



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:04 AM UTC

PDB ID : 8WGH / pdb_00008wgh
EMDB ID : EMD-37513
Title : Cryo-EM structure of the red-shifted *Fittonia albivenis* PSI-LHCI
Authors : Huang, G.Q.; Li, X.X.; Sui, S.F.; Qin, X.C.
Deposited on : 2023-09-21
Resolution : 2.40 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:

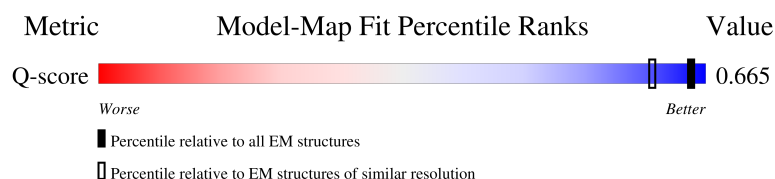
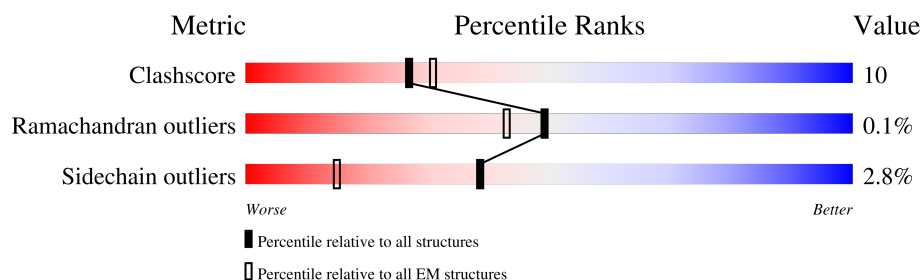
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.40 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.



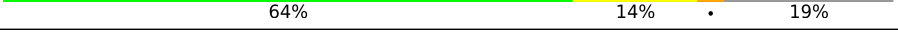
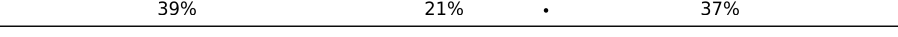
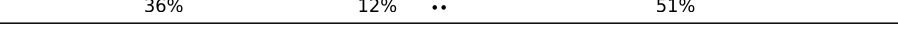
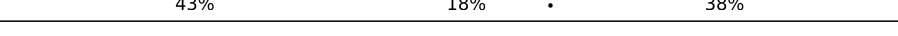
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	1	246	
2	2	265	
3	3	272	
4	4	248	

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	190	
9	E	151	
10	F	221	
11	G	145	
12	H	145	
13	I	36	
14	J	44	
15	K	132	
16	L	217	
17	N	173	
18	O	144	

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
19	CHL	1	301	X	-	-	-
19	CHL	1	306	X	-	-	-
19	CHL	2	301	X	-	-	-
19	CHL	2	305	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	2	307	X	-	-	-
19	CHL	2	314	X	-	-	-
19	CHL	3	306	X	-	-	-
19	CHL	4	305	X	-	-	-
19	CHL	4	306	X	-	-	-
19	CHL	4	307	X	-	-	-
19	CHL	4	315	X	-	-	-
20	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	303	X	-	-	-
20	CLA	1	304	X	-	-	-
20	CLA	1	305	X	-	-	-
20	CLA	1	307	X	-	-	-
20	CLA	1	308	X	-	-	-
20	CLA	1	309	X	-	-	-
20	CLA	1	310	X	-	-	-
20	CLA	1	311	X	-	-	-
20	CLA	1	312	X	-	-	-
20	CLA	1	313	X	-	-	-
20	CLA	1	314	X	-	-	-
20	CLA	1	321	X	-	-	-
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	313	X	-	-	-
20	CLA	3	301	X	-	-	-
20	CLA	3	302	X	-	-	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	4	301	X	-	-	-
20	CLA	4	302	X	-	-	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	841	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	F	802	X	-	-	-
20	CLA	F	804	X	-	-	-
20	CLA	F	805	X	-	-	-
20	CLA	G	603	X	-	-	-
20	CLA	G	604	X	-	-	-
20	CLA	G	605	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	205	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	303	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	307	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	N	203	X	-	-	-
20	CLA	O	201	X	-	-	-
20	CLA	O	202	X	-	-	-
20	CLA	O	203	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 38187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	199	Total	C	N	O	S	0	0
			1559	1016	261	278	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	209	Total	C	N	O	S	0	0
			1626	1068	264	289	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1727	1139	277	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	197	Total	C	N	O	S	0	0
			1568	1027	253	283	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5831	3820	989	1003	19		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	VAL	conflict	UNP A0A8A0WPY6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5854	3843	996	1002	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1116	714	193	206	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			511	324	92	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	153	Total	C	N	O	S	0	0
			1216	793	208	212	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	G	98	Total	C	N	O	0	0
			768	498	126	144		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	90	Total	C	N	O	0	0
			681	444	109	128		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	29	Total	C	N	O	S	0	0
			221	151	35	34	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O	S	0	0
			318	215	49	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	83	Total	C	N	O	S	0	0
			588	378	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1225	812	195	217	1		

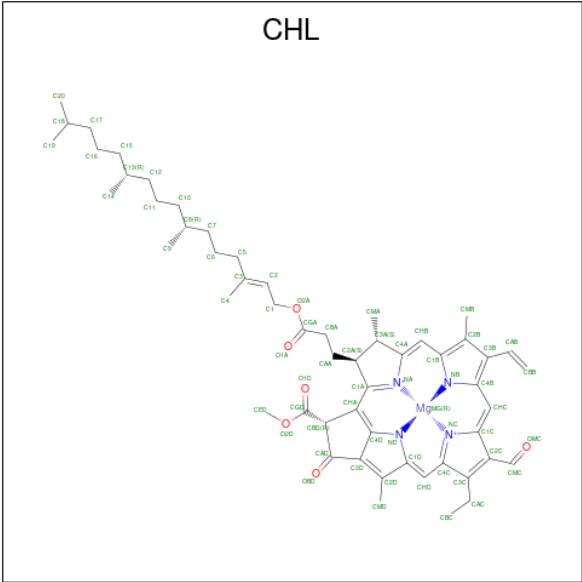
- Molecule 17 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			686	440	111	131	4		

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

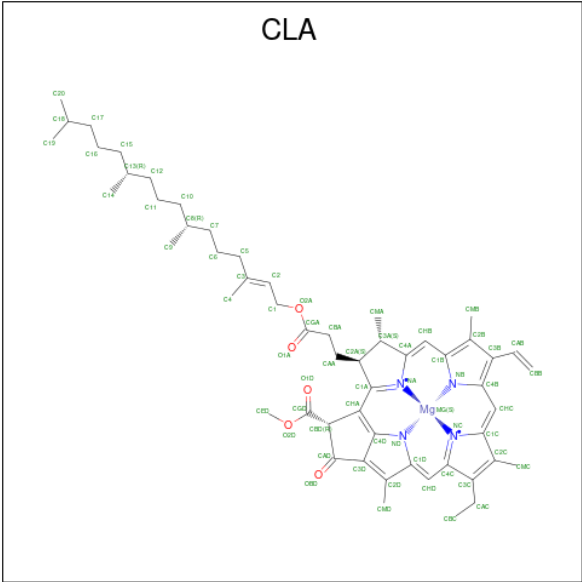
Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	89	Total	C	N	O	S	0	0
			705	475	112	117	1		

- Molecule 19 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
19	1	1	Total	C	Mg	N	O		0
			52	41	1	4	6		
19	1	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
19	2	1	Total	C	Mg	N	O		0
			53	42	1	4	6		
19	2	1	Total	C	Mg	N	O		0
			43	34	1	4	4		
19	2	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
19	2	1	Total	C	Mg	N	O		0
			51	40	1	4	6		
19	2	1	Total	C	Mg	N	O		0
			43	34	1	4	4		
19	3	1	Total	C	Mg	N	O		0
			47	36	1	4	6		
19	4	1	Total	C	Mg	N	O		0
			53	42	1	4	6		
19	4	1	Total	C	Mg	N	O		0
			51	40	1	4	6		
19	4	1	Total	C	Mg	N	O		0
			51	40	1	4	6		
19	4	1	Total	C	Mg	N	O		0
			43	34	1	4	4		

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
20	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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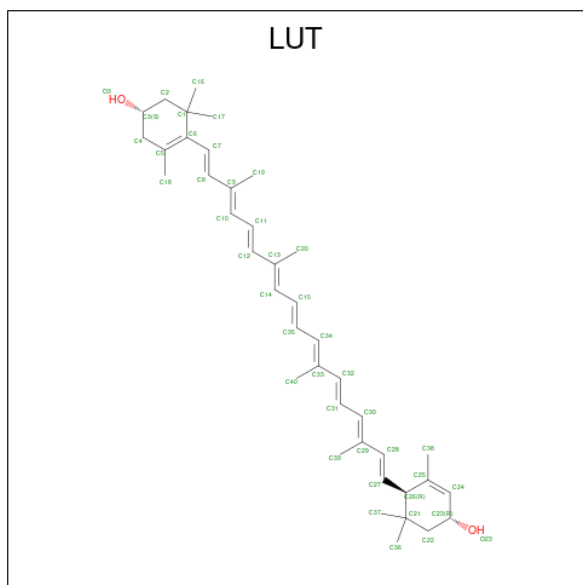
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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



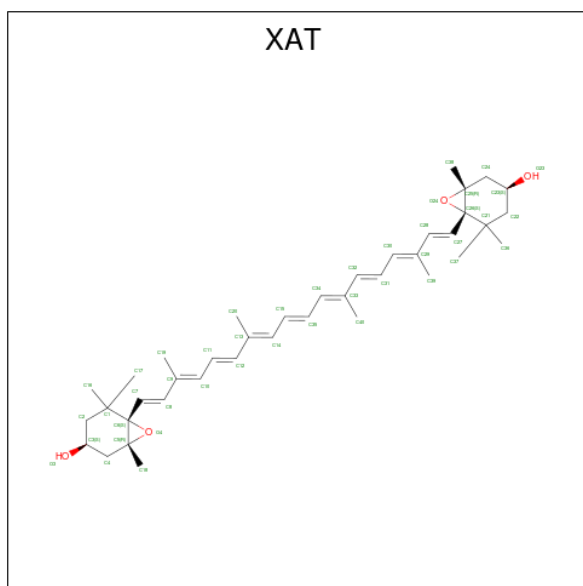
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	

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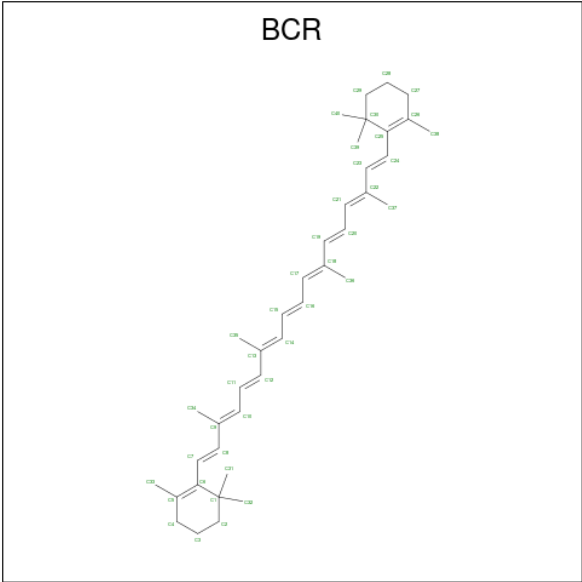
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	

- Molecule 22 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: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



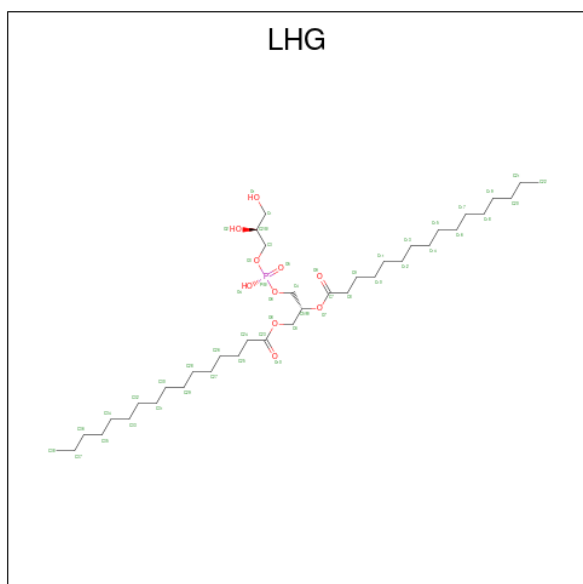
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	2	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

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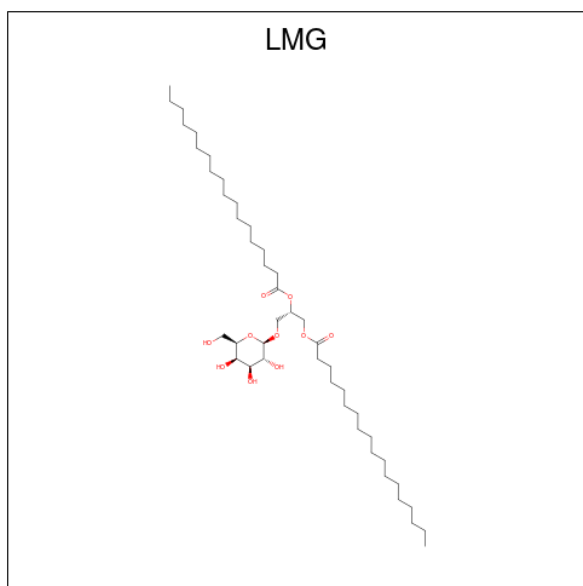
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



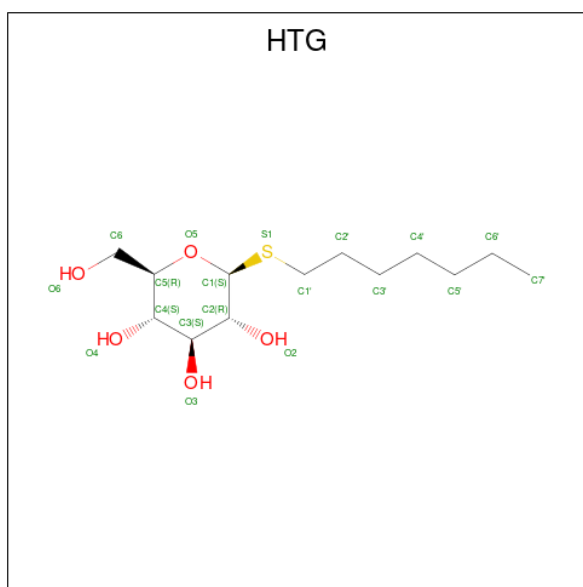
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			37	26	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



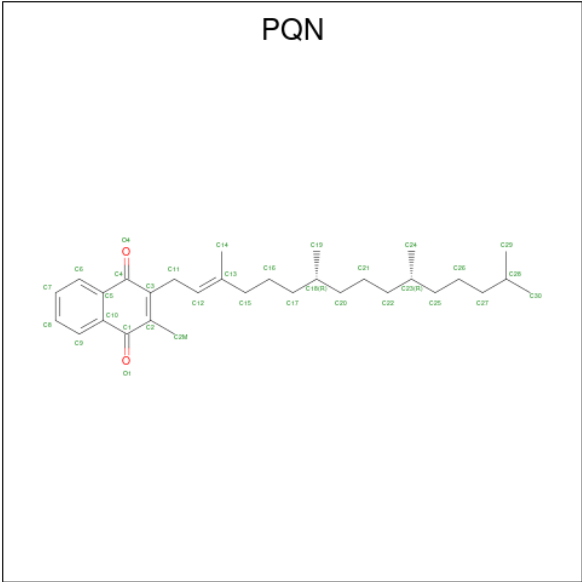
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			49	39	10	
25	1	1	Total	C	O	0
			44	34	10	
25	4	1	Total	C	O	0
			44	34	10	

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



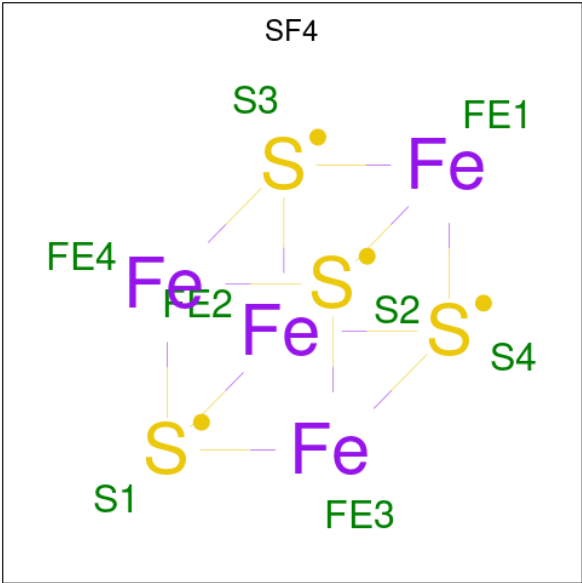
Mol	Chain	Residues	Atoms				AltConf
26	1	1	Total	C	O	S	0
			19	13	5	1	
26	4	1	Total	C	O	S	0
			19	13	5	1	
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	B	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	F	1	Total	C	O	S	0
			19	13	5	1	
26	G	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	
26	N	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



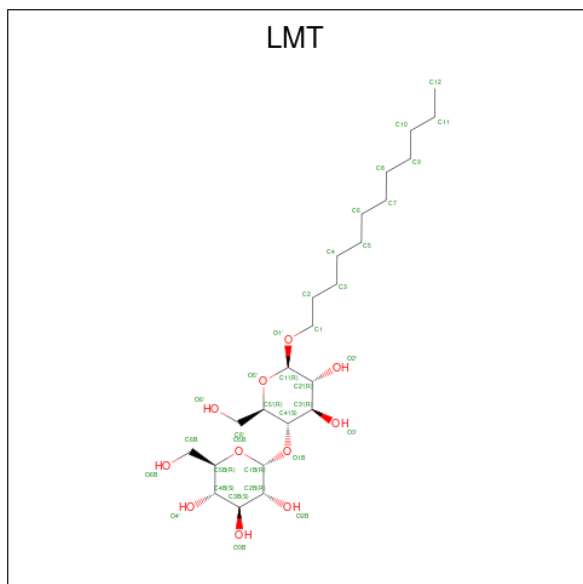
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

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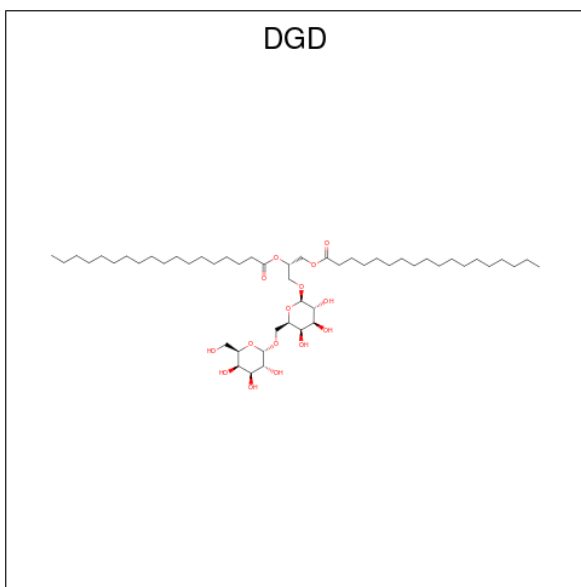
Mol	Chain	Residues	Atoms			AltConf
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			35	24	11	
29	G	1	Total	C	O	0
			35	24	11	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

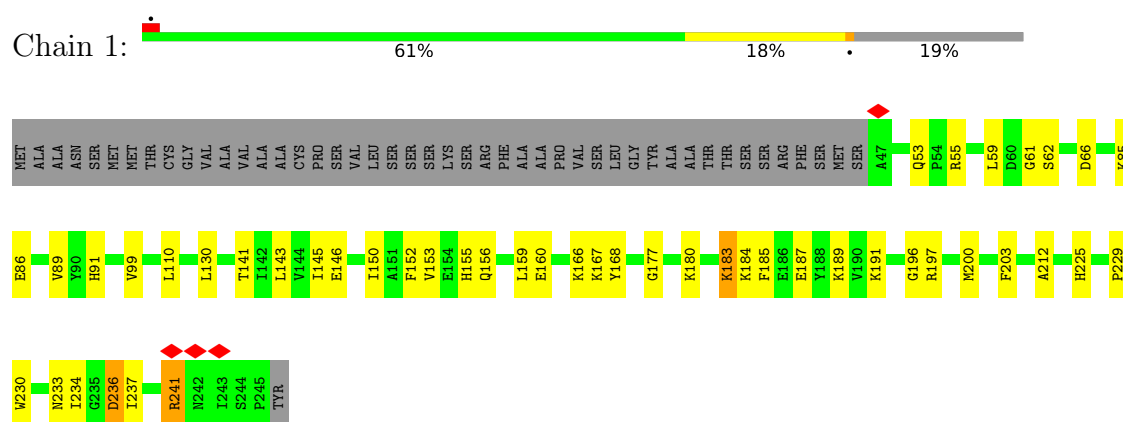


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	66	51	15	0

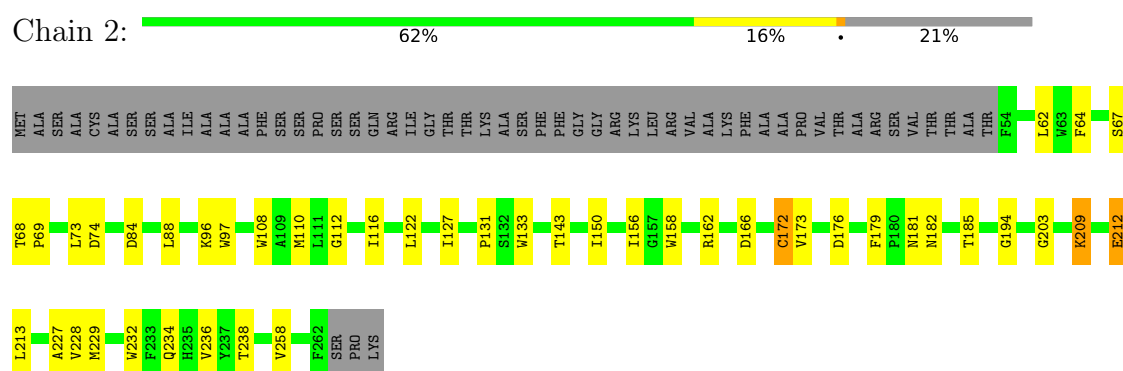
3 Residue-property plots [i](#)

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

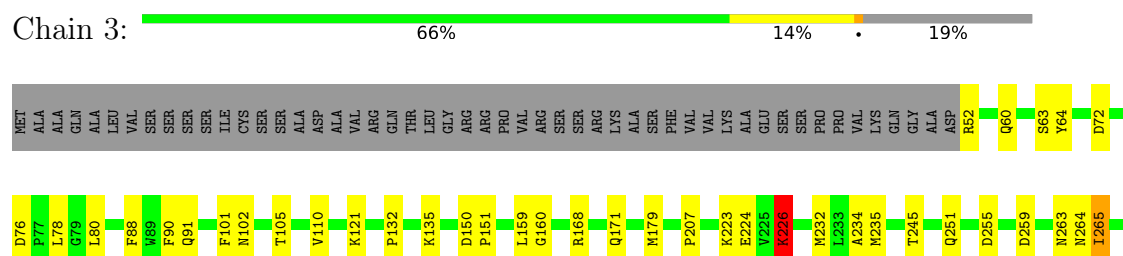
• Molecule 1: Chlorophyll a-b binding protein 1



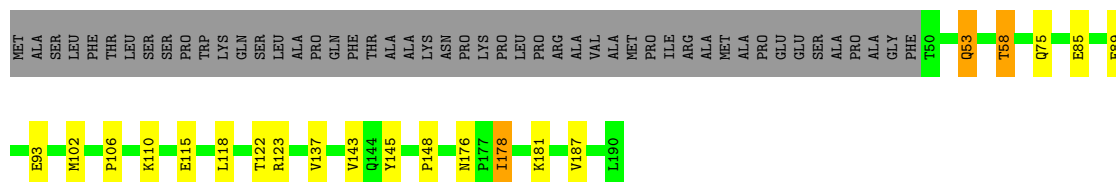
• Molecule 2: Chlorophyll a-b binding protein 2



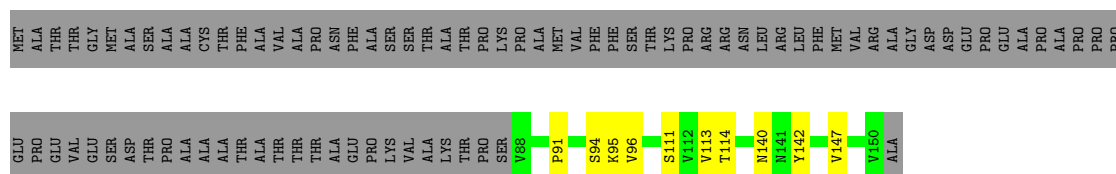
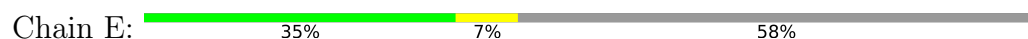
• Molecule 3: Chlorophyll a-b binding protein 3



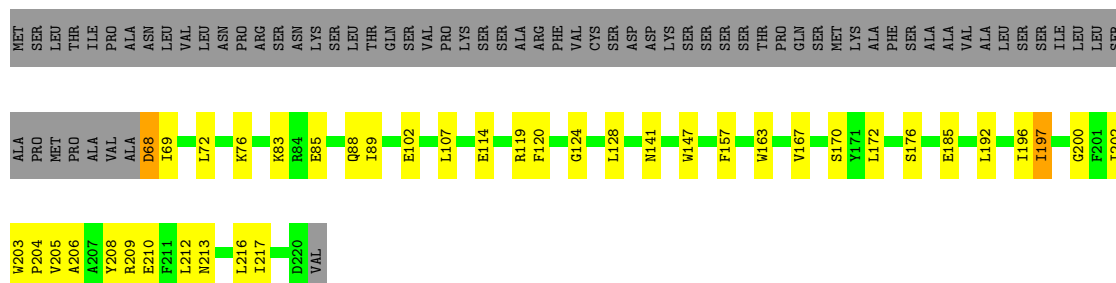
- Molecule 8: Photosystem I reaction center subunit II



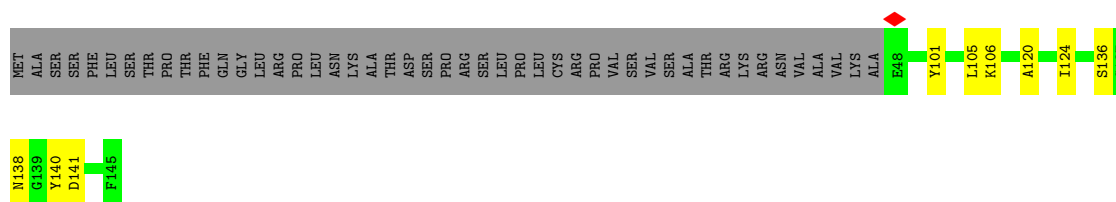
- Molecule 9: Photosystem I reaction center subunit IV



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

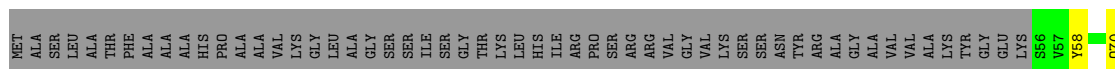


- Molecule 11: Photosystem I reaction center subunit VIII



- Molecule 12: Photosystem I reaction center subunit VI





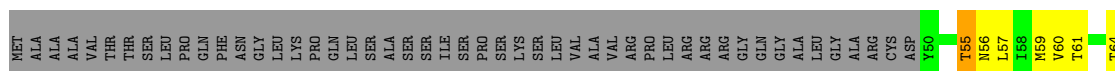
- Molecule 13: Photosystem I reaction center subunit VIII



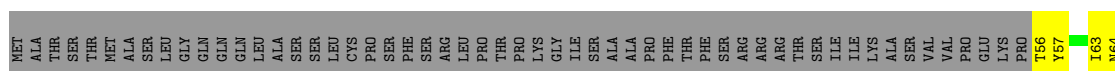
- Molecule 14: Photosystem I reaction center subunit IX



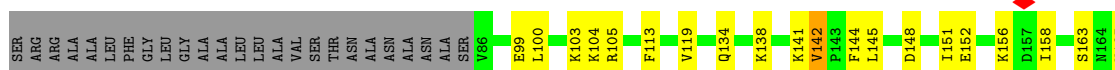
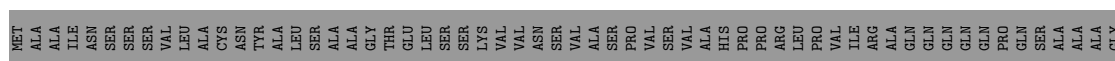
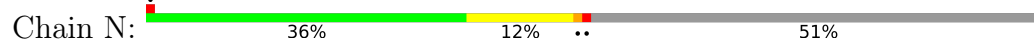
- Molecule 15: Photosystem I reaction center subunit psaK



- Molecule 16: Photosystem I reaction center subunit XI

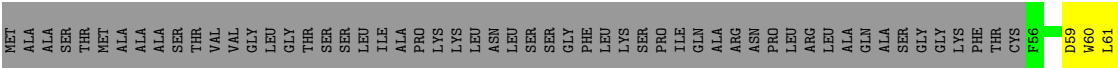


- Molecule 17: Photosystem I reaction center subunit N





• Molecule 18: Photosystem I reaction center subunit O



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.545	Depositor
Minimum map value	-2.048	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.146	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	324.75, 324.75, 324.75	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.17	0/1610	0.41	0/2195
2	2	0.34	1/1687 (0.1%)	0.50	2/2313 (0.1%)
3	3	0.27	1/1791 (0.1%)	0.46	0/2435
4	4	0.16	0/1621	0.41	0/2215
5	A	0.15	0/6029	0.37	0/8223
6	B	0.15	0/6066	0.39	0/8285
7	C	0.14	0/628	0.38	0/852
8	D	0.14	0/1143	0.40	0/1546
9	E	0.13	0/522	0.35	0/710
10	F	0.19	0/1246	0.50	0/1681
11	G	0.58	1/788 (0.1%)	0.48	0/1070
12	H	0.13	0/701	0.35	0/955
13	I	0.18	0/227	0.40	0/310
14	J	0.17	0/327	0.39	0/446
15	K	0.18	0/596	0.51	0/809
16	L	0.14	0/1263	0.36	0/1731
17	N	0.32	0/701	0.52	0/942
18	O	0.20	0/733	0.46	0/1001
All	All	0.21	3/27679 (0.0%)	0.42	2/37719 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	173	VAL	C-O	-6.69	1.16	1.24
11	G	141	ASP	C-O	-5.96	1.20	1.25
3	3	226	LYS	C-O	-5.96	1.16	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	172	CYS	N-CA-C	6.04	123.66	110.80
2	2	173	VAL	N-CA-C	5.13	120.02	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1559	0	1536	37	0
2	2	1626	0	1570	38	0
3	3	1727	0	1651	34	0
4	4	1568	0	1517	35	0
5	A	5831	0	5683	91	0
6	B	5854	0	5635	67	0
7	C	615	0	600	4	0
8	D	1116	0	1122	15	0
9	E	511	0	510	6	0
10	F	1216	0	1245	36	0
11	G	768	0	740	7	0
12	H	681	0	671	8	0
13	I	221	0	237	4	0
14	J	318	0	331	9	0
15	K	588	0	619	23	0
16	L	1225	0	1240	15	0
17	N	686	0	664	18	0
18	O	705	0	686	20	0
19	1	100	0	72	4	0
19	2	238	0	169	23	0
19	3	47	0	30	3	0
19	4	198	0	143	12	0
20	1	744	0	720	26	0
20	2	485	0	445	16	0
20	3	633	0	499	22	0
20	4	593	0	524	28	0
20	A	2610	0	2708	118	0
20	B	2361	0	2424	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	156	0	138	7	0
20	G	141	0	105	0	0
20	H	56	0	51	3	0
20	J	107	0	103	2	0
20	K	197	0	158	9	0
20	L	206	0	177	7	0
20	N	95	0	69	2	0
20	O	157	0	135	14	0
21	1	84	0	112	8	0
21	2	42	0	56	2	0
21	3	42	0	56	4	0
21	4	42	0	56	5	0
21	O	84	0	112	8	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	4	0
22	4	44	0	56	7	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	3	0
23	4	40	0	56	5	0
23	A	240	0	336	18	0
23	B	240	0	336	23	0
23	F	80	0	112	7	0
23	G	40	0	56	3	0
23	I	40	0	56	6	0
23	J	80	0	112	10	0
23	K	40	0	56	4	0
23	L	120	0	168	9	0
24	1	49	0	74	7	0
24	2	37	0	44	1	0
24	A	76	0	98	3	0
24	B	23	0	16	2	0
25	1	93	0	132	5	0
25	4	44	0	61	3	0
26	1	19	0	26	2	0
26	4	19	0	26	0	0
26	A	19	0	26	0	0
26	B	38	0	52	1	0
26	F	38	0	52	1	0
26	G	19	0	26	0	0
26	J	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	19	0	26	1	0
27	A	33	0	46	3	0
27	B	33	0	46	1	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	B	35	0	46	0	0
29	G	35	0	46	0	0
30	B	66	0	96	2	0
All	All	38187	0	37964	751	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 751 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)
10:F:217:ILE:HG13	20:F:802:CLA:O1A	1.45	1.16
20:1:309:CLA:HAB	21:1:315:LUT:H32	1.42	0.98
3:3:235:MET:HE2	22:3:316:XAT:H10	1.46	0.95
20:3:309:CLA:HBC2	20:3:309:CLA:HHD	1.50	0.93
20:B:831:CLA:HBB1	23:F:801:BCR:HC8	1.53	0.91

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	1	197/246 (80%)	194 (98%)	3 (2%)	0	100	100
2	2	207/265 (78%)	203 (98%)	3 (1%)	1 (0%)	24	37
3	3	218/272 (80%)	206 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	716 (98%)	14 (2%)	1 (0%)	48	64
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	139/190 (73%)	135 (97%)	4 (3%)	0	100	100
9	E	61/151 (40%)	59 (97%)	2 (3%)	0	100	100
10	F	151/221 (68%)	150 (99%)	1 (1%)	0	100	100
11	G	96/145 (66%)	95 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	87 (99%)	1 (1%)	0	100	100
13	I	27/36 (75%)	27 (100%)	0	0	100	100
14	J	38/44 (86%)	38 (100%)	0	0	100	100
15	K	81/132 (61%)	75 (93%)	5 (6%)	1 (1%)	10	16
16	L	160/217 (74%)	157 (98%)	3 (2%)	0	100	100
17	N	82/173 (47%)	76 (93%)	5 (6%)	1 (1%)	10	16
18	O	87/144 (60%)	85 (98%)	2 (2%)	0	100	100
All	All	3376/4194 (80%)	3289 (97%)	83 (2%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	172	CYS
6	B	362	ALA
17	N	167	TRP
15	K	96	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/198 (82%)	157 (97%)	5 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	168/208 (81%)	165 (98%)	3 (2%)	51	73
3	3	175/217 (81%)	170 (97%)	5 (3%)	37	60
4	4	168/207 (81%)	165 (98%)	3 (2%)	51	73
5	A	600/608 (99%)	584 (97%)	16 (3%)	39	62
6	B	598/599 (100%)	586 (98%)	12 (2%)	48	70
7	C	70/71 (99%)	68 (97%)	2 (3%)	37	60
8	D	121/159 (76%)	117 (97%)	4 (3%)	33	55
9	E	57/124 (46%)	57 (100%)	0	100	100
10	F	126/185 (68%)	118 (94%)	8 (6%)	16	29
11	G	84/125 (67%)	84 (100%)	0	100	100
12	H	72/110 (66%)	71 (99%)	1 (1%)	59	79
13	I	25/31 (81%)	23 (92%)	2 (8%)	11	19
14	J	34/38 (90%)	32 (94%)	2 (6%)	18	31
15	K	61/99 (62%)	59 (97%)	2 (3%)	33	55
16	L	129/176 (73%)	127 (98%)	2 (2%)	55	76
17	N	74/139 (53%)	67 (90%)	7 (10%)	8	13
18	O	73/114 (64%)	69 (94%)	4 (6%)	19	34
All	All	2797/3408 (82%)	2719 (97%)	78 (3%)	38	60

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	F	216	LEU
17	N	165	VAL
13	I	8	SER
16	L	112	LEU
18	O	73	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
5	A	599	ASN
16	L	58	GLN
6	B	218	HIS
15	K	79	ASN

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Mol	Chain	Res	Type
17	N	101	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

225 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	$\# Z > 2$
24	LHG	A	843	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
20	CLA	A	851	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
28	SF4	A	850	-	0,12,12	-	-	-		
20	CLA	3	312	-	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
20	CLA	2	313	-	47,51,73	1.37	7 (14%)	55,86,113	1.46	5 (9%)
21	LUT	1	319	-	42,43,43	0.67	0	51,60,60	1.83	14 (27%)
20	CLA	2	312	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	A	830	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	5 (7%)
20	CLA	B	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	1	311	1	56,60,73	1.30	7 (12%)	65,97,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	809	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
20	CLA	B	817	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
20	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)
20	CLA	A	806	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
20	CLA	B	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	6 (7%)
21	LUT	2	315	-	42,43,43	0.71	0	51,60,60	1.84	15 (29%)
20	CLA	B	809	6	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
19	CHL	4	315	-	37,51,74	4.32	23 (62%)	30,86,114	3.95	12 (40%)
20	CLA	A	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
20	CLA	K	201	15	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
20	CLA	A	836	-	55,59,73	1.30	8 (14%)	64,96,113	1.41	8 (12%)
19	CHL	4	305	-	47,61,74	3.97	23 (48%)	41,98,114	3.12	14 (34%)
20	CLA	L	302	16	49,53,73	1.37	8 (16%)	58,89,113	1.49	4 (6%)
20	CLA	3	314	-	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
26	HTG	4	320	-	19,19,19	1.02	2 (10%)	23,24,24	0.56	0
20	CLA	F	805	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	4 (6%)
20	CLA	3	308	3	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	O	203	-	64,68,73	1.22	7 (10%)	76,107,113	1.30	7 (9%)
20	CLA	2	308	2	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)
20	CLA	B	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
21	LUT	O	205	-	42,43,43	0.84	2 (4%)	51,60,60	2.06	12 (23%)
19	CHL	2	307	-	45,59,74	3.92	26 (57%)	40,96,114	3.67	19 (47%)
20	CLA	3	311	3	59,63,73	1.27	8 (13%)	70,101,113	1.33	6 (8%)
20	CLA	1	307	-	65,69,73	1.20	7 (10%)	77,108,113	1.29	5 (6%)
23	BCR	B	841	-	41,41,41	0.69	1 (2%)	56,56,56	1.90	14 (25%)
20	CLA	N	203	-	54,58,73	1.33	7 (12%)	64,95,113	1.39	6 (9%)
20	CLA	L	307	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	5 (8%)
23	BCR	4	318	-	41,41,41	0.63	0	56,56,56	3.43	23 (41%)
23	BCR	K	204	-	41,41,41	0.66	0	56,56,56	2.03	16 (28%)
20	CLA	1	312	1	69,73,73	1.18	6 (8%)	82,113,113	1.24	5 (6%)
20	CLA	A	835	5	49,53,73	1.38	8 (16%)	58,89,113	1.40	4 (6%)
20	CLA	A	833	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
20	CLA	B	820	-	54,58,73	1.31	8 (14%)	64,95,113	1.41	5 (7%)
26	HTG	N	201	-	19,19,19	0.98	2 (10%)	23,24,24	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	L	301	-	41,41,41	0.70	0	56,56,56	1.96	12 (21%)
20	CLA	1	302	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	B	832	-	62,66,73	1.23	7 (11%)	73,104,113	1.37	9 (12%)
25	LMG	4	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.02	3 (5%)
22	XAT	2	316	-	41,47,47	0.89	2 (4%)	54,74,74	2.56	21 (38%)
23	BCR	A	848	-	41,41,41	0.70	1 (2%)	56,56,56	1.90	14 (25%)
20	CLA	A	803	20	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
27	PQN	B	840	-	34,34,34	1.63	2 (5%)	43,45,45	1.17	4 (9%)
20	CLA	A	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
19	CHL	4	306	-	45,59,74	4.16	24 (53%)	40,96,114	3.08	18 (45%)
20	CLA	B	833	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
20	CLA	B	813	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
22	XAT	1	316	-	41,47,47	0.89	2 (4%)	54,74,74	2.51	19 (35%)
20	CLA	4	301	4	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
20	CLA	A	853	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
23	BCR	B	844	-	41,41,41	0.68	0	56,56,56	1.87	15 (26%)
23	BCR	A	845	-	41,41,41	0.69	0	56,56,56	1.95	17 (30%)
20	CLA	B	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
20	CLA	A	807	5	69,73,73	1.14	8 (11%)	82,113,113	1.29	8 (9%)
20	CLA	B	834	-	49,53,73	1.37	8 (16%)	58,89,113	1.42	6 (10%)
26	HTG	1	322	-	19,19,19	0.97	2 (10%)	23,24,24	1.03	3 (13%)
20	CLA	A	822	-	55,59,73	1.30	8 (14%)	64,96,113	1.35	7 (10%)
20	CLA	3	302	-	54,58,73	1.33	7 (12%)	64,95,113	1.35	6 (9%)
20	CLA	K	202	-	64,68,73	1.21	9 (14%)	76,107,113	1.35	8 (10%)
20	CLA	F	804	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
20	CLA	A	810	20	69,73,73	1.16	7 (10%)	82,113,113	1.24	4 (4%)
20	CLA	A	821	-	53,57,73	1.31	8 (15%)	61,93,113	1.41	5 (8%)
20	CLA	3	305	3	51,55,73	1.34	8 (15%)	60,91,113	1.38	4 (6%)
20	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
20	CLA	A	801	-	69,73,73	1.17	7 (10%)	82,113,113	1.40	8 (9%)
20	CLA	N	202	17	48,53,73	1.39	7 (14%)	56,89,113	1.40	4 (7%)
20	CLA	A	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	7 (8%)
20	CLA	A	813	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
20	CLA	2	310	24	45,49,73	1.39	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
20	CLA	A	814	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	6 (9%)
29	LMT	G	601	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
23	BCR	B	842	-	41,41,41	0.70	1 (2%)	56,56,56	2.04	19 (33%)
20	CLA	4	312	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	4 (4%)
23	BCR	A	846	-	41,41,41	0.71	0	56,56,56	1.98	15 (26%)
26	HTG	A	852	-	19,19,19	1.16	2 (10%)	23,24,24	1.41	3 (13%)
20	CLA	1	321	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	811	-	58,62,73	1.28	7 (12%)	68,99,113	1.31	5 (7%)
26	HTG	J	105	-	19,19,19	1.01	2 (10%)	23,24,24	0.55	0
20	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
19	CHL	2	301	2	47,61,74	4.13	30 (63%)	41,98,114	5.07	21 (51%)
20	CLA	4	313	-	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
23	BCR	A	847	-	41,41,41	0.65	0	56,56,56	2.01	17 (30%)
20	CLA	3	301	3	64,68,73	1.21	9 (14%)	76,107,113	1.29	5 (6%)
26	HTG	B	850	-	19,19,19	0.97	2 (10%)	23,24,24	0.81	0
23	BCR	J	102	-	41,41,41	0.65	0	56,56,56	1.98	17 (30%)
20	CLA	2	309	2	64,68,73	1.21	9 (14%)	76,107,113	1.28	6 (7%)
25	LMG	1	323	-	44,44,55	0.99	2 (4%)	52,52,63	1.05	3 (5%)
20	CLA	B	830	-	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
20	CLA	1	313	-	59,63,73	1.25	8 (13%)	70,101,113	1.35	5 (7%)
20	CLA	2	303	-	53,57,73	1.32	8 (15%)	61,93,113	1.39	4 (6%)
20	CLA	4	314	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	6 (9%)
20	CLA	K	203	-	50,54,73	1.35	8 (16%)	59,90,113	1.43	5 (8%)
20	CLA	3	303	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	5 (8%)
20	CLA	B	815	-	64,68,73	1.19	8 (12%)	76,107,113	1.31	6 (7%)
20	CLA	G	604	-	54,58,73	1.31	8 (14%)	64,95,113	1.40	6 (9%)
28	SF4	C	101	-	0,12,12	-	-	-	-	-
20	CLA	4	308	4	54,58,73	1.30	7 (12%)	64,95,113	1.39	6 (9%)
20	CLA	A	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
19	CHL	4	307	-	45,59,74	4.04	26 (57%)	40,96,114	3.66	13 (32%)
23	BCR	2	317	-	41,41,41	0.73	0	56,56,56	2.14	16 (28%)
20	CLA	B	811	-	58,62,73	1.35	8 (13%)	71,100,113	1.36	8 (11%)
20	CLA	B	810	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
23	BCR	L	305	-	41,41,41	0.68	0	56,56,56	2.10	14 (25%)
20	CLA	H	201	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	4	303	-	64,68,73	1.21	8 (12%)	76,107,113	1.31	5 (6%)
23	BCR	I	101	-	41,41,41	0.74	2 (4%)	56,56,56	2.09	17 (30%)
20	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
20	CLA	B	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
23	BCR	B	843	-	41,41,41	0.69	0	56,56,56	2.05	15 (26%)
20	CLA	J	103	14	46,50,73	1.40	8 (17%)	53,85,113	1.42	4 (7%)
20	CLA	1	304	-	56,60,73	1.29	8 (14%)	65,97,113	1.39	6 (9%)
24	LHG	B	849	-	22,22,48	1.20	2 (9%)	25,28,54	1.03	1 (4%)
20	CLA	B	835	-	55,59,73	1.30	8 (14%)	64,96,113	1.37	7 (10%)
22	XAT	4	317	-	41,47,47	0.89	1 (2%)	54,74,74	2.55	20 (37%)
20	CLA	A	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
20	CLA	G	605	11	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
27	PQN	A	842	-	34,34,34	1.66	2 (5%)	43,45,45	1.10	4 (9%)
20	CLA	2	311	2	56,60,73	1.29	7 (12%)	65,97,113	1.41	6 (9%)
26	HTG	G	602	-	19,19,19	0.99	2 (10%)	23,24,24	0.55	0
24	LHG	1	318	20	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
20	CLA	A	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
20	CLA	3	304	-	46,50,73	1.39	8 (17%)	53,85,113	1.45	6 (11%)
22	XAT	3	316	-	41,47,47	0.88	1 (2%)	54,74,74	2.65	21 (38%)
25	LMG	1	320	-	49,49,55	0.94	2 (4%)	57,57,63	1.03	3 (5%)
23	BCR	A	849	-	41,41,41	0.71	0	56,56,56	1.97	14 (25%)
20	CLA	B	816	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
20	CLA	B	823	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	7 (9%)
20	CLA	A	832	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
20	CLA	1	303	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
20	CLA	B	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
26	HTG	B	851	-	19,19,19	0.98	2 (10%)	23,24,24	0.51	0
20	CLA	G	603	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
20	CLA	A	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	F	802	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
20	CLA	A	834	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	L	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	A	802	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	A	818	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
19	CHL	2	306	-	42,56,74	4.11	22 (52%)	36,92,114	3.65	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	3	313	-	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
20	CLA	A	808	5	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
20	CLA	A	827	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
20	CLA	A	819	-	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
20	CLA	4	302	4	64,68,73	1.20	8 (12%)	76,107,113	1.31	7 (9%)
23	BCR	1	317	-	41,41,41	0.64	0	56,56,56	1.93	18 (32%)
20	CLA	A	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
20	CLA	K	205	15	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
23	BCR	F	801	-	41,41,41	0.66	0	56,56,56	1.81	14 (25%)
24	LHG	2	318	20	36,36,48	1.07	2 (5%)	39,42,54	1.14	3 (7%)
20	CLA	3	310	-	56,60,73	1.31	8 (14%)	65,97,113	1.37	5 (7%)
26	HTG	F	803	-	19,19,19	1.00	2 (10%)	23,24,24	0.55	0
28	SF4	C	102	-	0,12,12	-	-	-	-	-
20	CLA	4	309	4	64,68,73	1.20	9 (14%)	76,107,113	1.28	8 (10%)
20	CLA	O	201	24	56,60,73	1.29	8 (14%)	65,97,113	1.34	5 (7%)
20	CLA	2	304	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
20	CLA	3	309	-	50,54,73	1.78	12 (24%)	59,90,113	2.30	16 (27%)
19	CHL	2	305	-	37,51,74	4.34	23 (62%)	30,86,114	4.93	13 (43%)
20	CLA	B	827	-	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
20	CLA	3	307	3	54,58,73	1.30	8 (14%)	64,95,113	1.40	7 (10%)
20	CLA	A	820	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
23	BCR	B	845	-	41,41,41	0.66	0	56,56,56	2.00	17 (30%)
20	CLA	B	819	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
20	CLA	1	310	24	45,49,73	1.40	8 (17%)	54,84,113	1.49	6 (11%)
21	LUT	O	204	-	42,43,43	0.72	0	51,60,60	1.85	14 (27%)
24	LHG	A	844	20	26,26,48	1.26	2 (7%)	29,32,54	1.33	4 (13%)
20	CLA	J	101	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
20	CLA	1	309	1	64,68,73	1.18	7 (10%)	76,107,113	1.28	7 (9%)
20	CLA	1	308	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
20	CLA	A	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	8 (9%)
20	CLA	A	837	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	7 (8%)
20	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
20	CLA	B	804	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
20	CLA	B	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	8 (9%)
20	CLA	L	304	-	54,58,73	1.30	8 (14%)	64,95,113	1.38	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	1	301	1	46,60,74	3.94	18 (39%)	40,97,114	2.40	15 (37%)
20	CLA	2	302	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	5 (6%)
20	CLA	B	837	-	51,55,73	1.34	8 (15%)	60,91,113	1.38	5 (8%)
19	CHL	2	314	2	37,51,74	4.23	17 (45%)	30,86,114	2.88	12 (40%)
20	CLA	A	816	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
20	CLA	A	841	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
23	BCR	B	846	-	41,41,41	0.67	0	56,56,56	1.77	15 (26%)
20	CLA	B	806	6	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
23	BCR	J	104	-	41,41,41	0.65	0	56,56,56	1.98	14 (25%)
23	BCR	L	306	-	41,41,41	0.70	0	56,56,56	2.10	12 (21%)
21	LUT	3	315	-	42,43,43	0.71	0	51,60,60	1.71	15 (29%)
20	CLA	B	801	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
23	BCR	F	806	-	41,41,41	0.70	0	56,56,56	2.03	15 (26%)
20	CLA	B	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
19	CHL	3	306	-	41,55,74	4.17	27 (65%)	35,91,114	4.02	18 (51%)
30	DGD	B	848	-	67,67,67	0.84	2 (2%)	81,81,81	0.95	5 (6%)
20	CLA	1	305	-	56,60,73	1.30	8 (14%)	65,97,113	1.34	6 (9%)
23	BCR	A	854	-	41,41,41	0.66	0	56,56,56	1.95	12 (21%)
23	BCR	G	606	-	41,41,41	0.64	0	56,56,56	1.96	17 (30%)
20	CLA	A	829	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	6 (7%)
20	CLA	4	311	4	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
20	CLA	B	821	-	60,64,73	1.25	8 (13%)	71,102,113	1.33	5 (7%)
21	LUT	1	315	-	42,43,43	0.72	0	51,60,60	1.77	14 (27%)
26	HTG	F	807	-	19,19,19	0.96	2 (10%)	23,24,24	0.52	0
29	LMT	B	847	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	A	815	-	49,53,73	1.38	7 (14%)	58,89,113	1.42	4 (6%)
19	CHL	1	306	1	42,56,74	4.17	23 (54%)	36,92,114	3.11	16 (44%)
20	CLA	B	818	-	64,68,73	1.20	7 (10%)	76,107,113	1.28	4 (5%)
20	CLA	A	823	-	59,63,73	1.26	8 (13%)	70,101,113	1.32	6 (8%)
20	CLA	B	812	-	59,63,73	1.26	8 (13%)	70,101,113	1.33	5 (7%)
20	CLA	B	807	-	59,63,73	1.25	8 (13%)	70,101,113	1.33	6 (8%)
20	CLA	4	310	-	59,63,73	1.25	7 (11%)	70,101,113	1.27	5 (7%)
20	CLA	A	840	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
20	CLA	B	822	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	7 (8%)
21	LUT	4	316	-	42,43,43	0.72	0	51,60,60	1.74	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	3	317	-	41,41,41	0.63	0	56,56,56	2.01	16 (28%)
20	CLA	O	202	-	49,53,73	1.65	10 (20%)	58,89,113	1.87	8 (13%)
20	CLA	1	314	1	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
20	CLA	A	804	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
20	CLA	4	304	-	54,58,73	1.72	15 (27%)	64,95,113	3.32	20 (31%)

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
24	LHG	A	843	-	-	7/53/53/53	-
20	CLA	A	851	-	1/1/15/20	11/39/115/115	-
28	SF4	A	850	-	-	-	0/6/5/5
20	CLA	3	312	-	1/1/11/20	5/15/91/115	-
20	CLA	2	313	-	1/1/10/20	4/13/89/115	-
21	LUT	1	319	-	-	2/29/67/67	0/2/2/2
20	CLA	2	312	2	1/1/15/20	8/39/115/115	-
20	CLA	A	830	-	1/1/12/20	2/21/97/115	-
20	CLA	B	838	-	1/1/15/20	7/39/115/115	-
20	CLA	1	311	1	1/1/12/20	7/24/100/115	-
20	CLA	A	809	-	1/1/15/20	12/39/115/115	-
20	CLA	B	817	-	1/1/15/20	14/39/115/115	-
20	CLA	B	824	-	1/1/15/20	14/39/115/115	-
20	CLA	A	806	-	1/1/15/20	9/39/115/115	-
20	CLA	B	828	-	1/1/15/20	11/39/115/115	-
21	LUT	2	315	-	-	1/29/67/67	0/2/2/2
20	CLA	B	809	6	1/1/15/20	4/39/115/115	-
19	CHL	4	315	-	3/3/15/26	4/12/110/137	-
20	CLA	A	812	-	1/1/15/20	12/39/115/115	-
20	CLA	B	802	-	1/1/15/20	5/39/115/115	-
20	CLA	K	201	15	1/1/11/20	2/17/93/115	-
20	CLA	A	836	-	1/1/12/20	5/23/99/115	-
19	CHL	4	305	-	3/3/17/26	5/24/122/137	-
20	CLA	L	302	16	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	314	-	1/1/11/20	3/17/93/115	-
26	HTG	4	320	-	-	2/10/30/30	0/1/1/1
20	CLA	F	805	-	1/1/11/20	8/17/93/115	-
20	CLA	3	308	3	1/1/12/20	1/21/97/115	-
20	CLA	O	203	-	1/1/14/20	7/33/109/115	-
20	CLA	2	308	2	1/1/12/20	4/21/97/115	-
20	CLA	B	839	-	1/1/15/20	8/39/115/115	-
21	LUT	O	205	-	-	6/29/67/67	0/2/2/2
19	CHL	2	307	-	3/3/17/26	9/21/119/137	-
20	CLA	3	311	3	1/1/13/20	3/27/103/115	-
20	CLA	1	307	-	1/1/14/20	13/35/111/115	-
23	BCR	B	841	-	-	3/29/63/63	0/2/2/2
20	CLA	N	203	-	1/1/12/20	9/21/97/115	-
20	CLA	L	307	-	1/1/11/20	9/15/91/115	-
23	BCR	4	318	-	-	6/29/63/63	0/2/2/2
23	BCR	K	204	-	-	5/29/63/63	0/2/2/2
20	CLA	1	312	1	1/1/15/20	11/39/115/115	-
20	CLA	A	835	5	1/1/11/20	8/15/91/115	-
20	CLA	A	833	-	1/1/15/20	9/39/115/115	-
20	CLA	B	820	-	1/1/12/20	0/21/97/115	-
26	HTG	N	201	-	-	2/10/30/30	0/1/1/1
23	BCR	L	301	-	-	4/29/63/63	0/2/2/2
20	CLA	1	302	1	1/1/15/20	9/39/115/115	-
20	CLA	B	832	-	1/1/13/20	3/31/107/115	-
25	LMG	4	319	-	-	6/39/59/70	0/1/1/1
22	XAT	2	316	-	-	1/31/93/93	0/4/4/4
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	CLA	A	803	20	1/1/13/20	4/27/103/115	-
27	PQN	B	840	-	-	1/23/43/43	0/2/2/2
20	CLA	A	824	-	1/1/15/20	9/39/115/115	-
19	CHL	4	306	-	3/3/17/26	10/21/119/137	-
20	CLA	B	833	-	1/1/15/20	11/39/115/115	-
20	CLA	A	831	-	1/1/15/20	18/39/115/115	-
20	CLA	B	813	-	1/1/15/20	12/39/115/115	-
22	XAT	1	316	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	301	4	1/1/11/20	7/17/93/115	-
20	CLA	A	853	-	1/1/15/20	16/39/115/115	-
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
23	BCR	A	845	-	-	6/29/63/63	0/2/2/2
20	CLA	B	814	-	1/1/15/20	3/39/115/115	-
20	CLA	A	807	5	1/1/15/20	11/39/115/115	-
20	CLA	B	834	-	1/1/11/20	0/15/91/115	-
26	HTG	1	322	-	-	0/10/30/30	0/1/1/1
20	CLA	A	822	-	1/1/12/20	8/23/99/115	-
20	CLA	3	302	-	1/1/12/20	6/21/97/115	-
20	CLA	K	202	-	1/1/14/20	8/33/109/115	-
20	CLA	F	804	-	1/1/11/20	4/15/91/115	-
20	CLA	A	810	20	1/1/15/20	18/39/115/115	-
20	CLA	A	821	-	1/1/11/20	9/20/96/115	-
20	CLA	3	305	3	1/1/11/20	8/18/94/115	-
20	CLA	B	808	-	1/1/15/20	7/39/115/115	-
20	CLA	A	801	-	1/1/15/20	11/39/115/115	-
20	CLA	N	202	17	1/1/11/20	3/15/91/115	-
20	CLA	A	825	-	1/1/15/20	3/39/115/115	-
20	CLA	A	813	-	1/1/11/20	2/15/91/115	-
20	CLA	2	310	24	1/1/10/20	2/10/86/115	-
20	CLA	A	814	-	1/1/12/20	5/21/97/115	-
29	LMT	G	601	-	-	4/21/61/61	0/2/2/2
23	BCR	B	842	-	-	6/29/63/63	0/2/2/2
20	CLA	4	312	-	1/1/15/20	14/39/115/115	-
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
26	HTG	A	852	-	-	2/10/30/30	0/1/1/1
20	CLA	1	321	-	1/1/15/20	6/39/115/115	-
20	CLA	A	811	-	1/1/12/20	5/26/102/115	-
26	HTG	J	105	-	-	0/10/30/30	0/1/1/1
20	CLA	B	831	-	1/1/15/20	13/39/115/115	-
19	CHL	2	301	2	3/3/17/26	7/24/122/137	-
20	CLA	4	313	-	1/1/11/20	1/15/91/115	-
23	BCR	A	847	-	-	2/29/63/63	0/2/2/2
20	CLA	3	301	3	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	HTG	B	850	-	-	7/10/30/30	0/1/1/1
23	BCR	J	102	-	-	7/29/63/63	0/2/2/2
20	CLA	2	309	2	1/1/14/20	5/33/109/115	-
25	LMG	1	323	-	-	10/39/59/70	0/1/1/1
20	CLA	B	830	-	1/1/12/20	5/21/97/115	-
20	CLA	1	313	-	1/1/13/20	12/27/103/115	-
20	CLA	2	303	-	1/1/11/20	8/20/96/115	-
20	CLA	4	314	-	1/1/12/20	8/21/97/115	-
20	CLA	K	203	-	1/1/11/20	6/17/93/115	-
20	CLA	3	303	-	1/1/11/20	3/15/91/115	-
20	CLA	B	815	-	1/1/14/20	11/33/109/115	-
20	CLA	G	604	-	1/1/12/20	5/21/97/115	-
28	SF4	C	101	-	-	-	0/6/5/5
20	CLA	4	308	4	1/1/12/20	6/21/97/115	-
20	CLA	A	805	-	1/1/15/20	15/39/115/115	-
19	CHL	4	307	-	3/3/17/26	3/21/119/137	-
23	BCR	2	317	-	-	0/29/63/63	0/2/2/2
20	CLA	B	811	-	1/1/13/20	8/25/101/115	-
20	CLA	B	810	-	1/1/15/20	10/39/115/115	-
23	BCR	L	305	-	-	4/29/63/63	0/2/2/2
20	CLA	H	201	-	1/1/13/20	11/29/105/115	-
20	CLA	4	303	-	1/1/14/20	8/33/109/115	-
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
20	CLA	B	805	-	1/1/15/20	14/39/115/115	-
20	CLA	B	826	-	1/1/15/20	2/39/115/115	-
23	BCR	B	843	-	-	4/29/63/63	0/2/2/2
20	CLA	J	103	14	1/1/10/20	4/12/88/115	-
20	CLA	1	304	-	1/1/12/20	5/24/100/115	-
24	LHG	B	849	-	-	7/26/26/53	-
20	CLA	B	835	-	1/1/12/20	2/23/99/115	-
22	XAT	4	317	-	-	0/31/93/93	0/4/4/4
20	CLA	A	826	-	1/1/15/20	5/39/115/115	-
20	CLA	G	605	11	1/1/11/20	5/17/93/115	-
27	PQN	A	842	-	-	7/23/43/43	0/2/2/2
20	CLA	2	311	2	1/1/12/20	7/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	HTG	G	602	-	-	0/10/30/30	0/1/1/1
24	LHG	1	318	20	-	12/53/53/53	-
20	CLA	A	817	-	1/1/15/20	16/39/115/115	-
20	CLA	3	304	-	1/1/10/20	1/12/88/115	-
22	XAT	3	316	-	-	0/31/93/93	0/4/4/4
25	LMG	1	320	-	-	9/44/64/70	0/1/1/1
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
20	CLA	B	816	-	1/1/13/20	6/27/103/115	-
20	CLA	B	823	-	1/1/14/20	11/33/109/115	-
20	CLA	A	832	-	1/1/15/20	8/39/115/115	-
20	CLA	1	303	-	1/1/15/20	10/39/115/115	-
20	CLA	B	829	-	1/1/15/20	4/39/115/115	-
26	HTG	B	851	-	-	2/10/30/30	0/1/1/1
20	CLA	G	603	-	1/1/11/20	4/15/91/115	-
20	CLA	A	838	-	1/1/15/20	10/39/115/115	-
20	CLA	F	802	-	1/1/15/20	7/39/115/115	-
20	CLA	A	834	-	1/1/15/20	9/39/115/115	-
20	CLA	L	303	-	1/1/15/20	10/39/115/115	-
20	CLA	A	802	-	1/1/15/20	13/39/115/115	-
20	CLA	A	818	-	1/1/15/20	7/39/115/115	-
19	CHL	2	306	-	3/3/16/26	11/18/116/137	-
20	CLA	3	313	-	1/1/11/20	2/15/91/115	-
20	CLA	A	808	5	1/1/15/20	17/39/115/115	-
20	CLA	A	827	-	1/1/15/20	11/39/115/115	-
20	CLA	A	819	-	1/1/11/20	2/15/91/115	-
20	CLA	4	302	4	1/1/14/20	9/33/109/115	-
23	BCR	1	317	-	-	2/29/63/63	0/2/2/2
20	CLA	A	839	-	1/1/15/20	14/39/115/115	-
20	CLA	K	205	15	1/1/11/20	2/15/91/115	-
23	BCR	F	801	-	-	3/29/63/63	0/2/2/2
24	LHG	2	318	20	-	11/41/41/53	-
20	CLA	3	310	-	1/1/12/20	2/24/100/115	-
26	HTG	F	803	-	-	2/10/30/30	0/1/1/1
28	SF4	C	102	-	-	-	0/6/5/5
20	CLA	4	309	4	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	O	201	24	1/1/12/20	10/24/100/115	-
20	CLA	2	304	-	1/1/14/20	12/33/109/115	-
20	CLA	B	827	-	1/1/15/20	12/39/115/115	-
19	CHL	2	305	-	3/3/15/26	6/12/110/137	-
20	CLA	3	309	-	-	4/17/93/115	-
20	CLA	3	307	3	1/1/12/20	5/21/97/115	-
20	CLA	A	820	-	1/1/15/20	9/39/115/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
20	CLA	B	819	-	1/1/15/20	9/39/115/115	-
20	CLA	1	310	24	1/1/10/20	2/10/86/115	-
21	LUT	O	204	-	-	0/29/67/67	0/2/2/2
24	LHG	A	844	20	-	11/31/31/53	-
20	CLA	J	101	-	1/1/15/20	5/39/115/115	-
20	CLA	1	309	1	1/1/14/20	4/33/109/115	-
20	CLA	1	308	1	1/1/15/20	14/39/115/115	-
20	CLA	A	828	-	1/1/15/20	9/39/115/115	-
20	CLA	A	837	-	1/1/15/20	12/39/115/115	-
20	CLA	B	803	-	1/1/15/20	10/39/115/115	-
20	CLA	B	804	-	1/1/11/20	5/15/91/115	-
20	CLA	B	825	-	1/1/15/20	15/39/115/115	-
20	CLA	L	304	-	1/1/12/20	2/21/97/115	-
19	CHL	1	301	1	3/3/17/26	9/23/121/137	-
20	CLA	2	302	2	1/1/15/20	8/39/115/115	-
20	CLA	B	837	-	1/1/11/20	2/18/94/115	-
19	CHL	2	314	2	3/3/15/26	3/12/110/137	-
20	CLA	A	816	-	1/1/15/20	12/39/115/115	-
20	CLA	A	841	-	1/1/15/20	22/39/115/115	-
23	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	B	806	6	1/1/15/20	13/39/115/115	-
23	BCR	J	104	-	-	2/29/63/63	0/2/2/2
23	BCR	L	306	-	-	0/29/63/63	0/2/2/2
21	LUT	3	315	-	-	2/29/67/67	0/2/2/2
20	CLA	B	801	-	1/1/15/20	5/39/115/115	-
23	BCR	F	806	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	836	-	1/1/15/20	6/39/115/115	-
19	CHL	3	306	-	3/3/16/26	5/17/115/137	-
30	DGD	B	848	-	-	10/55/95/95	0/2/2/2
20	CLA	1	305	-	1/1/12/20	3/24/100/115	-
23	BCR	A	854	-	-	0/29/63/63	0/2/2/2
23	BCR	G	606	-	-	0/29/63/63	0/2/2/2
20	CLA	A	829	-	1/1/15/20	9/39/115/115	-
20	CLA	4	311	4	1/1/12/20	5/24/100/115	-
20	CLA	B	821	-	1/1/13/20	11/29/105/115	-
21	LUT	1	315	-	-	2/29/67/67	0/2/2/2
26	HTG	F	807	-	-	2/10/30/30	0/1/1/1
29	LMT	B	847	-	-	6/21/61/61	0/2/2/2
20	CLA	A	815	-	1/1/11/20	2/15/91/115	-
19	CHL	1	306	1	3/3/16/26	10/18/116/137	-
20	CLA	B	818	-	1/1/14/20	10/33/109/115	-
20	CLA	A	823	-	1/1/13/20	4/27/103/115	-
20	CLA	B	812	-	1/1/13/20	8/27/103/115	-
20	CLA	B	807	-	1/1/13/20	7/27/103/115	-
20	CLA	4	310	-	1/1/13/20	7/27/103/115	-
20	CLA	A	840	-	1/1/15/20	7/39/115/115	-
20	CLA	B	822	-	1/1/15/20	12/39/115/115	-
21	LUT	4	316	-	-	1/29/67/67	0/2/2/2
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
20	CLA	O	202	-	1/1/11/20	8/15/91/115	-
20	CLA	1	314	1	1/1/11/20	3/17/93/115	-
20	CLA	A	804	-	1/1/15/20	8/39/115/115	-
20	CLA	4	304	-	1/1/12/20	7/21/97/115	-

The worst 5 of 1534 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	301	CHL	C2C-C3C	11.03	1.47	1.36
19	1	306	CHL	C2C-C3C	10.71	1.46	1.36
19	4	306	CHL	C2C-C3C	10.62	1.46	1.36
19	4	315	CHL	C2C-C3C	10.56	1.46	1.36
19	2	301	CHL	C2C-C3C	10.50	1.46	1.36

The worst 5 of 1683 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	O2D-CGD-CBD	23.29	136.54	110.95
19	2	305	CHL	O2D-CGD-CBD	20.77	133.77	110.95
19	3	306	CHL	O2D-CGD-CBD	15.62	128.11	110.95
23	4	318	BCR	C32-C1-C6	-15.52	85.90	110.24
19	4	307	CHL	O2D-CGD-CBD	15.33	127.79	110.95

5 of 185 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	301	CHL	NC
19	1	301	CHL	ND
19	1	301	CHL	NA
19	1	306	CHL	NC
19	1	306	CHL	ND

5 of 1436 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C2-C3-C5-C6
19	1	301	CHL	C4-C3-C5-C6
19	1	306	CHL	C3A-C2A-CAA-CBA
19	1	306	CHL	C3C-C2C-CMC-OMC
19	1	306	CHL	CBD-CGD-O2D-CED

There are no ring outliers.

186 monomers are involved in 478 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	843	LHG	2	0
20	A	851	CLA	5	0
21	1	319	LUT	4	0
20	2	312	CLA	2	0
20	B	838	CLA	2	0
20	1	311	CLA	1	0
20	A	809	CLA	3	0
20	B	817	CLA	6	0
20	B	824	CLA	7	0
20	A	806	CLA	3	0
20	B	828	CLA	4	0
21	2	315	LUT	2	0
20	B	809	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	315	CHL	5	0
20	A	812	CLA	6	0
20	B	802	CLA	4	0
20	K	201	CLA	2	0
20	A	836	CLA	3	0
19	4	305	CHL	4	0
20	L	302	CLA	3	0
20	3	314	CLA	1	0
20	F	805	CLA	3	0
20	3	308	CLA	2	0
20	O	203	CLA	6	0
20	2	308	CLA	5	0
20	B	839	CLA	2	0
21	O	205	LUT	5	0
19	2	307	CHL	4	0
20	3	311	CLA	4	0
20	1	307	CLA	2	0
23	B	841	BCR	7	0
20	N	203	CLA	2	0
23	4	318	BCR	5	0
23	K	204	BCR	4	0
20	1	312	CLA	4	0
20	A	835	CLA	1	0
20	A	833	CLA	4	0
26	N	201	HTG	1	0
23	L	301	BCR	2	0
20	1	302	CLA	2	0
20	B	832	CLA	4	0
25	4	319	LMG	3	0
22	2	316	XAT	2	0
23	A	848	BCR	4	0
20	A	803	CLA	2	0
27	B	840	PQN	1	0
20	A	824	CLA	3	0
19	4	306	CHL	3	0
20	B	833	CLA	1	0
20	A	831	CLA	5	0
20	B	813	CLA	5	0
22	1	316	XAT	2	0
20	4	301	CLA	3	0
20	A	853	CLA	5	0
23	B	844	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	845	BCR	2	0
20	B	814	CLA	1	0
20	A	807	CLA	3	0
20	B	834	CLA	2	0
26	1	322	HTG	2	0
20	A	822	CLA	3	0
20	K	202	CLA	2	0
20	A	810	CLA	6	0
20	A	821	CLA	3	0
20	B	808	CLA	3	0
20	A	801	CLA	7	0
20	A	825	CLA	6	0
20	2	310	CLA	3	0
20	A	814	CLA	1	0
23	B	842	BCR	1	0
20	4	312	CLA	5	0
23	A	846	BCR	1	0
20	1	321	CLA	4	0
20	A	811	CLA	5	0
20	B	831	CLA	5	0
19	2	301	CHL	8	0
20	4	313	CLA	2	0
23	A	847	BCR	2	0
20	3	301	CLA	1	0
26	B	850	HTG	1	0
23	J	102	BCR	8	0
20	2	309	CLA	2	0
25	1	323	LMG	2	0
20	B	830	CLA	2	0
20	1	313	CLA	4	0
20	4	314	CLA	2	0
20	K	203	CLA	2	0
20	B	815	CLA	1	0
20	4	308	CLA	7	0
20	A	805	CLA	5	0
19	4	307	CHL	1	0
23	2	317	BCR	6	0
20	B	810	CLA	3	0
23	L	305	BCR	4	0
20	H	201	CLA	3	0
20	4	303	CLA	7	0
23	I	101	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	805	CLA	6	0
20	B	826	CLA	1	0
23	B	843	BCR	3	0
20	J	103	CLA	1	0
20	1	304	CLA	1	0
24	B	849	LHG	2	0
20	B	835	CLA	2	0
22	4	317	XAT	7	0
20	A	826	CLA	6	0
27	A	842	PQN	3	0
20	2	311	CLA	2	0
24	1	318	LHG	7	0
20	A	817	CLA	4	0
22	3	316	XAT	4	0
25	1	320	LMG	3	0
23	A	849	BCR	4	0
20	B	816	CLA	1	0
20	B	823	CLA	4	0
20	1	303	CLA	4	0
20	B	829	CLA	1	0
20	A	838	CLA	4	0
20	F	802	CLA	4	0
20	A	834	CLA	3	0
20	L	303	CLA	4	0
20	A	802	CLA	3	0
20	A	818	CLA	4	0
19	2	306	CHL	9	0
20	3	313	CLA	1	0
20	A	808	CLA	5	0
20	A	827	CLA	3	0
20	4	302	CLA	3	0
23	1	317	BCR	4	0
20	A	839	CLA	1	0
20	K	205	CLA	3	0
23	F	801	BCR	4	0
24	2	318	LHG	1	0
20	3	310	CLA	2	0
20	4	309	CLA	2	0
20	O	201	CLA	2	0
20	2	304	CLA	2	0
20	3	309	CLA	7	0
19	2	305	CHL	5	0

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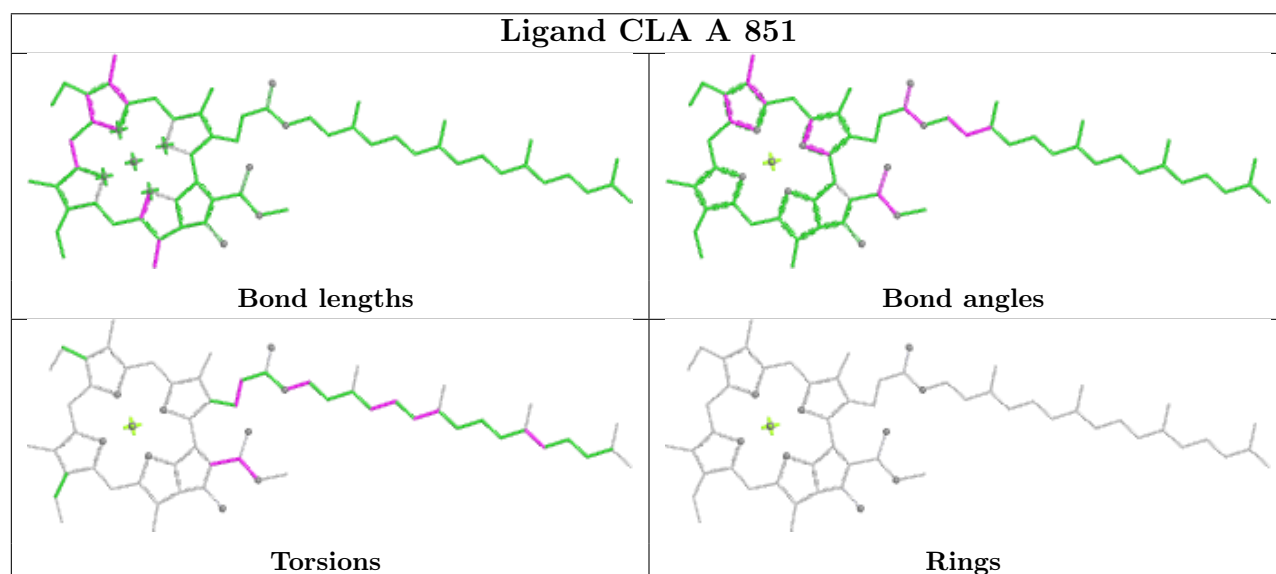
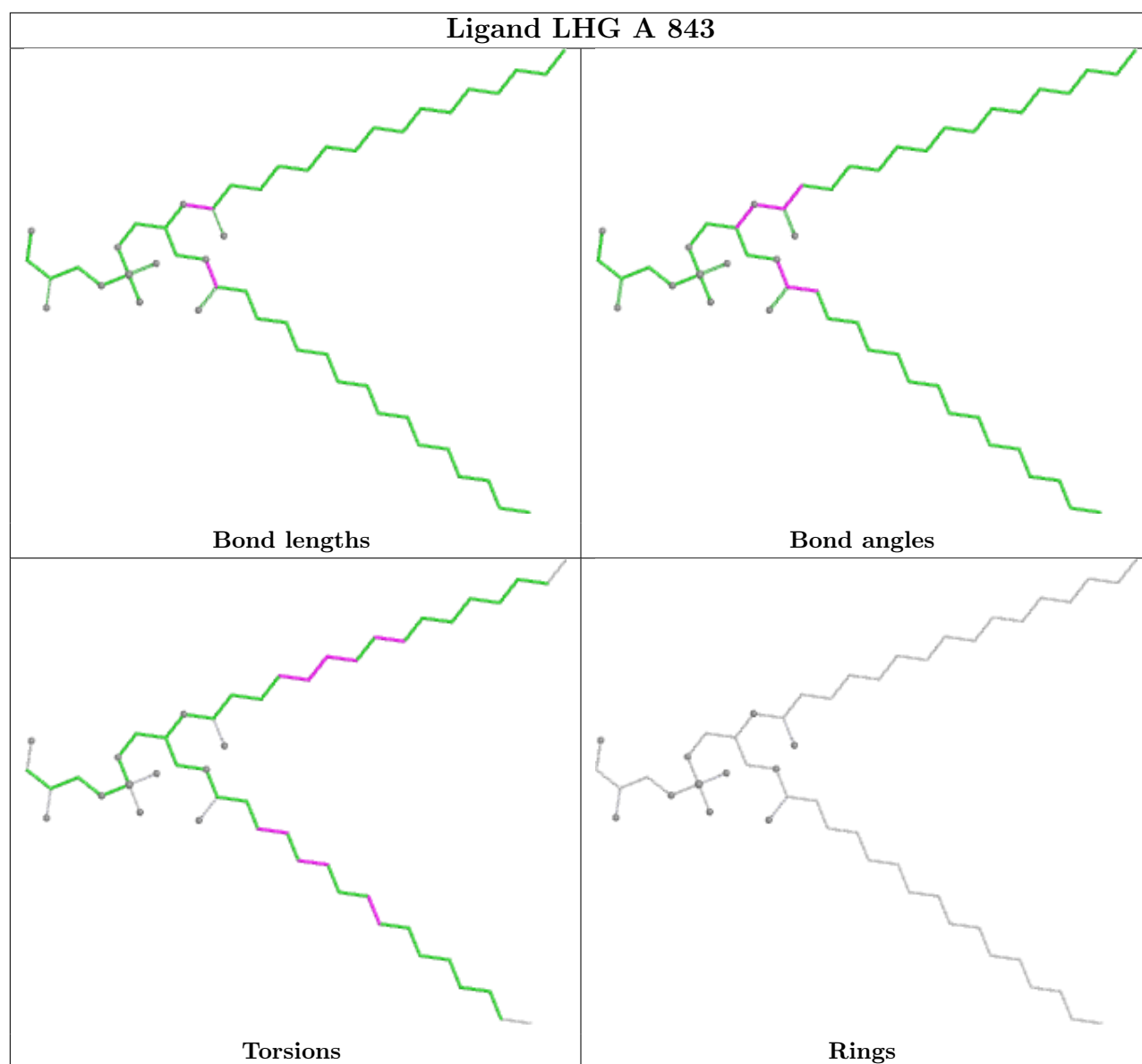
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	827	CLA	4	0
20	3	307	CLA	5	0
20	A	820	CLA	2	0
23	B	845	BCR	6	0
20	B	819	CLA	1	0
21	O	204	LUT	3	0
24	A	844	LHG	1	0
20	J	101	CLA	1	0
20	1	309	CLA	2	0
20	1	308	CLA	4	0
20	A	828	CLA	2	0
20	A	837	CLA	3	0
20	B	803	CLA	4	0
20	B	804	CLA	1	0
20	B	825	CLA	4	0
19	1	301	CHL	2	0
20	2	302	CLA	1	0
19	2	314	CHL	1	0
20	A	816	CLA	2	0
20	A	841	CLA	3	0
23	B	846	BCR	3	0
20	B	806	CLA	2	0
23	J	104	BCR	2	0
23	L	306	BCR	3	0
21	3	315	LUT	4	0
20	B	801	CLA	3	0
23	F	806	BCR	3	0
20	B	836	CLA	1	0
19	3	306	CHL	3	0
30	B	848	DGD	2	0
23	A	854	BCR	6	0
23	G	606	BCR	3	0
20	4	311	CLA	2	0
21	1	315	LUT	4	0
26	F	807	HTG	1	0
19	1	306	CHL	2	0
20	B	818	CLA	3	0
20	A	823	CLA	4	0
20	B	812	CLA	3	0
20	B	807	CLA	2	0
20	A	840	CLA	1	0
20	B	822	CLA	2	0

