



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:55 PM JST

PDB ID : 7XQP / pdb_00007xqp
EMDB ID : EMD-33401
Title : PSI-LHCI-LHCII-Lhcb9 supercomplex of *Physcomitrella patens*
Authors : Zhang, S.; Tang, K.L.; Li, X.Y.; Wang, W.D.; Yan, Q.J.; Shen, L.L.; Kuang, T.Y.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on : 2022-05-08
Resolution : 2.68 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>.

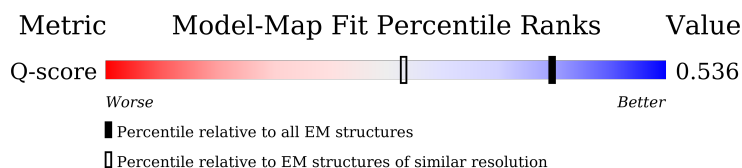
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

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ELECTRON MICROSCOPY

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	9255 (2.18 - 3.18)

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

Mol	Chain	Length	Quality of chain
1	A	742	87%13%
2	B	733	86%14%
3	C	80	81%19%
4	D	141	87%13%

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Mol	Chain	Length	Quality of chain
5	E	62	
6	F	159	
7	G	98	
8	H	95	
9	I	34	
10	J	41	
11	K	81	
12	L	163	
13	M	32	
14	O	89	
15	1	192	
15	5	192	
16	2	211	
16	6	211	
17	3	216	
17	7	216	
18	4	205	
18	8	205	
19	9	225	
20	a	227	
20	b	227	
20	c	227	

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
21	CLA	2	609	-	-	X	-
21	CLA	3	409	-	-	X	-
21	CLA	8	609	-	-	X	-
24	BCR	K	205	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5836	3827	993	997	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5849	3839	996	998	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			595	365	103	116	11		

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1104	707	196	198	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			487	309	87	91		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	159	Total	C	N	O	S	0	0
			1230	796	210	221	3		

- Molecule 7 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	95	Total	C	N	O	S	0	0
			740	476	125	138	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			566	356	98	109	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	163	Total	C	N	O	S	0	0
			1229	808	197	222	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O	S	0	0
			238	155	38	44	1		

- Molecule 14 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	89	Total	C	N	O	S	0	0
			702	472	115	114	1		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1478	965	247	265	1		
15	5	192	Total	C	N	O	S	0	0
			1475	962	247	265	1		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	211	Total	C	N	O	S	0	0
			1632	1062	274	292	4		
16	6	205	Total	C	N	O	S	0	0
			1587	1035	265	283	4		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	216	Total	C	N	O	S	0	0
			1670	1094	269	300	7		
17	7	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	205	Total	C	N	O	S	0	0
			1592	1033	266	288	5		
18	8	204	Total	C	N	O	S	0	0
			1585	1029	265	286	5		

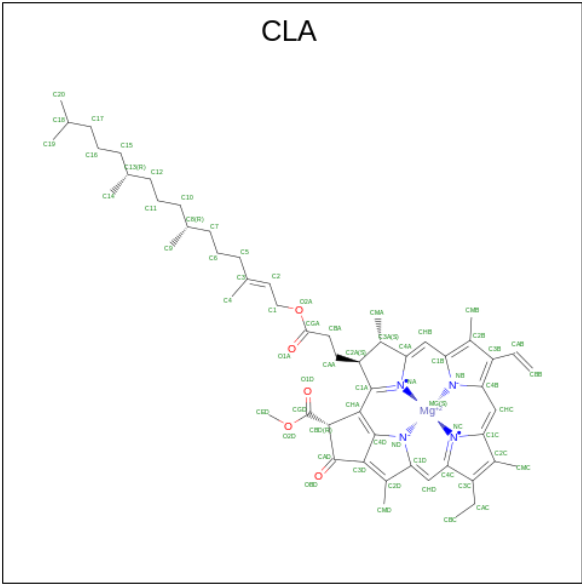
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	225	Total	C	N	O	S	0	0
			1747	1139	287	312	9		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	218	Total 1651	C 1069	N 268	O 309	S 5	0	0
20	b	218	Total 1651	C 1069	N 268	O 309	S 5	0	0
20	c	227	Total 1727	C 1110	N 284	O 327	P 1 S 5	0	0

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 55	C 45	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 45	C 35	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 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 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 53	C 43	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 65	C 55	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 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 63	C 53	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 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
			62	52	1	4	5	
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
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			44	34	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
			54	44	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
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			46	36	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
			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
			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
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 56	C 46	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 56	C 46	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	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 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 64	C 54	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 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	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	G	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	K	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	K	1	Total 44	C 34	Mg 1	N 4	O 5	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 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	O	1	Total 42	C 34	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 50	C 42	Mg 1	N 4	O 3	0
21	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	2	1	Total 51	C 42	Mg 1	N 4	O 4	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	7	1	Total 42	C 32	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	7	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	7	1	Total 36	C 30	Mg 1	N 4	O 1	0
21	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
21	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
21	8	1	Total 54	C 45	Mg 1	N 4	O 4	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	9	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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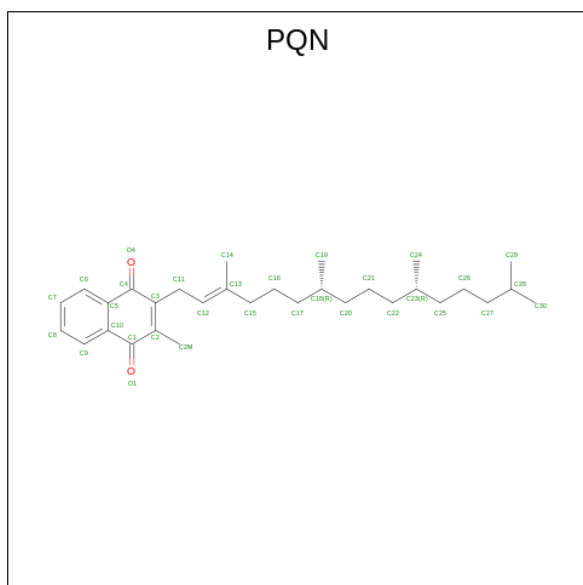
Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
21	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	c	1	Total 44	C 35	Mg 1	N 4	O 4	0

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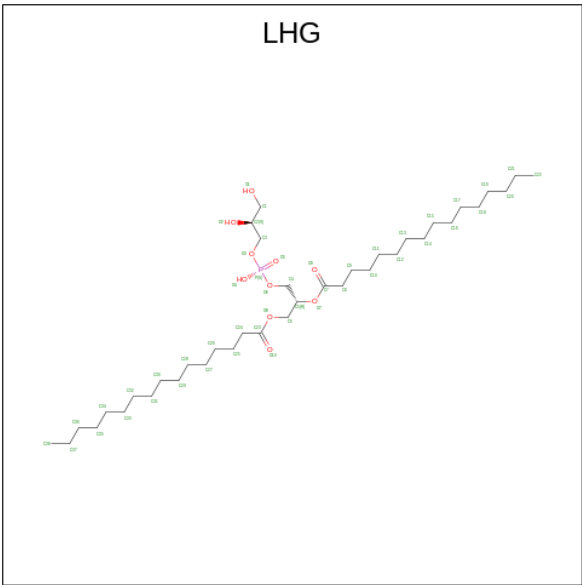
Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



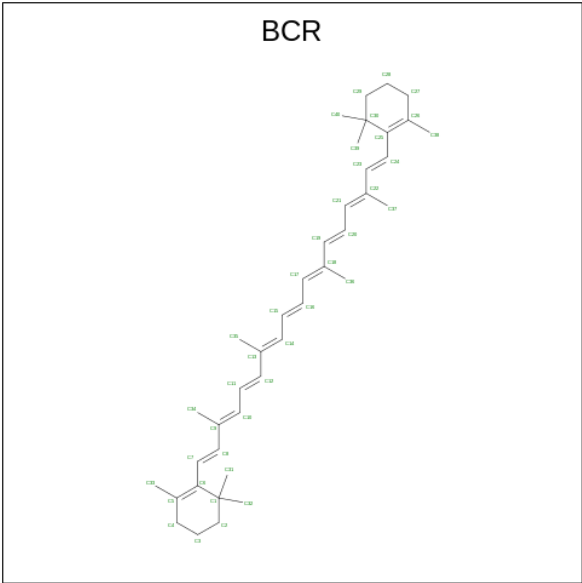
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			28	17	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	4	1	Total	C	O	P	0
			37	26	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	5	1	Total	C	O	P	0
			28	17	10	1	
23	6	1	Total	C	O	P	0
			35	24	10	1	
23	8	1	Total	C	O	P	0
			37	26	10	1	
23	9	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			49	38	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	c	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

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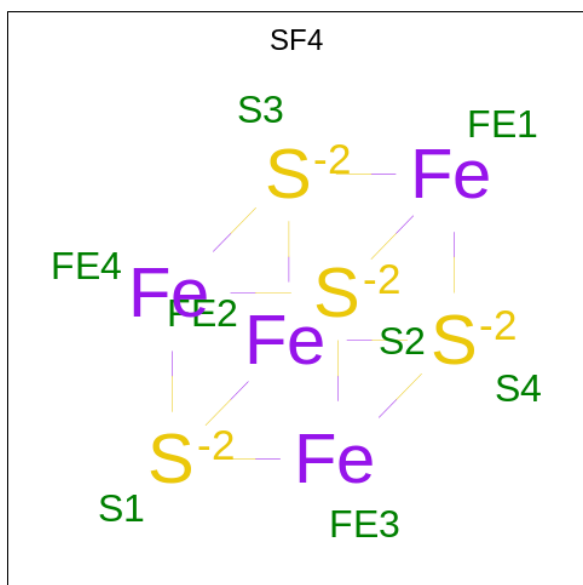
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	M	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	7	1	Total C 40 40	0

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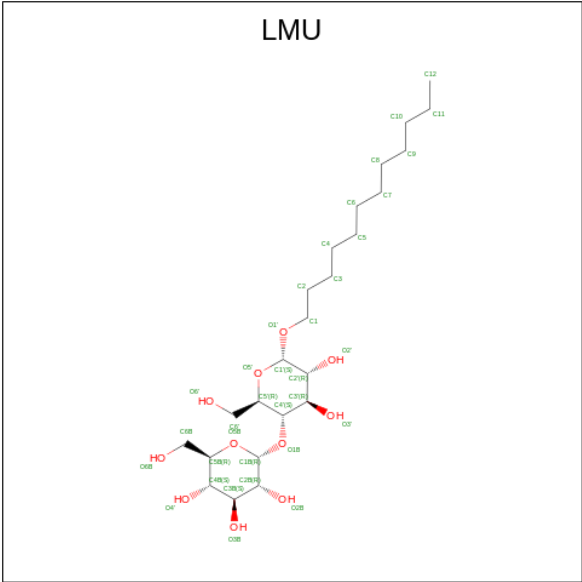
Mol	Chain	Residues	Atoms	AltConf
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



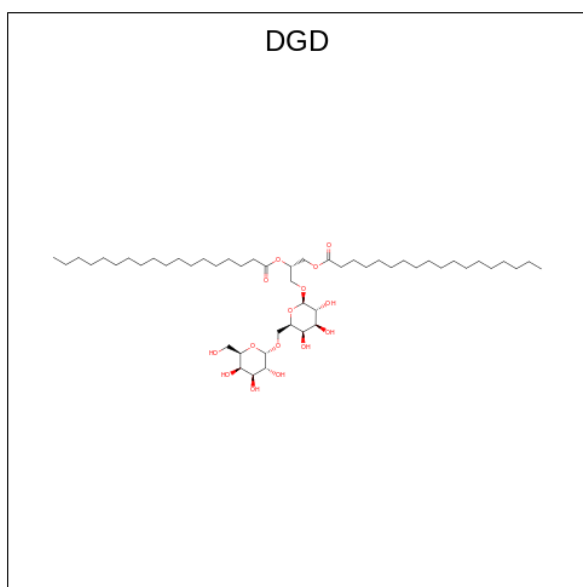
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).



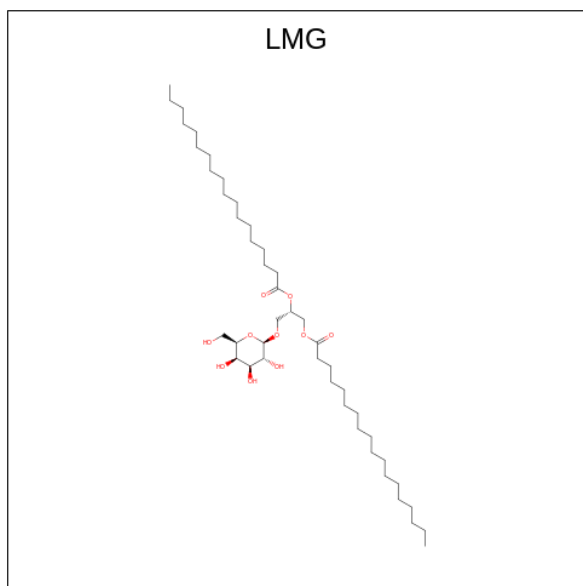
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	
26	A	1	Total	C	O	0
			35	24	11	
26	O	1	Total	C	O	0
			35	24	11	
26	3	1	Total	C	O	0
			35	24	11	
26	b	1	Total	C	O	0
			35	24	11	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



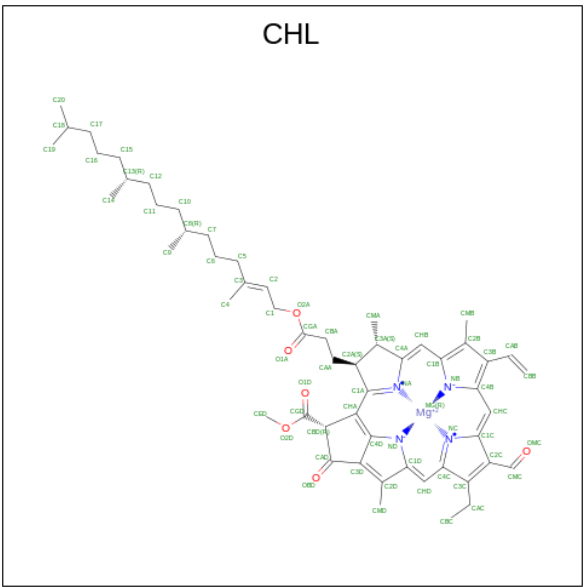
Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			30	20	10	

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Mol	Chain	Residues	Atoms			AltConf
28	2	1	Total	C	O	0
			13	7	6	
28	6	1	Total	C	O	0
			13	7	6	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



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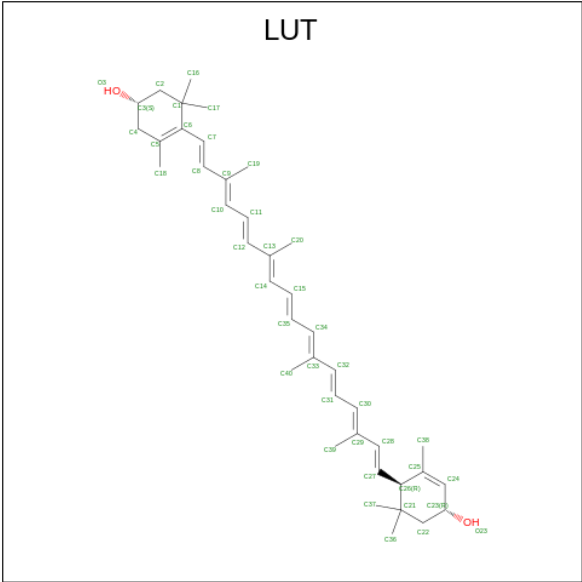
Mol	Chain	Residues	Atoms					AltConf
29	4	1	Total 41	C 32	Mg 1	N 4	O 4	0
29	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
29	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
29	6	1	Total 53	C 42	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	7	1	Total 40	C 32	Mg 1	N 4	O 3	0
29	8	1	Total 41	C 32	Mg 1	N 4	O 4	0
29	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	8	1	Total 42	C 33	Mg 1	N 4	O 4	0
29	9	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0
29	9	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			44	33	1	4	6	

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



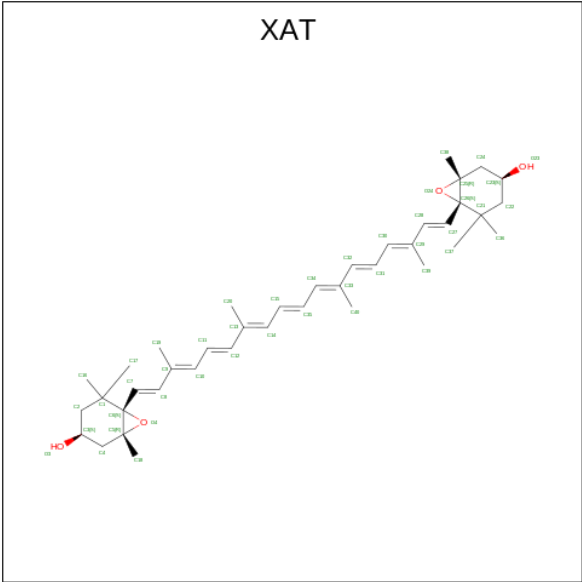
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	2	1	Total	C	O	0
			42	40	2	
30	3	1	Total	C	O	0
			42	40	2	
30	4	1	Total	C	O	0
			42	40	2	
30	5	1	Total	C	O	0
			42	40	2	
30	6	1	Total	C	O	0
			42	40	2	
30	7	1	Total	C	O	0
			42	40	2	
30	8	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	9	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	a	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	

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

- Molecule 31 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).



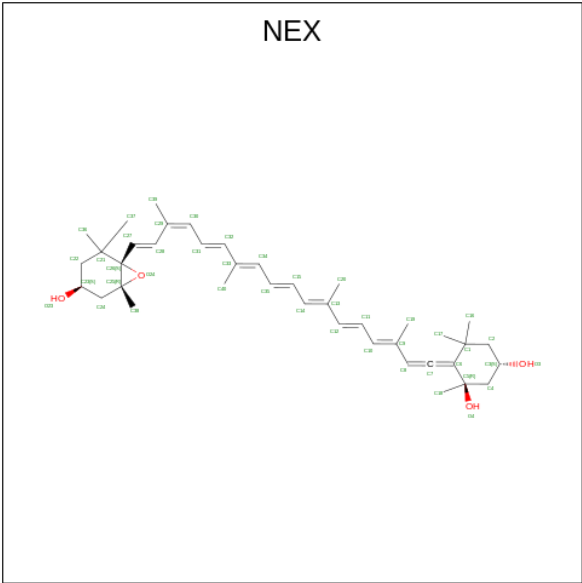
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			44	40	4	
31	2	1	Total	C	O	0
			44	40	4	
31	3	1	Total	C	O	0
			44	40	4	
31	4	1	Total	C	O	0
			44	40	4	
31	5	1	Total	C	O	0
			44	40	4	
31	6	1	Total	C	O	0
			44	40	4	
31	7	1	Total	C	O	0
			44	40	4	
31	8	1	Total	C	O	0
			44	40	4	
31	9	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			44	40	4	
31	c	1	Total	C	O	0
			44	40	4	

- Molecule 32 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: C₄₀H₅₆O₄).

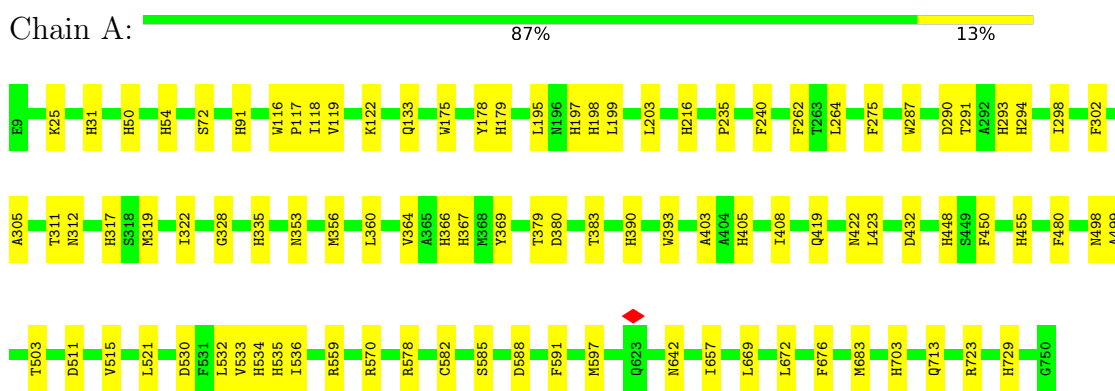


Mol	Chain	Residues	Atoms			AltConf
32	9	1	Total	C	O	0
			44	40	4	
32	b	1	Total	C	O	0
			44	40	4	
32	c	1	Total	C	O	0
			44	40	4	

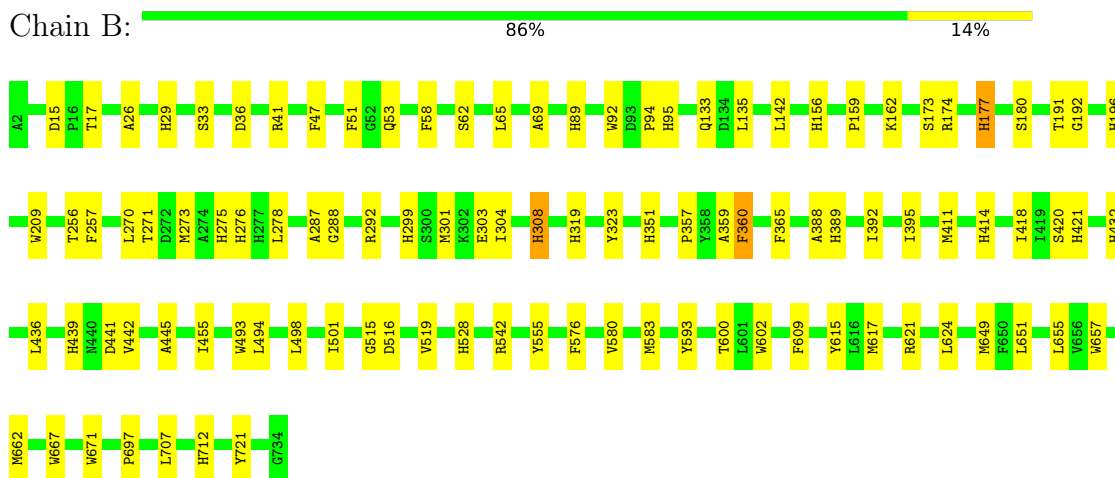
3 Residue-property plots

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

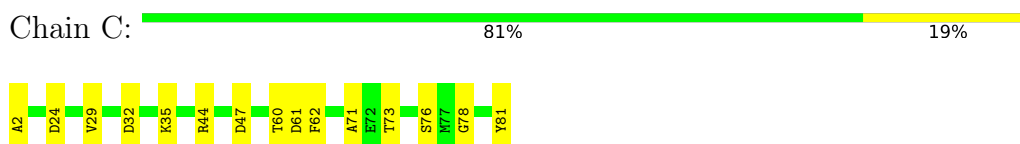
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Predicted protein PsaD

Chain D:  87% 13%



- Molecule 5: PsaE

Chain E:  85% 15%



- Molecule 6: PSI-F

Chain F:  89% 11%



- Molecule 7: PSI-G

Chain G:  5% 85% 15%



- Molecule 8: PsaH photosystem I reaction center subunit

Chain H:  93% 7%



- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  79% 21%



- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  88% 12%



- Molecule 11: PsaK

Chain K:  90% 10%



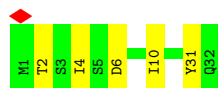
- Molecule 12: PSI subunit V

Chain L:  90% 10%



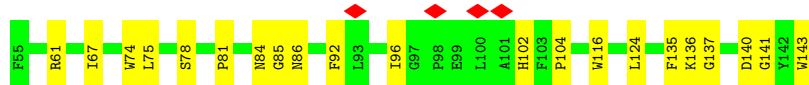
- Molecule 13: Photosystem I reaction center subunit XII

Chain M:  84% 16%



- Molecule 14: PsaO

Chain O:  76% 24%



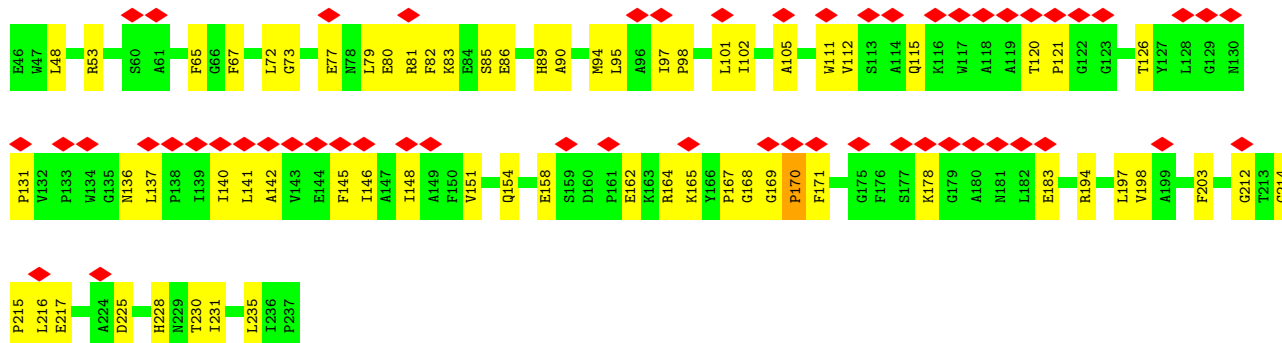
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 1:  84% 16%



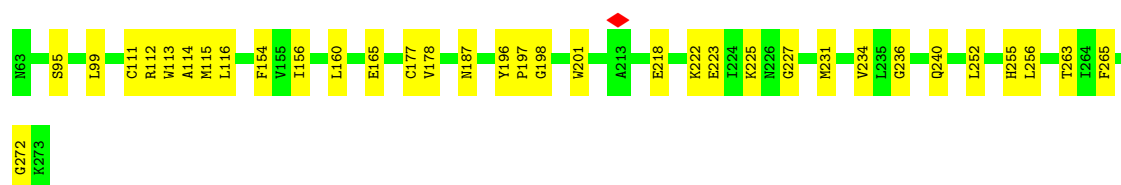
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5:  29% 66% 33%



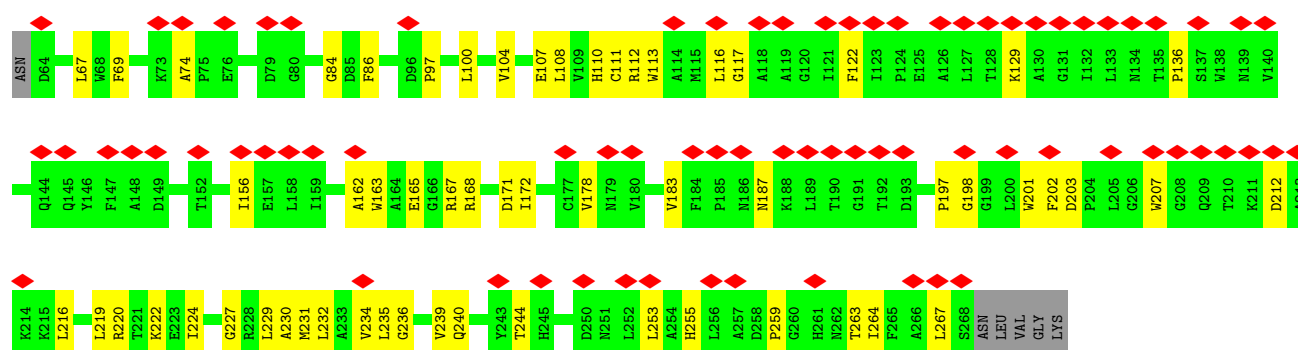
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  84% 16%



- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  36% 69% 28%



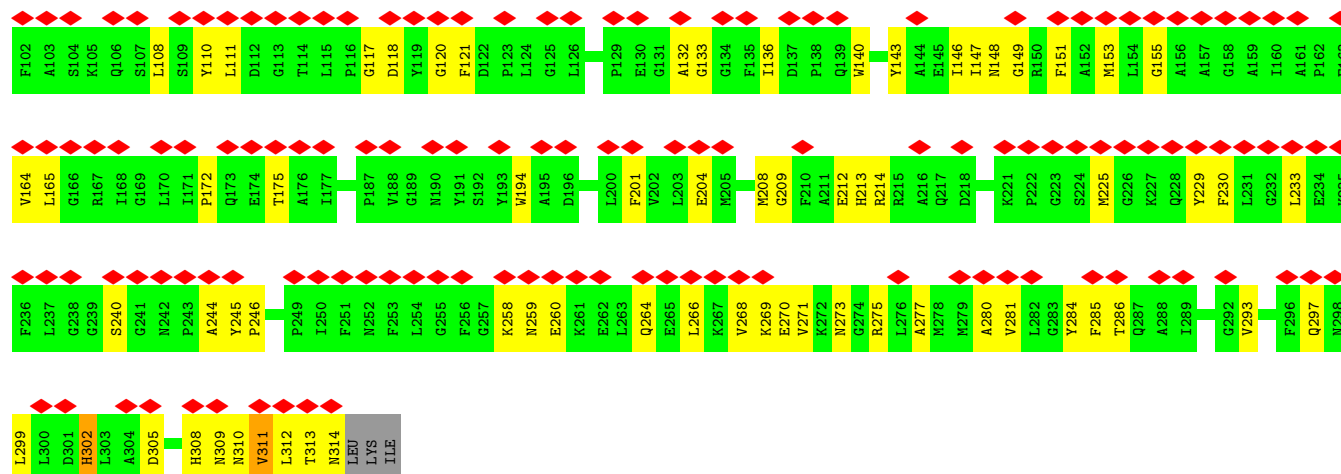
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 3:  89% 11%



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  62% 67% 31%



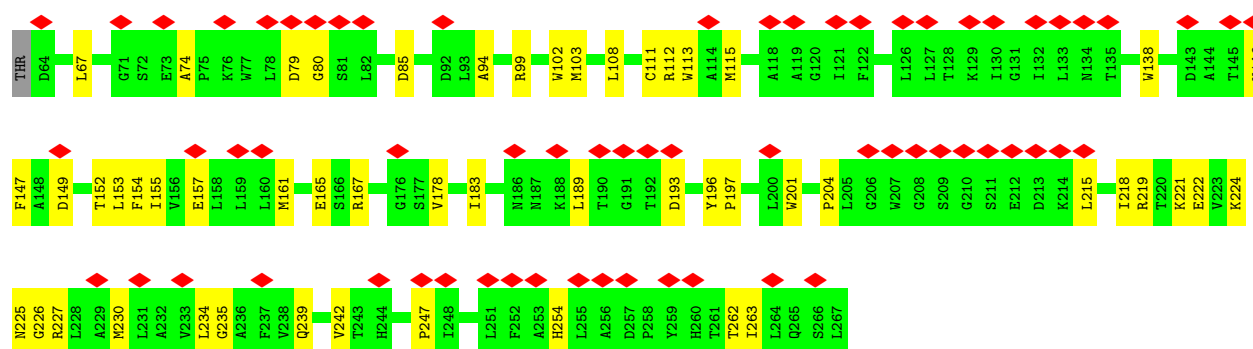
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:  85% 15%



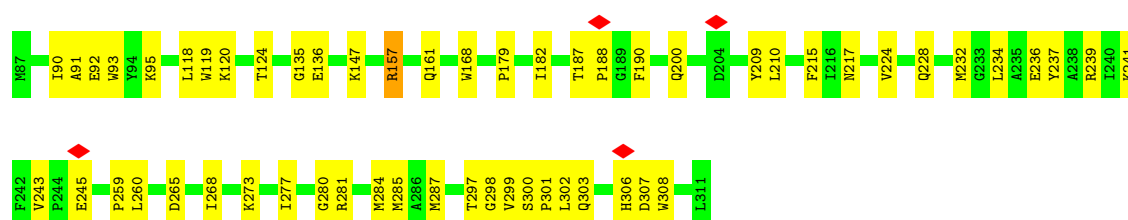
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  32% 74% 25%



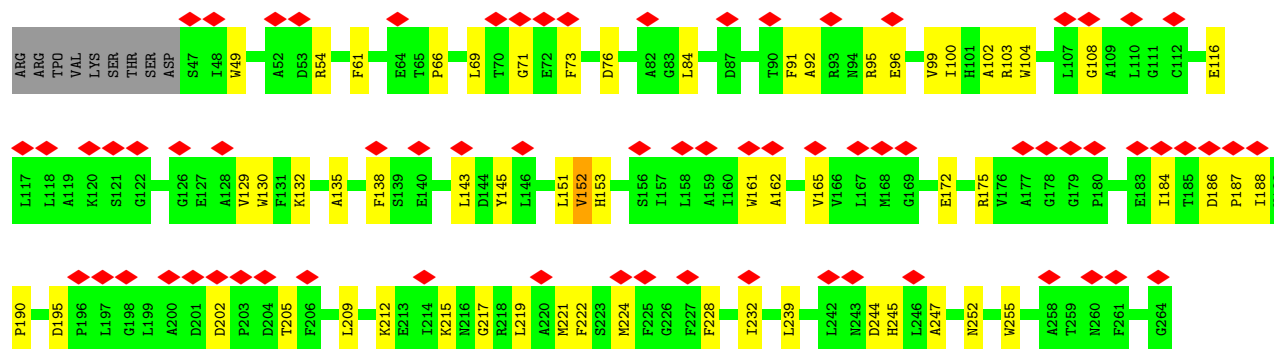
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9:  75% 24%

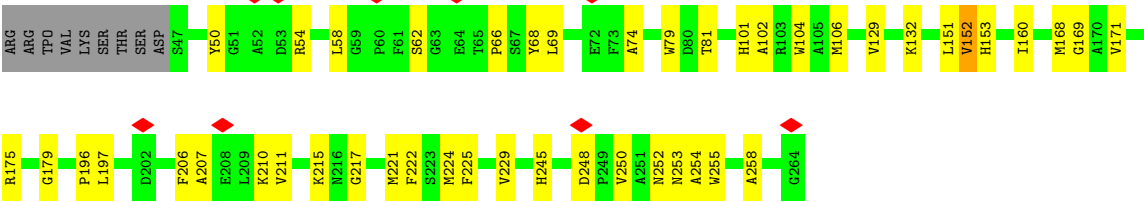
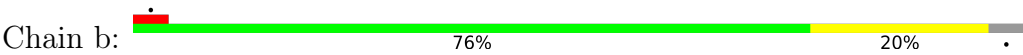


- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

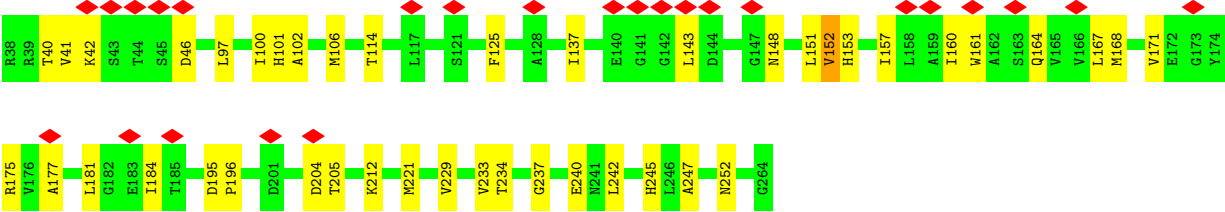
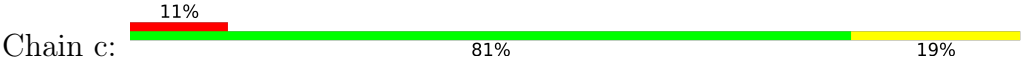
Chain a:  31% 70% 26%



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



● Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83777	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 ($e^-/\text{\AA}^2$)	78	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.400	Depositor
Minimum map value	-1.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	486.72003, 486.72003, 486.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: SF4, LMG, LHG, LMU, BCR, PQN, DGD, XAT, CLA, NEX, LUT, CHL, TPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/6031	0.33	0/8227
2	B	0.26	2/6063 (0.0%)	0.38	1/8274 (0.0%)
3	C	0.19	0/605	0.41	0/821
4	D	0.13	0/1132	0.38	1/1532 (0.1%)
5	E	0.12	0/498	0.23	0/677
6	F	0.15	0/1255	0.29	0/1696
7	G	0.20	0/767	0.38	0/1046
8	H	0.12	0/758	0.26	0/1022
9	I	0.15	0/273	0.37	0/373
10	J	0.14	0/334	0.25	0/457
11	K	0.13	0/572	0.23	0/773
12	L	0.14	0/1264	0.28	0/1727
13	M	0.24	0/239	0.26	0/322
14	O	0.17	0/729	0.37	0/997
15	1	0.20	0/1527	0.34	0/2088
15	5	0.18	0/1524	0.43	1/2084 (0.0%)
16	2	0.22	0/1683	0.41	0/2300
16	6	0.13	0/1638	0.31	0/2241
17	3	0.21	0/1721	0.40	0/2335
17	7	0.18	0/1695	0.39	0/2302
18	4	0.15	0/1641	0.29	0/2244
18	8	0.16	0/1634	0.31	0/2234
19	9	0.26	1/1801 (0.1%)	0.43	0/2451
20	a	0.18	0/1700	0.37	0/2316
20	b	0.15	0/1700	0.31	0/2316
20	c	0.14	0/1764	0.35	0/2399
All	All	0.19	3/40548 (0.0%)	0.35	3/55254 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	9	157	ARG	C-O	-6.48	1.16	1.24
2	B	177	HIS	CA-C	-5.34	1.46	1.52
2	B	308	HIS	CA-C	-5.26	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	PHE	CB-CA-C	9.86	119.59	109.83
4	D	173	LEU	N-CA-C	5.43	120.41	113.18
15	5	171	PHE	N-CA-C	-5.28	106.17	113.18

There are no chirality outliers.

There are no planarity outliers.

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	A	5836	0	5725	105	0
2	B	5849	0	5623	116	0
3	C	595	0	573	12	0
4	D	1104	0	1112	16	0
5	E	487	0	480	8	0
6	F	1230	0	1282	14	0
7	G	749	0	729	12	0
8	H	740	0	727	7	0
9	I	266	0	274	4	0
10	J	325	0	341	5	0
11	K	566	0	587	8	0
12	L	1229	0	1242	13	0
13	M	238	0	263	3	0
14	O	702	0	697	12	0
15	1	1478	0	1455	27	0
15	5	1475	0	1447	51	0
16	2	1632	0	1603	34	0
16	6	1587	0	1556	57	0
17	3	1670	0	1633	21	0
17	7	1644	0	1599	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	4	1592	0	1561	31	0
18	8	1585	0	1555	63	0
19	9	1747	0	1721	44	0
20	a	1651	0	1586	61	0
20	b	1651	0	1585	46	0
20	c	1727	0	1661	49	0
21	1	587	0	420	22	0
21	2	366	0	281	33	0
21	3	642	0	487	37	0
21	4	472	0	362	27	0
21	5	531	0	369	24	0
21	6	347	0	253	19	0
21	7	551	0	377	35	0
21	8	460	0	348	46	0
21	9	352	0	290	12	0
21	A	2422	0	2311	116	0
21	B	2312	0	2267	108	0
21	F	147	0	123	3	0
21	G	139	0	102	3	0
21	H	45	0	33	2	0
21	J	42	0	31	0	0
21	K	185	0	135	16	0
21	L	132	0	97	3	0
21	O	170	0	116	2	0
21	a	383	0	304	20	0
21	b	391	0	316	20	0
21	c	417	0	367	18	0
22	A	33	0	46	0	0
22	B	33	0	46	3	0
23	1	51	0	42	0	0
23	2	35	0	40	1	0
23	4	86	0	118	6	0
23	5	28	0	26	1	0
23	6	35	0	40	3	0
23	8	37	0	44	3	0
23	9	49	0	74	4	0
23	A	125	0	172	8	0
23	a	49	0	74	2	0
23	b	49	0	74	9	0
23	c	49	0	74	2	0
24	2	40	0	56	6	0
24	3	80	0	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	40	0	56	0	0
24	6	40	0	56	14	0
24	7	80	0	112	10	0
24	8	40	0	56	8	0
24	A	240	0	336	21	0
24	B	200	0	280	39	0
24	F	80	0	112	2	0
24	G	80	0	112	5	0
24	I	40	0	56	1	0
24	J	120	0	168	15	0
24	K	40	0	56	24	0
24	L	120	0	168	8	0
24	M	40	0	56	3	0
24	O	40	0	56	1	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	3	35	0	46	3	0
26	A	70	0	92	2	0
26	O	35	0	46	4	0
26	b	35	0	46	4	0
27	B	66	0	96	7	0
28	2	13	0	11	0	0
28	6	13	0	11	1	0
28	G	55	0	86	2	0
28	J	30	0	30	0	0
29	1	102	0	74	7	0
29	2	295	0	212	15	0
29	3	40	0	23	1	0
29	4	180	0	116	6	0
29	5	92	0	62	6	0
29	6	286	0	196	17	0
29	7	40	0	23	2	0
29	8	180	0	116	15	0
29	9	273	0	184	9	0
29	a	272	0	181	15	0
29	b	292	0	206	13	0
29	c	274	0	178	10	0
30	1	42	0	56	2	0
30	2	42	0	56	8	0
30	3	42	0	56	12	0
30	4	42	0	56	7	0
30	5	42	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	6	42	0	56	6	0
30	7	42	0	56	12	0
30	8	42	0	56	5	0
30	9	84	0	112	10	0
30	a	84	0	112	11	0
30	b	84	0	112	11	0
30	c	84	0	112	7	0
31	1	44	0	56	2	0
31	2	44	0	56	2	0
31	3	44	0	56	4	0
31	4	44	0	56	4	0
31	5	44	0	56	5	0
31	6	44	0	56	6	0
31	7	44	0	56	5	0
31	8	44	0	56	4	0
31	9	44	0	56	2	0
31	a	44	0	56	6	0
31	c	44	0	56	3	0
32	9	44	0	56	4	0
32	b	44	0	56	1	0
32	c	44	0	56	3	0
All	All	56417	0	54439	1292	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 12.

The worst 5 of 1292 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:409:CLA:C4	30:3:416:LUT:H28	1.47	1.43
21:A:852:CLA:O1D	21:B:801:CLA:H61	1.31	1.22
21:2:609:CLA:H43	30:2:616:LUT:H7	1.25	1.13
21:K:203:CLA:HMC2	24:K:205:BCR:H312	1.27	1.10
21:2:609:CLA:HBC2	21:2:609:CLA:HHD	1.30	1.10

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	A	740/742 (100%)	715 (97%)	25 (3%)	0	100	100
2	B	731/733 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	60/62 (97%)	60 (100%)	0	0	100	100
6	F	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
7	G	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
8	H	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
12	L	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	6
14	O	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
15	1	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
15	5	190/192 (99%)	176 (93%)	12 (6%)	2 (1%)	11	26
16	2	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
16	6	203/211 (96%)	199 (98%)	4 (2%)	0	100	100
17	3	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
17	7	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	24	45
18	4	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
18	8	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
19	9	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
20	a	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	24	45
20	b	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	24	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	c	224/227 (99%)	215 (96%)	8 (4%)	1 (0%)	30	51
All	All	5023/5104 (98%)	4800 (96%)	216 (4%)	7 (0%)	49	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	5	170	PRO
20	b	152	VAL
20	c	152	VAL
20	a	152	VAL
13	M	4	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/603 (100%)	602 (100%)	1 (0%)	87	95
2	B	595/595 (100%)	595 (100%)	0	100	100
3	C	67/67 (100%)	67 (100%)	0	100	100
4	D	115/115 (100%)	115 (100%)	0	100	100
5	E	52/52 (100%)	52 (100%)	0	100	100
6	F	129/129 (100%)	129 (100%)	0	100	100
7	G	78/78 (100%)	78 (100%)	0	100	100
8	H	77/77 (100%)	77 (100%)	0	100	100
9	I	30/30 (100%)	30 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	58 (100%)	0	100	100
12	L	126/126 (100%)	126 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
14	O	73/73 (100%)	73 (100%)	0	100	100
15	1	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	5	150/151 (99%)	149 (99%)	1 (1%)	76	89
16	2	168/168 (100%)	168 (100%)	0	100	100
16	6	163/168 (97%)	163 (100%)	0	100	100
17	3	169/169 (100%)	169 (100%)	0	100	100
17	7	166/169 (98%)	165 (99%)	1 (1%)	78	90
18	4	164/164 (100%)	164 (100%)	0	100	100
18	8	163/164 (99%)	162 (99%)	1 (1%)	78	90
19	9	179/179 (100%)	179 (100%)	0	100	100
20	a	165/173 (95%)	165 (100%)	0	100	100
20	b	165/173 (95%)	164 (99%)	1 (1%)	78	90
20	c	173/173 (100%)	173 (100%)	0	100	100
All	All	4041/4067 (99%)	4036 (100%)	5 (0%)	87	96

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

Mol	Chain	Res	Type
1	A	585	SER
15	5	115	GLN
17	7	302	HIS
18	8	165	GLU
20	b	68	TYR

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

Mol	Chain	Res	Type
16	6	187	ASN
19	9	105	GLN
16	6	240	GLN
16	6	261	HIS
20	b	153	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	$\# Z > 2$
20	TPO	c	40	20	8,10,11	1.58	1 (12%)	10,14,16	1.77	1 (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
20	TPO	c	40	20	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	40	TPO	P-O1P	3.35	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	40	TPO	P-OG1-CB	-4.89	108.44	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	c	40	TPO	CB-OG1-P-O2P
20	c	40	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

364 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	$\# Z > 2$
23	LHG	4	618	21	36,36,48	0.32	0	39,42,54	0.40	0
24	BCR	B	846	-	41,41,41	0.75	0	56,56,56	1.94	18 (32%)
21	CLA	1	304	15	59,63,73	1.35	9 (15%)	71,101,113	1.36	6 (8%)
29	CHL	4	607	-	55,59,74	2.14	18 (32%)	62,96,114	3.35	32 (51%)
21	CLA	A	802	-	56,60,73	1.39	9 (16%)	67,97,113	1.37	8 (11%)
21	CLA	c	603	20	59,63,73	1.35	8 (13%)	71,101,113	1.29	7 (9%)
29	CHL	8	605	18	45,49,74	2.28	18 (40%)	54,84,114	3.80	35 (64%)
21	CLA	5	607	-	47,52,73	1.51	7 (14%)	56,88,113	1.43	5 (8%)
23	LHG	1	319	21	27,27,48	0.35	0	30,33,54	0.47	0
21	CLA	a	611	-	51,55,73	1.45	7 (13%)	61,91,113	1.40	5 (8%)
21	CLA	a	614	20	45,49,73	1.53	8 (17%)	54,84,113	1.46	7 (12%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
23	LHG	A	845	21	26,26,48	0.33	0	29,32,54	0.44	0
29	CHL	4	606	-	50,54,74	2.28	18 (36%)	56,90,114	3.46	29 (51%)
21	CLA	7	408	-	45,49,73	1.52	6 (13%)	54,84,113	1.46	5 (9%)
21	CLA	a	604	-	50,55,73	1.46	8 (16%)	59,91,113	1.40	6 (10%)
29	CHL	2	605	-	50,54,74	2.28	18 (36%)	56,90,114	3.47	29 (51%)
29	CHL	4	605	-	45,49,74	2.27	18 (40%)	54,84,114	3.84	33 (61%)
29	CHL	6	602	-	57,61,74	2.14	18 (31%)	64,98,114	3.31	34 (53%)
21	CLA	8	609	23	49,53,73	1.70	9 (18%)	59,89,113	1.89	9 (15%)
21	CLA	5	611	15	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
29	CHL	c	608	20	50,54,74	2.30	20 (40%)	56,90,114	3.40	29 (51%)
21	CLA	A	803	-	56,60,73	1.37	9 (16%)	67,97,113	1.34	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	a	612	-	49,53,73	1.51	7 (14%)	59,89,113	1.43	5 (8%)
29	CHL	a	609	-	50,54,74	2.39	20 (40%)	56,90,114	3.36	29 (51%)
21	CLA	1	315	-	49,53,73	1.50	9 (18%)	59,89,113	1.45	6 (10%)
23	LHG	1	301	21	22,22,48	0.34	0	25,28,54	0.67	1 (4%)
29	CHL	6	601	16	48,52,74	2.39	20 (41%)	58,88,114	3.64	31 (53%)
31	XAT	1	318	-	39,47,47	1.67	8 (20%)	54,74,74	1.62	12 (22%)
21	CLA	K	203	11	48,52,73	1.55	11 (22%)	61,88,113	1.53	6 (9%)
21	CLA	A	840	1	69,73,73	1.22	9 (13%)	83,113,113	1.29	6 (7%)
21	CLA	A	832	1	49,53,73	1.46	8 (16%)	59,89,113	1.43	8 (13%)
30	LUT	9	614	-	42,43,43	1.63	8 (19%)	51,60,60	1.56	12 (23%)
21	CLA	b	304	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	5 (8%)
29	CHL	2	601	16	57,61,74	2.12	18 (31%)	64,98,114	3.30	34 (53%)
21	CLA	7	403	-	45,50,73	1.62	9 (20%)	57,86,113	1.52	7 (12%)
21	CLA	B	805	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)
21	CLA	3	408	17	63,67,73	1.32	9 (14%)	75,105,113	1.32	8 (10%)
21	CLA	5	608	15	44,48,73	1.59	8 (18%)	56,83,113	1.57	7 (12%)
21	CLA	7	414	-	43,48,73	1.56	8 (18%)	51,83,113	1.51	7 (13%)
26	LMU	b	301	-	36,36,36	0.37	0	47,47,47	0.76	0
21	CLA	A	809	1	63,67,73	1.29	9 (14%)	75,105,113	1.36	9 (12%)
29	CHL	9	606	19	50,54,74	2.28	19 (38%)	56,90,114	3.47	29 (51%)
21	CLA	B	813	-	47,52,73	1.49	8 (17%)	56,88,113	1.46	7 (12%)
21	CLA	A	841	1	69,73,73	1.25	9 (13%)	83,113,113	1.33	5 (6%)
21	CLA	A	830	1	56,60,73	1.57	9 (16%)	67,97,113	1.95	14 (20%)
21	CLA	8	603	-	47,52,73	1.53	8 (17%)	56,88,113	1.42	6 (10%)
29	CHL	6	607	-	55,59,74	2.23	20 (36%)	62,96,114	3.23	33 (53%)
29	CHL	8	607	-	55,59,74	2.18	19 (34%)	62,96,114	3.28	34 (54%)
30	LUT	c	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.57	11 (21%)
21	CLA	B	827	2	69,73,73	1.23	8 (11%)	83,113,113	1.23	6 (7%)
21	CLA	4	603	-	47,52,73	1.52	8 (17%)	56,88,113	1.42	6 (10%)
21	CLA	A	814	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	8 (9%)
22	PQN	A	843	-	34,34,34	0.39	0	42,45,45	0.43	0
21	CLA	7	401	17	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
21	CLA	1	306	-	43,48,73	1.54	8 (18%)	52,82,113	1.53	6 (11%)
21	CLA	B	820	2	50,54,73	1.46	8 (16%)	60,90,113	1.41	6 (10%)
21	CLA	2	609	16	55,59,73	1.49	7 (12%)	65,95,113	1.92	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	8	601	18	49,53,73	1.50	7 (14%)	59,89,113	1.42	5 (8%)
28	LMG	2	615	-	13,13,55	0.19	0	18,18,63	0.34	0
21	CLA	3	414	-	41,44,73	1.58	10 (24%)	49,77,113	1.49	5 (10%)
21	CLA	A	812	1	69,73,73	1.23	9 (13%)	83,113,113	1.24	8 (9%)
31	XAT	4	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.62	11 (20%)
21	CLA	1	314	15	41,46,73	1.66	10 (24%)	52,81,113	1.51	9 (17%)
21	CLA	B	819	2	47,51,73	1.48	10 (21%)	56,86,113	1.45	5 (8%)
29	CHL	5	606	15	50,54,74	2.33	20 (40%)	56,90,114	3.33	29 (51%)
30	LUT	5	615	-	42,43,43	1.67	8 (19%)	51,60,60	1.69	10 (19%)
23	LHG	A	844	-	48,48,48	0.27	0	51,54,54	0.35	0
30	LUT	b	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	9 (17%)
21	CLA	K	201	11	50,54,73	1.45	8 (16%)	60,90,113	1.44	4 (6%)
25	SF4	A	851	2,1	0,12,12	-	-	-	-	-
21	CLA	9	611	23	61,65,73	1.33	9 (14%)	73,103,113	1.34	6 (8%)
21	CLA	8	611	-	58,62,73	1.37	7 (12%)	69,99,113	1.33	6 (8%)
30	LUT	7	415	-	42,43,43	1.68	8 (19%)	51,60,60	1.77	13 (25%)
21	CLA	B	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
21	CLA	3	401	-	43,48,73	1.53	8 (18%)	51,83,113	1.59	7 (13%)
24	BCR	A	847	-	41,41,41	1.69	8 (19%)	56,56,56	1.39	9 (16%)
21	CLA	5	614	15	47,51,73	1.59	8 (17%)	60,87,113	1.51	6 (10%)
21	CLA	9	603	19	49,53,73	1.48	8 (16%)	59,89,113	1.47	4 (6%)
21	CLA	B	824	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	7 (8%)
21	CLA	B	840	23	69,73,73	1.23	8 (11%)	83,113,113	1.32	6 (7%)
22	PQN	B	841	-	34,34,34	0.40	0	42,45,45	0.37	0
21	CLA	A	808	1	49,53,73	1.47	8 (16%)	59,89,113	1.48	7 (11%)
21	CLA	B	815	2	57,62,73	1.37	10 (17%)	68,100,113	1.33	7 (10%)
24	BCR	A	849	-	41,41,41	1.70	8 (19%)	56,56,56	1.71	12 (21%)
21	CLA	A	835	1	54,58,73	1.38	7 (12%)	65,95,113	1.42	6 (9%)
21	CLA	O	202	-	40,46,73	1.61	9 (22%)	48,80,113	1.52	7 (14%)
21	CLA	2	603	16	49,53,73	1.50	9 (18%)	59,89,113	1.39	5 (8%)
21	CLA	2	608	16	59,63,73	1.33	8 (13%)	71,101,113	1.31	6 (8%)
21	CLA	6	608	16	49,53,73	1.50	7 (14%)	59,89,113	1.40	4 (6%)
21	CLA	8	608	18	47,51,73	1.62	10 (21%)	54,86,113	1.39	3 (5%)
21	CLA	b	303	20	63,67,73	1.32	8 (12%)	75,105,113	1.30	6 (8%)
21	CLA	1	316	15	47,51,73	1.59	10 (21%)	60,87,113	1.52	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	G	204	7	47,52,73	1.52	7 (14%)	56,88,113	1.44	4 (7%)
24	BCR	B	843	-	41,41,41	0.76	0	56,56,56	2.53	24 (42%)
21	CLA	B	817	2	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
21	CLA	G	203	7	54,58,73	1.42	9 (16%)	65,95,113	1.39	7 (10%)
21	CLA	b	315	20	49,53,73	1.49	8 (16%)	59,89,113	1.38	5 (8%)
21	CLA	4	604	-	47,51,73	1.49	8 (17%)	55,86,113	1.44	5 (9%)
24	BCR	B	844	-	41,41,41	0.71	0	56,56,56	2.10	22 (39%)
21	CLA	A	829	1	69,73,73	1.24	8 (11%)	83,113,113	1.22	6 (7%)
21	CLA	B	829	2	49,53,73	1.51	7 (14%)	59,89,113	1.55	6 (10%)
24	BCR	A	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.36	8 (14%)
21	CLA	A	822	1	48,52,73	1.50	9 (18%)	58,88,113	1.50	5 (8%)
21	CLA	c	602	20	64,68,73	1.30	10 (15%)	77,107,113	1.29	7 (9%)
21	CLA	8	612	18	47,51,73	1.50	7 (14%)	56,86,113	1.41	5 (8%)
21	CLA	L	302	12	49,53,73	1.48	9 (18%)	59,89,113	1.49	6 (10%)
24	BCR	O	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.67	11 (19%)
31	XAT	2	617	-	39,47,47	1.65	8 (20%)	54,74,74	1.60	11 (20%)
30	LUT	4	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.75	10 (19%)
24	BCR	L	306	-	41,41,41	1.72	8 (19%)	56,56,56	1.78	11 (19%)
21	CLA	c	613	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	4 (4%)
21	CLA	B	809	2	65,70,73	1.29	9 (13%)	77,109,113	1.26	5 (6%)
21	CLA	J	102	10	46,50,73	1.49	9 (19%)	55,85,113	1.45	5 (9%)
21	CLA	3	410	-	43,48,73	1.56	8 (18%)	51,83,113	1.46	6 (11%)
21	CLA	7	410	-	47,51,73	1.50	7 (14%)	56,86,113	1.43	4 (7%)
24	BCR	M	101	-	41,41,41	1.77	8 (19%)	56,56,56	1.83	12 (21%)
21	CLA	5	612	15	49,53,73	1.51	8 (16%)	59,89,113	1.44	5 (8%)
21	CLA	8	604	-	47,51,73	1.51	8 (17%)	55,86,113	1.46	6 (10%)
21	CLA	9	613	19	57,61,73	1.37	8 (14%)	68,98,113	1.40	6 (8%)
21	CLA	B	810	2	58,62,73	1.42	10 (17%)	73,100,113	1.40	8 (10%)
21	CLA	7	409	-	43,48,73	1.57	7 (16%)	51,83,113	1.50	5 (9%)
21	CLA	B	812	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	7 (8%)
21	CLA	4	601	18	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
29	CHL	2	602	16	57,61,74	2.14	18 (31%)	64,98,114	3.32	33 (51%)
21	CLA	c	612	20	48,52,73	1.49	8 (16%)	56,87,113	1.41	5 (8%)
21	CLA	A	833	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
21	CLA	B	833	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	K	204	11	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
21	CLA	F	304	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	8 (13%)
21	CLA	a	610	20	49,53,73	1.48	8 (16%)	59,89,113	1.44	5 (8%)
29	CHL	1	302	15	55,59,74	2.17	17 (30%)	62,96,114	3.31	33 (53%)
29	CHL	6	605	-	50,54,74	2.30	19 (38%)	56,90,114	3.46	30 (53%)
21	CLA	4	610	23	49,53,73	1.47	8 (16%)	59,89,113	1.46	4 (6%)
21	CLA	3	415	17	43,48,73	1.54	8 (18%)	51,83,113	1.44	6 (11%)
24	BCR	F	303	-	41,41,41	1.72	8 (19%)	56,56,56	1.50	11 (19%)
24	BCR	J	103	-	41,41,41	1.76	8 (19%)	56,56,56	1.58	11 (19%)
21	CLA	A	815	-	49,53,73	1.47	8 (16%)	59,89,113	1.47	7 (11%)
21	CLA	B	832	2	60,64,73	1.33	10 (16%)	72,102,113	1.42	9 (12%)
21	CLA	A	804	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	7 (8%)
21	CLA	B	828	2	56,60,73	1.38	10 (17%)	67,97,113	1.37	7 (10%)
21	CLA	7	402	17	49,53,73	1.50	8 (16%)	59,89,113	1.42	4 (6%)
21	CLA	6	609	-	46,50,73	1.50	9 (19%)	55,85,113	1.54	7 (12%)
21	CLA	6	612	16	49,53,73	1.52	6 (12%)	59,89,113	1.47	5 (8%)
21	CLA	A	805	1	59,63,73	1.34	9 (15%)	71,101,113	1.33	6 (8%)
21	CLA	B	822	2	49,53,73	1.48	10 (20%)	59,89,113	1.47	4 (6%)
21	CLA	c	610	20	49,53,73	1.47	7 (14%)	59,89,113	1.45	8 (13%)
26	LMU	A	853	-	36,36,36	0.39	0	47,47,47	0.80	1 (2%)
29	CHL	c	607	-	50,54,74	2.34	20 (40%)	56,90,114	3.36	30 (53%)
21	CLA	G	202	-	49,53,73	1.47	8 (16%)	59,89,113	1.51	5 (8%)
29	CHL	9	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.46	28 (50%)
24	BCR	8	616	-	41,41,41	1.75	8 (19%)	56,56,56	1.49	9 (16%)
21	CLA	3	402	17	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
21	CLA	4	608	18	47,51,73	1.59	9 (19%)	54,86,113	1.40	4 (7%)
24	BCR	6	618	-	41,41,41	1.73	8 (19%)	56,56,56	1.65	10 (17%)
21	CLA	A	823	1	60,64,73	1.35	10 (16%)	72,102,113	1.32	7 (9%)
21	CLA	A	834	1	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
21	CLA	4	611	18	48,52,73	1.51	8 (16%)	58,88,113	1.47	5 (8%)
21	CLA	a	603	20	45,49,73	1.52	8 (17%)	54,84,113	1.49	6 (11%)
29	CHL	a	601	20	50,54,74	2.35	20 (40%)	56,90,114	3.36	28 (50%)
21	CLA	1	308	-	47,52,73	1.52	9 (19%)	56,88,113	1.46	6 (10%)
29	CHL	b	309	-	53,57,74	2.20	17 (32%)	59,93,114	3.39	31 (52%)
24	BCR	2	618	-	41,41,41	1.71	8 (19%)	56,56,56	1.55	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	7	418	-	41,41,41	1.73	8 (19%)	56,56,56	1.98	12 (21%)
21	CLA	A	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
32	NEX	b	318	-	38,46,46	1.61	7 (18%)	50,70,70	1.59	8 (16%)
24	BCR	K	205	-	41,41,41	0.74	0	56,56,56	2.13	19 (33%)
21	CLA	F	302	-	65,69,73	1.28	9 (13%)	78,108,113	1.35	8 (10%)
21	CLA	A	801	1	56,60,73	1.76	9 (16%)	67,97,113	2.15	17 (25%)
21	CLA	3	403	17	59,63,73	1.37	9 (15%)	71,101,113	1.34	4 (5%)
21	CLA	4	602	18	61,66,73	1.32	8 (13%)	72,104,113	1.34	8 (11%)
21	CLA	B	821	2	59,63,73	1.33	8 (13%)	71,101,113	1.38	6 (8%)
24	BCR	G	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	10 (17%)
24	BCR	A	850	-	41,41,41	1.70	8 (19%)	56,56,56	1.78	9 (16%)
21	CLA	A	807	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	4 (4%)
21	CLA	6	604	-	49,53,73	1.50	7 (14%)	59,89,113	1.40	4 (6%)
21	CLA	3	406	17	43,48,73	1.61	10 (23%)	54,83,113	1.53	7 (12%)
24	BCR	F	301	-	41,41,41	1.67	8 (19%)	56,56,56	1.56	9 (16%)
31	XAT	a	618	-	39,47,47	1.68	8 (20%)	54,74,74	1.77	11 (20%)
24	BCR	A	846	-	41,41,41	1.71	8 (19%)	56,56,56	1.63	9 (16%)
28	LMG	J	105	-	30,30,55	0.26	0	38,38,63	0.35	0
30	LUT	a	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.57	10 (19%)
21	CLA	A	819	1	69,73,73	1.24	9 (13%)	83,113,113	1.27	7 (8%)
21	CLA	A	818	1	56,60,73	1.43	10 (17%)	67,97,113	1.41	8 (11%)
29	CHL	b	310	-	55,60,74	2.17	19 (34%)	61,97,114	3.28	32 (52%)
29	CHL	6	606	-	50,54,74	2.29	19 (38%)	56,90,114	3.43	30 (53%)
29	CHL	8	606	-	50,54,74	2.35	20 (40%)	56,90,114	3.30	28 (50%)
23	LHG	c	619	21	48,48,48	0.26	0	51,54,54	0.31	0
30	LUT	8	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.68	9 (17%)
21	CLA	A	813	1	58,62,73	1.34	9 (15%)	69,99,113	1.44	6 (8%)
21	CLA	B	806	2	67,71,73	1.25	8 (11%)	80,110,113	1.30	6 (7%)
21	CLA	A	817	1	69,73,73	1.22	8 (11%)	83,113,113	1.31	6 (7%)
29	CHL	2	607	-	55,59,74	2.17	18 (32%)	62,96,114	3.35	32 (51%)
21	CLA	A	825	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
21	CLA	6	613	16	46,50,73	1.52	8 (17%)	55,85,113	1.45	6 (10%)
21	CLA	5	613	15	41,46,73	1.67	8 (19%)	52,81,113	1.56	7 (13%)
29	CHL	9	601	19	47,51,74	2.31	19 (40%)	52,86,114	3.49	29 (55%)
21	CLA	B	825	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	816	1	46,50,73	1.48	8 (17%)	55,85,113	1.46	7 (12%)
31	XAT	c	617	-	39,47,47	1.67	8 (20%)	54,74,74	1.66	10 (18%)
29	CHL	a	606	-	50,54,74	2.32	19 (38%)	56,90,114	3.38	30 (53%)
24	BCR	L	305	-	41,41,41	1.71	8 (19%)	56,56,56	1.46	8 (14%)
21	CLA	7	407	17	47,52,73	2.29	13 (27%)	56,88,113	3.75	20 (35%)
24	BCR	3	419	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	12 (21%)
21	CLA	9	612	19	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
21	CLA	7	404	-	44,49,73	1.55	8 (18%)	52,84,113	1.47	4 (7%)
23	LHG	5	617	-	27,27,48	0.35	0	30,33,54	0.44	0
31	XAT	8	615	-	39,47,47	1.71	8 (20%)	54,74,74	1.67	9 (16%)
21	CLA	8	618	-	45,49,73	1.52	8 (17%)	54,84,113	1.49	7 (12%)
21	CLA	4	612	18	59,63,73	1.36	8 (13%)	71,101,113	1.34	7 (9%)
21	CLA	B	839	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
21	CLA	5	605	-	43,48,73	1.56	9 (20%)	52,82,113	1.47	6 (11%)
21	CLA	7	411	-	57,62,73	1.39	7 (12%)	68,100,113	1.30	7 (10%)
21	CLA	B	803	2	59,63,73	1.34	9 (15%)	71,101,113	1.36	6 (8%)
21	CLA	5	610	-	41,46,73	1.66	9 (21%)	52,81,113	1.60	8 (15%)
21	CLA	b	314	20	57,61,73	1.38	9 (15%)	68,98,113	1.38	7 (10%)
29	CHL	b	308	-	57,61,74	2.14	18 (31%)	64,98,114	3.33	34 (53%)
29	CHL	b	302	20	50,54,74	2.32	20 (40%)	56,90,114	3.32	27 (48%)
21	CLA	B	836	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	7 (8%)
29	CHL	3	407	-	43,48,74	2.36	16 (37%)	51,83,114	3.51	30 (58%)
21	CLA	5	603	15	49,53,73	1.50	9 (18%)	59,89,113	1.39	5 (8%)
24	BCR	G	201	-	41,41,41	1.70	8 (19%)	56,56,56	1.53	9 (16%)
21	CLA	6	611	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	6 (11%)
29	CHL	2	614	-	50,54,74	2.27	19 (38%)	56,90,114	3.44	30 (53%)
29	CHL	6	614	-	50,54,74	2.35	20 (40%)	56,90,114	3.32	30 (53%)
21	CLA	7	405	17	43,48,73	1.63	8 (18%)	54,83,113	1.54	7 (12%)
24	BCR	3	418	-	41,41,41	1.69	8 (19%)	56,56,56	1.47	9 (16%)
21	CLA	c	611	23	62,66,73	1.31	9 (14%)	74,104,113	1.33	6 (8%)
21	CLA	7	413	-	41,44,73	1.60	8 (19%)	49,77,113	1.46	6 (12%)
21	CLA	c	614	20	49,53,73	1.49	9 (18%)	59,89,113	1.35	5 (8%)
23	LHG	6	619	-	34,34,48	0.31	0	37,40,54	0.37	0
29	CHL	9	605	19	50,54,74	2.32	20 (40%)	56,90,114	3.41	29 (51%)
21	CLA	B	826	2	56,60,73	1.37	9 (16%)	67,97,113	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	5	604	-	53,57,73	1.43	7 (13%)	62,93,113	1.41	5 (8%)
23	LHG	8	617	21	36,36,48	0.31	0	39,42,54	0.36	0
29	CHL	7	406	-	43,48,74	2.51	20 (46%)	51,83,114	3.62	28 (54%)
21	CLA	a	602	-	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
21	CLA	A	820	1	48,52,73	1.51	9 (18%)	58,88,113	1.47	5 (8%)
21	CLA	1	311	23	41,46,73	1.65	9 (21%)	52,81,113	1.58	8 (15%)
26	LMU	A	856	-	36,36,36	0.38	0	47,47,47	0.74	1 (2%)
21	CLA	B	831	2	60,64,73	1.34	8 (13%)	72,102,113	1.32	9 (12%)
21	CLA	6	603	16	49,53,73	1.51	7 (14%)	59,89,113	1.45	5 (8%)
23	LHG	a	617	-	48,48,48	0.26	0	51,54,54	0.35	0
29	CHL	b	307	-	50,54,74	2.28	18 (36%)	56,90,114	3.49	28 (50%)
21	CLA	A	824	1	59,63,73	1.35	9 (15%)	71,101,113	1.35	7 (9%)
21	CLA	B	804	2	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
21	CLA	H	201	8	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
21	CLA	c	604	-	49,53,73	1.49	9 (18%)	59,89,113	1.47	5 (8%)
30	LUT	b	317	-	42,43,43	1.62	8 (19%)	51,60,60	1.55	10 (19%)
29	CHL	a	607	-	47,51,74	2.27	18 (38%)	52,86,114	3.57	30 (57%)
23	LHG	A	855	-	48,48,48	0.27	0	51,54,54	0.37	0
29	CHL	1	307	15	55,59,74	2.17	18 (32%)	62,96,114	3.38	33 (53%)
21	CLA	1	303	15	65,69,73	1.28	9 (13%)	78,108,113	1.33	6 (7%)
21	CLA	1	310	15	46,51,73	1.51	9 (19%)	55,87,113	1.44	6 (10%)
21	CLA	9	610	19	58,62,73	1.35	9 (15%)	69,99,113	1.36	8 (11%)
21	CLA	3	409	17	56,60,73	1.59	10 (17%)	67,97,113	2.11	18 (26%)
21	CLA	A	811	-	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
21	CLA	a	613	-	61,65,73	1.34	7 (11%)	73,103,113	1.34	8 (10%)
21	CLA	A	828	1	64,68,73	1.28	9 (14%)	77,107,113	1.24	8 (10%)
21	CLA	A	852	-	56,60,73	1.38	9 (16%)	67,97,113	1.35	9 (13%)
29	CHL	9	607	-	50,54,74	2.29	18 (36%)	56,90,114	3.41	28 (50%)
21	CLA	O	201	23	46,50,73	1.48	9 (19%)	55,85,113	1.49	5 (9%)
24	BCR	L	301	-	41,41,41	1.69	8 (19%)	56,56,56	1.43	9 (16%)
21	CLA	K	202	-	54,58,73	1.40	8 (14%)	65,95,113	1.53	10 (15%)
21	CLA	A	842	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
21	CLA	5	602	15	65,69,73	1.29	8 (12%)	78,108,113	1.29	6 (7%)
21	CLA	1	312	15	49,53,73	1.50	9 (18%)	59,89,113	1.41	5 (8%)
21	CLA	A	810	1	49,53,73	1.47	9 (18%)	59,89,113	1.47	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	J	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	10 (17%)
21	CLA	2	611	16	45,49,73	1.51	8 (17%)	54,84,113	1.51	8 (14%)
30	LUT	3	416	-	42,43,43	1.64	7 (16%)	51,60,60	1.68	11 (21%)
26	LMU	O	206	-	36,36,36	0.40	0	47,47,47	0.69	0
29	CHL	c	609	20	47,52,74	2.41	20 (42%)	53,88,114	3.27	26 (49%)
31	XAT	3	417	-	39,47,47	1.67	8 (20%)	54,74,74	1.60	9 (16%)
29	CHL	4	614	18	46,50,74	2.37	17 (36%)	51,85,114	3.62	29 (56%)
21	CLA	B	801	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	31 (37%)
21	CLA	1	313	15	49,53,73	1.48	9 (18%)	59,89,113	1.45	7 (11%)
26	LMU	3	420	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
31	XAT	5	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.56	8 (14%)
30	LUT	9	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.59	11 (21%)
21	CLA	b	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	4 (6%)
21	CLA	L	304	-	46,50,73	1.49	9 (19%)	55,85,113	1.46	5 (9%)
21	CLA	3	405	-	44,49,73	1.53	10 (22%)	52,84,113	1.49	4 (7%)
21	CLA	4	609	18	56,60,73	1.66	11 (19%)	67,97,113	2.17	16 (23%)
21	CLA	B	808	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
21	CLA	b	313	20	49,53,73	1.49	9 (18%)	59,89,113	1.40	6 (10%)
21	CLA	1	305	-	53,57,73	1.42	9 (16%)	62,93,113	1.42	7 (11%)
29	CHL	a	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.44	30 (53%)
21	CLA	A	839	1	49,53,73	1.50	9 (18%)	59,89,113	1.48	5 (8%)
23	LHG	4	619	-	48,48,48	0.28	0	51,54,54	0.62	1 (1%)
32	NEX	c	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.61	9 (18%)
21	CLA	B	814	2	64,68,73	1.30	9 (14%)	77,107,113	1.36	6 (7%)
32	NEX	9	617	-	38,46,46	1.61	7 (18%)	50,70,70	1.60	8 (16%)
21	CLA	B	816	2	56,60,73	1.39	10 (17%)	67,97,113	1.44	7 (10%)
24	BCR	B	842	-	41,41,41	1.71	8 (19%)	56,56,56	1.44	8 (14%)
31	XAT	9	616	-	39,47,47	1.73	8 (20%)	54,74,74	2.33	15 (27%)
21	CLA	7	412	-	43,48,73	1.61	6 (13%)	51,83,113	1.47	6 (11%)
30	LUT	1	317	-	42,43,43	1.69	8 (19%)	51,60,60	1.70	9 (17%)
21	CLA	B	823	-	69,73,73	1.25	9 (13%)	83,113,113	1.39	7 (8%)
24	BCR	7	417	-	41,41,41	1.73	8 (19%)	56,56,56	1.52	9 (16%)
21	CLA	B	835	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	9 (10%)
21	CLA	B	807	2	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
29	CHL	c	601	20	53,57,74	2.20	17 (32%)	59,93,114	3.39	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	9	618	21	48,48,48	0.27	0	51,54,54	0.33	0
21	CLA	B	811	2	49,53,73	1.53	9 (18%)	59,89,113	1.54	5 (8%)
21	CLA	9	602	19	57,61,73	1.38	10 (17%)	68,98,113	1.38	7 (10%)
21	CLA	2	612	16	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
21	CLA	8	602	18	61,66,73	1.33	7 (11%)	72,104,113	1.30	8 (11%)
21	CLA	9	604	-	49,53,73	1.48	10 (20%)	59,89,113	1.48	6 (10%)
24	BCR	J	104	-	41,41,41	0.92	1 (2%)	56,56,56	2.29	20 (35%)
29	CHL	2	606	-	50,54,74	2.25	18 (36%)	56,90,114	3.46	29 (51%)
21	CLA	3	412	17	57,62,73	1.38	9 (15%)	68,100,113	1.31	6 (8%)
21	CLA	3	404	-	45,50,73	1.60	10 (22%)	57,86,113	1.55	8 (14%)
21	CLA	O	204	-	43,48,73	1.56	7 (16%)	51,83,113	1.41	5 (9%)
21	CLA	B	838	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
28	LMG	6	615	-	13,13,55	0.20	0	18,18,63	0.49	0
24	BCR	4	617	-	41,41,41	1.72	8 (19%)	56,56,56	1.46	9 (16%)
31	XAT	7	416	-	39,47,47	1.70	8 (20%)	54,74,74	1.70	12 (22%)
21	CLA	A	806	1	69,73,73	1.23	10 (14%)	83,113,113	1.30	4 (4%)
21	CLA	2	604	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	6 (10%)
27	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	0.98	3 (3%)
21	CLA	L	303	-	49,53,73	1.47	8 (16%)	59,89,113	1.48	7 (11%)
21	CLA	A	838	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	8 (9%)
21	CLA	O	203	-	53,58,73	1.39	8 (15%)	65,94,113	1.39	7 (10%)
24	BCR	A	854	-	41,41,41	1.69	8 (19%)	56,56,56	1.44	8 (14%)
28	LMG	G	206	-	55,55,55	0.21	0	63,63,63	0.26	0
29	CHL	9	609	-	50,54,74	2.29	19 (38%)	56,90,114	3.48	31 (55%)
21	CLA	B	834	-	49,53,73	1.46	8 (16%)	59,89,113	1.49	9 (15%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
24	BCR	I	101	-	41,41,41	1.73	8 (19%)	56,56,56	1.49	10 (17%)
29	CHL	c	605	-	46,51,74	2.35	19 (41%)	53,86,114	3.53	27 (50%)
30	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	12 (23%)
30	LUT	6	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.66	12 (23%)
21	CLA	A	837	1	55,59,73	1.42	9 (16%)	66,96,113	1.30	7 (10%)
29	CHL	8	613	-	46,50,74	2.41	19 (41%)	51,85,114	3.47	28 (54%)
21	CLA	B	837	2	67,72,73	1.25	8 (11%)	80,112,113	1.28	5 (6%)
21	CLA	F	305	6	45,49,73	1.50	9 (20%)	54,84,113	1.49	5 (9%)
24	BCR	B	845	-	41,41,41	1.71	8 (19%)	56,56,56	1.48	8 (14%)
23	LHG	b	319	21	48,48,48	0.27	0	51,54,54	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	b	311	20	58,62,73	1.35	8 (13%)	69,99,113	1.36	9 (13%)
21	CLA	A	836	1	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
29	CHL	c	606	20	50,54,74	2.31	20 (40%)	56,90,114	3.36	29 (51%)
30	LUT	c	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.50	10 (19%)
29	CHL	a	605	20	48,53,74	2.38	20 (41%)	53,89,114	3.35	28 (52%)
21	CLA	A	827	1	67,72,73	1.26	7 (10%)	80,112,113	1.30	6 (7%)
21	CLA	2	613	16	46,50,73	1.50	9 (19%)	55,85,113	1.45	6 (10%)
31	XAT	6	617	-	39,47,47	1.73	8 (20%)	54,74,74	1.79	12 (22%)
21	CLA	A	831	1	59,63,73	1.34	9 (15%)	71,101,113	1.40	6 (8%)
29	CHL	5	601	15	50,54,74	2.27	18 (36%)	56,90,114	3.43	30 (53%)
21	CLA	4	613	18	47,51,73	1.48	9 (19%)	56,86,113	1.43	6 (10%)
23	LHG	2	619	21	34,34,48	0.33	0	37,40,54	0.41	0
29	CHL	b	306	20	50,54,74	2.32	20 (40%)	56,90,114	3.39	29 (51%)
21	CLA	A	821	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	9 (10%)
21	CLA	3	411	17	47,51,73	1.49	9 (19%)	56,86,113	1.43	5 (8%)
21	CLA	8	610	-	48,52,73	1.52	8 (16%)	58,88,113	1.44	5 (8%)
21	CLA	b	312	23	49,53,73	1.49	6 (12%)	59,89,113	1.41	4 (6%)
21	CLA	1	309	15	45,49,73	1.64	9 (20%)	54,84,113	2.16	17 (31%)
21	CLA	B	830	2	60,64,73	1.33	9 (15%)	72,102,113	1.30	7 (9%)
21	CLA	B	818	-	62,66,73	1.31	10 (16%)	74,104,113	1.33	6 (8%)
21	CLA	5	609	-	46,51,73	1.54	9 (19%)	55,87,113	1.43	5 (9%)
21	CLA	2	610	23	45,50,73	1.51	8 (17%)	56,85,113	1.47	5 (8%)
21	CLA	6	610	-	45,50,73	1.54	8 (17%)	56,85,113	1.43	5 (8%)
21	CLA	3	413	17	43,48,73	1.55	8 (18%)	51,83,113	1.46	5 (9%)
30	LUT	a	615	-	42,43,43	1.64	7 (16%)	51,60,60	1.63	10 (19%)

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
23	LHG	4	618	21	-	9/41/41/53	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
21	CLA	1	304	15	-	5/27/103/115	-
29	CHL	4	607	-	-	4/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	802	-	-	3/24/100/115	-
21	CLA	c	603	20	-	6/27/103/115	-
29	CHL	8	605	18	-	4/10/86/117	-
21	CLA	5	607	-	-	4/13/89/115	-
23	LHG	1	319	21	-	7/32/32/53	-
21	CLA	a	611	-	-	8/18/94/115	-
21	CLA	a	614	20	-	4/10/86/115	-
25	SF4	C	101	3	-	-	0/6/5/5
23	LHG	A	845	21	-	6/31/31/53	-
29	CHL	4	606	-	-	4/17/93/117	-
21	CLA	7	408	-	-	4/10/86/115	-
21	CLA	a	604	-	-	10/17/93/115	-
29	CHL	2	605	-	-	3/17/93/117	-
29	CHL	4	605	-	-	2/10/86/117	-
29	CHL	6	602	-	-	9/26/102/117	-
21	CLA	8	609	23	-	6/15/91/115	-
21	CLA	5	611	15	-	5/15/91/115	-
29	CHL	c	608	20	-	7/17/93/117	-
21	CLA	A	803	-	-	7/24/100/115	-
21	CLA	a	612	-	-	7/15/91/115	-
29	CHL	a	609	-	-	5/17/93/117	-
21	CLA	1	315	-	-	6/15/91/115	-
23	LHG	1	301	21	-	7/26/26/53	-
29	CHL	6	601	16	-	6/13/89/117	-
31	XAT	1	318	-	-	0/31/93/93	0/4/4/4
21	CLA	K	203	11	-	2/13/89/115	-
21	CLA	A	840	1	-	16/39/115/115	-
21	CLA	A	832	1	-	5/15/91/115	-
30	LUT	9	614	-	-	2/29/67/67	0/2/2/2
21	CLA	b	304	-	-	4/15/91/115	-
29	CHL	2	601	16	-	10/26/102/117	-
21	CLA	7	403	-	-	2/9/85/115	-
21	CLA	B	805	-	-	19/39/115/115	-
21	CLA	3	408	17	-	7/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	608	15	-	4/8/84/115	-
21	CLA	7	414	-	-	2/8/84/115	-
26	LMU	b	301	-	-	6/21/61/61	0/2/2/2
21	CLA	A	809	1	-	5/32/108/115	-
29	CHL	9	606	19	-	6/17/93/117	-
21	CLA	B	813	-	-	2/13/89/115	-
21	CLA	A	841	1	-	18/39/115/115	-
21	CLA	A	830	1	-	4/24/100/115	-
21	CLA	8	603	-	-	4/13/89/115	-
29	CHL	6	607	-	-	5/23/99/117	-
29	CHL	8	607	-	-	5/23/99/117	-
30	LUT	c	616	-	-	0/29/67/67	0/2/2/2
21	CLA	B	827	2	-	12/39/115/115	-
21	CLA	4	603	-	-	6/13/89/115	-
21	CLA	A	814	1	-	10/39/115/115	-
22	PQN	A	843	-	-	1/23/43/43	0/2/2/2
21	CLA	7	401	17	-	8/15/91/115	-
21	CLA	1	306	-	-	4/10/82/115	-
21	CLA	B	820	2	-	5/17/93/115	-
21	CLA	2	609	16	-	9/22/98/115	-
21	CLA	8	601	18	-	11/15/91/115	-
28	LMG	2	615	-	-	1/4/24/70	0/1/1/1
21	CLA	3	414	-	-	2/2/74/115	-
21	CLA	A	812	1	-	6/39/115/115	-
31	XAT	4	616	-	-	0/31/93/93	0/4/4/4
21	CLA	1	314	15	-	2/4/80/115	-
21	CLA	B	819	2	-	4/13/89/115	-
29	CHL	5	606	15	-	5/17/93/117	-
30	LUT	5	615	-	-	7/29/67/67	0/2/2/2
23	LHG	A	844	-	-	10/53/53/53	-
30	LUT	b	316	-	-	2/29/67/67	0/2/2/2
21	CLA	K	201	11	-	6/17/93/115	-
25	SF4	A	851	2,1	-	-	0/6/5/5
21	CLA	9	611	23	-	9/30/106/115	-
21	CLA	8	611	-	-	15/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LUT	7	415	-	-	6/29/67/67	0/2/2/2
21	CLA	B	802	-	-	21/39/115/115	-
21	CLA	3	401	-	-	0/8/84/115	-
24	BCR	A	847	-	-	0/29/63/63	0/2/2/2
21	CLA	5	614	15	-	5/11/87/115	-
21	CLA	9	603	19	-	4/15/91/115	-
21	CLA	B	824	-	-	10/39/115/115	-
21	CLA	B	840	23	-	6/39/115/115	-
22	PQN	B	841	-	-	1/23/43/43	0/2/2/2
21	CLA	A	808	1	-	3/15/91/115	-
21	CLA	B	815	2	-	5/25/101/115	-
24	BCR	A	849	-	-	3/29/63/63	0/2/2/2
21	CLA	A	835	1	-	2/21/97/115	-
21	CLA	O	202	-	-	2/6/78/115	-
21	CLA	2	603	16	-	8/15/91/115	-
21	CLA	2	608	16	-	8/27/103/115	-
21	CLA	6	608	16	-	7/15/91/115	-
21	CLA	8	608	18	-	5/9/87/115	-
21	CLA	b	303	20	-	12/32/108/115	-
21	CLA	1	316	15	-	4/11/87/115	-
21	CLA	G	204	7	-	4/13/89/115	-
24	BCR	B	843	-	-	12/29/63/63	0/2/2/2
21	CLA	B	817	2	-	20/39/115/115	-
21	CLA	G	203	7	-	9/21/97/115	-
21	CLA	b	315	20	-	12/15/91/115	-
21	CLA	4	604	-	-	3/11/88/115	-
24	BCR	B	844	-	-	11/29/63/63	0/2/2/2
21	CLA	A	829	1	-	9/39/115/115	-
21	CLA	B	829	2	-	2/15/91/115	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	822	1	-	1/13/89/115	-
21	CLA	c	602	20	-	7/33/109/115	-
21	CLA	8	612	18	-	4/13/89/115	-
21	CLA	L	302	12	-	7/15/91/115	-
24	BCR	O	205	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	XAT	2	617	-	-	0/31/93/93	0/4/4/4
30	LUT	4	615	-	-	4/29/67/67	0/2/2/2
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
21	CLA	c	613	-	-	13/39/115/115	-
21	CLA	B	809	2	-	13/35/111/115	-
21	CLA	J	102	10	-	10/12/88/115	-
21	CLA	3	410	-	-	3/8/84/115	-
21	CLA	7	410	-	-	5/13/89/115	-
24	BCR	M	101	-	-	8/29/63/63	0/2/2/2
21	CLA	5	612	15	-	6/15/91/115	-
21	CLA	8	604	-	-	8/11/88/115	-
21	CLA	9	613	19	-	8/25/101/115	-
21	CLA	B	810	2	-	3/25/101/115	-
21	CLA	7	409	-	-	1/8/84/115	-
21	CLA	B	812	2	-	21/39/115/115	-
21	CLA	4	601	18	-	4/15/91/115	-
29	CHL	2	602	16	-	9/26/102/117	-
21	CLA	c	612	20	-	5/13/90/115	-
21	CLA	A	833	1	-	9/39/115/115	-
21	CLA	B	833	-	-	3/15/91/115	-
21	CLA	K	204	11	-	7/15/91/115	-
21	CLA	F	304	-	-	1/15/91/115	-
21	CLA	a	610	20	-	4/15/91/115	-
29	CHL	1	302	15	-	8/23/99/117	-
29	CHL	6	605	-	-	3/17/93/117	-
21	CLA	4	610	23	-	2/15/91/115	-
21	CLA	3	415	17	-	1/8/84/115	-
24	BCR	F	303	-	-	0/29/63/63	0/2/2/2
24	BCR	J	103	-	-	3/29/63/63	0/2/2/2
21	CLA	A	815	-	-	5/15/91/115	-
21	CLA	B	832	2	-	7/29/105/115	-
21	CLA	A	804	1	-	9/39/115/115	-
21	CLA	B	828	2	-	6/24/100/115	-
21	CLA	7	402	17	-	11/15/91/115	-
21	CLA	6	609	-	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	612	16	-	7/15/91/115	-
21	CLA	A	805	1	-	6/27/103/115	-
21	CLA	B	822	2	-	6/15/91/115	-
21	CLA	c	610	20	-	7/15/91/115	-
26	LMU	A	853	-	-	0/21/61/61	0/2/2/2
29	CHL	c	607	-	-	3/17/93/117	-
21	CLA	G	202	-	-	6/15/91/115	-
29	CHL	9	608	-	-	5/17/93/117	-
24	BCR	8	616	-	-	6/29/63/63	0/2/2/2
21	CLA	3	402	17	-	5/33/109/115	-
21	CLA	4	608	18	-	0/9/87/115	-
24	BCR	6	618	-	-	4/29/63/63	0/2/2/2
21	CLA	A	823	1	-	9/29/105/115	-
21	CLA	A	834	1	-	10/39/115/115	-
21	CLA	4	611	18	-	4/13/89/115	-
21	CLA	a	603	20	-	2/10/86/115	-
29	CHL	a	601	20	-	4/17/93/117	-
21	CLA	1	308	-	-	5/13/89/115	-
29	CHL	b	309	-	-	5/21/97/117	-
24	BCR	2	618	-	-	3/29/63/63	0/2/2/2
24	BCR	7	418	-	-	6/29/63/63	0/2/2/2
21	CLA	A	826	-	-	9/39/115/115	-
32	NEX	b	318	-	-	2/27/83/83	0/3/3/3
24	BCR	K	205	-	-	3/29/63/63	0/2/2/2
21	CLA	F	302	-	-	10/35/111/115	-
21	CLA	A	801	1	-	7/24/100/115	-
21	CLA	3	403	17	-	8/27/103/115	-
21	CLA	4	602	18	-	10/30/106/115	-
21	CLA	B	821	2	-	4/27/103/115	-
24	BCR	G	205	-	-	2/29/63/63	0/2/2/2
24	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	CLA	A	807	1	-	11/39/115/115	-
21	CLA	6	604	-	-	6/15/91/115	-
21	CLA	3	406	17	-	0/8/84/115	-
24	BCR	F	301	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	XAT	a	618	-	-	1/31/93/93	0/4/4/4
24	BCR	A	846	-	-	4/29/63/63	0/2/2/2
28	LMG	J	105	-	-	5/25/45/70	0/1/1/1
30	LUT	a	616	-	-	4/29/67/67	0/2/2/2
21	CLA	A	819	1	-	16/39/115/115	-
21	CLA	A	818	1	-	8/24/100/115	-
29	CHL	b	310	-	-	2/24/100/117	-
29	CHL	6	606	-	-	5/17/93/117	-
29	CHL	8	606	-	-	5/17/93/117	-
23	LHG	c	619	21	-	6/53/53/53	-
30	LUT	8	614	-	-	4/29/67/67	0/2/2/2
21	CLA	A	813	1	-	4/26/102/115	-
21	CLA	B	806	2	-	13/37/113/115	-
21	CLA	A	817	1	-	19/39/115/115	-
29	CHL	2	607	-	-	4/23/99/117	-
21	CLA	A	825	-	-	11/39/115/115	-
21	CLA	6	613	16	-	6/12/88/115	-
21	CLA	5	613	15	-	2/4/80/115	-
29	CHL	9	601	19	-	2/14/90/117	-
21	CLA	B	825	2	-	12/39/115/115	-
21	CLA	A	816	1	-	3/12/88/115	-
31	XAT	c	617	-	-	1/31/93/93	0/4/4/4
29	CHL	a	606	-	-	5/17/93/117	-
24	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	7	407	17	-	5/13/89/115	-
24	BCR	3	419	-	-	8/29/63/63	0/2/2/2
21	CLA	9	612	19	-	4/15/91/115	-
21	CLA	7	404	-	-	3/10/86/115	-
23	LHG	5	617	-	-	7/32/32/53	-
31	XAT	8	615	-	-	0/31/93/93	0/4/4/4
21	CLA	8	618	-	-	5/10/86/115	-
21	CLA	4	612	18	-	7/27/103/115	-
21	CLA	B	839	2	-	12/39/115/115	-
21	CLA	5	605	-	-	6/10/82/115	-
21	CLA	7	411	-	-	9/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	803	2	-	7/27/103/115	-
21	CLA	5	610	-	-	0/4/80/115	-
21	CLA	b	314	20	-	9/25/101/115	-
29	CHL	b	308	-	-	7/26/102/117	-
29	CHL	b	302	20	-	8/17/93/117	-
21	CLA	B	836	-	-	16/39/115/115	-
29	CHL	3	407	-	-	0/8/84/117	-
21	CLA	5	603	15	-	5/15/91/115	-
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
21	CLA	6	611	-	-	5/10/86/115	-
29	CHL	2	614	-	-	4/17/93/117	-
29	CHL	6	614	-	-	5/17/93/117	-
21	CLA	7	405	17	-	3/8/84/115	-
24	BCR	3	418	-	-	4/29/63/63	0/2/2/2
21	CLA	c	611	23	-	11/31/107/115	-
21	CLA	7	413	-	-	0/2/74/115	-
21	CLA	c	614	20	-	7/15/91/115	-
23	LHG	6	619	-	-	5/39/39/53	-
29	CHL	9	605	19	-	2/17/93/117	-
21	CLA	B	826	2	-	9/24/100/115	-
21	CLA	5	604	-	-	8/20/96/115	-
23	LHG	8	617	21	-	9/41/41/53	-
29	CHL	7	406	-	-	0/8/84/117	-
21	CLA	a	602	-	-	11/33/109/115	-
21	CLA	A	820	1	-	3/13/89/115	-
21	CLA	1	311	23	-	0/4/80/115	-
26	LMU	A	856	-	-	3/21/61/61	0/2/2/2
21	CLA	B	831	2	-	9/29/105/115	-
21	CLA	6	603	16	-	8/15/91/115	-
23	LHG	a	617	-	-	10/53/53/53	-
29	CHL	b	307	-	-	3/17/93/117	-
21	CLA	A	824	1	-	13/27/103/115	-
21	CLA	B	804	2	-	13/39/115/115	-
21	CLA	H	201	8	-	6/15/91/115	-
21	CLA	c	604	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LUT	b	317	-	-	2/29/67/67	0/2/2/2
29	CHL	a	607	-	-	1/14/90/117	-
23	LHG	A	855	-	-	7/53/53/53	-
29	CHL	1	307	15	-	2/23/99/117	-
21	CLA	1	303	15	-	17/35/111/115	-
21	CLA	1	310	15	-	3/11/87/115	-
21	CLA	9	610	19	-	3/26/102/115	-
21	CLA	3	409	17	-	10/24/100/115	-
21	CLA	A	811	-	-	3/15/91/115	-
21	CLA	a	613	-	-	6/30/106/115	-
21	CLA	A	828	1	-	14/33/109/115	-
21	CLA	A	852	-	-	6/24/100/115	-
29	CHL	9	607	-	-	7/17/93/117	-
21	CLA	O	201	23	-	4/12/88/115	-
24	BCR	L	301	-	-	4/29/63/63	0/2/2/2
21	CLA	K	202	-	-	2/21/97/115	-
21	CLA	A	842	-	-	16/39/115/115	-
21	CLA	5	602	15	-	17/35/111/115	-
21	CLA	1	312	15	-	5/15/91/115	-
21	CLA	A	810	1	-	4/15/91/115	-
24	BCR	J	101	-	-	7/29/63/63	0/2/2/2
21	CLA	2	611	16	-	0/10/86/115	-
30	LUT	3	416	-	-	5/29/67/67	0/2/2/2
26	LMU	O	206	-	-	5/21/61/61	0/2/2/2
29	CHL	c	609	20	-	7/13/89/117	-
31	XAT	3	417	-	-	0/31/93/93	0/4/4/4
29	CHL	4	614	18	-	2/12/88/117	-
21	CLA	B	801	2	-	15/39/115/115	-
21	CLA	1	313	15	-	6/15/91/115	-
26	LMU	3	420	-	-	3/21/61/61	0/2/2/2
31	XAT	5	616	-	-	4/31/93/93	0/4/4/4
30	LUT	9	615	-	-	2/29/67/67	0/2/2/2
21	CLA	b	305	-	-	6/15/91/115	-
21	CLA	L	304	-	-	4/12/88/115	-
21	CLA	3	405	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	609	18	-	10/24/100/115	-
21	CLA	B	808	2	-	7/39/115/115	-
21	CLA	b	313	20	-	8/15/91/115	-
21	CLA	1	305	-	-	9/20/96/115	-
29	CHL	a	608	-	-	5/17/93/117	-
21	CLA	A	839	1	-	2/15/91/115	-
23	LHG	4	619	-	-	11/53/53/53	-
32	NEX	c	618	-	-	2/27/83/83	0/3/3/3
21	CLA	B	814	2	-	8/33/109/115	-
32	NEX	9	617	-	-	2/27/83/83	0/3/3/3
21	CLA	B	816	2	-	6/24/100/115	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
31	XAT	9	616	-	-	8/31/93/93	0/4/4/4
21	CLA	7	412	-	-	2/8/84/115	-
30	LUT	1	317	-	-	4/29/67/67	0/2/2/2
21	CLA	B	823	-	-	12/39/115/115	-
24	BCR	7	417	-	-	2/29/63/63	0/2/2/2
21	CLA	B	835	2	-	8/39/115/115	-
21	CLA	B	807	2	-	18/39/115/115	-
29	CHL	c	601	20	-	5/21/97/117	-
23	LHG	9	618	21	-	10/53/53/53	-
21	CLA	B	811	2	-	3/15/91/115	-
21	CLA	9	602	19	-	5/25/101/115	-
21	CLA	2	612	16	-	8/15/91/115	-
21	CLA	8	602	18	-	8/30/106/115	-
21	CLA	9	604	-	-	7/15/91/115	-
24	BCR	J	104	-	-	9/29/63/63	0/2/2/2
29	CHL	2	606	-	-	2/17/93/117	-
21	CLA	3	412	17	-	11/25/101/115	-
21	CLA	3	404	-	-	0/9/85/115	-
21	CLA	O	204	-	-	3/8/84/115	-
21	CLA	B	838	-	-	10/39/115/115	-
28	LMG	6	615	-	-	3/4/24/70	0/1/1/1
24	BCR	4	617	-	-	4/29/63/63	0/2/2/2
31	XAT	7	416	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	806	1	-	20/39/115/115	-
21	CLA	2	604	-	-	4/15/91/115	-
27	DGD	B	847	-	-	16/55/95/95	0/2/2/2
21	CLA	L	303	-	-	3/15/91/115	-
21	CLA	A	838	1	-	13/39/115/115	-
21	CLA	O	203	-	-	4/19/95/115	-
24	BCR	A	854	-	-	0/29/63/63	0/2/2/2
28	LMG	G	206	-	-	10/50/70/70	0/1/1/1
29	CHL	9	609	-	-	5/17/93/117	-
21	CLA	B	834	-	-	5/15/91/115	-
25	SF4	C	102	3	-	-	0/6/5/5
24	BCR	I	101	-	-	4/29/63/63	0/2/2/2
29	CHL	c	605	-	-	3/11/87/117	-
30	LUT	2	616	-	-	4/29/67/67	0/2/2/2
30	LUT	6	616	-	-	2/29/67/67	0/2/2/2
21	CLA	A	837	1	-	9/23/99/115	-
29	CHL	8	613	-	-	4/12/88/117	-
21	CLA	B	837	2	-	12/37/113/115	-
21	CLA	F	305	6	-	3/10/86/115	-
24	BCR	B	845	-	-	2/29/63/63	0/2/2/2
23	LHG	b	319	21	-	8/53/53/53	-
21	CLA	b	311	20	-	9/26/102/115	-
21	CLA	A	836	1	-	4/15/91/115	-
29	CHL	c	606	20	-	4/17/93/117	-
30	LUT	c	615	-	-	1/29/67/67	0/2/2/2
29	CHL	a	605	20	-	4/15/91/117	-
21	CLA	A	827	1	-	17/37/113/115	-
21	CLA	2	613	16	-	3/12/88/115	-
31	XAT	6	617	-	-	6/31/93/93	0/4/4/4
21	CLA	A	831	1	-	8/27/103/115	-
29	CHL	5	601	15	-	7/17/93/117	-
21	CLA	4	613	18	-	2/13/89/115	-
23	LHG	2	619	21	-	7/39/39/53	-
29	CHL	b	306	20	-	6/17/93/117	-
21	CLA	A	821	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	411	17	-	3/13/89/115	-
21	CLA	8	610	-	-	8/13/89/115	-
21	CLA	b	312	23	-	4/15/91/115	-
21	CLA	1	309	15	-	3/10/86/115	-
21	CLA	B	830	2	-	12/29/105/115	-
21	CLA	B	818	-	-	11/31/107/115	-
21	CLA	5	609	-	-	3/11/87/115	-
21	CLA	2	610	23	-	2/9/85/115	-
21	CLA	6	610	-	-	1/9/85/115	-
21	CLA	3	413	17	-	2/8/84/115	-
30	LUT	a	615	-	-	5/29/67/67	0/2/2/2

The worst 5 of 3303 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	407	CLA	C1D-ND	8.02	1.47	1.37
21	A	801	CLA	C1D-ND	6.31	1.45	1.37
29	3	407	CHL	C3A-C2A	-6.07	1.48	1.54
29	6	601	CHL	C3C-C2C	5.75	1.47	1.36
21	B	801	CLA	C3C-C2C	5.39	1.48	1.36

The worst 5 of 3660 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	407	CLA	CAC-C3C-C4C	16.81	146.62	124.81
21	7	407	CLA	C1D-ND-C4D	-10.68	98.75	106.33
29	a	601	CHL	C1D-ND-C4D	10.07	113.49	106.33
29	9	601	CHL	C1D-ND-C4D	10.04	113.47	106.33
29	c	609	CHL	C1D-ND-C4D	10.00	113.44	106.33

There are no chirality outliers.

5 of 2134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	801	CLA	CBD-CGD-O2D-CED
21	A	802	CLA	C2B-C3B-CAB-CBB
21	A	802	CLA	C4B-C3B-CAB-CBB
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

307 monomers are involved in 867 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	618	LHG	5	0
24	B	846	BCR	8	0
21	1	304	CLA	2	0
29	4	607	CHL	4	0
21	A	802	CLA	4	0
21	c	603	CLA	4	0
29	8	605	CHL	4	0
21	5	607	CLA	3	0
21	a	611	CLA	4	0
21	a	614	CLA	1	0
23	A	845	LHG	1	0
29	4	606	CHL	1	0
21	7	408	CLA	2	0
21	a	604	CLA	1	0
29	6	602	CHL	3	0
21	8	609	CLA	26	0
29	c	608	CHL	3	0
21	A	803	CLA	2	0
21	a	612	CLA	1	0
29	a	609	CHL	3	0
21	1	315	CLA	1	0
29	6	601	CHL	3	0
31	1	318	XAT	2	0
21	K	203	CLA	9	0
21	A	840	CLA	8	0
21	A	832	CLA	1	0
30	9	614	LUT	3	0
21	b	304	CLA	4	0
29	2	601	CHL	2	0
21	B	805	CLA	4	0
21	3	408	CLA	5	0
26	b	301	LMU	4	0
21	A	809	CLA	1	0
29	9	606	CHL	1	0
21	B	813	CLA	3	0
21	A	841	CLA	4	0
21	A	830	CLA	3	0
21	8	603	CLA	1	0
29	6	607	CHL	5	0
29	8	607	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	c	616	LUT	4	0
21	B	827	CLA	9	0
21	A	814	CLA	1	0
21	7	401	CLA	7	0
21	1	306	CLA	2	0
21	2	609	CLA	23	0
21	A	812	CLA	5	0
31	4	616	XAT	4	0
21	1	314	CLA	1	0
21	B	819	CLA	1	0
29	5	606	CHL	3	0
30	5	615	LUT	2	0
23	A	844	LHG	3	0
30	b	316	LUT	6	0
21	K	201	CLA	5	0
21	9	611	CLA	5	0
21	8	611	CLA	5	0
30	7	415	LUT	12	0
21	B	802	CLA	3	0
21	3	401	CLA	2	0
24	A	847	BCR	3	0
21	5	614	CLA	1	0
21	B	824	CLA	3	0
21	B	840	CLA	1	0
22	B	841	PQN	3	0
21	A	808	CLA	2	0
21	B	815	CLA	2	0
24	A	849	BCR	4	0
21	A	835	CLA	2	0
21	O	202	CLA	1	0
21	2	603	CLA	1	0
21	2	608	CLA	2	0
21	6	608	CLA	2	0
21	8	608	CLA	2	0
21	b	303	CLA	3	0
21	G	204	CLA	1	0
24	B	843	BCR	20	0
21	B	817	CLA	8	0
21	b	315	CLA	1	0
24	B	844	BCR	6	0
21	A	829	CLA	2	0
21	B	829	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	822	CLA	3	0
21	c	602	CLA	3	0
21	8	612	CLA	2	0
21	L	302	CLA	2	0
24	O	205	BCR	1	0
31	2	617	XAT	2	0
30	4	615	LUT	7	0
24	L	306	BCR	3	0
21	c	613	CLA	4	0
21	B	809	CLA	4	0
21	7	410	CLA	2	0
24	M	101	BCR	3	0
21	5	612	CLA	1	0
21	8	604	CLA	3	0
21	9	613	CLA	2	0
21	B	810	CLA	1	0
21	B	812	CLA	1	0
21	4	601	CLA	2	0
29	2	602	CHL	3	0
21	c	612	CLA	2	0
21	A	833	CLA	5	0
21	K	204	CLA	1	0
21	F	304	CLA	2	0
21	a	610	CLA	5	0
29	1	302	CHL	2	0
29	6	605	CHL	1	0
21	3	415	CLA	2	0
24	J	103	BCR	3	0
21	B	832	CLA	4	0
21	A	804	CLA	3	0
21	B	828	CLA	3	0
21	7	402	CLA	9	0
21	6	609	CLA	4	0
21	6	612	CLA	2	0
21	A	805	CLA	4	0
21	B	822	CLA	2	0
21	c	610	CLA	2	0
29	c	607	CHL	1	0
21	G	202	CLA	2	0
29	9	608	CHL	1	0
24	8	616	BCR	8	0
21	3	402	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	618	BCR	14	0
21	A	823	CLA	1	0
21	A	834	CLA	4	0
21	4	611	CLA	1	0
29	a	601	CHL	1	0
21	1	308	CLA	1	0
29	b	309	CHL	3	0
24	2	618	BCR	6	0
24	7	418	BCR	4	0
21	A	826	CLA	2	0
32	b	318	NEX	1	0
24	K	205	BCR	24	0
21	F	302	CLA	1	0
21	A	801	CLA	1	0
21	4	602	CLA	5	0
21	B	821	CLA	1	0
24	G	205	BCR	2	0
24	A	850	BCR	1	0
21	A	807	CLA	2	0
21	6	604	CLA	7	0
24	F	301	BCR	2	0
31	a	618	XAT	6	0
24	A	846	BCR	1	0
30	a	616	LUT	7	0
21	A	819	CLA	6	0
21	A	818	CLA	7	0
29	b	310	CHL	3	0
29	6	606	CHL	1	0
29	8	606	CHL	2	0
23	c	619	LHG	2	0
30	8	614	LUT	5	0
21	A	813	CLA	1	0
21	B	806	CLA	2	0
21	A	817	CLA	3	0
29	2	607	CHL	3	0
21	A	825	CLA	3	0
21	6	613	CLA	1	0
29	9	601	CHL	2	0
21	B	825	CLA	2	0
21	A	816	CLA	1	0
31	c	617	XAT	3	0
29	a	606	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L	305	BCR	2	0
21	7	407	CLA	18	0
24	3	419	BCR	1	0
21	9	612	CLA	1	0
21	7	404	CLA	3	0
23	5	617	LHG	1	0
31	8	615	XAT	4	0
21	8	618	CLA	2	0
21	4	612	CLA	1	0
21	B	839	CLA	4	0
21	5	605	CLA	2	0
21	7	411	CLA	2	0
21	B	803	CLA	2	0
21	b	314	CLA	4	0
29	b	308	CHL	2	0
29	b	302	CHL	2	0
21	B	836	CLA	4	0
29	3	407	CHL	1	0
21	5	603	CLA	3	0
24	G	201	BCR	4	0
21	6	611	CLA	1	0
29	2	614	CHL	5	0
29	6	614	CHL	4	0
24	3	418	BCR	6	0
21	c	611	CLA	1	0
21	c	614	CLA	2	0
23	6	619	LHG	3	0
29	9	605	CHL	2	0
21	B	826	CLA	1	0
21	5	604	CLA	2	0
23	8	617	LHG	3	0
29	7	406	CHL	2	0
21	a	602	CLA	5	0
21	A	820	CLA	1	0
26	A	856	LMU	2	0
21	B	831	CLA	6	0
21	6	603	CLA	2	0
23	a	617	LHG	2	0
29	b	307	CHL	2	0
21	A	824	CLA	3	0
21	B	804	CLA	2	0
21	H	201	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	c	604	CLA	3	0
30	b	317	LUT	5	0
29	a	607	CHL	5	0
23	A	855	LHG	4	0
29	1	307	CHL	5	0
21	1	303	CLA	2	0
21	1	310	CLA	1	0
21	9	610	CLA	1	0
21	3	409	CLA	21	0
21	a	613	CLA	3	0
21	A	828	CLA	3	0
21	A	852	CLA	6	0
29	9	607	CHL	1	0
24	L	301	BCR	3	0
21	K	202	CLA	1	0
21	A	842	CLA	7	0
21	5	602	CLA	10	0
21	1	312	CLA	1	0
21	A	810	CLA	4	0
24	J	101	BCR	4	0
30	3	416	LUT	12	0
26	O	206	LMU	4	0
29	c	609	CHL	3	0
31	3	417	XAT	4	0
29	4	614	CHL	1	0
21	B	801	CLA	9	0
21	1	313	CLA	1	0
26	3	420	LMU	3	0
31	5	616	XAT	5	0
30	9	615	LUT	7	0
21	4	609	CLA	16	0
21	B	808	CLA	2	0
29	a	608	CHL	3	0
23	4	619	LHG	1	0
32	c	618	NEX	3	0
21	B	814	CLA	4	0
32	9	617	NEX	4	0
21	B	816	CLA	5	0
24	B	842	BCR	3	0
31	9	616	XAT	2	0
30	1	317	LUT	2	0
21	B	823	CLA	3	0

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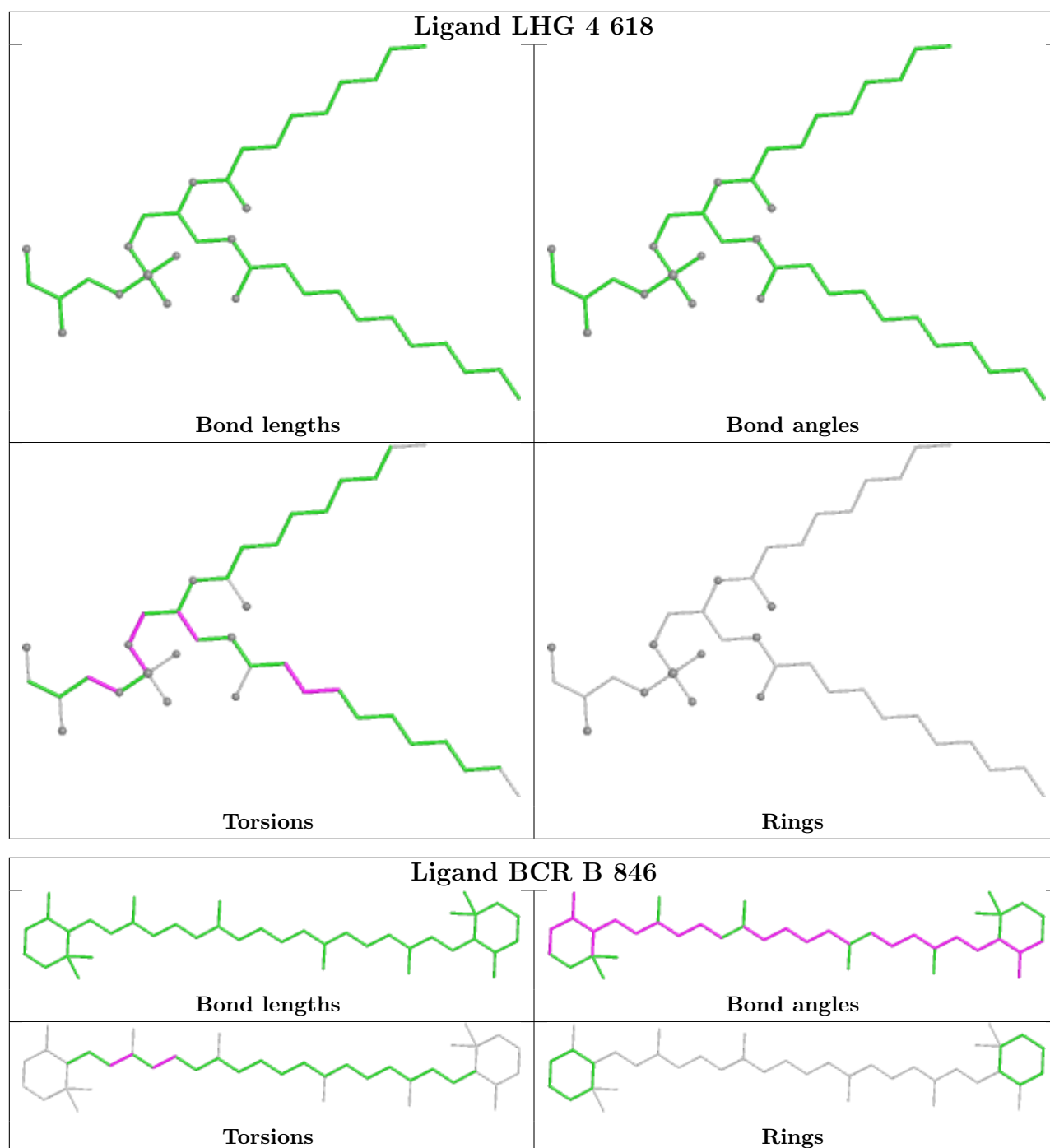
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	B	835	CLA	2	0
21	B	807	CLA	5	0
23	9	618	LHG	4	0
21	B	811	CLA	1	0
21	9	602	CLA	3	0
21	8	602	CLA	4	0
24	J	104	BCR	8	0
29	2	606	CHL	2	0
21	3	412	CLA	1	0
21	3	404	CLA	4	0
21	B	838	CLA	1	0
28	6	615	LMG	1	0
31	7	416	XAT	5	0
21	A	806	CLA	3	0
21	2	604	CLA	3	0
27	B	847	DGD	7	0
21	L	303	CLA	1	0
21	A	838	CLA	3	0
21	O	203	CLA	1	0
24	A	854	BCR	13	0
28	G	206	LMG	2	0
29	9	609	CHL	2	0
24	I	101	BCR	1	0
29	c	605	CHL	1	0
30	2	616	LUT	8	0
30	6	616	LUT	6	0
21	A	837	CLA	3	0
29	8	613	CHL	4	0
21	B	837	CLA	6	0
24	B	845	BCR	3	0
23	b	319	LHG	9	0
21	b	311	CLA	6	0
21	A	836	CLA	1	0
29	c	606	CHL	2	0
30	c	615	LUT	3	0
29	a	605	CHL	1	0
21	A	827	CLA	5	0
21	2	613	CLA	2	0
31	6	617	XAT	6	0
21	A	831	CLA	1	0
29	5	601	CHL	3	0

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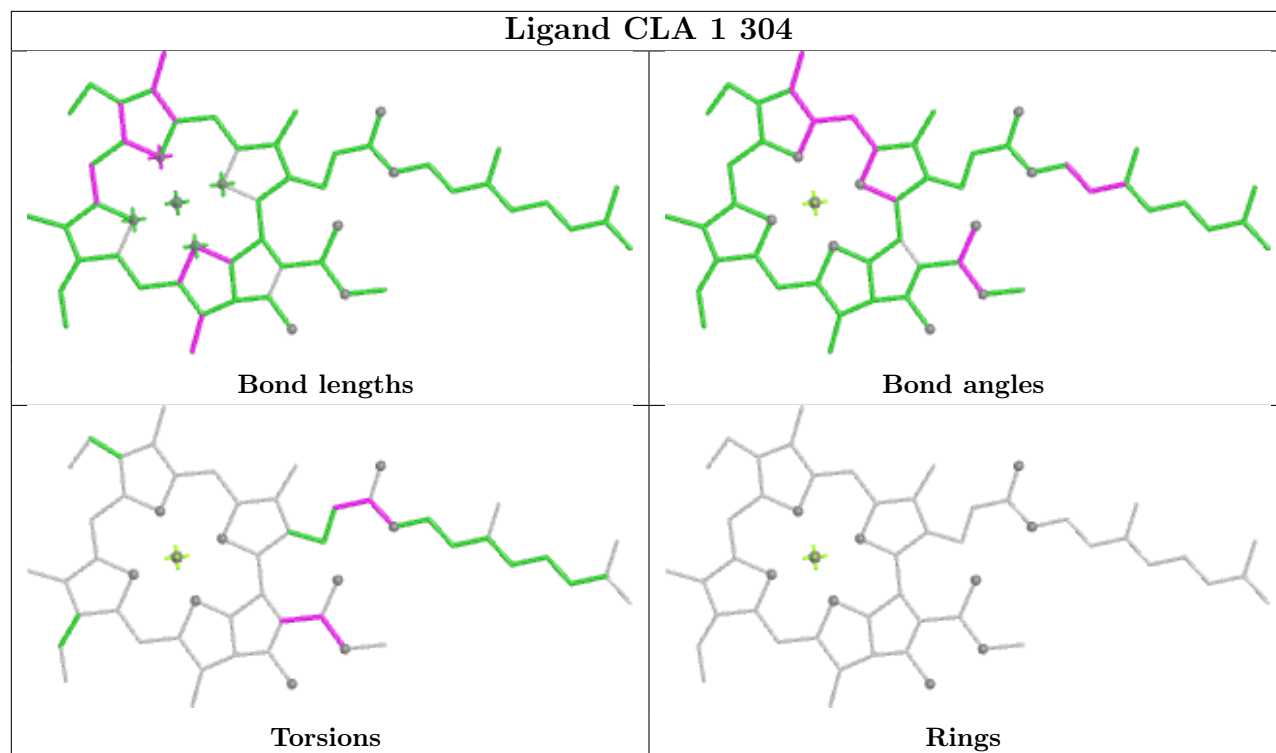
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	4	613	CLA	2	0
23	2	619	LHG	1	0
29	b	306	CHL	2	0
21	A	821	CLA	7	0
21	3	411	CLA	1	0
21	8	610	CLA	1	0
21	b	312	CLA	3	0
21	1	309	CLA	10	0
21	B	830	CLA	4	0
21	B	818	CLA	1	0
21	5	609	CLA	2	0
21	2	610	CLA	2	0
21	6	610	CLA	1	0
21	3	413	CLA	1	0
30	a	615	LUT	4	0

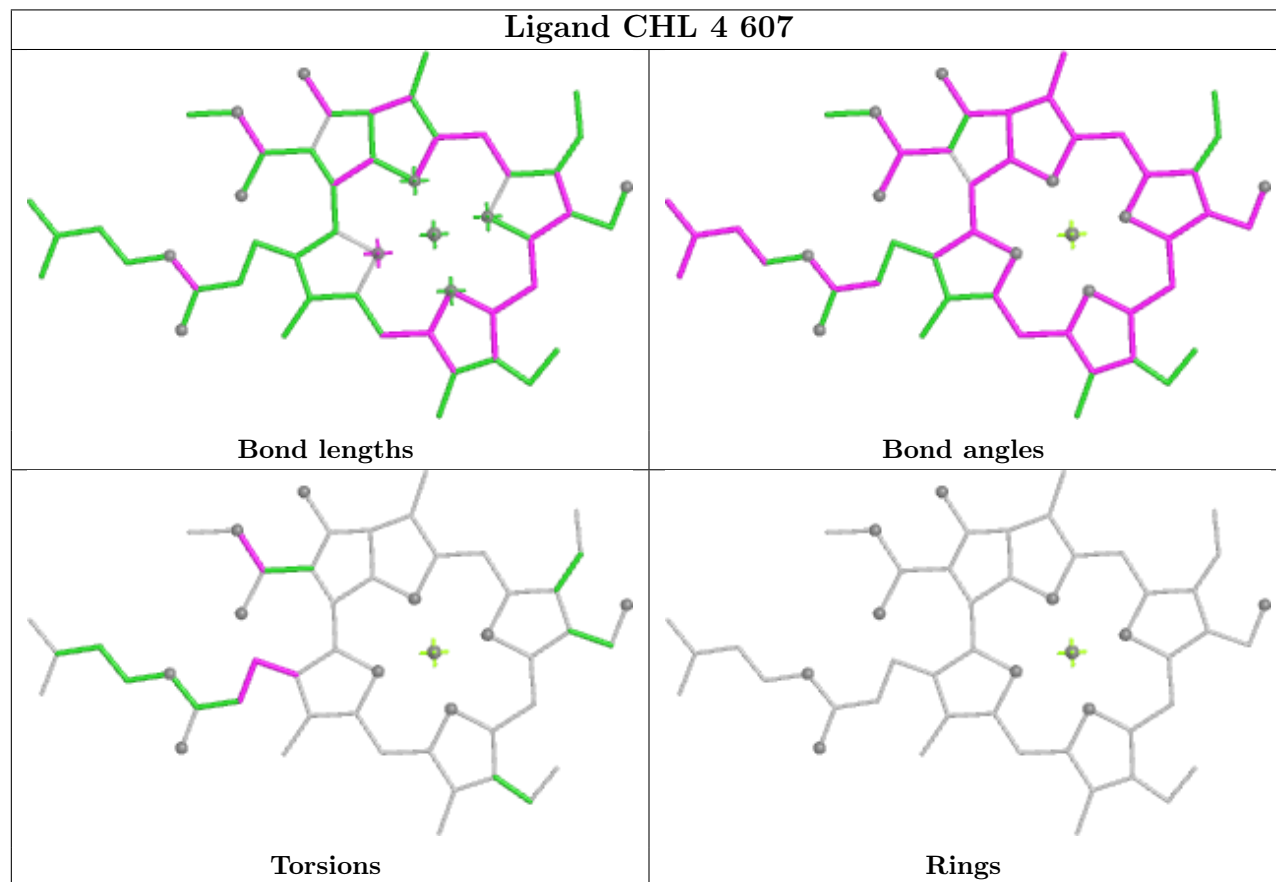
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



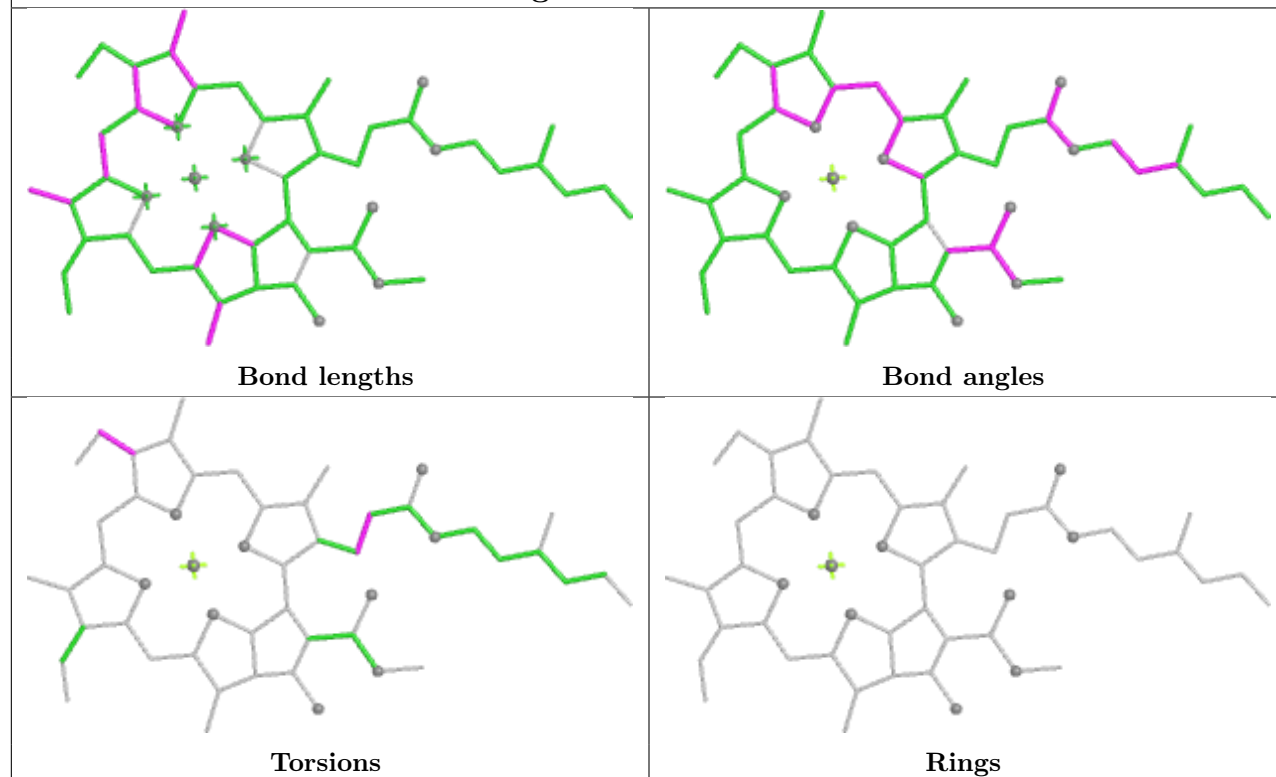
Ligand CLA 1 304



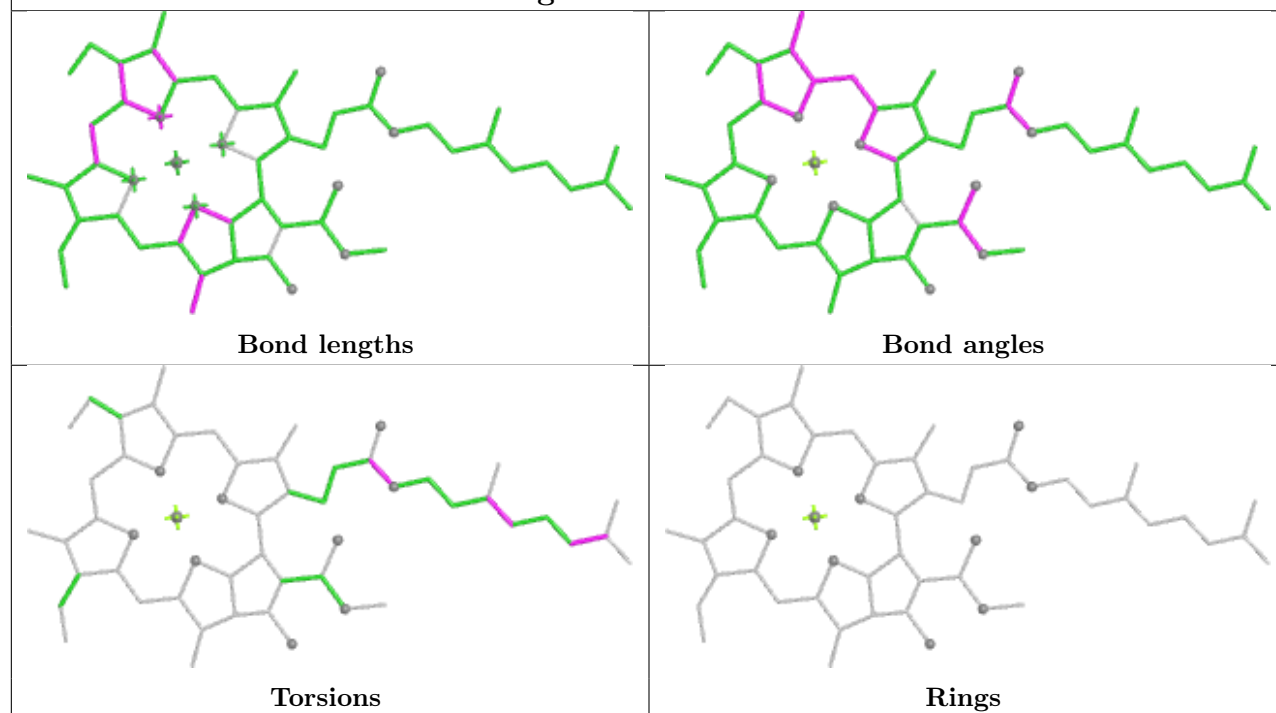
Ligand CHL 4 607



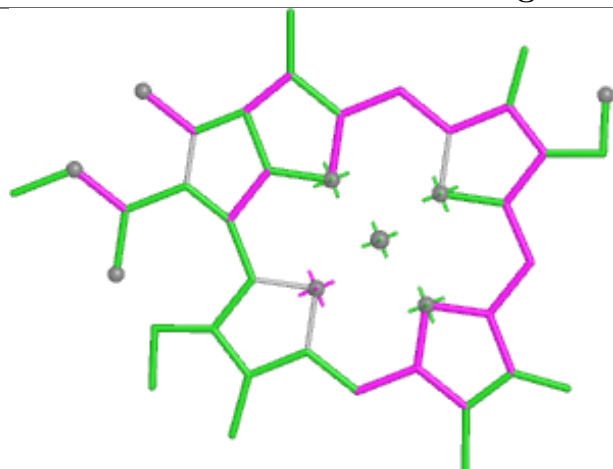
Ligand CLA A 802



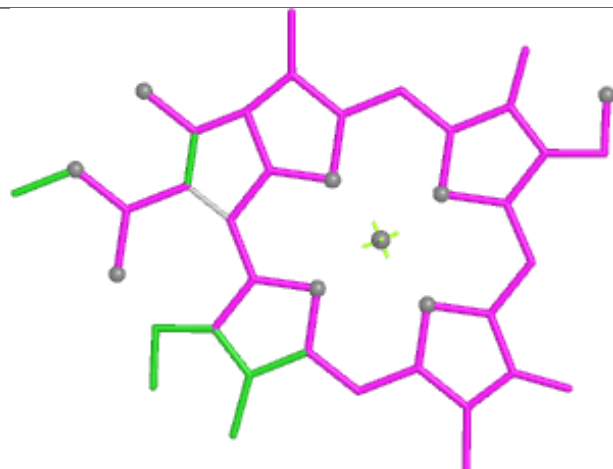
Ligand CLA c 603



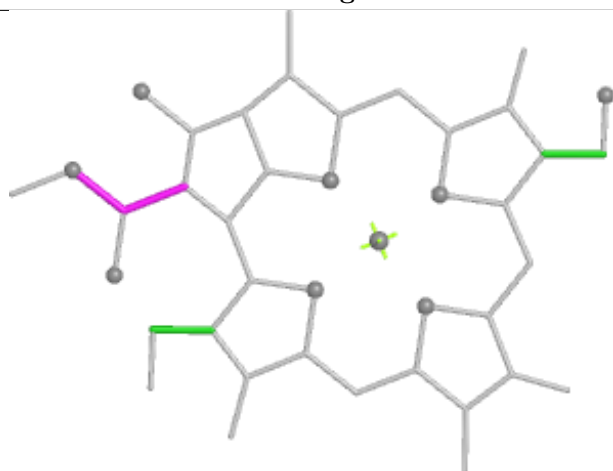
Ligand CHL 8 605



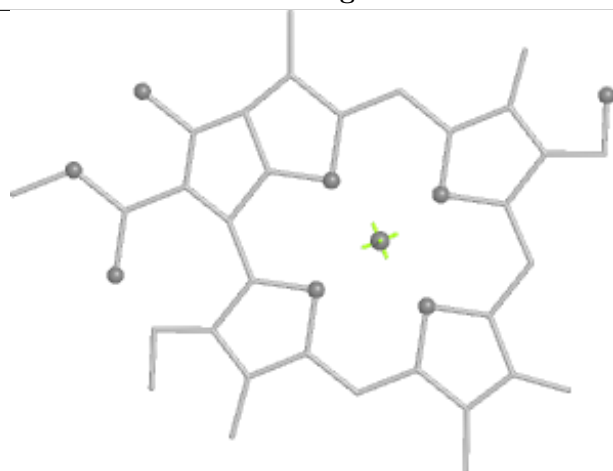
Bond lengths



Bond angles

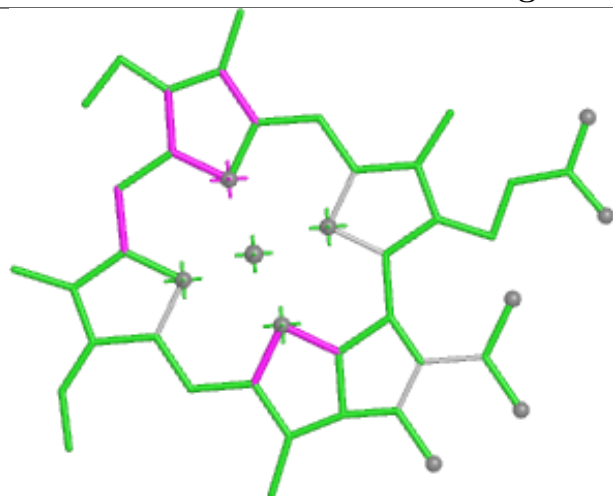


Torsions

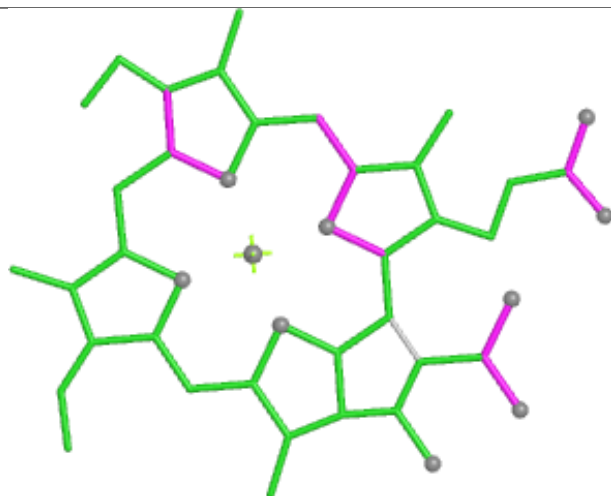


Rings

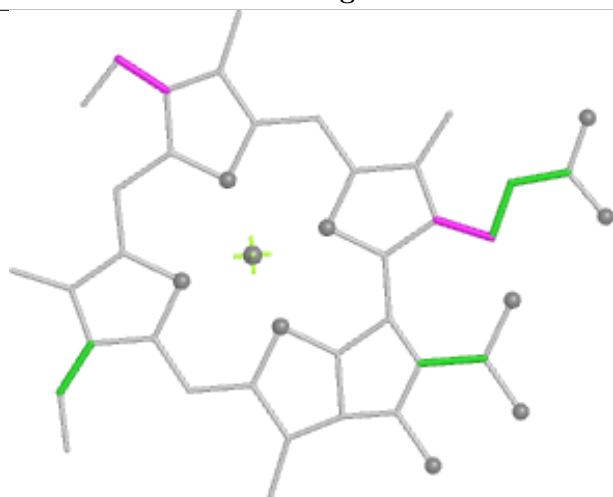
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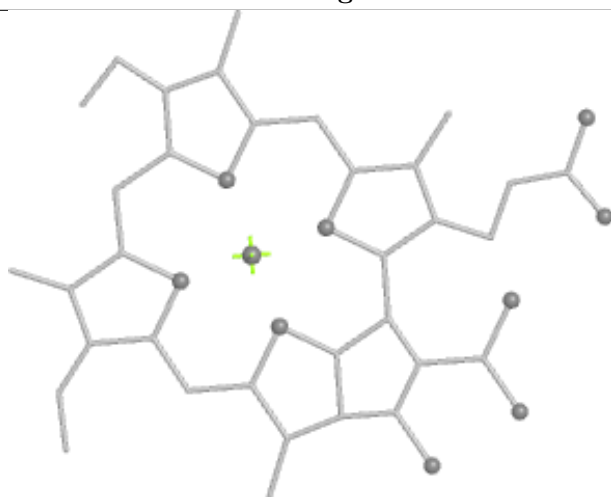
Bond lengths



