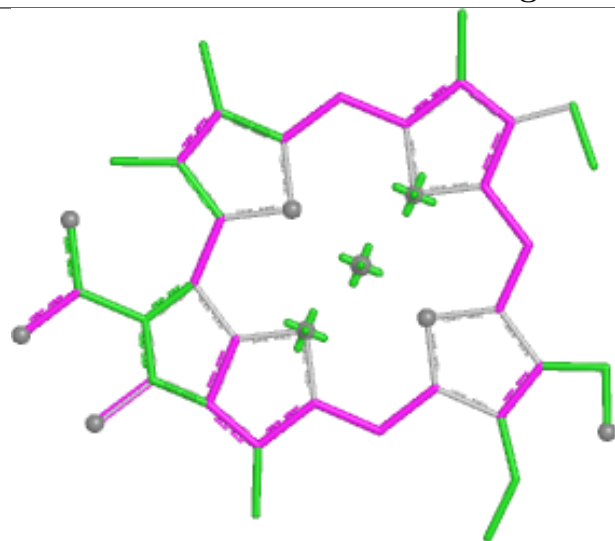




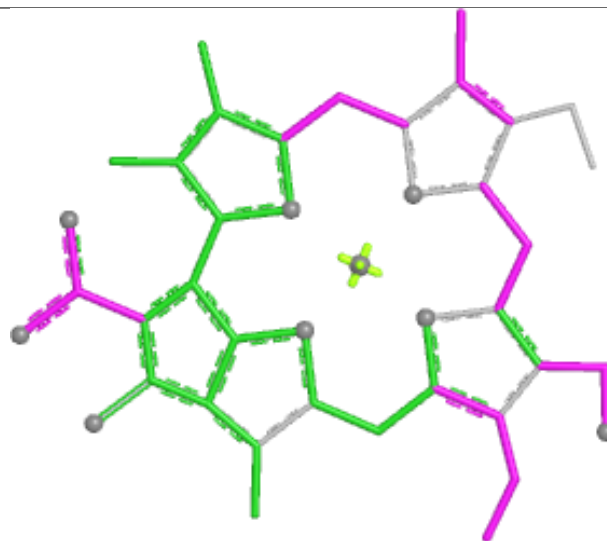




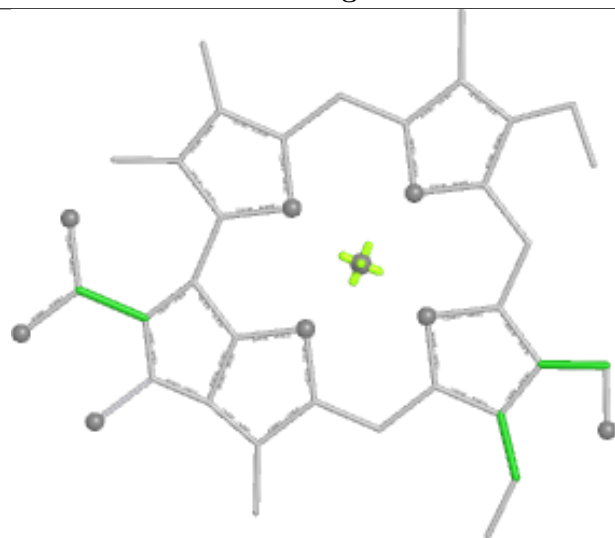
Ligand CHL 1 606



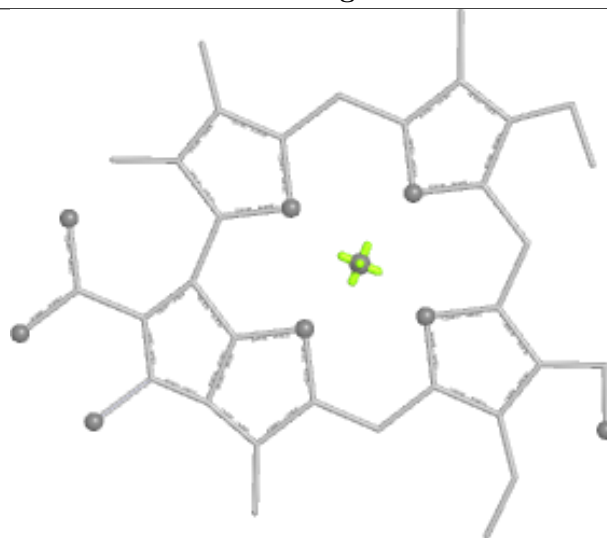
Bond lengths



Bond angles

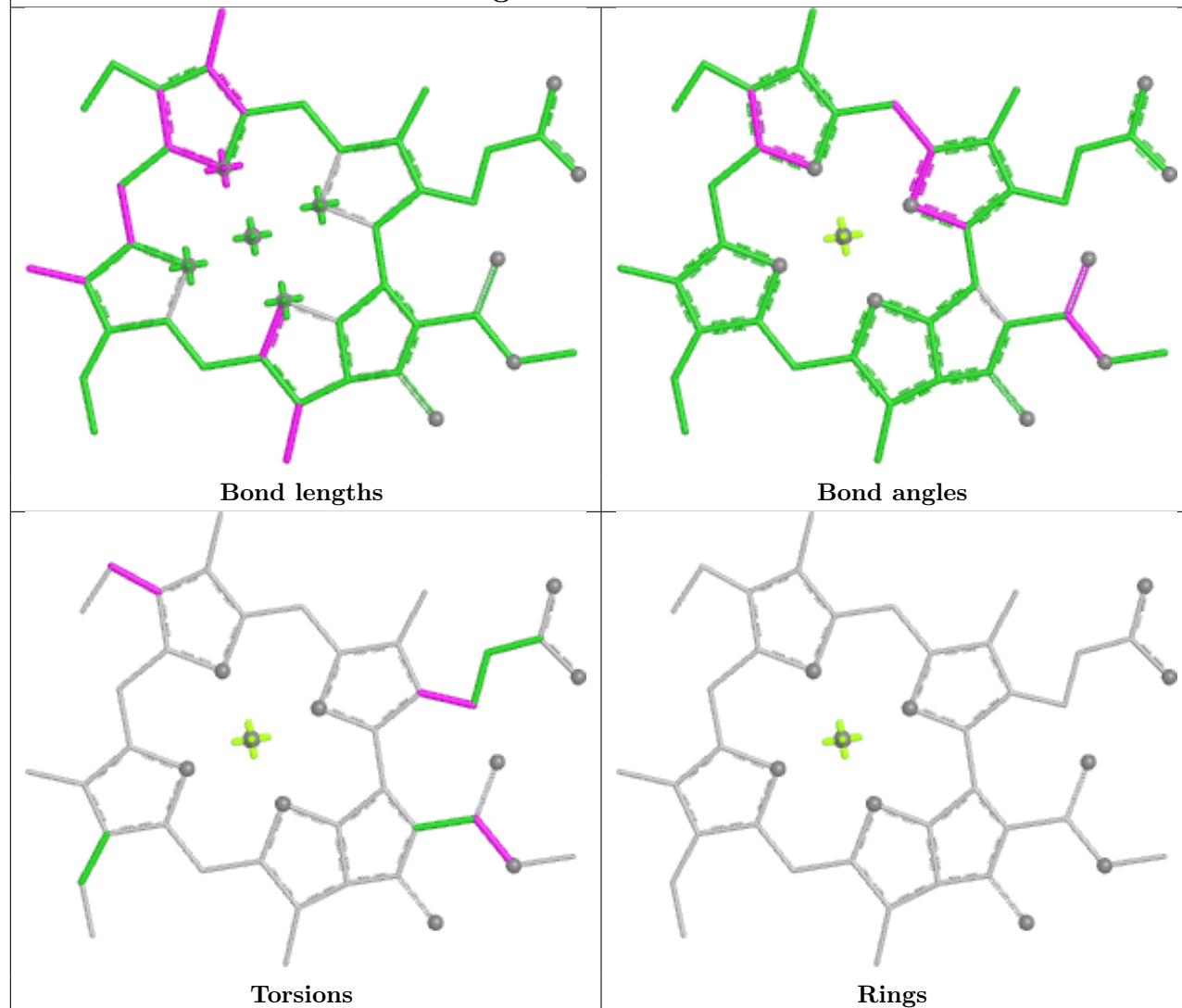


Torsions

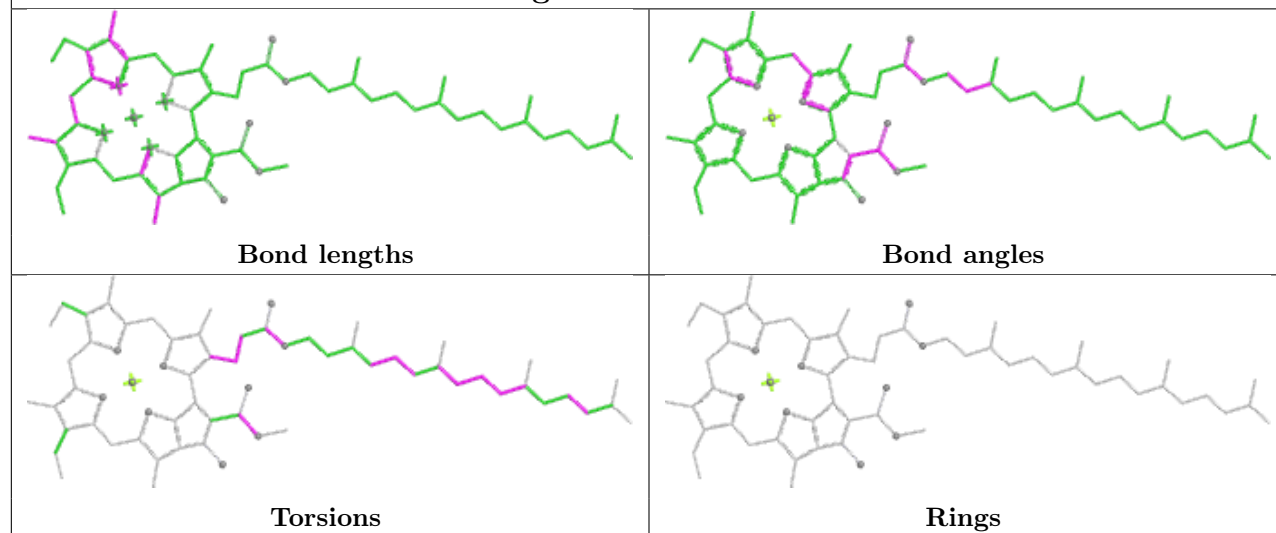


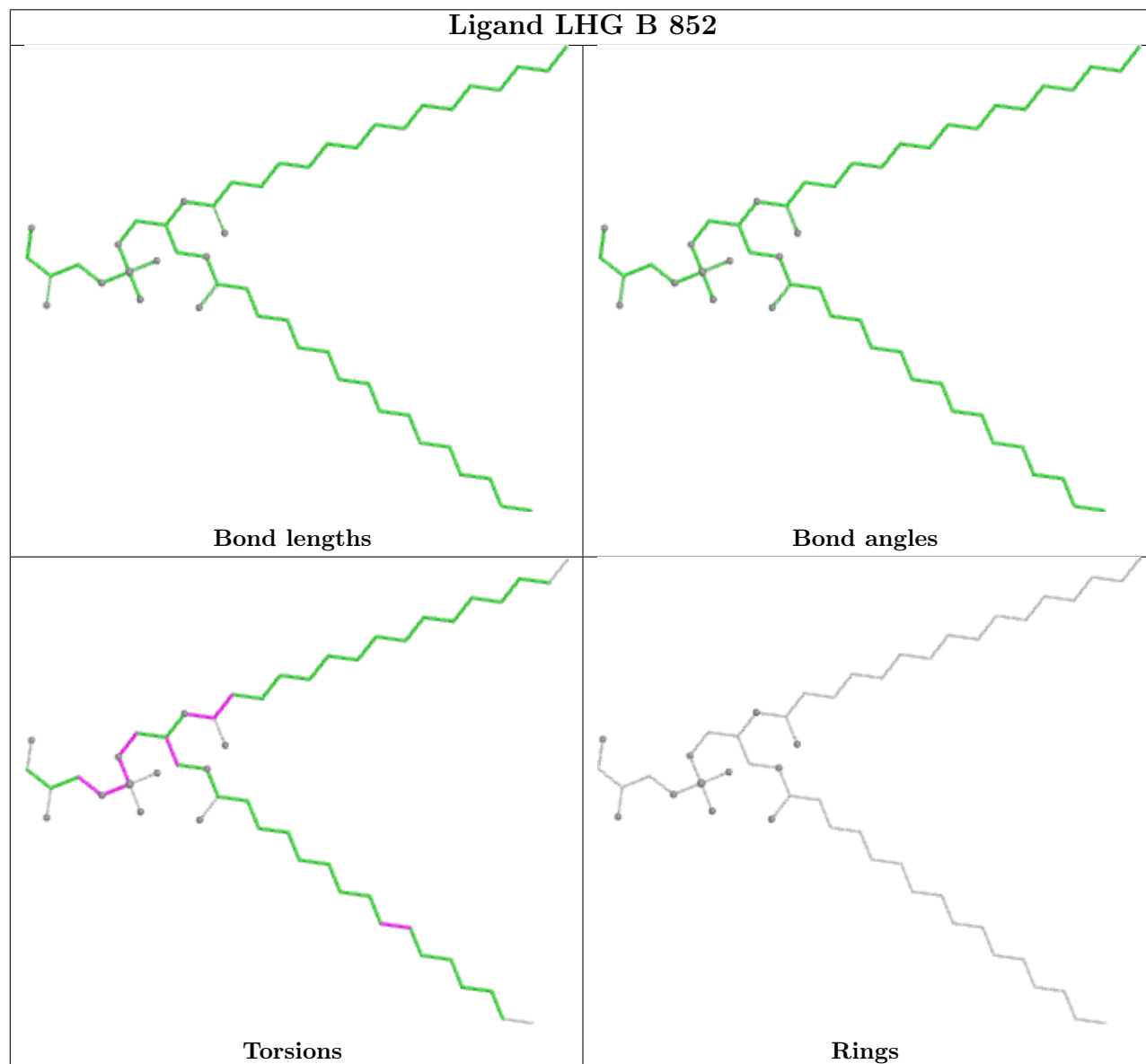
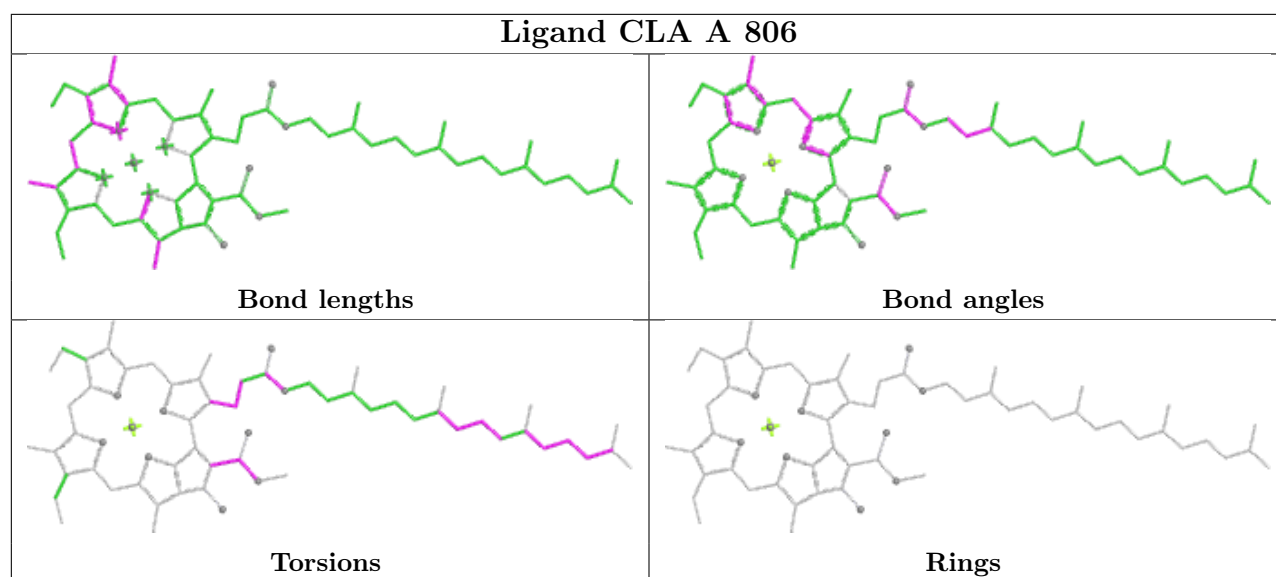
Rings

