



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:19 PM JST

PDB ID : 8J6Z / pdb_00008j6z
EMDB ID : EMD-36021
Title : Cryo-EM structure of the Arabidopsis thaliana photosystem I(PSI-LHCII-ST2)
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2023-04-26
Resolution : 2.79 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

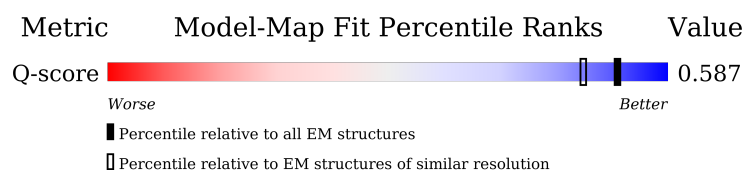
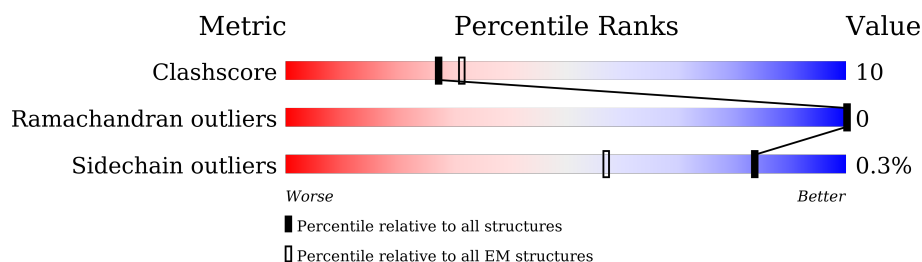
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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.



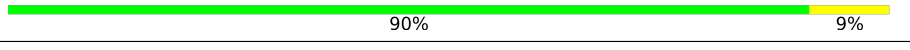
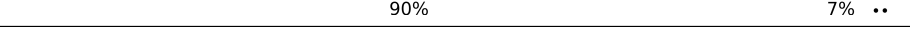
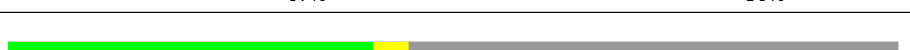
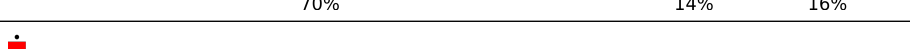
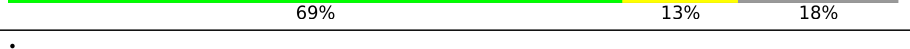
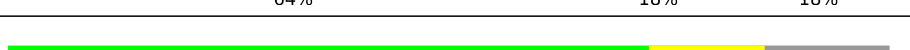
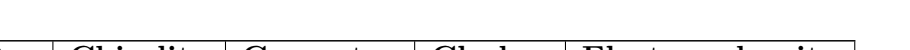
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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

Mol	Chain	Length	Quality of chain
1	1	241	 66% 14% 20%
2	2	257	 67% 11% 22%
3	3	273	 70% 10% 20%
4	4	251	 72% 6% 22%

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	204	
9	E	143	
10	F	221	
11	G	160	
12	H	145	
13	I	37	
14	J	44	
15	K	130	
16	L	219	
17	O	140	
18	x	267	
18	y	267	
19	z	265	

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
28	SF4	A	854	-	-	X	-
28	SF4	C	101	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 43924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	193	Total	C	N	O	S	0	0
			1496	975	248	268	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	218	Total	C	N	O	S	0	0
			1666	1088	270	303	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	737	Total	C	N	O	S	0	0
			5807	3807	986	996	18		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	152	Total	C	N	O	S	0	0
			1208	789	207	209	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	90	Total	C	N	O	S	0	0
			693	451	112	130			

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	86	Total	C	N	O	S	0	0
			686	456	114	115	1		

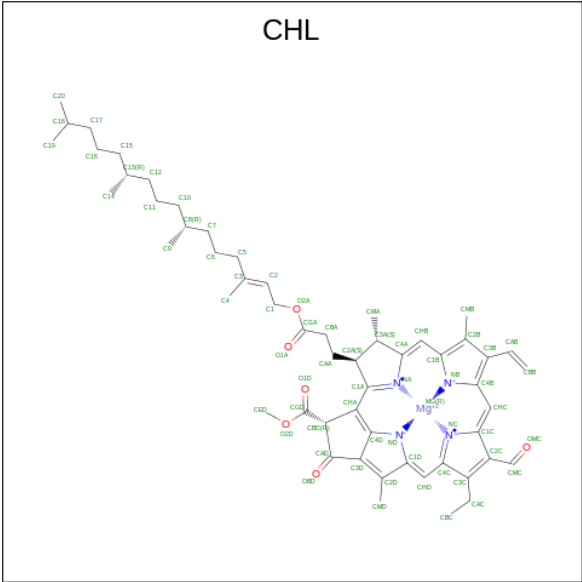
- Molecule 18 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	x	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
18	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	z	227	Total	C	N	O	P	S	0	0
			1759	1140	286	327	1	5		

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



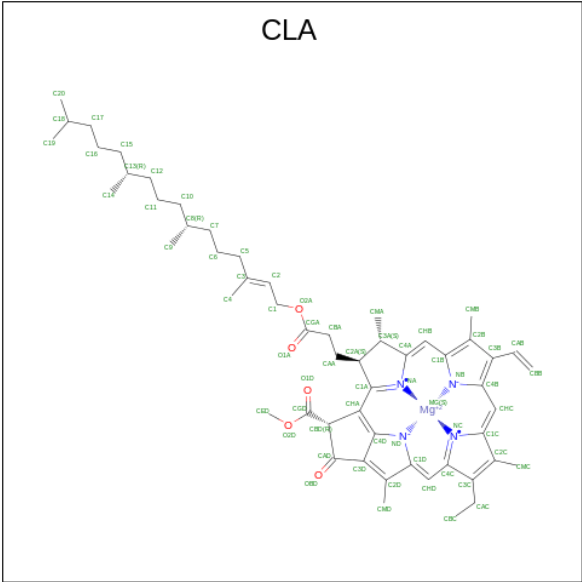
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	x	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	y	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	y	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
20	z	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
20	z	1	Total	C	Mg	N	O	0
			52	41	1	4	6	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 56	C 46	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	F	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	J	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	K	1	Total 37	C 31	Mg 1	N 4	O 1	0
21	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	K	1	Total 39	C 31	Mg 1	N 4	O 3	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

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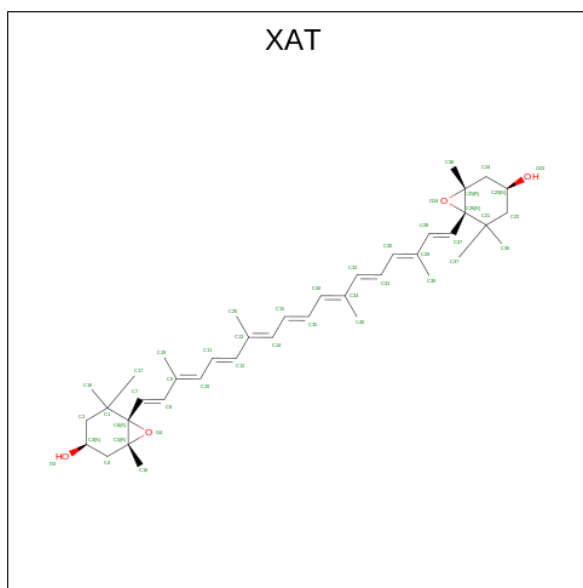
Mol	Chain	Residues	Atoms					AltConf
21	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	x	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	x	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	y	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	y	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	y	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

- 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: C₄₀H₅₆O₄).



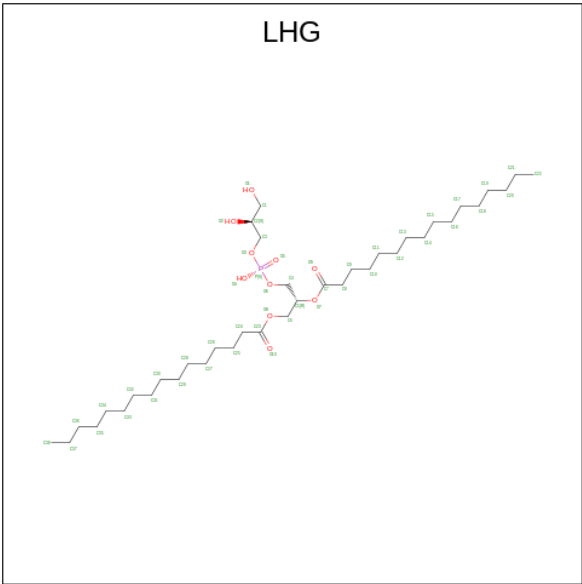
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	
22	x	1	Total	C	O	0
			44	40	4	

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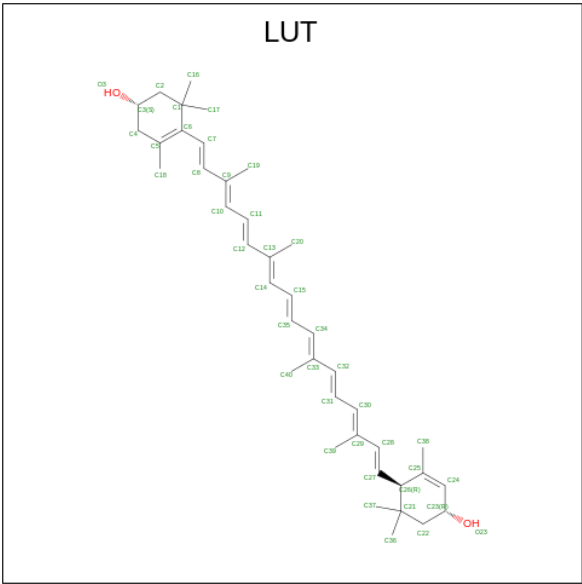
Mol	Chain	Residues	Atoms			AltConf
22	y	1	Total	C	O	0
			44	40	4	
22	z	1	Total	C	O	0
			44	40	4	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



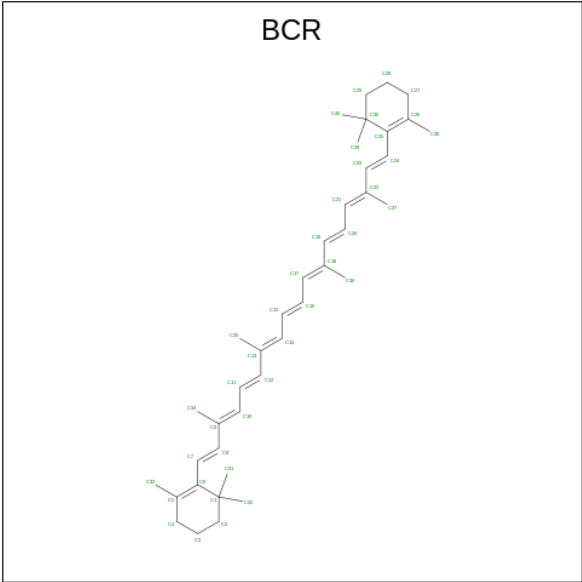
Mol	Chain	Residues	Atoms				AltConf
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			37	26	10	1	
23	A	1	Total	C	O	P	0
			30	19	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			38	27	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	x	1	Total	C	O	P	0
			49	38	10	1	
23	y	1	Total	C	O	P	0
			49	38	10	1	
23	z	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 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
24	1	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	2	1	Total	C	O	0
			42	40	2	
24	3	1	Total	C	O	0
			42	40	2	
24	4	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	x	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	y	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	
24	z	1	Total	C	O	0
			42	40	2	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



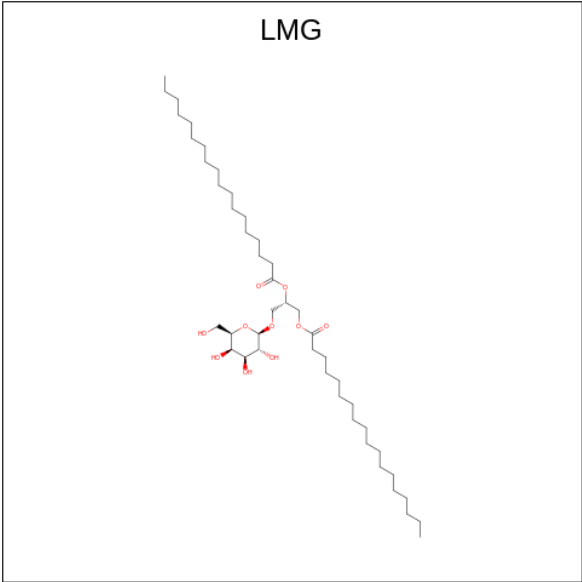
Mol	Chain	Residues	Atoms		AltConf
25	3	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	

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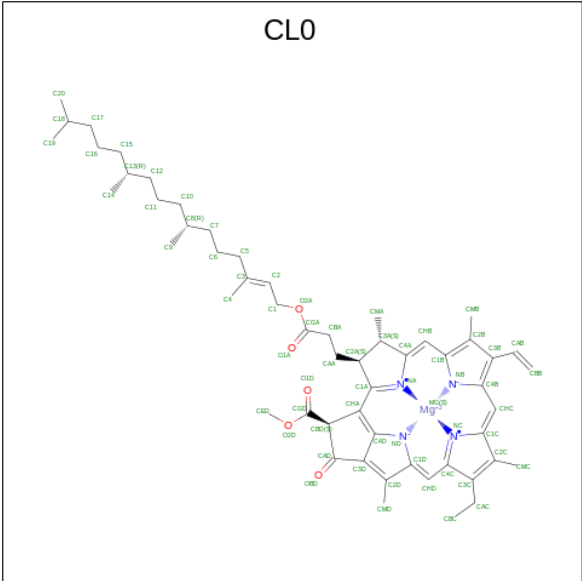
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	O	1	Total C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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



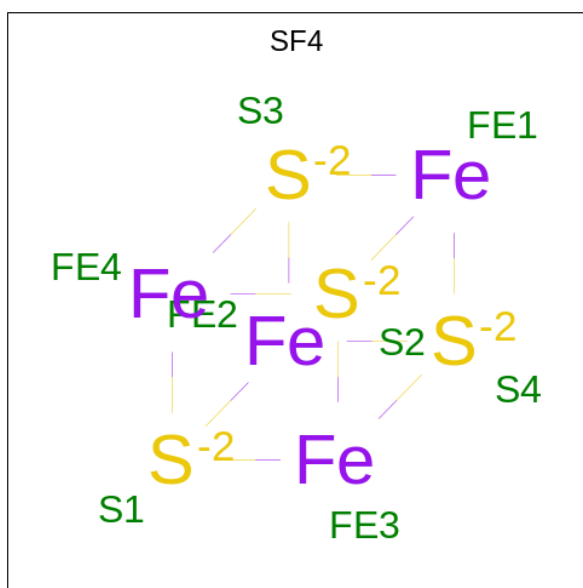
Mol	Chain	Residues	Atoms			AltConf
26	4	1	Total	C	O	0
			39	29	10	
26	4	1	Total	C	O	0
			33	23	10	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



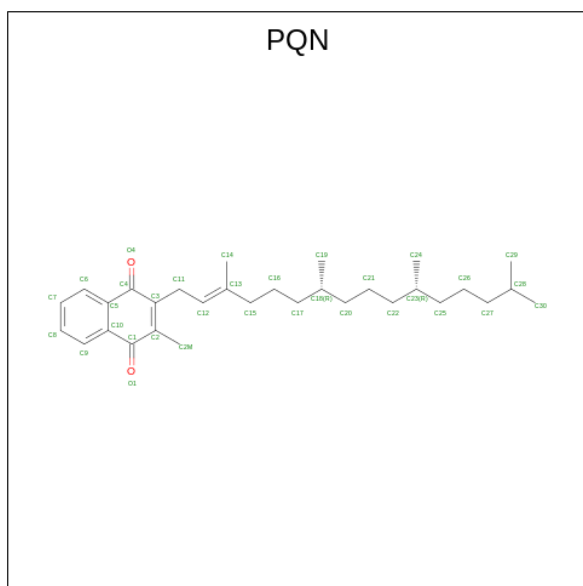
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			61	53	1	4	3	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



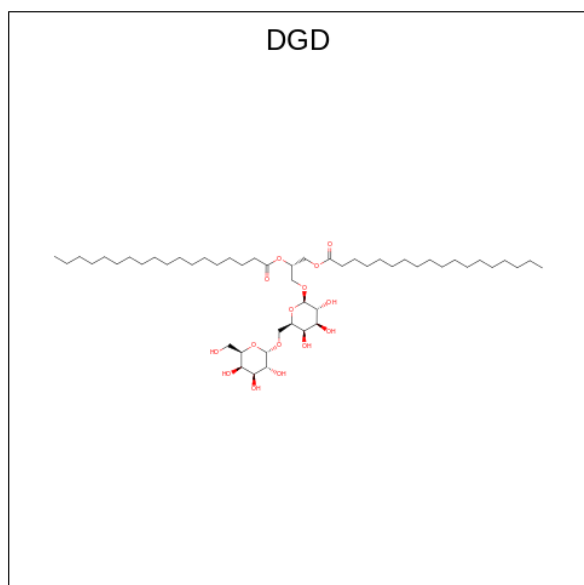
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$).



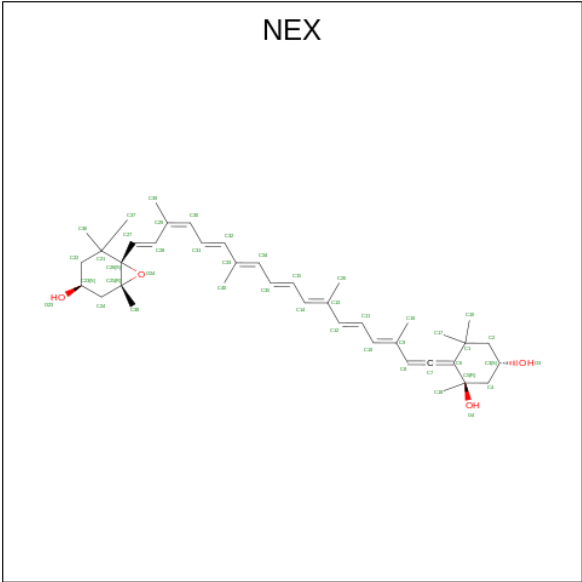
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

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



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

- Molecule 31 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).

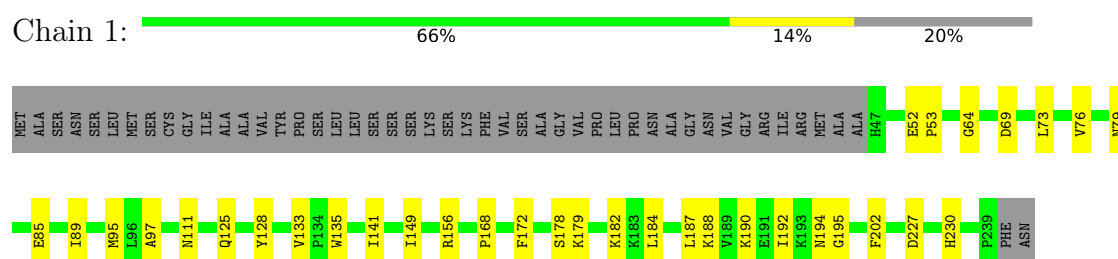


Mol	Chain	Residues	Atoms			AltConf
31	x	1	Total	C	O	0
			44	40	4	
31	y	1	Total	C	O	0
			44	40	4	
31	z	1	Total	C	O	0
			44	40	4	

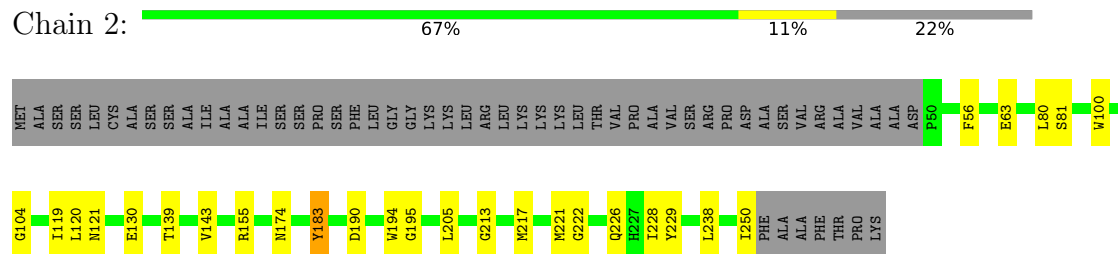
3 Residue-property plots

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

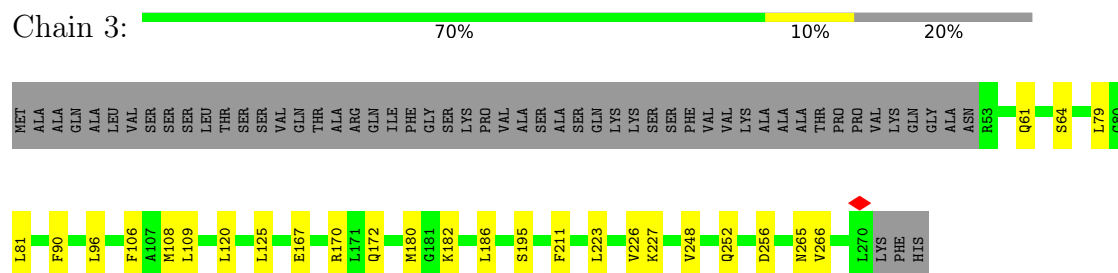
- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic



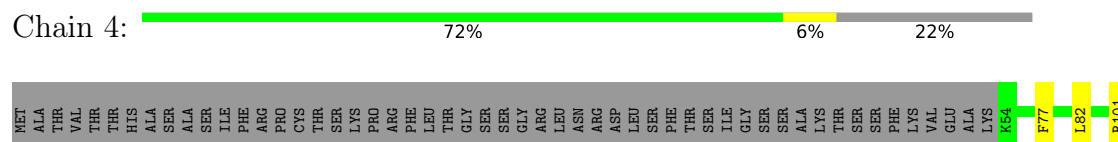
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

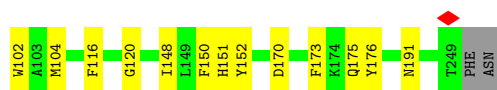


- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic



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





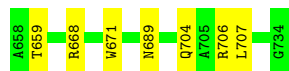
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 91% 8%



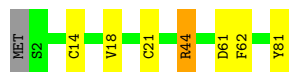
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 90% 9%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 90% 7%



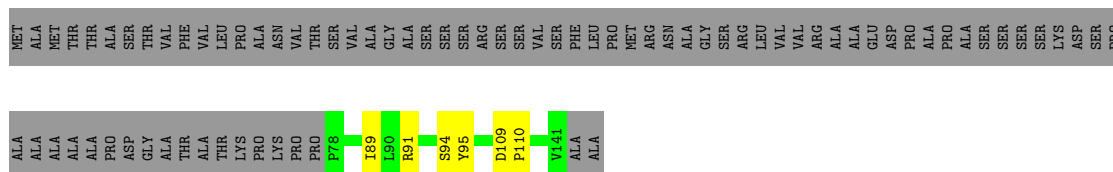
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D: 67% 30%



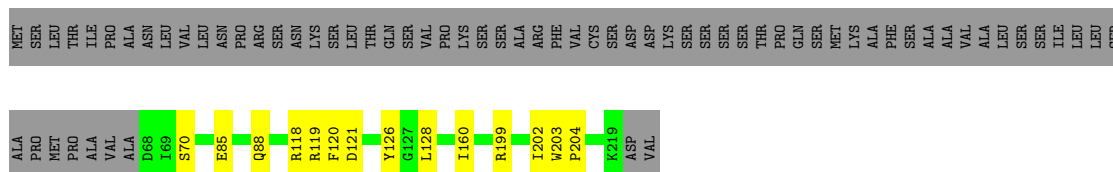
- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

Chain E:  41% 55%



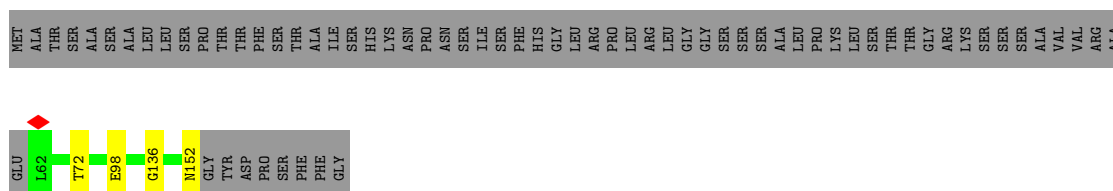
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:  62% 6% 31%



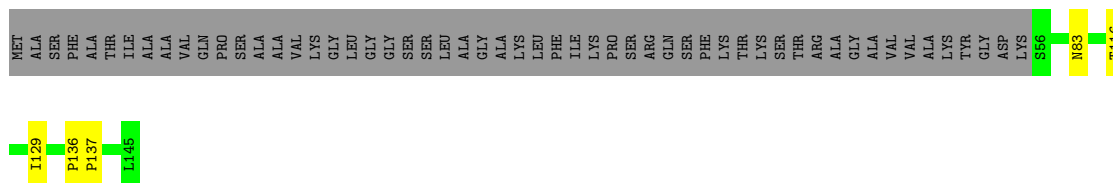
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G:  54% 43%



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

Chain H:  59% 38%



- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  70% 14% 16%

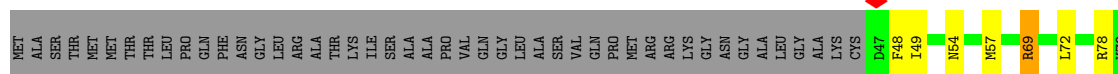


- Molecule 14: Photosystem I reaction center subunit IX

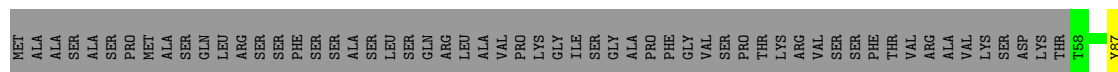
Chain J:  66% 27% 7%



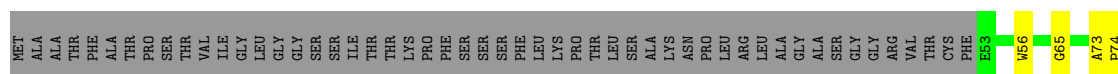
- Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic



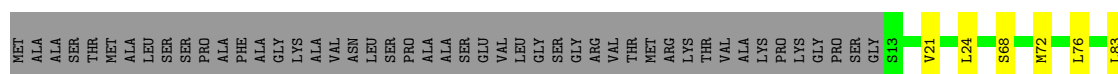
- Molecule 16: Photosystem I reaction center subunit XI, chloroplastic



- Molecule 17: Photosystem I subunit O

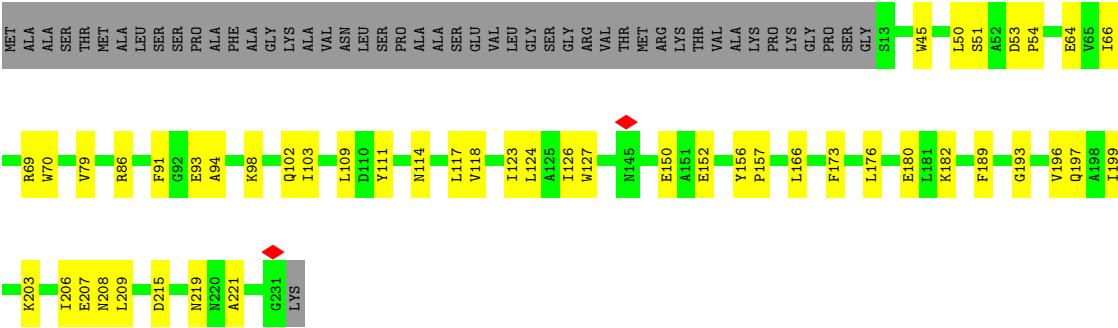


- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic

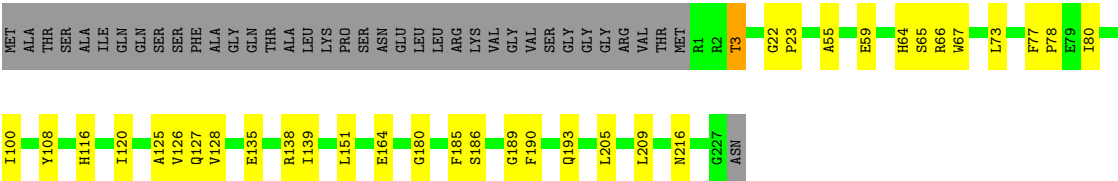


- Molecule 18: Chlorophyll a-b binding protein 2, chloroplastic





● Molecule 19: Chlorophyll a-b binding protein 2.1, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188490	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	38.962	Depositor
Minimum map value	-20.964	Depositor
Average map value	0.022	Depositor
Map value standard deviation	1.157	Depositor
Recommended contour level	3.59	Depositor
Map size ($\text{\AA}$)	365.232, 365.232, 365.232	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.18	0/1546	0.36	0/2110
2	2	0.43	0/1622	0.74	2/2219 (0.1%)
3	3	0.20	0/1717	0.37	0/2336
4	4	0.17	0/1599	0.32	0/2178
5	A	0.25	0/6005	0.47	3/8194 (0.0%)
6	B	0.26	0/6065	0.50	2/8279 (0.0%)
7	C	0.62	0/629	1.15	2/852 (0.2%)
8	D	0.45	0/1157	0.78	3/1563 (0.2%)
9	E	0.17	0/528	0.40	0/715
10	F	0.15	0/1238	0.37	0/1670
11	G	0.18	0/724	0.38	0/981
12	H	0.37	0/713	0.61	0/968
13	I	0.16	0/245	0.34	0/333
14	J	0.15	0/336	0.36	0/458
15	K	0.53	0/599	0.92	2/809 (0.2%)
16	L	0.21	0/1244	0.49	0/1700
17	O	0.20	0/710	0.37	0/969
18	x	0.35	0/1716	0.65	0/2336
18	y	0.45	0/1716	0.83	0/2336
19	z	0.26	0/1802	0.52	0/2450
All	All	0.30	0/31911	0.56	14/43456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	1
7	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	44	ARG	NE-CZ-NH2	6.80	125.33	119.20
8	D	164	ASP	CA-CB-CG	6.02	118.62	112.60
6	B	668	ARG	N-CA-C	5.93	117.74	111.28
15	K	78	ARG	NE-CZ-NH2	5.86	124.48	119.20
8	D	150	ARG	NE-CZ-NH2	5.69	124.32	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	578	ARG	Sidechain
7	C	44	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1496	0	1471	33	0
2	2	1566	0	1519	31	0
3	3	1666	0	1627	23	0
4	4	1551	0	1508	20	0
5	A	5807	0	5657	44	0
6	B	5854	0	5645	63	0
7	C	616	0	595	6	0
8	D	1128	0	1134	2	0
9	E	517	0	526	4	0
10	F	1208	0	1243	12	0
11	G	708	0	700	2	0
12	H	693	0	690	4	0
13	I	239	0	258	4	0
14	J	327	0	342	12	0
15	K	593	0	614	18	0
16	L	1207	0	1209	9	0
17	O	686	0	677	7	0
18	x	1666	0	1593	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	y	1666	0	1593	58	0
19	z	1759	0	1693	29	0
20	1	93	0	62	7	0
20	2	226	0	150	10	0
20	3	45	0	30	2	0
20	4	169	0	100	5	0
20	x	293	0	212	29	0
20	y	296	0	215	29	0
20	z	295	0	213	20	0
21	1	496	0	354	22	0
21	2	434	0	352	36	0
21	3	498	0	377	23	0
21	4	527	0	412	18	0
21	A	2533	0	2495	112	0
21	B	2284	0	2242	97	0
21	F	149	0	123	9	0
21	G	132	0	97	2	0
21	H	60	0	59	4	0
21	J	51	0	41	1	0
21	K	167	0	116	15	0
21	L	155	0	138	7	0
21	O	141	0	110	1	0
21	x	436	0	403	12	0
21	y	427	0	384	34	0
21	z	438	0	409	15	0
22	1	44	0	56	12	0
22	2	44	0	56	4	0
22	4	44	0	54	6	0
22	x	44	0	56	4	0
22	y	44	0	56	9	0
22	z	44	0	56	5	0
23	1	49	0	74	12	0
23	2	37	0	44	2	0
23	A	79	0	104	8	0
23	B	87	0	120	5	0
23	x	49	0	74	3	0
23	y	49	0	74	5	0
23	z	49	0	74	6	0
24	1	42	0	56	3	0
24	2	84	0	112	11	0
24	3	42	0	56	8	0
24	4	42	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	x	84	0	112	3	0
24	y	84	0	112	7	0
24	z	84	0	112	10	0
25	3	40	0	56	5	0
25	4	40	0	56	6	0
25	A	240	0	336	27	0
25	B	320	0	448	47	0
25	F	40	0	56	2	0
25	G	40	0	56	4	0
25	I	40	0	56	1	0
25	J	40	0	56	5	0
25	K	80	0	112	10	0
25	L	120	0	168	15	0
25	O	80	0	112	2	0
26	4	72	0	84	0	0
27	A	61	0	68	14	0
28	A	8	0	0	2	0
28	C	16	0	0	3	0
29	A	33	0	46	2	0
29	B	33	0	46	2	0
30	B	66	0	96	5	0
31	x	44	0	56	3	0
31	y	44	0	56	4	0
31	z	44	0	56	1	0
All	All	43924	0	42922	847	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 847 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:y:182:LYS:HE2	21:y:611:CLA:O1D	1.51	1.08
4:4:77:PHE:HE2	22:4:617:XAT:H383	1.22	1.05
4:4:77:PHE:CE2	22:4:617:XAT:H383	1.91	1.05
18:y:180:GLU:OE1	21:y:610:CLA:C1B	2.10	1.00
21:A:803:CLA:HBA2	6:B:655:LEU:HB2	1.52	0.90

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	191/241 (79%)	190 (100%)	1 (0%)	0	100	100
2	2	199/257 (77%)	196 (98%)	3 (2%)	0	100	100
3	3	216/273 (79%)	214 (99%)	2 (1%)	0	100	100
4	4	194/251 (77%)	190 (98%)	4 (2%)	0	100	100
5	A	735/750 (98%)	723 (98%)	12 (2%)	0	100	100
6	B	730/734 (100%)	718 (98%)	12 (2%)	0	100	100
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	141/204 (69%)	137 (97%)	4 (3%)	0	100	100
9	E	62/143 (43%)	61 (98%)	1 (2%)	0	100	100
10	F	150/221 (68%)	148 (99%)	2 (1%)	0	100	100
11	G	89/160 (56%)	88 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	88 (100%)	0	0	100	100
13	I	29/37 (78%)	29 (100%)	0	0	100	100
14	J	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
15	K	82/130 (63%)	81 (99%)	1 (1%)	0	100	100
16	L	158/219 (72%)	156 (99%)	2 (1%)	0	100	100
17	O	84/140 (60%)	83 (99%)	1 (1%)	0	100	100
18	x	217/267 (81%)	212 (98%)	5 (2%)	0	100	100
18	y	217/267 (81%)	209 (96%)	8 (4%)	0	100	100
19	z	224/265 (84%)	211 (94%)	13 (6%)	0	100	100
All	All	3923/4829 (81%)	3845 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/190 (80%)	152 (99%)	1 (1%)	76	91
2	2	163/205 (80%)	162 (99%)	1 (1%)	78	92
3	3	167/211 (79%)	166 (99%)	1 (1%)	78	92
4	4	163/210 (78%)	163 (100%)	0	100	100
5	A	598/610 (98%)	598 (100%)	0	100	100
6	B	599/600 (100%)	597 (100%)	2 (0%)	86	95
7	C	70/71 (99%)	69 (99%)	1 (1%)	59	85
8	D	121/170 (71%)	120 (99%)	1 (1%)	73	90
9	E	57/114 (50%)	57 (100%)	0	100	100
10	F	125/185 (68%)	125 (100%)	0	100	100
11	G	77/133 (58%)	76 (99%)	1 (1%)	61	86
12	H	75/113 (66%)	75 (100%)	0	100	100
13	I	27/33 (82%)	27 (100%)	0	100	100
14	J	36/39 (92%)	36 (100%)	0	100	100
15	K	61/95 (64%)	61 (100%)	0	100	100
16	L	126/174 (72%)	126 (100%)	0	100	100
17	O	72/114 (63%)	72 (100%)	0	100	100
18	x	167/201 (83%)	167 (100%)	0	100	100
18	y	167/201 (83%)	166 (99%)	1 (1%)	78	92
19	z	179/208 (86%)	178 (99%)	1 (1%)	78	92
All	All	3203/3877 (83%)	3193 (100%)	10 (0%)	84	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	G	98	GLU
18	y	152	GLU
19	z	139	ILE

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Mol	Chain	Res	Type
6	B	65	LEU
6	B	294	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	114	ASN
6	B	389	HIS
19	z	27	ASN
6	B	289	HIS
6	B	439	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
19	TPO	z	3	19	8,10,11	1.07	0	10,14,16	1.92	2 (20%)

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
19	TPO	z	3	19	-	2/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	3	TPO	P-OG1-CB	-5.31	107.17	123.21
19	z	3	TPO	CG2-CB-CA	-2.07	109.09	113.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	z	3	TPO	O-C-CA-CB
19	z	3	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	z	3	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

263 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	$\# Z > 2$
21	CLA	B	835	-	46,50,73	1.51	9 (19%)	55,85,113	1.46	6 (10%)
20	CHL	1	601	1	55,60,74	2.18	20 (36%)	61,97,114	2.91	25 (40%)
21	CLA	y	612	-	49,53,73	1.48	10 (20%)	59,89,113	1.46	5 (8%)
25	BCR	O	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.49	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	845	23	54,58,73	1.41	10 (18%)	65,95,113	1.50	8 (12%)
21	CLA	K	201	15	42,45,73	1.56	10 (23%)	50,78,113	1.54	5 (10%)
21	CLA	z	613	19	69,73,73	1.23	9 (13%)	83,113,113	1.35	6 (7%)
21	CLA	z	612	-	49,53,73	1.48	10 (20%)	59,89,113	1.45	6 (10%)
21	CLA	1	608	1	44,48,73	1.59	10 (22%)	56,83,113	1.57	8 (14%)
21	CLA	B	810	6	69,73,73	1.24	9 (13%)	83,113,113	1.32	9 (10%)
21	CLA	B	830	-	47,51,73	1.47	9 (19%)	56,86,113	1.47	5 (8%)
31	NEX	y	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.64	9 (18%)
21	CLA	y	613	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	6 (10%)
21	CLA	A	832	5	54,58,73	1.39	9 (16%)	65,95,113	1.46	8 (12%)
21	CLA	3	608	-	45,49,73	1.52	10 (22%)	54,84,113	1.70	11 (20%)
21	CLA	B	814	6	69,73,73	1.22	8 (11%)	83,113,113	1.36	8 (9%)
21	CLA	A	824	5	45,49,73	1.50	9 (20%)	54,84,113	1.57	9 (16%)
20	CHL	2	601	2	51,55,74	2.14	18 (35%)	57,91,114	3.24	25 (43%)
21	CLA	A	817	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
31	NEX	z	618	-	38,46,46	1.63	7 (18%)	50,70,70	1.60	9 (18%)
21	CLA	1	613	-	41,46,73	1.65	10 (24%)	52,81,113	1.62	9 (17%)
25	BCR	4	618	-	41,41,41	1.72	8 (19%)	56,56,56	1.69	11 (19%)
20	CHL	2	615	2	47,51,74	2.26	19 (40%)	52,86,114	3.13	22 (42%)
21	CLA	A	840	5	56,60,73	1.39	8 (14%)	67,97,113	1.41	7 (10%)
21	CLA	2	608	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	5 (8%)
21	CLA	A	806	5	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
28	SF4	C	102	7	0,12,12	-	-	-	-	-
20	CHL	x	608	18	46,50,74	2.31	18 (39%)	51,85,114	3.26	23 (45%)
21	CLA	B	809	6	69,73,73	1.24	9 (13%)	83,113,113	1.33	7 (8%)
21	CLA	A	822	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
21	CLA	x	612	-	49,53,73	1.46	9 (18%)	59,89,113	1.46	6 (10%)
21	CLA	B	840	6	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
21	CLA	1	609	-	46,50,73	1.50	10 (21%)	55,85,113	1.77	9 (16%)
25	BCR	G	204	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	10 (17%)
21	CLA	B	804	6	45,49,73	1.49	8 (17%)	54,84,113	1.58	7 (12%)
21	CLA	B	836	6	54,58,73	1.40	10 (18%)	65,95,113	3.45	11 (16%)
21	CLA	K	203	-	49,53,73	1.47	9 (18%)	59,89,113	1.60	9 (15%)
21	CLA	4	610	-	46,50,73	1.49	10 (21%)	55,85,113	1.44	5 (9%)
21	CLA	A	838	5	55,59,73	1.38	10 (18%)	66,96,113	1.41	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	J	101	-	55,59,73	1.41	7 (12%)	66,96,113	1.40	6 (9%)
24	LUT	1	616	-	42,43,43	1.69	7 (16%)	51,60,60	2.07	13 (25%)
21	CLA	1	612	1	50,54,73	1.47	10 (20%)	60,90,113	1.57	7 (11%)
21	CLA	3	605	-	45,49,73	1.58	10 (22%)	57,84,113	1.59	8 (14%)
21	CLA	4	609	4	58,62,73	1.35	10 (17%)	69,99,113	1.38	9 (13%)
21	CLA	G	201	-	49,53,73	1.49	8 (16%)	59,89,113	1.48	5 (8%)
21	CLA	1	611	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	5 (8%)
21	CLA	x	613	18	63,67,73	1.31	10 (15%)	75,105,113	1.36	6 (8%)
25	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.55	10 (17%)
20	CHL	3	606	-	49,53,74	2.23	18 (36%)	59,89,114	2.89	23 (38%)
21	CLA	B	824	-	69,73,73	1.25	7 (10%)	83,113,113	1.35	6 (7%)
26	LMG	4	620	-	33,33,55	0.26	0	41,41,63	0.59	1 (2%)
21	CLA	H	201	12	64,68,73	1.30	7 (10%)	77,107,113	1.30	4 (5%)
21	CLA	2	609	-	51,55,73	1.43	10 (19%)	61,91,113	1.46	5 (8%)
25	BCR	A	853	-	41,41,41	1.81	8 (19%)	56,56,56	1.78	14 (25%)
25	BCR	O	204	-	41,41,41	1.73	8 (19%)	56,56,56	1.53	9 (16%)
21	CLA	B	831	6	47,51,73	1.45	7 (14%)	56,86,113	1.52	7 (12%)
21	CLA	B	806	6	69,73,73	1.23	8 (11%)	83,113,113	1.30	8 (9%)
25	BCR	I	101	-	41,41,41	1.72	8 (19%)	56,56,56	1.52	9 (16%)
21	CLA	B	828	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
31	NEX	x	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.86	13 (26%)
24	LUT	y	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.72	11 (21%)
21	CLA	3	601	-	64,68,73	1.28	8 (12%)	77,107,113	1.34	6 (7%)
21	CLA	A	823	5	46,50,73	1.48	7 (15%)	55,85,113	1.51	6 (10%)
25	BCR	A	851	-	41,41,41	1.85	9 (21%)	56,56,56	2.71	20 (35%)
21	CLA	A	811	5	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
21	CLA	A	829	5	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
21	CLA	y	611	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	4 (6%)
20	CHL	z	606	-	50,54,74	2.29	20 (40%)	56,90,114	3.04	19 (33%)
23	LHG	B	852	-	48,48,48	0.27	0	51,54,54	0.34	0
21	CLA	A	818	5	64,68,73	1.28	10 (15%)	77,107,113	4.90	8 (10%)
21	CLA	A	839	5	59,63,73	1.33	8 (13%)	71,101,113	1.41	7 (9%)
25	BCR	B	848	-	41,41,41	1.72	8 (19%)	56,56,56	1.56	11 (19%)
21	CLA	A	841	5	69,73,73	1.22	8 (11%)	83,113,113	1.33	7 (8%)
21	CLA	B	818	6	64,68,73	1.28	10 (15%)	77,107,113	1.37	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	y	608	-	53,57,74	2.20	20 (37%)	59,93,114	2.96	20 (33%)
21	CLA	1	605	-	50,54,73	1.47	10 (20%)	60,90,113	1.45	5 (8%)
21	CLA	B	813	-	69,73,73	1.24	10 (14%)	83,113,113	1.44	9 (10%)
21	CLA	y	614	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	5 (6%)
21	CLA	A	816	5	46,50,73	1.48	9 (19%)	55,85,113	1.50	4 (7%)
21	CLA	B	827	6	69,73,73	1.23	9 (13%)	83,113,113	1.32	6 (7%)
20	CHL	x	605	-	57,61,74	2.06	18 (31%)	64,98,114	3.00	25 (39%)
21	CLA	z	614	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	6 (7%)
21	CLA	3	609	-	57,62,73	1.38	10 (17%)	68,100,113	1.38	7 (10%)
20	CHL	y	609	18	57,61,74	2.29	19 (33%)	64,98,114	2.90	26 (40%)
20	CHL	4	606	-	45,49,74	2.25	15 (33%)	57,84,114	3.15	23 (40%)
21	CLA	K	204	15	50,54,73	1.47	10 (20%)	60,90,113	1.47	6 (10%)
25	BCR	B	846	-	41,41,41	1.76	8 (19%)	56,56,56	1.73	11 (19%)
21	CLA	3	610	3	43,48,73	1.56	9 (20%)	51,83,113	1.55	5 (9%)
21	CLA	1	607	-	47,52,73	1.50	9 (19%)	56,88,113	1.50	4 (7%)
25	BCR	B	844	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	13 (23%)
21	CLA	A	835	5	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
21	CLA	B	825	-	66,70,73	1.25	9 (13%)	79,109,113	1.39	10 (12%)
21	CLA	x	604	-	56,60,73	1.38	9 (16%)	67,97,113	1.46	8 (11%)
20	CHL	4	607	-	50,54,74	2.21	20 (40%)	56,90,114	3.14	22 (39%)
22	XAT	2	617	-	39,47,47	1.79	8 (20%)	54,74,74	2.18	16 (29%)
20	CHL	2	605	-	46,50,74	2.23	16 (34%)	52,85,114	3.18	21 (40%)
21	CLA	4	602	4	64,68,73	1.28	10 (15%)	77,107,113	1.33	9 (11%)
21	CLA	4	604	-	47,51,73	1.59	10 (21%)	60,87,113	1.53	7 (11%)
21	CLA	F	302	-	55,59,73	1.40	9 (16%)	66,96,113	1.50	6 (9%)
21	CLA	B	829	6	60,64,73	1.33	10 (16%)	72,102,113	1.41	8 (11%)
24	LUT	z	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.76	10 (19%)
21	CLA	A	830	-	69,73,73	1.24	10 (14%)	83,113,113	1.45	9 (10%)
21	CLA	x	610	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	5 (6%)
24	LUT	x	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.84	11 (21%)
21	CLA	K	206	15	41,47,73	1.57	9 (21%)	49,81,113	1.53	7 (14%)
21	CLA	x	614	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	6 (10%)
21	CLA	1	602	1	58,62,73	1.35	10 (17%)	69,99,113	1.38	6 (8%)
28	SF4	A	854	5,6	0,12,12	-	-	-	-	-
20	CHL	x	606	-	50,54,74	2.19	18 (36%)	56,90,114	3.13	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	833	6	49,53,73	1.47	8 (16%)	59,89,113	1.57	10 (16%)
21	CLA	x	611	23	49,53,73	1.47	9 (18%)	59,89,113	1.48	7 (11%)
21	CLA	B	821	6	51,55,73	1.43	9 (17%)	61,91,113	1.55	10 (16%)
20	CHL	x	609	18	50,54,74	2.25	20 (40%)	56,90,114	3.06	23 (41%)
21	CLA	B	817	6	63,67,73	1.29	9 (14%)	75,105,113	1.37	5 (6%)
23	LHG	x	619	21	48,48,48	0.28	0	51,54,54	0.34	0
21	CLA	4	608	4	49,53,73	1.48	9 (18%)	59,89,113	1.47	5 (8%)
21	CLA	A	814	5	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
21	CLA	B	832	6	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)
24	LUT	3	613	-	42,43,43	1.68	8 (19%)	51,60,60	2.01	14 (27%)
21	CLA	L	304	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
21	CLA	y	610	18	62,66,73	1.31	9 (14%)	74,104,113	1.36	7 (9%)
24	LUT	x	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.58	11 (21%)
21	CLA	2	604	-	47,51,73	1.49	9 (19%)	55,86,113	1.52	5 (9%)
21	CLA	B	822	6	69,73,73	1.27	9 (13%)	83,113,113	1.45	8 (9%)
21	CLA	A	804	5	69,73,73	1.23	10 (14%)	83,113,113	1.44	9 (10%)
21	CLA	A	836	5	49,53,73	1.46	9 (18%)	59,89,113	1.50	6 (10%)
30	DGD	B	850	-	67,67,67	0.83	2 (2%)	81,81,81	0.97	3 (3%)
24	LUT	y	615	-	42,43,43	1.65	7 (16%)	51,60,60	2.14	13 (25%)
21	CLA	A	833	5	60,64,73	1.33	9 (15%)	72,102,113	1.37	6 (8%)
21	CLA	A	844	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	6 (7%)
21	CLA	B	808	6	69,73,73	1.22	10 (14%)	83,113,113	1.39	7 (8%)
21	CLA	B	837	6	69,73,73	1.23	7 (10%)	83,113,113	1.36	7 (8%)
24	LUT	4	616	-	42,43,43	1.62	8 (19%)	51,60,60	1.57	10 (19%)
25	BCR	J	102	-	41,41,41	1.75	8 (19%)	56,56,56	1.76	13 (23%)
21	CLA	4	601	4	50,54,73	1.46	10 (20%)	60,90,113	1.42	5 (8%)
24	LUT	z	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.80	11 (21%)
21	CLA	z	611	-	49,53,73	1.47	10 (20%)	59,89,113	1.48	4 (6%)
25	BCR	L	305	-	41,41,41	1.77	8 (19%)	56,56,56	1.79	15 (26%)
21	CLA	2	610	23	41,45,73	2.52	13 (31%)	47,76,113	1.34	5 (10%)
21	CLA	B	812	6	47,51,73	1.48	10 (21%)	56,86,113	1.46	5 (8%)
25	BCR	A	849	-	41,41,41	1.76	8 (19%)	56,56,56	2.00	13 (23%)
25	BCR	L	306	-	41,41,41	1.77	8 (19%)	56,56,56	2.04	16 (28%)
21	CLA	A	828	5	69,73,73	1.24	8 (11%)	83,113,113	1.32	8 (9%)
24	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	2.13	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	A	850	-	41,41,41	1.82	8 (19%)	56,56,56	1.93	12 (21%)
21	CLA	B	803	-	69,73,73	1.23	8 (11%)	83,113,113	1.35	6 (7%)
21	CLA	4	611	-	44,49,73	1.53	10 (22%)	52,84,113	1.48	5 (9%)
21	CLA	G	203	11	49,53,73	1.47	8 (16%)	59,89,113	1.48	6 (10%)
21	CLA	y	604	-	55,59,73	1.38	9 (16%)	66,96,113	1.46	8 (12%)
21	CLA	A	831	5	69,73,73	1.23	9 (13%)	83,113,113	1.31	5 (6%)
21	CLA	F	301	-	61,65,73	1.34	8 (13%)	73,103,113	1.32	7 (9%)
21	CLA	B	819	-	59,63,73	1.34	9 (15%)	71,101,113	1.44	8 (11%)
21	CLA	O	203	-	41,46,73	1.66	10 (24%)	52,81,113	1.62	9 (17%)
21	CLA	B	802	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	8 (9%)
21	CLA	z	602	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
23	LHG	A	847	21	29,29,48	0.35	0	32,35,54	0.49	0
21	CLA	A	825	5	59,63,73	1.34	9 (15%)	71,101,113	1.36	8 (11%)
21	CLA	B	826	6	66,70,73	1.27	10 (15%)	79,109,113	1.34	6 (7%)
20	CHL	y	605	18	46,50,74	2.34	17 (36%)	51,85,114	3.19	22 (43%)
21	CLA	A	802	-	69,73,73	1.24	11 (15%)	83,113,113	1.41	9 (10%)
21	CLA	z	610	-	49,53,73	1.47	10 (20%)	59,89,113	1.49	7 (11%)
21	CLA	3	611	-	41,44,73	1.59	9 (21%)	49,77,113	1.52	7 (14%)
25	BCR	B	801	-	41,41,41	1.79	8 (19%)	56,56,56	1.82	14 (25%)
21	CLA	A	826	-	69,73,73	1.24	9 (13%)	83,113,113	1.32	4 (4%)
21	CLA	O	202	17	40,46,73	1.58	10 (25%)	48,80,113	1.55	7 (14%)
21	CLA	A	810	5	54,58,73	1.41	9 (16%)	65,95,113	1.60	11 (16%)
21	CLA	A	808	5	54,58,73	1.40	9 (16%)	65,95,113	1.44	8 (12%)
21	CLA	A	827	-	63,67,73	1.29	9 (14%)	75,105,113	1.38	6 (8%)
21	CLA	A	815	5	49,53,73	1.45	8 (16%)	59,89,113	1.54	6 (10%)
20	CHL	z	607	-	56,60,74	2.10	18 (32%)	63,97,114	3.08	26 (41%)
21	CLA	2	611	-	48,52,73	1.52	8 (16%)	58,88,113	1.47	6 (10%)
21	CLA	2	613	2	47,51,73	1.49	9 (19%)	56,86,113	1.45	6 (10%)
21	CLA	1	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.51	7 (11%)
21	CLA	x	602	-	69,73,73	1.24	10 (14%)	83,113,113	1.36	6 (7%)
21	CLA	3	604	-	44,49,73	1.53	10 (22%)	52,84,113	1.47	5 (9%)
25	BCR	L	301	-	41,41,41	1.77	8 (19%)	56,56,56	2.30	12 (21%)
21	CLA	B	811	6	58,62,73	1.40	10 (17%)	73,100,113	1.48	6 (8%)
20	CHL	2	606	-	47,51,74	2.23	17 (36%)	52,86,114	3.17	21 (40%)
21	CLA	3	602	-	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SF4	C	101	7	0,12,12	-	-	-		
25	BCR	K	205	-	41,41,41	1.73	8 (19%)	56,56,56	2.02	16 (28%)
20	CHL	z	609	-	57,61,74	2.28	19 (33%)	64,98,114	2.88	24 (37%)
21	CLA	B	841	23	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
23	LHG	z	619	-	48,48,48	0.29	0	51,54,54	0.38	0
21	CLA	2	602	2	69,73,73	1.24	10 (14%)	83,113,113	1.30	6 (7%)
23	LHG	A	846	-	48,48,48	0.28	0	51,54,54	0.35	0
21	CLA	2	612	2	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
22	XAT	y	617	-	39,47,47	1.73	8 (20%)	54,74,74	2.01	14 (25%)
20	CHL	x	607	-	57,61,74	2.17	18 (31%)	64,98,114	2.91	26 (40%)
25	BCR	B	849	-	41,41,41	1.76	8 (19%)	56,56,56	1.92	13 (23%)
20	CHL	4	615	4	44,49,74	2.25	18 (40%)	51,84,114	3.23	21 (41%)
21	CLA	B	815	6	47,51,73	1.46	9 (19%)	56,86,113	1.52	5 (8%)
21	CLA	L	303	16	69,73,73	1.23	9 (13%)	83,113,113	1.37	7 (8%)
21	CLA	A	843	-	69,73,73	1.22	8 (11%)	83,113,113	1.33	4 (4%)
21	CLA	B	820	6	54,58,73	1.39	9 (16%)	65,95,113	1.48	9 (13%)
20	CHL	z	601	19	57,61,74	2.20	19 (33%)	64,98,114	2.94	27 (42%)
21	CLA	y	602	18	69,73,73	1.24	10 (14%)	83,113,113	1.31	6 (7%)
29	PQN	A	855	-	34,34,34	0.40	0	42,45,45	0.42	0
21	CLA	B	807	6	56,60,73	1.35	8 (14%)	67,97,113	1.45	7 (10%)
20	CHL	z	608	-	53,57,74	2.14	19 (35%)	59,93,114	3.04	24 (40%)
21	CLA	F	303	10	45,49,73	1.54	8 (17%)	54,84,113	1.51	6 (11%)
21	CLA	A	834	5	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
21	CLA	A	837	5	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
21	CLA	A	807	5	69,73,73	1.25	9 (13%)	83,113,113	1.26	7 (8%)
21	CLA	4	613	4	49,53,73	1.47	10 (20%)	59,89,113	1.69	7 (11%)
21	CLA	4	603	-	48,52,73	1.56	11 (22%)	61,88,113	1.52	7 (11%)
21	CLA	y	603	18	57,61,73	1.37	10 (17%)	68,98,113	1.41	7 (10%)
25	BCR	3	614	-	41,41,41	1.73	8 (19%)	56,56,56	1.58	12 (21%)
22	XAT	1	614	-	39,47,47	0.82	1 (2%)	54,74,74	3.18	19 (35%)
20	CHL	x	601	18	57,61,74	2.22	19 (33%)	64,98,114	2.88	26 (40%)
21	CLA	B	834	6	64,68,73	1.31	9 (14%)	77,107,113	1.34	6 (7%)
21	CLA	B	805	6	69,73,73	1.24	9 (13%)	83,113,113	1.33	7 (8%)
21	CLA	z	603	-	61,65,73	1.31	9 (14%)	73,103,113	1.40	5 (6%)
21	CLA	1	603	1	58,62,73	1.35	10 (17%)	69,99,113	1.38	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	4	605	-	44,49,74	2.29	17 (38%)	49,84,114	3.20	22 (44%)
21	CLA	3	607	-	49,53,73	1.49	9 (18%)	59,89,113	1.47	6 (10%)
21	CLA	A	813	5	58,62,73	1.37	10 (17%)	69,99,113	1.41	7 (10%)
21	CLA	G	202	-	46,50,73	1.50	9 (19%)	55,85,113	1.47	5 (9%)
25	BCR	A	848	-	41,41,41	1.75	8 (19%)	56,56,56	1.69	12 (21%)
26	LMG	4	619	-	39,39,55	0.23	0	47,47,63	0.24	0
21	CLA	A	819	5	63,67,73	1.31	10 (15%)	75,105,113	1.34	7 (9%)
25	BCR	K	202	-	41,41,41	1.74	8 (19%)	56,56,56	2.07	15 (26%)
21	CLA	3	603	-	49,53,73	1.50	8 (16%)	59,89,113	1.45	7 (11%)
21	CLA	A	809	5	69,73,73	1.21	8 (11%)	83,113,113	1.36	8 (9%)
21	CLA	3	612	-	43,48,73	1.51	8 (18%)	51,83,113	1.63	7 (13%)
21	CLA	z	604	-	55,59,73	1.40	9 (16%)	66,96,113	1.44	8 (12%)
20	CHL	y	607	-	57,61,74	2.10	18 (31%)	64,98,114	2.98	27 (42%)
21	CLA	B	838	6	51,55,73	1.44	10 (19%)	61,91,113	1.47	7 (11%)
23	LHG	1	615	21	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
21	CLA	2	603	-	47,52,73	1.50	10 (21%)	56,88,113	1.58	8 (14%)
21	CLA	O	201	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
22	XAT	z	617	-	39,47,47	1.66	8 (20%)	54,74,74	1.76	12 (22%)
20	CHL	2	607	-	55,59,74	2.10	18 (32%)	62,96,114	3.00	25 (40%)
21	CLA	x	603	18	64,68,73	1.28	9 (14%)	77,107,113	1.37	8 (10%)
21	CLA	A	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)
27	CL0	A	801	5	66,69,73	1.89	17 (25%)	79,107,113	4.28	32 (40%)
29	PQN	B	842	-	34,34,34	0.42	0	42,45,45	0.42	0
21	CLA	A	805	5,21	56,60,73	1.37	8 (14%)	67,97,113	1.43	9 (13%)
21	CLA	B	823	6	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
20	CHL	z	605	-	46,50,74	2.34	17 (36%)	51,85,114	3.22	24 (47%)
20	CHL	y	601	18	57,61,74	2.23	19 (33%)	64,98,114	2.92	26 (40%)
22	XAT	4	617	-	39,47,47	5.32	25 (64%)	54,74,74	5.60	38 (70%)
21	CLA	A	842	5	69,73,73	1.24	8 (11%)	83,113,113	1.43	10 (12%)
21	CLA	A	821	5	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
21	CLA	A	812	21	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
24	LUT	2	619	-	42,43,43	1.67	8 (19%)	51,60,60	1.93	12 (23%)
23	LHG	B	851	21	37,37,48	0.31	0	40,43,54	0.51	0
25	BCR	F	304	-	41,41,41	1.87	8 (19%)	56,56,56	2.16	16 (28%)
21	CLA	B	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHL	y	606	-	50,54,74	2.26	18 (36%)	56,90,114	3.16	22 (39%)
21	CLA	1	610	23	41,46,73	1.66	11 (26%)	52,81,113	1.59	7 (13%)
23	LHG	2	618	21	36,36,48	0.32	0	39,42,54	0.50	0
21	CLA	4	614	4	54,58,73	1.40	9 (16%)	65,95,113	1.48	7 (10%)
21	CLA	B	816	6	59,63,73	1.33	8 (13%)	71,101,113	1.45	8 (11%)
21	CLA	4	612	4	61,65,73	1.32	10 (16%)	73,103,113	1.40	8 (10%)
20	CHL	1	606	-	44,49,74	2.45	19 (43%)	48,84,114	3.10	22 (45%)
25	BCR	B	843	-	41,41,41	1.74	8 (19%)	56,56,56	2.05	14 (25%)
21	CLA	L	302	16	49,53,73	1.48	9 (18%)	59,89,113	1.51	7 (11%)
23	LHG	y	619	-	48,48,48	0.29	0	51,54,54	0.35	0
25	BCR	A	852	-	41,41,41	1.75	9 (21%)	56,56,56	1.94	14 (25%)
25	BCR	B	845	-	41,41,41	1.79	8 (19%)	56,56,56	1.89	13 (23%)
22	XAT	x	617	-	39,47,47	1.74	8 (20%)	54,74,74	2.05	14 (25%)
21	CLA	A	820	5	69,73,73	1.24	10 (14%)	83,113,113	1.37	9 (10%)

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
21	CLA	B	835	-	-	6/12/88/115	-
20	CHL	1	601	1	-	7/24/100/117	-
21	CLA	y	612	-	-	8/15/91/115	-
25	BCR	O	205	-	-	0/29/63/63	0/2/2/2
21	CLA	A	845	23	-	10/21/97/115	-
21	CLA	K	201	15	-	2/4/76/115	-
21	CLA	z	613	19	-	15/39/115/115	-
21	CLA	z	612	-	-	4/15/91/115	-
21	CLA	1	608	1	-	3/8/84/115	-
21	CLA	B	810	6	-	16/39/115/115	-
21	CLA	B	830	-	-	3/13/89/115	-
31	NEX	y	618	-	-	2/27/83/83	0/3/3/3
21	CLA	y	613	-	-	7/15/91/115	-
21	CLA	A	832	5	-	6/21/97/115	-
21	CLA	3	608	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	814	6	-	17/39/115/115	-
21	CLA	A	824	5	-	4/10/86/115	-
20	CHL	2	601	2	-	6/19/95/117	-
21	CLA	A	817	-	-	2/15/91/115	-
31	NEX	z	618	-	-	2/27/83/83	0/3/3/3
21	CLA	1	613	-	-	0/4/80/115	-
25	BCR	4	618	-	-	8/29/63/63	0/2/2/2
20	CHL	2	615	2	-	2/14/90/117	-
21	CLA	A	840	5	-	5/24/100/115	-
21	CLA	2	608	-	-	7/15/91/115	-
21	CLA	A	806	5	-	14/39/115/115	-
28	SF4	C	102	7	-	-	0/6/5/5
20	CHL	x	608	18	-	3/12/88/117	-
21	CLA	B	809	6	-	15/39/115/115	-
21	CLA	A	822	-	-	11/39/115/115	-
21	CLA	x	612	-	-	8/15/91/115	-
21	CLA	B	840	6	-	13/39/115/115	-
21	CLA	1	609	-	-	5/11/87/115	-
25	BCR	G	204	-	-	4/29/63/63	0/2/2/2
21	CLA	B	804	6	-	2/10/86/115	-
21	CLA	B	836	6	-	7/21/97/115	-
21	CLA	K	203	-	-	7/15/91/115	-
21	CLA	4	610	-	-	6/12/88/115	-
21	CLA	A	838	5	-	10/23/99/115	-
21	CLA	J	101	-	-	8/23/99/115	-
24	LUT	1	616	-	-	2/29/67/67	0/2/2/2
21	CLA	1	612	1	-	7/17/93/115	-
21	CLA	3	605	-	-	6/10/86/115	-
21	CLA	4	609	4	-	6/26/102/115	-
21	CLA	G	201	-	-	9/15/91/115	-
21	CLA	1	611	-	-	6/15/91/115	-
21	CLA	x	613	18	-	13/32/108/115	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
20	CHL	3	606	-	-	5/15/91/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	824	-	-	12/39/115/115	-
26	LMG	4	620	-	-	8/28/48/70	0/1/1/1
21	CLA	H	201	12	-	16/33/109/115	-
21	CLA	2	609	-	-	9/18/94/115	-
25	BCR	A	853	-	-	5/29/63/63	0/2/2/2
25	BCR	O	204	-	-	2/29/63/63	0/2/2/2
21	CLA	B	831	6	-	2/13/89/115	-
21	CLA	B	806	6	-	16/39/115/115	-
25	BCR	I	101	-	-	0/29/63/63	0/2/2/2
21	CLA	B	828	-	-	15/39/115/115	-
31	NEX	x	618	-	-	8/27/83/83	0/3/3/3
24	LUT	y	616	-	-	6/29/67/67	0/2/2/2
21	CLA	3	601	-	-	17/33/109/115	-
21	CLA	A	823	5	-	5/12/88/115	-
25	BCR	A	851	-	-	8/29/63/63	0/2/2/2
21	CLA	A	811	5	-	13/39/115/115	-
21	CLA	A	829	5	-	17/39/115/115	-
21	CLA	y	611	-	-	7/15/91/115	-
20	CHL	z	606	-	-	6/17/93/117	-
23	LHG	B	852	-	-	17/53/53/53	-
21	CLA	A	818	5	-	16/33/109/115	-
21	CLA	A	839	5	-	7/27/103/115	-
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	841	5	-	17/39/115/115	-
21	CLA	B	818	6	-	11/33/109/115	-
20	CHL	y	608	-	-	8/21/97/117	-
21	CLA	1	605	-	-	8/17/93/115	-
21	CLA	B	813	-	-	12/39/115/115	-
21	CLA	y	614	-	-	20/39/115/115	-
21	CLA	A	816	5	-	2/12/88/115	-
21	CLA	B	827	6	-	18/39/115/115	-
20	CHL	x	605	-	-	13/26/102/117	-
21	CLA	z	614	-	-	13/39/115/115	-
21	CLA	3	609	-	-	5/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	y	609	18	-	18/26/102/117	-
20	CHL	4	606	-	-	2/10/86/117	-
21	CLA	K	204	15	-	10/17/93/115	-
25	BCR	B	846	-	-	8/29/63/63	0/2/2/2
21	CLA	3	610	3	-	2/8/84/115	-
21	CLA	1	607	-	-	9/13/89/115	-
25	BCR	B	844	-	-	12/29/63/63	0/2/2/2
21	CLA	A	835	5	-	22/39/115/115	-
21	CLA	B	825	-	-	13/36/112/115	-
21	CLA	x	604	-	-	8/24/100/115	-
20	CHL	4	607	-	-	5/17/93/117	-
22	XAT	2	617	-	-	15/31/93/93	0/4/4/4
20	CHL	2	605	-	-	2/12/88/117	-
21	CLA	4	602	4	-	6/33/109/115	-
21	CLA	4	604	-	-	6/11/87/115	-
21	CLA	F	302	-	-	8/23/99/115	-
21	CLA	B	829	6	-	7/29/105/115	-
24	LUT	z	615	-	-	4/29/67/67	0/2/2/2
21	CLA	A	830	-	-	14/39/115/115	-
21	CLA	x	610	-	-	17/39/115/115	-
24	LUT	x	616	-	-	2/29/67/67	0/2/2/2
21	CLA	K	206	15	-	2/8/80/115	-
21	CLA	x	614	-	-	7/15/91/115	-
21	CLA	1	602	1	-	7/26/102/115	-
28	SF4	A	854	5,6	-	-	0/6/5/5
20	CHL	x	606	-	-	6/17/93/117	-
21	CLA	B	833	6	-	4/15/91/115	-
21	CLA	x	611	23	-	2/15/91/115	-
21	CLA	B	821	6	-	3/18/94/115	-
20	CHL	x	609	18	-	5/17/93/117	-
21	CLA	B	817	6	-	13/32/108/115	-
23	LHG	x	619	21	-	7/53/53/53	-
21	CLA	4	608	4	-	6/15/91/115	-
21	CLA	A	814	5	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	832	6	-	16/39/115/115	-
24	LUT	3	613	-	-	7/29/67/67	0/2/2/2
21	CLA	L	304	-	-	3/15/91/115	-
21	CLA	y	610	18	-	13/31/107/115	-
24	LUT	x	615	-	-	0/29/67/67	0/2/2/2
21	CLA	2	604	-	-	6/11/88/115	-
21	CLA	B	822	6	-	25/39/115/115	-
21	CLA	A	804	5	-	20/39/115/115	-
21	CLA	A	836	5	-	6/15/91/115	-
30	DGD	B	850	-	-	14/55/95/95	0/2/2/2
24	LUT	y	615	-	-	5/29/67/67	0/2/2/2
21	CLA	A	833	5	-	5/29/105/115	-
21	CLA	A	844	-	-	11/39/115/115	-
21	CLA	B	808	6	-	17/39/115/115	-
21	CLA	B	837	6	-	9/39/115/115	-
24	LUT	4	616	-	-	2/29/67/67	0/2/2/2
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	4	601	4	-	5/17/93/115	-
24	LUT	z	616	-	-	3/29/67/67	0/2/2/2
21	CLA	z	611	-	-	2/15/91/115	-
25	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	2	610	23	-	2/10/70/115	-
21	CLA	B	812	6	-	0/13/89/115	-
25	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	BCR	L	306	-	-	5/29/63/63	0/2/2/2
21	CLA	A	828	5	-	12/39/115/115	-
24	LUT	2	616	-	-	7/29/67/67	0/2/2/2
25	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	CLA	B	803	-	-	15/39/115/115	-
21	CLA	4	611	-	-	4/10/86/115	-
21	CLA	G	203	11	-	3/15/91/115	-
21	CLA	y	604	-	-	9/23/99/115	-
21	CLA	A	831	5	-	8/39/115/115	-
21	CLA	F	301	-	-	13/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	819	-	-	7/27/103/115	-
21	CLA	O	203	-	-	0/4/80/115	-
21	CLA	B	802	-	-	16/39/115/115	-
21	CLA	z	602	-	-	13/39/115/115	-
23	LHG	A	847	21	-	3/34/34/53	-
21	CLA	A	825	5	-	14/27/103/115	-
21	CLA	B	826	6	-	7/36/112/115	-
20	CHL	y	605	18	-	2/12/88/117	-
21	CLA	A	802	-	-	19/39/115/115	-
21	CLA	z	610	-	-	5/15/91/115	-
21	CLA	3	611	-	-	2/2/74/115	-
25	BCR	B	801	-	-	6/29/63/63	0/2/2/2
21	CLA	A	826	-	-	10/39/115/115	-
21	CLA	O	202	17	-	0/6/78/115	-
21	CLA	A	810	5	-	6/21/97/115	-
21	CLA	A	808	5	-	3/21/97/115	-
21	CLA	A	827	-	-	5/32/108/115	-
21	CLA	A	815	5	-	8/15/91/115	-
20	CHL	z	607	-	-	7/25/101/117	-
21	CLA	2	611	-	-	6/13/89/115	-
21	CLA	2	613	2	-	6/13/89/115	-
21	CLA	1	604	-	-	10/20/96/115	-
21	CLA	x	602	-	-	13/39/115/115	-
21	CLA	3	604	-	-	2/10/86/115	-
25	BCR	L	301	-	-	3/29/63/63	0/2/2/2
21	CLA	B	811	6	-	10/25/101/115	-
20	CHL	2	606	-	-	2/14/90/117	-
21	CLA	3	602	-	-	13/27/103/115	-
28	SF4	C	101	7	-	-	0/6/5/5
25	BCR	K	205	-	-	8/29/63/63	0/2/2/2
20	CHL	z	609	-	-	15/26/102/117	-
21	CLA	B	841	23	-	23/39/115/115	-
23	LHG	z	619	-	-	10/53/53/53	-
21	CLA	2	602	2	-	16/39/115/115	-
23	LHG	A	846	-	-	4/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	612	2	-	21/39/115/115	-
22	XAT	y	617	-	-	4/31/93/93	0/4/4/4
20	CHL	x	607	-	-	11/26/102/117	-
25	BCR	B	849	-	-	7/29/63/63	0/2/2/2
20	CHL	4	615	4	-	1/10/86/117	-
21	CLA	B	815	6	-	2/13/89/115	-
21	CLA	L	303	16	-	10/39/115/115	-
21	CLA	A	843	-	-	13/39/115/115	-
21	CLA	B	820	6	-	7/21/97/115	-
20	CHL	z	601	19	-	10/26/102/117	-
21	CLA	y	602	18	-	21/39/115/115	-
29	PQN	A	855	-	-	1/23/43/43	0/2/2/2
21	CLA	B	807	6	-	4/24/100/115	-
20	CHL	z	608	-	-	4/21/97/117	-
21	CLA	F	303	10	-	4/10/86/115	-
21	CLA	A	834	5	-	9/39/115/115	-
21	CLA	A	837	5	-	4/15/91/115	-
21	CLA	A	807	5	-	13/39/115/115	-
21	CLA	4	613	4	-	7/15/91/115	-
21	CLA	4	603	-	-	4/13/89/115	-
21	CLA	y	603	18	-	7/25/101/115	-
25	BCR	3	614	-	-	5/29/63/63	0/2/2/2
22	XAT	1	614	-	-	9/31/93/93	0/4/4/4
20	CHL	x	601	18	-	13/26/102/117	-
21	CLA	B	834	6	-	9/33/109/115	-
21	CLA	B	805	6	-	13/39/115/115	-
21	CLA	z	603	-	-	8/30/106/115	-
21	CLA	1	603	1	-	8/26/102/115	-
20	CHL	4	605	-	-	2/10/86/117	-
21	CLA	3	607	-	-	4/15/91/115	-
21	CLA	A	813	5	-	9/26/102/115	-
21	CLA	G	202	-	-	3/12/88/115	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
26	LMG	4	619	-	-	6/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	819	5	-	17/32/108/115	-
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	3	603	-	-	7/15/91/115	-
21	CLA	A	809	5	-	9/39/115/115	-
21	CLA	3	612	-	-	3/8/84/115	-
21	CLA	z	604	-	-	12/23/99/115	-
20	CHL	y	607	-	-	12/26/102/117	-
21	CLA	B	838	6	-	1/18/94/115	-
23	LHG	1	615	21	-	30/53/53/53	-
21	CLA	2	603	-	-	5/13/89/115	-
21	CLA	O	201	-	-	17/39/115/115	-
22	XAT	z	617	-	-	0/31/93/93	0/4/4/4
20	CHL	2	607	-	-	7/23/99/117	-
21	CLA	x	603	18	-	10/33/109/115	-
21	CLA	A	803	-	-	20/39/115/115	-
27	CL0	A	801	5	-	16/33/105/115	-
29	PQN	B	842	-	-	6/23/43/43	0/2/2/2
21	CLA	A	805	5,21	-	7/24/100/115	-
21	CLA	B	823	6	-	7/15/91/115	-
20	CHL	z	605	-	-	4/12/88/117	-
20	CHL	y	601	18	-	12/26/102/117	-
22	XAT	4	617	-	-	1/31/93/93	0/4/4/4
21	CLA	A	842	5	-	12/39/115/115	-
21	CLA	A	821	5	-	4/15/91/115	-
21	CLA	A	812	21	-	22/39/115/115	-
24	LUT	2	619	-	-	4/29/67/67	0/2/2/2
23	LHG	B	851	21	-	5/42/42/53	-
25	BCR	F	304	-	-	13/29/63/63	0/2/2/2
21	CLA	B	839	-	-	10/39/115/115	-
20	CHL	y	606	-	-	4/17/93/117	-
21	CLA	1	610	23	-	0/4/80/115	-
23	LHG	2	618	21	-	10/41/41/53	-
21	CLA	4	614	4	-	9/21/97/115	-
21	CLA	B	816	6	-	6/27/103/115	-
21	CLA	4	612	4	-	12/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	1	606	-	-	0/10/86/117	-
25	BCR	B	843	-	-	1/29/63/63	0/2/2/2
21	CLA	L	302	16	-	1/15/91/115	-
23	LHG	y	619	-	-	11/53/53/53	-
25	BCR	A	852	-	-	13/29/63/63	0/2/2/2
25	BCR	B	845	-	-	9/29/63/63	0/2/2/2
22	XAT	x	617	-	-	8/31/93/93	0/4/4/4
21	CLA	A	820	5	-	17/39/115/115	-

The worst 5 of 2496 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	617	XAT	O4-C5	-12.41	1.28	1.46
21	2	610	CLA	C1A-NA	12.18	1.40	1.29
22	4	617	XAT	O24-C25	-10.96	1.30	1.46
22	4	617	XAT	C4-C3	-9.80	1.38	1.52
22	4	617	XAT	C2-C3	-8.85	1.39	1.52

The worst 5 of 2492 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	818	CLA	O2D-CGD-CBD	25.89	157.28	111.27
21	A	818	CLA	O2D-CGD-O1D	-25.26	74.45	123.84
22	4	617	XAT	O24-C25-C24	23.78	131.25	113.38
21	A	818	CLA	O1D-CGD-CBD	-20.36	82.83	124.48
27	A	801	CL0	C1D-ND-C4D	-17.19	94.13	106.33

There are no chirality outliers.

5 of 2087 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	2	605	CHL	C3C-C2C-CMC-OMC
20	2	607	CHL	C1A-C2A-CAA-CBA
20	2	607	CHL	CBD-CGD-O2D-CED
20	3	606	CHL	C2A-CAA-CBA-CGA
20	3	606	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

222 monomers are involved in 693 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	601	CHL	7	0
21	y	612	CLA	1	0
21	A	845	CLA	3	0
21	K	201	CLA	6	0
21	z	613	CLA	3	0
21	1	608	CLA	1	0
21	B	830	CLA	2	0
31	y	618	NEX	4	0
21	3	608	CLA	3	0
21	B	814	CLA	5	0
21	A	824	CLA	2	0
20	2	601	CHL	1	0
31	z	618	NEX	1	0
25	4	618	BCR	6	0
20	2	615	CHL	3	0
21	A	840	CLA	1	0
21	2	608	CLA	3	0
21	A	806	CLA	4	0
28	C	102	SF4	1	0
20	x	608	CHL	1	0
21	B	809	CLA	3	0
21	A	822	CLA	2	0
21	B	840	CLA	2	0
21	1	609	CLA	9	0
25	G	204	BCR	4	0
21	B	836	CLA	2	0
21	4	610	CLA	1	0
21	A	838	CLA	1	0
21	J	101	CLA	1	0
24	1	616	LUT	3	0
21	3	605	CLA	1	0
21	4	609	CLA	6	0
21	G	201	CLA	2	0
21	1	611	CLA	1	0
21	x	613	CLA	2	0
25	B	847	BCR	2	0
20	3	606	CHL	2	0
21	B	824	CLA	8	0
21	H	201	CLA	4	0
21	2	609	CLA	10	0
25	A	853	BCR	9	0
25	O	204	BCR	2	0
21	B	831	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	806	CLA	4	0
25	I	101	BCR	1	0
21	B	828	CLA	8	0
31	x	618	NEX	3	0
24	y	616	LUT	5	0
21	3	601	CLA	4	0
21	A	823	CLA	3	0
25	A	851	BCR	6	0
21	A	811	CLA	3	0
21	A	829	CLA	8	0
21	y	611	CLA	3	0
20	z	606	CHL	1	0
23	B	852	LHG	2	0
21	A	818	CLA	6	0
21	A	839	CLA	1	0
25	B	848	BCR	2	0
21	A	841	CLA	4	0
21	B	818	CLA	4	0
20	y	608	CHL	6	0
21	1	605	CLA	3	0
21	B	813	CLA	5	0
21	y	614	CLA	5	0
21	B	827	CLA	3	0
20	x	605	CHL	3	0
21	z	614	CLA	6	0
21	3	609	CLA	5	0
20	y	609	CHL	6	0
21	K	204	CLA	4	0
25	B	846	BCR	6	0
21	3	610	CLA	1	0
21	1	607	CLA	2	0
25	B	844	BCR	6	0
21	A	835	CLA	4	0
21	B	825	CLA	3	0
21	x	604	CLA	2	0
20	4	607	CHL	1	0
22	2	617	XAT	4	0
20	2	605	CHL	5	0
21	4	602	CLA	2	0
21	F	302	CLA	7	0
24	z	615	LUT	2	0
21	A	830	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	x	610	CLA	5	0
24	x	616	LUT	2	0
21	K	206	CLA	5	0
21	x	614	CLA	1	0
21	1	602	CLA	4	0
28	A	854	SF4	2	0
20	x	606	CHL	2	0
21	B	833	CLA	1	0
21	B	821	CLA	1	0
20	x	609	CHL	4	0
21	B	817	CLA	2	0
23	x	619	LHG	3	0
21	4	608	CLA	2	0
21	A	814	CLA	1	0
21	B	832	CLA	5	0
24	3	613	LUT	8	0
21	y	610	CLA	16	0
24	x	615	LUT	1	0
21	2	604	CLA	8	0
21	B	822	CLA	7	0
21	A	804	CLA	8	0
30	B	850	DGD	5	0
24	y	615	LUT	2	0
21	A	833	CLA	2	0
21	A	844	CLA	3	0
21	B	808	CLA	4	0
21	B	837	CLA	2	0
24	4	616	LUT	2	0
25	J	102	BCR	5	0
21	4	601	CLA	2	0
24	z	616	LUT	8	0
25	L	305	BCR	7	0
25	A	849	BCR	2	0
25	L	306	BCR	5	0
21	A	828	CLA	2	0
24	2	616	LUT	5	0
25	A	850	BCR	5	0
21	B	803	CLA	5	0
21	y	604	CLA	2	0
21	A	831	CLA	3	0
21	F	301	CLA	2	0
21	B	819	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	802	CLA	10	0
21	z	602	CLA	3	0
23	A	847	LHG	1	0
21	A	825	CLA	2	0
21	B	826	CLA	2	0
20	y	605	CHL	1	0
21	A	802	CLA	6	0
21	z	610	CLA	1	0
25	B	801	BCR	9	0
21	A	826	CLA	3	0
21	A	810	CLA	1	0
21	A	808	CLA	1	0
21	A	827	CLA	1	0
21	A	815	CLA	1	0
20	z	607	CHL	2	0
21	2	611	CLA	1	0
21	2	613	CLA	2	0
21	1	604	CLA	3	0
21	x	602	CLA	1	0
25	L	301	BCR	3	0
21	B	811	CLA	2	0
20	2	606	CHL	1	0
21	3	602	CLA	1	0
28	C	101	SF4	2	0
25	K	205	BCR	5	0
20	z	609	CHL	3	0
21	B	841	CLA	1	0
23	z	619	LHG	6	0
21	2	602	CLA	8	0
23	A	846	LHG	7	0
21	2	612	CLA	3	0
22	y	617	XAT	9	0
20	x	607	CHL	8	0
25	B	849	BCR	7	0
20	4	615	CHL	2	0
21	L	303	CLA	3	0
21	A	843	CLA	2	0
21	B	820	CLA	1	0
20	z	601	CHL	10	0
21	y	602	CLA	6	0
29	A	855	PQN	2	0
20	z	608	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	807	CLA	2	0
21	4	613	CLA	2	0
21	4	603	CLA	1	0
21	y	603	CLA	3	0
25	3	614	BCR	5	0
22	1	614	XAT	12	0
20	x	601	CHL	12	0
21	B	834	CLA	2	0
21	B	805	CLA	7	0
20	4	605	CHL	2	0
21	3	607	CLA	5	0
21	A	813	CLA	2	0
25	A	848	BCR	3	0
21	A	819	CLA	3	0
25	K	202	BCR	5	0
21	3	603	CLA	2	0
21	A	809	CLA	5	0
21	3	612	CLA	2	0
21	z	604	CLA	2	0
20	y	607	CHL	4	0
21	B	838	CLA	2	0
23	1	615	LHG	12	0
21	2	603	CLA	1	0
21	O	201	CLA	1	0
22	z	617	XAT	5	0
21	x	603	CLA	1	0
21	A	803	CLA	8	0
27	A	801	CL0	14	0
29	B	842	PQN	2	0
21	A	805	CLA	1	0
21	B	823	CLA	2	0
20	z	605	CHL	2	0
20	y	601	CHL	10	0
22	4	617	XAT	6	0
21	A	842	CLA	6	0
21	A	821	CLA	1	0
21	A	812	CLA	6	0
24	2	619	LUT	6	0
23	B	851	LHG	3	0
25	F	304	BCR	2	0
21	B	839	CLA	1	0
20	y	606	CHL	2	0

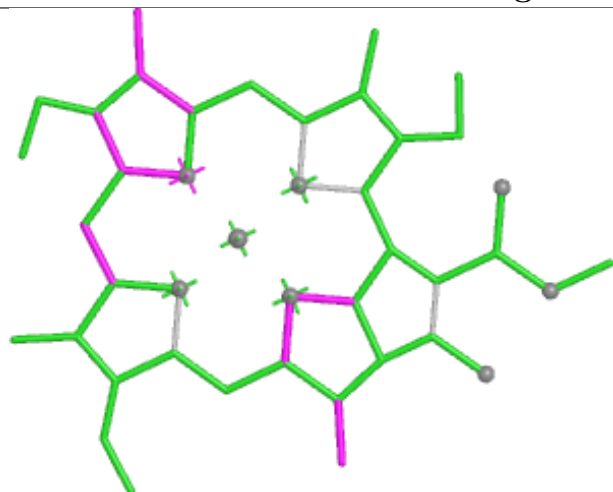
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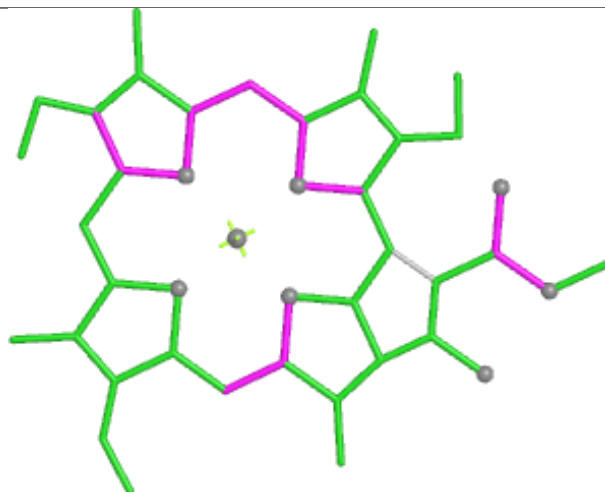
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2	618	LHG	2	0
21	4	614	CLA	1	0
21	B	816	CLA	1	0
21	4	612	CLA	1	0
25	B	843	BCR	6	0
21	L	302	CLA	4	0
23	y	619	LHG	5	0
25	A	852	BCR	2	0
25	B	845	BCR	9	0
22	x	617	XAT	4	0
21	A	820	CLA	6	0