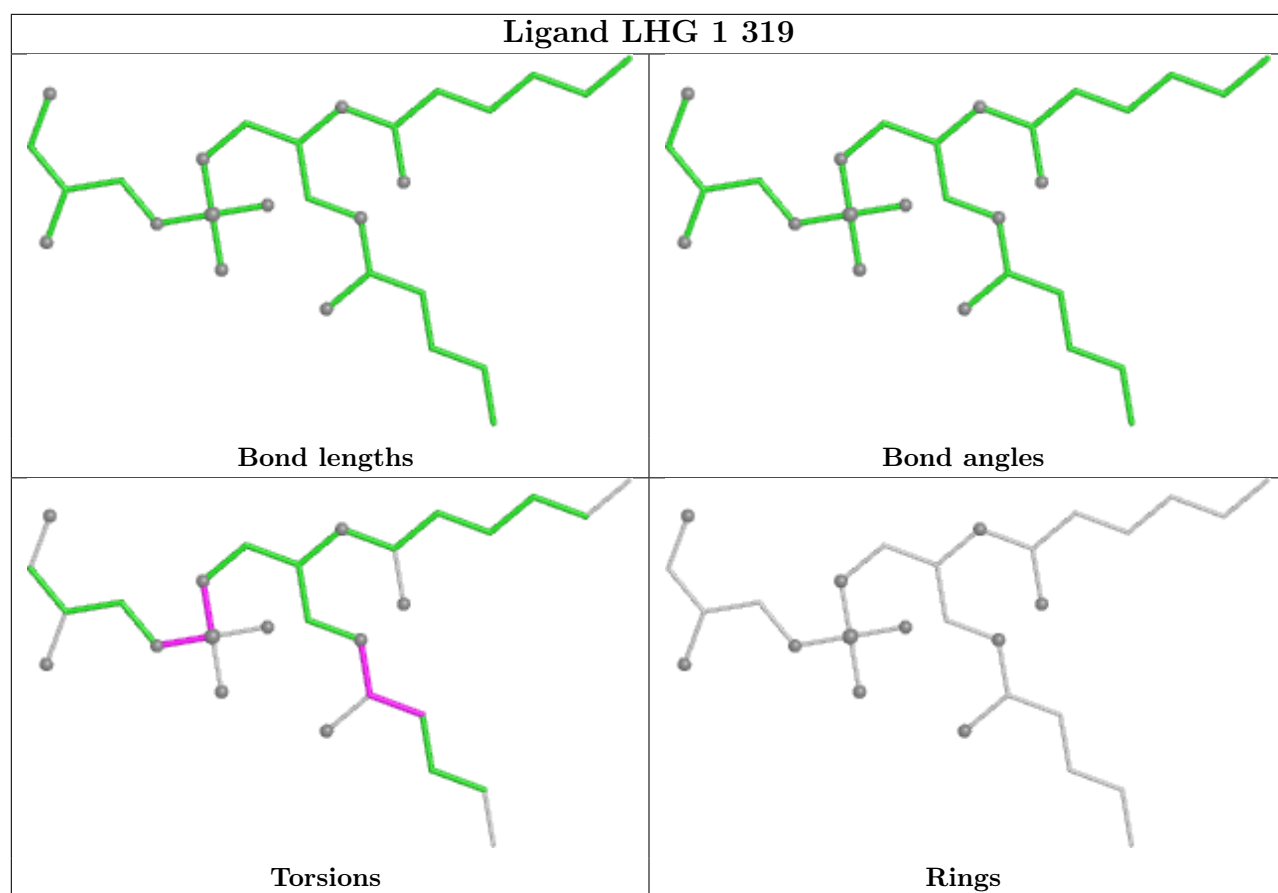
Bond angles



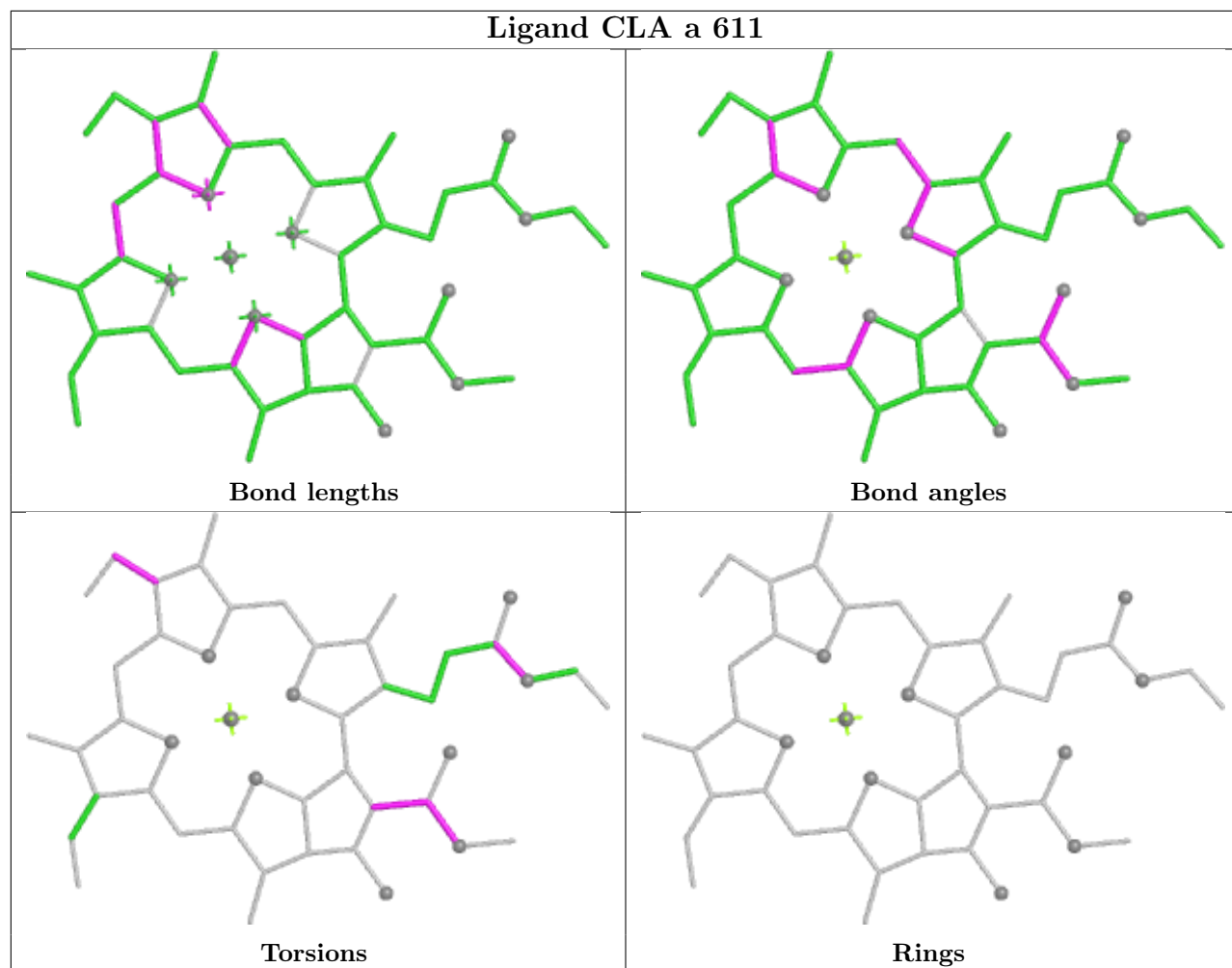
Torsions



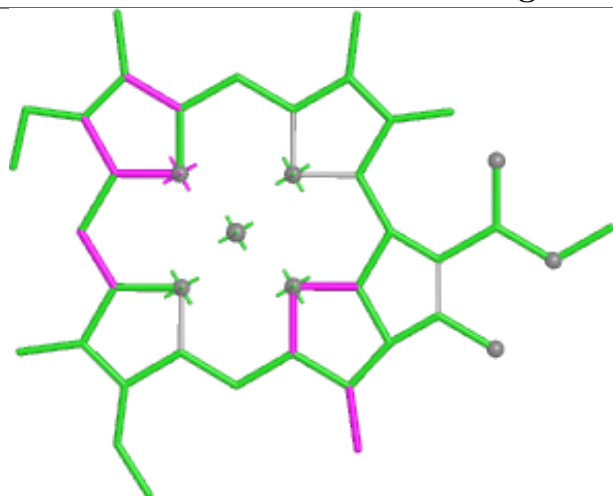
Rings



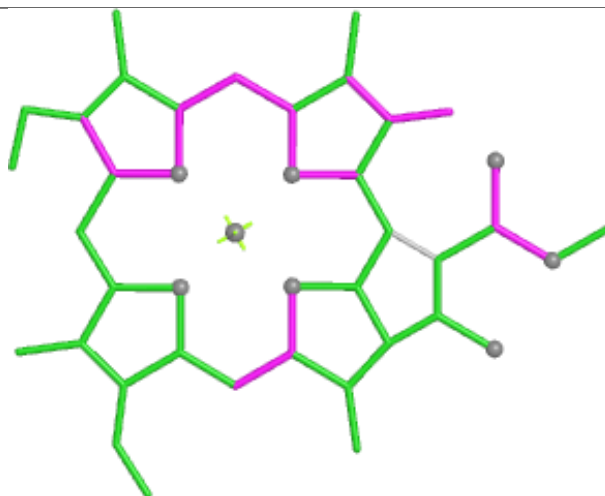
Ligand CLA a 611



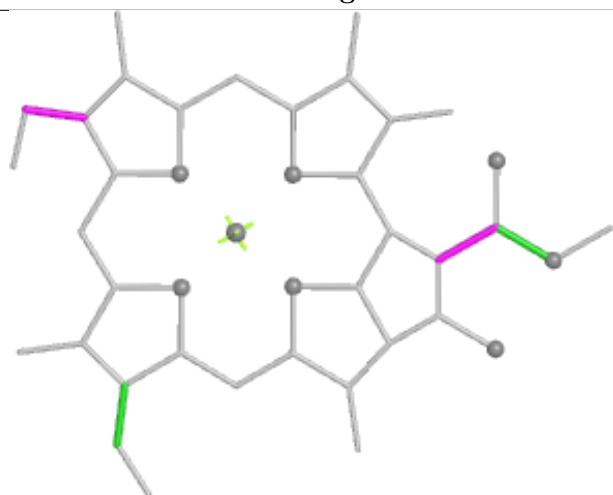
Ligand CLA a 614



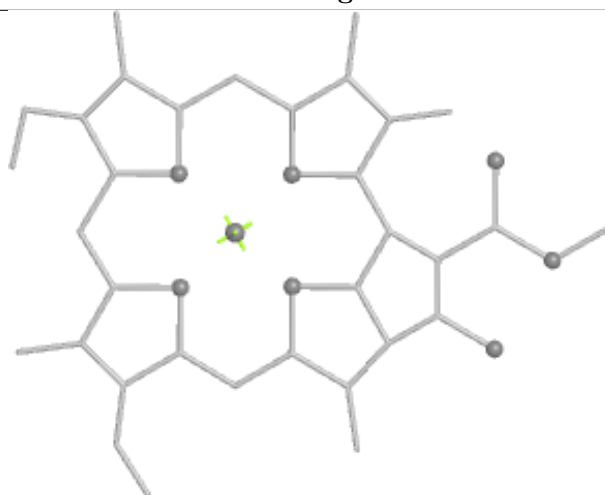
Bond lengths



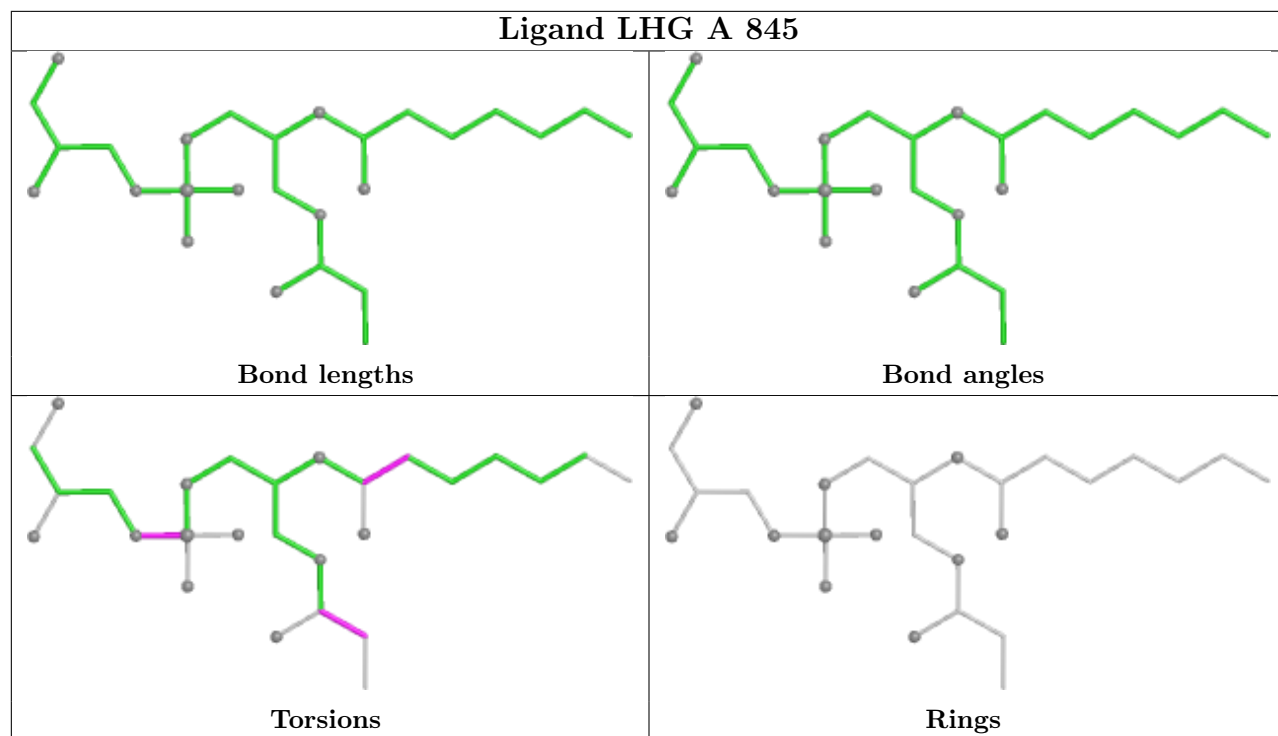
Bond angles



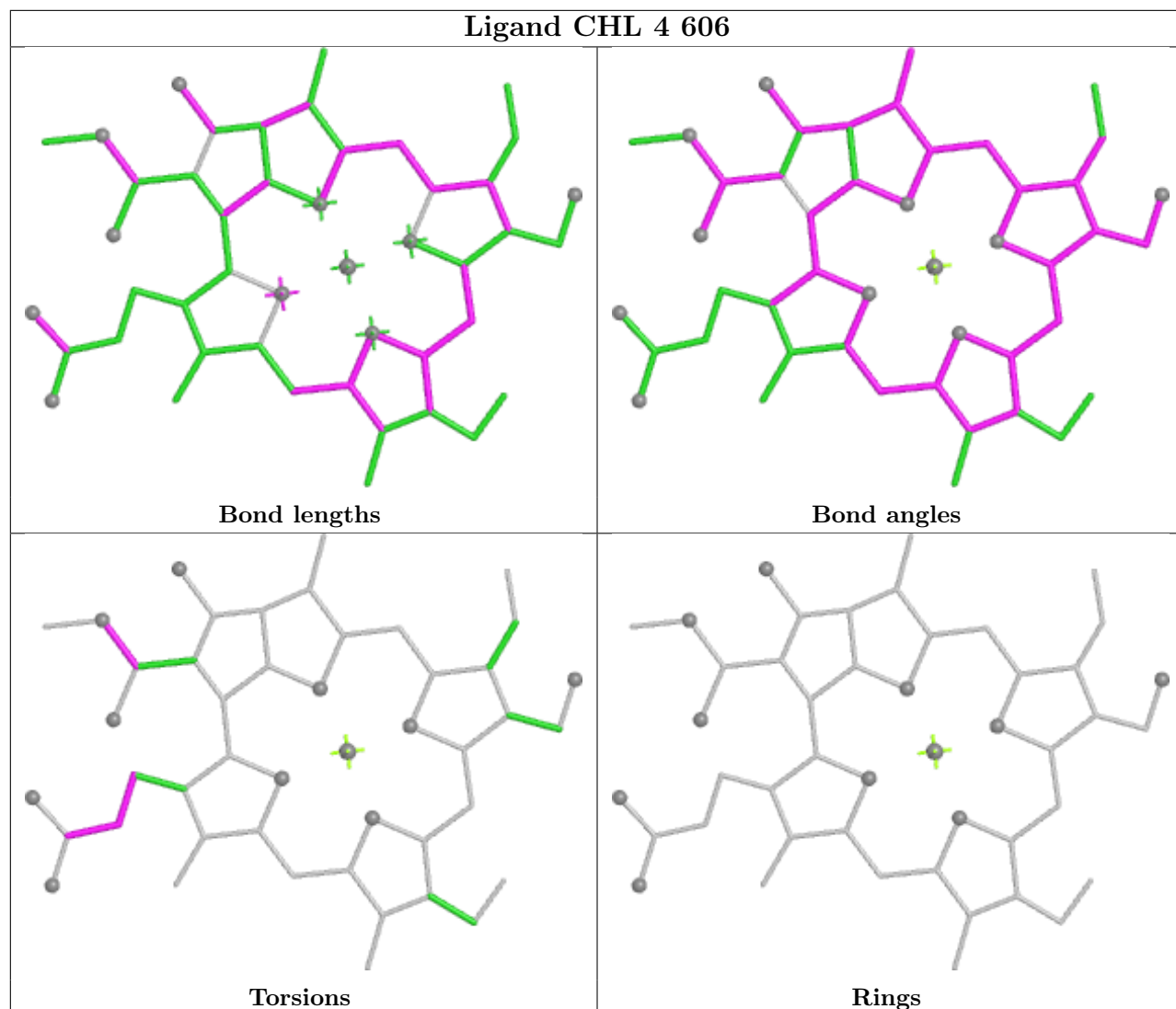
Torsions



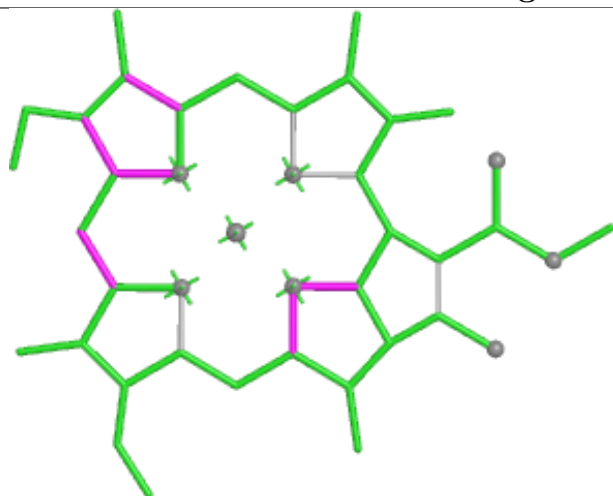
Rings



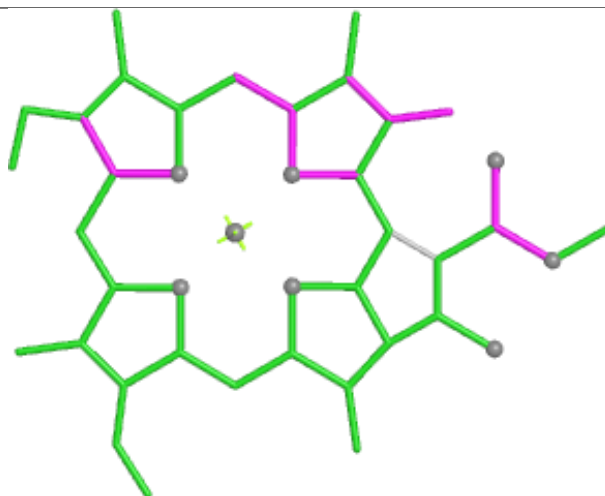
Ligand CHL 4 606



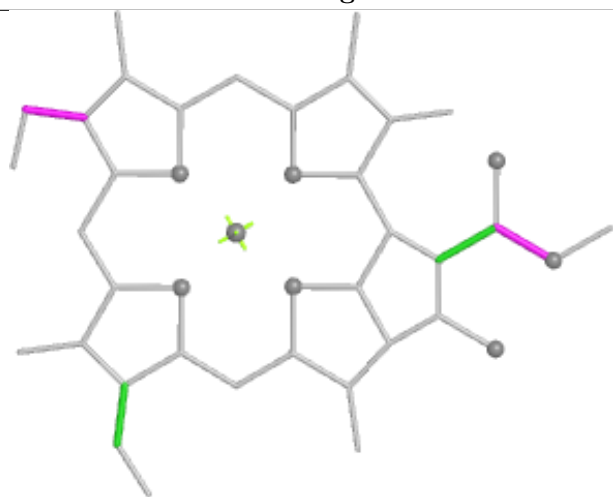
Ligand CLA 7 408



Bond lengths



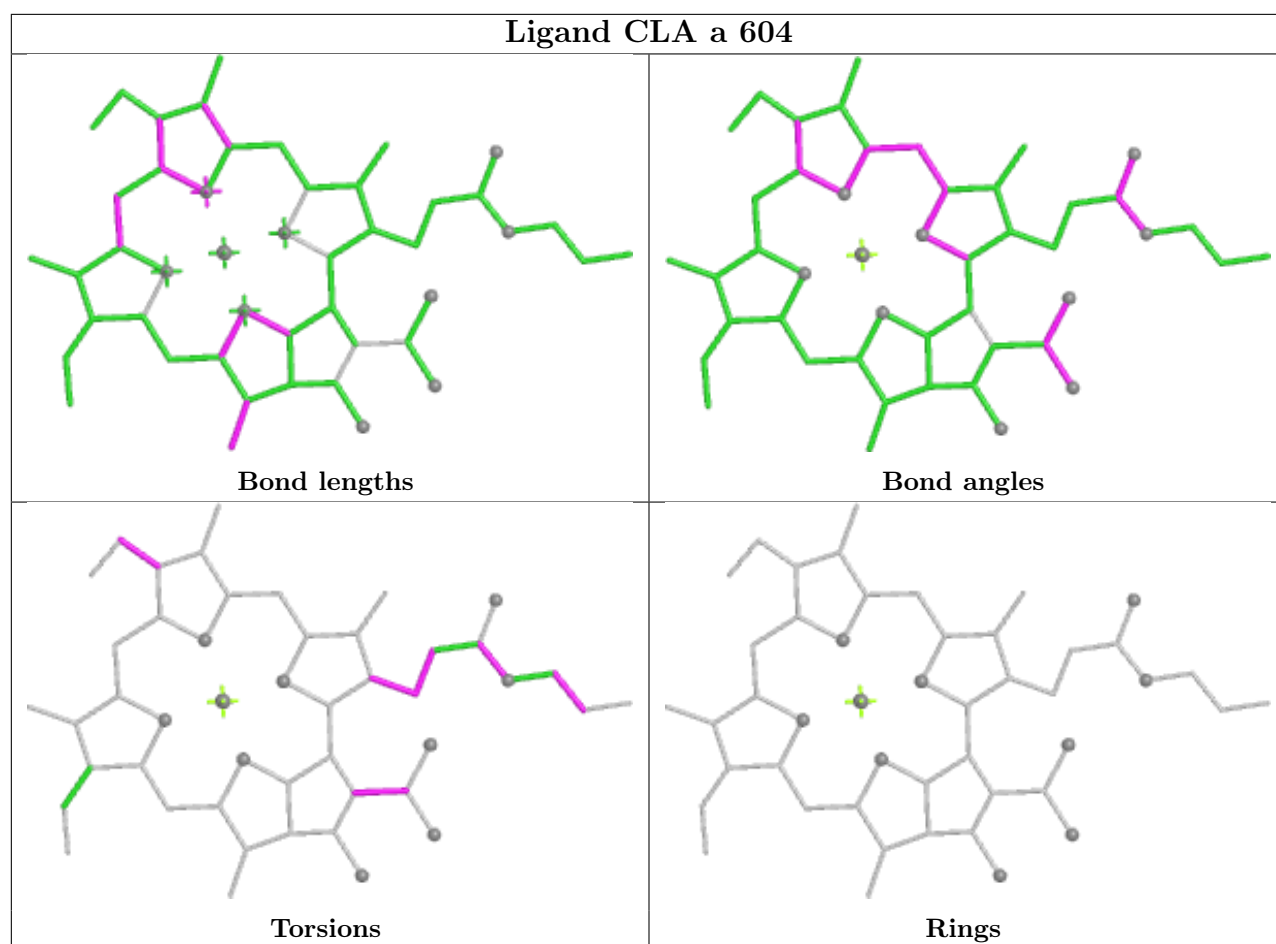
Bond angles



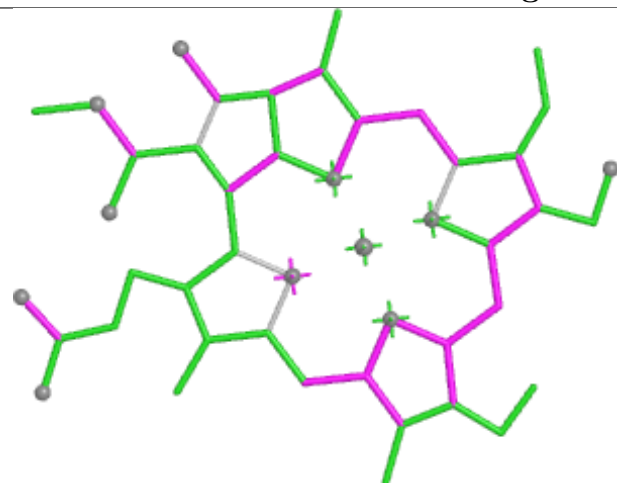
Torsions



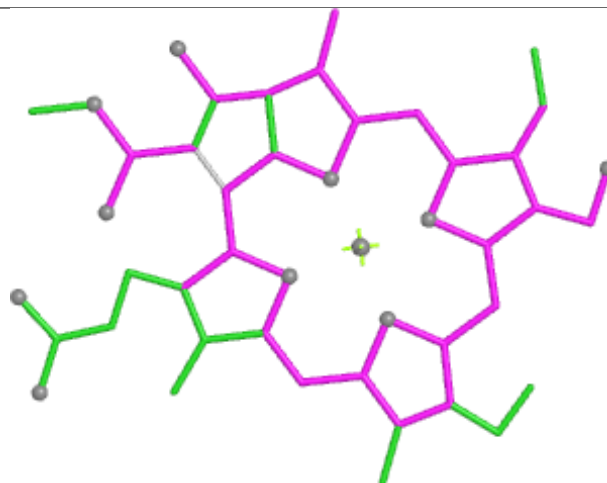
Rings



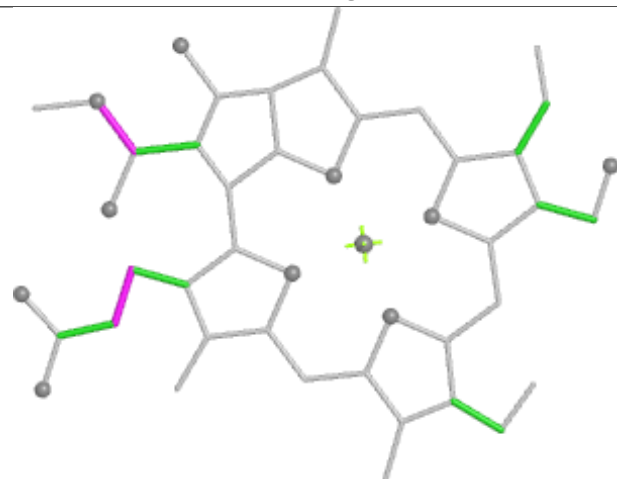
Ligand CHL 2 605



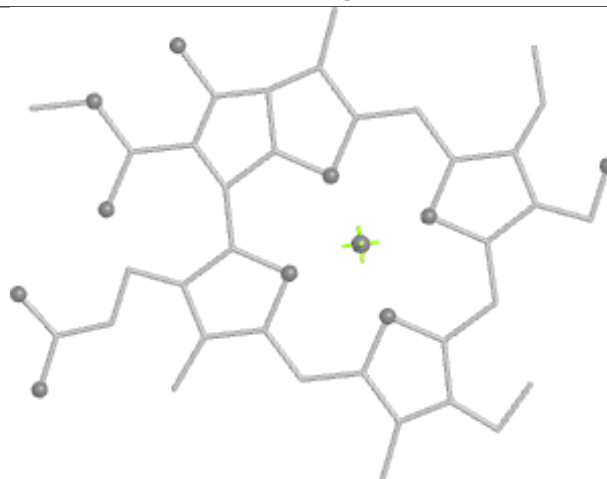
Bond lengths



Bond angles

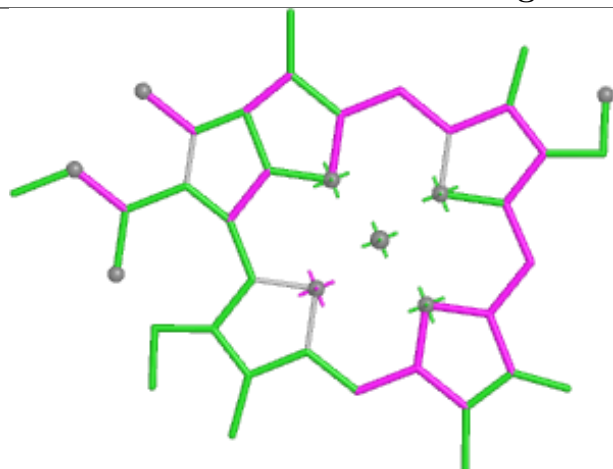


Torsions

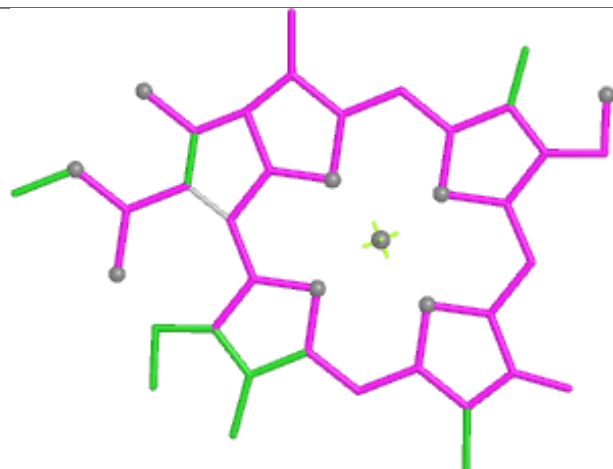


Rings

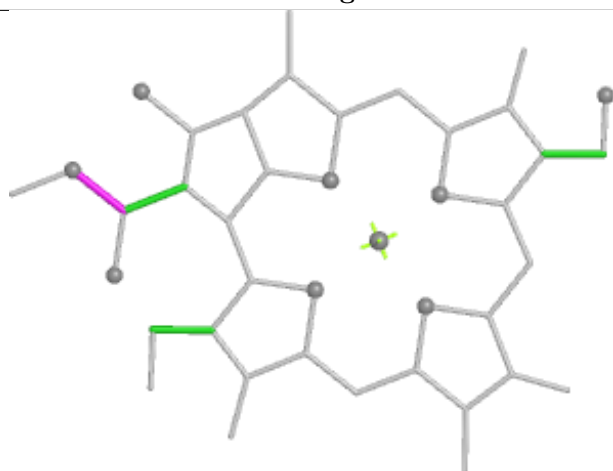
Ligand CHL 4 605



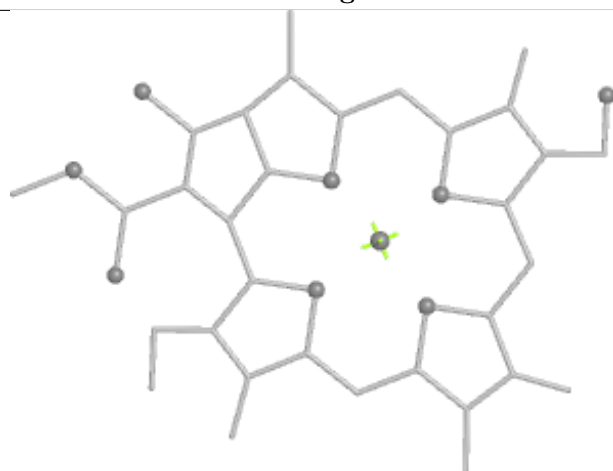
Bond lengths



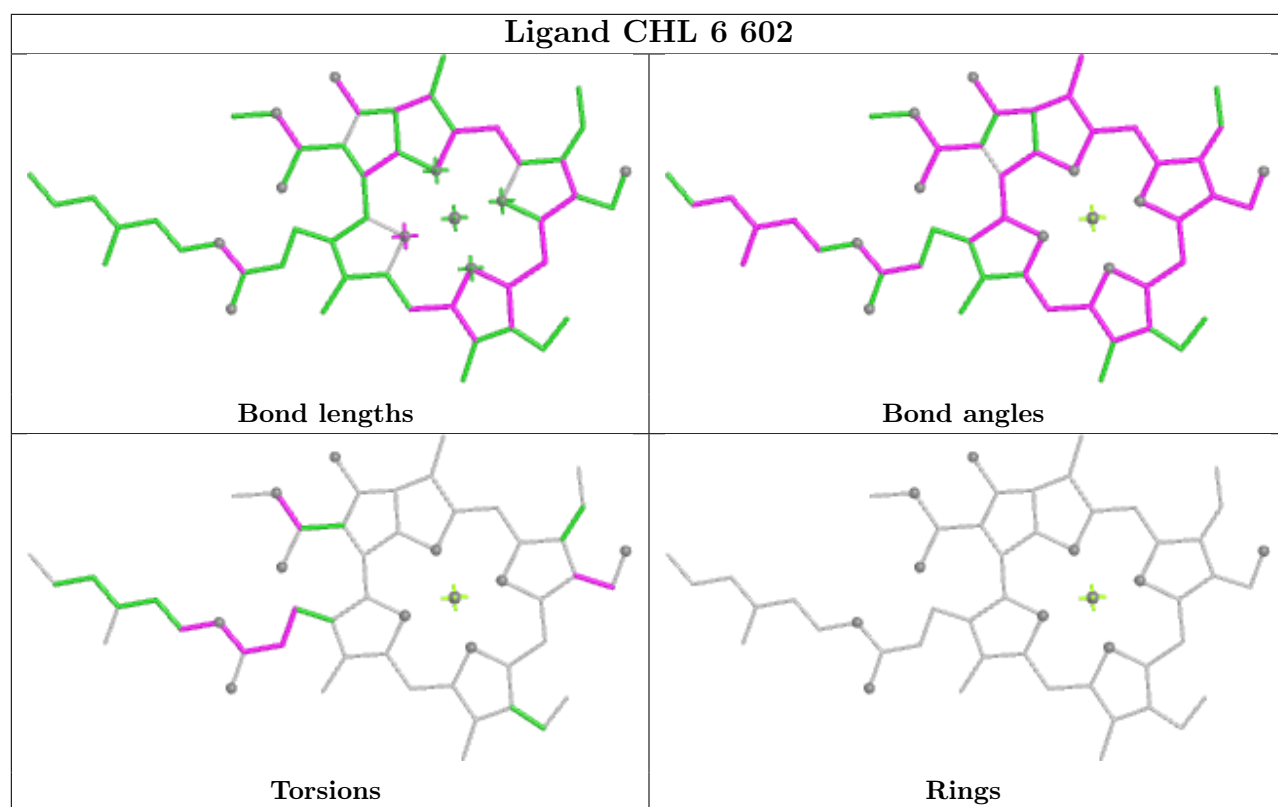
Bond angles



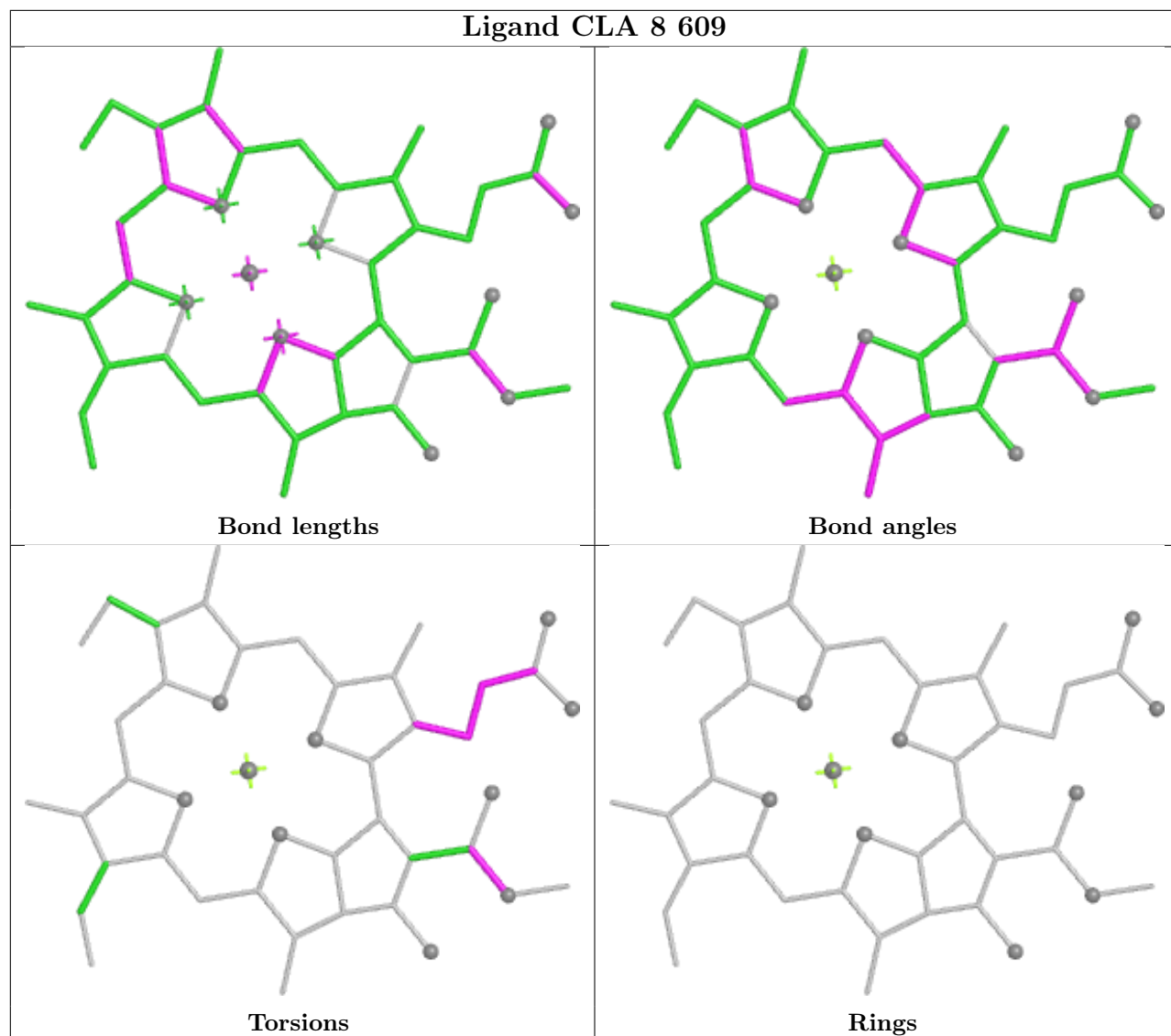
Torsions



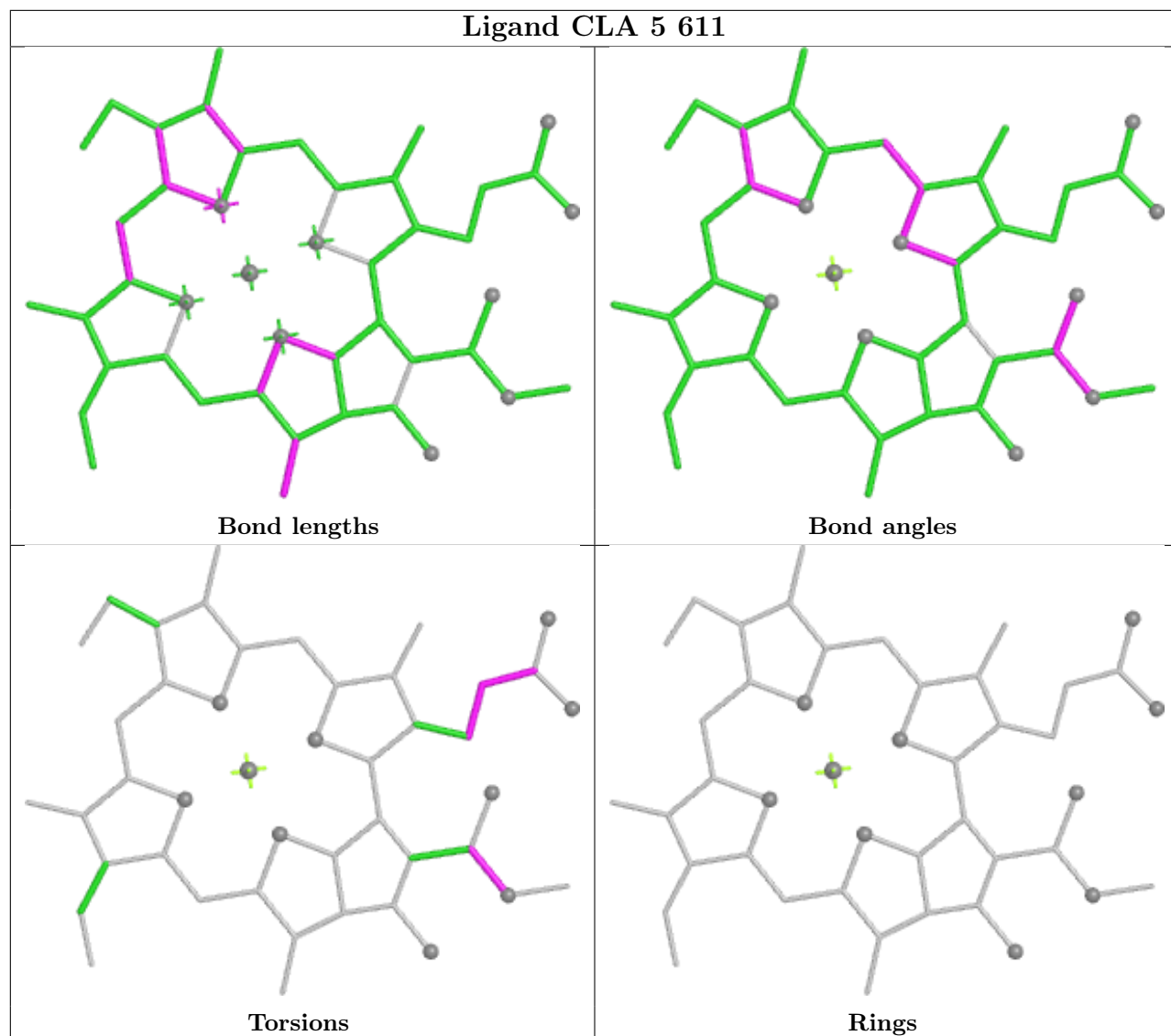
Rings



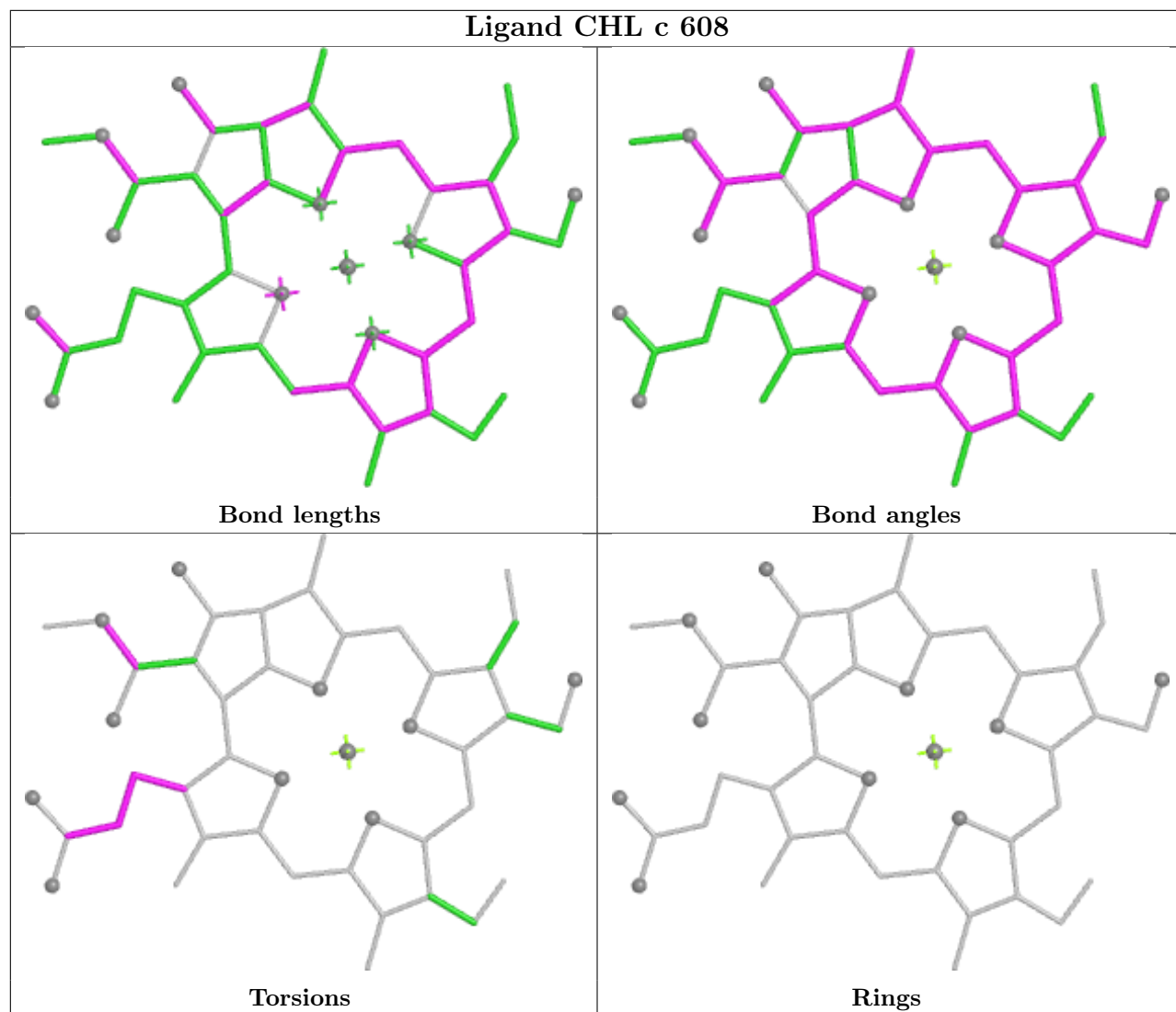
Ligand CLA 8 609

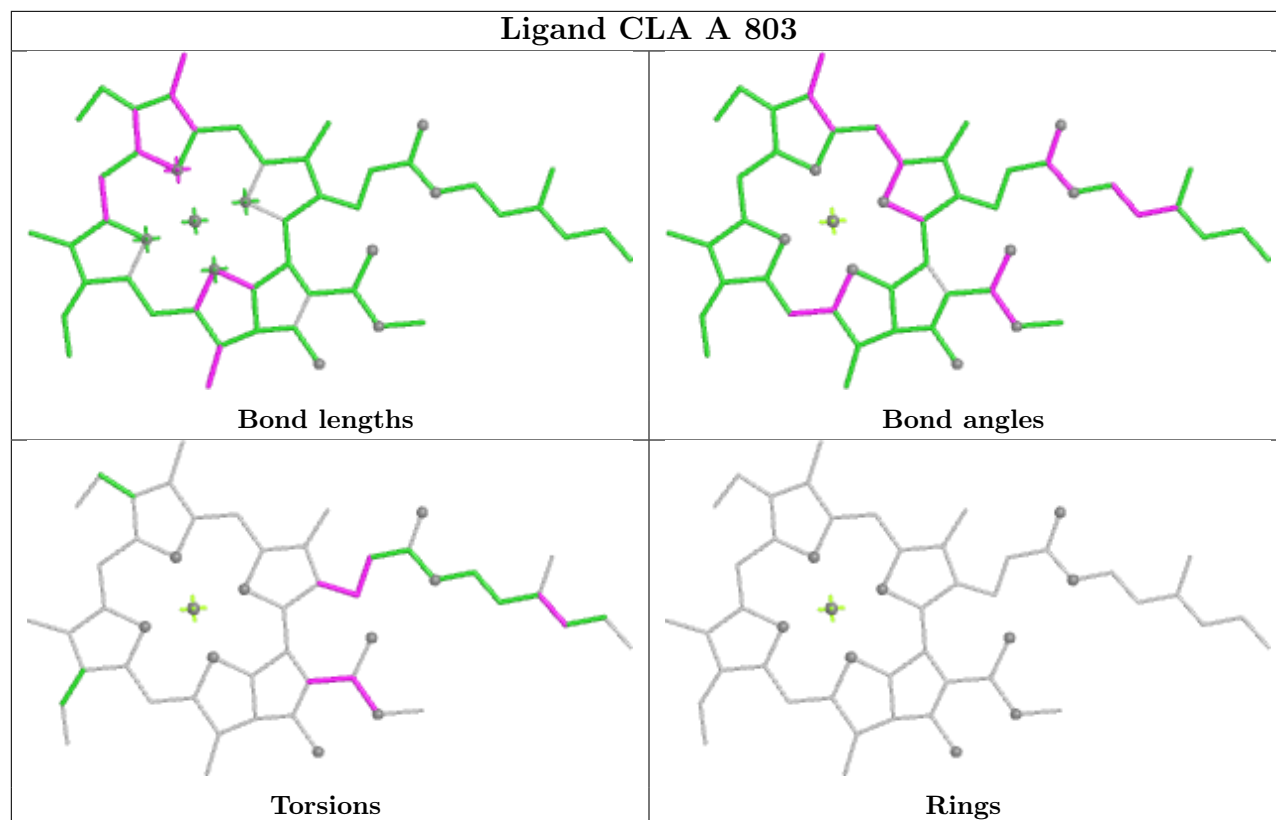


Ligand CLA 5 611

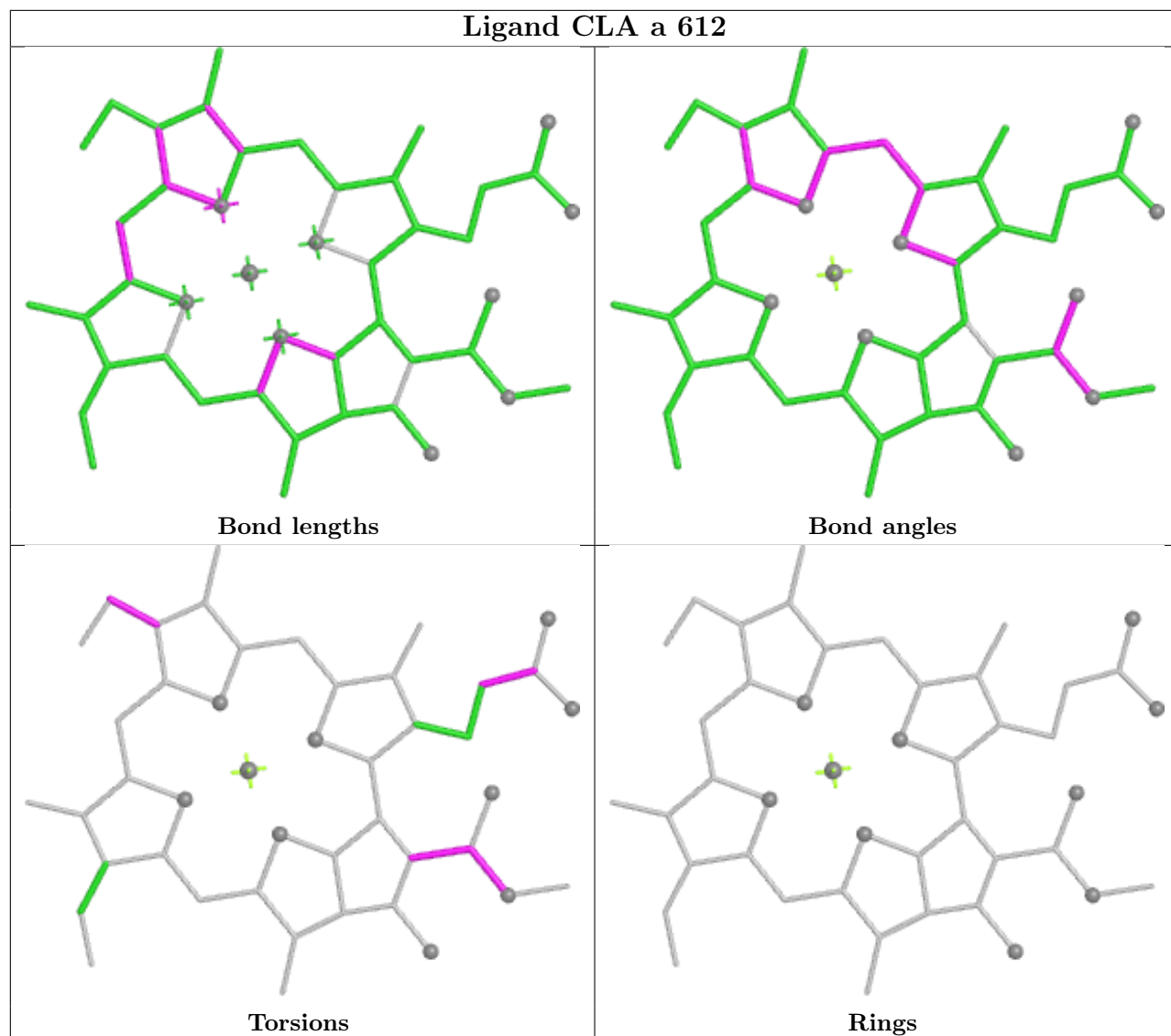


Ligand CHL c 608

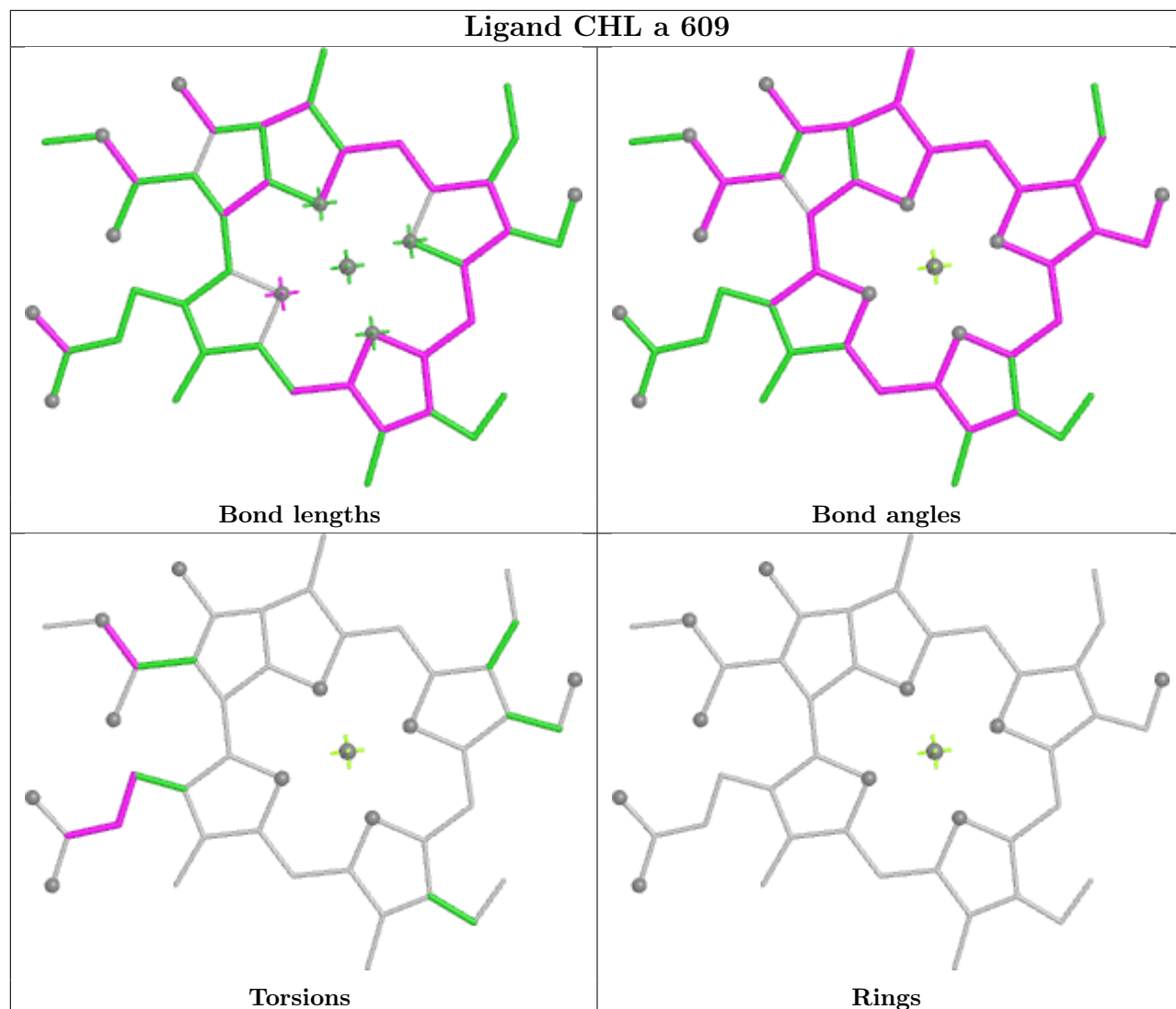




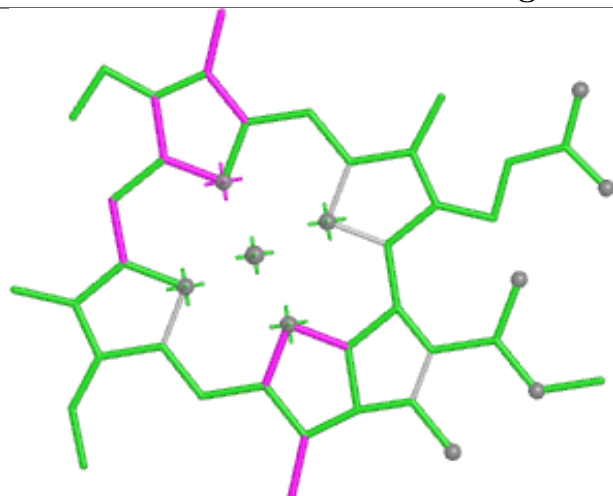
Ligand CLA a 612



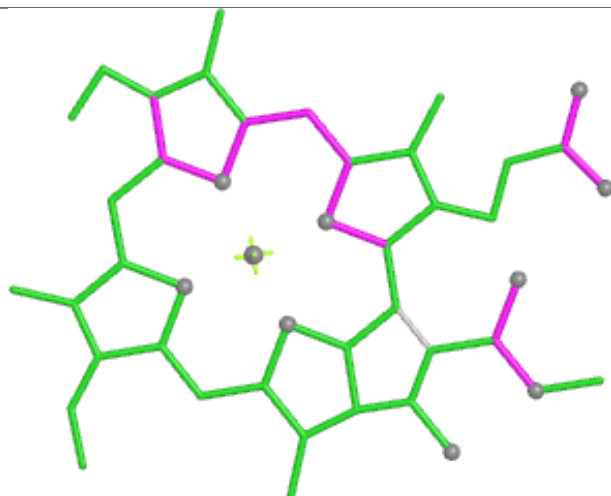
Ligand CHL a 609



Ligand CLA 1 315



Bond lengths



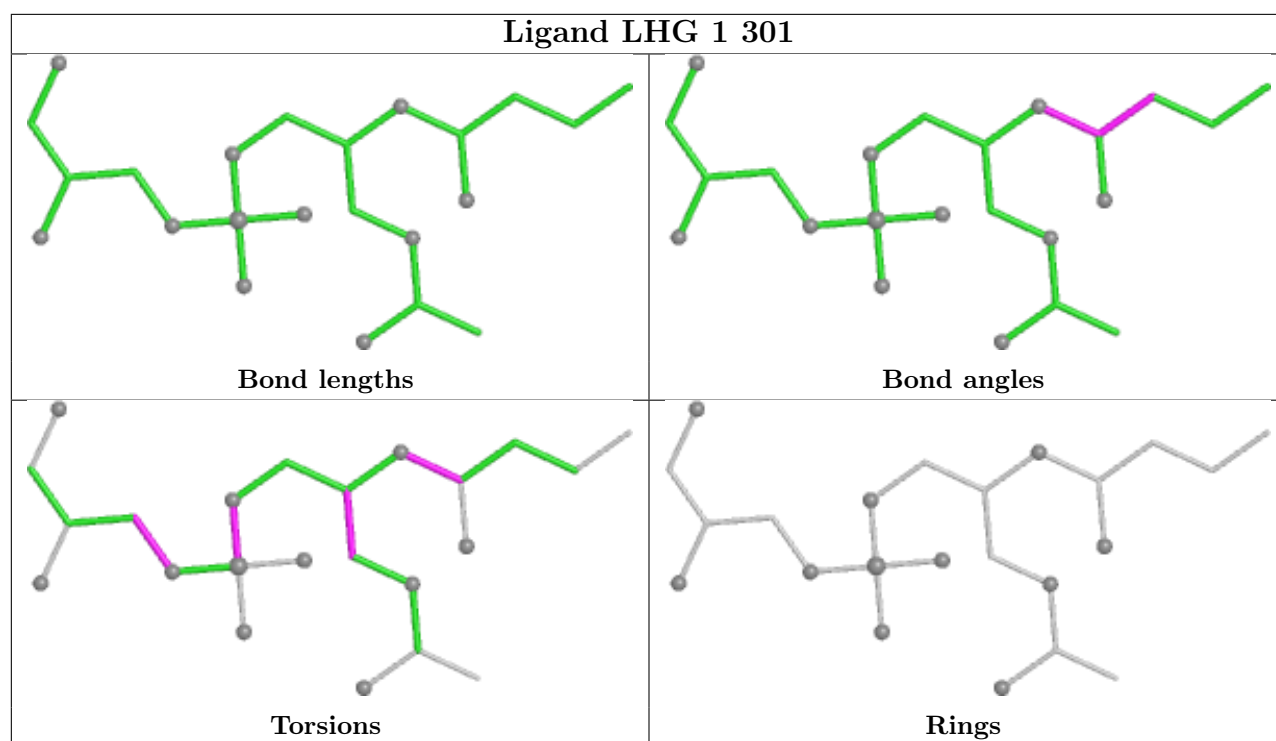
Bond angles



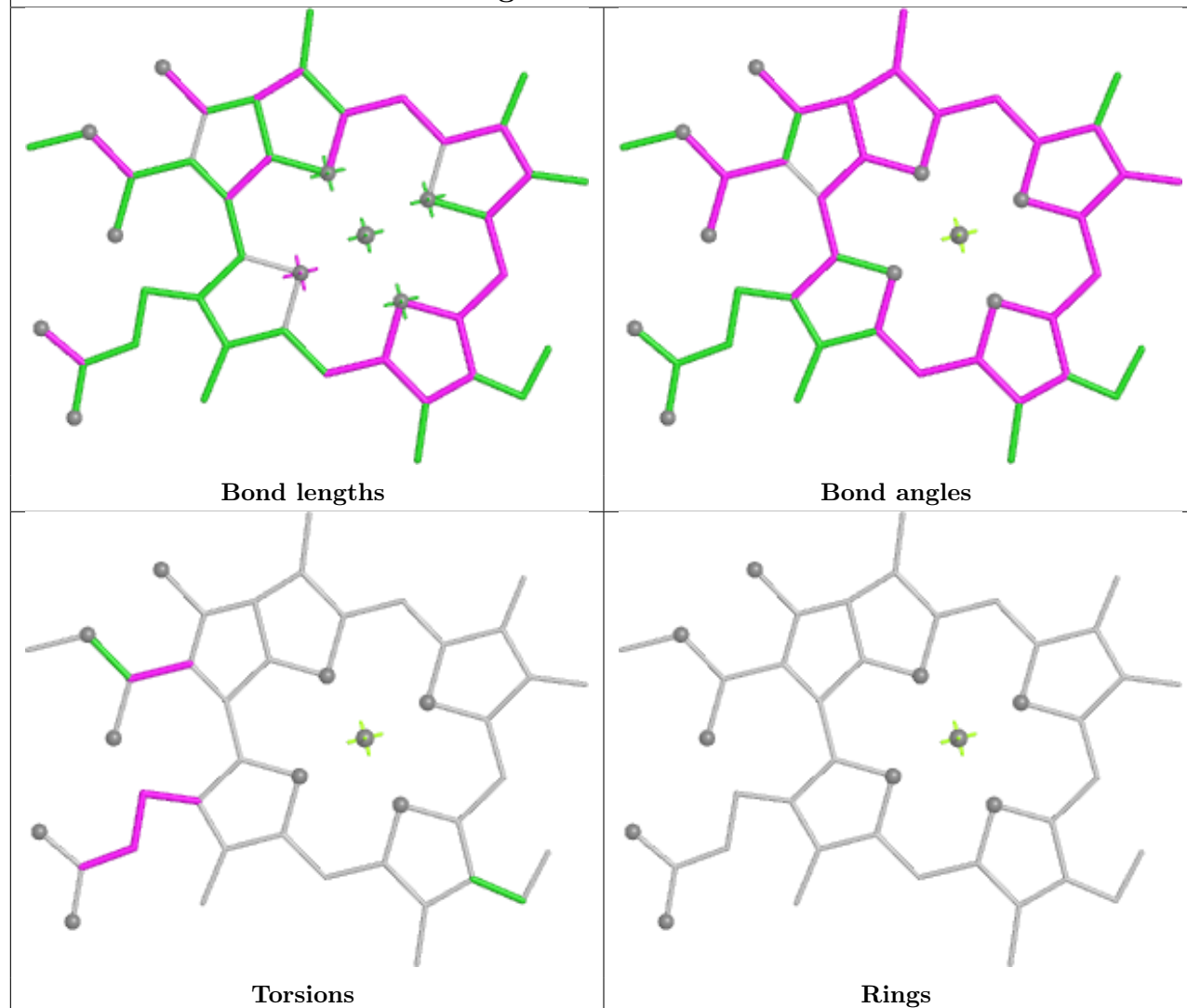
Torsions



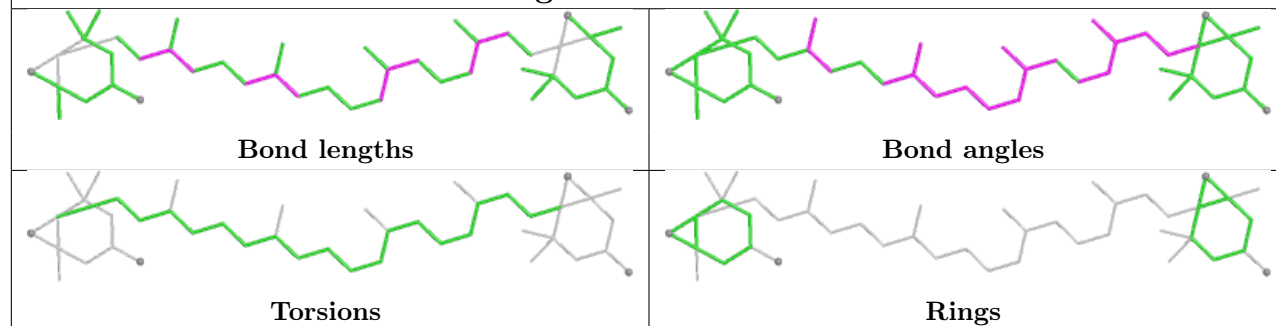
Rings



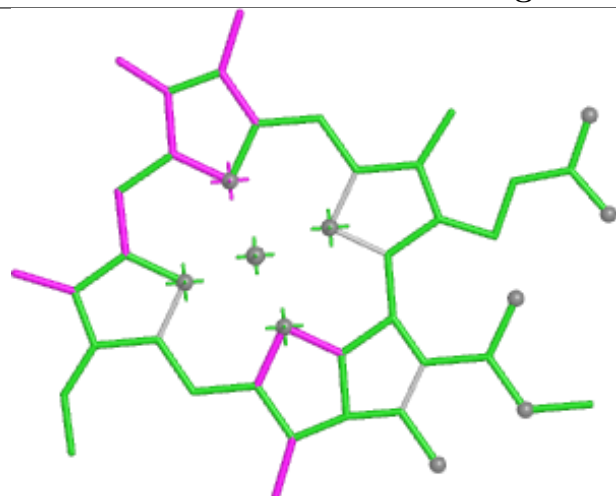
Ligand CHL 6 601



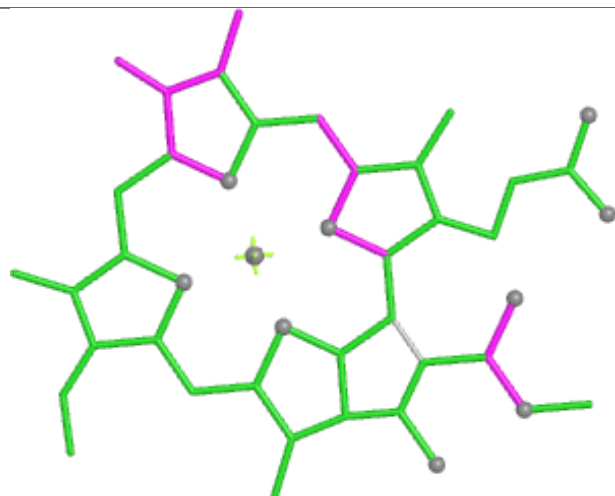
Ligand XAT 1 318



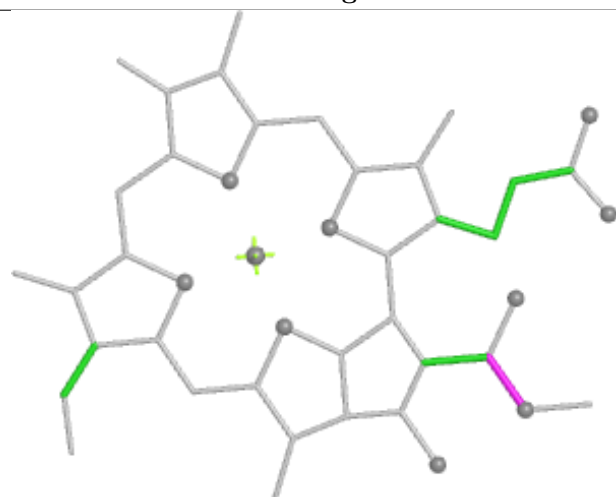
Ligand CLA K 203



Bond lengths



Bond angles

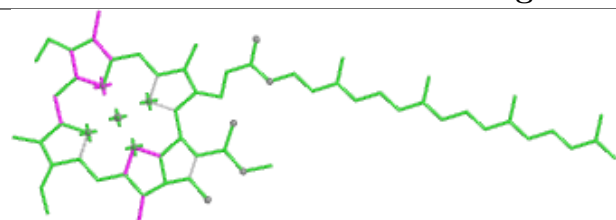


Torsions

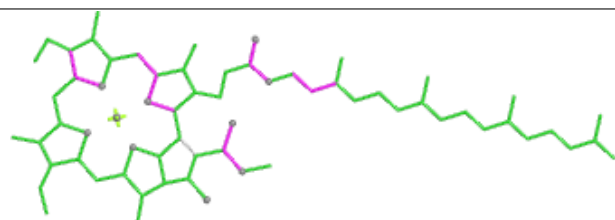


Rings

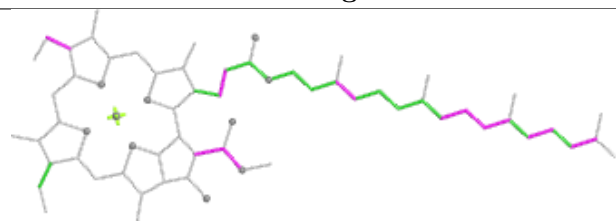
Ligand CLA A 840



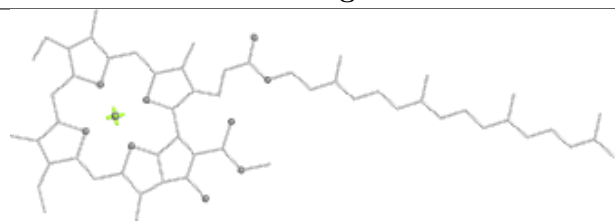
Bond lengths



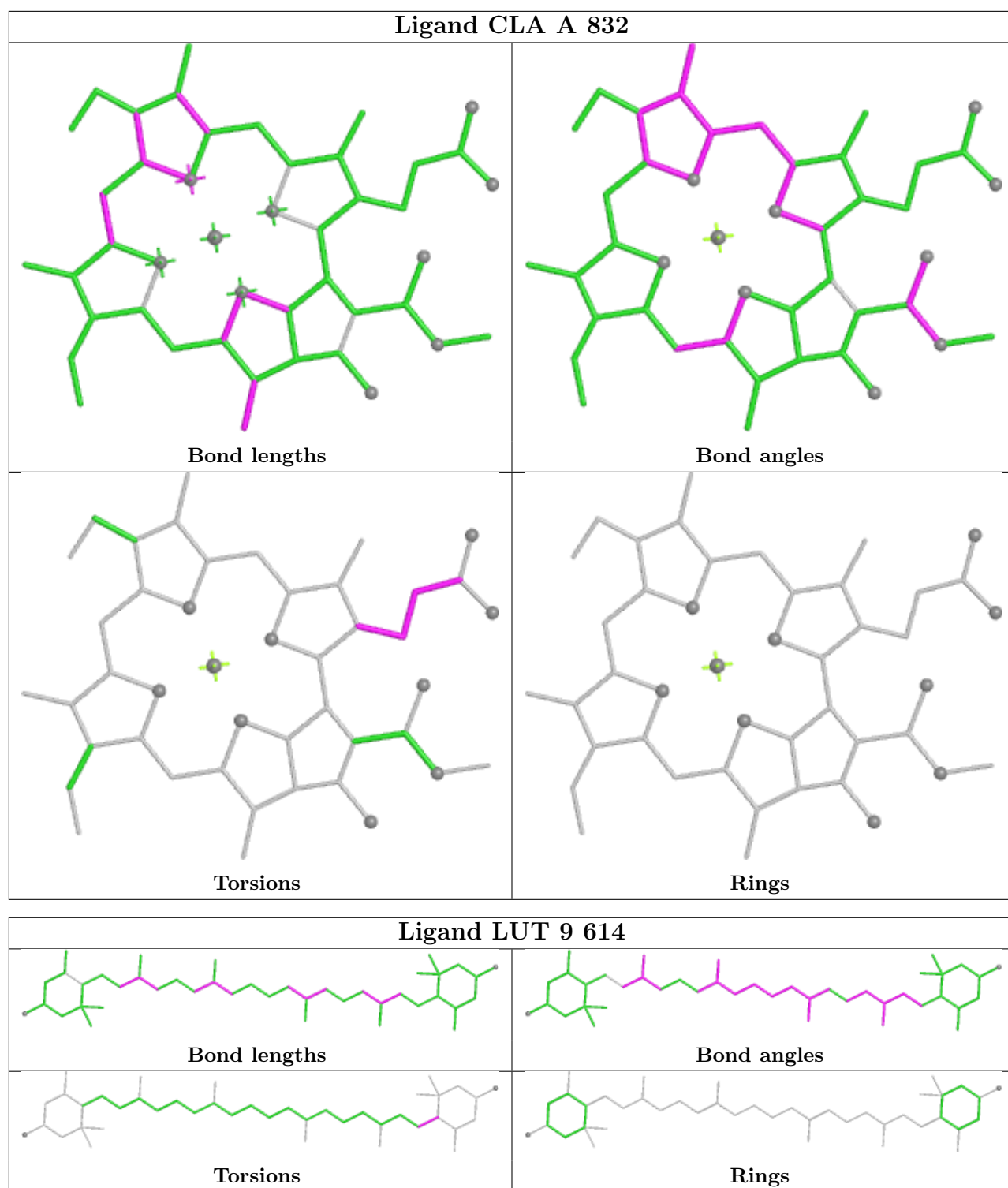
Bond angles



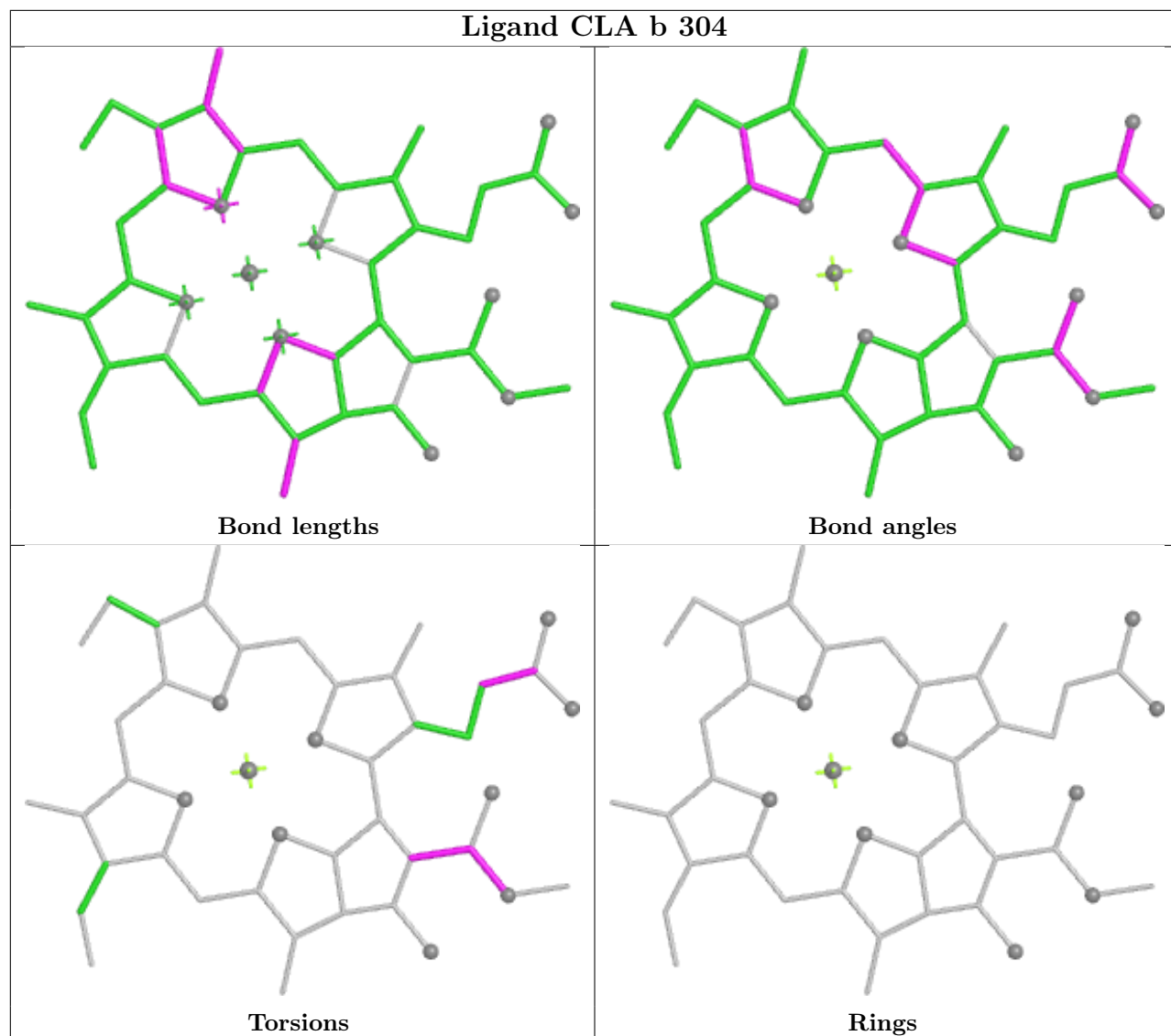
Torsions

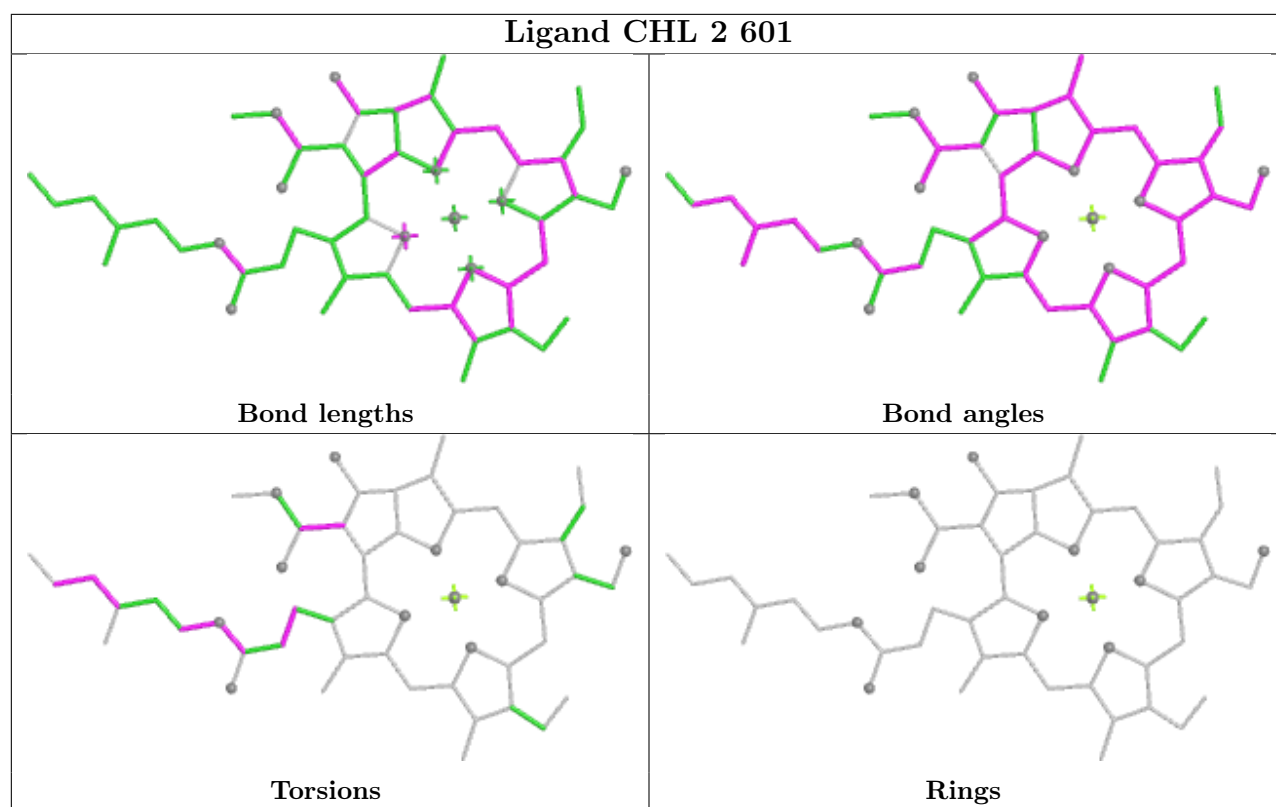


Rings

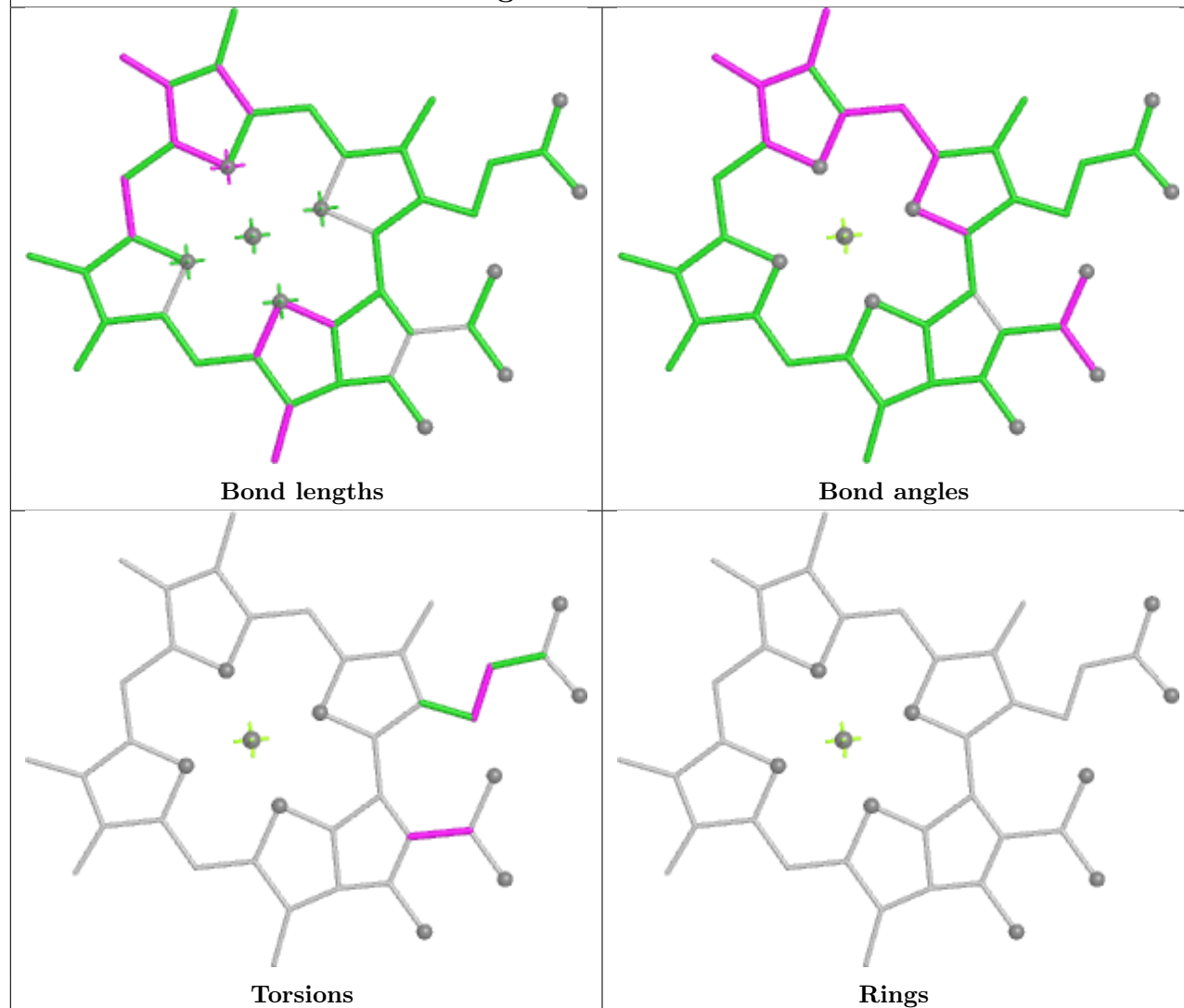


Ligand CLA b 304

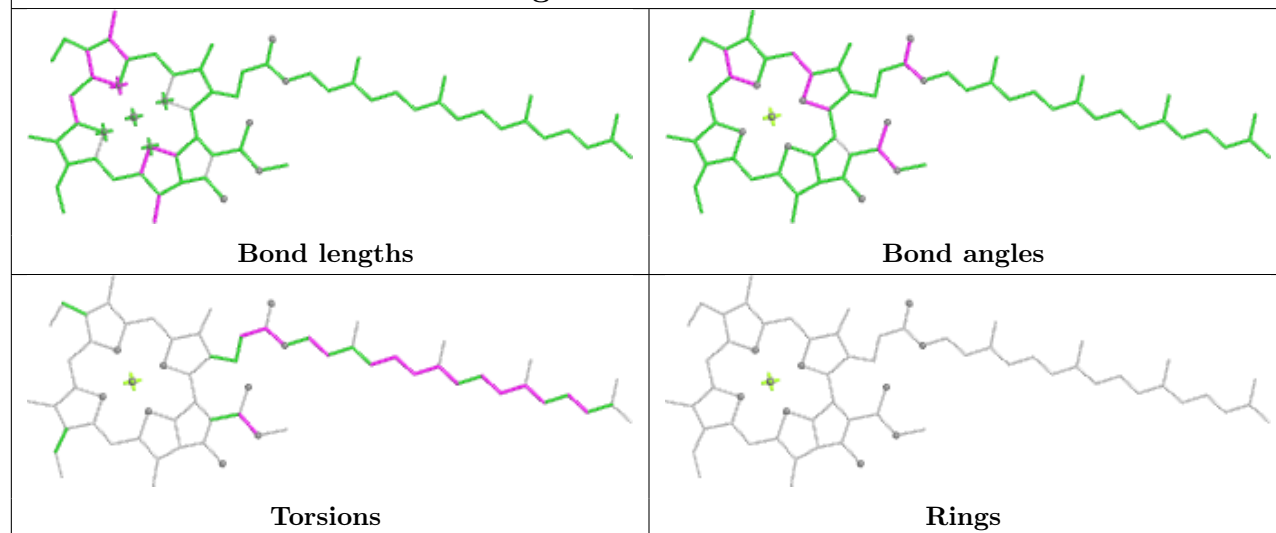




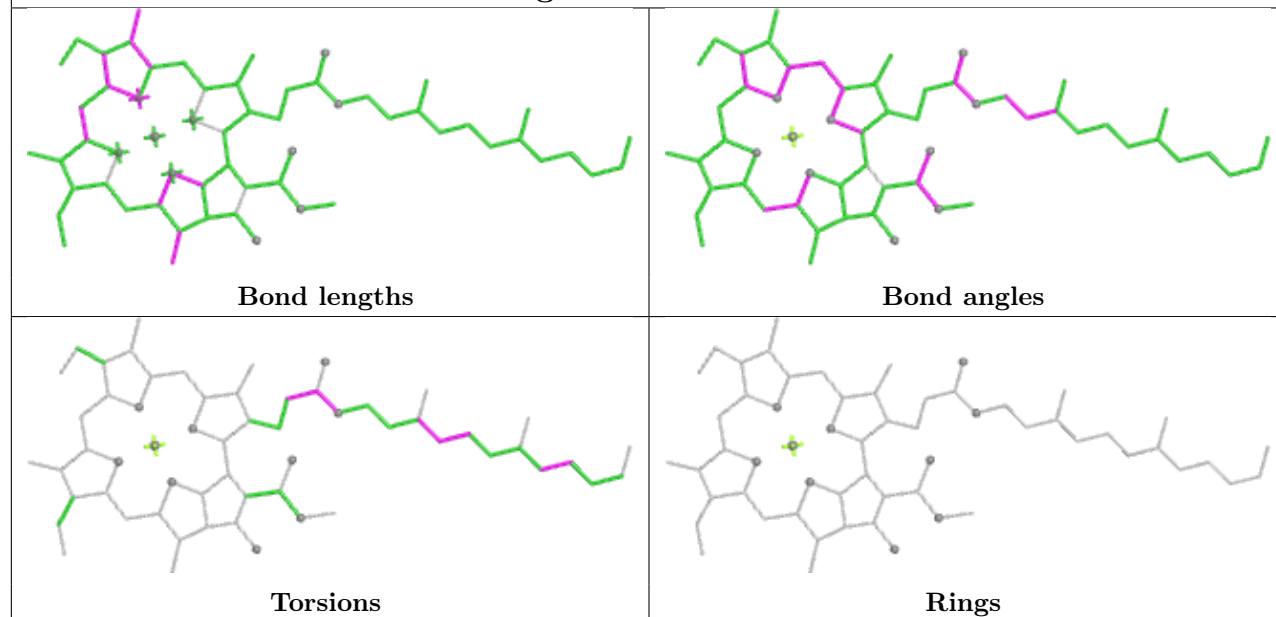
Ligand CLA 7 403



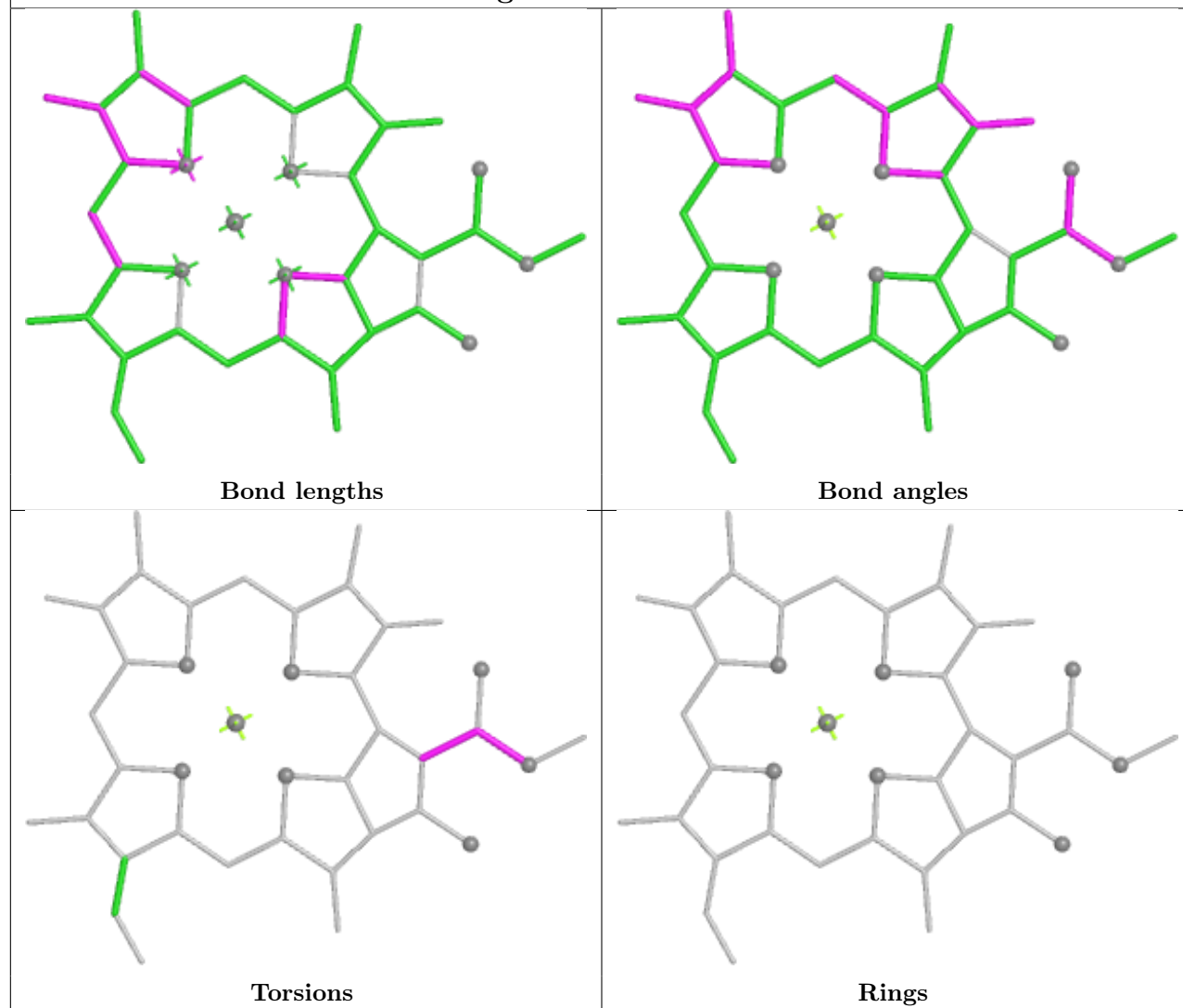
Ligand CLA B 805



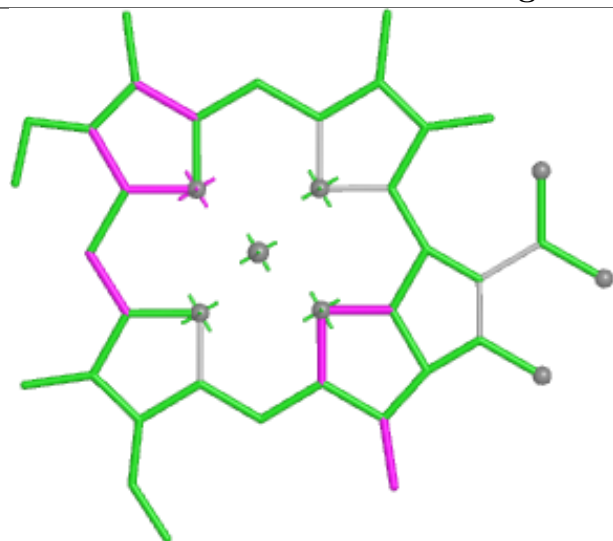
Ligand CLA 3 408



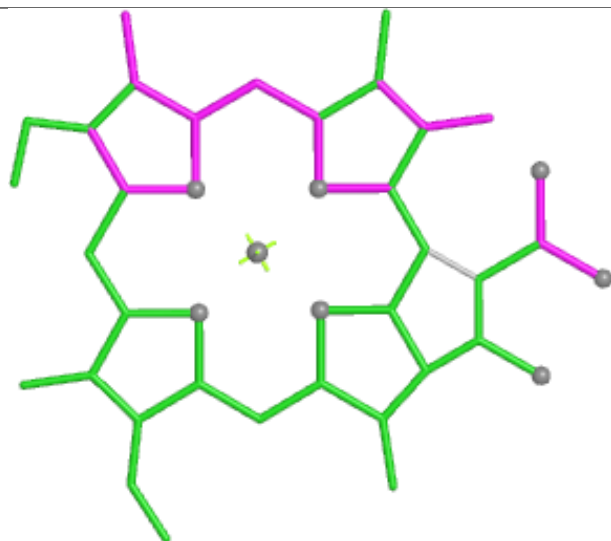
Ligand CLA 5 608



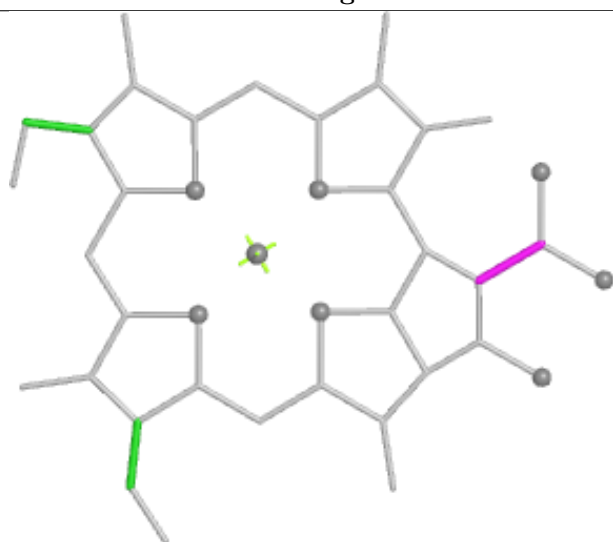
Ligand CLA 7 414



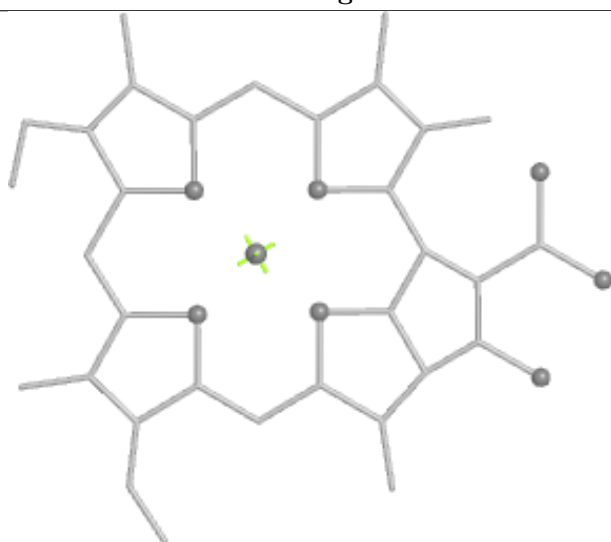
Bond lengths



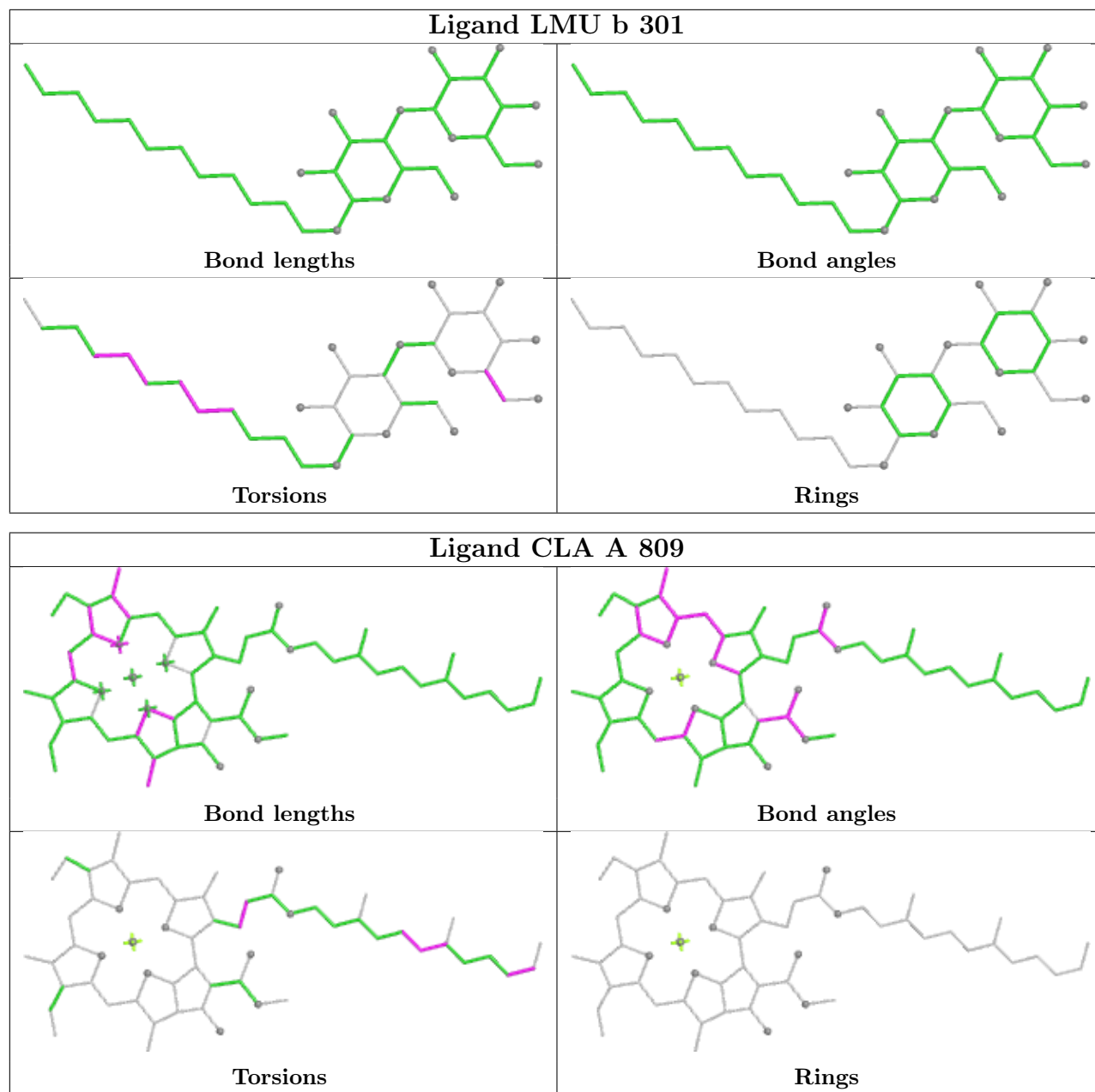
Bond angles



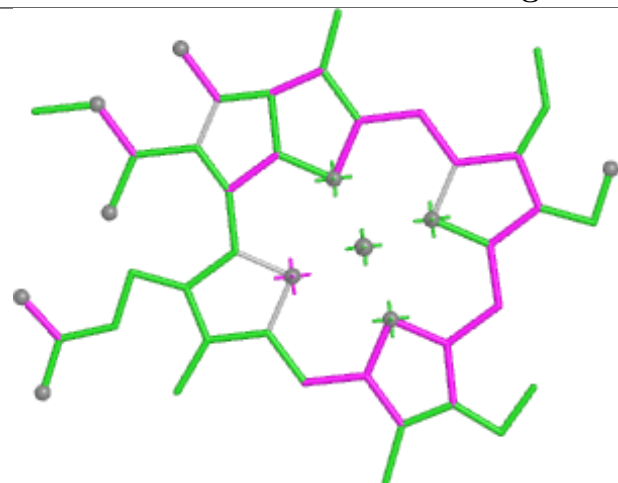
Torsions



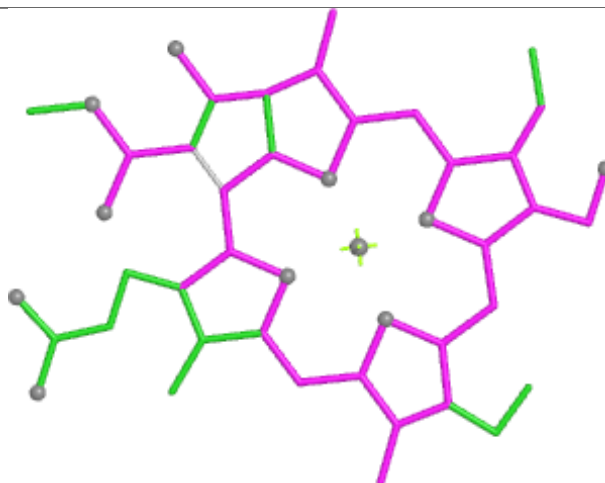
Rings



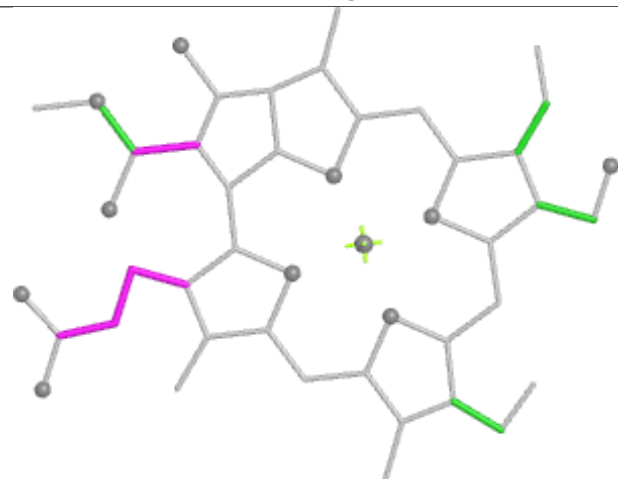
Ligand CHL 9 606



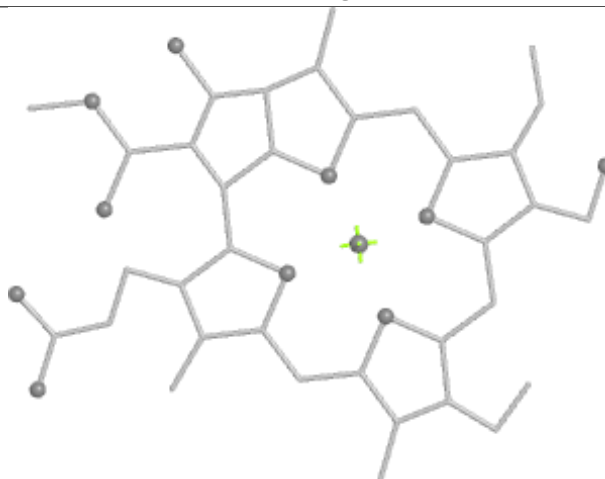
Bond lengths



Bond angles

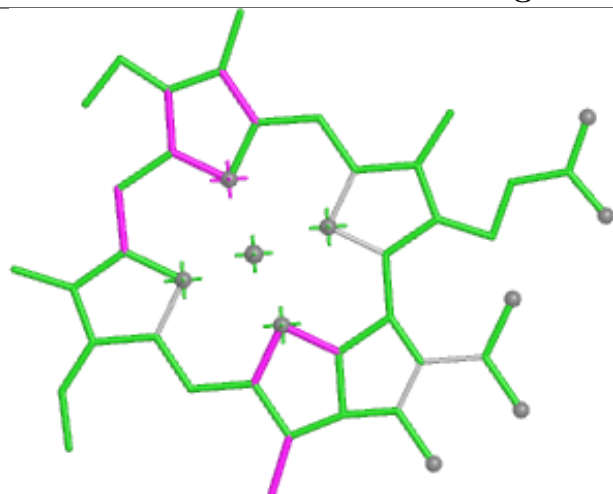


Torsions

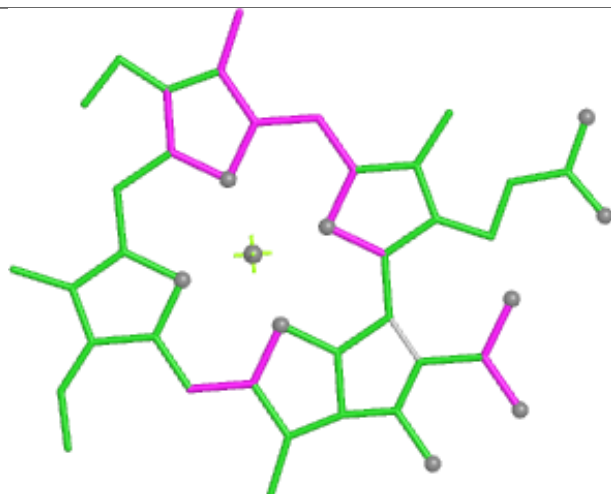


Rings

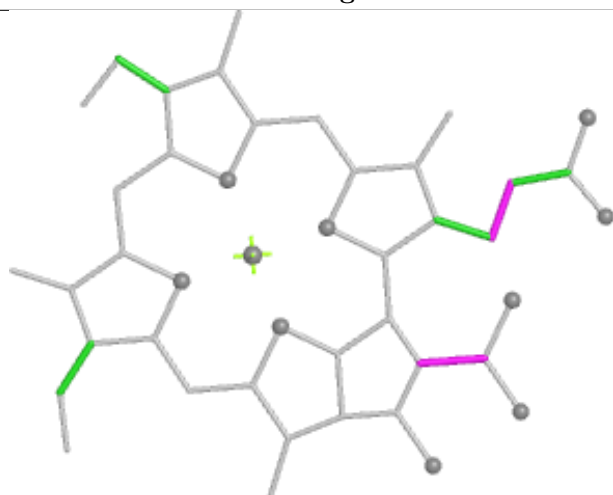
Ligand CLA B 813



Bond lengths



Bond angles

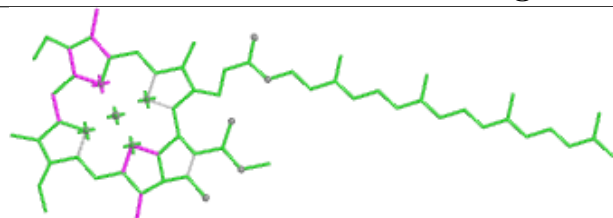


Torsions

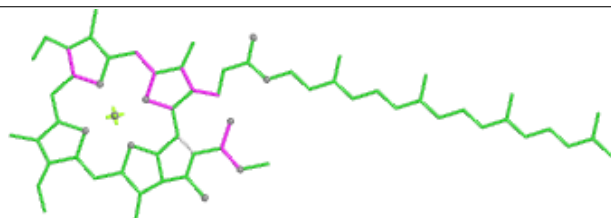


Rings

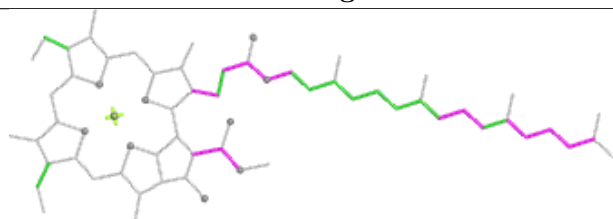
Ligand CLA A 841



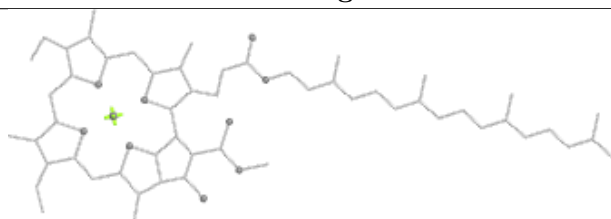
Bond lengths



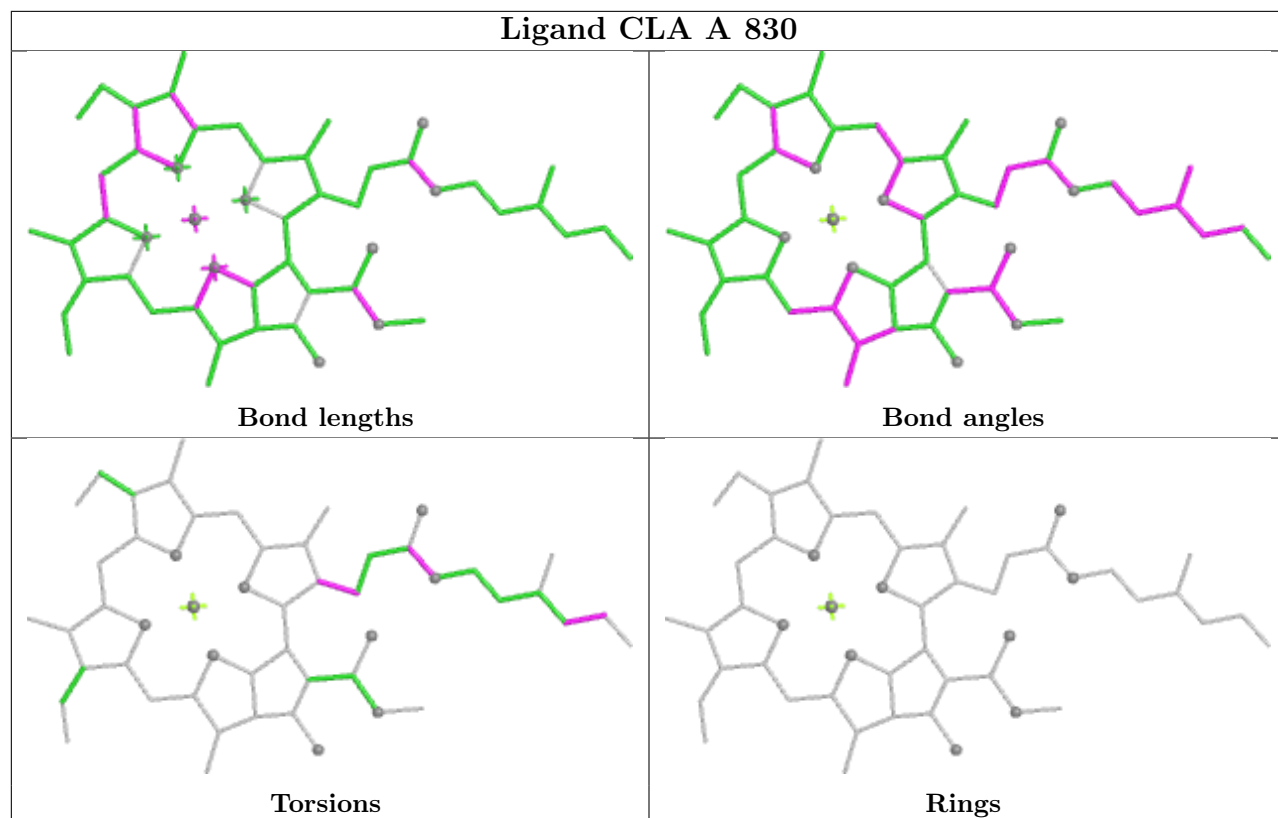
Bond angles



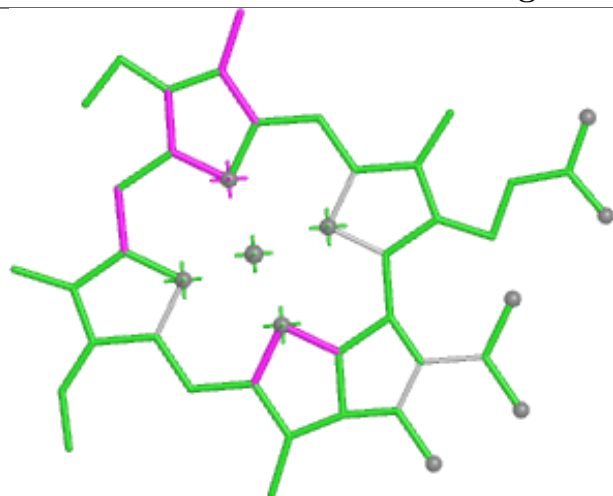
Torsions



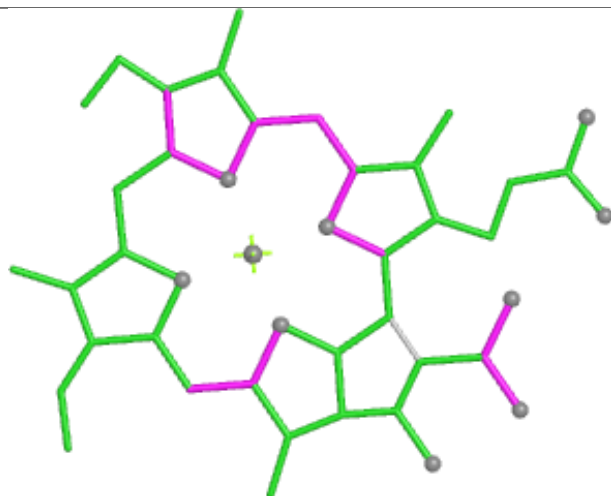
Rings



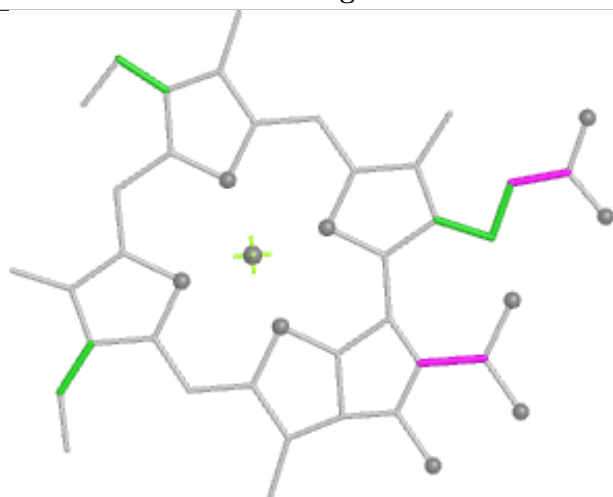
Ligand CLA 8 603



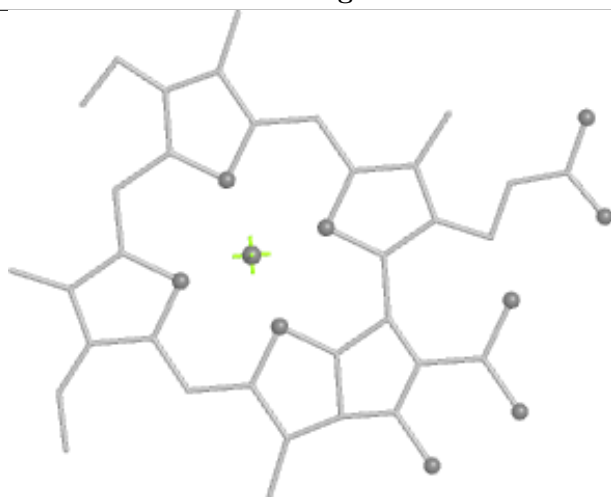
Bond lengths



Bond angles

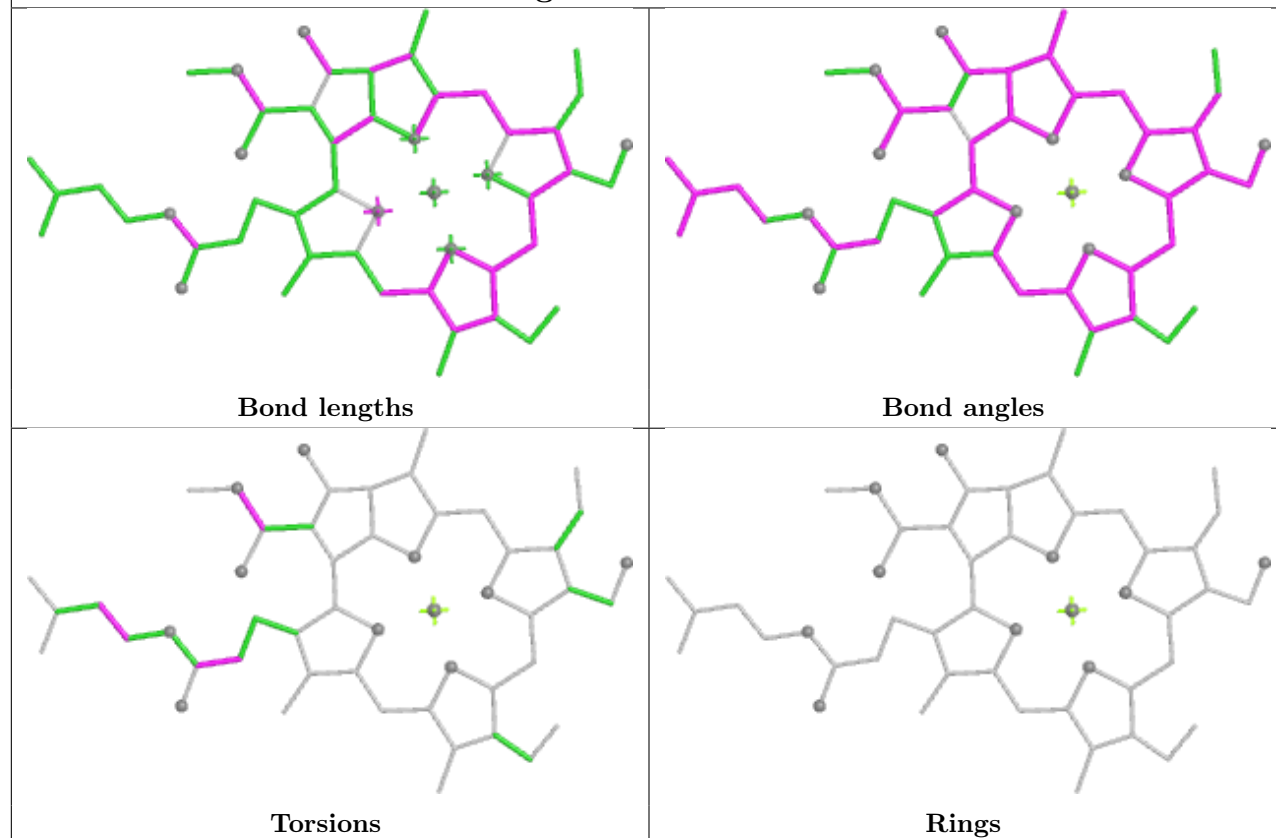


Torsions

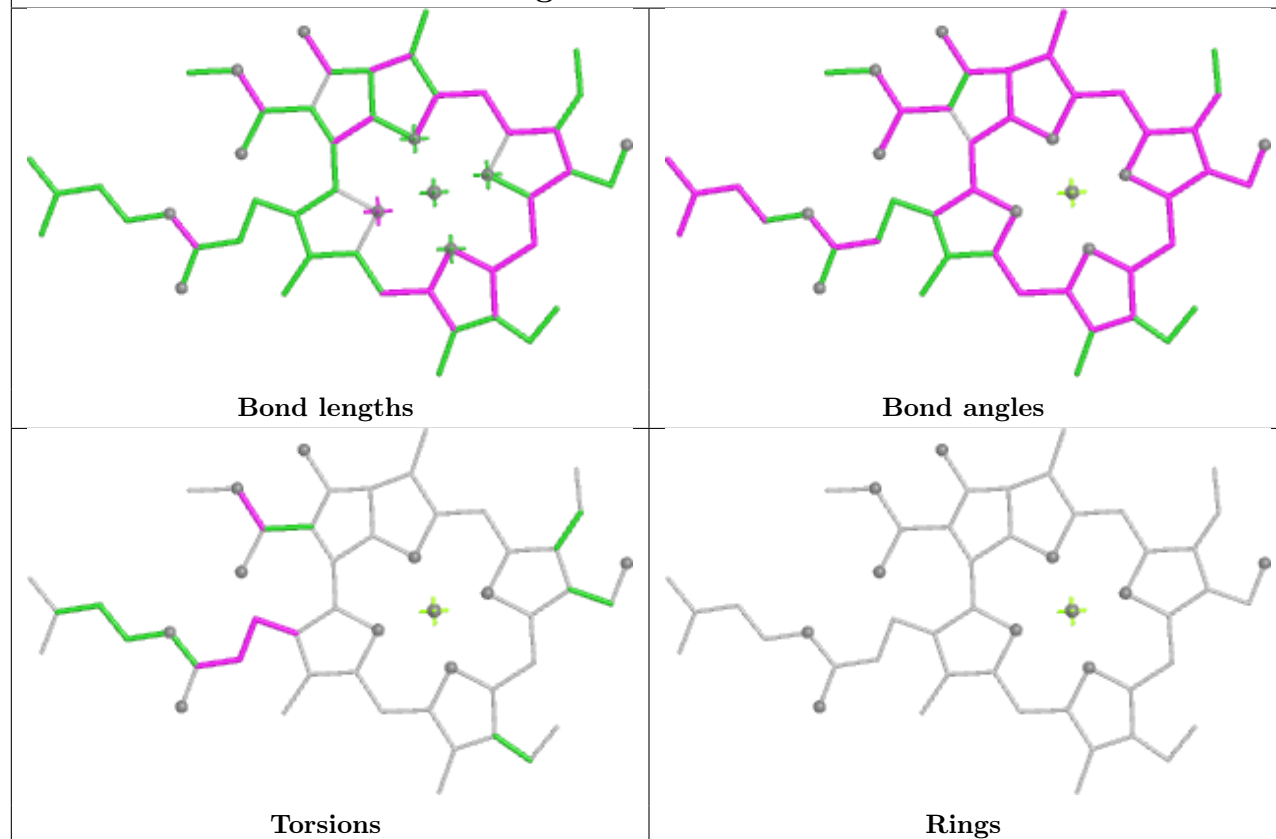


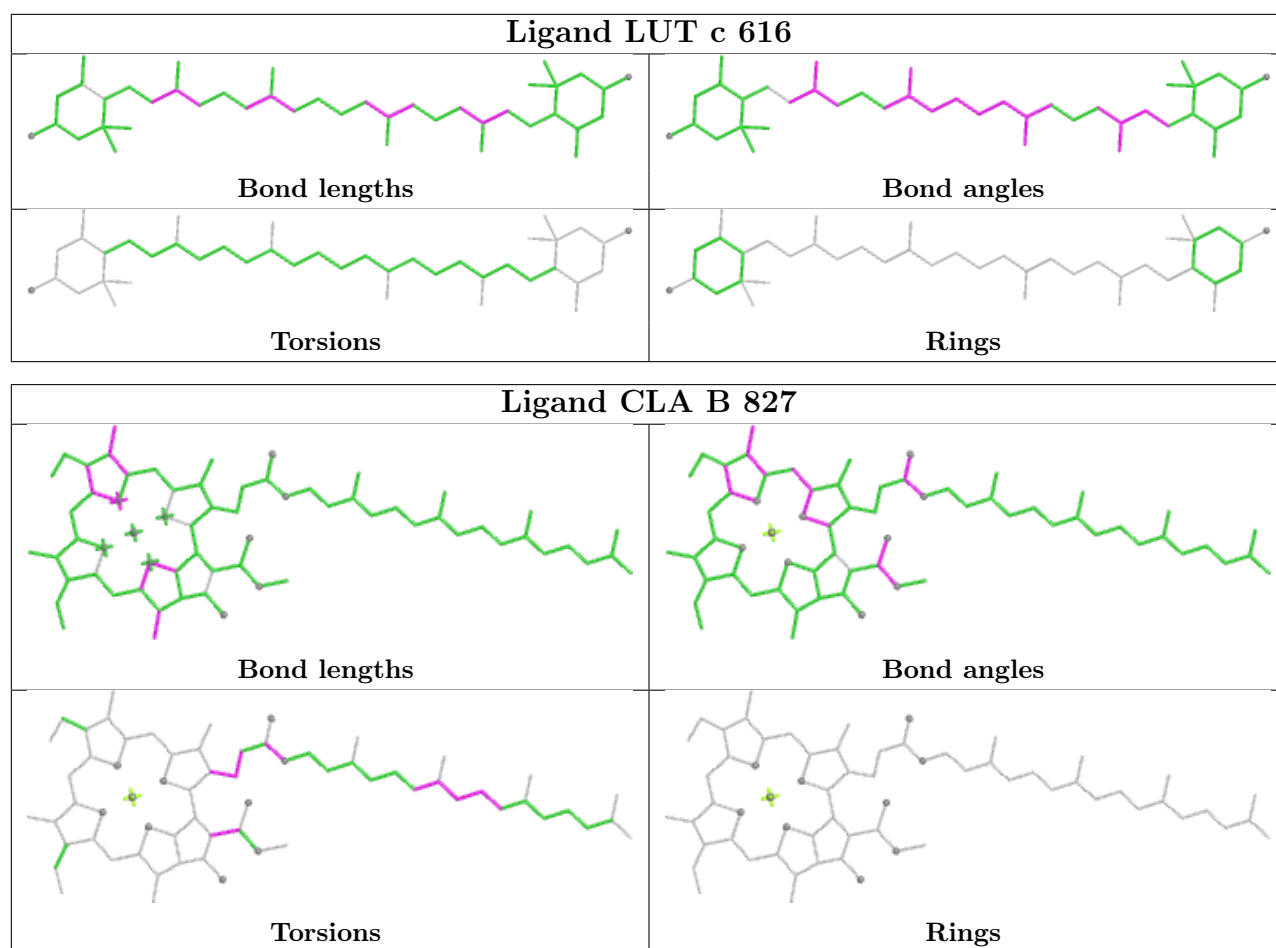
Rings

Ligand CHL 6 607

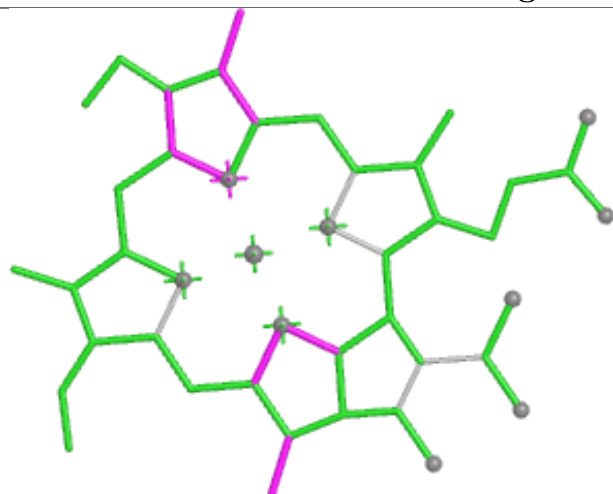


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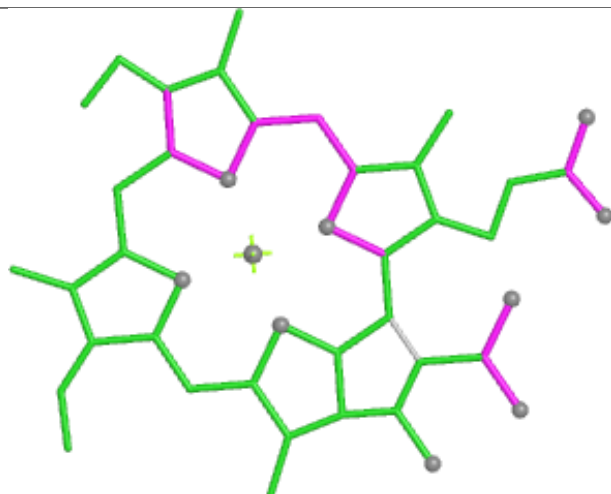




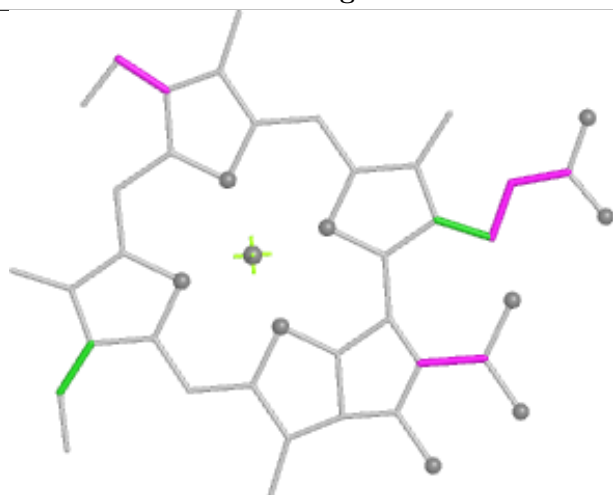
Ligand CLA 4 603



Bond lengths



Bond angles

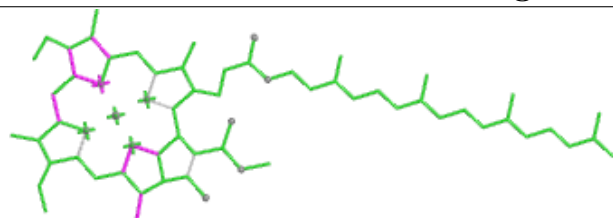


Torsions

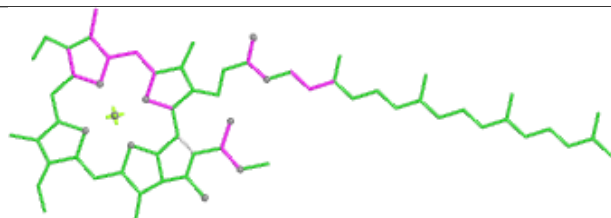


Rings

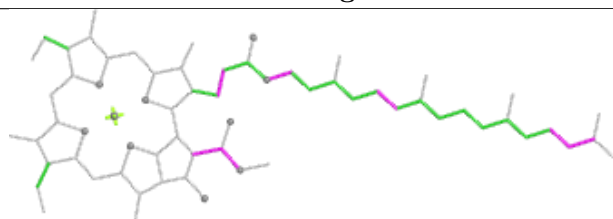
Ligand CLA A 814



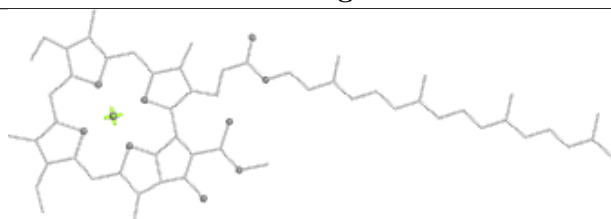
Bond lengths



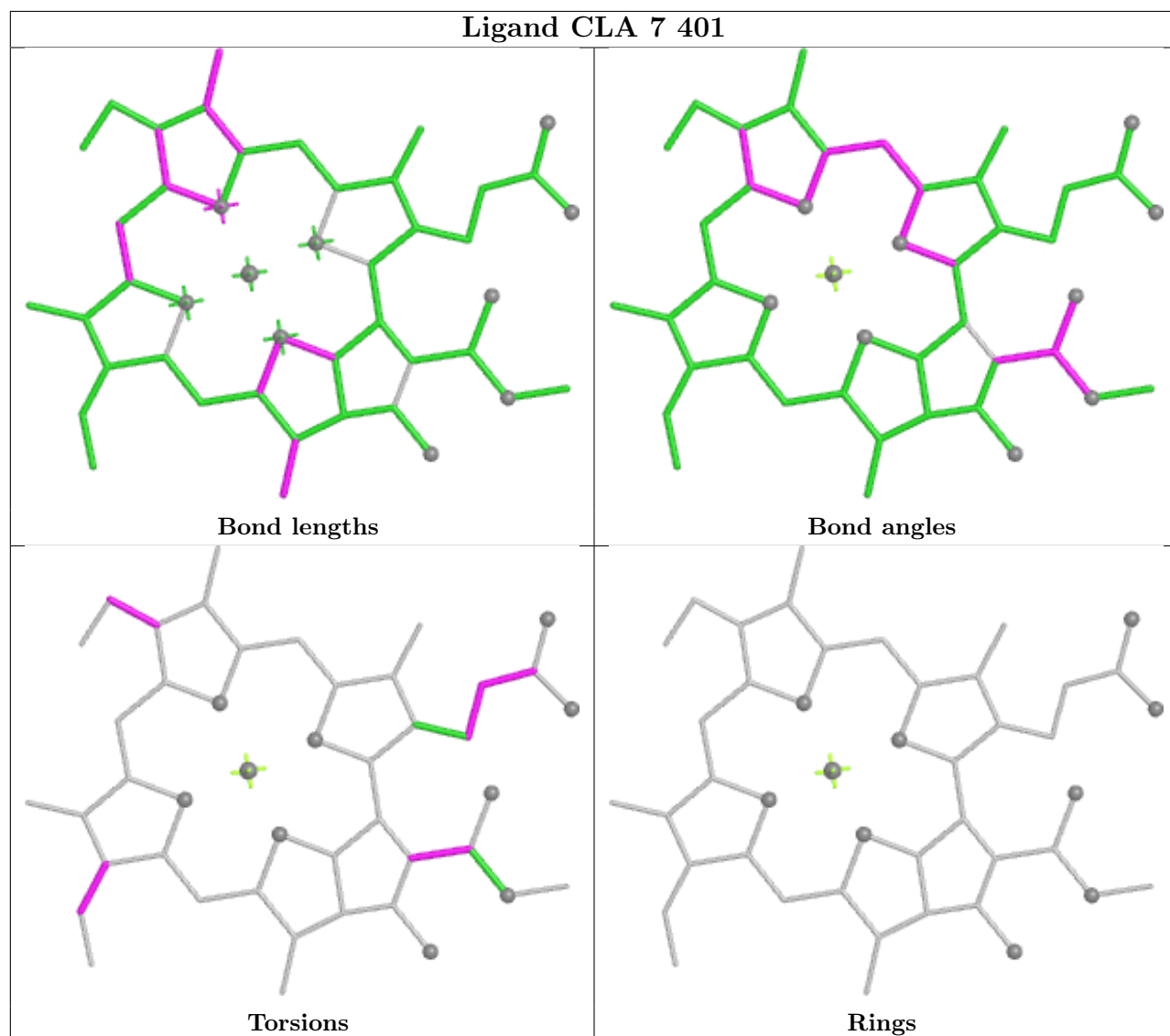
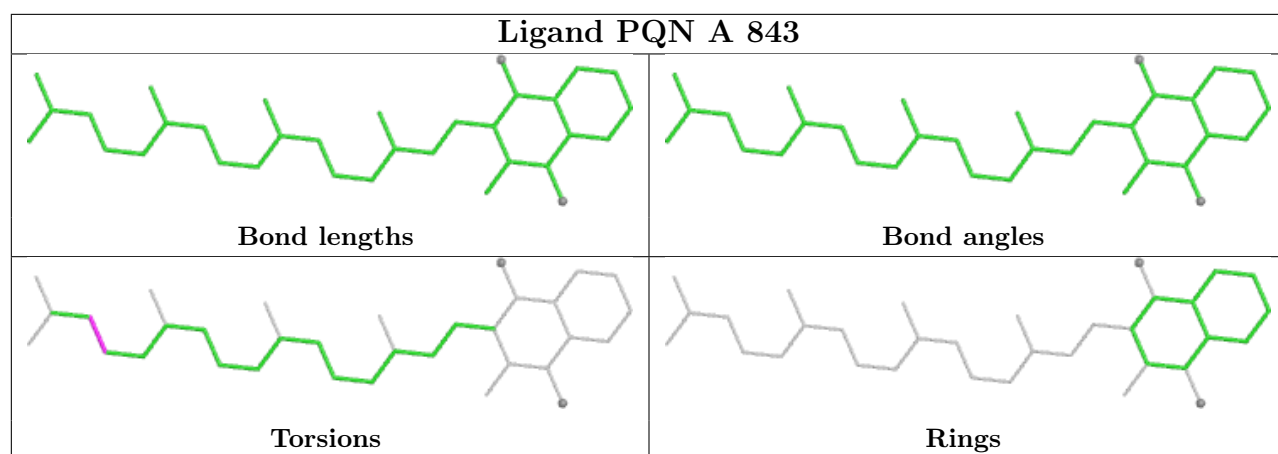
Bond angles