Ligand CLA B 823

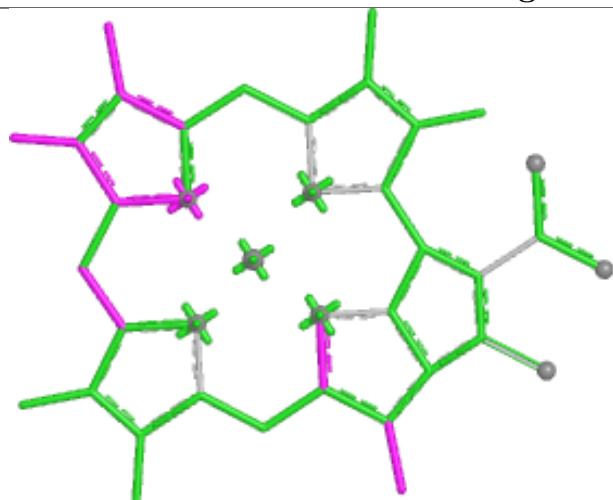


Ligand CLA B 802

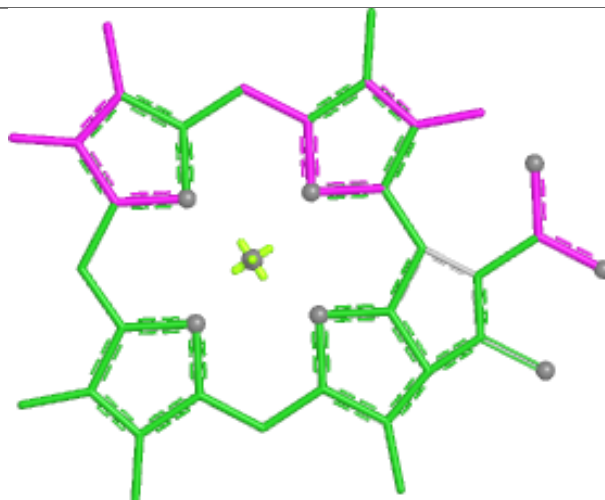




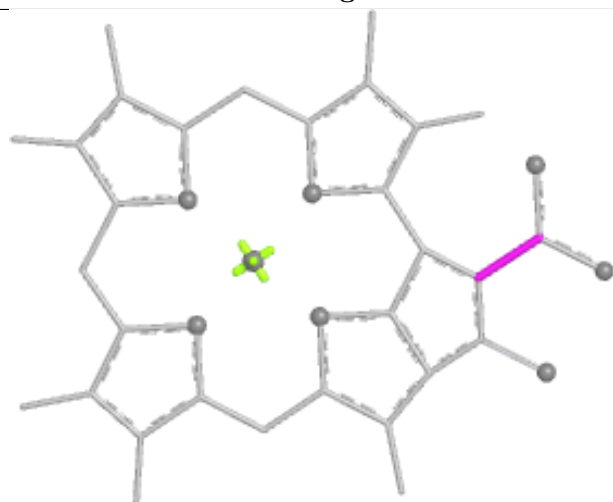
Ligand CLA 1 613



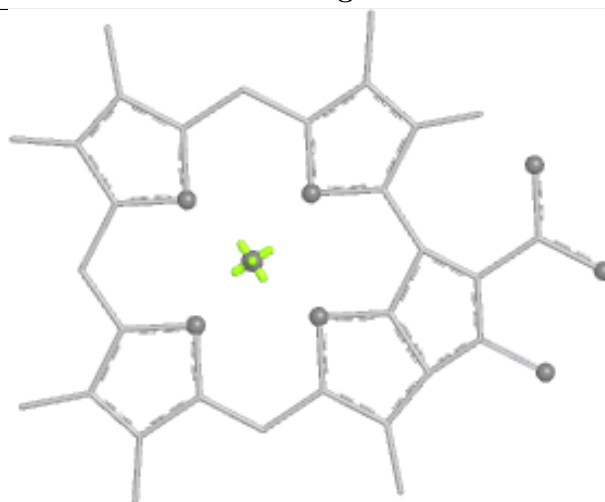
Bond lengths



Bond angles

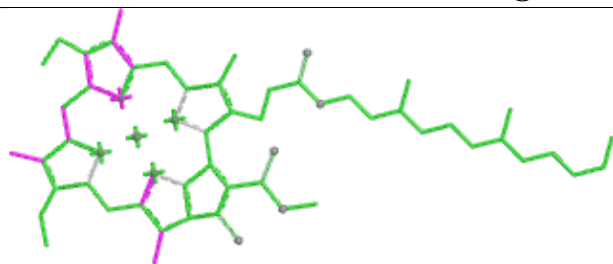


Torsions

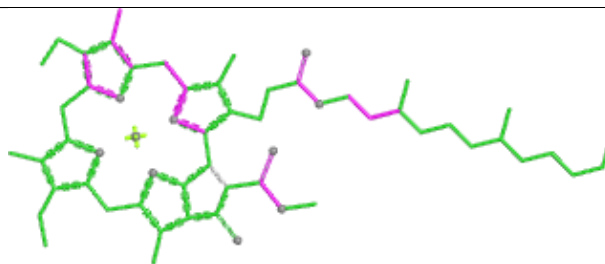


Rings

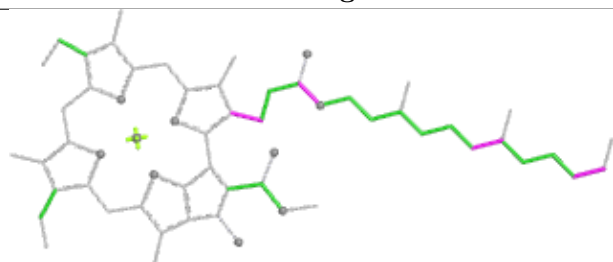
Ligand CLA A 827



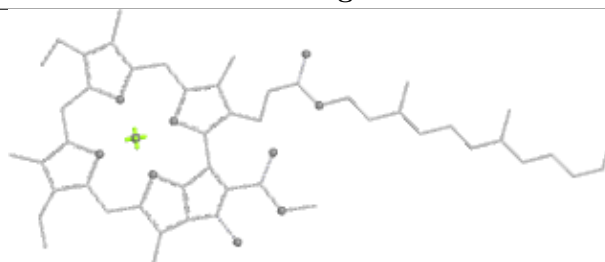
Bond lengths



Bond angles

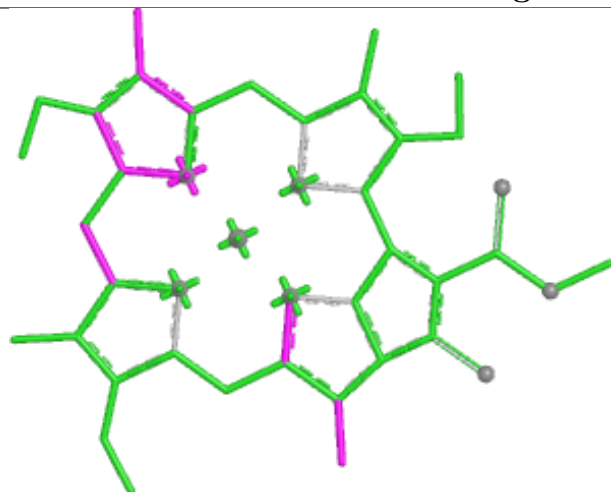


Torsions

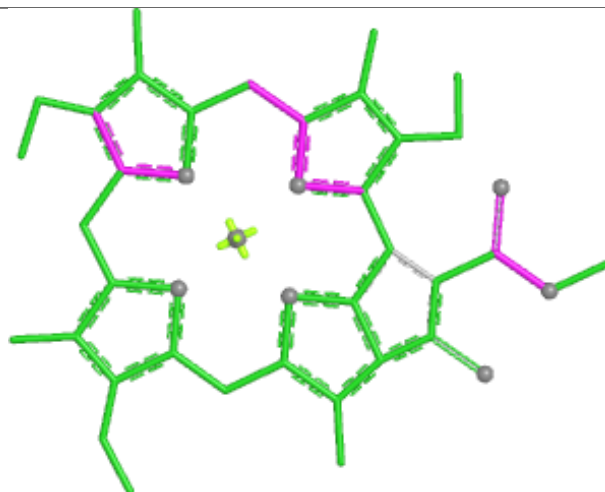


Rings

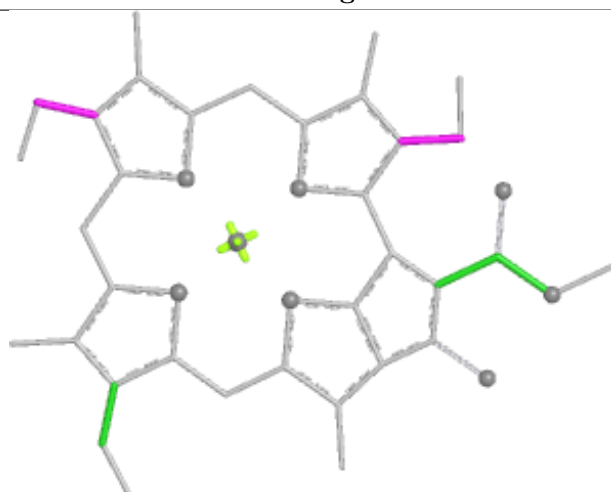
Ligand CLA G 202



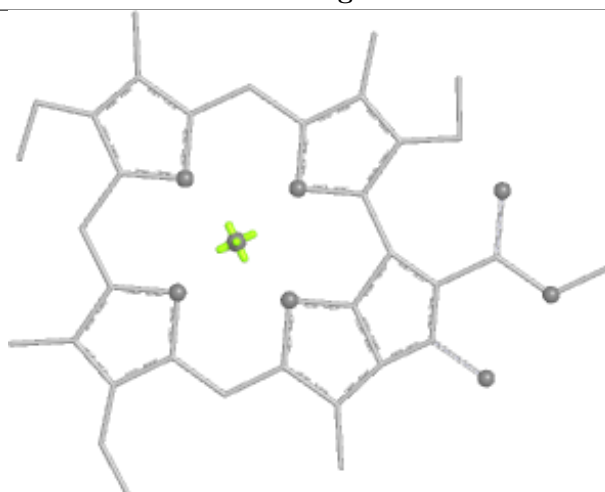
Bond lengths



Bond angles

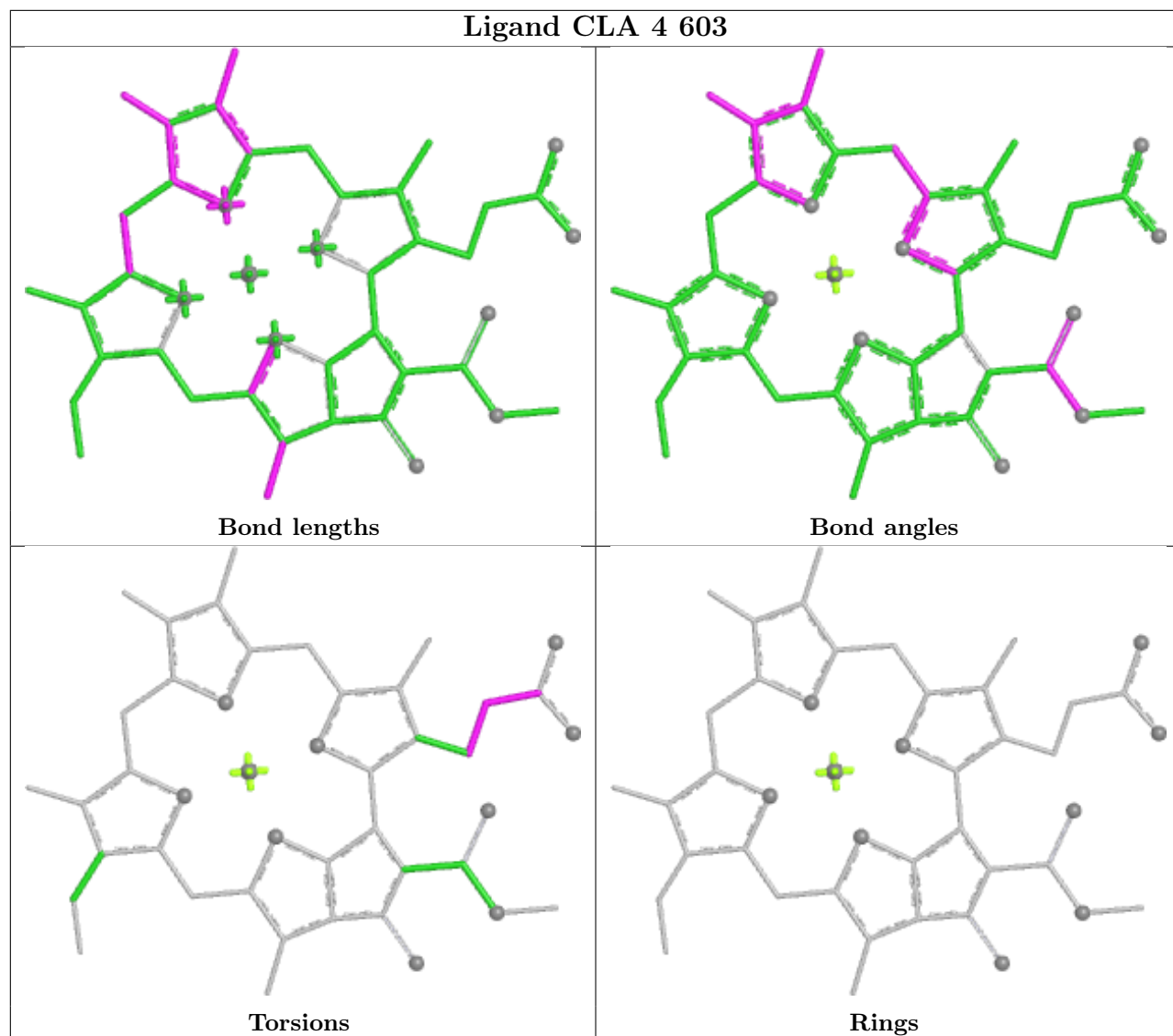


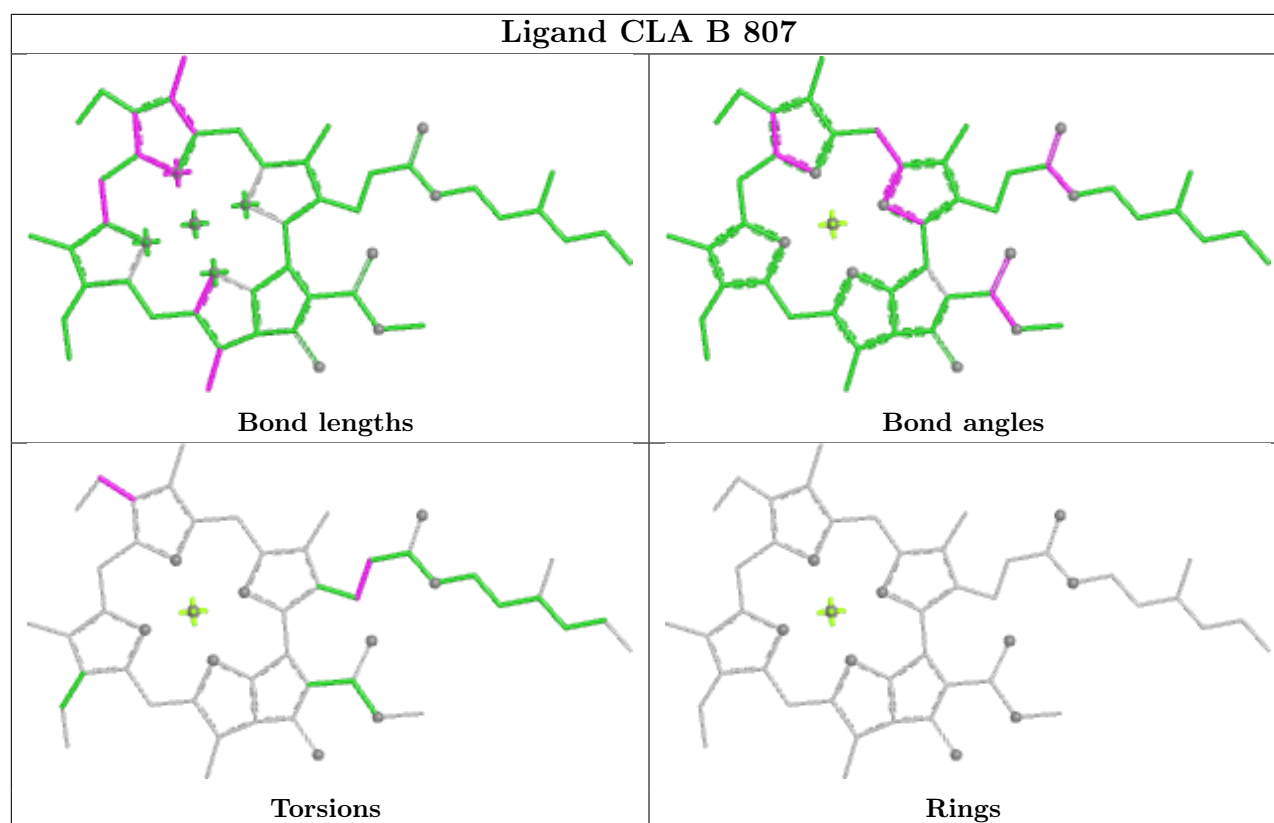
Torsions



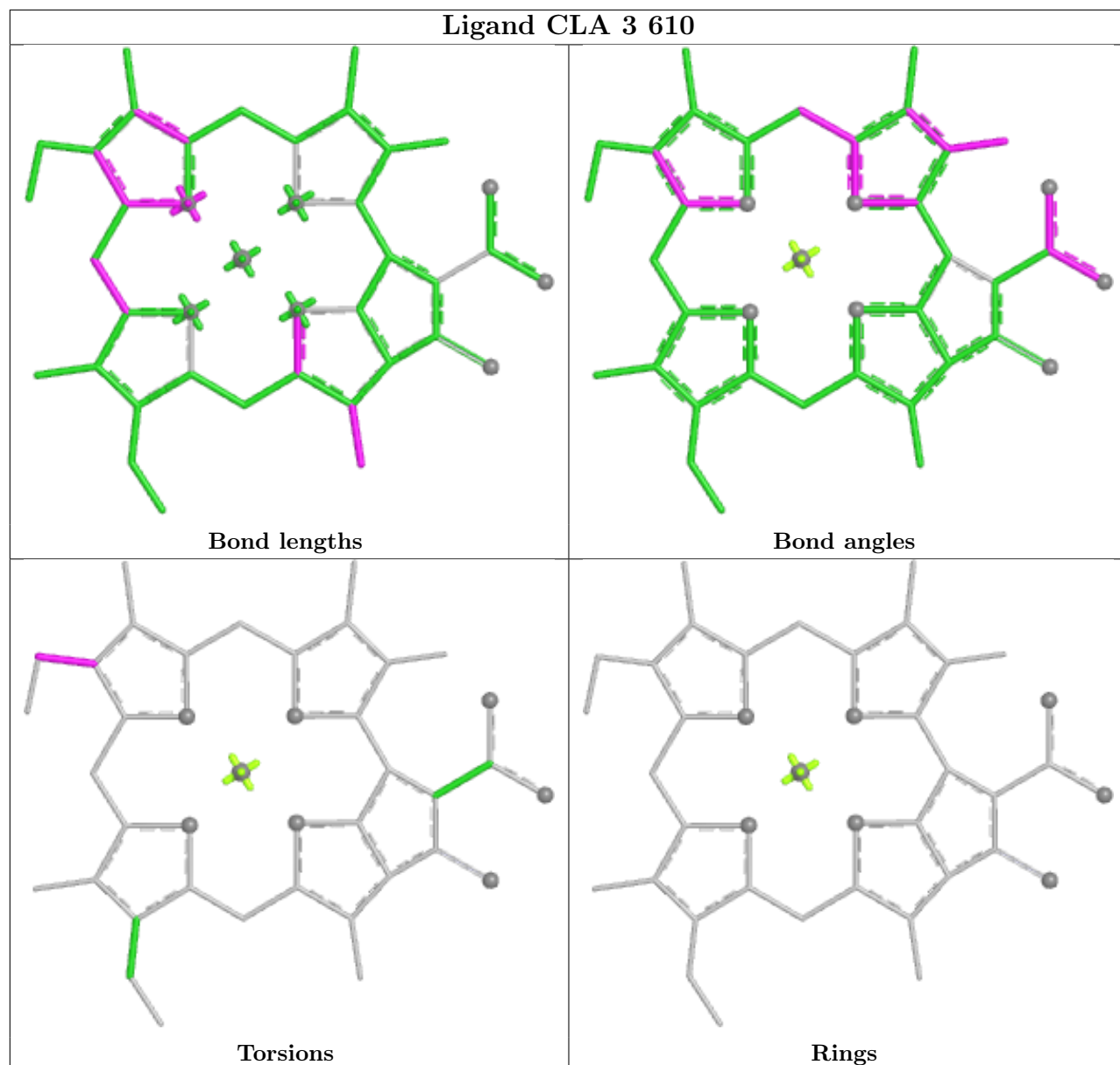
Rings

Ligand CLA 4 603

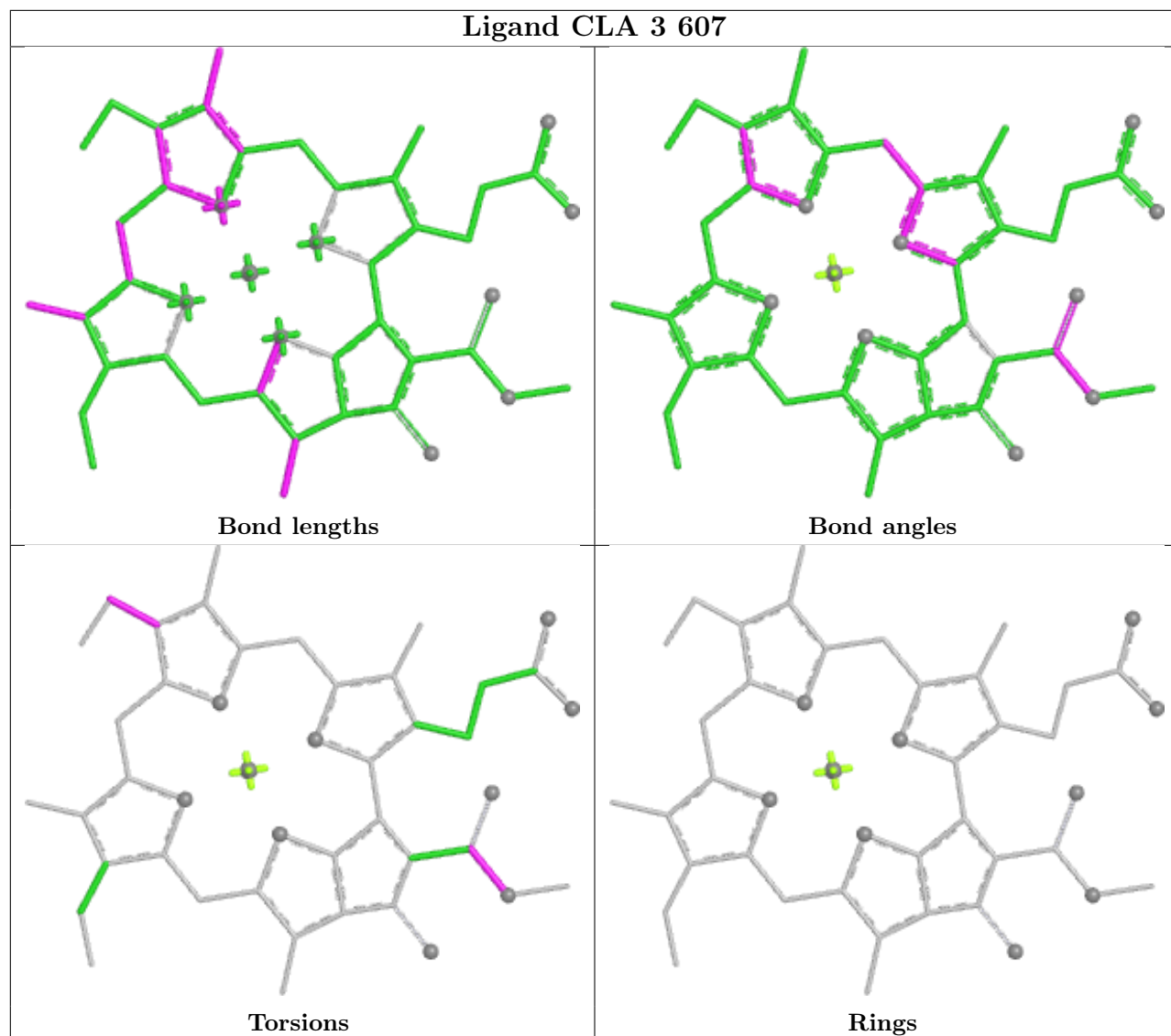




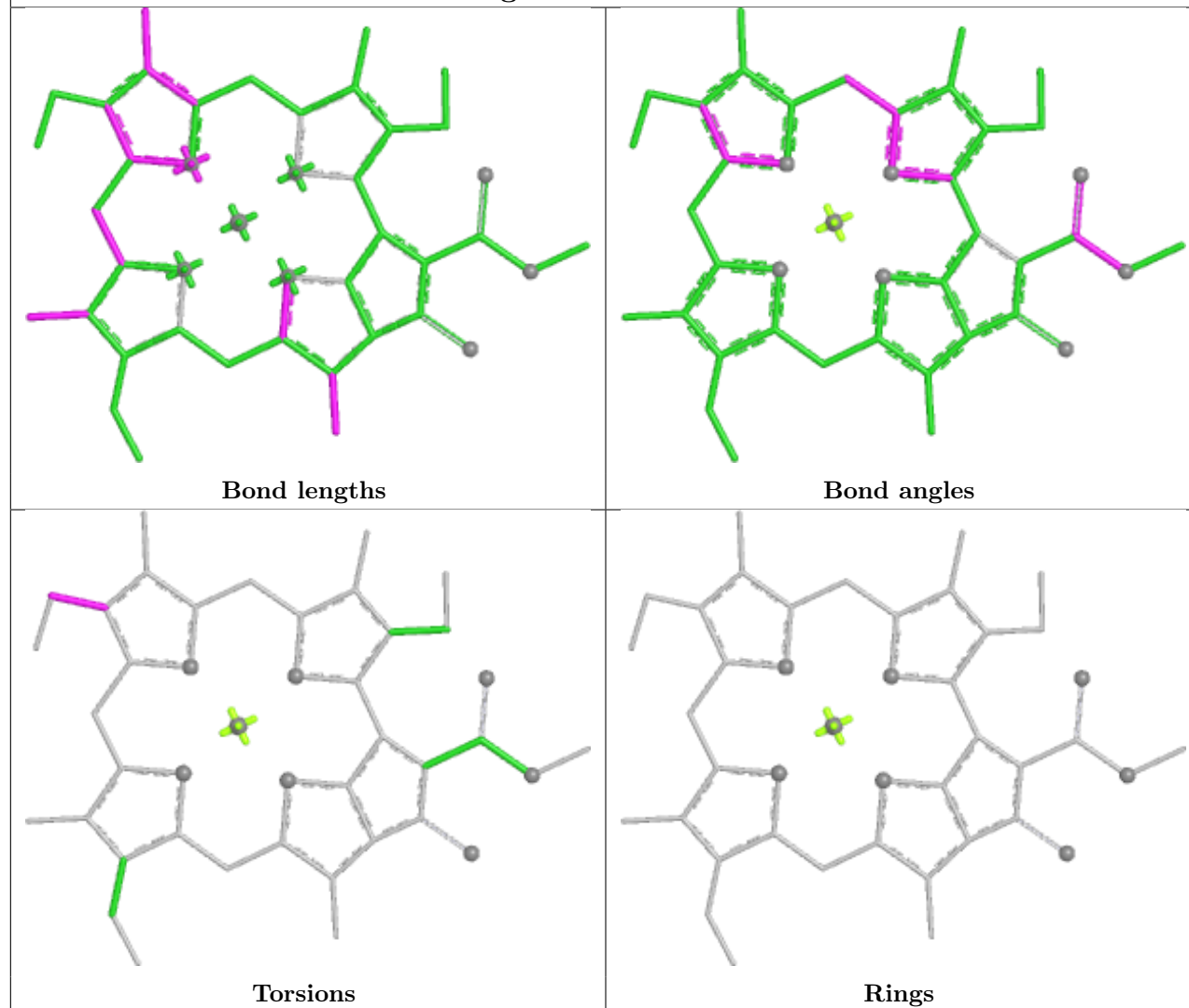
Ligand CLA 3 610



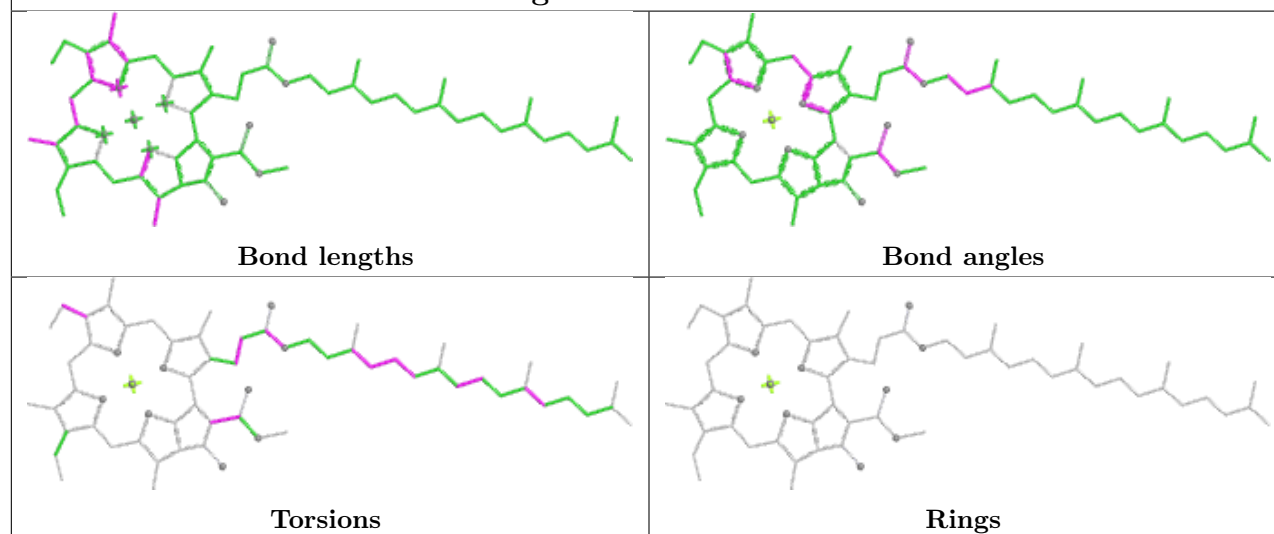
Ligand CLA 3 607



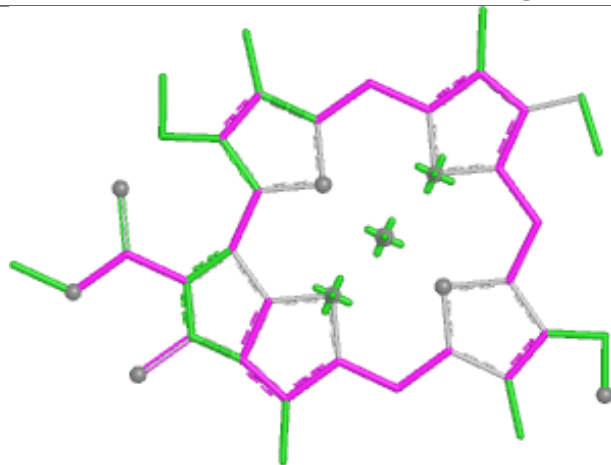
Ligand CLA 4 610



Ligand CLA A 844



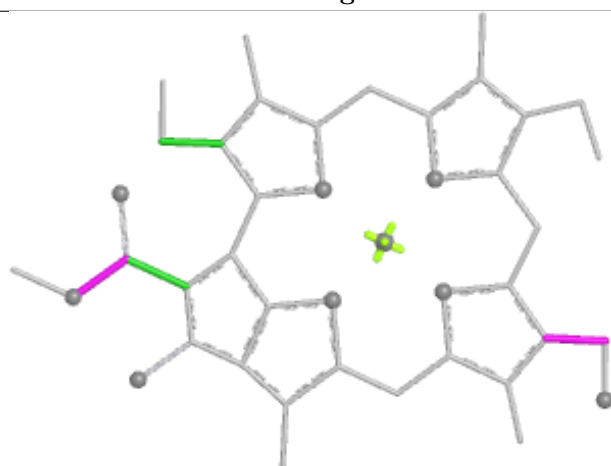
Ligand CHL 2 605



Bond lengths



Bond angles

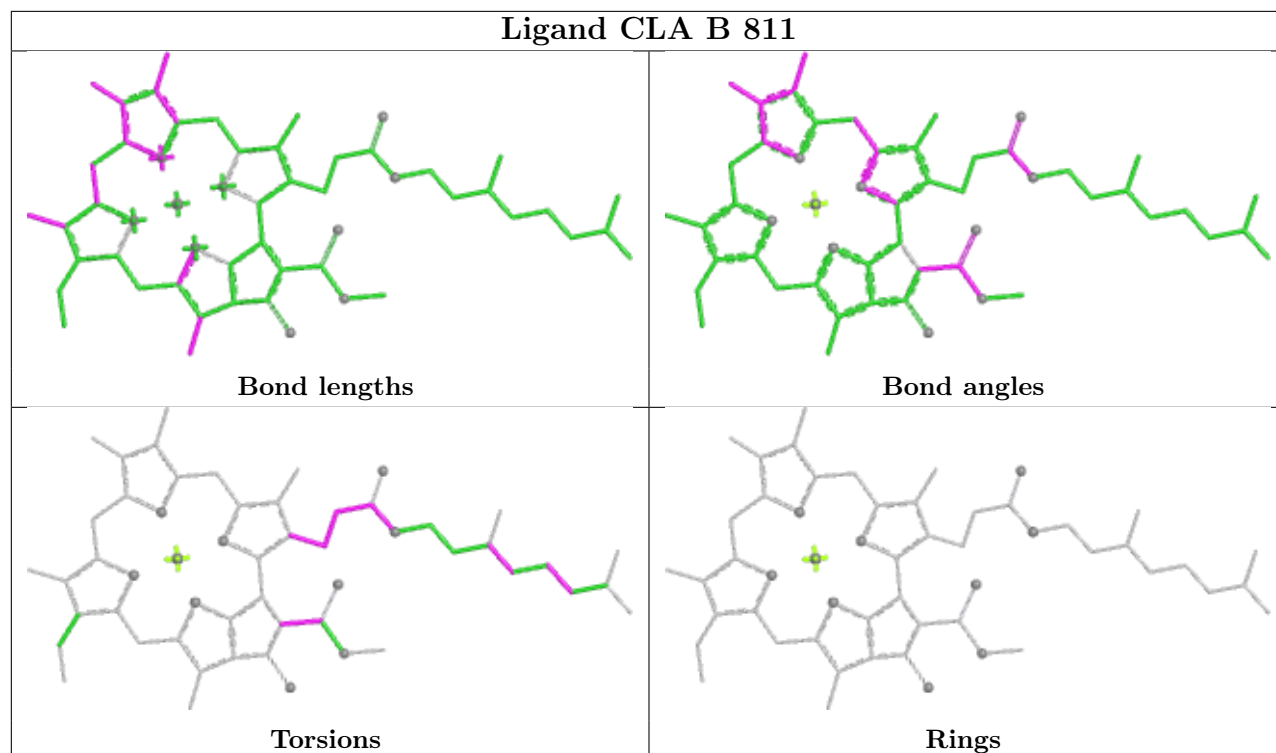


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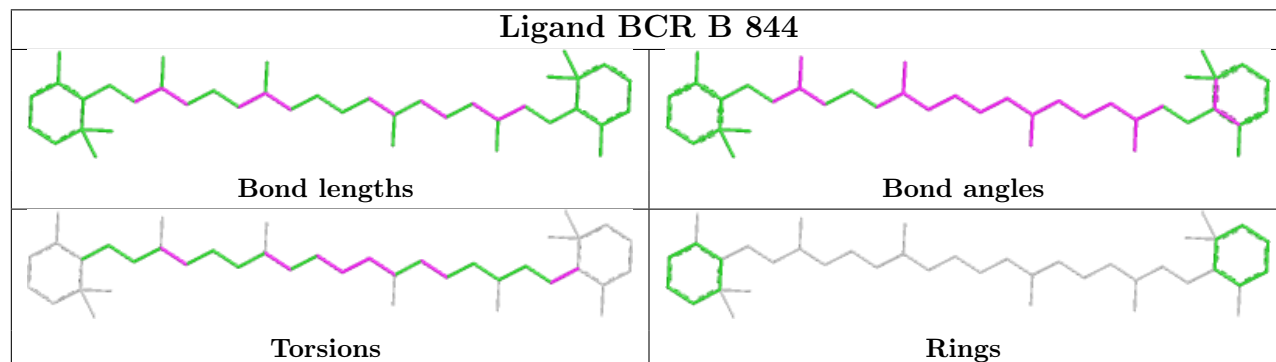


Rings

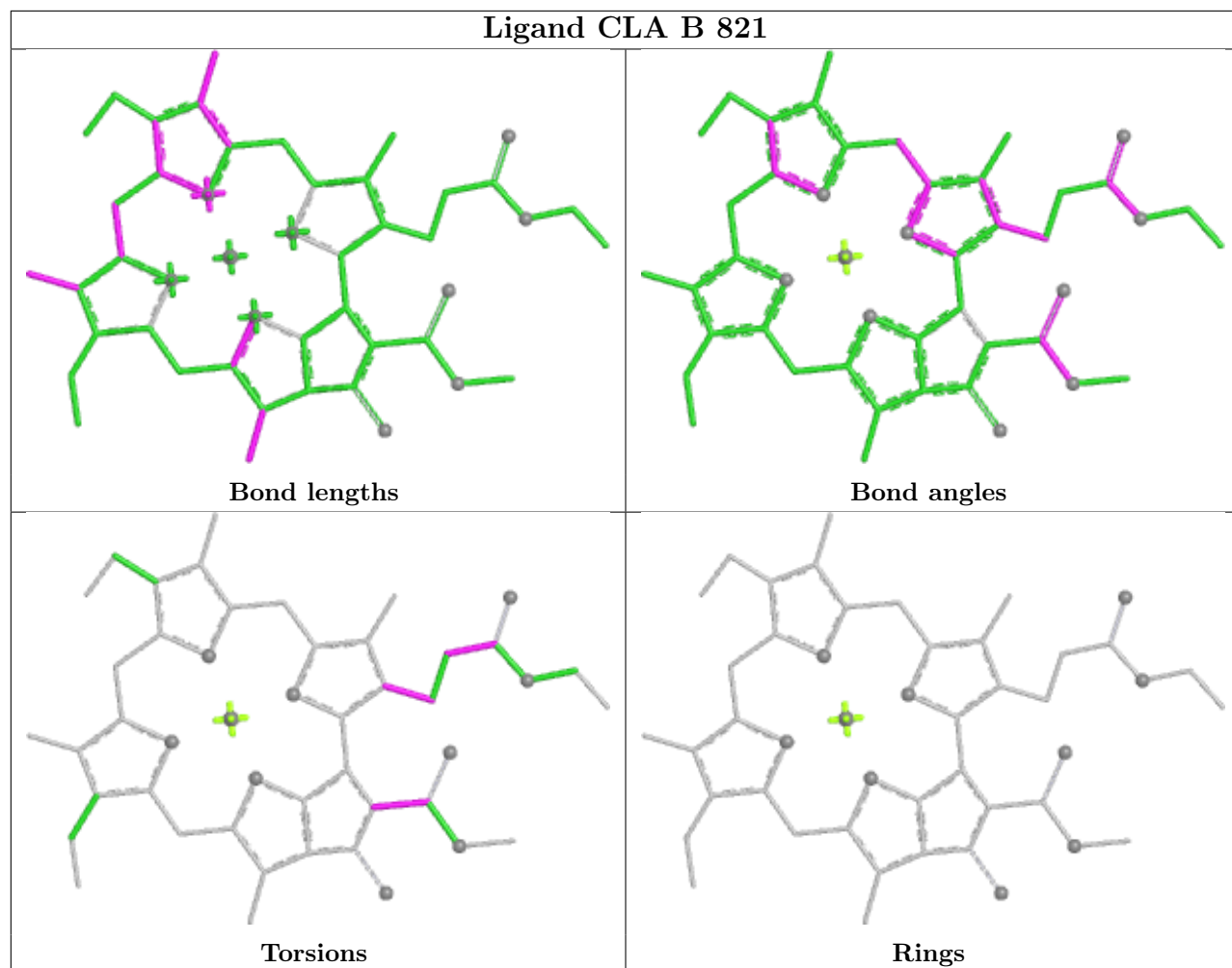
Ligand CLA B 811



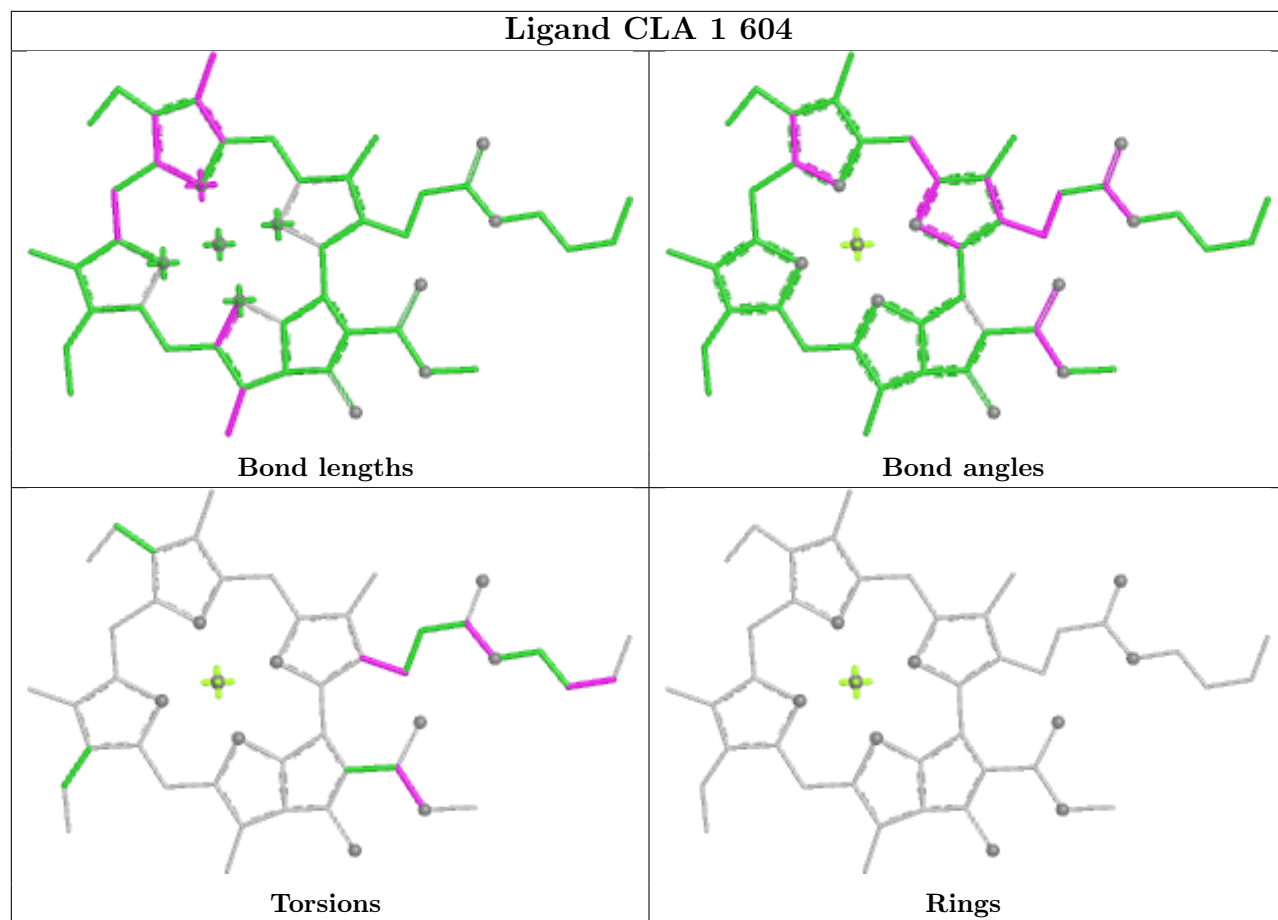
Ligand BCR B 844



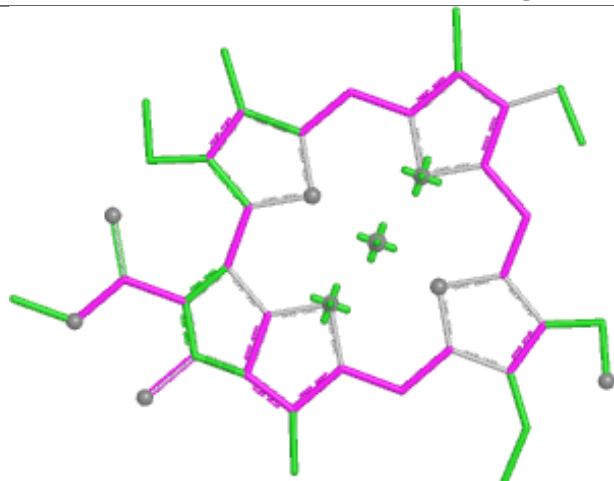
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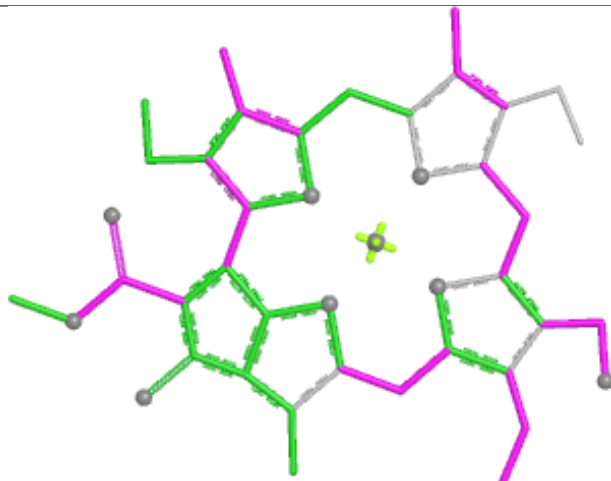
Ligand CLA 1 604



