



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 04:33 PM EDT

PDB ID : 9MGZ / pdb_00009mgz
EMDB ID : EMD-48264
Title : Dunaliella tertiolecta PSI-LHCI-TID1 supercomplex
Authors : Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on : 2024-12-11
Resolution : 2.80 Å(reported)
Based on initial model : 6SL5

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:

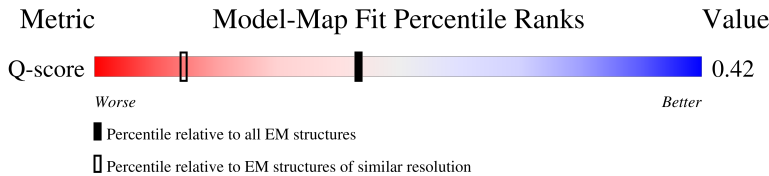
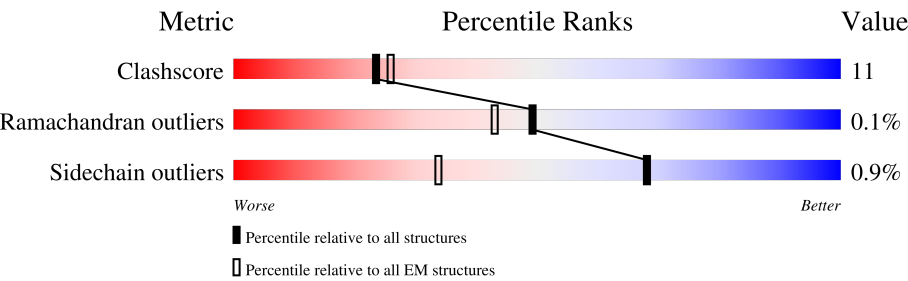
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



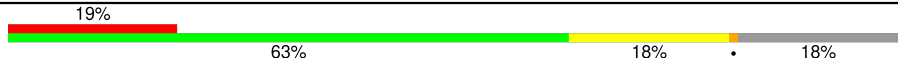
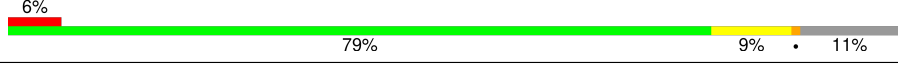
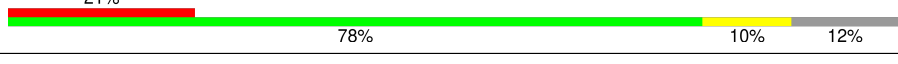
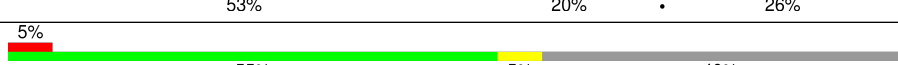
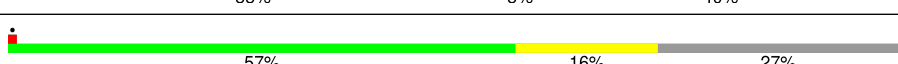
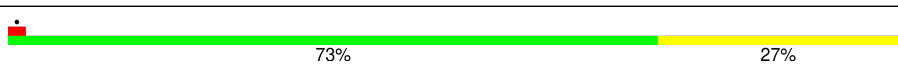
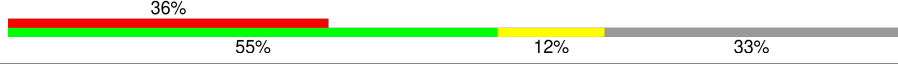
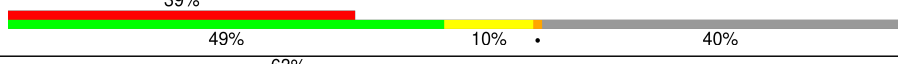
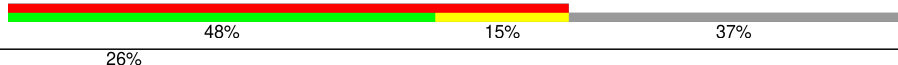
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	1	228	48% 71%15%14%
1	a	228	10% 73%13%14%
2	3	286	5% 61%17%21%
3	7	255	67%18%15%