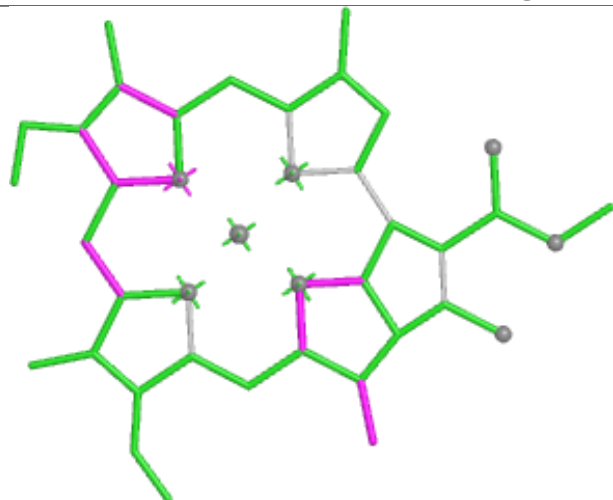
Torsions



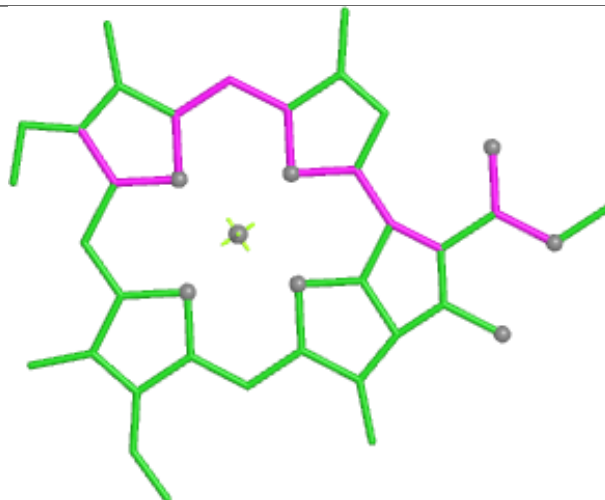
Rings



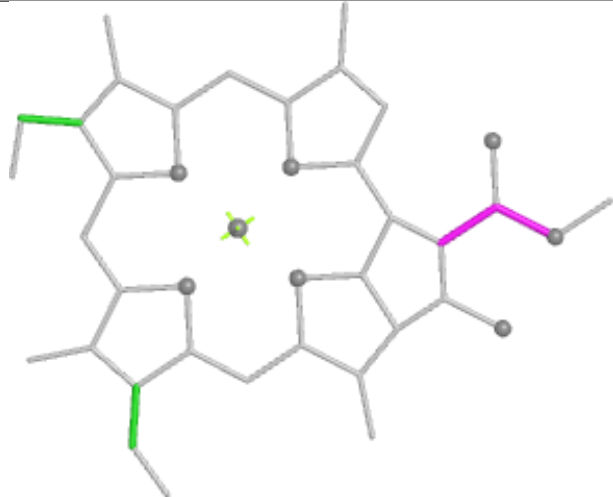
Ligand CLA 1 306



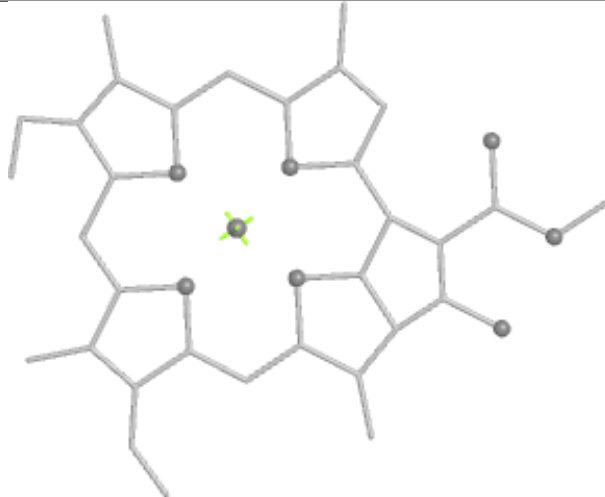
Bond lengths



Bond angles

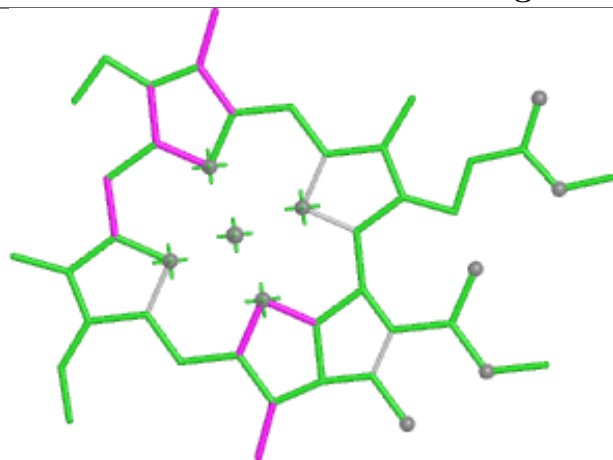


Torsions

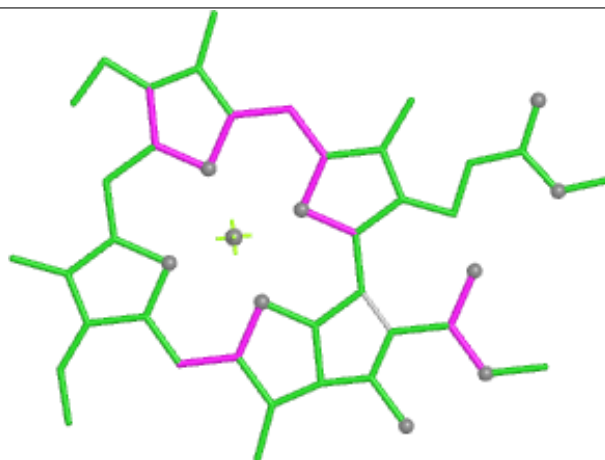


Rings

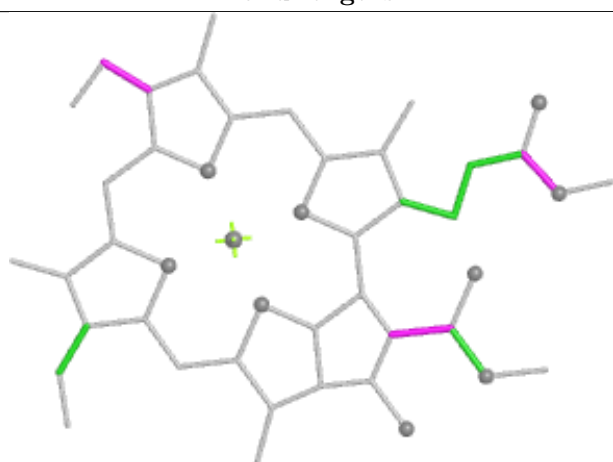
Ligand CLA B 820



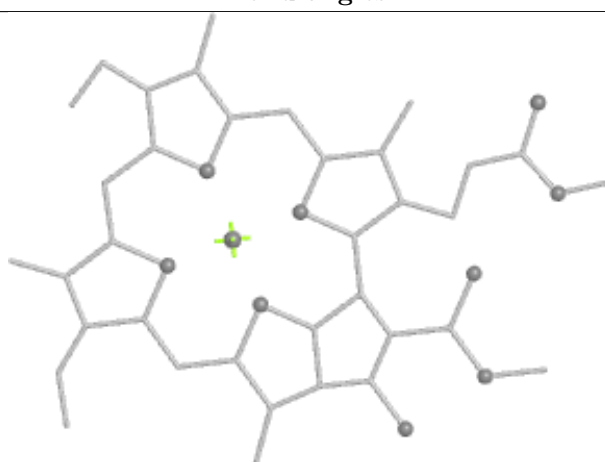
Bond lengths



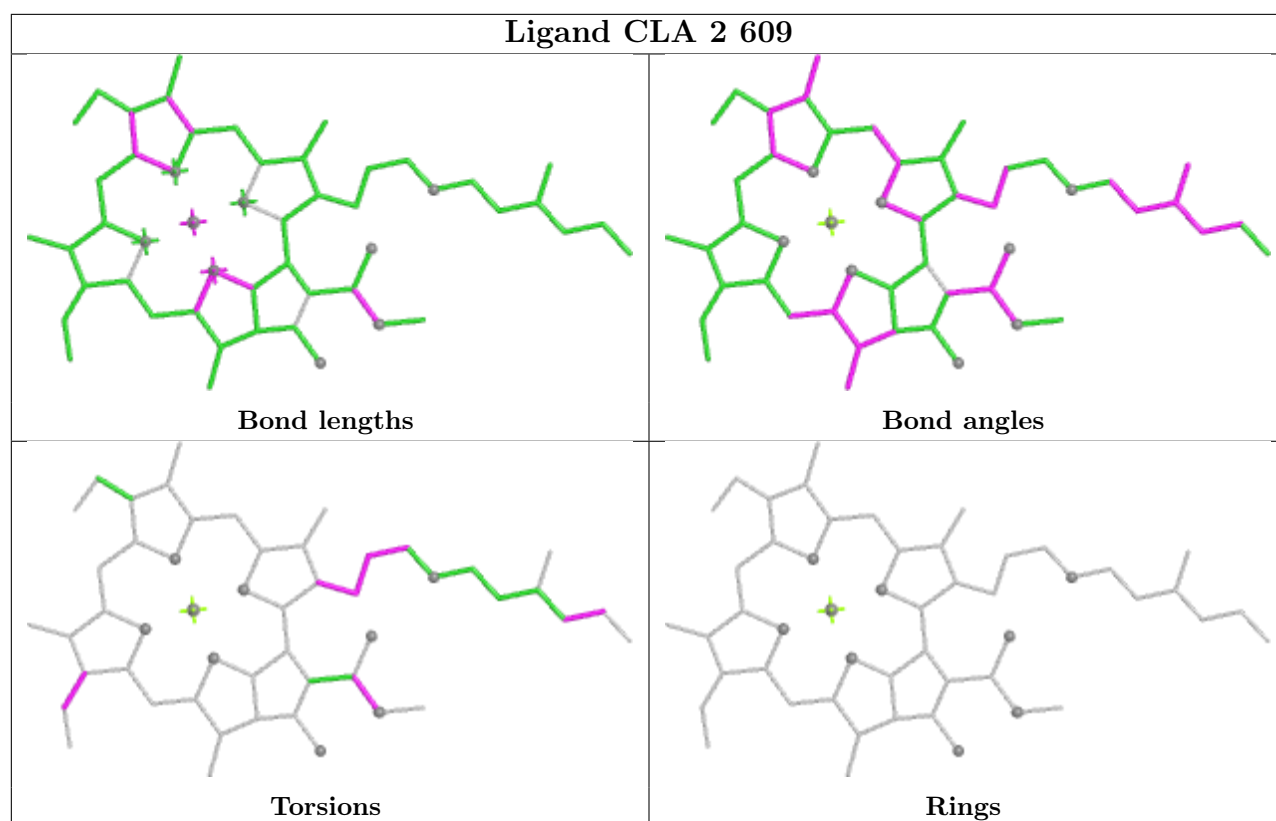
Bond angles



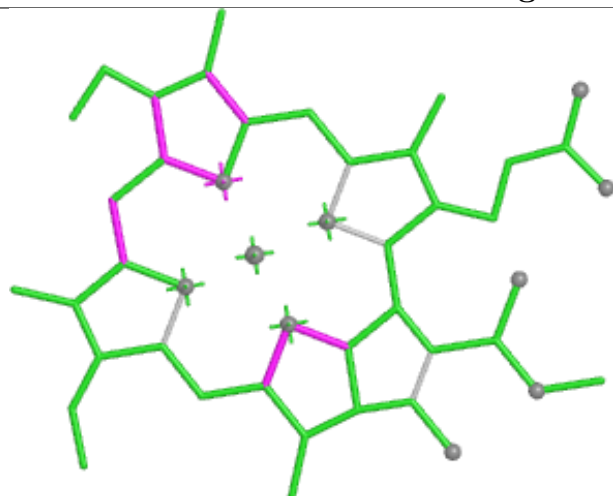
Torsions



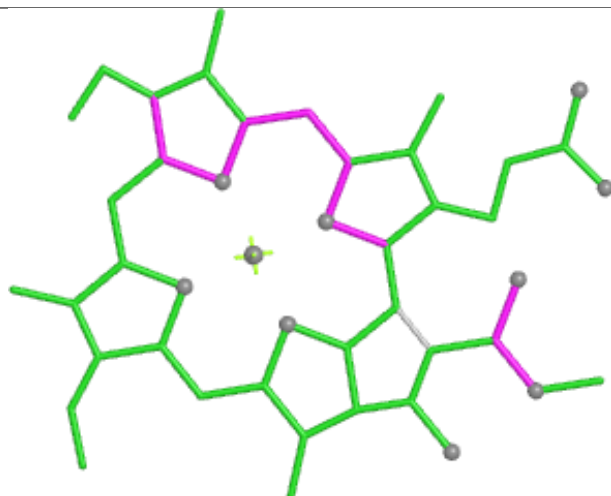
Rings



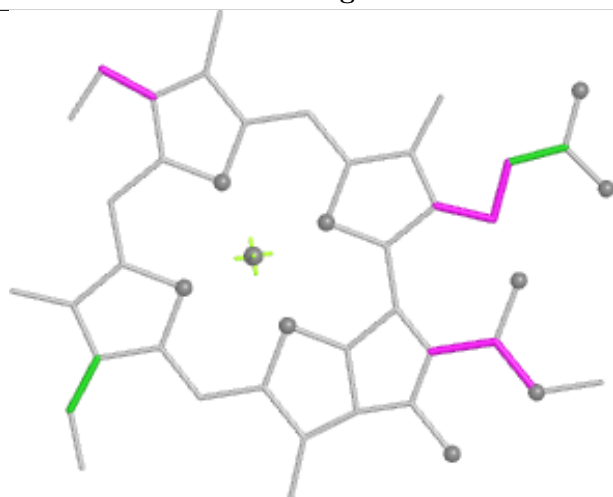
Ligand CLA 8 601



Bond lengths



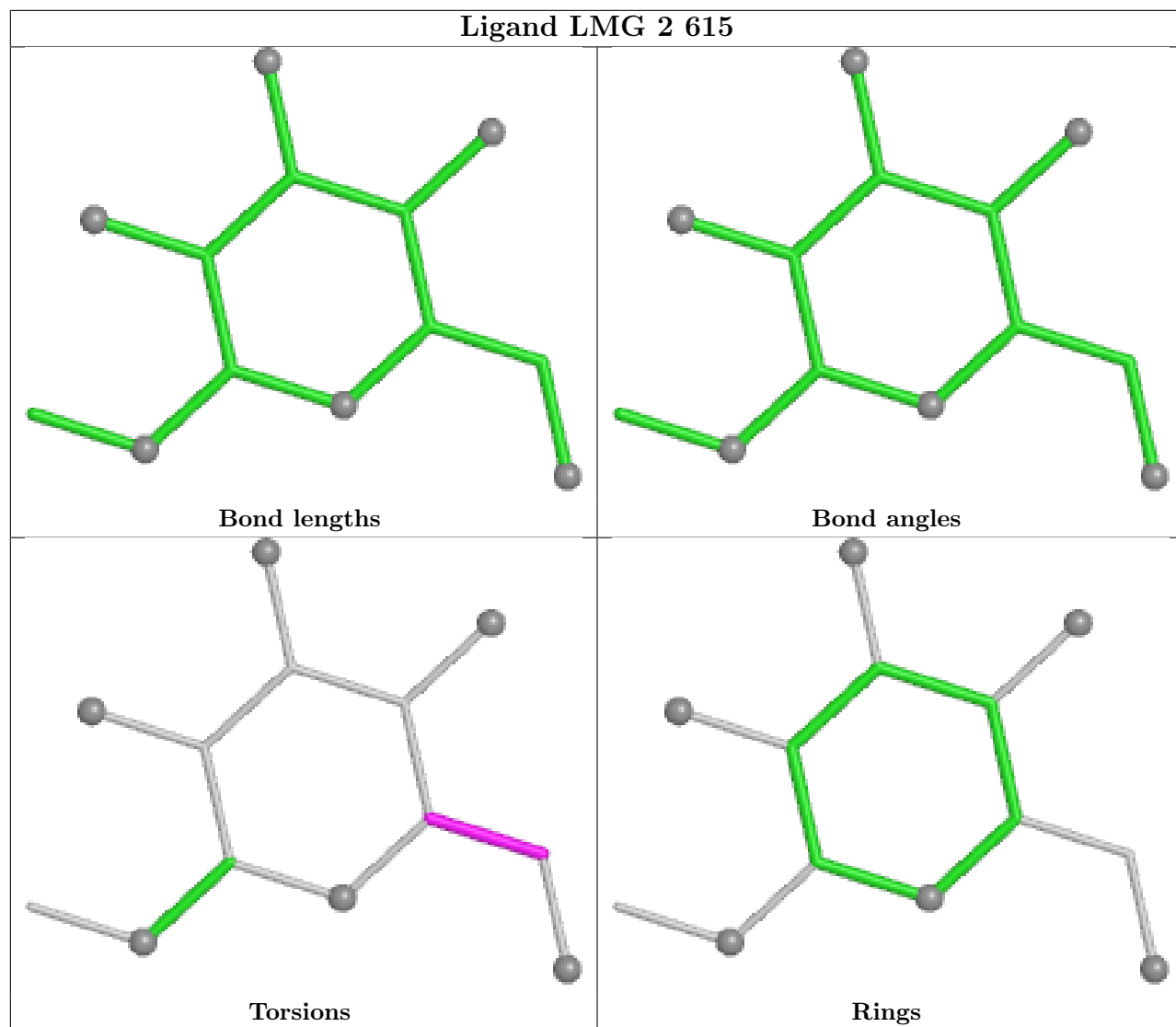
Bond angles



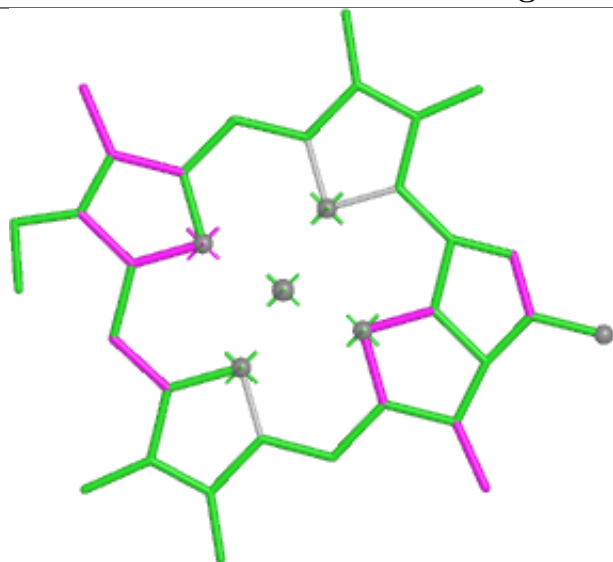
Torsions



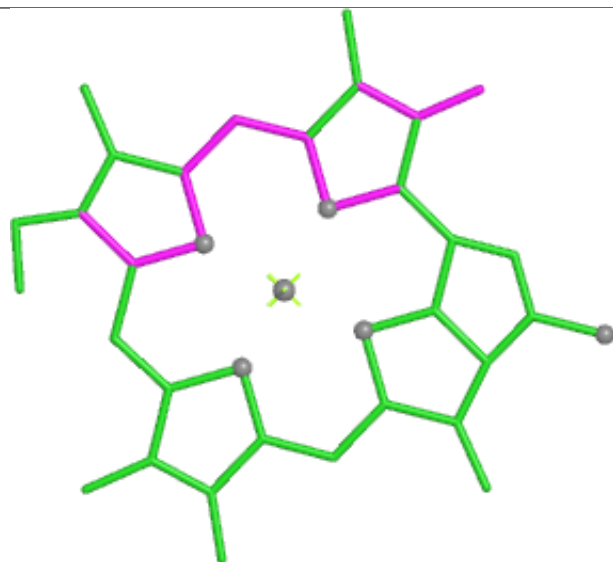
Rings



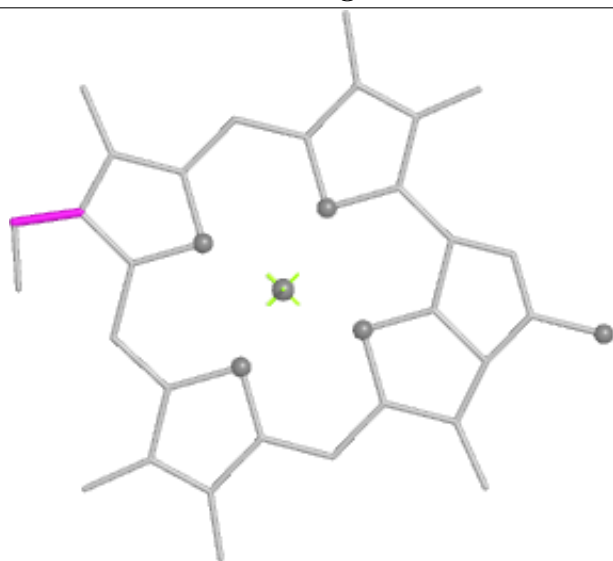
Ligand CLA 3 414



Bond lengths



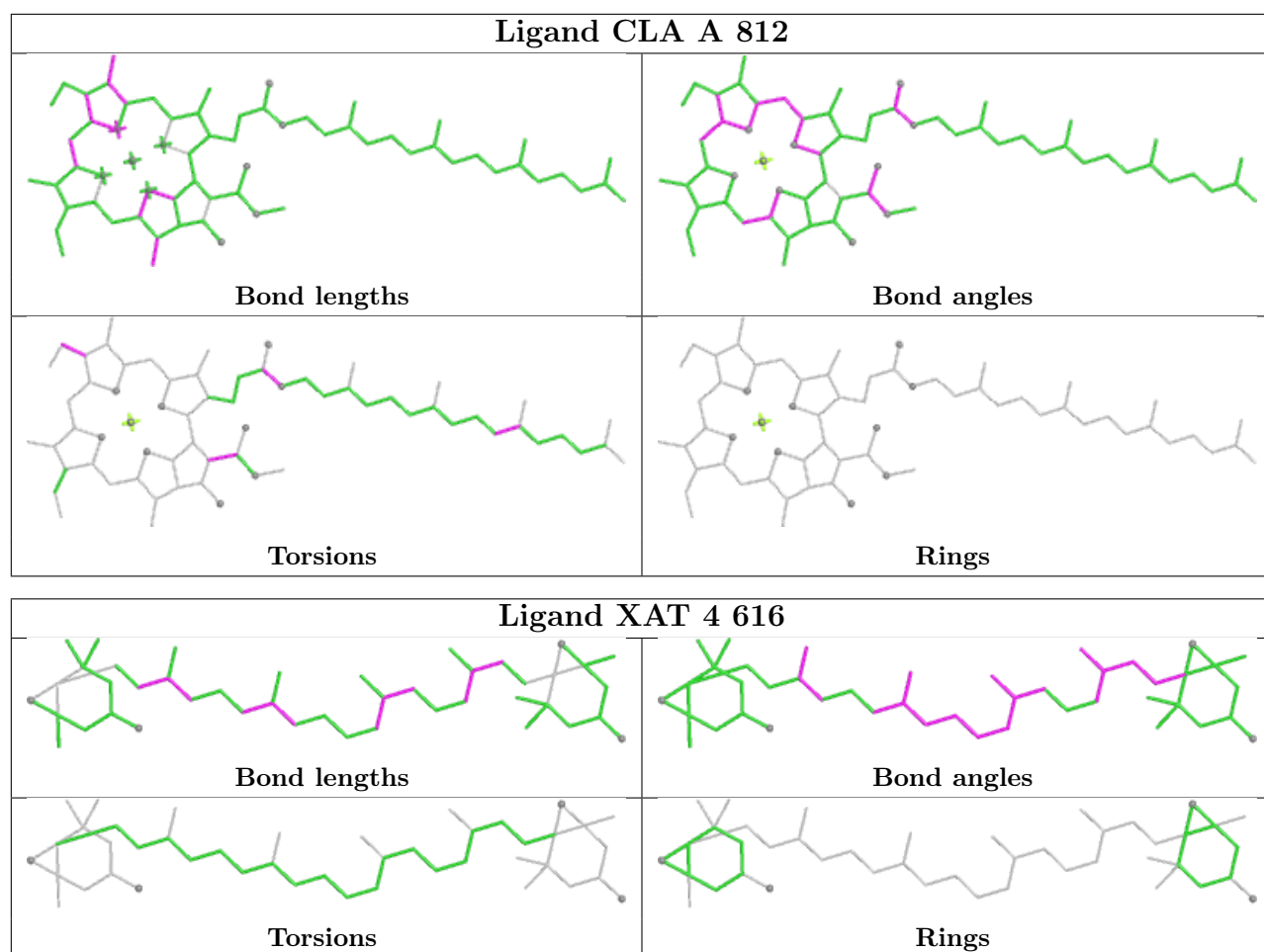
Bond angles



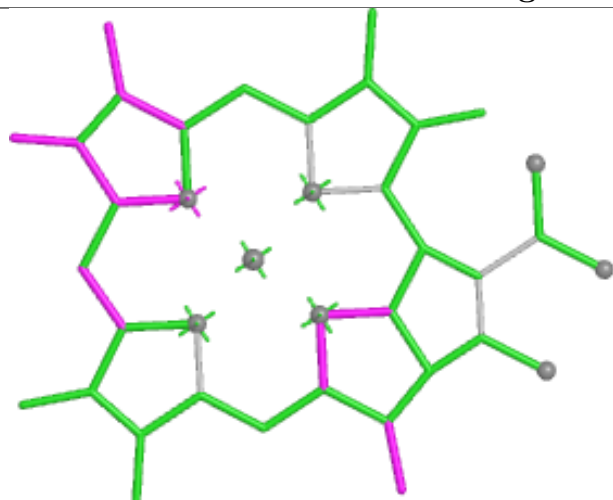
Torsions



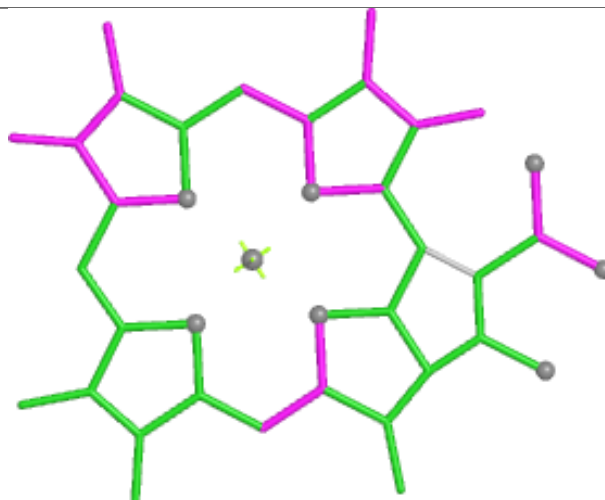
Rings



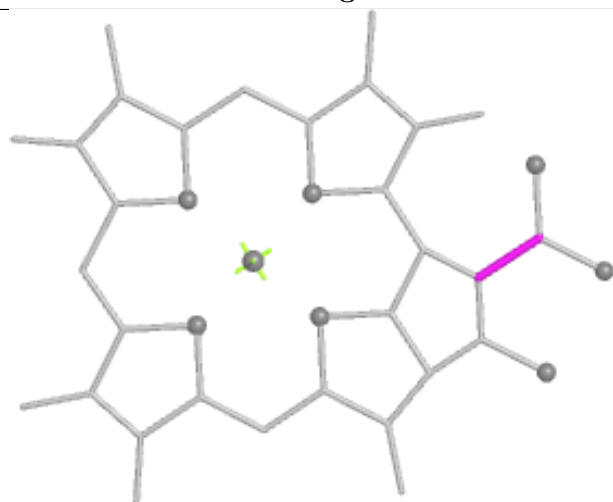
Ligand CLA 1 314



Bond lengths



Bond angles

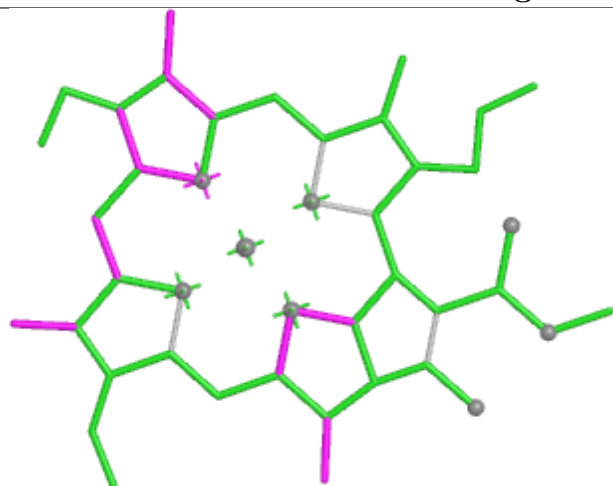


Torsions

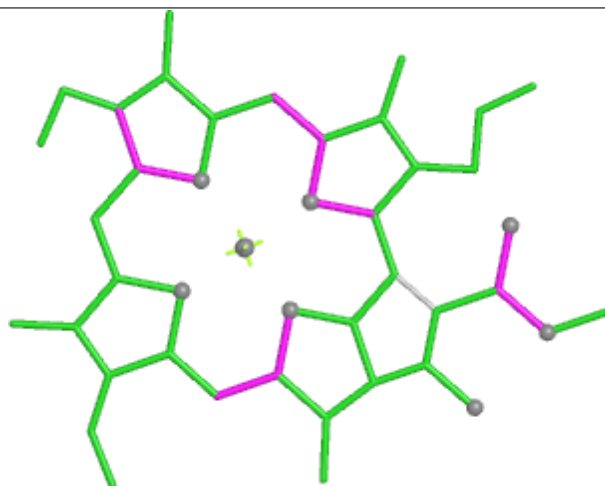


Rings

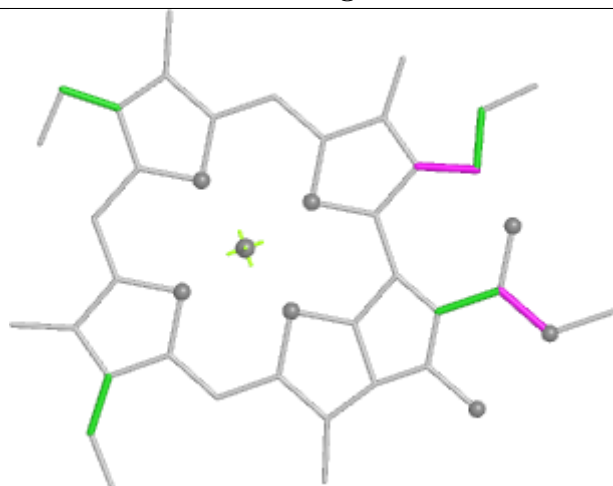
Ligand CLA B 819



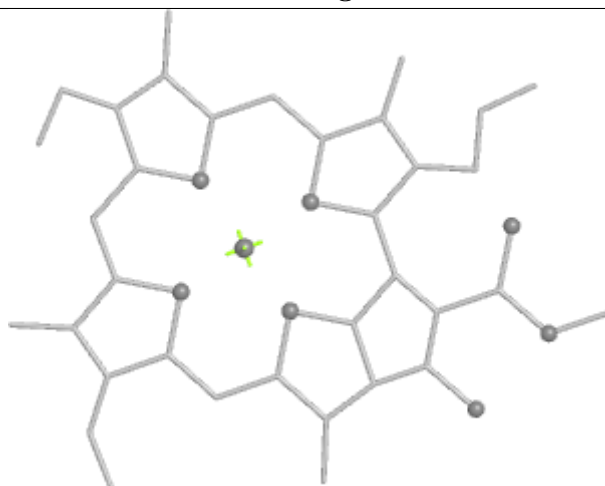
Bond lengths



Bond angles

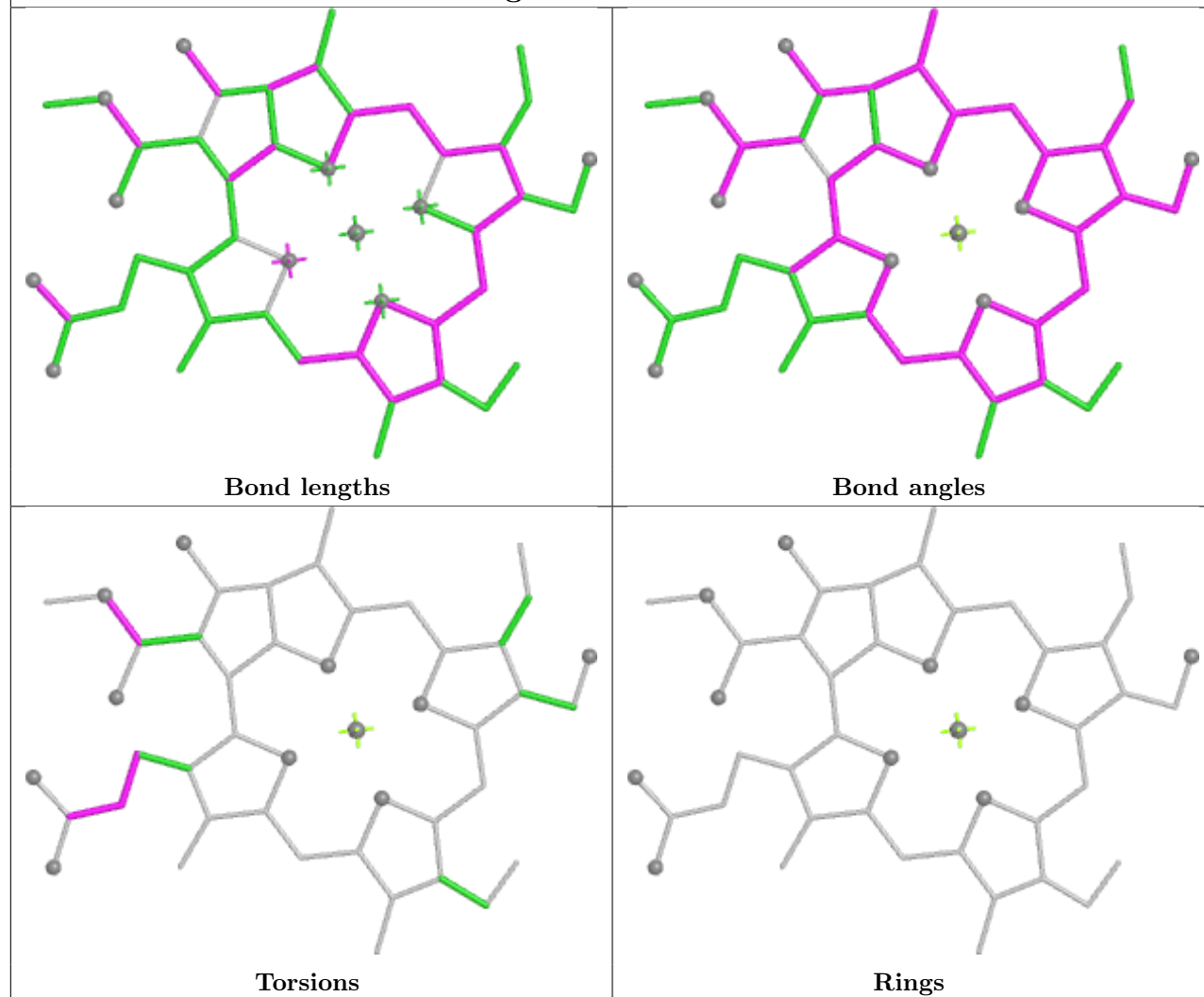


Torsions

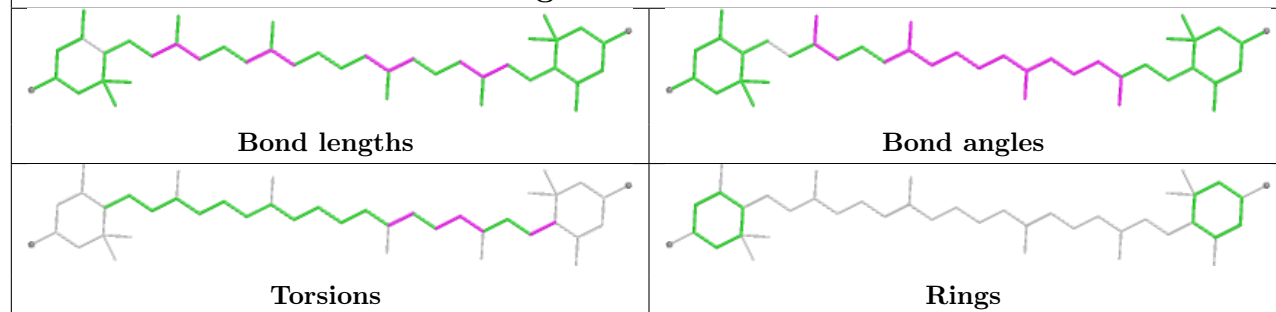


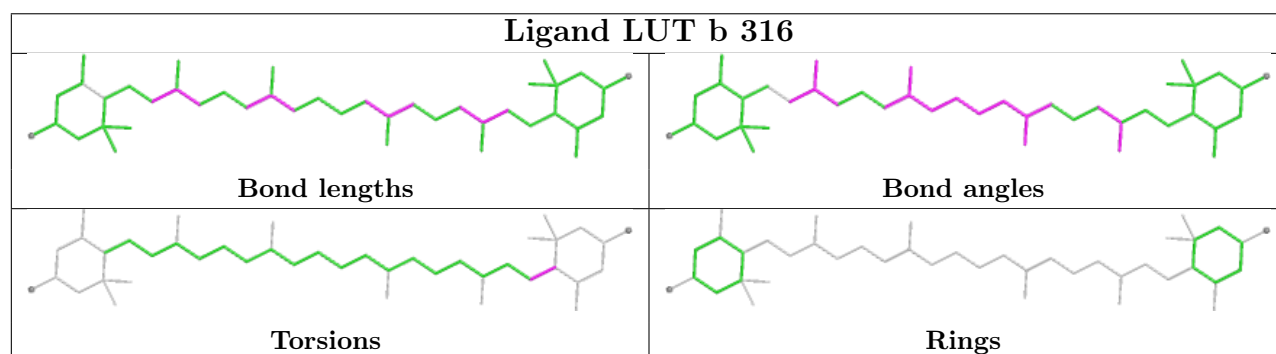
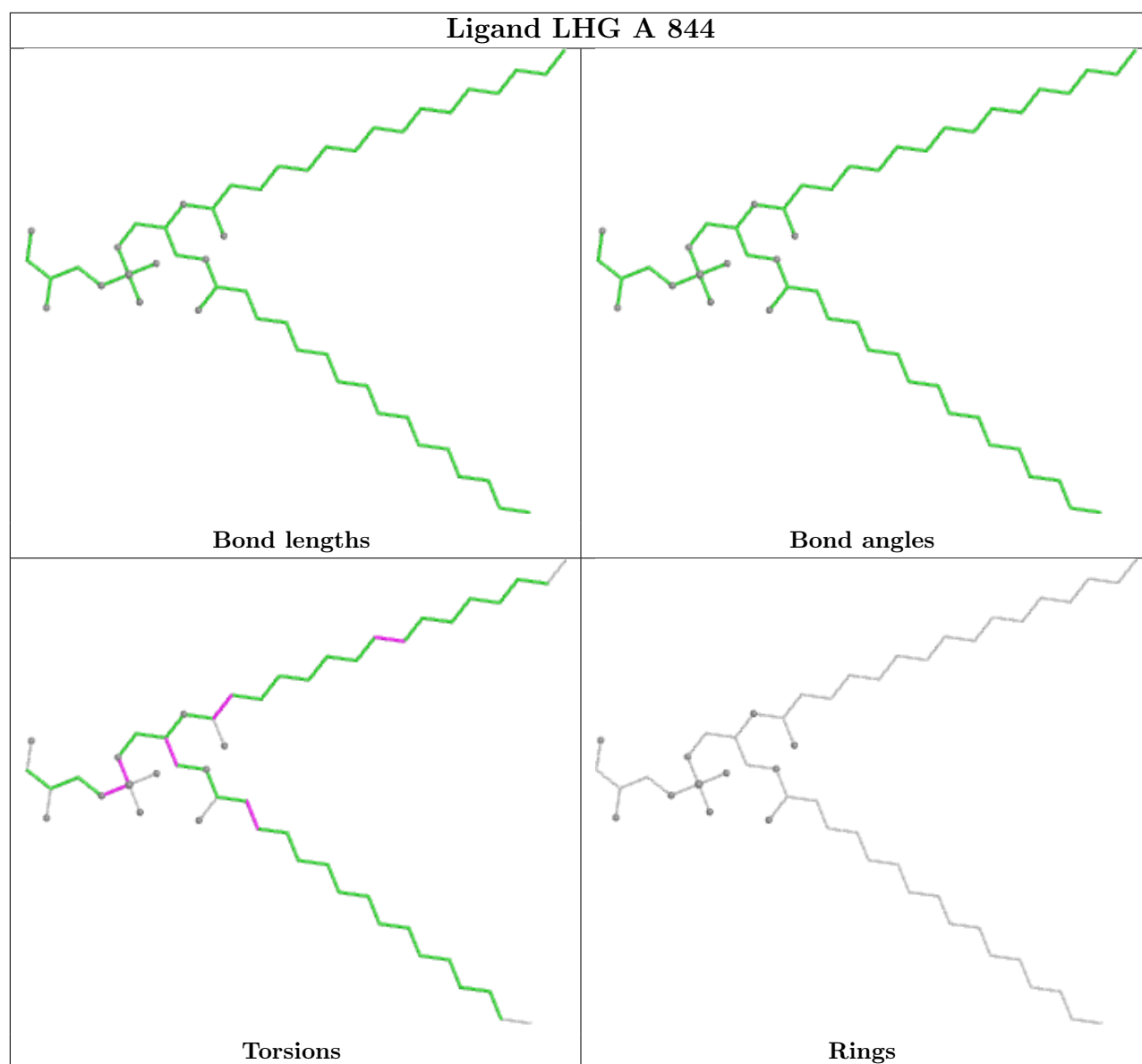
Rings

Ligand CHL 5 606

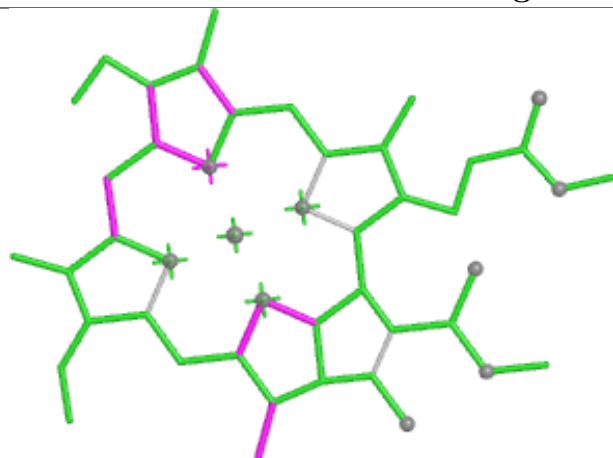


Ligand LUT 5 615

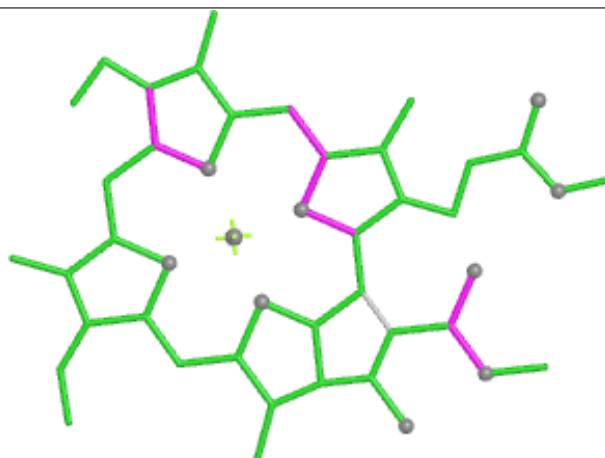




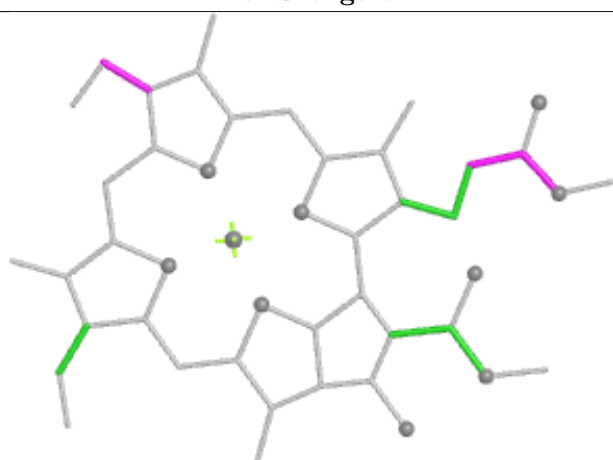
Ligand CLA K 201



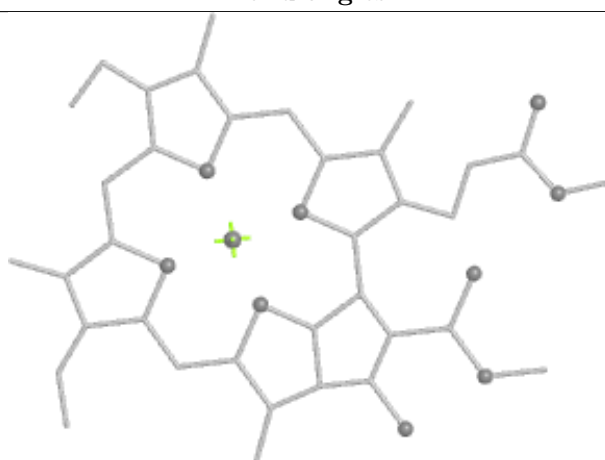
Bond lengths



Bond angles

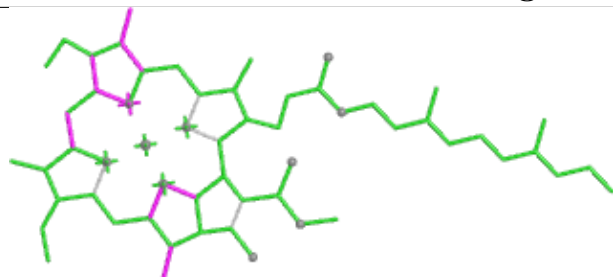


Torsions

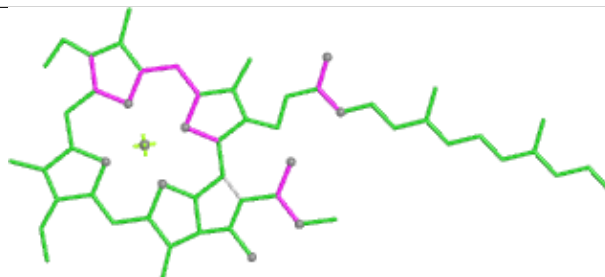


Rings

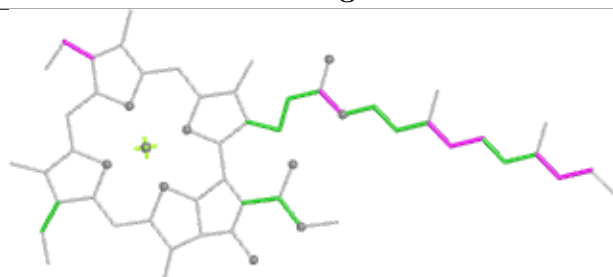
Ligand CLA 9 611



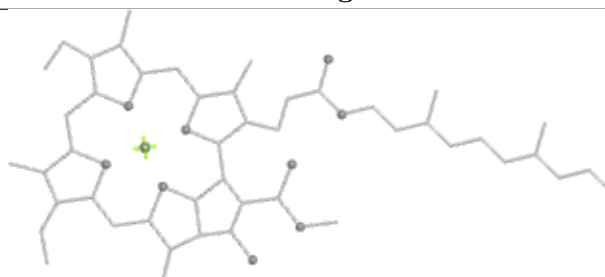
Bond lengths



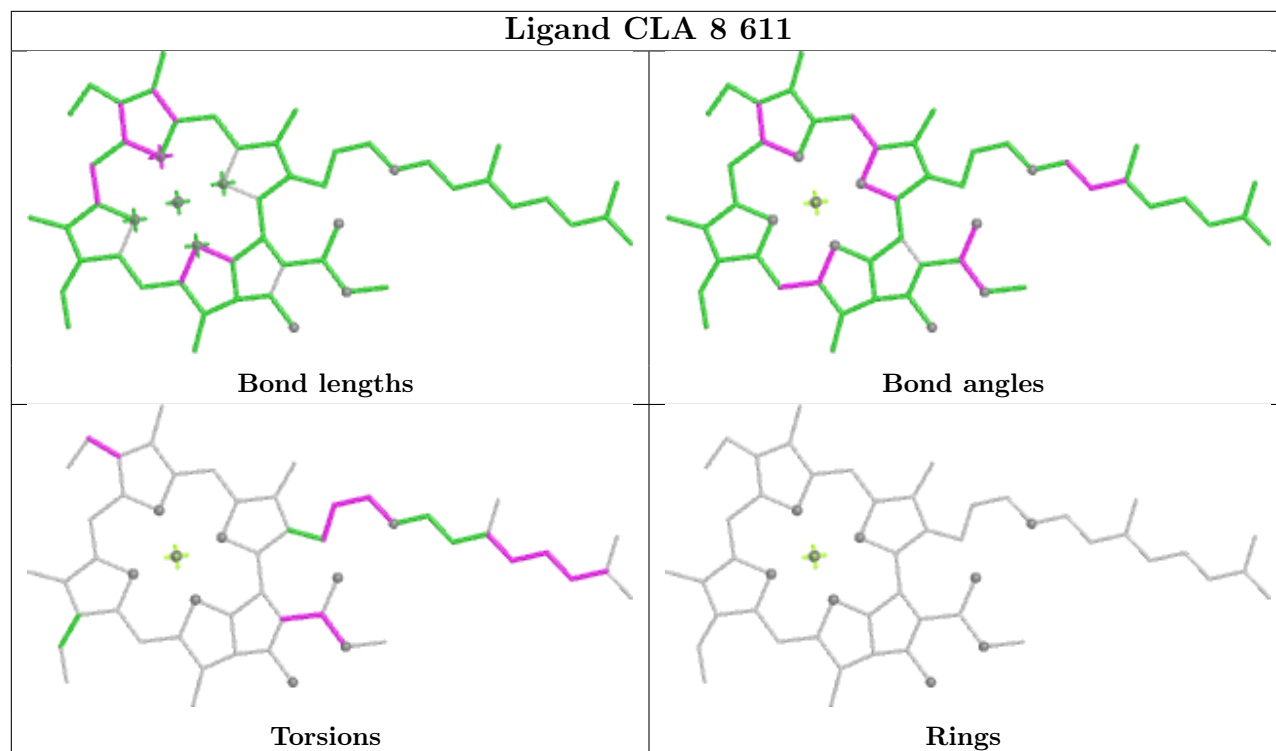
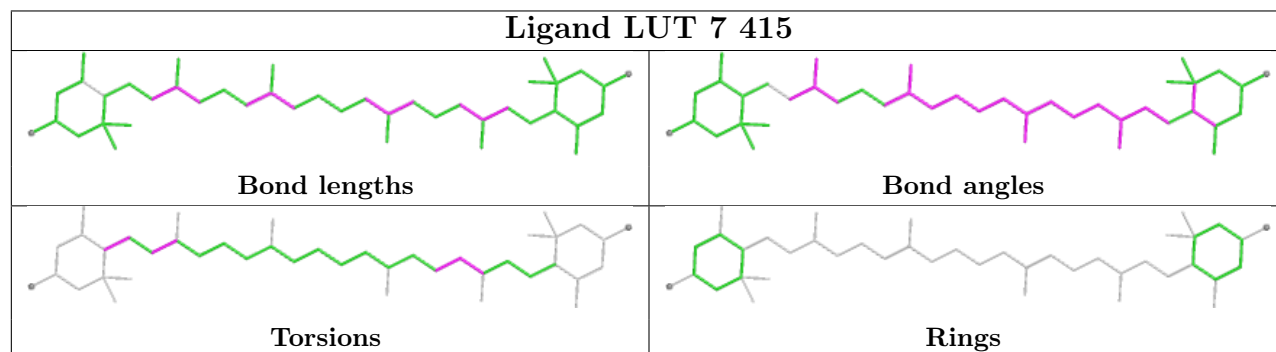
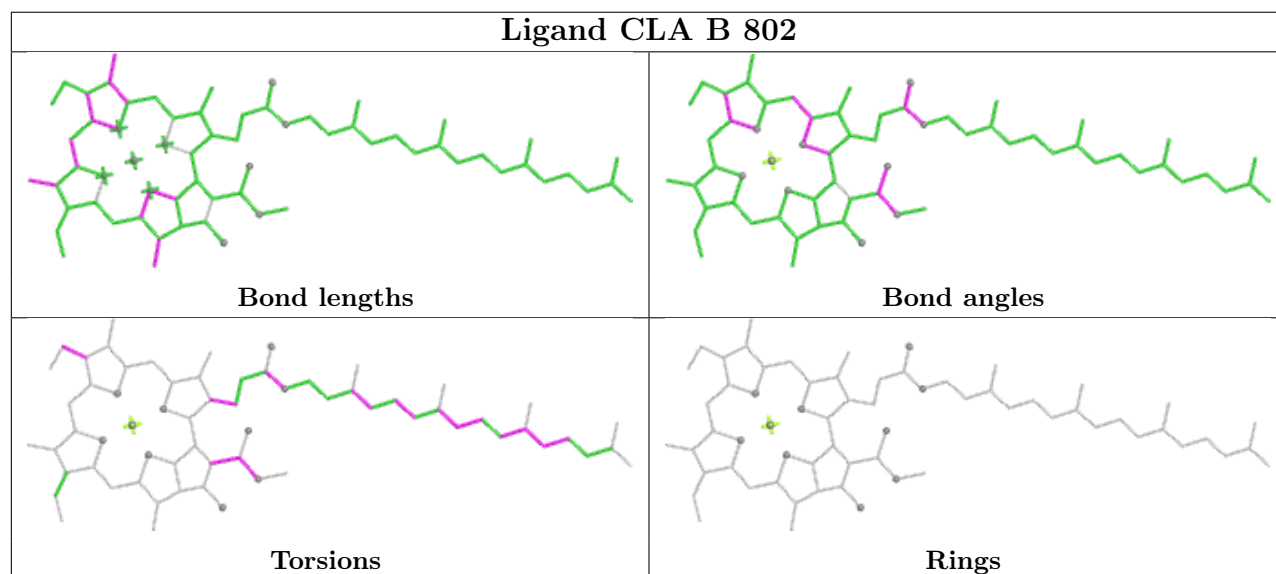
Bond angles



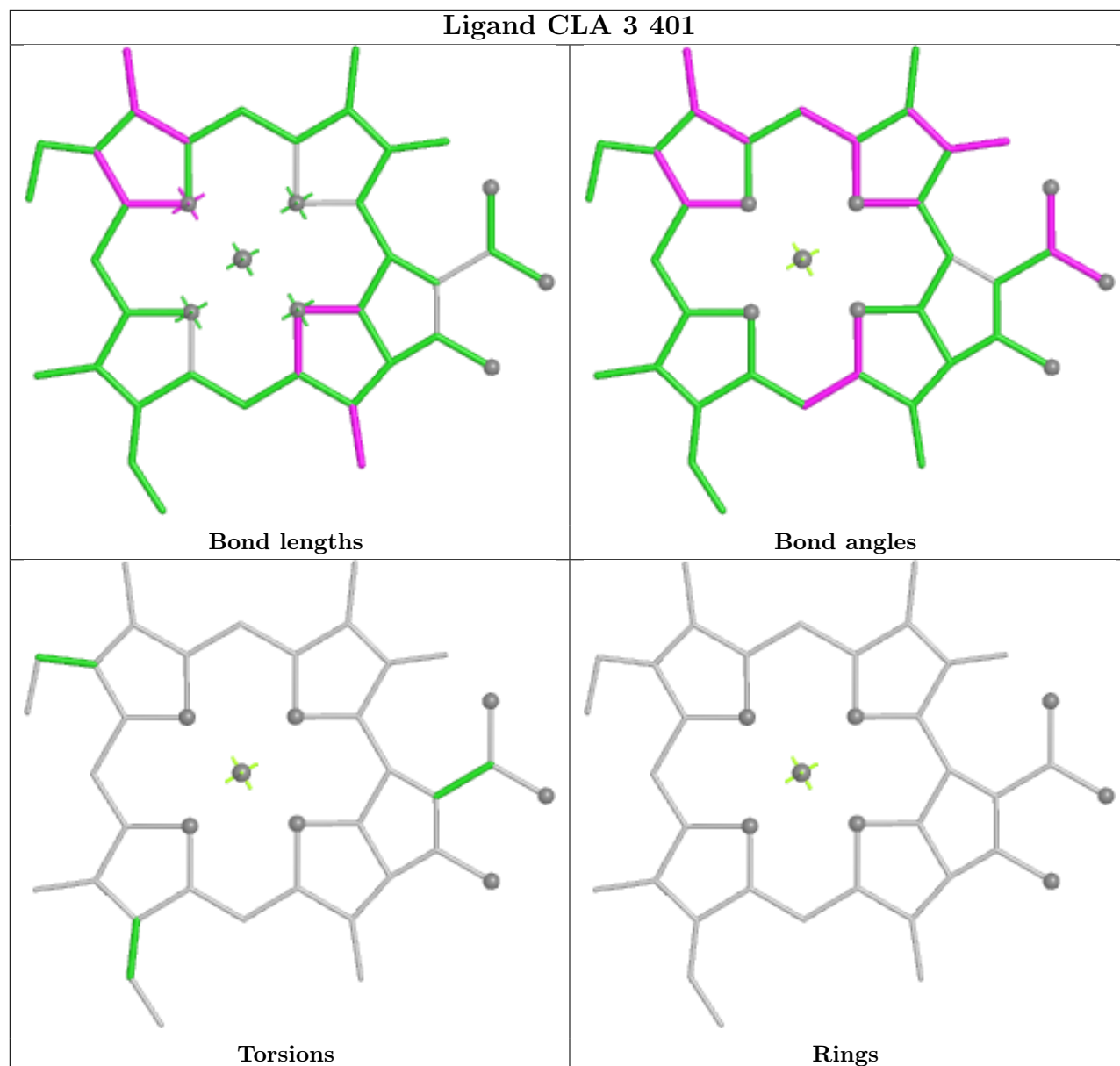
Torsions



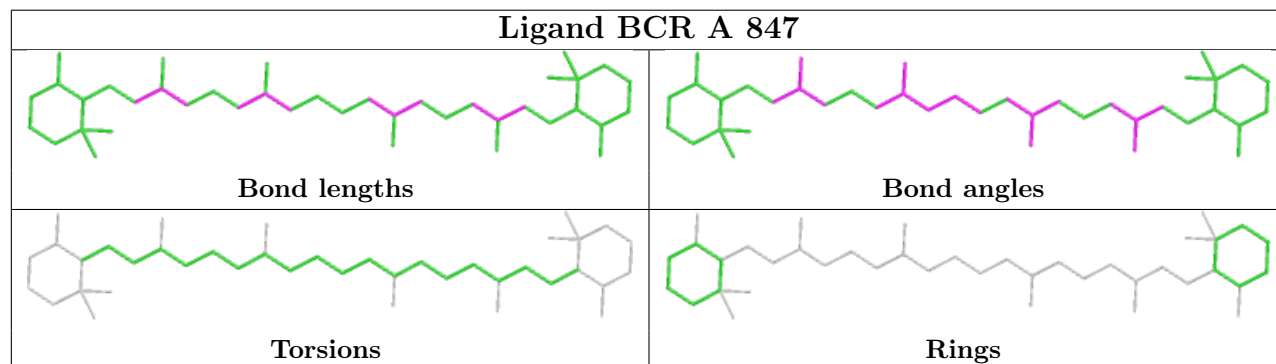
Rings

Ligand CLA 8 611**Ligand LUT 7 415****Ligand CLA B 802**

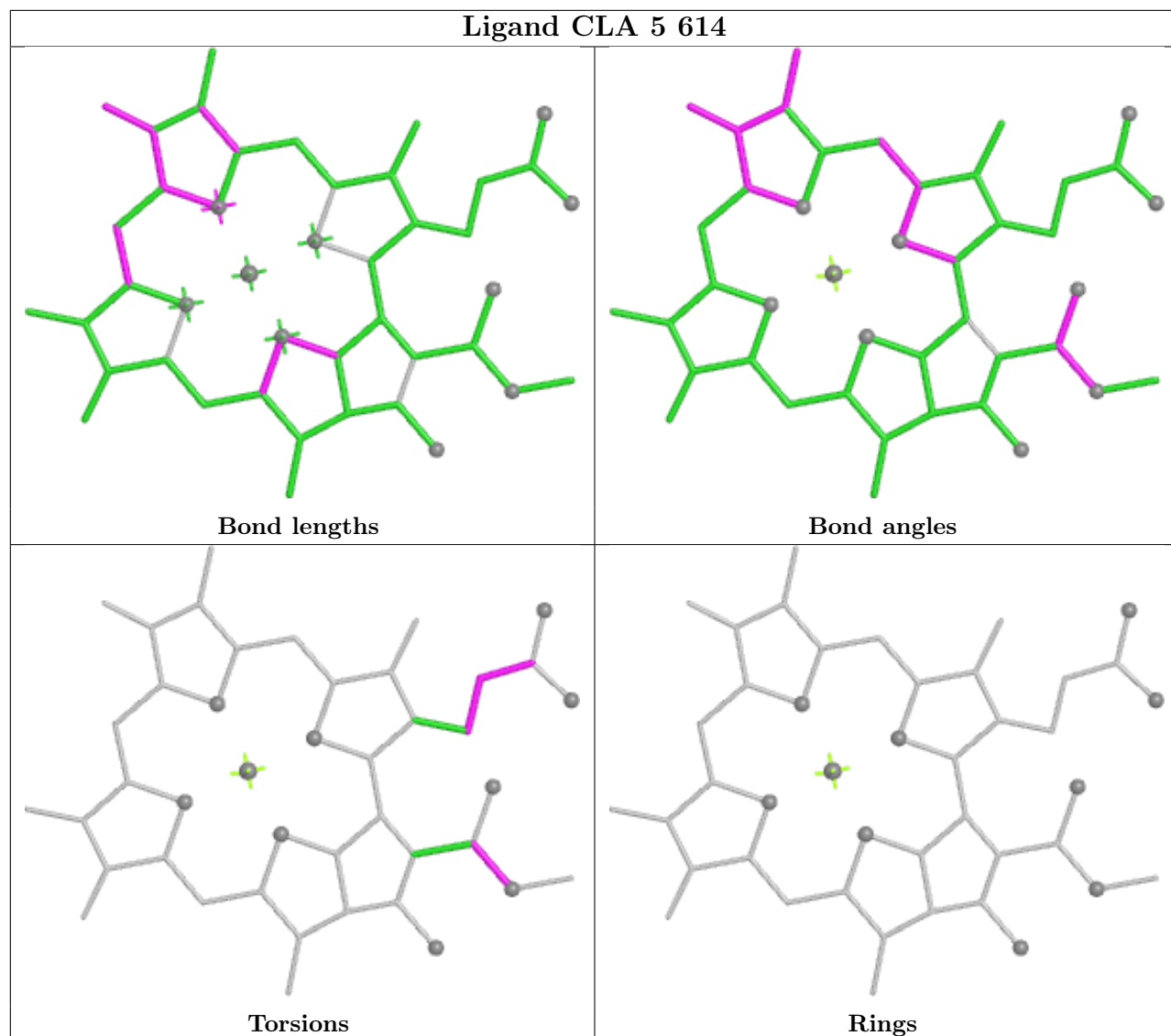
Ligand CLA 3 401



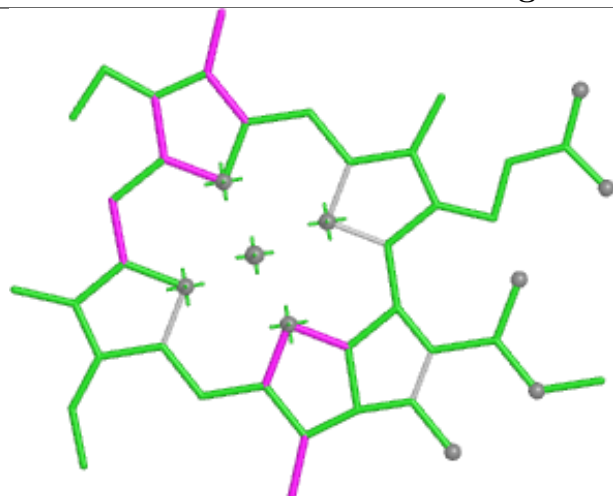
Ligand BCR A 847



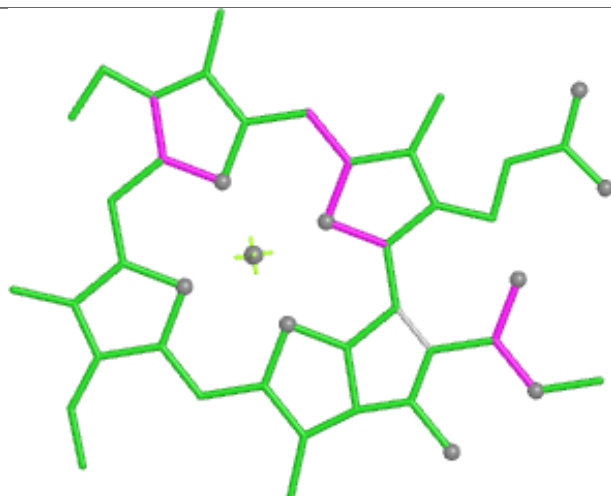
Ligand CLA 5 614



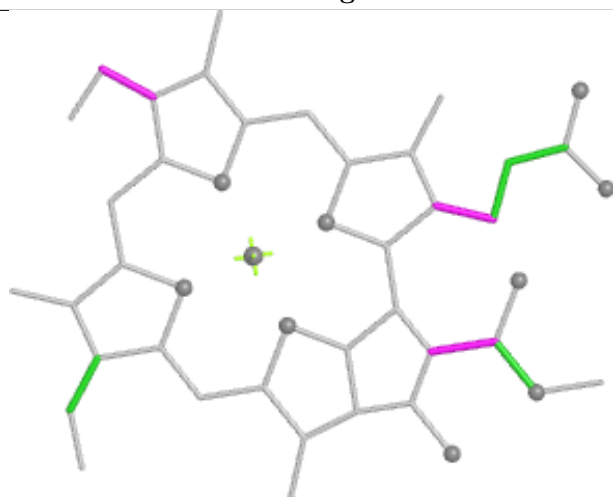
Ligand CLA 9 603



Bond lengths



Bond angles

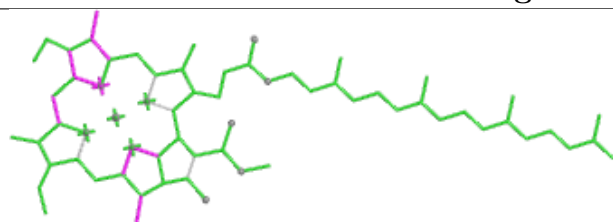


Torsions

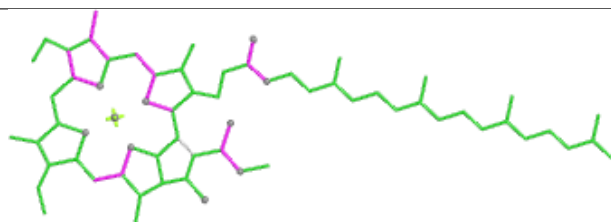


Rings

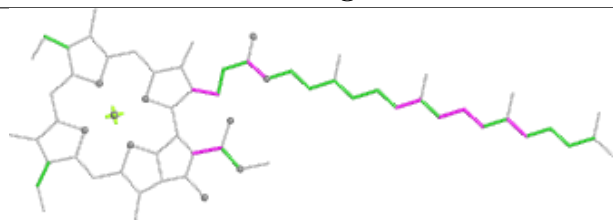
Ligand CLA B 824



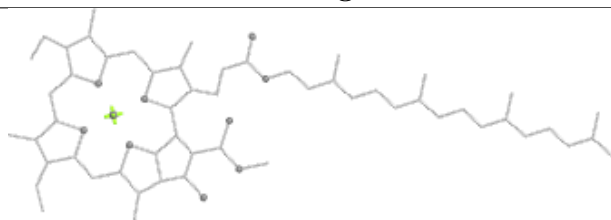
Bond lengths



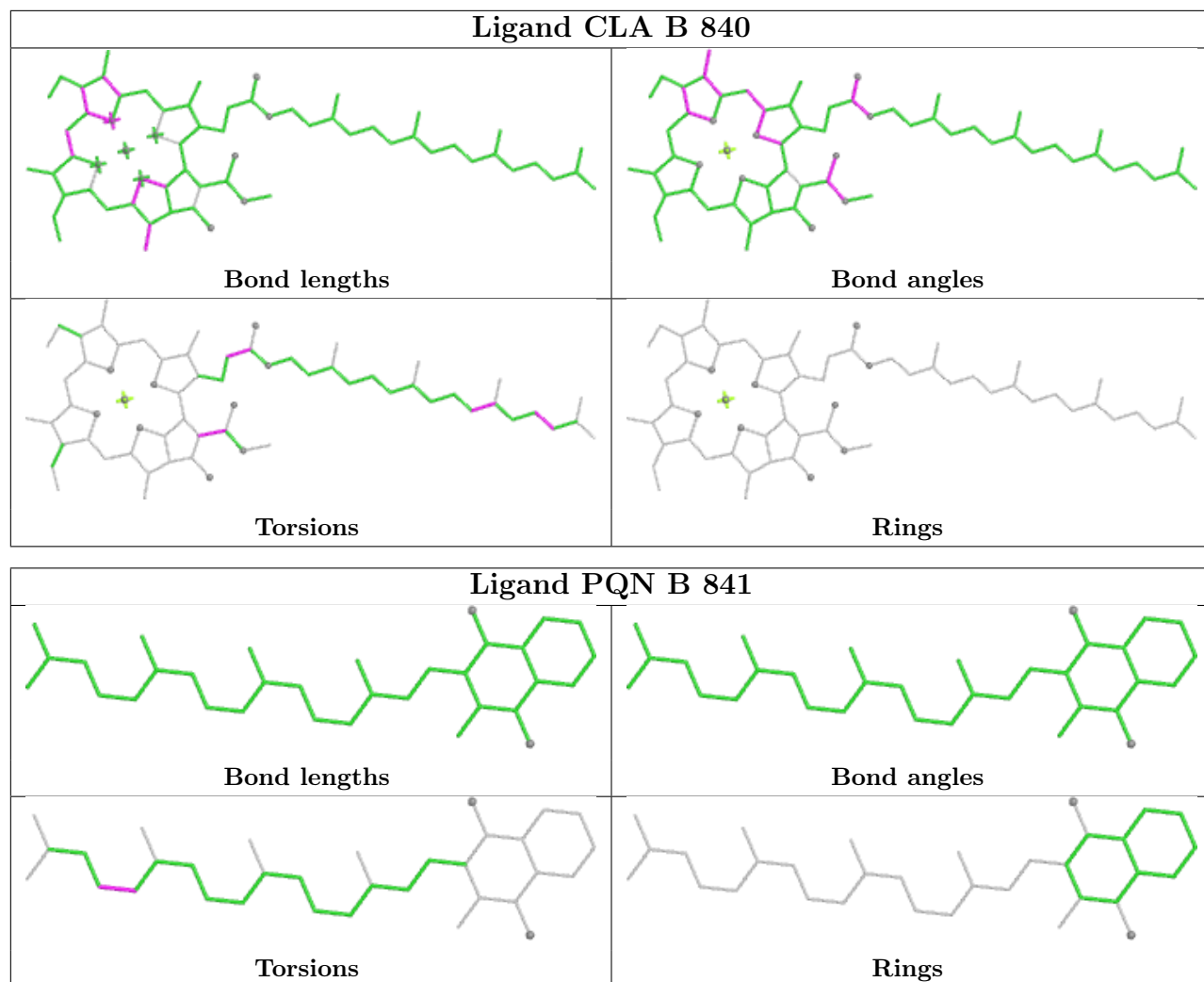
Bond angles



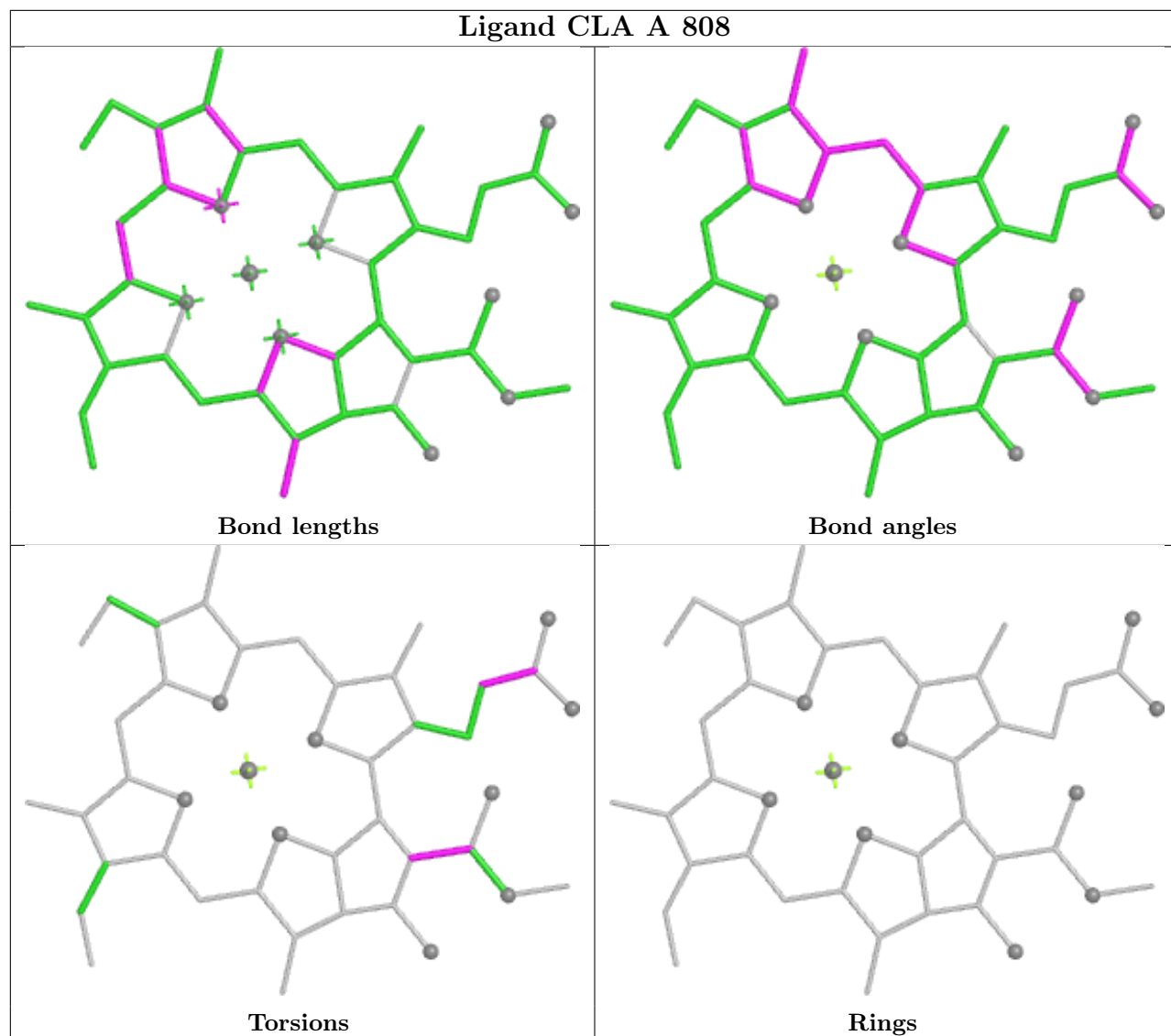
Torsions

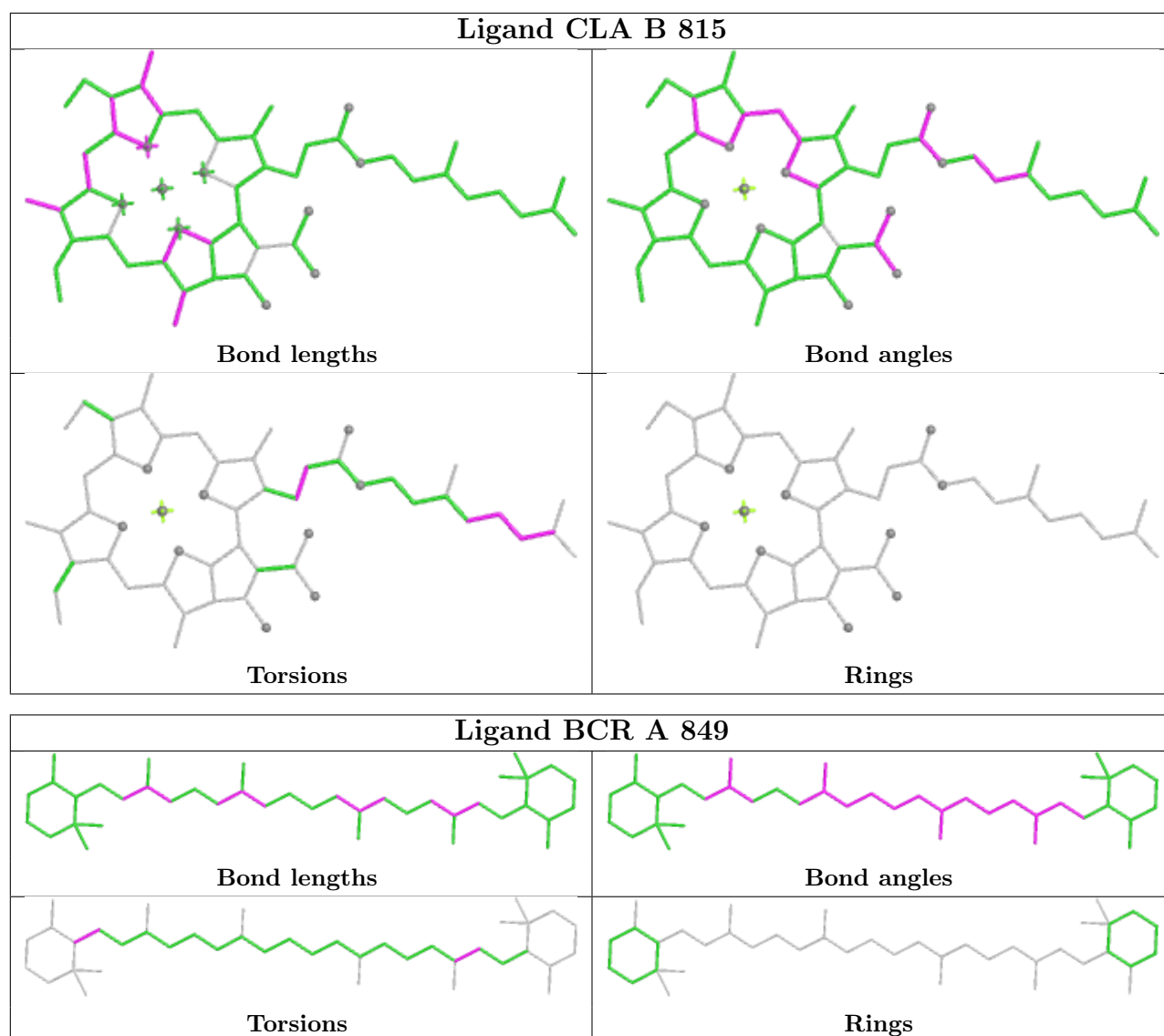


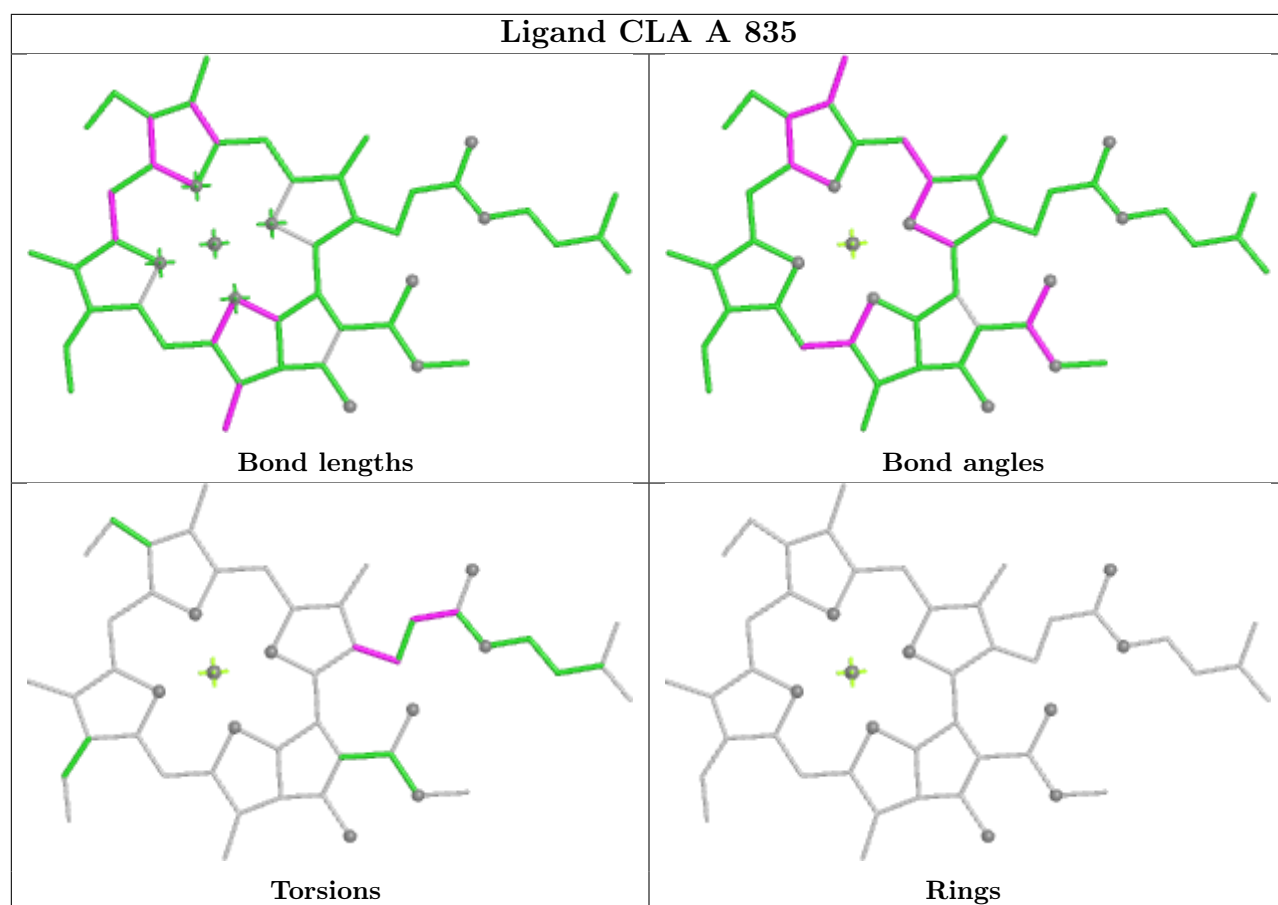
Rings



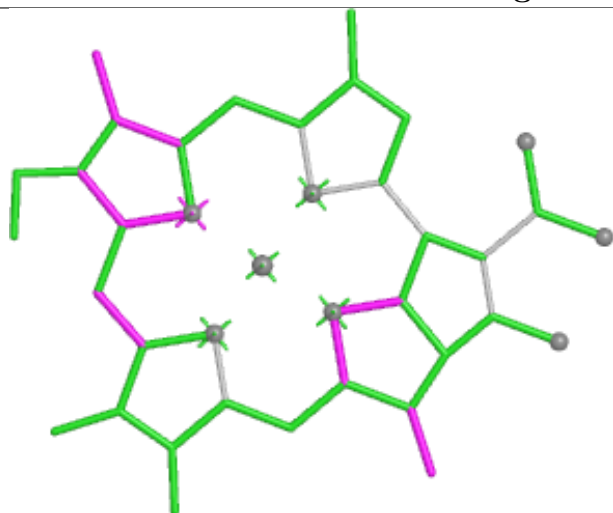
Ligand CLA A 808



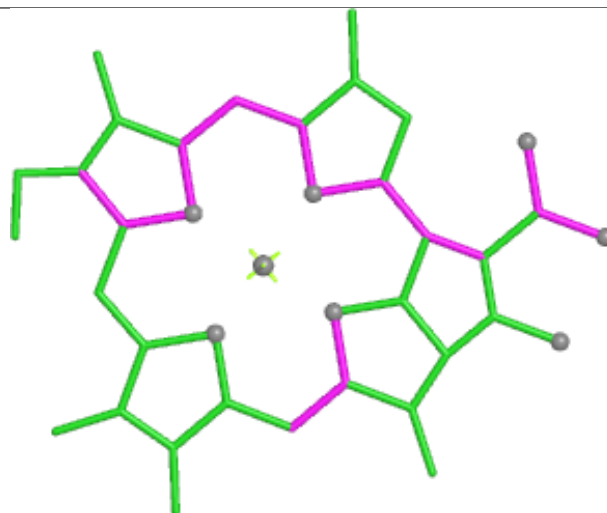




Ligand CLA O 202



Bond lengths



Bond angles

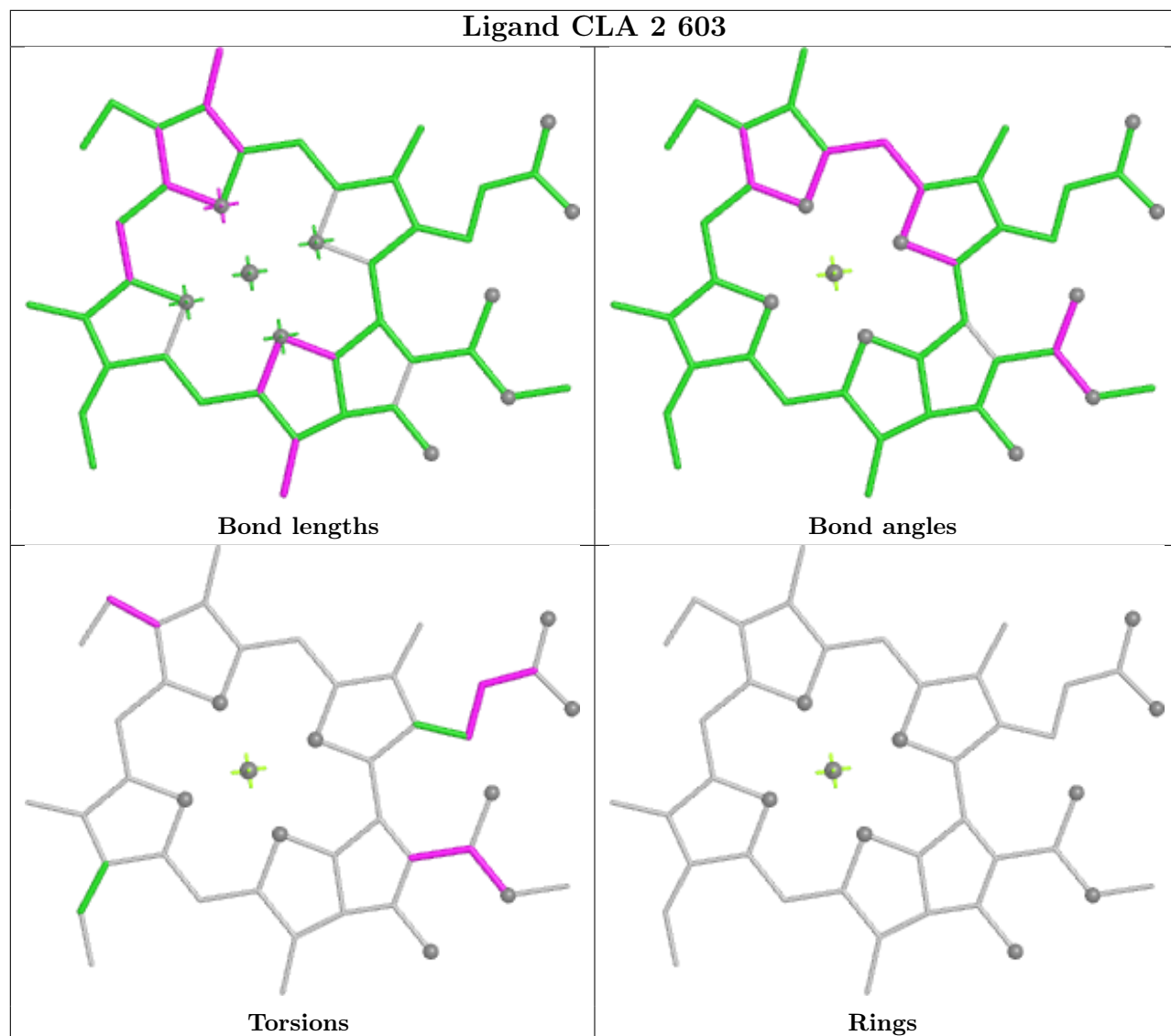


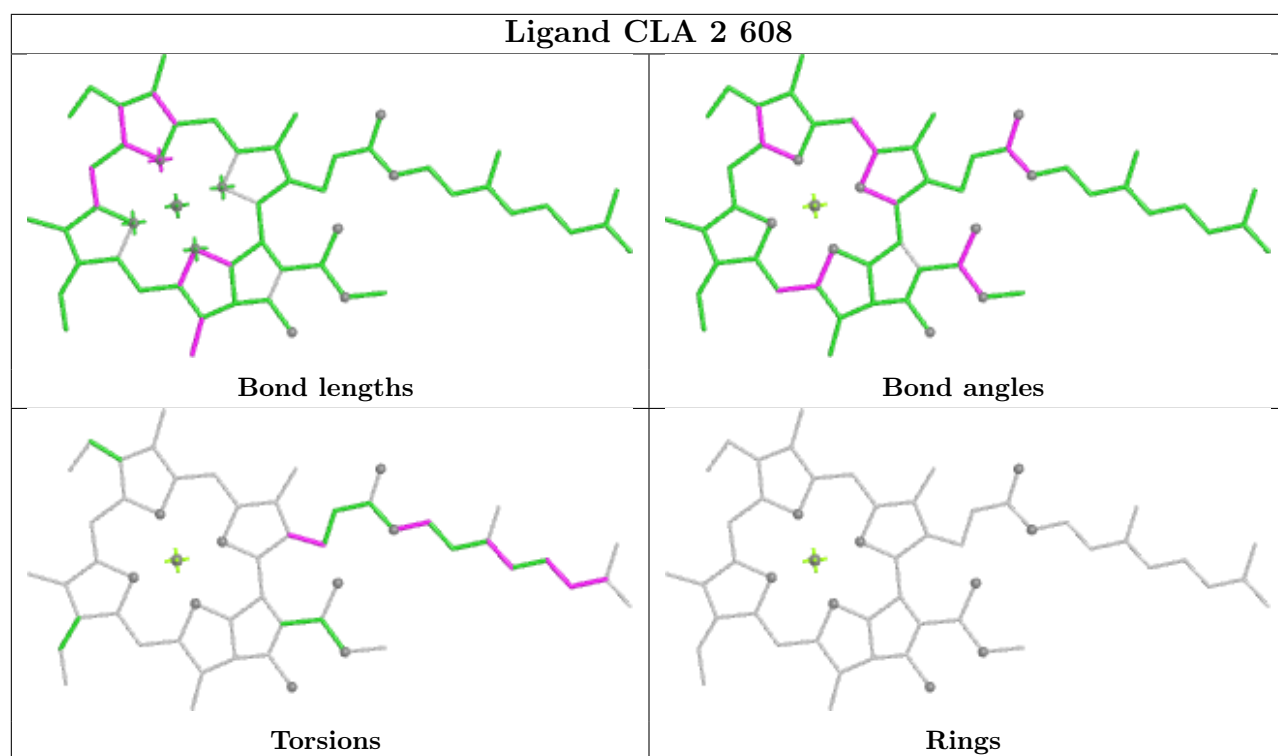
Torsions



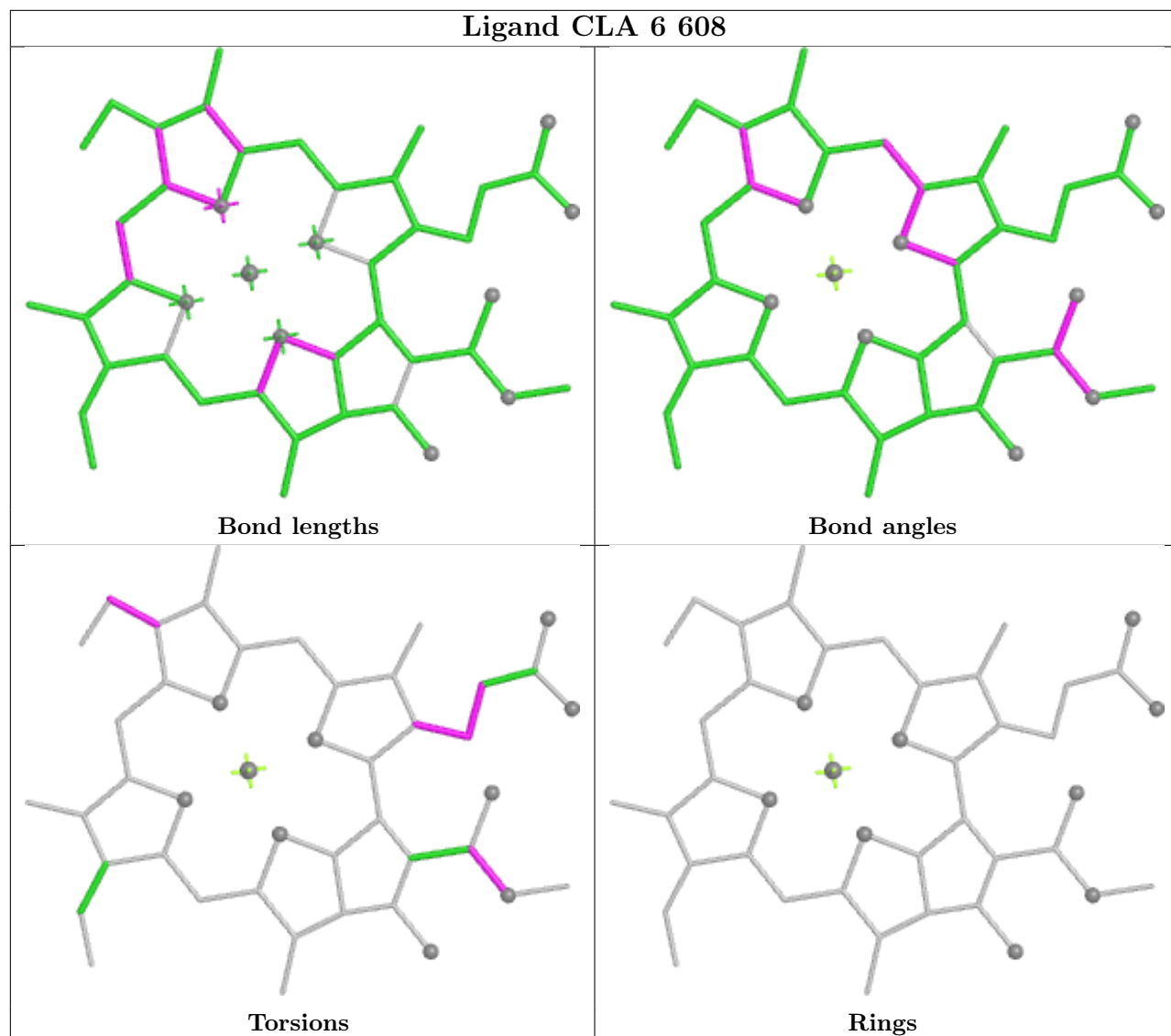
Rings

Ligand CLA 2 603

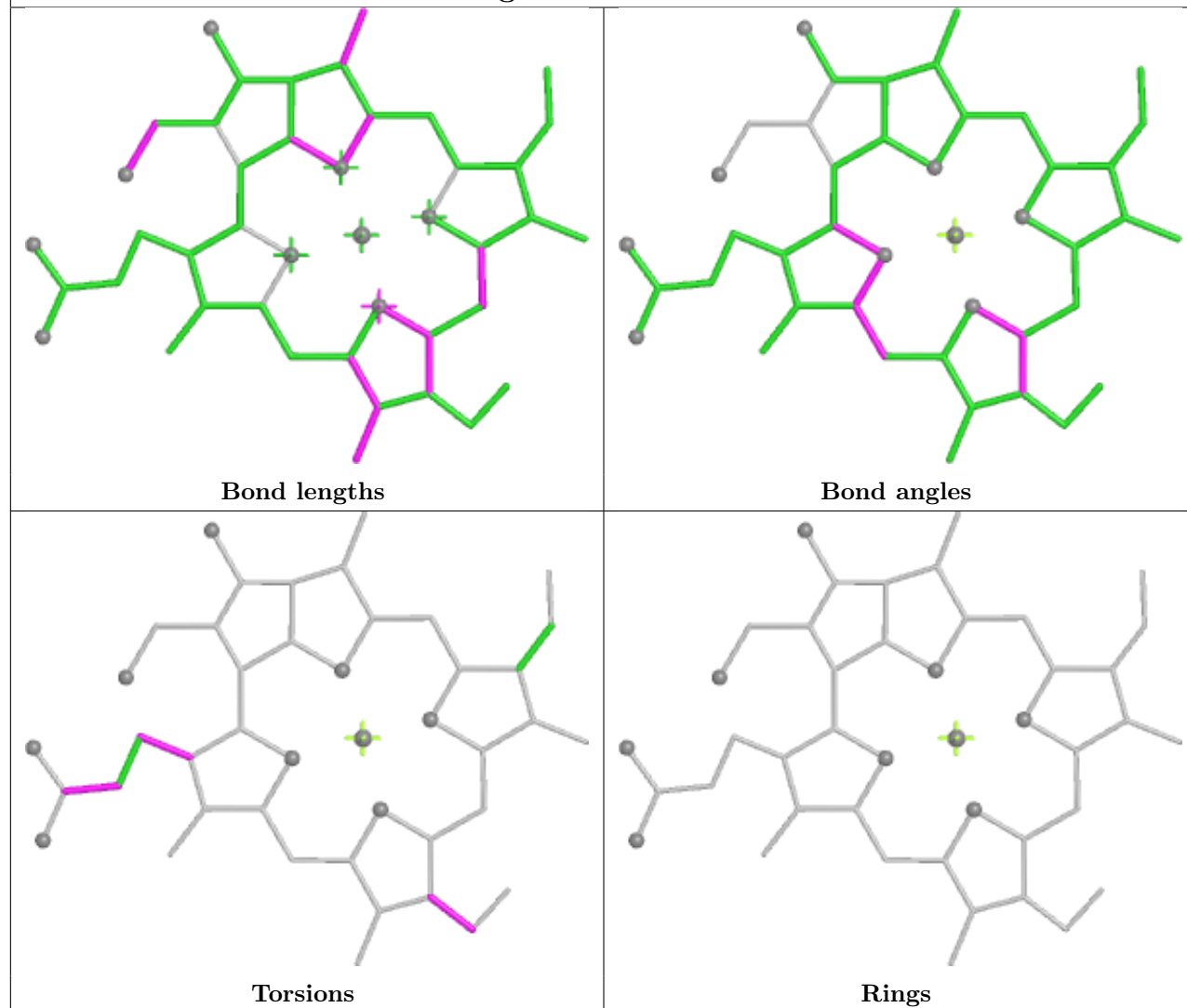




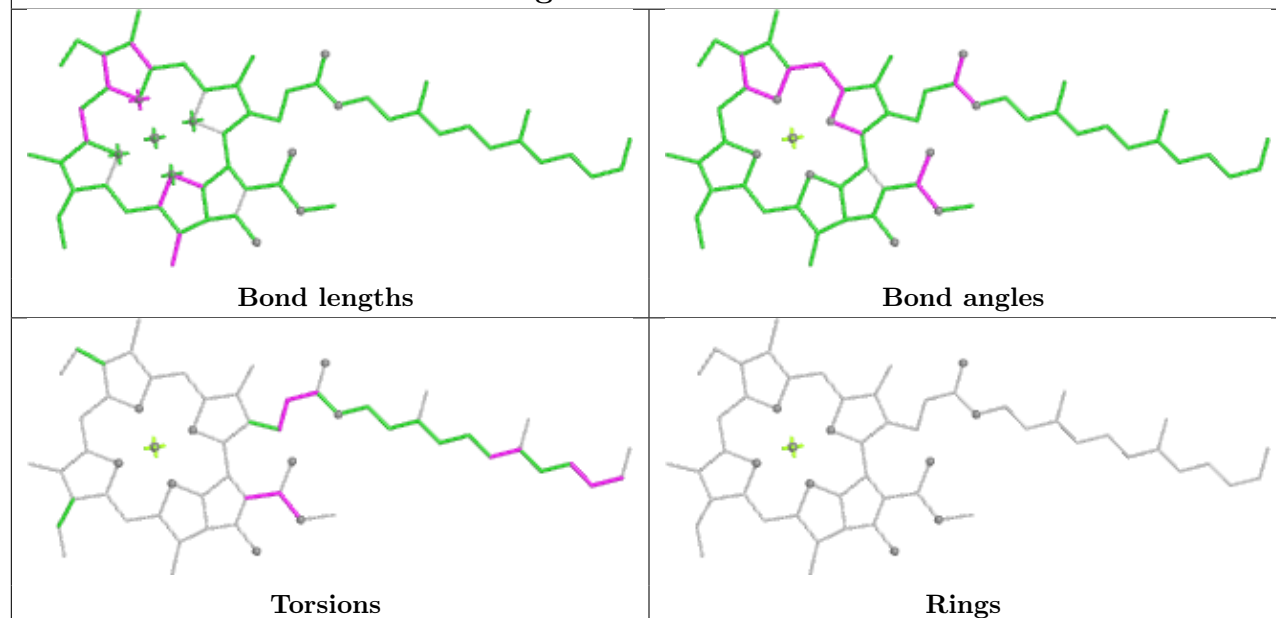
Ligand CLA 6 608



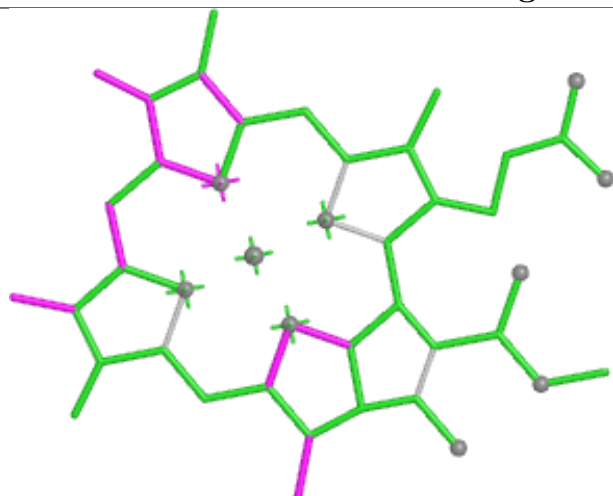
Ligand CLA 8 608



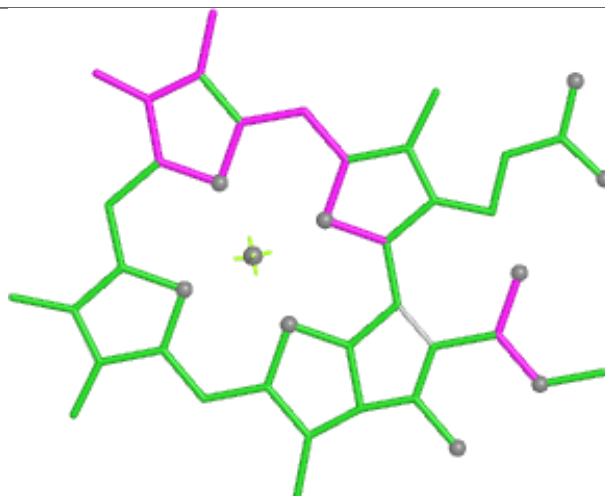
Ligand CLA b 303



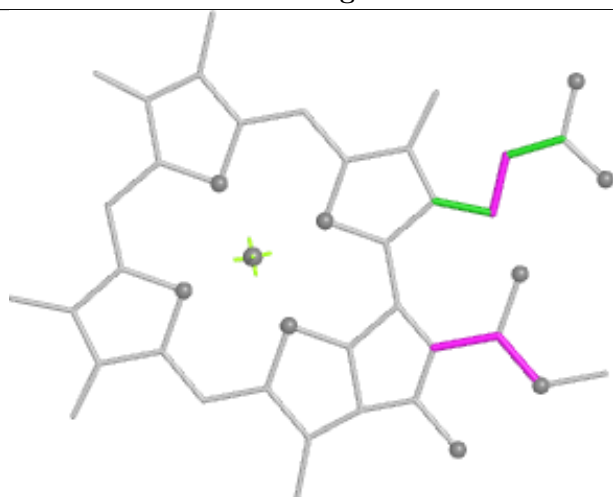
Ligand CLA 1 316



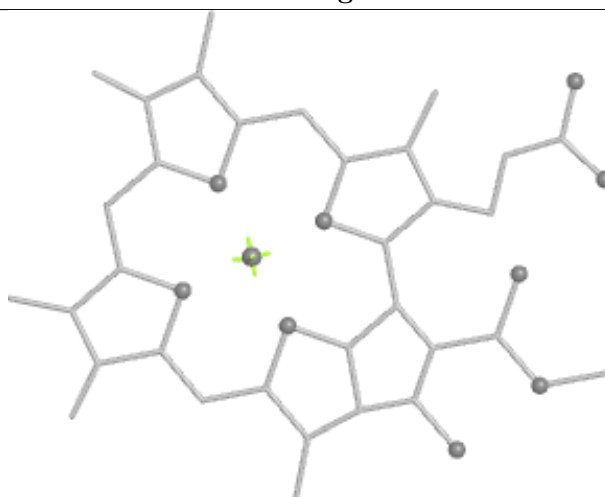
Bond lengths



Bond angles

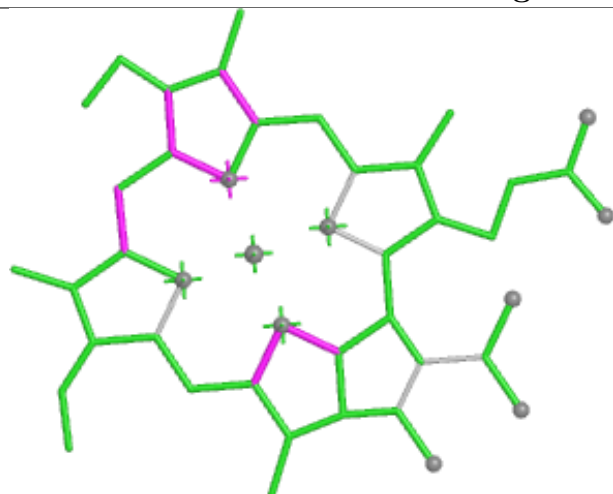


Torsions

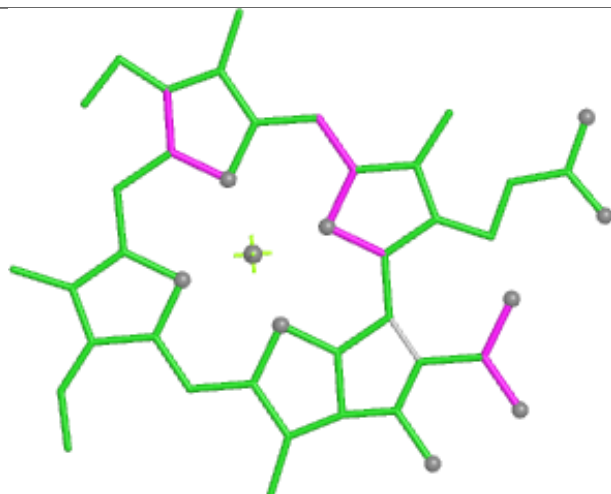


Rings

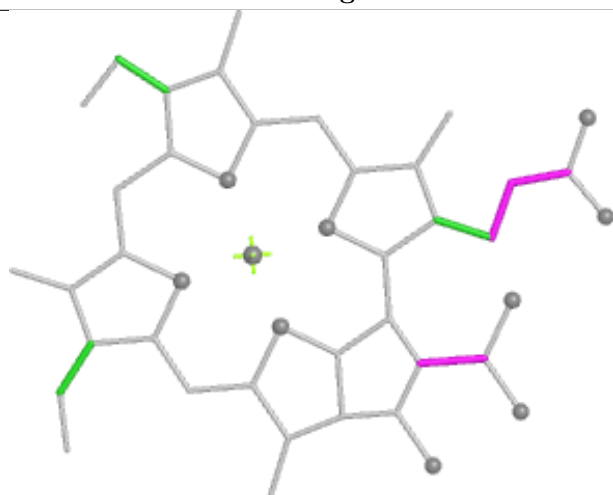
Ligand CLA G 204



Bond lengths



Bond angles

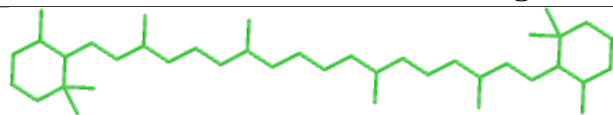


Torsions

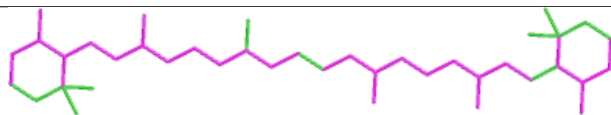


Rings

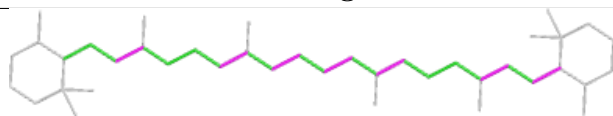
Ligand BCR B 843



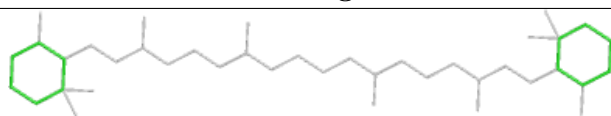
Bond lengths



Bond angles

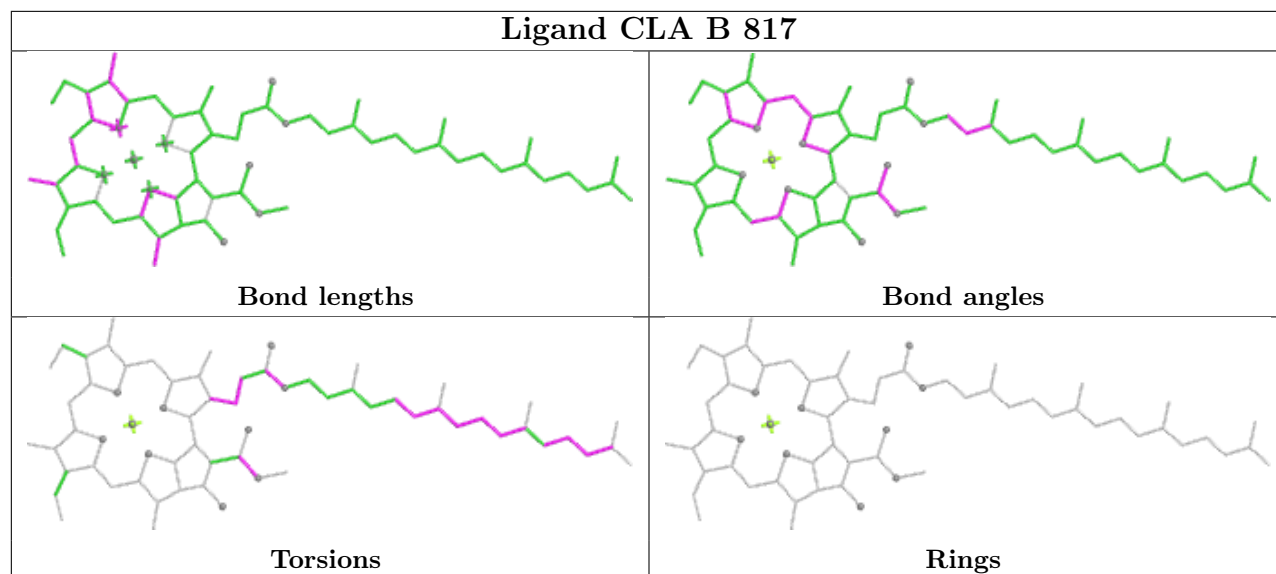


Torsions

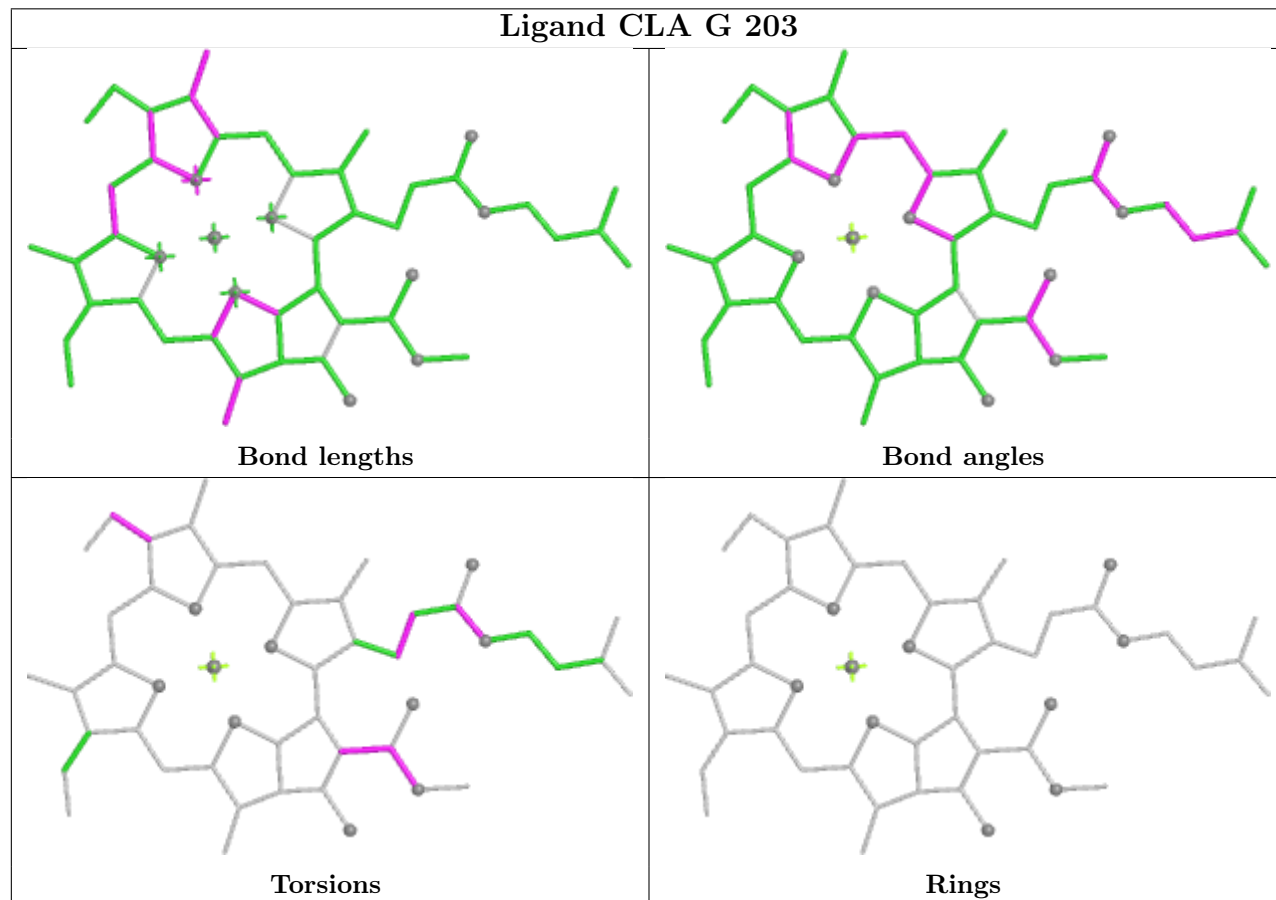


Rings

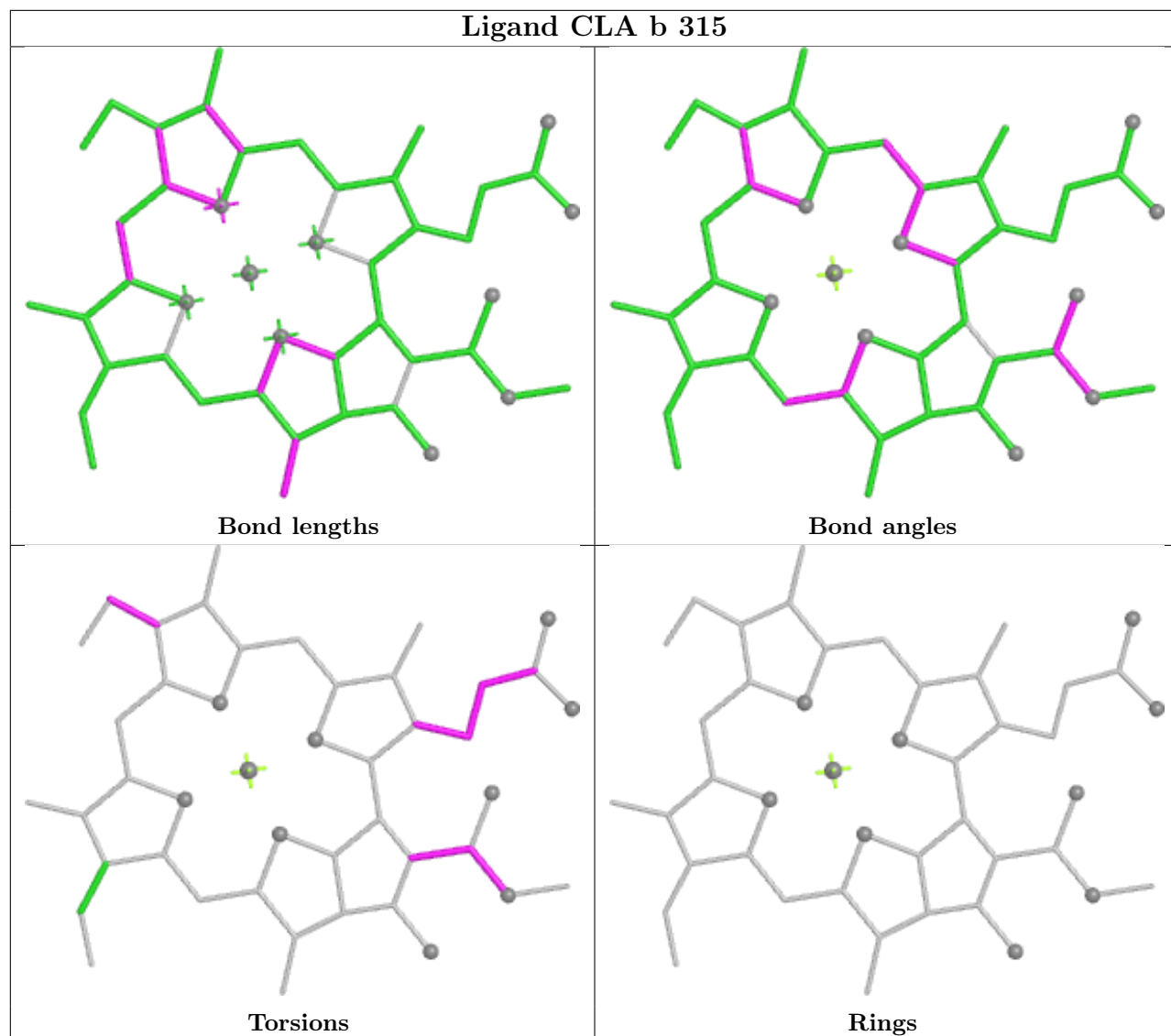
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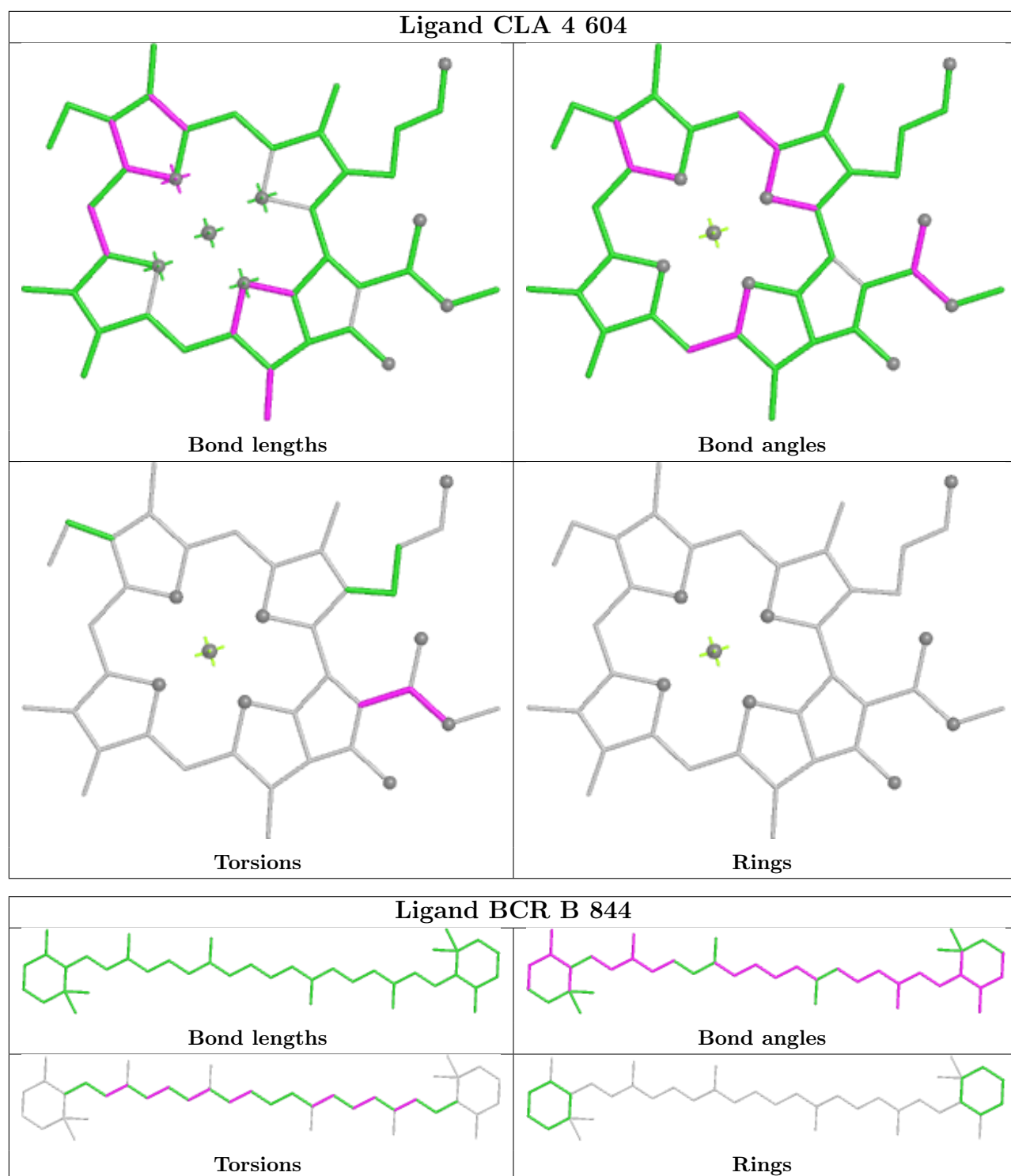


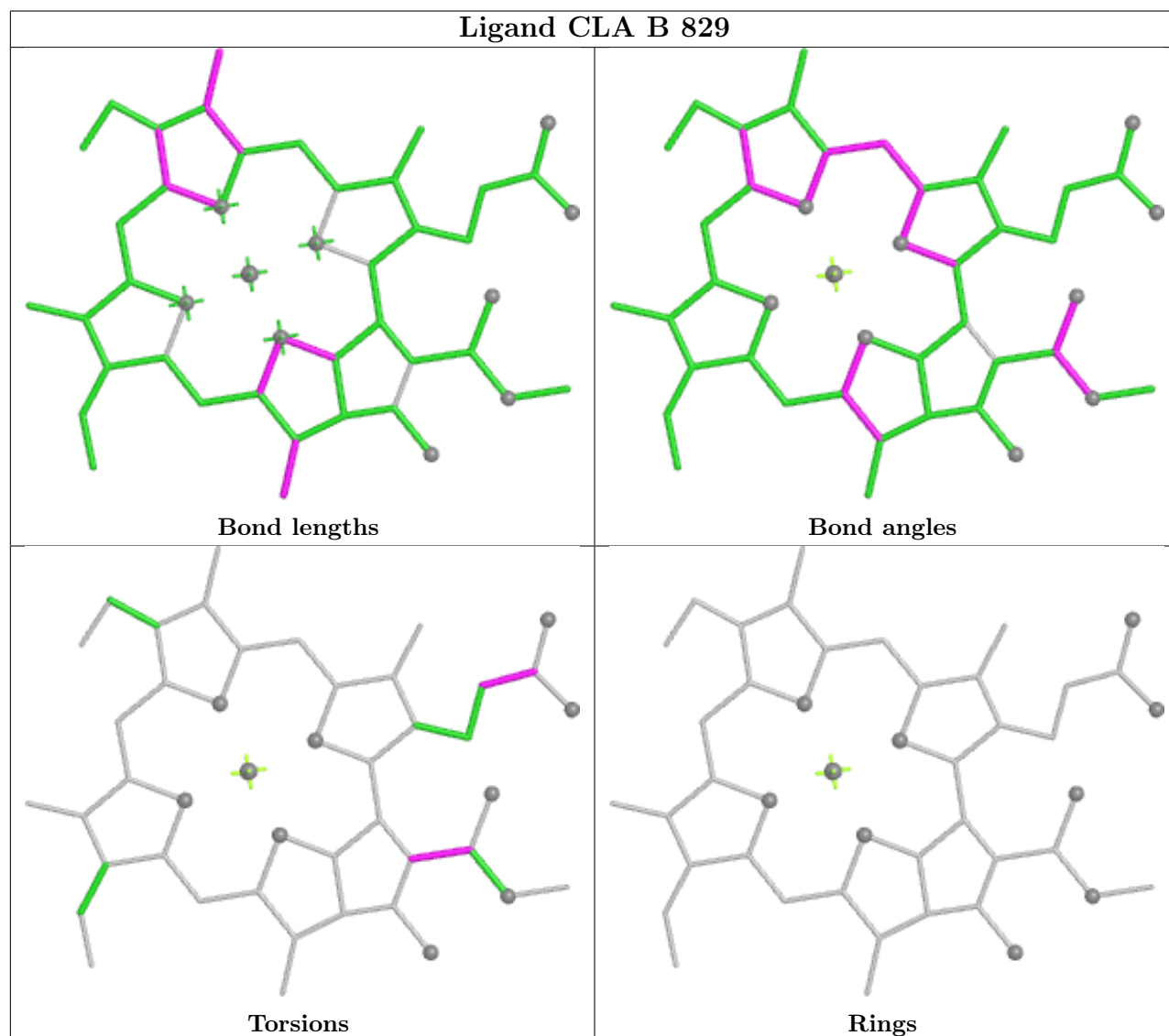
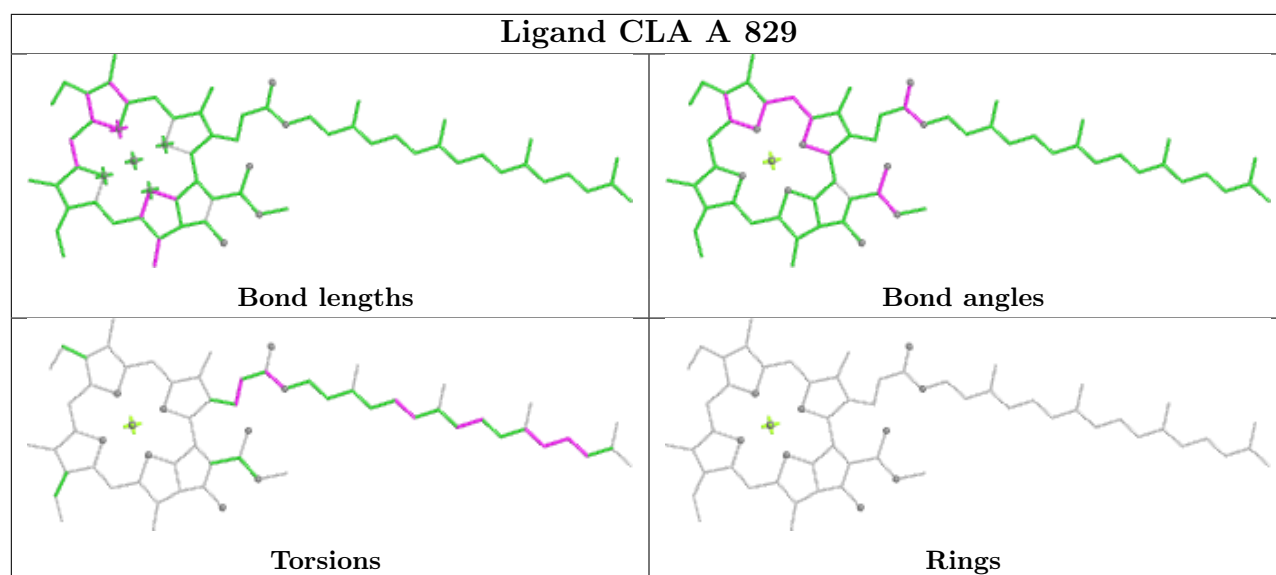
Ligand CLA G 203

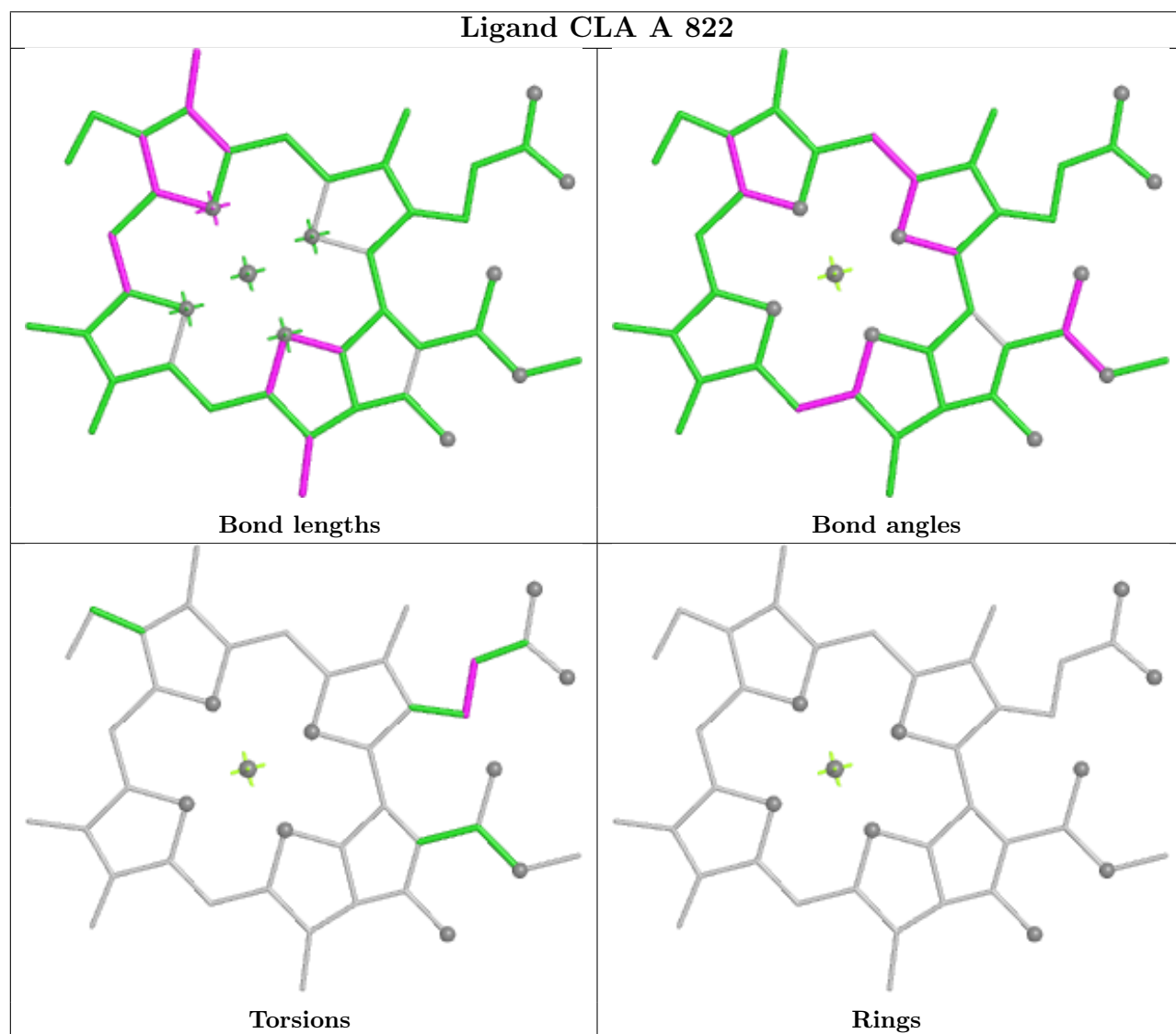
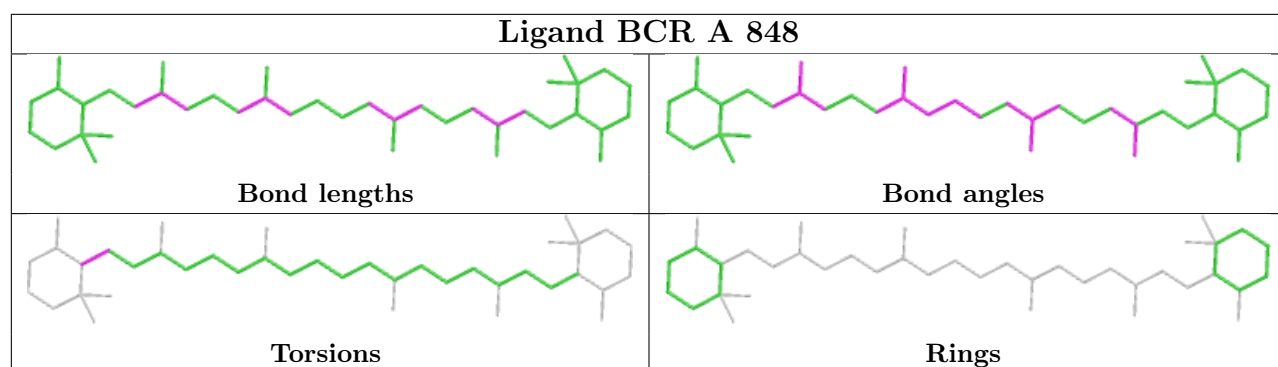


Ligand CLA b 315

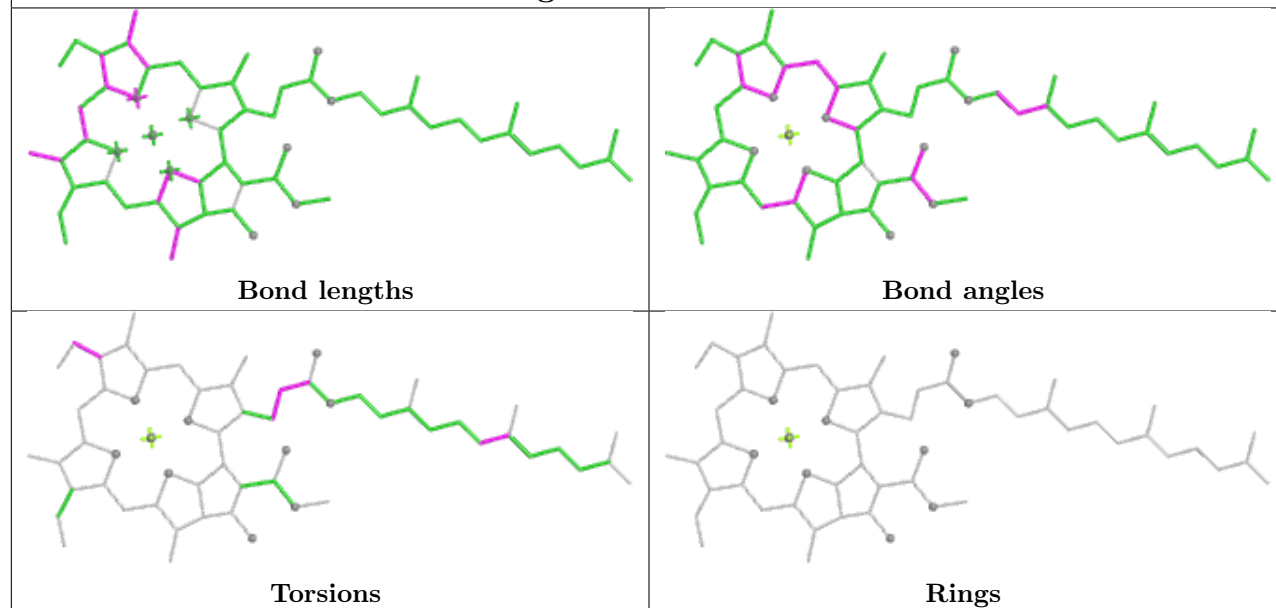




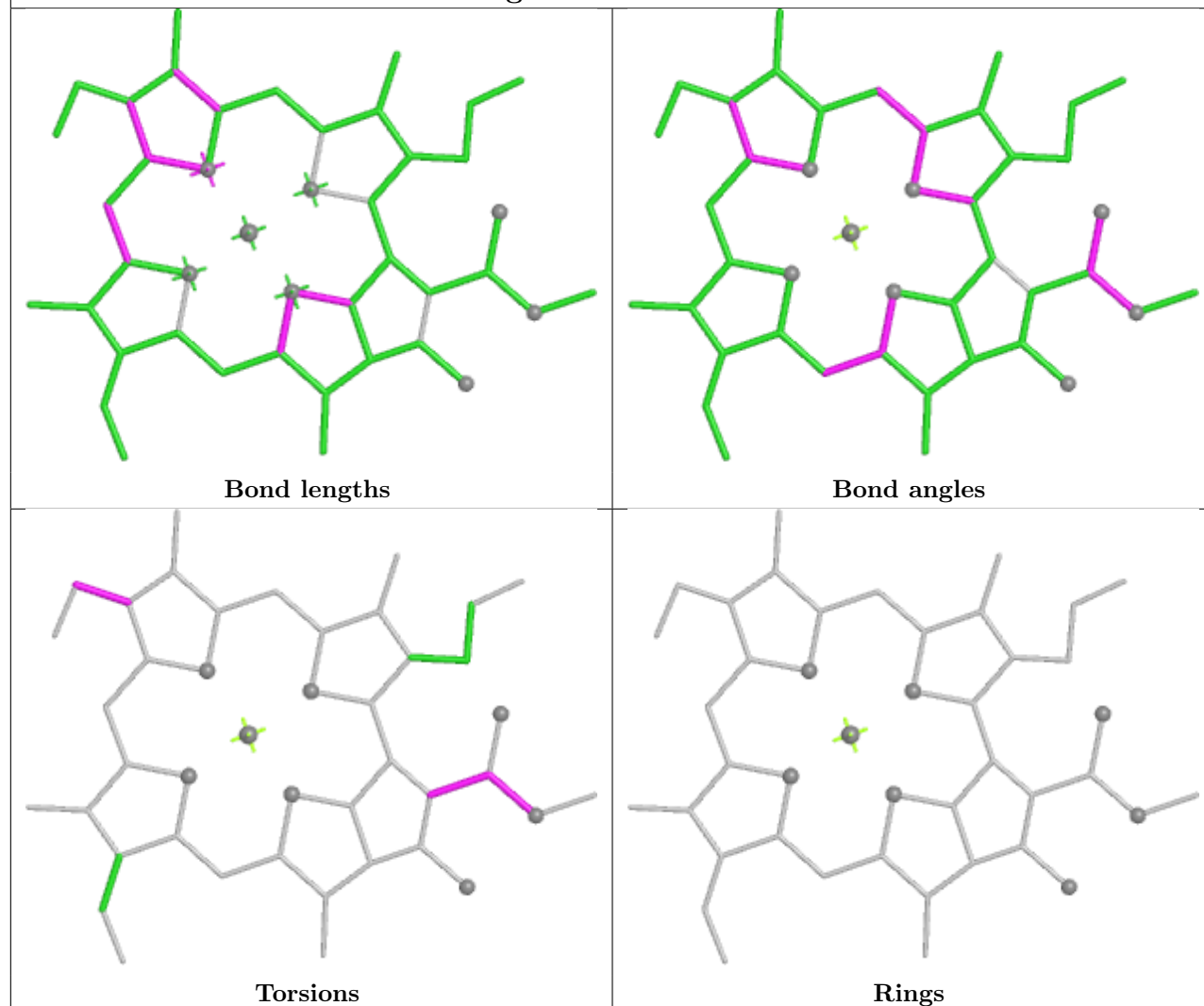




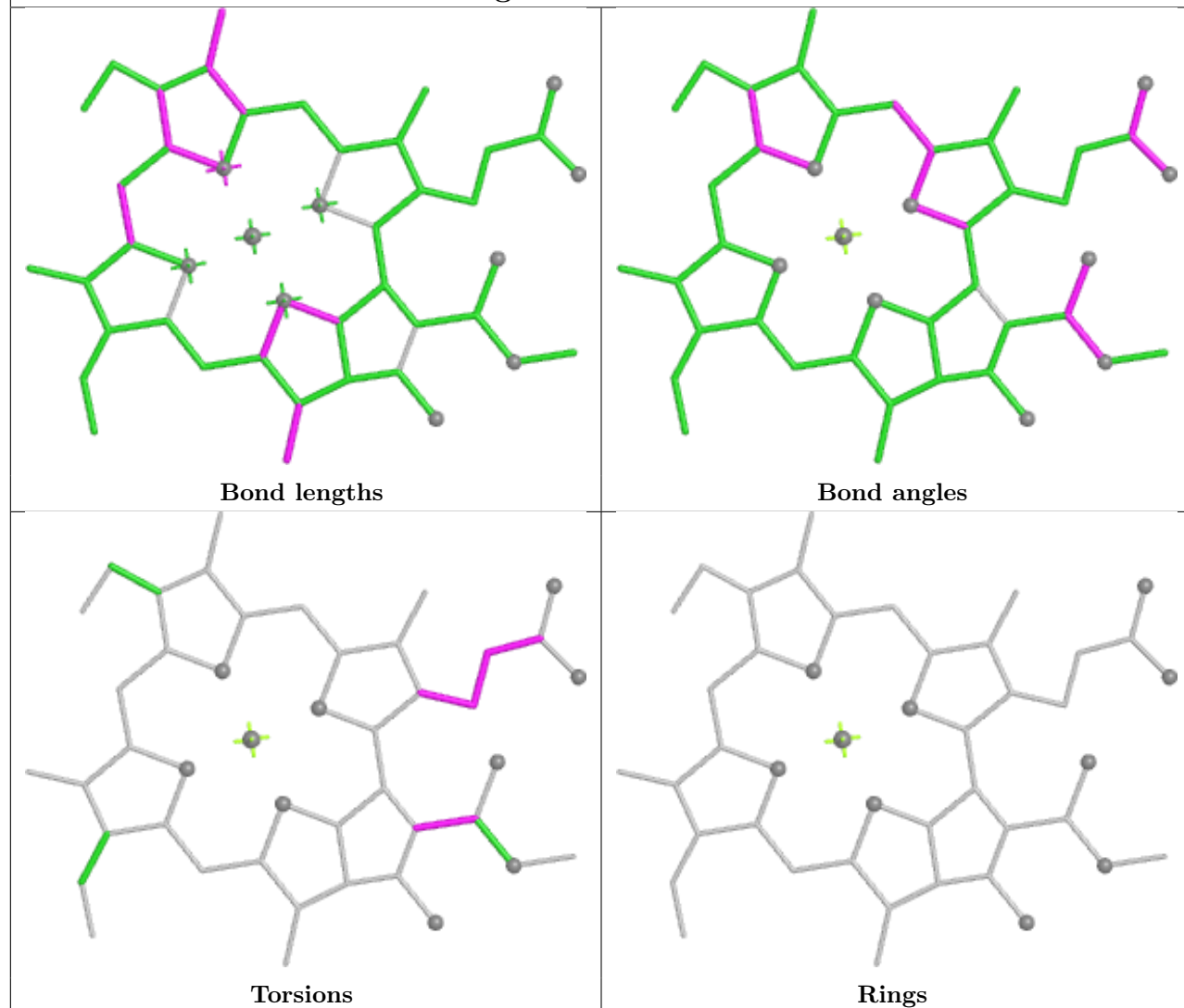
Ligand CLA c 602



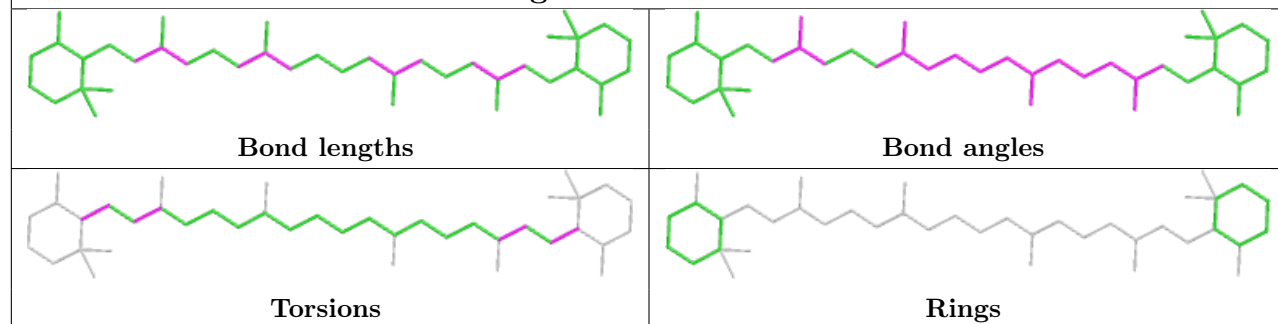
Ligand CLA 8 612

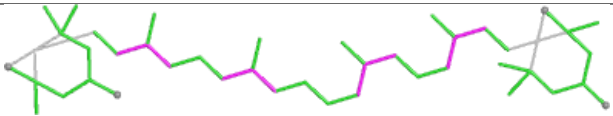
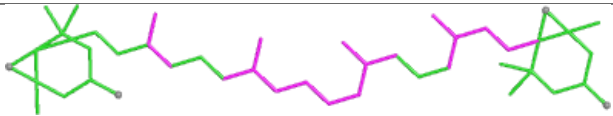
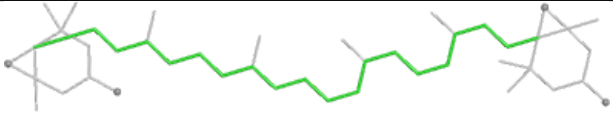
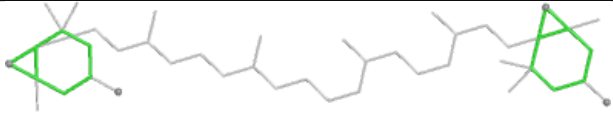


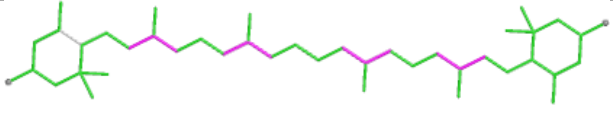
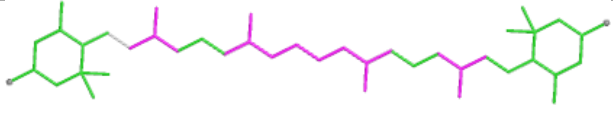
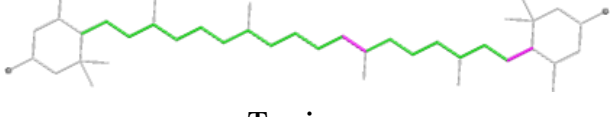
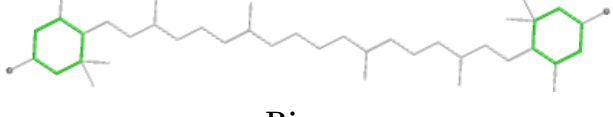
Ligand CLA L 302

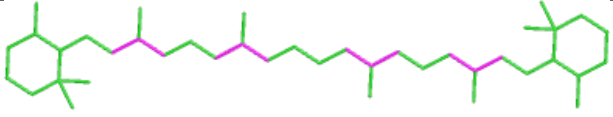
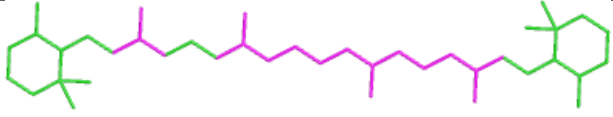
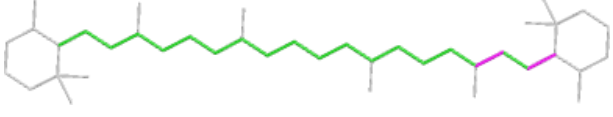
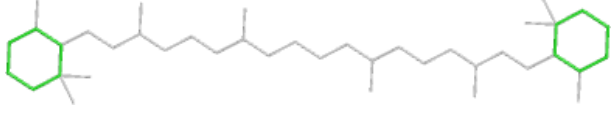


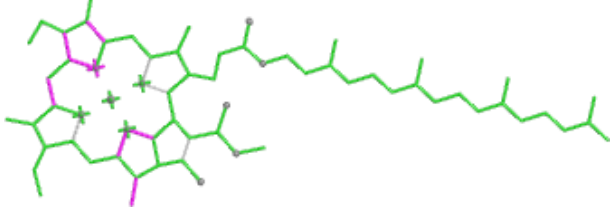
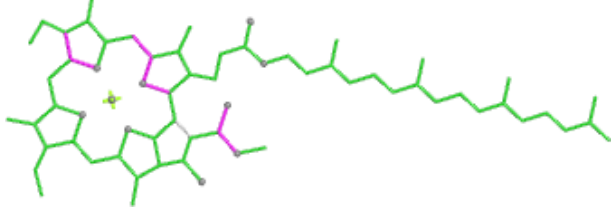
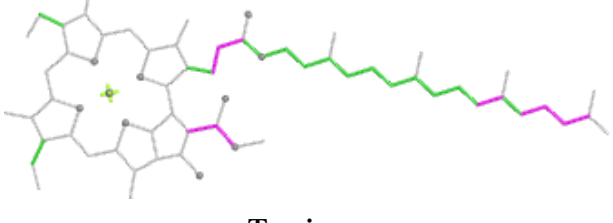
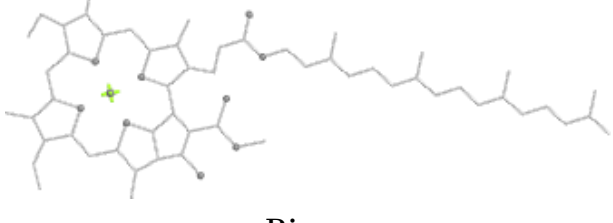
Ligand BCR O 205

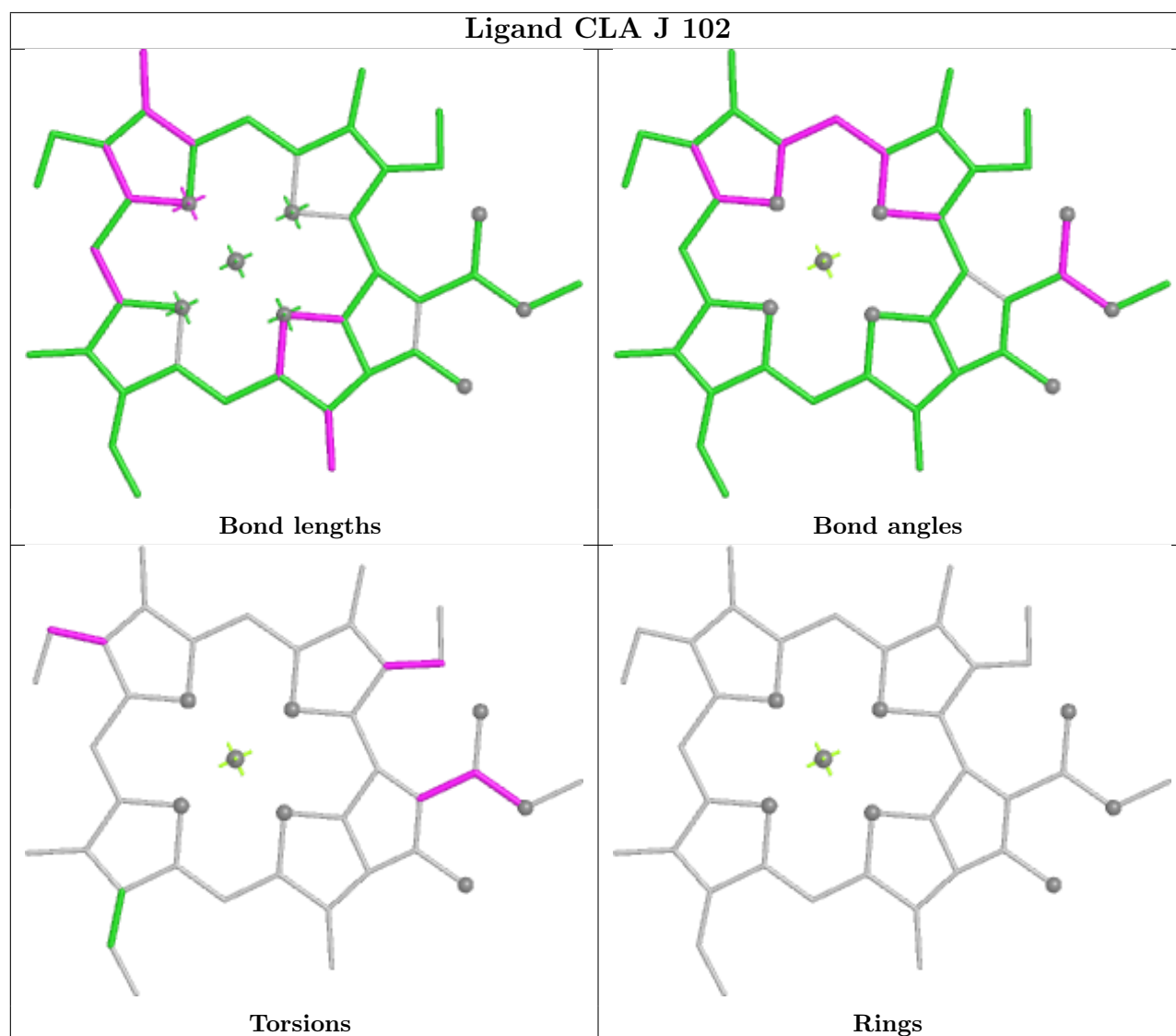
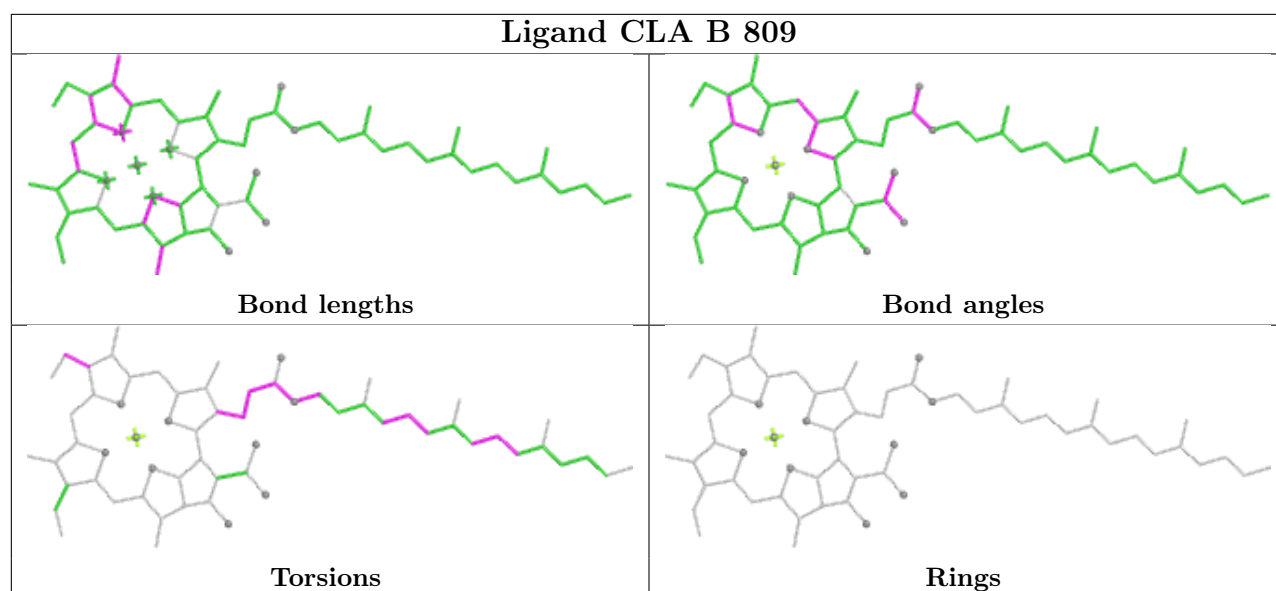


Ligand XAT 2 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

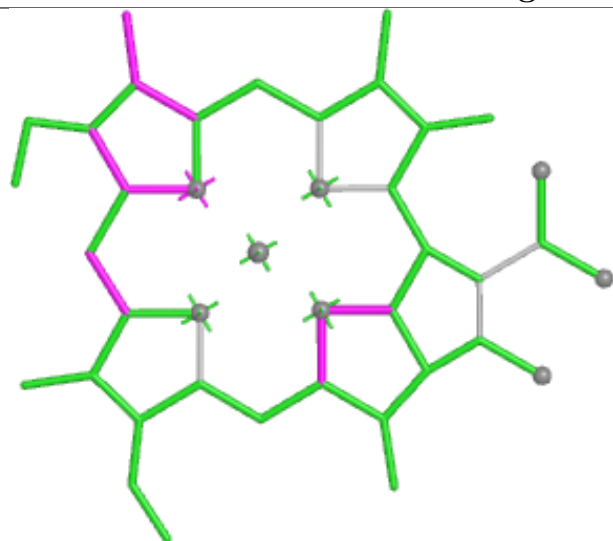
Ligand LUT 4 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