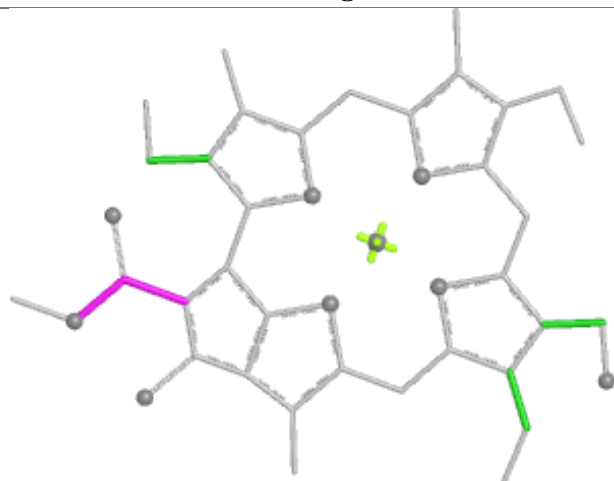
Ligand CHL 2 615



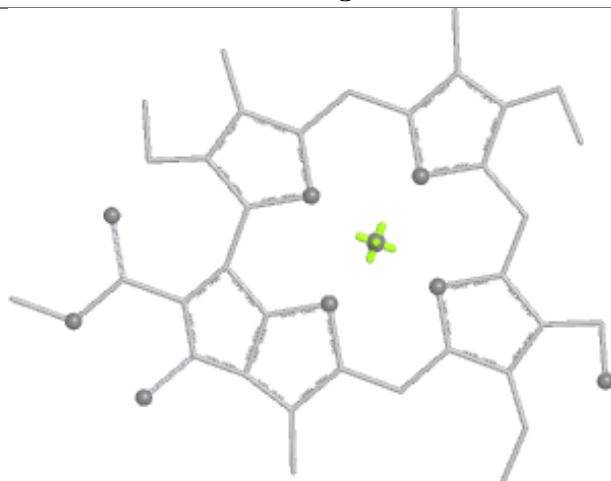
Bond lengths



Bond angles

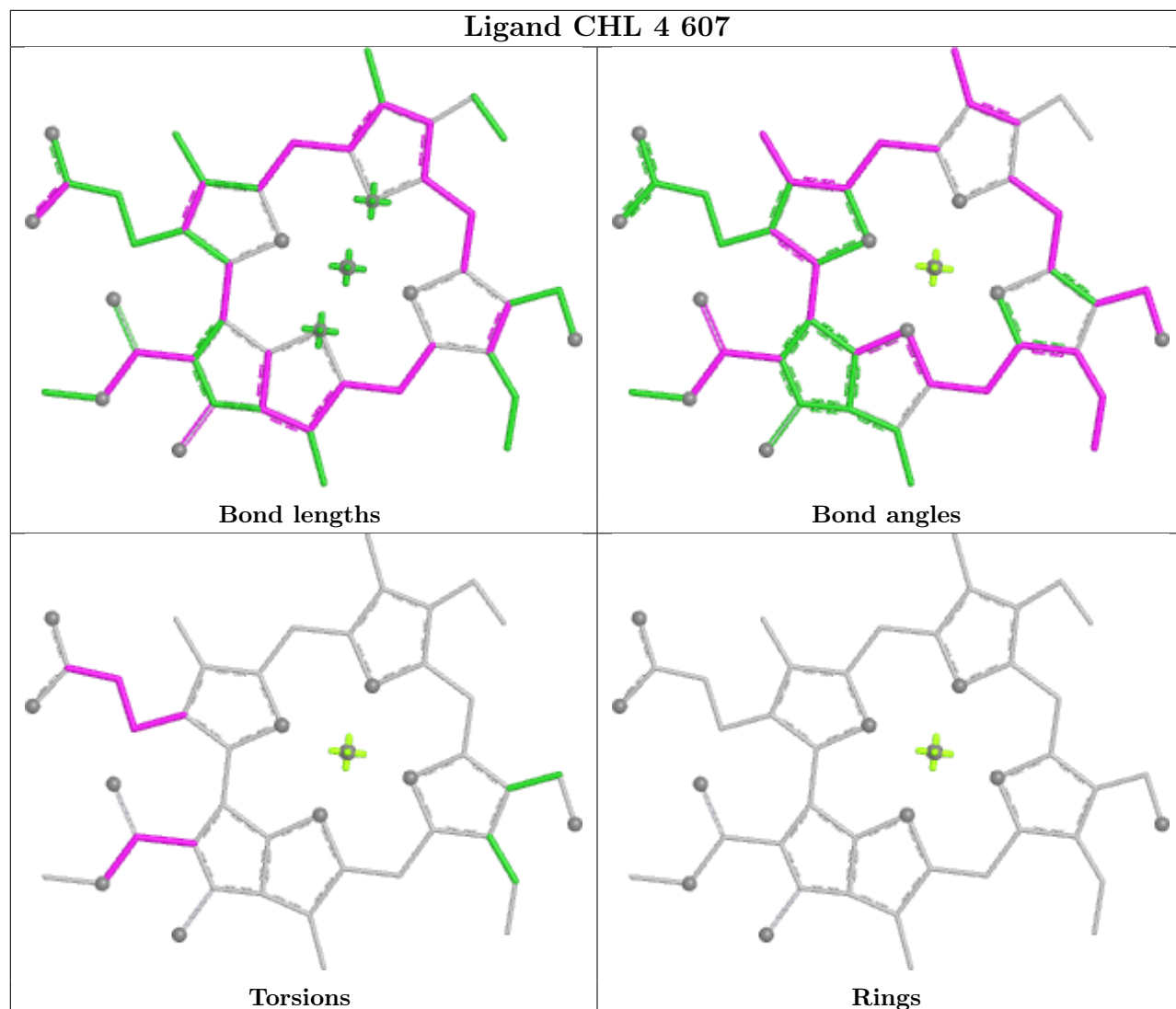


Torsions

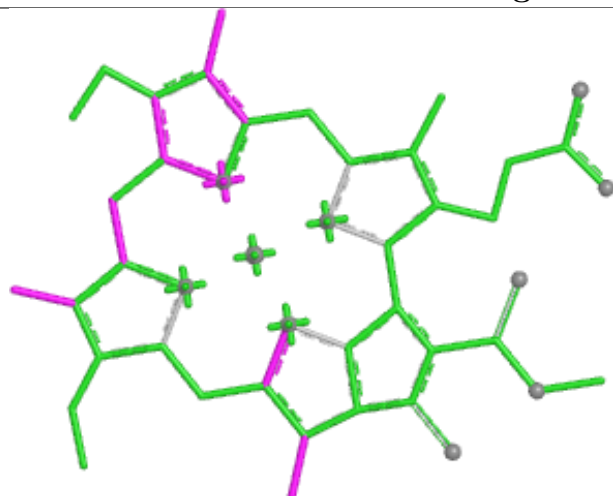


Rings

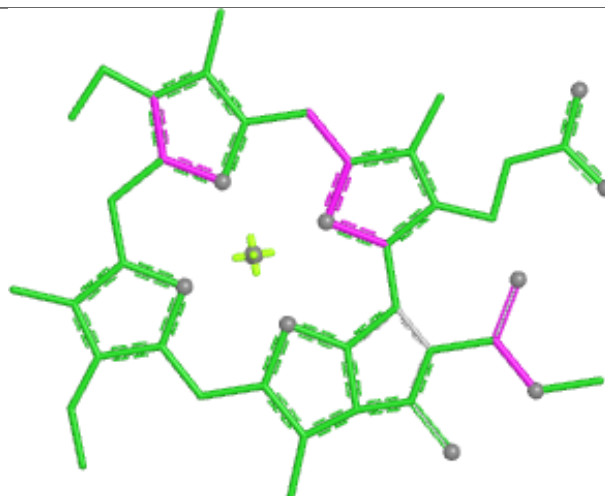
Ligand CHL 4 607



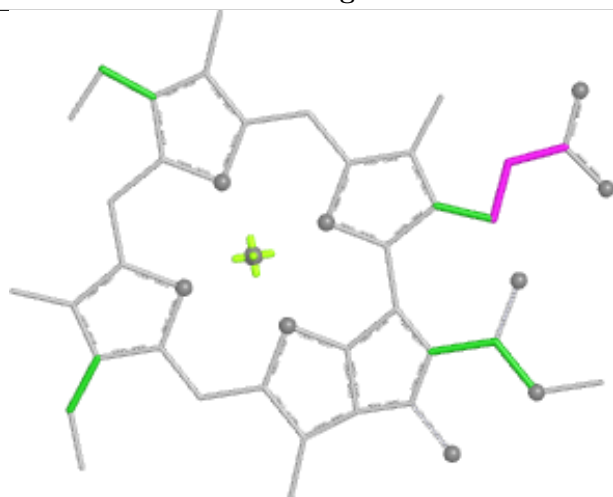
Ligand CLA G 203



Bond lengths



Bond angles

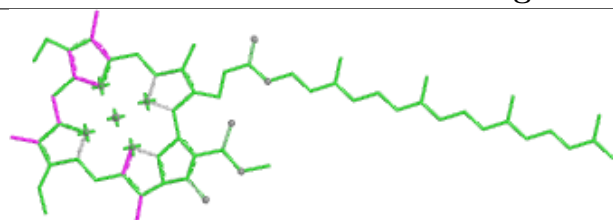


Torsions

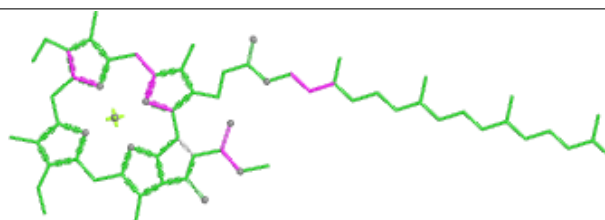


Rings

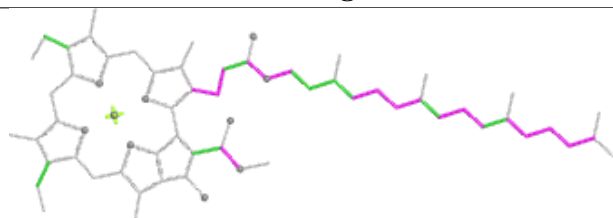
Ligand CLA A 812



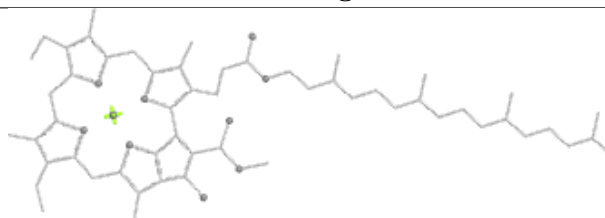
Bond lengths



Bond angles

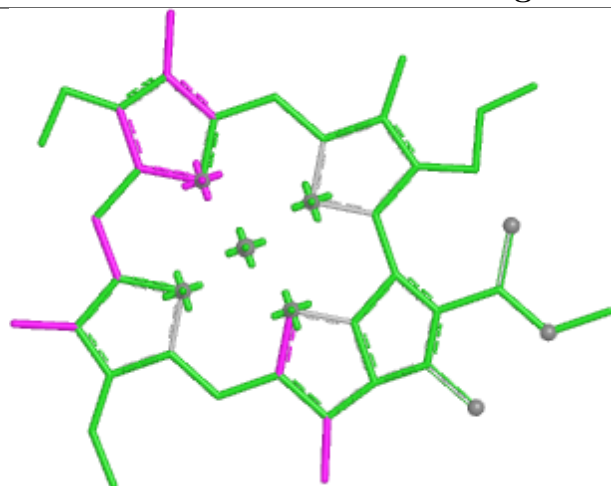


Torsions

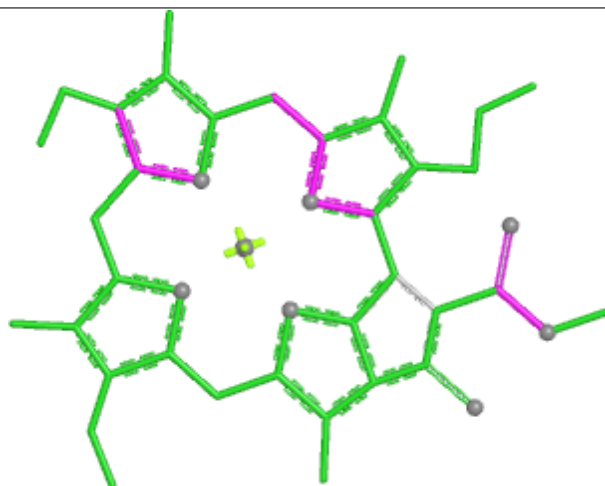


Rings

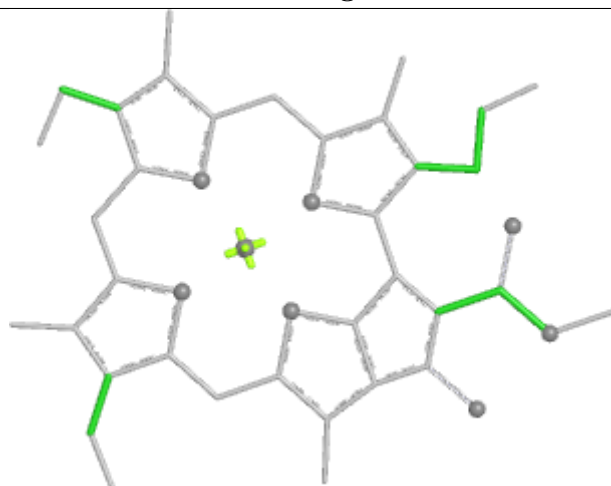
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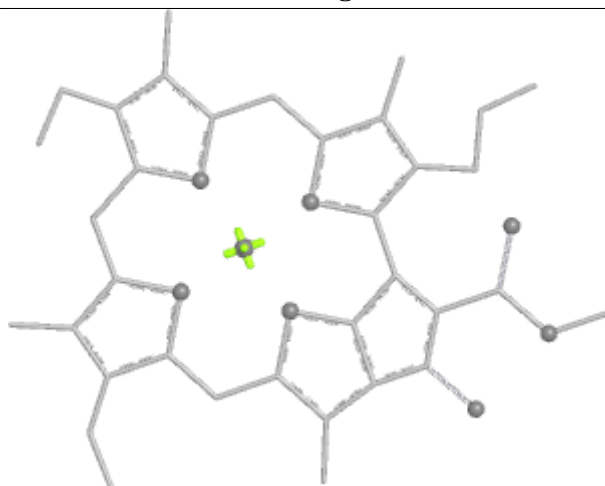
Bond lengths