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Mol	Chain	Length	Quality of chain
3	c	255	
4	8	254	
4	b	254	
5	A	751	
6	B	735	
7	C	81	
8	D	193	
9	E	111	
10	F	227	
11	J	41	
12	K	123	
13	T	350	
14	L	198	
15	I	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CHL	3	301	X	-	-	-
16	CHL	3	322	X	-	-	-
18	LUT	1	615	X	-	-	-
18	LUT	3	315	X	-	-	-
18	LUT	7	315	X	-	-	-
18	LUT	8	316	X	-	-	-
18	LUT	T	413	X	-	-	-
18	LUT	a	615	X	-	-	-
18	LUT	b	615	X	-	-	-
18	LUT	c	314	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 44202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		
1	a	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	226	Total	C	N	O	S	0	0
			1719	1120	282	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	217	Total	C	N	O	S	0	0
			1669	1078	281	304	6		
3	c	209	Total	C	N	O	S	0	0
			1607	1037	271	293	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	226	Total	C	N	O	S	0	0
			1721	1108	286	320	7		
4	b	224	Total	C	N	O	S	0	0
			1710	1102	284	317	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	67	Total	C	N	O	0	0
			535	340	94	101		

- Molecule 10 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

- Molecule 13 is a protein called TIDI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	210	Total	C	N	O	S	0	0
			1639	1062	271	298	8		

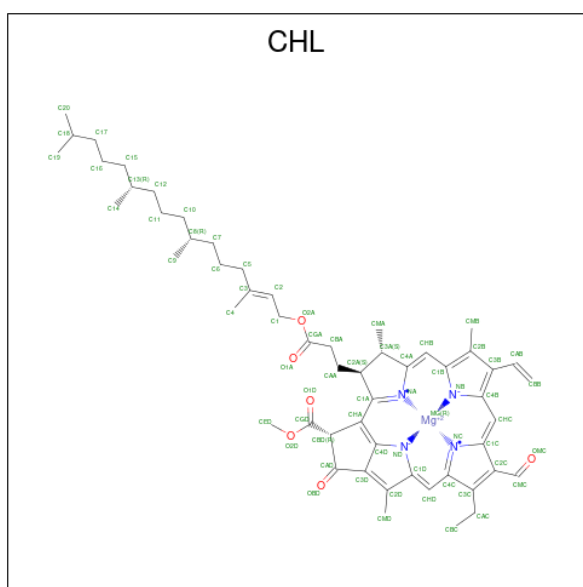
- Molecule 14 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	124	Total	C	N	O	S	0	0
			894	582	147	160	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			274	191	40	42	1		

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
16	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
17	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
17	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	T	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
17	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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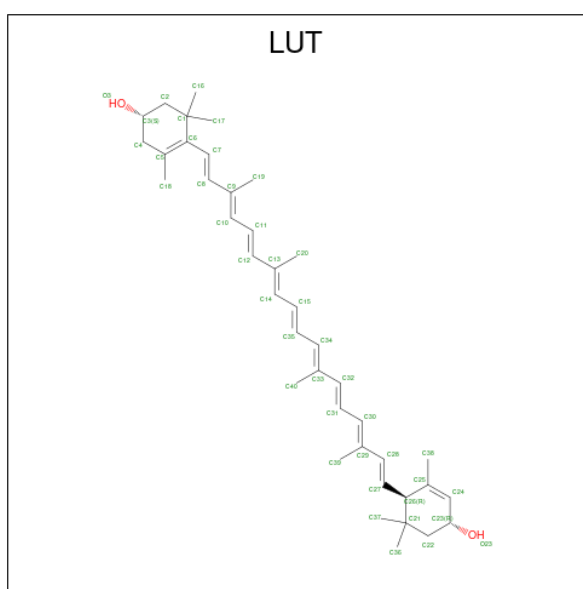
Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	c	1	Total 50	C 40	Mg 1	N 4	O 5	0

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

- Molecule 18 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



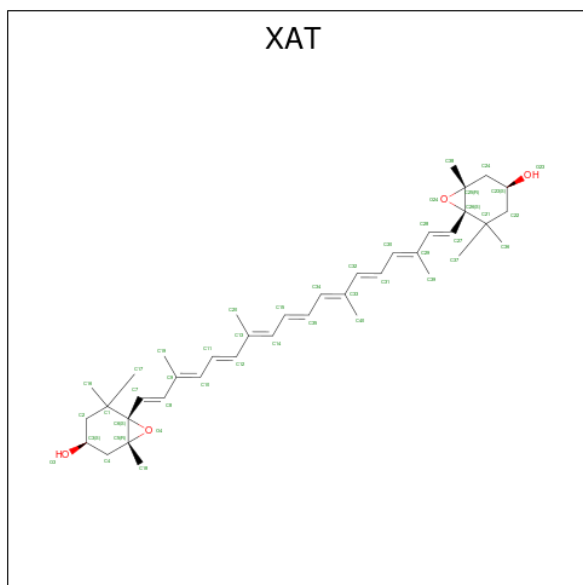
Mol	Chain	Residues	Atoms				AltConf
18	1	1	Total	C	O		0
			42	40	2		
18	3	1	Total	C	O		0
			42	40	2		
18	7	1	Total	C	O		0
			42	40	2		
18	8	1	Total	C	O		0
			42	40	2		
18	T	1	Total	C	O		0
			42	40	2		
18	a	1	Total	C	O		0
			42	40	2		
18	b	1	Total	C	O		0
			42	40	2		