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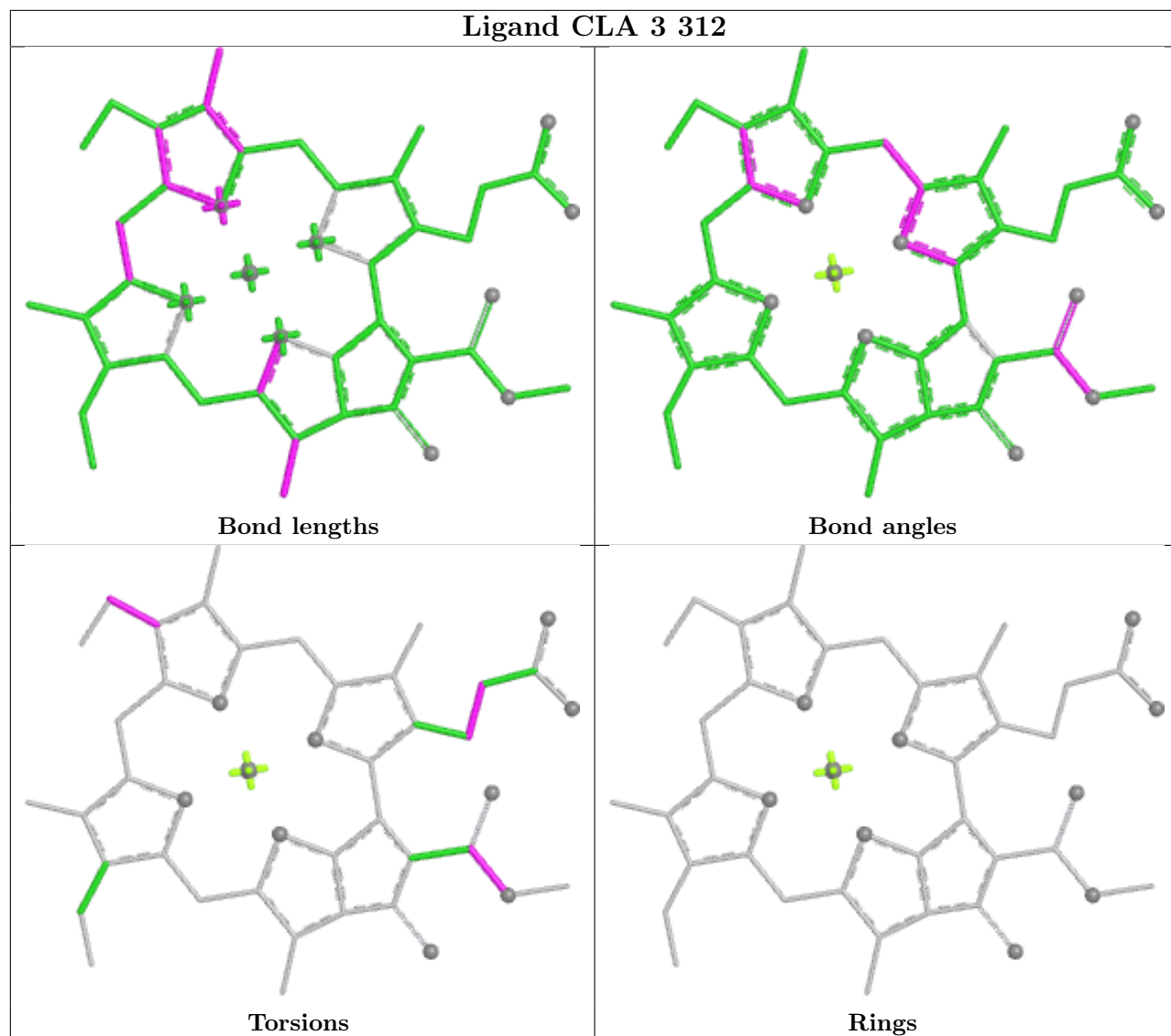
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4	316	LUT	5	0
23	3	317	BCR	3	0
20	O	202	CLA	6	0
20	A	804	CLA	4	0
20	4	304	CLA	2	0

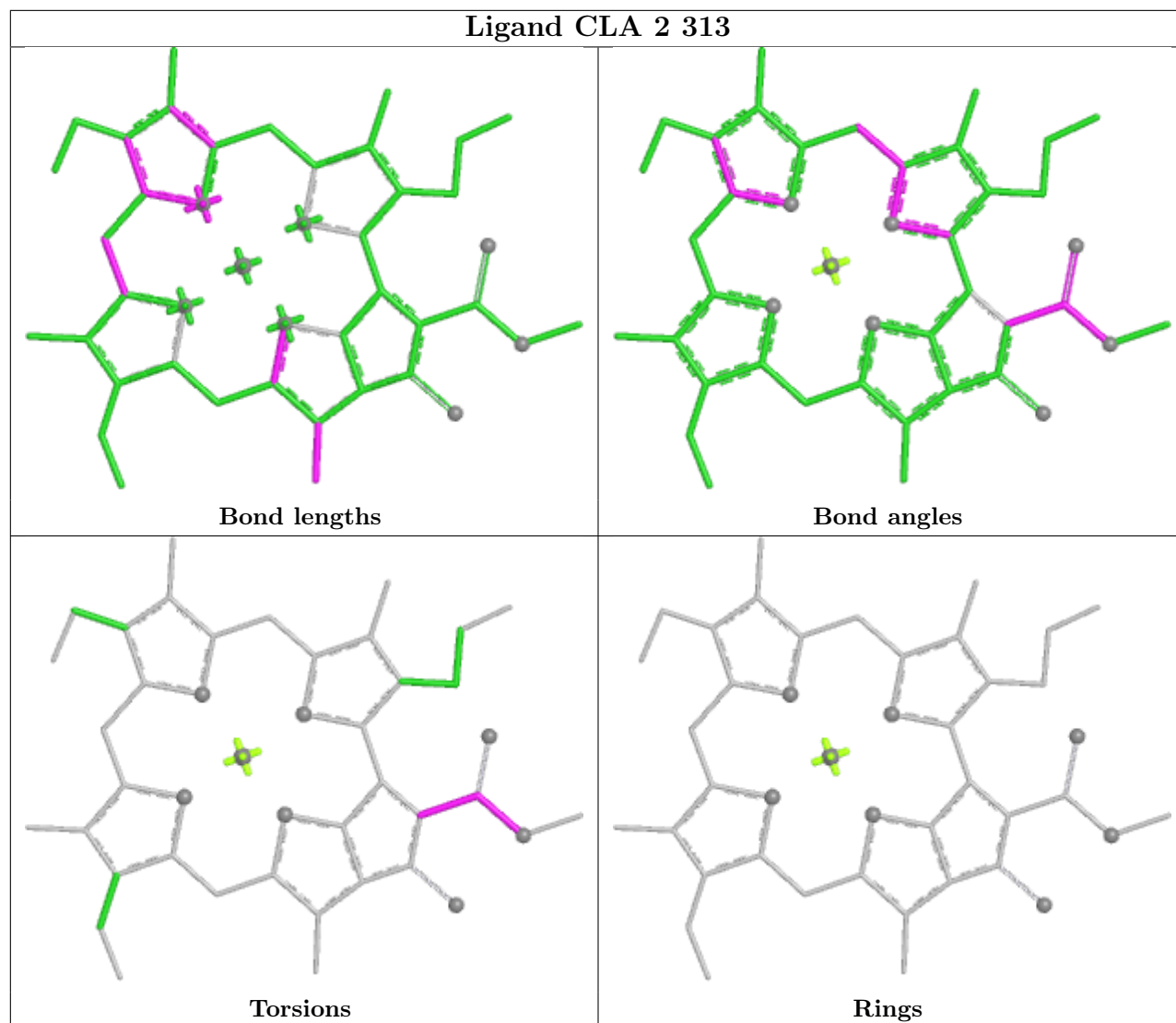
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



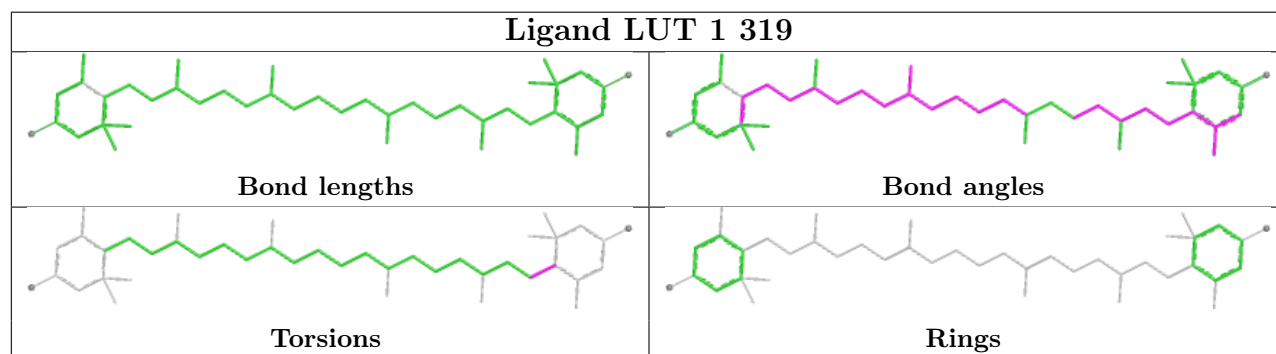
Ligand CLA 3 312



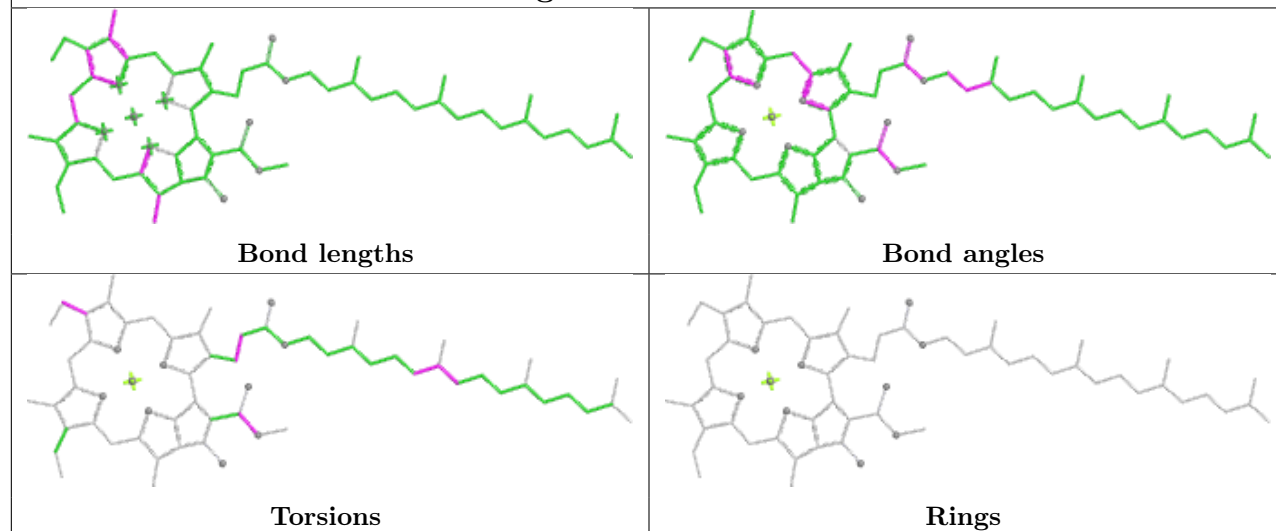
Ligand CLA 2 313



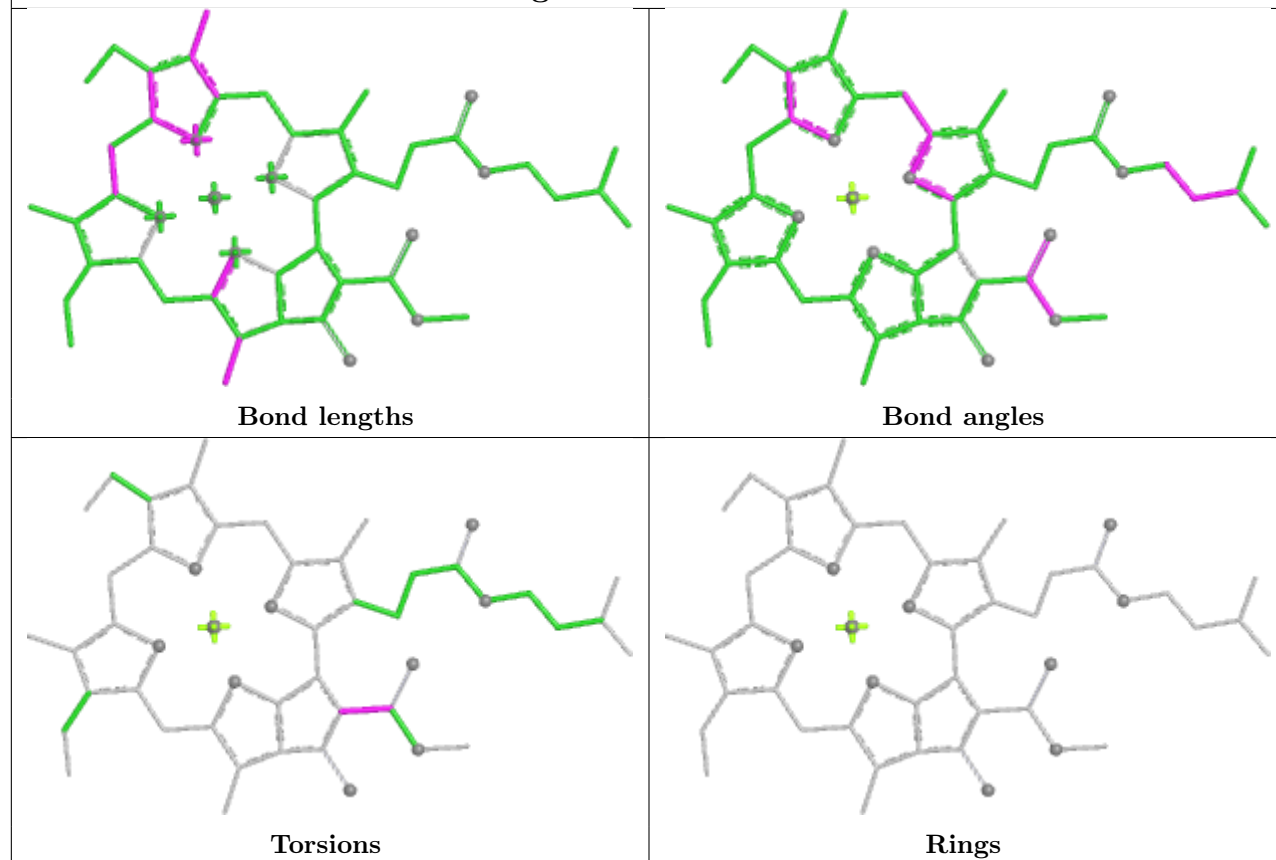
Ligand LUT 1 319

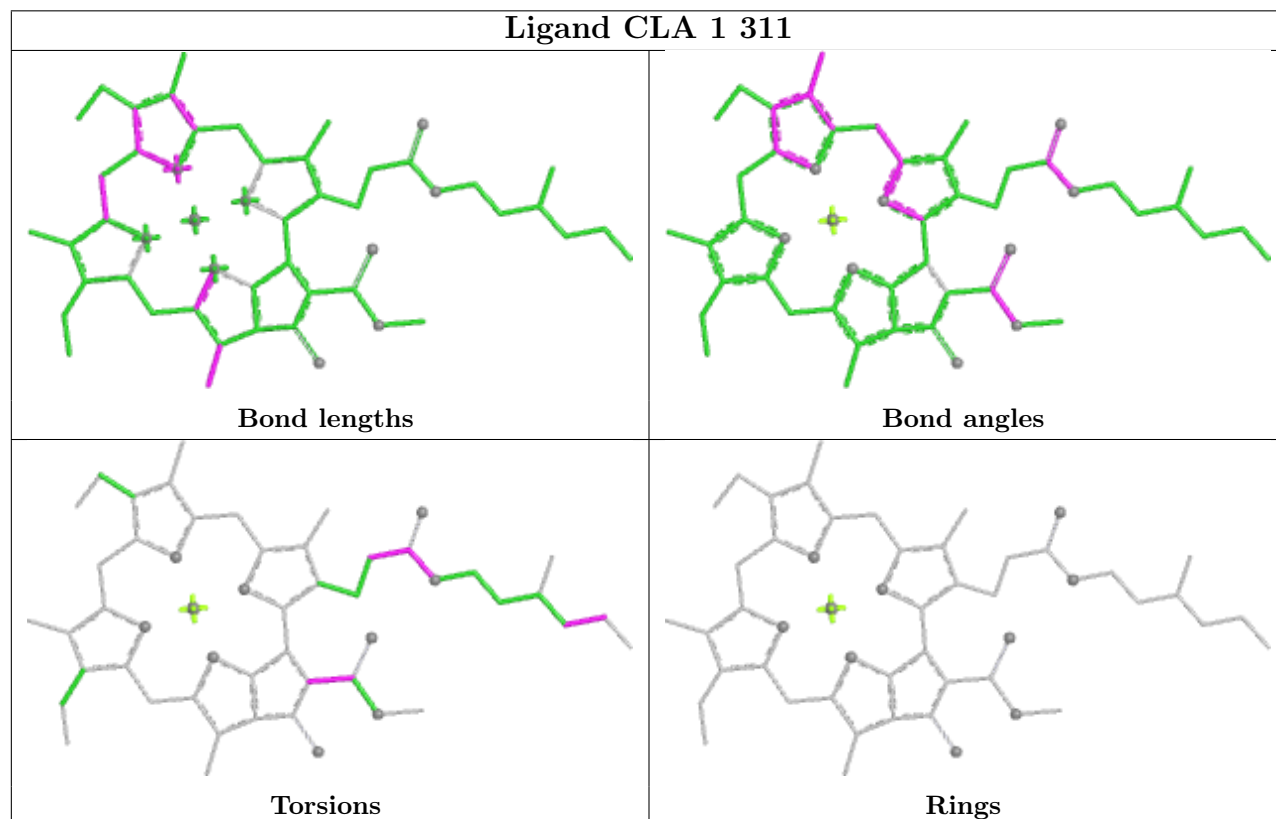
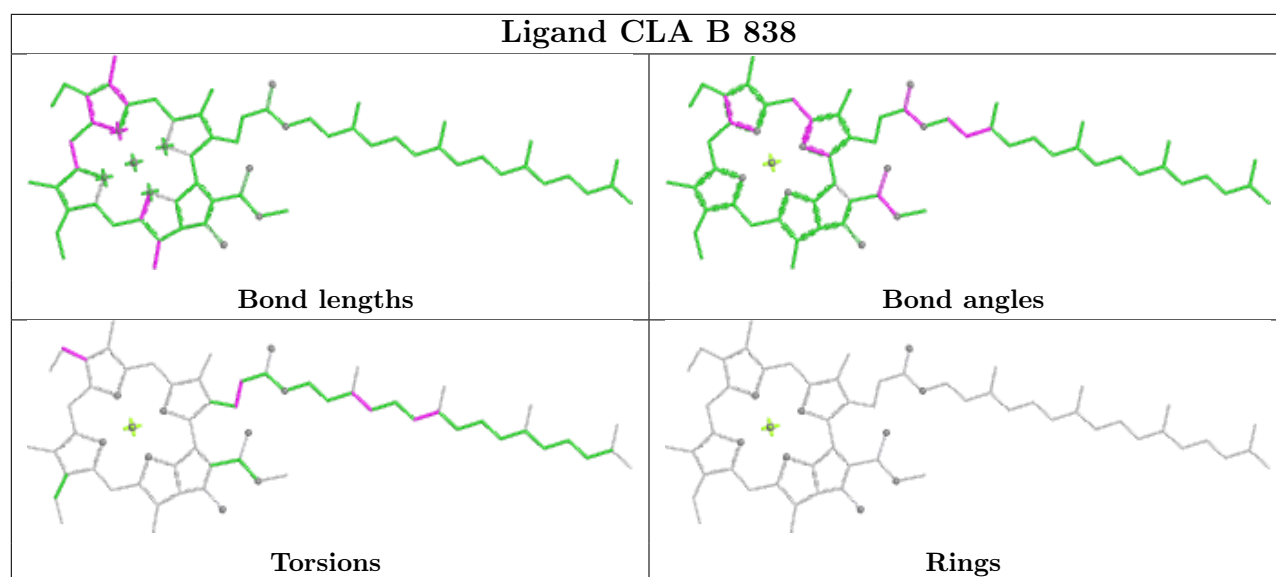


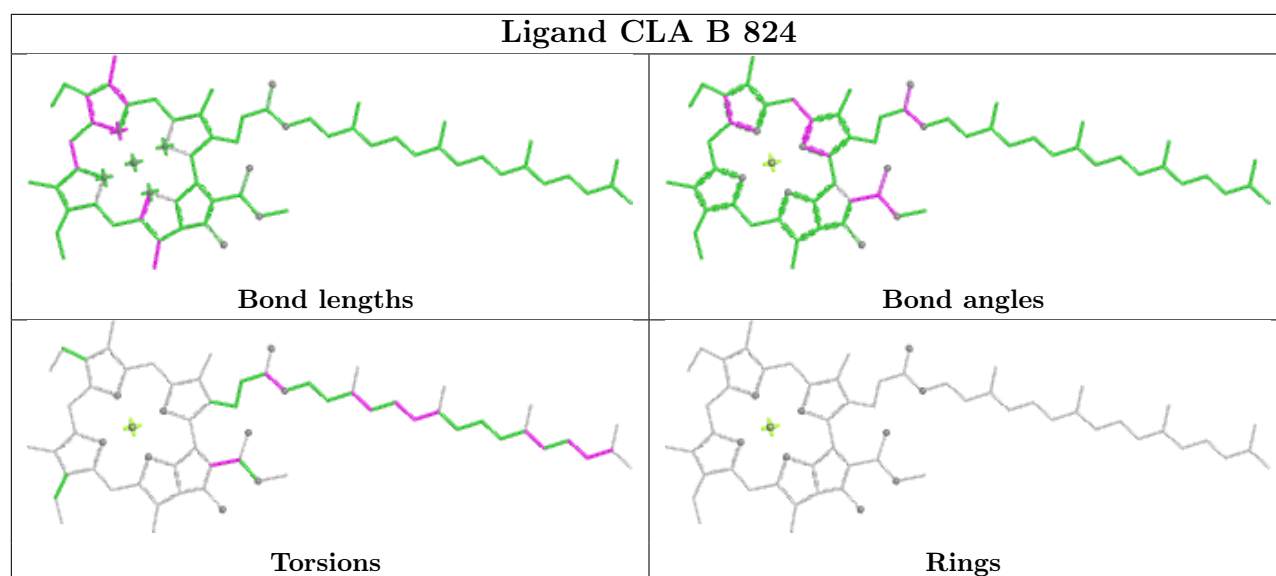
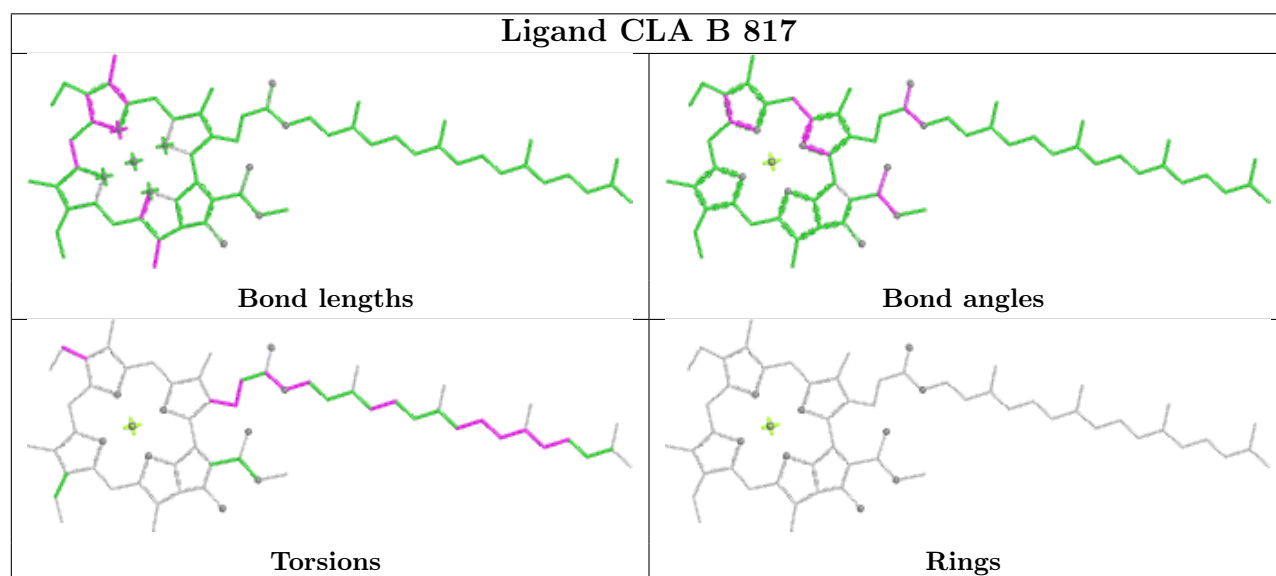
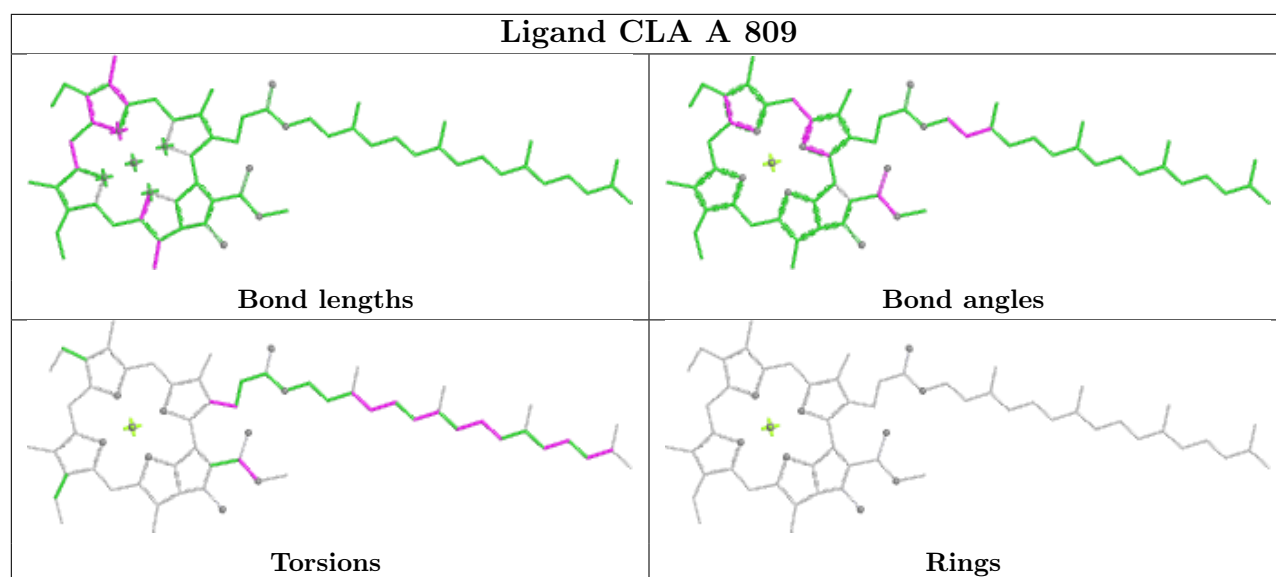
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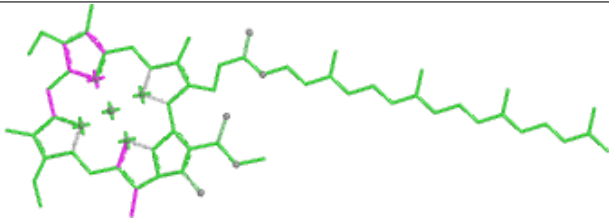
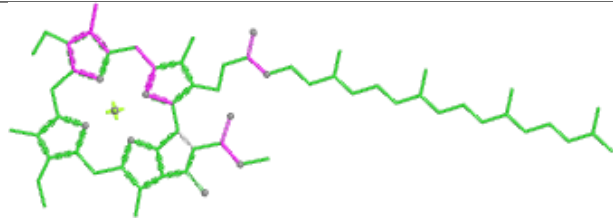
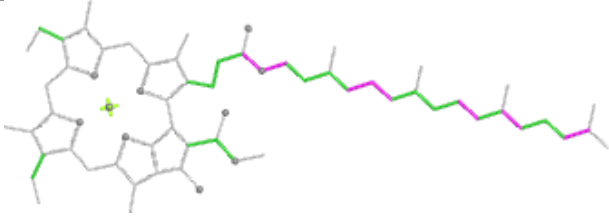
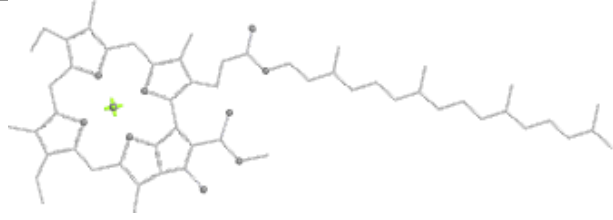
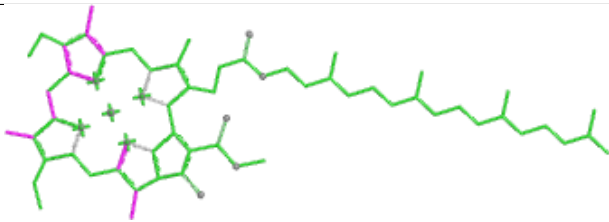
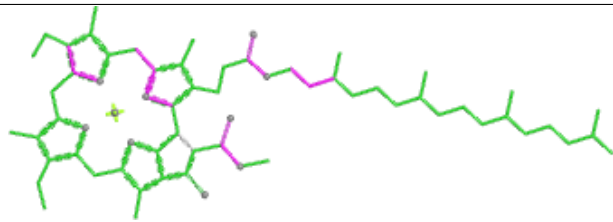
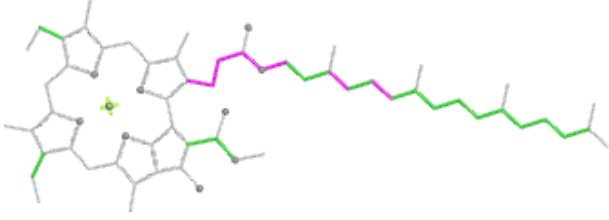
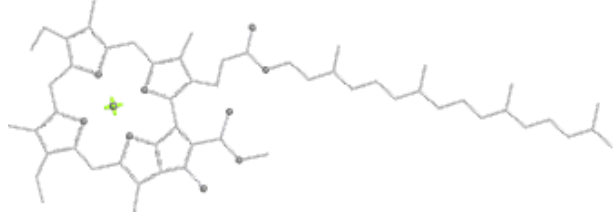
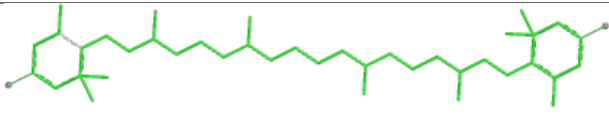
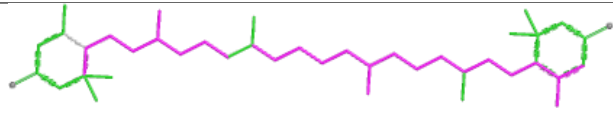
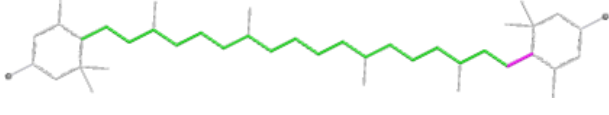
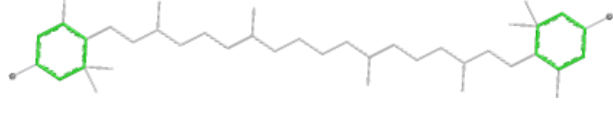


Ligand CLA A 830

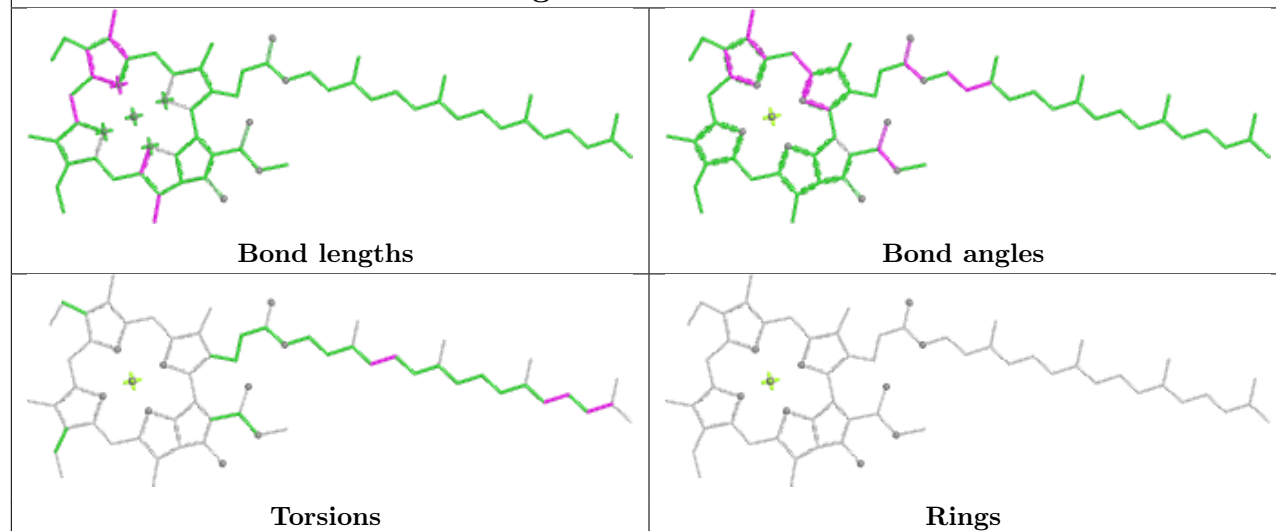




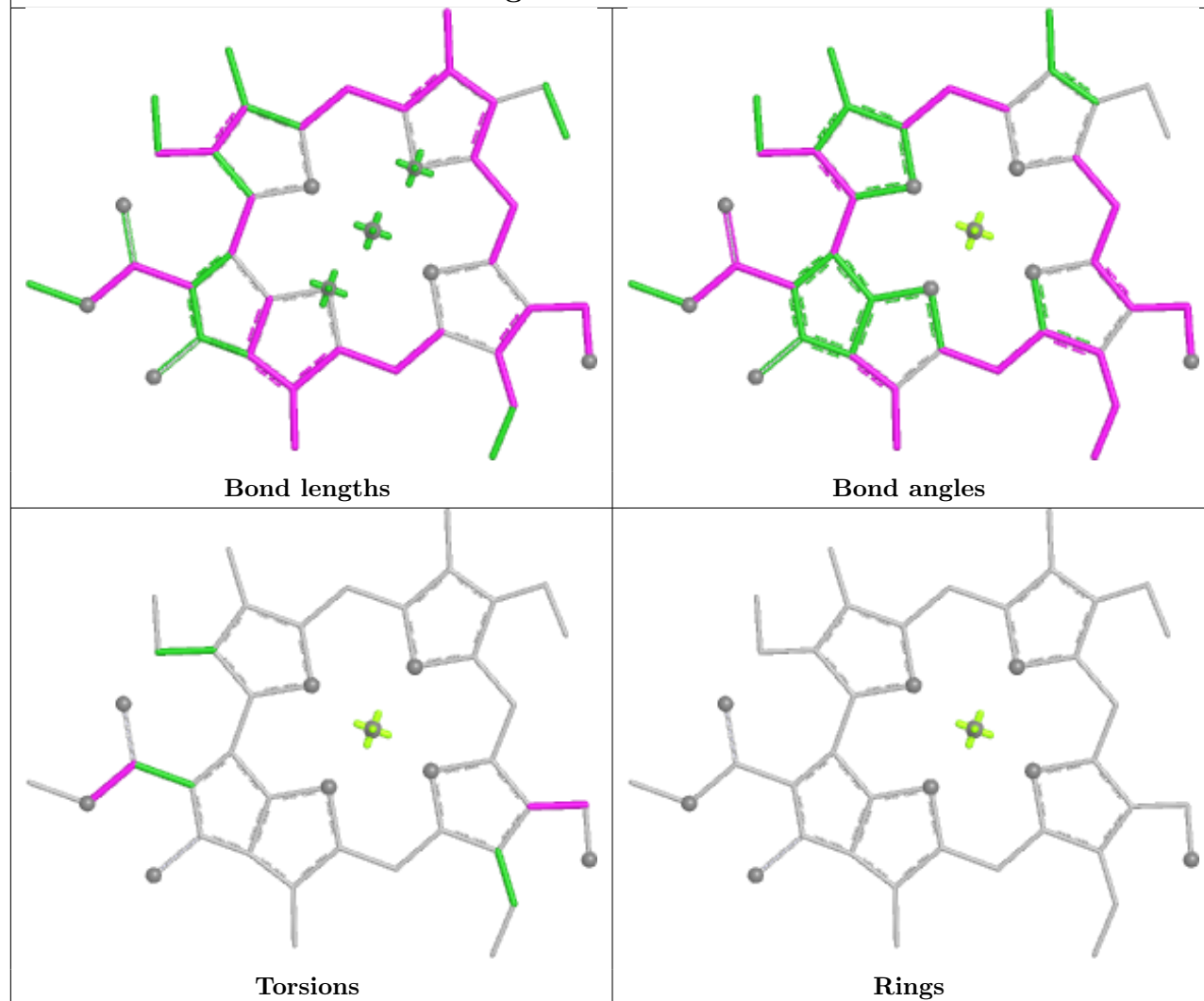


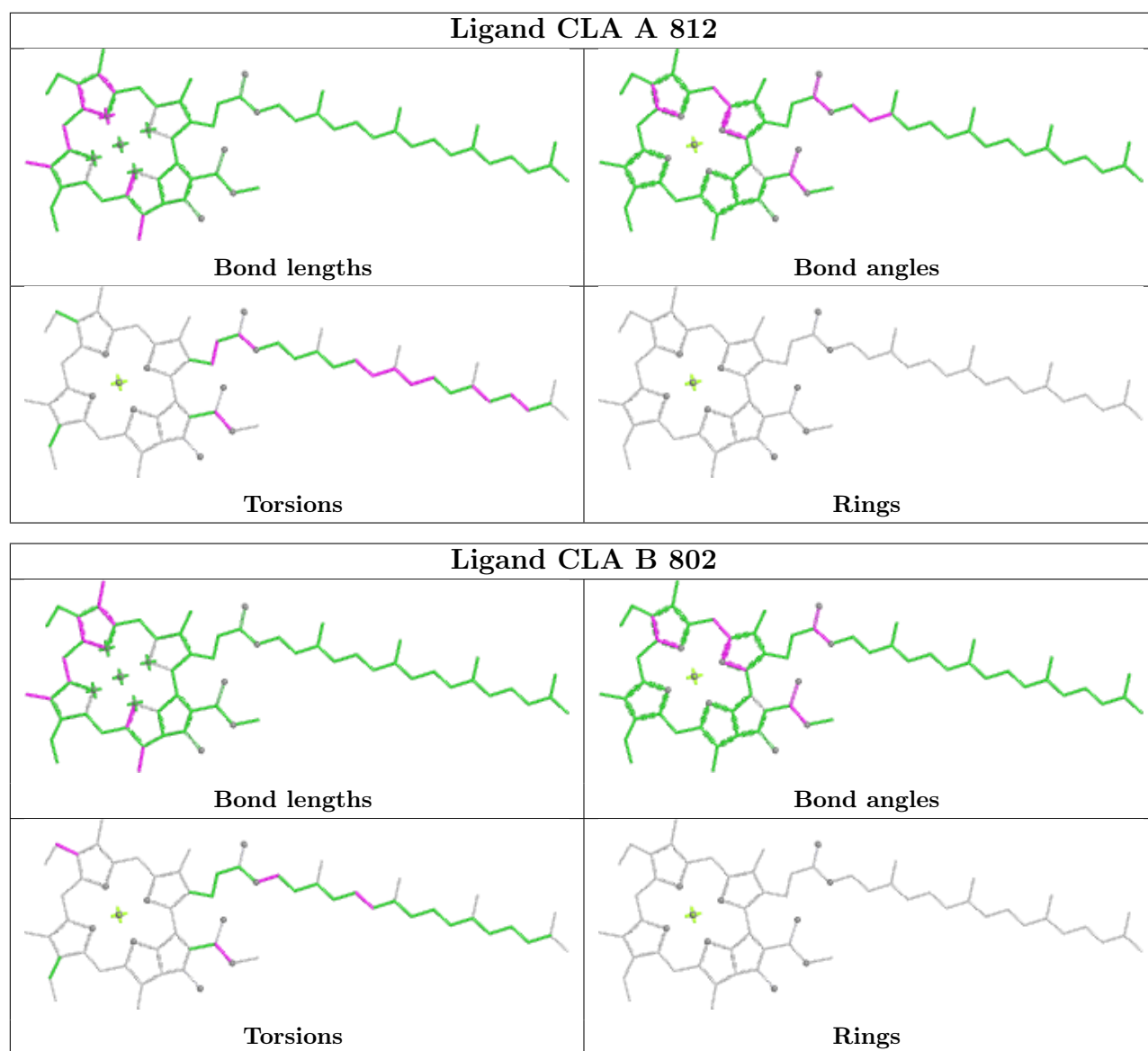
Ligand CLA A 806	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand CLA B 828	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand LUT 2 315	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings

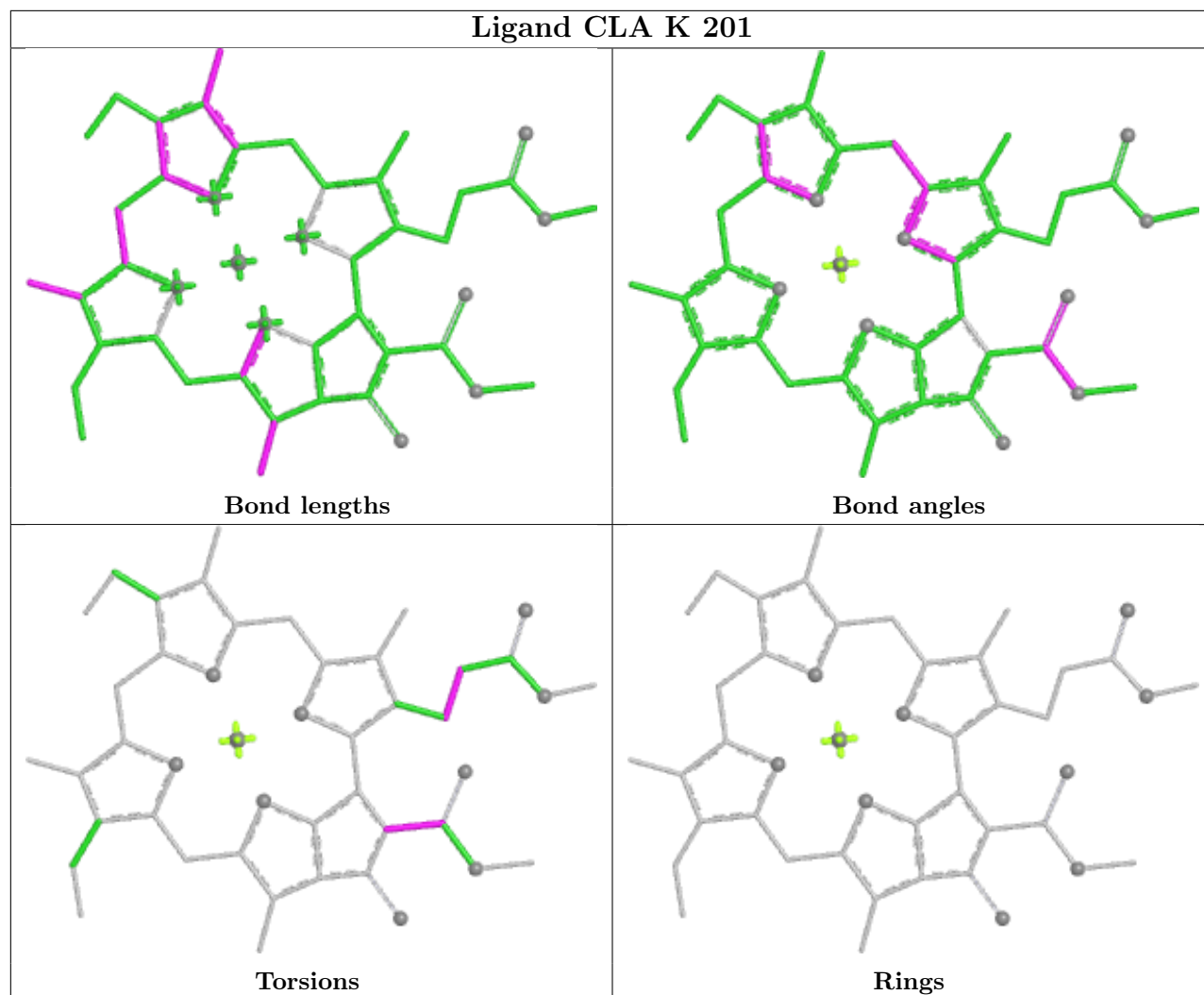
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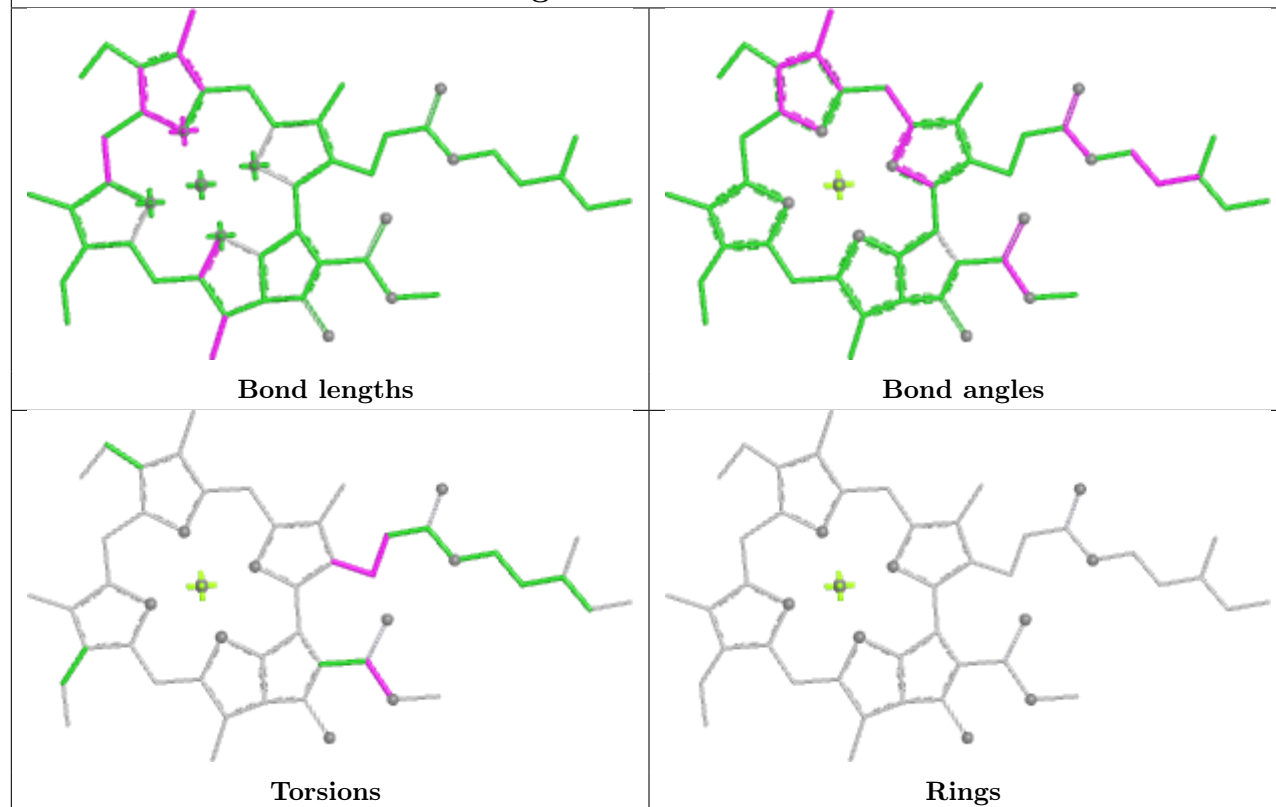
Ligand CHL 4 315



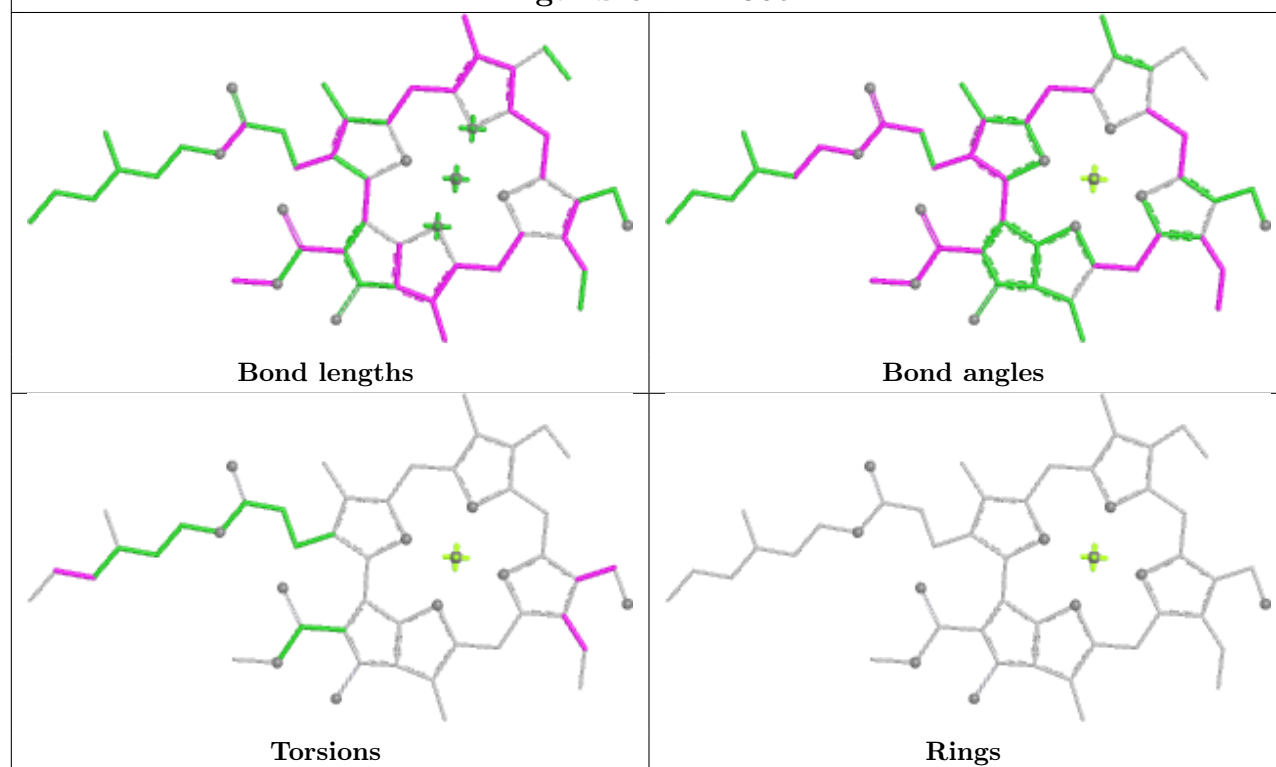


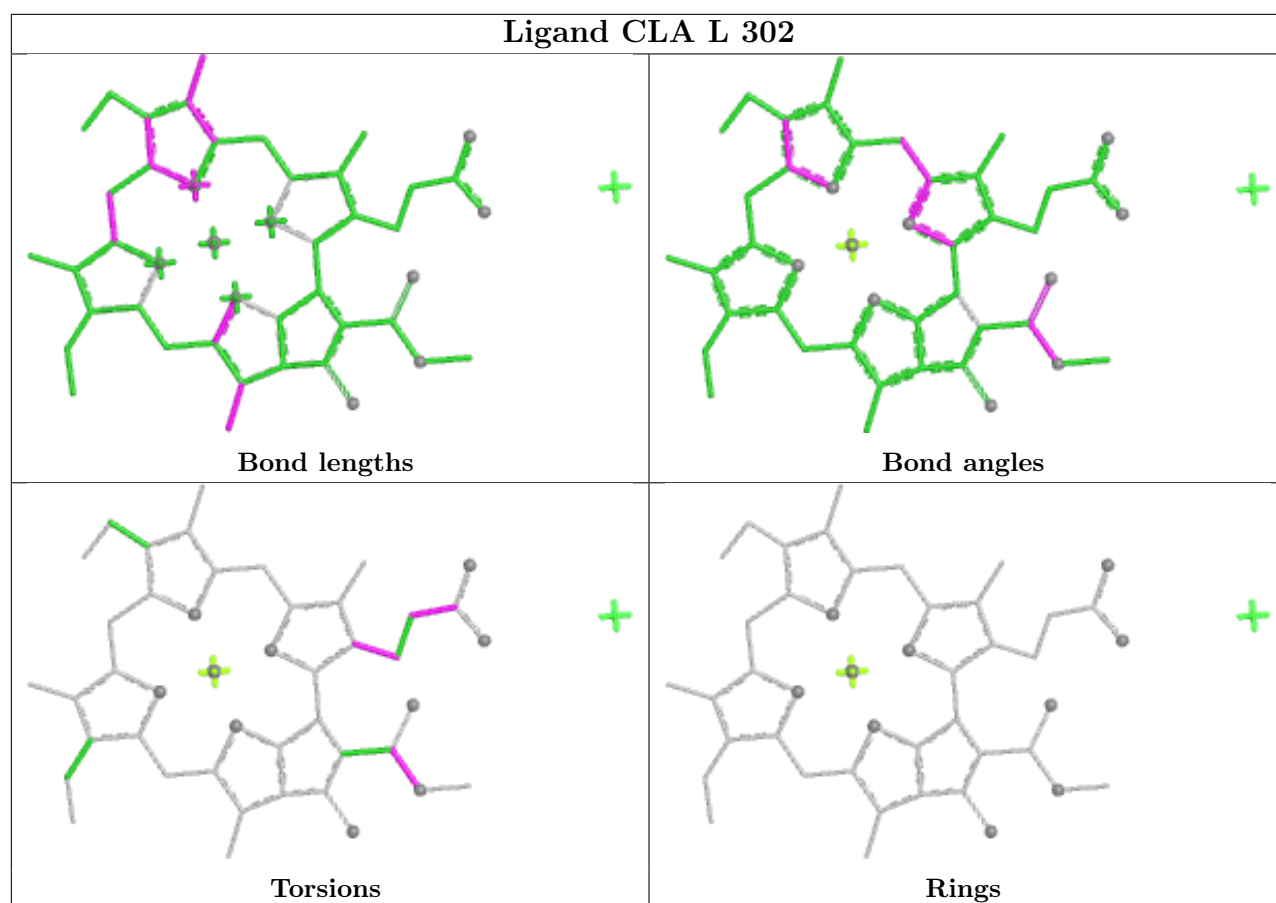


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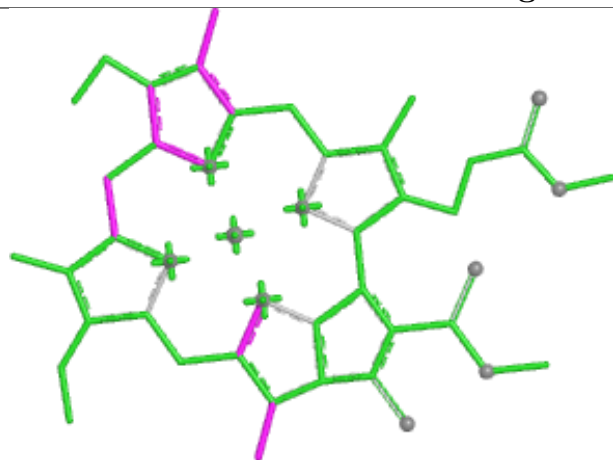


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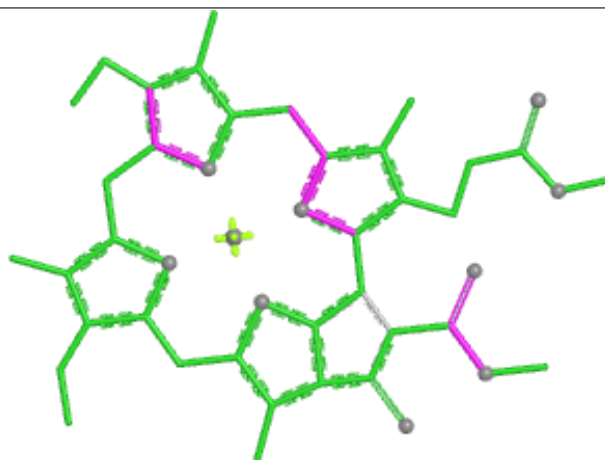




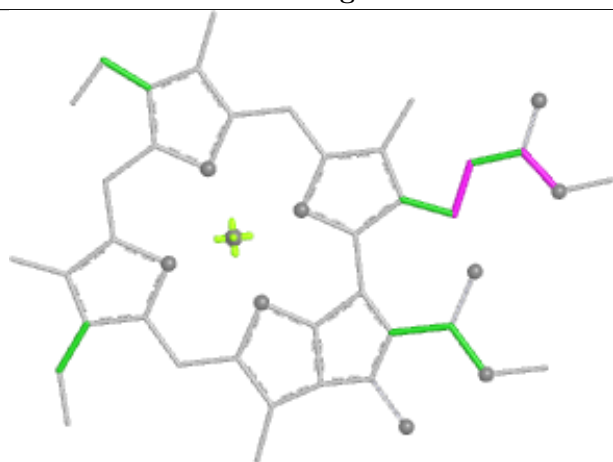
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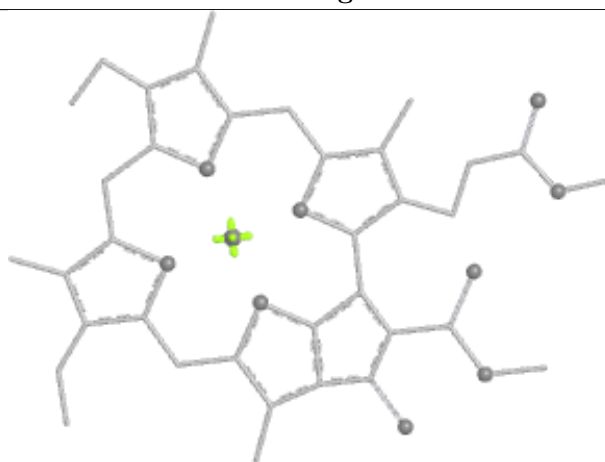
Bond lengths



Bond angles

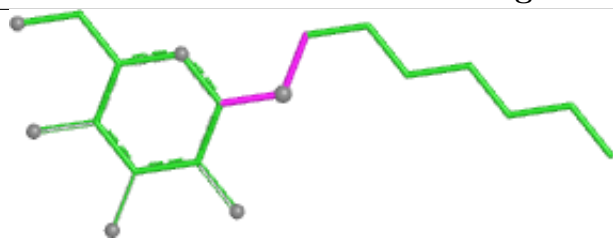


Torsions

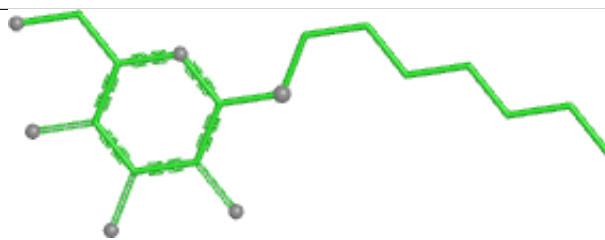


Rings

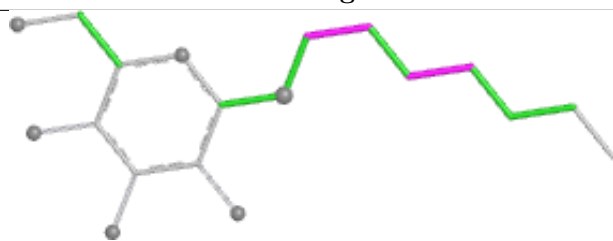
Ligand HTG 4 320



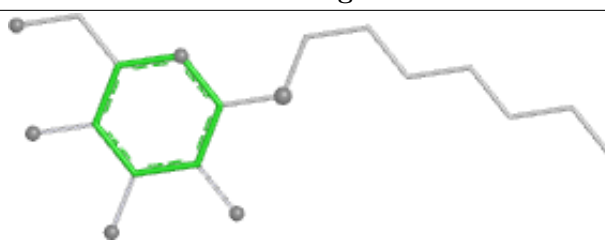
Bond lengths



Bond angles

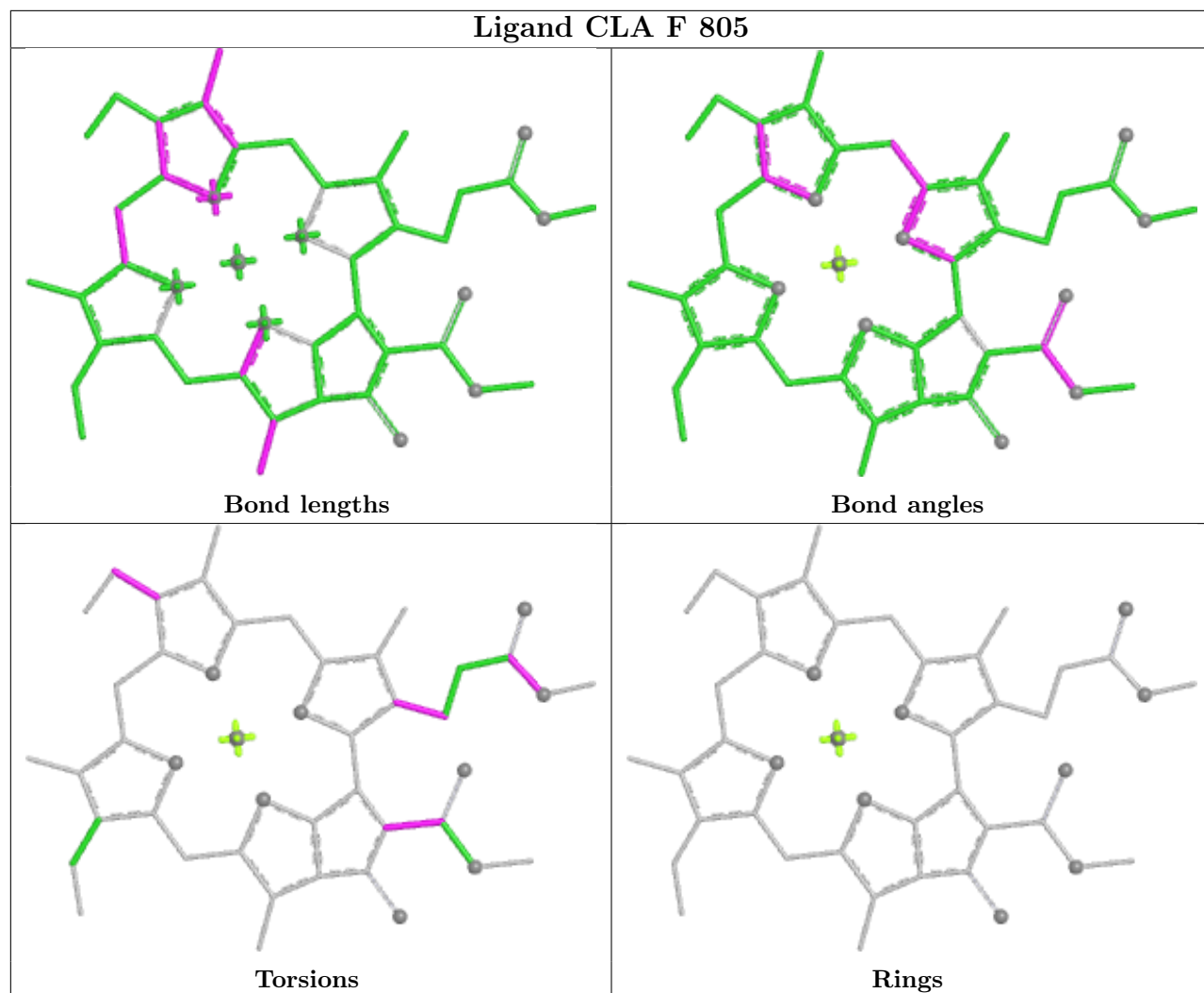


Torsions

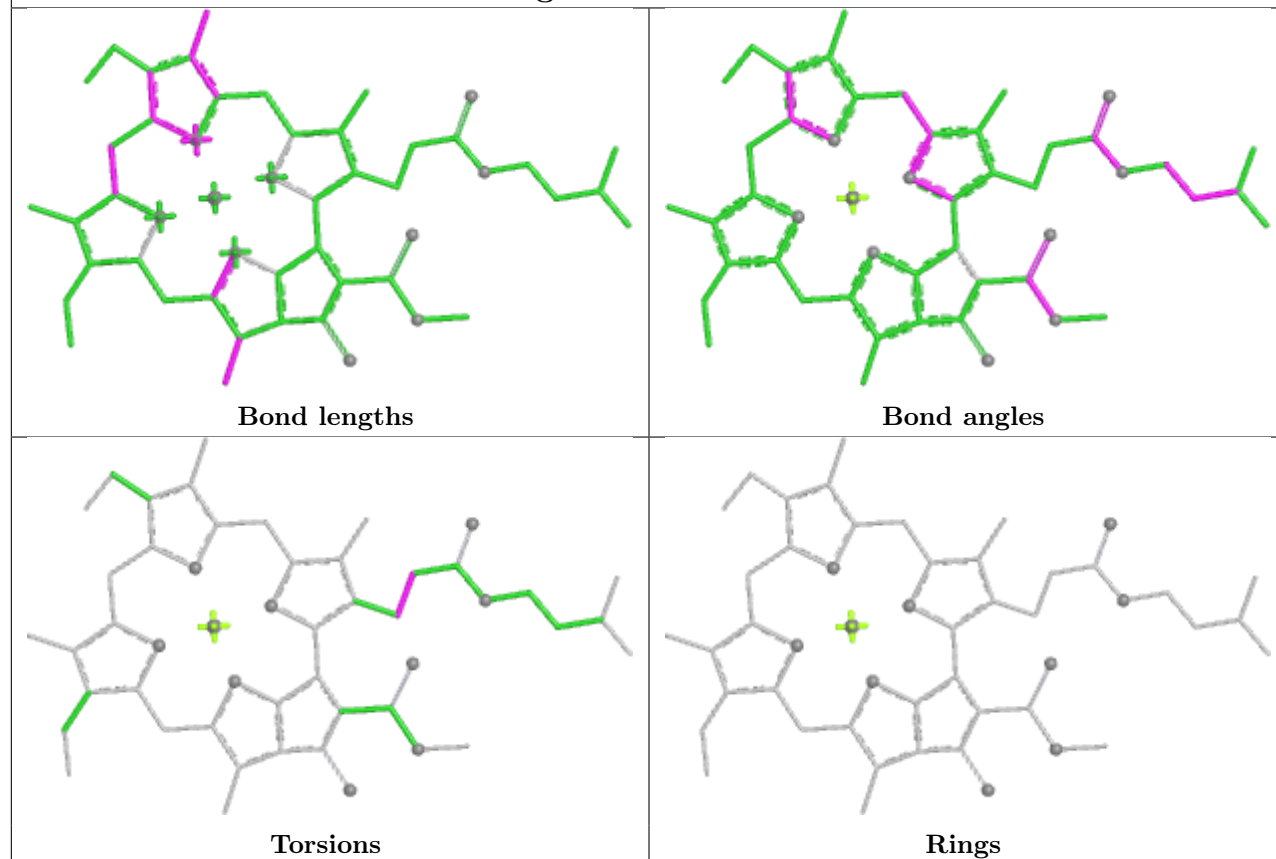


Rings

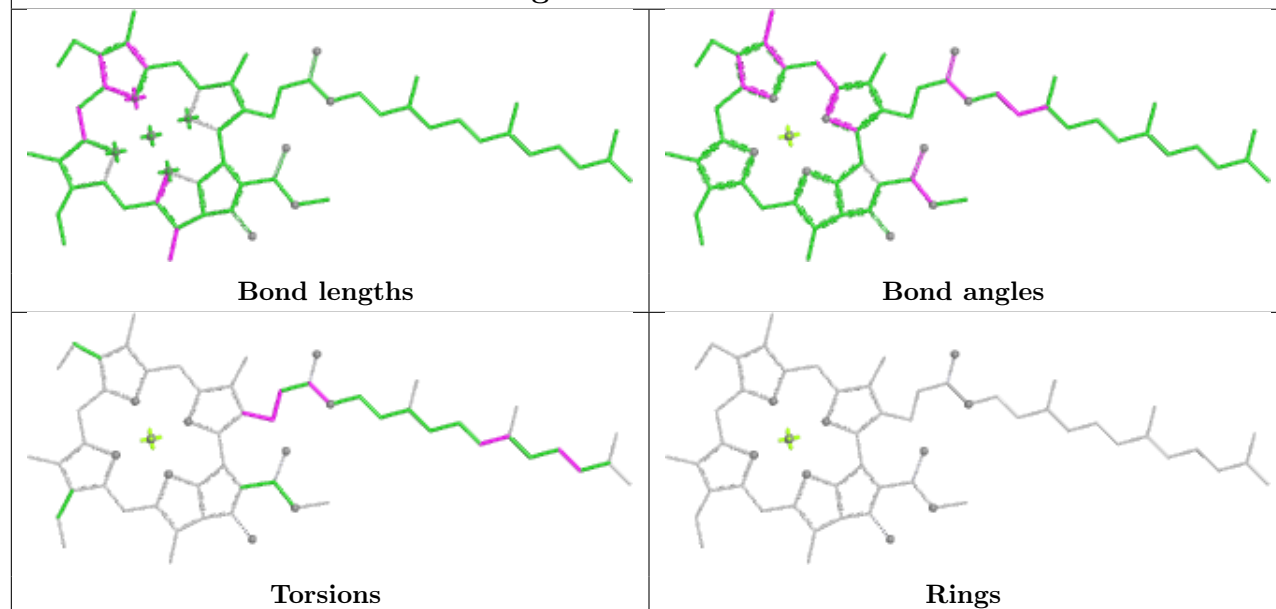
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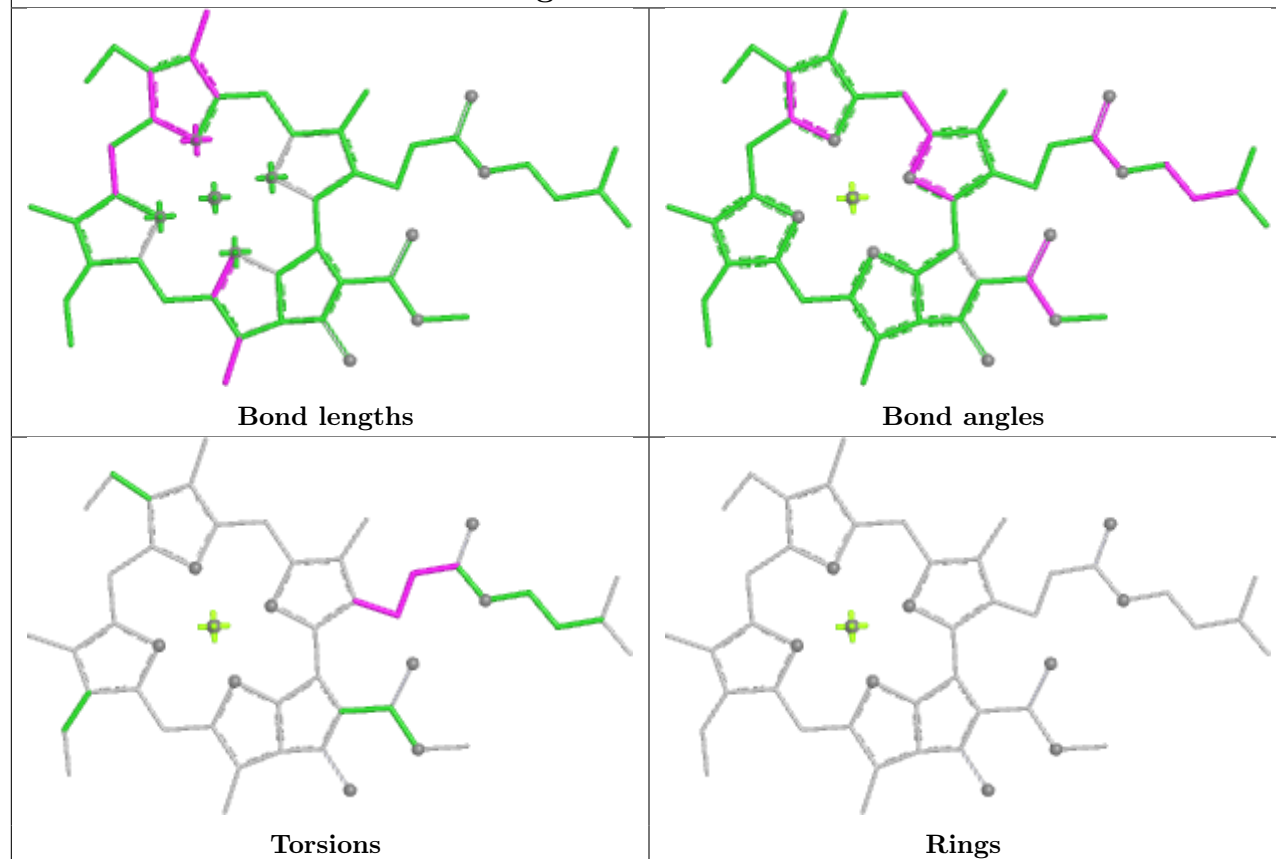
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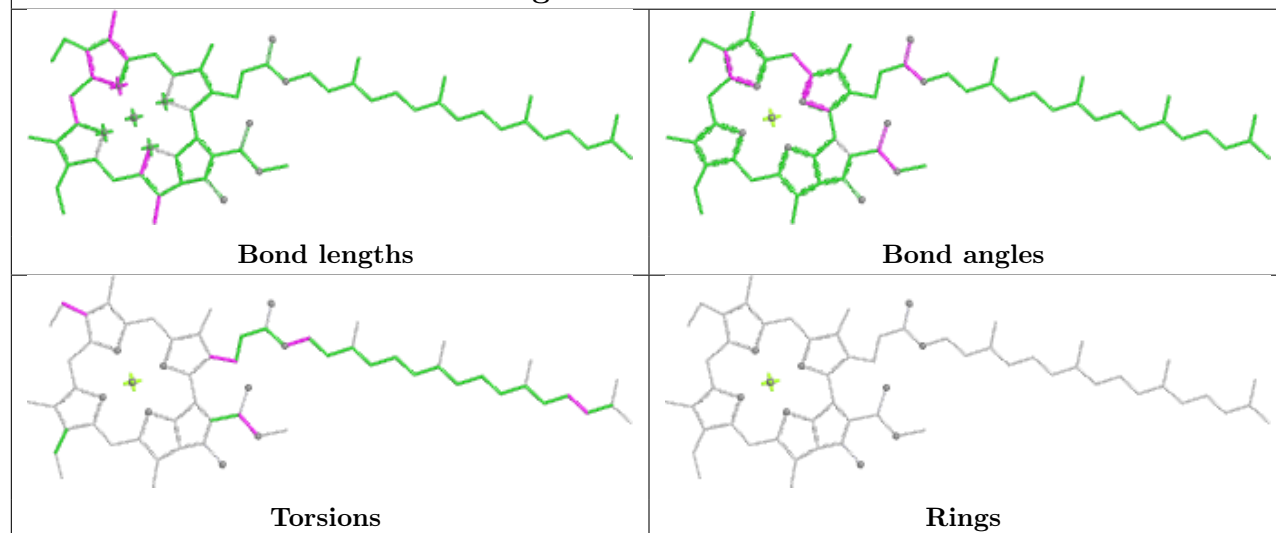
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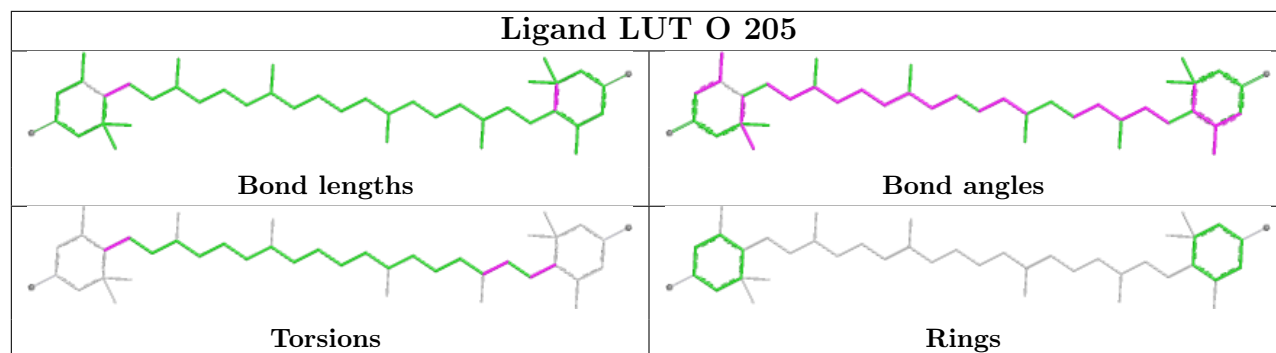
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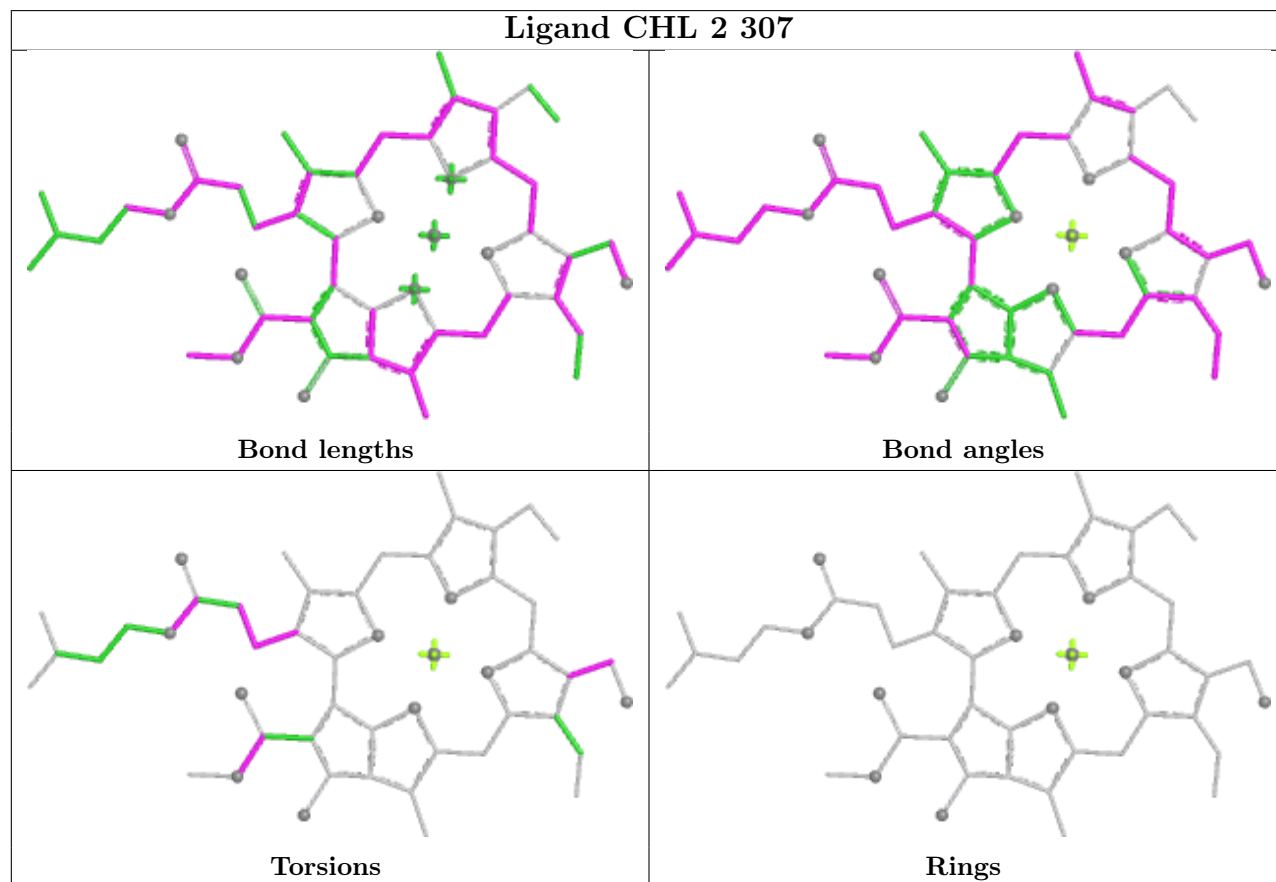
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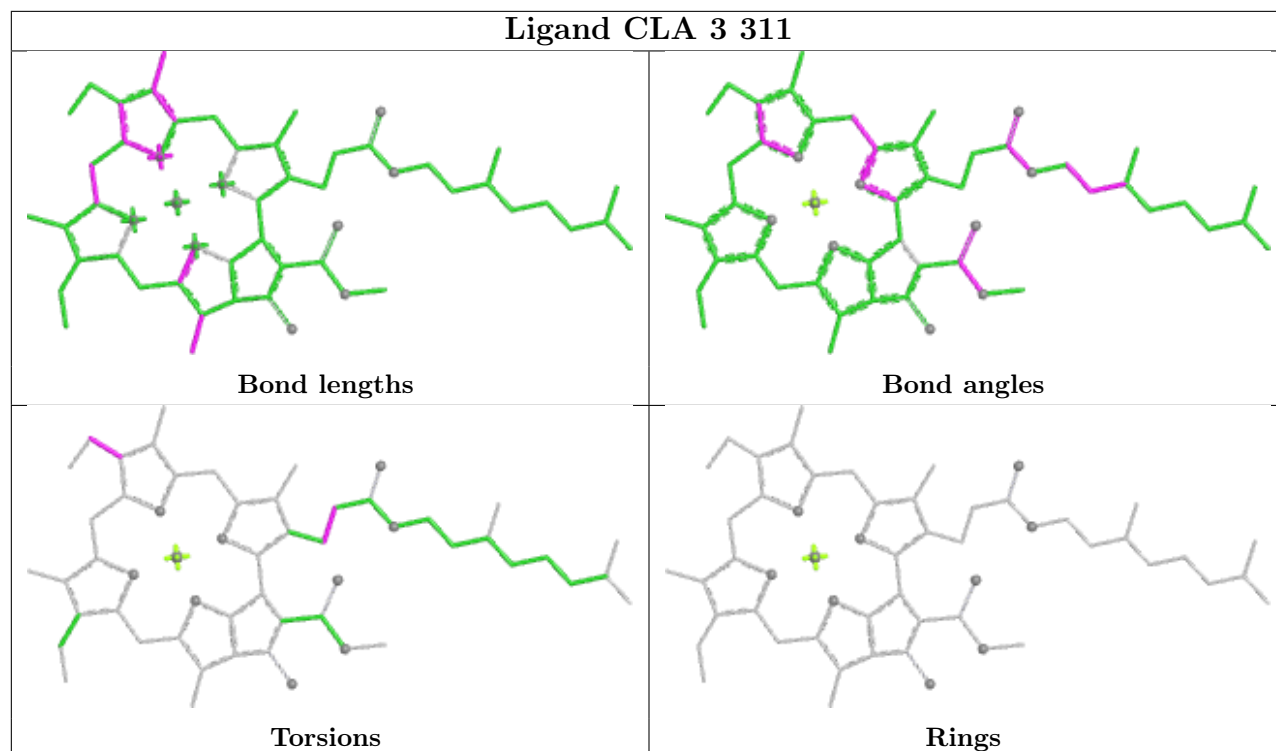
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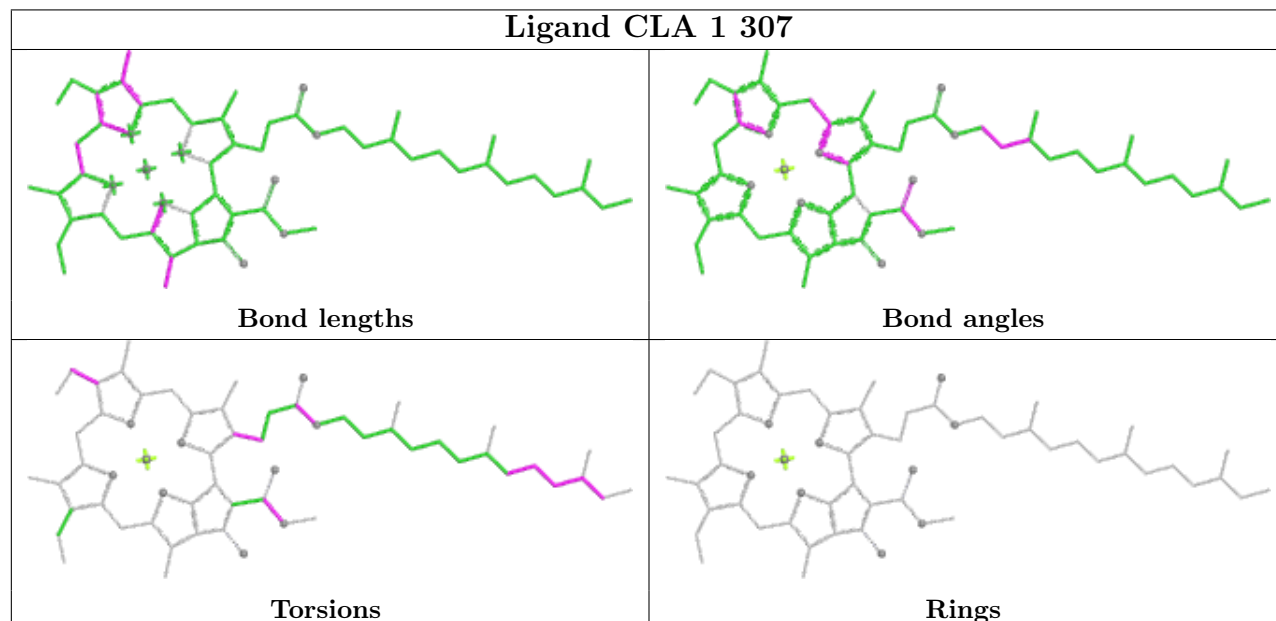
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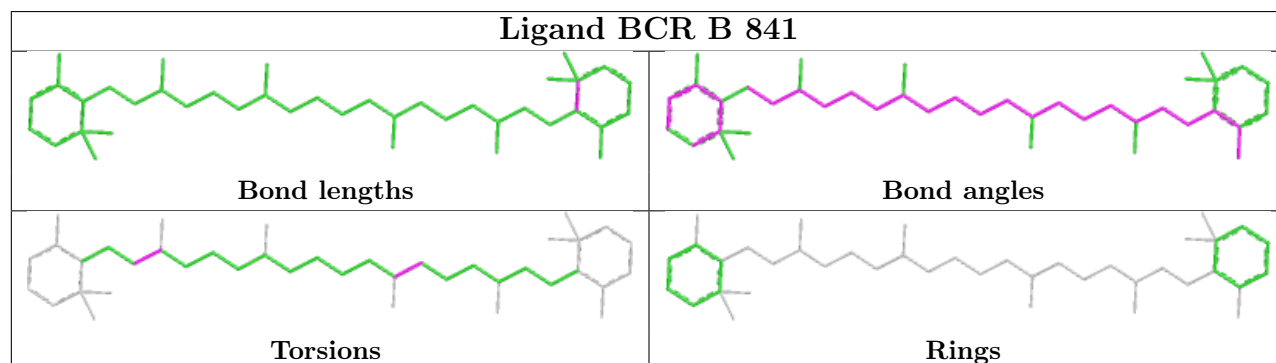
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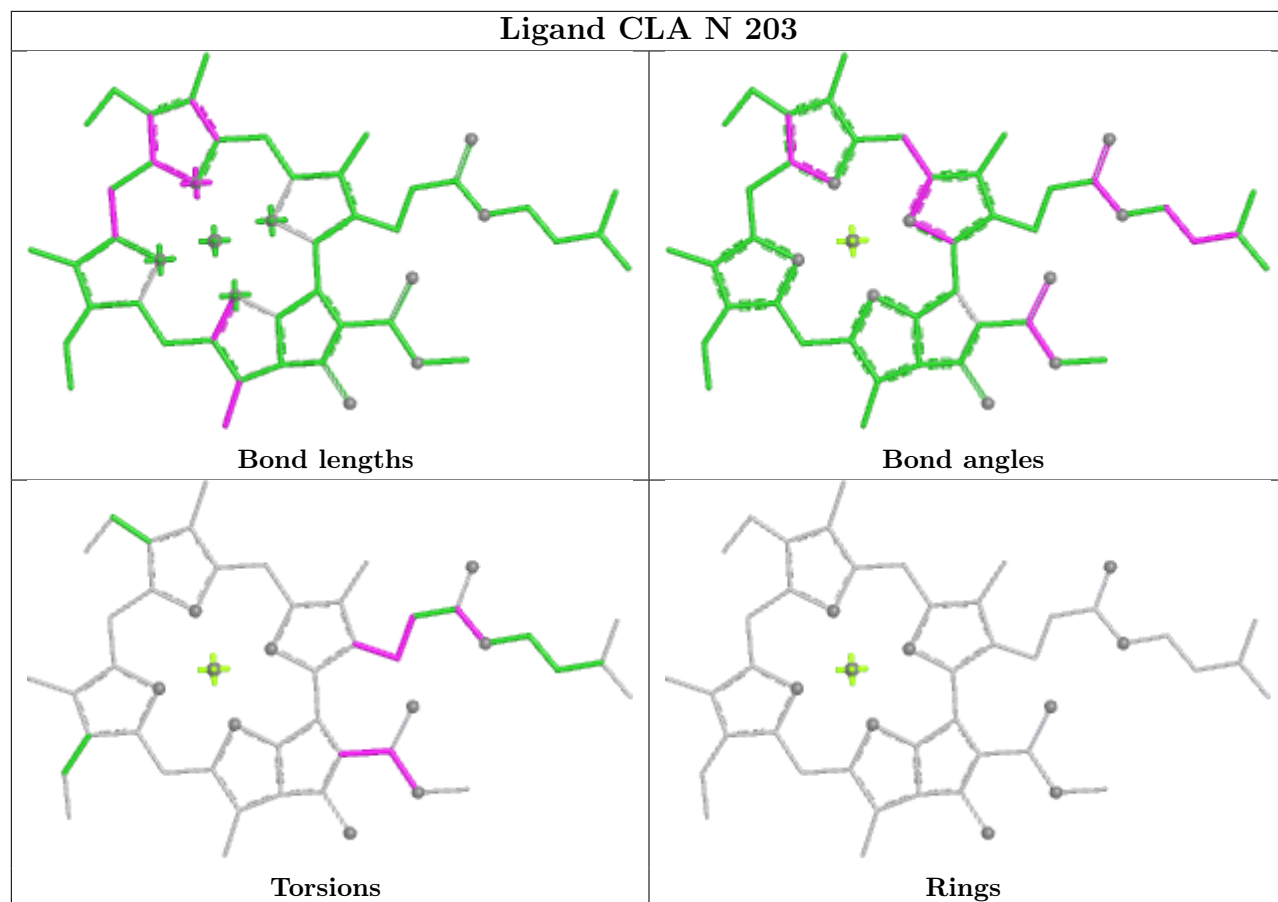


