



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:34 PM UTC

PDB ID : 7EWK / pdb_00007ewk
EMDB ID : EMD-31350
Title : Barley photosystem I-LHCI-Lhca6 supercomplex
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2021-05-25
Resolution : 3.88 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:

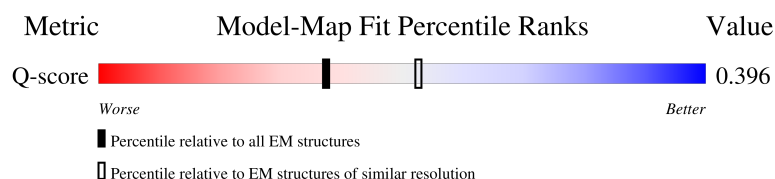
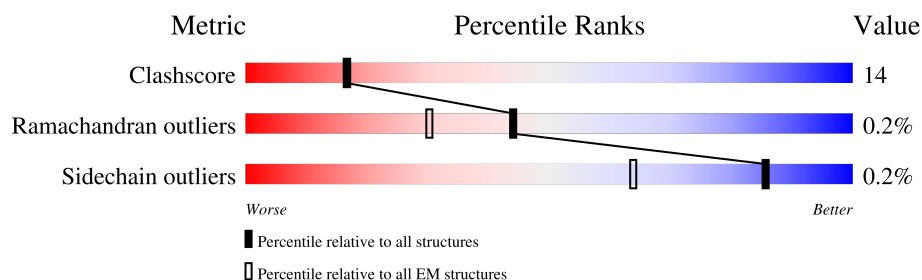
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.88 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	8773 (3.38 - 4.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	 73% 27%
2	B	733	 72% 28%
3	C	81	 62% 38%
4	D	142	 68% 32%

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Mol	Chain	Length	Quality of chain
5	E	68	
6	F	158	
7	H	61	
8	I	30	
9	J	42	
10	K	84	
11	L	146	
12	1	193	
13	3	222	
14	4	197	
15	6	211	

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
16	CL0	A	801	X	-	-	-
17	CLA	1	504	X	-	-	-
17	CLA	1	506	X	-	-	-
17	CLA	1	507	X	-	-	-
17	CLA	1	508	X	-	-	-
17	CLA	1	509	X	-	-	-
17	CLA	1	510	X	-	-	-
17	CLA	1	511	X	-	-	-
17	CLA	1	513	X	-	-	-
17	CLA	1	515	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	3	314	X	-	-	-
17	CLA	3	316	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	305	X	-	-	-
17	CLA	4	306	X	-	-	-
17	CLA	4	307	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	311	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	315	X	-	-	-
17	CLA	4	317	X	-	-	-
17	CLA	6	504	X	-	-	-
17	CLA	6	506	X	-	-	-
17	CLA	6	507	X	-	-	-
17	CLA	6	508	X	-	-	-
17	CLA	6	509	X	-	-	-
17	CLA	6	510	X	-	-	-
17	CLA	6	511	X	-	-	-
17	CLA	6	514	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-
17	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	852	X	-	-	-
17	CLA	A	853	X	-	-	-
17	CLA	B	801	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	B	843	X	-	-	-
17	CLA	F	802	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	102	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	205	X	-	-	-
17	CLA	L	302	X	-	-	-
17	CLA	L	303	X	-	-	-
17	CLA	L	304	X	-	-	-
24	LUT	1	502	X	-	-	-
25	CHL	1	512	X	-	-	-
25	CHL	1	514	X	-	-	-
25	CHL	1	517	X	-	-	-
25	CHL	3	313	X	-	-	-
25	CHL	4	313	X	-	-	-
25	CHL	4	314	X	-	-	-
25	CHL	4	316	X	-	-	-
25	CHL	6	512	X	-	-	-
25	CHL	6	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	6	515	X	-	-	-
25	CHL	6	517	X	-	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 32765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5798	3797	987	996	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5840	3832	991	1003	14		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			613	377	105	119	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1112	714	195	200	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			540	341	99	100		

- Molecule 6 is a protein called Photosystem I reaction center subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1188	768	203	216	1		

- Molecule 7 is a protein called Photosystem I reaction center subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			447	298	73	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	30	Total	C	N	O	S	0	0
			235	163	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			332	225	51	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			576	361	101	110	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	146	Total	C	N	O	0	0
			1090	720	174	196		

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	193	Total	C	N	O	S	0	0
			1484	965	248	269	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	222	Total	C	N	O	S	0	0
			1672	1097	272	298	5		

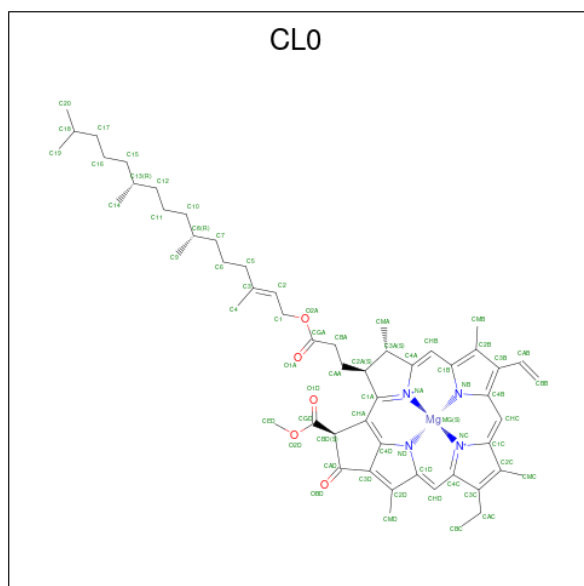
- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

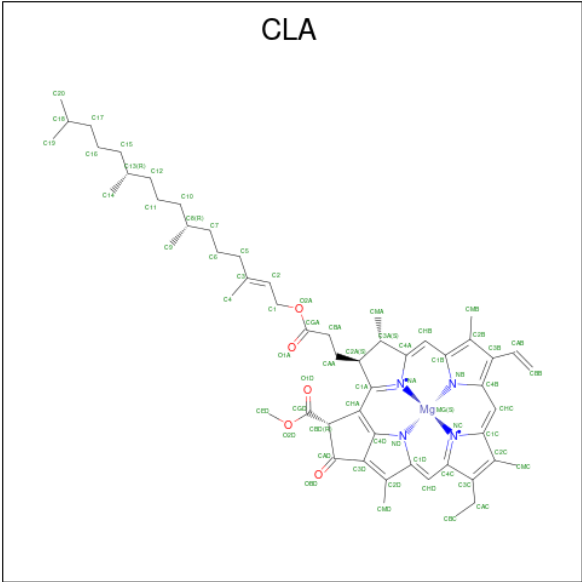
Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	197	Total	C	N	O	S	0	0
			1529	991	253	282	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	211	Total	C	N	O	S	0	0
			1655	1088	274	285	8		

- Molecule 16 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).





Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
17	A	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
17	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
17	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	B	1	Total 42	C 33	Mg 1	N 4	O 4	0
17	B	1	Total 38	C 31	Mg 1	N 4	O 2	0
17	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
17	B	1	Total 54	C 45	Mg 1	N 4	O 4	0
17	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	B	1	Total 40	C 32	Mg 1	N 4	O 3	0
17	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
17	B	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
17	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
17	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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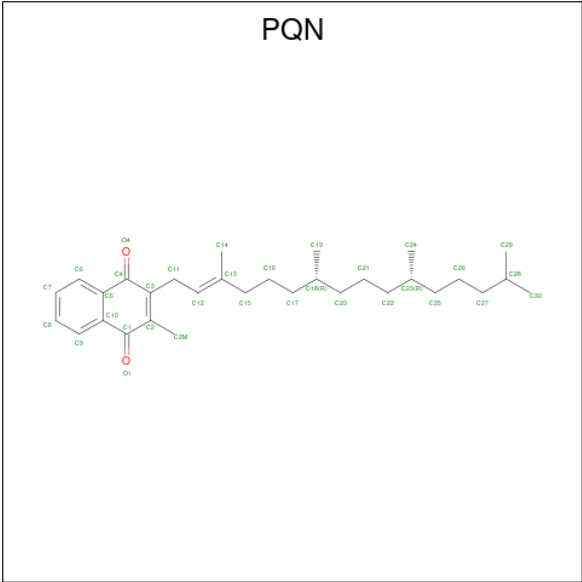
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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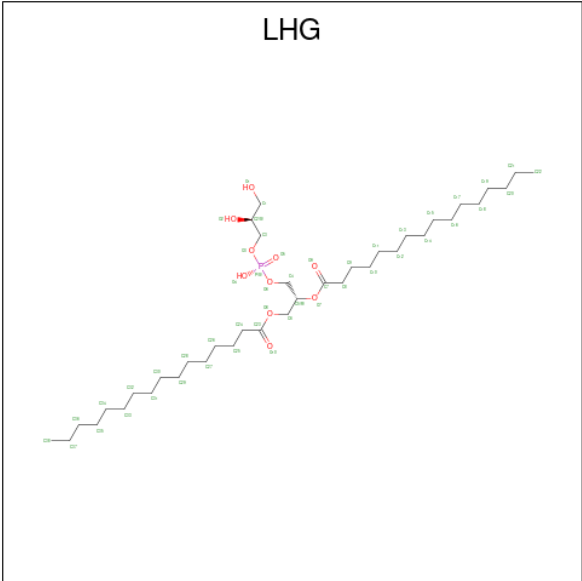
Mol	Chain	Residues	Atoms					AltConf
17	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
17	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
17	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			14	12	2	
18	B	1	Total	C	O	0
			16	14	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



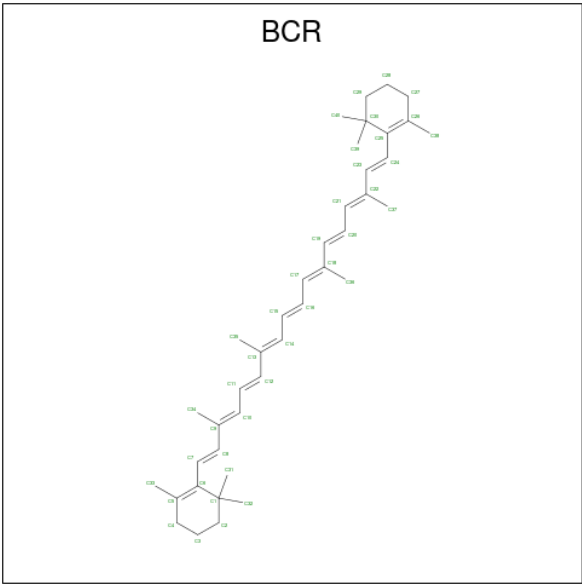
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			40	29	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			25	15	9	1	
19	B	1	Total	C	O	P	0
			38	27	10	1	
19	1	1	Total	C	O	P	0
			49	38	10	1	
19	6	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



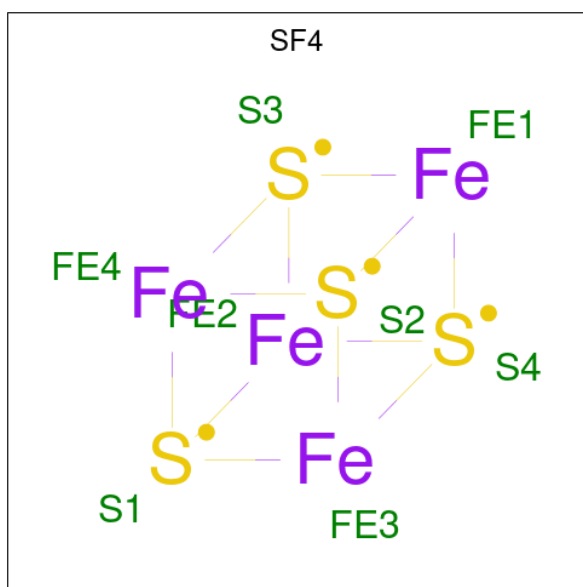
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	

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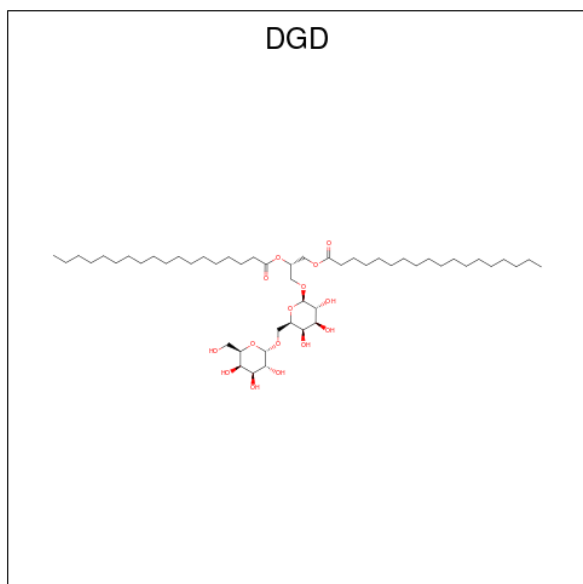
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 39 39	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	1	1	Total C 11 11	0
20	3	1	Total C 40 40	0
20	4	1	Total C 40 40	0
20	6	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



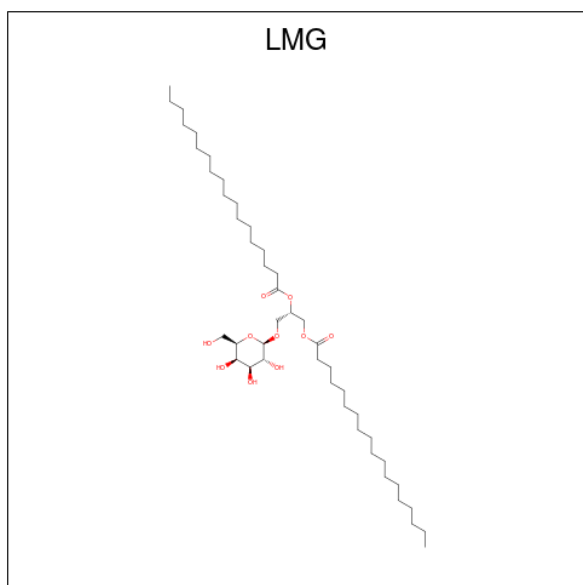
Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



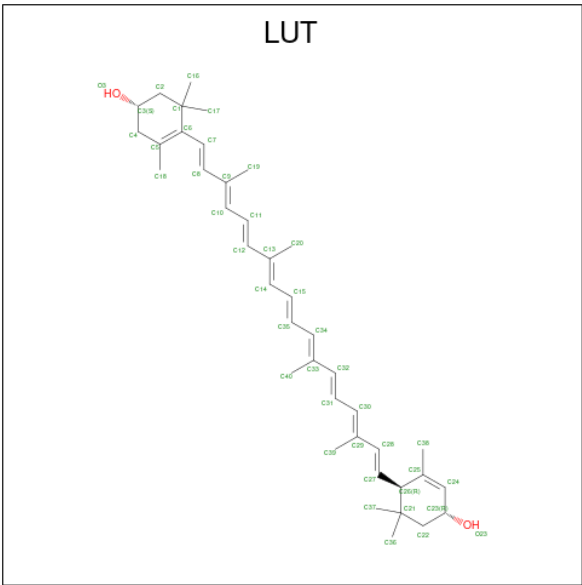
Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			52	37	15	
22	J	1	Total	C	O	0
			66	51	15	

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



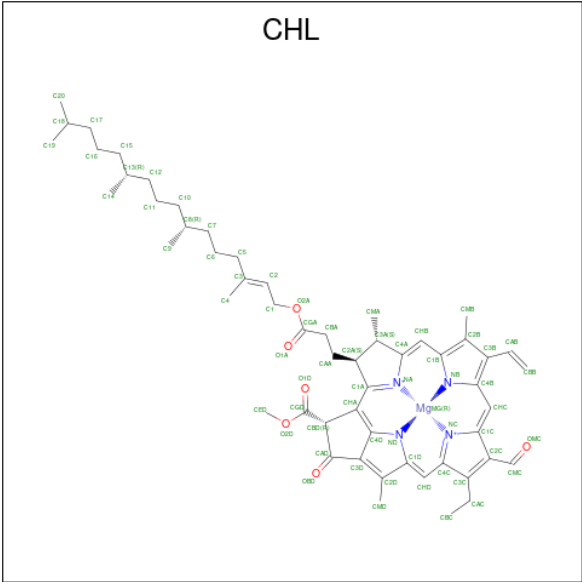
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total	C	O	0
			30	20	10	
23	4	1	Total	C	O	0
			18	10	8	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



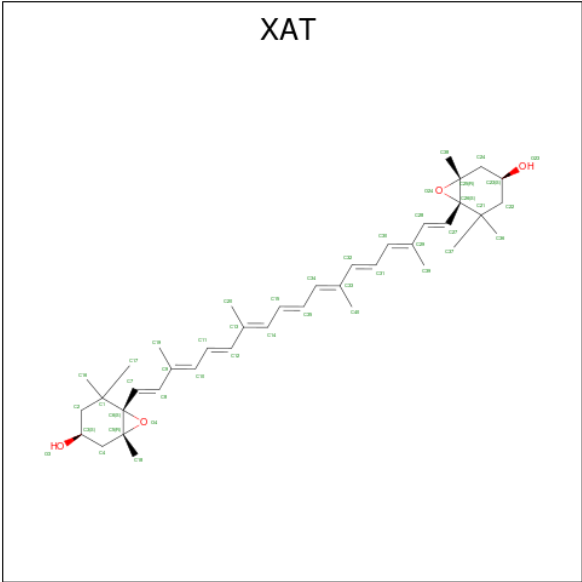
Mol	Chain	Residues	Atoms			AltConf
24	1	1	Total	C	O	0
			42	40	2	
24	1	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	4	1	Total	C	O	0
			42	40	2	
24	6	1	Total	C	O	0
			42	40	2	

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
25	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
25	6	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
25	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 26 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).

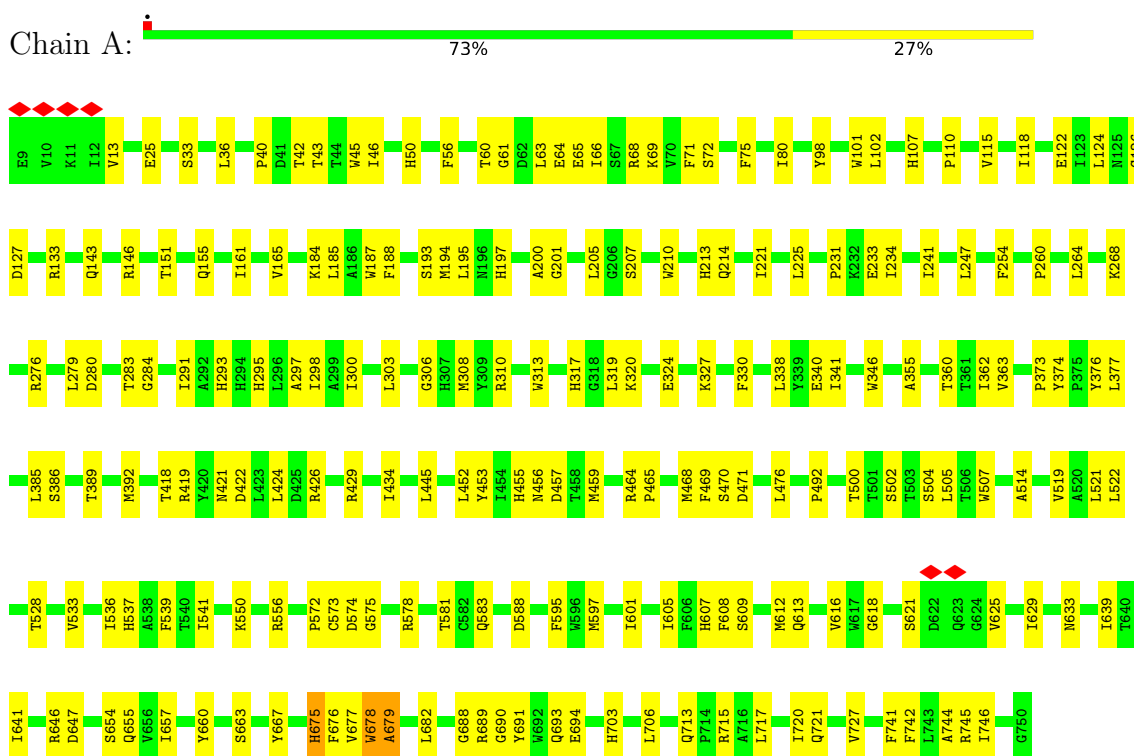


Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			44	40	4	
26	6	1	Total	C	O	0
			44	40	4	

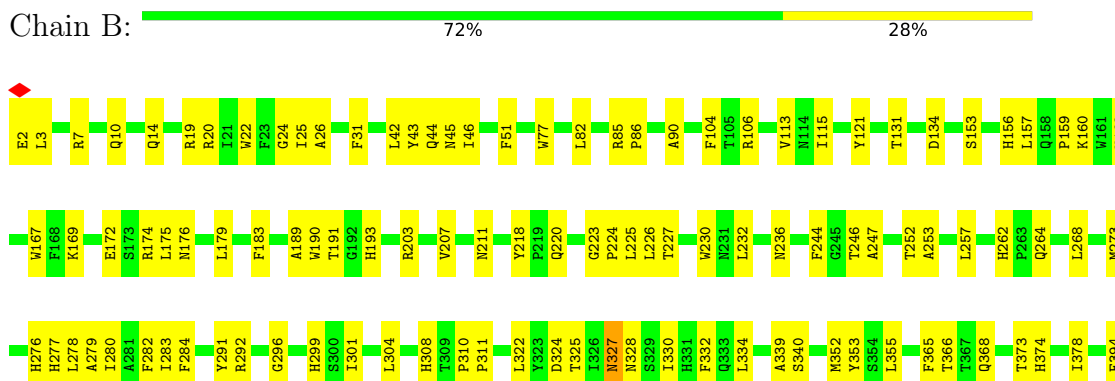
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

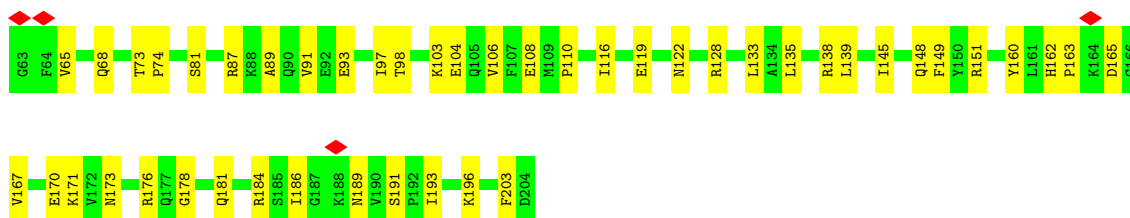




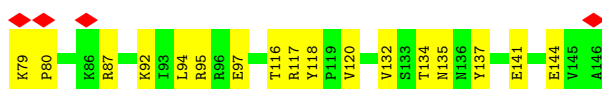
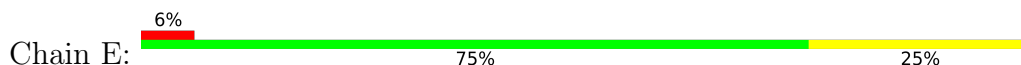
• Molecule 3: Photosystem I iron-sulfur center



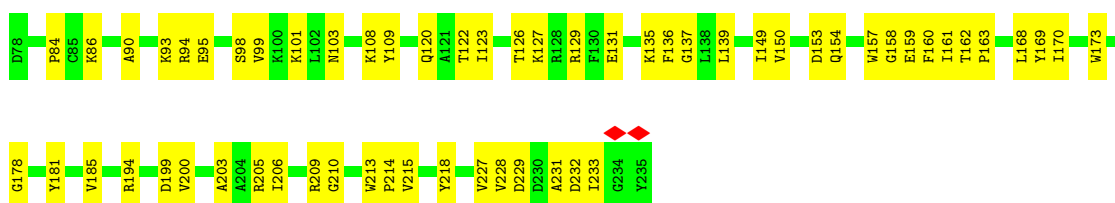
• Molecule 4: Photosystem I reaction center subunit D



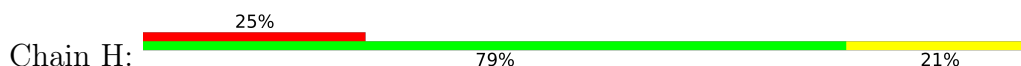
• Molecule 5: Photosystem I reaction center subunit E

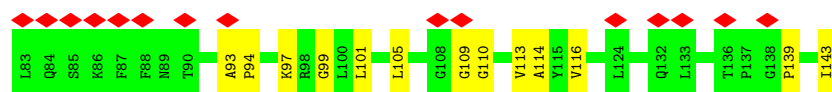


• Molecule 6: Photosystem I reaction center subunit F

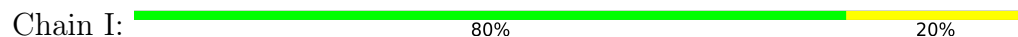


• Molecule 7: Photosystem I reaction center subunit H

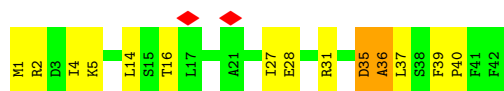




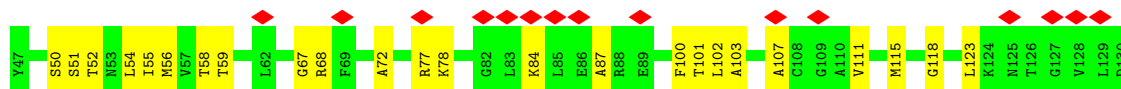
• Molecule 8: Photosystem I reaction center subunit VIII



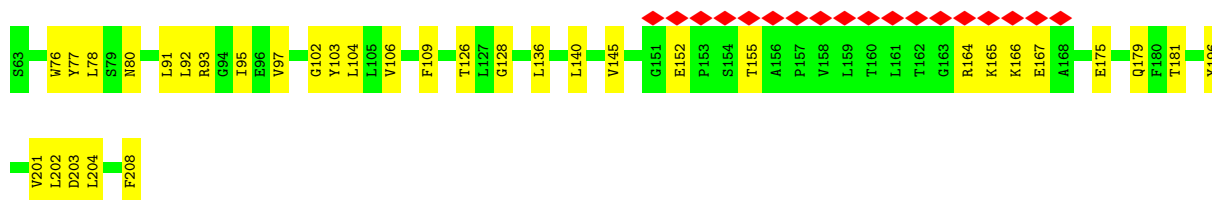
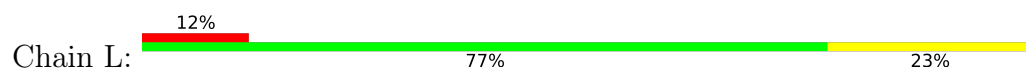
• Molecule 9: Photosystem I reaction center subunit IX



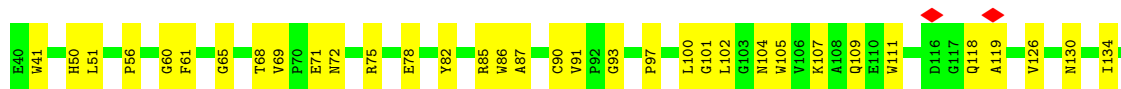
• Molecule 10: Photosystem I reaction center subunit K



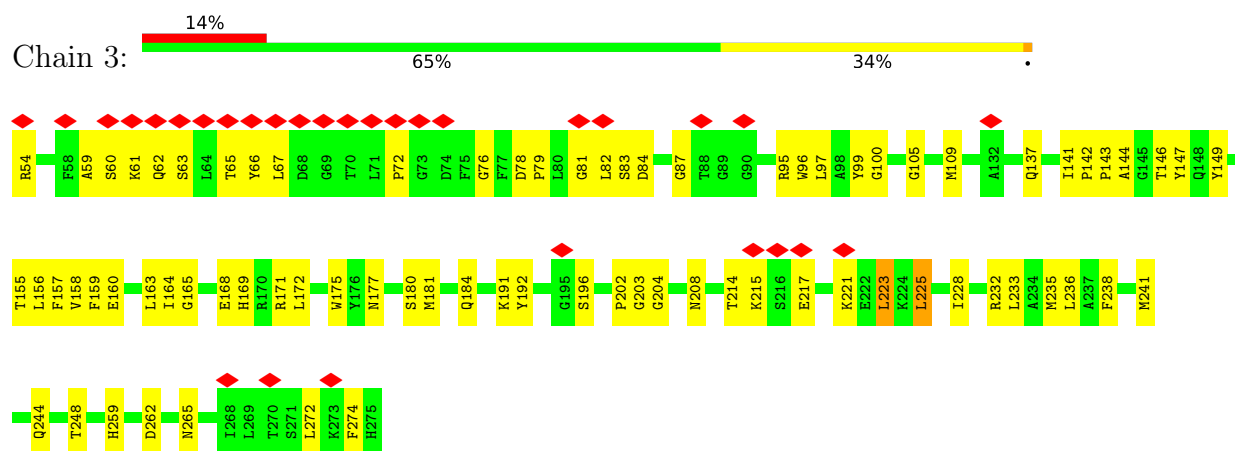
• Molecule 11: Photosystem I reaction center subunit L



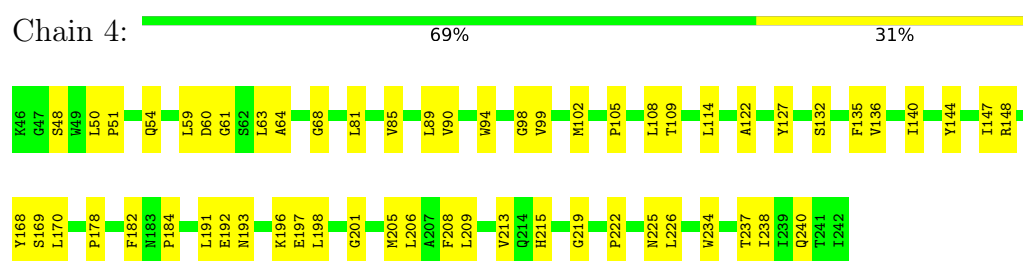
• Molecule 12: Chlorophyll a-b binding protein Lhca1



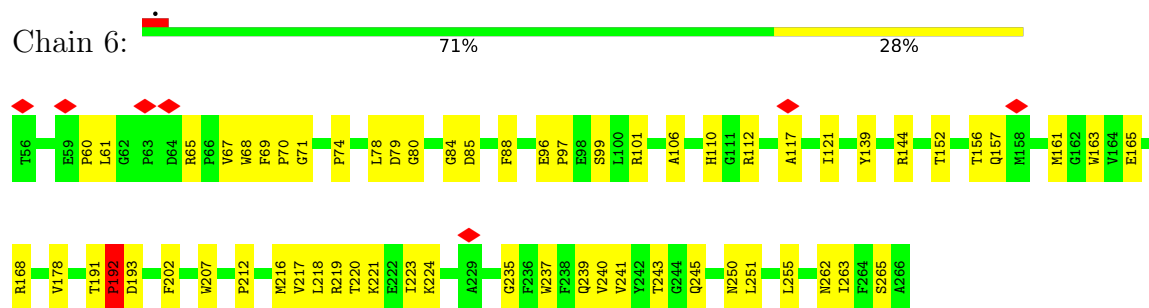
- Molecule 13: Chlorophyll a-b binding protein Lhca3



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



- Molecule 15: Chlorophyll a-b binding protein Lhca6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.561	Depositor
Minimum map value	-1.733	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	4/5993 (0.1%)	0.39	2/8178 (0.0%)
2	B	0.31	5/6052 (0.1%)	0.37	1/8267 (0.0%)
3	C	0.20	0/624	0.40	0/844
4	D	0.15	0/1141	0.43	0/1540
5	E	0.17	0/553	0.40	0/751
6	F	0.15	0/1214	0.40	0/1643
7	H	0.13	0/460	0.38	0/623
8	I	0.21	0/241	0.40	0/327
9	J	0.13	0/342	0.41	0/465
10	K	0.16	0/581	0.46	0/786
11	L	0.15	0/1122	0.34	0/1537
12	1	0.20	0/1535	0.45	0/2097
13	3	0.29	1/1727 (0.1%)	0.52	1/2353 (0.0%)
14	4	0.16	0/1577	0.38	0/2153
15	6	0.18	0/1723	0.47	3/2358 (0.1%)
All	All	0.24	10/24885 (0.0%)	0.41	7/33922 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	J	0	1
12	1	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	TRP	C-O	-11.08	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	TRP	CA-C	-9.13	1.41	1.52
1	A	679	ALA	CA-C	-7.51	1.43	1.52
1	A	678	TRP	C-O	-6.16	1.16	1.24
2	B	657	TRP	CA-CB	-6.14	1.43	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	225	LEU	N-CA-C	-11.77	98.42	111.14
2	B	657	TRP	CB-CA-C	-7.86	98.55	110.88
1	A	677	VAL	O-C-N	7.21	128.95	121.89
15	6	192	PRO	N-CA-C	7.00	126.89	112.47
15	6	192	PRO	CA-C-N	-6.70	108.73	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1	231	ILE	Peptide
9	J	35	ASP	Peptide

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	A	5798	0	5613	169	0
2	B	5840	0	5580	175	0
3	C	613	0	607	30	0
4	D	1112	0	1113	40	0
5	E	540	0	539	12	0
6	F	1188	0	1178	42	0
7	H	447	0	472	9	0
8	I	235	0	261	6	0
9	J	332	0	335	16	0
10	K	576	0	584	18	0
11	L	1090	0	1075	29	0
12	1	1484	0	1410	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	3	1672	0	1575	66	0
14	4	1529	0	1448	49	0
15	6	1655	0	1530	54	0
16	A	61	0	62	5	0
17	1	474	0	373	20	0
17	3	543	0	404	20	0
17	4	525	0	424	21	0
17	6	447	0	371	21	0
17	A	2028	0	1626	68	0
17	B	1921	0	1521	67	0
17	F	41	0	29	1	0
17	J	83	0	59	0	0
17	K	162	0	112	3	0
17	L	145	0	118	6	0
18	A	14	0	7	1	0
18	B	16	0	10	6	0
19	1	49	0	74	7	0
19	6	35	0	40	1	0
19	A	65	0	77	2	0
19	B	38	0	46	1	0
20	1	11	0	16	1	0
20	3	40	0	56	3	0
20	4	40	0	56	5	0
20	6	40	0	56	4	0
20	A	280	0	392	23	0
20	B	239	0	333	14	0
20	F	80	0	112	2	0
20	I	80	0	112	5	0
20	J	40	0	56	3	0
20	K	40	0	56	1	0
20	L	80	0	112	4	0
21	B	8	0	0	0	0
21	C	16	0	0	1	0
22	B	52	0	62	2	0
22	J	66	0	96	2	0
23	4	18	0	12	0	0
23	J	30	0	30	1	0
24	1	84	0	111	11	0
24	3	84	0	112	11	0
24	4	42	0	56	10	0
24	6	42	0	56	5	0
25	1	137	0	91	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	46	0	31	1	0
25	4	141	0	97	2	0
25	6	183	0	121	7	0
26	4	44	0	56	4	0
26	6	44	0	56	8	0
All	All	32765	0	31017	891	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 14.

The worst 5 of 891 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:LEU:HB2	18:B:844:PQN:H6	1.62	0.81
3:C:54:CYS:SG	3:C:55:GLU:N	2.61	0.72
6:F:215:VAL:O	6:F:218:TYR:HB3	1.89	0.72
12:1:90:CYS:CB	24:1:502:LUT:H392	2.21	0.70
15:6:67:VAL:HG22	15:6:69:PHE:H	1.57	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	740/742 (100%)	684 (92%)	56 (8%)	0	100	100
2	B	731/733 (100%)	680 (93%)	51 (7%)	0	100	100
3	C	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
4	D	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
5	E	66/68 (97%)	61 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	156/158 (99%)	148 (95%)	8 (5%)	0	100	100
7	H	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
8	I	28/30 (93%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	38 (95%)	1 (2%)	1 (2%)	4	29
10	K	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
11	L	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
12	1	191/193 (99%)	171 (90%)	18 (9%)	2 (1%)	12	45
13	3	220/222 (99%)	193 (88%)	27 (12%)	0	100	100
14	4	195/197 (99%)	183 (94%)	12 (6%)	0	100	100
15	6	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	12	45
All	All	3080/3110 (99%)	2834 (92%)	241 (8%)	5 (0%)	44	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	6	191	THR
15	6	192	PRO
9	J	36	ALA
12	1	101	GLY
12	1	221	PRO

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	A	588/600 (98%)	587 (100%)	1 (0%)	87	87
2	B	589/600 (98%)	588 (100%)	1 (0%)	87	87
3	C	71/71 (100%)	71 (100%)	0	100	100
4	D	118/119 (99%)	118 (100%)	0	100	100
5	E	58/59 (98%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	115/127 (91%)	115 (100%)	0	100	100
7	H	47/49 (96%)	47 (100%)	0	100	100
8	I	27/27 (100%)	27 (100%)	0	100	100
9	J	34/36 (94%)	34 (100%)	0	100	100
10	K	56/61 (92%)	55 (98%)	1 (2%)	51	67
11	L	110/115 (96%)	110 (100%)	0	100	100
12	1	147/155 (95%)	147 (100%)	0	100	100
13	3	159/176 (90%)	158 (99%)	1 (1%)	78	80
14	4	156/164 (95%)	156 (100%)	0	100	100
15	6	162/172 (94%)	162 (100%)	0	100	100
All	All	2437/2531 (96%)	2433 (100%)	4 (0%)	85	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	HIS
2	B	327	ASN
10	K	123	LEU
13	3	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	80	ASN
14	4	67	ASN
12	1	72	ASN
13	3	208	ASN
14	4	225	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

196 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
17	CLA	B	837	-	46,50,73	1.40	8 (17%)	53,85,113	1.42	4 (7%)
24	LUT	1	502	-	42,43,43	2.48	1 (2%)	51,60,60	1.66	7 (13%)
19	LHG	A	844	-	39,39,48	1.01	2 (5%)	42,45,54	1.25	4 (9%)
17	CLA	K	203	-	45,49,73	1.41	8 (17%)	54,84,113	1.51	6 (11%)
17	CLA	K	202	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	6 (10%)
21	SF4	B	802	-	0,12,12	-	-	-	-	-
17	CLA	B	803	-	43,49,73	1.36	8 (18%)	48,83,113	1.36	4 (8%)
20	BCR	B	847	-	41,41,41	0.74	0	56,56,56	2.22	17 (30%)
17	CLA	F	802	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	5 (9%)
17	CLA	B	842	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	6 (11%)
17	CLA	6	514	-	44,48,73	1.43	8 (18%)	51,82,113	1.54	6 (11%)
24	LUT	1	501	-	42,43,43	0.80	0	51,60,60	2.00	13 (25%)
17	CLA	4	307	-	64,68,73	1.21	9 (14%)	76,107,113	1.33	8 (10%)
20	BCR	A	851	-	41,41,41	0.69	0	56,56,56	2.17	18 (32%)
25	CHL	1	517	-	37,51,74	4.34	18 (48%)	30,86,114	2.50	9 (30%)
17	CLA	3	311	-	52,56,73	1.33	8 (15%)	61,92,113	1.38	5 (8%)
17	CLA	A	829	-	62,66,73	1.23	8 (12%)	73,104,113	1.32	6 (8%)
17	CLA	B	833	-	47,51,73	1.37	9 (19%)	55,86,113	1.38	4 (7%)
17	CLA	3	309	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	6 (9%)
17	CLA	3	314	-	44,48,73	1.41	8 (18%)	51,82,113	1.59	7 (13%)
20	BCR	4	301	-	41,41,41	0.73	0	56,56,56	1.85	12 (21%)
17	CLA	A	828	-	47,51,73	1.37	9 (19%)	53,85,113	1.44	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	827	-	44,48,73	1.41	9 (20%)	50,82,113	1.48	6 (12%)
17	CLA	4	308	-	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
17	CLA	3	315	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	6 (10%)
17	CLA	A	803	17	56,60,73	1.28	9 (16%)	65,97,113	1.40	6 (9%)
17	CLA	B	807	-	45,49,73	1.40	9 (20%)	54,84,113	1.47	9 (16%)
21	SF4	C	101	-	0,12,12	-	-	-	-	-
17	CLA	B	809	-	56,60,73	1.28	9 (16%)	65,97,113	1.35	5 (7%)
17	CLA	B	832	-	44,48,73	1.43	9 (20%)	51,82,113	1.57	6 (11%)
17	CLA	4	315	14	45,49,73	1.41	8 (17%)	54,84,113	1.52	6 (11%)
17	CLA	B	822	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	5 (9%)
17	CLA	A	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
17	CLA	B	805	-	41,46,73	1.44	9 (21%)	47,79,113	1.69	8 (17%)
17	CLA	6	504	-	42,47,73	1.58	7 (16%)	53,81,113	1.70	9 (16%)
17	CLA	3	312	13	64,68,73	1.21	7 (10%)	76,107,113	1.30	7 (9%)
17	CLA	B	830	-	43,47,73	1.54	10 (23%)	52,81,113	1.58	9 (17%)
17	CLA	B	828	-	45,49,73	1.40	9 (20%)	54,84,113	1.56	5 (9%)
20	BCR	F	803	-	41,41,41	0.76	1 (2%)	56,56,56	2.16	17 (30%)
20	BCR	A	847	-	41,41,41	0.75	1 (2%)	56,56,56	1.91	17 (30%)
17	CLA	A	808	1	45,49,73	1.41	9 (20%)	54,84,113	1.52	6 (11%)
17	CLA	A	835	1	44,50,73	1.43	9 (20%)	56,85,113	1.36	5 (8%)
17	CLA	A	815	-	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
17	CLA	A	853	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	7 (12%)
17	CLA	B	812	-	44,48,73	1.44	10 (22%)	51,82,113	1.58	6 (11%)
17	CLA	J	102	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
17	CLA	B	834	-	47,51,73	1.36	8 (17%)	55,86,113	1.46	5 (9%)
17	CLA	1	510	-	50,54,73	1.35	9 (18%)	59,90,113	1.35	4 (6%)
17	CLA	B	843	19	40,46,73	1.46	9 (22%)	52,80,113	1.48	5 (9%)
17	CLA	B	806	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	5 (9%)
17	CLA	A	811	-	45,49,73	1.39	9 (20%)	54,84,113	1.49	6 (11%)
17	CLA	L	304	-	49,53,73	1.37	8 (16%)	58,89,113	1.40	5 (8%)
17	CLA	A	824	-	60,64,73	1.23	9 (15%)	71,102,113	1.32	7 (9%)
17	CLA	B	813	-	58,62,73	1.36	10 (17%)	71,100,113	1.36	7 (9%)
17	CLA	A	817	-	42,47,73	1.44	9 (21%)	49,81,113	1.51	5 (10%)
17	CLA	A	827	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	6 (11%)
17	CLA	A	831	-	60,64,73	1.22	9 (15%)	71,102,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	B	845	-	41,41,41	0.74	1 (2%)	56,56,56	2.15	17 (30%)
17	CLA	3	308	-	46,50,73	1.41	8 (17%)	53,85,113	1.47	6 (11%)
20	BCR	B	849	-	41,41,41	0.77	2 (4%)	56,56,56	2.03	16 (28%)
17	CLA	A	807	-	46,50,73	1.40	9 (19%)	53,85,113	1.50	5 (9%)
17	CLA	1	509	-	54,58,73	1.54	8 (14%)	64,95,113	1.91	17 (26%)
18	PQN	A	842	-	15,15,34	1.49	2 (13%)	20,22,45	0.84	0
17	CLA	B	836	-	62,66,73	1.23	8 (12%)	69,103,113	1.28	4 (5%)
17	CLA	A	813	-	46,50,73	1.40	9 (19%)	53,85,113	1.40	5 (9%)
17	CLA	B	801	-	68,72,73	1.23	10 (14%)	83,112,113	1.32	8 (9%)
17	CLA	B	817	-	47,51,73	1.37	9 (19%)	55,86,113	1.42	4 (7%)
17	CLA	1	513	-	56,60,73	1.32	6 (10%)	65,97,113	1.34	7 (10%)
19	LHG	A	845	-	24,24,48	0.97	1 (4%)	26,29,54	1.29	3 (11%)
17	CLA	K	205	-	42,47,73	1.50	8 (19%)	48,81,113	1.45	5 (10%)
19	LHG	6	516	-	34,34,48	1.09	2 (5%)	37,40,54	1.16	3 (8%)
17	CLA	B	824	-	46,50,73	1.39	8 (17%)	53,85,113	1.45	4 (7%)
19	LHG	B	852	17	37,37,48	1.05	2 (5%)	40,43,54	1.18	3 (7%)
17	CLA	1	515	-	44,48,73	1.48	9 (20%)	51,82,113	1.52	6 (11%)
20	BCR	L	305	-	41,41,41	0.71	0	56,56,56	2.17	14 (25%)
17	CLA	B	840	-	45,49,73	1.38	9 (20%)	54,84,113	1.52	7 (12%)
20	BCR	3	303	-	41,41,41	0.74	1 (2%)	56,56,56	2.03	18 (32%)
17	CLA	3	304	-	41,46,73	1.65	9 (21%)	50,79,113	1.58	10 (20%)
17	CLA	A	825	-	45,49,73	1.38	9 (20%)	54,84,113	1.49	7 (12%)
20	BCR	A	848	-	41,41,41	0.75	1 (2%)	56,56,56	2.16	21 (37%)
26	XAT	4	303	-	41,47,47	0.87	2 (4%)	54,74,74	2.65	20 (37%)
17	CLA	A	836	-	55,59,73	1.30	9 (16%)	64,96,113	1.37	6 (9%)
17	CLA	3	305	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	7 (10%)
17	CLA	A	841	-	45,49,73	1.41	9 (20%)	54,84,113	1.51	6 (11%)
26	XAT	6	502	-	41,47,47	0.92	2 (4%)	54,74,74	2.78	22 (40%)
17	CLA	B	816	-	42,46,73	1.42	9 (21%)	49,79,113	1.42	5 (10%)
17	CLA	B	810	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
17	CLA	A	802	-	44,48,73	1.42	9 (20%)	51,82,113	1.49	5 (9%)
25	CHL	1	512	-	41,55,74	4.24	19 (46%)	35,91,114	2.34	11 (31%)
17	CLA	J	101	-	45,49,73	1.52	9 (20%)	54,84,113	1.42	5 (9%)
17	CLA	A	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.30	4 (5%)
17	CLA	4	312	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PQN	B	844	-	17,17,34	2.17	2 (11%)	22,24,45	1.34	4 (18%)
17	CLA	3	307	13	44,48,73	1.46	8 (18%)	51,82,113	1.49	6 (11%)
17	CLA	A	832	-	47,51,73	1.38	8 (17%)	55,86,113	1.38	5 (9%)
17	CLA	6	506	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	4 (4%)
20	BCR	I	102	-	41,41,41	0.68	0	56,56,56	2.17	17 (30%)
20	BCR	J	103	-	41,41,41	0.76	1 (2%)	56,56,56	2.11	17 (30%)
17	CLA	A	834	-	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
17	CLA	3	306	-	45,49,73	1.42	8 (17%)	54,84,113	1.54	6 (11%)
20	BCR	B	848	-	41,41,41	0.76	1 (2%)	56,56,56	2.05	16 (28%)
17	CLA	A	810	17	59,63,73	1.27	9 (15%)	70,101,113	1.34	5 (7%)
17	CLA	A	840	-	45,49,73	1.39	9 (20%)	54,84,113	1.51	5 (9%)
20	BCR	L	301	-	41,41,41	0.75	1 (2%)	56,56,56	2.04	18 (32%)
17	CLA	1	507	12	44,48,73	1.50	10 (22%)	55,83,113	1.57	8 (14%)
17	CLA	B	835	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	6 (10%)
17	CLA	4	306	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
17	CLA	B	823	-	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
17	CLA	A	821	-	46,50,73	1.38	9 (19%)	53,85,113	1.44	5 (9%)
17	CLA	1	505	-	50,54,73	1.32	8 (16%)	59,90,113	1.29	8 (13%)
24	LUT	4	302	-	42,43,43	0.72	0	51,60,60	2.02	16 (31%)
17	CLA	6	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.25	5 (6%)
20	BCR	6	503	-	41,41,41	0.70	0	56,56,56	3.70	30 (53%)
17	CLA	B	820	-	54,58,73	1.31	9 (16%)	64,95,113	1.43	5 (7%)
17	CLA	B	818	-	59,63,73	1.24	9 (15%)	70,101,113	1.32	4 (5%)
17	CLA	4	317	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	7 (10%)
17	CLA	L	302	-	44,48,73	1.52	10 (22%)	55,83,113	1.62	7 (12%)
17	CLA	3	316	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	4 (6%)
16	CL0	A	801	-	55,69,73	2.42	6 (10%)	58,107,113	2.28	15 (25%)
17	CLA	B	811	2	55,59,73	1.32	9 (16%)	64,96,113	1.40	7 (10%)
20	BCR	A	854	-	41,41,41	0.69	0	56,56,56	2.26	20 (35%)
20	BCR	A	850	-	41,41,41	0.81	2 (4%)	56,56,56	2.32	20 (35%)
17	CLA	4	309	-	54,58,73	1.30	9 (16%)	64,95,113	1.30	4 (6%)
17	CLA	6	507	-	55,59,73	1.31	8 (14%)	64,96,113	1.39	5 (7%)
17	CLA	A	823	-	46,50,73	1.47	10 (21%)	56,85,113	1.51	8 (14%)
17	CLA	6	509	-	54,58,73	1.32	9 (16%)	64,95,113	1.38	6 (9%)
24	LUT	3	302	-	42,43,43	0.71	0	51,60,60	2.02	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LUT	3	301	-	42,43,43	0.75	1 (2%)	51,60,60	2.11	11 (21%)
17	CLA	1	506	-	59,63,73	1.25	8 (13%)	70,101,113	1.26	6 (8%)
17	CLA	B	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
17	CLA	A	820	-	45,49,73	1.39	9 (20%)	54,84,113	1.50	6 (11%)
17	CLA	4	311	-	50,54,73	1.36	8 (16%)	59,90,113	1.35	4 (6%)
17	CLA	4	305	-	54,58,73	1.33	9 (16%)	64,95,113	1.36	6 (9%)
20	BCR	A	849	-	41,41,41	0.73	0	56,56,56	2.07	15 (26%)
17	CLA	A	814	-	46,50,73	1.39	9 (19%)	53,85,113	1.45	4 (7%)
17	CLA	A	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
19	LHG	1	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	4 (7%)
17	CLA	A	837	-	59,63,73	1.23	9 (15%)	70,101,113	1.41	8 (11%)
25	CHL	4	314	-	45,59,74	3.83	19 (42%)	40,96,114	2.49	15 (37%)
20	BCR	B	850	-	40,40,41	0.75	0	54,54,56	2.08	14 (25%)
17	CLA	A	819	-	49,53,73	1.36	9 (18%)	58,89,113	1.47	5 (8%)
17	CLA	L	303	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	6 (7%)
17	CLA	A	833	-	45,49,73	1.39	8 (17%)	54,84,113	1.47	6 (11%)
17	CLA	A	818	-	43,47,73	1.71	7 (16%)	49,81,113	1.99	11 (22%)
20	BCR	1	503	-	11,11,41	0.68	0	15,16,56	1.99	5 (33%)
25	CHL	3	313	-	38,54,74	4.11	17 (44%)	31,89,114	1.95	9 (29%)
17	CLA	B	841	-	45,49,73	1.38	9 (20%)	54,84,113	1.51	5 (9%)
24	LUT	6	501	-	42,43,43	0.74	0	51,60,60	2.04	15 (29%)
17	CLA	B	825	-	46,50,73	1.39	9 (19%)	53,85,113	1.42	4 (7%)
17	CLA	B	808	-	58,62,73	1.26	7 (12%)	68,99,113	1.35	7 (10%)
17	CLA	6	505	-	56,60,73	1.30	9 (16%)	65,97,113	1.39	4 (6%)
25	CHL	4	313	-	41,55,74	4.21	19 (46%)	35,91,114	2.24	10 (28%)
17	CLA	B	819	-	45,49,73	1.39	9 (20%)	54,84,113	1.47	6 (11%)
17	CLA	A	852	-	61,65,73	1.24	8 (13%)	72,103,113	1.33	6 (8%)
23	LMG	4	318	-	18,18,55	1.57	2 (11%)	22,23,63	1.58	2 (9%)
17	CLA	A	822	-	45,49,73	1.39	9 (20%)	54,84,113	1.54	5 (9%)
17	CLA	6	511	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	5 (7%)
17	CLA	A	805	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
17	CLA	6	508	-	44,48,73	1.42	9 (20%)	53,83,113	1.50	4 (7%)
17	CLA	1	504	-	45,49,73	1.44	9 (20%)	52,84,113	1.61	7 (13%)
17	CLA	A	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	7 (10%)
17	CLA	B	829	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	838	-	56,60,73	1.27	9 (16%)	65,97,113	1.42	7 (10%)
17	CLA	B	838	-	44,48,73	1.41	9 (20%)	51,82,113	1.52	6 (11%)
17	CLA	B	804	-	42,50,73	1.85	8 (19%)	50,83,113	2.14	8 (16%)
20	BCR	K	204	-	41,41,41	0.66	0	56,56,56	2.10	19 (33%)
17	CLA	B	831	-	60,64,73	1.26	8 (13%)	71,102,113	1.35	5 (7%)
17	CLA	A	843	-	53,57,73	1.41	9 (16%)	65,94,113	1.44	7 (10%)
17	CLA	A	806	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	7 (12%)
22	DGD	J	104	-	67,67,67	0.85	2 (2%)	81,81,81	0.86	3 (3%)
17	CLA	3	310	-	45,49,73	1.42	7 (15%)	54,84,113	1.44	4 (7%)
17	CLA	B	821	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
17	CLA	1	508	-	69,73,73	1.17	9 (13%)	82,113,113	1.21	4 (4%)
17	CLA	A	812	-	41,47,73	1.44	9 (21%)	50,80,113	1.54	7 (14%)
17	CLA	B	815	-	47,51,73	1.37	8 (17%)	55,86,113	1.33	4 (7%)
17	CLA	A	830	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	6 (9%)
17	CLA	B	839	-	45,49,73	1.40	8 (17%)	54,84,113	1.54	6 (11%)
25	CHL	6	512	-	41,55,74	4.25	19 (46%)	35,91,114	2.31	10 (28%)
21	SF4	C	102	-	0,12,12	-	-	-	-	-
22	DGD	B	851	-	53,53,67	0.93	2 (3%)	67,67,81	1.07	3 (4%)
25	CHL	6	513	-	42,56,74	4.12	19 (45%)	36,92,114	2.34	11 (30%)
17	CLA	4	304	-	43,47,73	1.52	8 (18%)	52,81,113	1.66	10 (19%)
17	CLA	4	310	-	46,50,73	1.41	8 (17%)	53,85,113	1.45	5 (9%)
20	BCR	B	846	-	41,41,41	0.74	0	56,56,56	1.95	14 (25%)
17	CLA	K	201	-	41,45,73	1.47	10 (24%)	50,78,113	1.45	4 (8%)
17	CLA	A	826	-	68,72,73	1.24	10 (14%)	83,112,113	1.34	8 (9%)
20	BCR	F	801	-	41,41,41	0.72	0	56,56,56	2.25	20 (35%)
20	BCR	I	101	-	41,41,41	0.77	1 (2%)	56,56,56	2.30	19 (33%)
25	CHL	4	316	-	37,51,74	4.23	18 (48%)	30,86,114	2.34	11 (36%)
20	BCR	A	846	-	41,41,41	0.78	2 (4%)	56,56,56	2.20	16 (28%)
25	CHL	6	515	-	35,49,74	4.34	17 (48%)	30,83,114	2.28	11 (36%)
25	CHL	1	514	-	41,55,74	4.22	18 (43%)	35,91,114	2.18	11 (31%)
25	CHL	6	517	15	41,55,74	4.13	19 (46%)	35,91,114	2.32	13 (37%)
17	CLA	B	814	-	47,51,73	1.37	9 (19%)	55,86,113	1.43	4 (7%)
17	CLA	1	511	-	42,47,73	1.46	8 (19%)	50,80,113	1.51	6 (12%)
23	LMG	J	105	-	30,30,55	1.21	2 (6%)	38,38,63	1.21	3 (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
17	CLA	B	837	-	1/1/10/20	4/12/88/115	-
24	LUT	1	502	-	1/1/12/27	8/29/67/67	0/2/2/2
19	LHG	A	844	-	-	8/44/44/53	-
17	CLA	K	203	-	1/1/10/20	4/10/86/115	-
17	CLA	K	202	-	1/1/11/20	10/15/91/115	-
21	SF4	B	802	-	-	-	0/6/5/5
17	CLA	B	803	-	1/1/10/20	2/12/88/115	-
20	BCR	B	847	-	-	6/29/63/63	0/2/2/2
17	CLA	F	802	-	1/1/10/20	4/10/86/115	-
17	CLA	B	842	-	1/1/10/20	2/10/86/115	-
17	CLA	6	514	-	1/1/9/20	2/10/82/115	-
24	LUT	1	501	-	-	2/29/67/67	0/2/2/2
17	CLA	4	307	-	1/1/14/20	9/33/109/115	-
25	CHL	1	517	-	3/3/15/26	4/12/110/137	-
20	BCR	A	851	-	-	4/29/63/63	0/2/2/2
17	CLA	3	311	-	1/1/11/20	10/19/95/115	-
17	CLA	A	829	-	1/1/13/20	13/31/107/115	-
17	CLA	B	833	-	1/1/10/20	3/13/89/115	-
17	CLA	3	309	-	1/1/12/20	5/21/97/115	-
17	CLA	3	314	-	1/1/9/20	2/10/82/115	-
20	BCR	4	301	-	-	6/29/63/63	0/2/2/2
17	CLA	A	828	-	1/1/10/20	3/12/88/115	-
17	CLA	B	827	-	1/1/9/20	0/10/82/115	-
17	CLA	4	308	-	1/1/10/20	4/10/86/115	-
17	CLA	3	315	-	-	8/15/91/115	-
17	CLA	A	803	17	1/1/12/20	4/24/100/115	-
17	CLA	B	807	-	1/1/10/20	2/10/86/115	-
21	SF4	C	101	-	-	-	0/6/5/5
17	CLA	B	809	-	1/1/12/20	3/24/100/115	-
17	CLA	B	832	-	1/1/9/20	3/10/82/115	-
17	CLA	4	315	14	1/1/10/20	2/10/86/115	-
17	CLA	B	822	-	1/1/10/20	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	804	-	1/1/15/20	17/39/115/115	-
17	CLA	B	805	-	1/1/8/20	0/4/78/115	-
17	CLA	6	504	-	1/1/10/20	4/8/84/115	-
17	CLA	3	312	13	1/1/14/20	11/33/109/115	-
17	CLA	B	830	-	1/1/9/20	2/8/80/115	-
17	CLA	B	828	-	1/1/10/20	6/10/86/115	-
20	BCR	F	803	-	-	2/29/63/63	0/2/2/2
20	BCR	A	847	-	-	0/29/63/63	0/2/2/2
17	CLA	A	808	1	1/1/10/20	6/10/86/115	-
17	CLA	A	835	1	1/1/10/20	4/9/85/115	-
17	CLA	A	815	-	1/1/11/20	8/15/91/115	-
17	CLA	A	853	-	1/1/11/20	6/15/91/115	-
17	CLA	B	812	-	1/1/9/20	4/10/82/115	-
17	CLA	J	102	-	1/1/10/20	6/12/88/115	-
17	CLA	B	834	-	1/1/10/20	4/13/89/115	-
17	CLA	1	510	-	1/1/11/20	9/17/93/115	-
17	CLA	B	843	19	1/1/9/20	0/4/80/115	-
17	CLA	B	806	-	1/1/10/20	0/10/86/115	-
17	CLA	A	811	-	1/1/10/20	4/10/86/115	-
17	CLA	L	304	-	1/1/11/20	6/15/91/115	-
17	CLA	A	824	-	1/1/13/20	8/29/105/115	-
17	CLA	B	813	-	1/1/13/20	10/25/101/115	-
17	CLA	A	817	-	1/1/9/20	0/4/82/115	-
17	CLA	A	827	-	1/1/10/20	1/10/86/115	-
17	CLA	A	831	-	1/1/13/20	5/29/105/115	-
20	BCR	B	845	-	-	7/29/63/63	0/2/2/2
17	CLA	3	308	-	1/1/10/20	4/12/88/115	-
20	BCR	B	849	-	-	0/29/63/63	0/2/2/2
17	CLA	A	807	-	1/1/10/20	6/12/88/115	-
17	CLA	1	509	-	1/1/12/20	6/21/97/115	-
18	PQN	A	842	-	-	-	0/2/2/2
17	CLA	B	836	-	1/1/12/20	11/31/103/115	-
17	CLA	A	813	-	1/1/10/20	2/12/88/115	-
17	CLA	B	801	-	1/1/15/20	10/37/113/115	-
17	CLA	B	817	-	1/1/10/20	7/13/89/115	-
17	CLA	1	513	-	1/1/12/20	5/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	A	845	-	-	8/28/28/53	-
17	CLA	K	205	-	1/1/9/20	2/8/80/115	-
19	LHG	6	516	-	-	5/39/39/53	-
17	CLA	B	824	-	1/1/10/20	5/12/88/115	-
19	LHG	B	852	17	-	13/42/42/53	-
17	CLA	1	515	-	1/1/9/20	2/10/82/115	-
20	BCR	L	305	-	-	2/29/63/63	0/2/2/2
17	CLA	B	840	-	1/1/10/20	4/10/86/115	-
20	BCR	3	303	-	-	6/29/63/63	0/2/2/2
17	CLA	3	304	-	1/1/10/20	1/7/84/115	-
17	CLA	A	825	-	1/1/10/20	0/10/86/115	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
26	XAT	4	303	-	-	2/31/93/93	0/4/4/4
17	CLA	A	836	-	1/1/12/20	4/23/99/115	-
17	CLA	3	305	-	1/1/12/20	8/24/100/115	-
17	CLA	A	841	-	1/1/10/20	4/10/86/115	-
26	XAT	6	502	-	-	6/31/93/93	0/4/4/4
17	CLA	B	816	-	1/1/8/20	1/6/78/115	-
17	CLA	B	810	-	1/1/15/20	14/39/115/115	-
17	CLA	A	802	-	1/1/9/20	4/10/82/115	-
25	CHL	1	512	-	3/3/16/26	3/17/115/137	-
17	CLA	J	101	-	1/1/10/20	6/10/86/115	-
17	CLA	A	816	-	1/1/14/20	11/33/109/115	-
17	CLA	4	312	-	1/1/10/20	4/10/86/115	-
18	PQN	B	844	-	-	0/3/23/43	0/2/2/2
17	CLA	3	307	13	-	2/10/82/115	-
17	CLA	A	832	-	1/1/10/20	7/13/89/115	-
17	CLA	6	506	-	1/1/15/20	16/39/115/115	-
20	BCR	I	102	-	-	8/29/63/63	0/2/2/2
20	BCR	J	103	-	-	2/29/63/63	0/2/2/2
17	CLA	A	834	-	1/1/11/20	4/15/91/115	-
17	CLA	3	306	-	1/1/10/20	5/10/86/115	-
20	BCR	B	848	-	-	0/29/63/63	0/2/2/2
17	CLA	A	810	17	1/1/13/20	12/27/103/115	-
17	CLA	A	840	-	1/1/10/20	0/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	L	301	-	-	2/29/63/63	0/2/2/2
17	CLA	1	507	12	1/1/10/20	2/8/84/115	-
17	CLA	B	835	-	1/1/11/20	7/15/91/115	-
17	CLA	4	306	-	1/1/15/20	15/39/115/115	-
17	CLA	B	823	-	1/1/10/20	4/10/86/115	-
17	CLA	A	821	-	1/1/10/20	4/12/88/115	-
17	CLA	1	505	-	-	3/17/93/115	-
24	LUT	4	302	-	-	2/29/67/67	0/2/2/2
17	CLA	6	510	-	1/1/14/20	10/33/109/115	-
20	BCR	6	503	-	-	5/29/63/63	0/2/2/2
17	CLA	B	820	-	1/1/12/20	11/21/97/115	-
17	CLA	B	818	-	1/1/13/20	6/27/103/115	-
17	CLA	4	317	-	1/1/12/20	7/21/97/115	-
17	CLA	L	302	-	1/1/10/20	2/8/84/115	-
17	CLA	3	316	-	1/1/11/20	9/17/93/115	-
16	CL0	A	801	-	3/3/18/25	6/33/125/135	-
17	CLA	B	811	2	1/1/12/20	6/23/99/115	-
20	BCR	A	854	-	-	4/29/63/63	0/2/2/2
20	BCR	A	850	-	-	6/29/63/63	0/2/2/2
17	CLA	4	309	-	1/1/12/20	7/21/97/115	-
17	CLA	6	507	-	1/1/12/20	8/23/99/115	-
17	CLA	A	823	-	1/1/10/20	2/11/87/115	-
17	CLA	6	509	-	1/1/12/20	7/21/97/115	-
24	LUT	3	302	-	-	5/29/67/67	0/2/2/2
24	LUT	3	301	-	-	6/29/67/67	0/2/2/2
17	CLA	1	506	-	1/1/13/20	12/27/103/115	-
17	CLA	B	826	-	1/1/15/20	11/39/115/115	-
17	CLA	A	820	-	1/1/10/20	3/10/86/115	-
17	CLA	4	311	-	1/1/11/20	6/17/93/115	-
17	CLA	4	305	-	1/1/12/20	8/21/97/115	-
20	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	CLA	A	814	-	1/1/10/20	5/12/88/115	-
17	CLA	A	839	-	1/1/15/20	14/39/115/115	-
19	LHG	1	516	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	837	-	1/1/13/20	9/27/103/115	-
25	CHL	4	314	-	3/3/17/26	3/21/119/137	-
20	BCR	B	850	-	-	2/27/61/63	0/2/2/2
17	CLA	A	819	-	1/1/11/20	5/15/91/115	-
17	CLA	L	303	-	1/1/14/20	9/33/109/115	-
17	CLA	A	833	-	1/1/10/20	4/10/86/115	-
17	CLA	A	818	-	1/1/9/20	2/8/80/115	-
20	BCR	1	503	-	-	1/1/19/63	0/1/1/2
25	CHL	3	313	-	3/3/15/26	11/17/111/137	-
17	CLA	B	841	-	1/1/10/20	2/10/86/115	-
24	LUT	6	501	-	-	3/29/67/67	0/2/2/2
17	CLA	B	825	-	1/1/10/20	2/12/88/115	-
17	CLA	B	808	-	1/1/12/20	6/25/101/115	-
25	CHL	4	313	-	3/3/16/26	7/17/115/137	-
17	CLA	6	505	-	-	11/24/100/115	-
17	CLA	B	819	-	1/1/10/20	4/10/86/115	-
17	CLA	A	852	-	1/1/13/20	10/30/106/115	-
23	LMG	4	318	-	-	11/11/28/70	0/1/1/1
17	CLA	A	822	-	1/1/10/20	2/10/86/115	-
17	CLA	6	511	-	1/1/12/20	9/21/97/115	-
17	CLA	A	805	-	1/1/11/20	5/17/93/115	-
17	CLA	6	508	-	1/1/10/20	2/8/84/115	-
17	CLA	1	504	-	1/1/10/20	6/10/86/115	-
17	CLA	A	809	-	1/1/12/20	6/21/97/115	-
17	CLA	B	829	-	1/1/12/20	7/21/97/115	-
17	CLA	A	838	-	1/1/12/20	5/24/100/115	-
17	CLA	B	838	-	1/1/9/20	3/10/82/115	-
17	CLA	B	804	-	1/1/9/20	3/11/84/115	-
20	BCR	K	204	-	-	9/29/63/63	0/2/2/2
17	CLA	B	831	-	1/1/13/20	4/29/105/115	-
17	CLA	A	843	-	1/1/12/20	7/19/95/115	-
17	CLA	A	806	-	1/1/10/20	2/10/86/115	-
22	DGD	J	104	-	-	14/55/95/95	0/2/2/2
17	CLA	3	310	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	821	-	1/1/13/20	7/27/103/115	-
17	CLA	1	508	-	1/1/15/20	16/39/115/115	-
17	CLA	A	812	-	1/1/8/20	3/7/79/115	-
17	CLA	B	815	-	1/1/10/20	5/13/89/115	-
17	CLA	A	830	-	1/1/12/20	7/21/97/115	-
17	CLA	B	839	-	1/1/10/20	2/10/86/115	-
25	CHL	6	512	-	3/3/16/26	5/17/115/137	-
25	CHL	6	513	-	3/3/16/26	4/18/116/137	-
22	DGD	B	851	-	-	10/41/81/95	0/2/2/2
21	SF4	C	102	-	-	-	0/6/5/5
17	CLA	4	304	-	1/1/9/20	2/8/80/115	-
17	CLA	4	310	-	1/1/10/20	6/12/88/115	-
20	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	CLA	K	201	-	1/1/8/20	2/4/76/115	-
17	CLA	A	826	-	1/1/15/20	16/37/113/115	-
20	BCR	F	801	-	-	2/29/63/63	0/2/2/2
20	BCR	I	101	-	-	5/29/63/63	0/2/2/2
25	CHL	4	316	-	3/3/15/26	4/12/110/137	-
20	BCR	A	846	-	-	5/29/63/63	0/2/2/2
25	CHL	6	515	-	3/3/14/26	3/10/104/137	-
25	CHL	1	514	-	3/3/16/26	7/17/115/137	-
25	CHL	6	517	15	3/3/16/26	2/17/115/137	-
17	CLA	B	814	-	1/1/10/20	2/13/89/115	-
17	CLA	1	511	-	1/1/8/20	4/10/79/115	-
23	LMG	J	105	-	-	5/25/45/70	0/1/1/1

The worst 5 of 1433 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	502	LUT	C24-C25	15.30	1.51	1.33
25	1	512	CHL	C2C-C3C	11.22	1.47	1.36
25	6	512	CHL	C2C-C3C	11.20	1.47	1.36
25	1	514	CHL	C2C-C3C	10.96	1.47	1.36
25	1	517	CHL	C2C-C3C	10.90	1.46	1.36

The worst 5 of 1526 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	503	BCR	C40-C30-C25	-12.78	90.20	110.24
16	A	801	CL0	C1B-CHB-C4A	10.77	130.76	120.23
17	B	804	CLA	C4A-NA-C1A	9.90	111.20	106.68
25	1	517	CHL	O2D-CGD-CBD	9.73	121.63	110.95
20	6	503	BCR	C20-C21-C22	-9.61	113.80	127.28

5 of 170 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	A	801	CL0	ND
16	A	801	CL0	NA
16	A	801	CL0	NC
17	A	802	CLA	ND
17	A	803	CLA	ND

5 of 1039 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	801	CL0	CHA-CBD-CGD-O2D
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CBD-CGD-O2D-CED
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	807	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

158 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	502	LUT	6	0
19	A	844	LHG	1	0
17	K	203	CLA	1	0
17	K	202	CLA	1	0
17	B	803	CLA	2	0
20	B	847	BCR	1	0
17	F	802	CLA	1	0
17	B	842	CLA	1	0
17	6	514	CLA	2	0
24	1	501	LUT	5	0
17	4	307	CLA	4	0
20	A	851	BCR	5	0
25	1	517	CHL	2	0
17	3	311	CLA	1	0
17	A	829	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	833	CLA	1	0
17	3	314	CLA	5	0
20	4	301	BCR	5	0
17	A	828	CLA	2	0
17	B	827	CLA	1	0
17	4	308	CLA	2	0
17	3	315	CLA	4	0
17	A	803	CLA	3	0
17	B	807	CLA	4	0
21	C	101	SF4	1	0
17	B	809	CLA	1	0
17	B	832	CLA	2	0
17	A	804	CLA	3	0
17	B	805	CLA	2	0
17	6	504	CLA	1	0
17	3	312	CLA	2	0
17	B	828	CLA	1	0
20	F	803	BCR	1	0
20	A	847	BCR	2	0
17	A	808	CLA	1	0
17	A	815	CLA	1	0
17	A	853	CLA	2	0
17	B	834	CLA	2	0
17	1	510	CLA	2	0
17	B	843	CLA	1	0
17	B	806	CLA	1	0
17	A	811	CLA	1	0
17	L	304	CLA	3	0
17	A	824	CLA	1	0
17	B	813	CLA	2	0
17	A	817	CLA	2	0
17	A	827	CLA	2	0
20	B	845	BCR	1	0
20	B	849	BCR	4	0
17	A	807	CLA	1	0
17	1	509	CLA	3	0
18	A	842	PQN	1	0
17	A	813	CLA	2	0
17	B	801	CLA	4	0
17	1	513	CLA	1	0
19	A	845	LHG	1	0
17	K	205	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	516	LHG	1	0
19	B	852	LHG	1	0
17	1	515	CLA	3	0
20	L	305	BCR	3	0
17	B	840	CLA	3	0
20	3	303	BCR	3	0
17	3	304	CLA	3	0
17	A	825	CLA	2	0
20	A	848	BCR	2	0
26	4	303	XAT	4	0
17	A	836	CLA	2	0
17	3	305	CLA	1	0
26	6	502	XAT	8	0
17	B	816	CLA	2	0
17	B	810	CLA	3	0
25	1	512	CHL	1	0
17	A	816	CLA	1	0
17	4	312	CLA	2	0
18	B	844	PQN	6	0
17	3	307	CLA	3	0
17	6	506	CLA	6	0
20	I	102	BCR	4	0
20	J	103	BCR	3	0
17	A	834	CLA	1	0
20	B	848	BCR	4	0
17	A	810	CLA	5	0
20	L	301	BCR	1	0
17	1	507	CLA	1	0
17	B	835	CLA	4	0
17	4	306	CLA	7	0
17	B	823	CLA	1	0
17	A	821	CLA	2	0
17	1	505	CLA	1	0
24	4	302	LUT	10	0
17	6	510	CLA	4	0
20	6	503	BCR	4	0
17	B	820	CLA	2	0
17	B	818	CLA	4	0
17	4	317	CLA	1	0
17	L	302	CLA	2	0
17	3	316	CLA	1	0
16	A	801	CL0	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	854	BCR	4	0
20	A	850	BCR	2	0
17	4	309	CLA	1	0
17	6	509	CLA	2	0
24	3	302	LUT	6	0
24	3	301	LUT	5	0
17	1	506	CLA	5	0
17	B	826	CLA	3	0
17	4	305	CLA	2	0
20	A	849	BCR	4	0
17	A	814	CLA	1	0
17	A	839	CLA	4	0
19	1	516	LHG	7	0
17	A	837	CLA	3	0
20	B	850	BCR	4	0
17	A	819	CLA	1	0
17	L	303	CLA	1	0
17	A	833	CLA	2	0
17	A	818	CLA	3	0
20	1	503	BCR	1	0
25	3	313	CHL	1	0
24	6	501	LUT	5	0
17	B	808	CLA	3	0
17	6	505	CLA	2	0
25	4	313	CHL	1	0
17	B	819	CLA	5	0
17	A	852	CLA	4	0
17	6	511	CLA	6	0
17	A	805	CLA	1	0
17	1	504	CLA	5	0
17	A	809	CLA	5	0
17	B	829	CLA	1	0
17	A	838	CLA	6	0
17	B	838	CLA	2	0
17	B	804	CLA	7	0
20	K	204	BCR	1	0
17	B	831	CLA	2	0
17	A	843	CLA	2	0
22	J	104	DGD	2	0
17	3	310	CLA	1	0
17	B	821	CLA	5	0
17	A	812	CLA	5	0

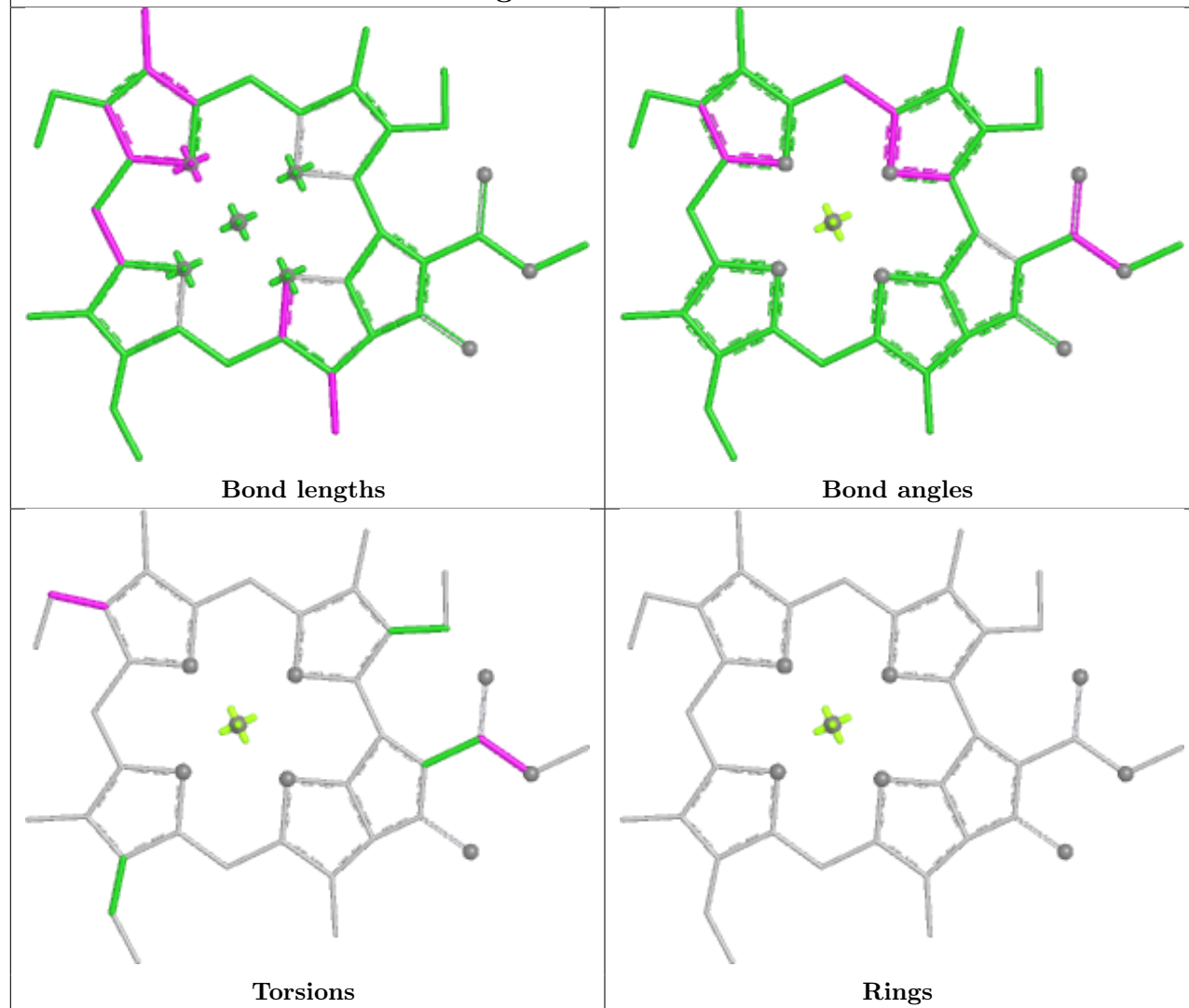
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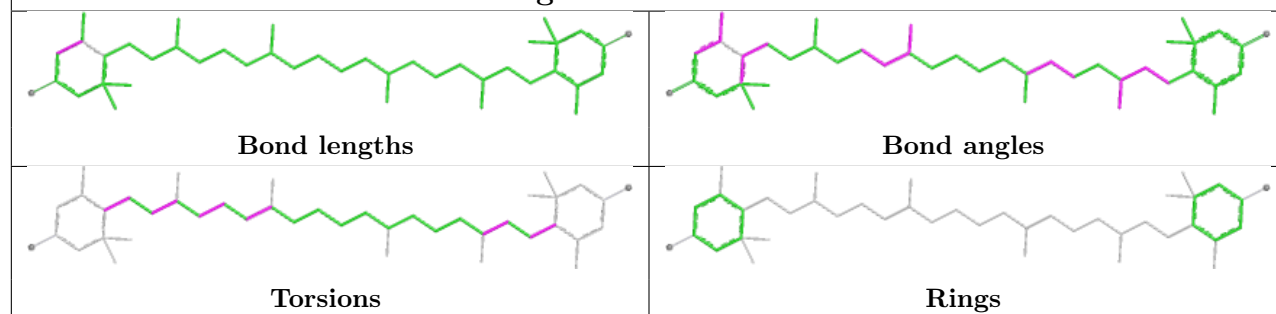
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	815	CLA	1	0
17	A	830	CLA	2	0
17	B	839	CLA	3	0
25	6	512	CHL	3	0
22	B	851	DGD	2	0
25	6	513	CHL	2	0
17	4	304	CLA	2	0
17	4	310	CLA	1	0
17	A	826	CLA	3	0
20	F	801	BCR	1	0
20	I	101	BCR	1	0
25	4	316	CHL	1	0
20	A	846	BCR	5	0
25	6	515	CHL	1	0
25	1	514	CHL	4	0
25	6	517	CHL	1	0
23	J	105	LMG	1	0

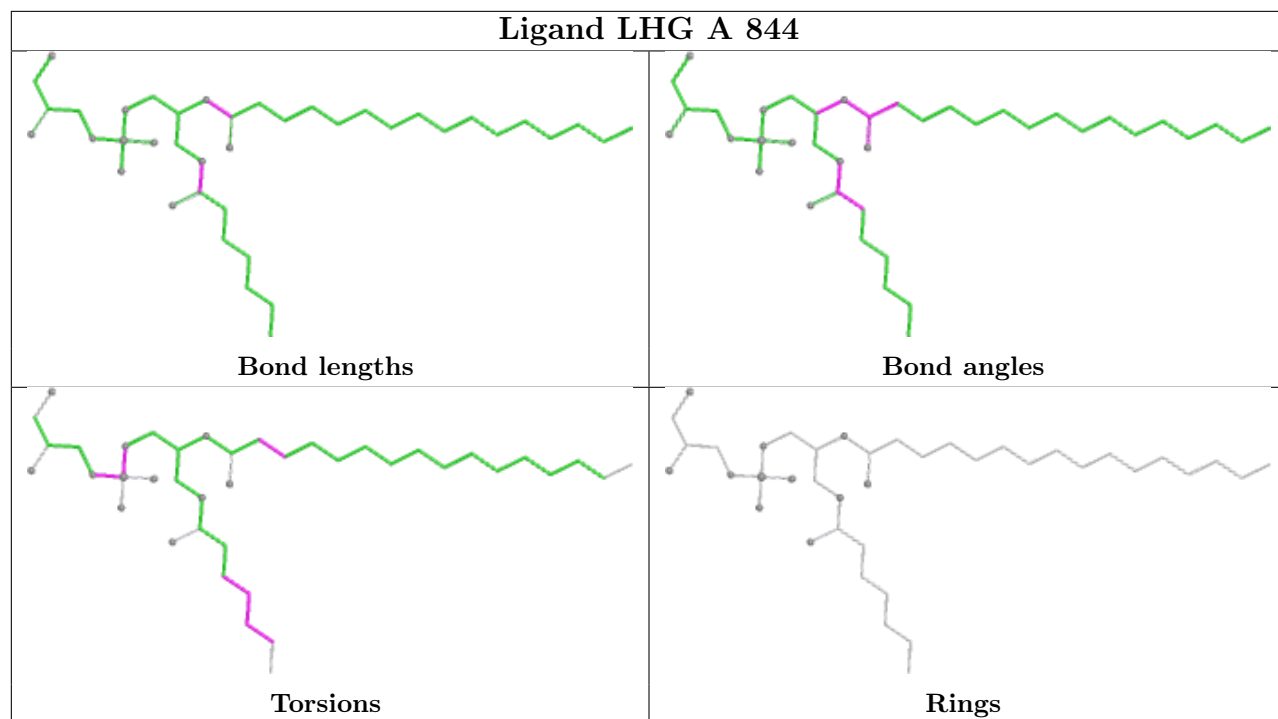
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA B 837