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

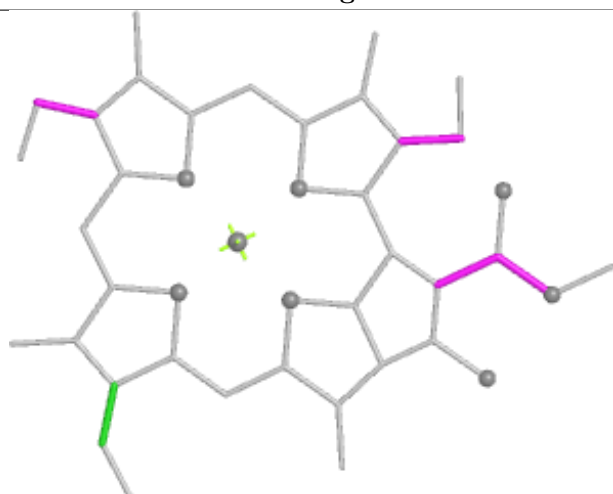
Ligand CLA B 835



Bond lengths



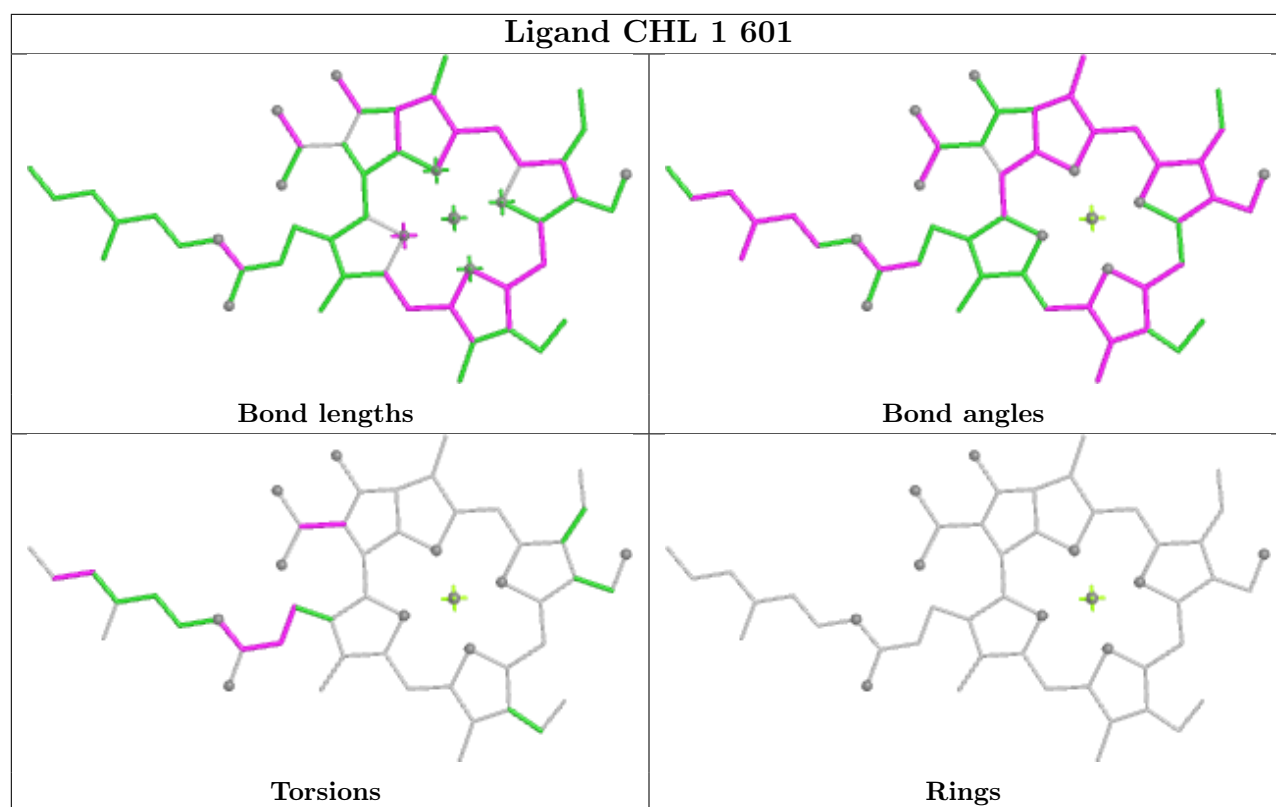
Bond angles



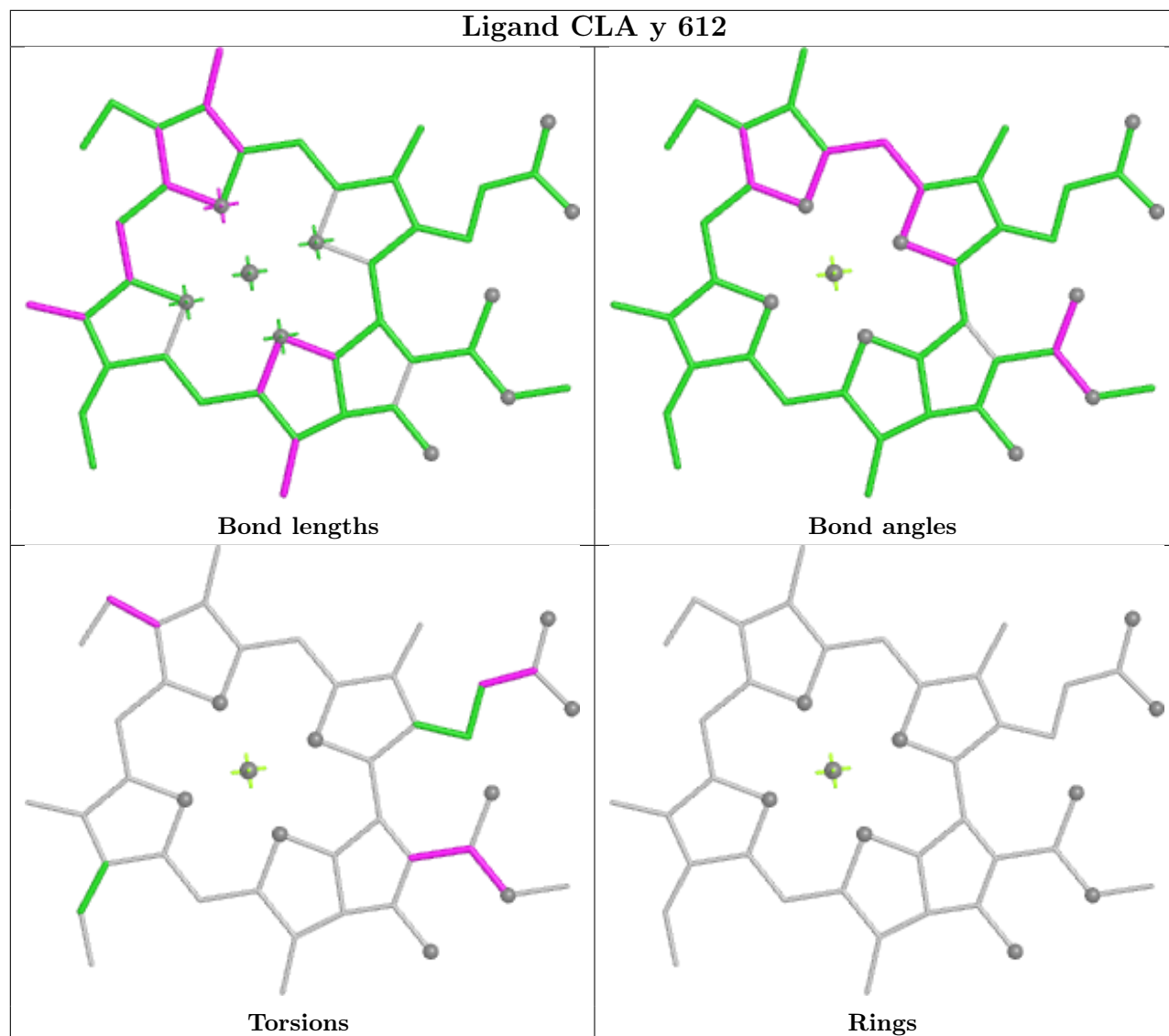
Torsions



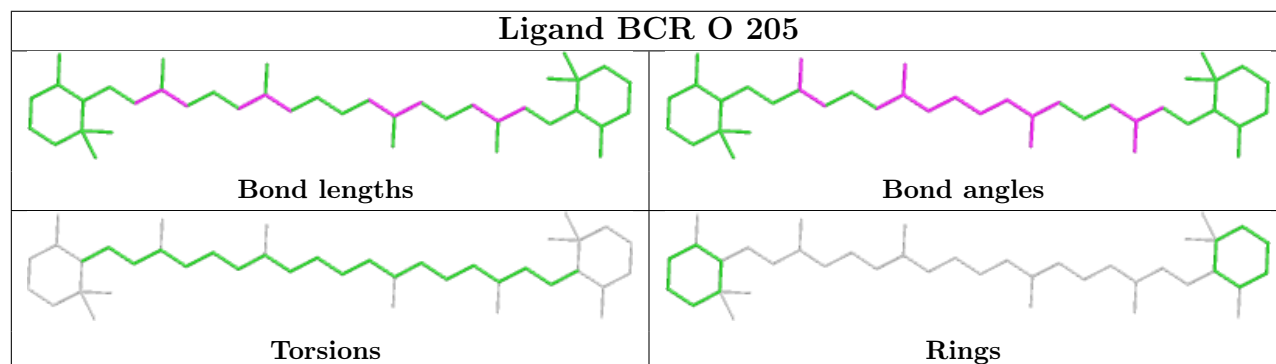
Rings

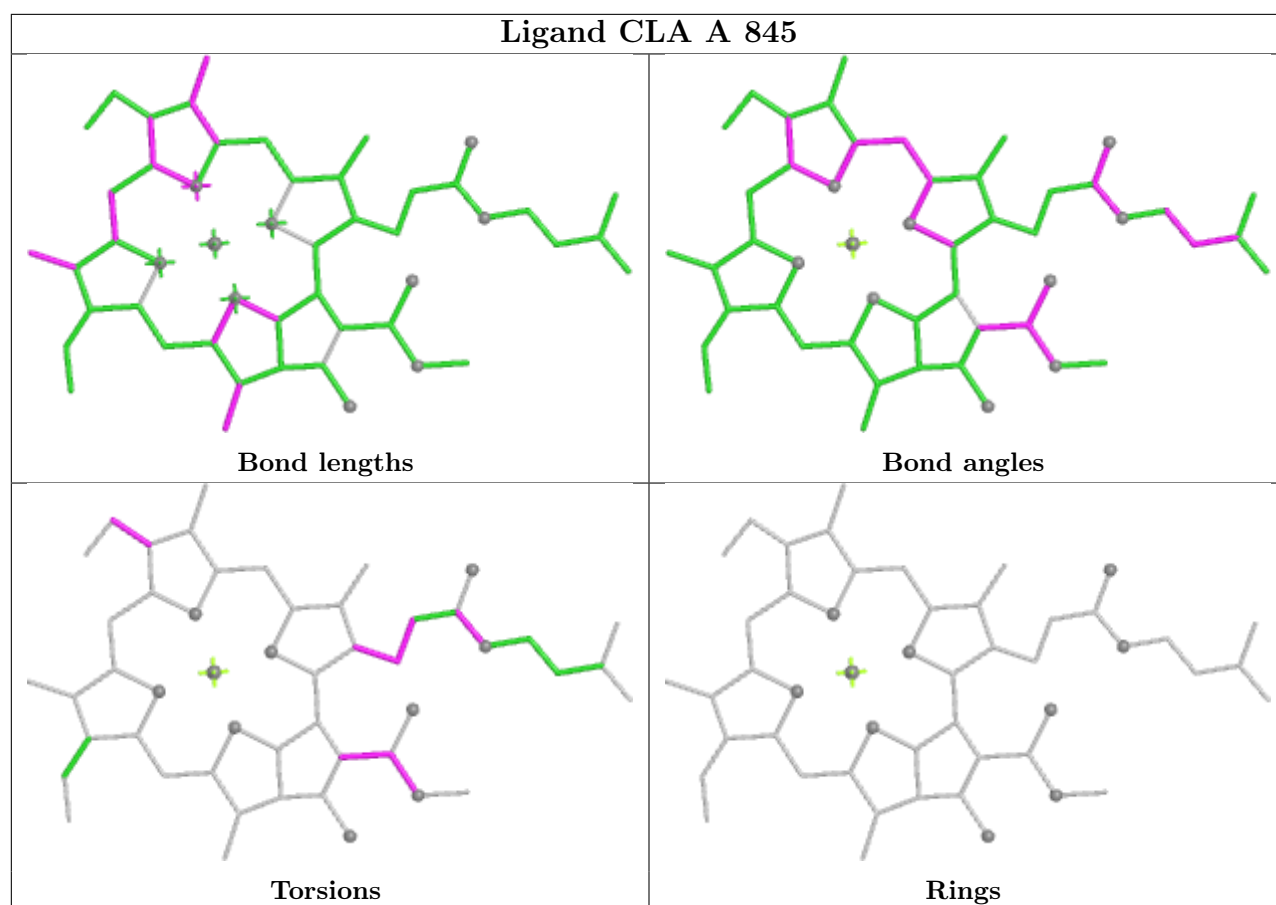


Ligand CLA y 612

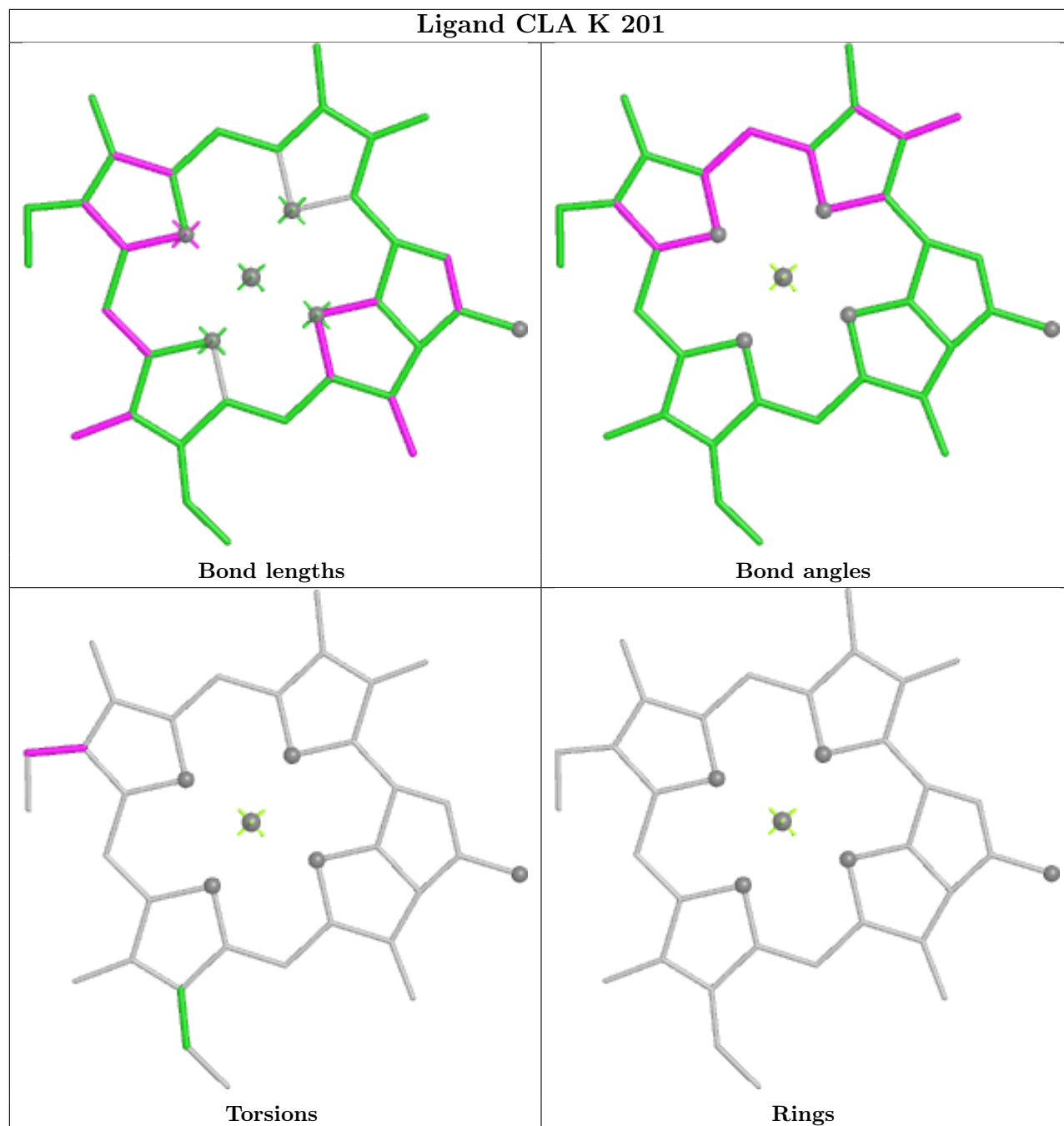


Ligand BCR O 205

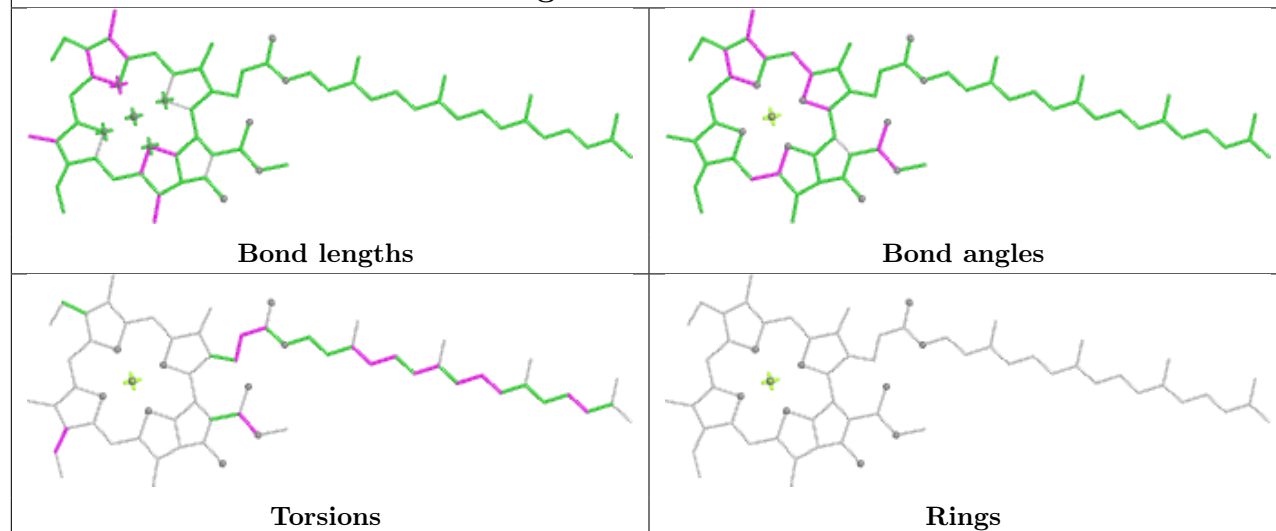




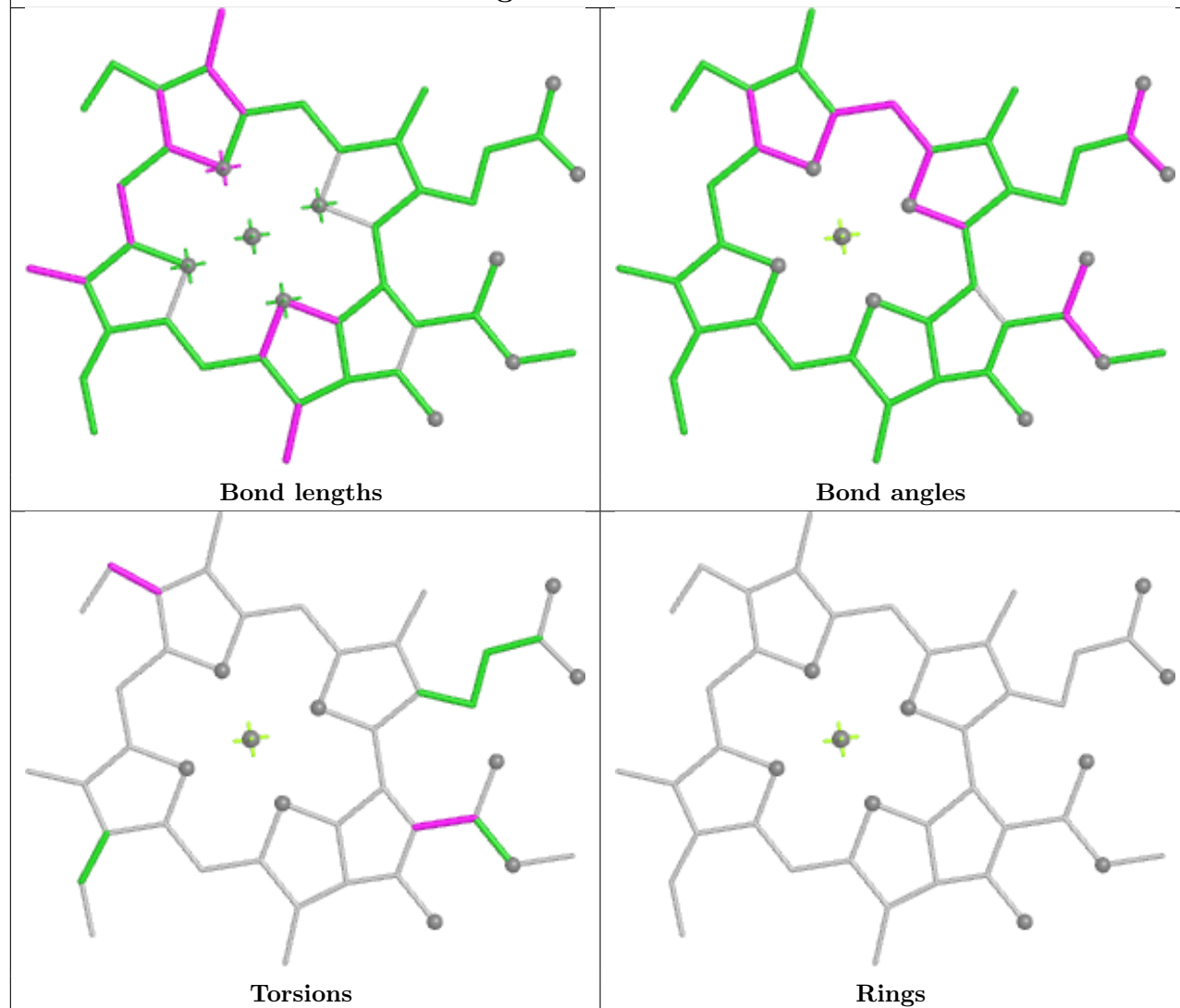
Ligand CLA K 201



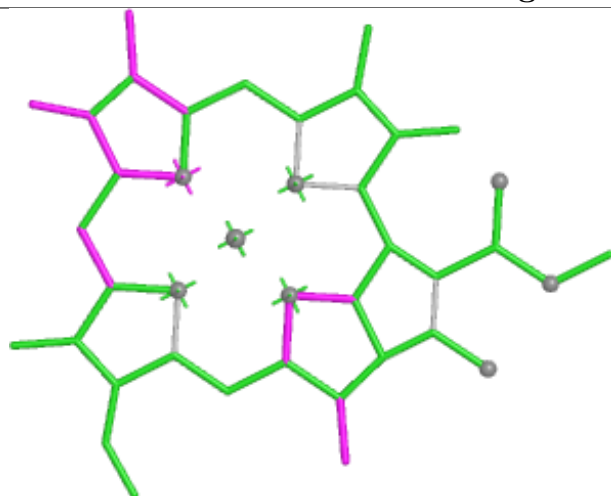
Ligand CLA z 613



Ligand CLA z 612



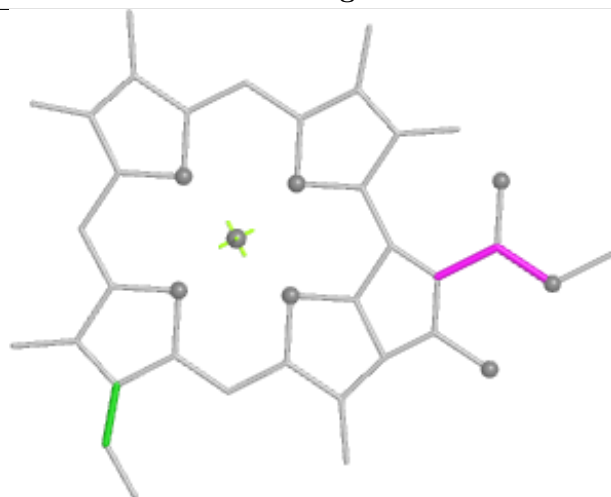
Ligand CLA 1 608



Bond lengths



Bond angles

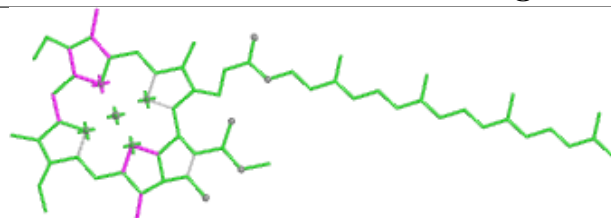


Torsions

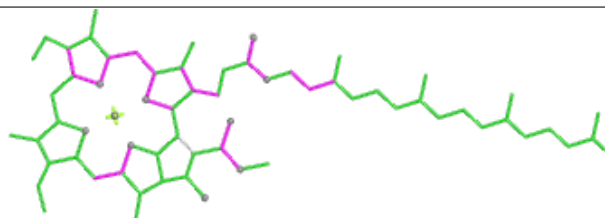


Rings

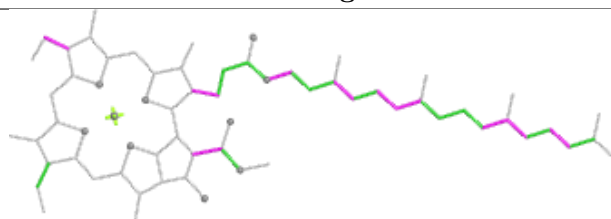
Ligand CLA B 810



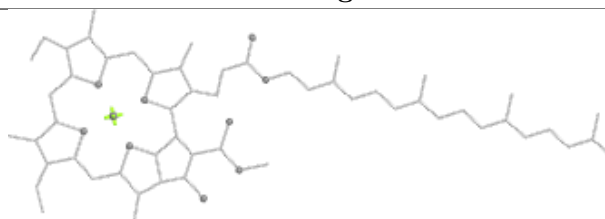
Bond lengths



Bond angles

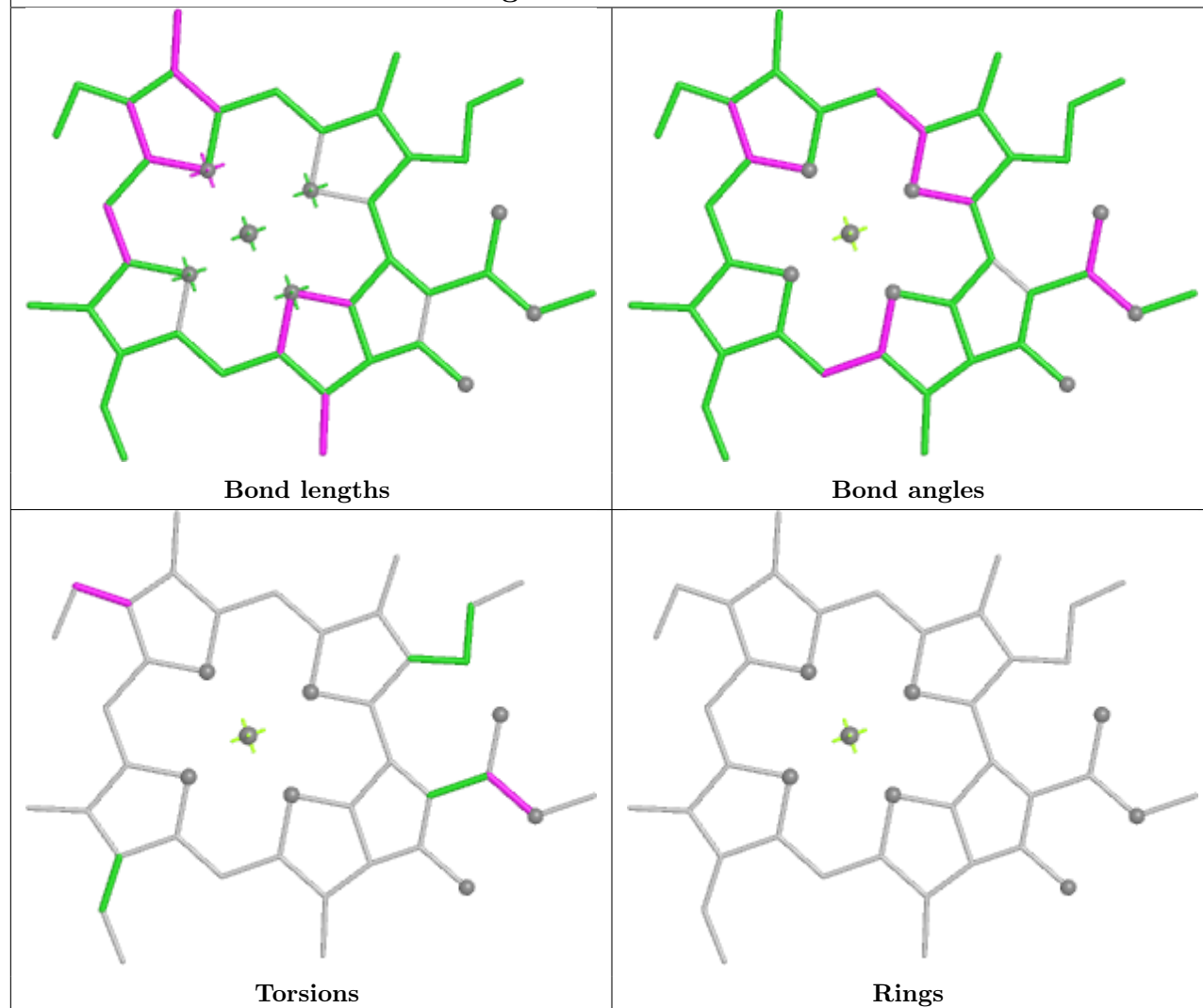


Torsions

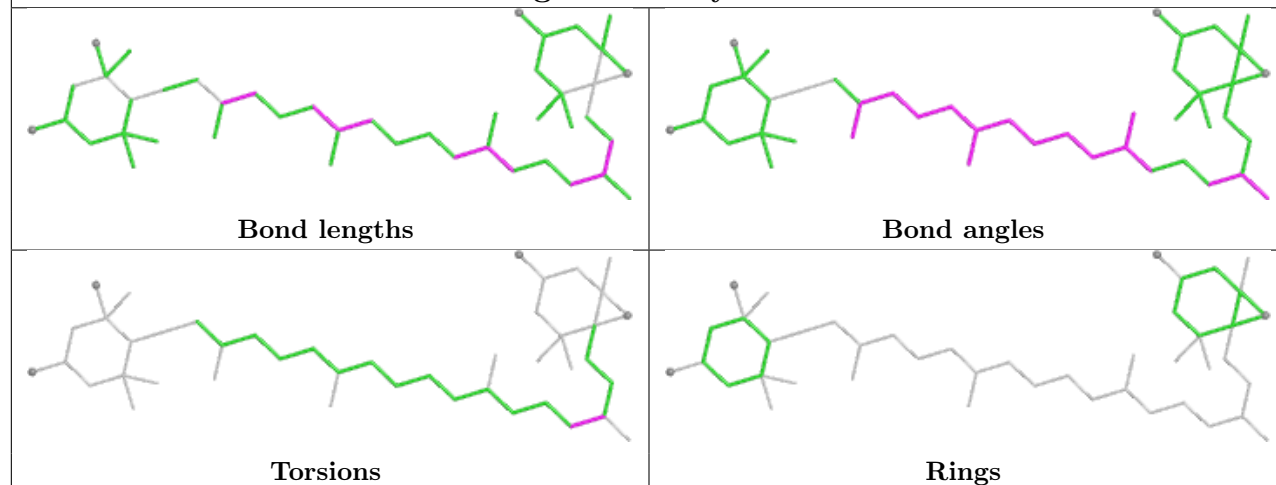


Rings

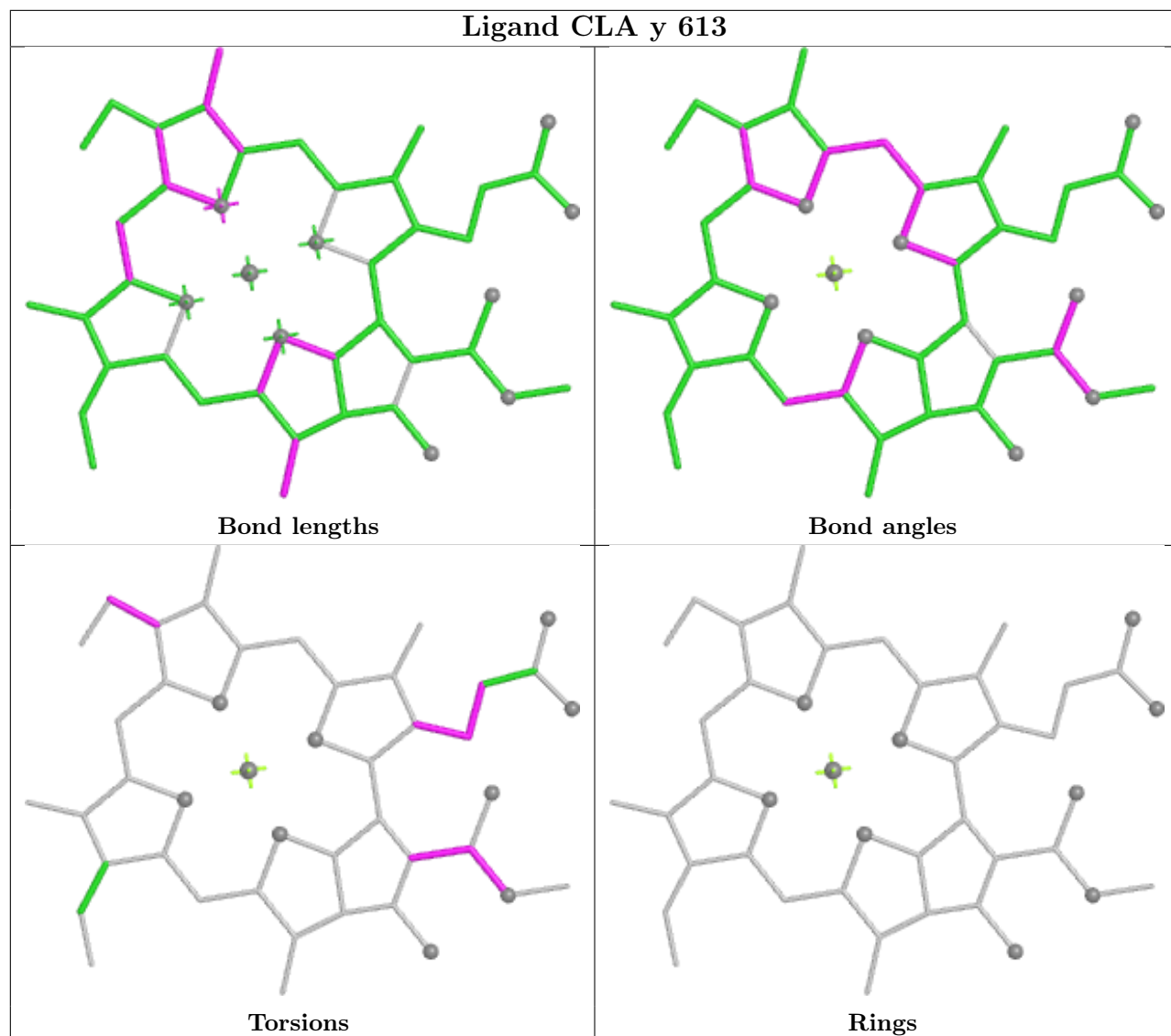
Ligand CLA B 830

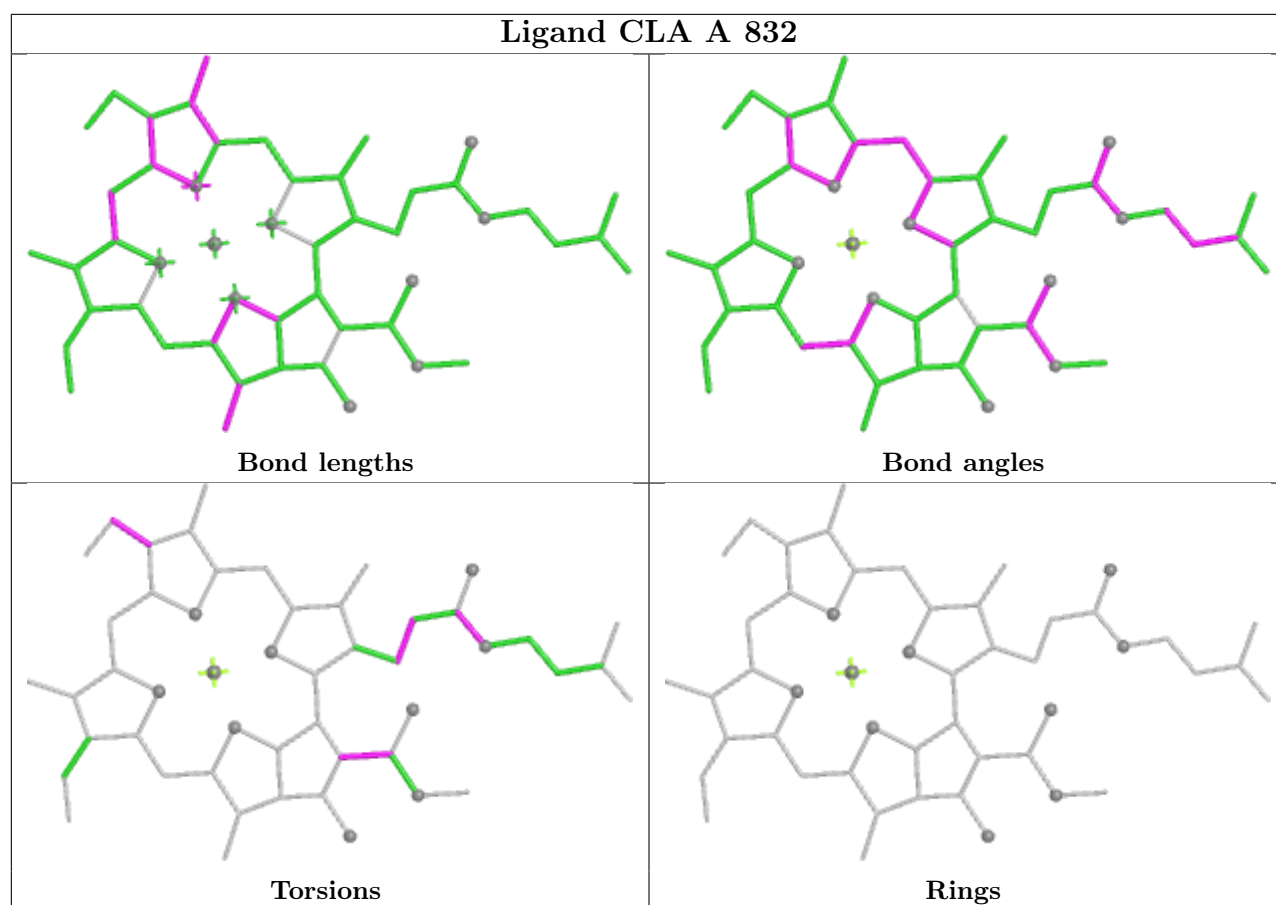


Ligand NEX y 618

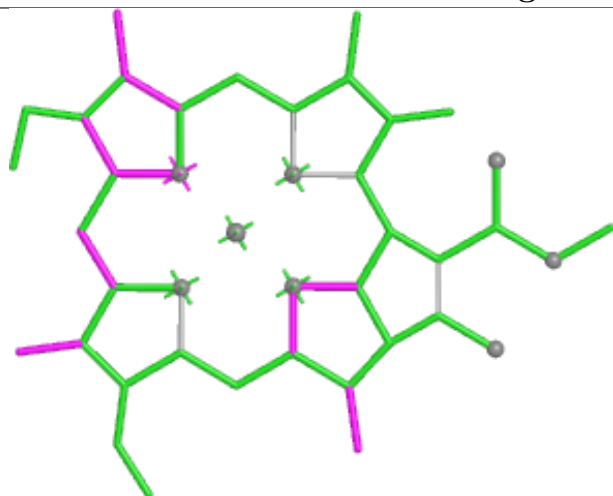


Ligand CLA y 613

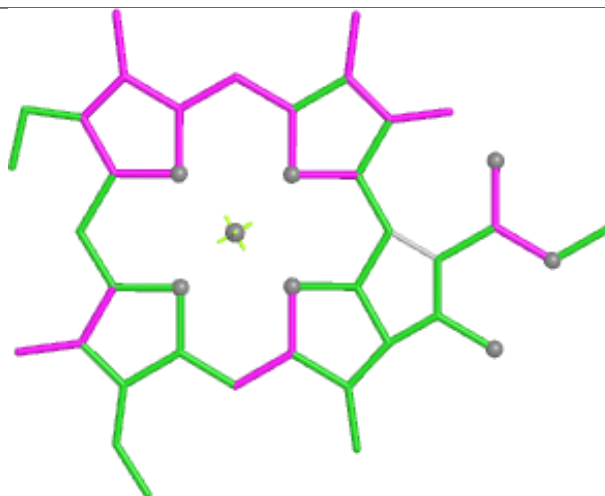




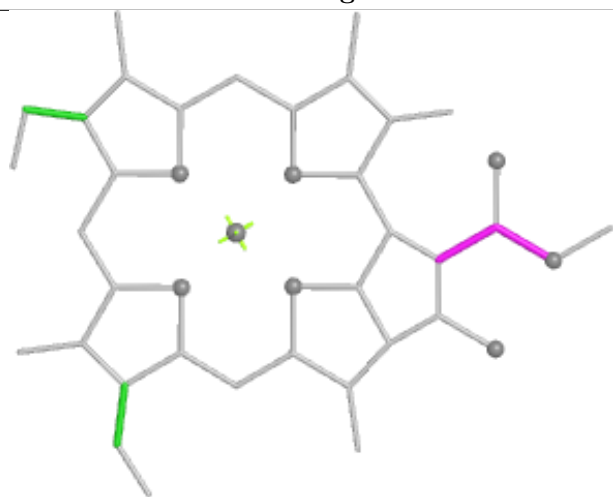
Ligand CLA 3 608



Bond lengths



Bond angles

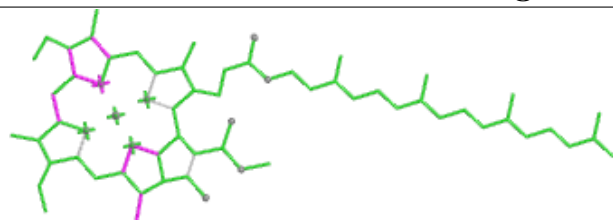


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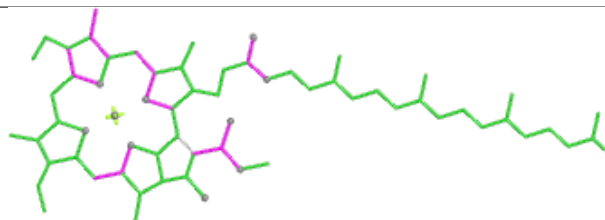


Rings

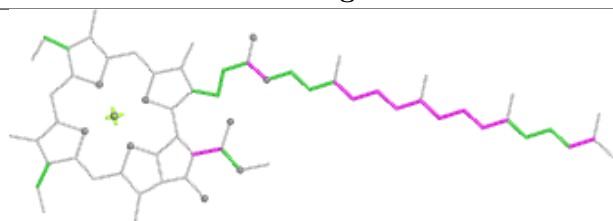
Ligand CLA B 814



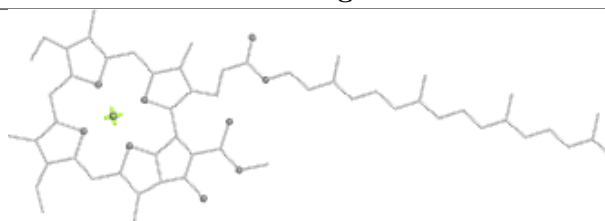
Bond lengths



Bond angles

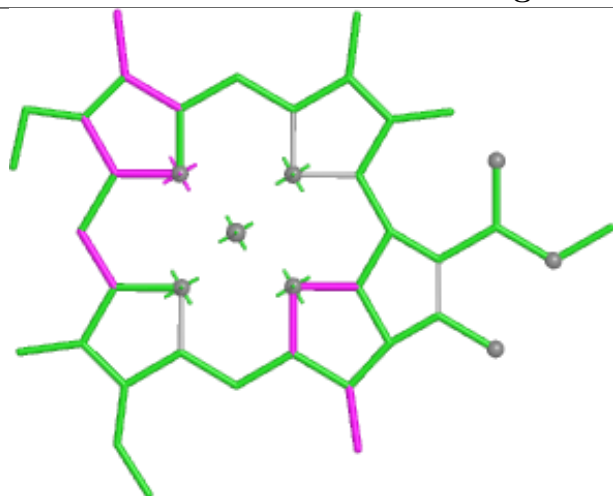


Torsions

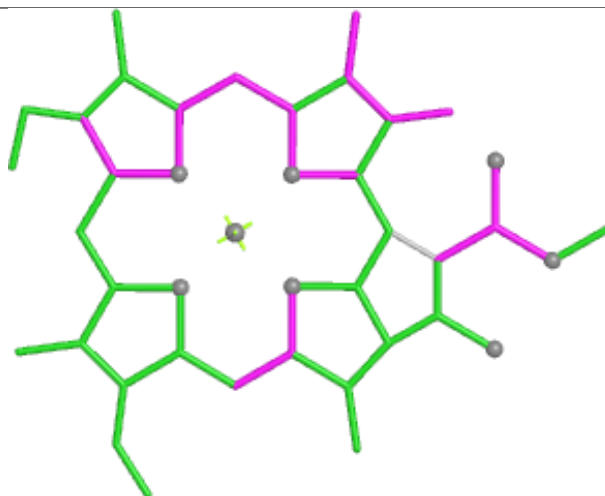


Rings

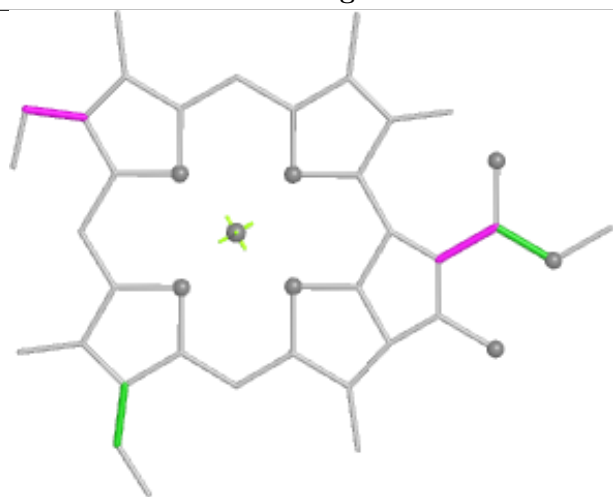
Ligand CLA A 824



Bond lengths



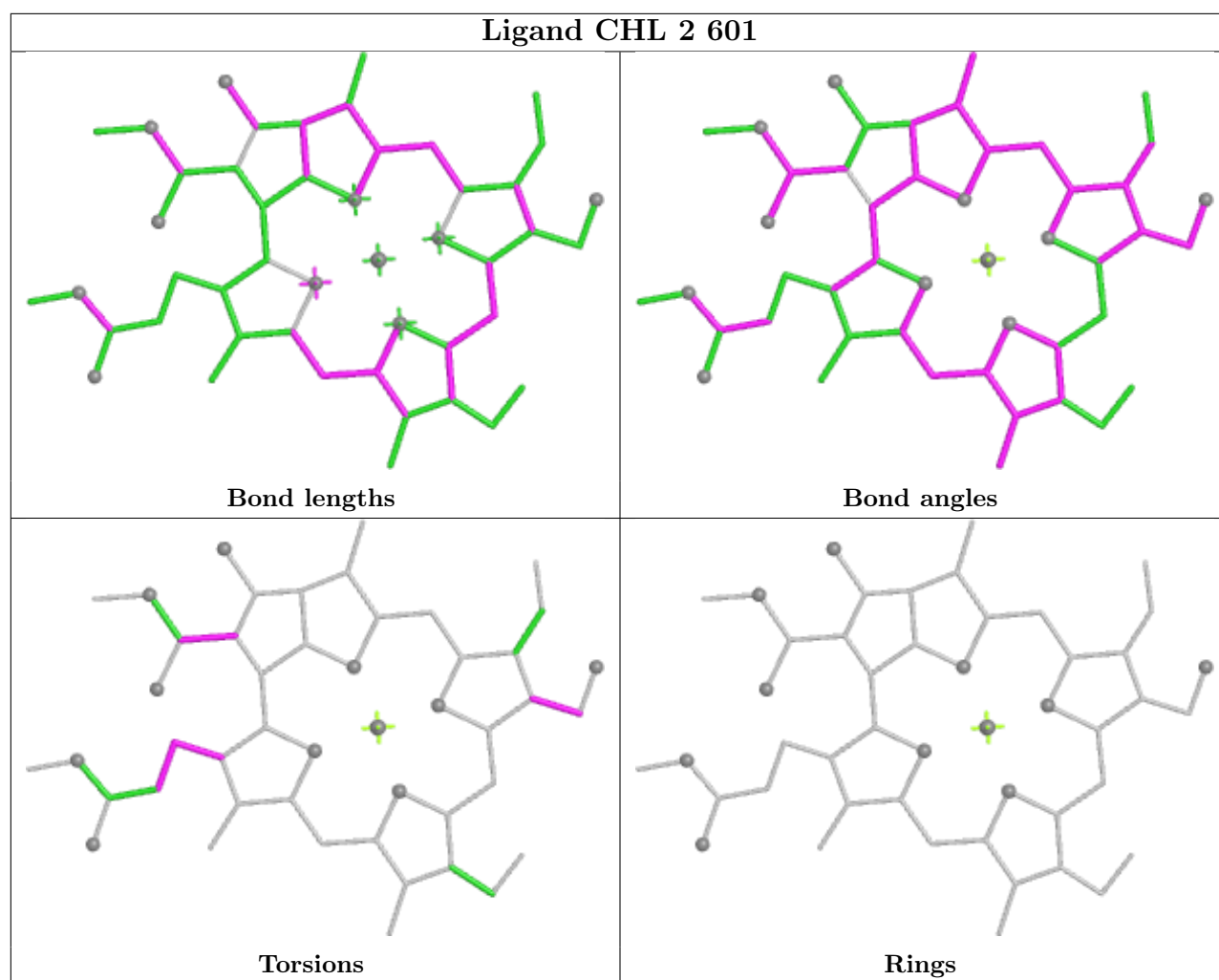
Bond angles

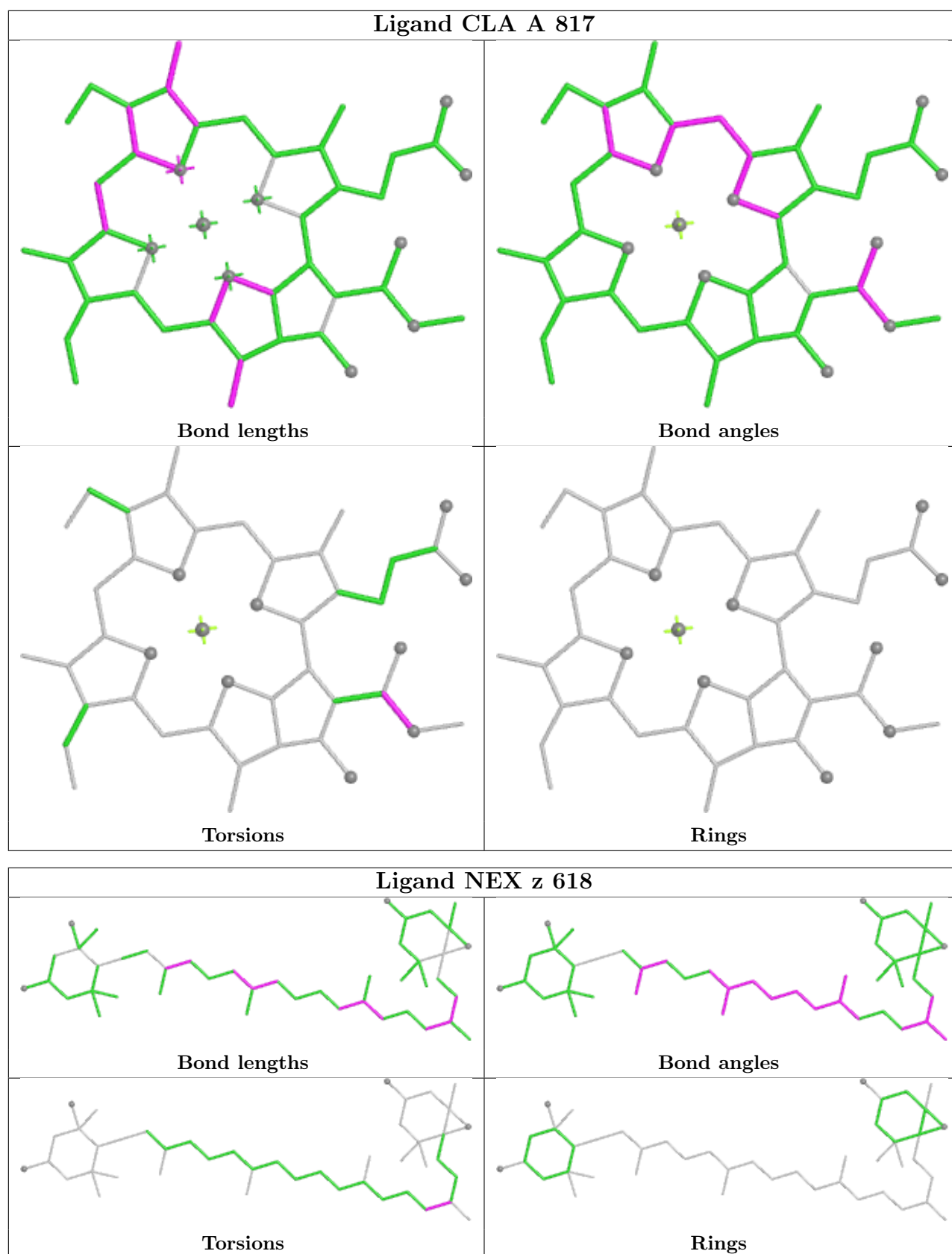


Torsions

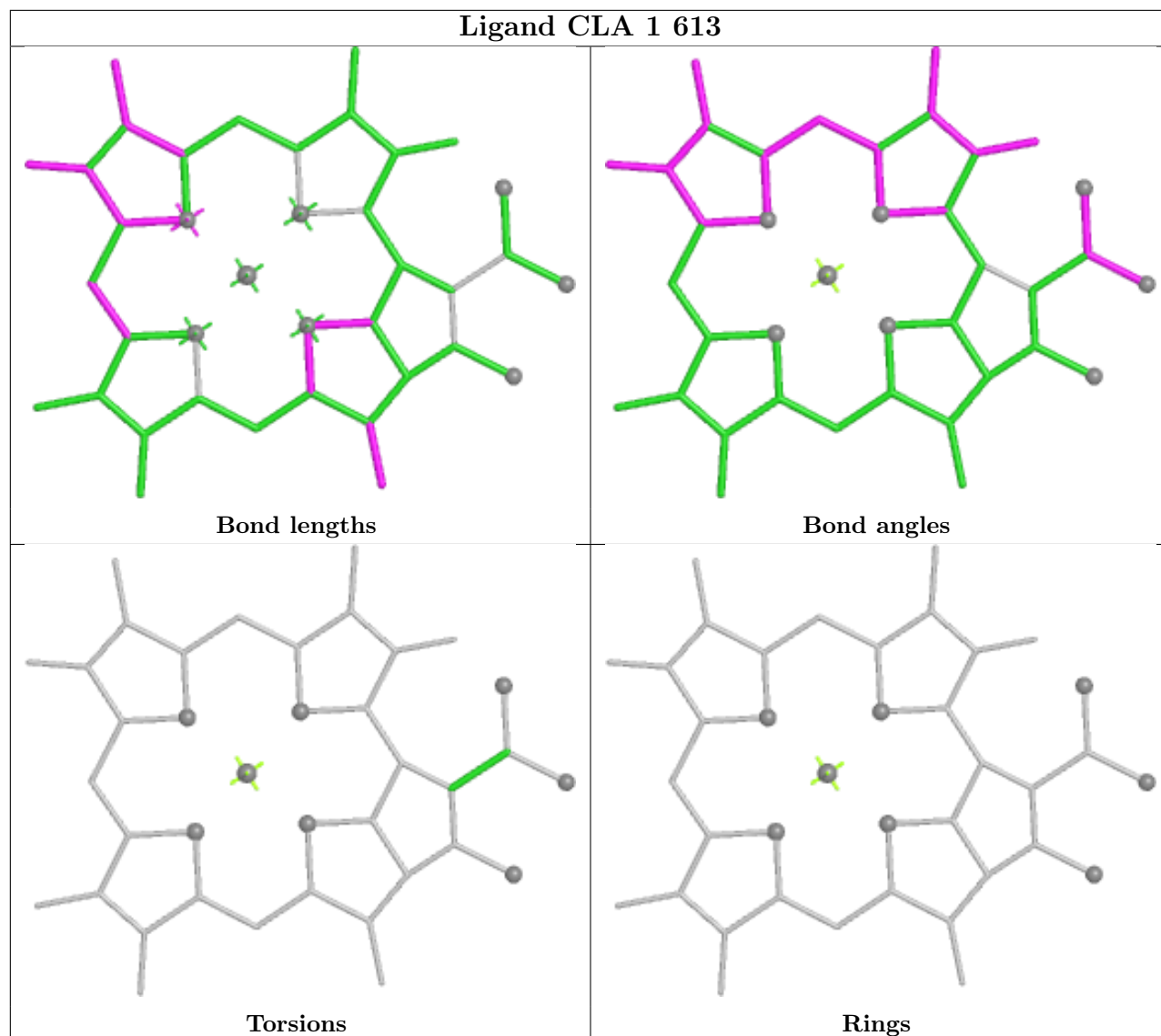


Rings

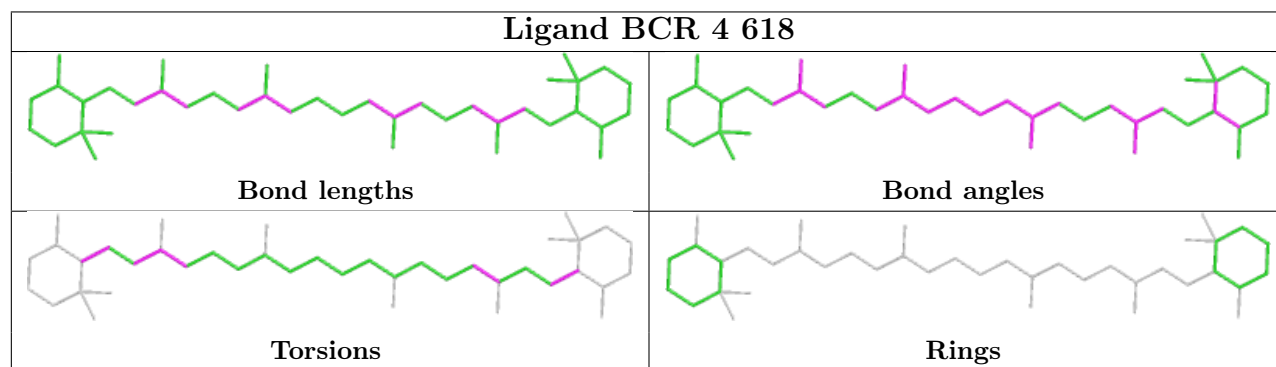




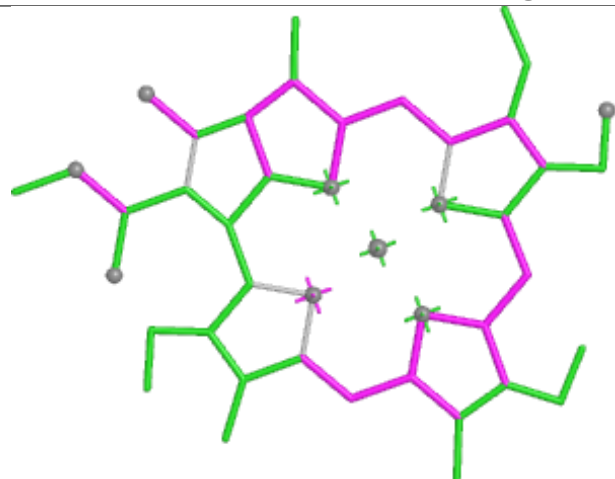
Ligand CLA 1 613



Ligand BCR 4 618



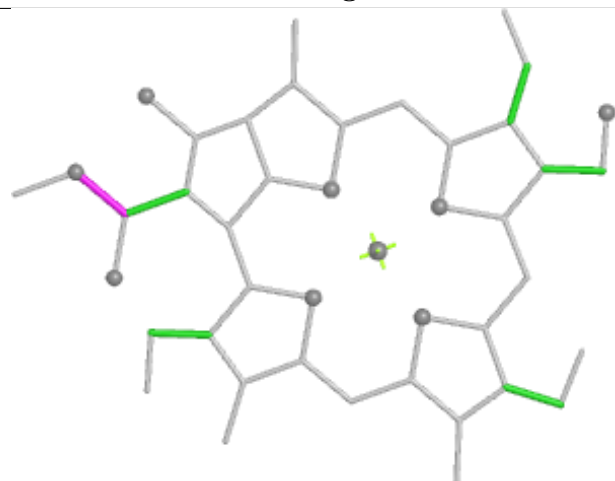
Ligand CHL 2 615



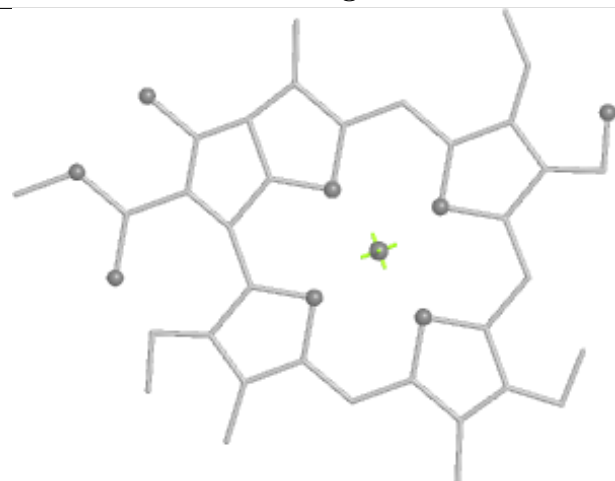
Bond lengths



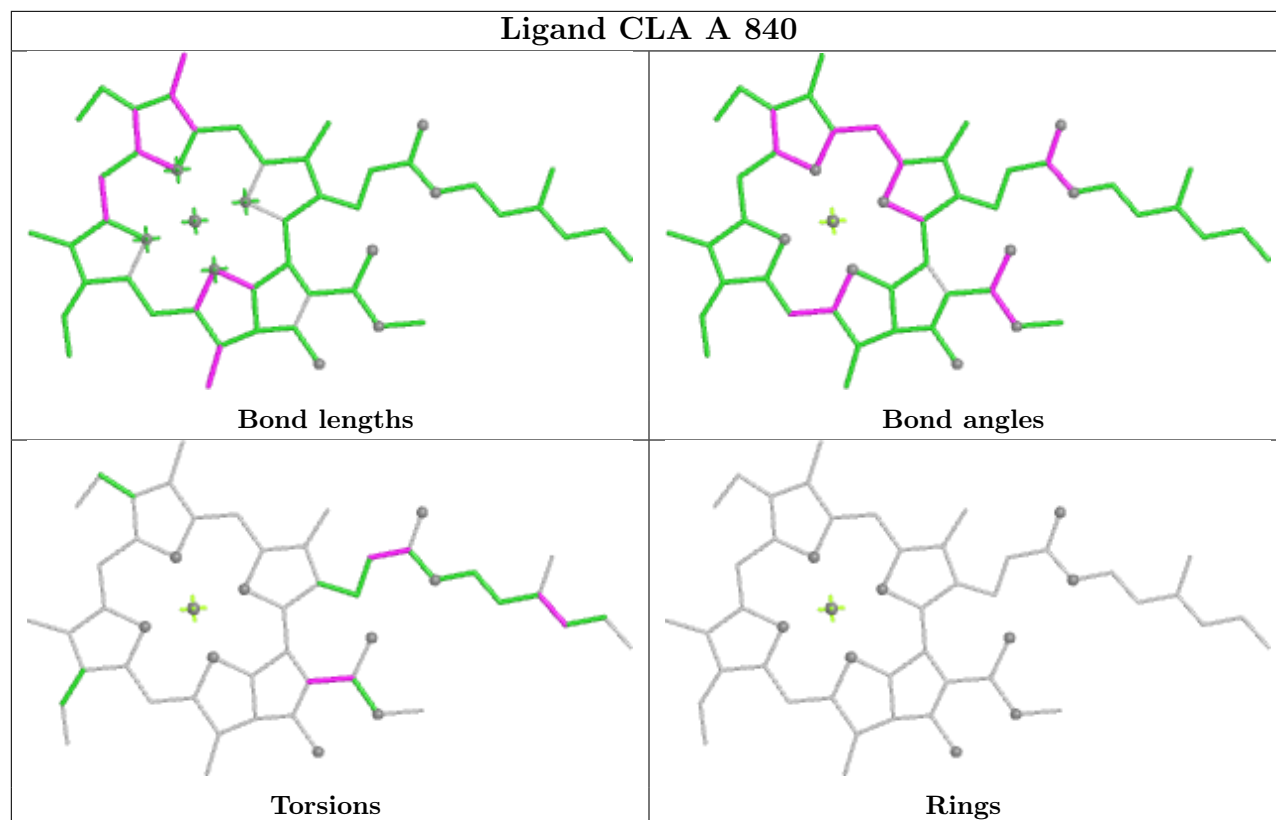
Bond angles



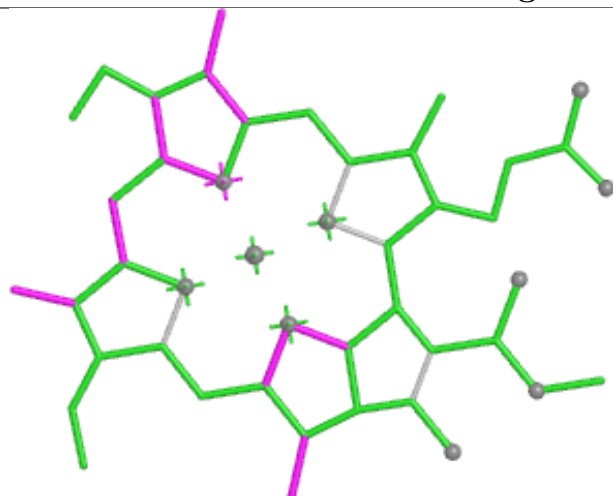
Torsions



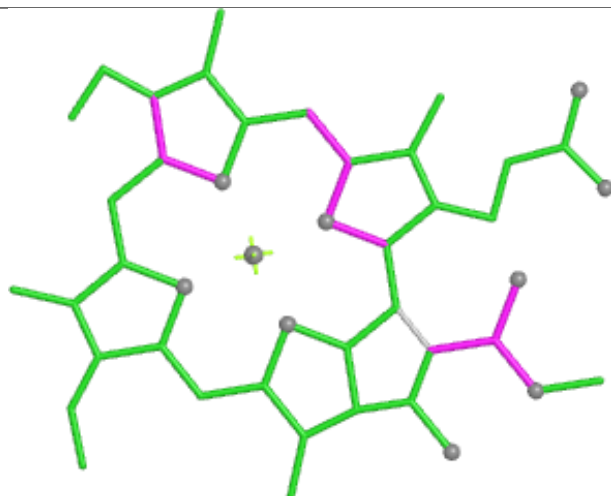
Rings



Ligand CLA 2 608



Bond lengths



Bond angles

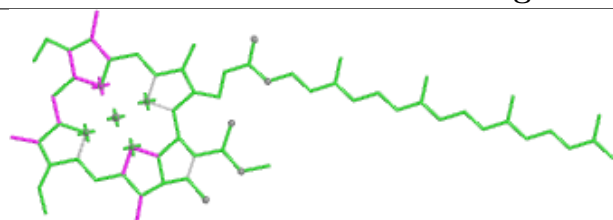


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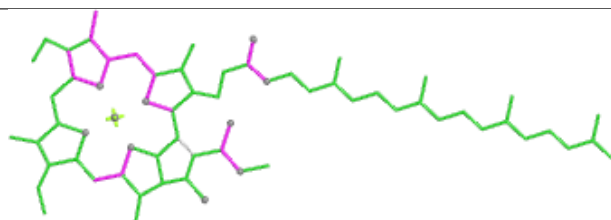


Rings

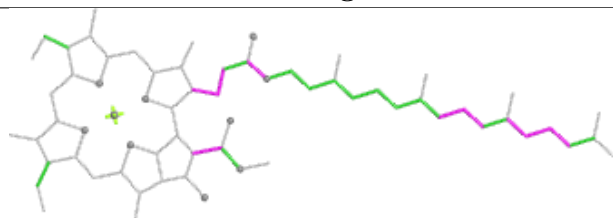
Ligand CLA A 806



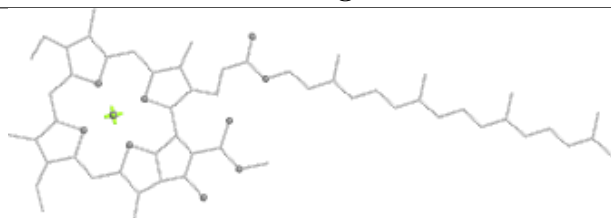
Bond lengths



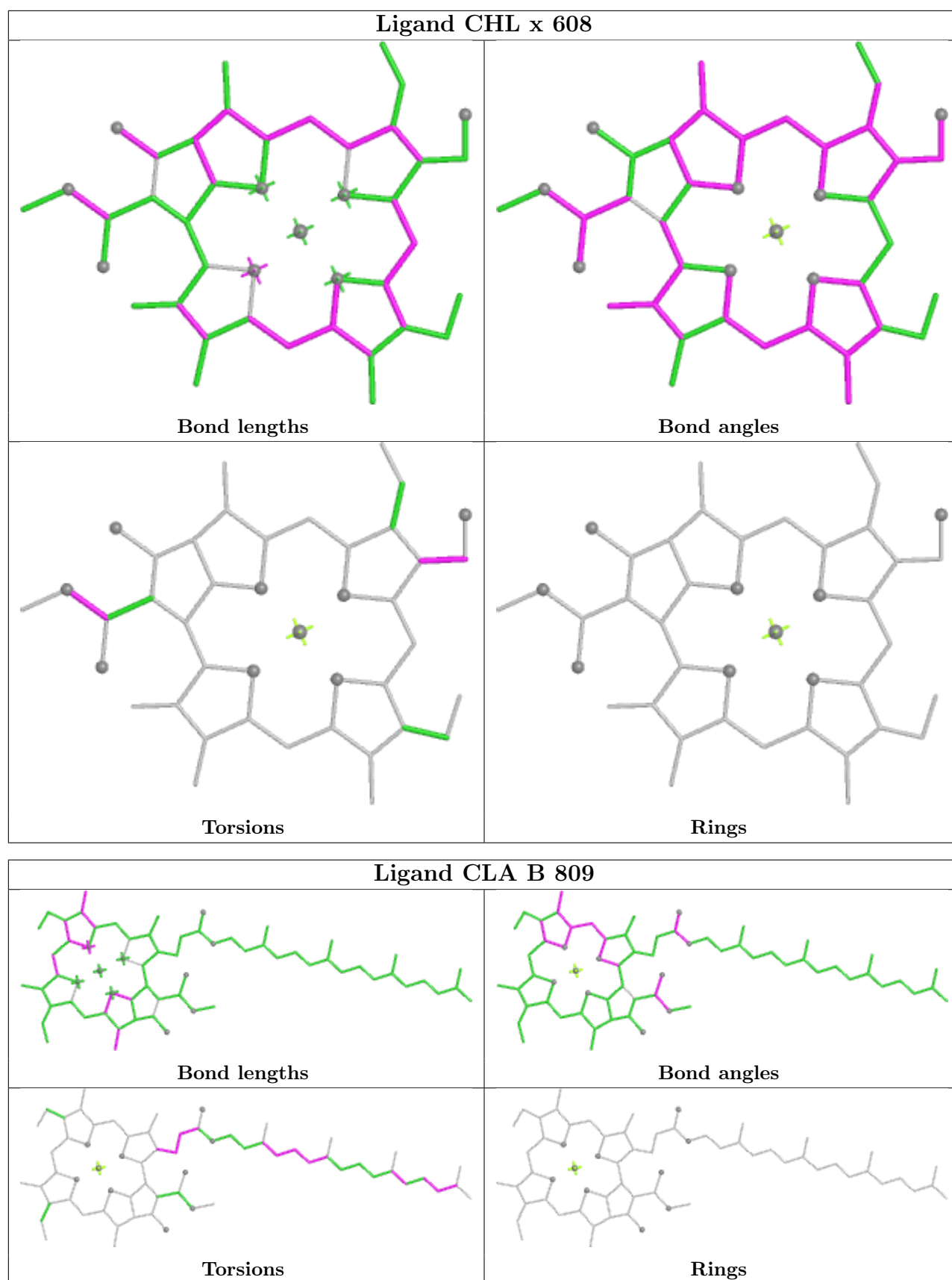
Bond angles

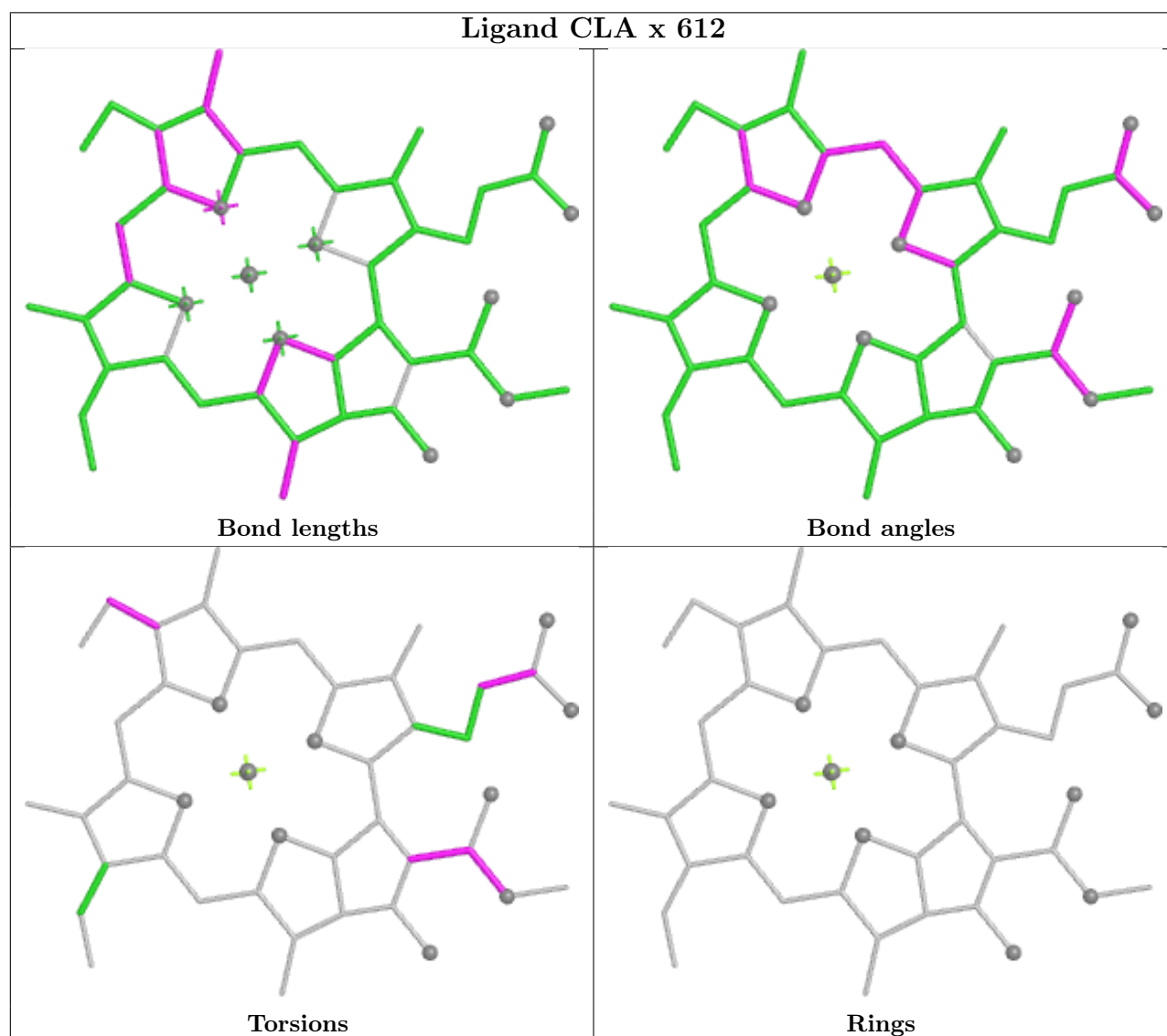
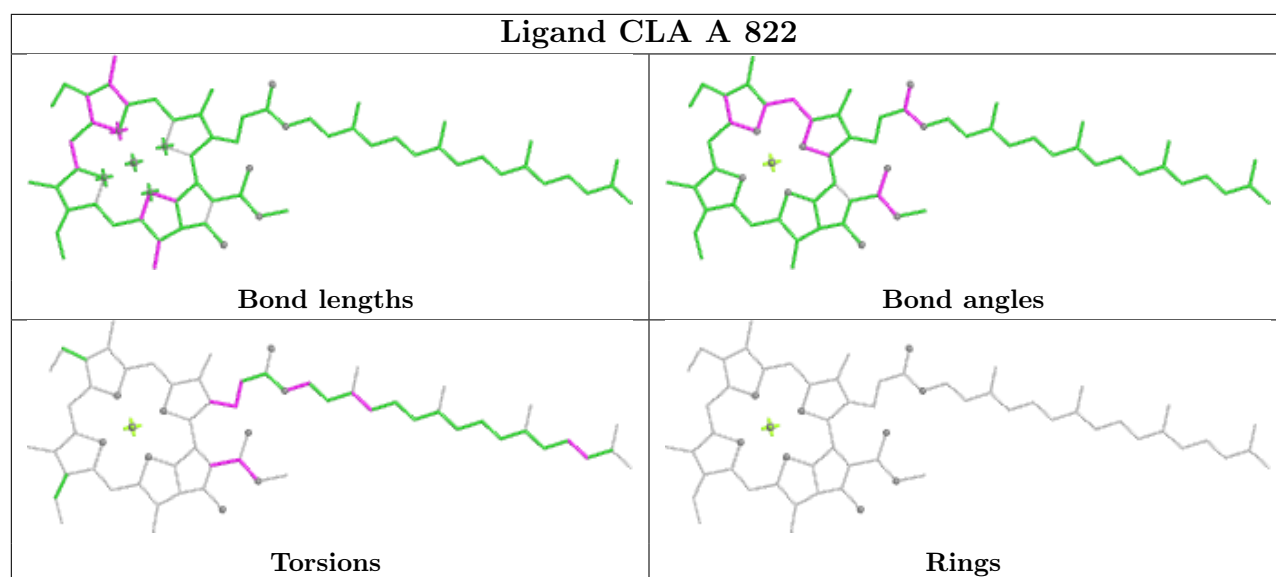


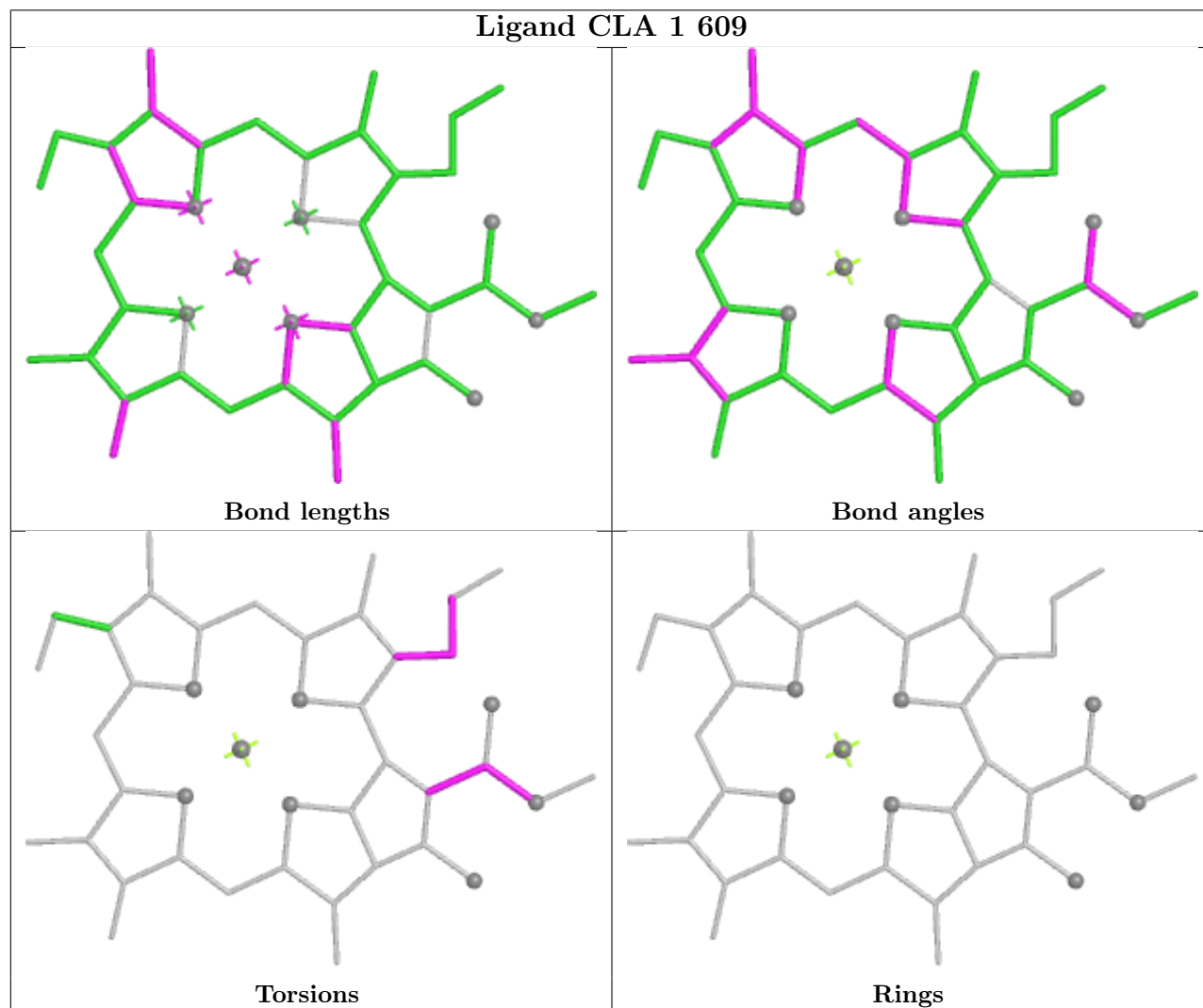
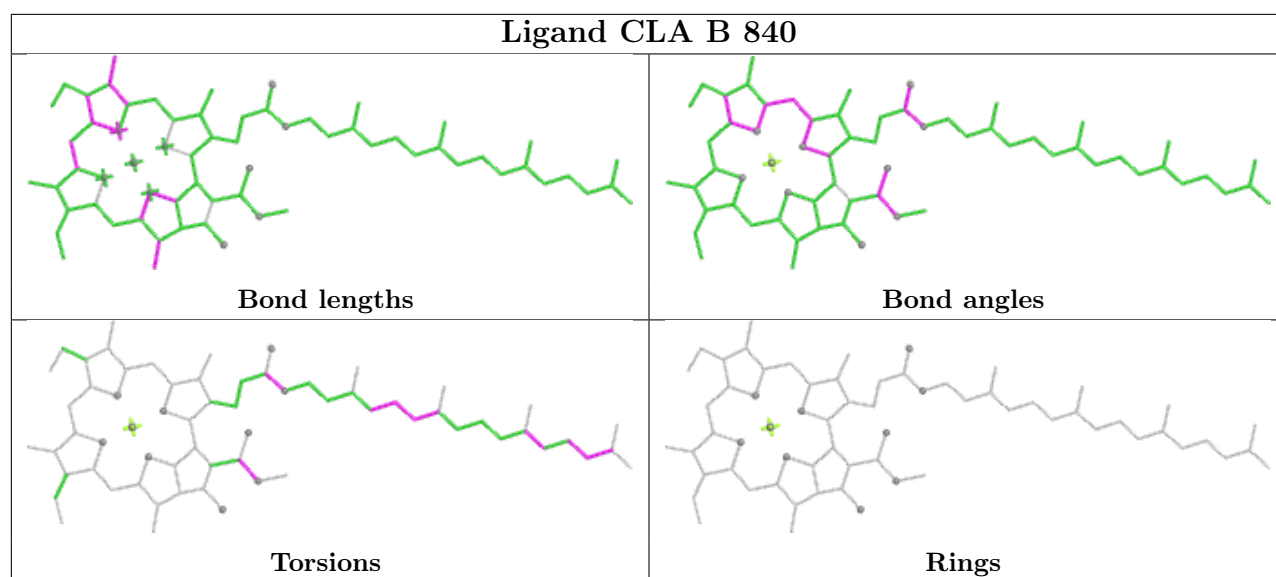
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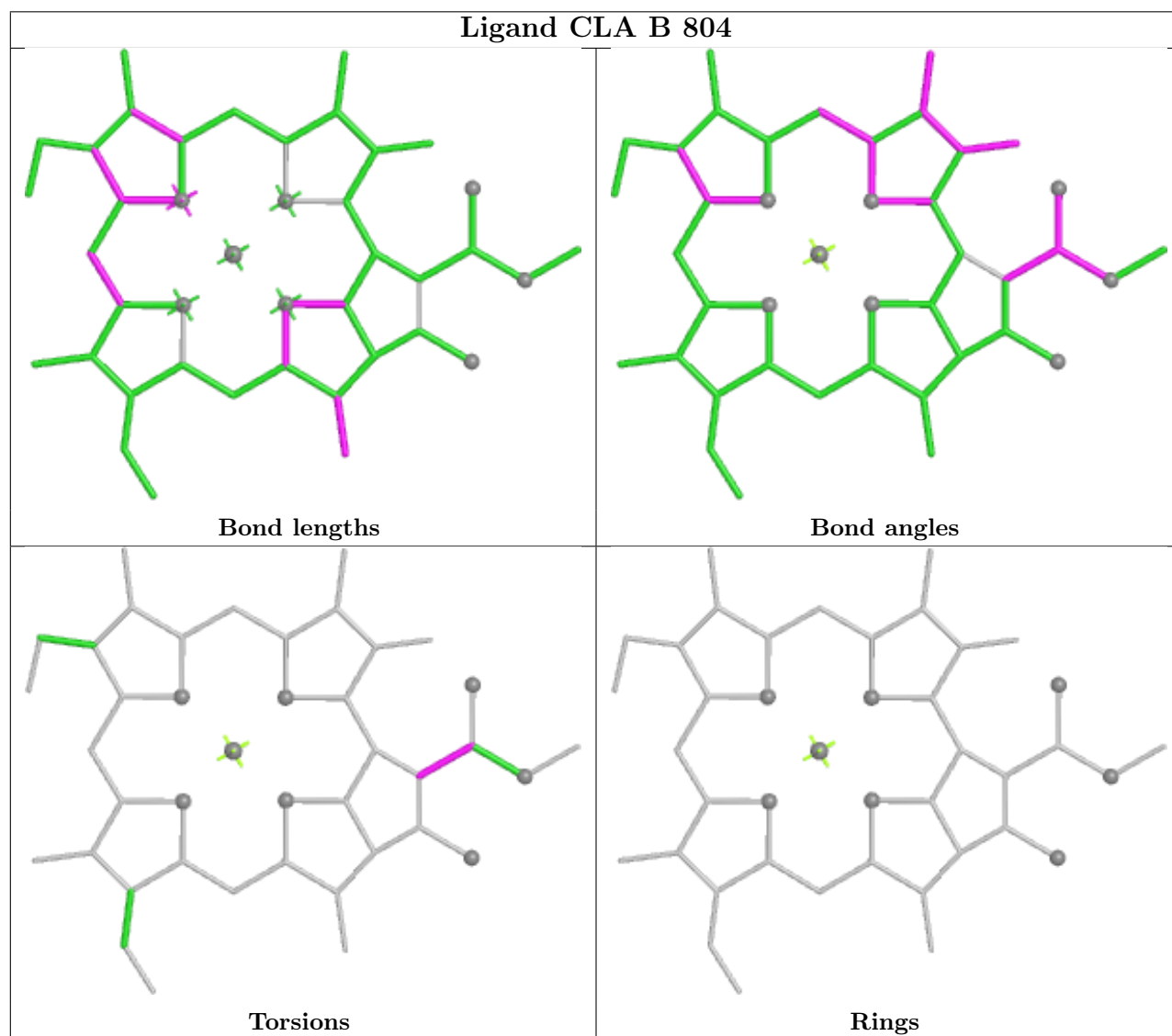
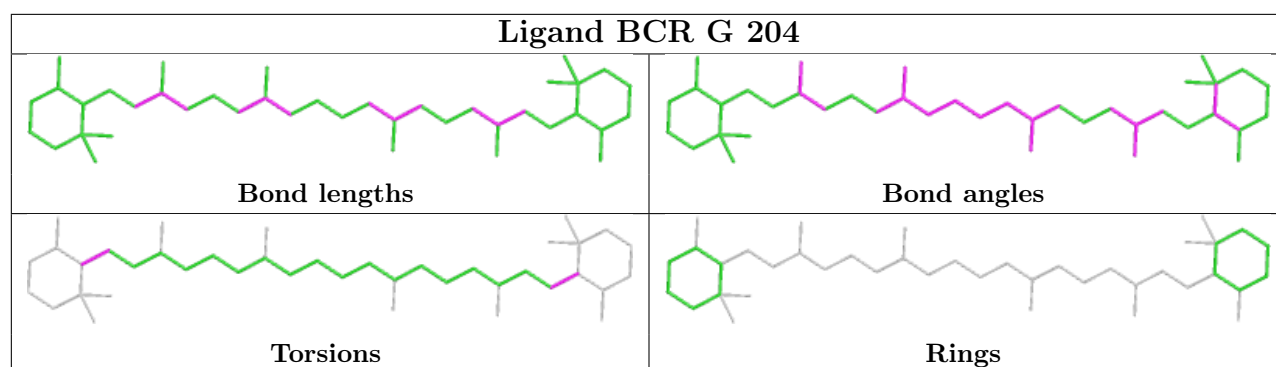


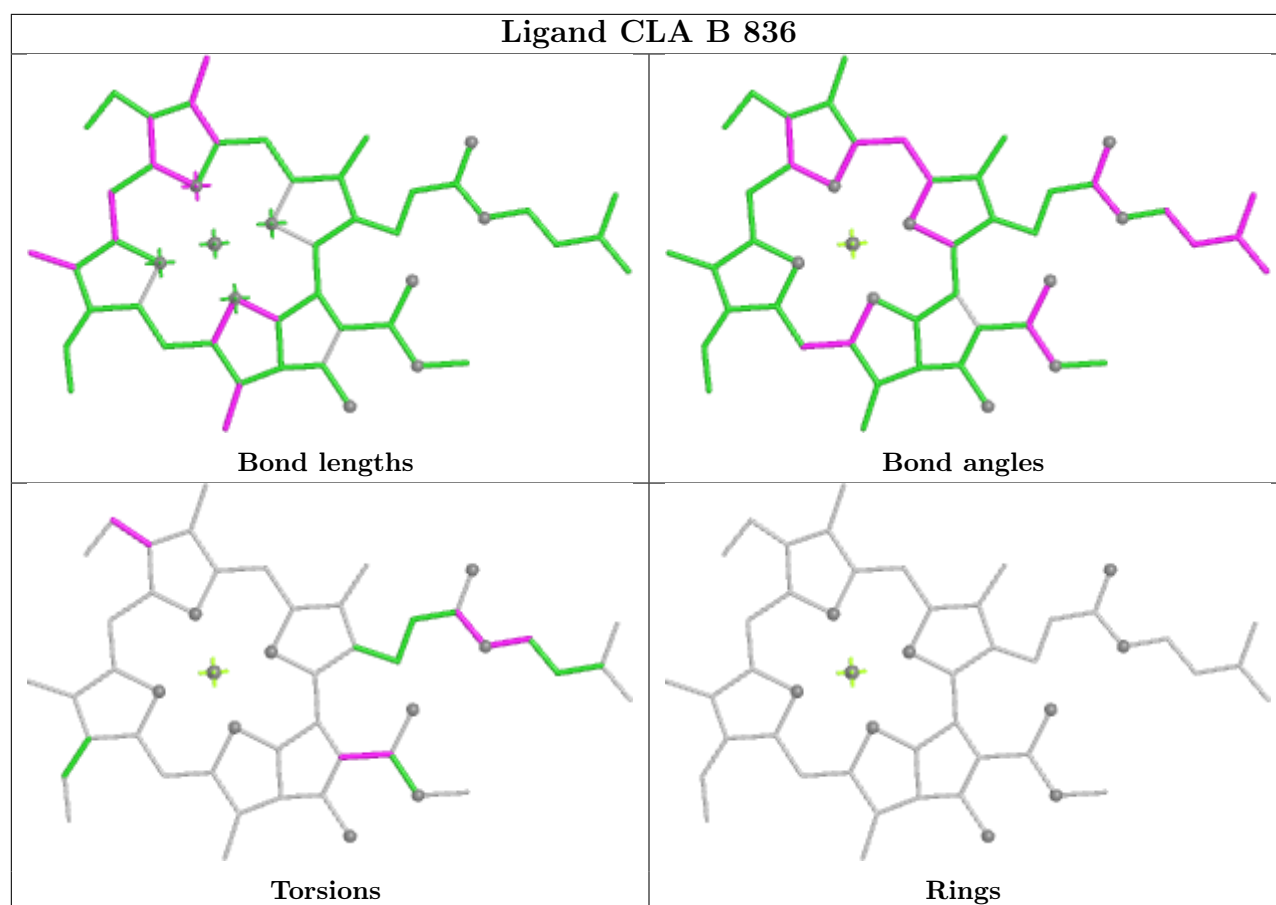
Rings

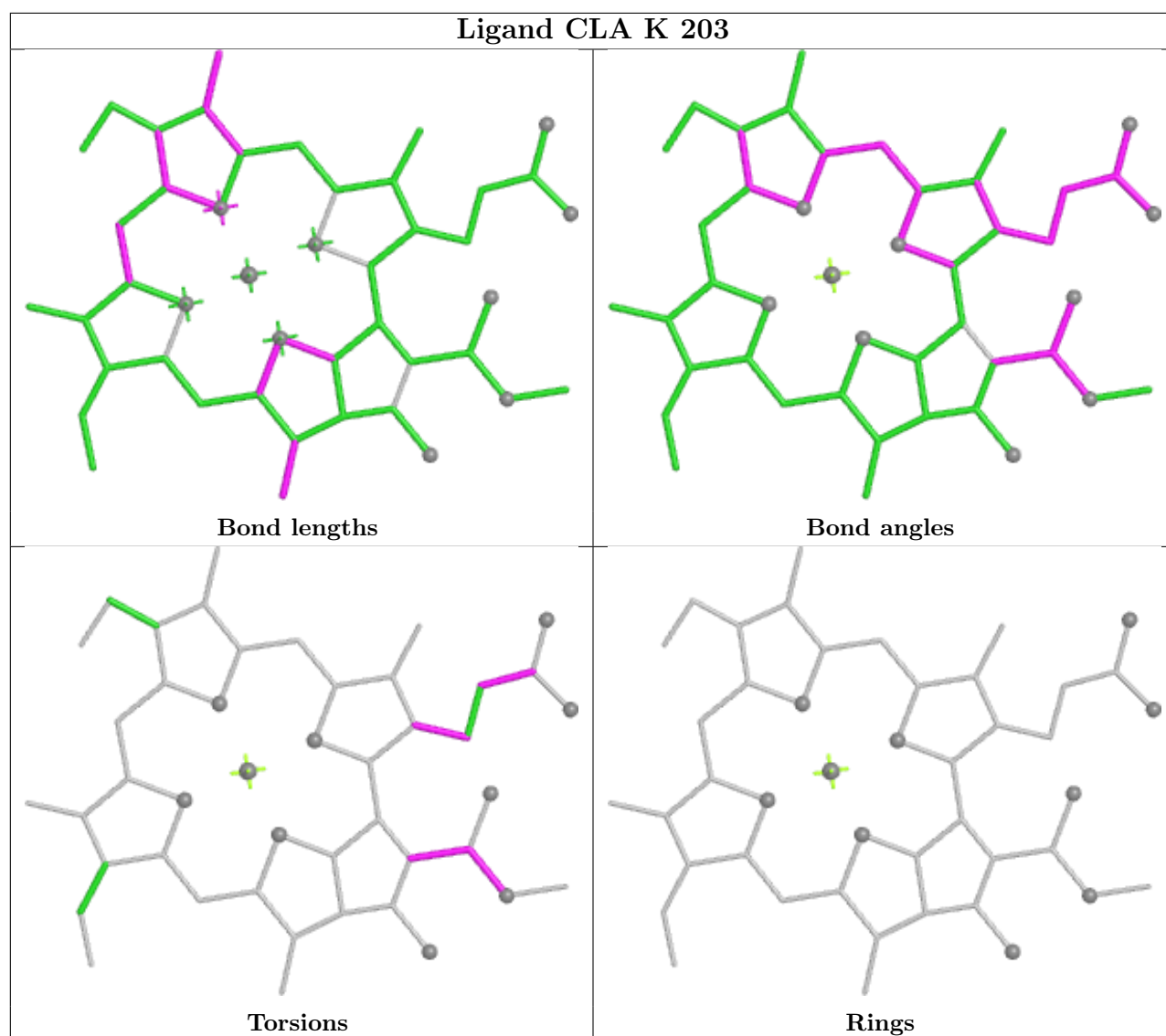




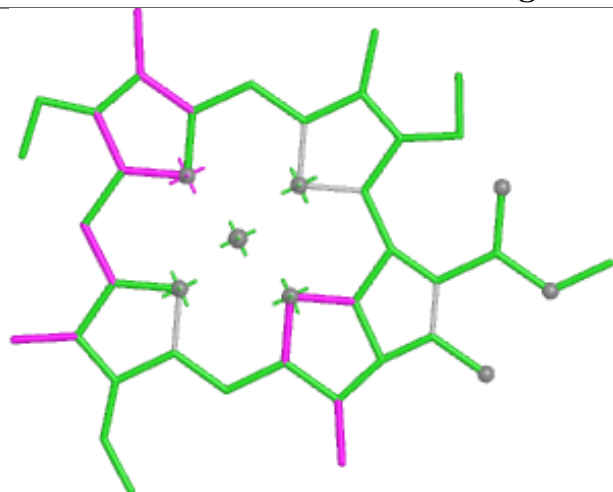




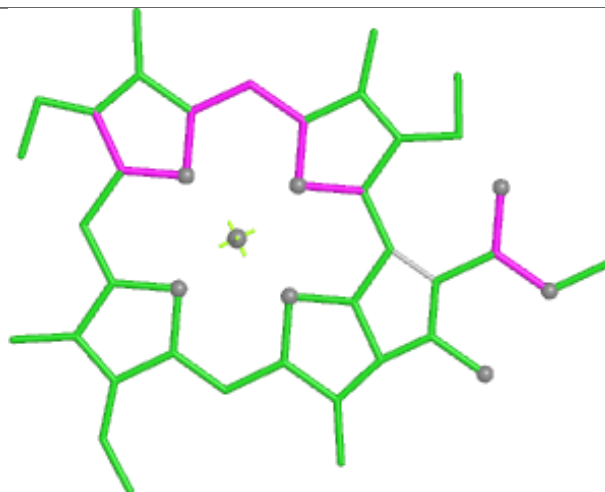




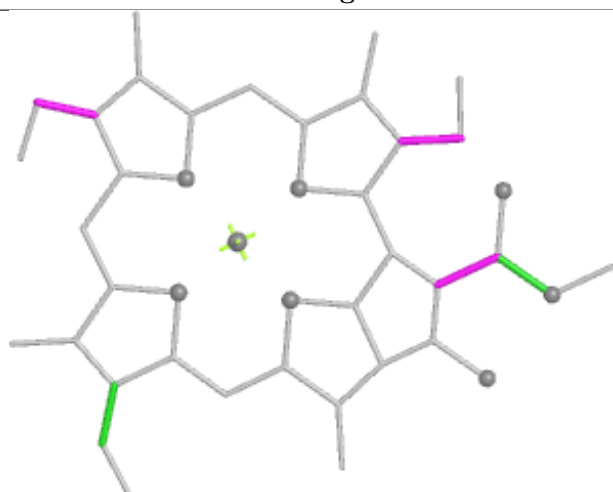
Ligand CLA 4 610



Bond lengths



Bond angles

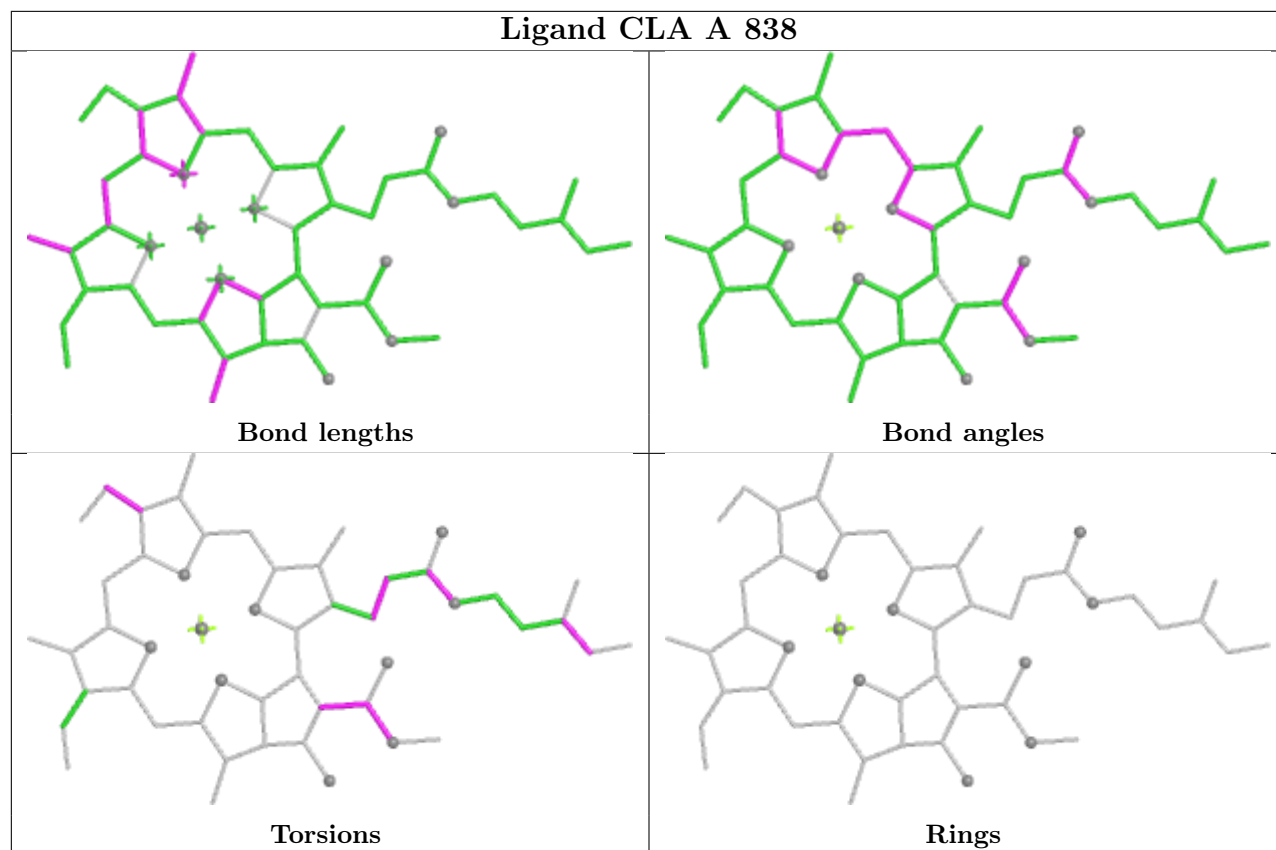


Torsions

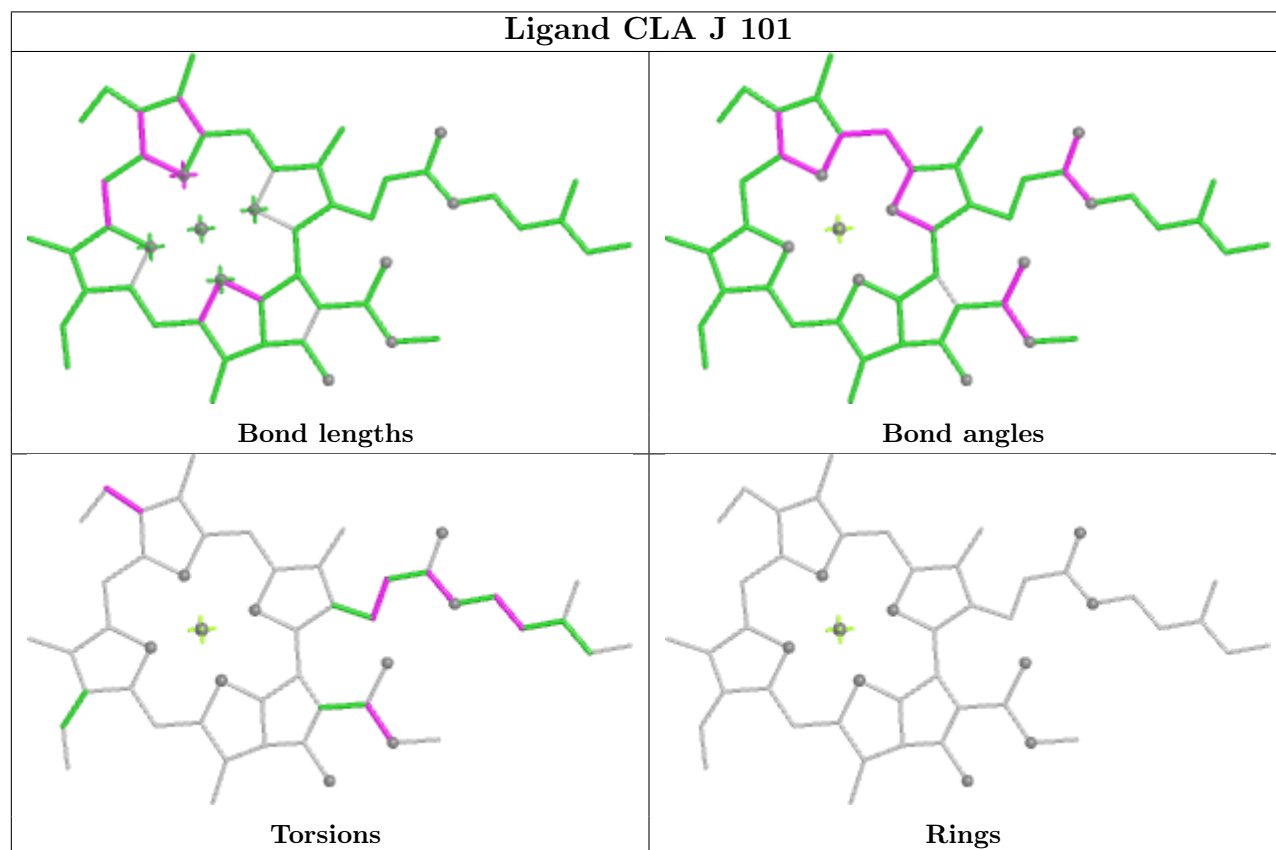


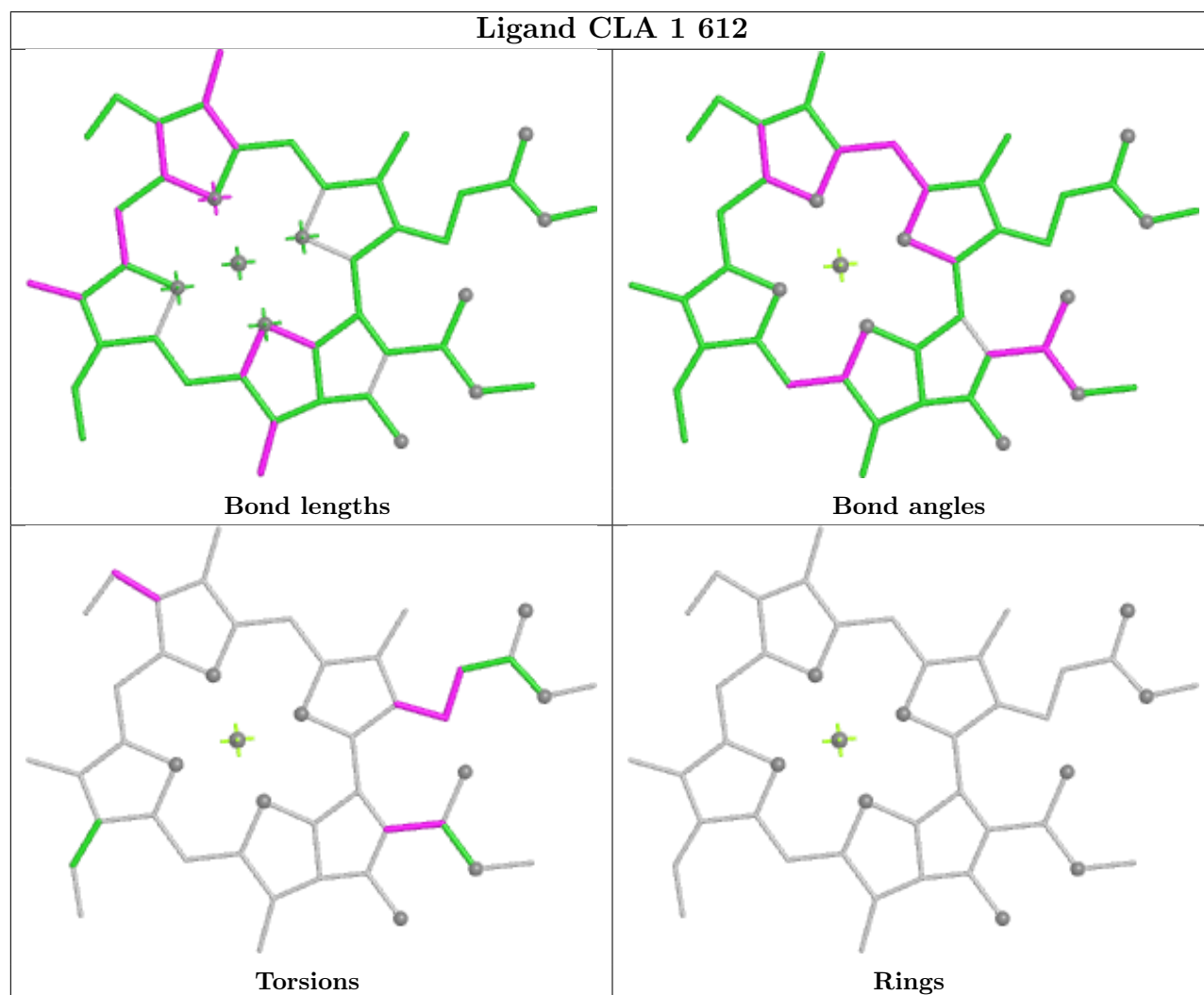
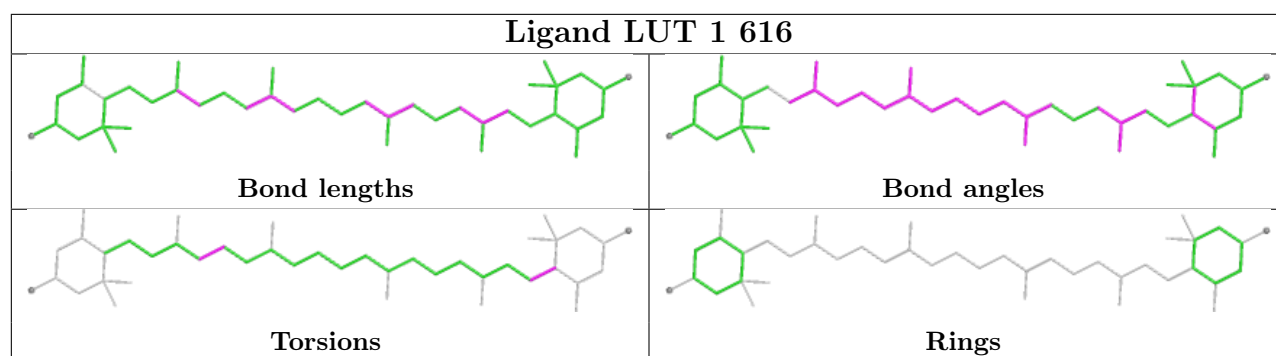
Rings