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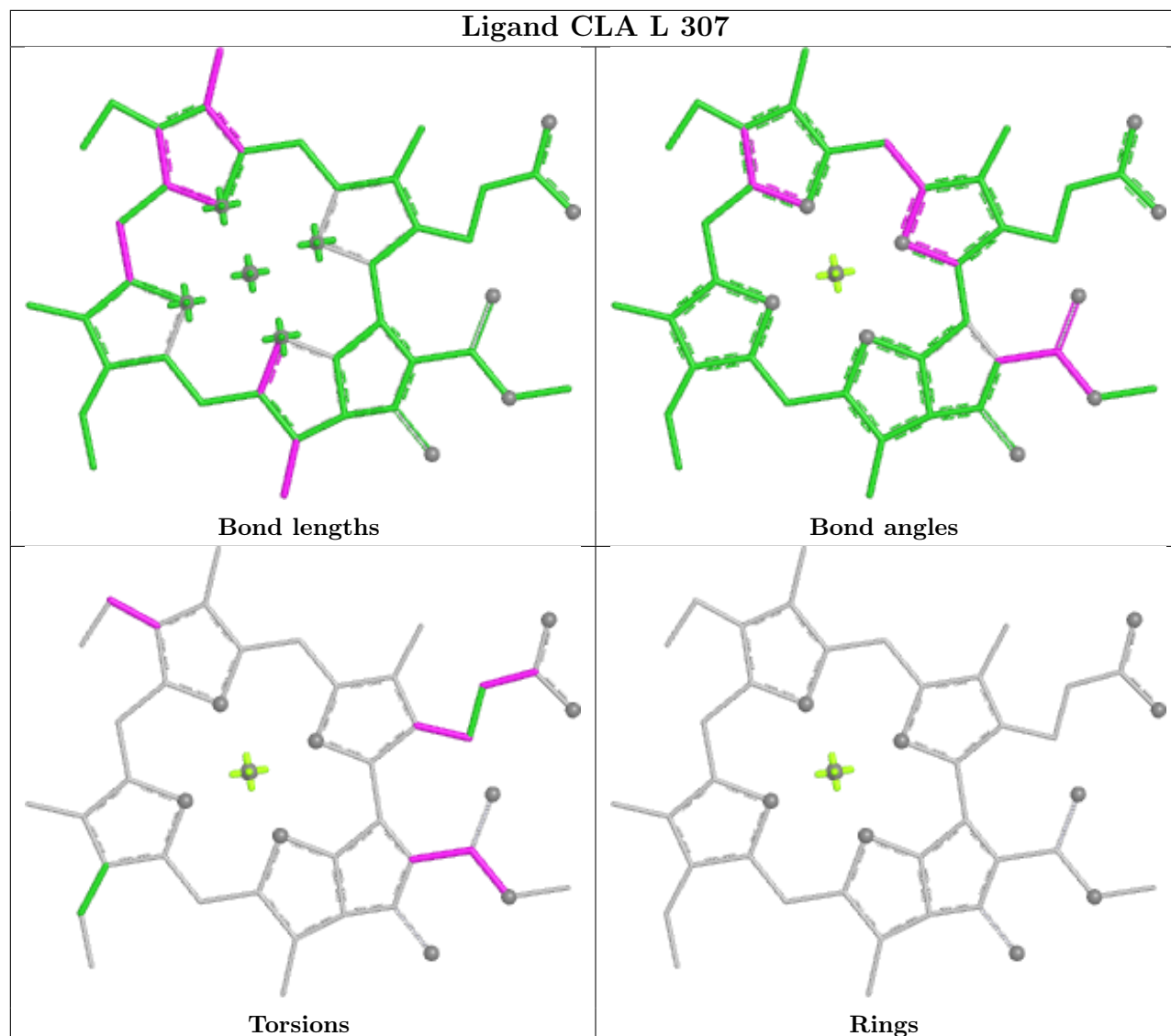


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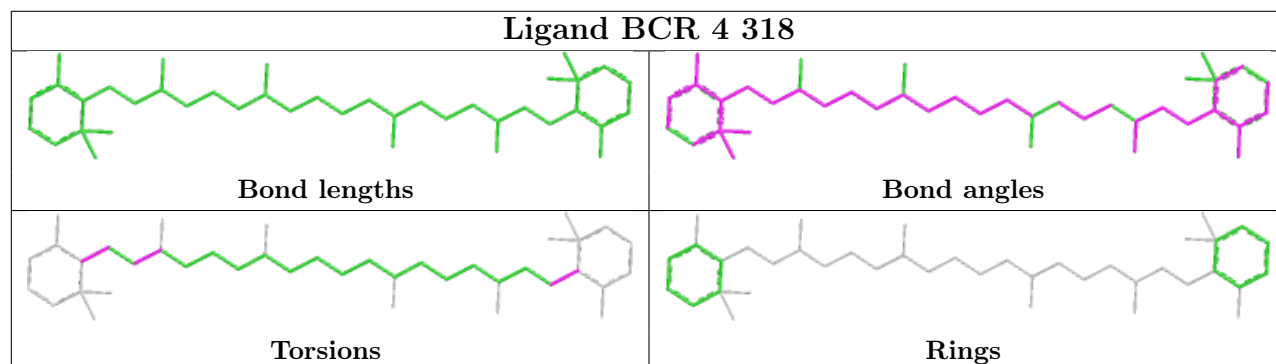


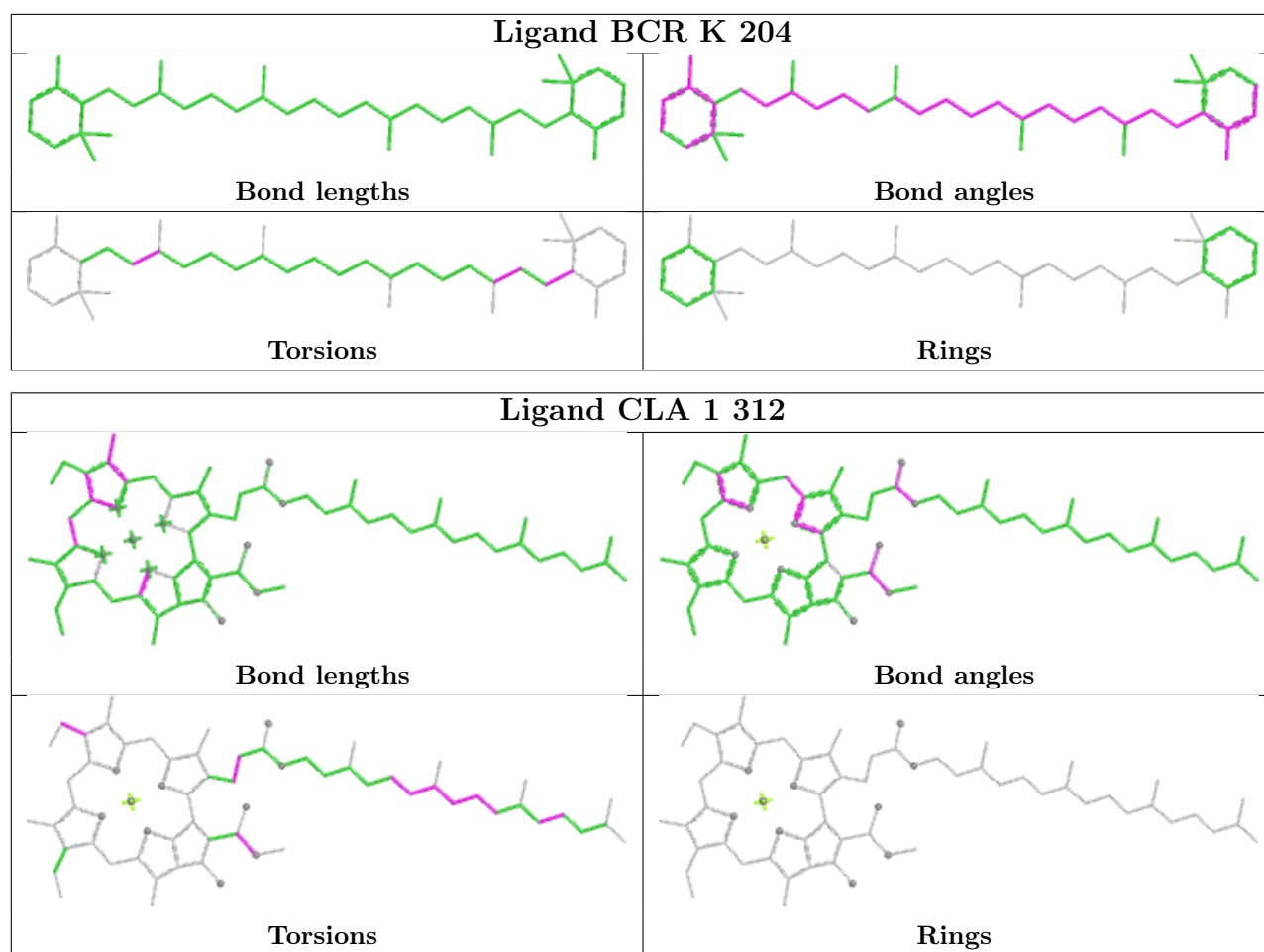


Ligand CLA L 307

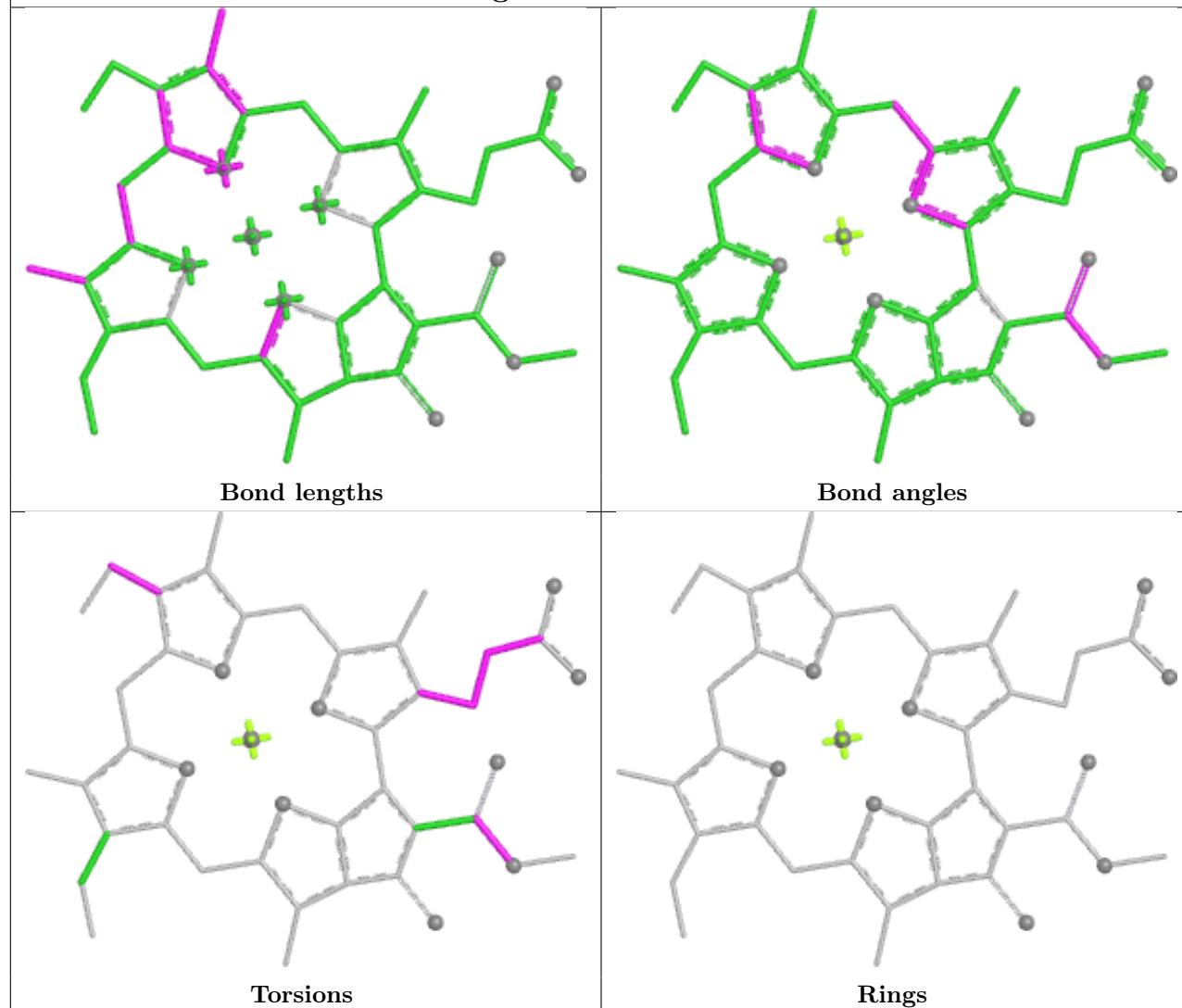


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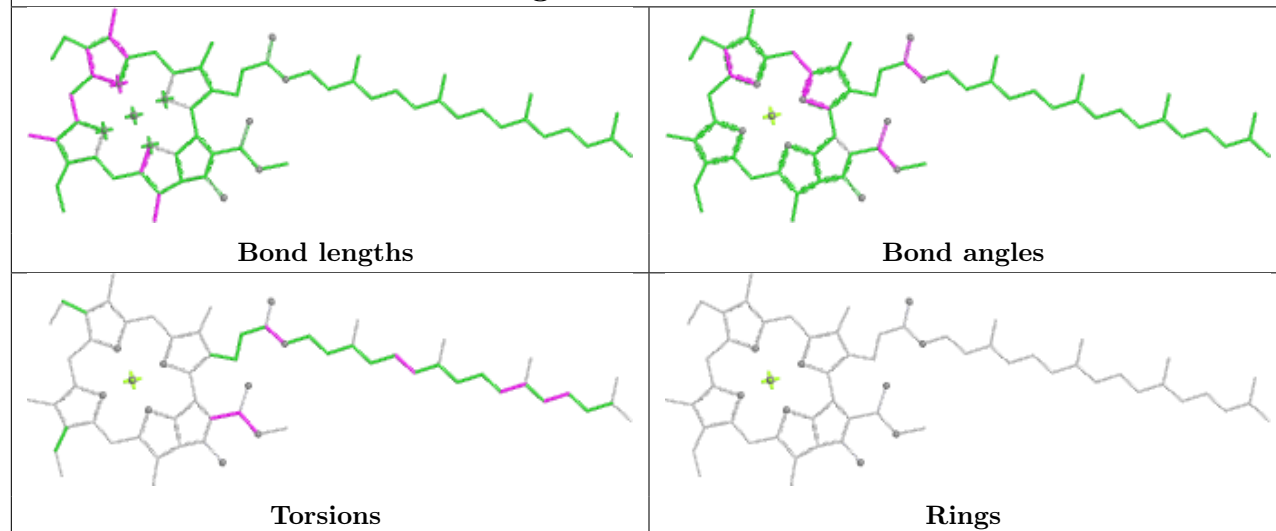




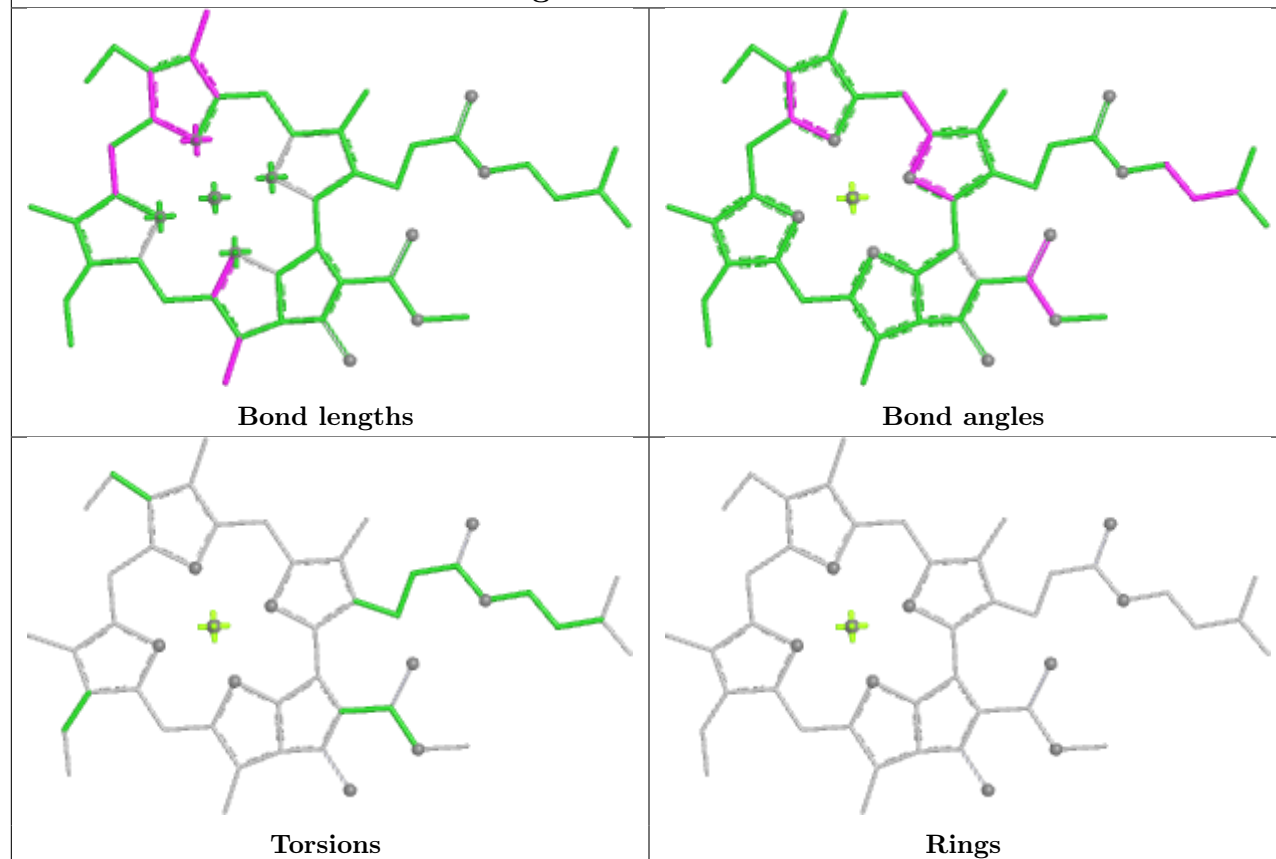
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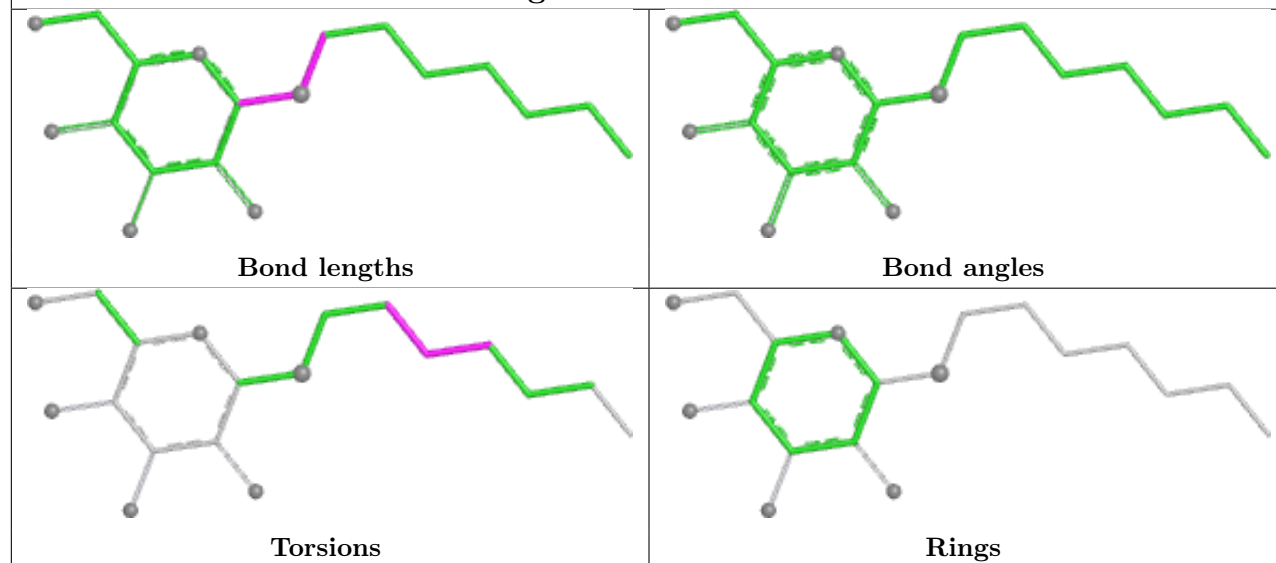
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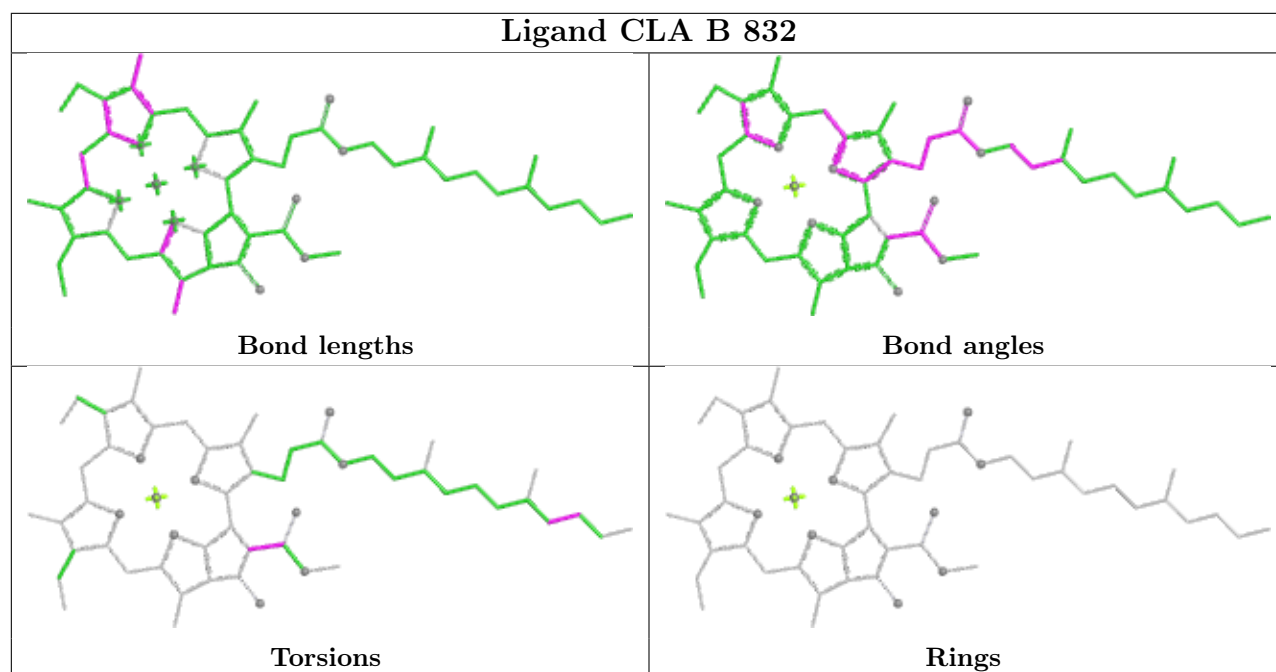
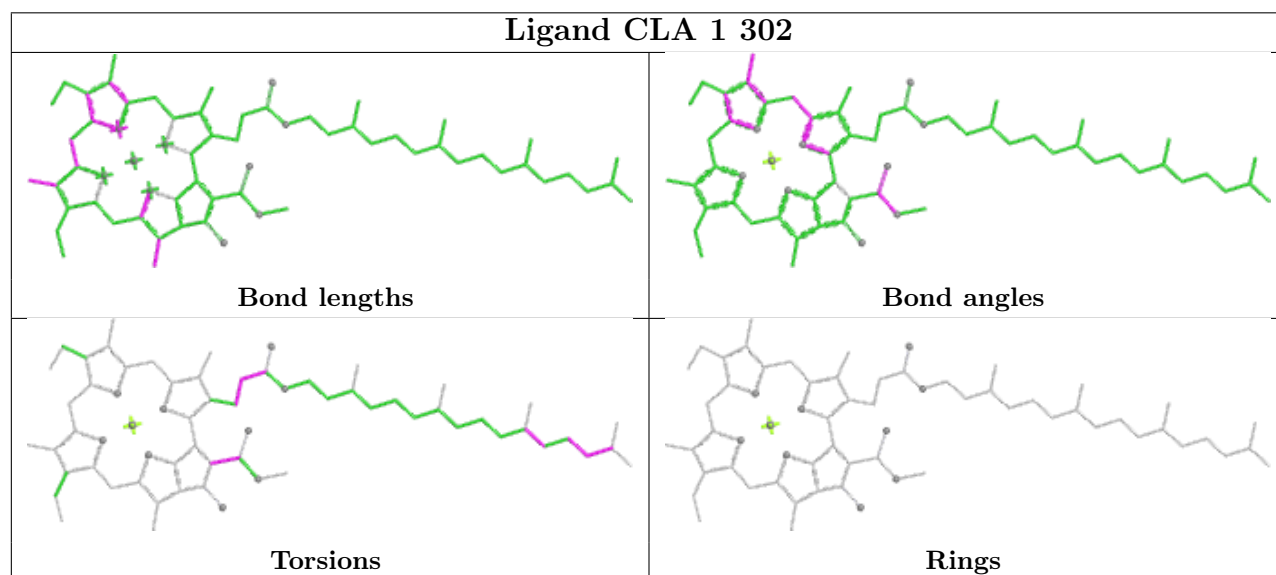
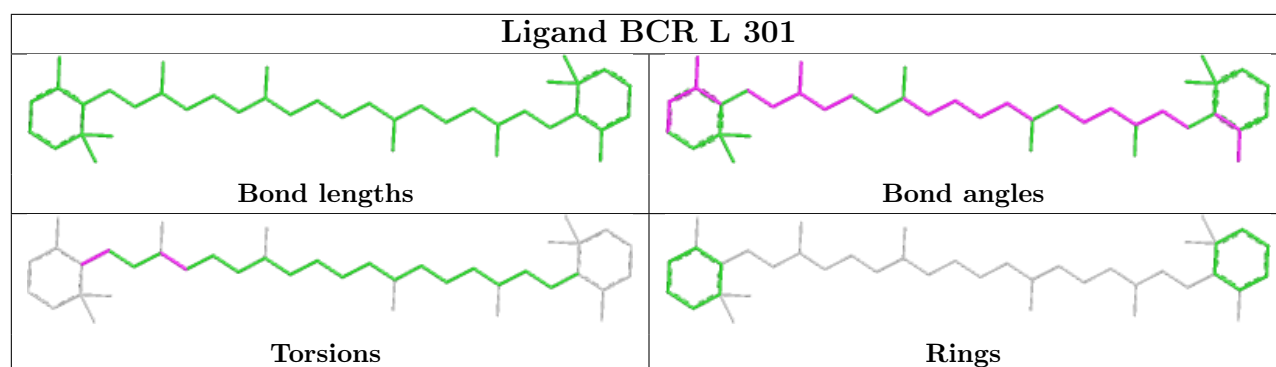


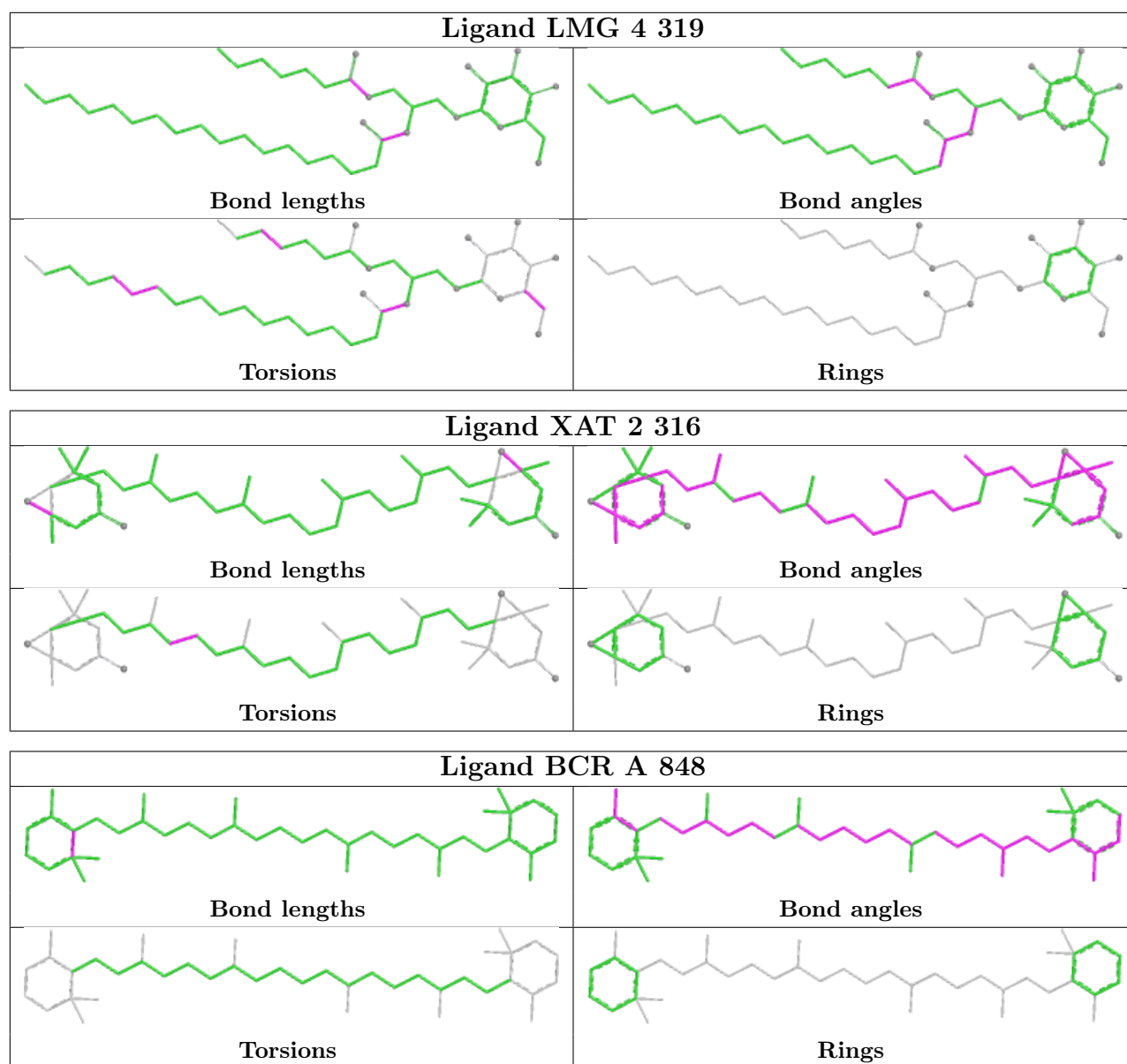
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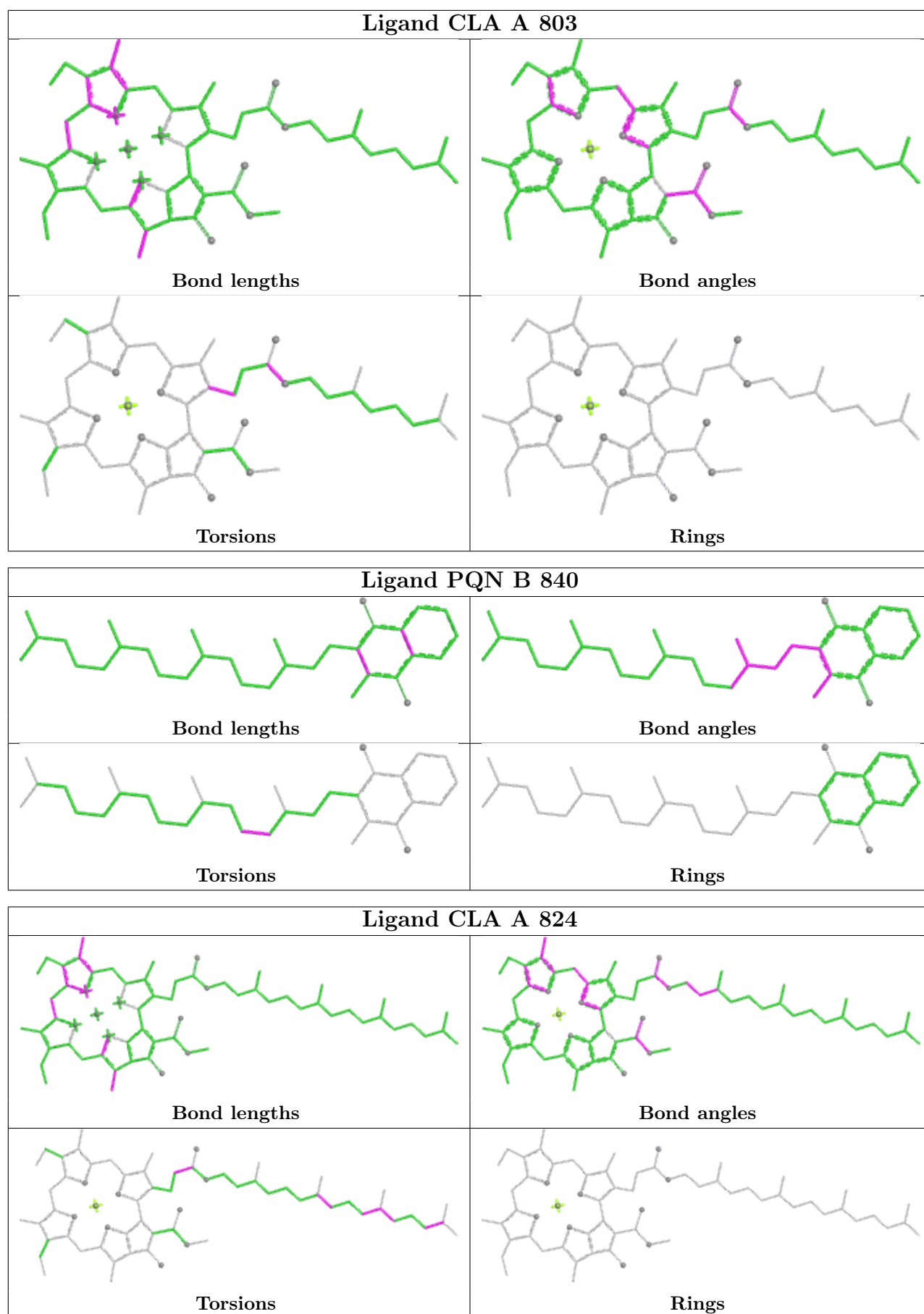


Ligand HTG N 201

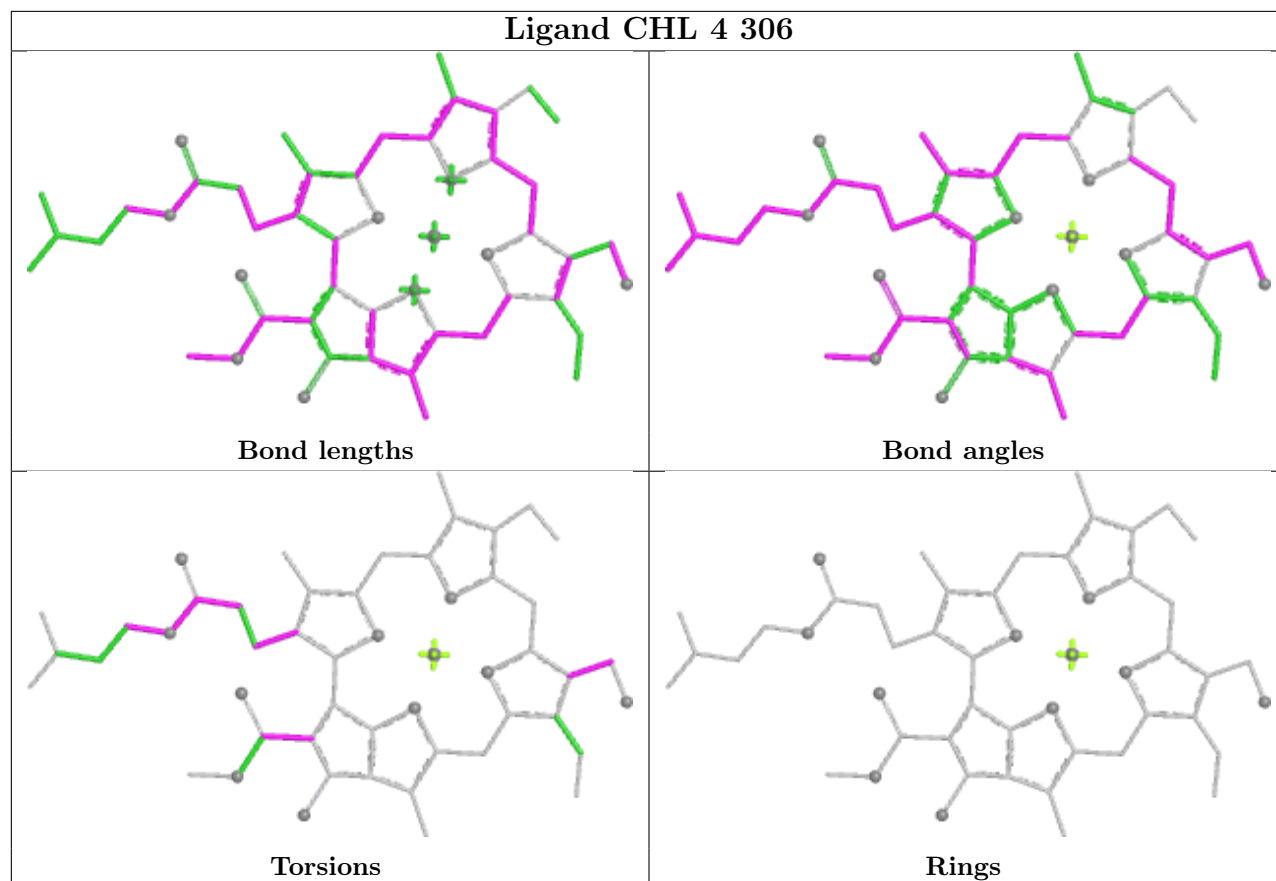




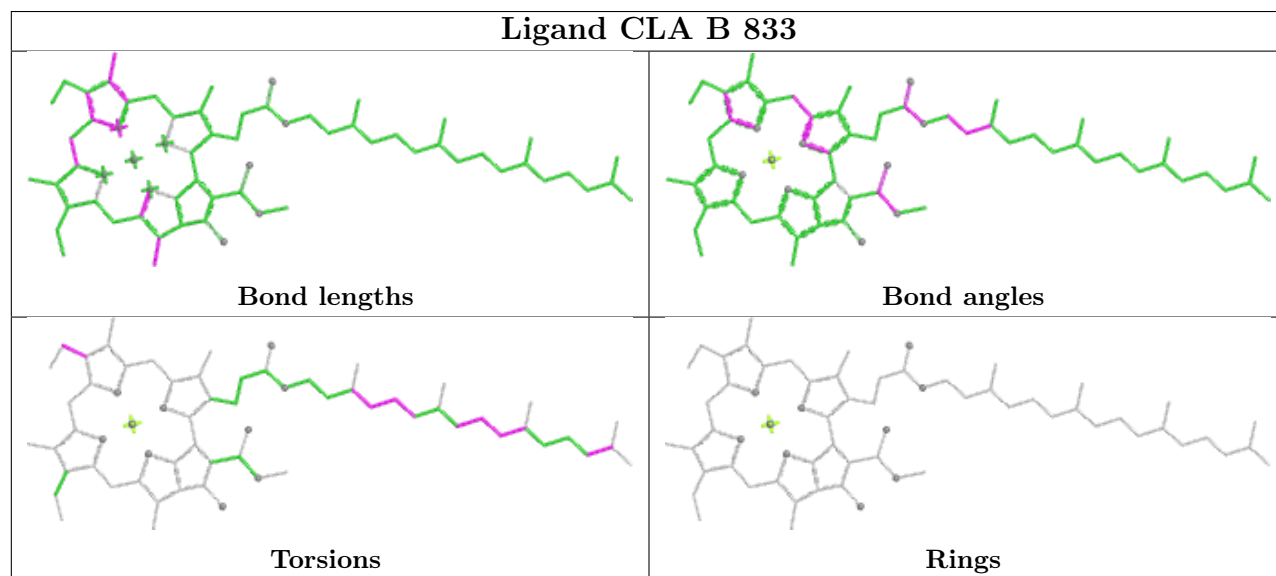


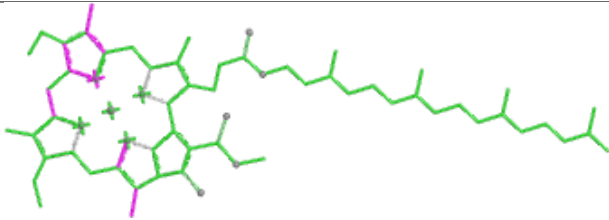
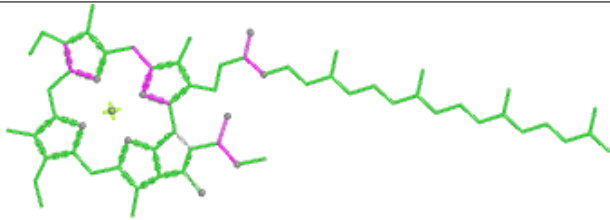
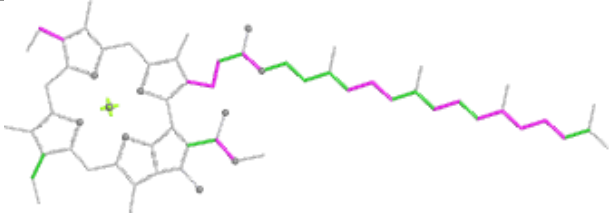
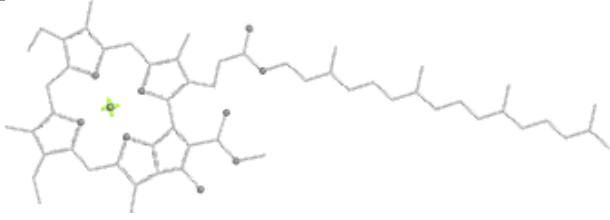


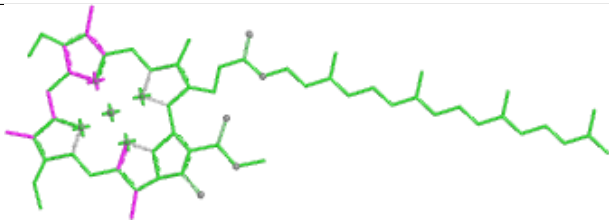
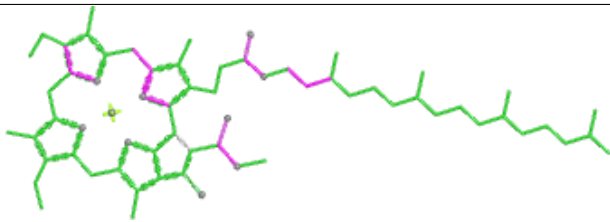
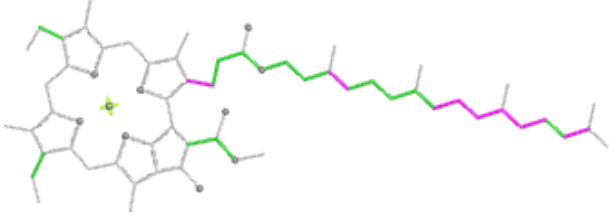
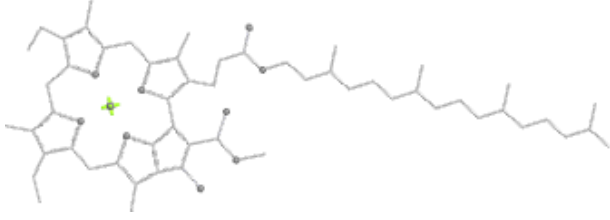
Ligand CHL 4 306

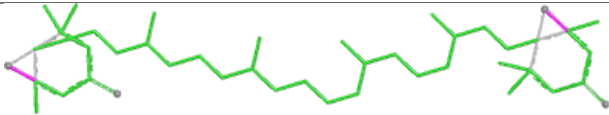
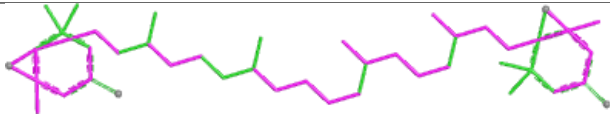
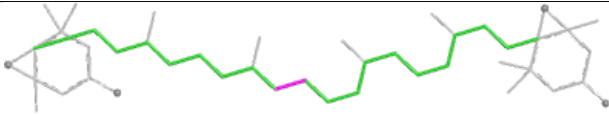
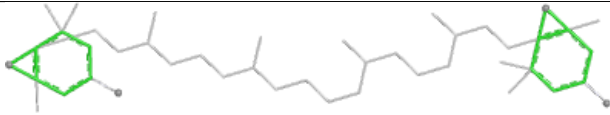


Ligand CLA B 833

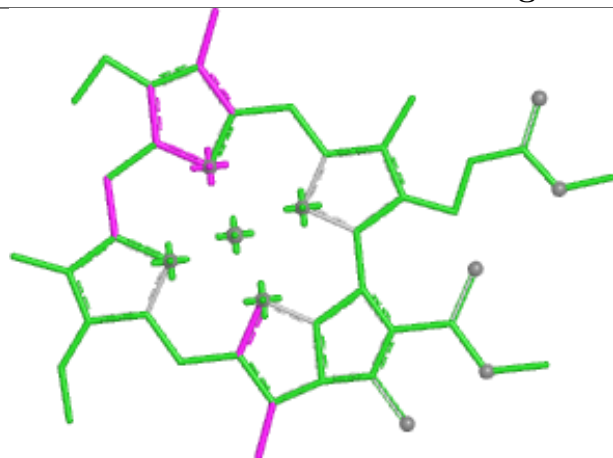


Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

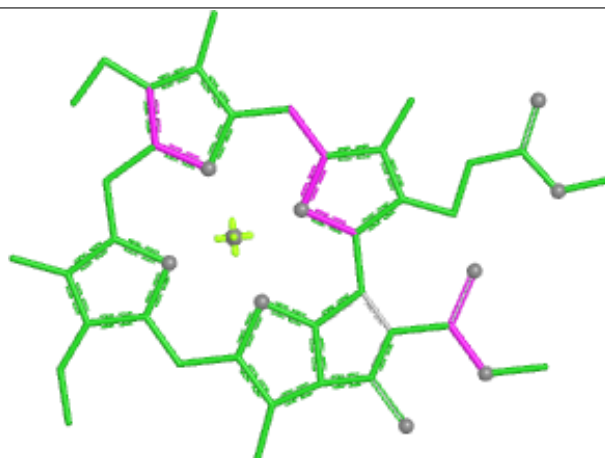
Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 1 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

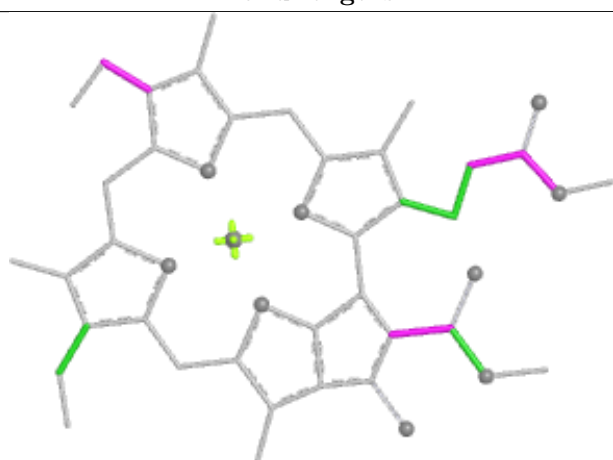
Ligand CLA 4 301



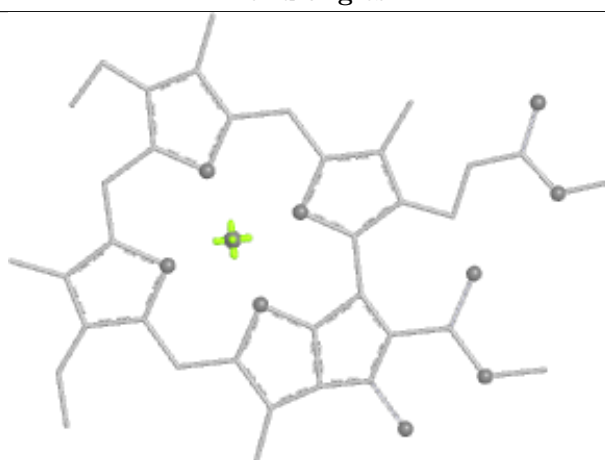
Bond lengths



Bond angles

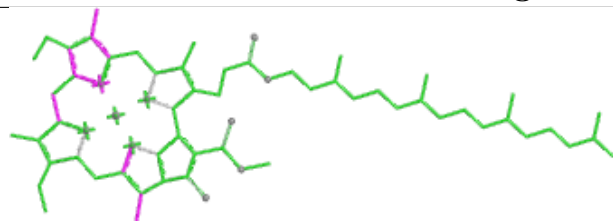


Torsions

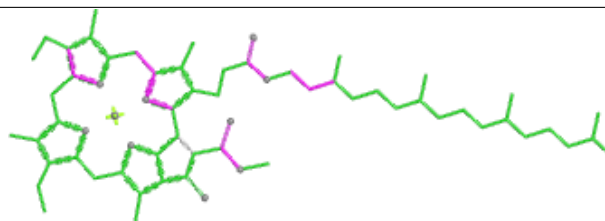


Rings

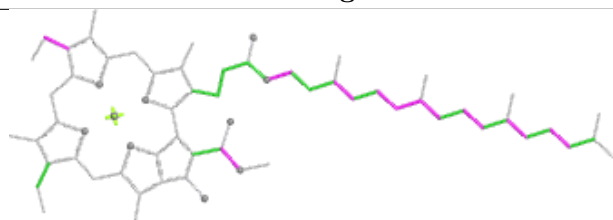
Ligand CLA A 853



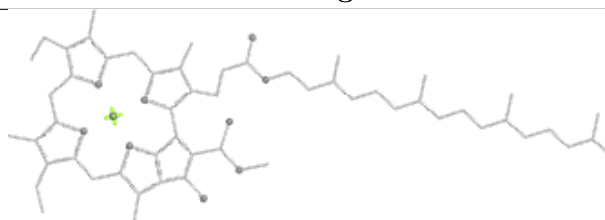
Bond lengths



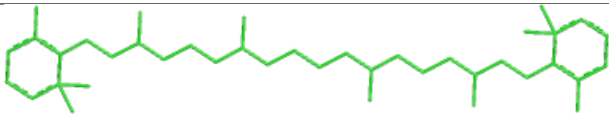
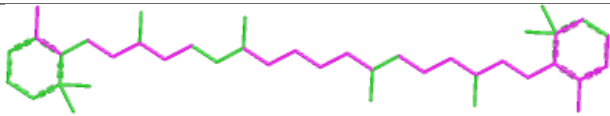
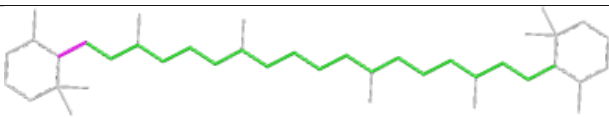
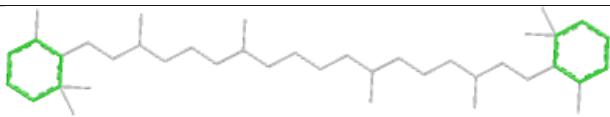
Bond angles

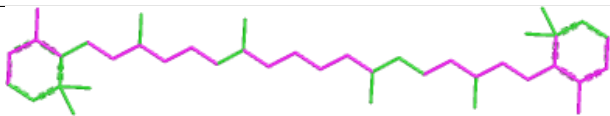
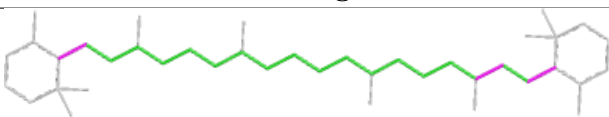
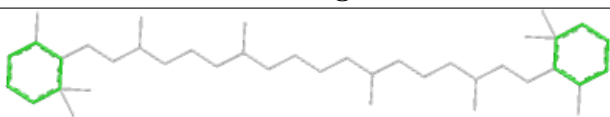


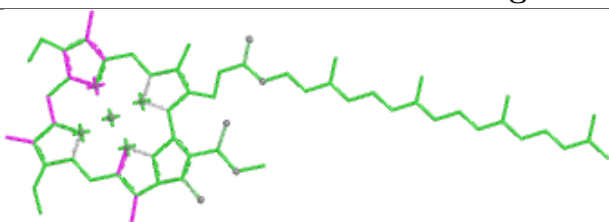
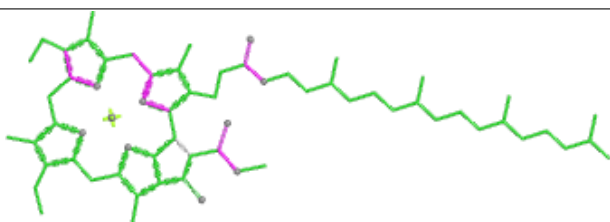
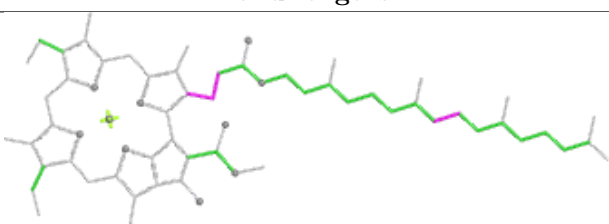
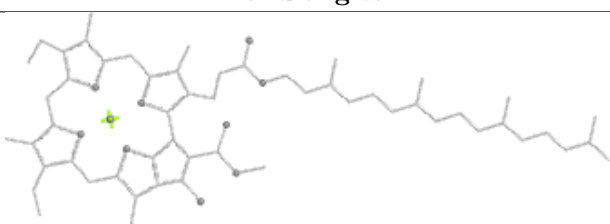
Torsions

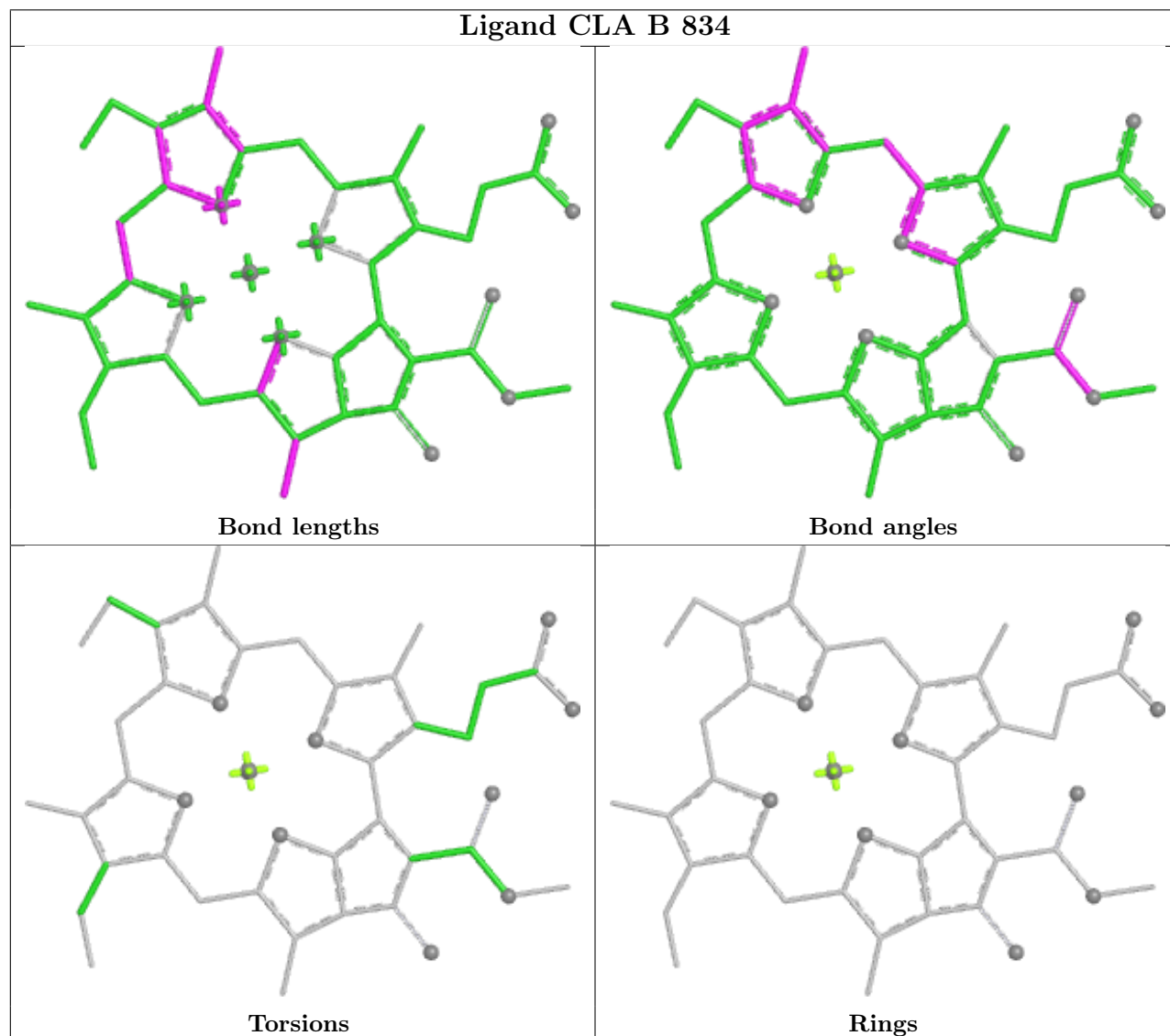
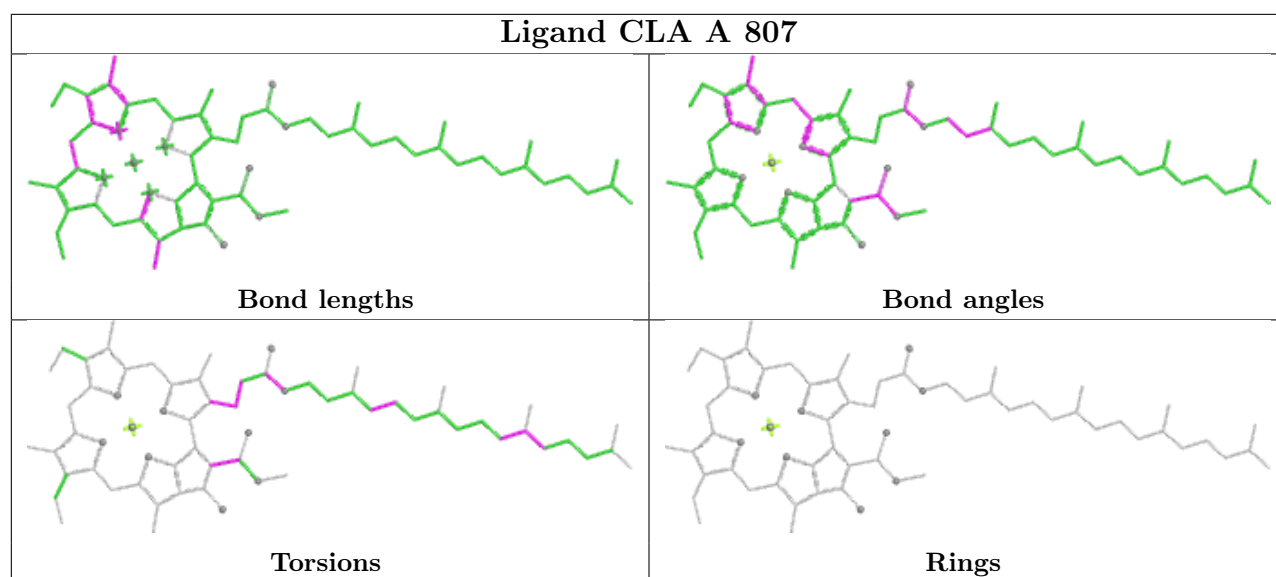


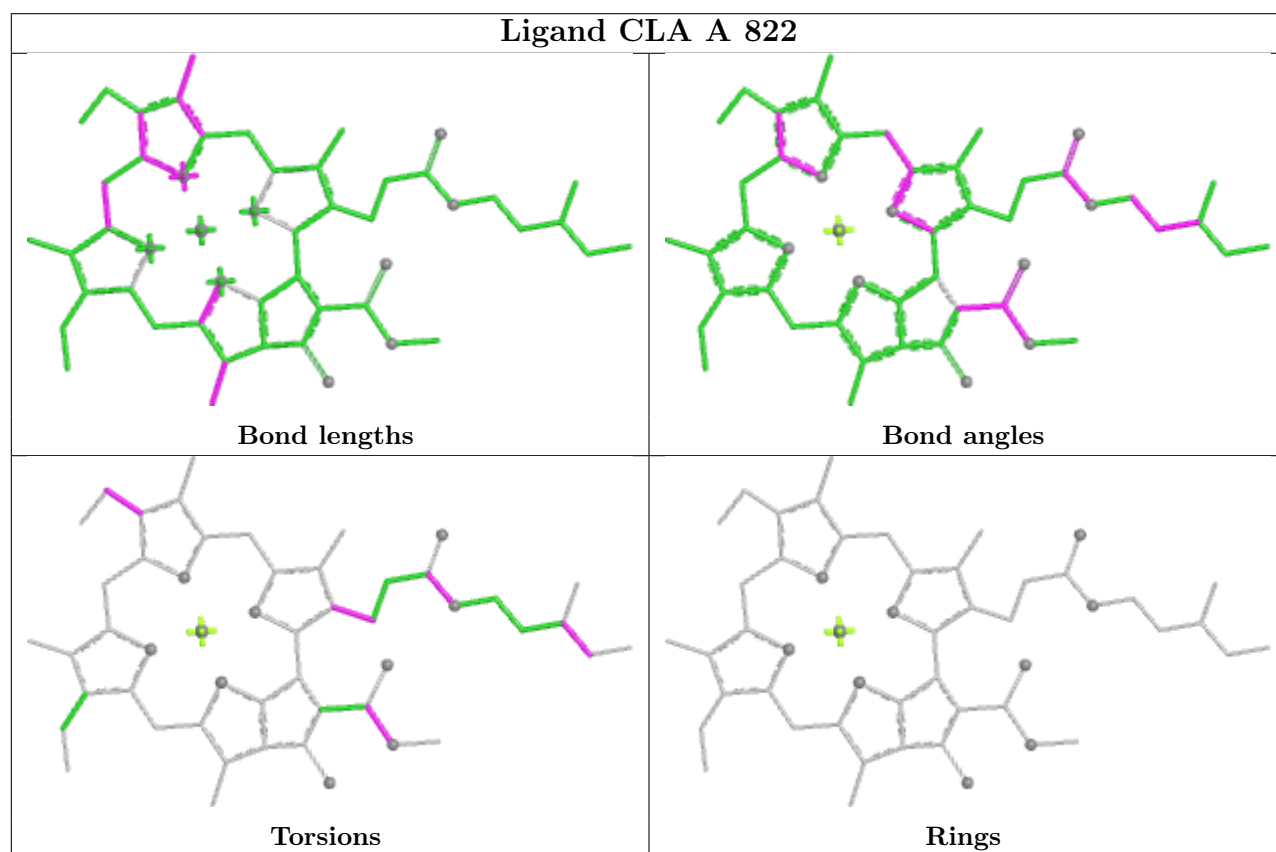
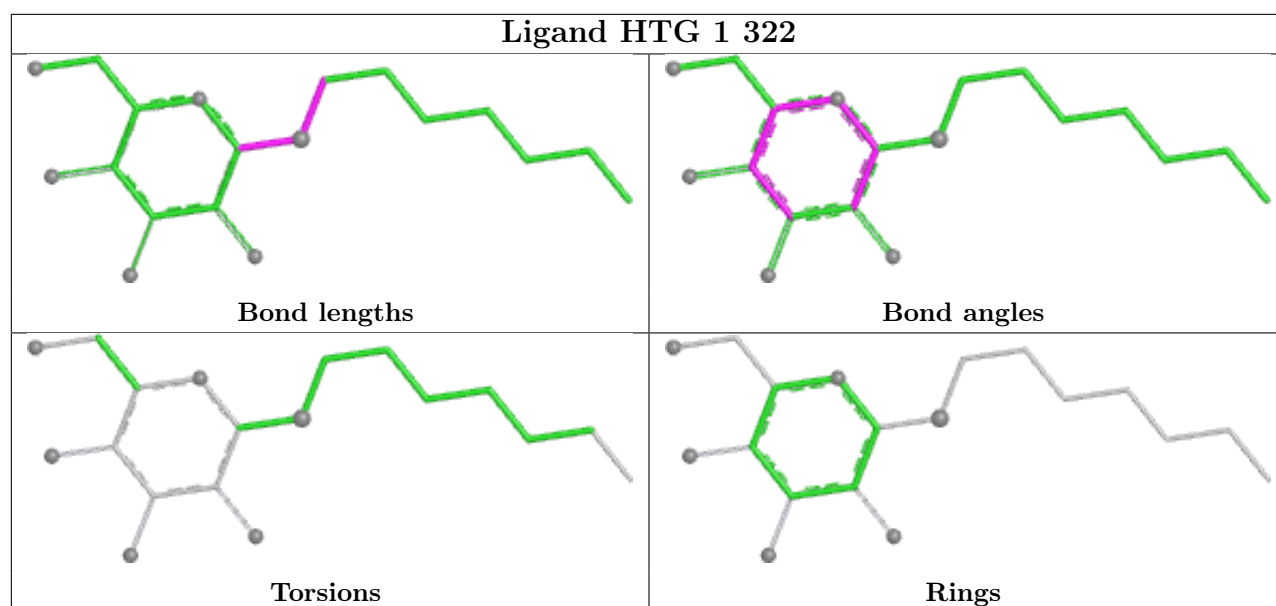
Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

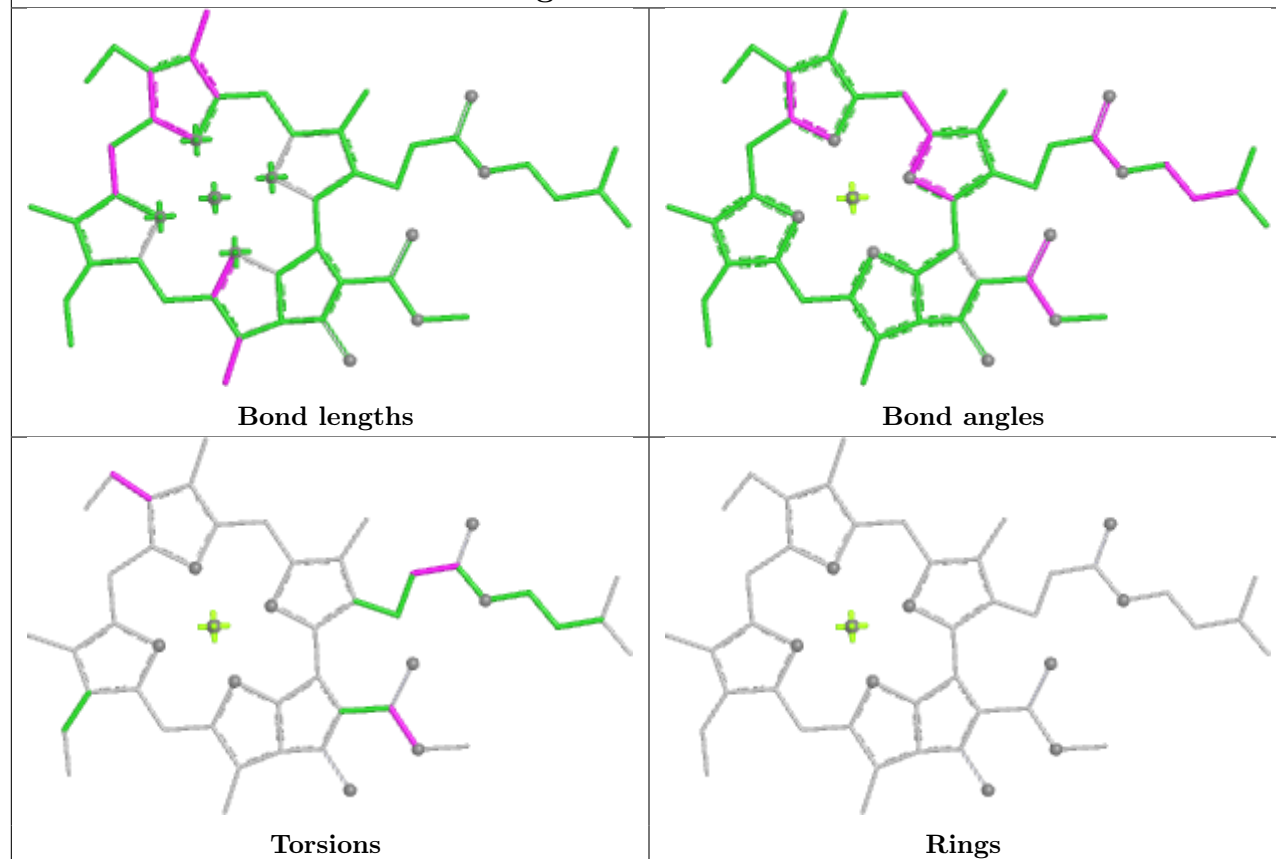
Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

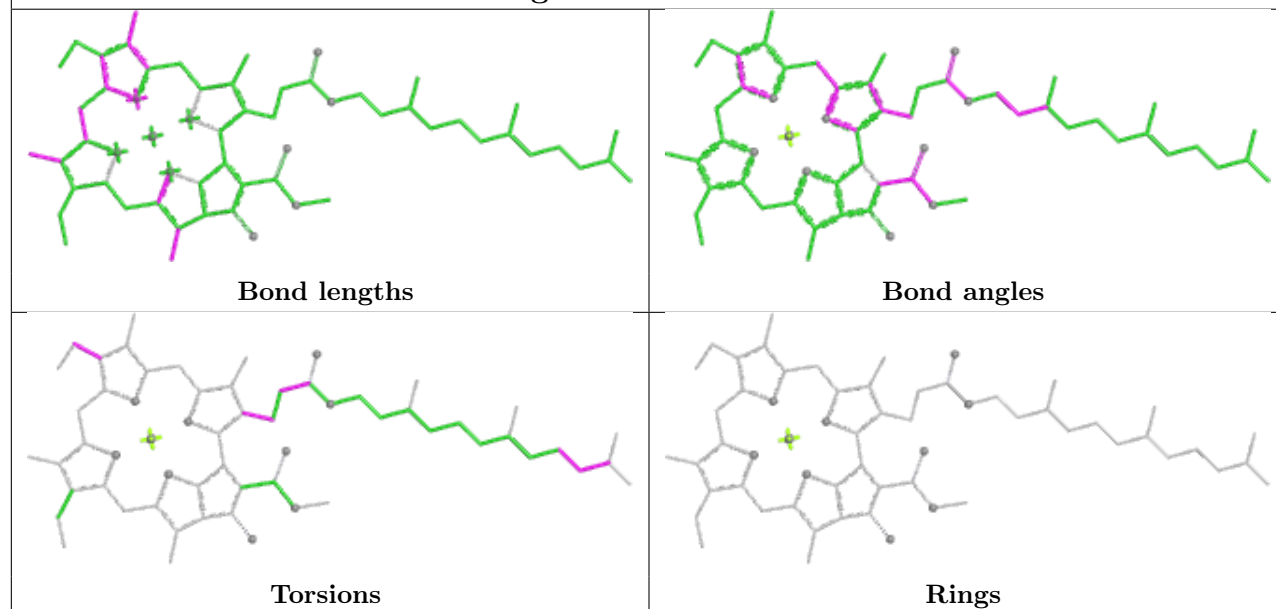




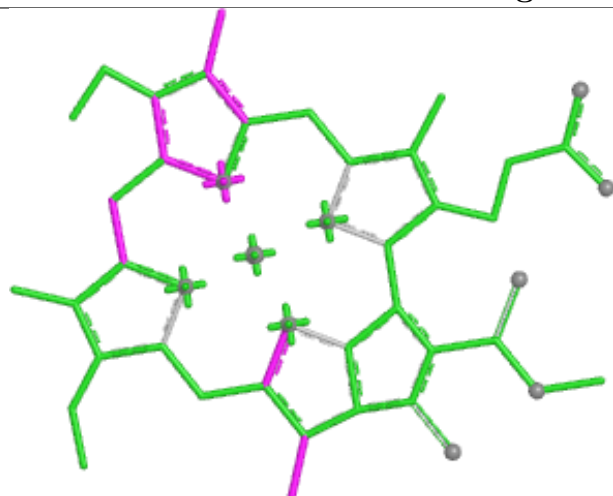
Ligand CLA 3 302



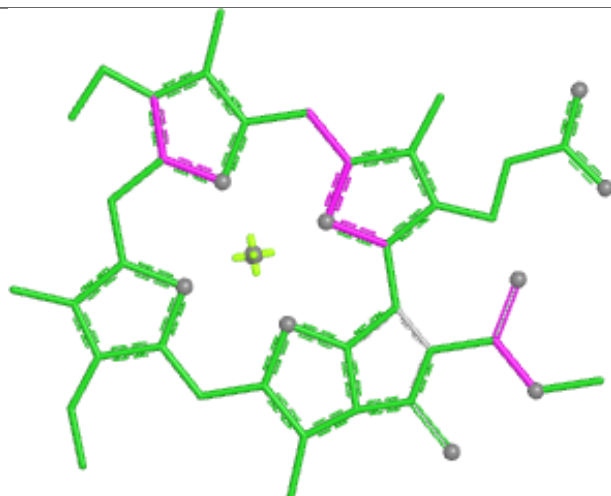
Ligand CLA K 202



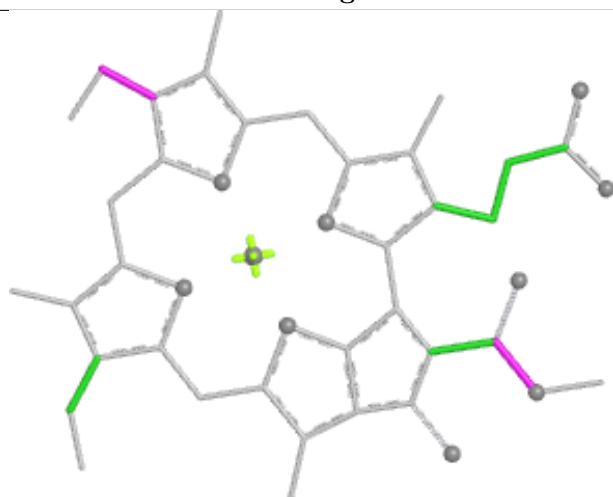
Ligand CLA F 804



Bond lengths



Bond angles

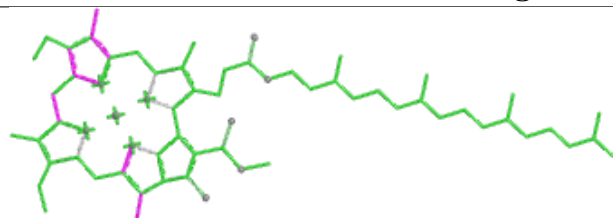


Torsions

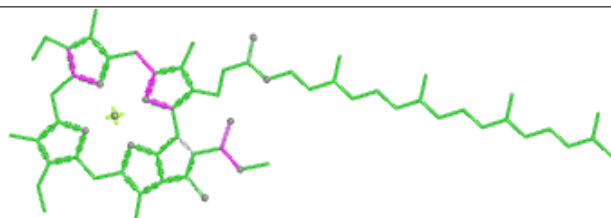


Rings

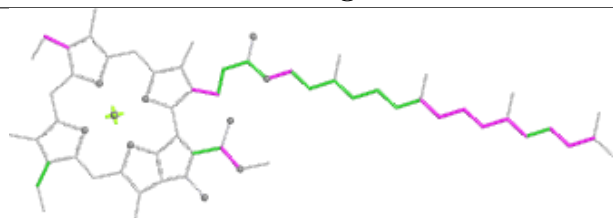
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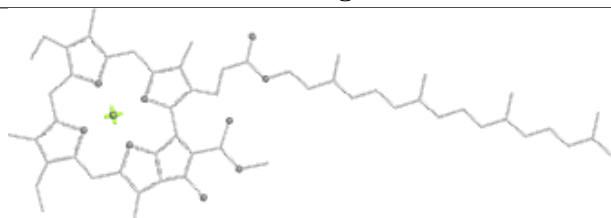
Bond lengths