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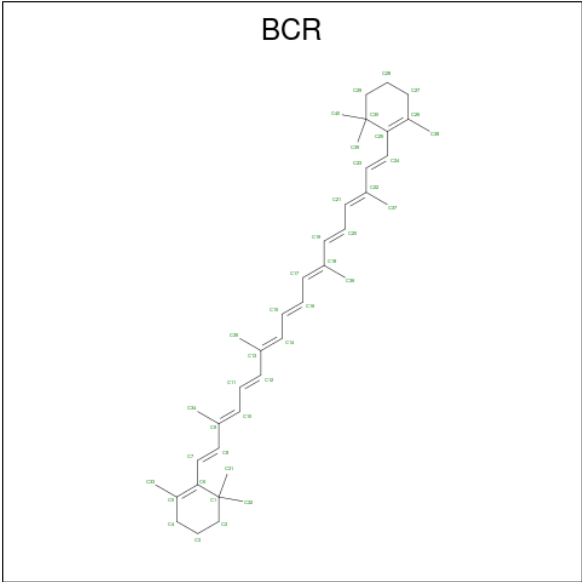
Mol	Chain	Residues	Atoms			AltConf
18	c	1	Total	C	O	0
			42	40	2	

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



Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	3	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	T	1	Total	C	O	0
			44	40	4	
19	a	1	Total	C	O	0
			44	40	4	
19	b	1	Total	C	O	0
			44	40	4	
19	c	1	Total	C	O	0
			44	40	4	

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



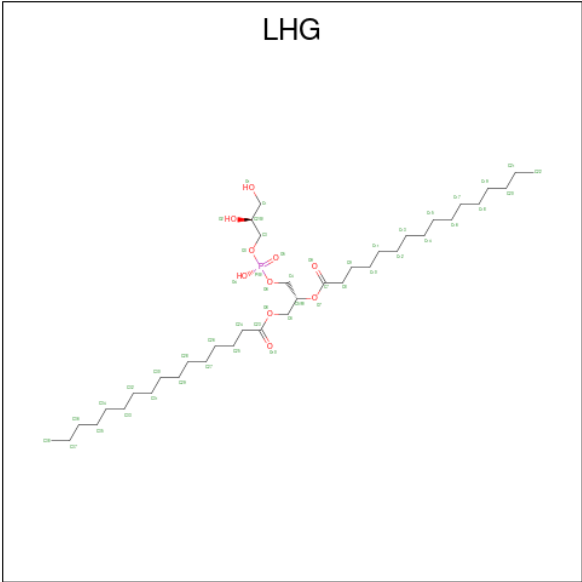
Mol	Chain	Residues	Atoms		AltConf
20	1	1	Total	C	0
			40	40	
20	3	1	Total	C	0
			40	40	
20	3	1	Total	C	0
			40	40	
20	3	1	Total	C	0
			40	40	
20	7	1	Total	C	0
			40	40	
20	8	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	

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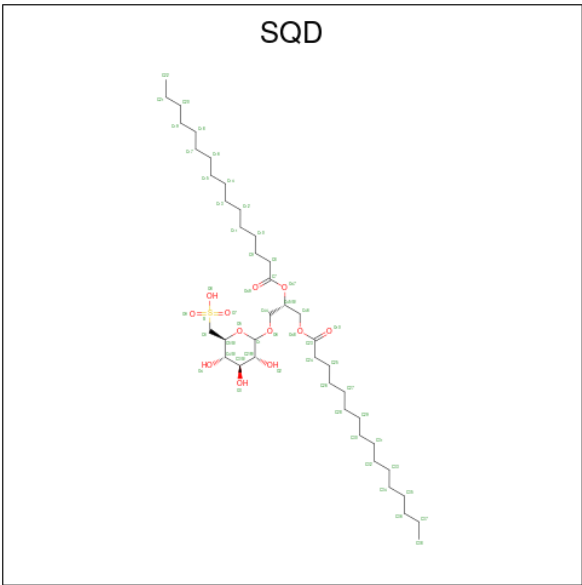
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	I	1	Total C 40 40	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