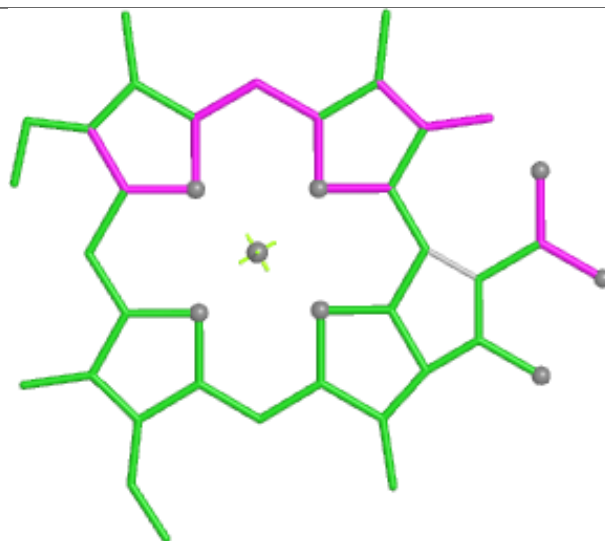
Ligand CLA c 613	
	
Bond lengths	Bond angles
	
Torsions	Rings



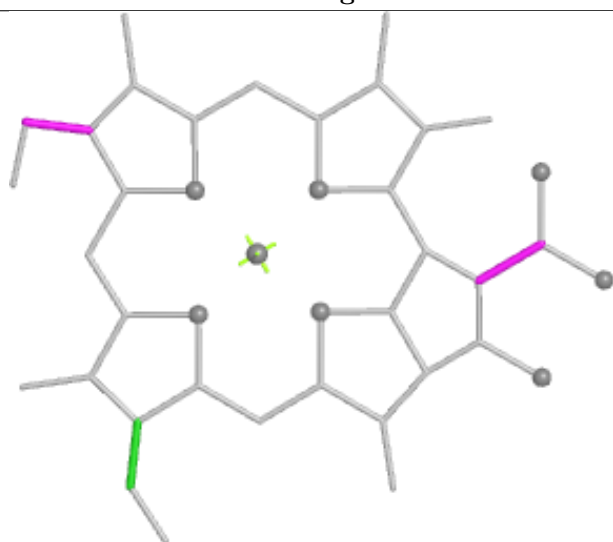
Ligand CLA 3 410



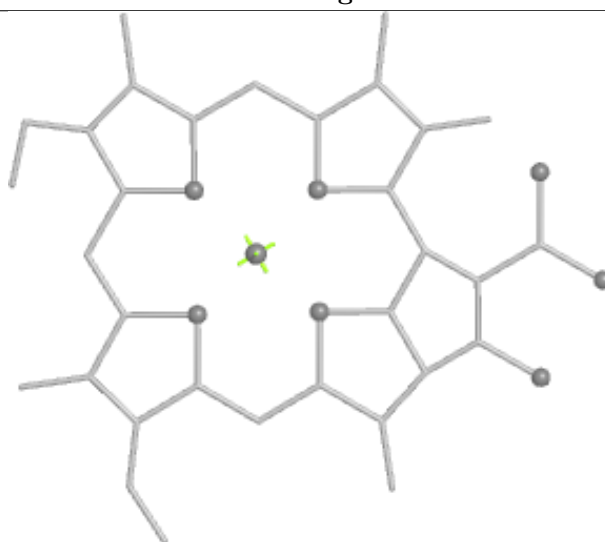
Bond lengths



Bond angles

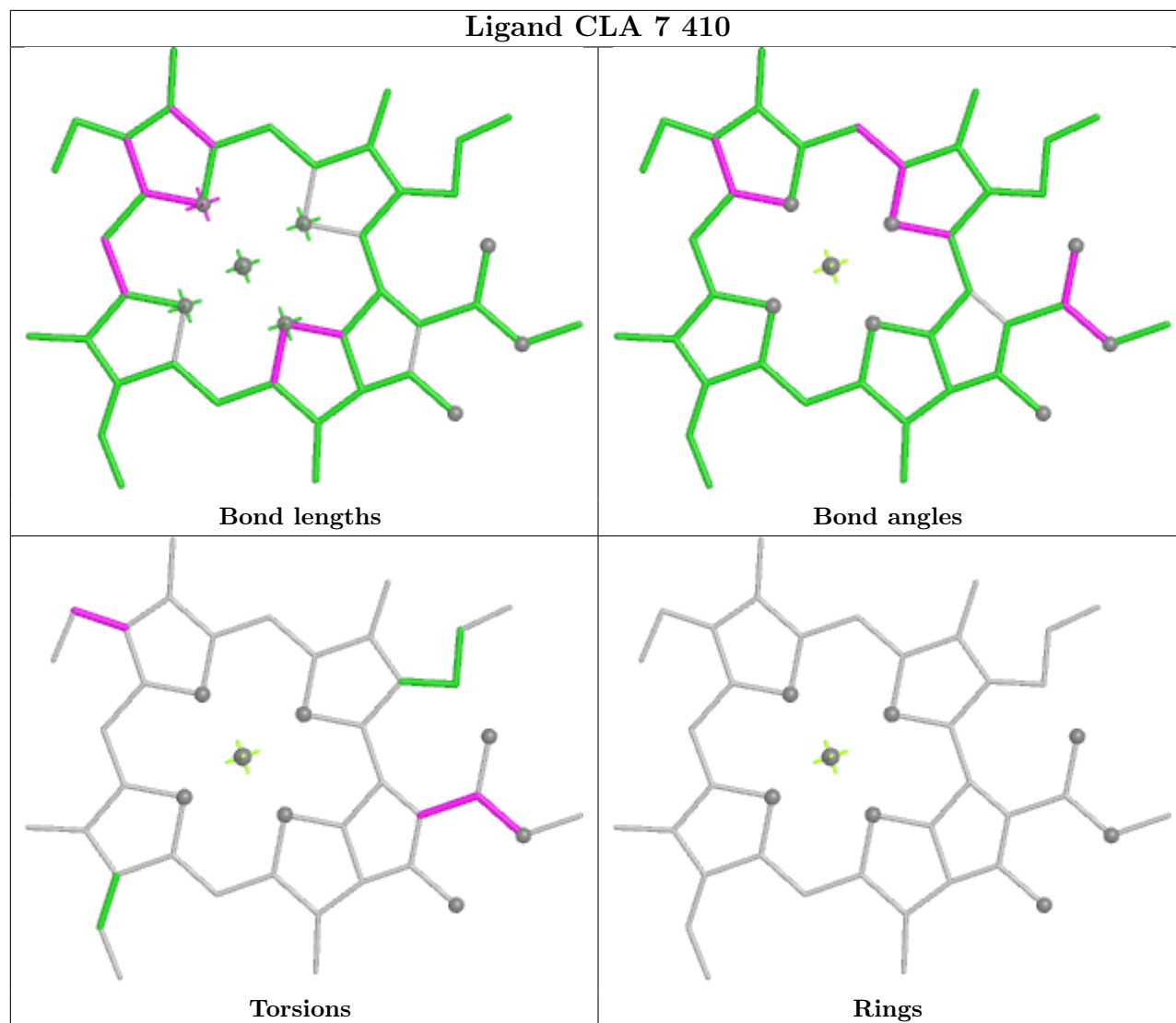


Torsions

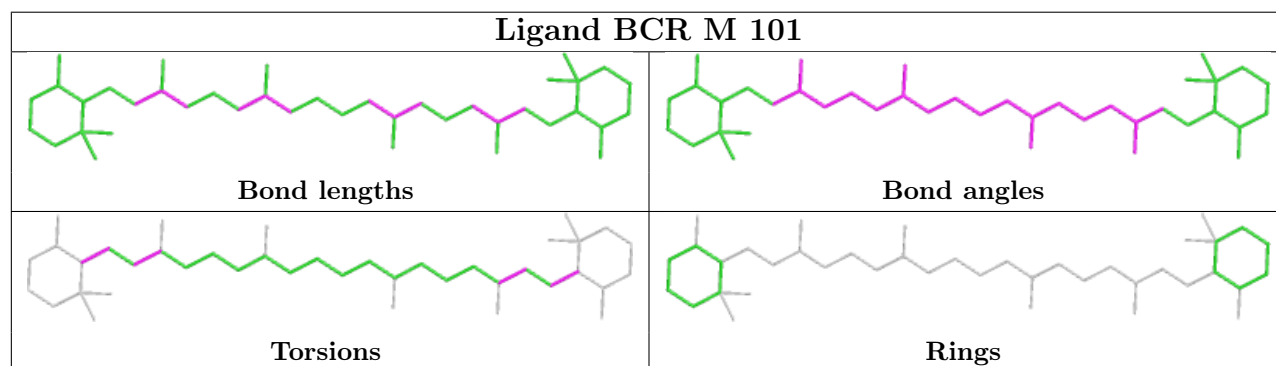


Rings

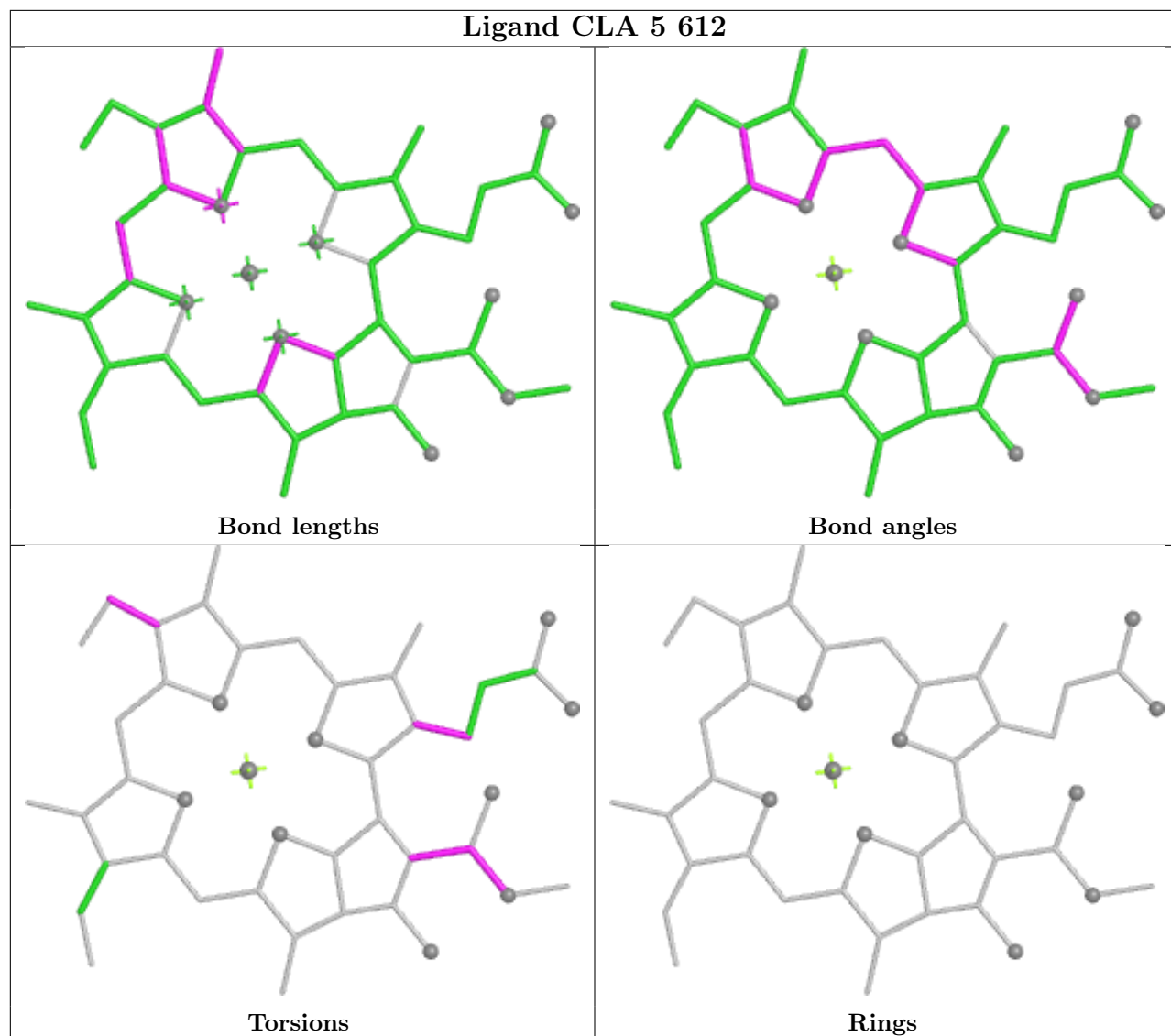
Ligand CLA 7 410



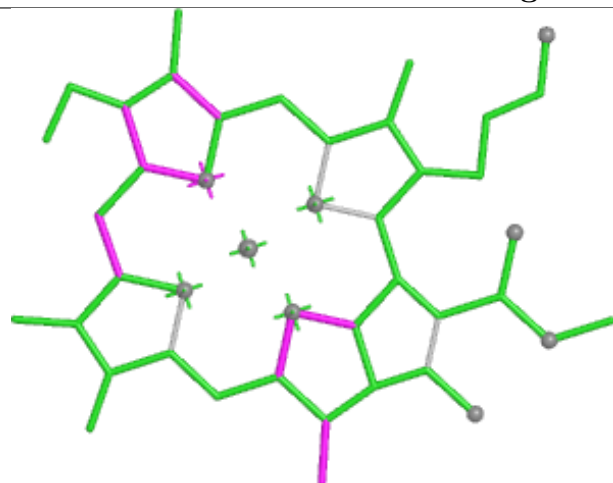
Ligand BCR M 101



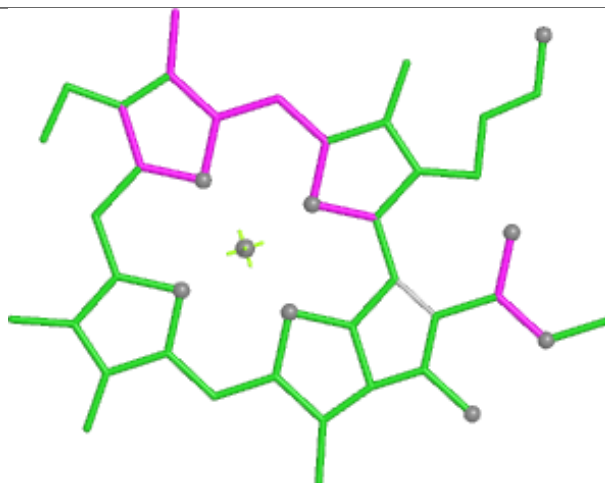
Ligand CLA 5 612



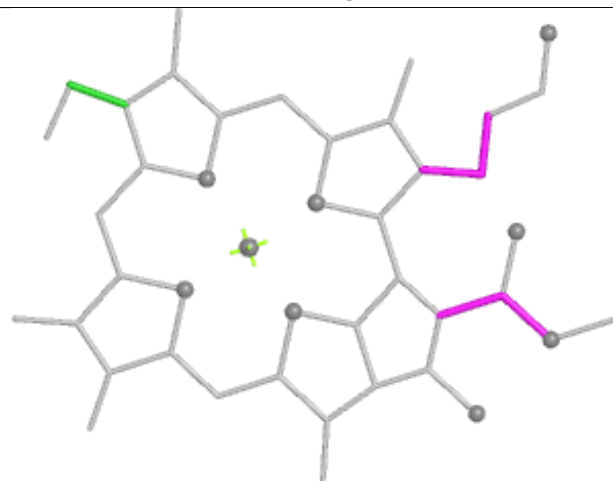
Ligand CLA 8 604



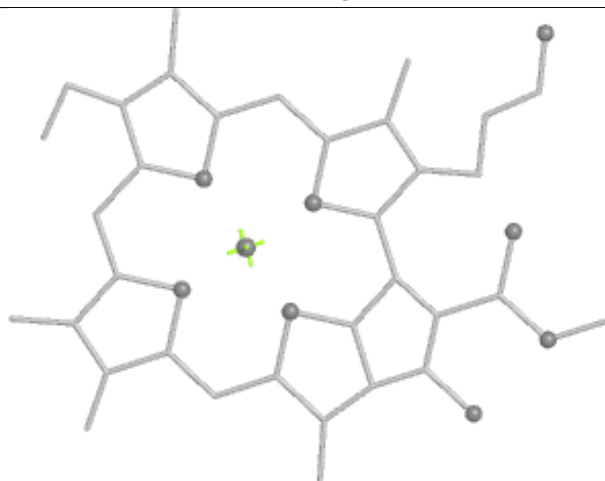
Bond lengths



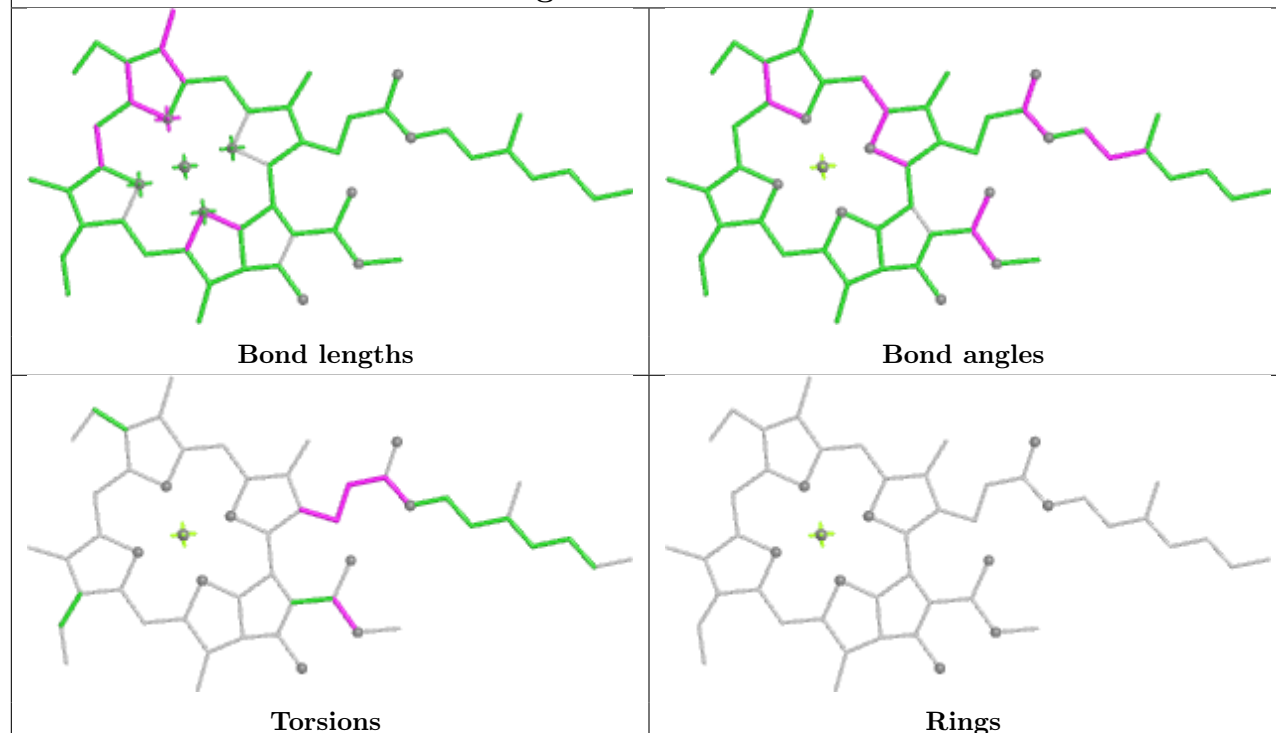
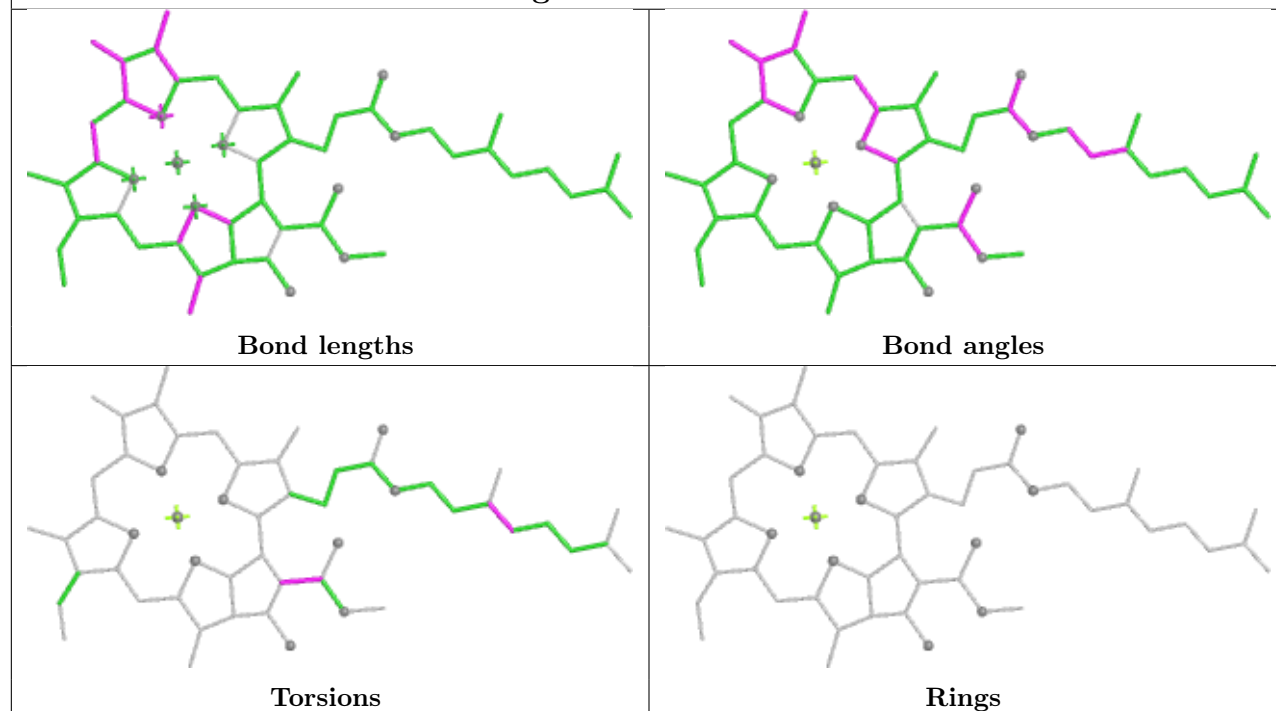
Bond angles



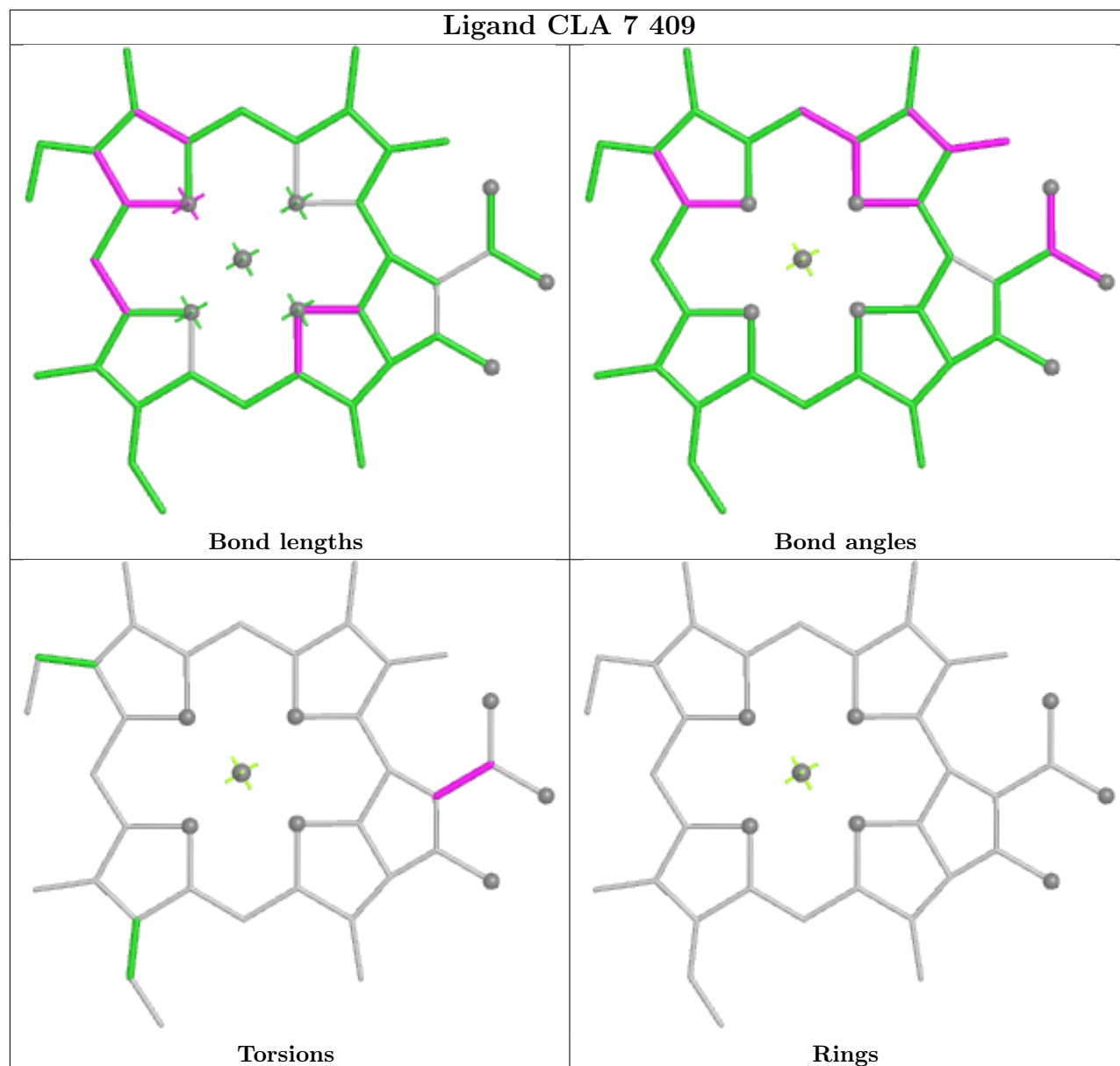
Torsions



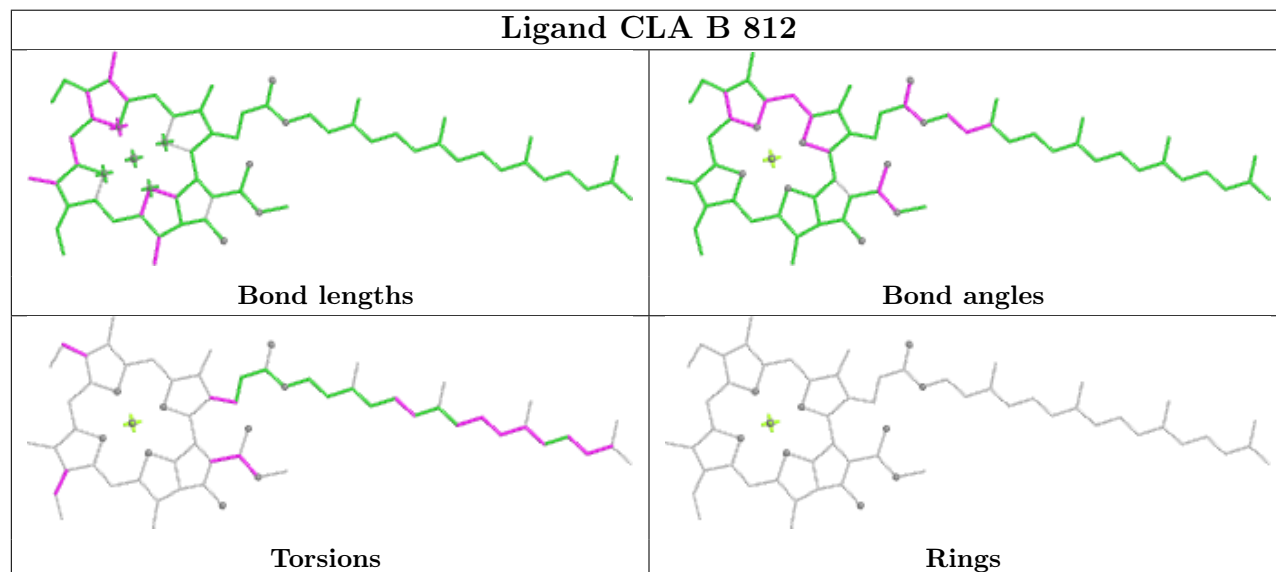
Rings

Ligand CLA 9 613**Ligand CLA B 810**

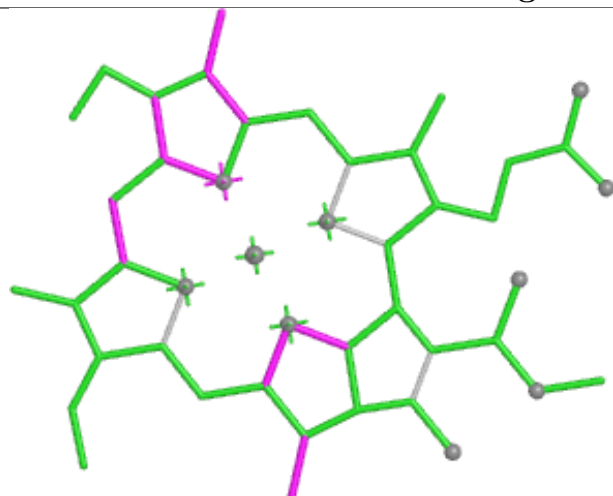
Ligand CLA 7 409



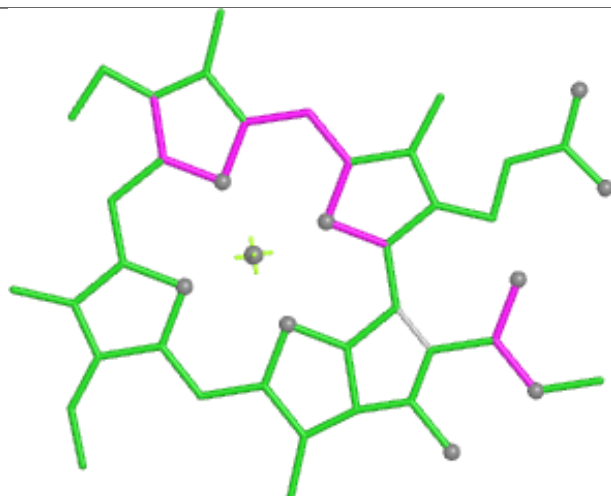
Ligand CLA B 812



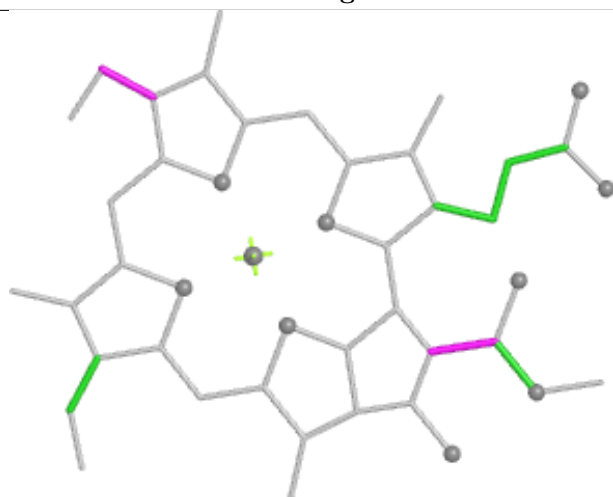
Ligand CLA 4 601



Bond lengths



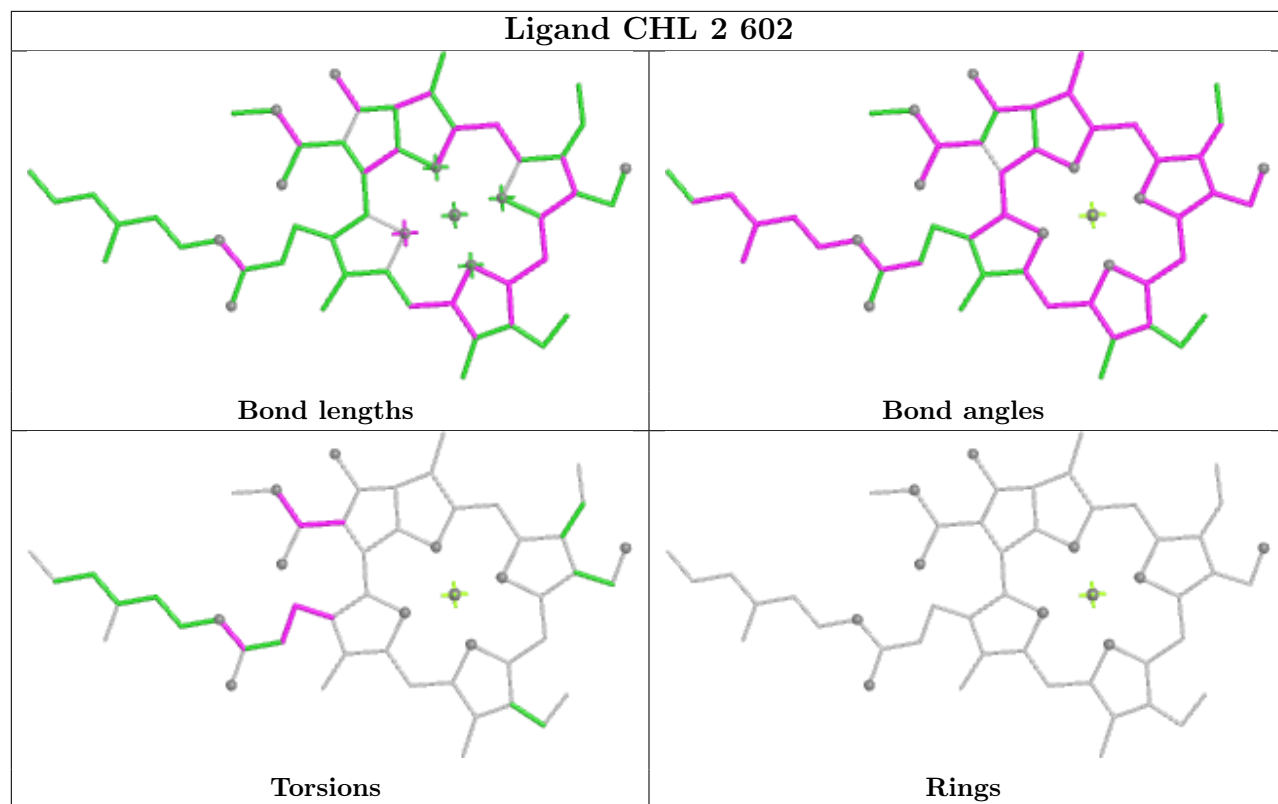
Bond angles



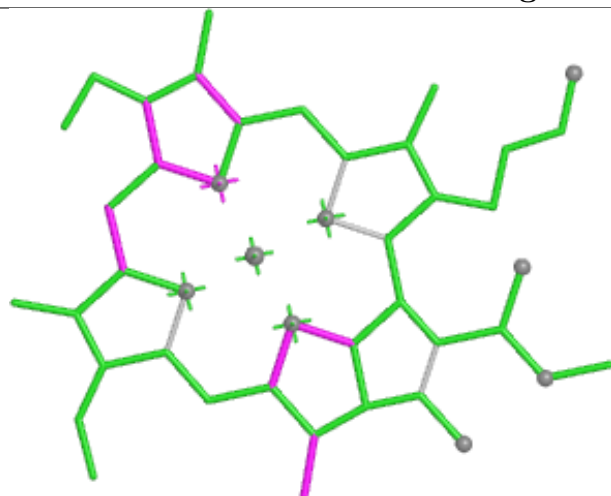
Torsions



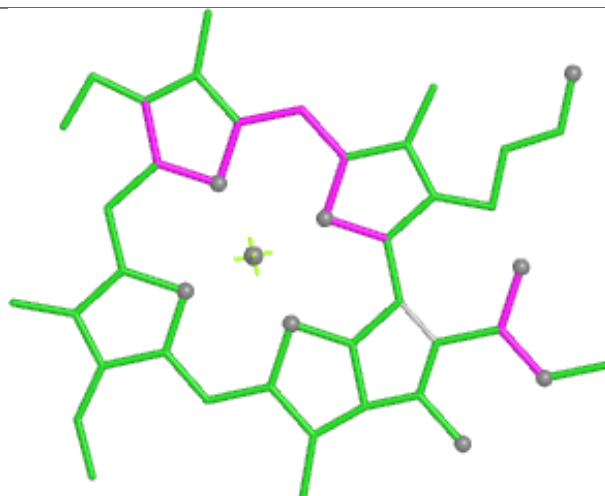
Rings



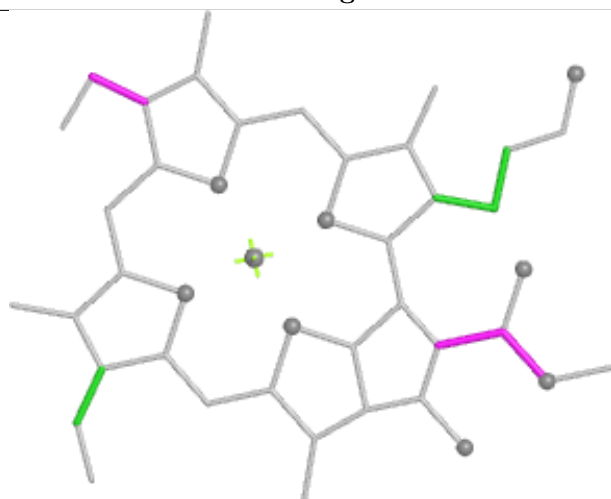
Ligand CLA c 612



Bond lengths



Bond angles

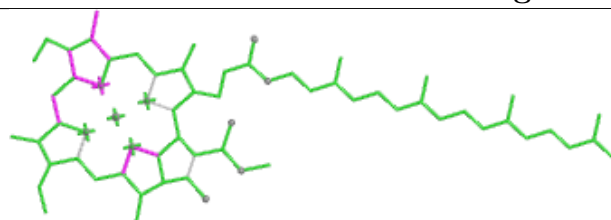


Torsions

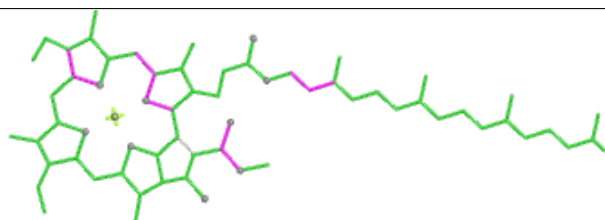


Rings

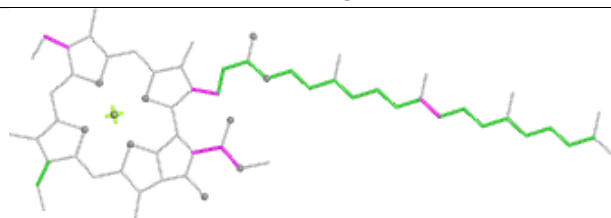
Ligand CLA A 833



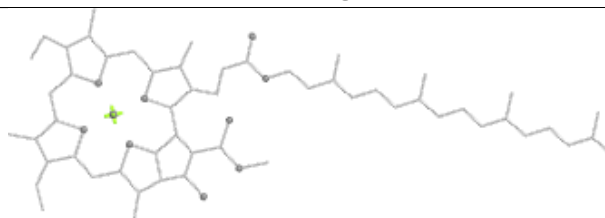
Bond lengths



Bond angles

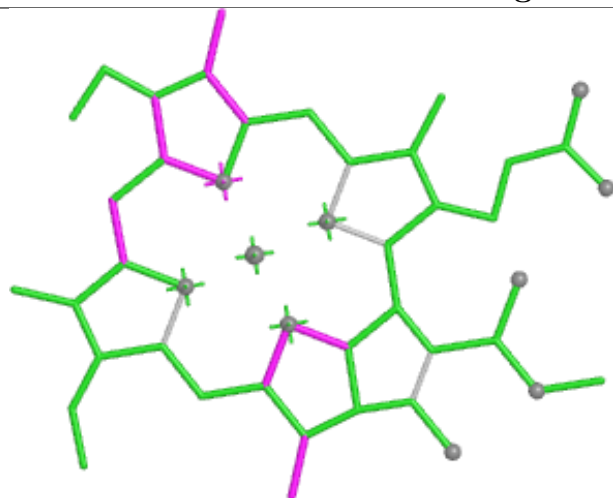


Torsions

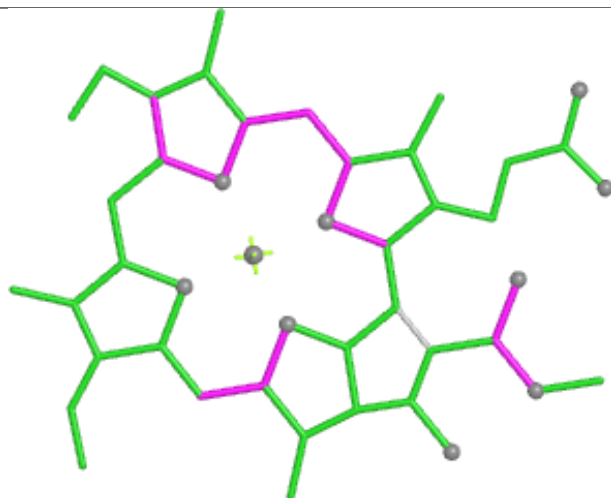


Rings

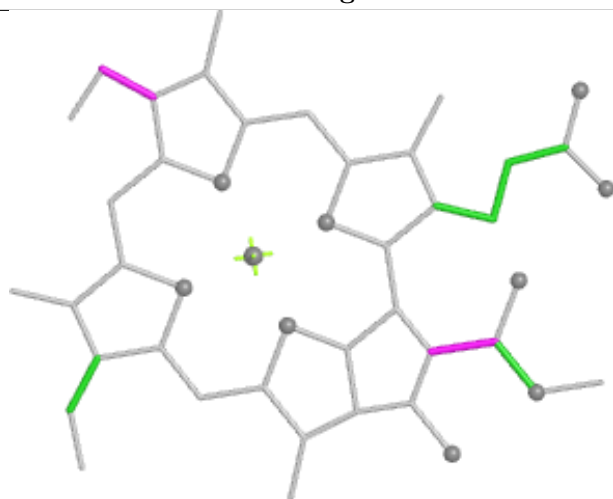
Ligand CLA B 833



Bond lengths



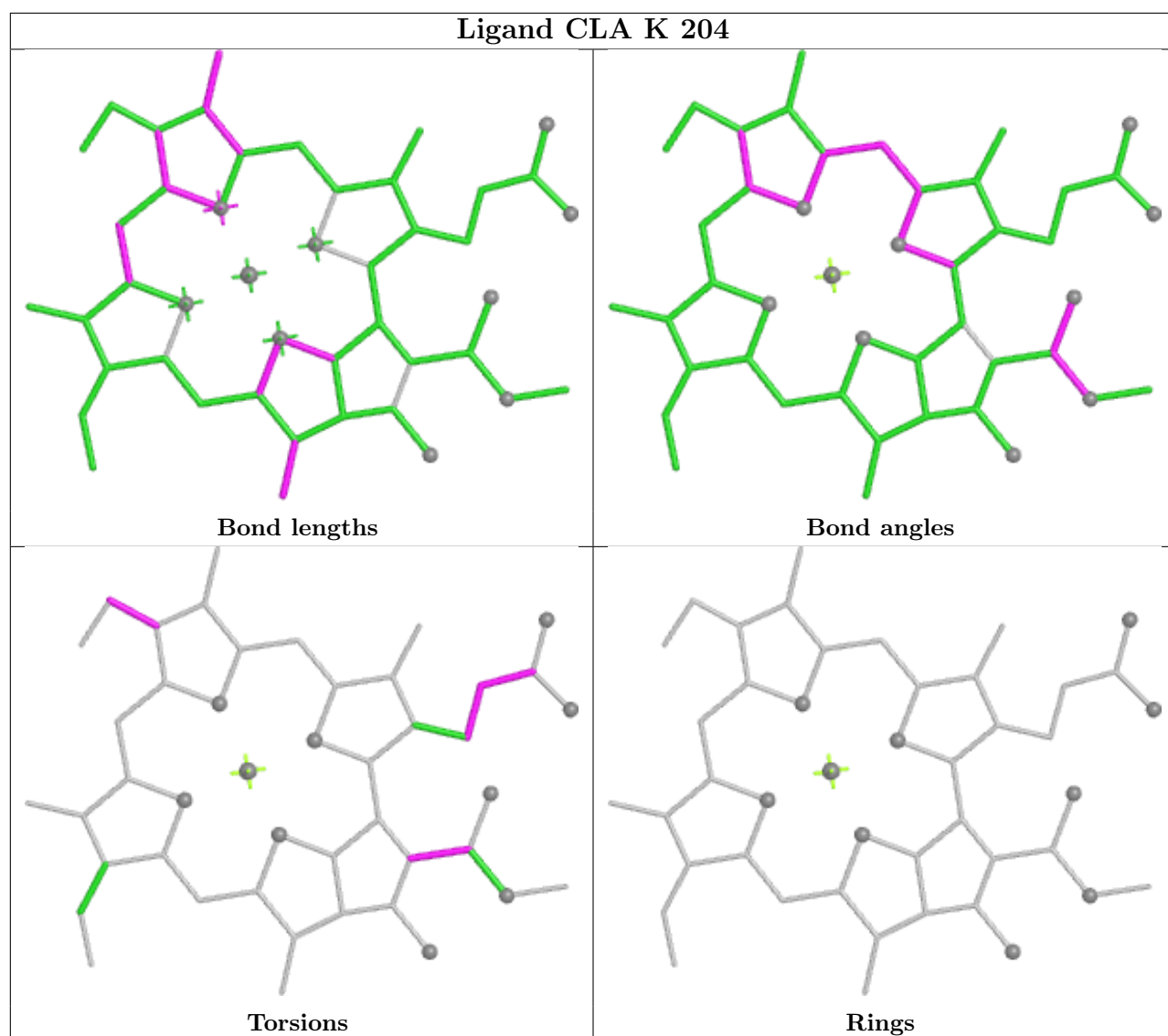
Bond angles



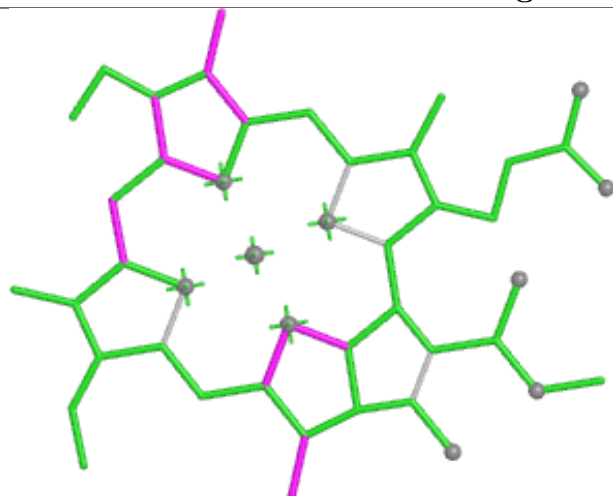
Torsions



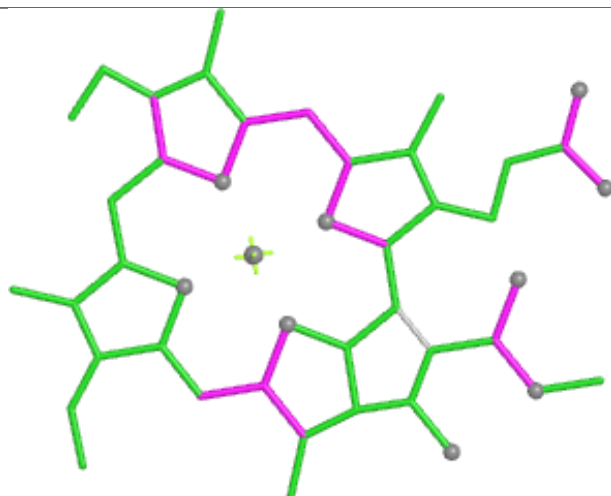
Rings



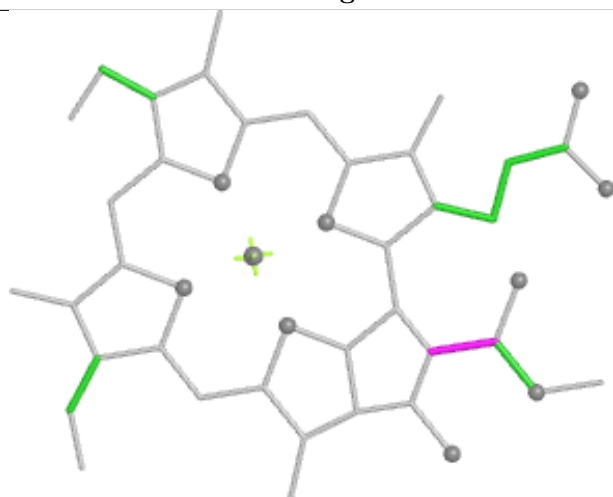
Ligand CLA F 304



Bond lengths



Bond angles

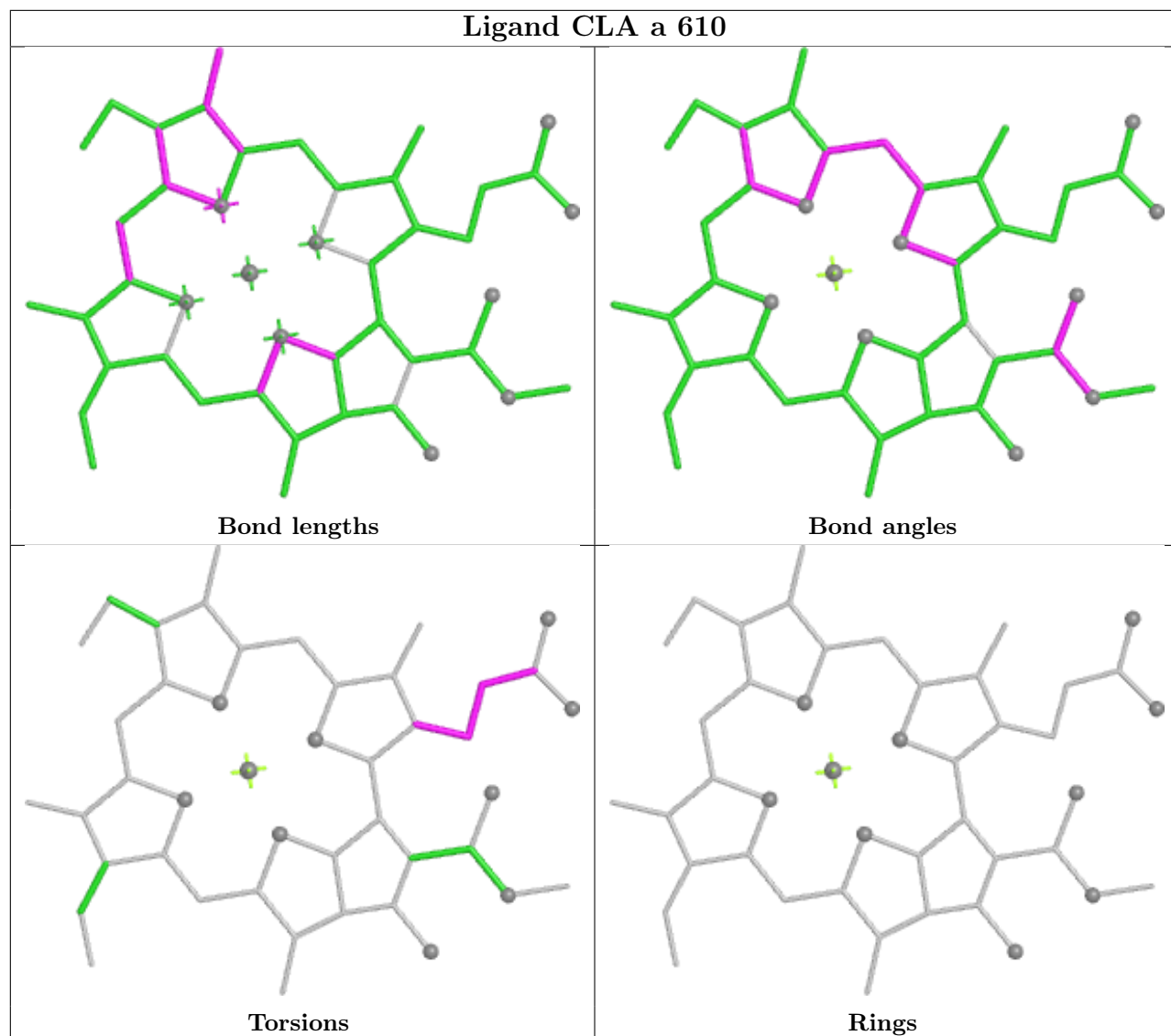


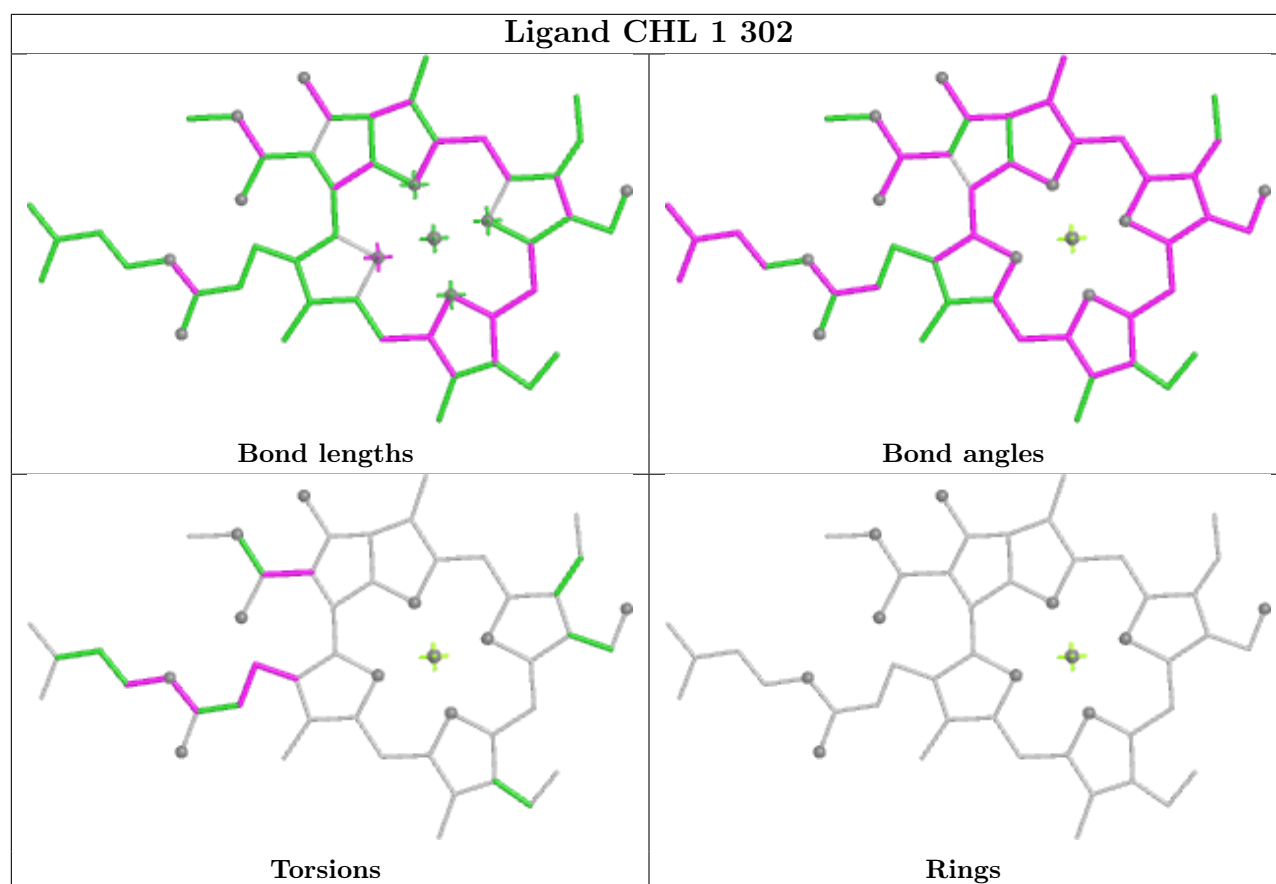
Torsions



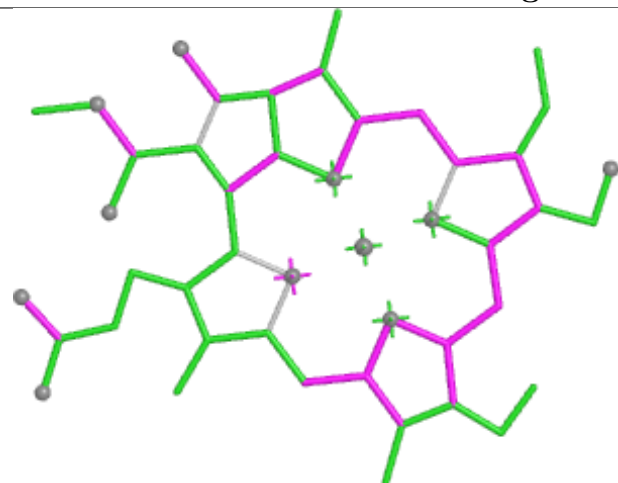
Rings

Ligand CLA a 610

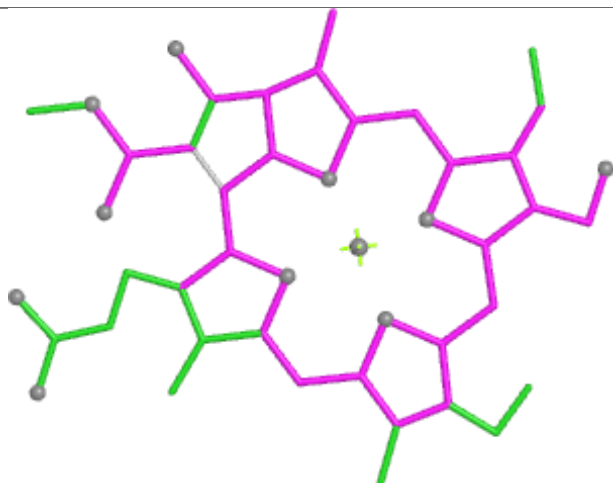




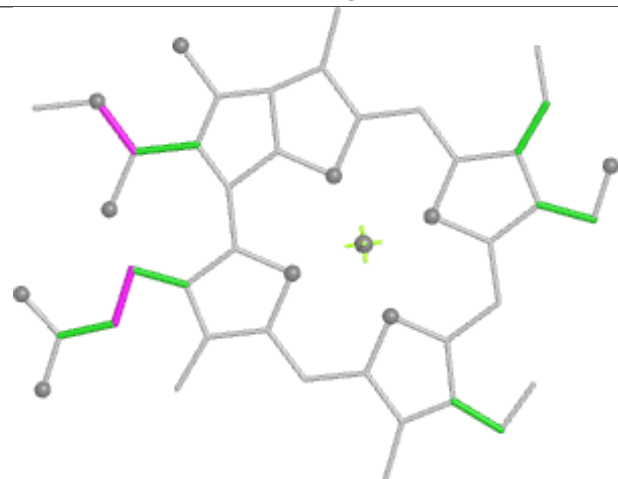
Ligand CHL 6 605



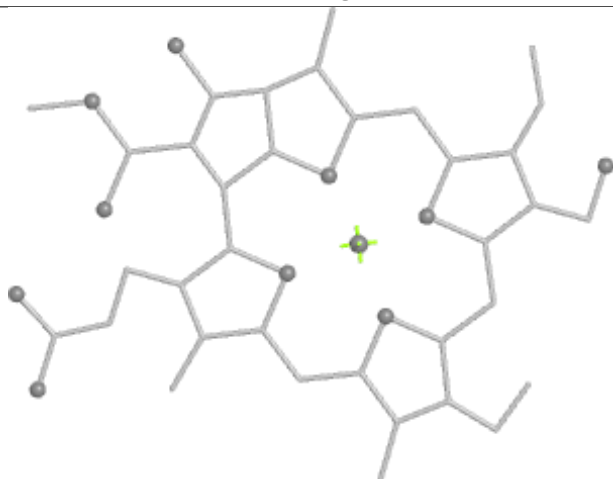
Bond lengths



Bond angles

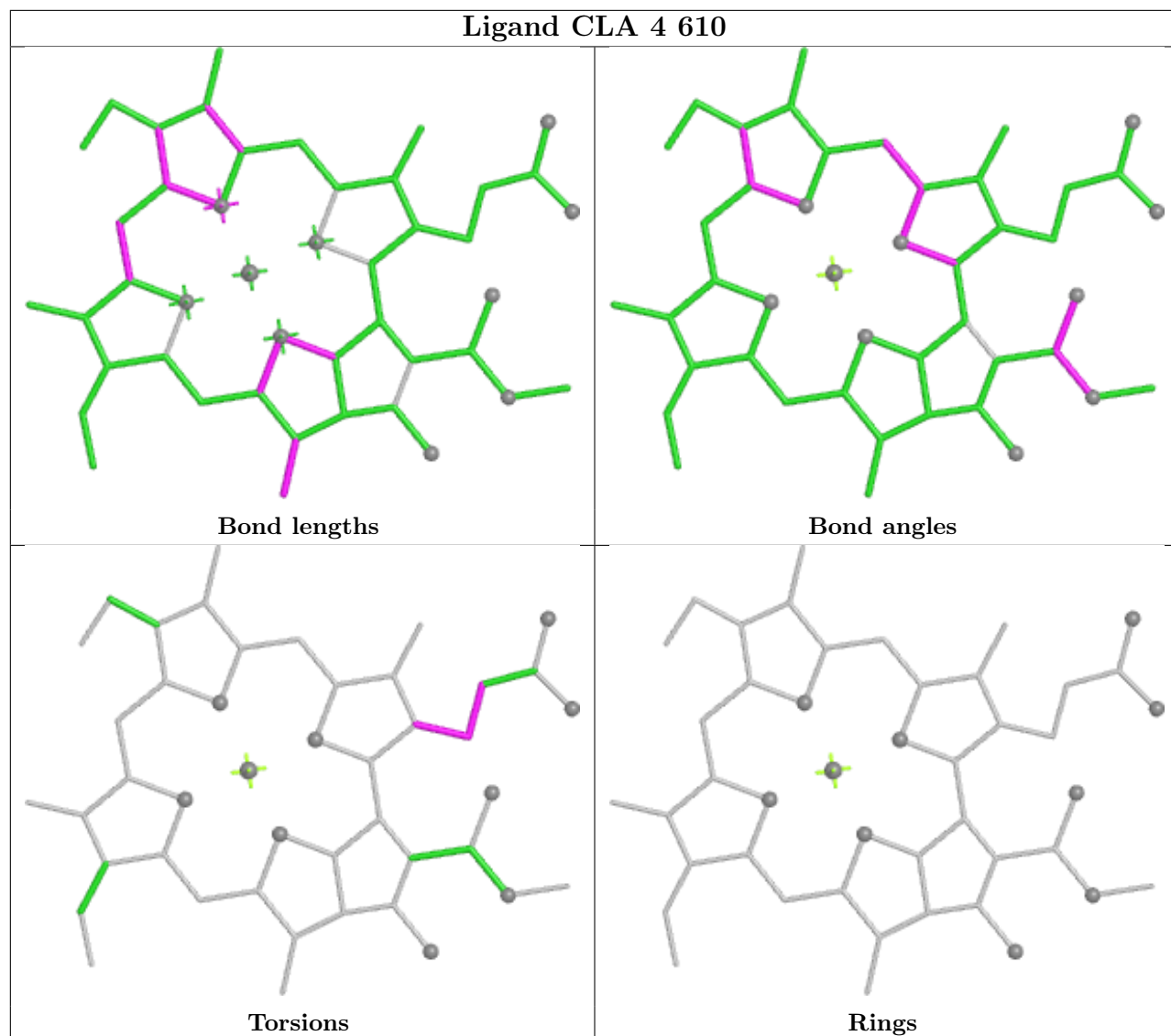


Torsions

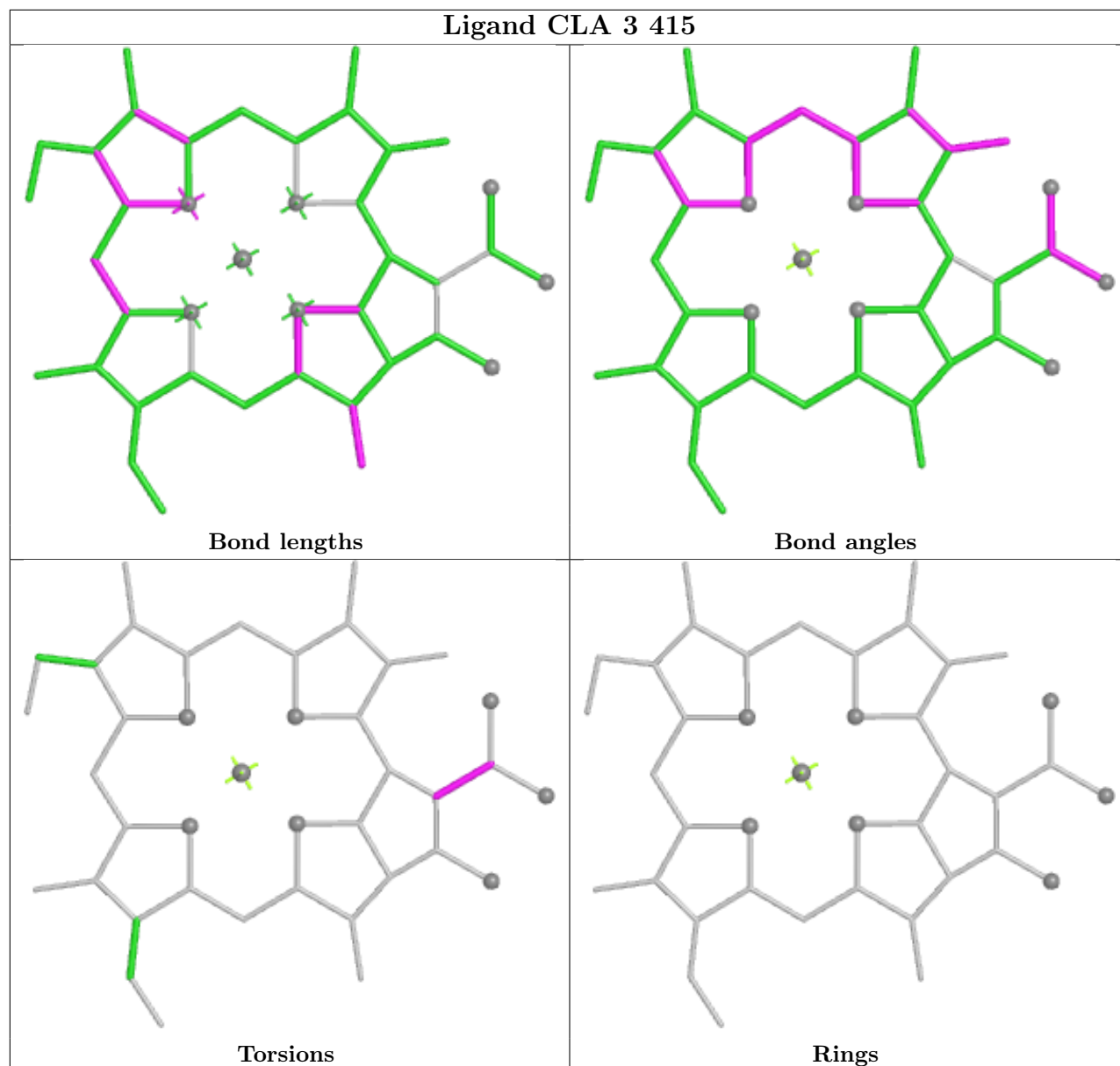


Rings

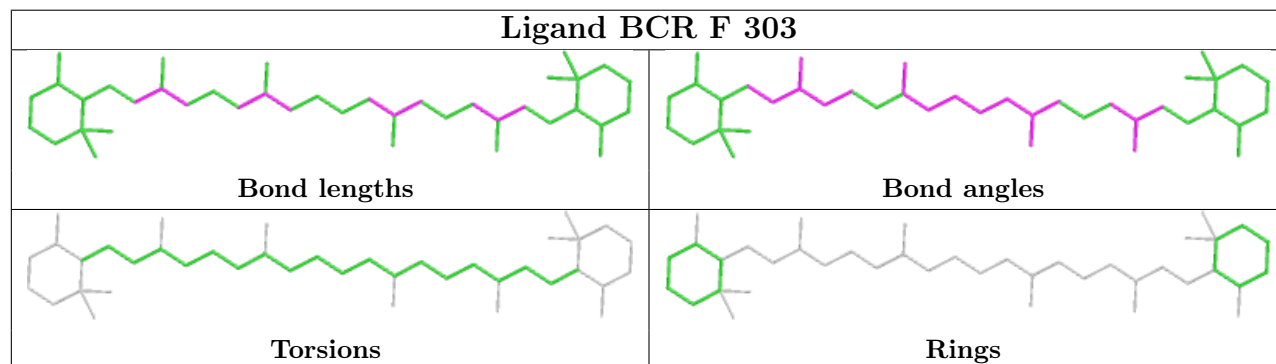
Ligand CLA 4 610

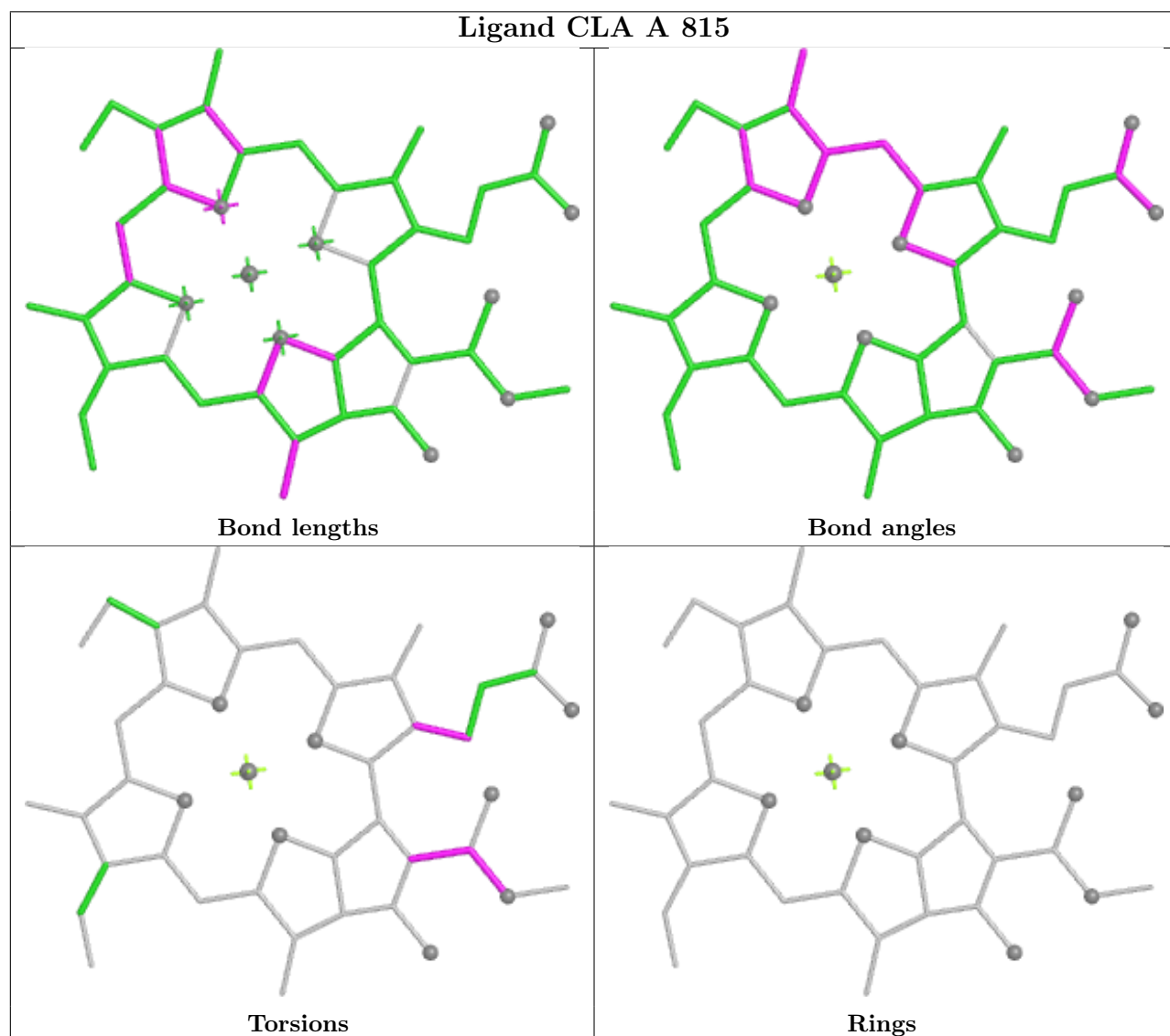
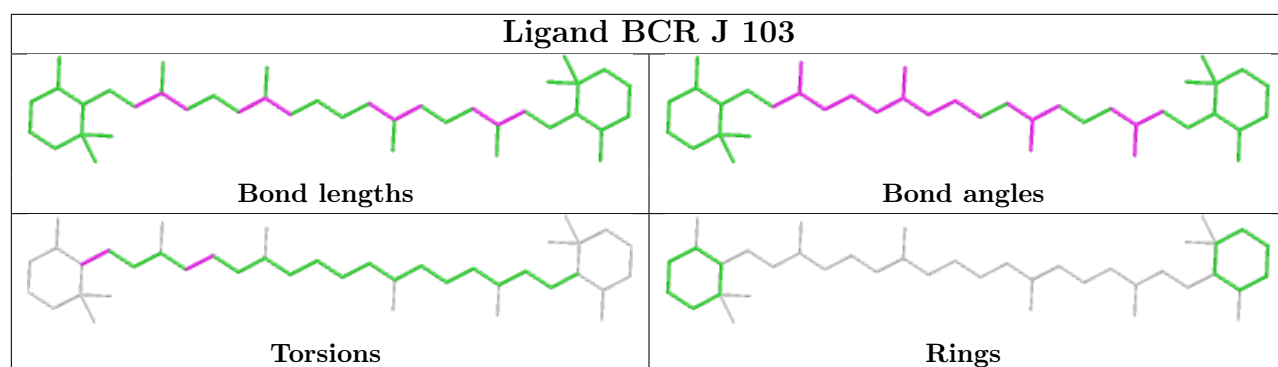


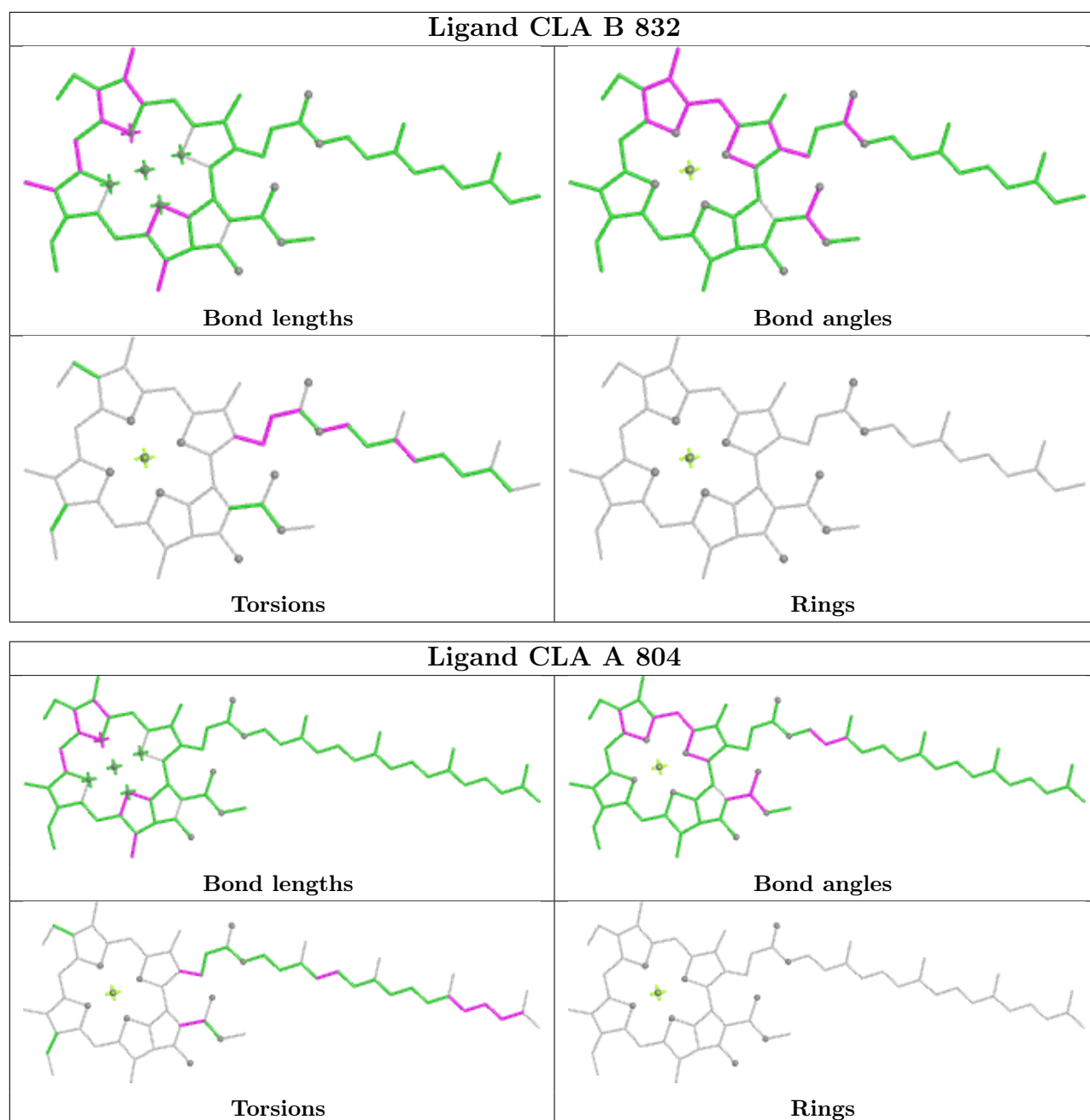
Ligand CLA 3 415

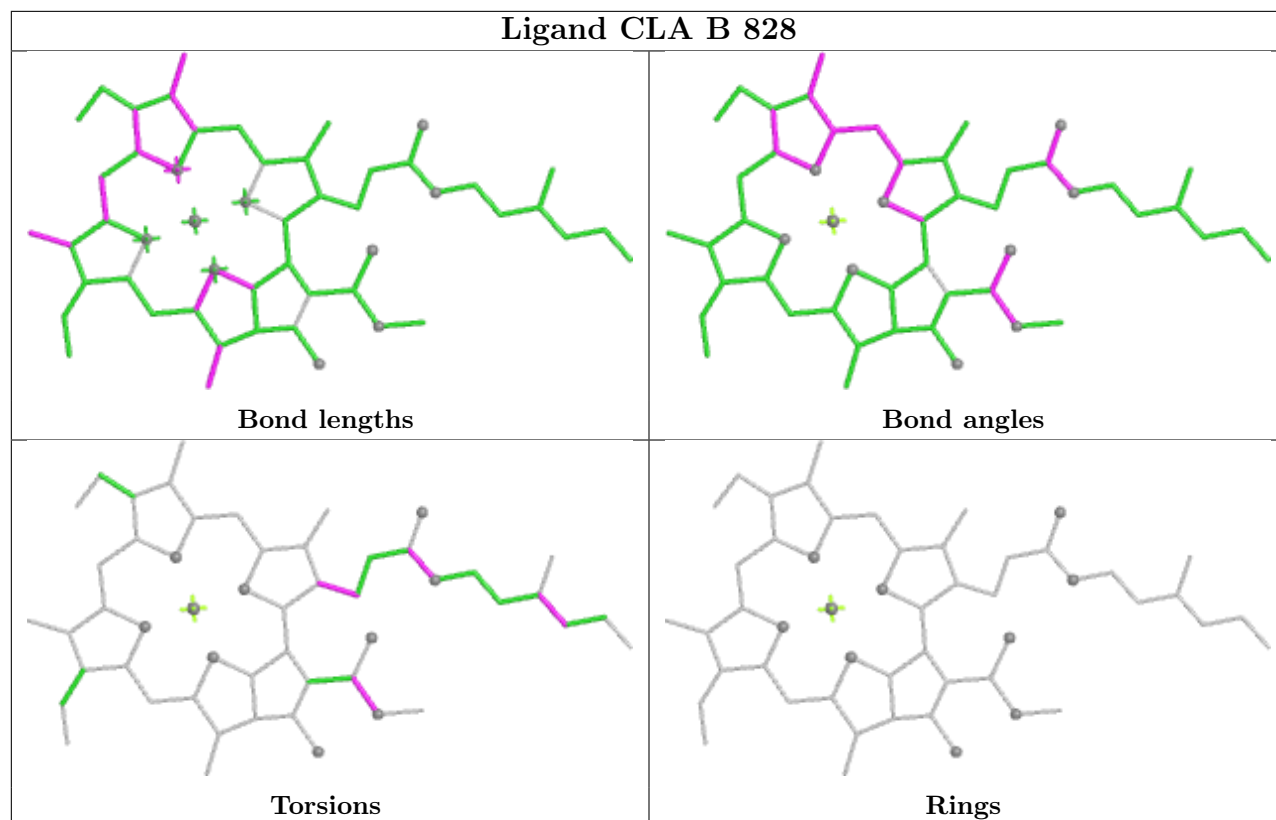


Ligand BCR F 303

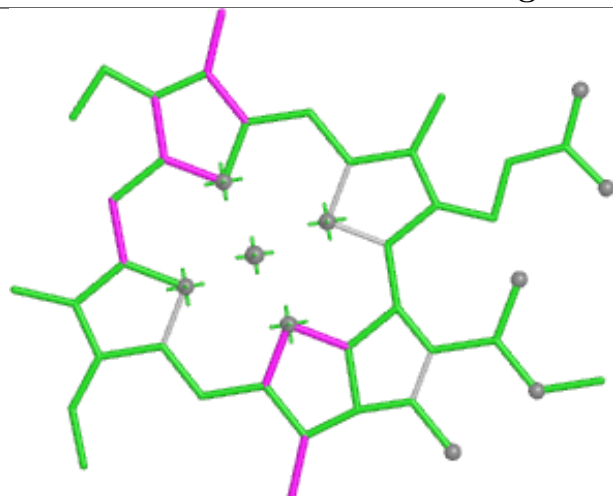




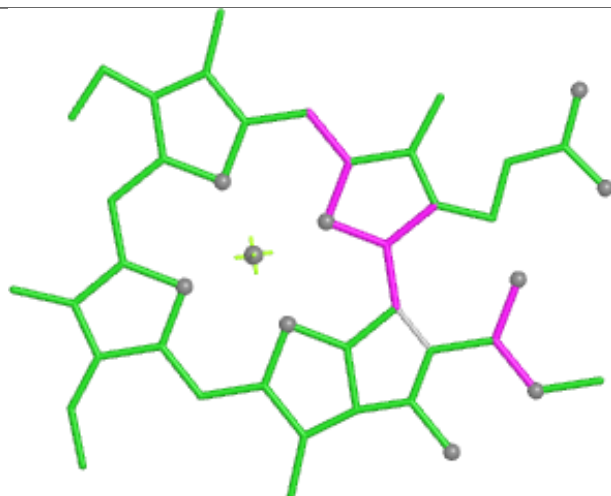




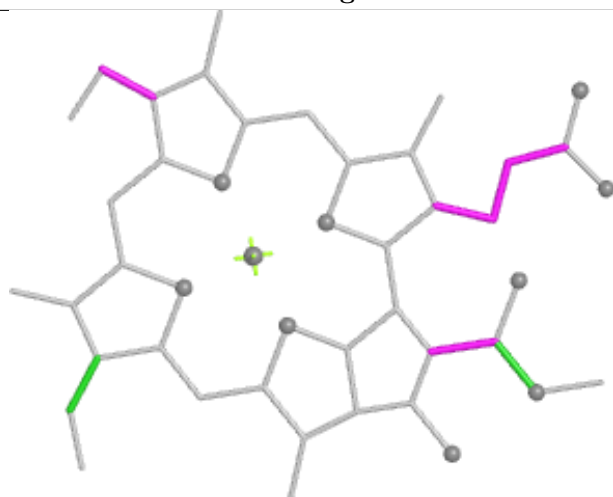
Ligand CLA 7 402



Bond lengths



Bond angles

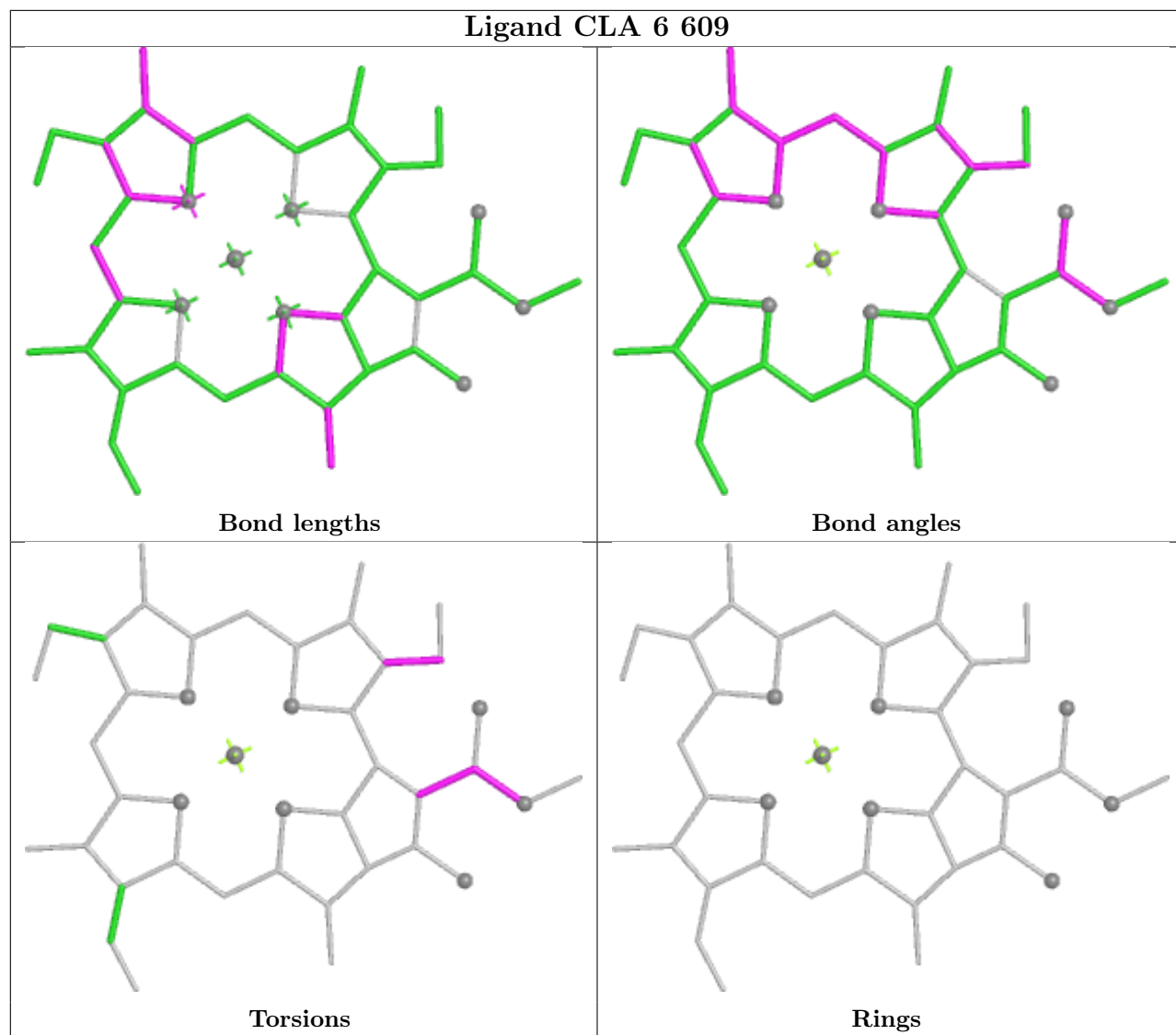


Torsions

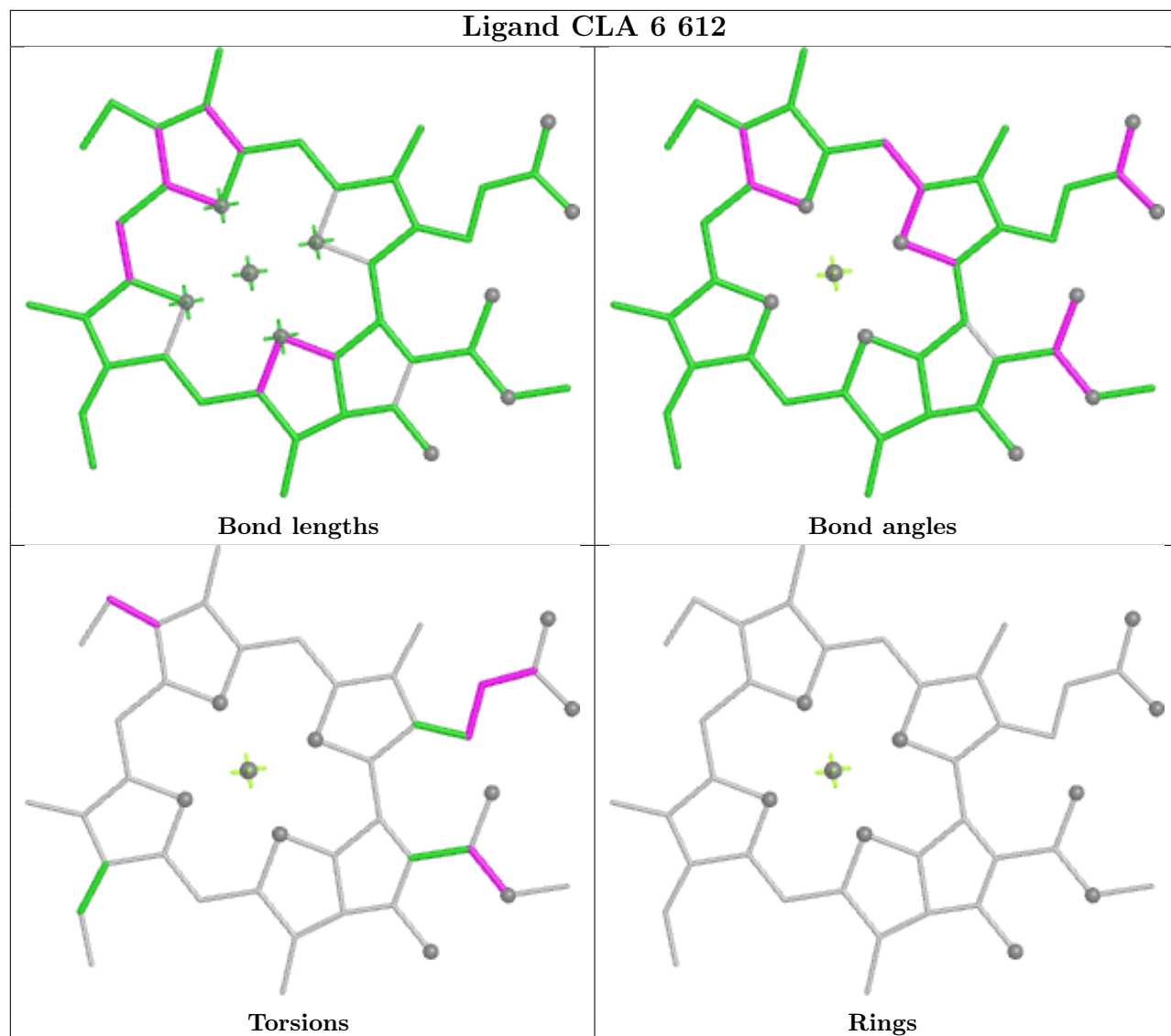


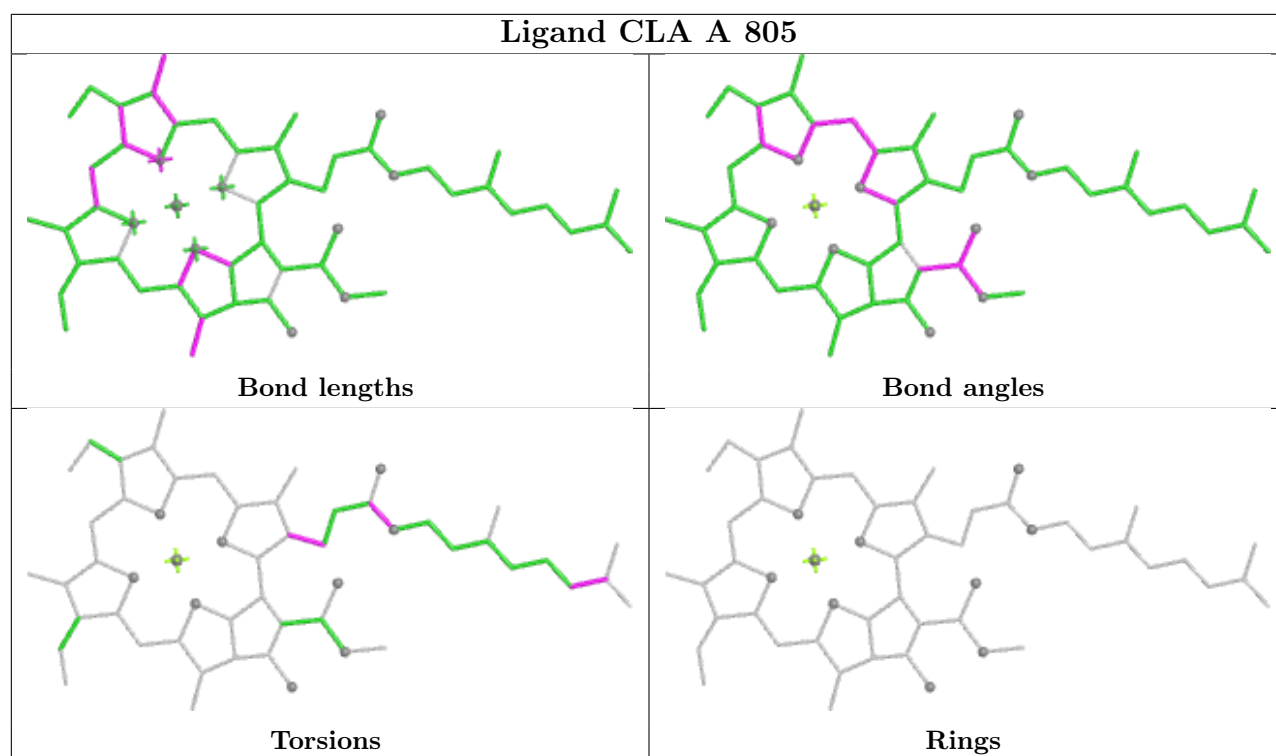
Rings

Ligand CLA 6 609

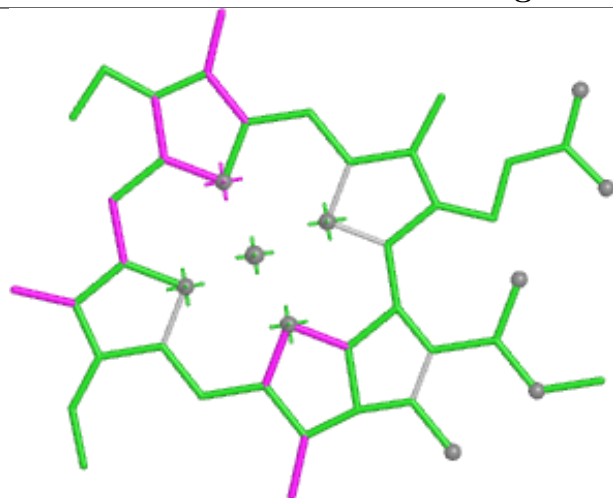


Ligand CLA 6 612

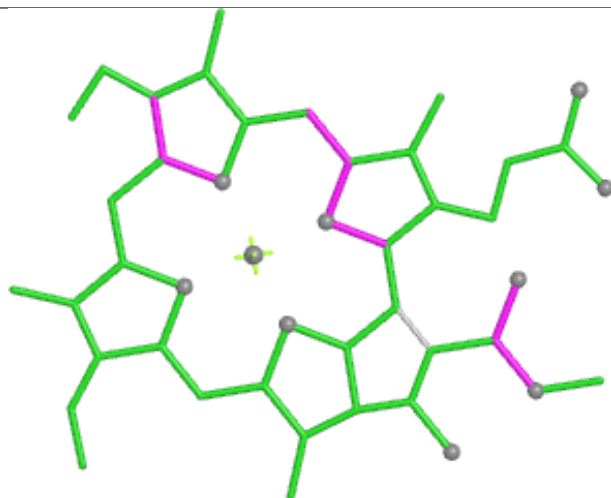




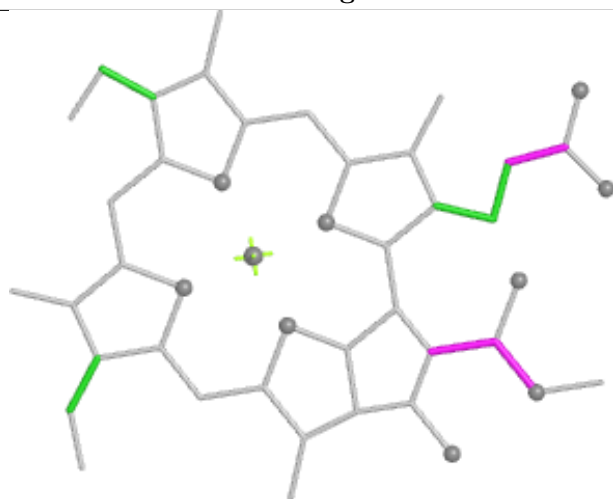
Ligand CLA B 822



Bond lengths



Bond angles

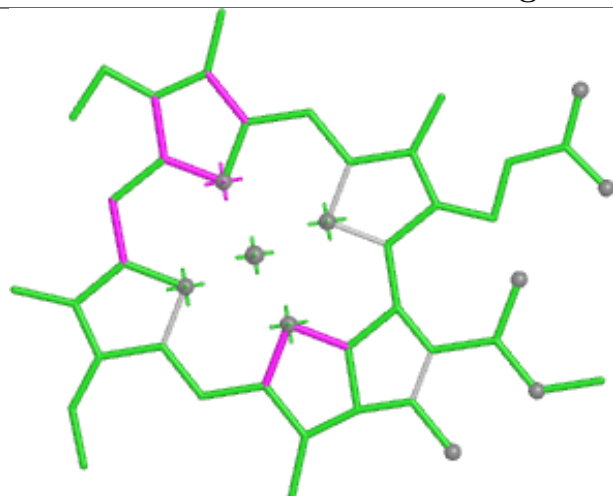


Torsions

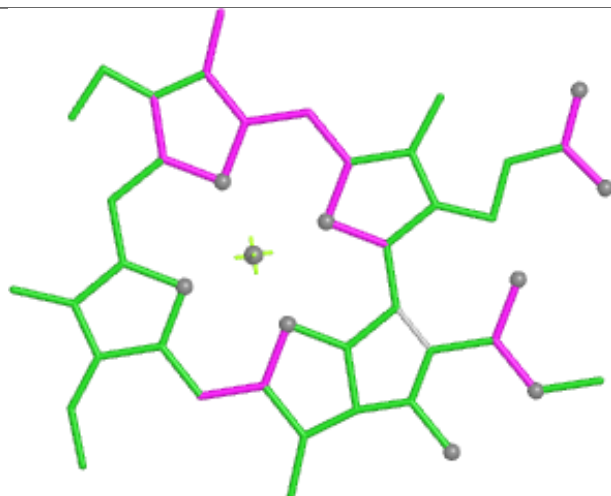


Rings

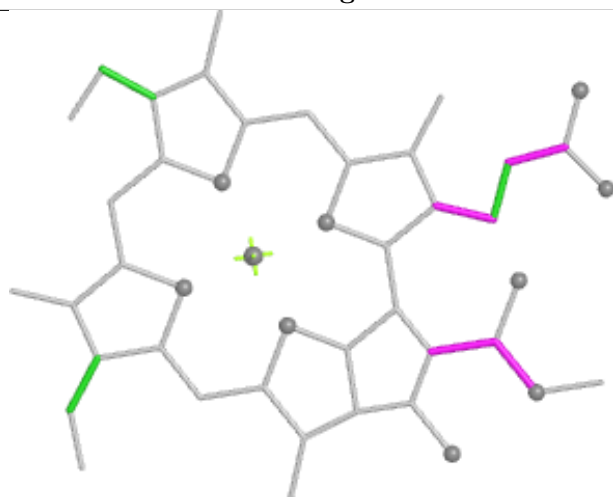
Ligand CLA c 610



Bond lengths



Bond angles

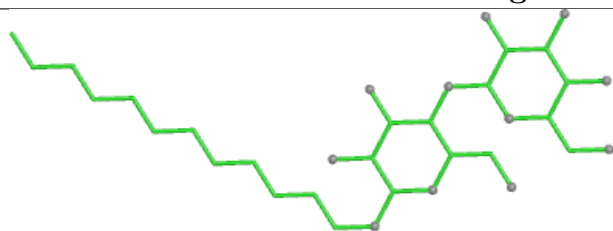


Torsions

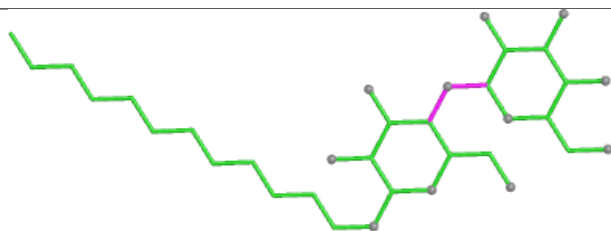


Rings

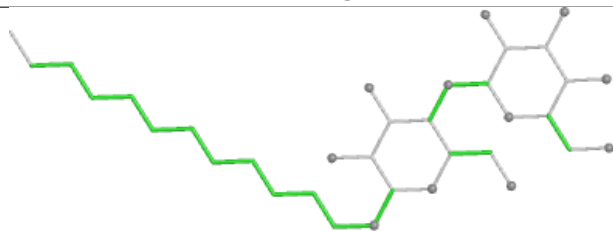
Ligand LMU A 853



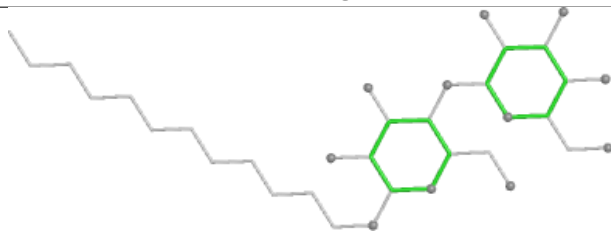
Bond lengths



Bond angles

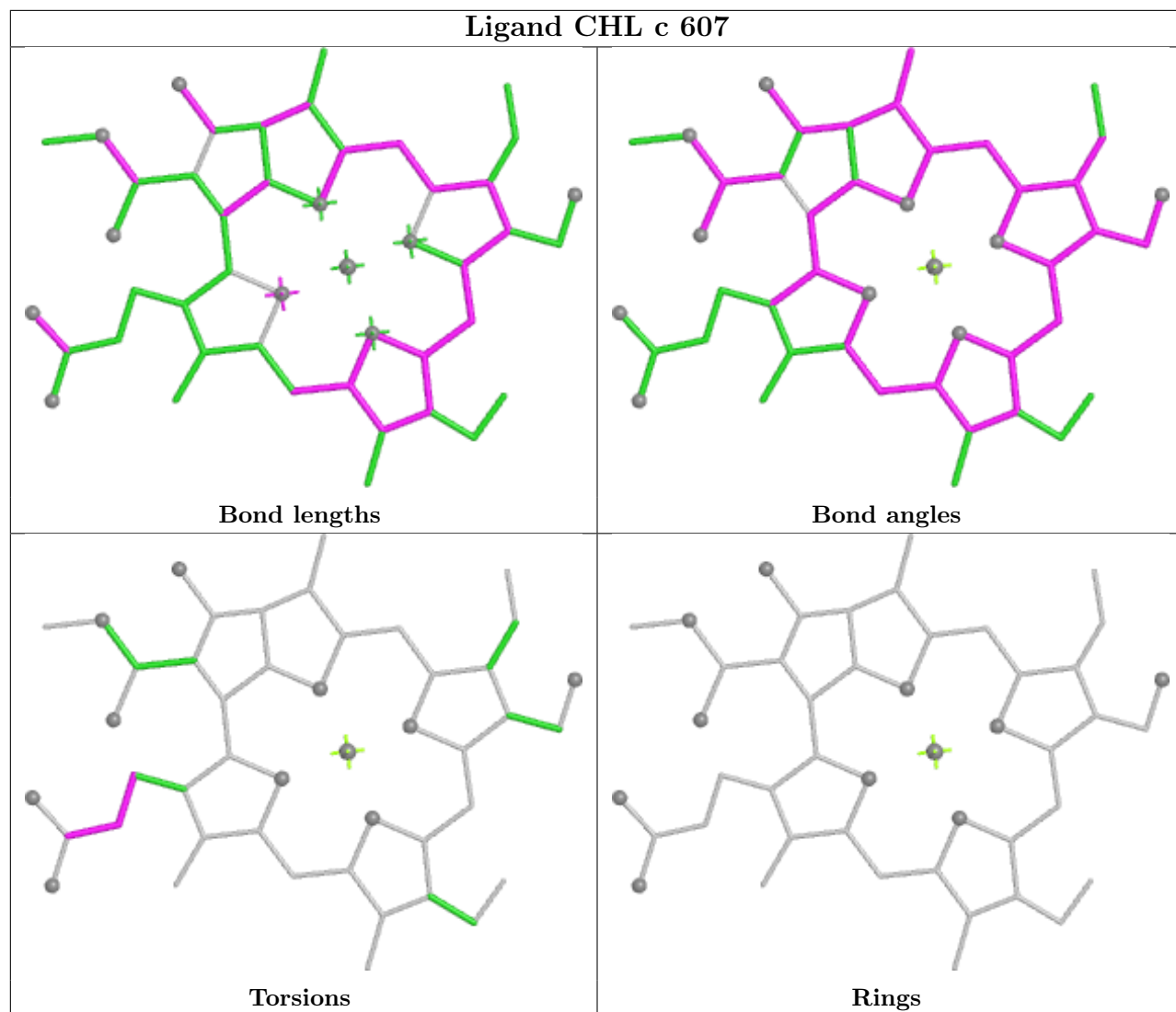


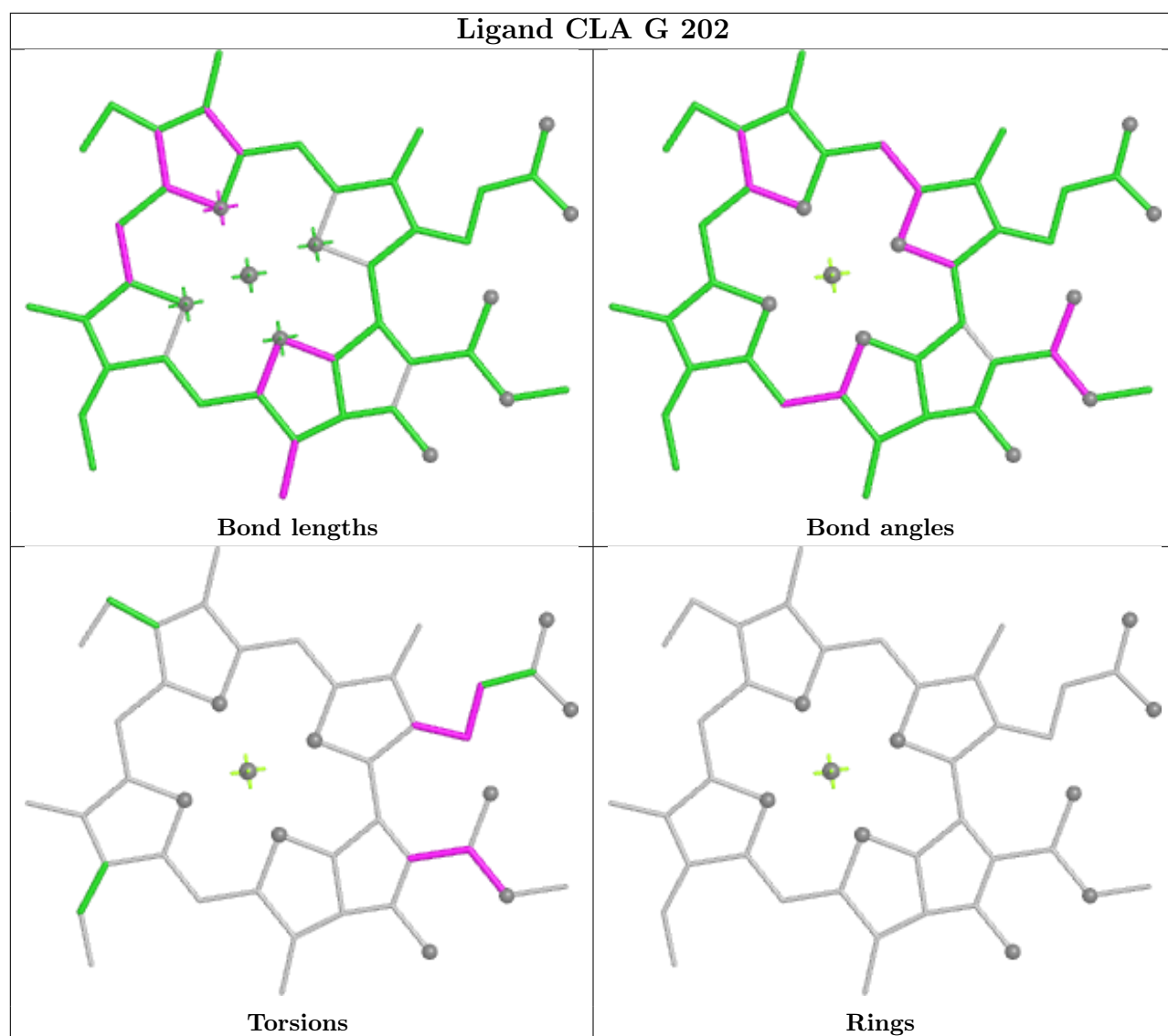
Torsions



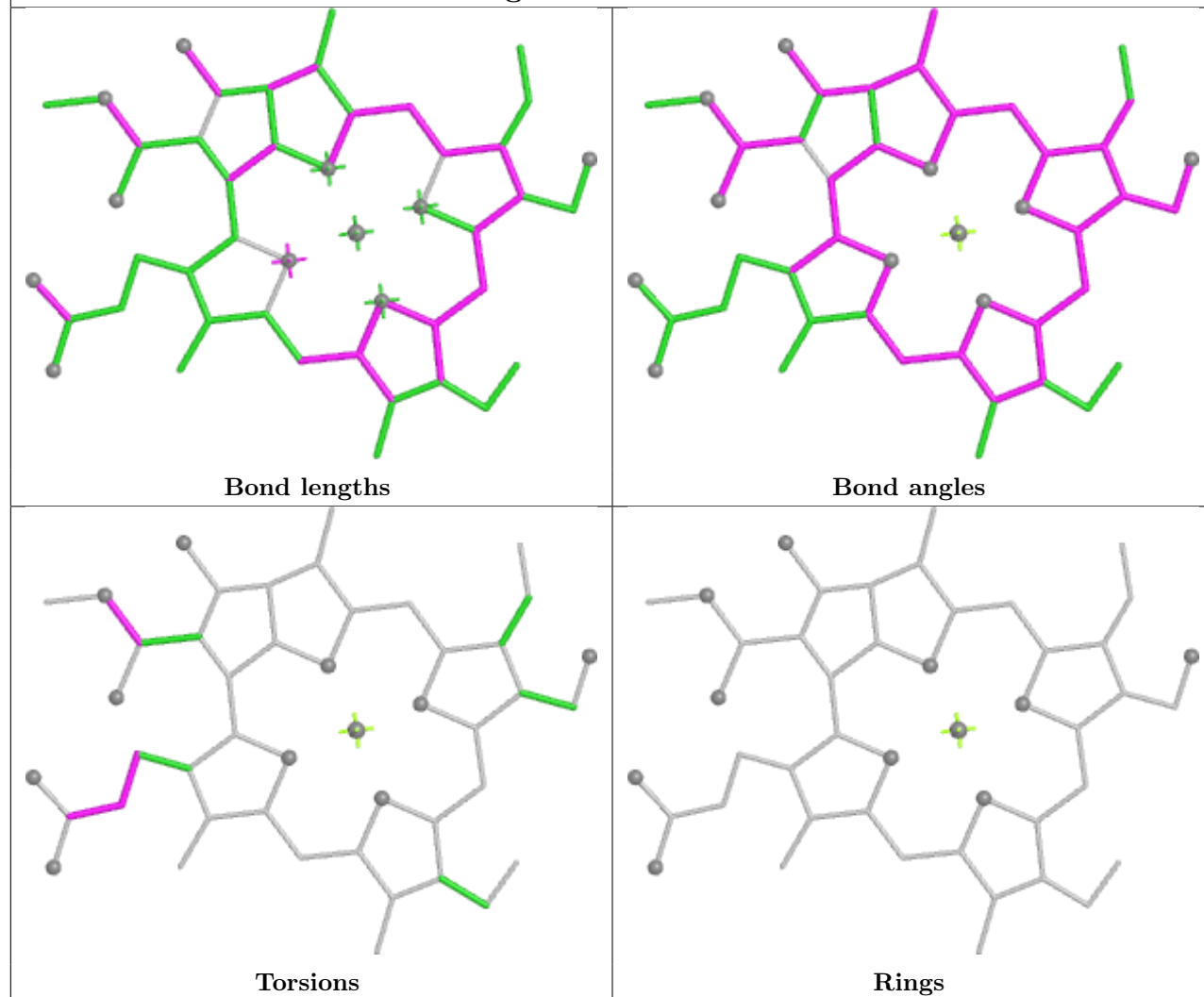
Rings

Ligand CHL c 607

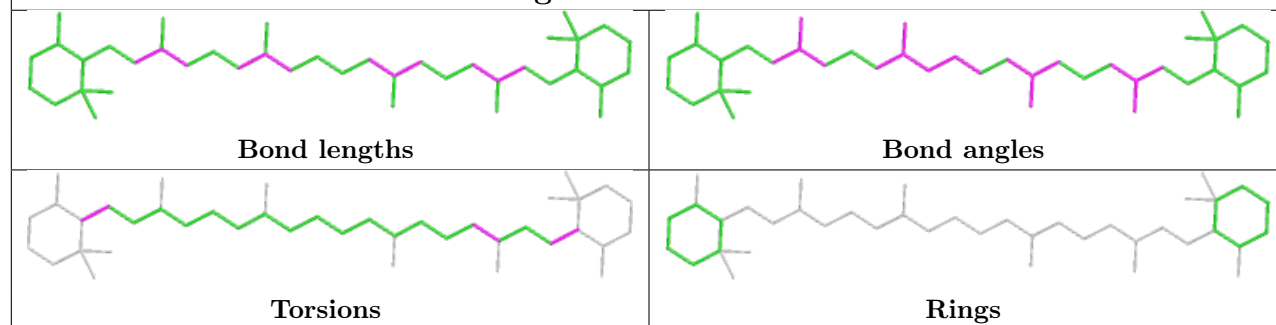




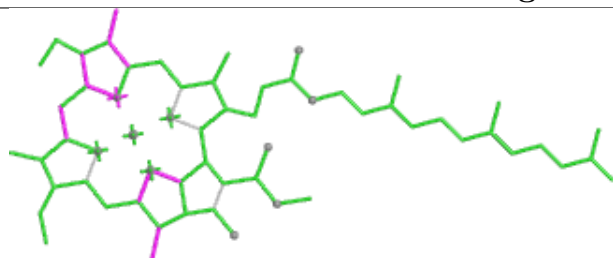
Ligand CHL 9 608



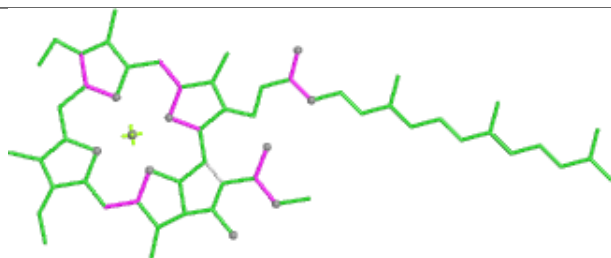
Ligand BCR 8 616



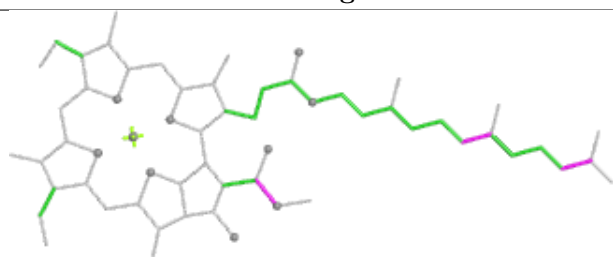
Ligand CLA 3 402



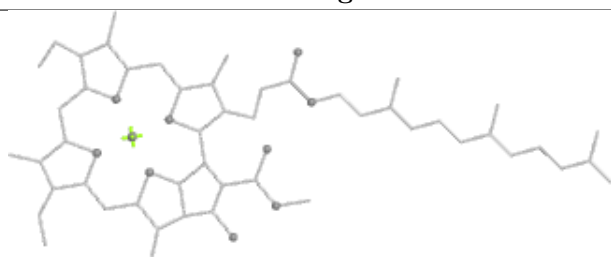
Bond lengths



Bond angles

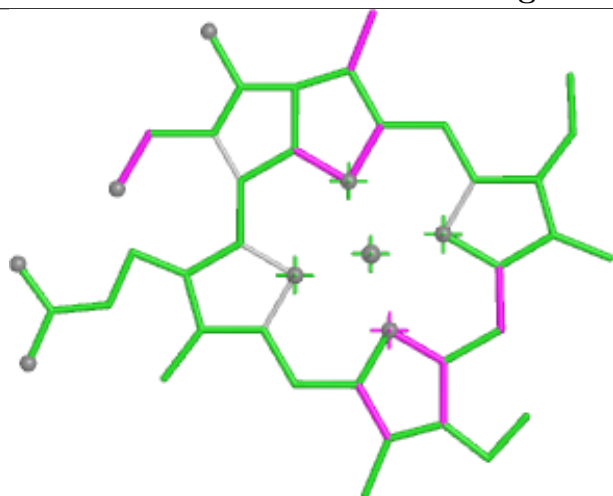


Torsions

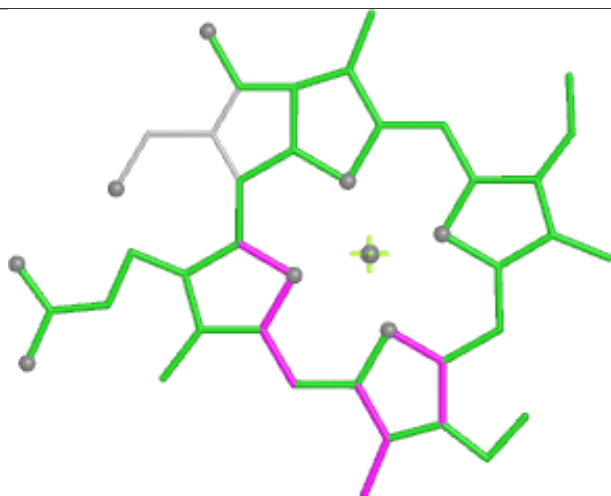


Rings

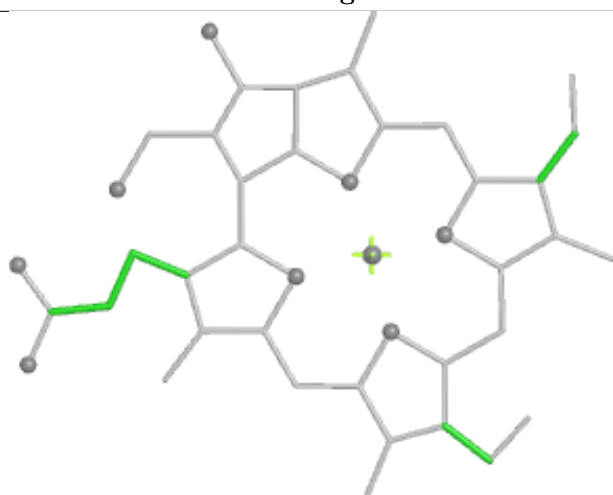
Ligand CLA 4 608



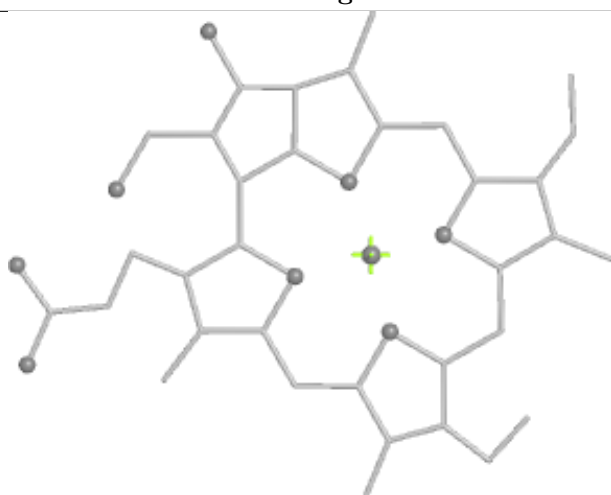
Bond lengths



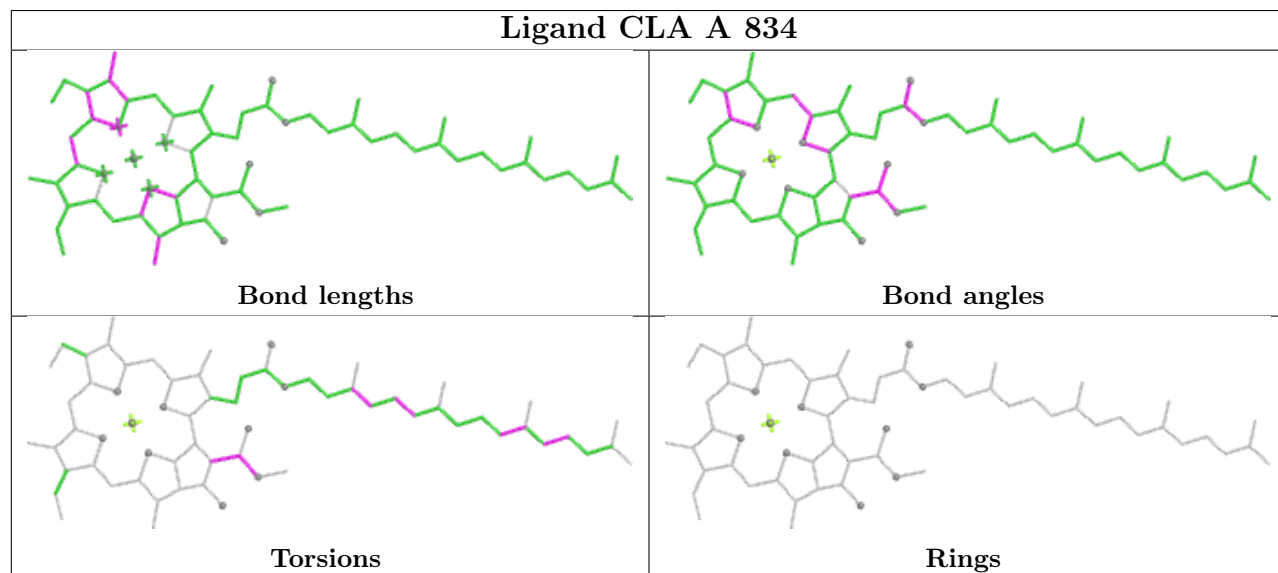
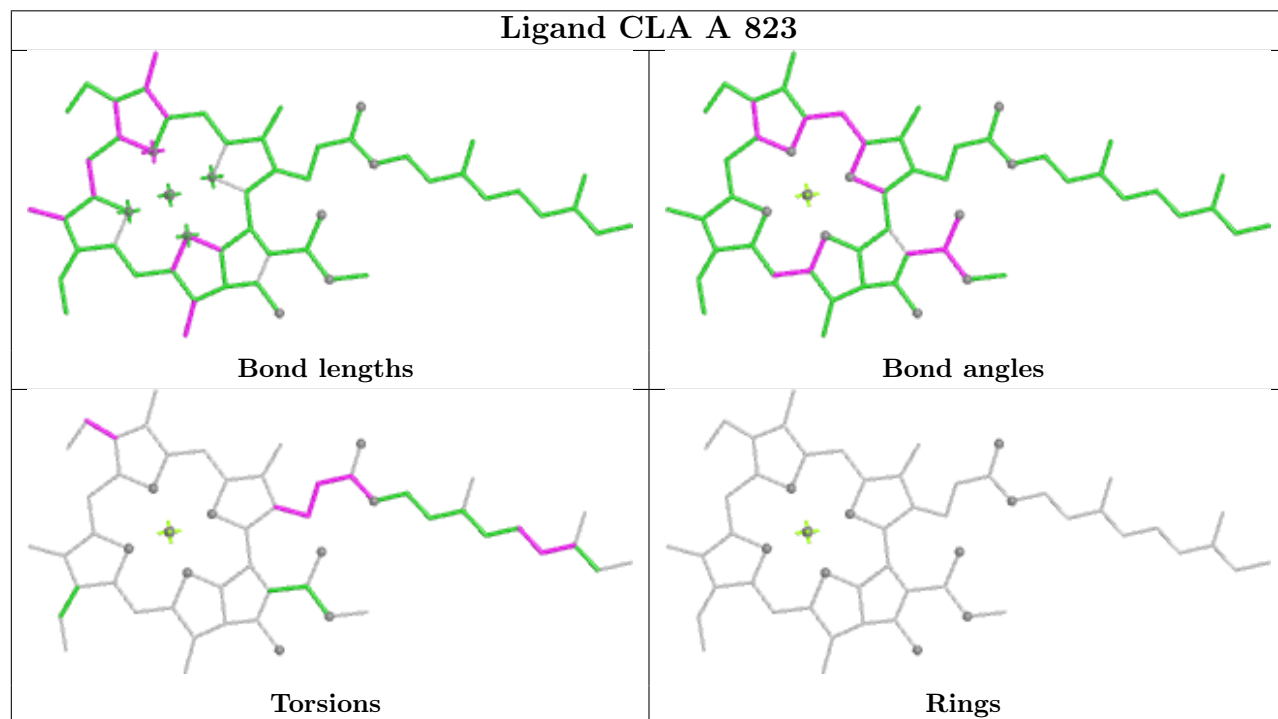
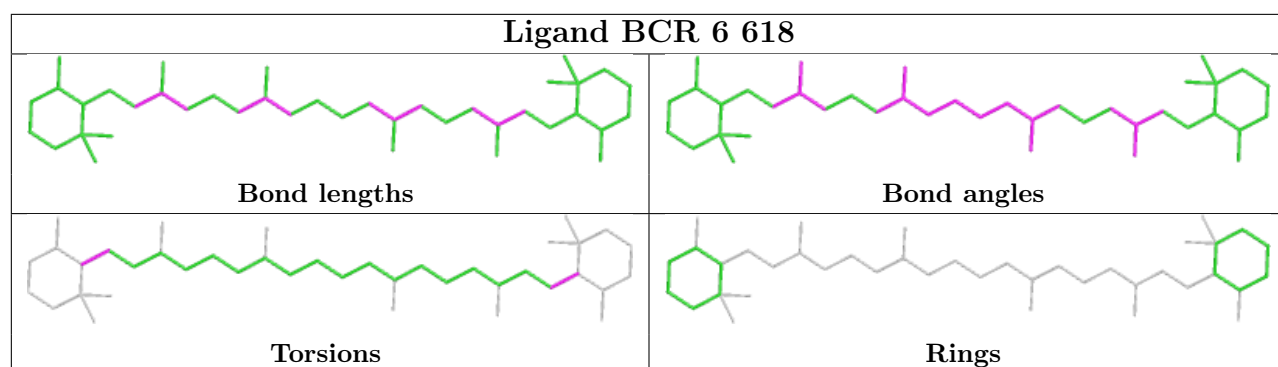
Bond angles



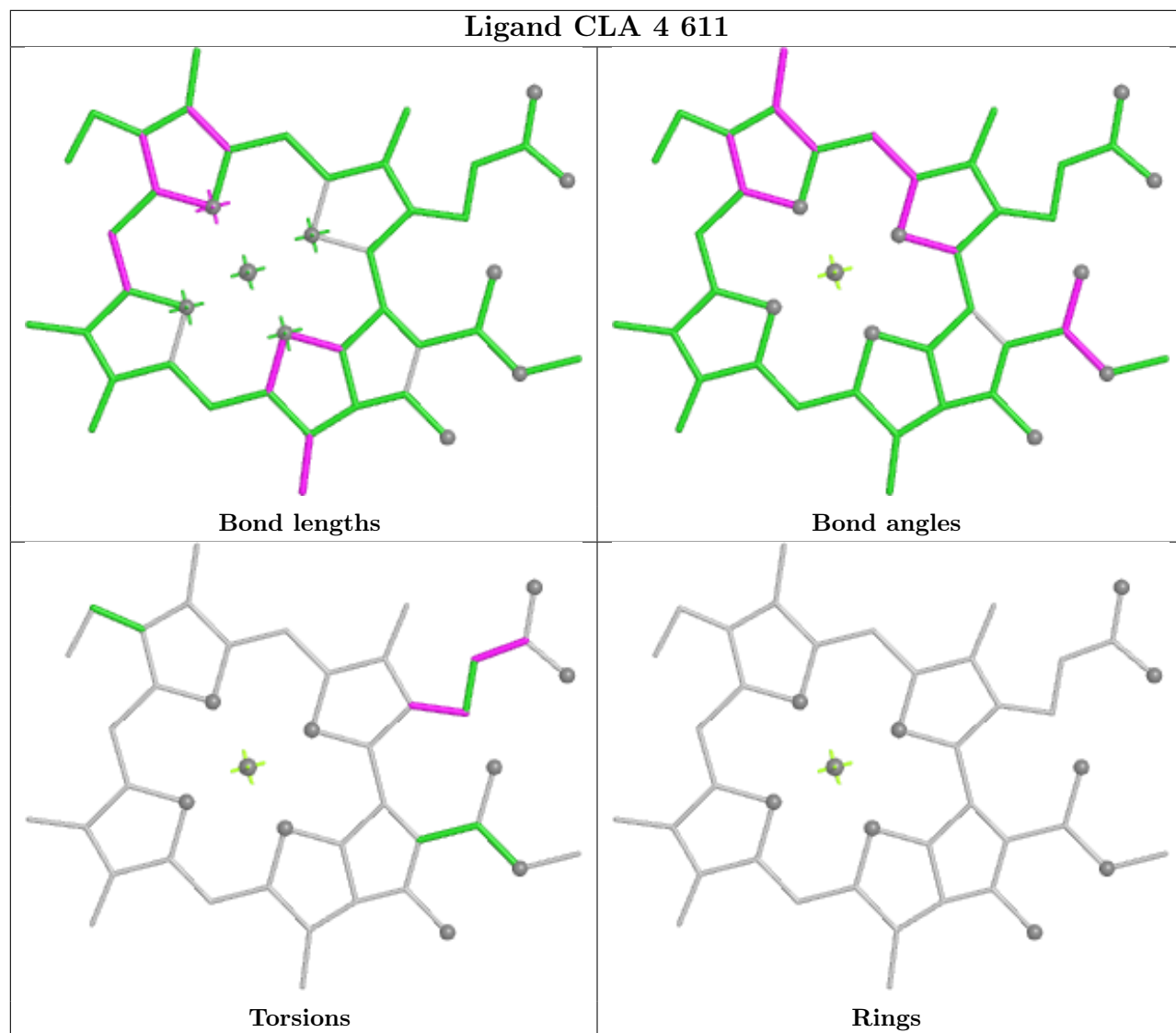
Torsions



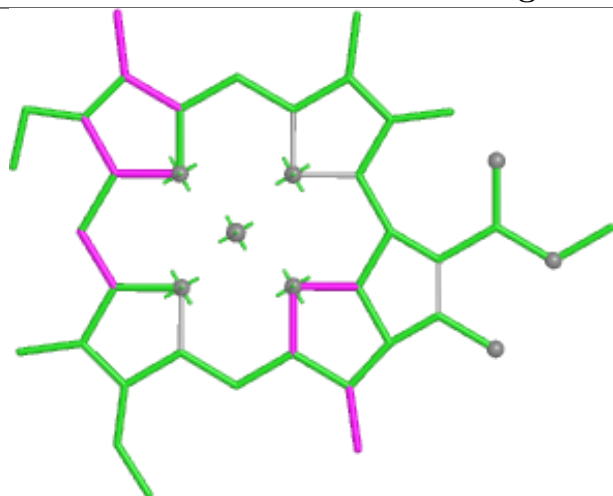
Rings



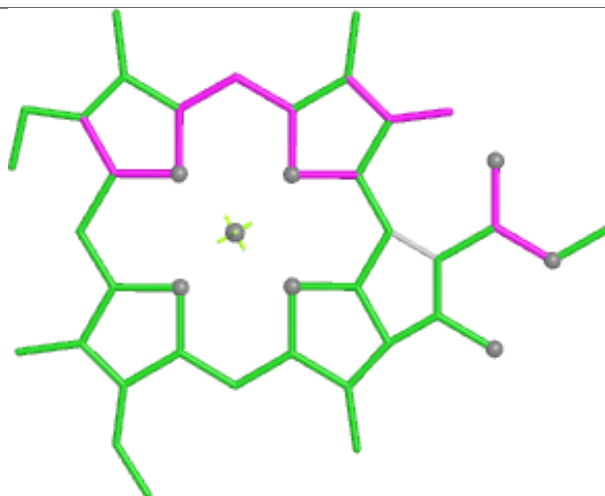
Ligand CLA 4 611



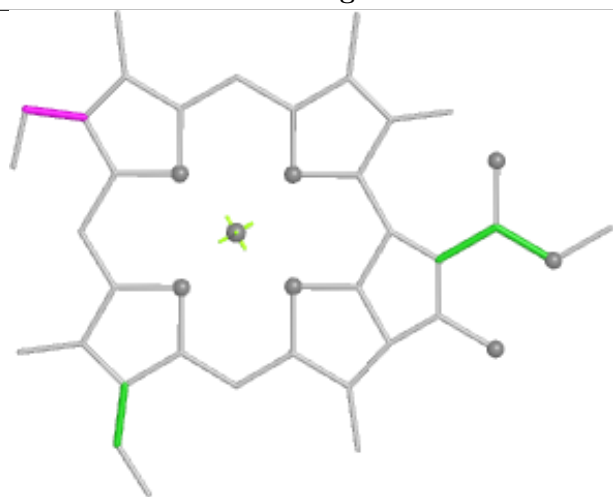
Ligand CLA a 603



Bond lengths



Bond angles

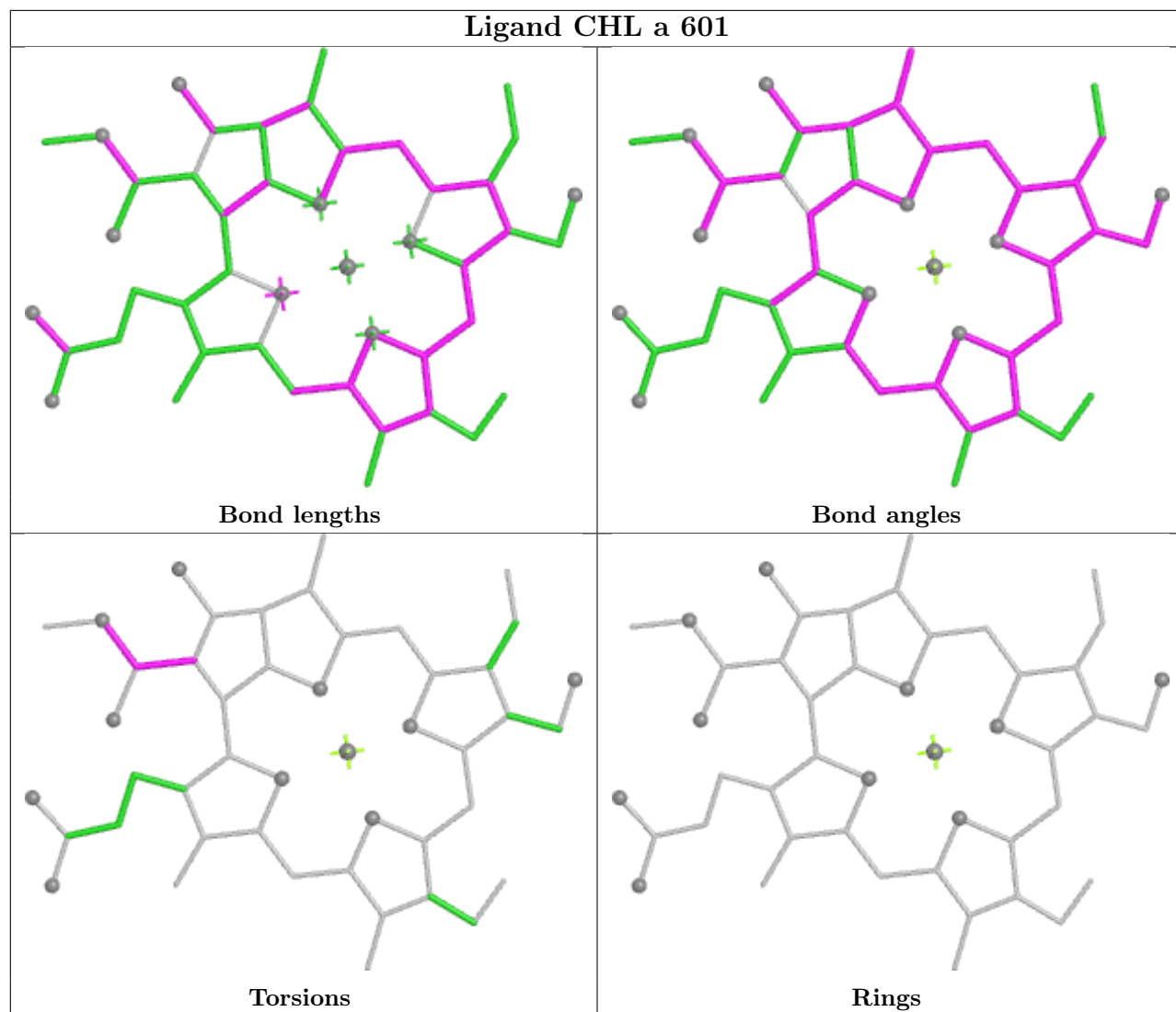


Torsions

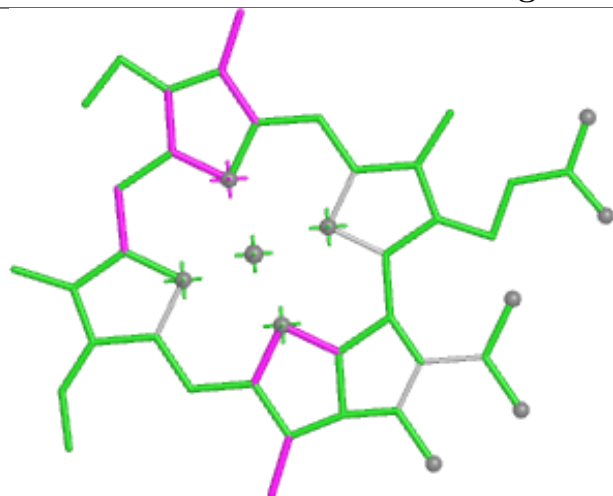


Rings

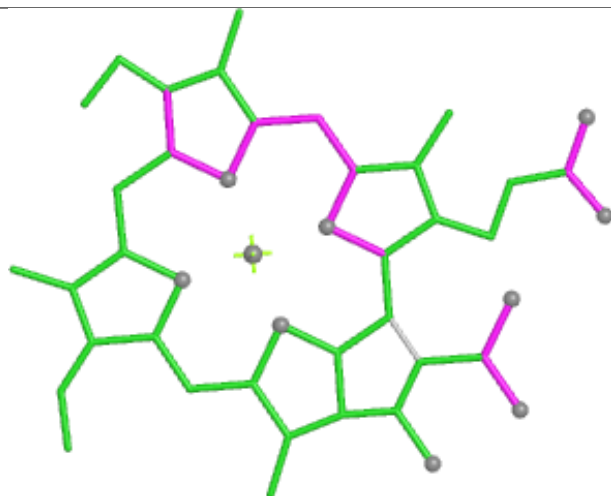
Ligand CHL a 601



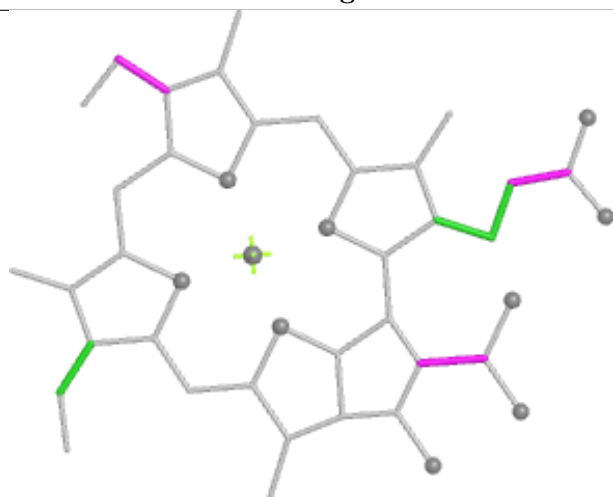
Ligand CLA 1 308



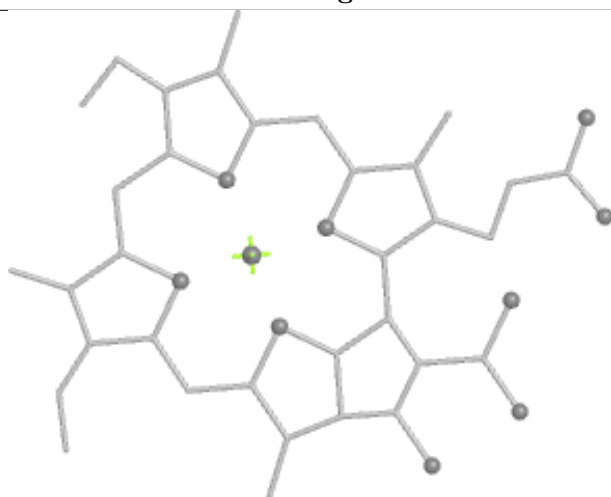
Bond lengths



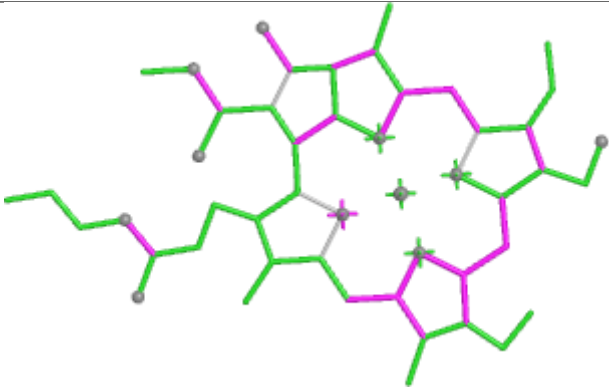
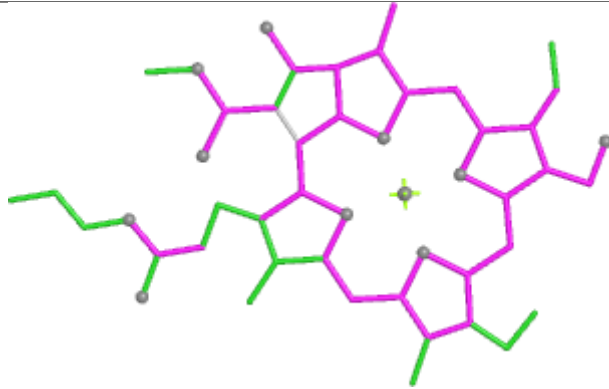
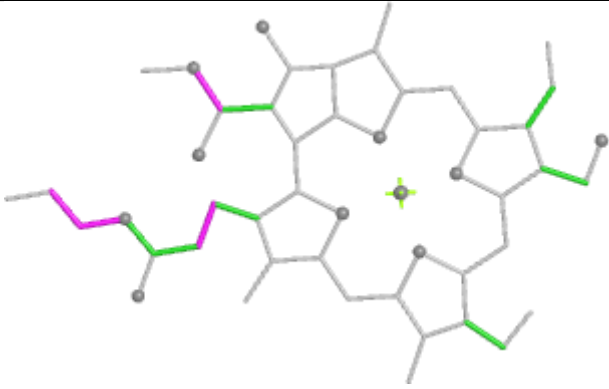
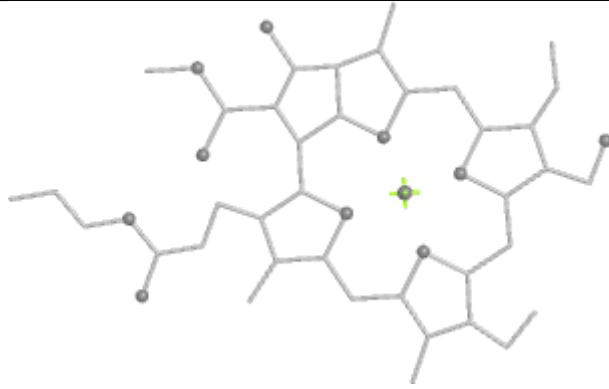
Bond angles