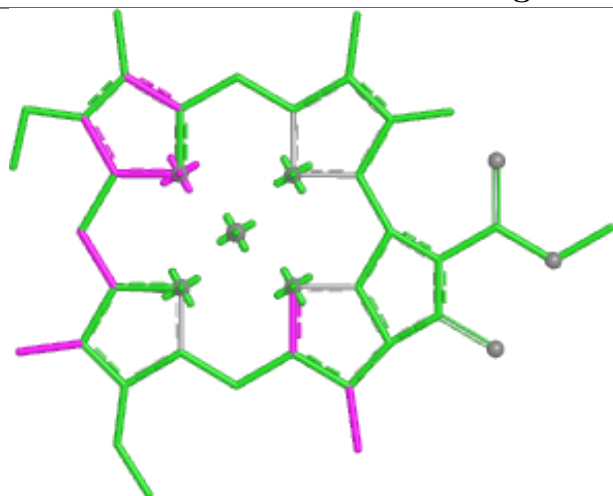


Ligand LUT 1 502

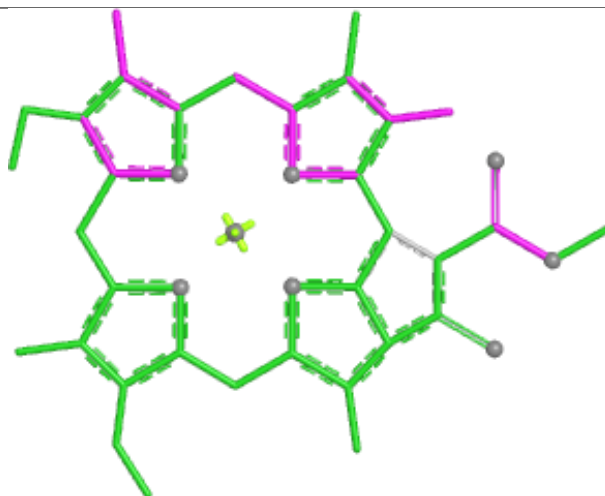




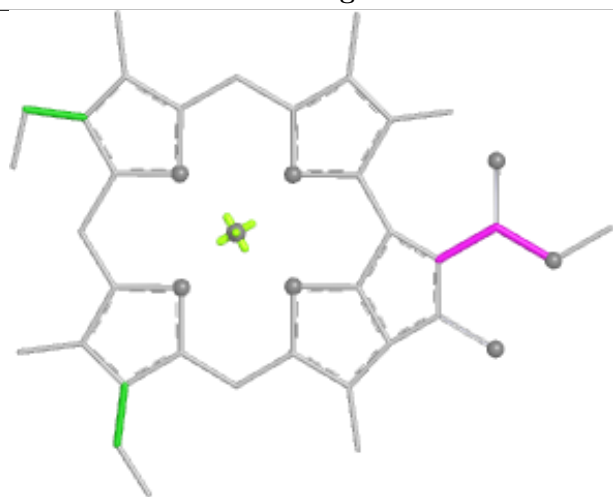
Ligand CLA K 203



Bond lengths



Bond angles

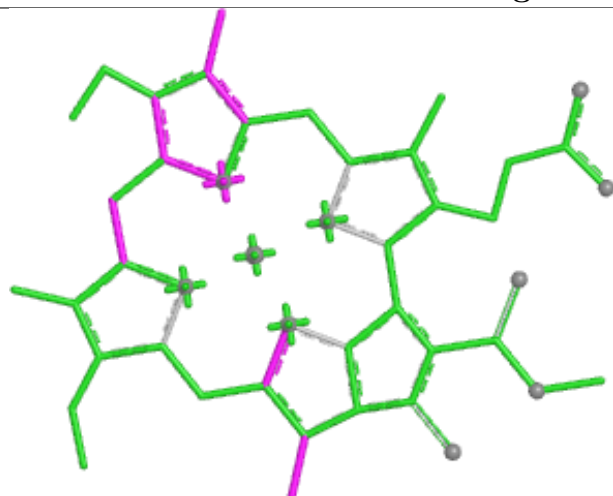


Torsions

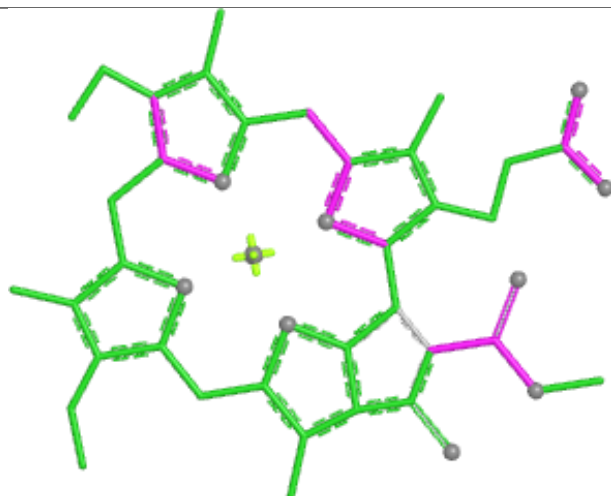


Rings

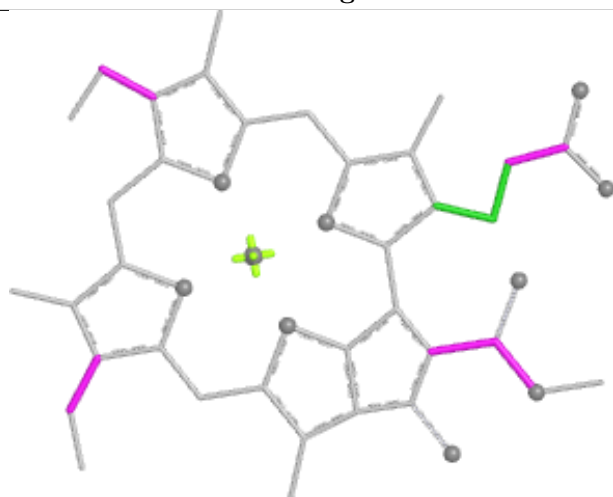
Ligand CLA K 202



Bond lengths



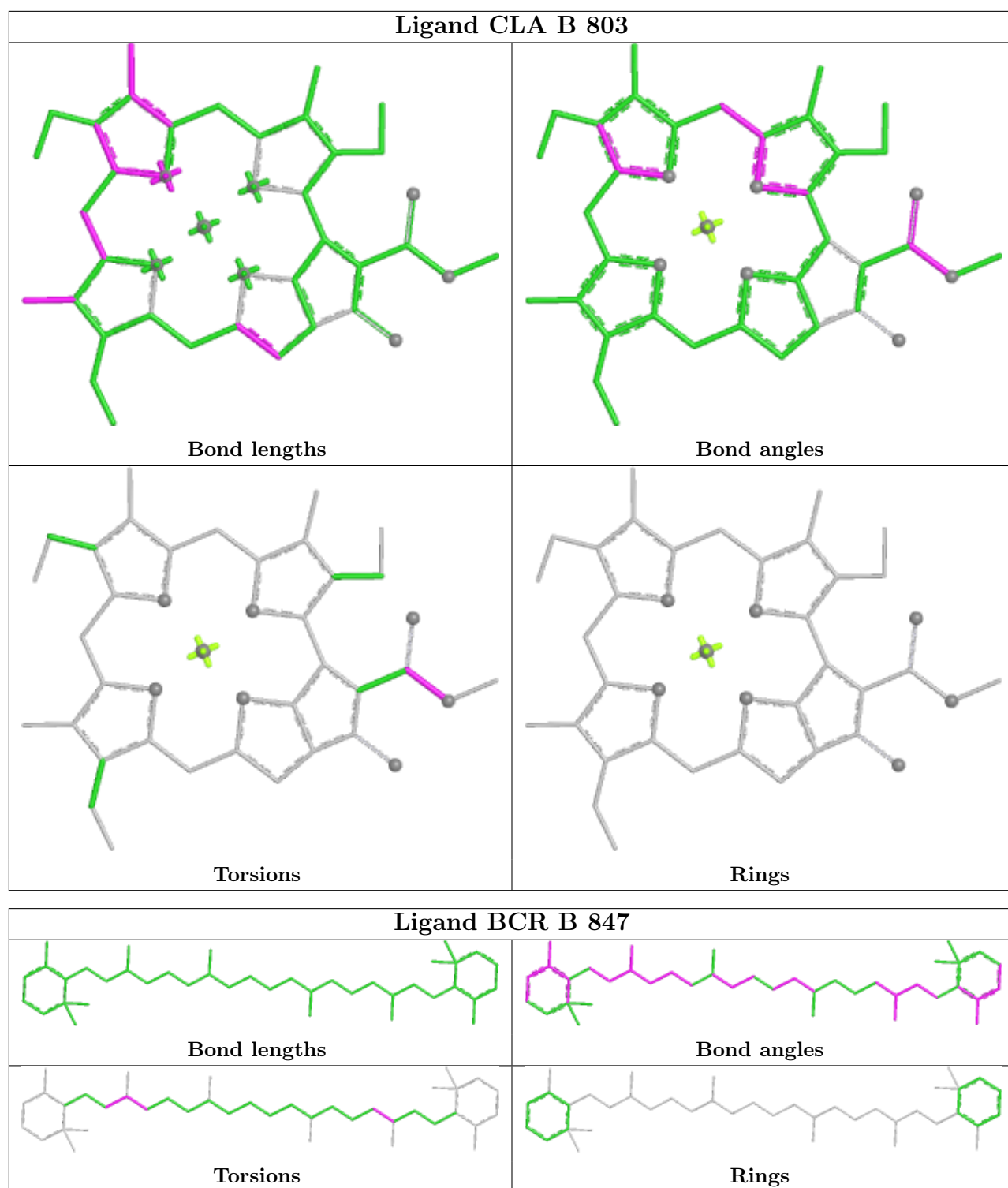
Bond angles



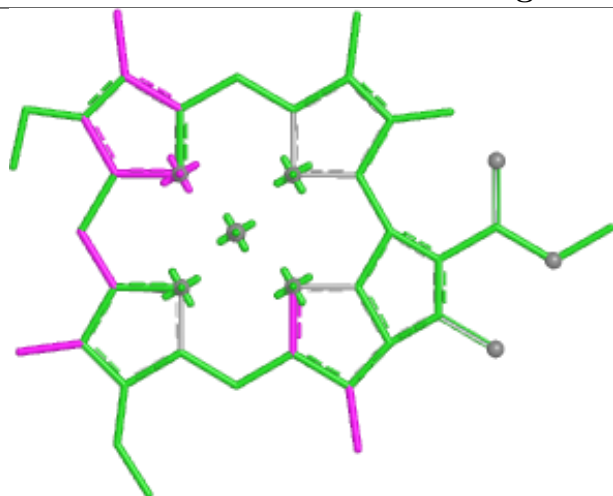
Torsions



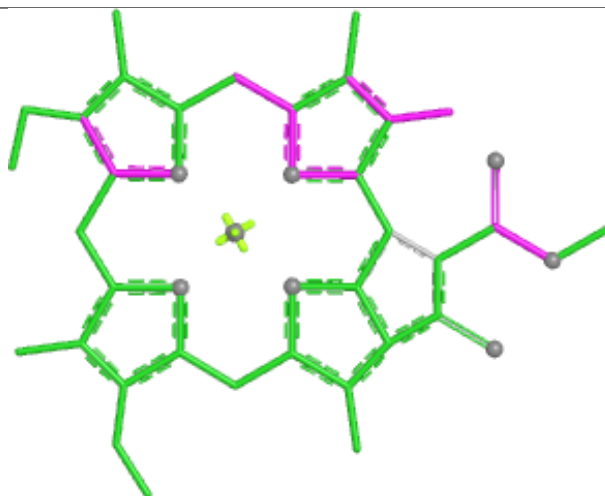
Rings



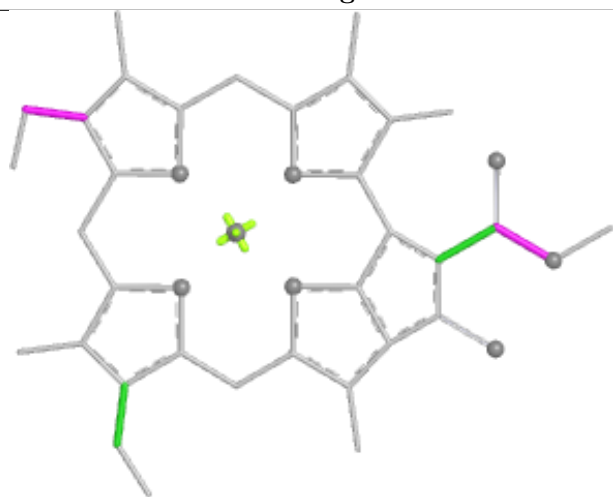
Ligand CLA F 802



Bond lengths



Bond angles

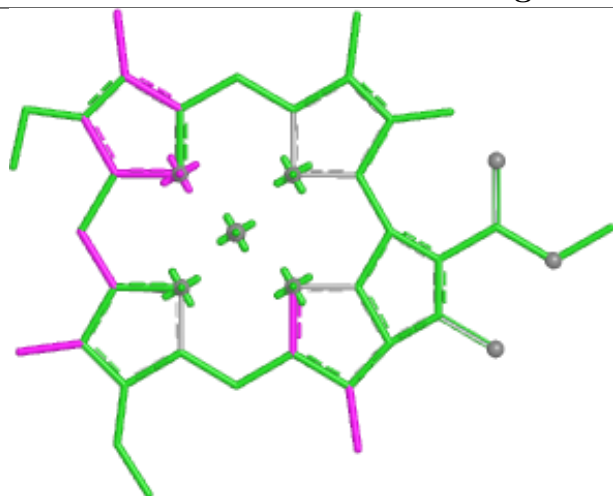


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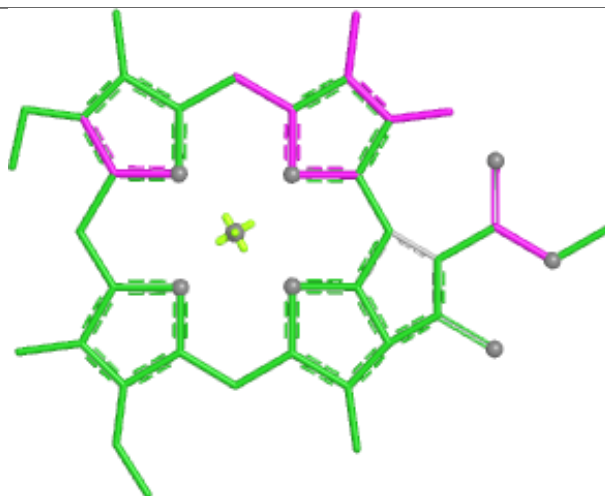


Rings

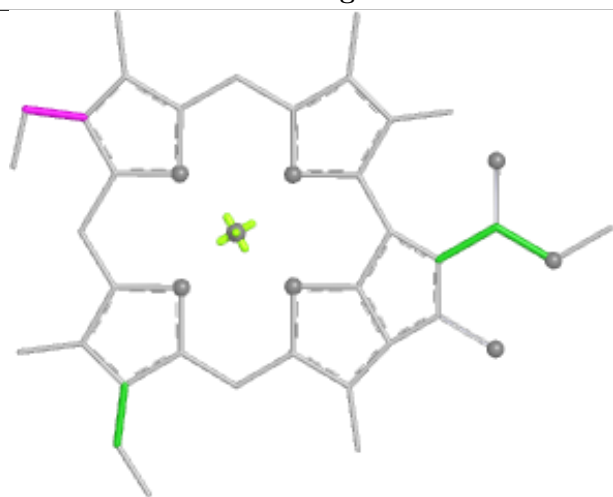
Ligand CLA B 842



Bond lengths



Bond angles

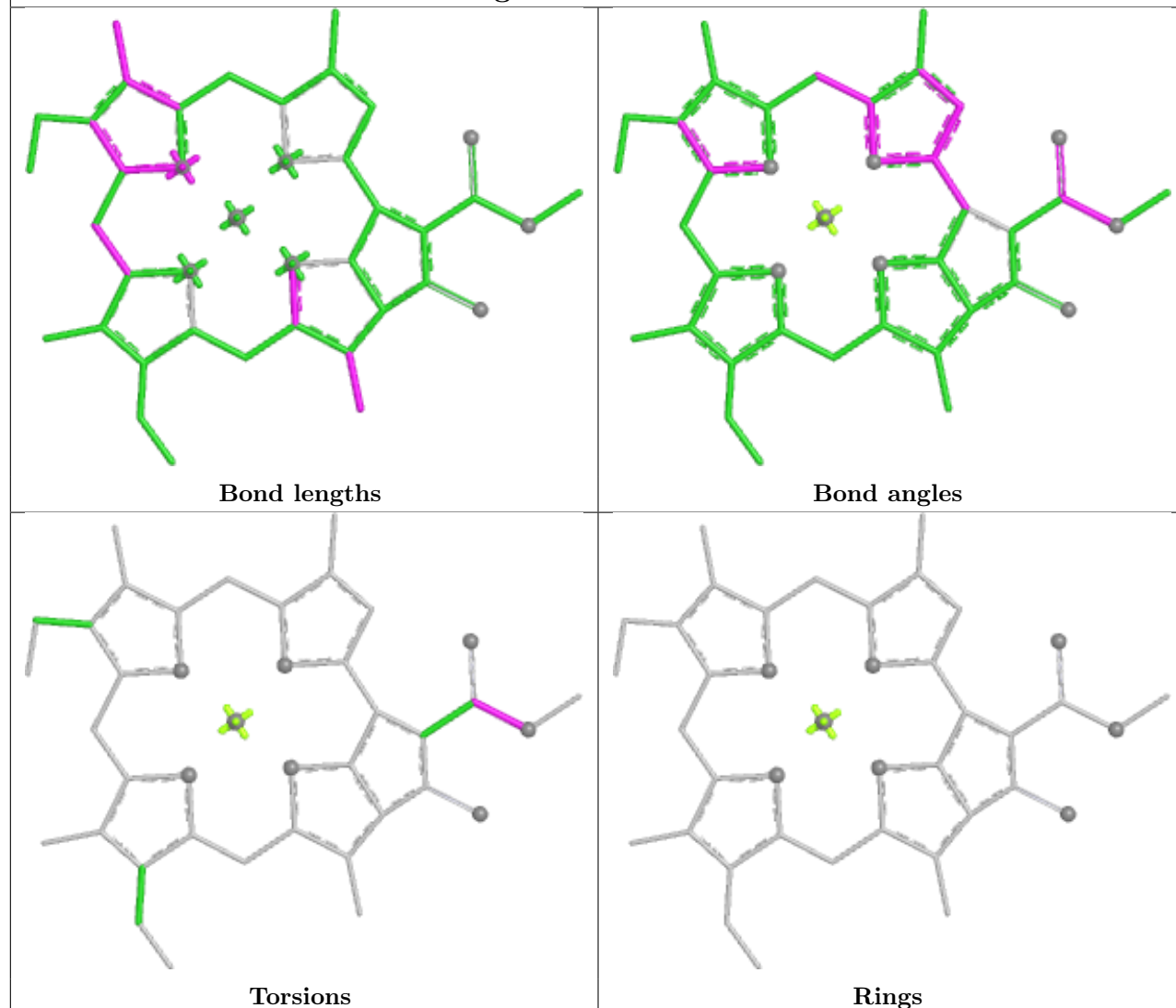


Torsions

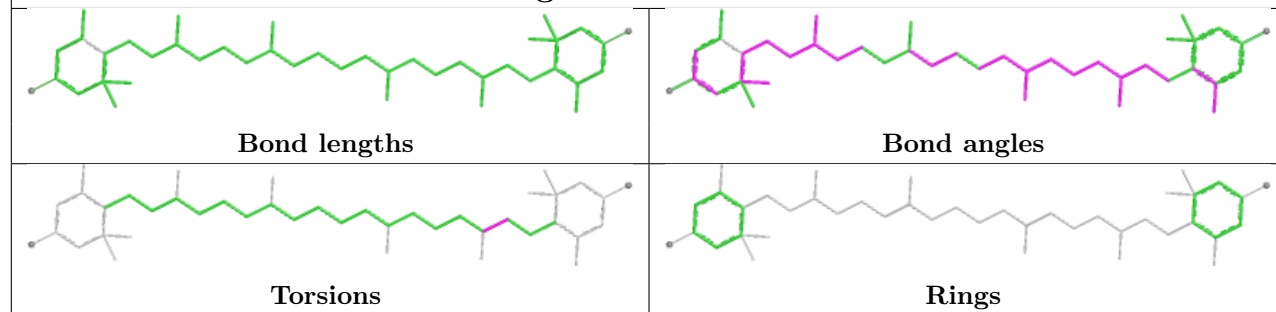


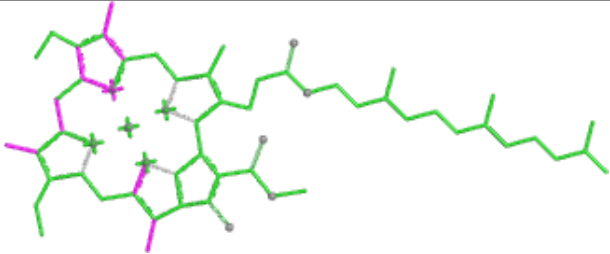
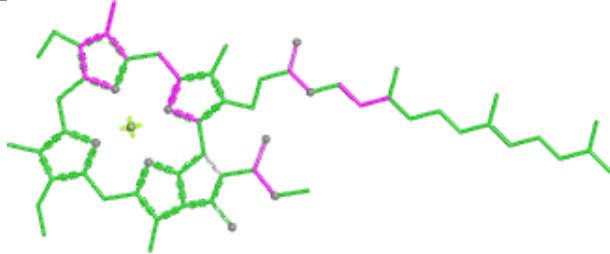
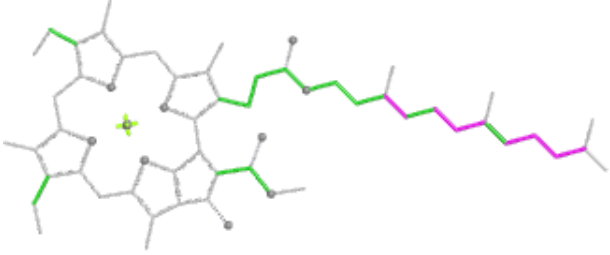
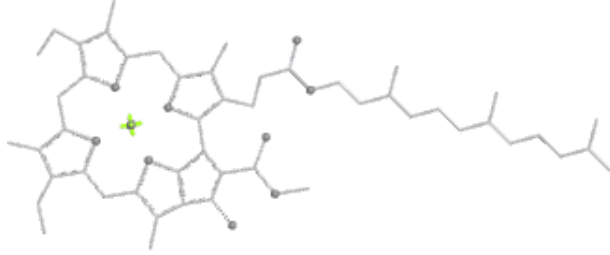
Rings

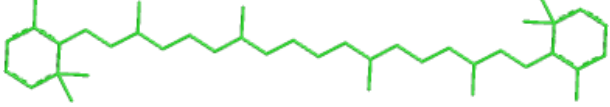
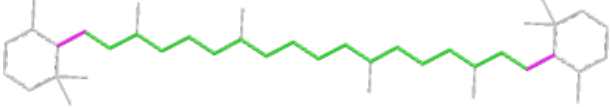
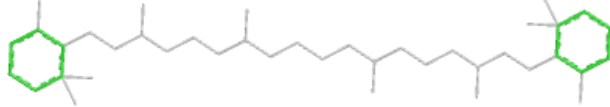
Ligand CLA 6 514



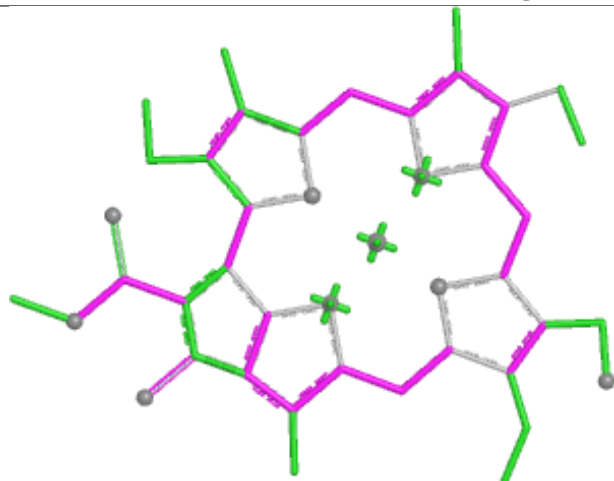
Ligand LUT 1 501



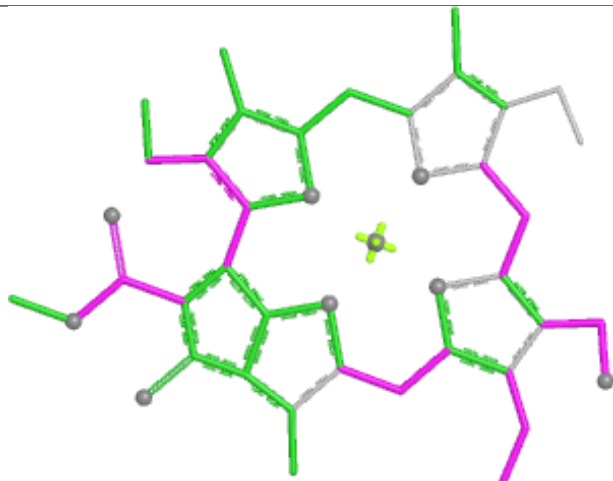
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

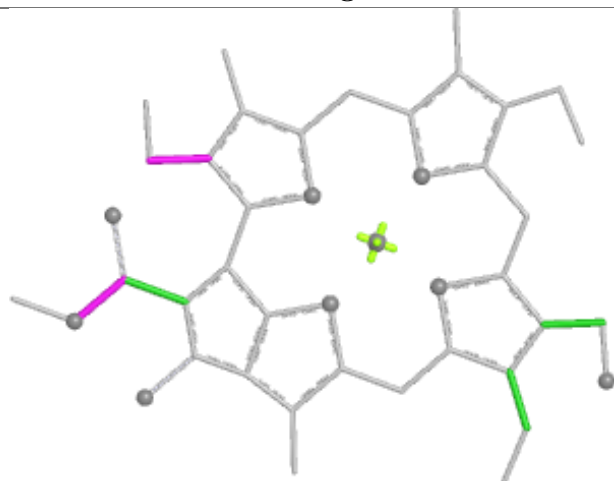
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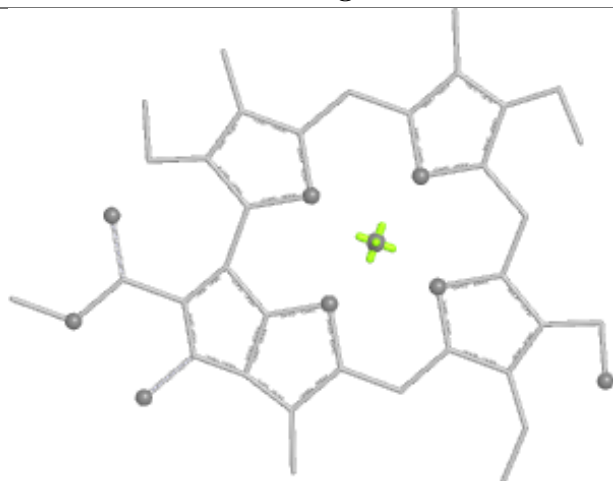
Bond lengths



Bond angles

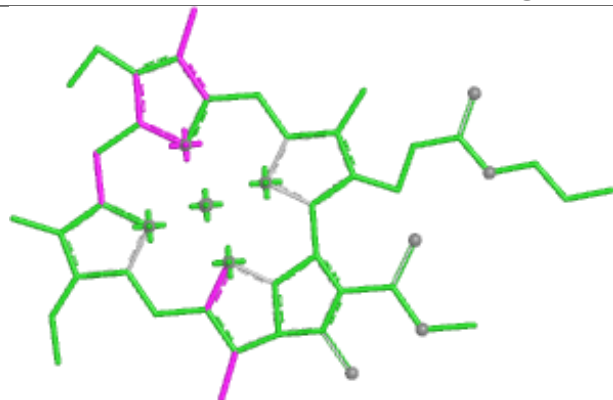


Torsions

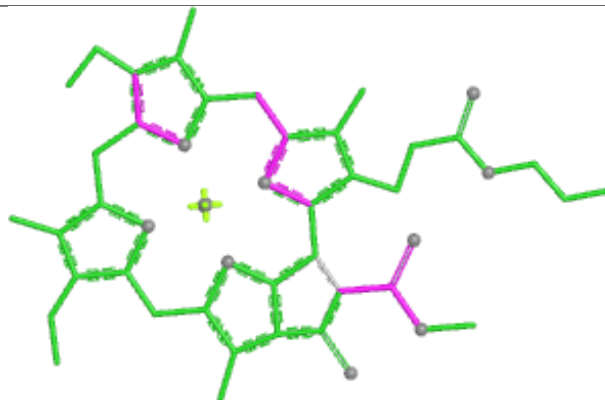


Rings

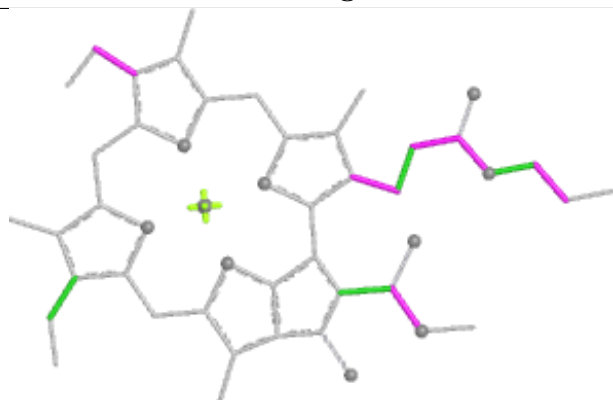
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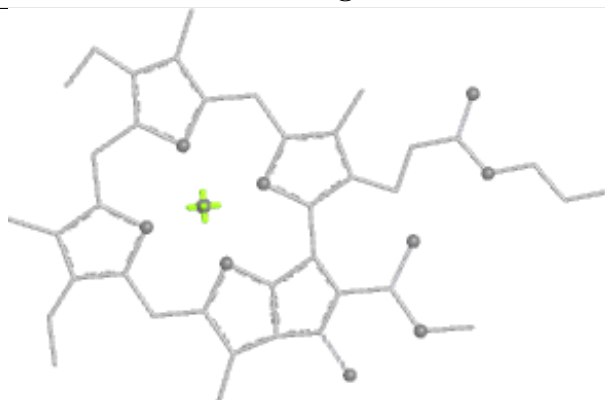
Bond lengths



Bond angles

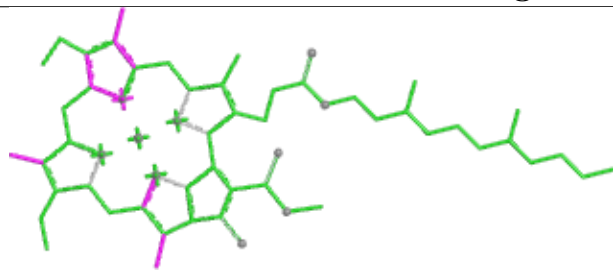


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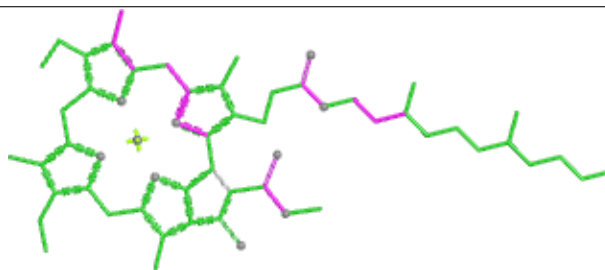


Rings

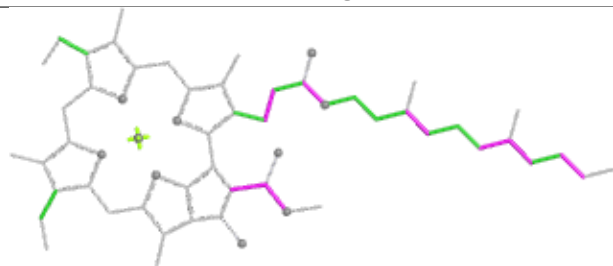
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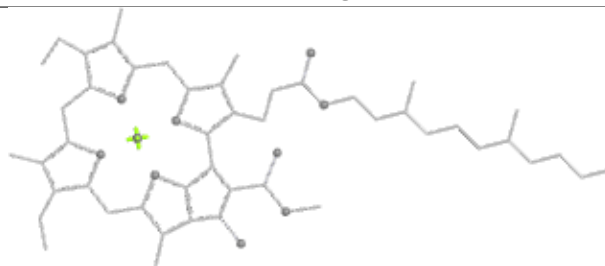
Bond lengths



Bond angles

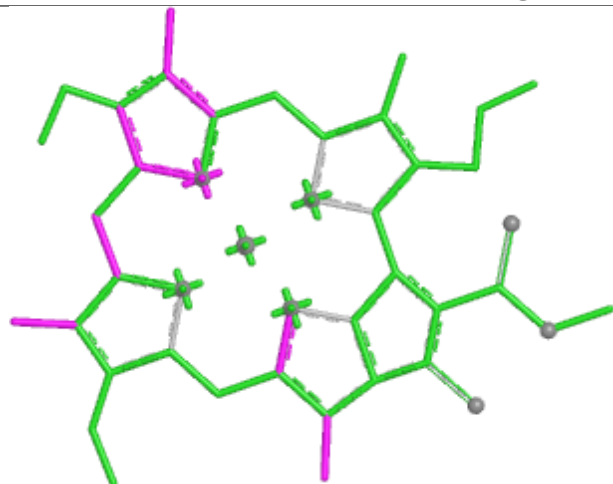


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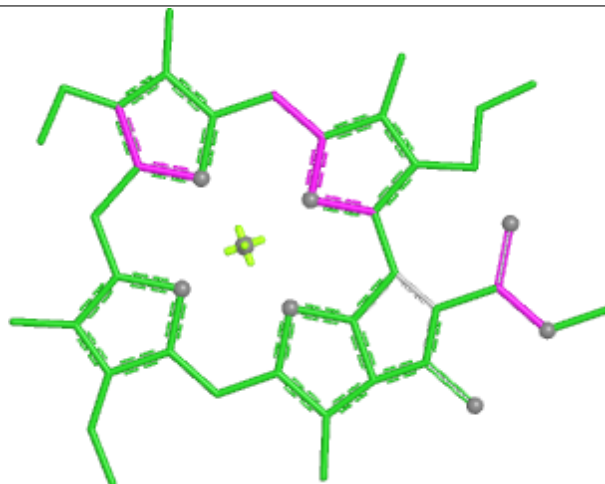


Rings

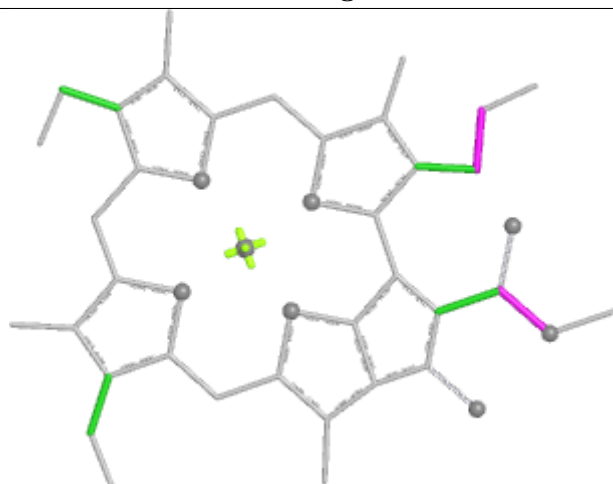
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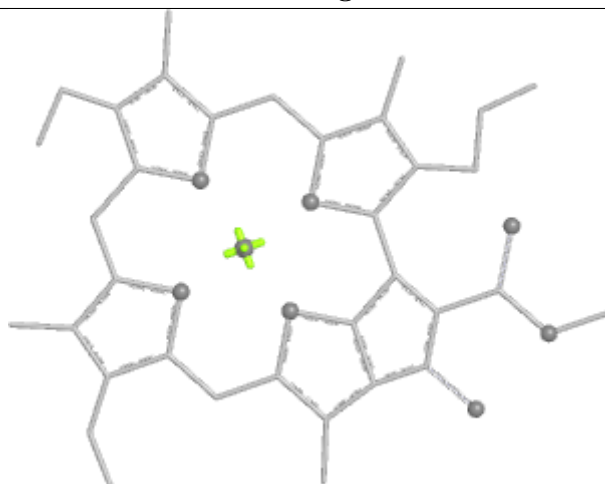
Bond lengths



Bond angles

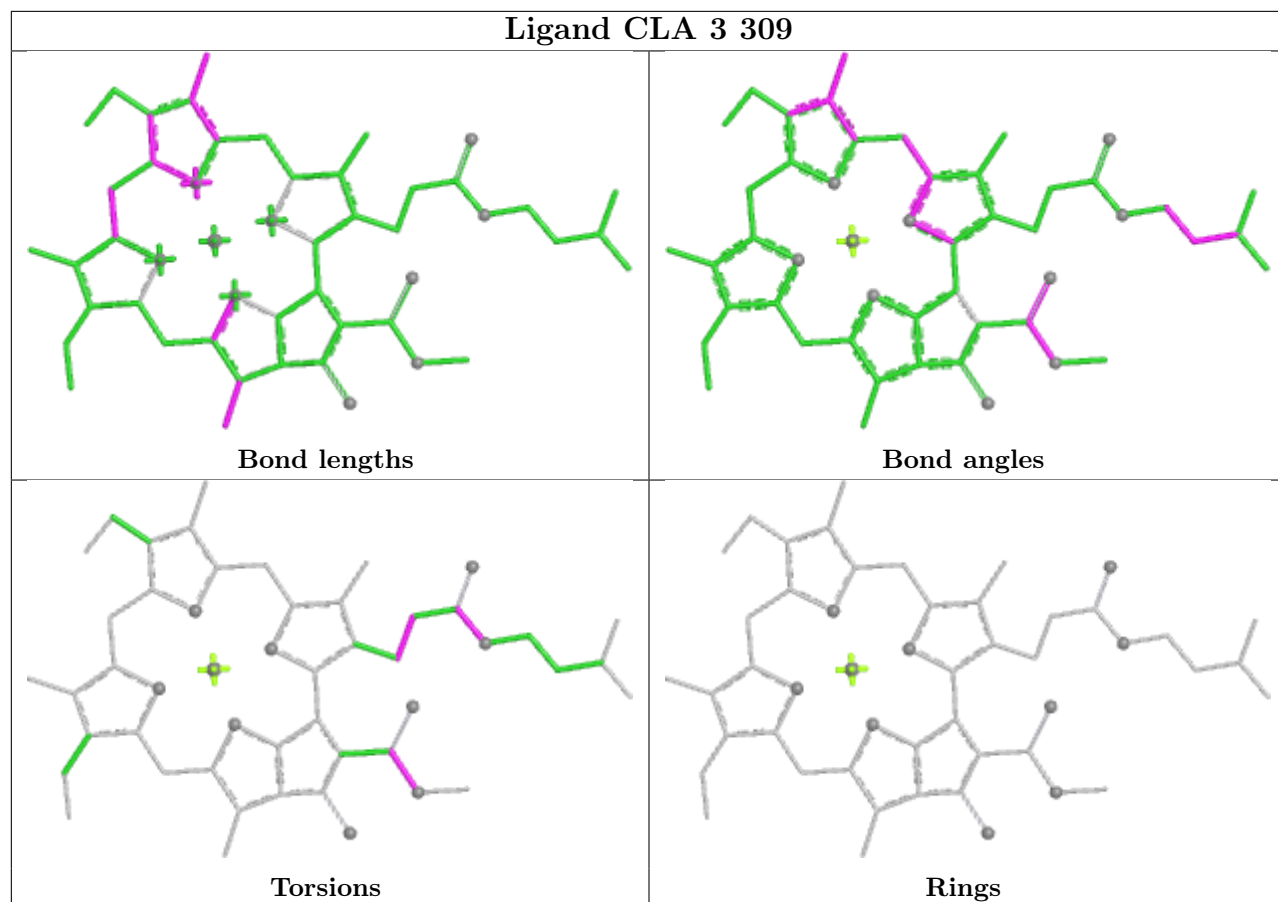


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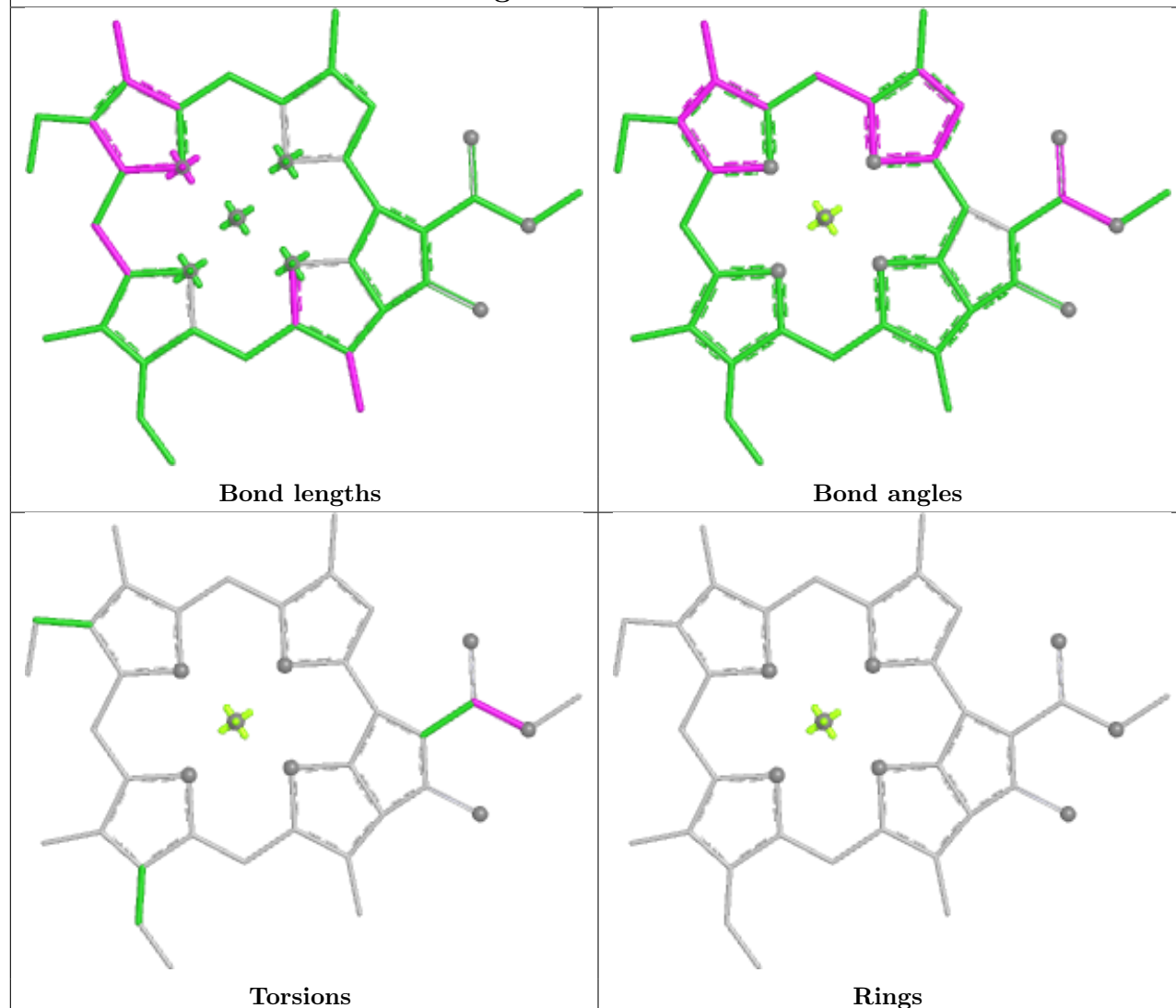


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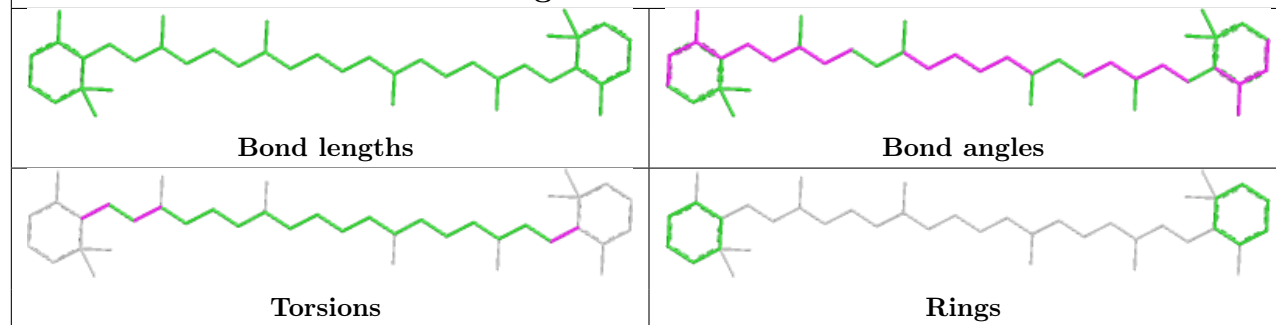
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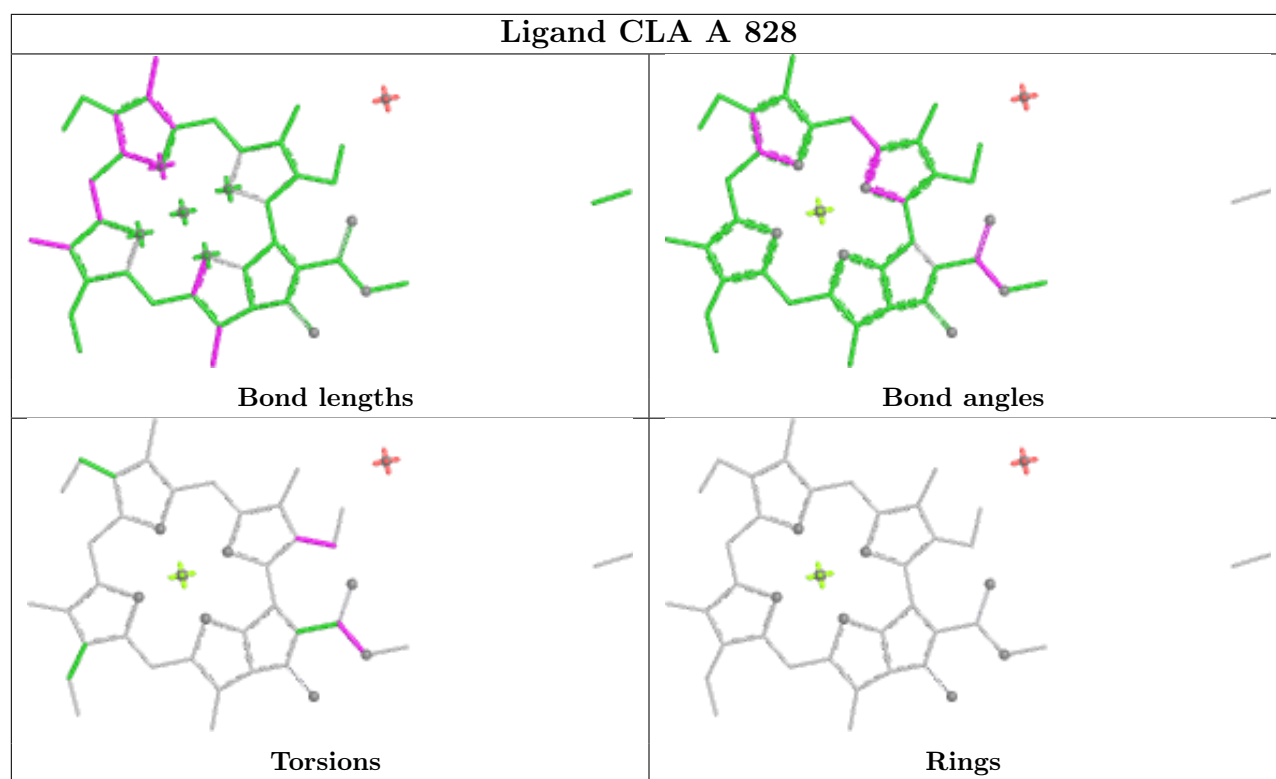


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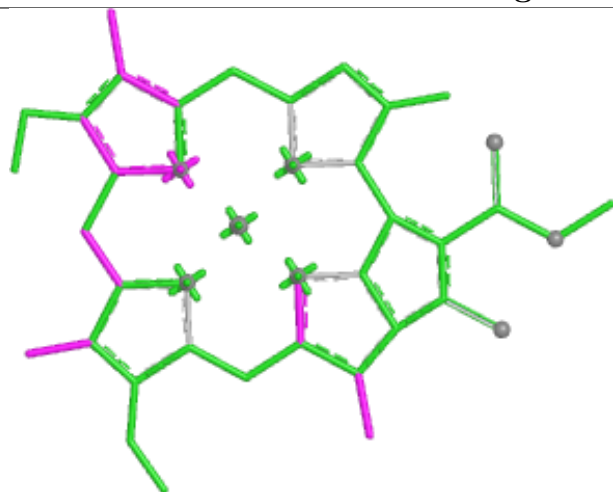