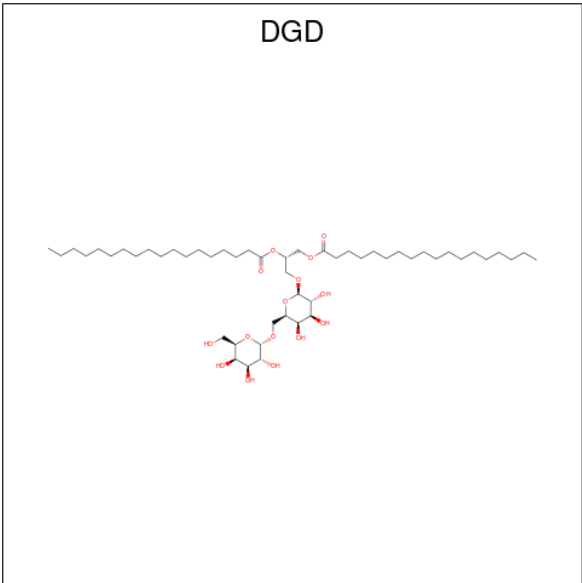
Mol	Chain	Residues	Atoms				AltConf
21	1	1	Total	C	O	P	0
			27	16	10	1	
21	1	1	Total	C	O	P	0
			31	20	10	1	
21	7	1	Total	C	O	P	0
			34	23	10	1	
21	8	1	Total	C	O	P	0
			30	19	10	1	
21	A	1	Total	C	O	P	0
			36	25	10	1	
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			30	20	9	1	
21	F	1	Total	C	O	P	0
			31	20	10	1	
21	a	1	Total	C	O	P	0
			23	13	9	1	
21	a	1	Total	C	O	P	0
			23	12	10	1	
21	b	1	Total	C	O	P	0
			21	10	10	1	
21	c	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
22	3	1	35	22	12	1	0

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



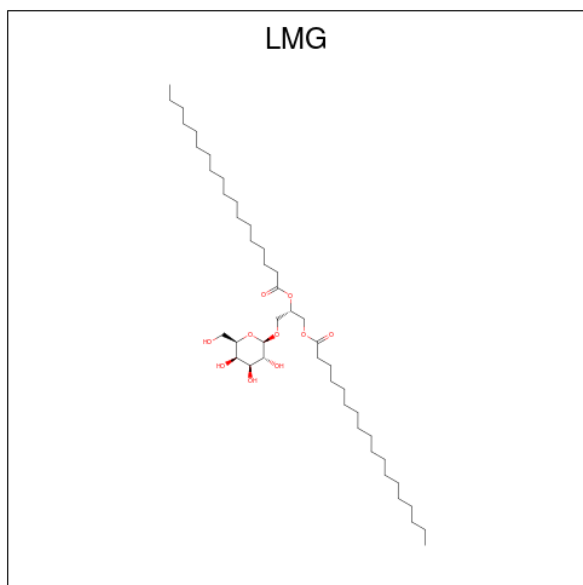
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	3	1	50	35	15	0
23	8	1	39	24	15	0

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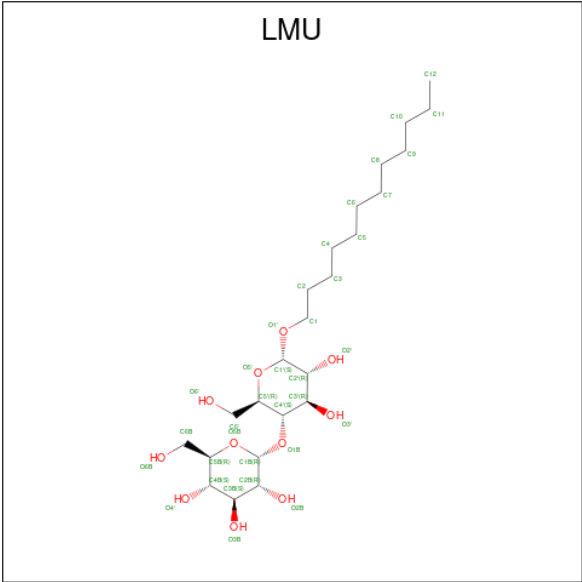
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			61	46	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