Bond angles

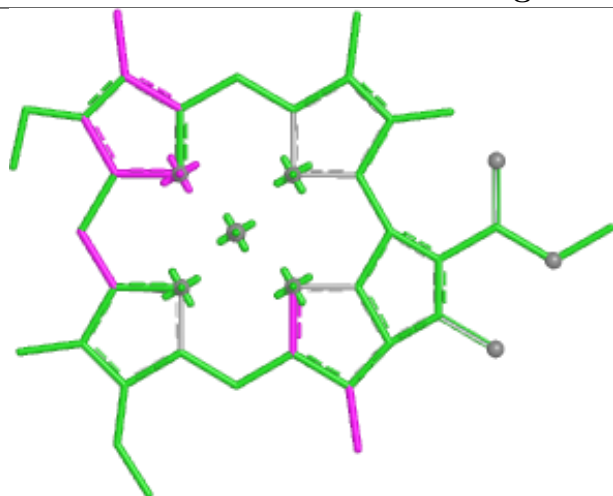


Torsions

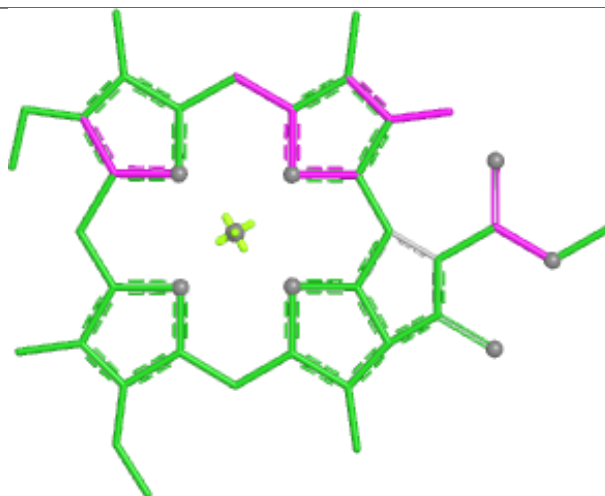


Rings

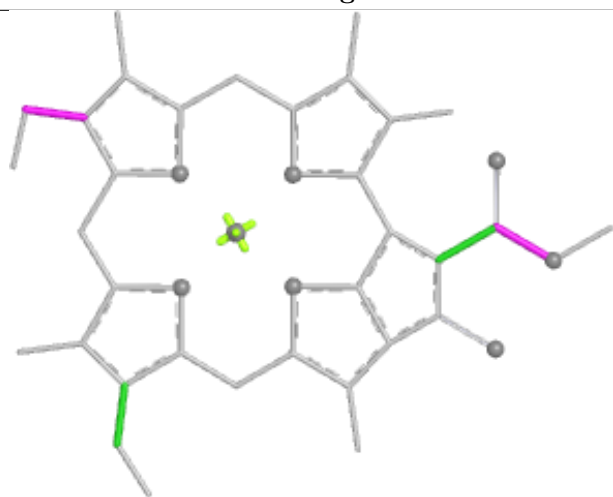
Ligand CLA A 824



Bond lengths



Bond angles

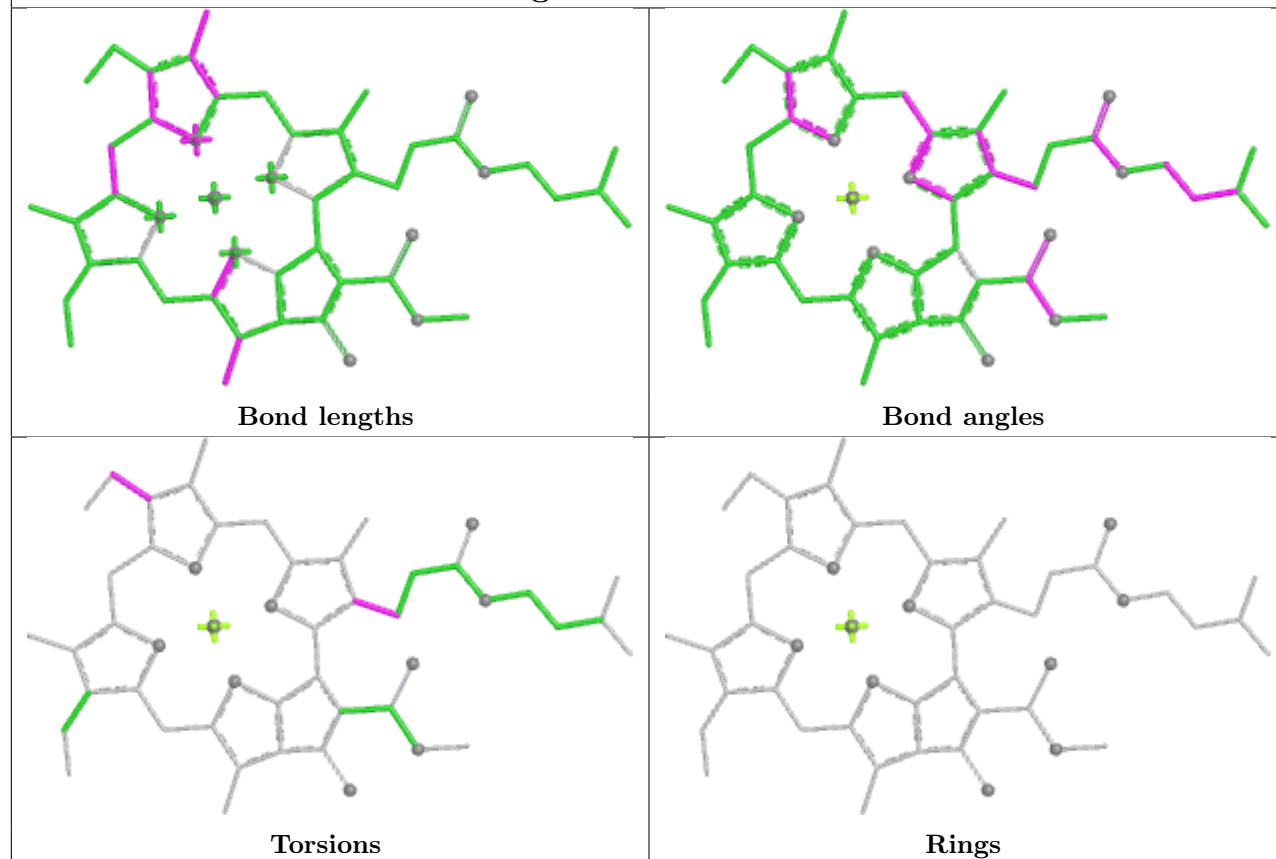


Torsions

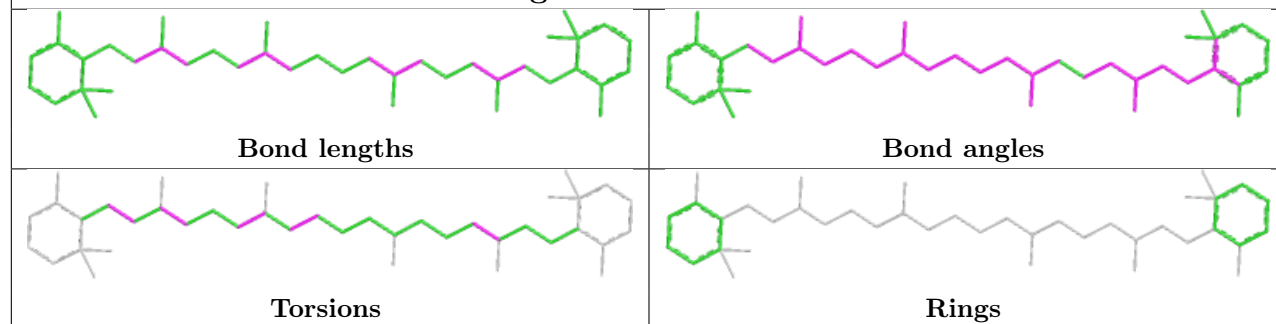


Rings

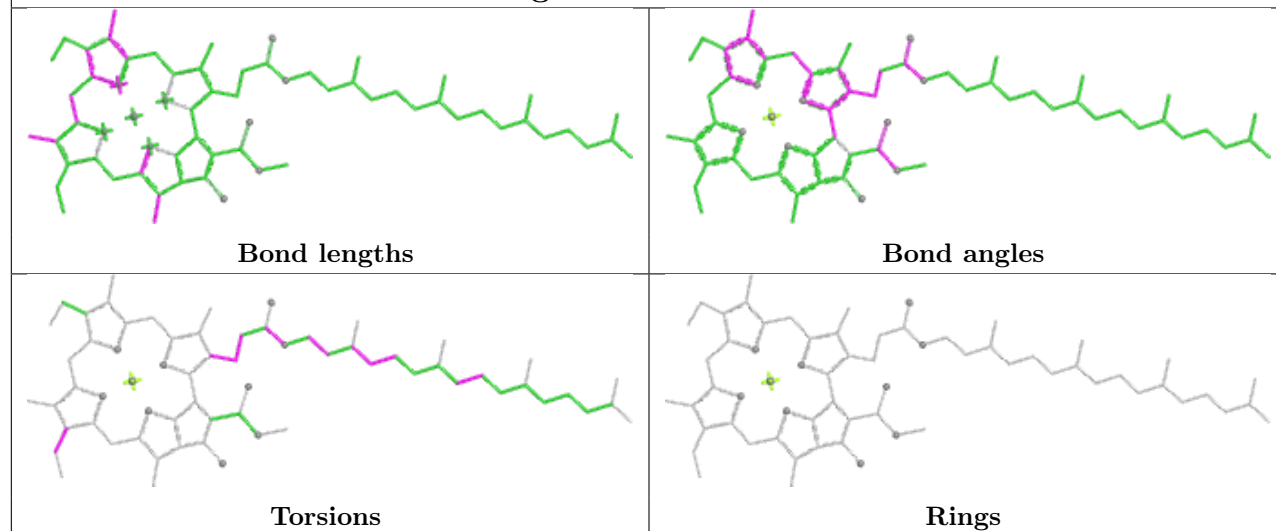
Ligand CLA A 810



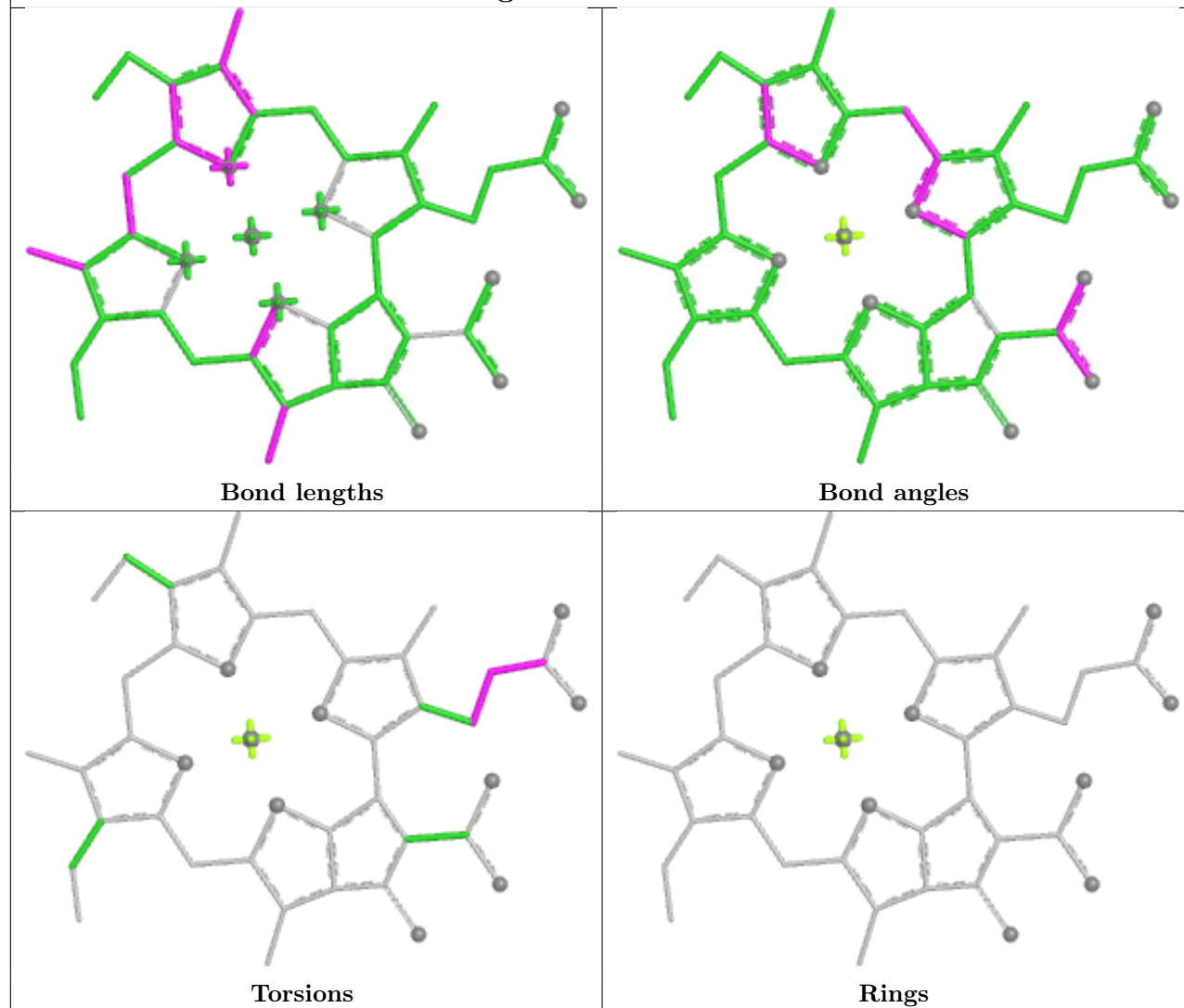
Ligand BCR A 851



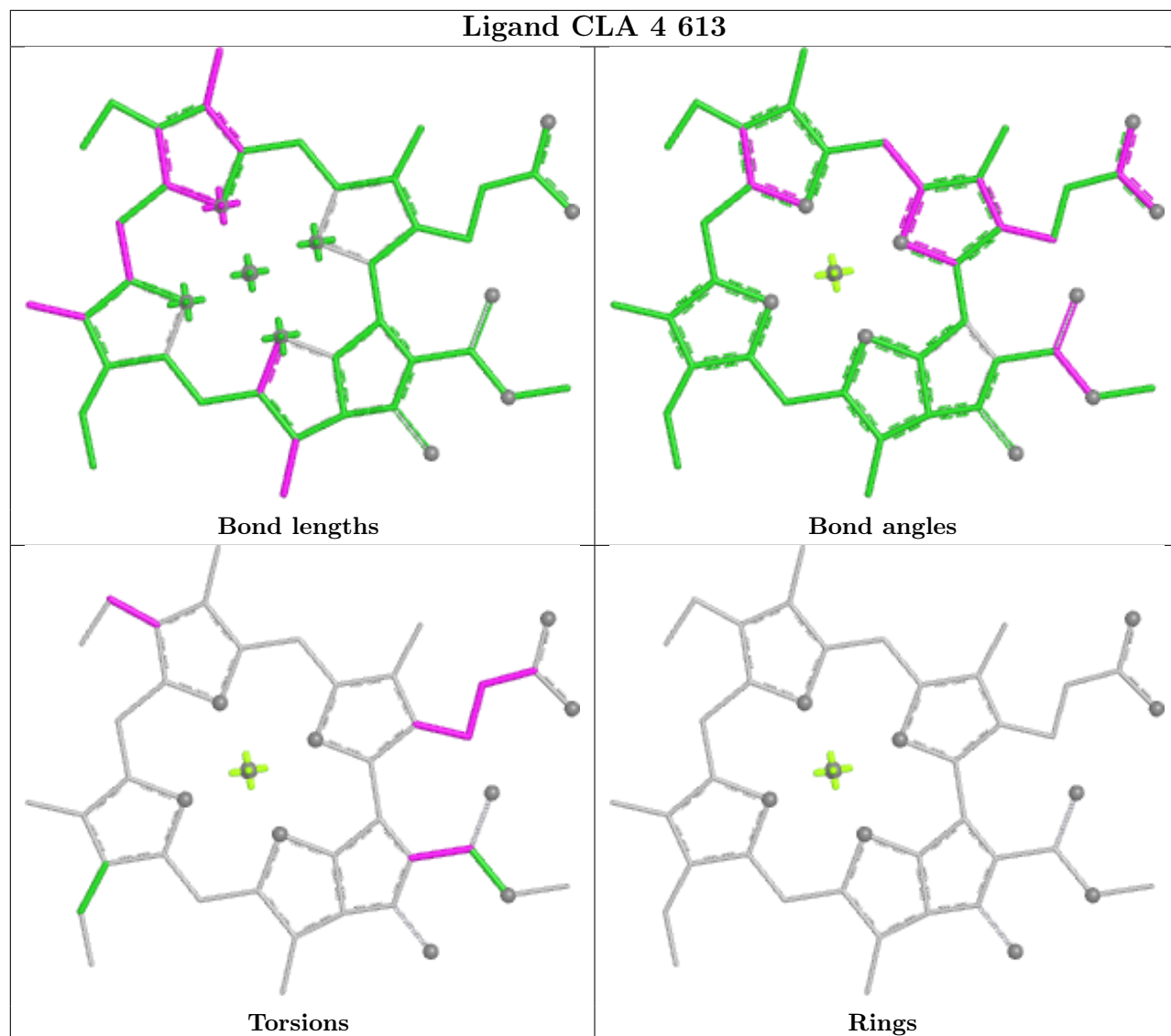
Ligand CLA A 830



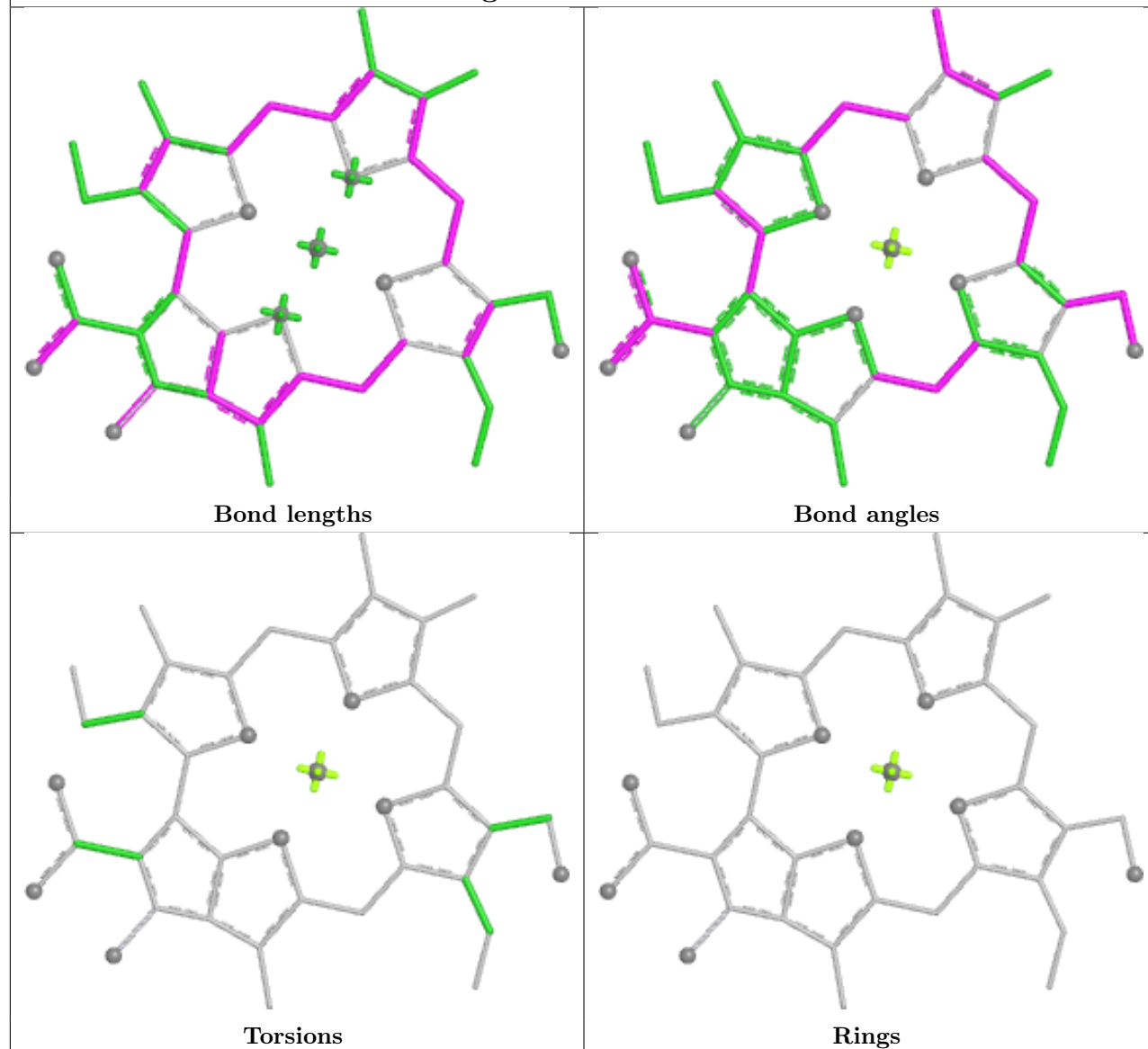
Ligand CLA 2 603



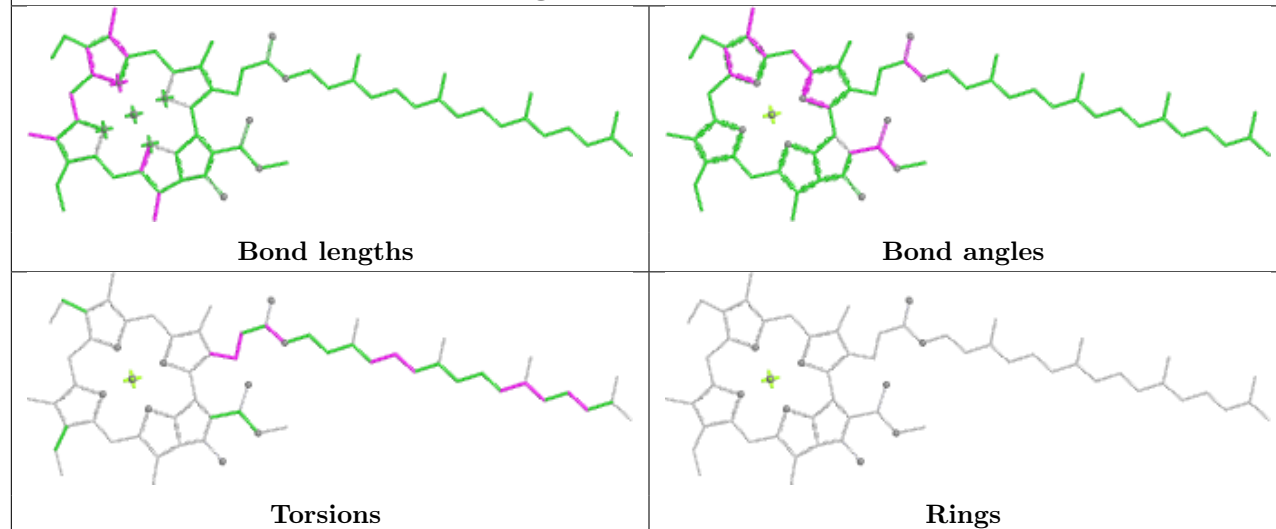
Ligand CLA 4 613

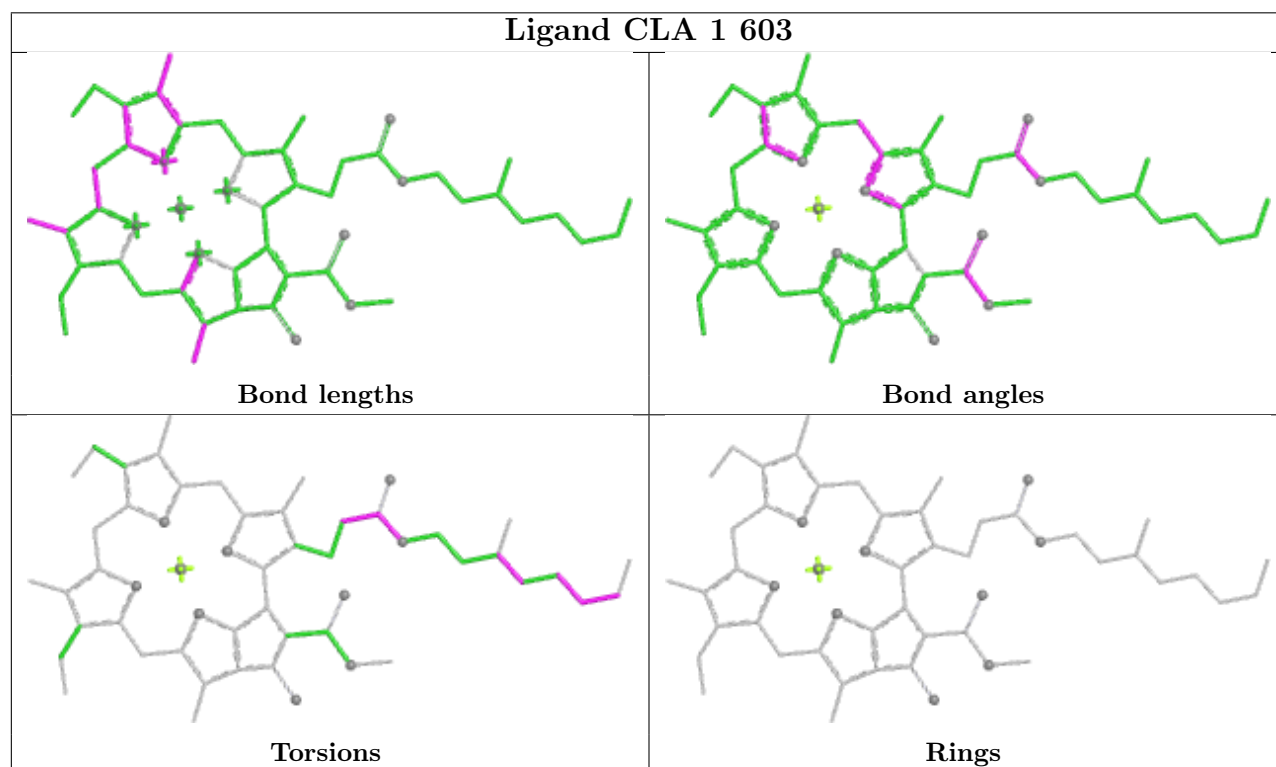
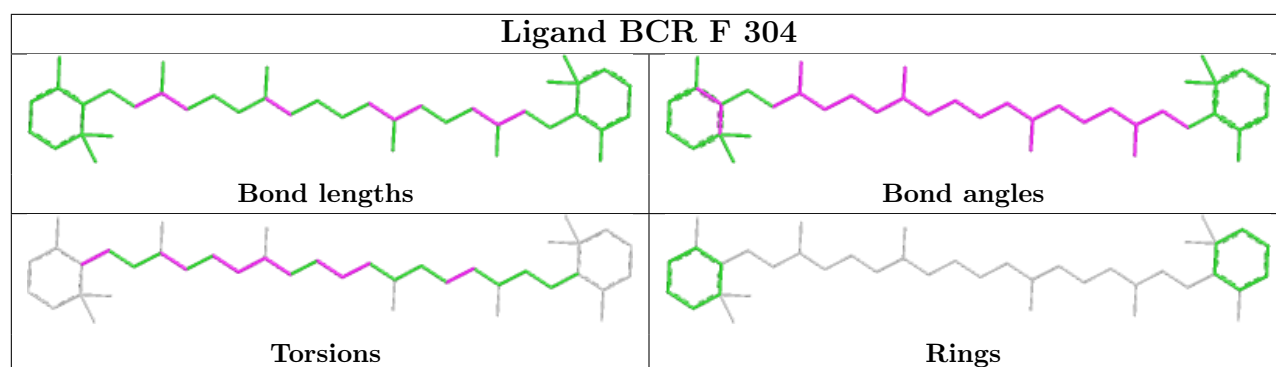


Ligand CHL 4 615

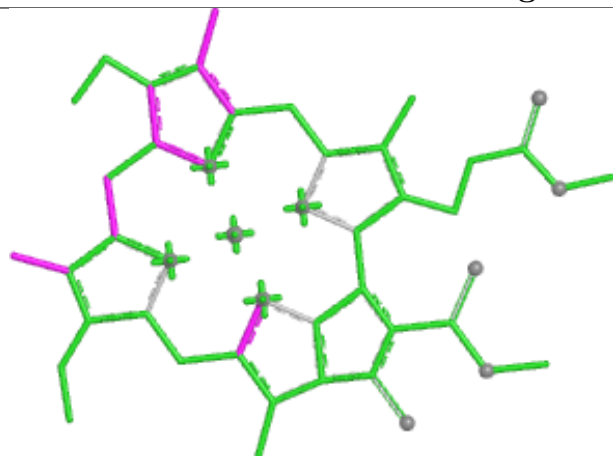


Ligand CLA B 837

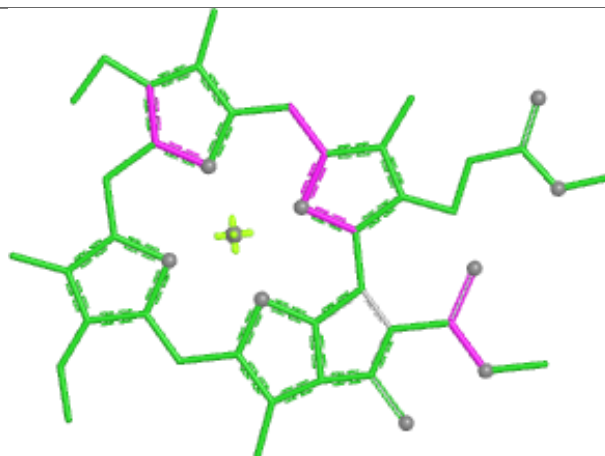




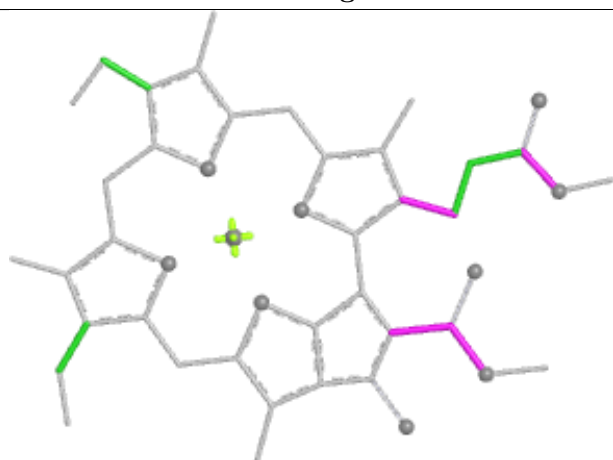
Ligand CLA 1 605



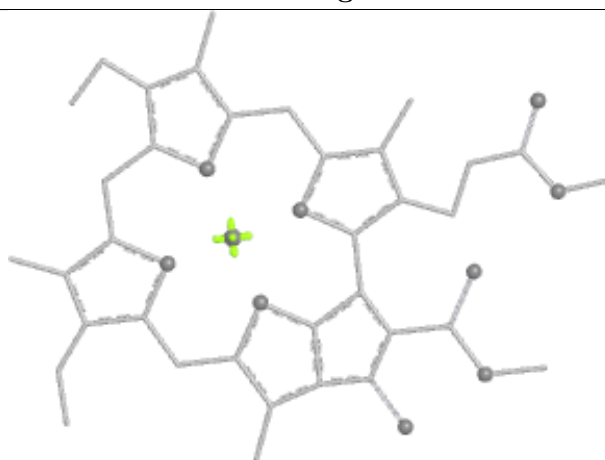
Bond lengths



Bond angles

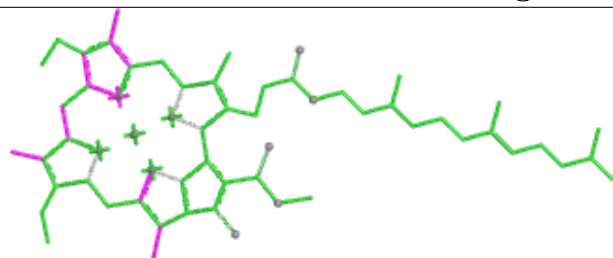


Torsions

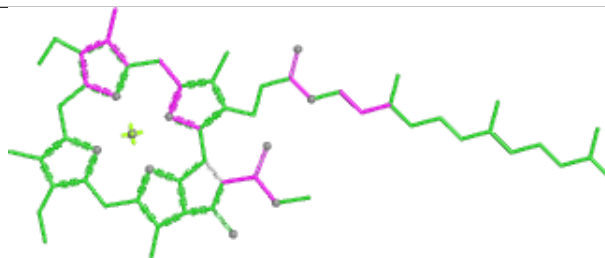


Rings

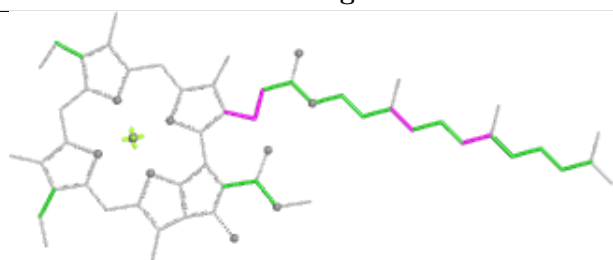
Ligand CLA B 818



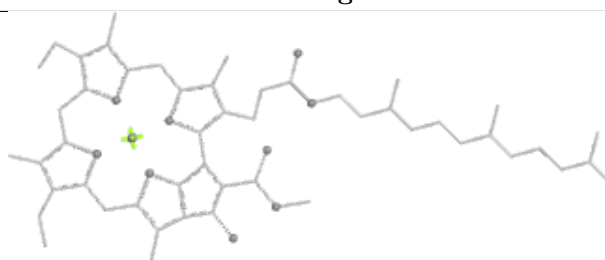
Bond lengths



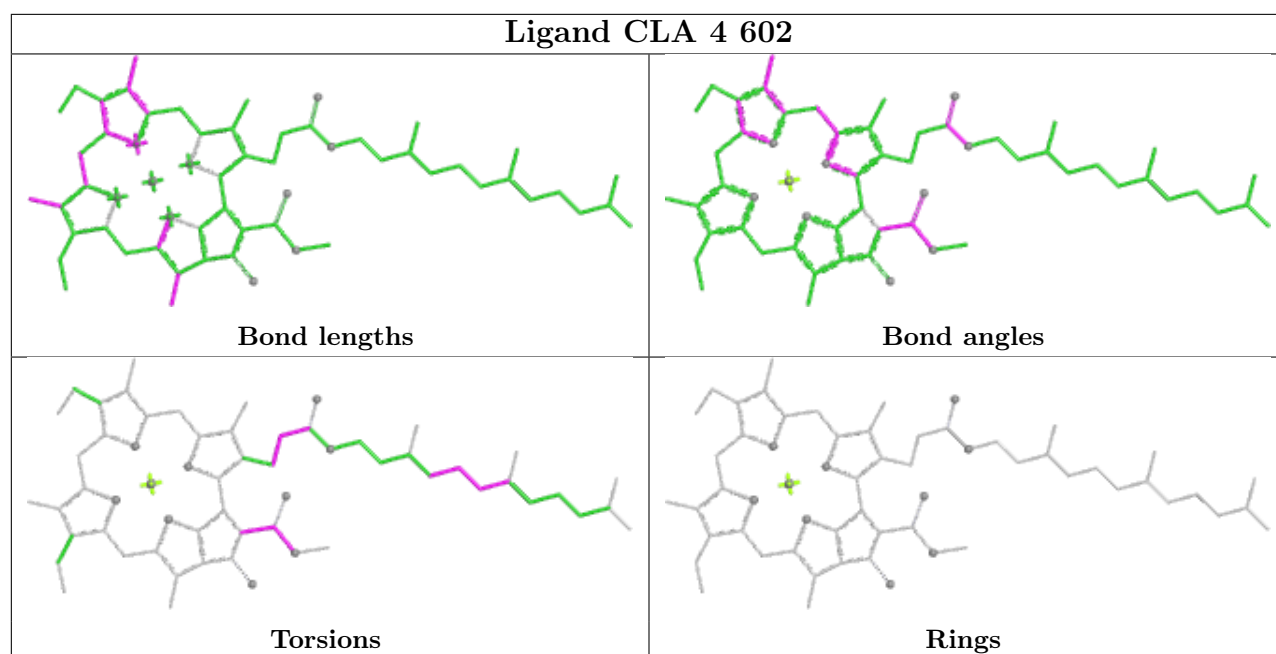
Bond angles

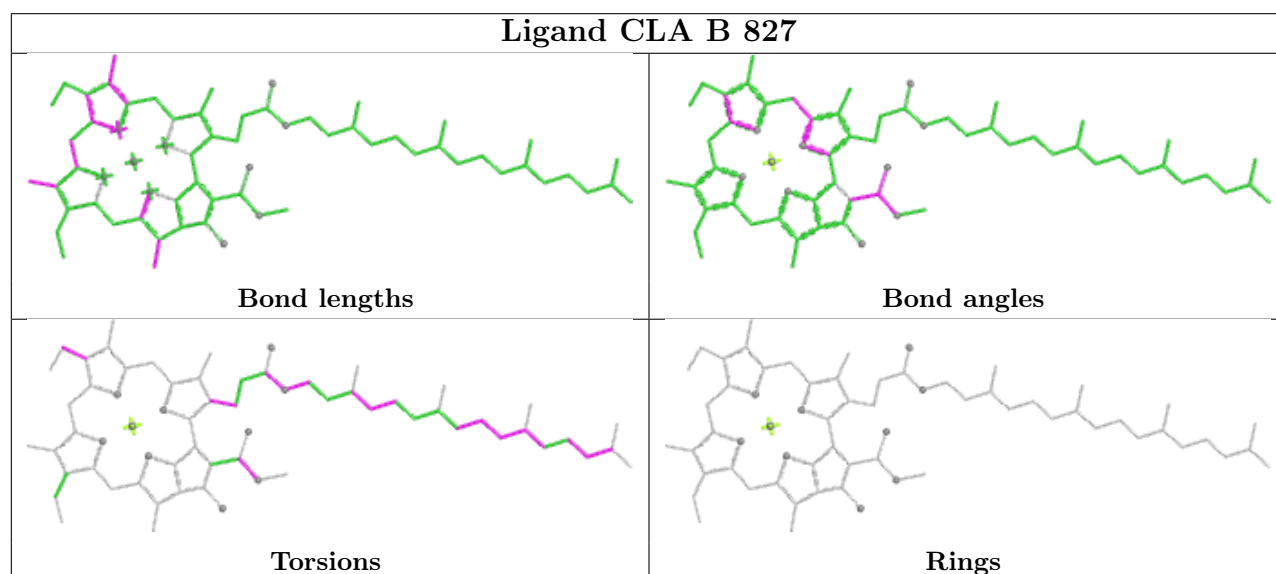
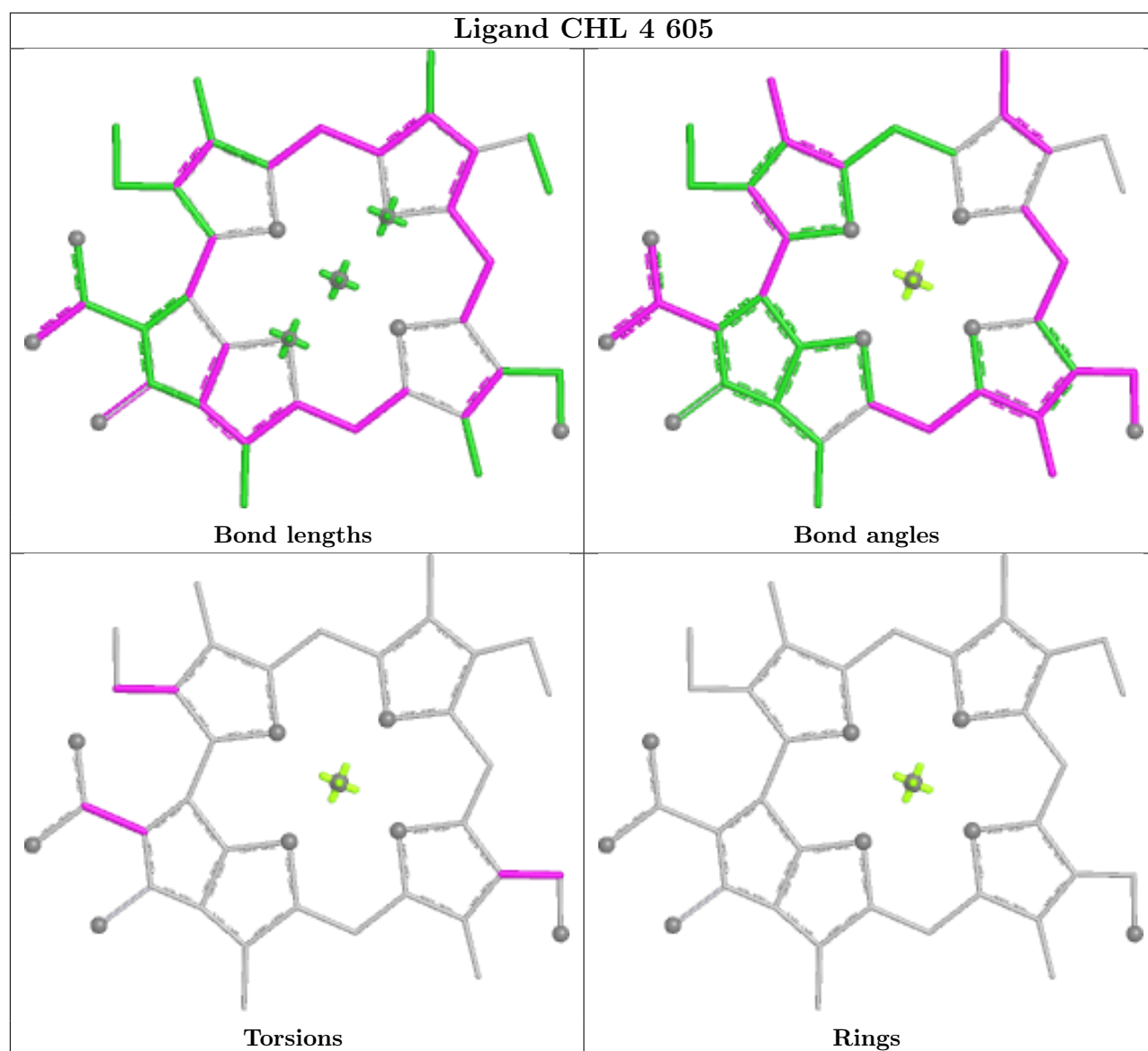


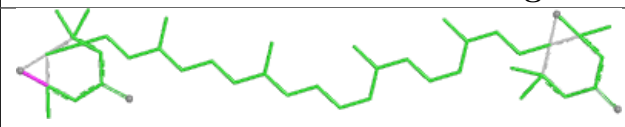
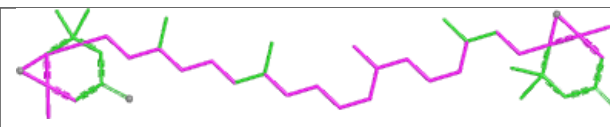
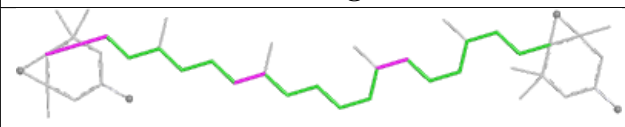
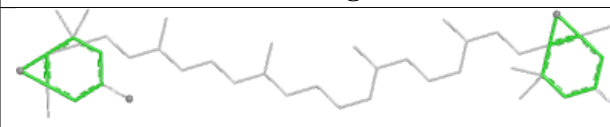
Torsions

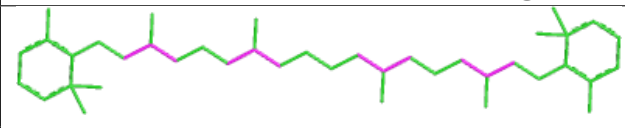
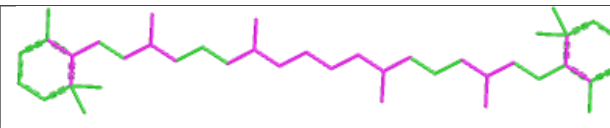
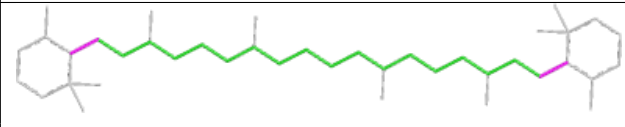
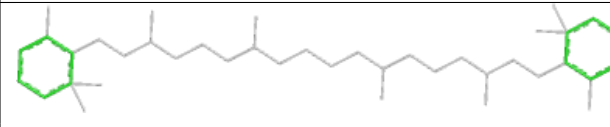