Ligand BCR 4 301

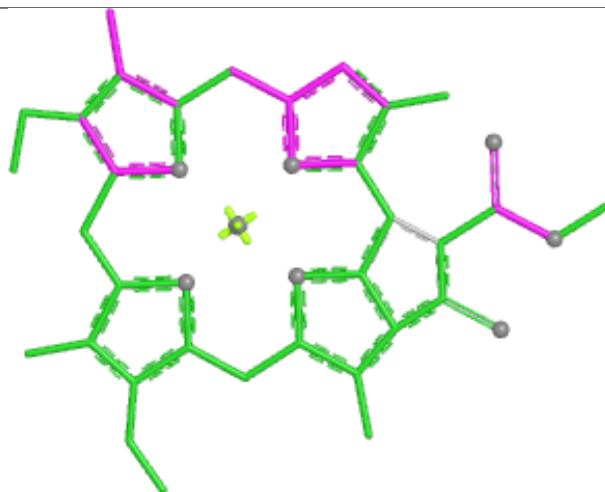




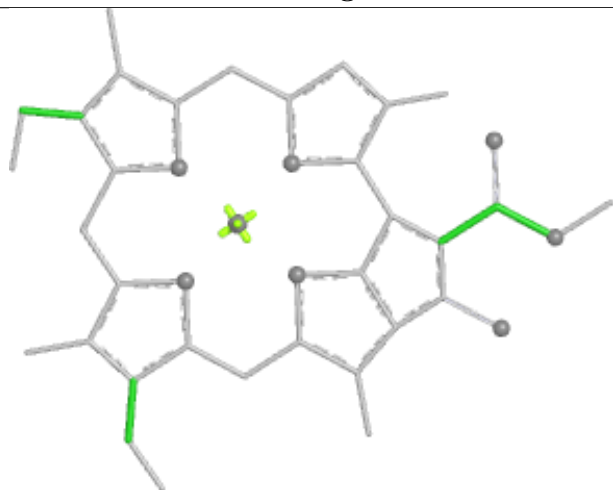
Ligand CLA B 827



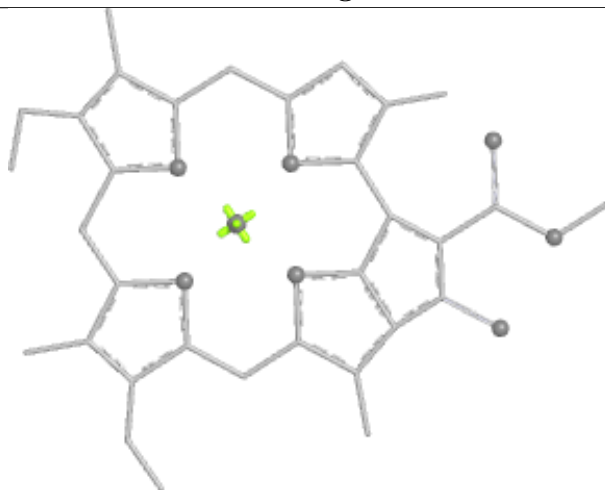
Bond lengths



Bond angles

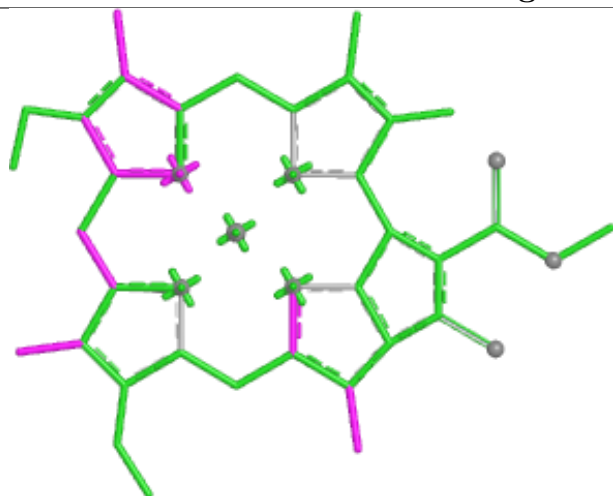


Torsions

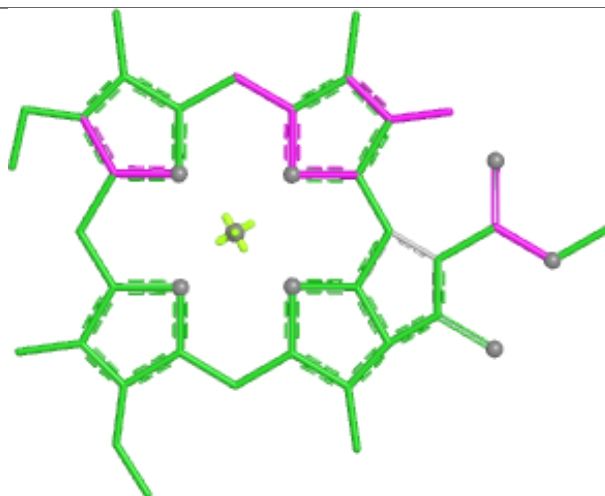


Rings

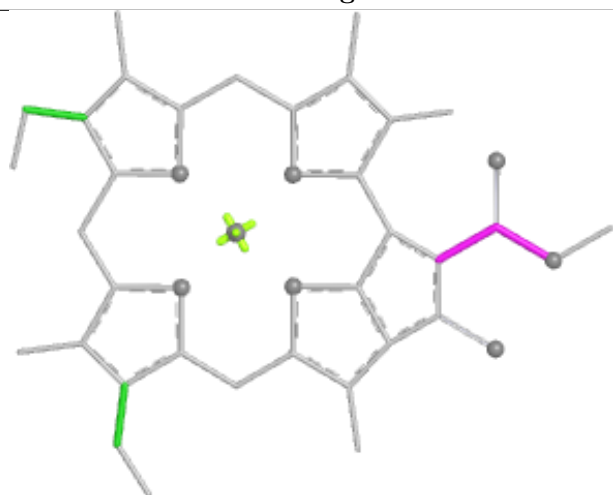
Ligand CLA 4 308



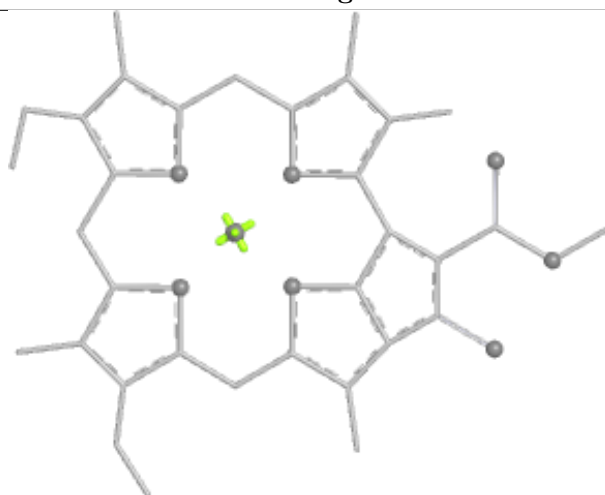
Bond lengths



Bond angles

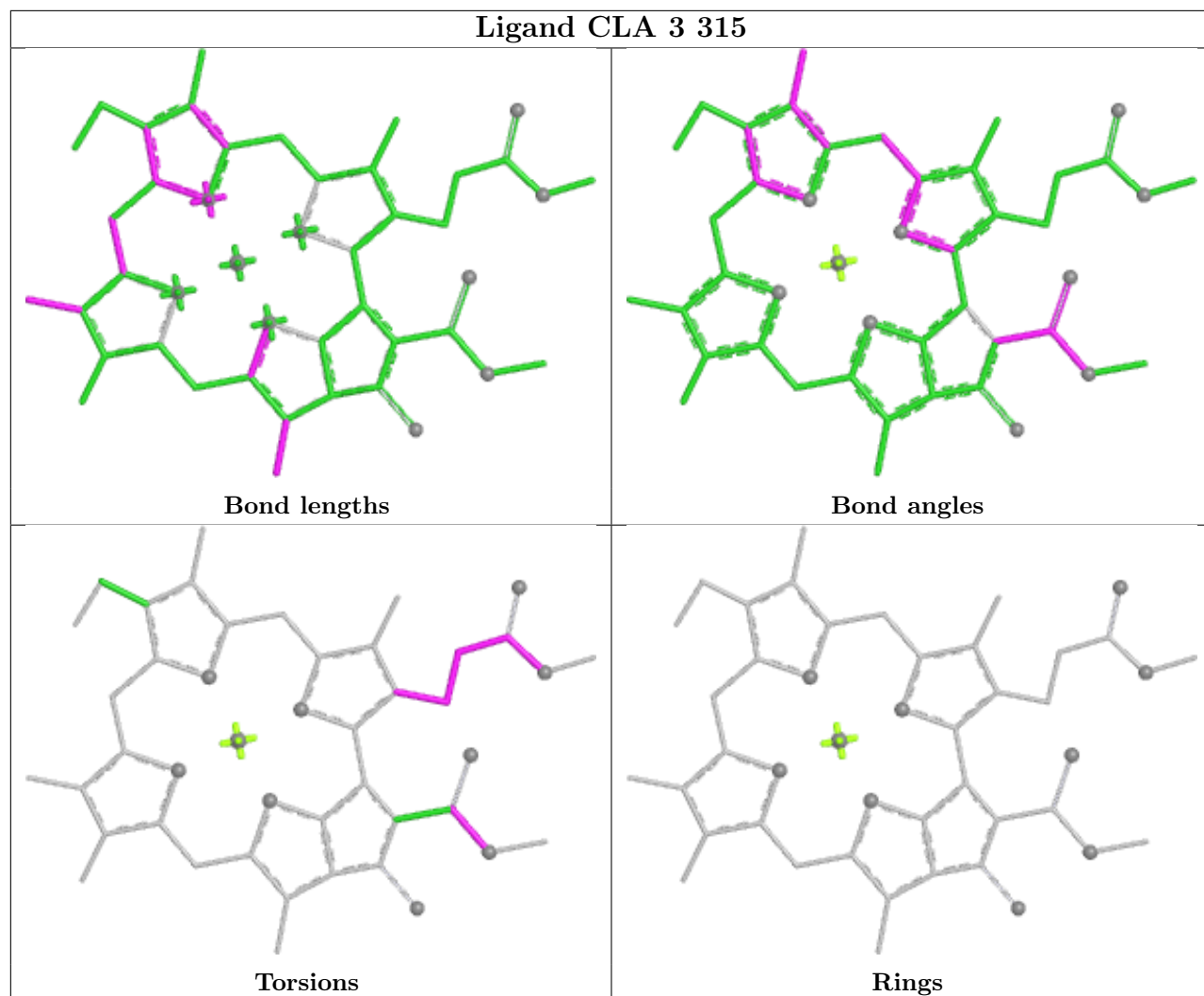


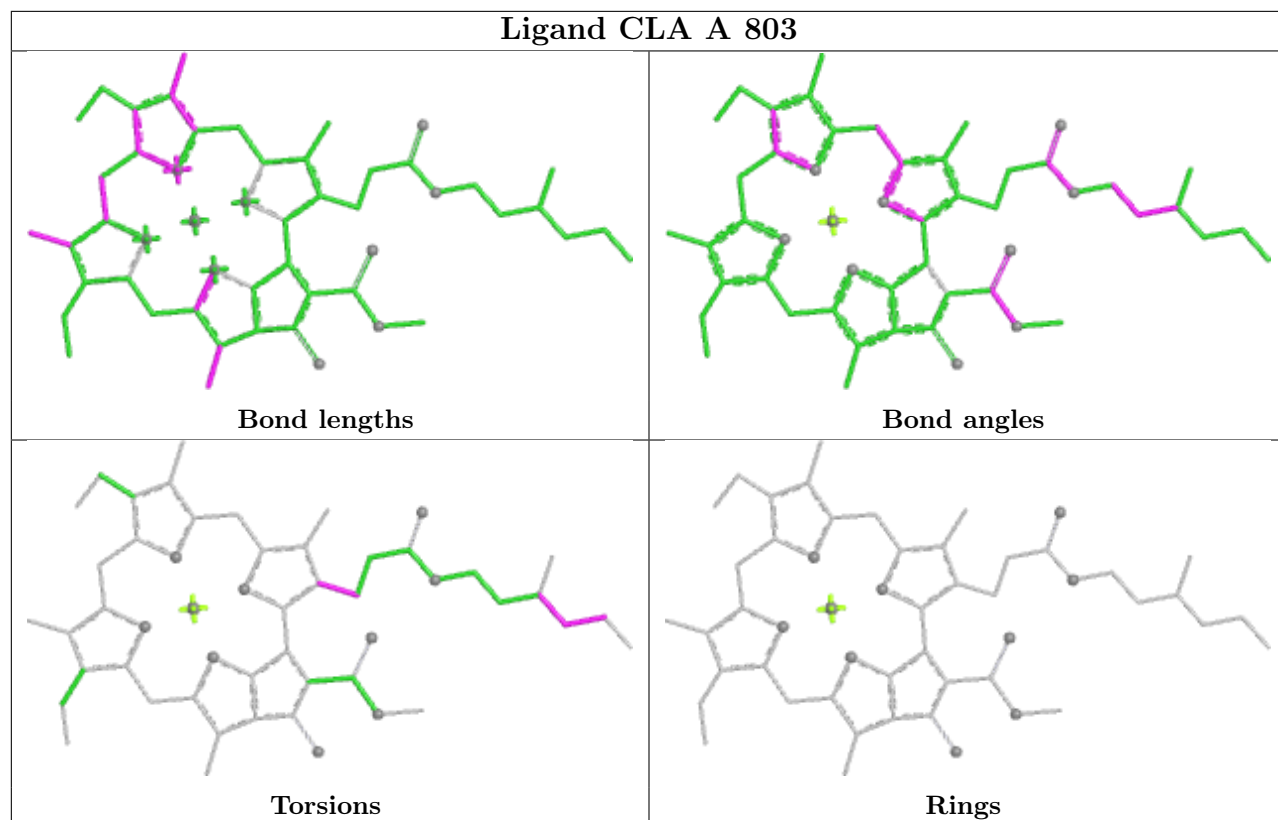
Torsions



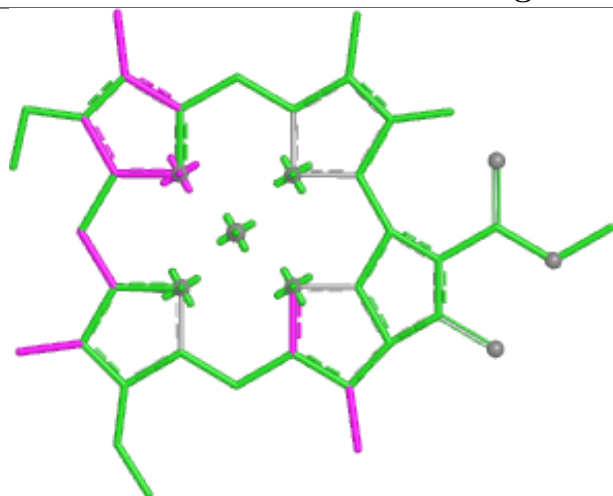
Rings

Ligand CLA 3 315

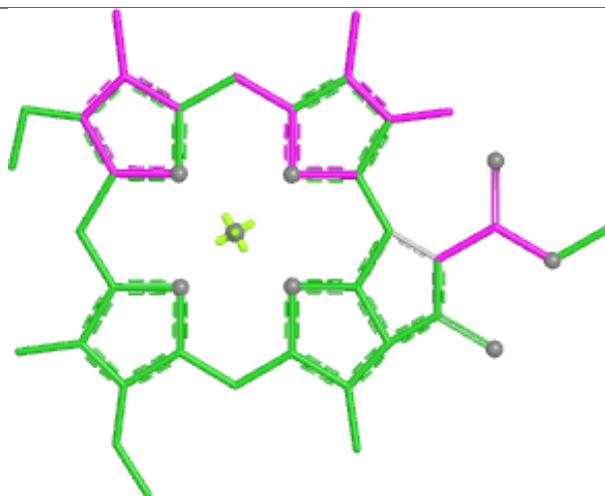




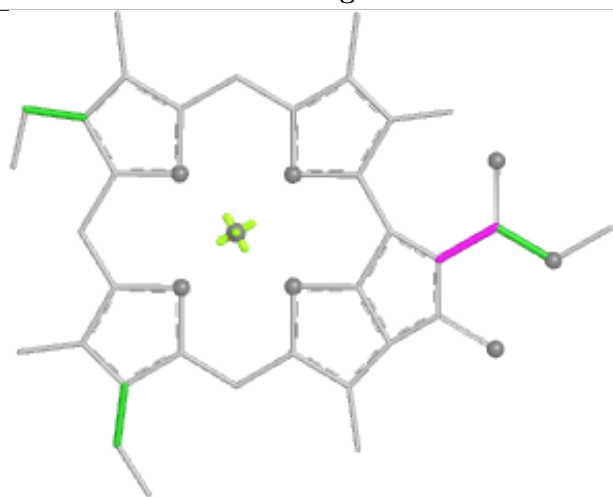
Ligand CLA B 807



Bond lengths



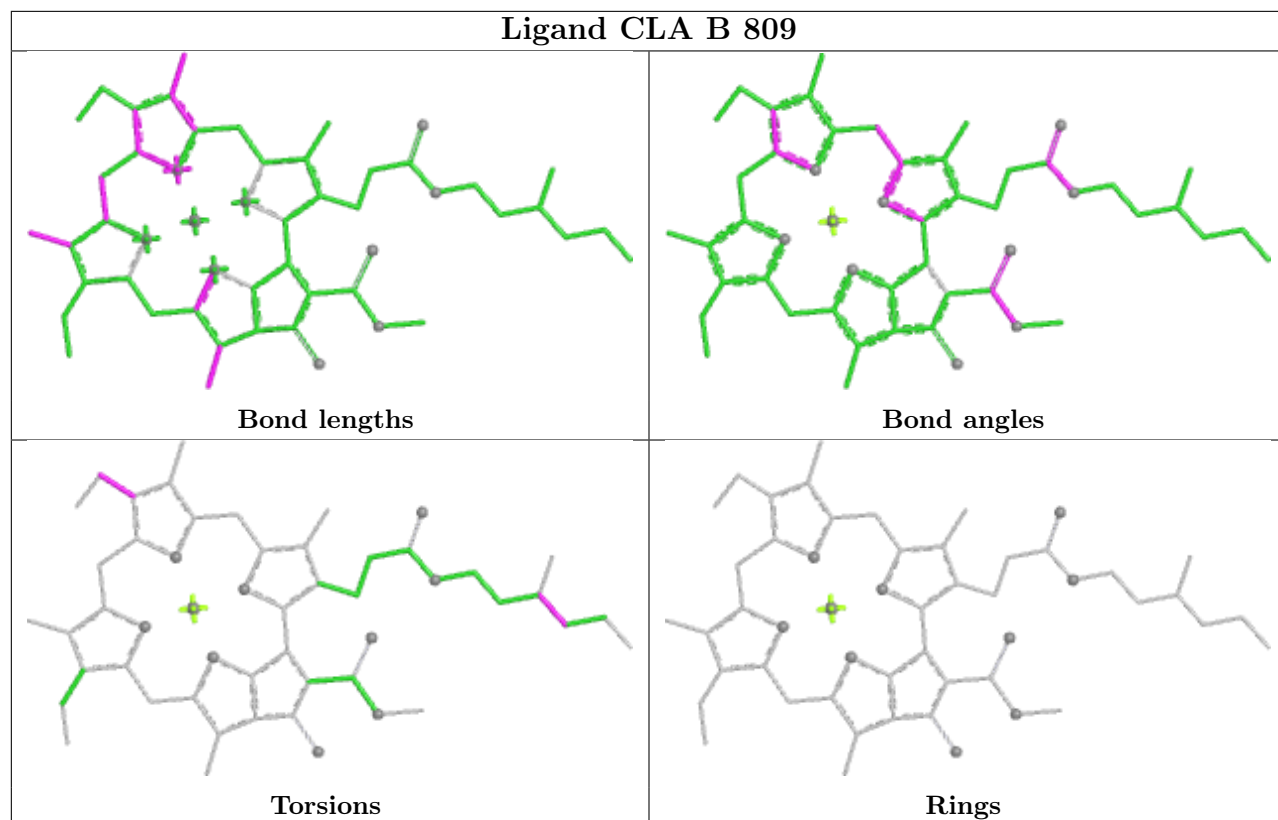
Bond angles



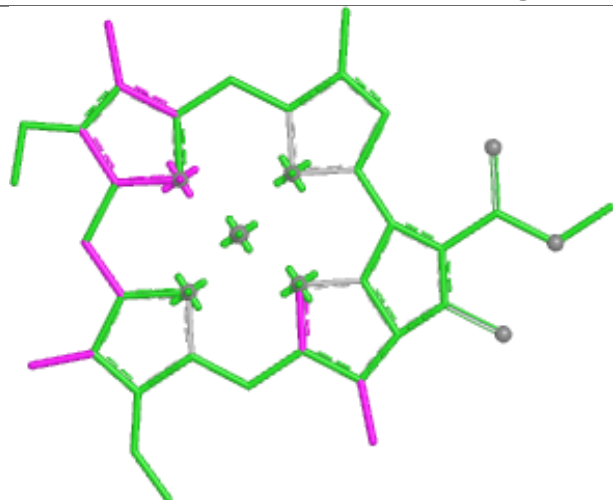
Torsions



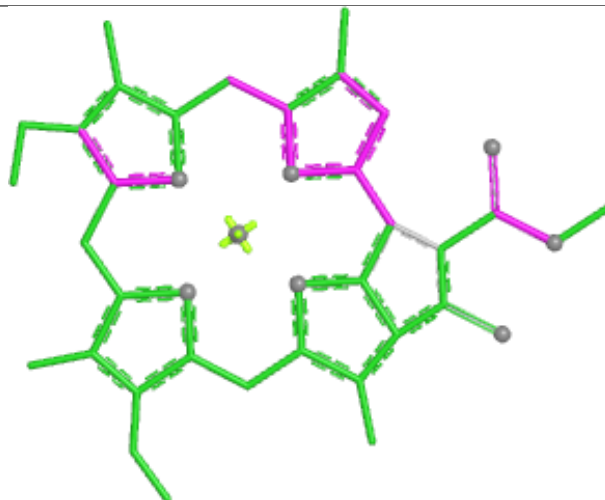
Rings



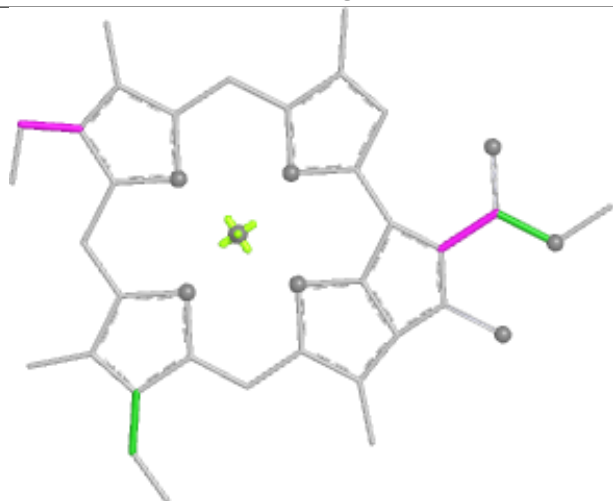
Ligand CLA B 832



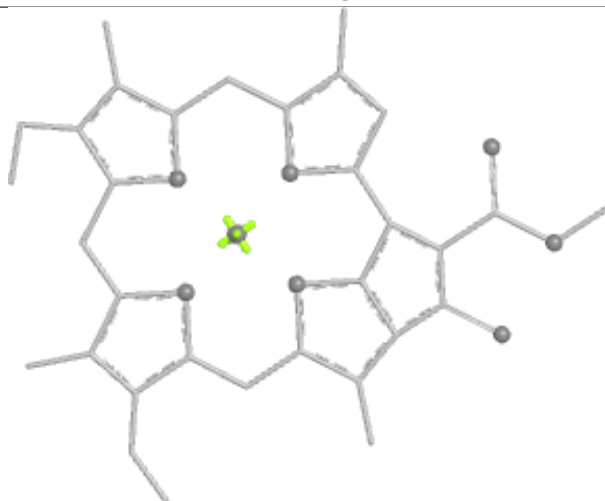
Bond lengths



Bond angles

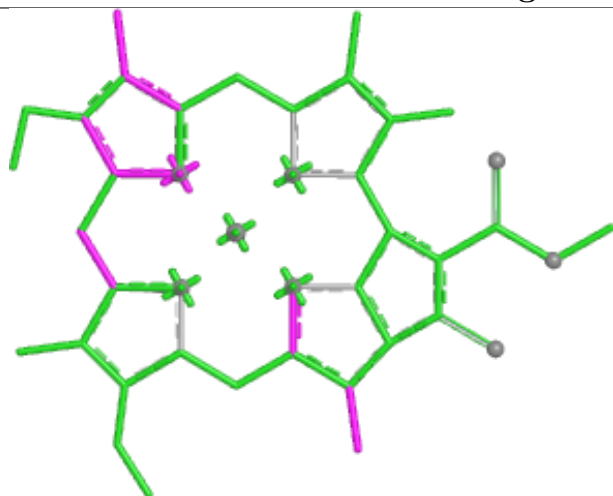


Torsions

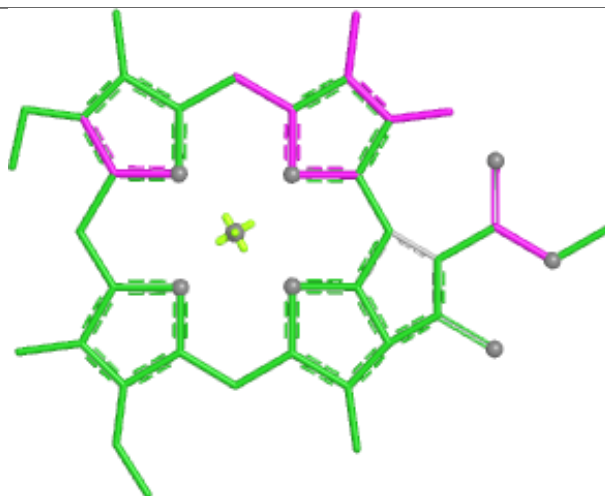


Rings

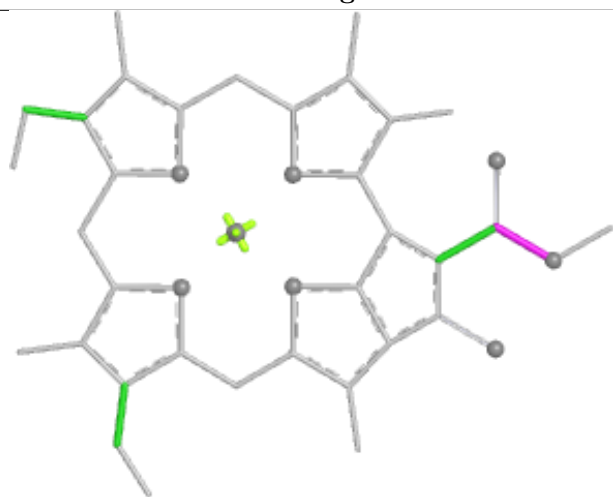
Ligand CLA 4 315



Bond lengths



Bond angles

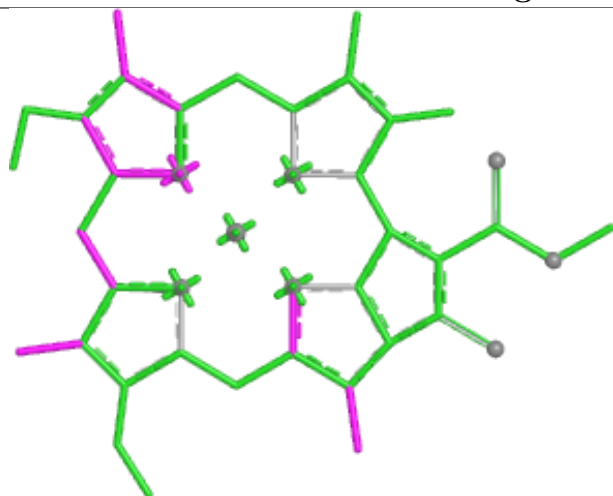


Torsions

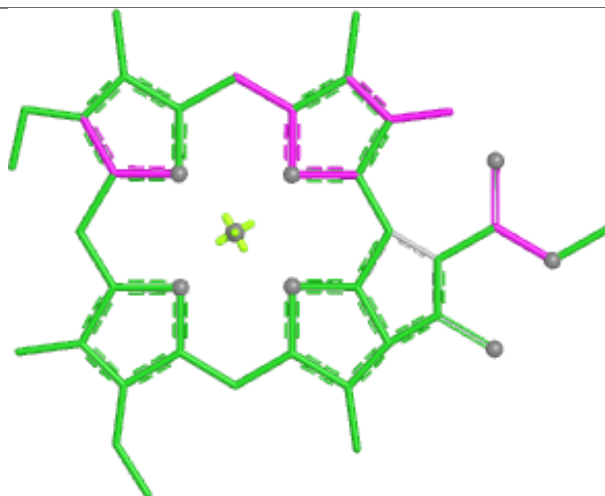


Rings

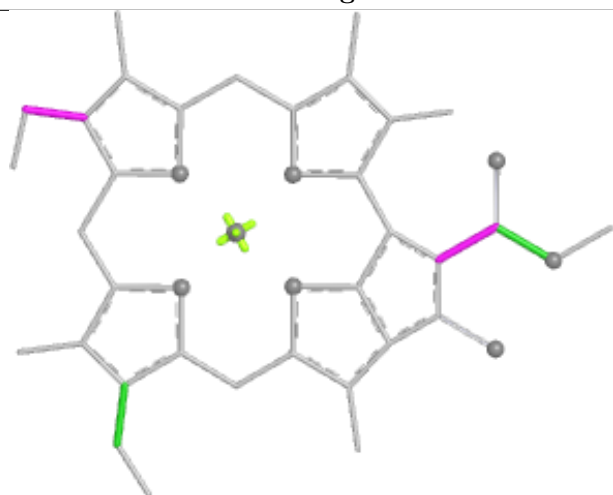
Ligand CLA B 822



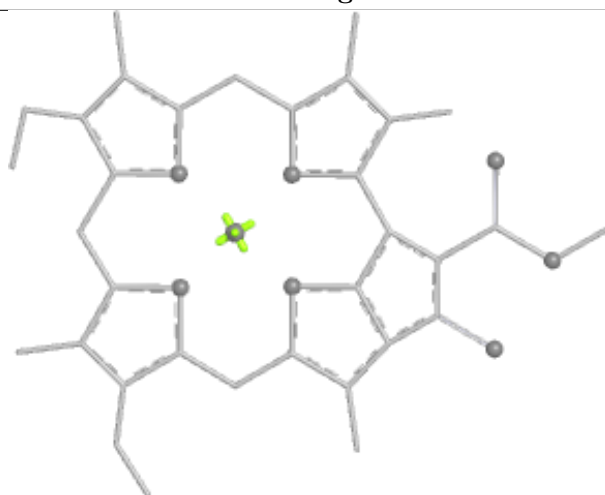
Bond lengths



Bond angles

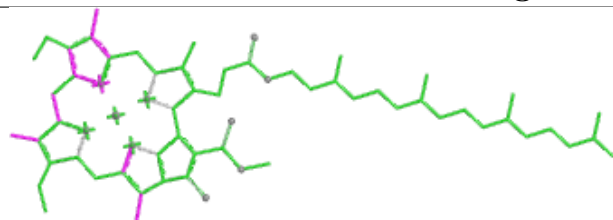


Torsions

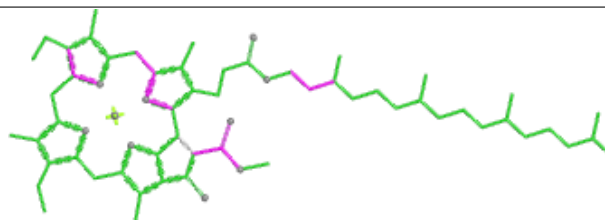


Rings

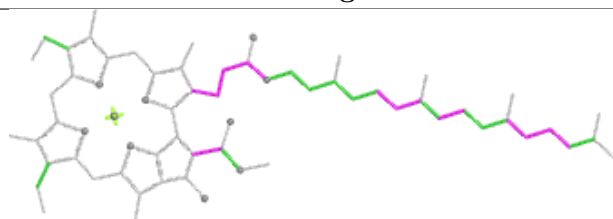
Ligand CLA A 804



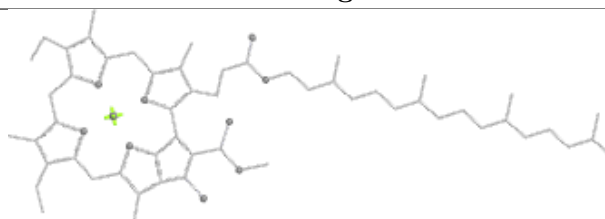
Bond lengths



Bond angles

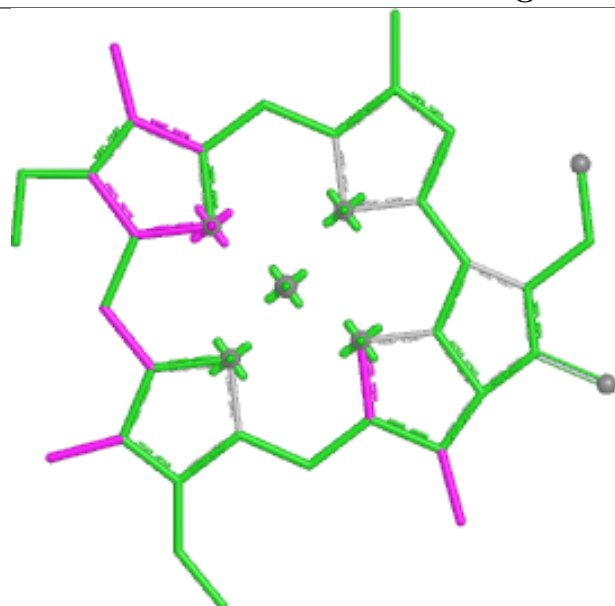


Torsions

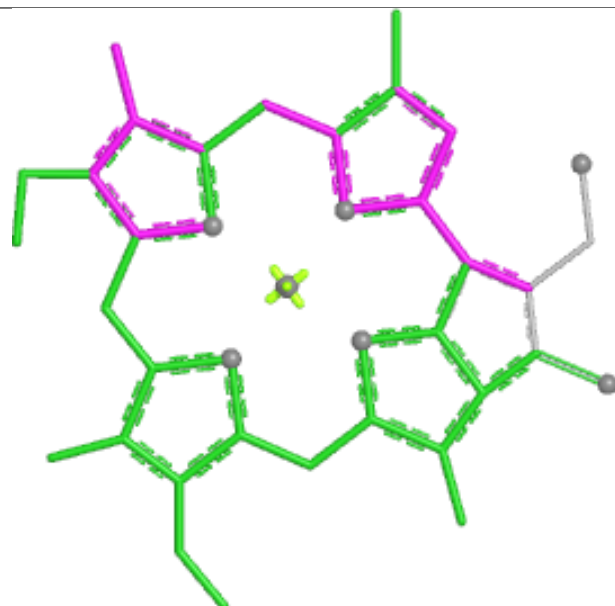


Rings

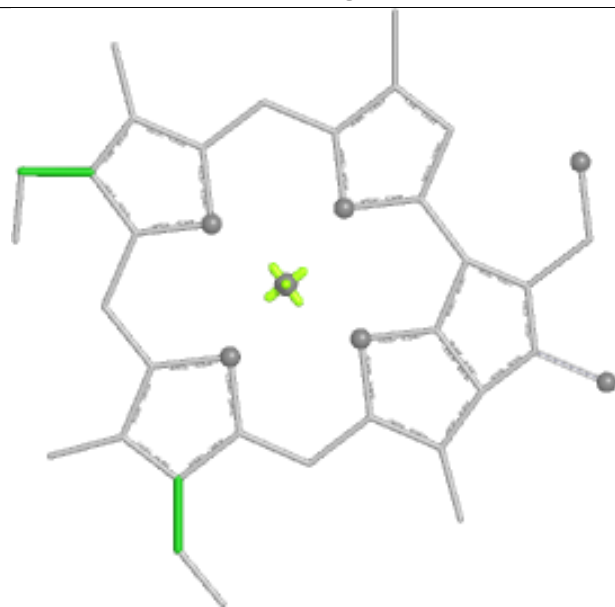
Ligand CLA B 805



Bond lengths



Bond angles

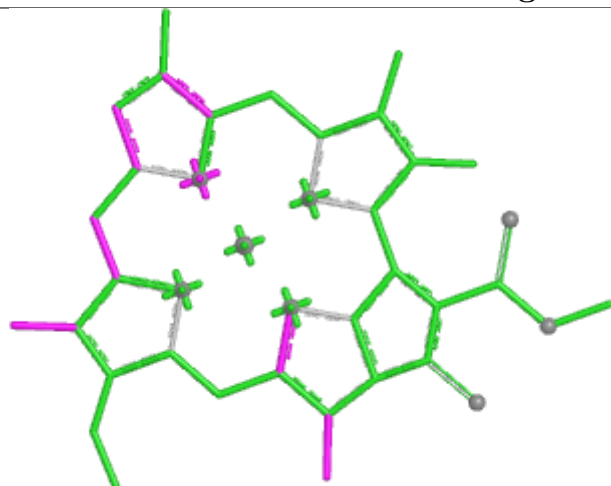


Torsions

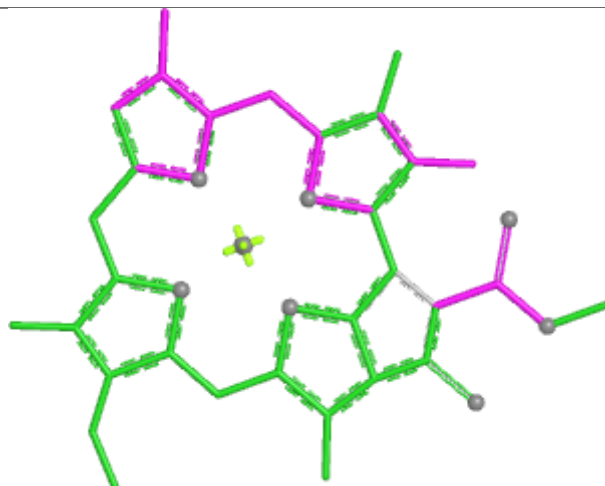


Rings

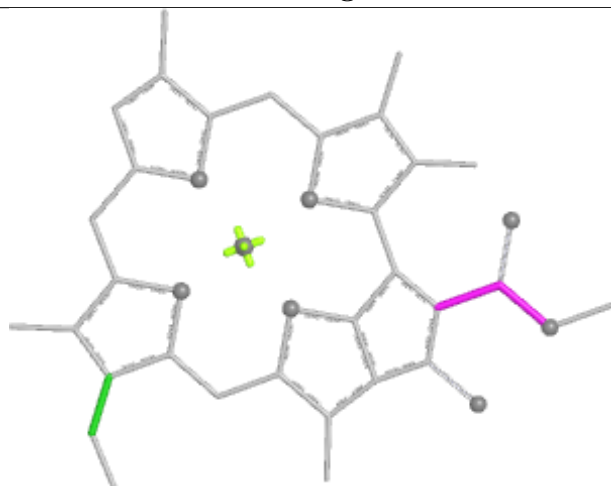
Ligand CLA 6 504



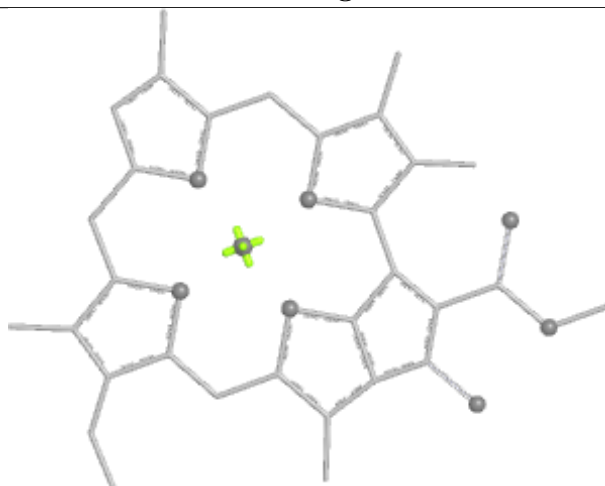
Bond lengths



Bond angles

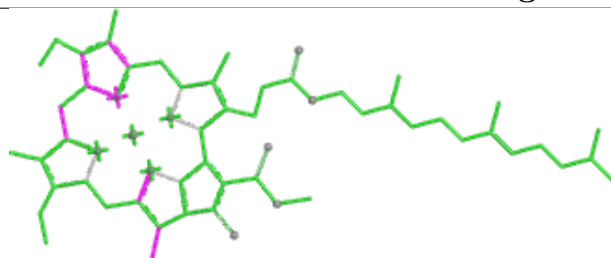


Torsions

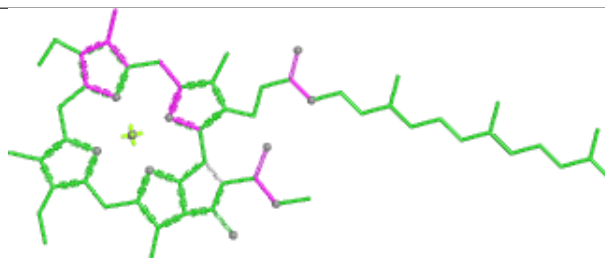


Rings

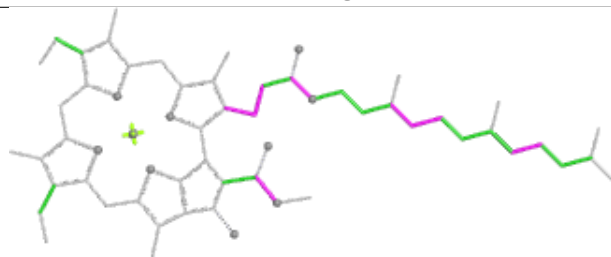
Ligand CLA 3 312



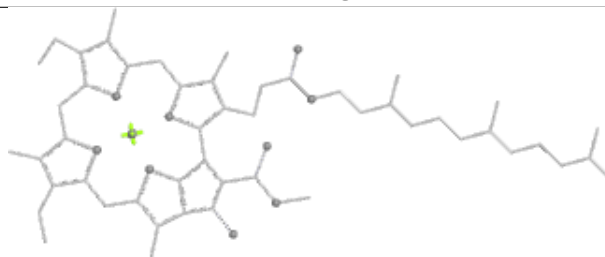
Bond lengths



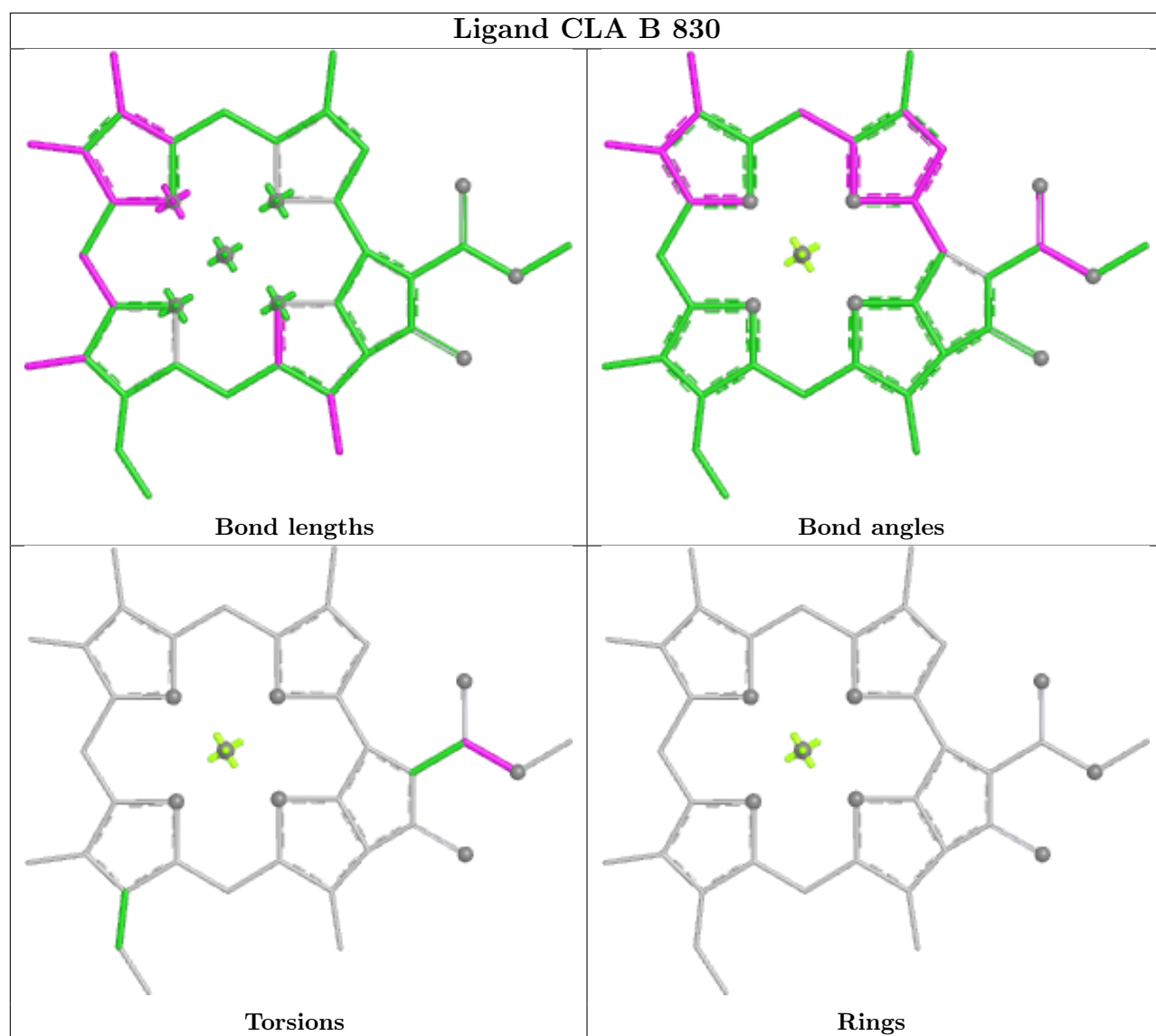
Bond angles



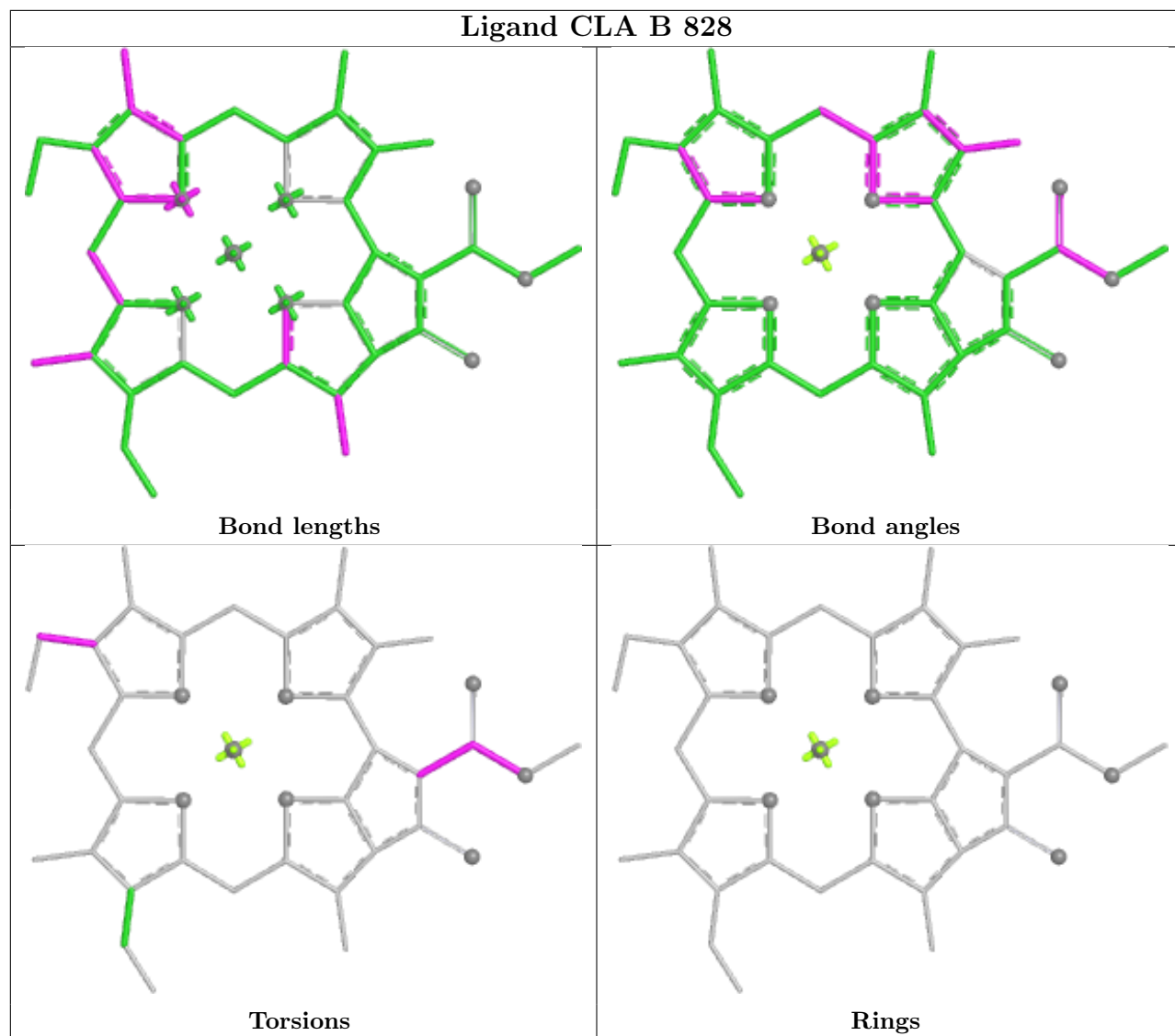
Torsions



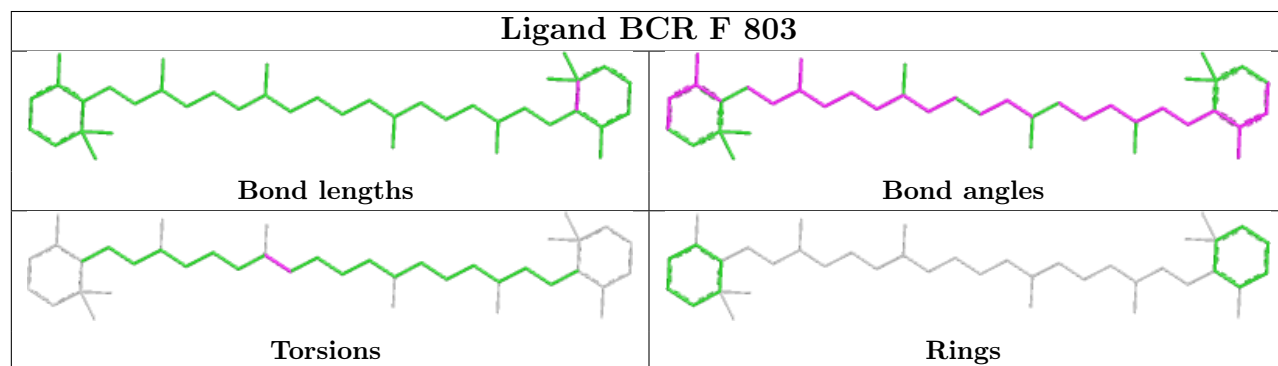
Rings

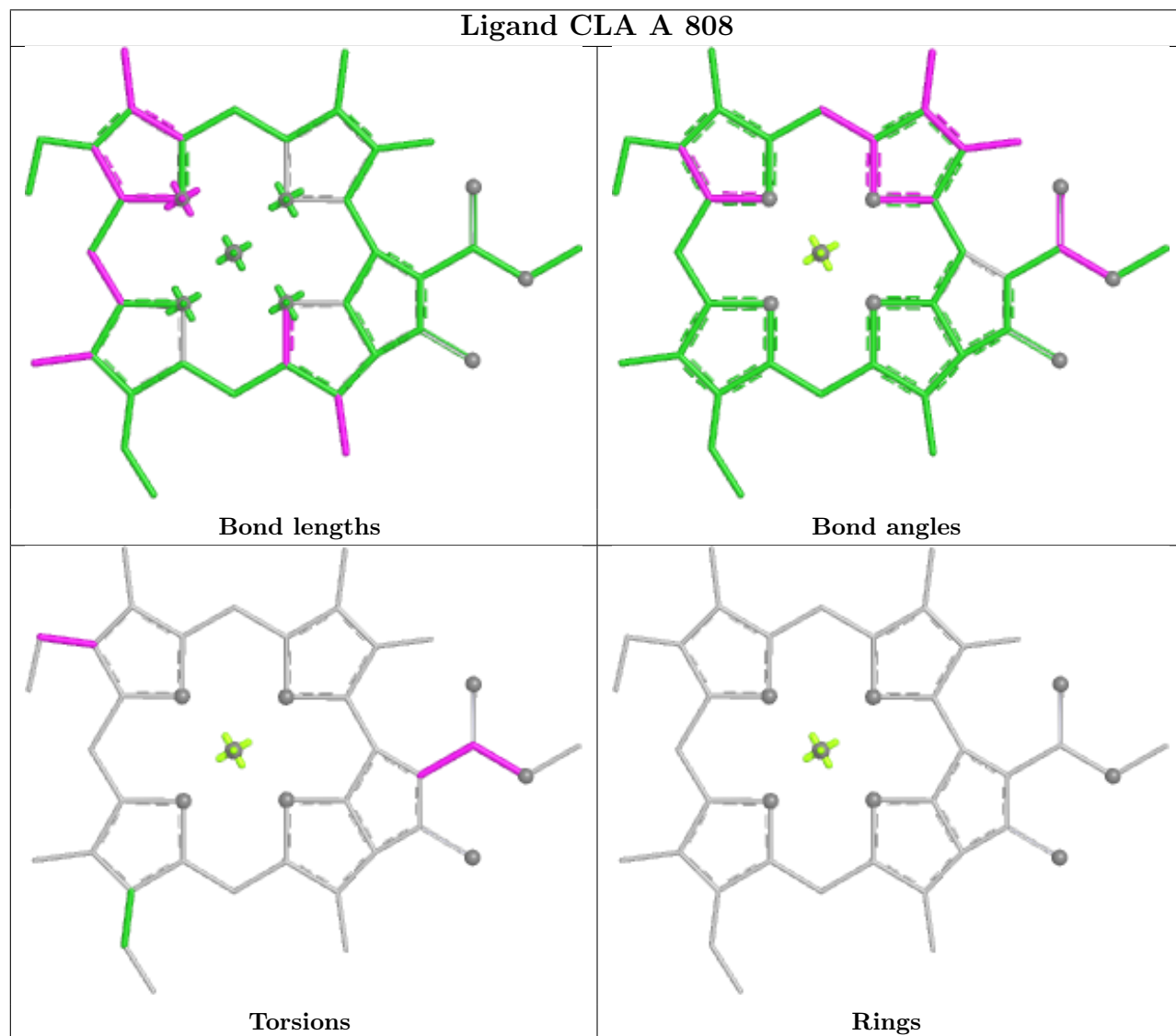
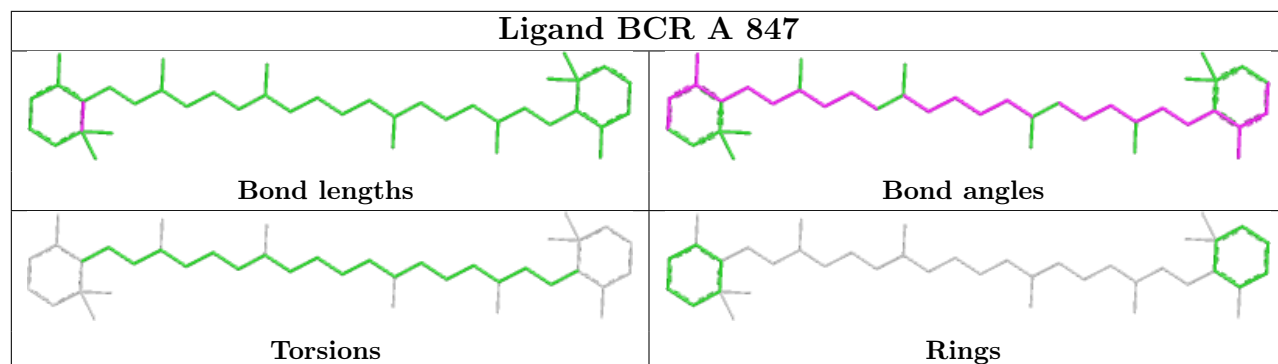