Bond angles

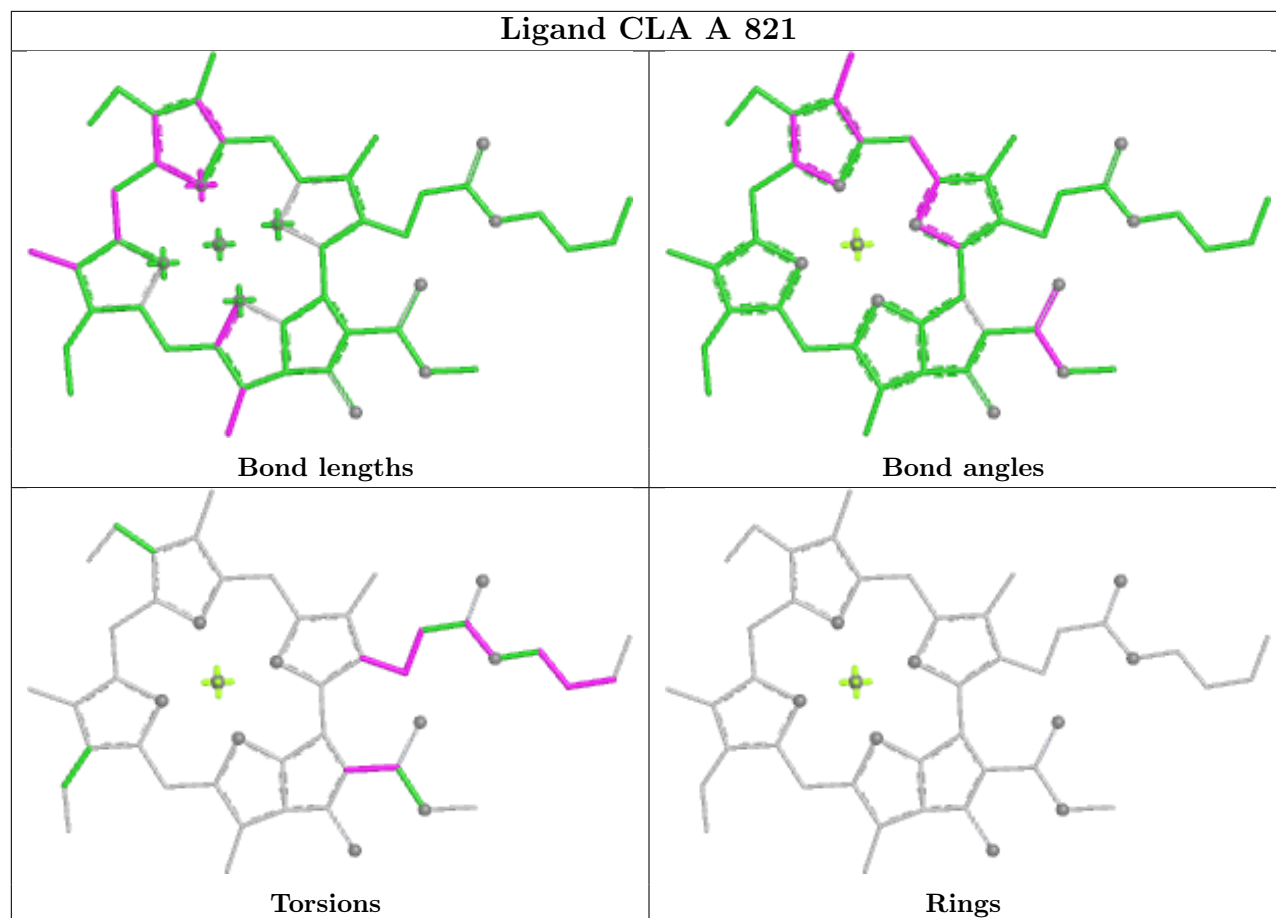


Torsions

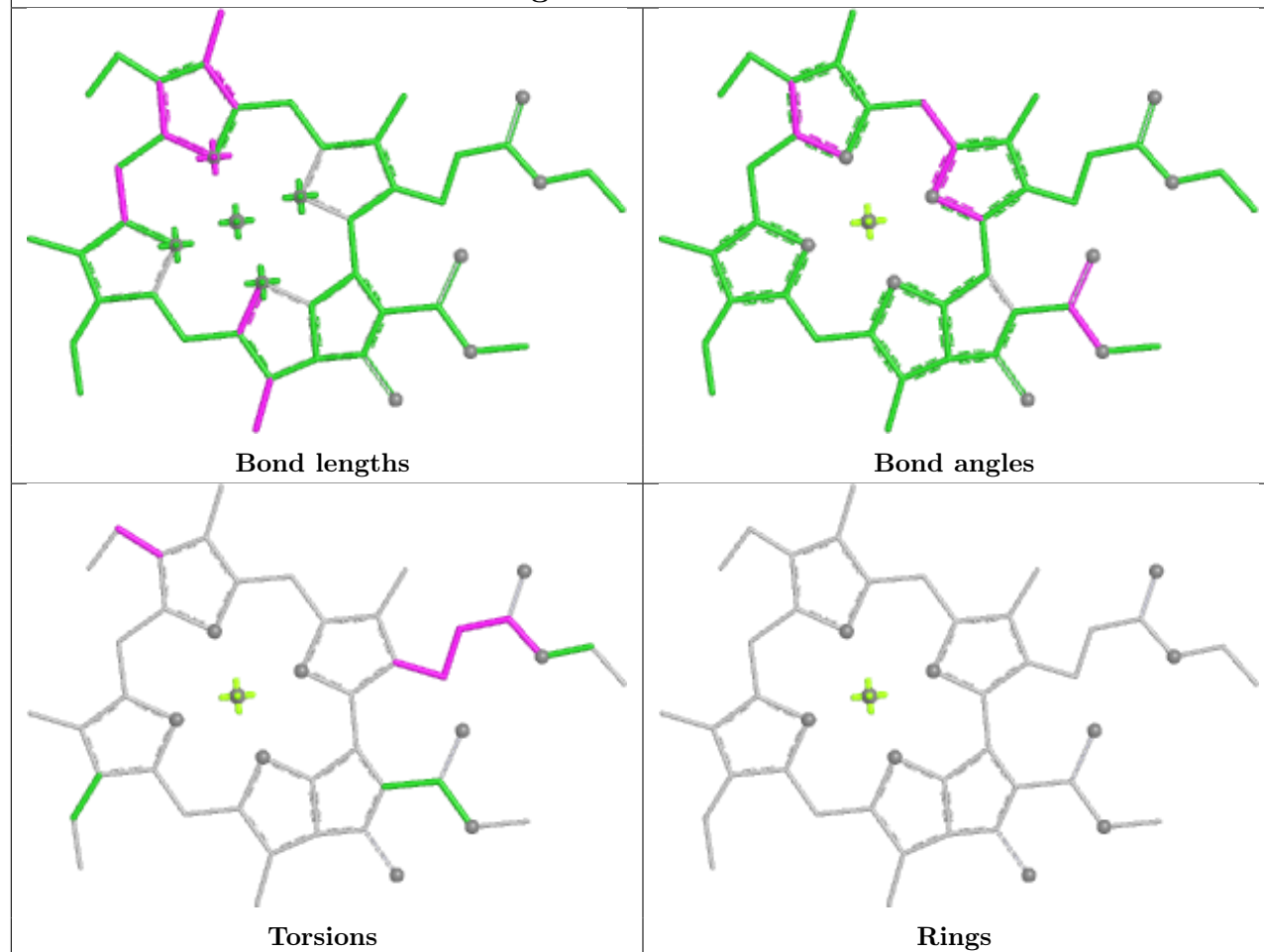


Rings

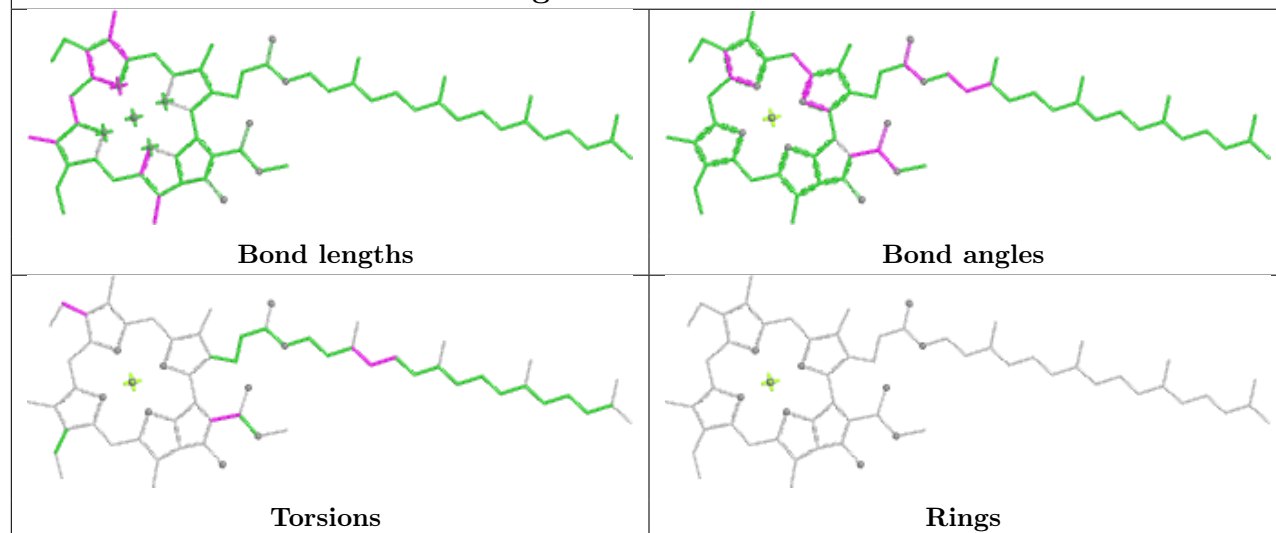
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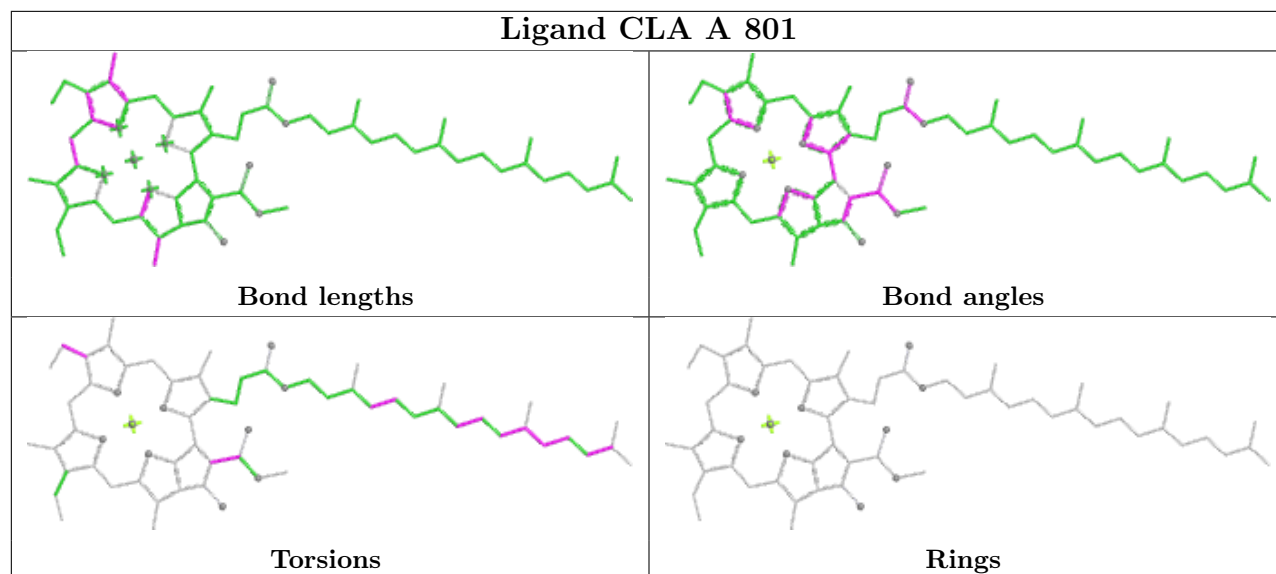
Ligand CLA 3 305



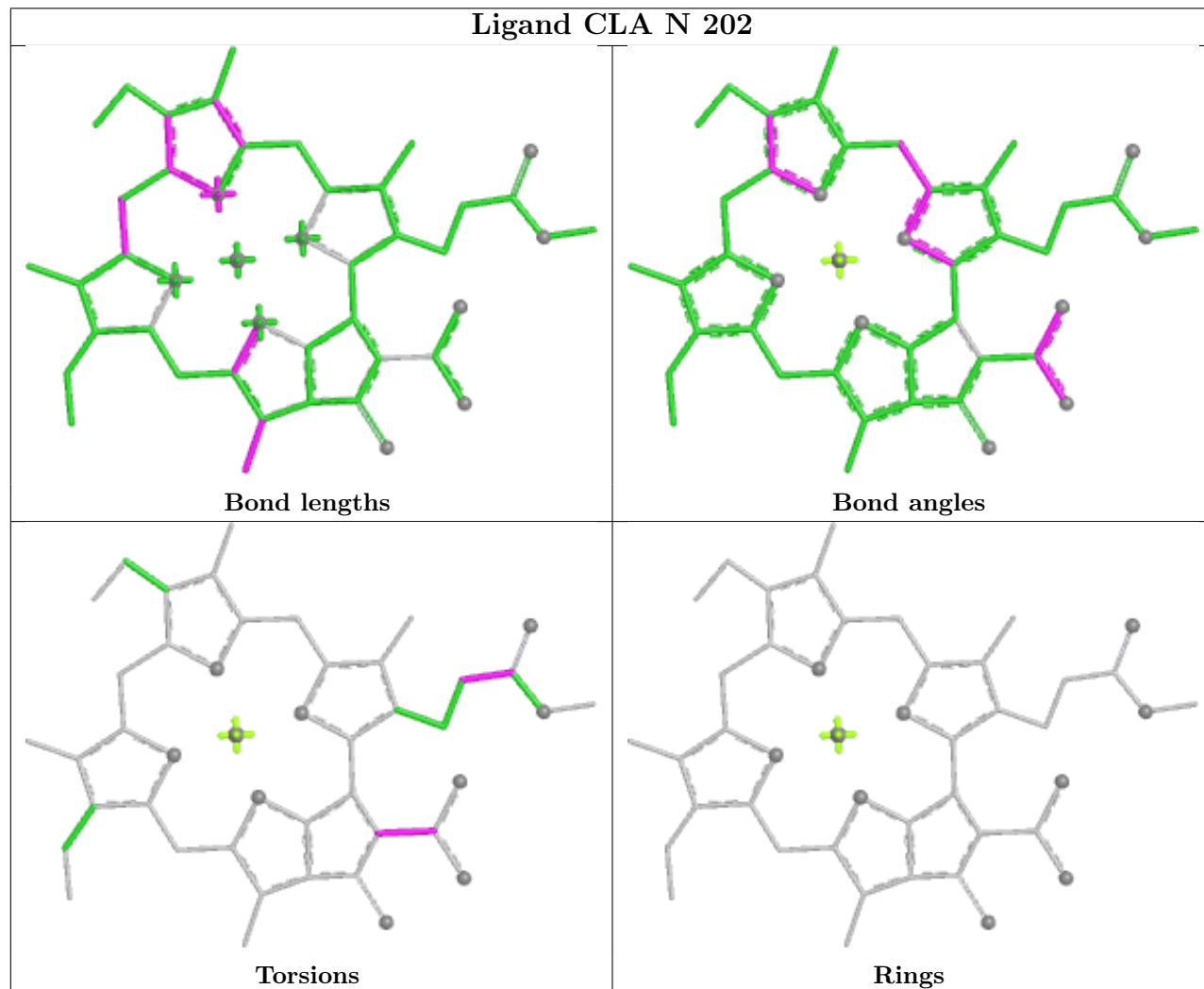
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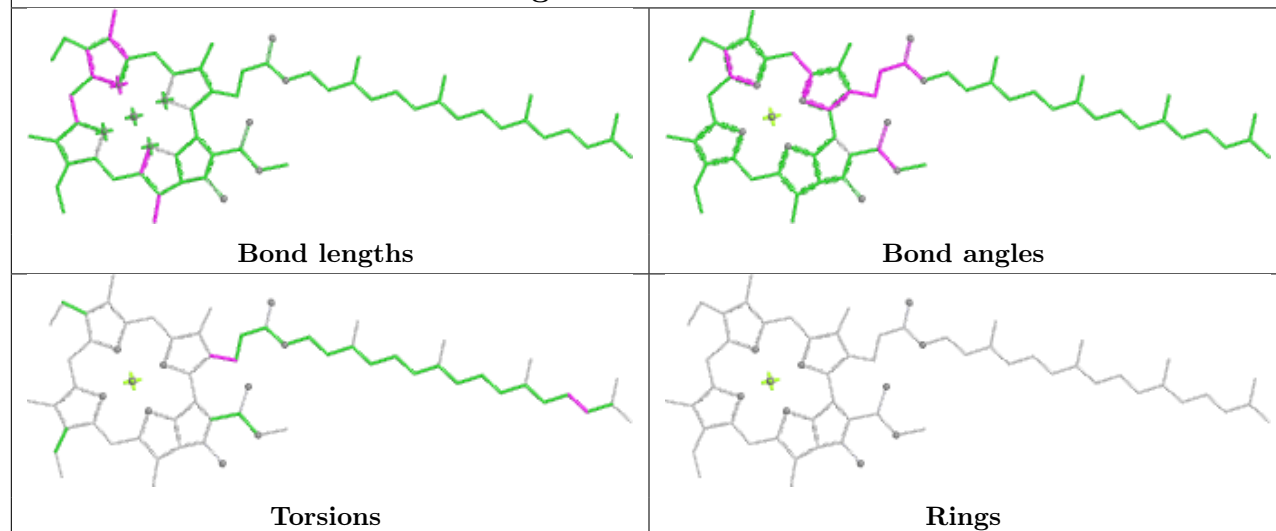
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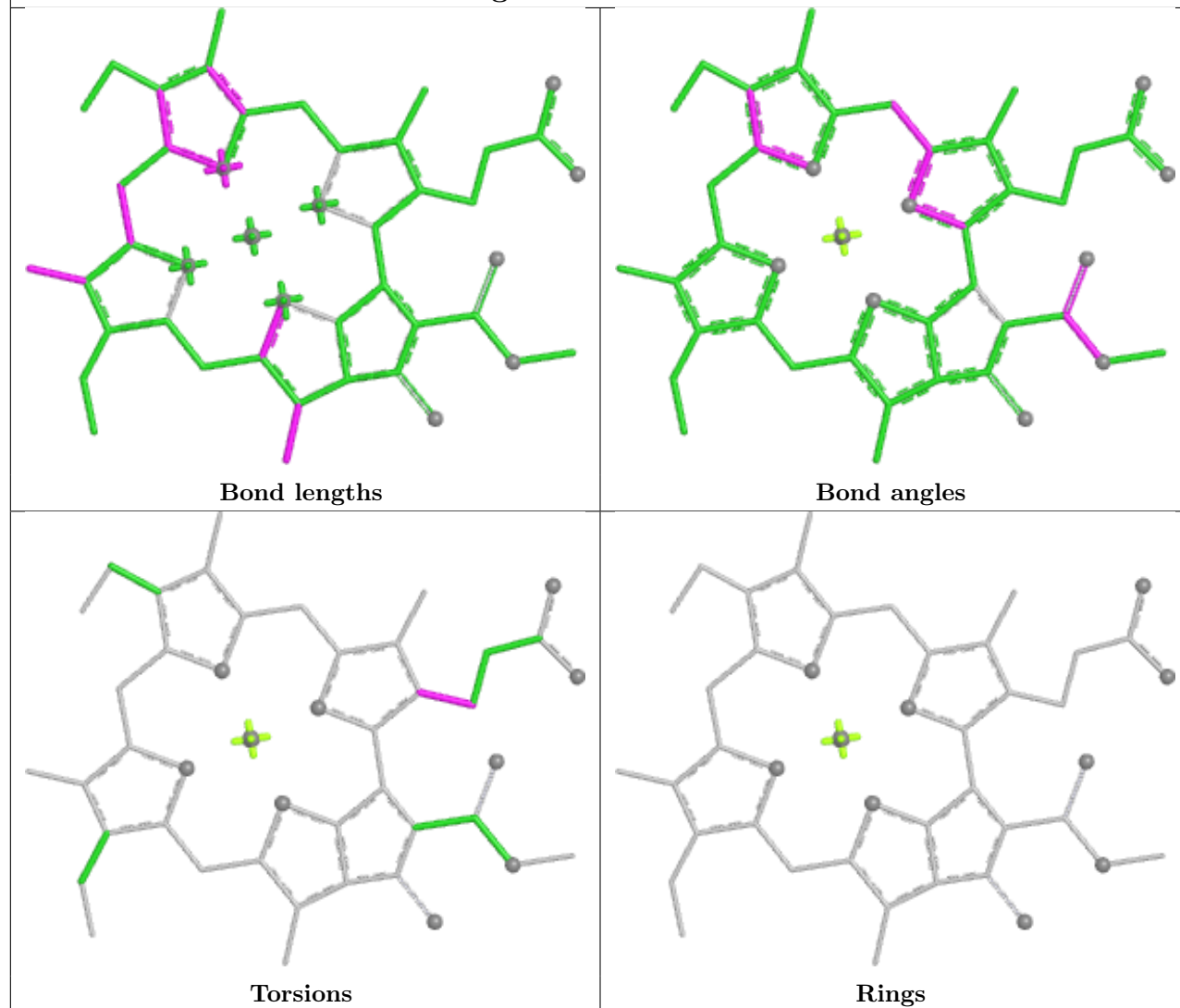
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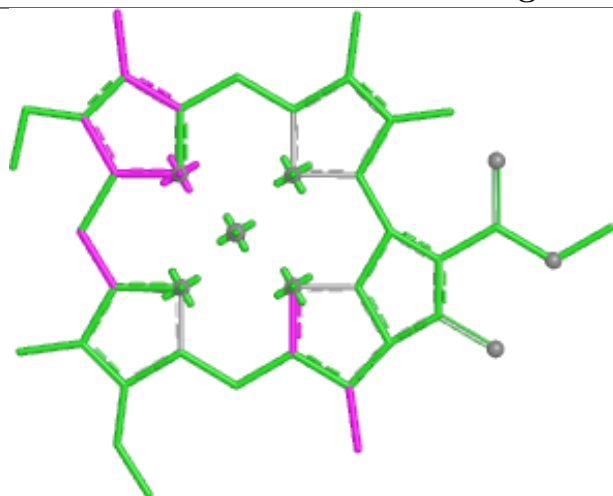
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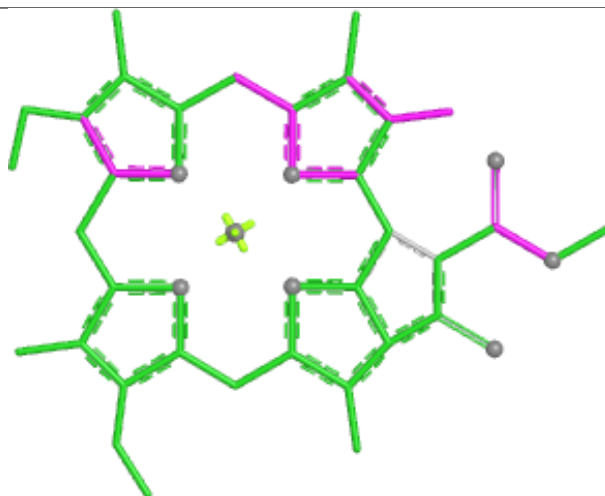
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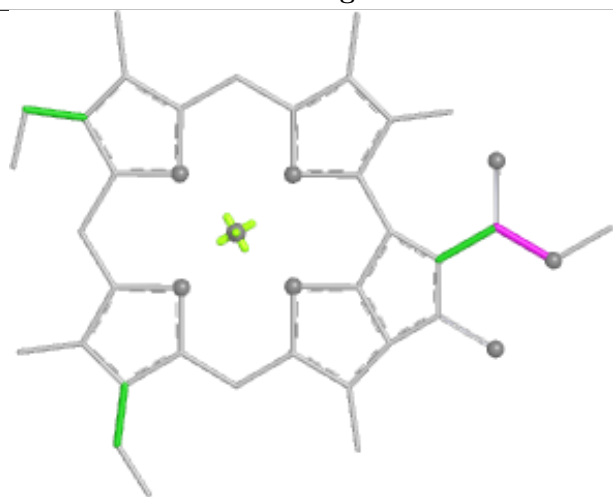
Ligand CLA 2 310



Bond lengths



Bond angles

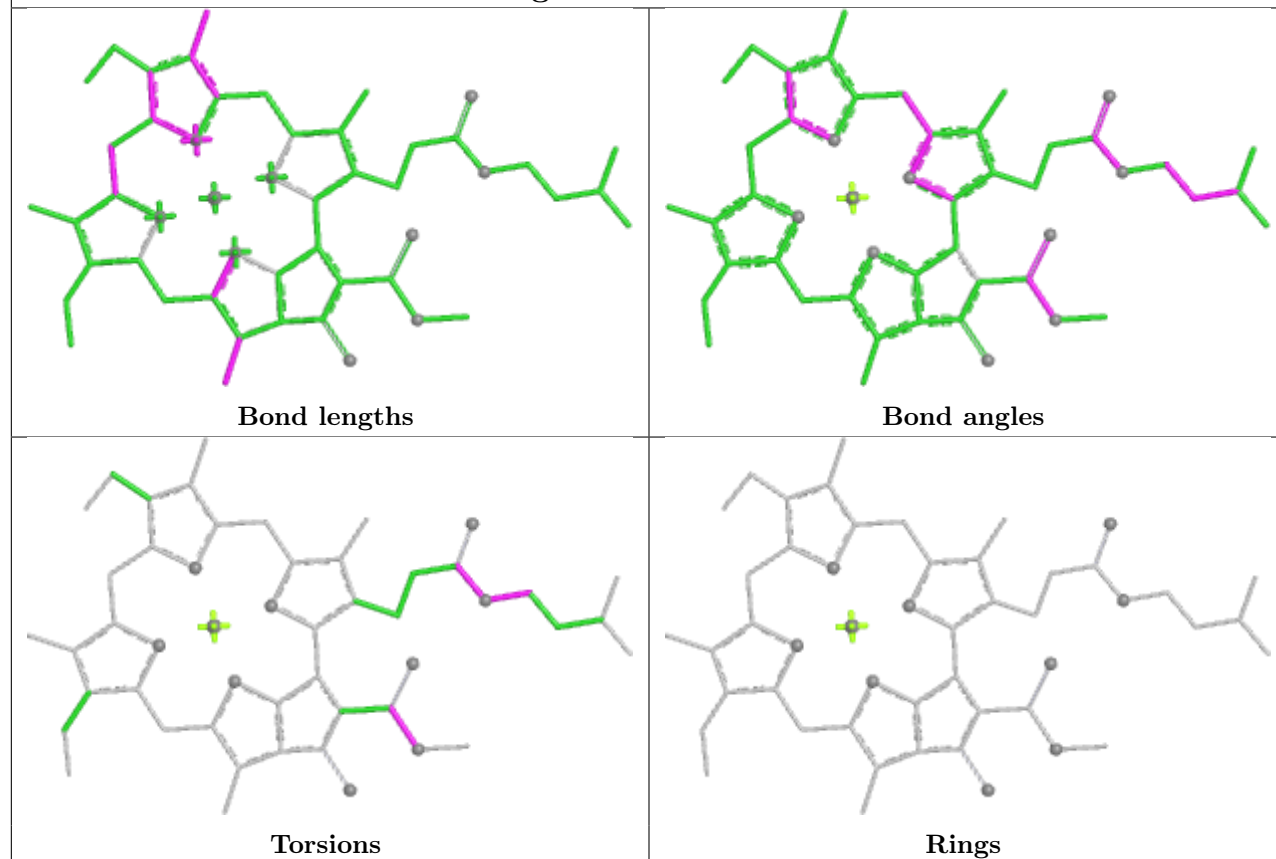


Torsions

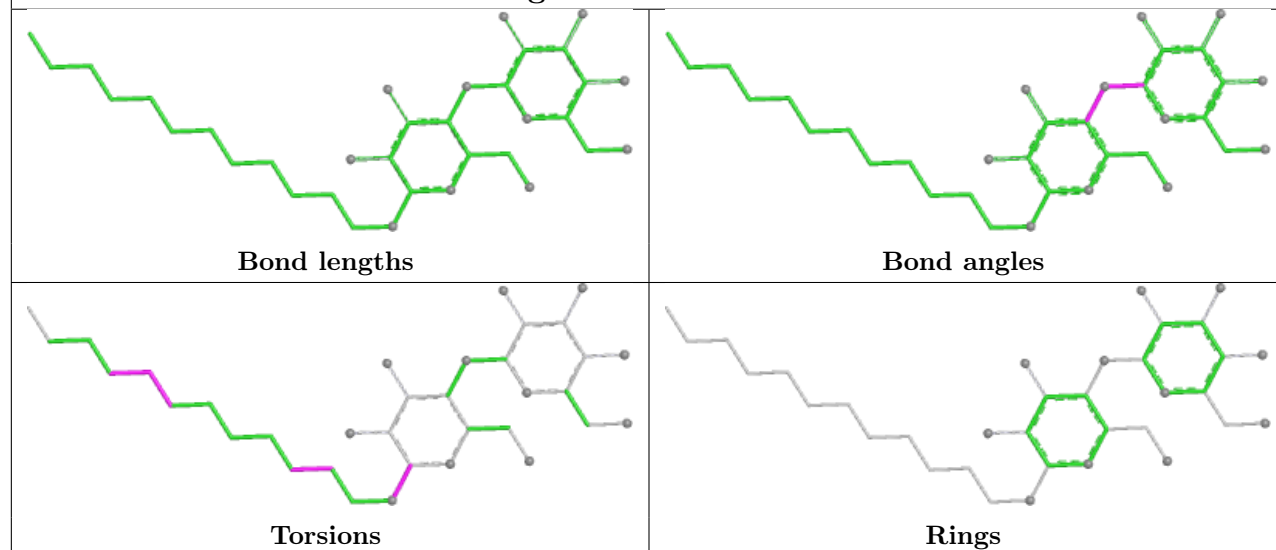


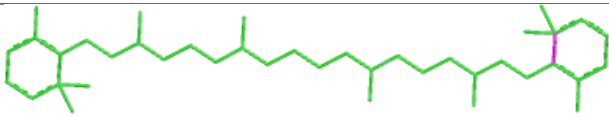
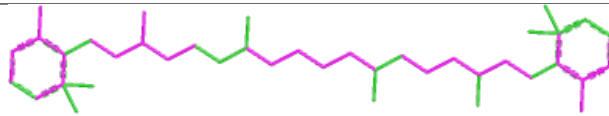
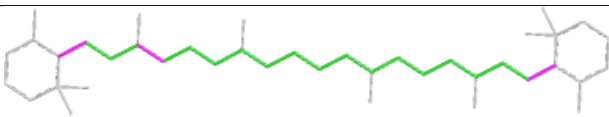
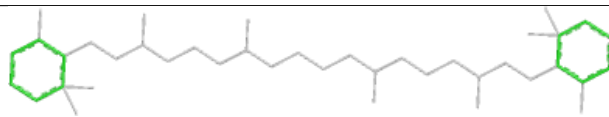
Rings

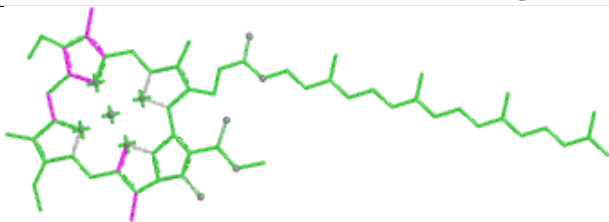
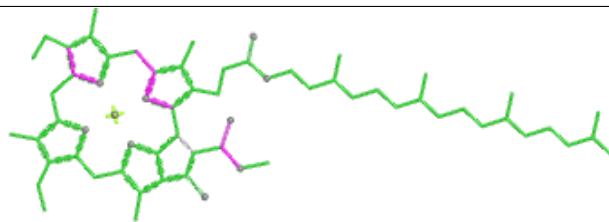
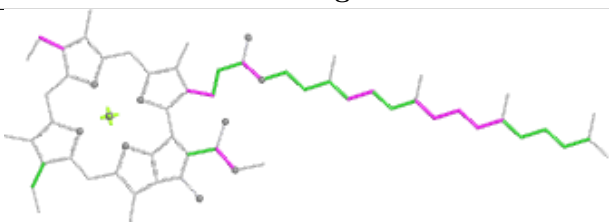
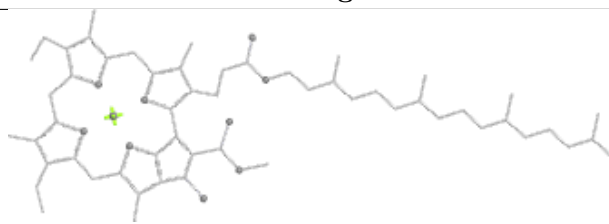
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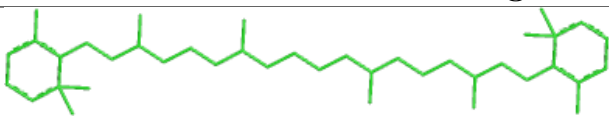
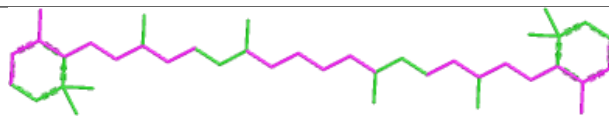
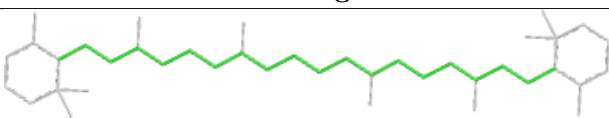
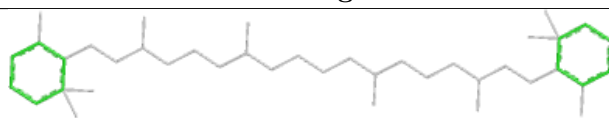


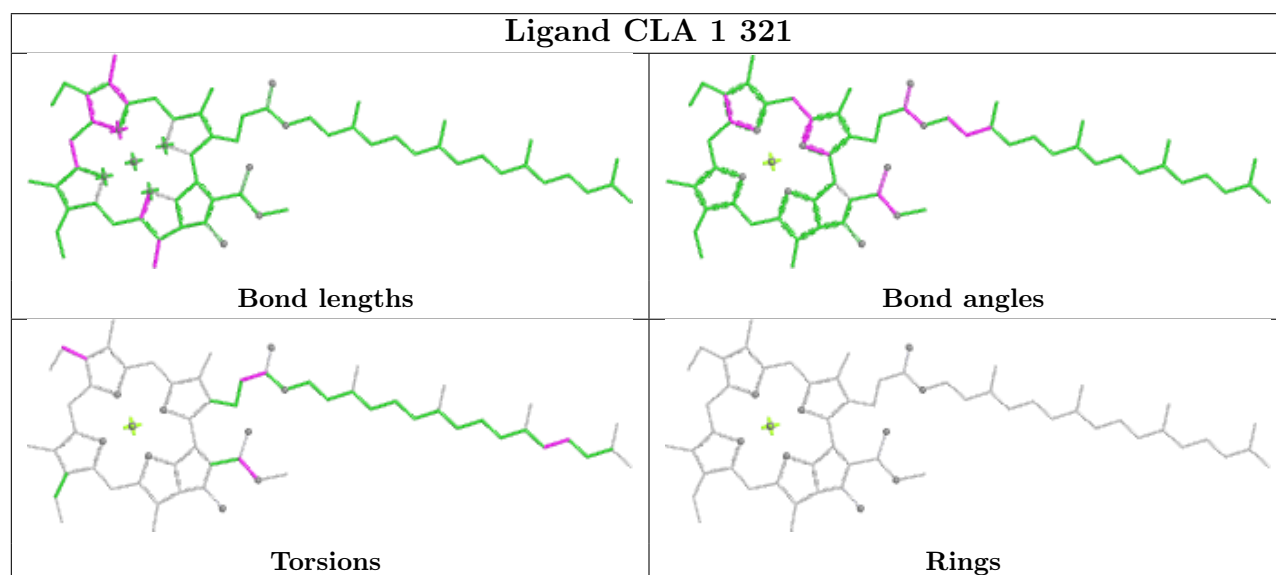
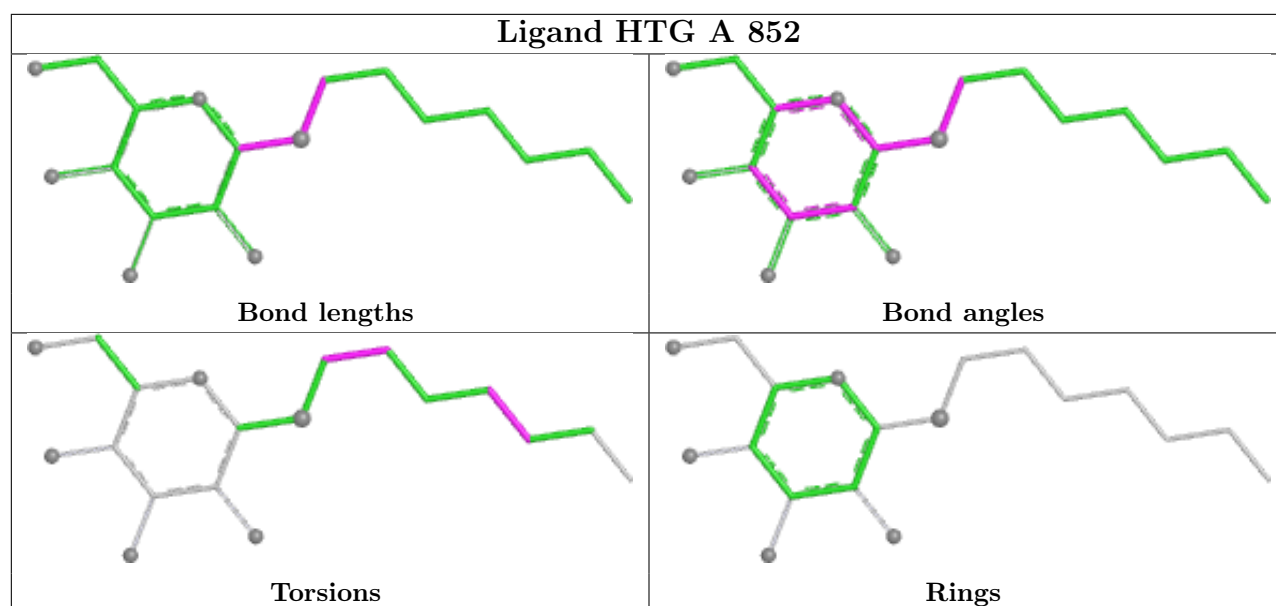
Ligand LMT G 601



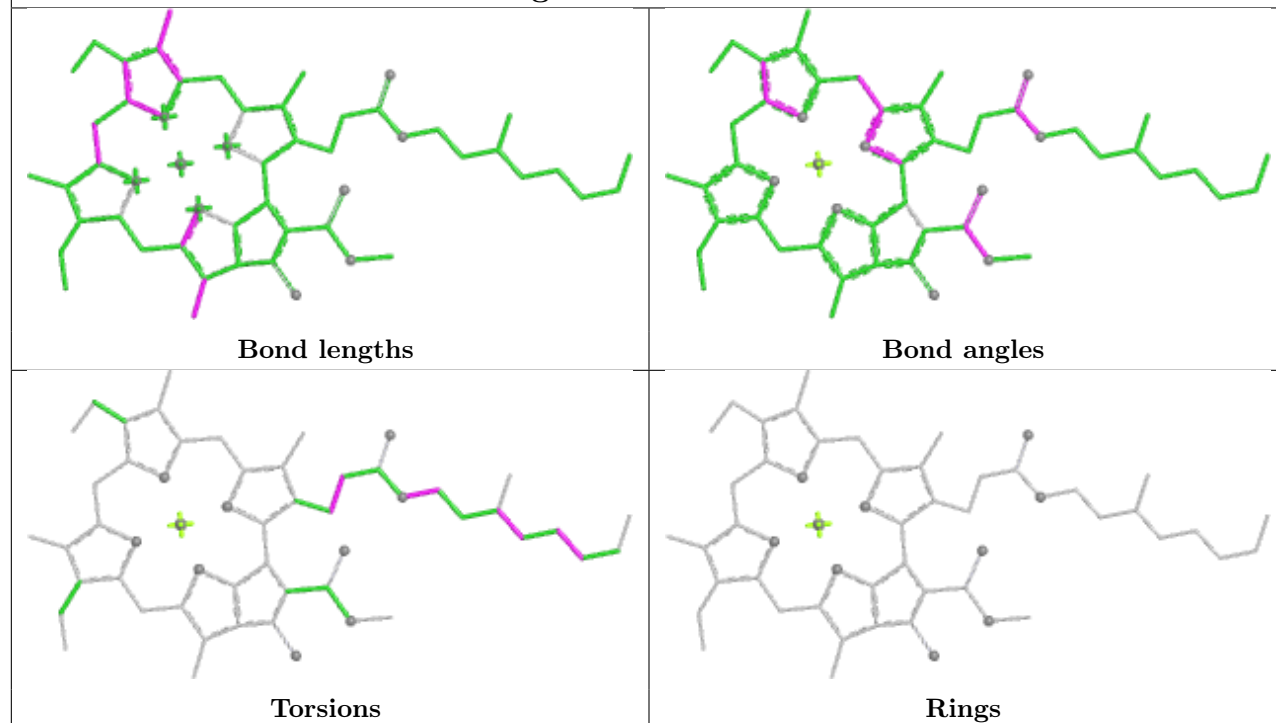
Ligand BCR B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

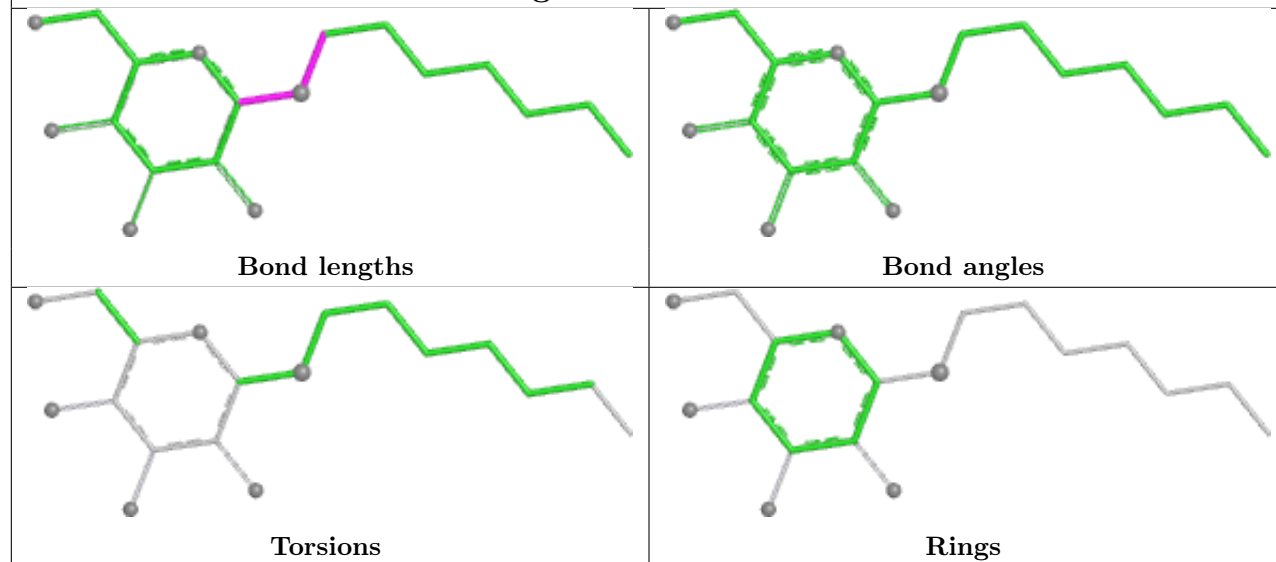
Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

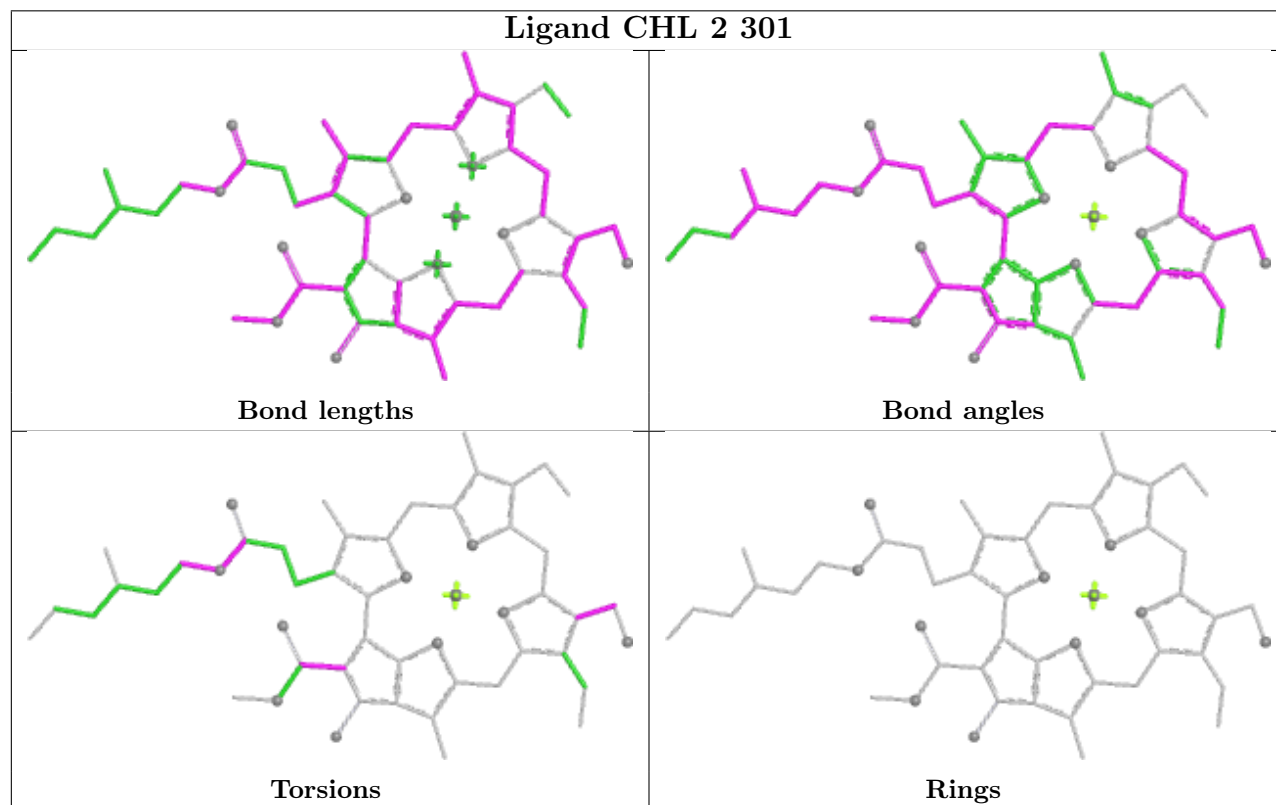
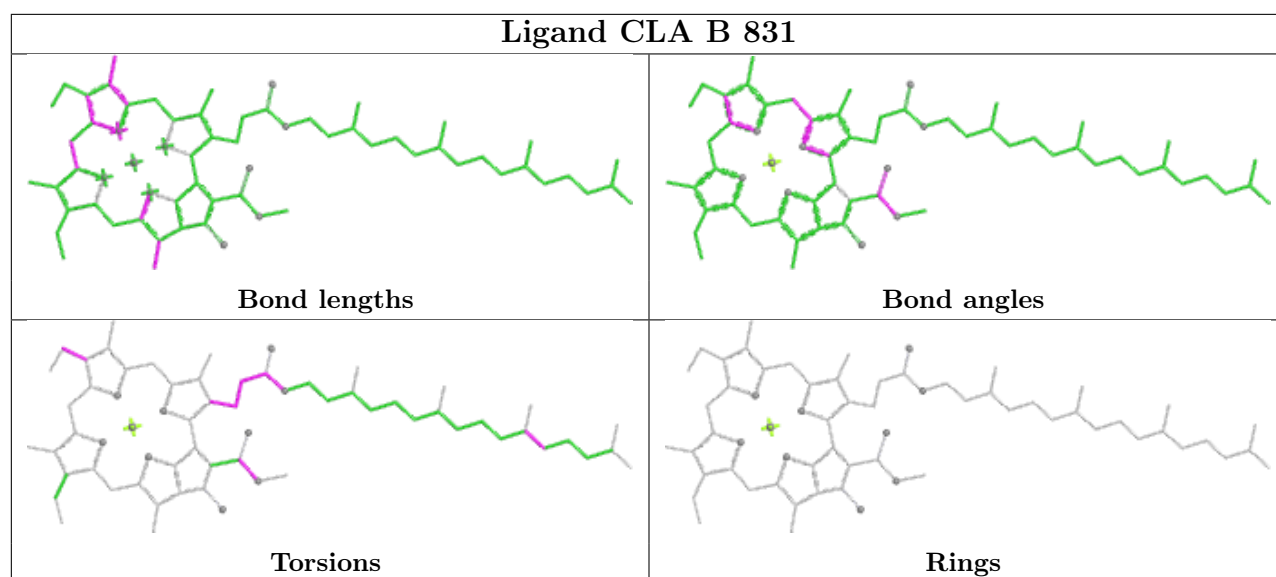


Ligand CLA A 811

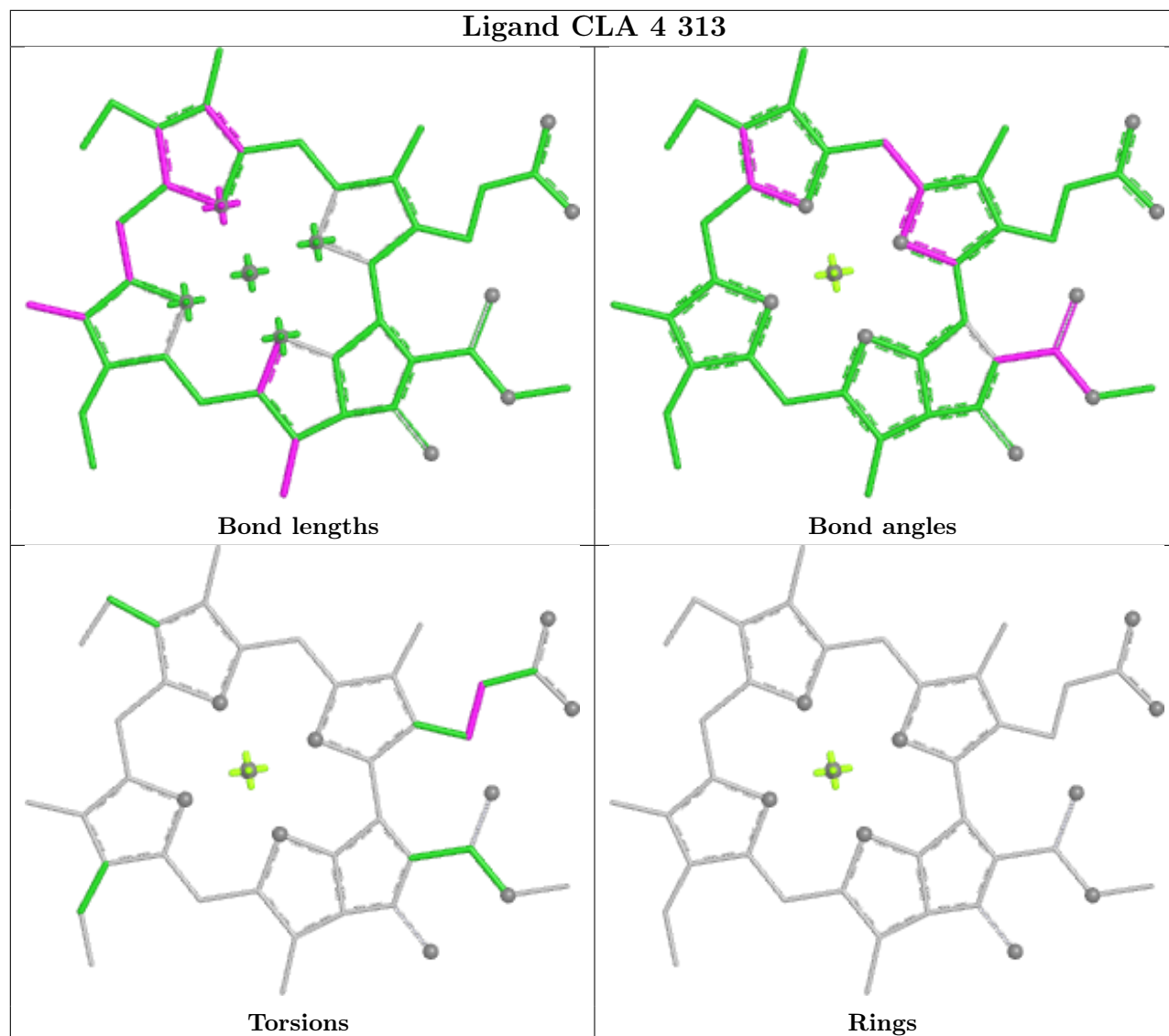


Ligand HTG J 105

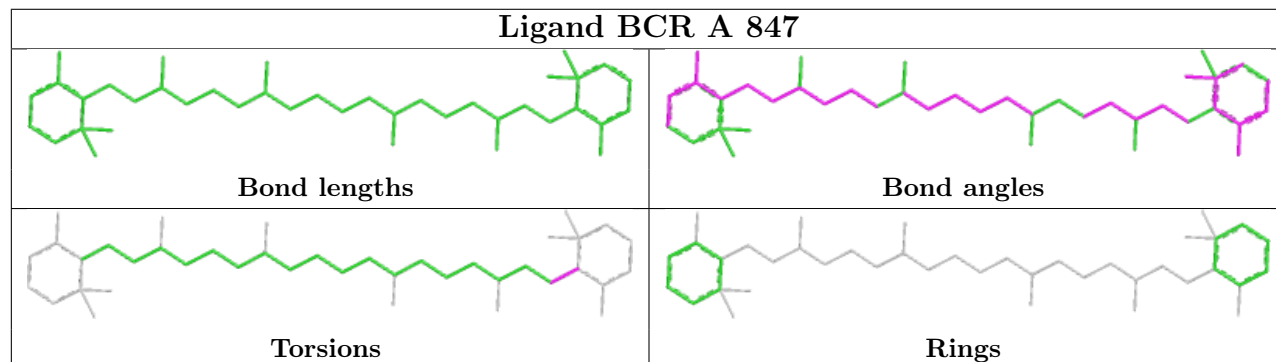


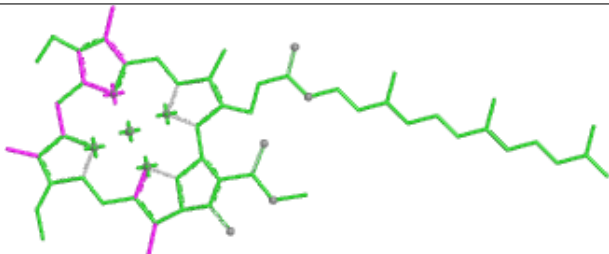
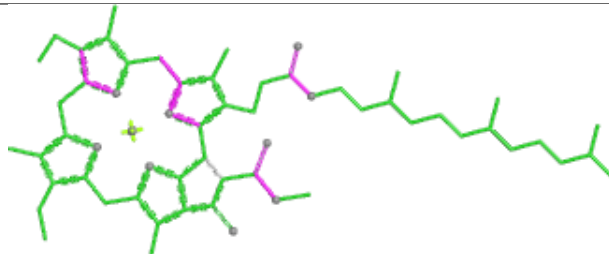
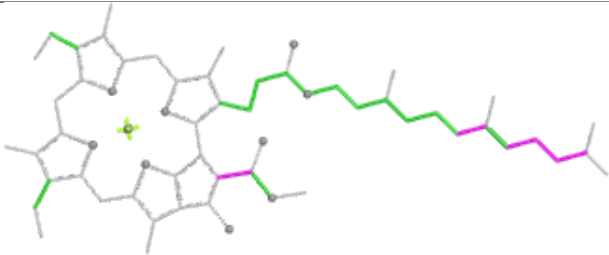
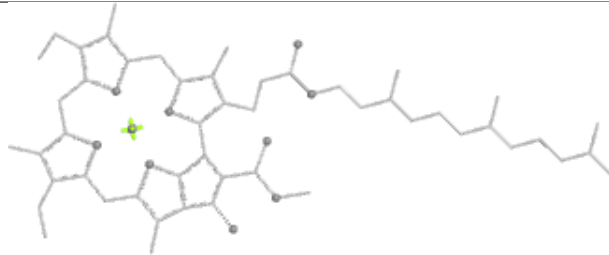
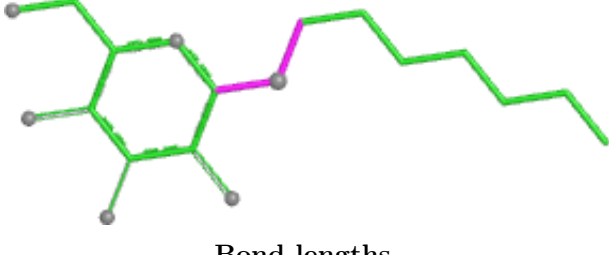
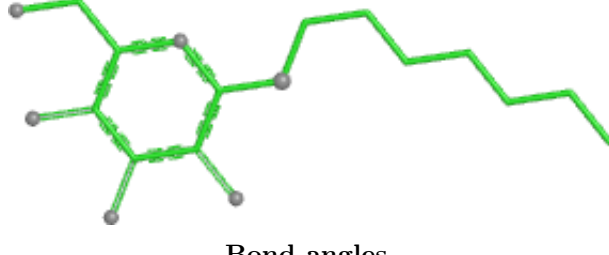
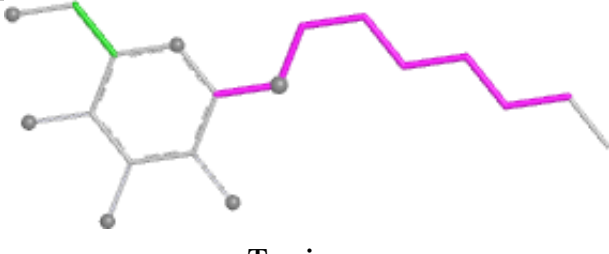
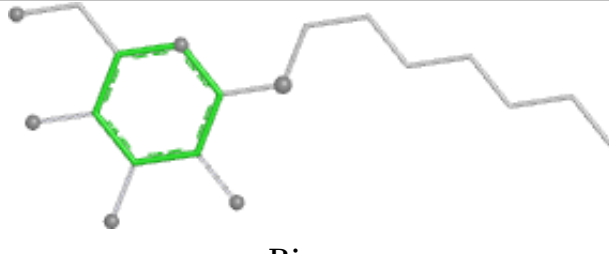
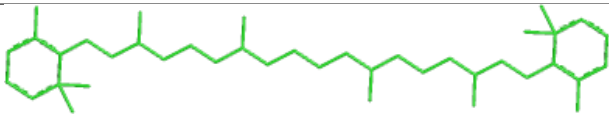
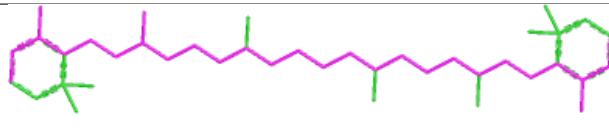
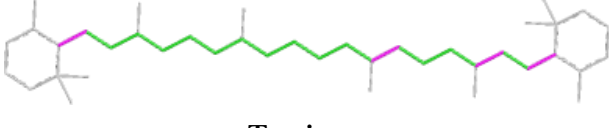
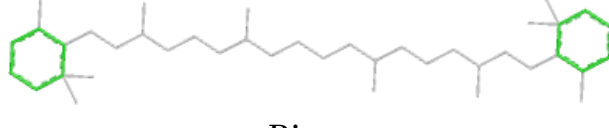


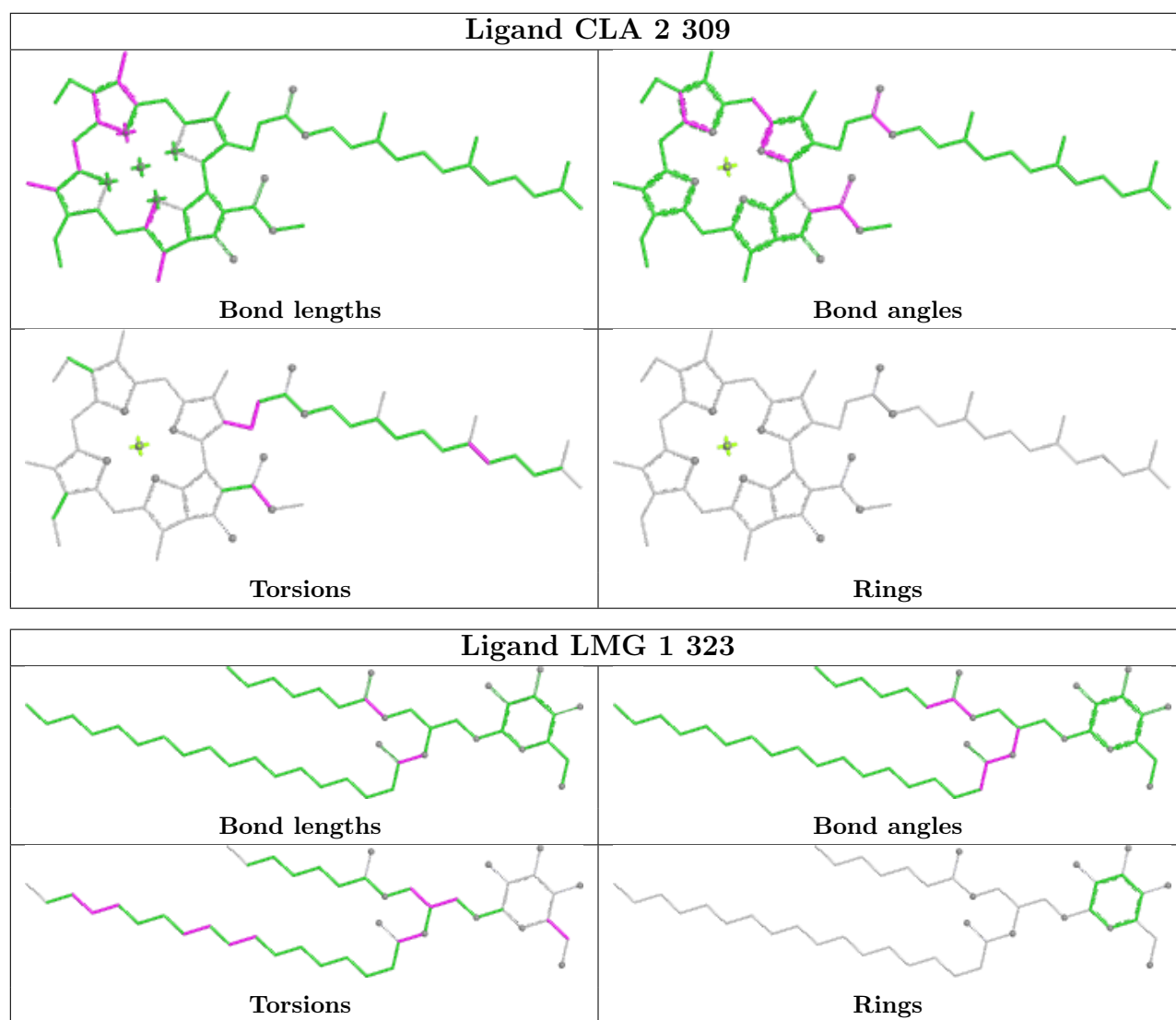
Ligand CLA 4 313



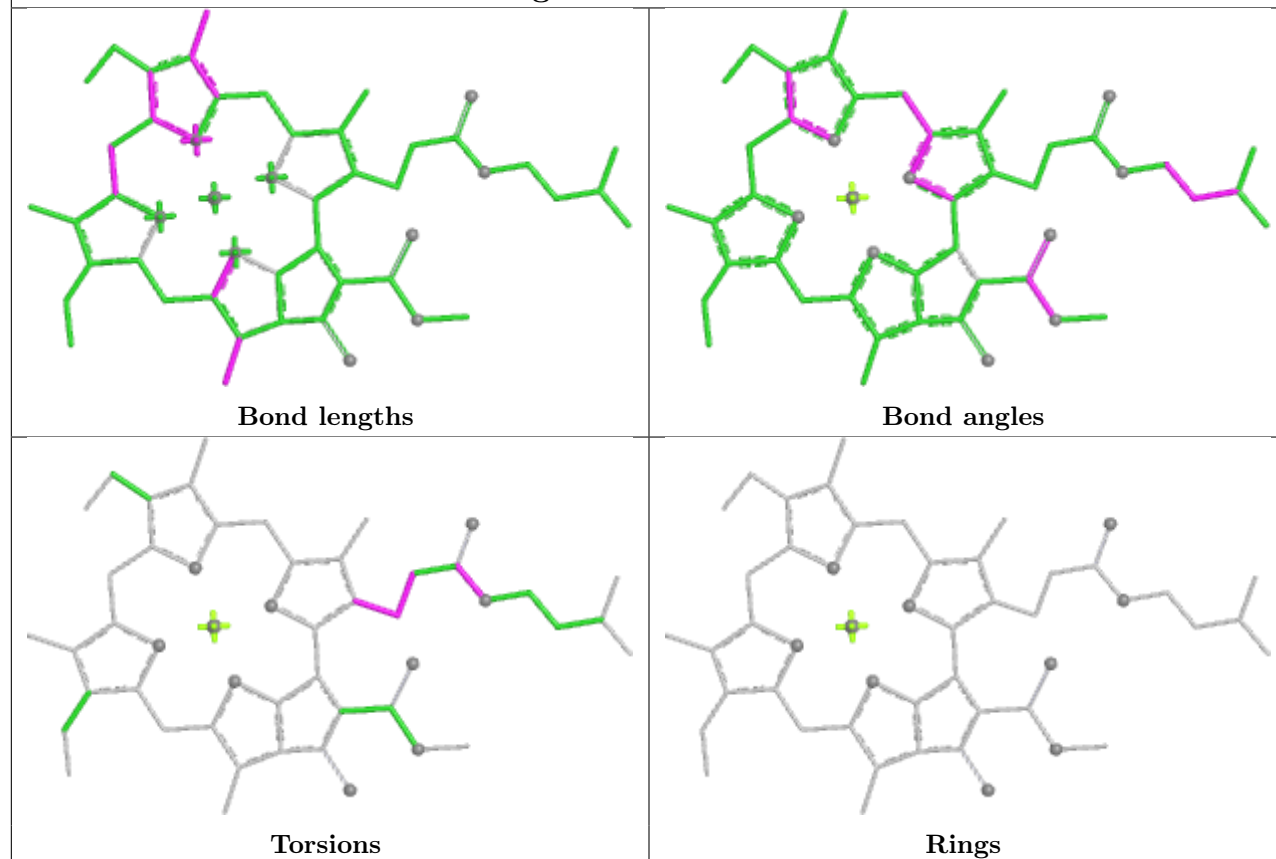
Ligand BCR A 847



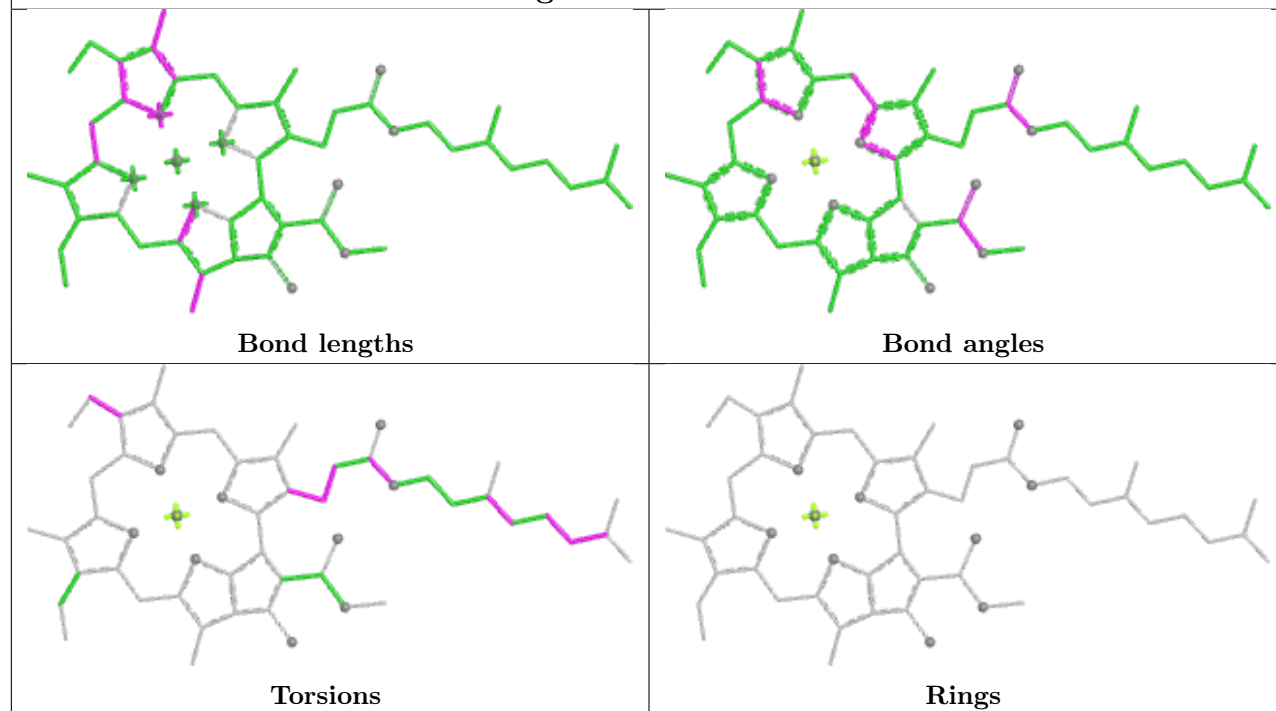
Ligand CLA 3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand HTG B 850	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



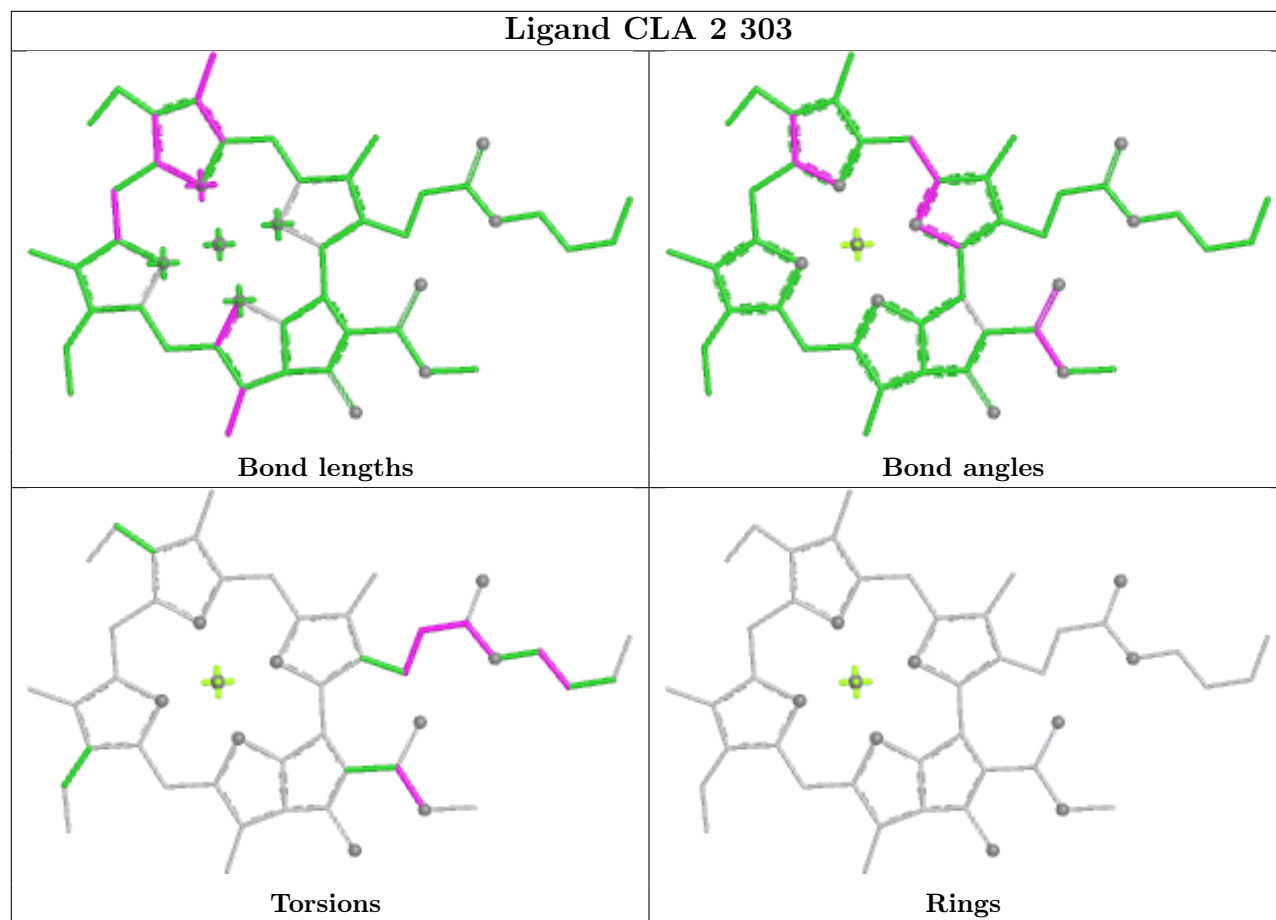
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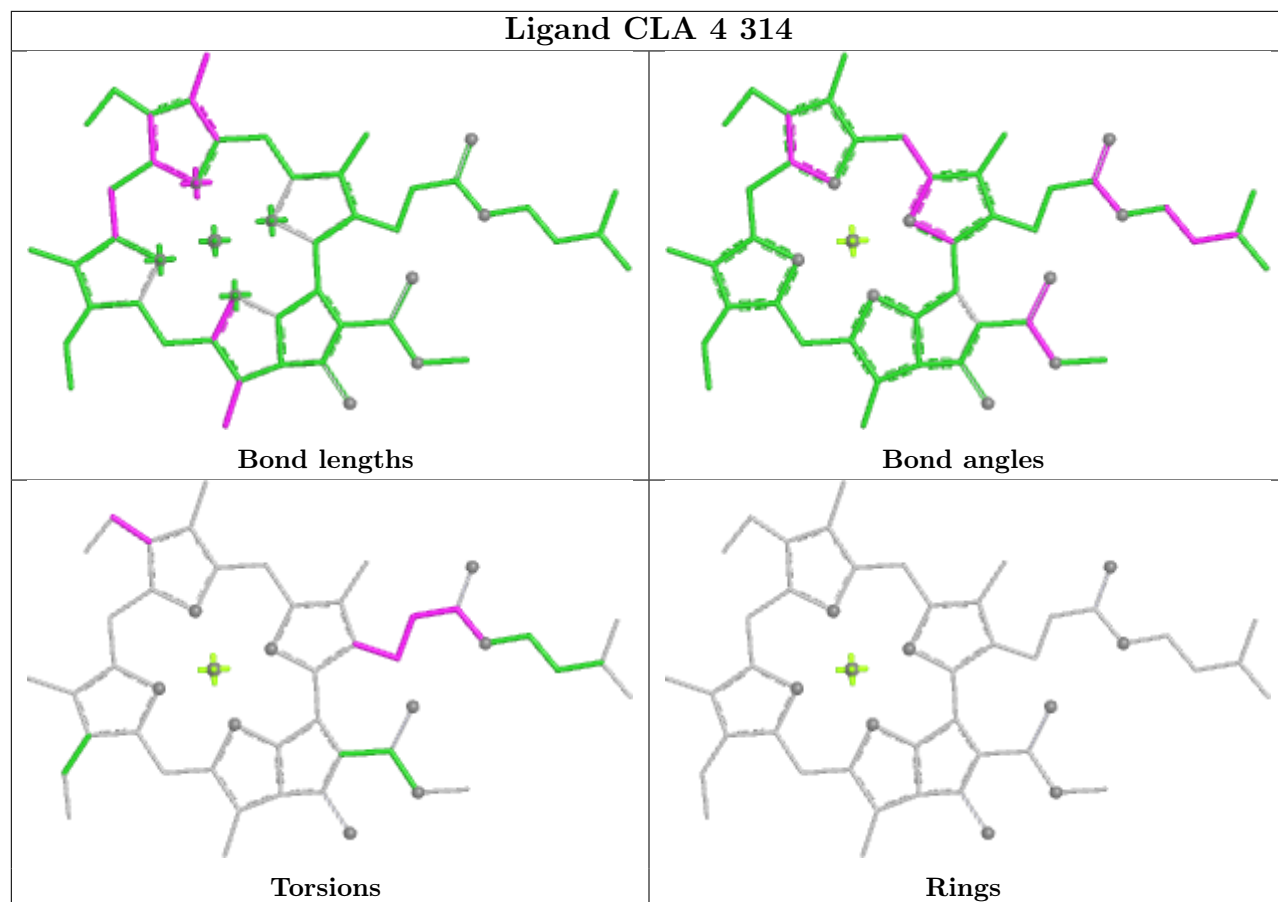
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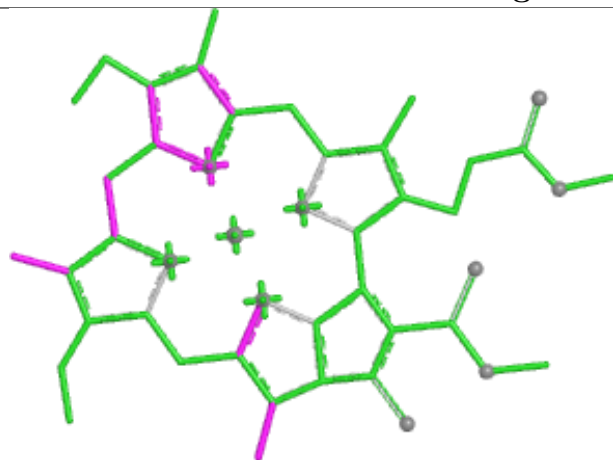
Ligand CLA 2 303