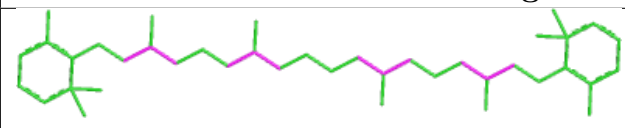
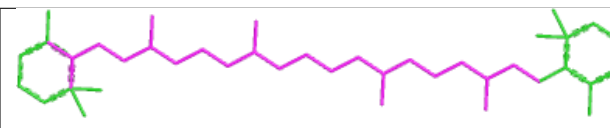
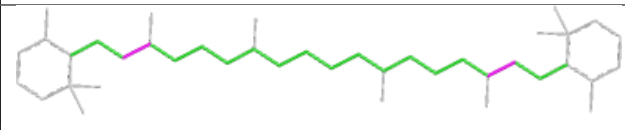
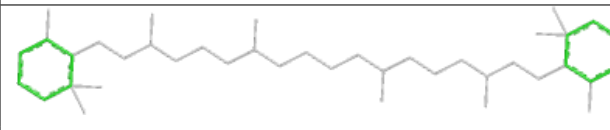
Rings

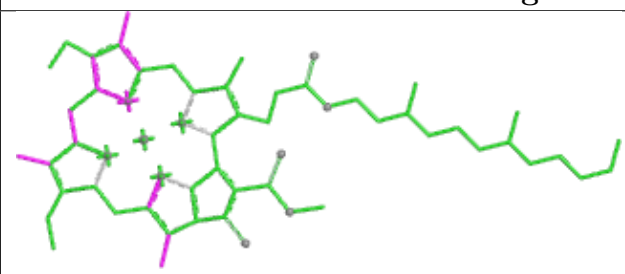
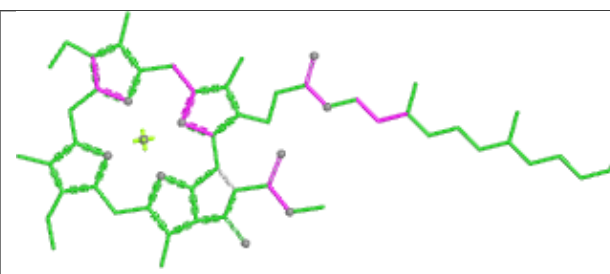
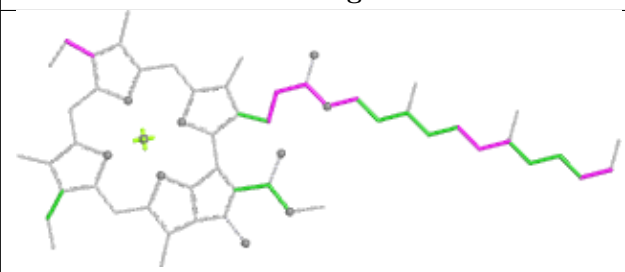
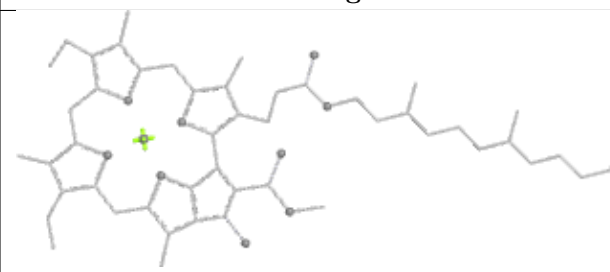


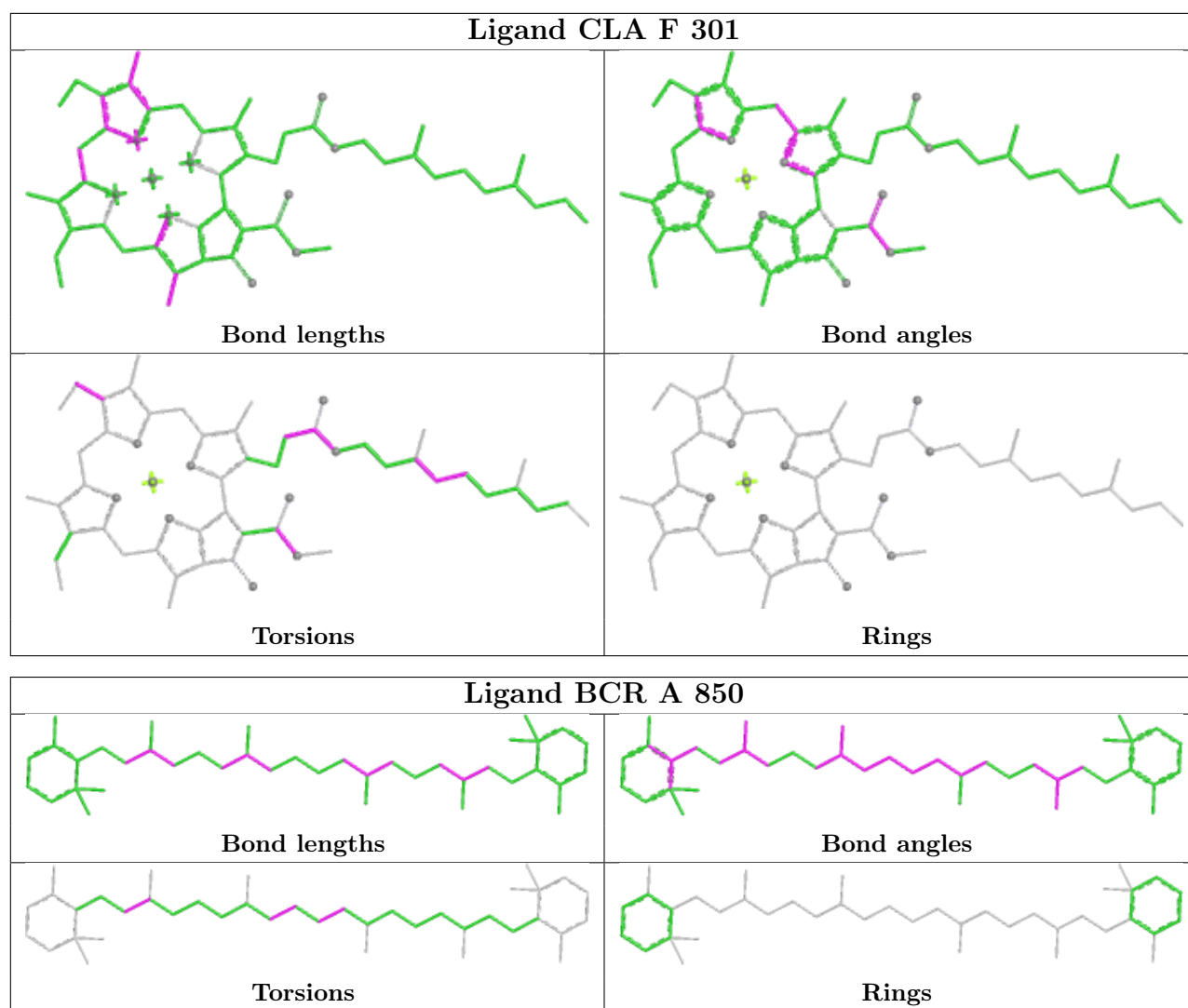


Ligand XAT 1 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

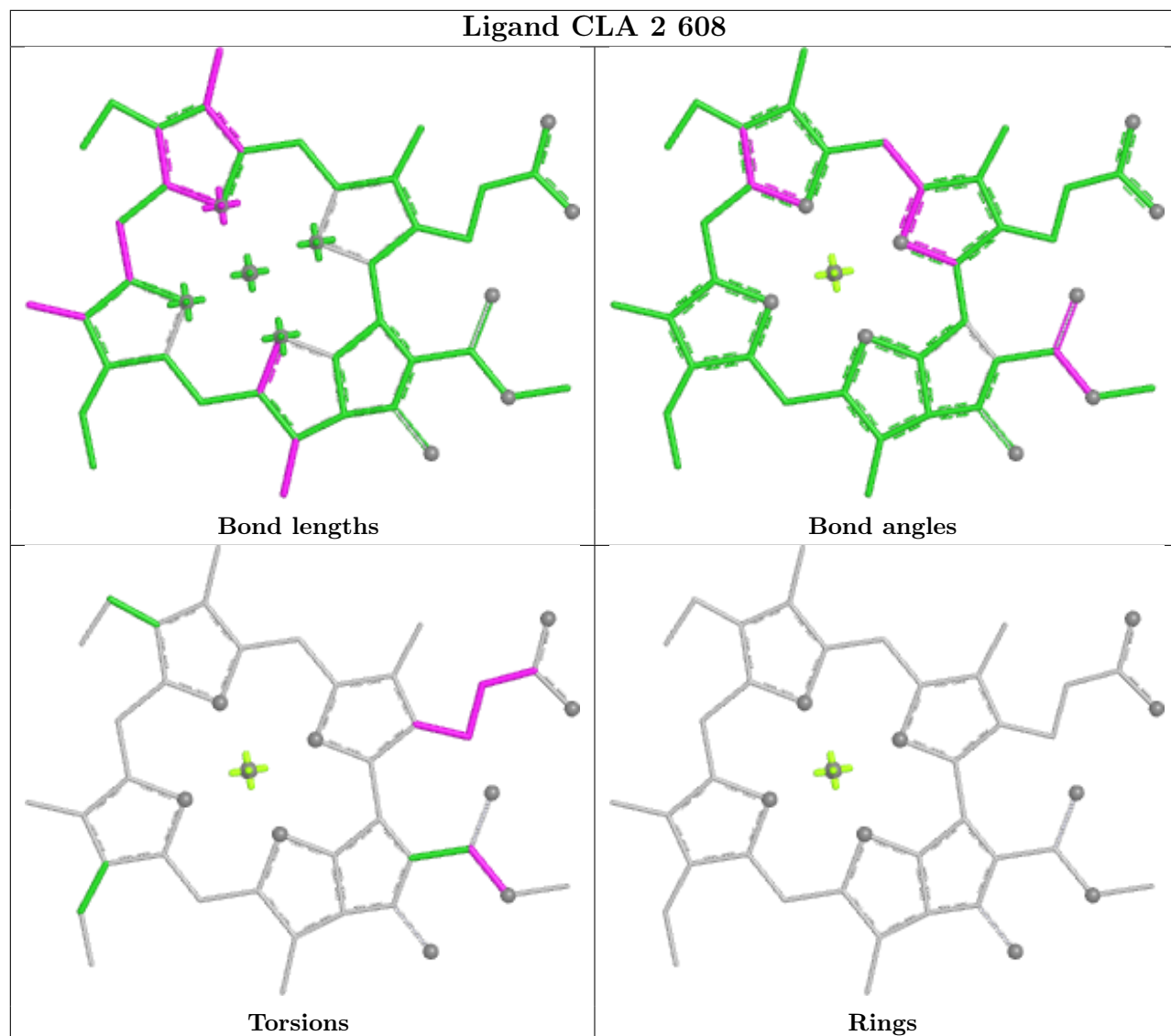
Ligand BCR G 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

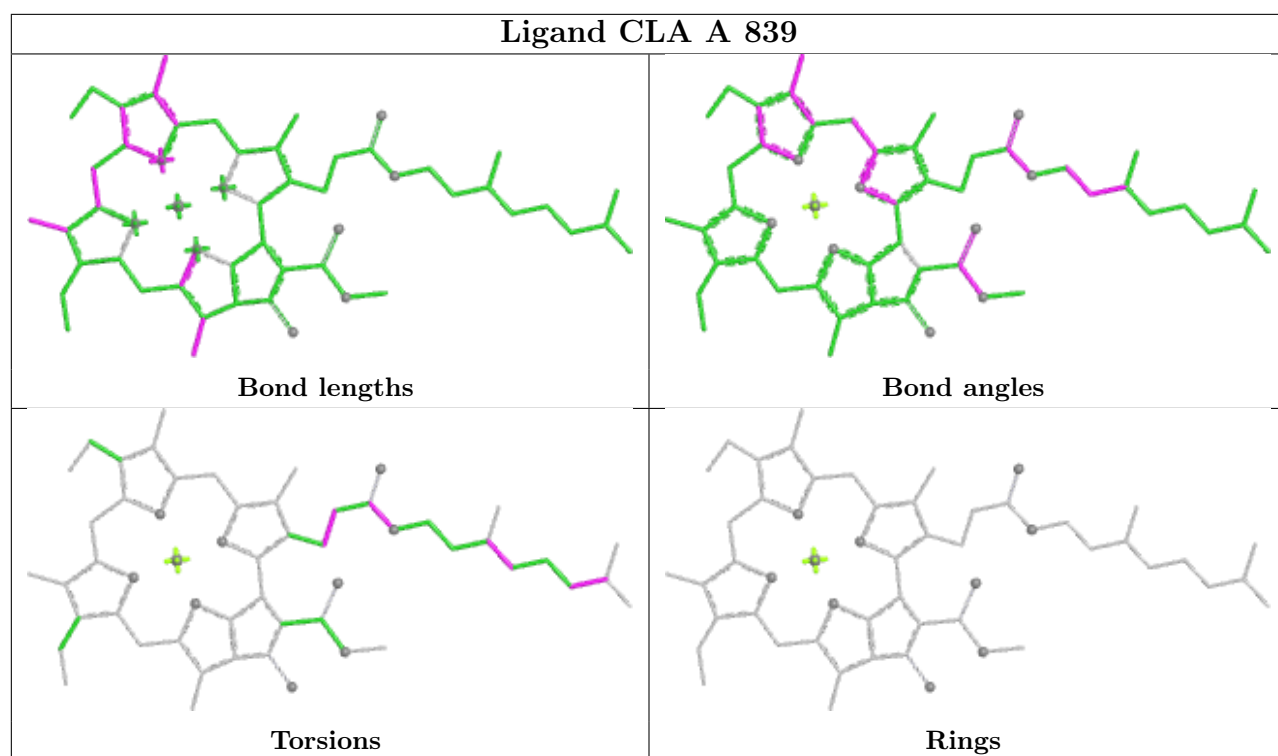
Ligand BCR L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

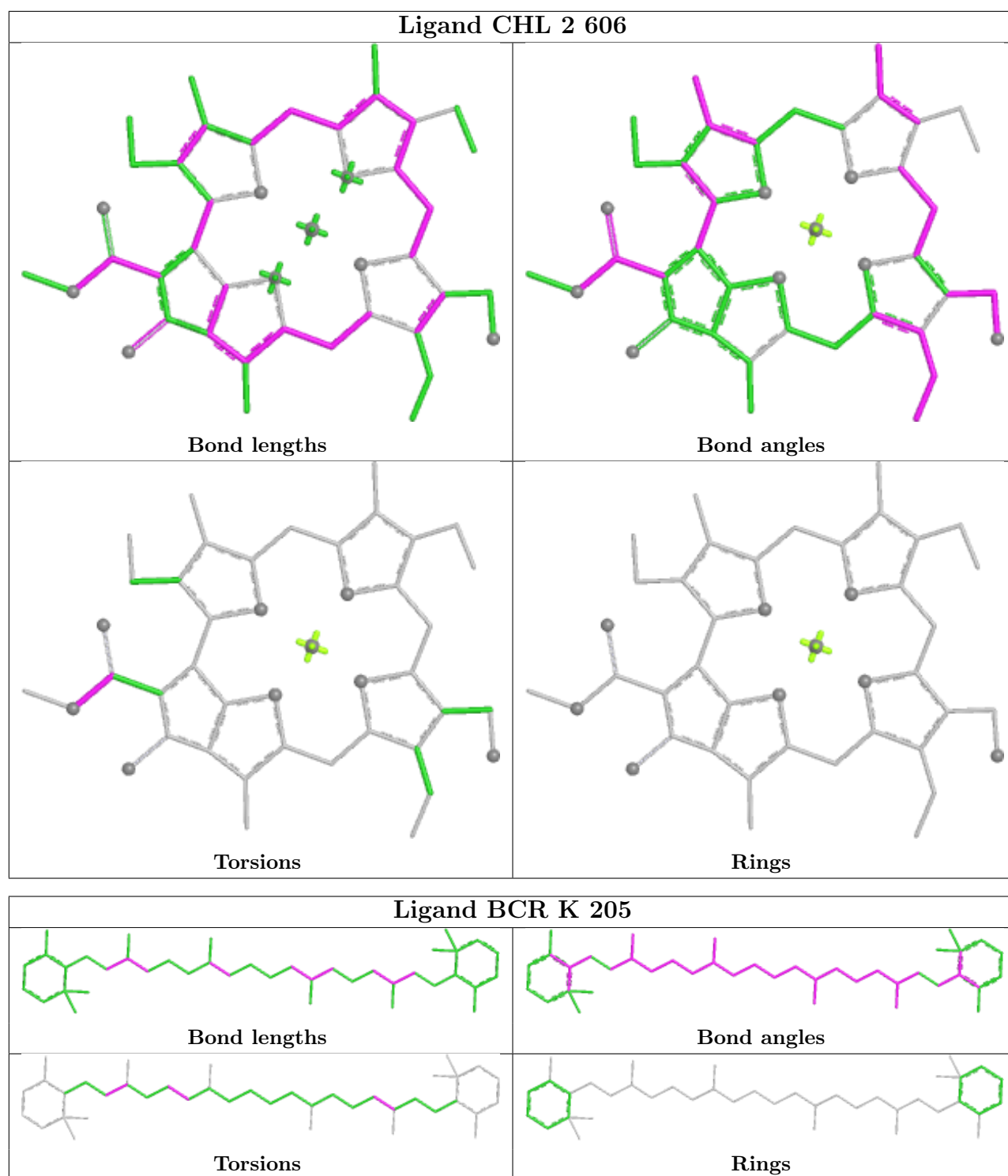
Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