Ligand CLA A 838

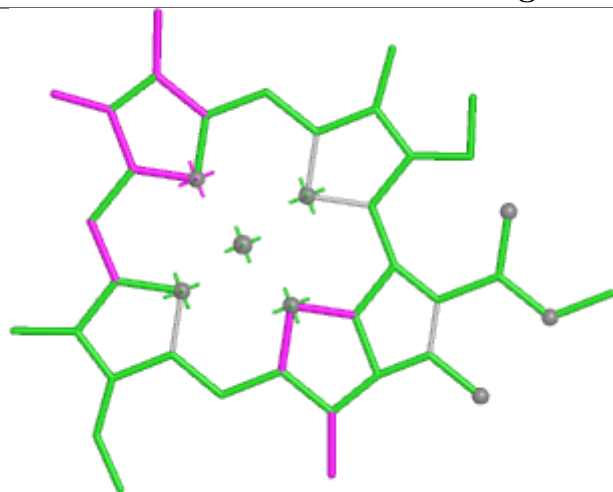


Ligand CLA J 101

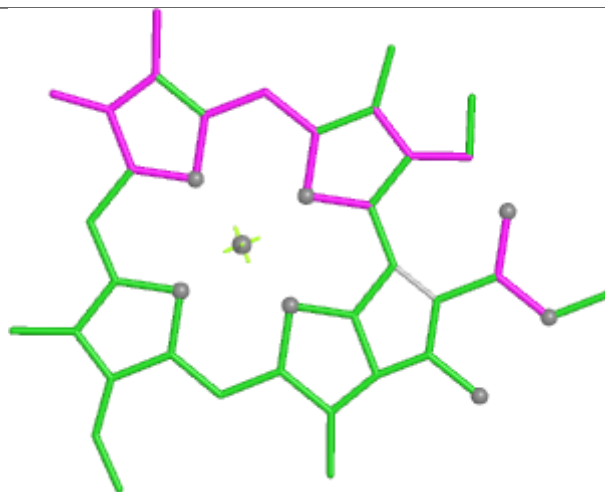




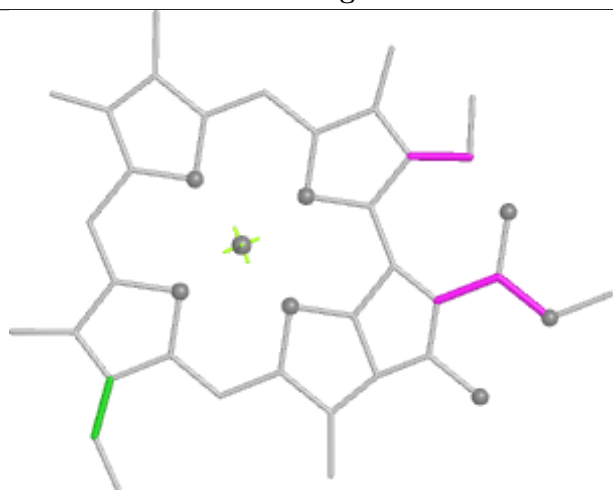
Ligand CLA 3 605



Bond lengths



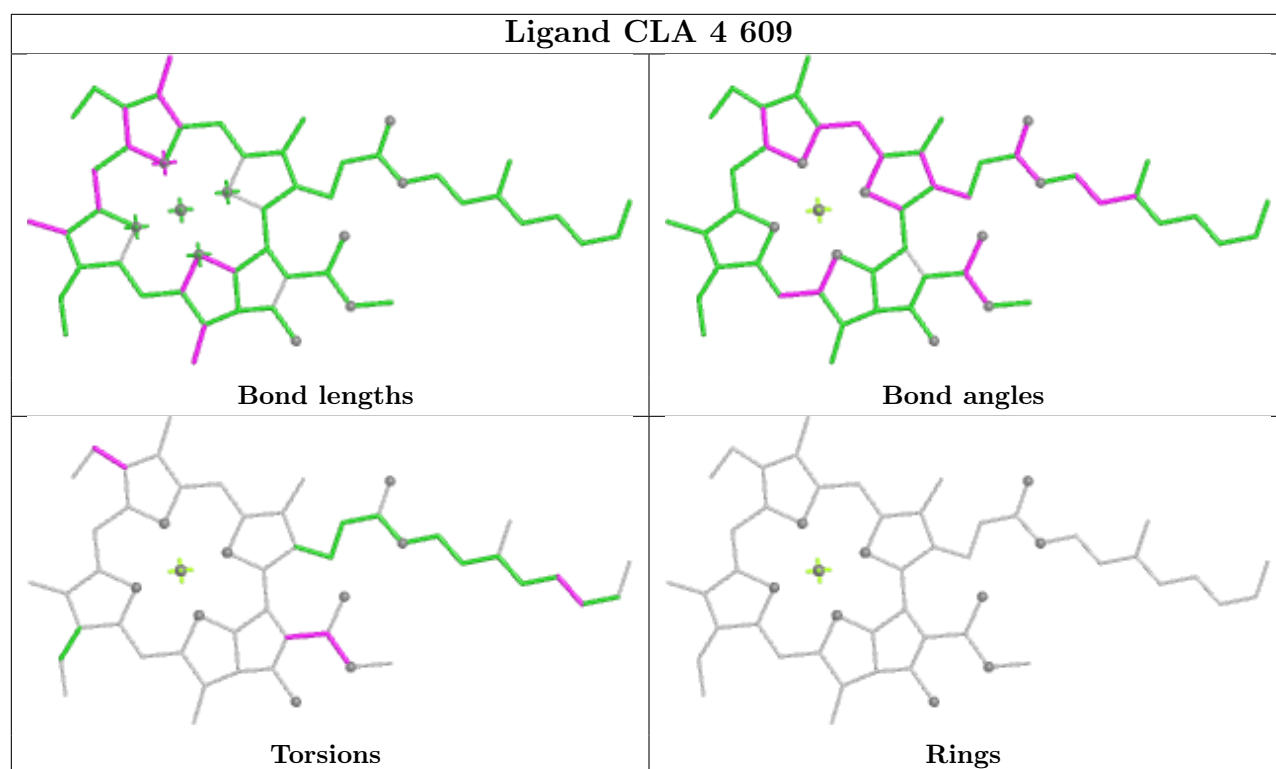
Bond angles

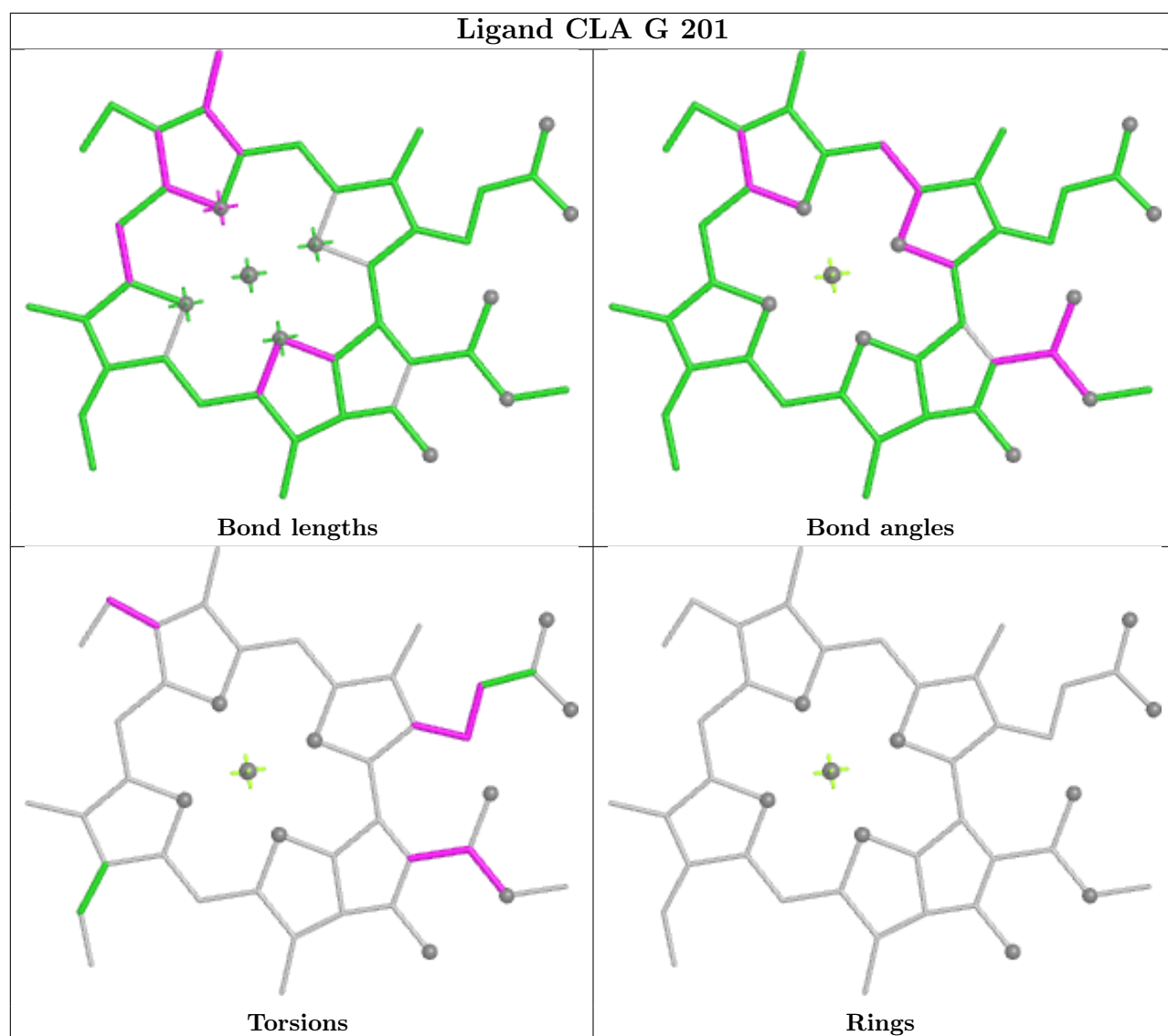


Torsions

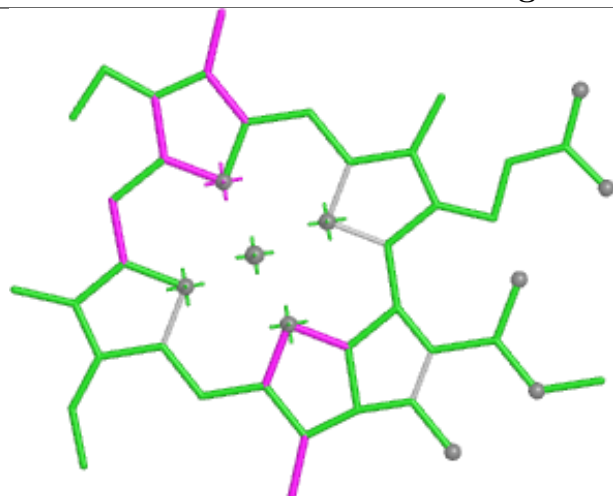


Rings

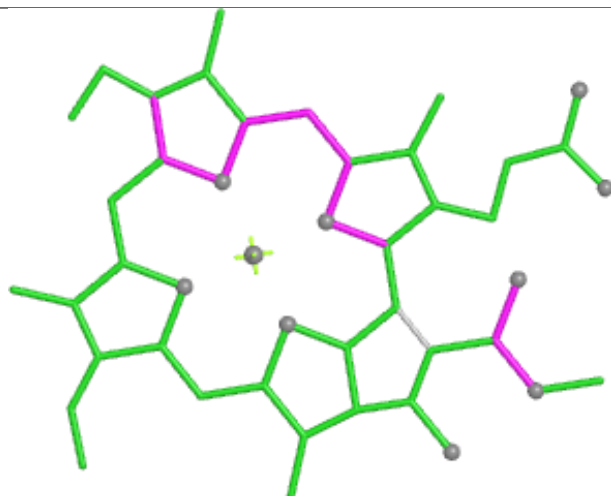




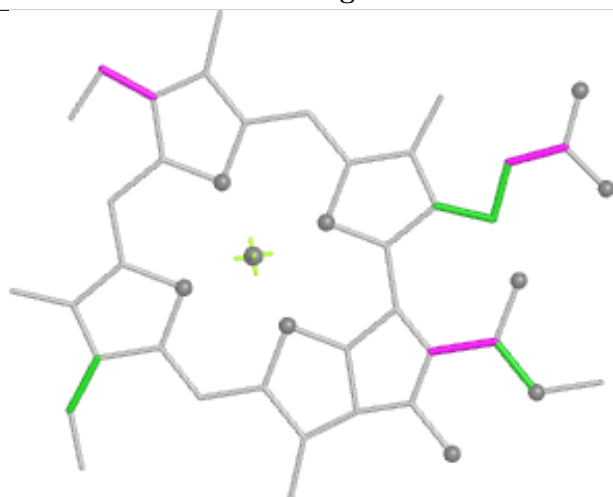
Ligand CLA 1 611



Bond lengths



Bond angles

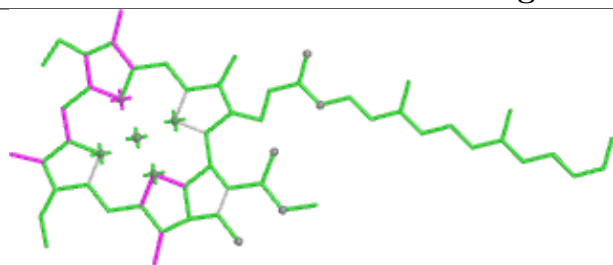


Torsions

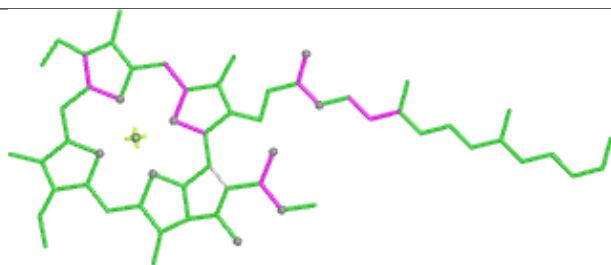


Rings

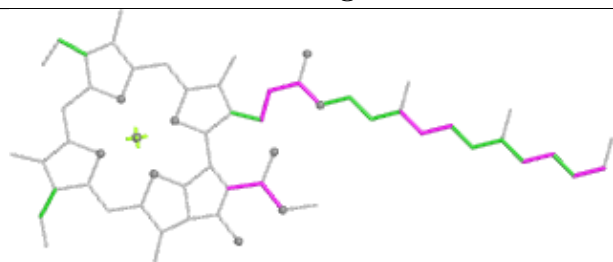
Ligand CLA x 613



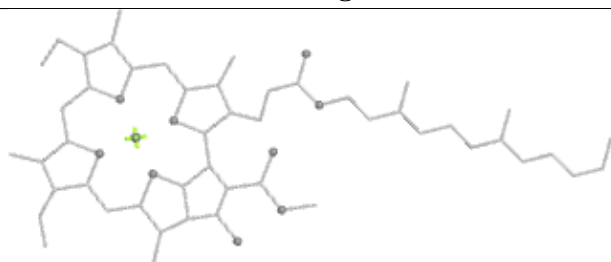
Bond lengths



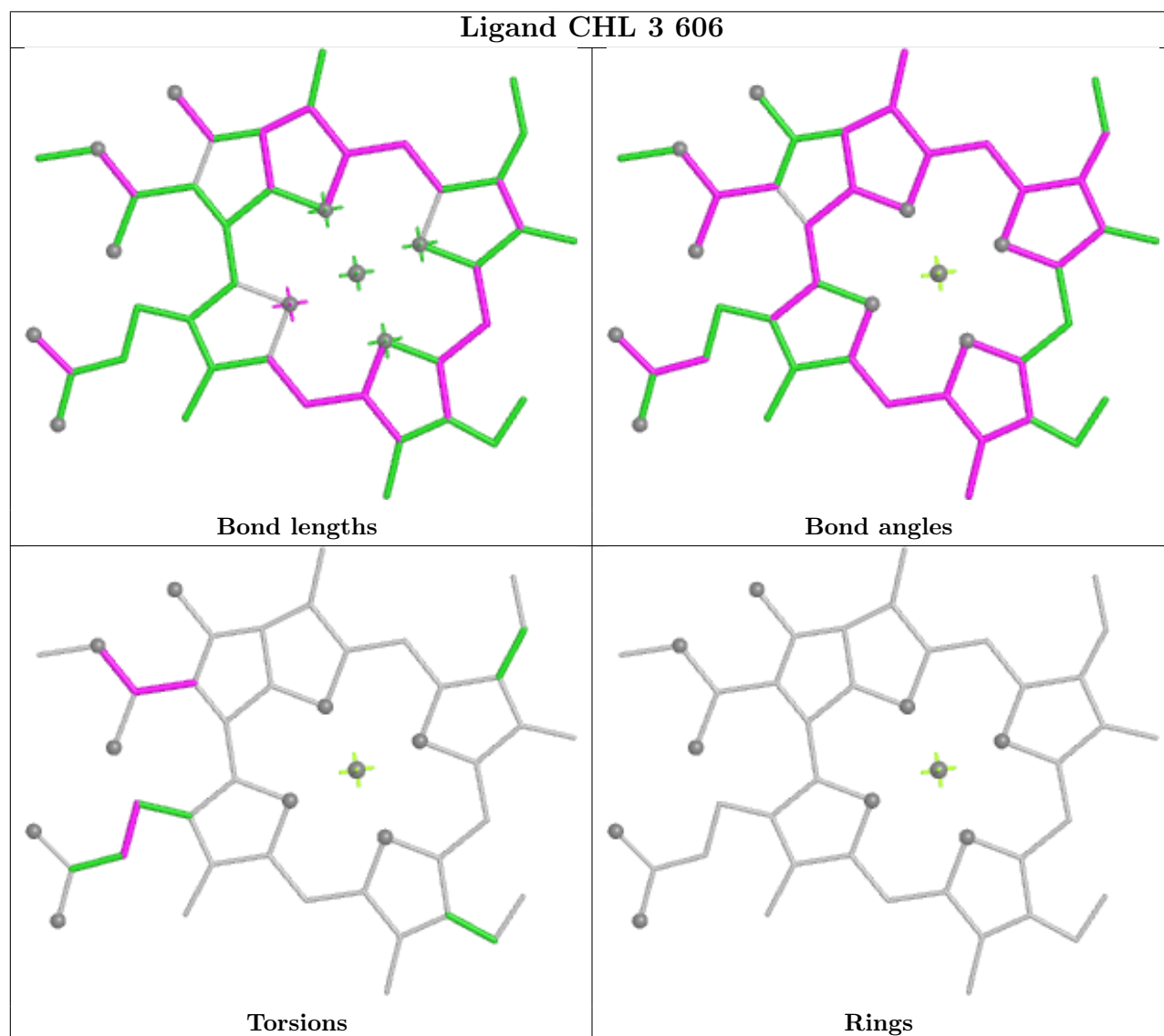
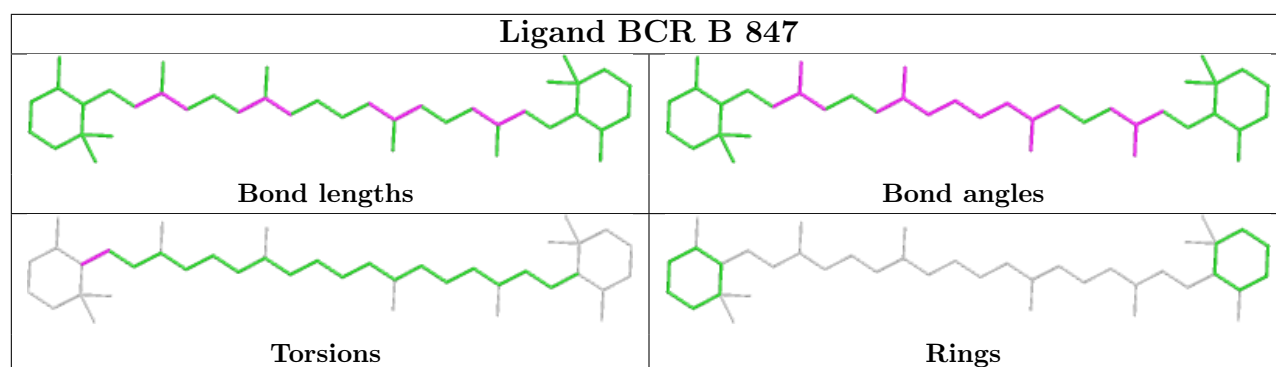
Bond angles

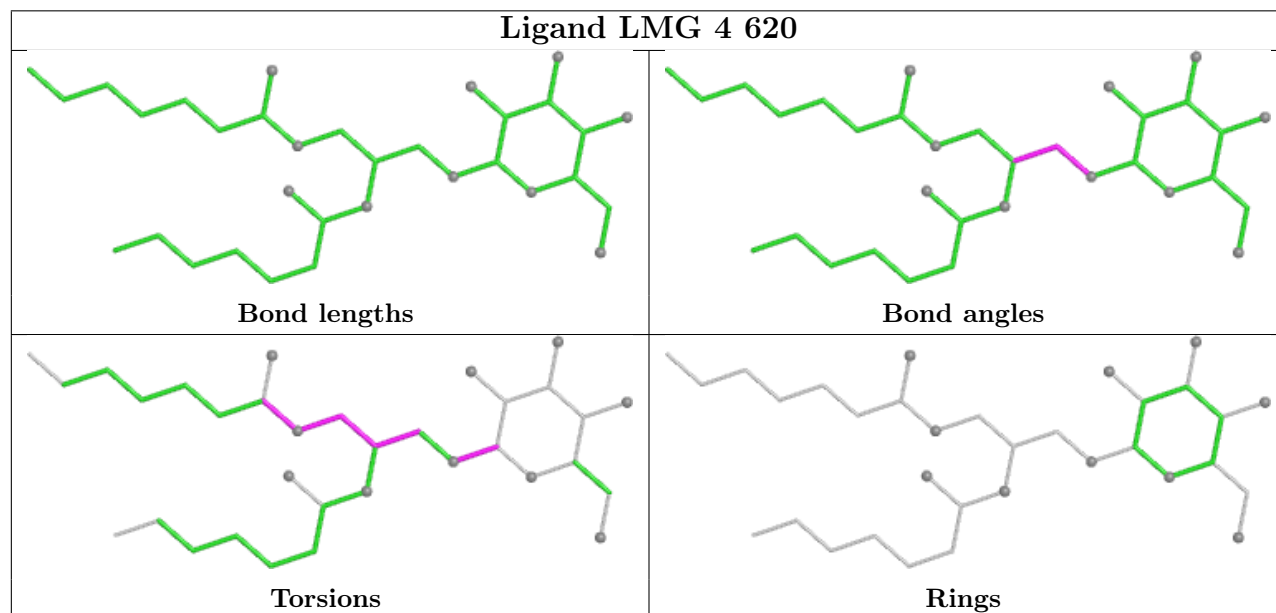
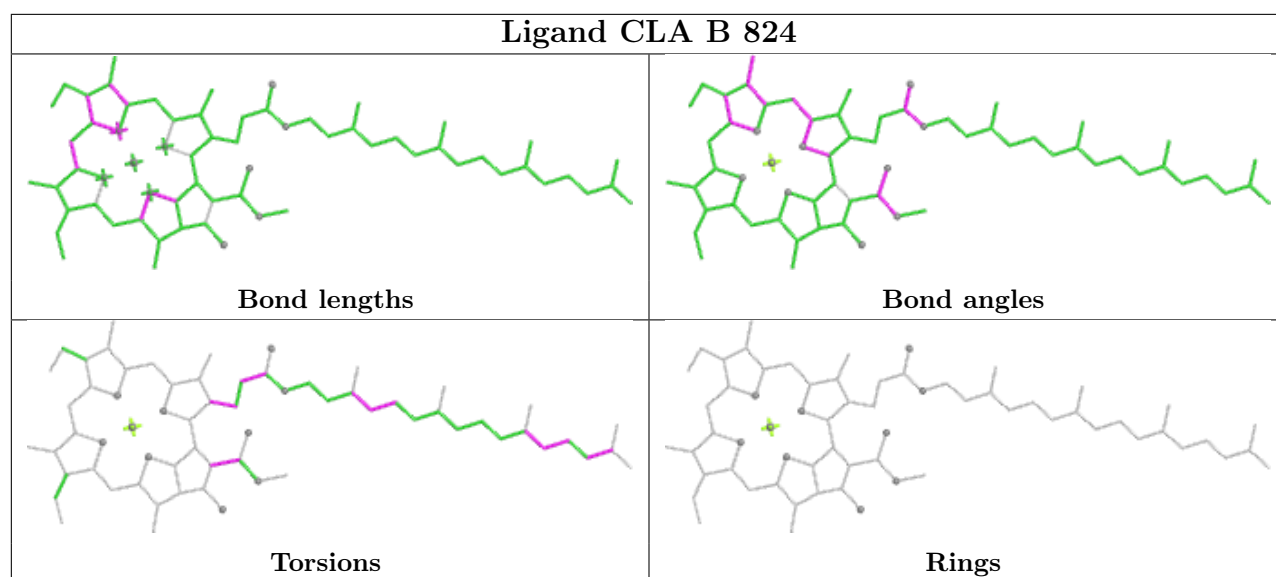


Torsions

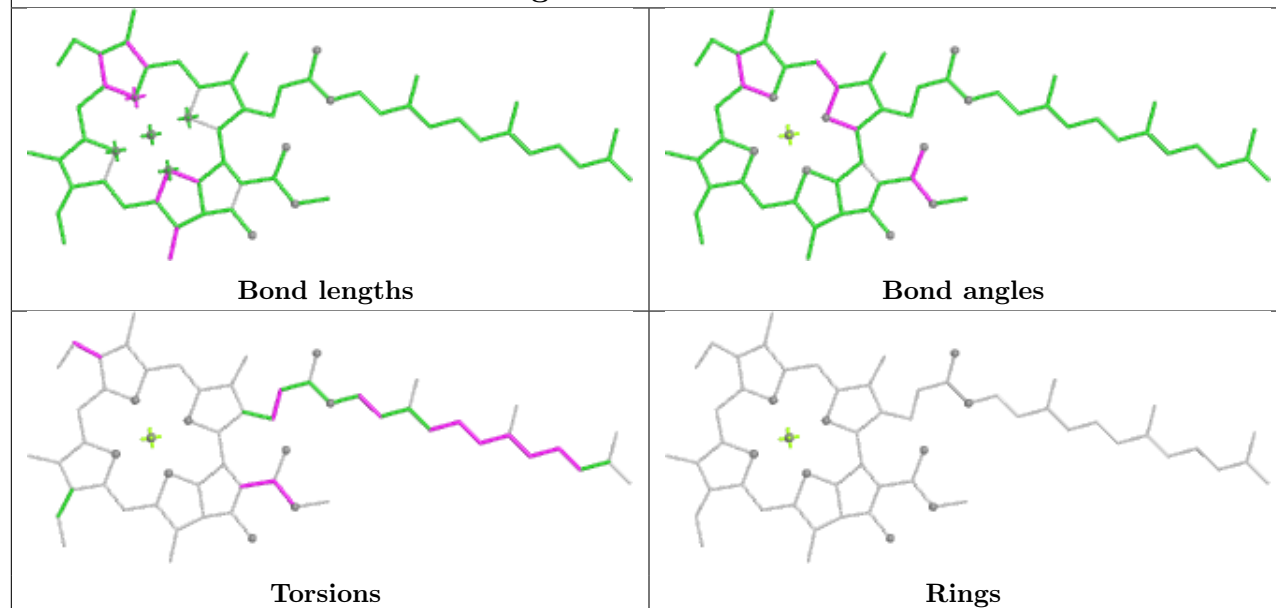


Rings

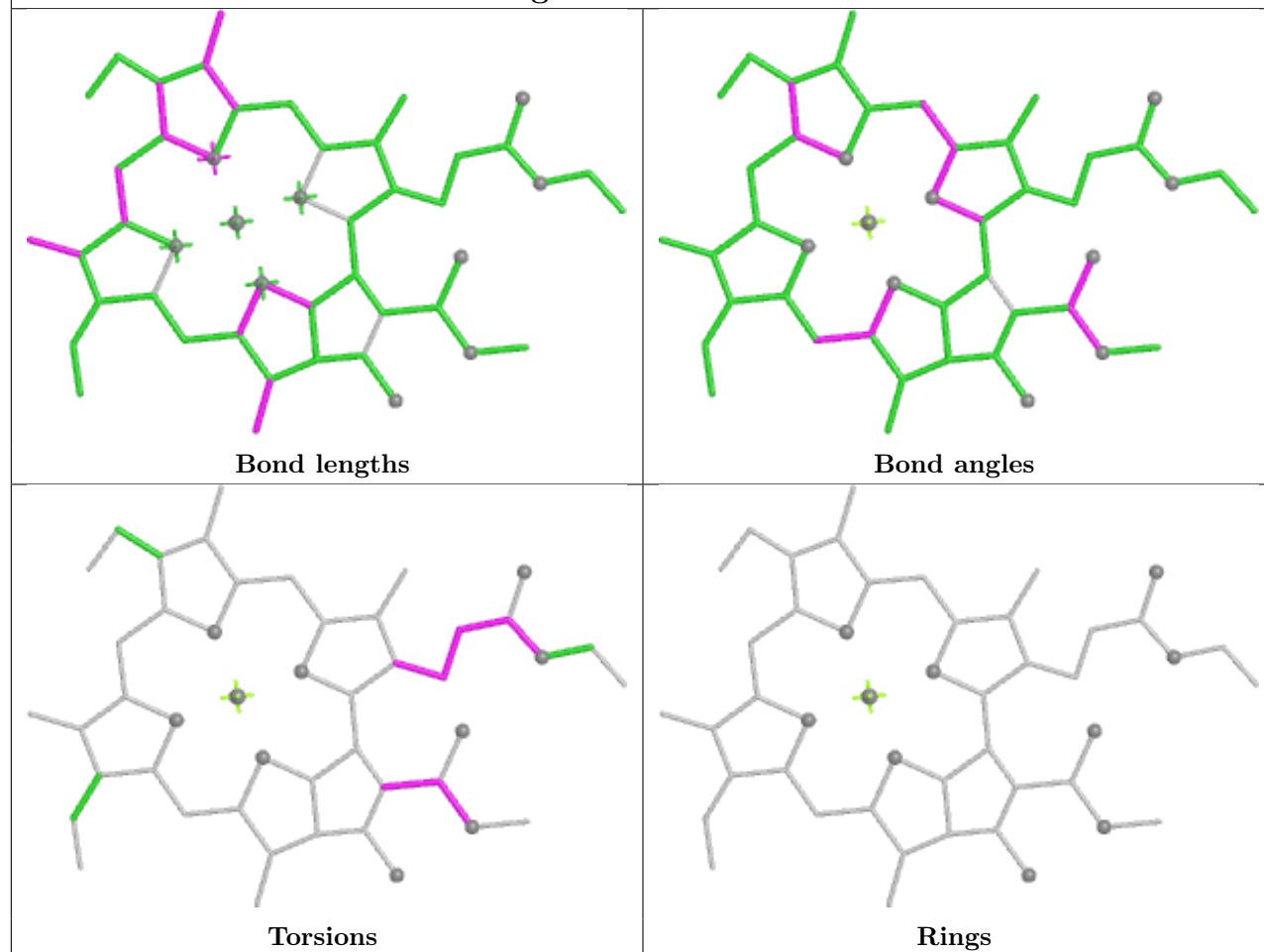


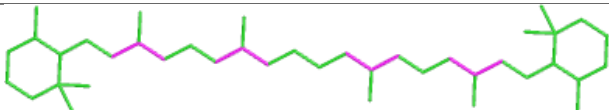
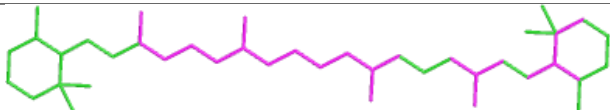
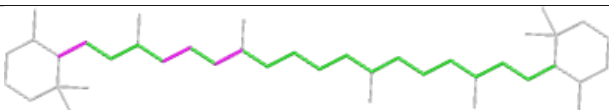
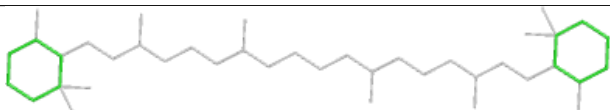
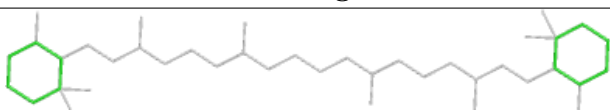


Ligand CLA H 201

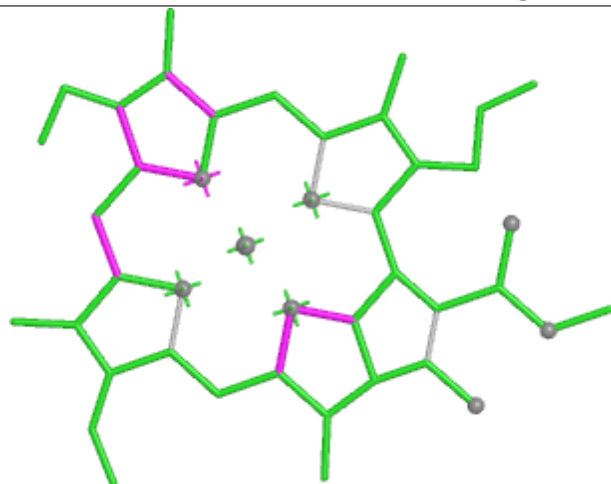


Ligand CLA 2 609

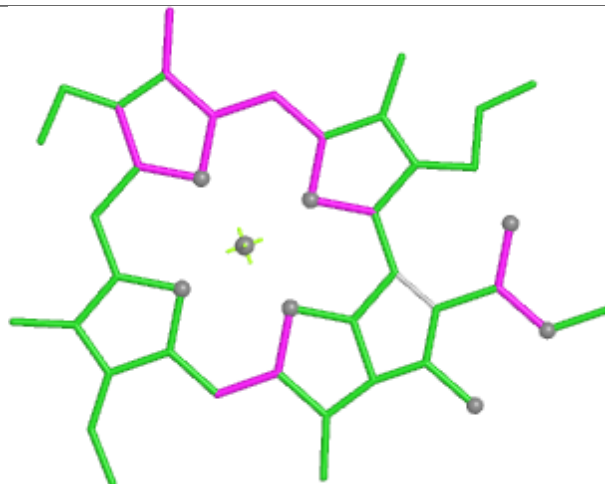


Ligand BCR A 853			
	Bond lengths		
	Torsions		
Ligand BCR O 204			
	Bond lengths		
	Torsions		

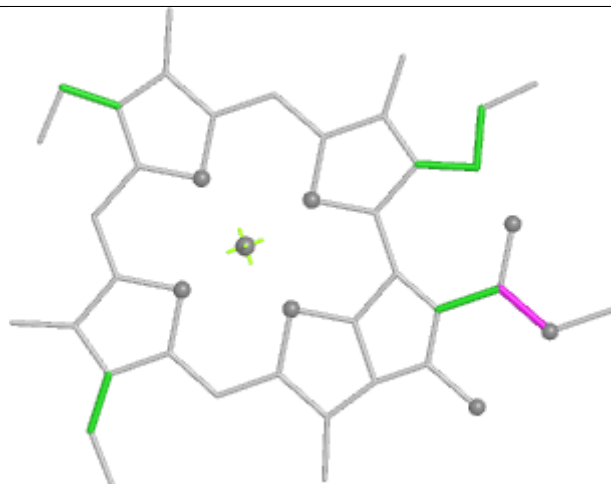
Ligand CLA B 831



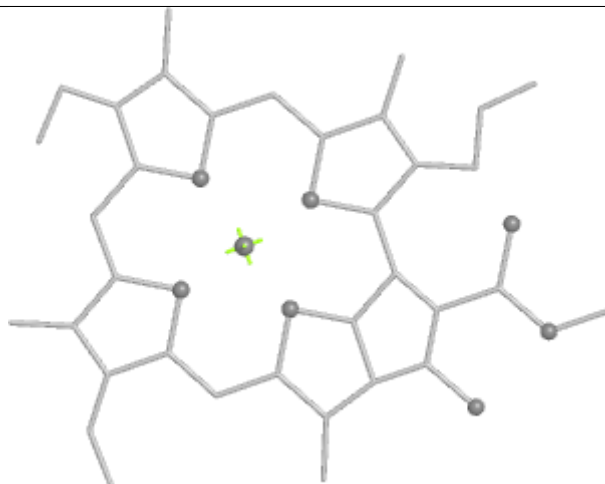
Bond lengths



Bond angles

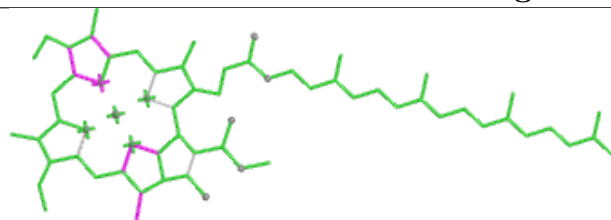


Torsions

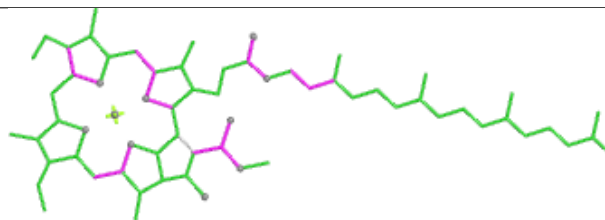


Rings

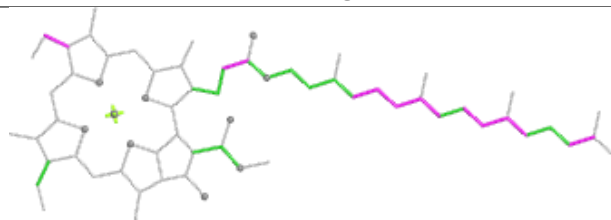
Ligand CLA B 806



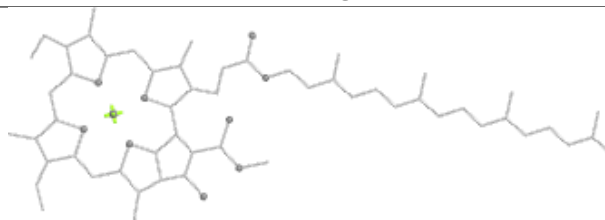
Bond lengths



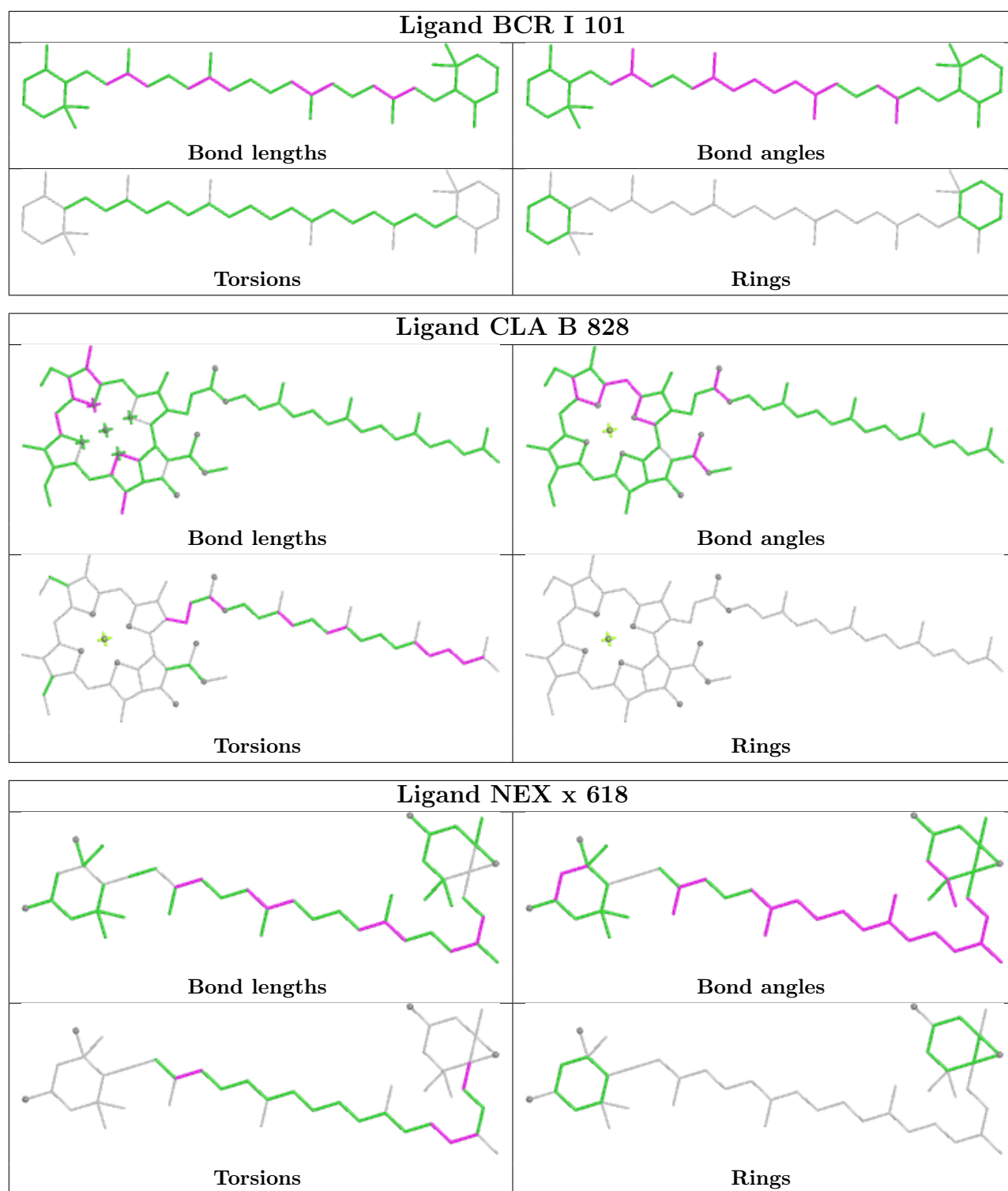
Bond angles

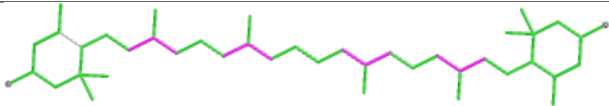
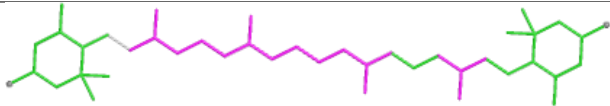
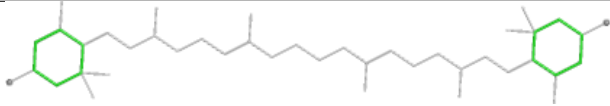


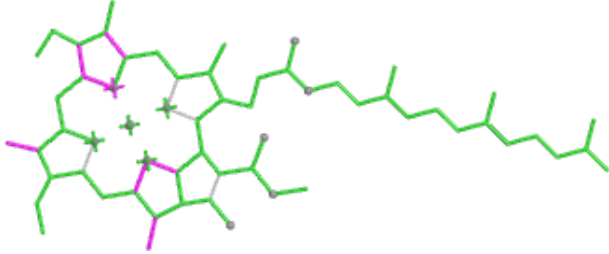
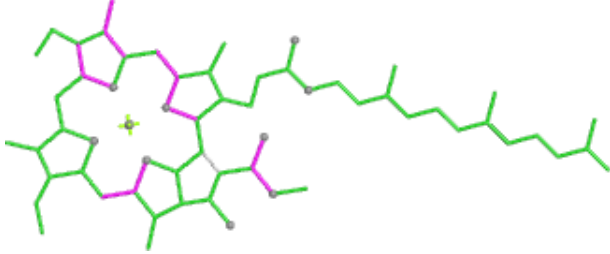
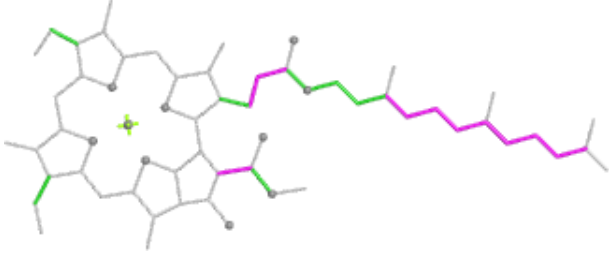
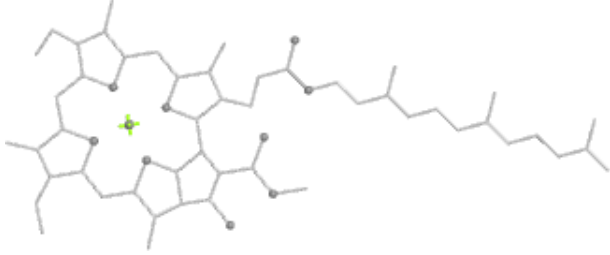
Torsions



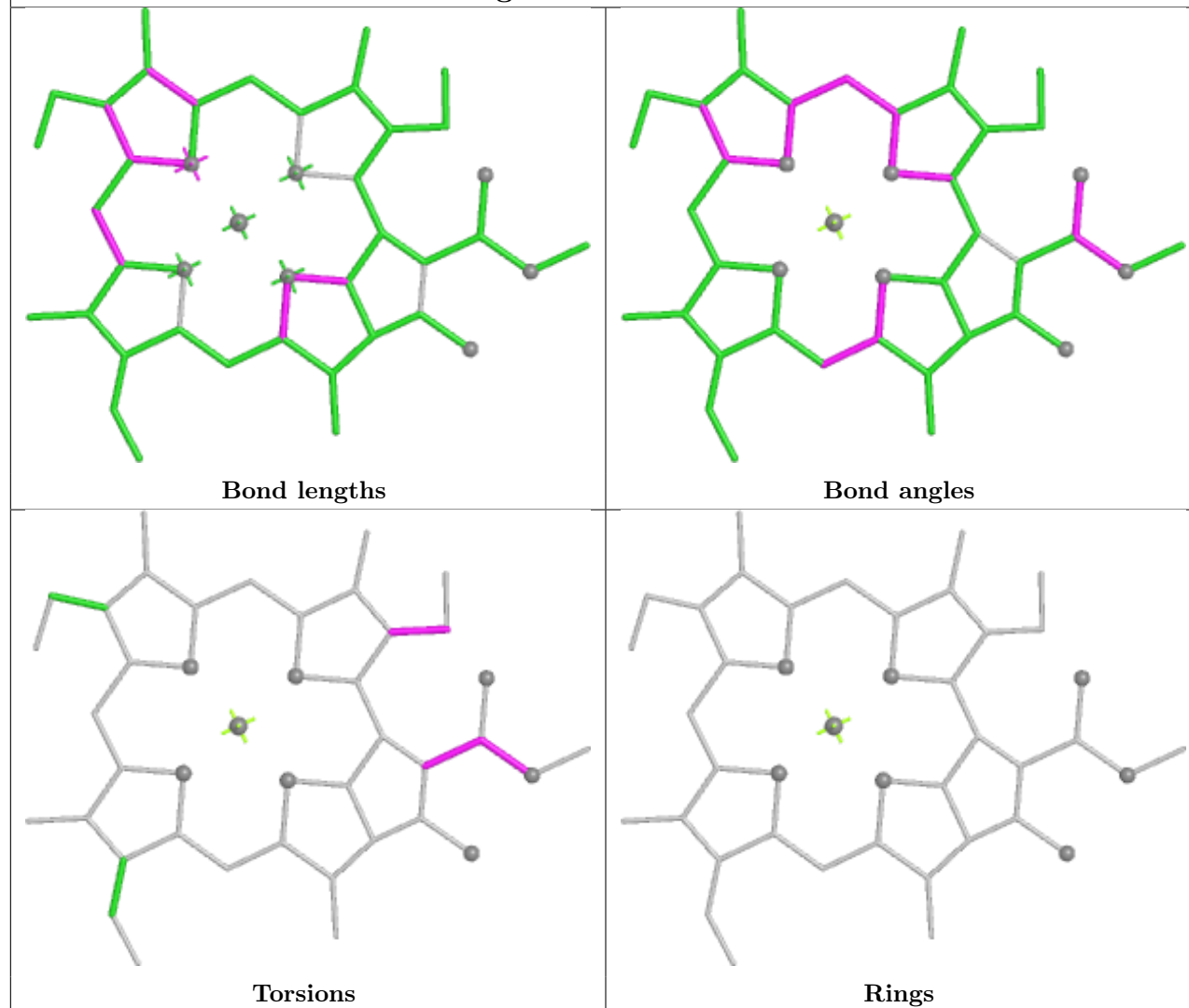
Rings



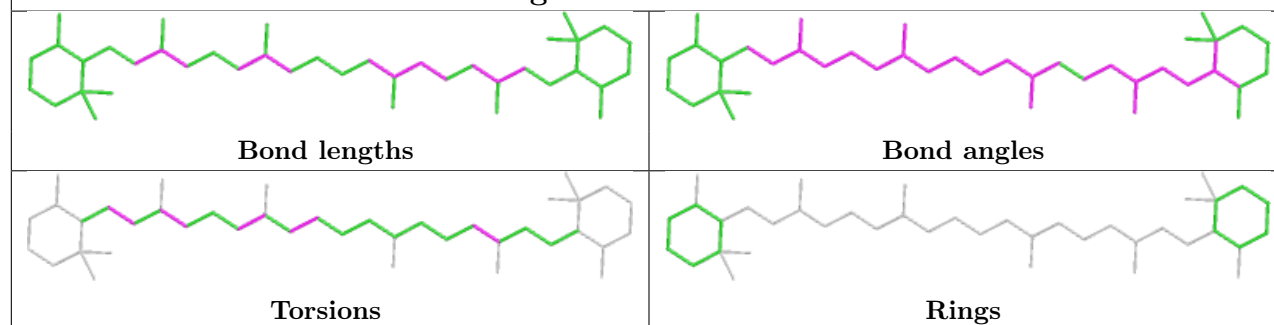
Ligand LUT y 616	
	Bond lengths
	Bond angles
	Torsions
	Rings

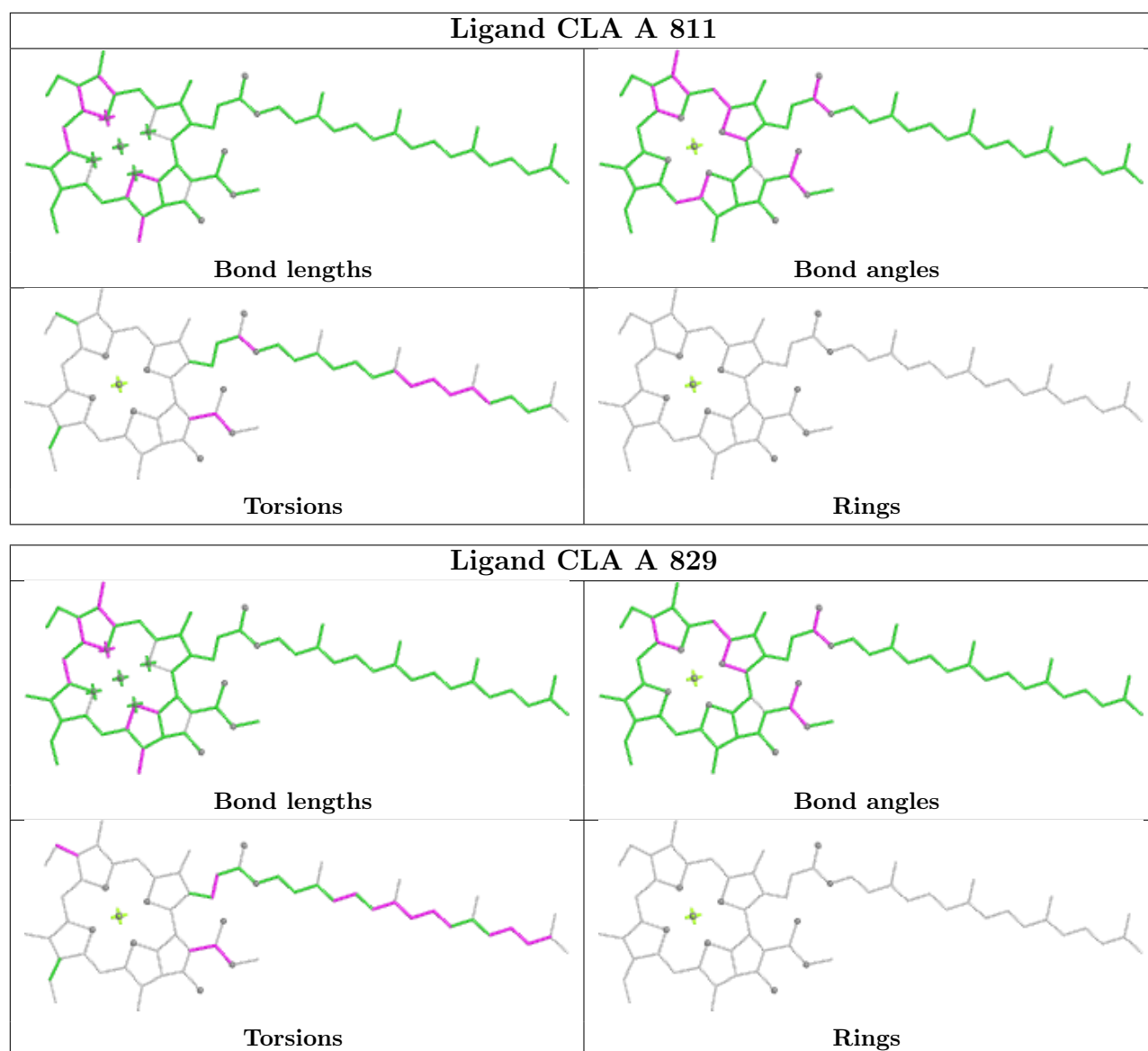
Ligand CLA 3 601	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand CLA A 823

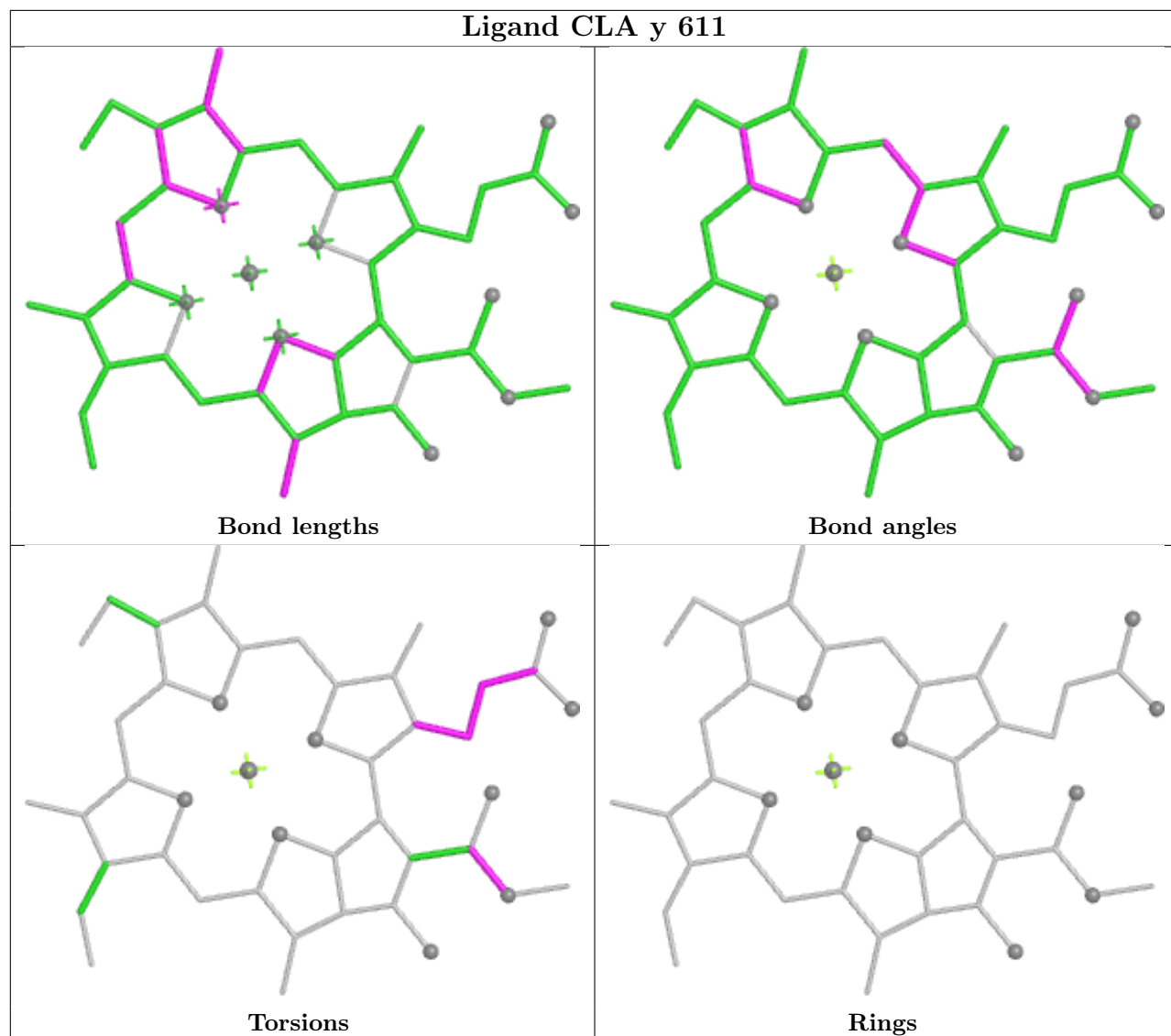


Ligand BCR A 851

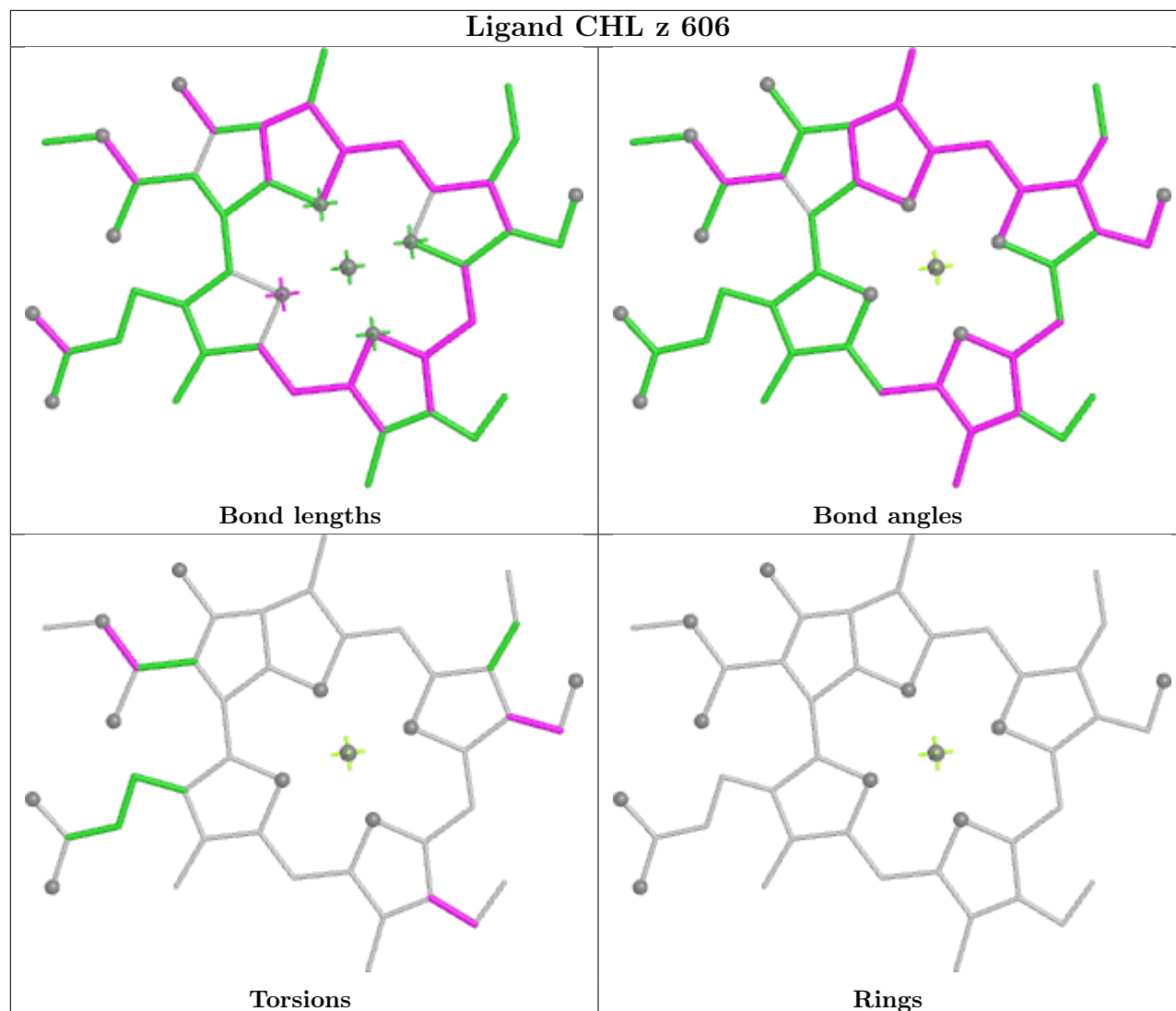


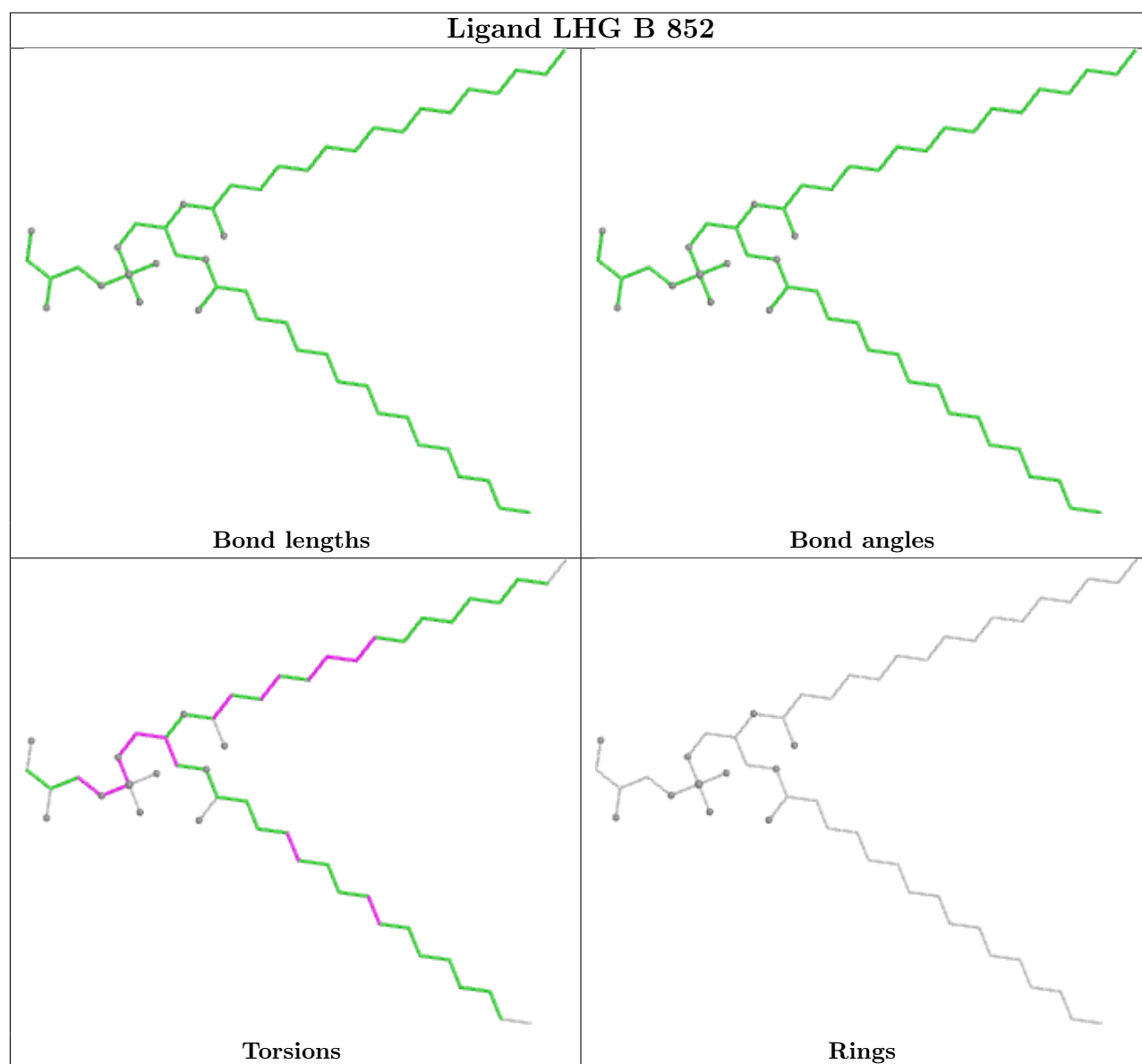


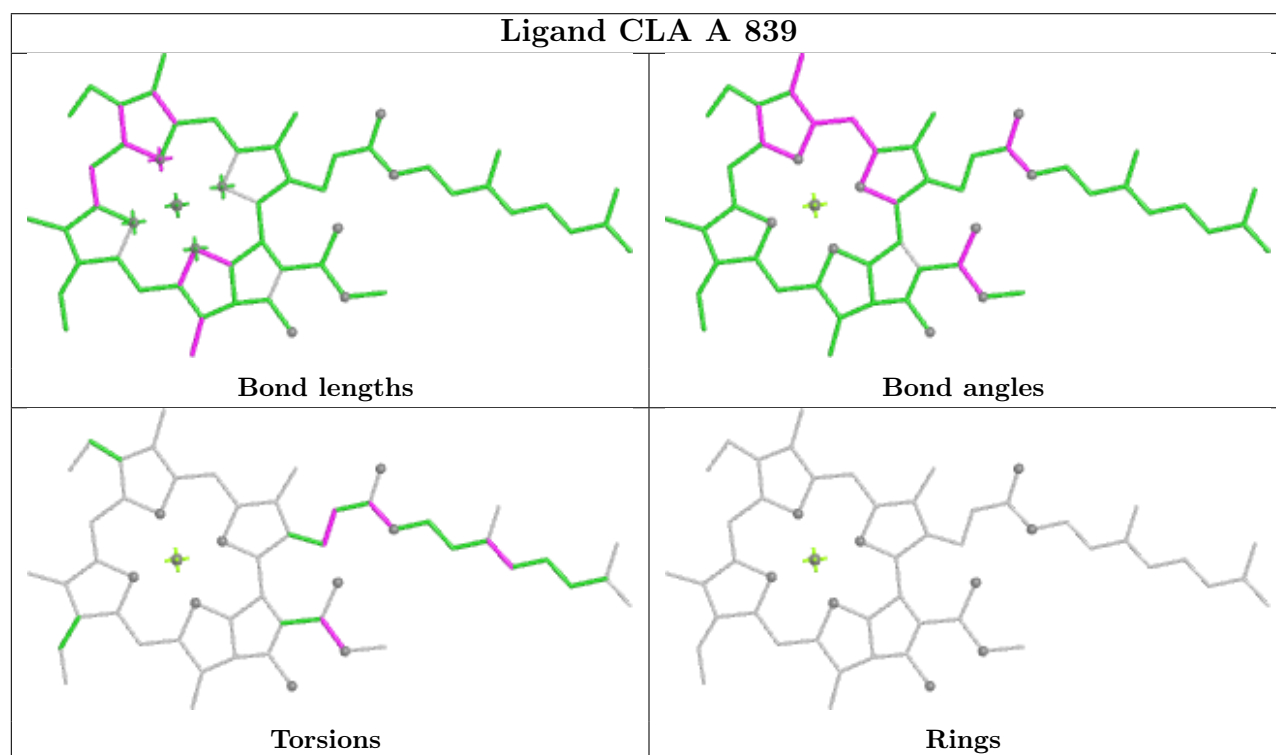
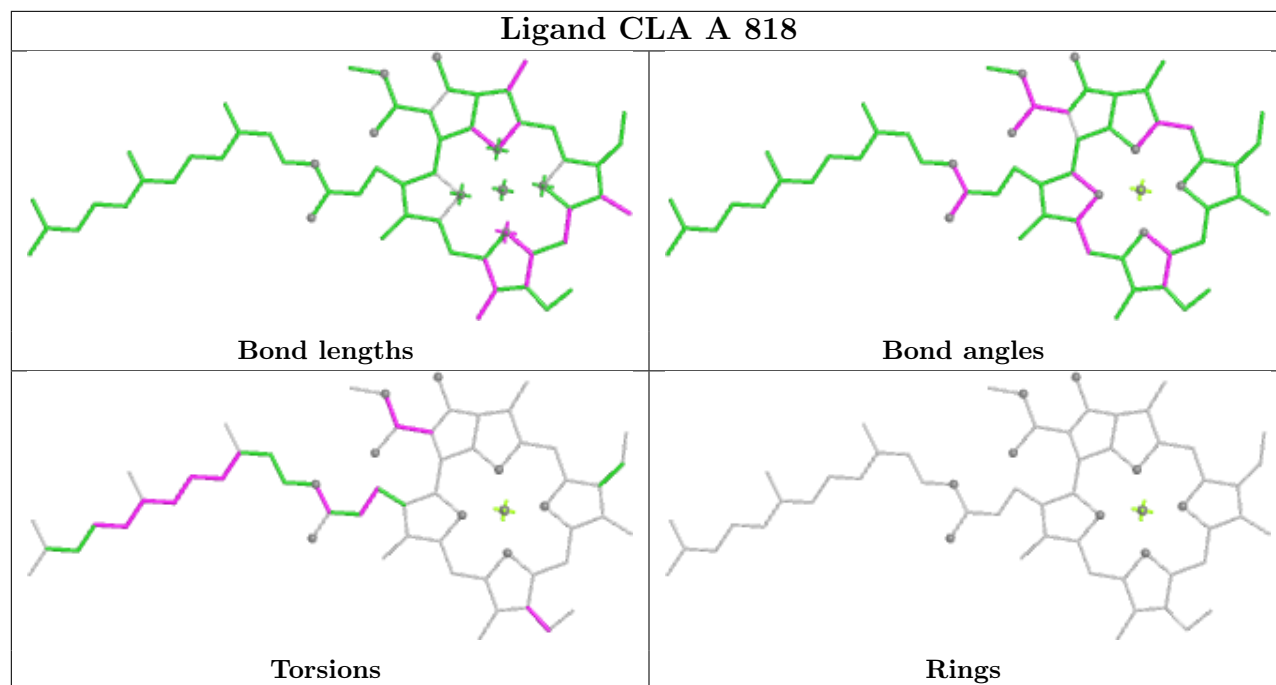
Ligand CLA y 611

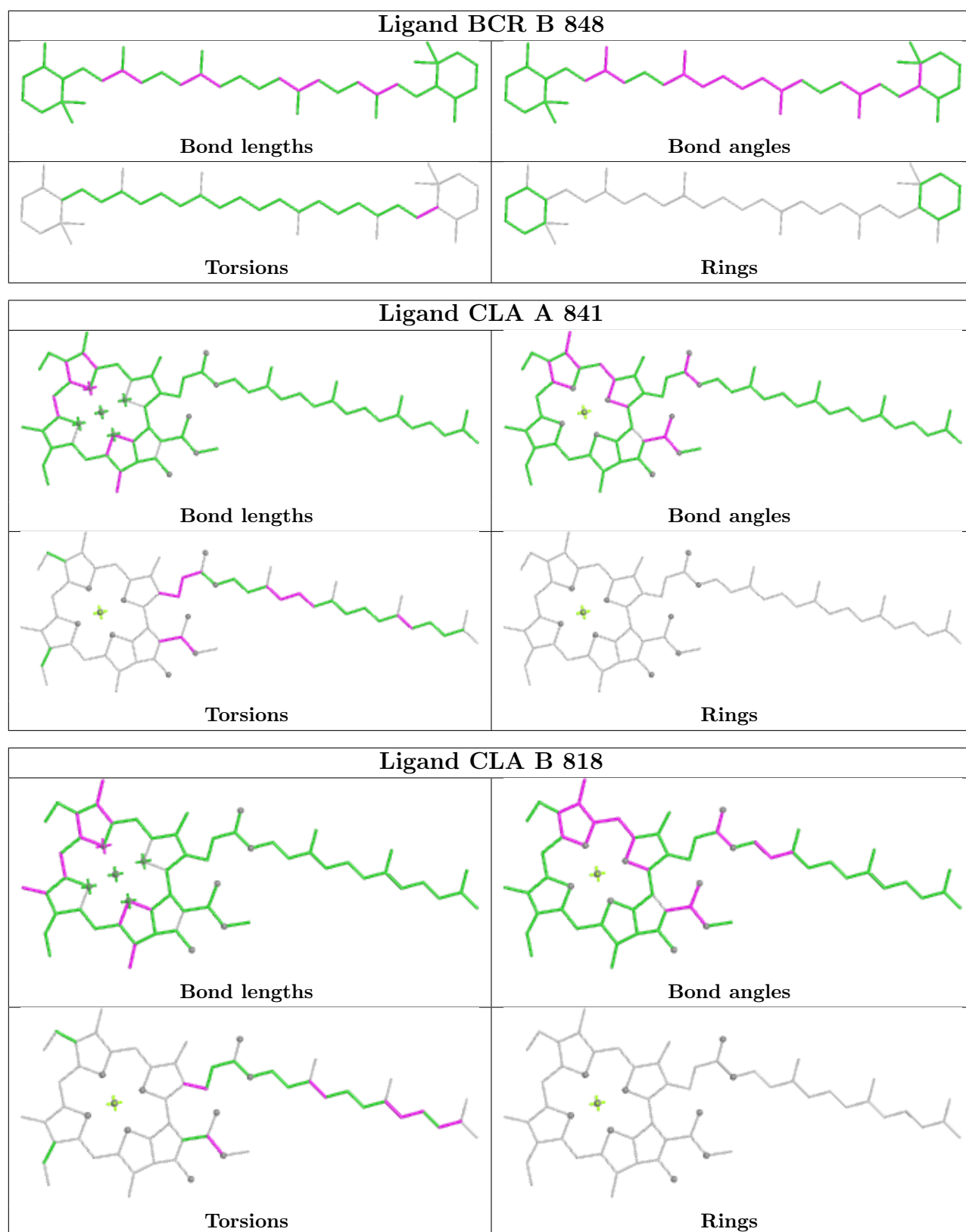


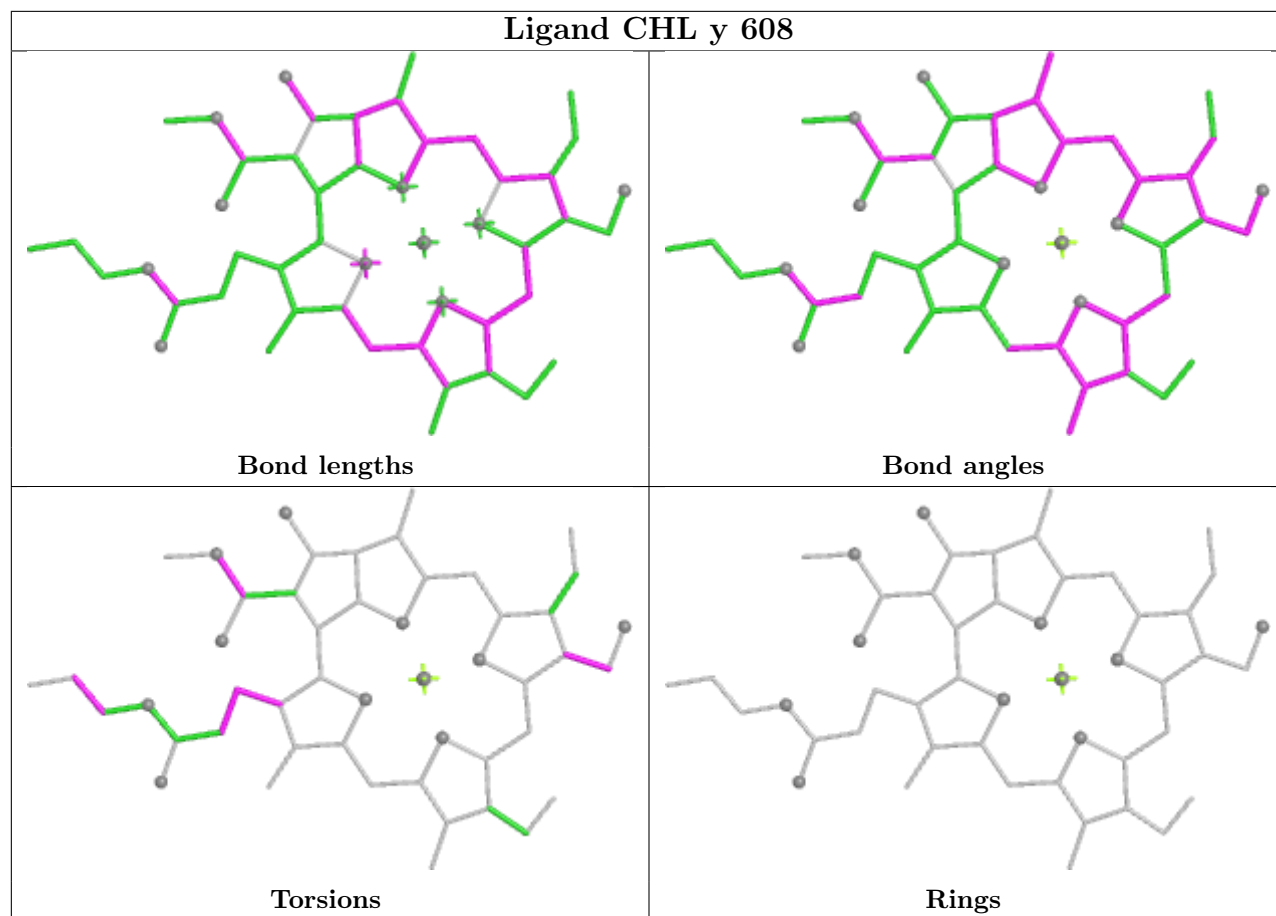
Ligand CHL z 606



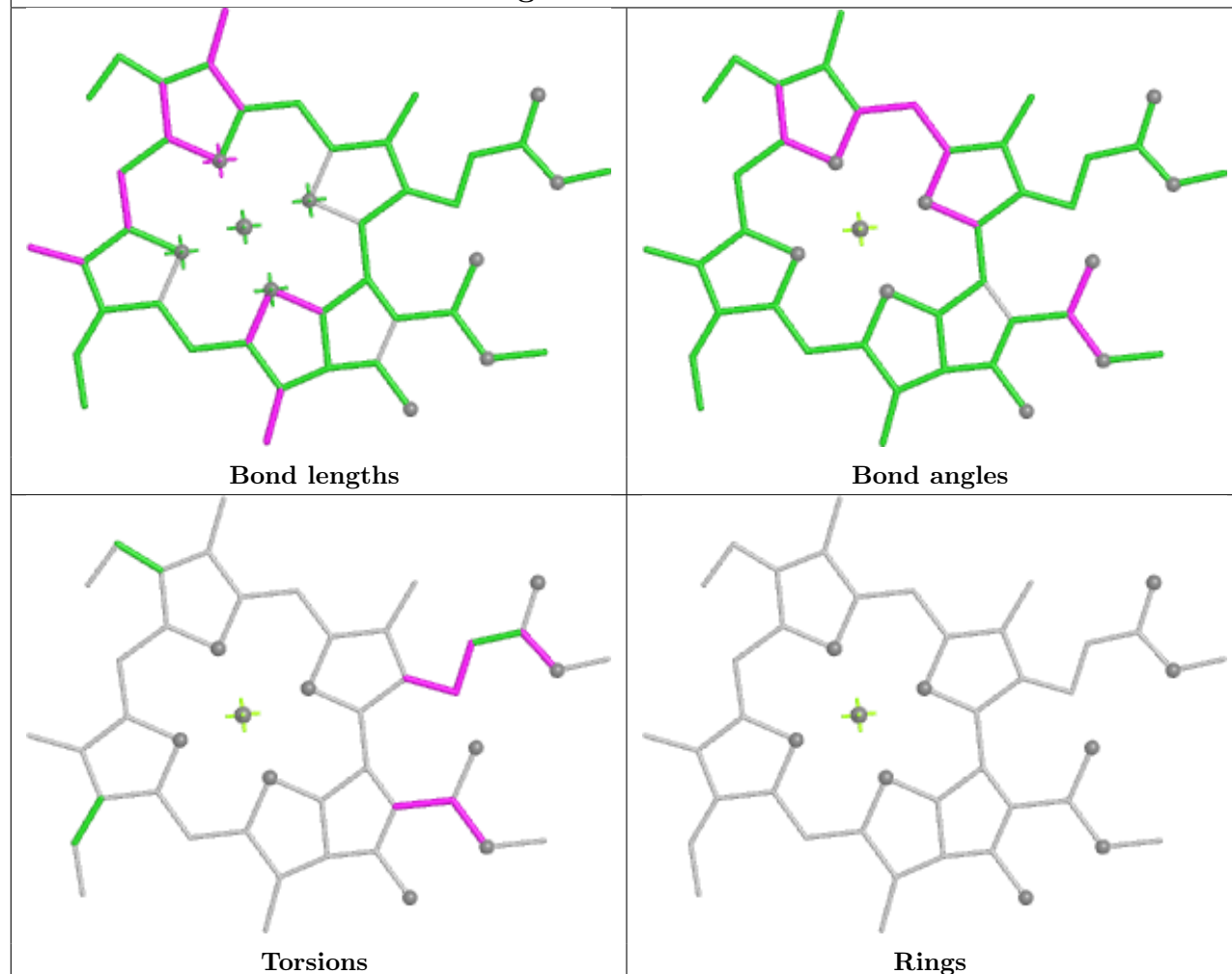




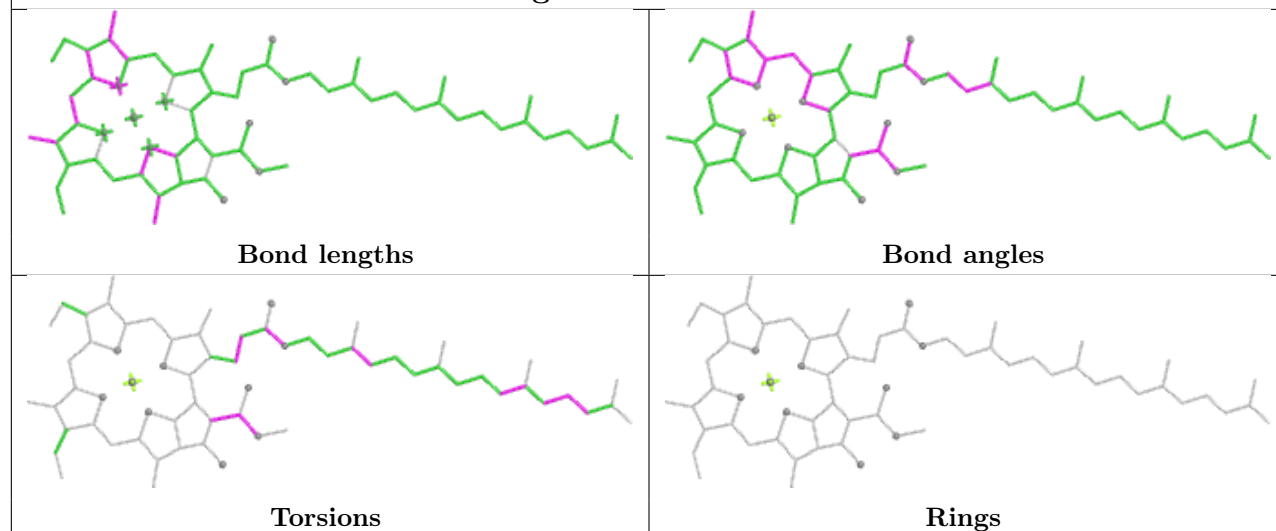


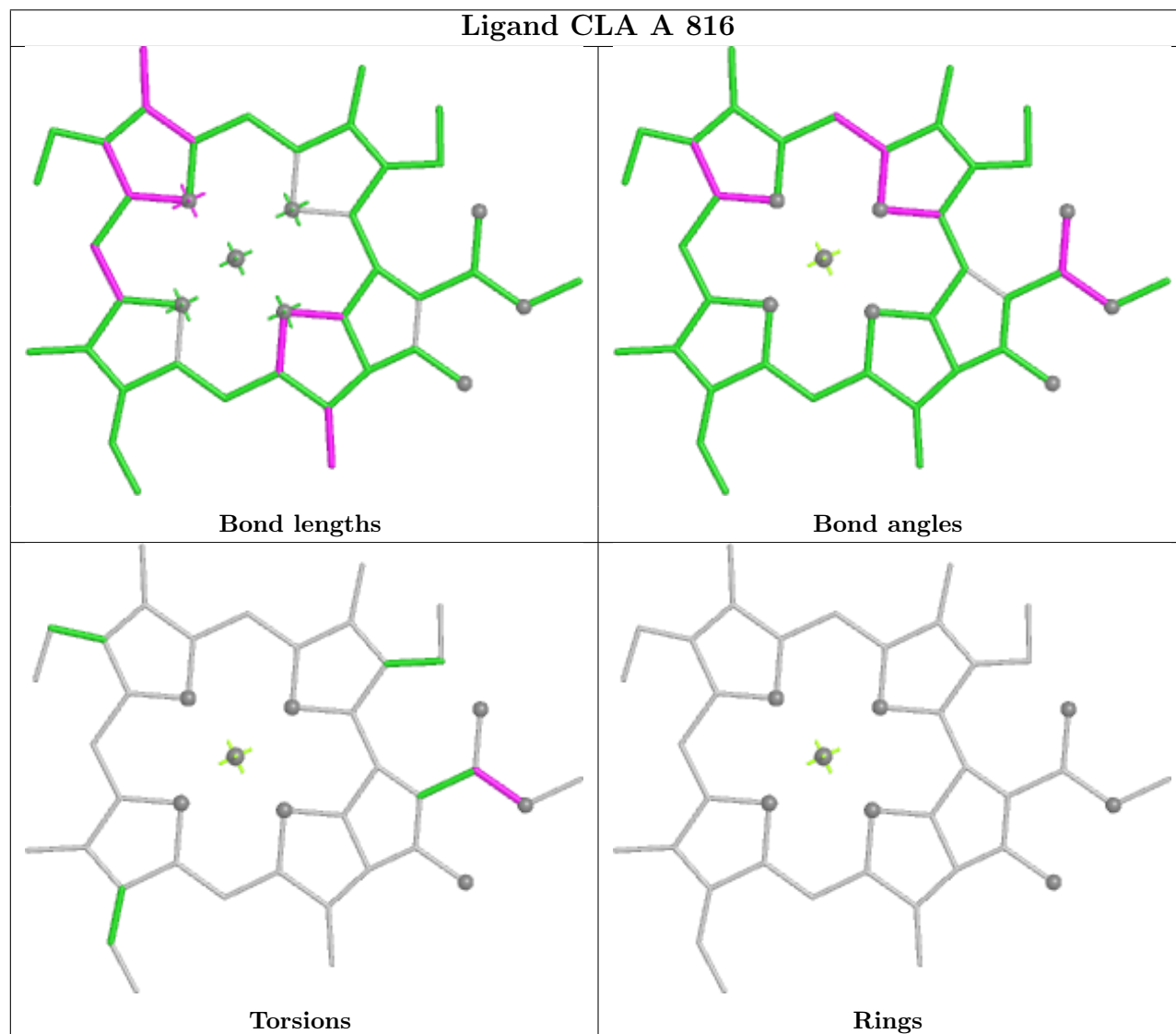
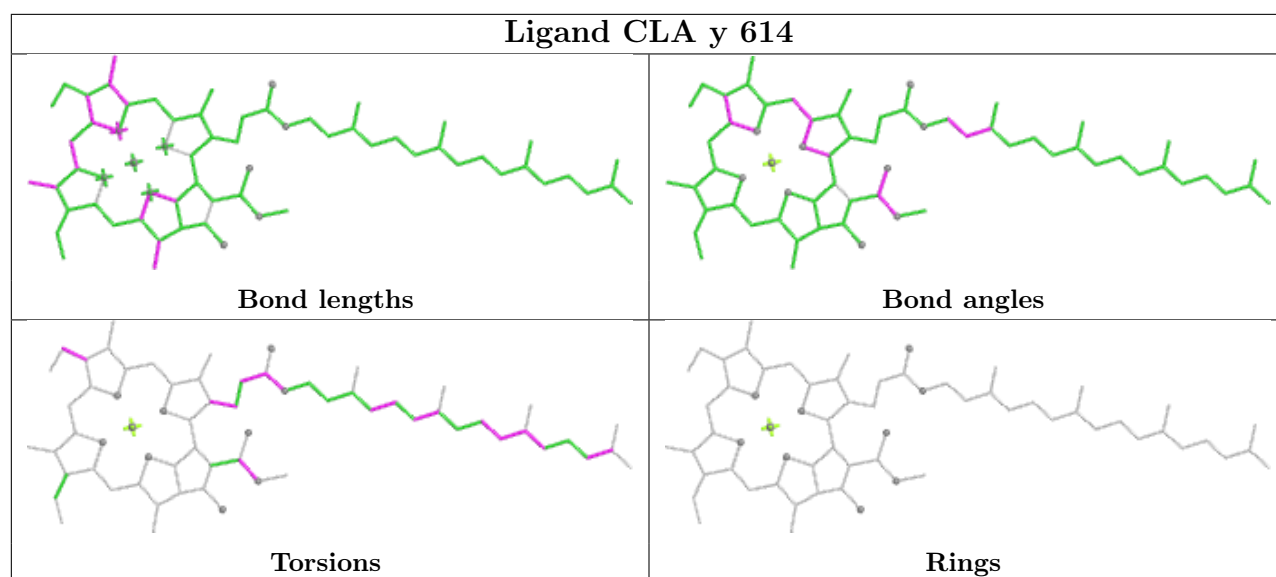


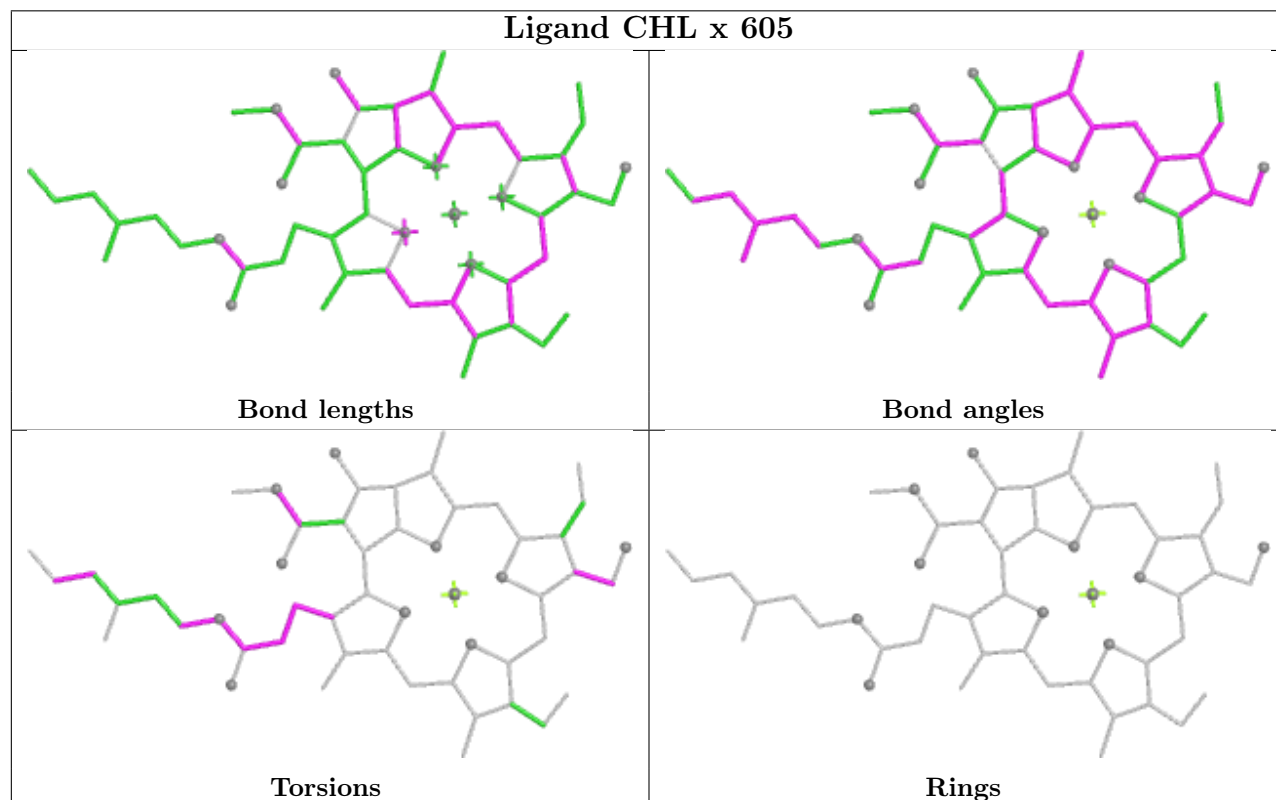
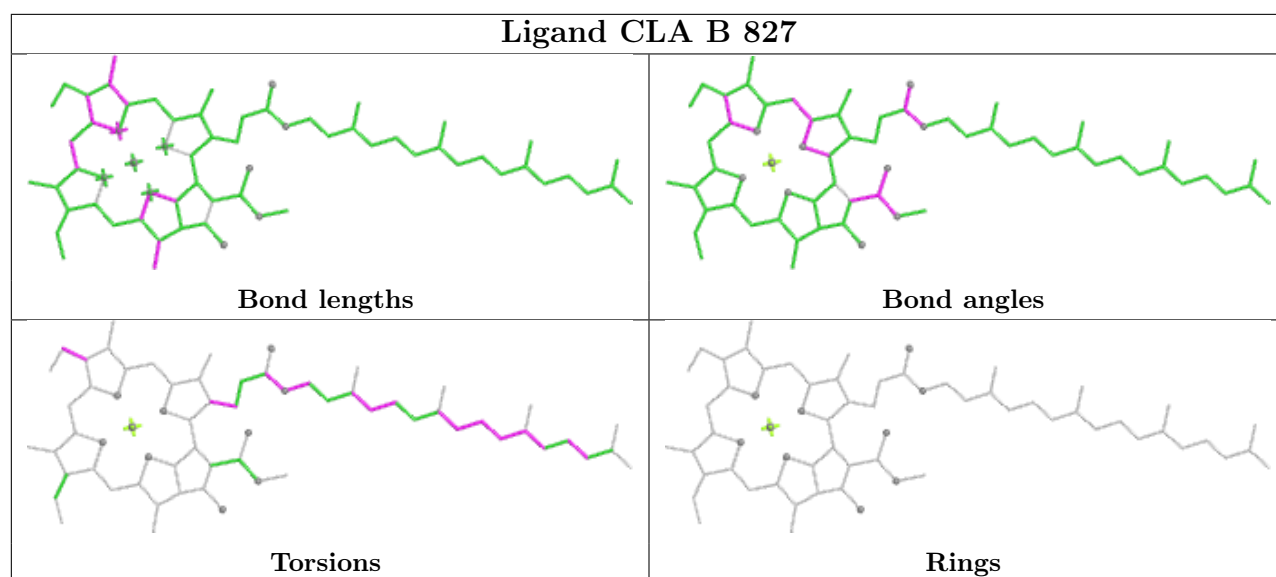
Ligand CLA 1 605