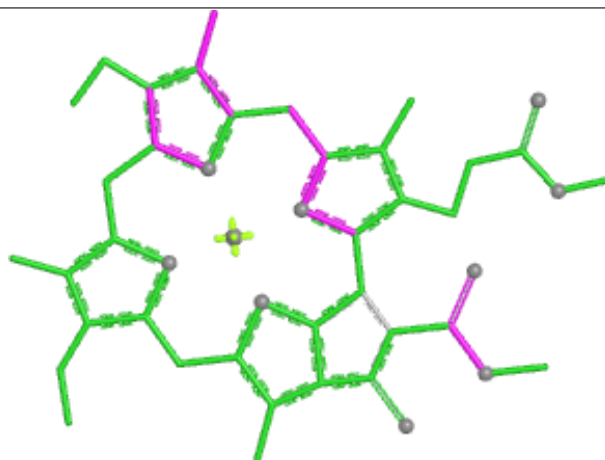
Ligand CLA 4 314



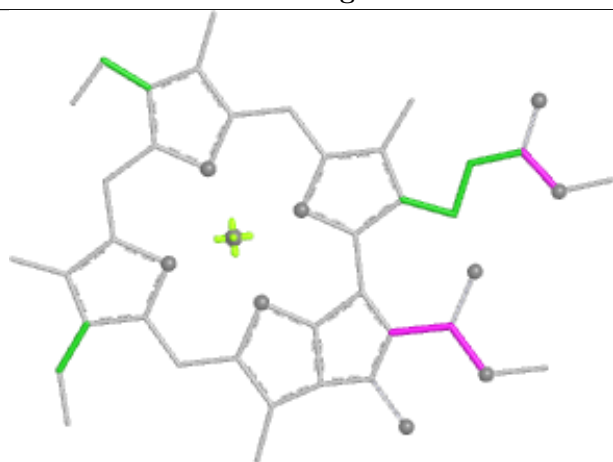
Ligand CLA K 203



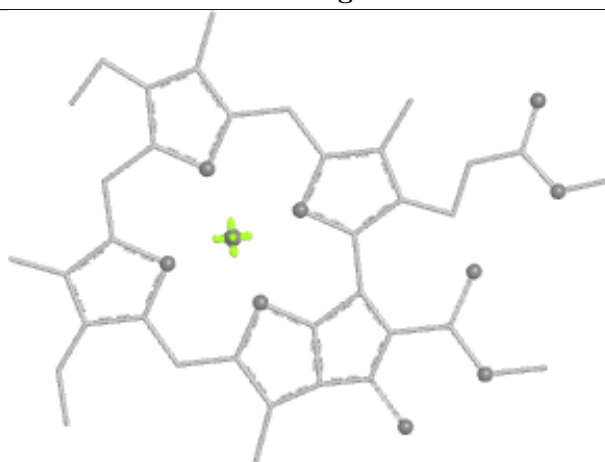
Bond lengths



Bond angles

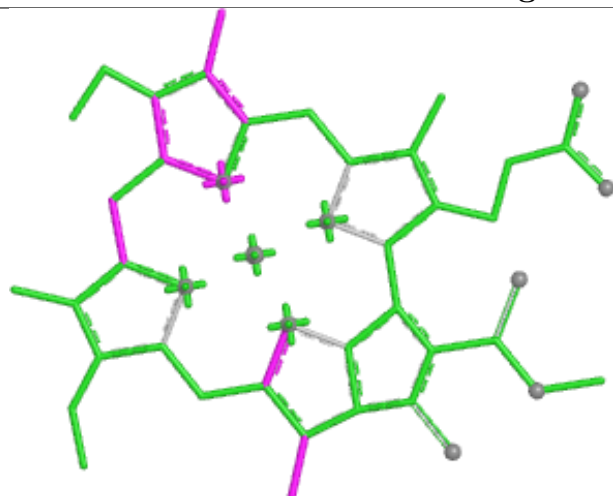


Torsions

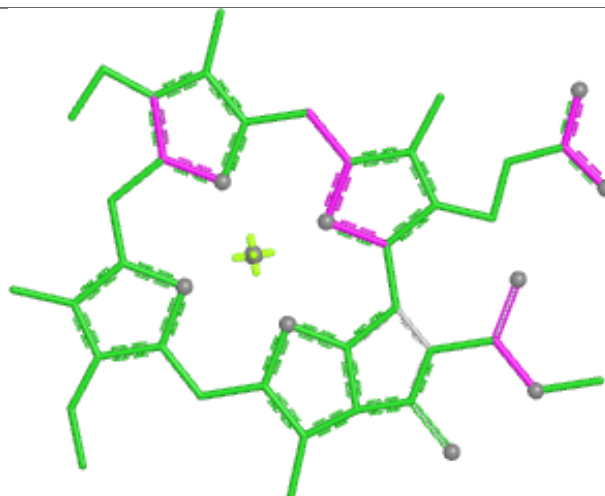


Rings

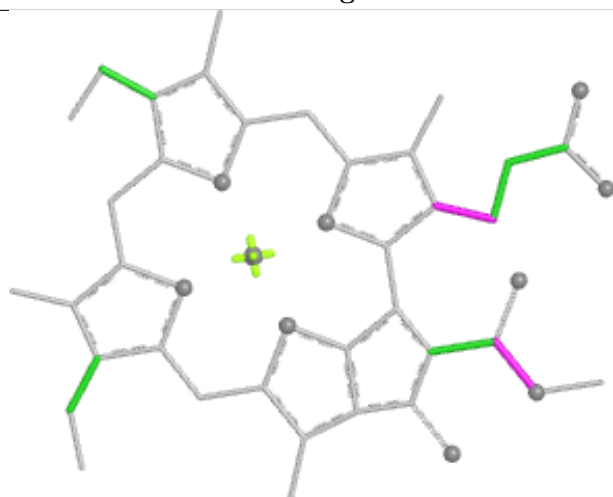
Ligand CLA 3 303



Bond lengths



Bond angles

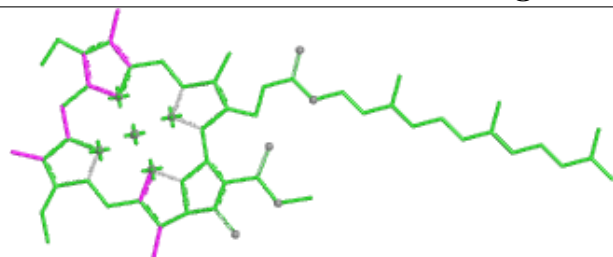


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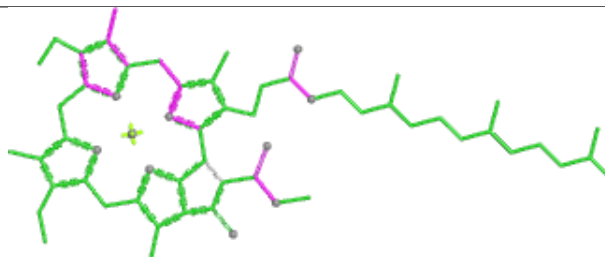


Rings

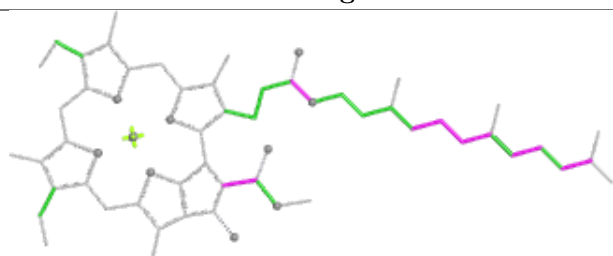
Ligand CLA B 815



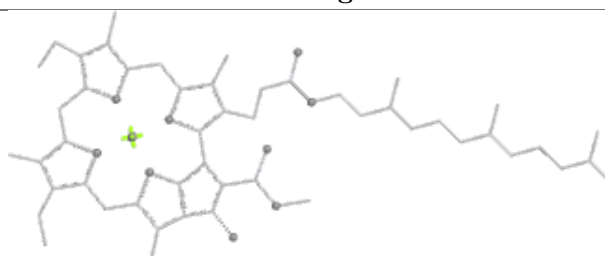
Bond lengths



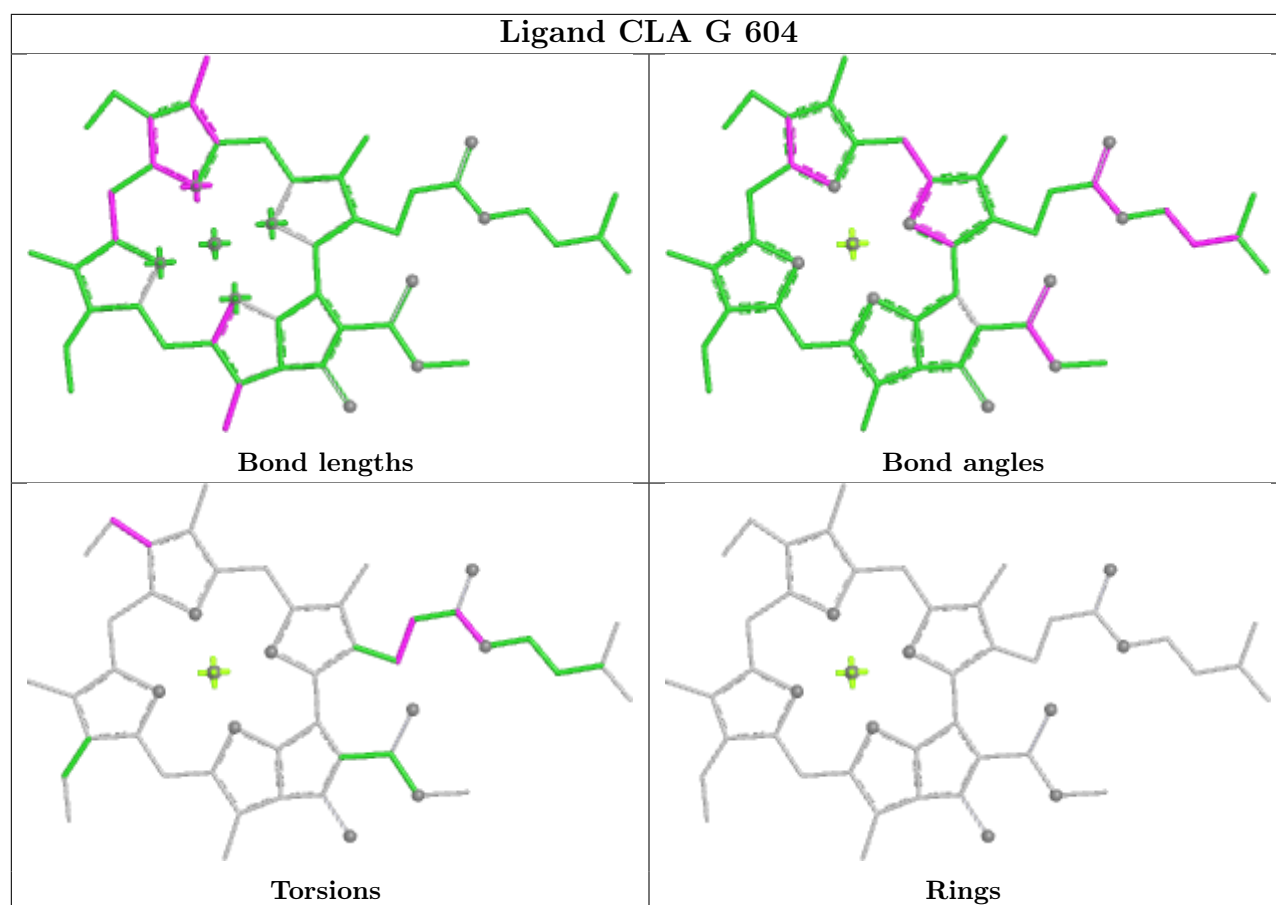
Bond angles



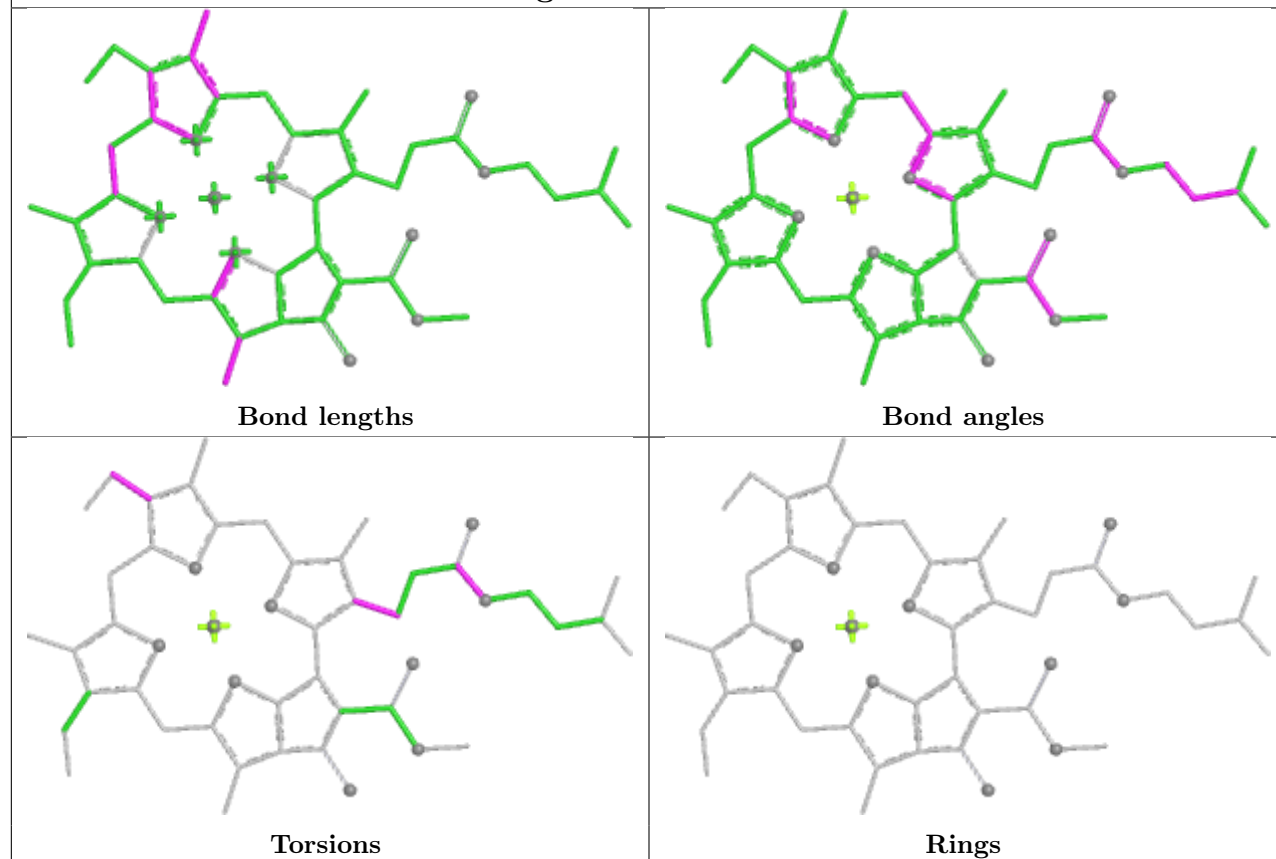
Torsions



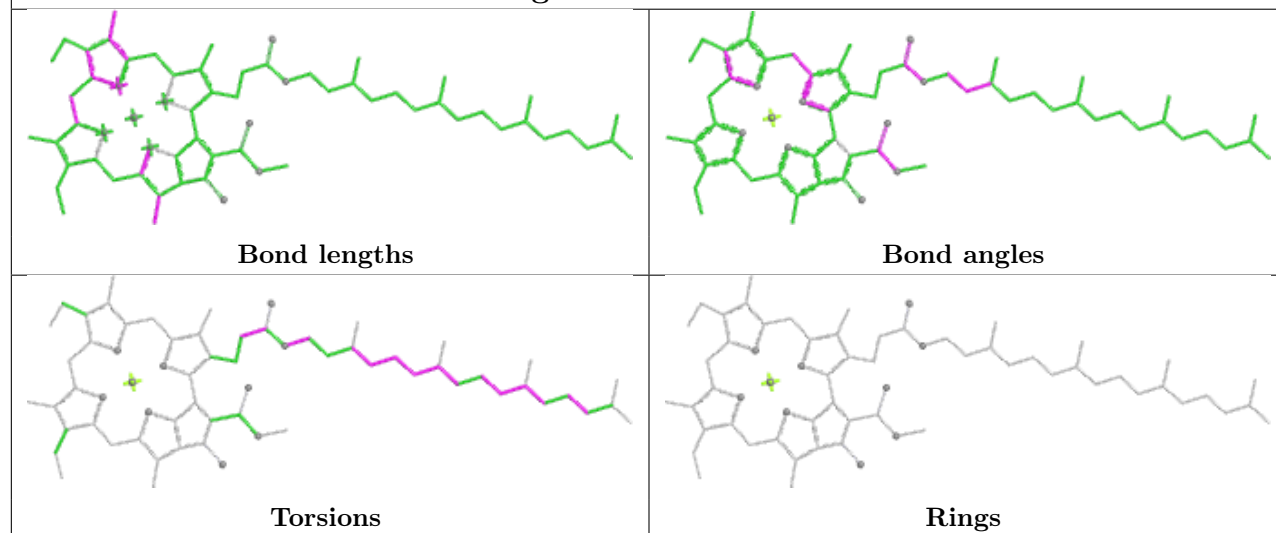
Rings

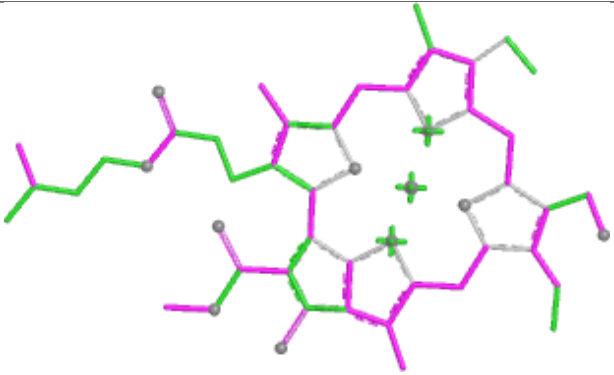
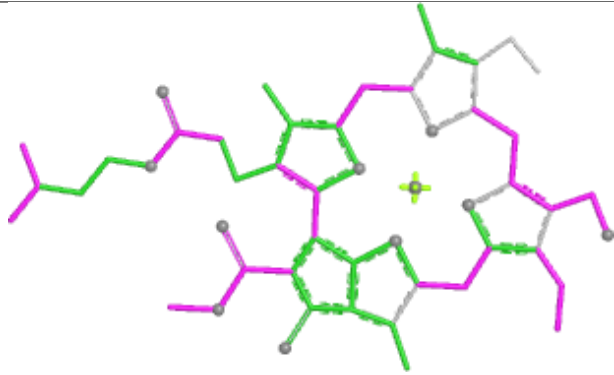
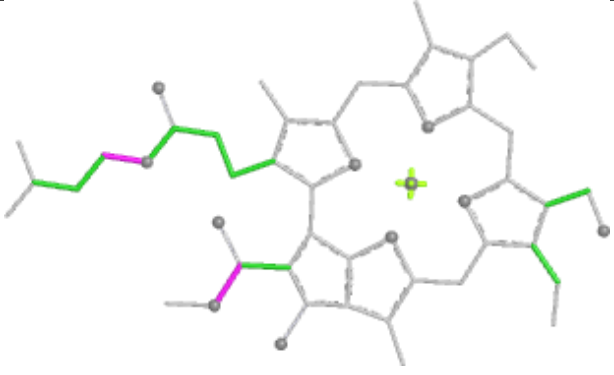
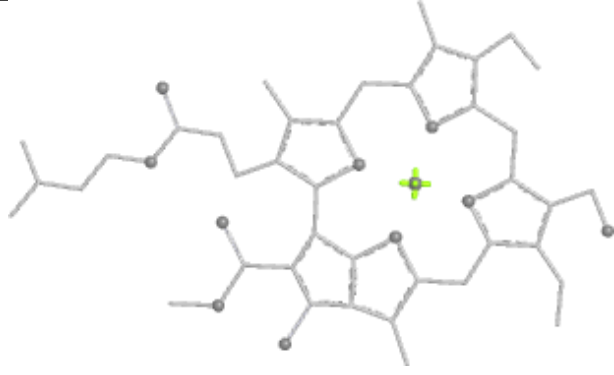
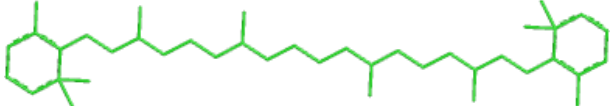
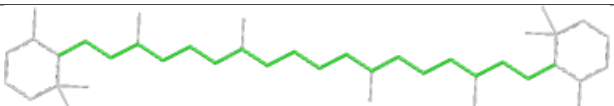
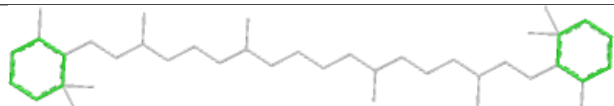


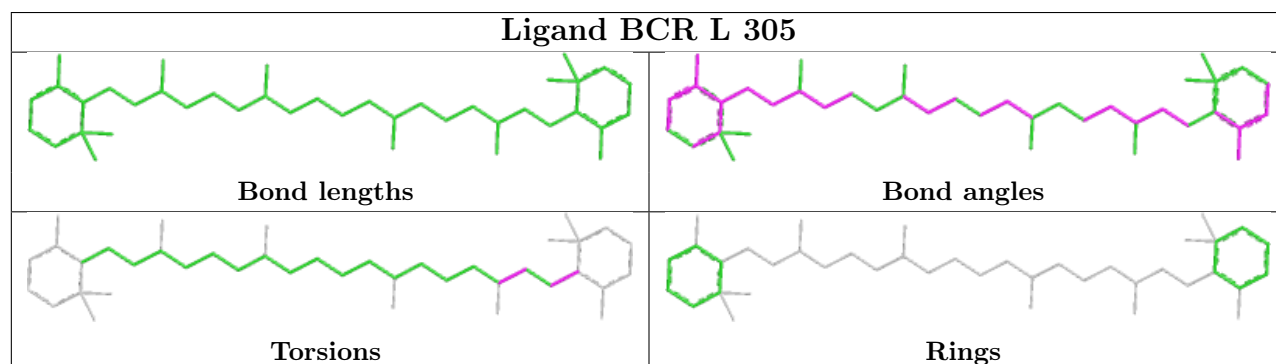
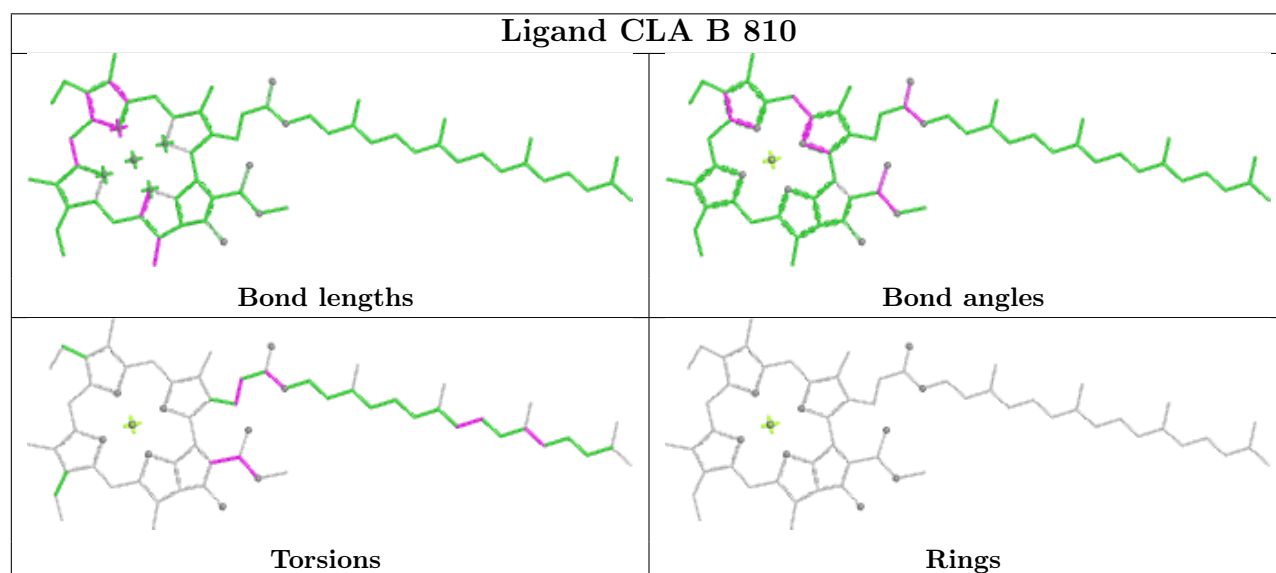
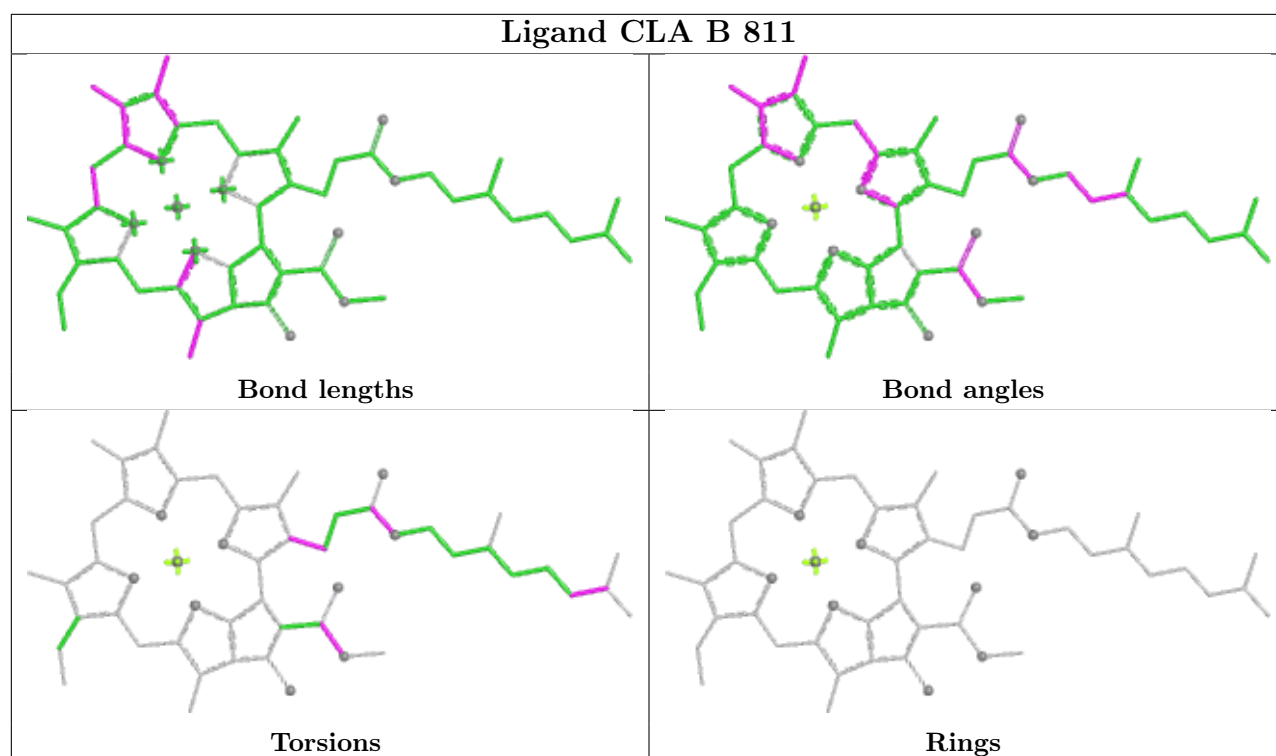
Ligand CLA 4 308

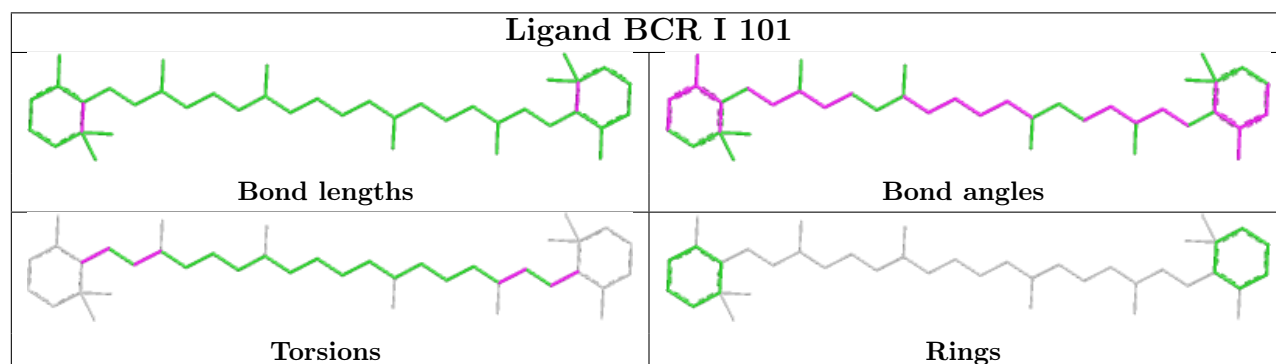
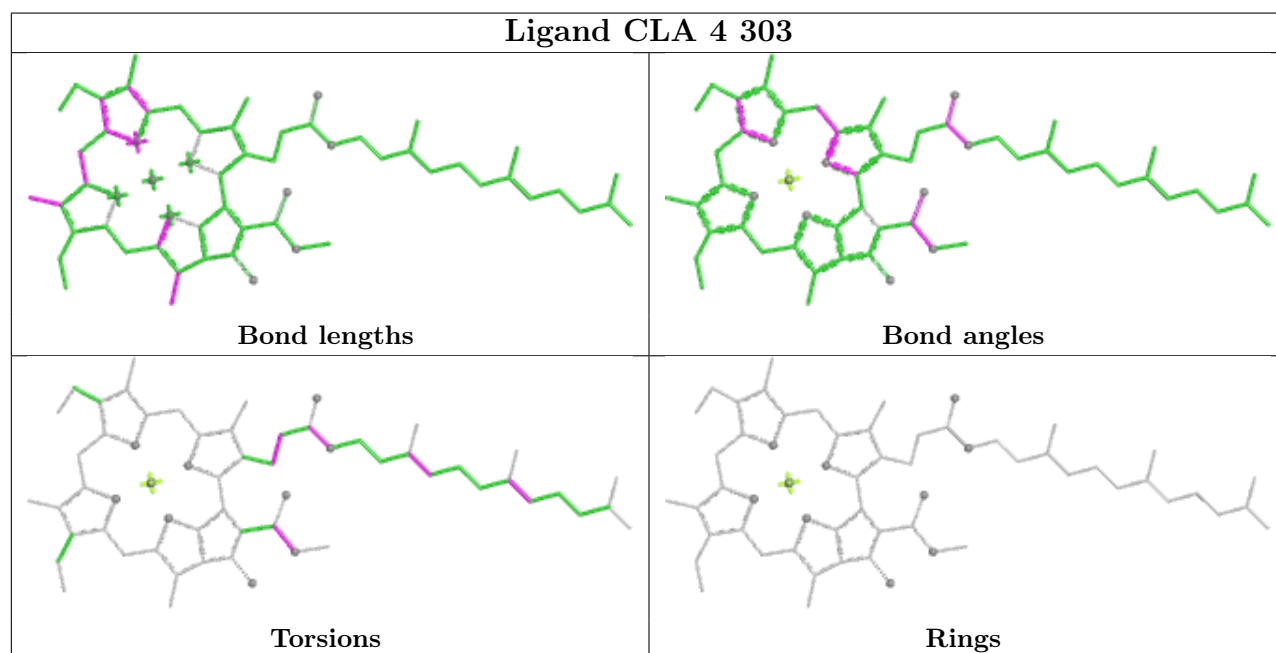
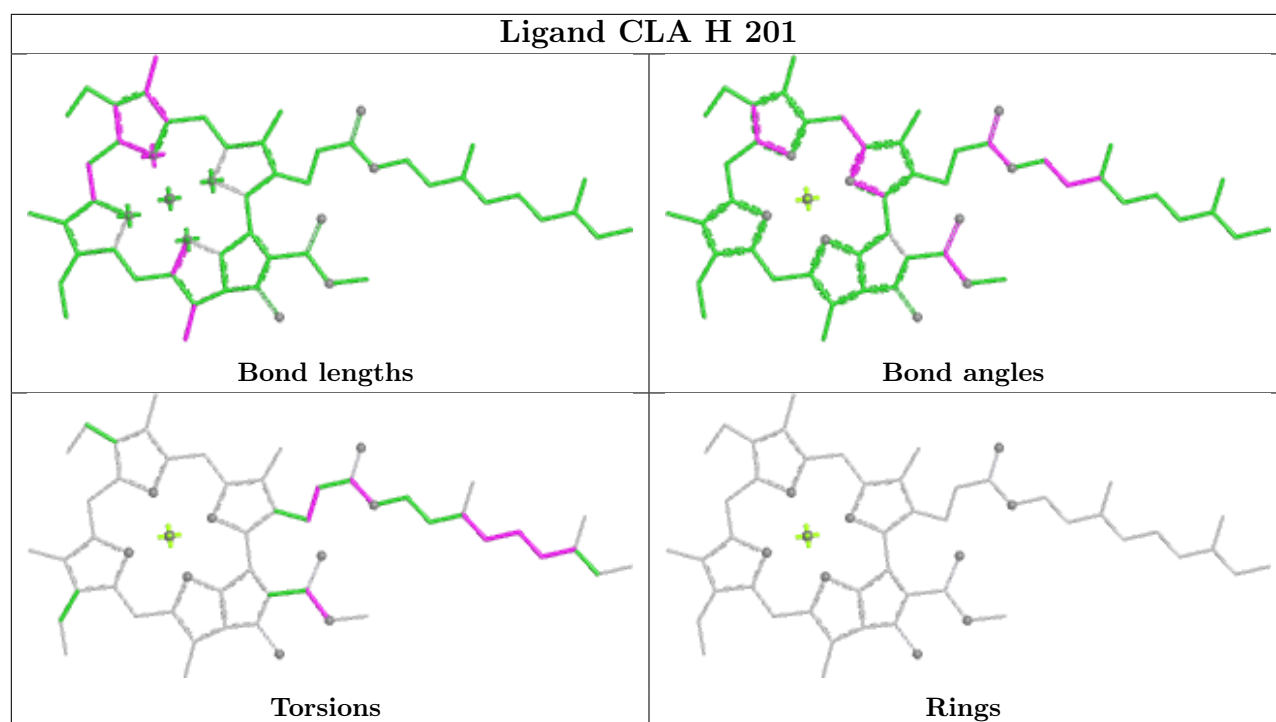


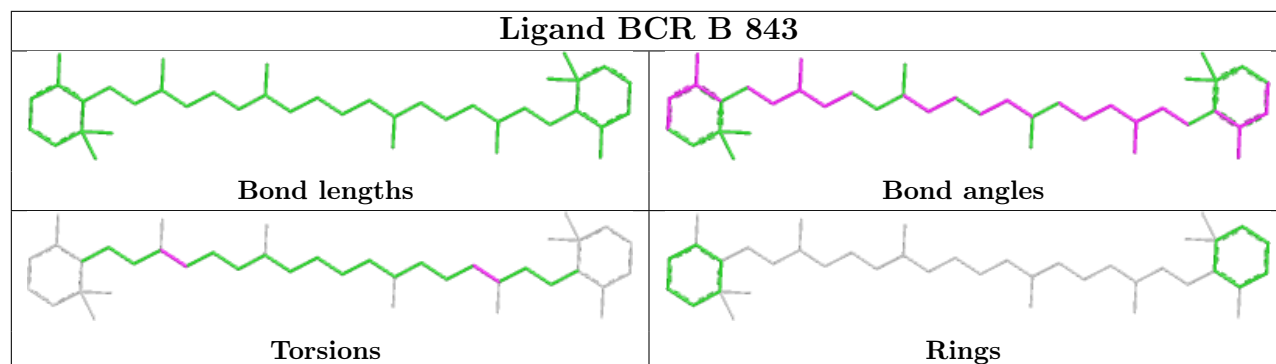
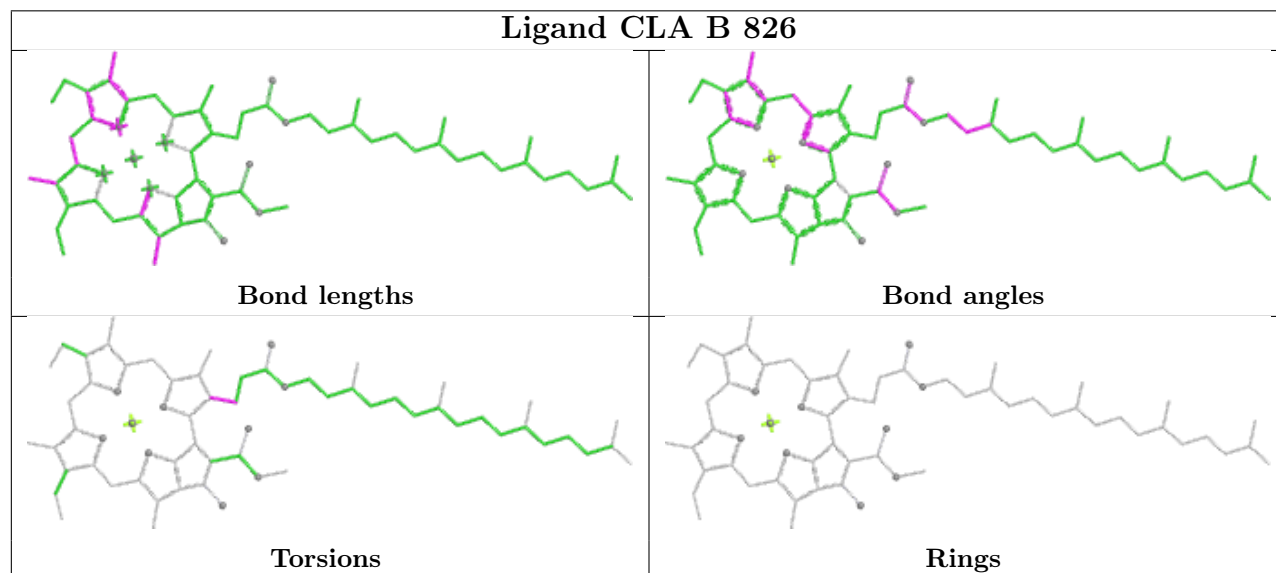
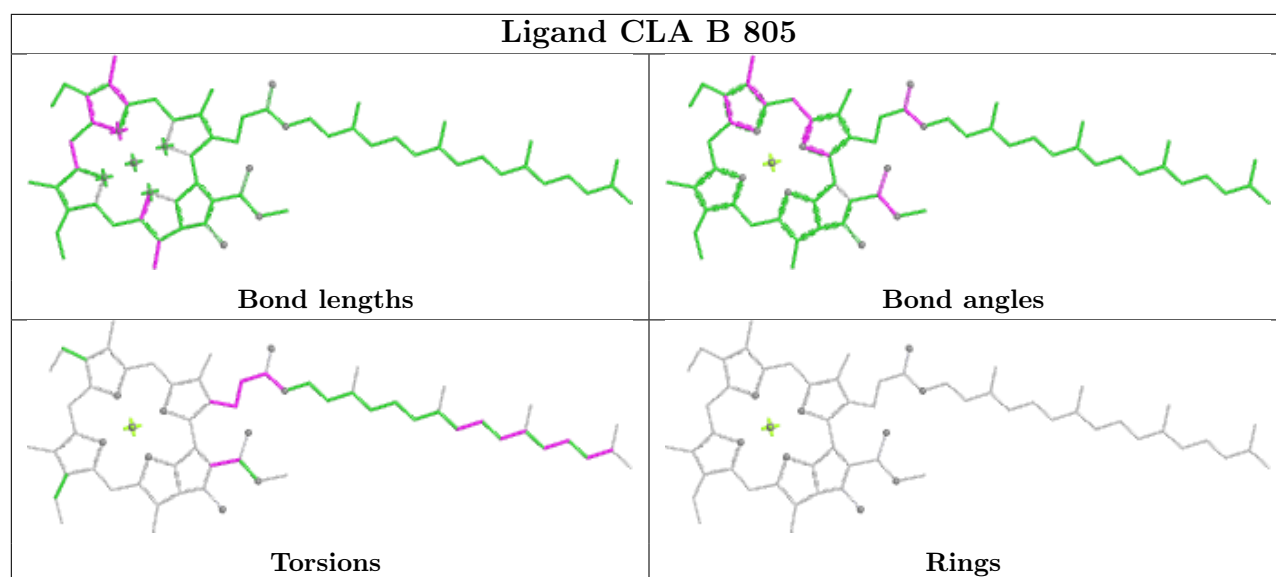
Ligand CLA A 805



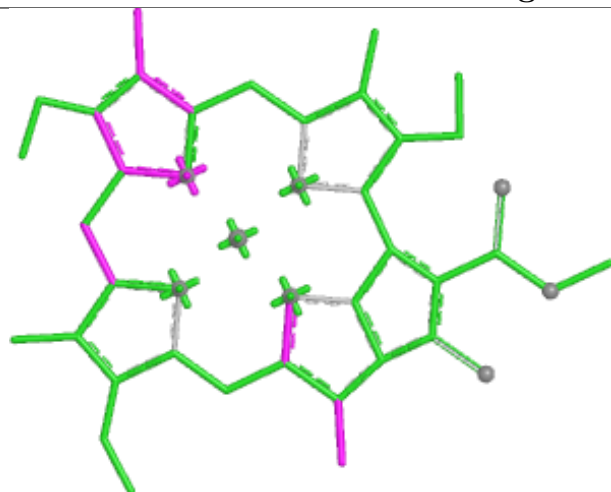
Ligand CHL 4 307	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR 2 317	
	
Bond lengths	Bond angles
	
Torsions	Rings



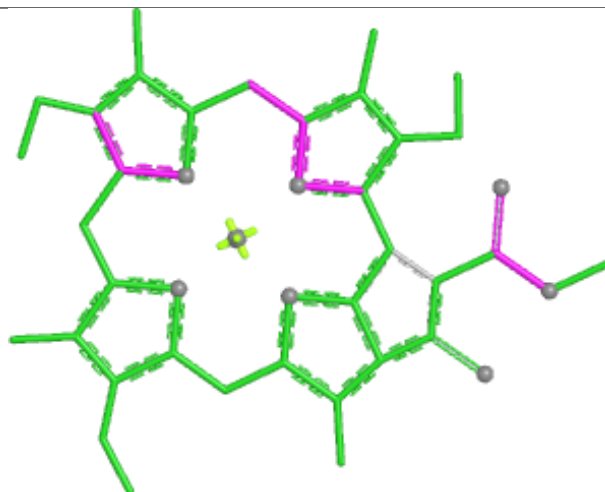




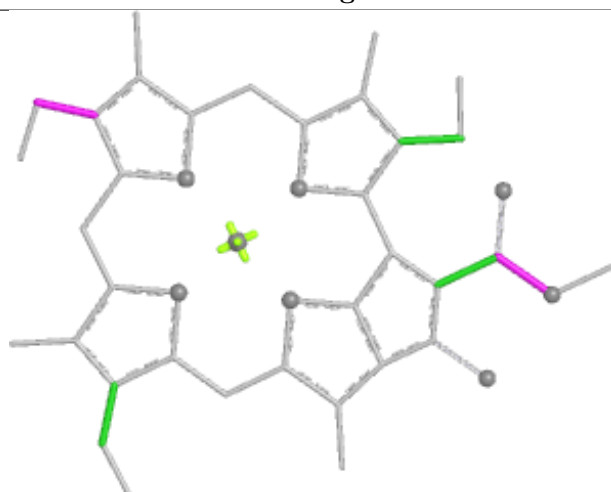
Ligand CLA J 103



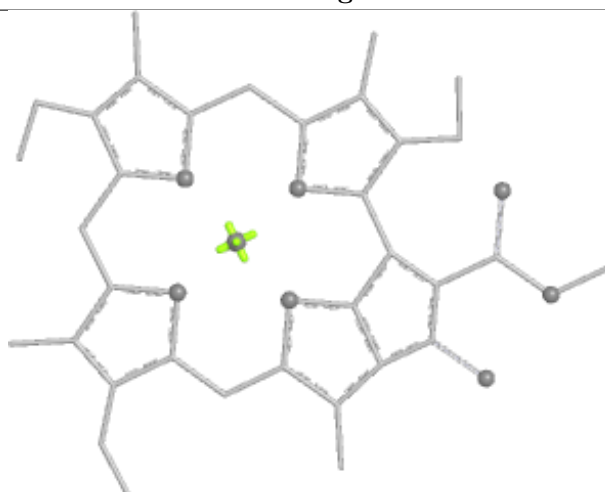
Bond lengths



Bond angles

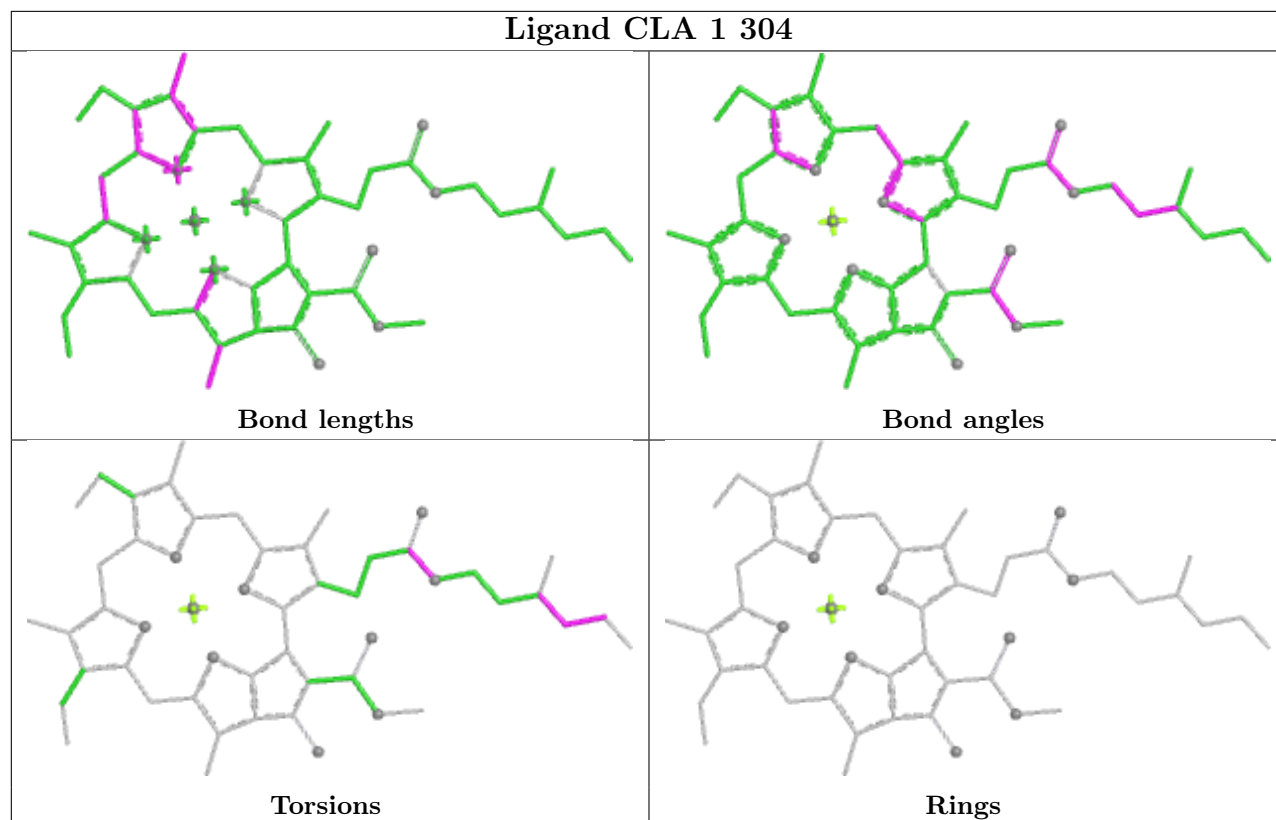


Torsions

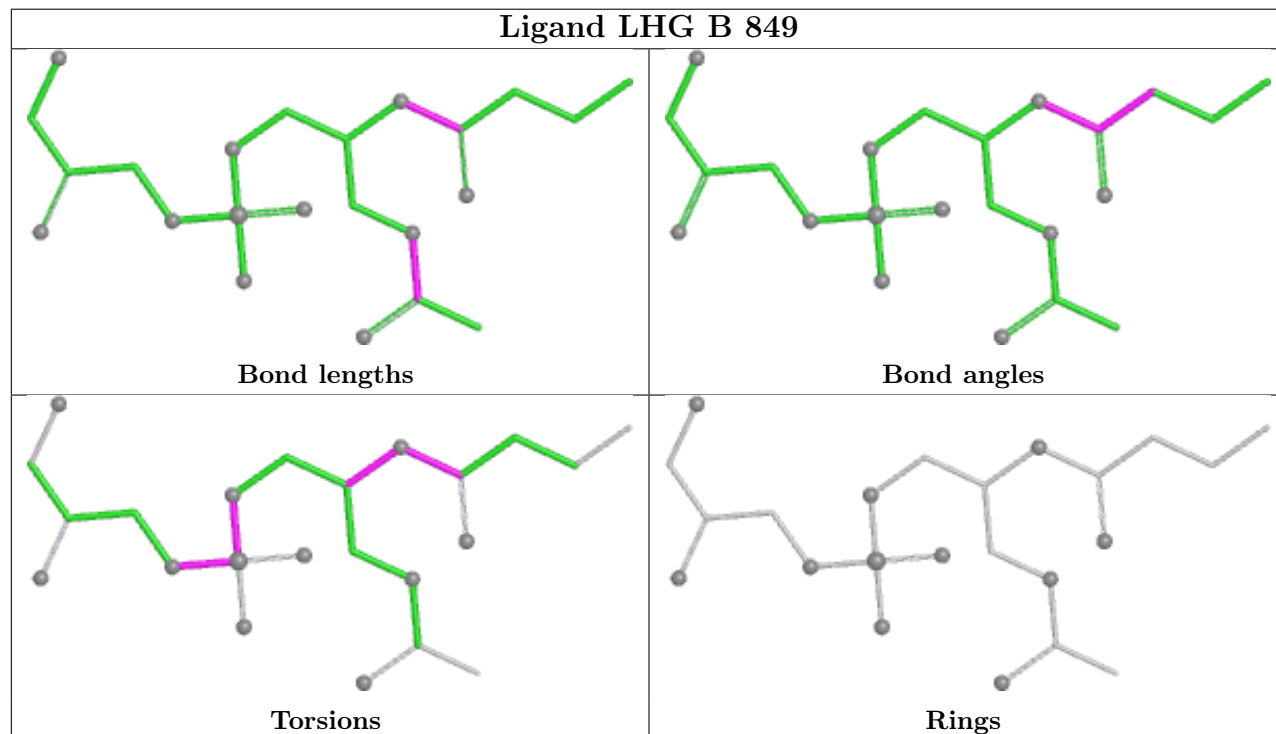


Rings

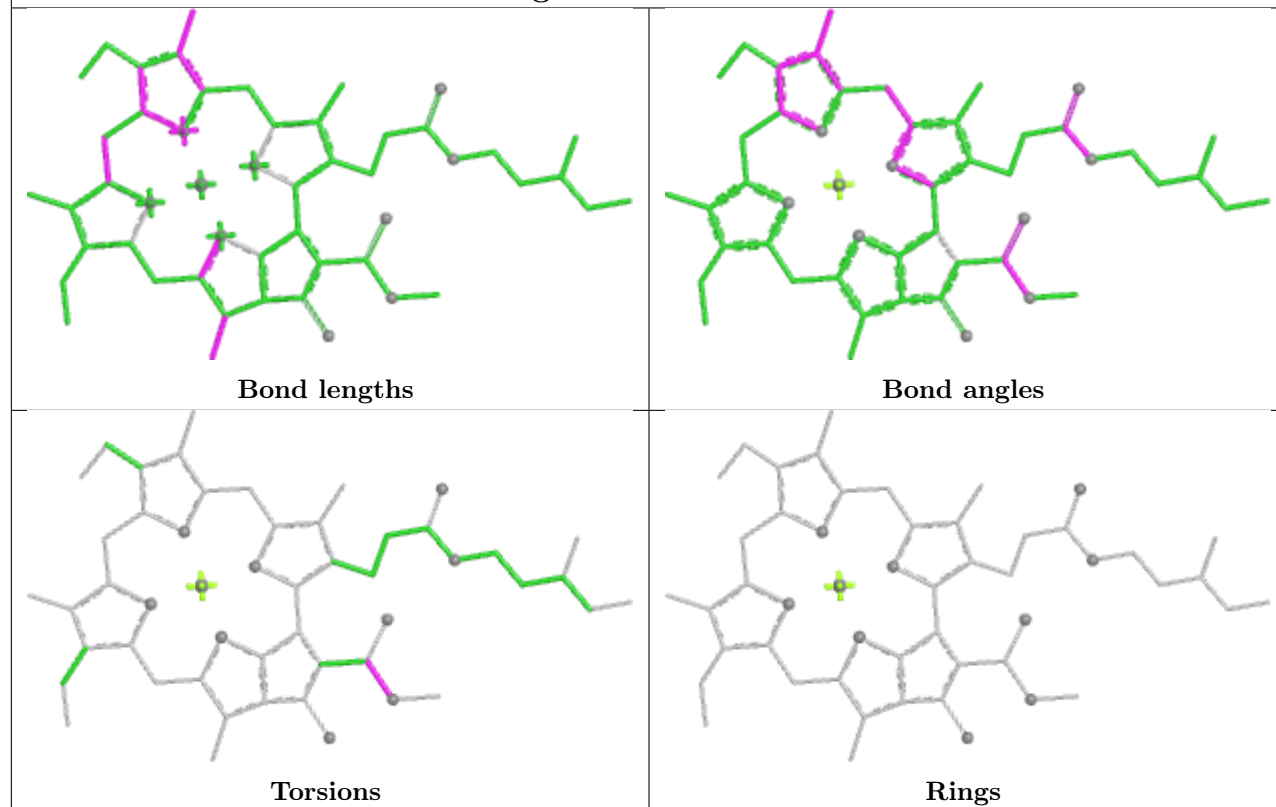
Ligand CLA 1 304



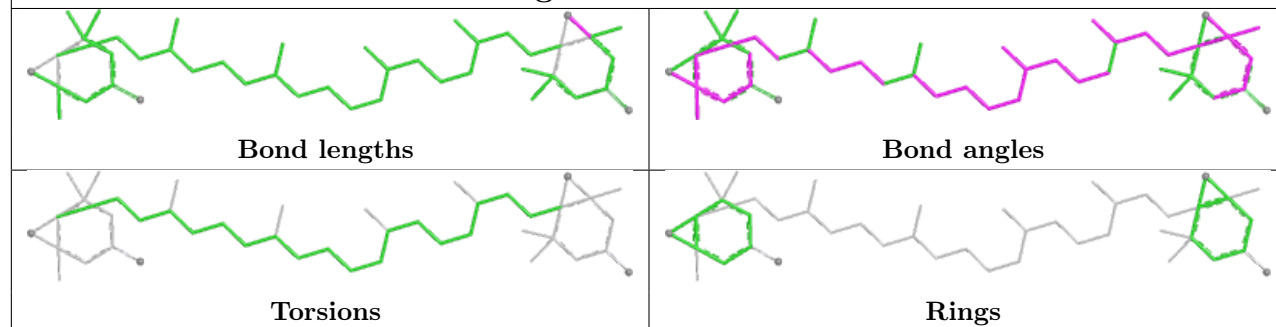
Ligand LHG B 849



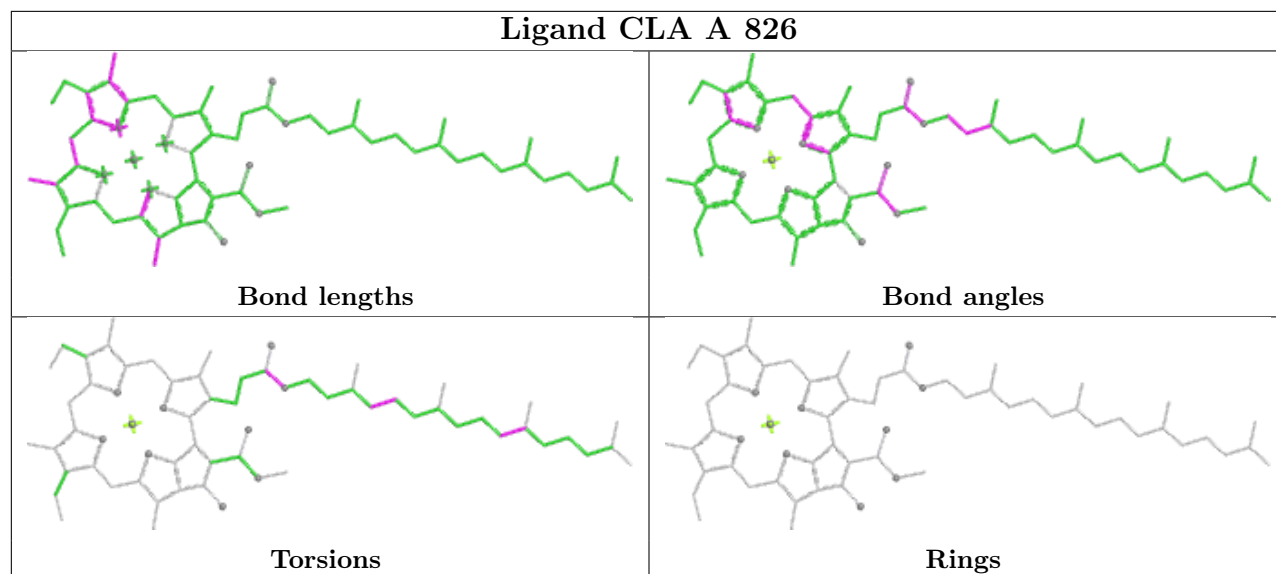
Ligand CLA B 835



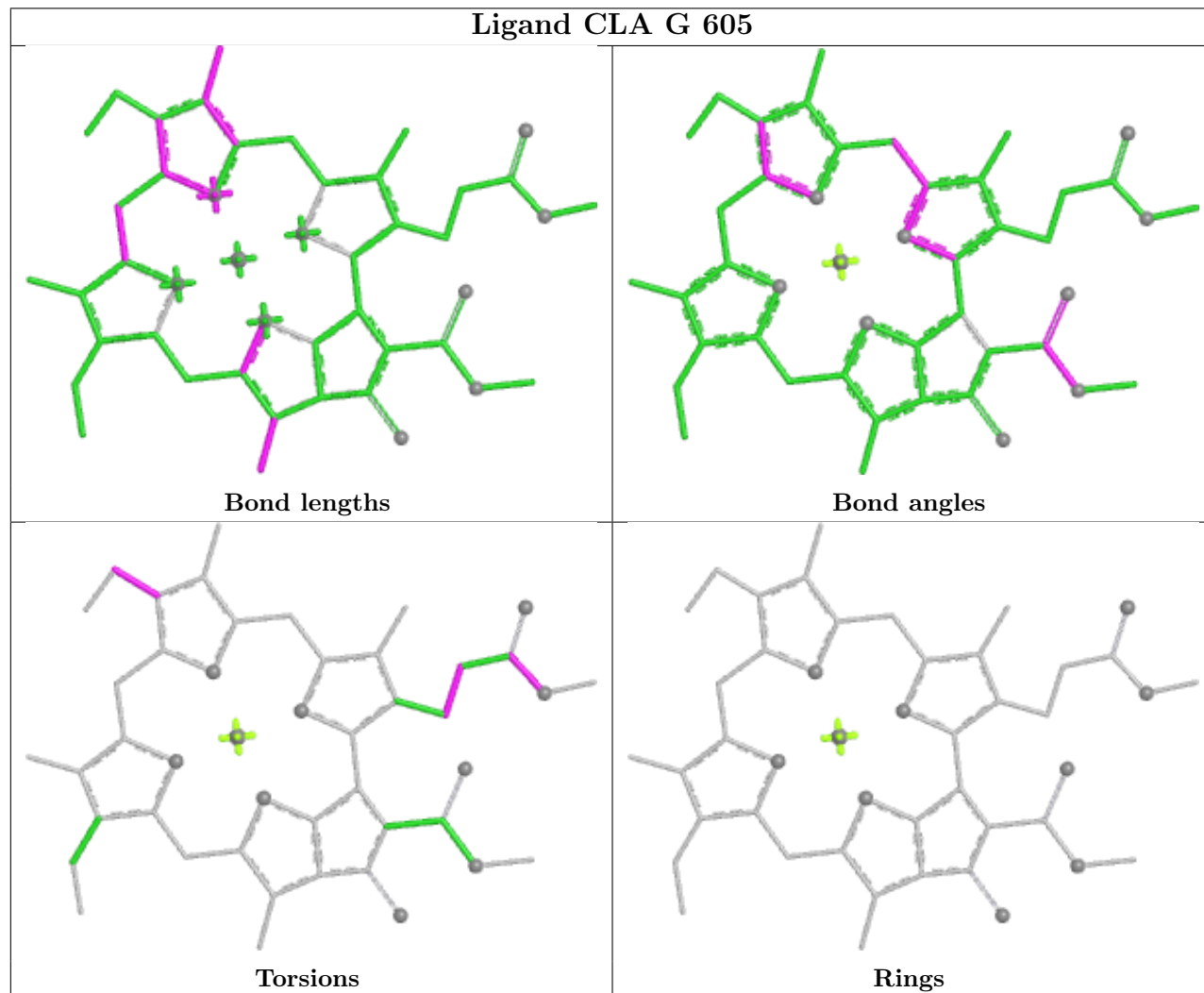
Ligand XAT 4 317

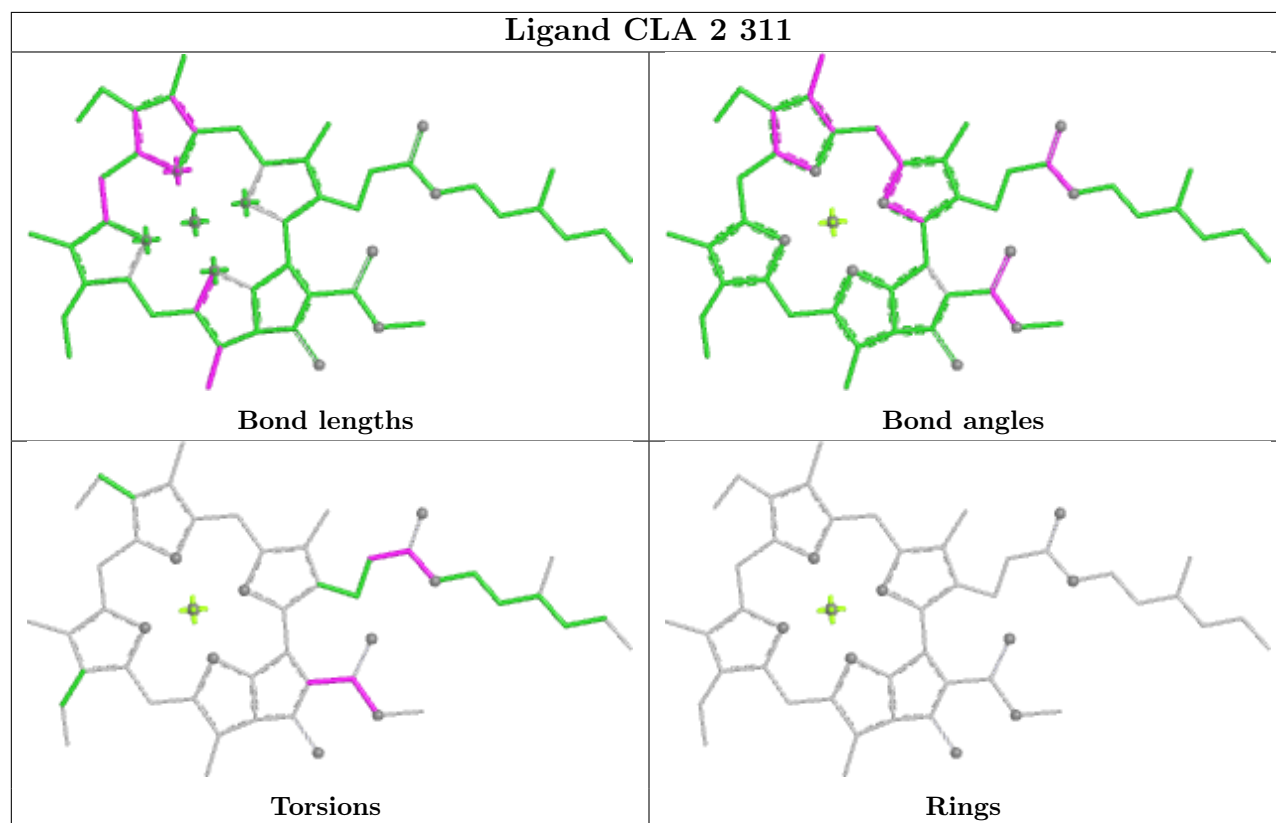
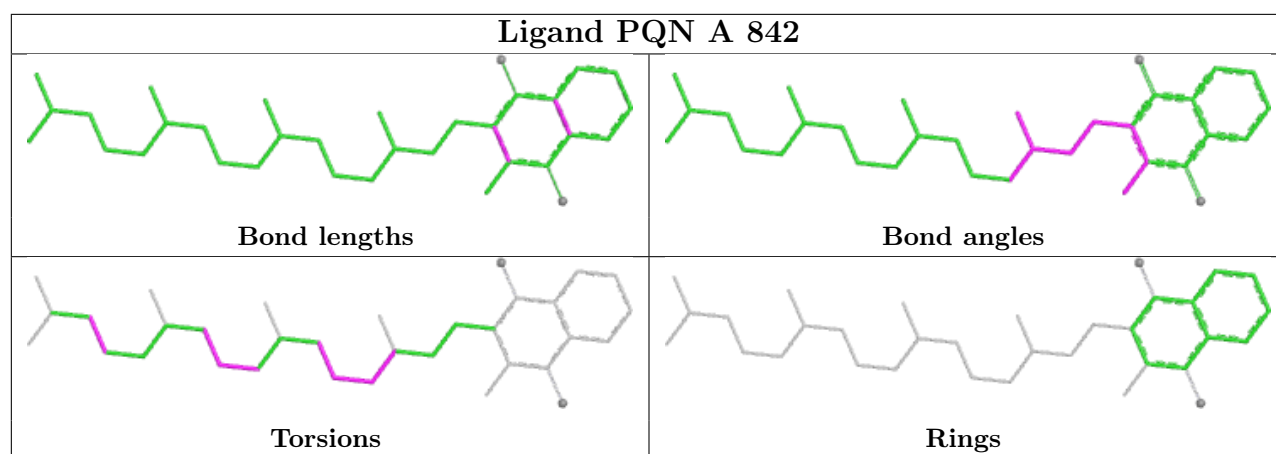


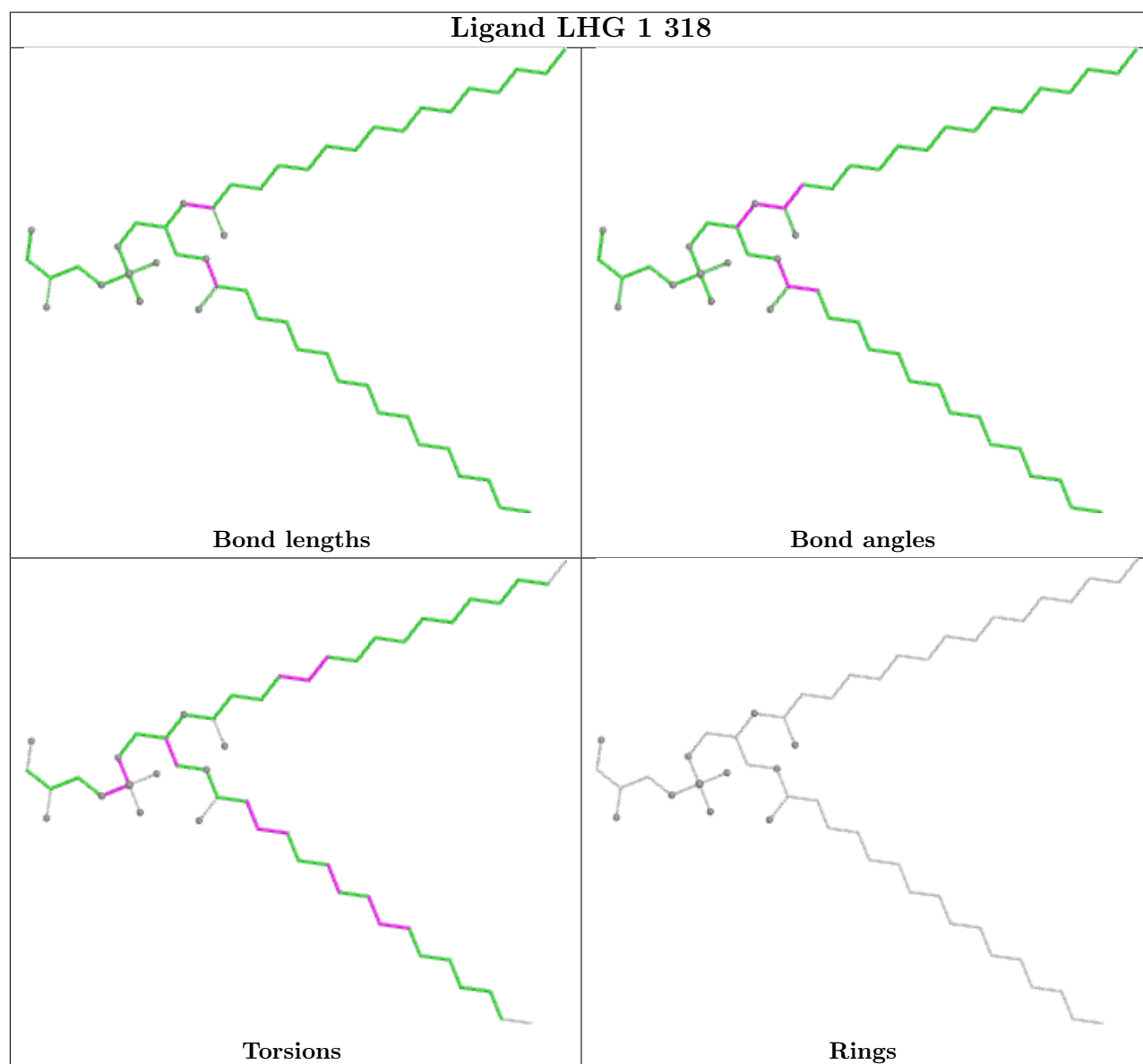
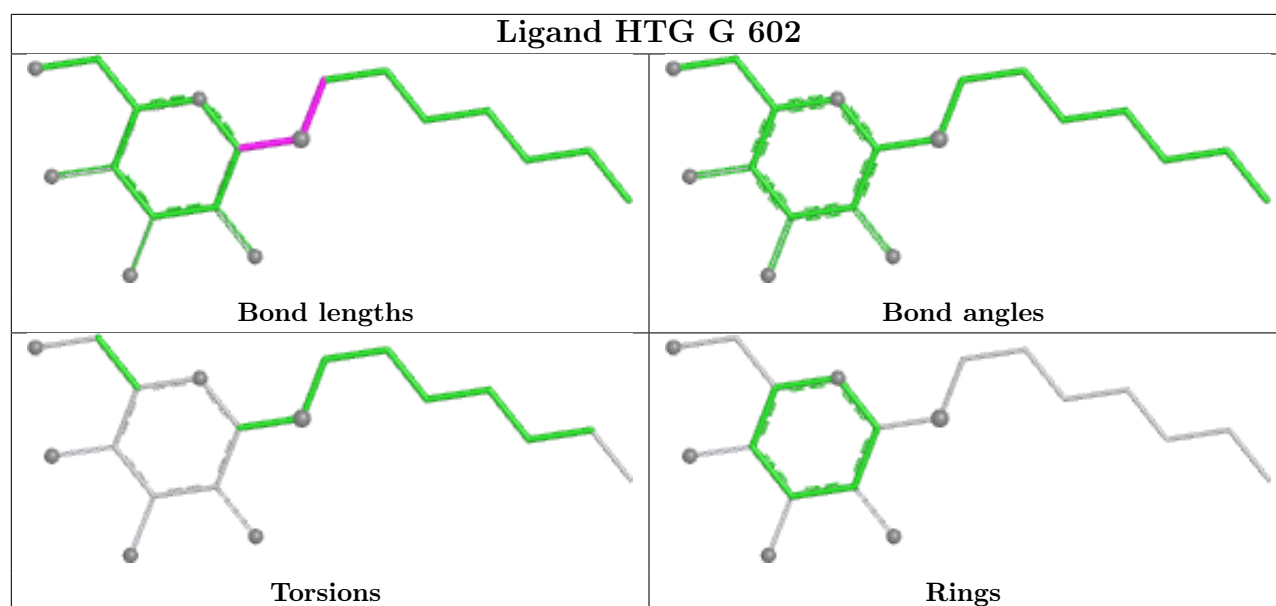
Ligand CLA A 826



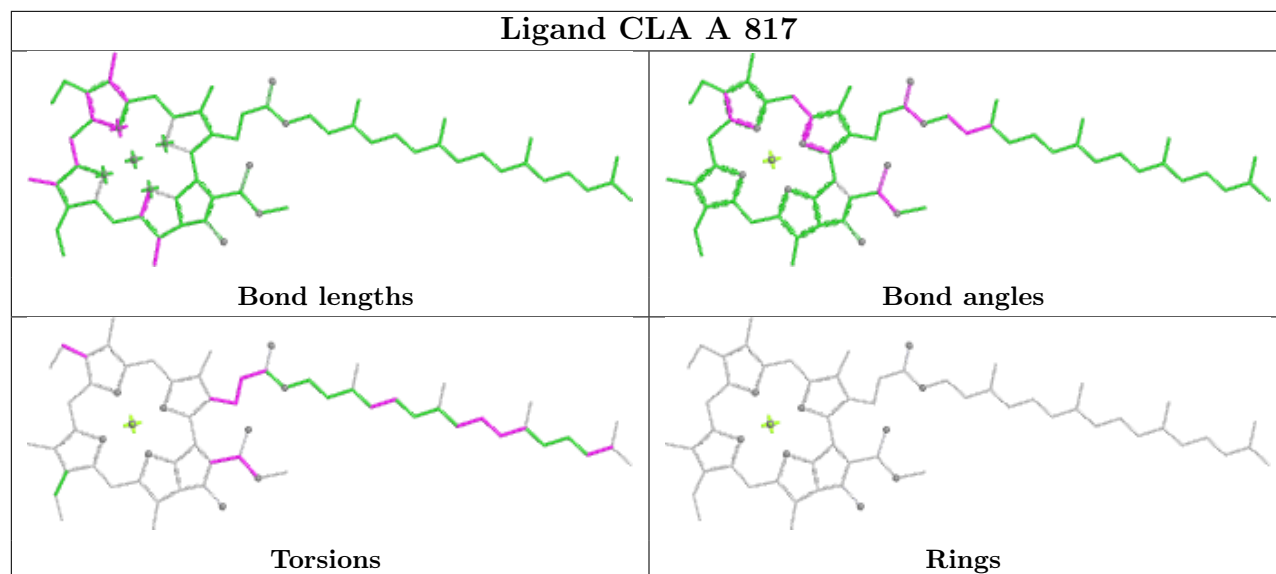
Ligand CLA G 605



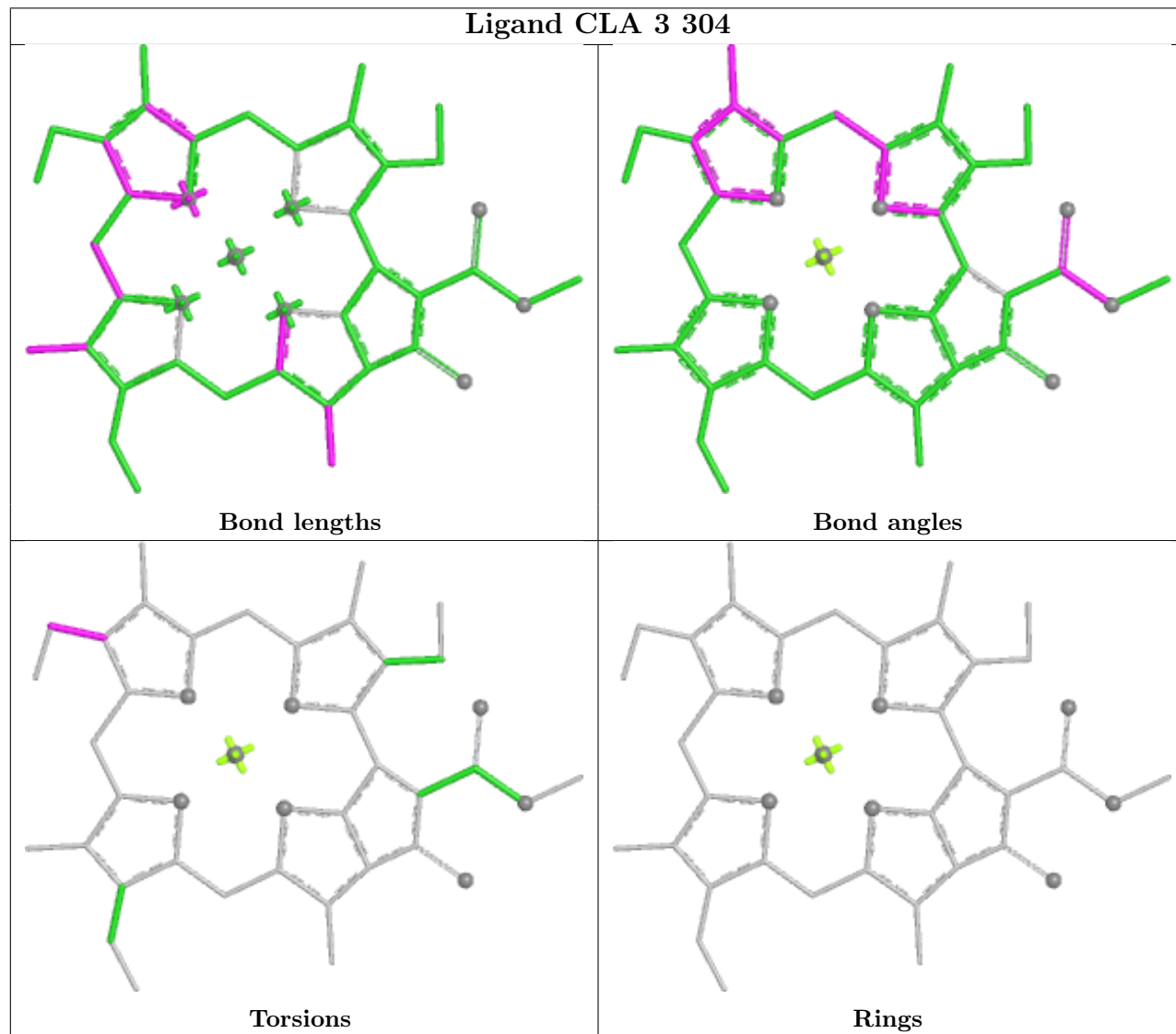


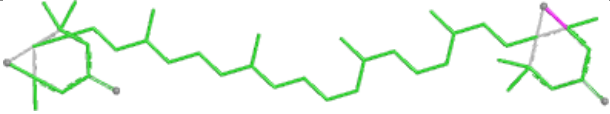
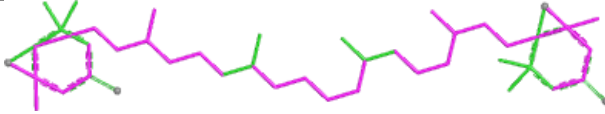
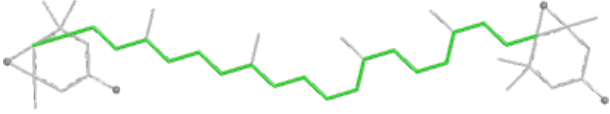
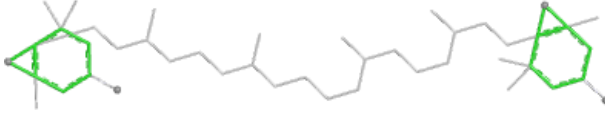
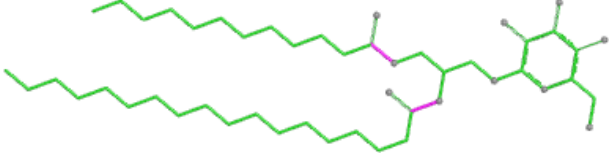
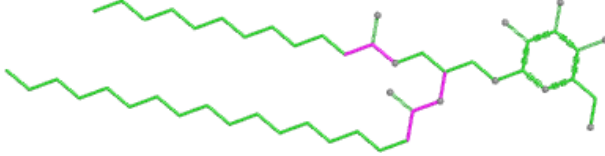
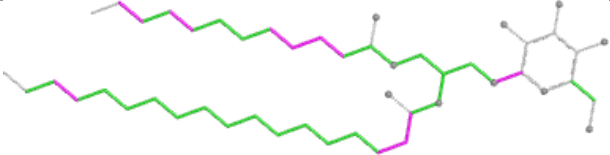
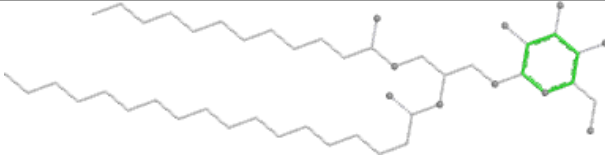
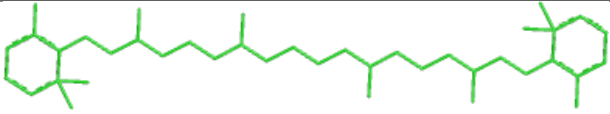
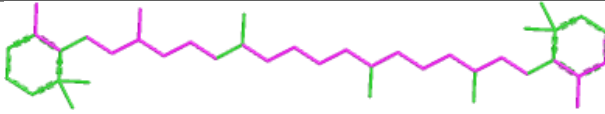
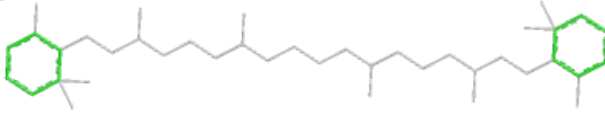