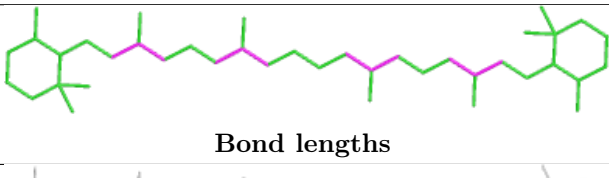
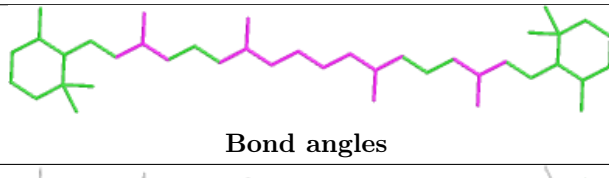
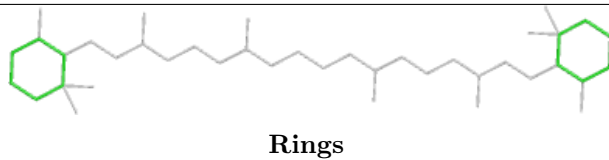


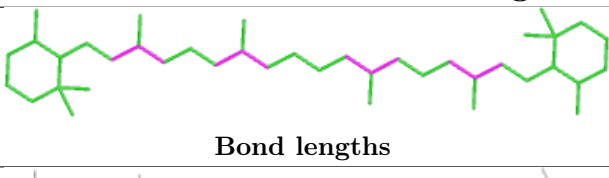
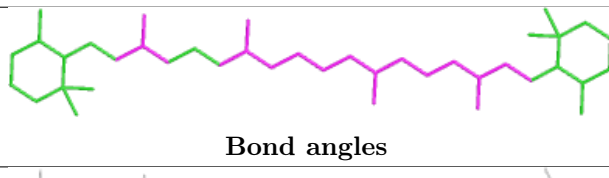
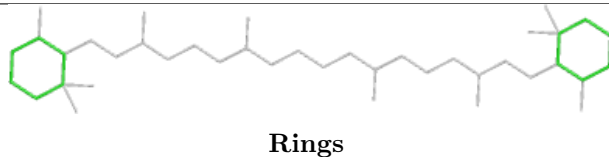
Torsions

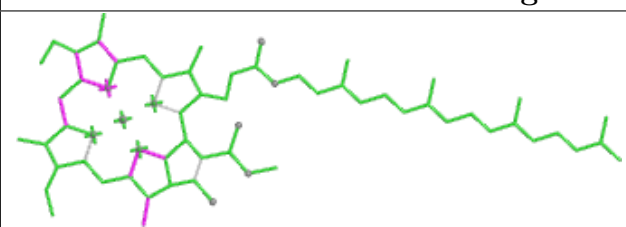
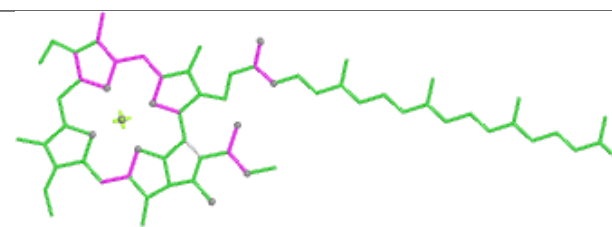
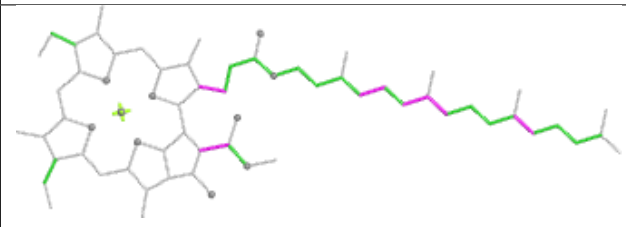
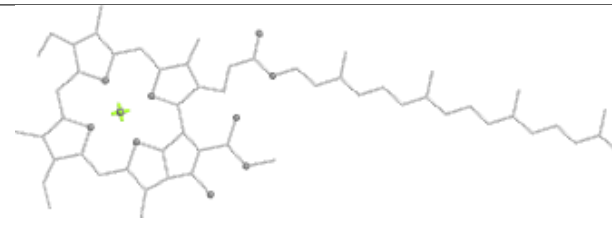


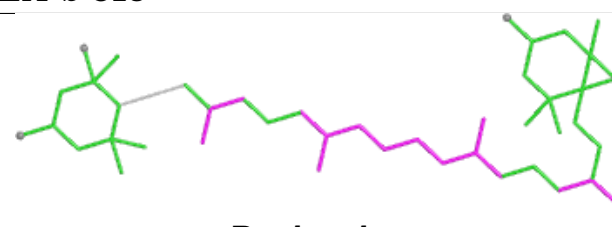
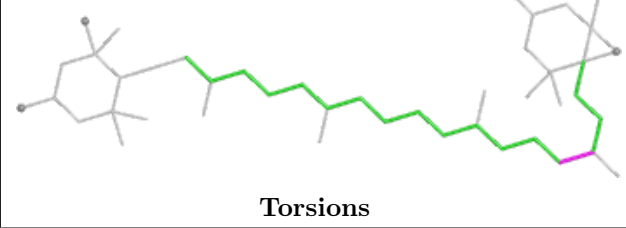
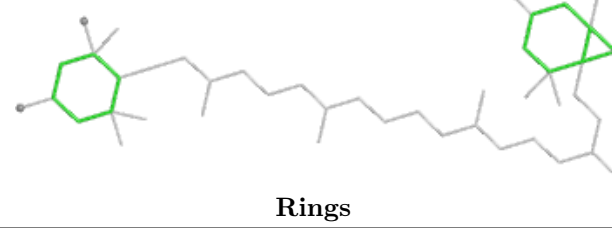
Rings

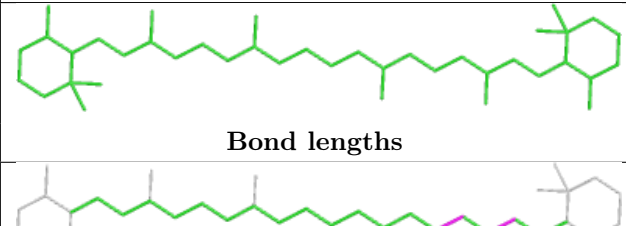
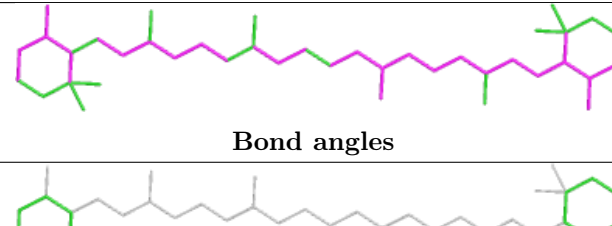
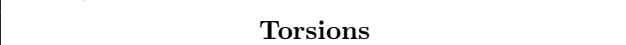
Ligand CHL b 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 2 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

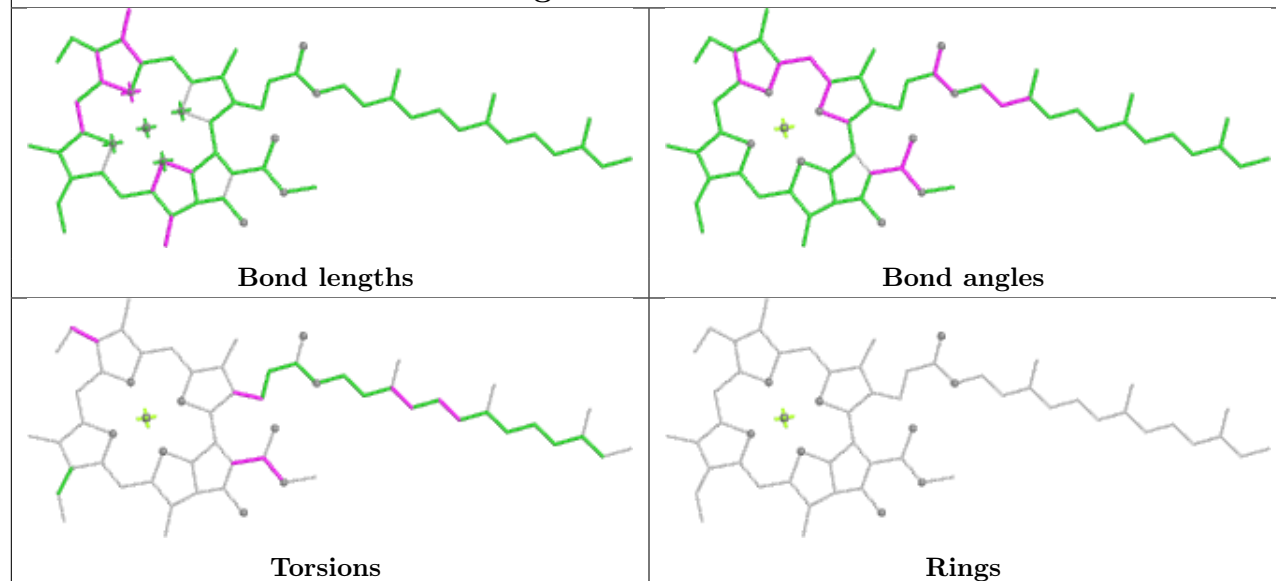
Ligand BCR 7 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

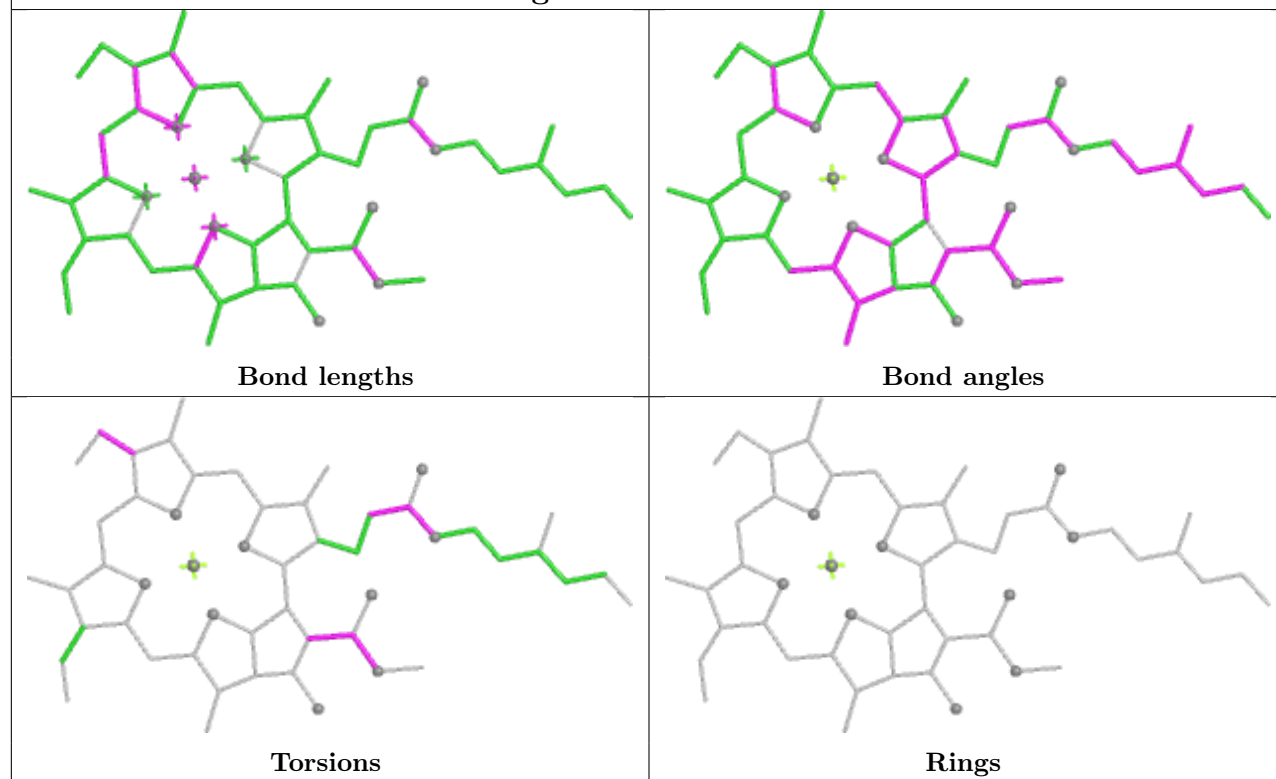
Ligand NEX b 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

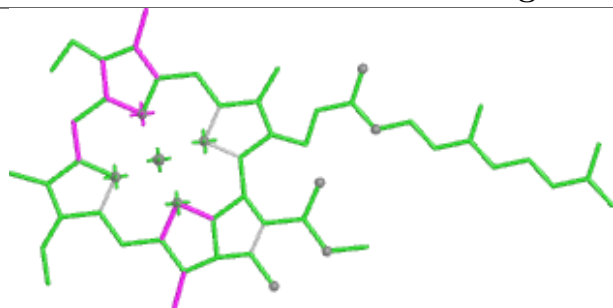
Ligand BCR K 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA F 302

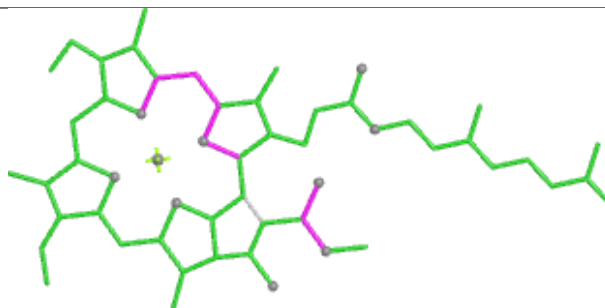


Ligand CLA A 801

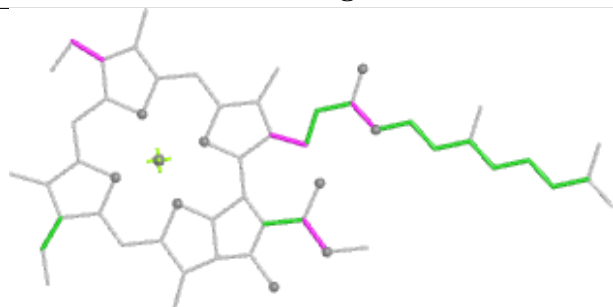


Ligand CLA 3 403

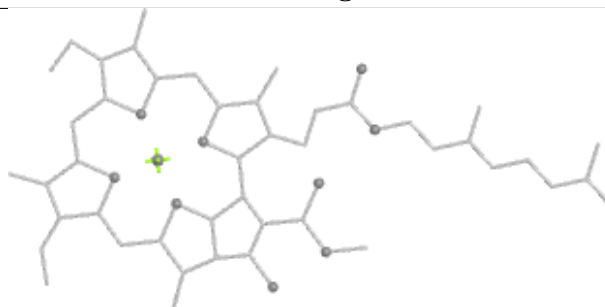
Bond lengths



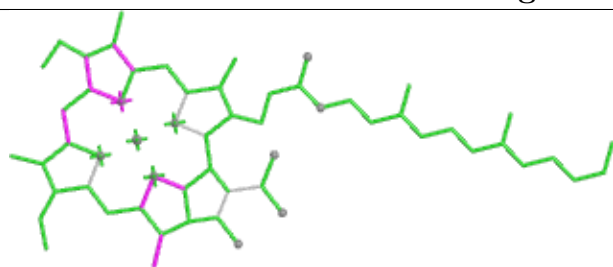
Bond angles



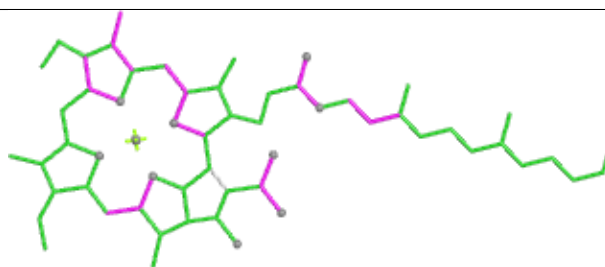
Torsions



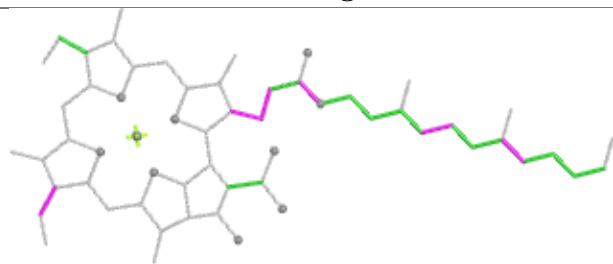
Rings

Ligand CLA 4 602

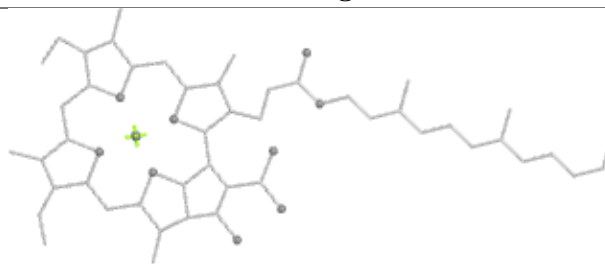
Bond lengths



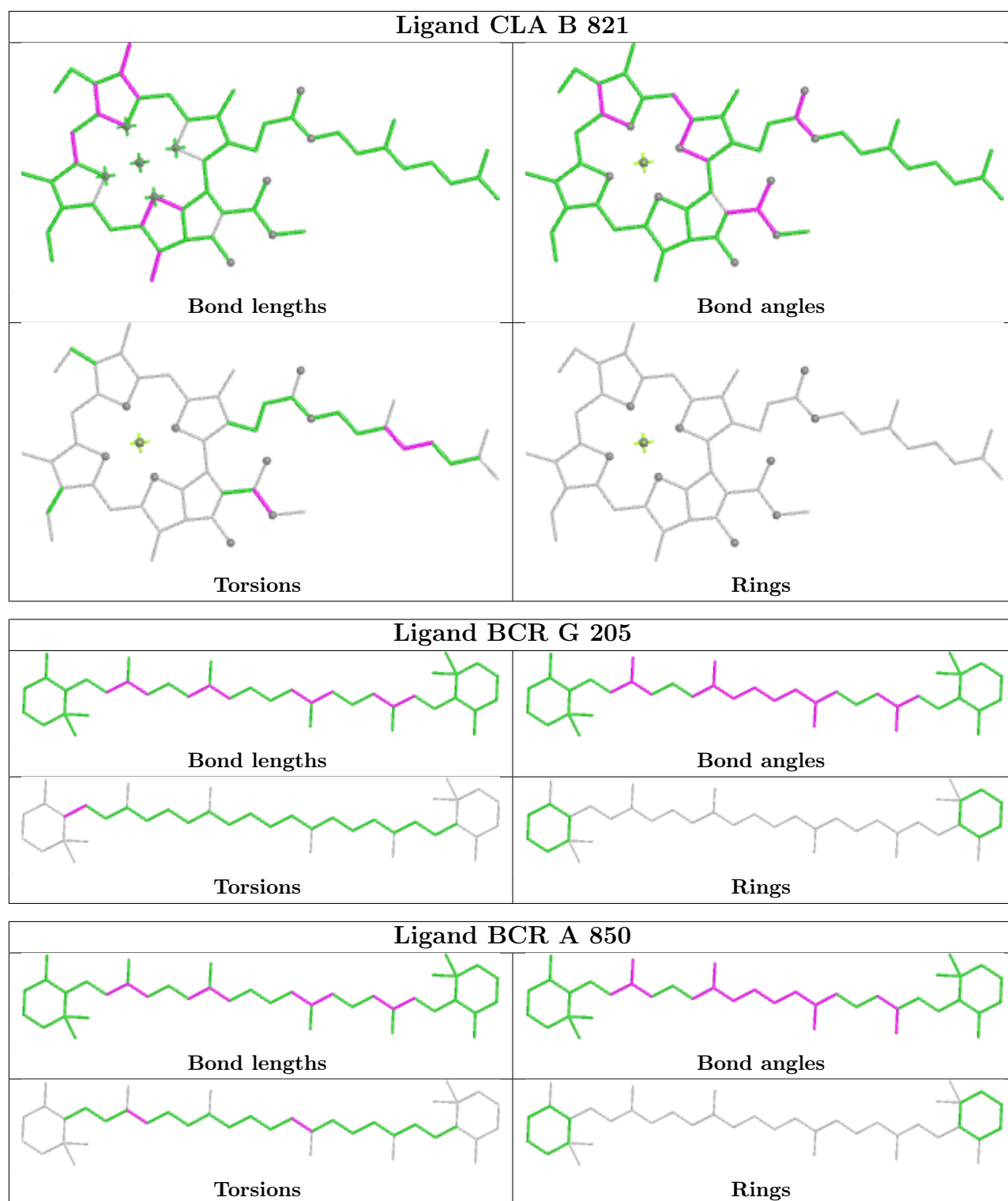
Bond angles

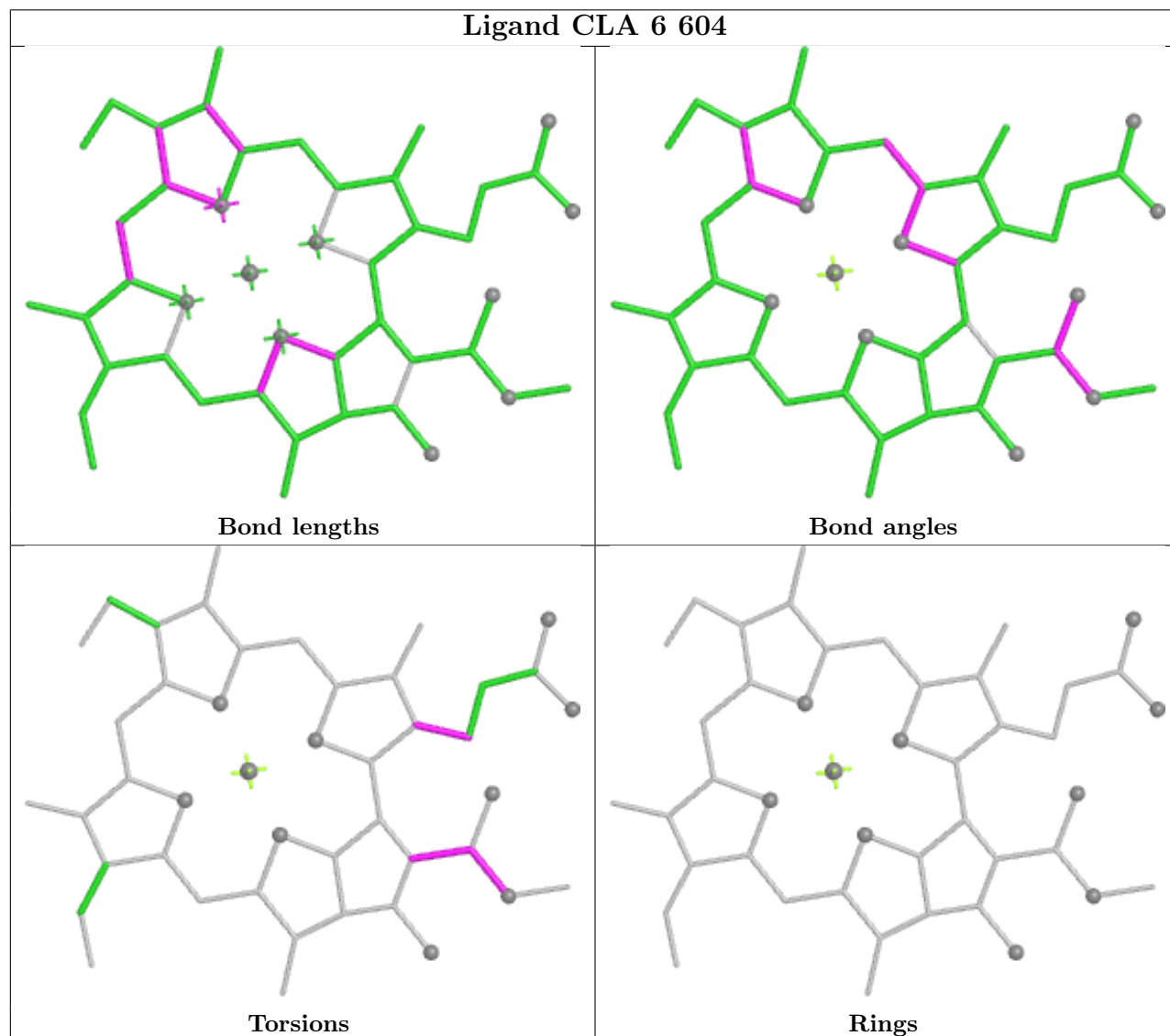
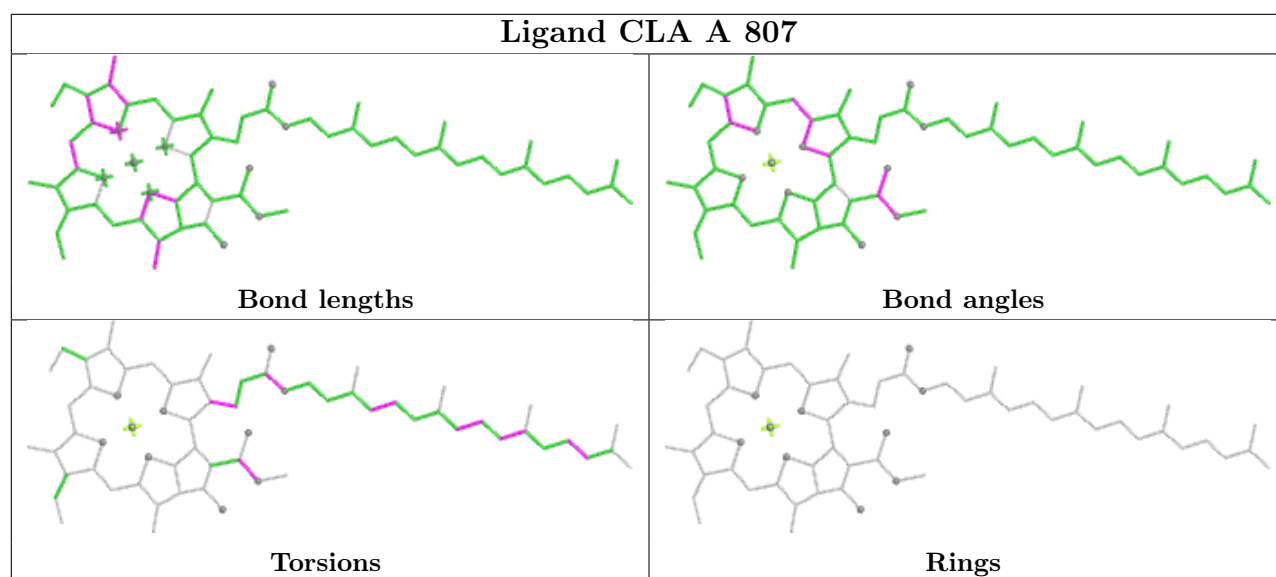


Torsions

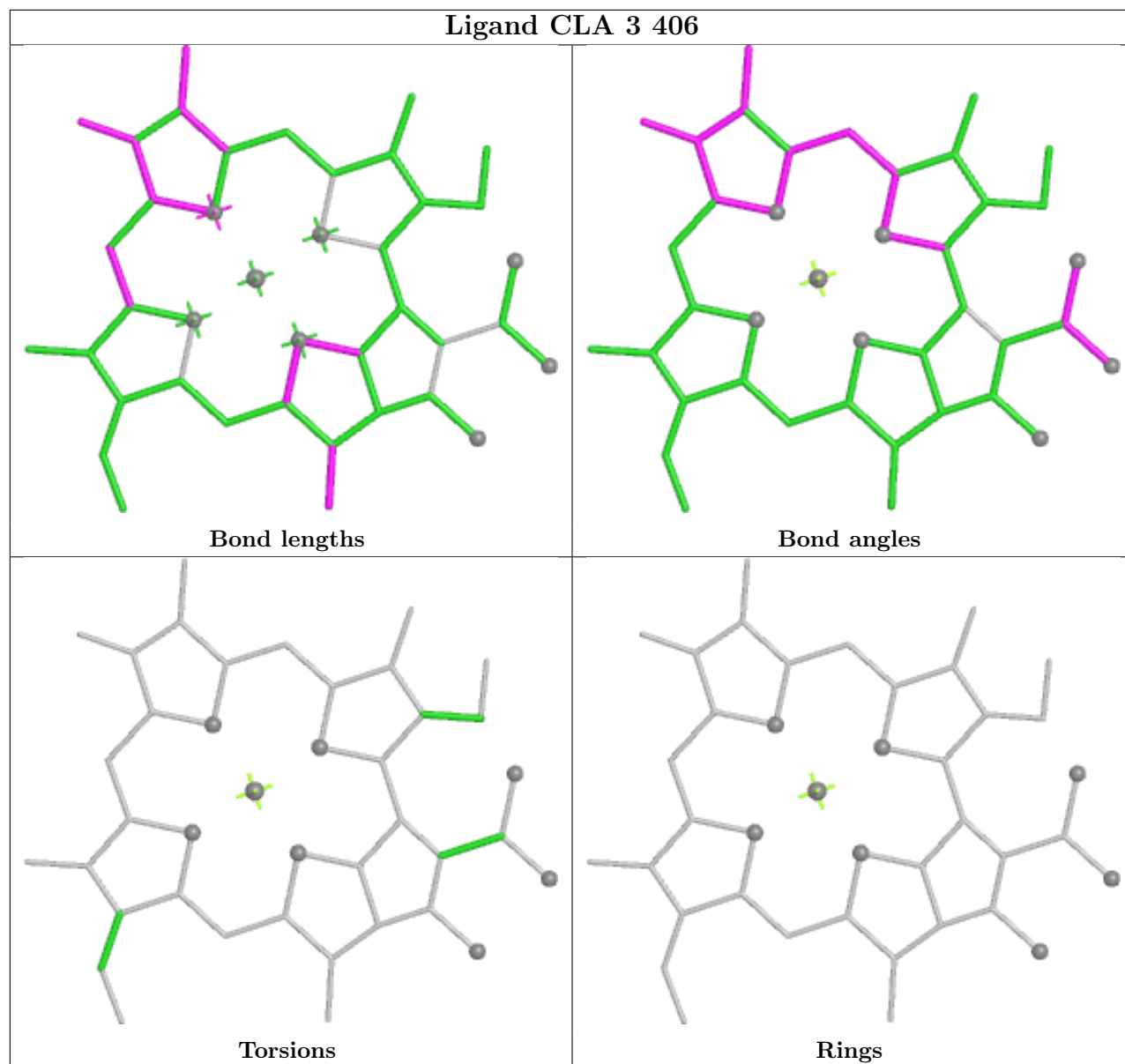


Rings

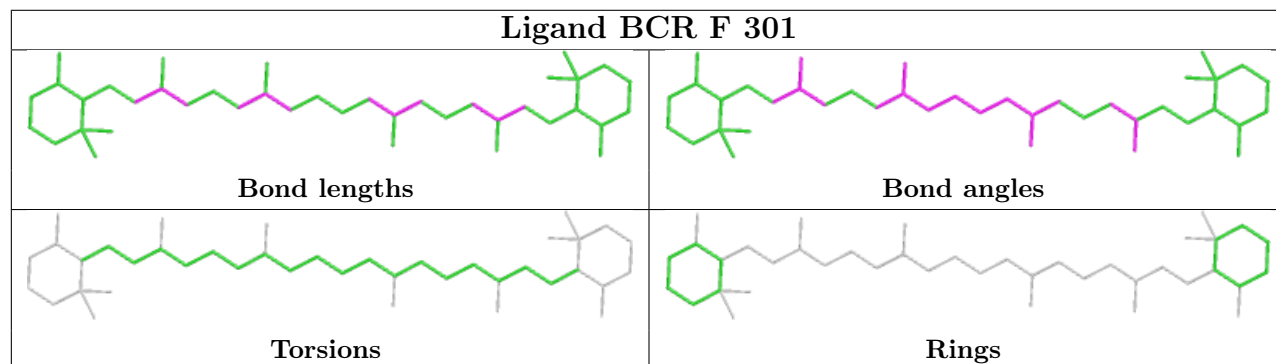


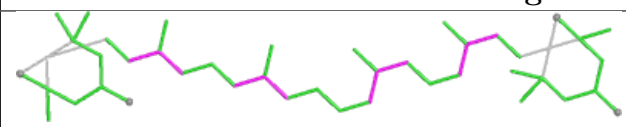
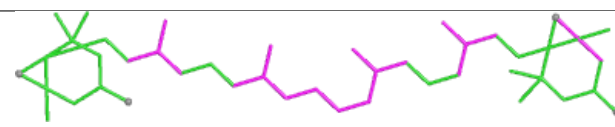
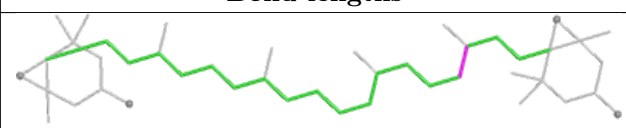
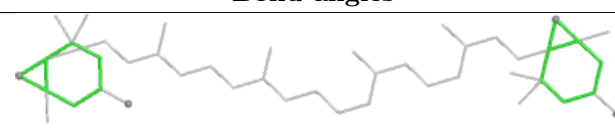


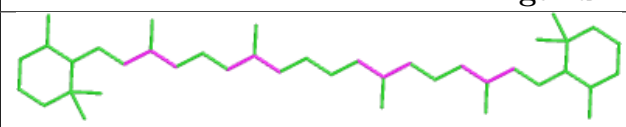
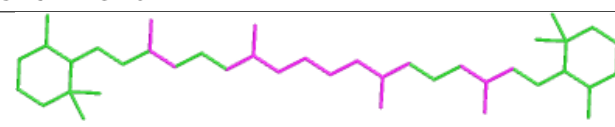
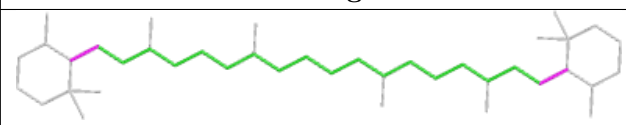
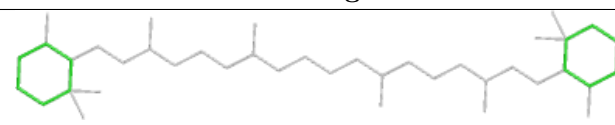
Ligand CLA 3 406

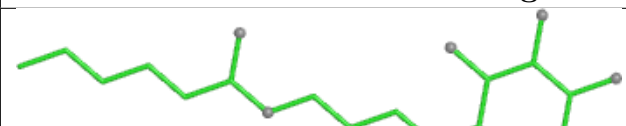
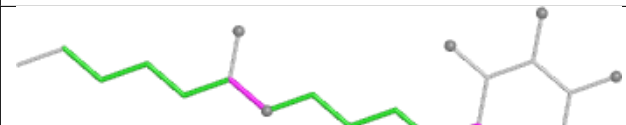
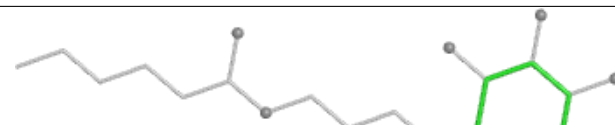


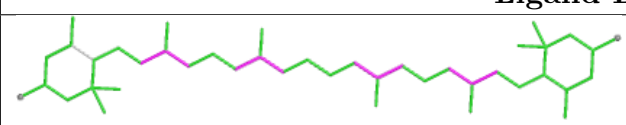
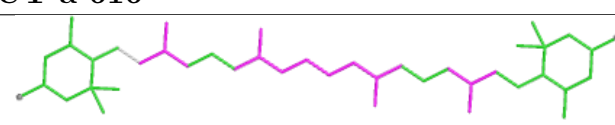
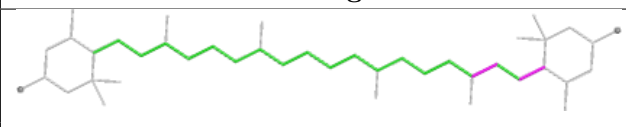
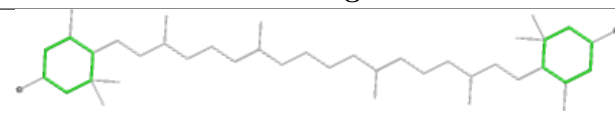
Ligand BCR F 301

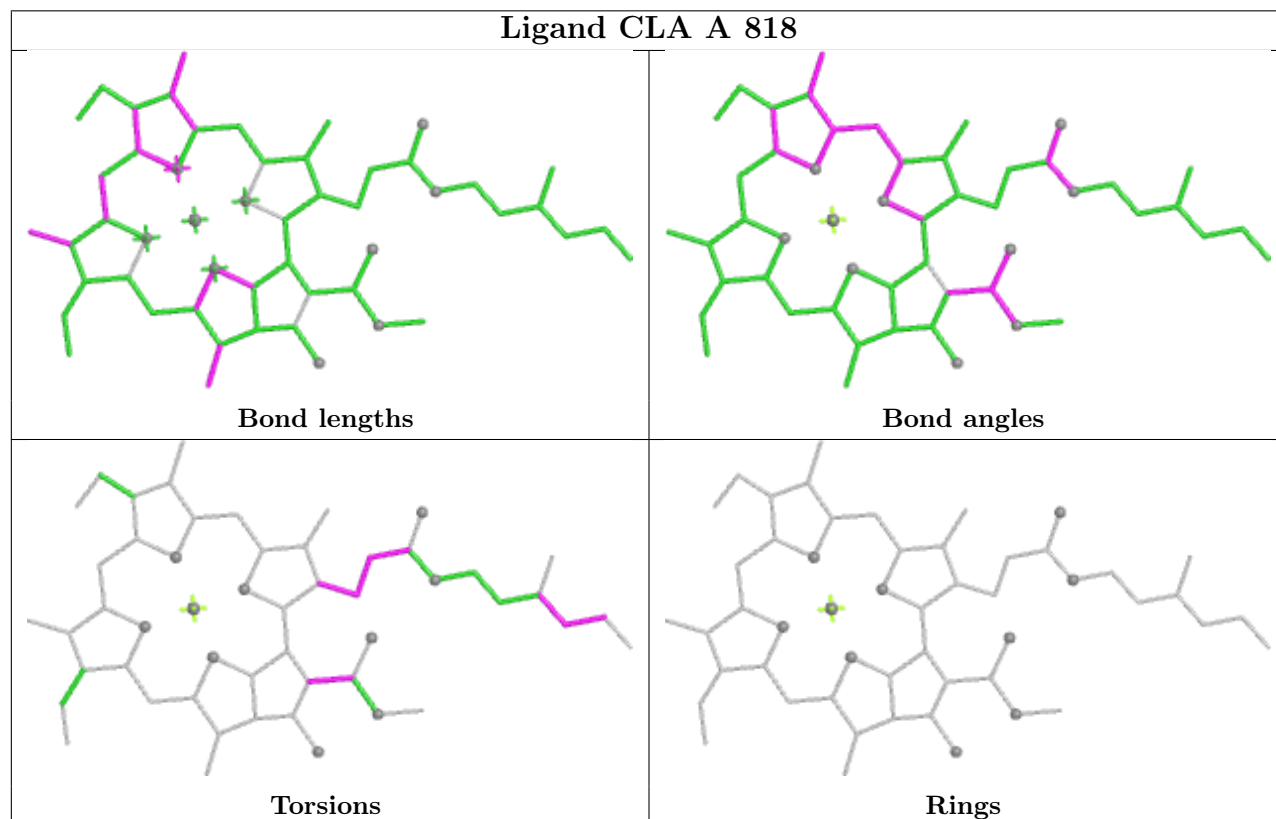
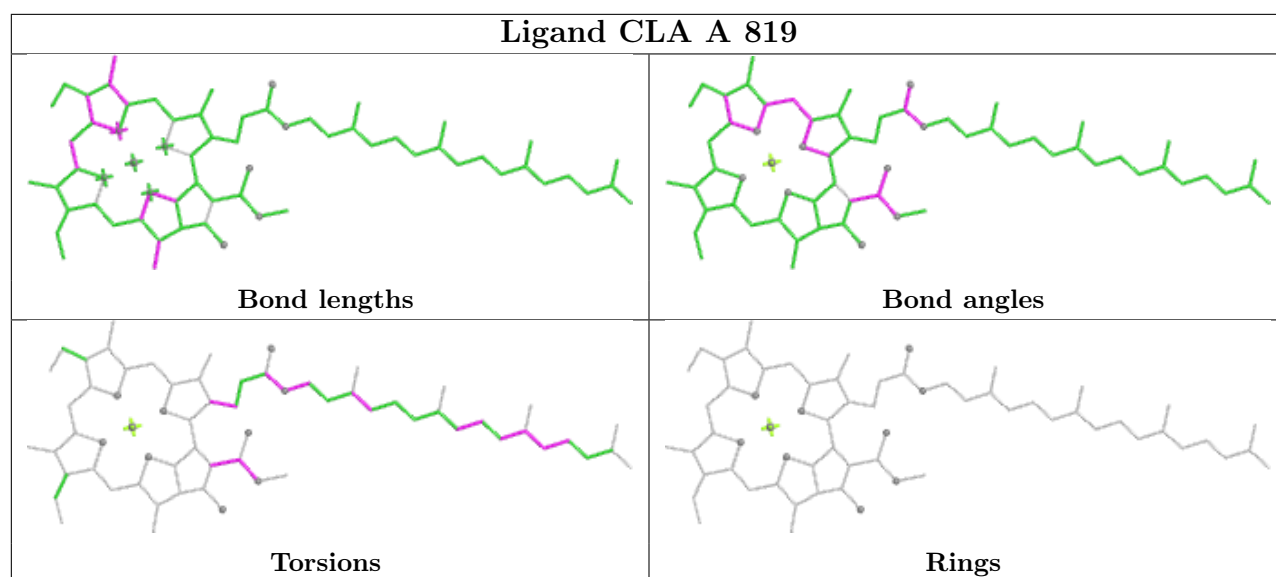


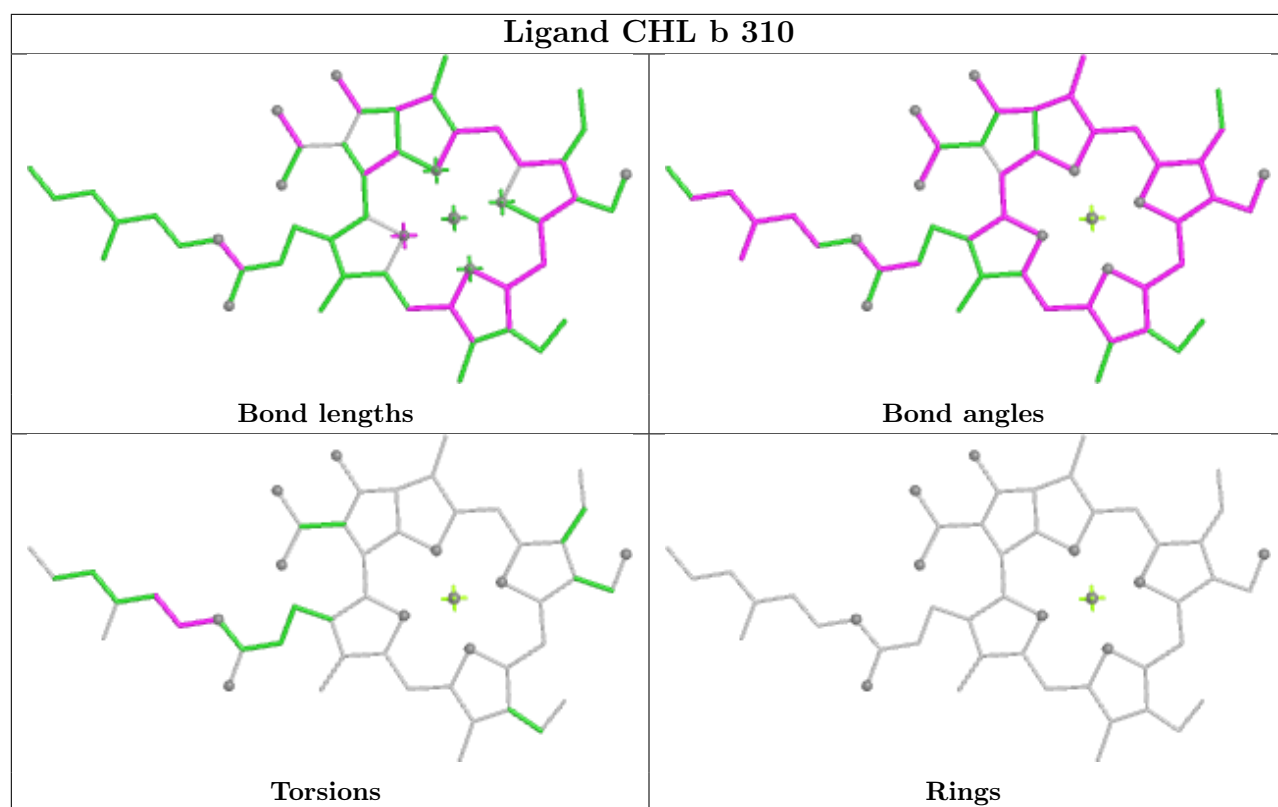
Ligand XAT a 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

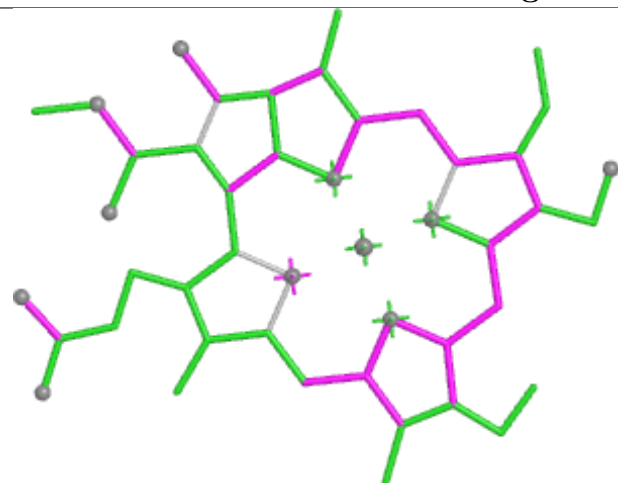
Ligand LMG J 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT a 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

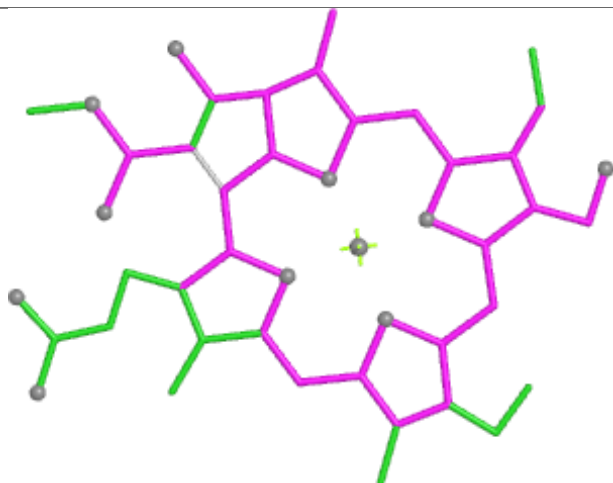




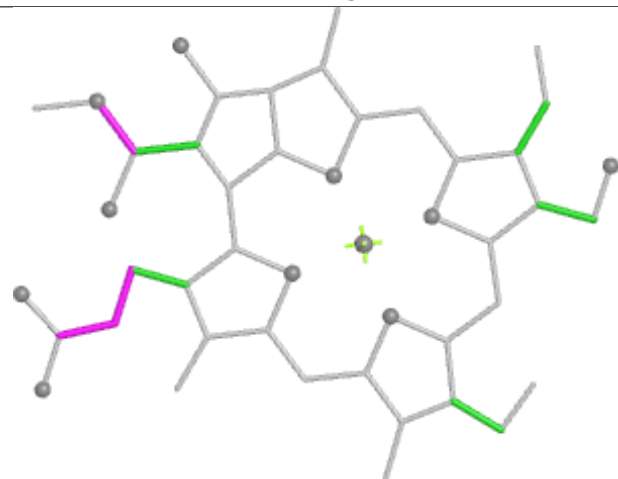
Ligand CHL 6 606



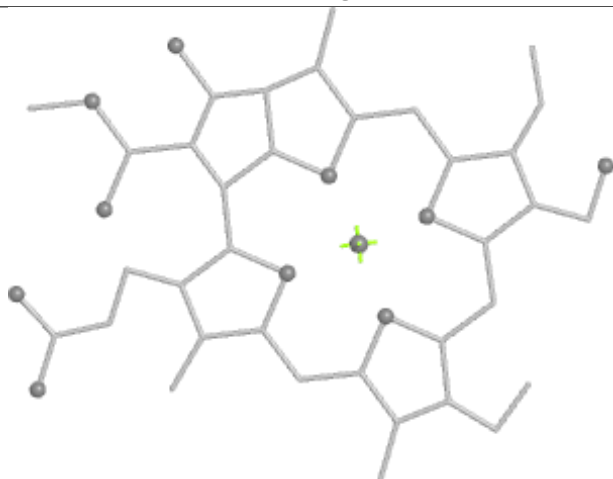
Bond lengths



Bond angles

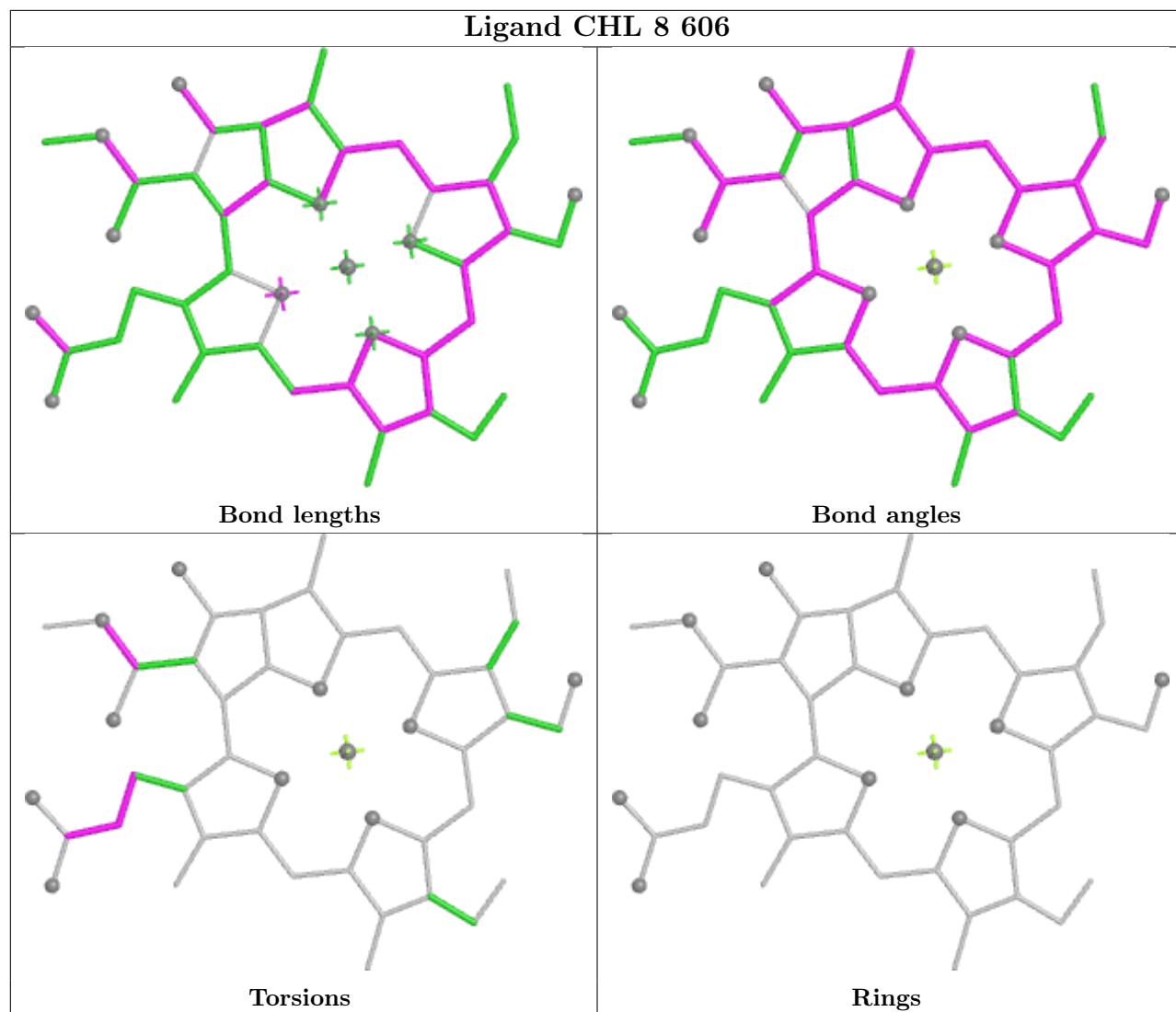


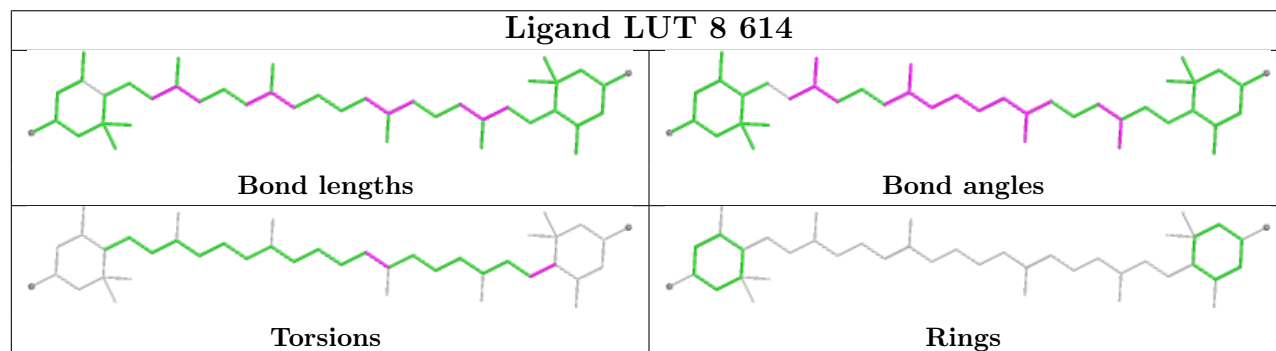
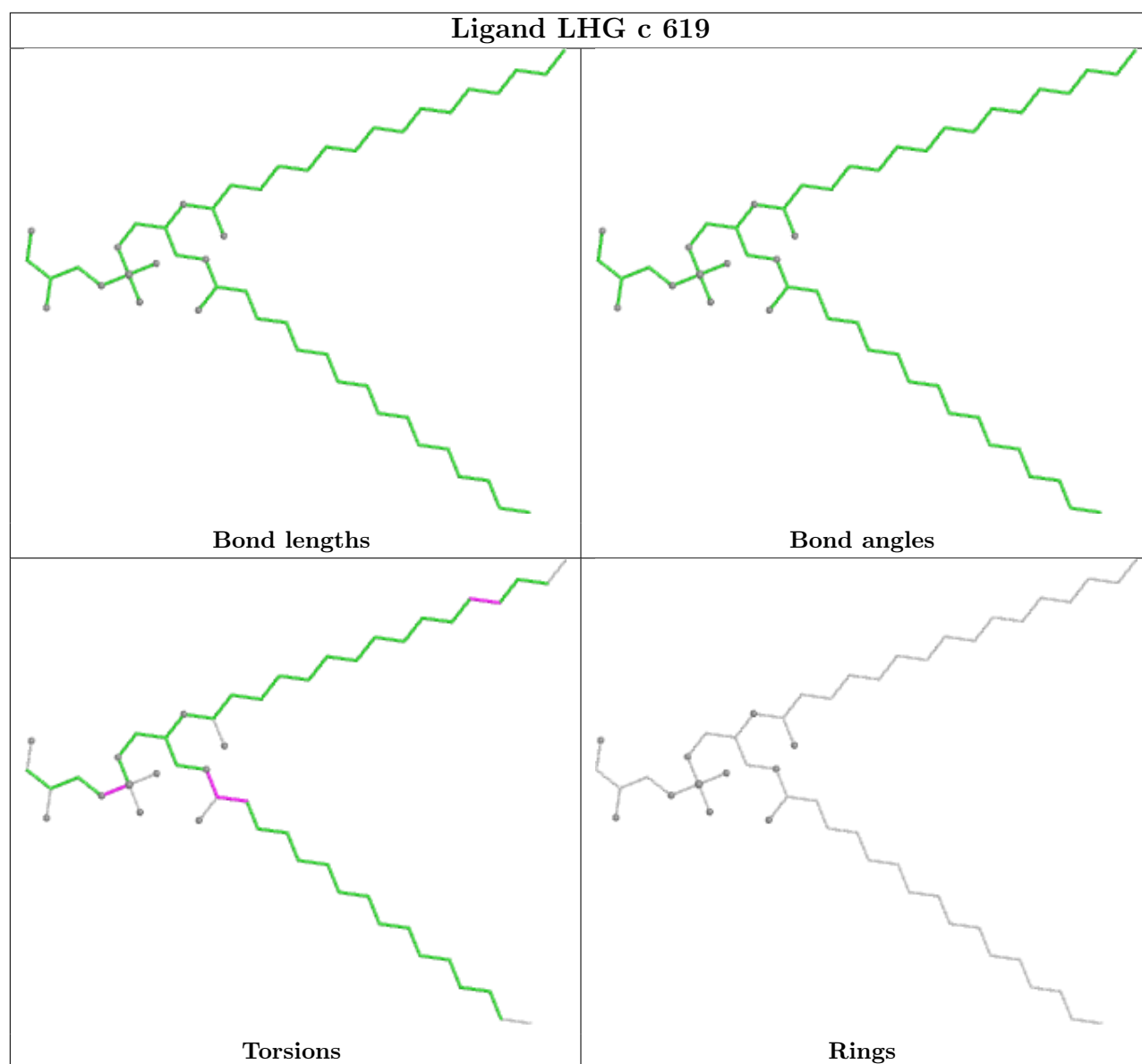
Torsions

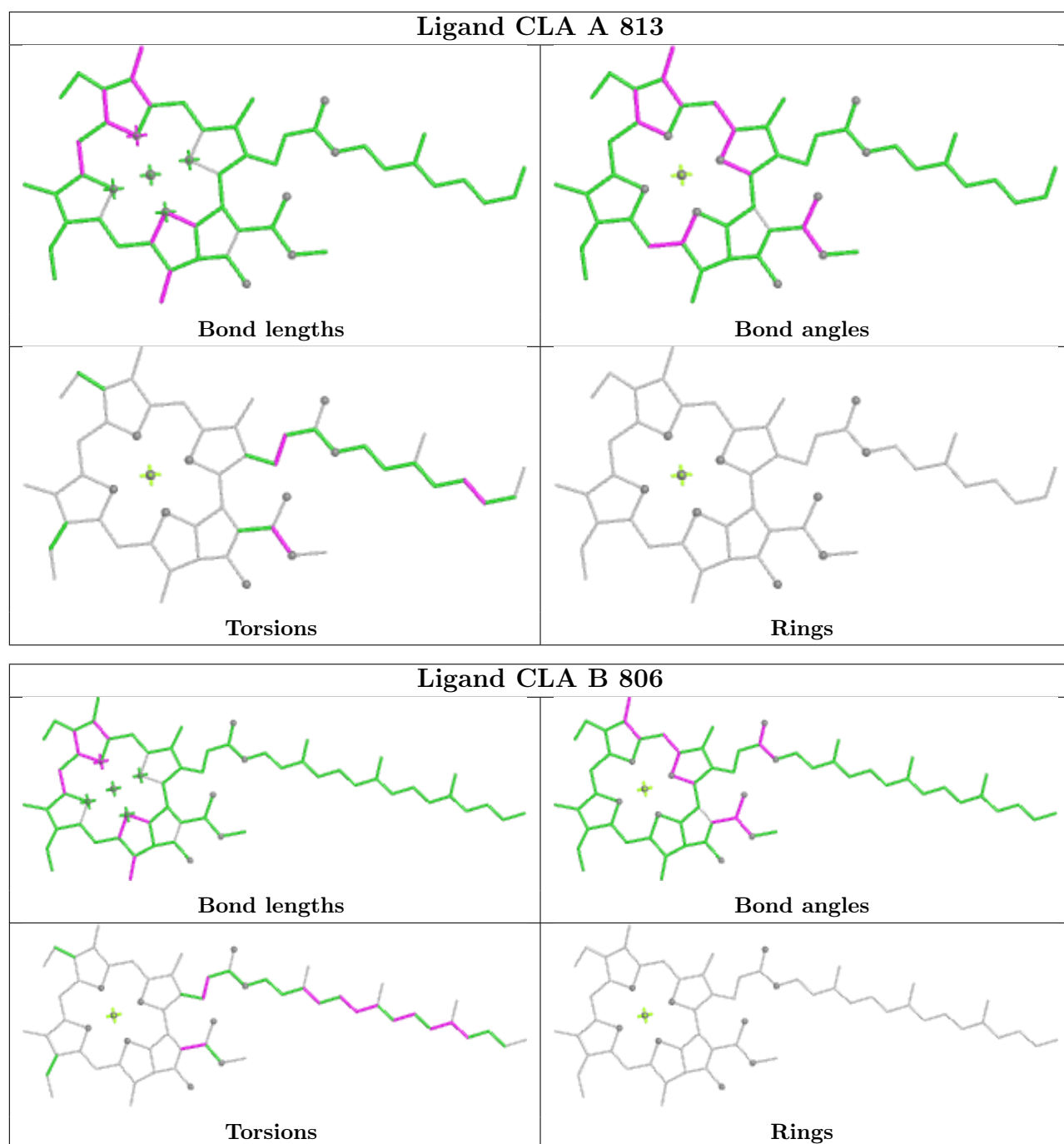


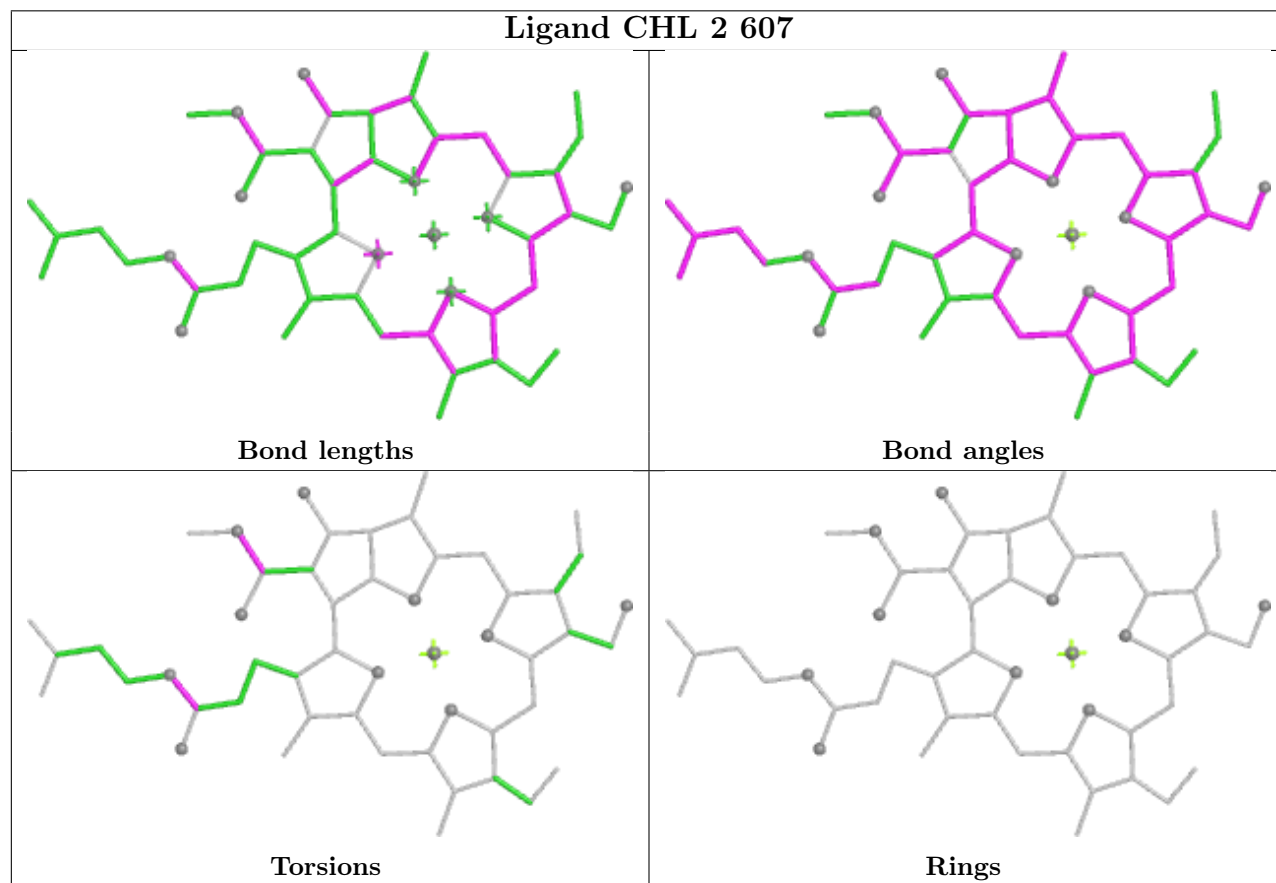
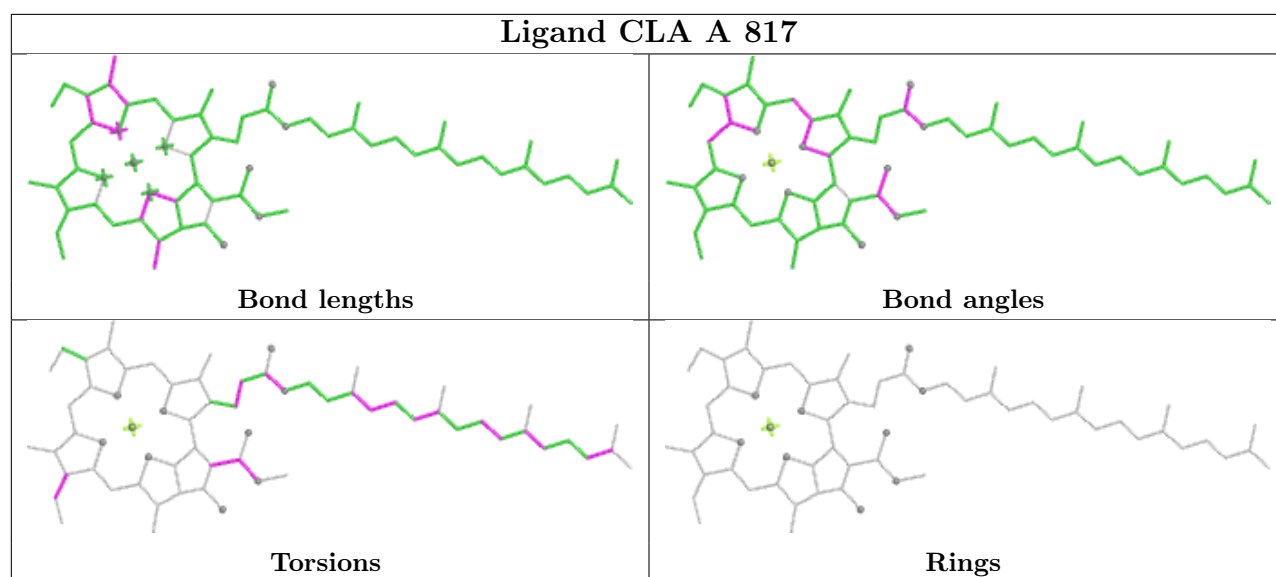
Rings

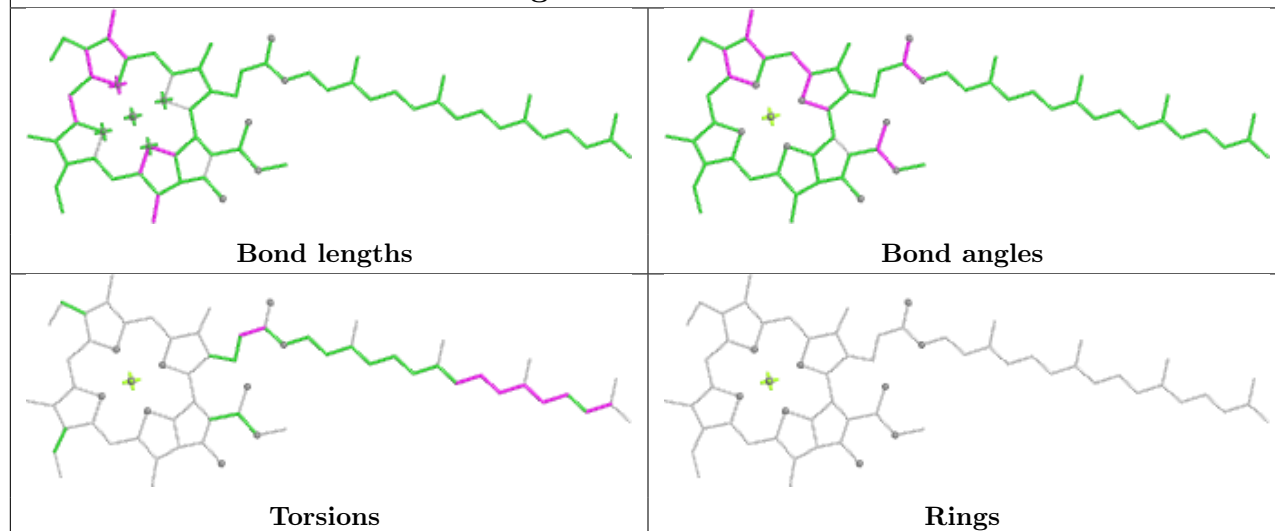
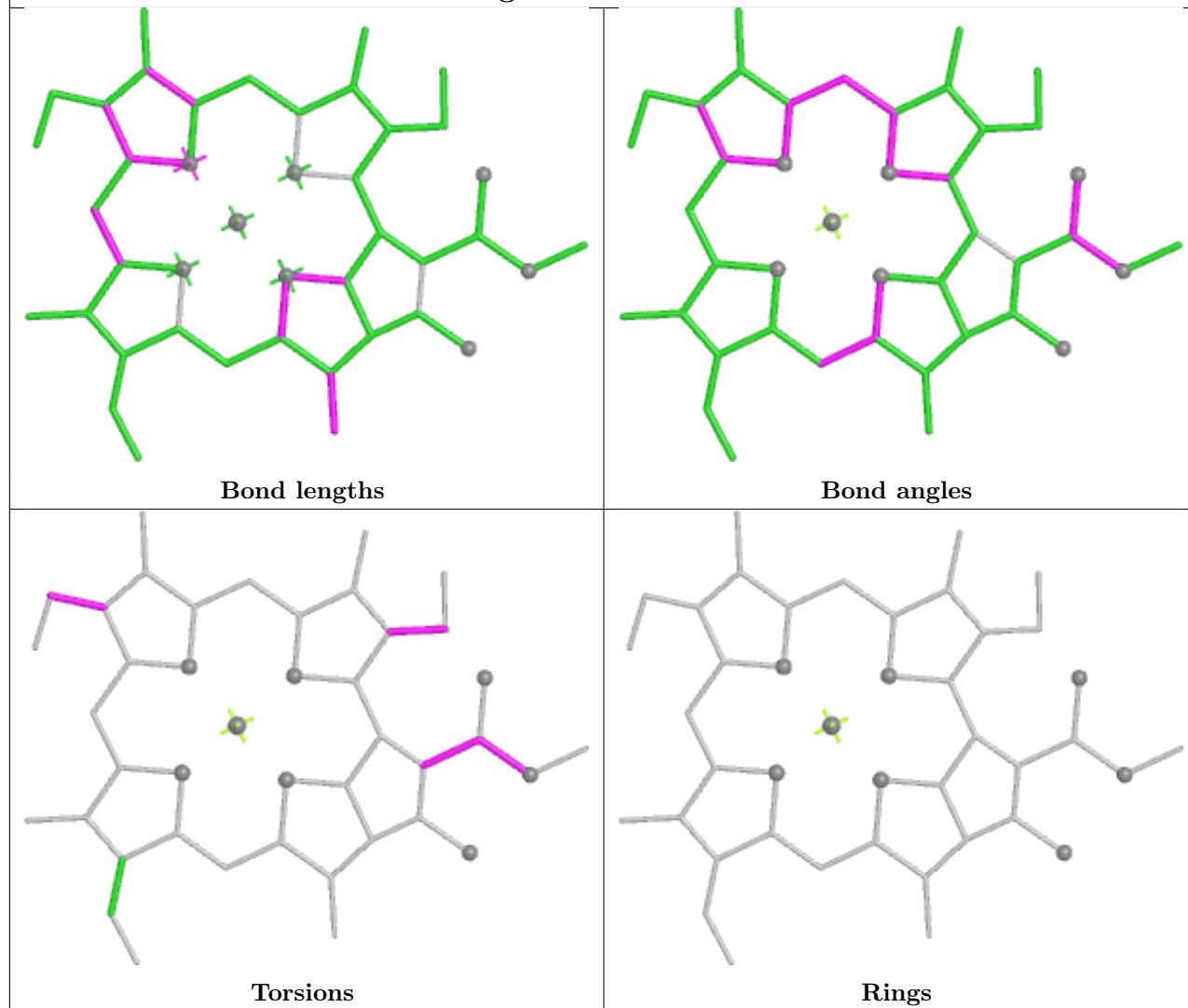
Ligand CHL 8 606