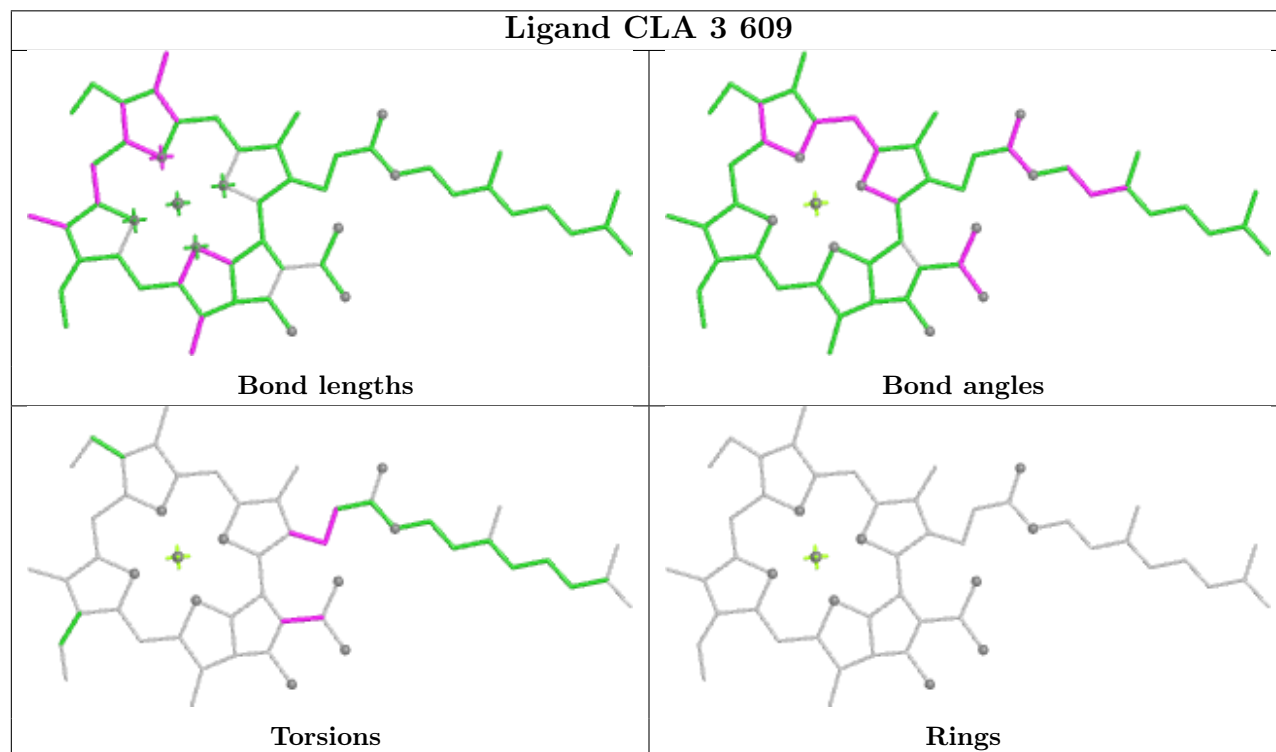
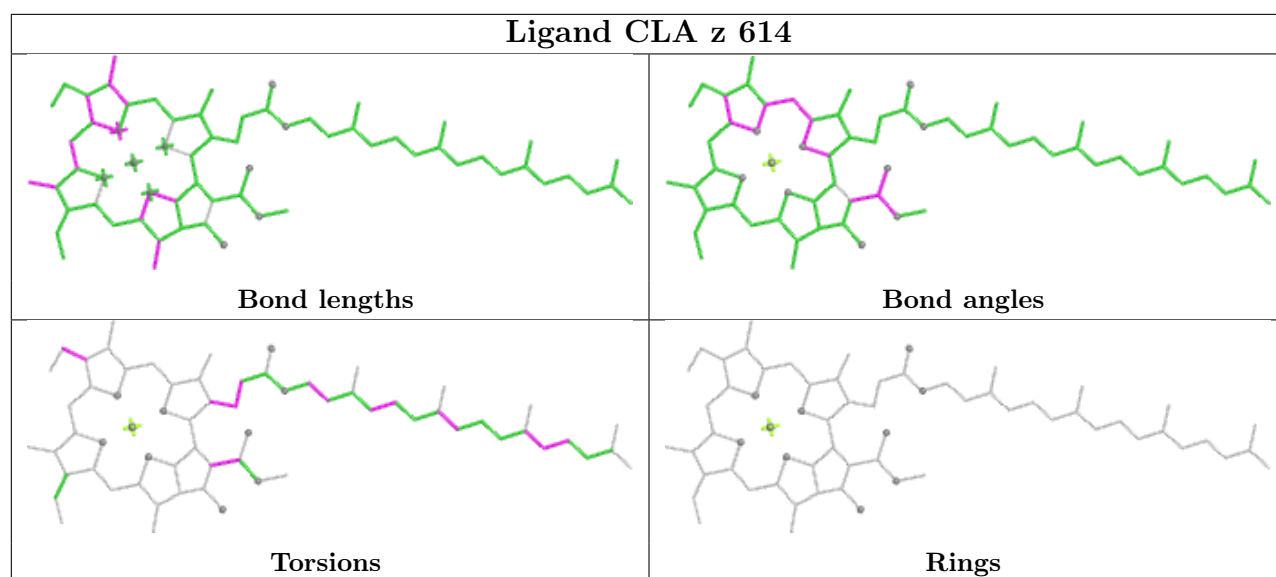


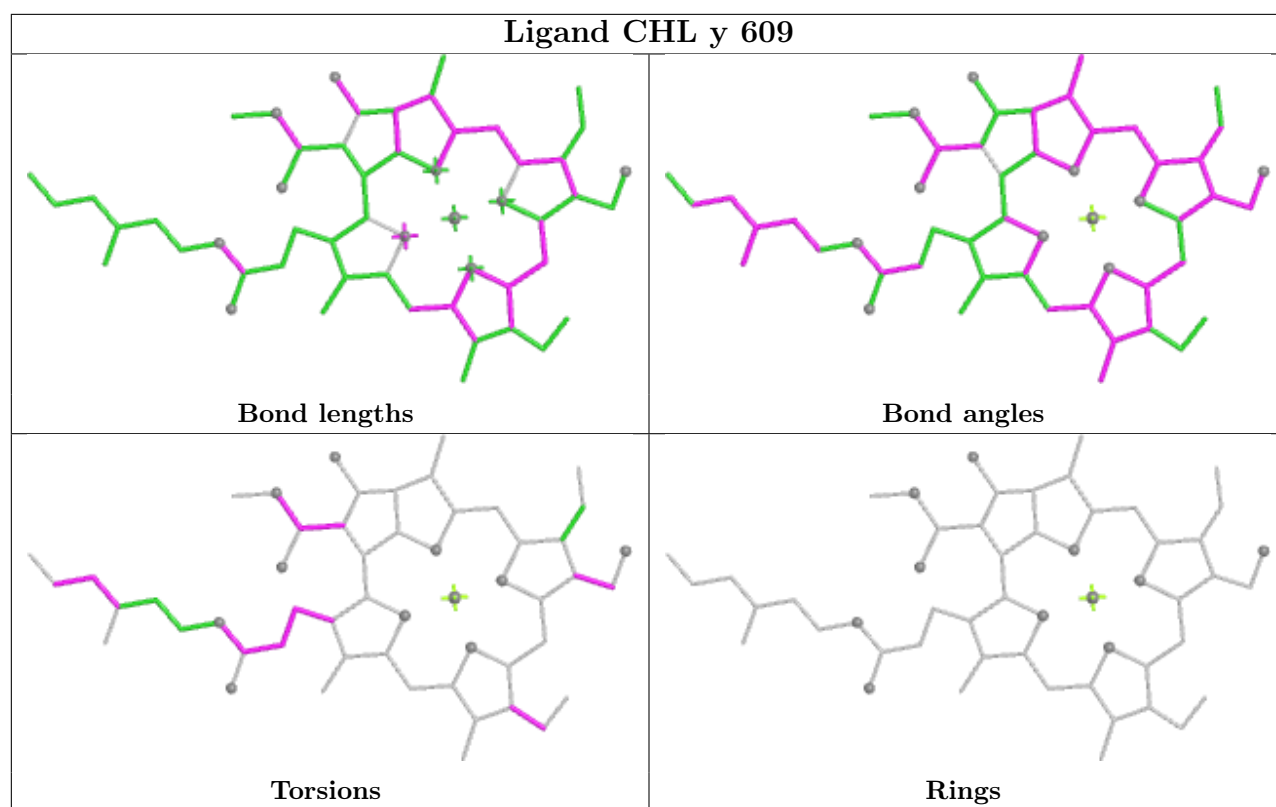
Ligand CLA B 813



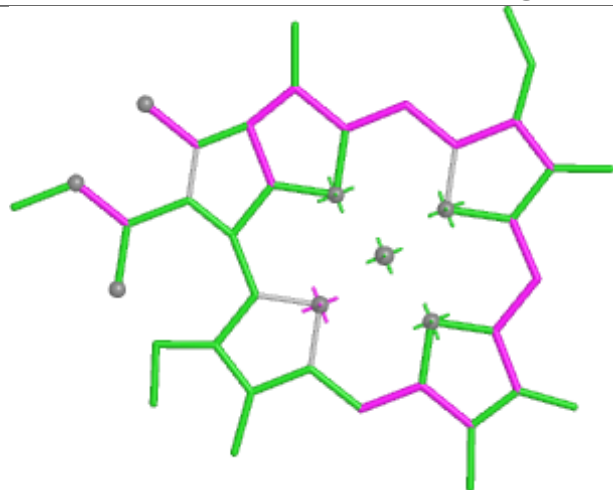




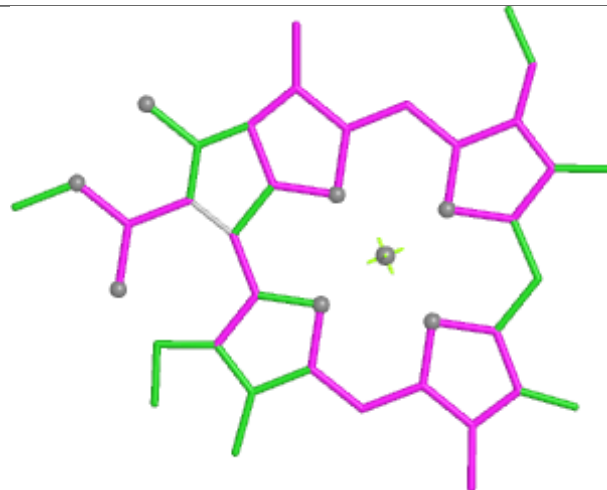




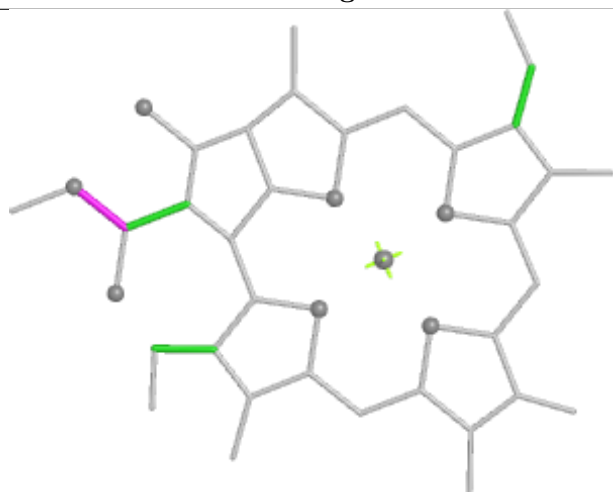
Ligand CHL 4 606



Bond lengths



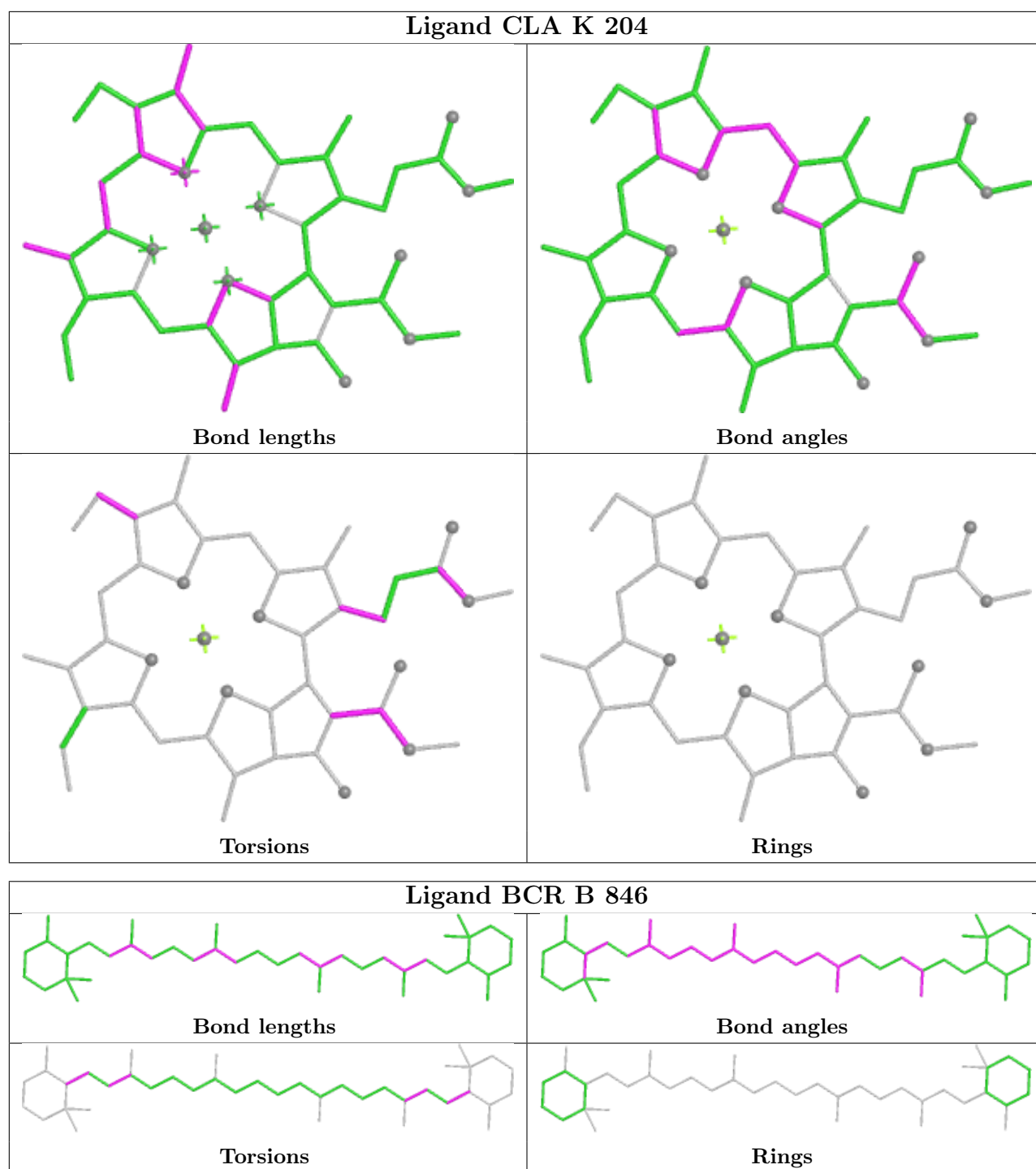
Bond angles



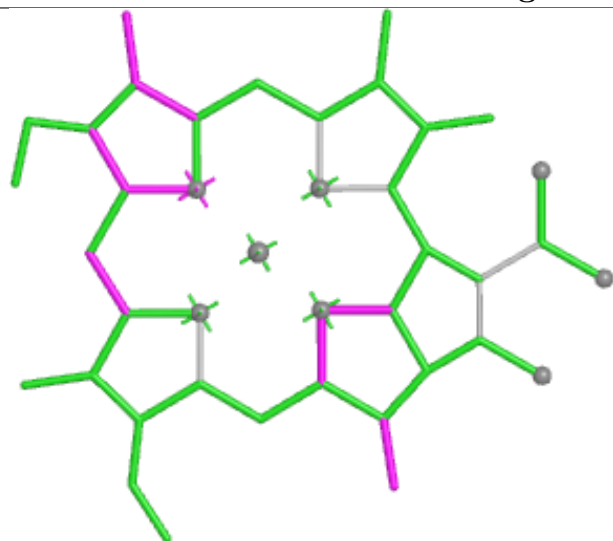
Torsions



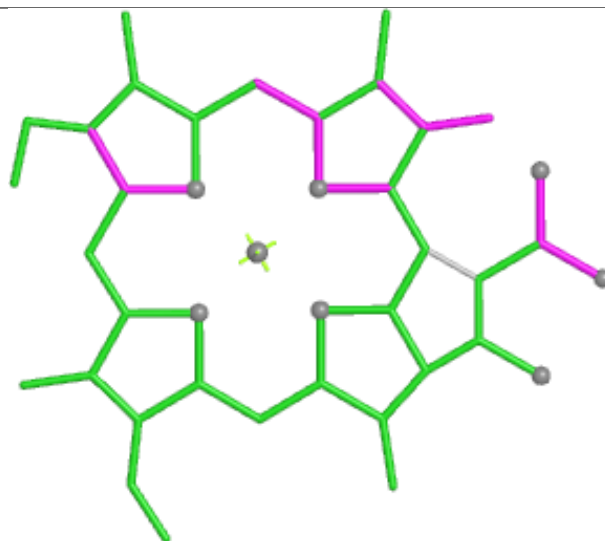
Rings



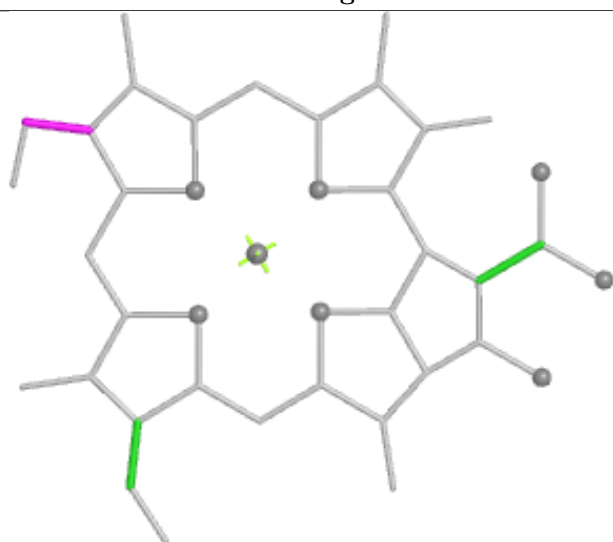
Ligand CLA 3 610



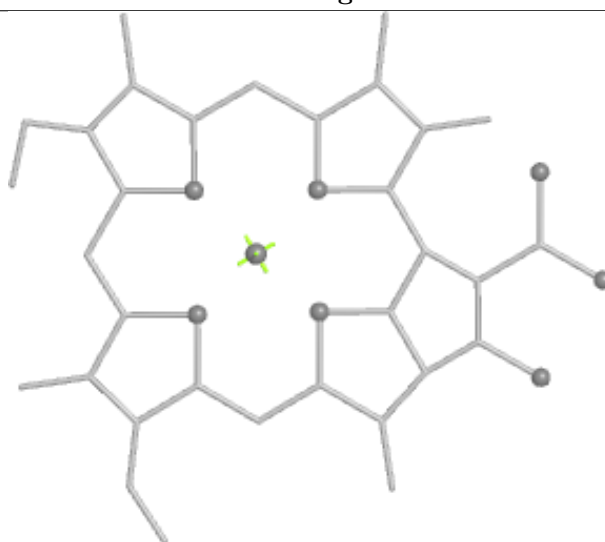
Bond lengths



Bond angles

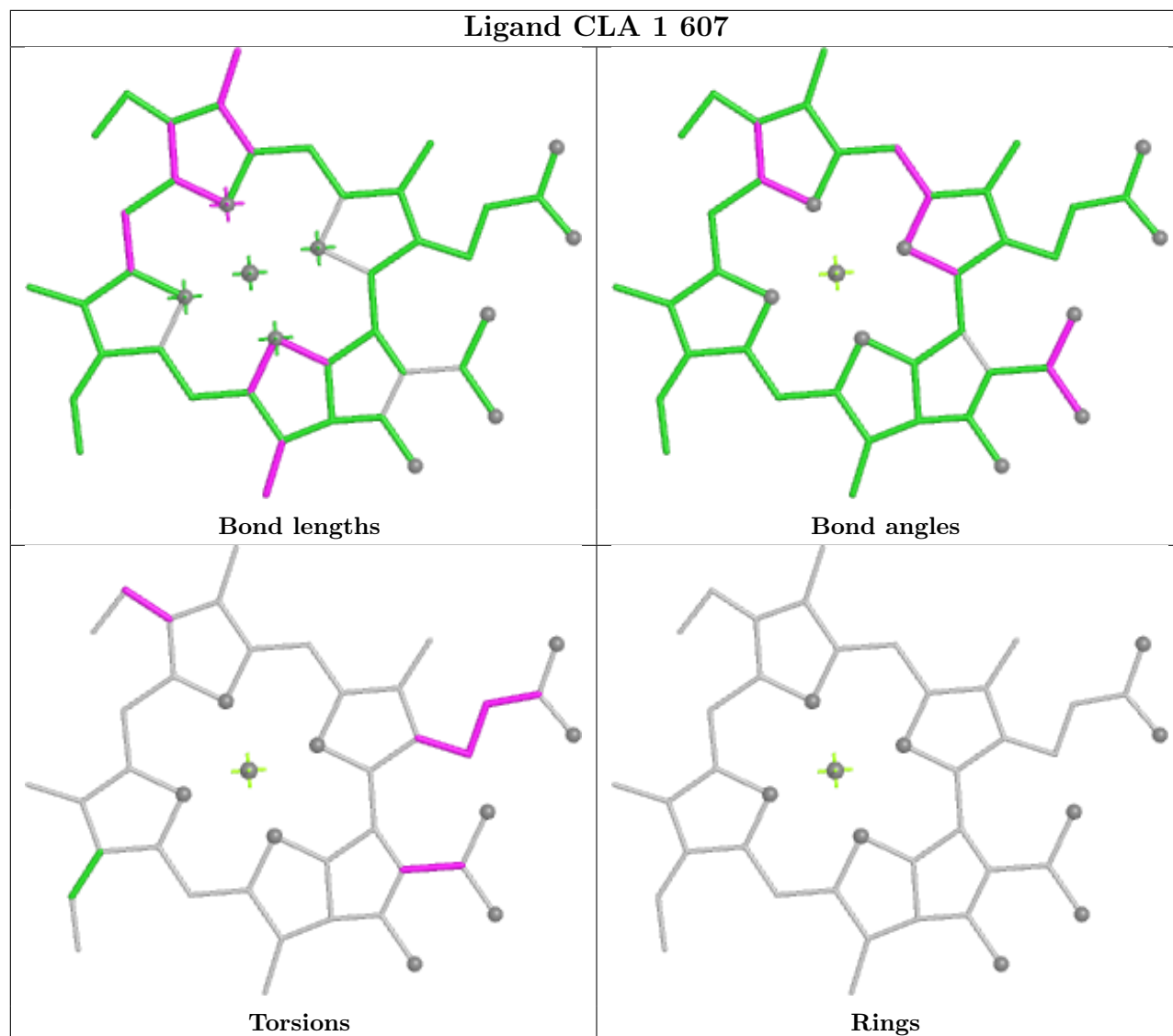


Torsions

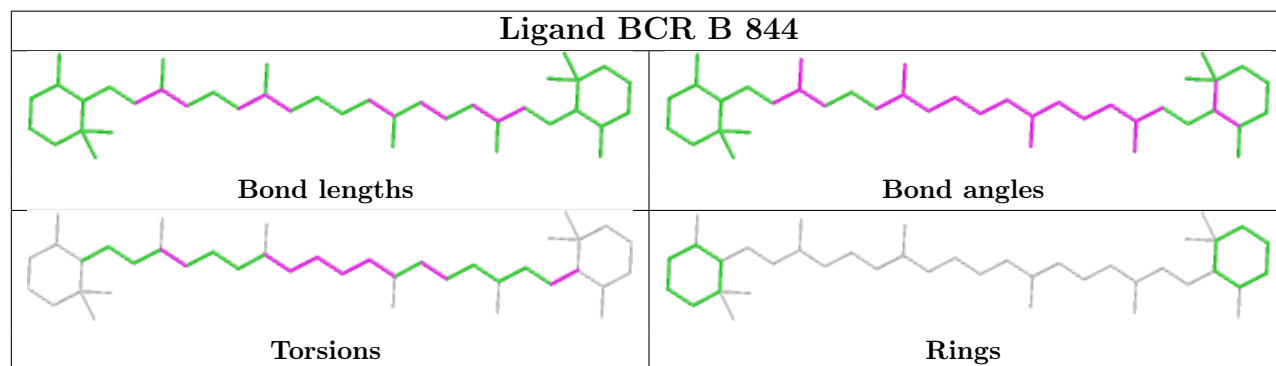


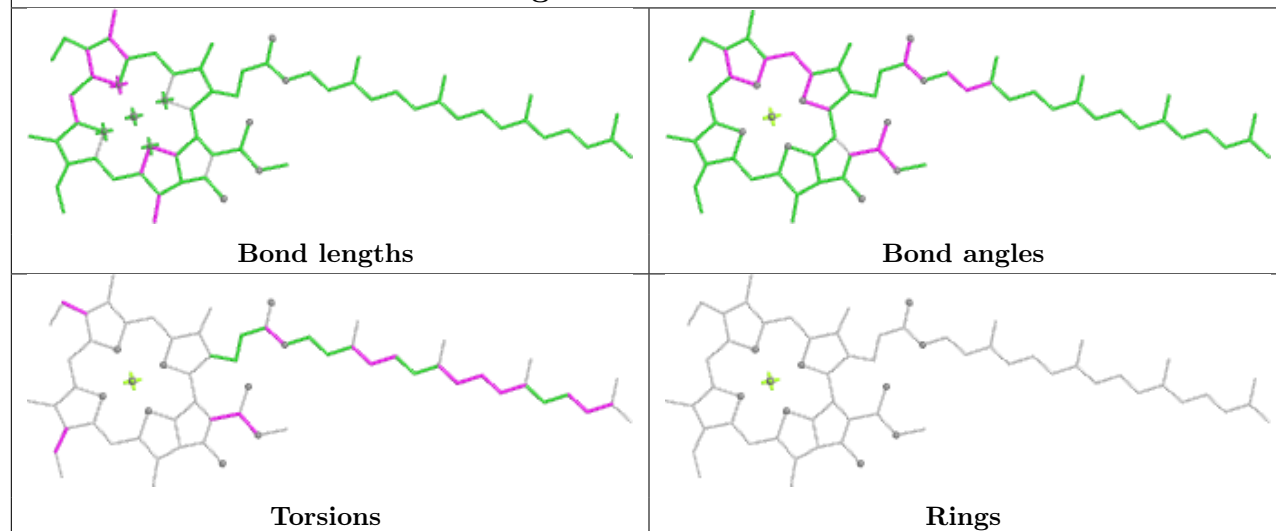
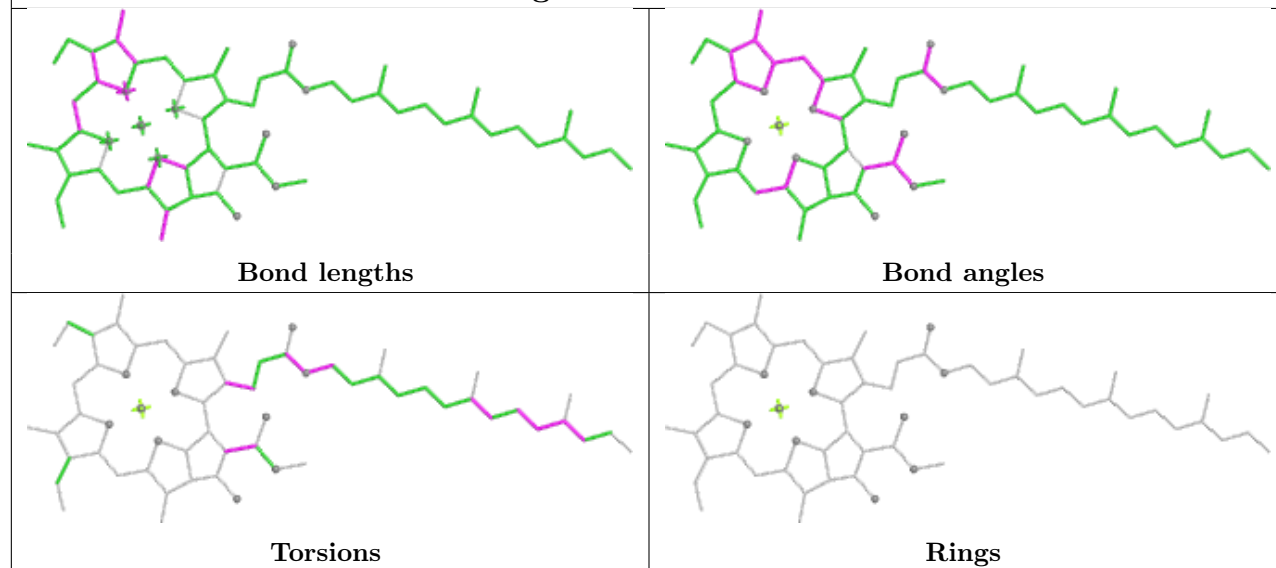
Rings

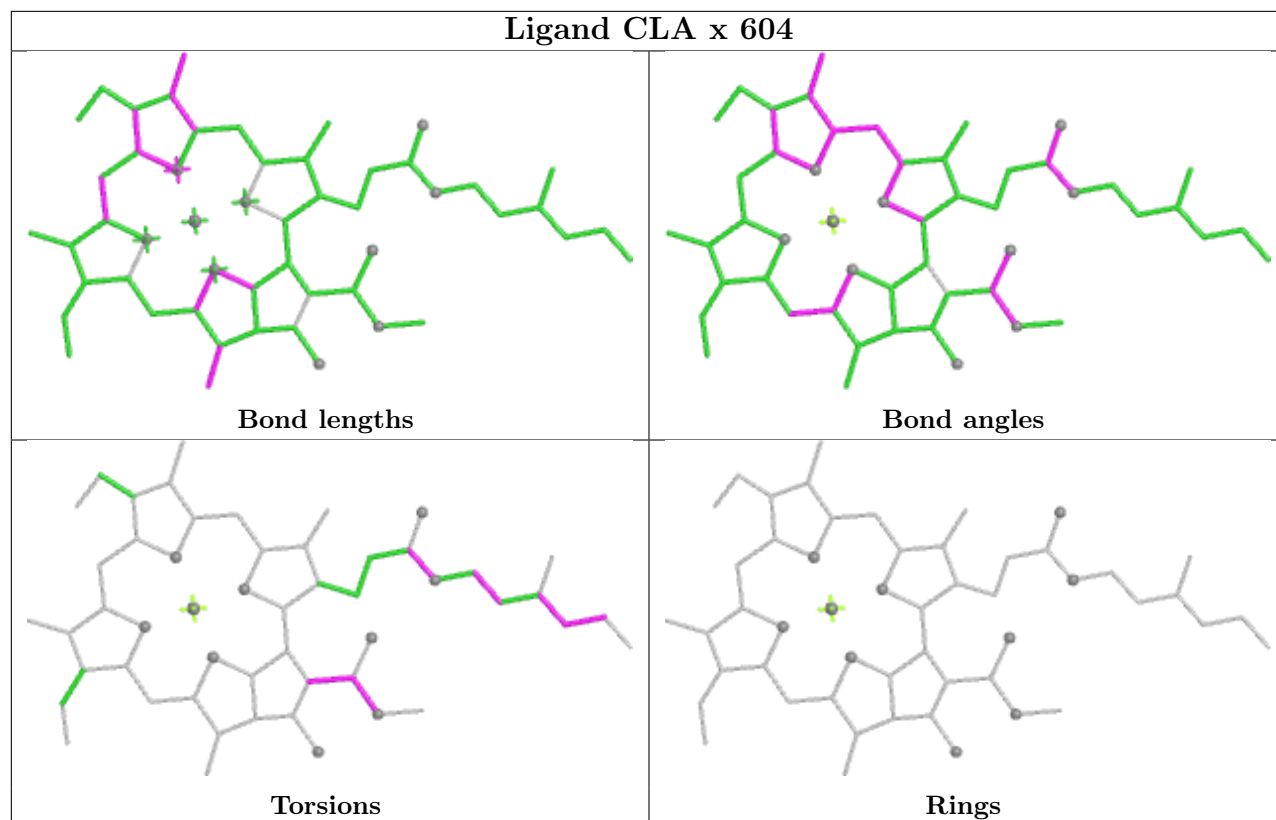
Ligand CLA 1 607



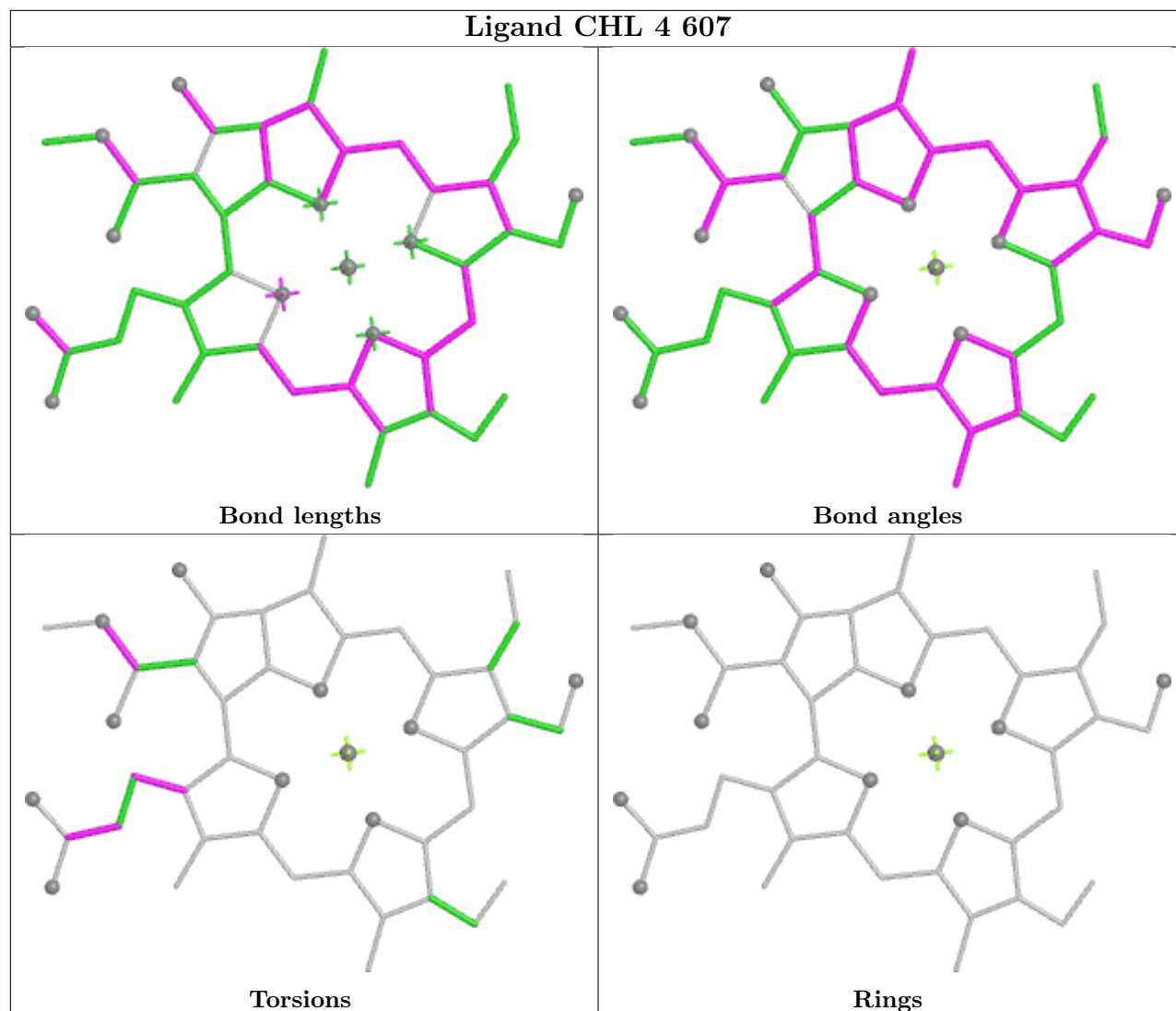
Ligand BCR B 844



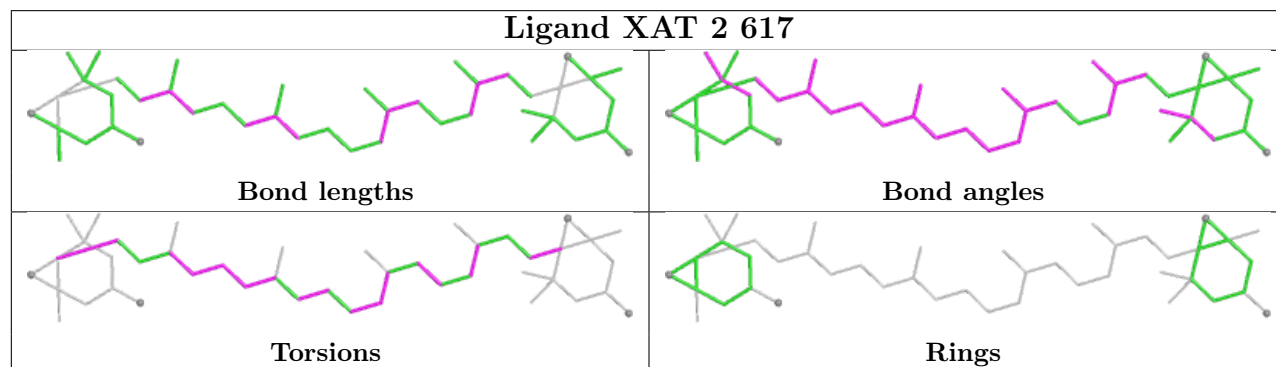
Ligand CLA A 835**Ligand CLA B 825**



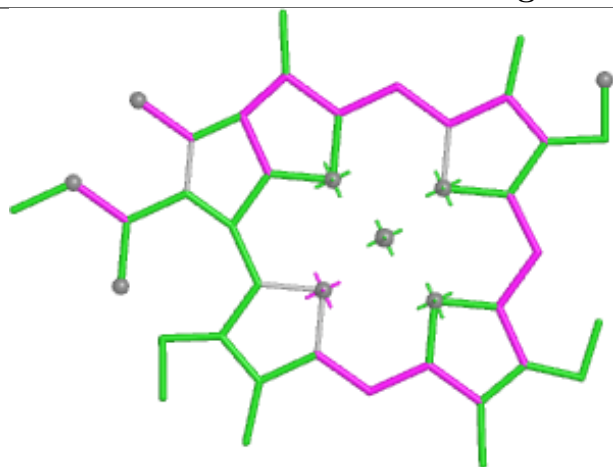
Ligand CHL 4 607



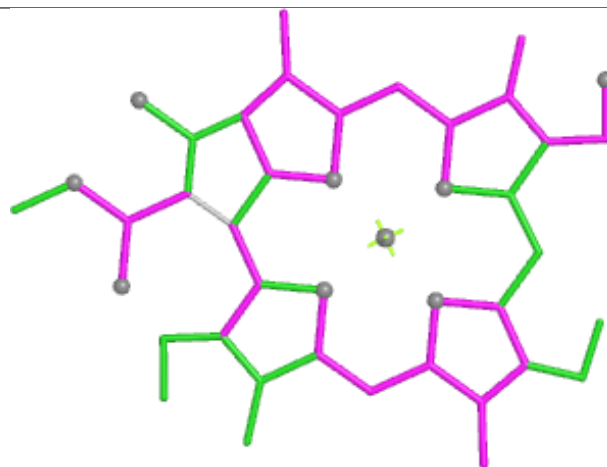
Ligand XAT 2 617



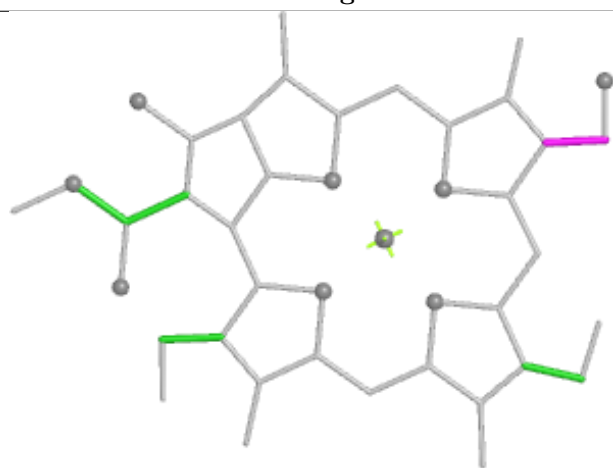
Ligand CHL 2 605



Bond lengths



Bond angles

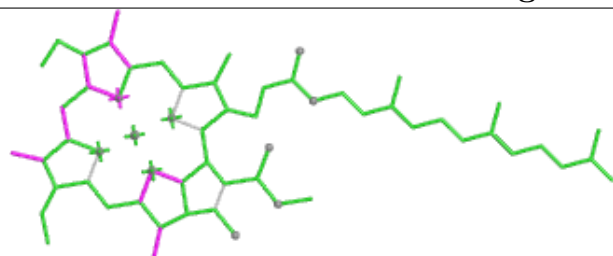


Torsions

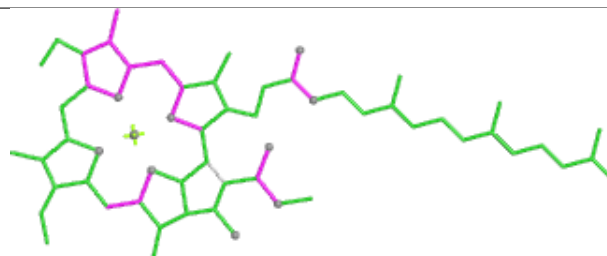


Rings

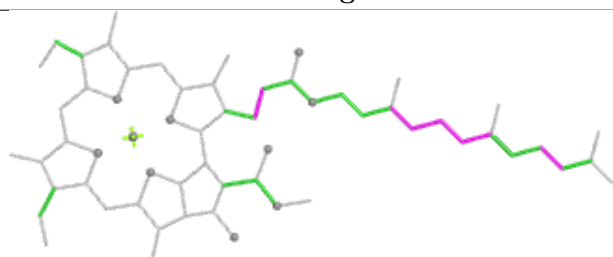
Ligand CLA 4 602



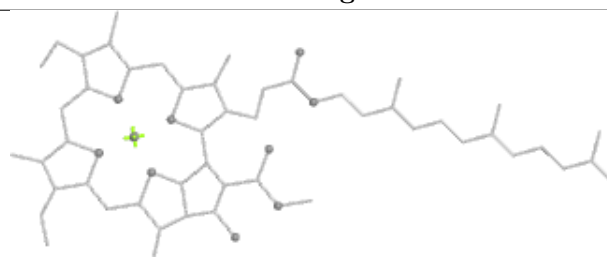
Bond lengths



Bond angles

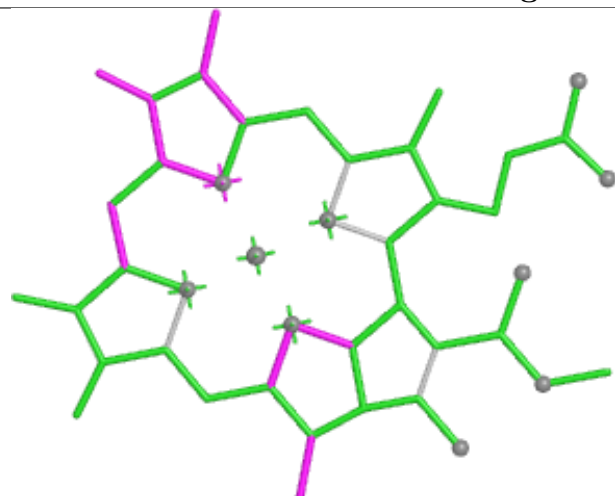


Torsions

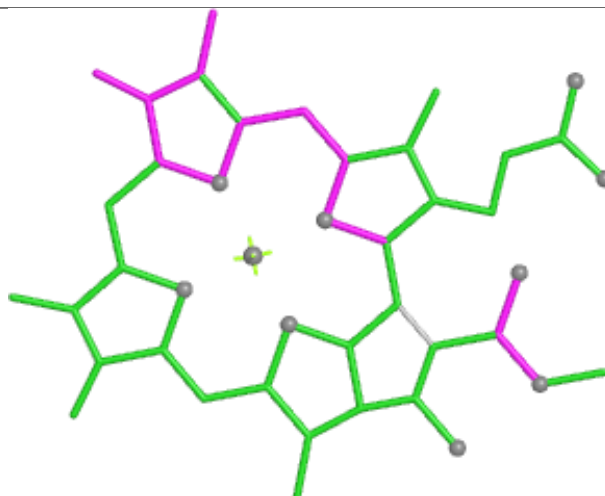


Rings

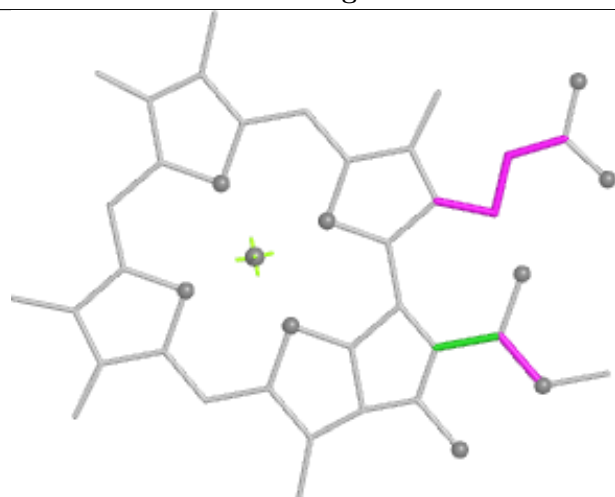
Ligand CLA 4 604



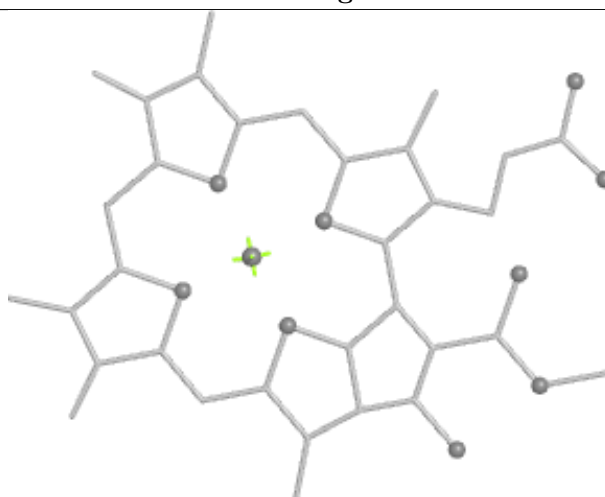
Bond lengths



Bond angles

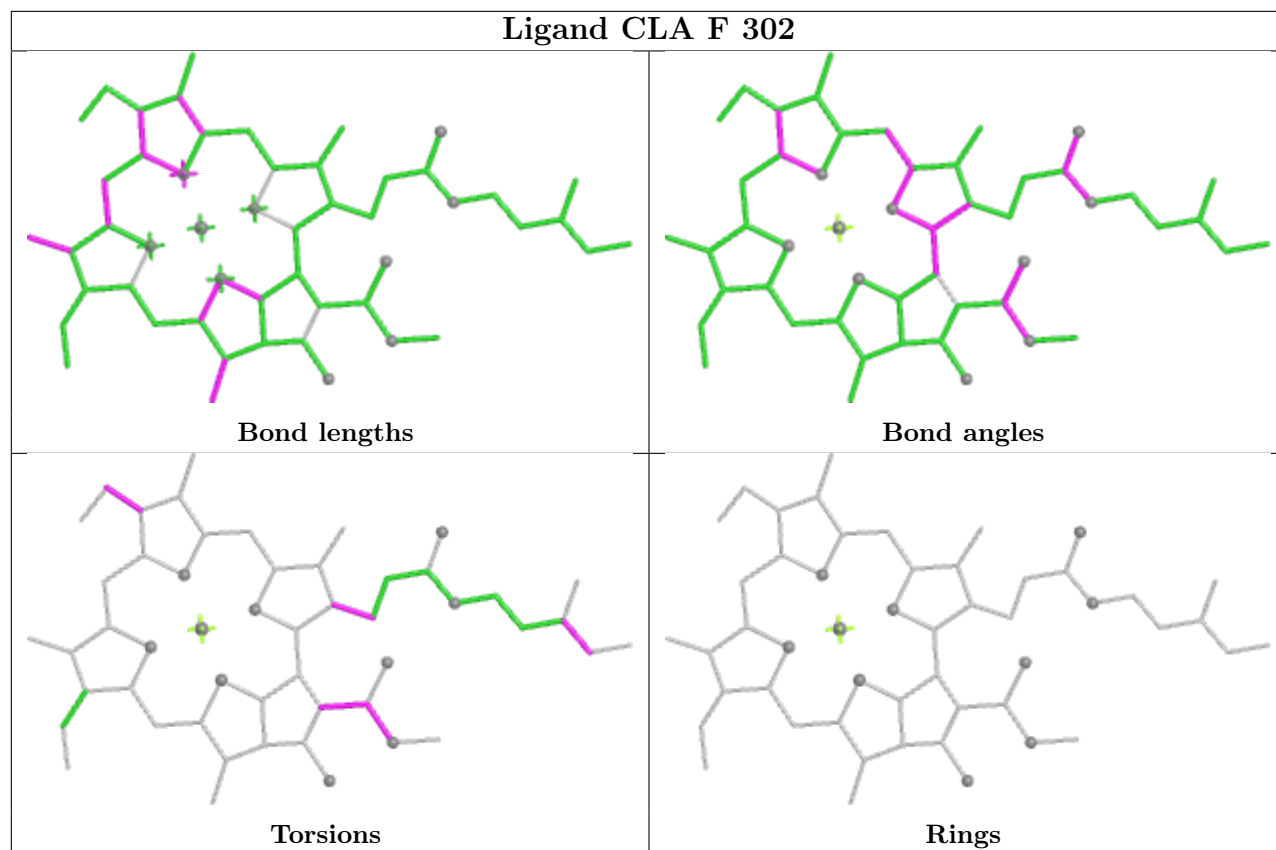


Torsions

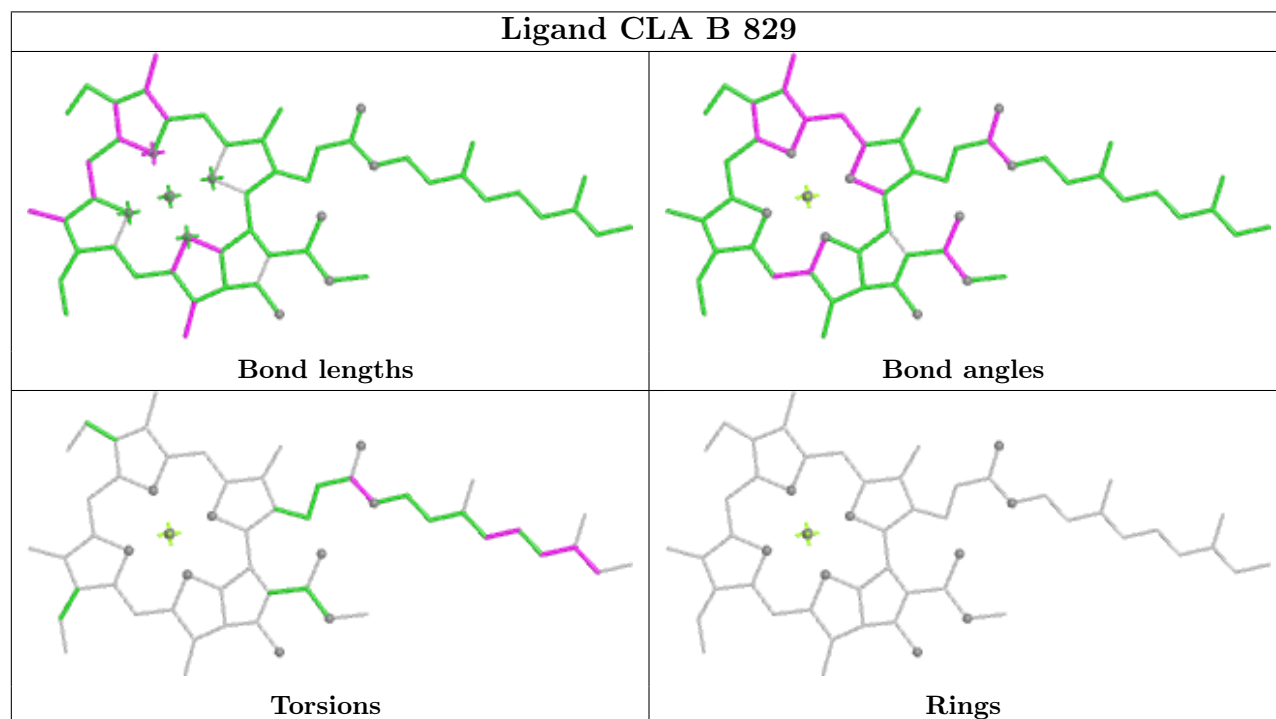


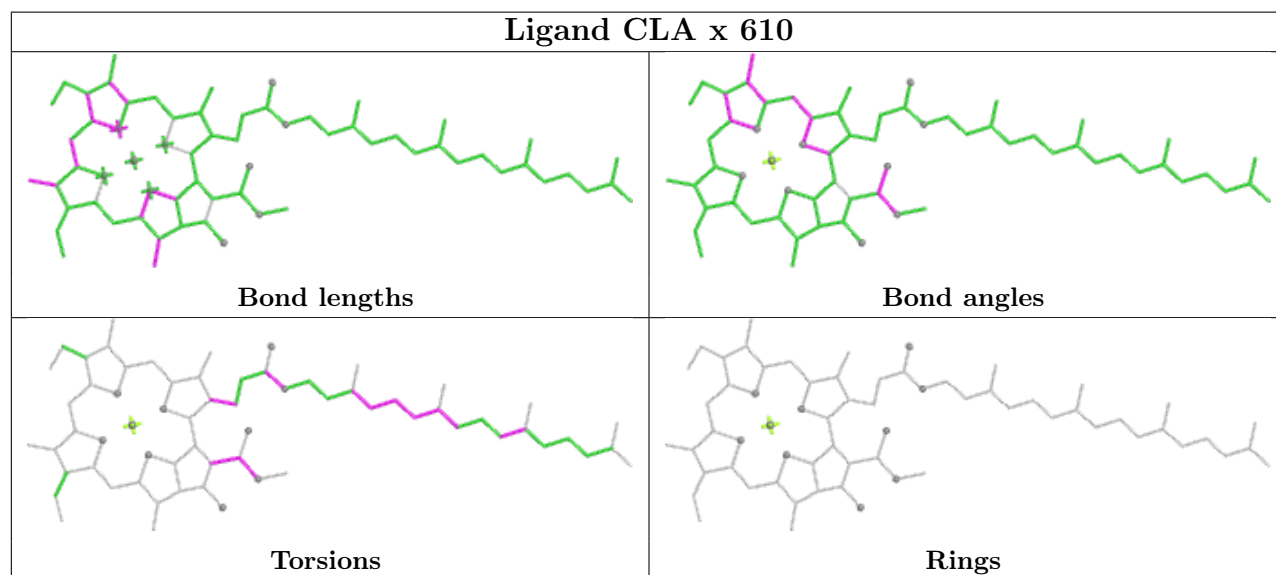
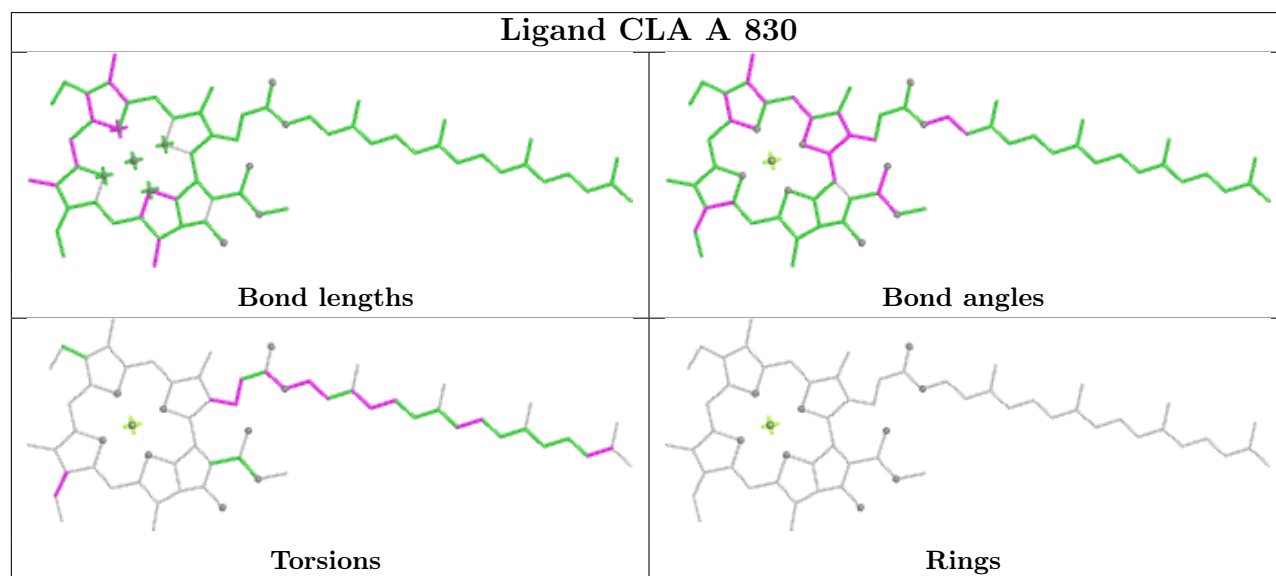
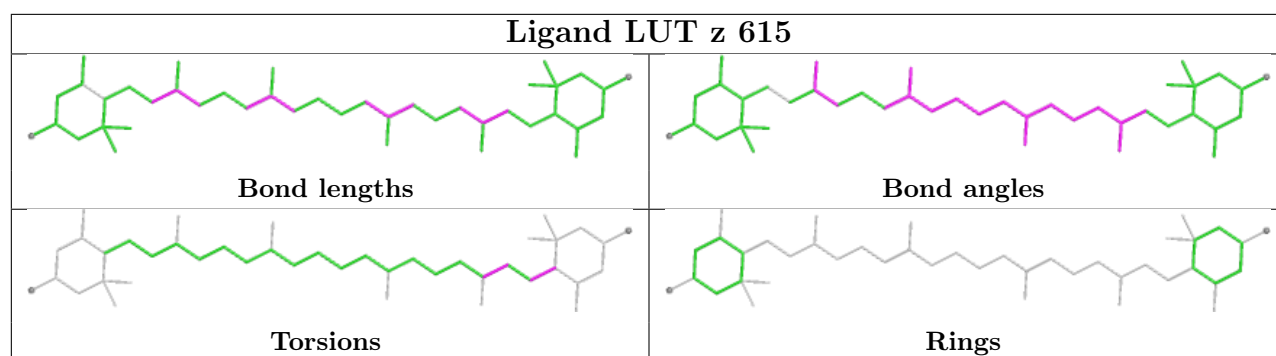
Rings

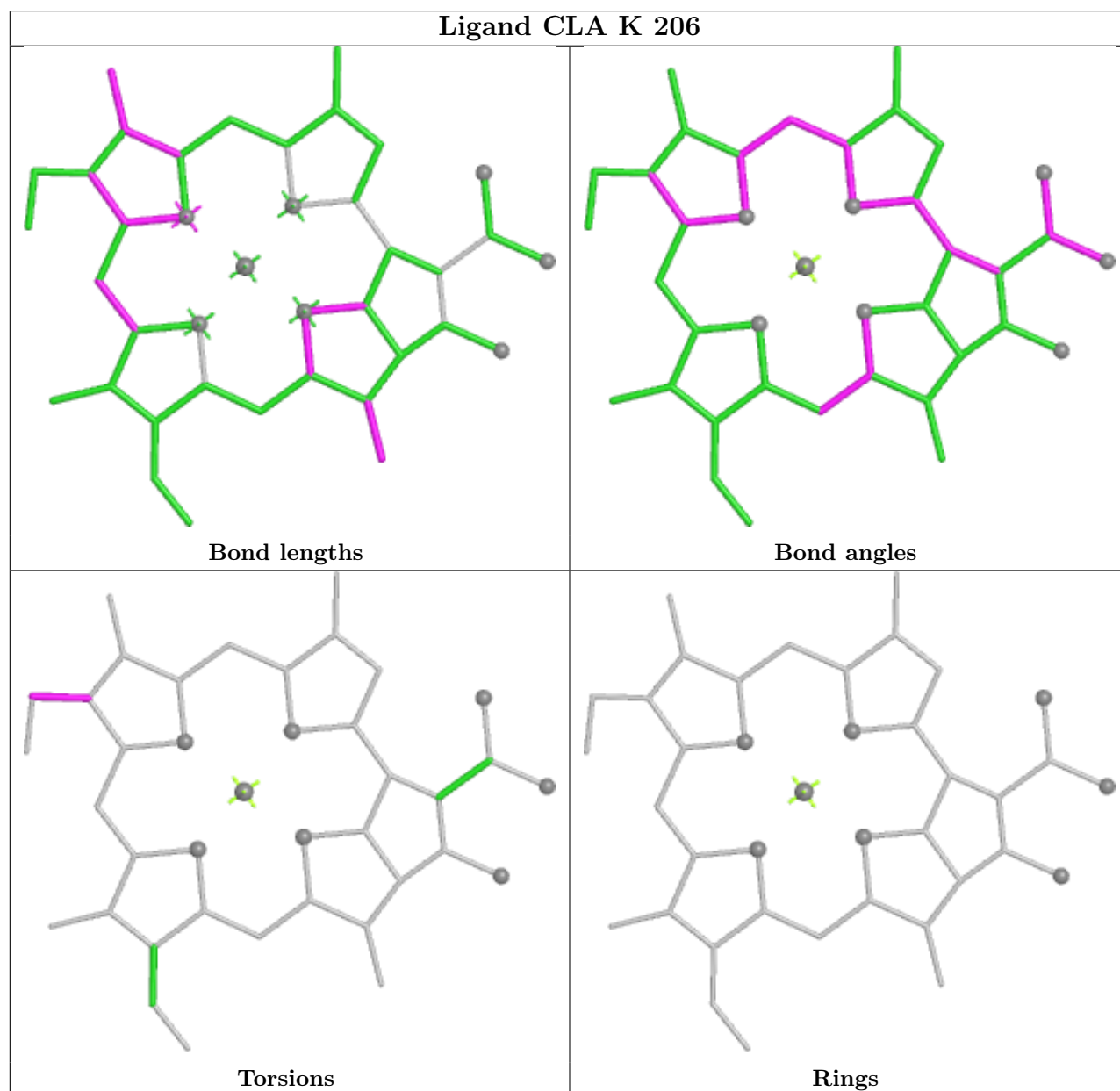
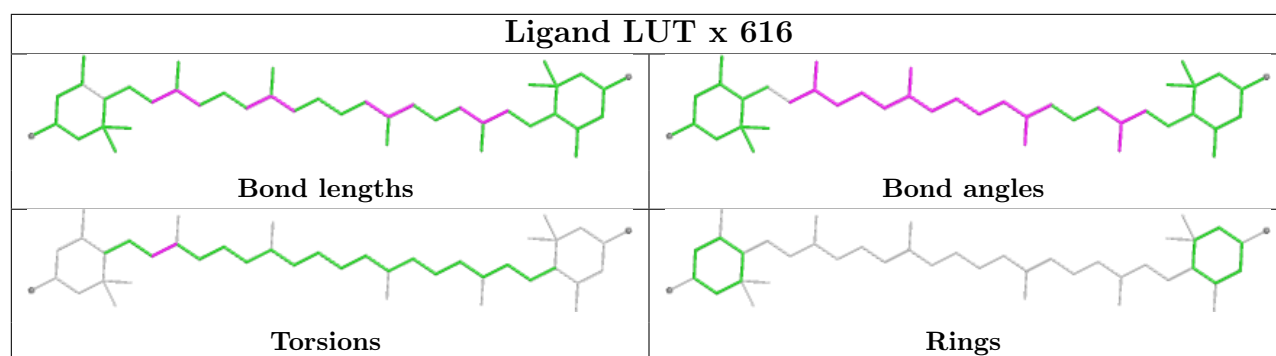
Ligand CLA F 302

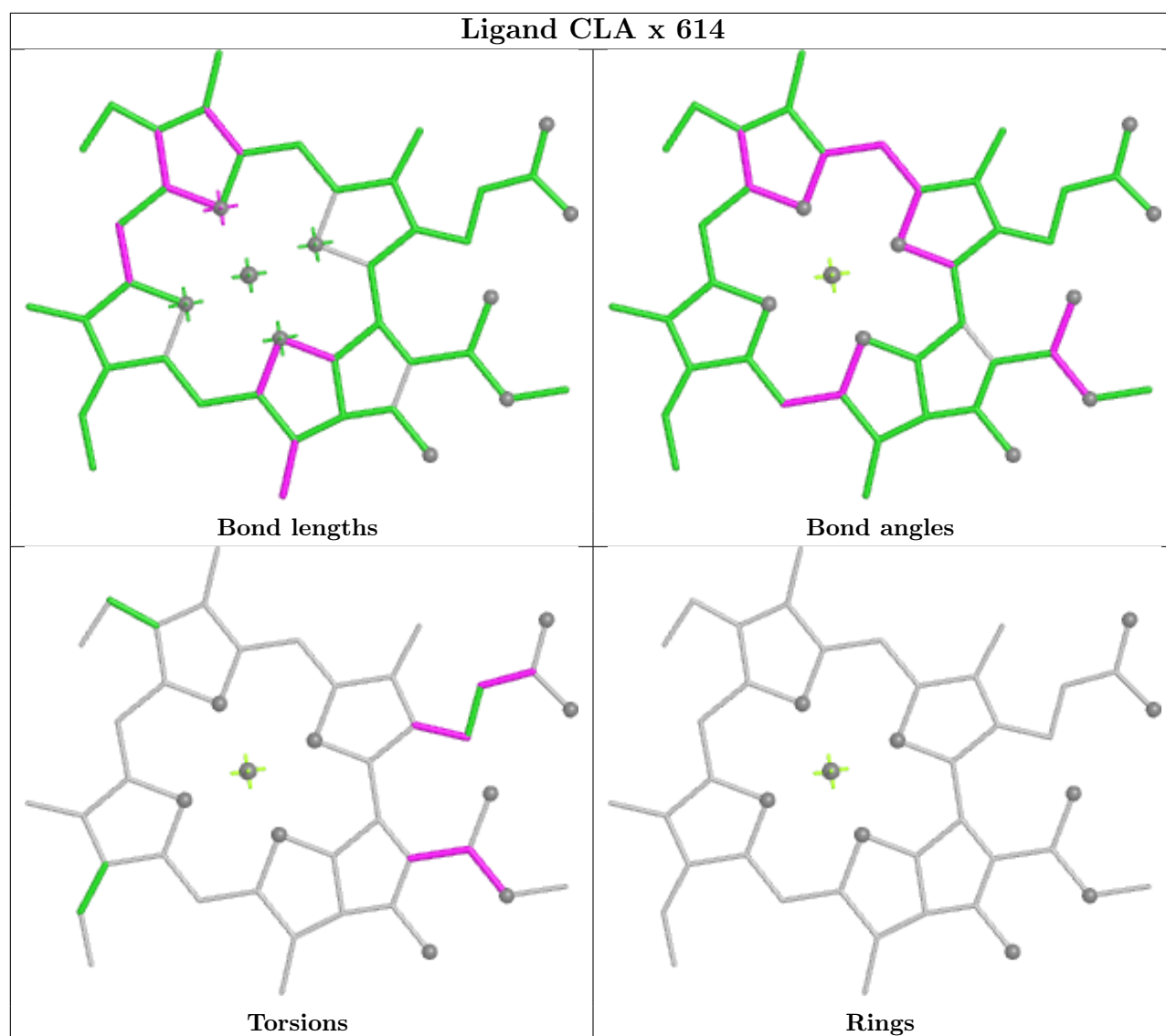


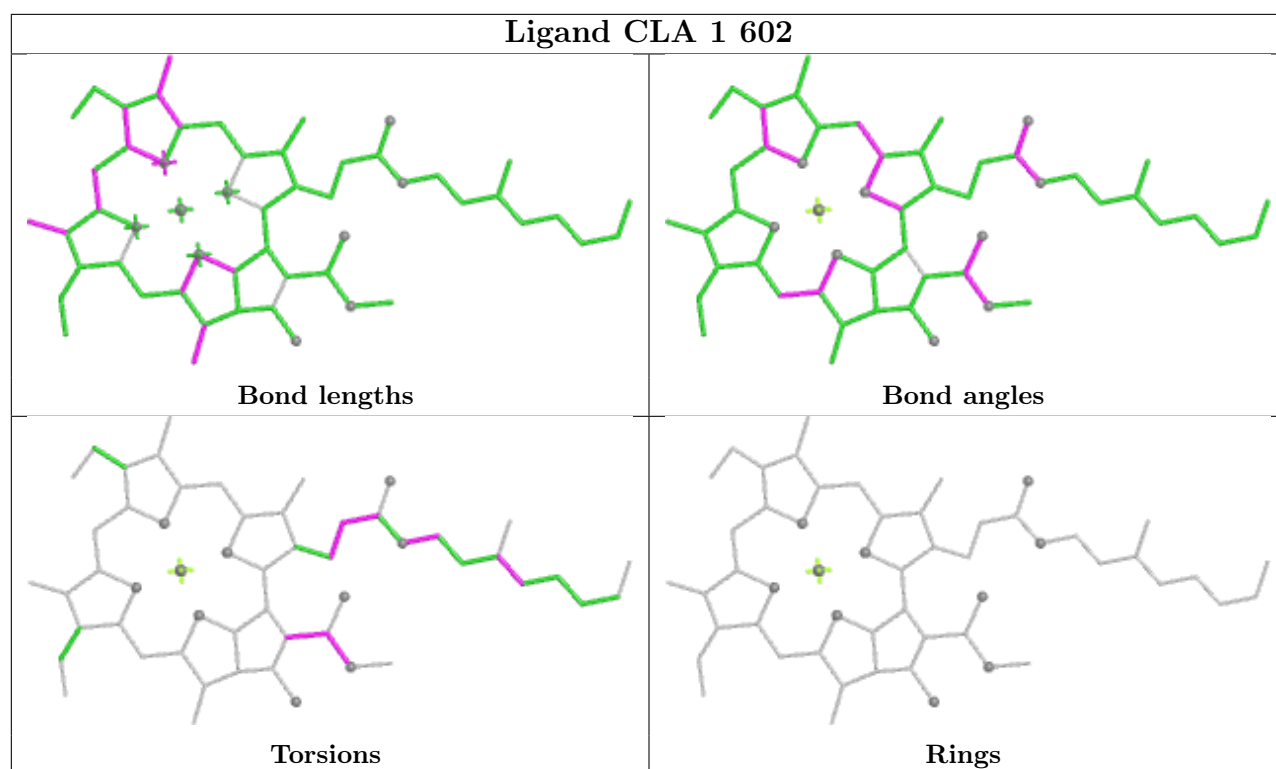
Ligand CLA B 829



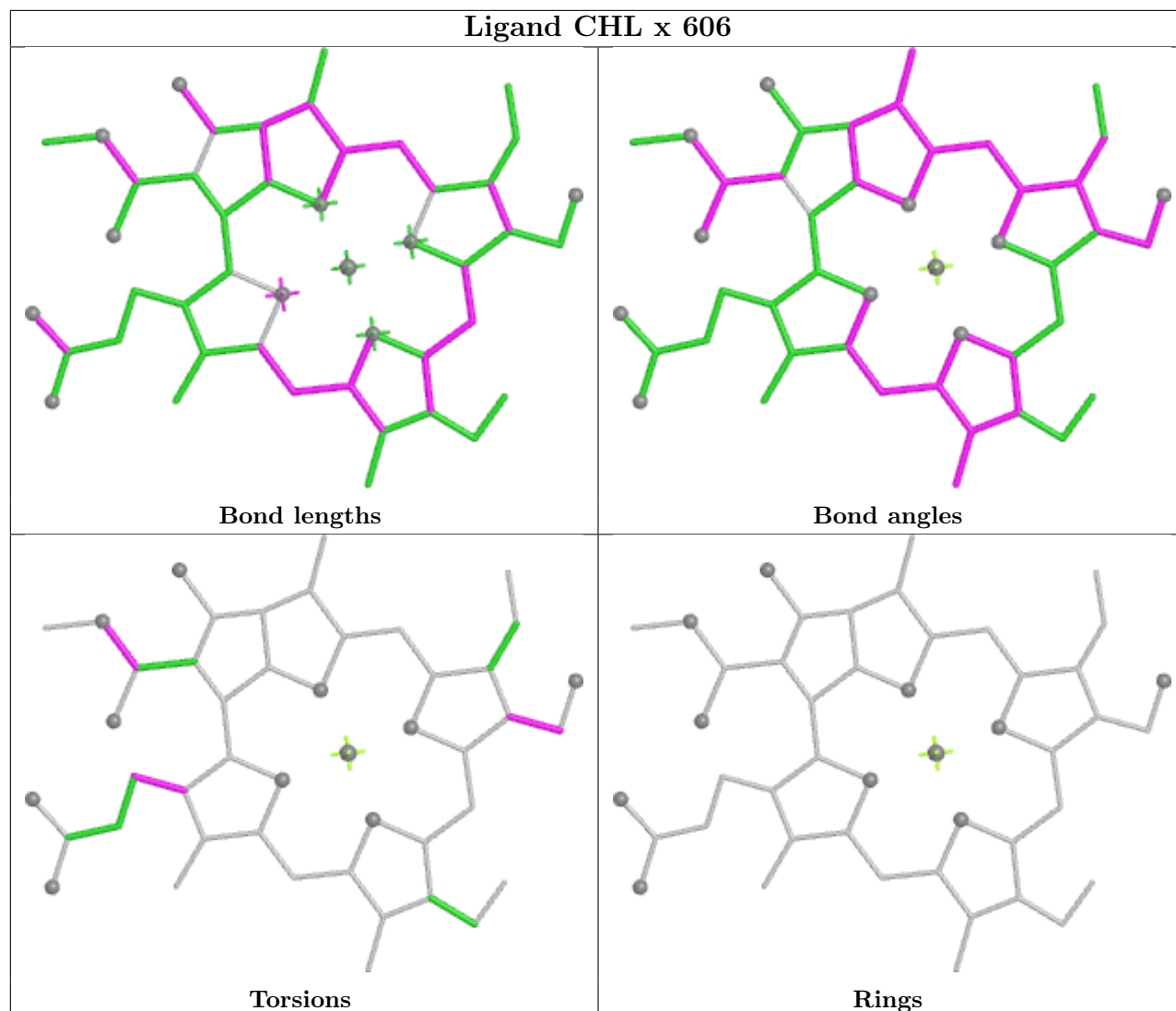




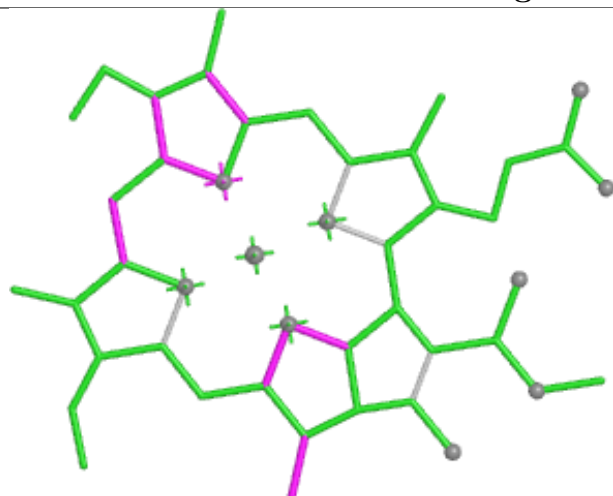




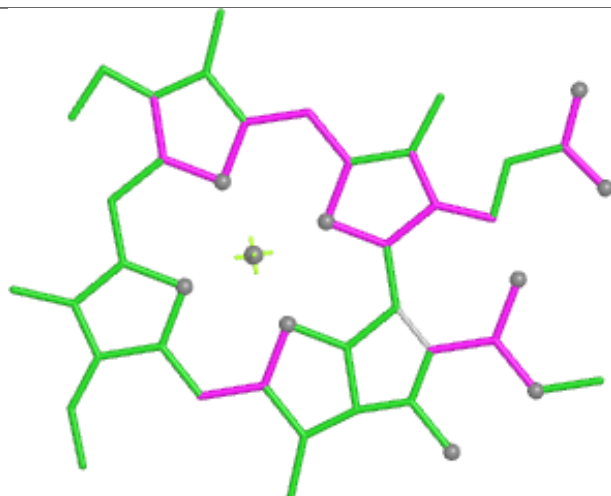
Ligand CHL x 606



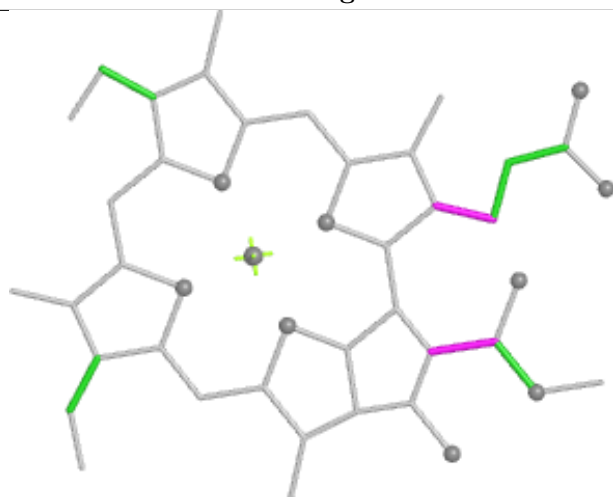
Ligand CLA B 833



Bond lengths



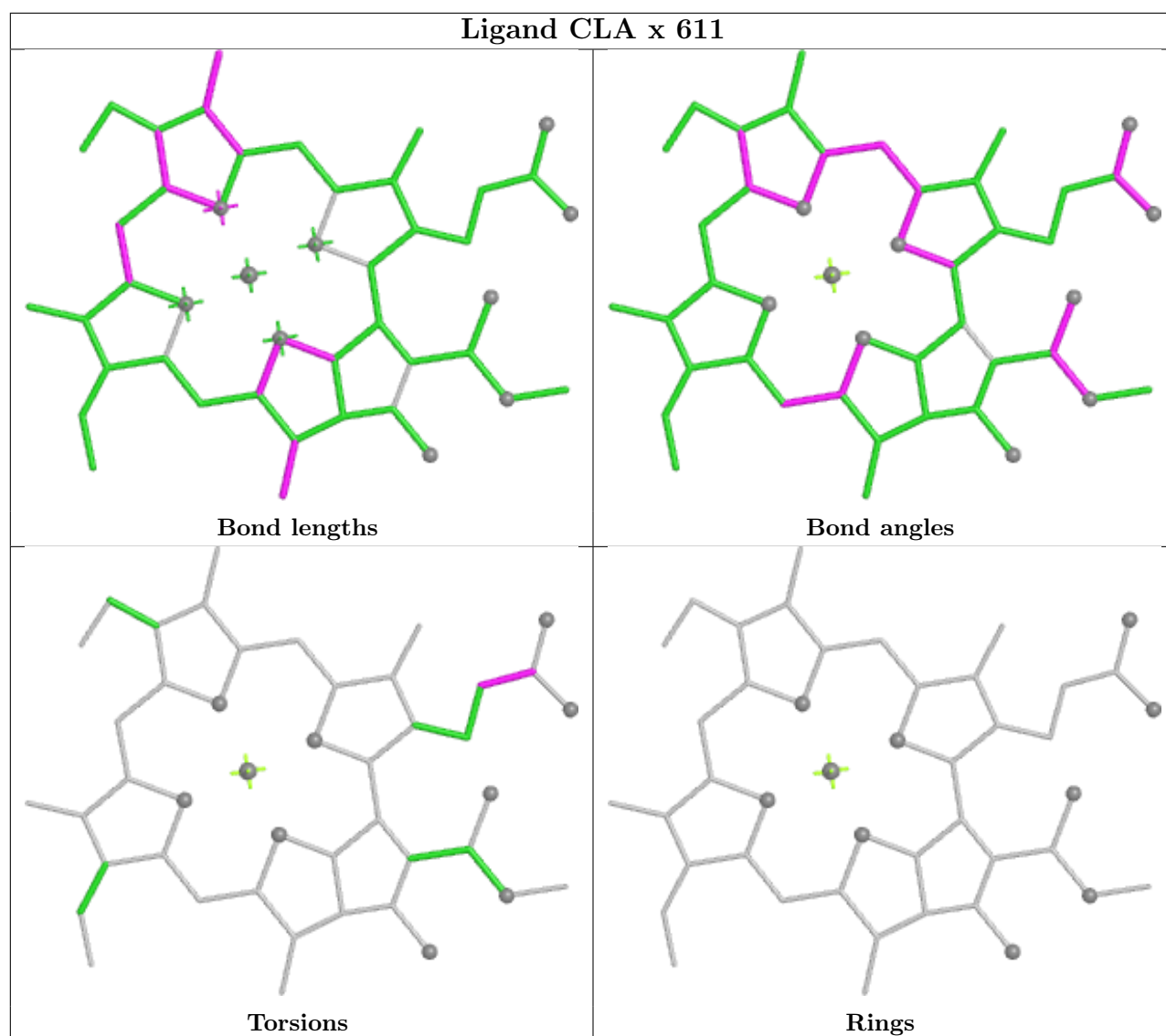
Bond angles



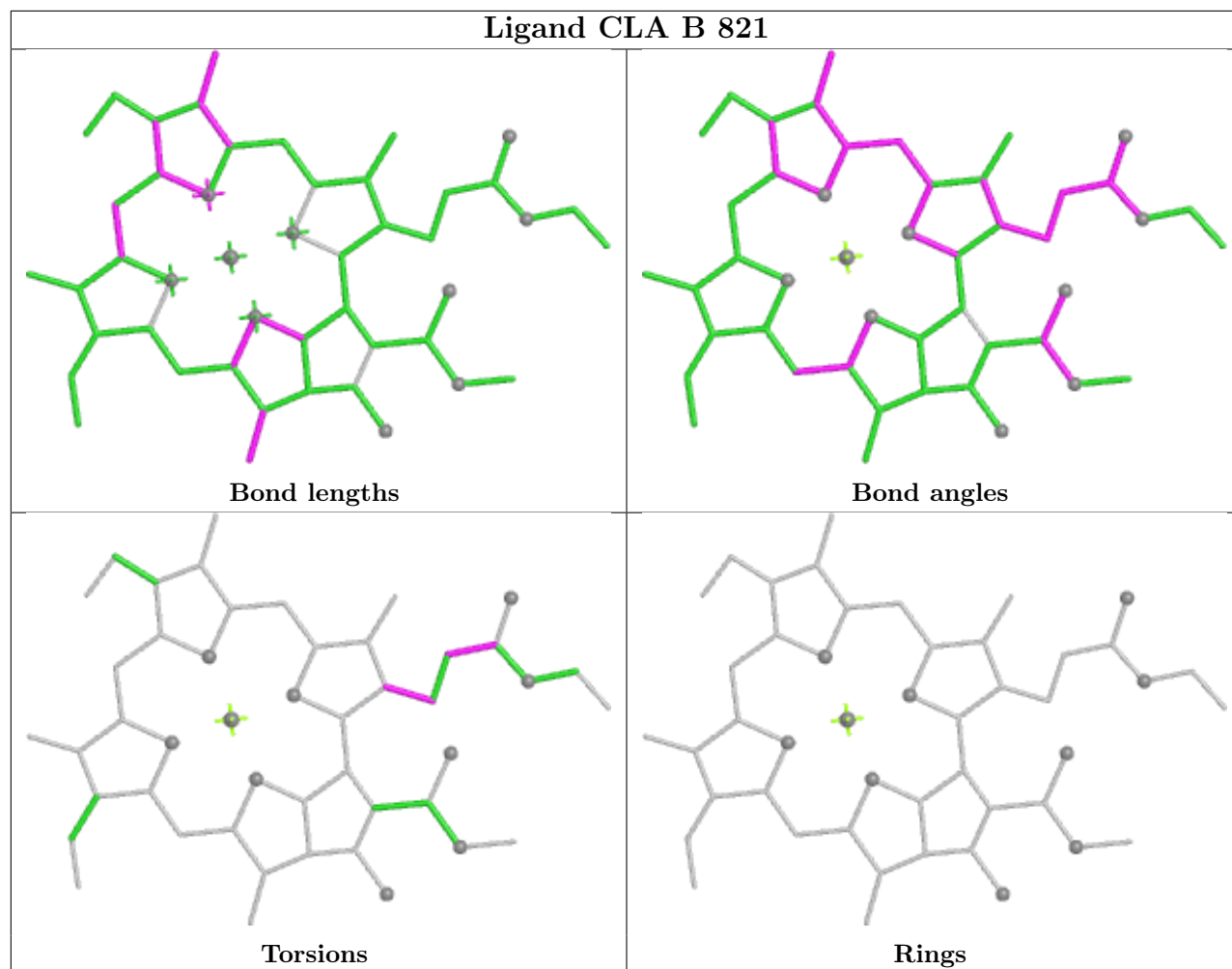
Torsions



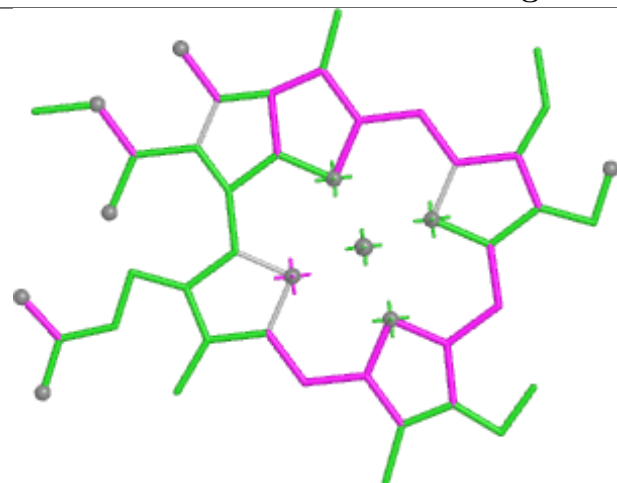
Rings



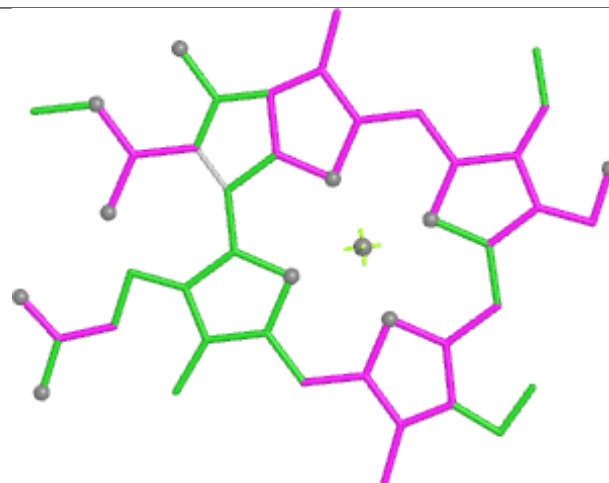
Ligand CLA B 821



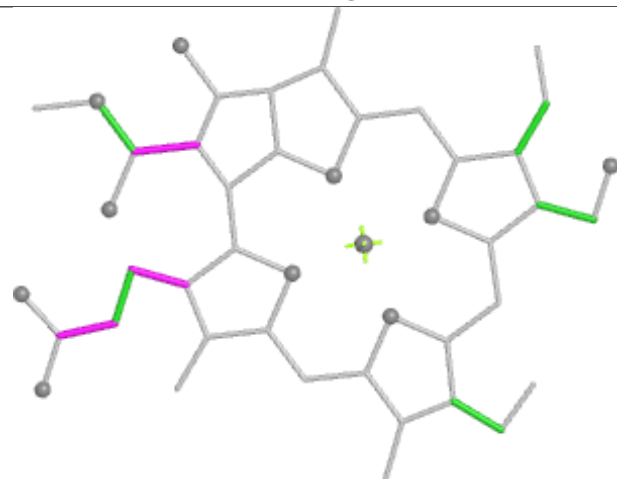
Ligand CHL x 609



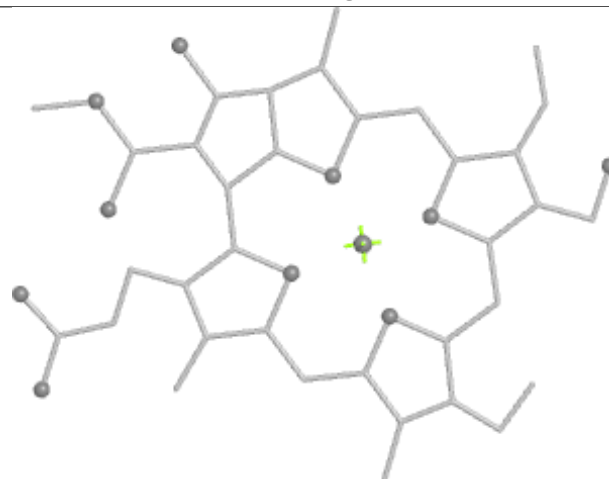
Bond lengths



Bond angles

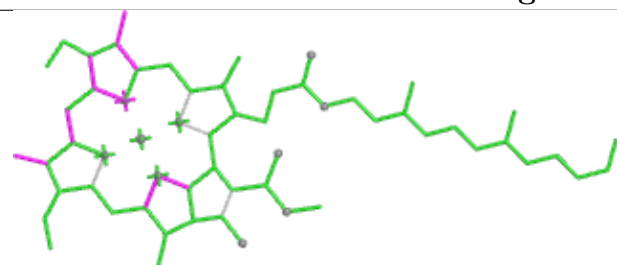


Torsions

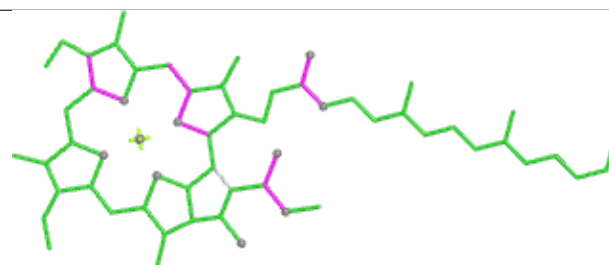


Rings

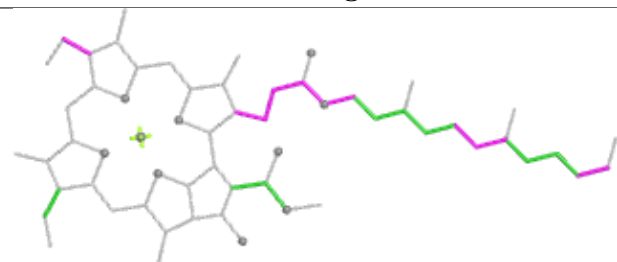
Ligand CLA B 817



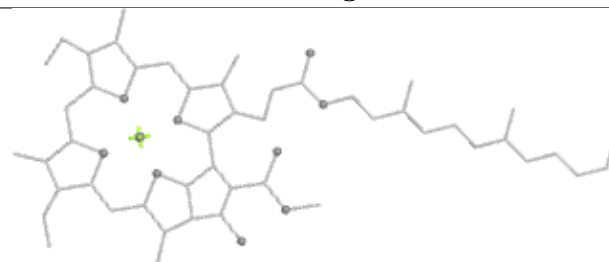
Bond lengths



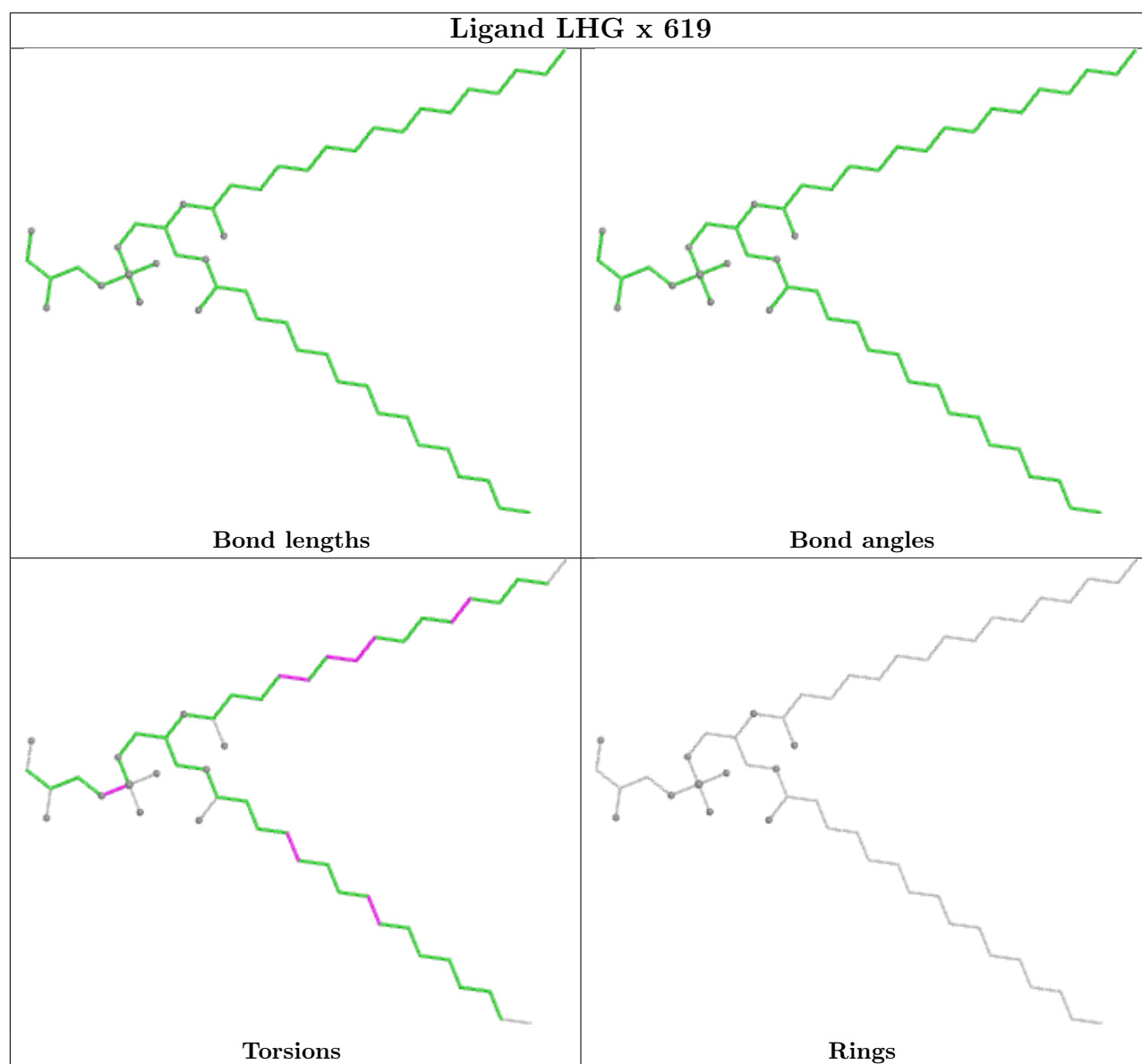
Bond angles



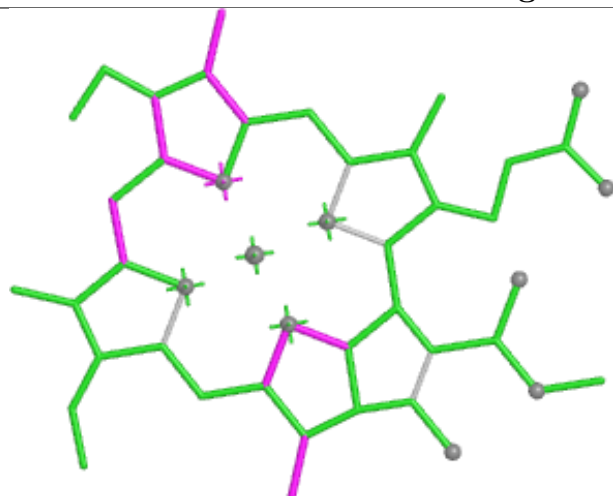
Torsions



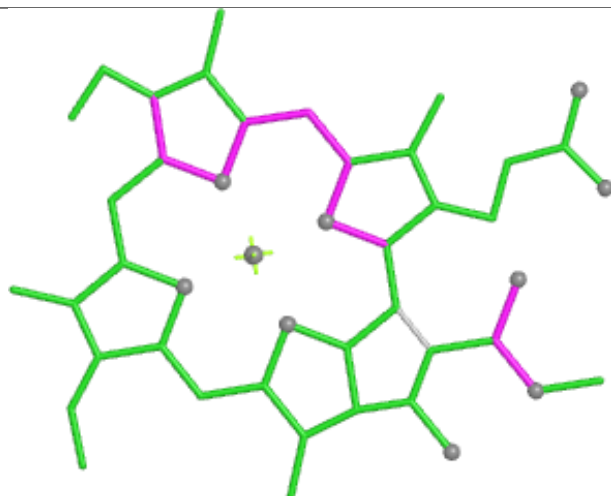
Rings



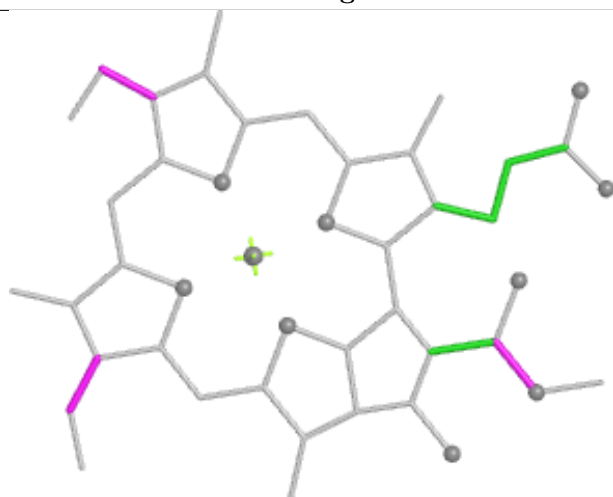
Ligand CLA 4 608



Bond lengths



Bond angles

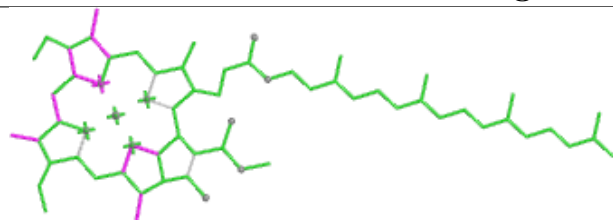


Torsions

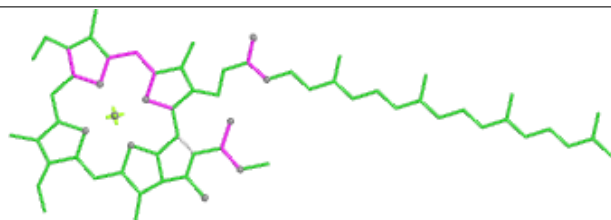


Rings

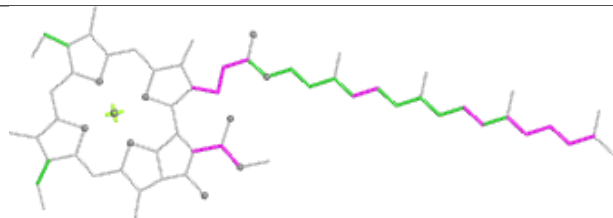
Ligand CLA A 814



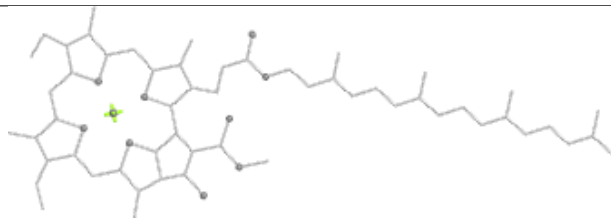
Bond lengths



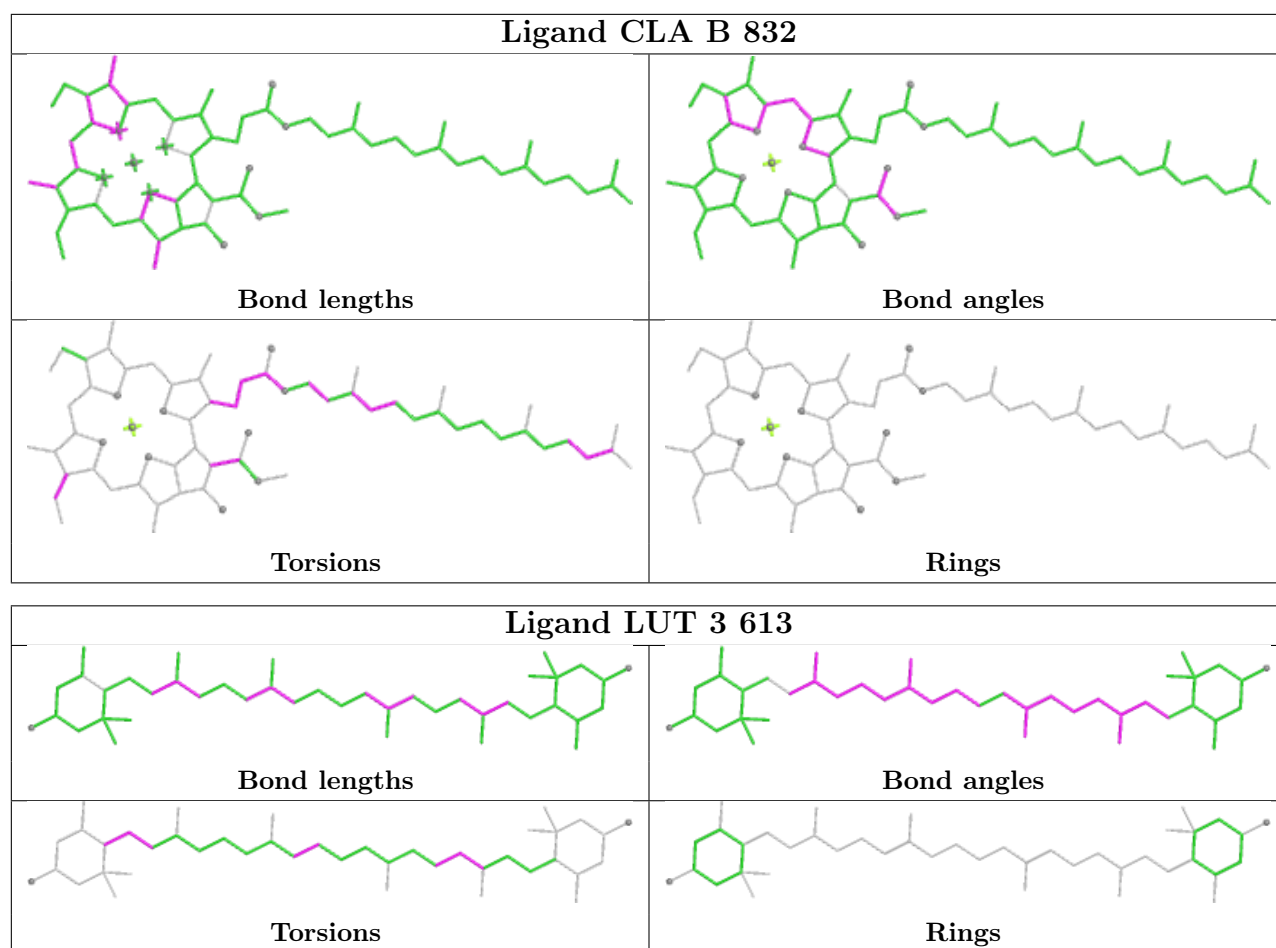
Bond angles



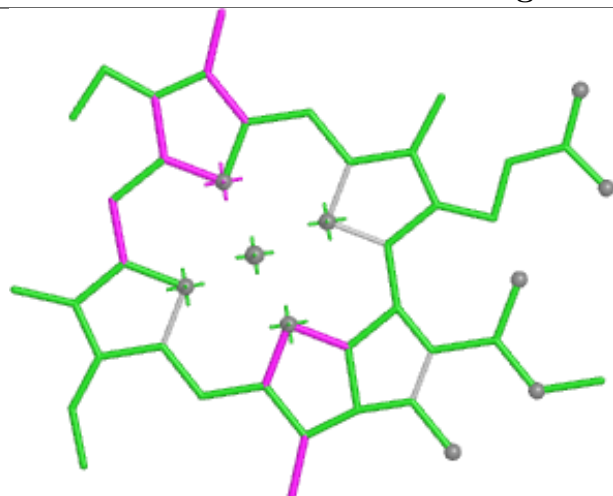
Torsions



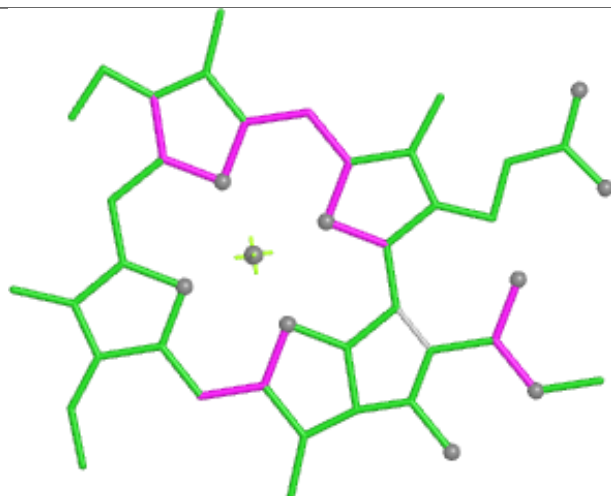
Rings



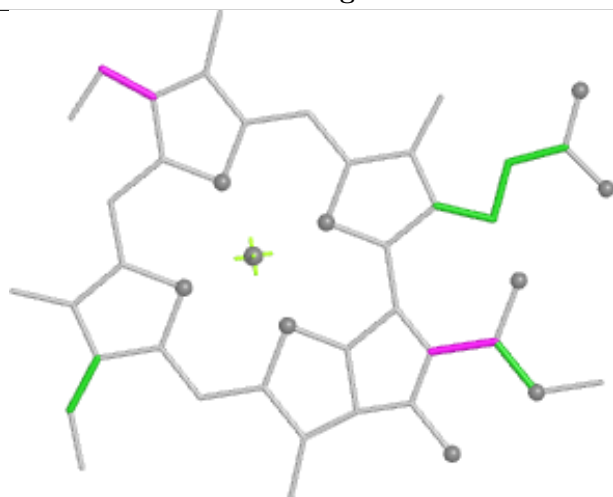
Ligand CLA L 304



Bond lengths



Bond angles

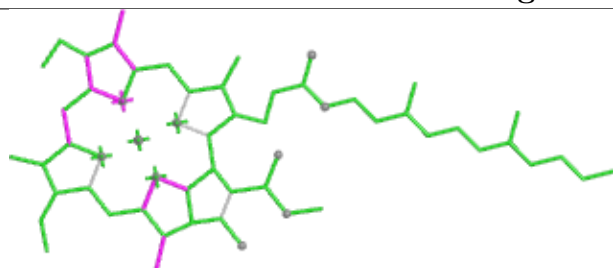


Torsions

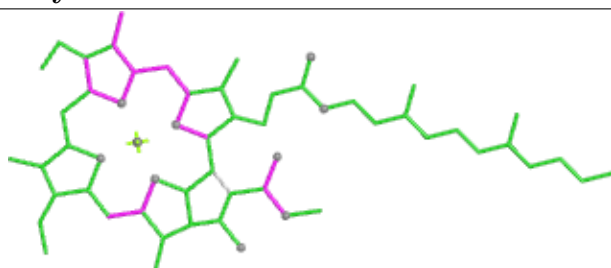


Rings

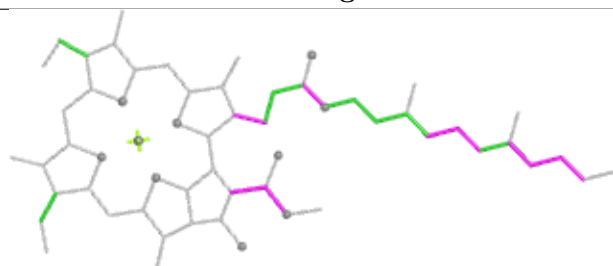
Ligand CLA y 610



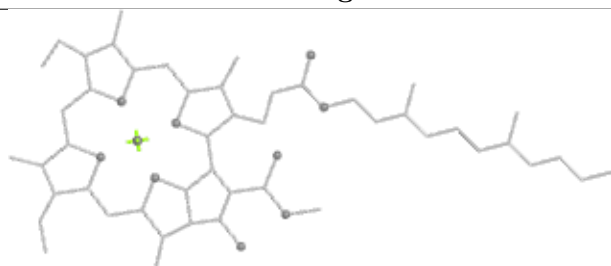
Bond lengths



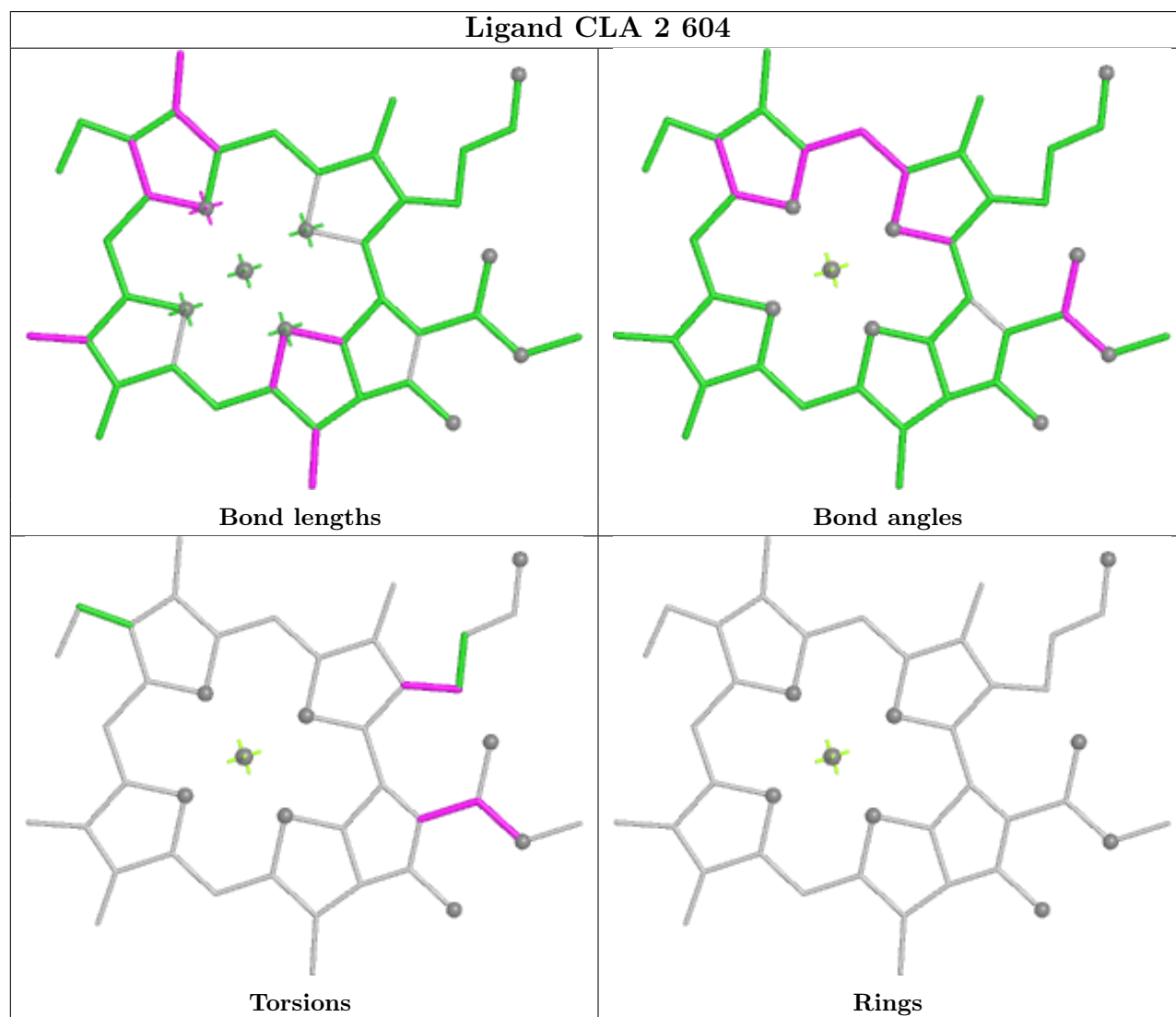
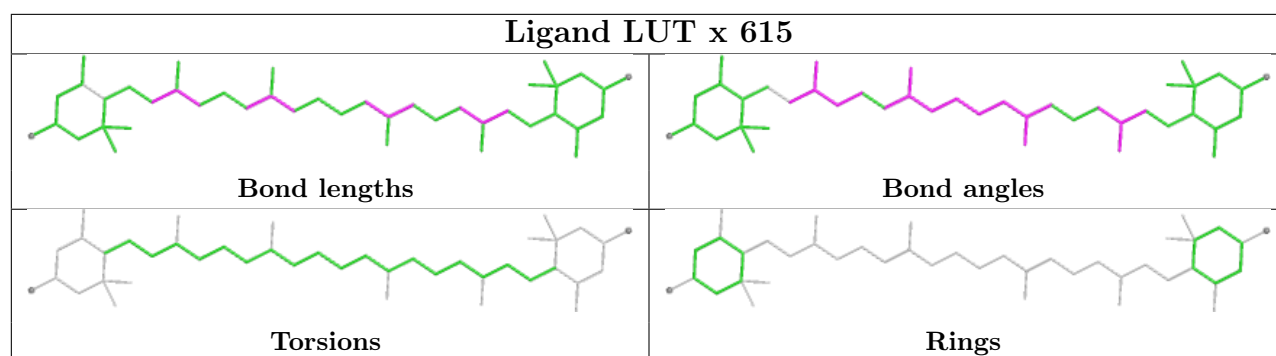
Bond angles