Ligand CLA A 817

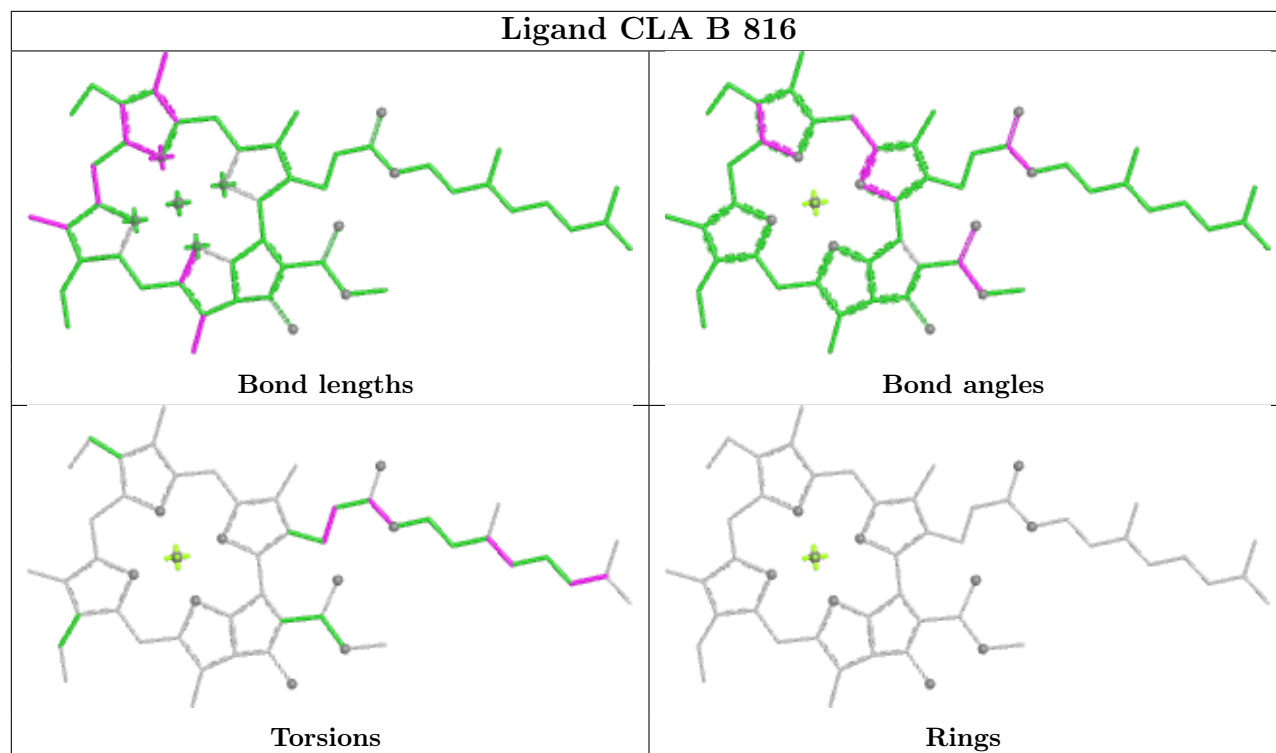


Ligand CLA 3 304

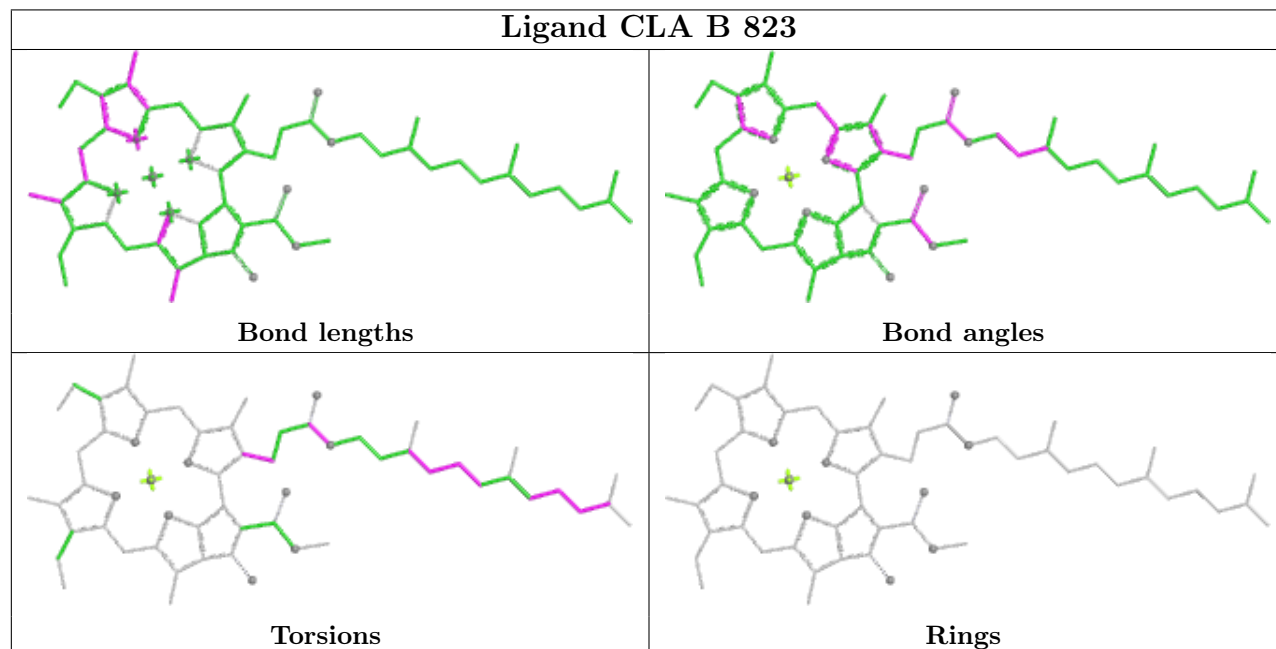


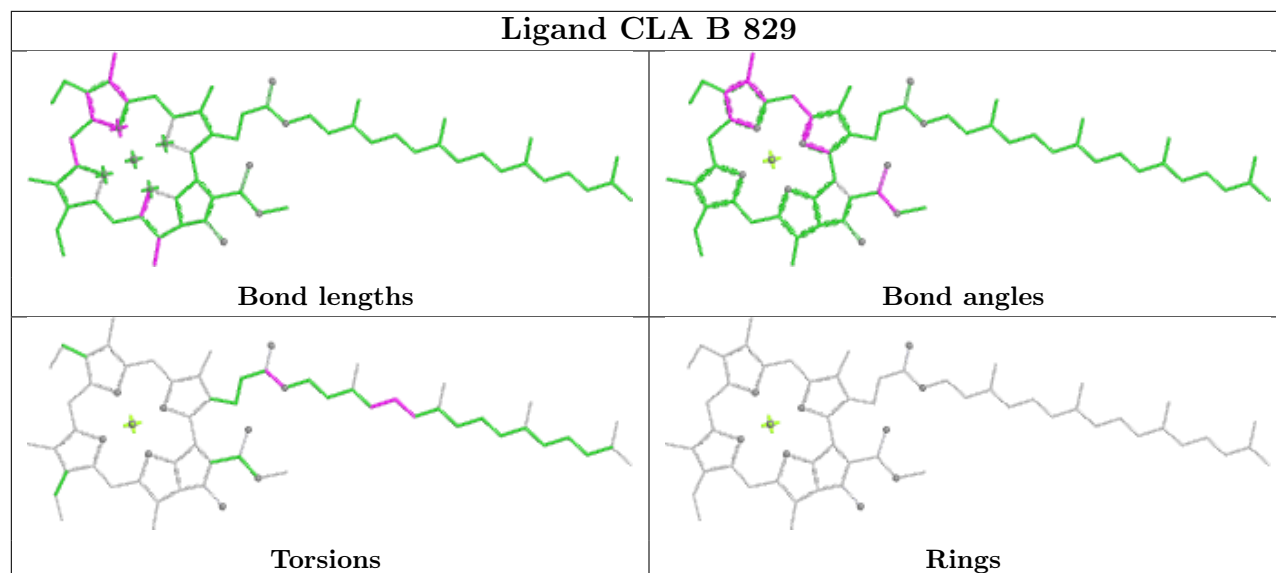
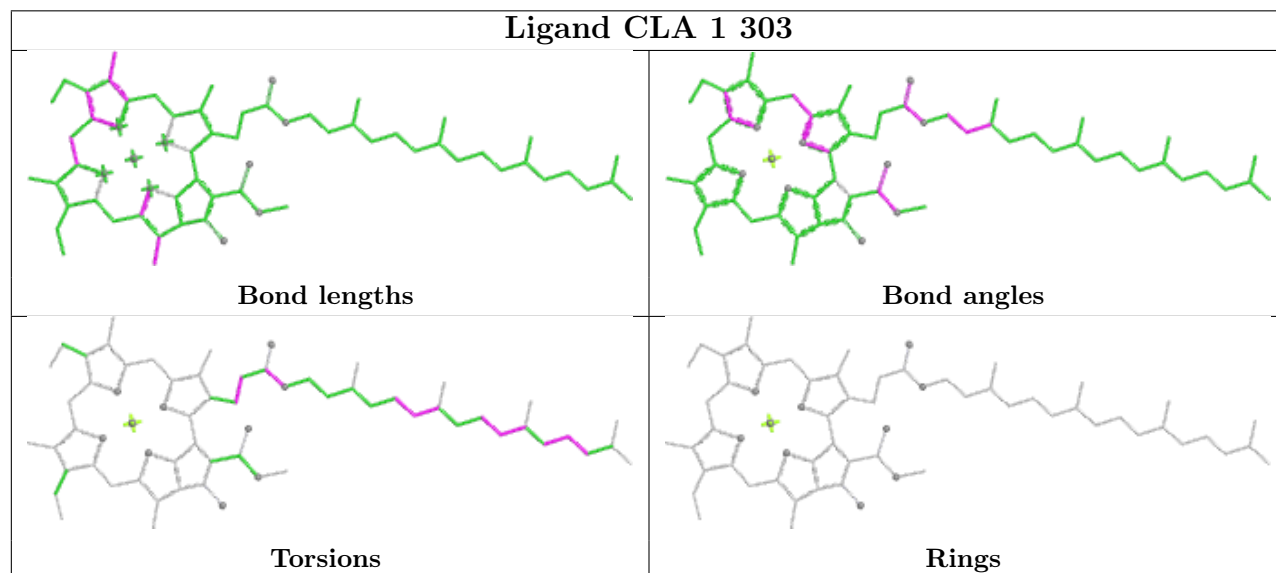
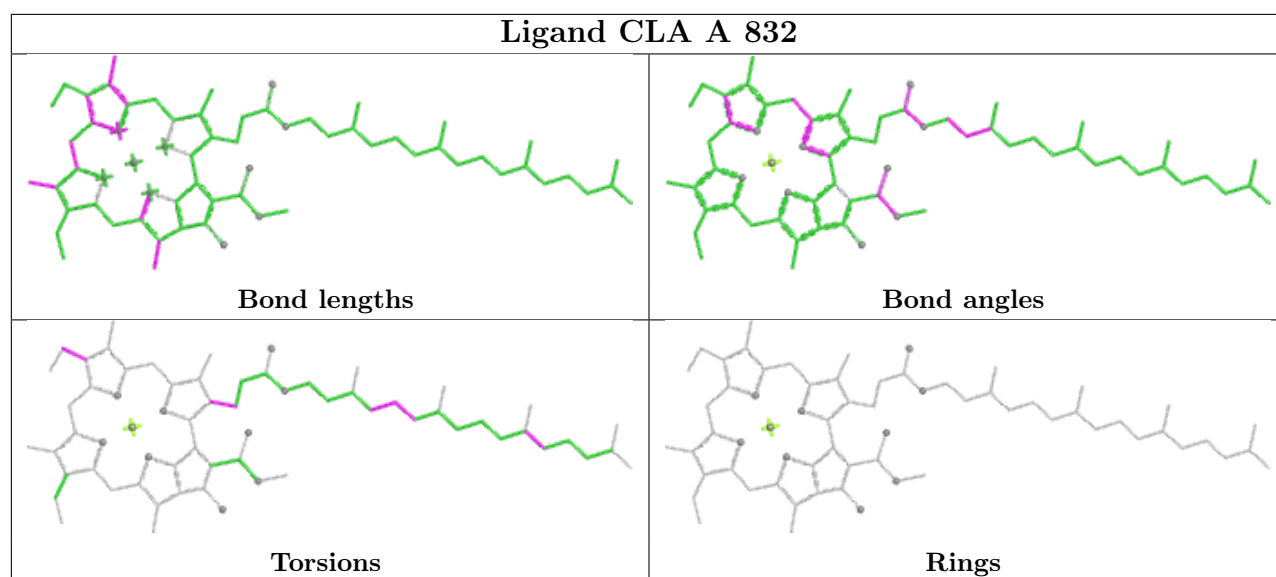
Ligand XAT 3 316	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 1 320	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

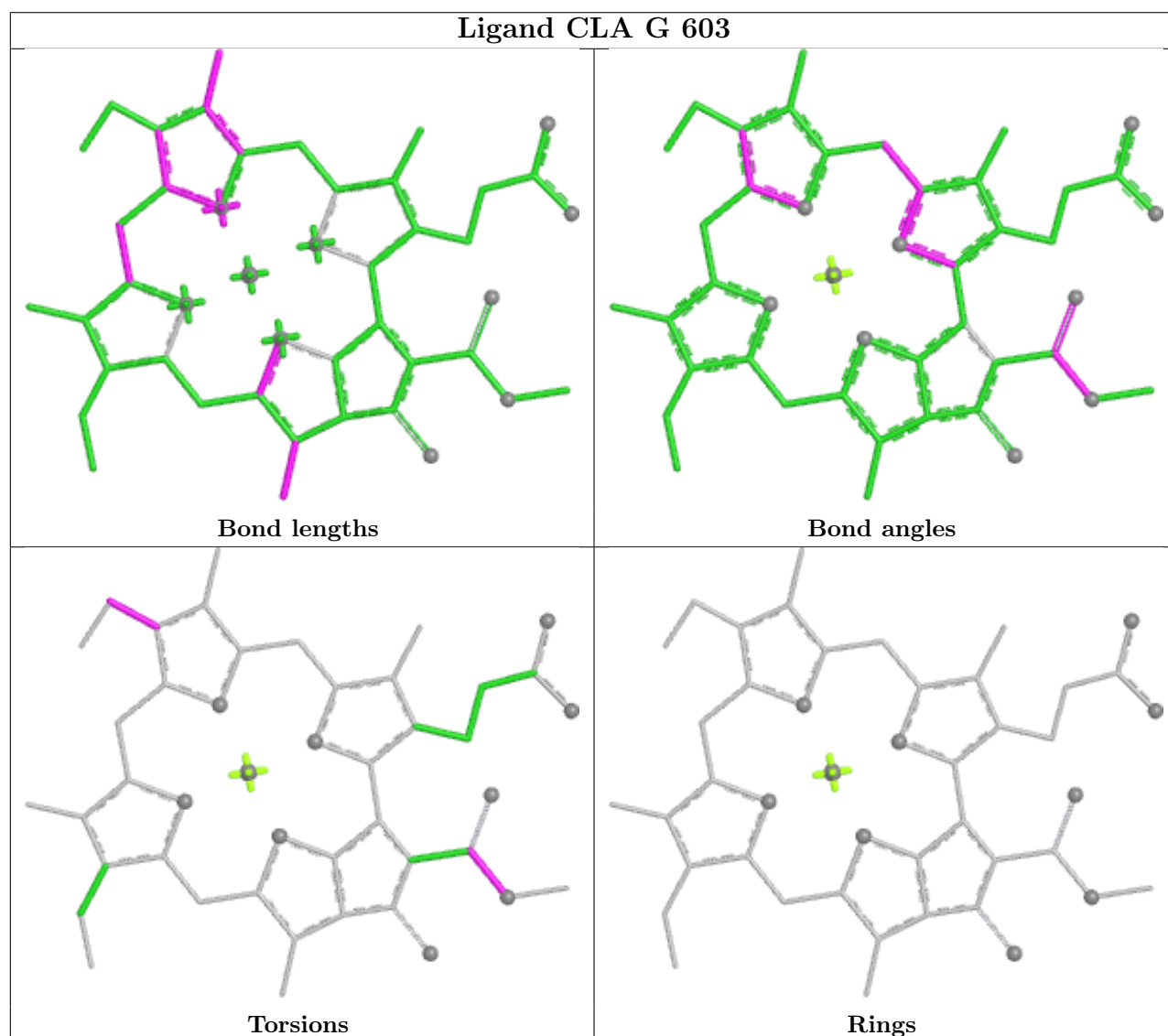
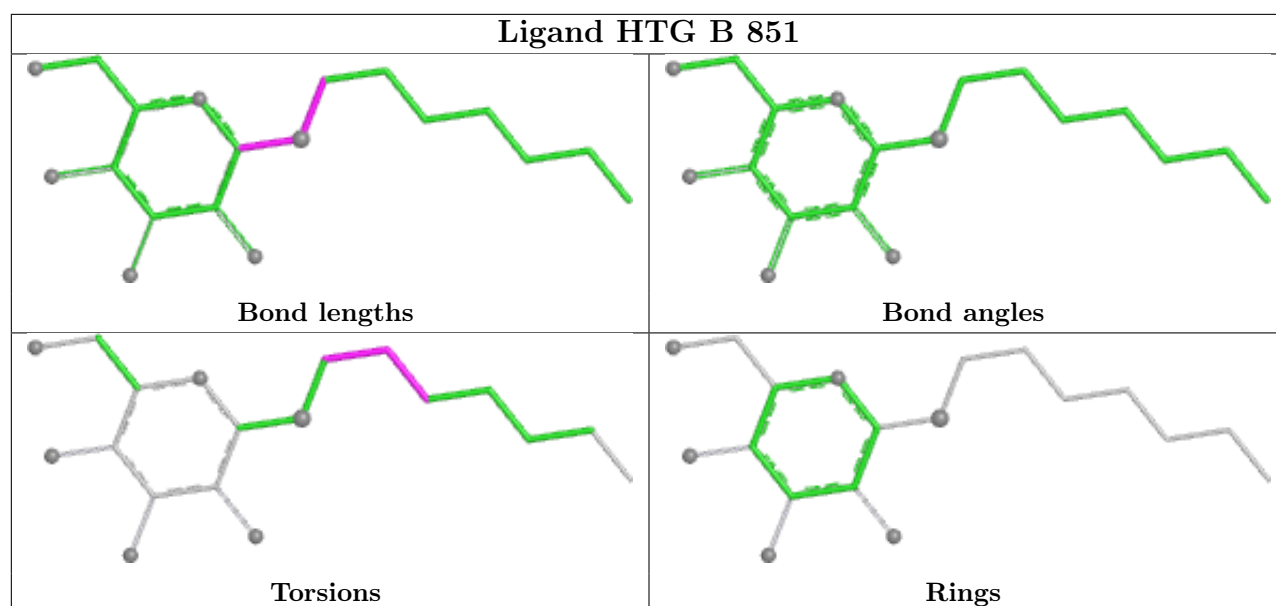
Ligand CLA B 816

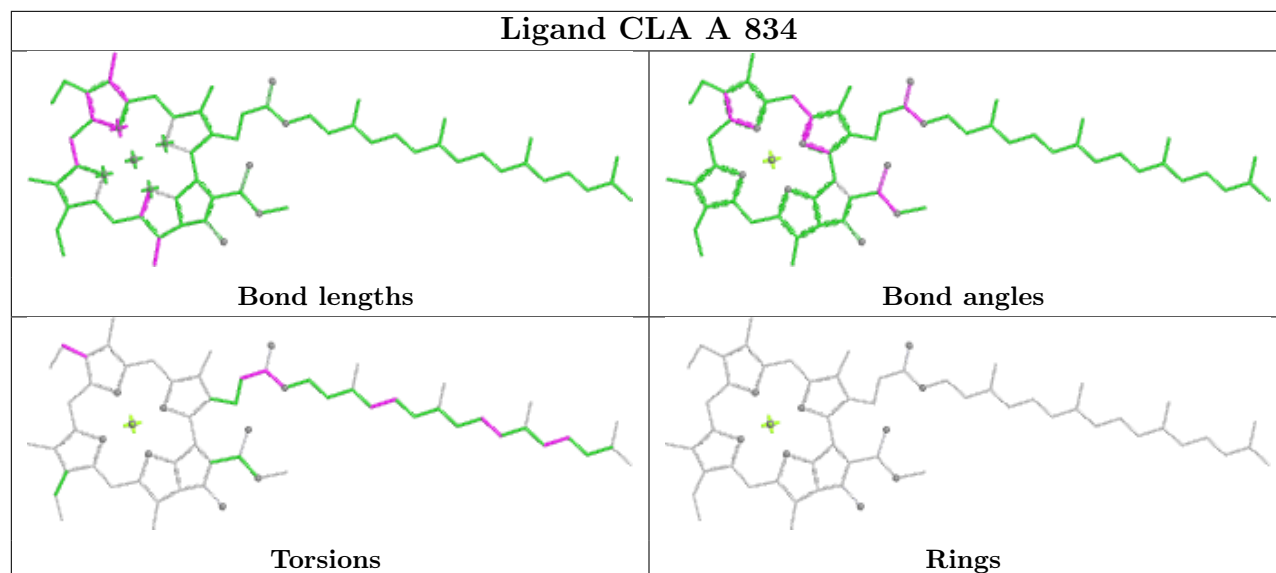
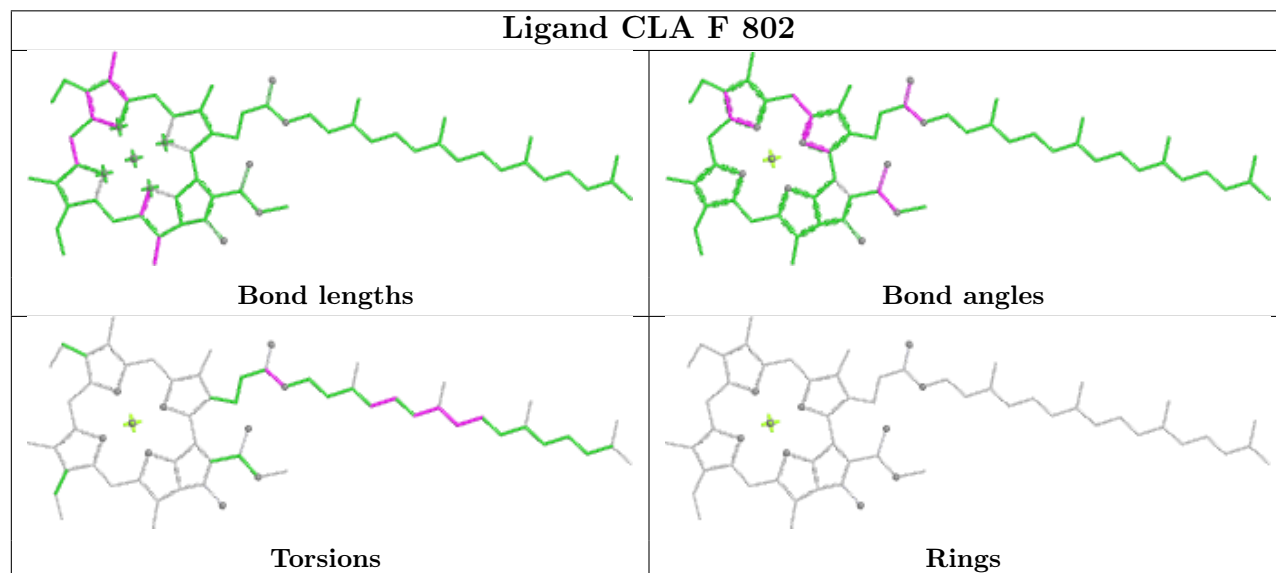
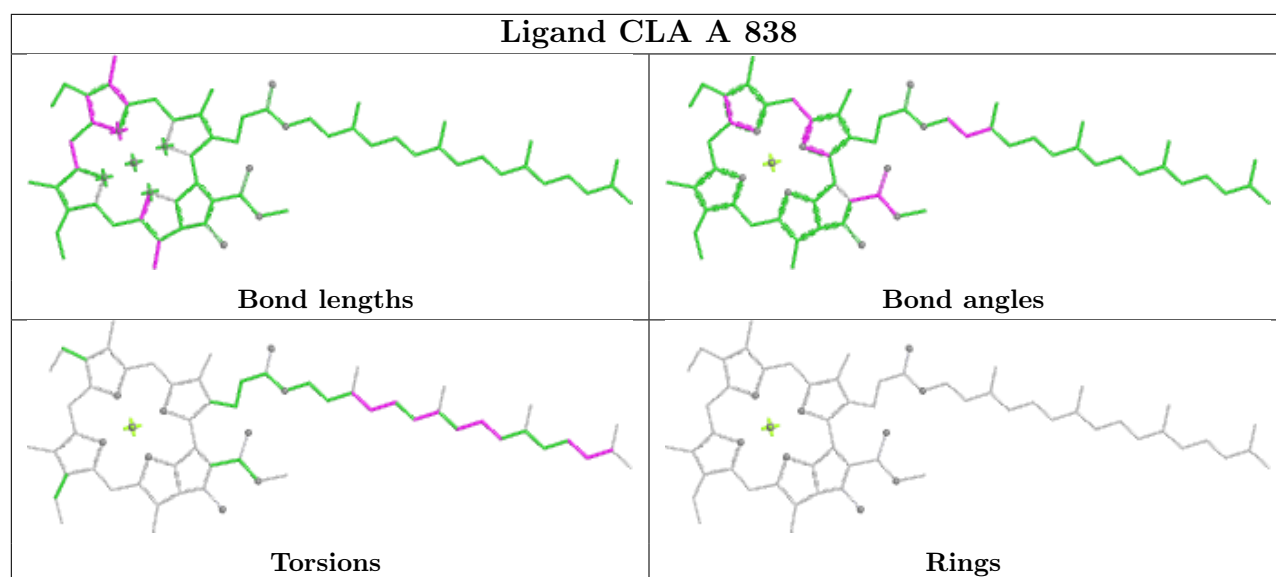


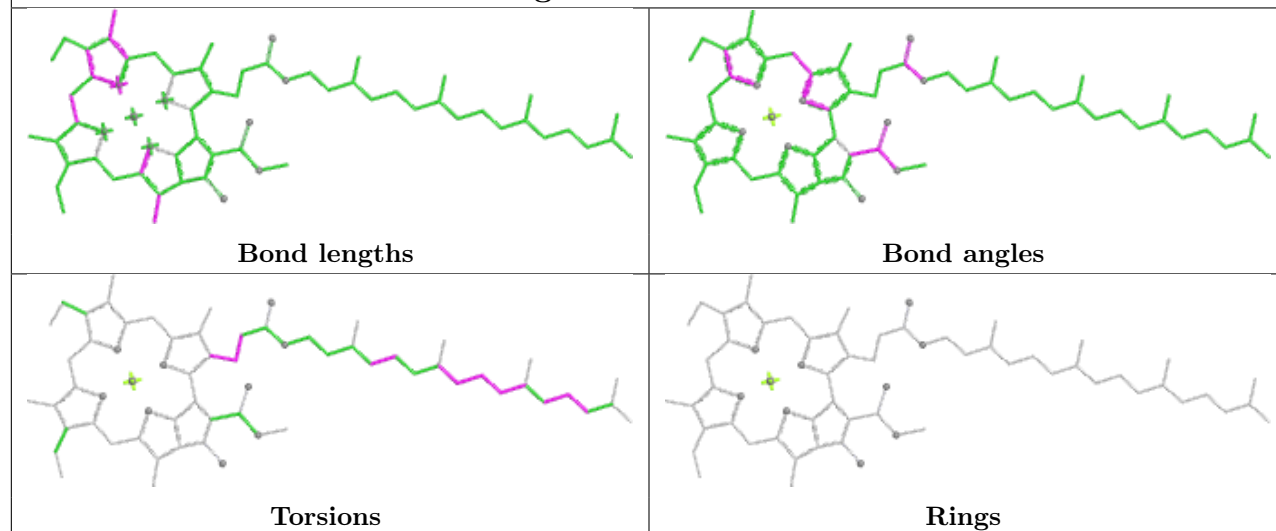
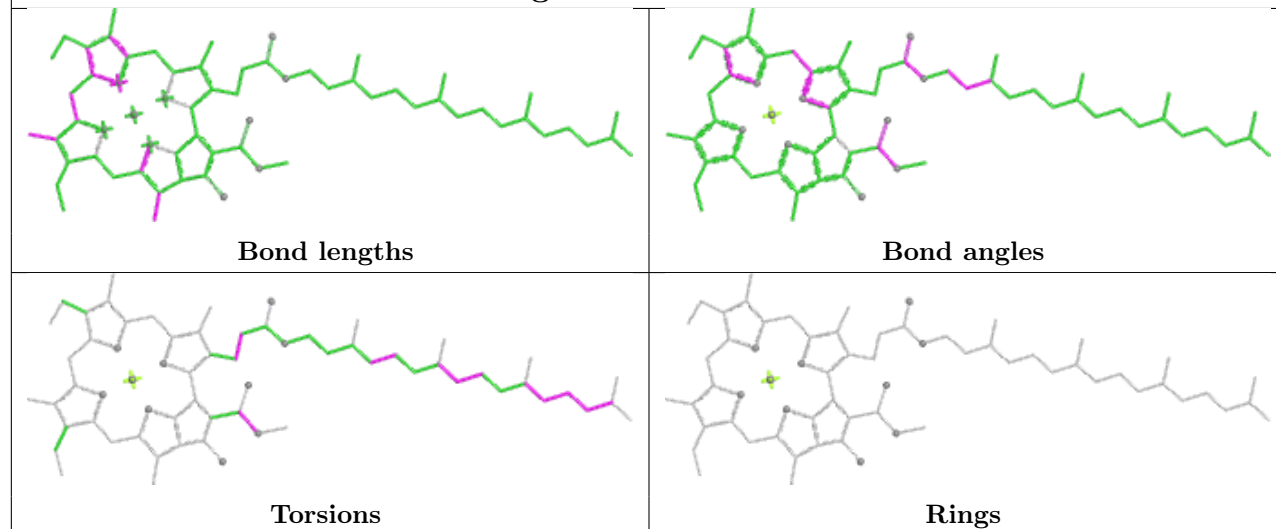
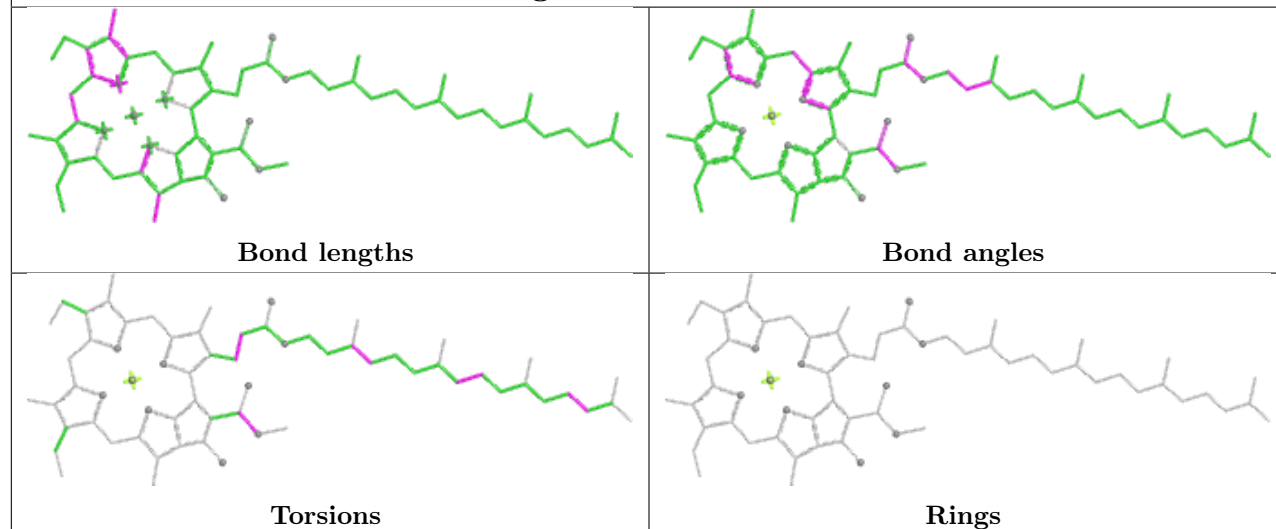
Ligand CLA B 823



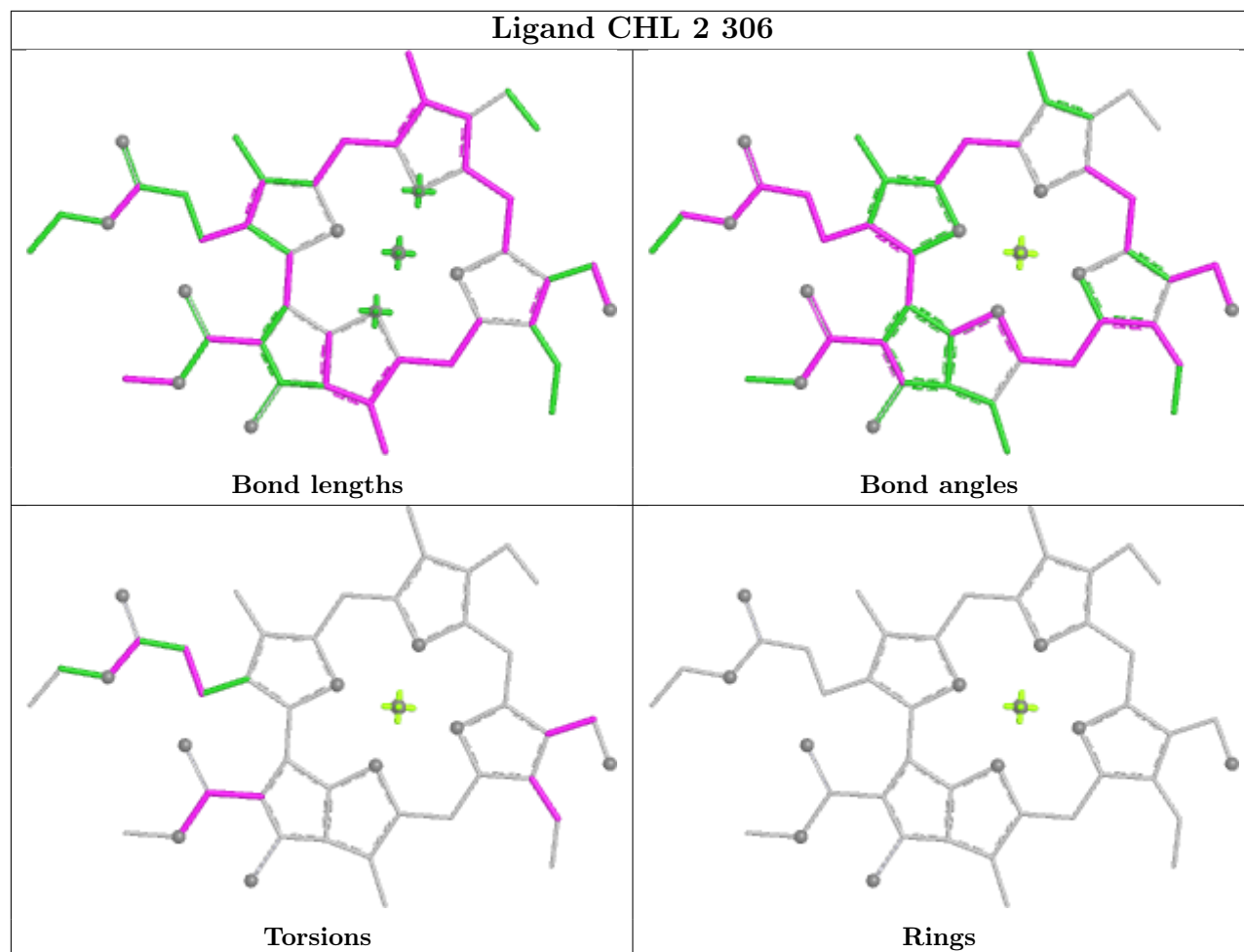




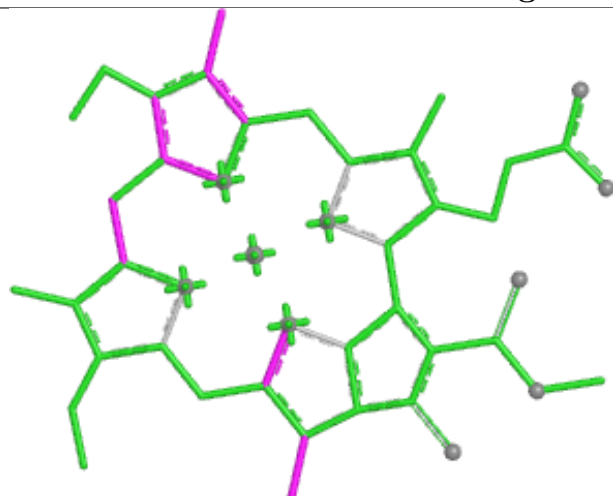


Ligand CLA L 303**Ligand CLA A 802****Ligand CLA A 818**

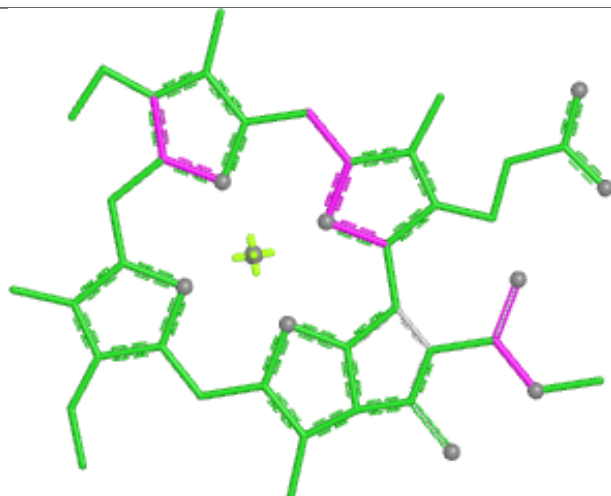
Ligand CHL 2 306



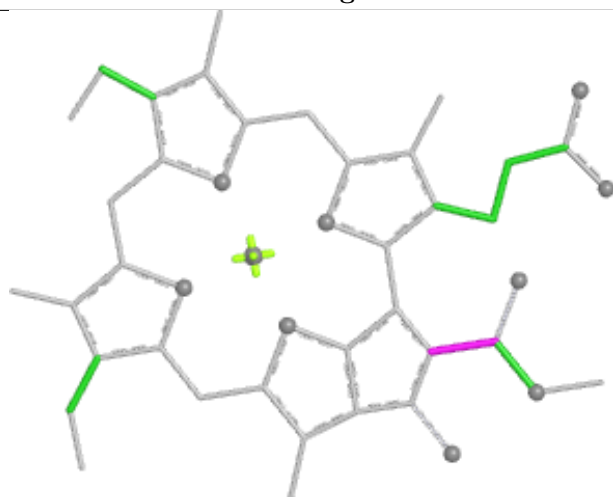
Ligand CLA 3 313



Bond lengths



Bond angles

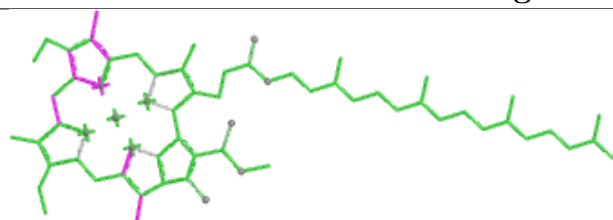


Torsions

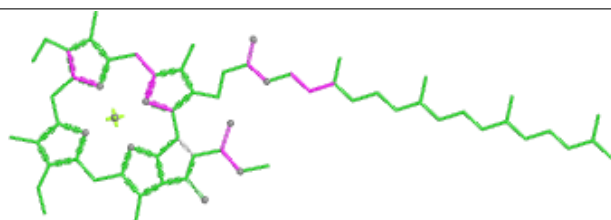


Rings

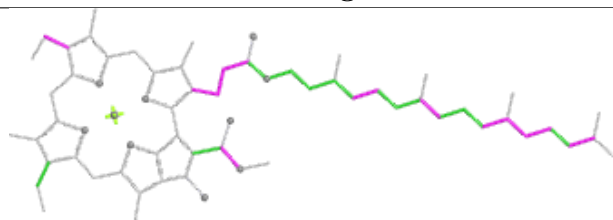
Ligand CLA A 808



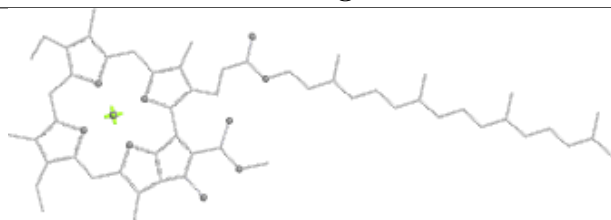
Bond lengths



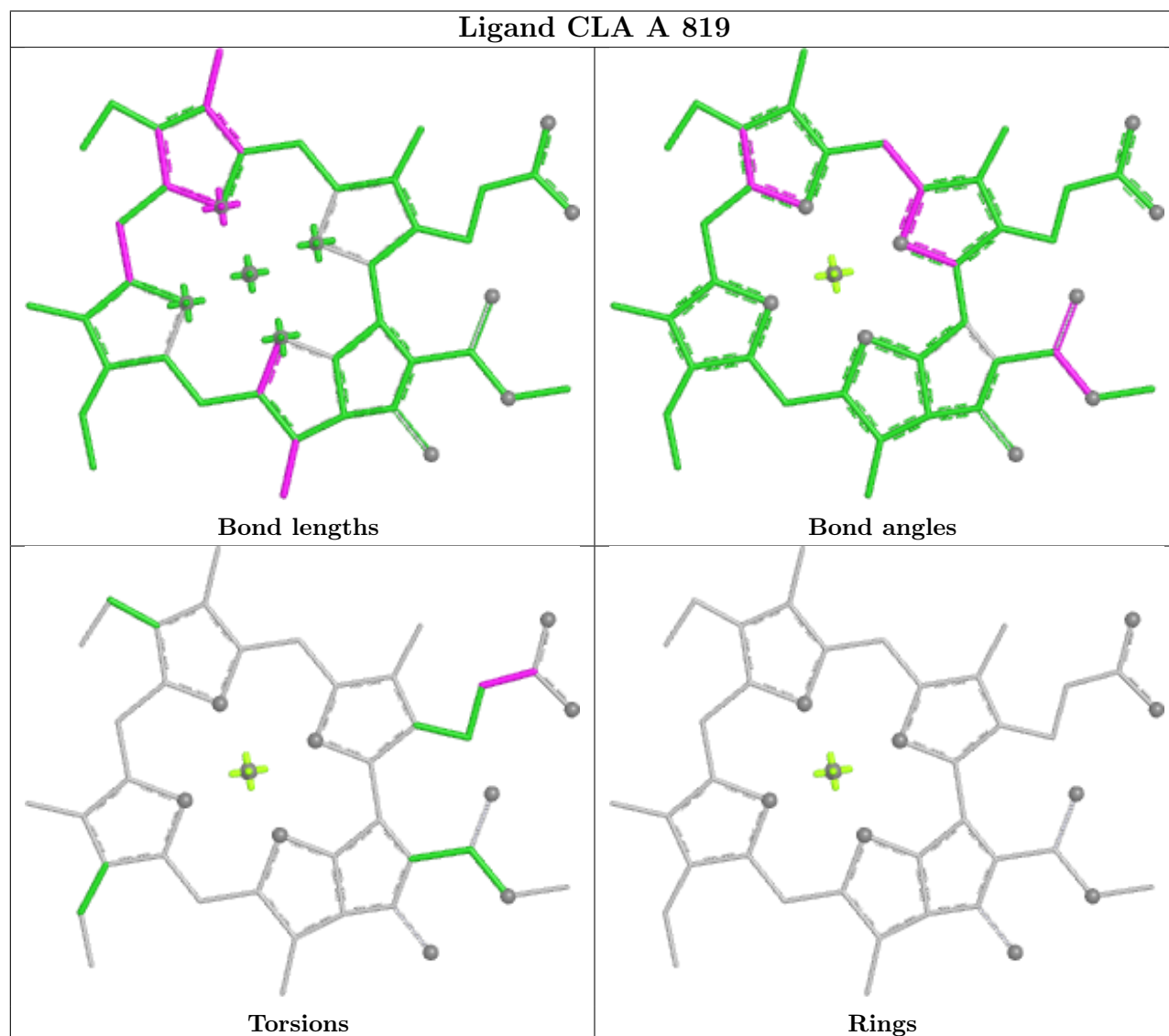
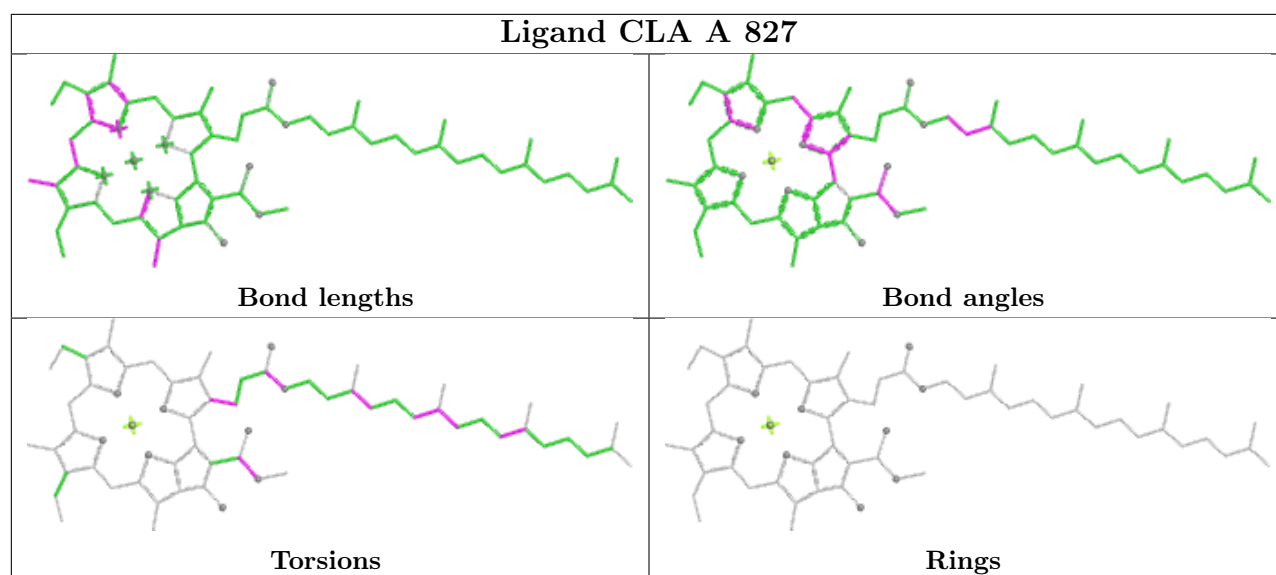
Bond angles

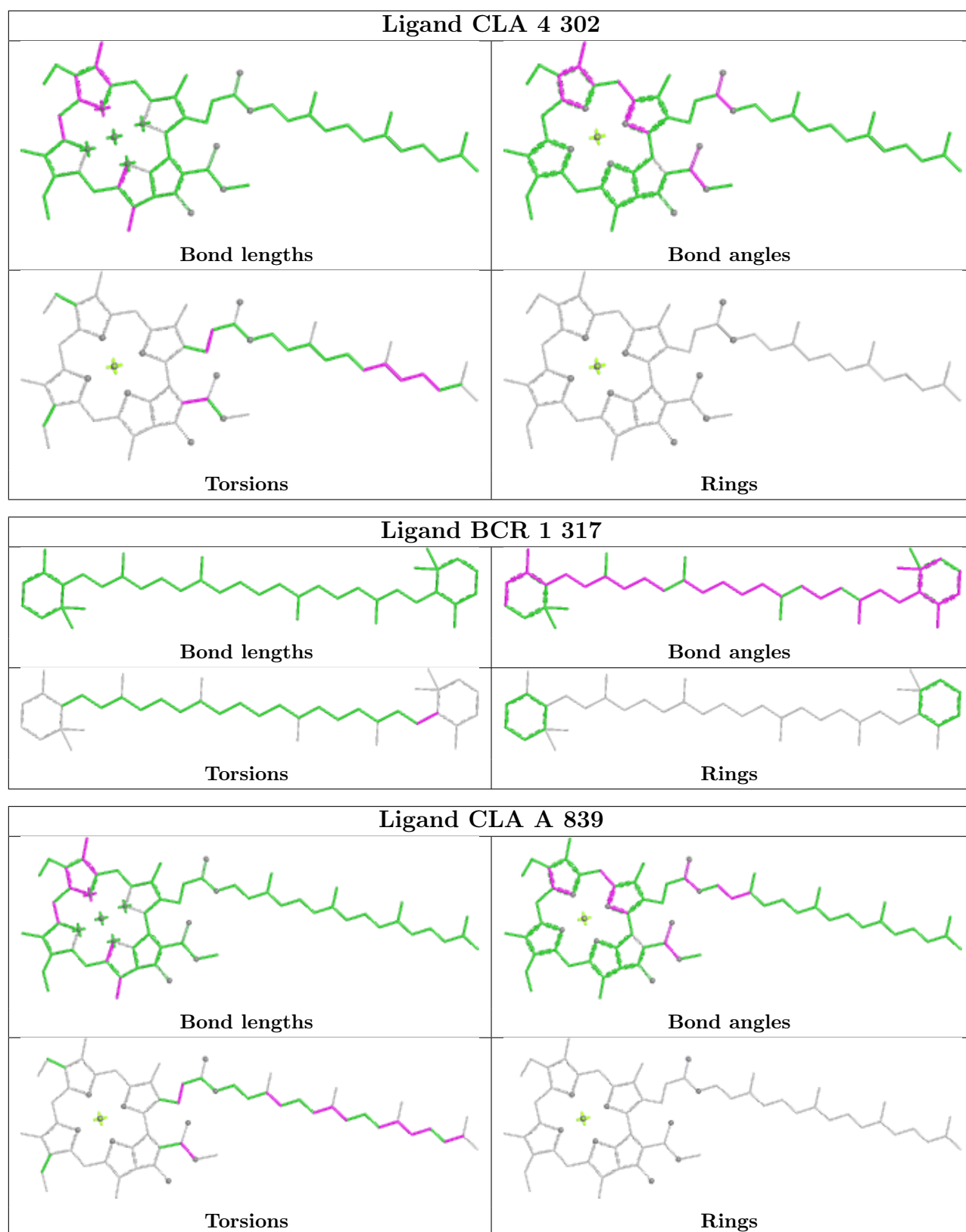


Torsions

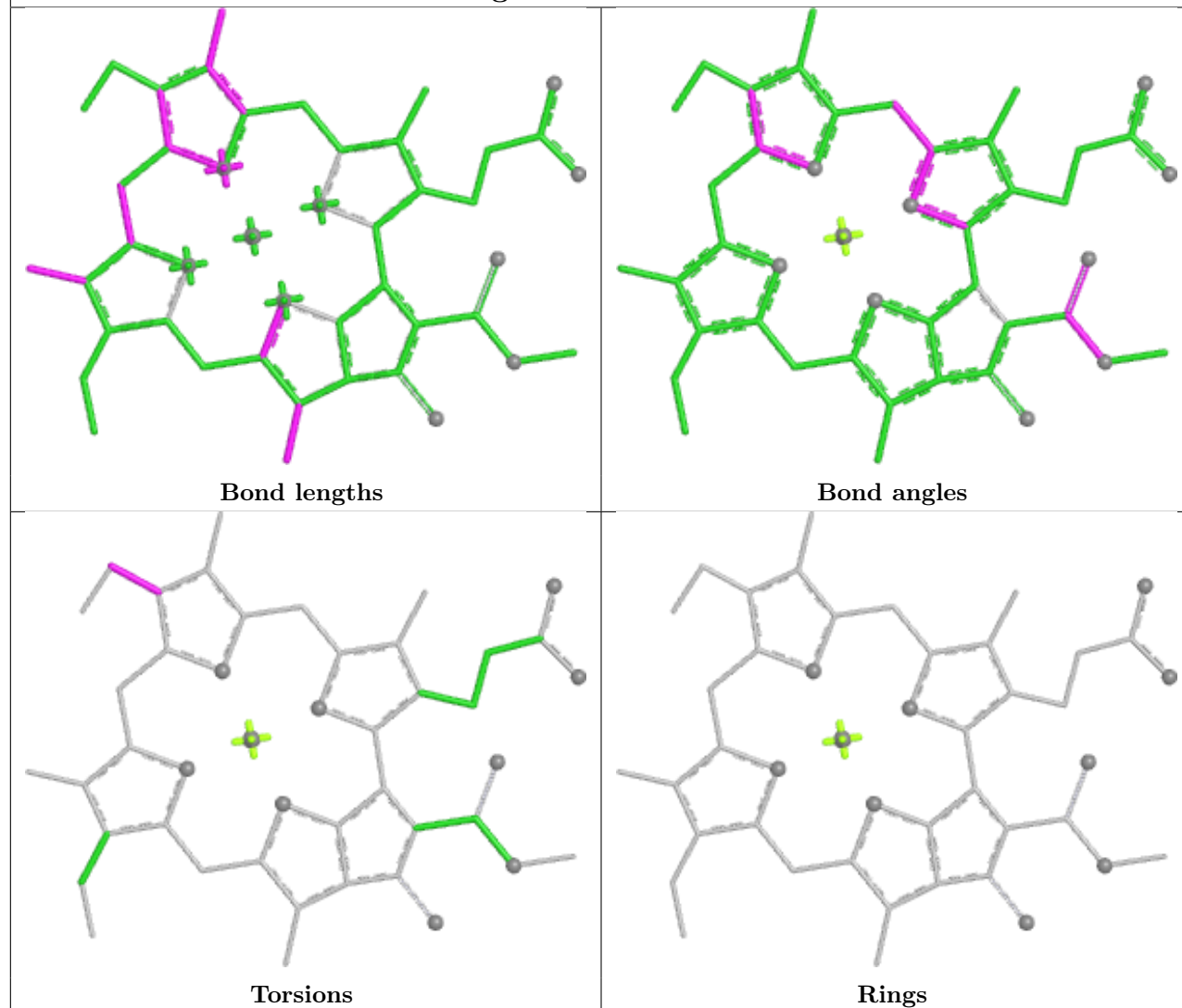


Rings

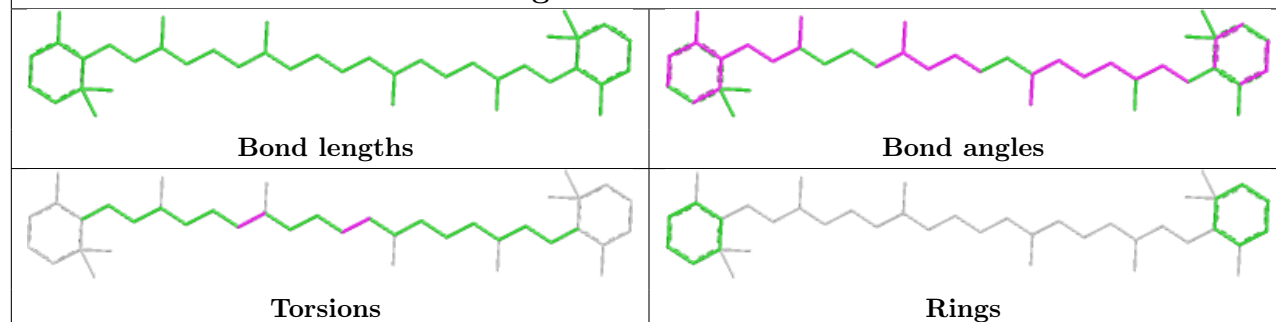


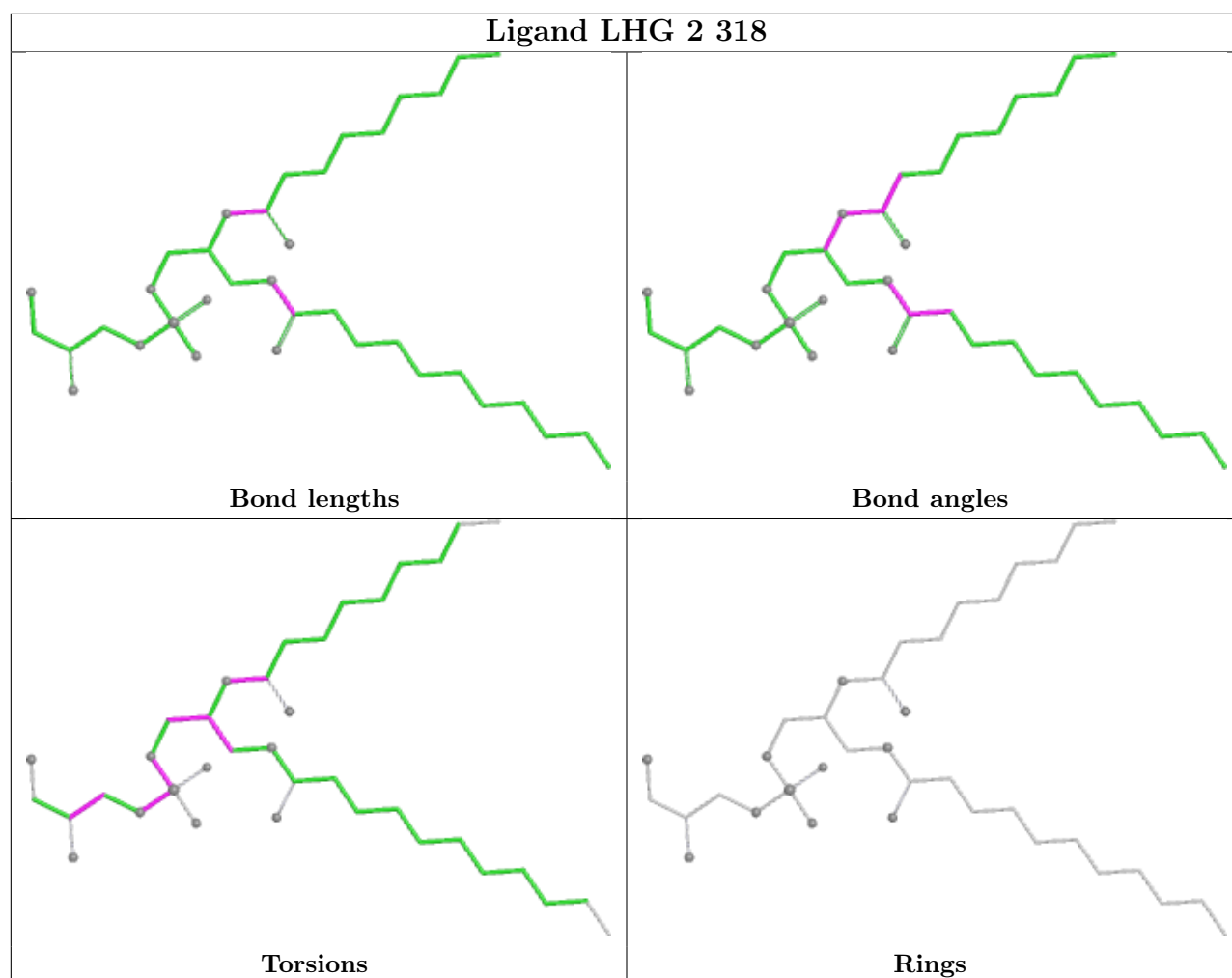


Ligand CLA K 205

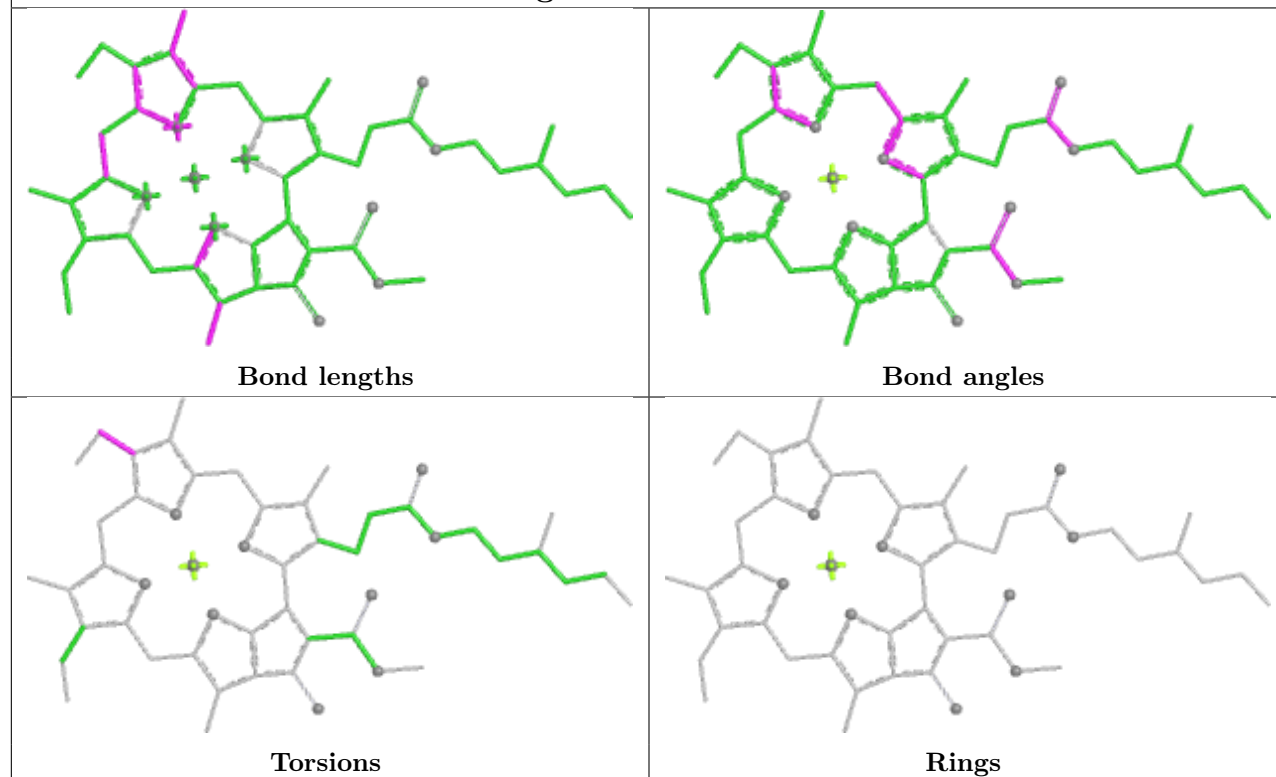


Ligand BCR F 801

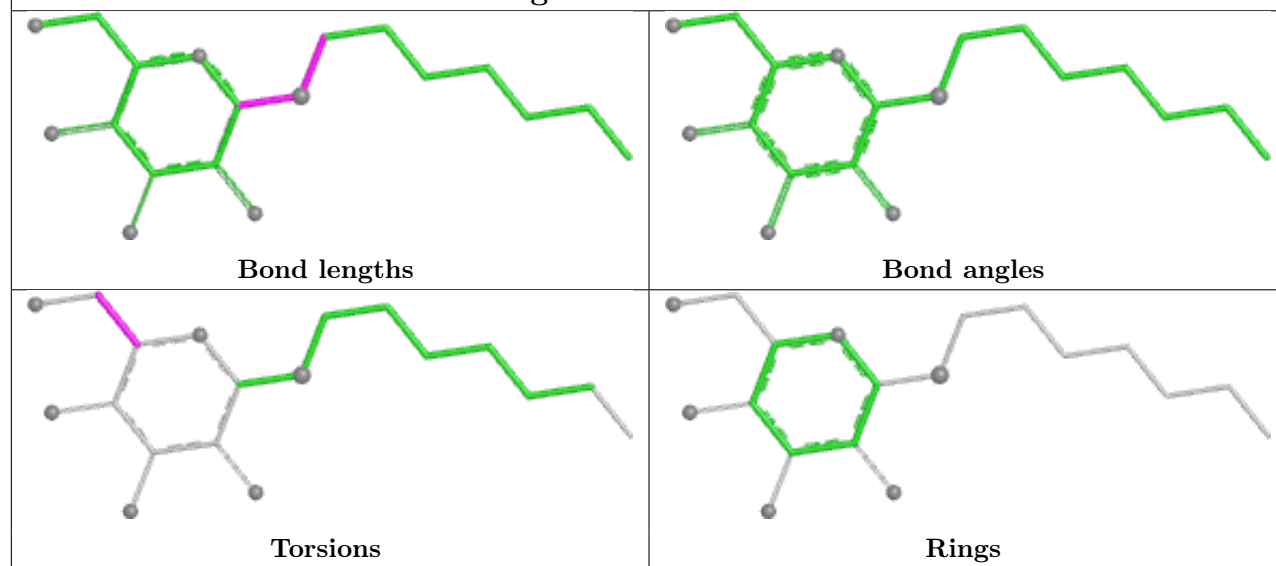




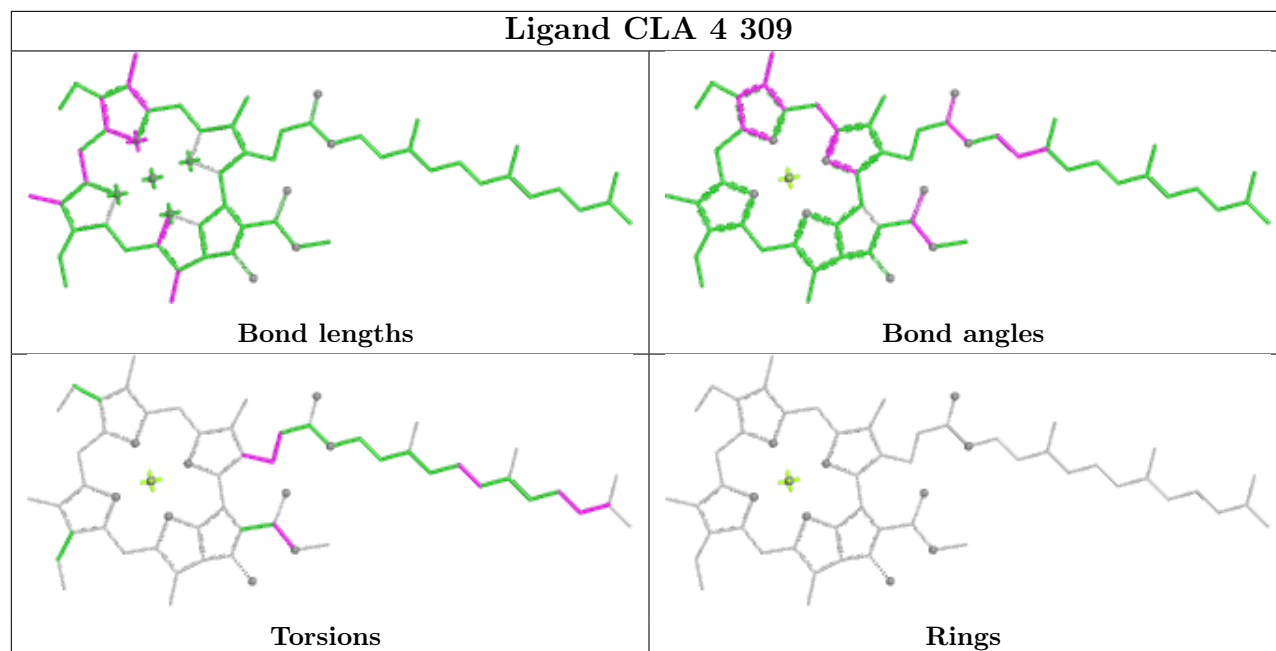
Ligand CLA 3 310



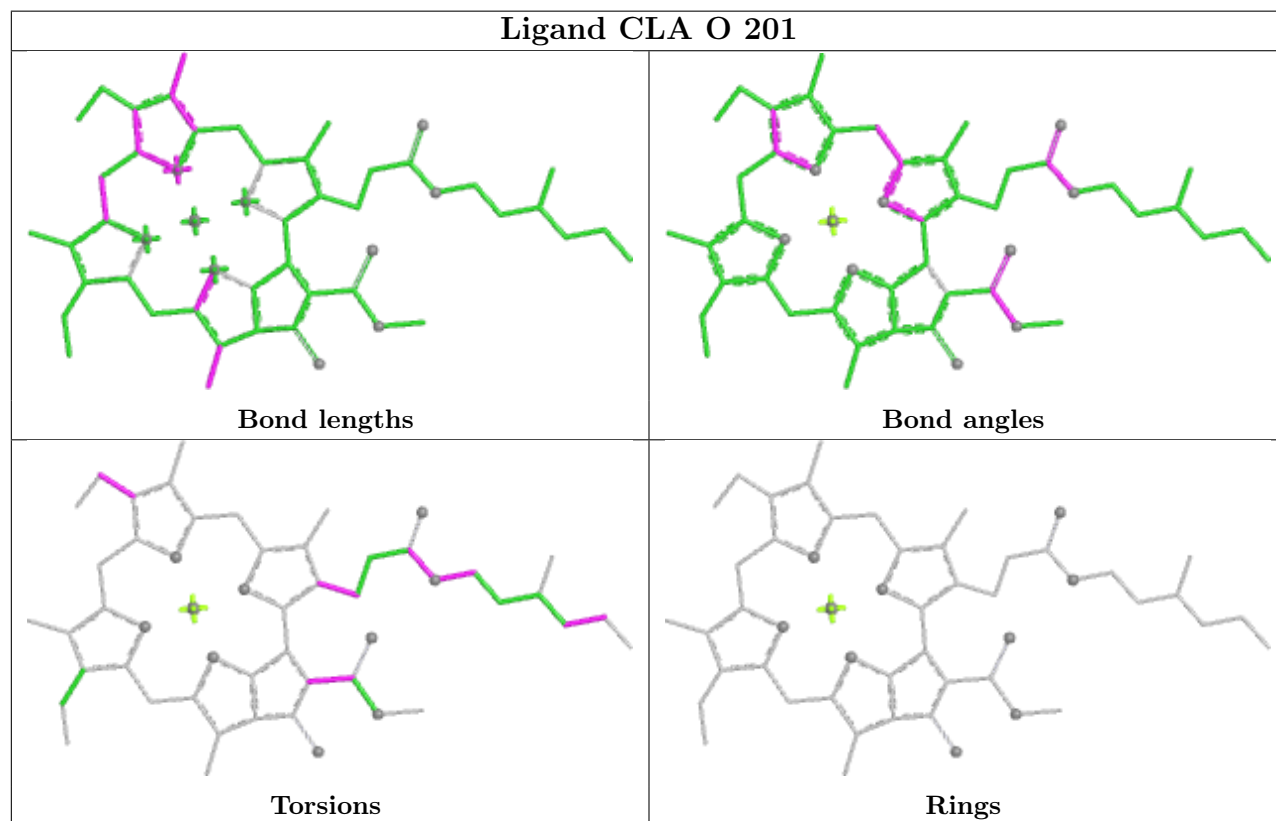
Ligand HTG F 803



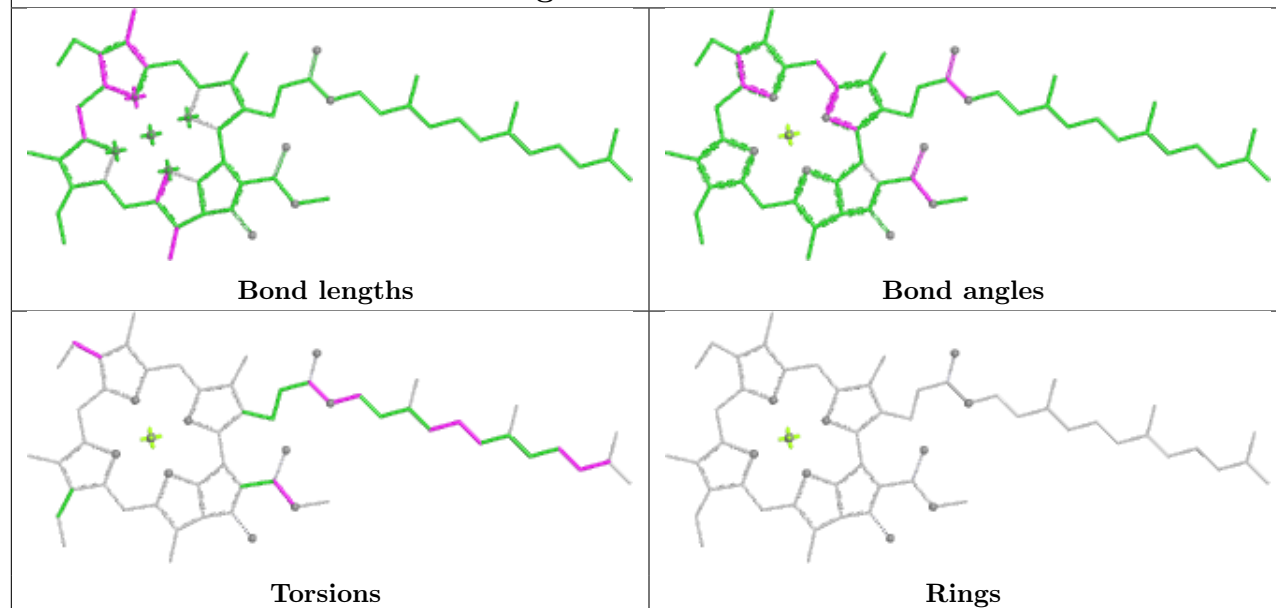
Ligand CLA 4 309



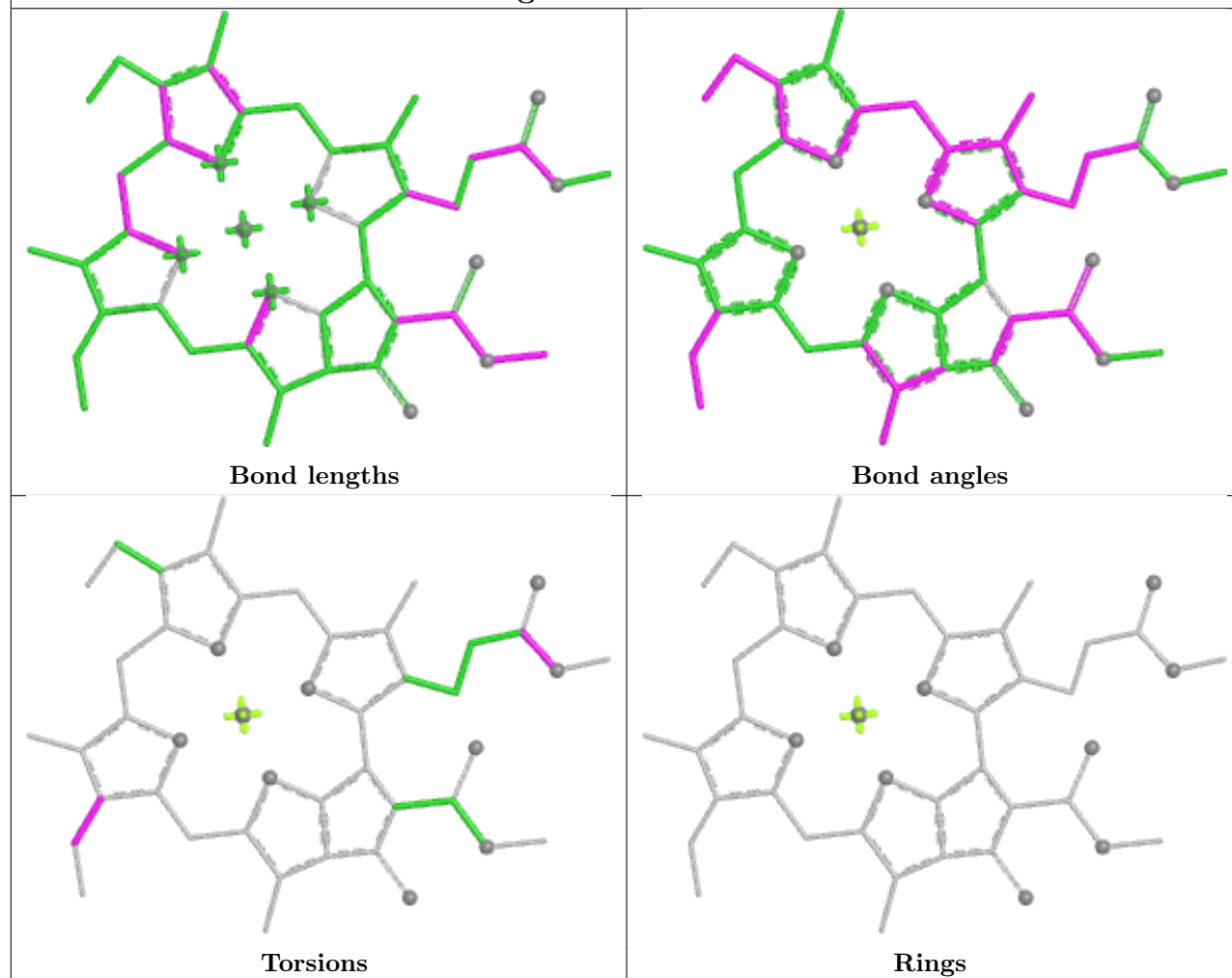
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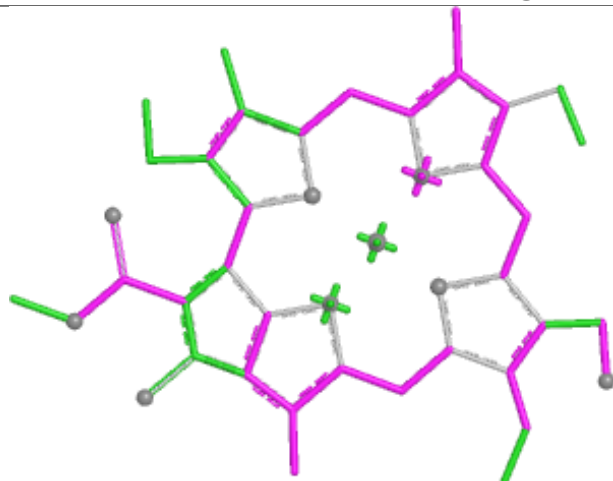
Ligand CLA 2 304