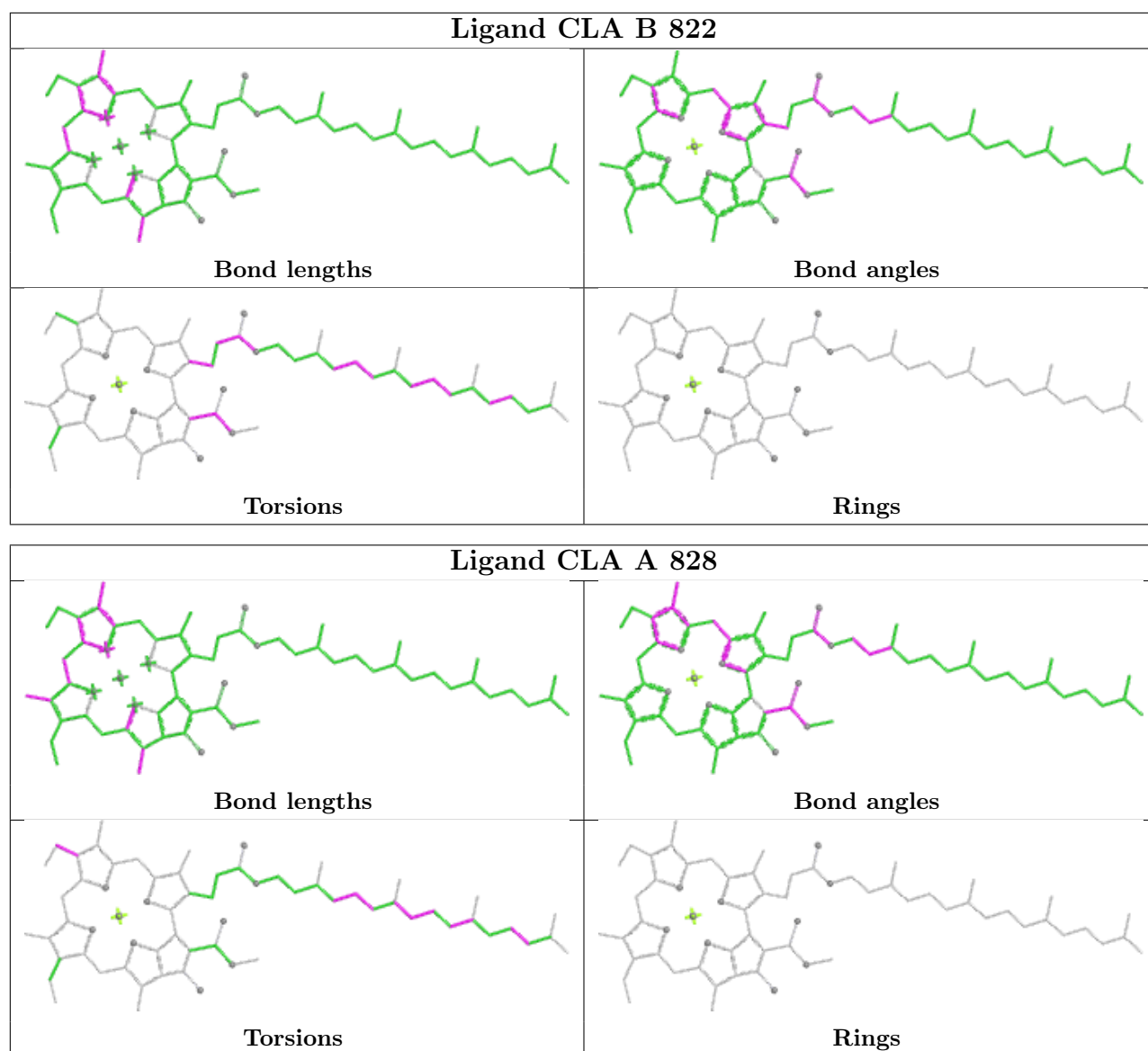


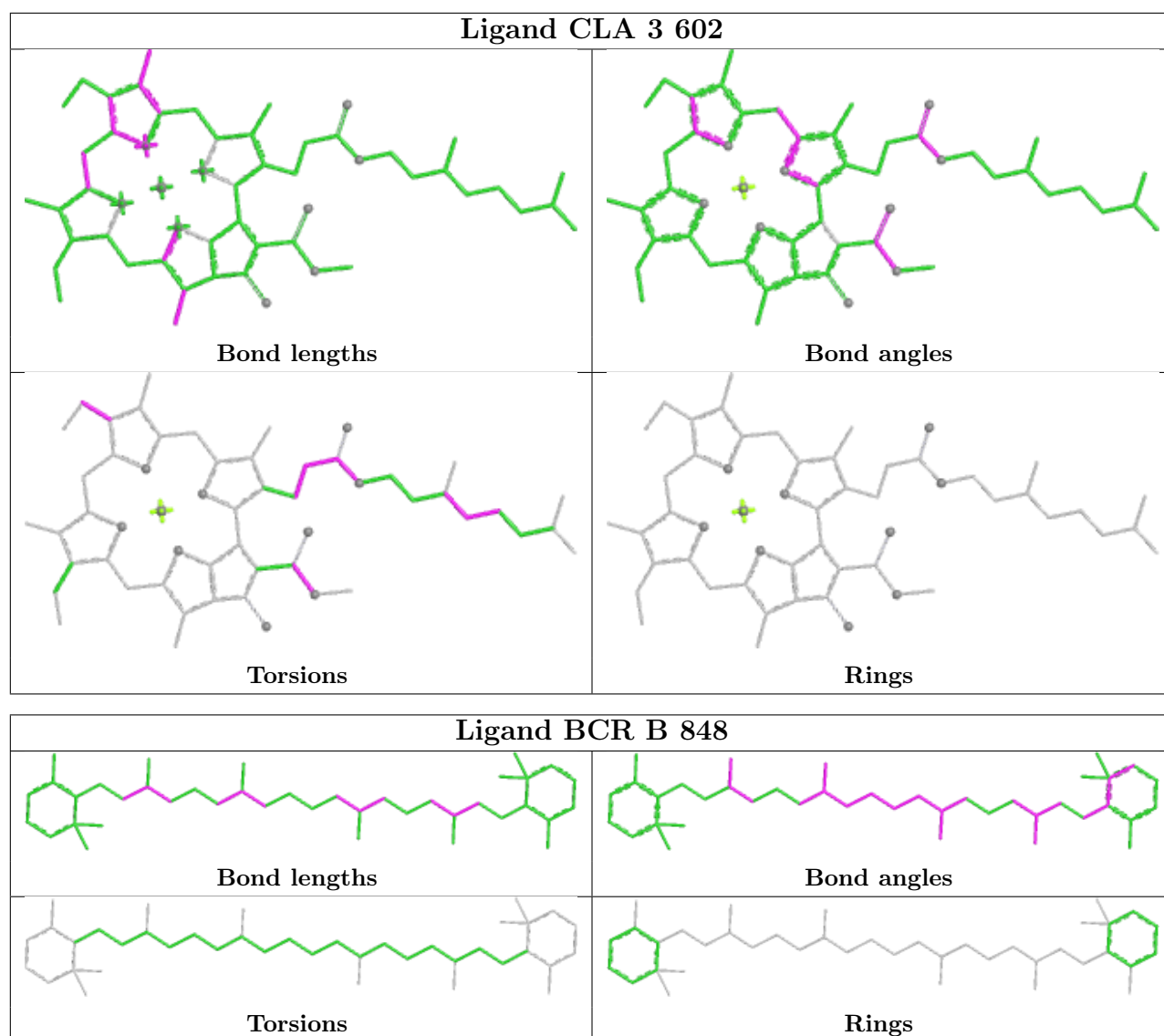
Ligand CLA 2 608

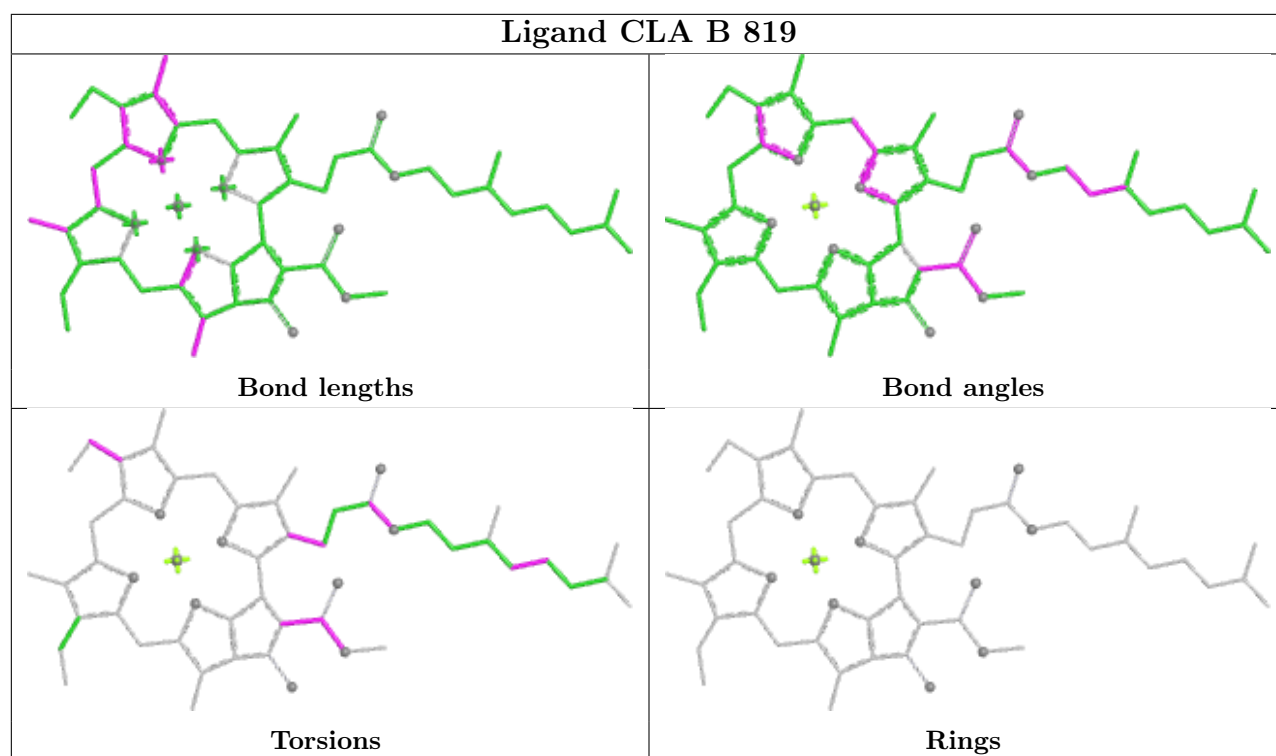


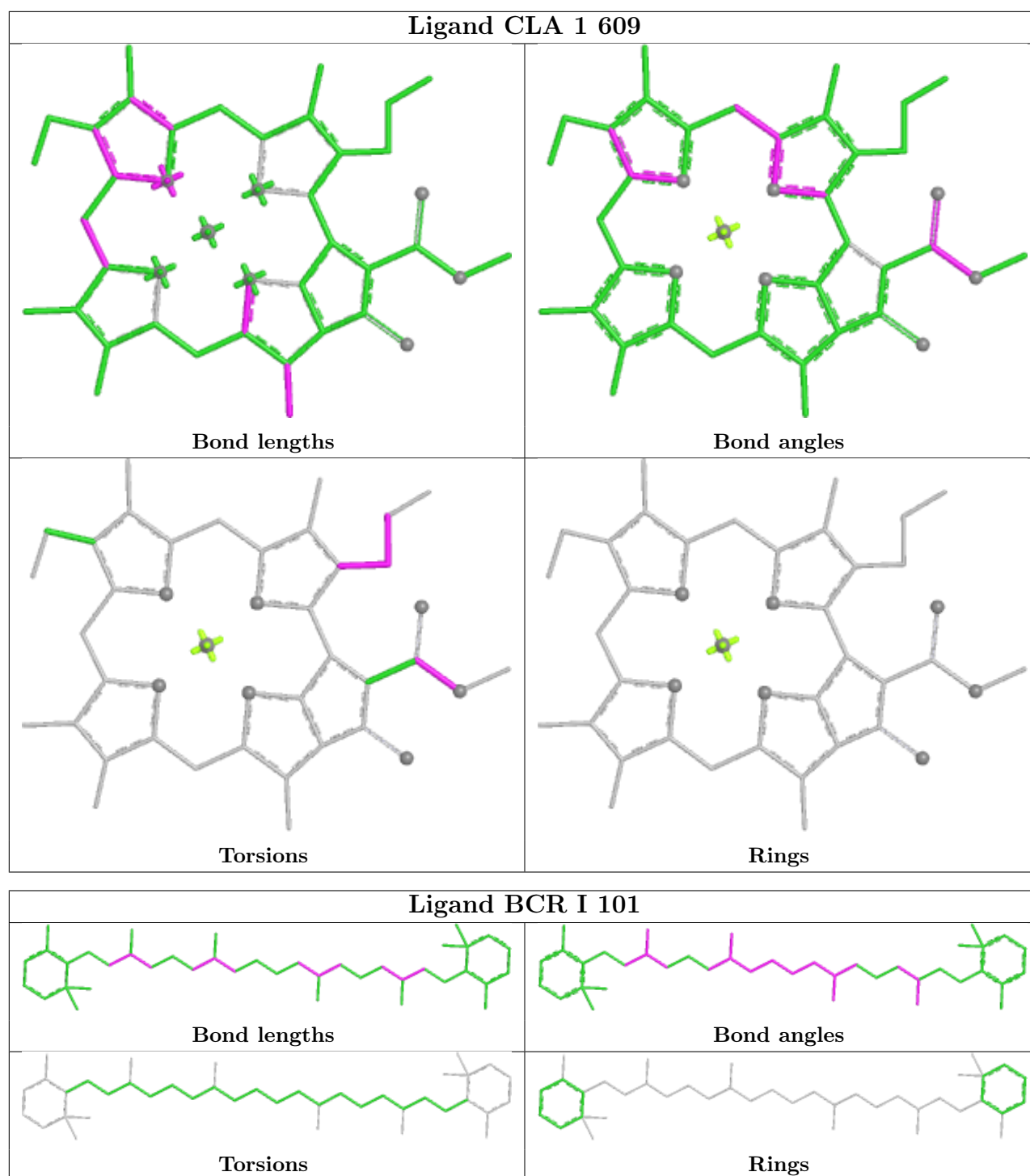


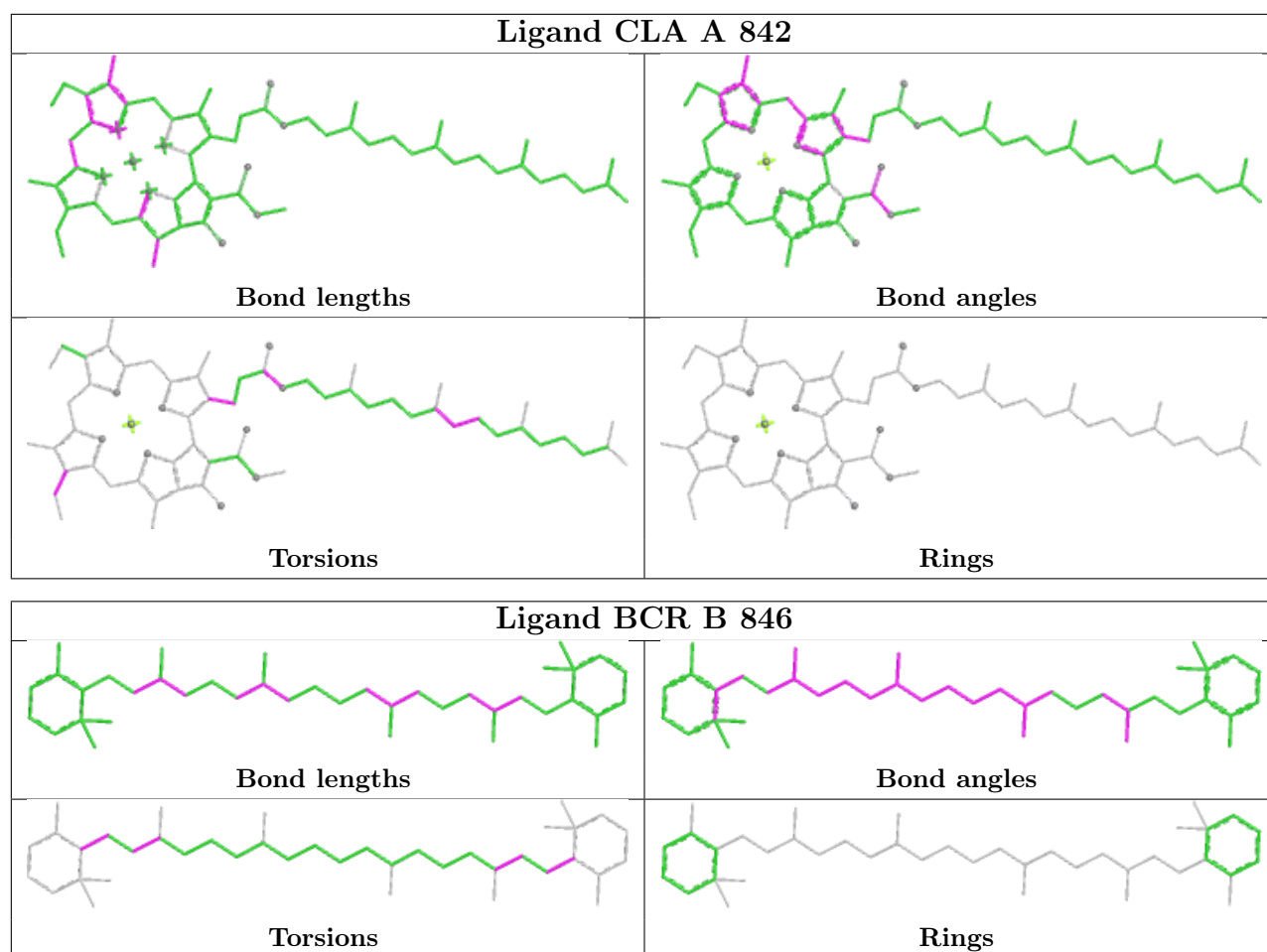




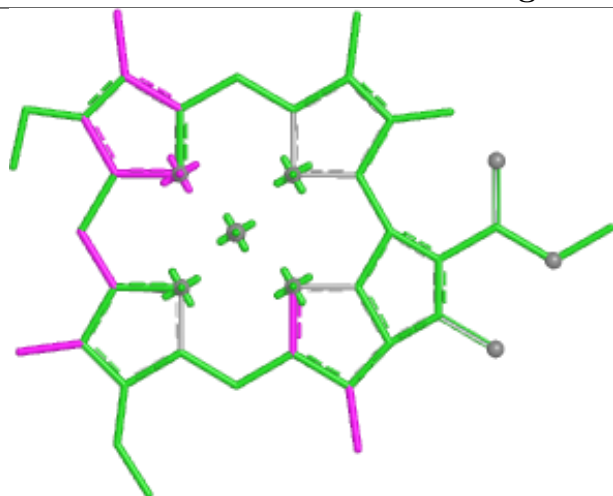




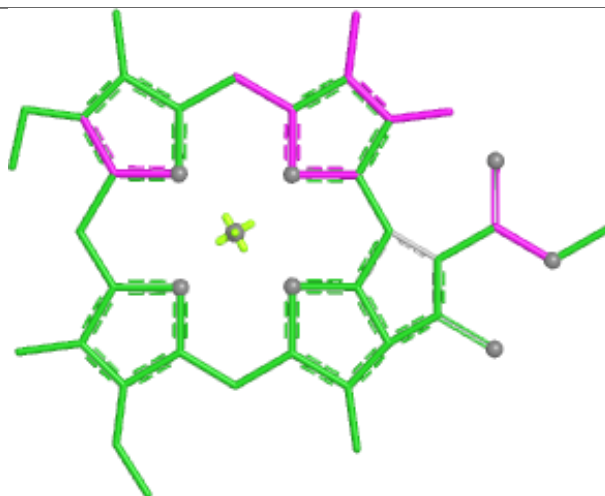




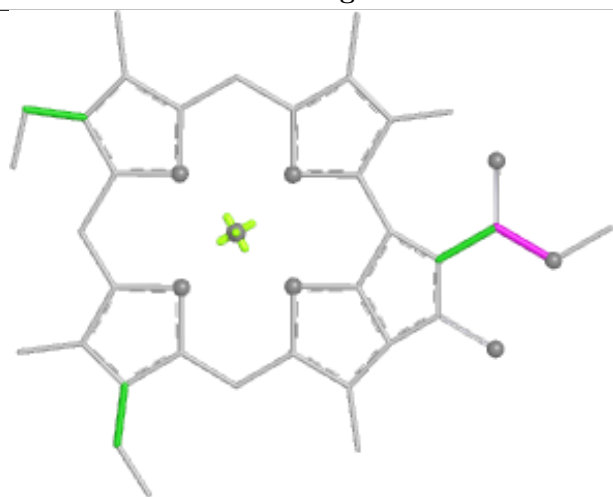
Ligand CLA 3 608



Bond lengths



Bond angles

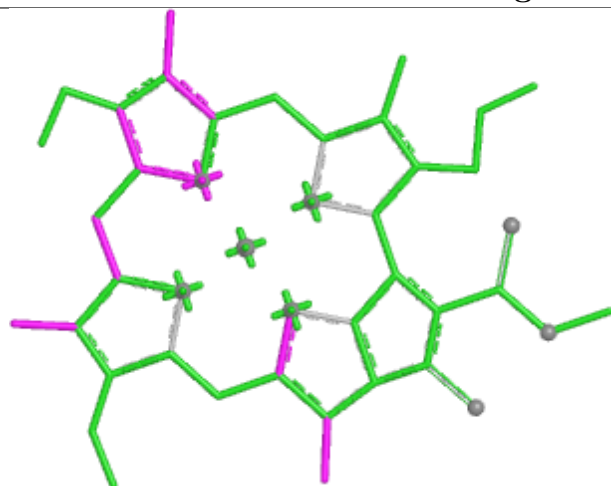


Torsions

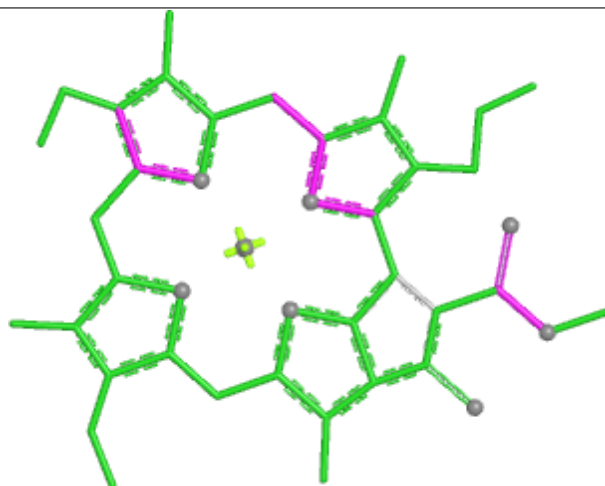


Rings

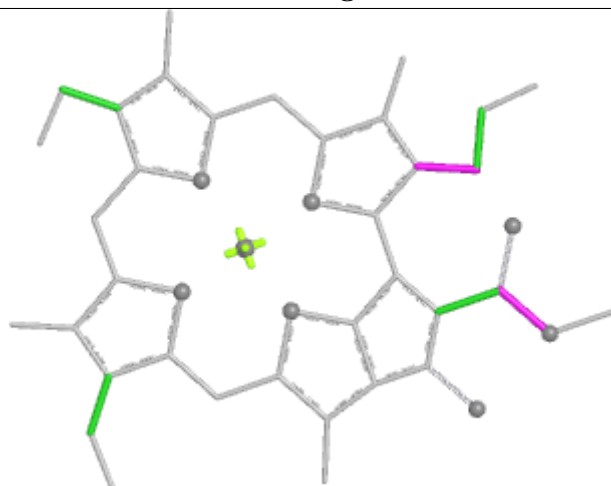
Ligand CLA B 815



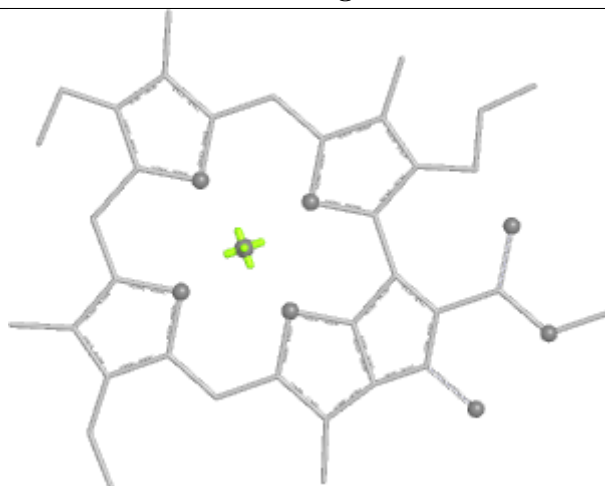
Bond lengths



Bond angles

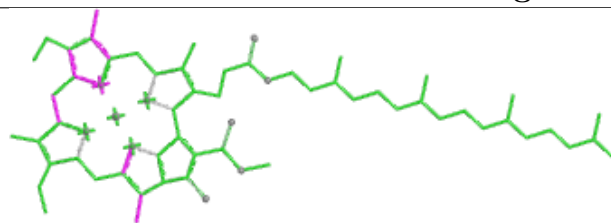


Torsions

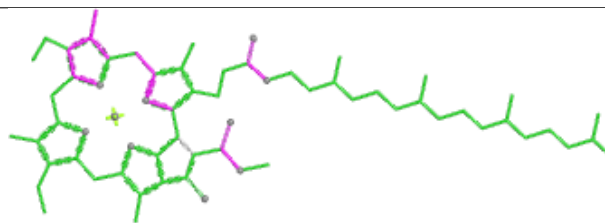


Rings

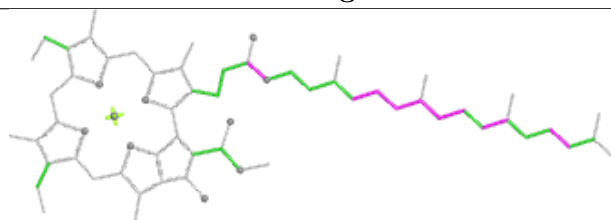
Ligand CLA A 826



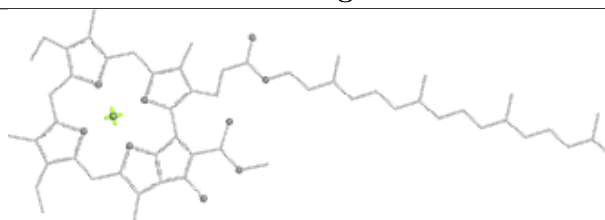
Bond lengths



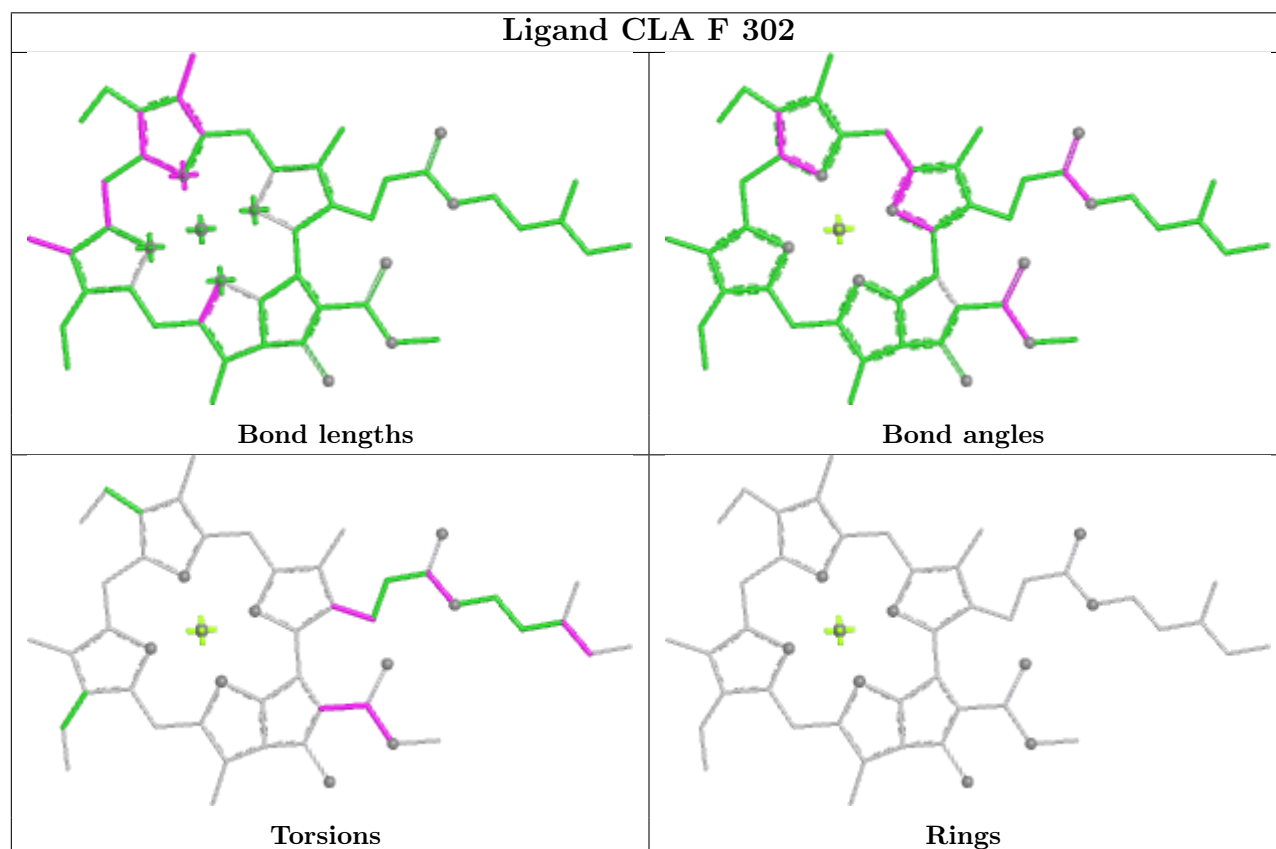
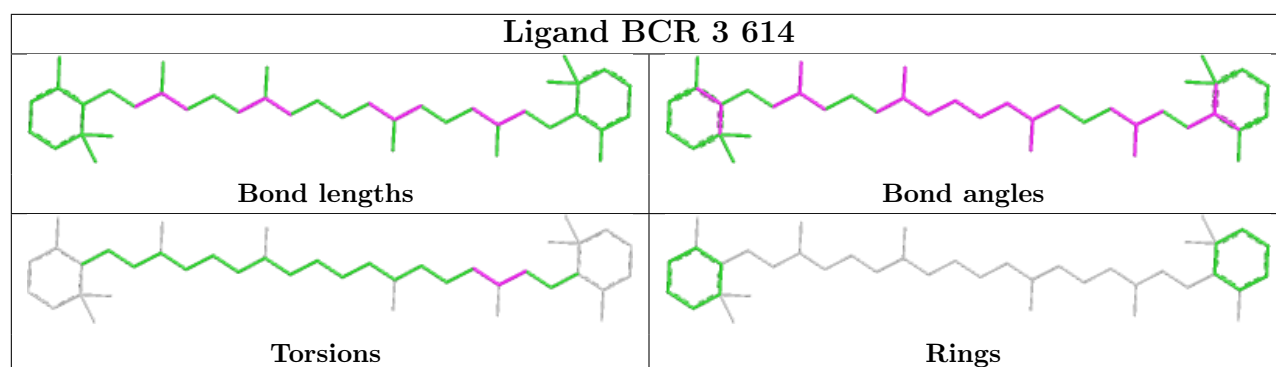
Bond angles

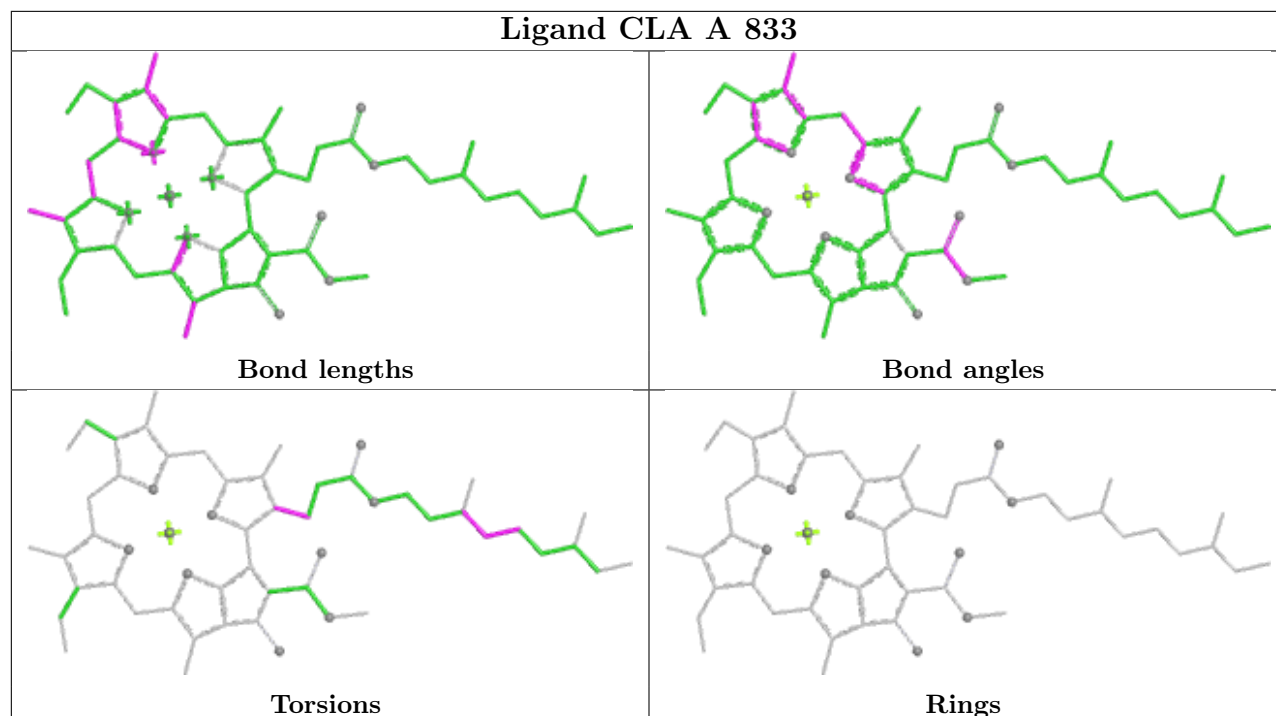
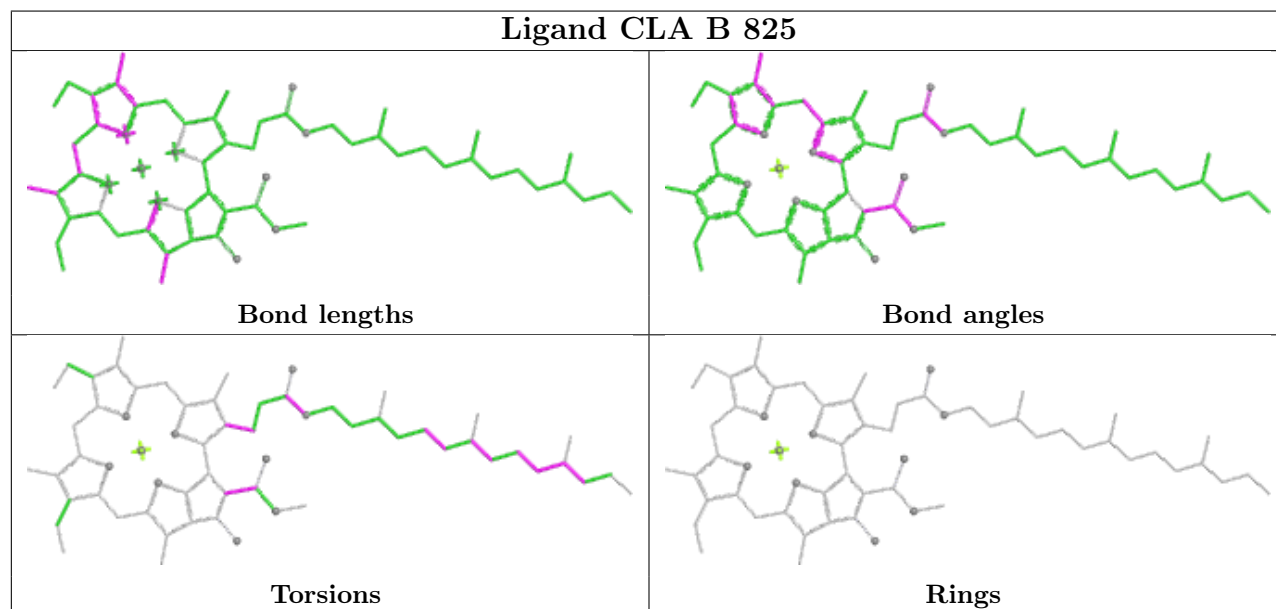