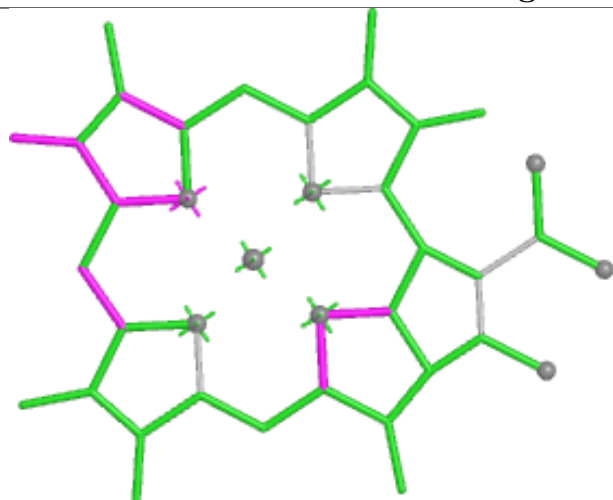




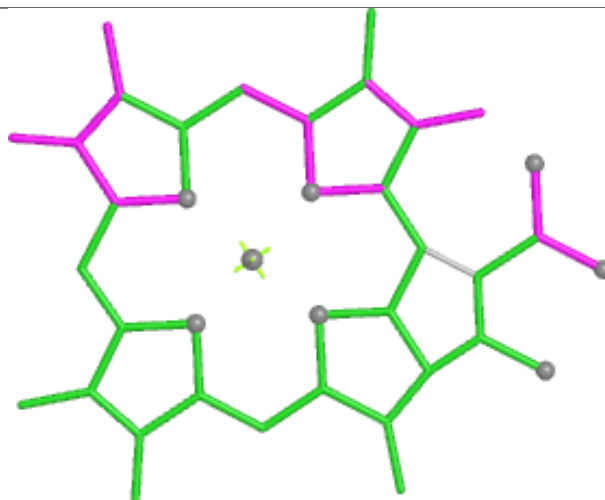


Ligand CLA A 825**Ligand CLA 6 613**

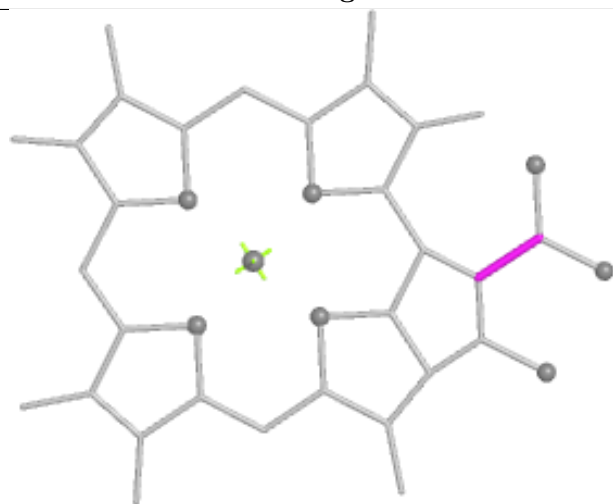
Ligand CLA 5 613



Bond lengths



Bond angles

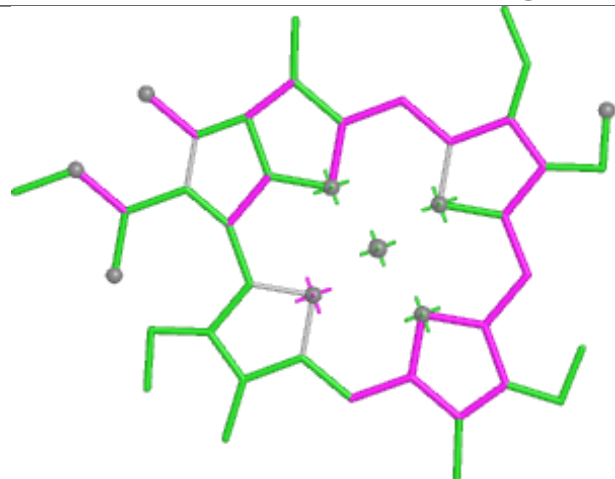


Torsions

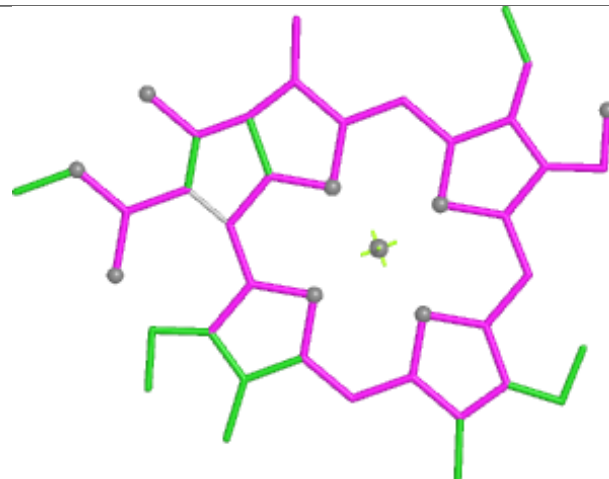


Rings

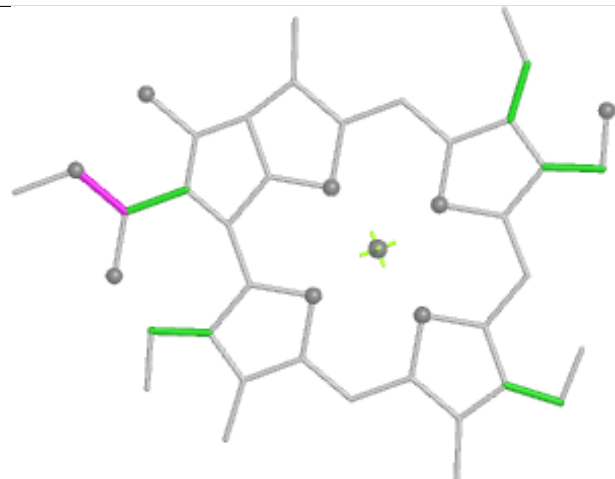
Ligand CHL 9 601



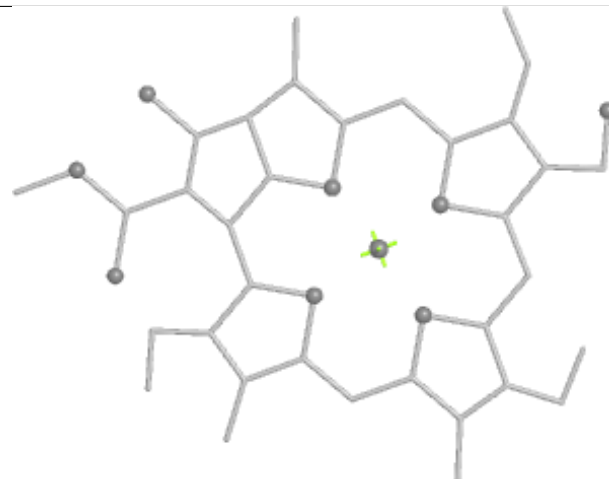
Bond lengths



Bond angles

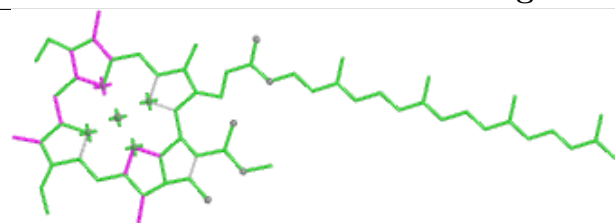


Torsions

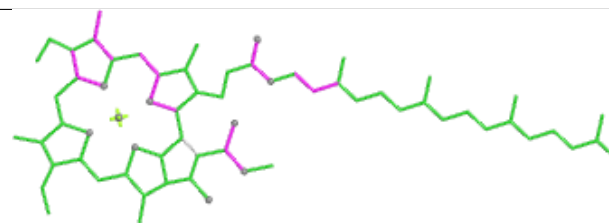


Rings

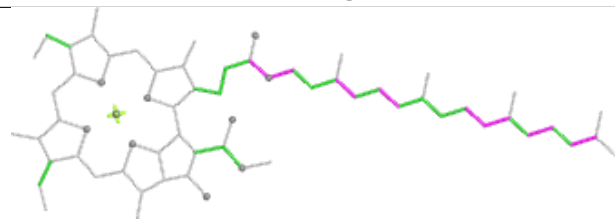
Ligand CLA B 825



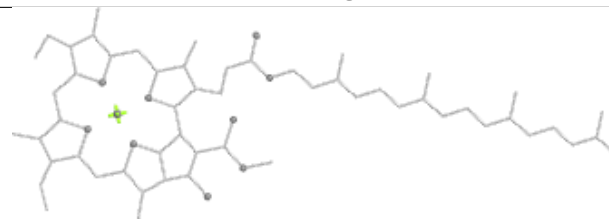
Bond lengths



Bond angles

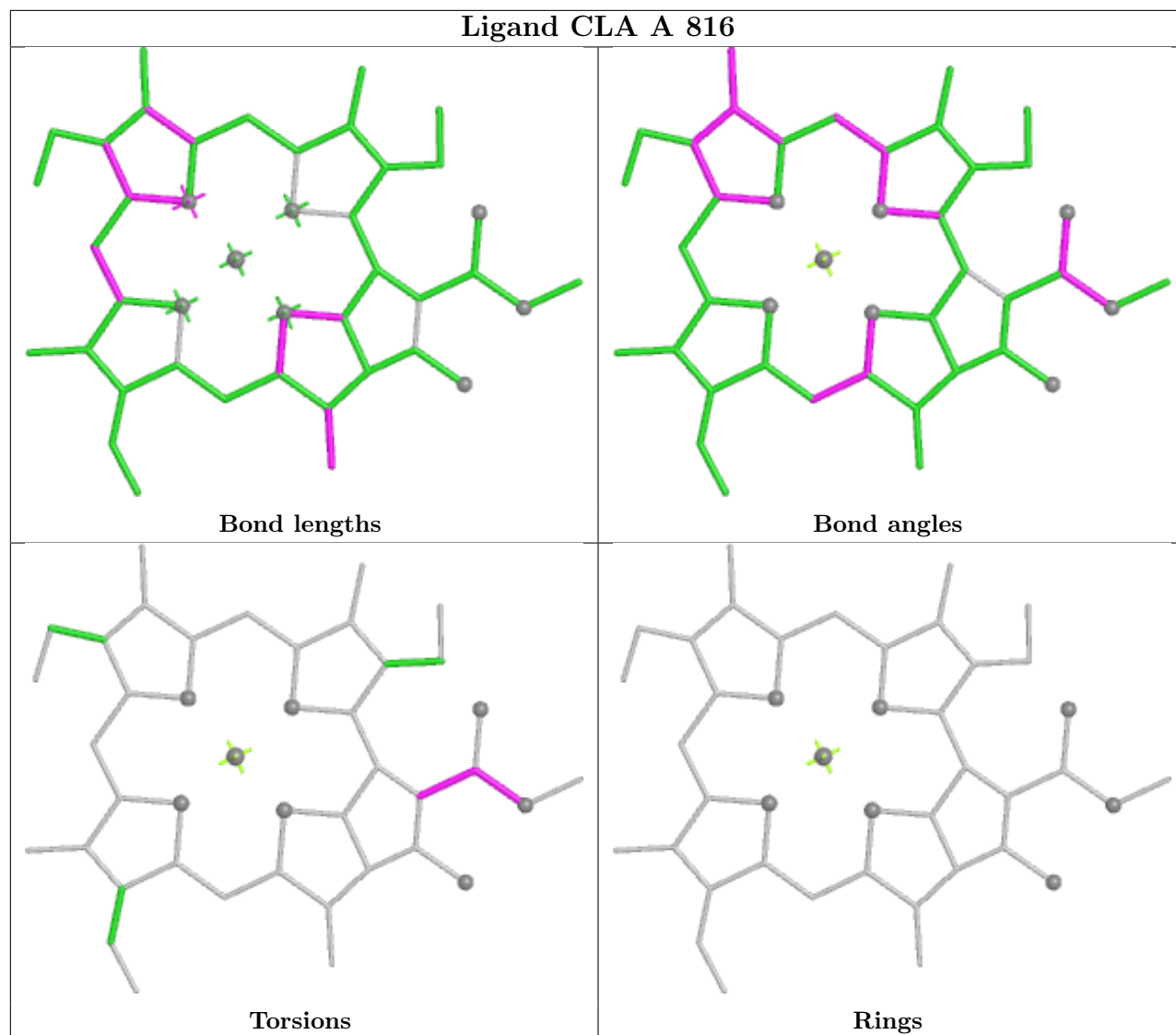


Torsions

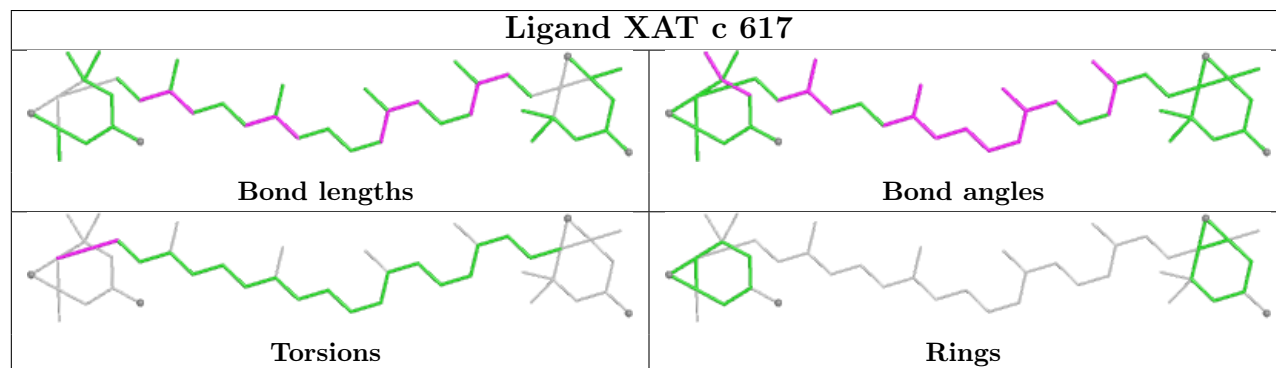


Rings

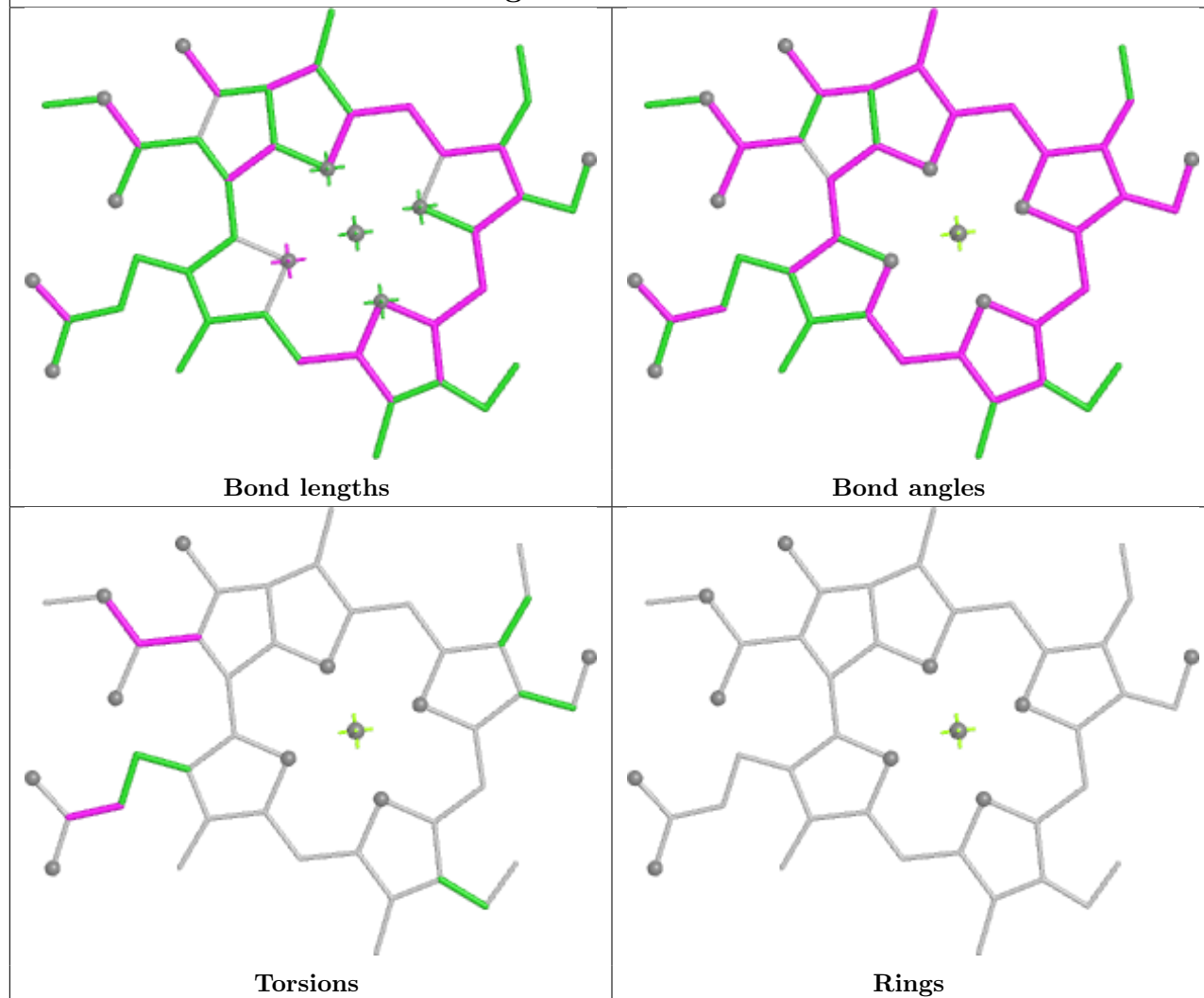
Ligand CLA A 816



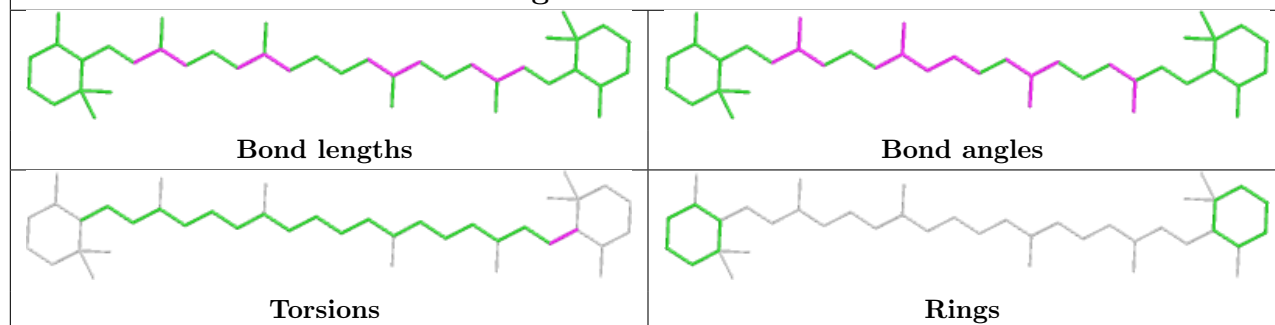
Ligand XAT c 617



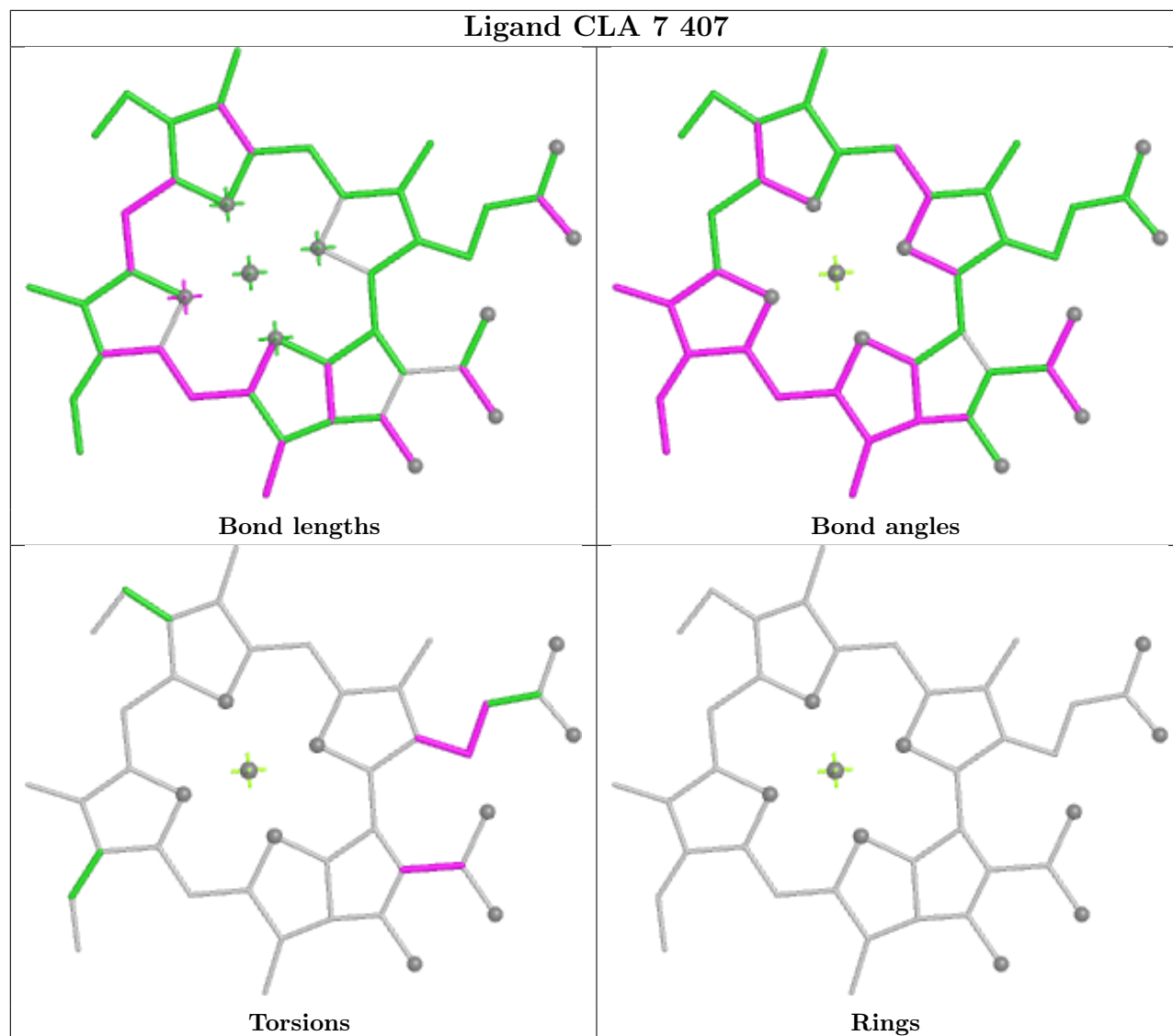
Ligand CHL a 606



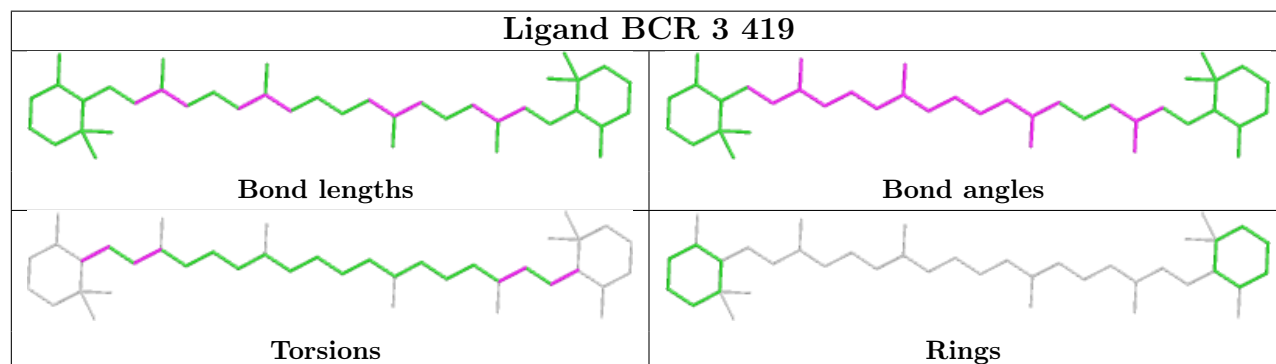
Ligand BCR L 305



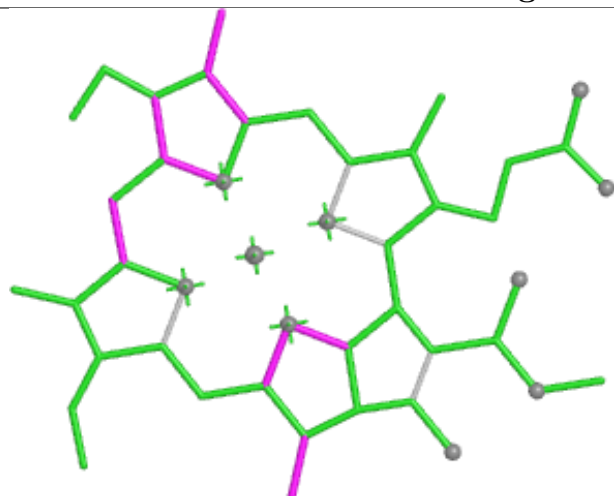
Ligand CLA 7 407



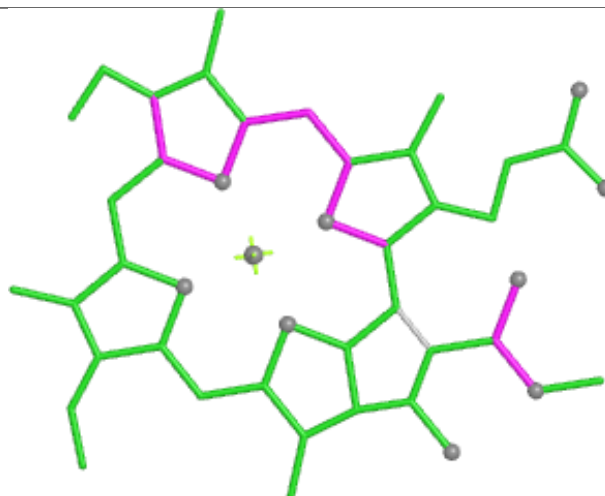
Ligand BCR 3 419



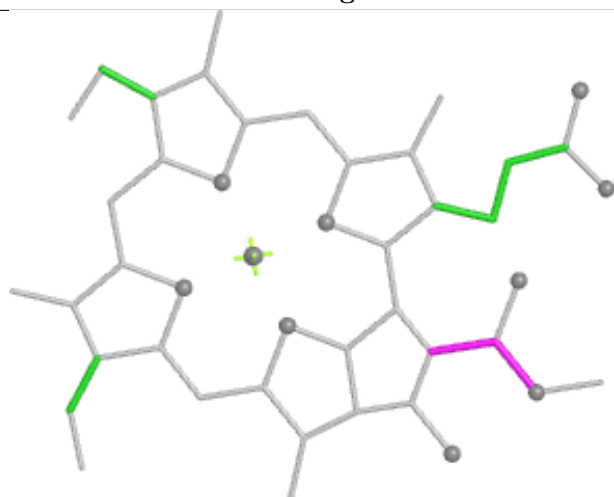
Ligand CLA 9 612



Bond lengths



Bond angles

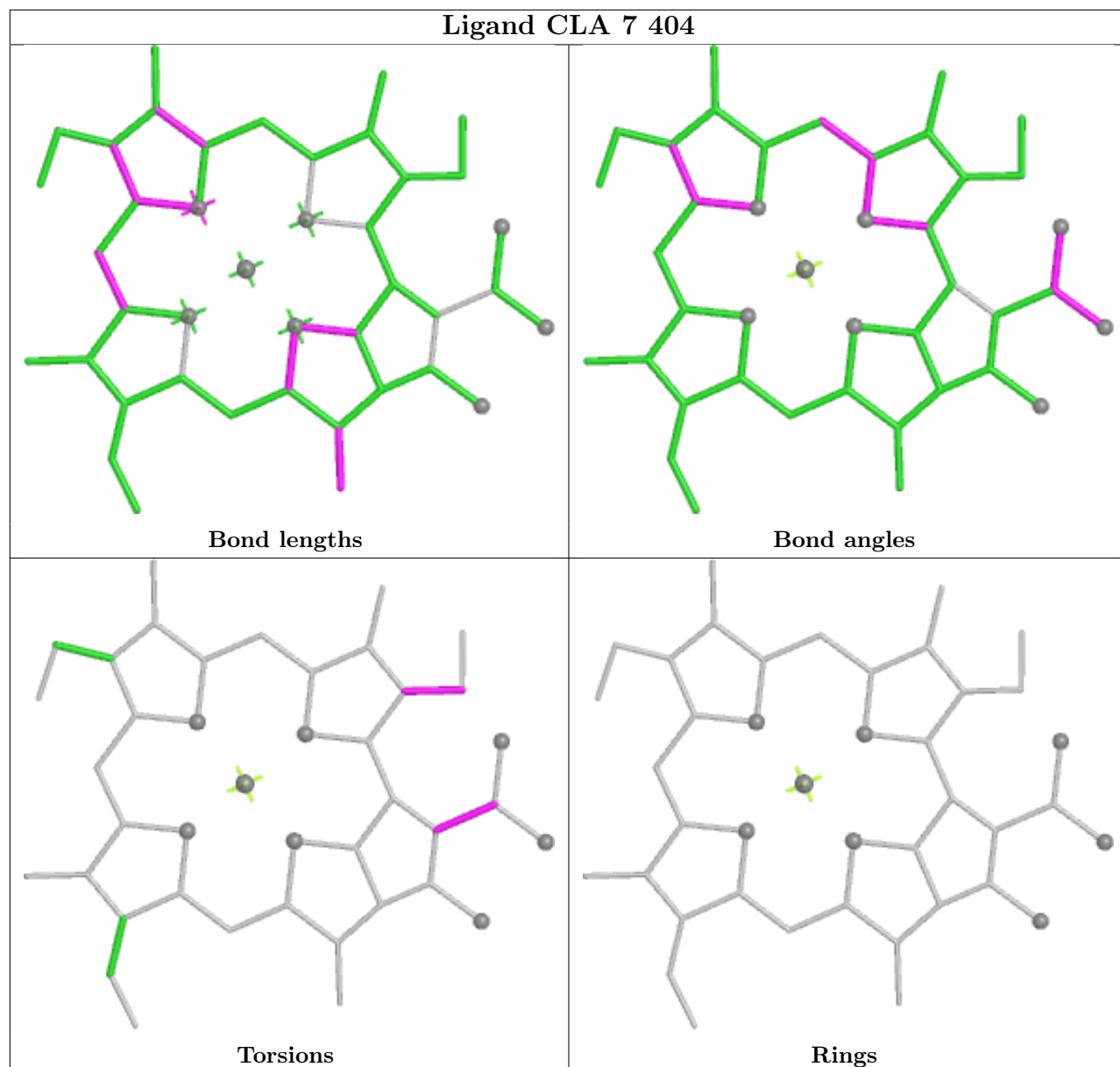


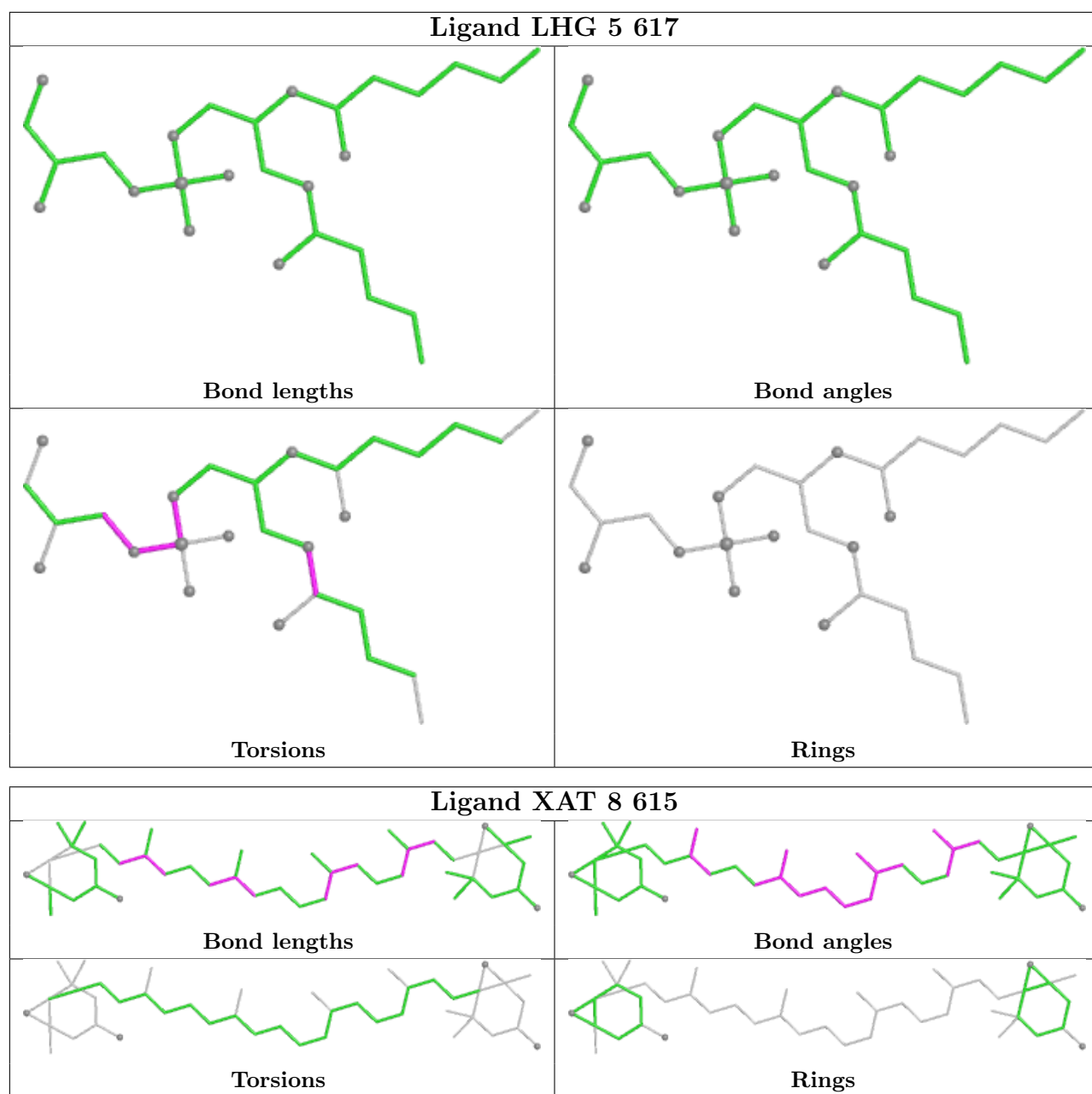
Torsions



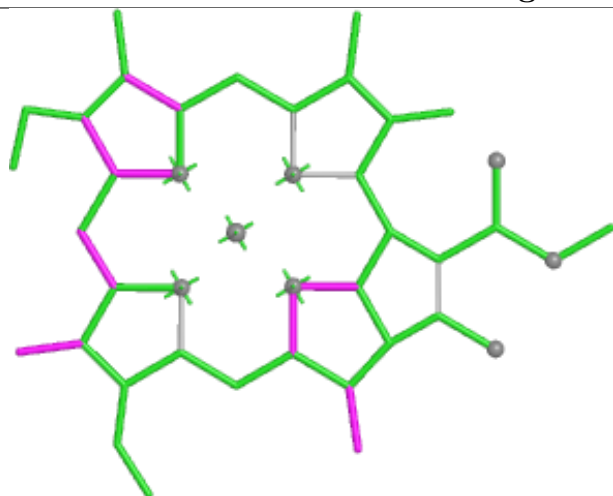
Rings

Ligand CLA 7 404





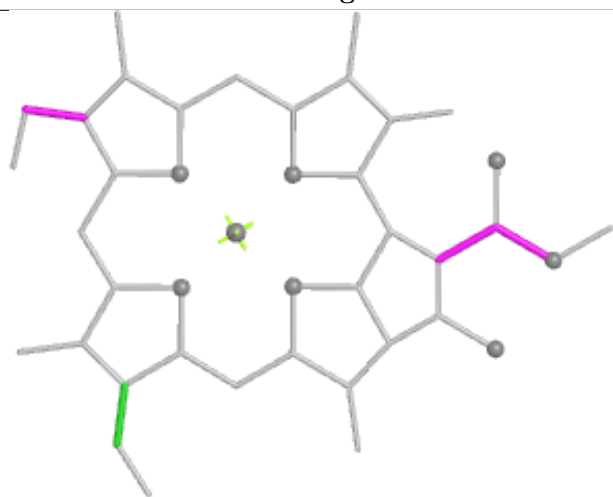
Ligand CLA 8 618



Bond lengths



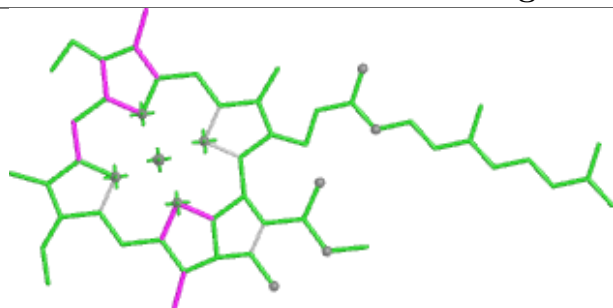
Bond angles



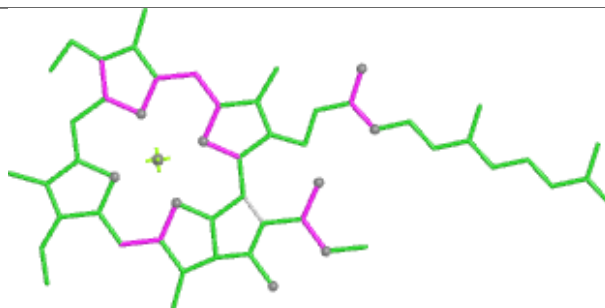
Torsions



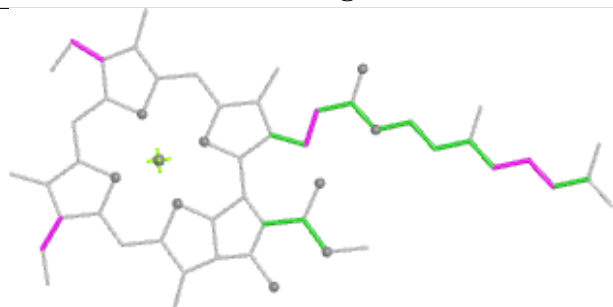
Rings

Ligand CLA 4 612

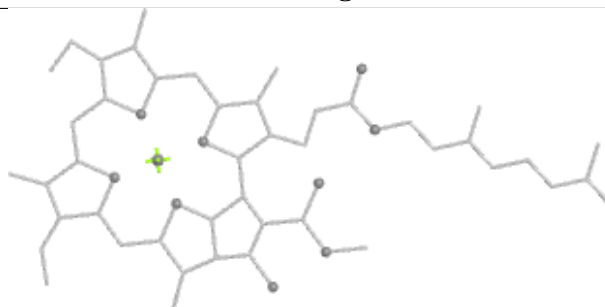
Bond lengths



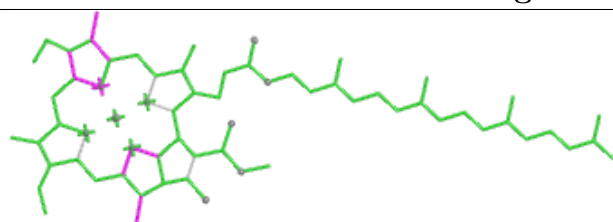
Bond angles



Torsions



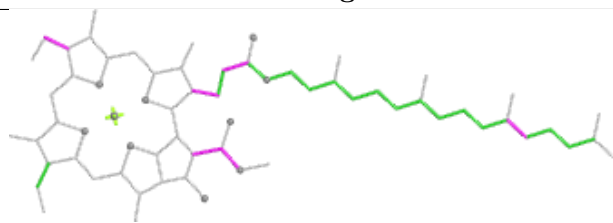
Rings

Ligand CLA B 839

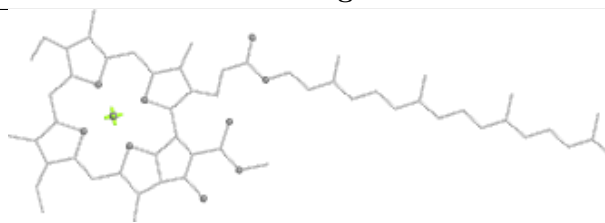
Bond lengths



Bond angles

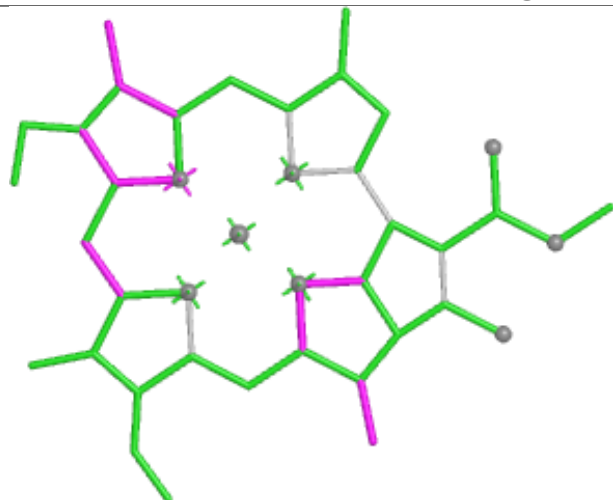


Torsions

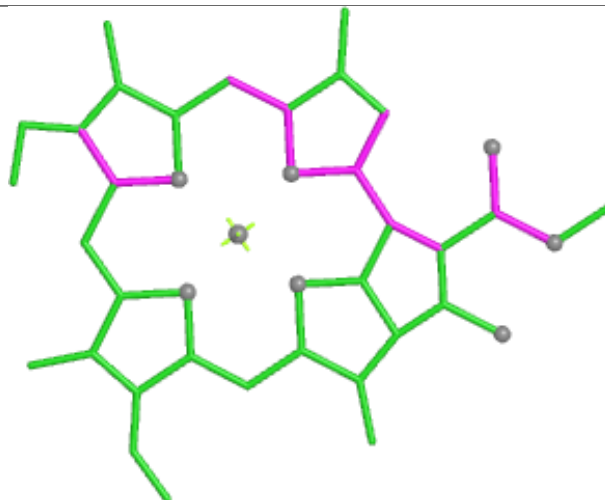


Rings

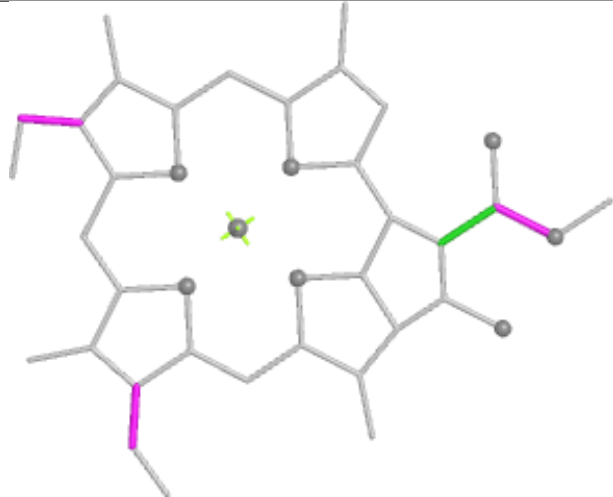
Ligand CLA 5 605



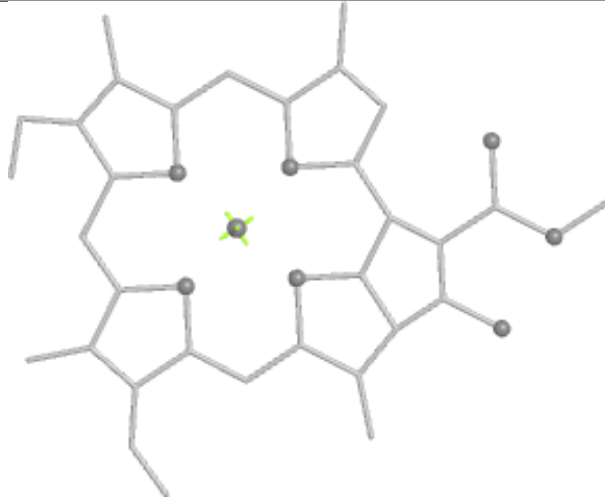
Bond lengths



Bond angles

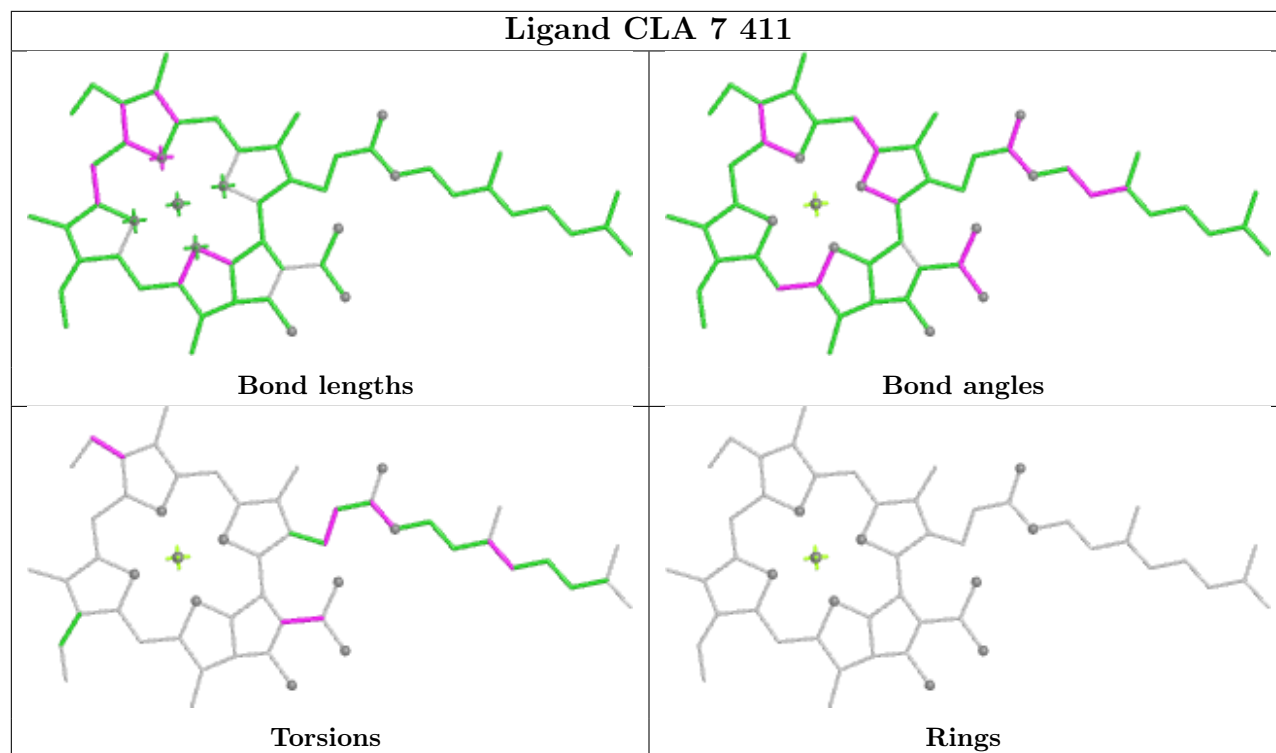


Torsions

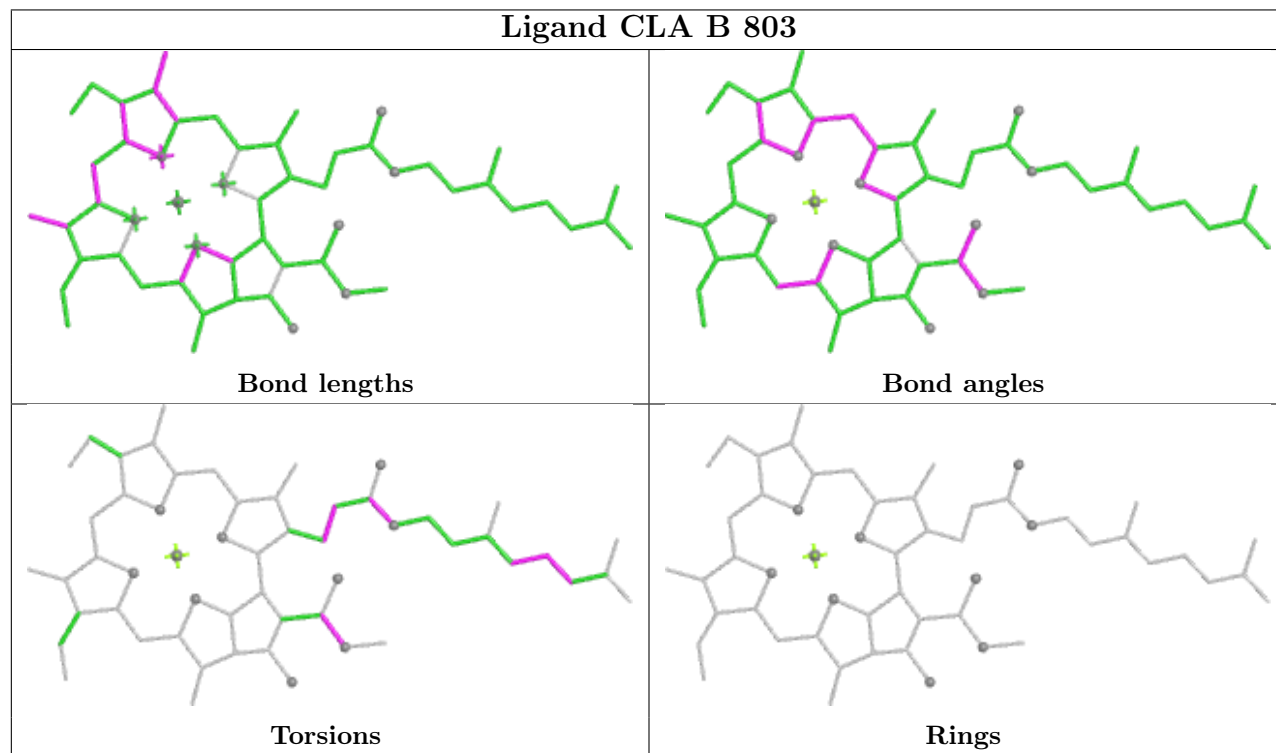


Rings

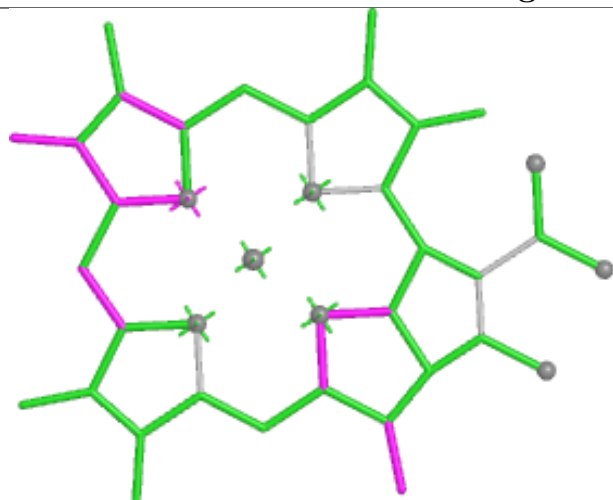
Ligand CLA 7 411



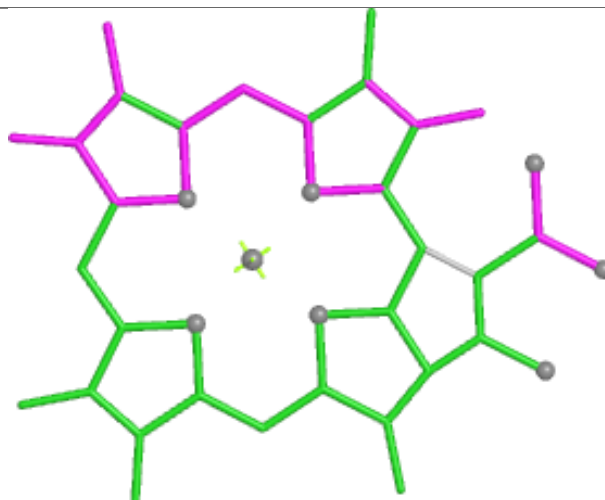
Ligand CLA B 803



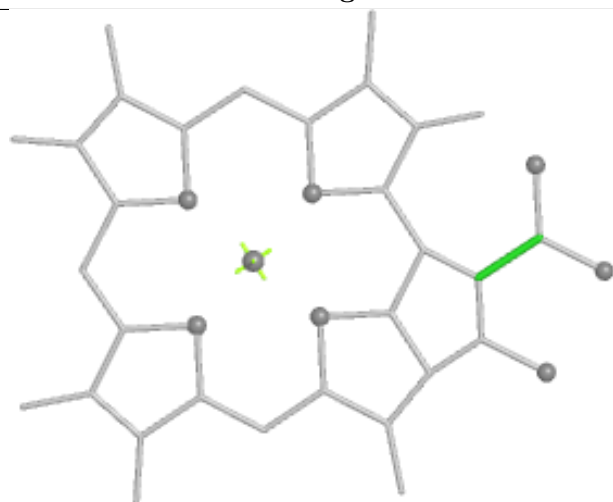
Ligand CLA 5 610



Bond lengths



Bond angles

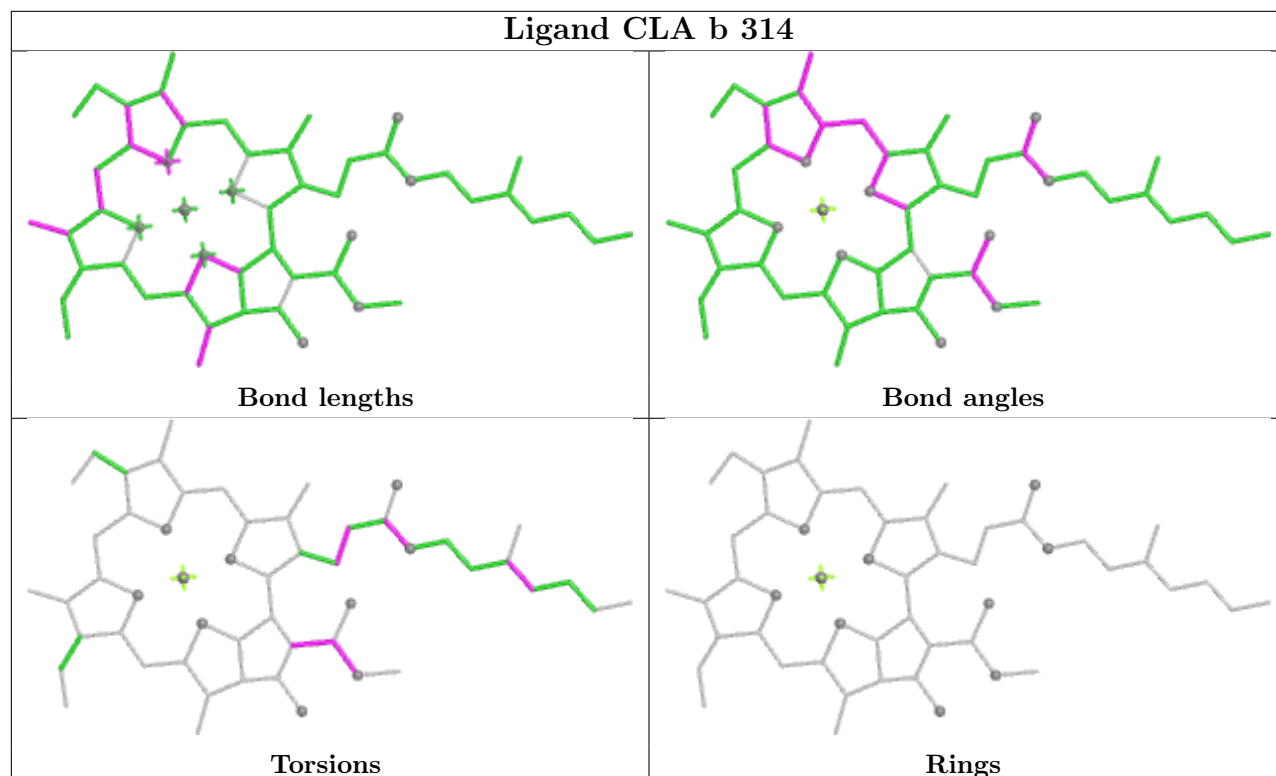


Torsions

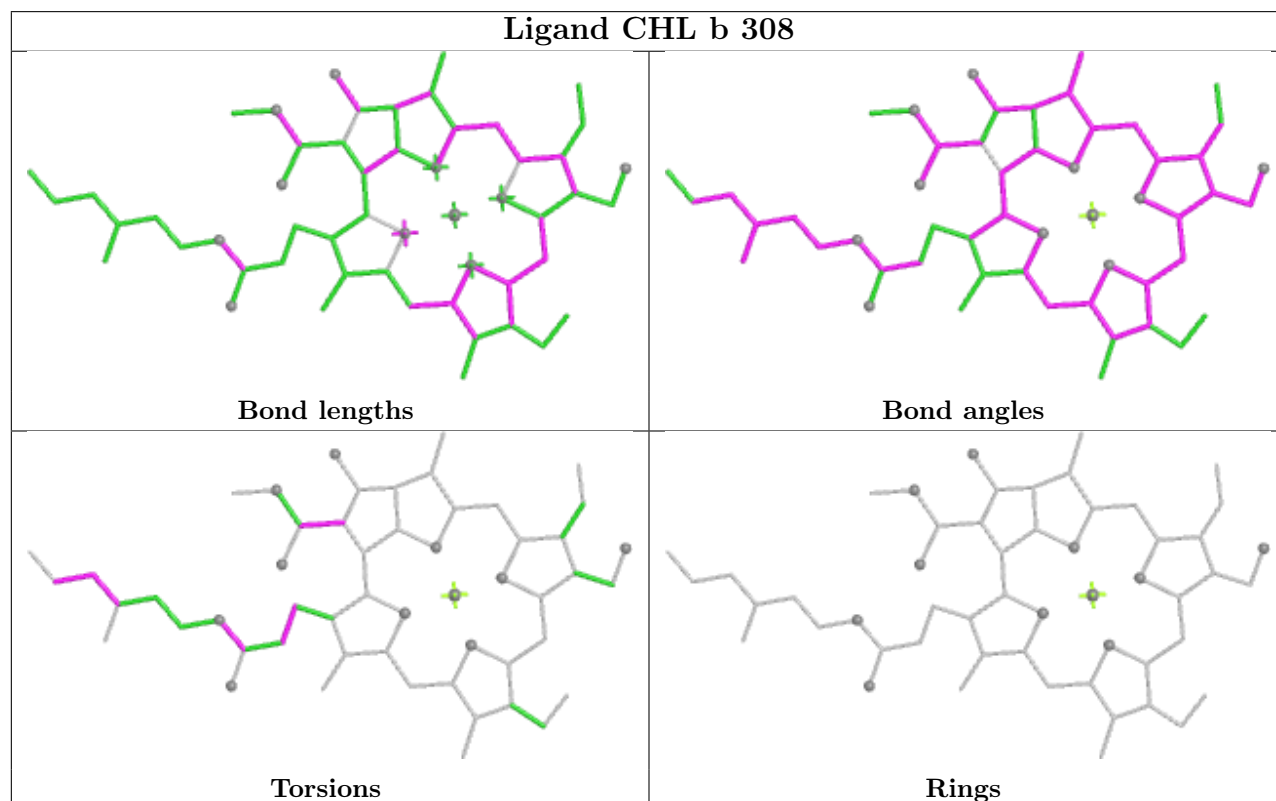


Rings

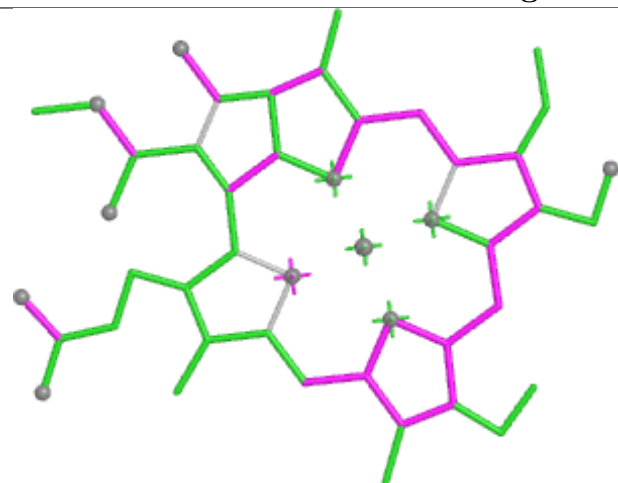
Ligand CLA b 314



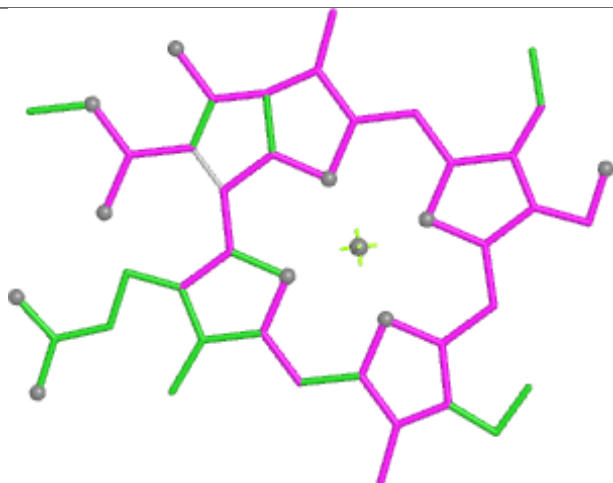
Ligand CHL b 308



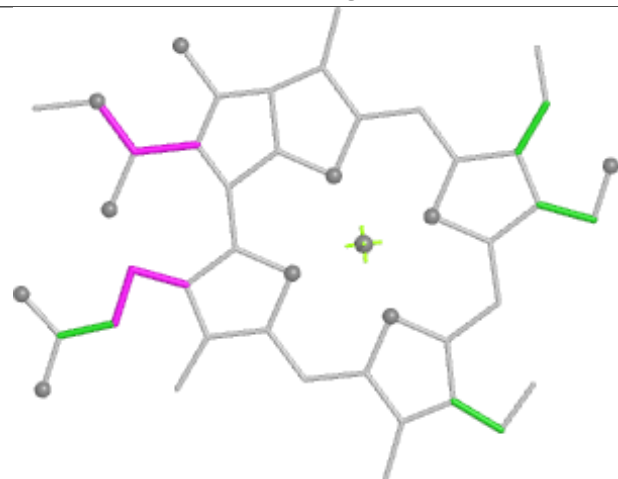
Ligand CHL b 302



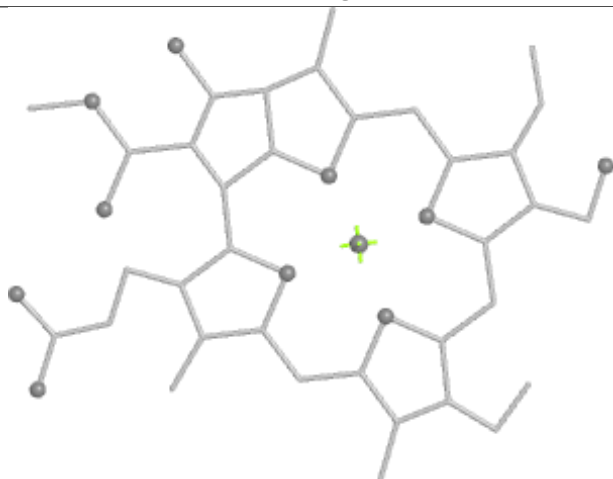
Bond lengths



Bond angles

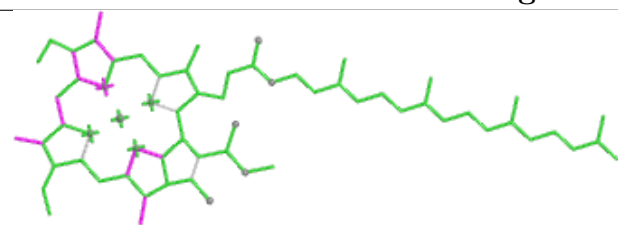


Torsions

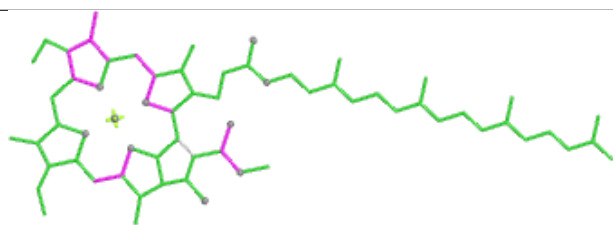


Rings

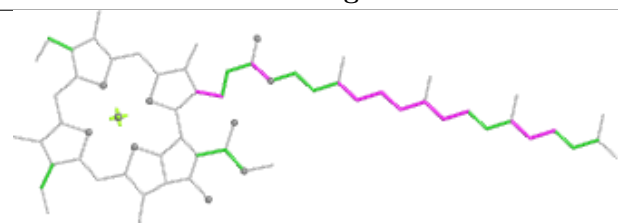
Ligand CLA B 836



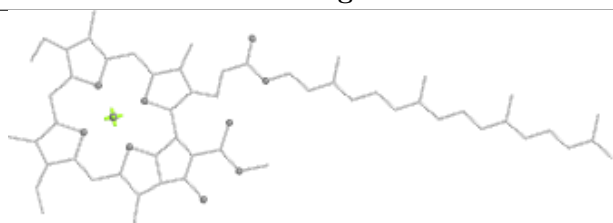
Bond lengths



Bond angles

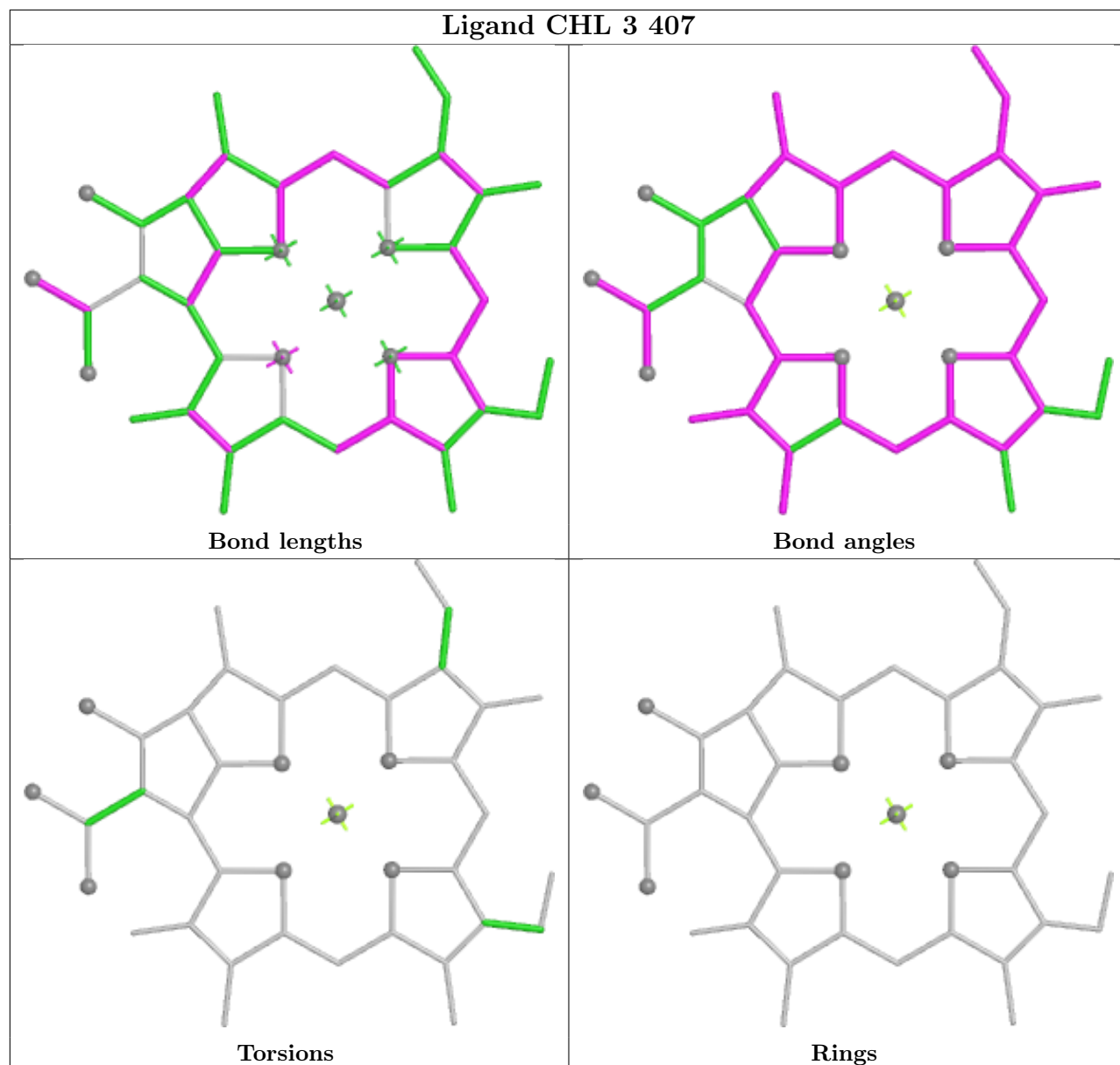


Torsions

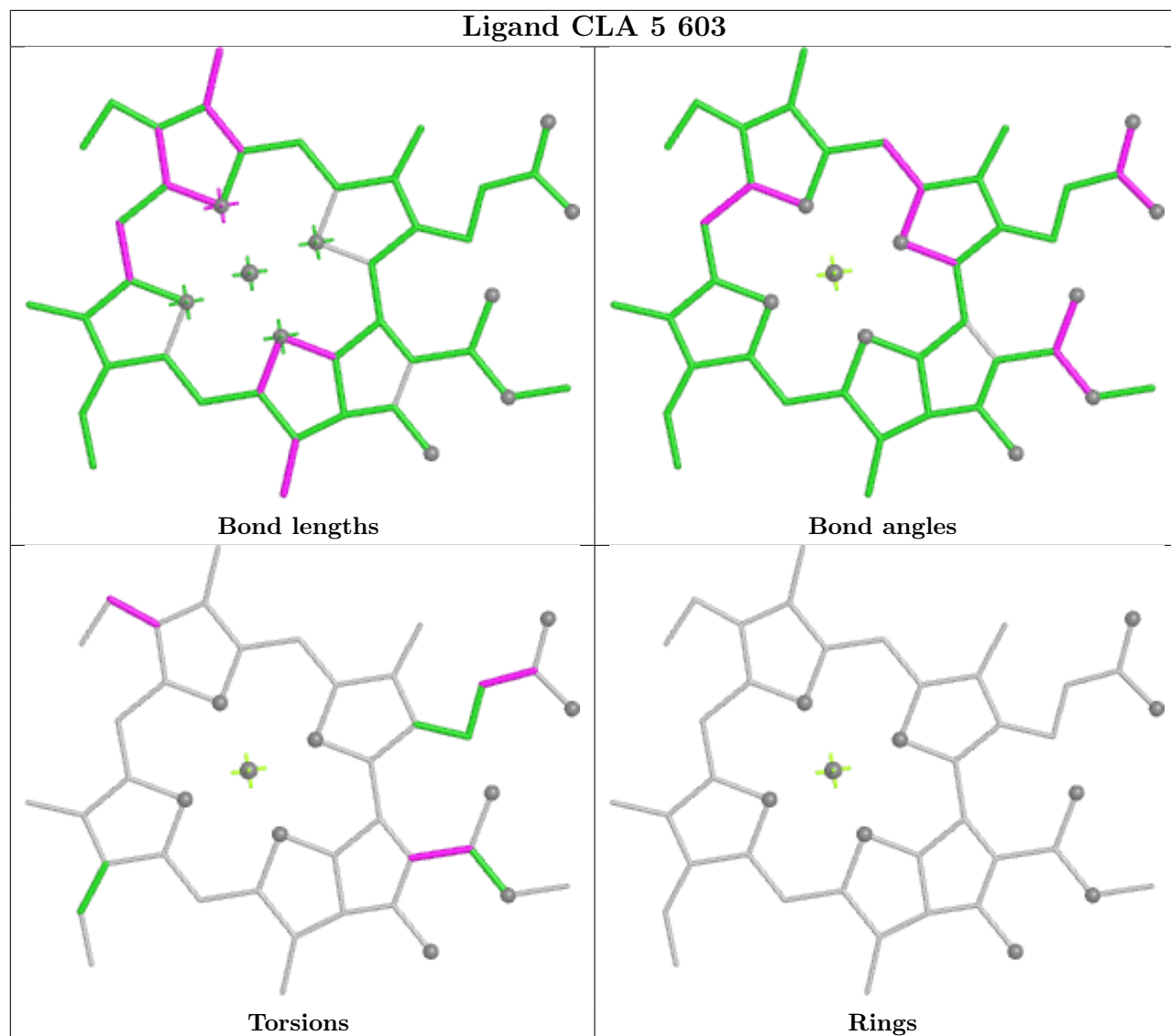


Rings

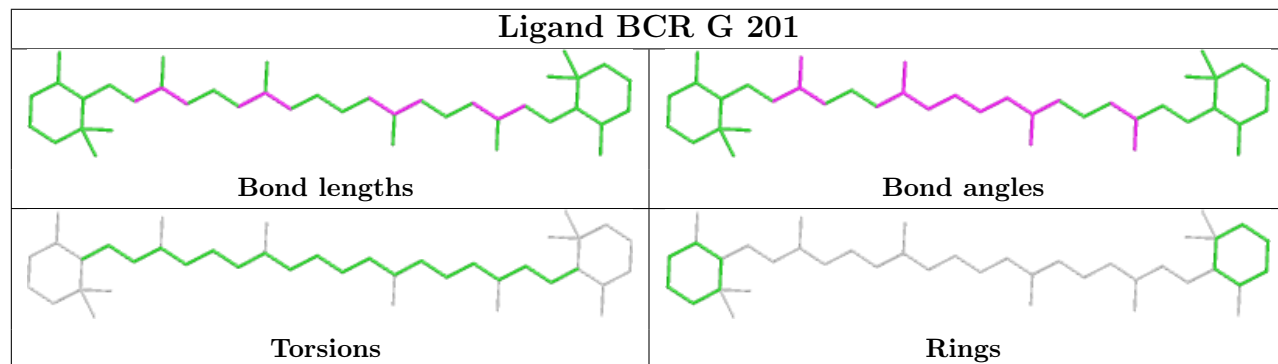
Ligand CHL 3 407



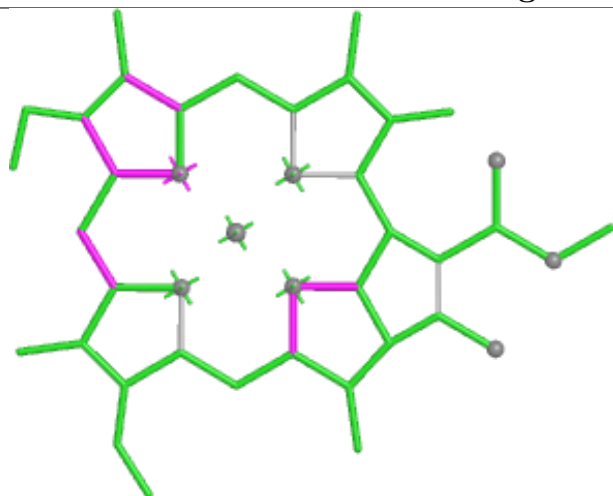
Ligand CLA 5 603



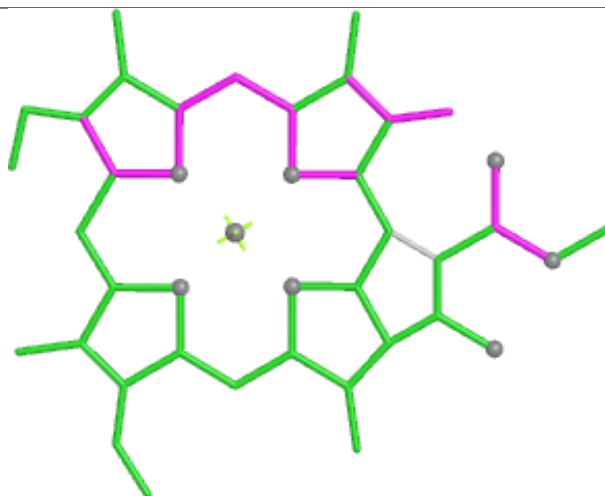
Ligand BCR G 201



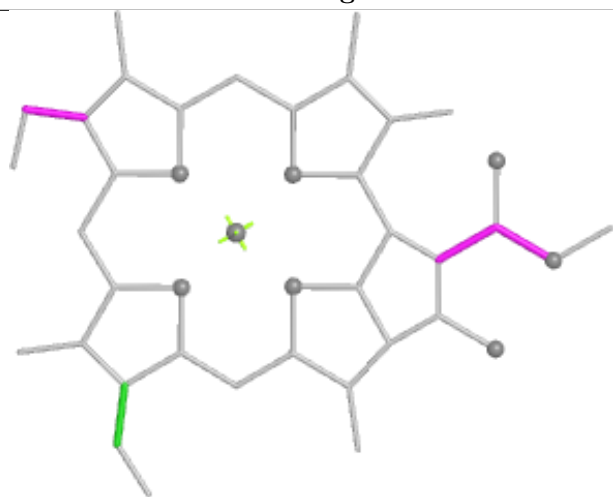
Ligand CLA 6 611



Bond lengths



Bond angles

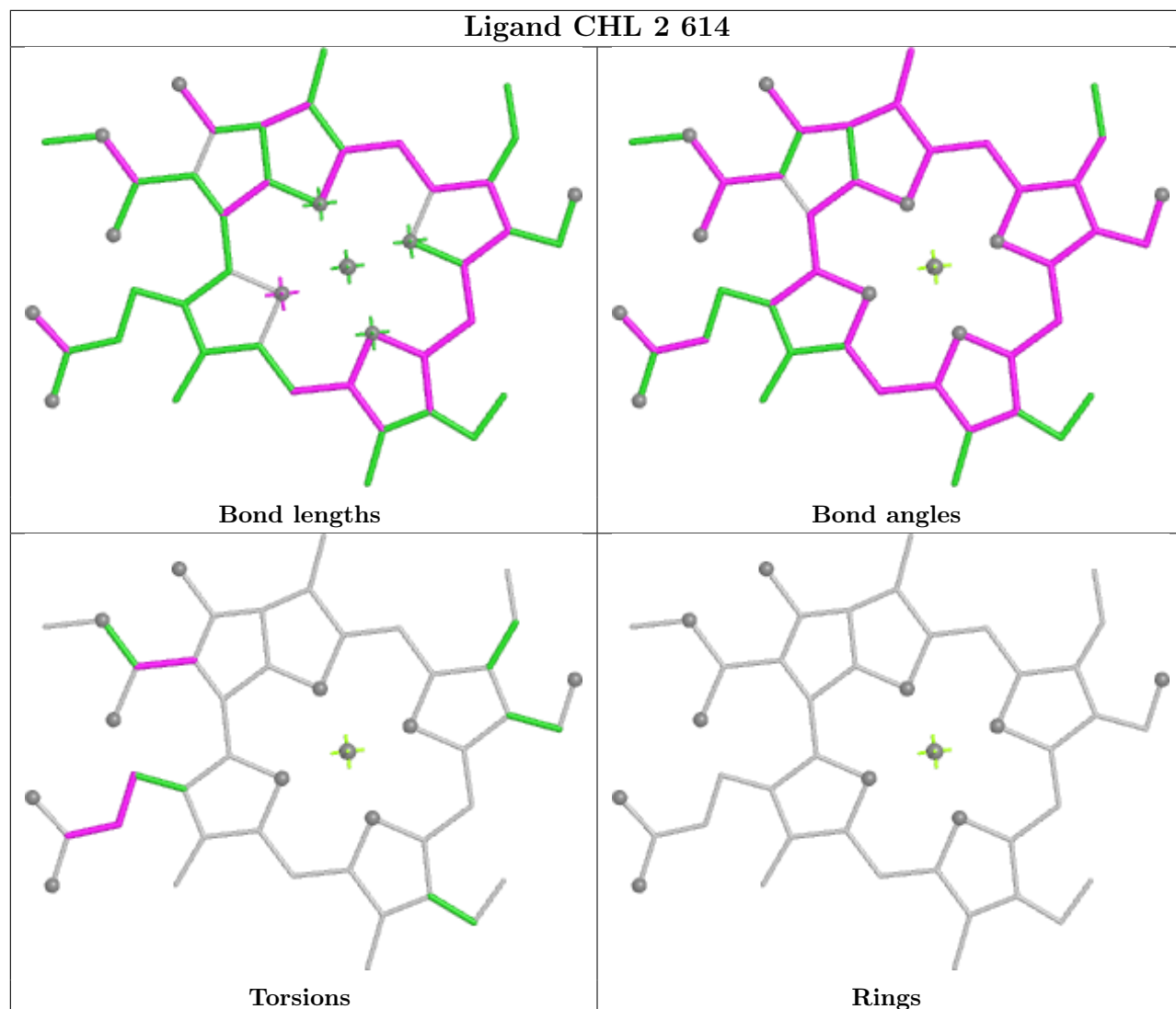


Torsions

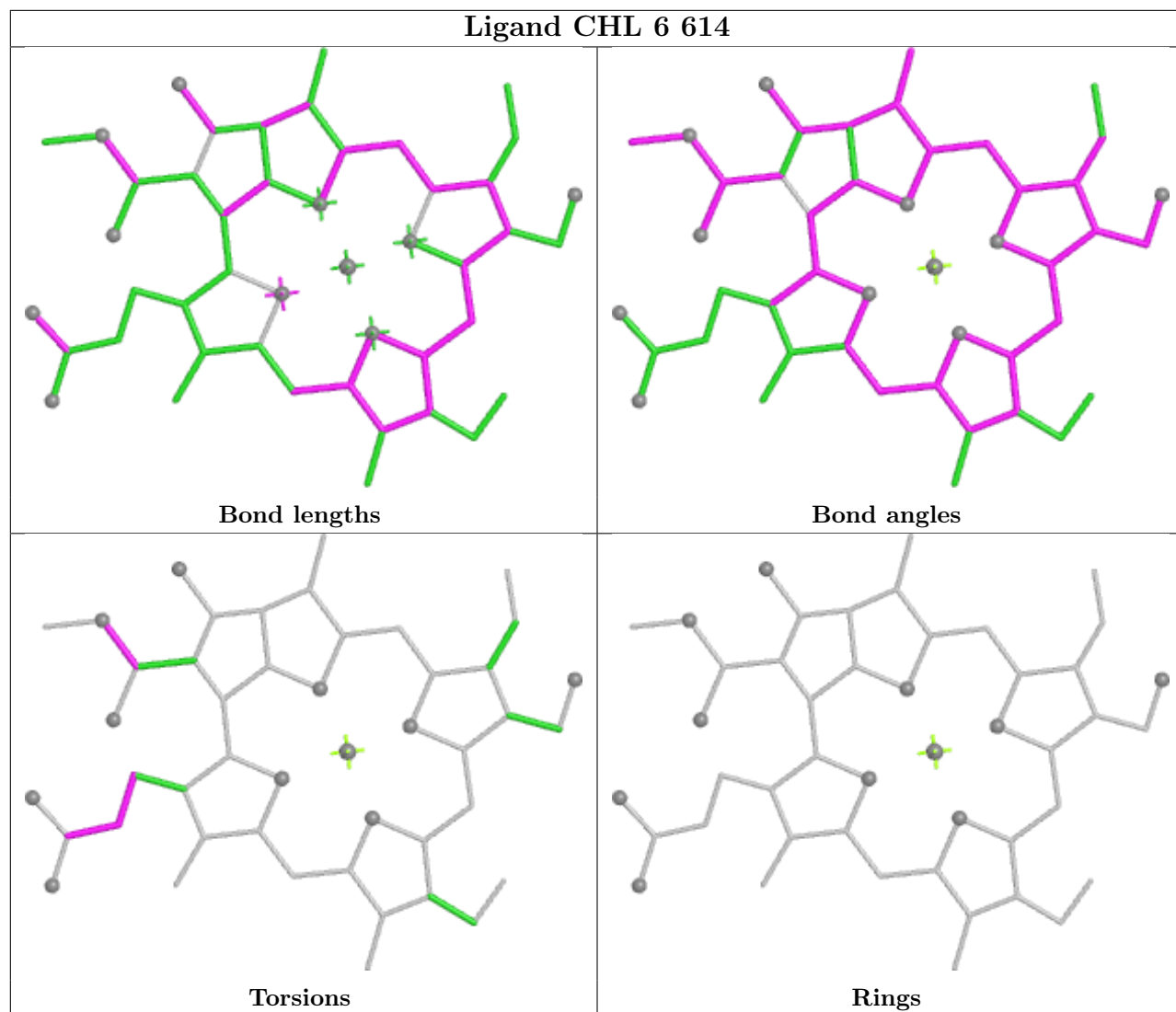


Rings

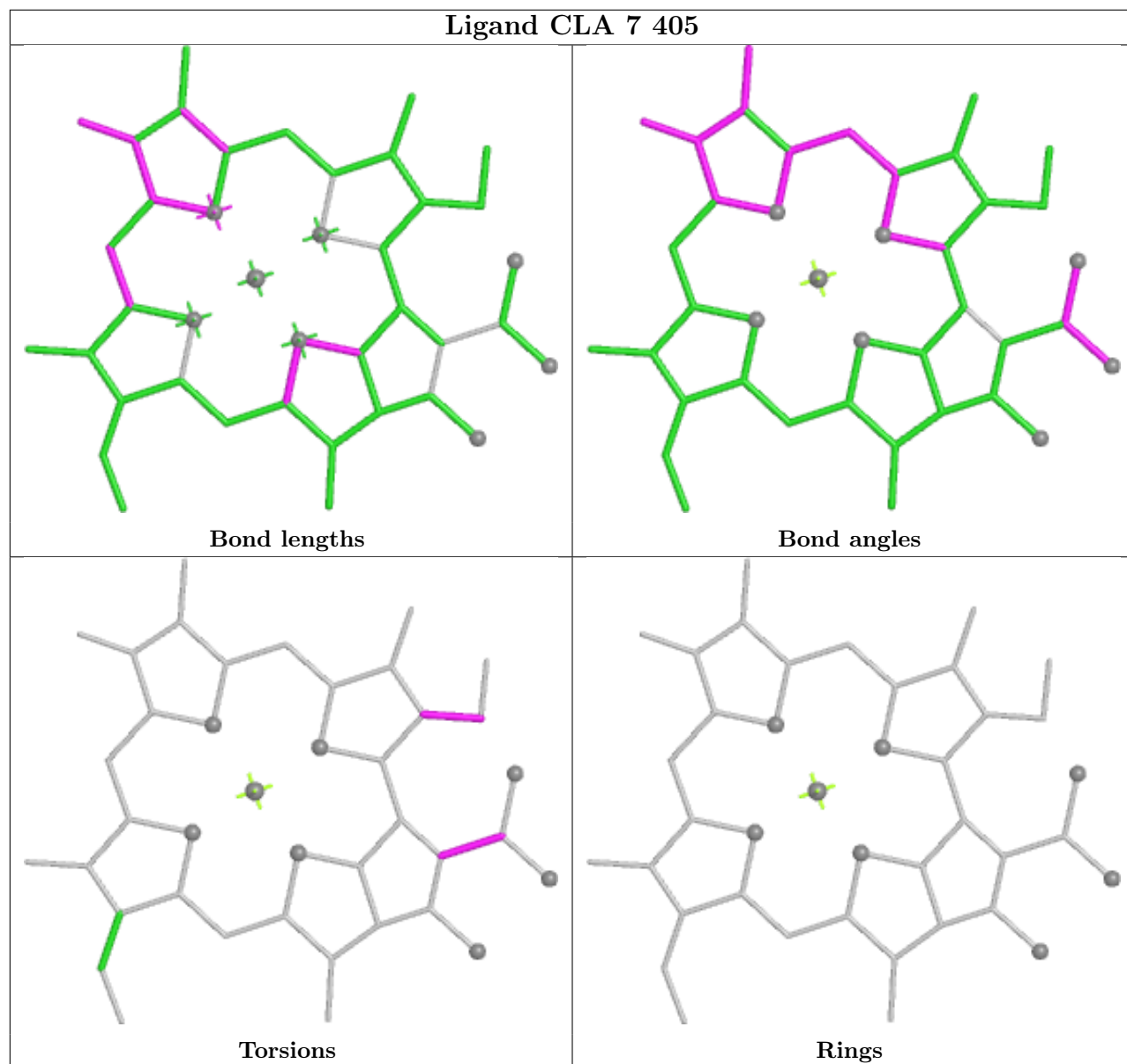
Ligand CHL 2 614



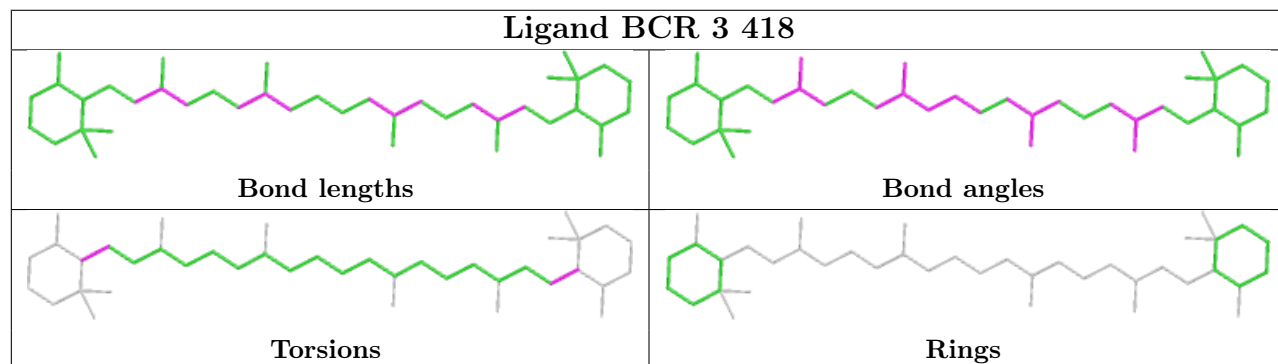
Ligand CHL 6 614

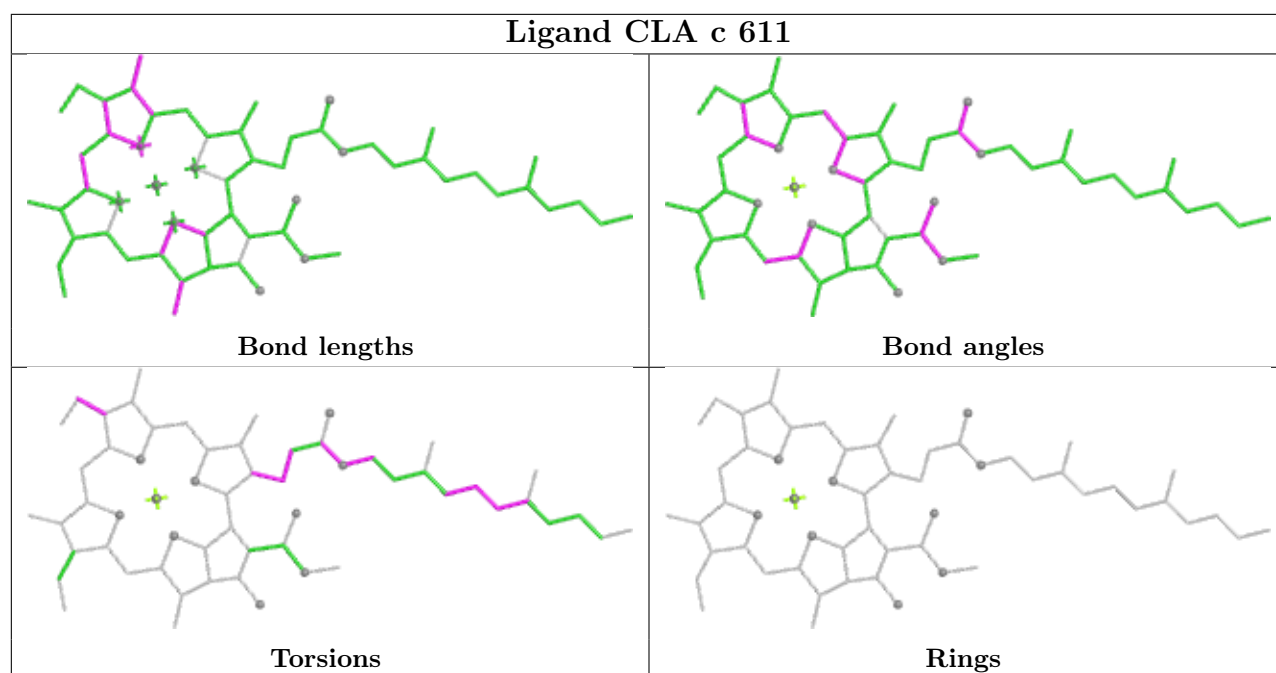


Ligand CLA 7 405



Ligand BCR 3 418

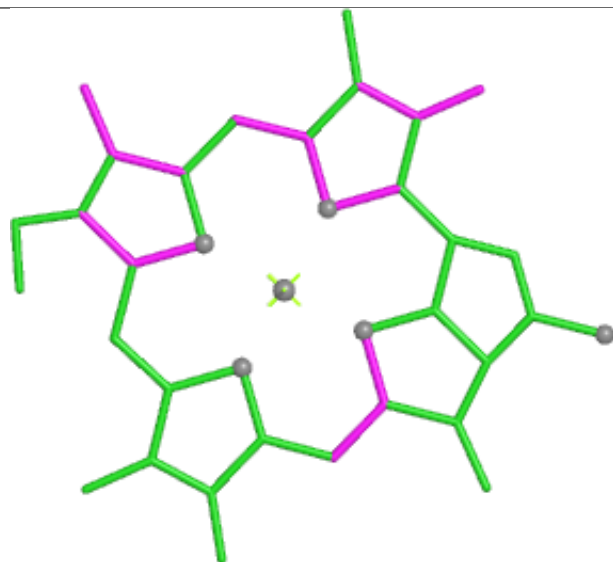




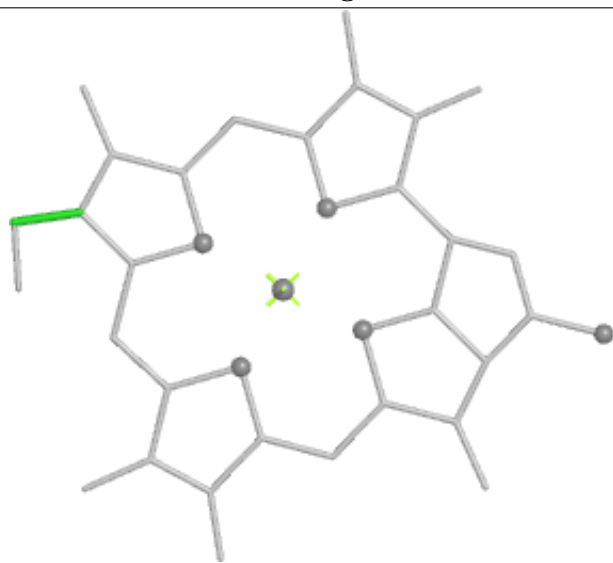
Ligand CLA 7 413



Bond lengths



Bond angles

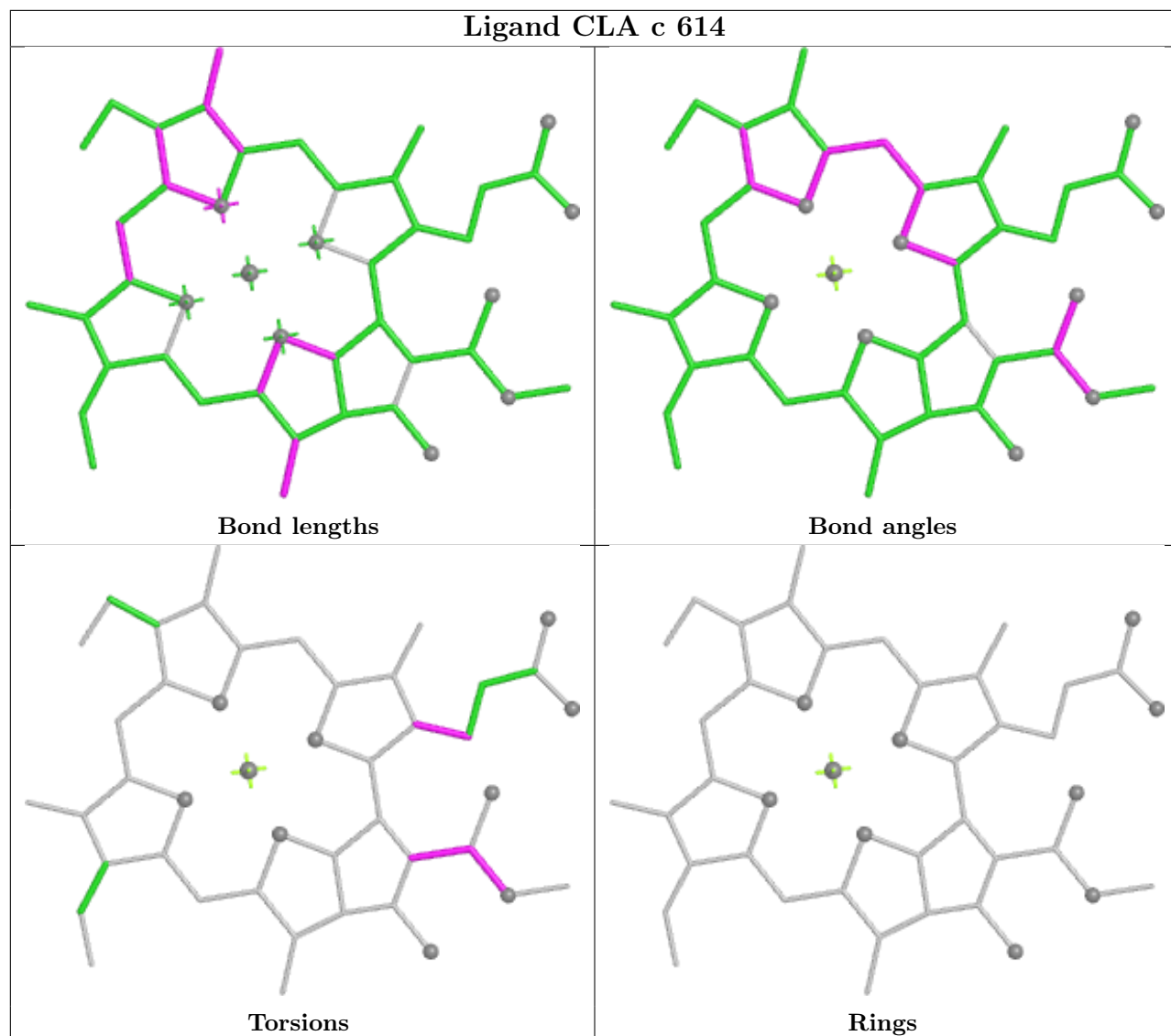


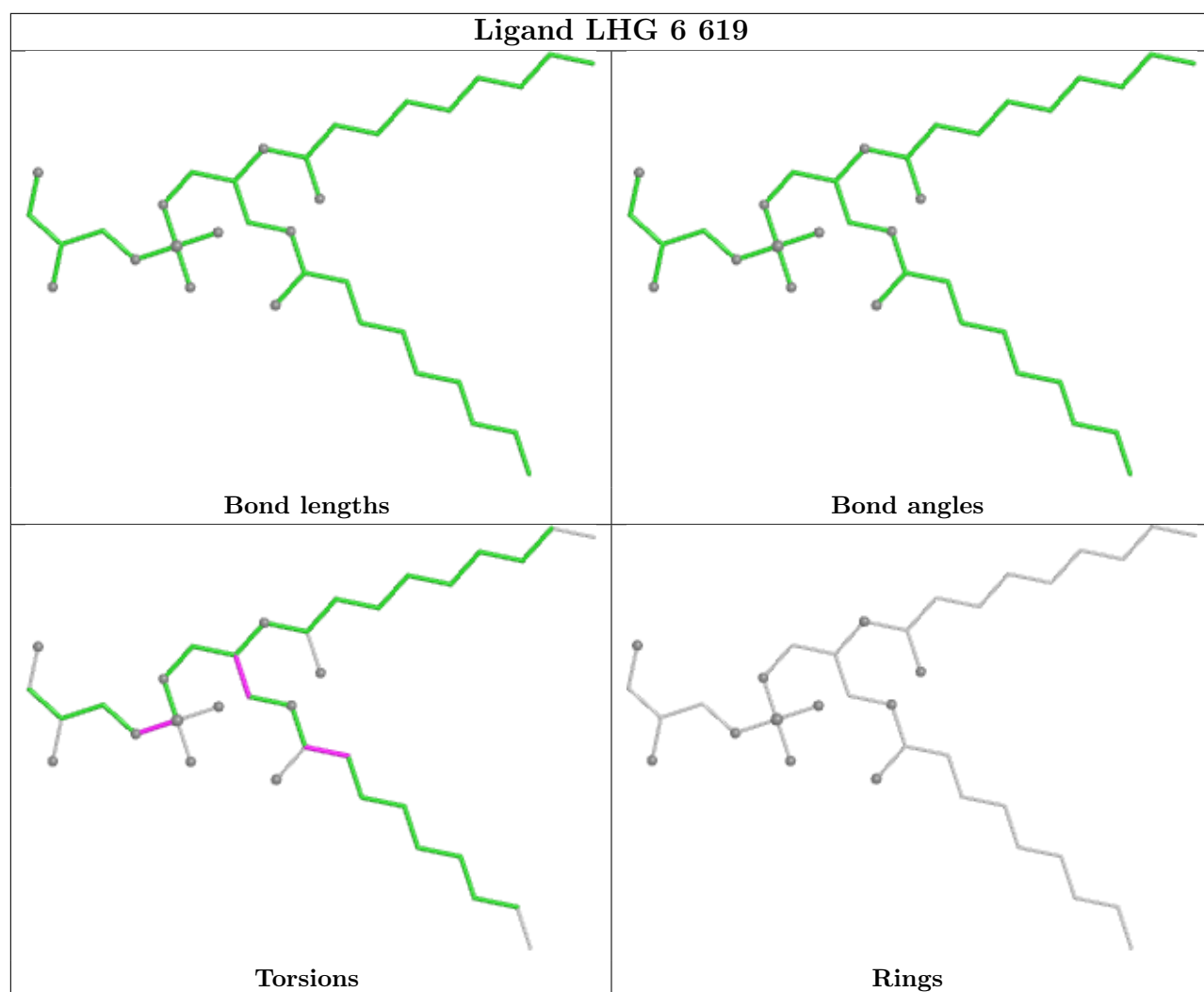
Torsions



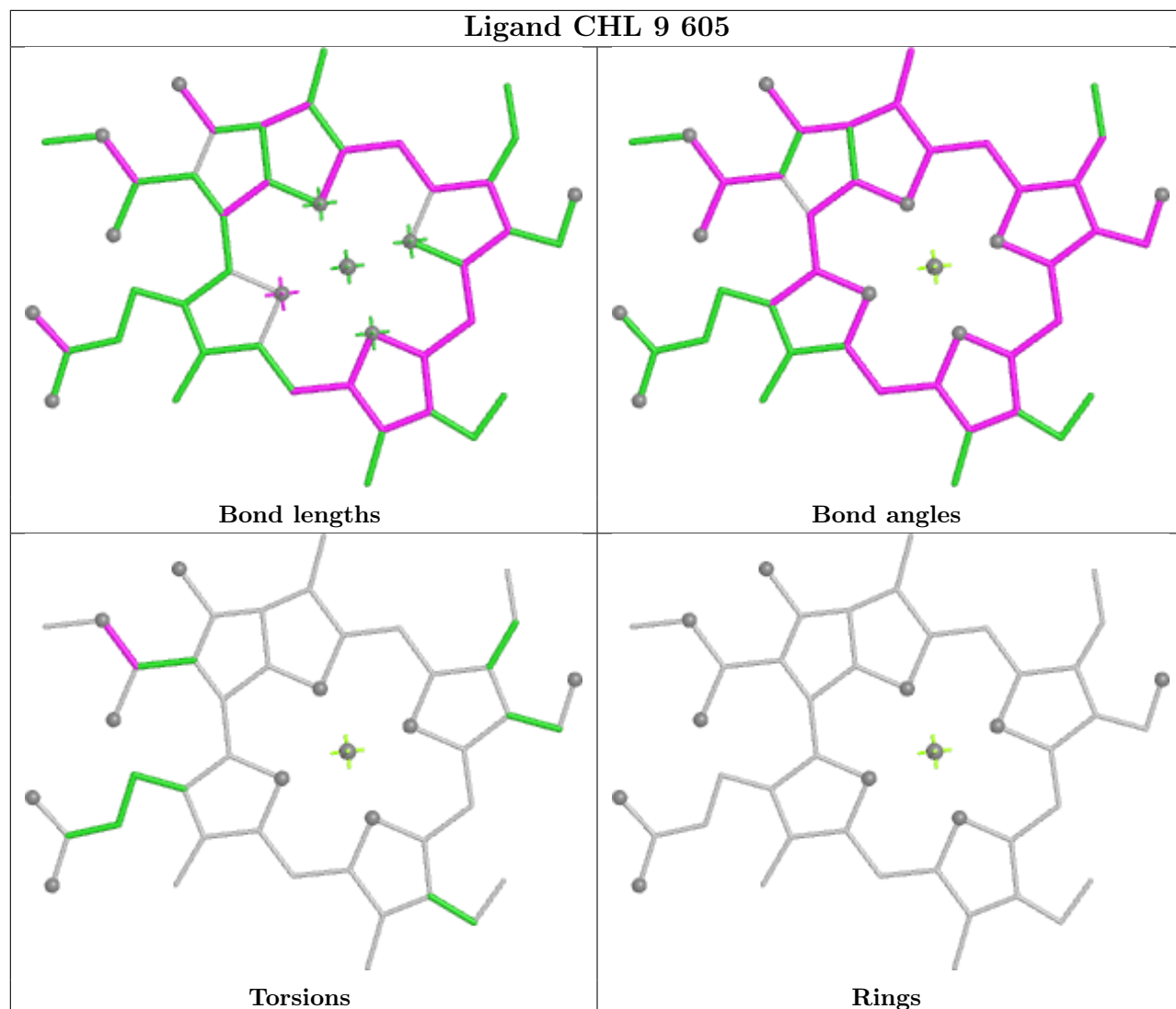
Rings

Ligand CLA c 614

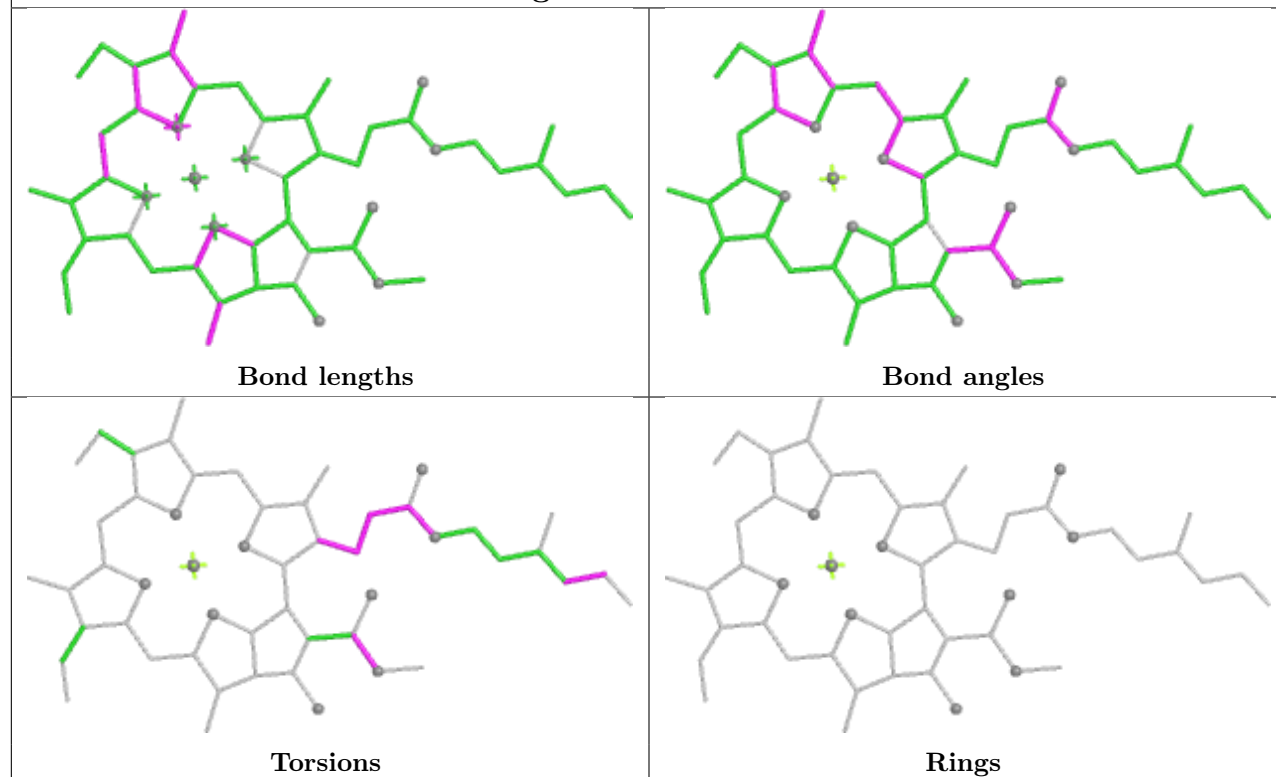




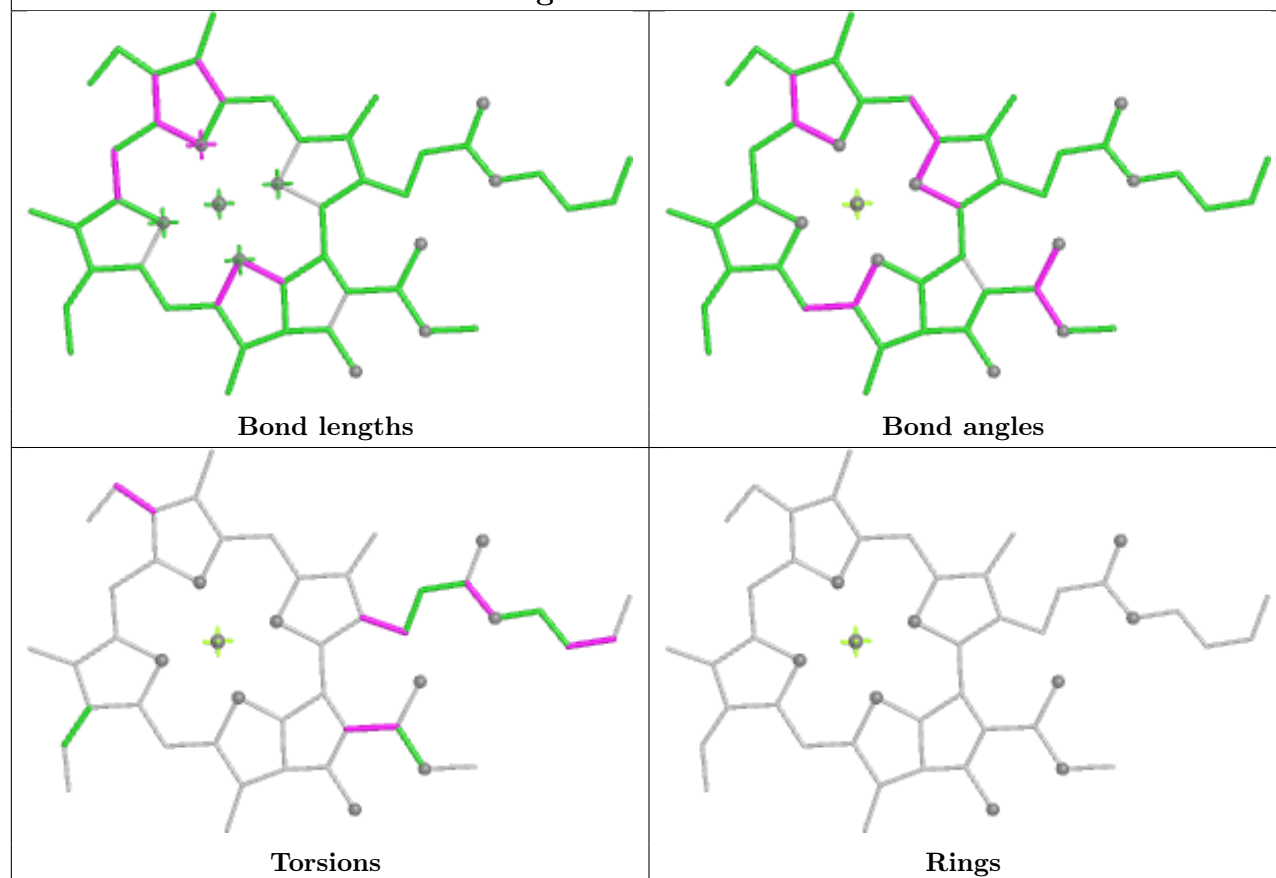
Ligand CHL 9 605

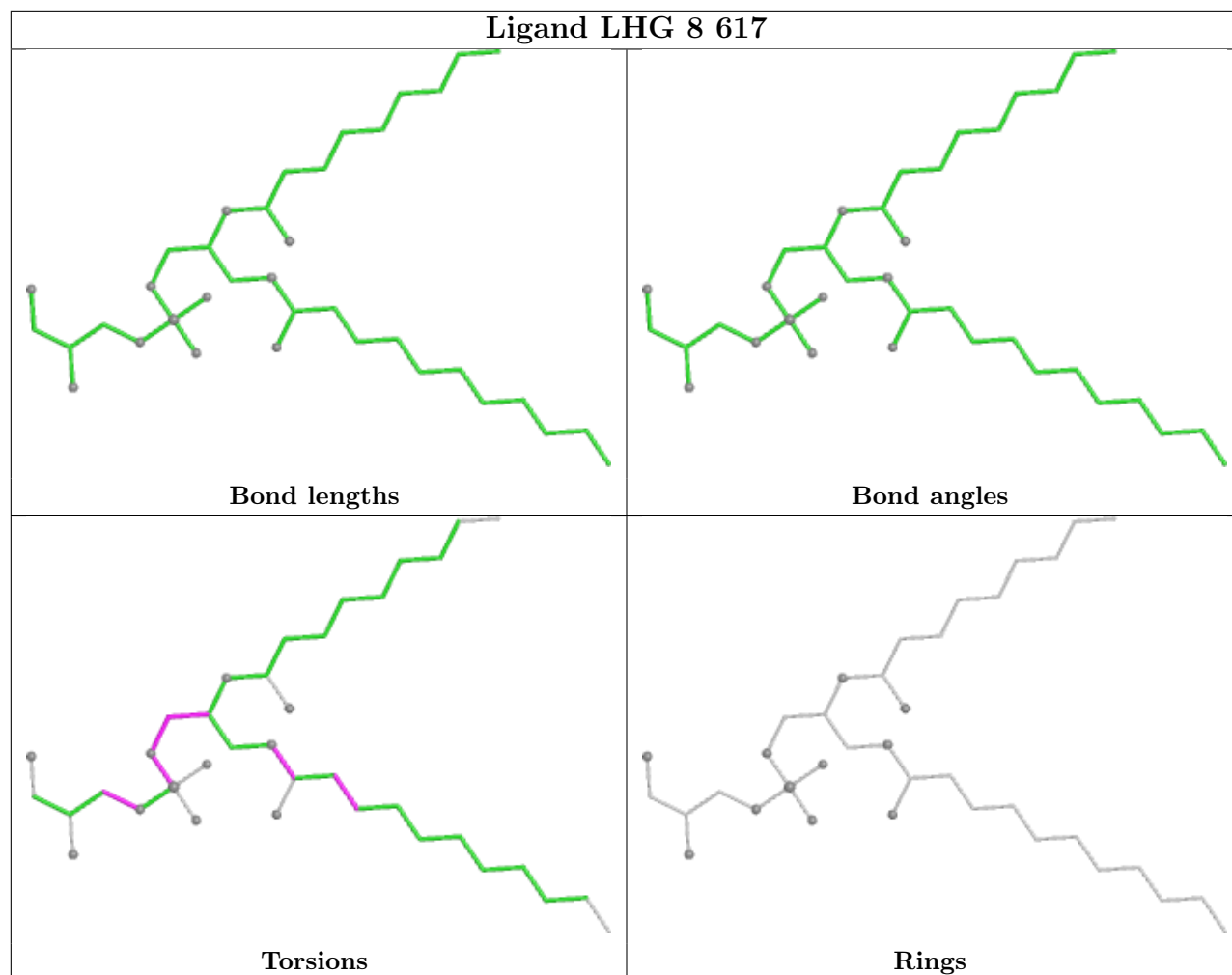


Ligand CLA B 826

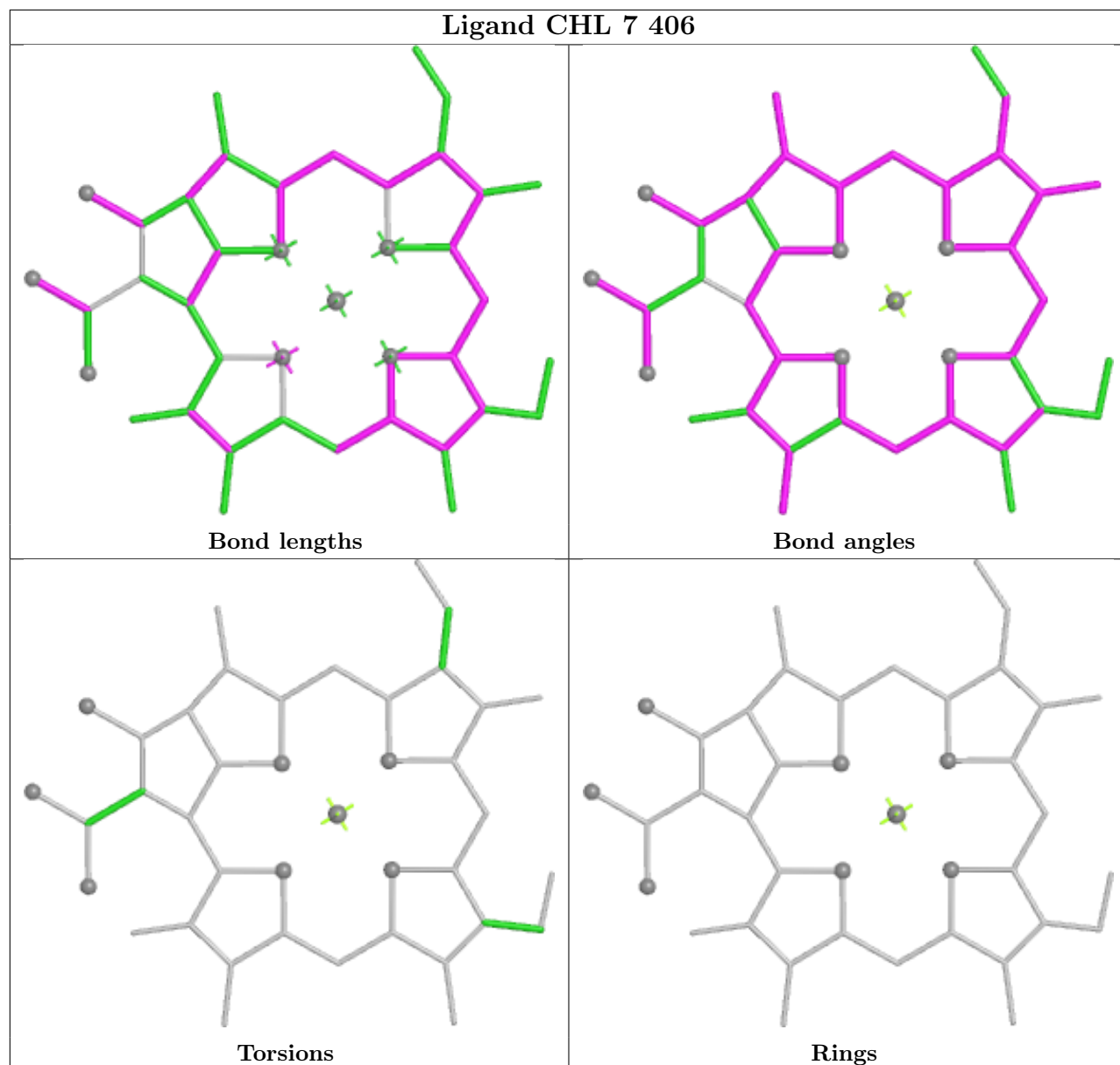


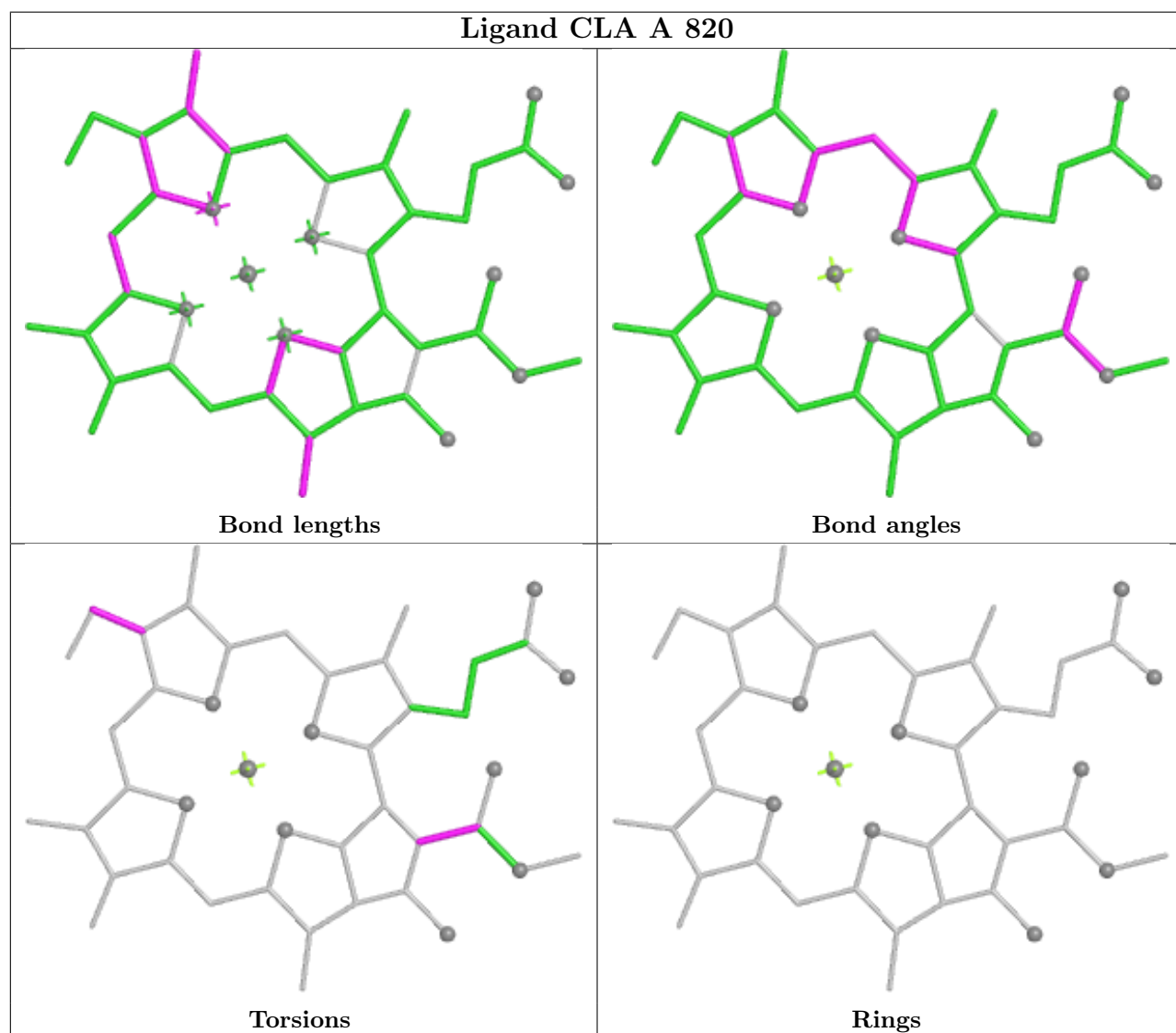
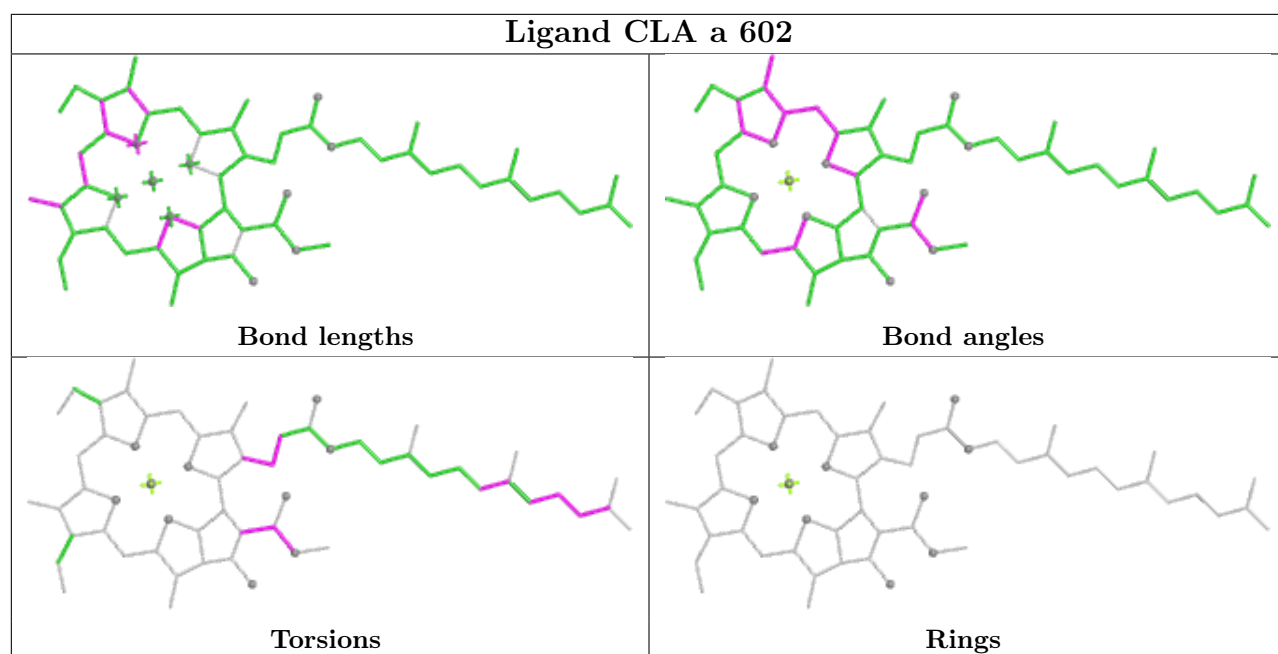
Ligand CLA 5 604



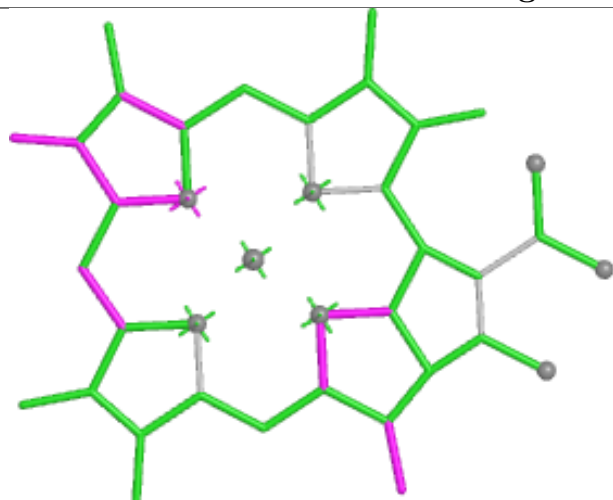


Ligand CHL 7 406

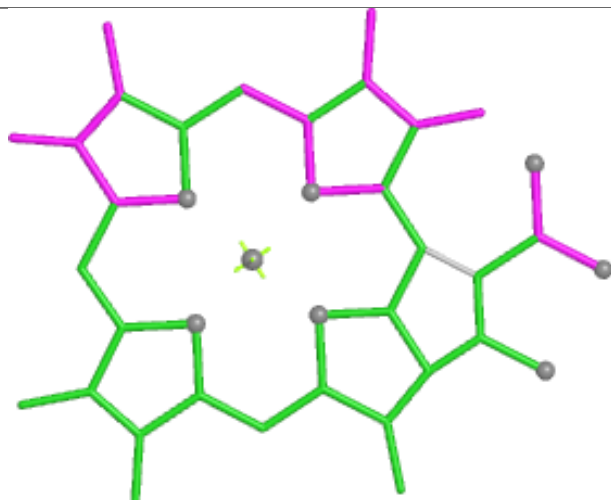




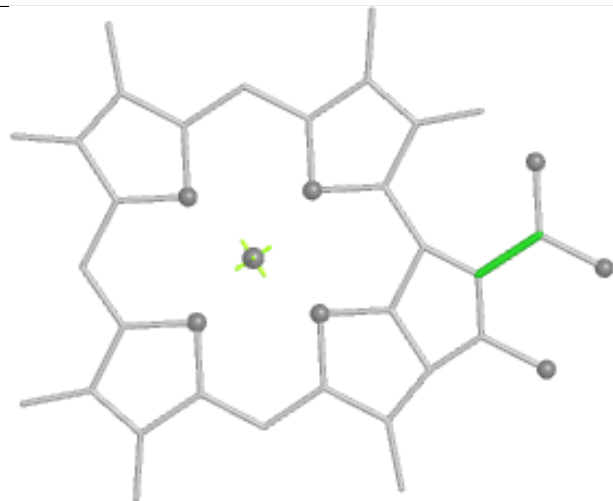
Ligand CLA 1 311



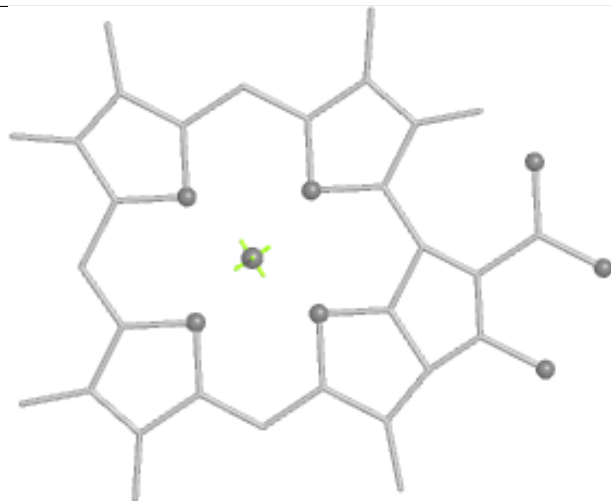
Bond lengths



Bond angles

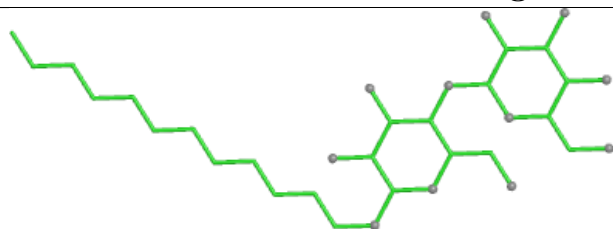


Torsions

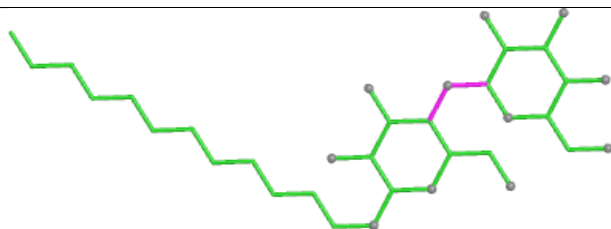


Rings

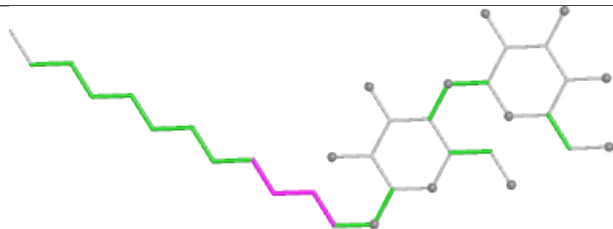
Ligand LMU A 856



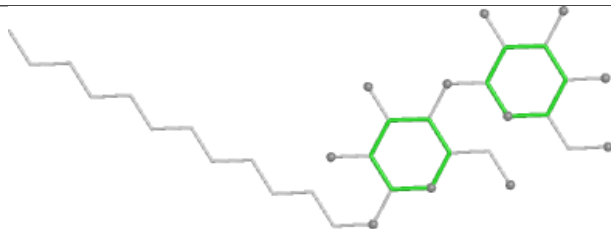
Bond lengths



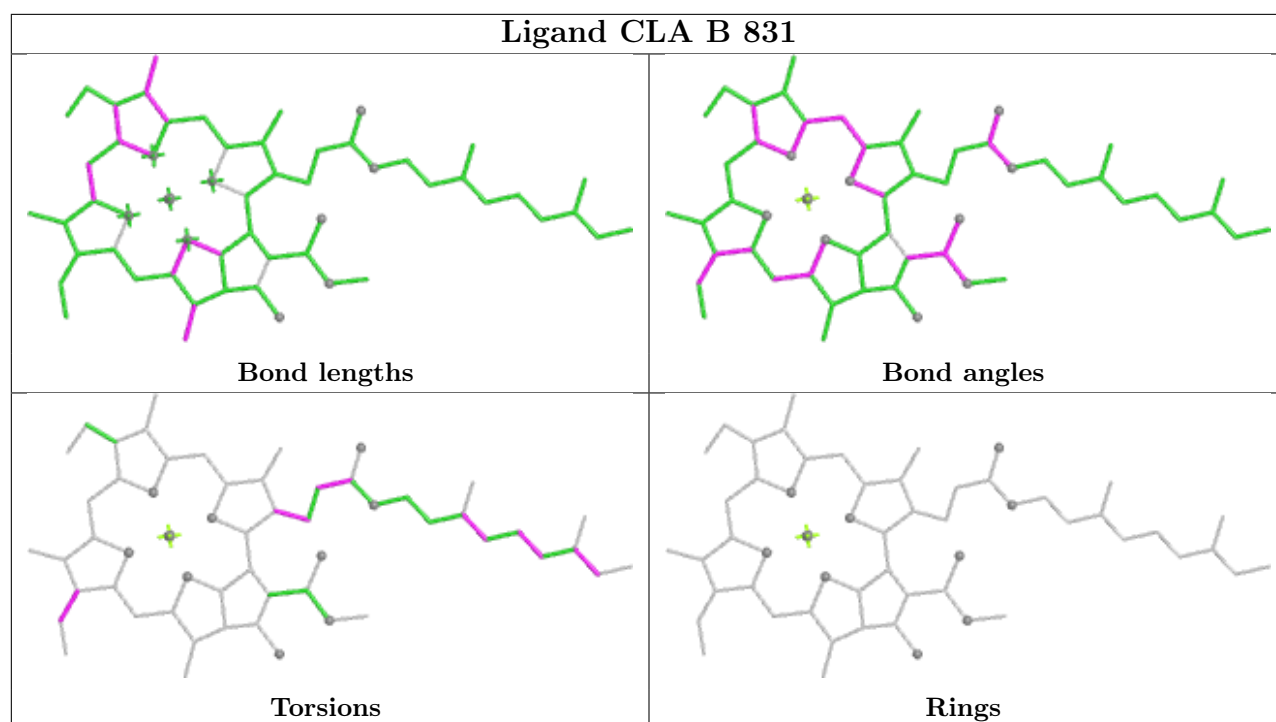
Bond angles



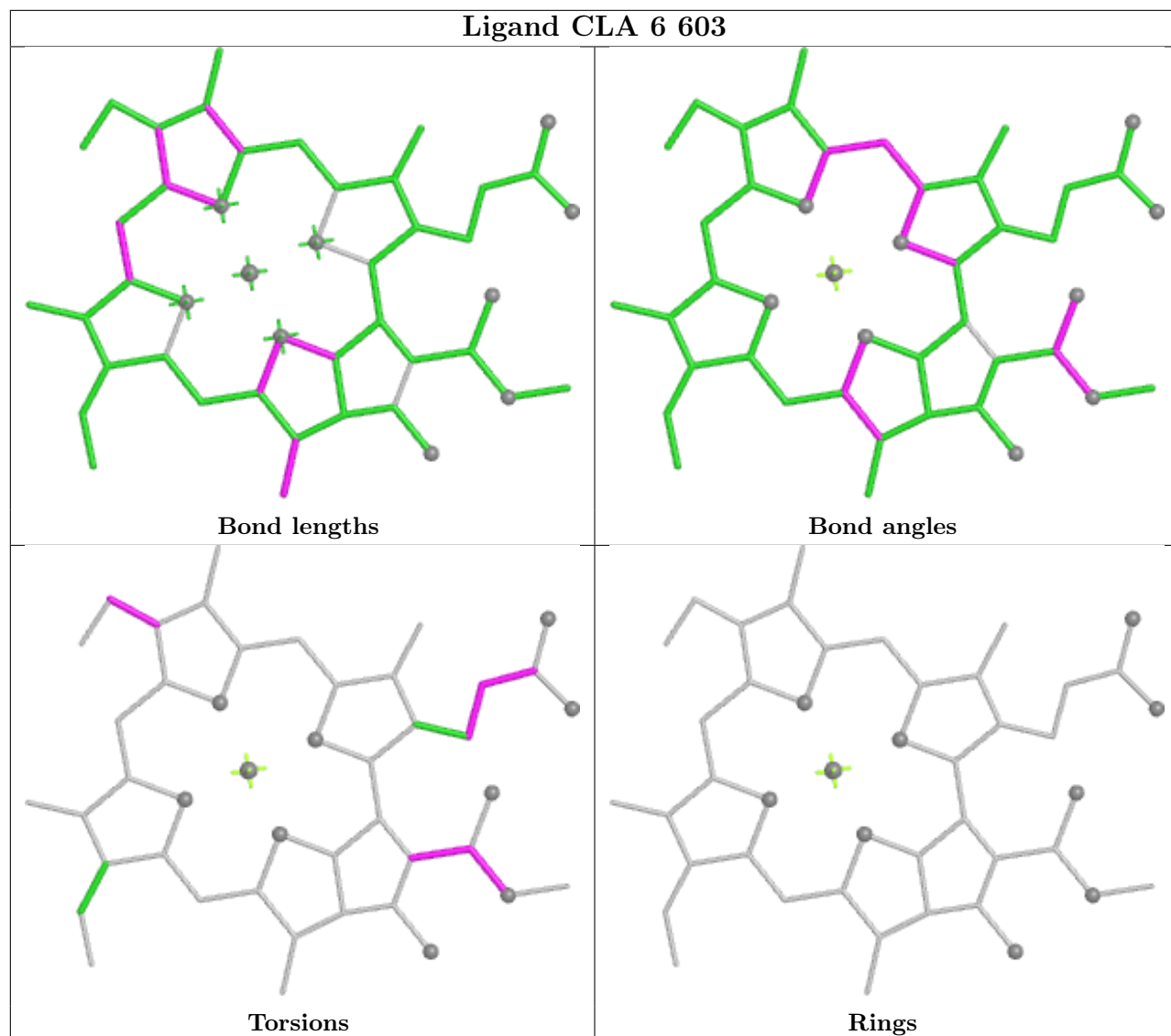
Torsions

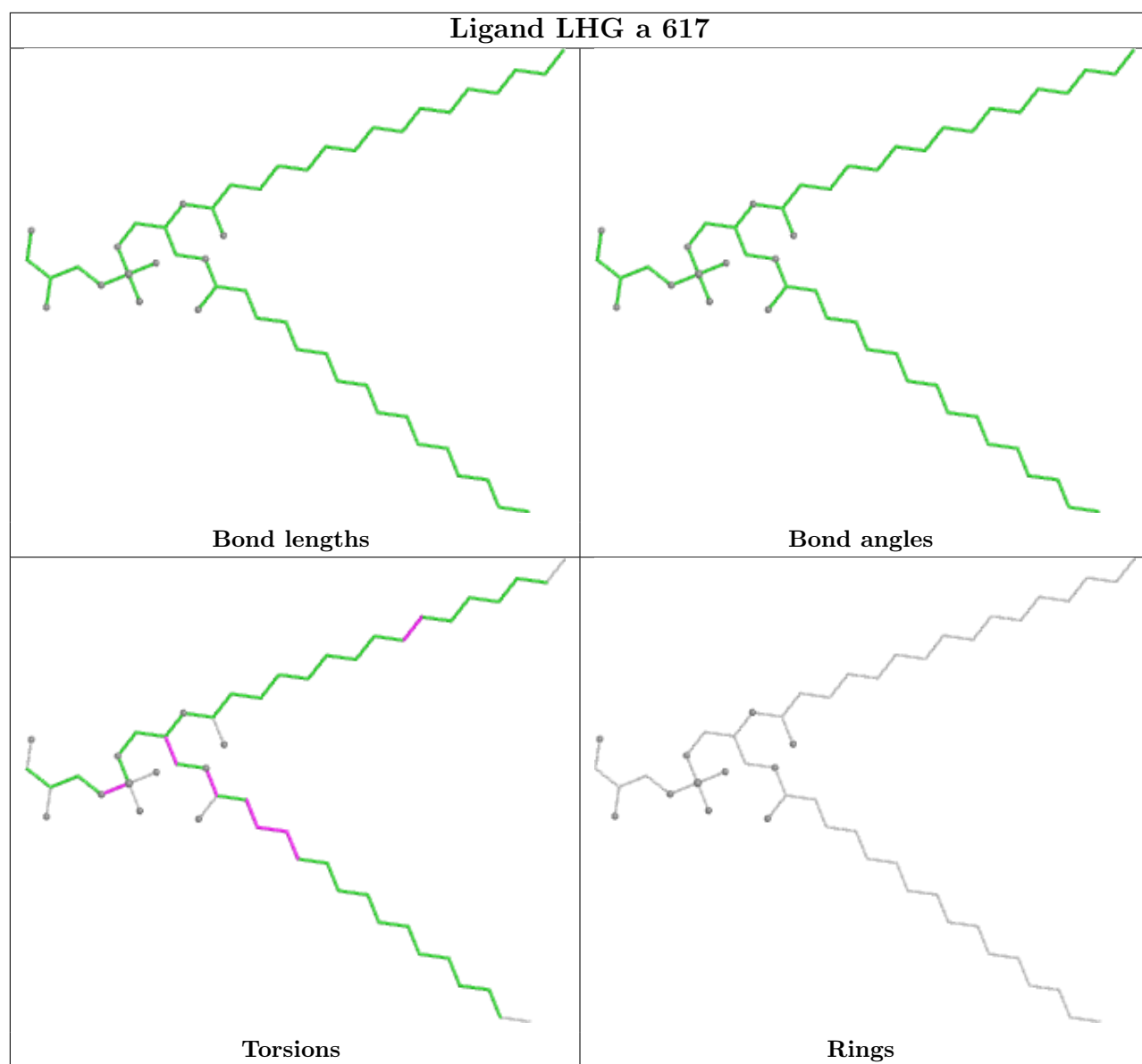


Rings

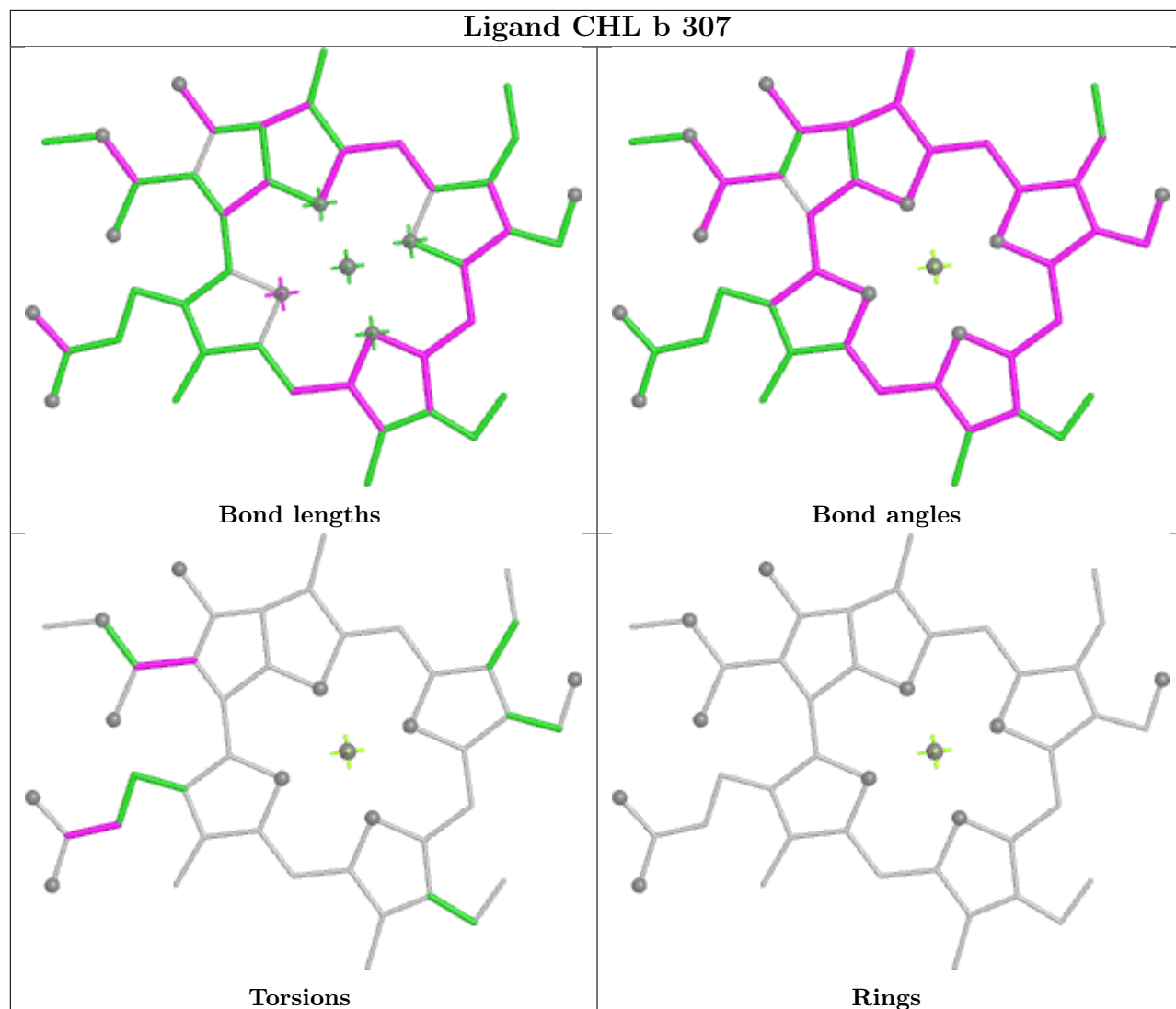


Ligand CLA 6 603

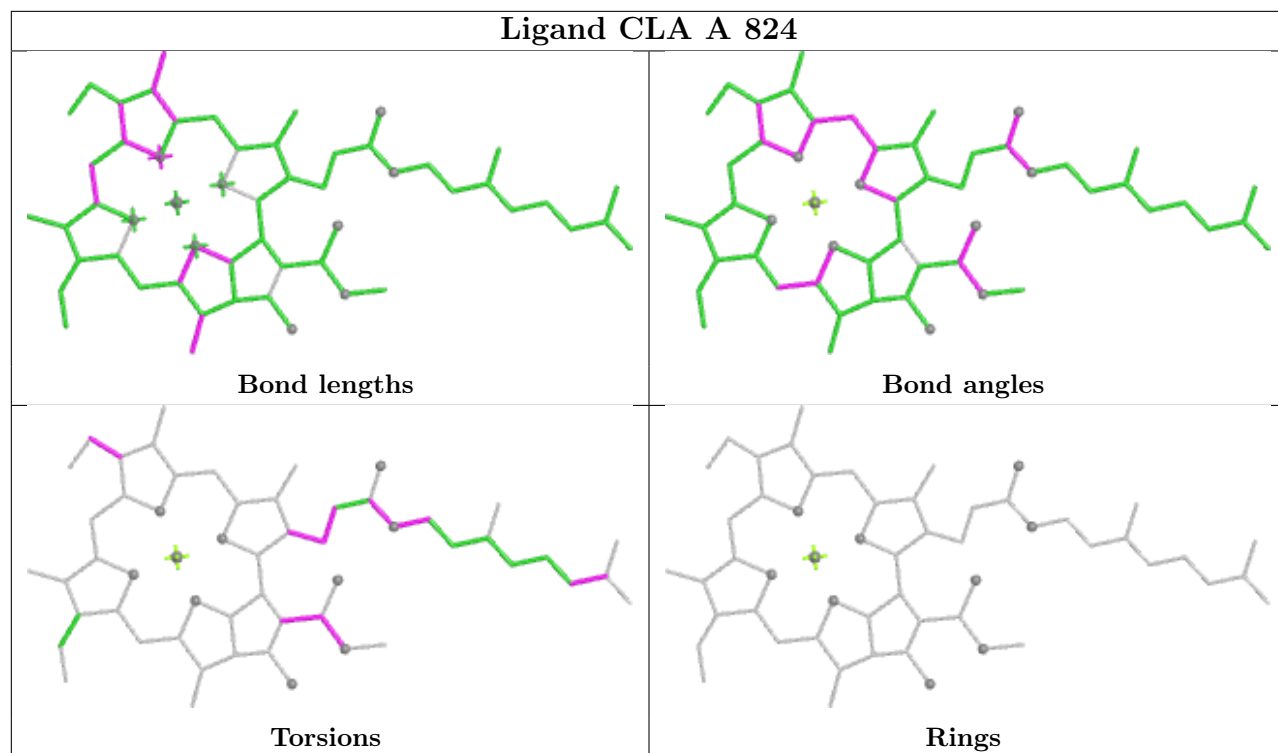




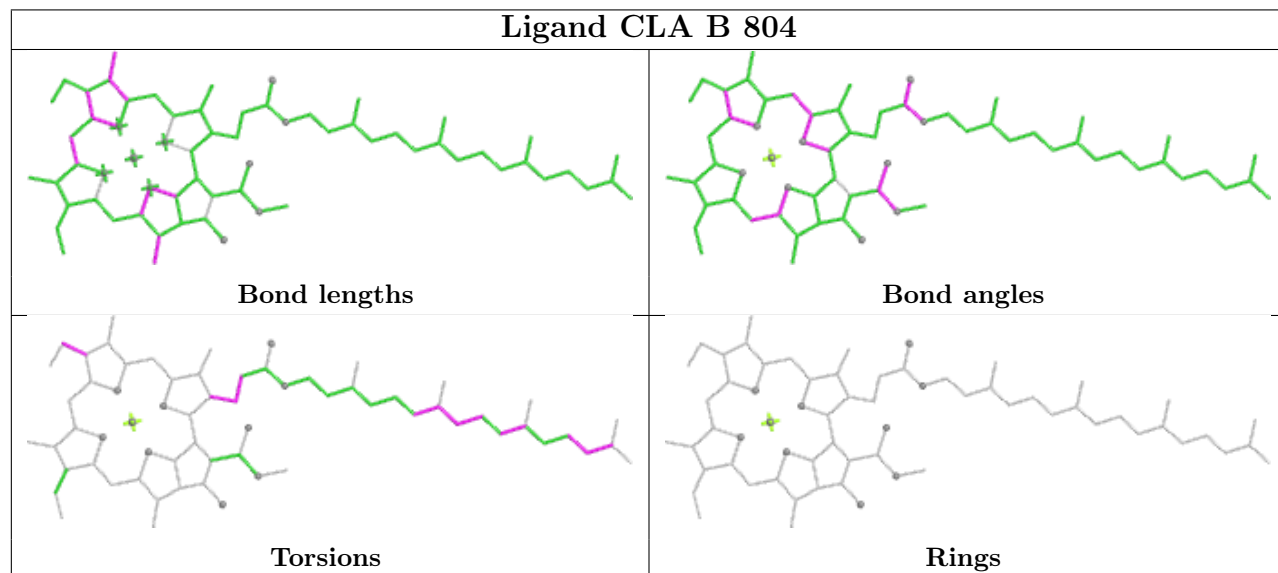
Ligand CHL b 307

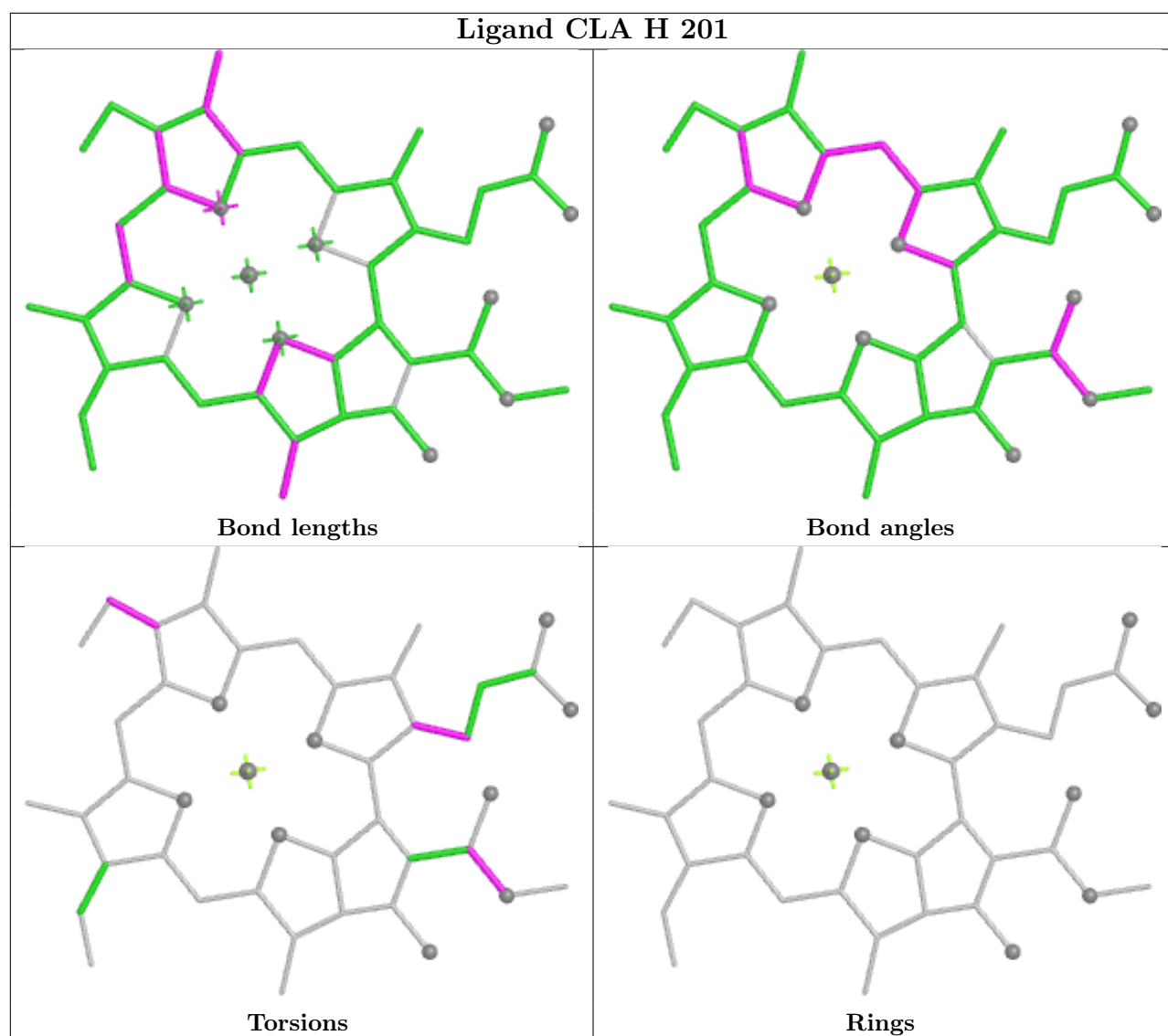


Ligand CLA A 824

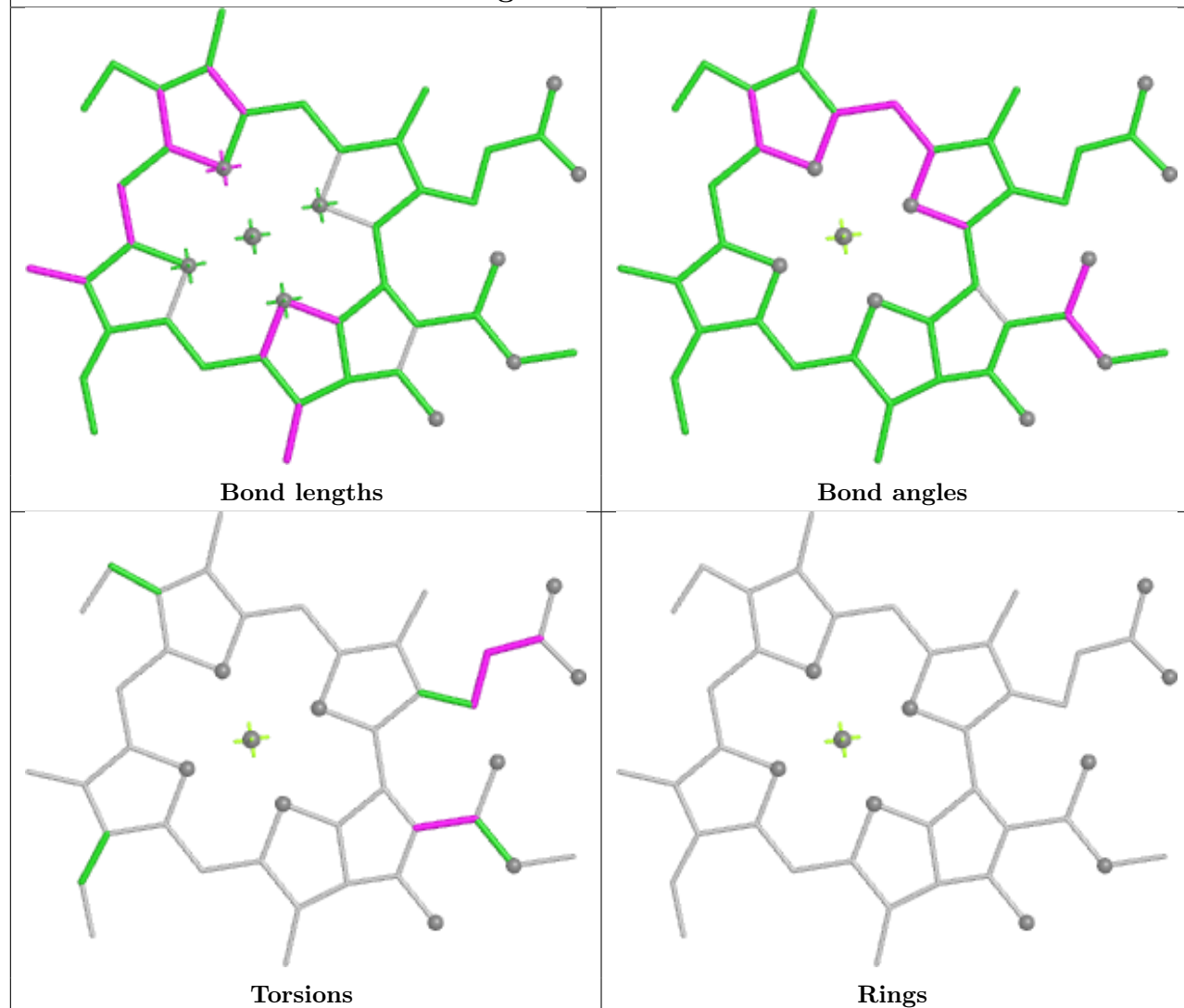


Ligand CLA B 804

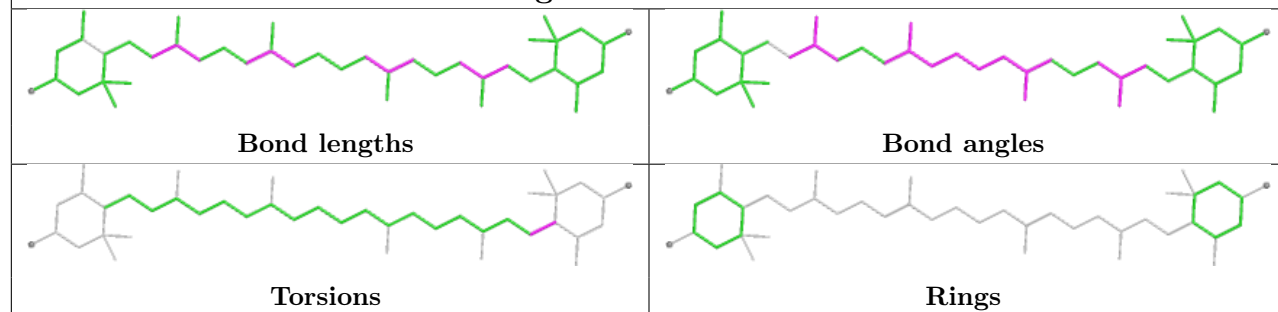


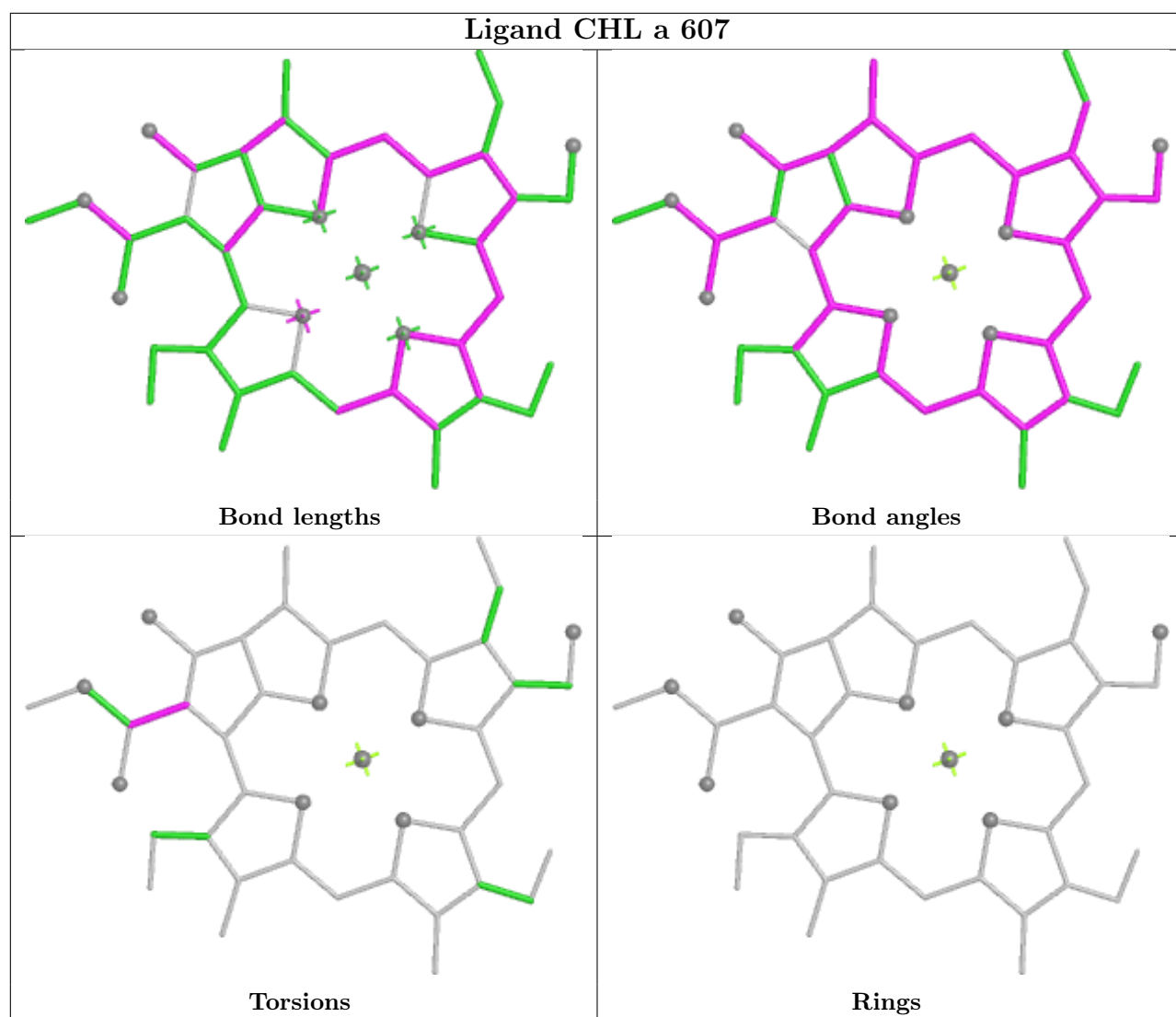


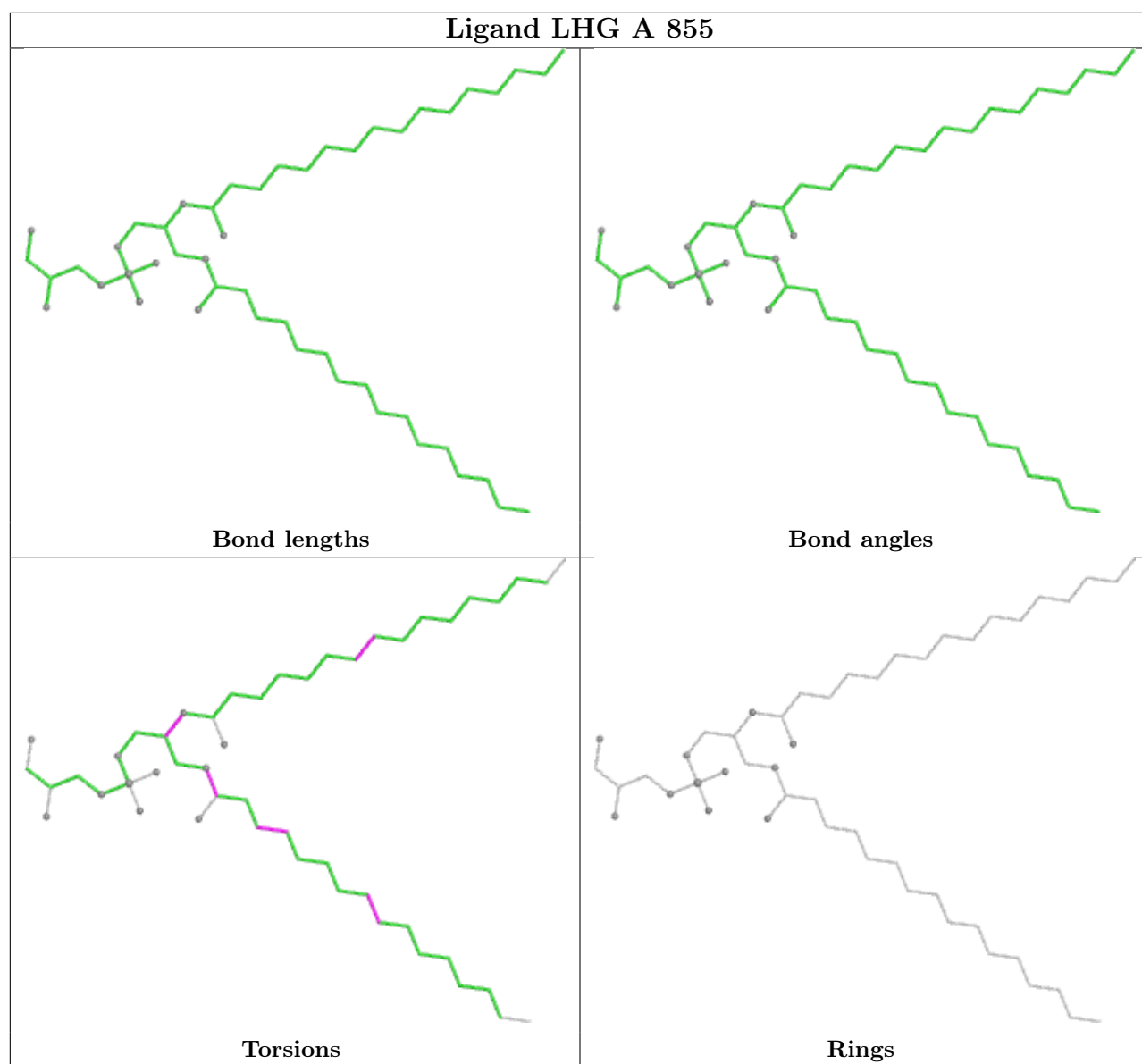
Ligand CLA c 604



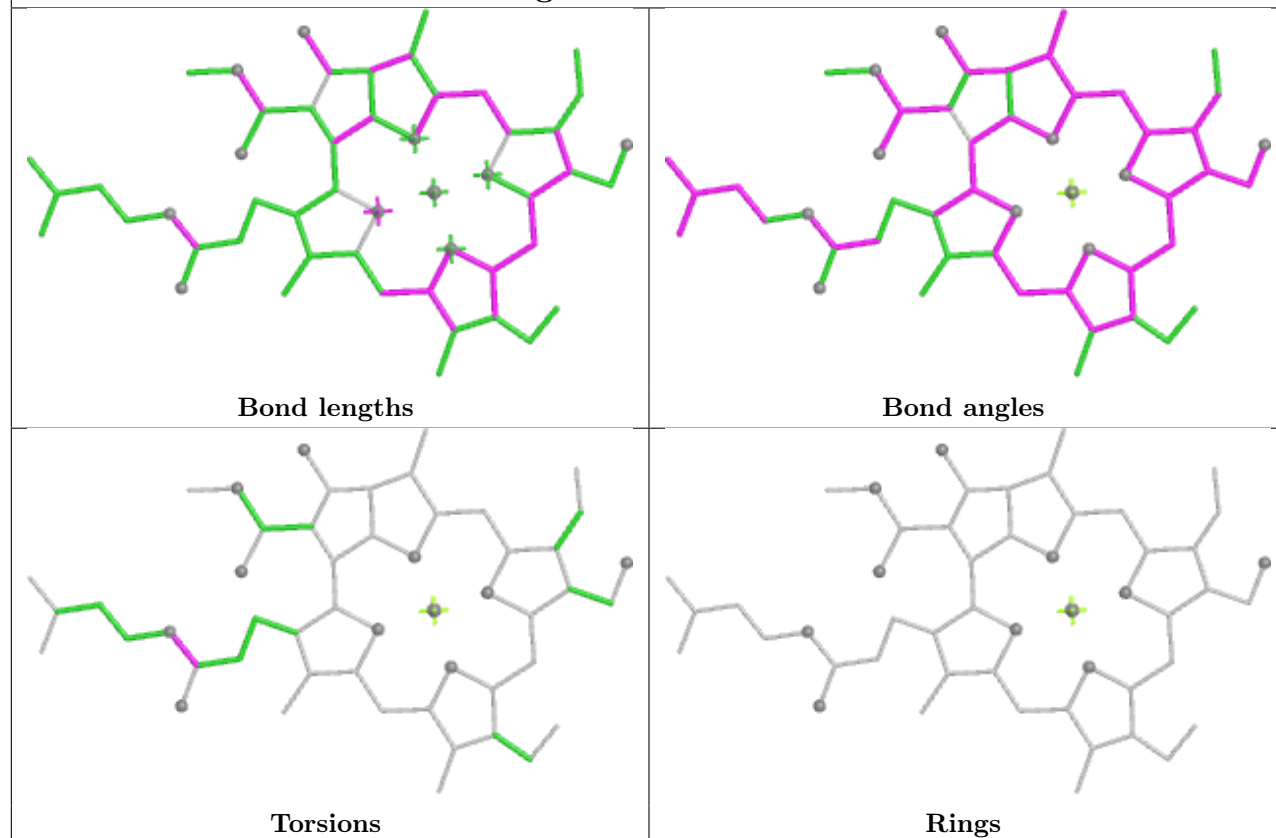
Ligand LUT b 317



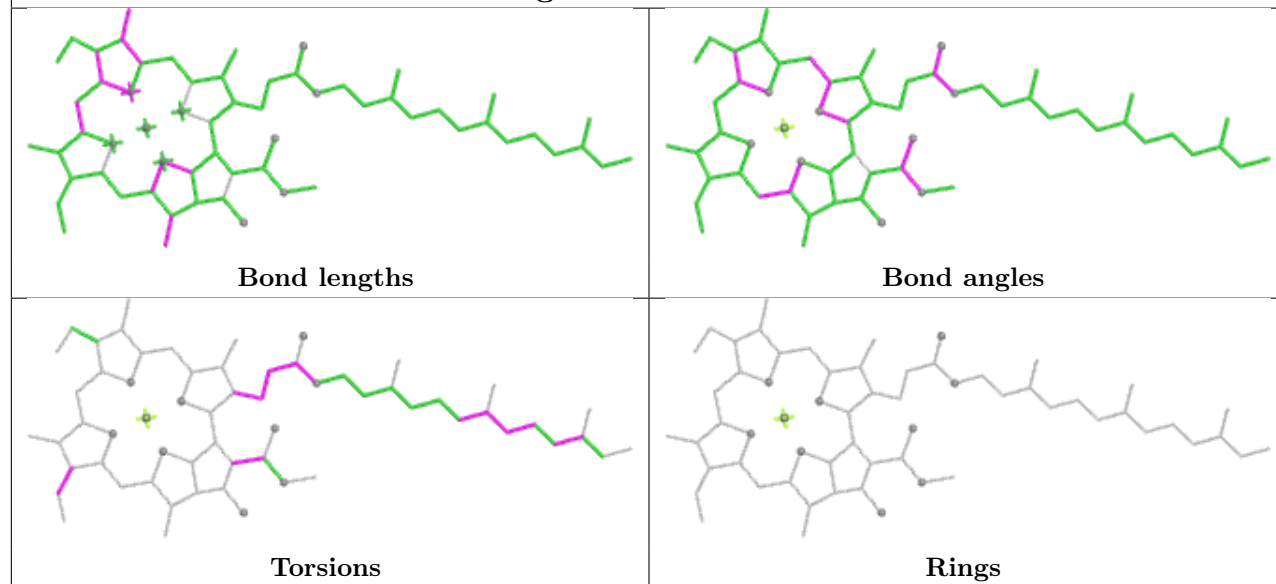




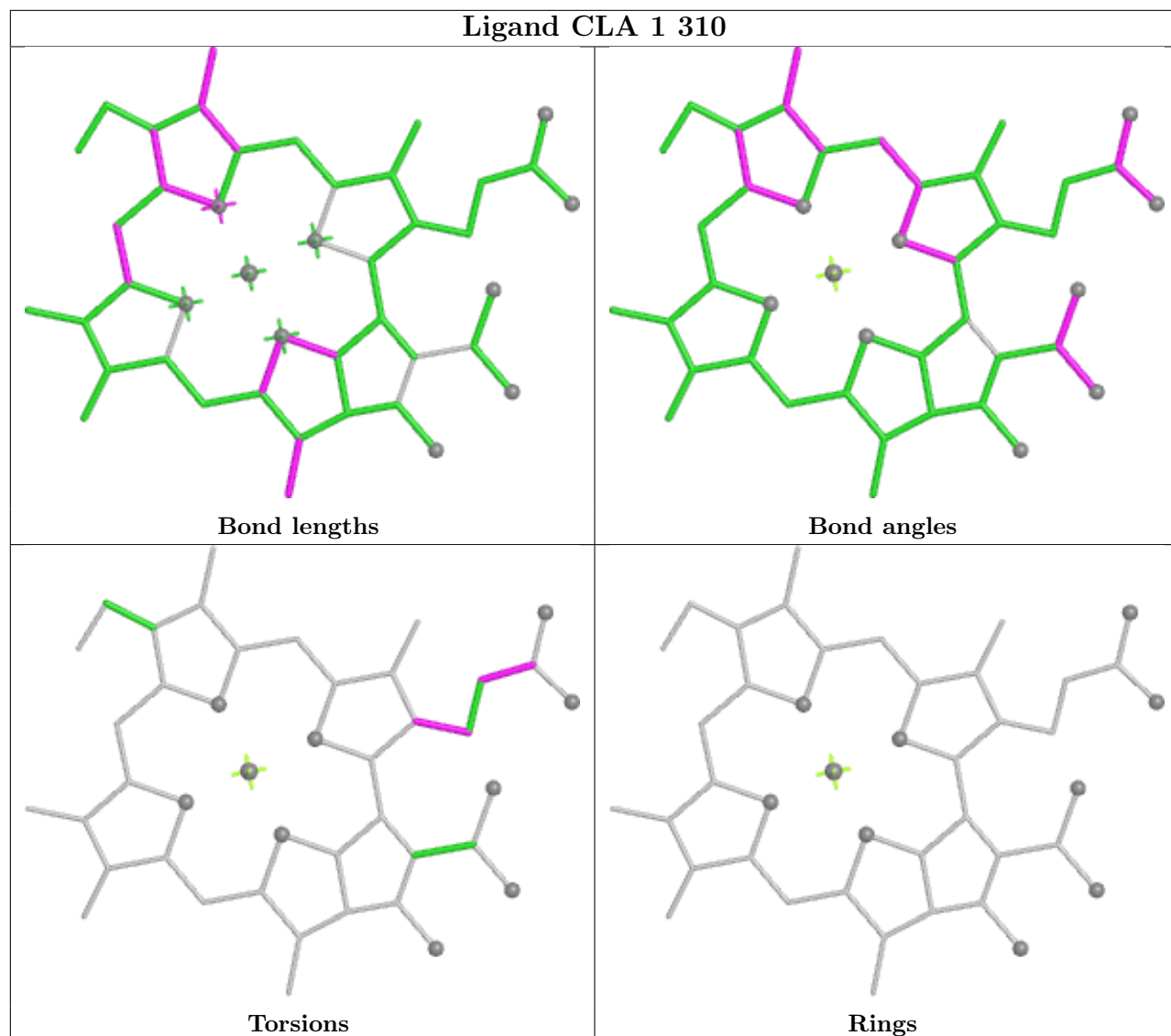
Ligand CHL 1 307



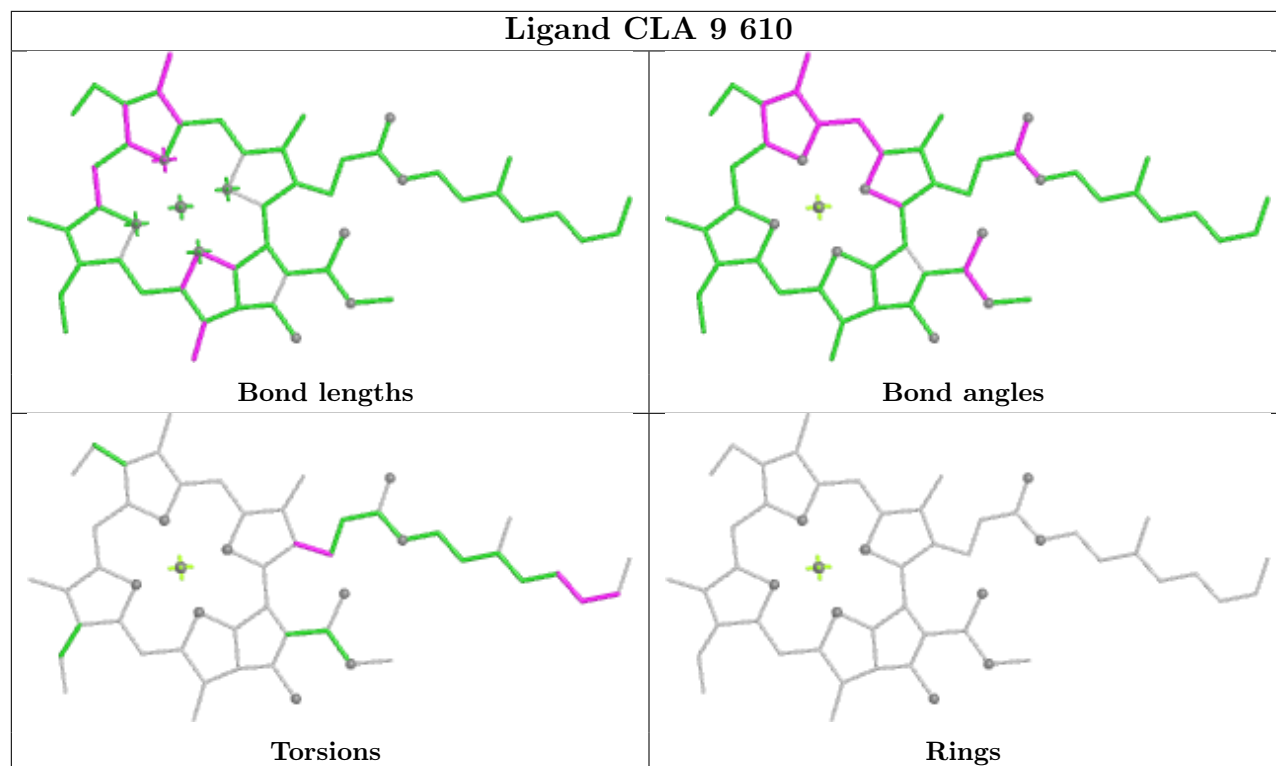
Ligand CLA 1 303



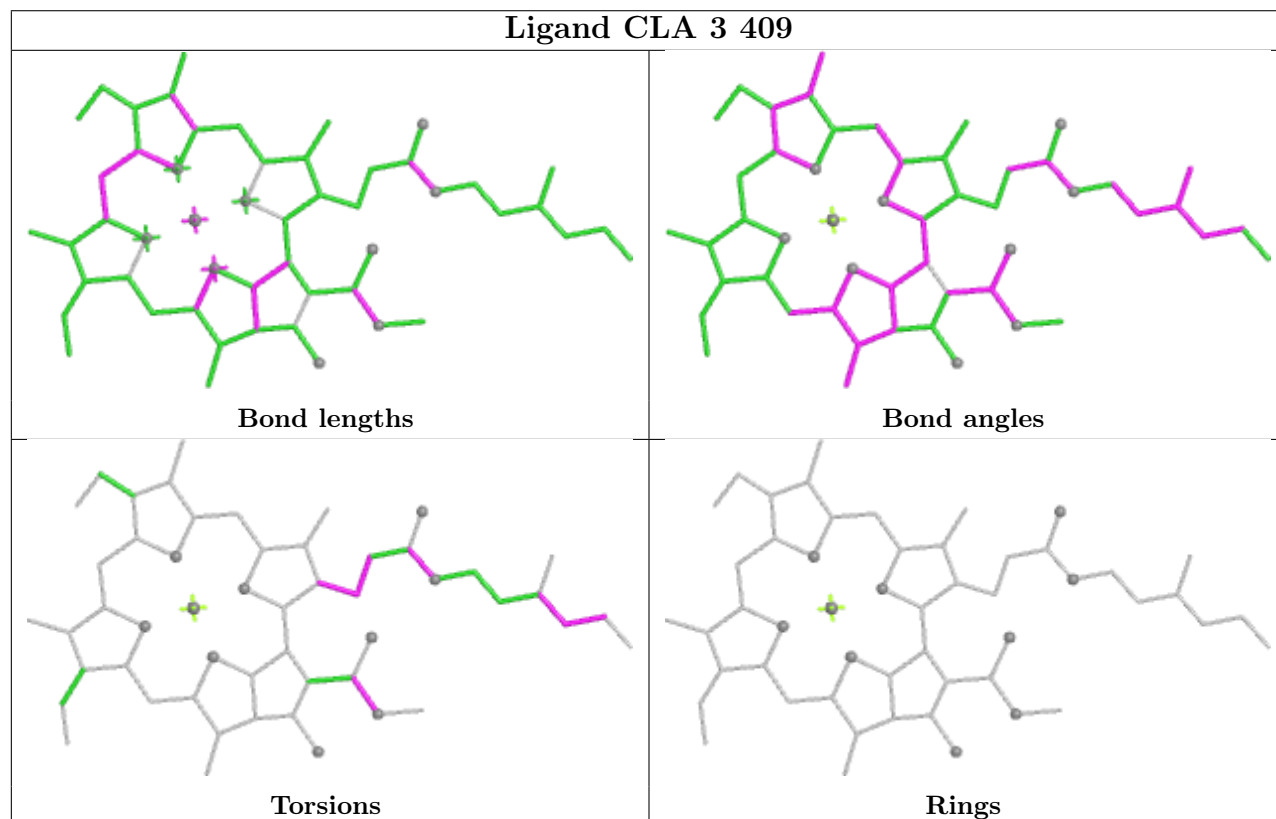
Ligand CLA 1 310



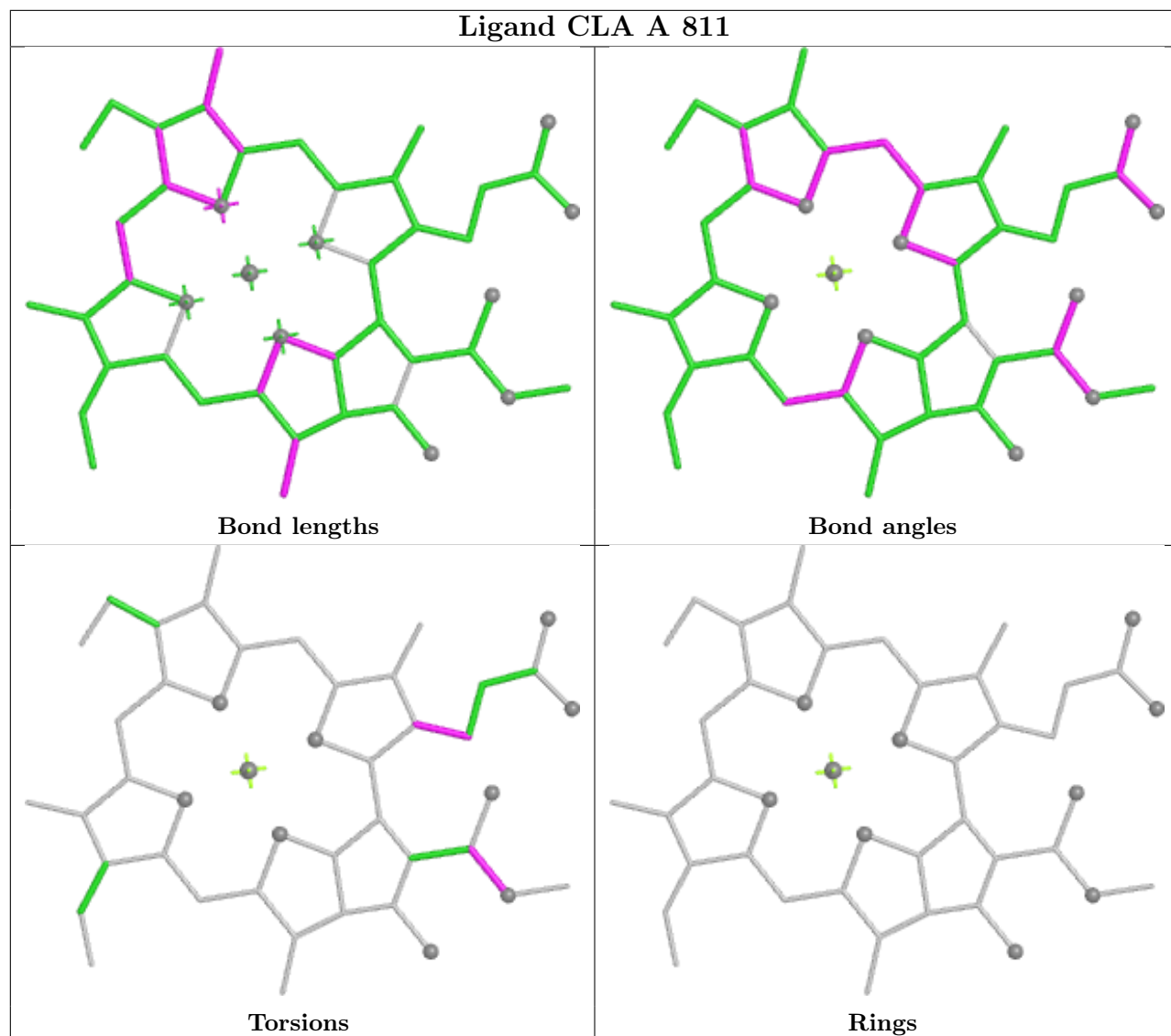
Ligand CLA 9 610

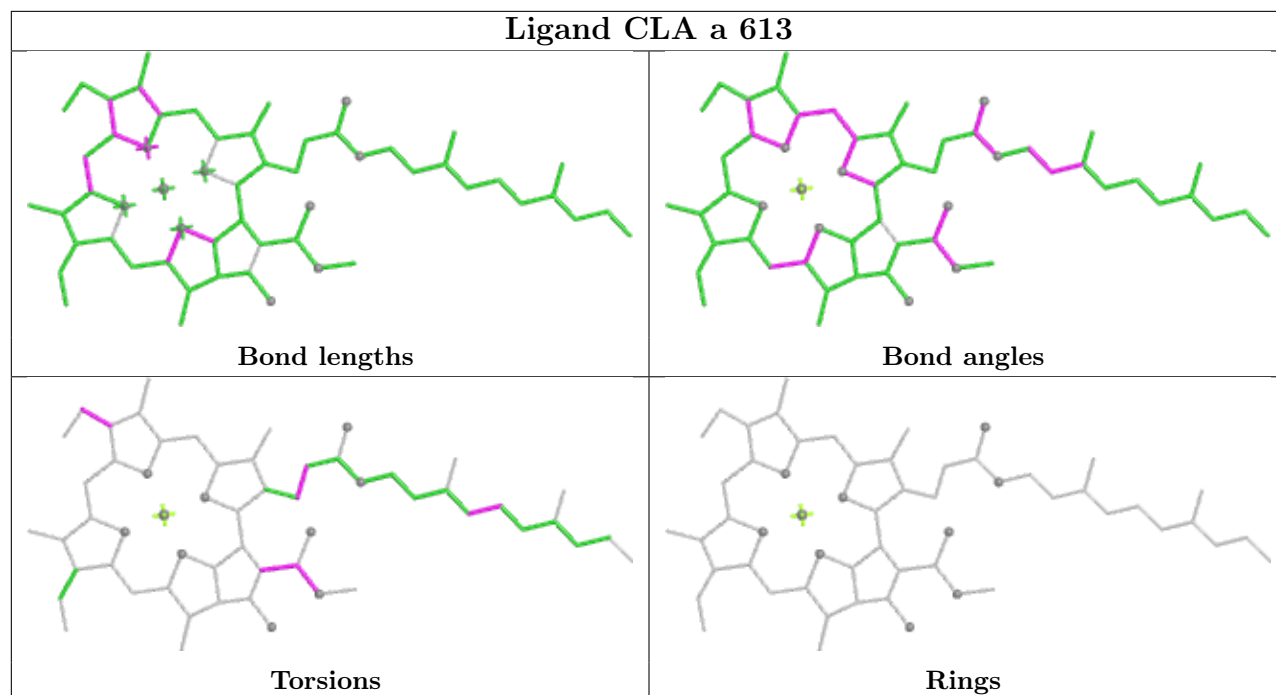
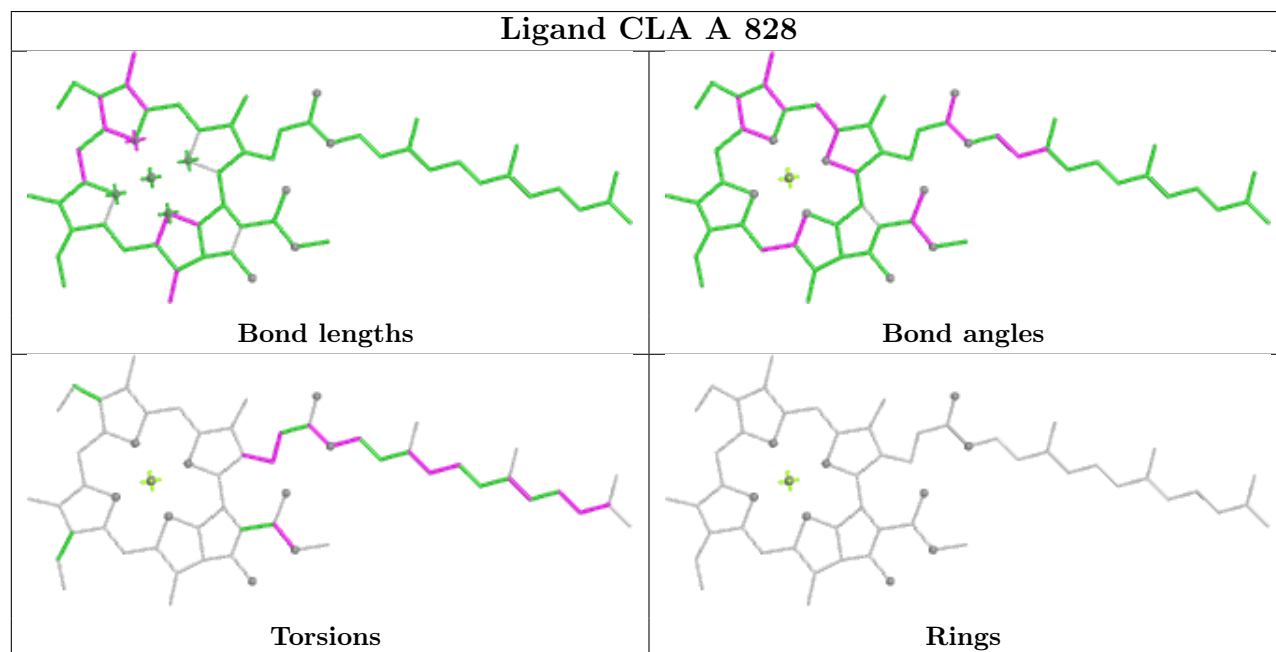


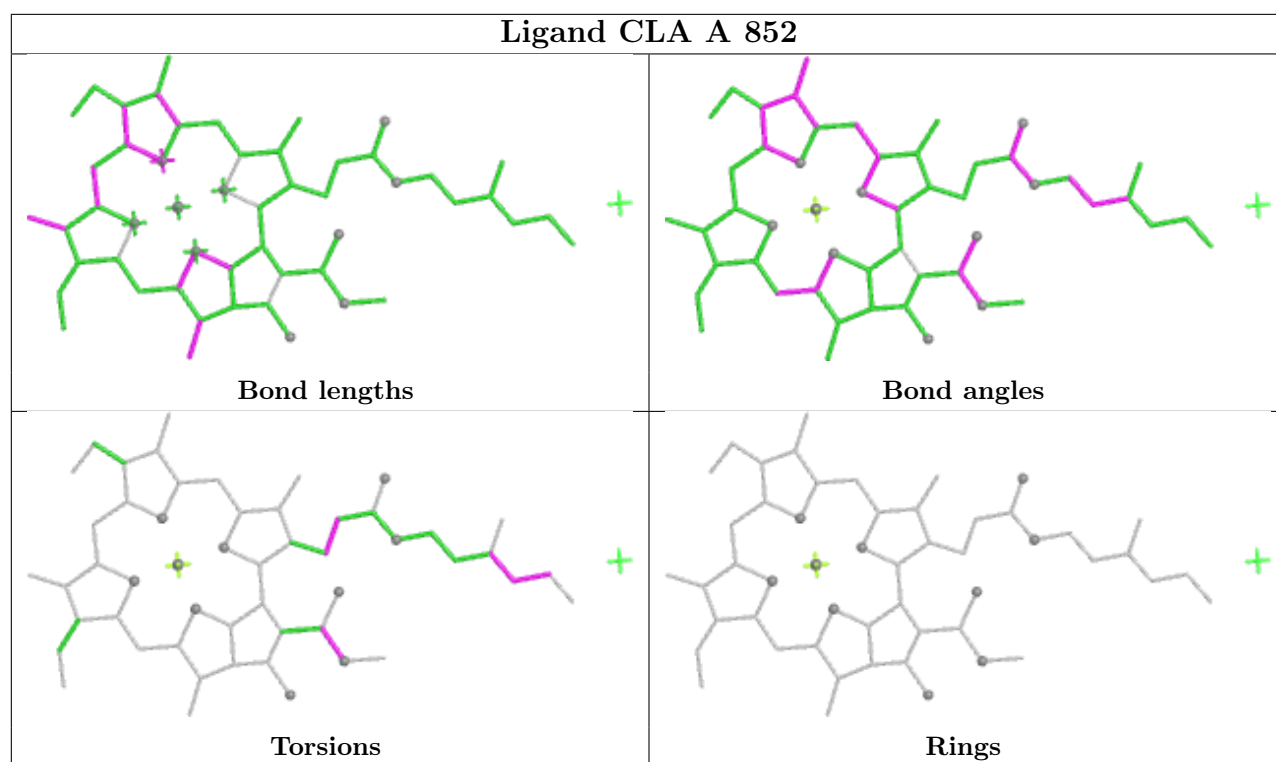
Ligand CLA 3 409



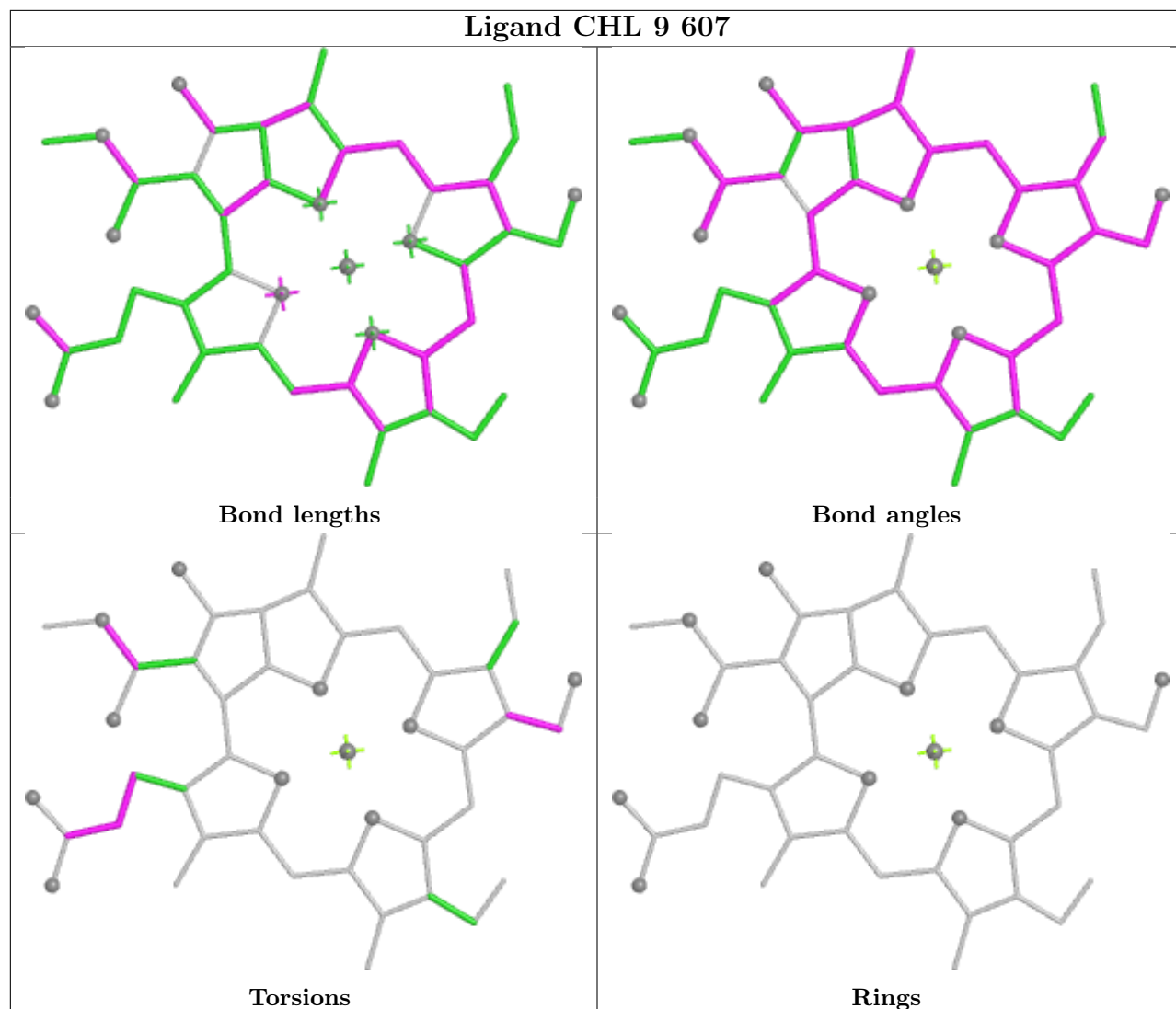
Ligand CLA A 811



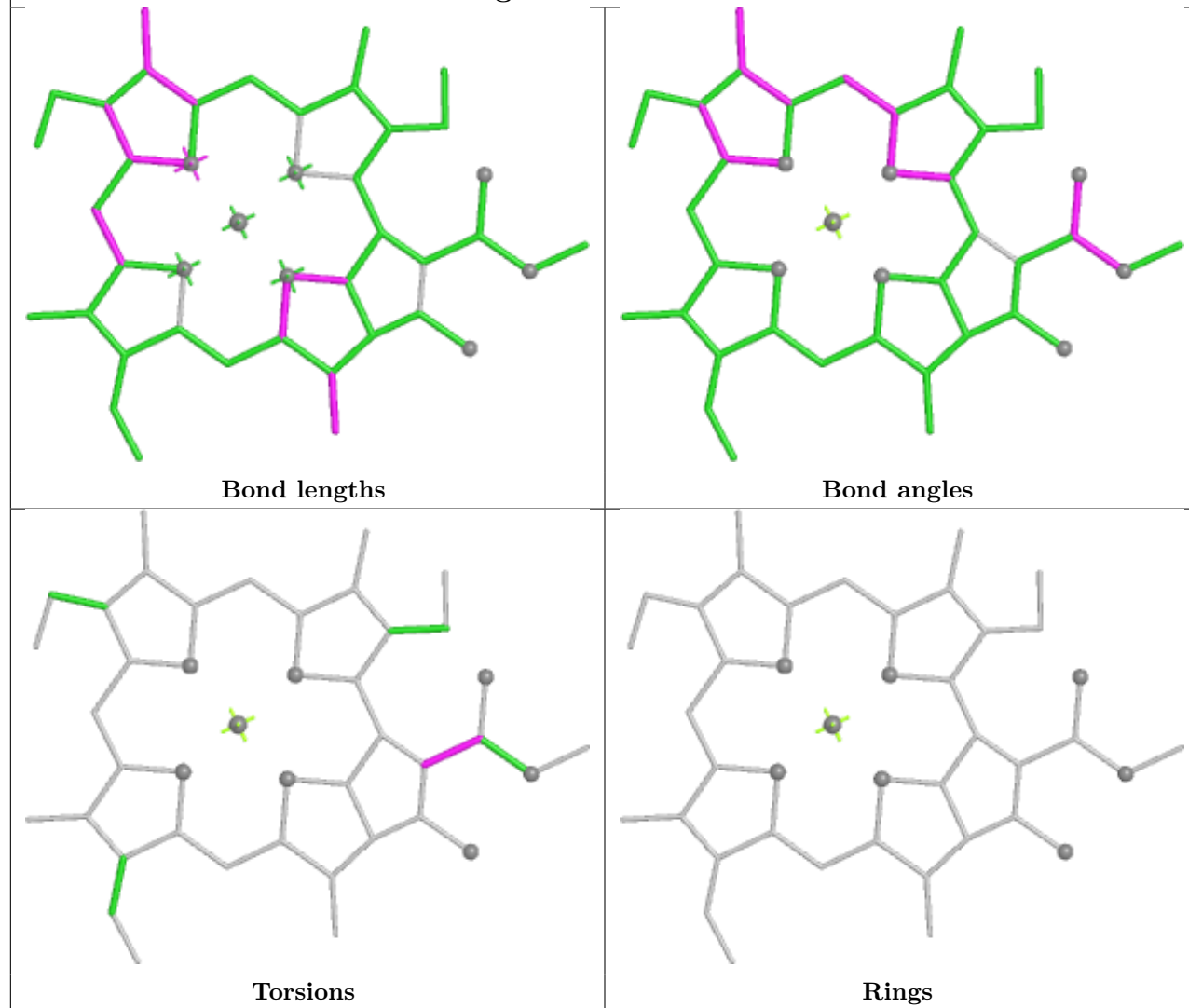
Ligand CLA a 613**Ligand CLA A 828**



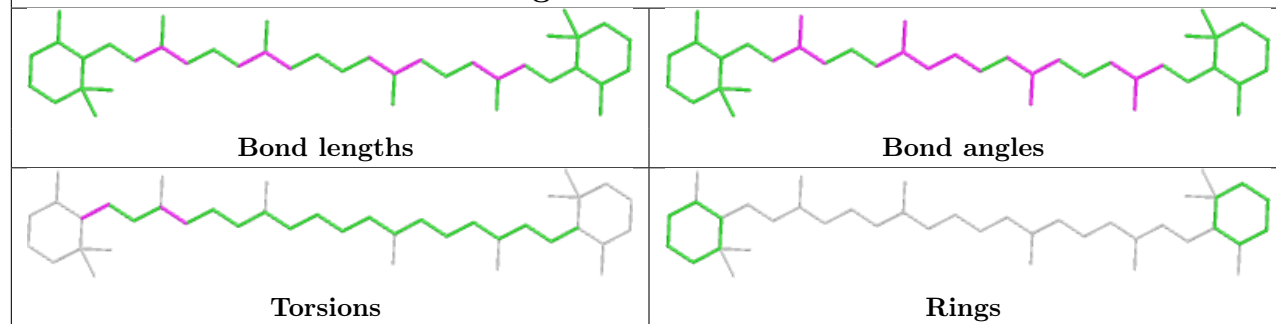
Ligand CHL 9 607



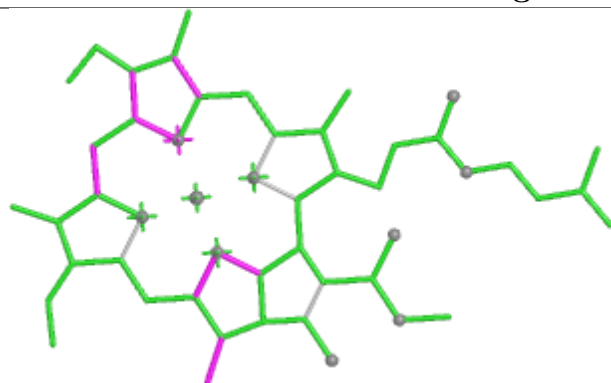
Ligand CLA O 201



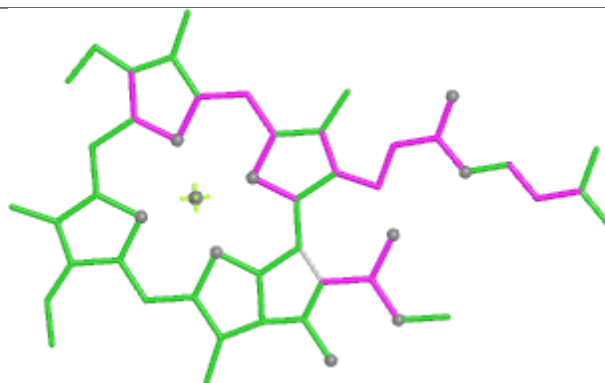
Ligand BCR L 301



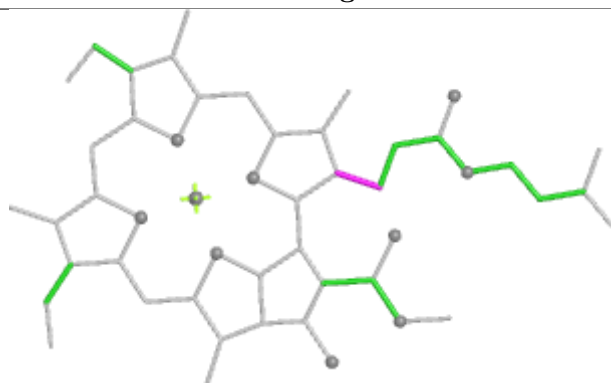
Ligand CLA K 202



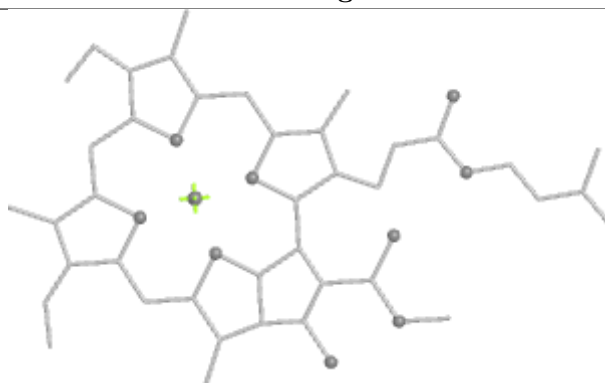
Bond lengths



Bond angles

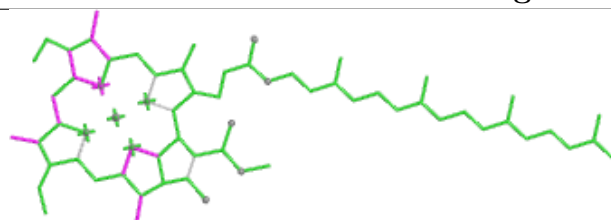


Torsions

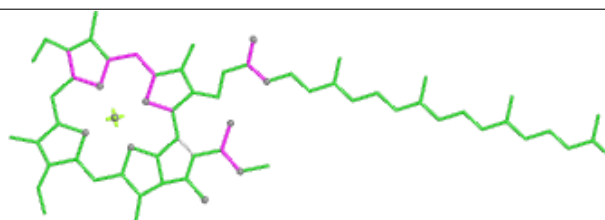


Rings

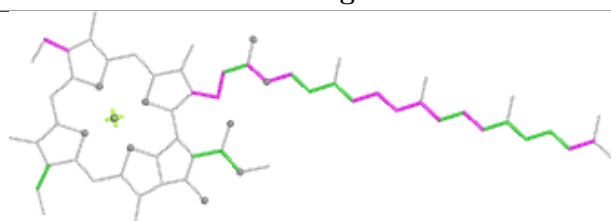
Ligand CLA A 842



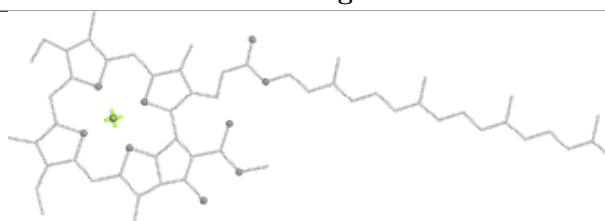
Bond lengths



Bond angles

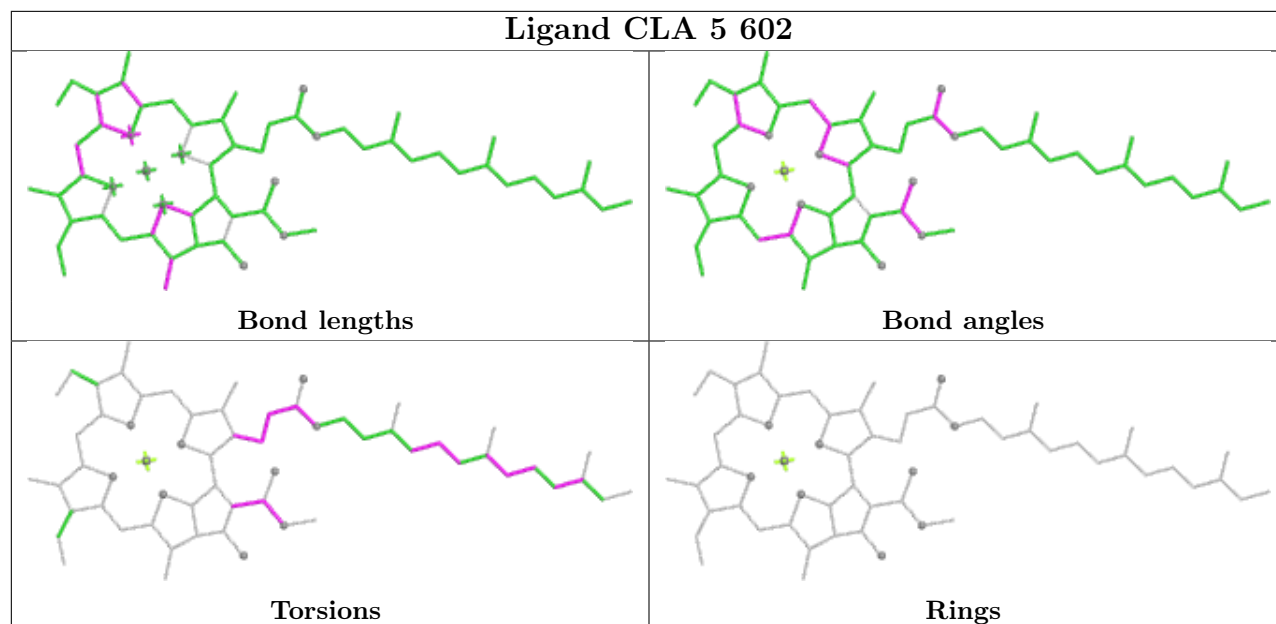


Torsions

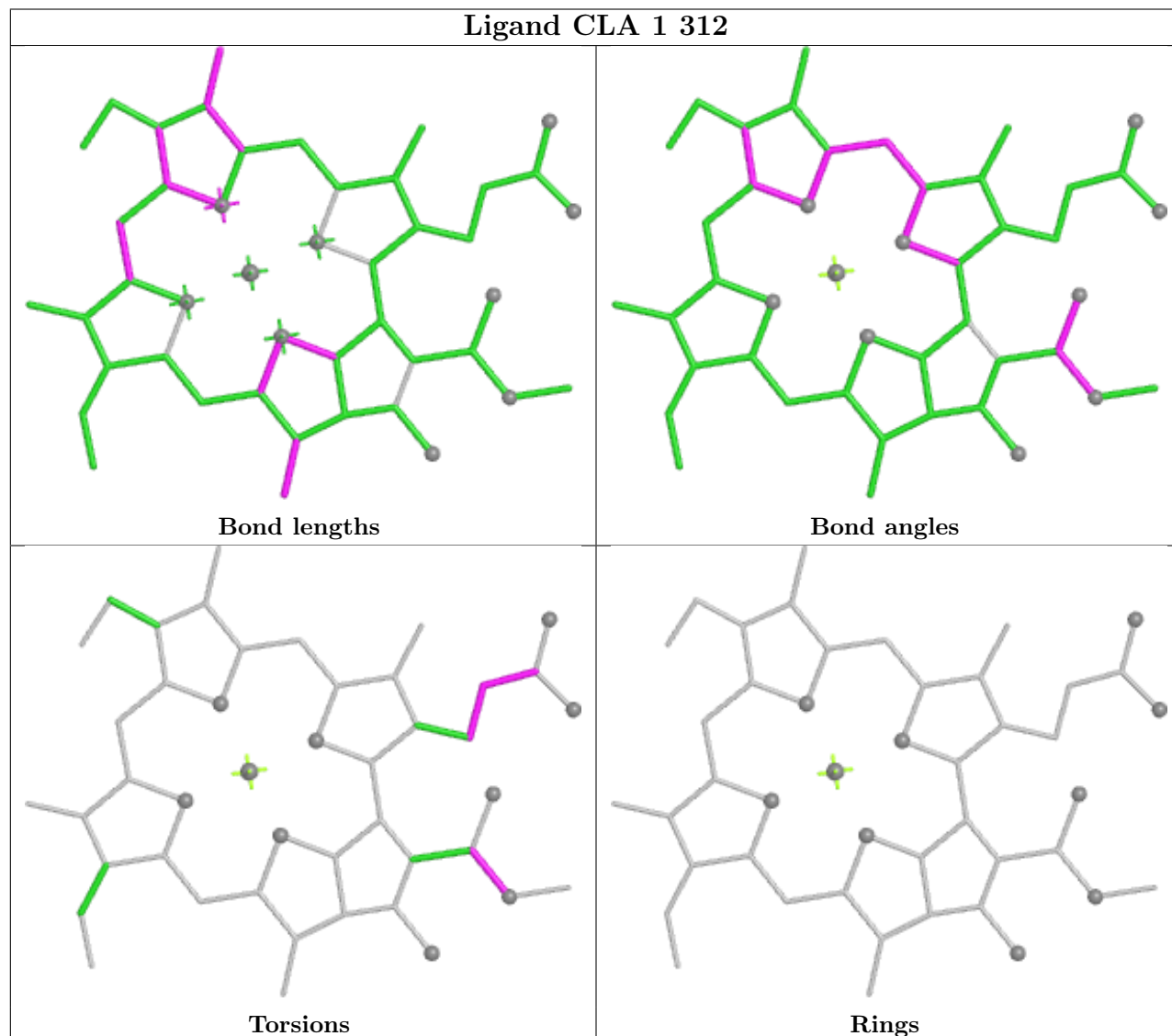


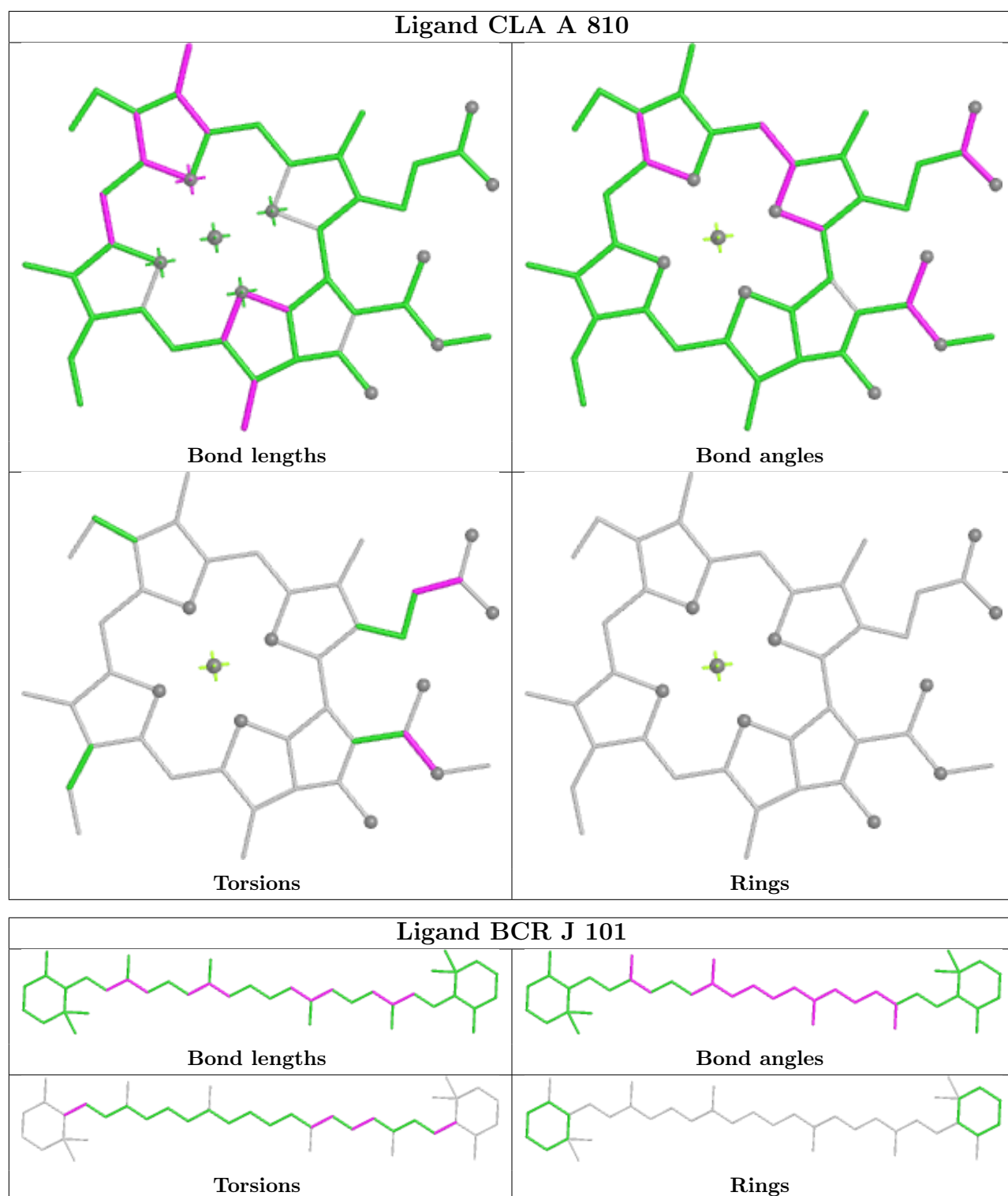
Rings

Ligand CLA 5 602

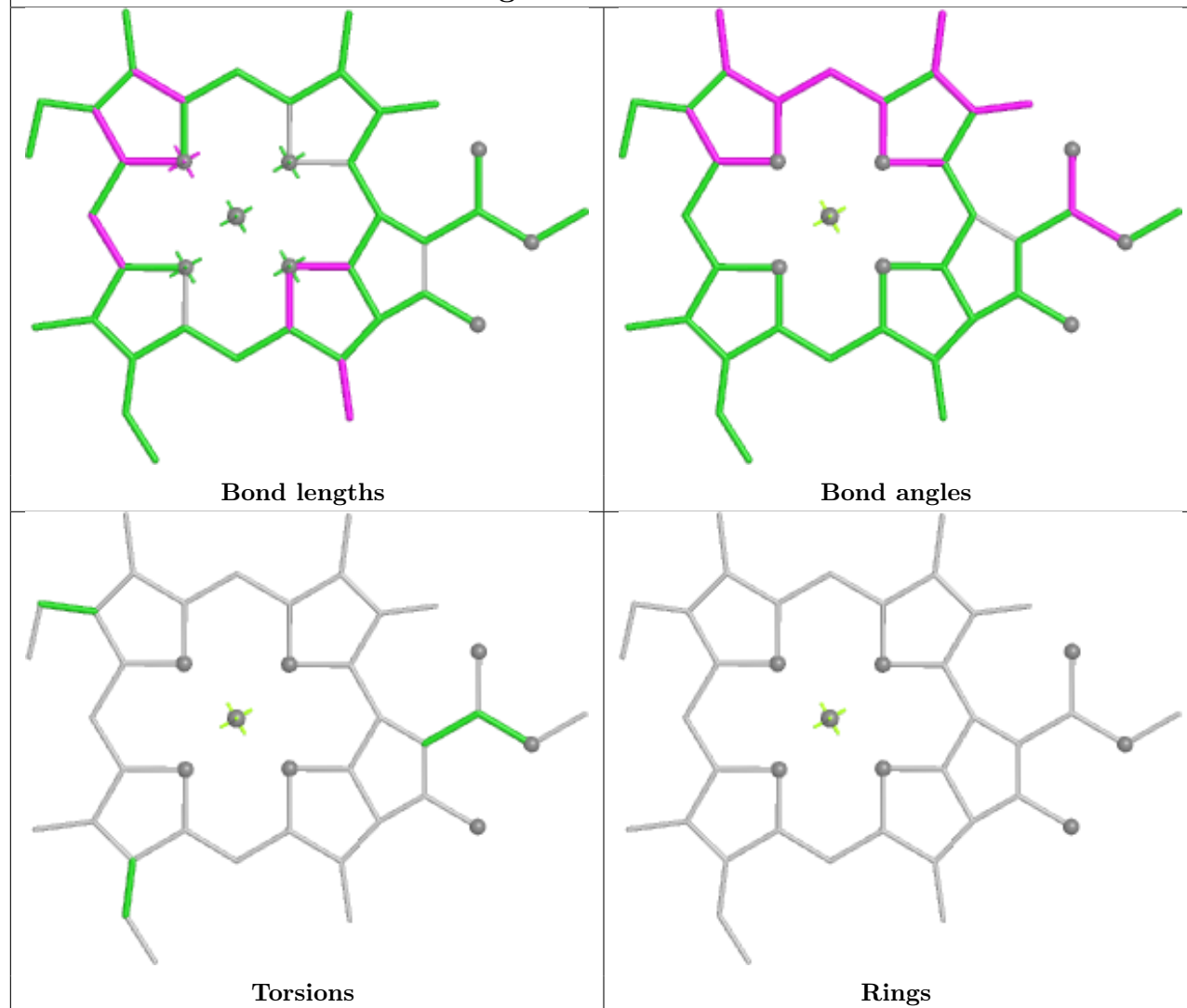


Ligand CLA 1 312

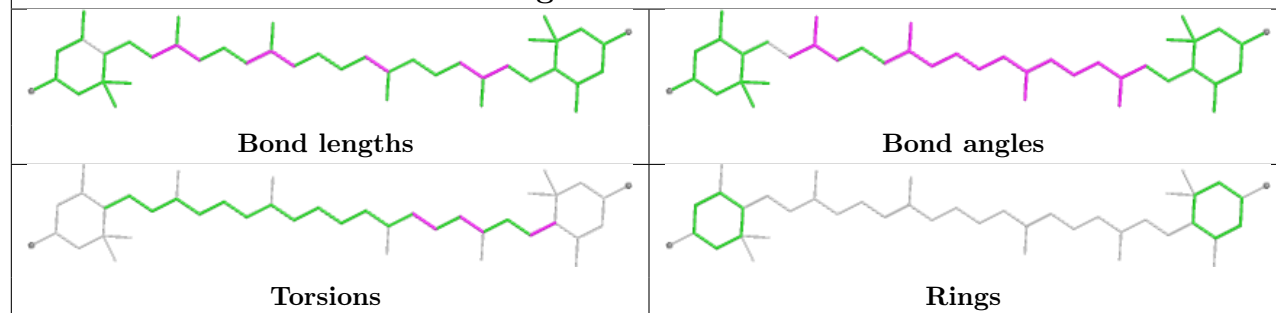


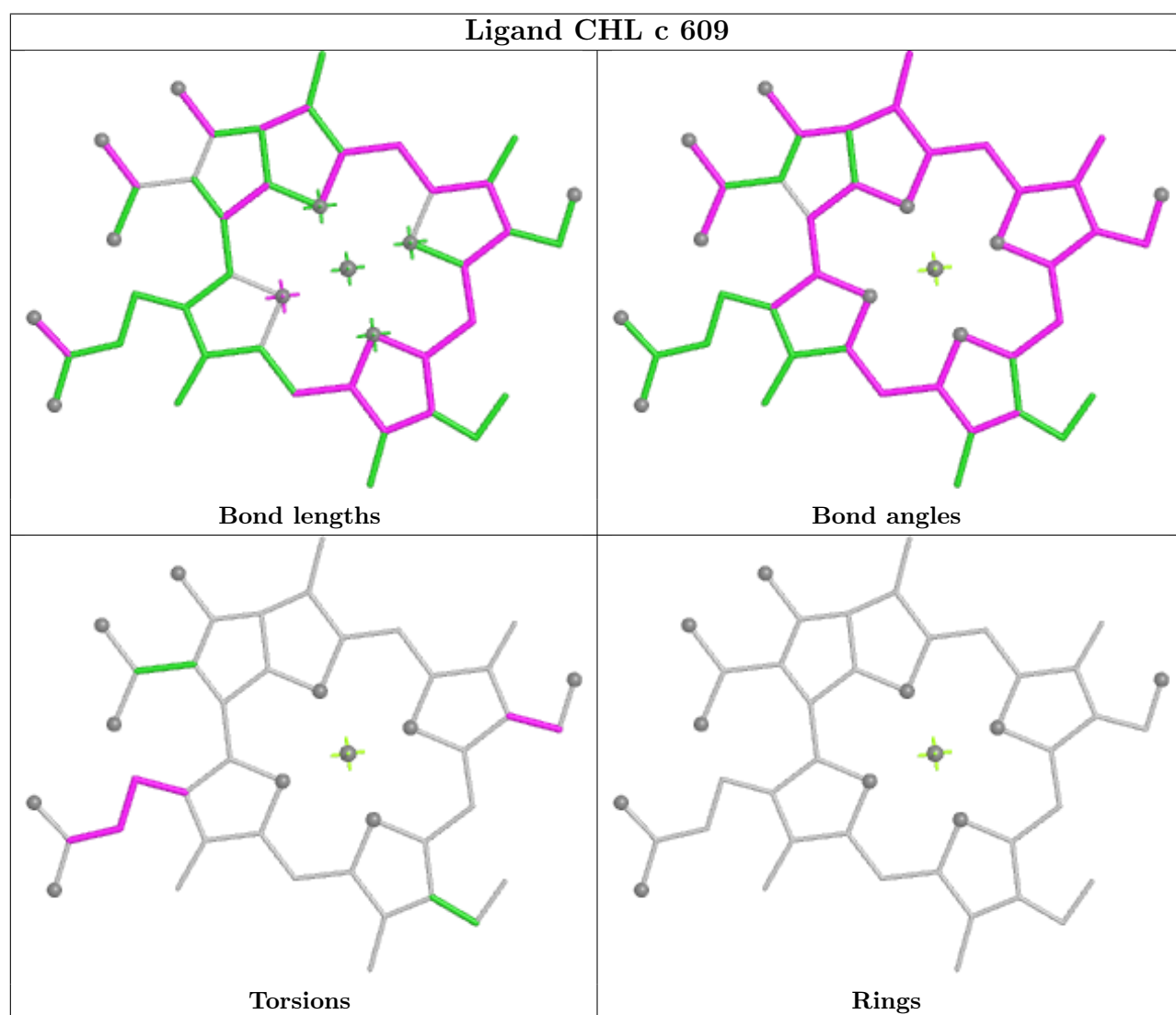
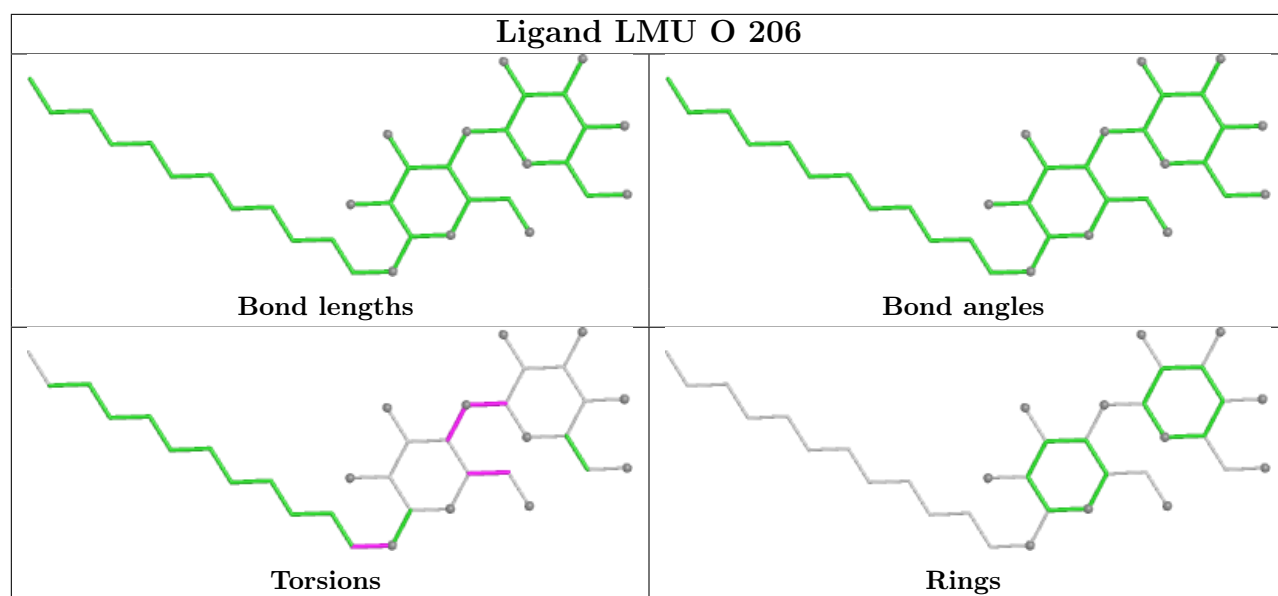