Ligand CLA B 828

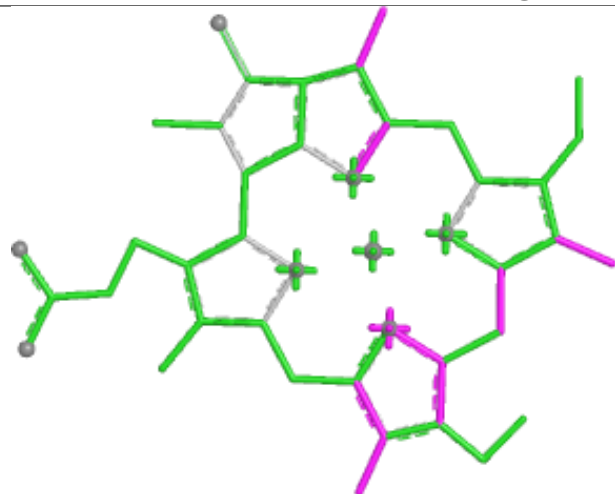


Ligand BCR F 803

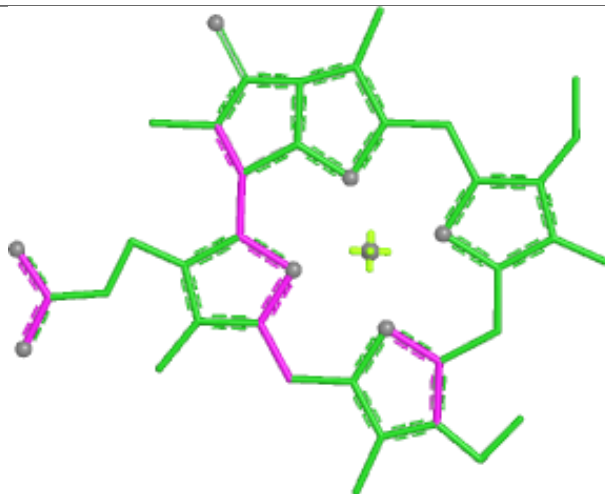




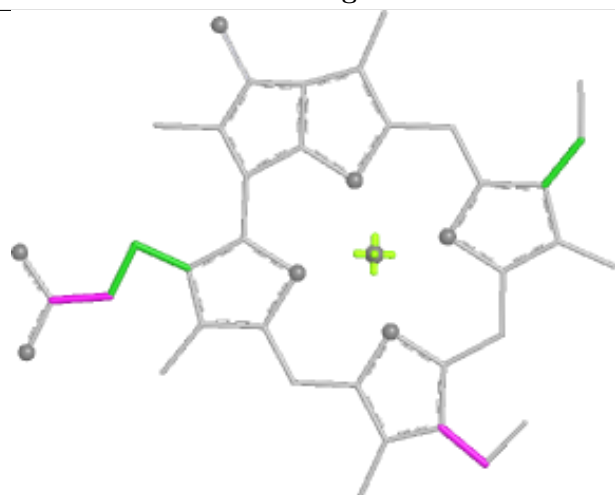
Ligand CLA A 835



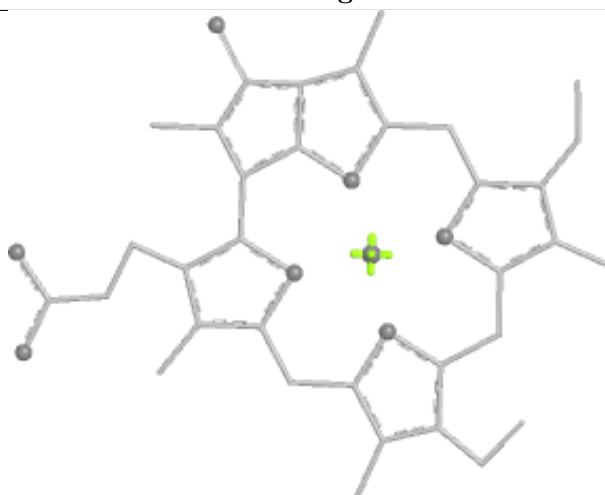
Bond lengths



Bond angles

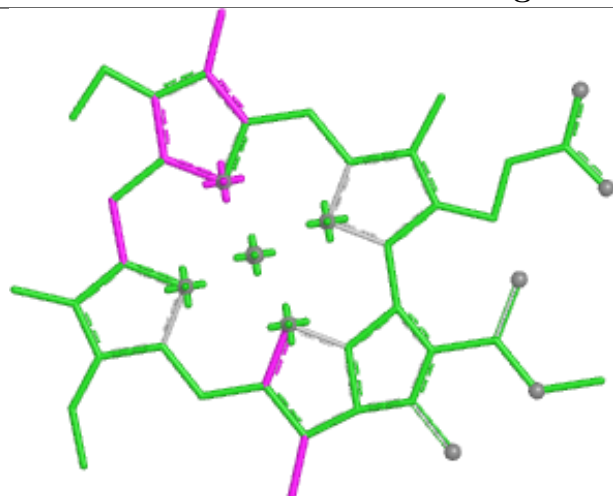


Torsions

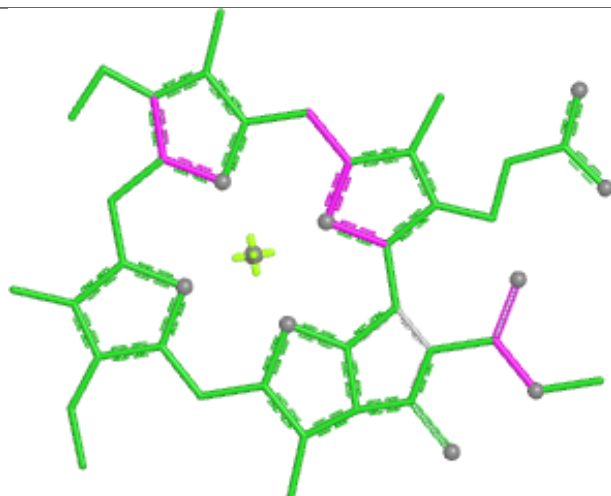


Rings

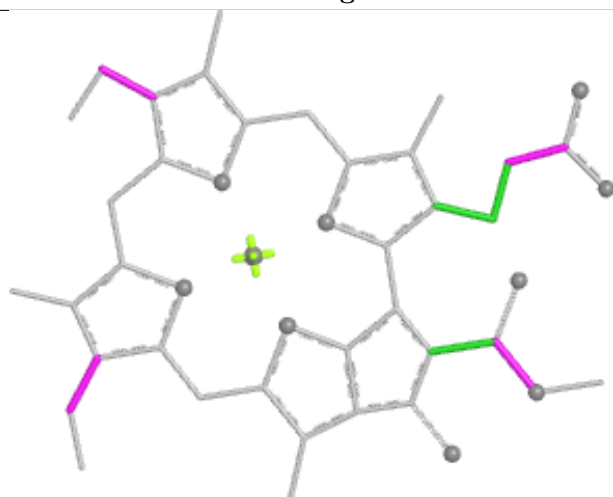
Ligand CLA A 815



Bond lengths



Bond angles

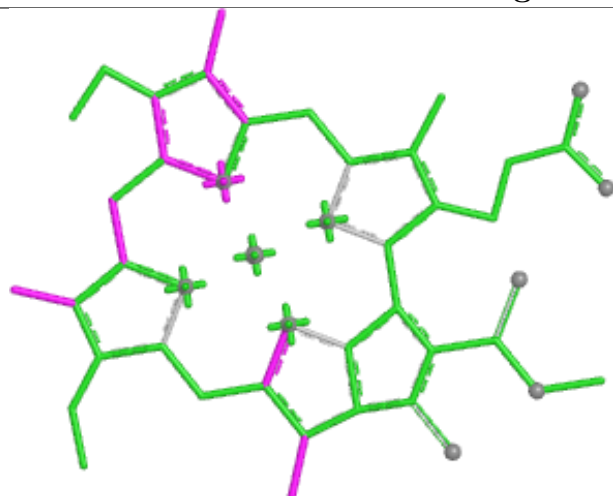


Torsions

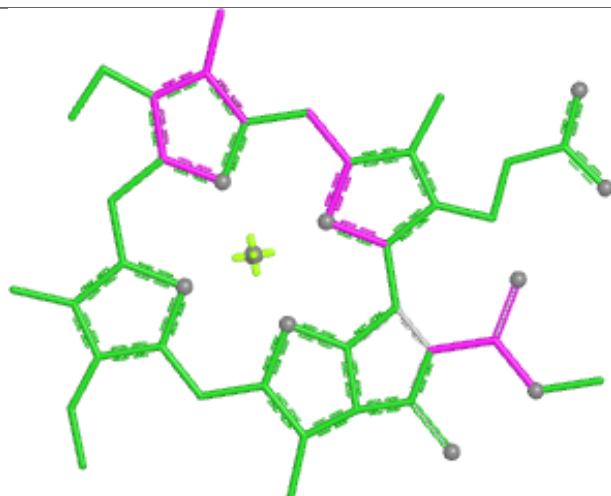


Rings

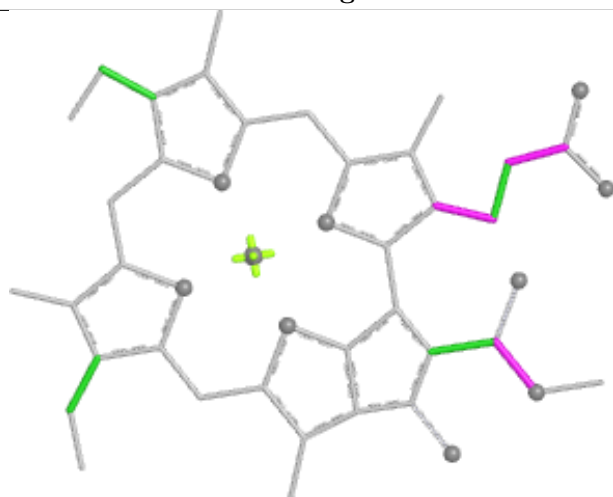
Ligand CLA A 853



Bond lengths



Bond angles

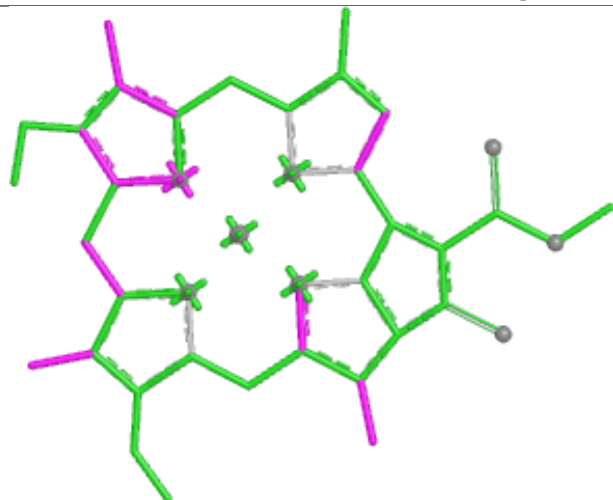


Torsions

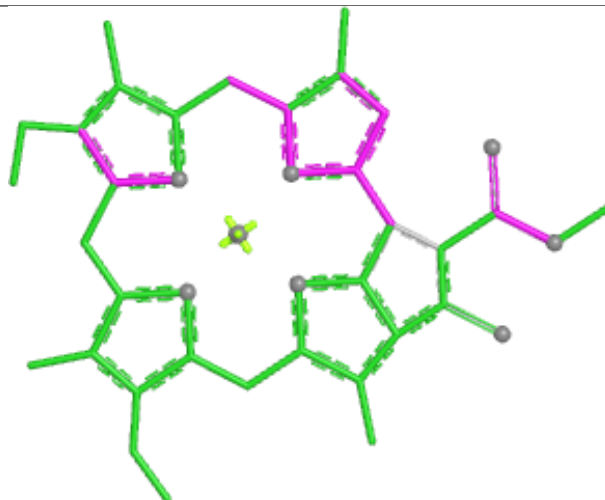


Rings

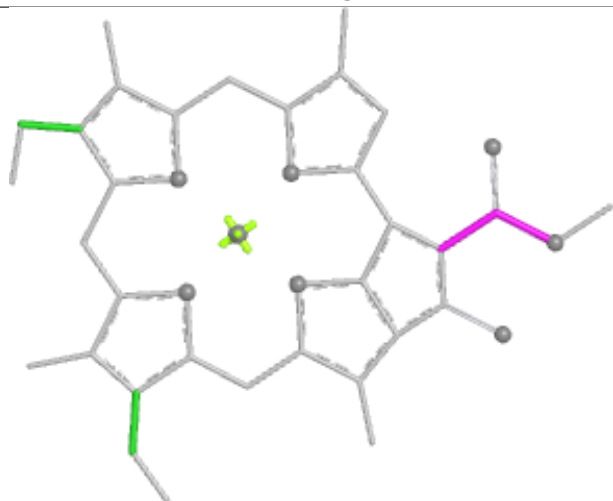
Ligand CLA B 812



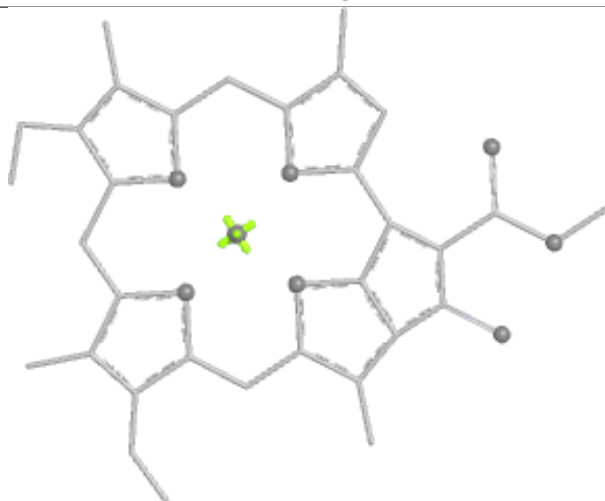
Bond lengths



Bond angles

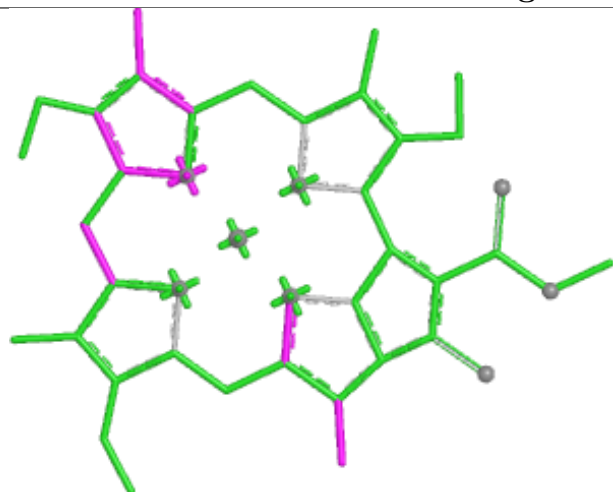


Torsions

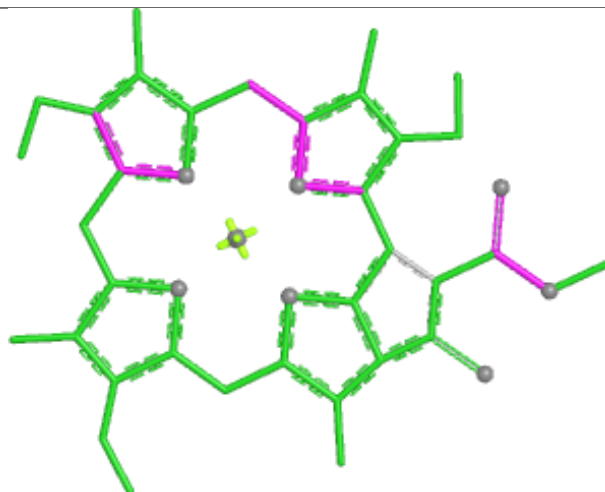


Rings

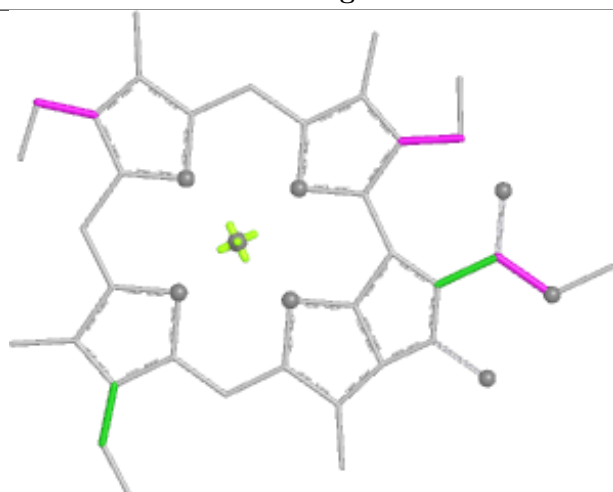
Ligand CLA J 102



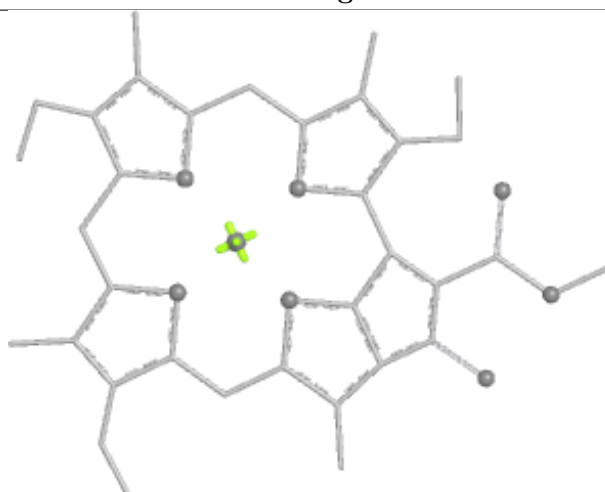
Bond lengths



Bond angles

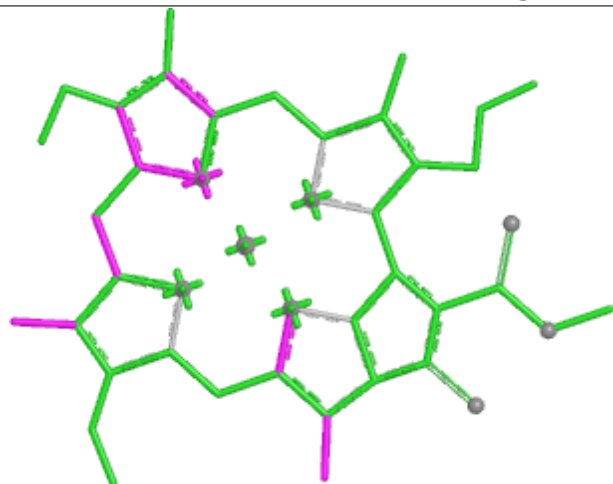


Torsions

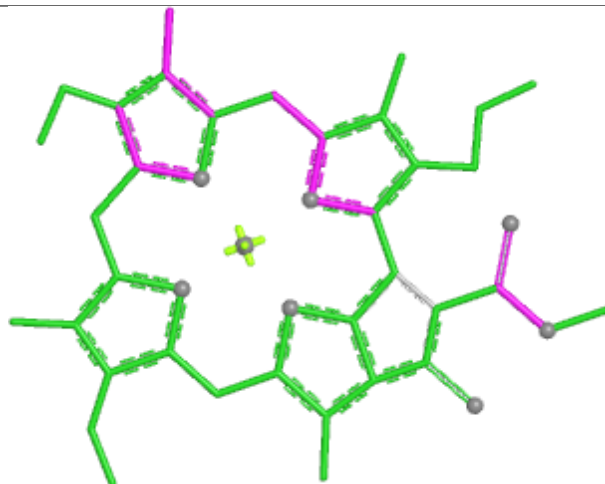


Rings

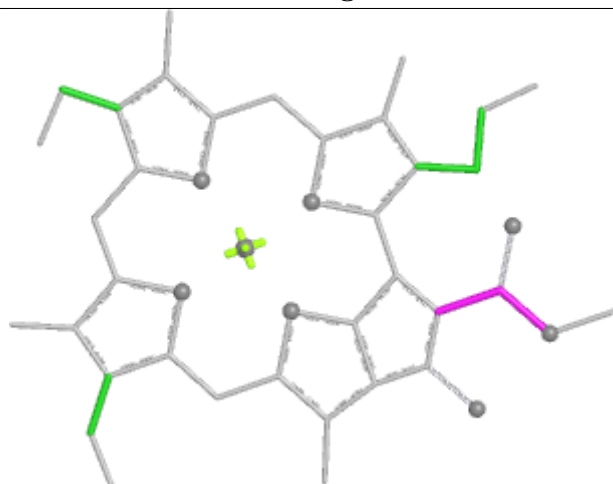
Ligand CLA B 834



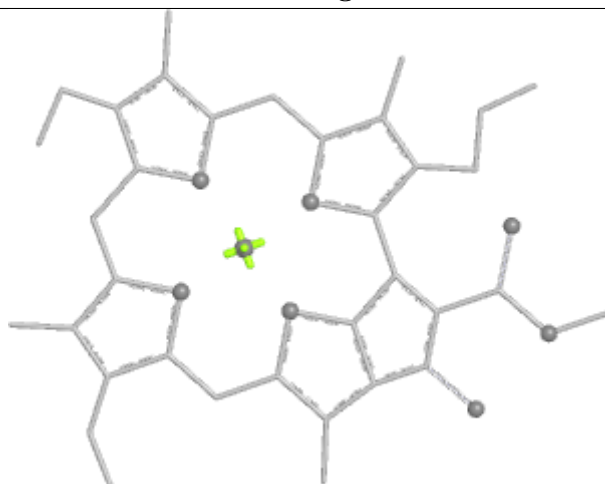
Bond lengths



Bond angles

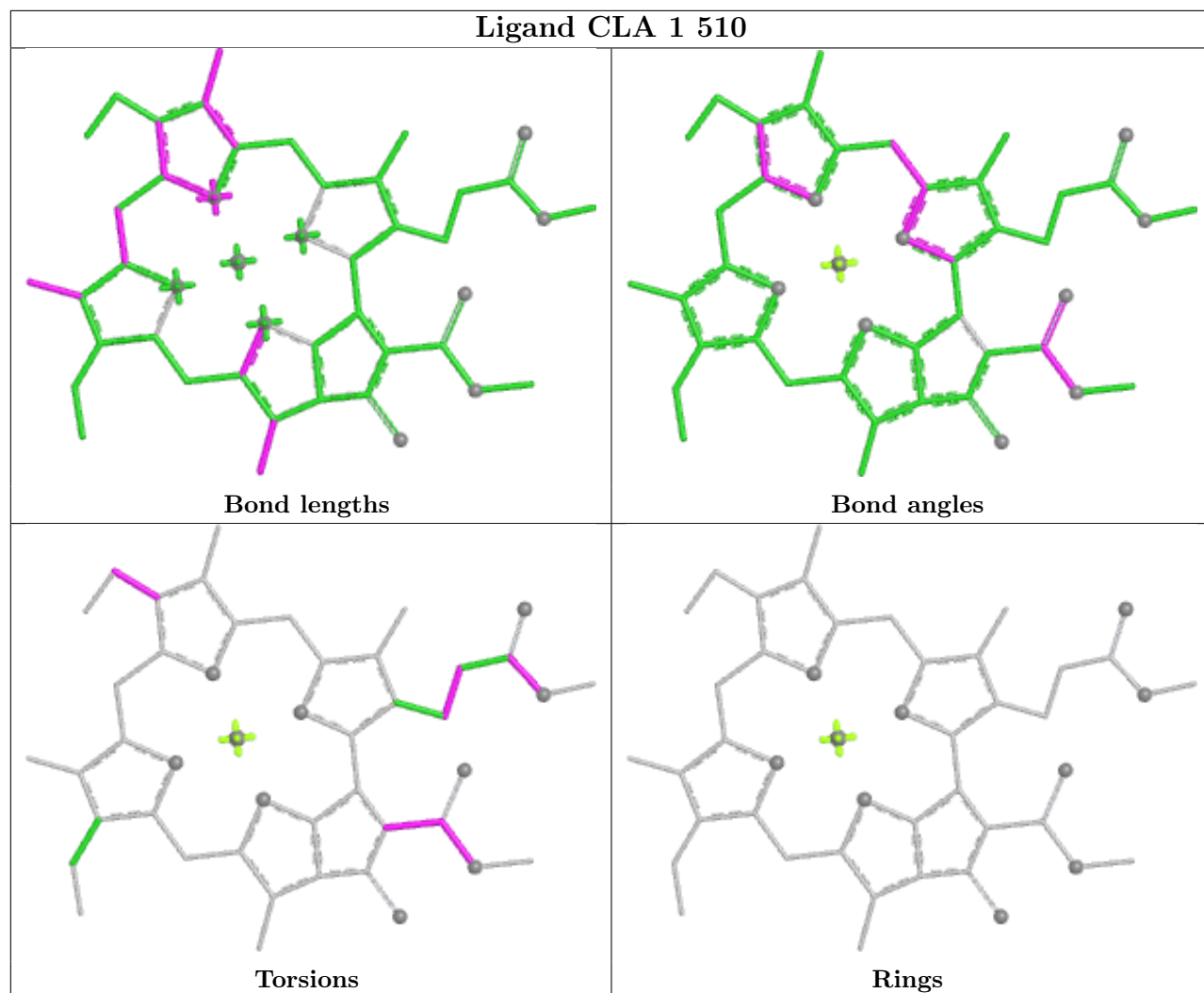


Torsions

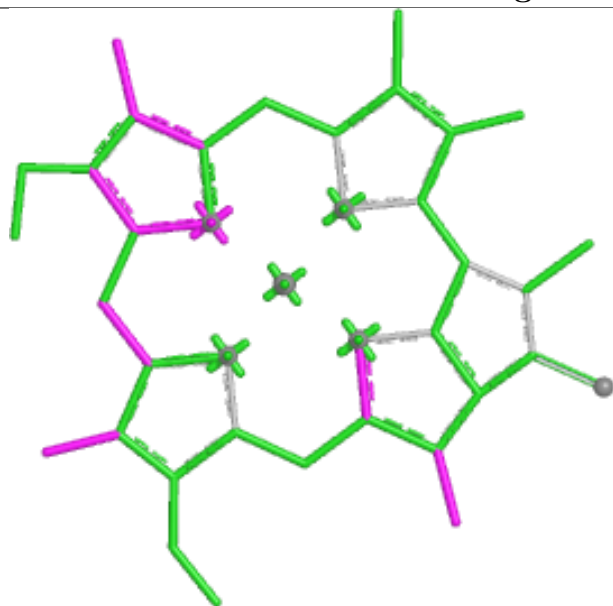


Rings

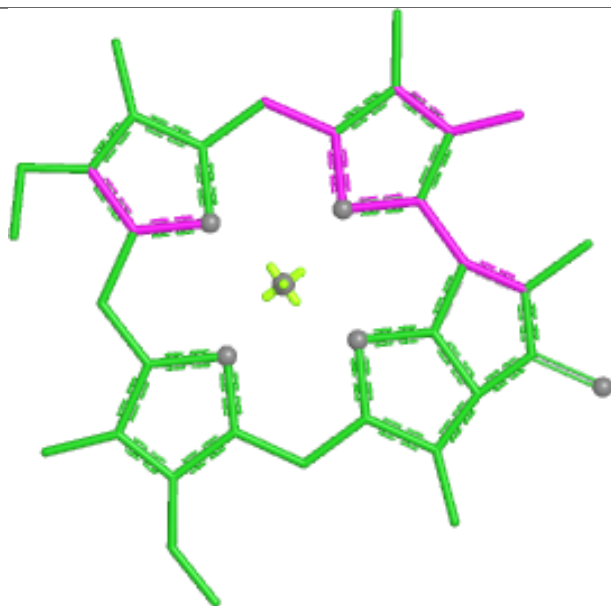
Ligand CLA 1 510



Ligand CLA B 843



Bond lengths



Bond angles

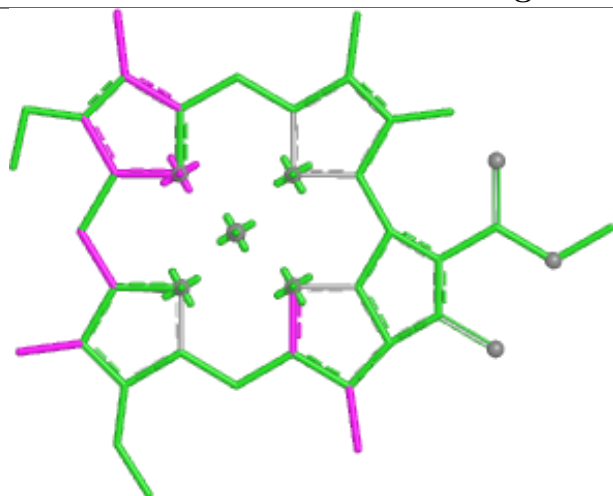


Torsions

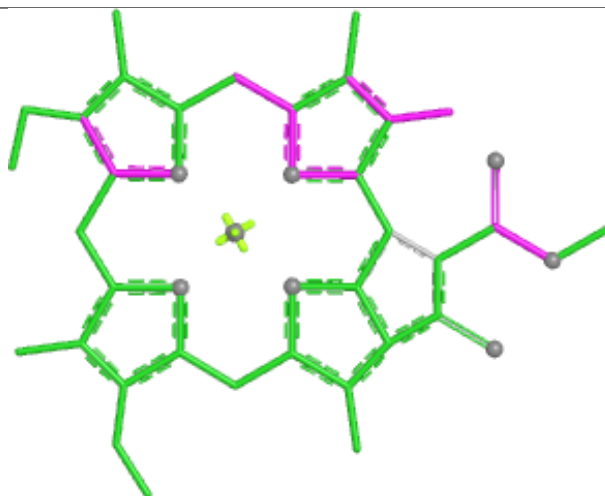


Rings

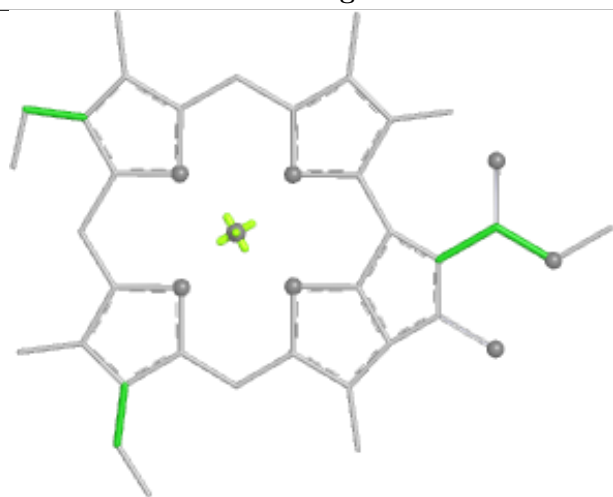
Ligand CLA B 806



Bond lengths



Bond angles

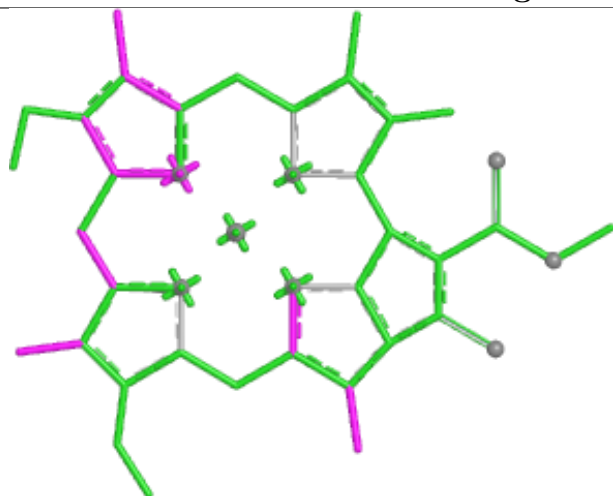


Torsions

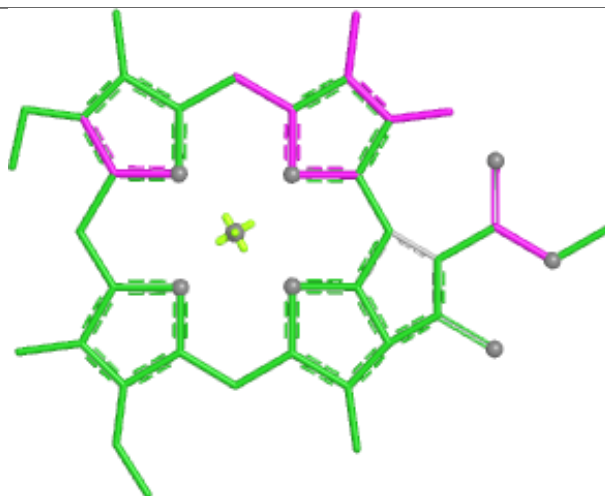


Rings

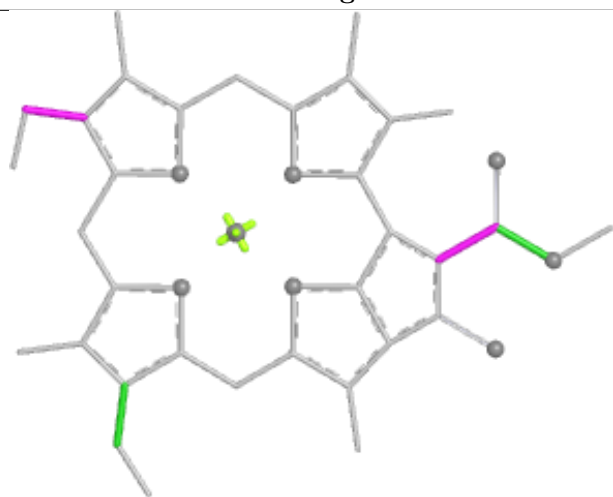
Ligand CLA A 811



Bond lengths



Bond angles

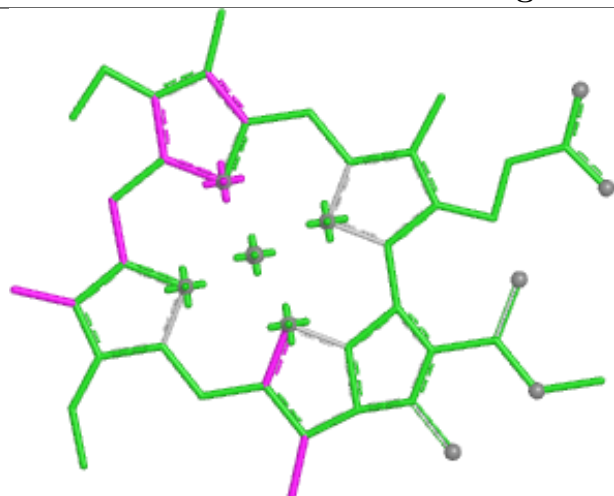


Torsions

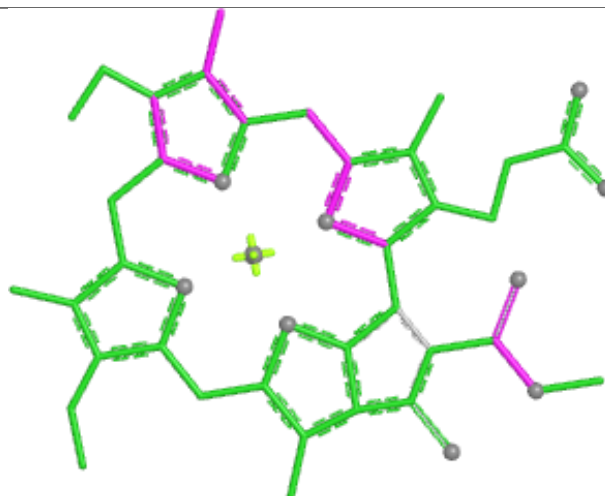


Rings

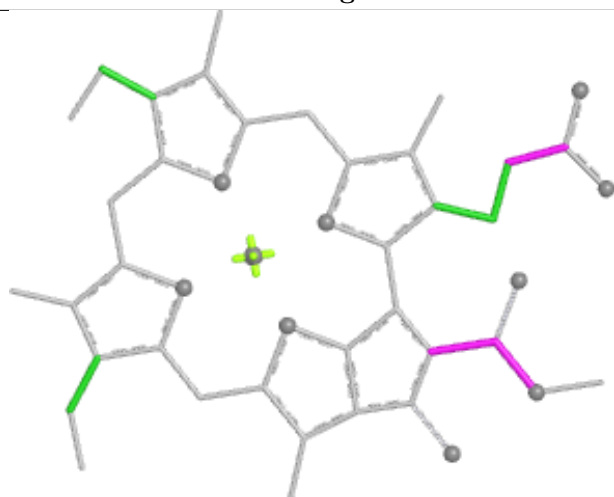
Ligand CLA L 304



Bond lengths



Bond angles

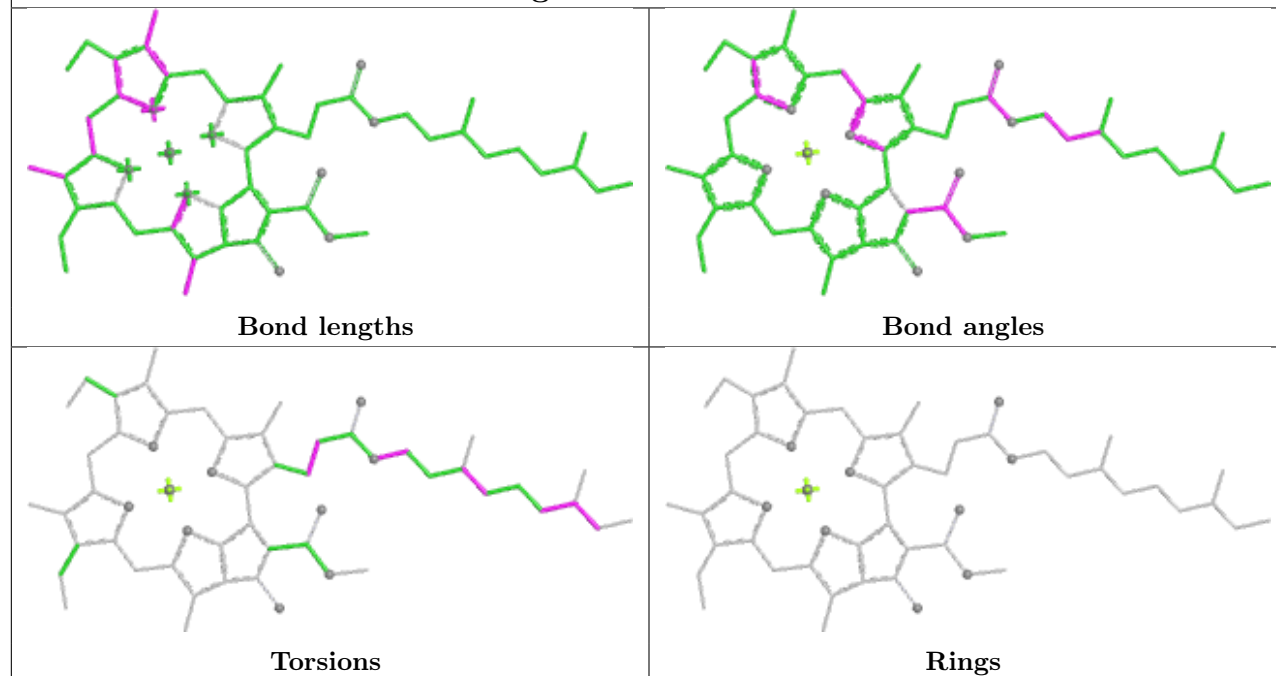


Torsions

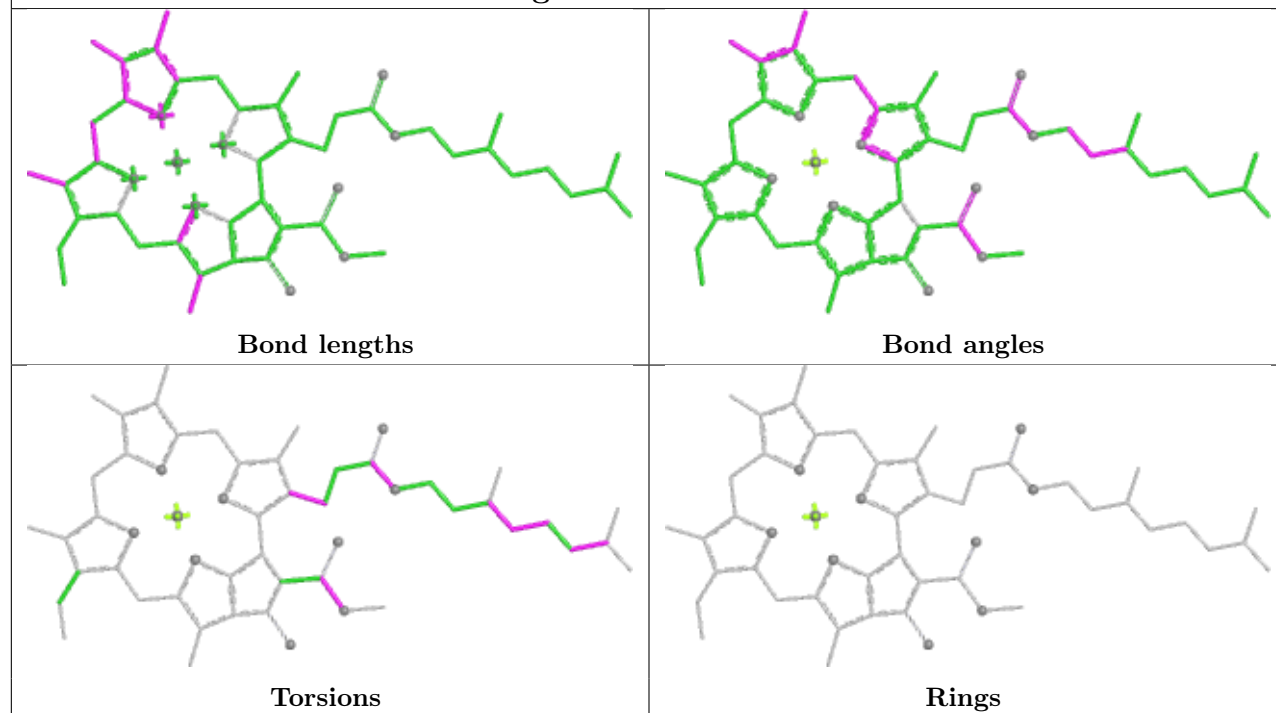


Rings

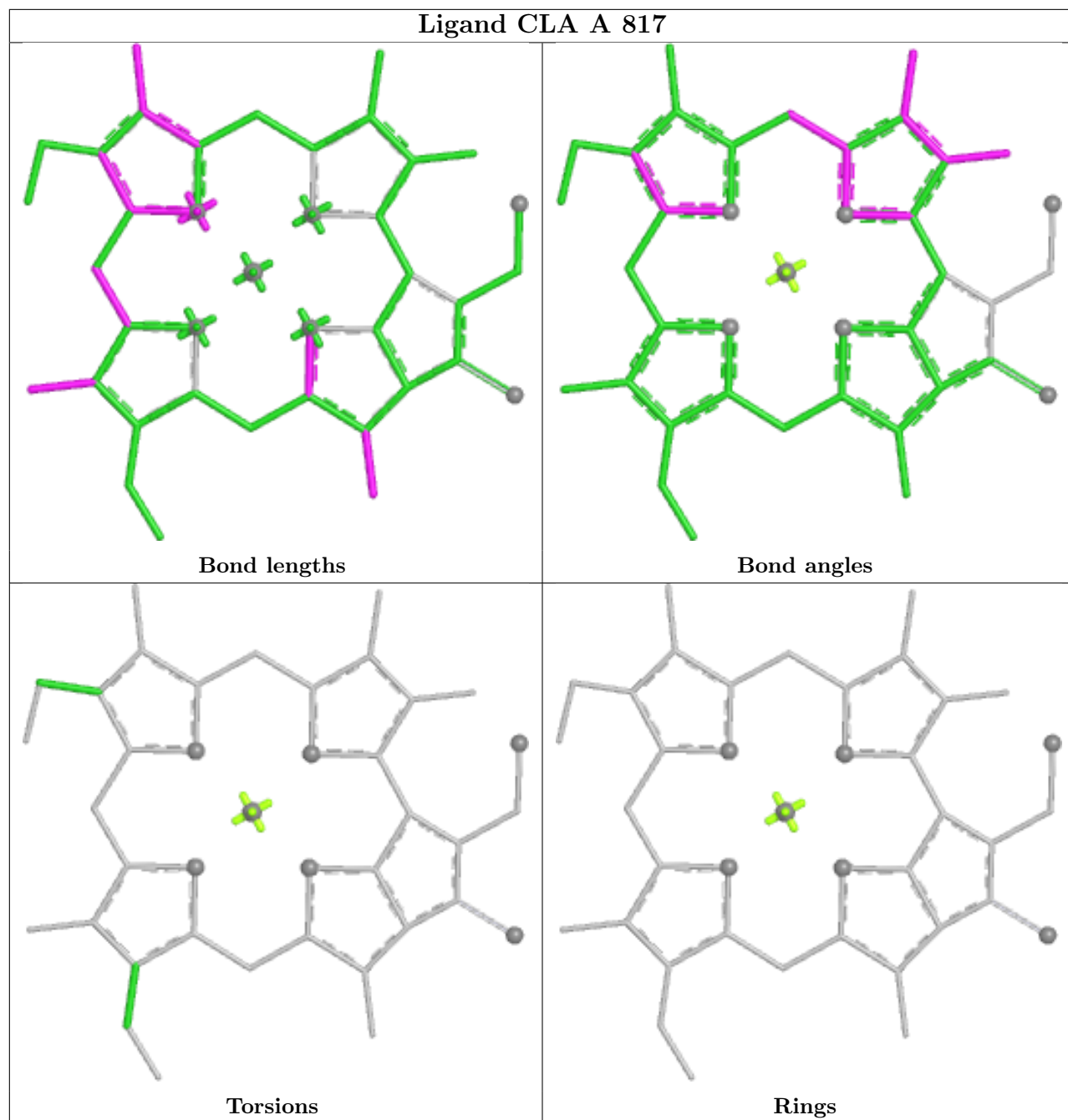
Ligand CLA A 824



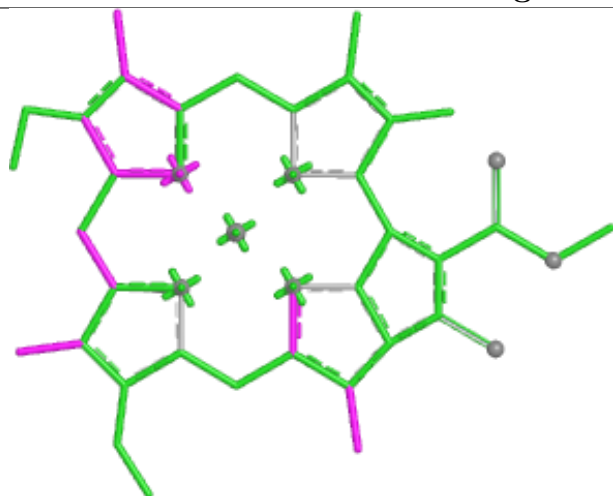
Ligand CLA B 813



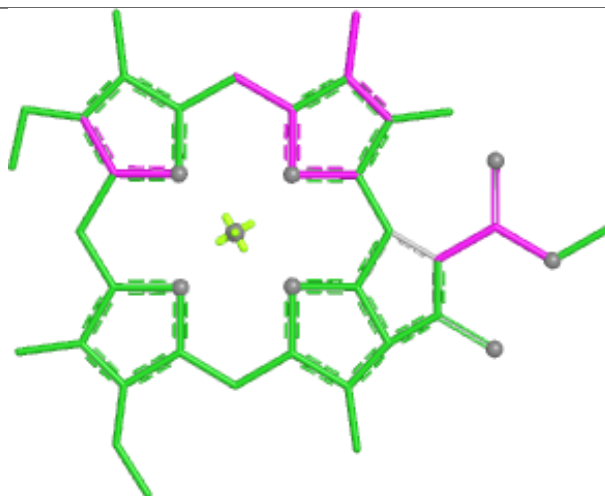
Ligand CLA A 817



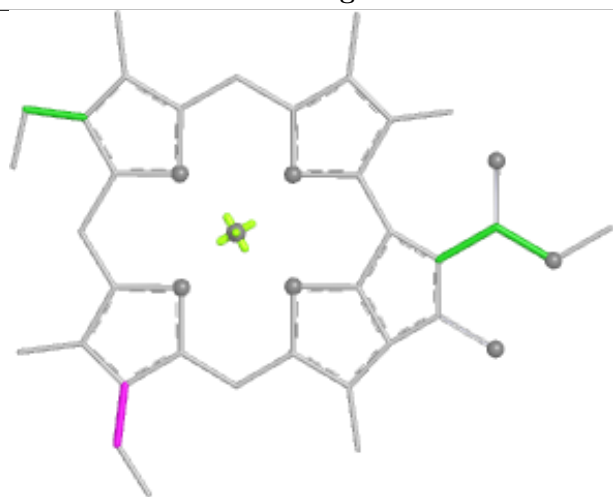
Ligand CLA A 827



Bond lengths



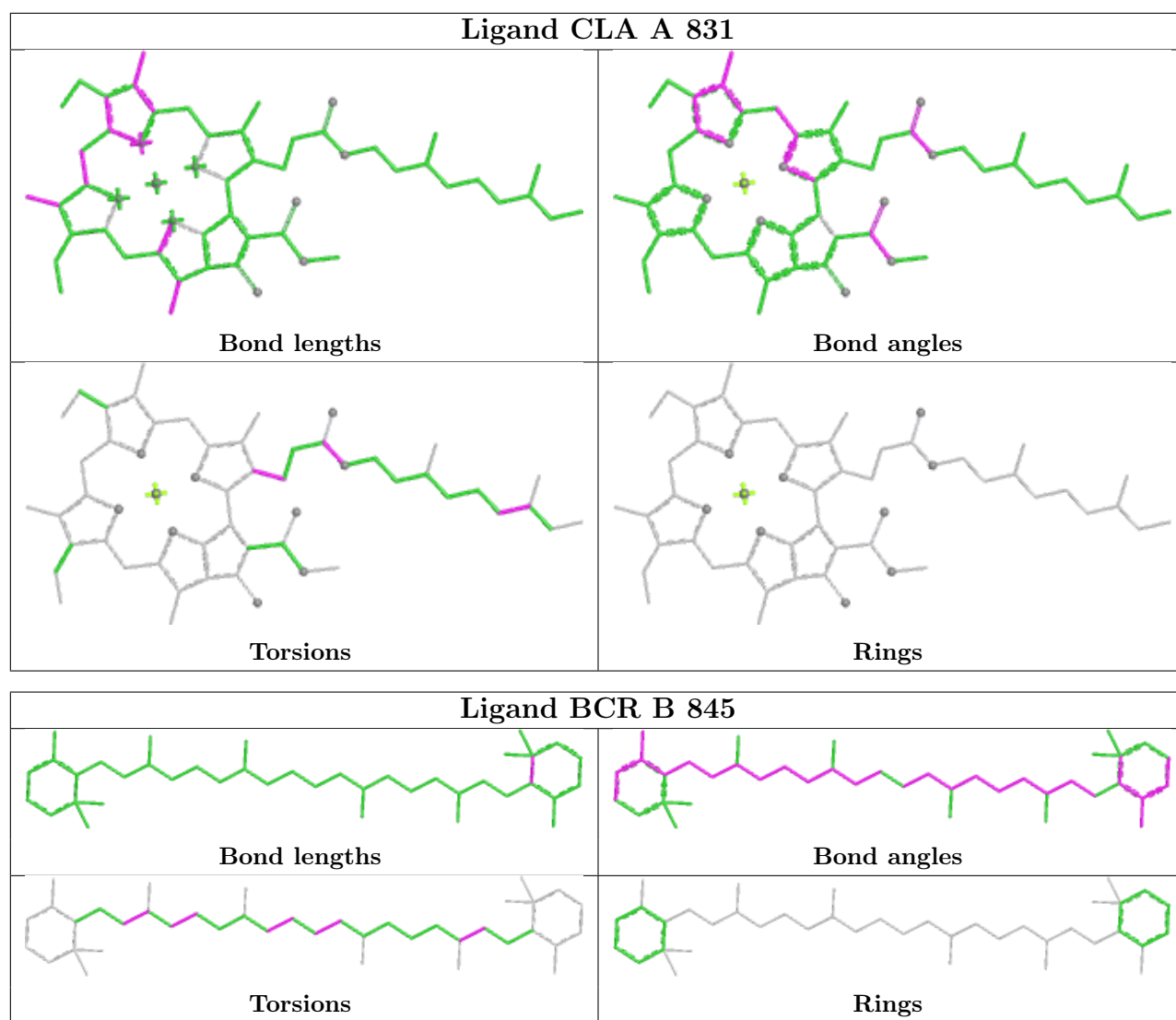
Bond angles



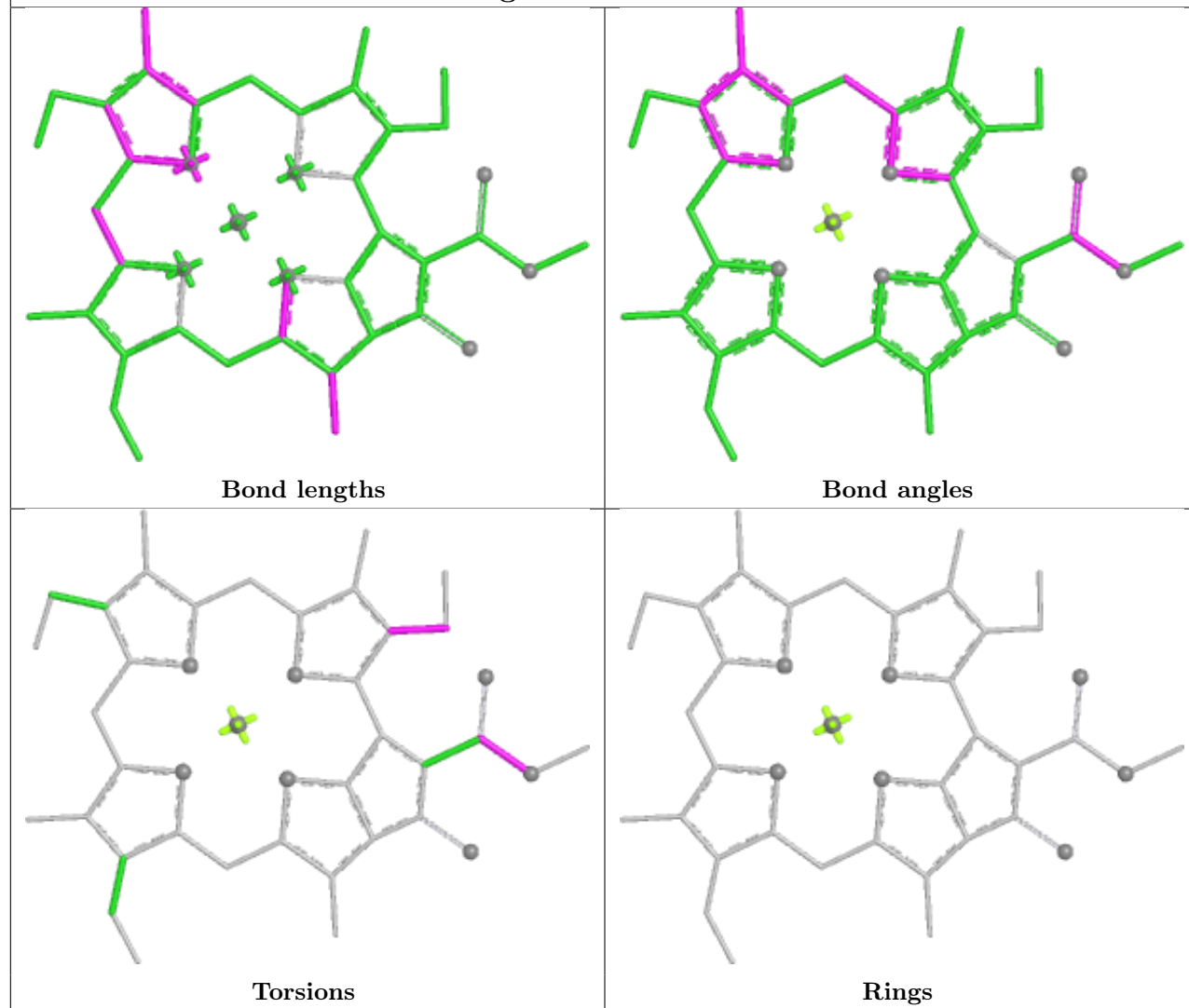
Torsions



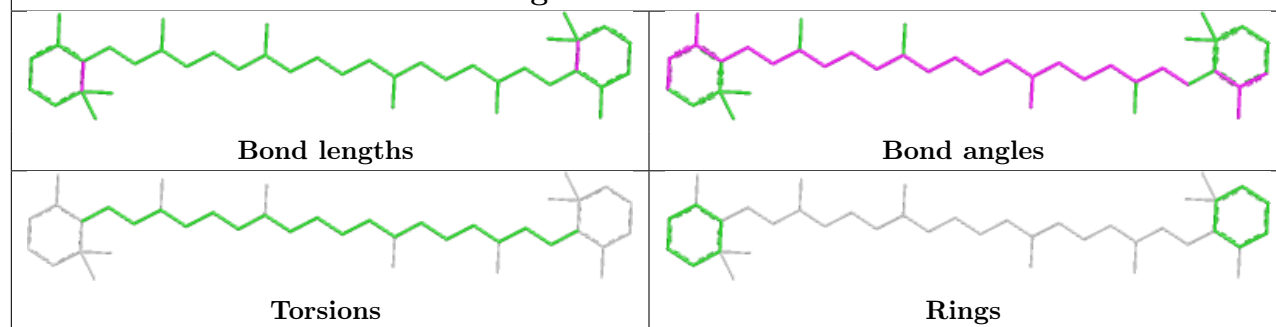
Rings



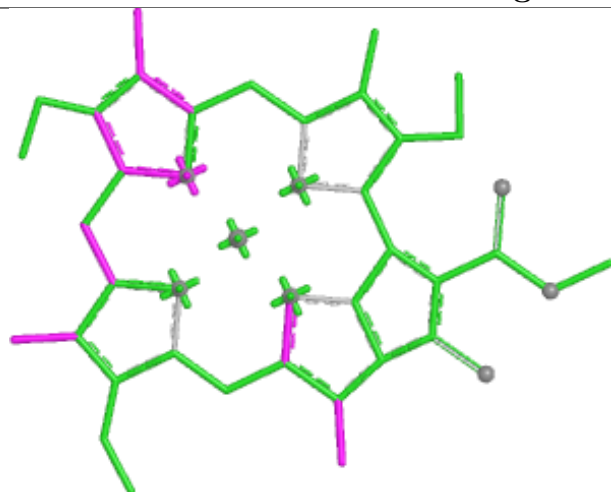
Ligand CLA 3 308



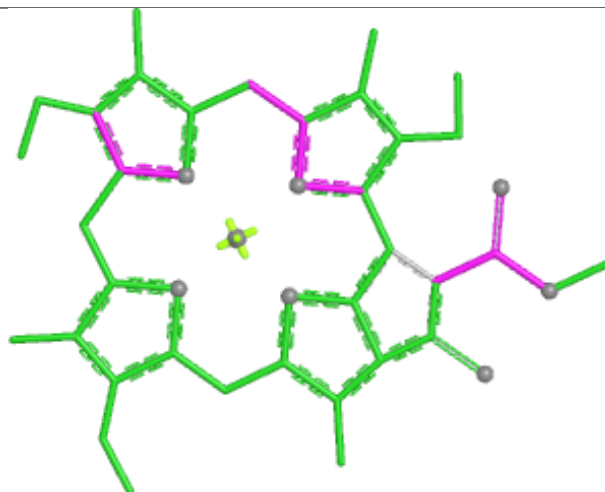
Ligand BCR B 849



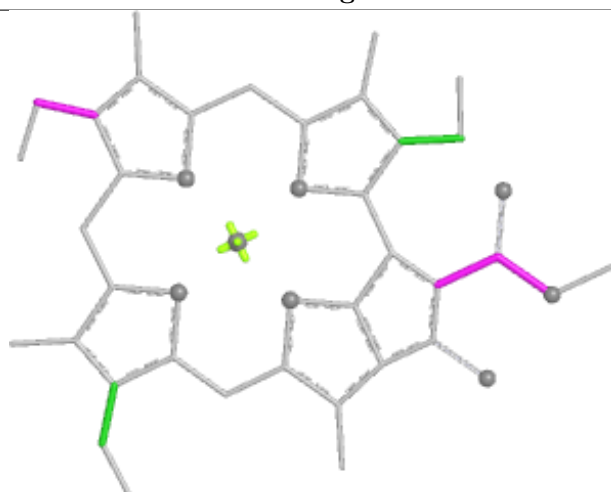
Ligand CLA A 807



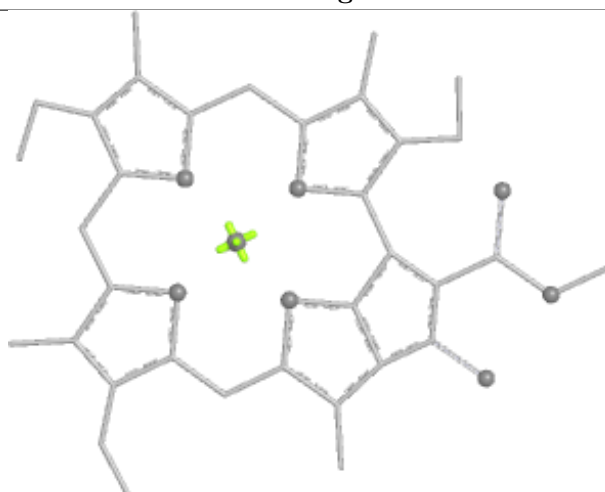
Bond lengths



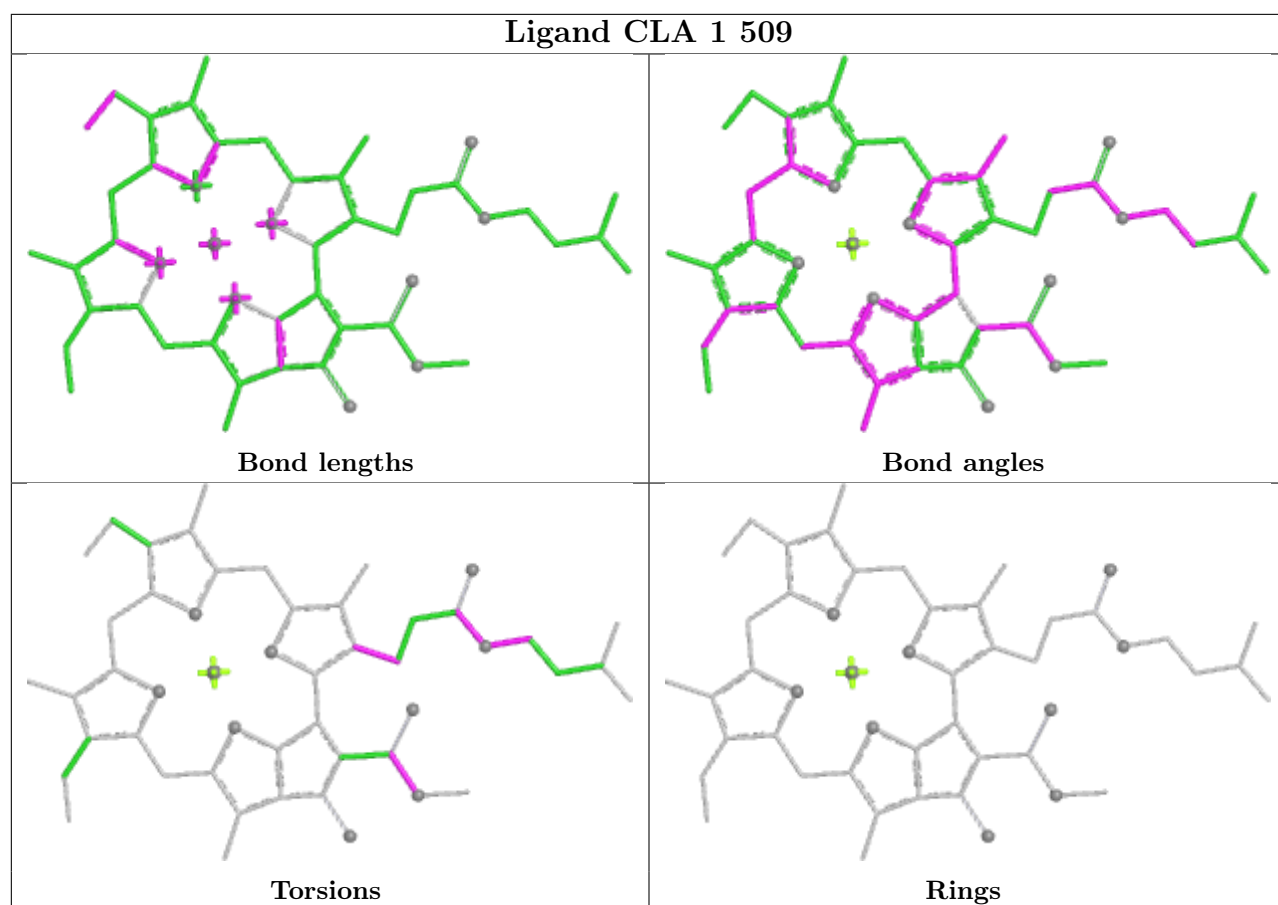
Bond angles

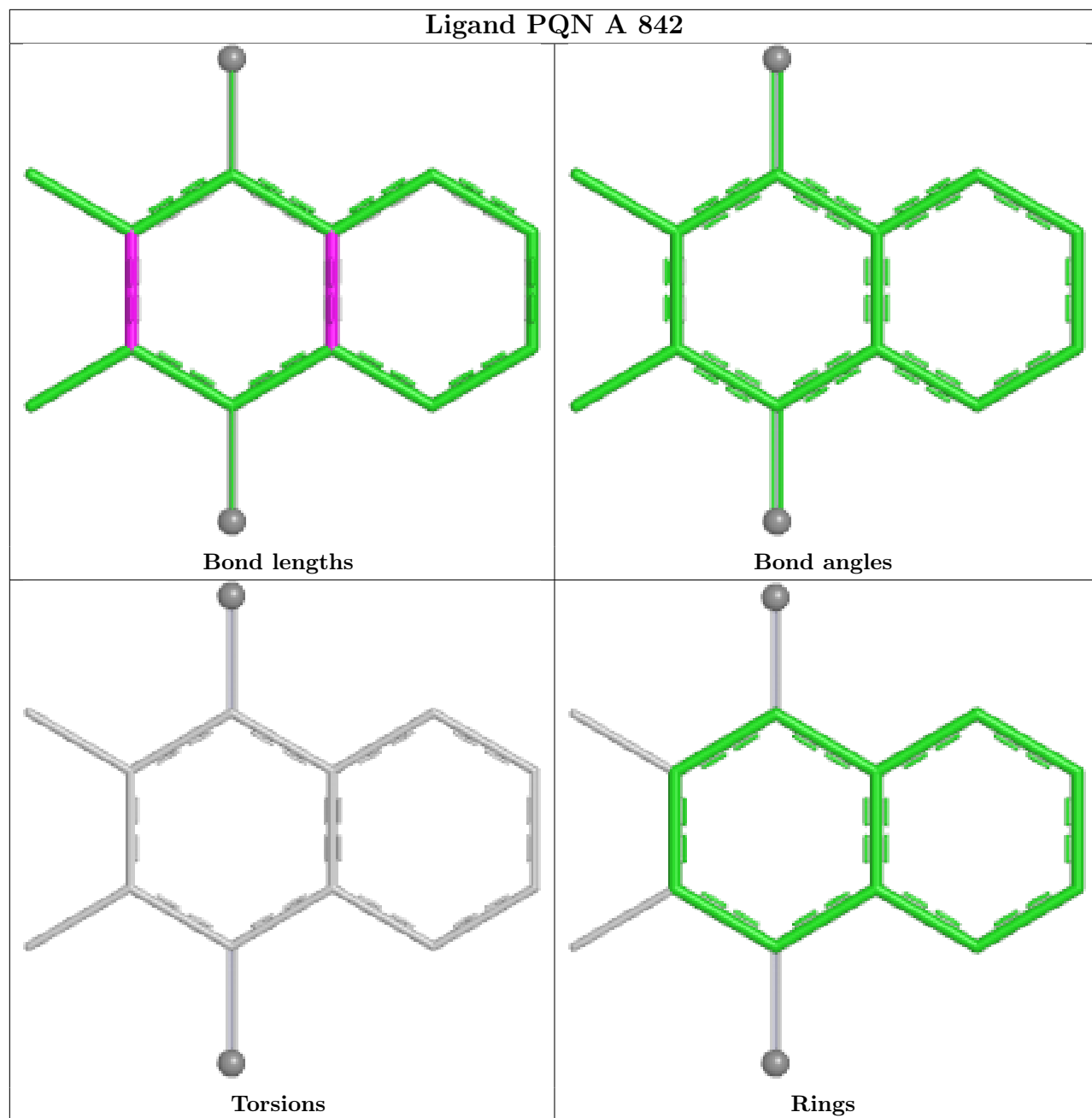


Torsions

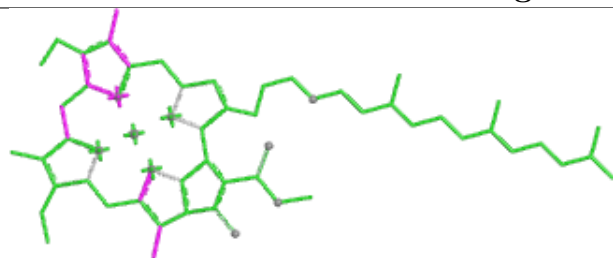


Rings

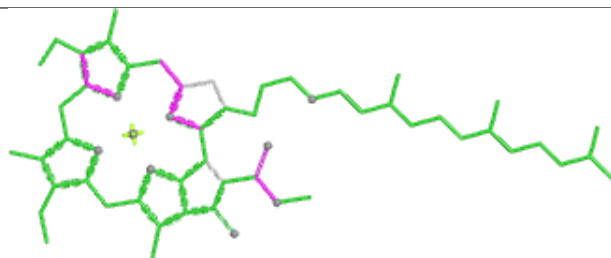




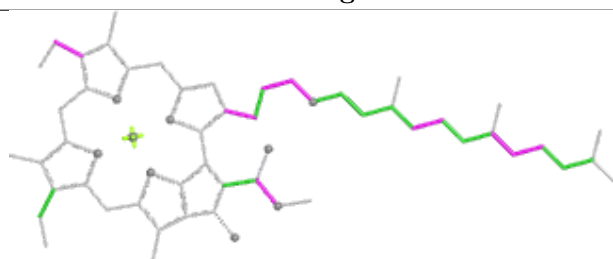
Ligand CLA B 836



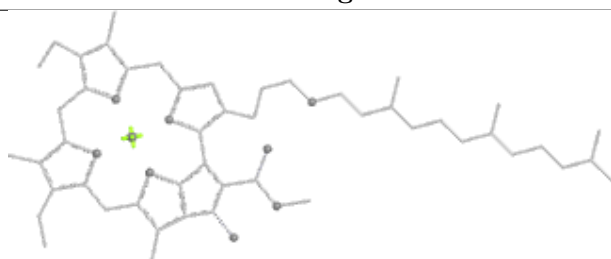
Bond lengths



Bond angles

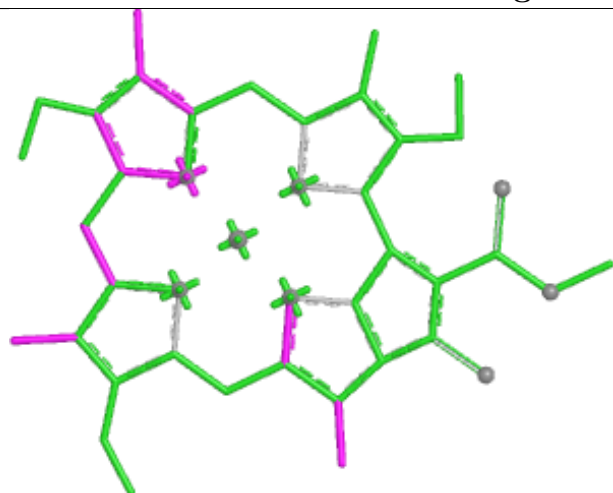


Torsions

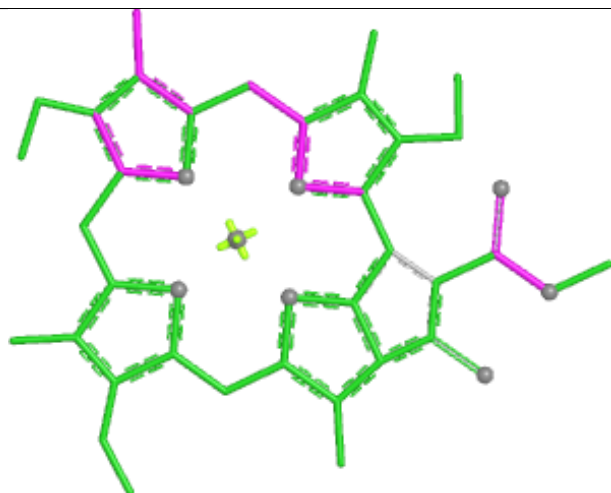


Rings

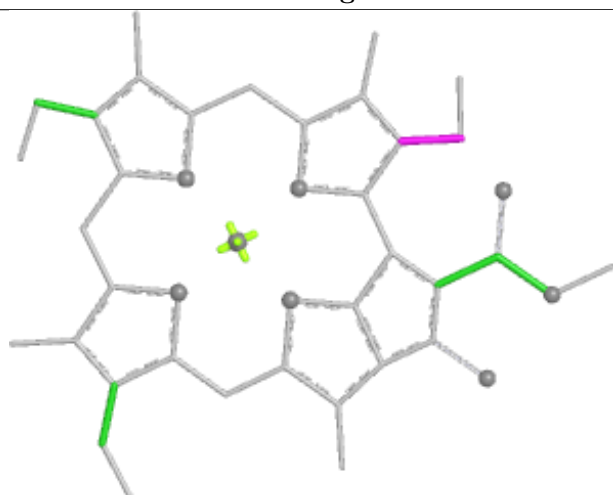
Ligand CLA A 813



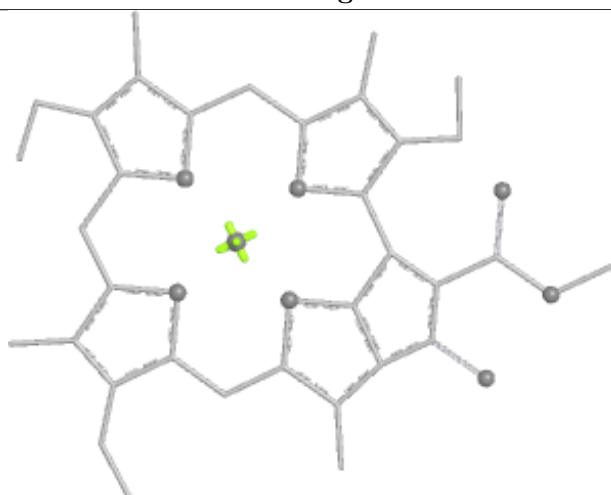
Bond lengths



Bond angles

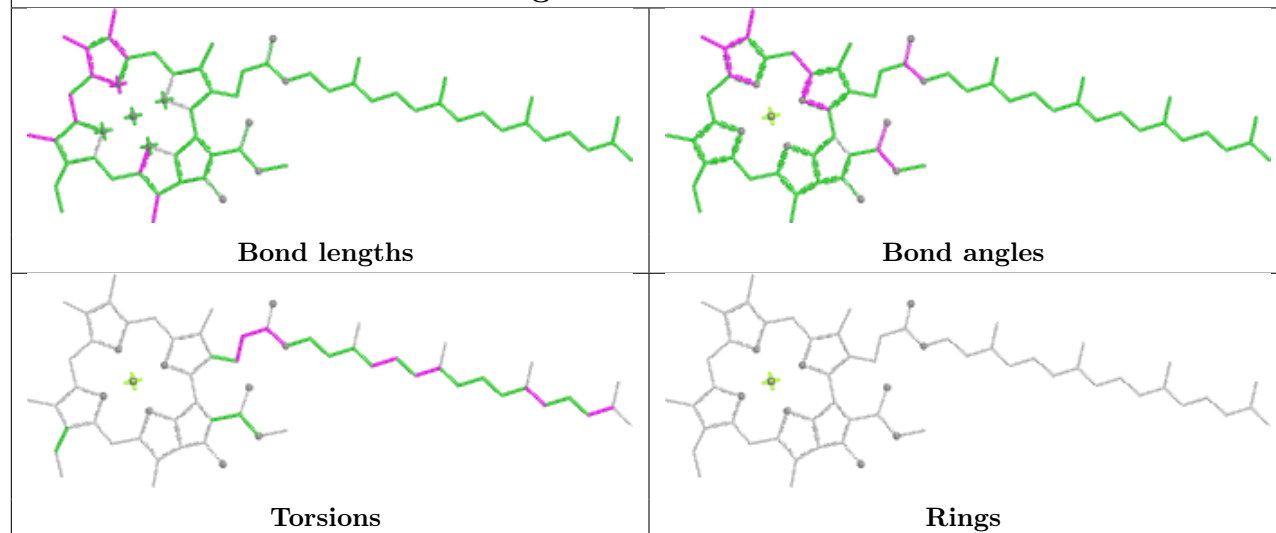


Torsions

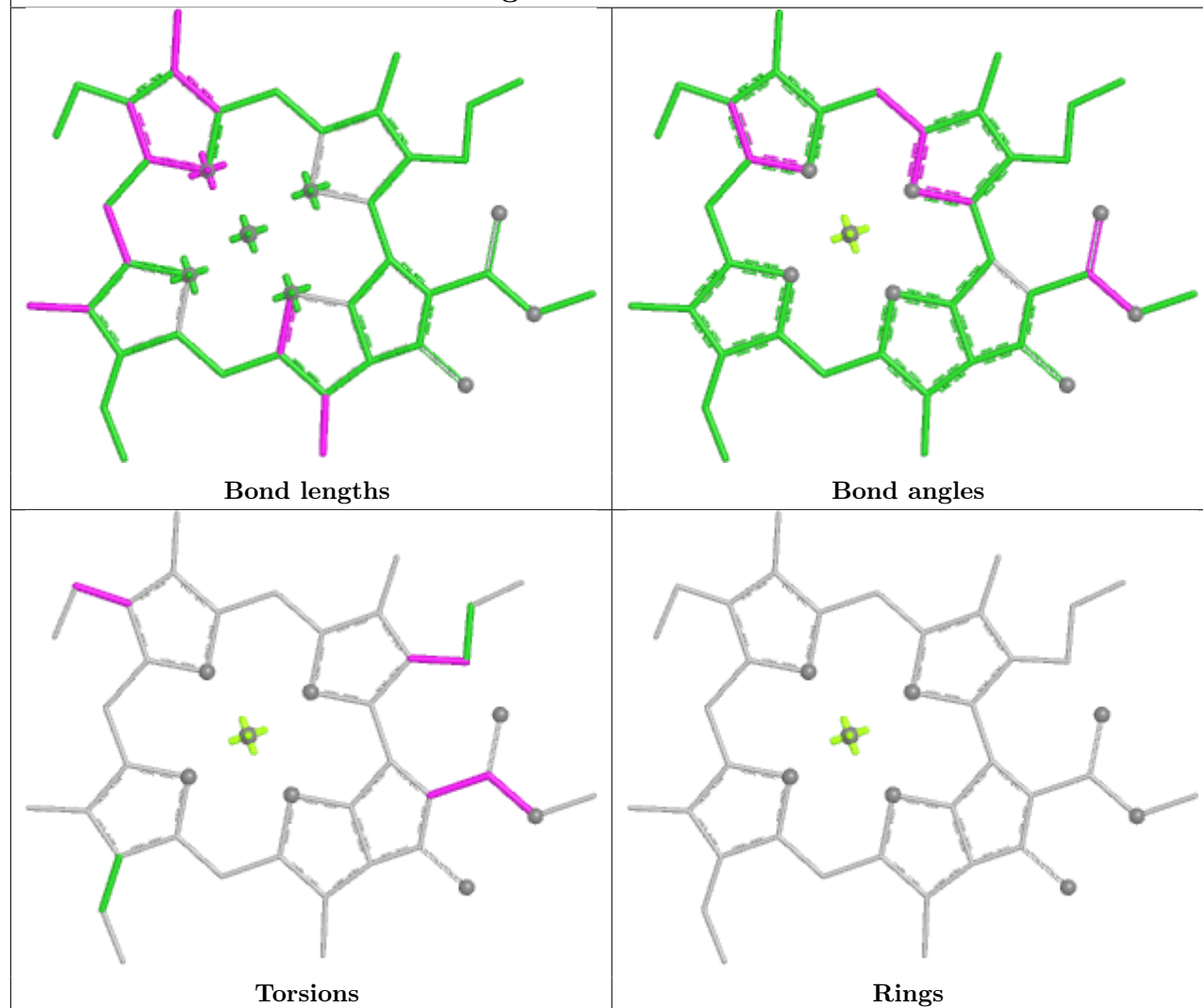


Rings

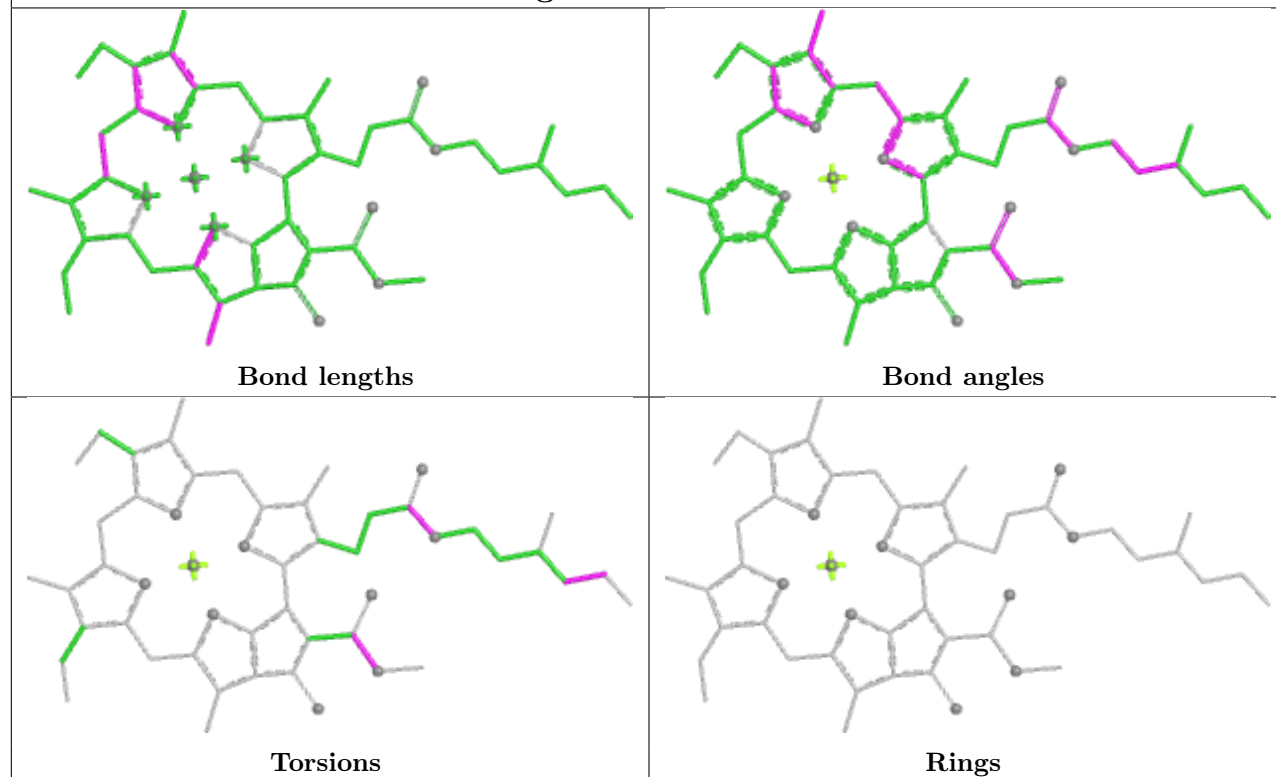
Ligand CLA B 801



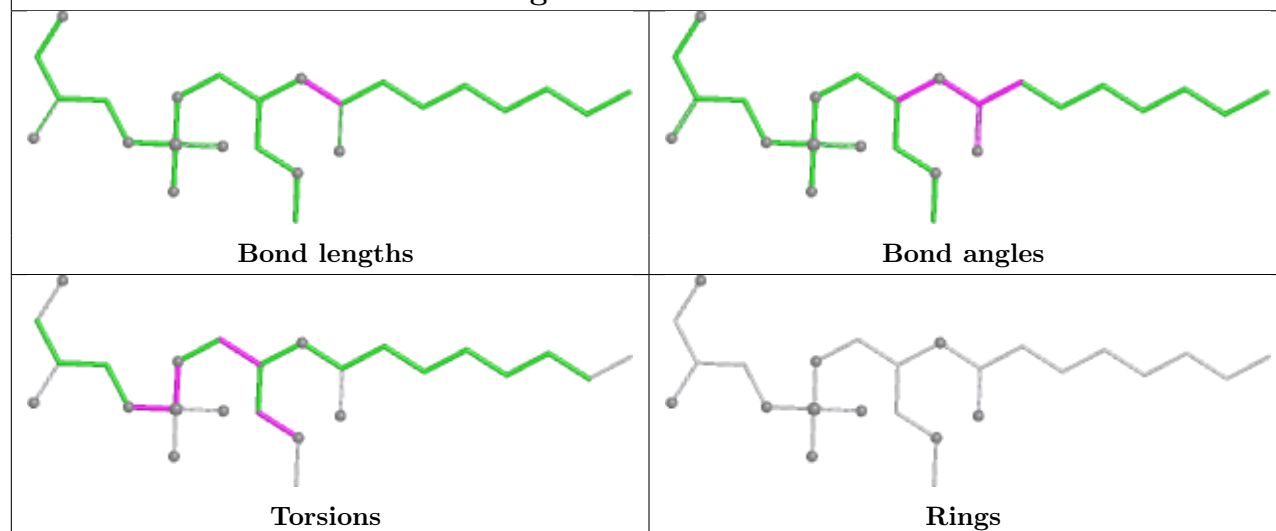
Ligand CLA B 817



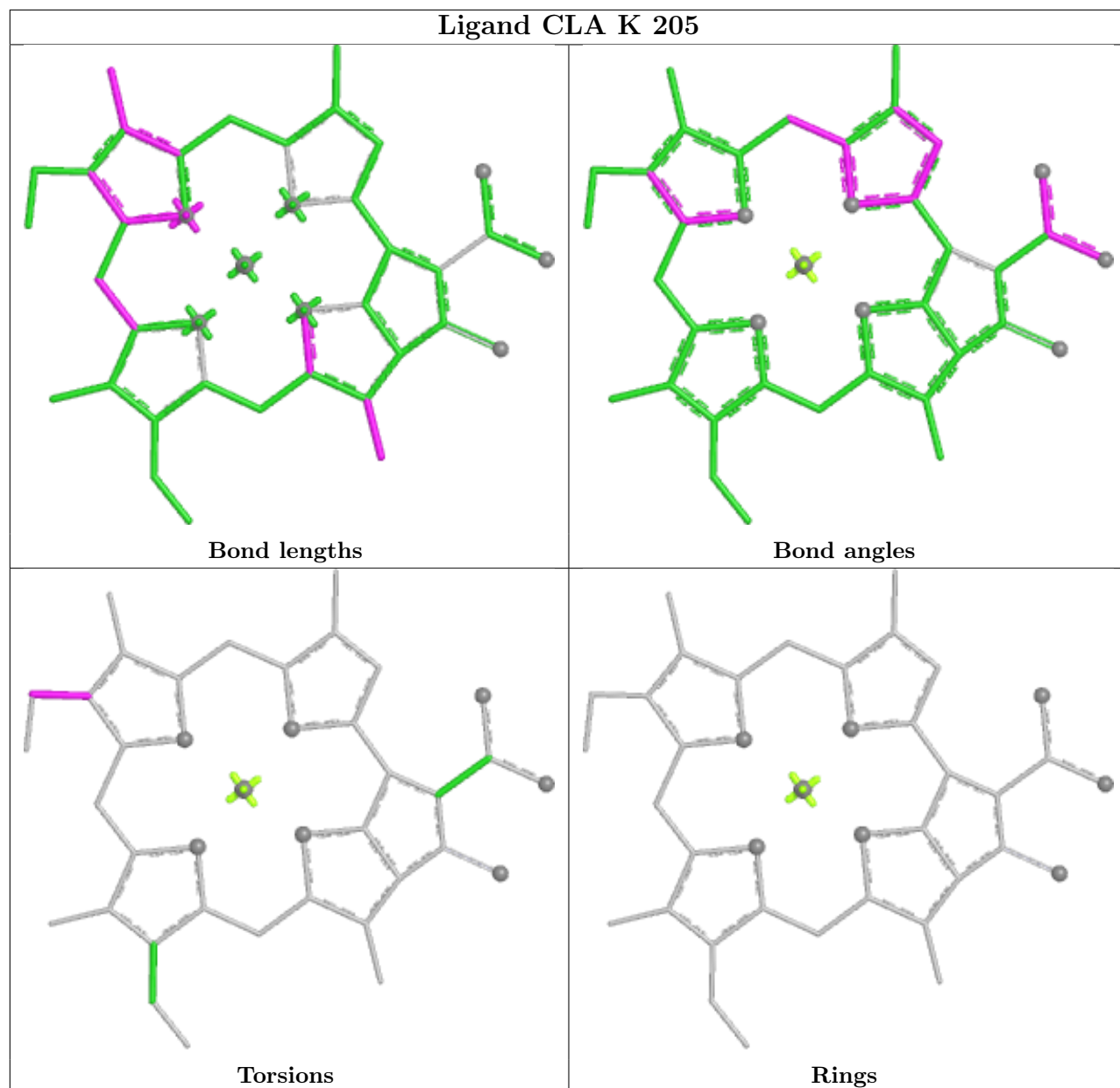
Ligand CLA 1 513

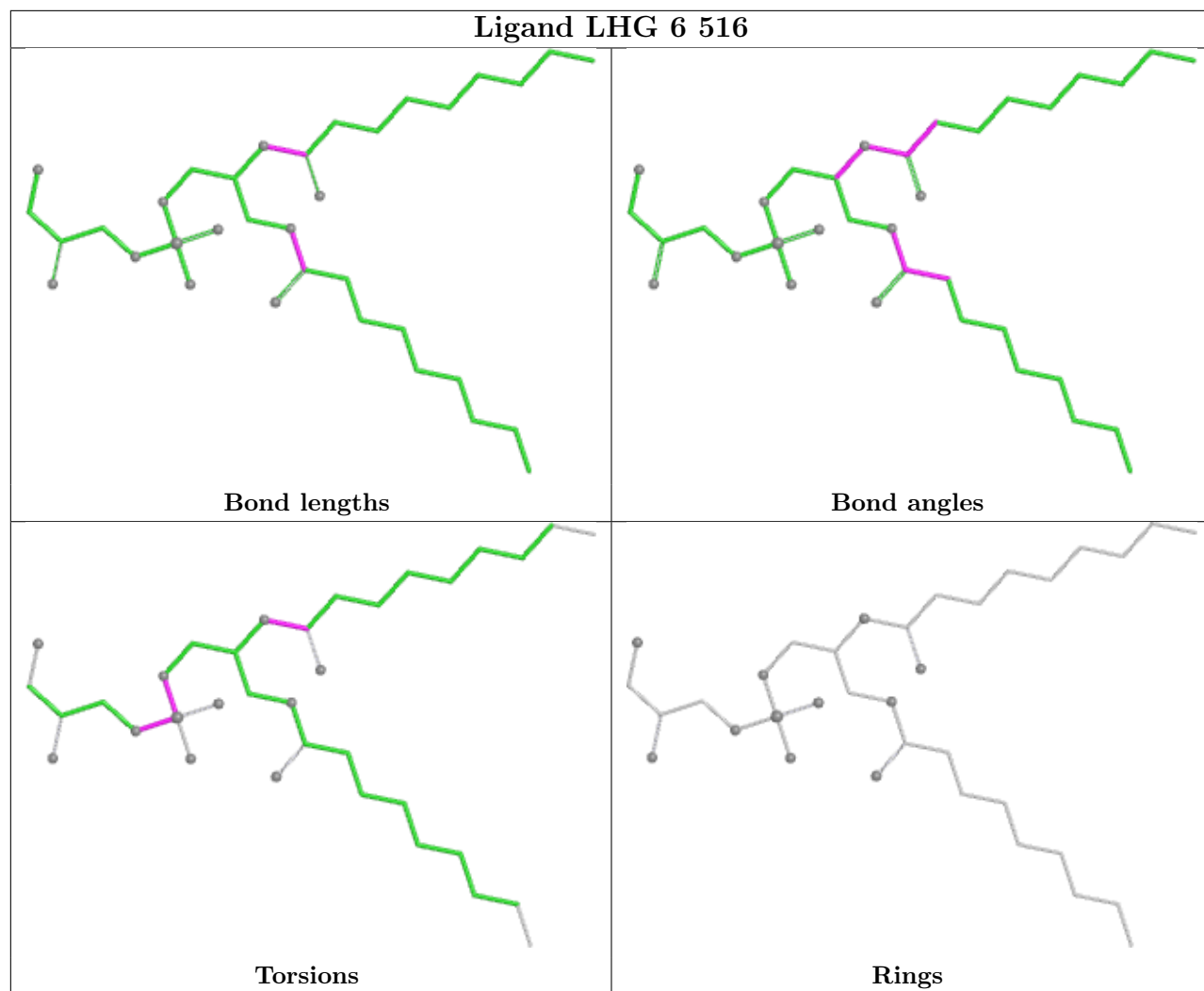


Ligand LHG A 845

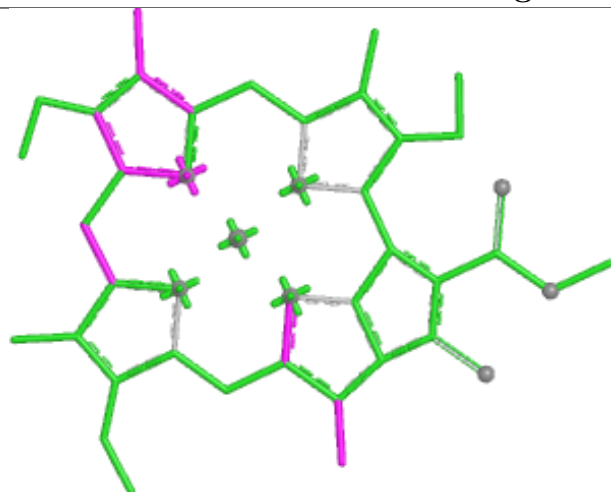


Ligand CLA K 205

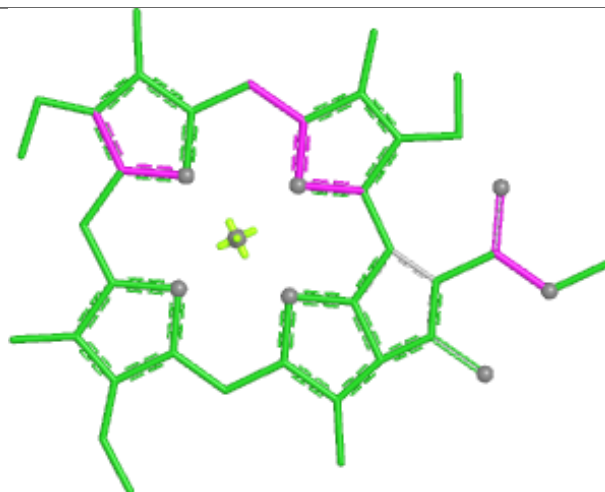




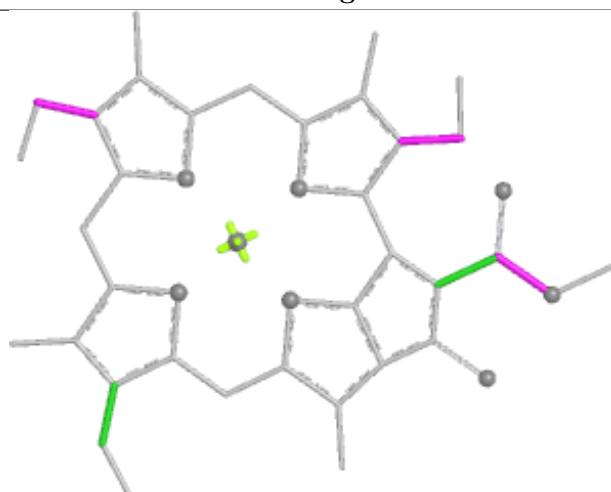
Ligand CLA B 824



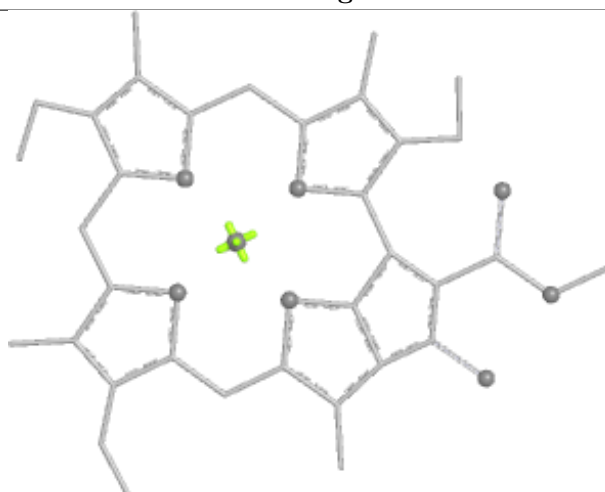
Bond lengths



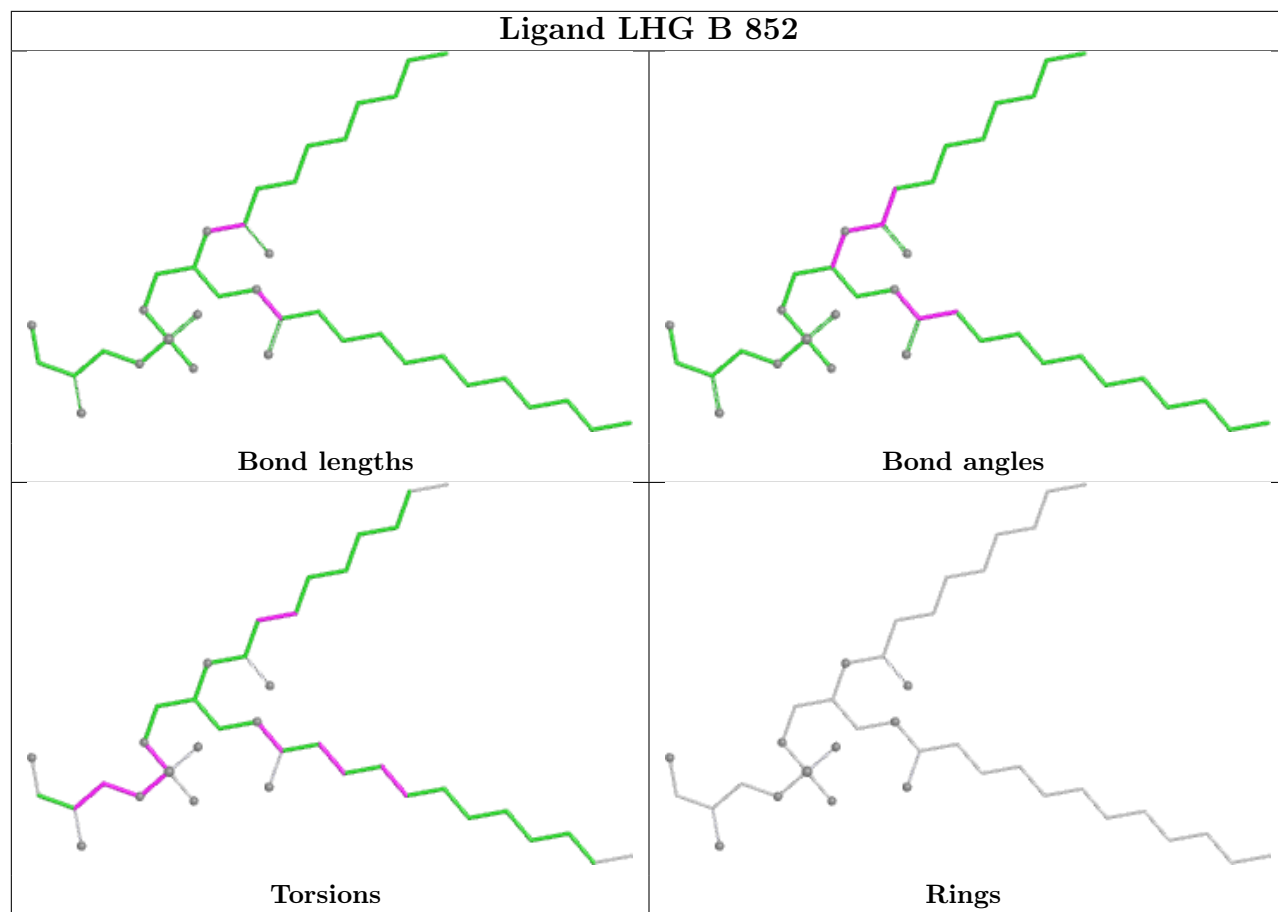
Bond angles



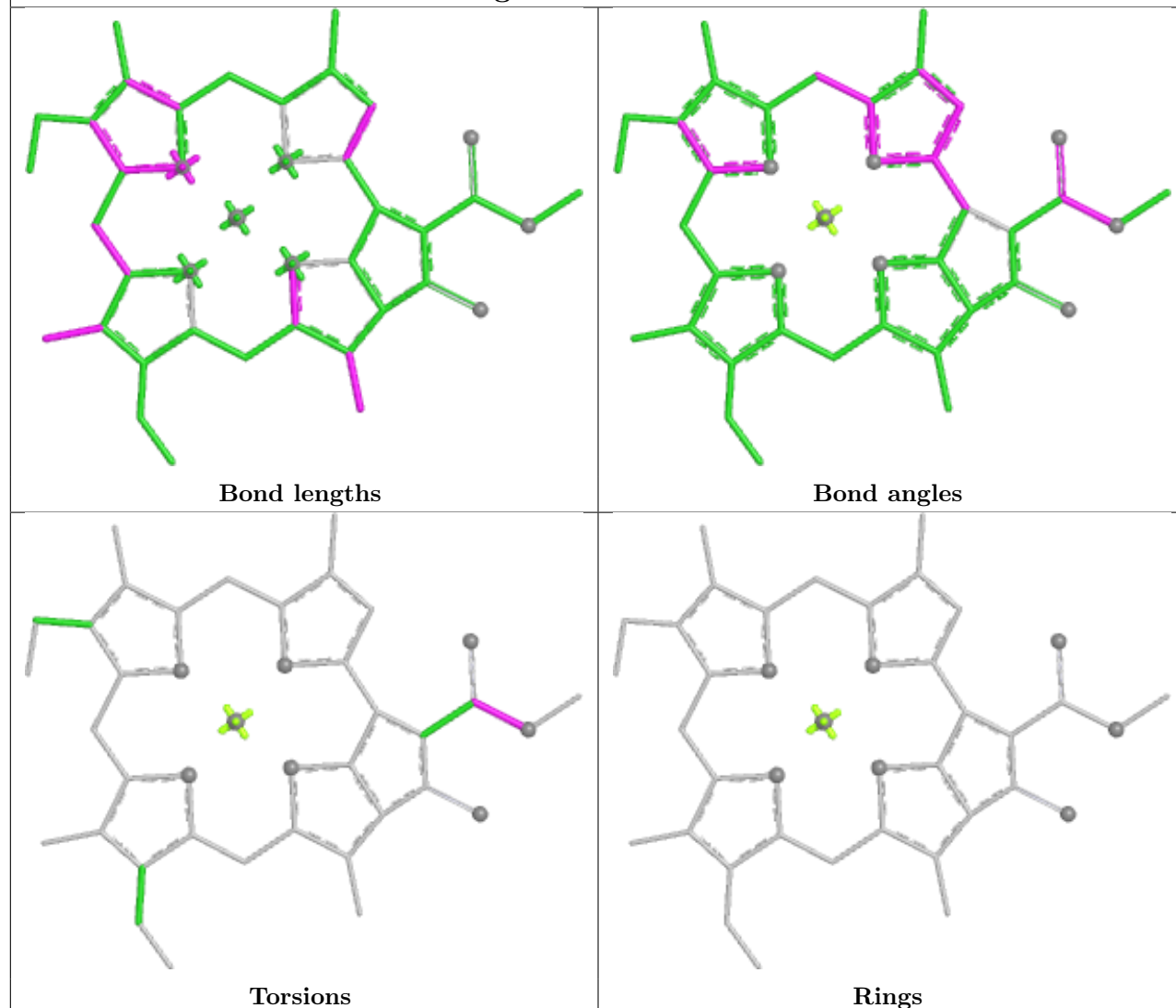
Torsions



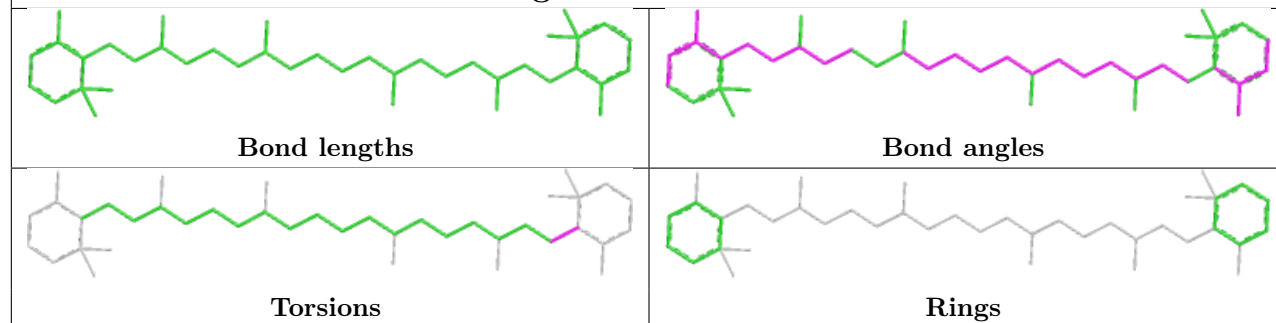
Rings



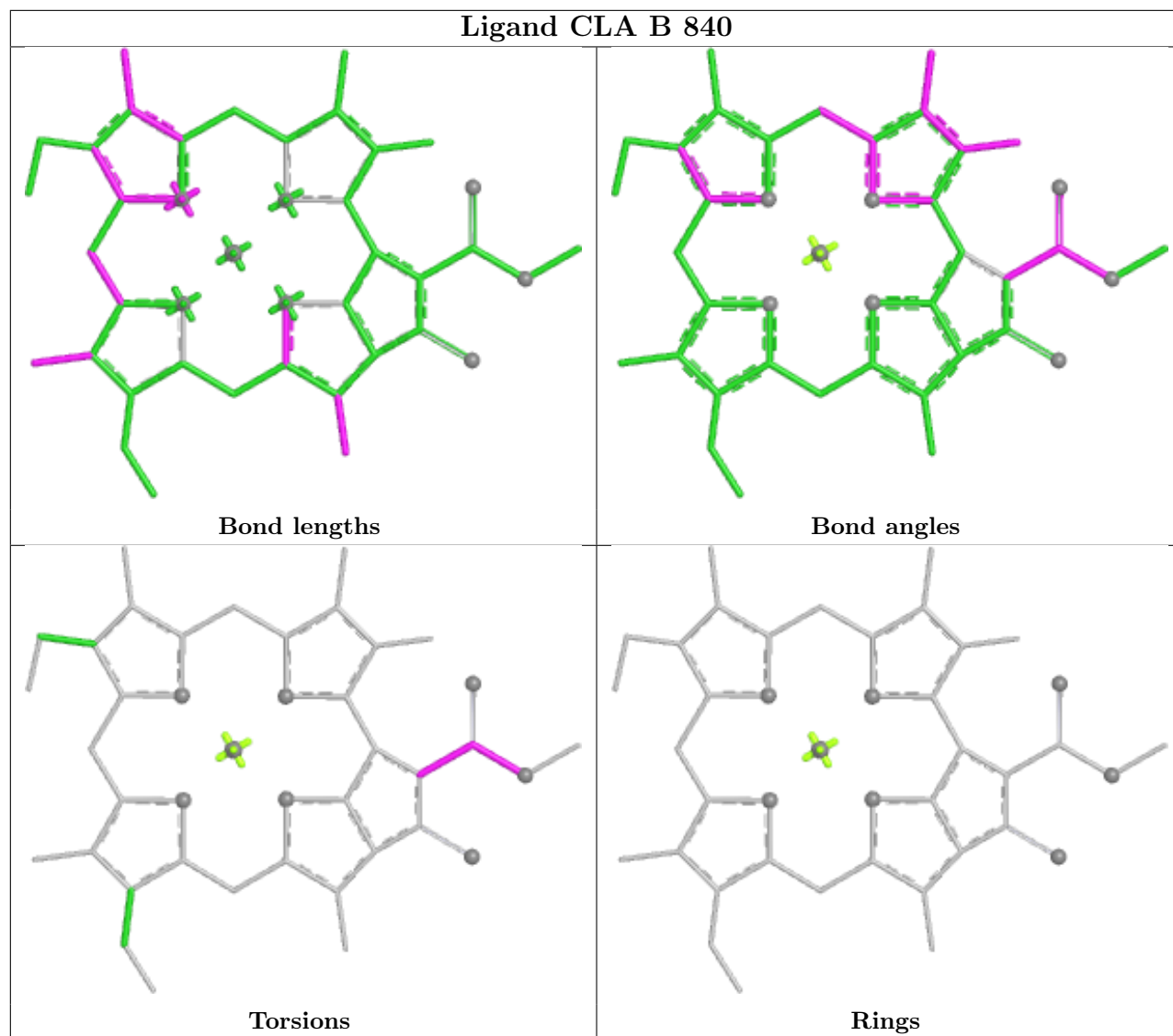
Ligand CLA 1 515



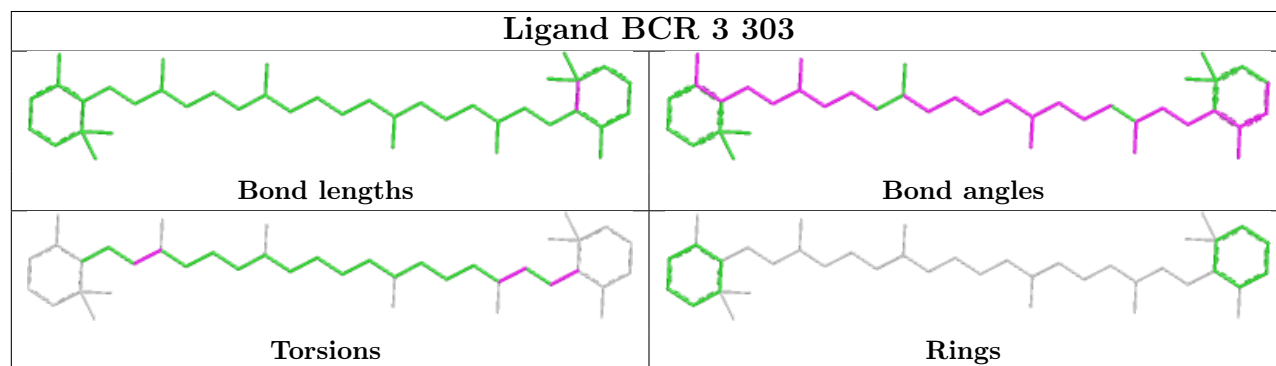
Ligand BCR L 305



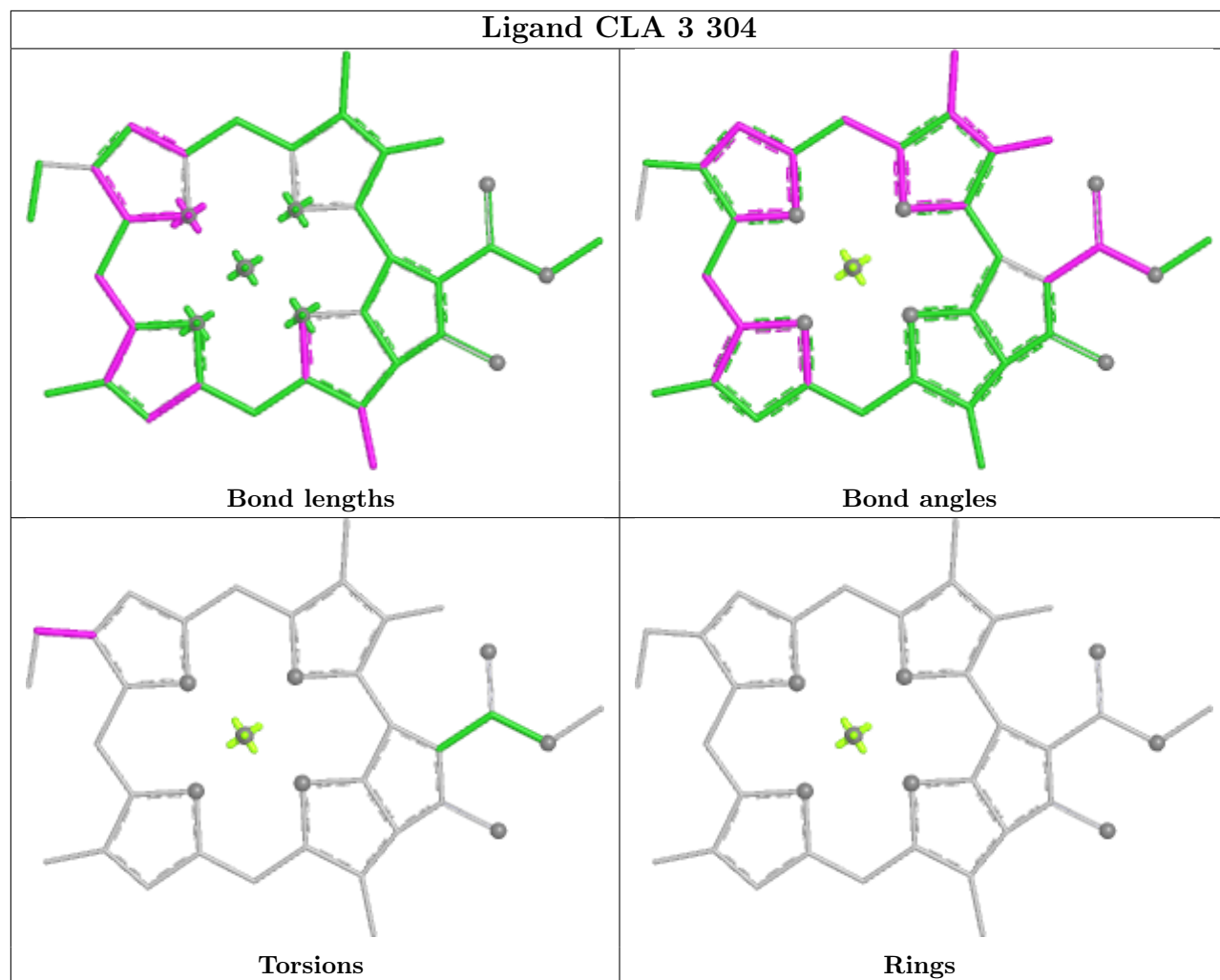
Ligand CLA B 840



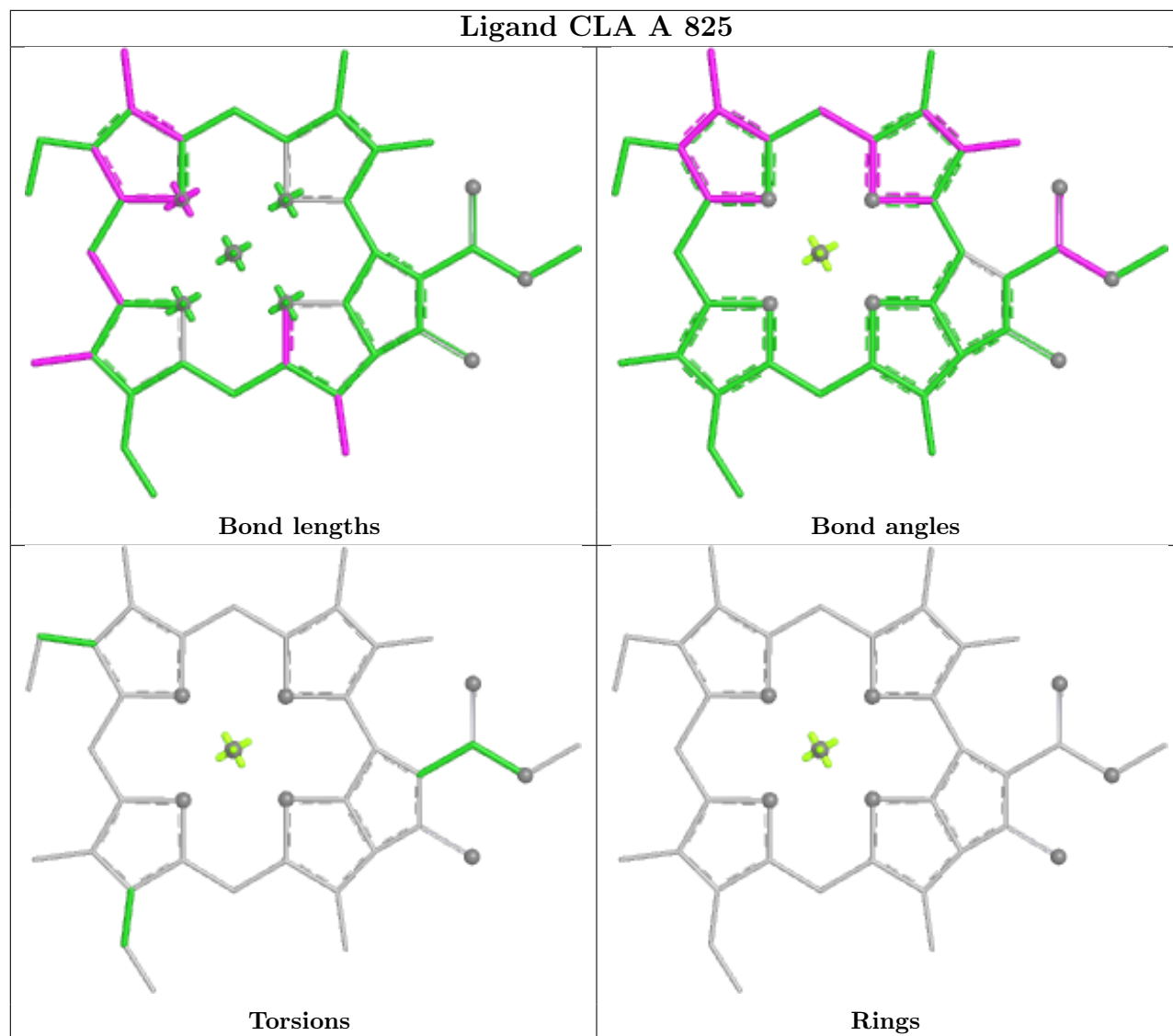
Ligand BCR 3 303



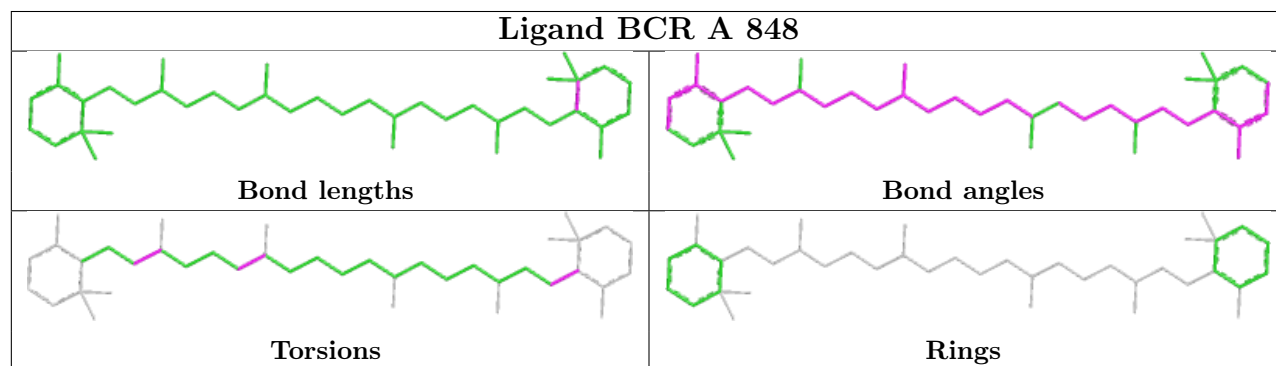
Ligand CLA 3 304

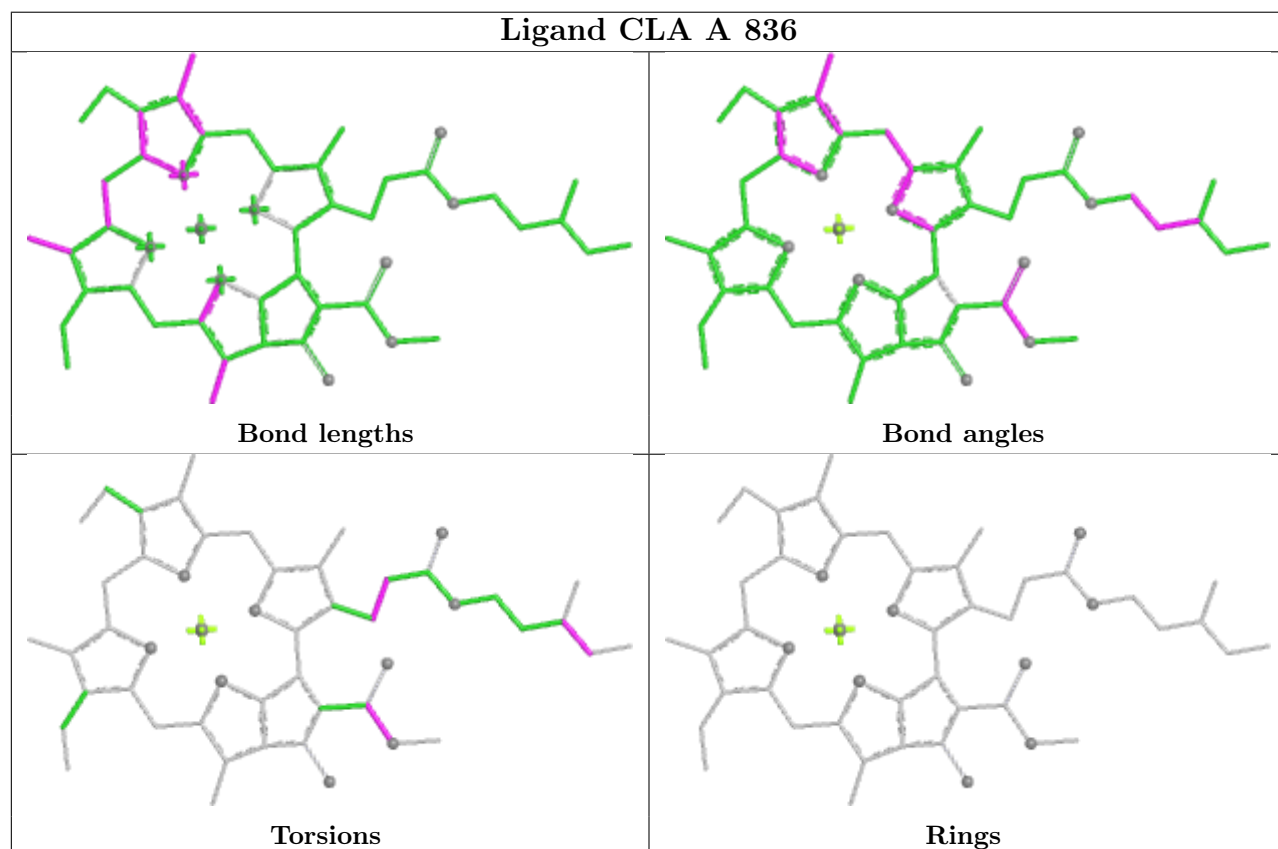
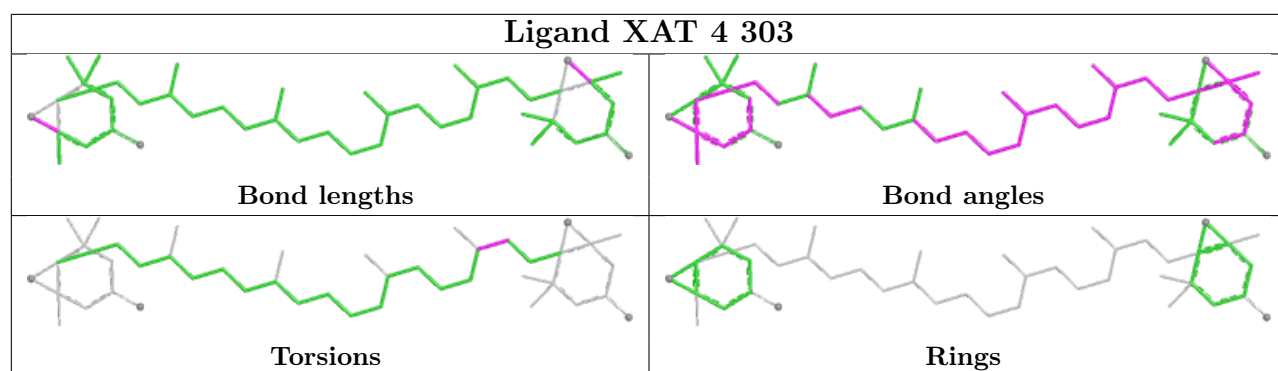