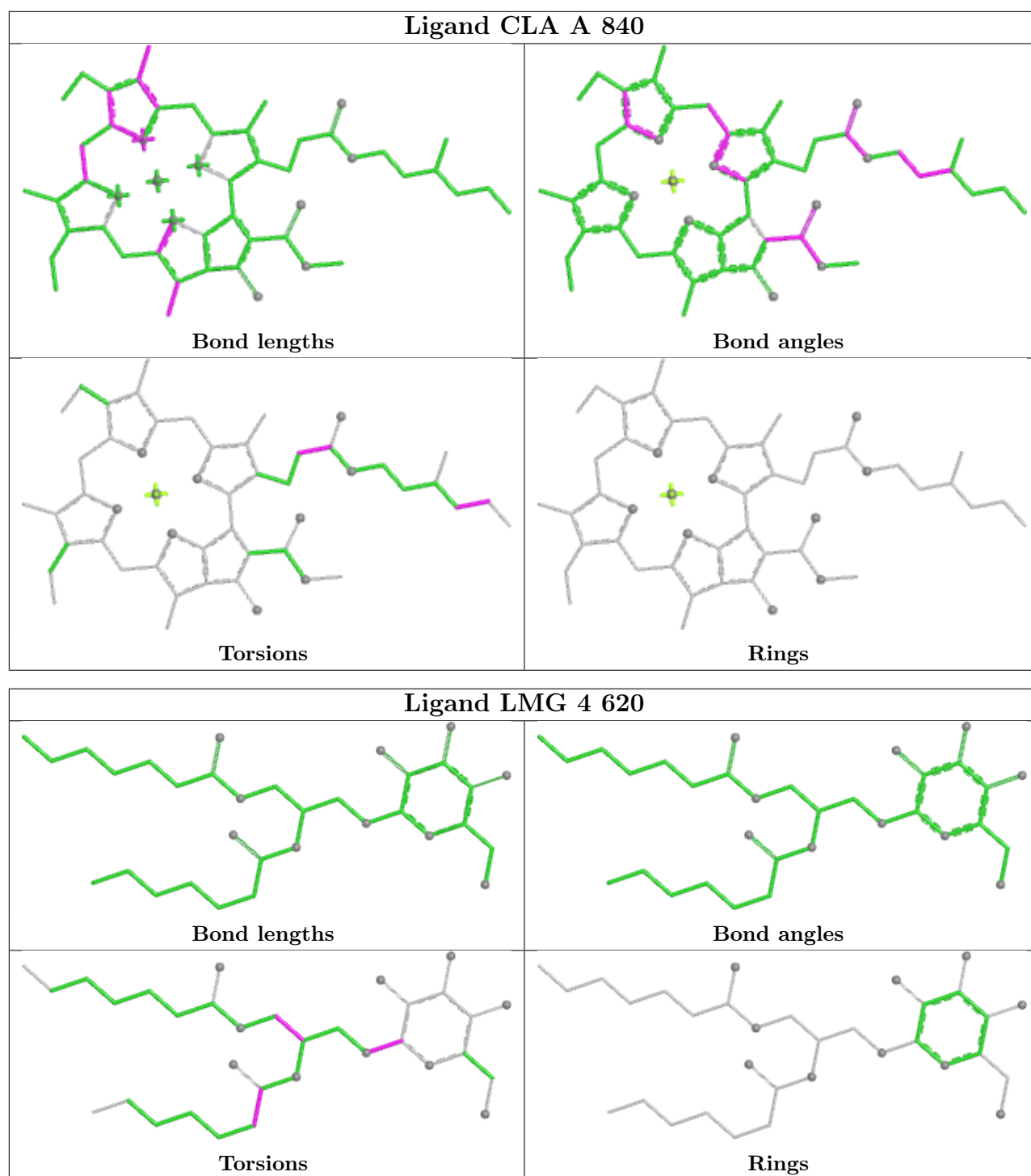
Torsions



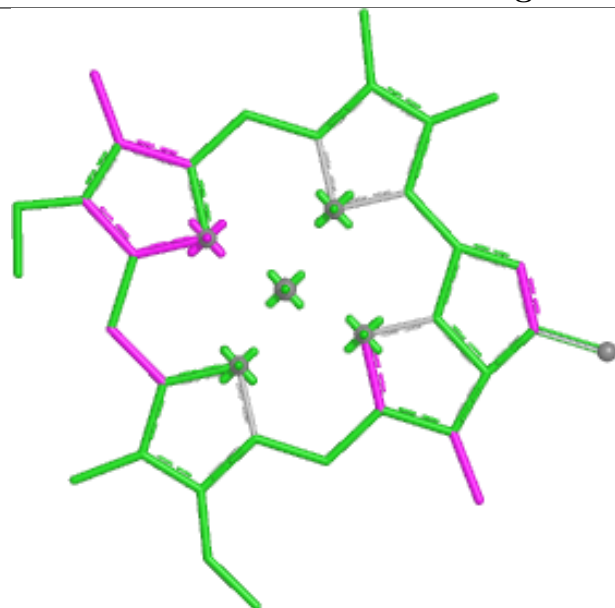
Rings



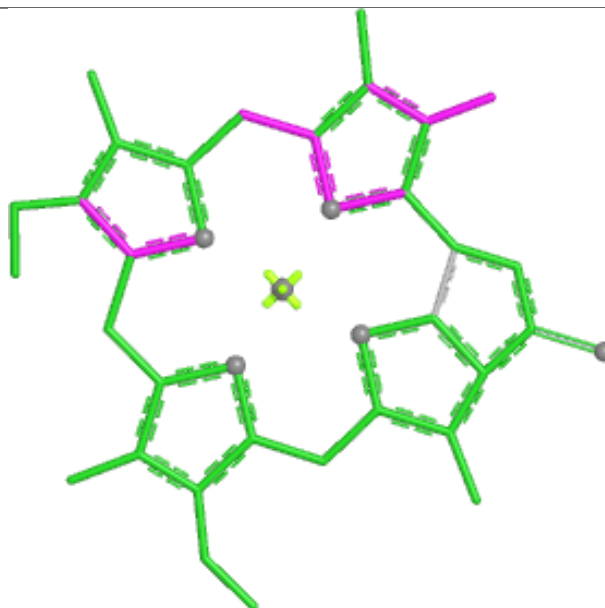
Ligand CLA A 833**Ligand CLA B 825**



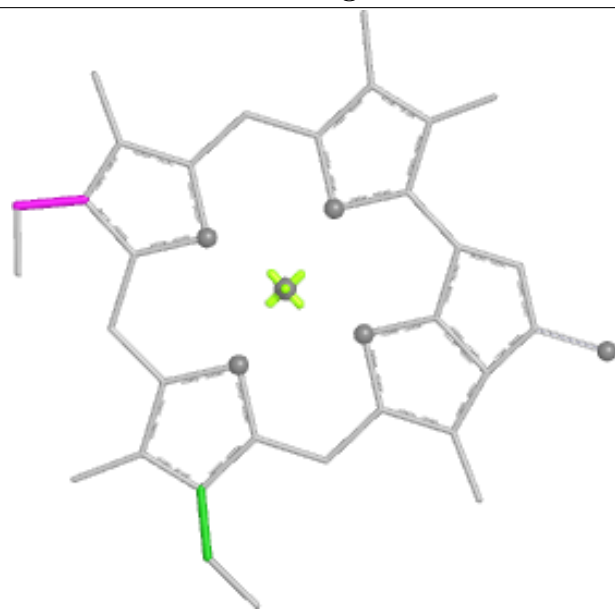
Ligand CLA K 201



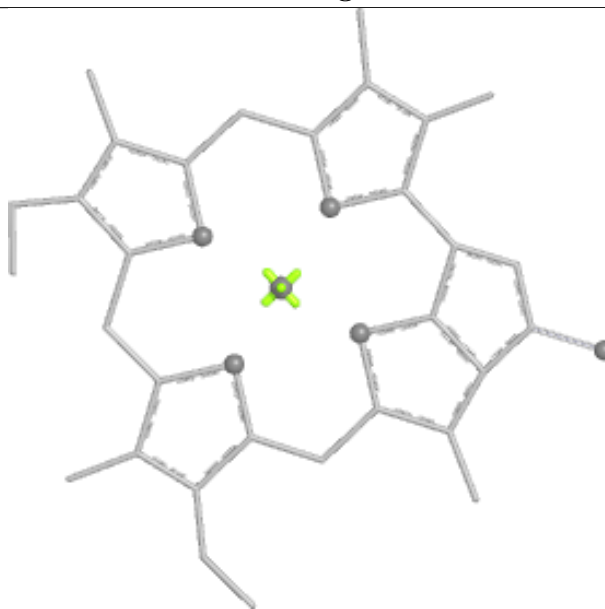
Bond lengths



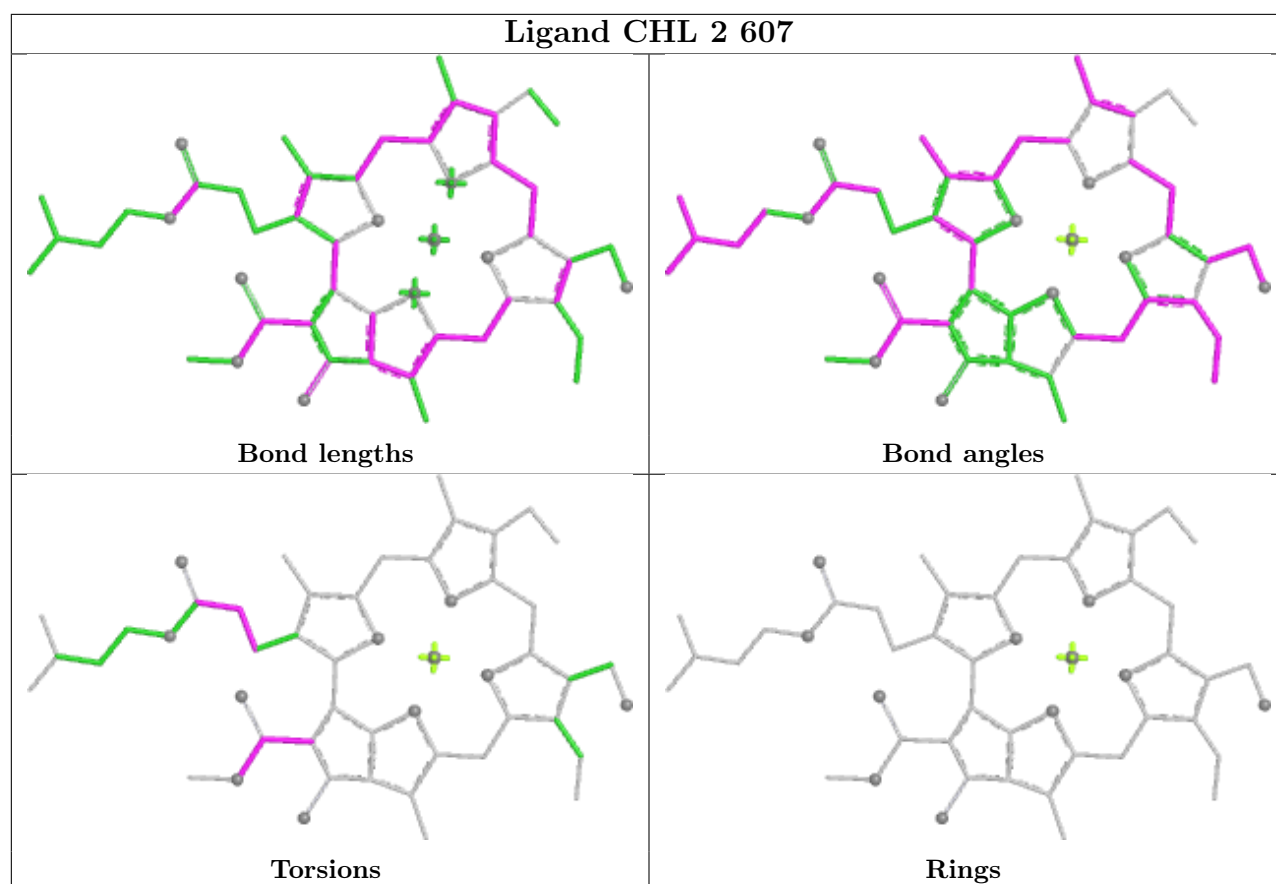
Bond angles



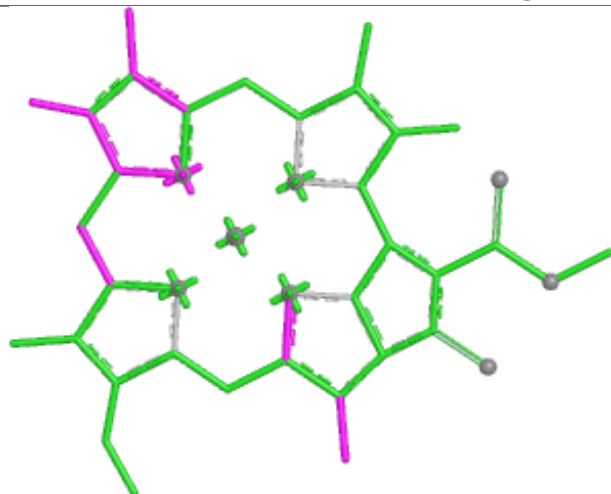
Torsions



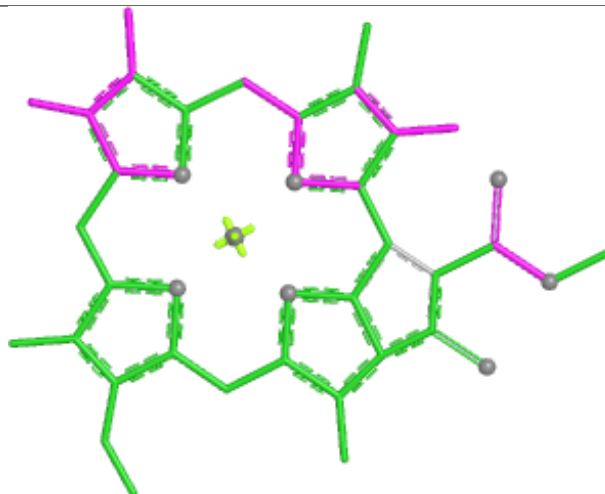
Rings



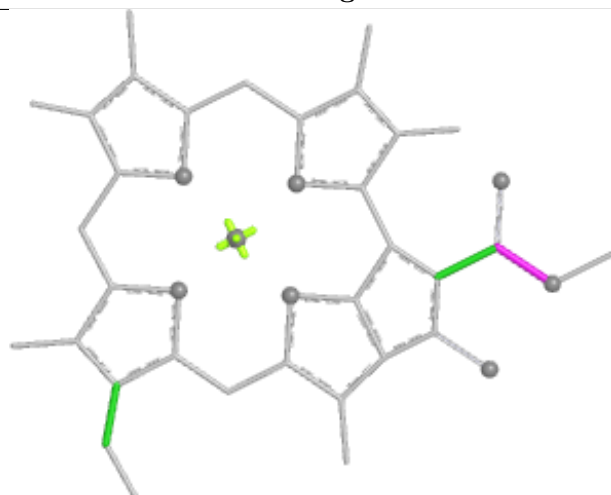
Ligand CLA 1 608



Bond lengths



Bond angles

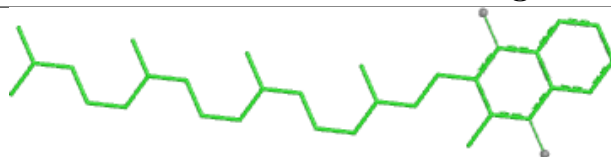


Torsions

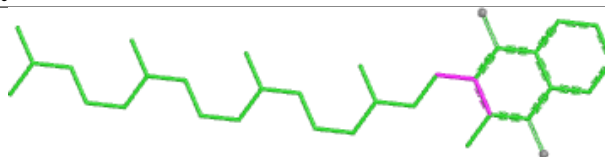


Rings

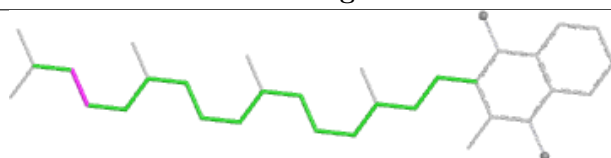
Ligand PQN A 855



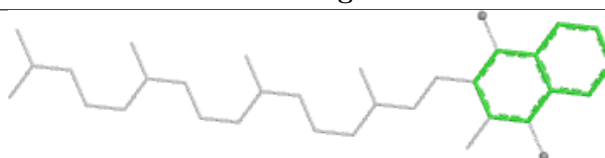
Bond lengths



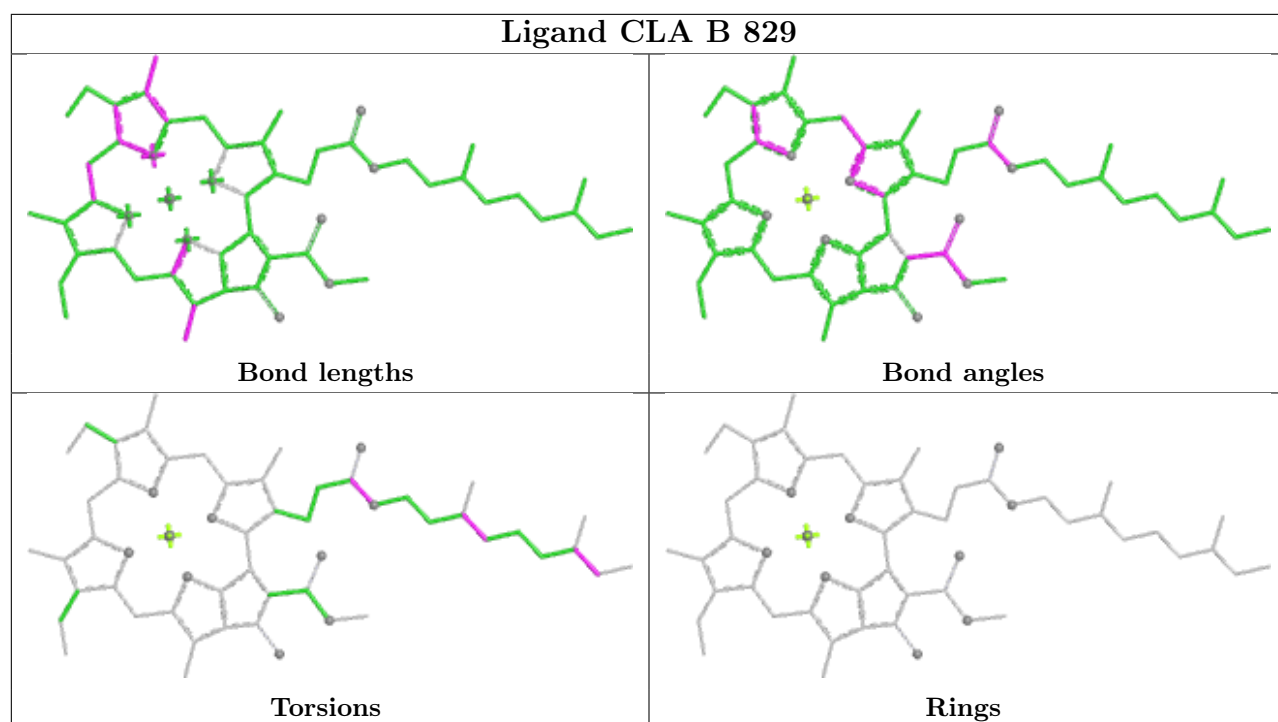
Bond angles



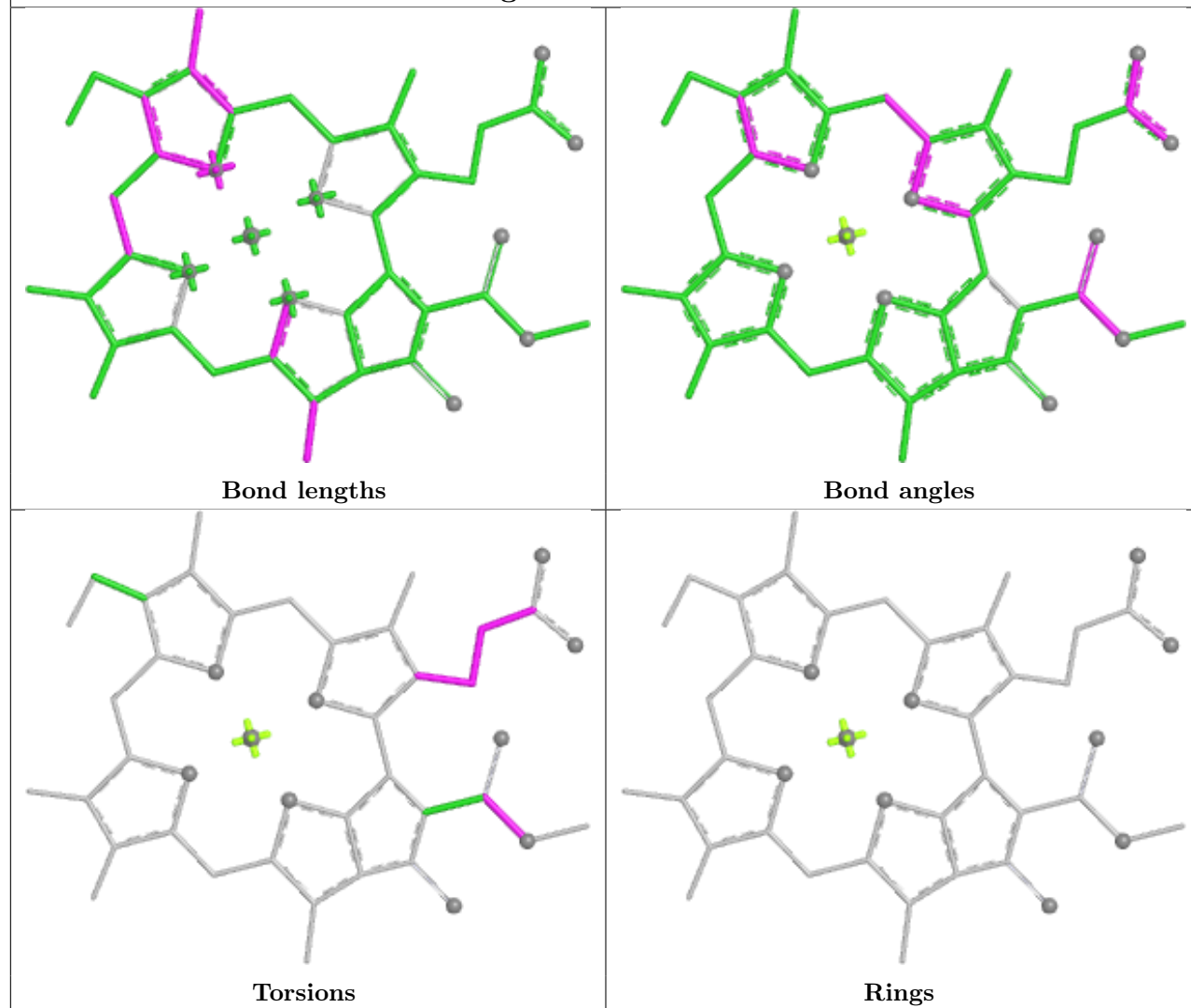
Torsions



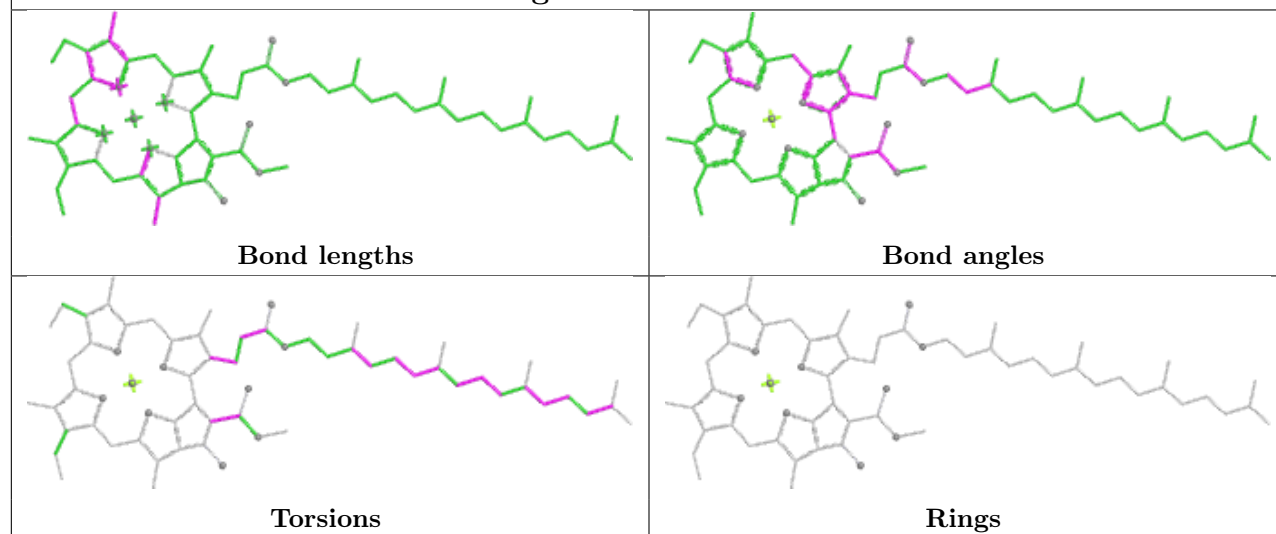
Rings



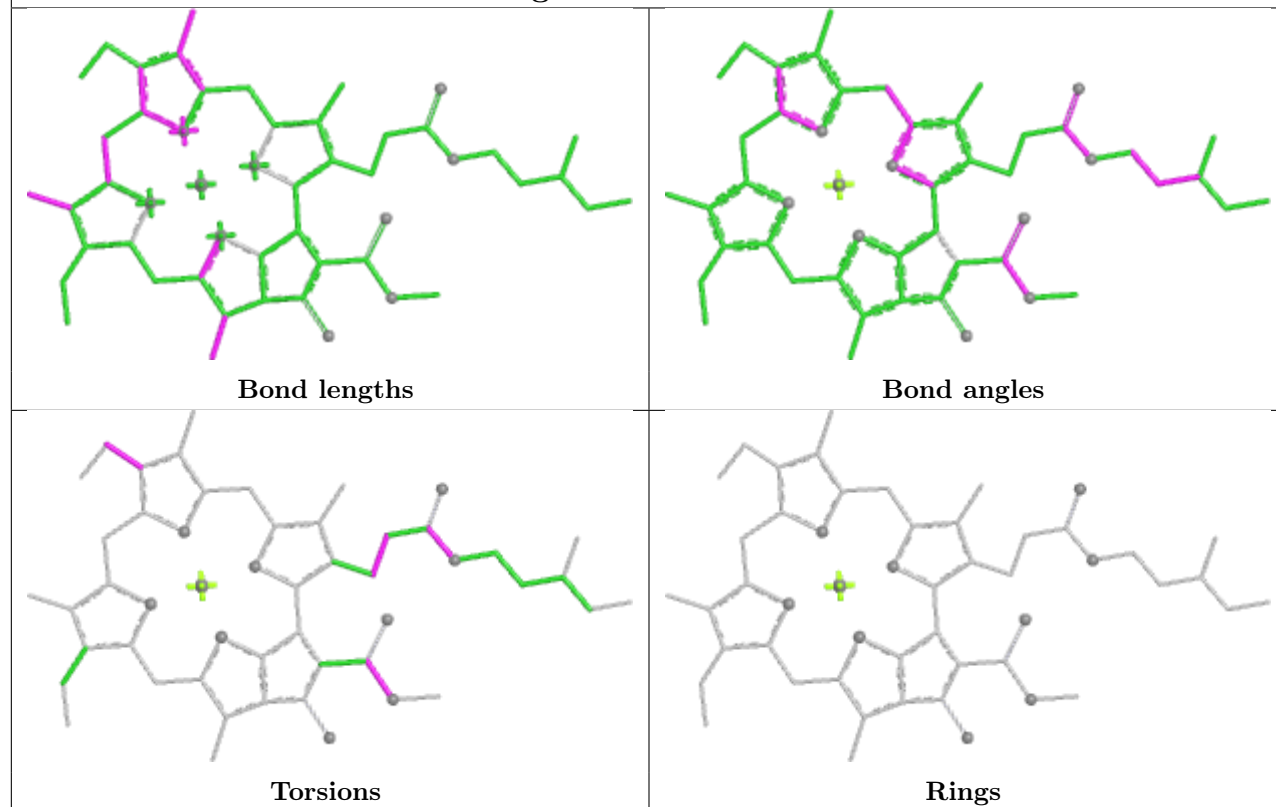
Ligand CLA 2 611



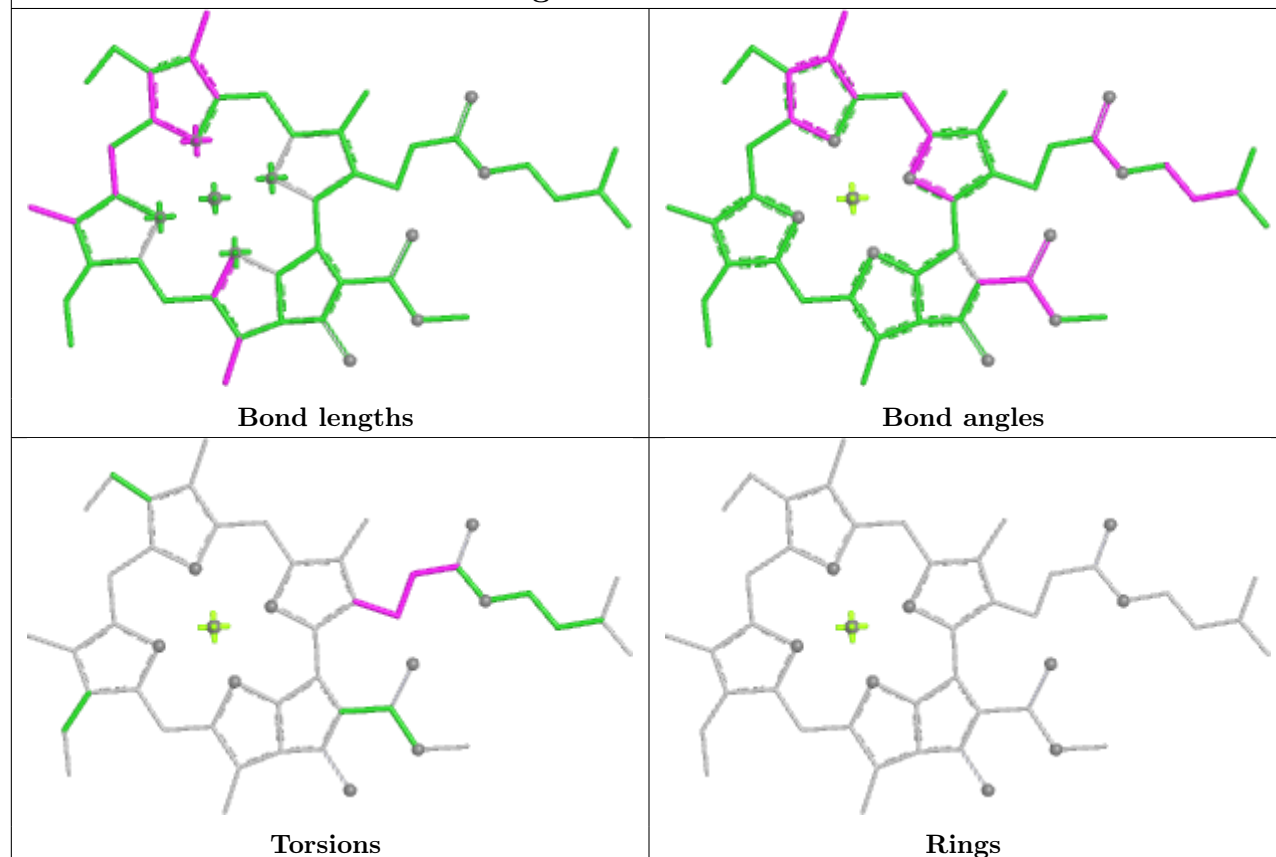
Ligand CLA A 804



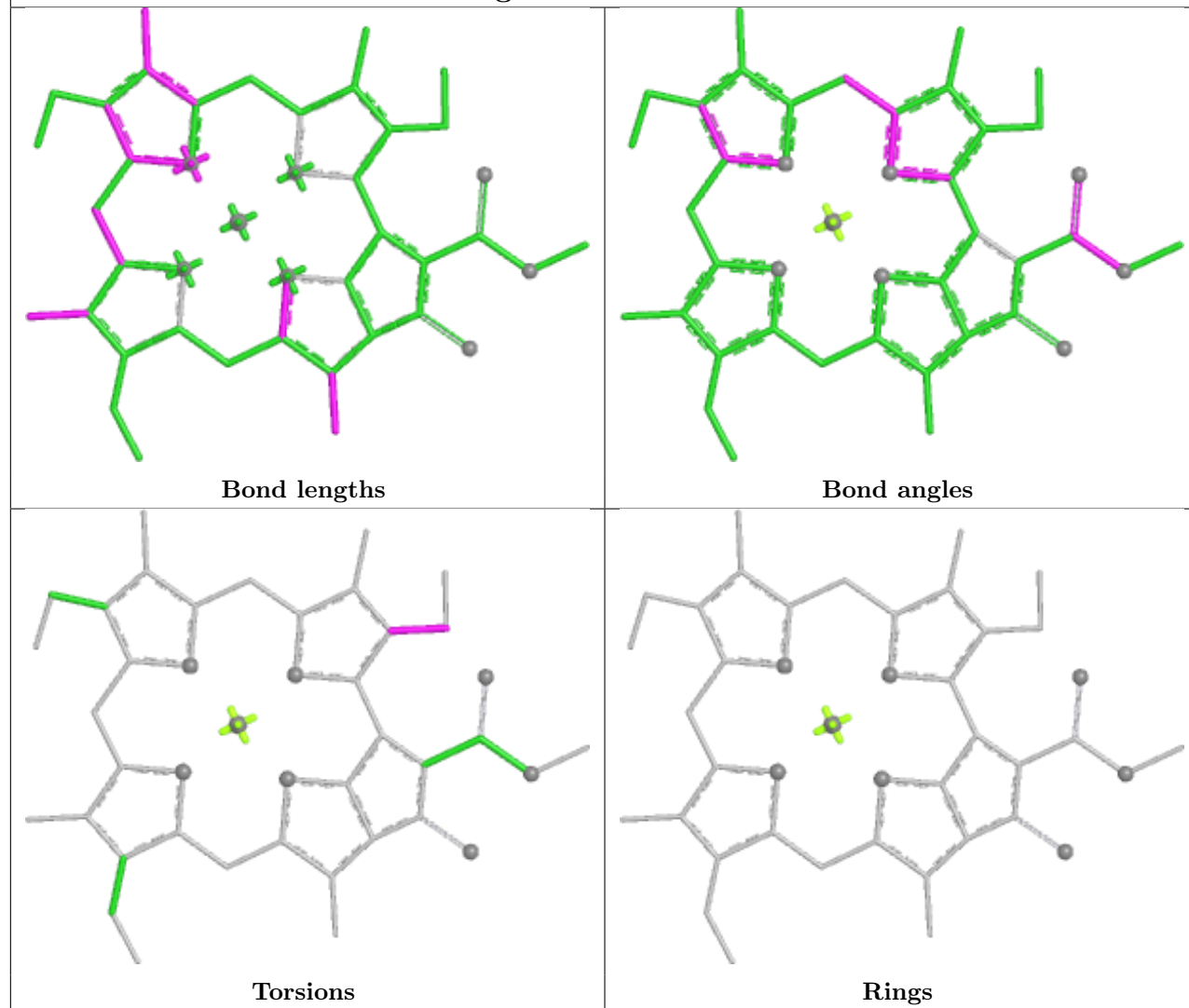
Ligand CLA A 838



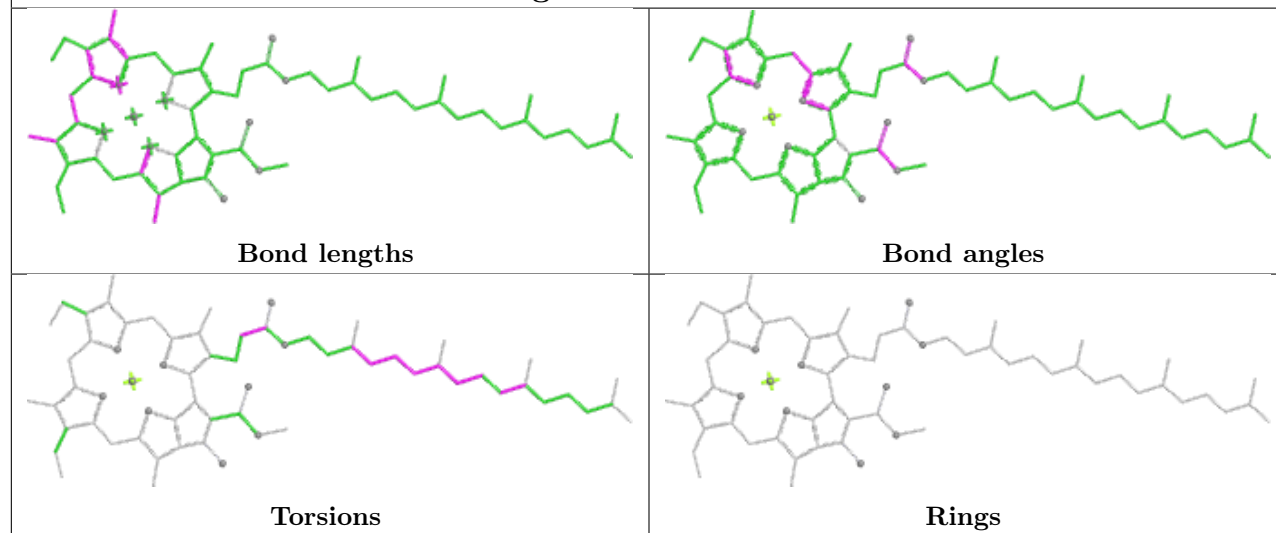
Ligand CLA B 820

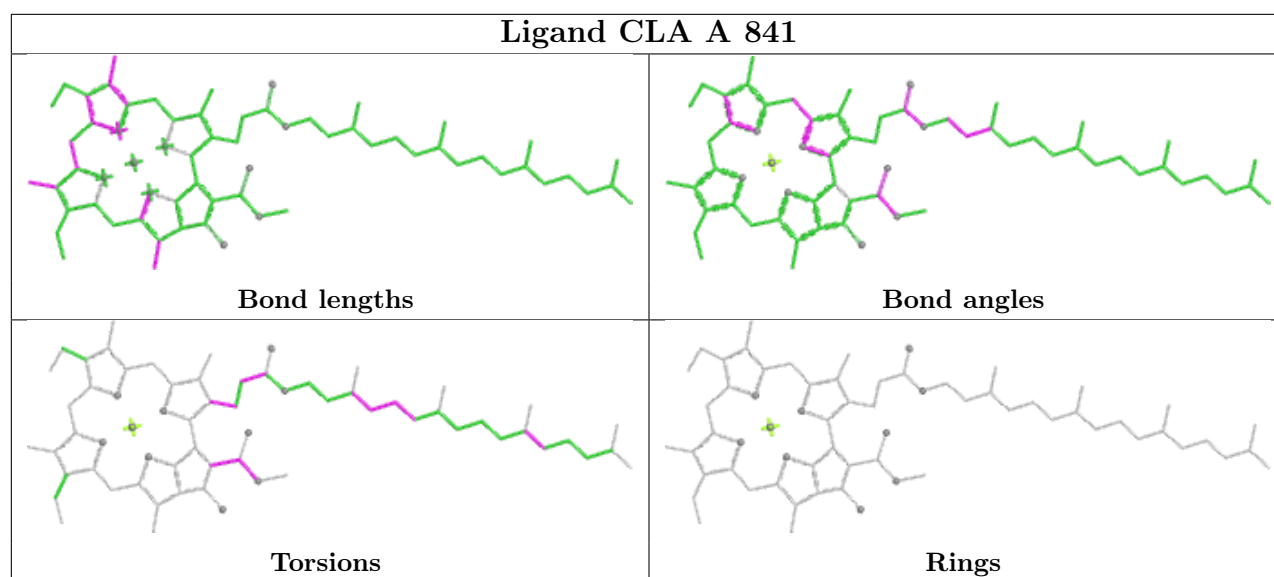


Ligand CLA A 816



Ligand CLA B 806





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

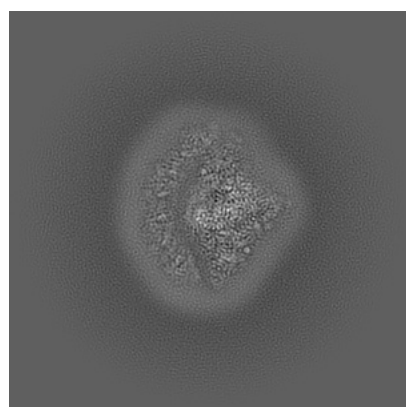
6 Map visualisation [i](#)