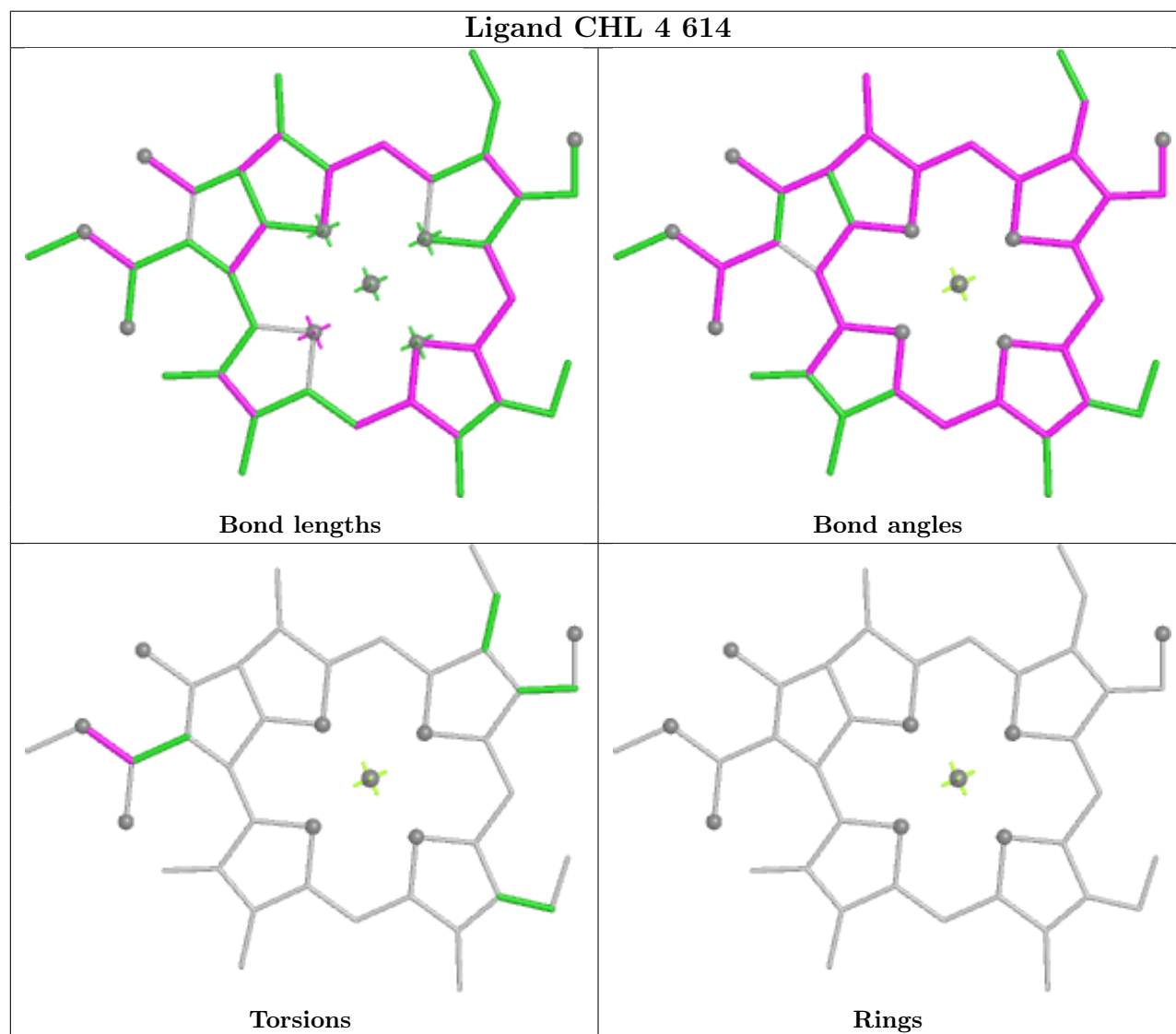
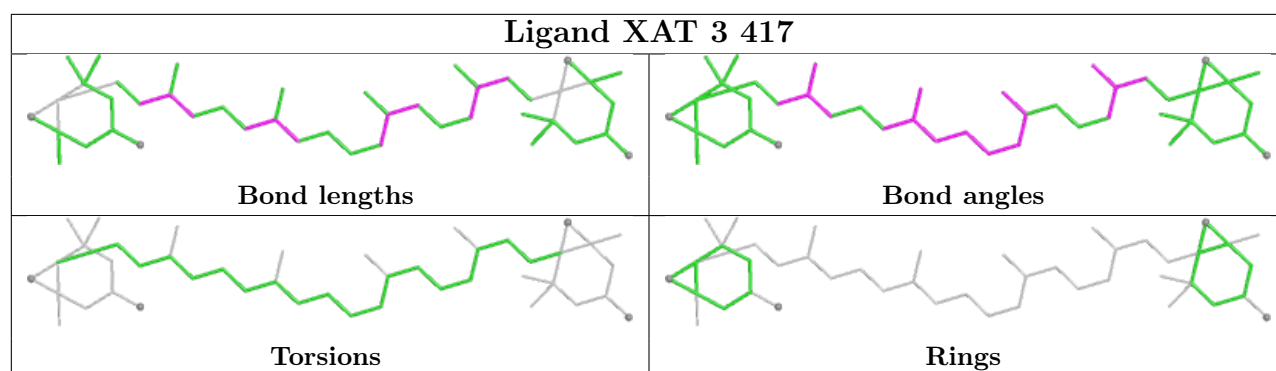
Ligand CLA 2 611



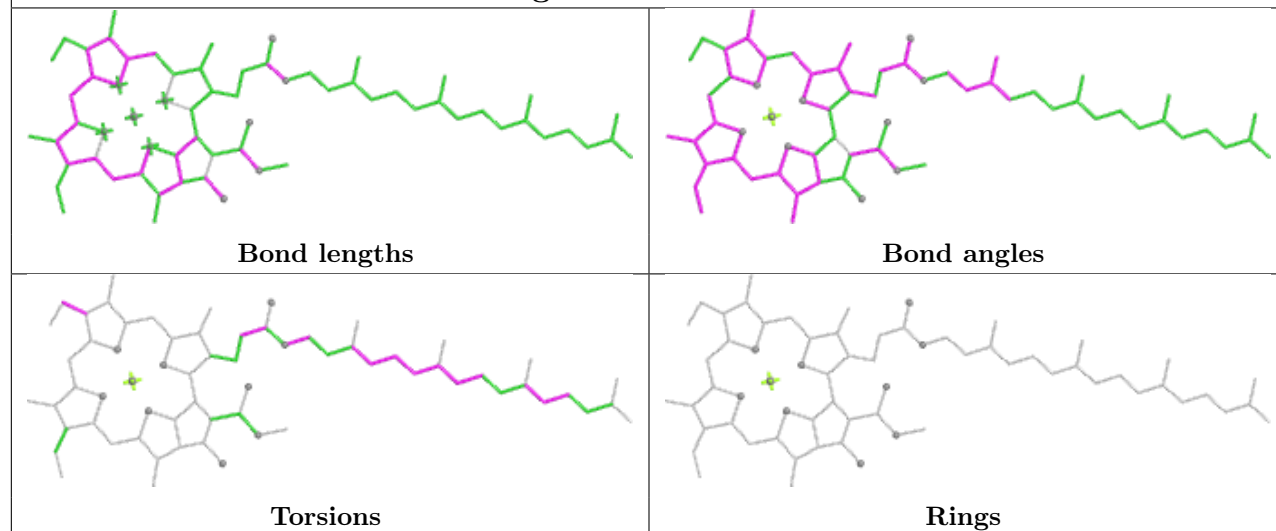
Ligand LUT 3 416



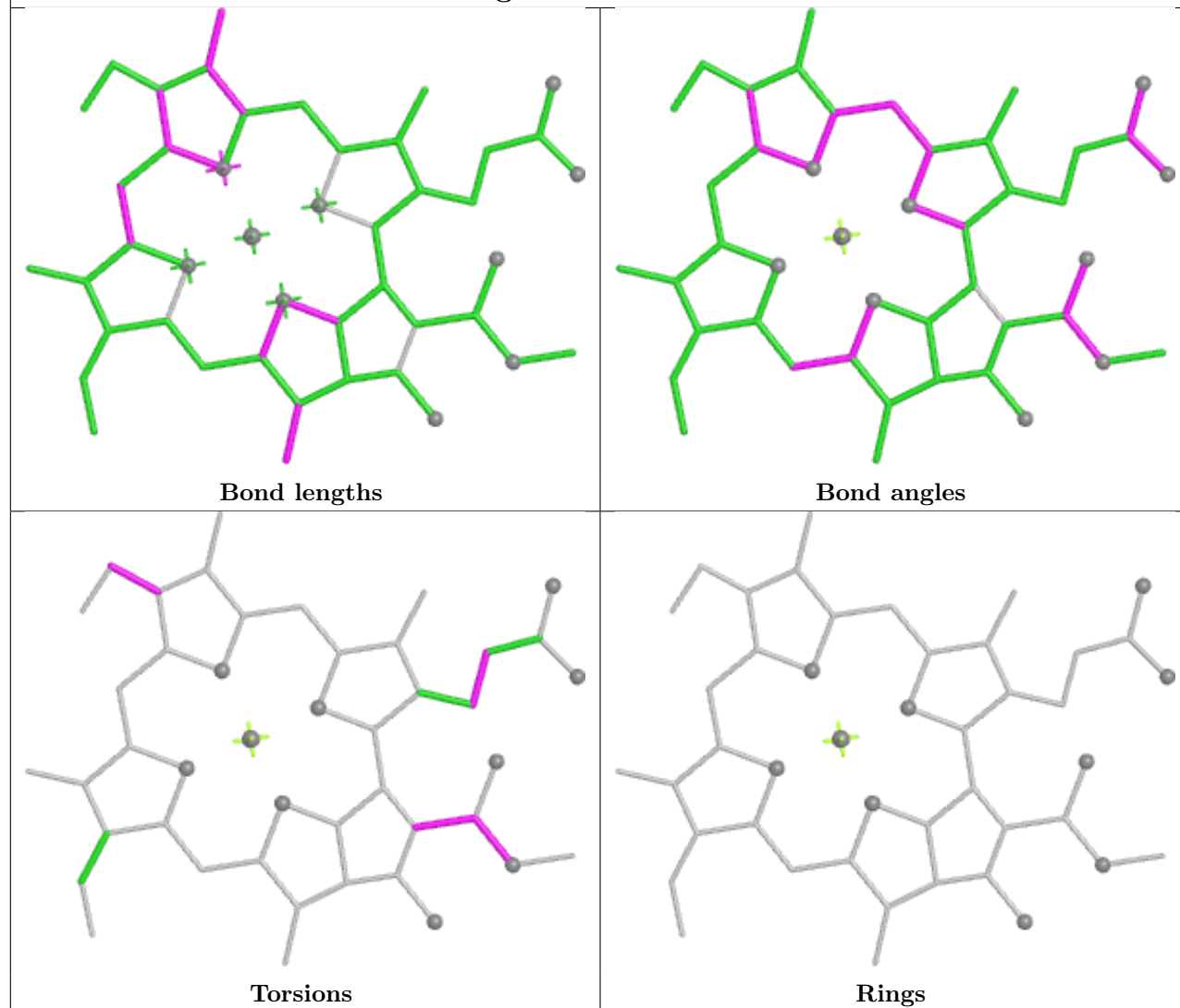


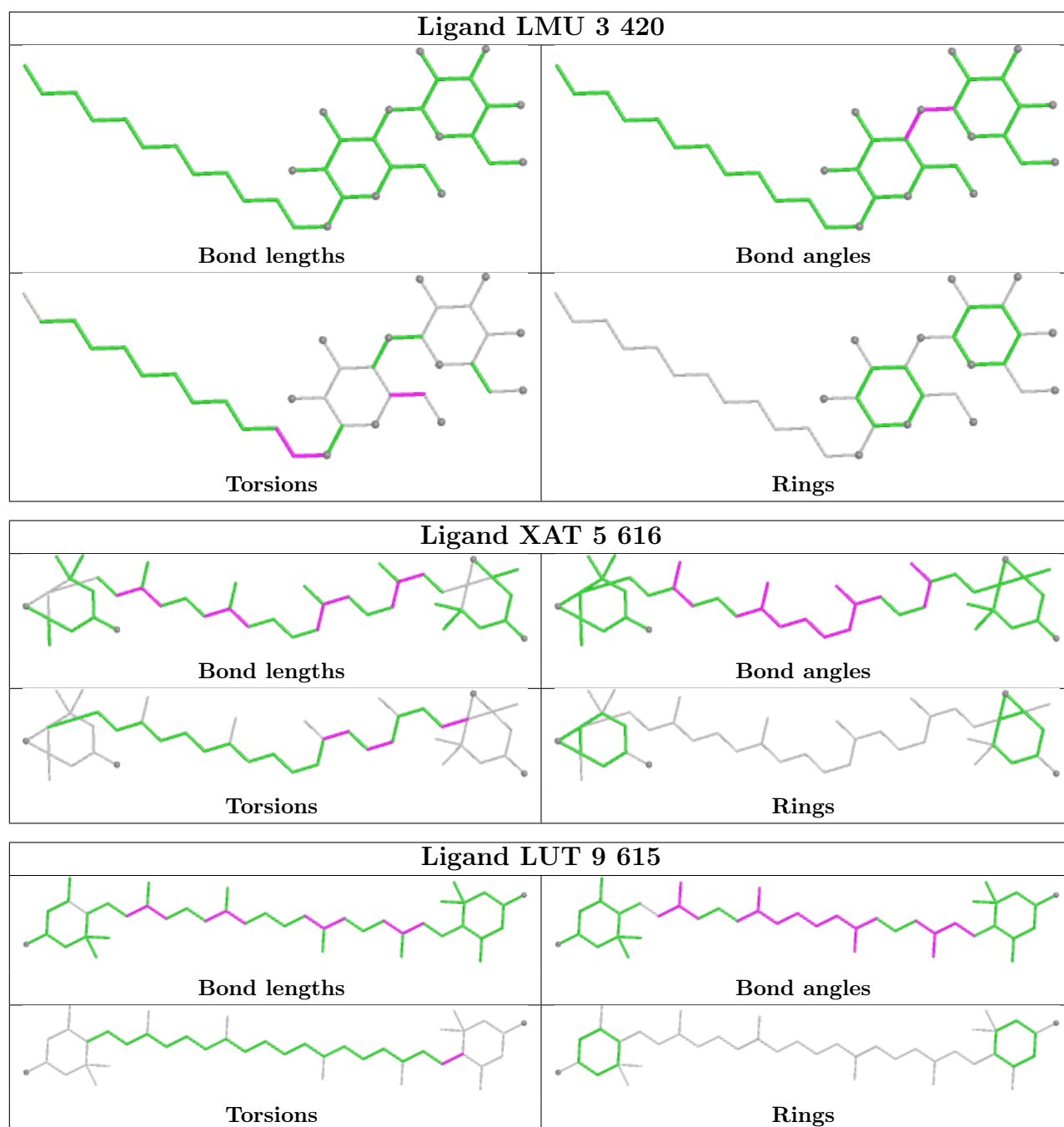


Ligand CLA B 801

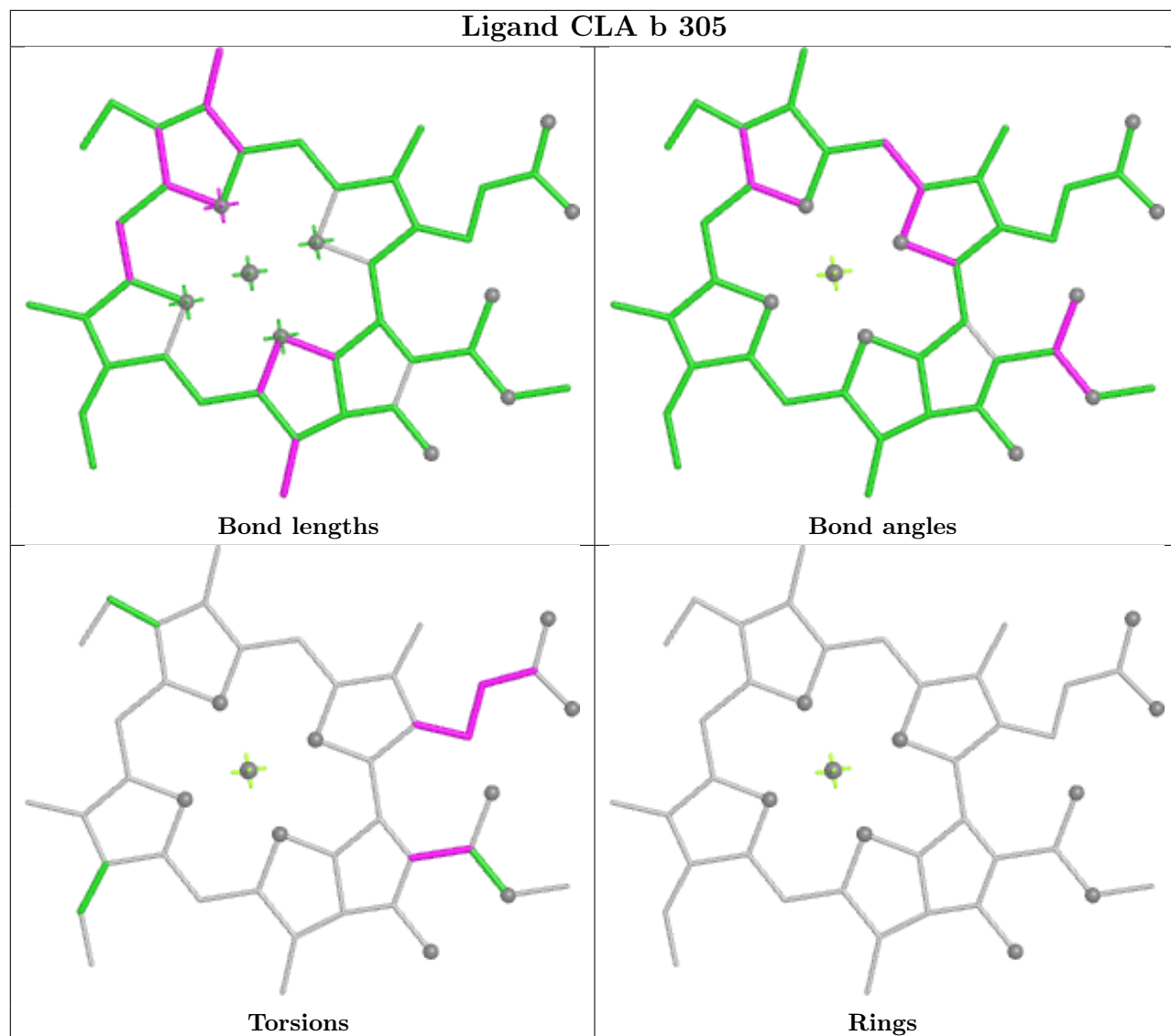


Ligand CLA 1 313

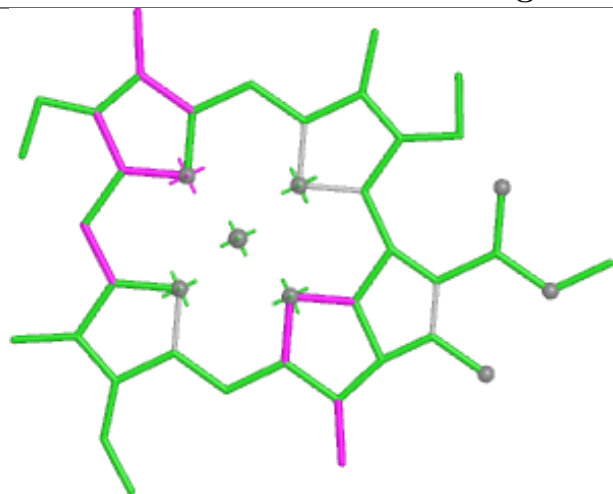




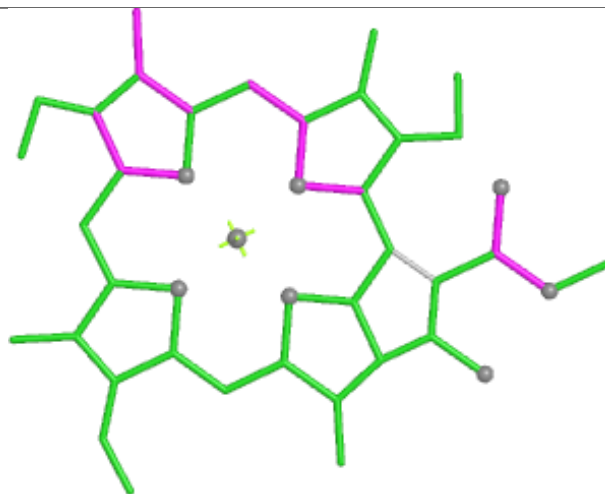
Ligand CLA b 305



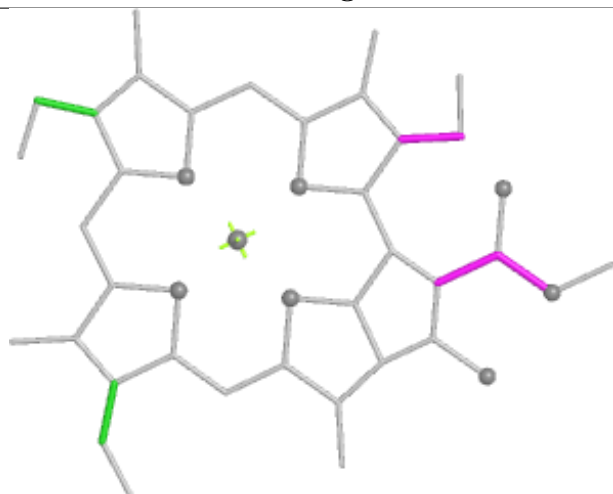
Ligand CLA L 304



Bond lengths



Bond angles

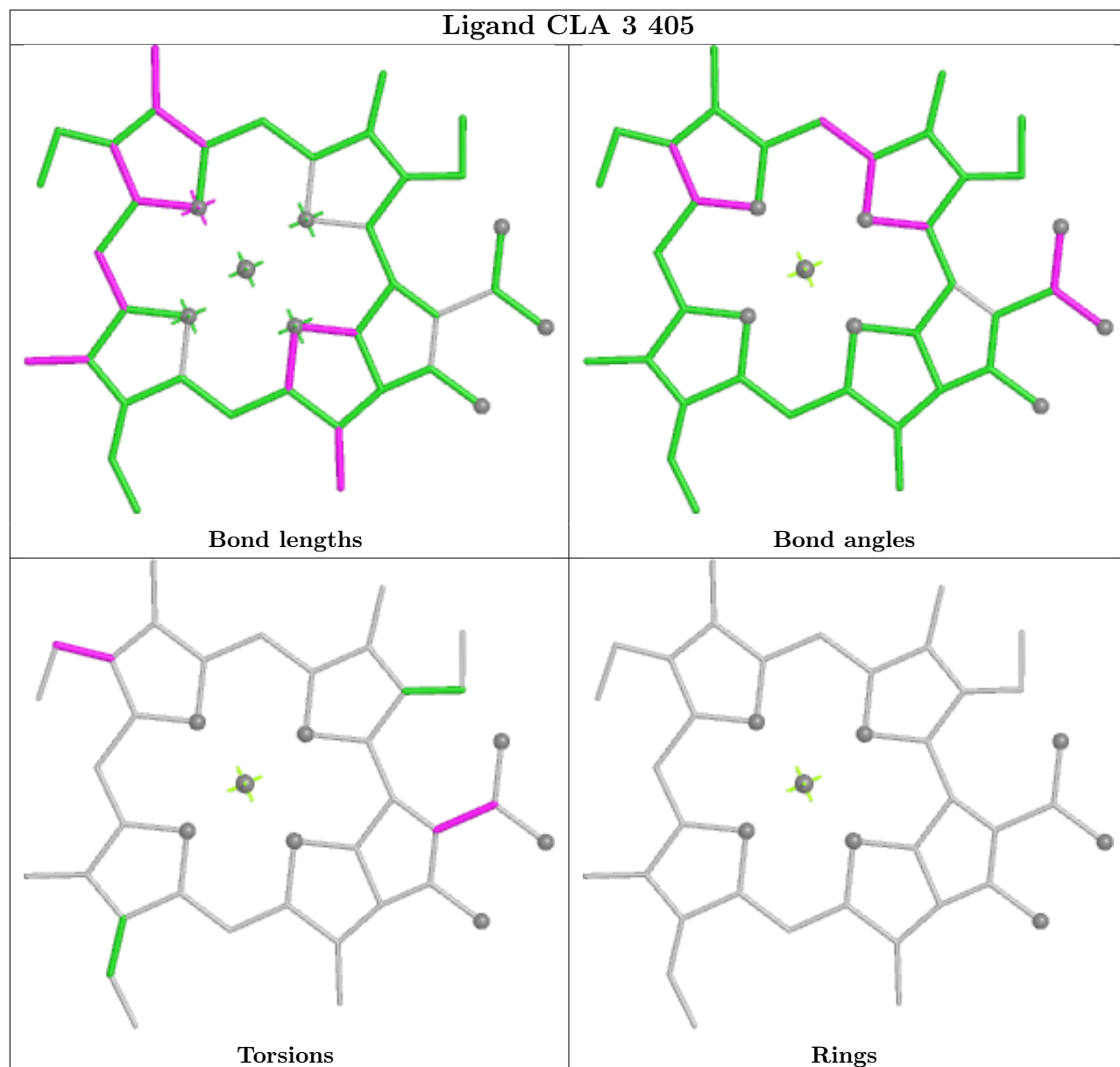


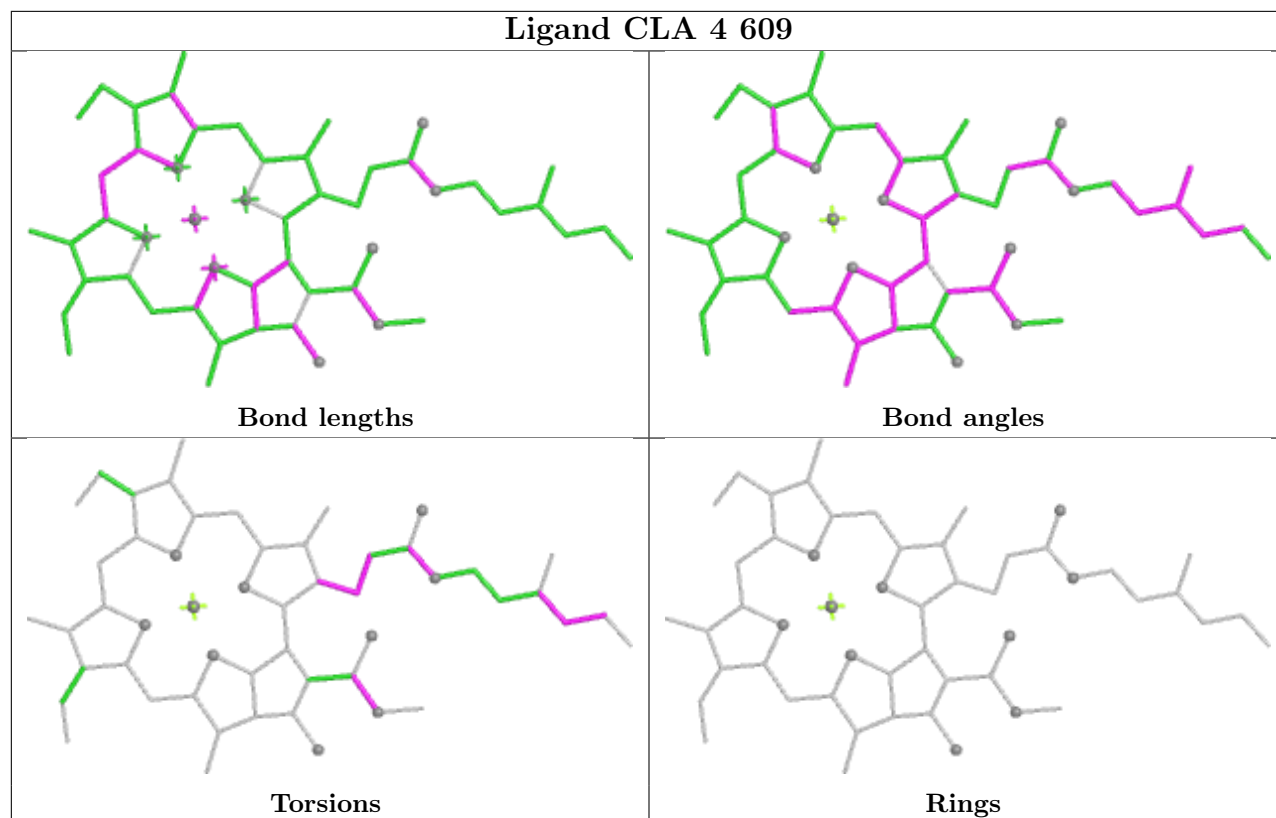
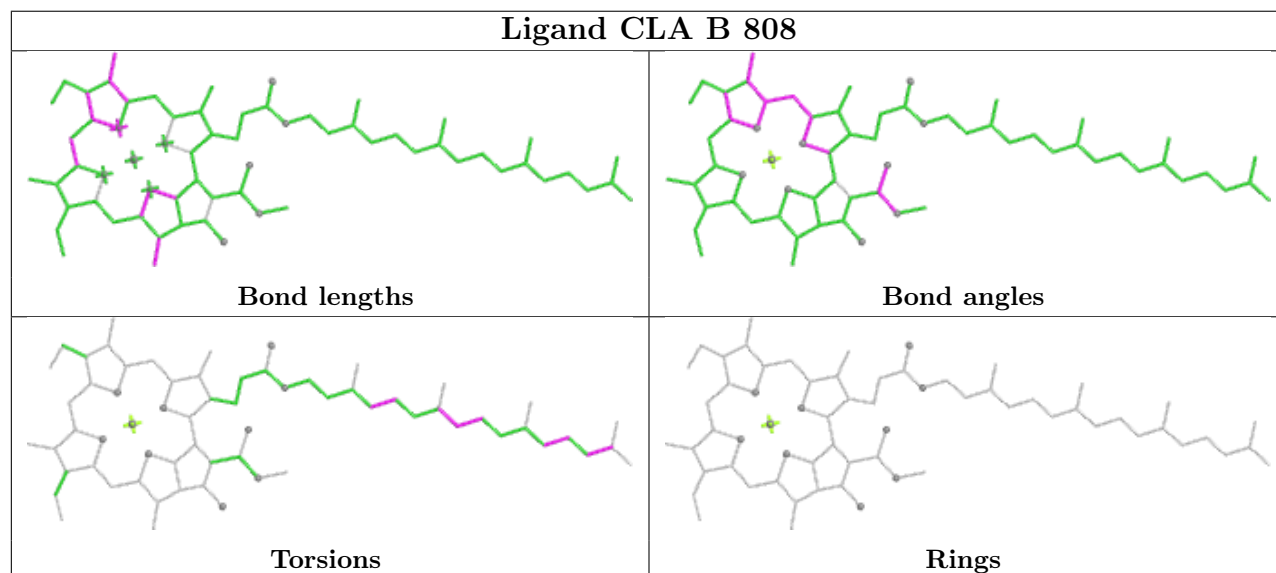
Torsions



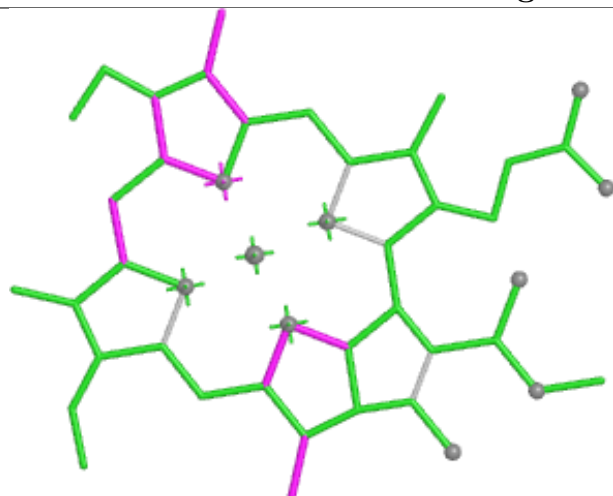
Rings

Ligand CLA 3 405

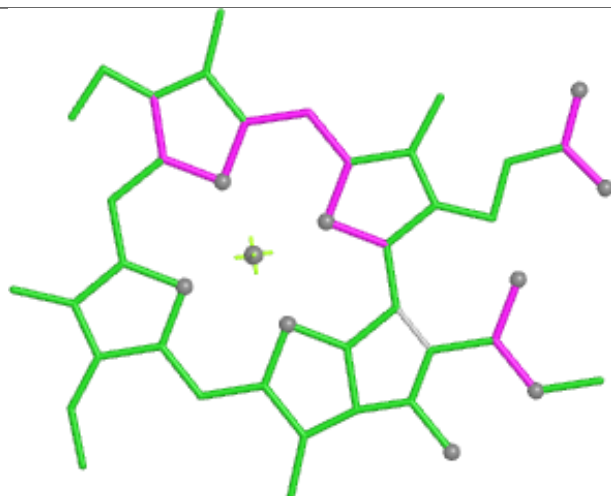


Ligand CLA 4 609**Ligand CLA B 808**

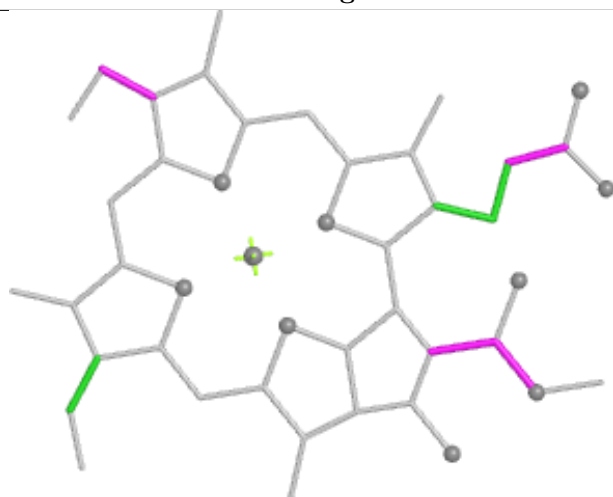
Ligand CLA b 313



Bond lengths



Bond angles

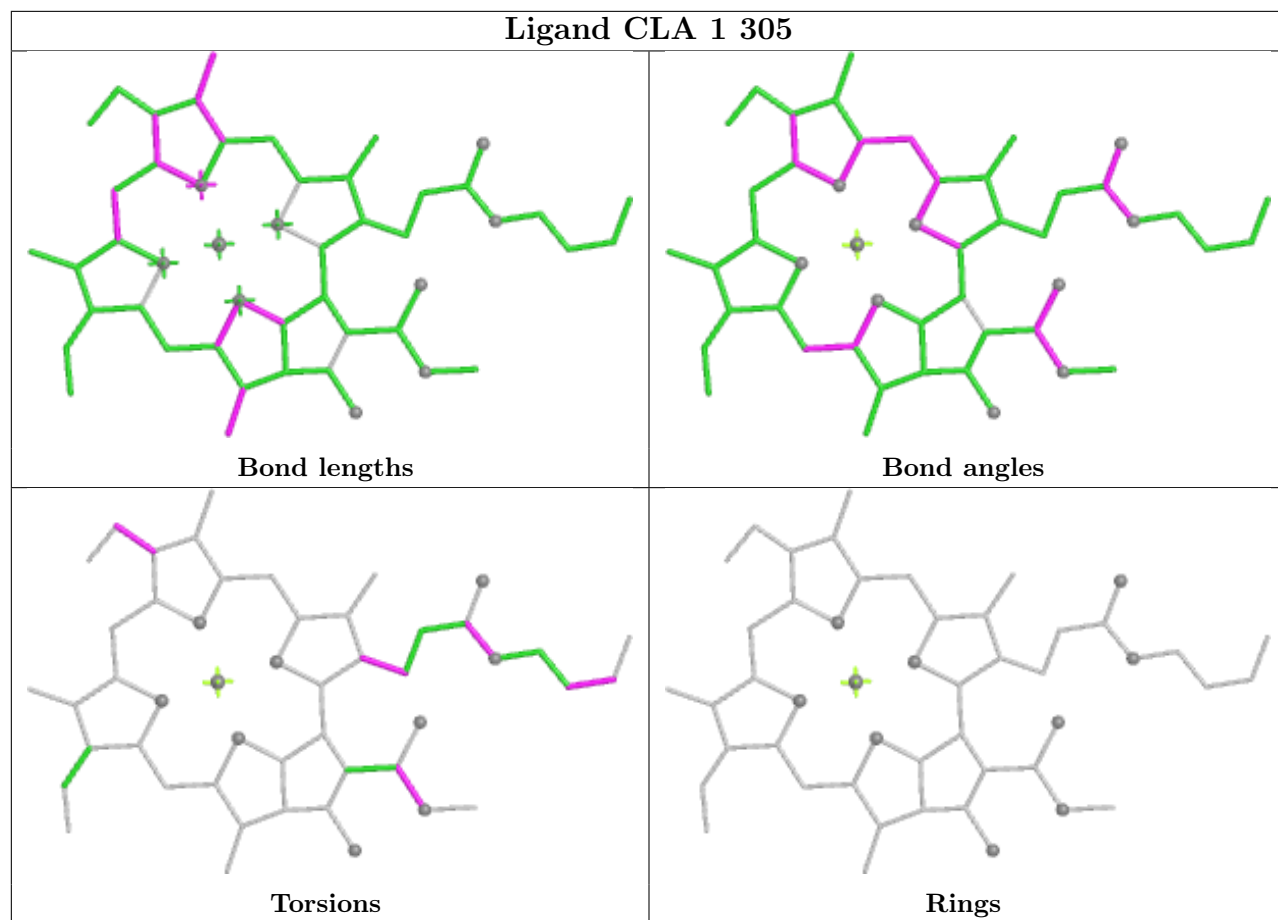


Torsions

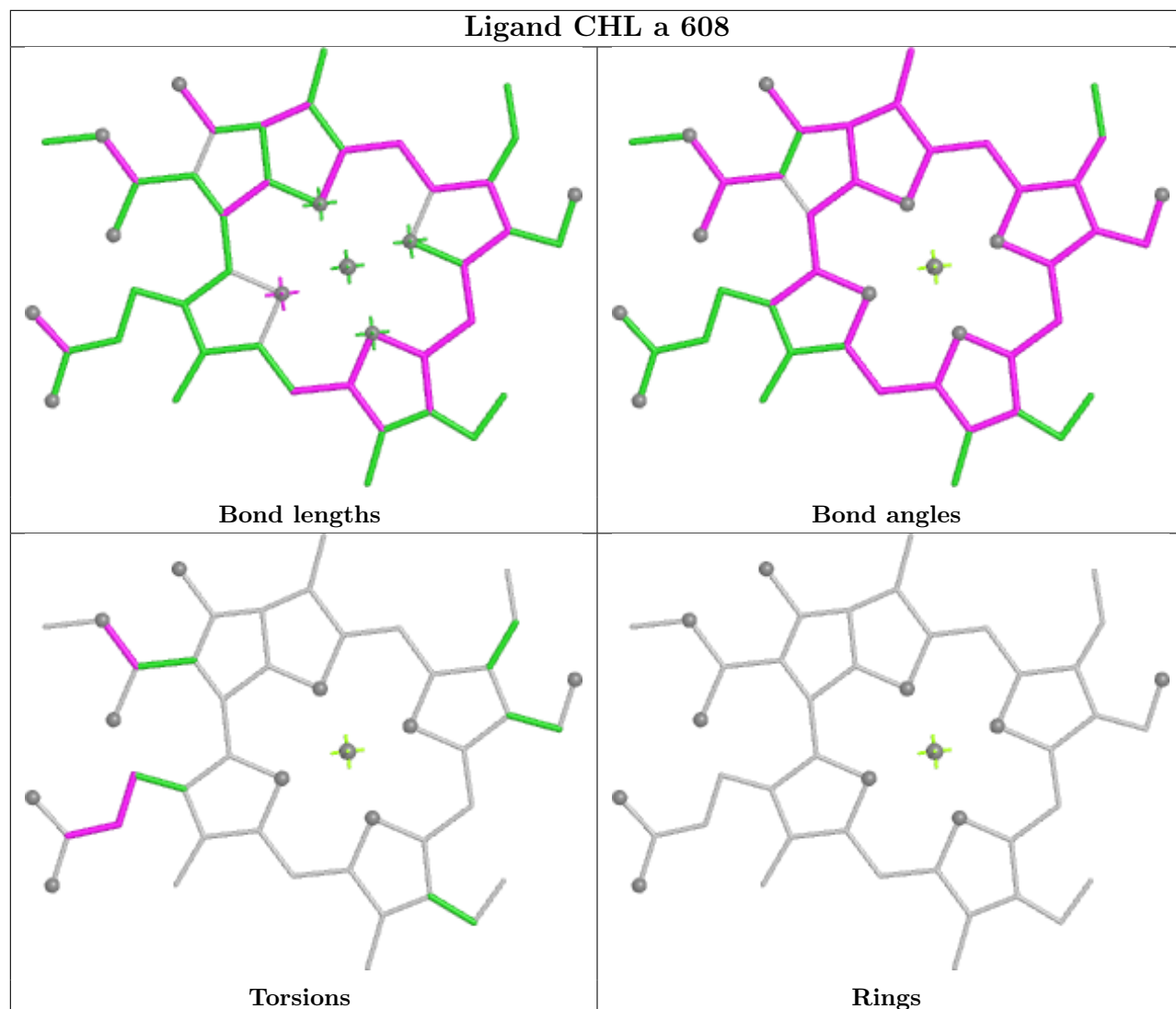


Rings

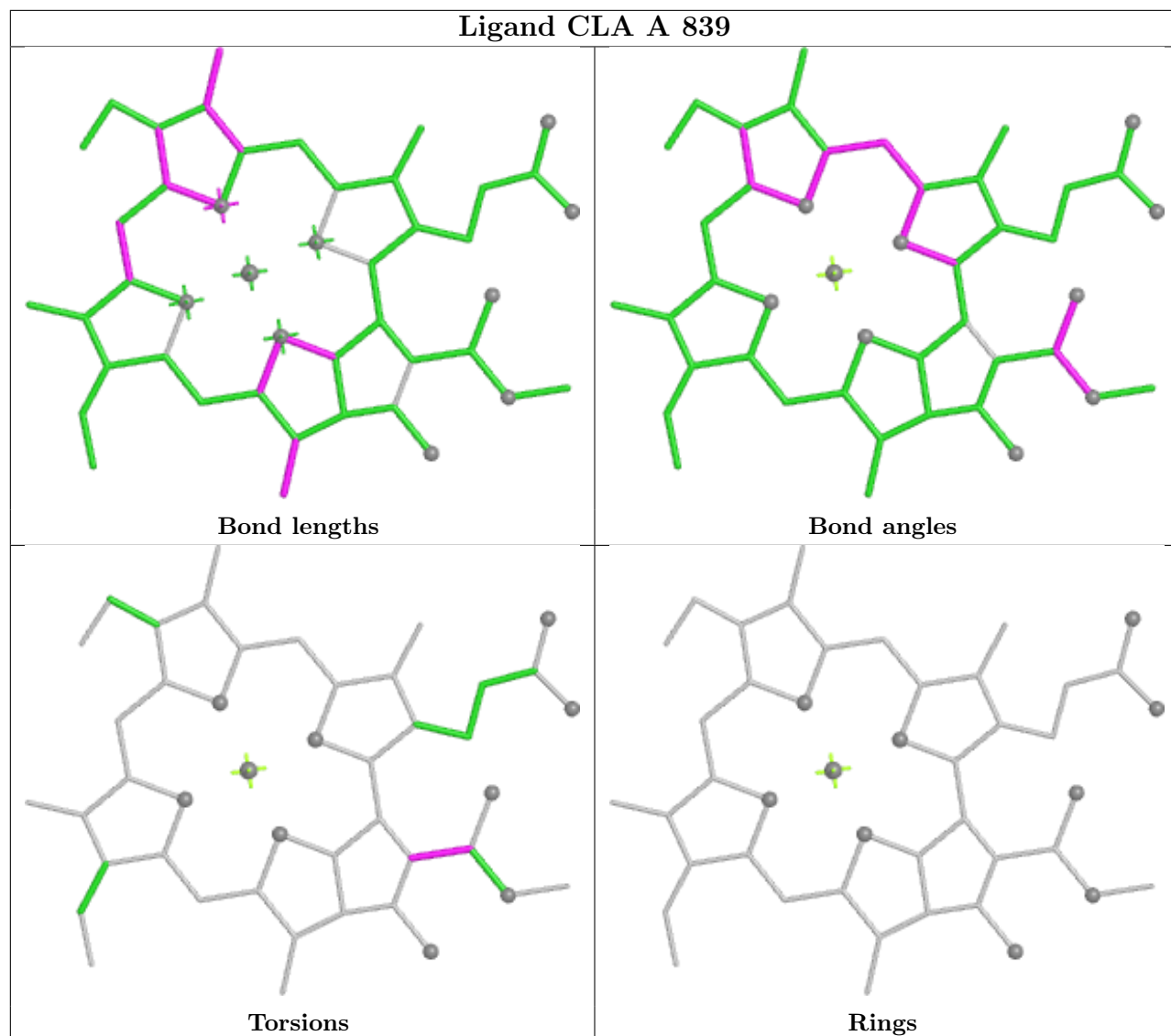
Ligand CLA 1 305

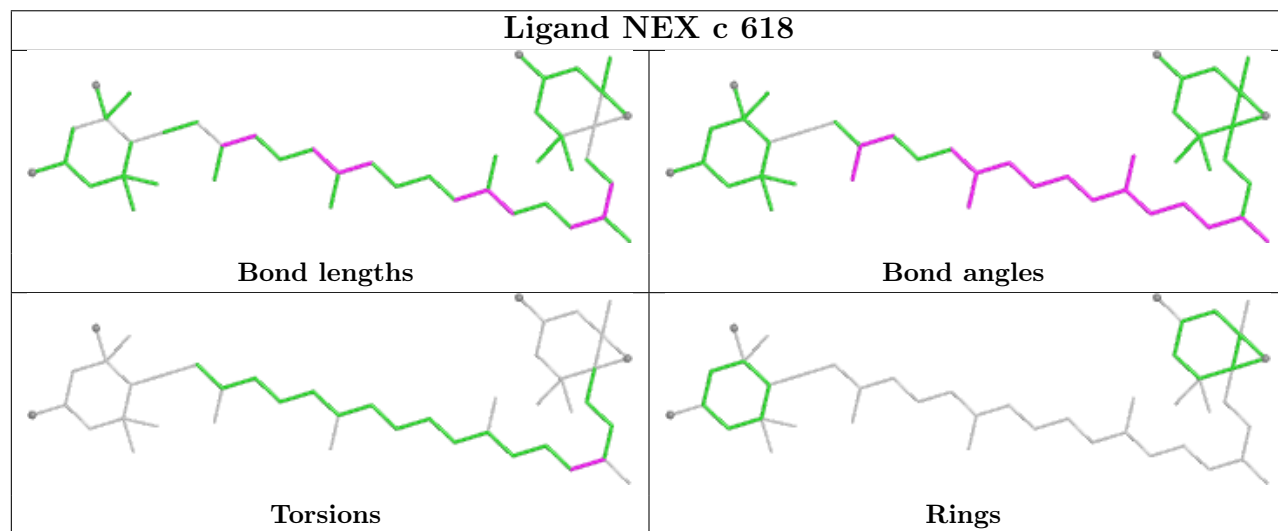
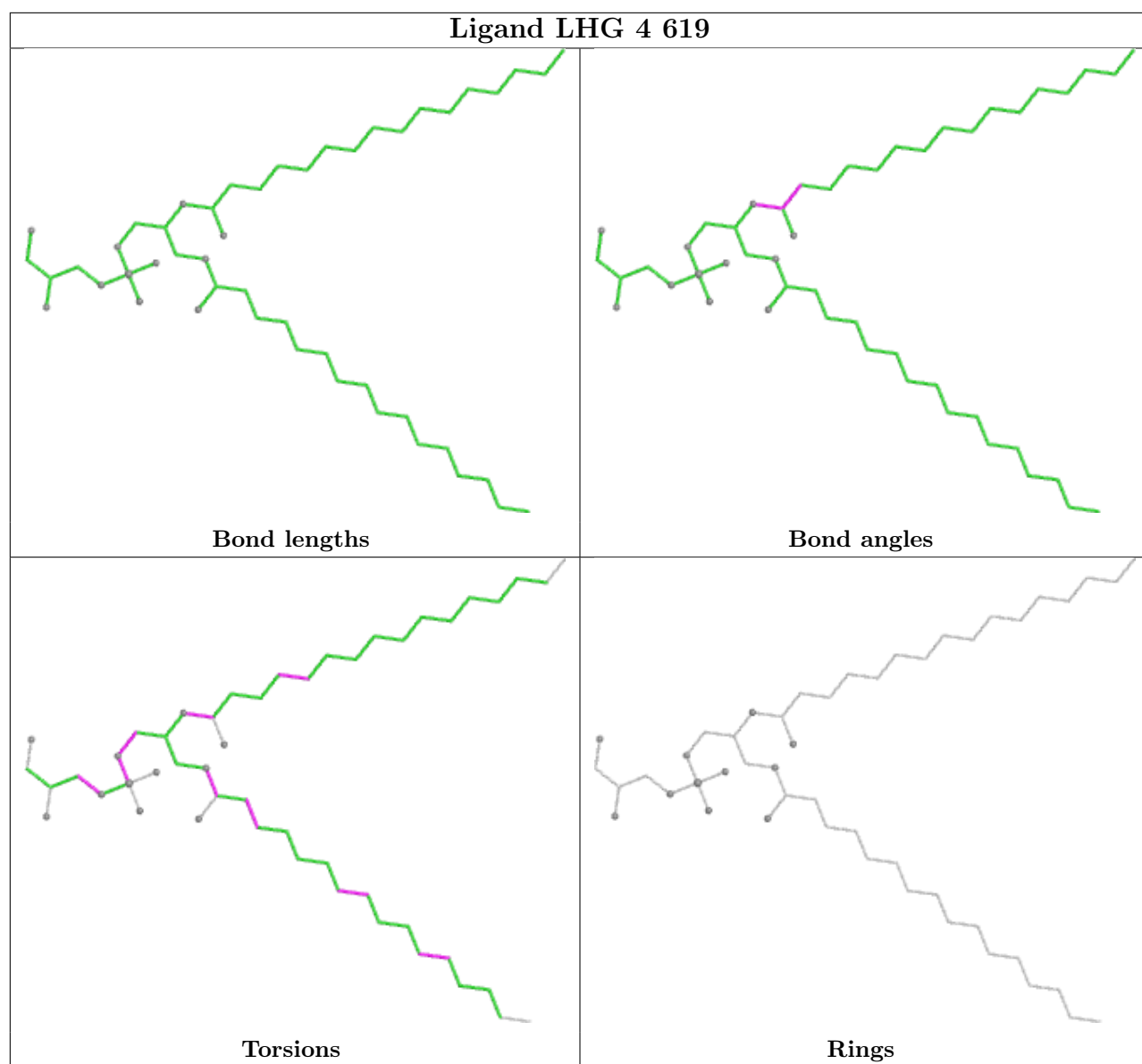


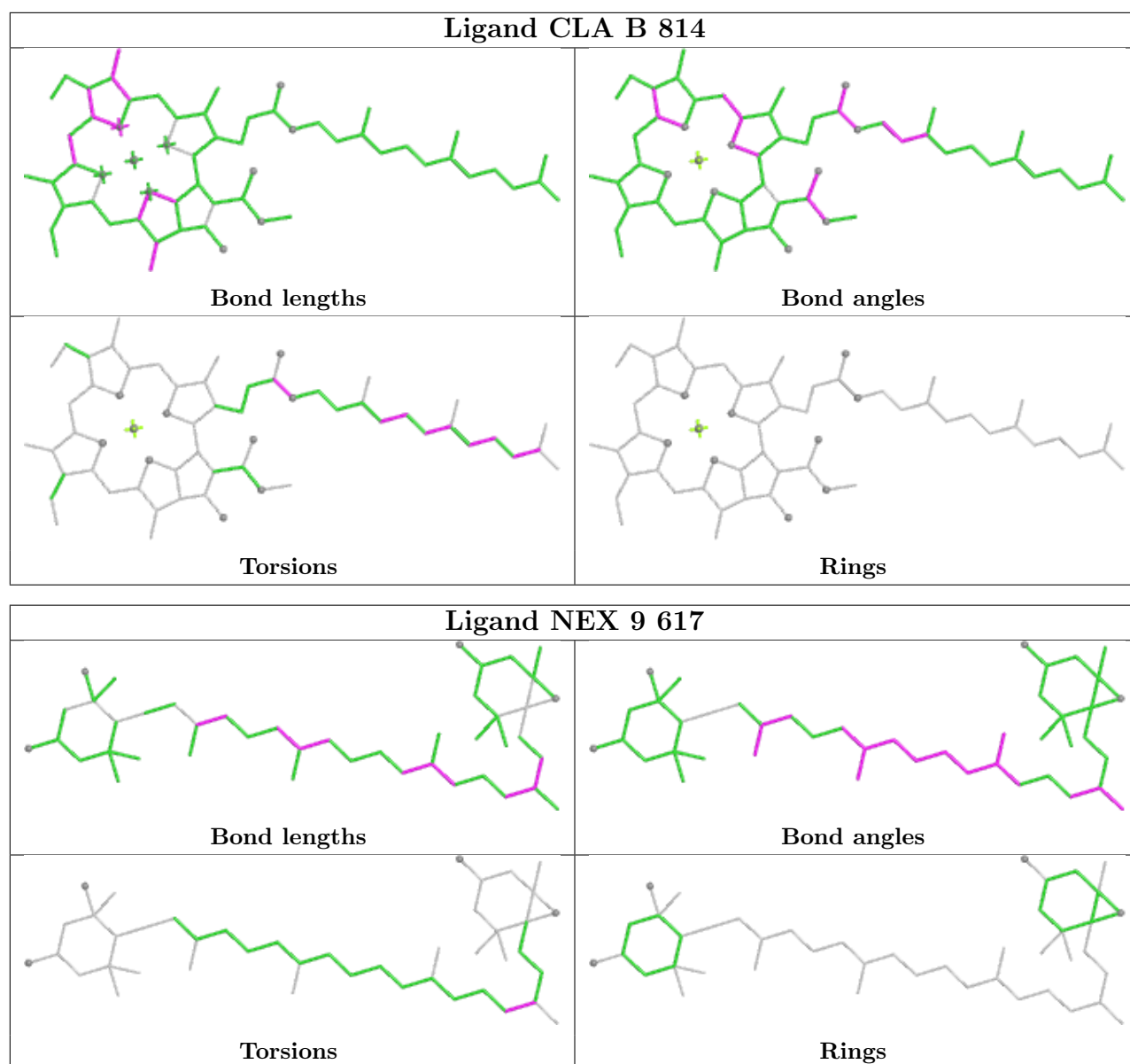
Ligand CHL a 608

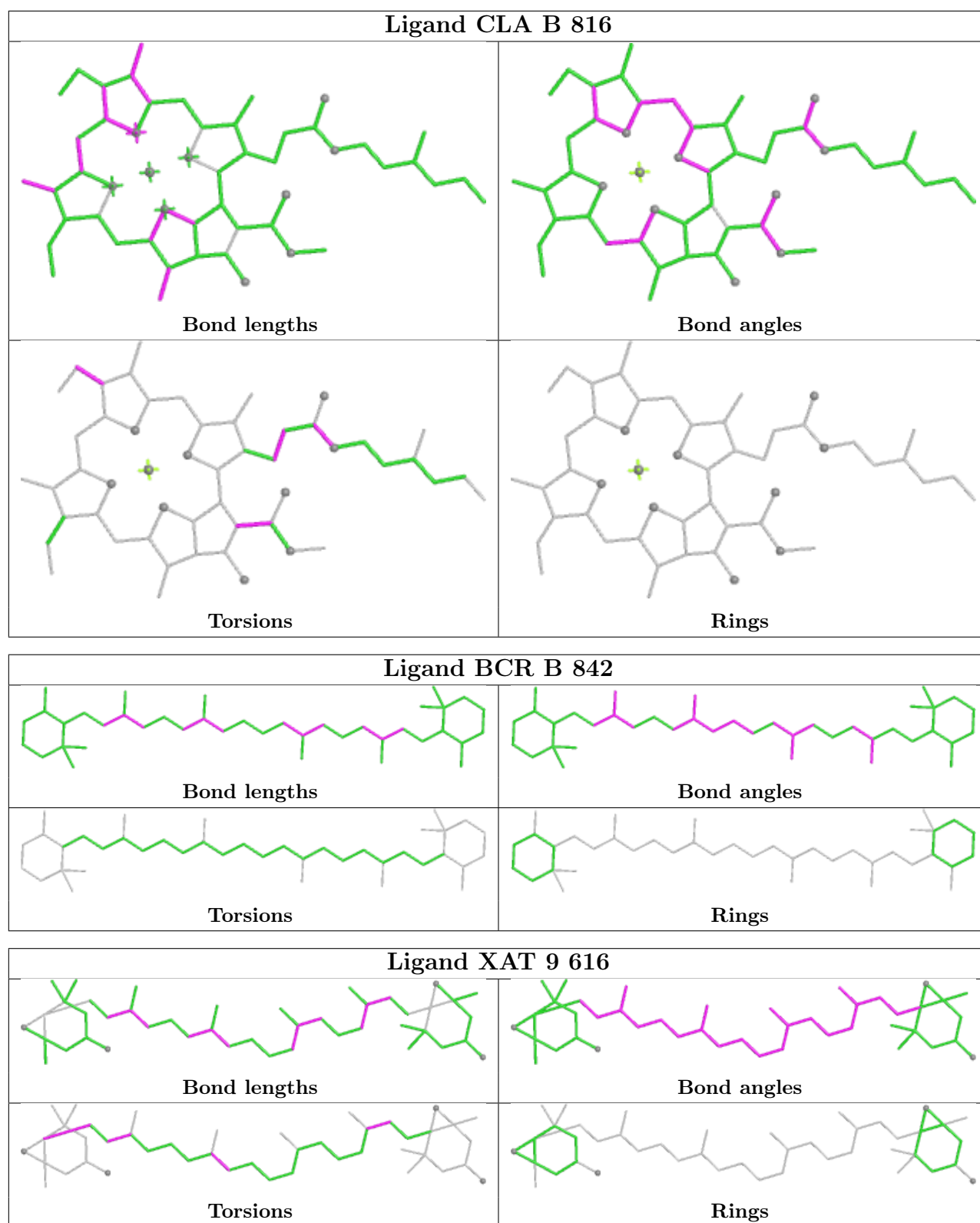


Ligand CLA A 839

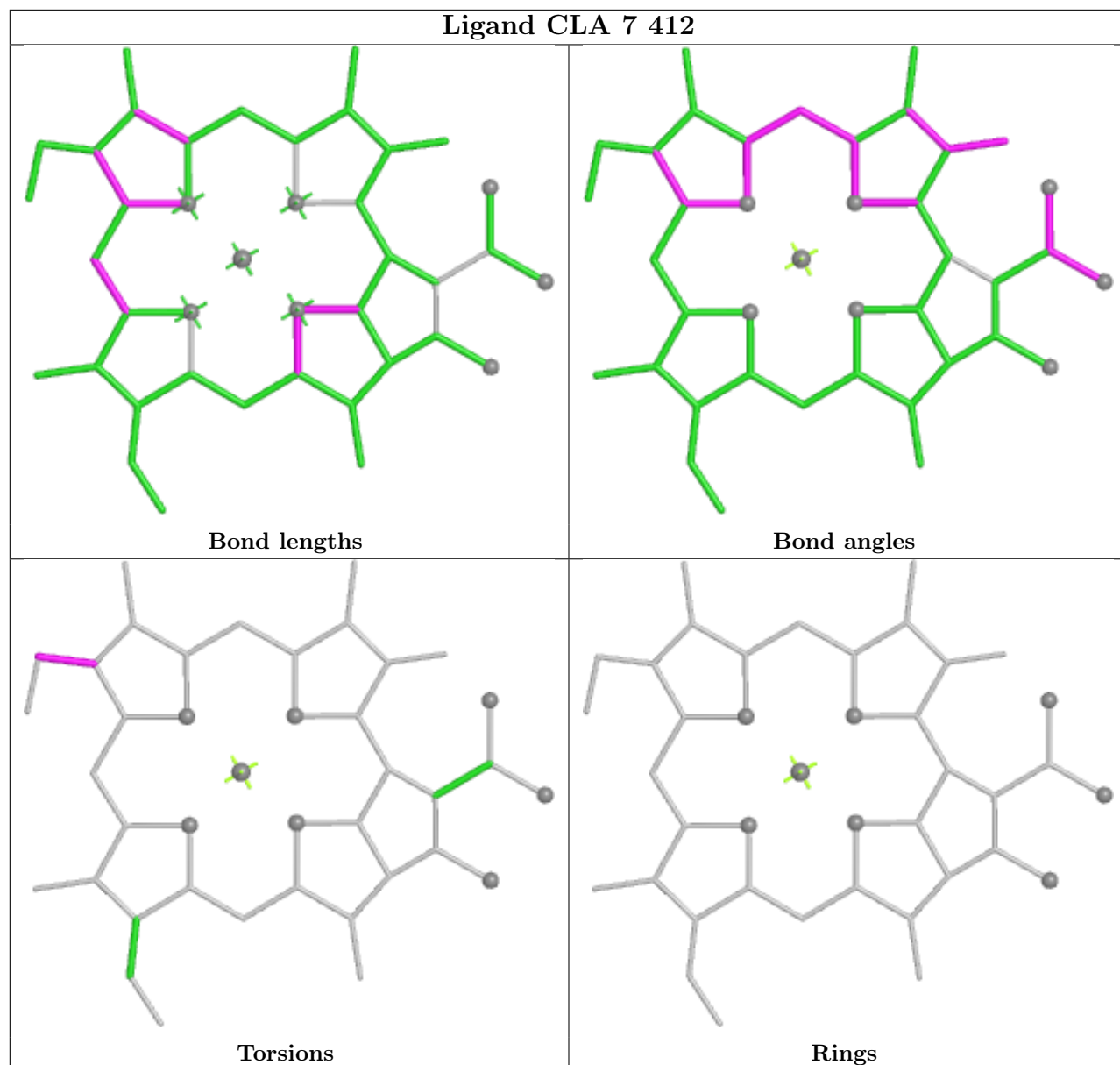




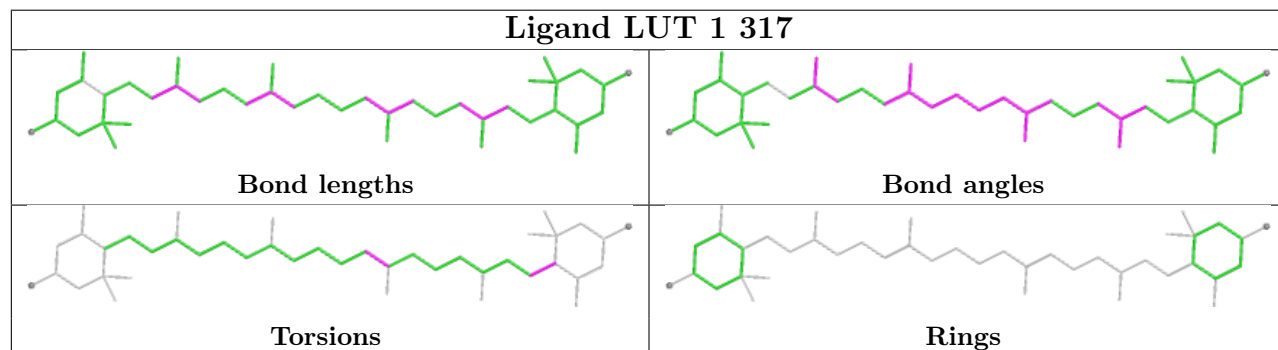


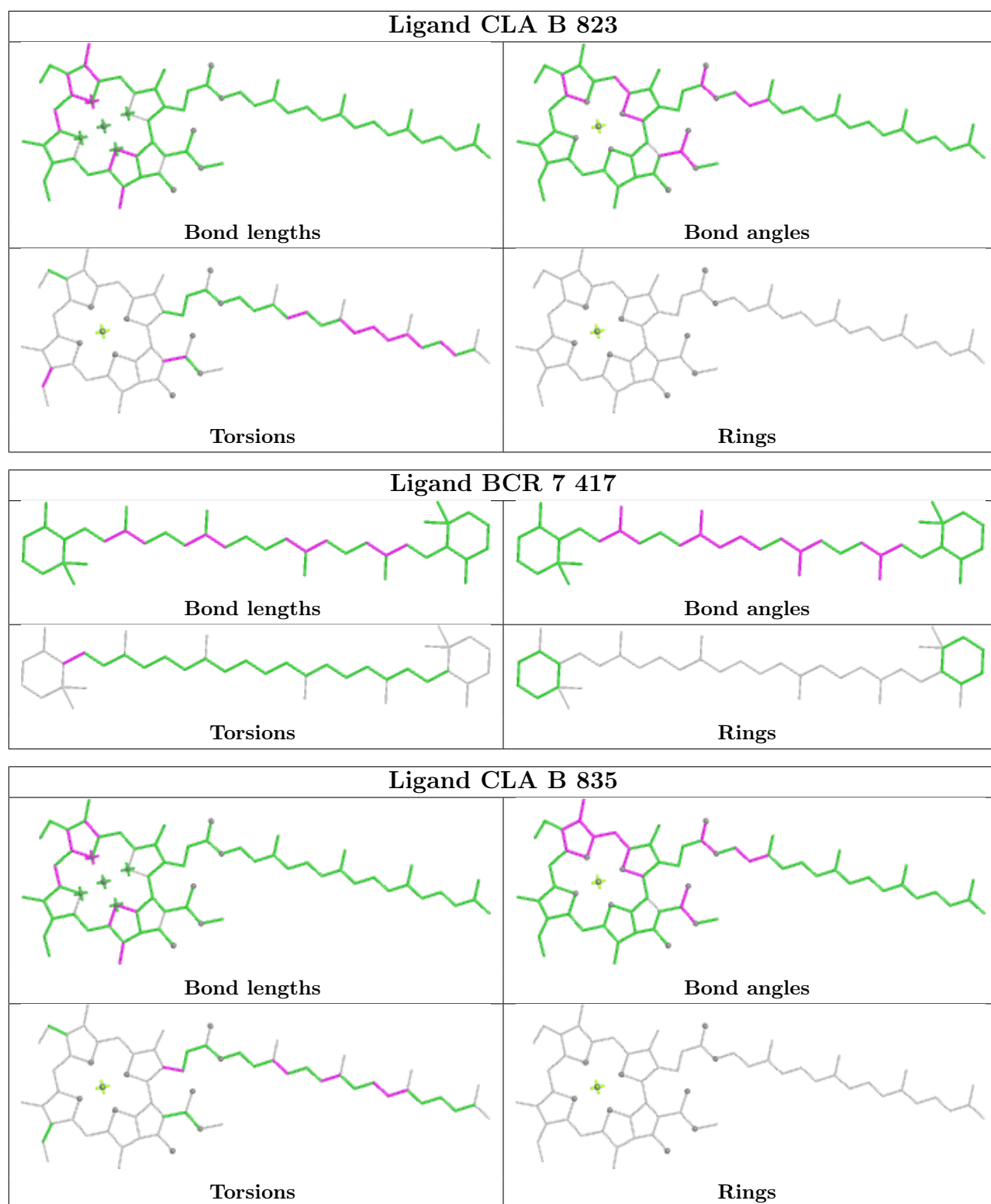


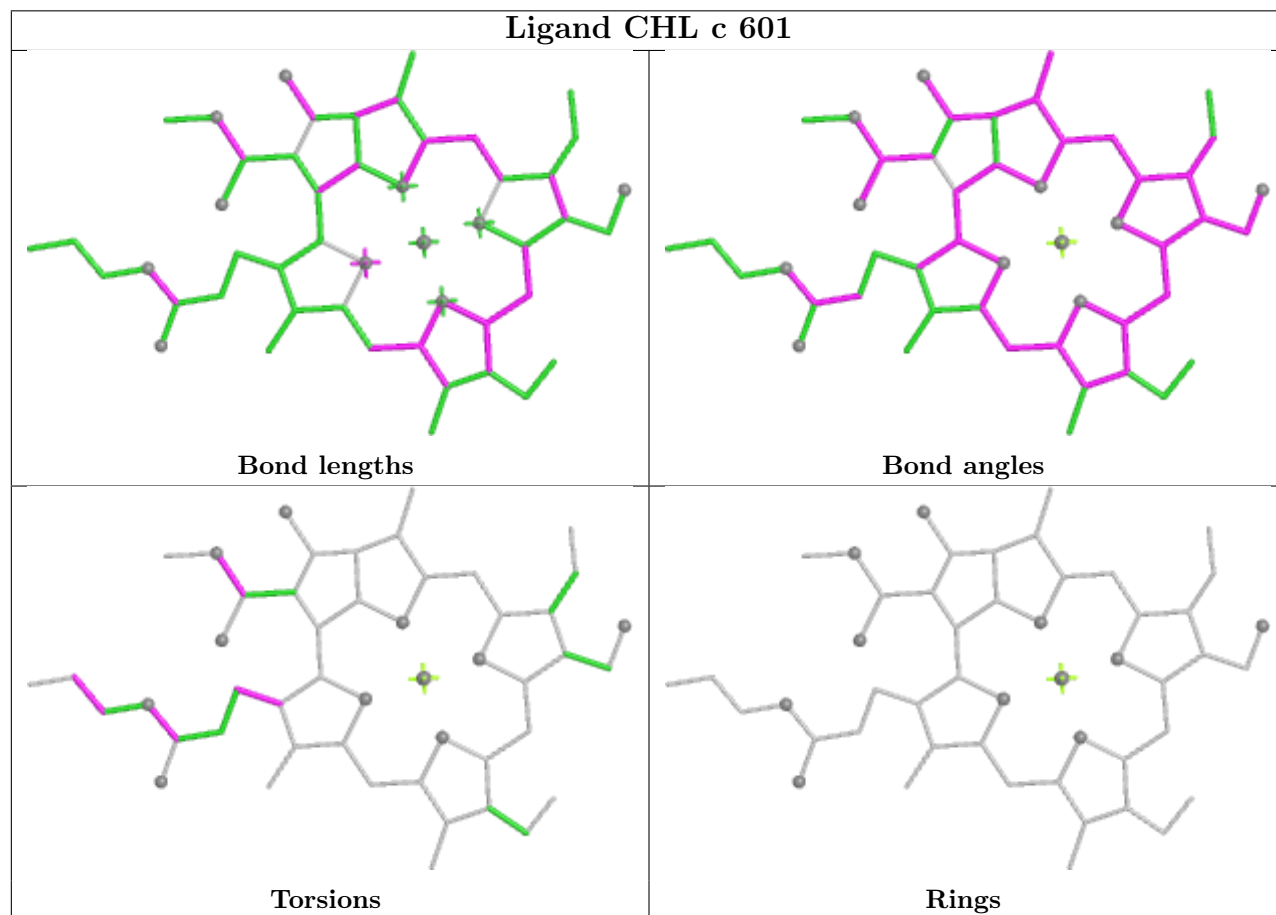
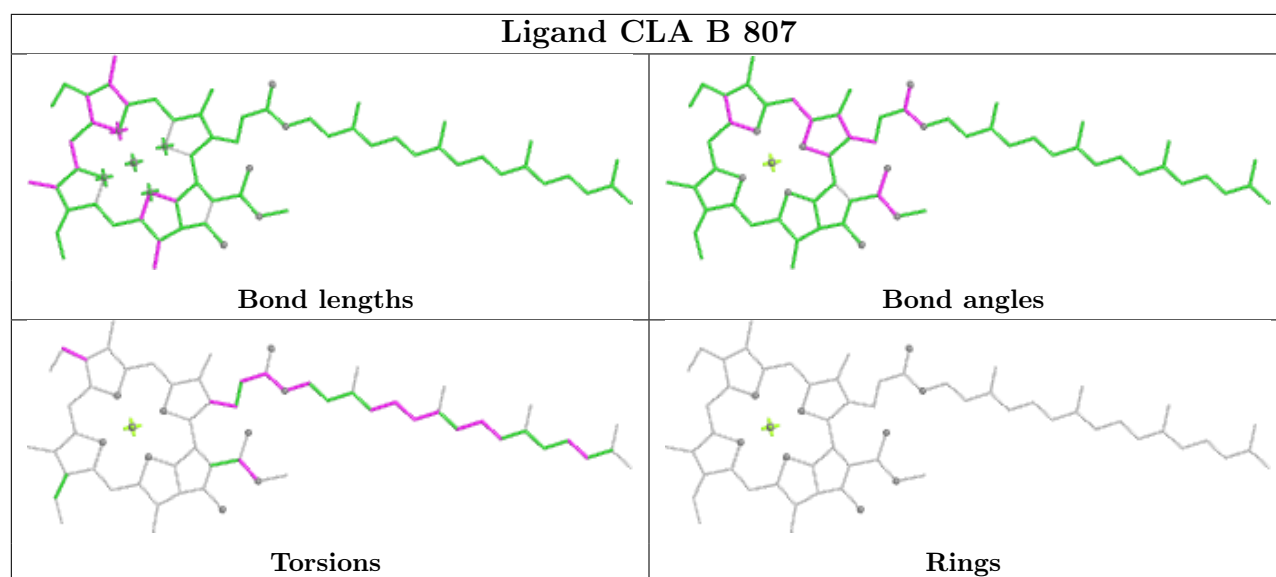
Ligand CLA 7 412

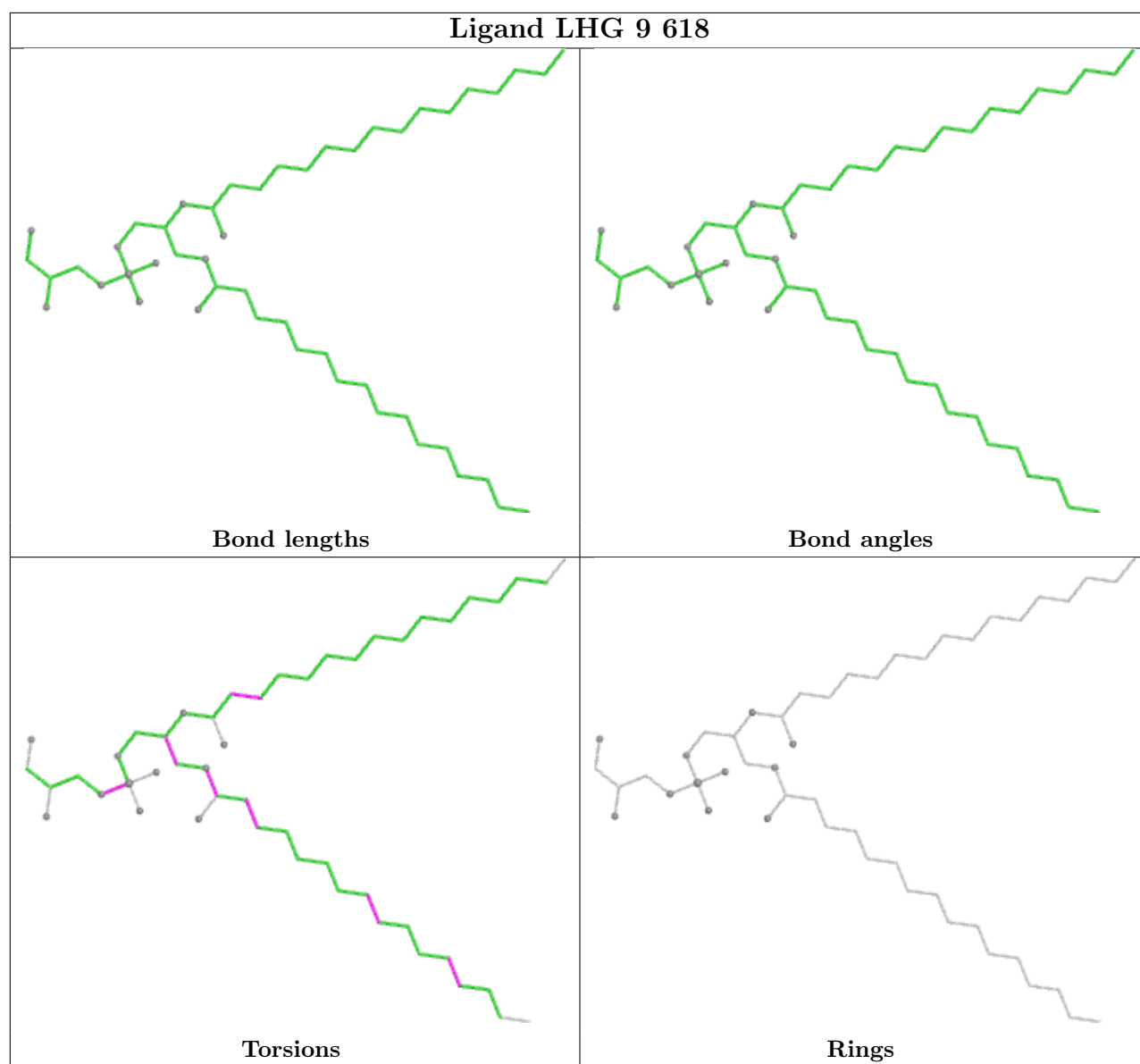


Ligand LUT 1 317

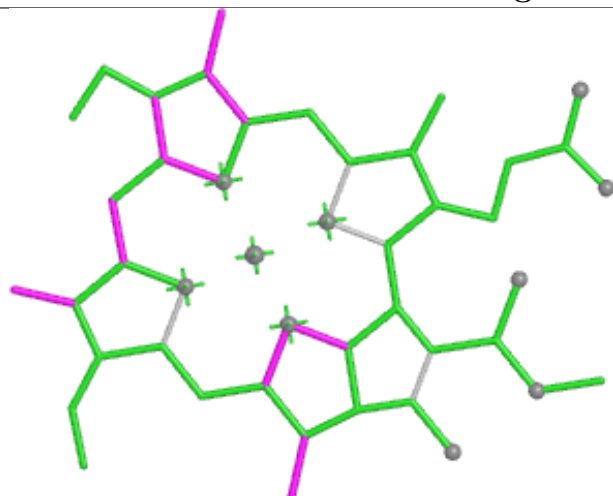




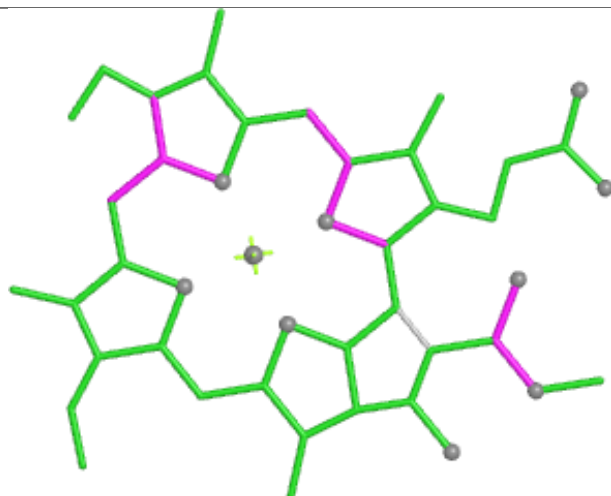




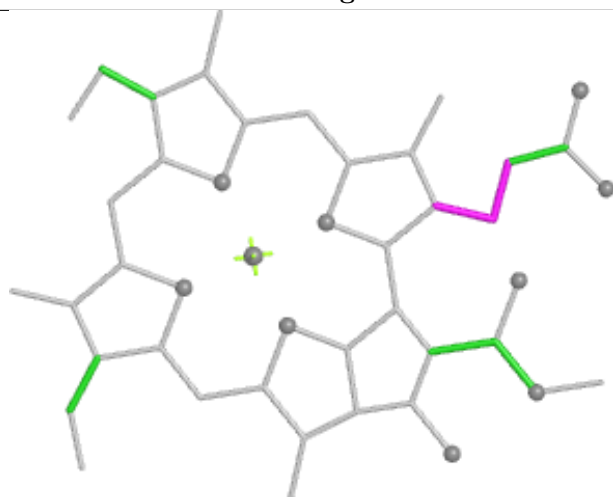
Ligand CLA B 811



Bond lengths



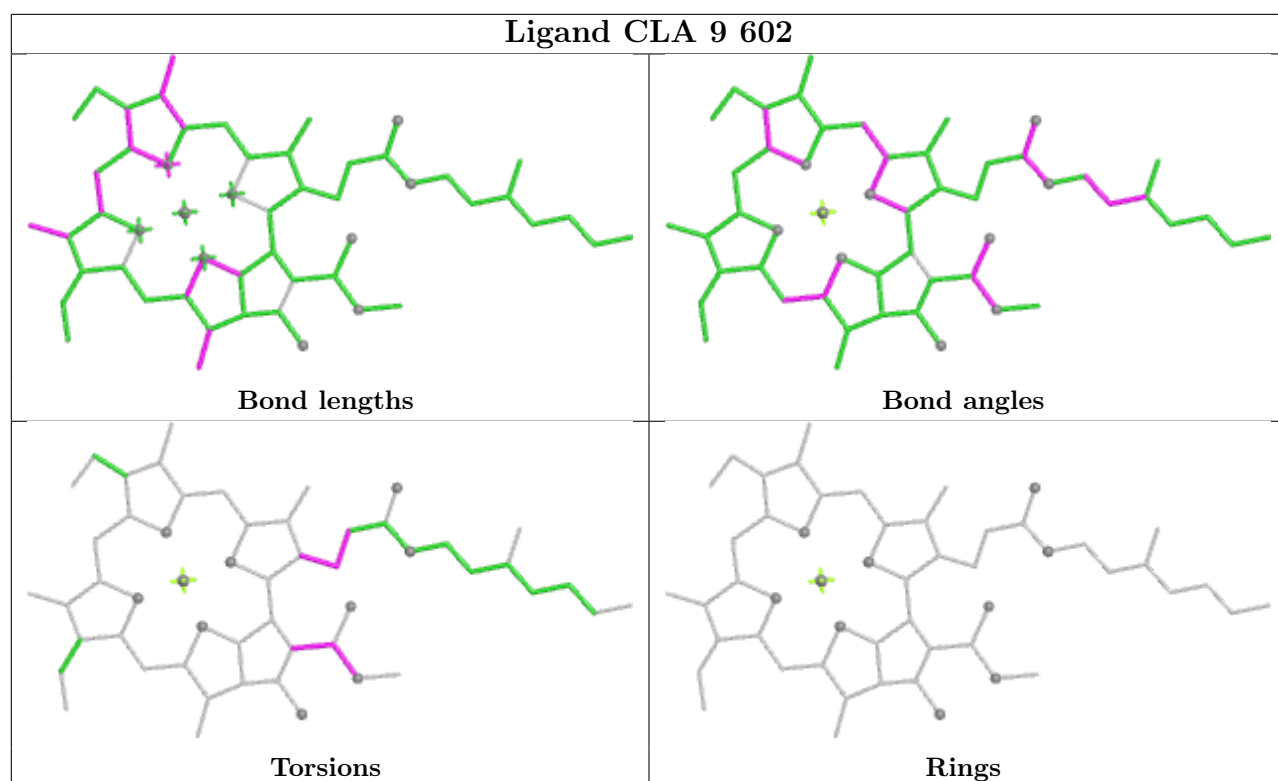
Bond angles



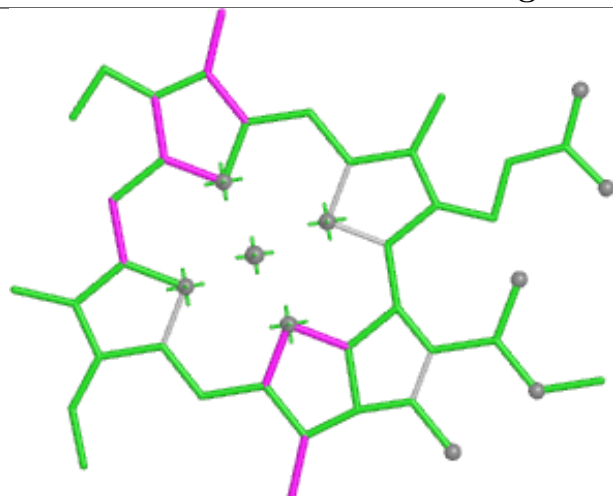
Torsions



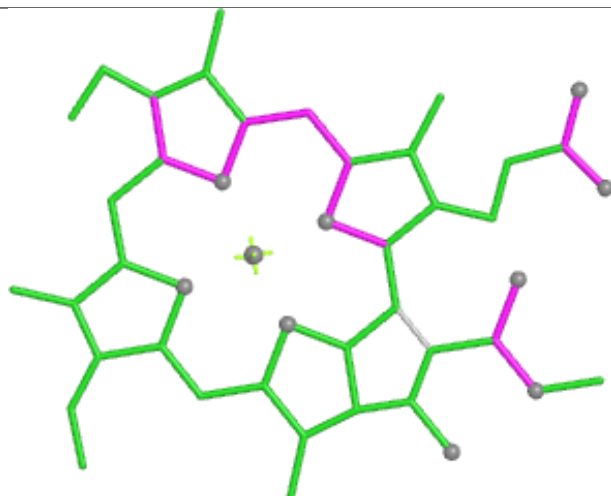
Rings



Ligand CLA 2 612



Bond lengths



Bond angles

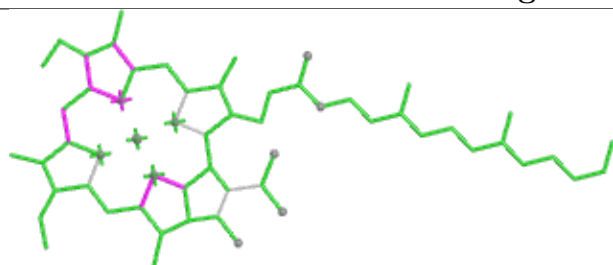


Torsions

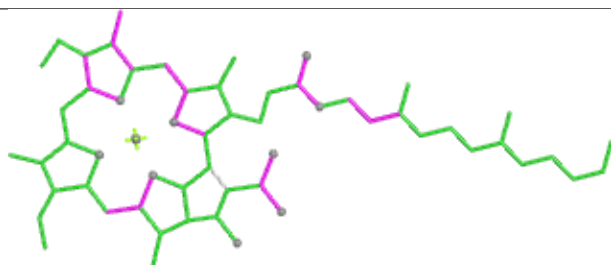


Rings

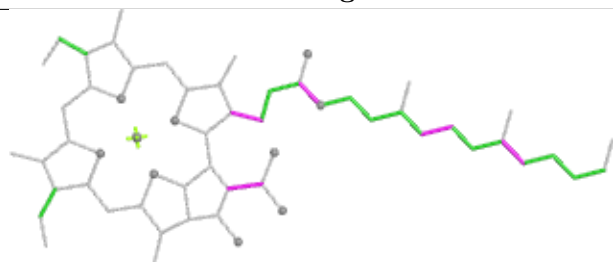
Ligand CLA 8 602



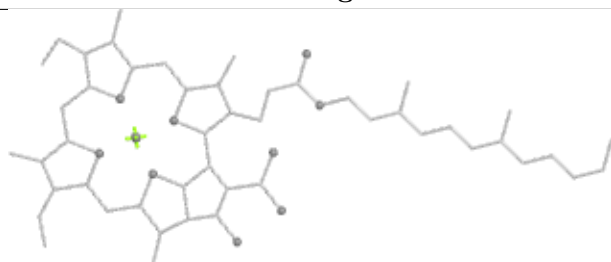
Bond lengths



Bond angles

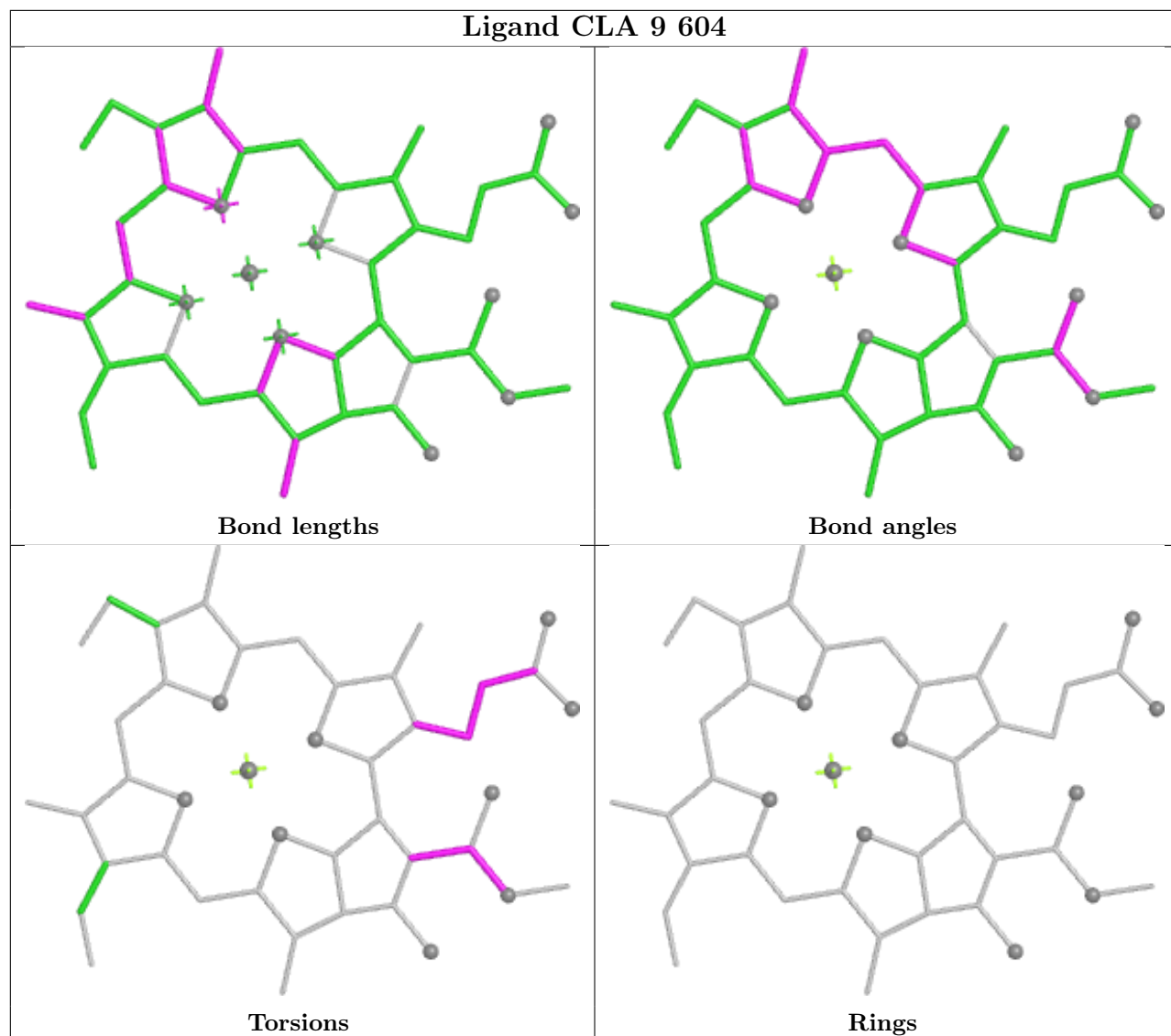


Torsions

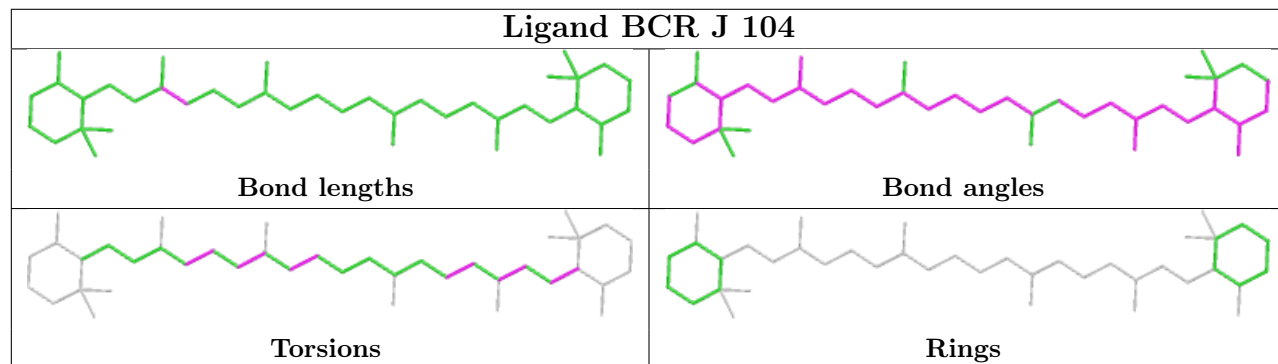


Rings

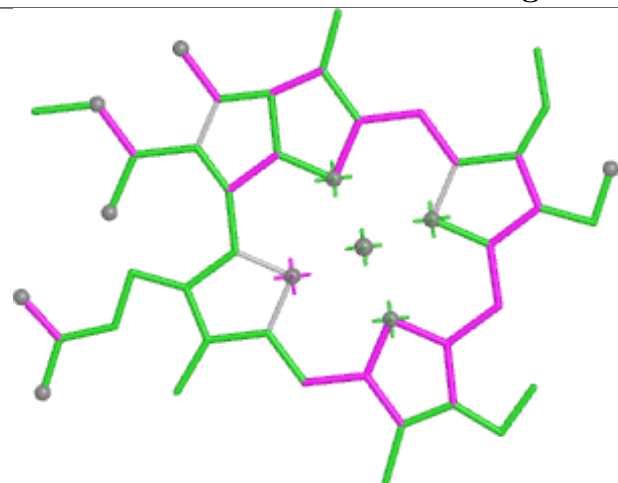
Ligand CLA 9 604



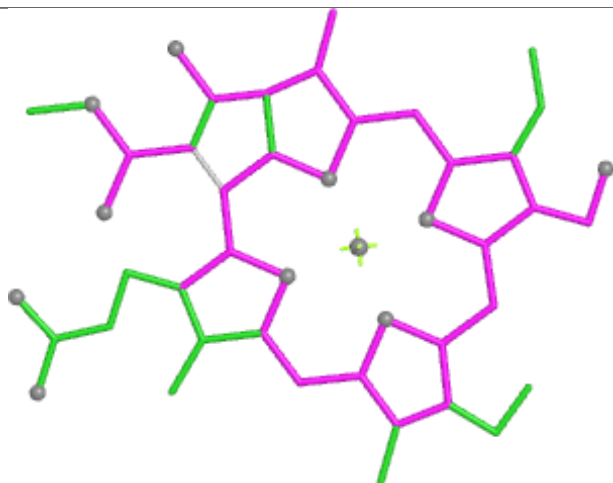
Ligand BCR J 104



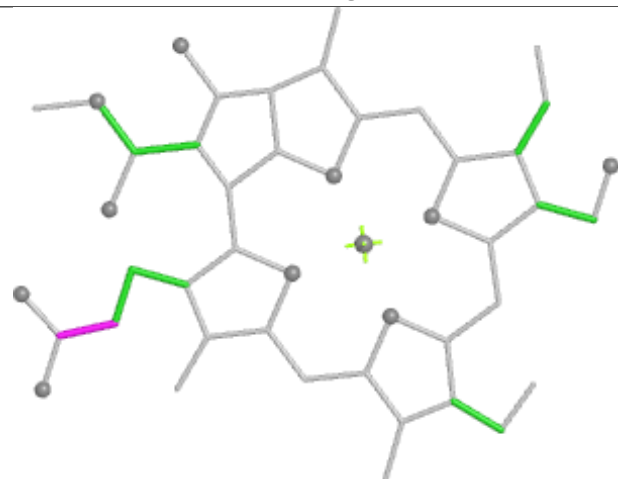
Ligand CHL 2 606



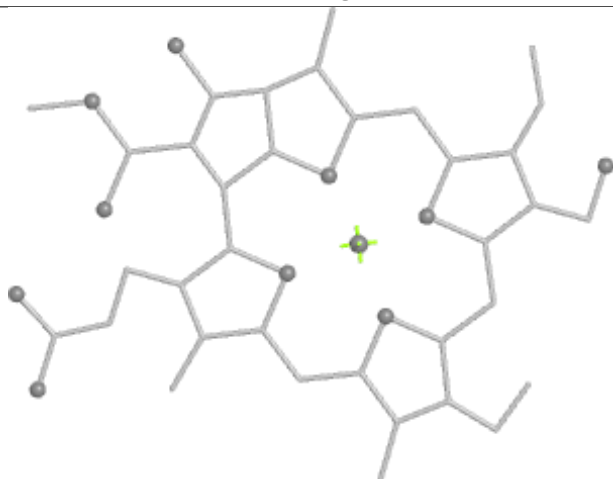
Bond lengths



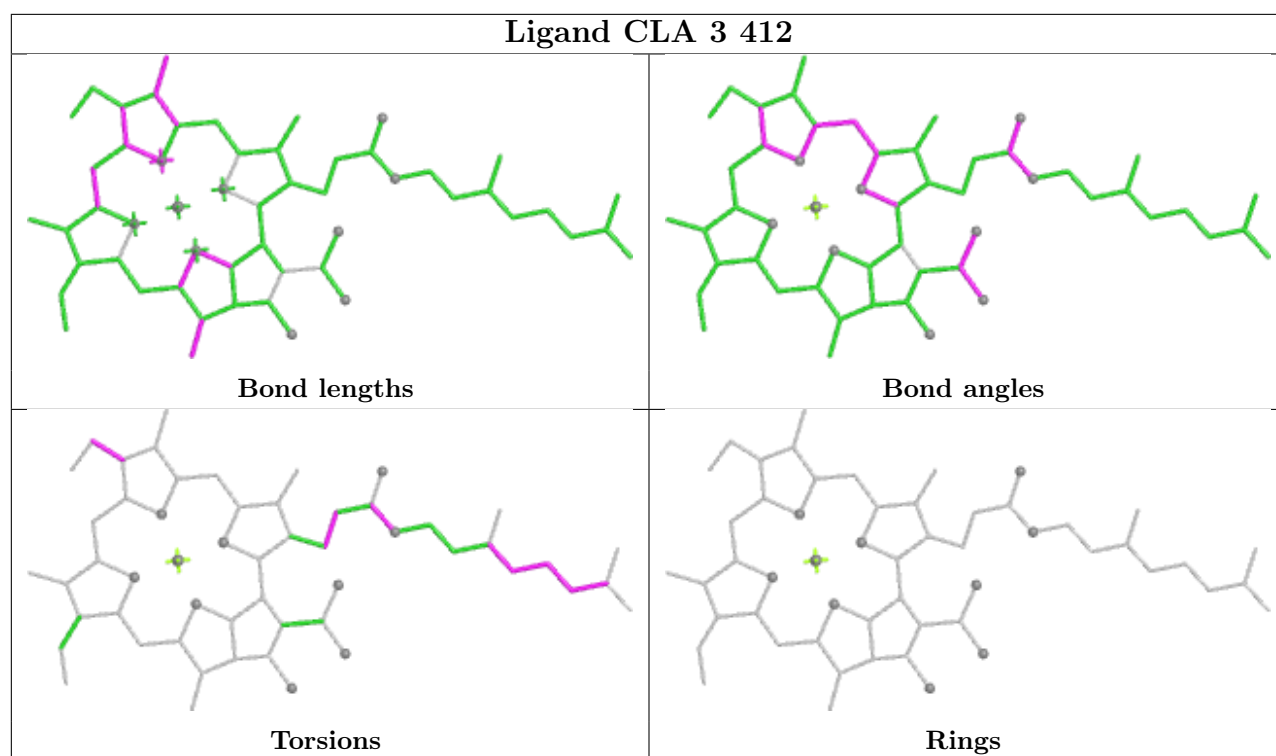
Bond angles



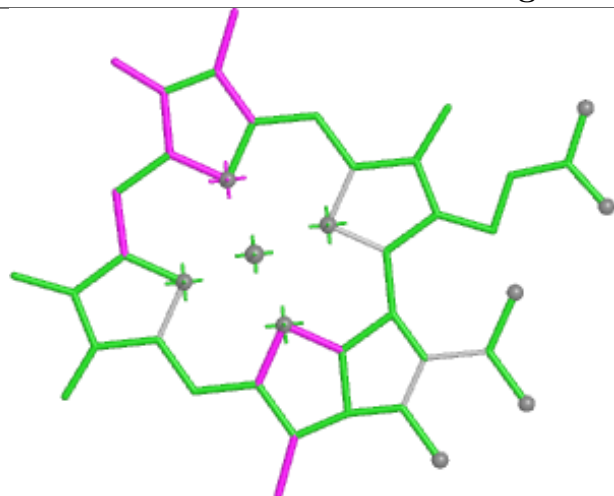
Torsions



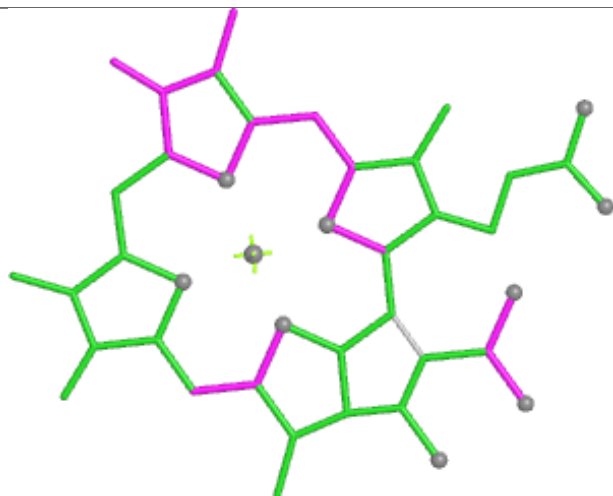
Rings



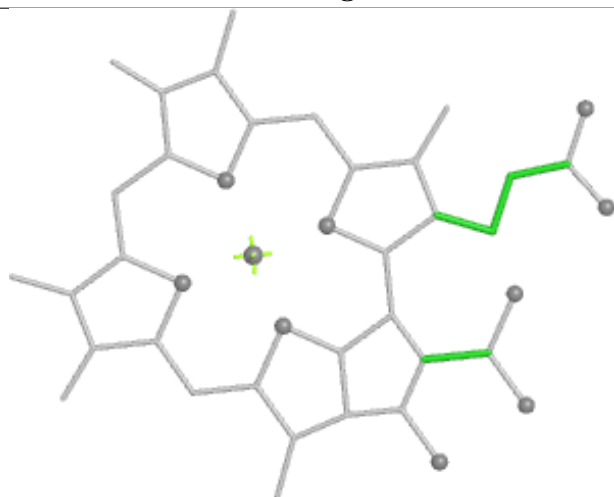
Ligand CLA 3 404



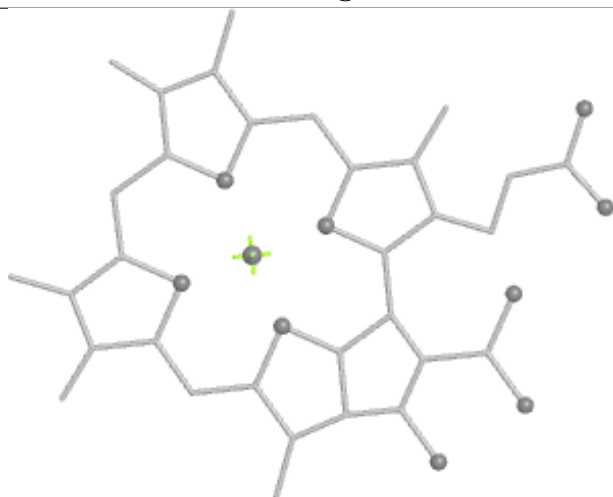
Bond lengths



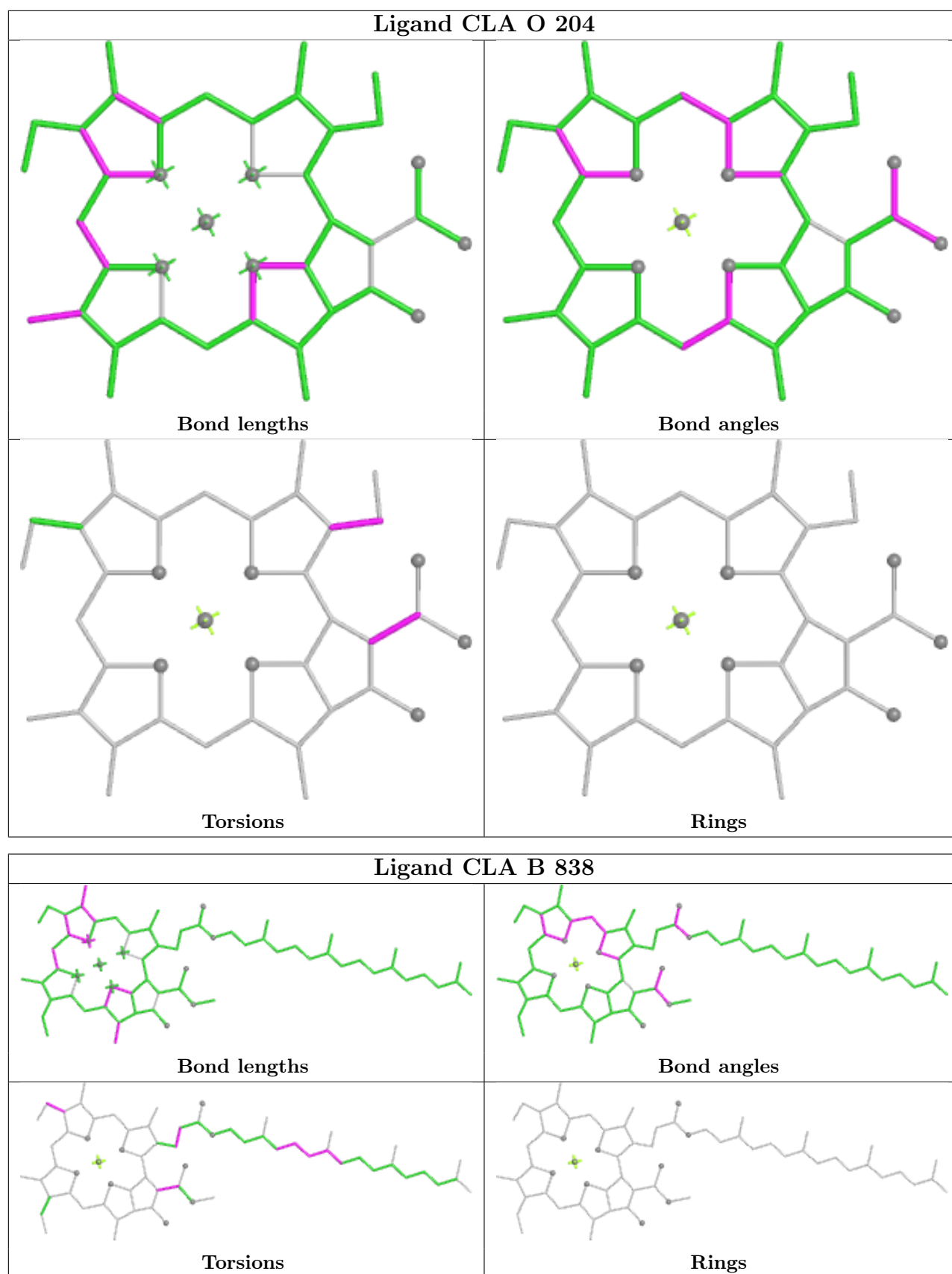
Bond angles



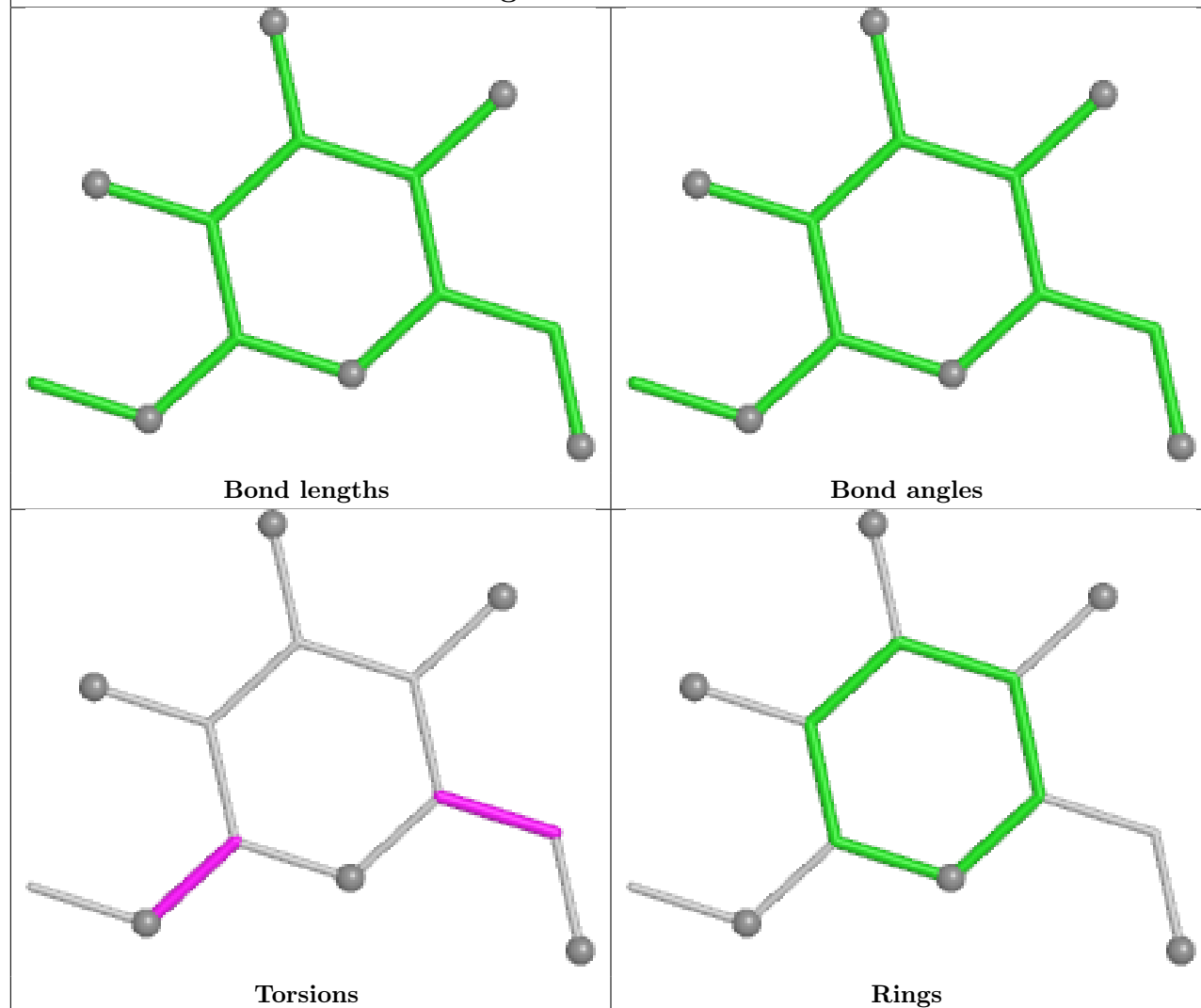
Torsions



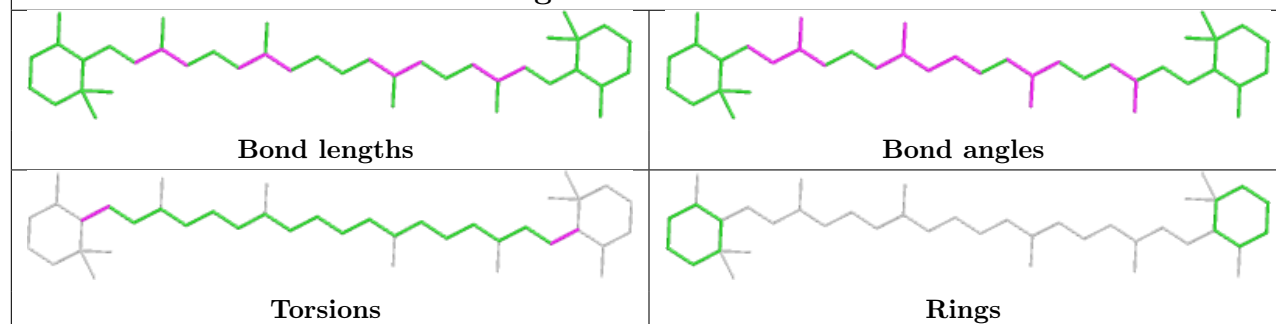
Rings

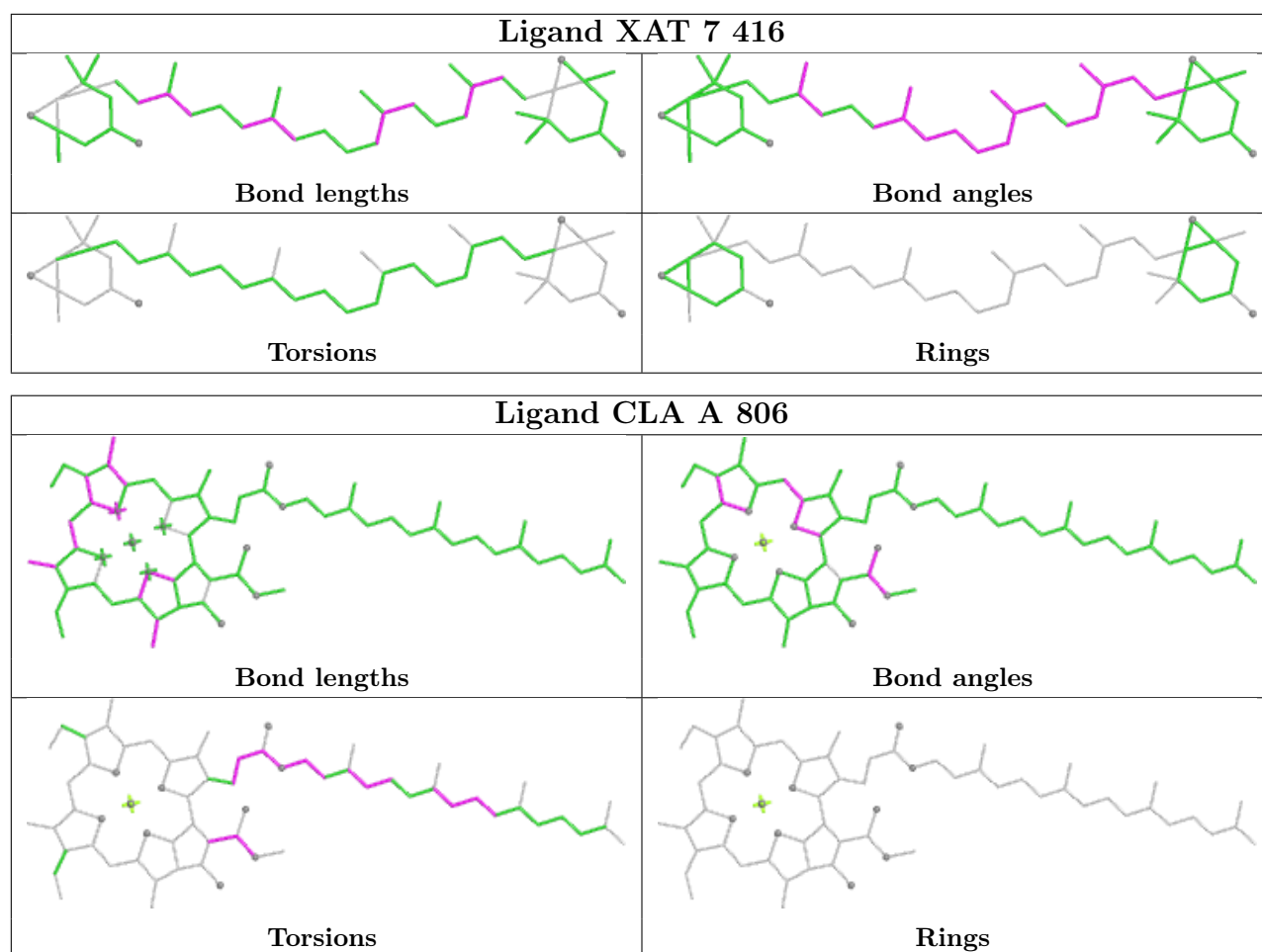


Ligand LMG 6 615

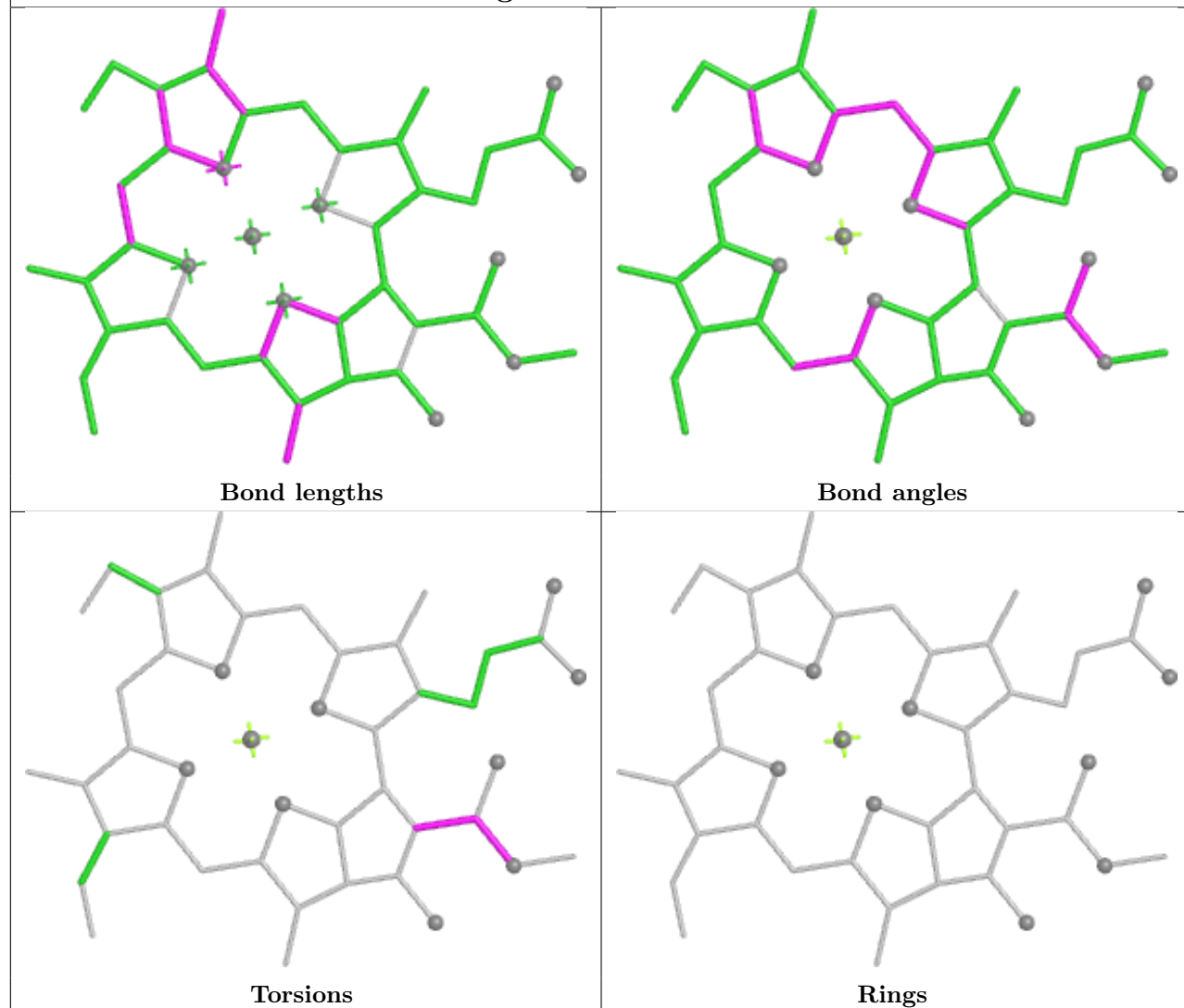


Ligand BCR 4 617

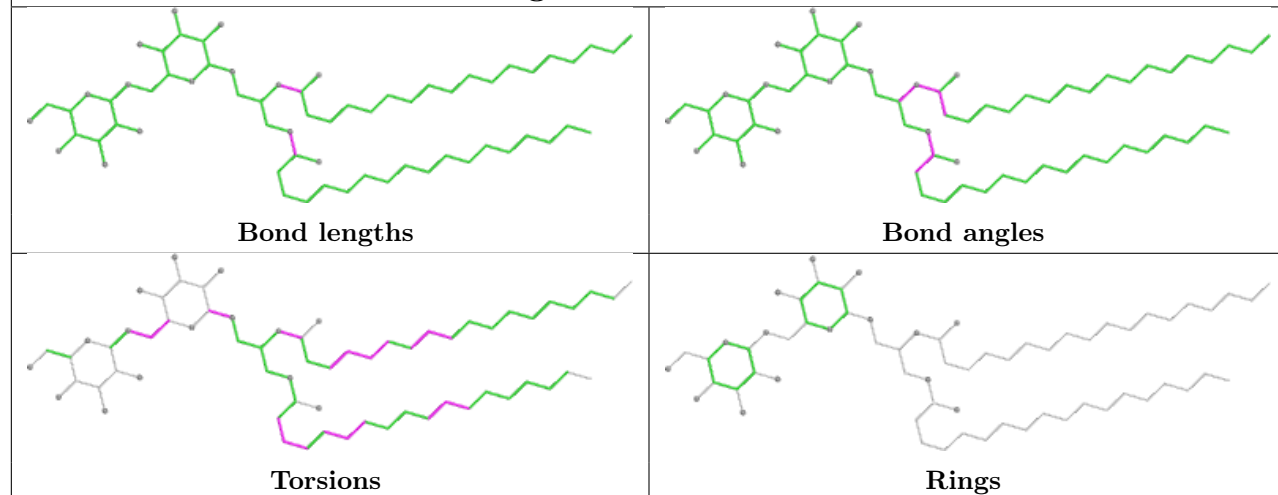




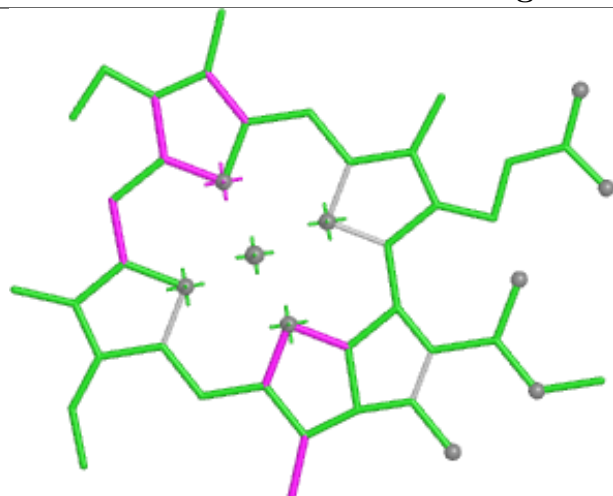
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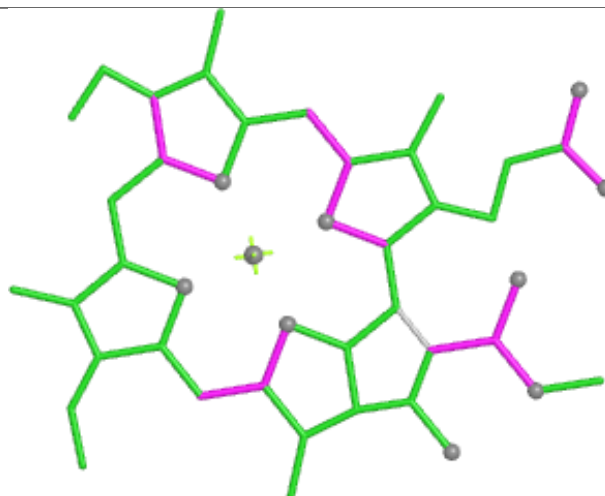
Ligand DGD B 847



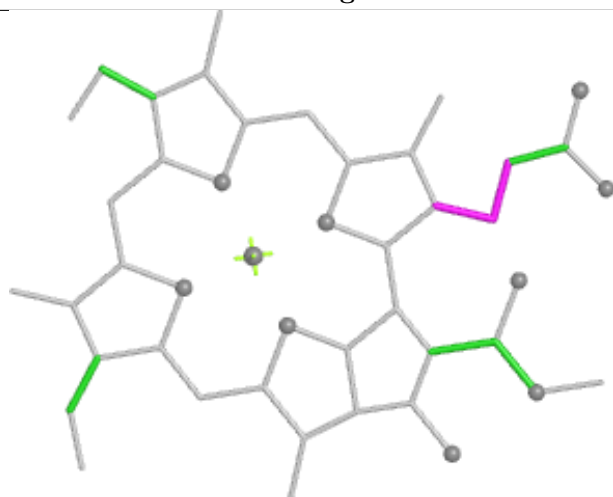
Ligand CLA L 303



Bond lengths



Bond angles

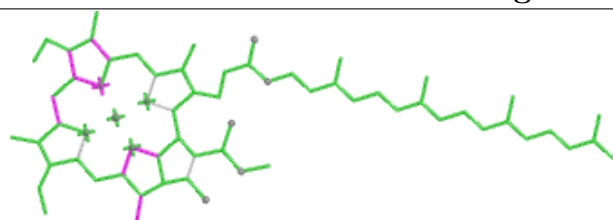


Torsions

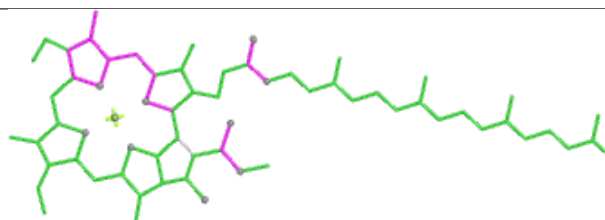


Rings

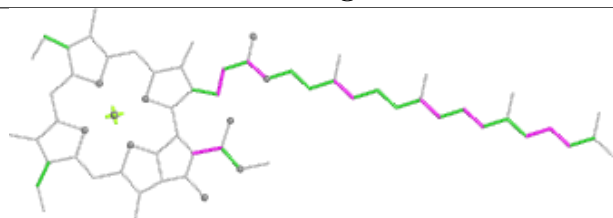
Ligand CLA A 838



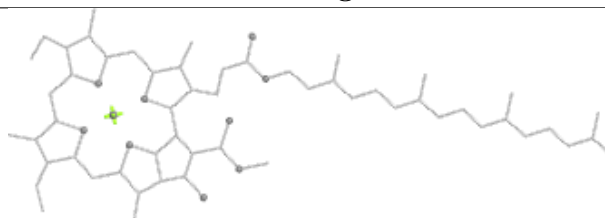
Bond lengths



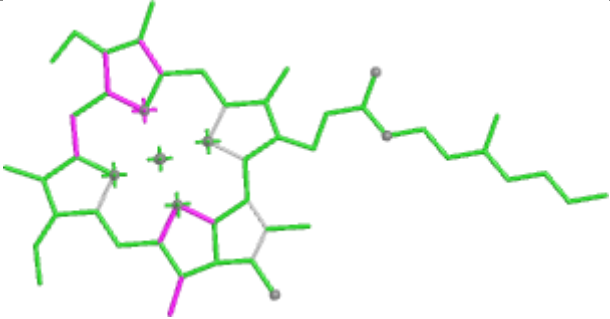
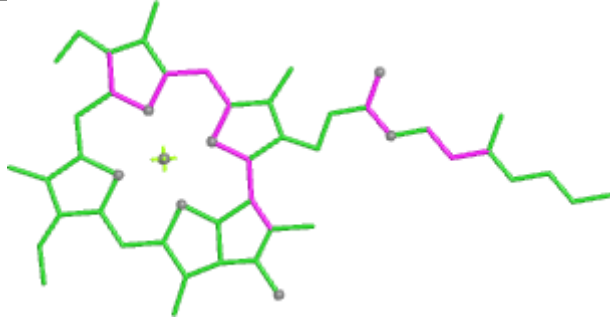
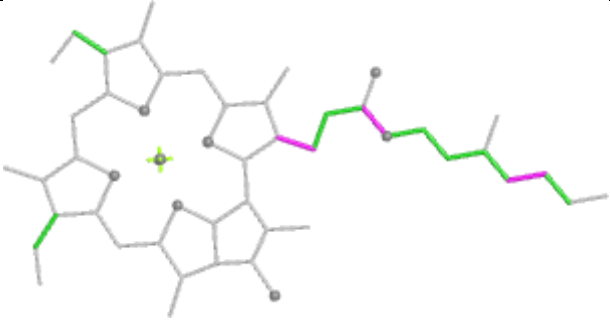
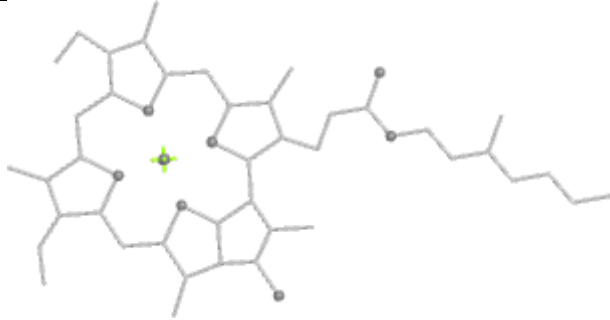
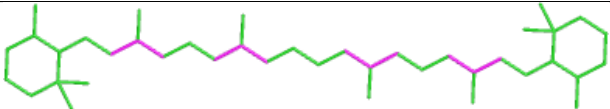
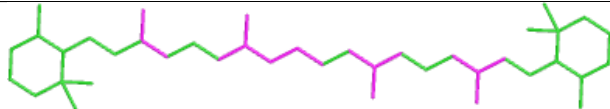
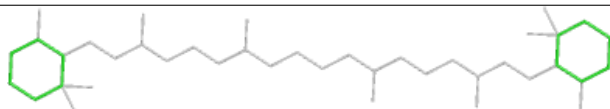
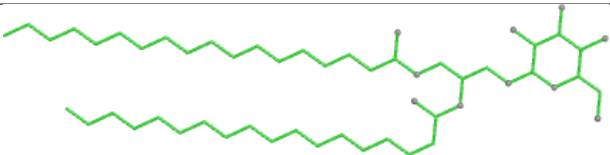
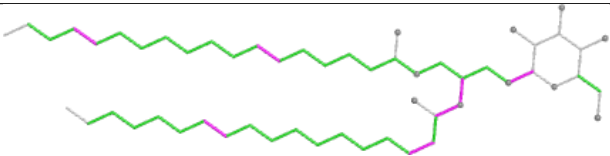
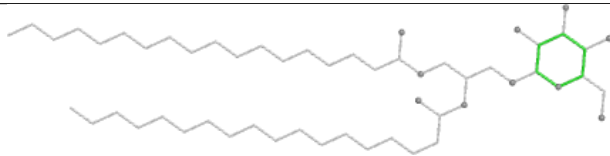
Bond angles