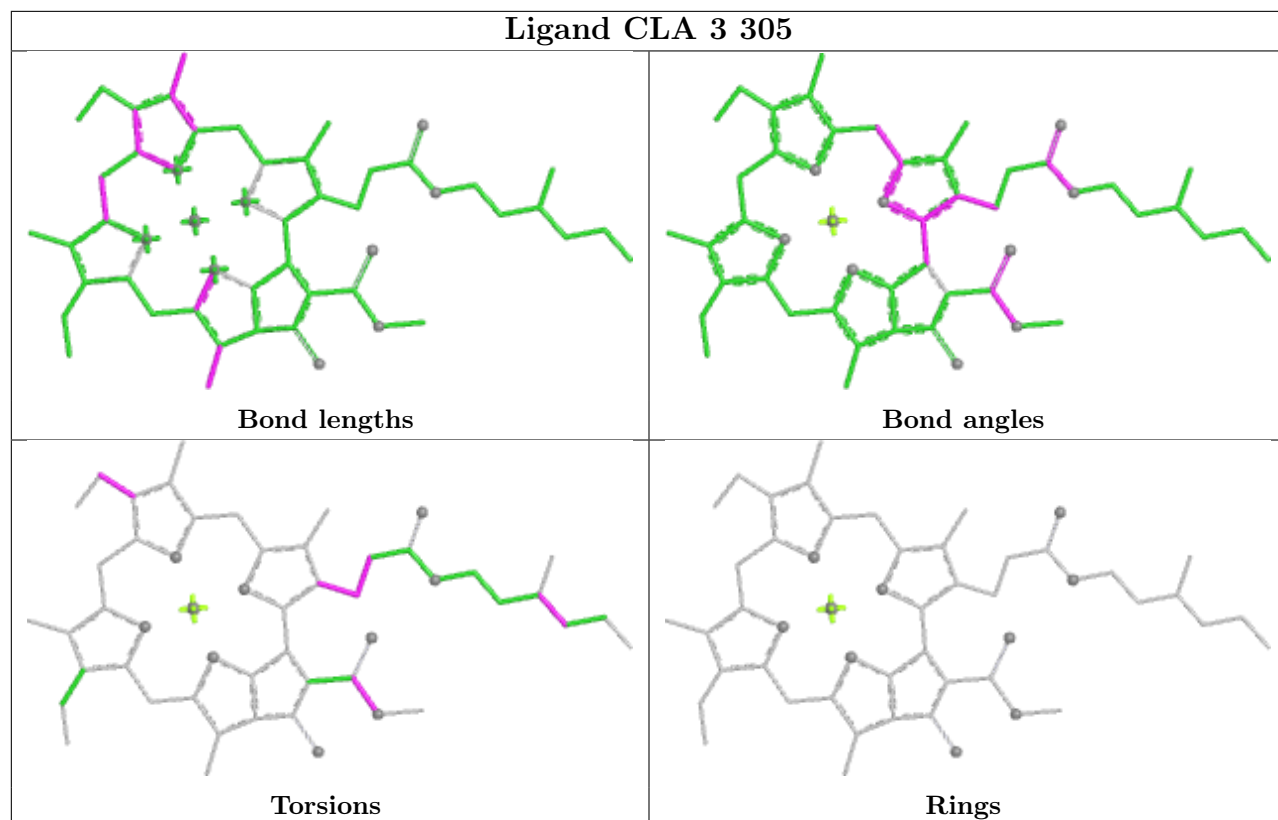
Ligand CLA A 825



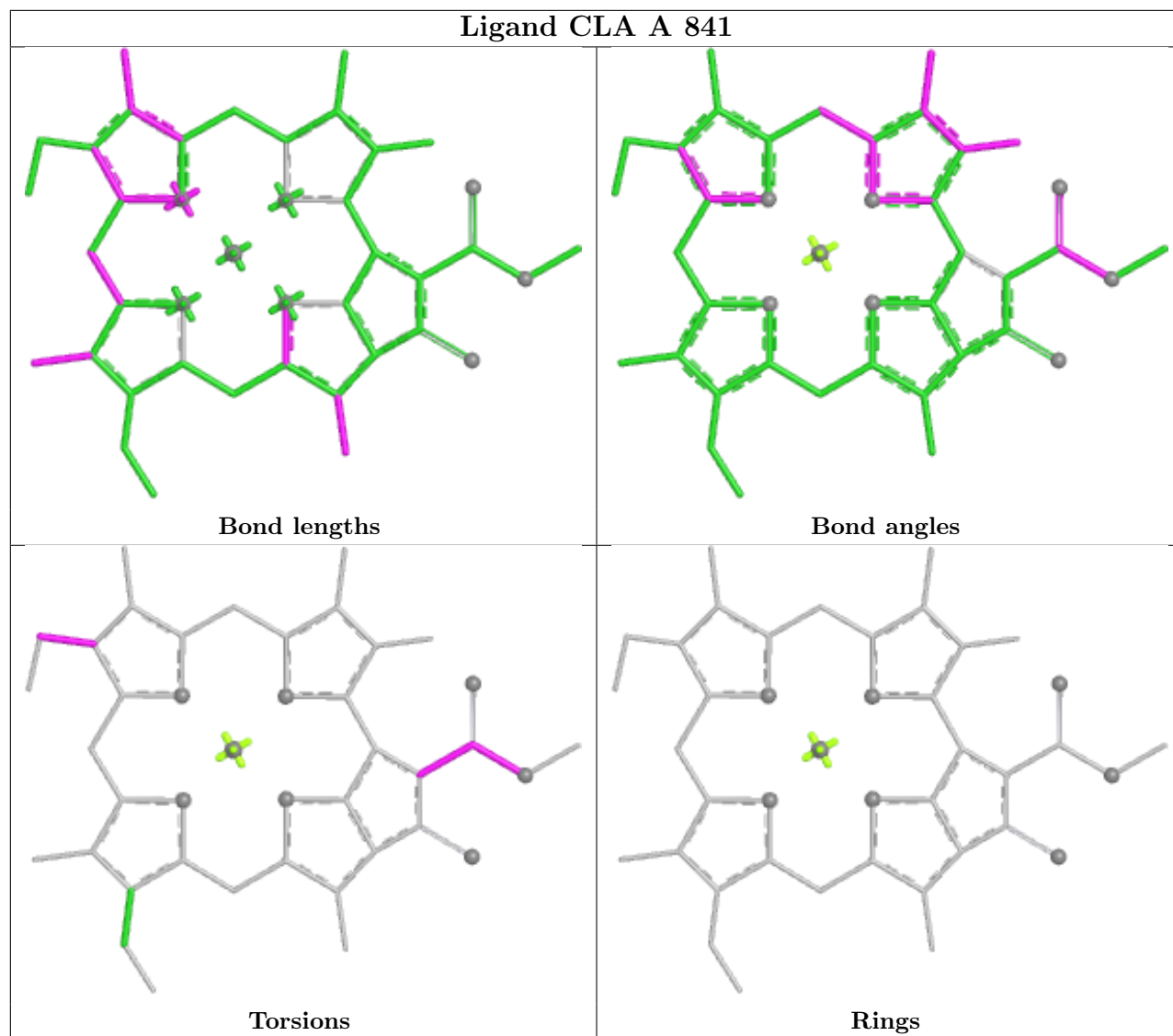
Ligand BCR A 848



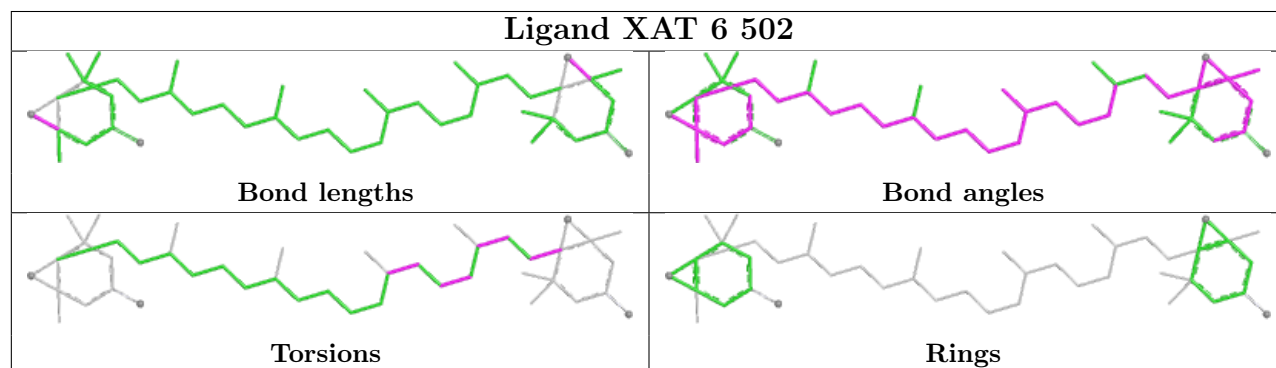




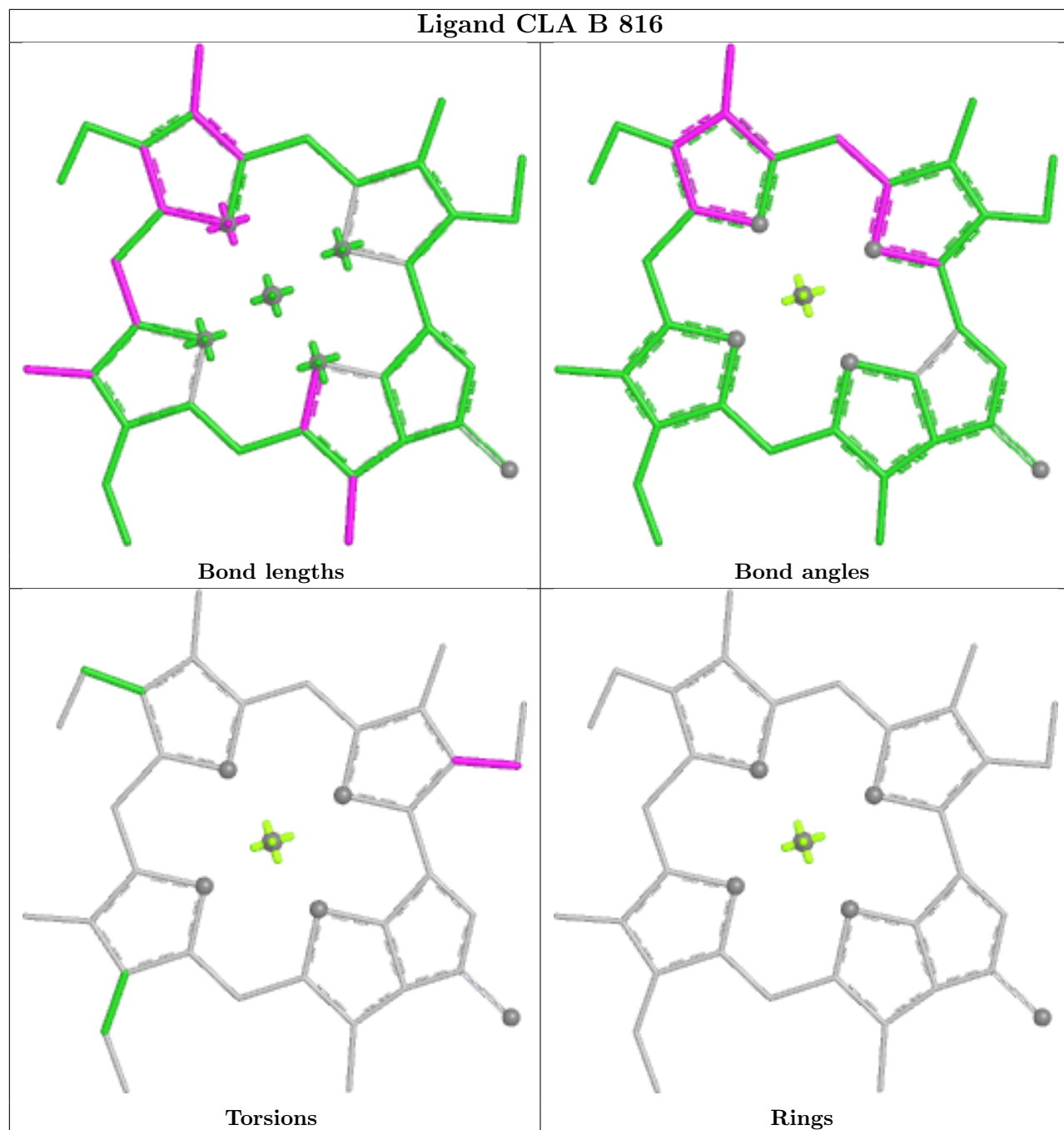
Ligand CLA A 841



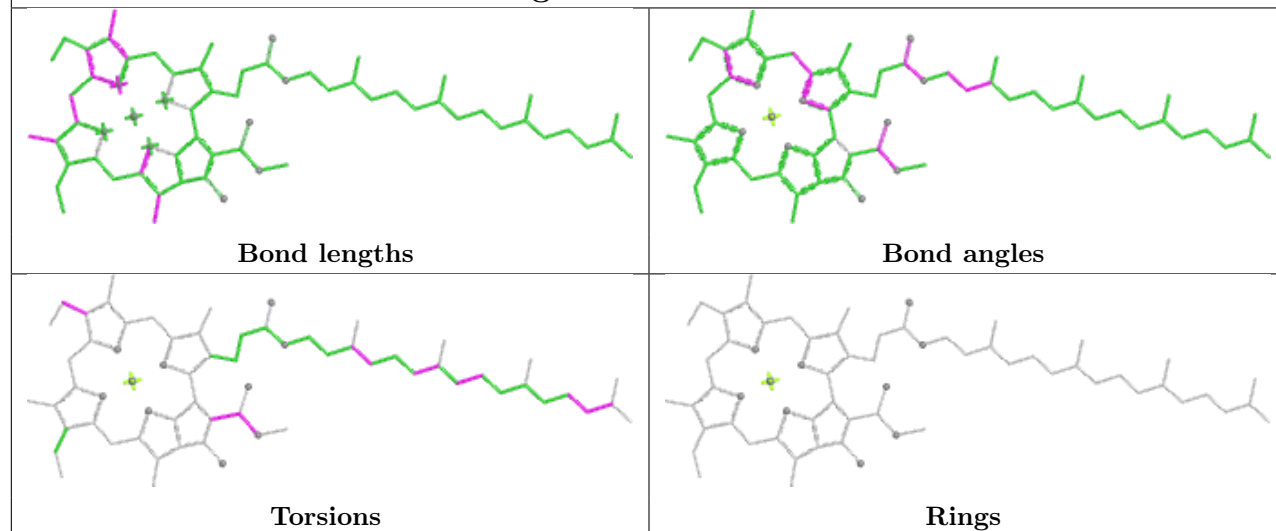
Ligand XAT 6 502



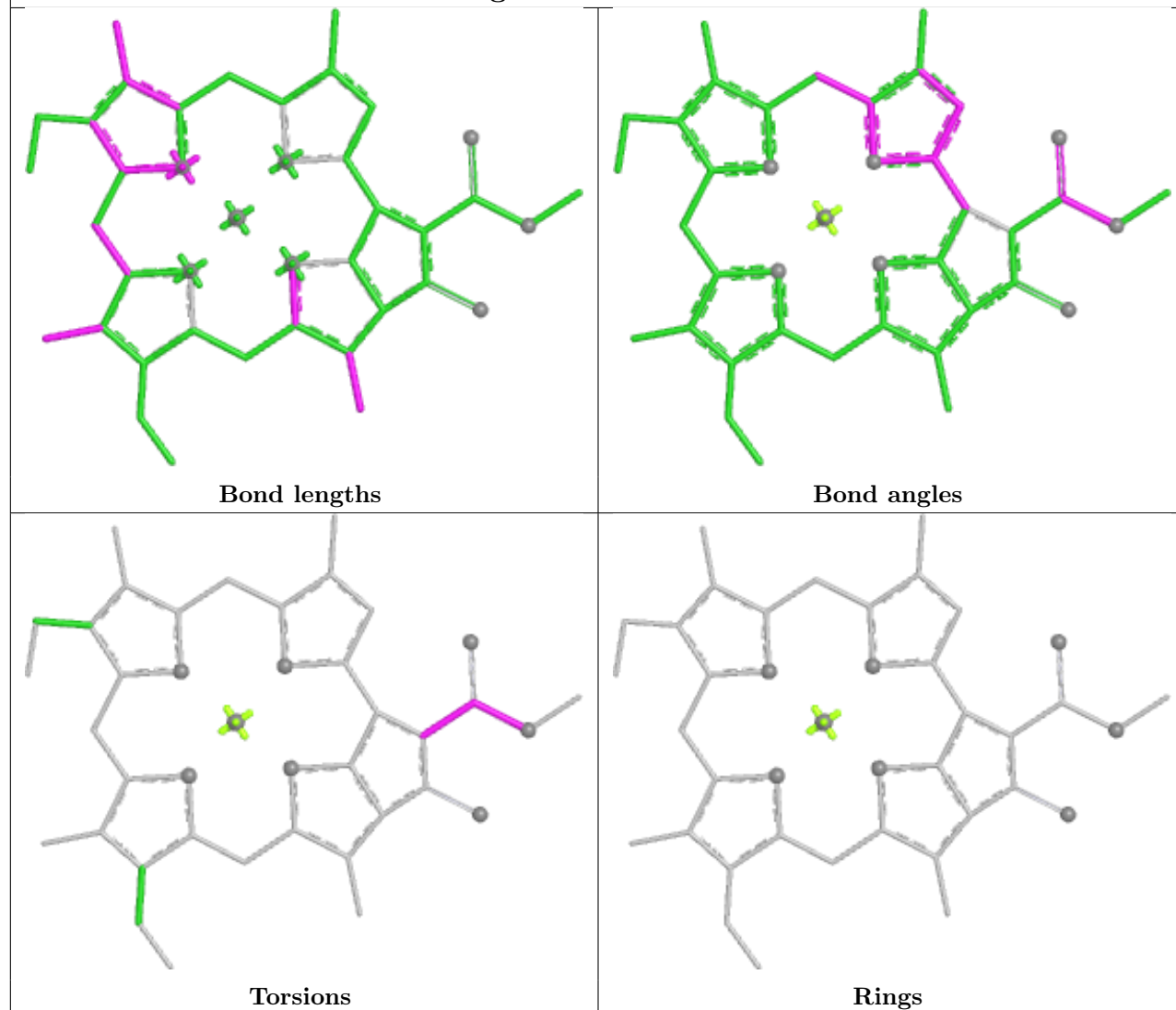
Ligand CLA B 816



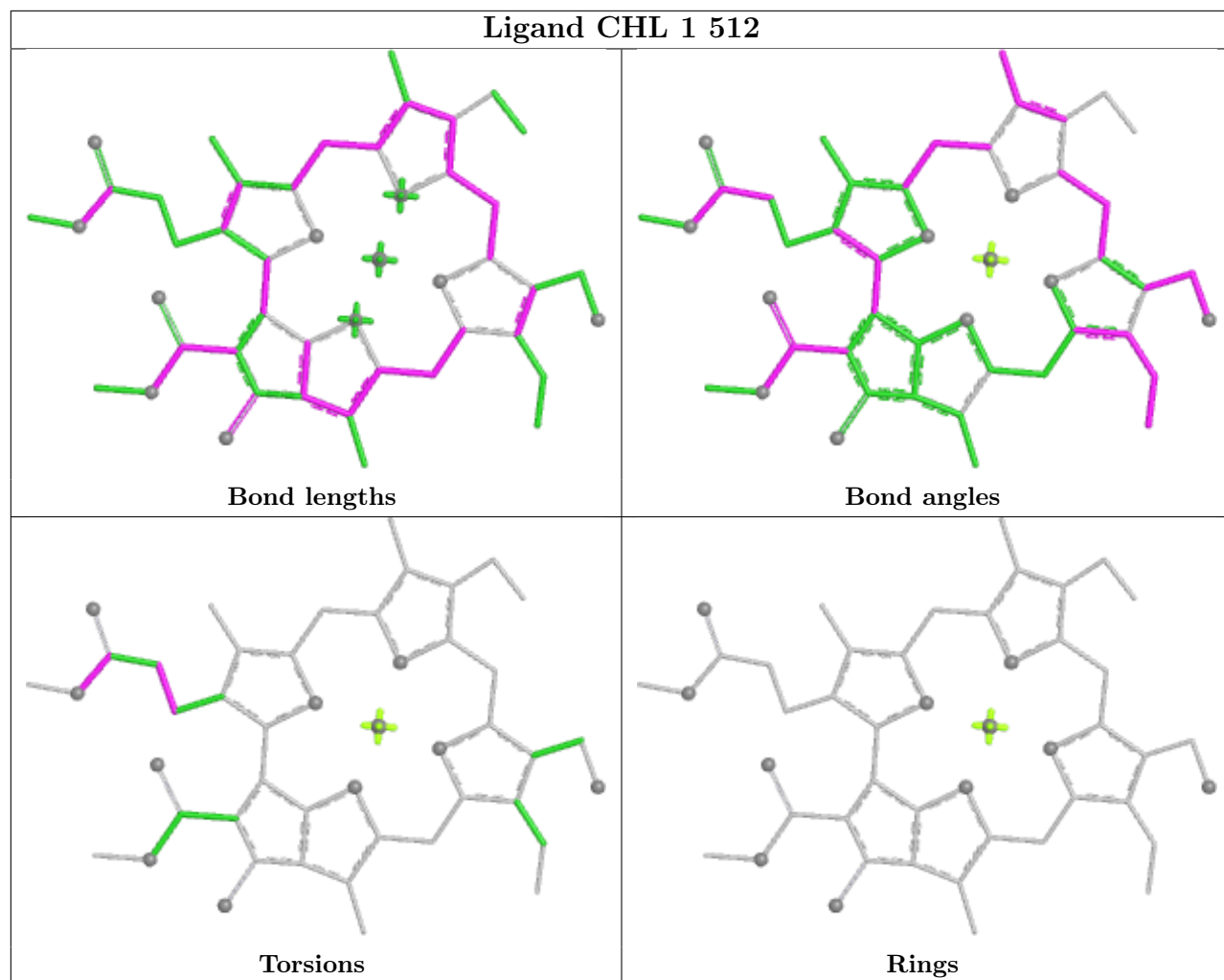
Ligand CLA B 810



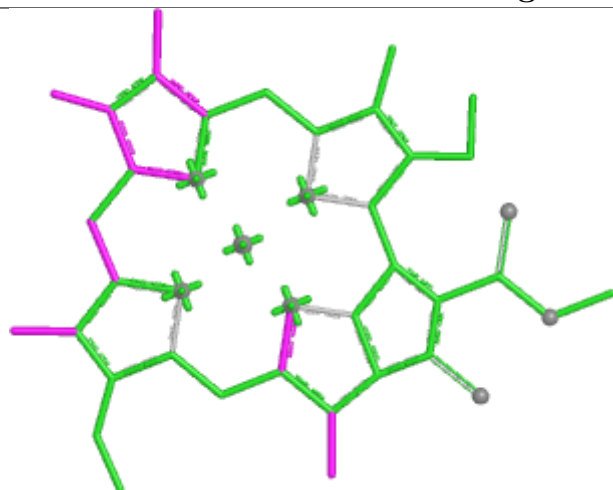
Ligand CLA A 802



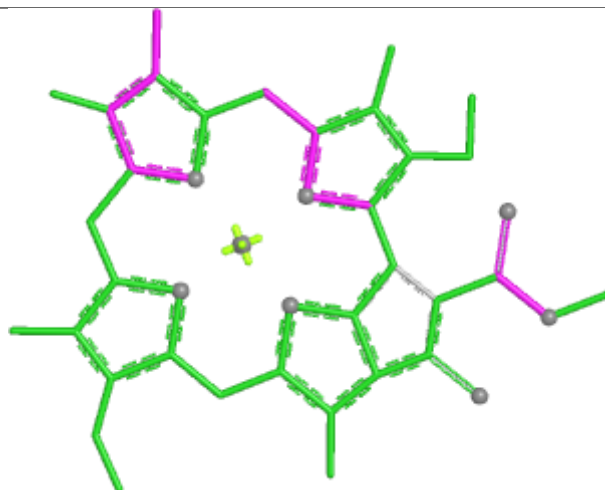
Ligand CHL 1 512



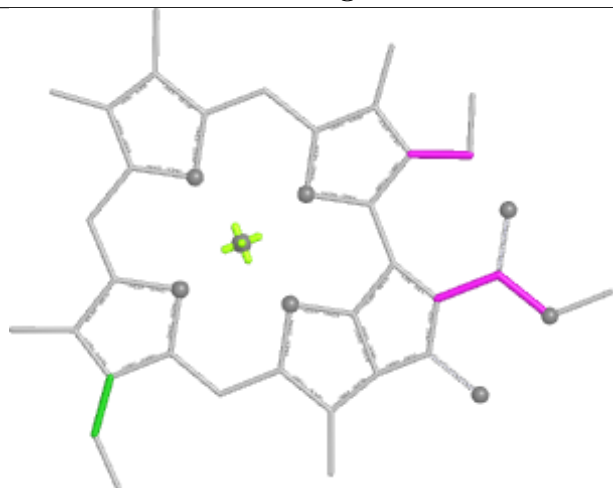
Ligand CLA J 101



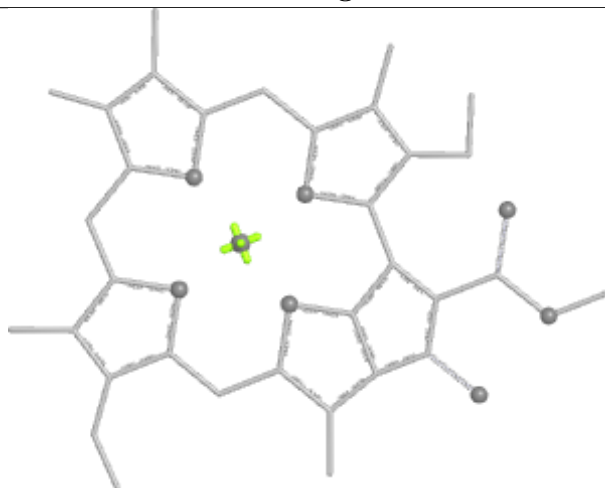
Bond lengths



Bond angles

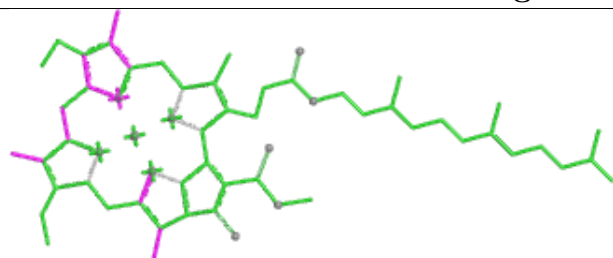


Torsions

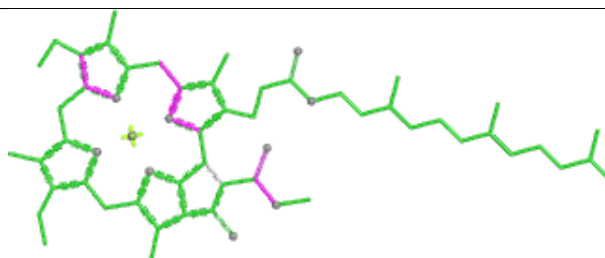


Rings

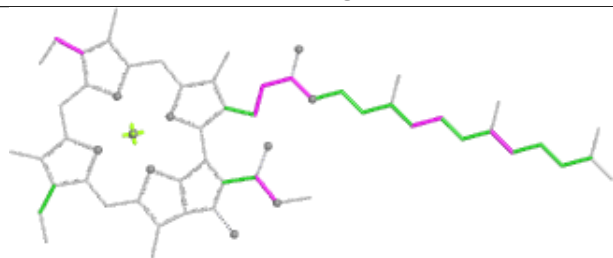
Ligand CLA A 816



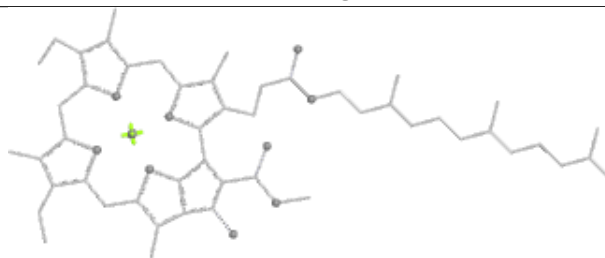
Bond lengths



Bond angles

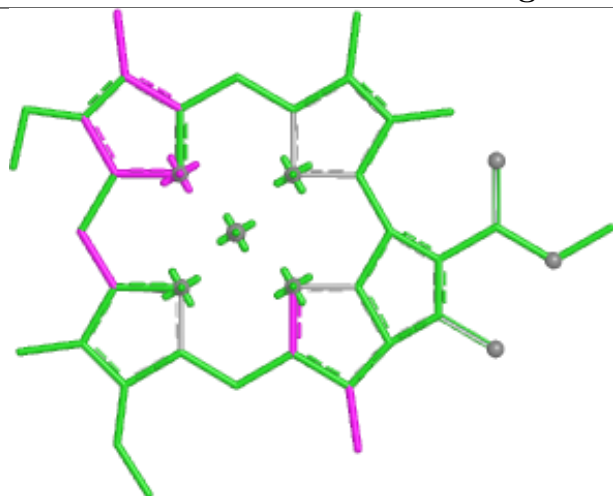


Torsions

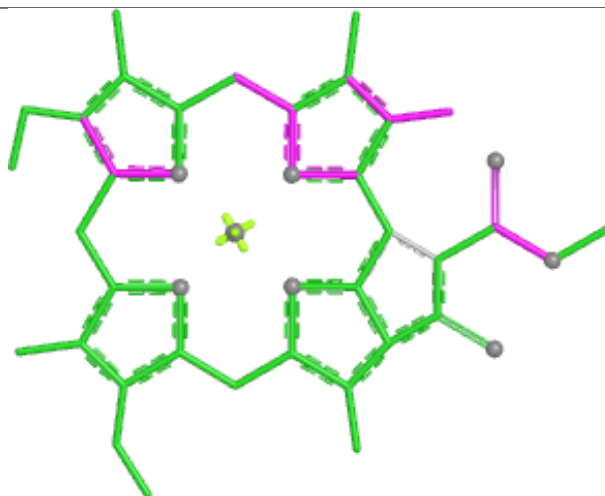


Rings

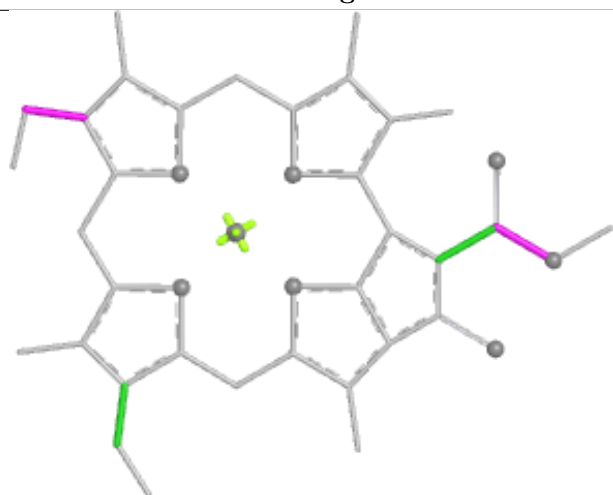
Ligand CLA 4 312



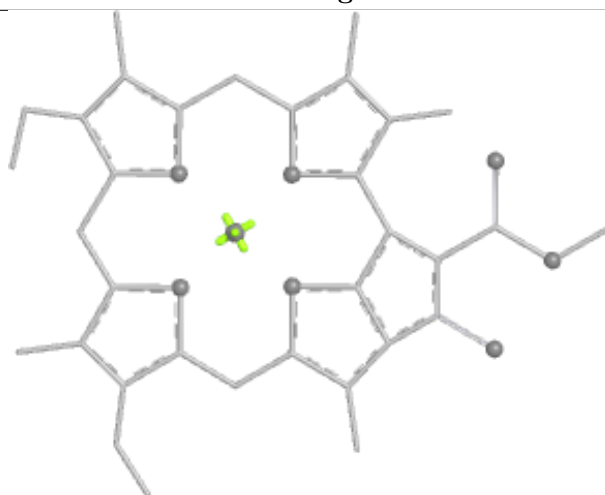
Bond lengths



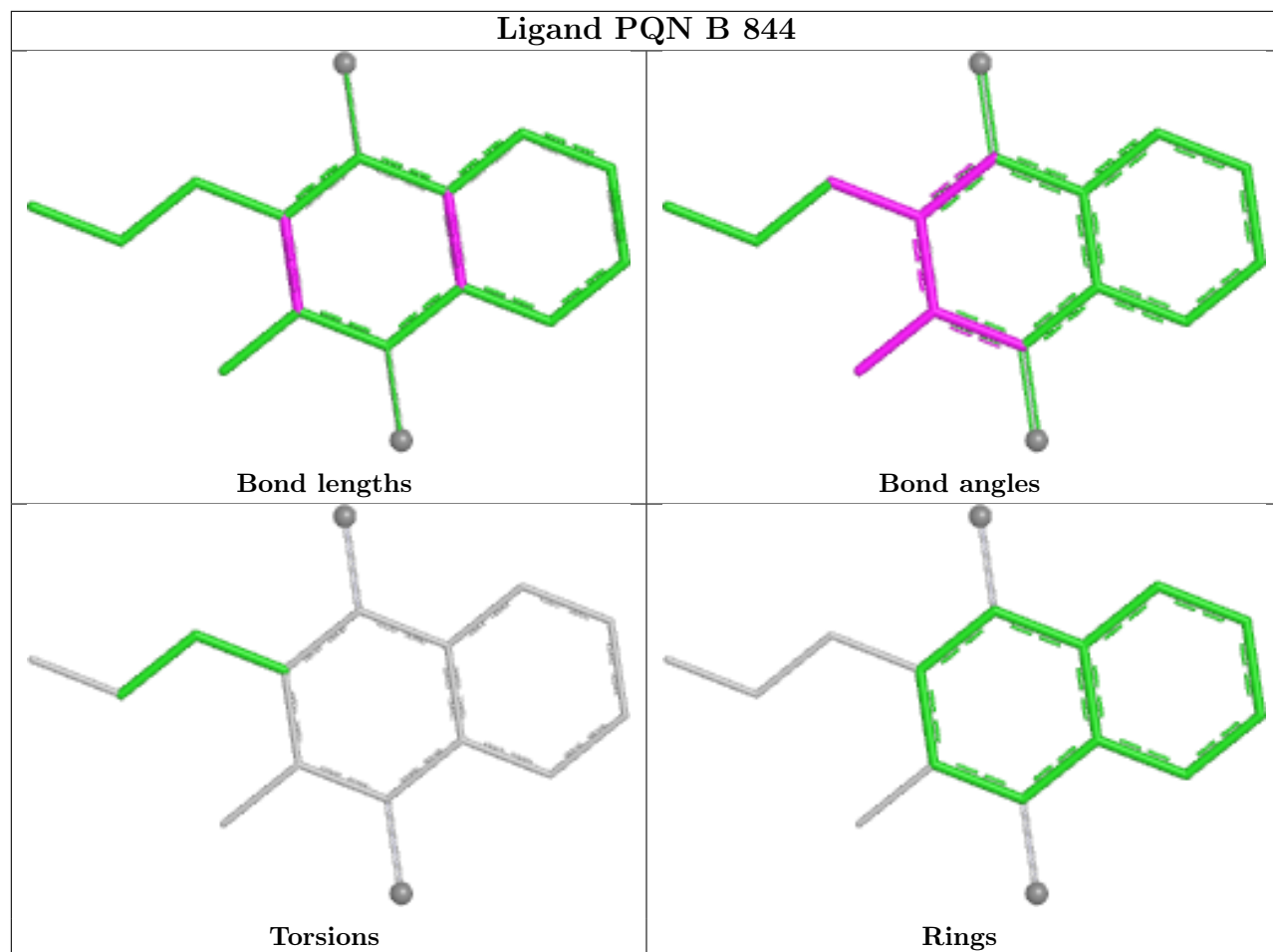
Bond angles



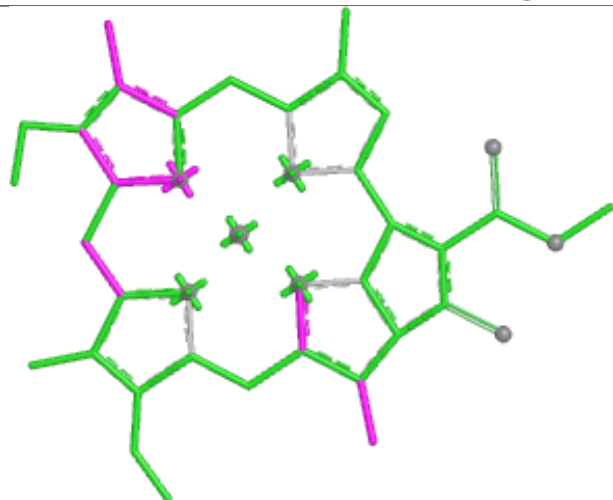
Torsions



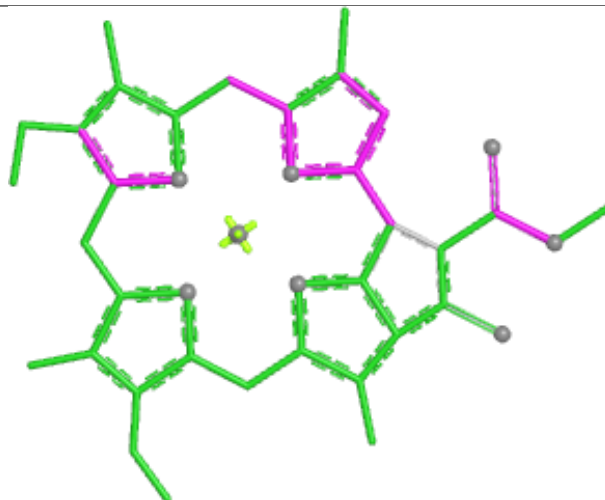
Rings



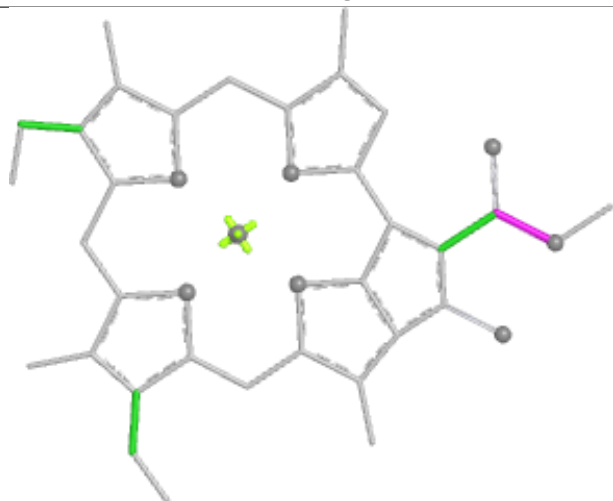
Ligand CLA 3 307



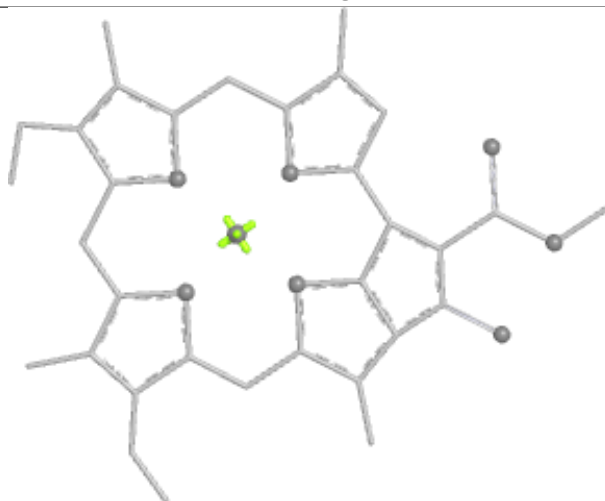
Bond lengths



Bond angles

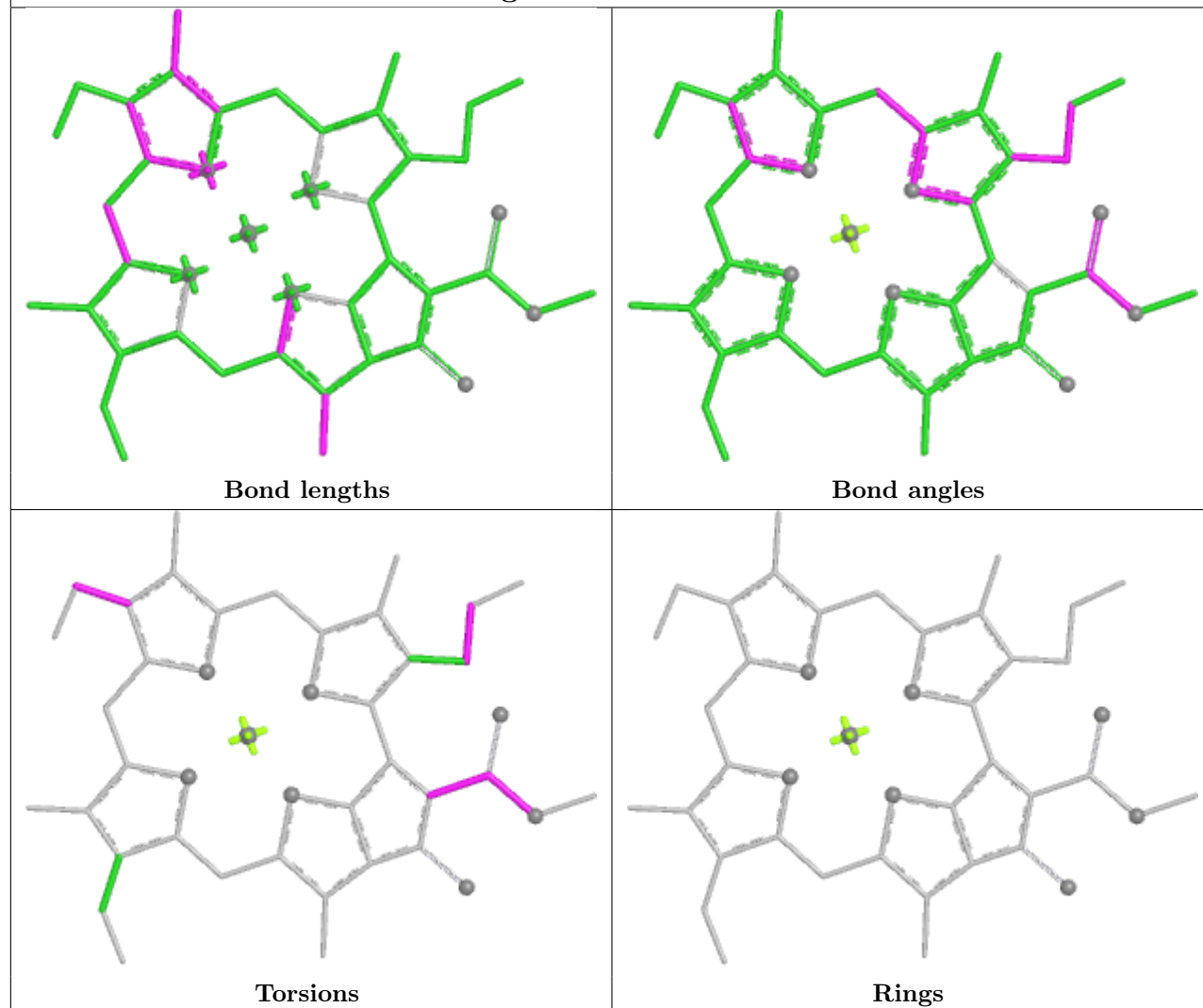


Torsions

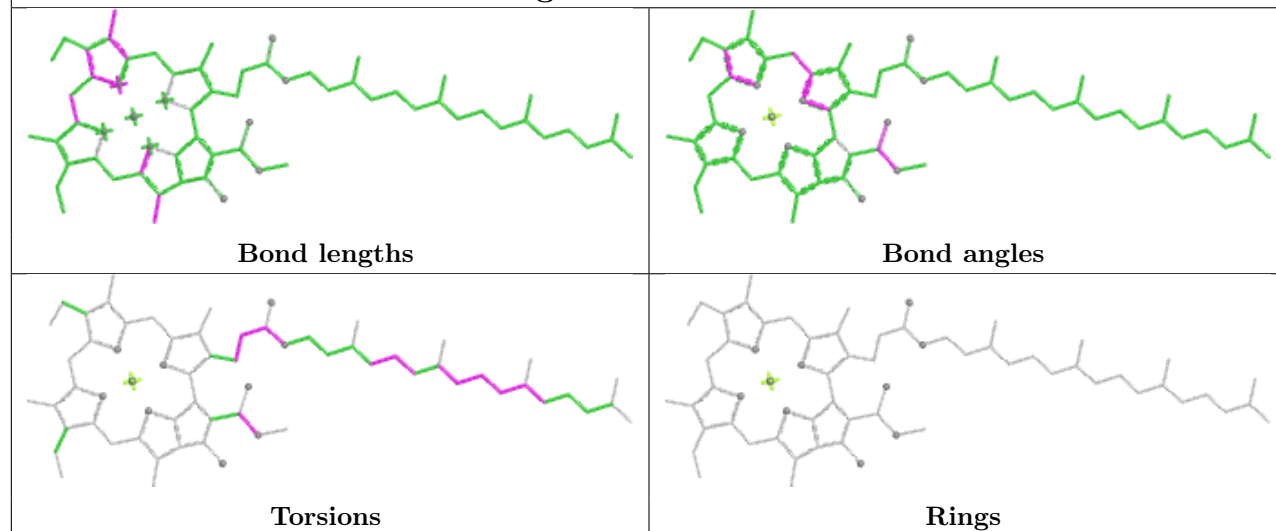


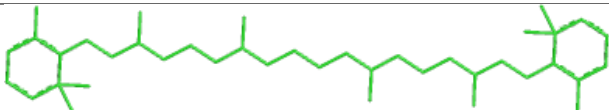
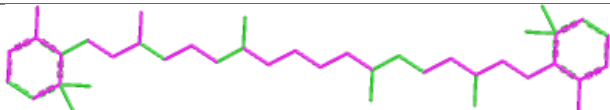
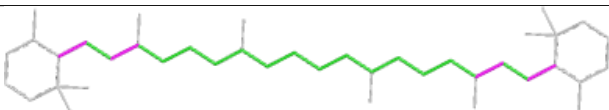
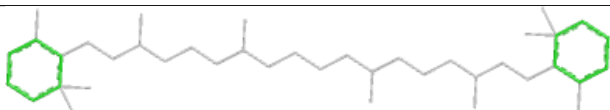
Rings

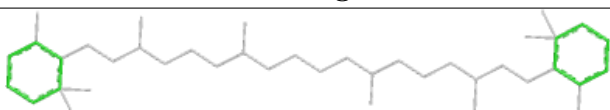
Ligand CLA A 832



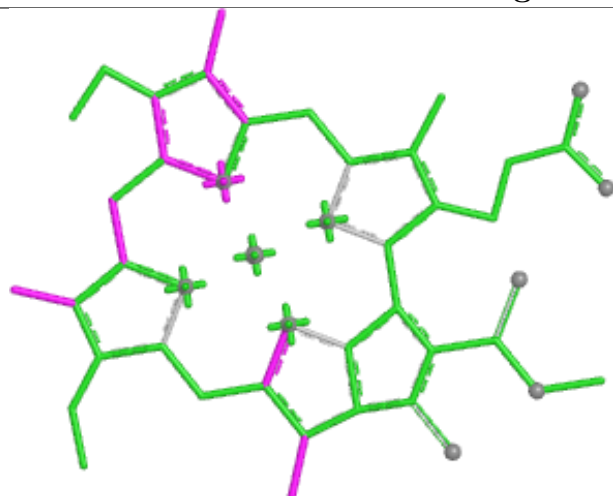
Ligand CLA 6 506



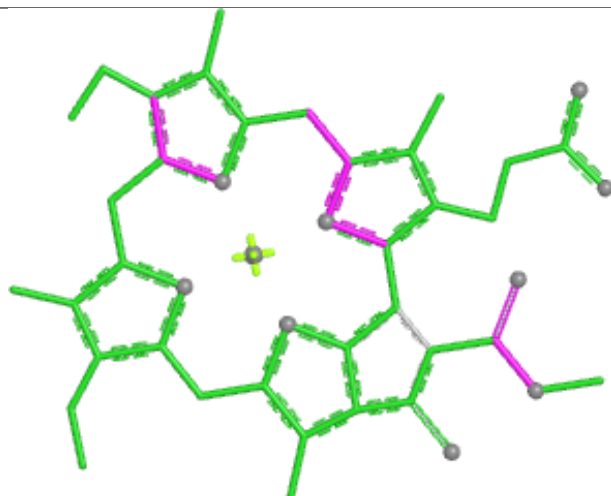
Ligand BCR I 102	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR J 103	
	Bond lengths
	Bond angles
	Torsions
	Rings

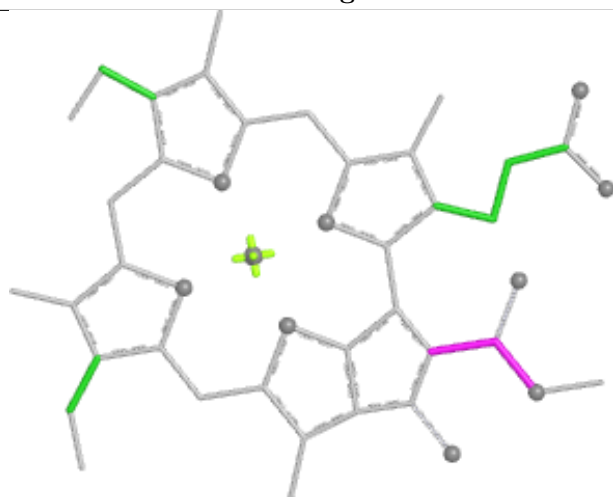
Ligand CLA A 834



Bond lengths



Bond angles

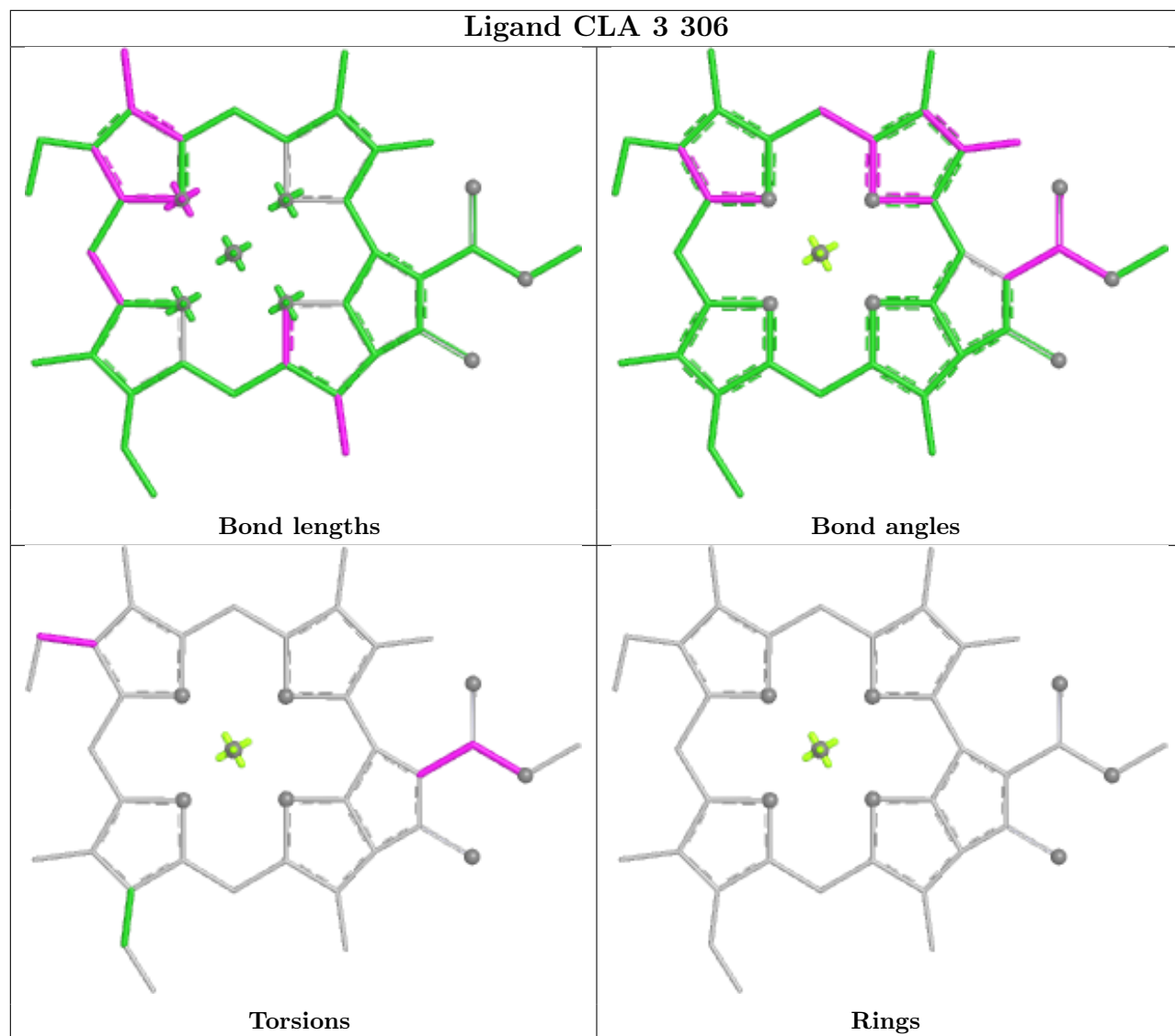


Torsions

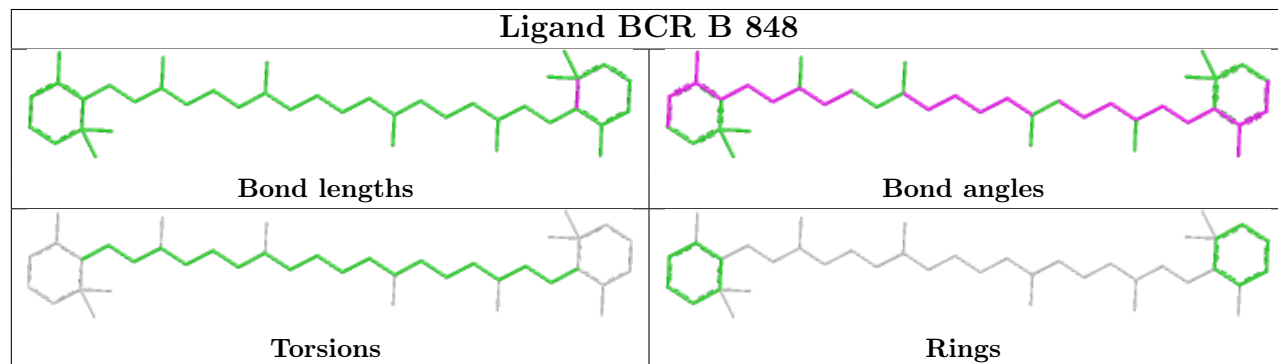


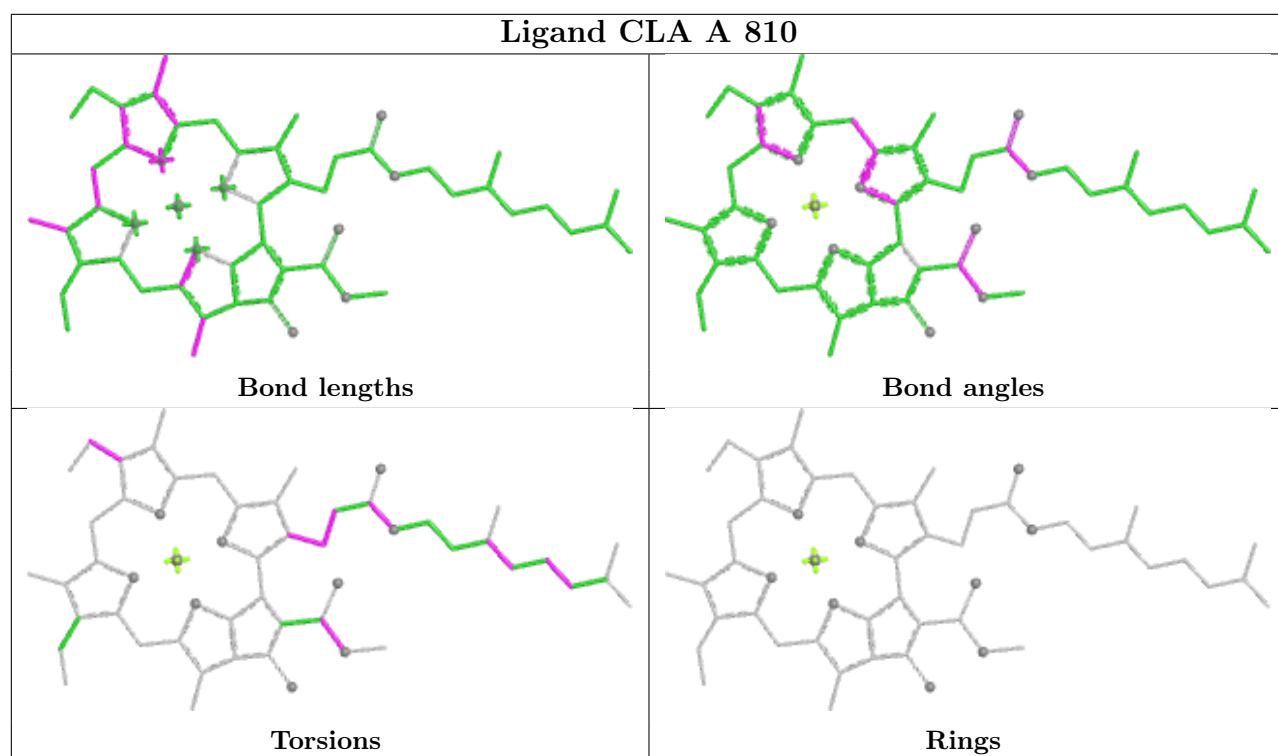
Rings

Ligand CLA 3 306

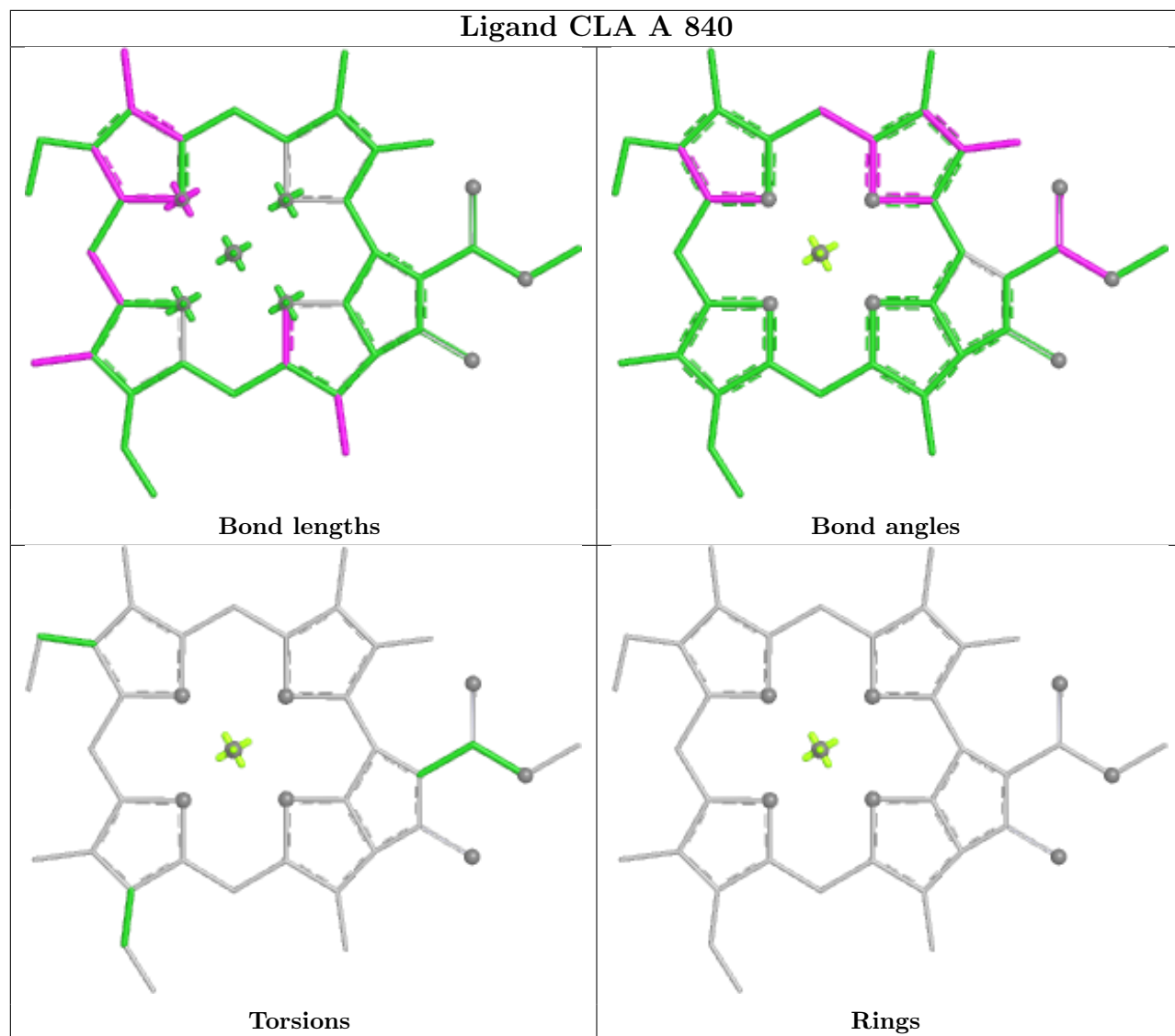


Ligand BCR B 848

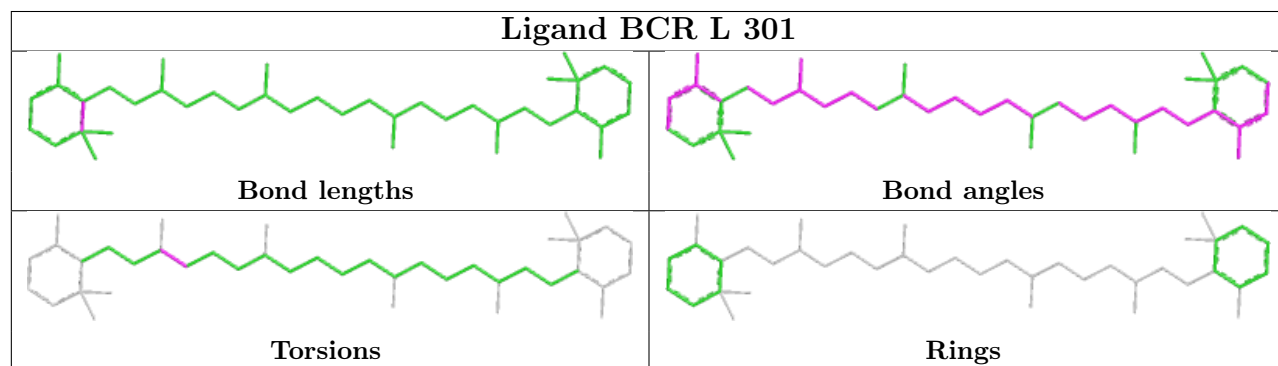




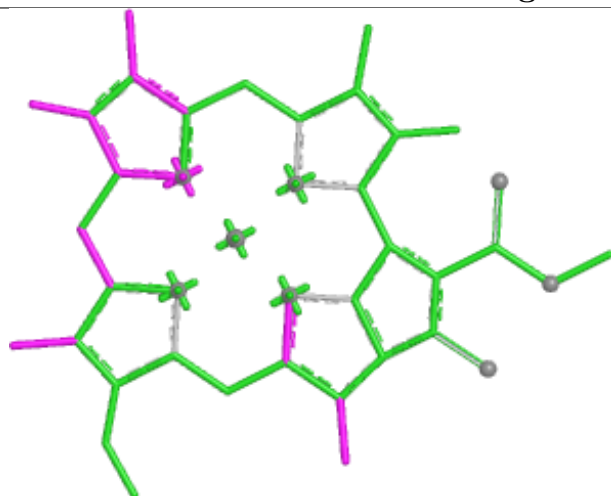
Ligand CLA A 840



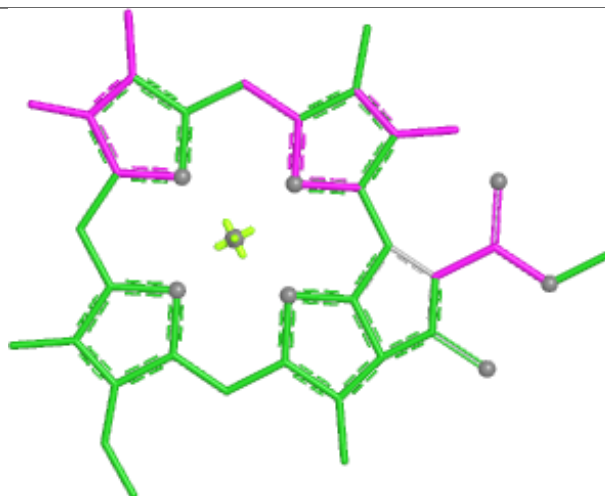
Ligand BCR L 301



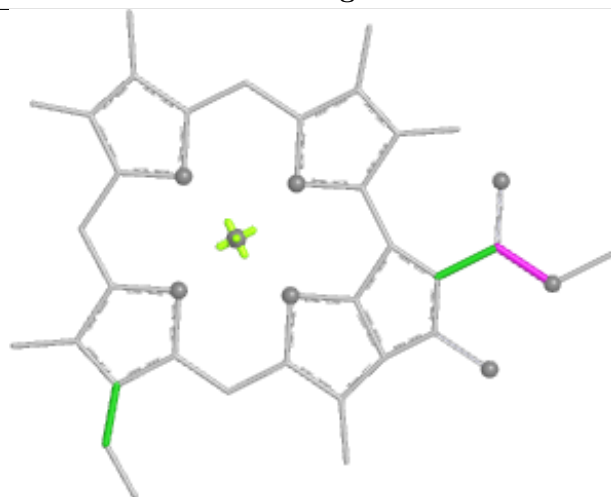
Ligand CLA 1 507



Bond lengths



Bond angles

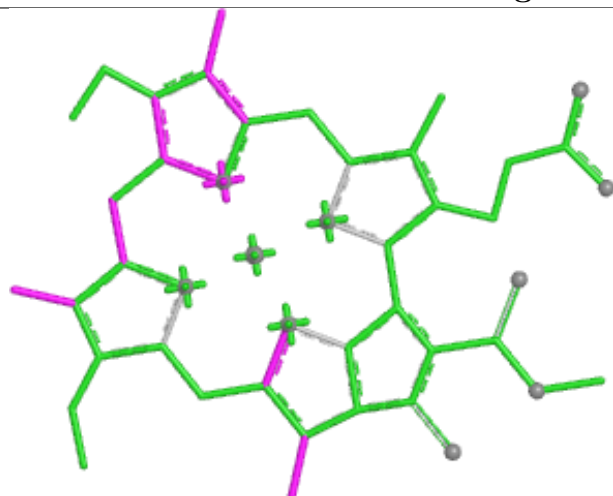


Torsions

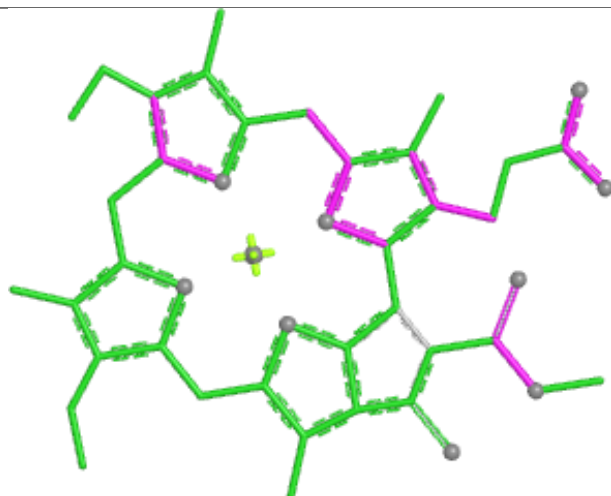


Rings

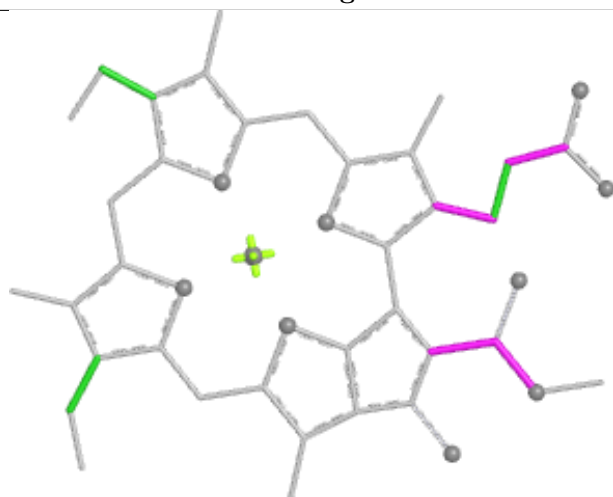
Ligand CLA B 835



Bond lengths



Bond angles

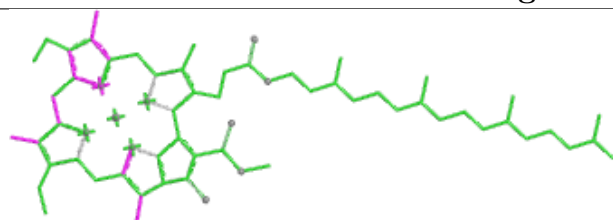


Torsions

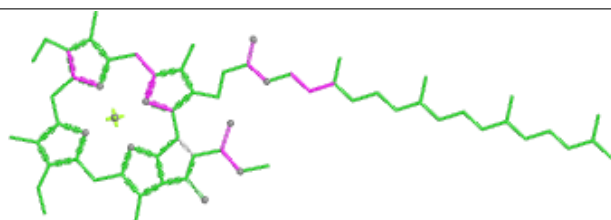


Rings

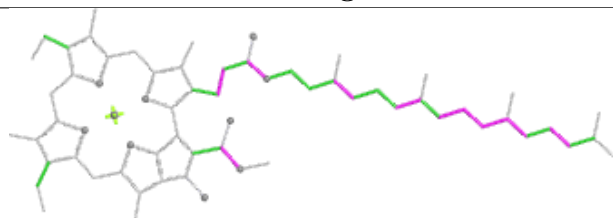
Ligand CLA 4 306



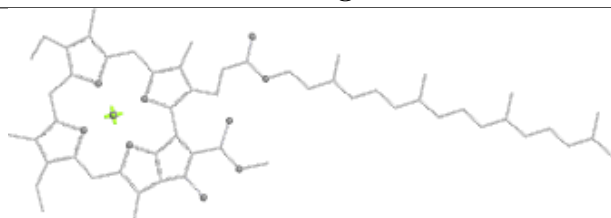
Bond lengths



Bond angles

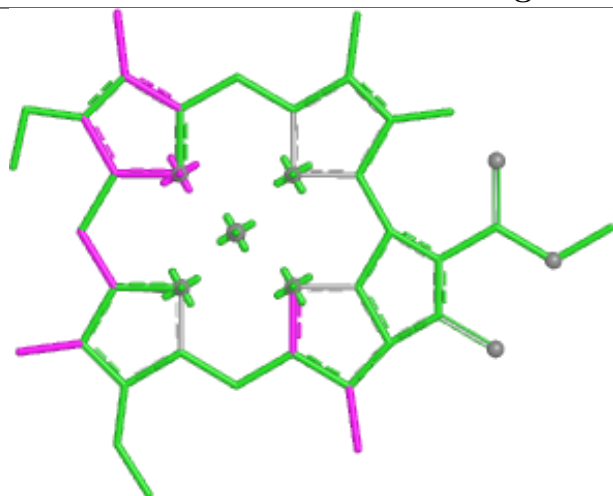


Torsions

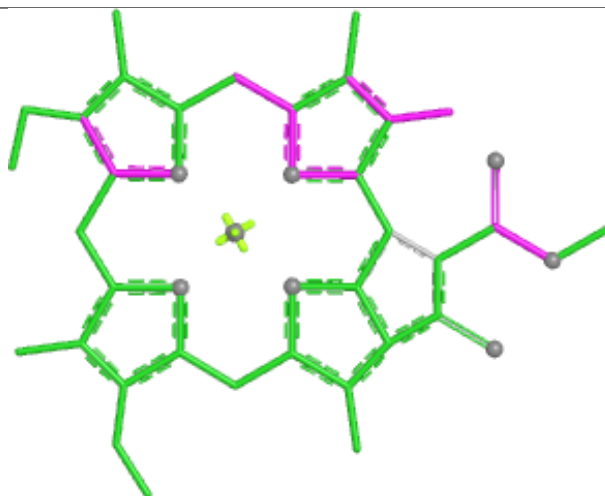


Rings

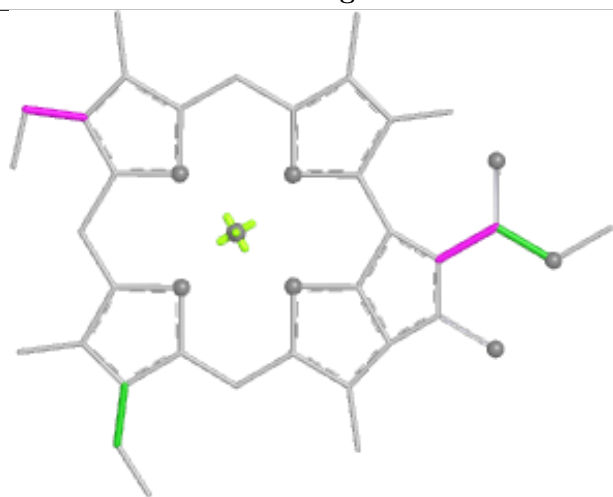
Ligand CLA B 823



Bond lengths



Bond angles

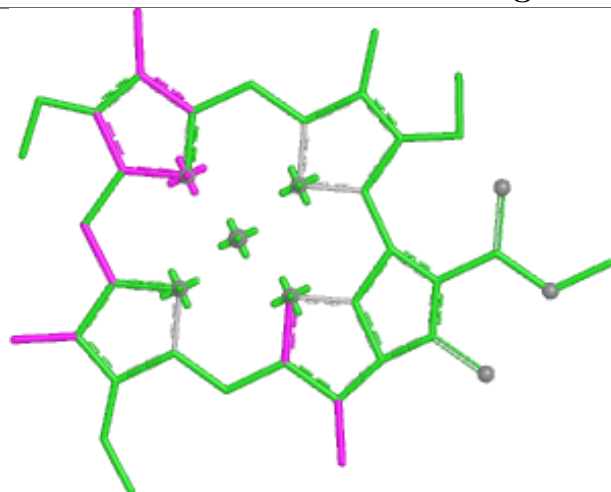


Torsions



Rings

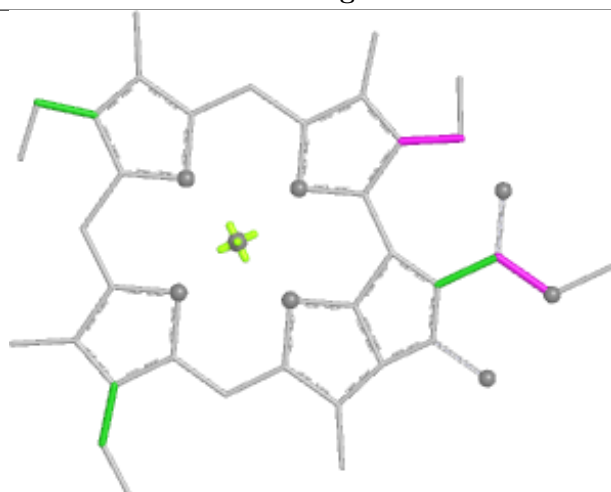
Ligand CLA A 821



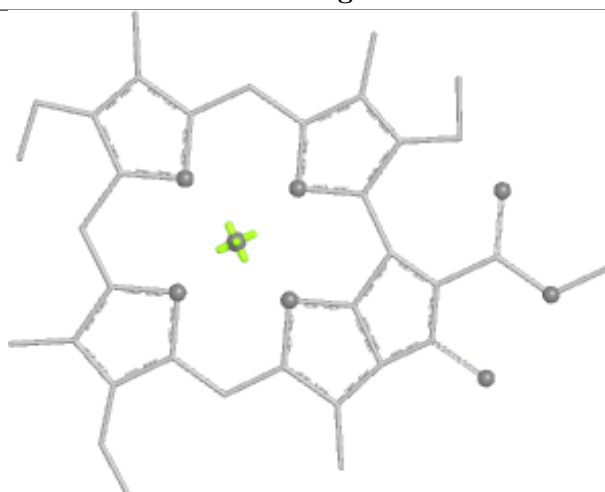
Bond lengths



Bond angles

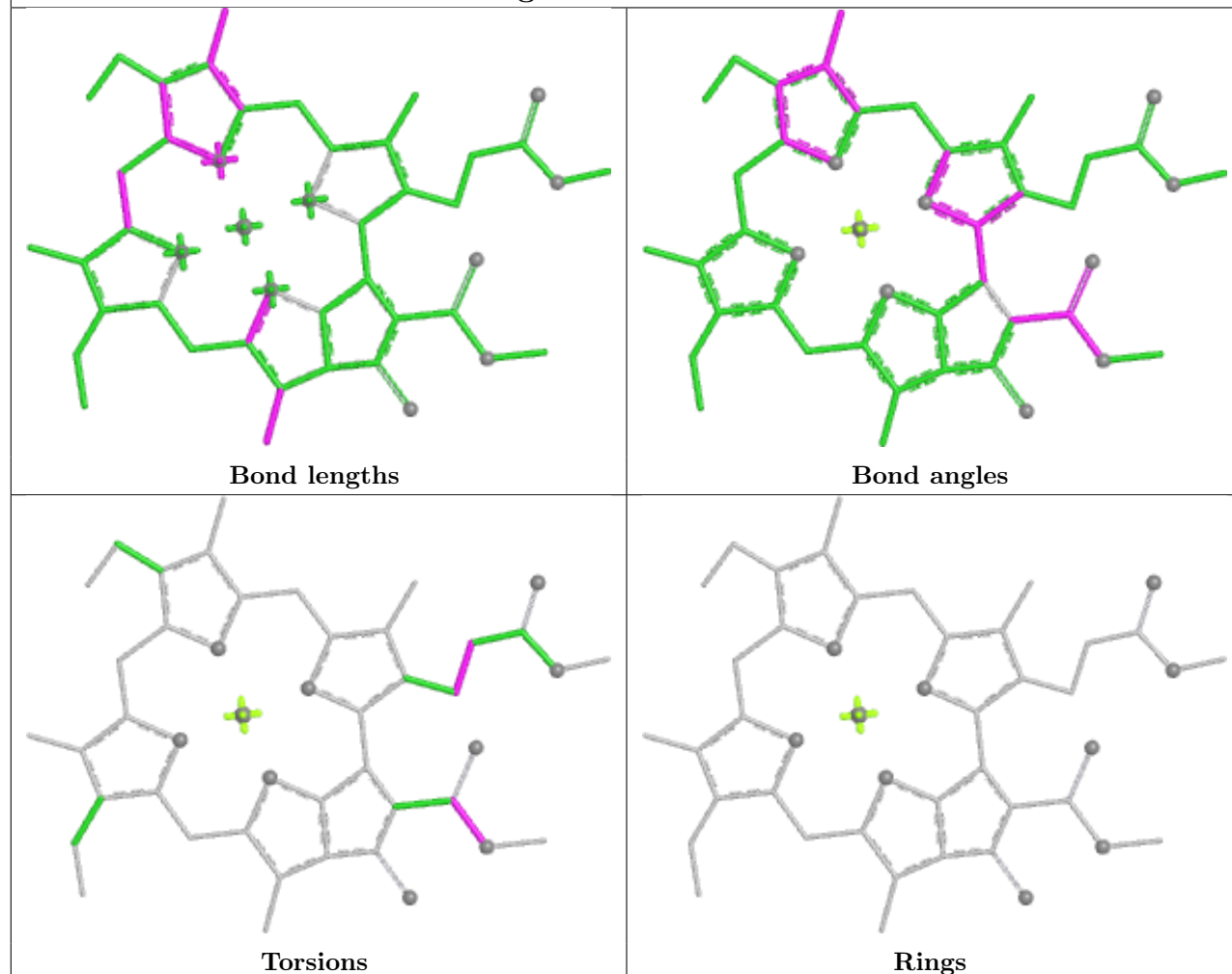


Torsions

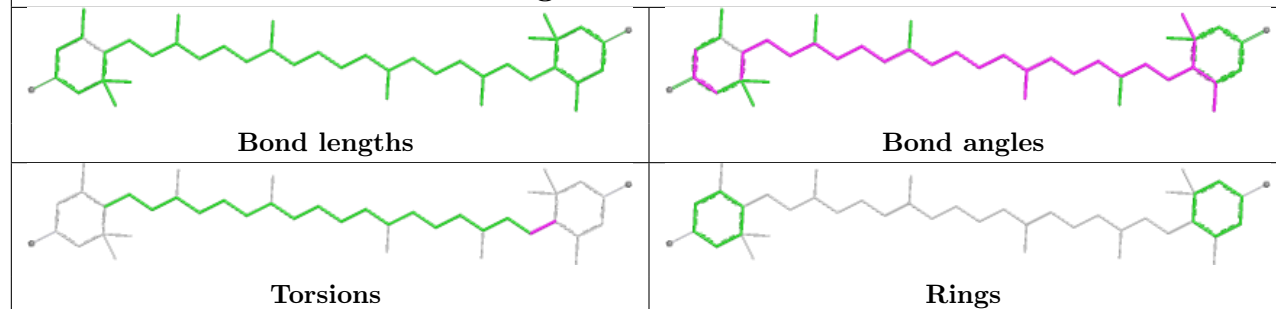


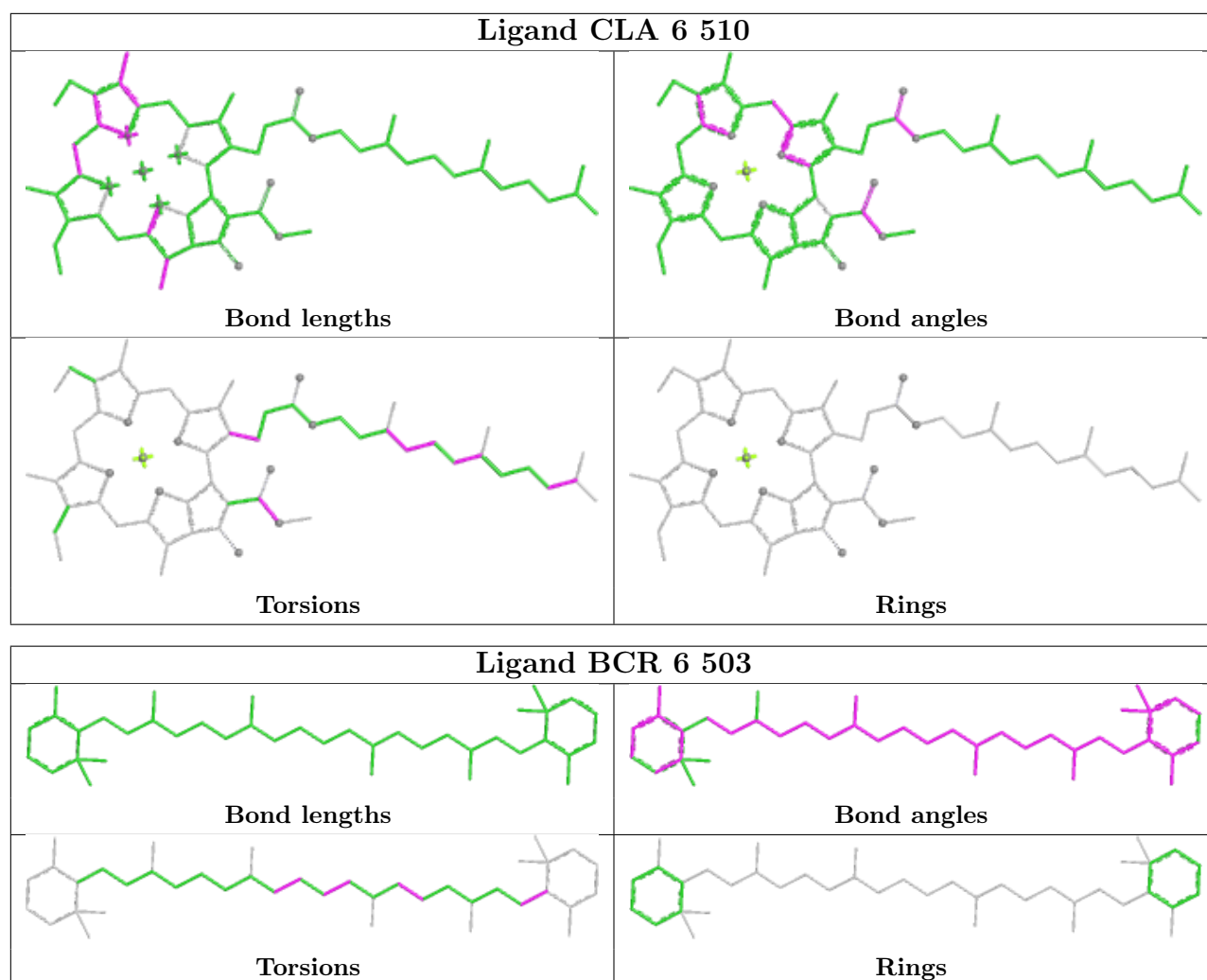
Rings

Ligand CLA 1 505

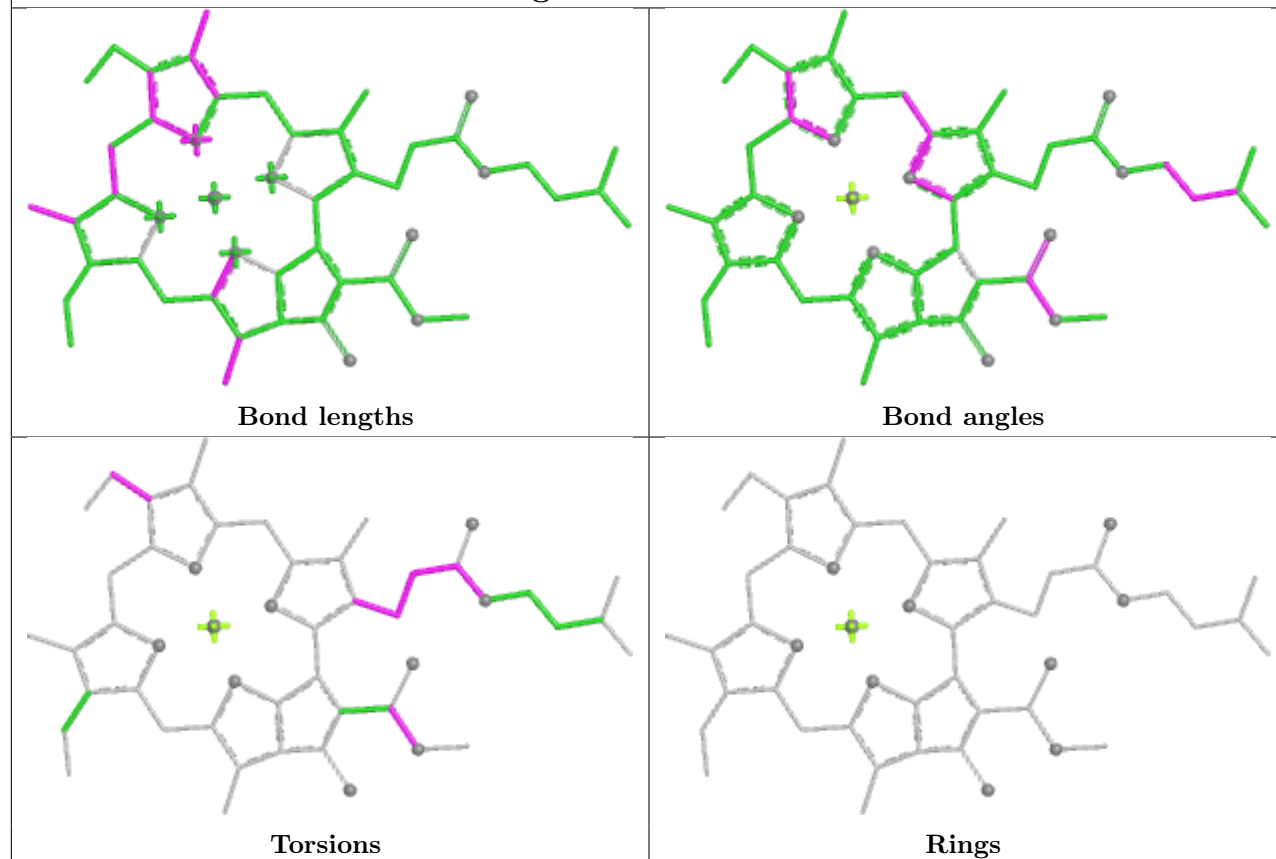


Ligand LUT 4 302

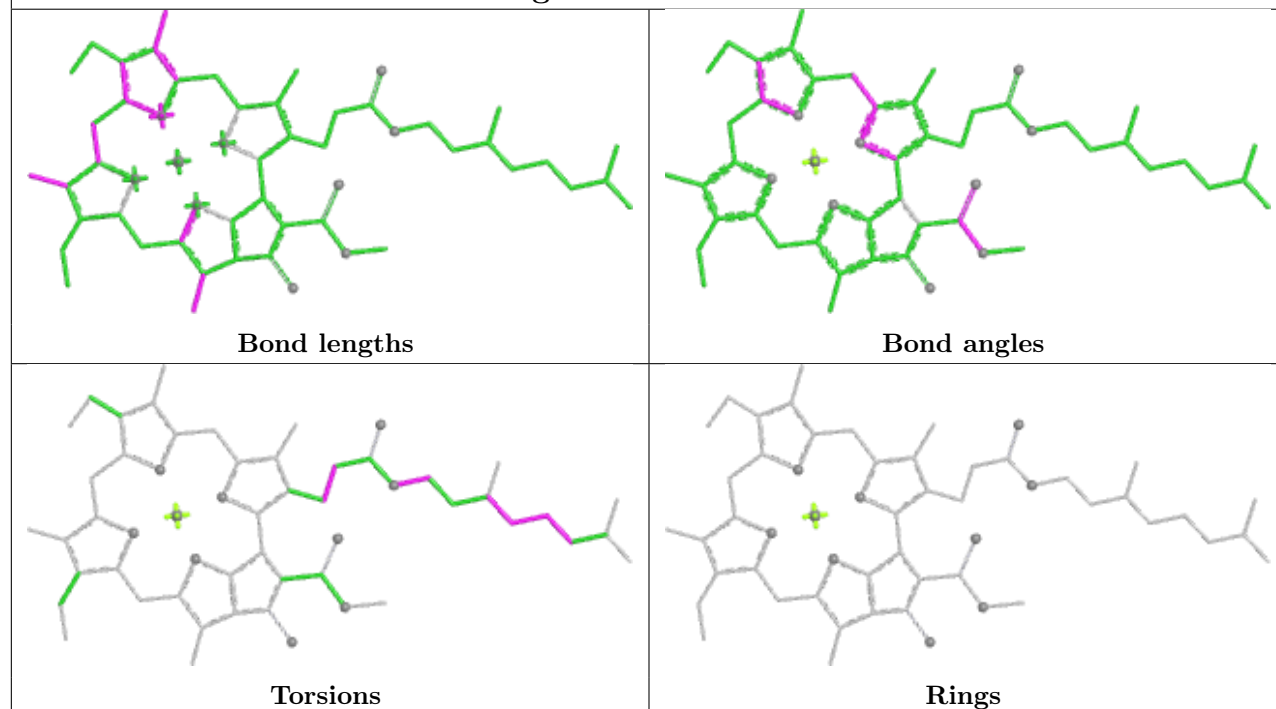




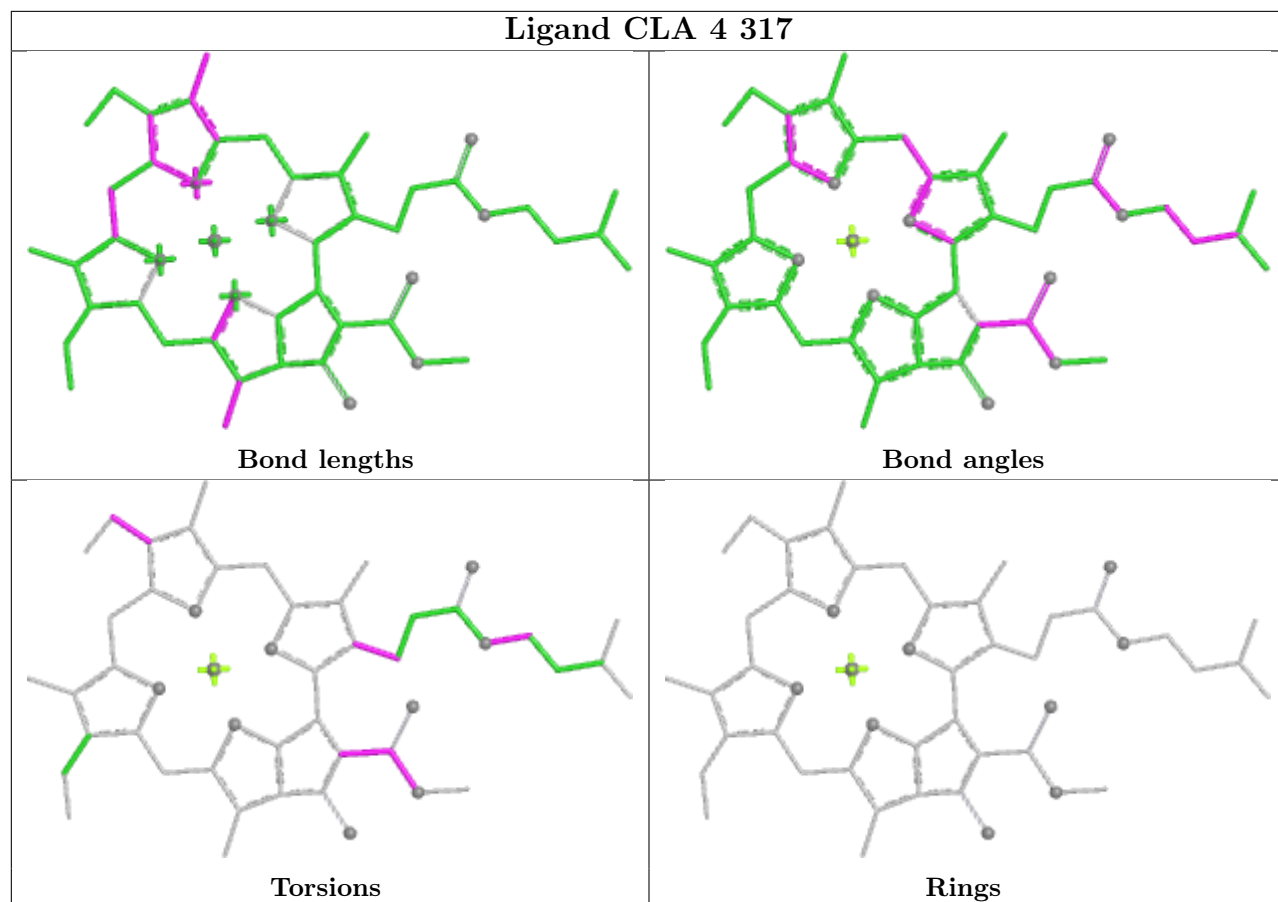
Ligand CLA B 820



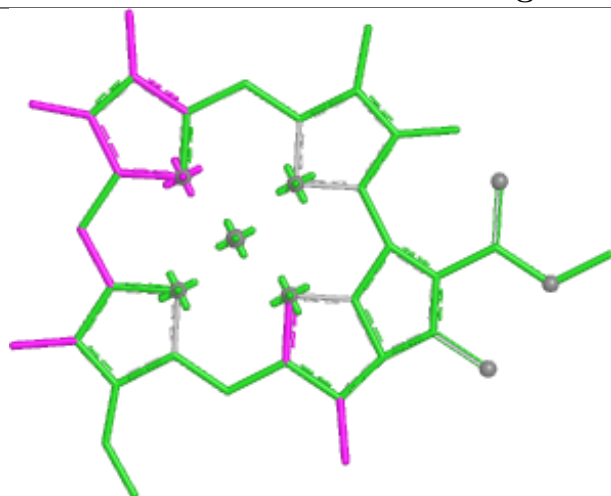
Ligand CLA B 818



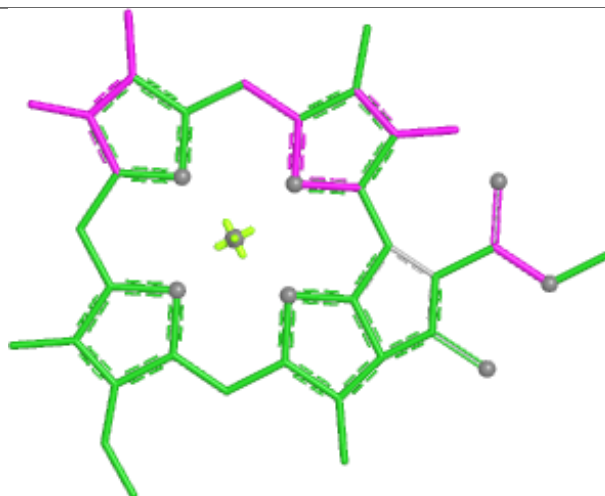
Ligand CLA 4 317



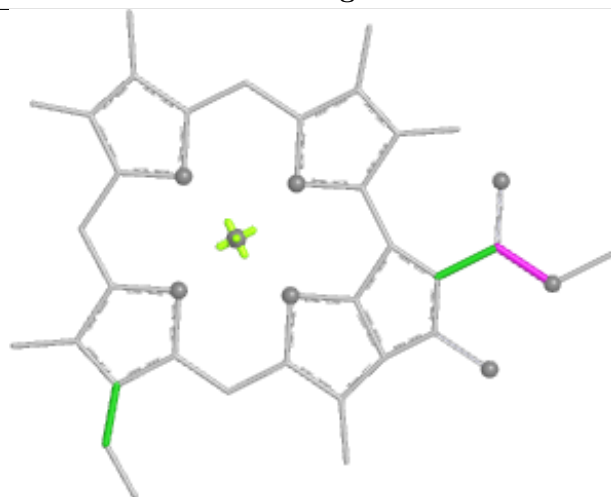
Ligand CLA L 302



Bond lengths



Bond angles

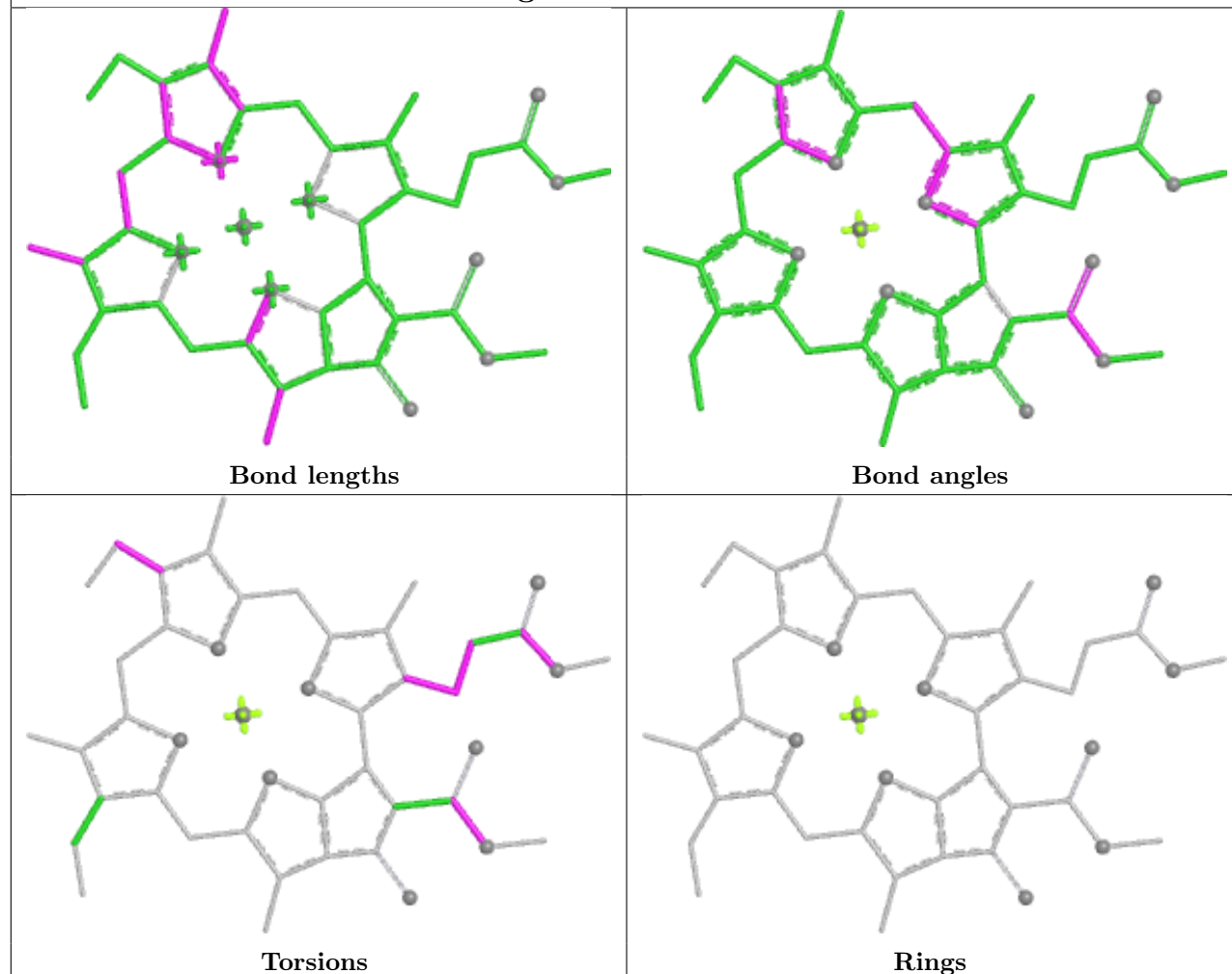


Torsions

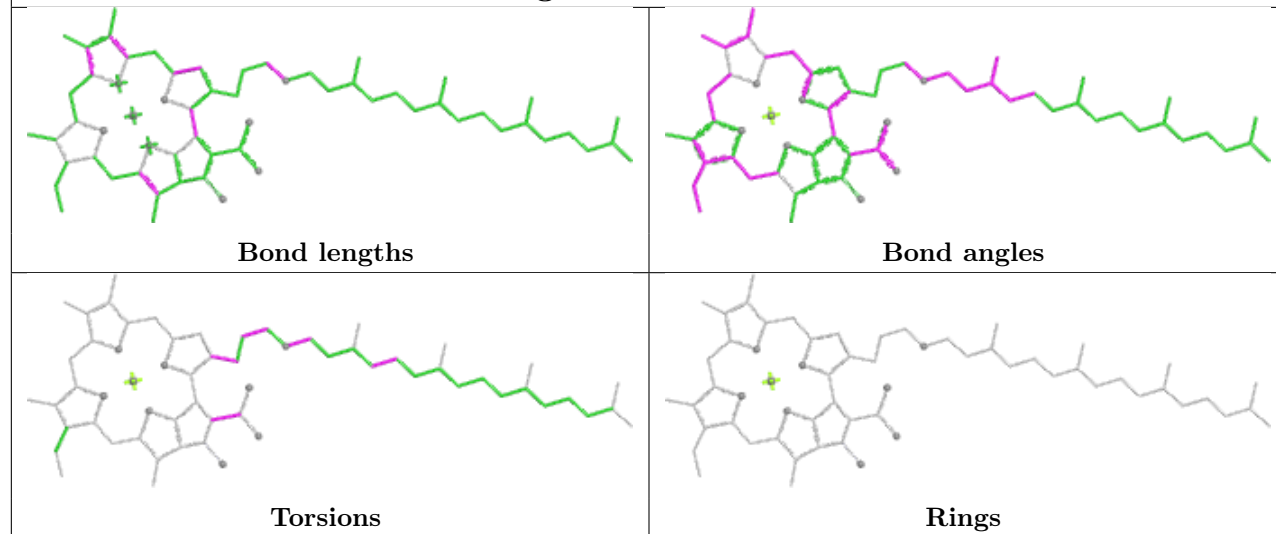


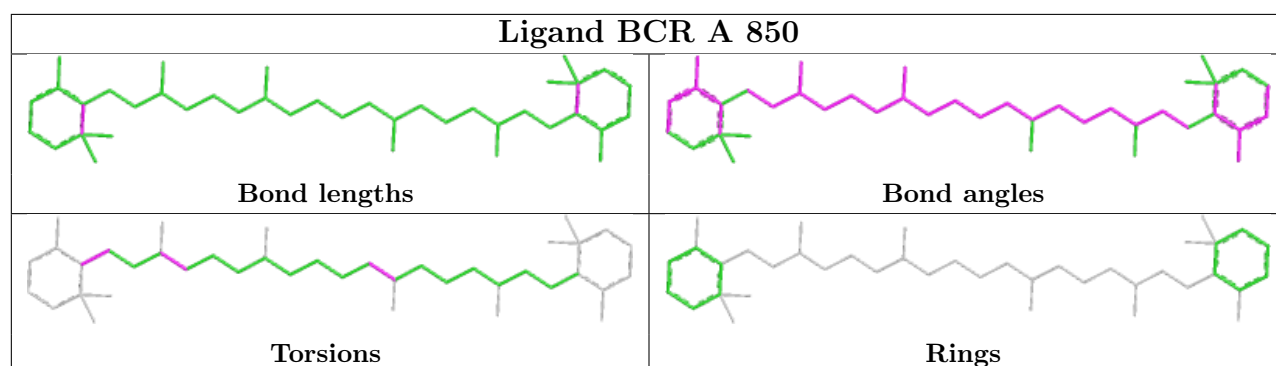
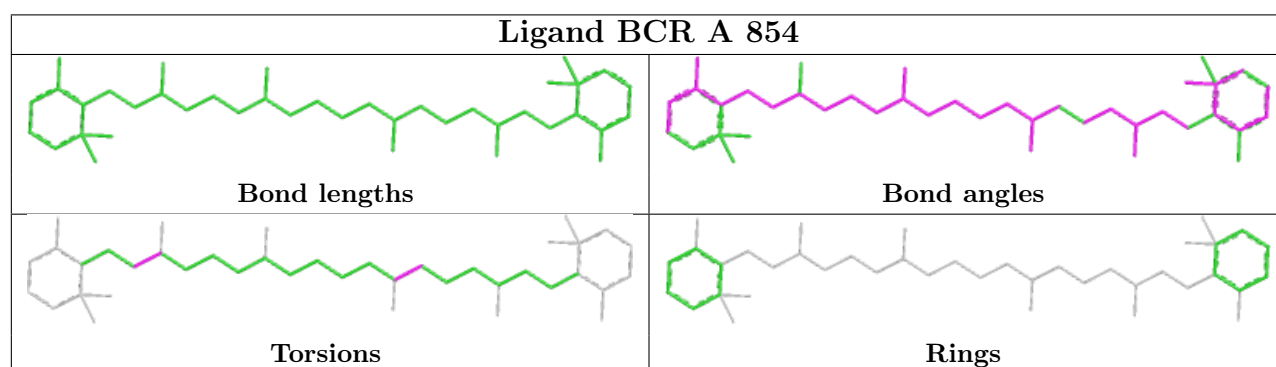
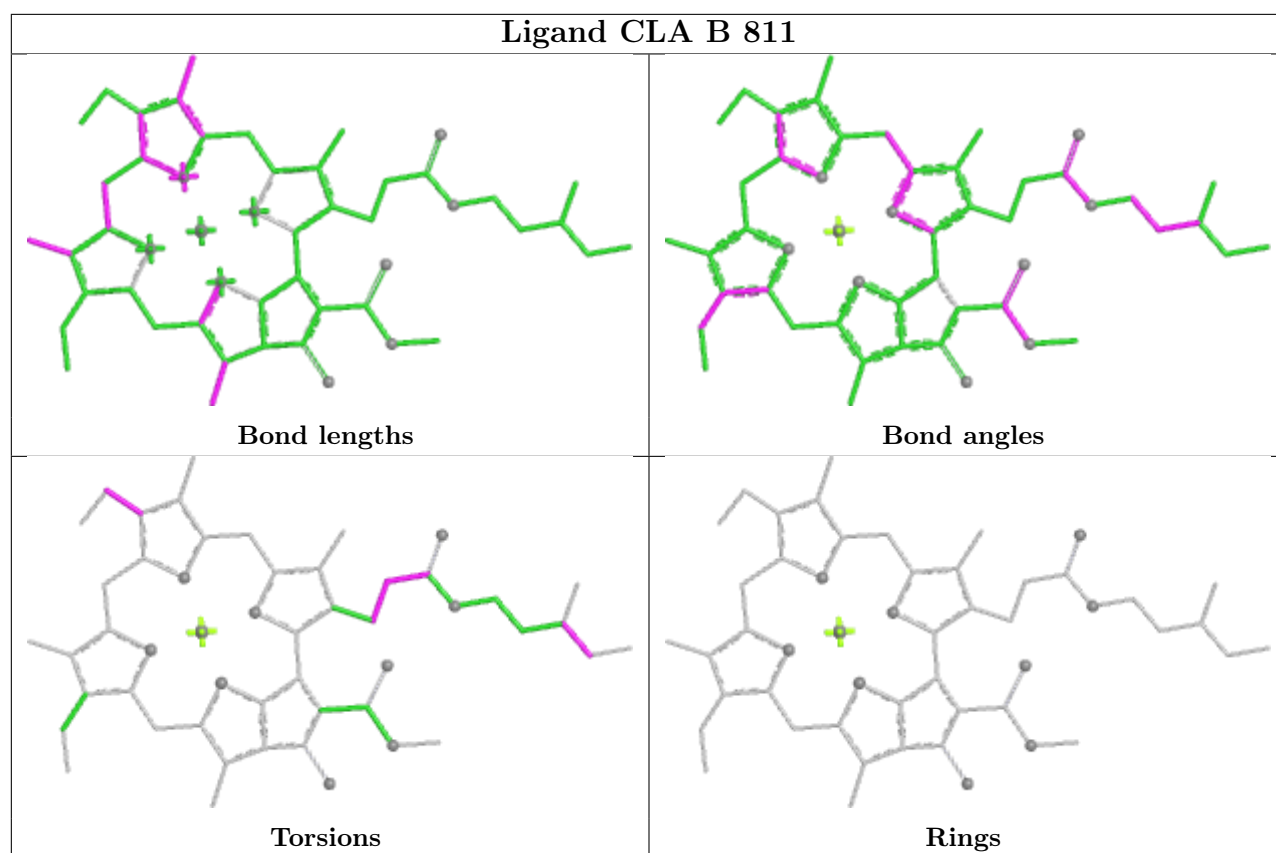
Rings