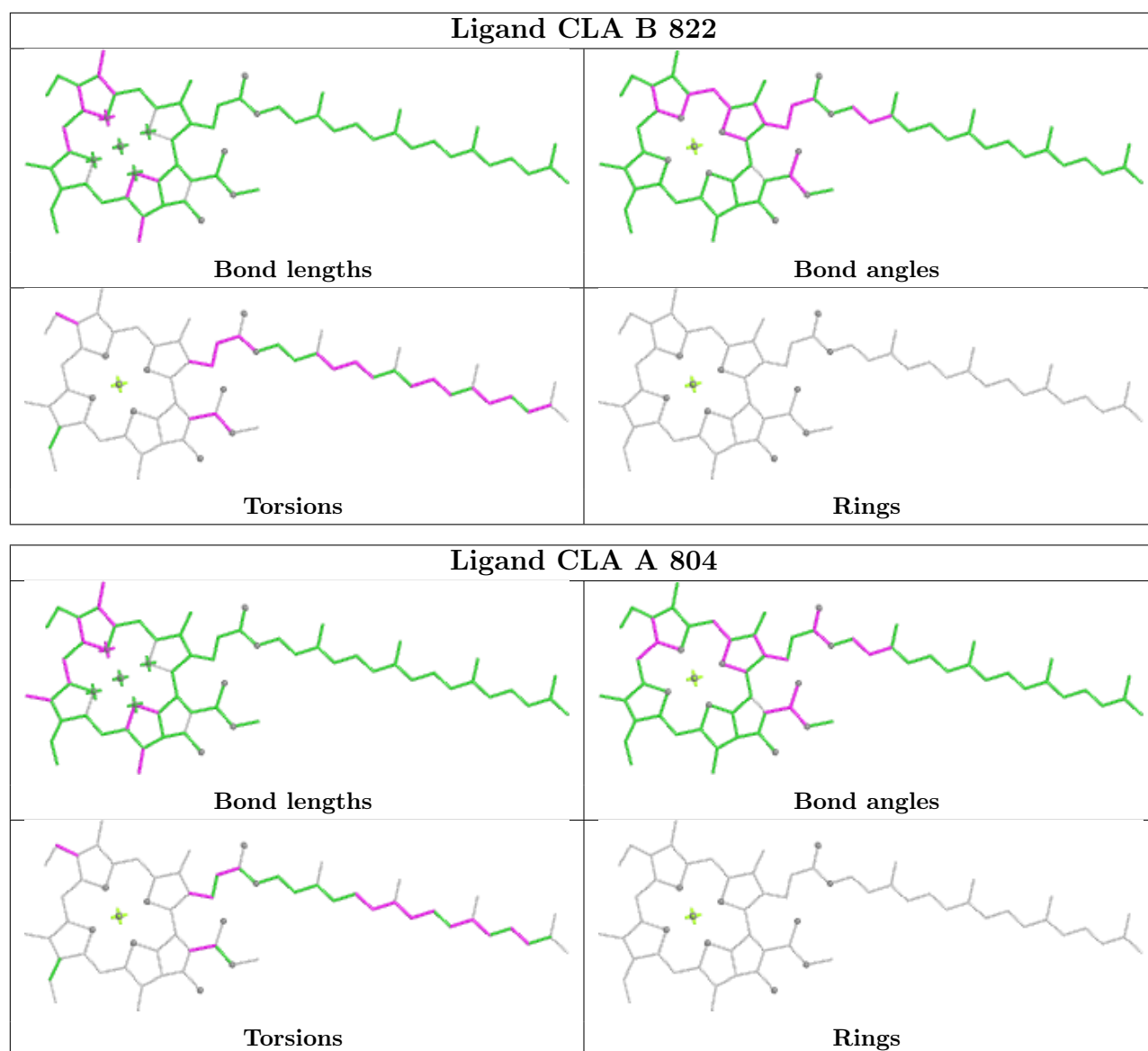


Torsions

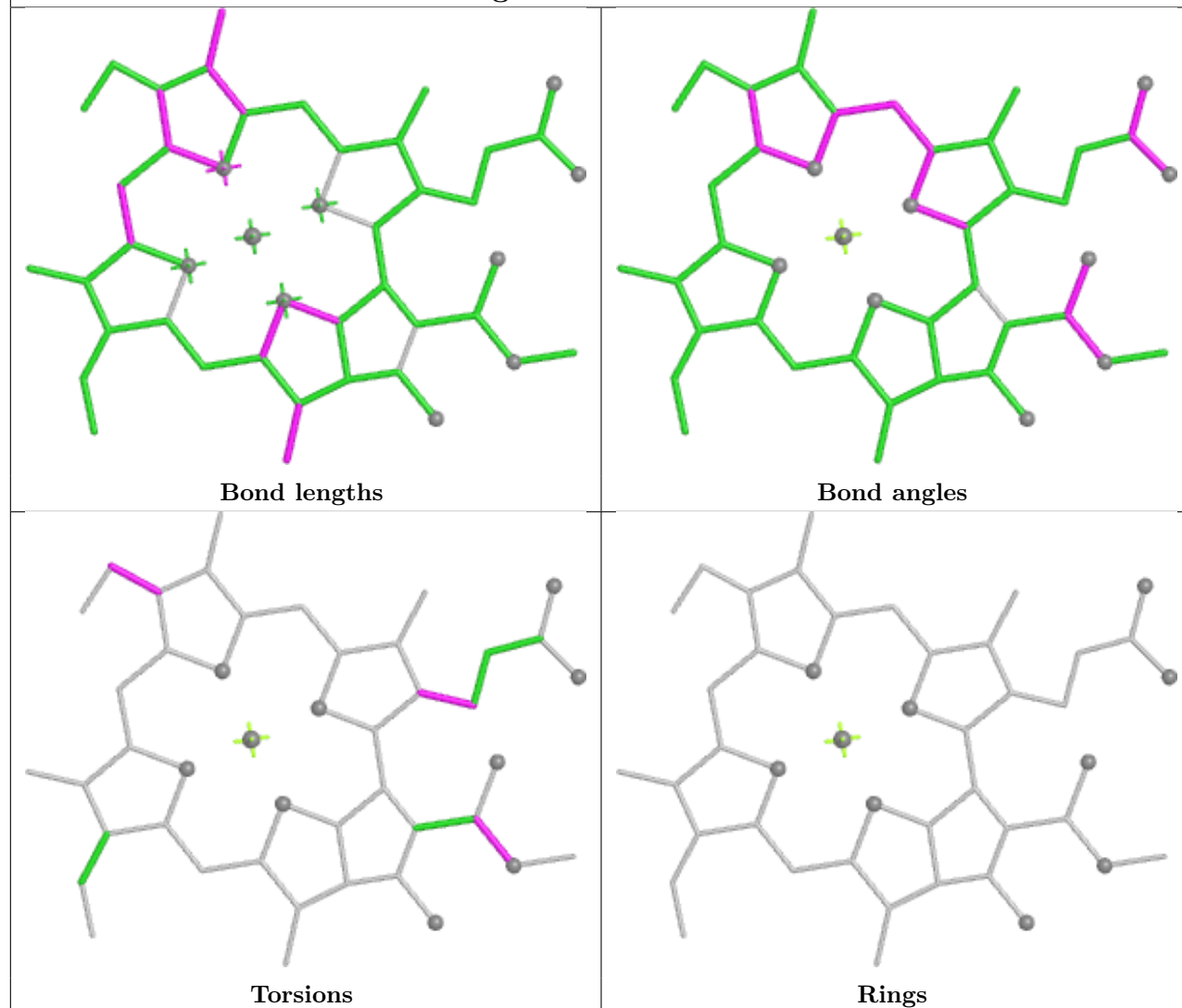


Rings

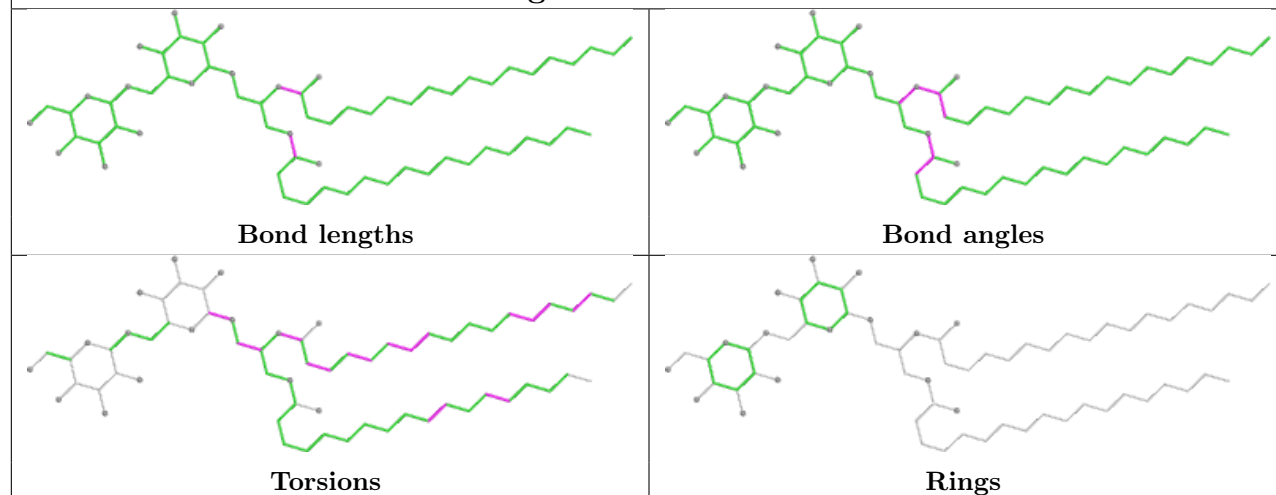


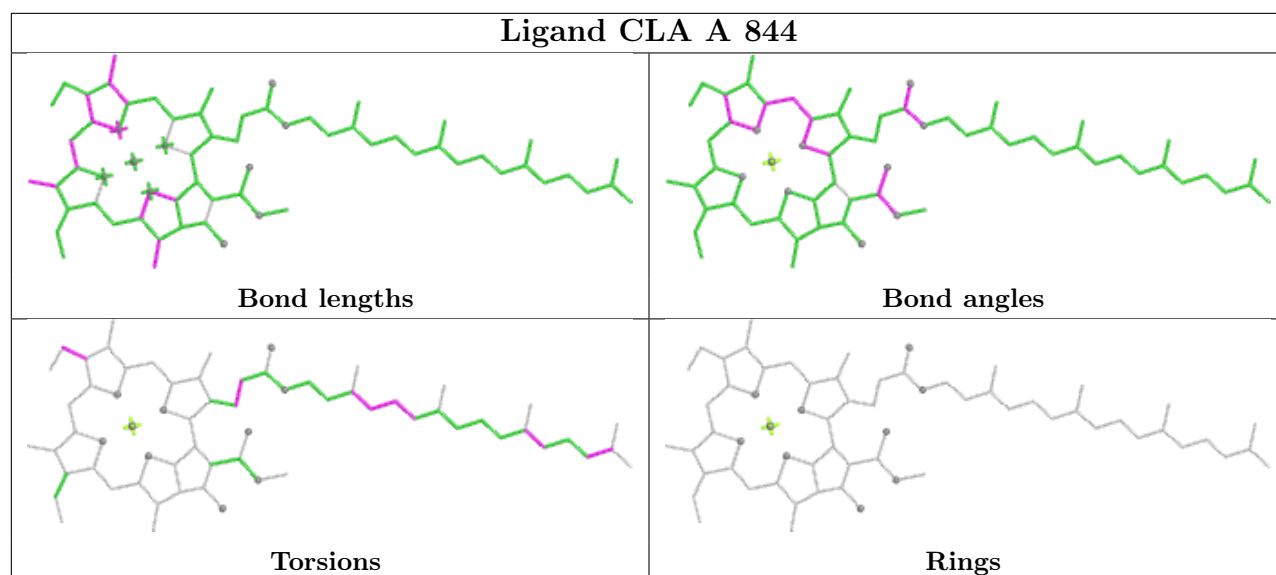
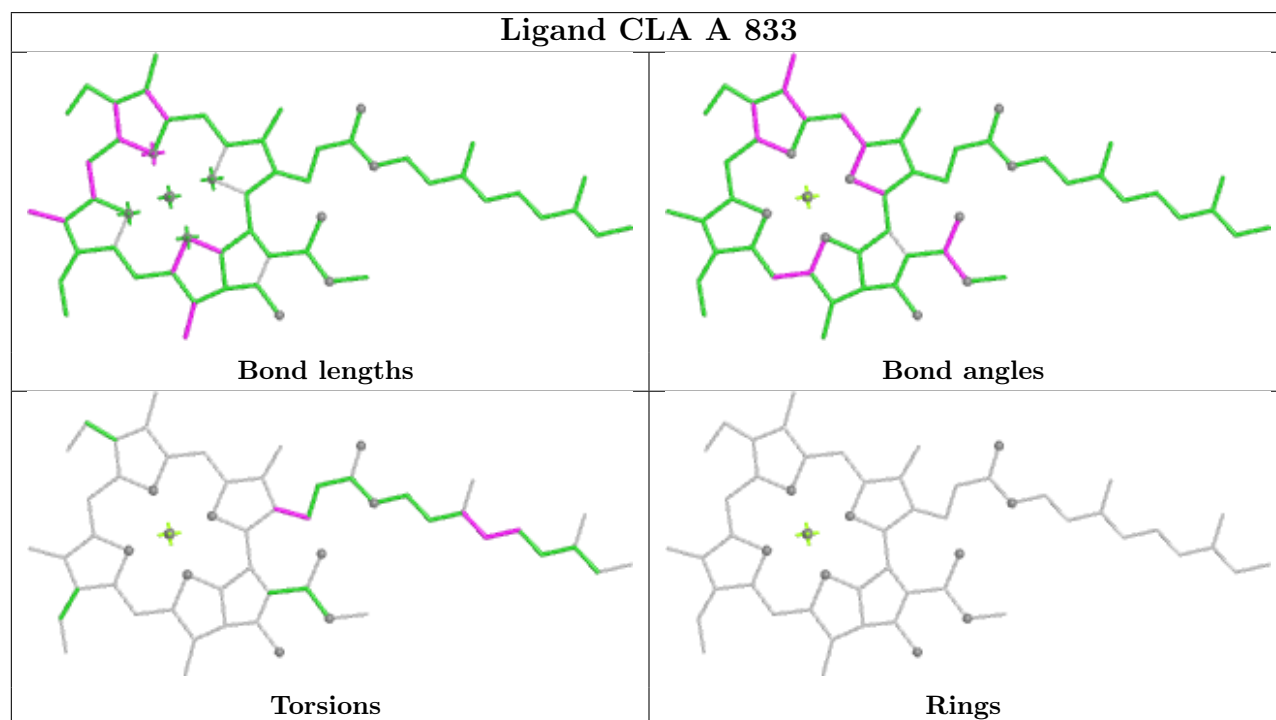
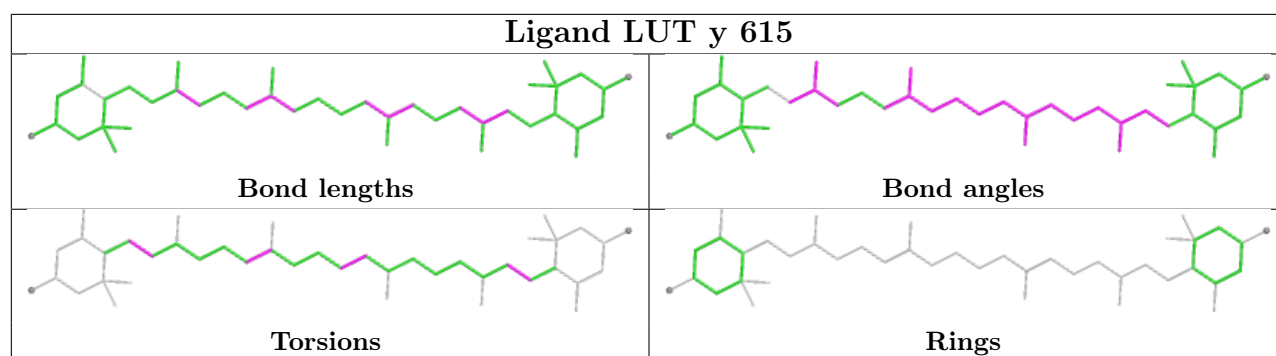


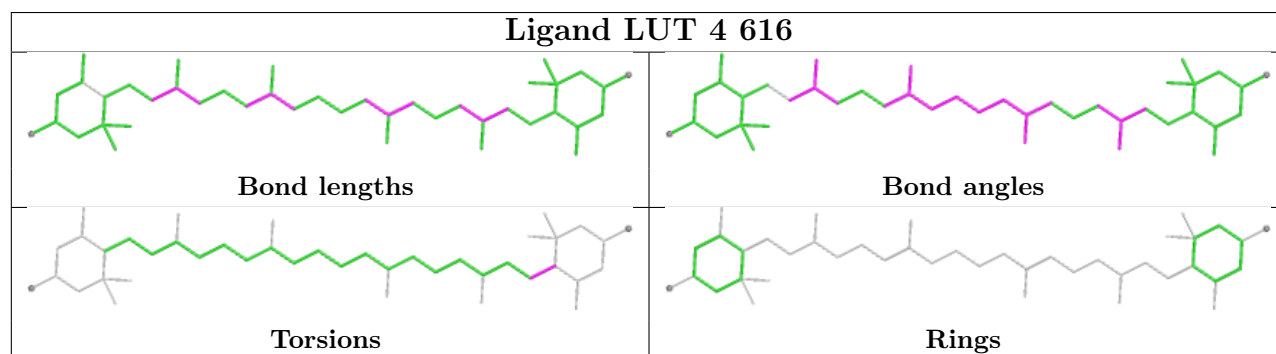
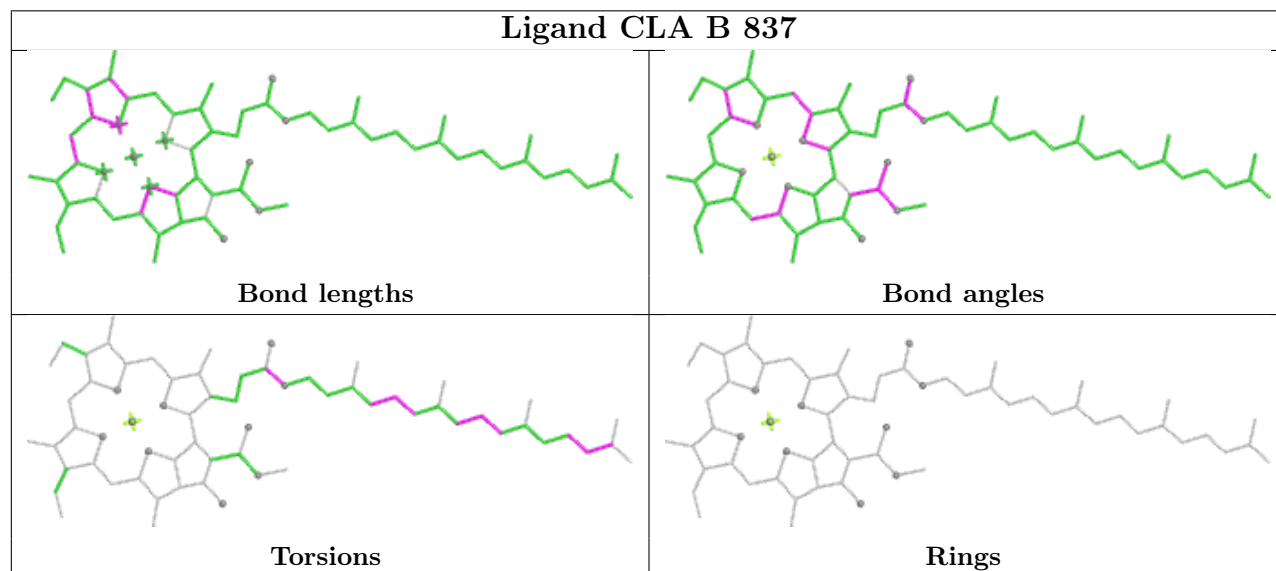
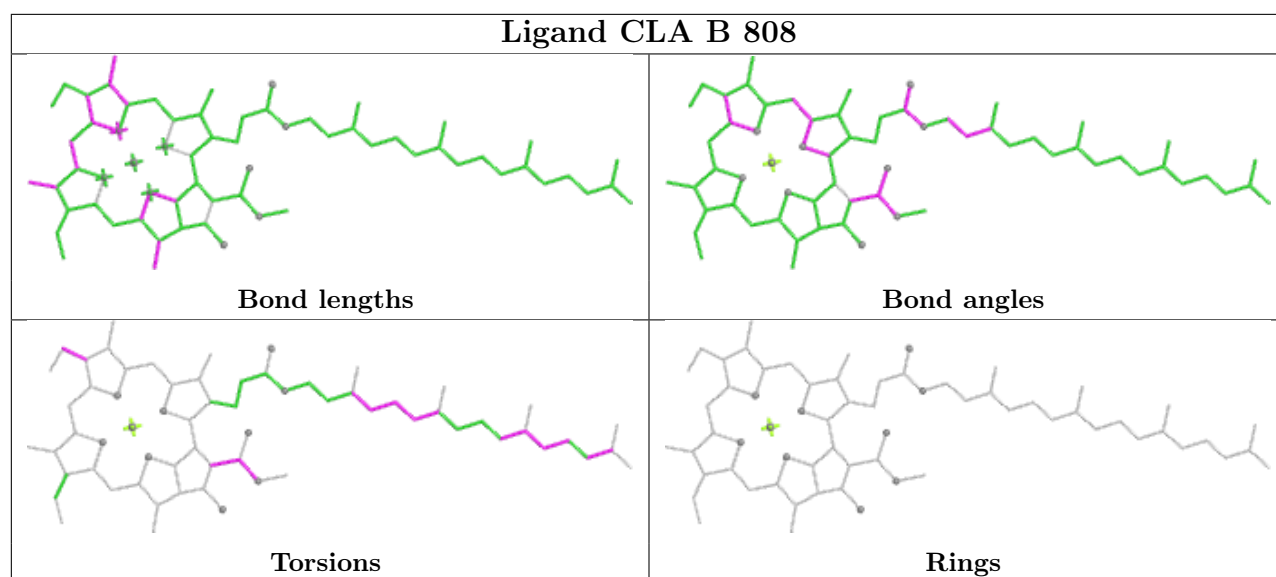
Ligand CLA A 836

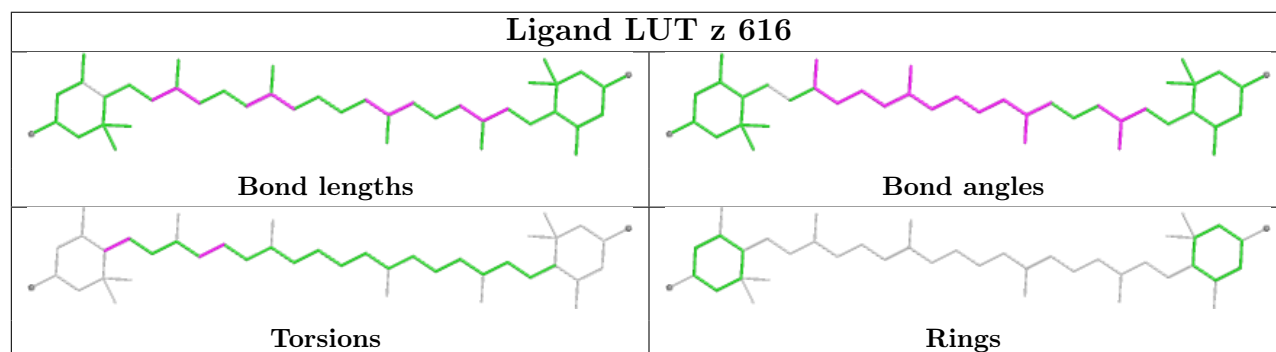
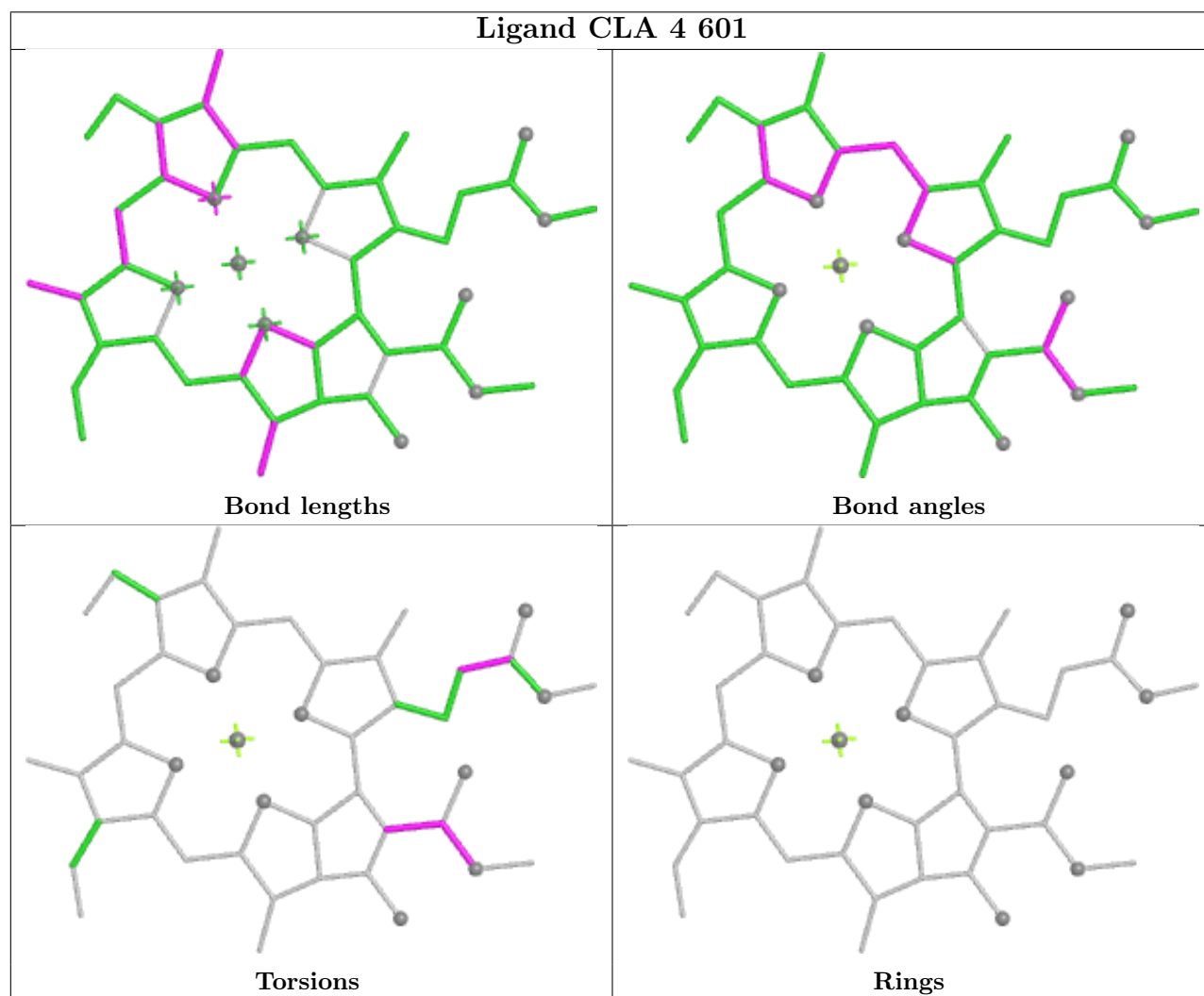
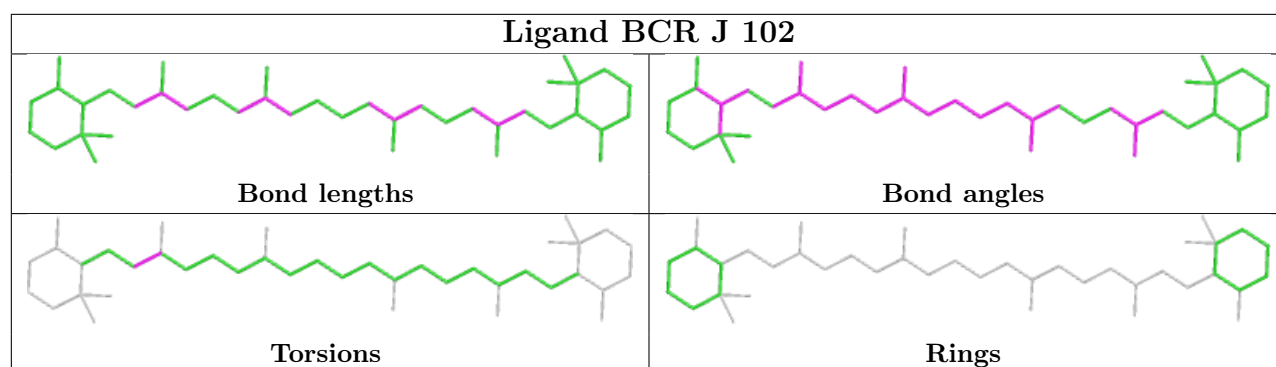


Ligand DGD B 850

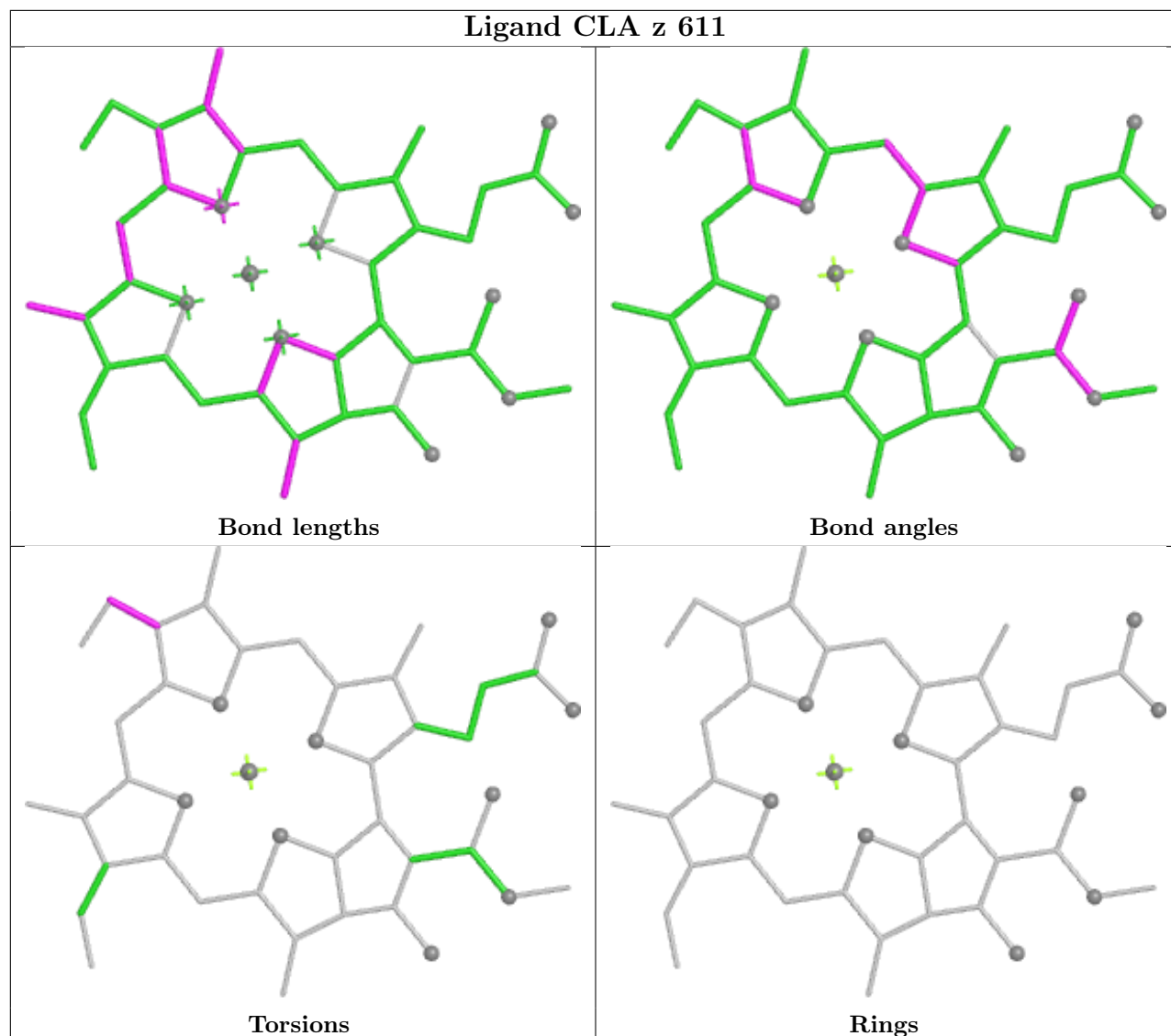




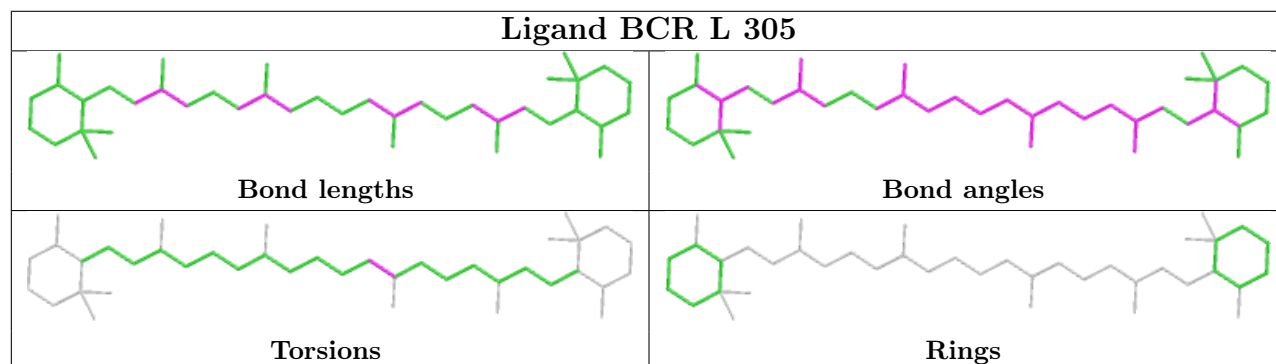




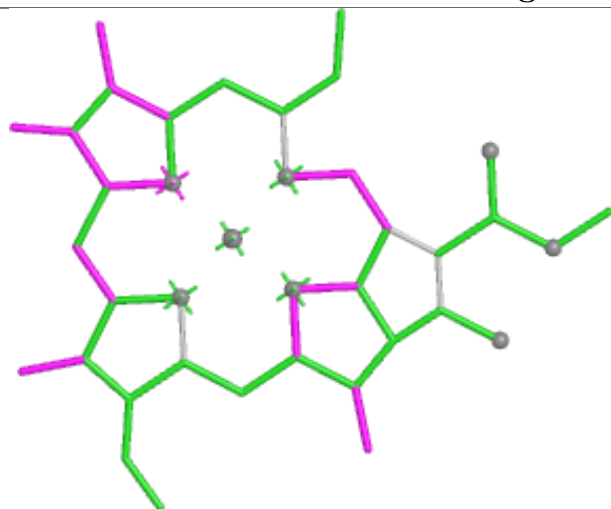
Ligand CLA z 611



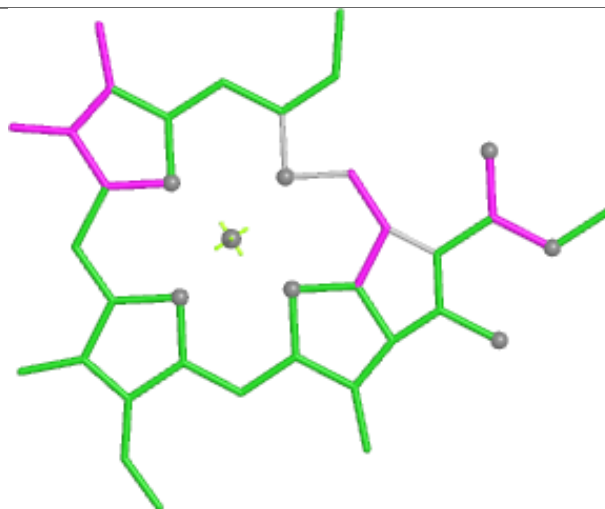
Ligand BCR L 305



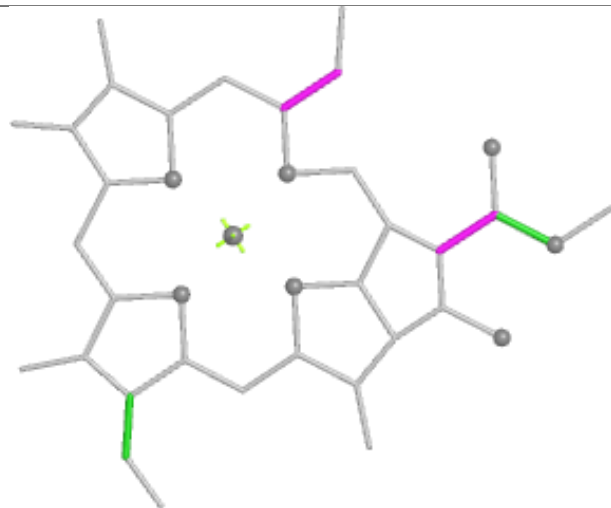
Ligand CLA 2 610



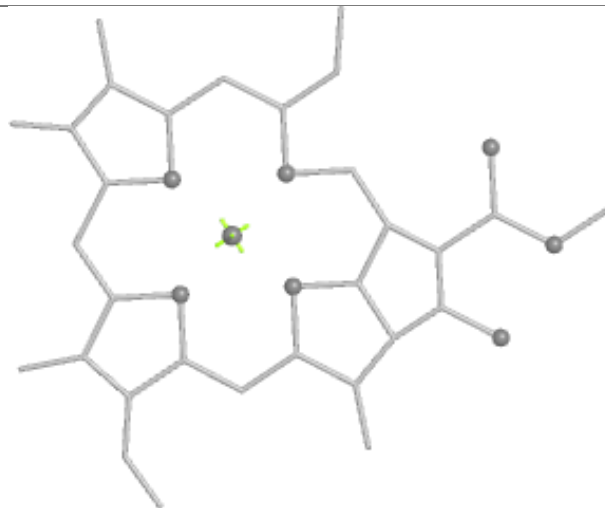
Bond lengths



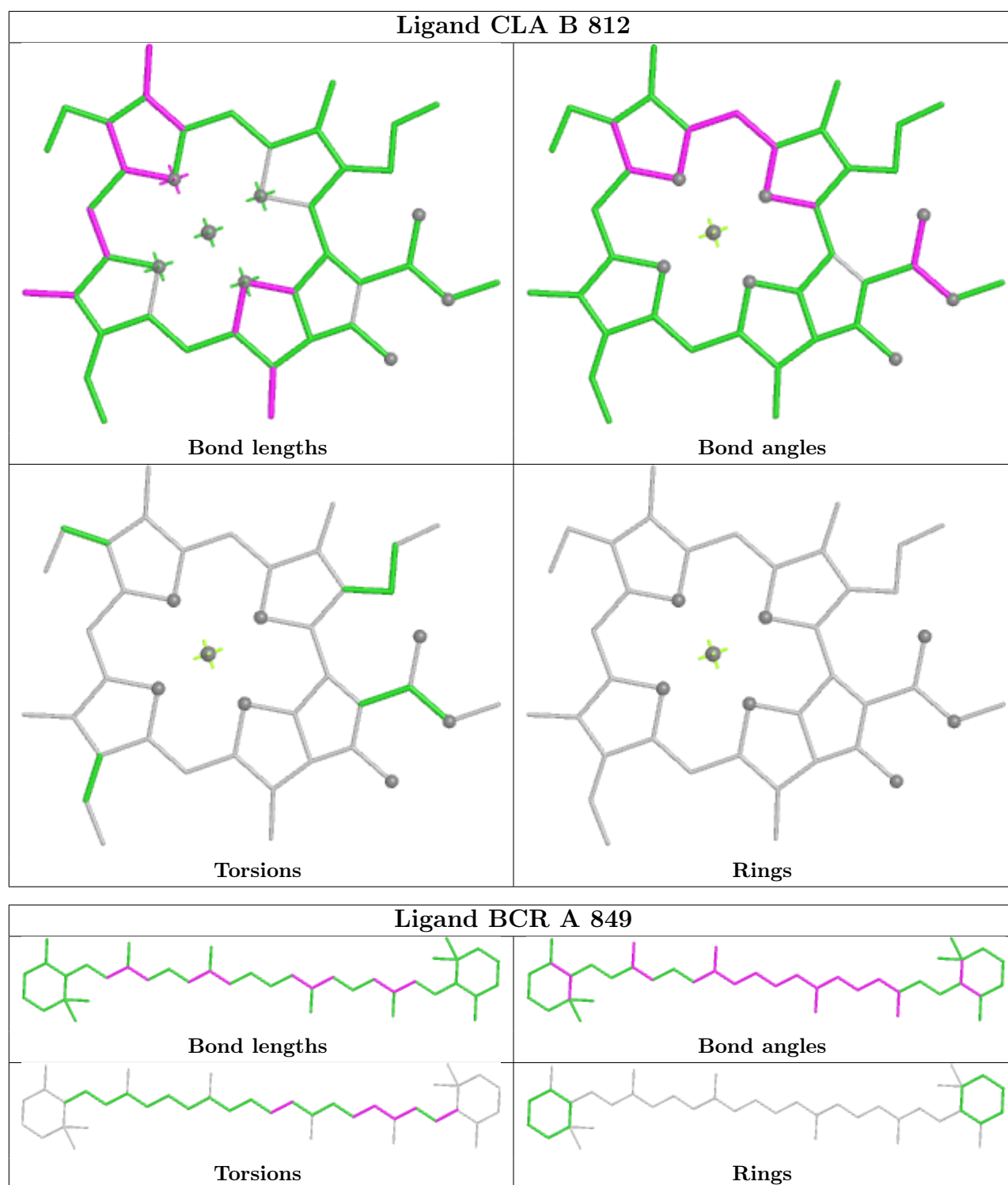
Bond angles

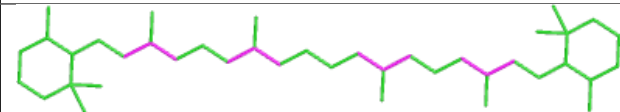
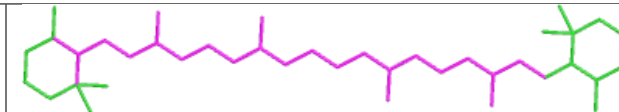
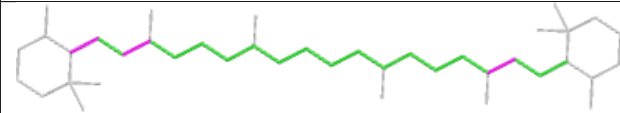
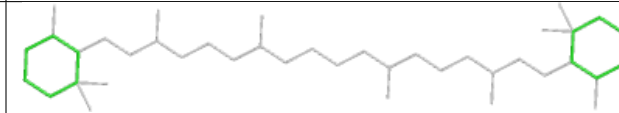


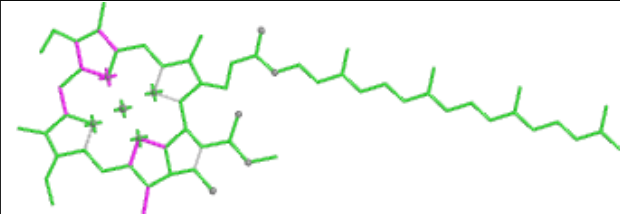
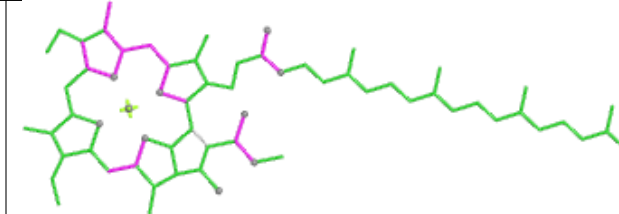
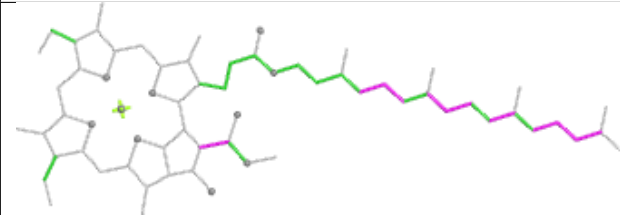
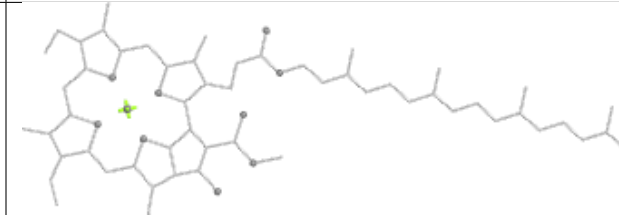
Torsions

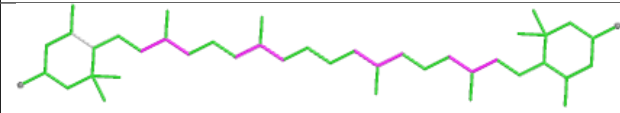
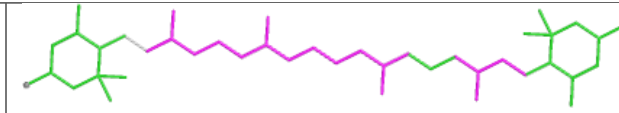
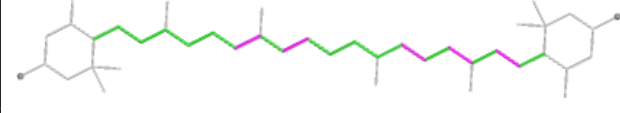
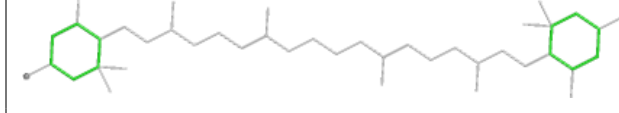


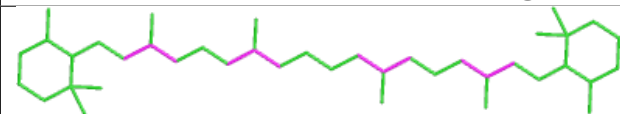
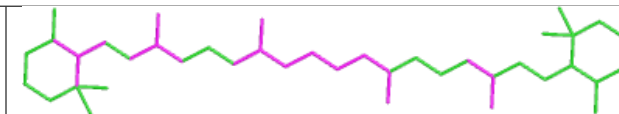
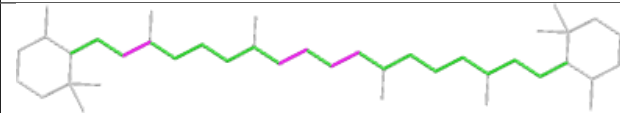
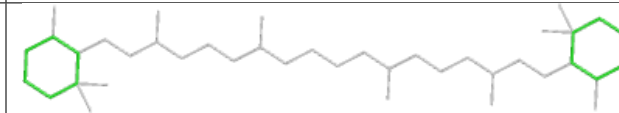
Rings



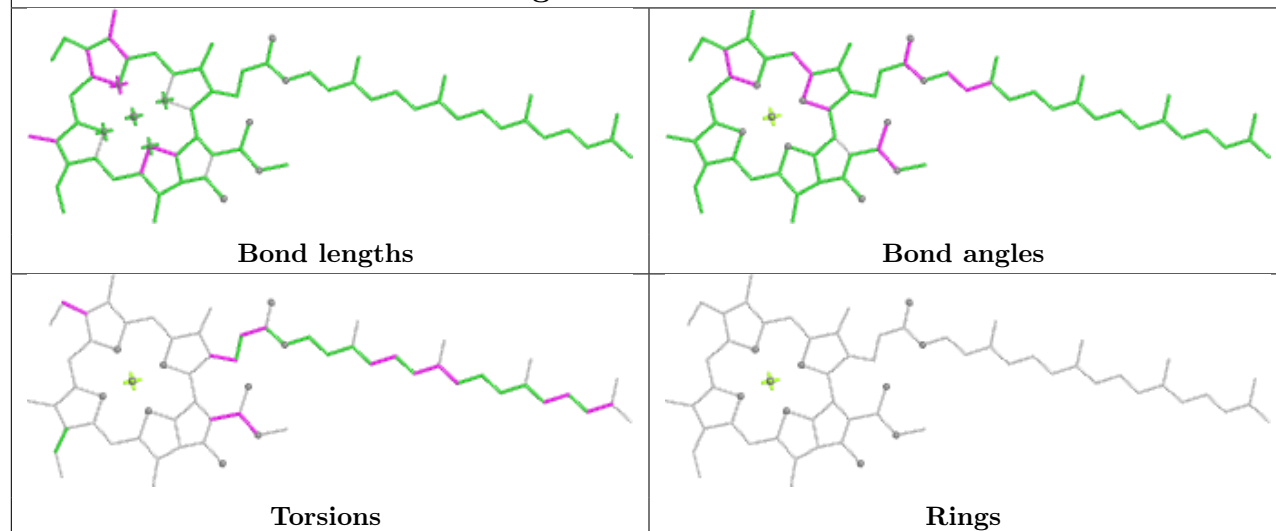
Ligand BCR L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

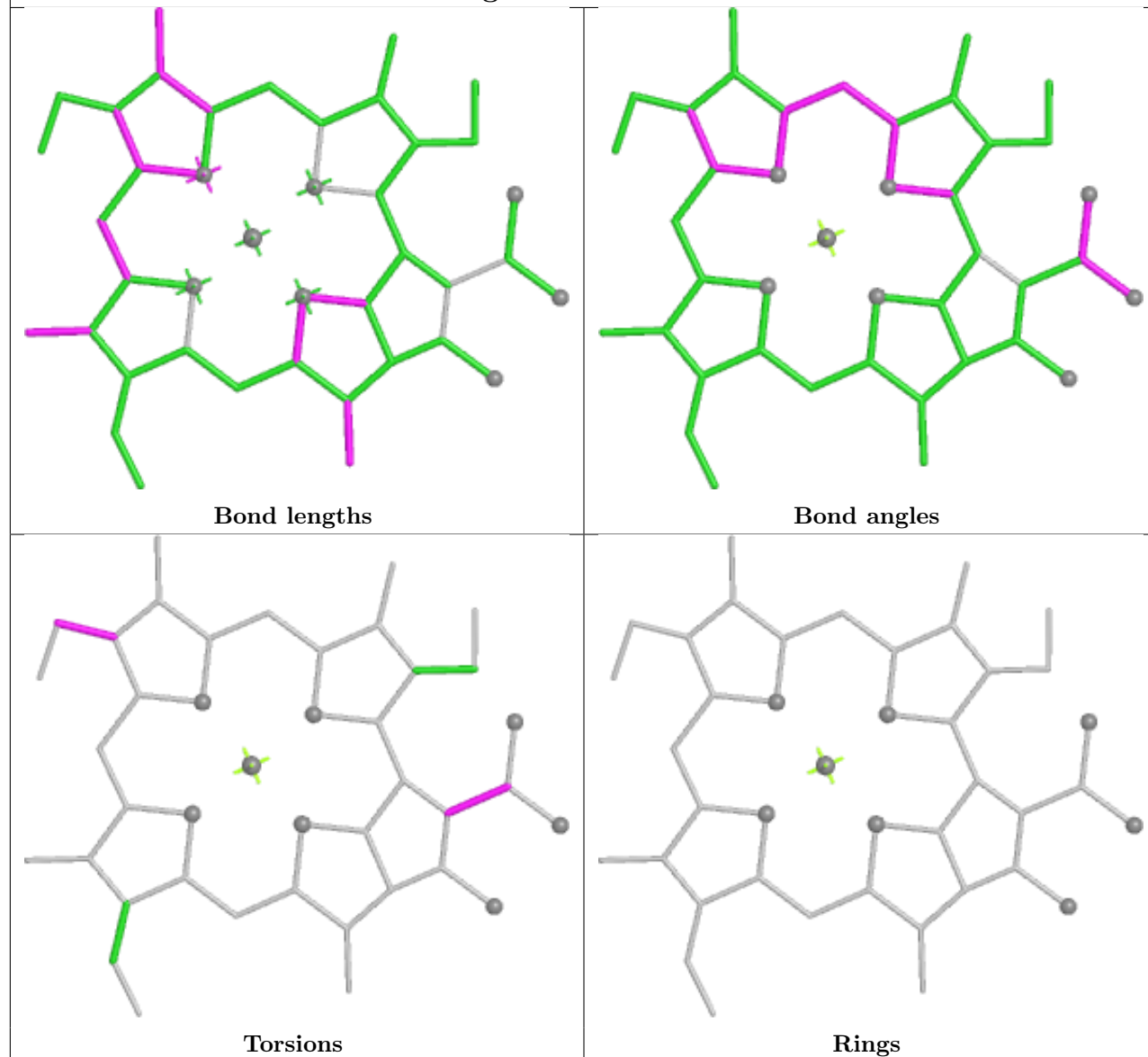
Ligand LUT 2 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

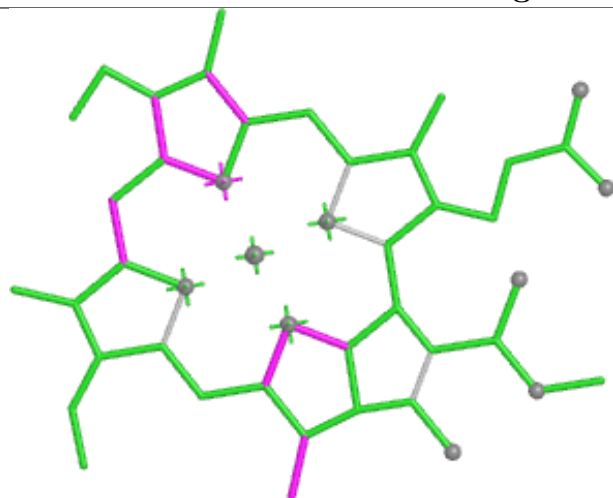
Ligand CLA B 803



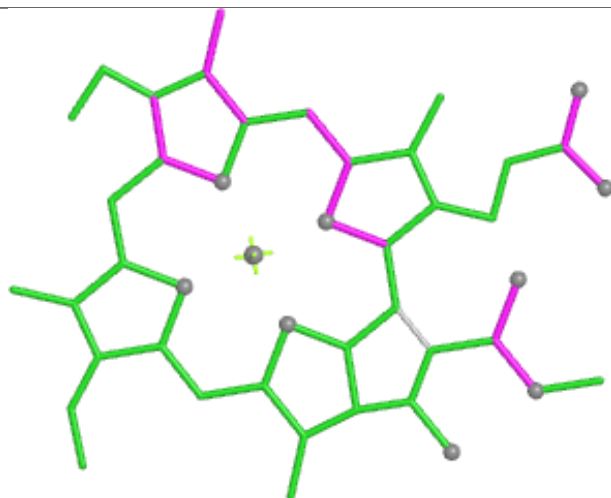
Ligand CLA 4 611



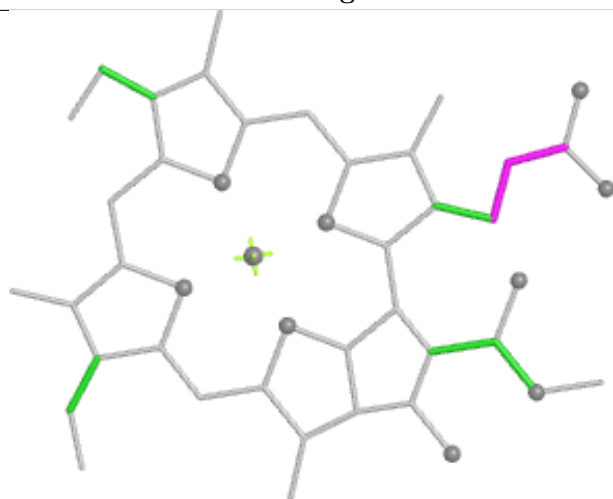
Ligand CLA G 203



Bond lengths



Bond angles

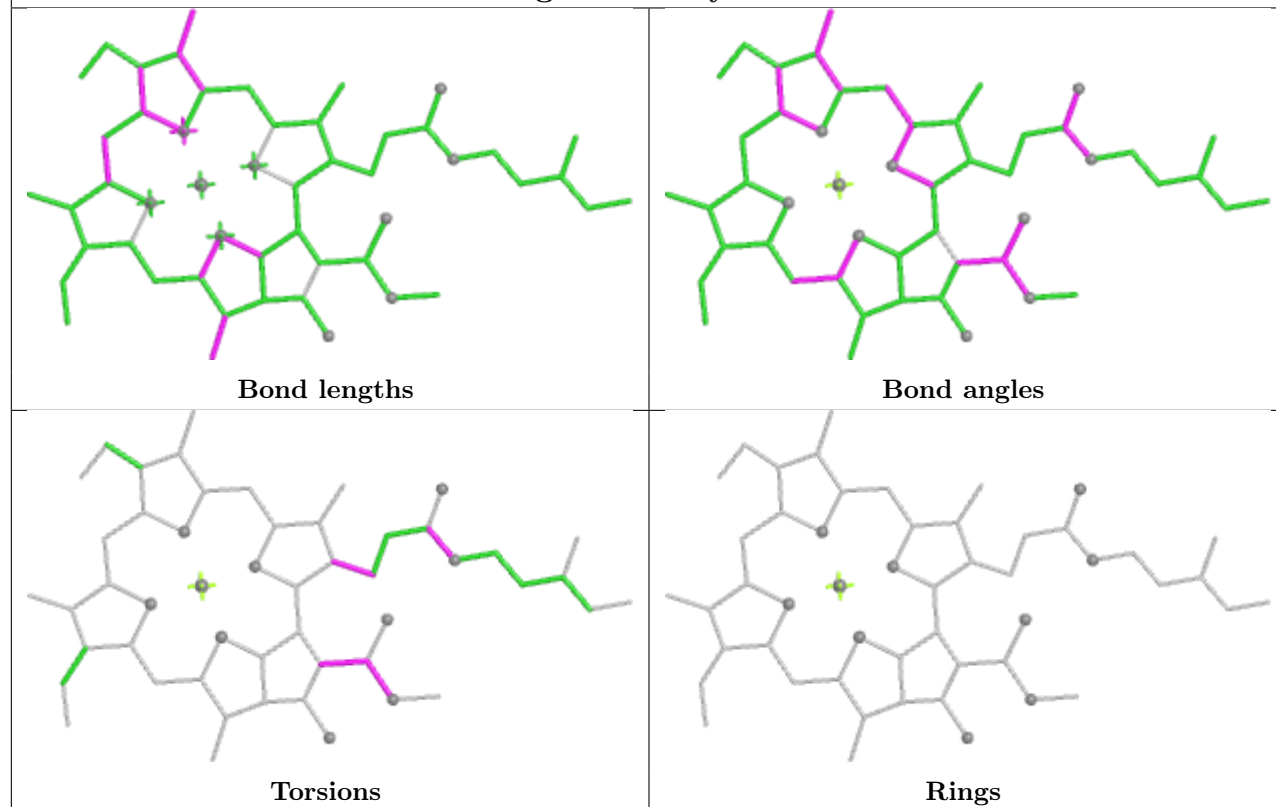


Torsions

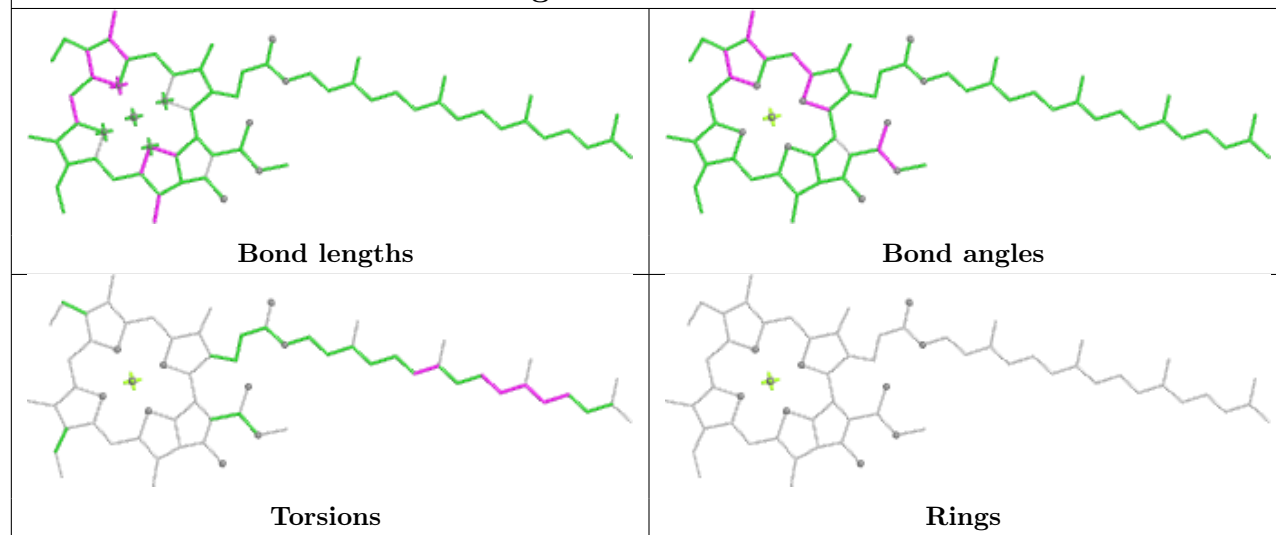


Rings

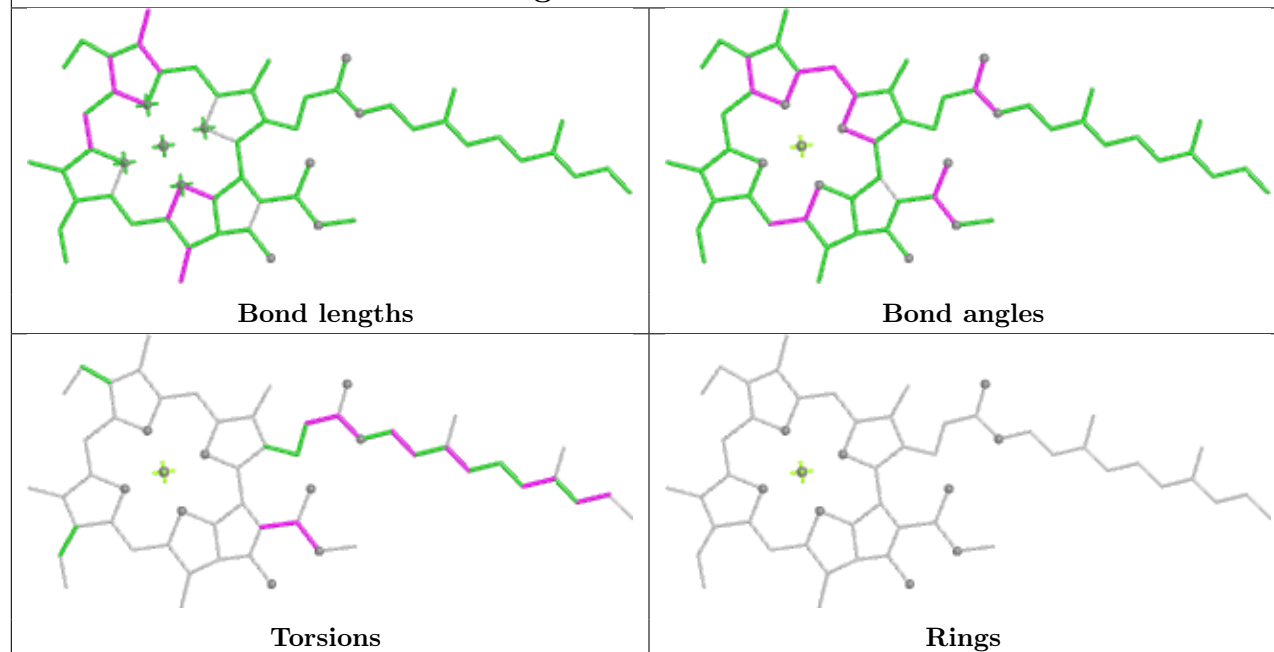
Ligand CLA y 604



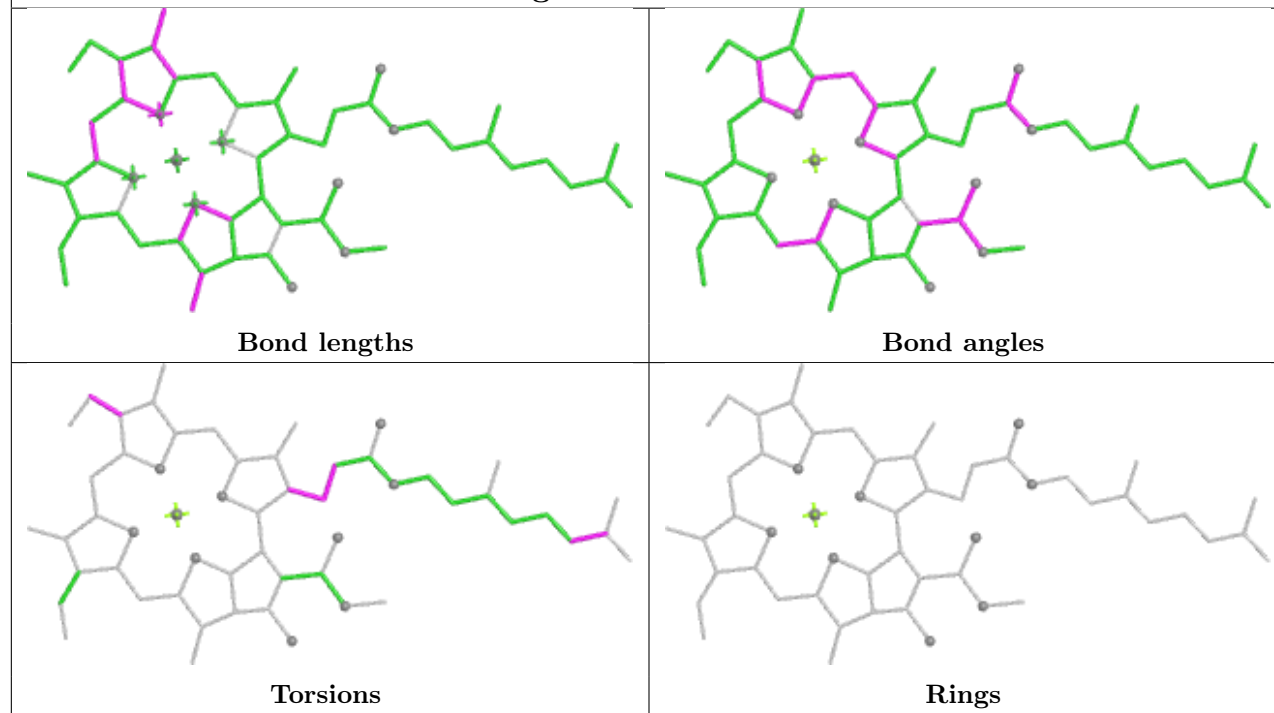
Ligand CLA A 831



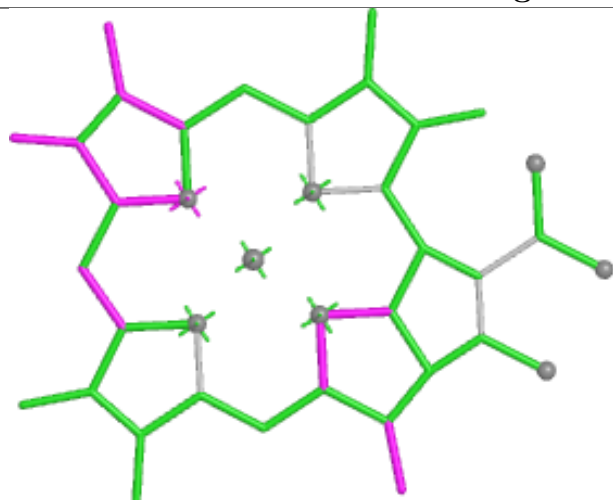
Ligand CLA F 301



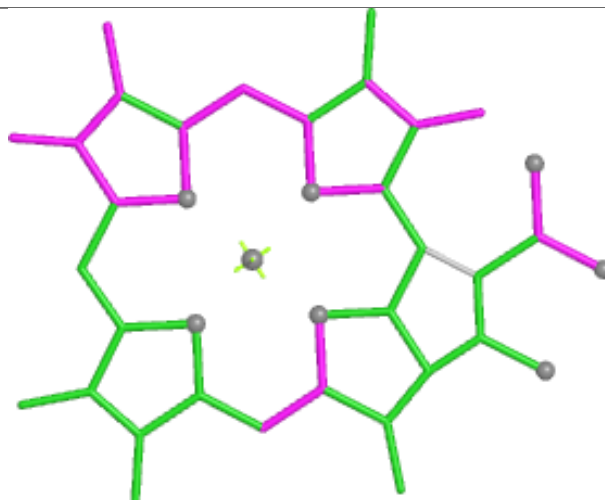
Ligand CLA B 819



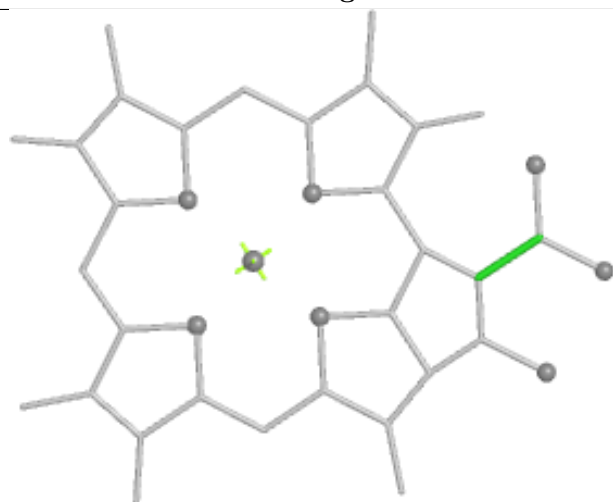
Ligand CLA O 203



Bond lengths



Bond angles

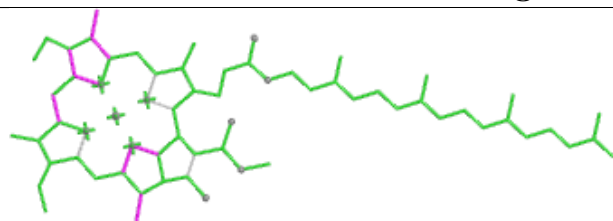


Torsions

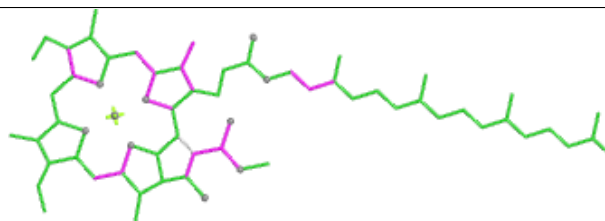


Rings

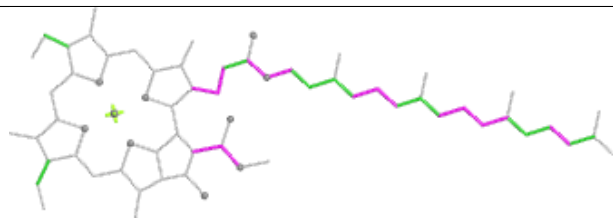
Ligand CLA B 802



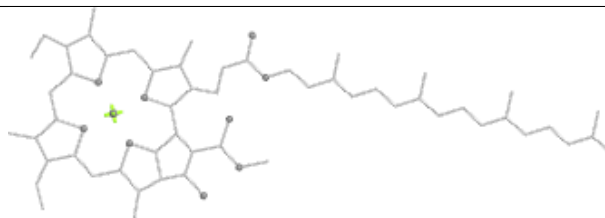
Bond lengths



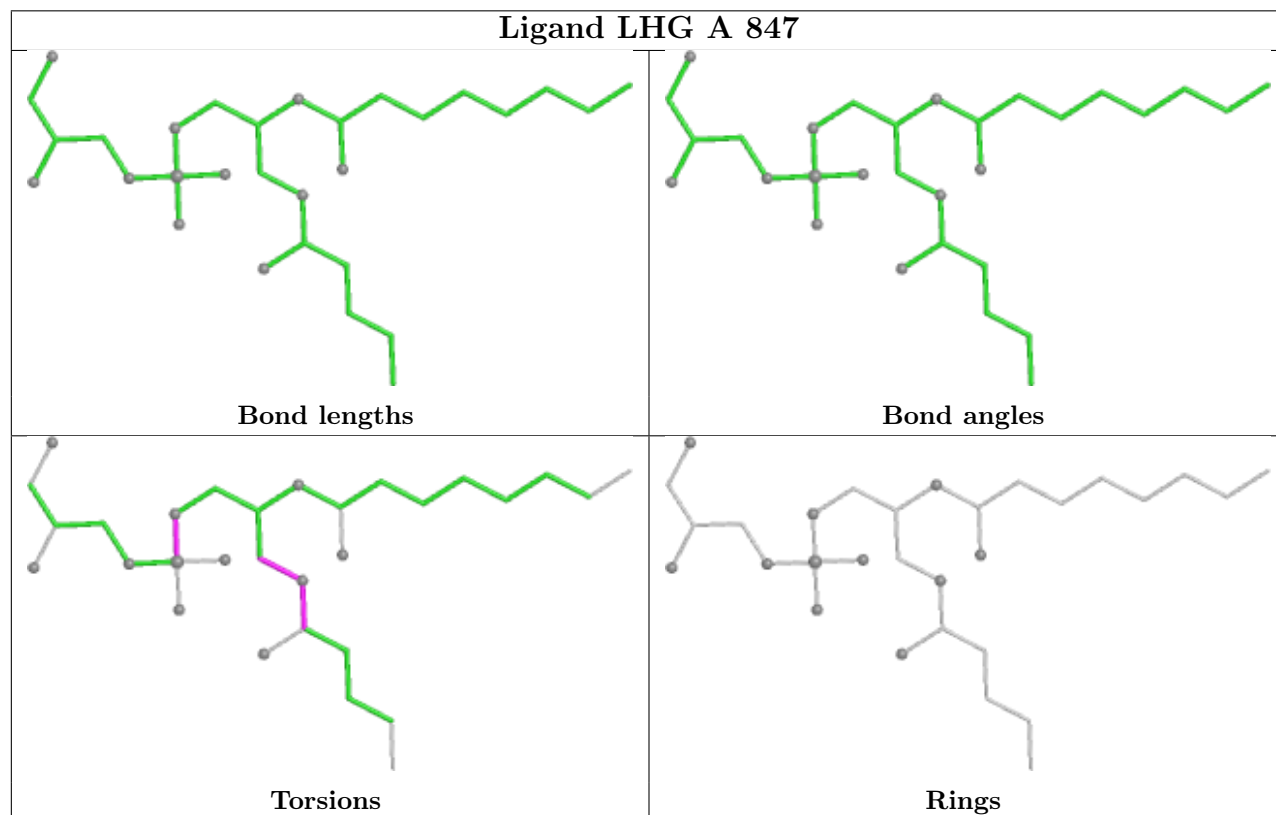
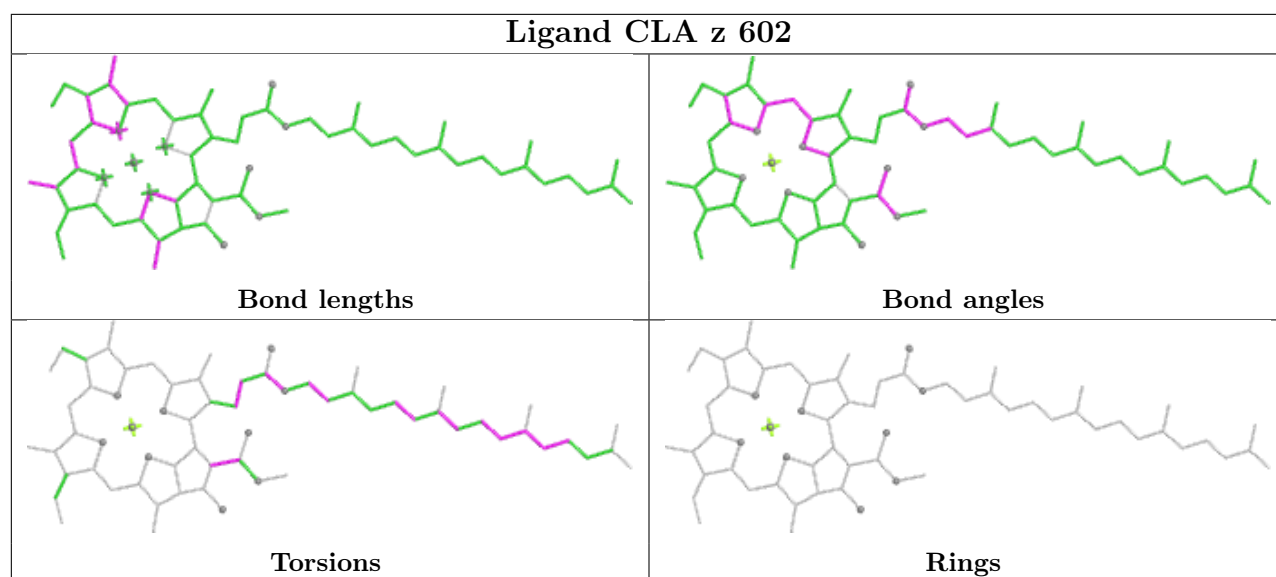
Bond angles

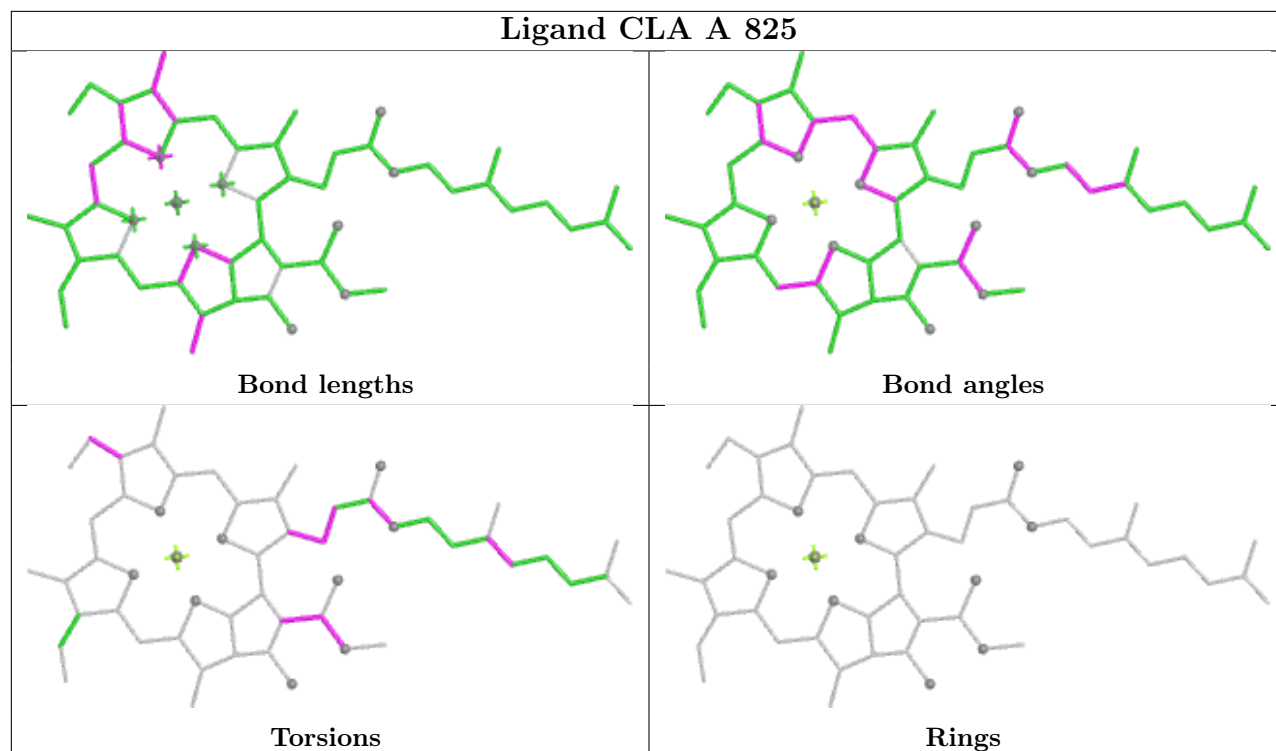
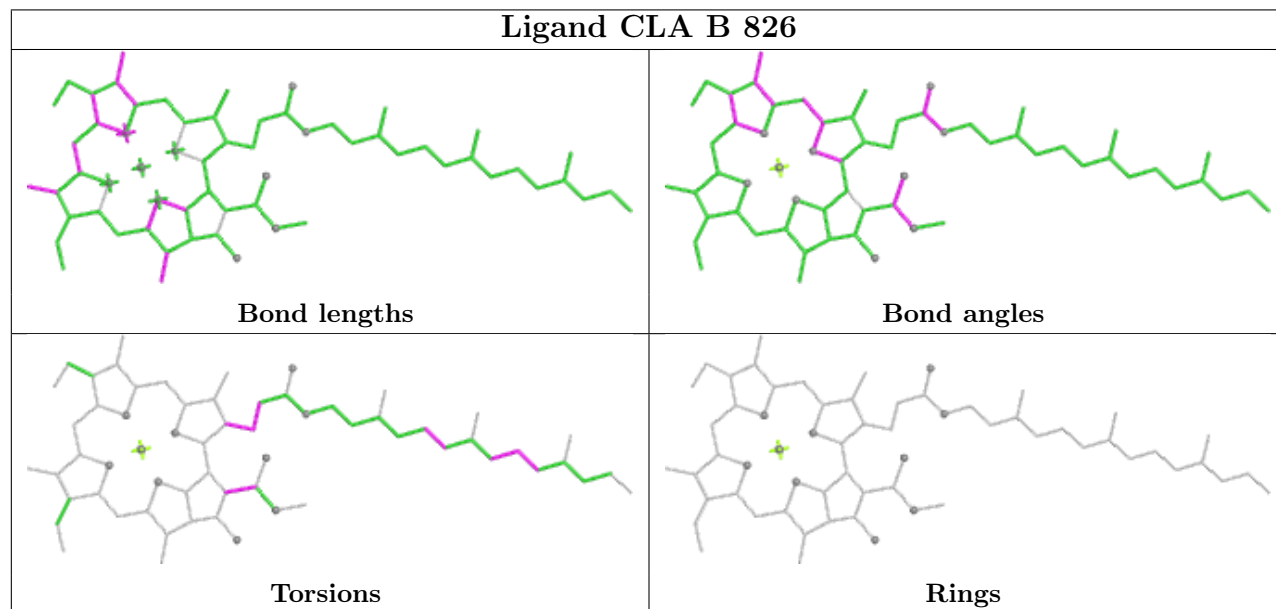