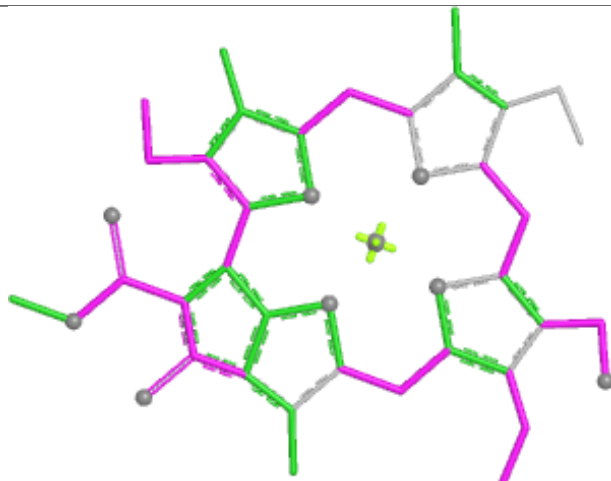
Ligand CLA 3 309



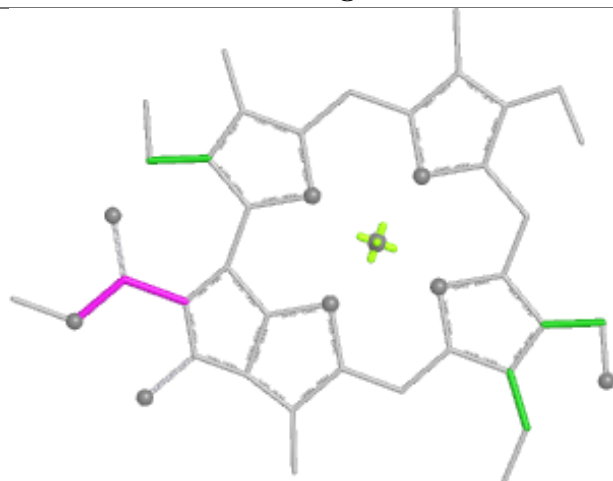
Ligand CHL 2 305



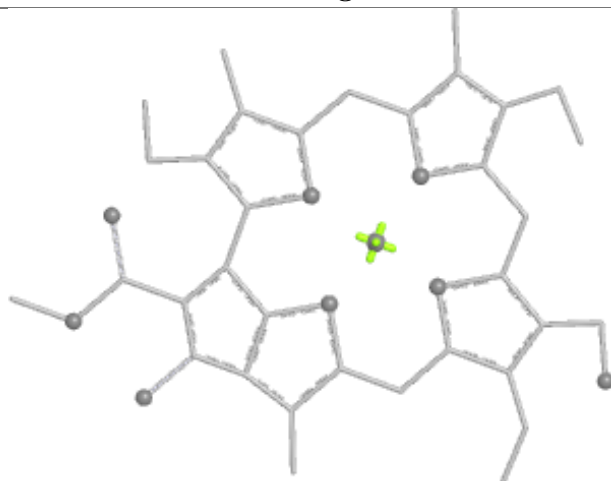
Bond lengths



Bond angles

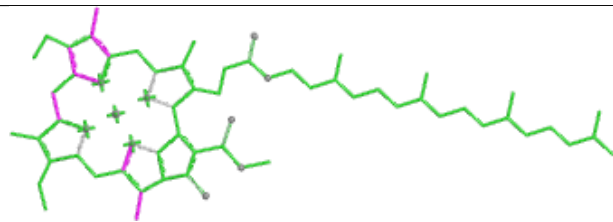


Torsions

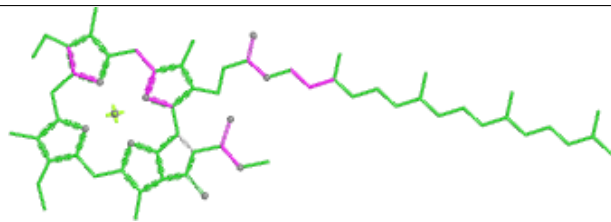


Rings

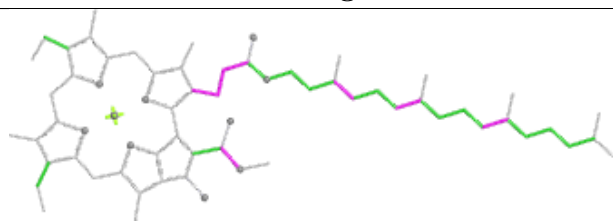
Ligand CLA B 827



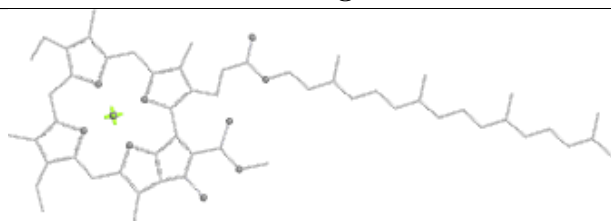
Bond lengths



Bond angles

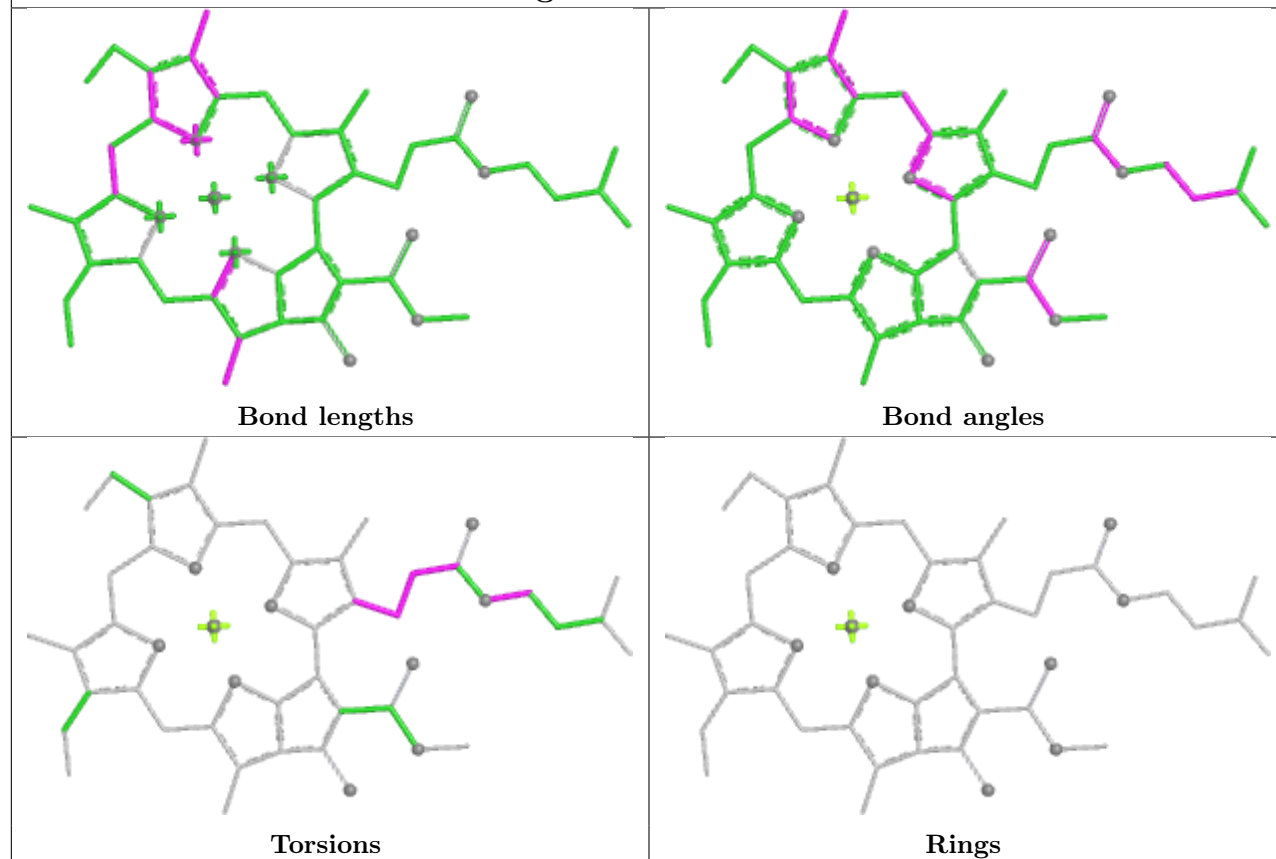


Torsions

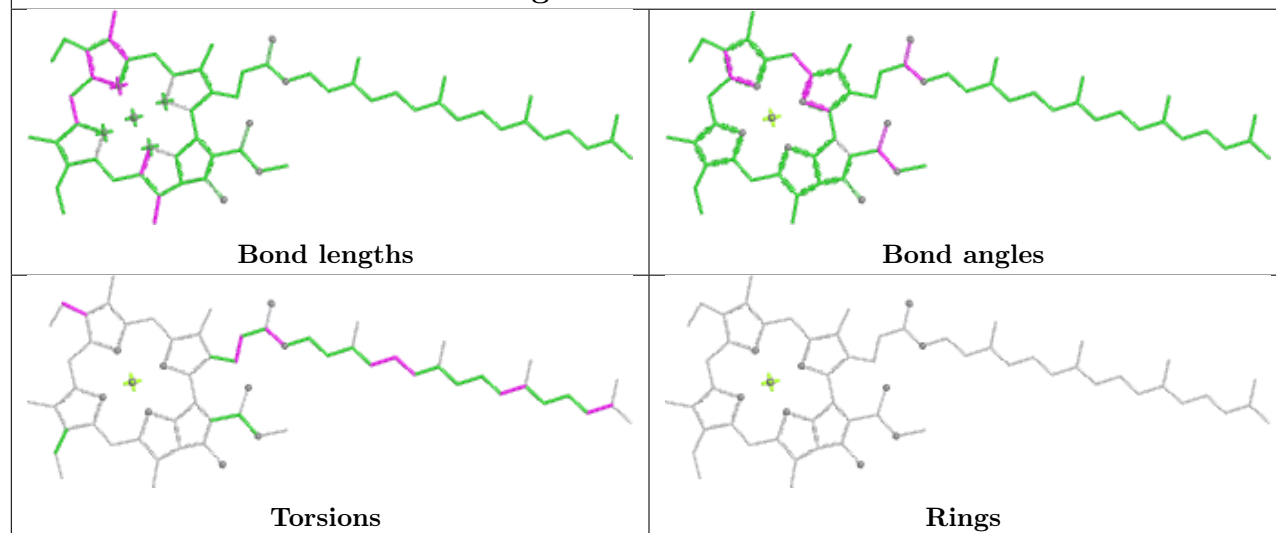


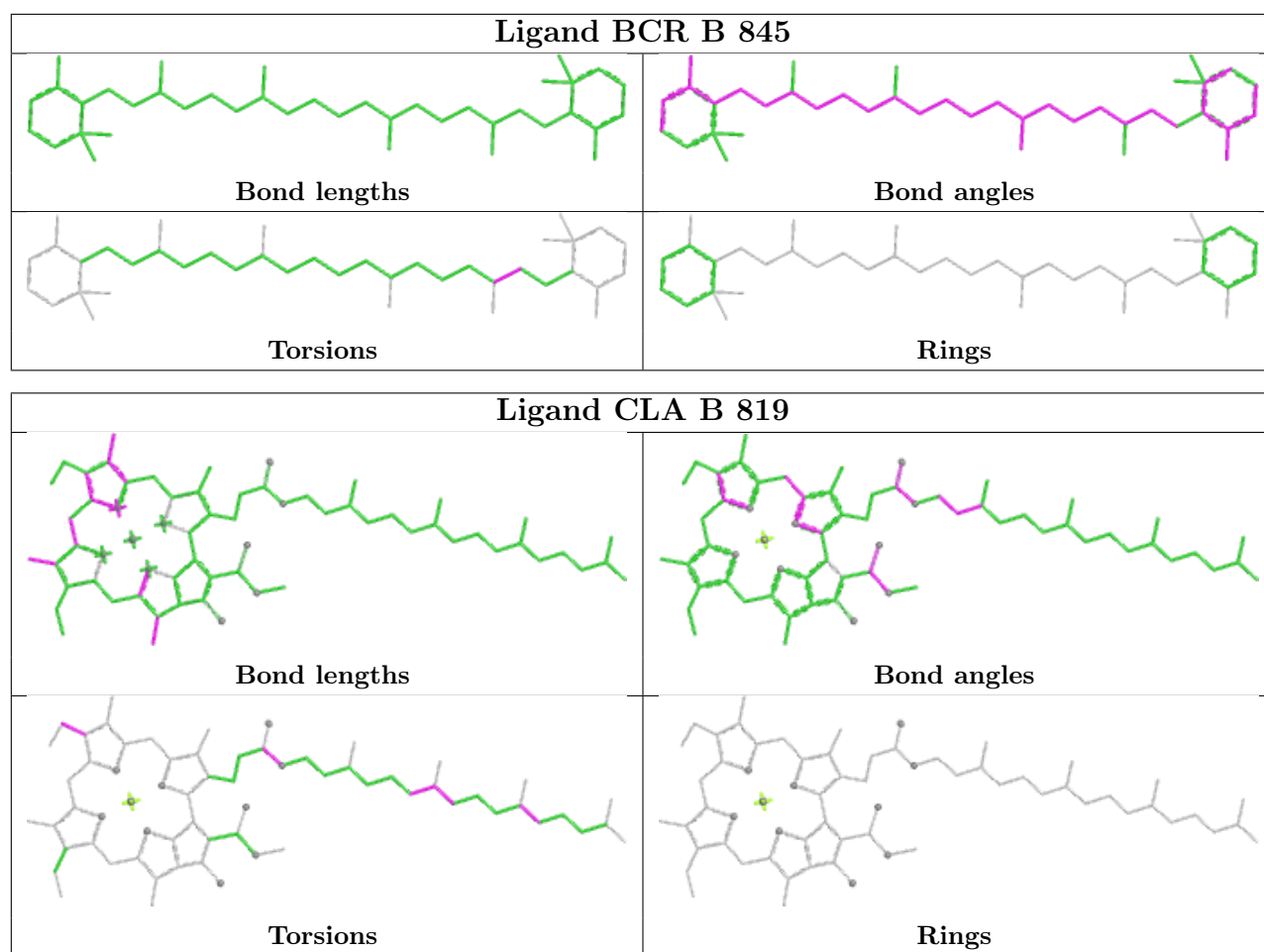
Rings

Ligand CLA 3 307

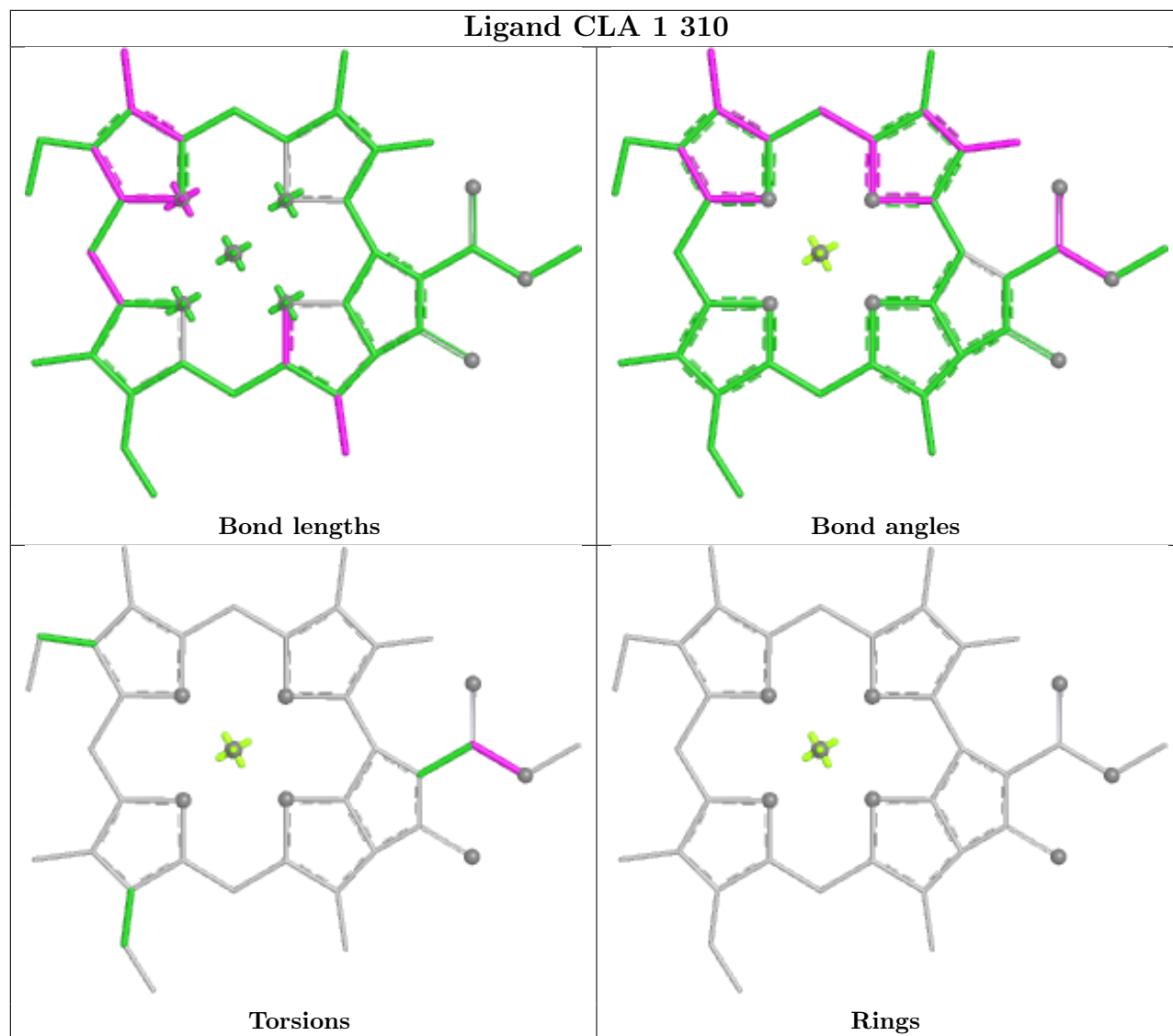


Ligand CLA A 820

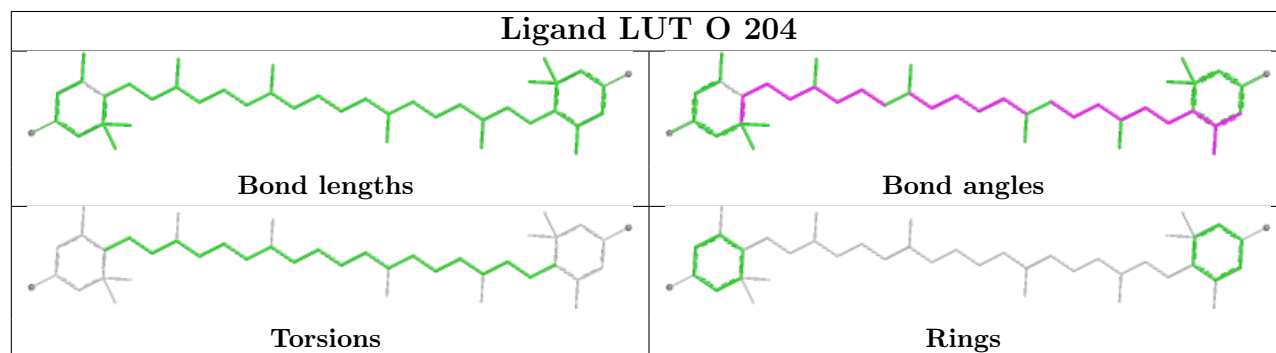


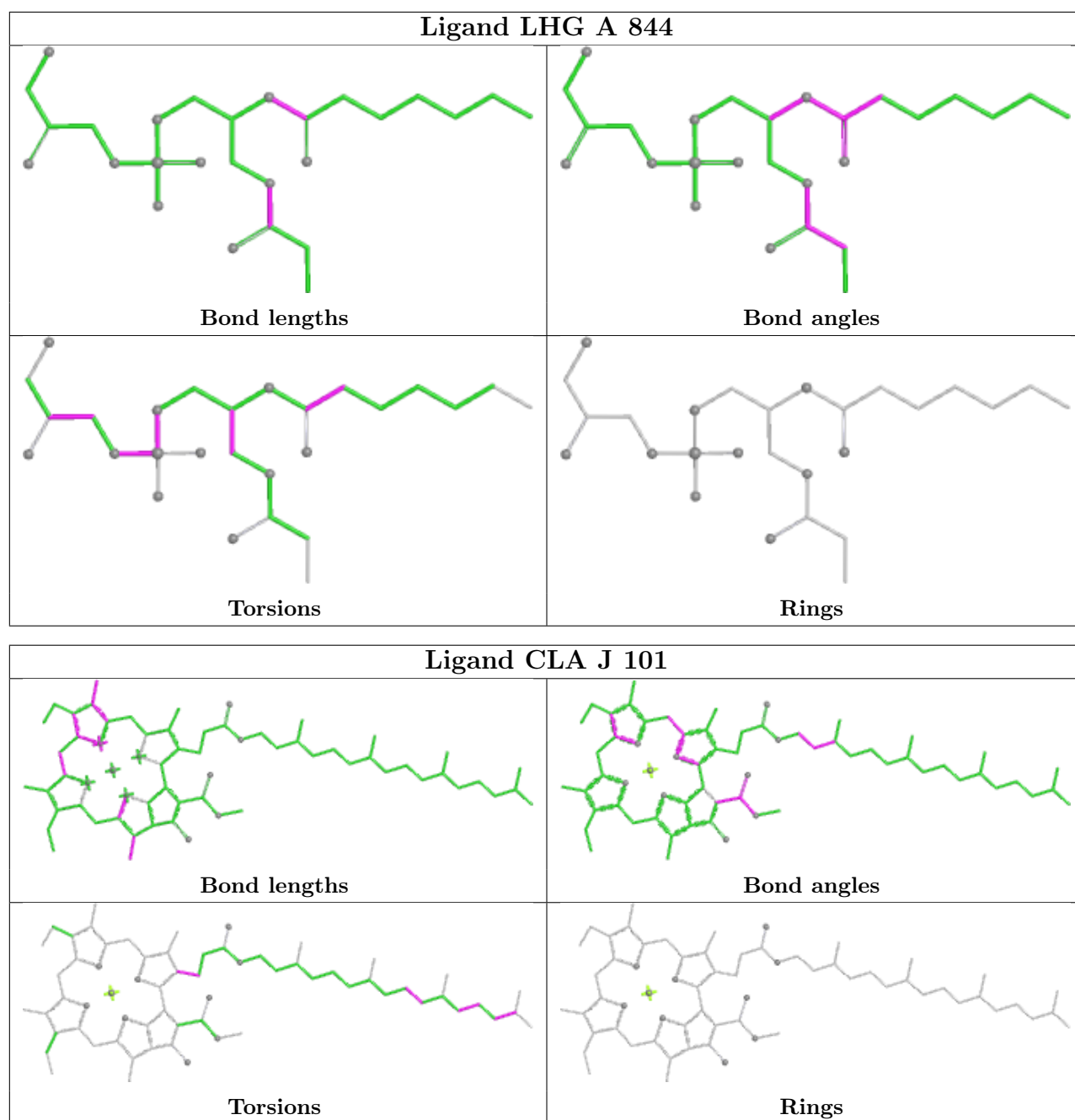


Ligand CLA 1 310

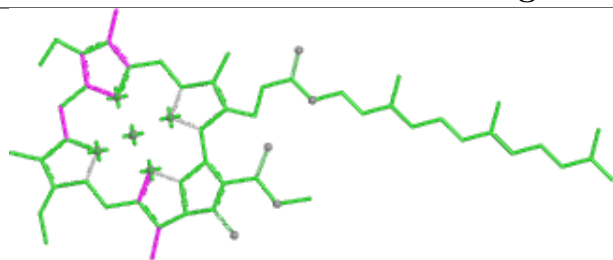


Ligand LUT O 204

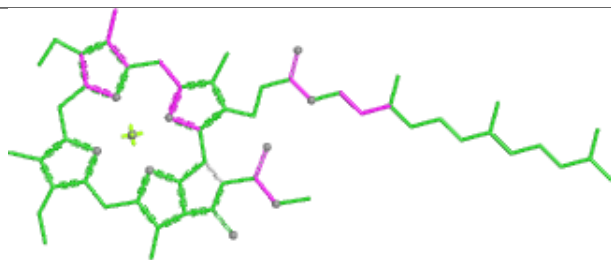




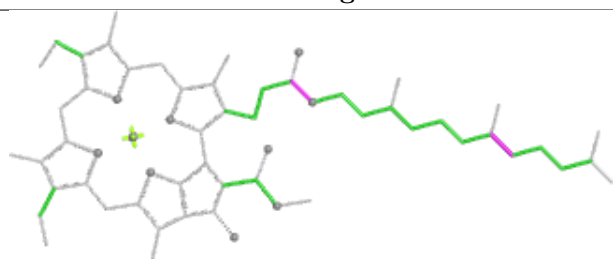
Ligand CLA 1 309



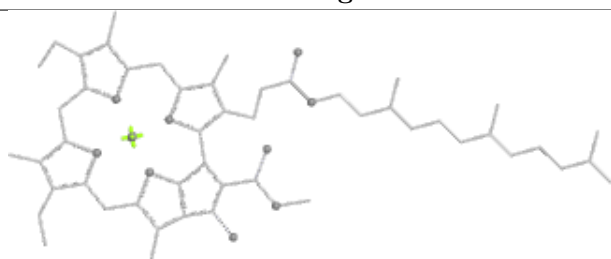
Bond lengths



Bond angles

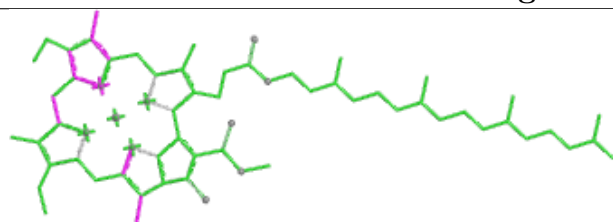


Torsions

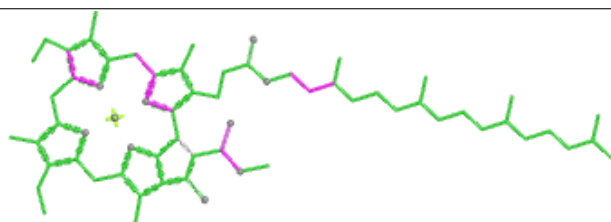


Rings

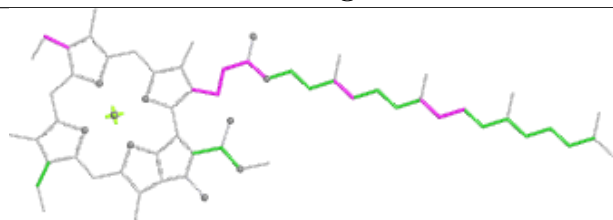
Ligand CLA 1 308



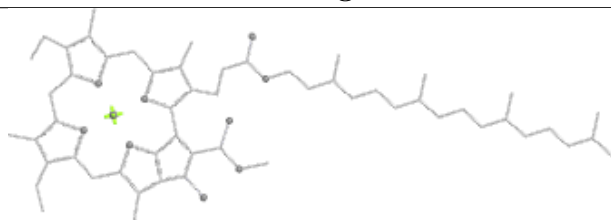
Bond lengths



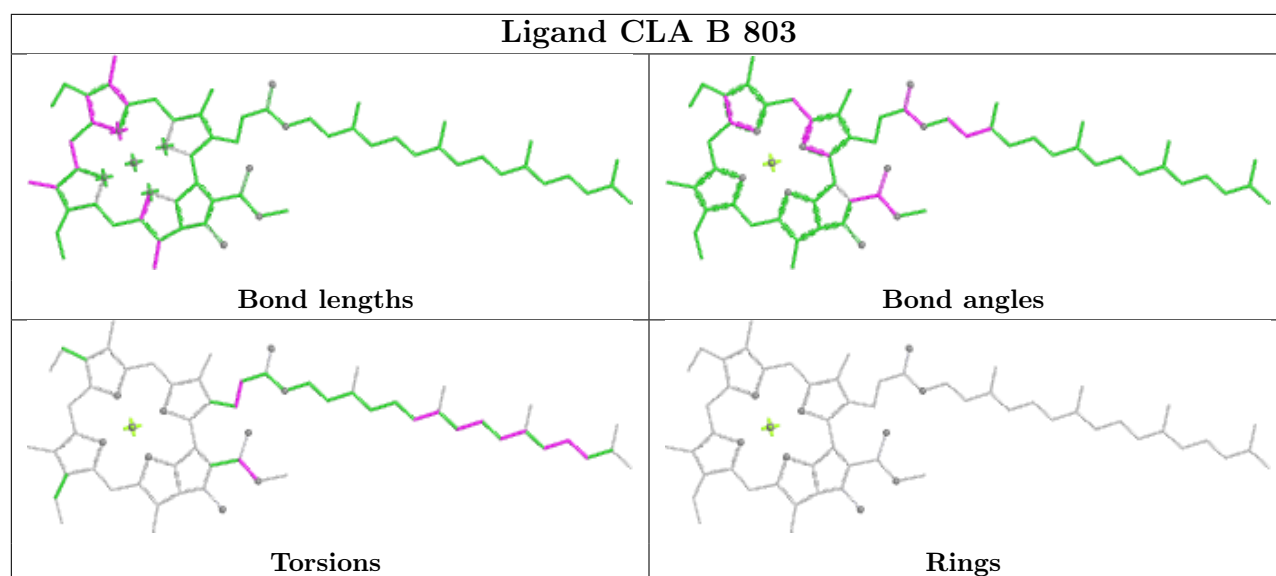
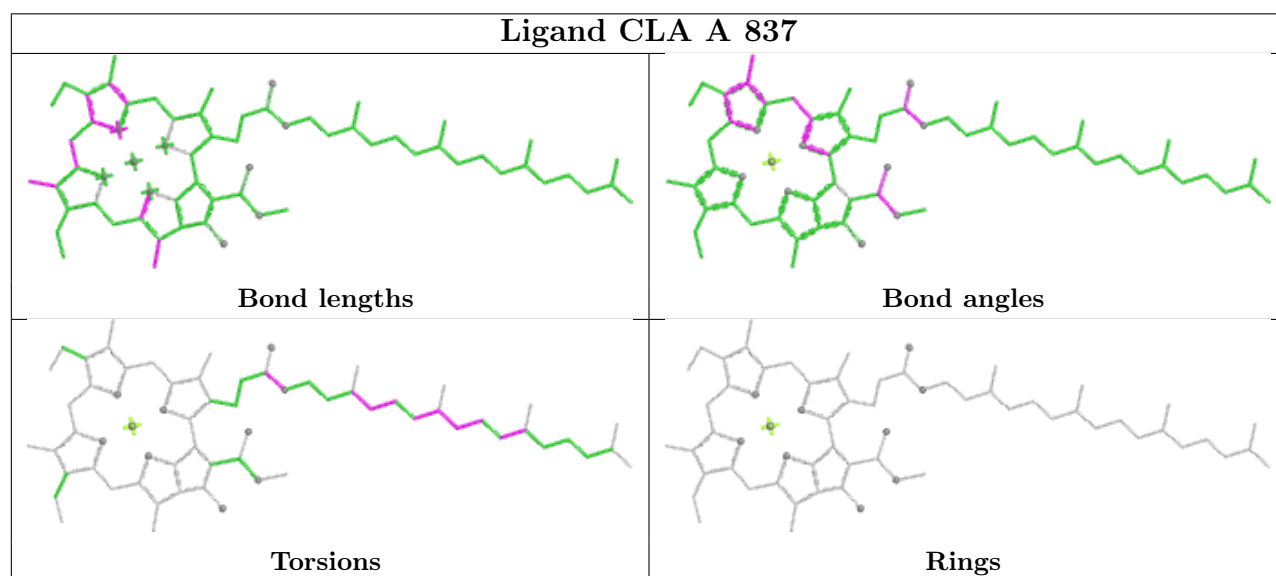
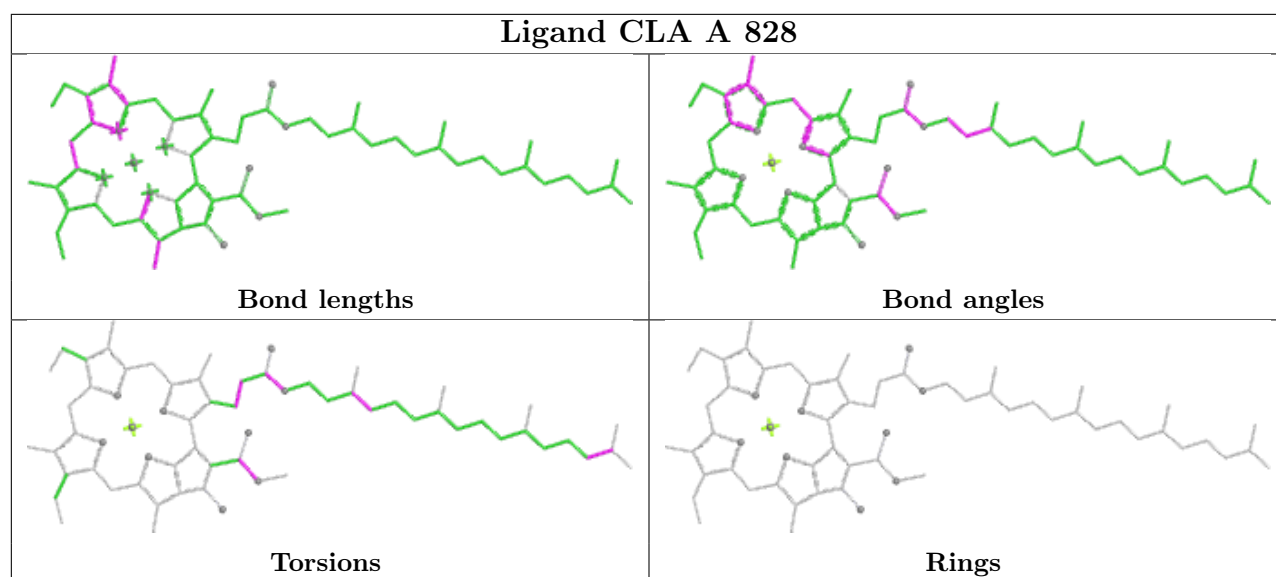
Bond angles



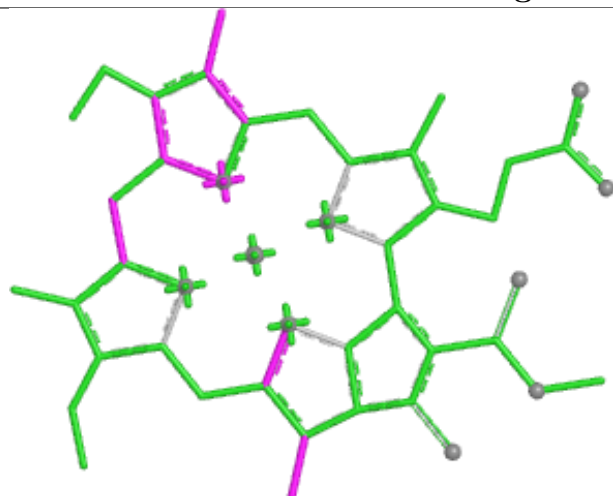
Torsions



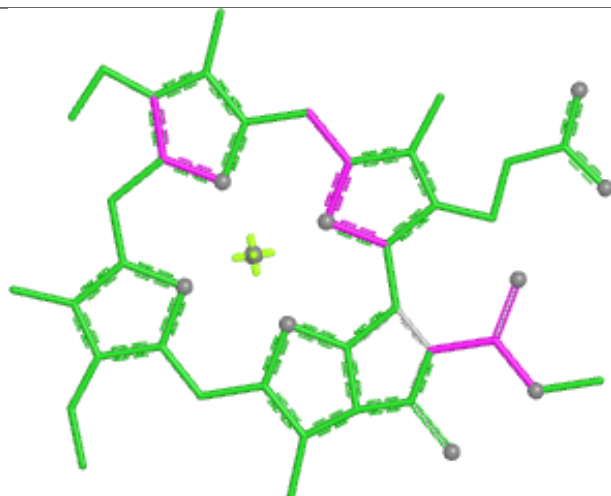
Rings



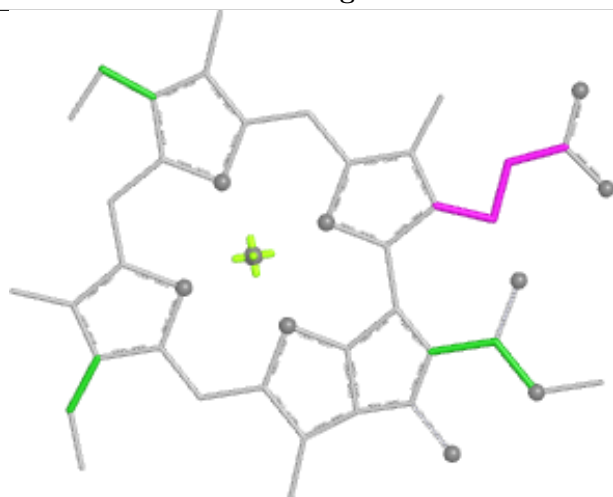
Ligand CLA B 804



Bond lengths



Bond angles

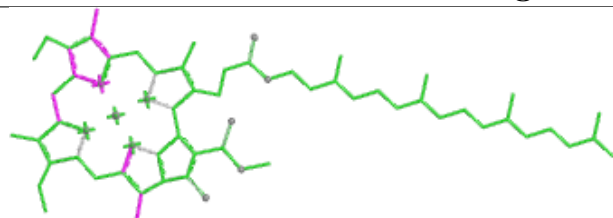


Torsions

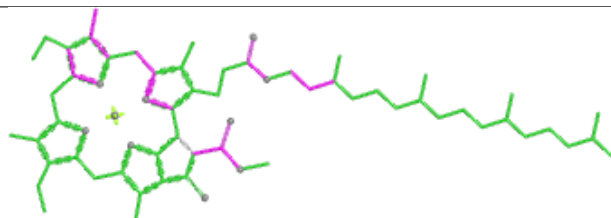


Rings

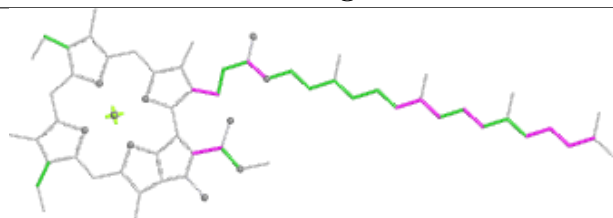
Ligand CLA B 825



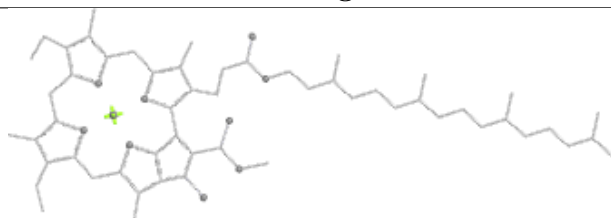
Bond lengths



Bond angles

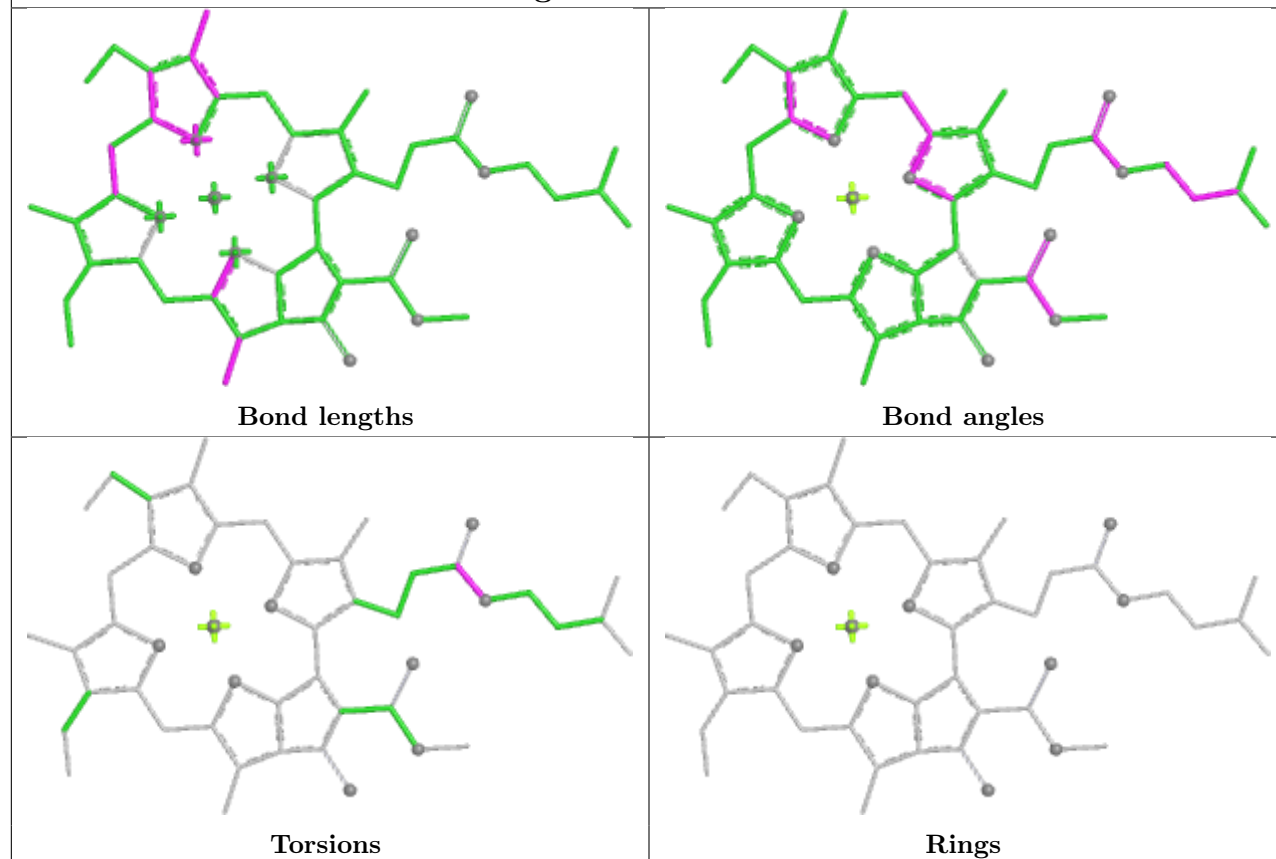


Torsions

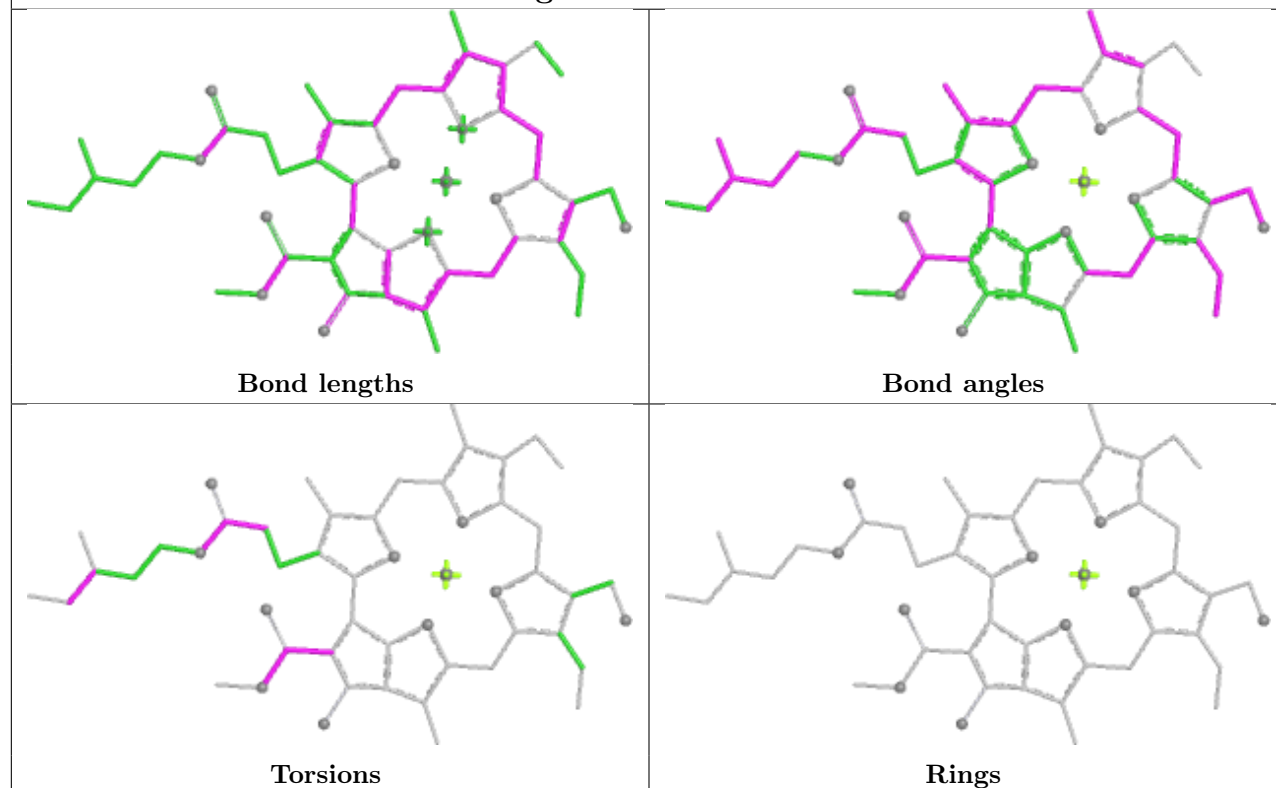


Rings

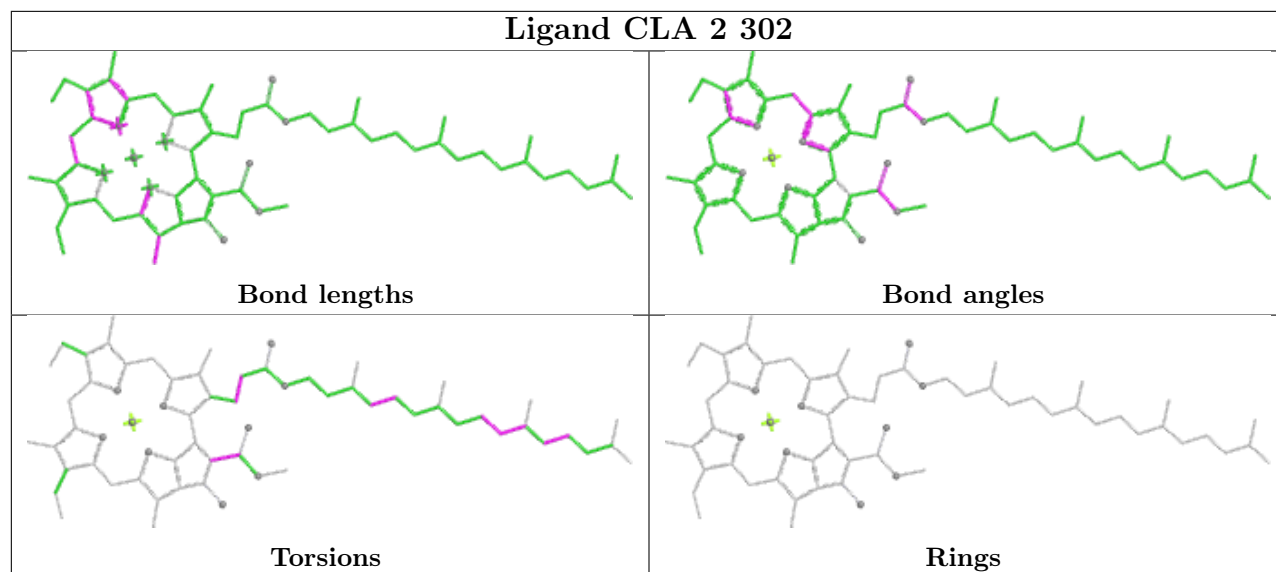
Ligand CLA L 304



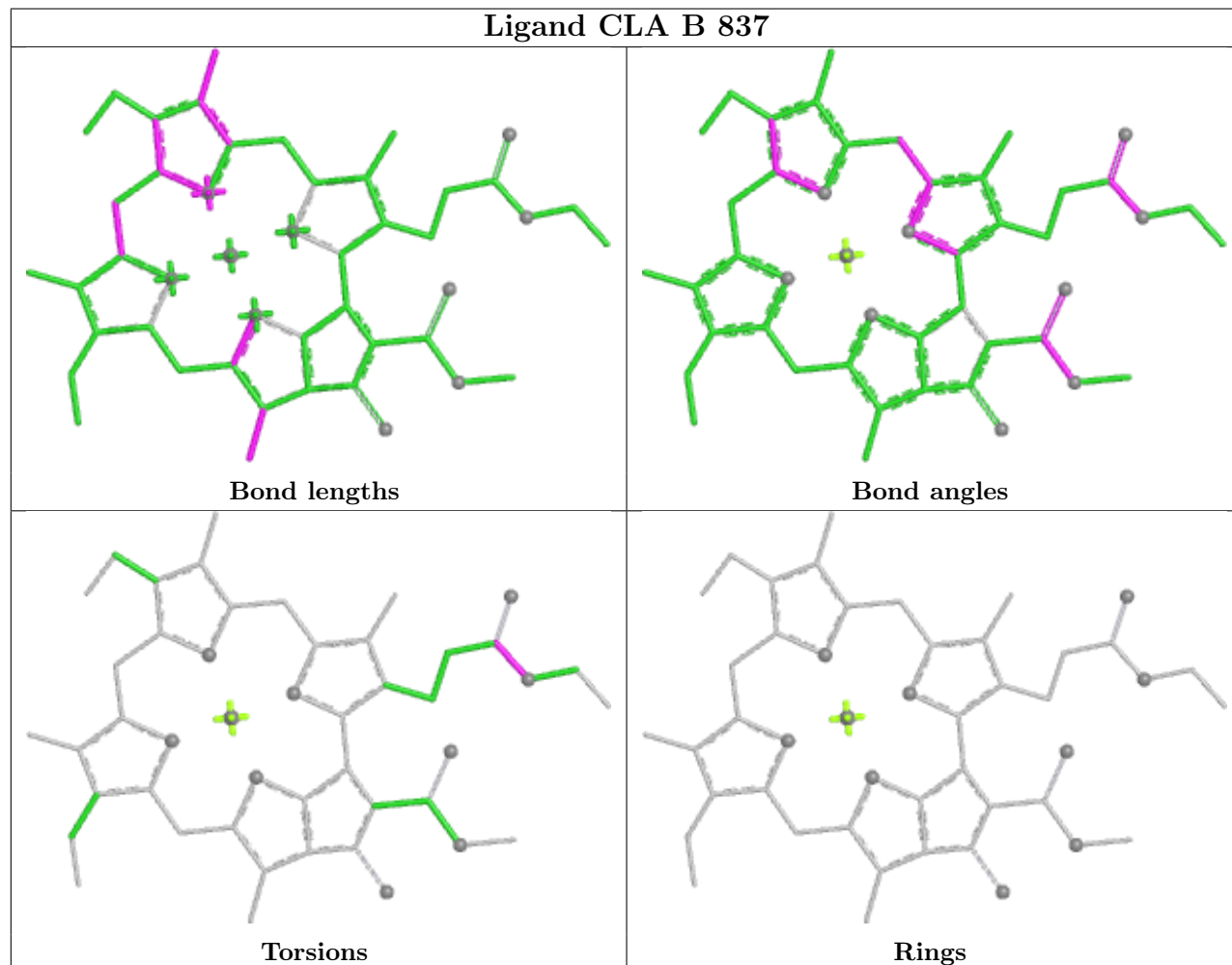
Ligand CHL 1 301



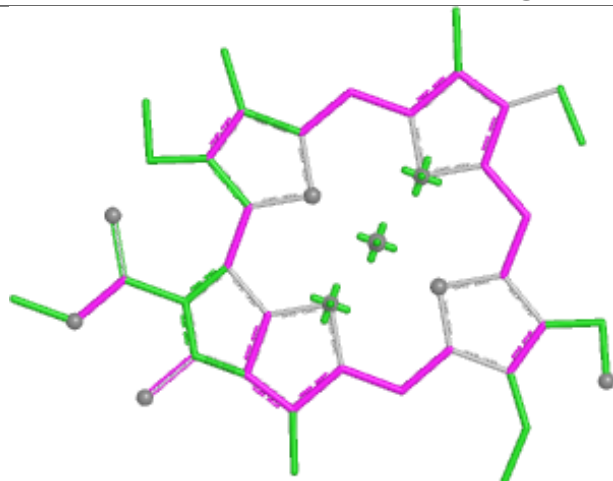
Ligand CLA 2 302



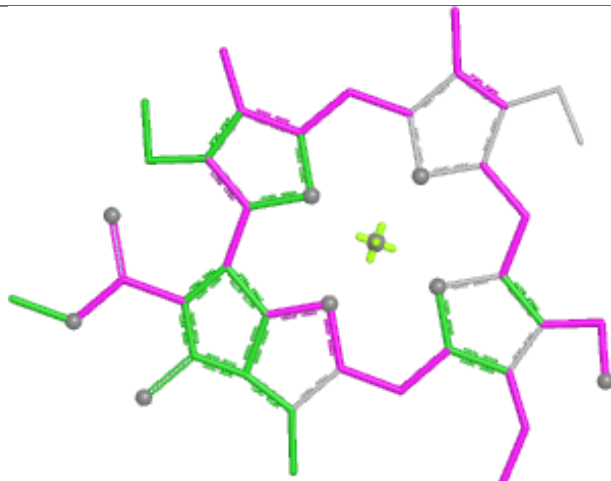
Ligand CLA B 837



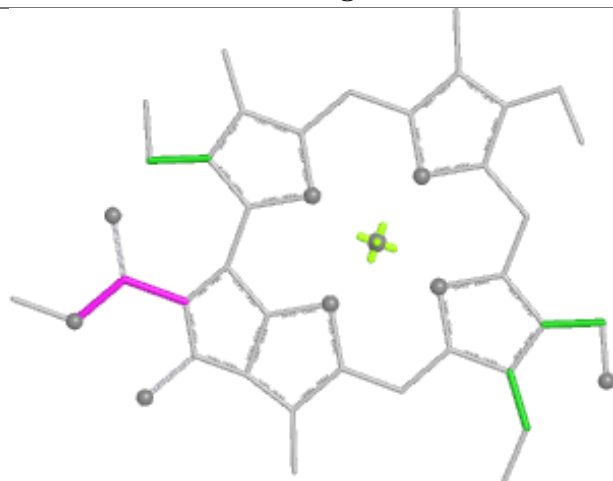
Ligand CHL 2 314



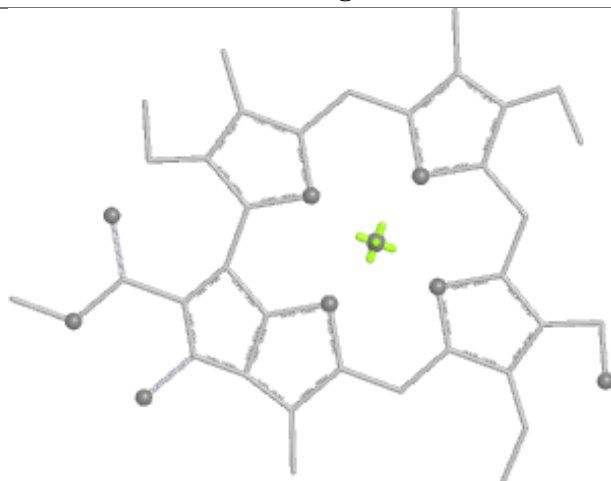
Bond lengths



Bond angles

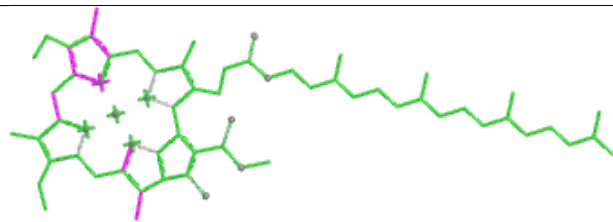


Torsions

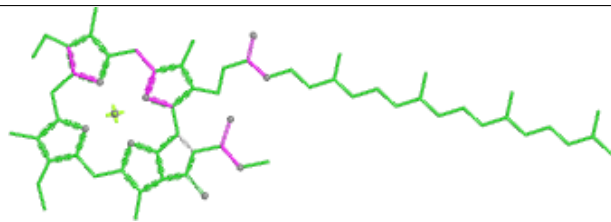


Rings

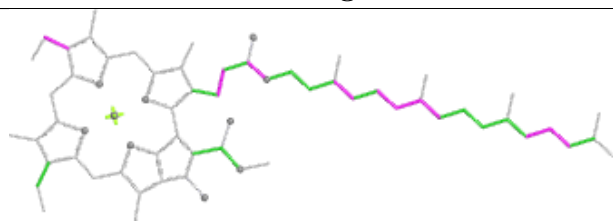
Ligand CLA A 816



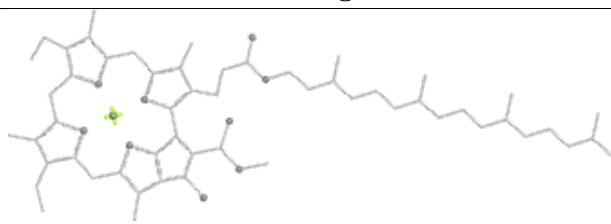
Bond lengths



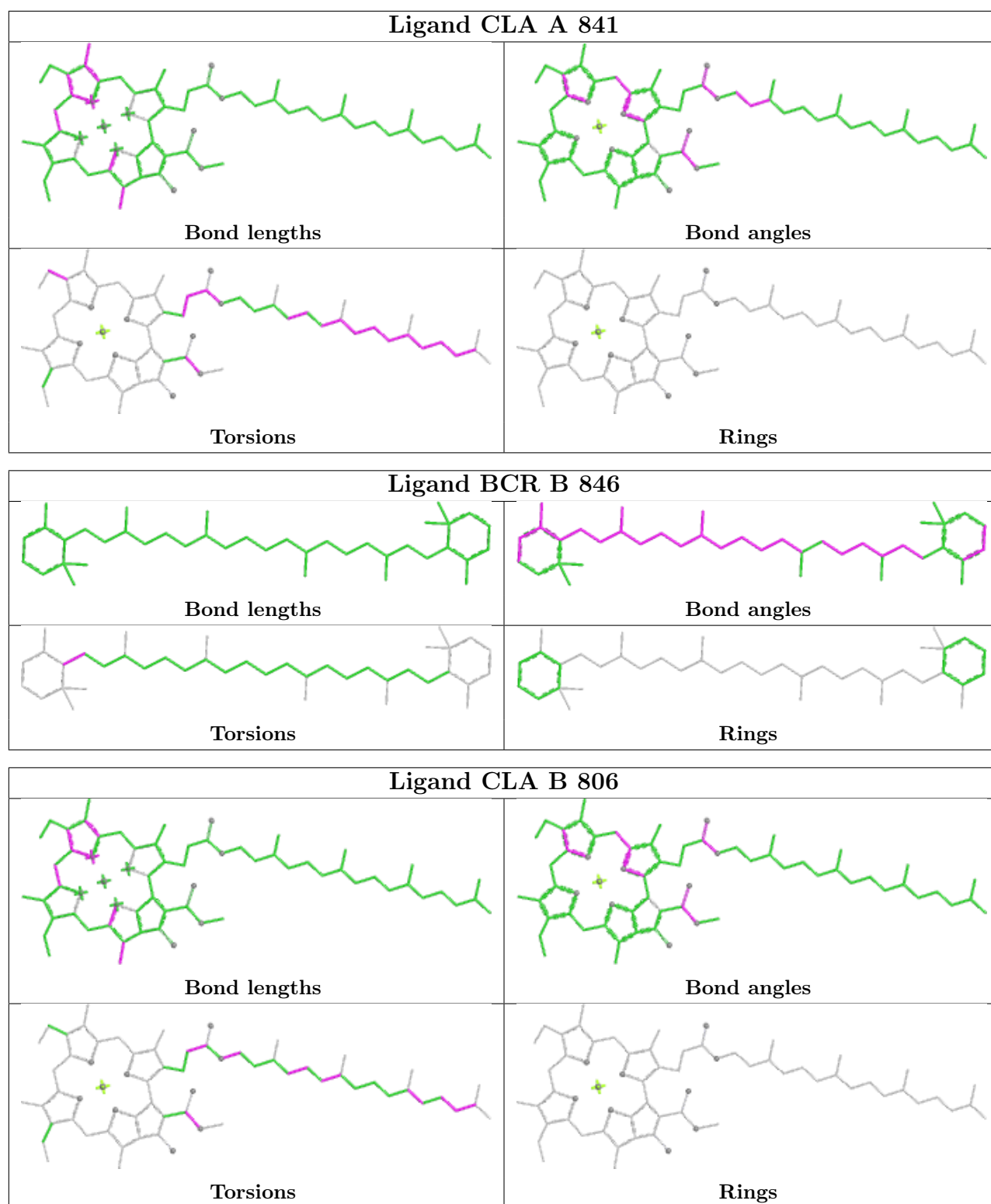
Bond angles

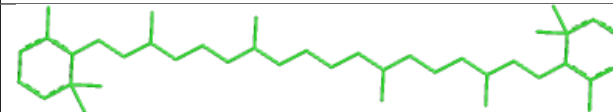
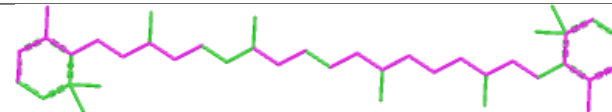
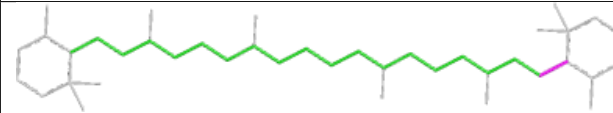
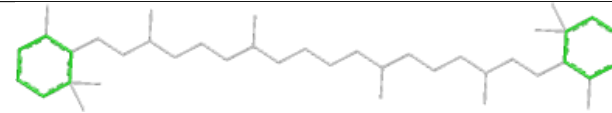


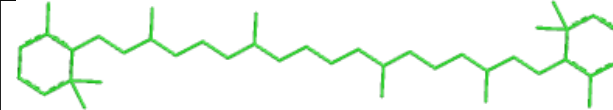
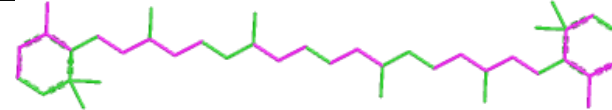
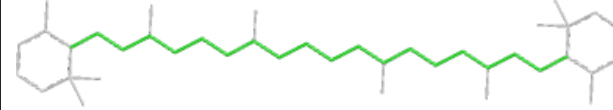
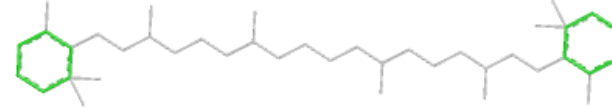
Torsions

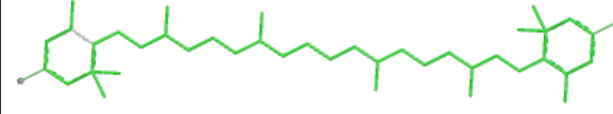
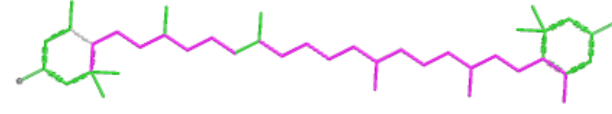
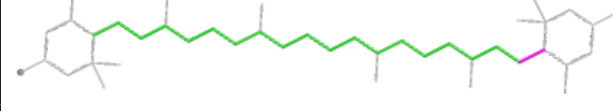
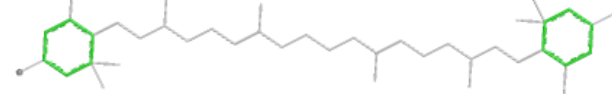


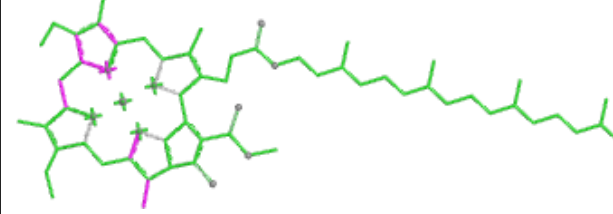
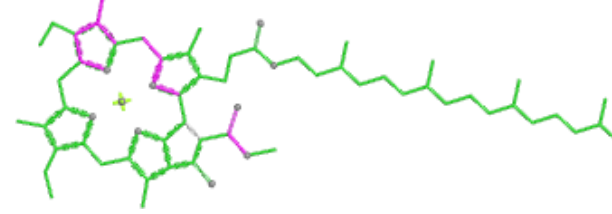
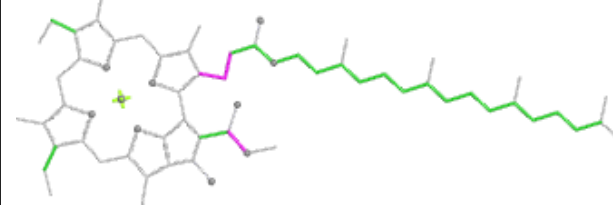
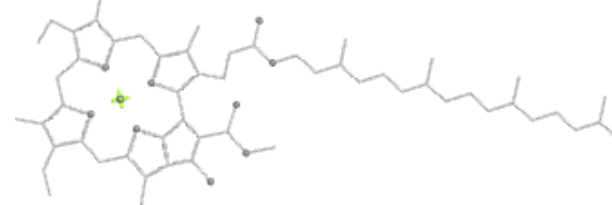
Rings

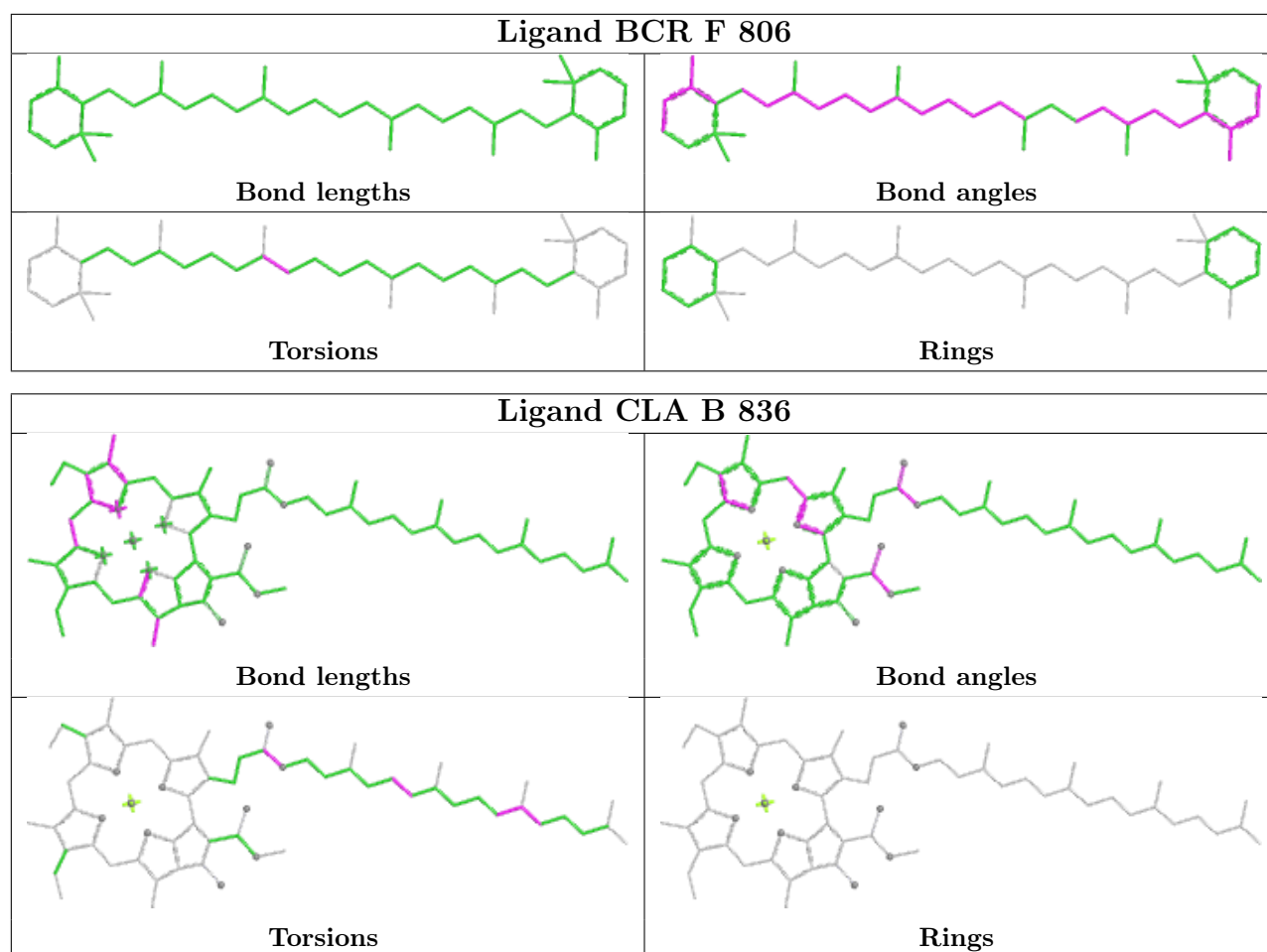


Ligand BCR J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

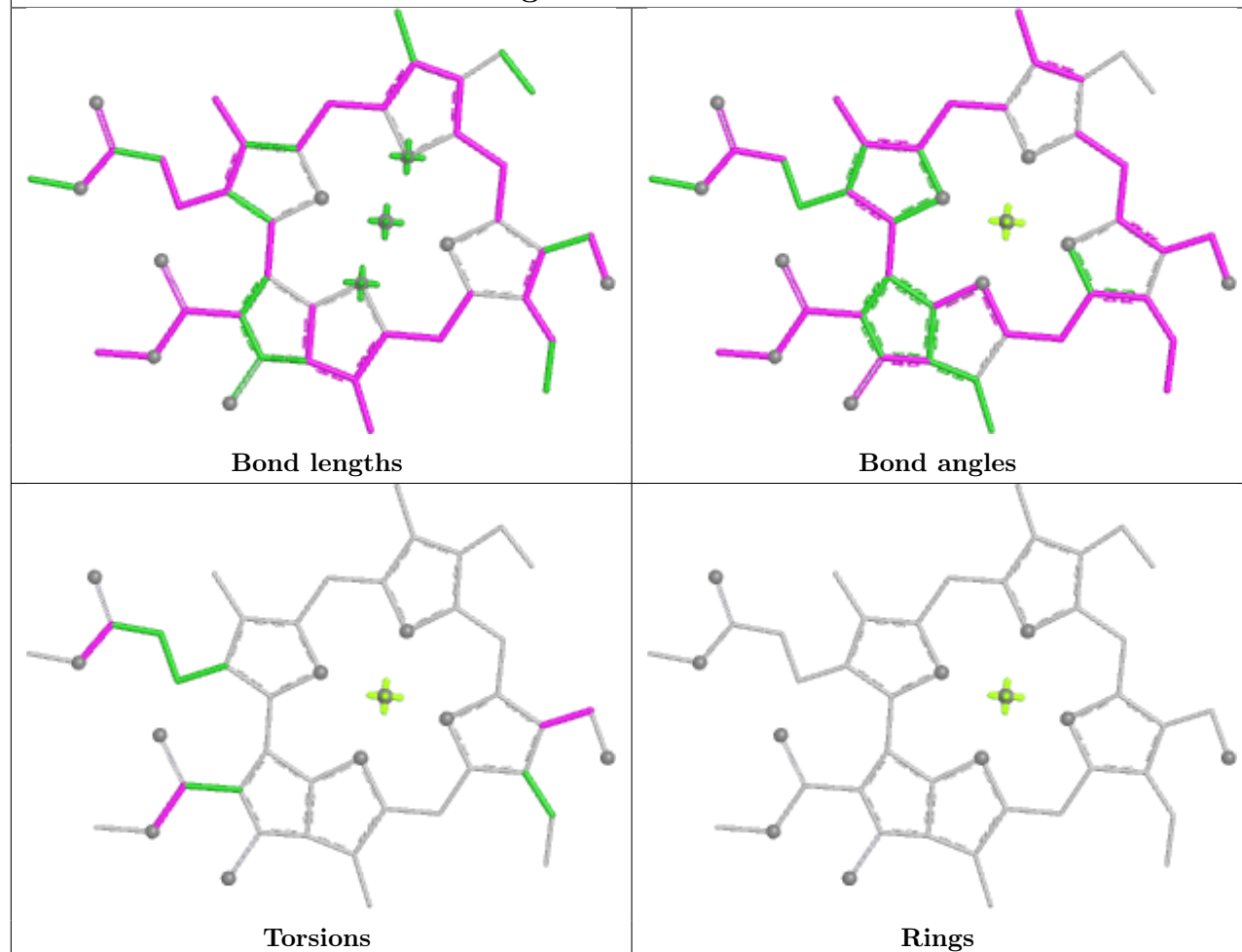
Ligand BCR L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

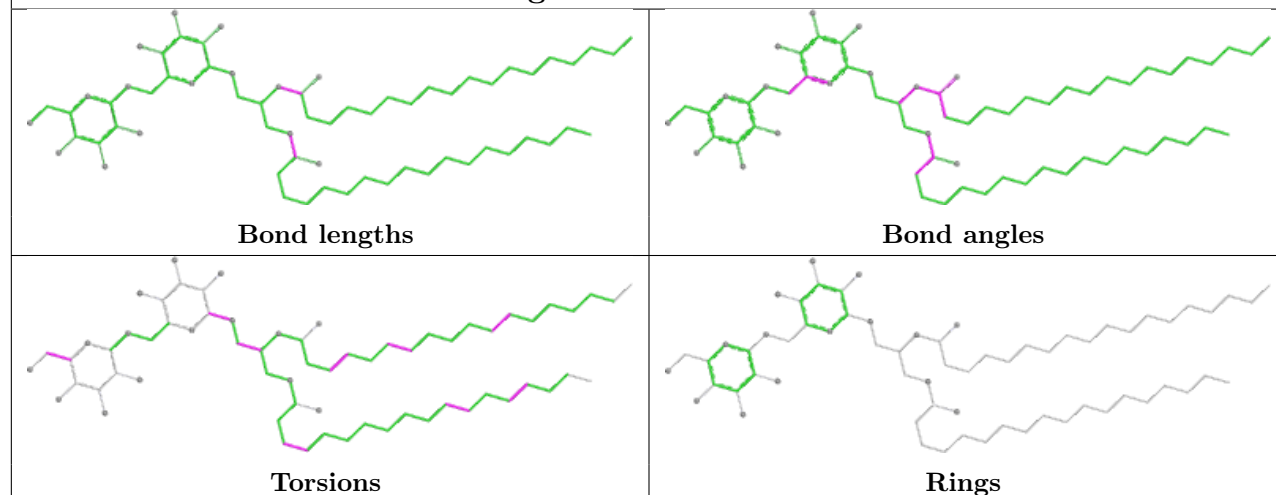
Ligand CLA B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

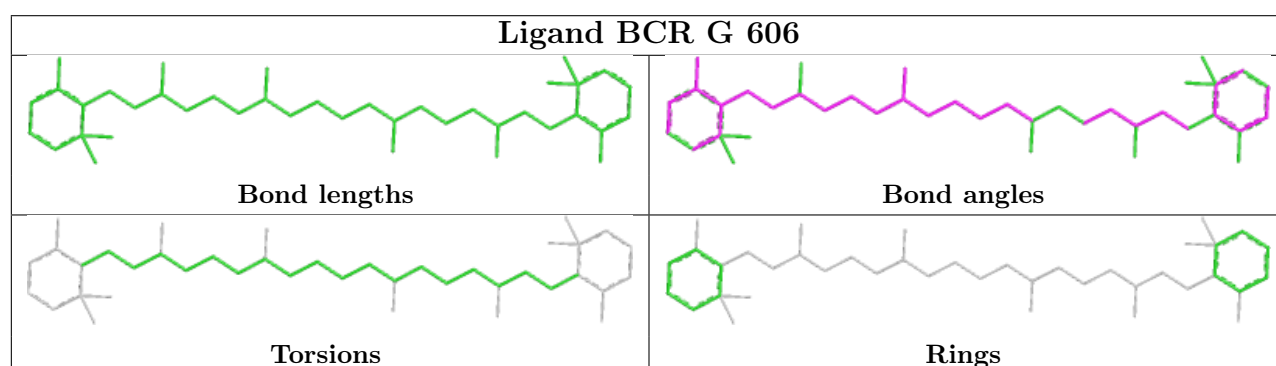
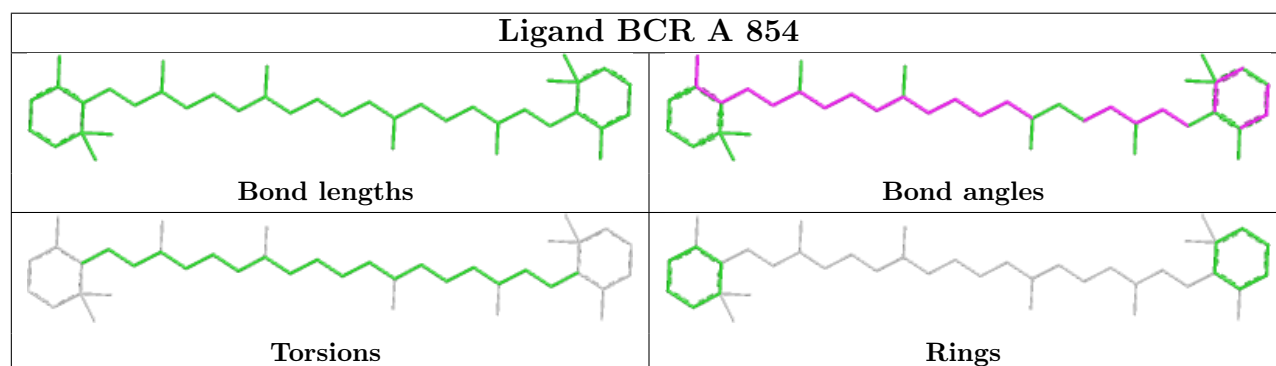
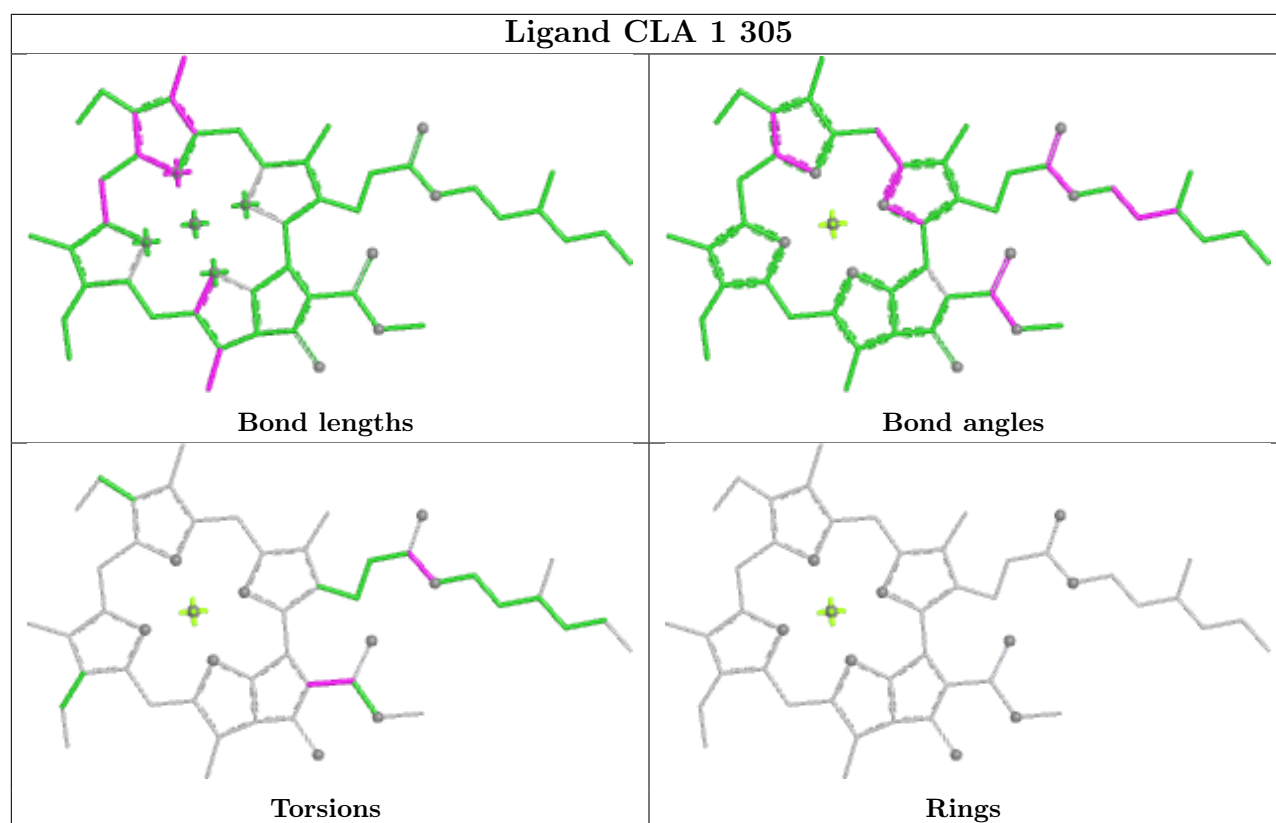


Ligand CHL 3 306

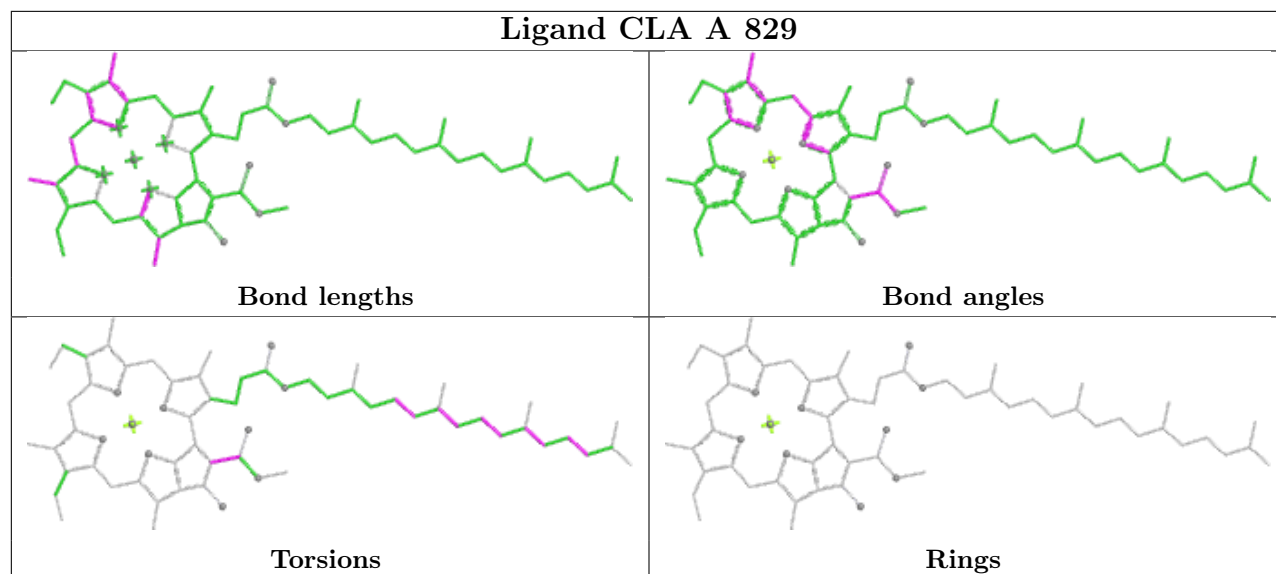


Ligand DGD B 848

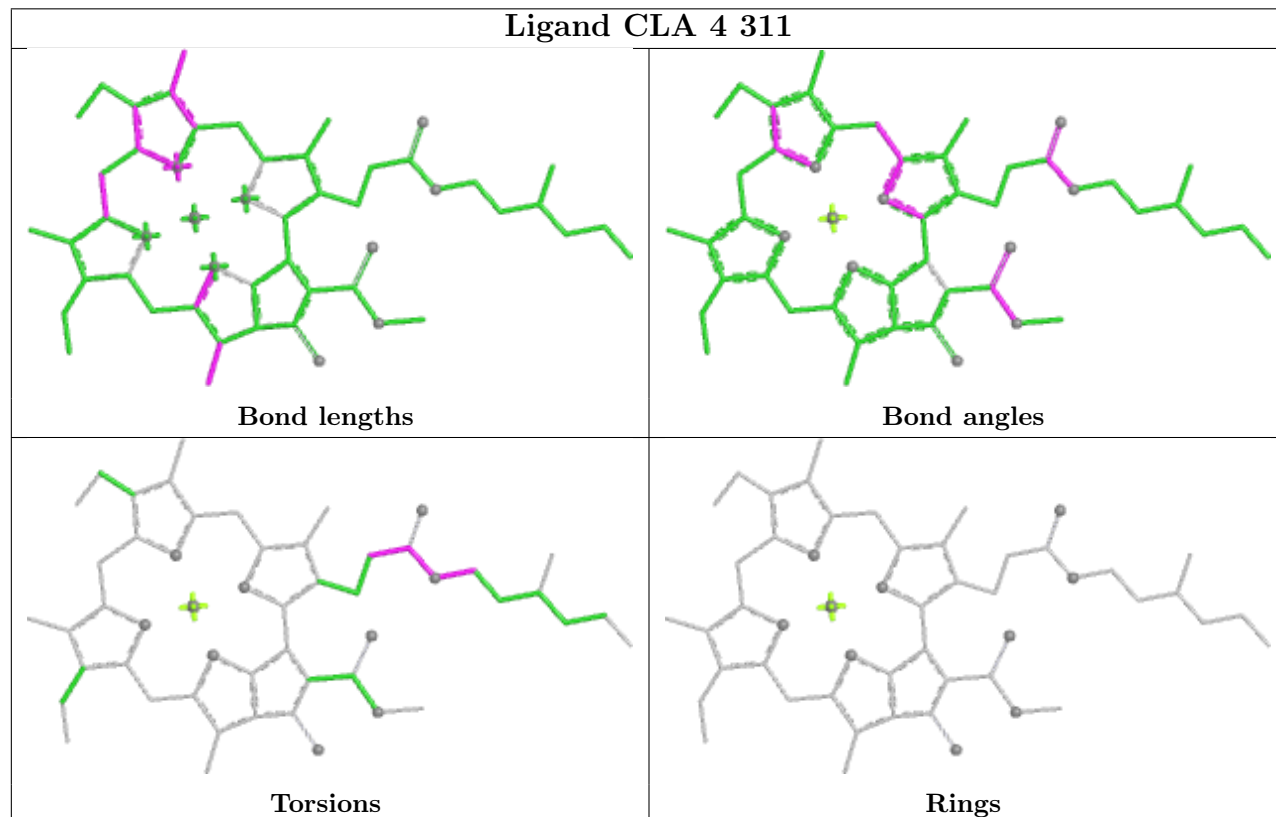


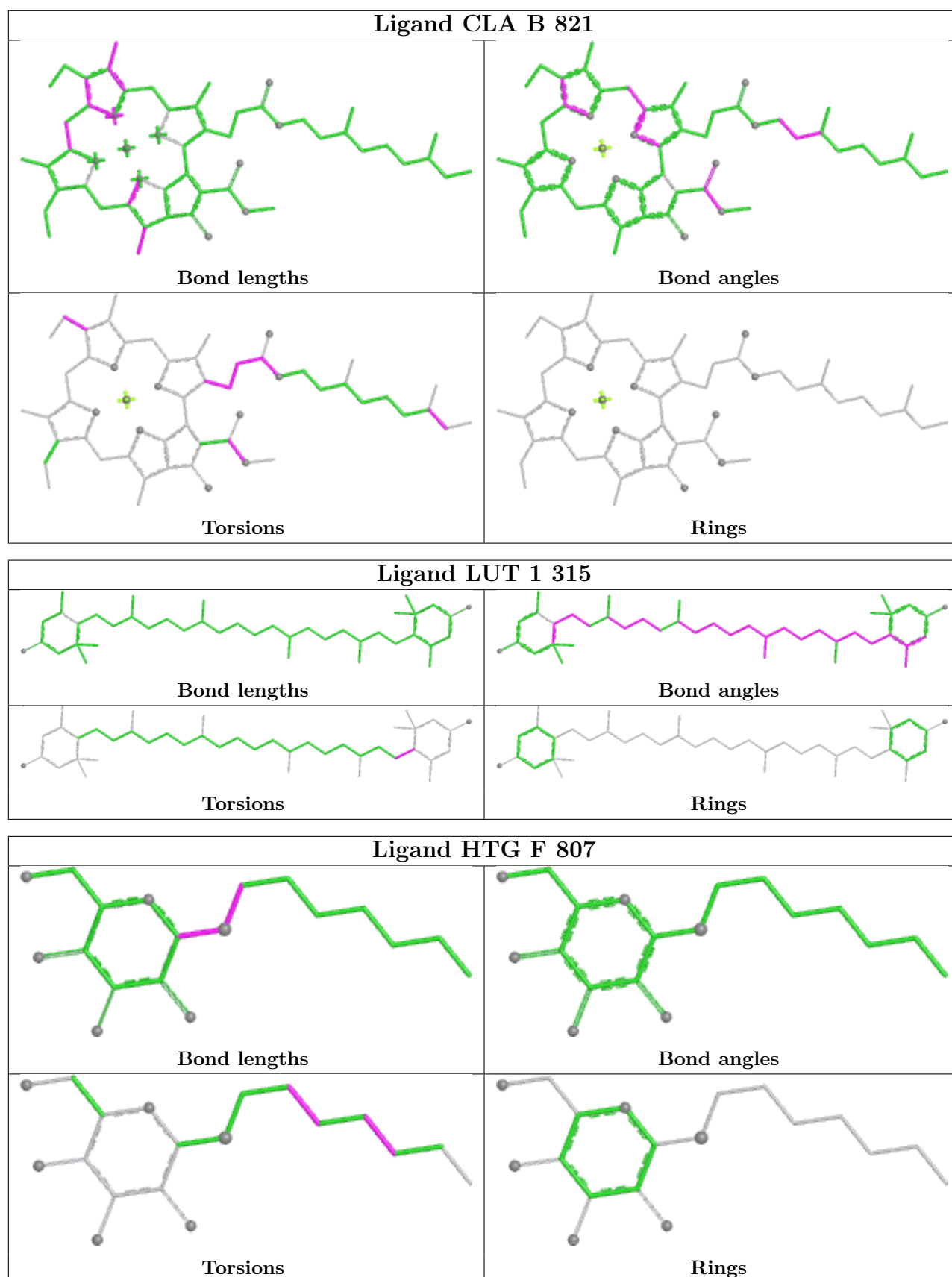


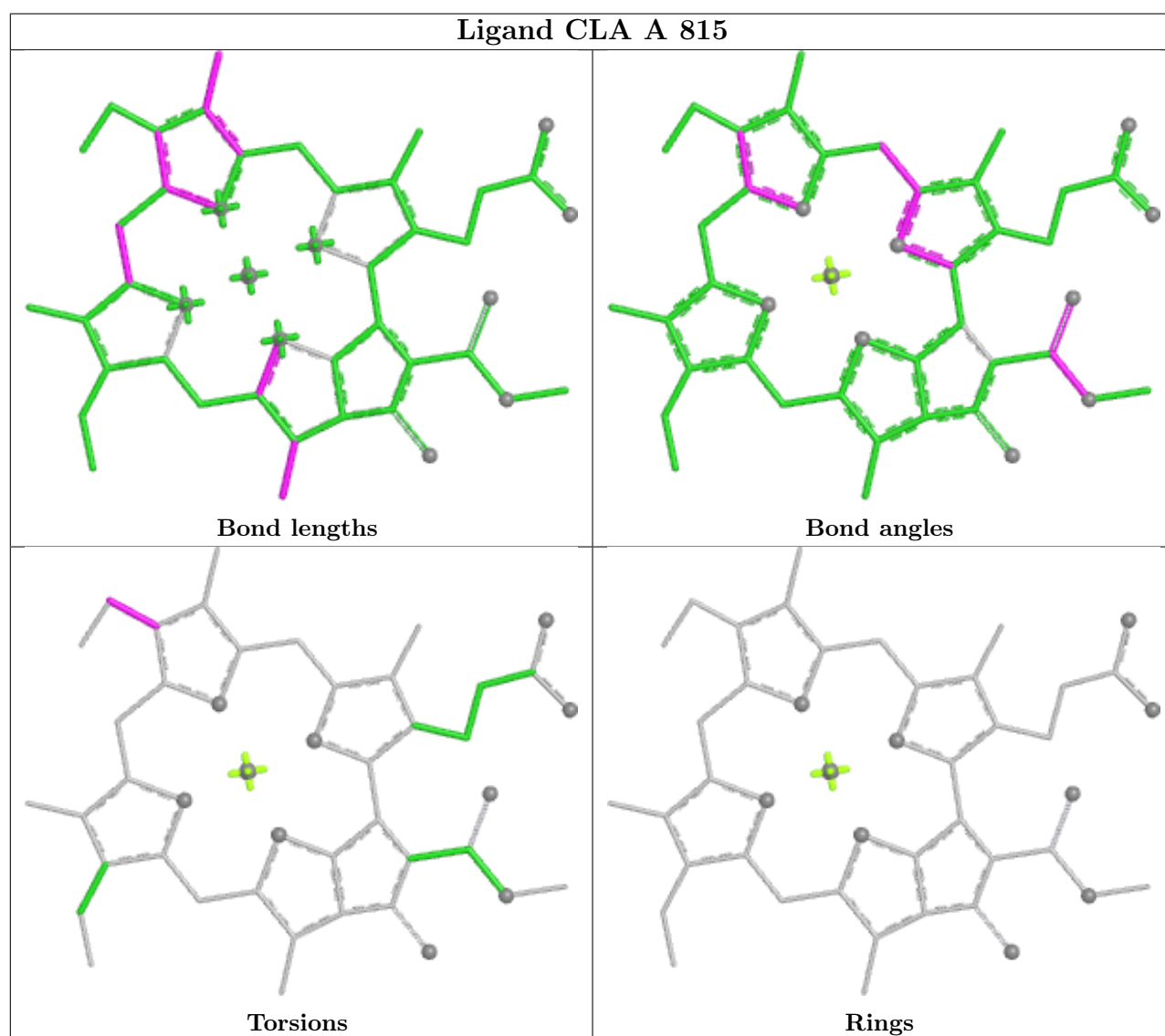
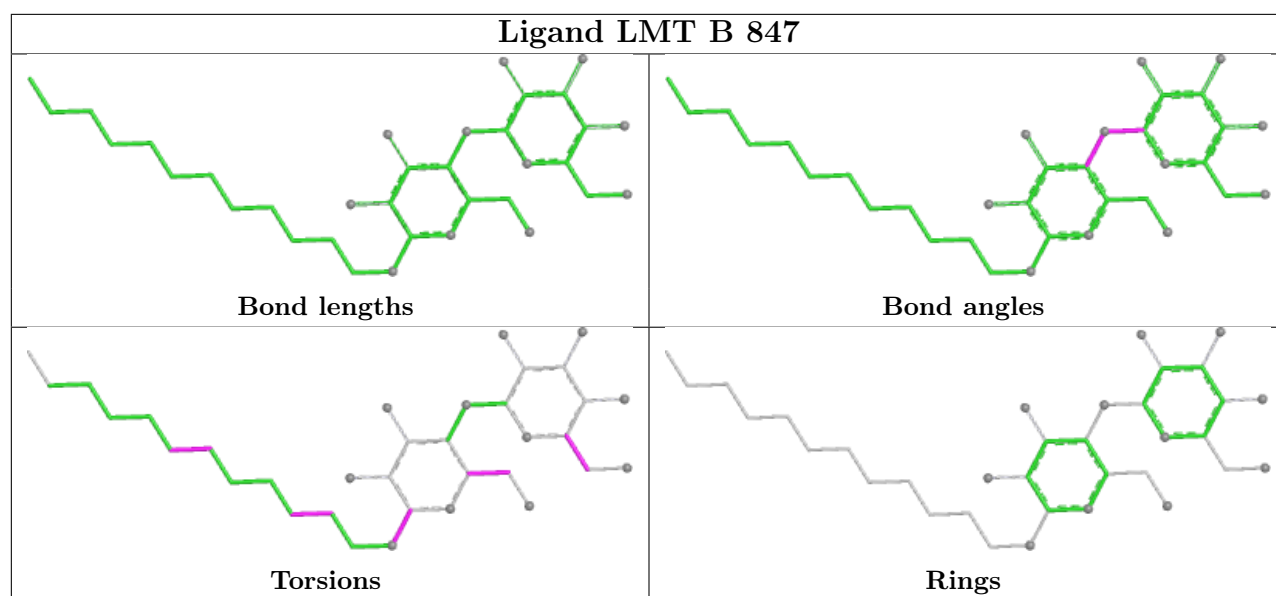
Ligand CLA A 829