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

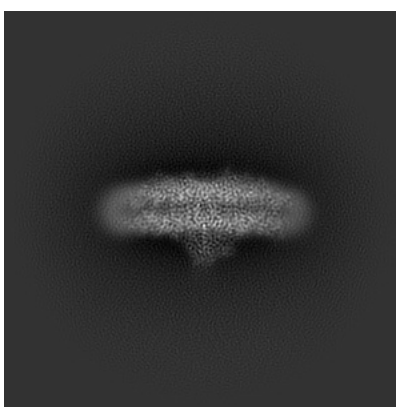
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

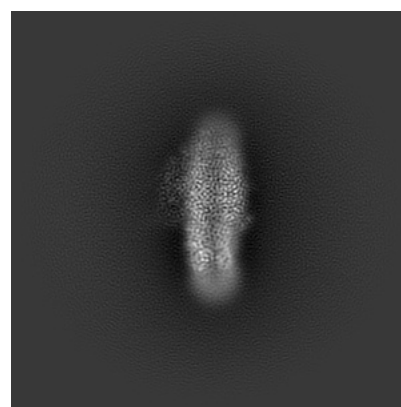
6.1.1 Primary map



X



Y

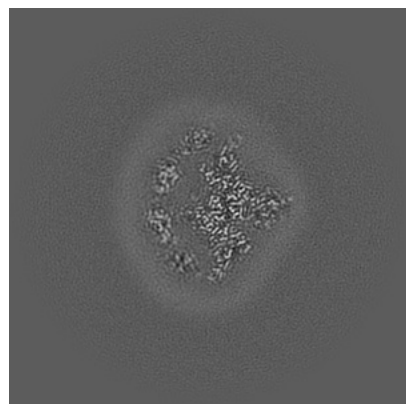


Z

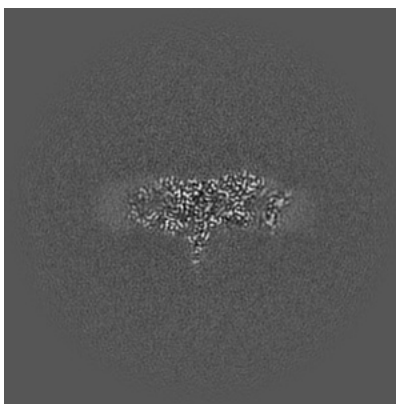
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

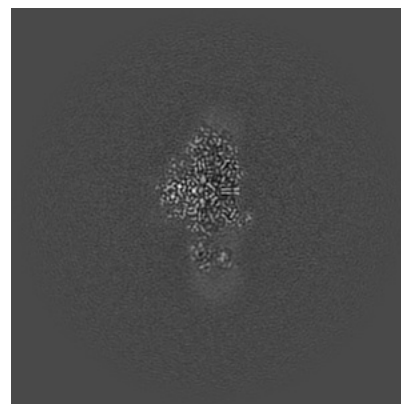
6.2.1 Primary map



X Index: 192



Y Index: 192

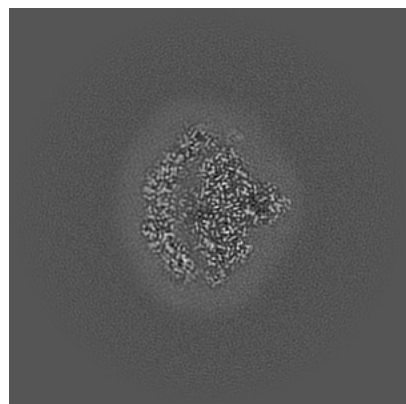


Z Index: 192

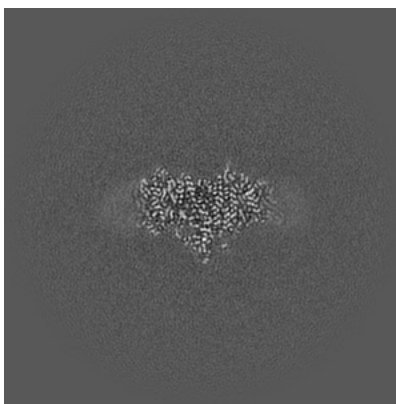
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

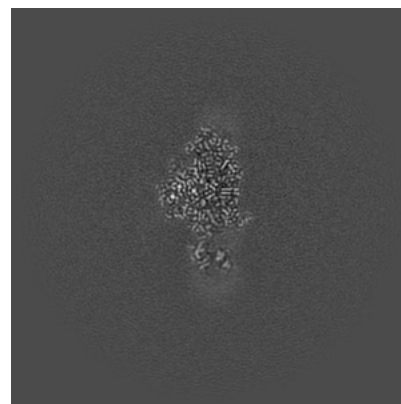
6.3.1 Primary map



X Index: 182



Y Index: 211

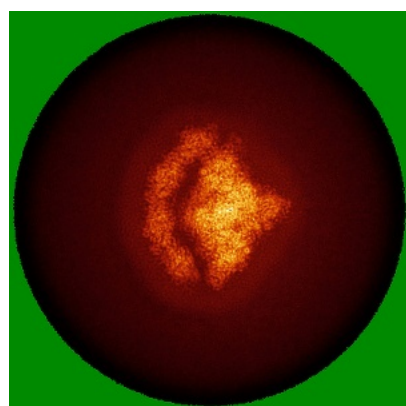


Z Index: 191

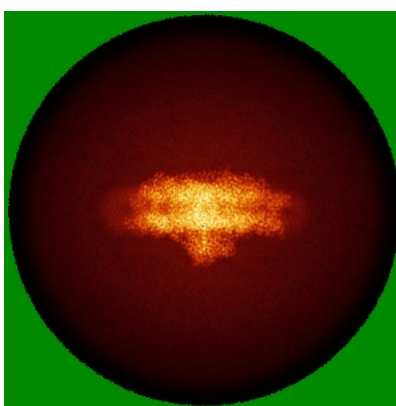
The images above show the largest variance slices of the map in three orthogonal directions.

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

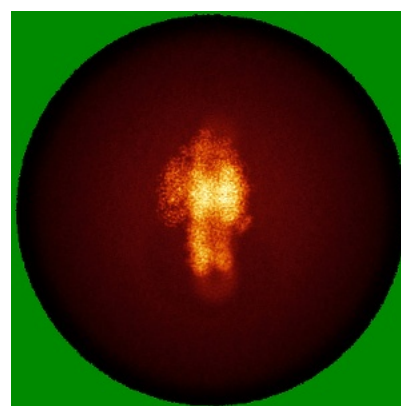
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

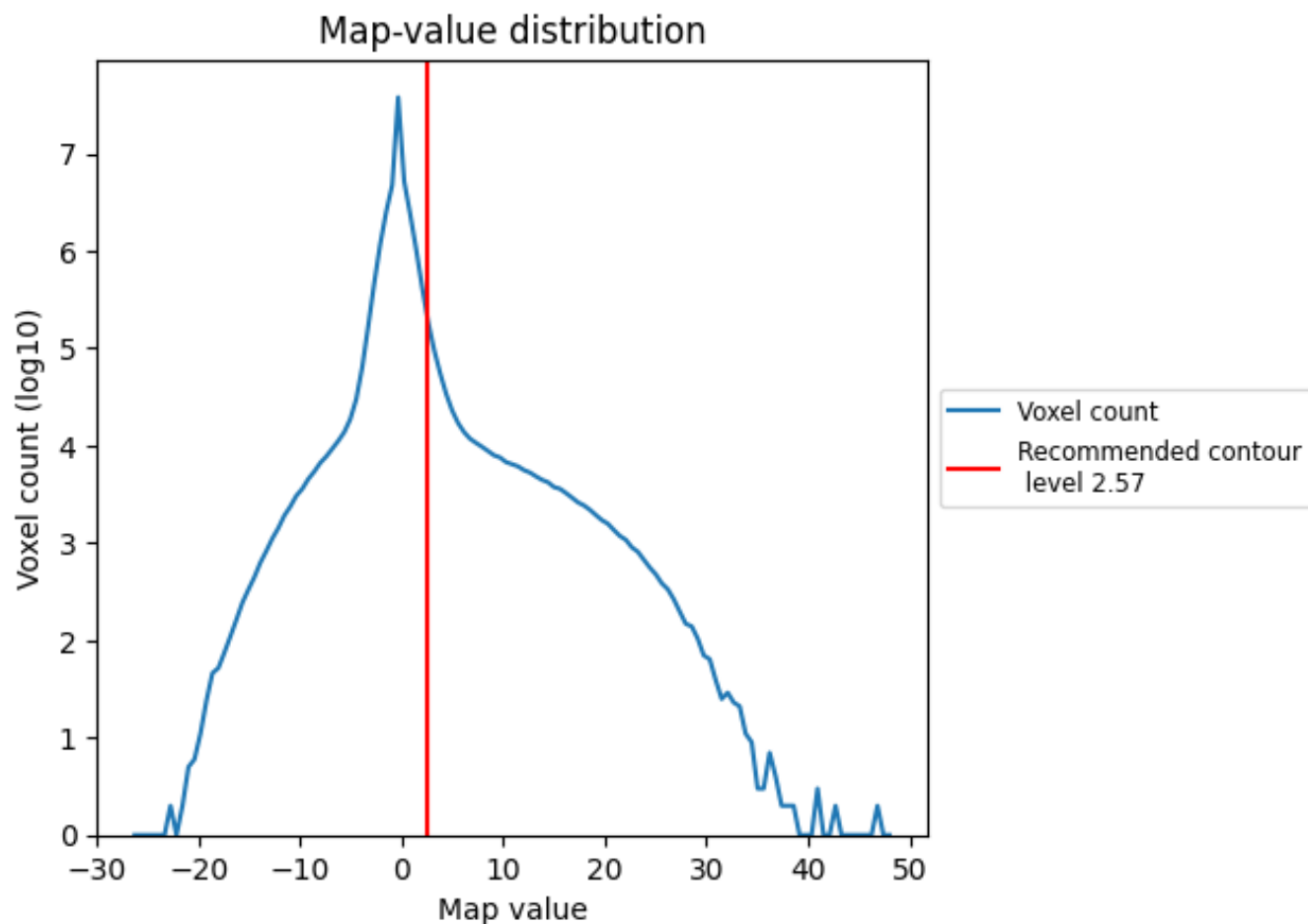
6.6 Mask visualisation

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

7 Map analysis [i](#)

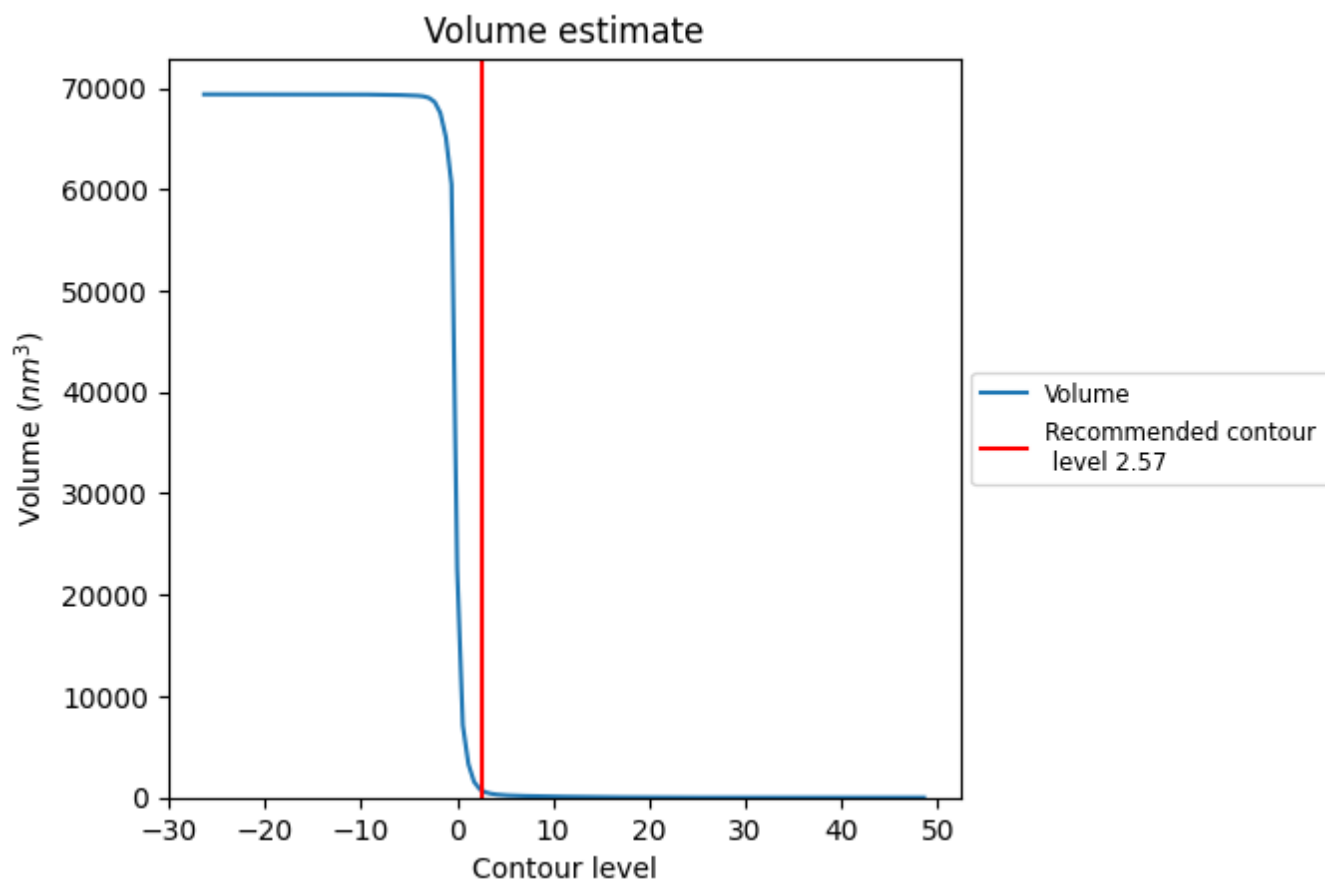
This section contains the results of statistical analysis of the map.

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.

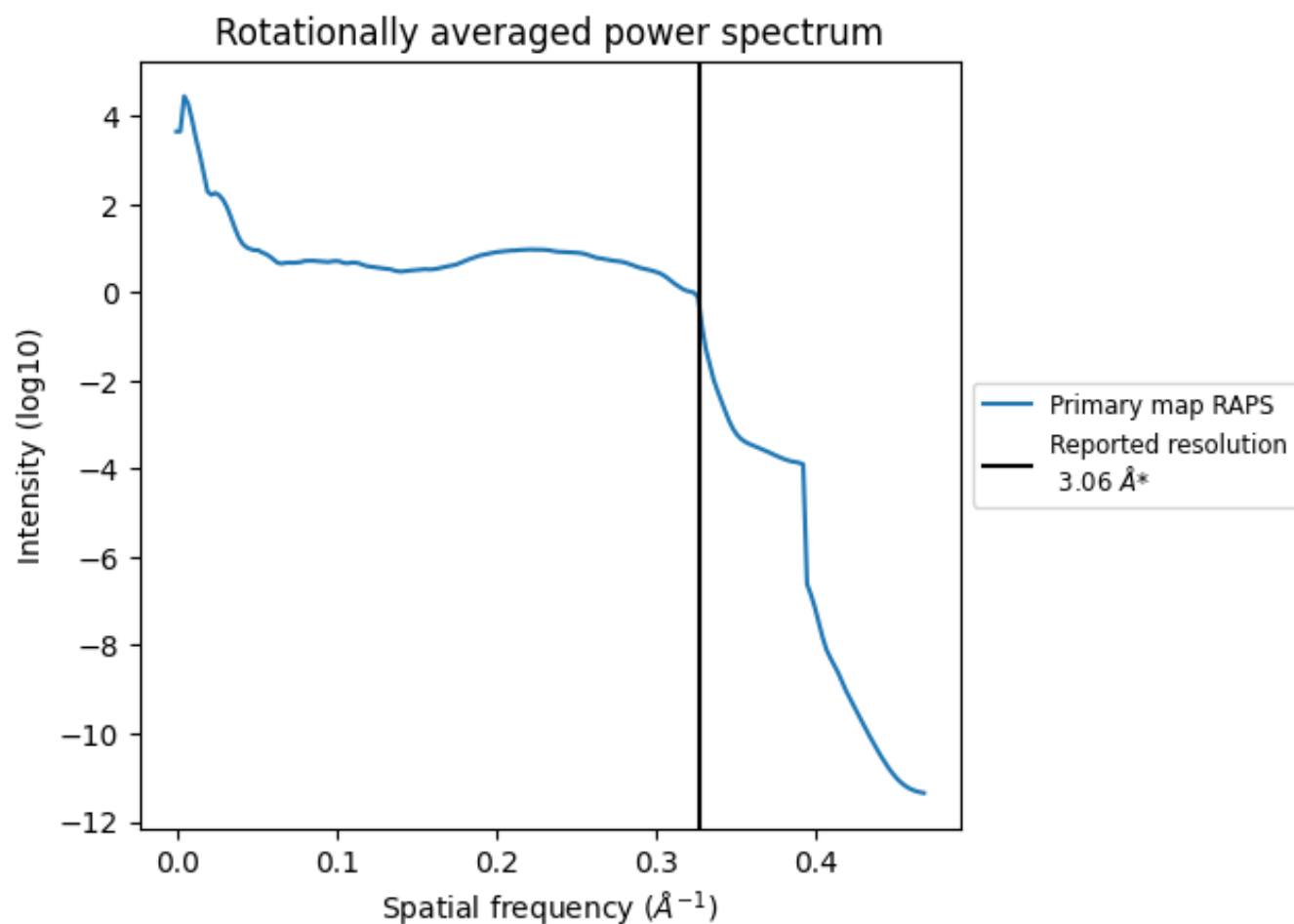
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm³; this corresponds to an approximate mass of 654 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

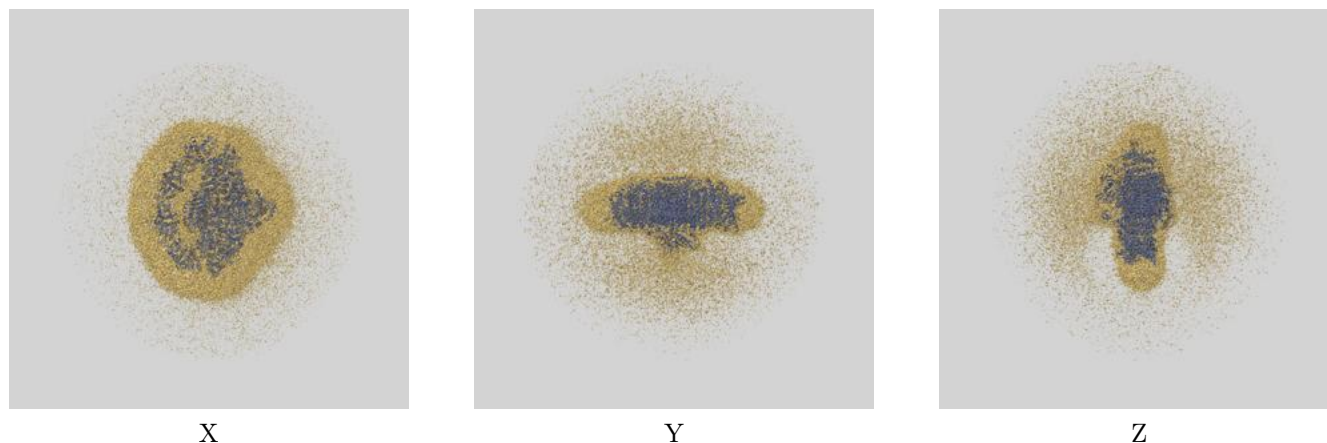
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

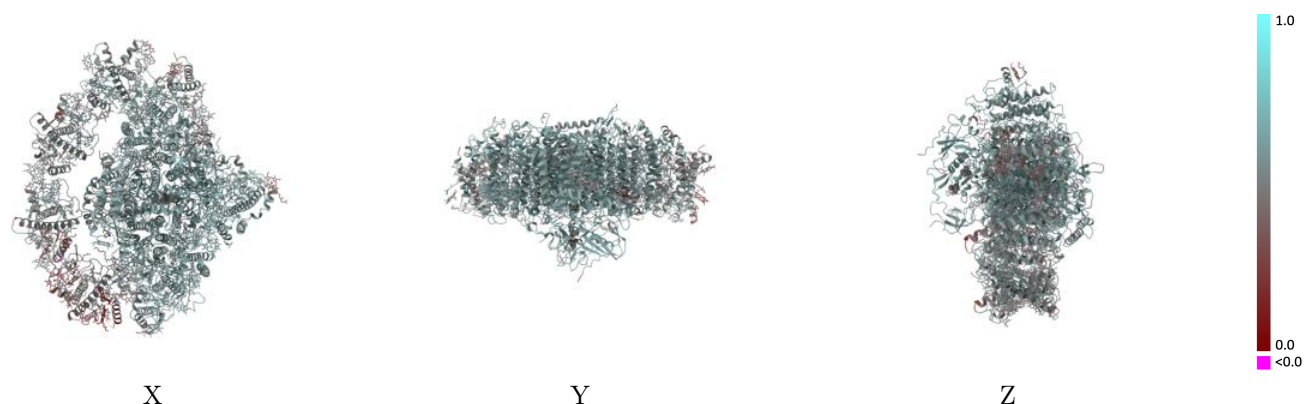
This section contains information regarding the fit between EMDB map EMD-36036 and PDB model 8J7A. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



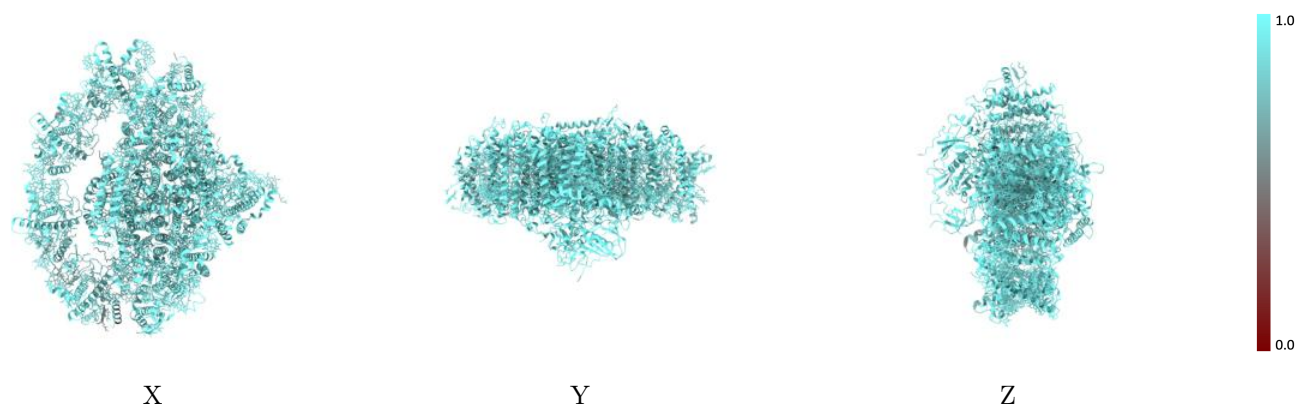
The images above show the 3D surface view of the map at the recommended contour level 2.57 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



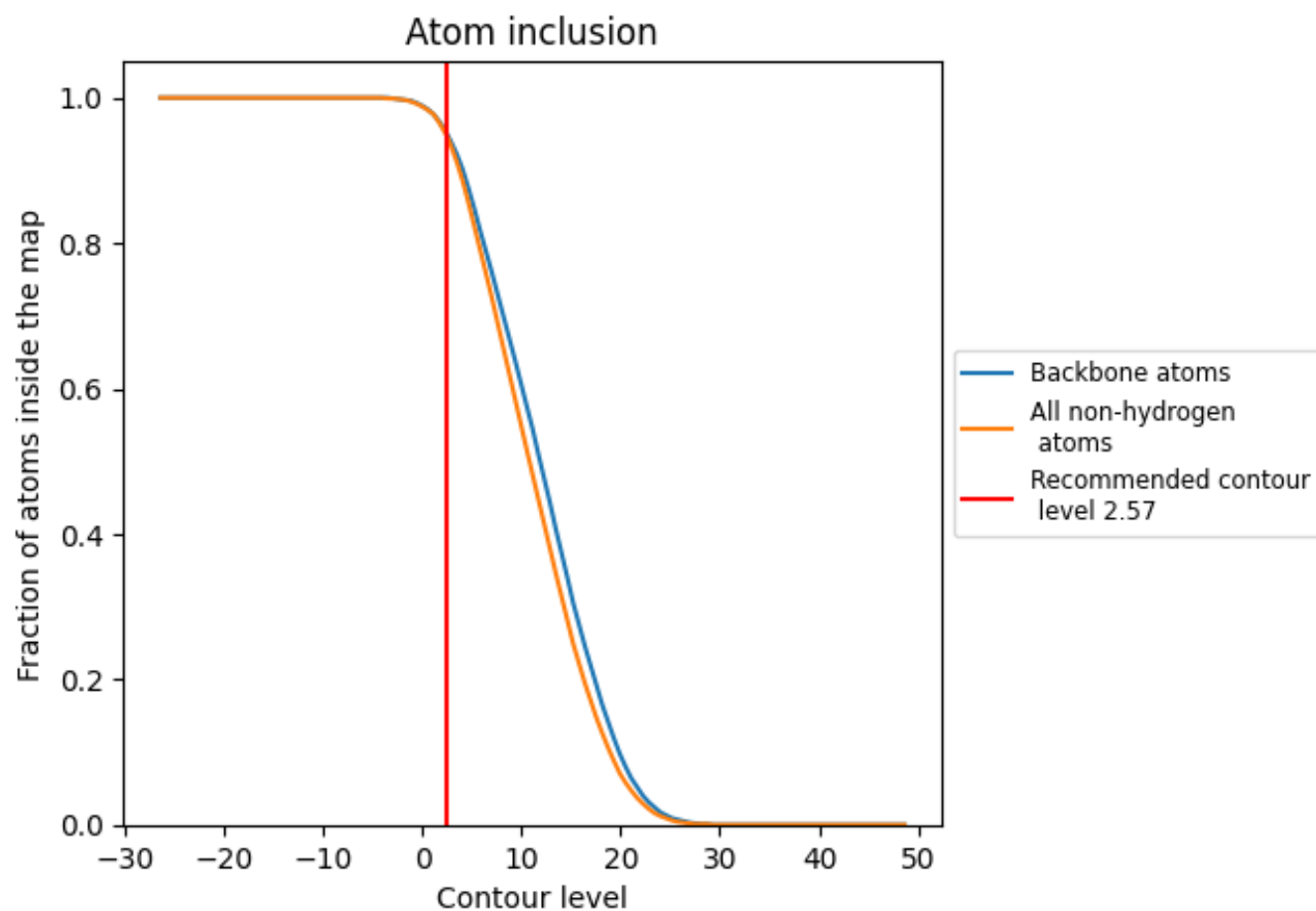
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.57).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.57) and Q-score for the entire model and for each chain.

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

1.0

0.0

<0.0