Ligand CLA 3 316

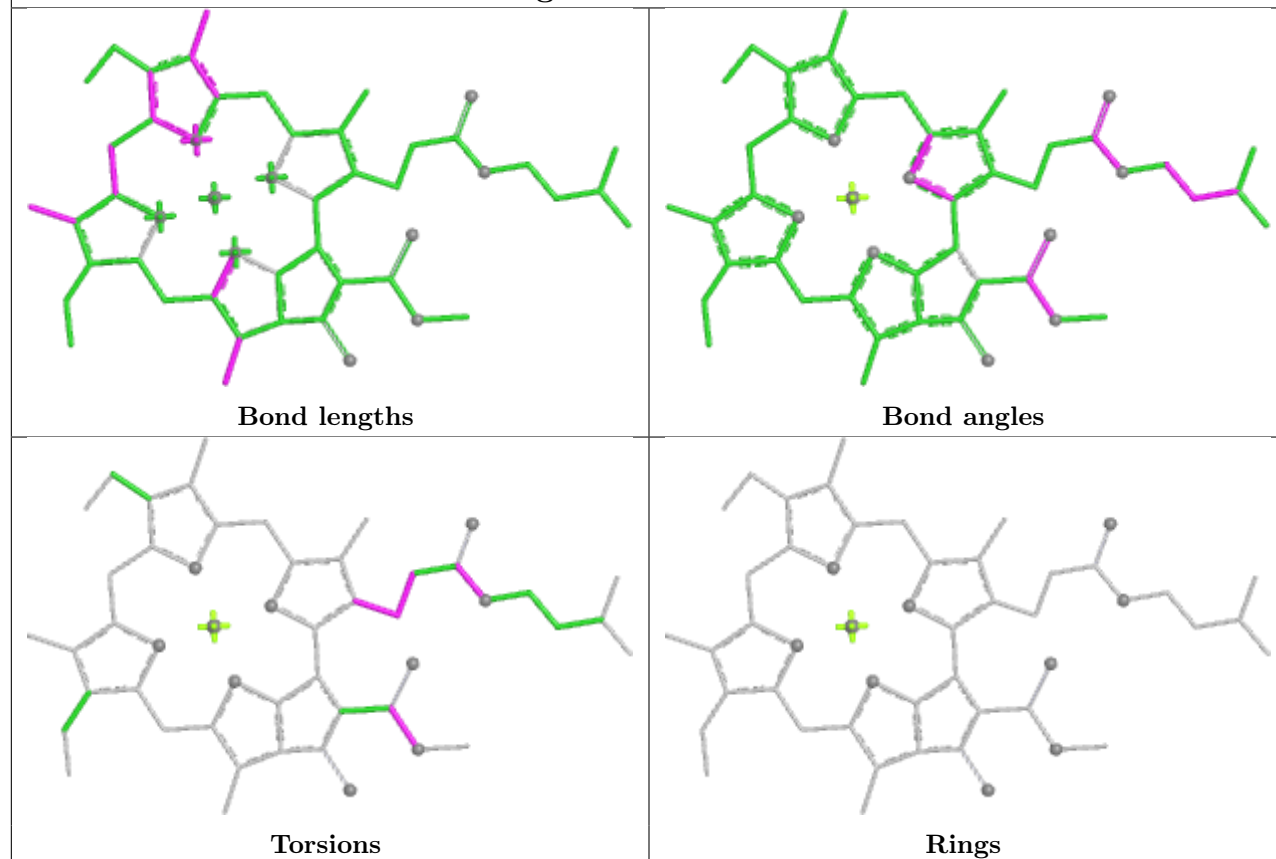


Ligand CL0 A 801

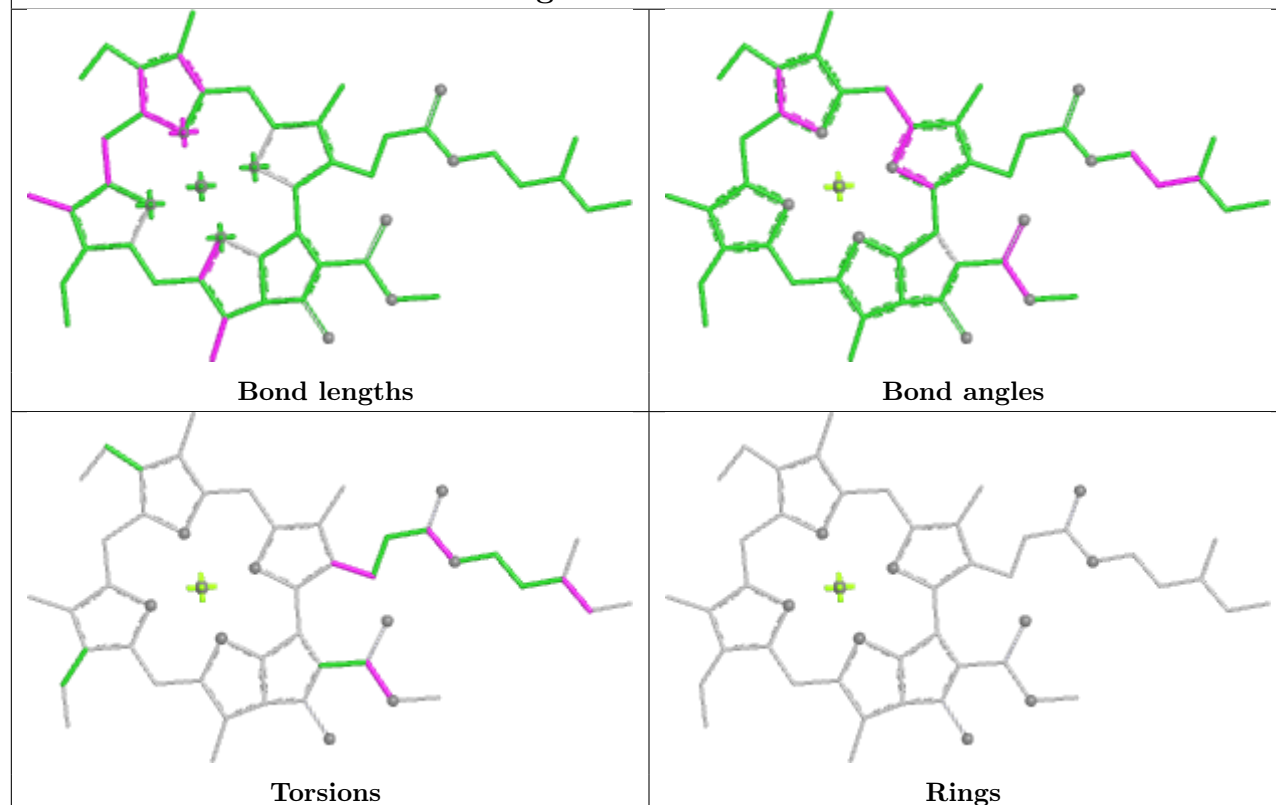




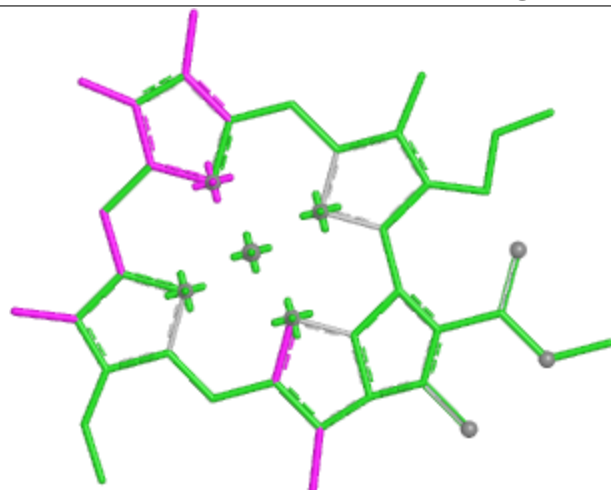
Ligand CLA 4 309



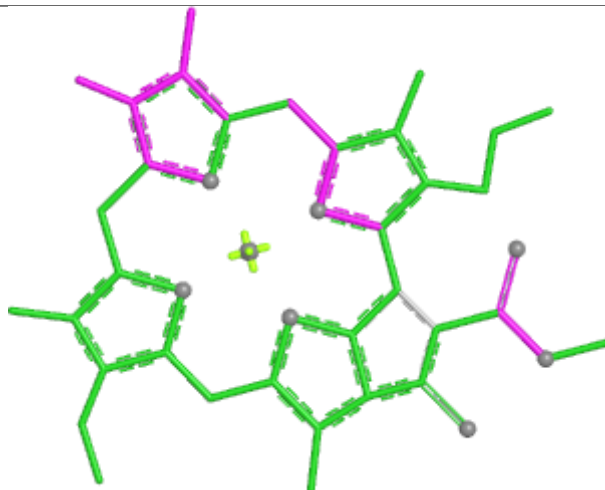
Ligand CLA 6 507



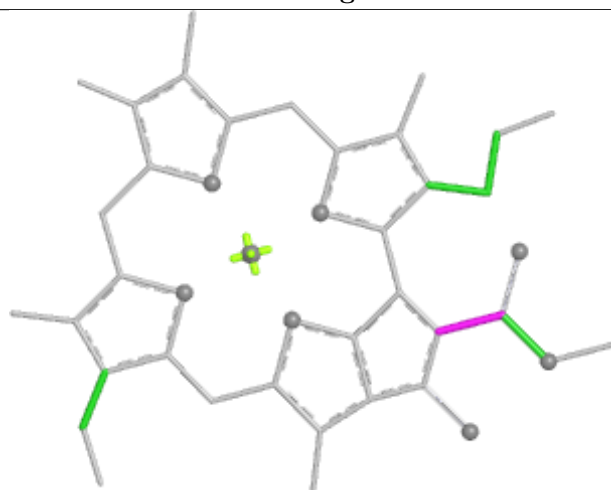
Ligand CLA A 823



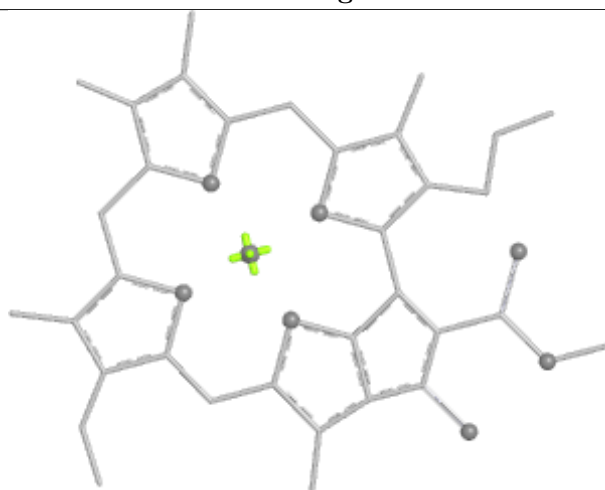
Bond lengths



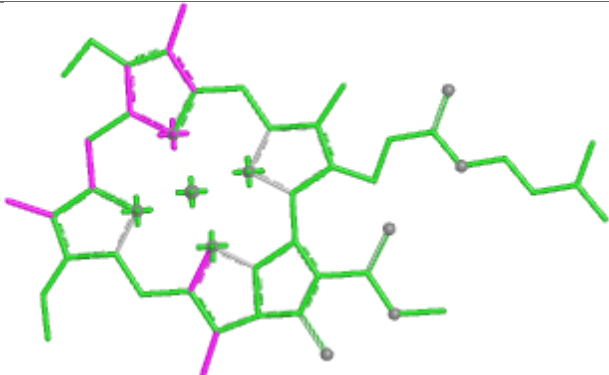
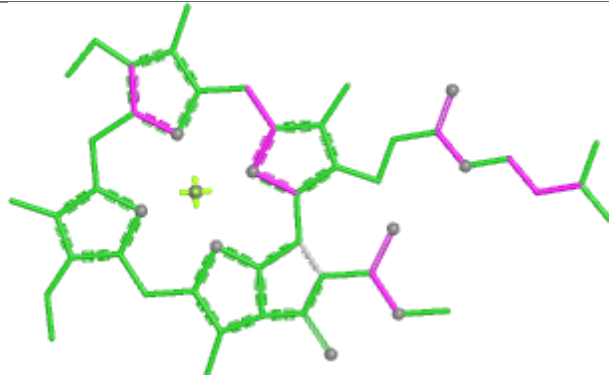
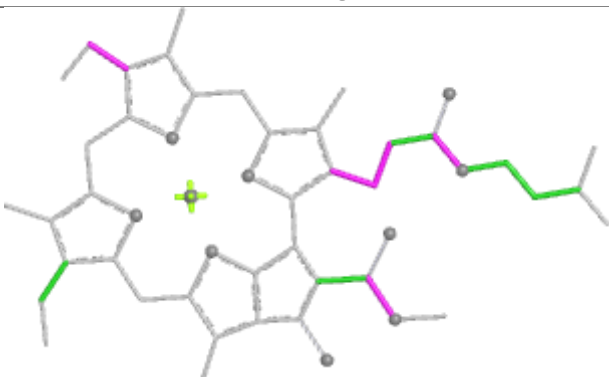
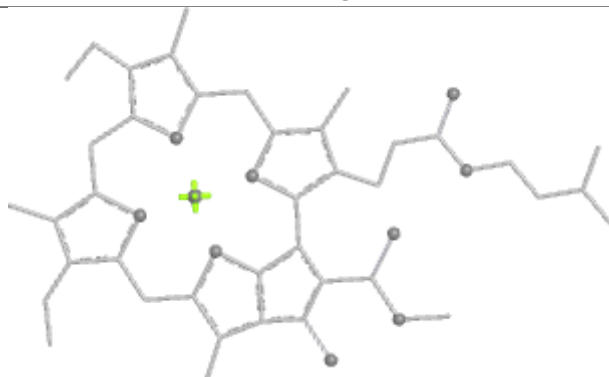
Bond angles

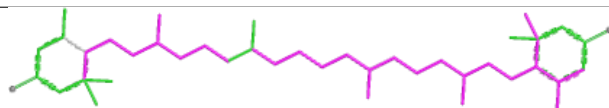
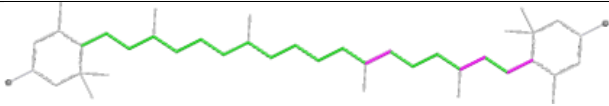
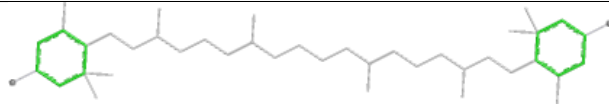


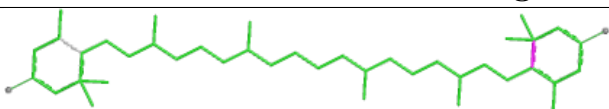
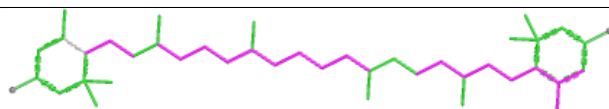
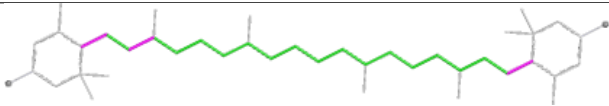
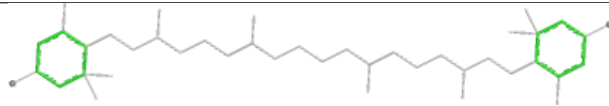
Torsions

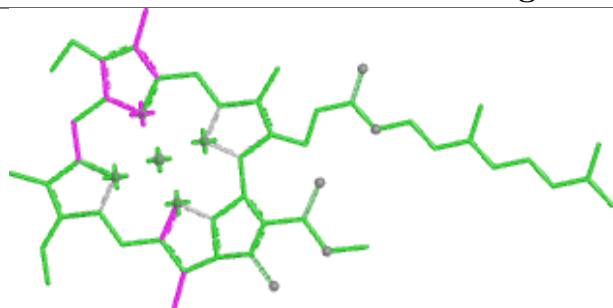


Rings

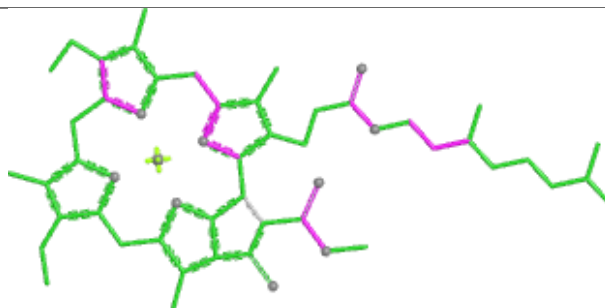
Ligand CLA 6 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

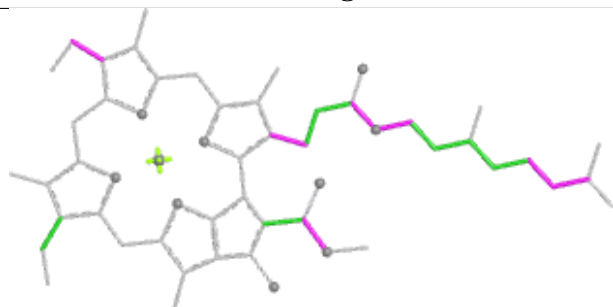
Ligand LUT 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 506

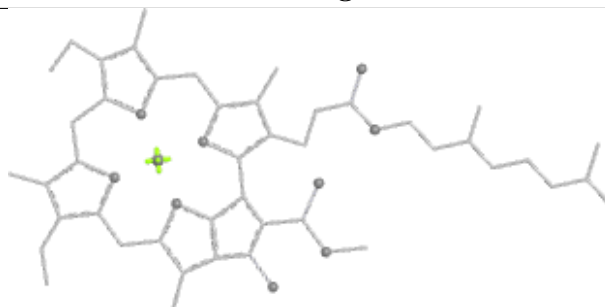
Bond lengths



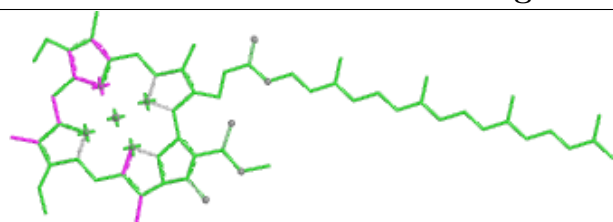
Bond angles



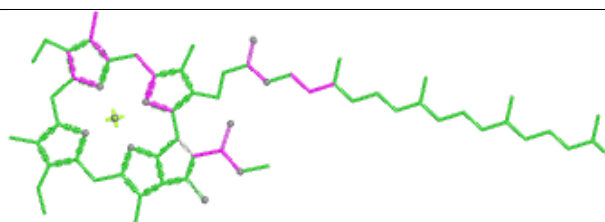
Torsions



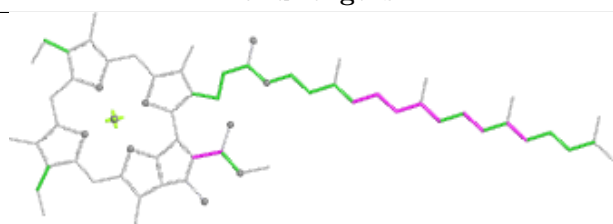
Rings

Ligand CLA B 826

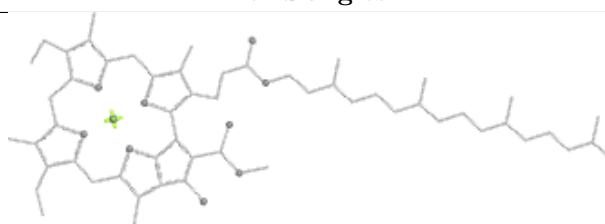
Bond lengths



Bond angles

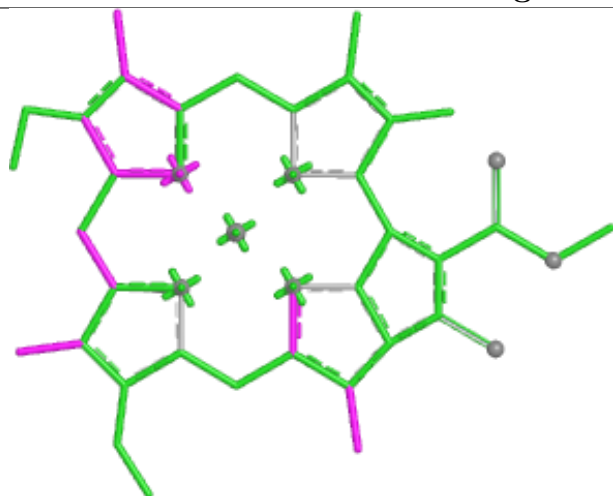


Torsions

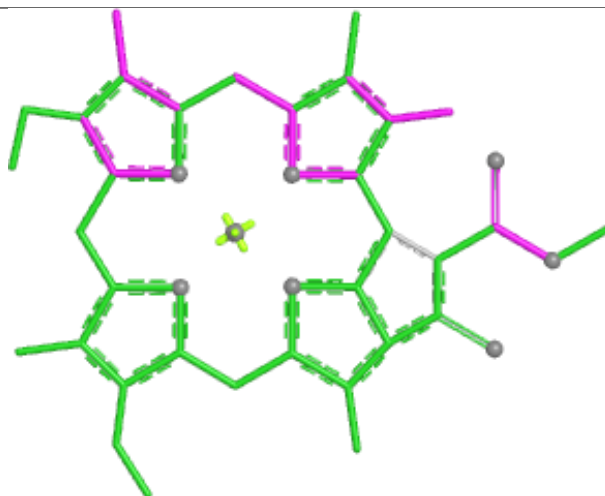


Rings

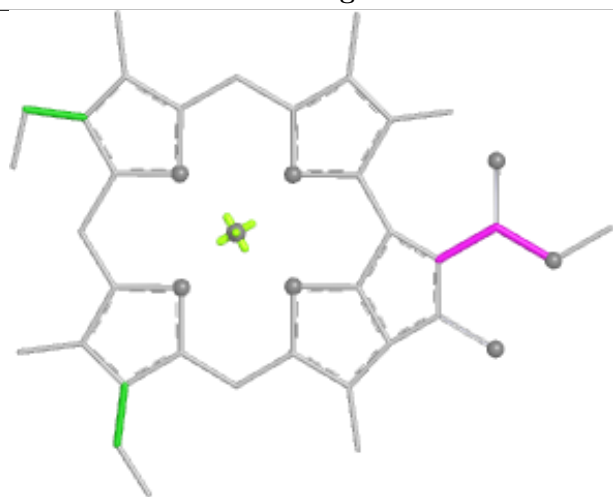
Ligand CLA A 820



Bond lengths



Bond angles

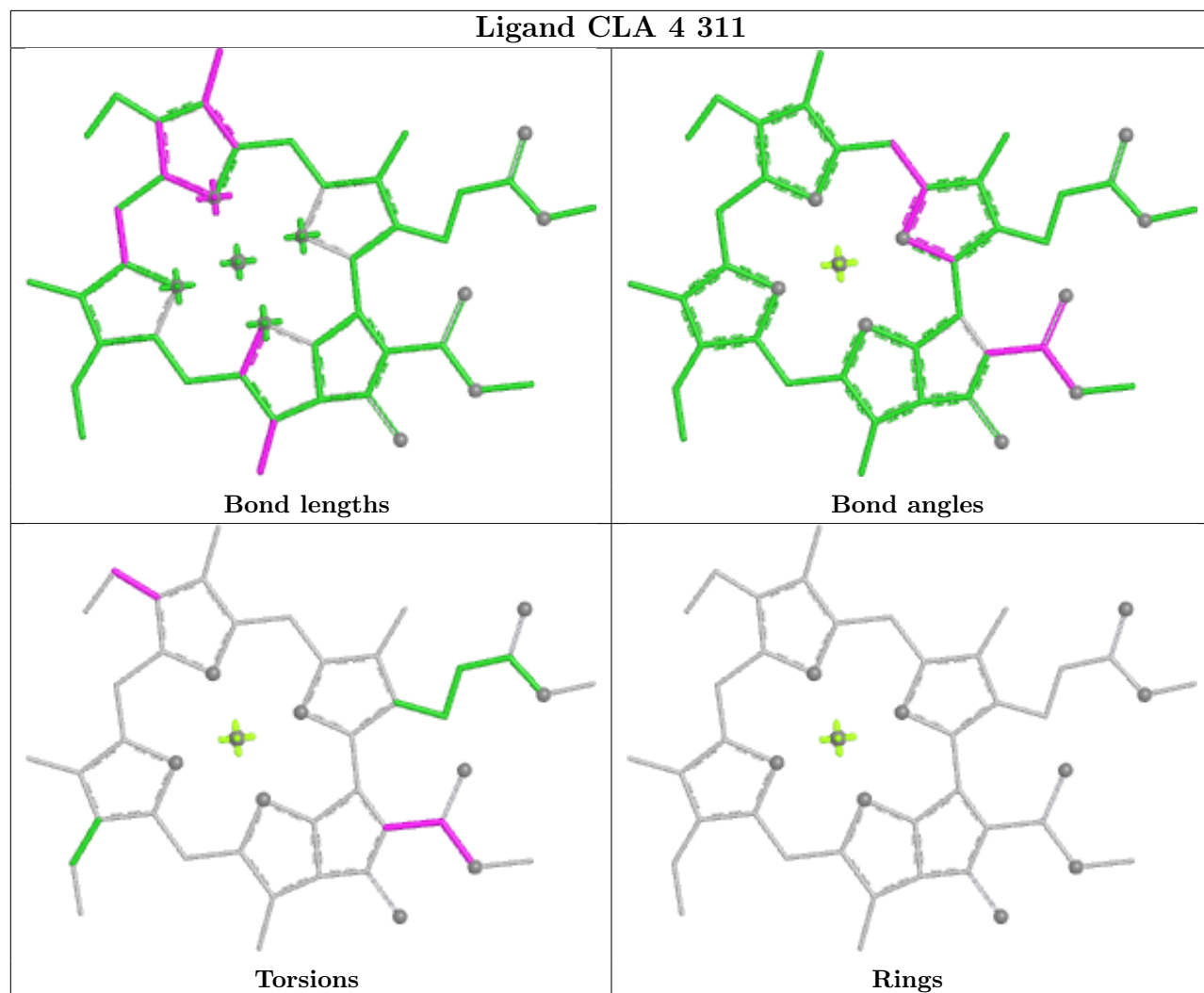


Torsions

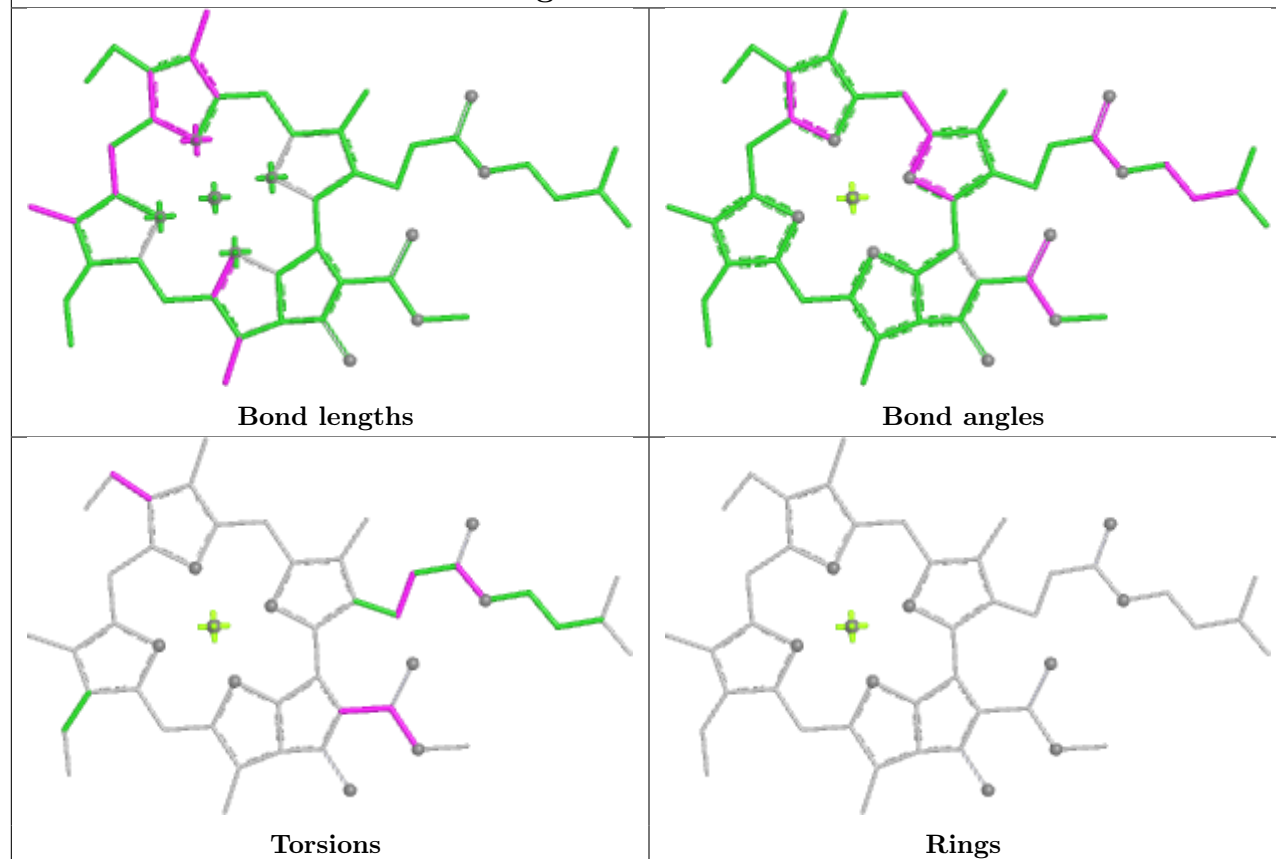


Rings

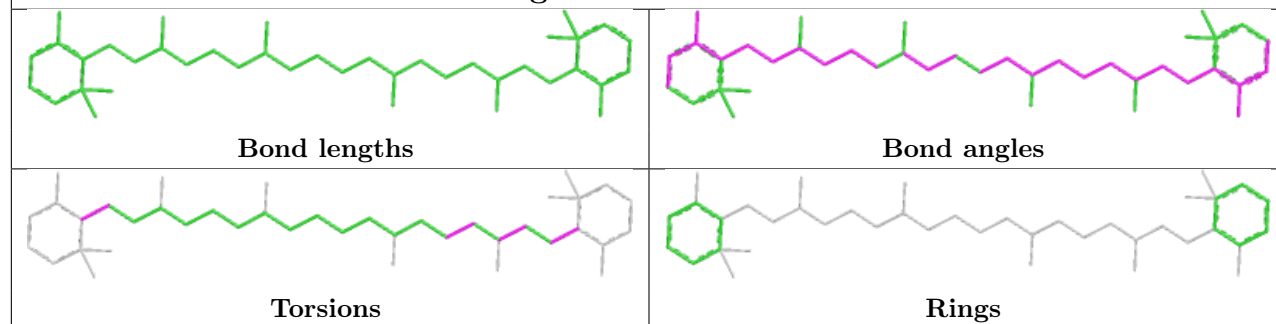
Ligand CLA 4 311



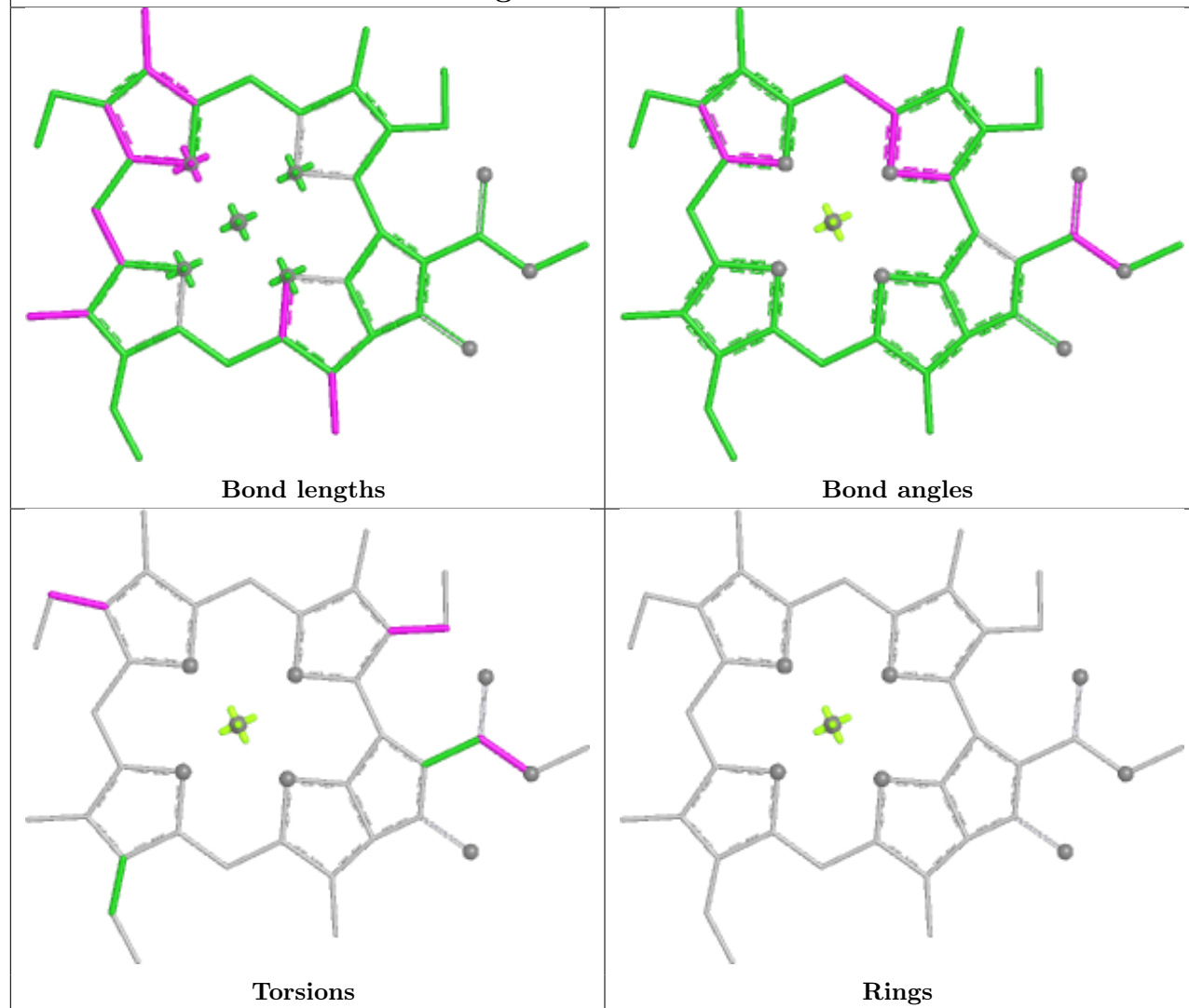
Ligand CLA 4 305



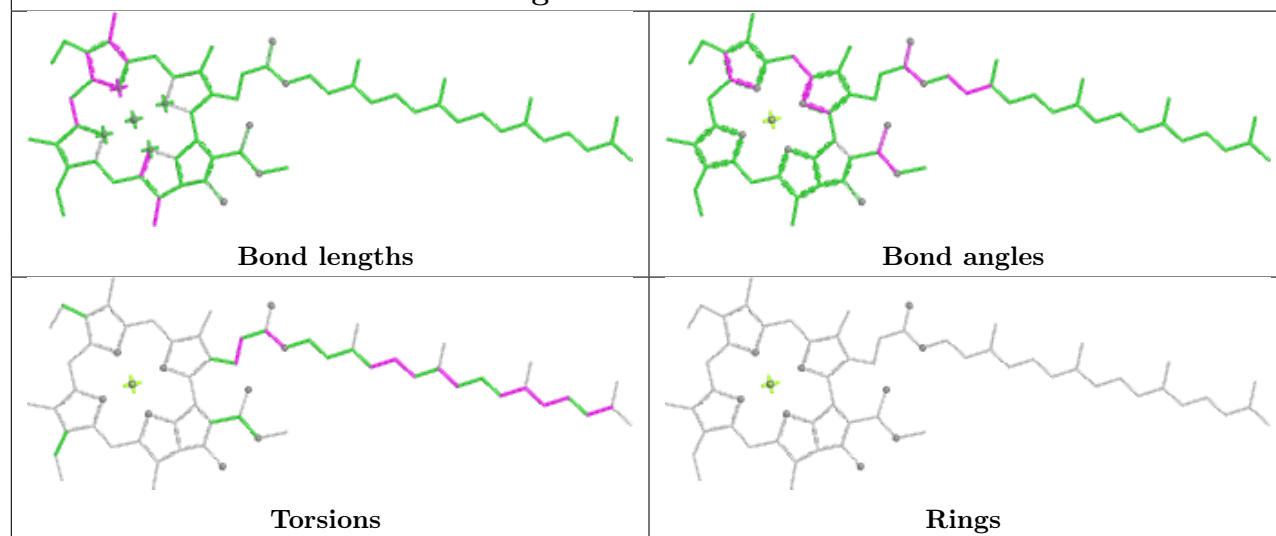
Ligand BCR A 849

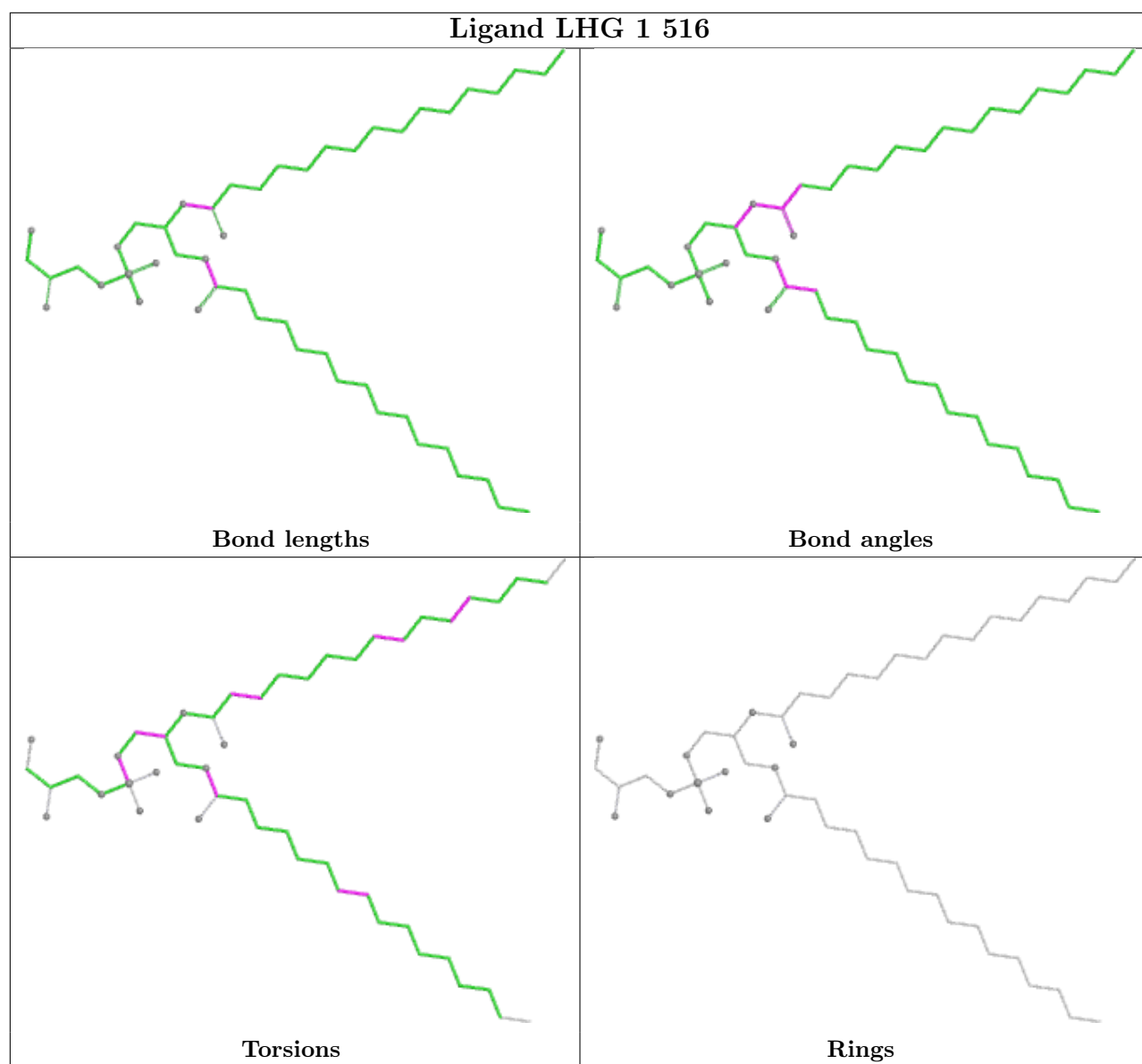


Ligand CLA A 814

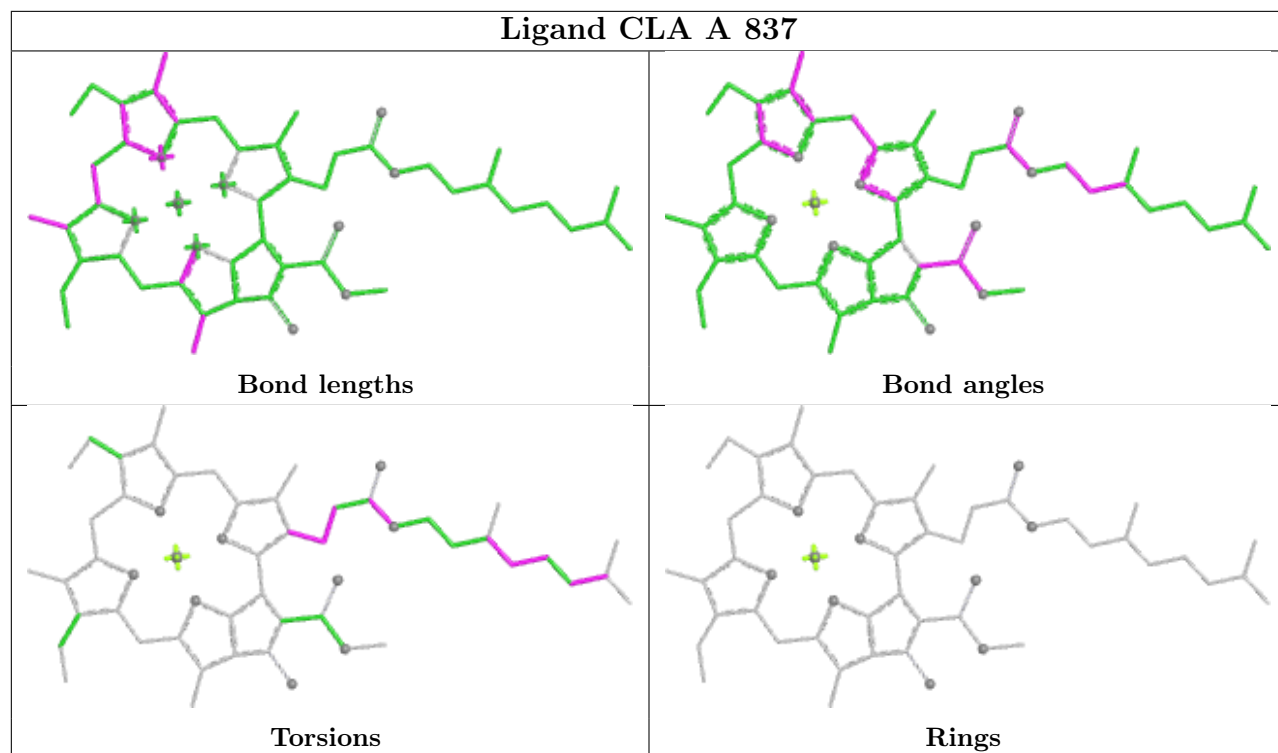


Ligand CLA A 839

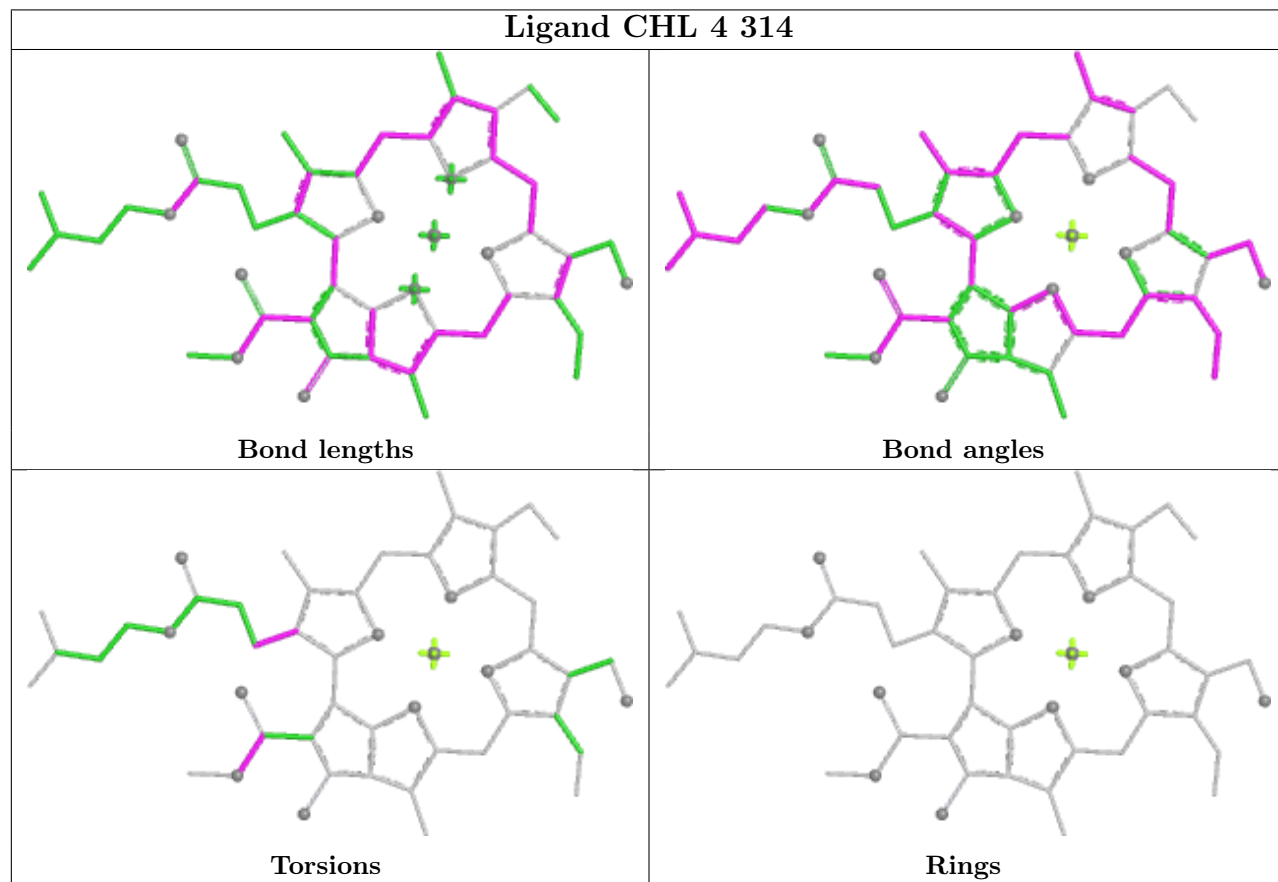


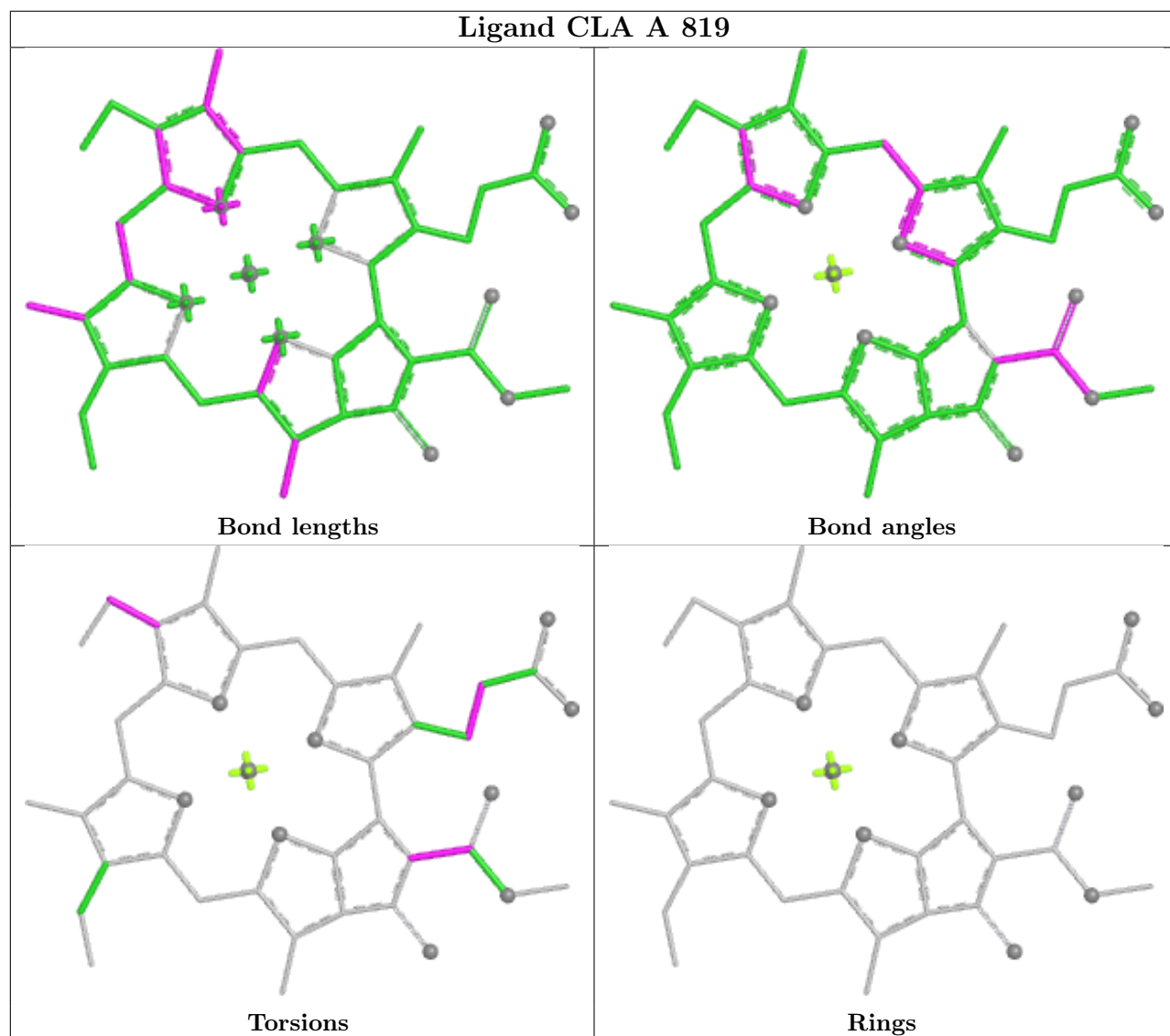
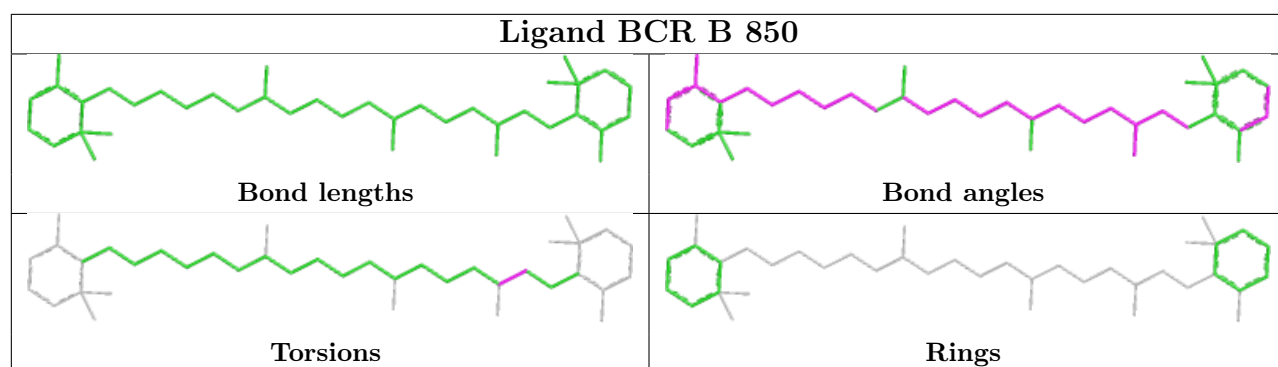