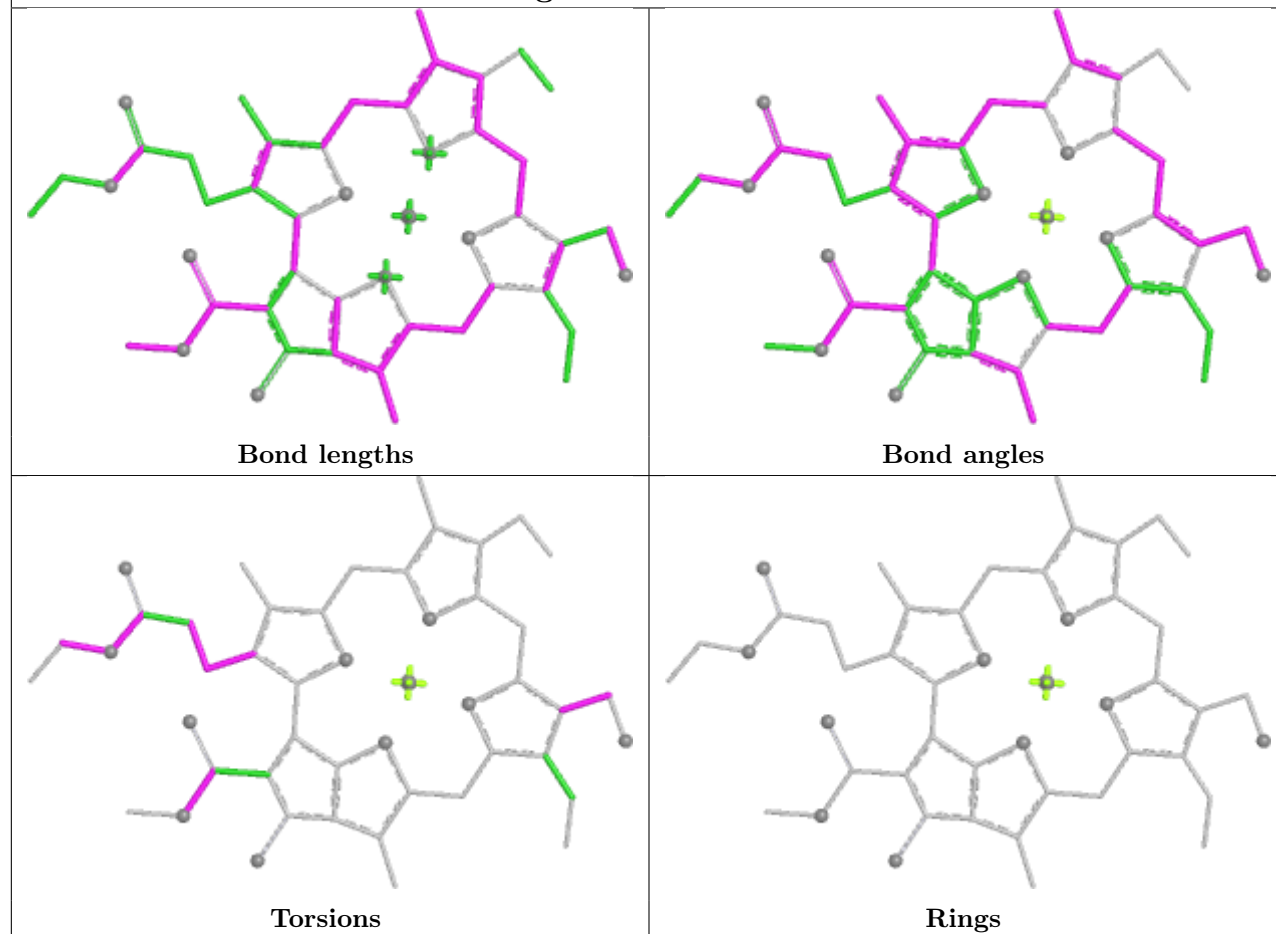
Ligand CLA 4 311



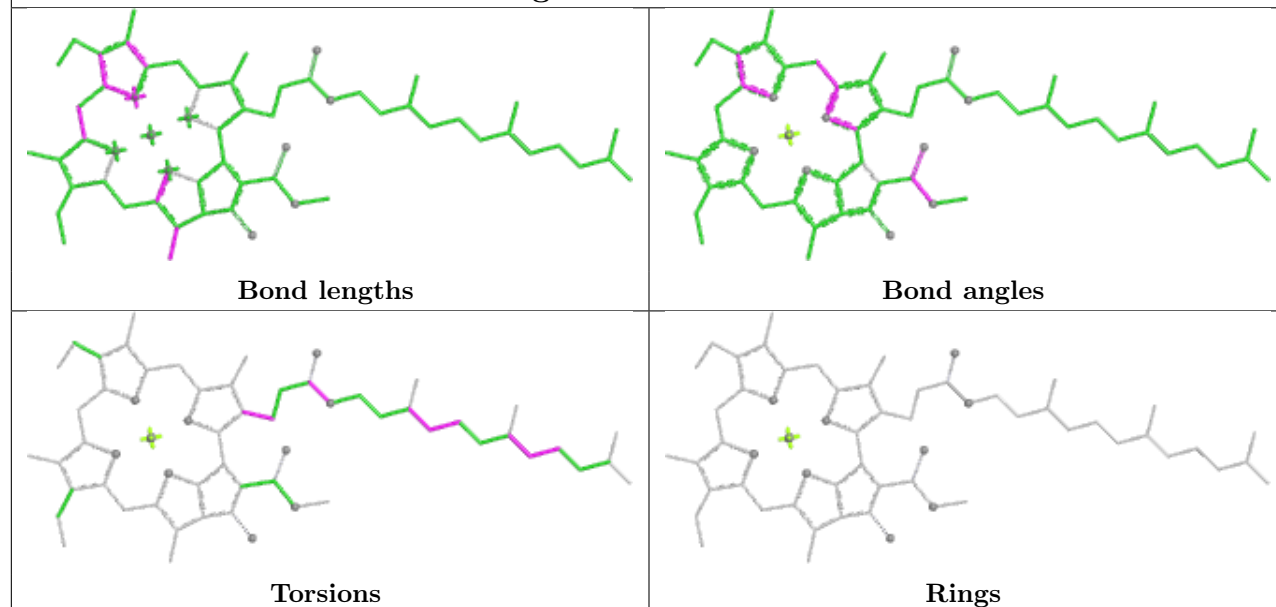




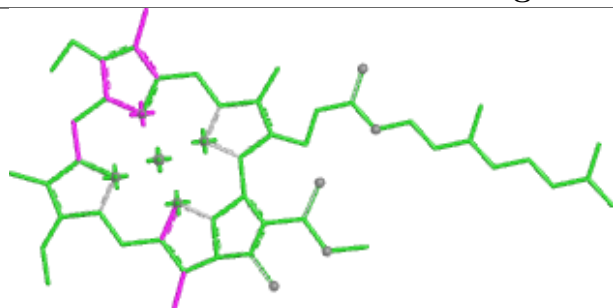
Ligand CHL 1 306



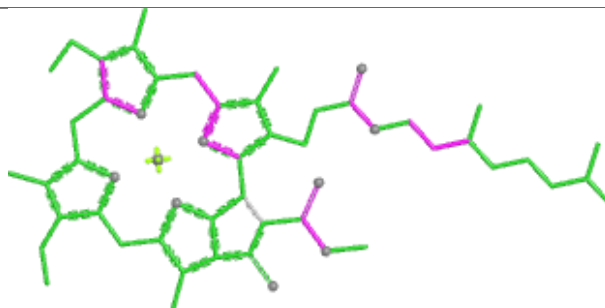
Ligand CLA B 818



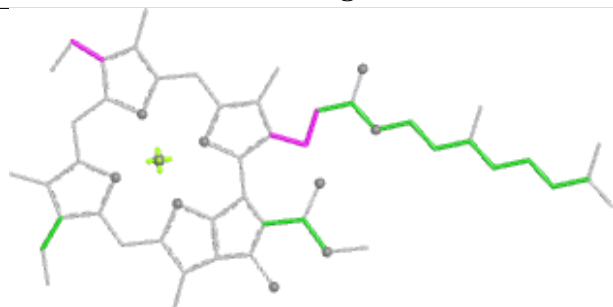
Ligand CLA A 823



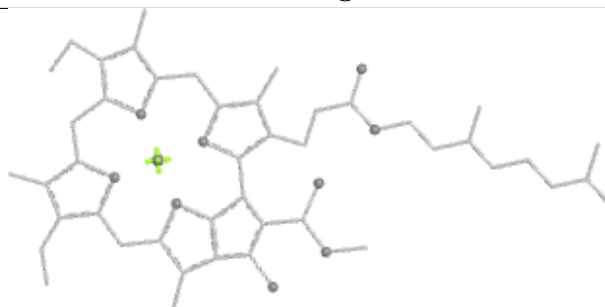
Bond lengths



Bond angles

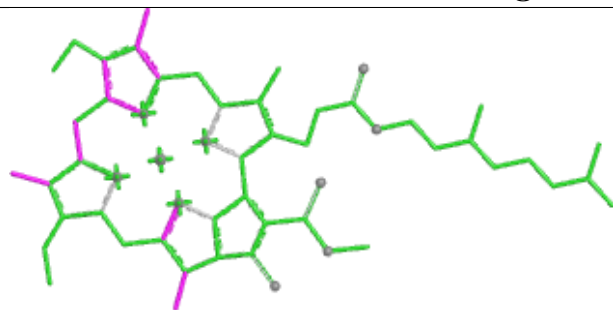


Torsions

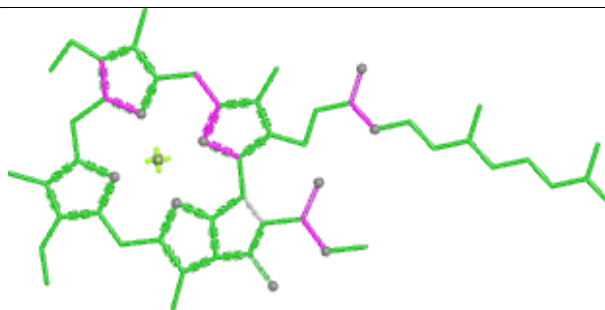


Rings

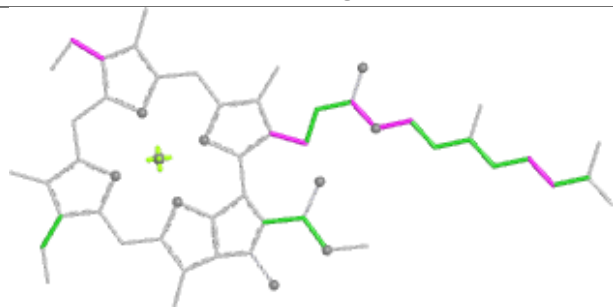
Ligand CLA B 812



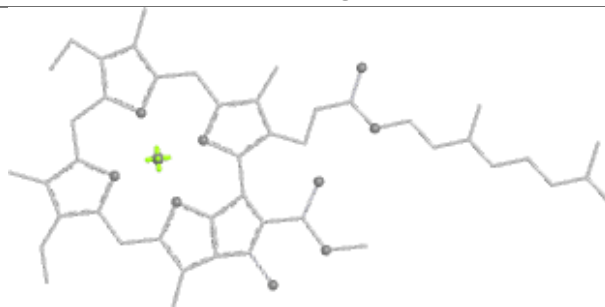
Bond lengths



Bond angles

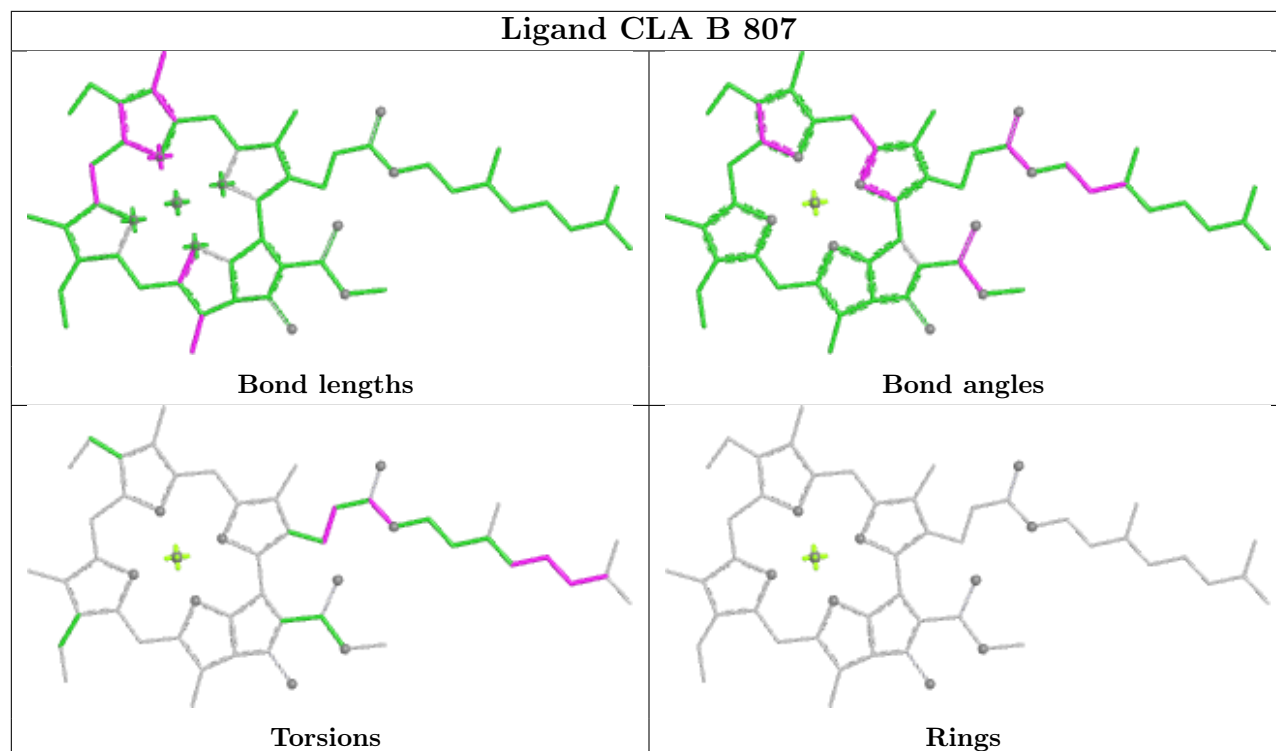


Torsions

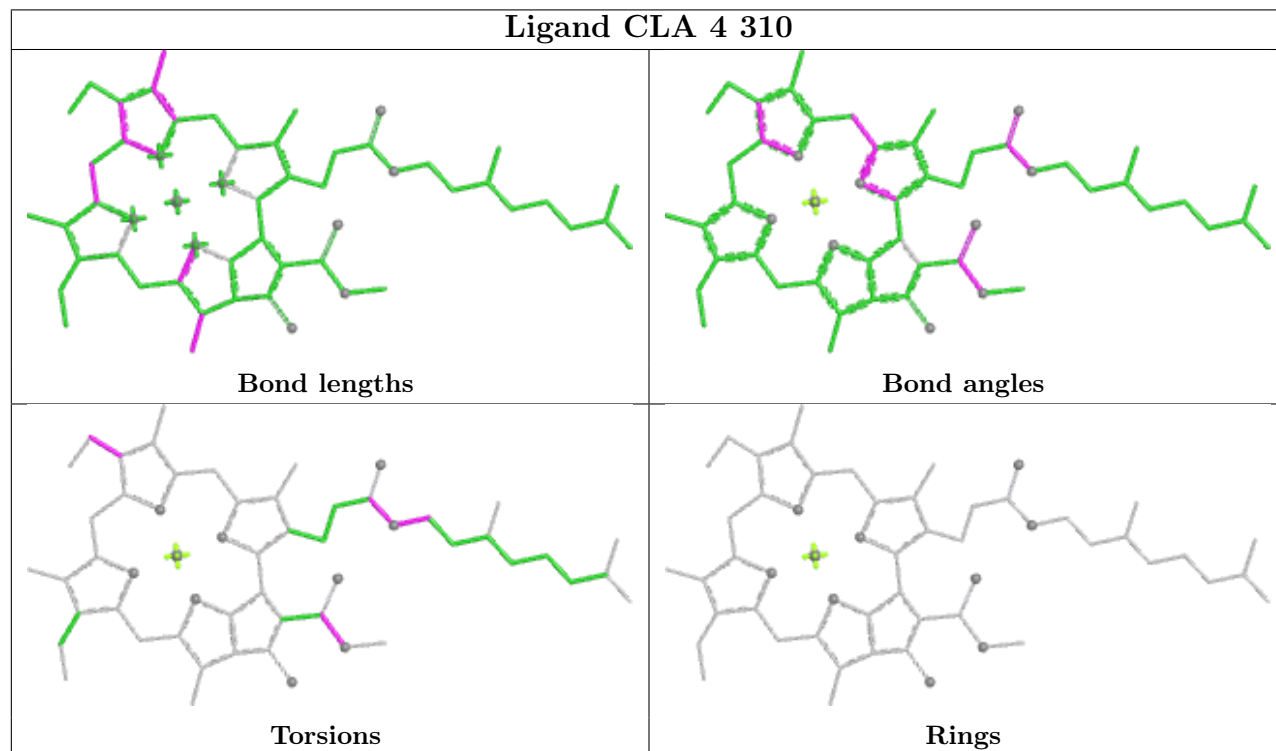


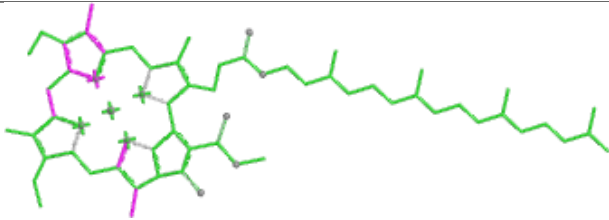
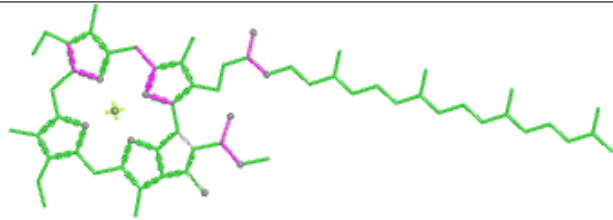
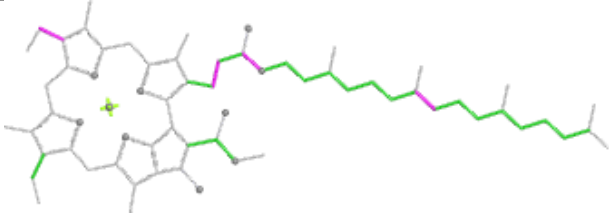
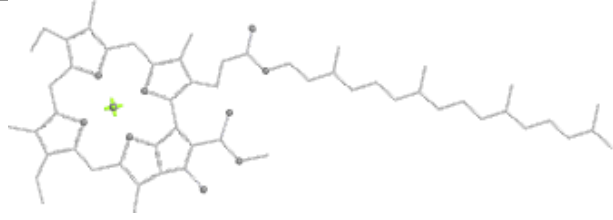
Rings

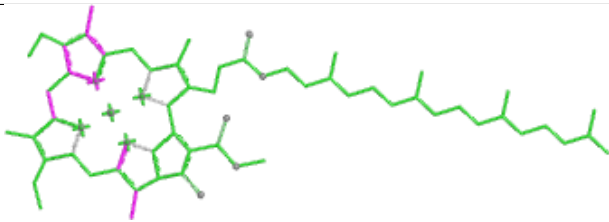
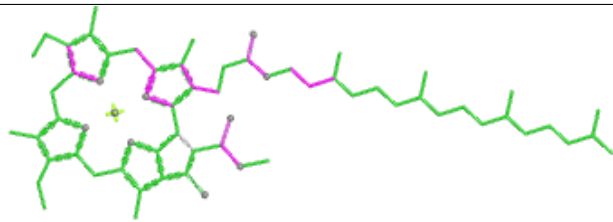
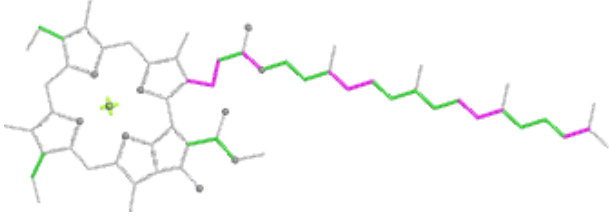
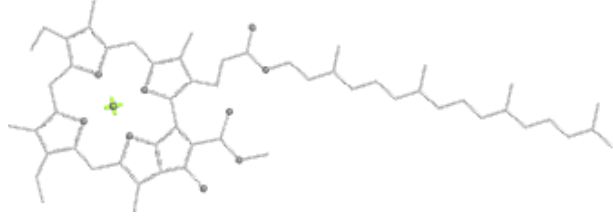
Ligand CLA B 807

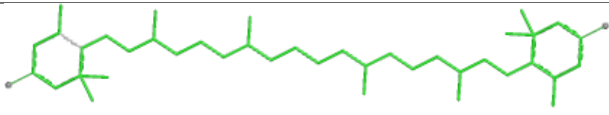
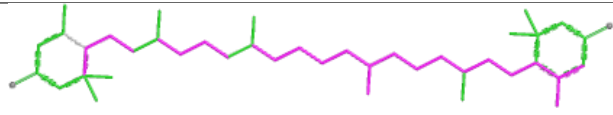
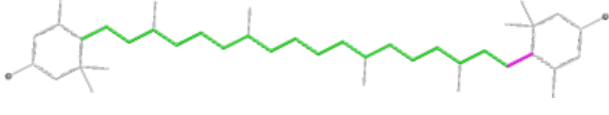
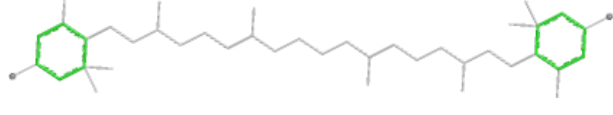


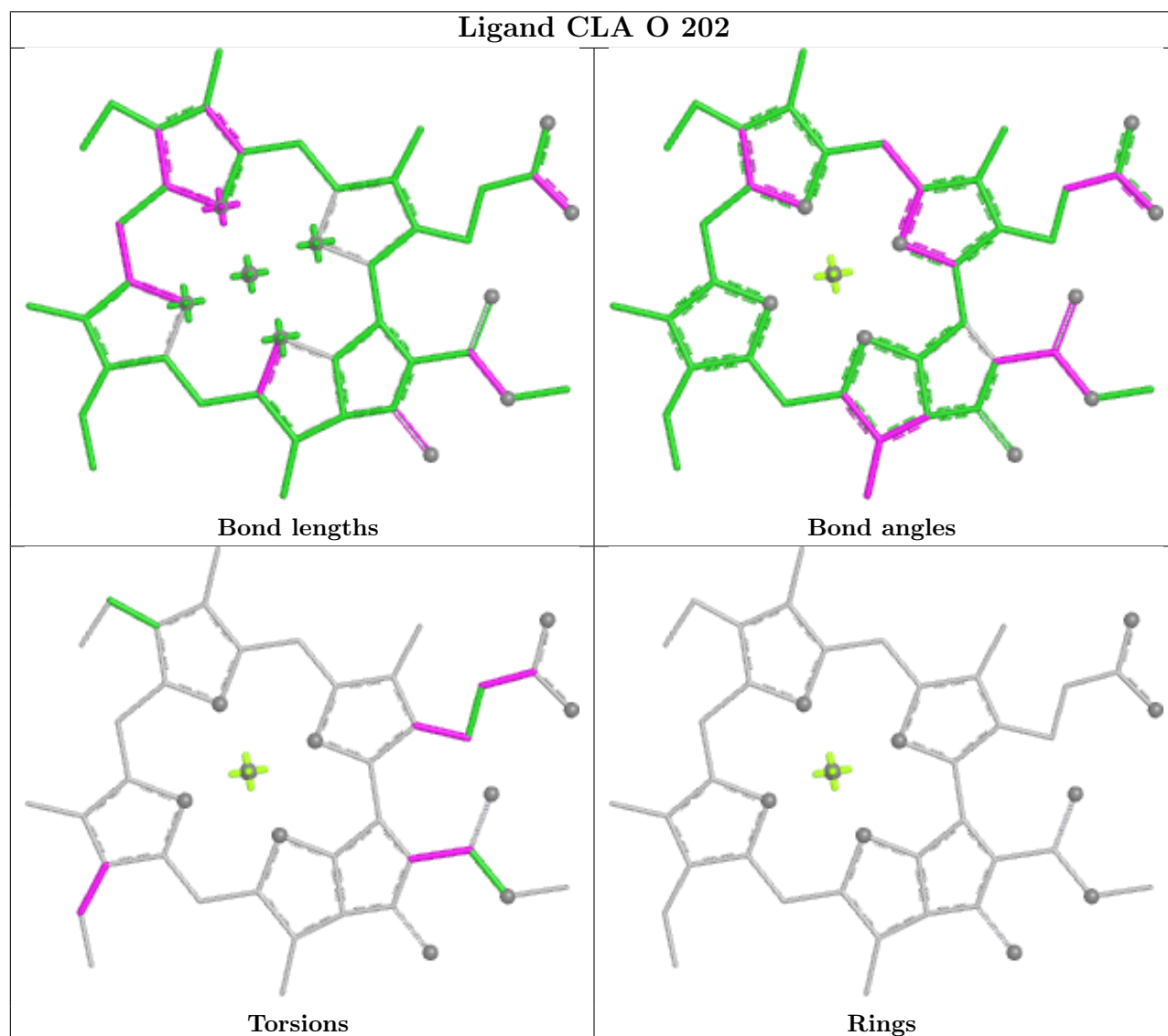
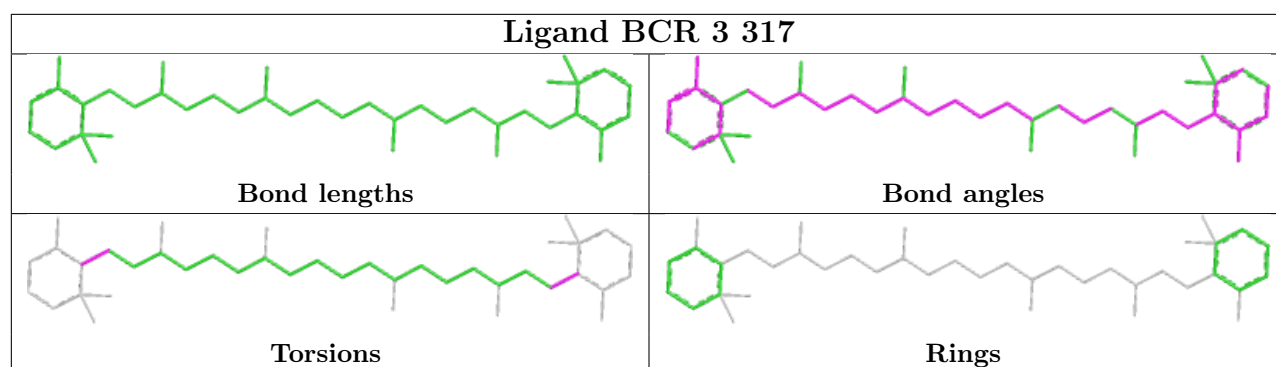
Ligand CLA 4 310



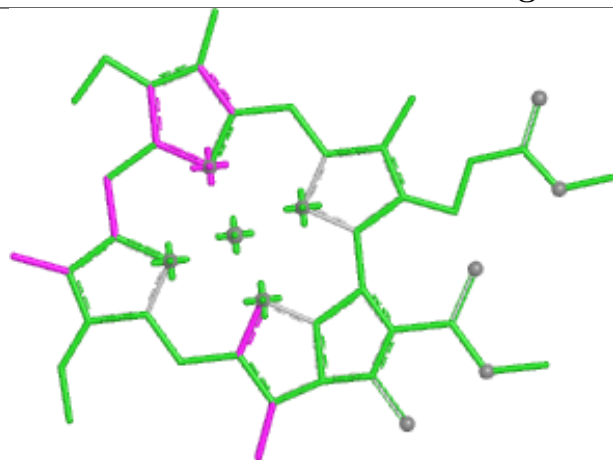
Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

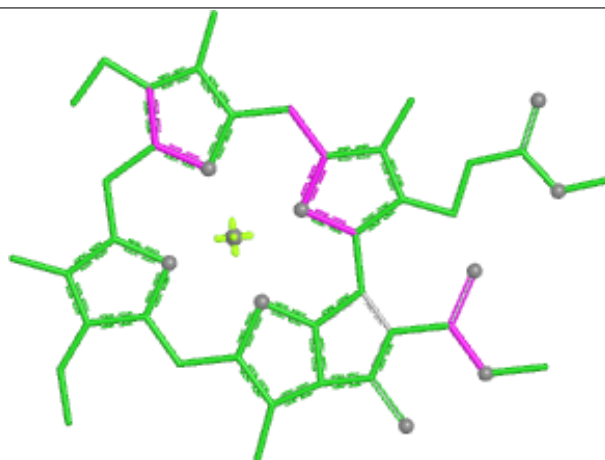
Ligand LUT 4 316	
	
Bond lengths	Bond angles
	
Torsions	Rings



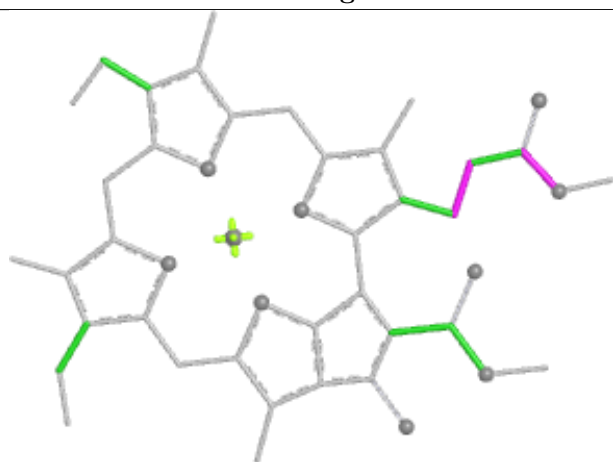
Ligand CLA 1 314



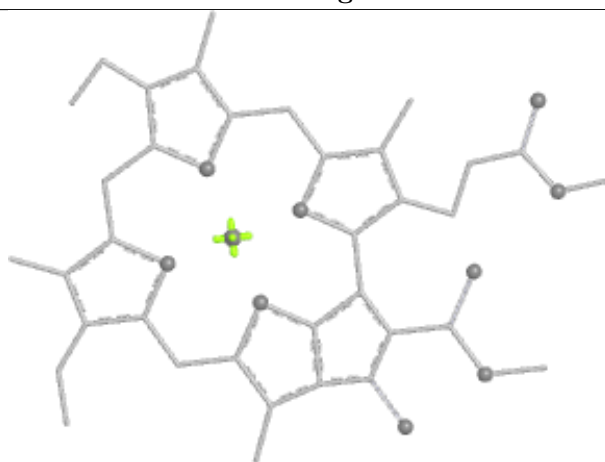
Bond lengths



Bond angles

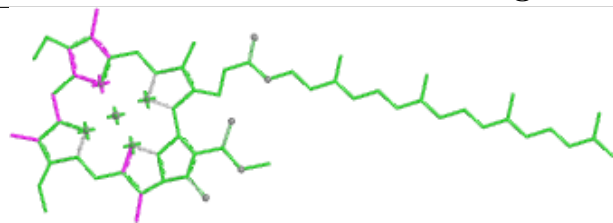


Torsions

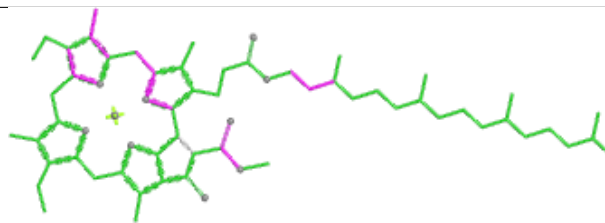


Rings

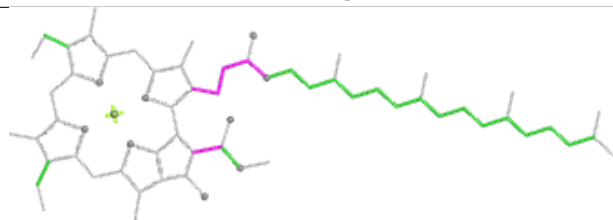
Ligand CLA A 804



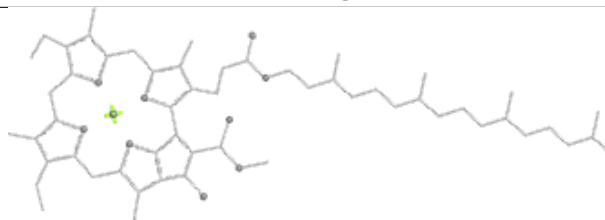
Bond lengths



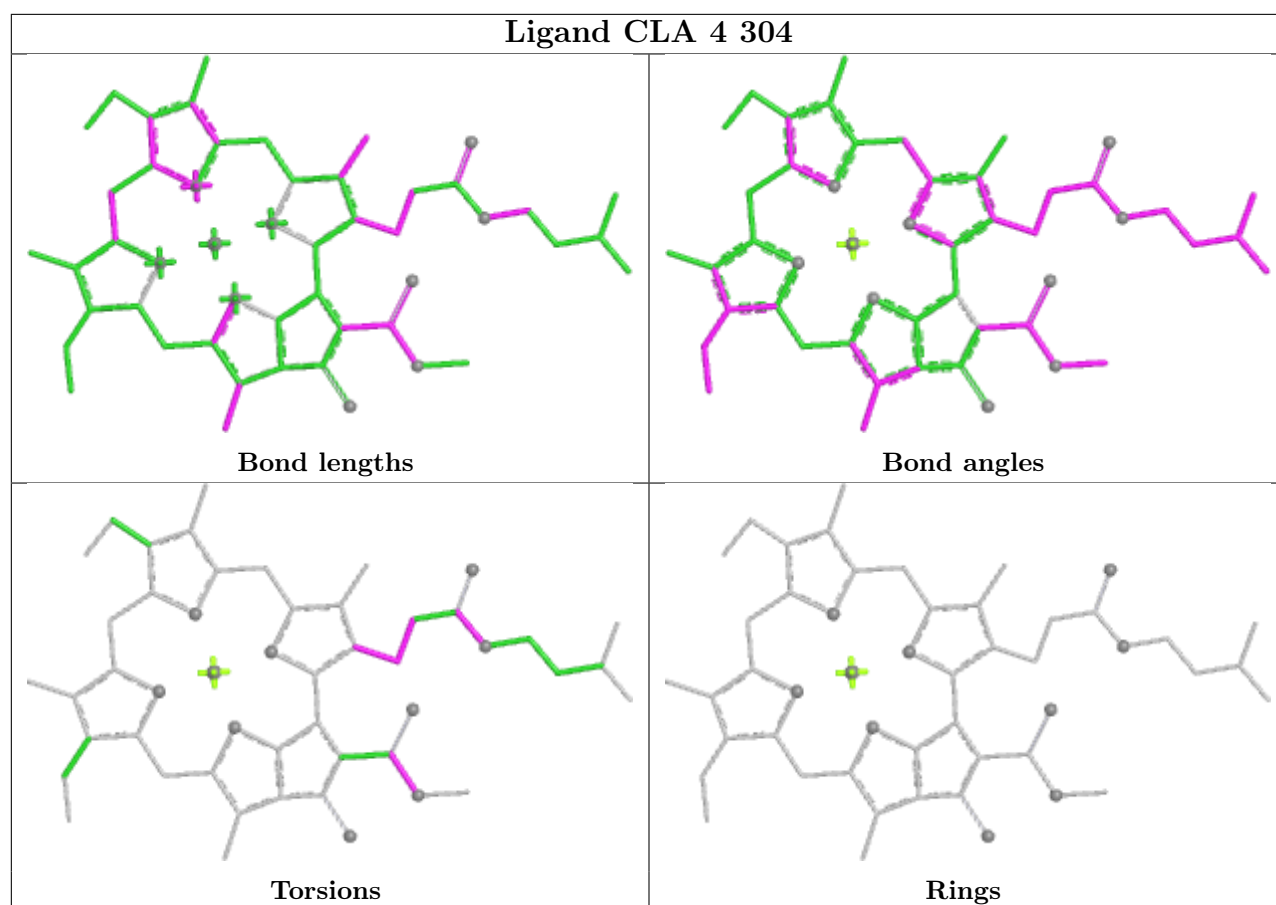
Bond angles



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.

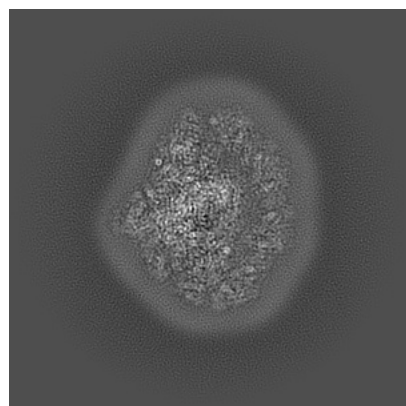
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37513. These allow visual inspection of the internal detail of the map and identification of artifacts.

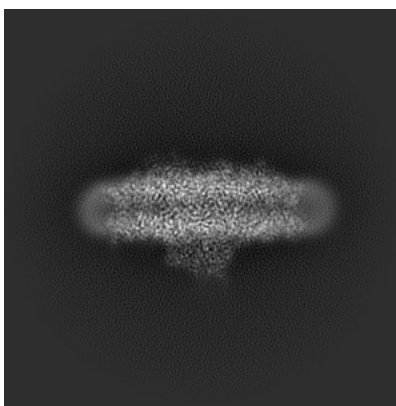
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

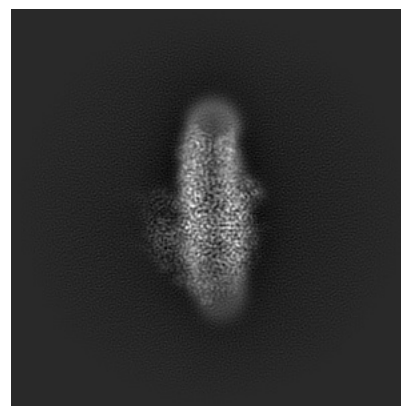
6.1.1 Primary map



X

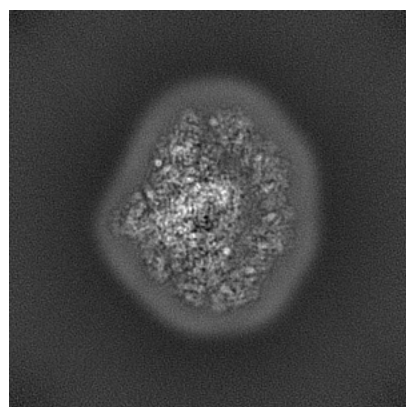


Y

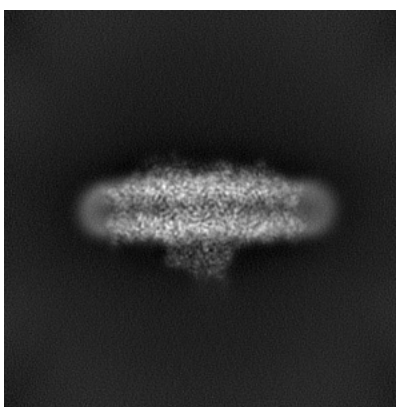


Z

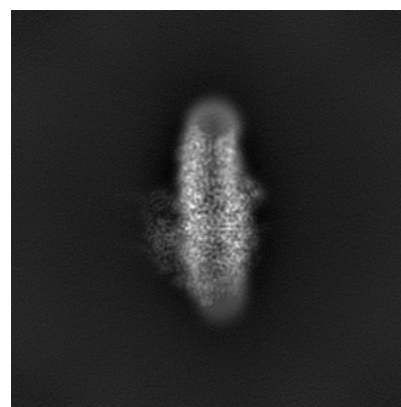
6.1.2 Raw map



X



Y

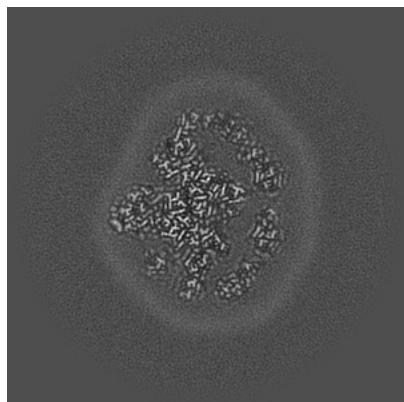


Z

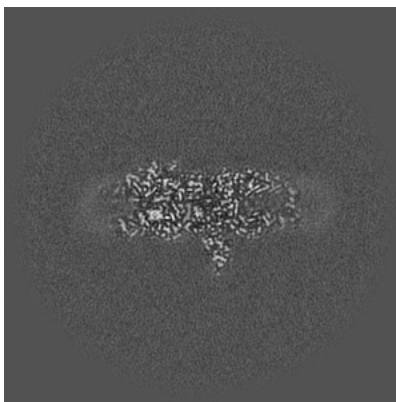
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

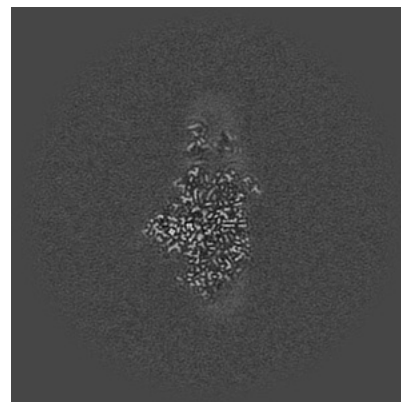
6.2.1 Primary map



X Index: 150

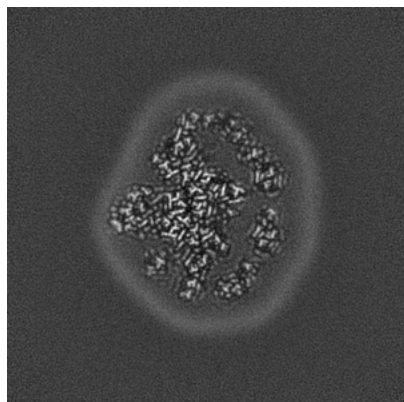


Y Index: 150

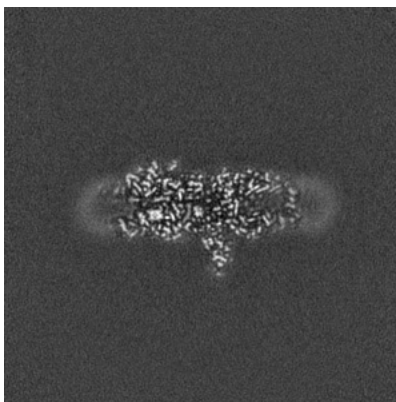


Z Index: 150

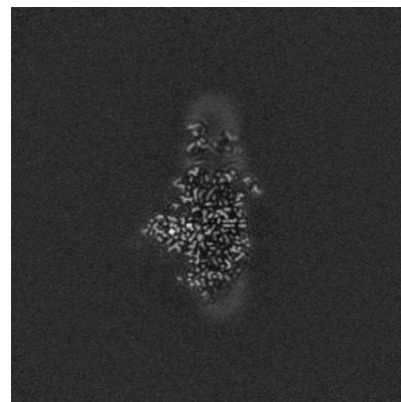
6.2.2 Raw map



X Index: 150



Y Index: 150

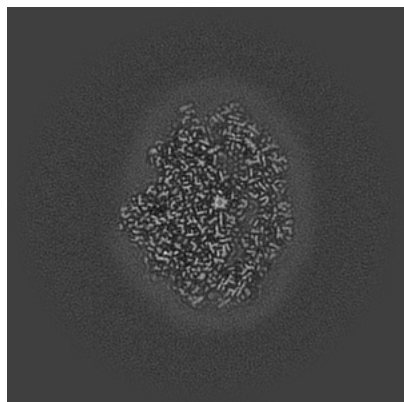


Z Index: 150

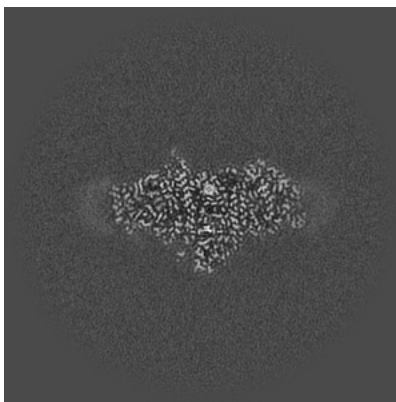
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

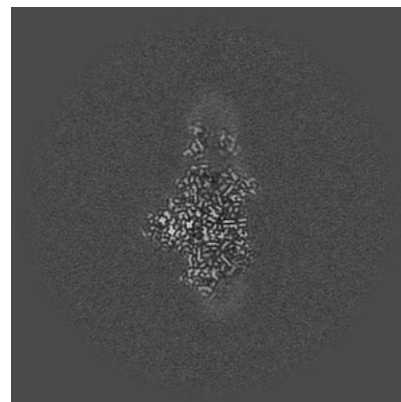
6.3.1 Primary map



X Index: 138

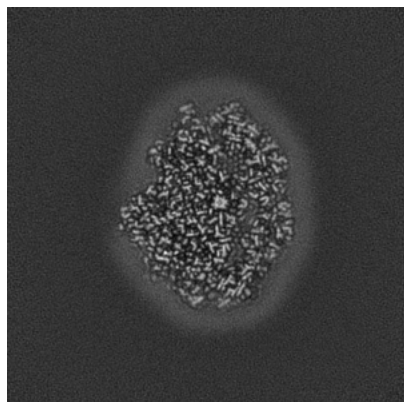


Y Index: 135

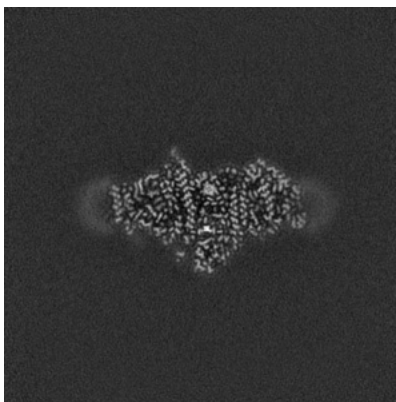


Z Index: 152

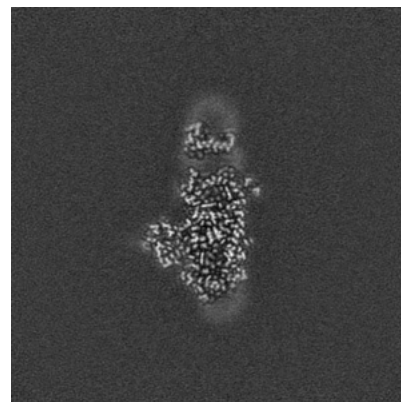
6.3.2 Raw map



X Index: 138



Y Index: 135

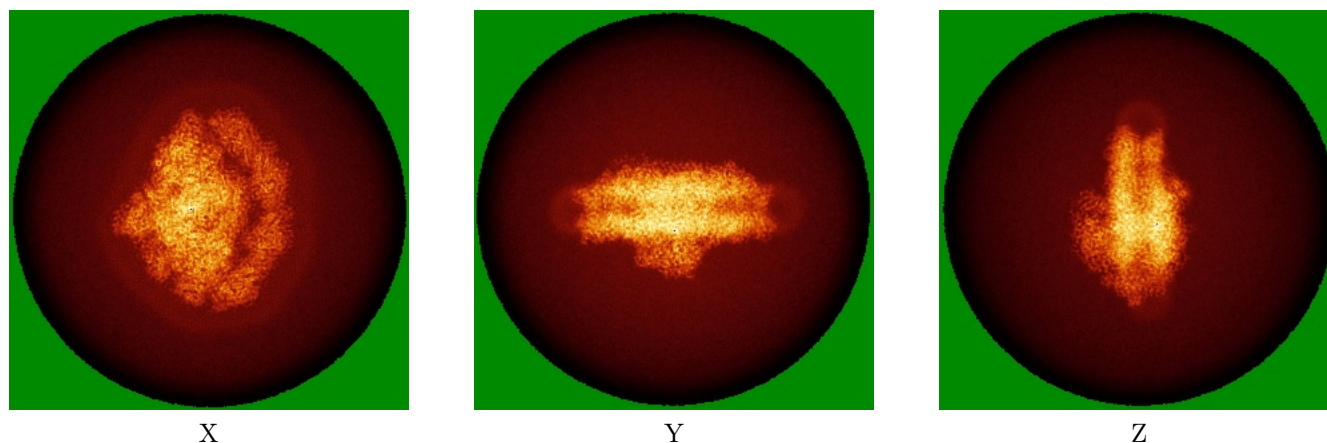


Z Index: 145

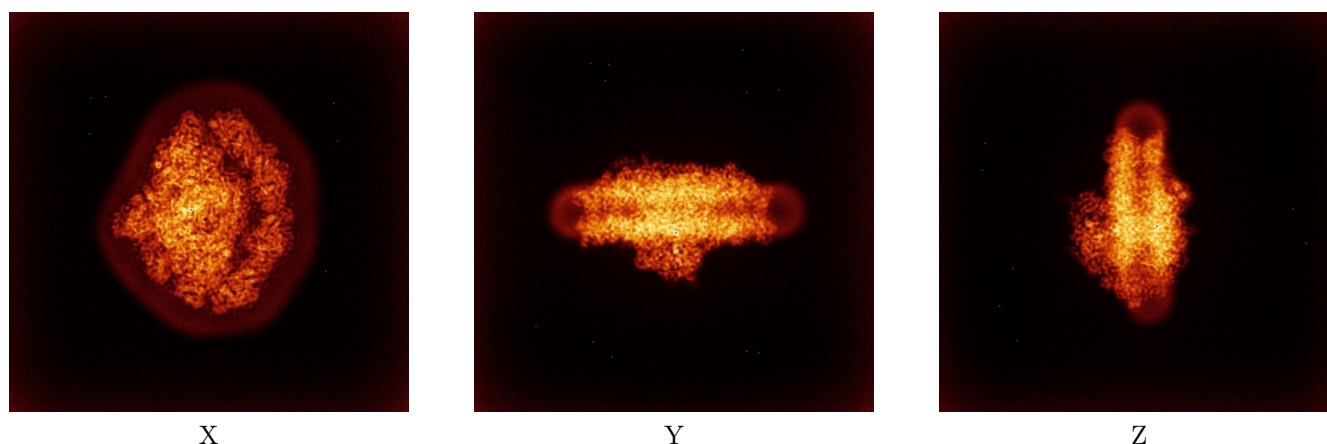
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

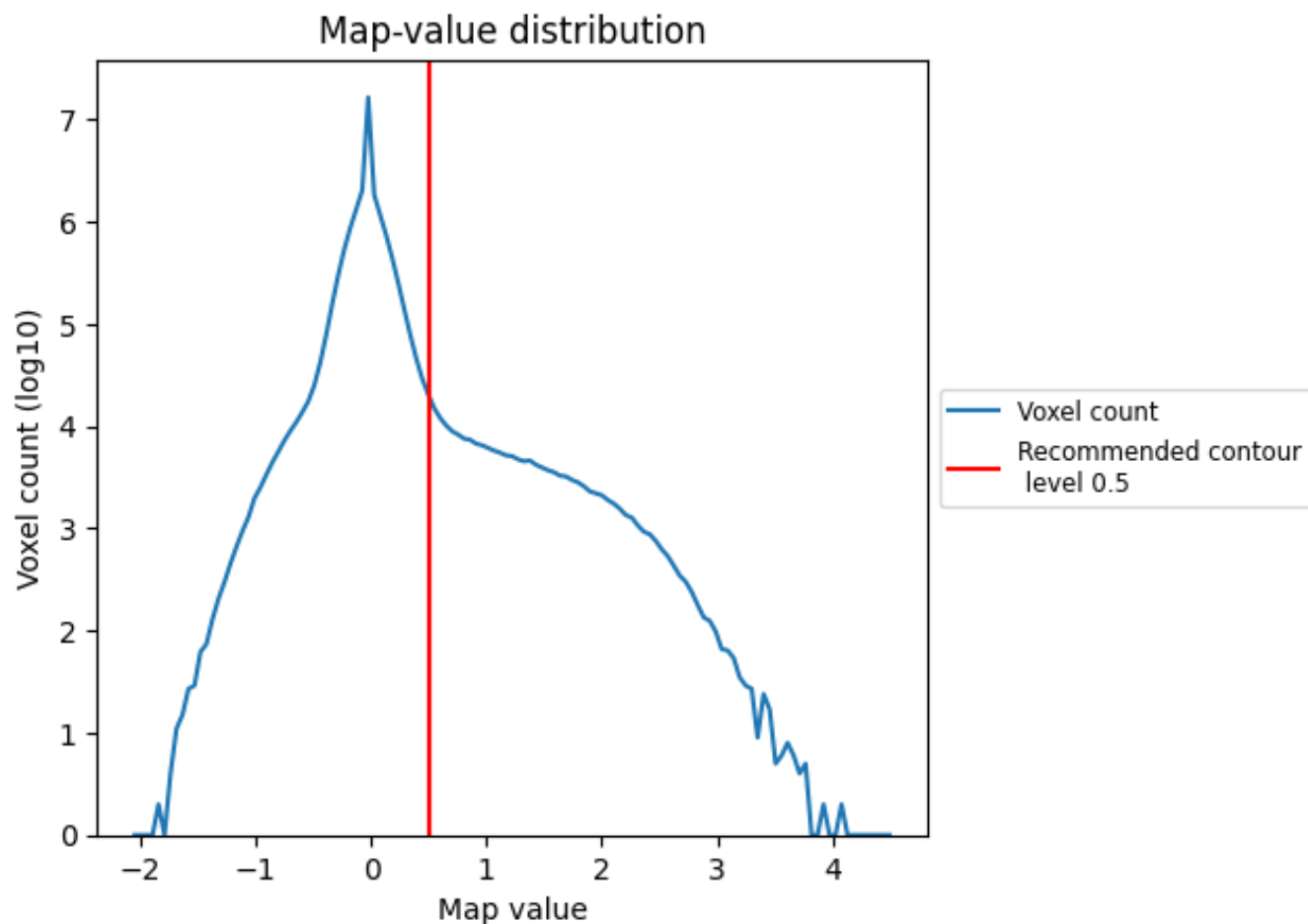
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

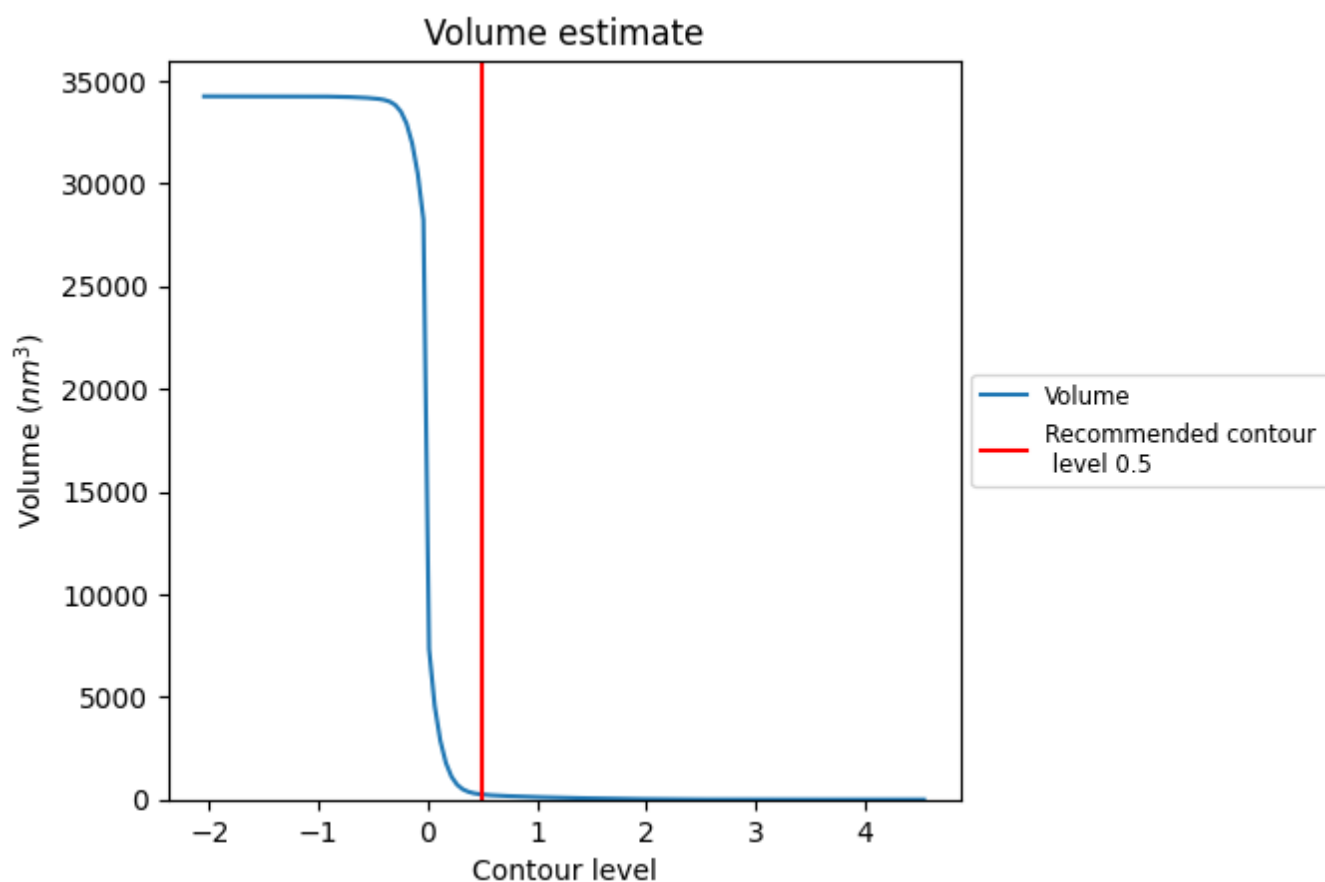
This section contains the results of statistical analysis of the map.

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.

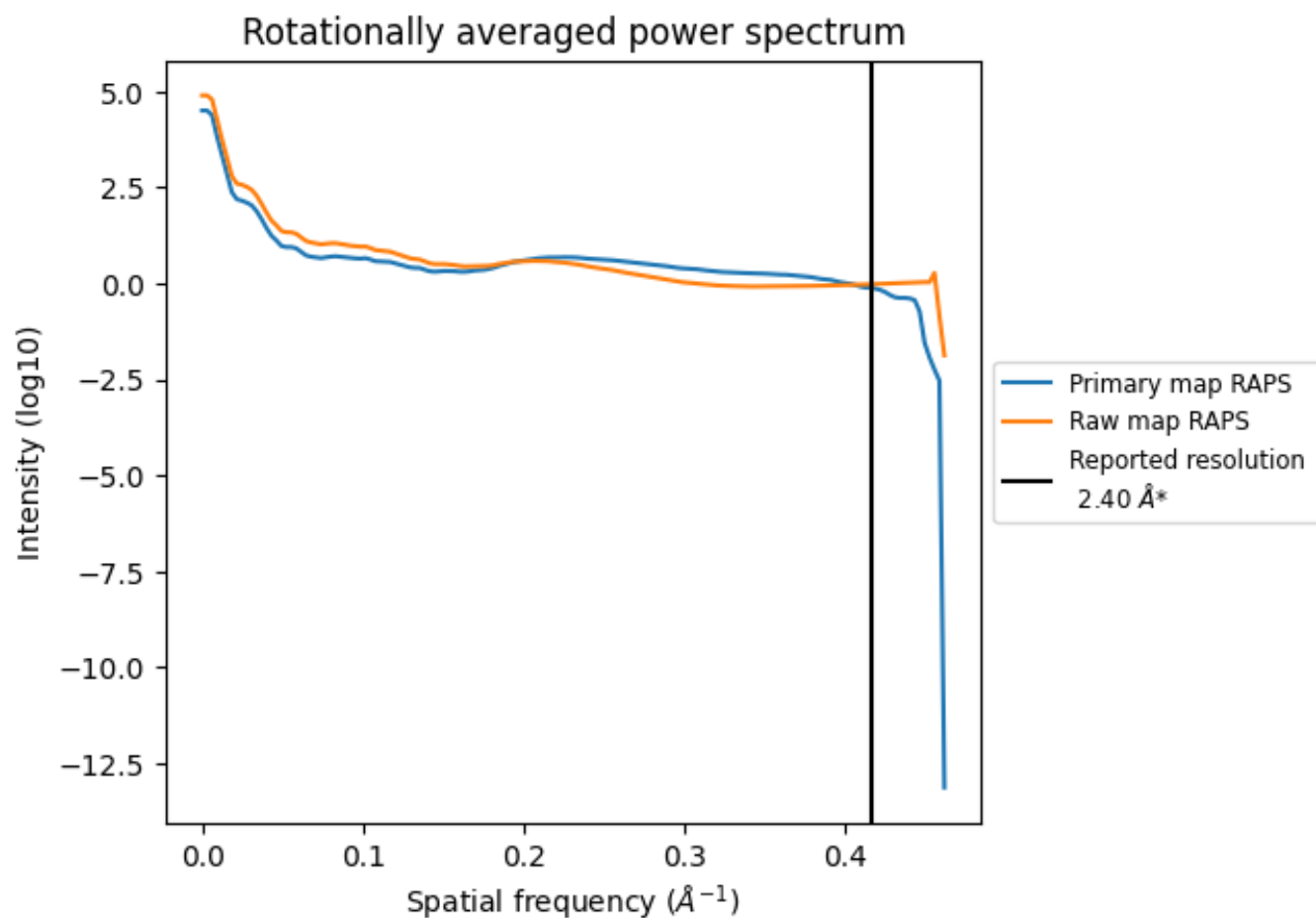
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 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 ⓘ

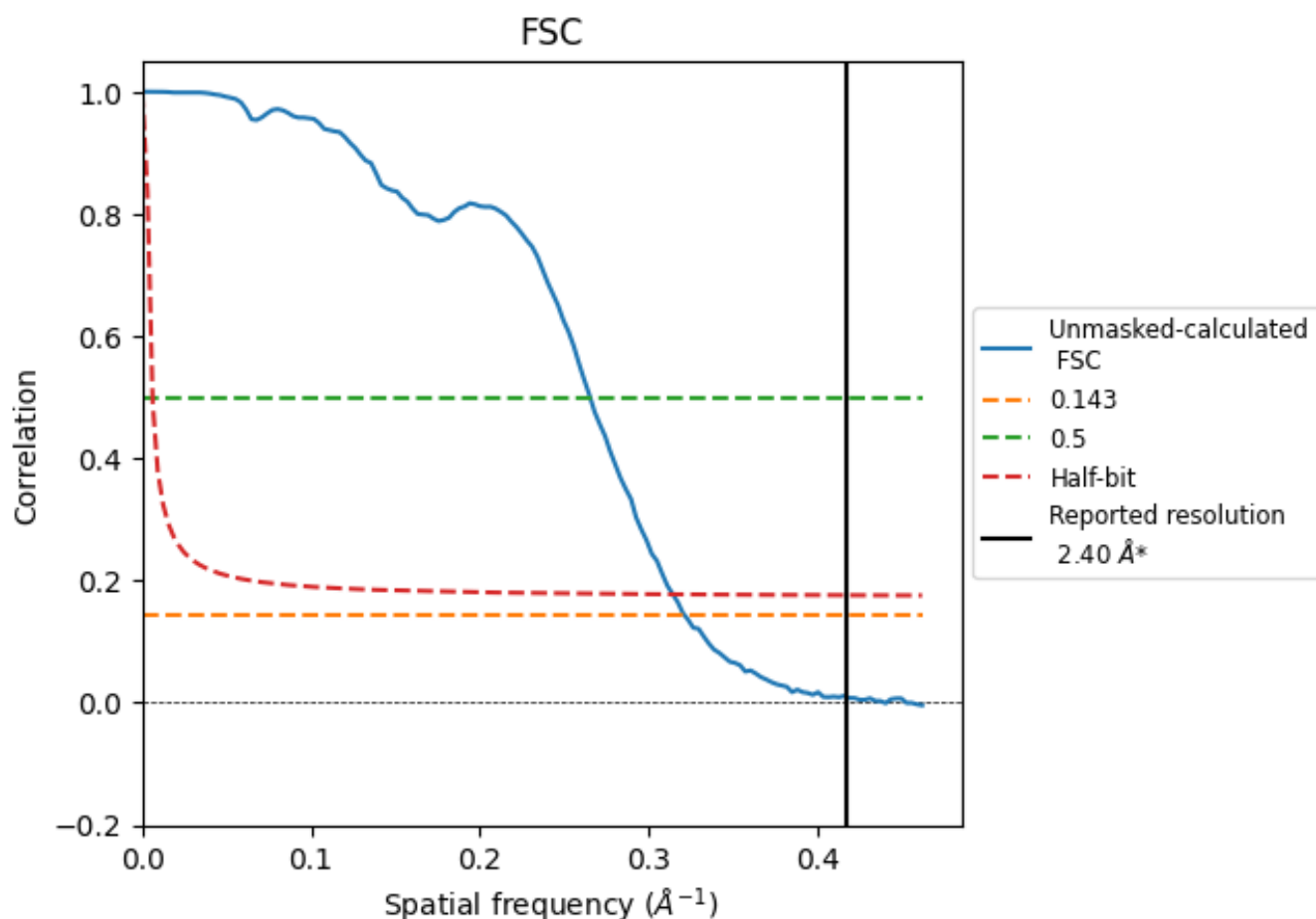


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

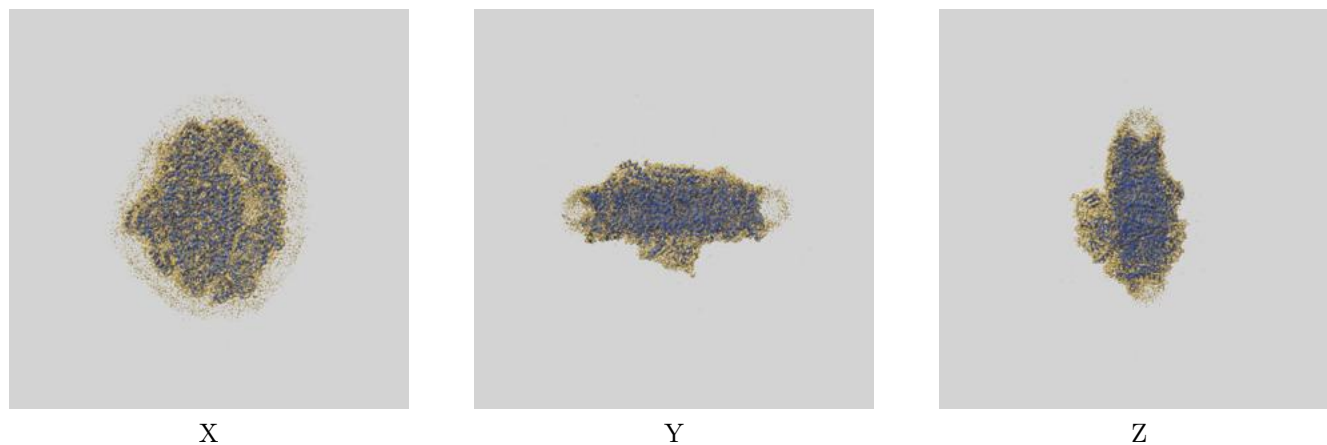
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.77	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

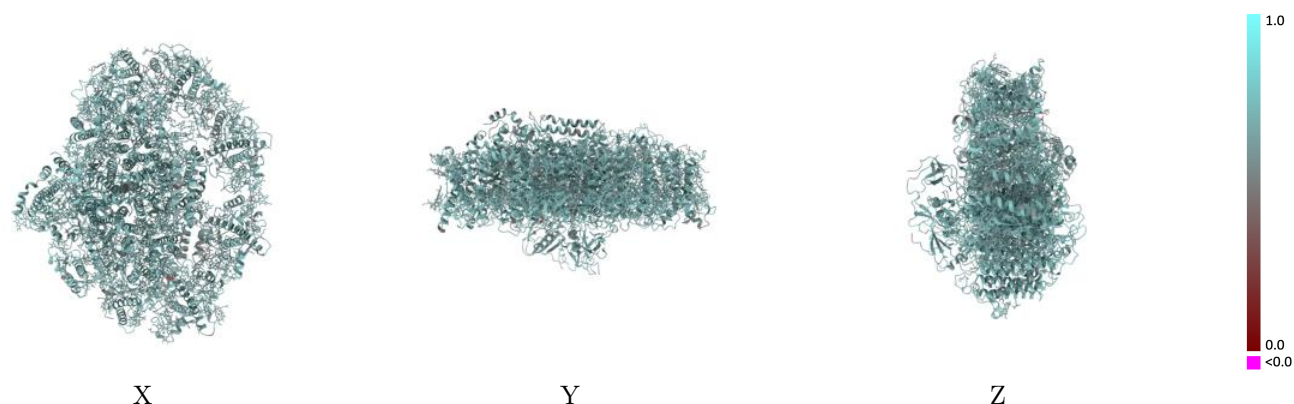
This section contains information regarding the fit between EMDB map EMD-37513 and PDB model 8WGH. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

9.1 Map-model overlay [i](#)



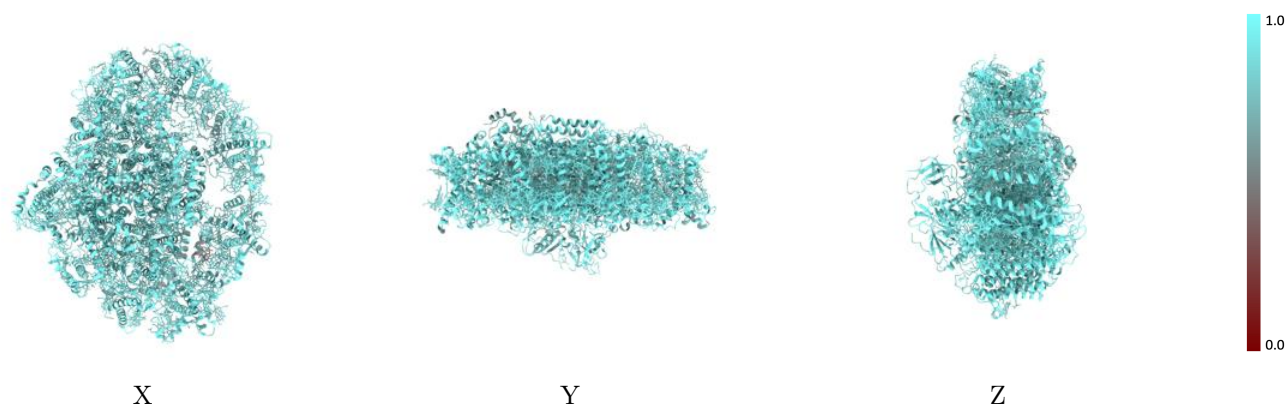
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



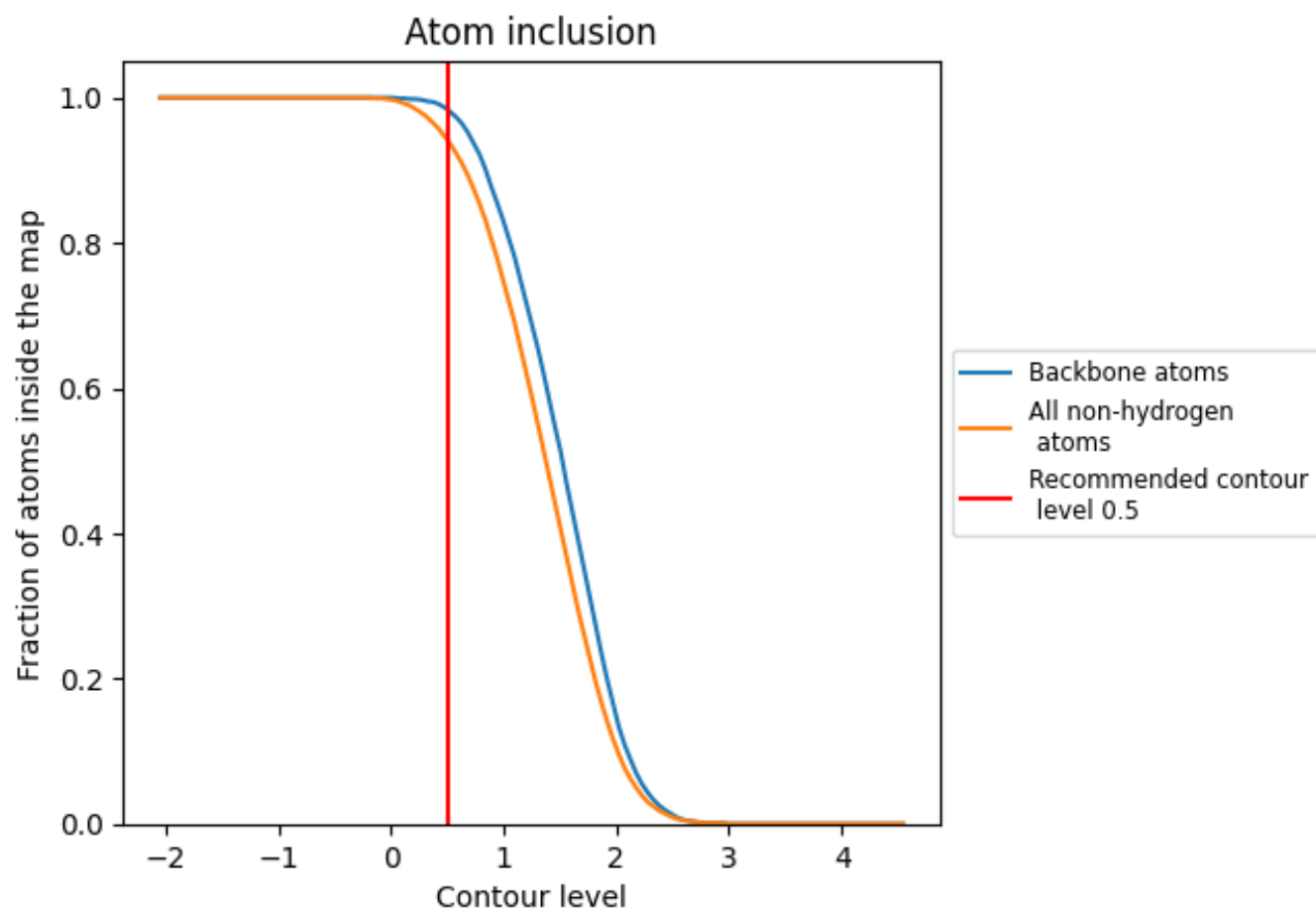
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.6650
1	0.8880	0.6340
2	0.9220	0.6460
3	0.9360	0.6530
4	0.9280	0.6510
A	0.9670	0.6860
B	0.9650	0.6840
C	0.9850	0.6840
D	0.9580	0.6720
E	0.9390	0.6500
F	0.9160	0.6430
G	0.9150	0.6500
H	0.9320	0.6570
I	0.9660	0.6760
J	0.9490	0.6680
K	0.9180	0.6310
L	0.9580	0.6750
N	0.7530	0.5770
O	0.9270	0.6460

1.0
0.0
-0.0