Torsions

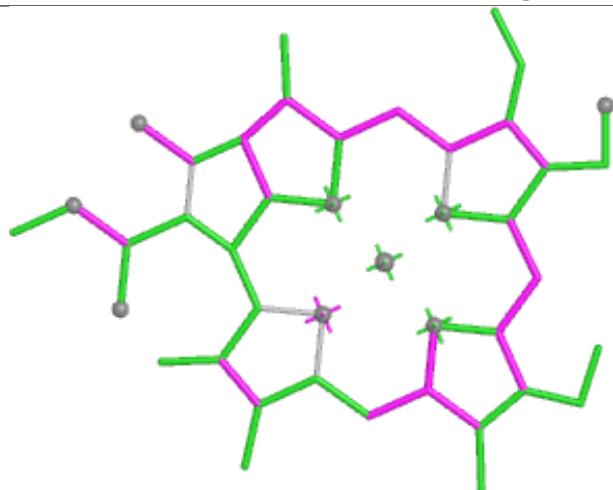


Rings

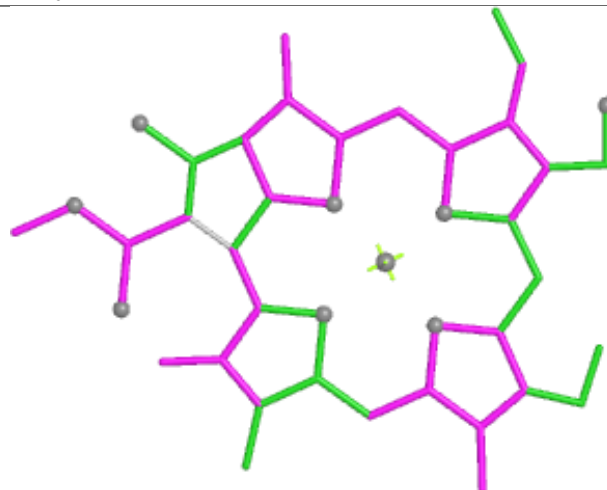


Ligand CLA A 825**Ligand CLA B 826**

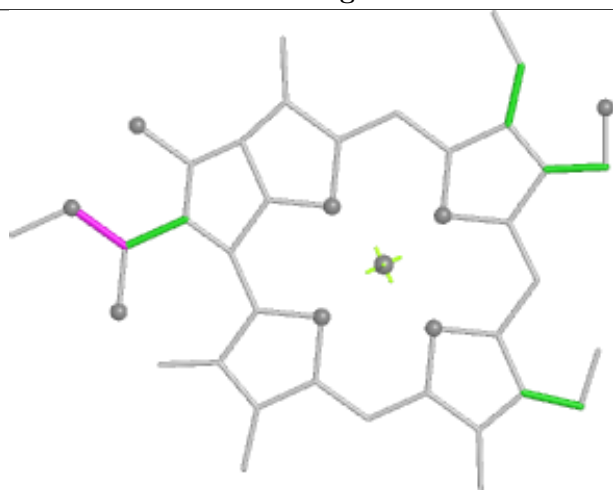
Ligand CHL y 605



Bond lengths



Bond angles

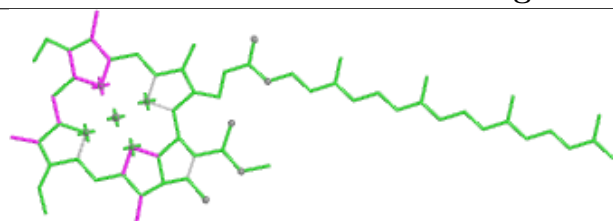


Torsions

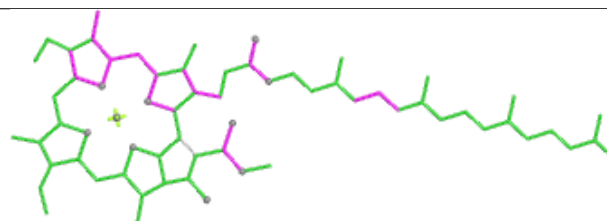


Rings

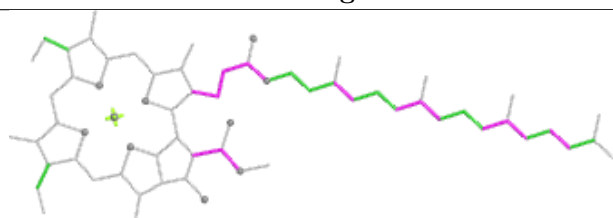
Ligand CLA A 802



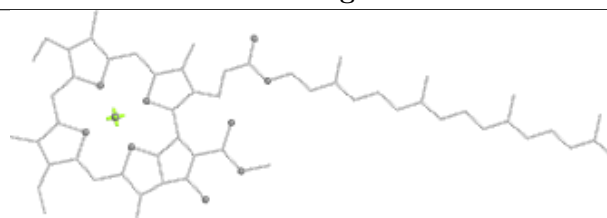
Bond lengths



Bond angles

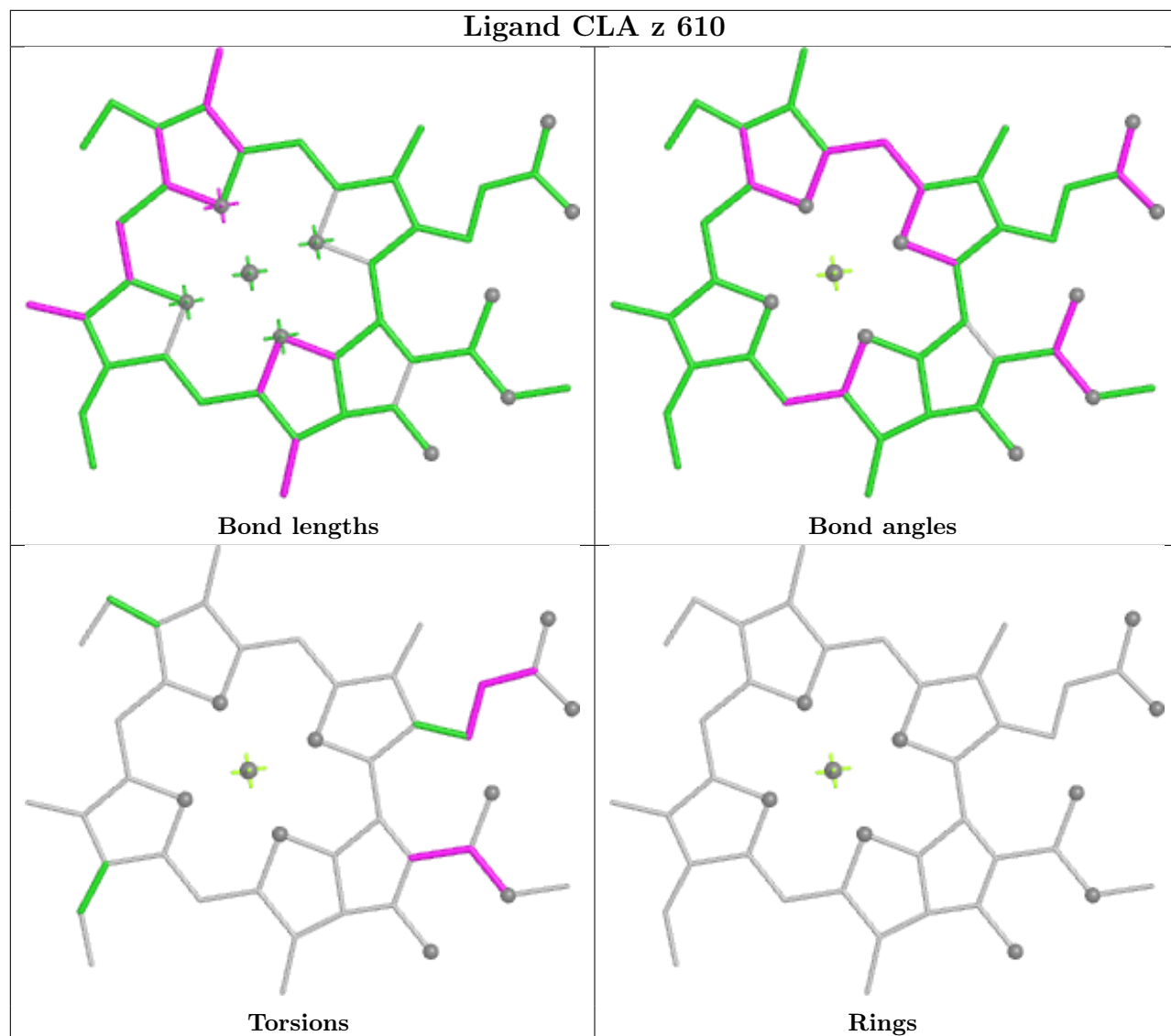


Torsions

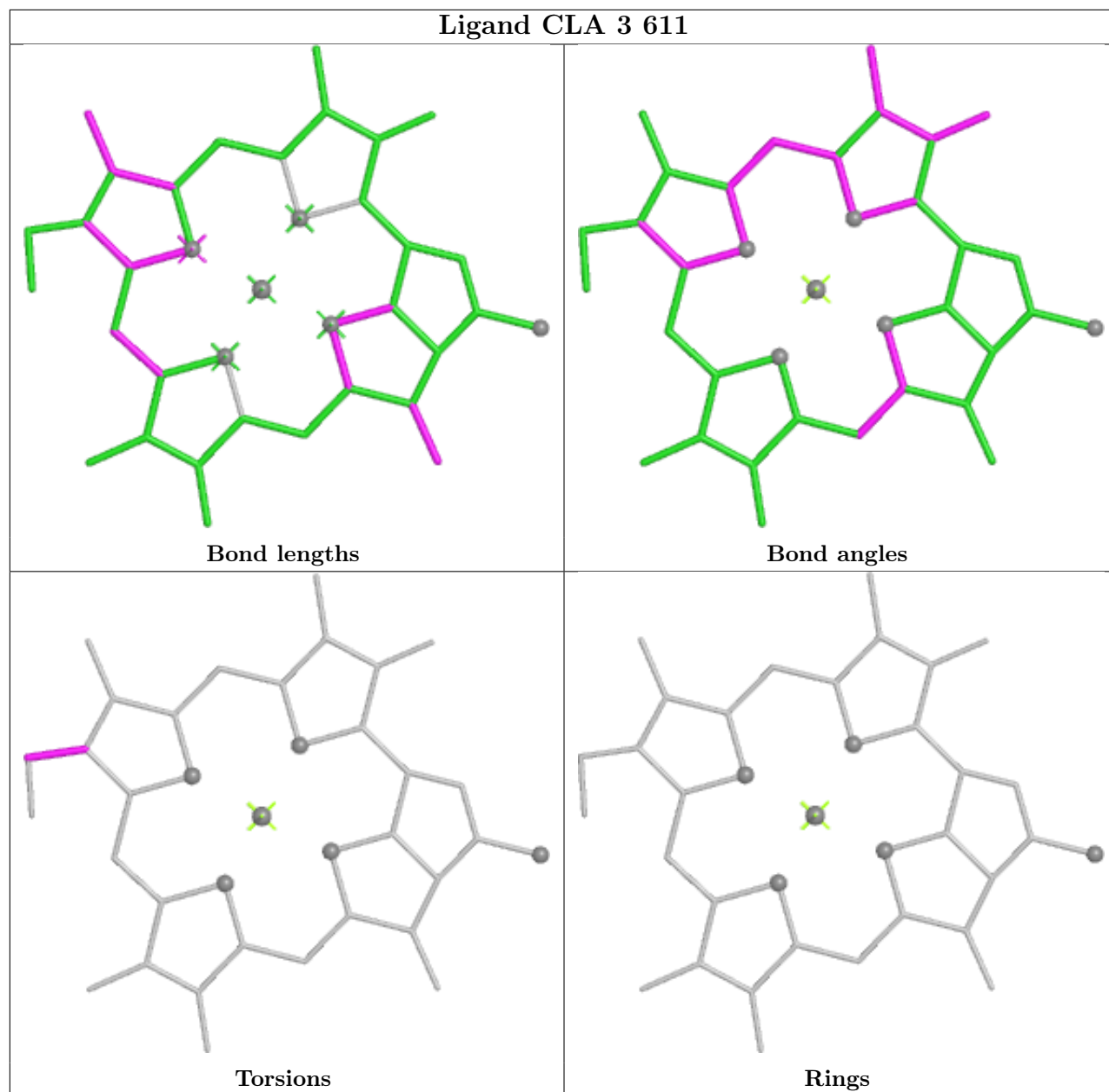


Rings

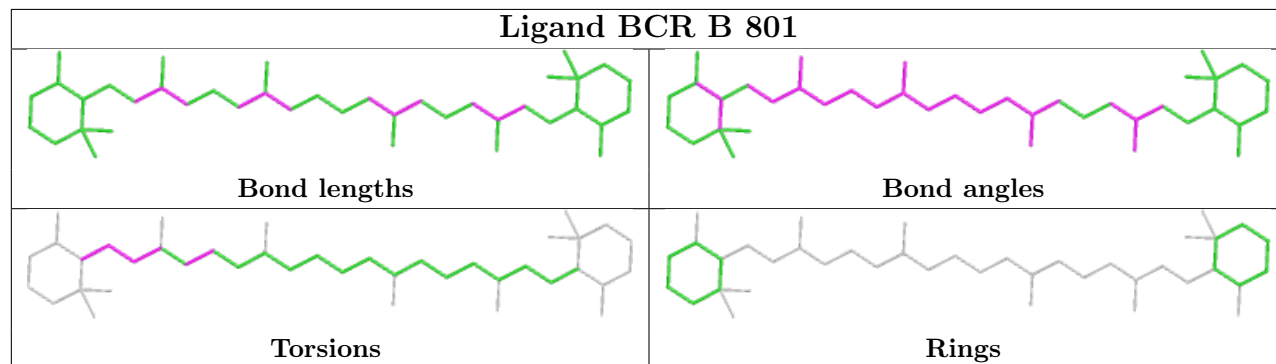
Ligand CLA z 610



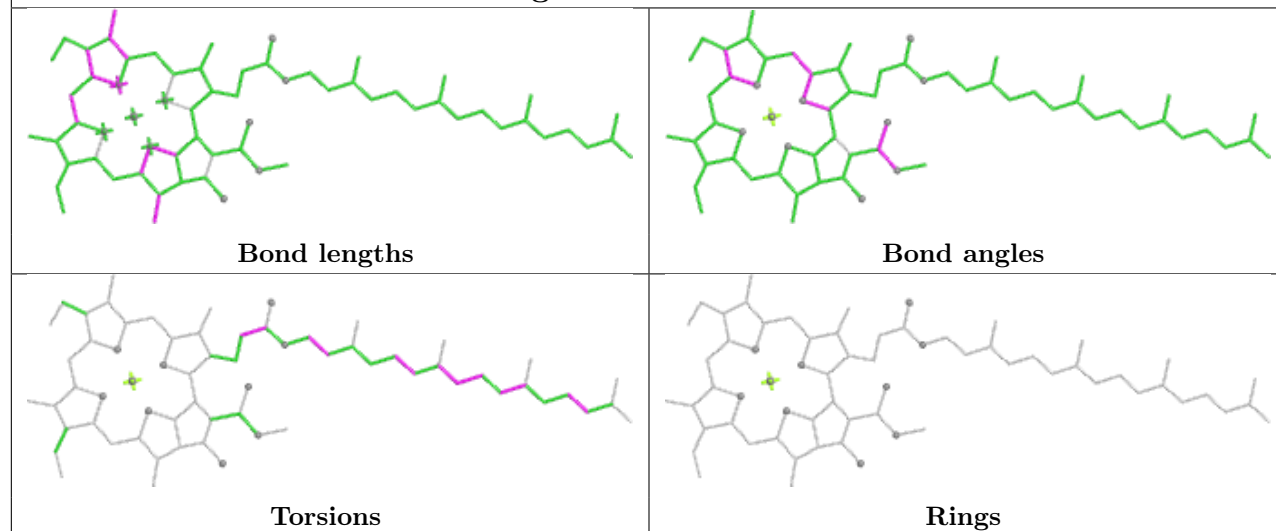
Ligand CLA 3 611



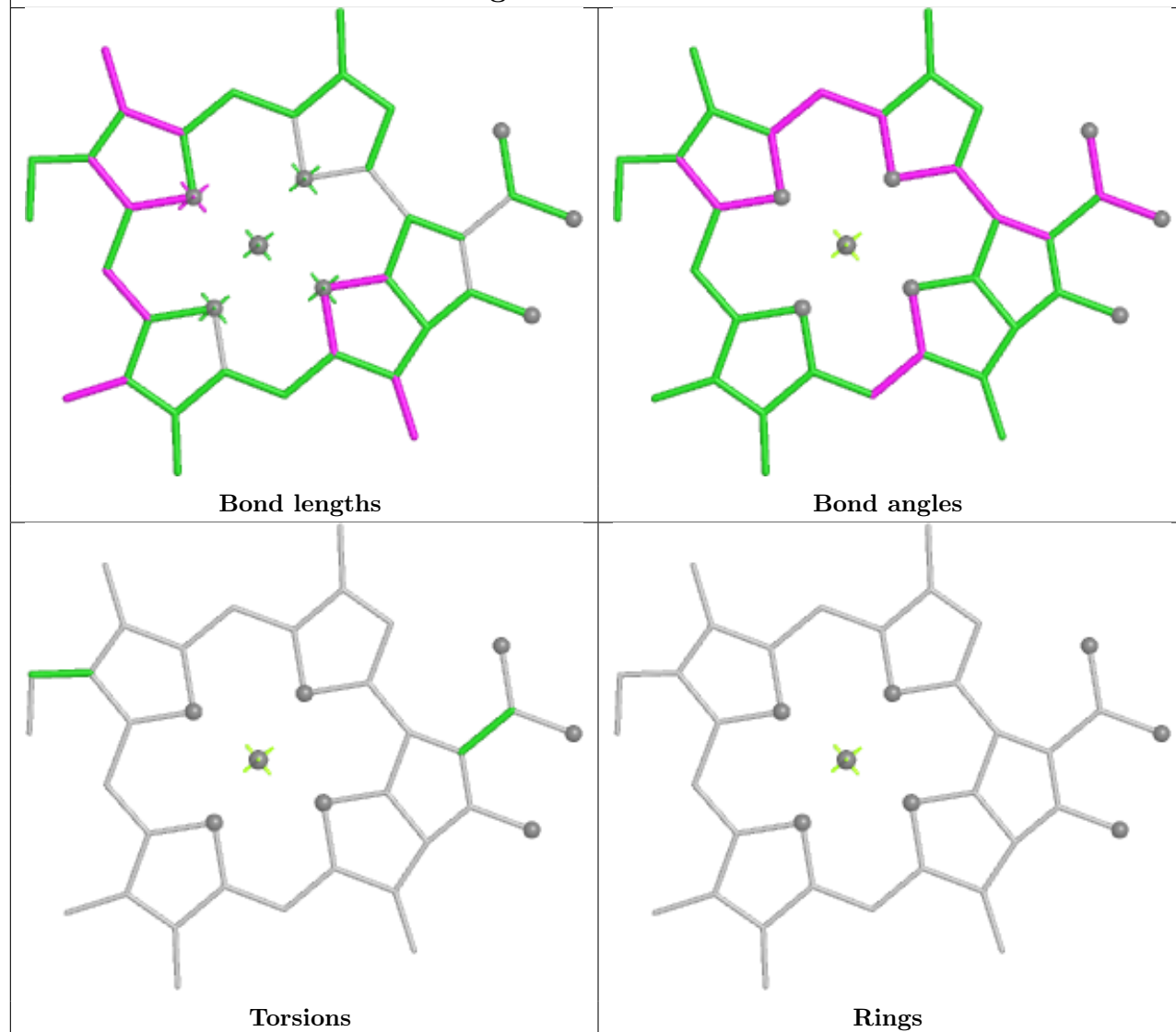
Ligand BCR B 801

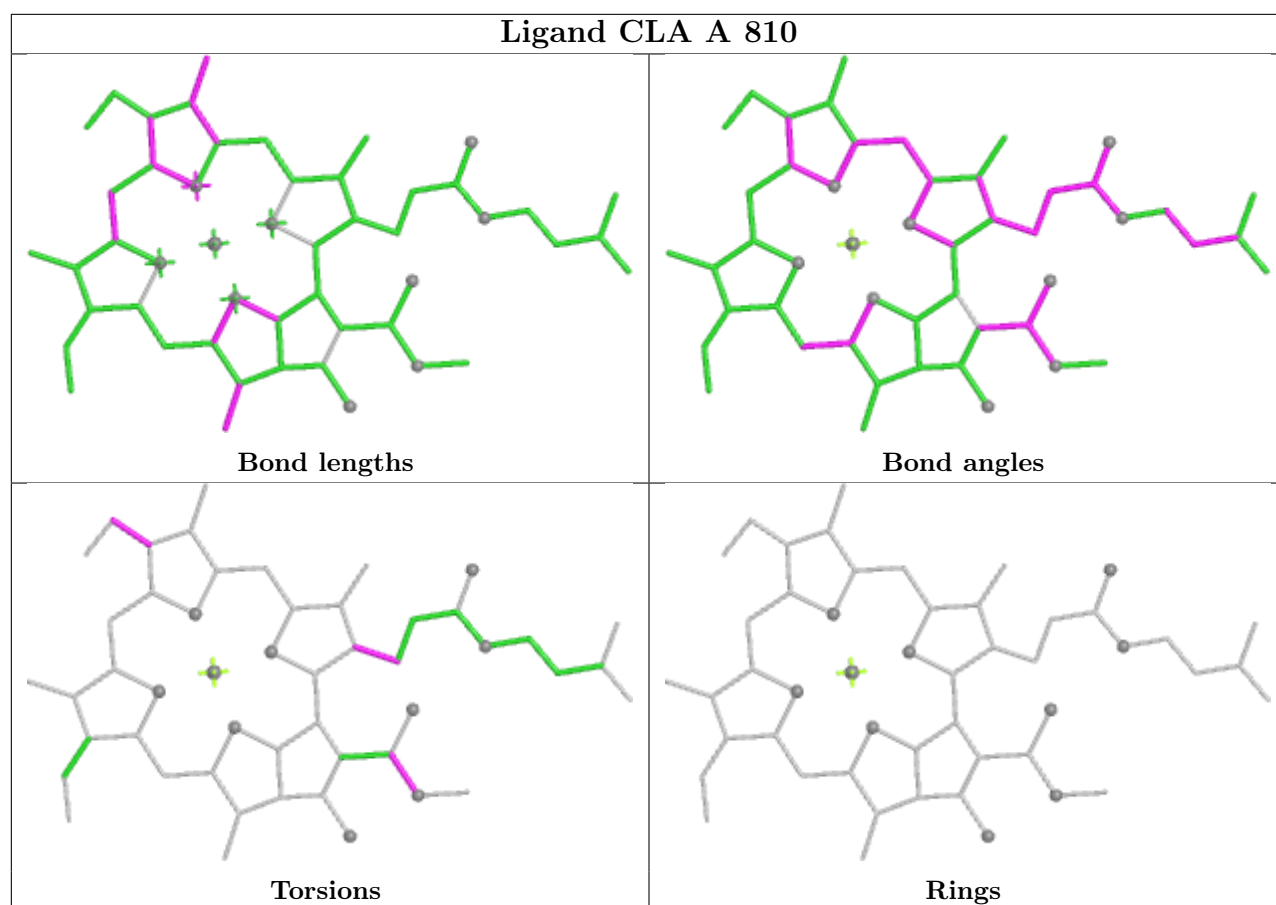


Ligand CLA A 826

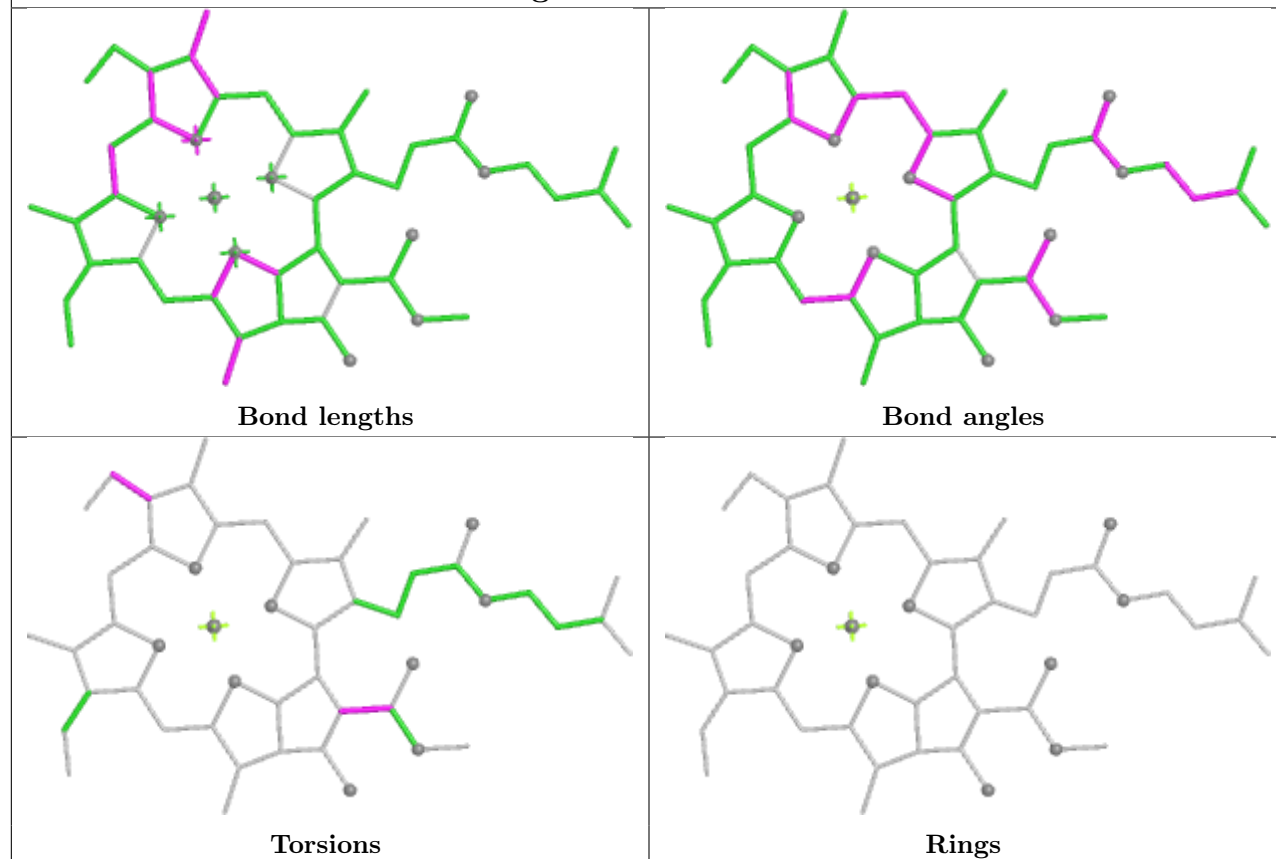


Ligand CLA O 202

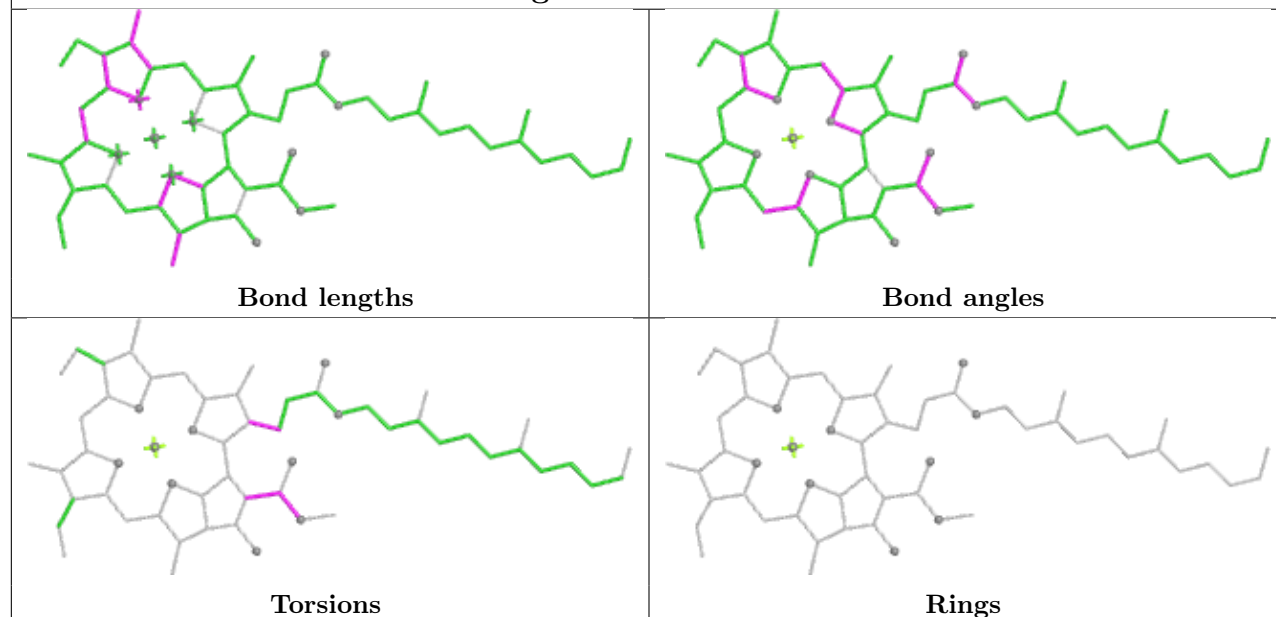




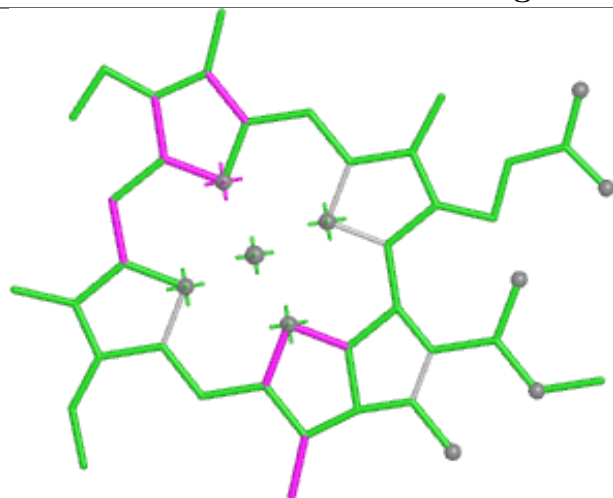
Ligand CLA A 808



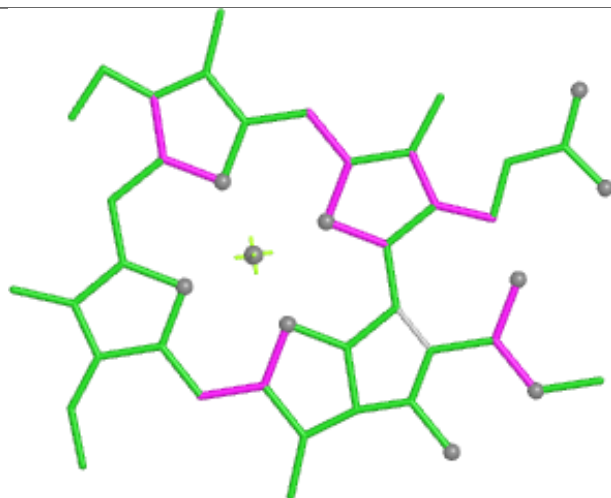
Ligand CLA A 827



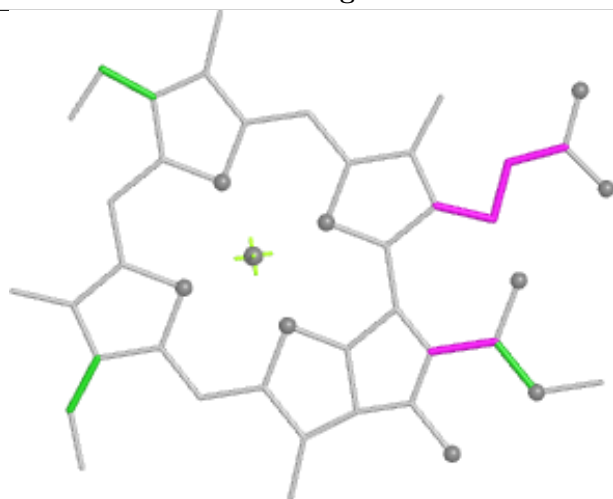
Ligand CLA A 815



Bond lengths



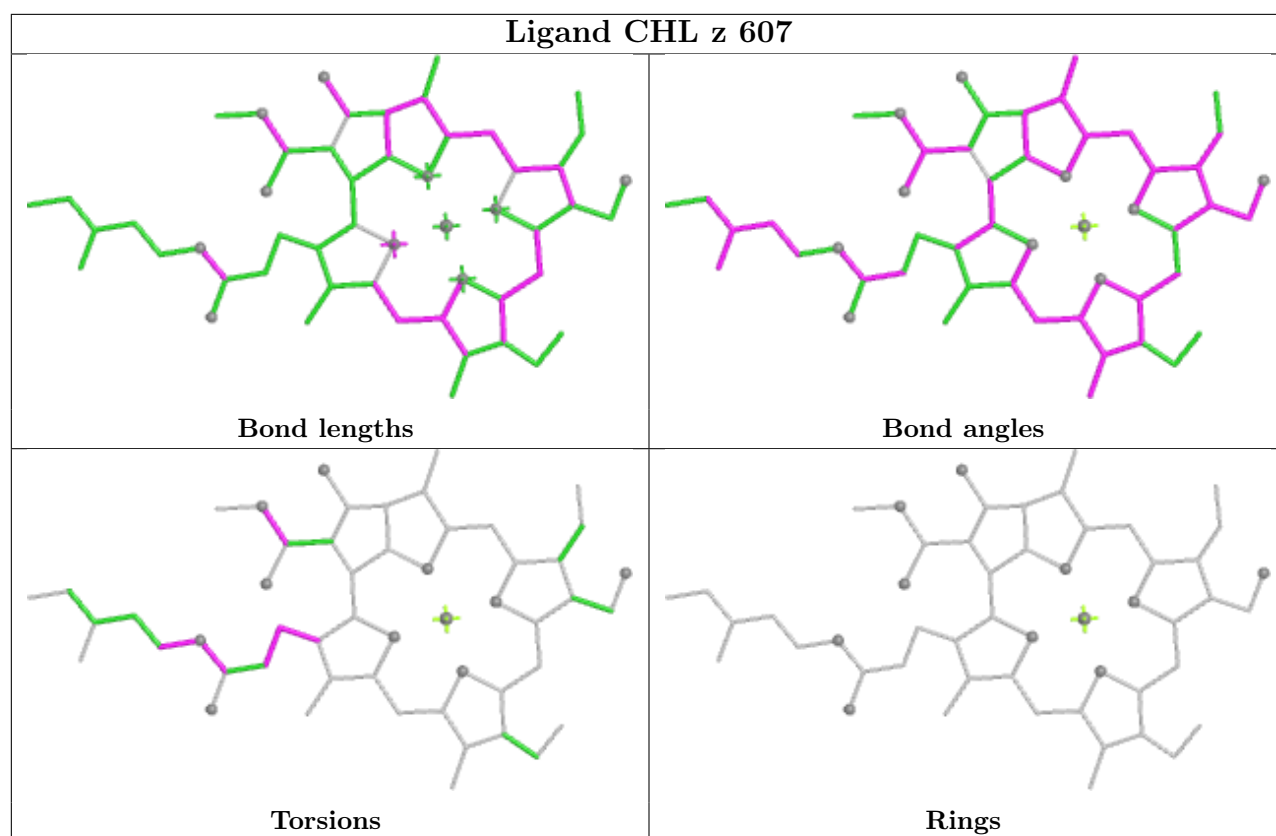
Bond angles



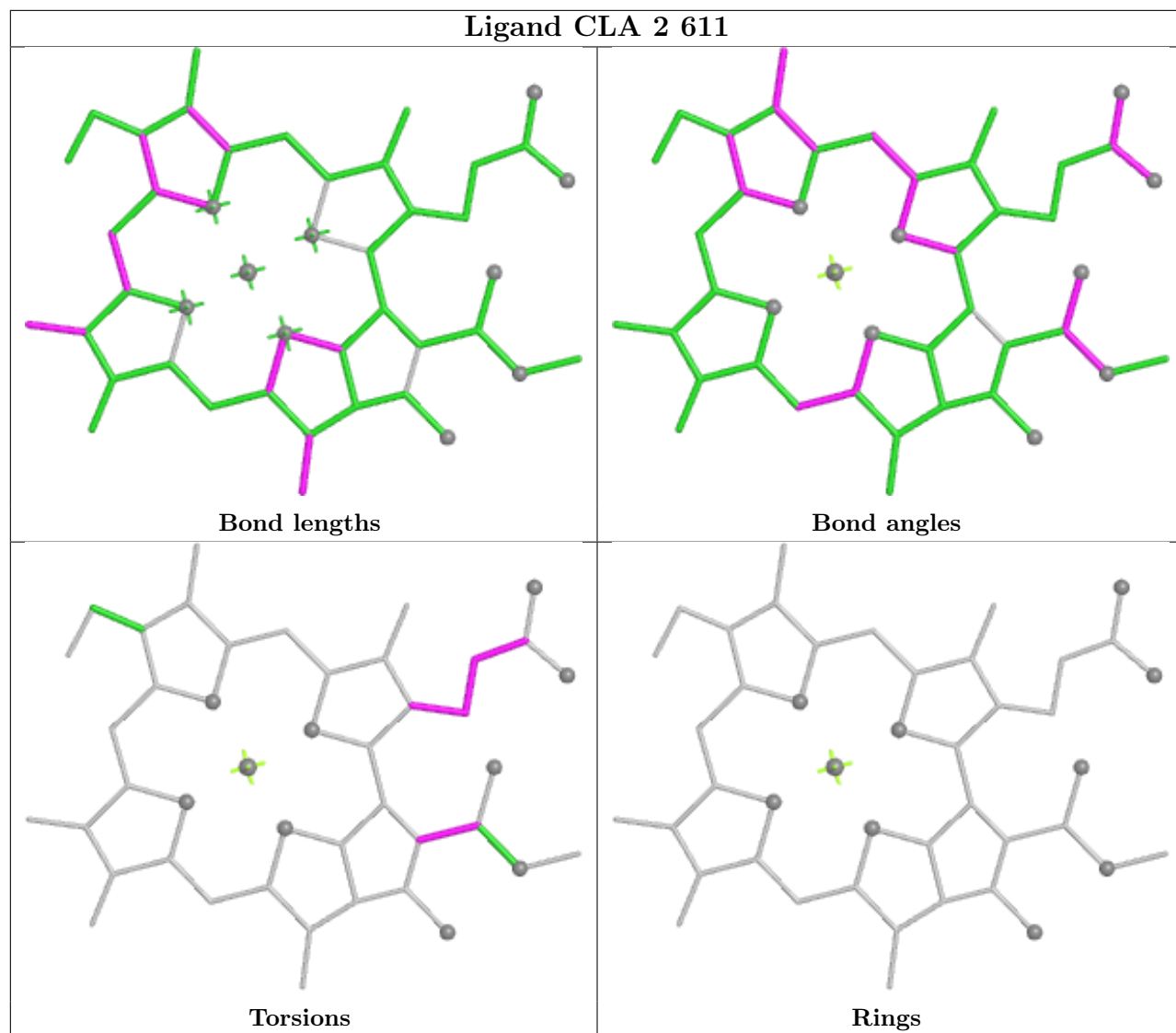
Torsions



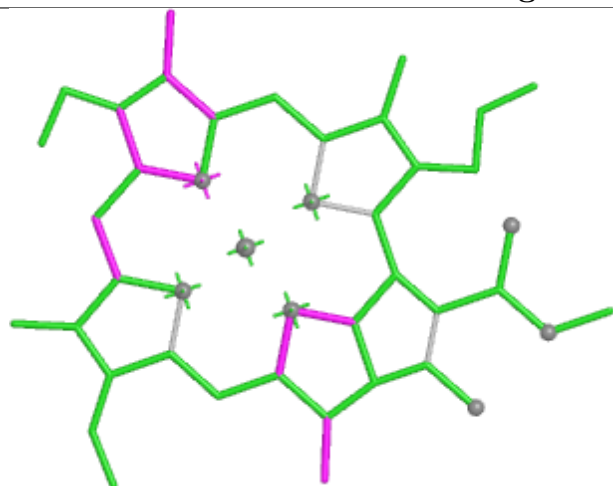
Rings



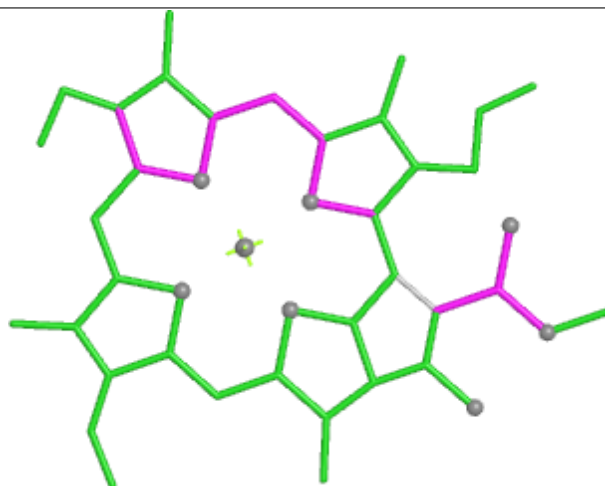
Ligand CLA 2 611



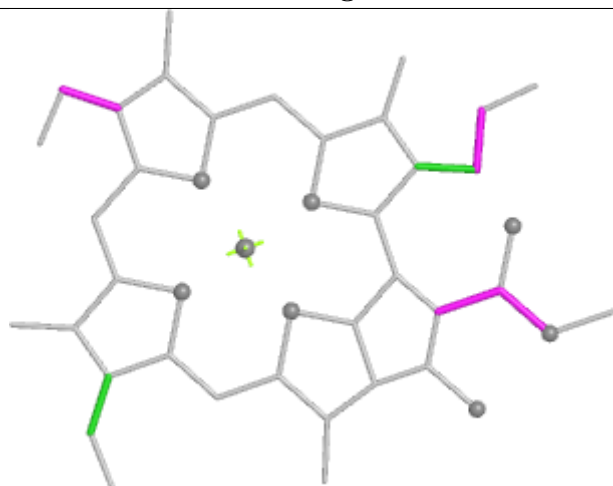
Ligand CLA 2 613



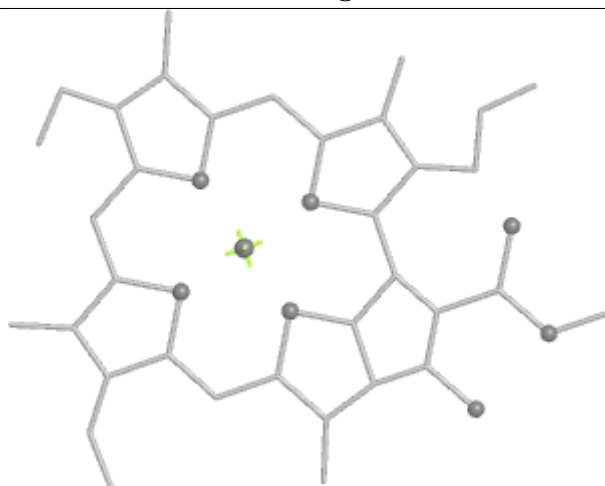
Bond lengths



Bond angles

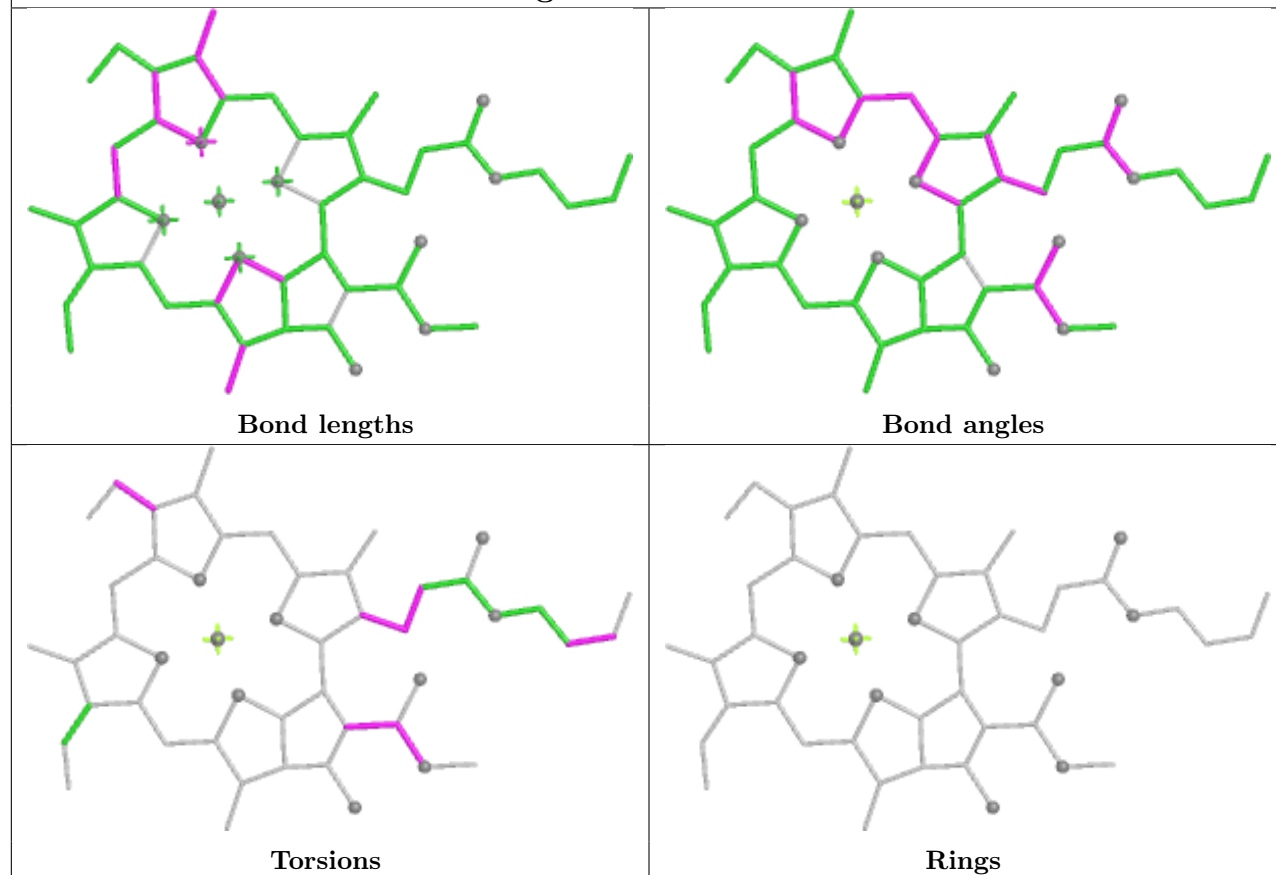


Torsions

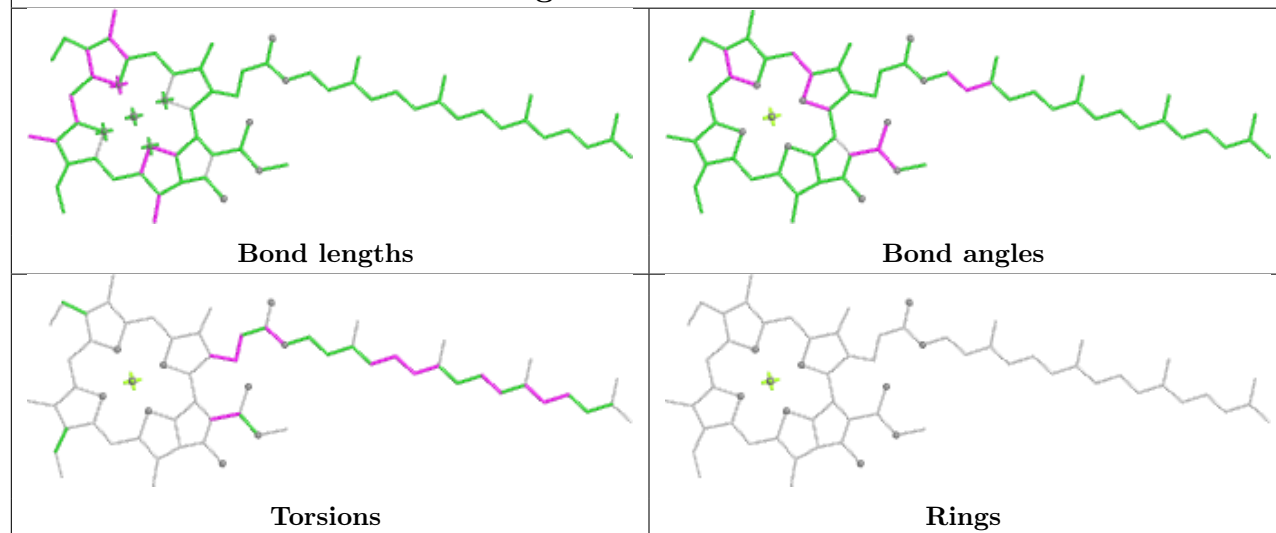


Rings

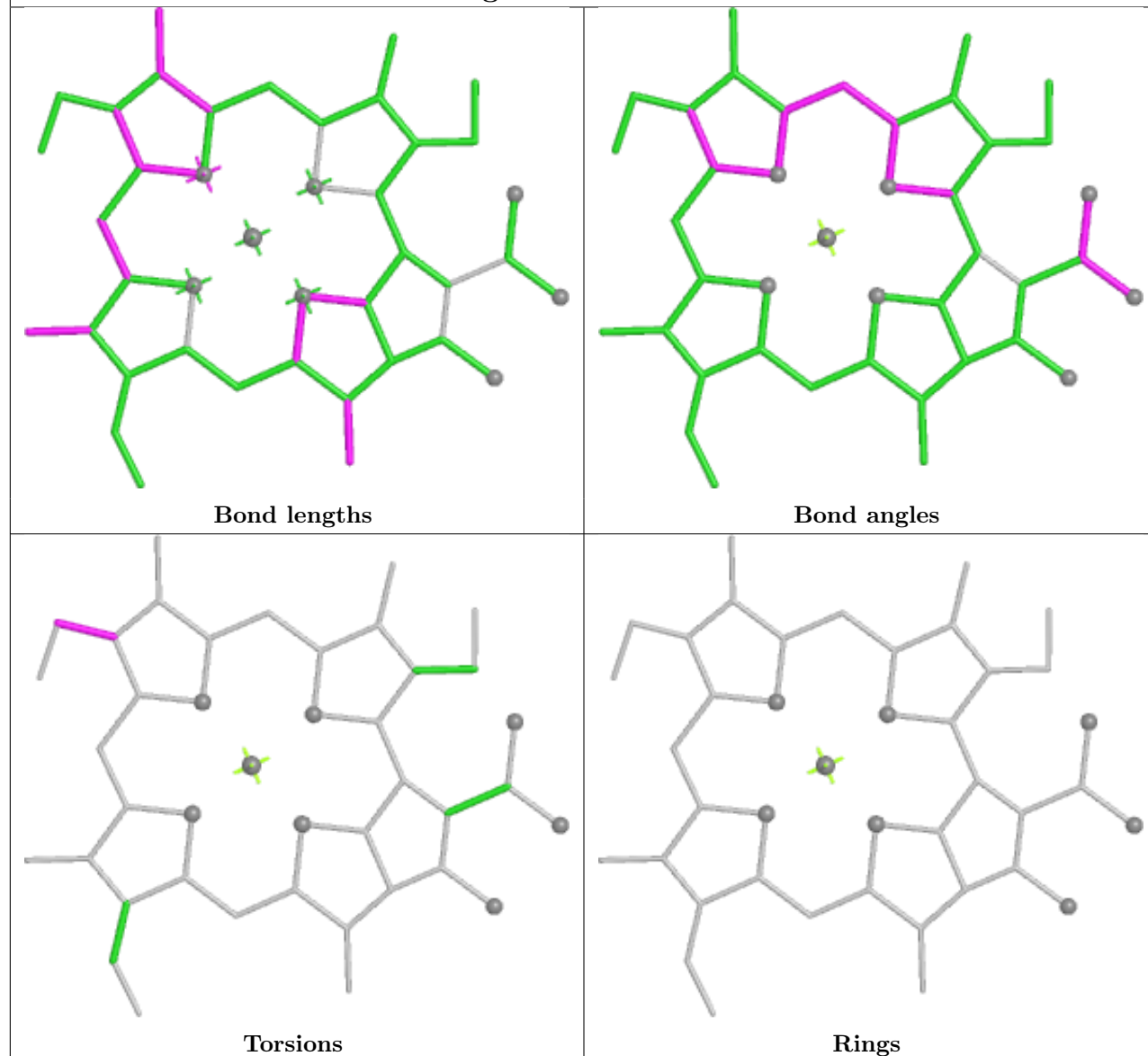
Ligand CLA 1 604



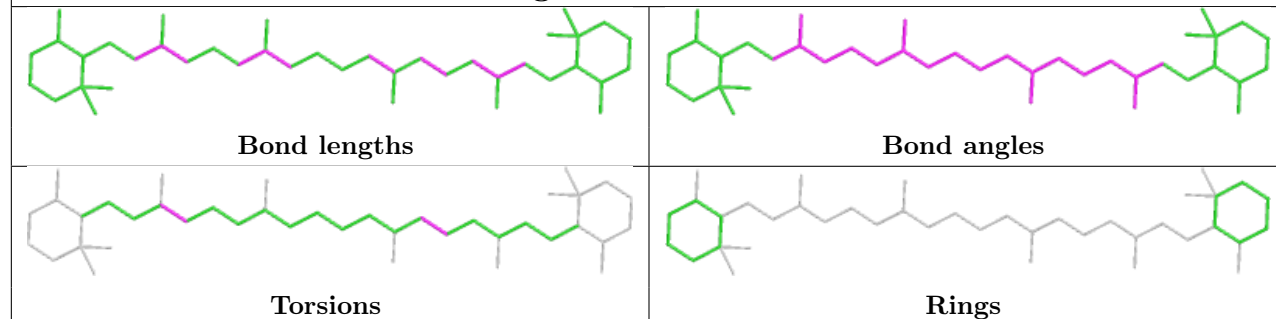
Ligand CLA x 602

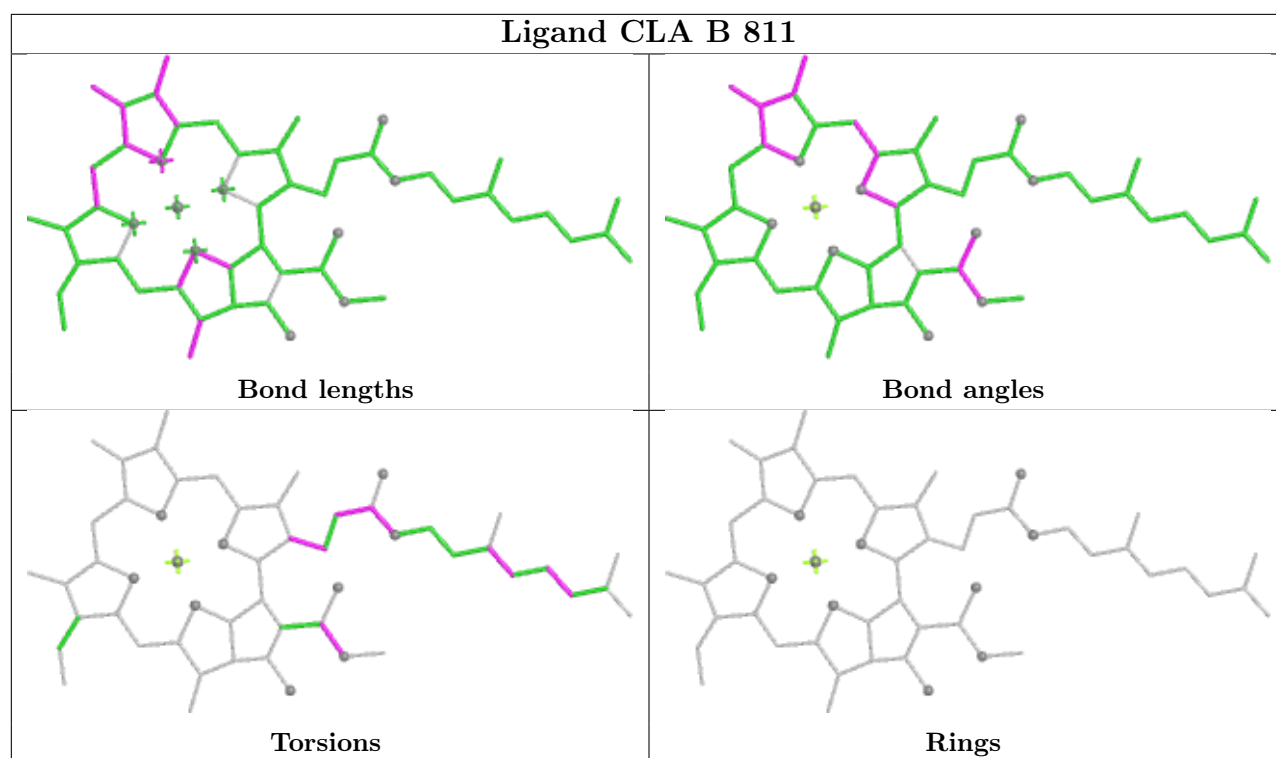


Ligand CLA 3 604

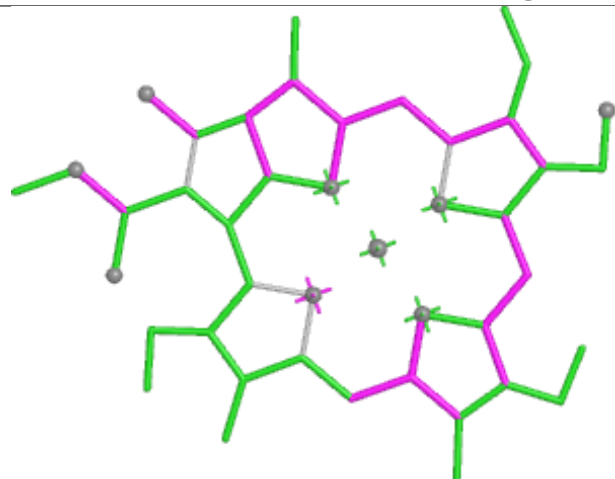


Ligand BCR L 301

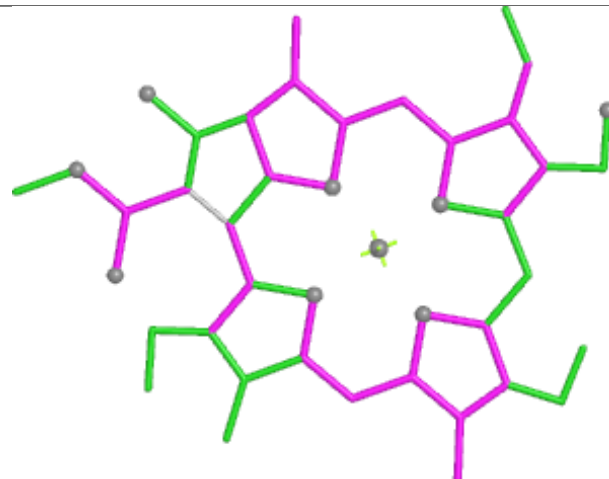




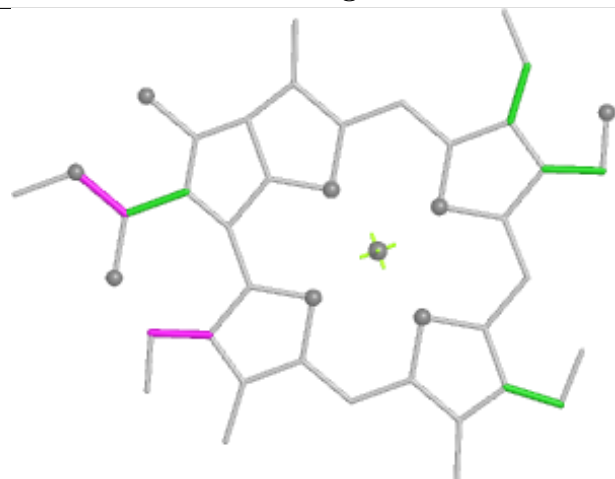
Ligand CHL 2 606



Bond lengths



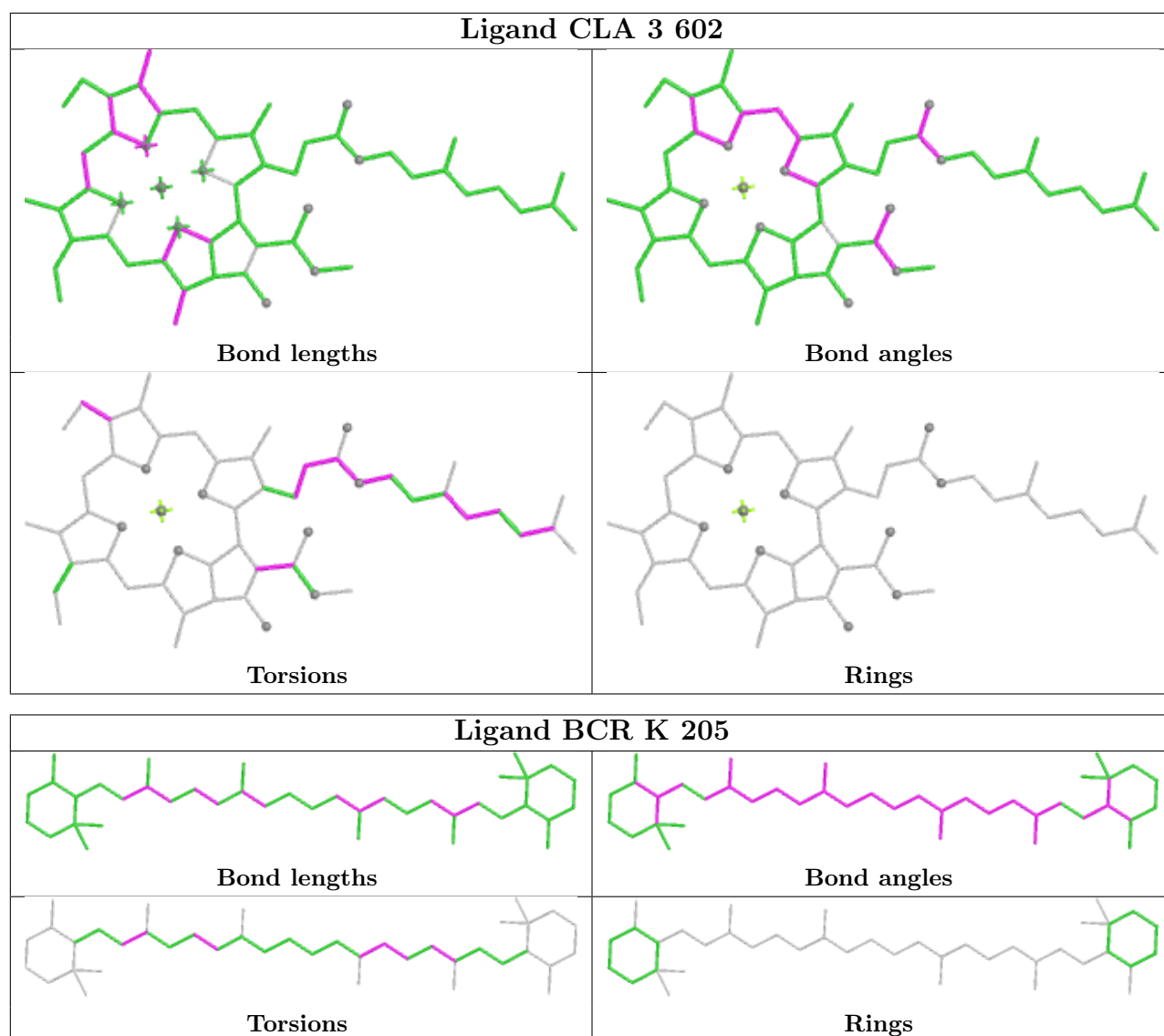
Bond angles

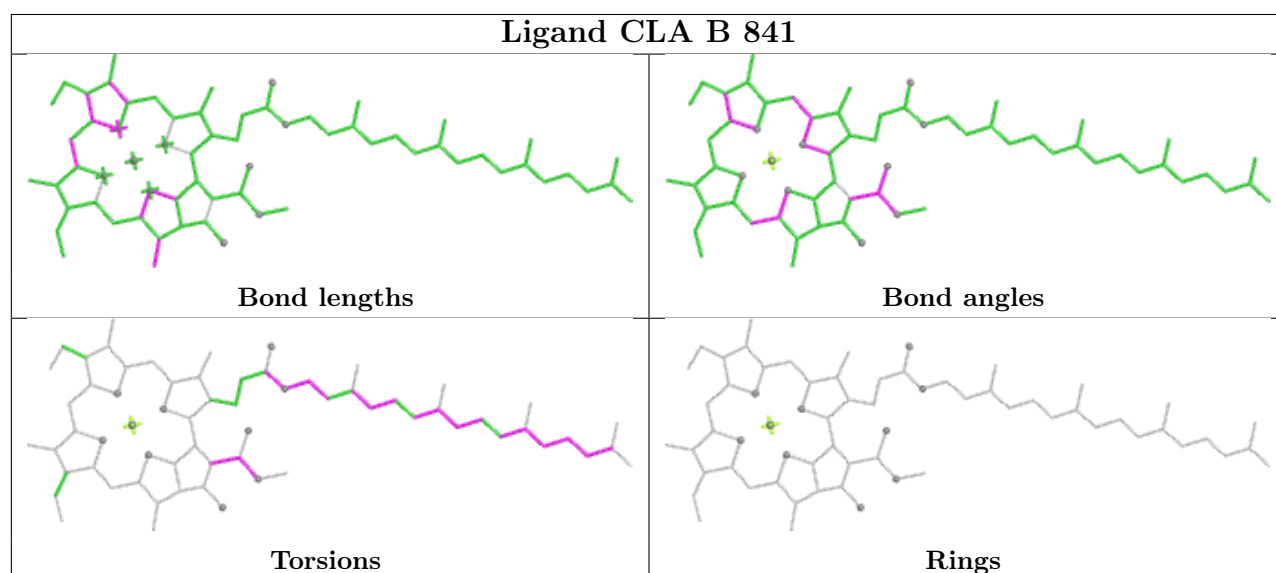
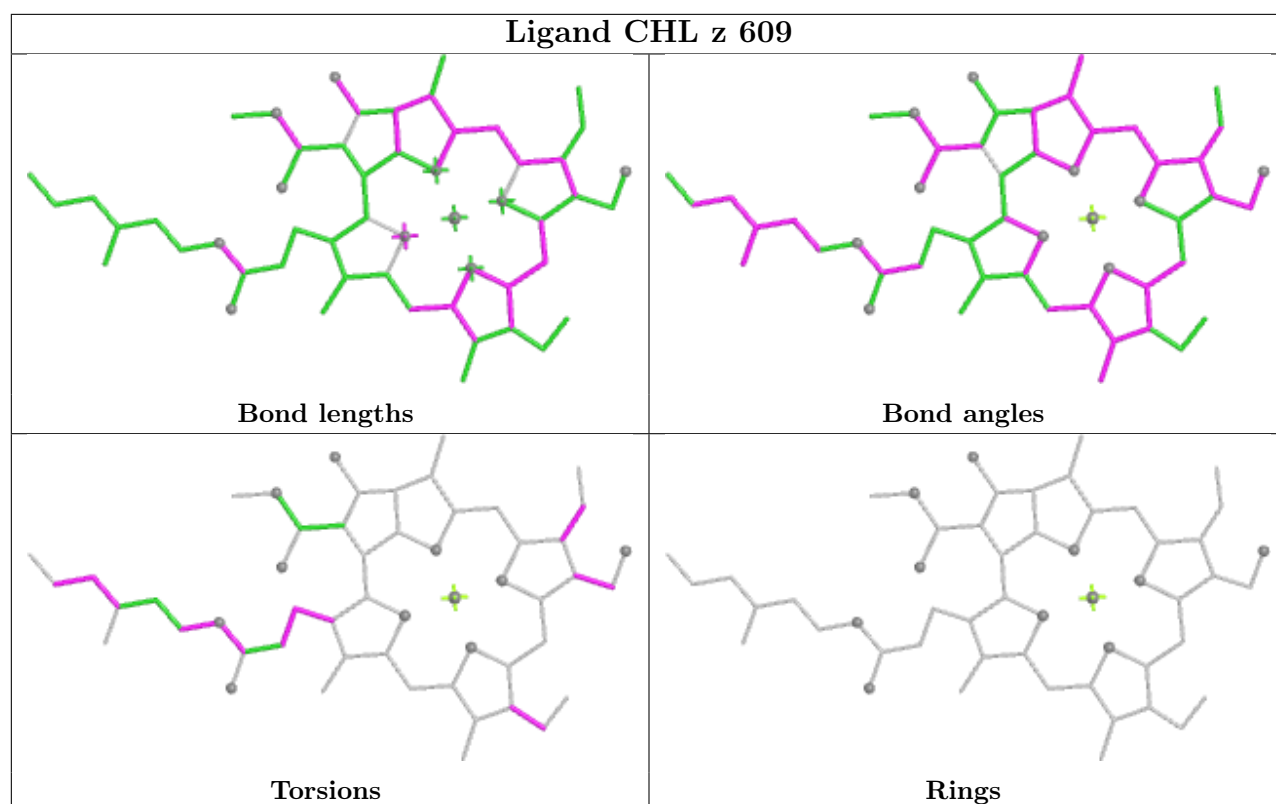


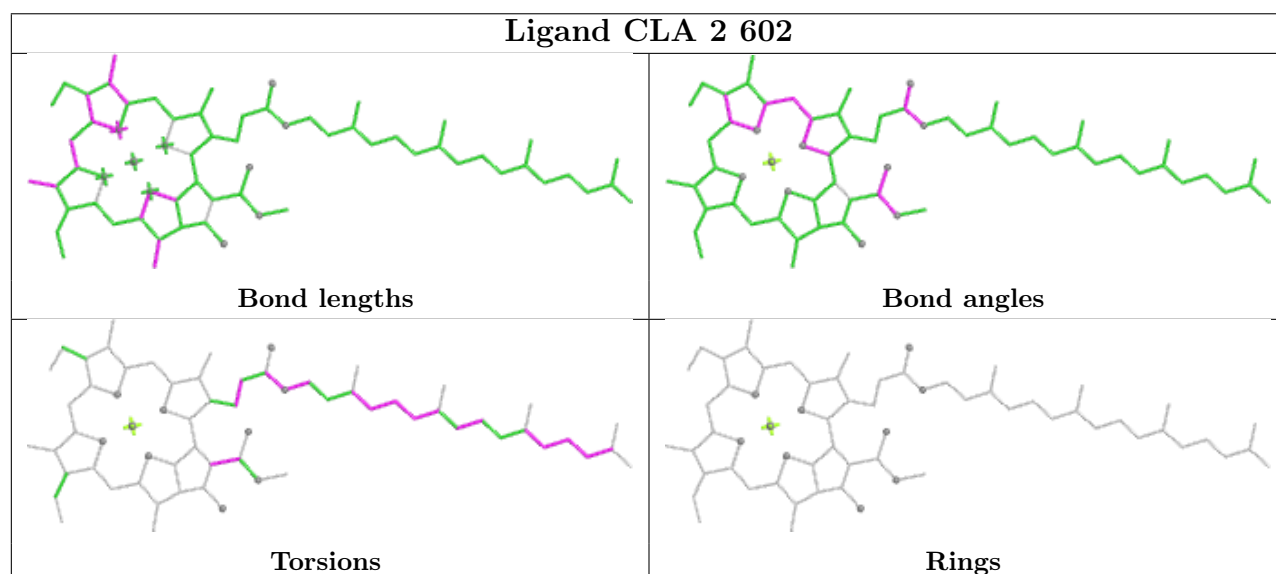
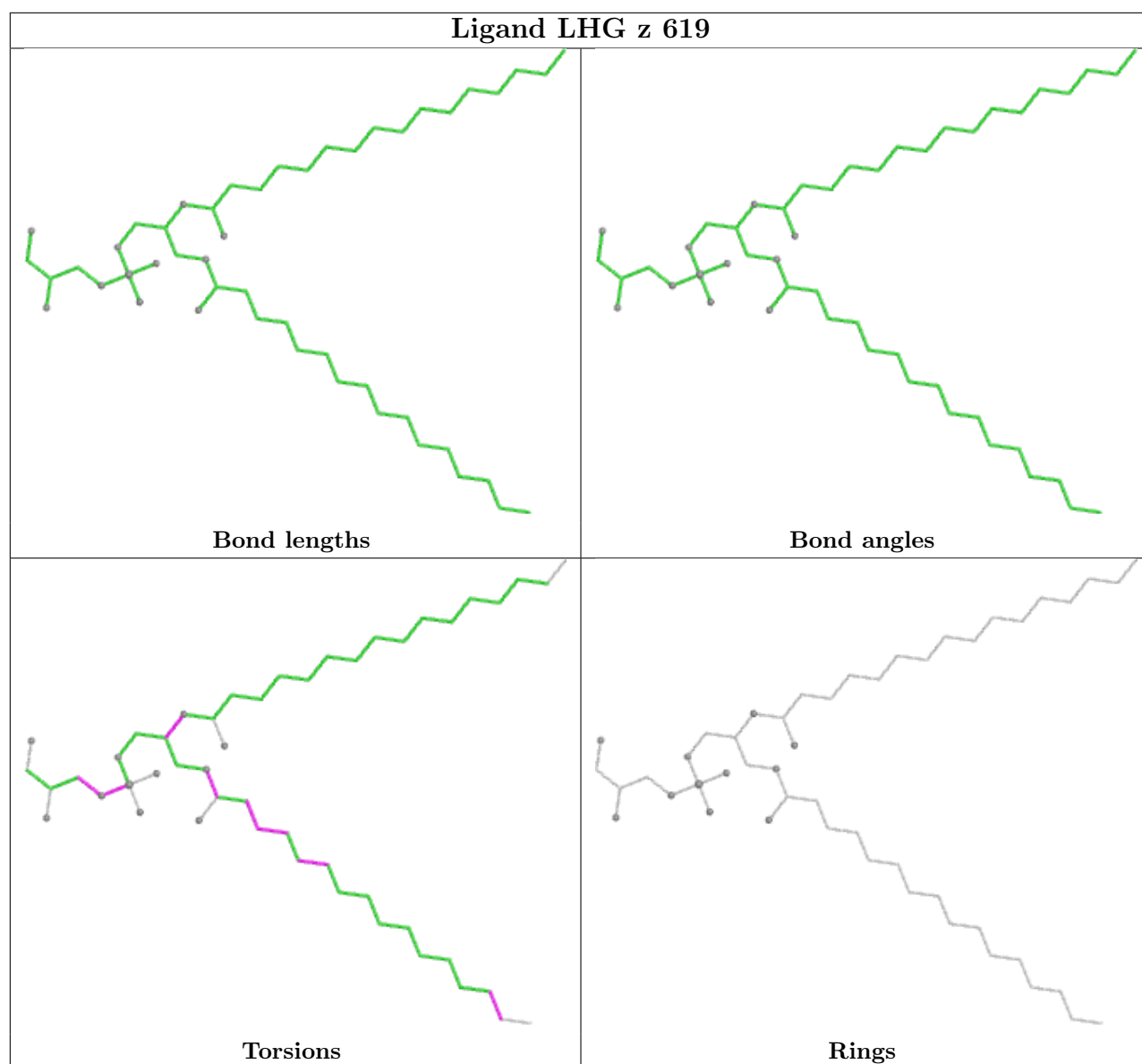
Torsions

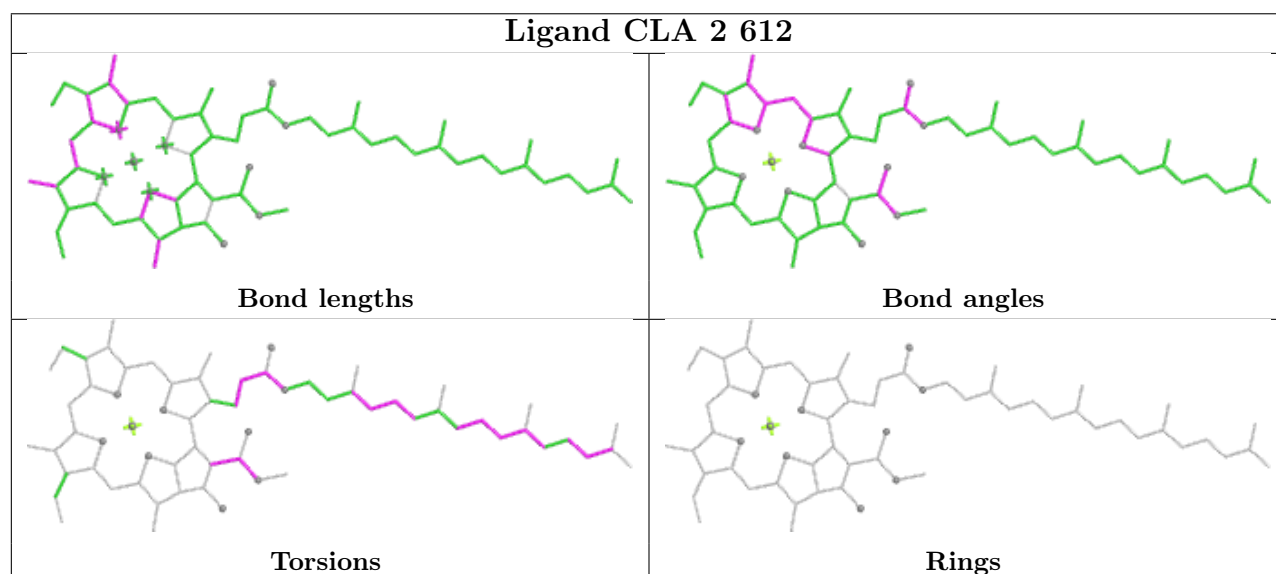
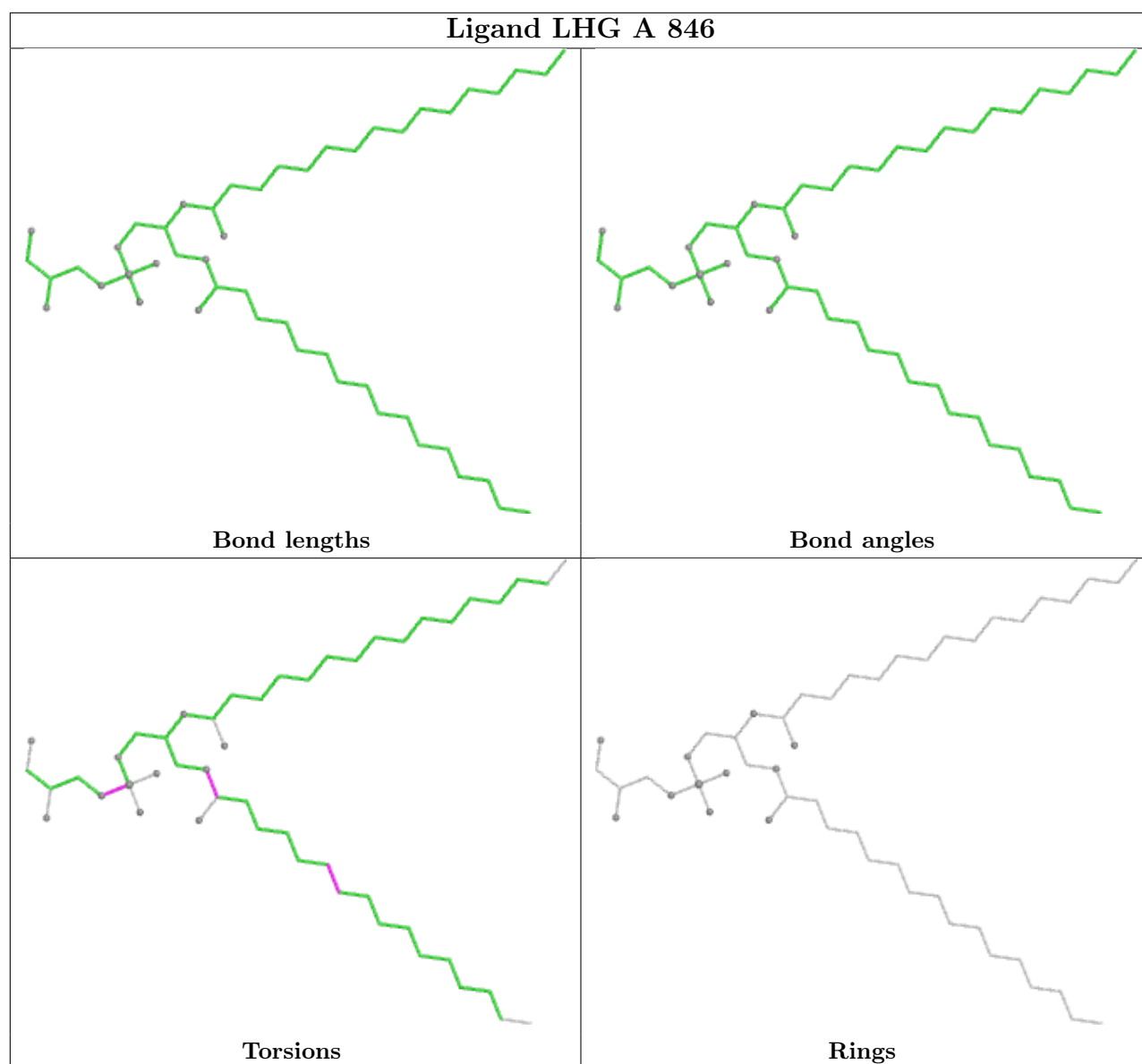


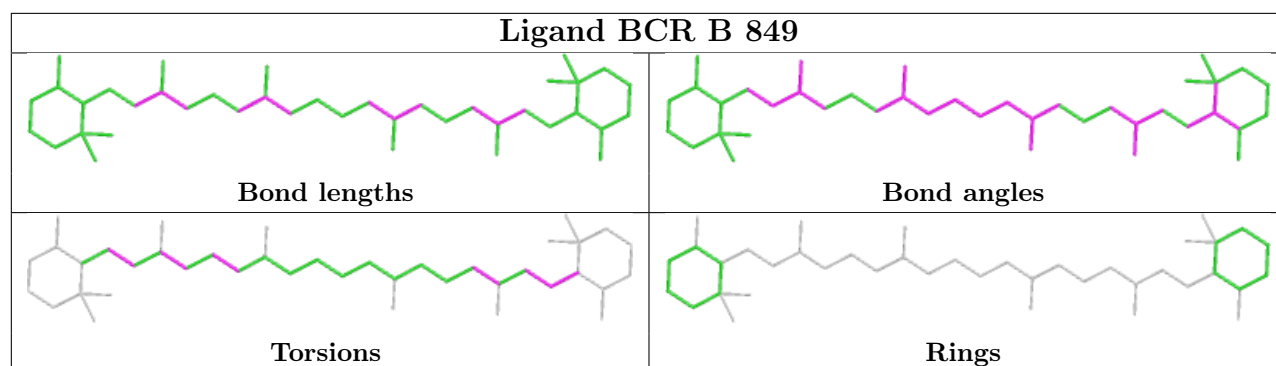
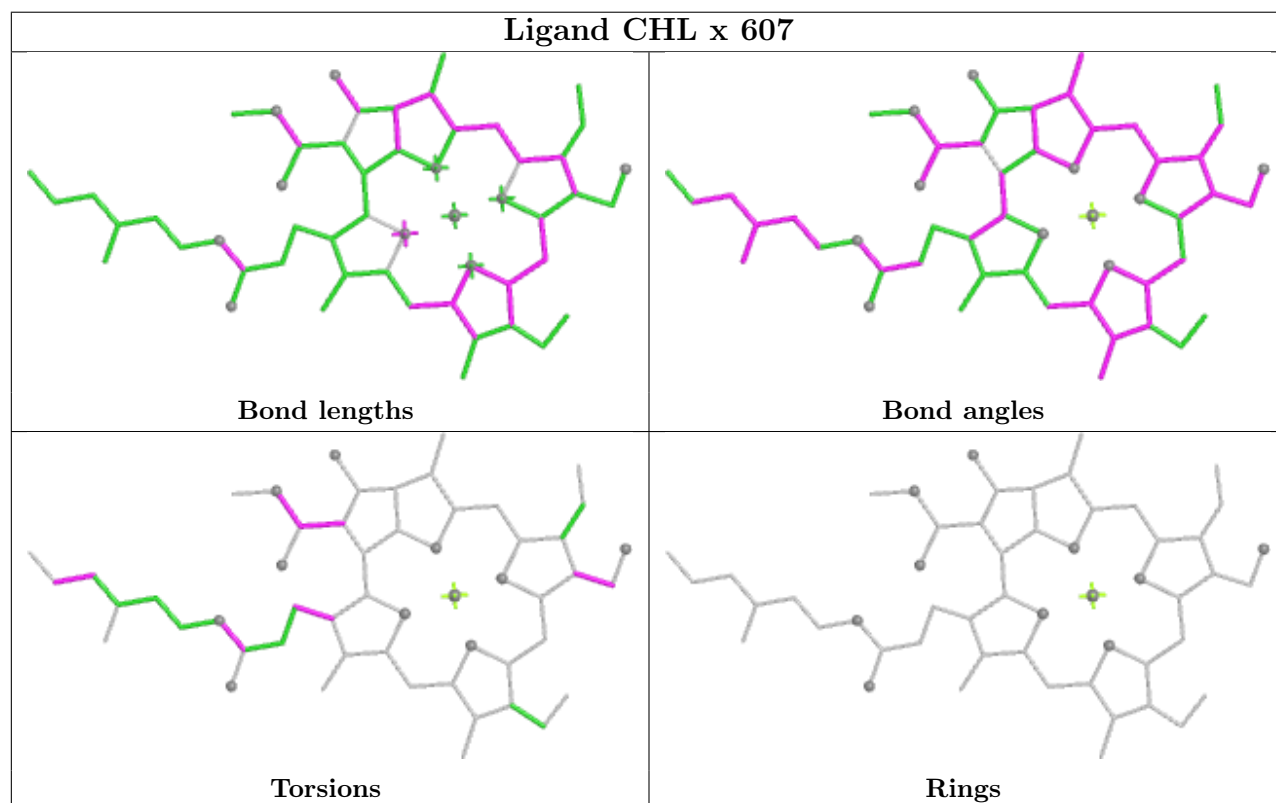
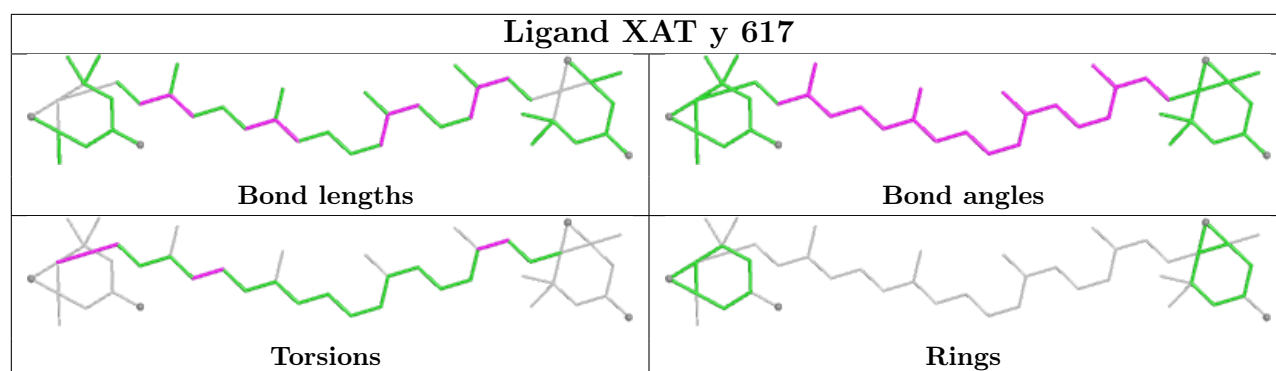
Rings



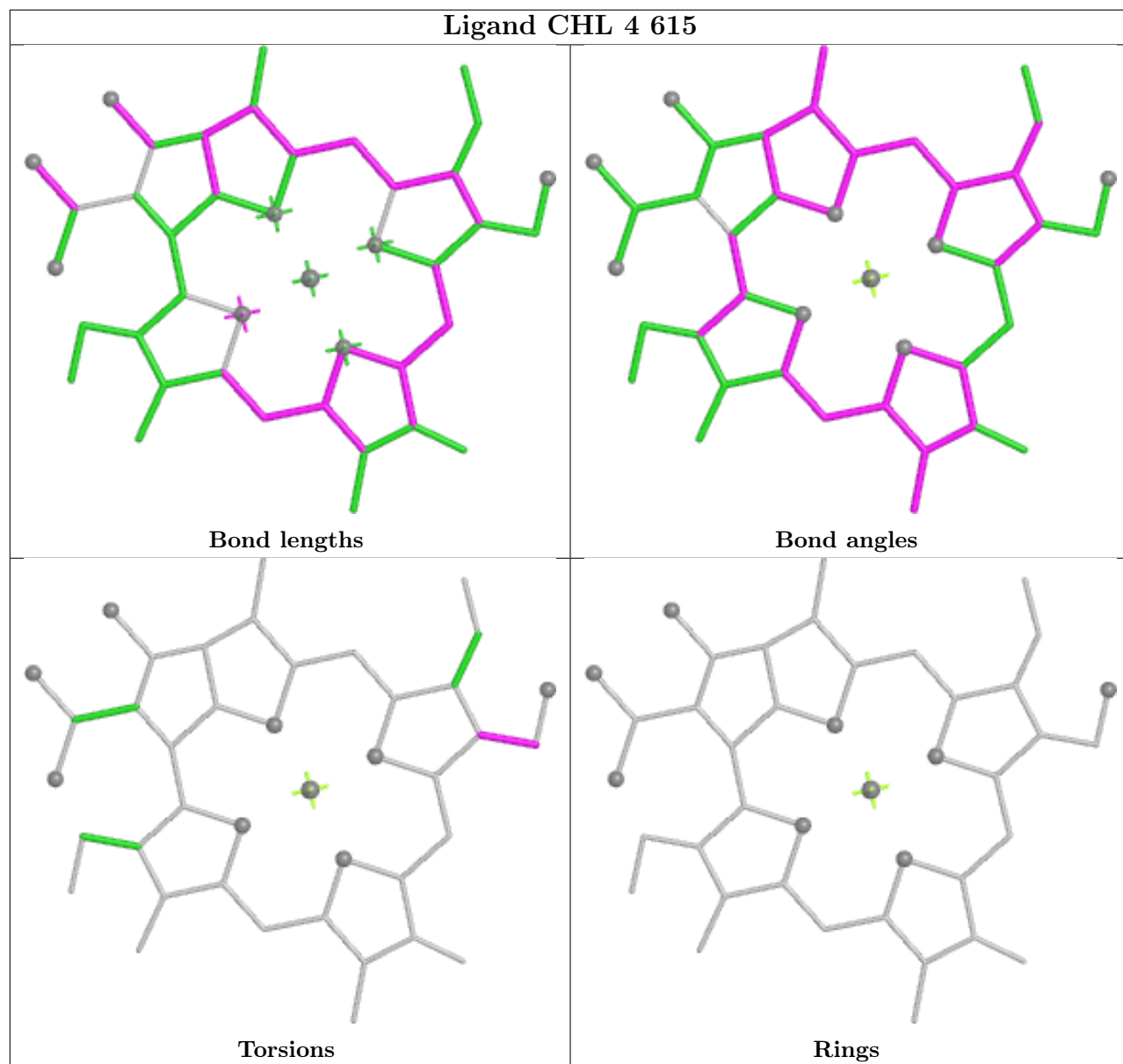




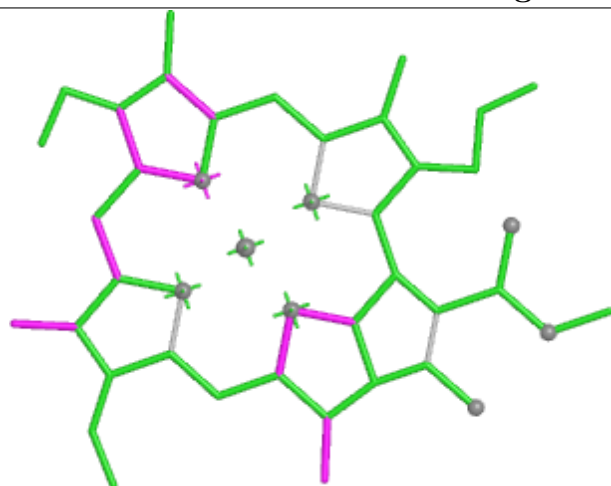




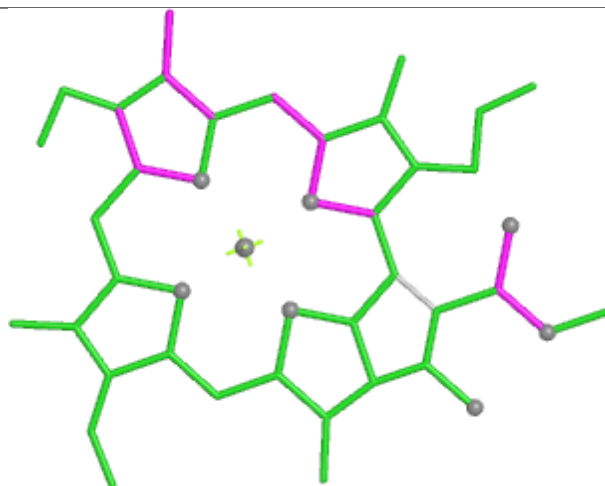
Ligand CHL 4 615



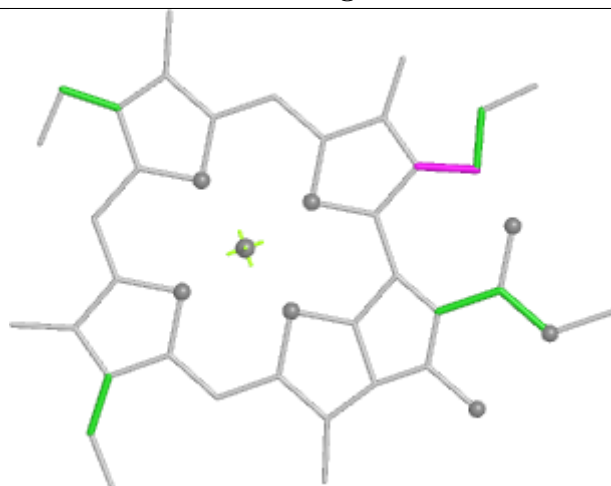
Ligand CLA B 815



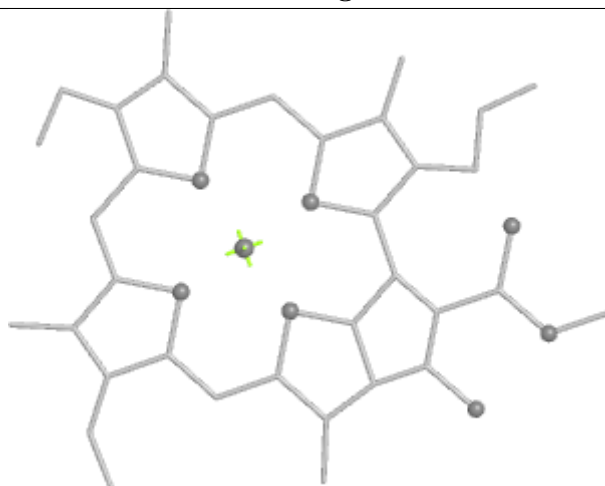
Bond lengths



Bond angles

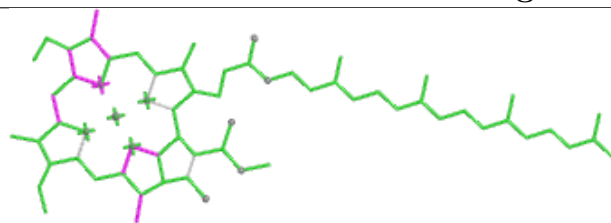


Torsions

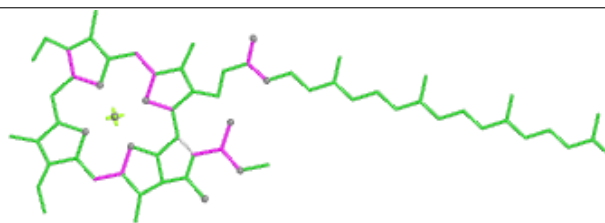


Rings

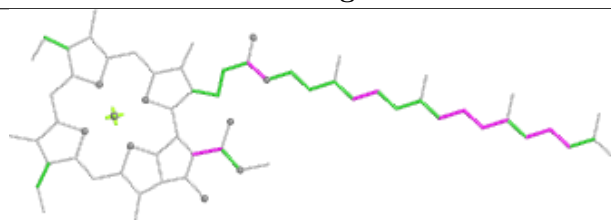
Ligand CLA L 303



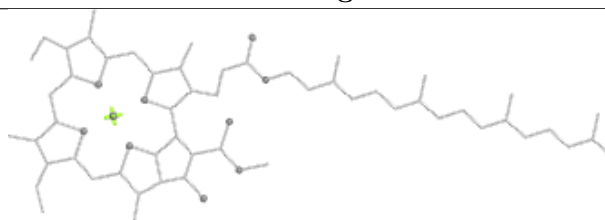
Bond lengths



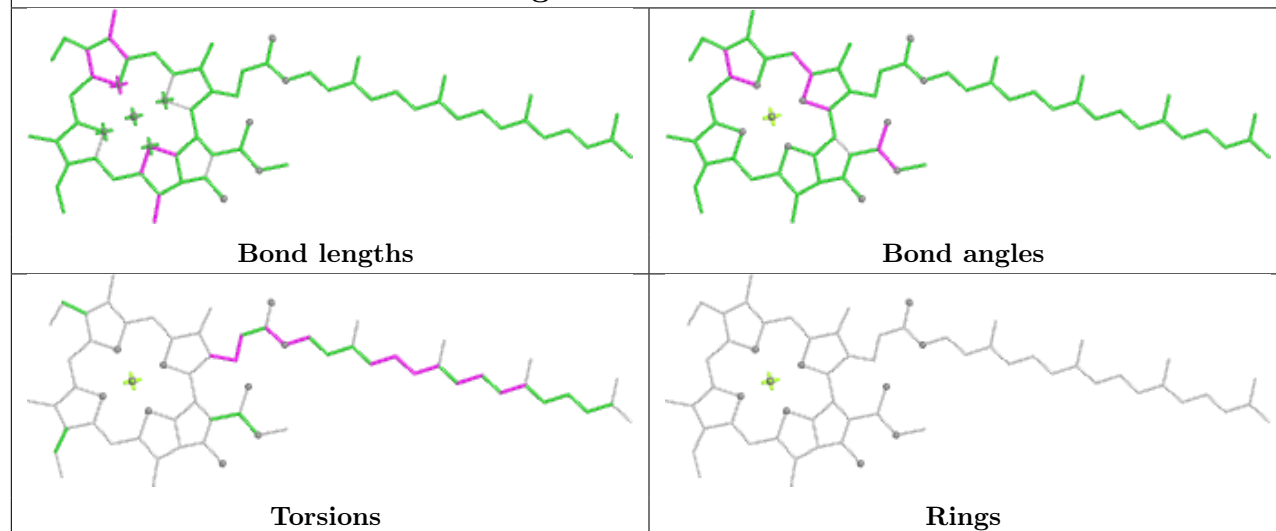
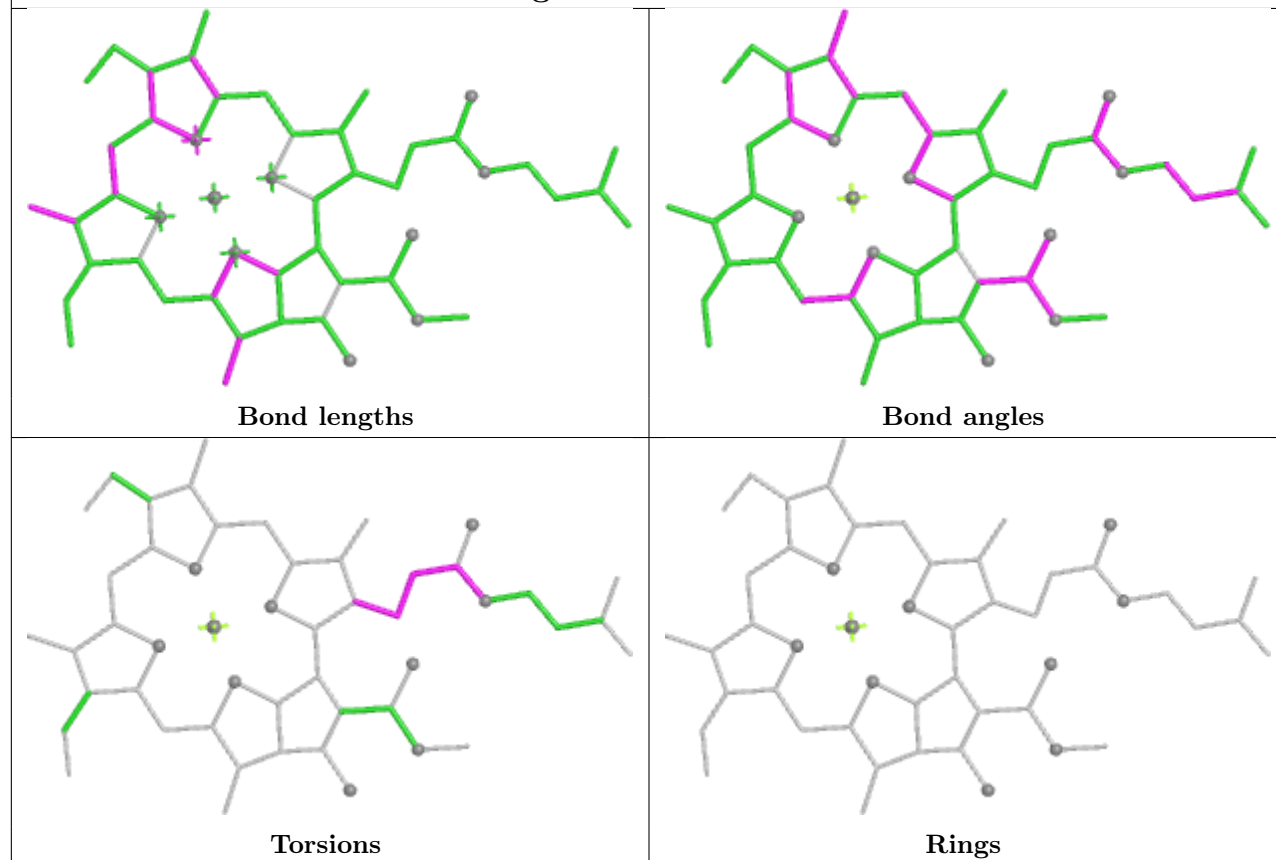
Bond angles