Ligand CLA A 837

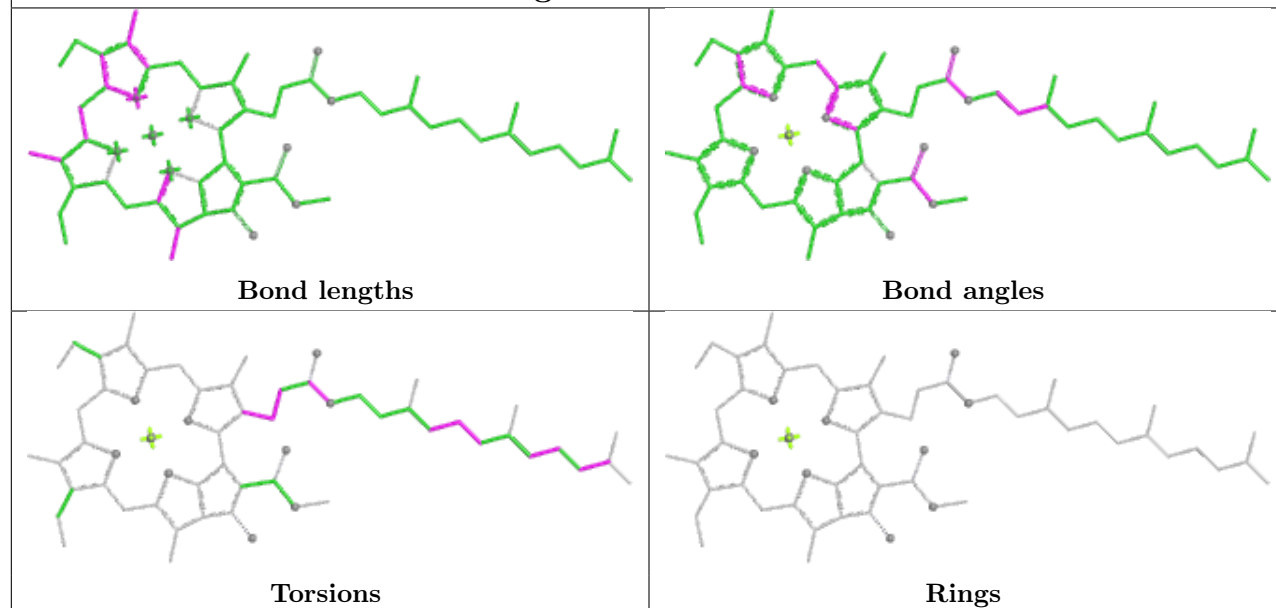


Ligand CHL 4 314

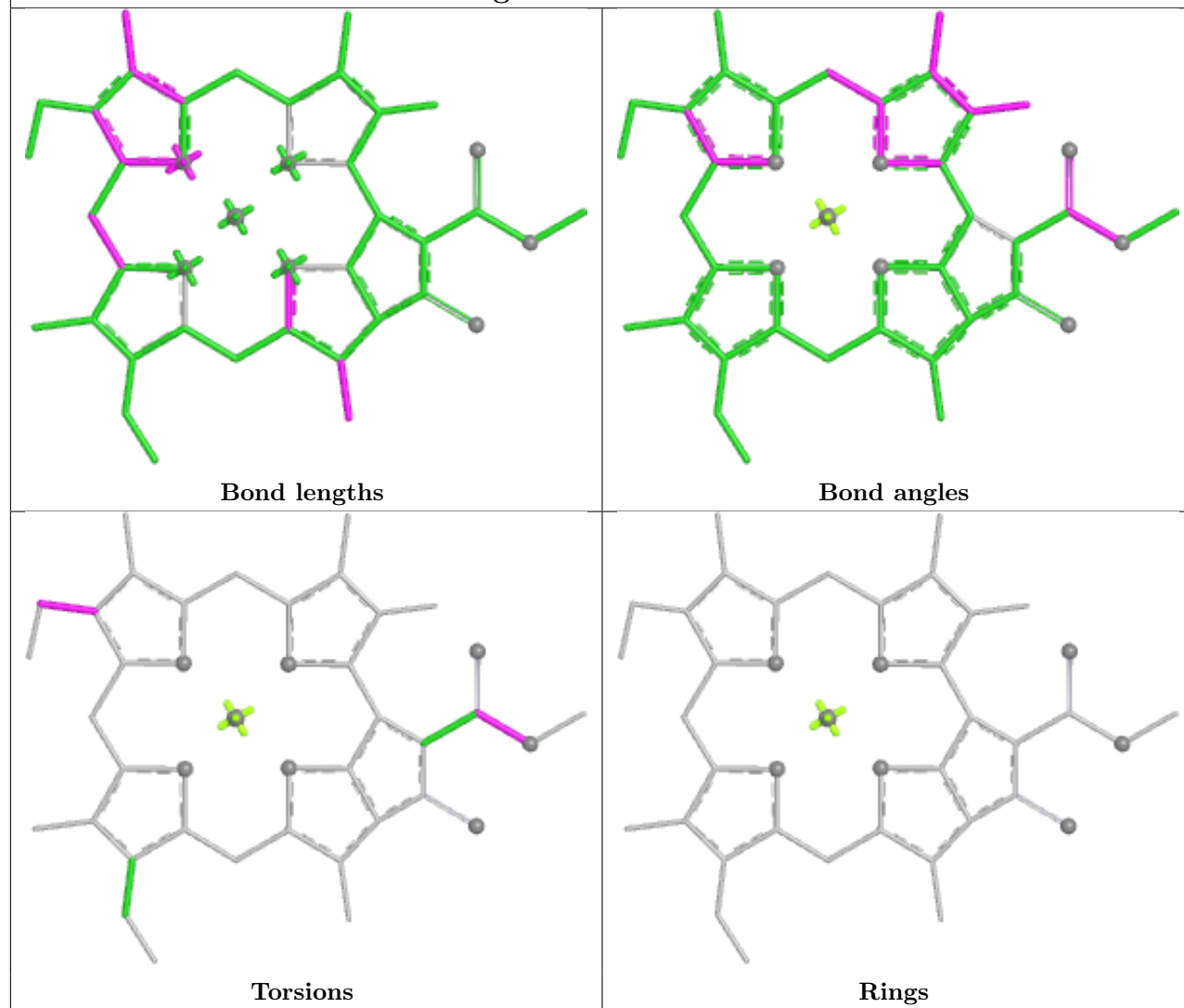




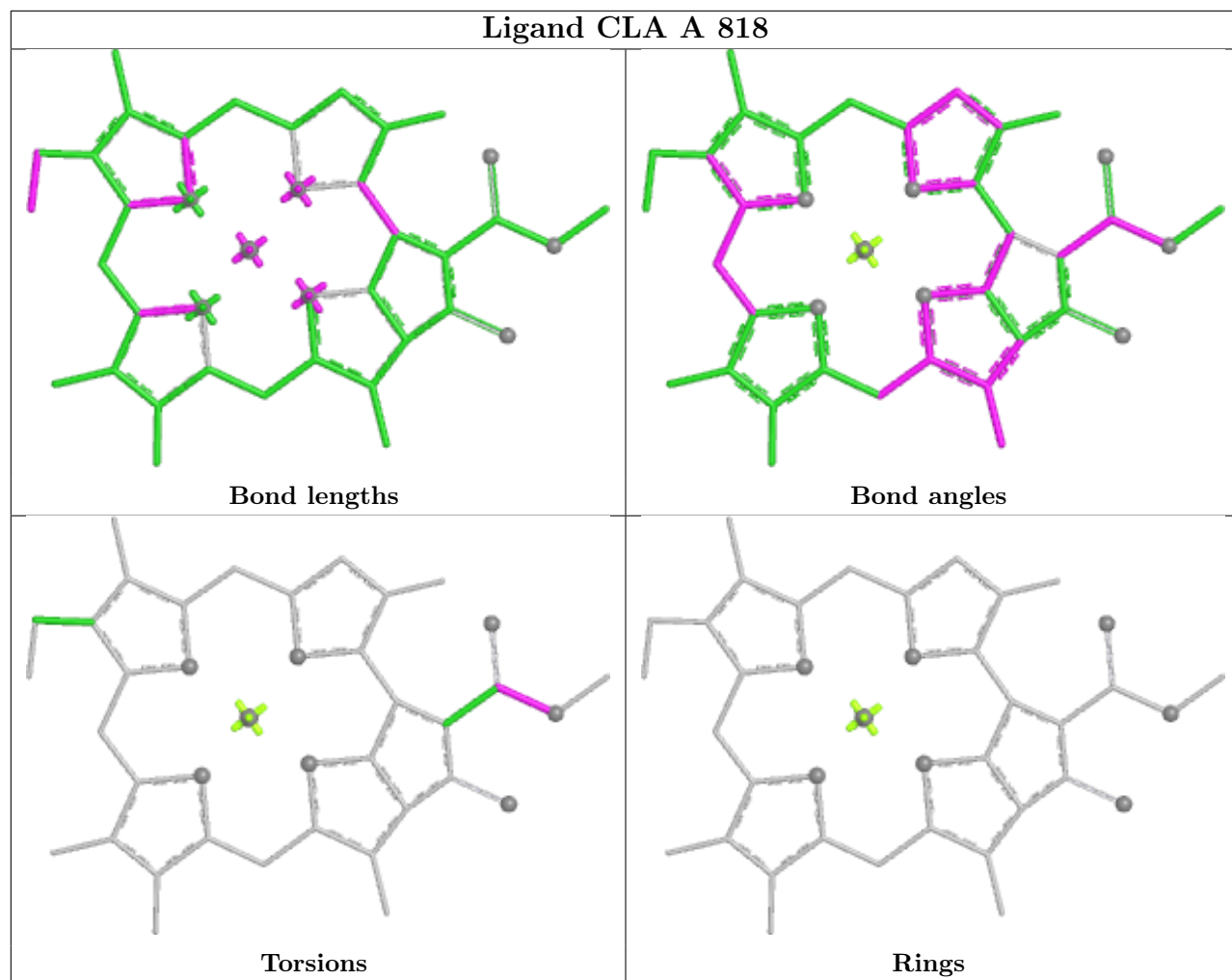
Ligand CLA L 303



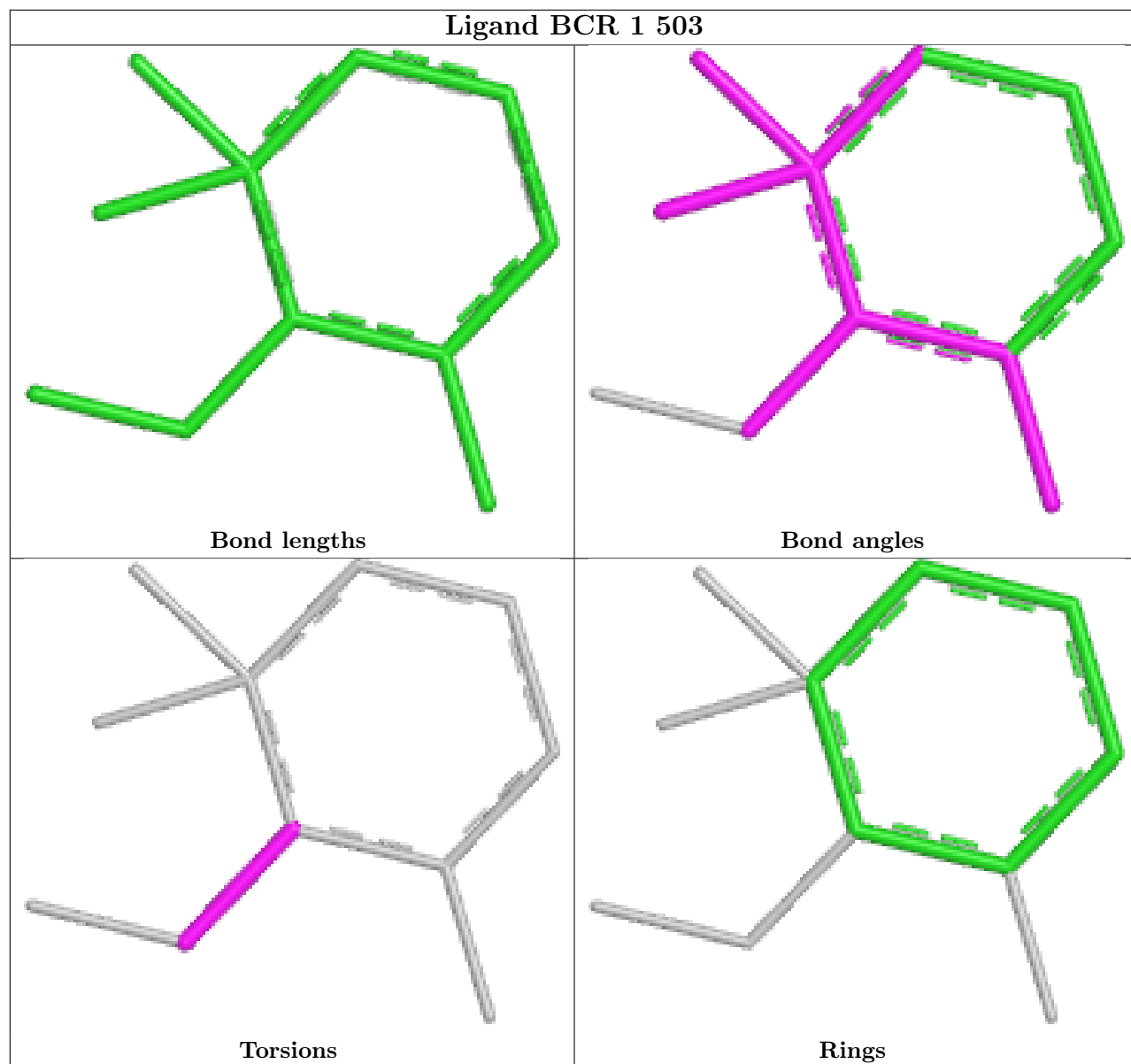
Ligand CLA A 833



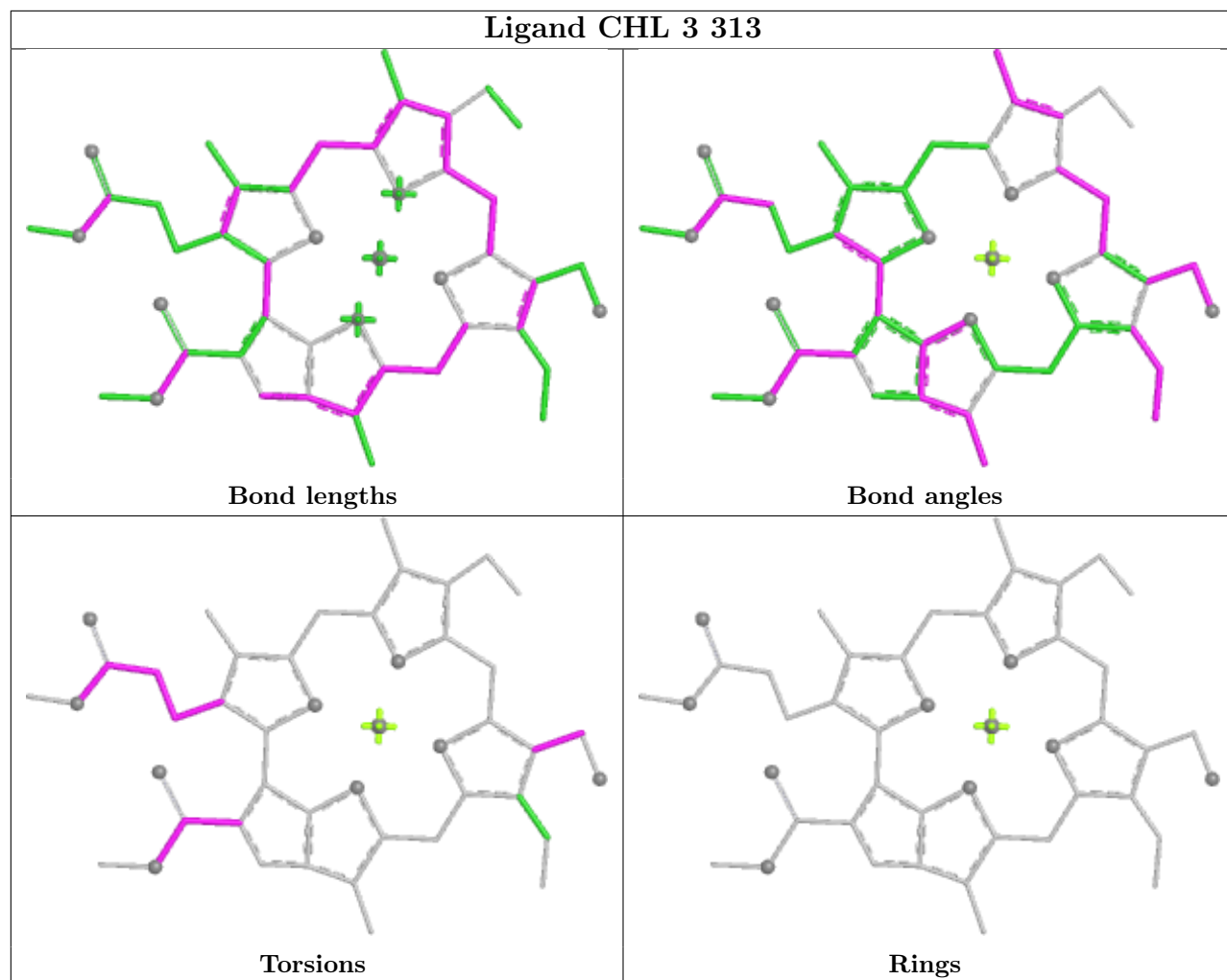
Ligand CLA A 818



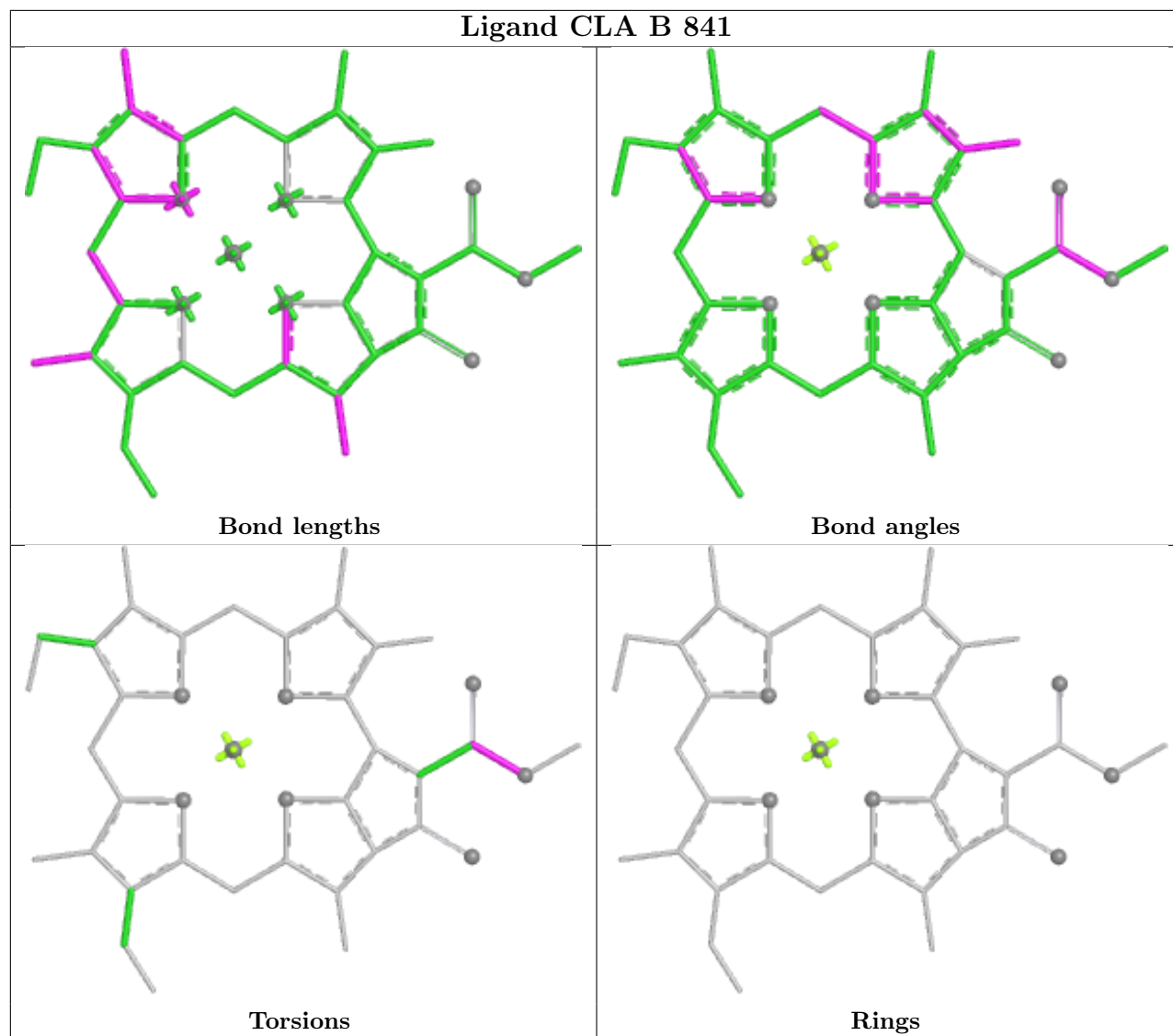
Ligand BCR 1 503



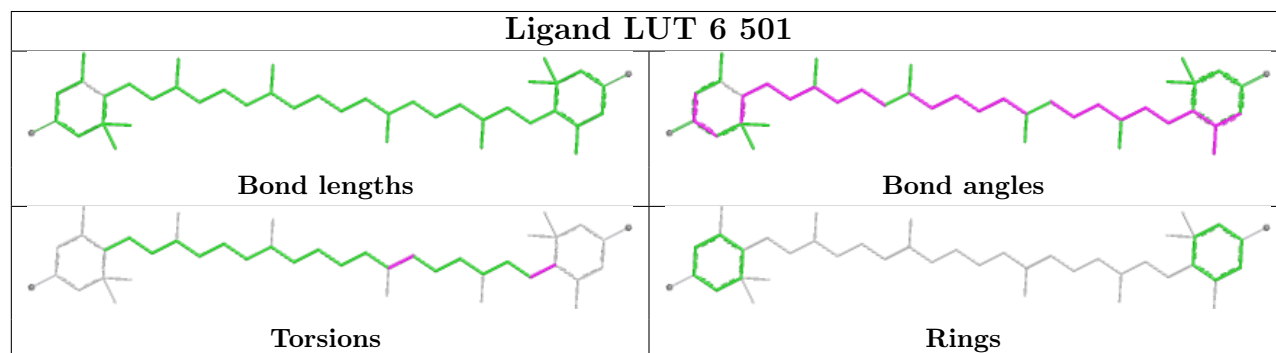
Ligand CHL 3 313



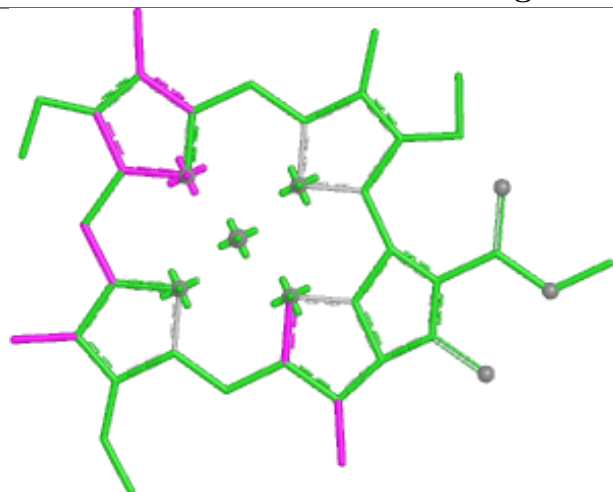
Ligand CLA B 841



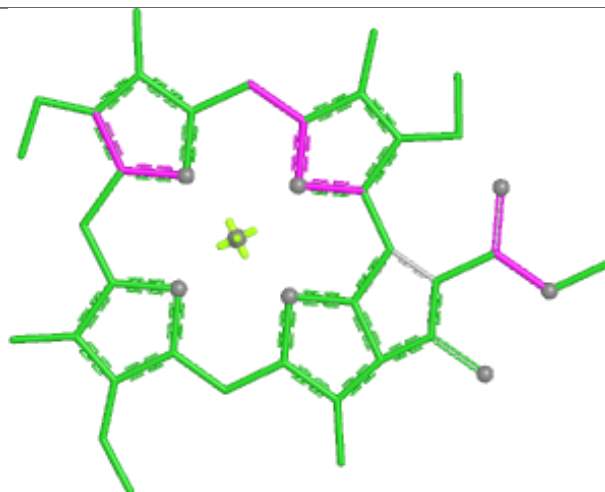
Ligand LUT 6 501



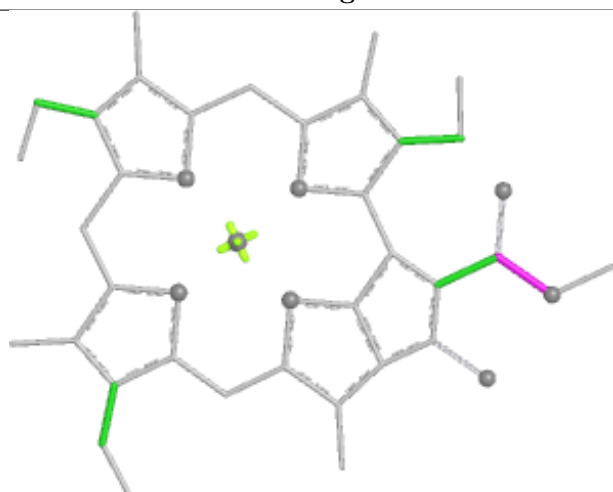
Ligand CLA B 825



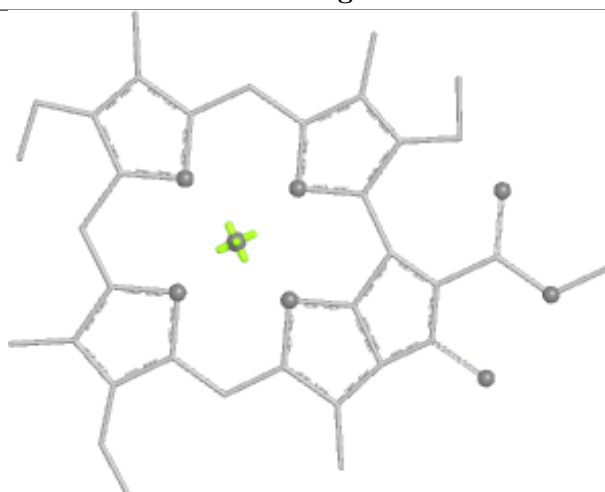
Bond lengths



Bond angles

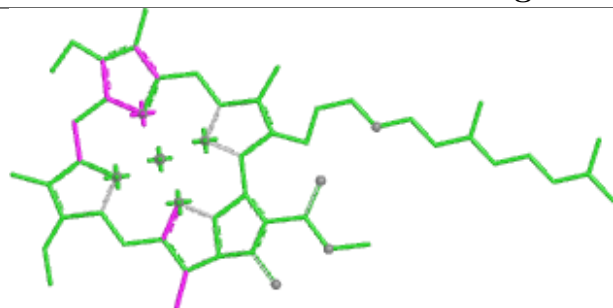


Torsions

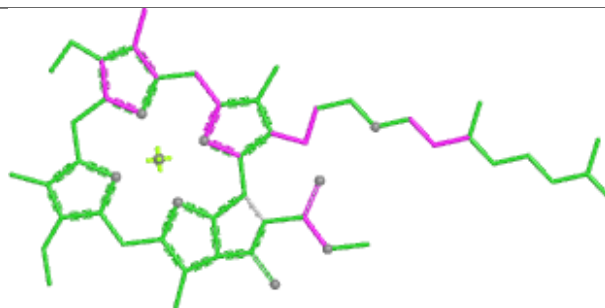


Rings

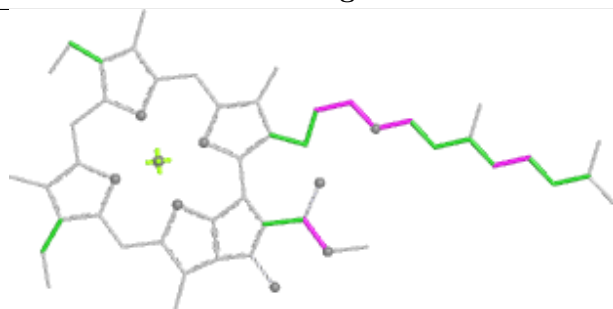
Ligand CLA B 808



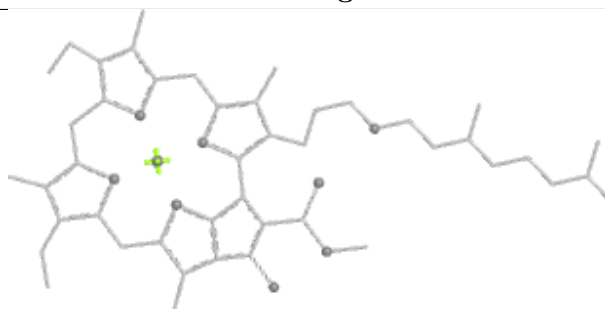
Bond lengths



Bond angles

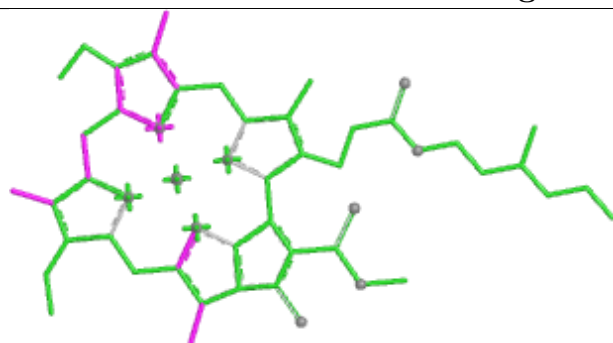


Torsions

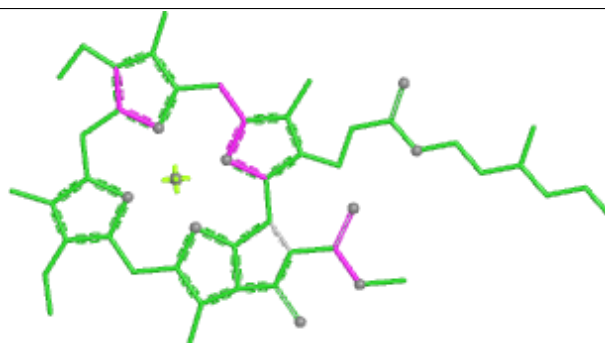


Rings

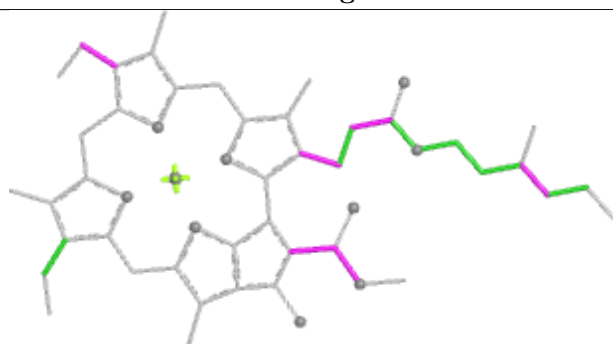
Ligand CLA 6 505



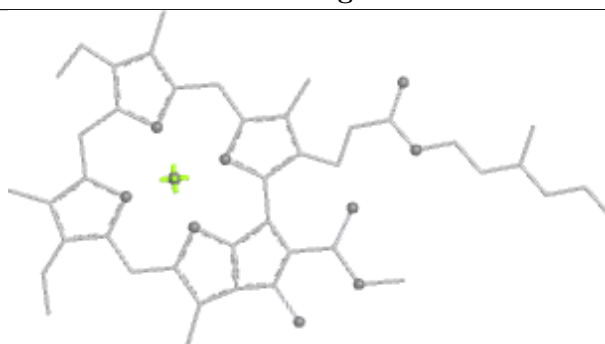
Bond lengths



Bond angles

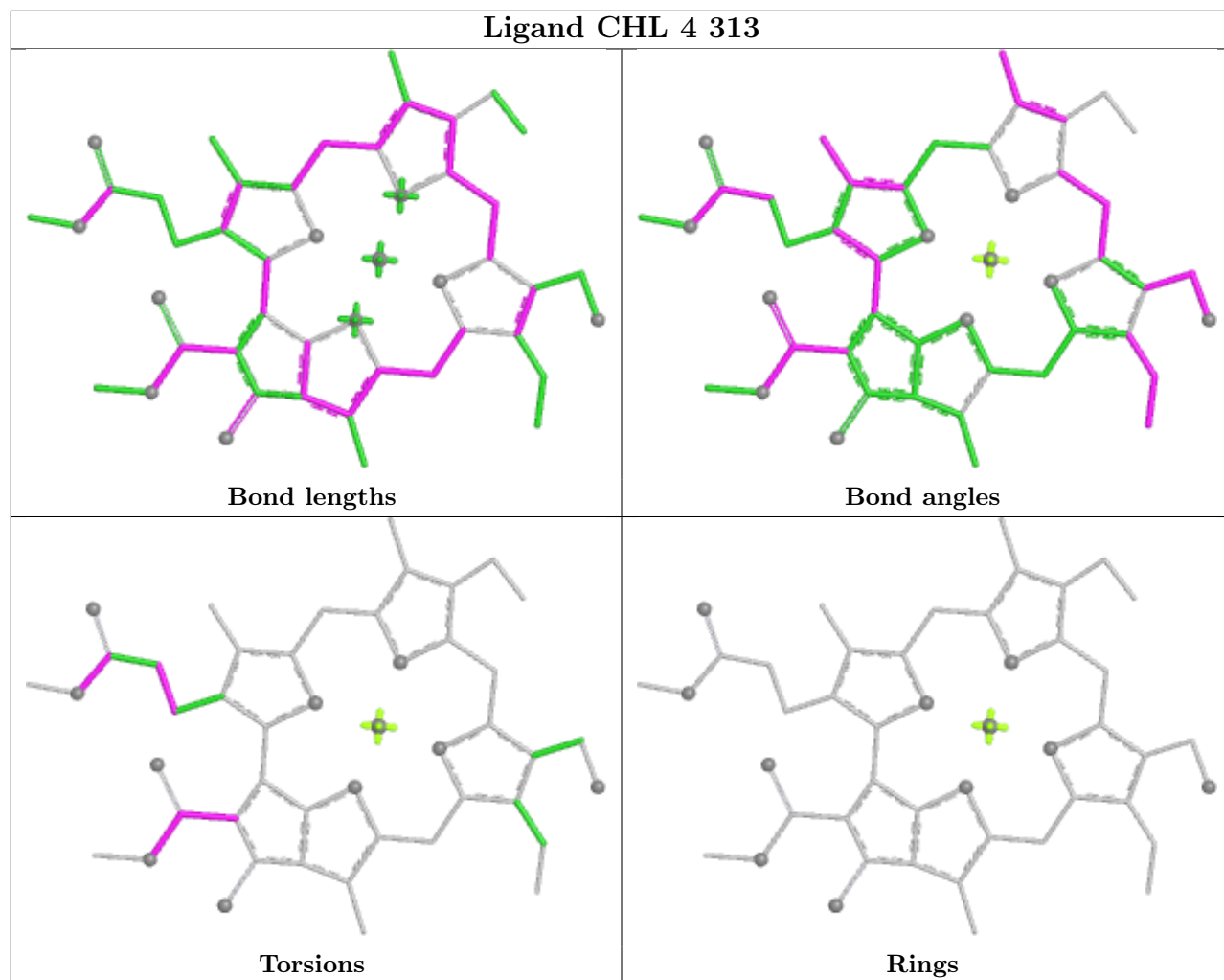


Torsions

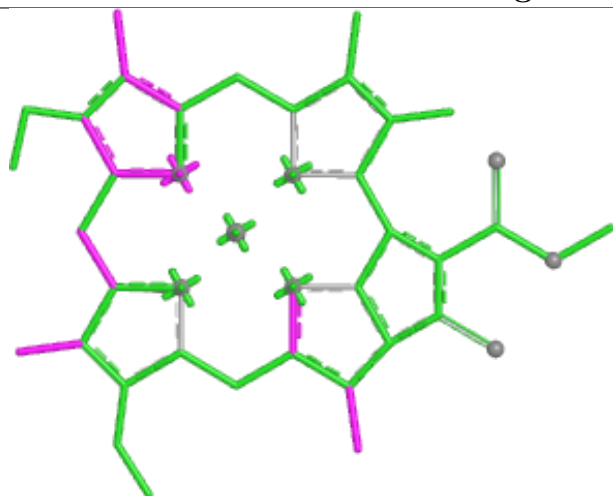


Rings

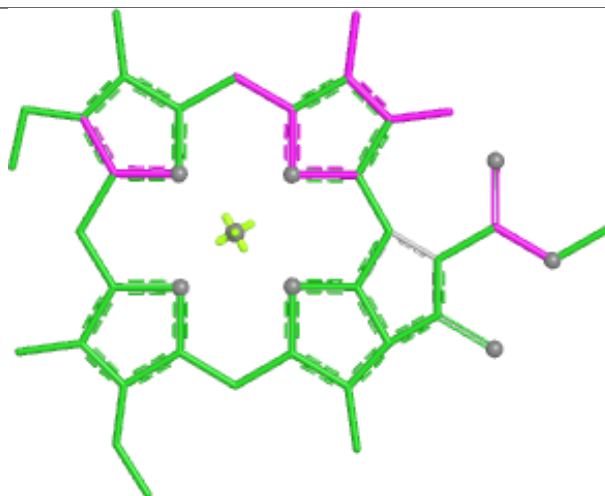
Ligand CHL 4 313



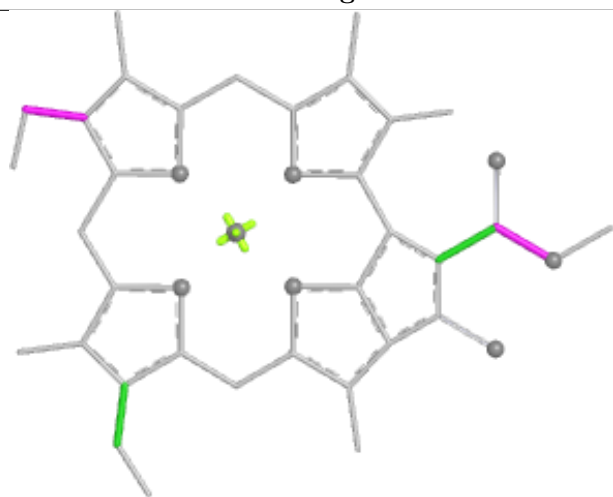
Ligand CLA B 819



Bond lengths



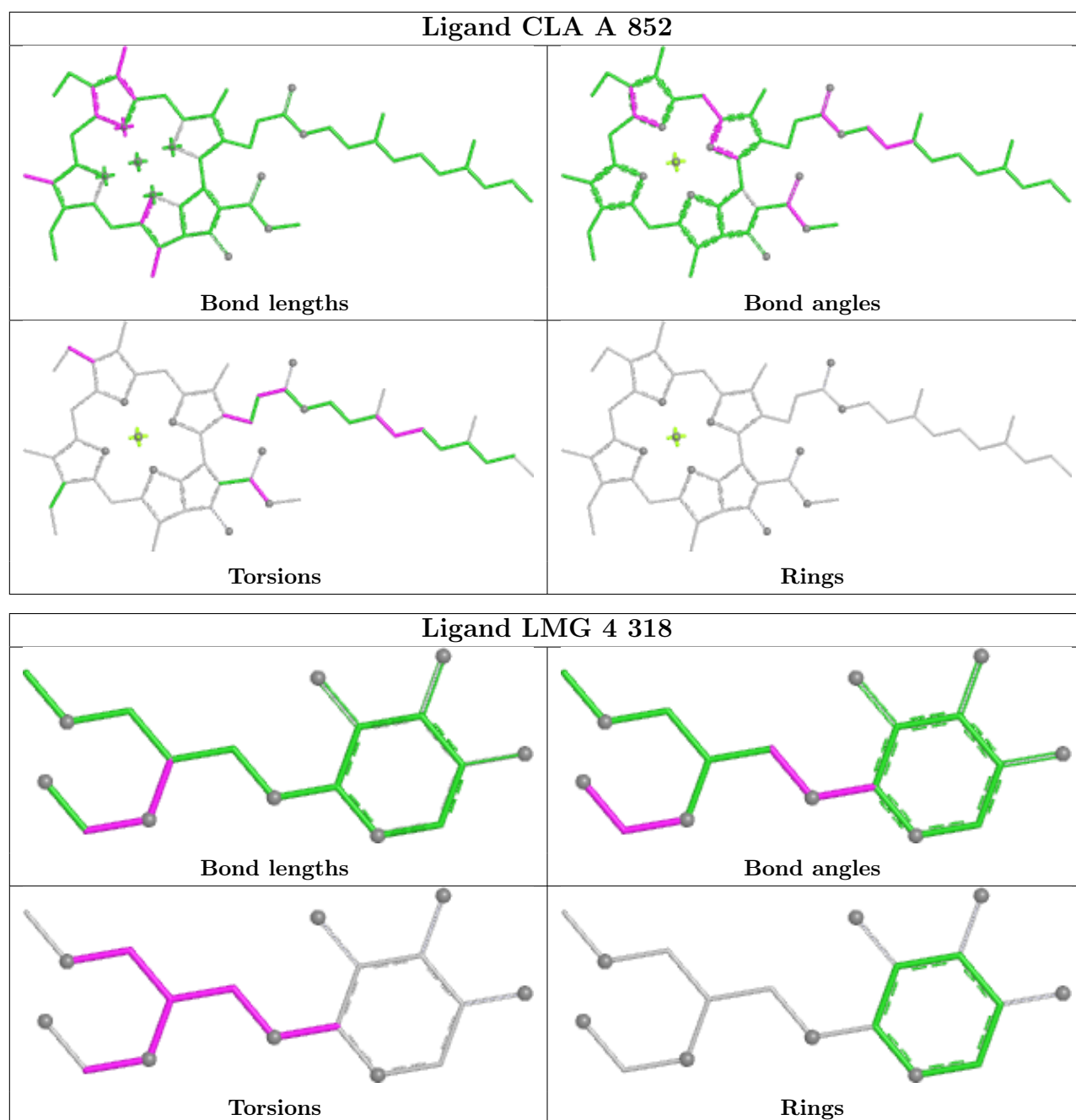
Bond angles



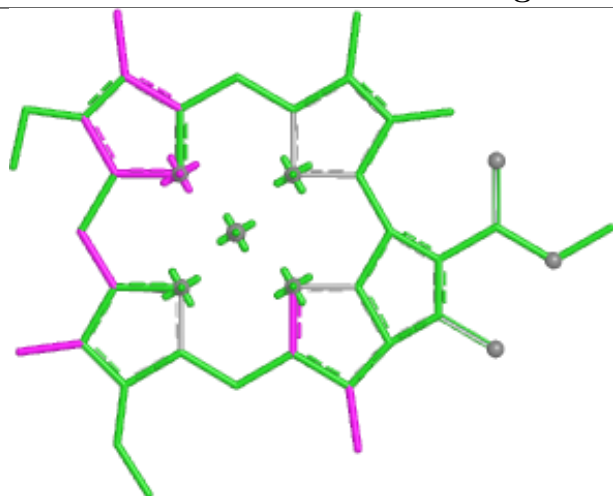
Torsions



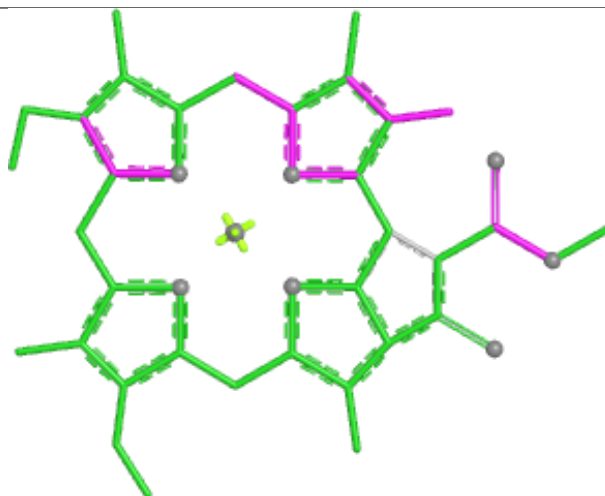
Rings



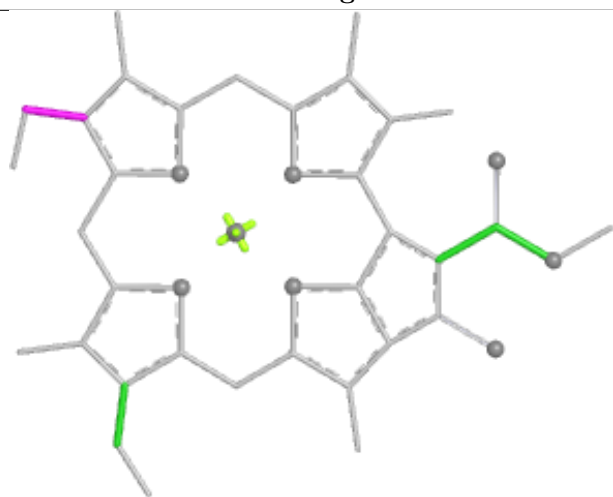
Ligand CLA A 822



Bond lengths



Bond angles

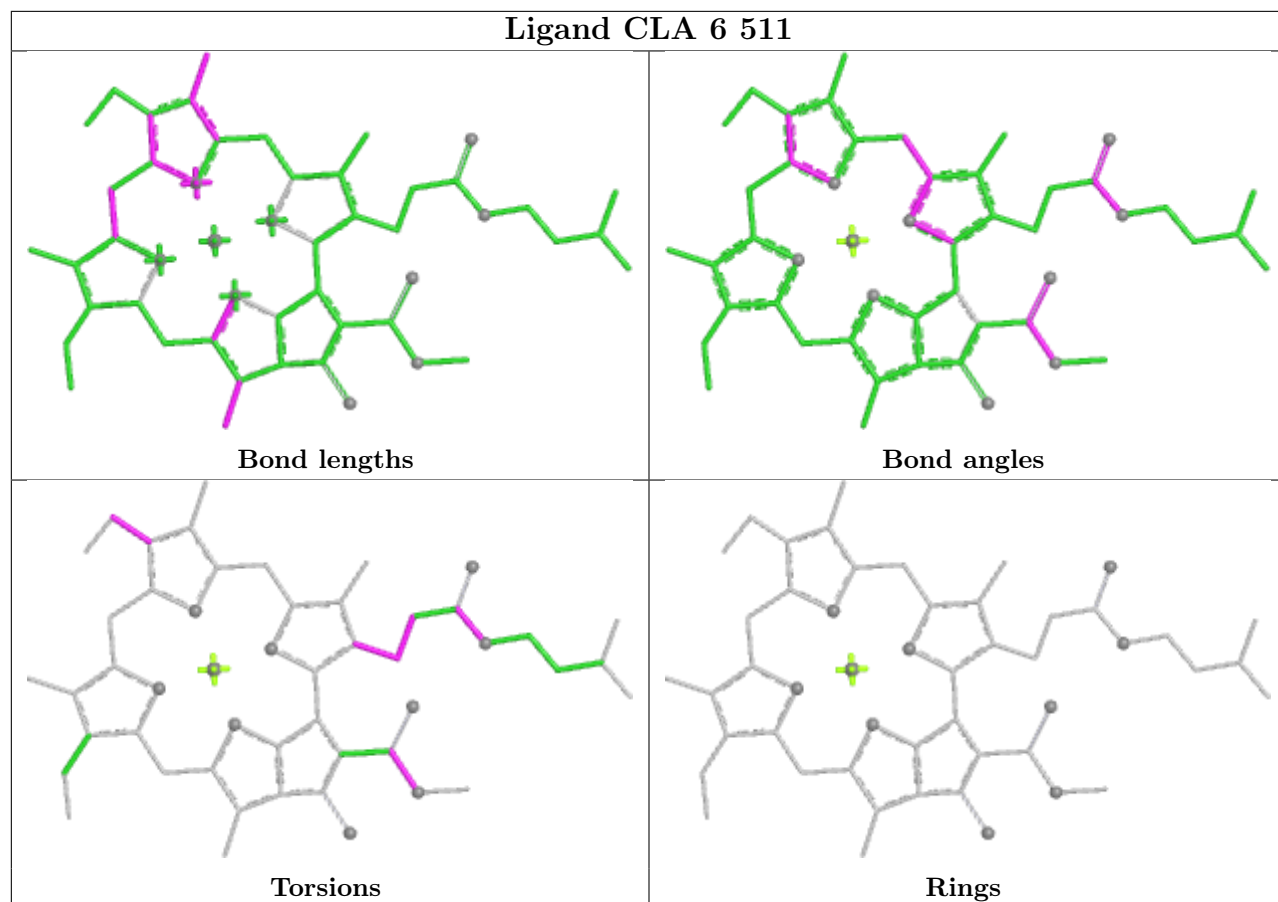


Torsions

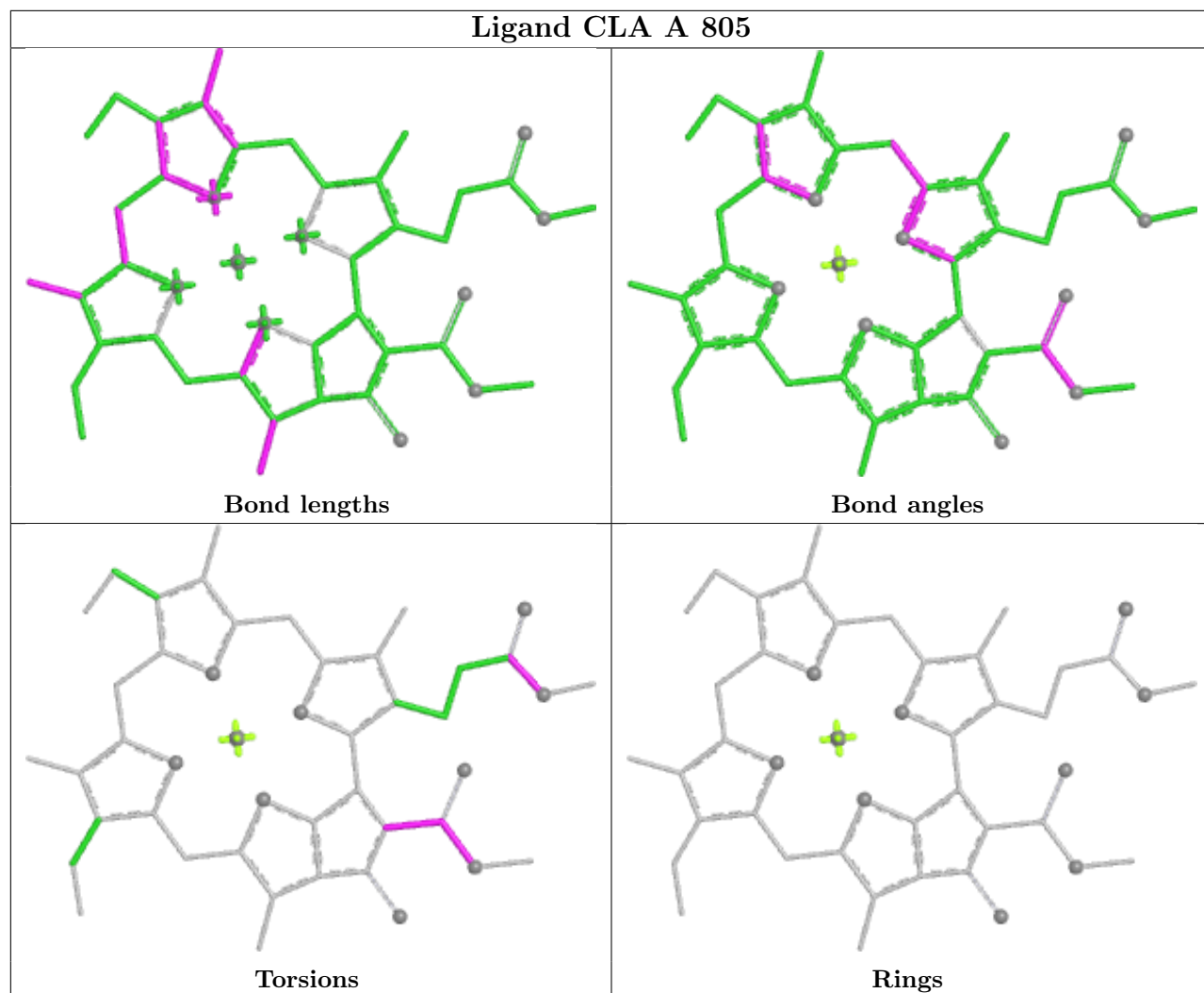


Rings

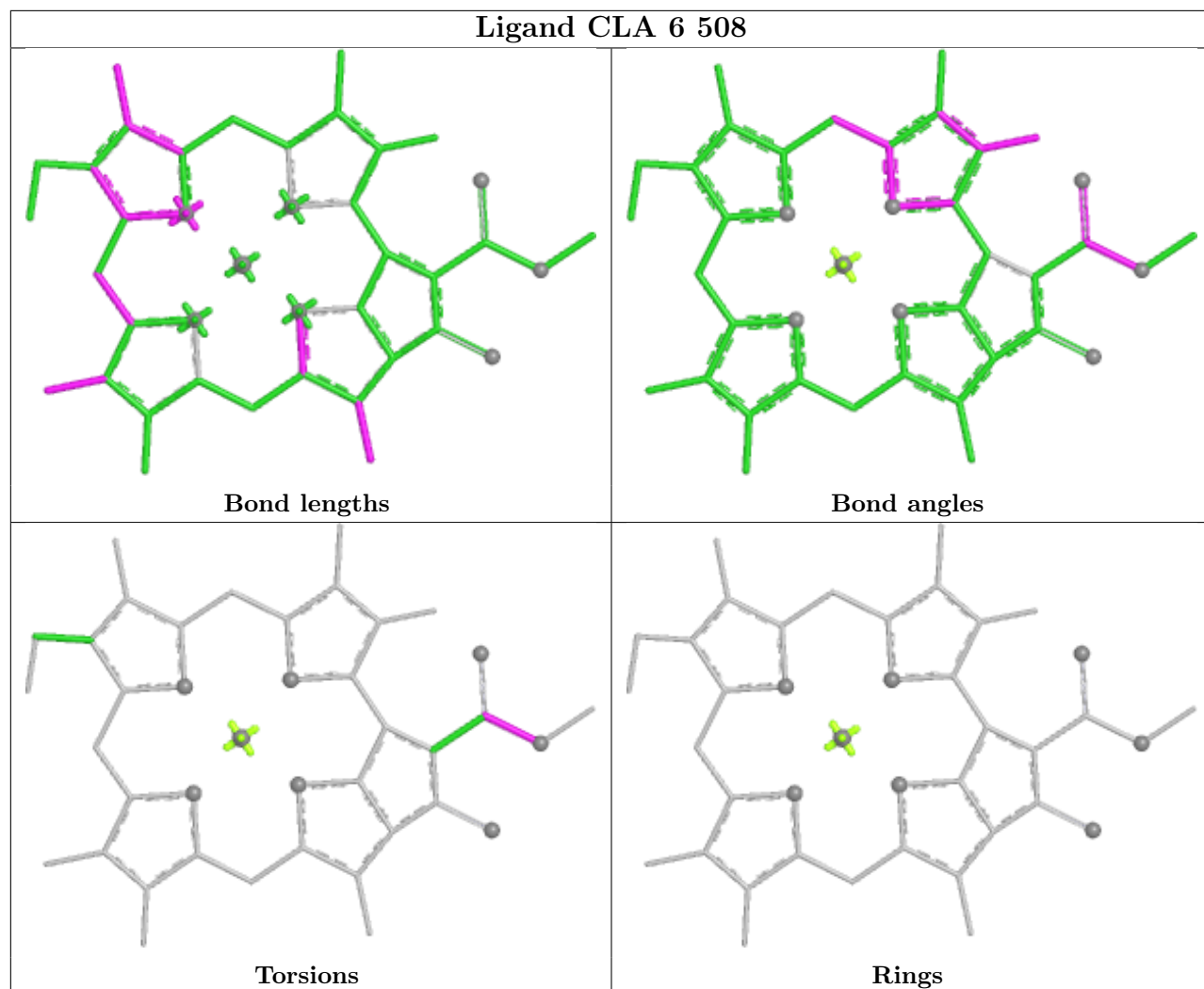
Ligand CLA 6 511



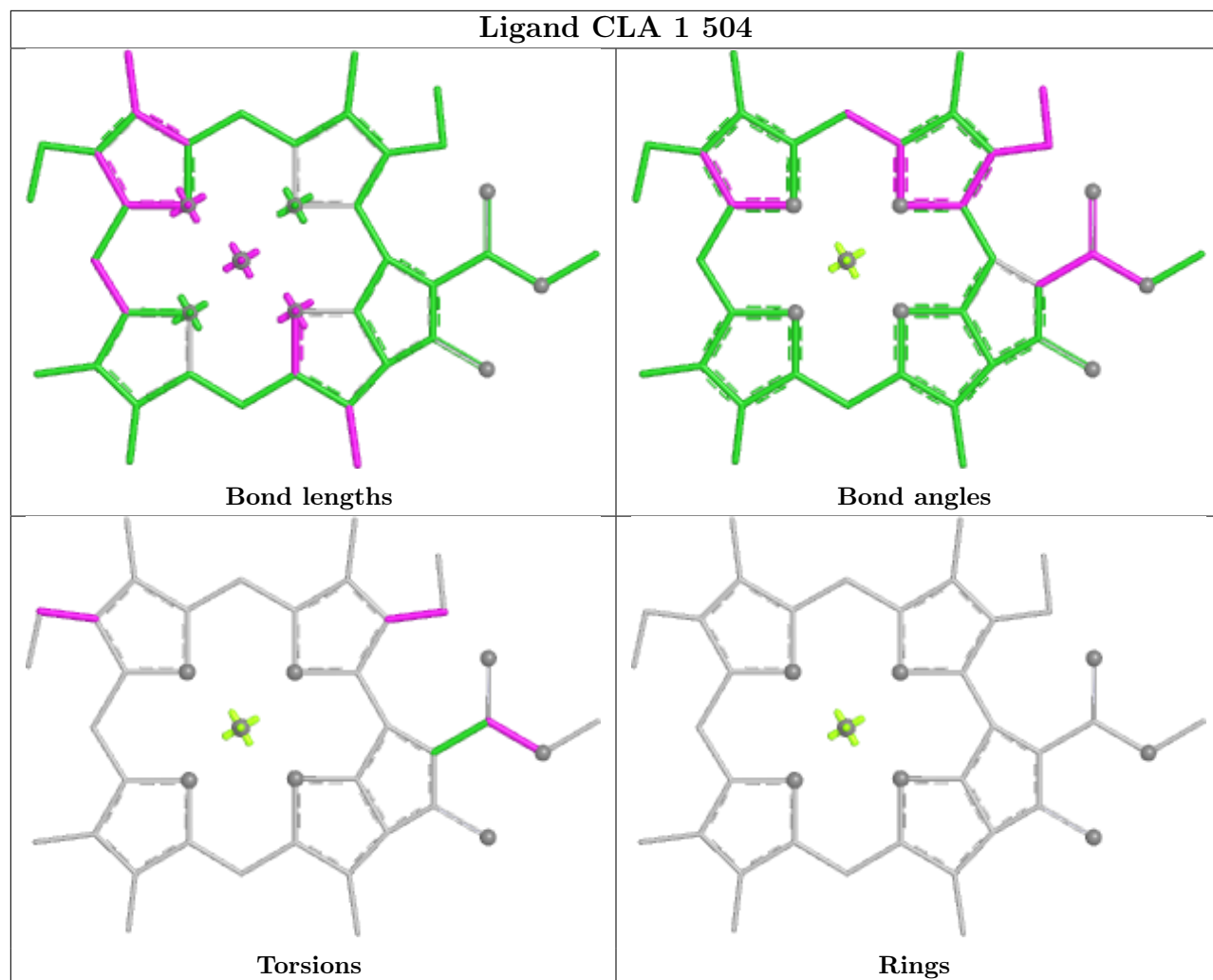
Ligand CLA A 805



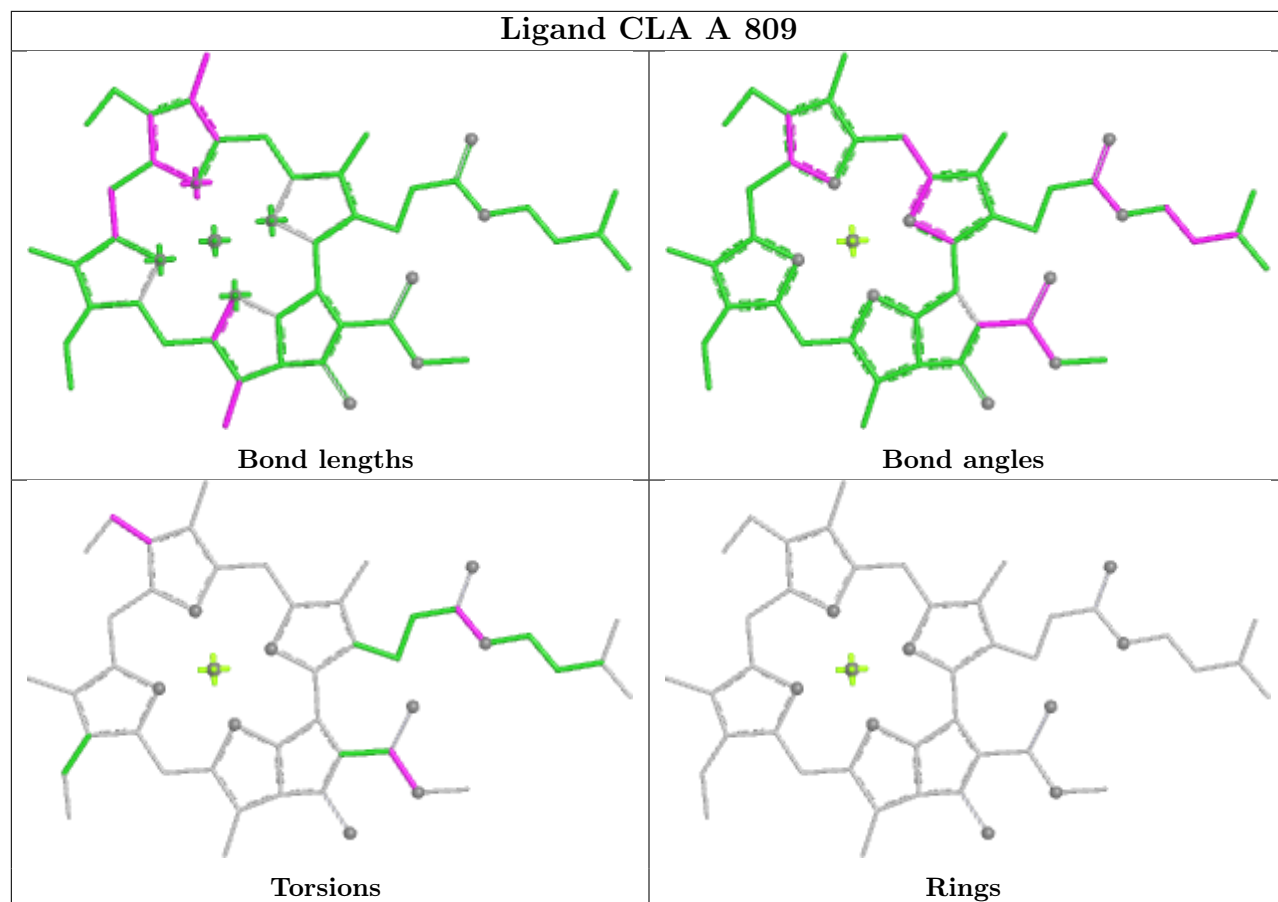
Ligand CLA 6 508



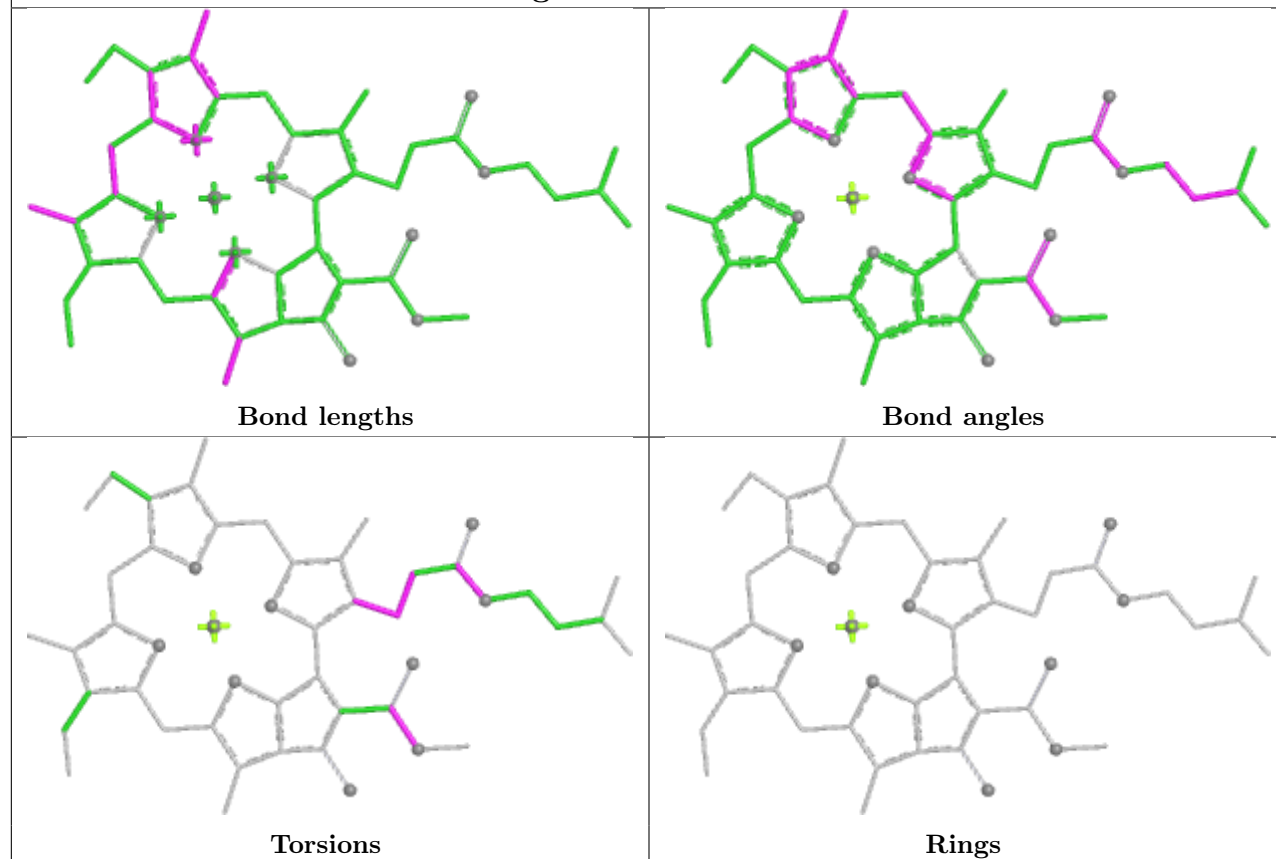
Ligand CLA 1 504



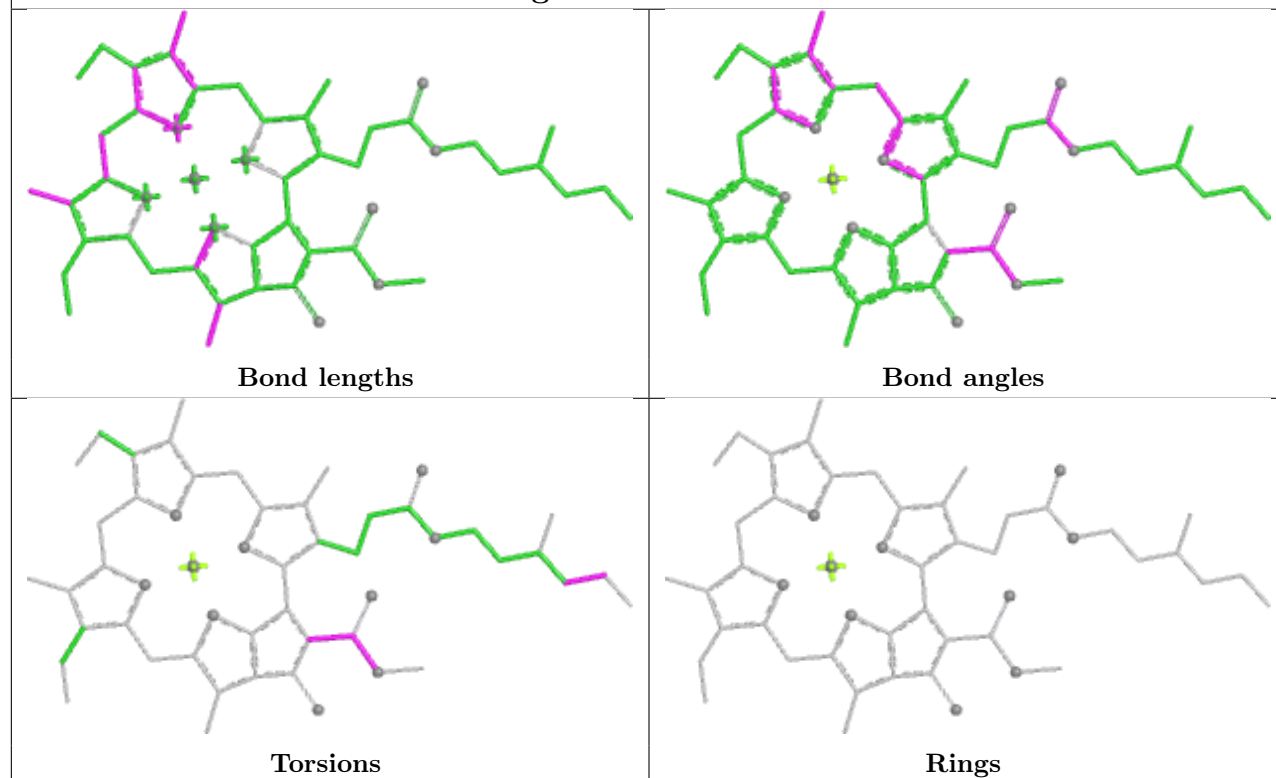
Ligand CLA A 809



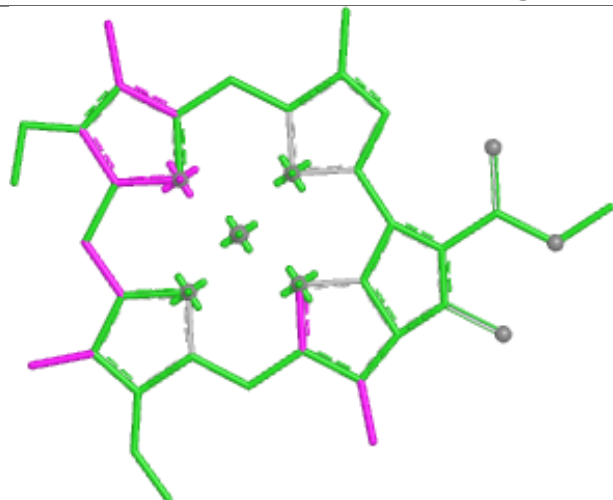
Ligand CLA B 829



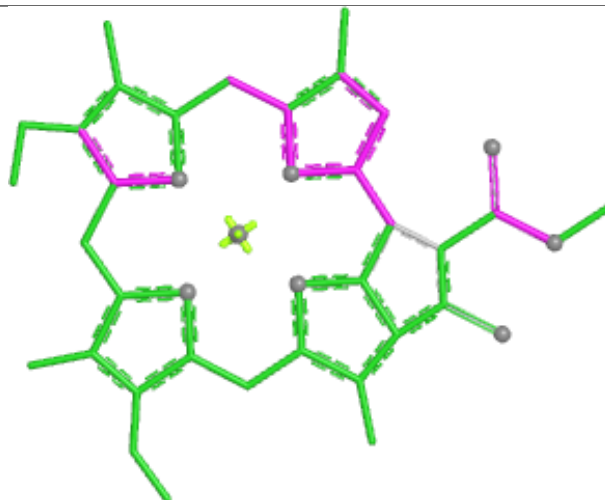
Ligand CLA A 838



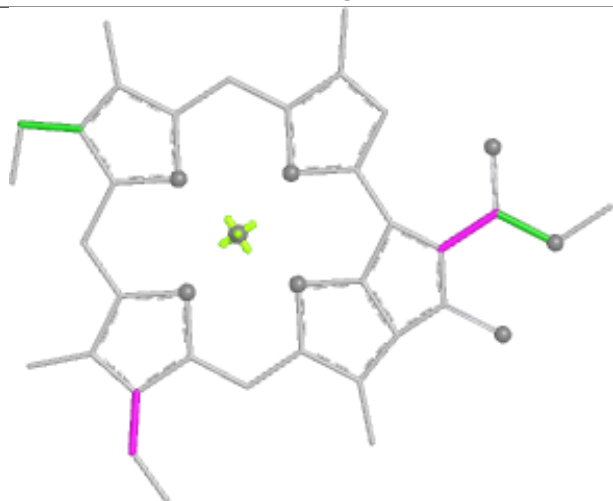
Ligand CLA B 838



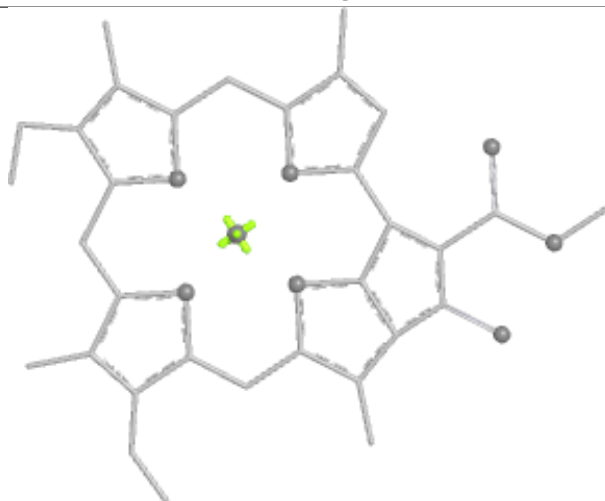
Bond lengths



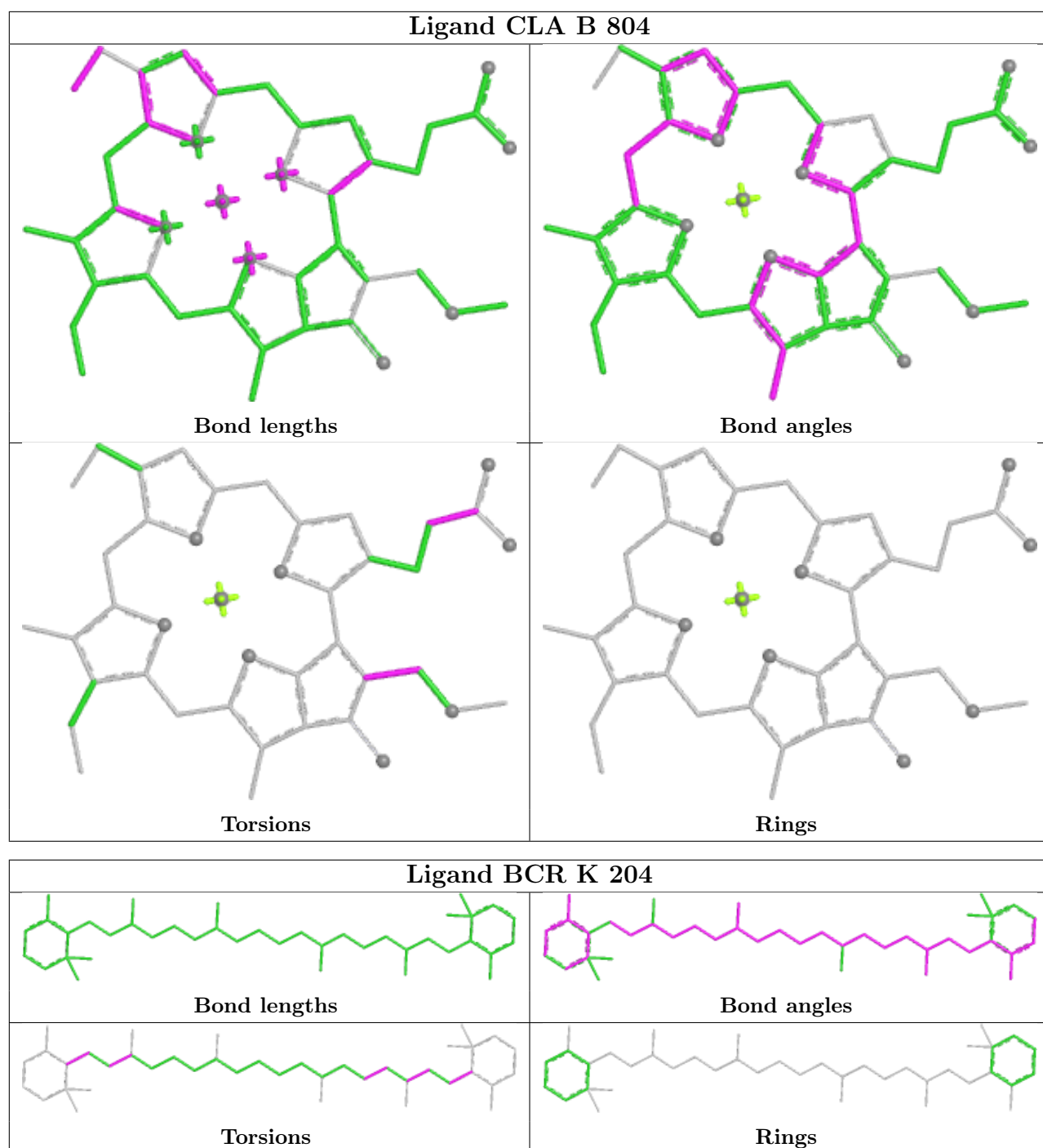
Bond angles



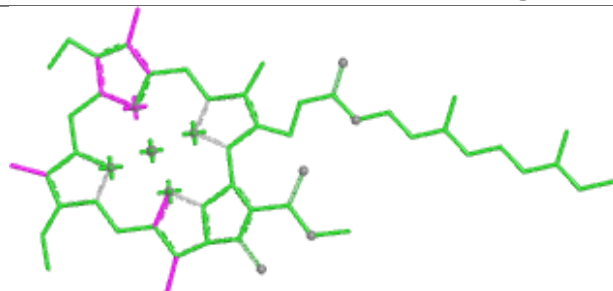
Torsions



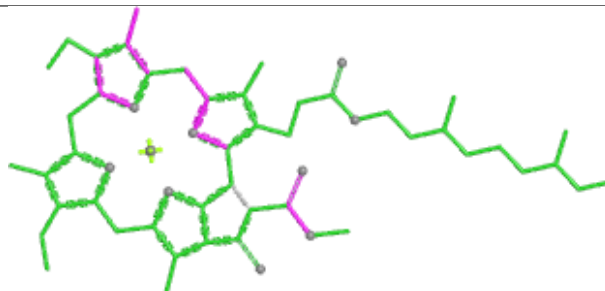
Rings



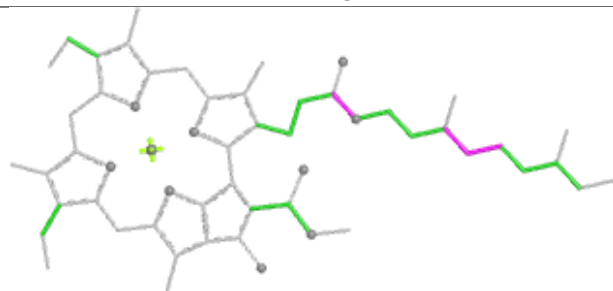
Ligand CLA B 831



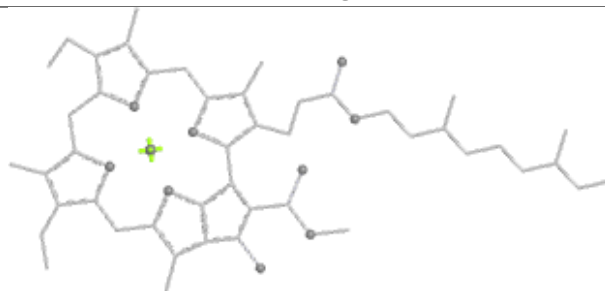
Bond lengths



Bond angles

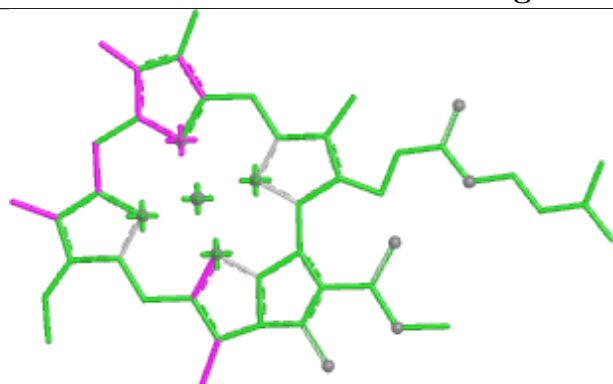


Torsions

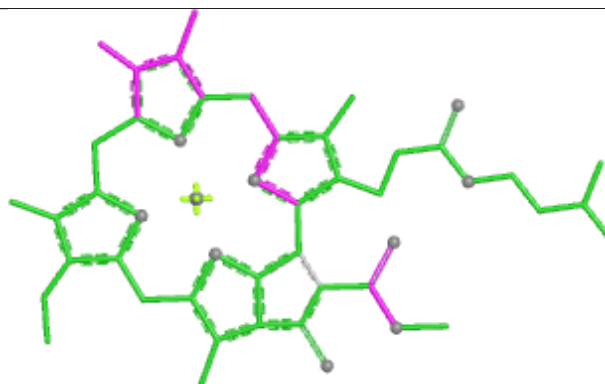


Rings

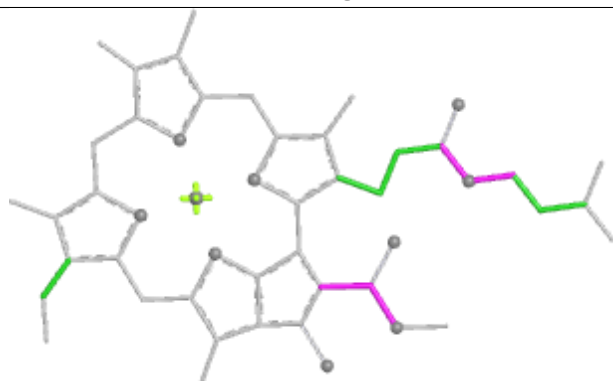
Ligand CLA A 843



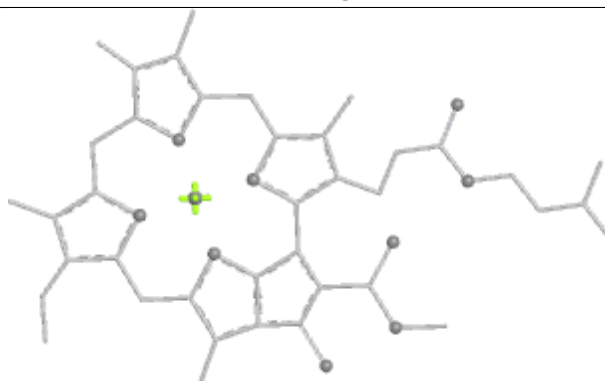
Bond lengths



Bond angles

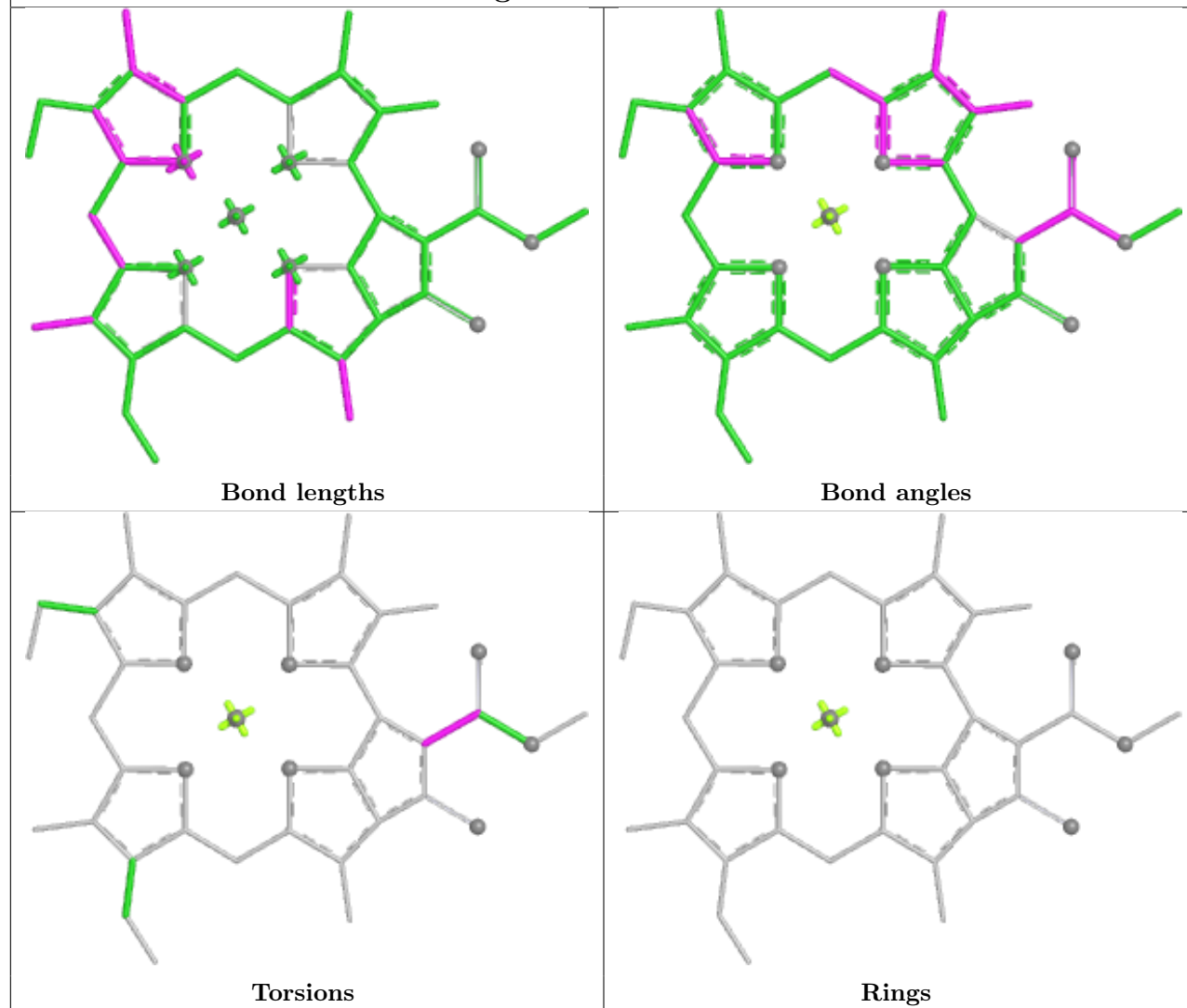


Torsions

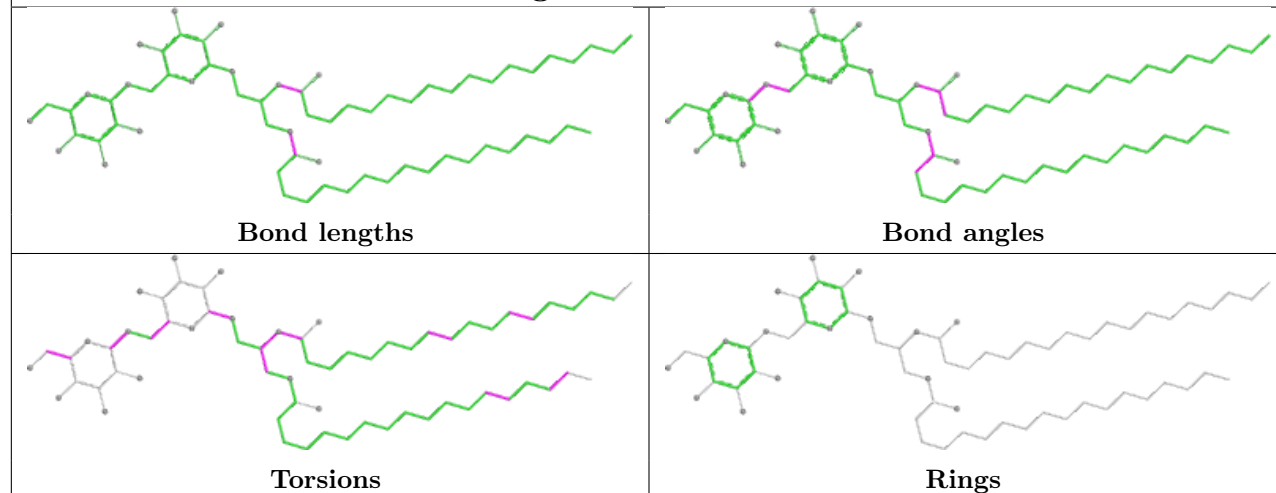


Rings

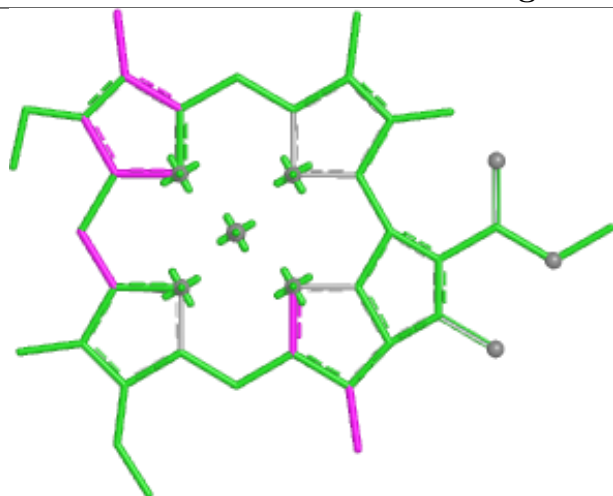
Ligand CLA A 806



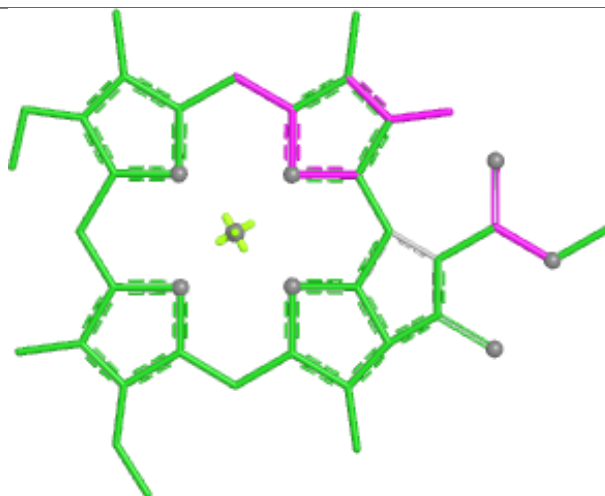
Ligand DGD J 104



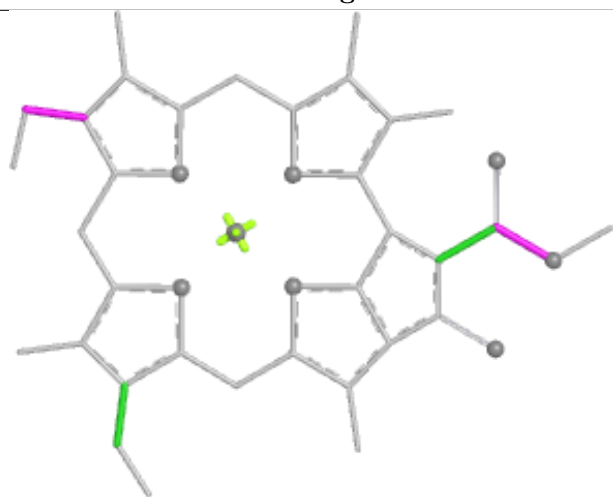
Ligand CLA 3 310



Bond lengths



Bond angles

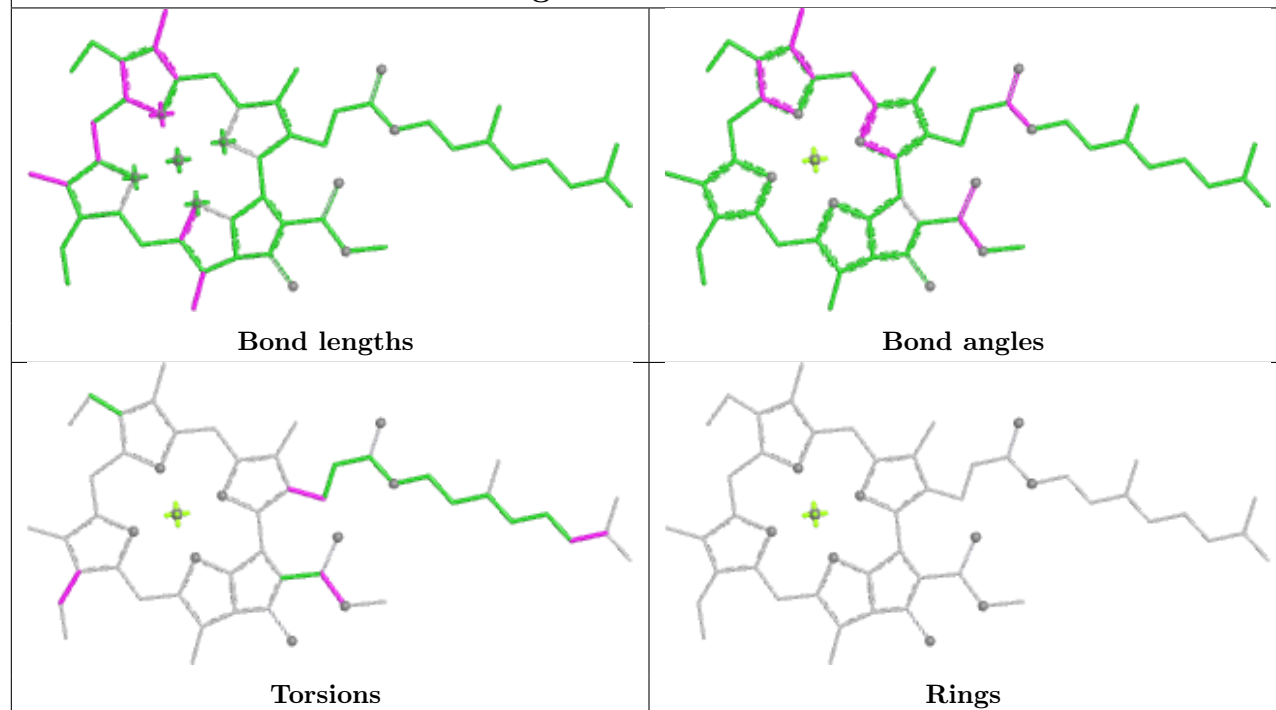


Torsions

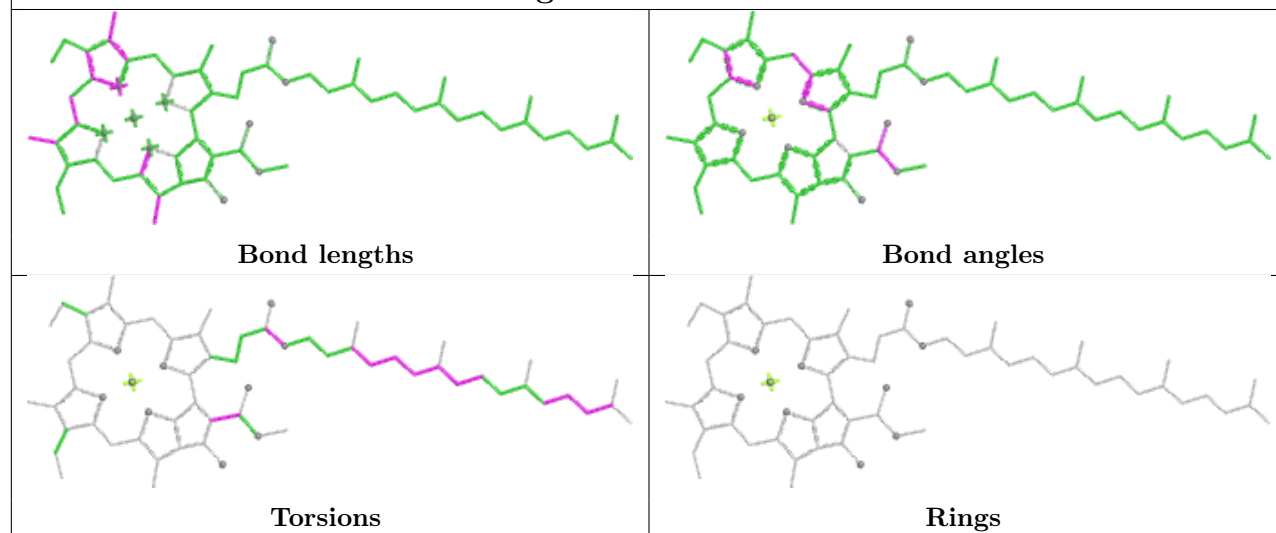


Rings

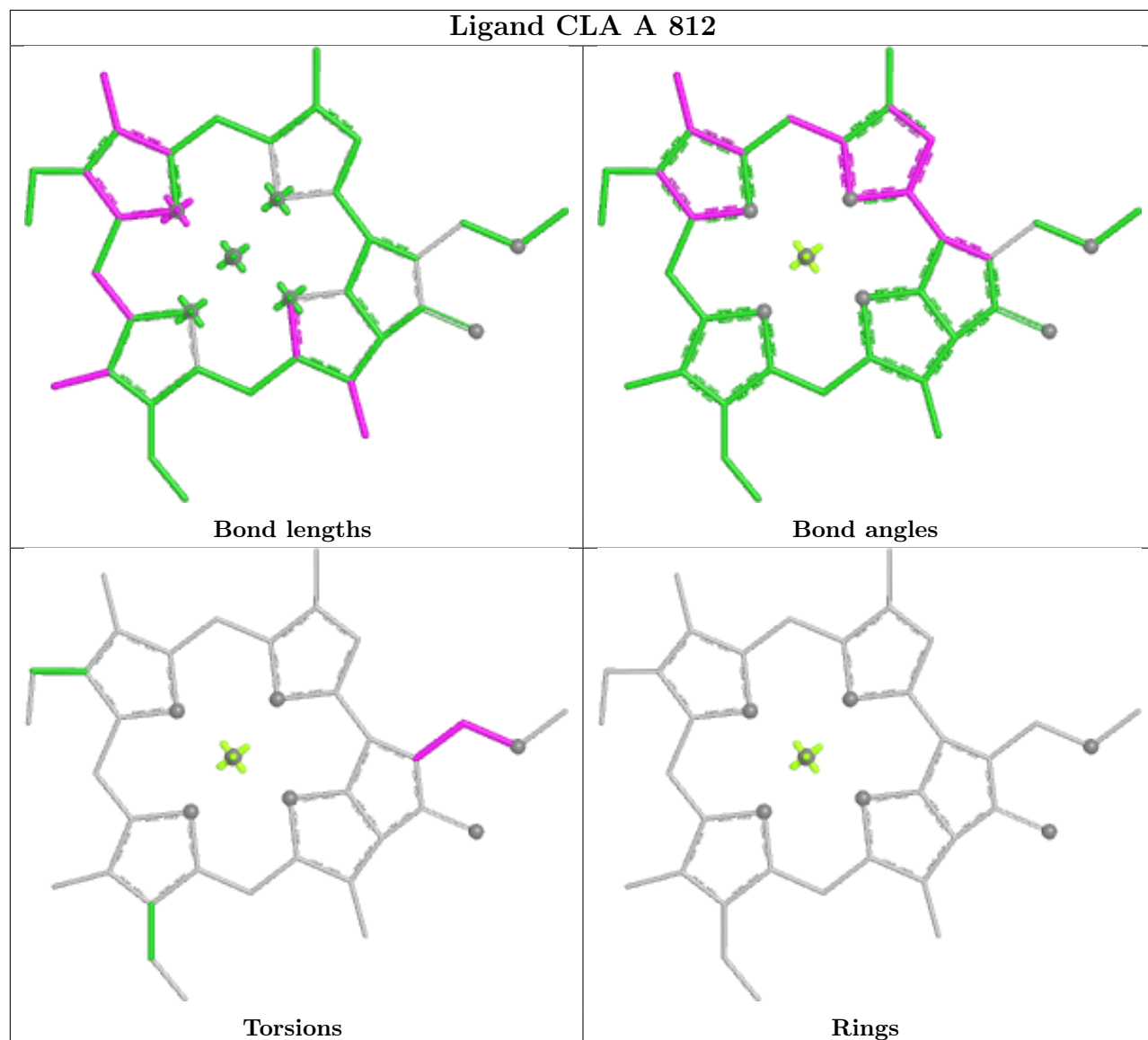
Ligand CLA B 821



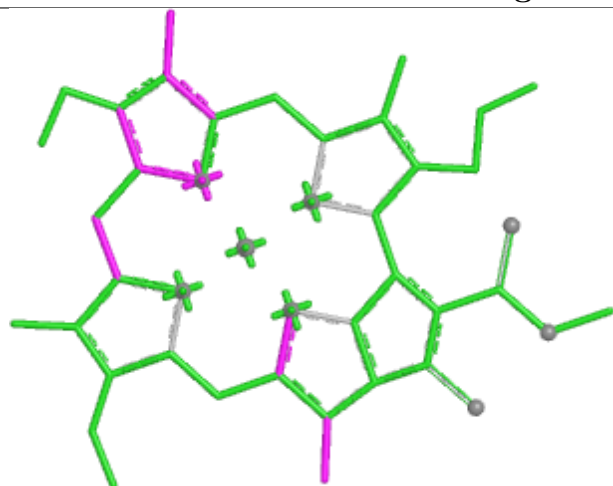
Ligand CLA 1 508



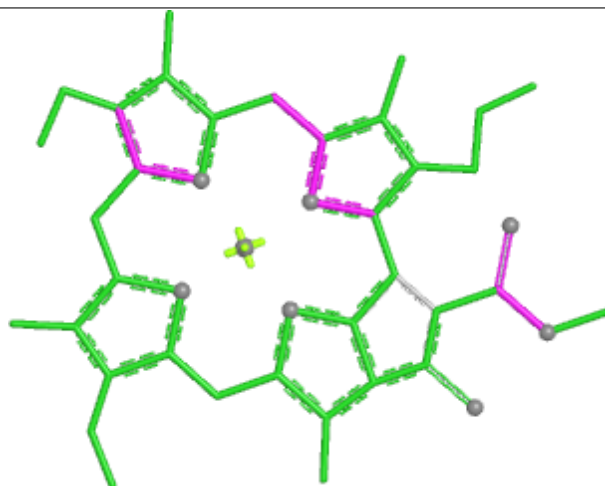
Ligand CLA A 812



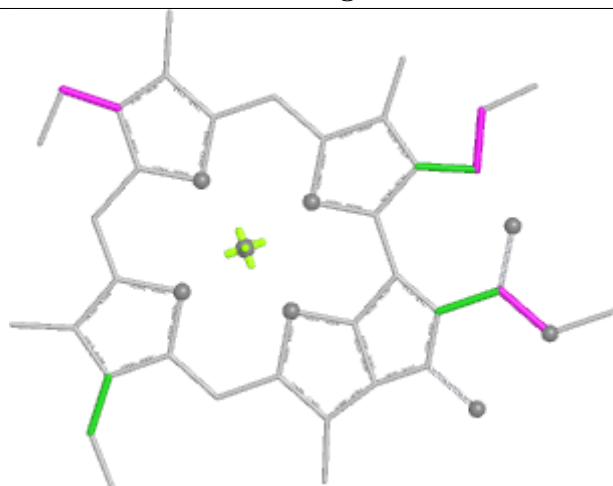
Ligand CLA B 815



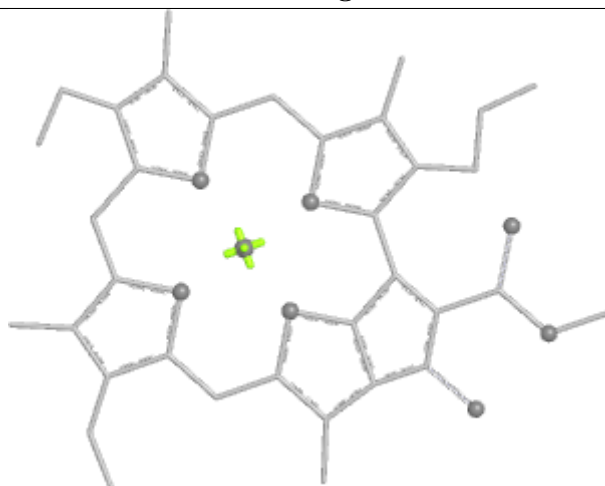
Bond lengths



Bond angles

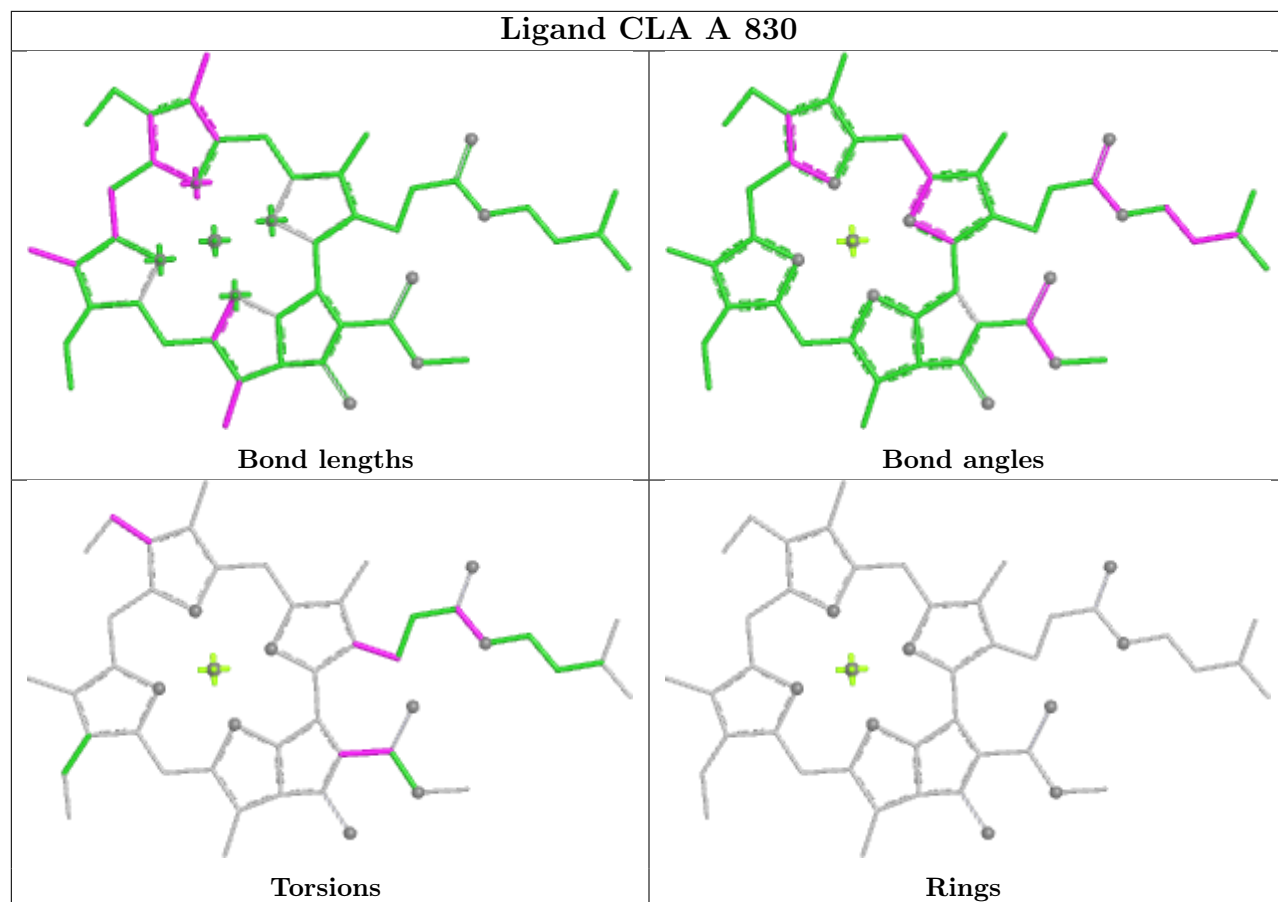


Torsions

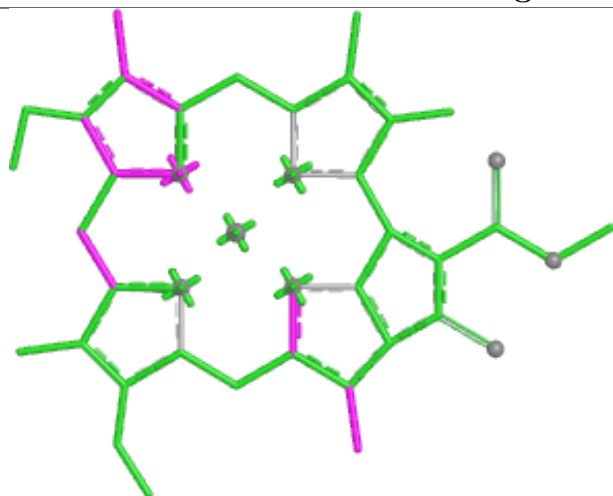


Rings

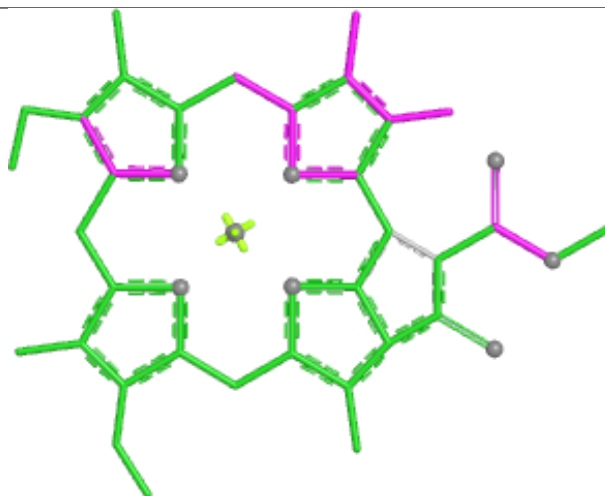
Ligand CLA A 830



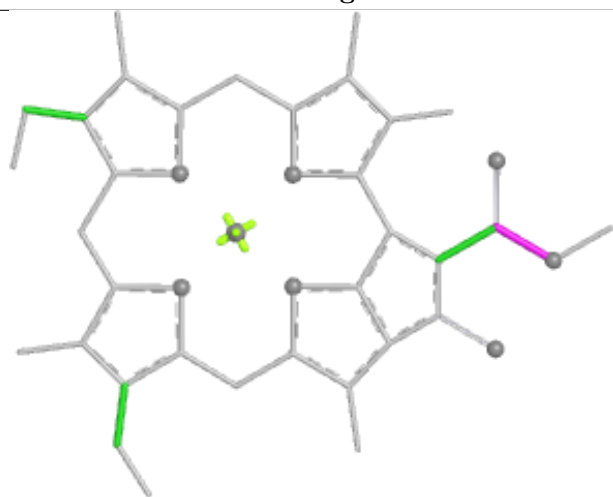
Ligand CLA B 839



Bond lengths



Bond angles

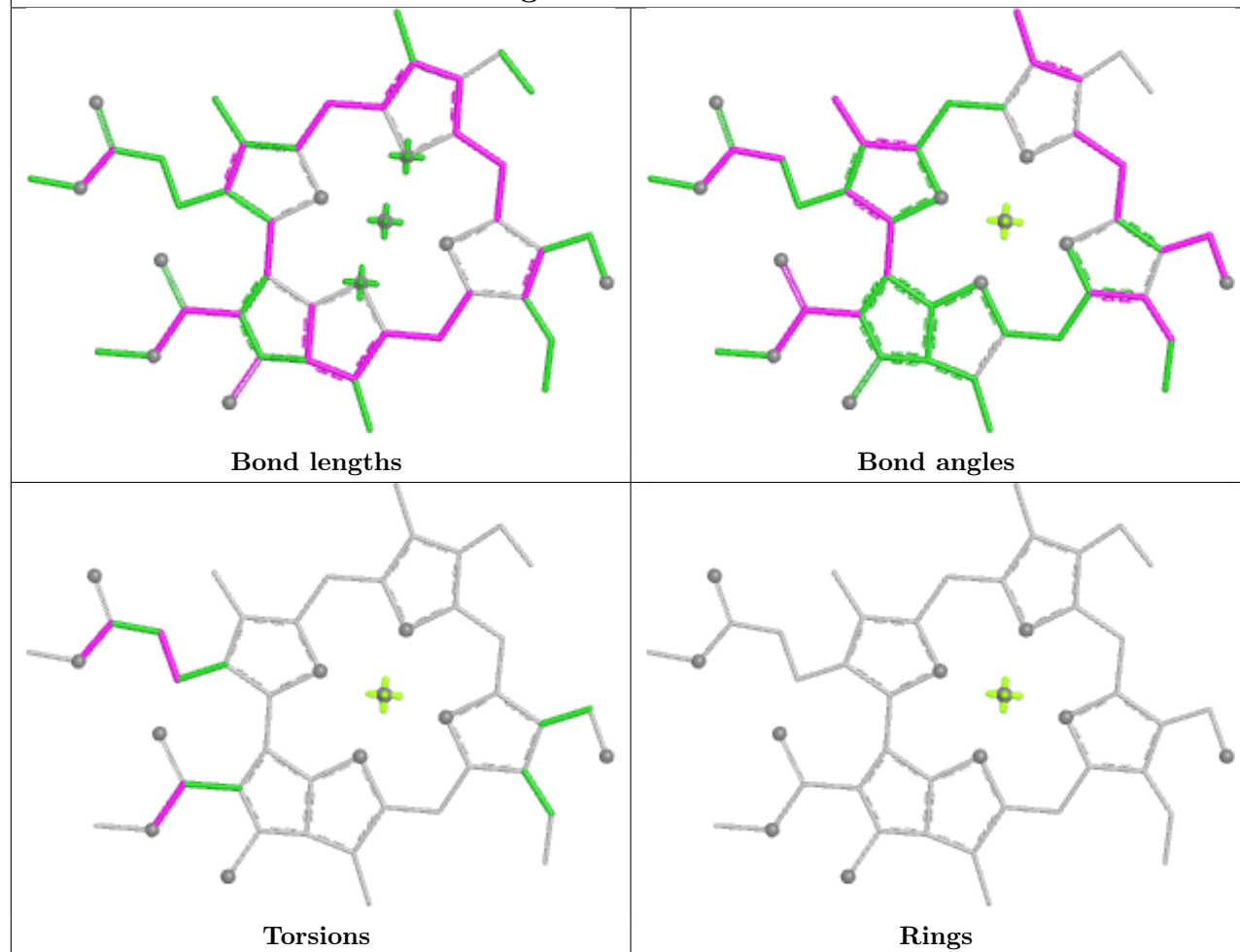


Torsions

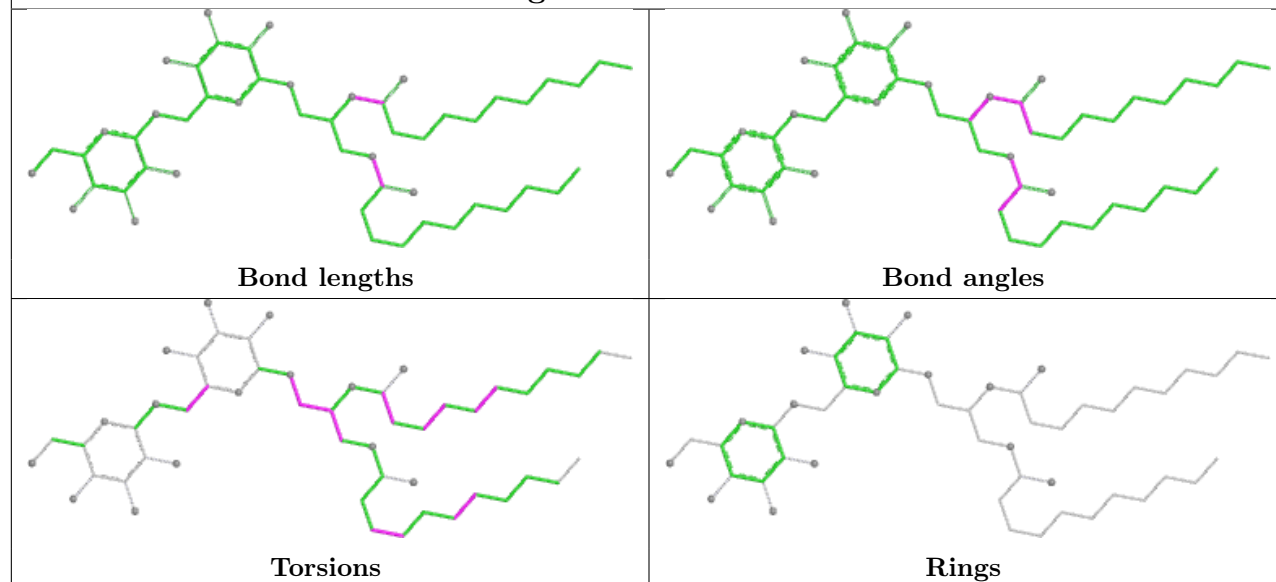


Rings

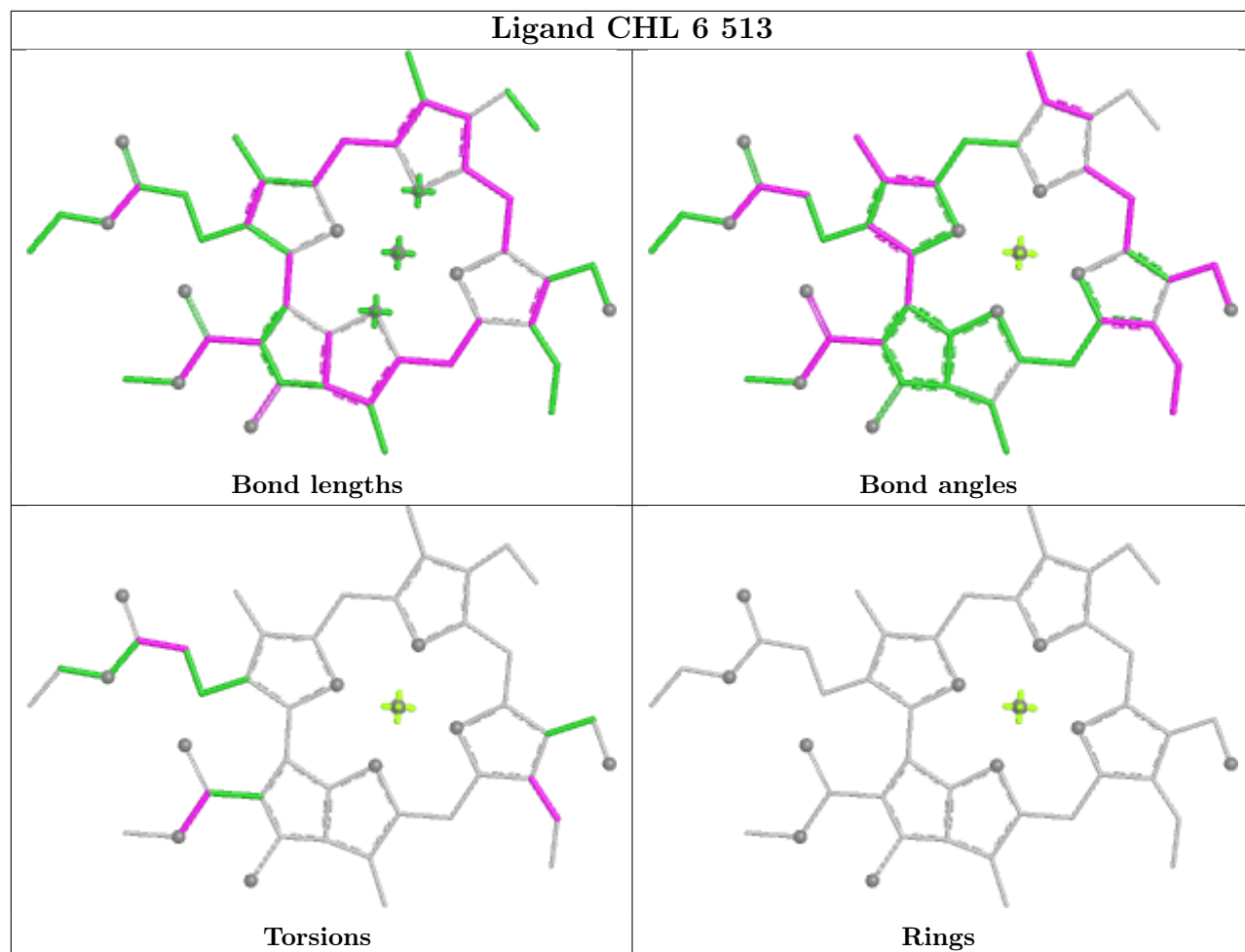
Ligand CHL 6 512



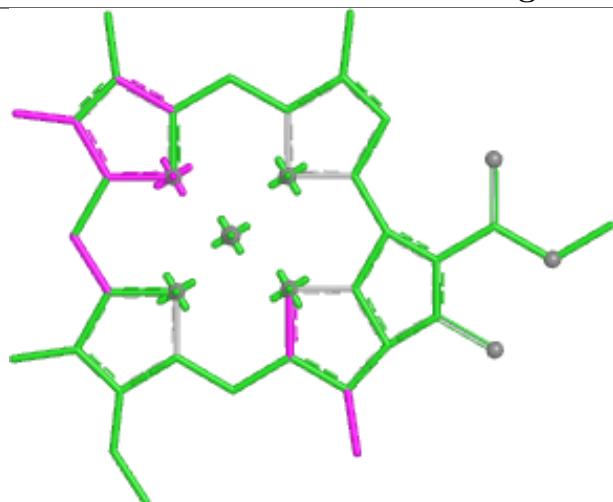
Ligand DGD B 851



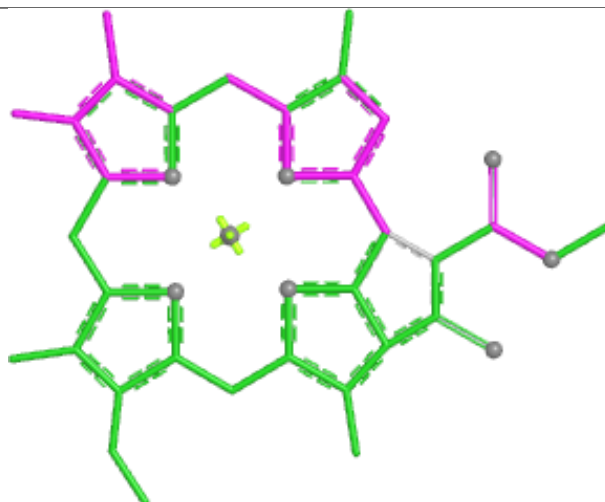
Ligand CHL 6 513



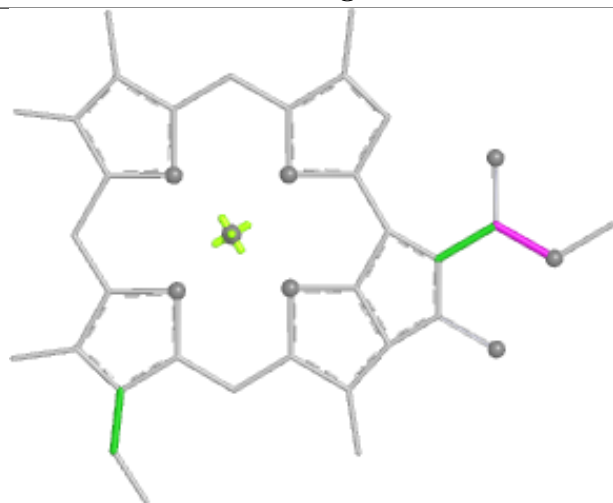
Ligand CLA 4 304



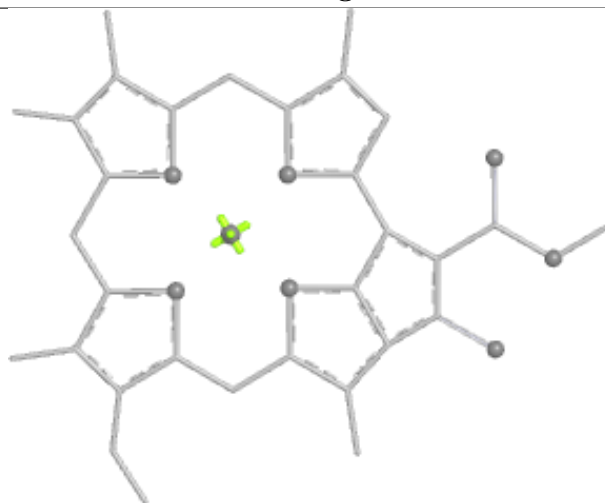
Bond lengths



Bond angles

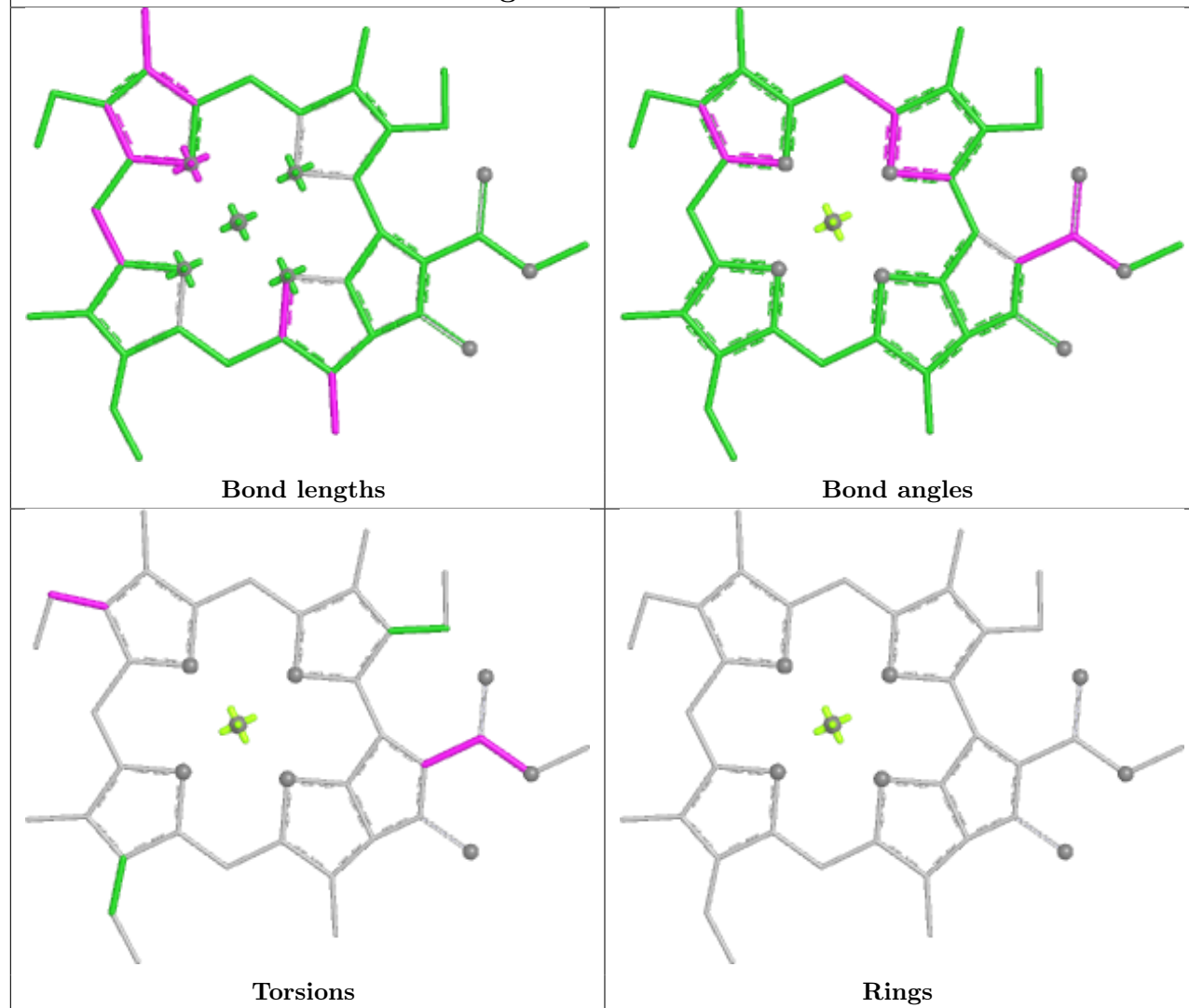


Torsions

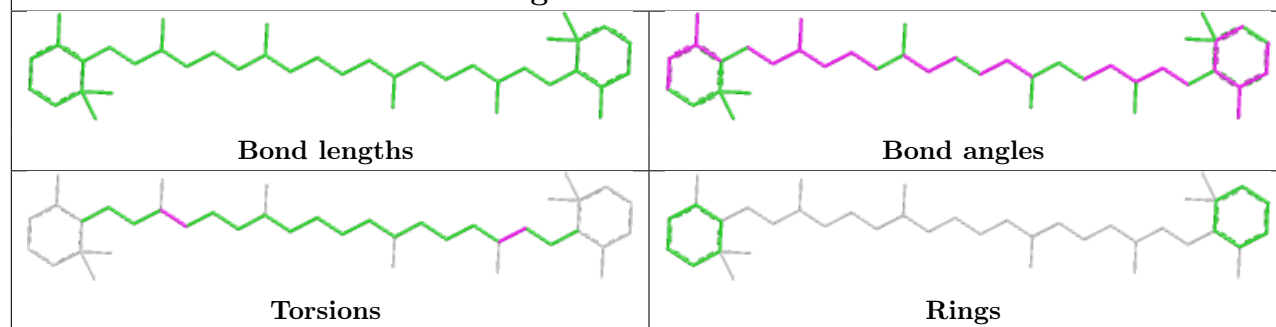


Rings

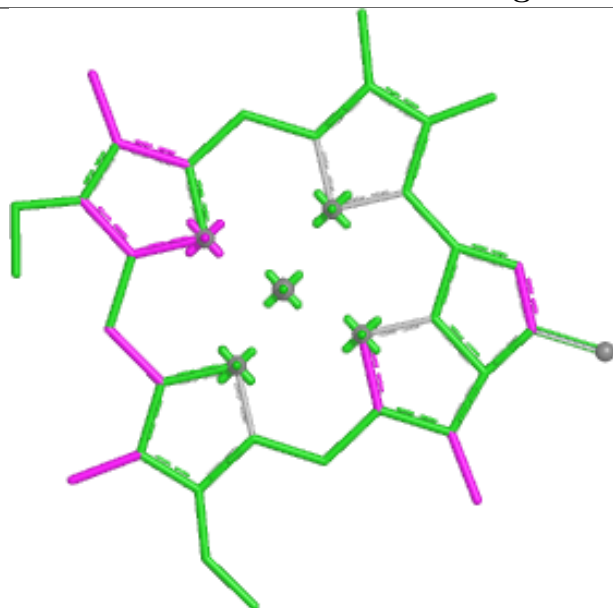
Ligand CLA 4 310



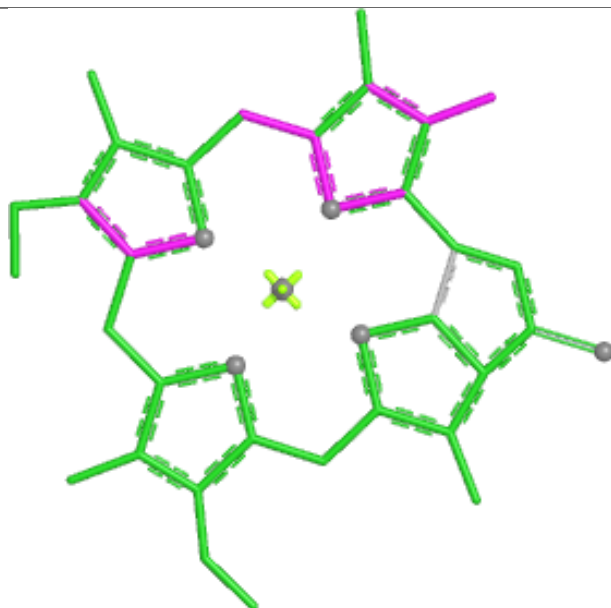
Ligand BCR B 846



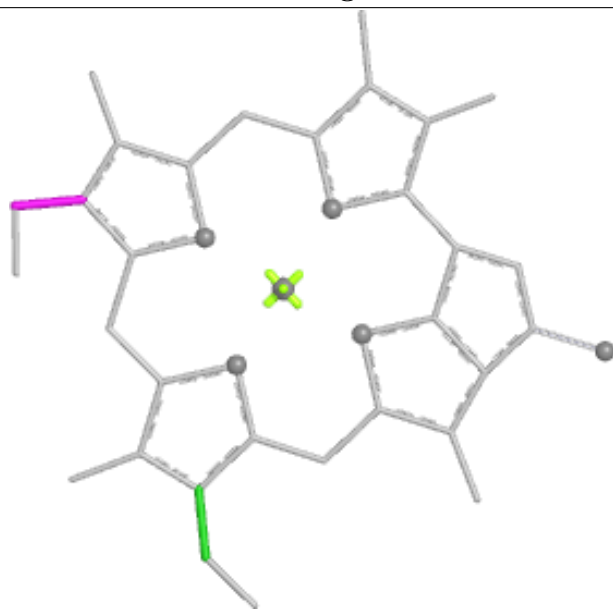
Ligand CLA K 201