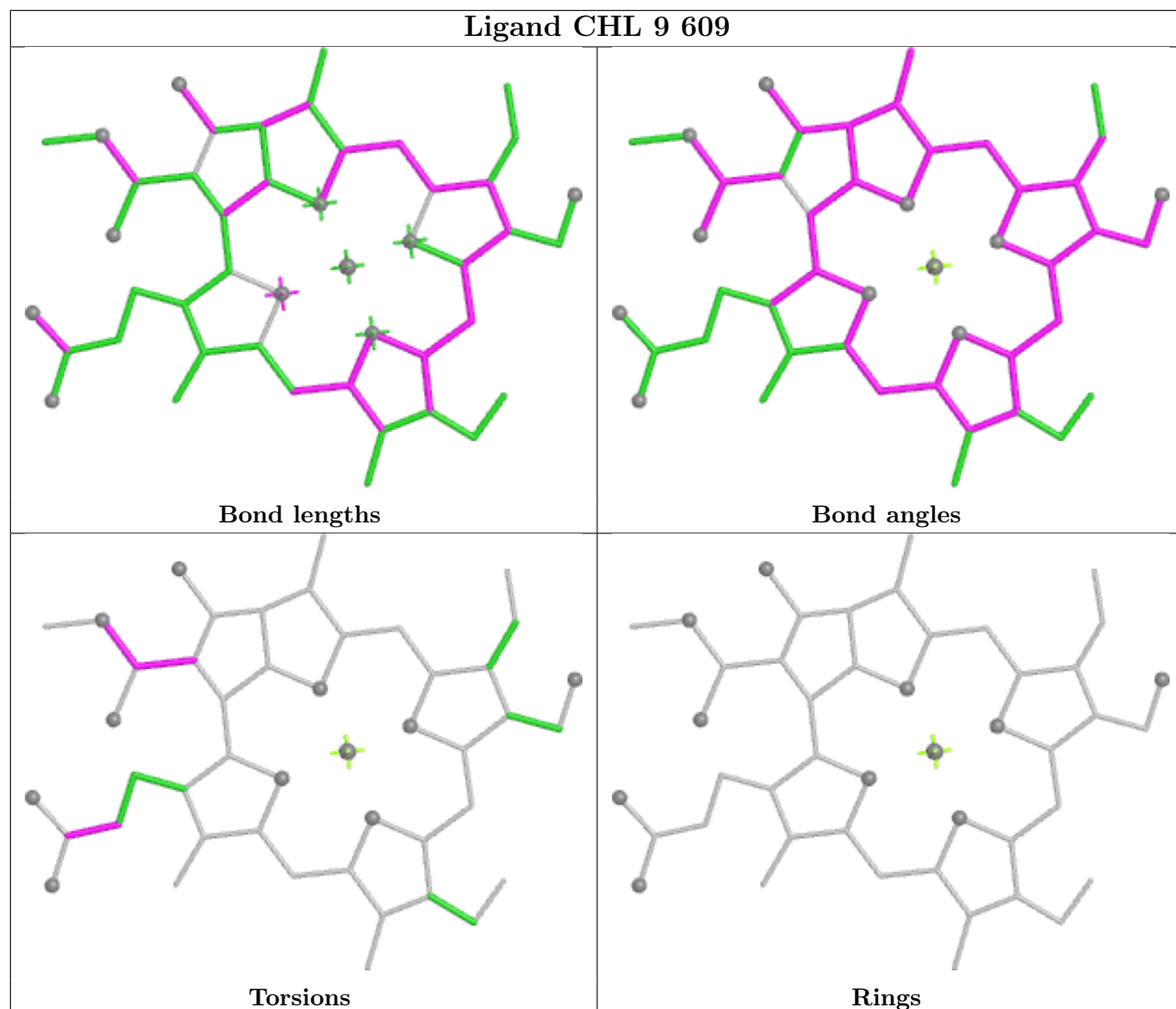
Torsions



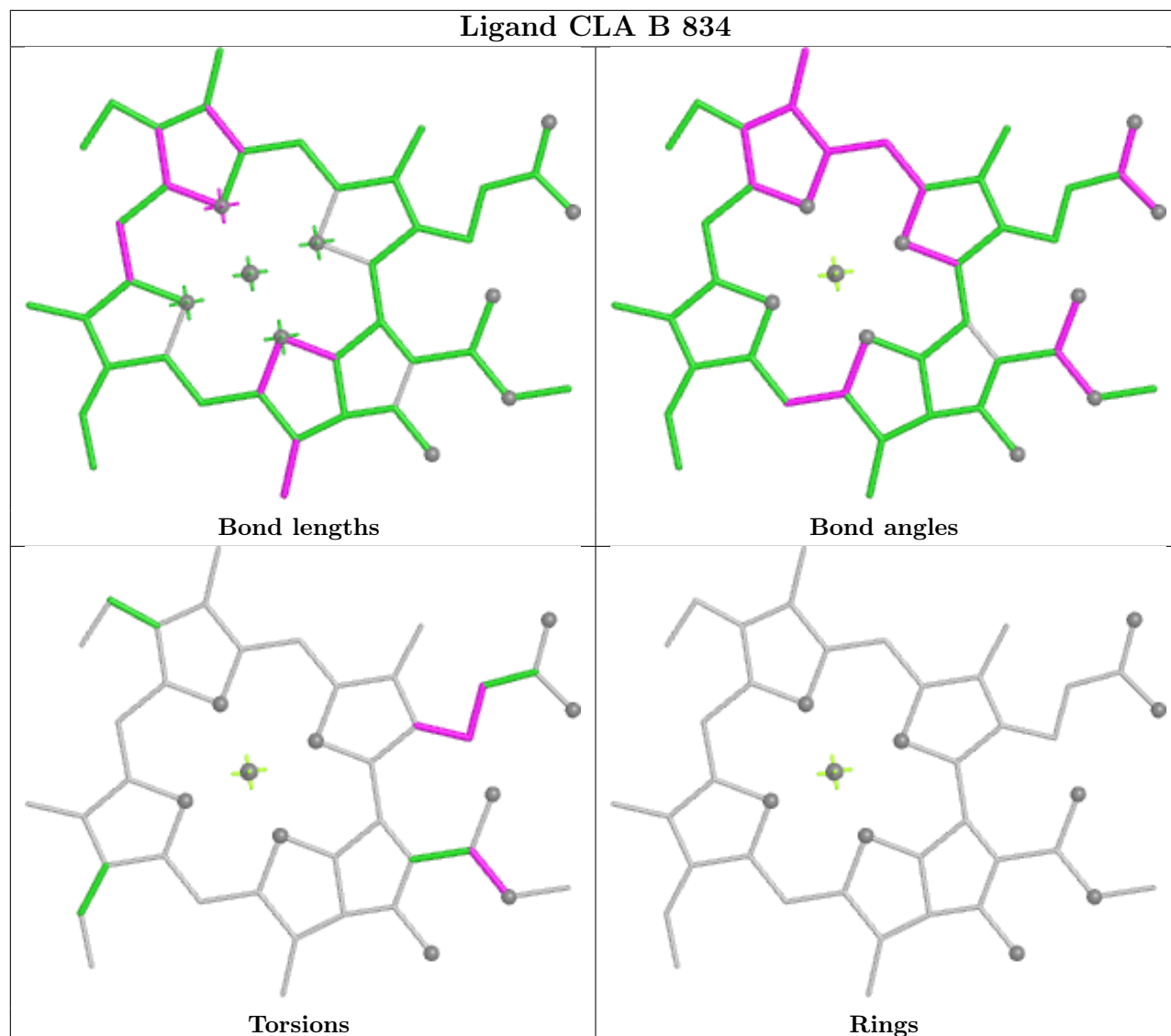
Rings

Ligand CLA O 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG G 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

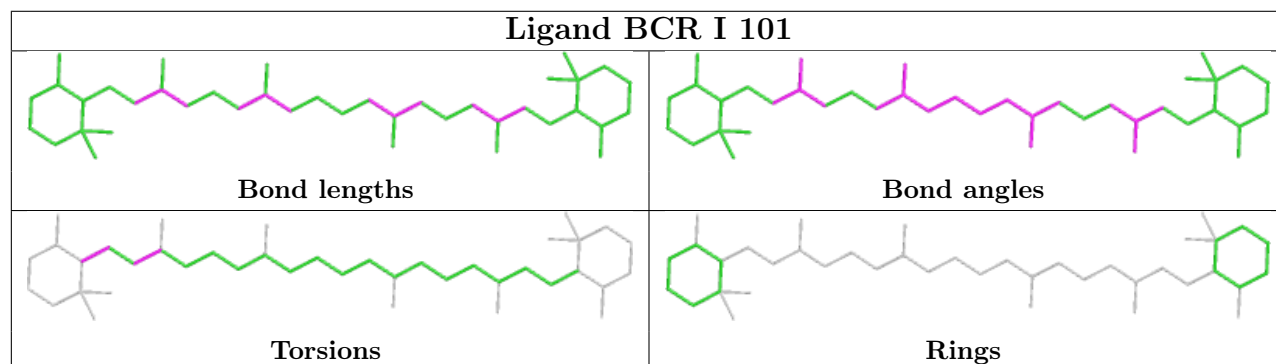
Ligand CHL 9 609

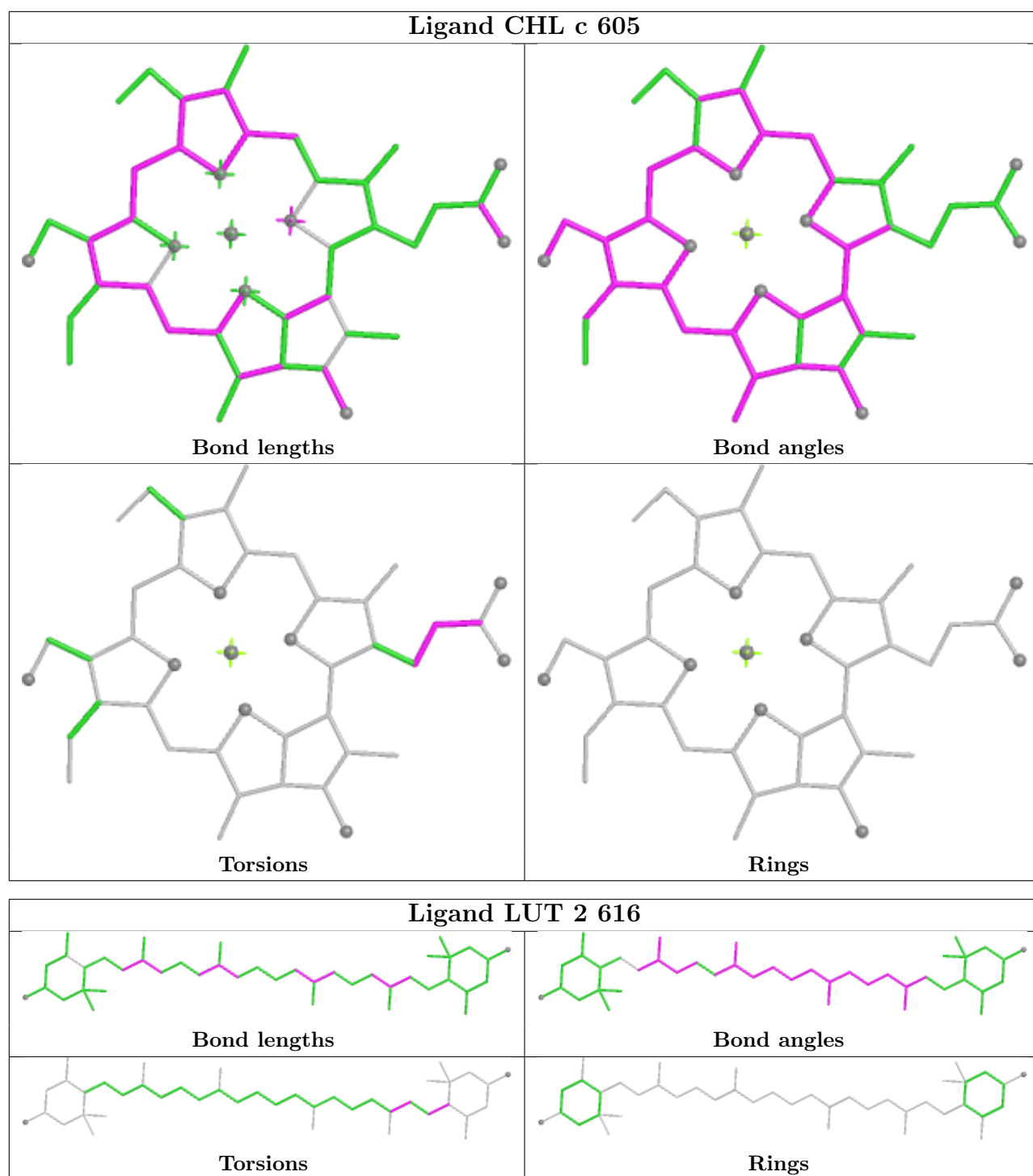


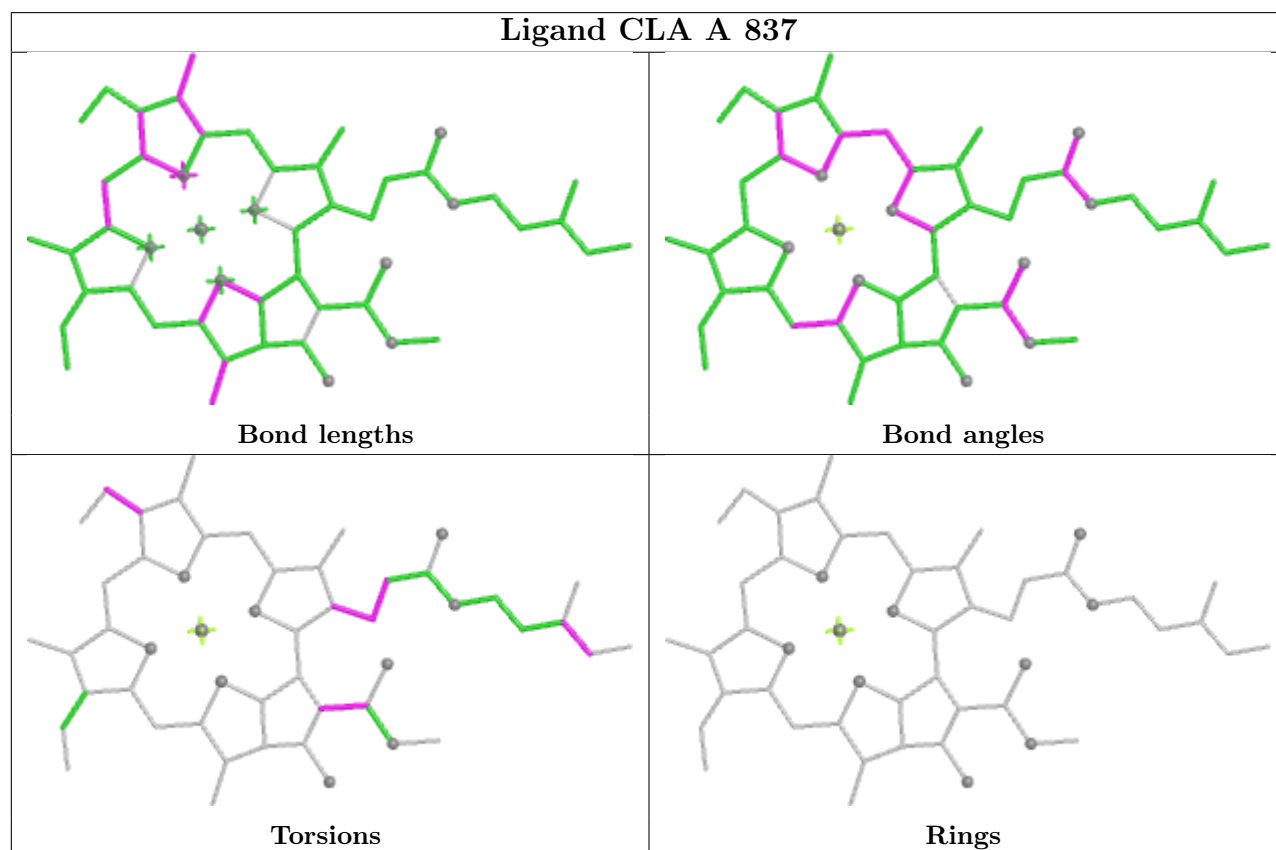
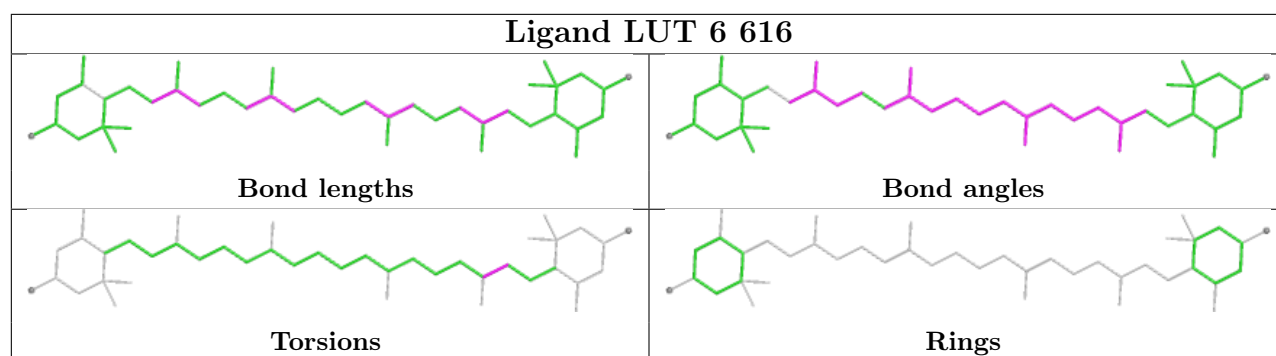
Ligand CLA B 834



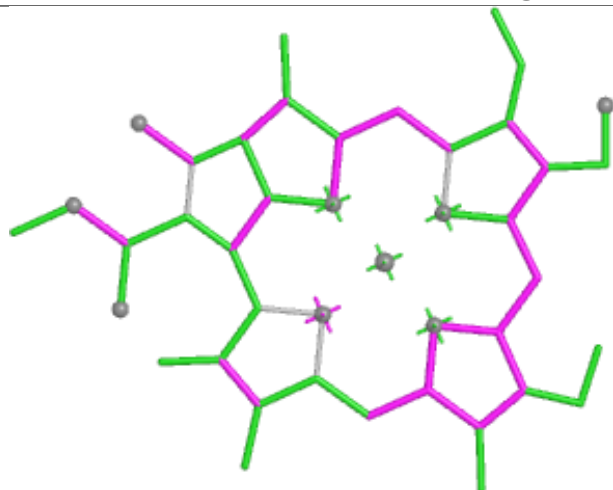
Ligand BCR I 101



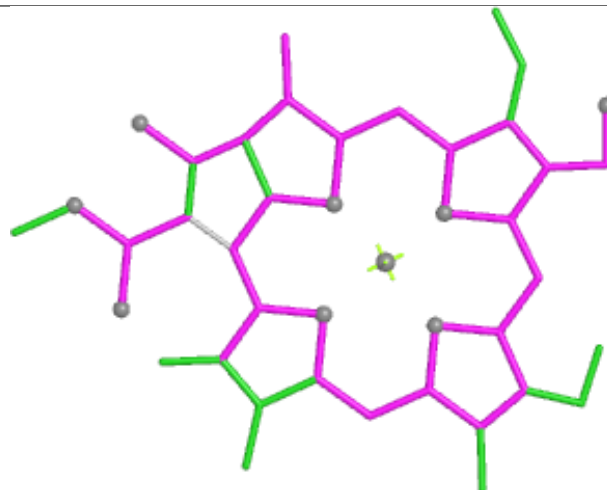




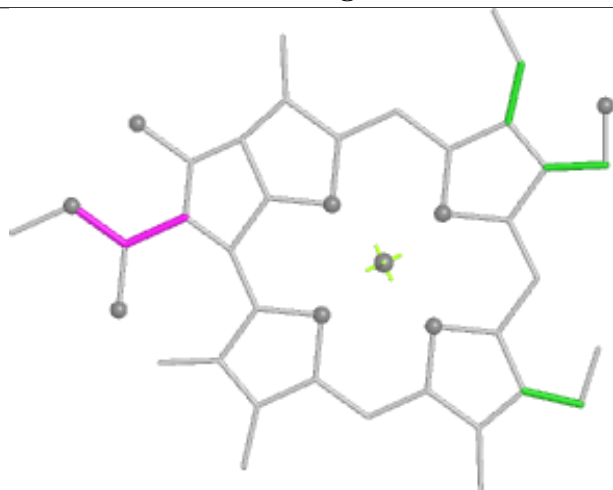
Ligand CHL 8 613



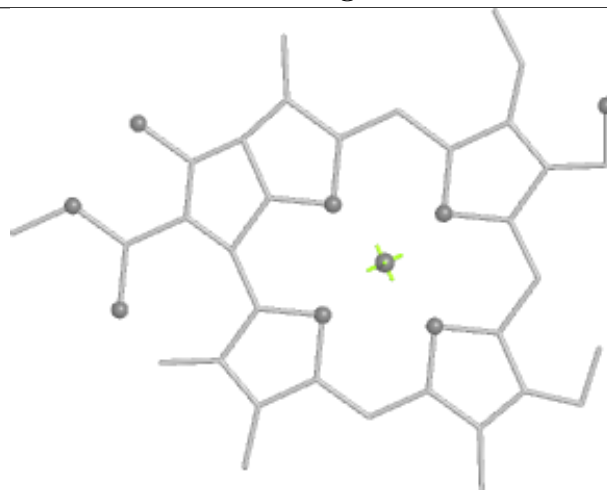
Bond lengths



Bond angles

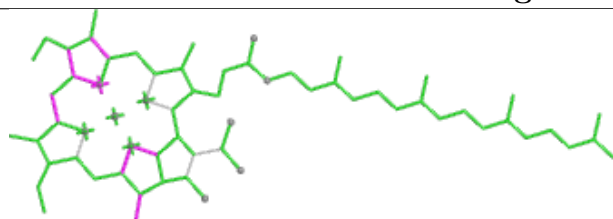


Torsions

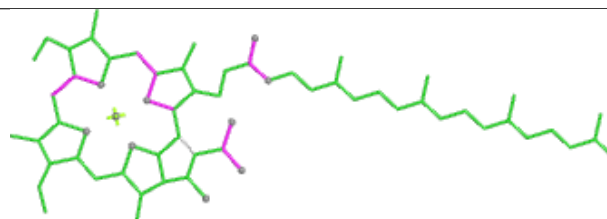


Rings

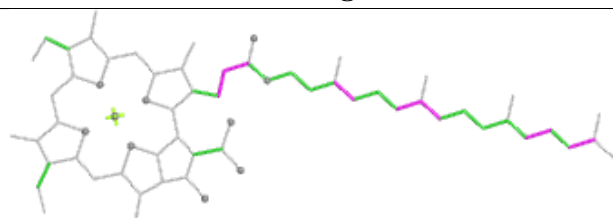
Ligand CLA B 837



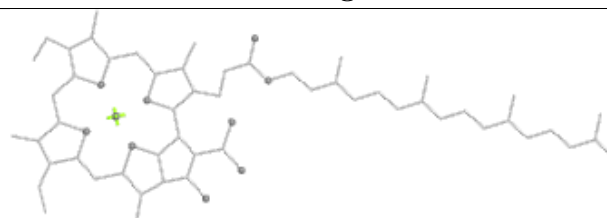
Bond lengths



Bond angles

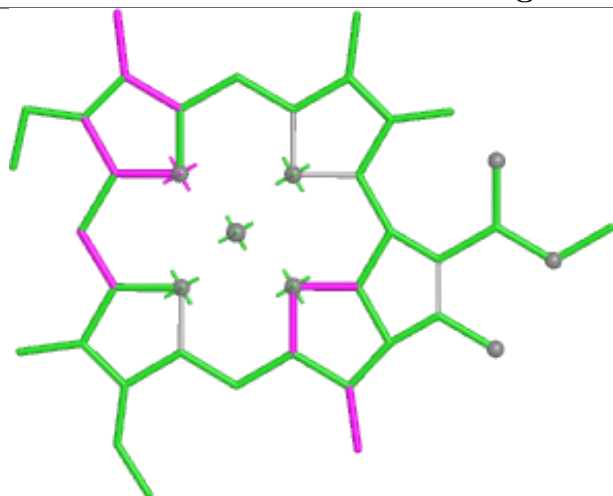


Torsions

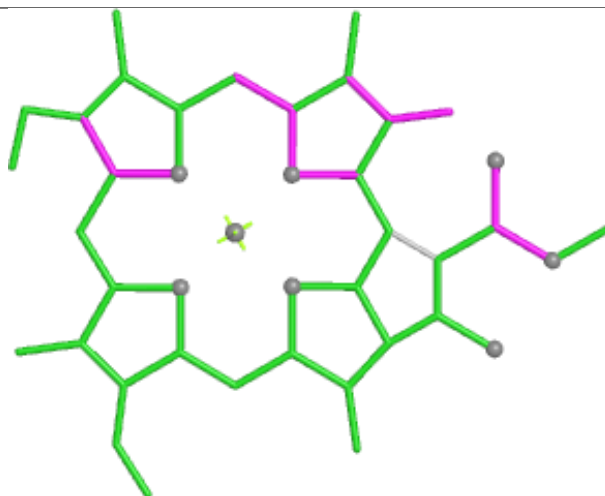


Rings

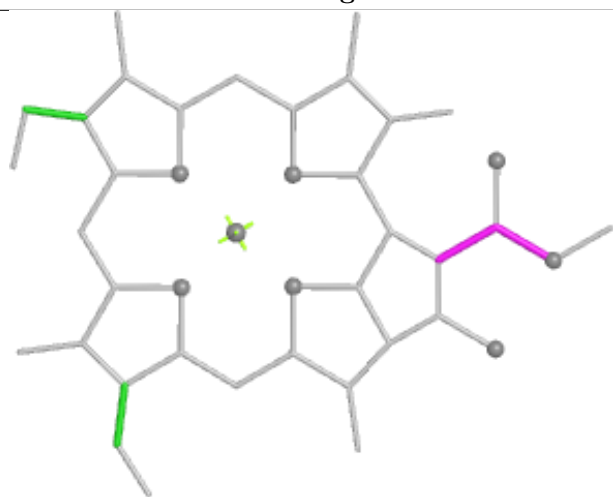
Ligand CLA F 305



Bond lengths



Bond angles

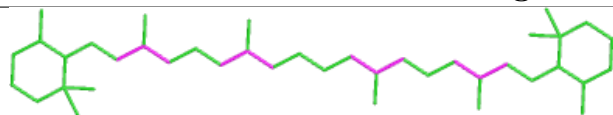


Torsions

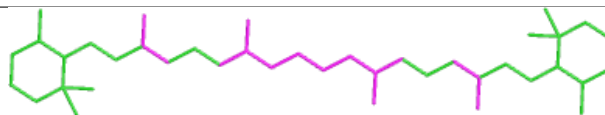


Rings

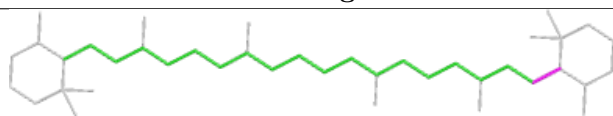
Ligand BCR B 845



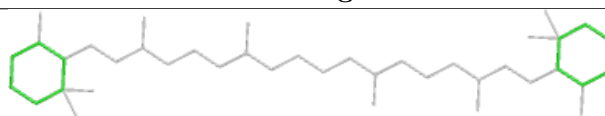
Bond lengths



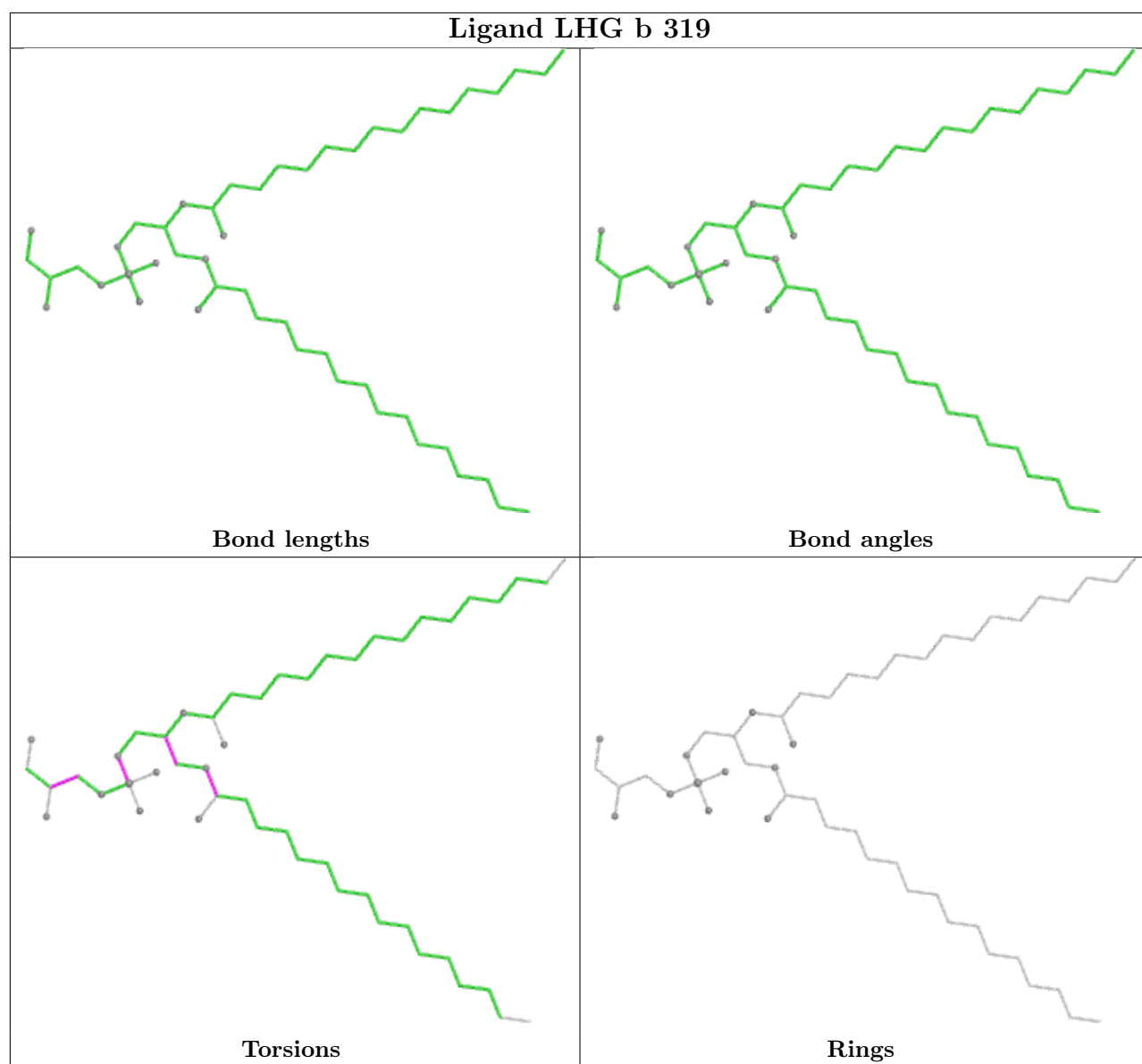
Bond angles

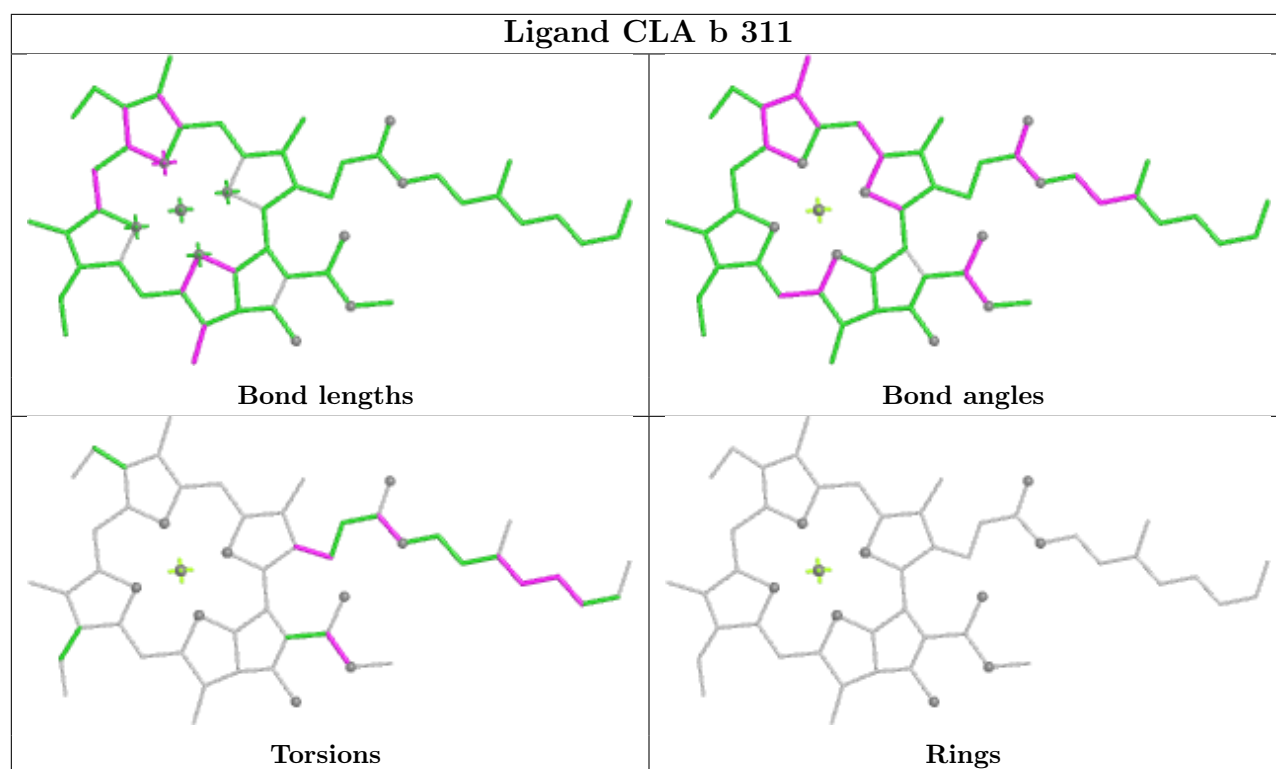


Torsions

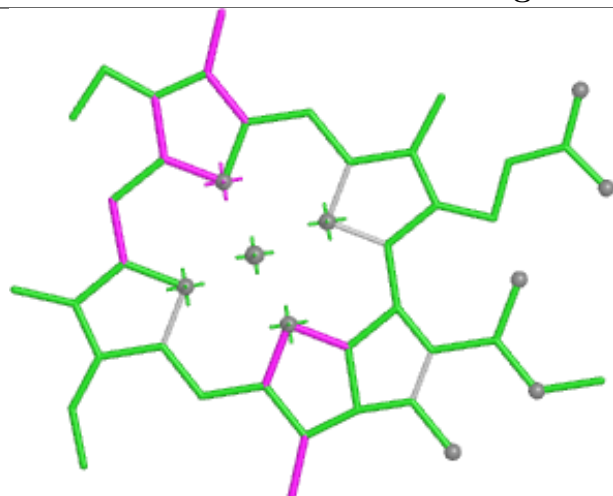


Rings

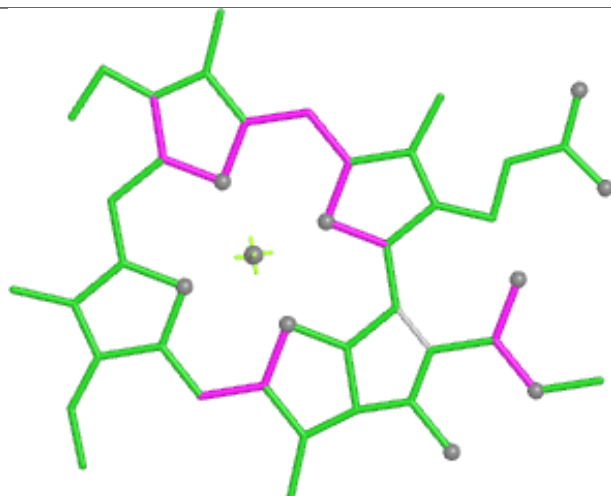




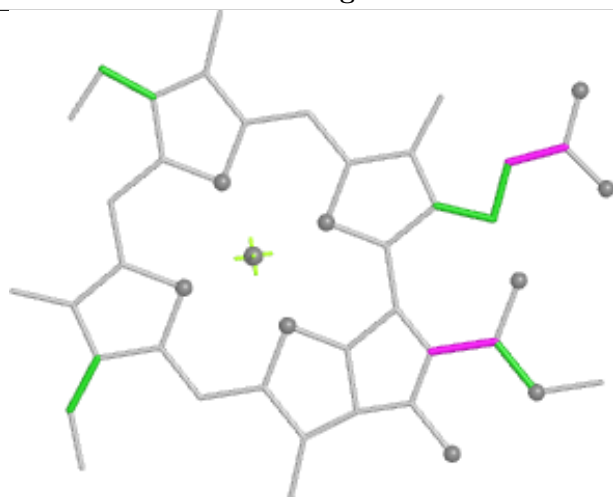
Ligand CLA A 836



Bond lengths



Bond angles

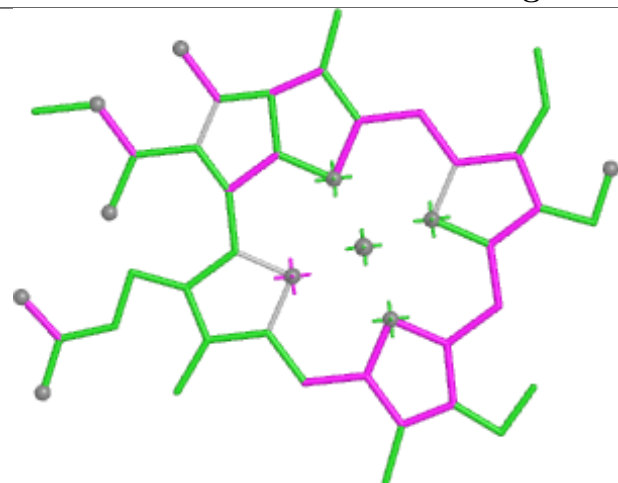


Torsions

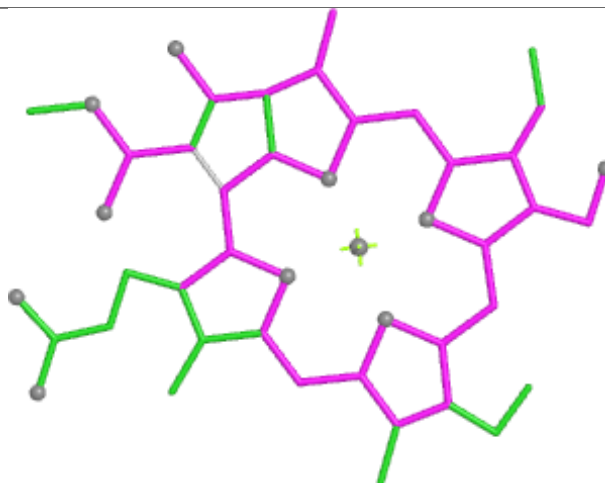


Rings

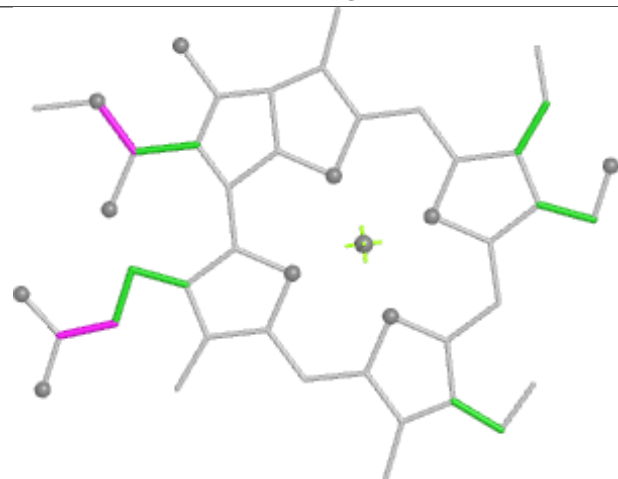
Ligand CHL c 606



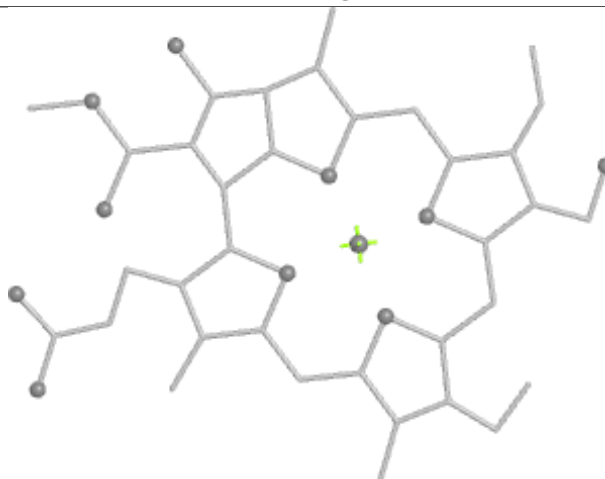
Bond lengths



Bond angles



Torsions

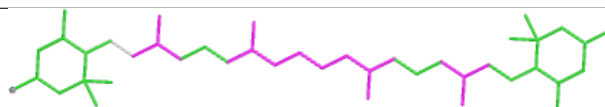


Rings

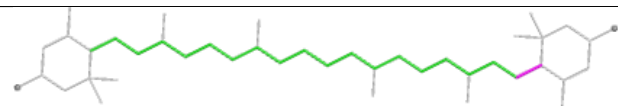
Ligand LUT c 615



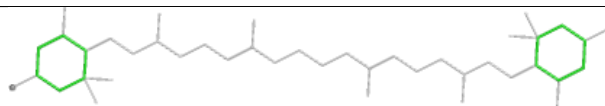
Bond lengths



Bond angles

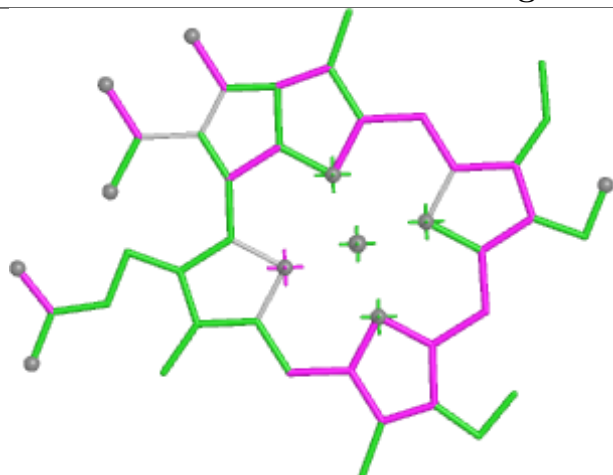


Torsions

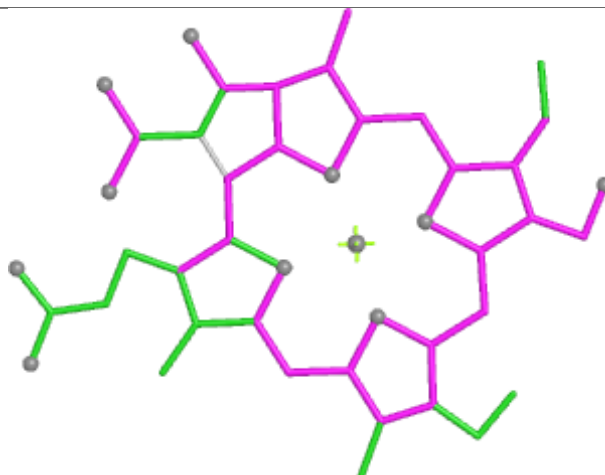


Rings

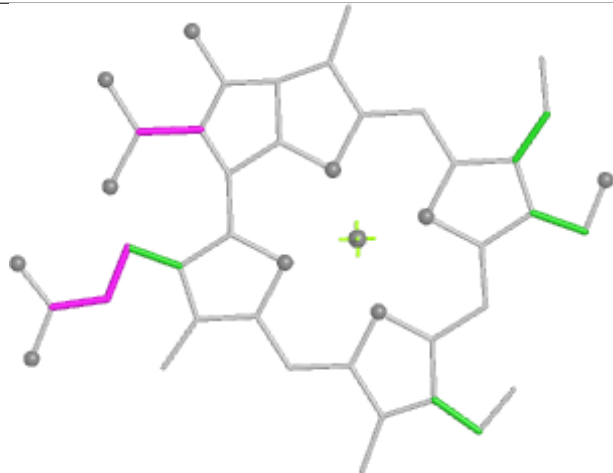
Ligand CHL a 605



Bond lengths



Bond angles

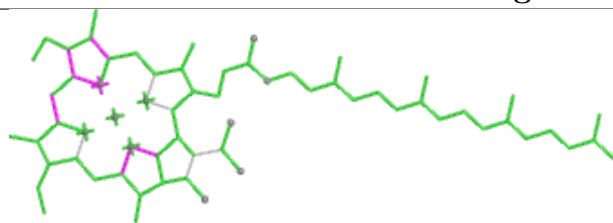


Torsions

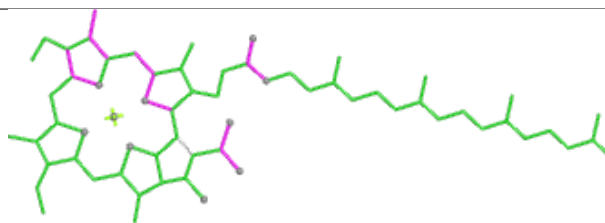


Rings

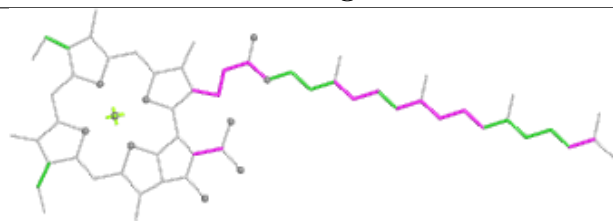
Ligand CLA A 827



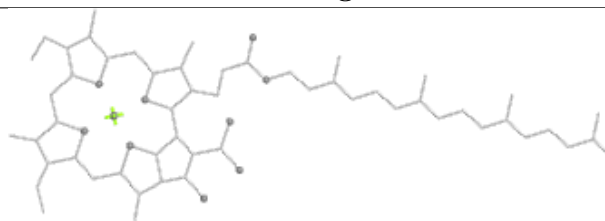
Bond lengths



Bond angles

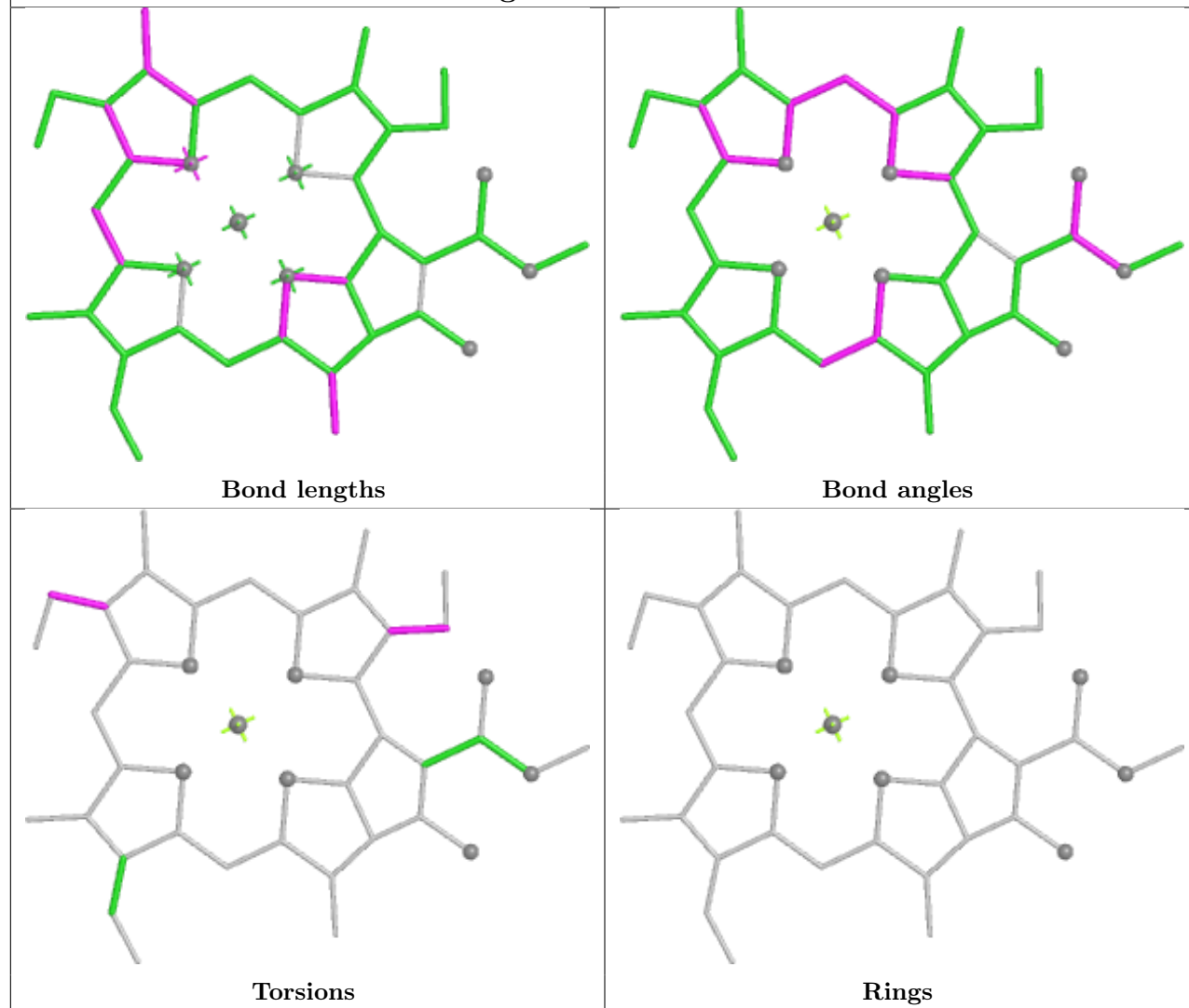


Torsions

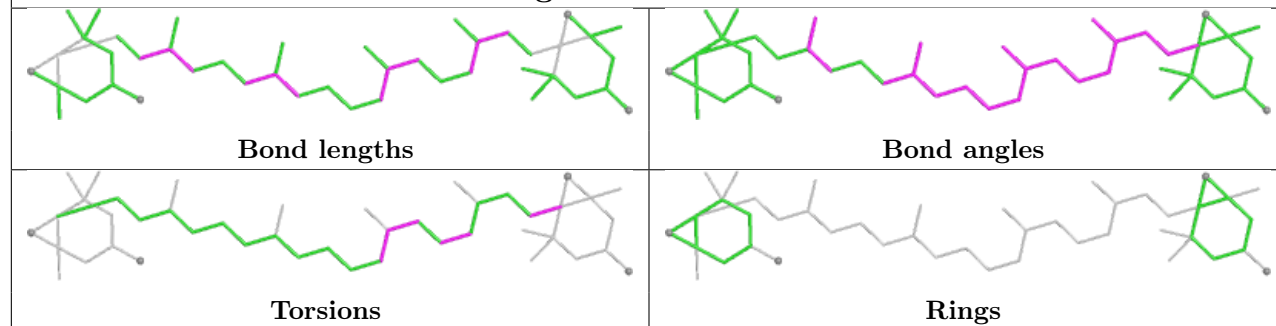


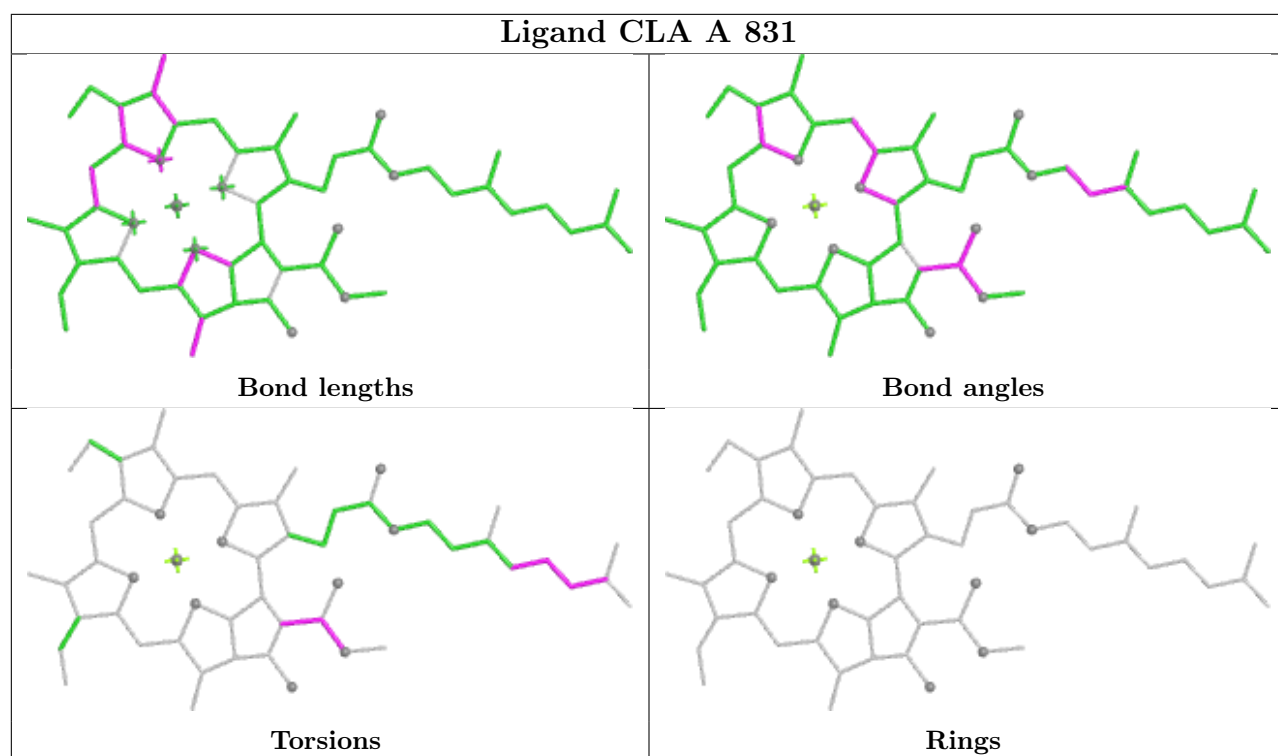
Rings

Ligand CLA 2 613

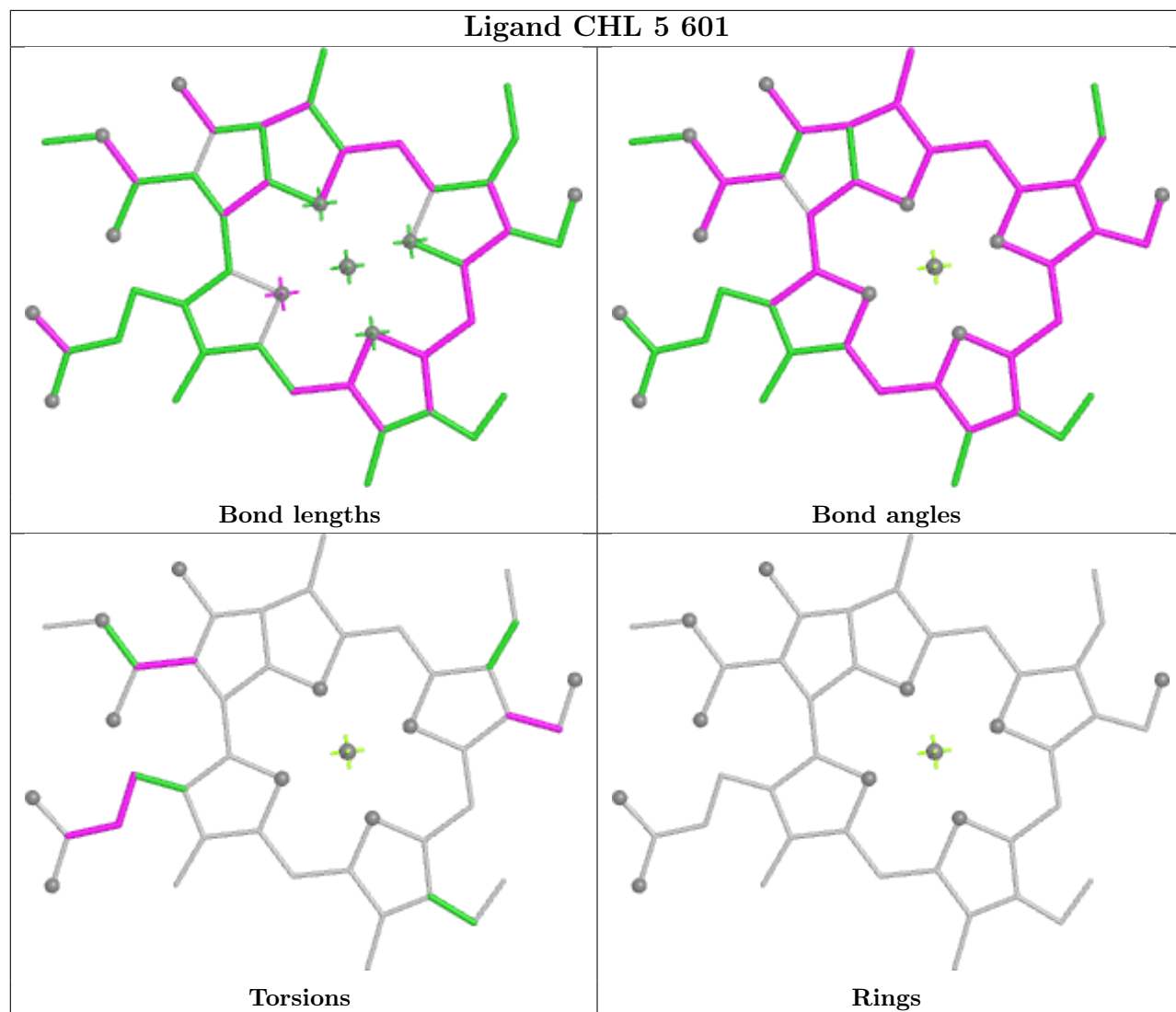


Ligand XAT 6 617

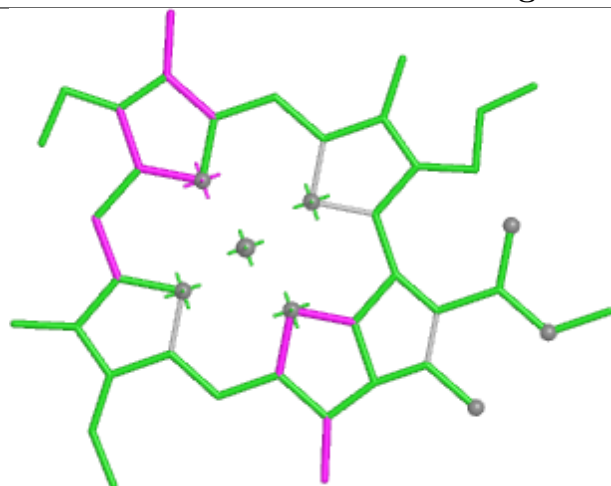




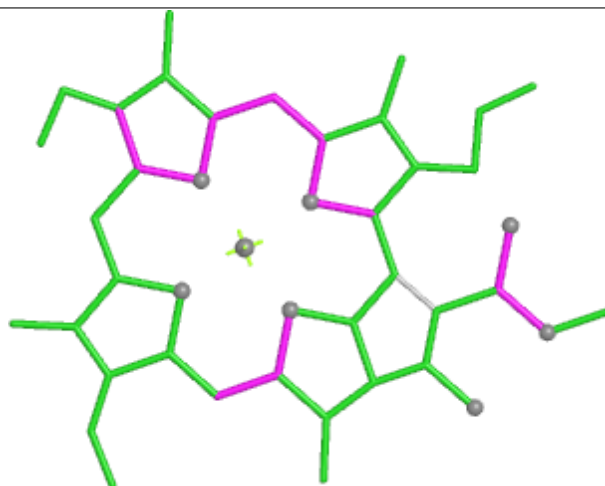
Ligand CHL 5 601



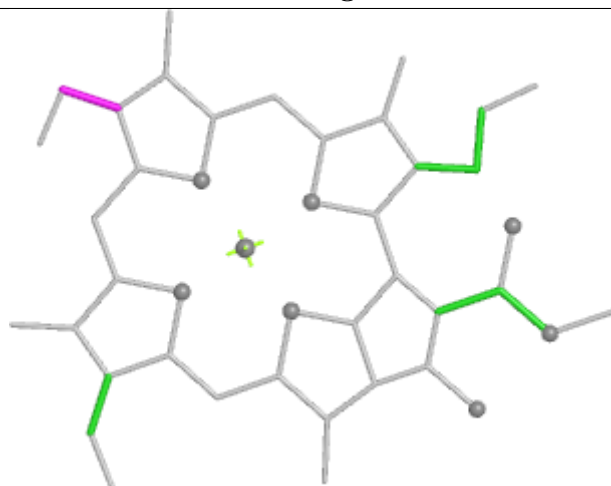
Ligand CLA 4 613



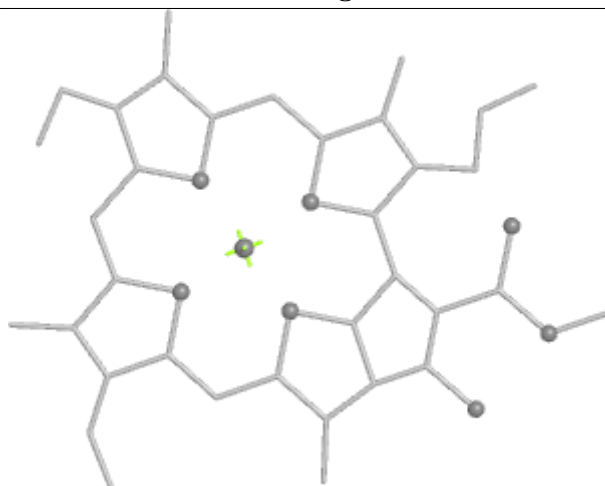
Bond lengths



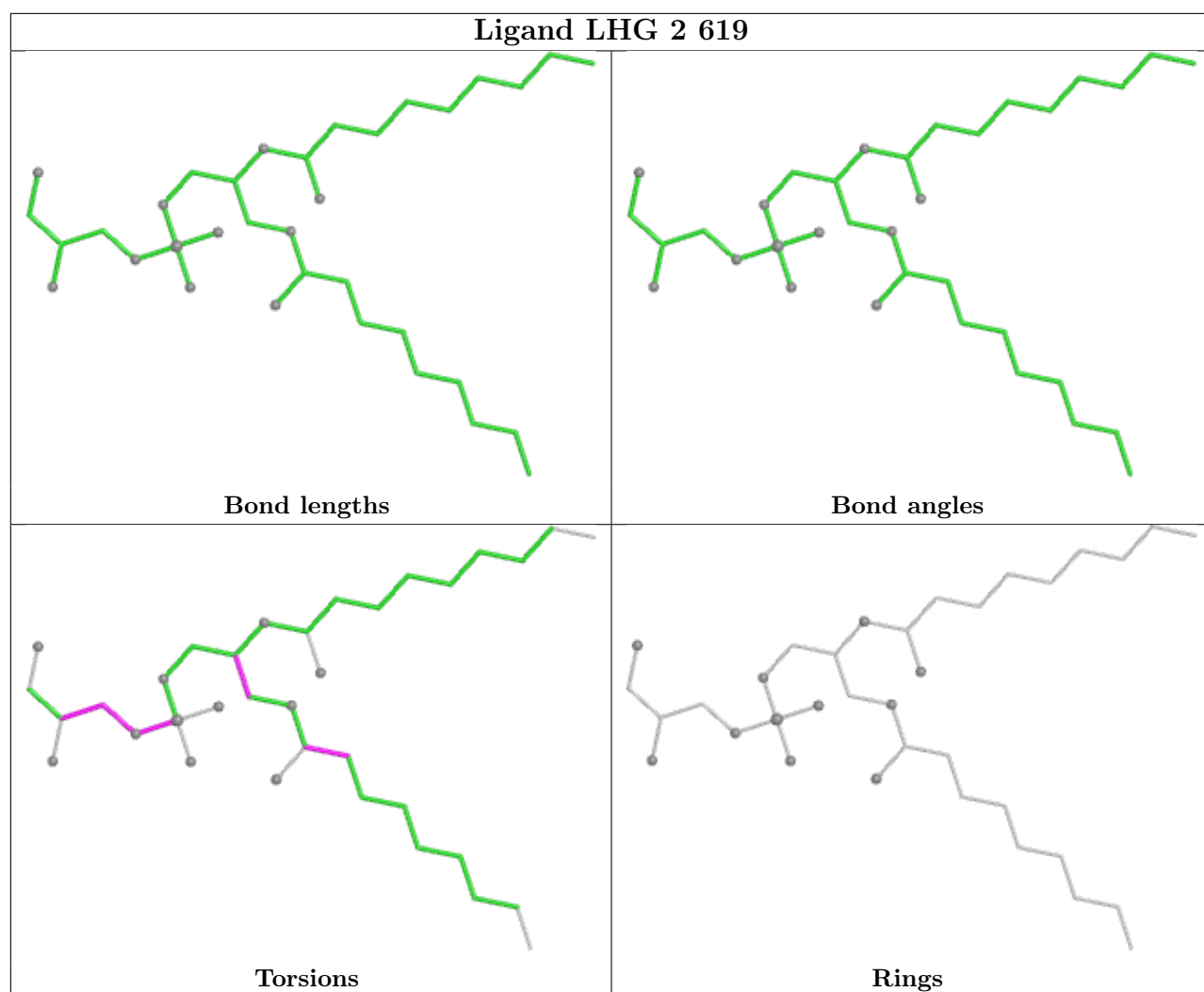
Bond angles



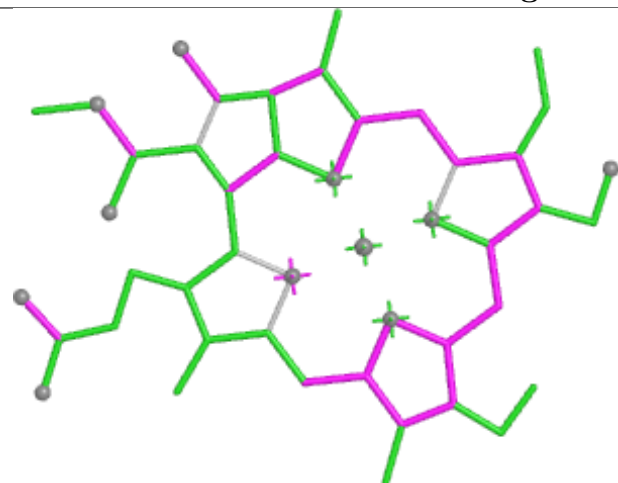
Torsions



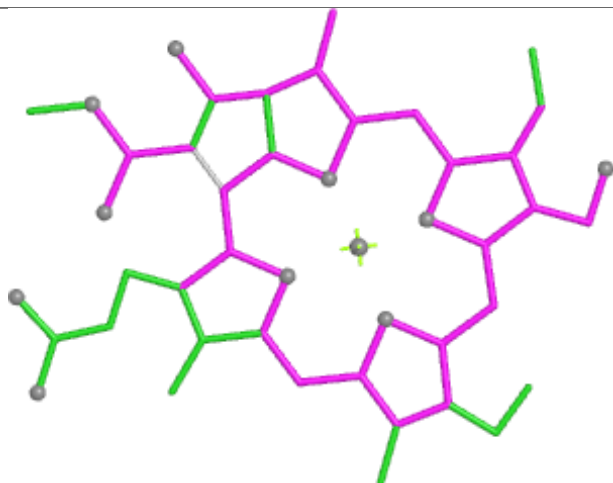
Rings



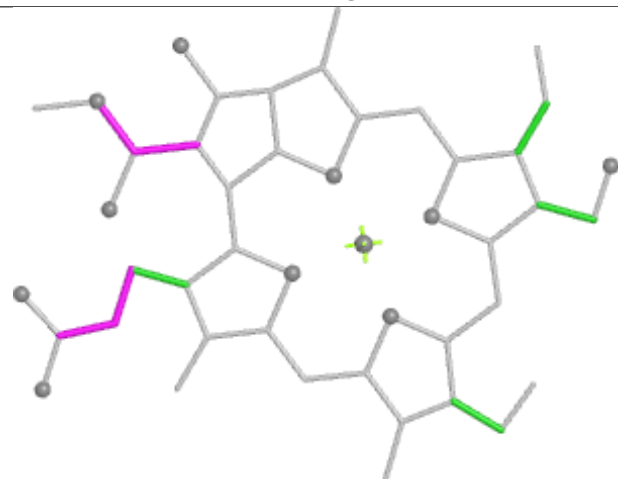
Ligand CHL b 306



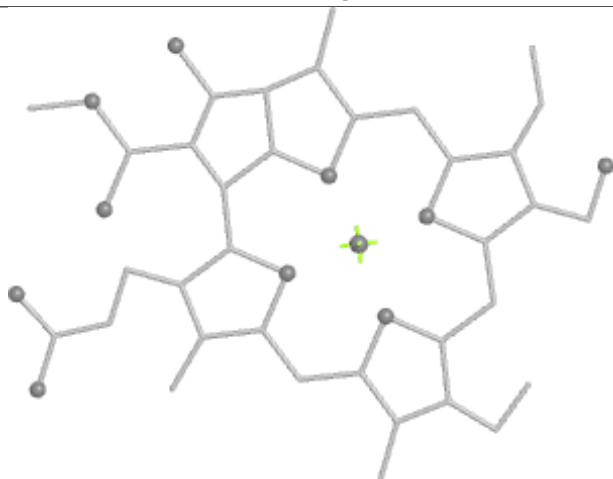
Bond lengths



Bond angles

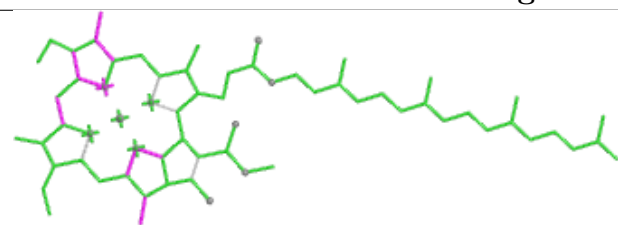


Torsions

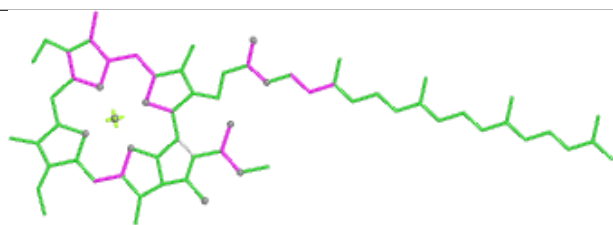


Rings

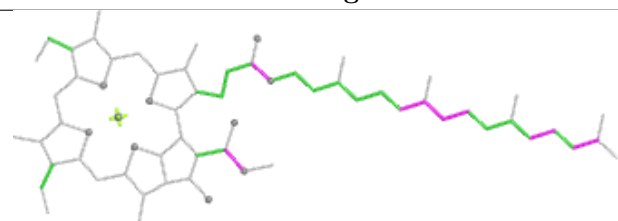
Ligand CLA A 821



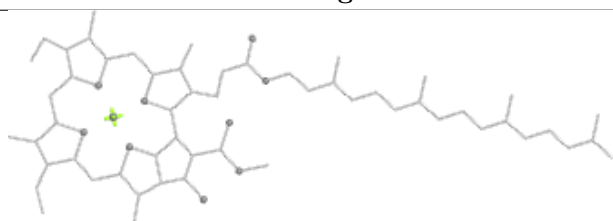
Bond lengths



Bond angles

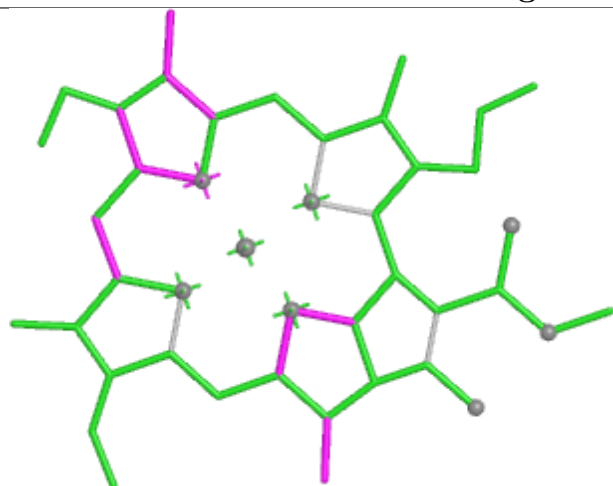


Torsions

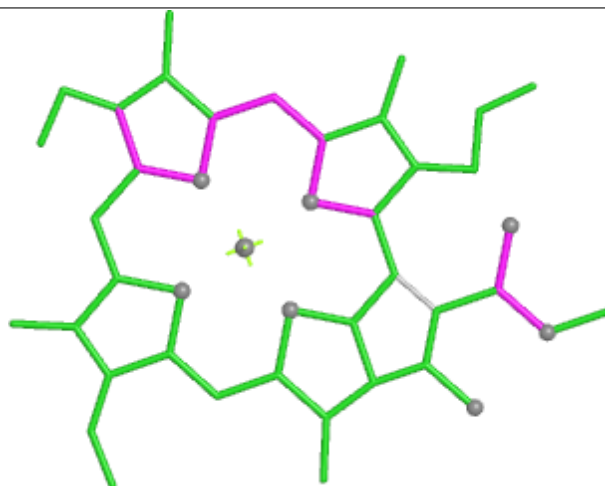


Rings

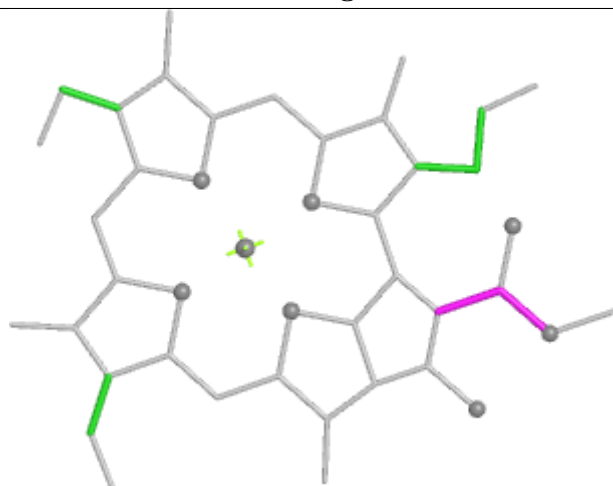
Ligand CLA 3 411



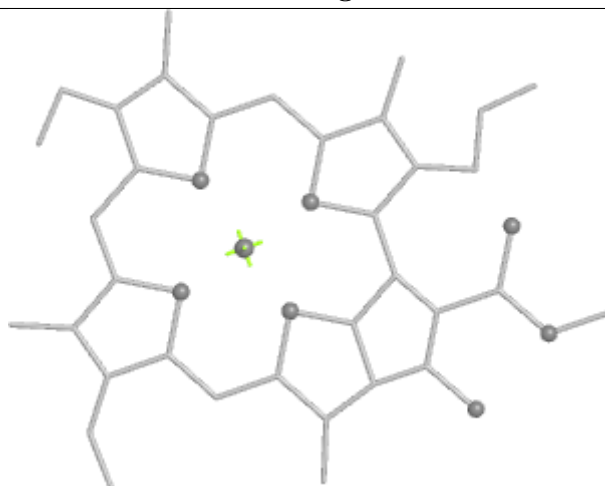
Bond lengths



Bond angles

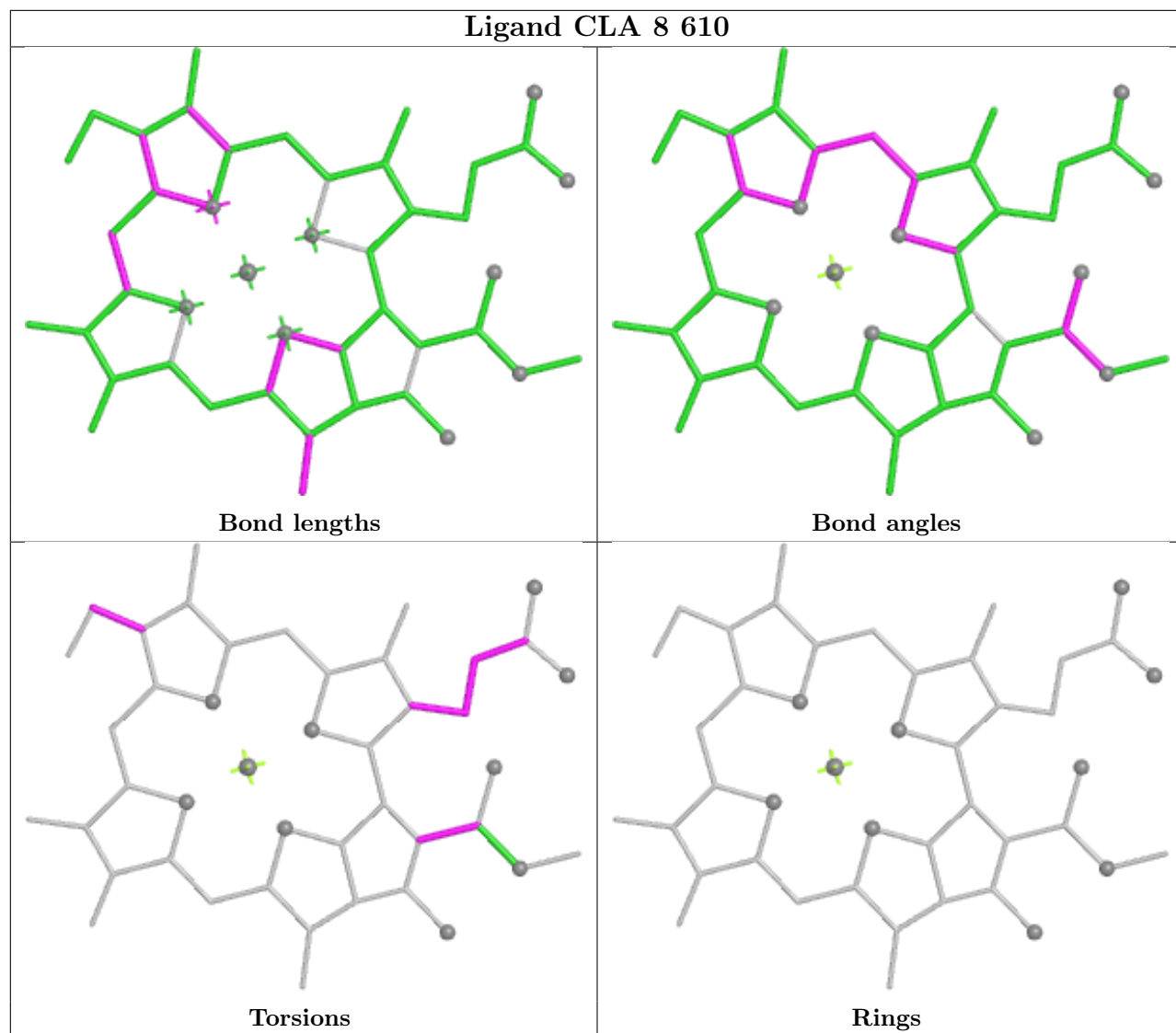


Torsions

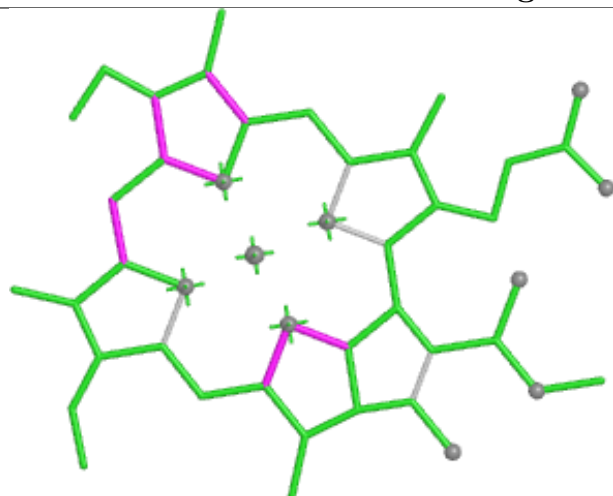


Rings

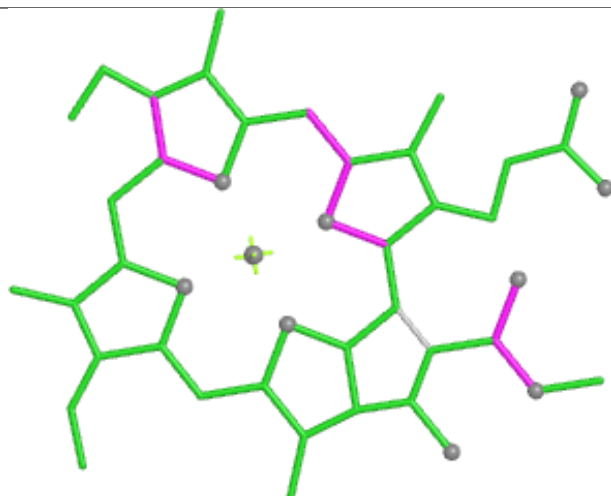
Ligand CLA 8 610



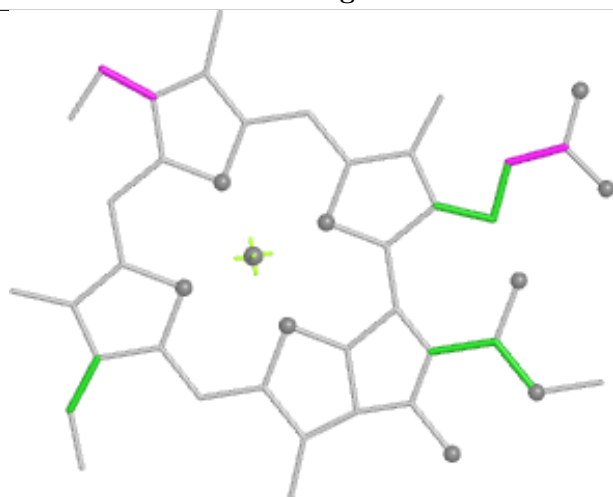
Ligand CLA b 312



Bond lengths



Bond angles

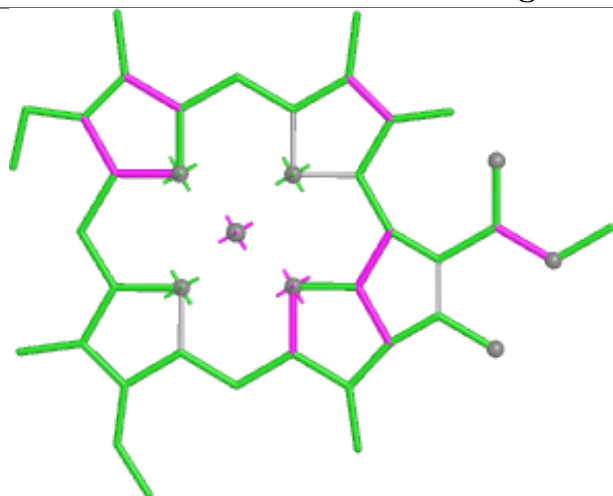


Torsions



Rings

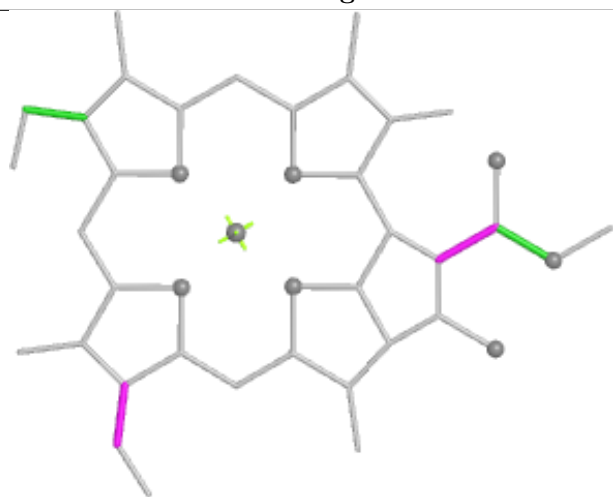
Ligand CLA 1 309



Bond lengths



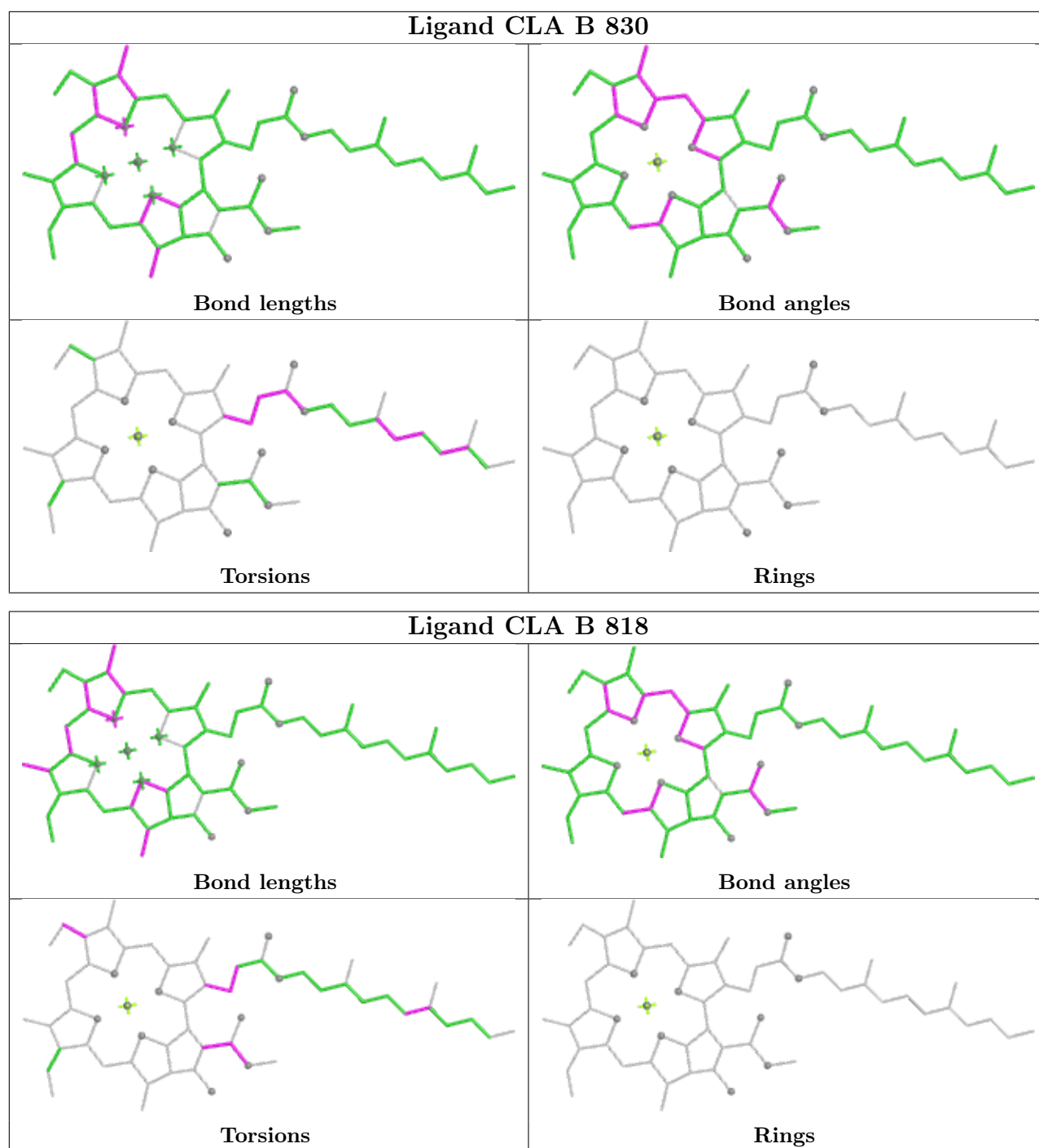
Bond angles



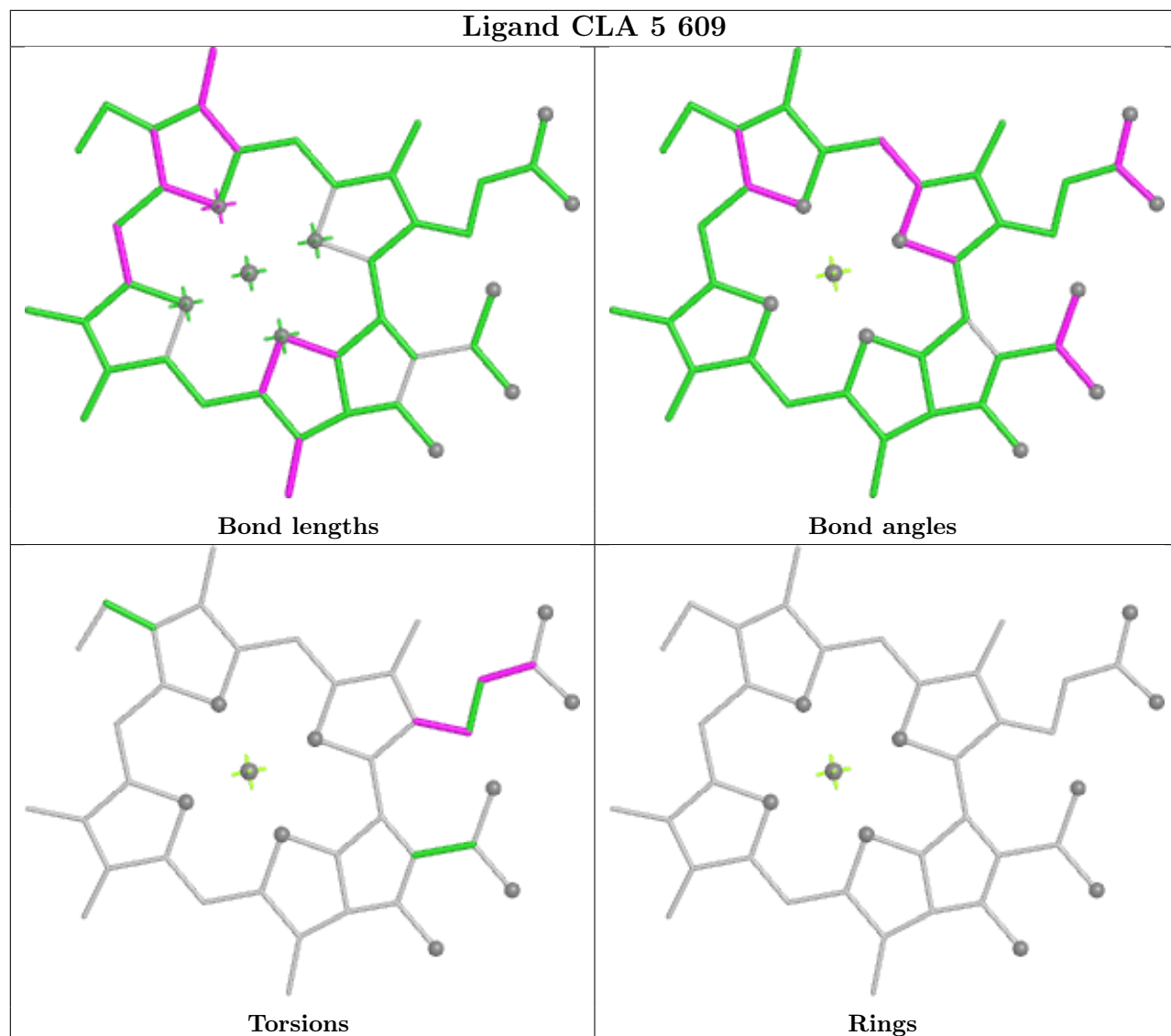
Torsions



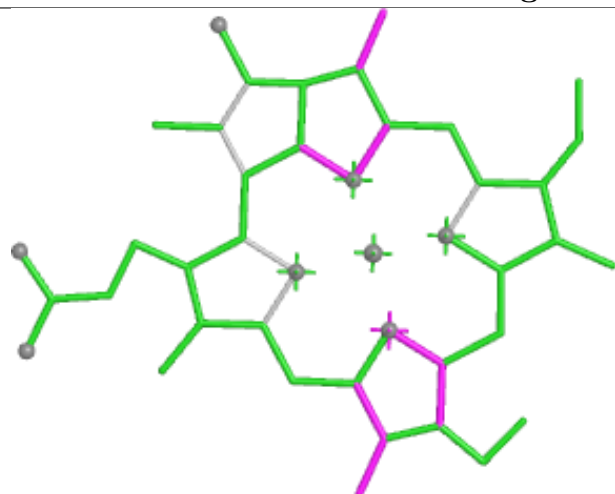
Rings



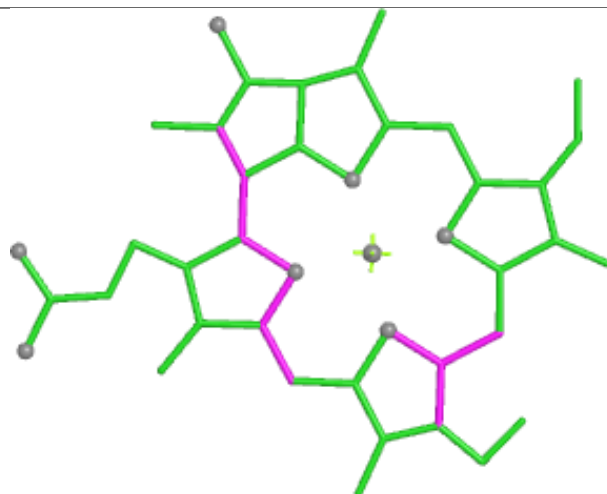
Ligand CLA 5 609



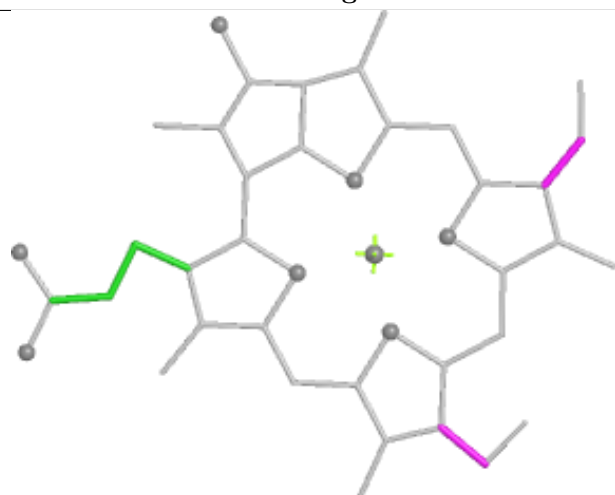
Ligand CLA 2 610



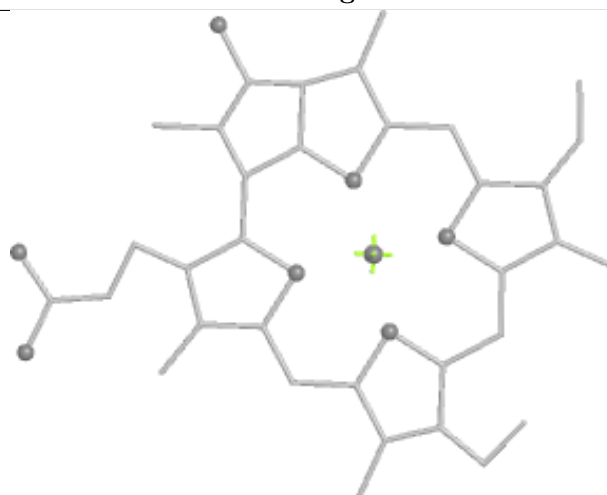
Bond lengths



Bond angles

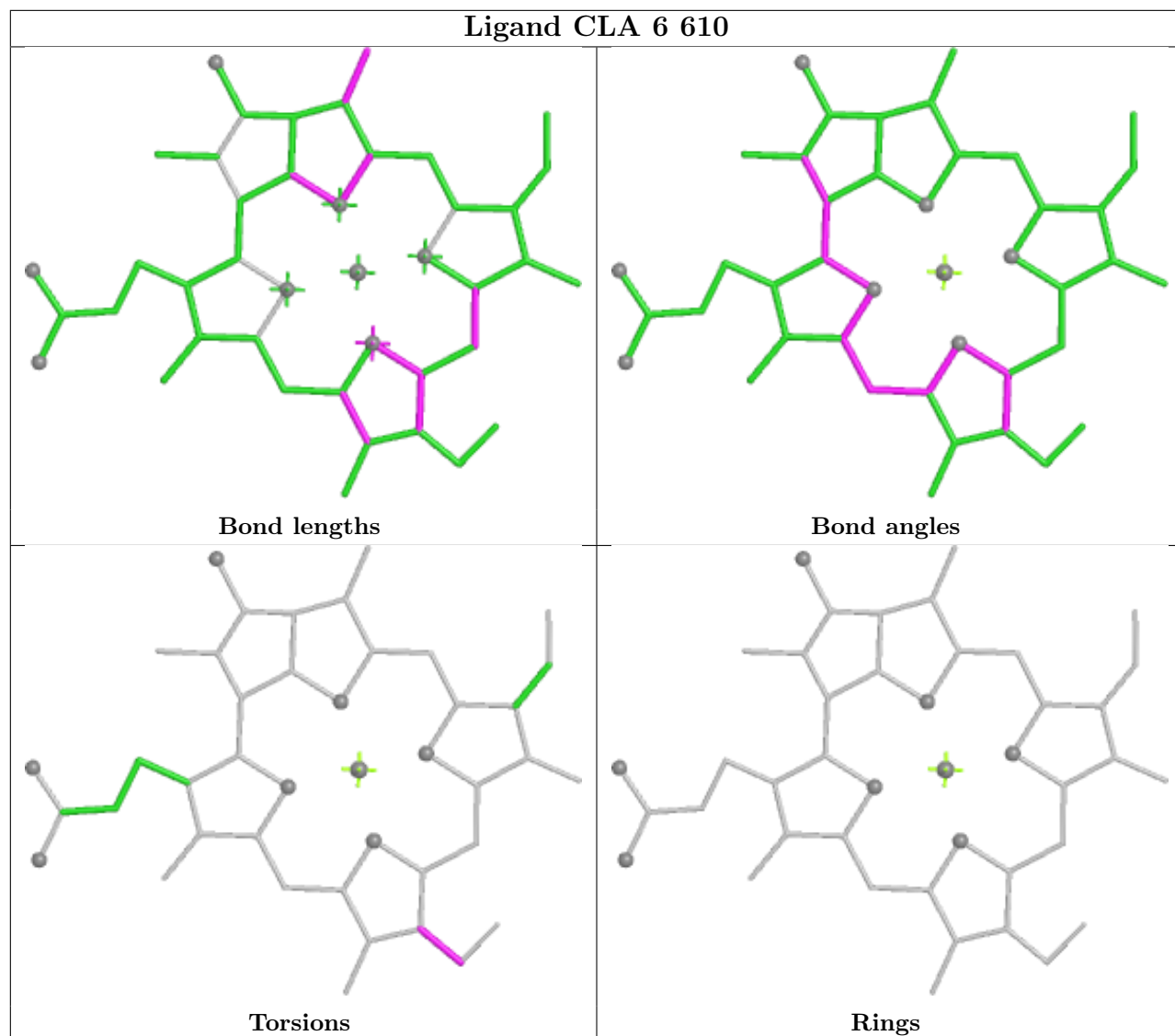


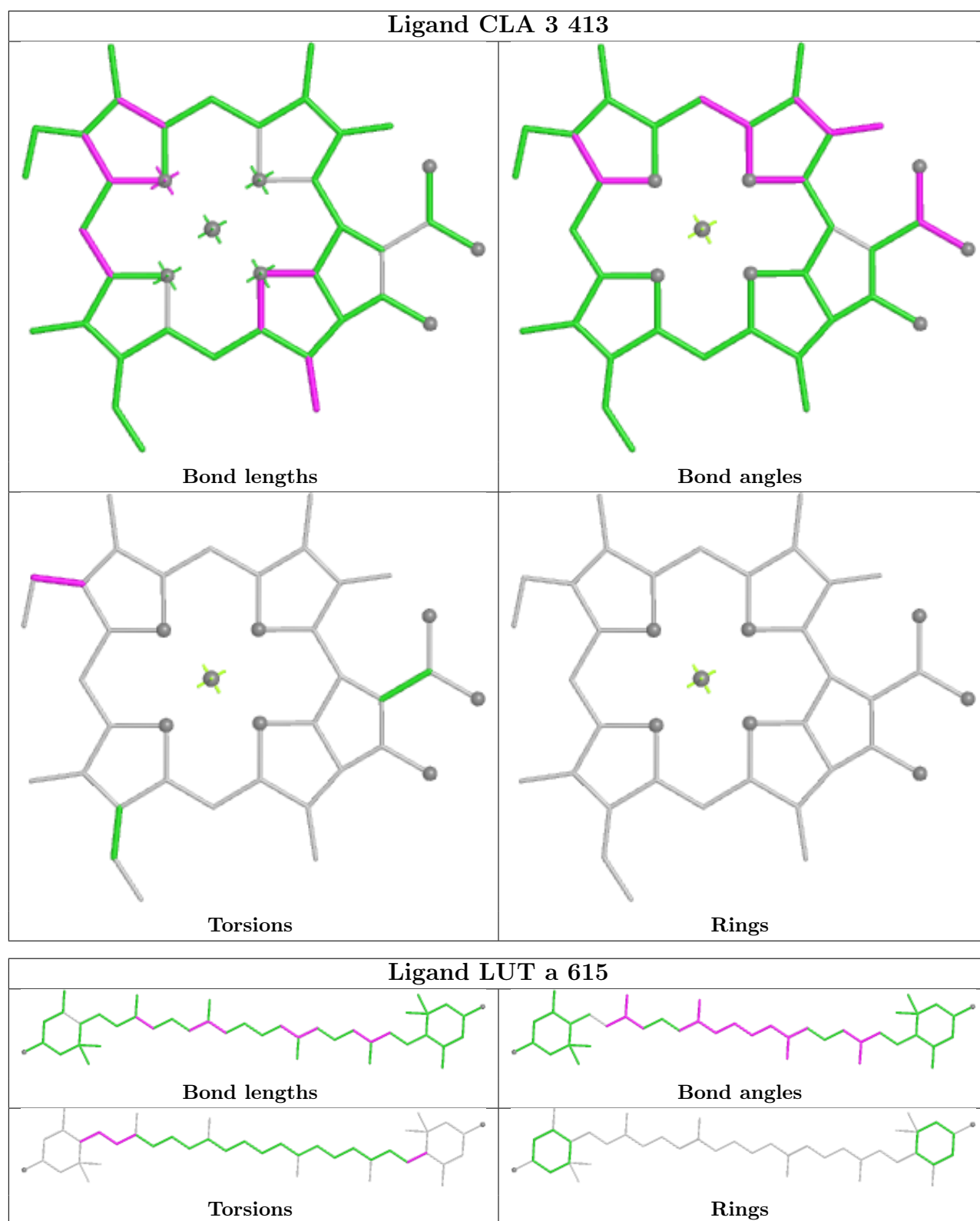
Torsions



Rings

Ligand CLA 6 610





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

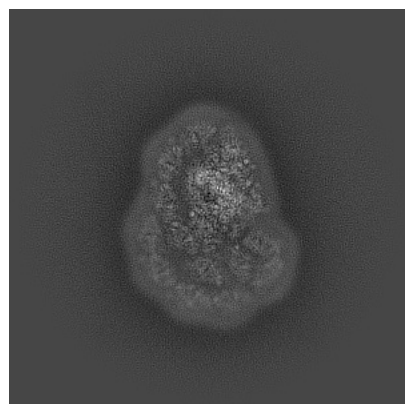
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33401. These allow visual inspection of the internal detail of the map and identification of artifacts.

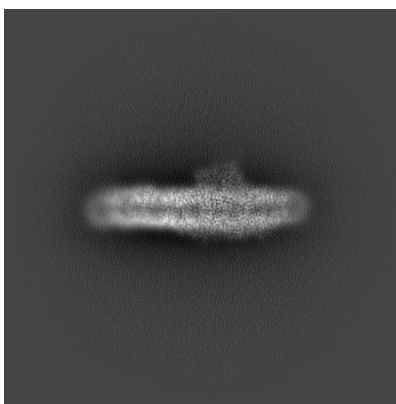
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

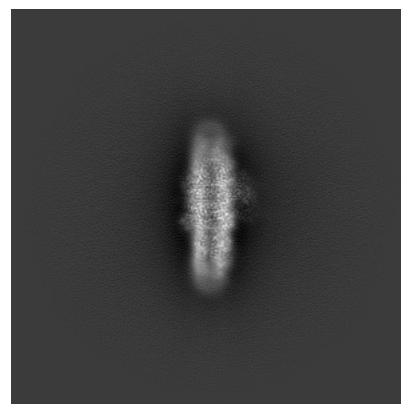
6.1.1 Primary map



X

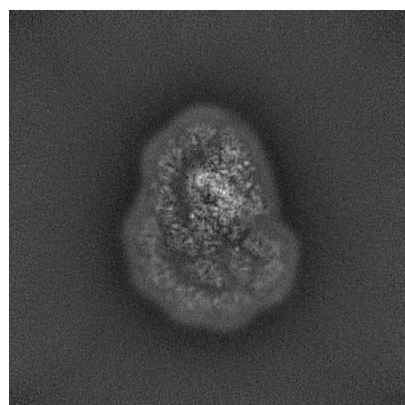


Y

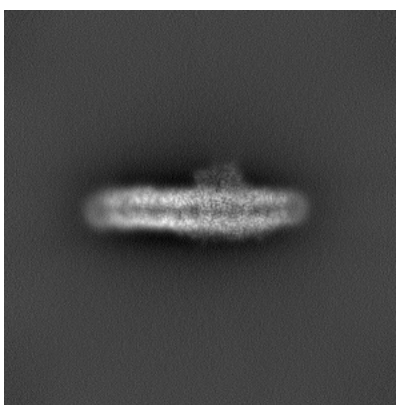


Z

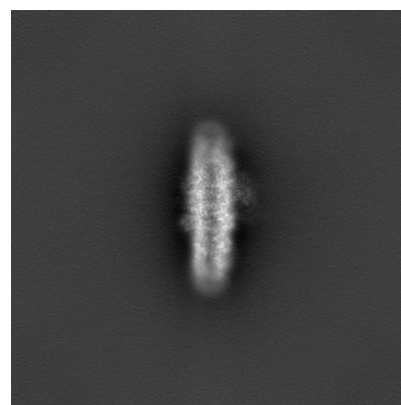
6.1.2 Raw map



X



Y

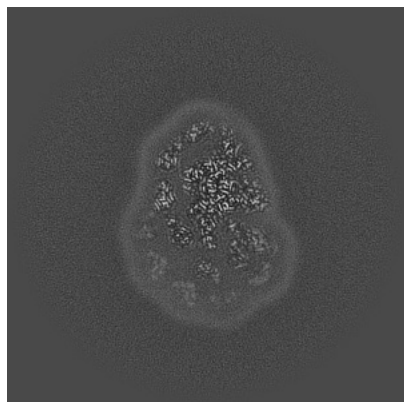


Z

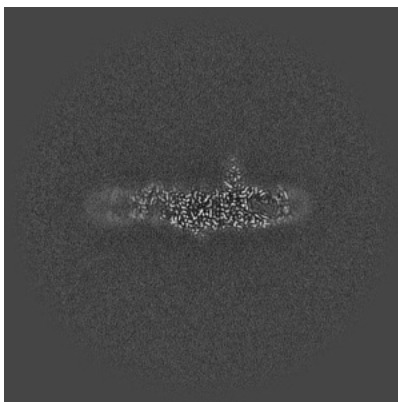
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

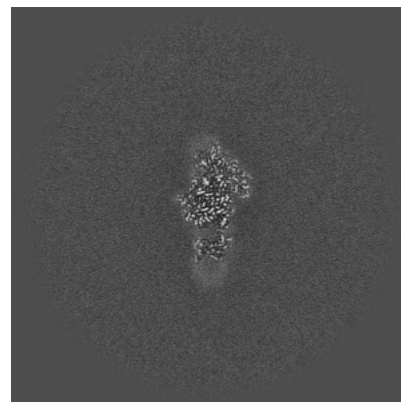
6.2.1 Primary map



X Index: 240

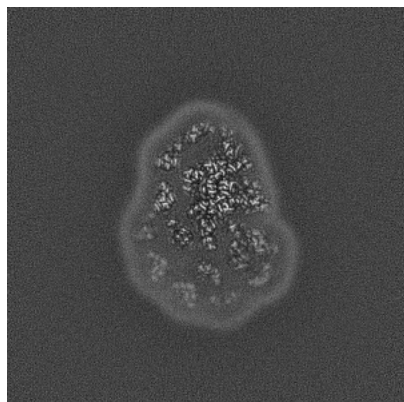


Y Index: 240

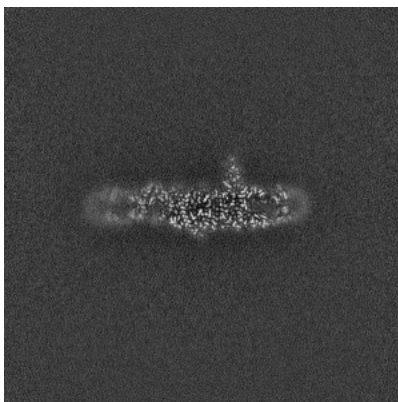


Z Index: 240

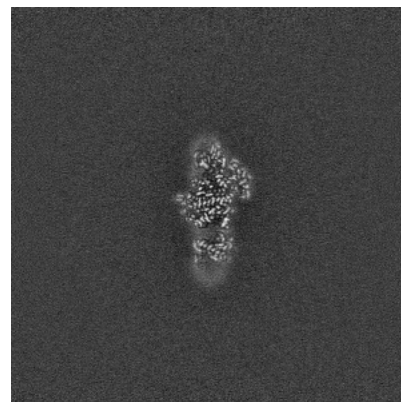
6.2.2 Raw map



X Index: 240



Y Index: 240

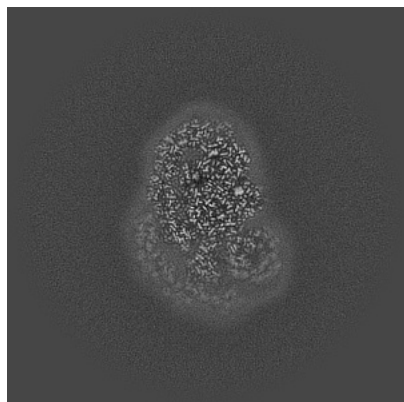


Z Index: 240

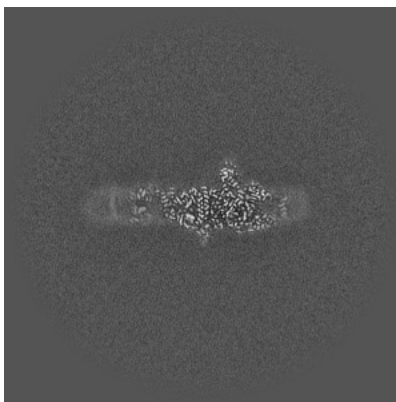
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

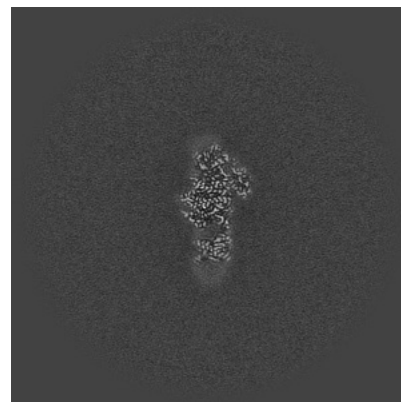
6.3.1 Primary map



X Index: 252

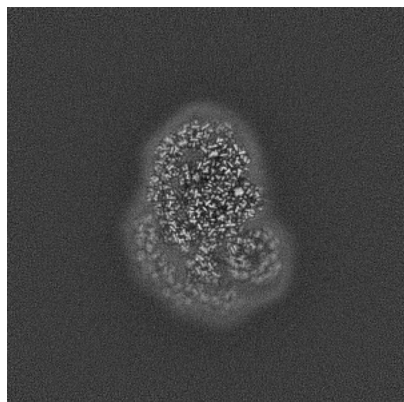


Y Index: 247

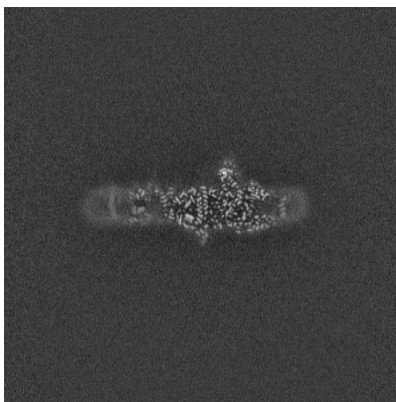


Z Index: 243

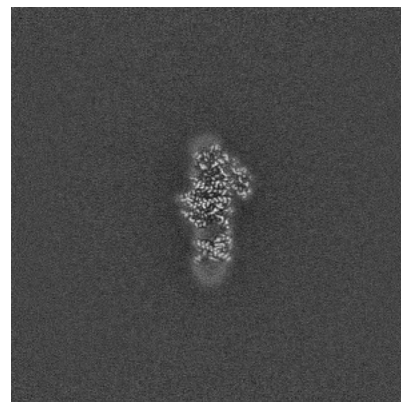
6.3.2 Raw map



X Index: 252



Y Index: 247

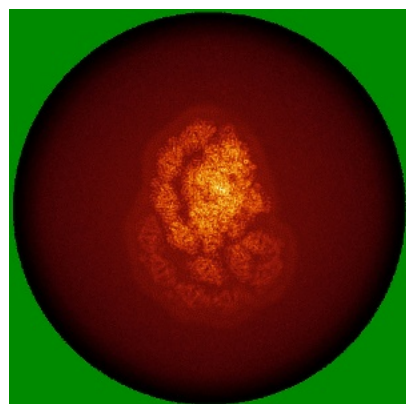


Z Index: 242

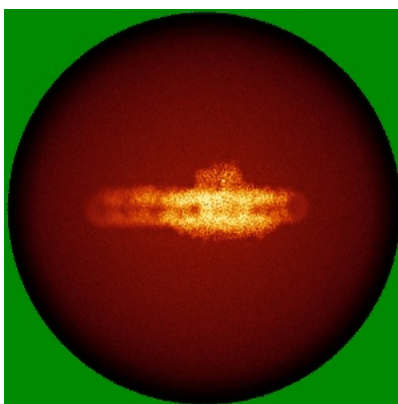
The images above show the largest variance slices of the map in three orthogonal directions.

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

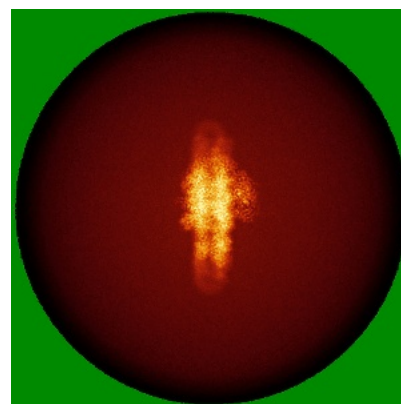
6.4.1 Primary map



X

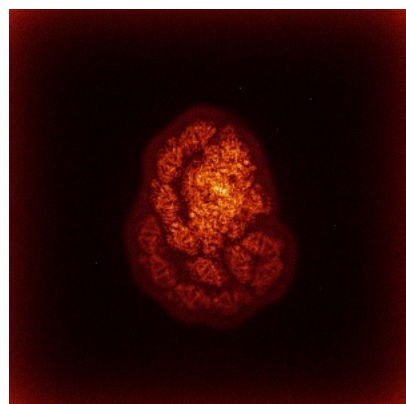


Y

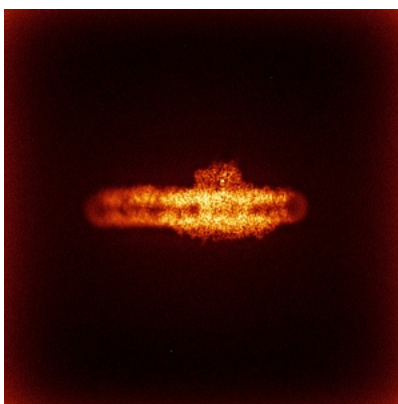


Z

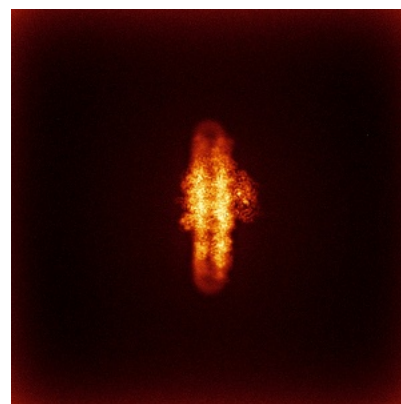
6.4.2 Raw map



X



Y

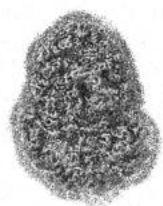


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

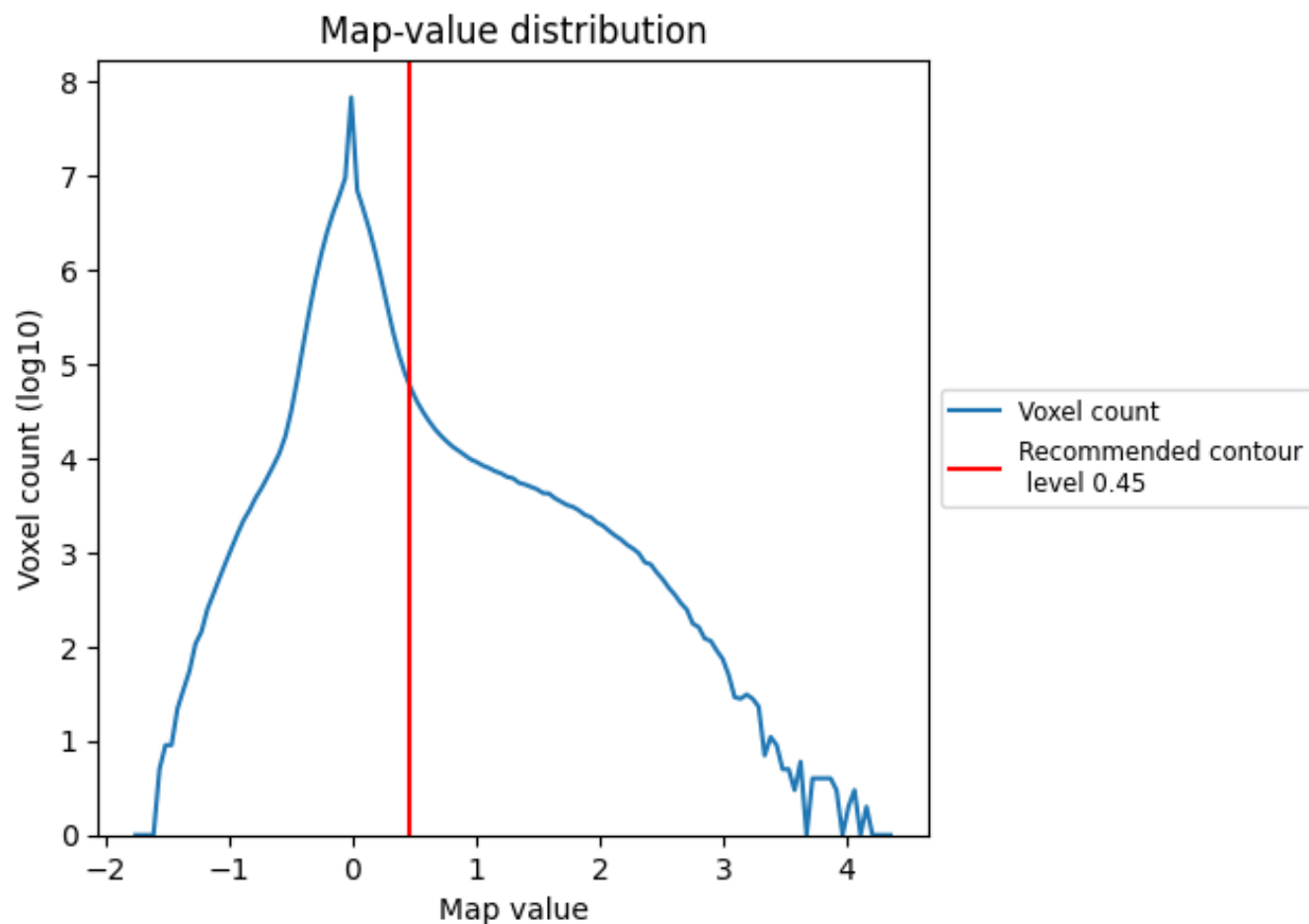
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

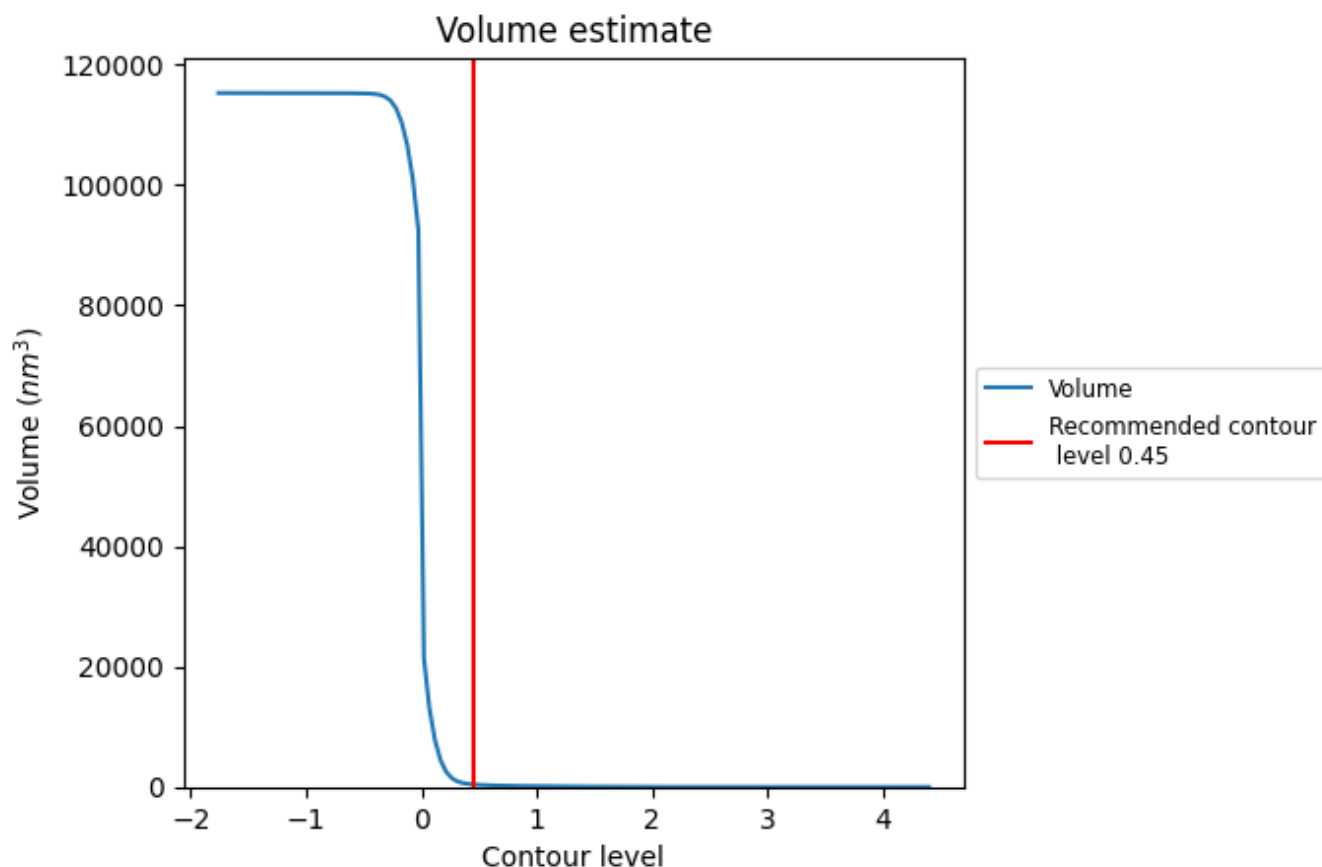
This section contains the results of statistical analysis of the map.

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.

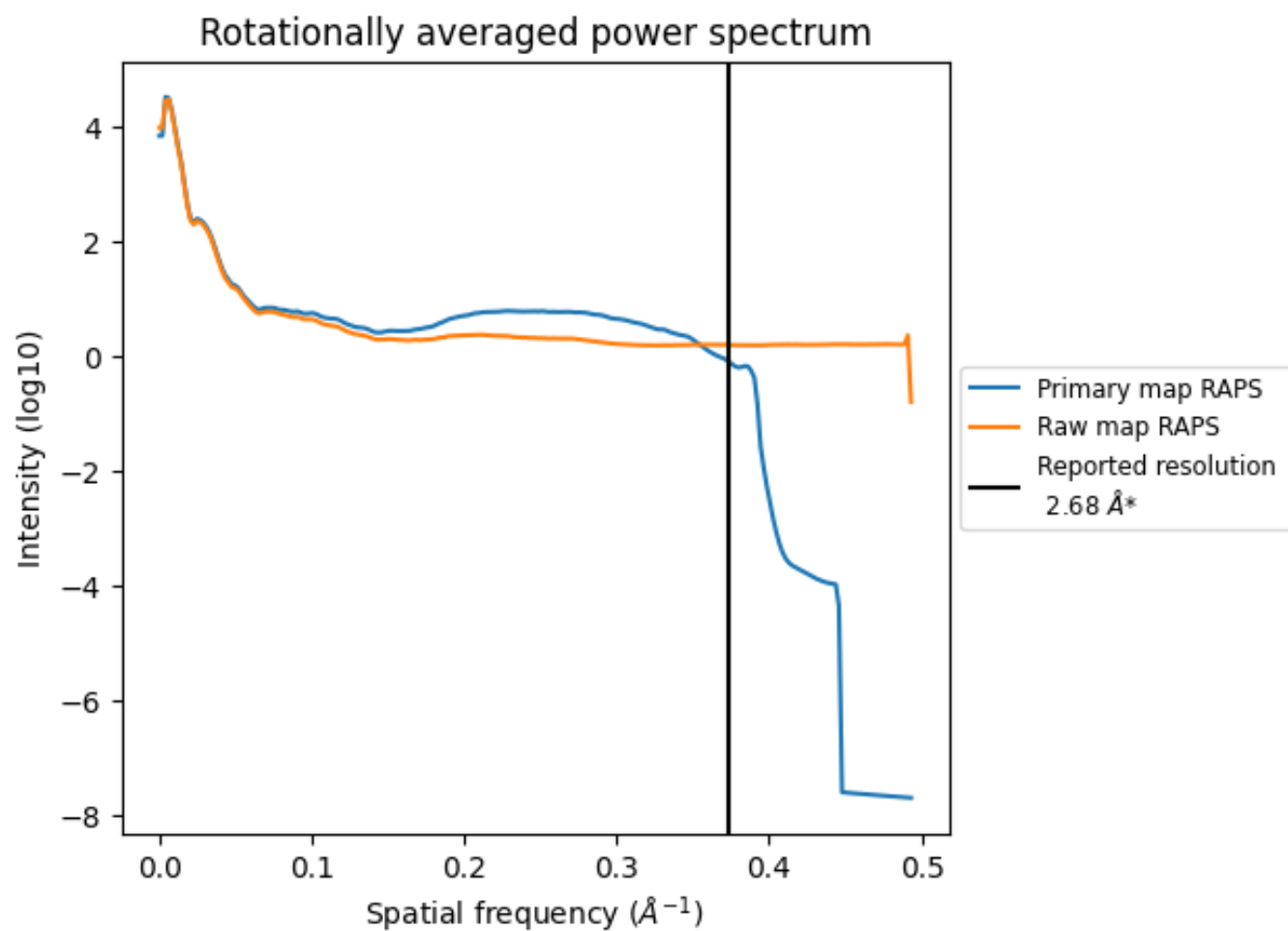
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 378 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 ⓘ

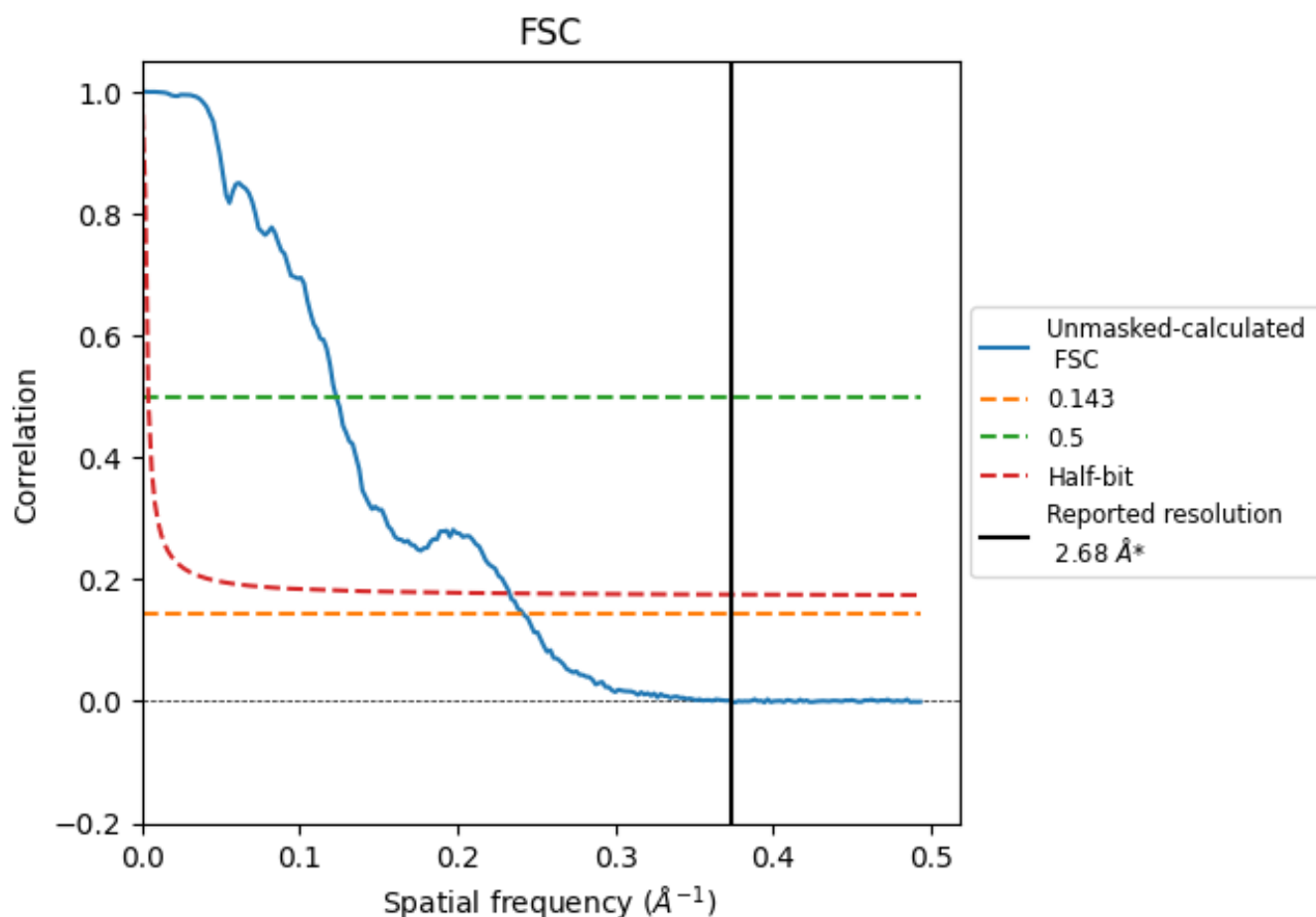


*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8.2 Resolution estimates [i](#)

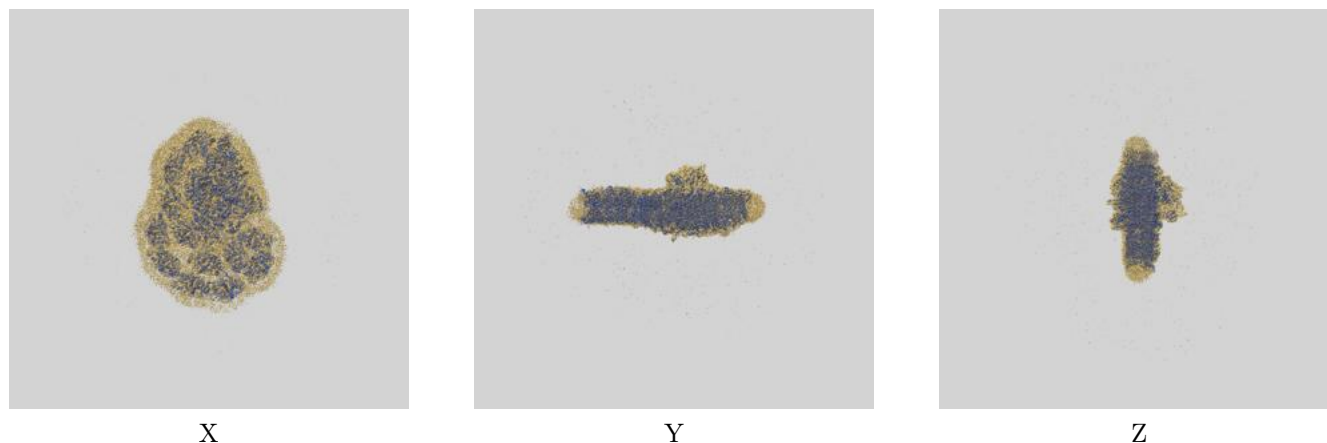
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	8.13	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

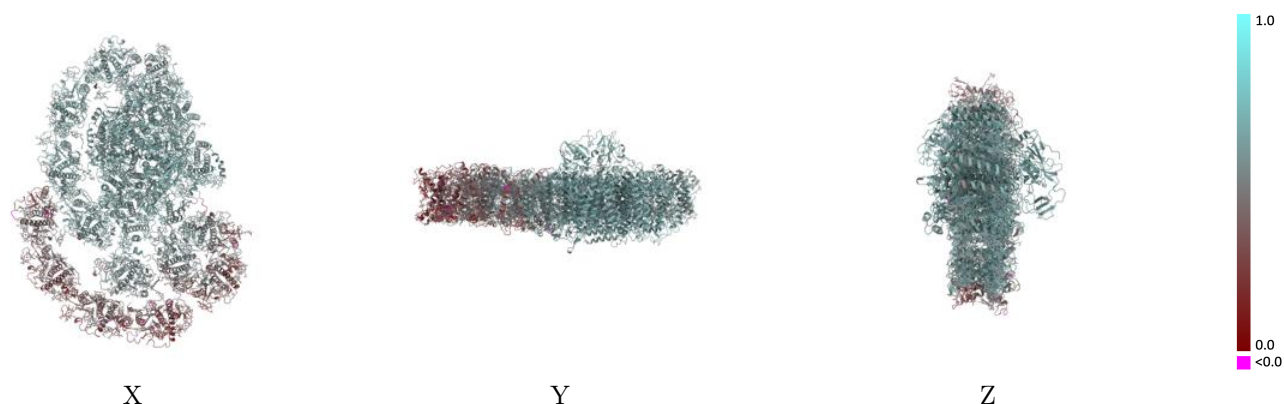
This section contains information regarding the fit between EMDB map EMD-33401 and PDB model 7XQP. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



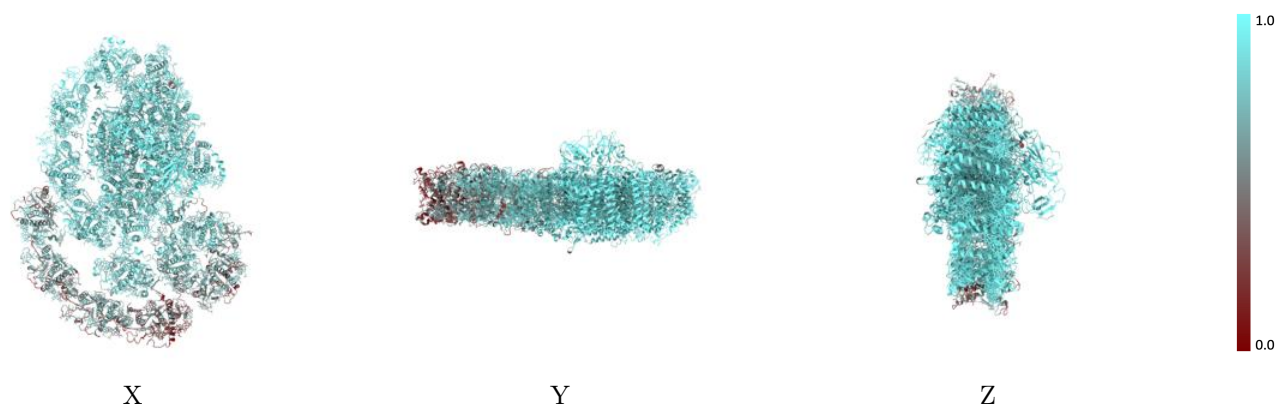
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



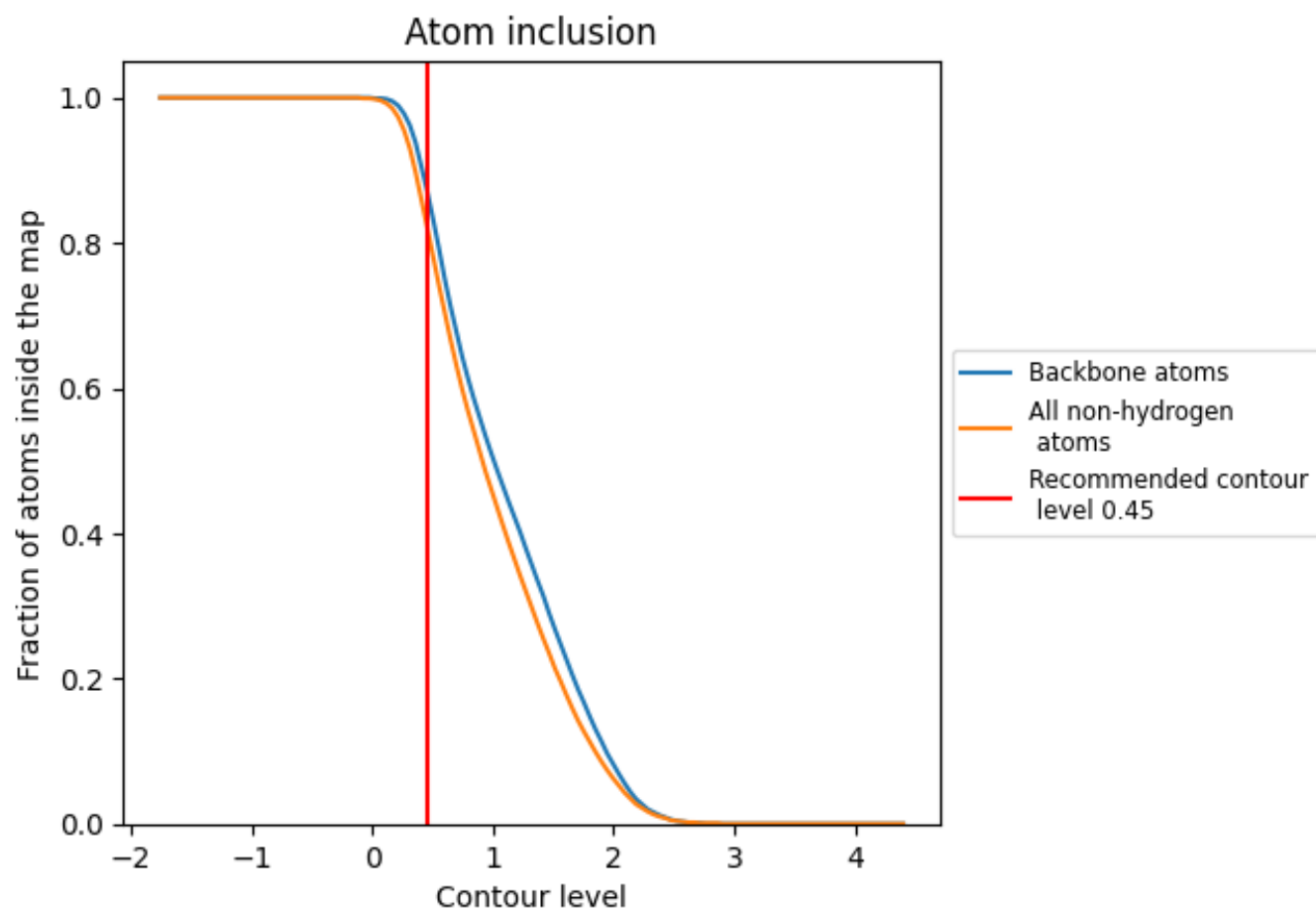
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5360
1	 0.9160	 0.5760
2	 0.9220	 0.5910
3	 0.9350	 0.6030
4	 0.9200	 0.5810
5	 0.5830	 0.3590
6	 0.5300	 0.3330
7	 0.3390	 0.2870
8	 0.5420	 0.3320
9	 0.8250	 0.5250
A	 0.9620	 0.6340
B	 0.9610	 0.6300
C	 0.9730	 0.6210
D	 0.9470	 0.6150
E	 0.9410	 0.6070
F	 0.9220	 0.6030
G	 0.7980	 0.5530
H	 0.8880	 0.5780
I	 0.9470	 0.6180
J	 0.9350	 0.6110
K	 0.9400	 0.6090
L	 0.9430	 0.6120
M	 0.8980	 0.5880
O	 0.8320	 0.5260
a	 0.5470	 0.3560
b	 0.7680	 0.4910
c	 0.7450	 0.4660