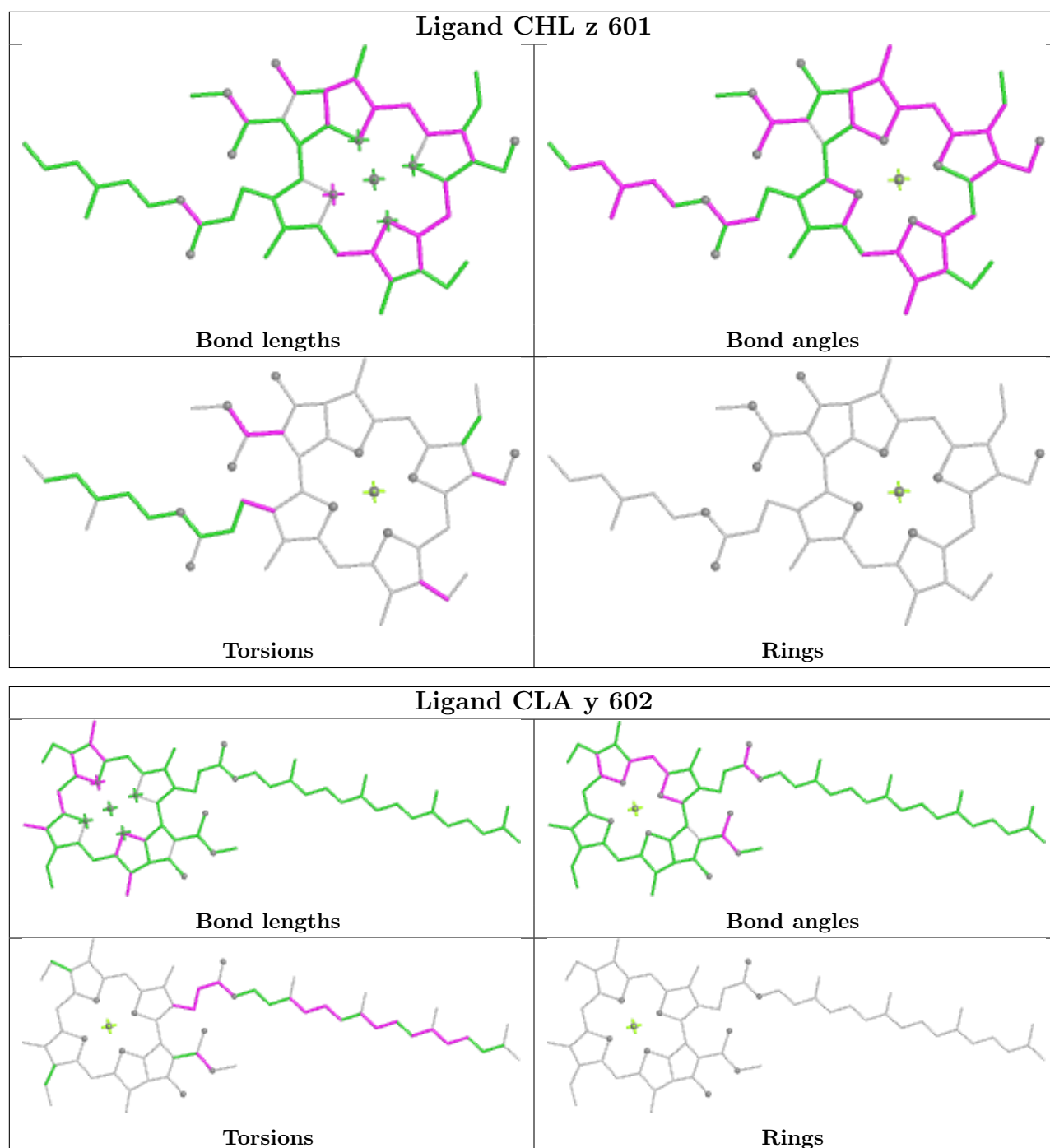


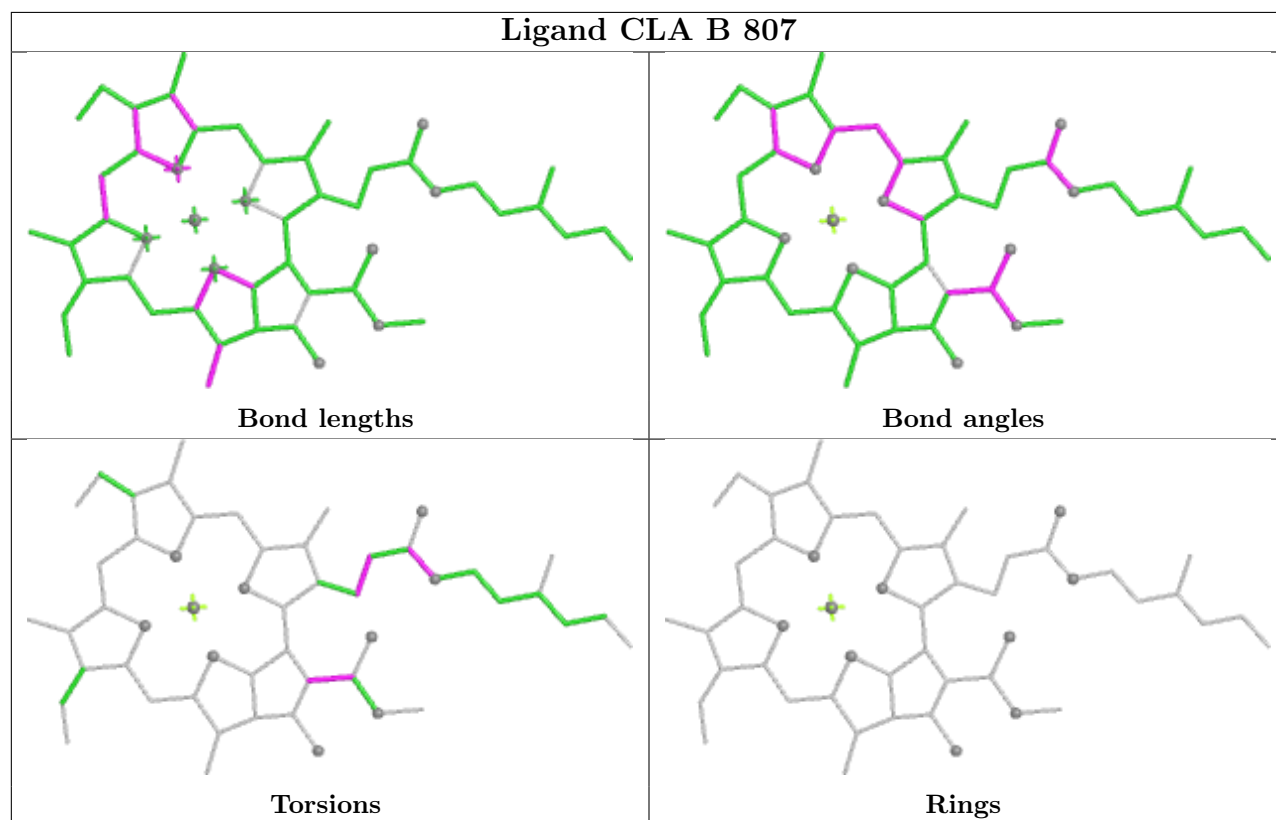
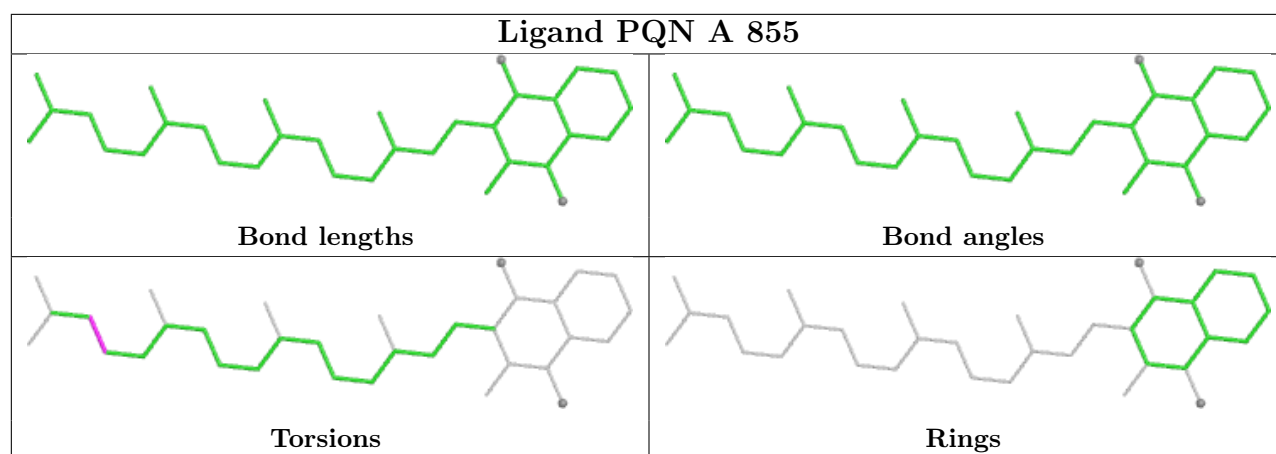
Torsions

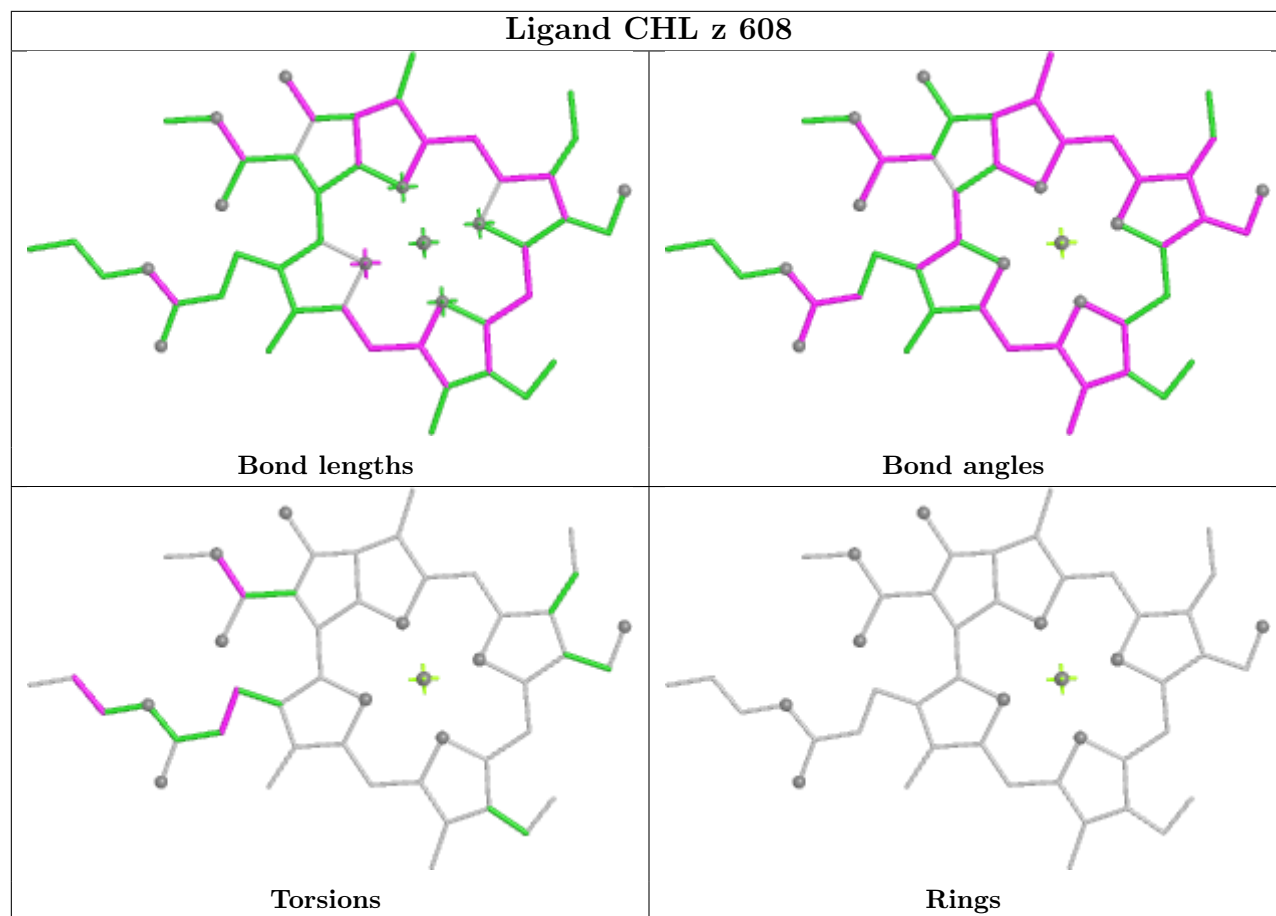


Rings

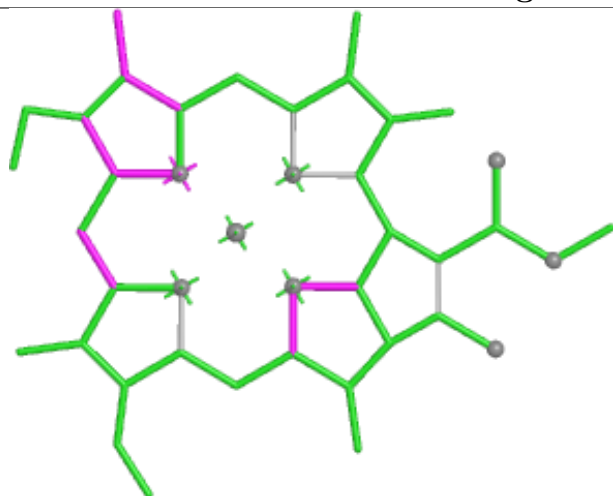
Ligand CLA A 843**Ligand CLA B 820**



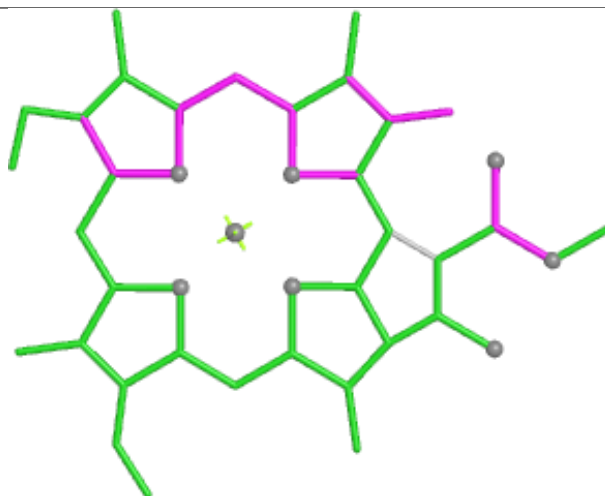




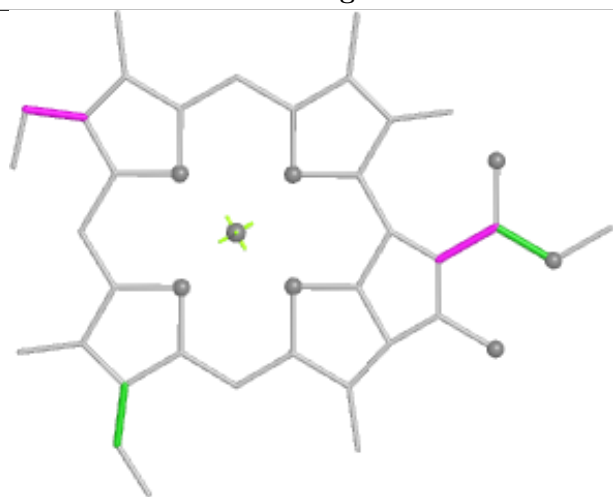
Ligand CLA F 303



Bond lengths



Bond angles

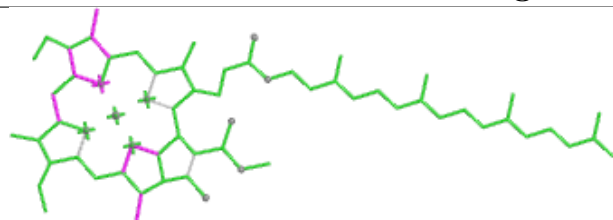


Torsions

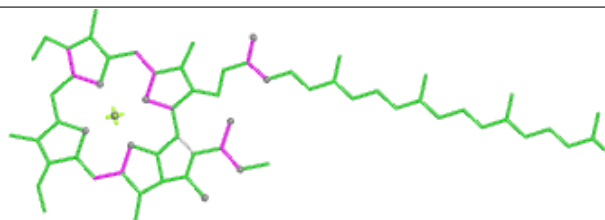


Rings

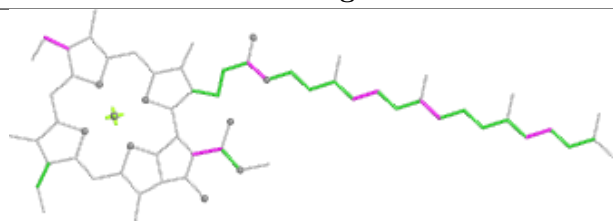
Ligand CLA A 834



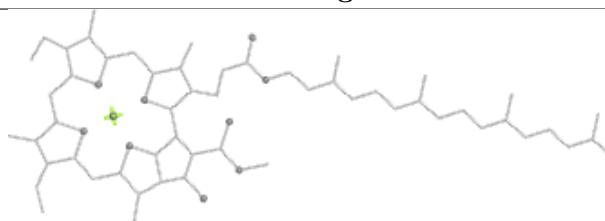
Bond lengths



Bond angles

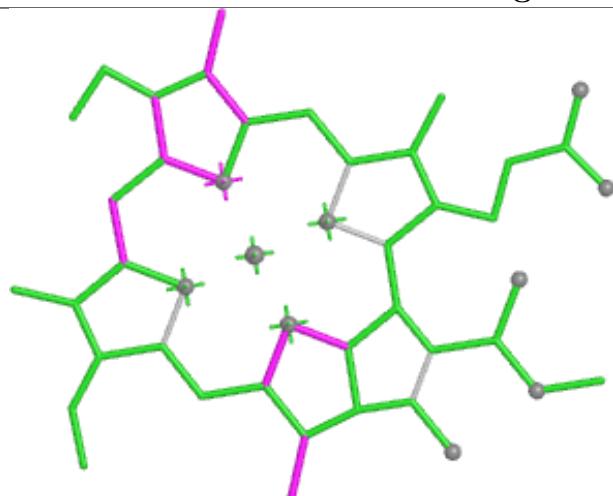


Torsions

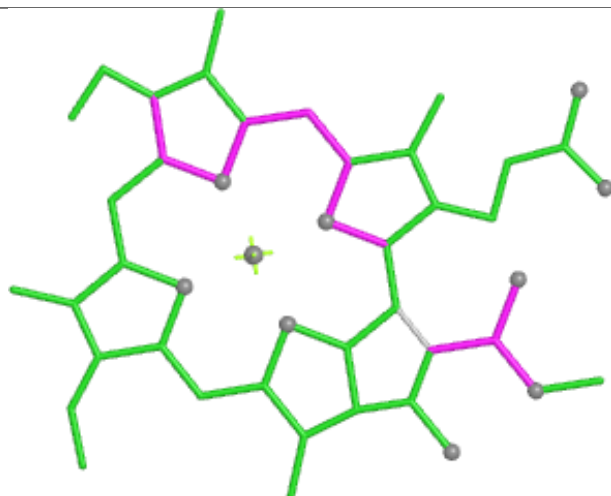


Rings

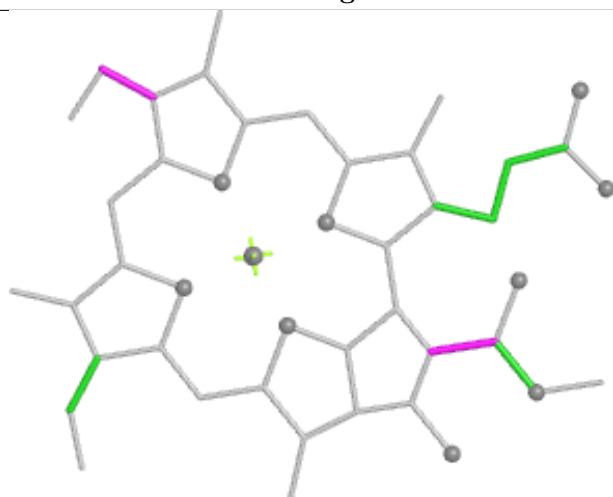
Ligand CLA A 837



Bond lengths



Bond angles

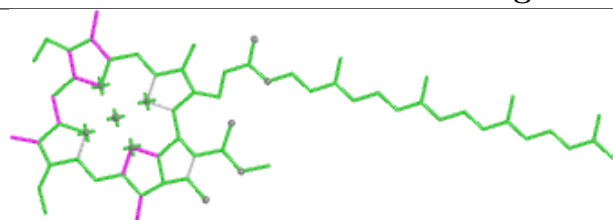


Torsions

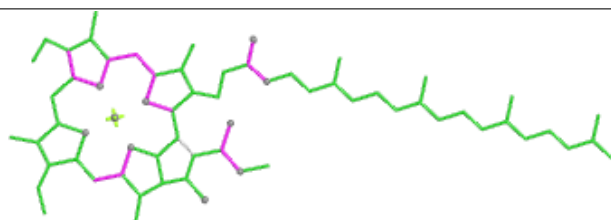


Rings

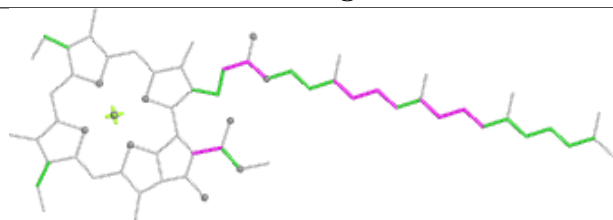
Ligand CLA A 807



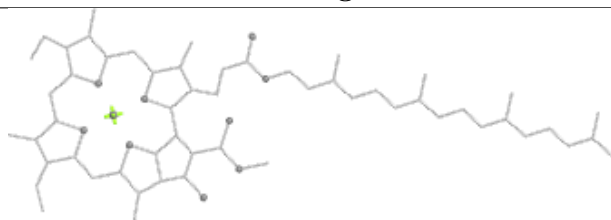
Bond lengths



Bond angles

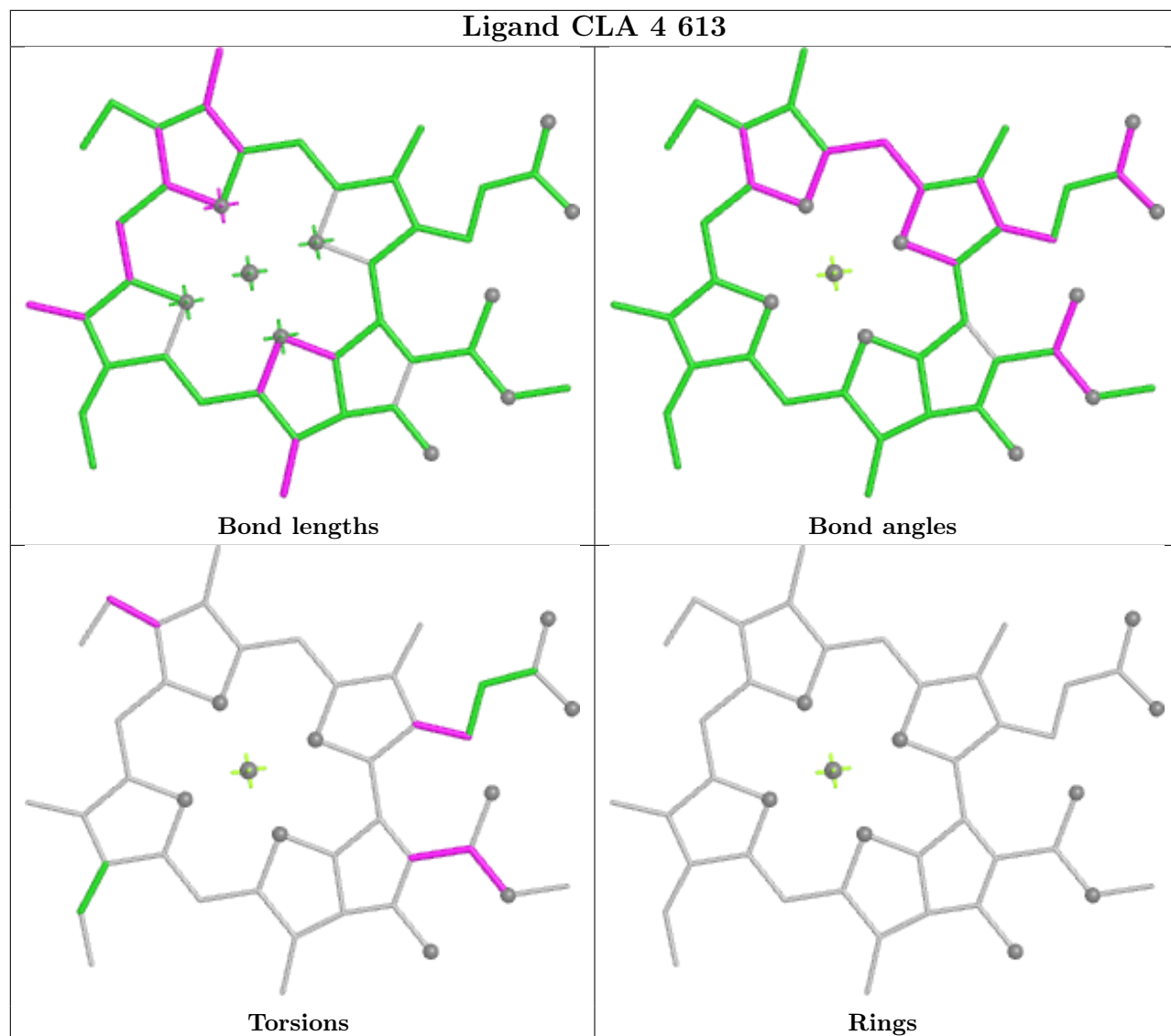


Torsions

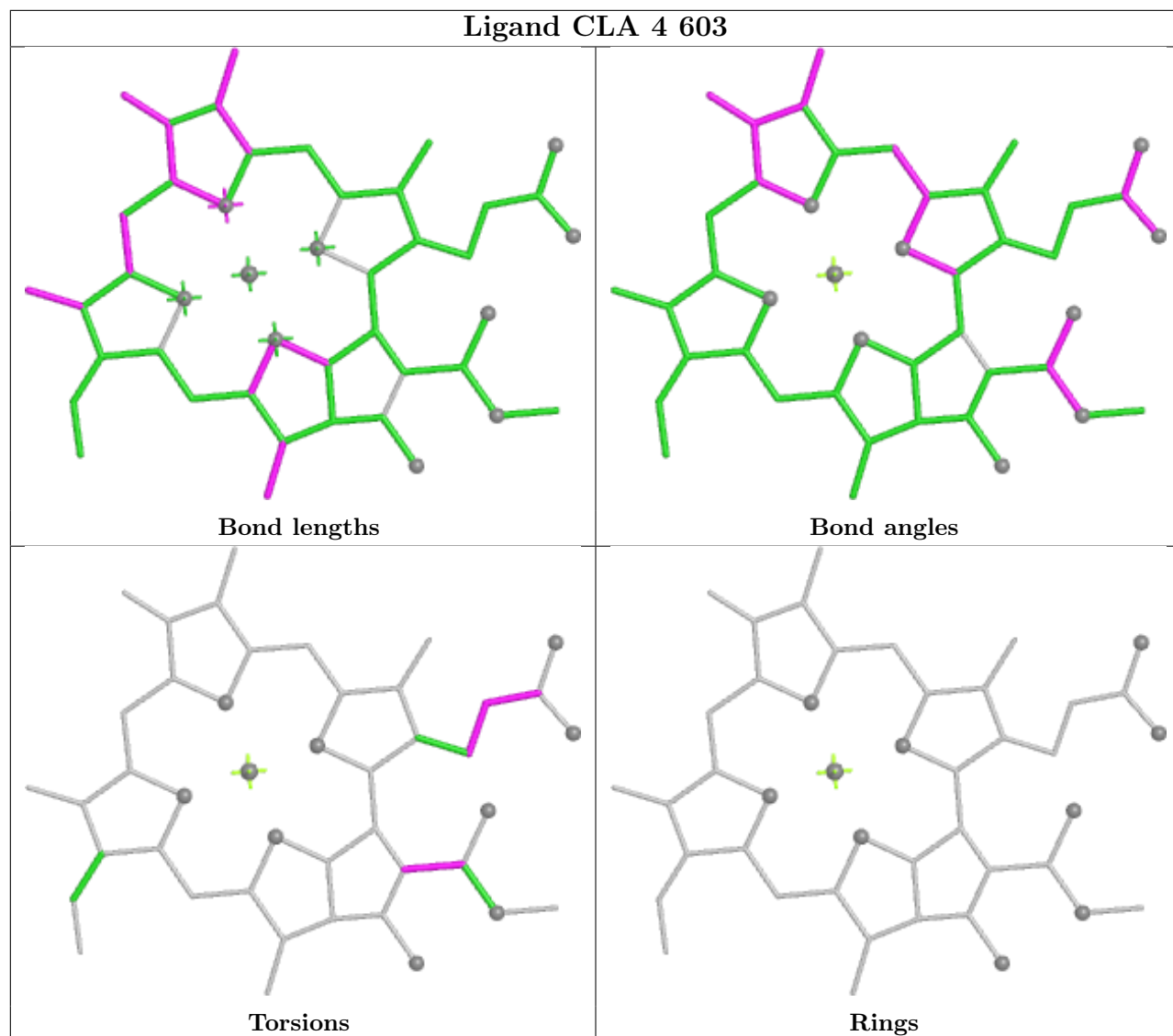


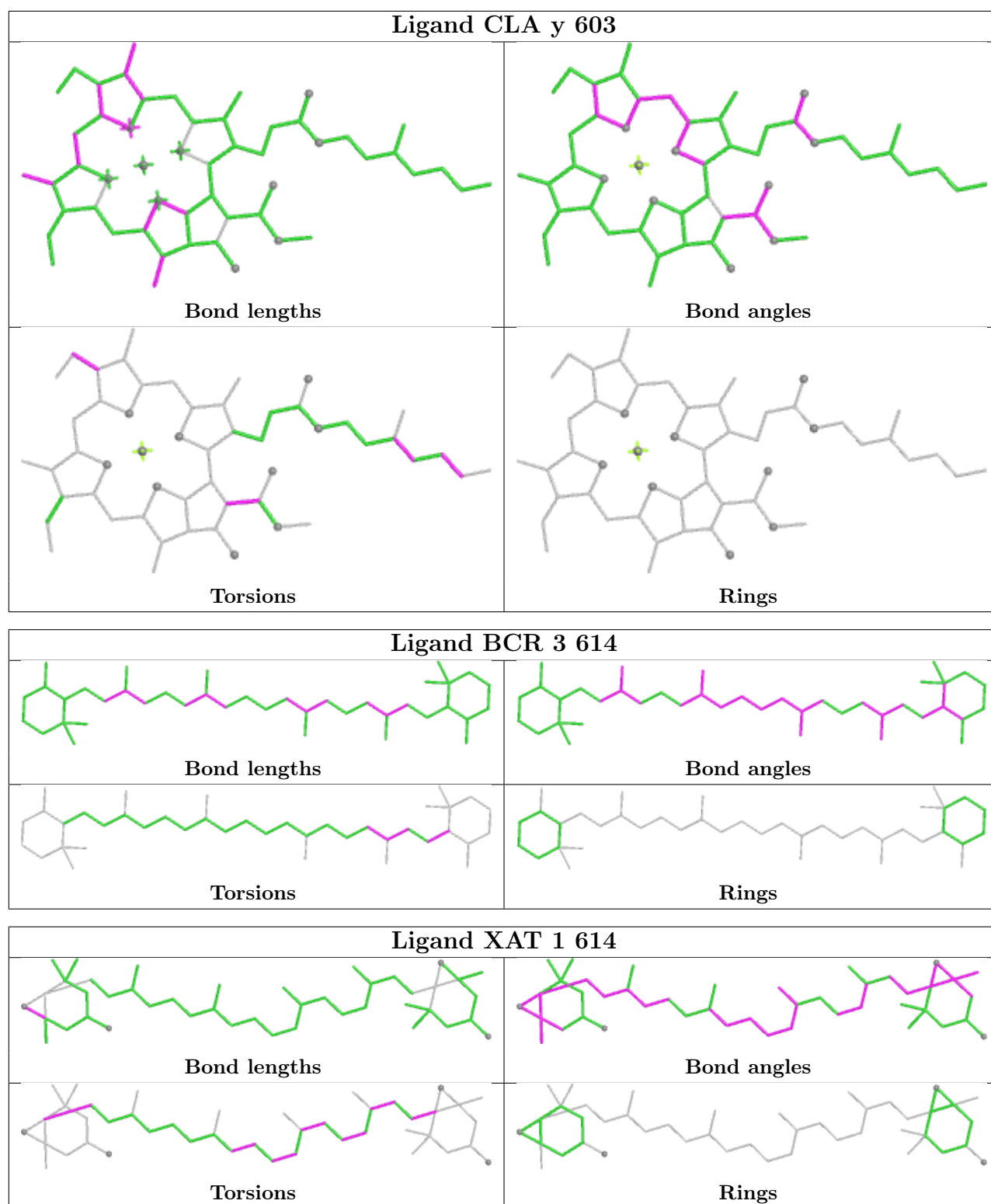
Rings

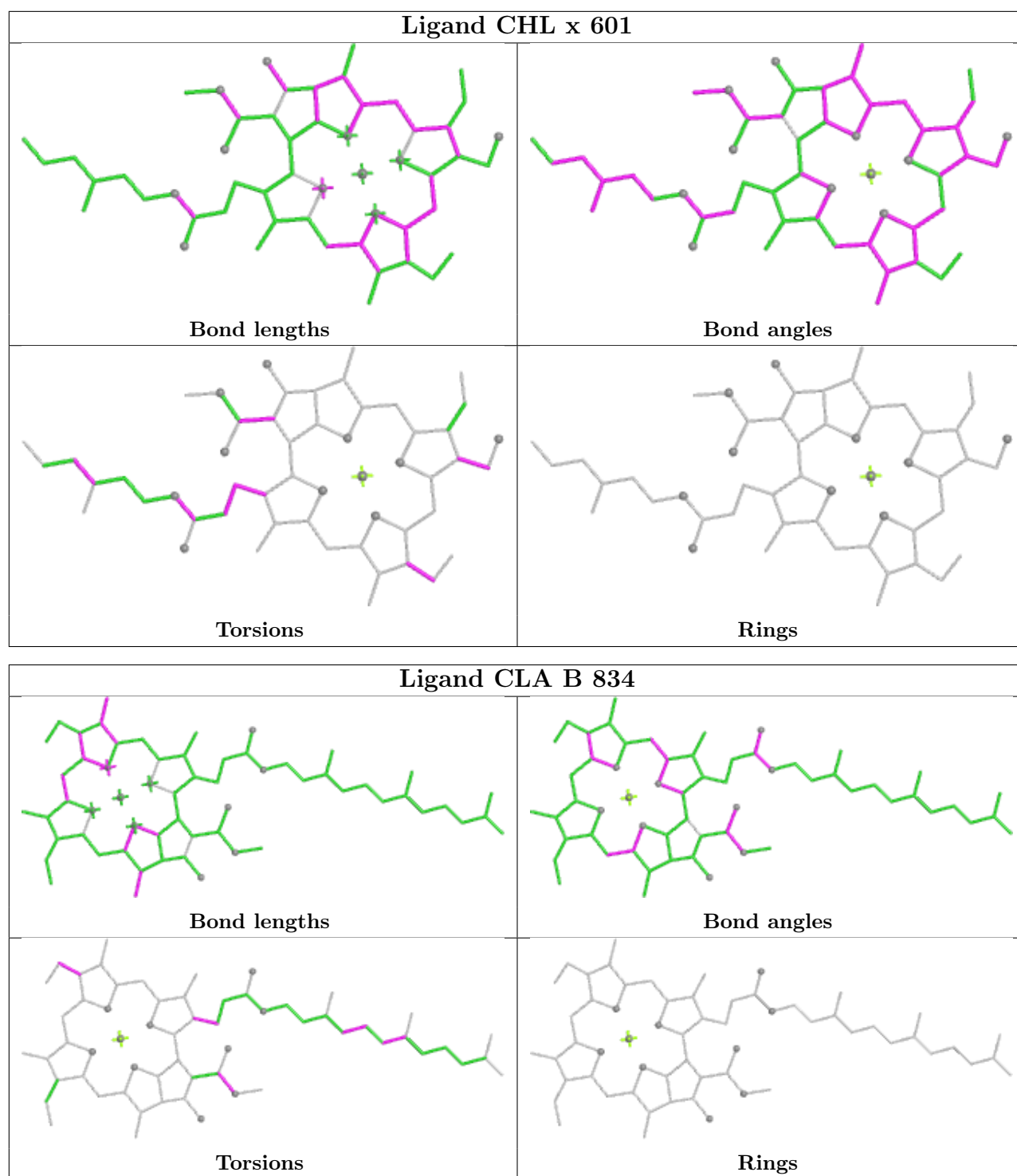
Ligand CLA 4 613

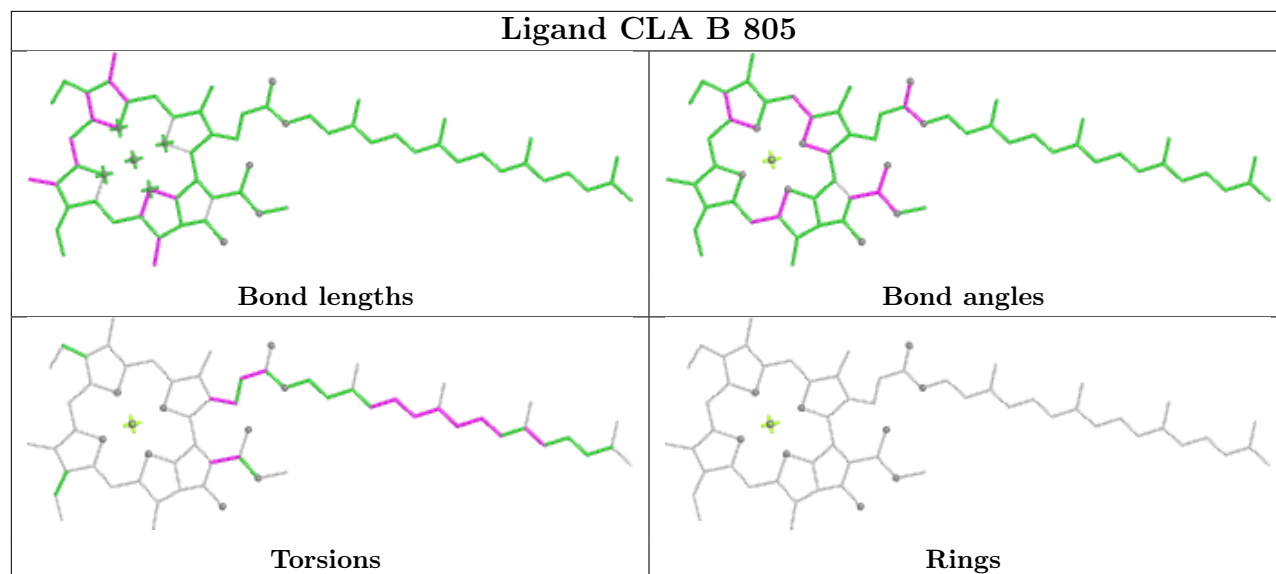
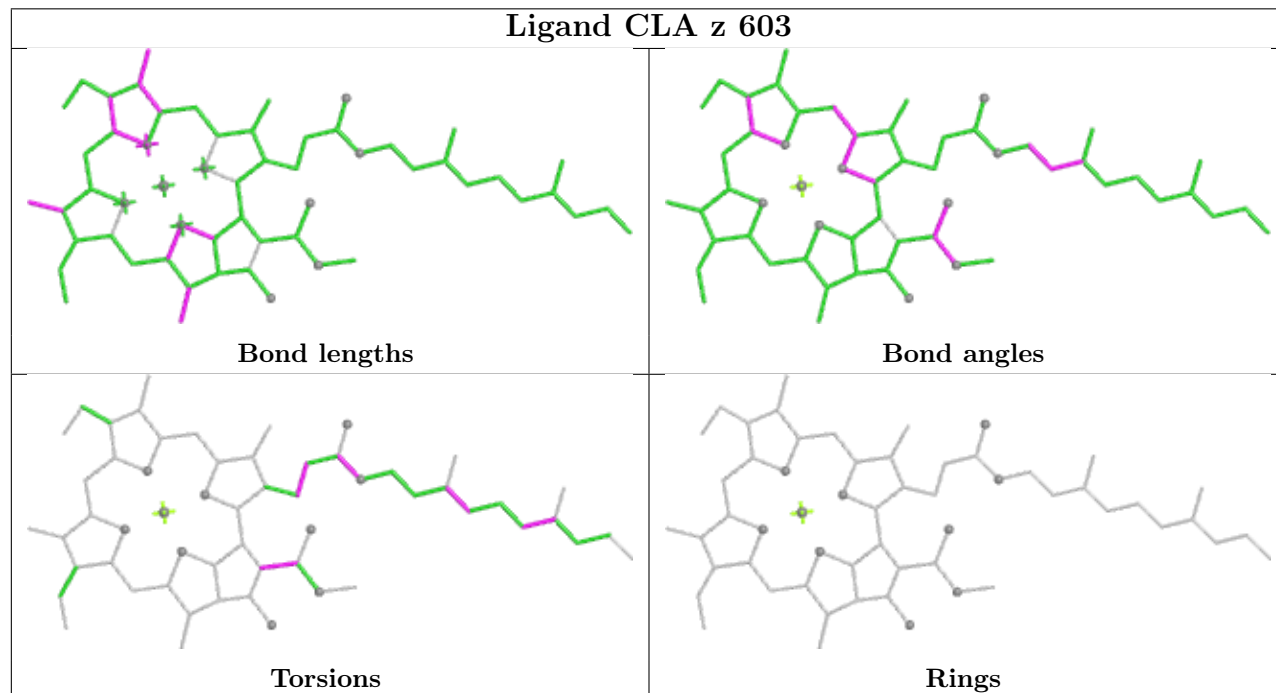


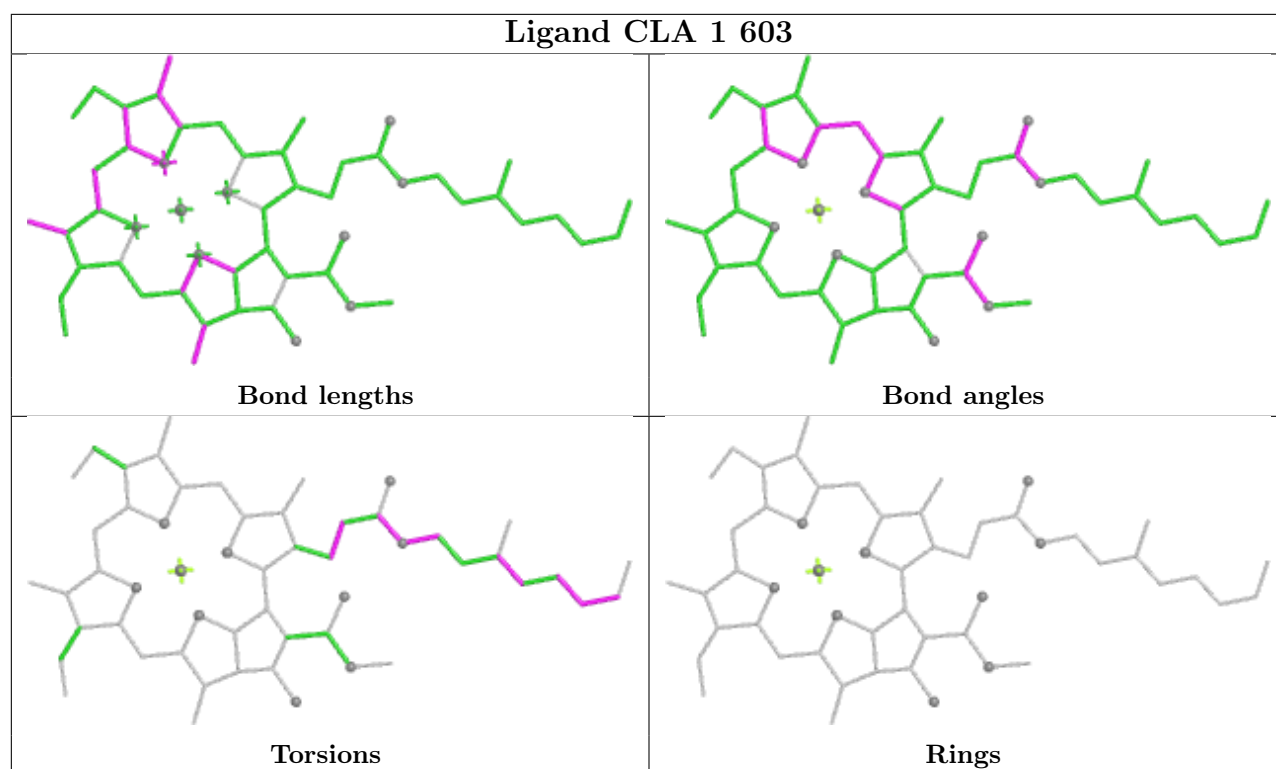
Ligand CLA 4 603



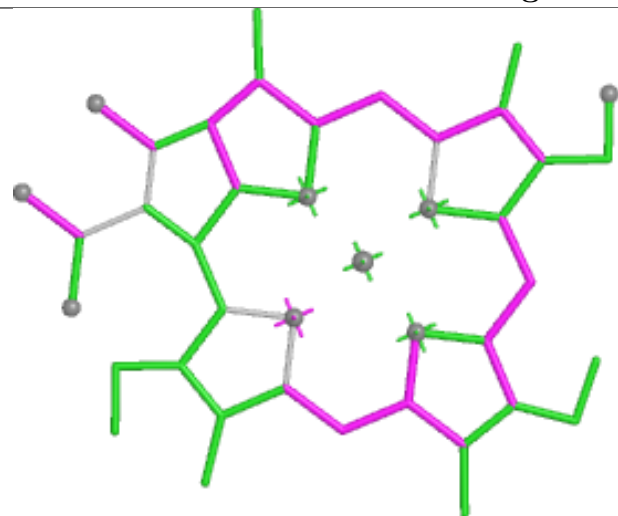




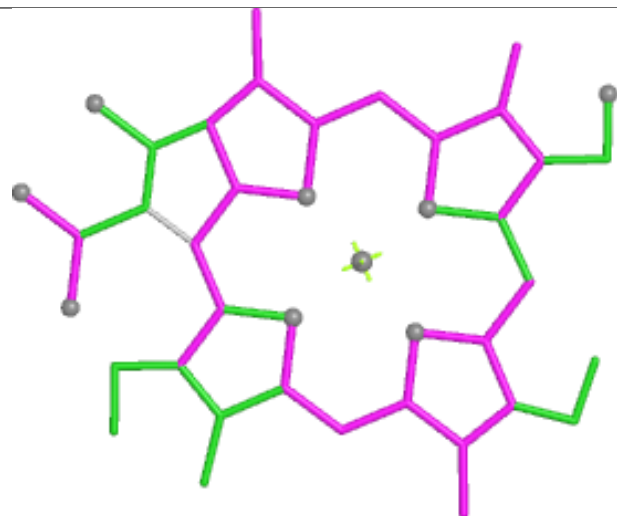
Ligand CLA B 805**Ligand CLA z 603**



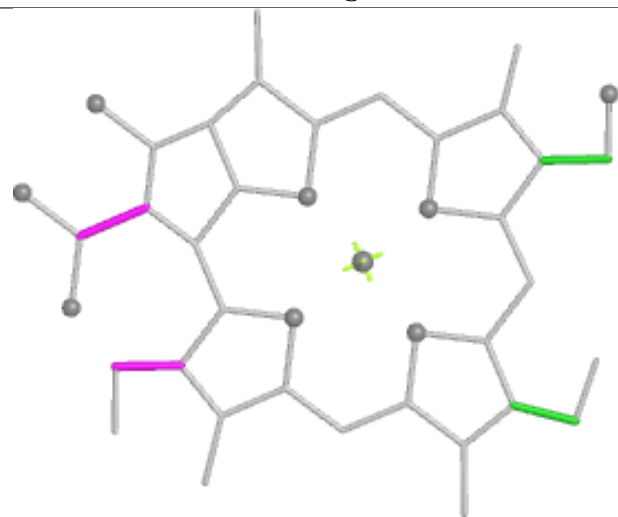
Ligand CHL 4 605



Bond lengths



Bond angles

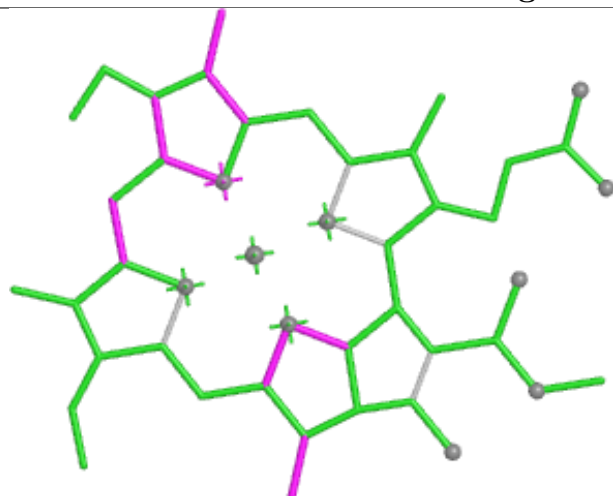


Torsions

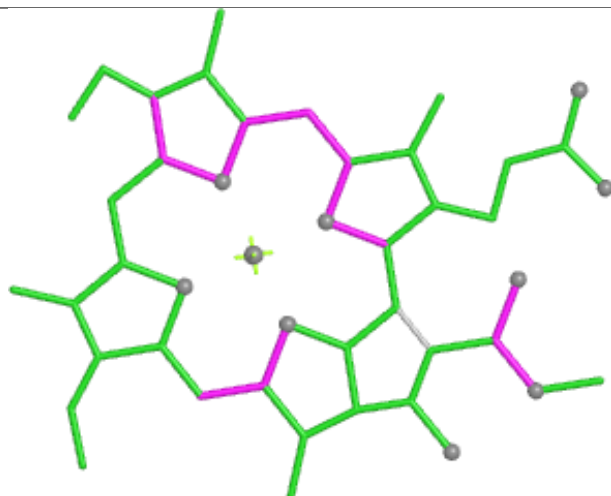


Rings

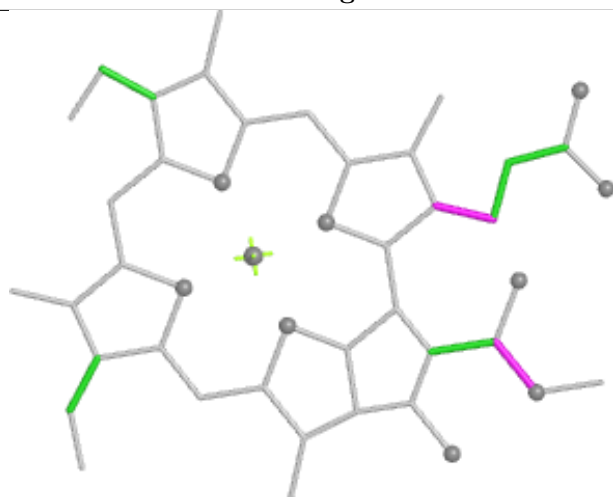
Ligand CLA 3 607



Bond lengths



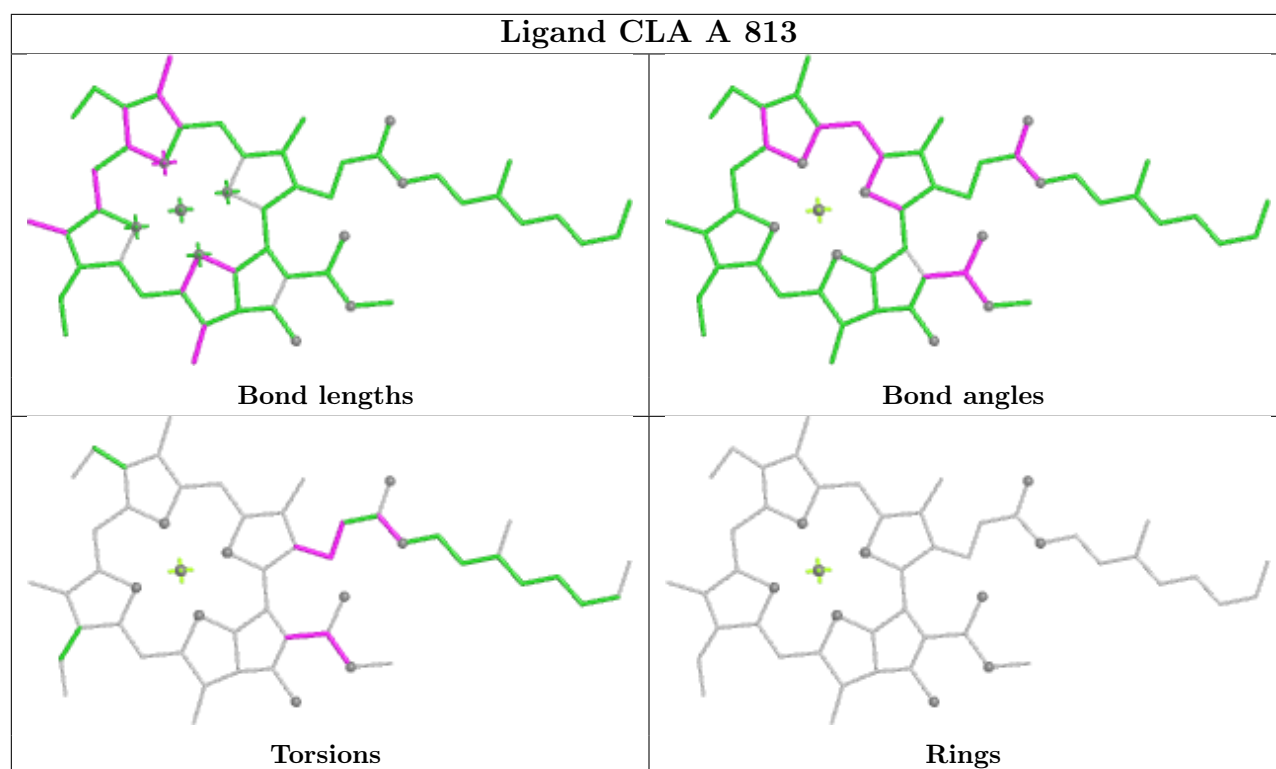
Bond angles



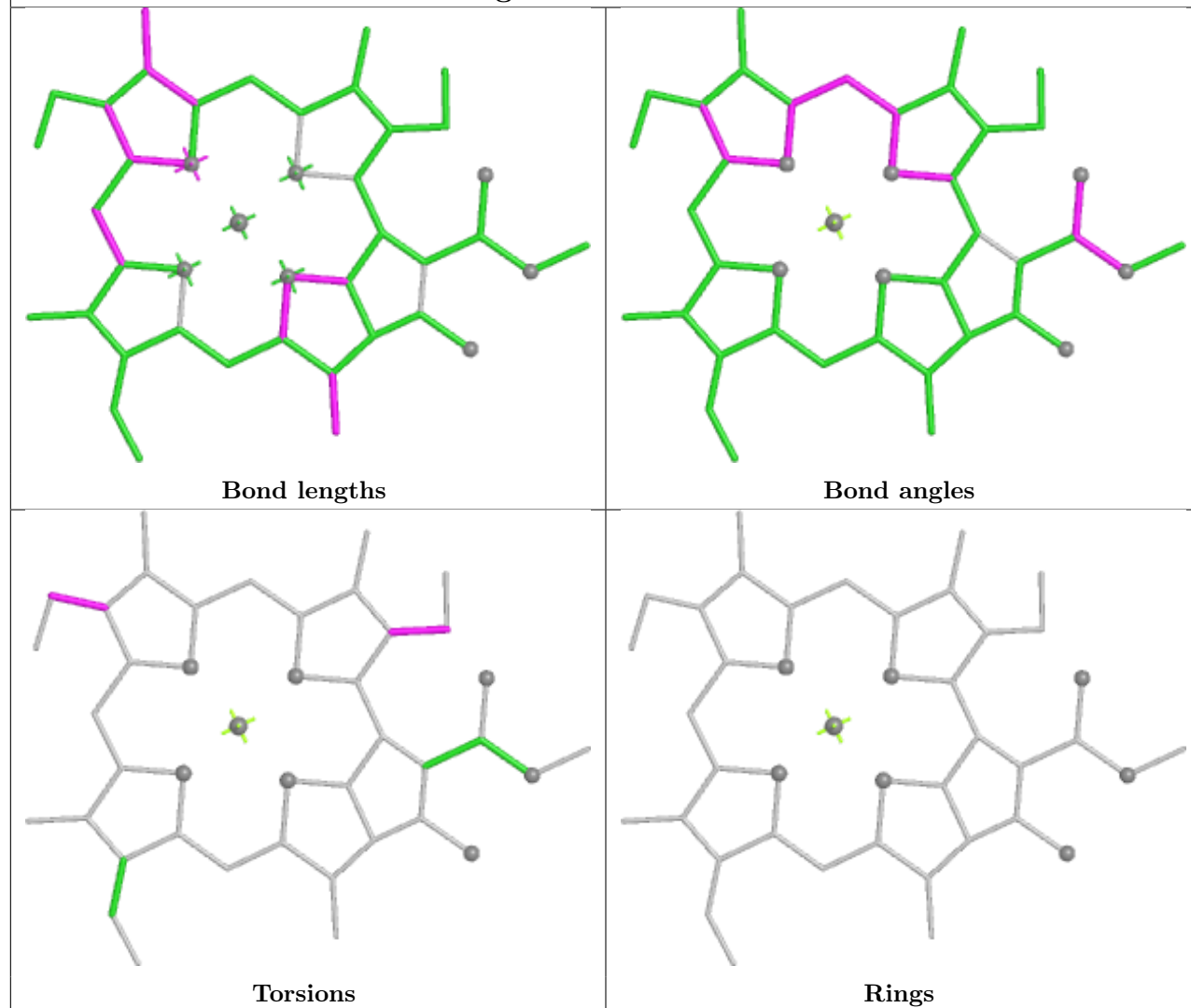
Torsions



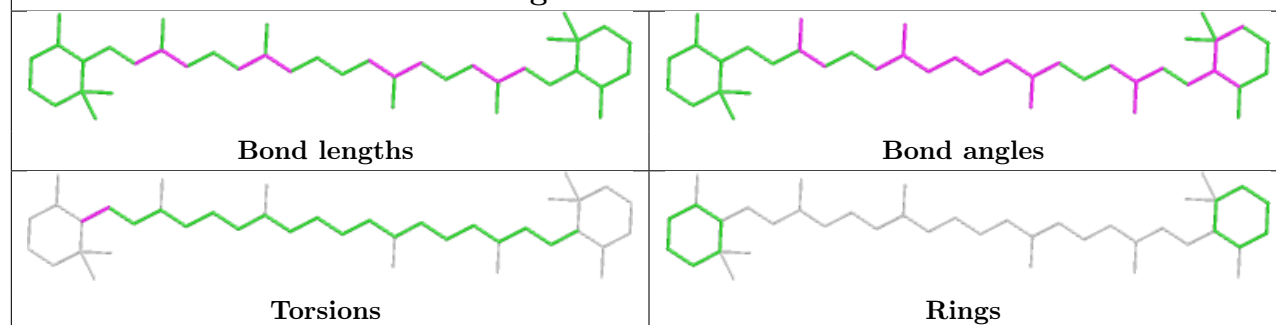
Rings

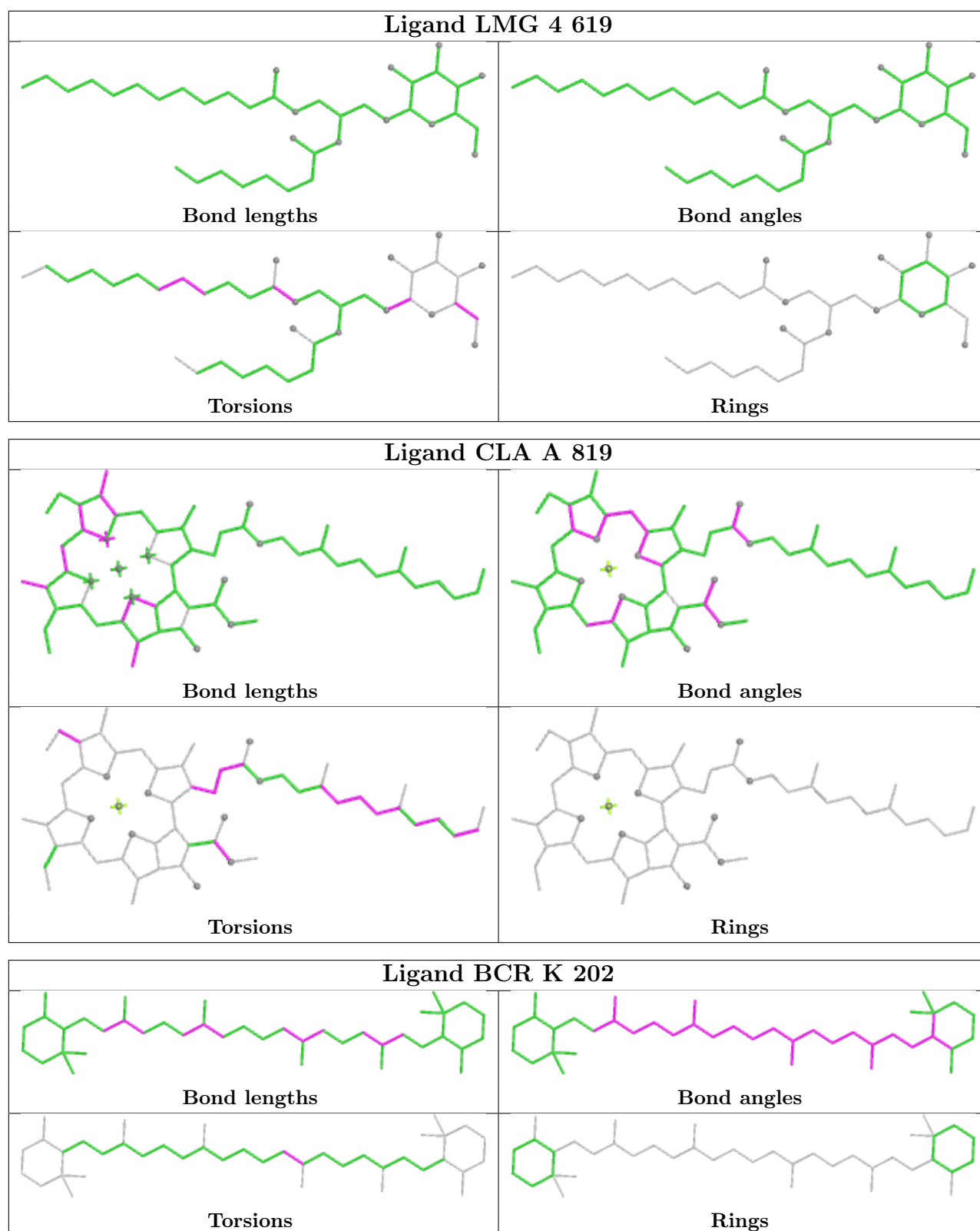


Ligand CLA G 202

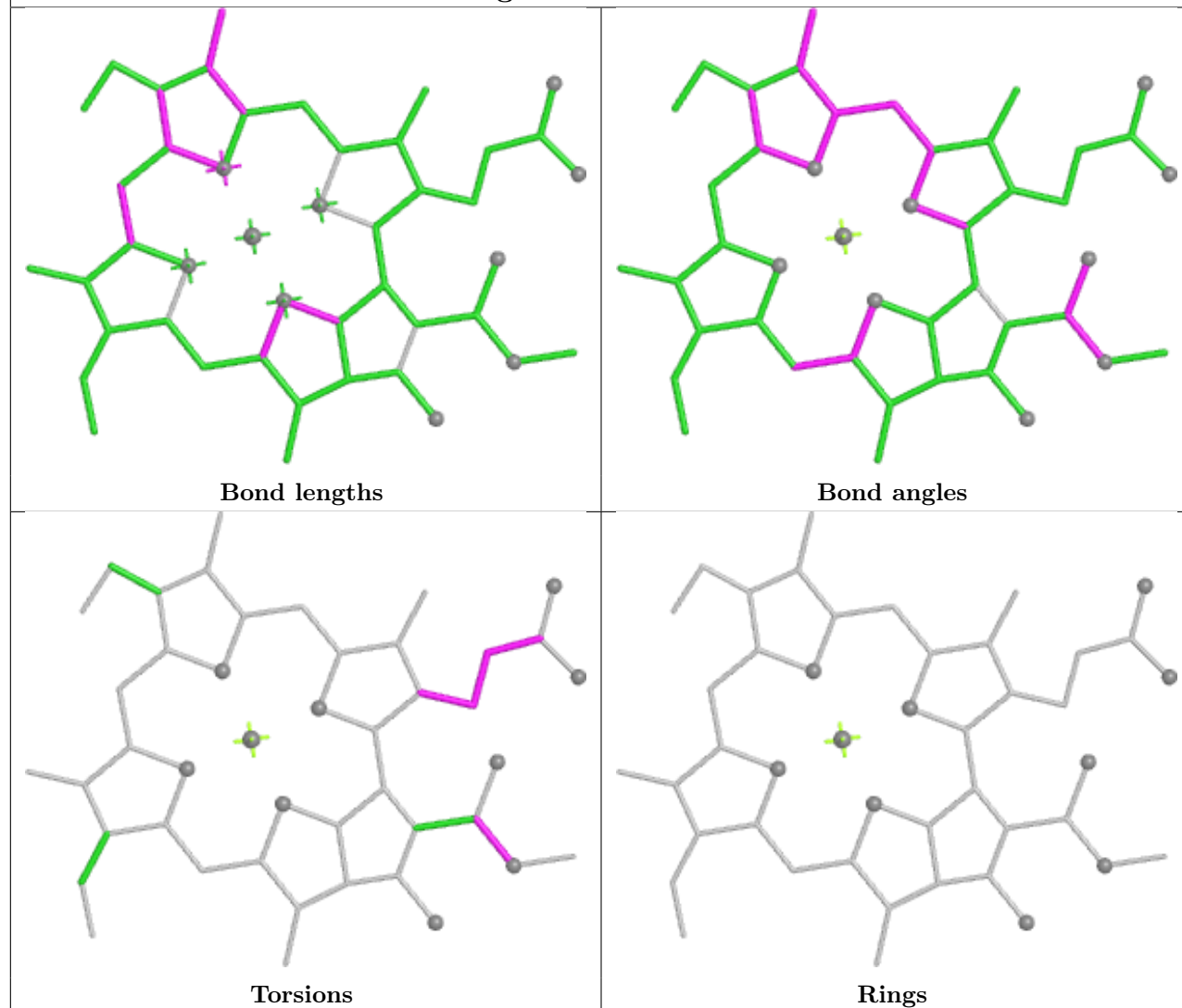


Ligand BCR A 848

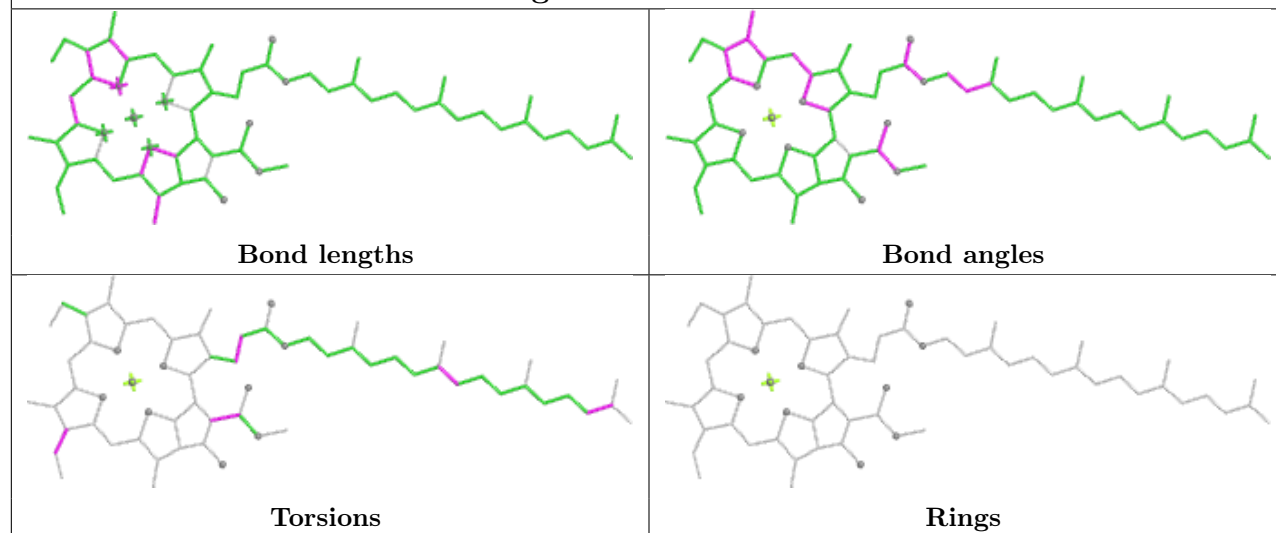




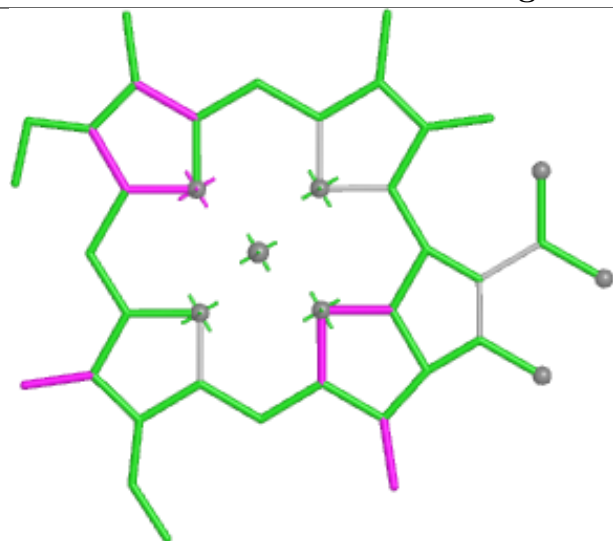
Ligand CLA 3 603



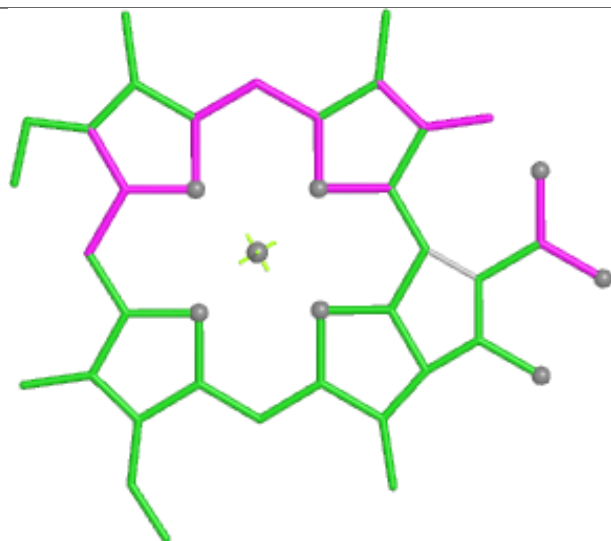
Ligand CLA A 809



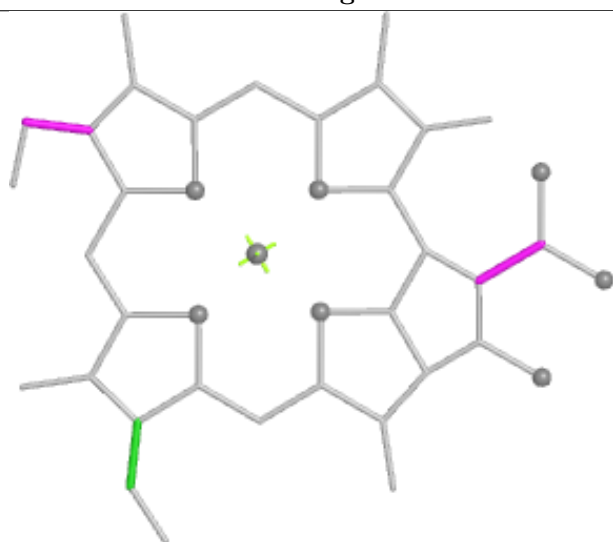
Ligand CLA 3 612



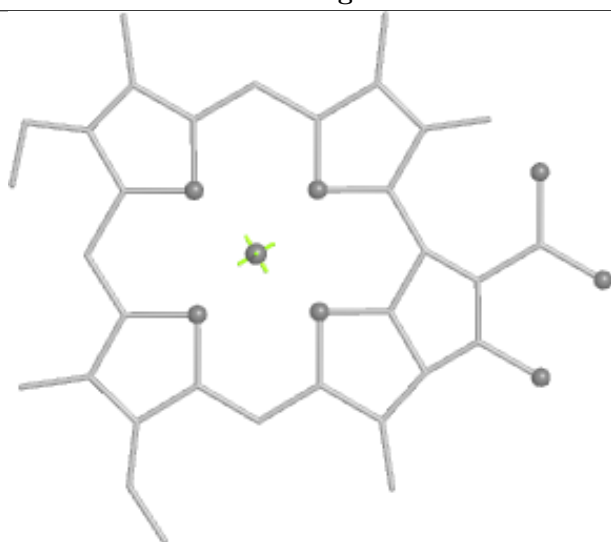
Bond lengths



Bond angles

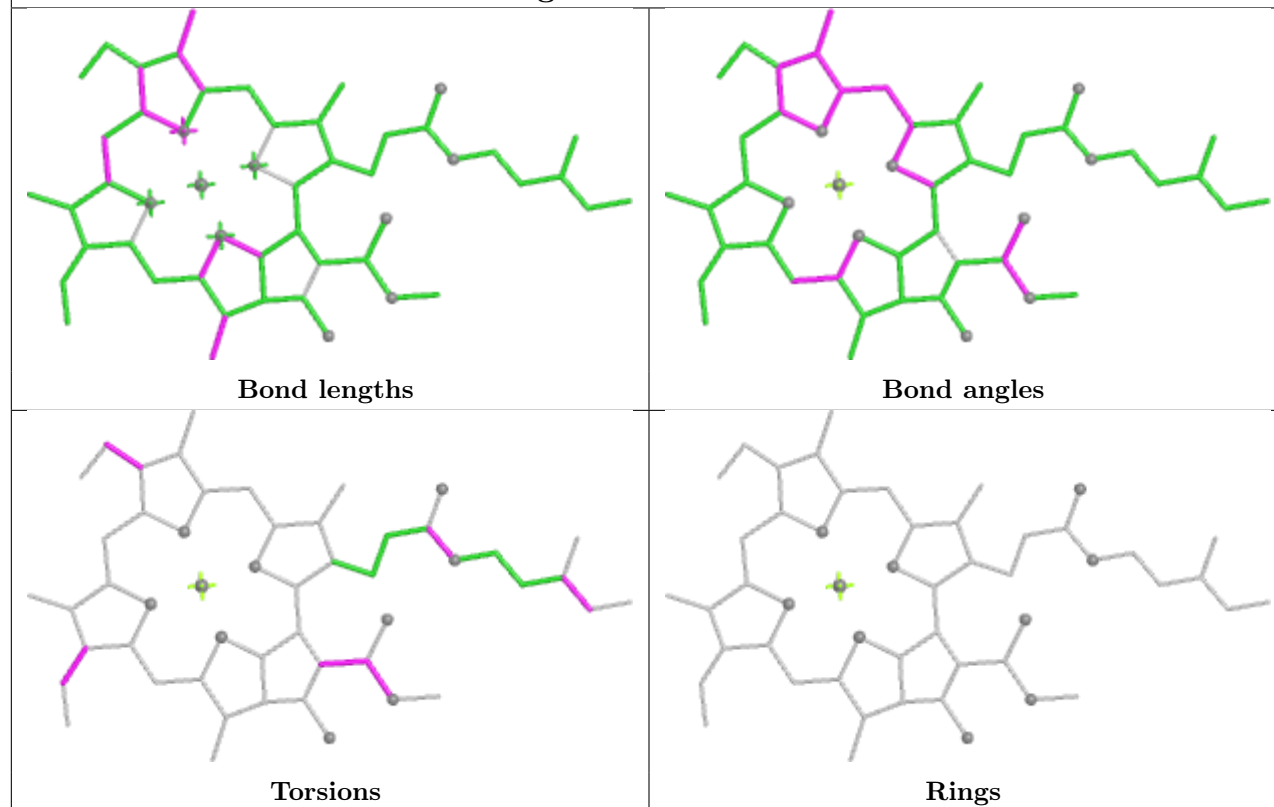


Torsions

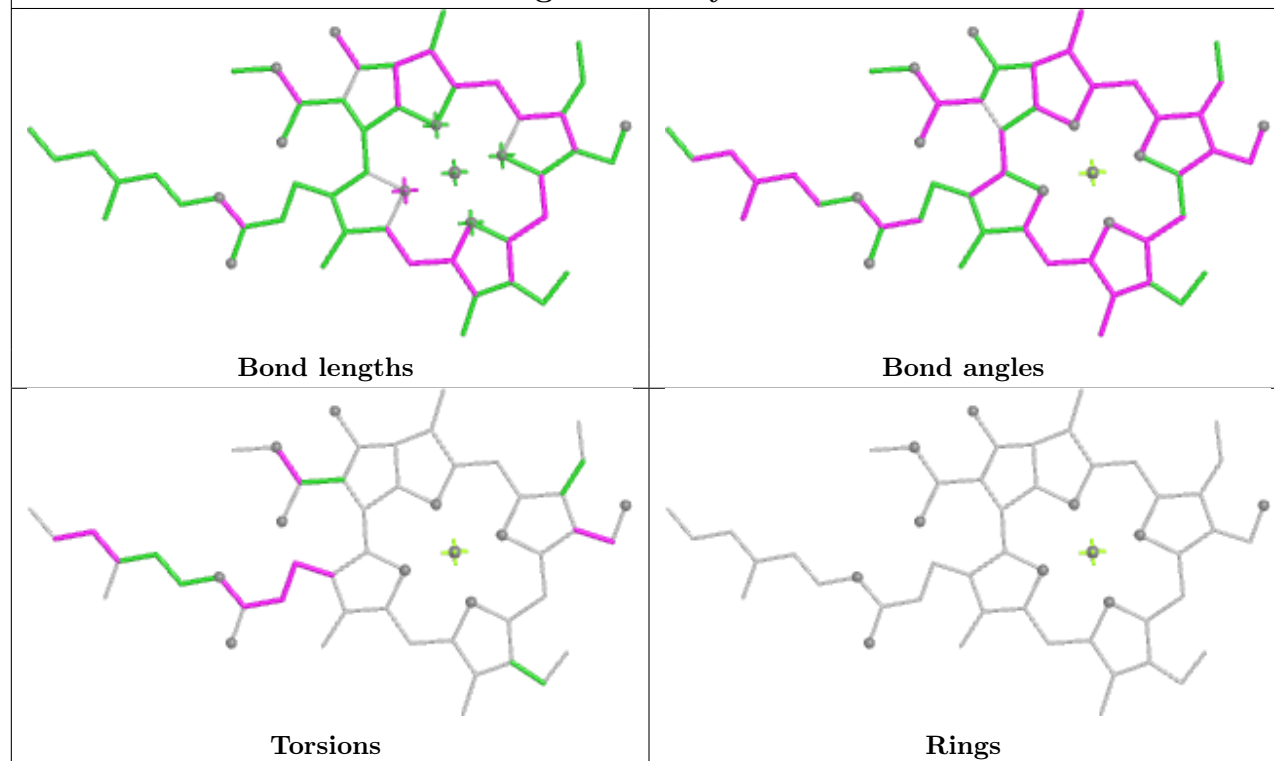


Rings

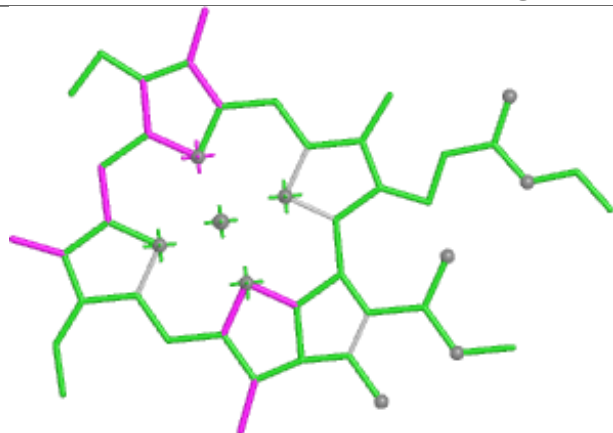
Ligand CLA z 604



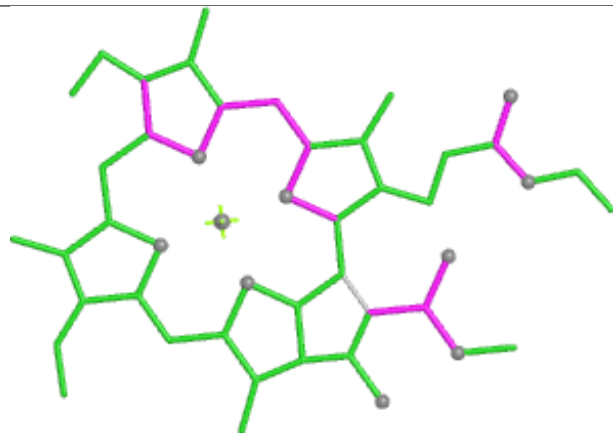
Ligand CHL y 607



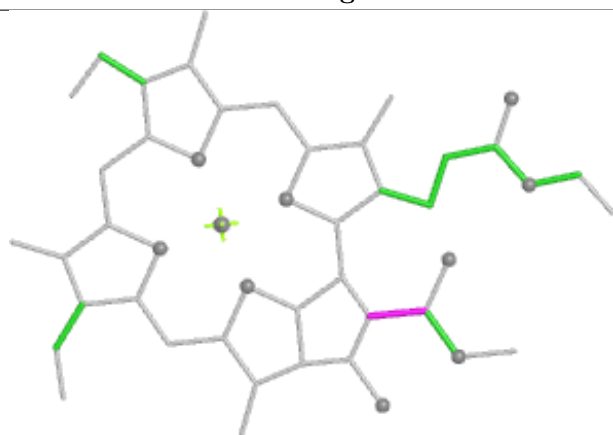
Ligand CLA B 838



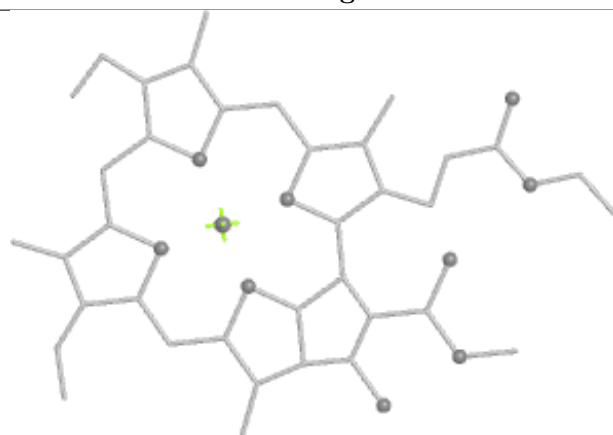
Bond lengths



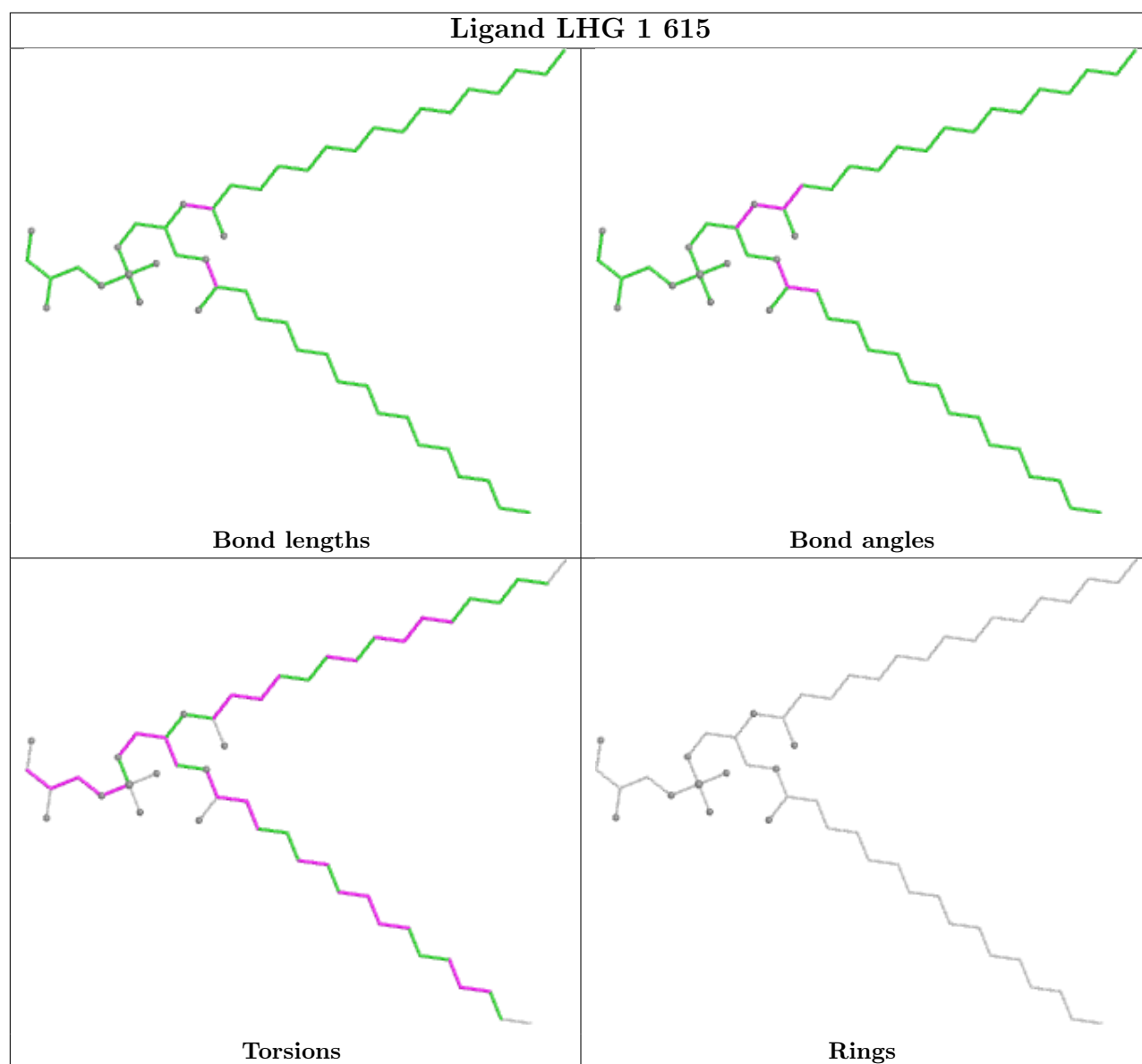
Bond angles



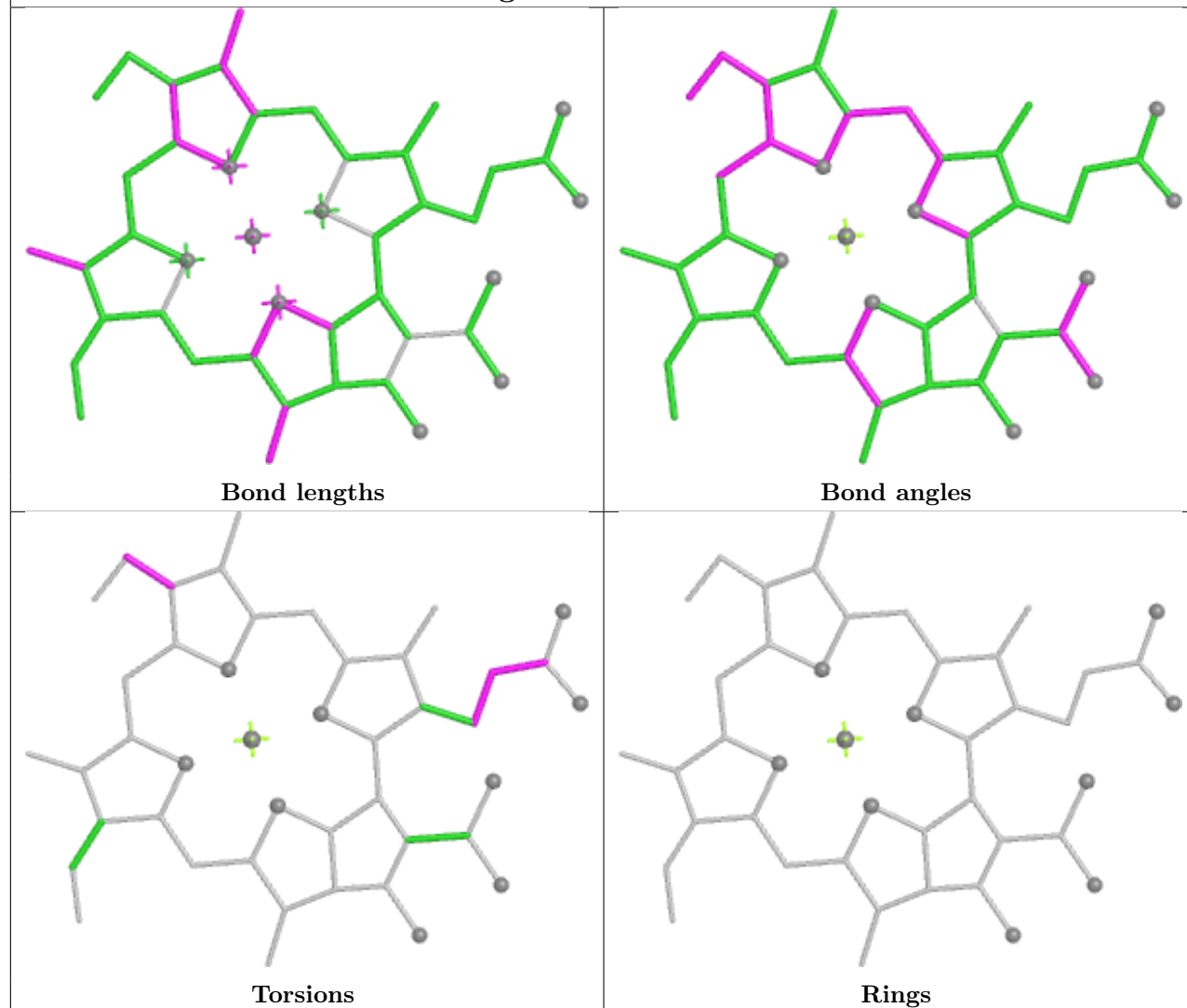
Torsions



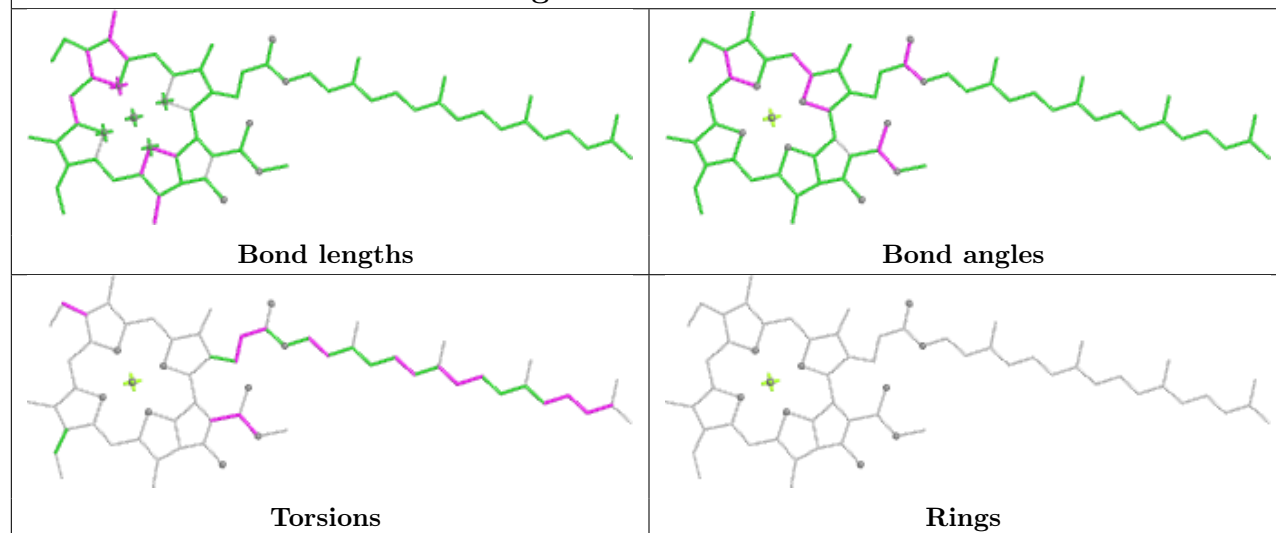
Rings

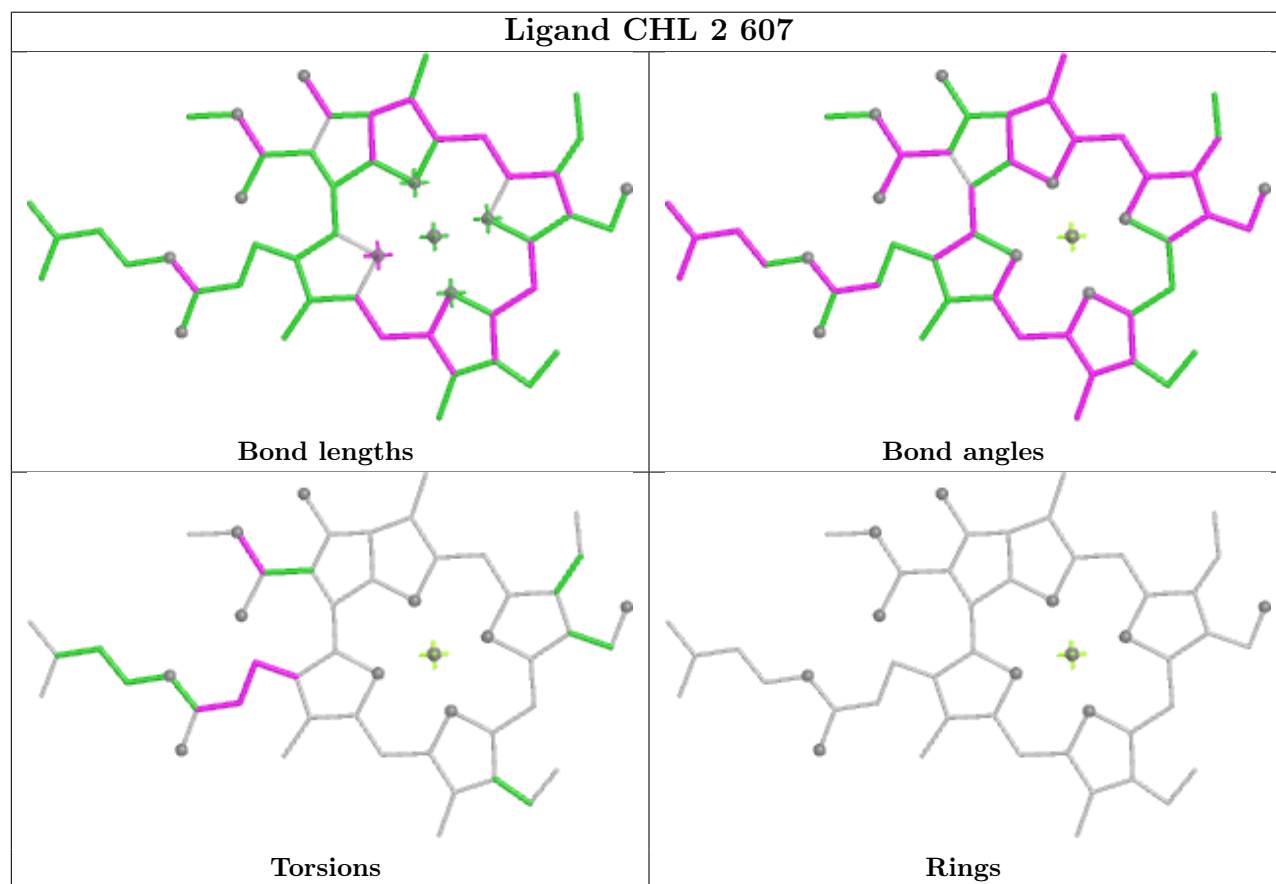
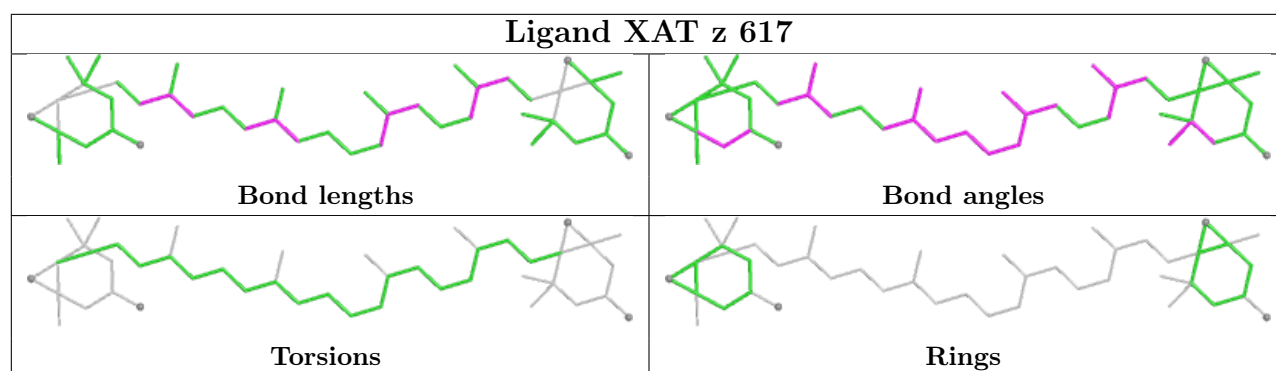