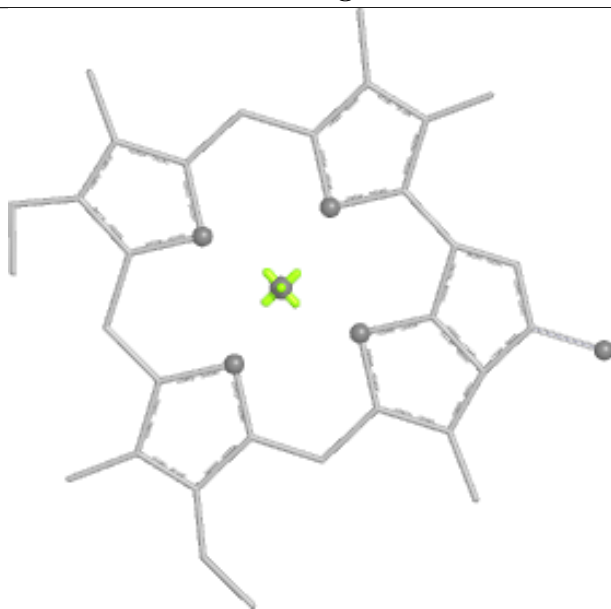
Bond lengths



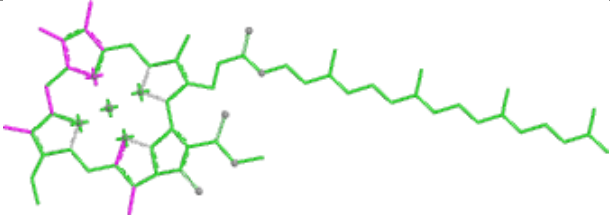
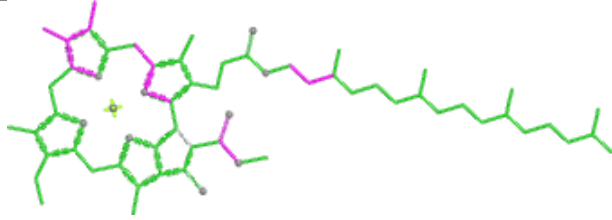
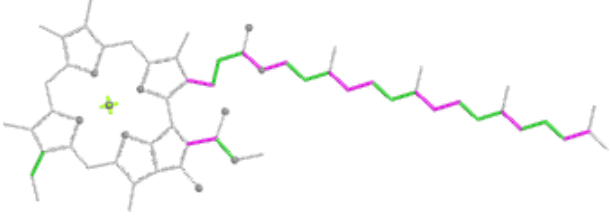
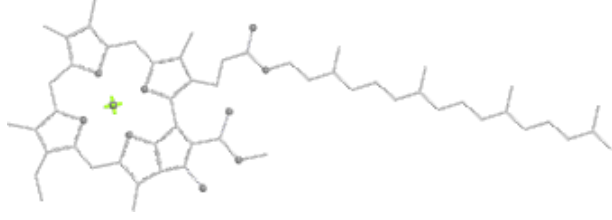
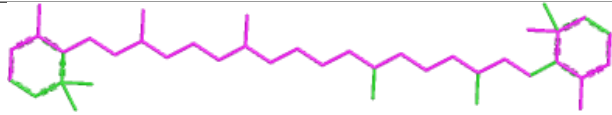
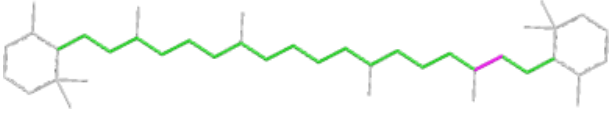
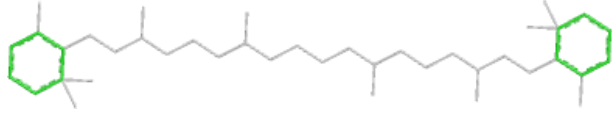
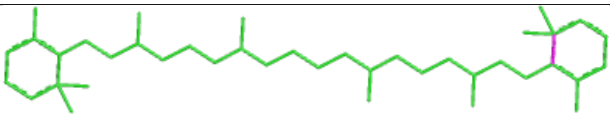
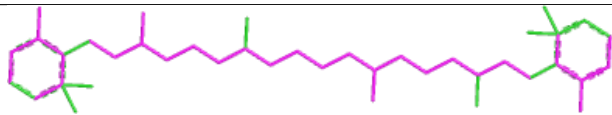
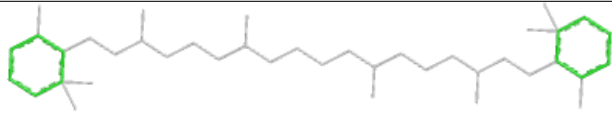
Bond angles



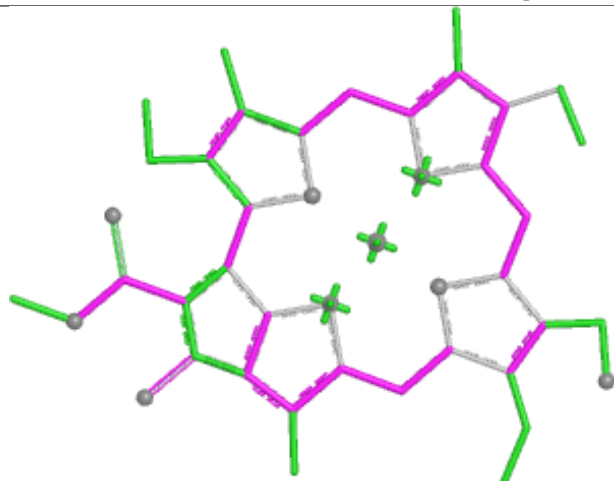
Torsions



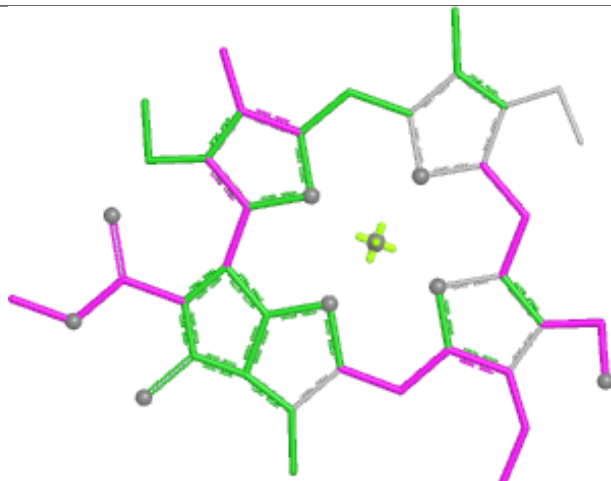
Rings

Ligand CLA A 826	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 801	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

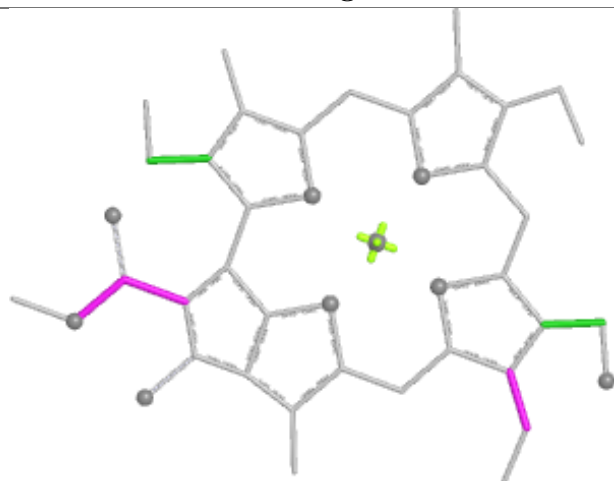
Ligand CHL 4 316



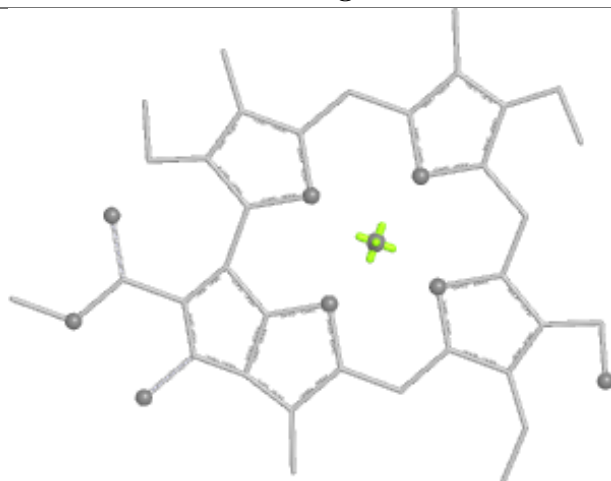
Bond lengths



Bond angles

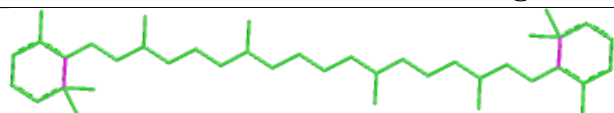


Torsions

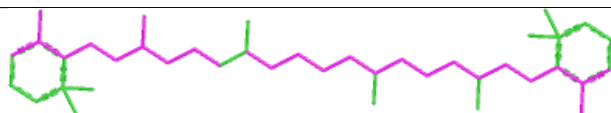


Rings

Ligand BCR A 846



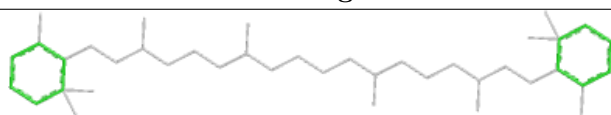
Bond lengths



Bond angles

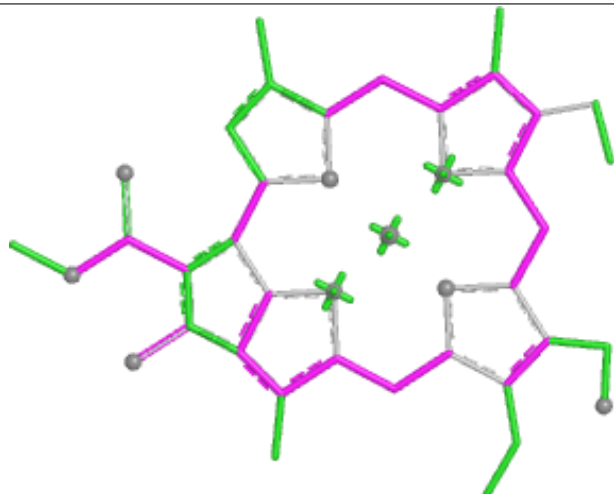


Torsions

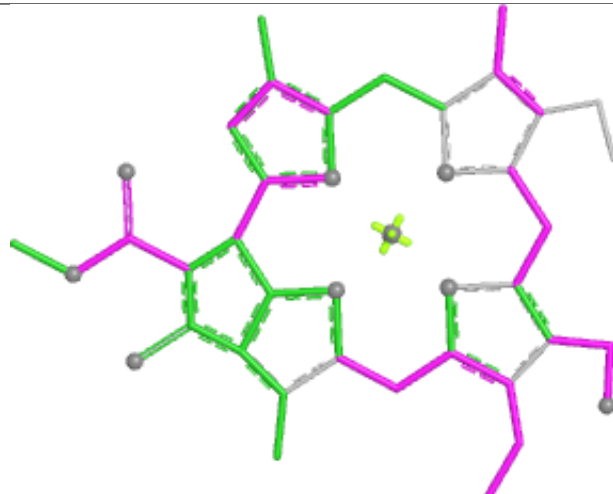


Rings

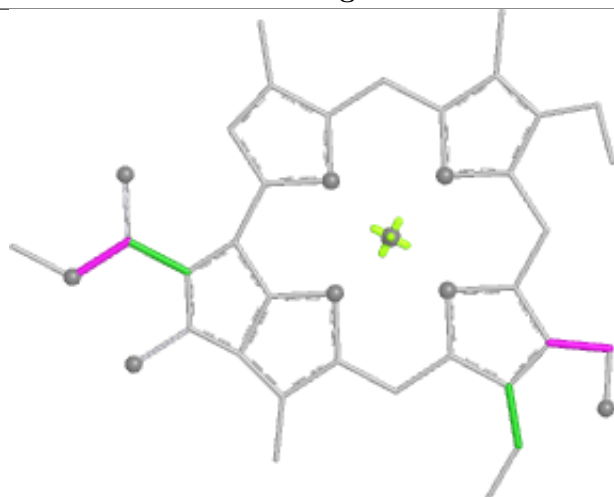
Ligand CHL 6 515



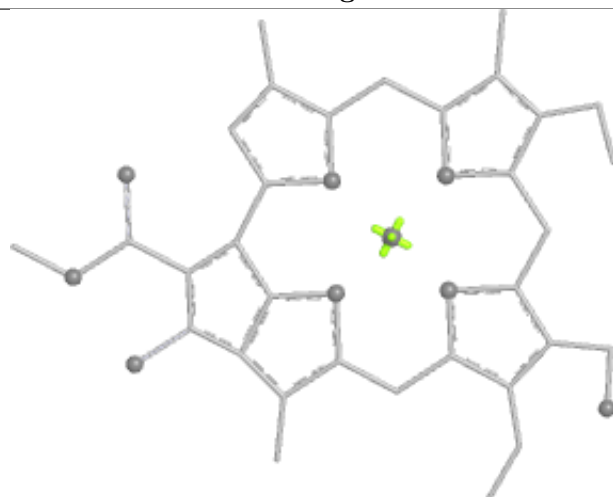
Bond lengths



Bond angles

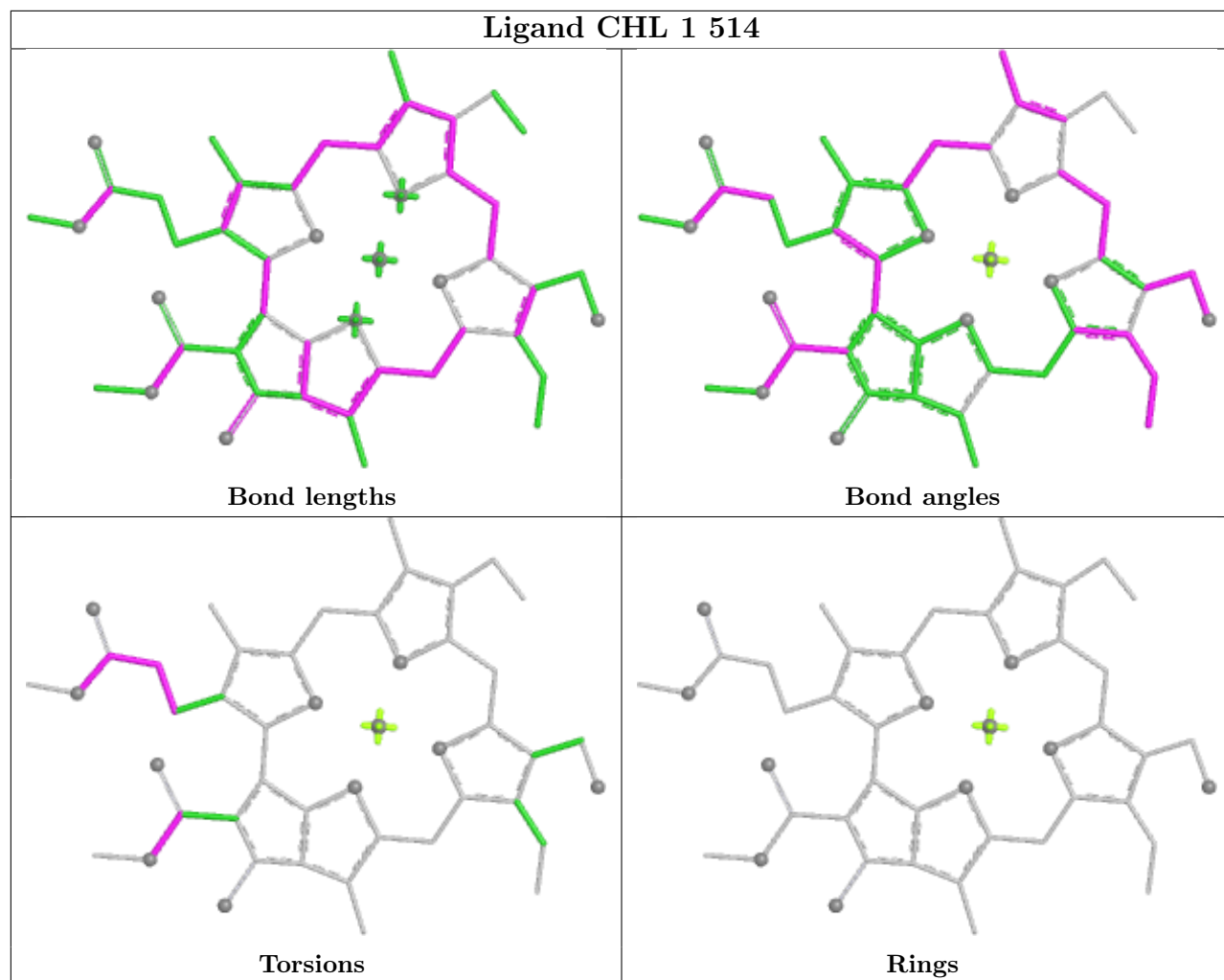


Torsions

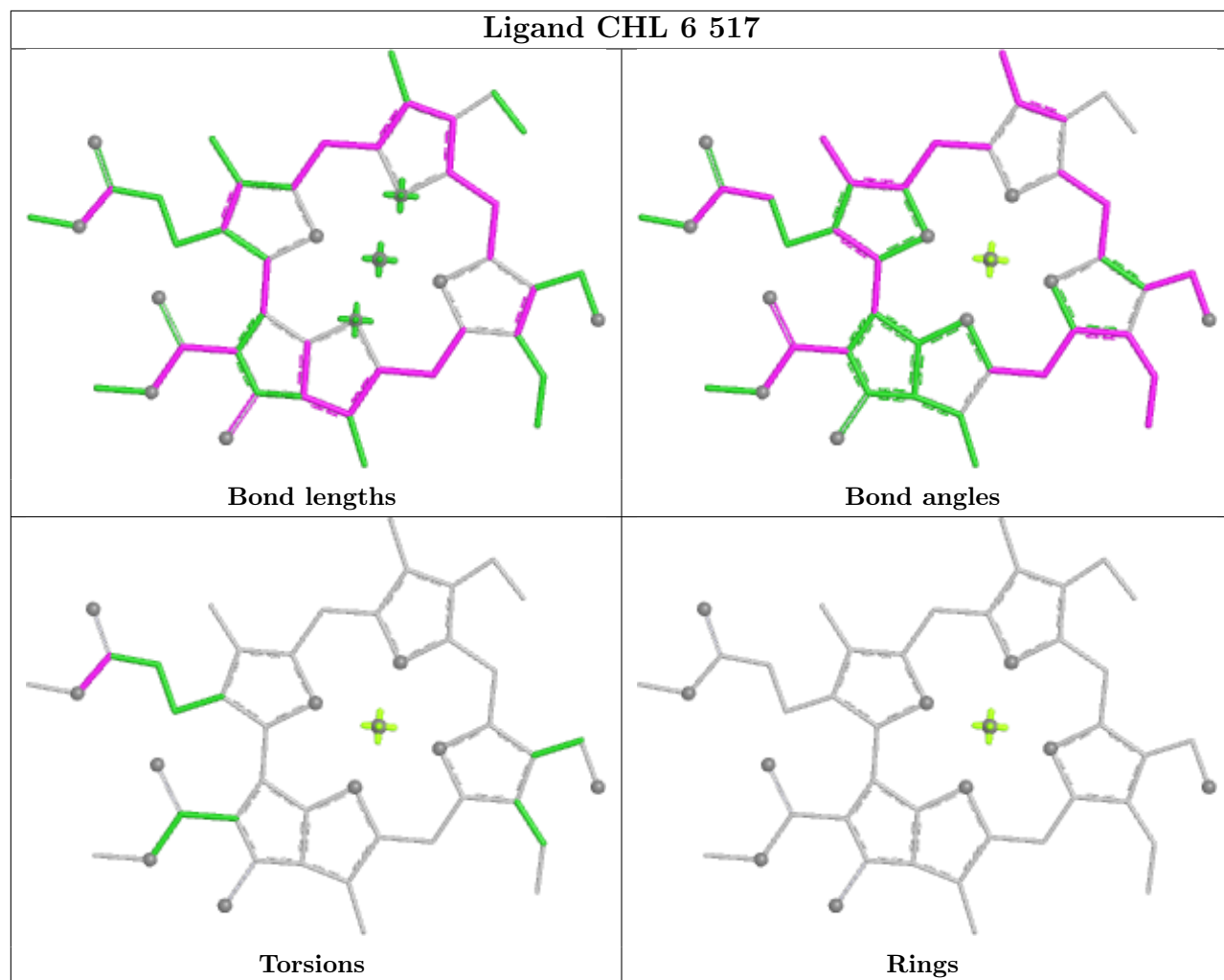


Rings

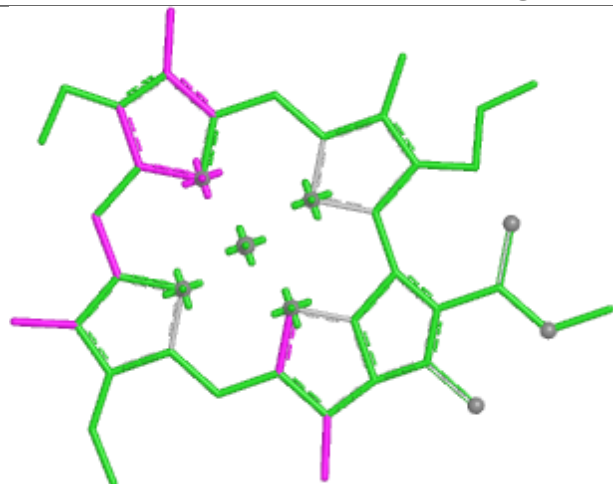
Ligand CHL 1 514



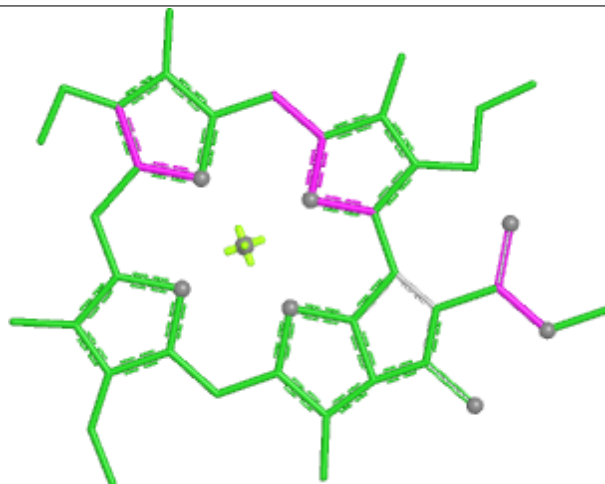
Ligand CHL 6 517



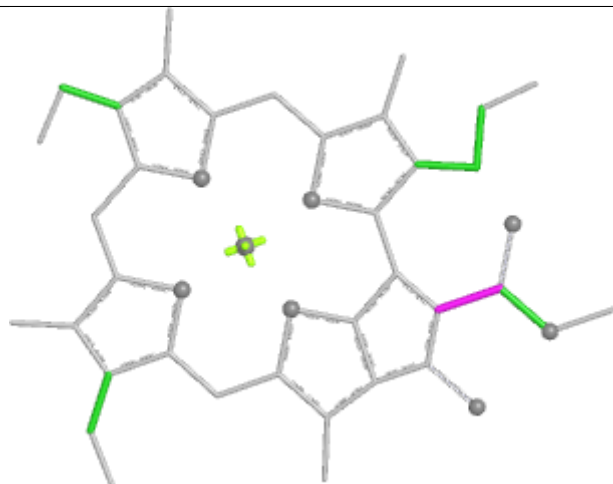
Ligand CLA B 814



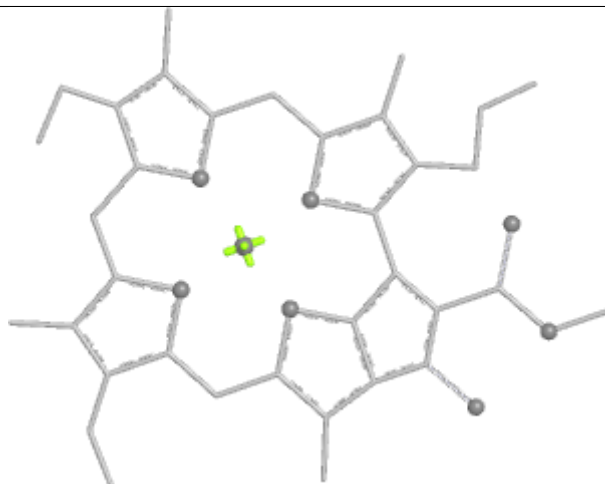
Bond lengths



Bond angles

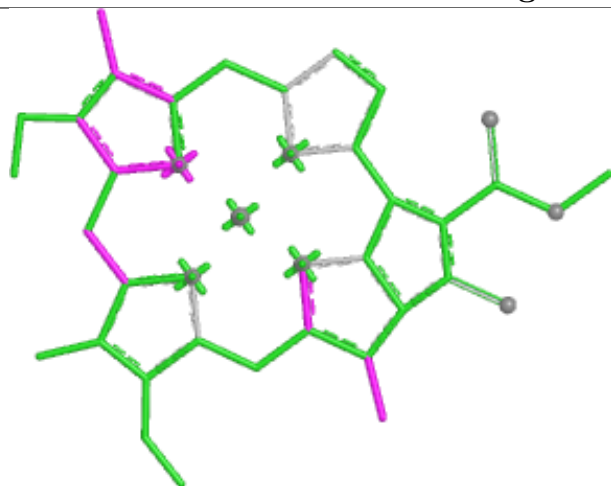


Torsions

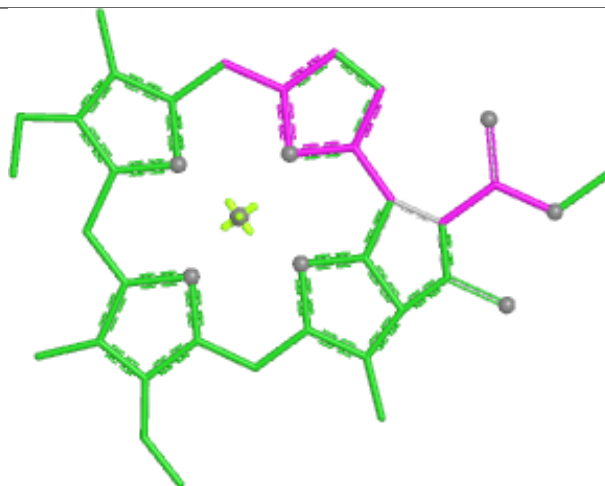


Rings

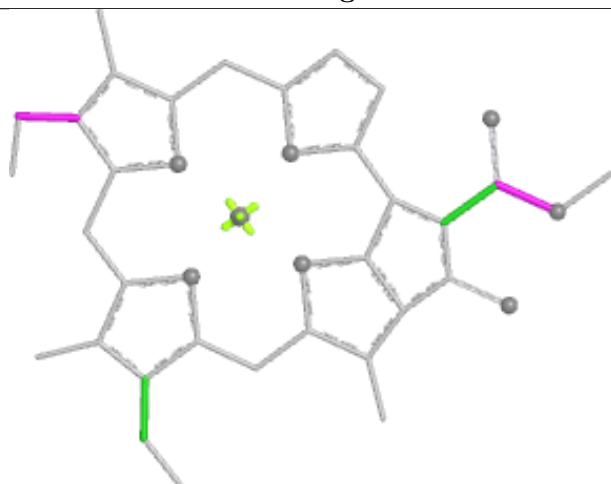
Ligand CLA 1 511



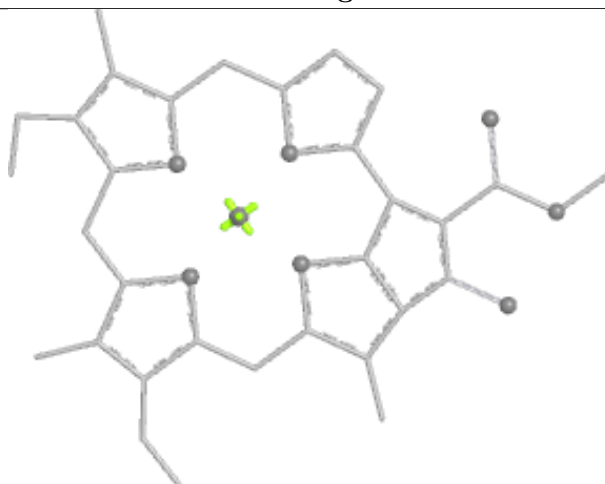
Bond lengths



Bond angles

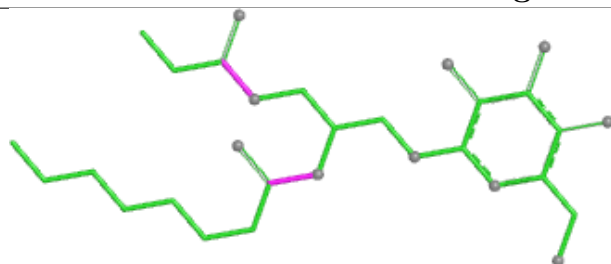


Torsions

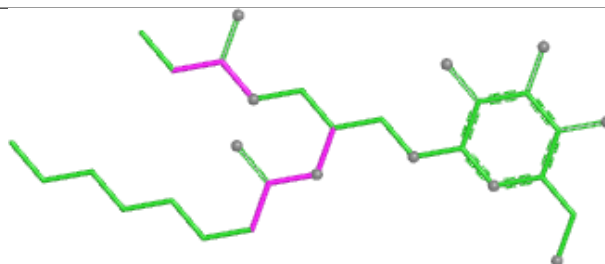


Rings

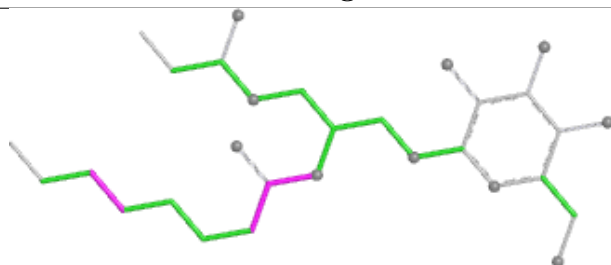
Ligand LMG J 105



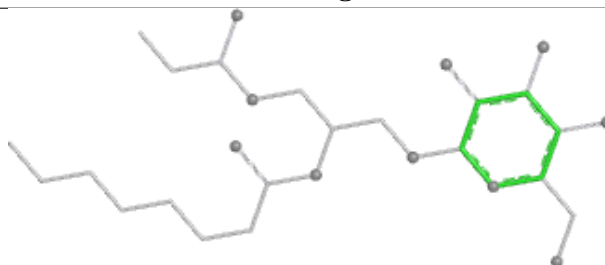
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

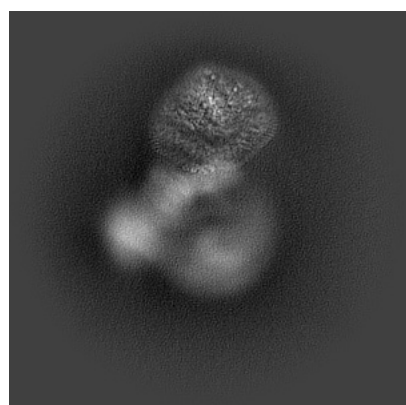
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31350. These allow visual inspection of the internal detail of the map and identification of artifacts.

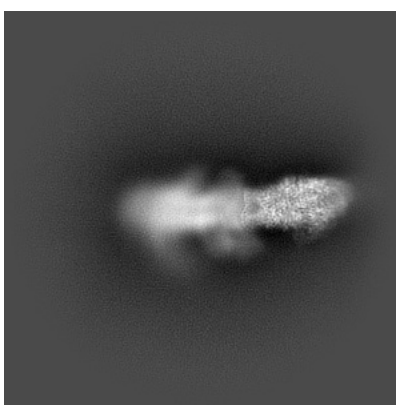
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

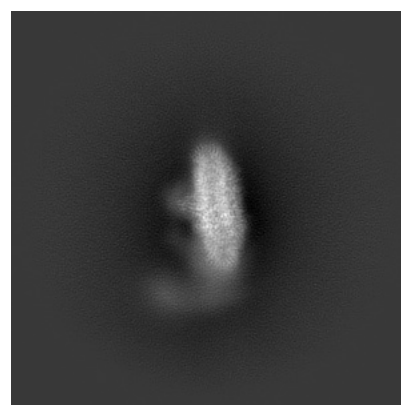
6.1.1 Primary map



X



Y

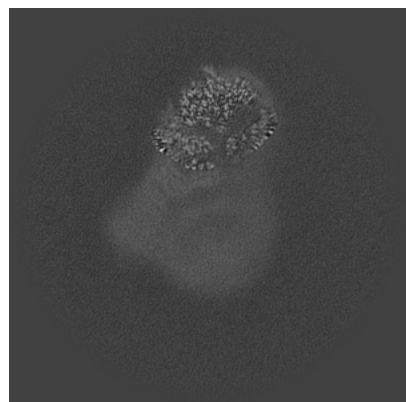


Z

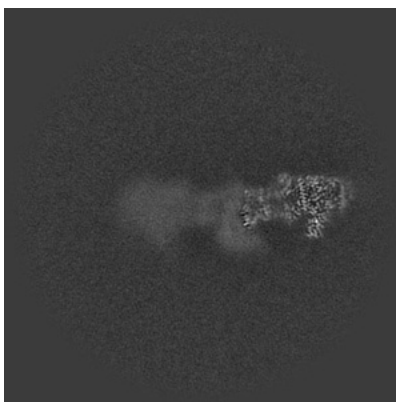
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

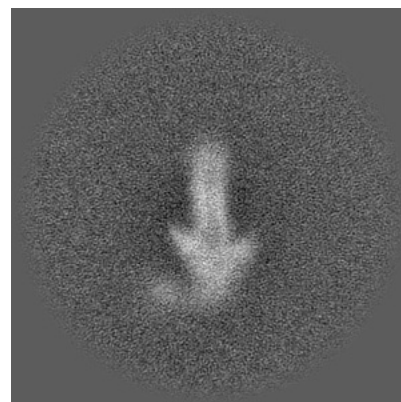
6.2.1 Primary map



X Index: 220



Y Index: 220

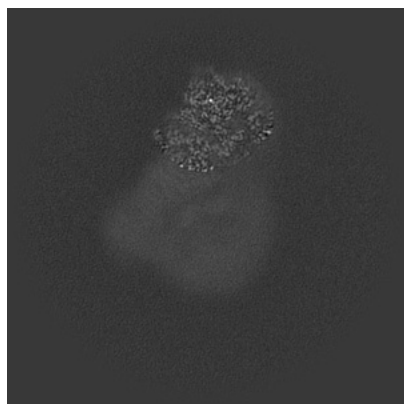


Z Index: 220

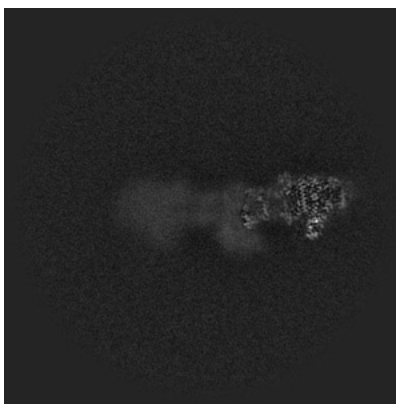
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

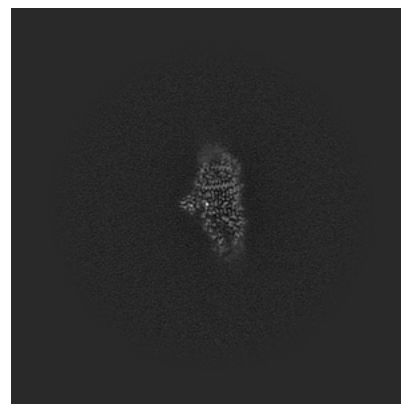
6.3.1 Primary map



X Index: 215



Y Index: 221

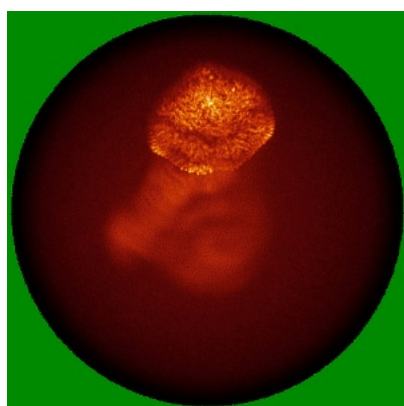


Z Index: 338

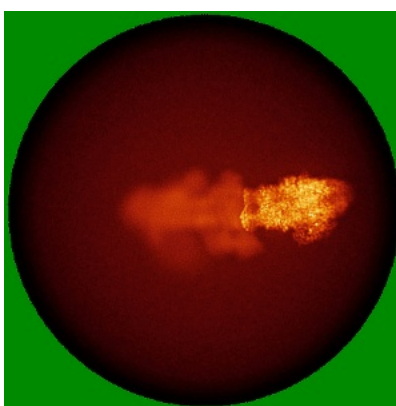
The images above show the largest variance slices of the map in three orthogonal directions.

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

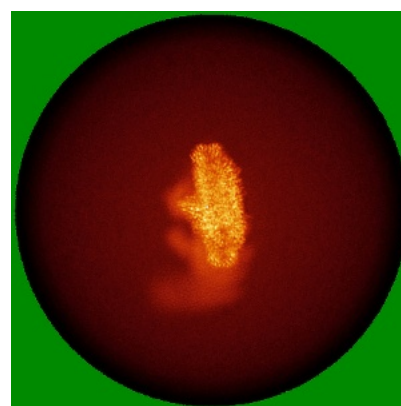
6.4.1 Primary map



X



Y

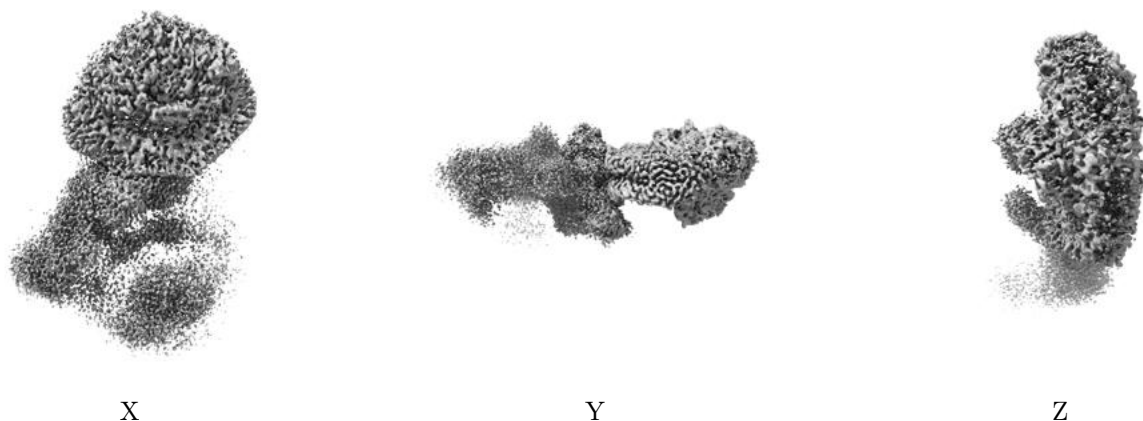


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

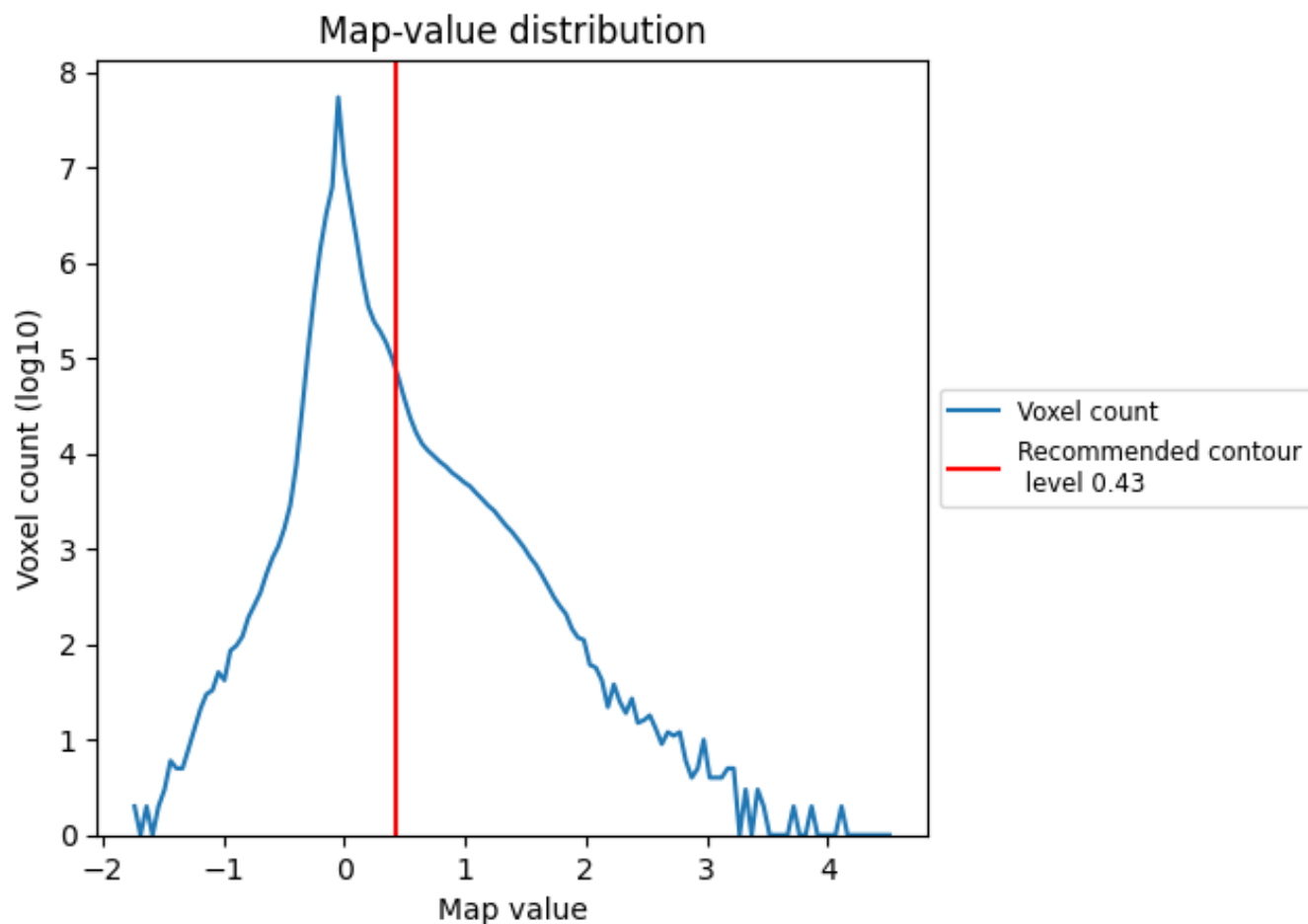
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

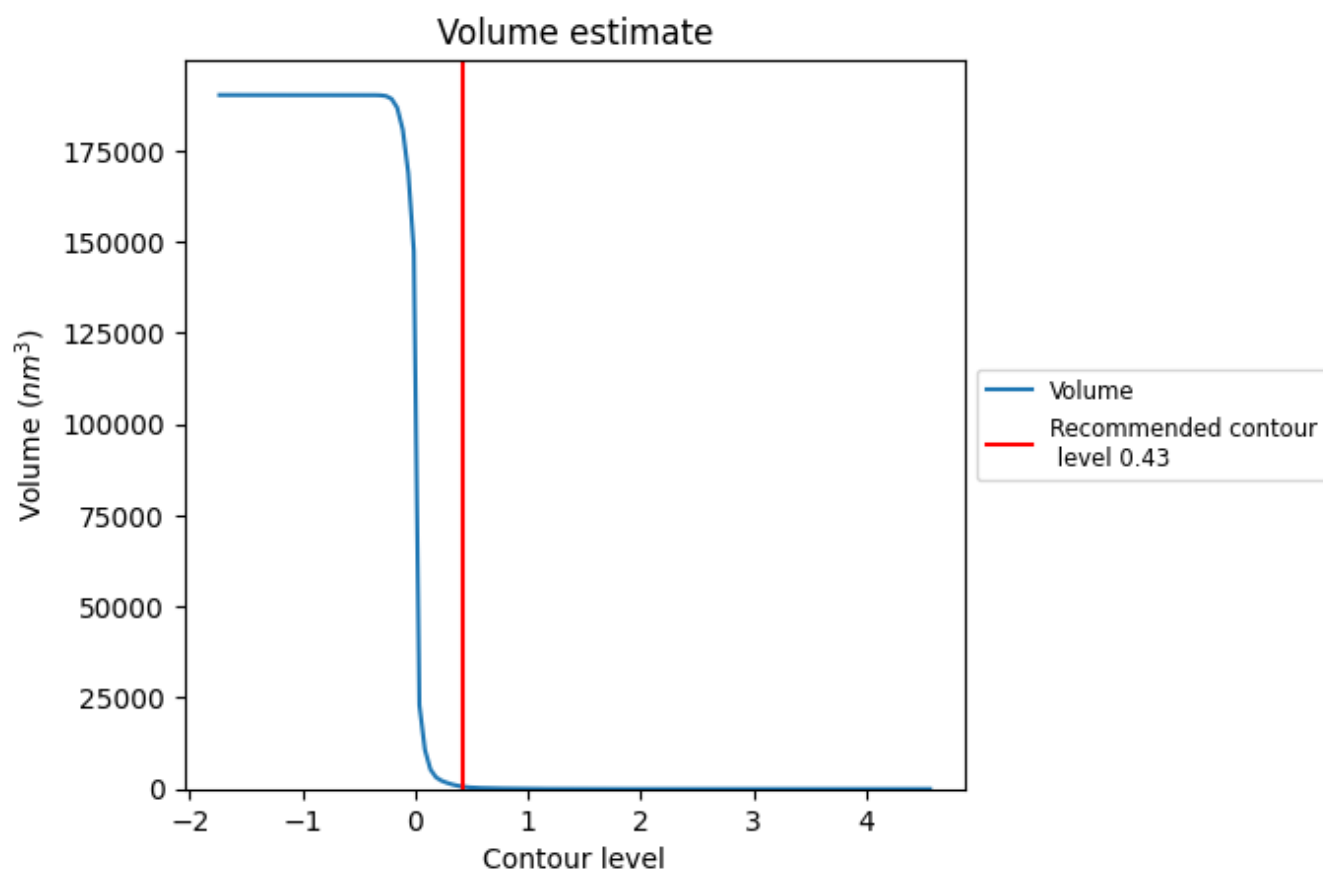
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

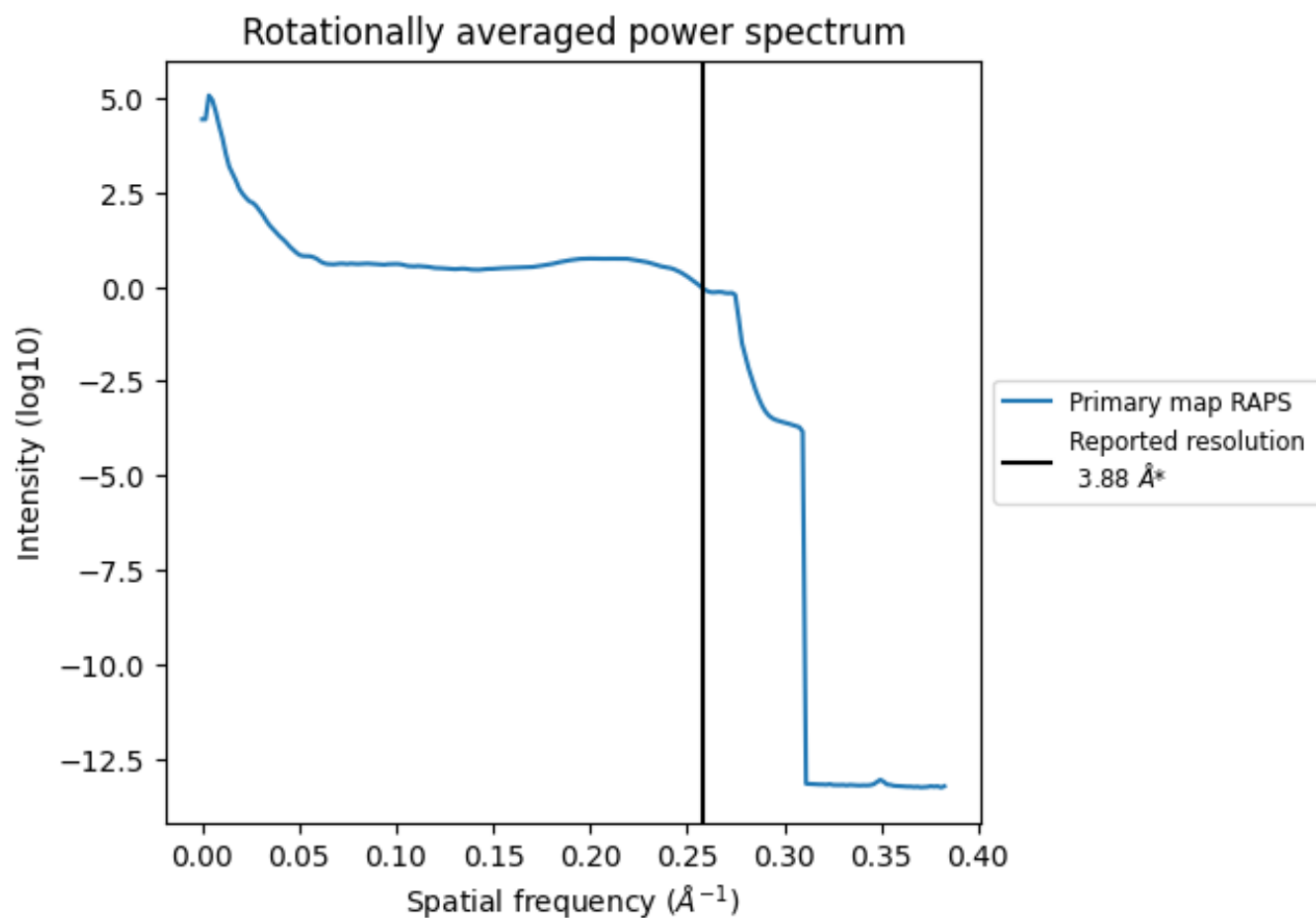
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 598 nm^3 ; this corresponds to an approximate mass of 540 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 0.258 Å⁻¹

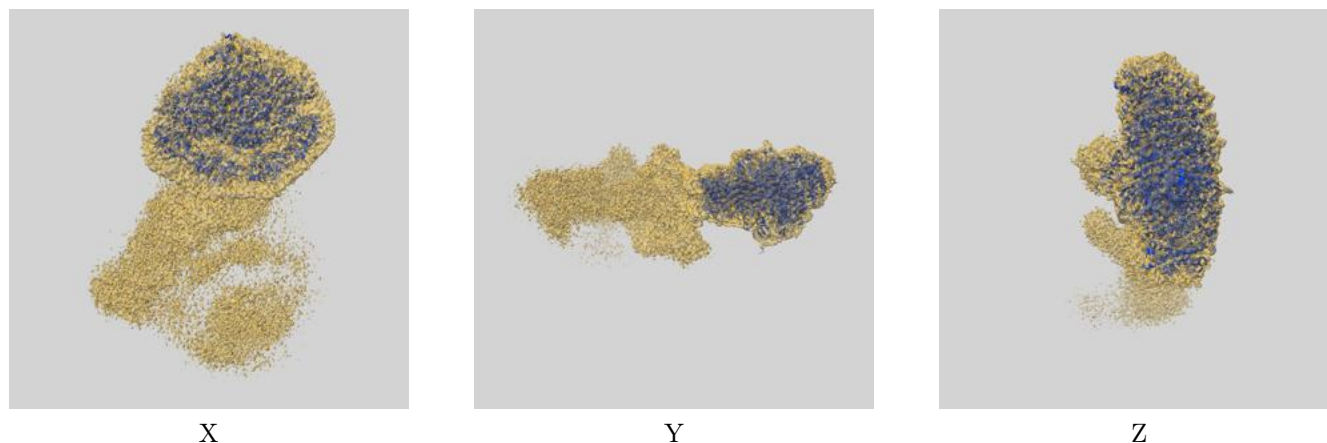
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

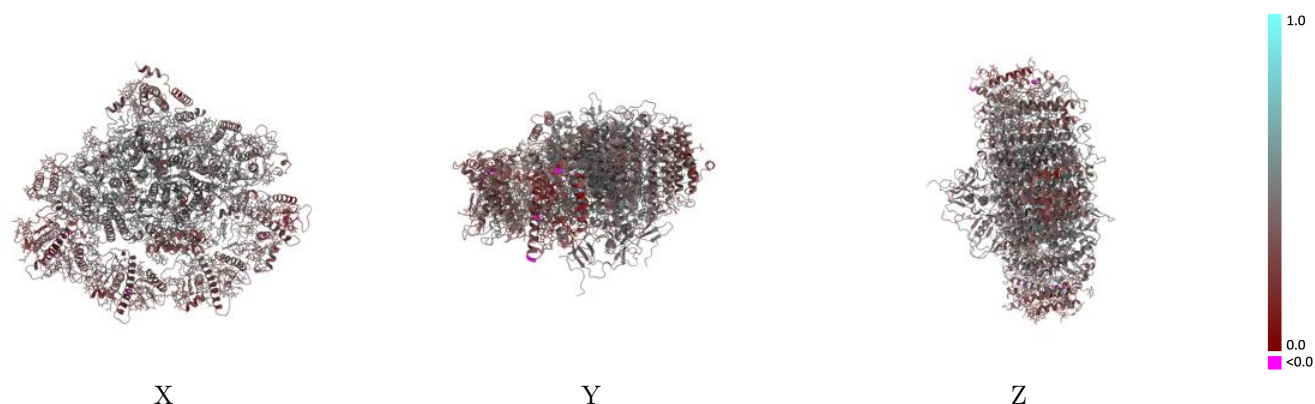
This section contains information regarding the fit between EMDB map EMD-31350 and PDB model 7EWK. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



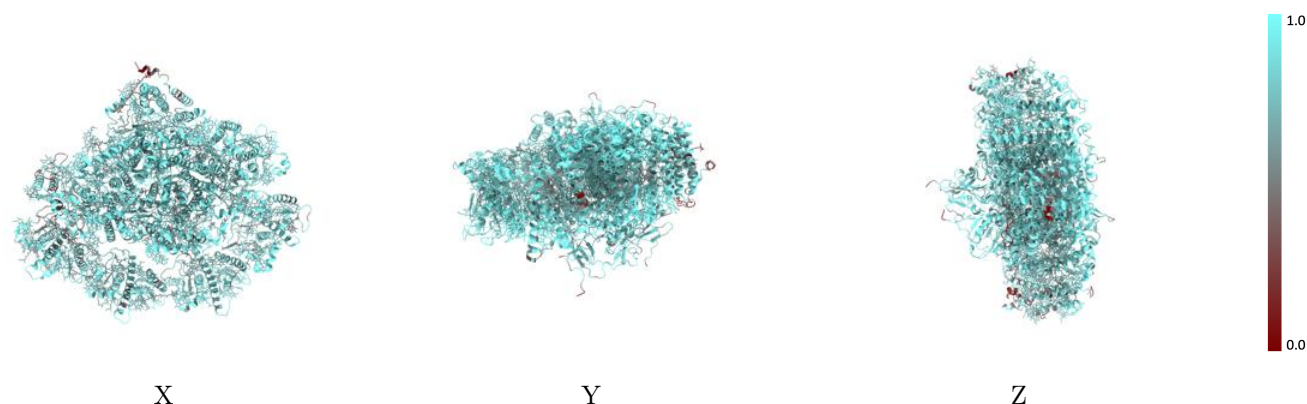
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



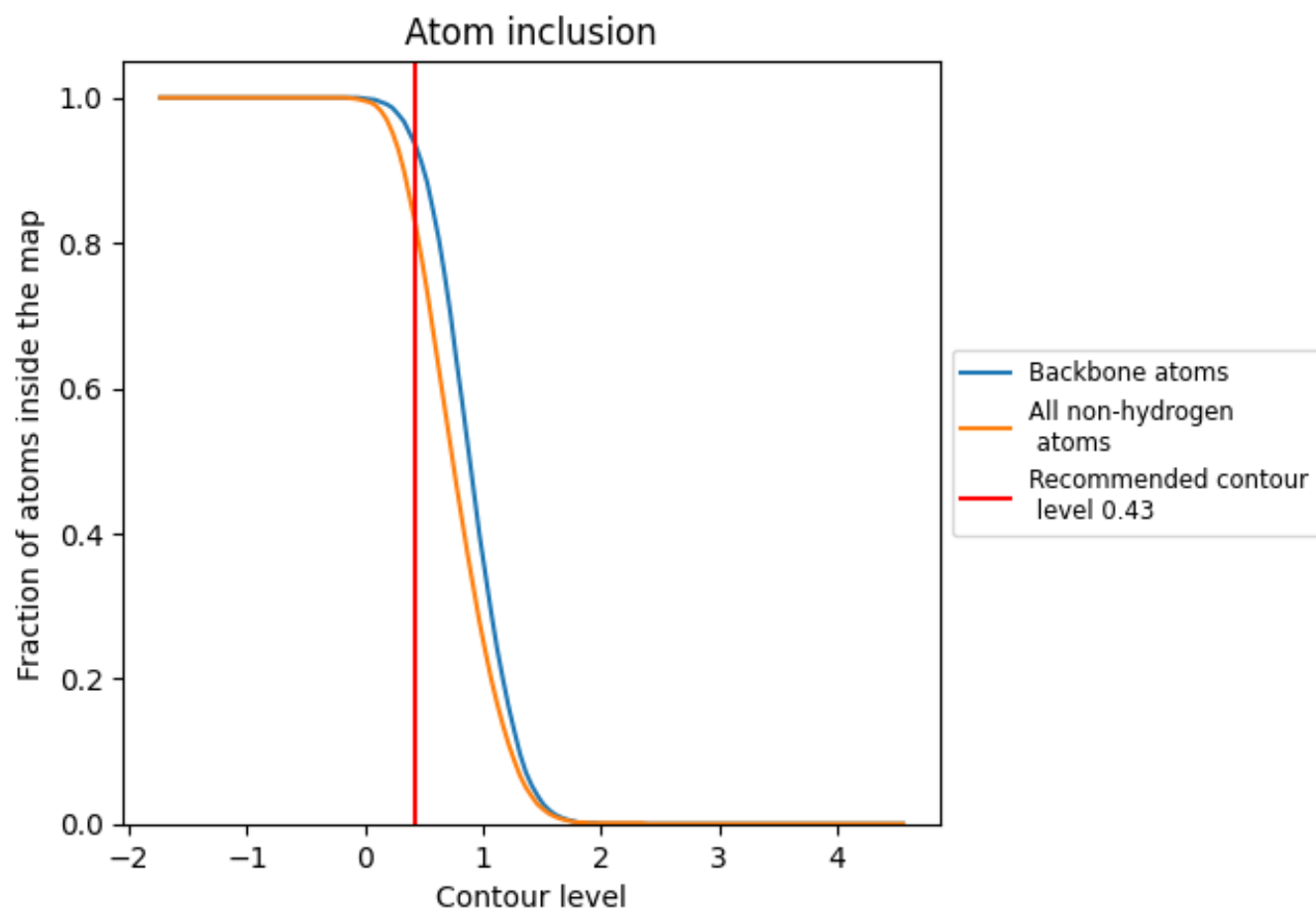
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3960
1	0.8130	0.3100
3	0.7240	0.2960
4	0.8440	0.3590
6	0.8200	0.3440
A	0.8500	0.4450
B	0.8690	0.4350
C	0.9140	0.4250
D	0.8180	0.4190
E	0.7990	0.4320
F	0.8380	0.3750
H	0.6350	0.3430
I	0.7740	0.4220
J	0.7400	0.3940
K	0.6770	0.3280
L	0.7240	0.3620