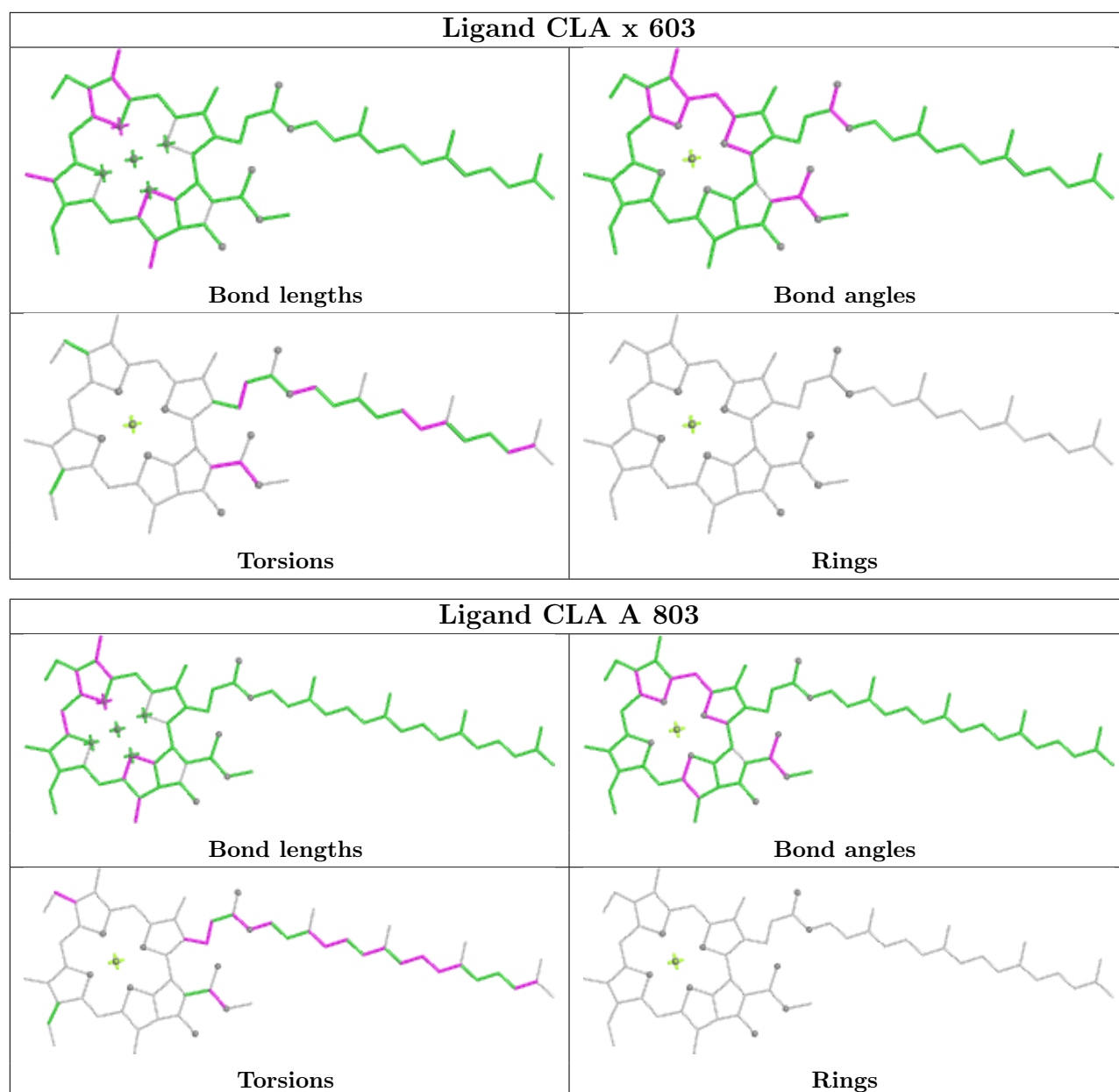
Ligand CLA 2 603

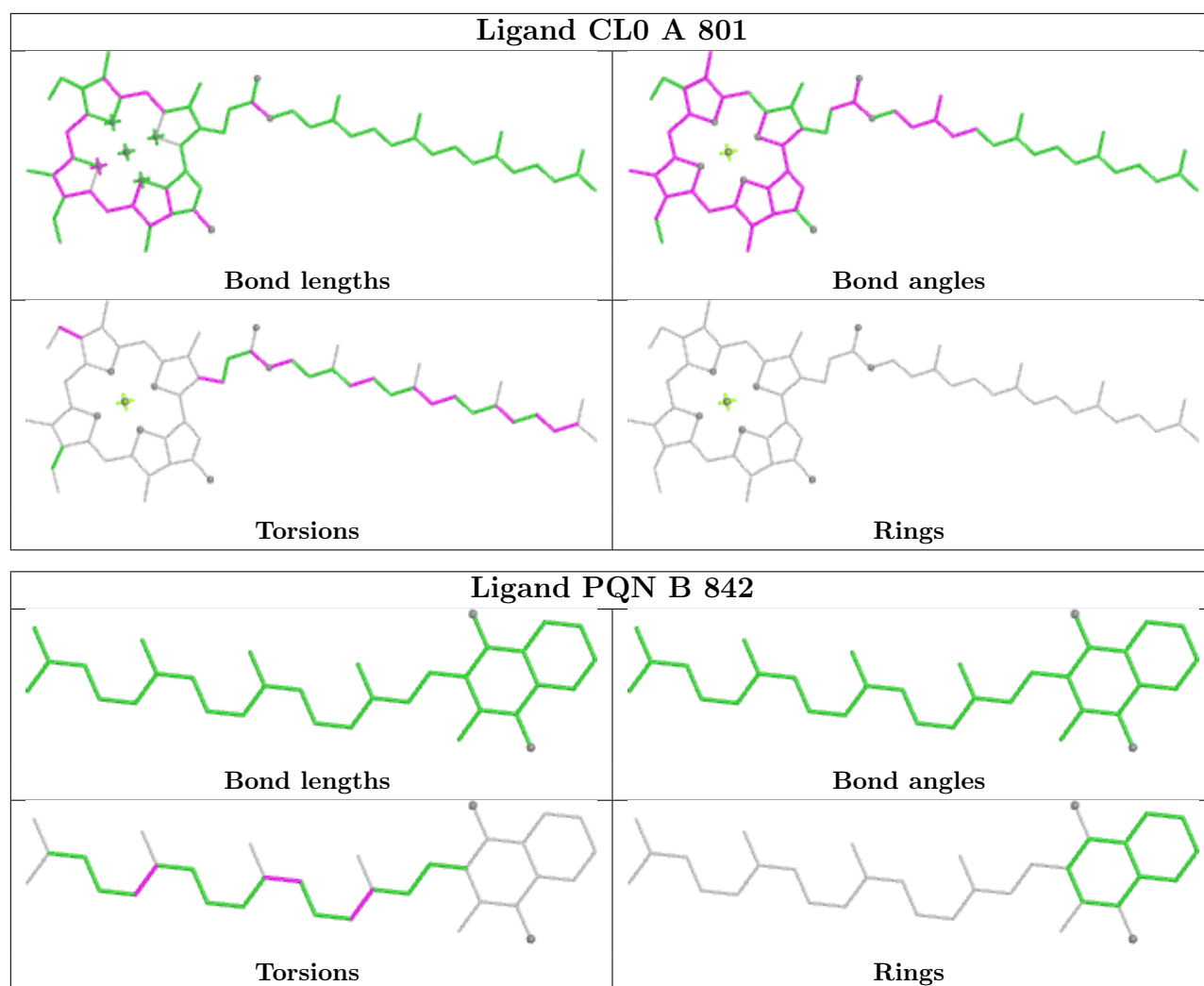


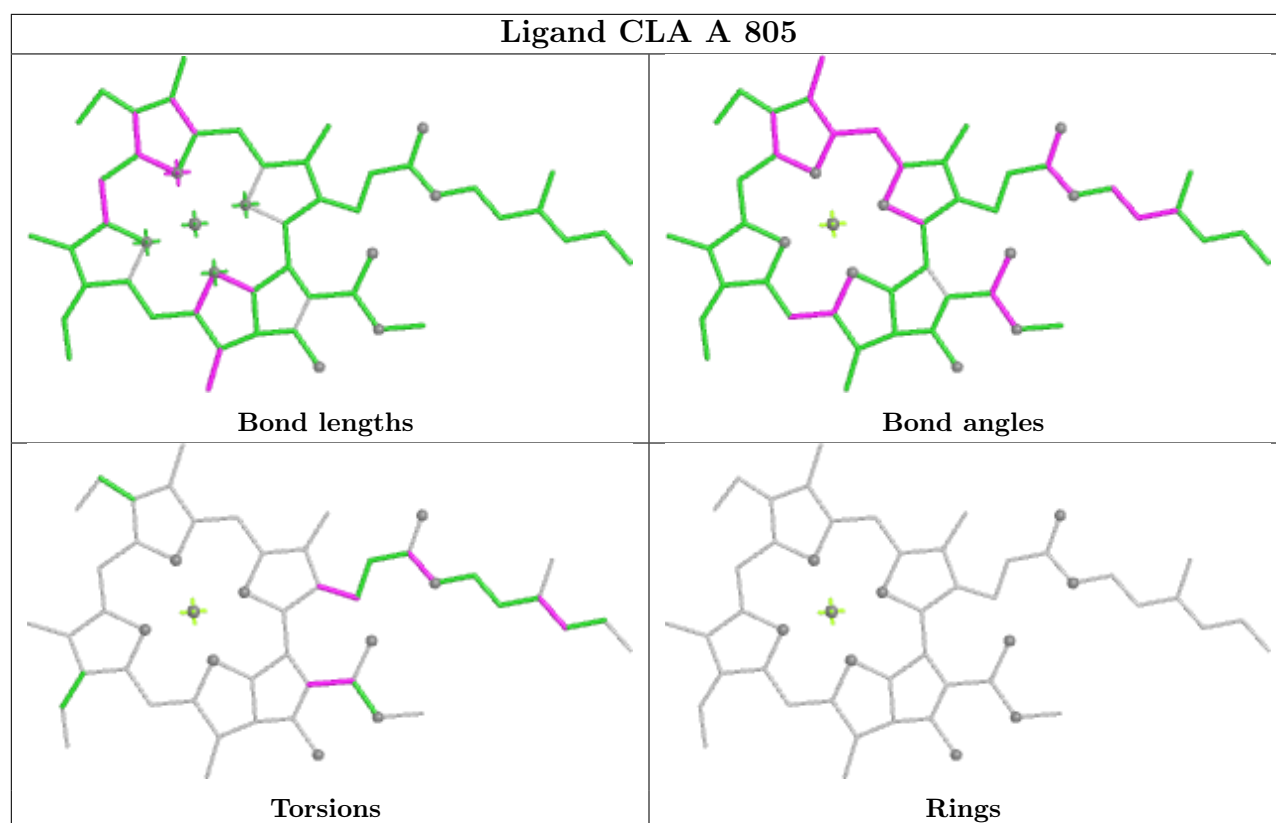
Ligand CLA O 201



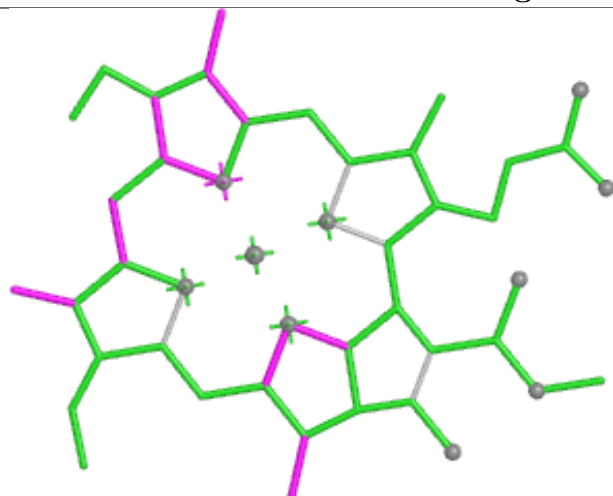




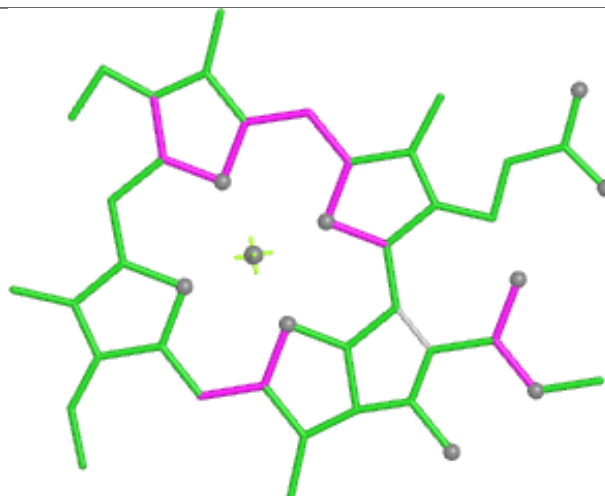




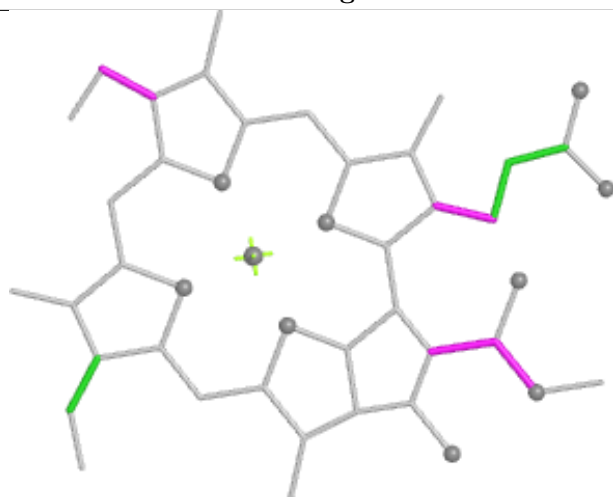
Ligand CLA B 823



Bond lengths



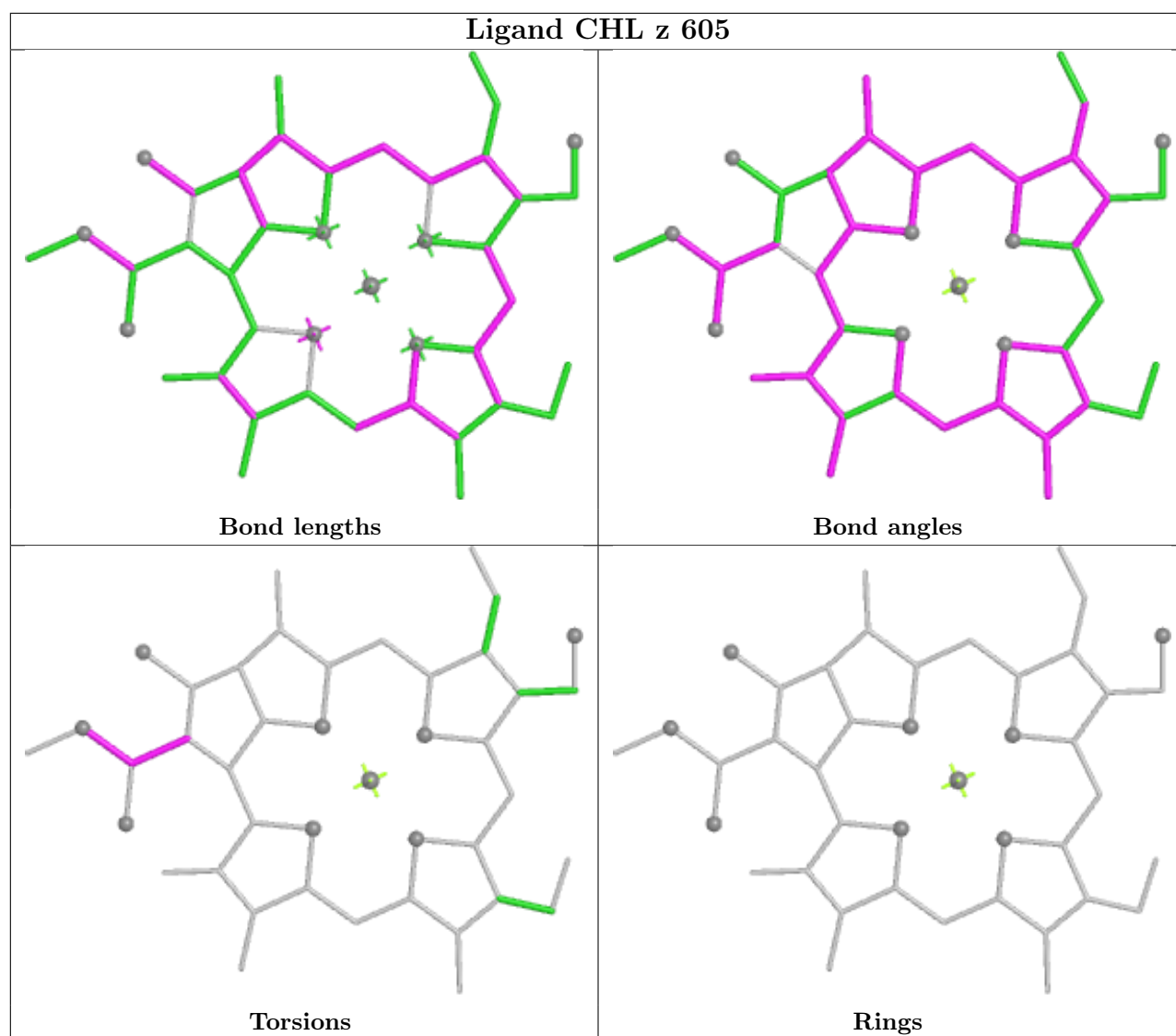
Bond angles

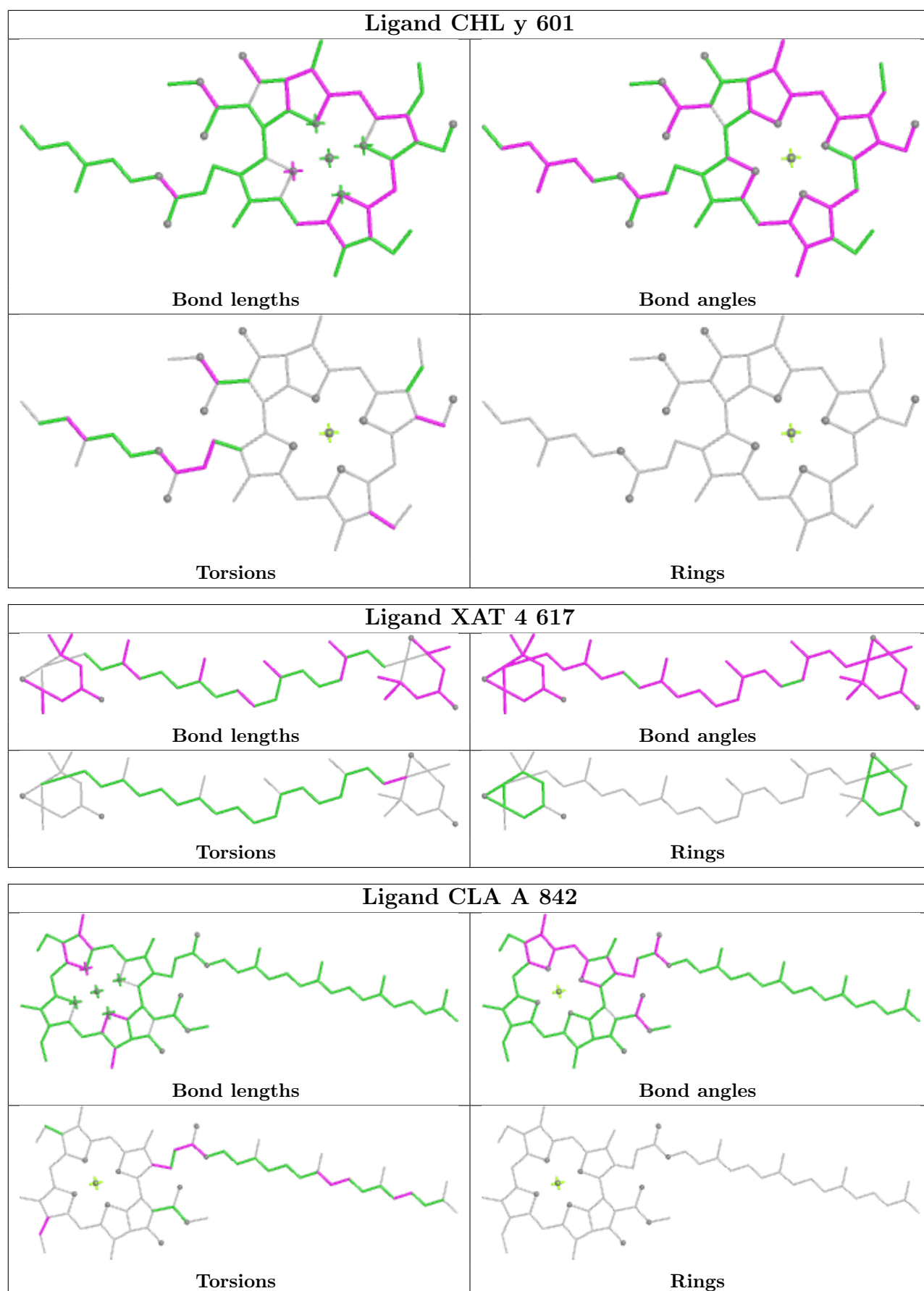


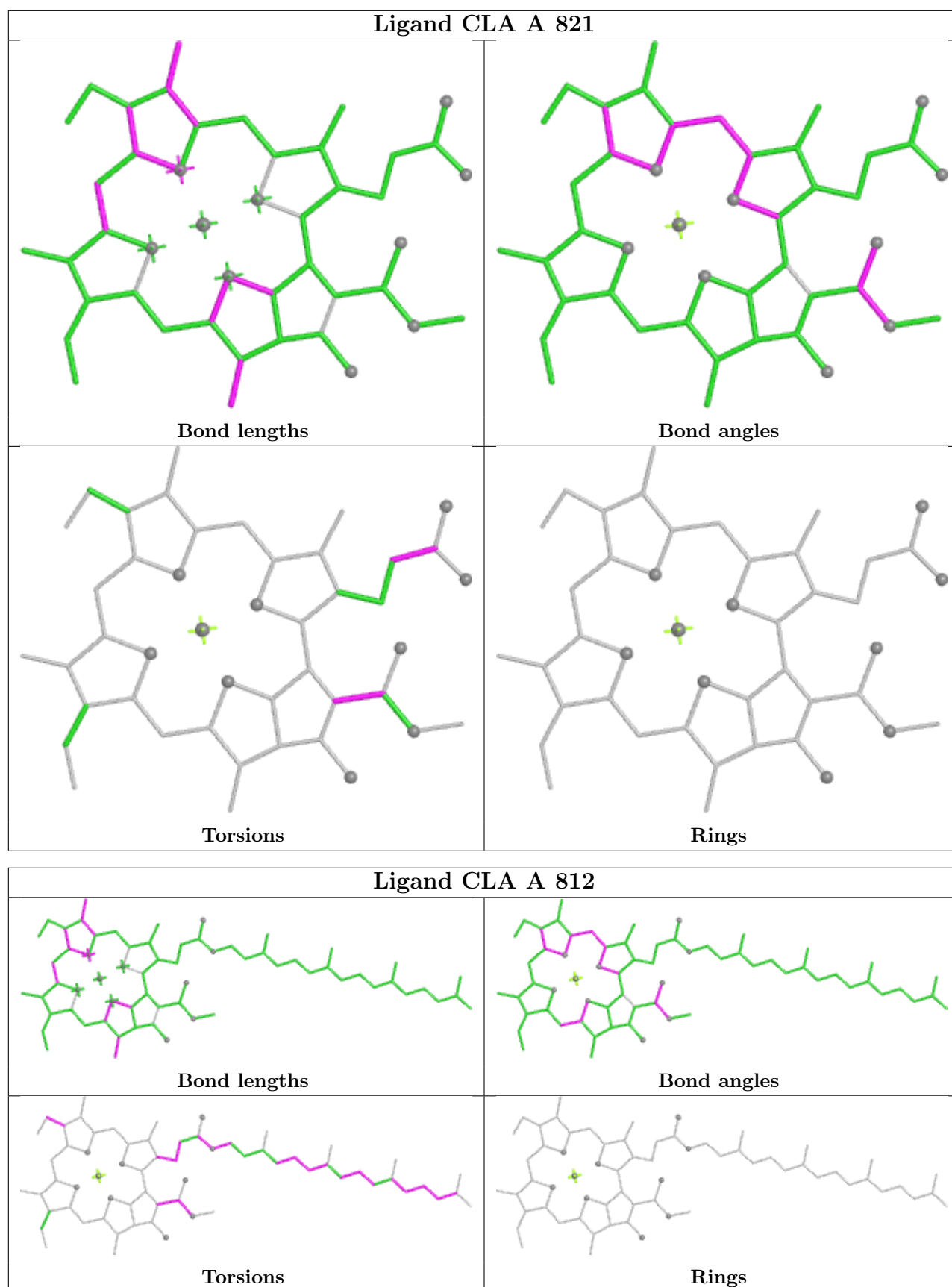
Torsions

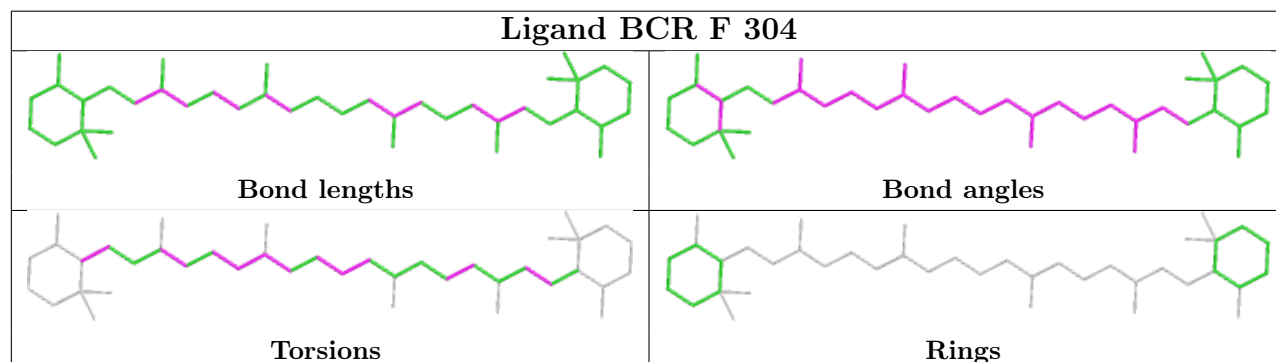
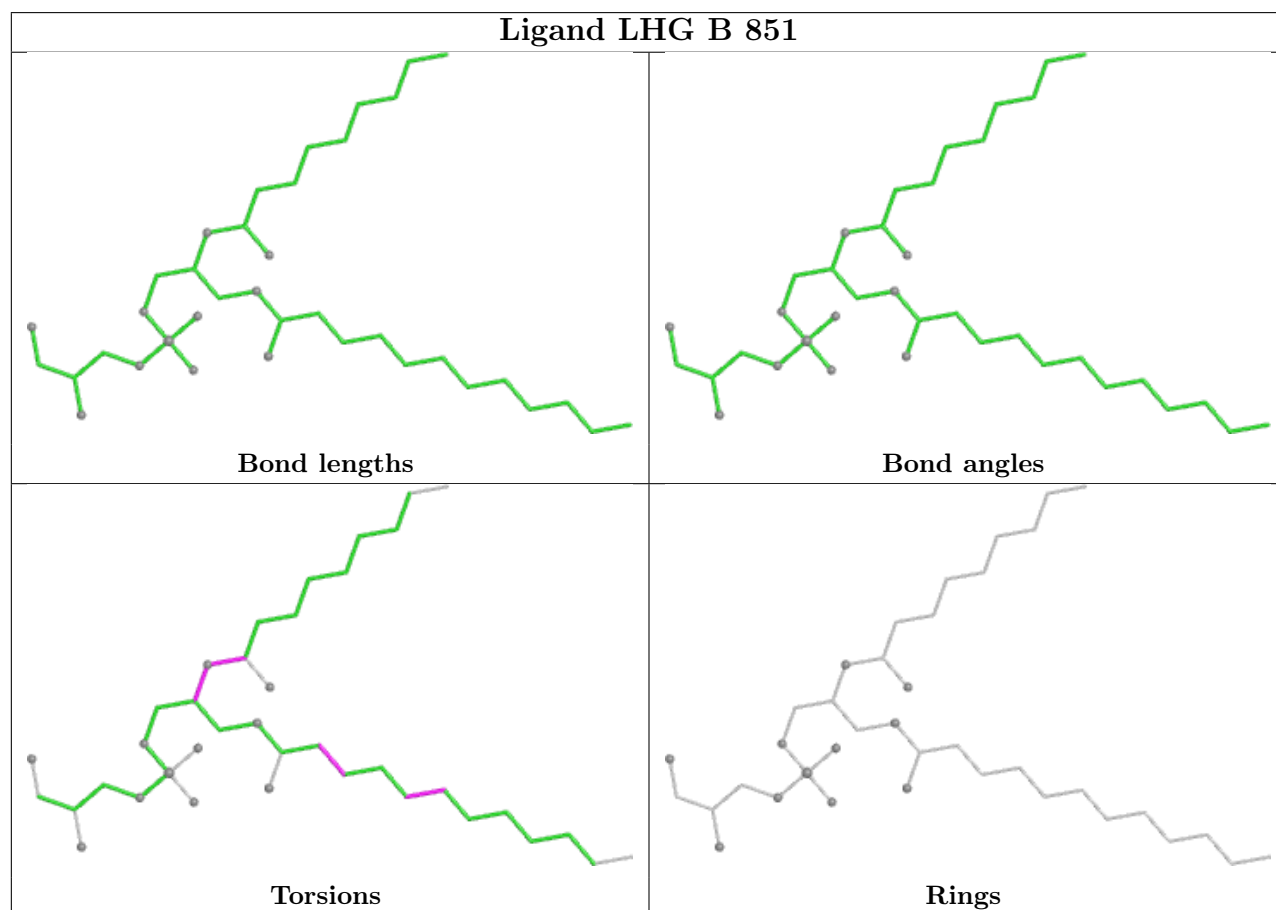
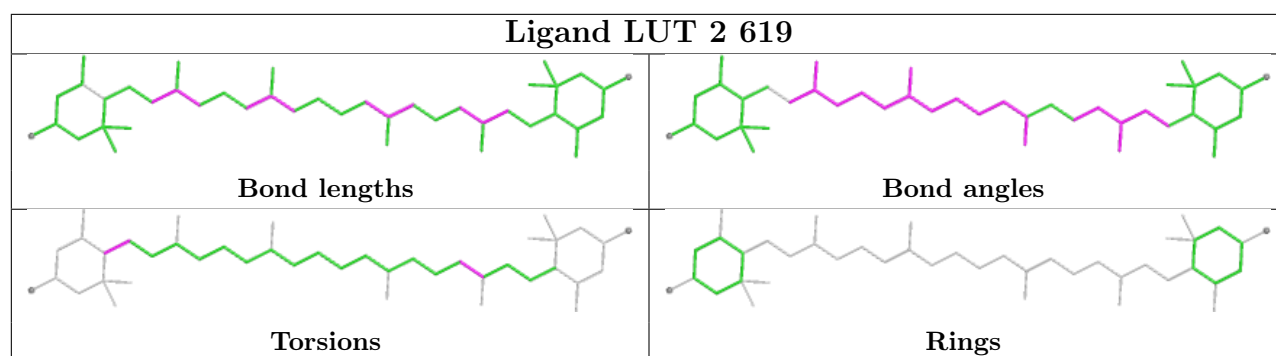


Rings

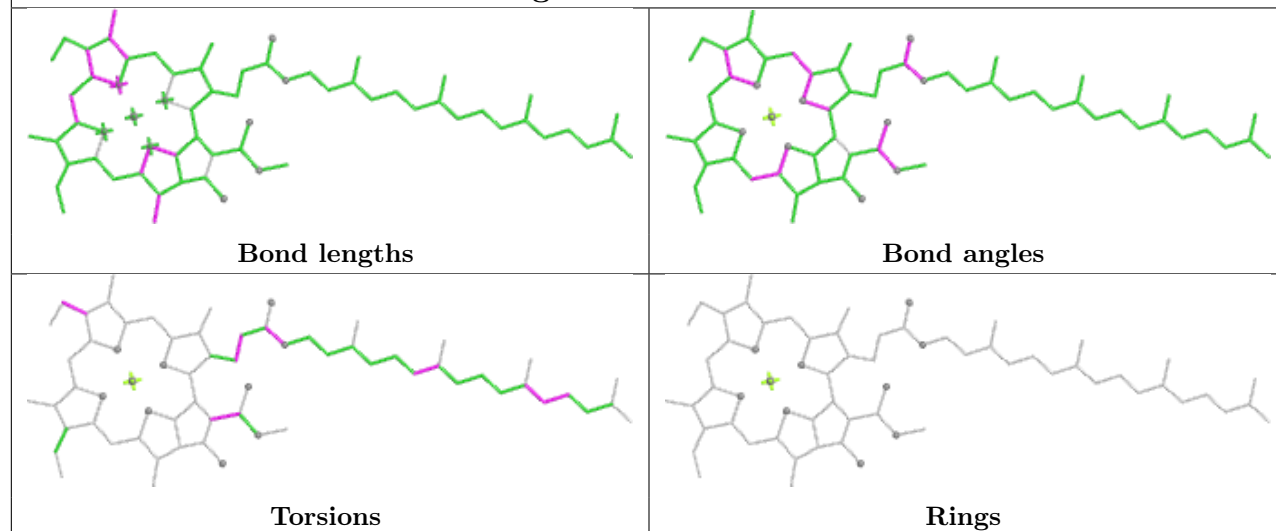




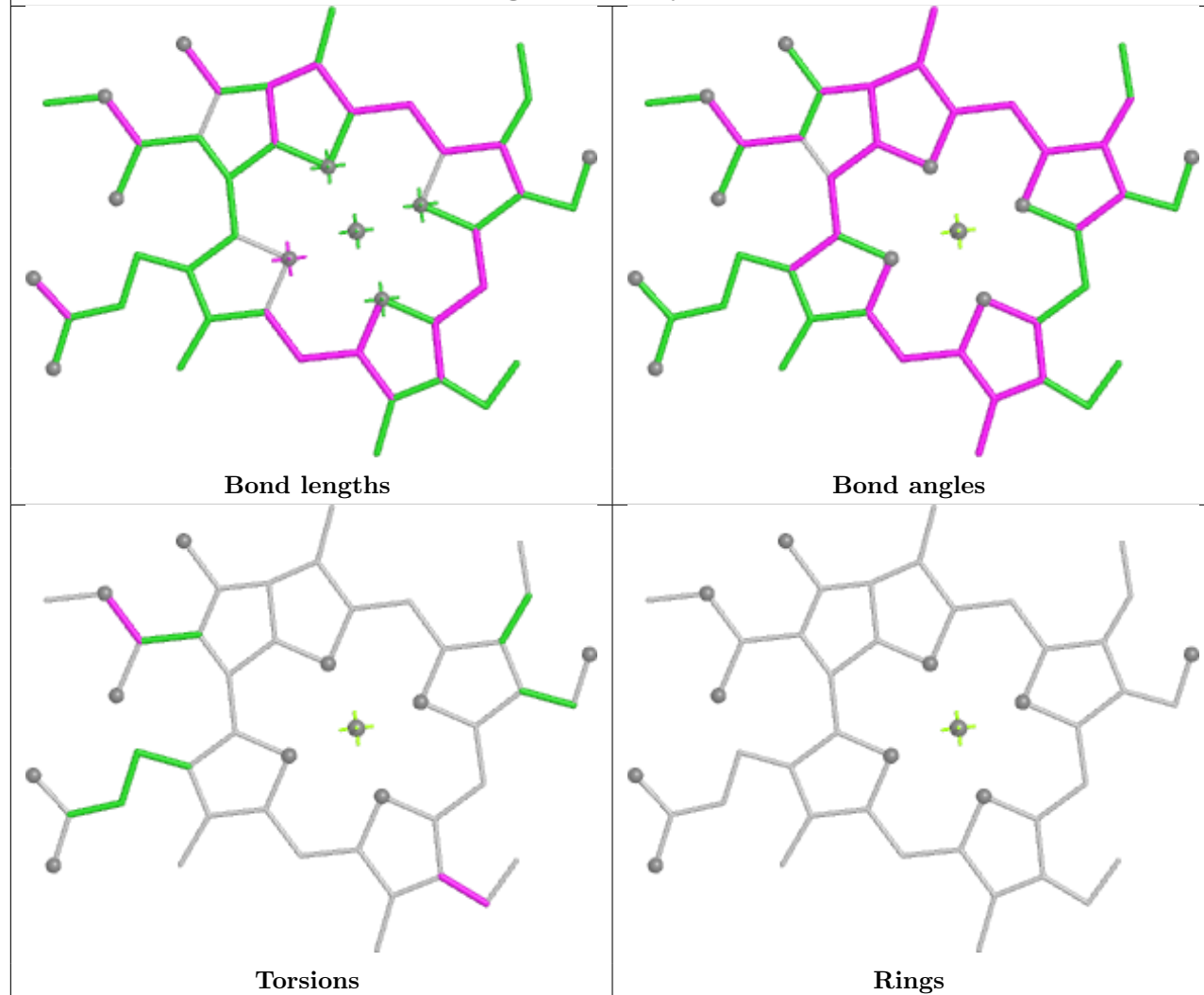




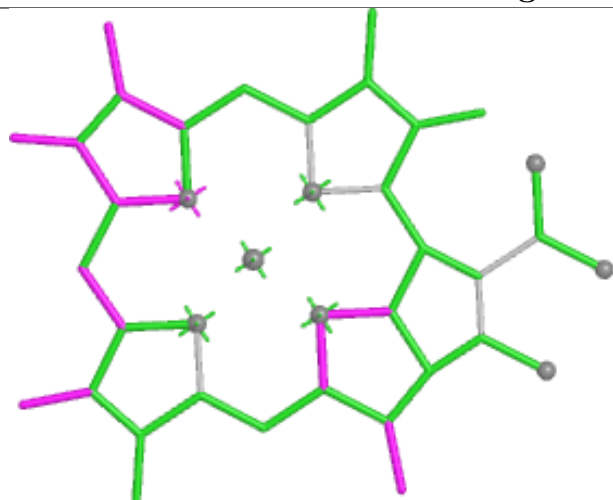
Ligand CLA B 839



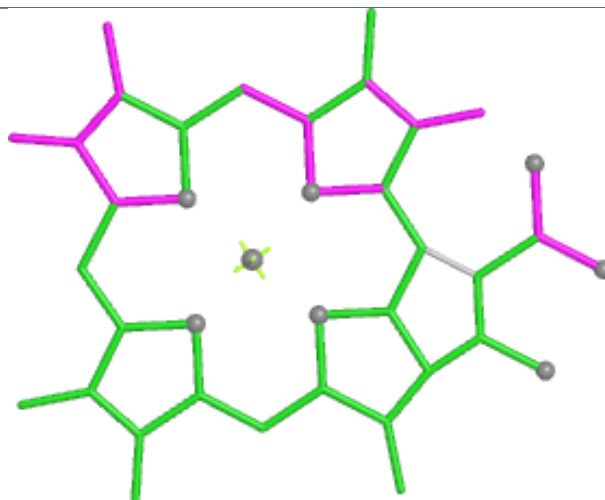
Ligand CHL y 606



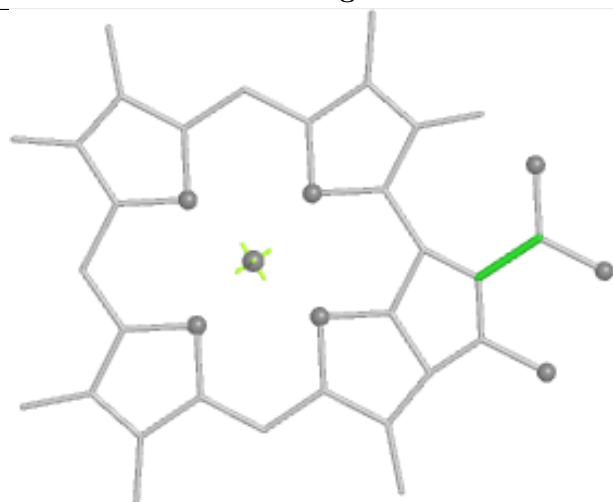
Ligand CLA 1 610



Bond lengths



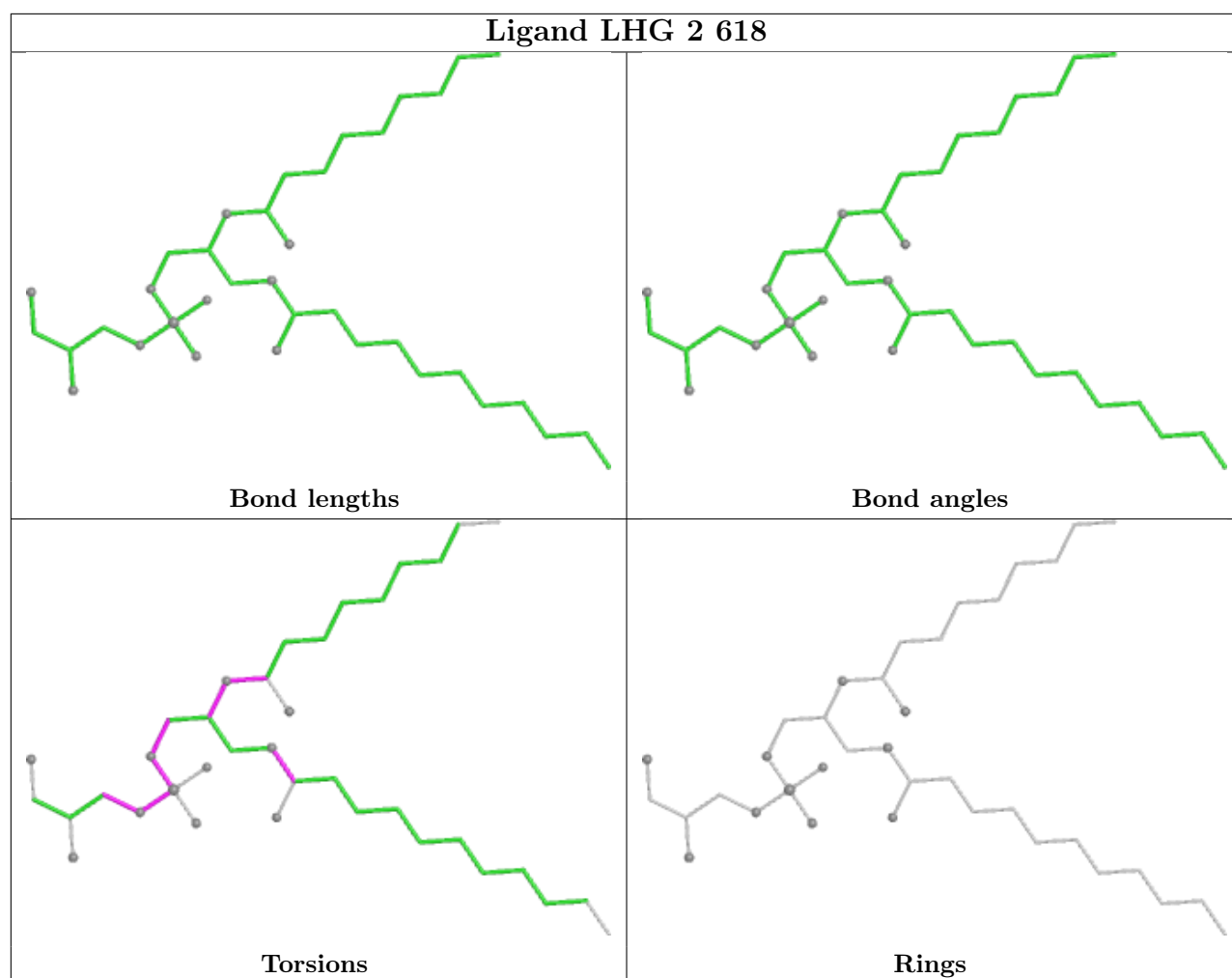
Bond angles



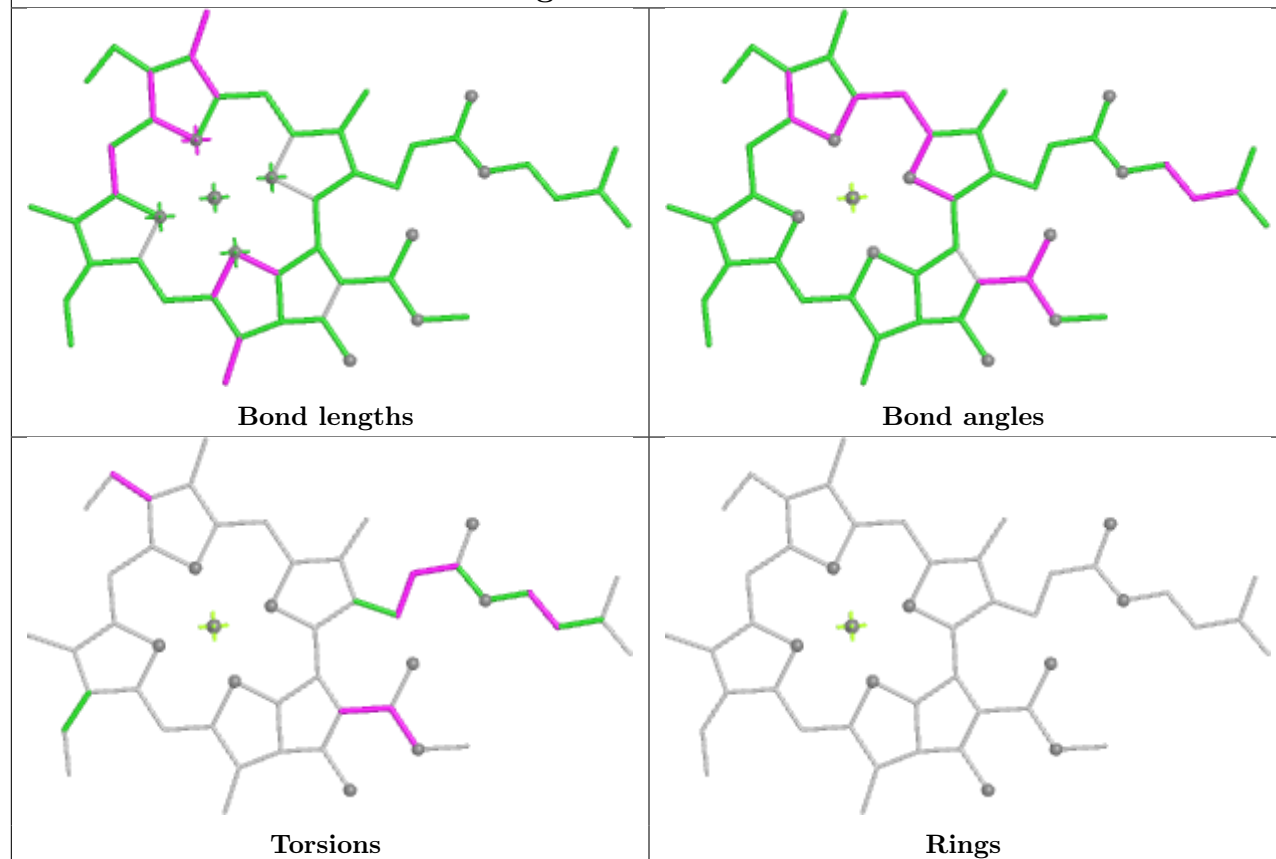
Torsions



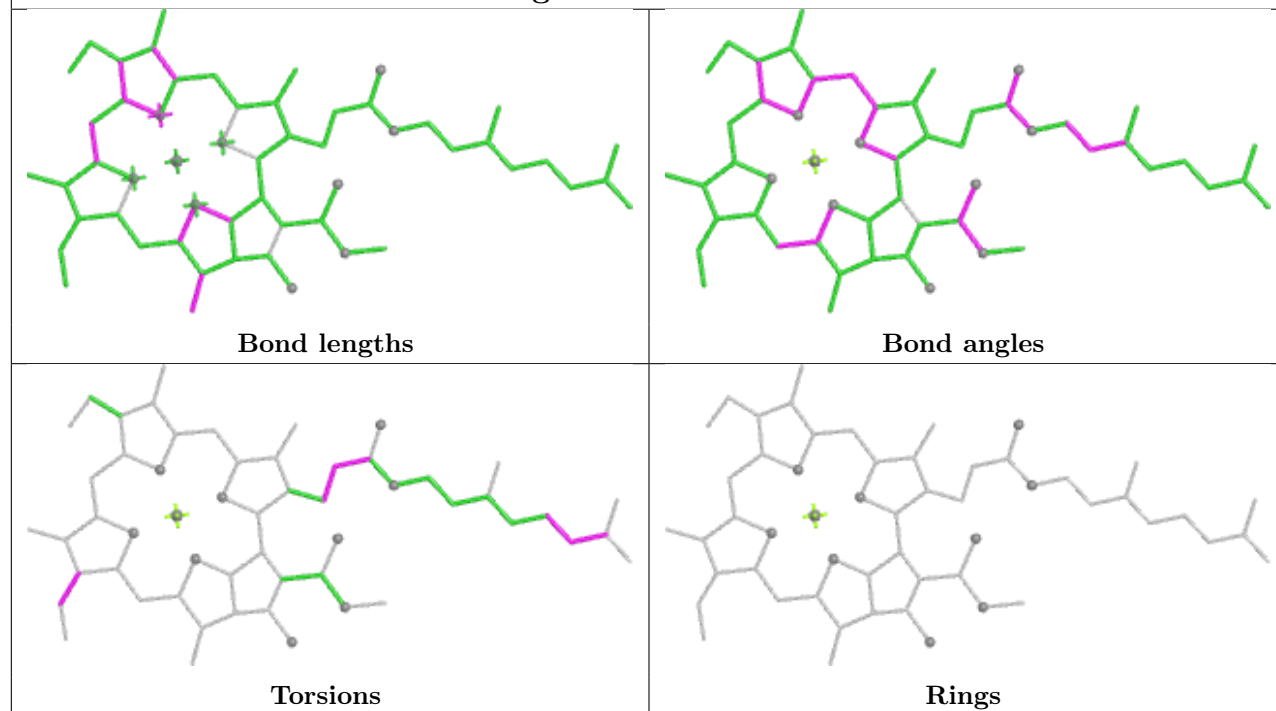
Rings

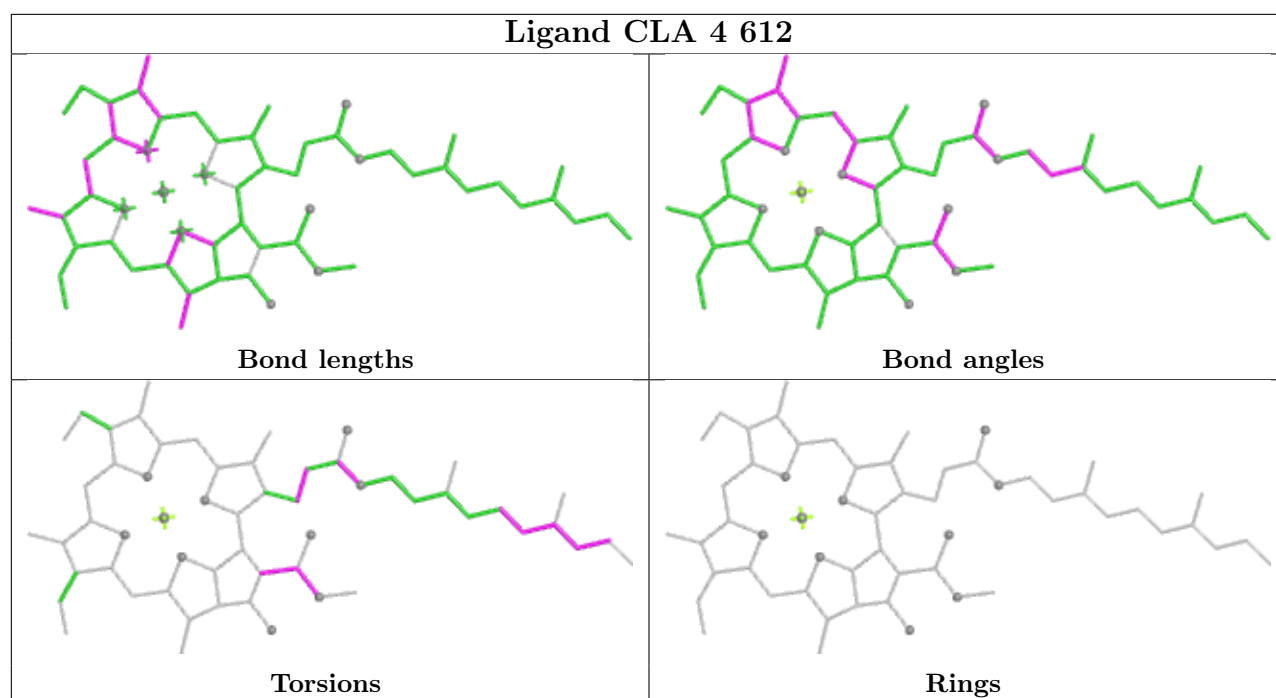


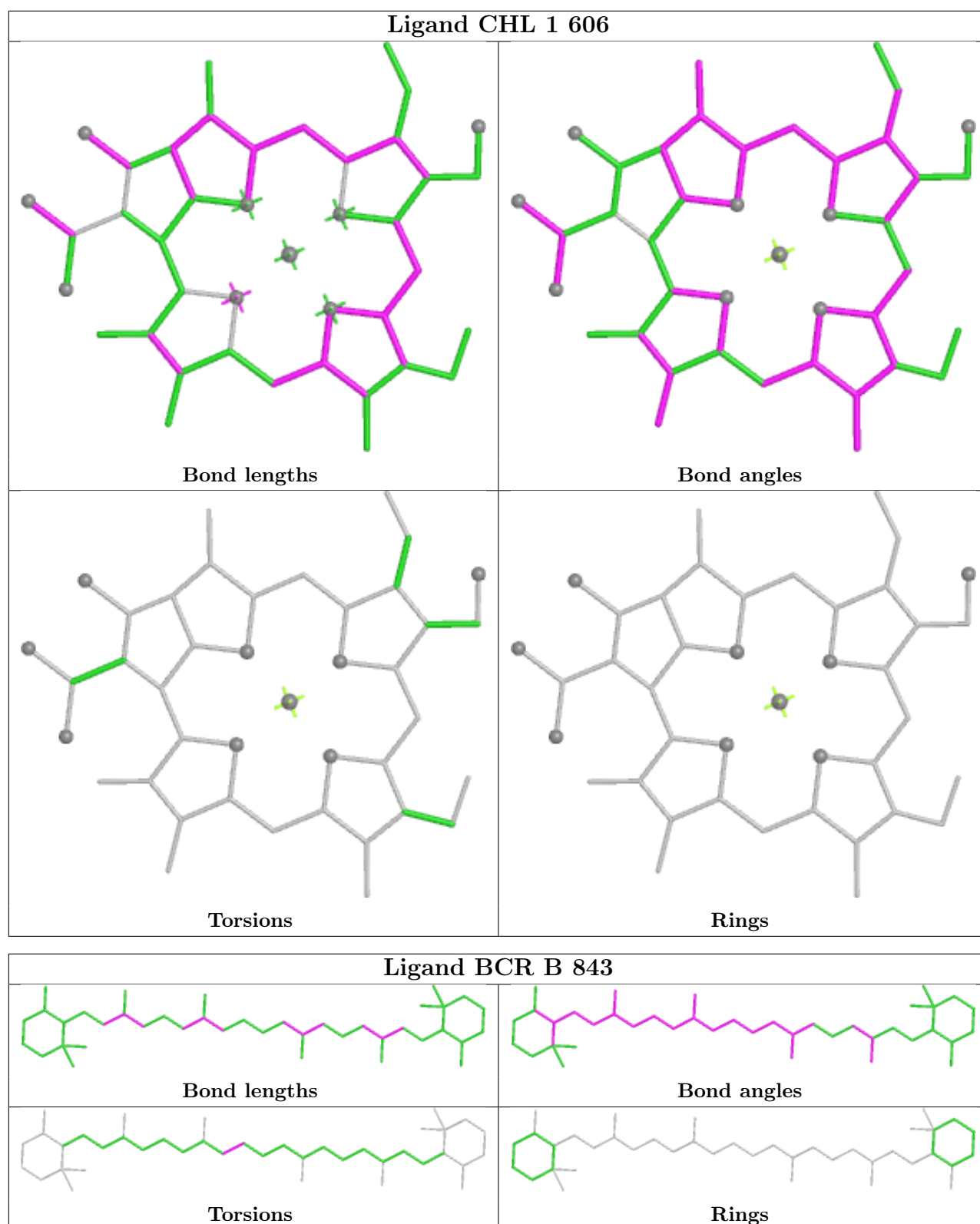
Ligand CLA 4 614



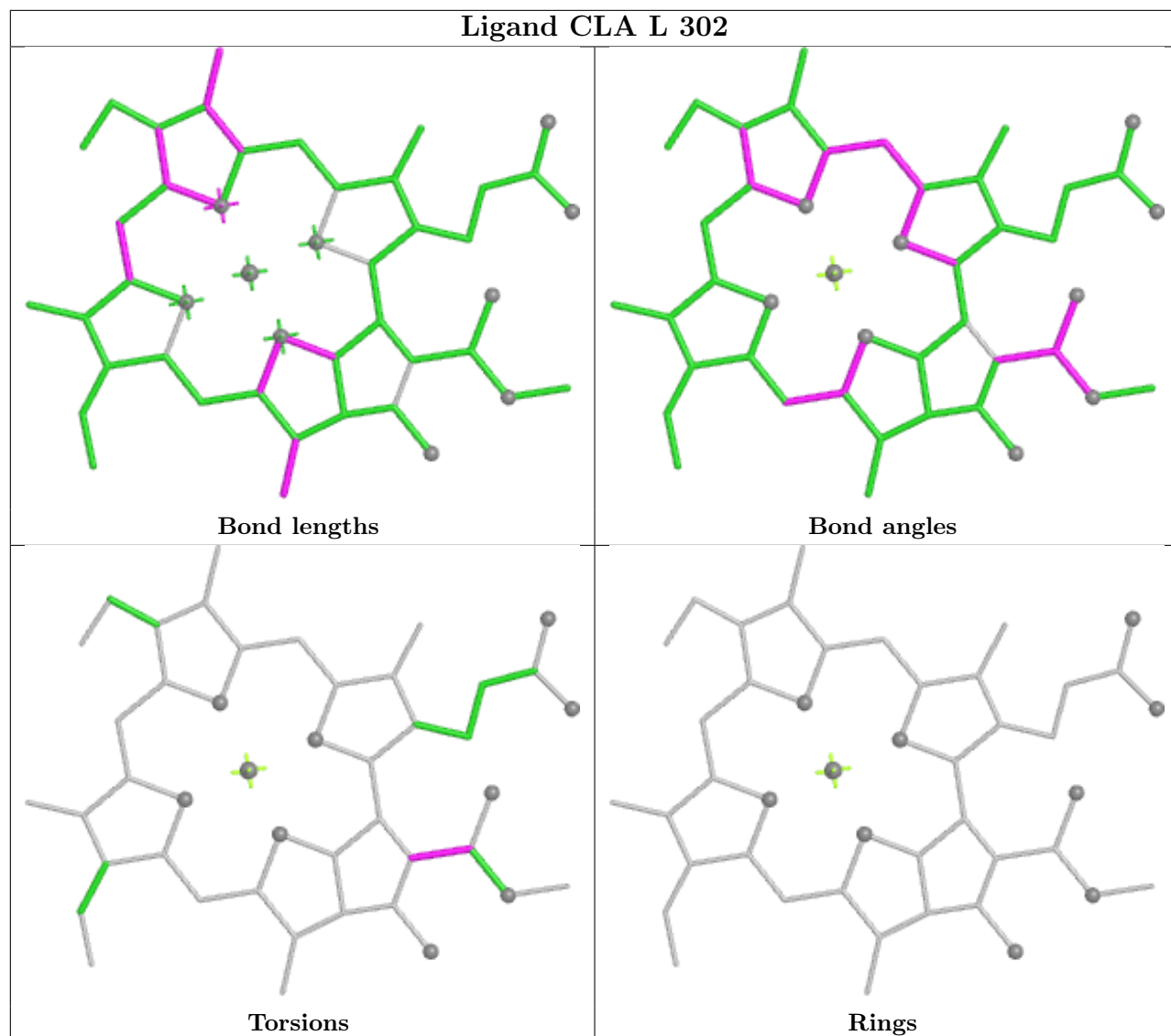
Ligand CLA B 816

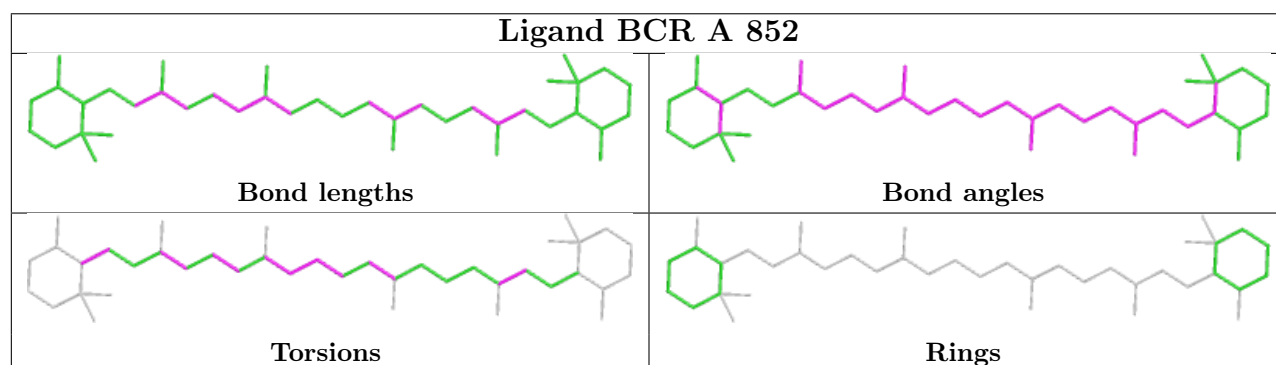
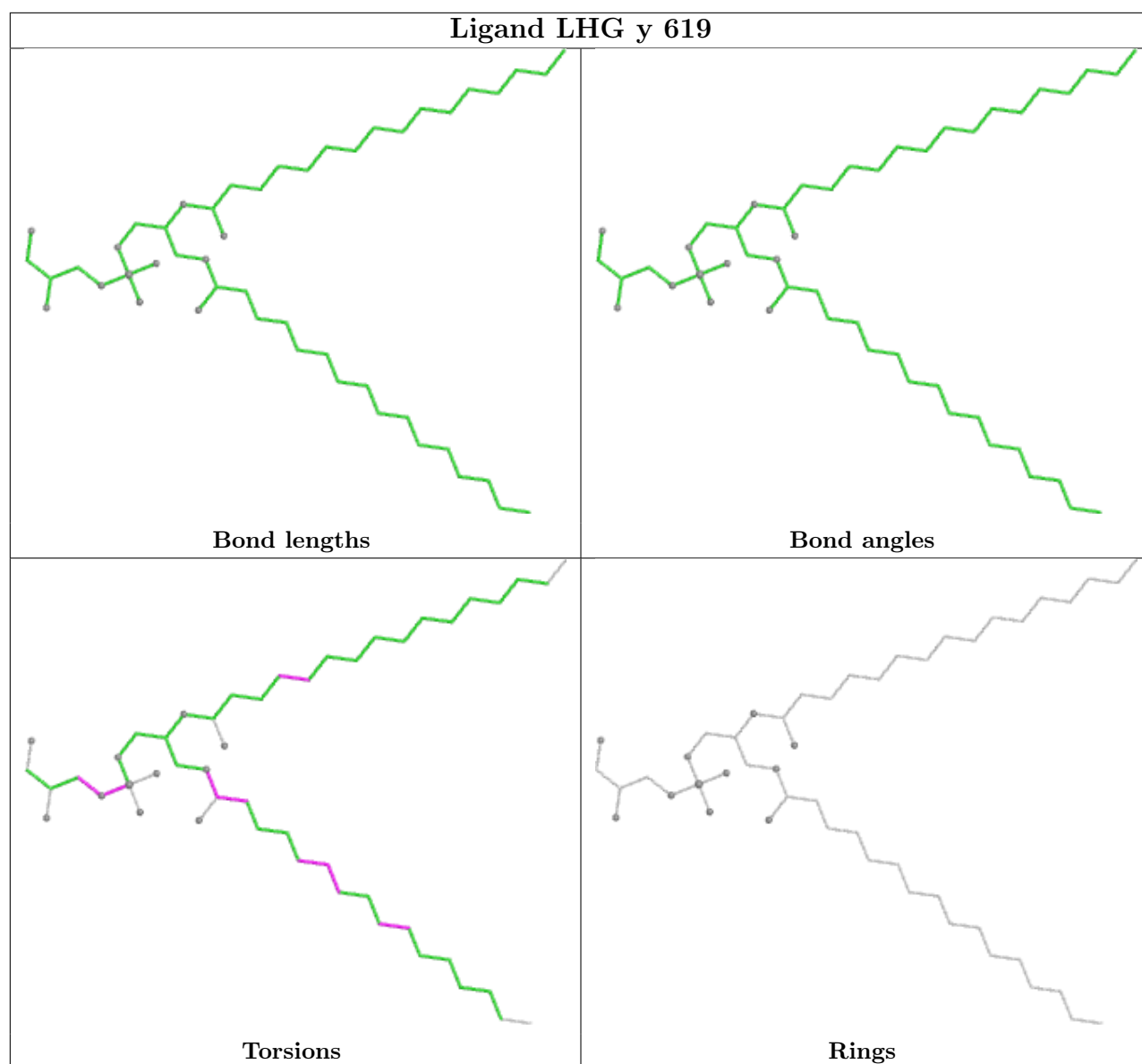


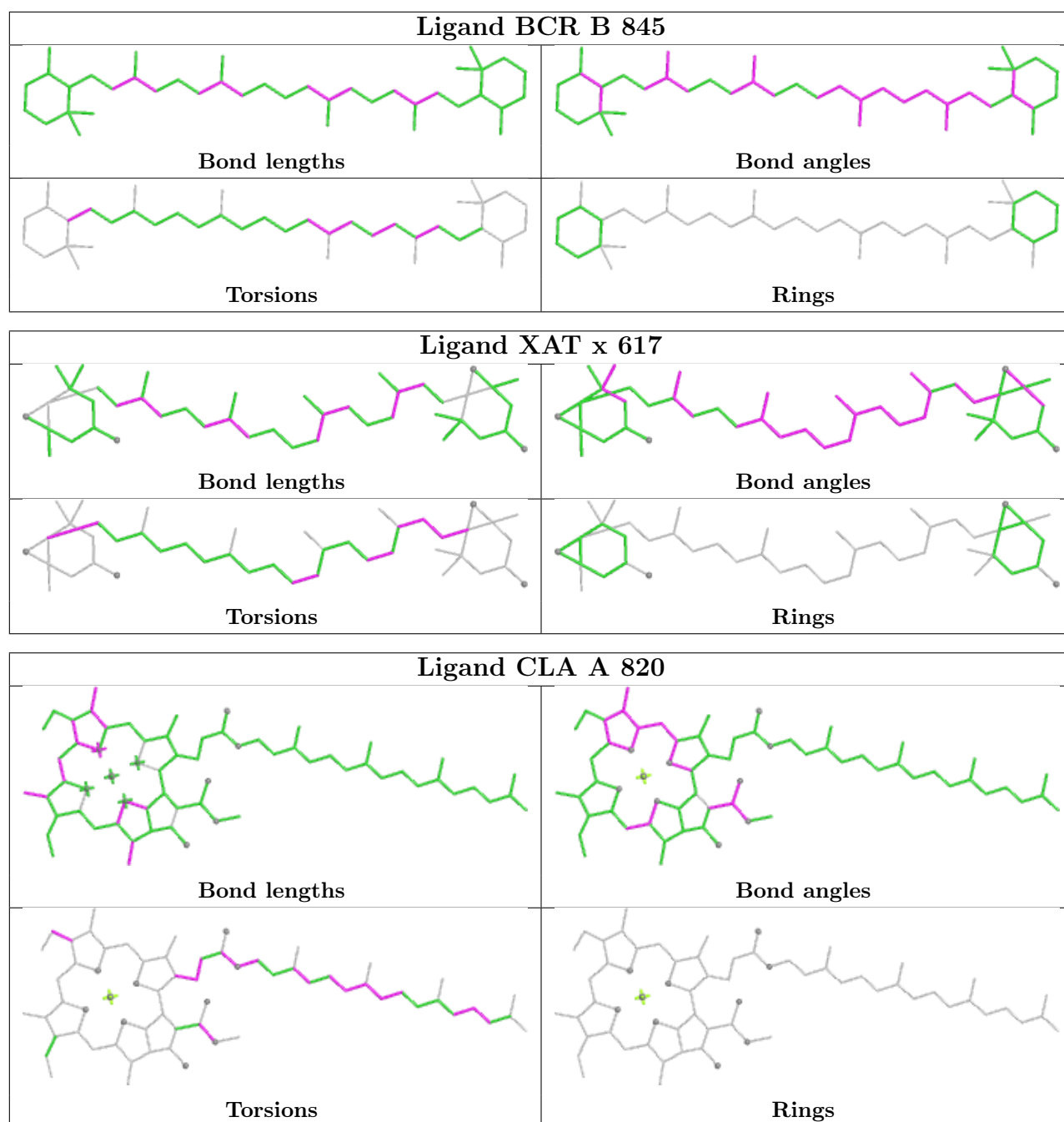




Ligand CLA L 302







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.

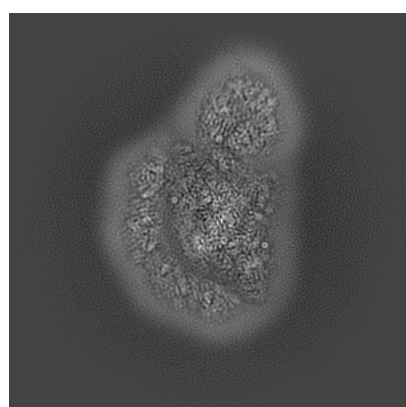
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36021. These allow visual inspection of the internal detail of the map and identification of artifacts.

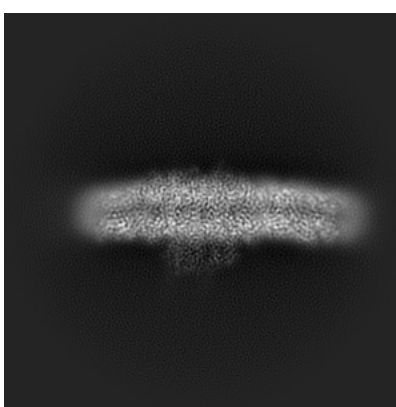
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

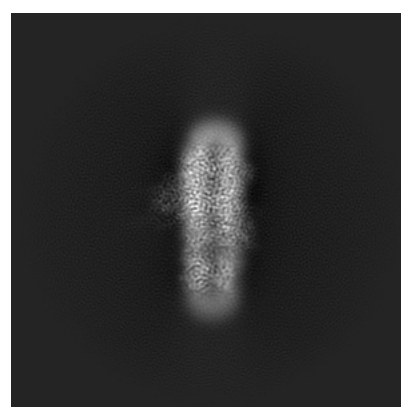
6.1.1 Primary map



X



Y

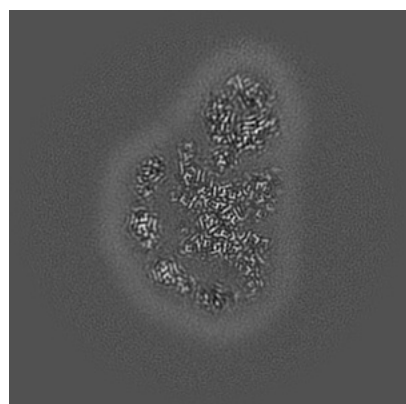


Z

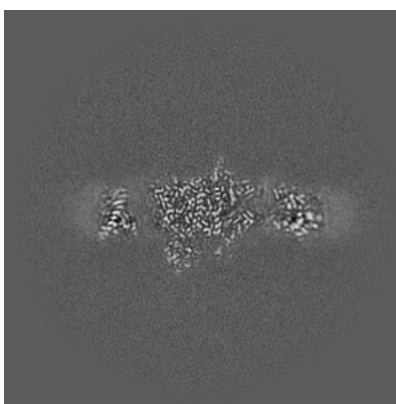
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

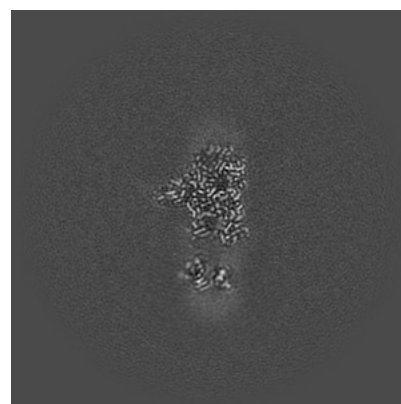
6.2.1 Primary map



X Index: 168



Y Index: 168

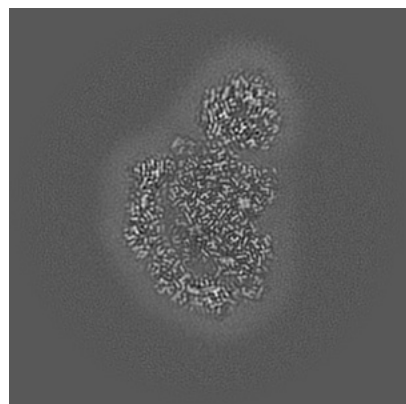


Z Index: 168

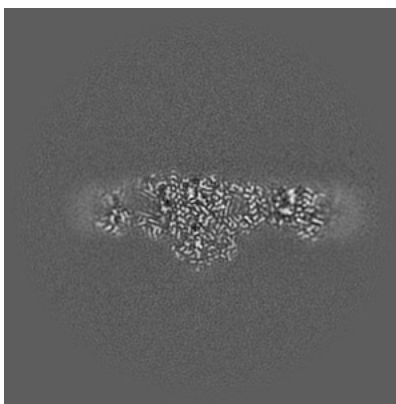
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

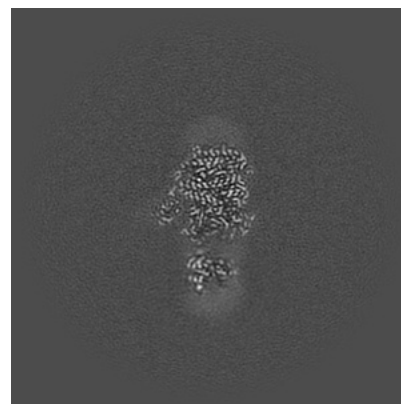
6.3.1 Primary map



X Index: 157



Y Index: 180

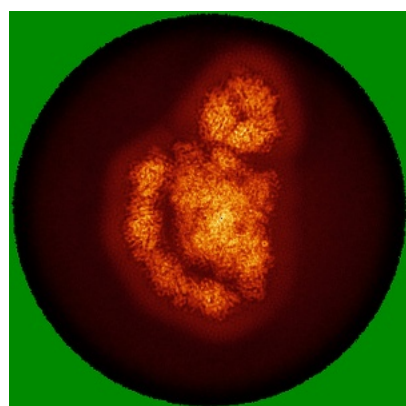


Z Index: 142

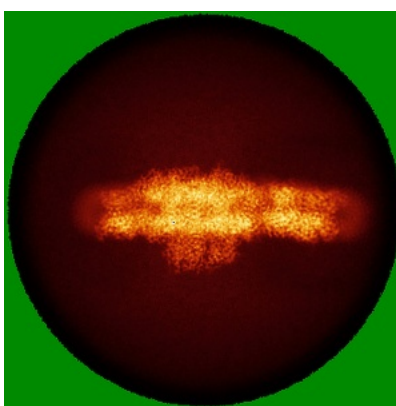
The images above show the largest variance slices of the map in three orthogonal directions.

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

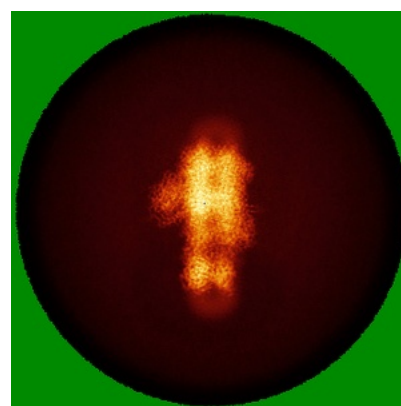
6.4.1 Primary map



X



Y

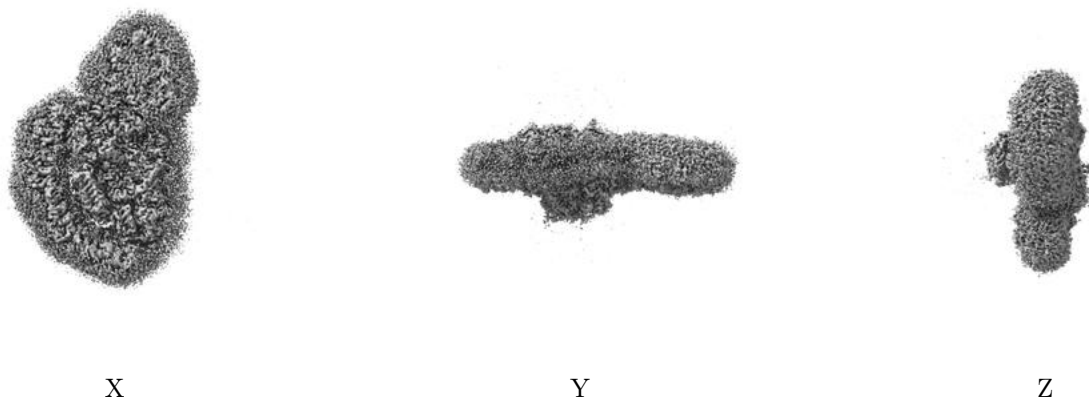


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.59. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

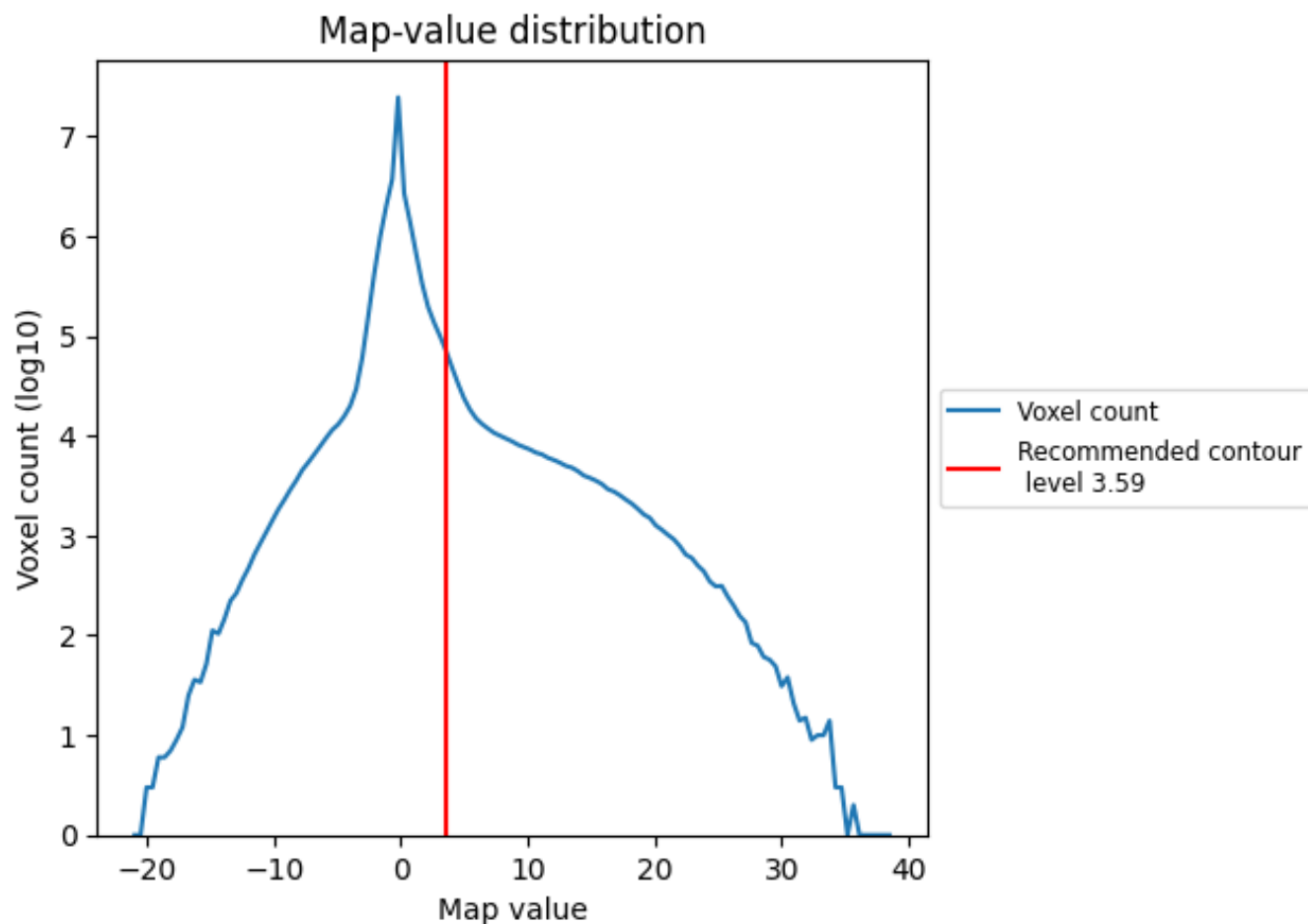
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

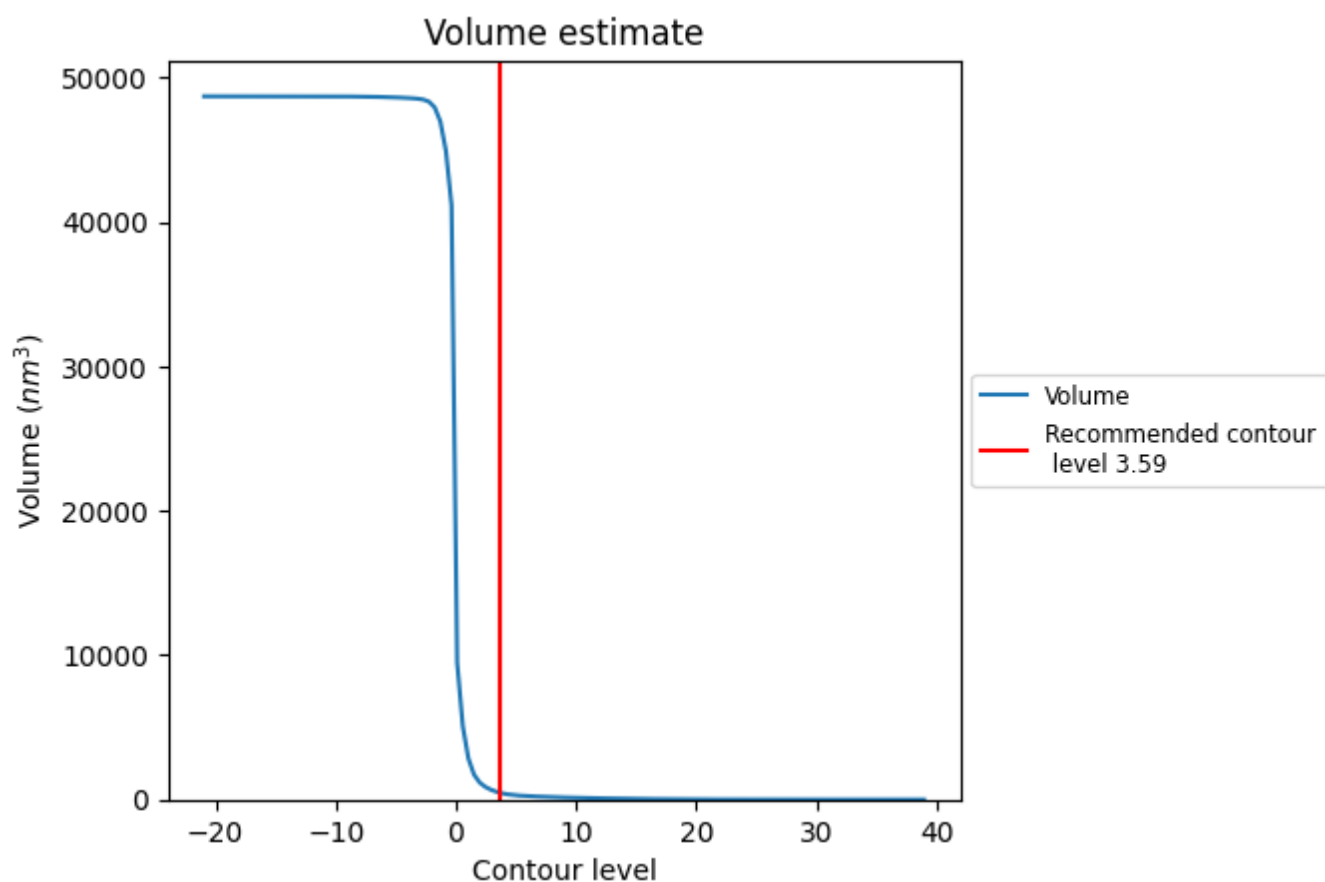
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

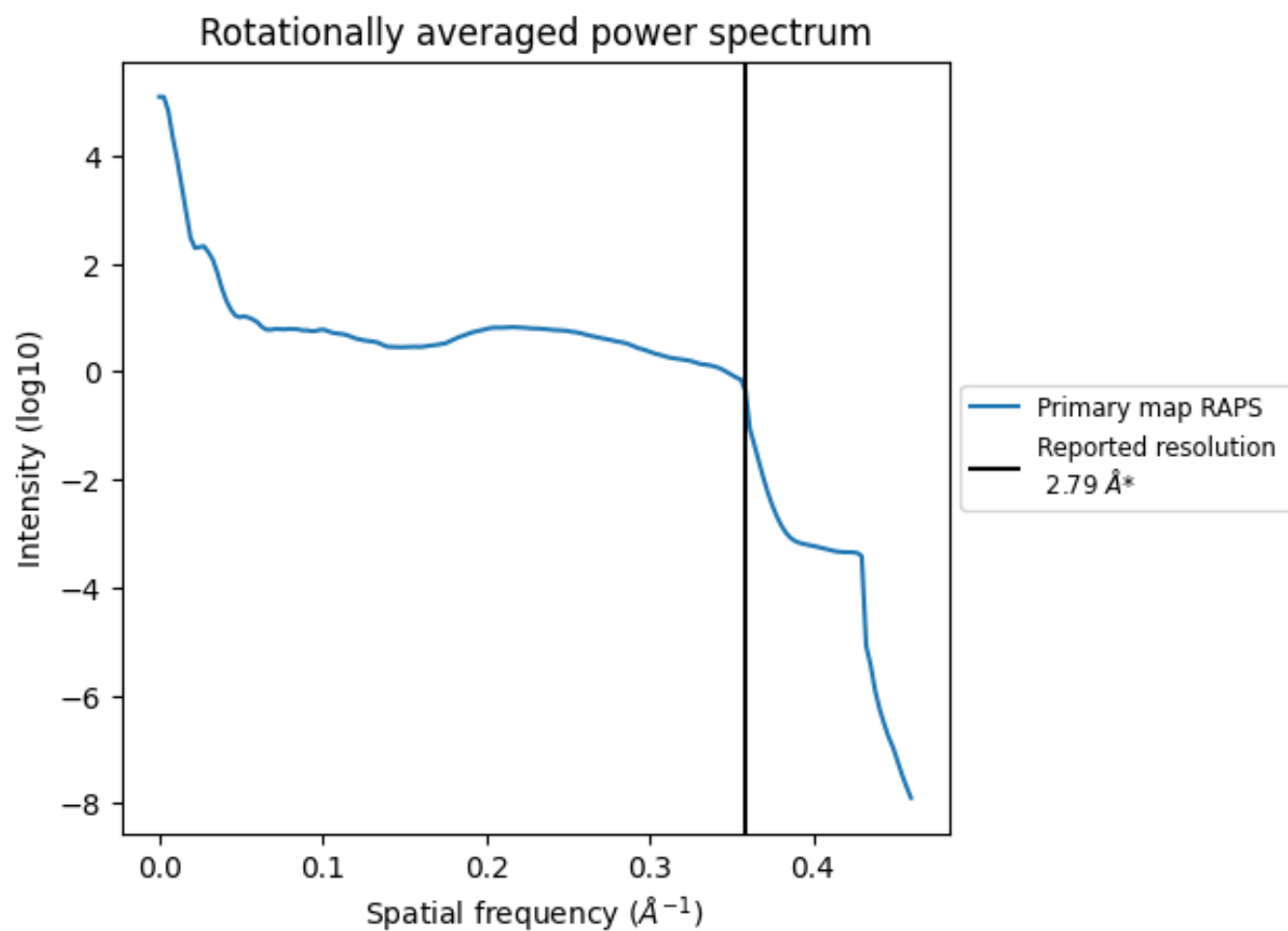
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm³; this corresponds to an approximate mass of 444 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 0.358 Å⁻¹

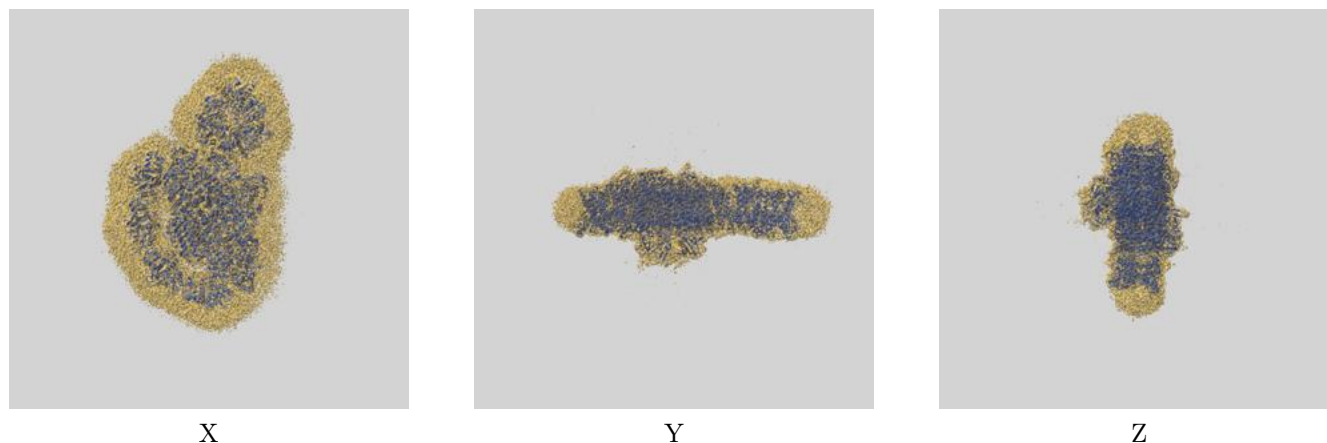
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

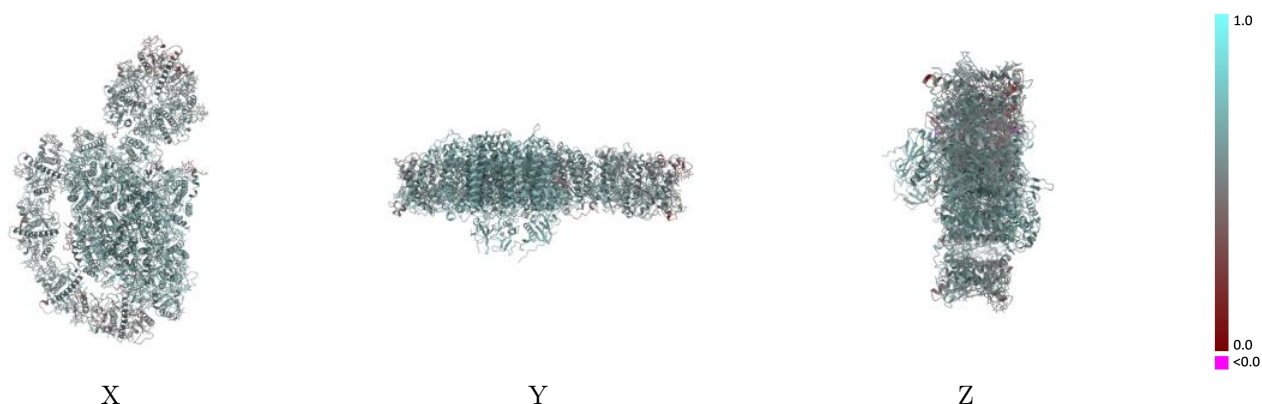
This section contains information regarding the fit between EMDB map EMD-36021 and PDB model 8J6Z. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



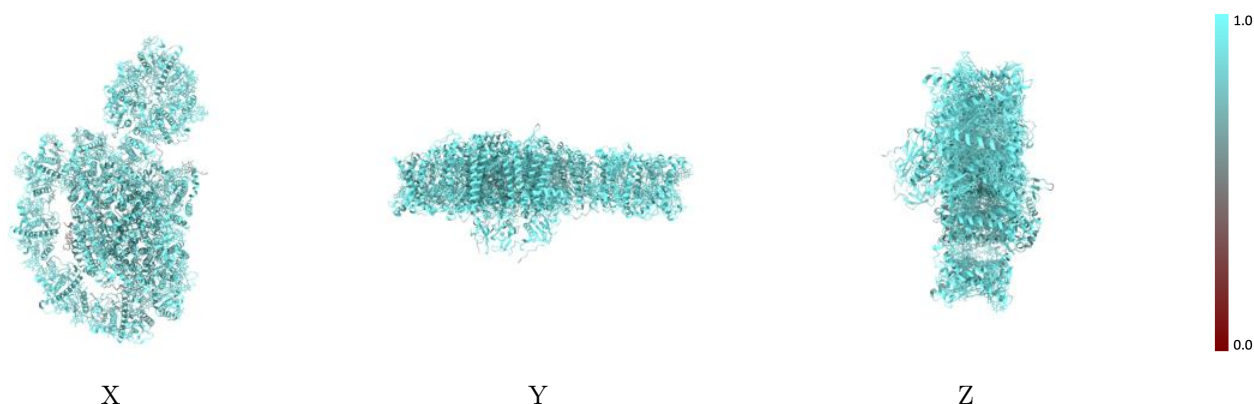
The images above show the 3D surface view of the map at the recommended contour level 3.59 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



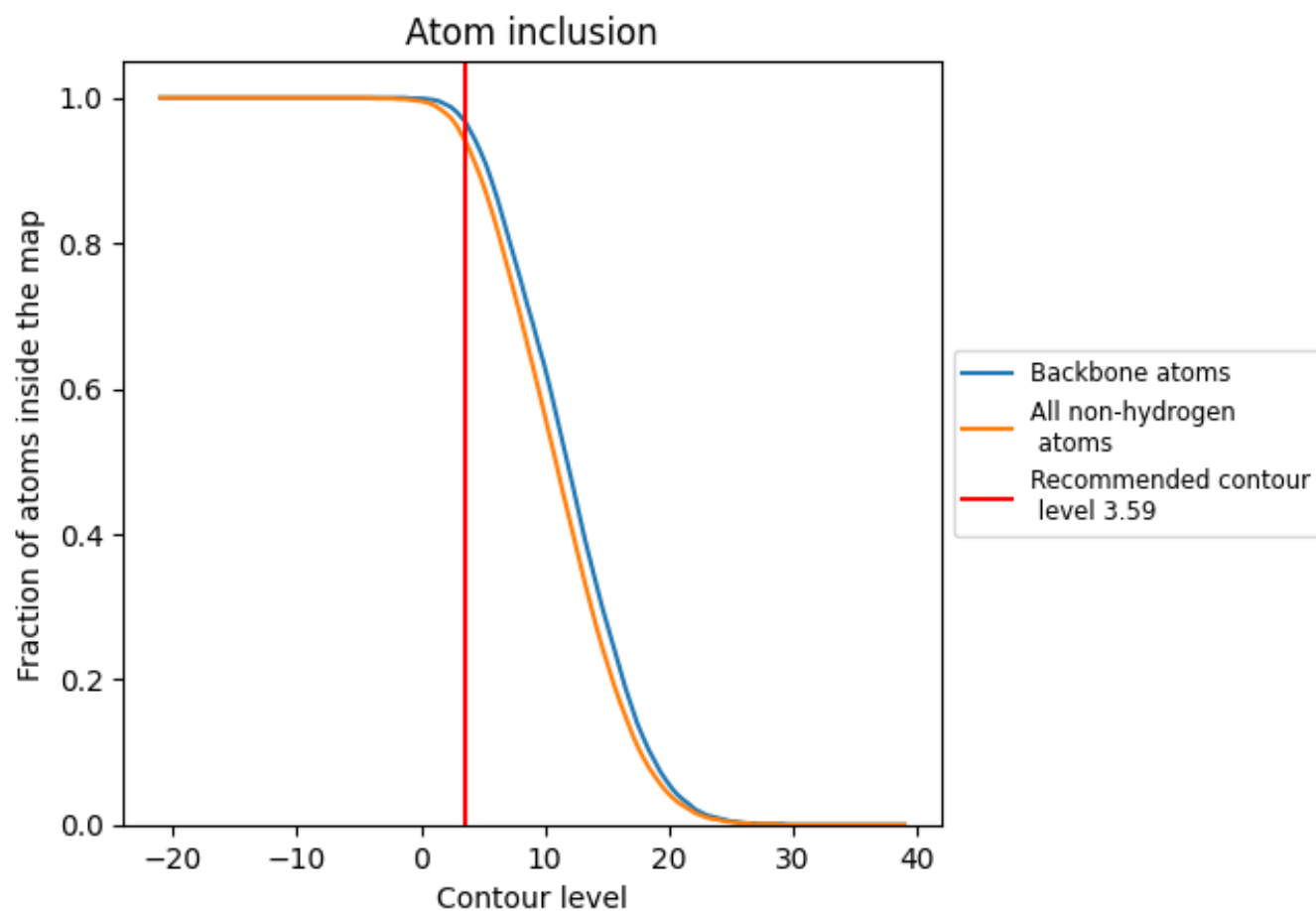
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.59).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (3.59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.5870
1	0.9140	0.5120
2	0.9470	0.5510
3	0.9300	0.5400
4	0.9350	0.5600
A	0.9480	0.6270
B	0.9600	0.6330
C	0.9790	0.6360
D	0.9550	0.6250
E	0.9480	0.6200
F	0.8810	0.5920
G	0.9060	0.5880
H	0.9160	0.5880
I	0.9680	0.6200
J	0.7920	0.5530
K	0.8900	0.5620
L	0.9590	0.6250
O	0.9570	0.5820
x	0.9460	0.5470
y	0.9200	0.4890
z	0.9480	0.5580

1.0

0.0

<0.0