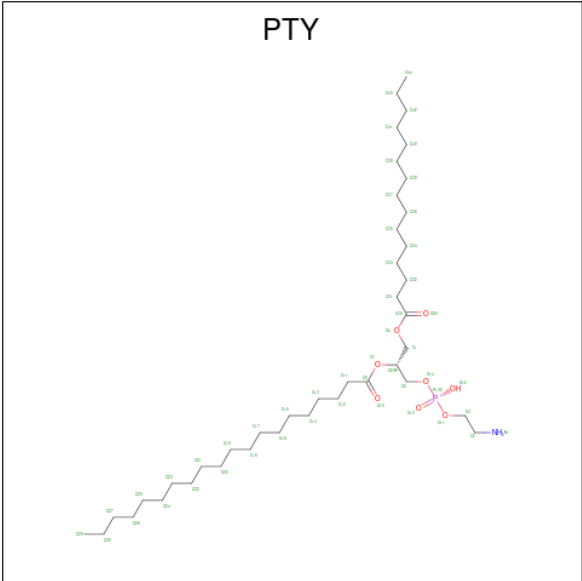
Mol	Chain	Residues	Atoms			AltConf
24	7	1	Total	C	O	0
			50	40	10	
24	A	1	Total	C	O	0
			32	22	10	
24	F	1	Total	C	O	0
			29	19	10	

- Molecule 25 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
25	7	1	Total	C	O	0
			35	24	11	
25	A	1	Total	C	O	0
			35	24	11	

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



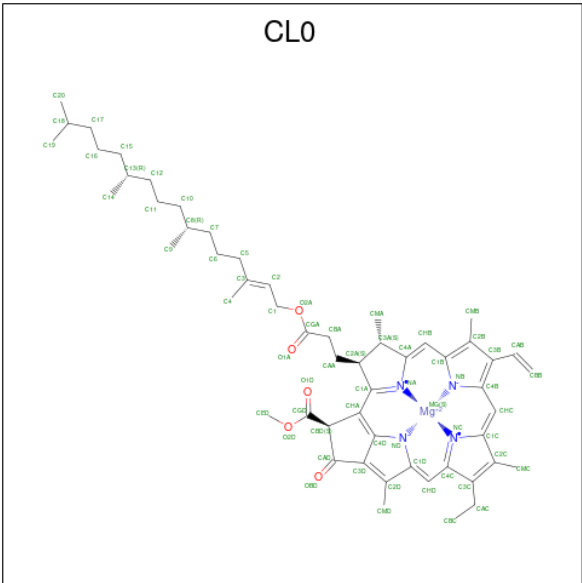
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	N	O	P	0
			21	11	1	8	1	

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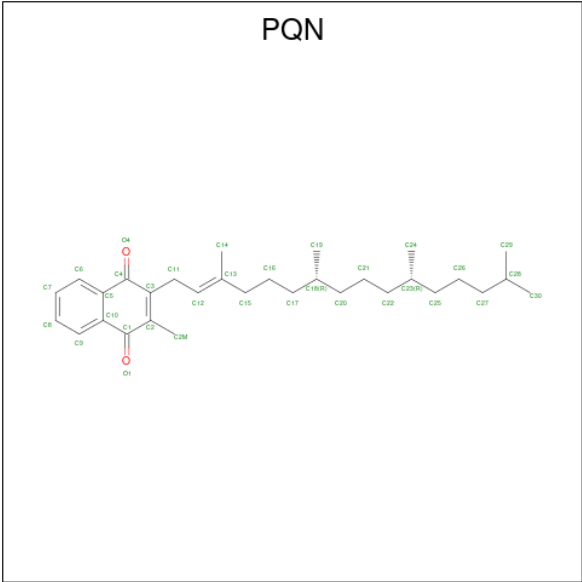
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
26	F	1	Total	C	N	O	P	0
			33	23	1	8	1	
26	F	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



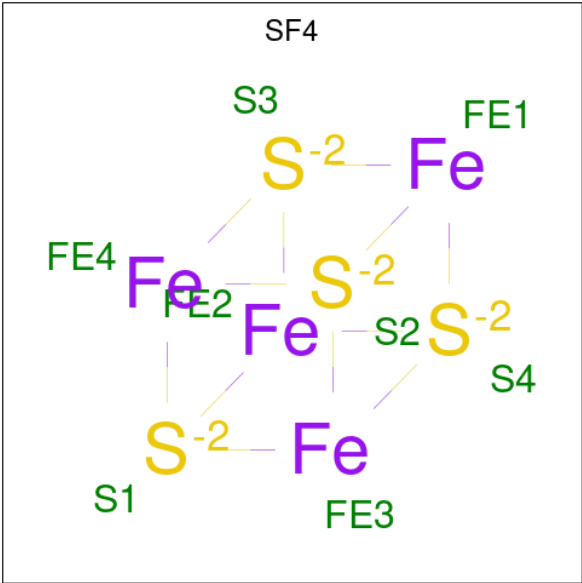
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



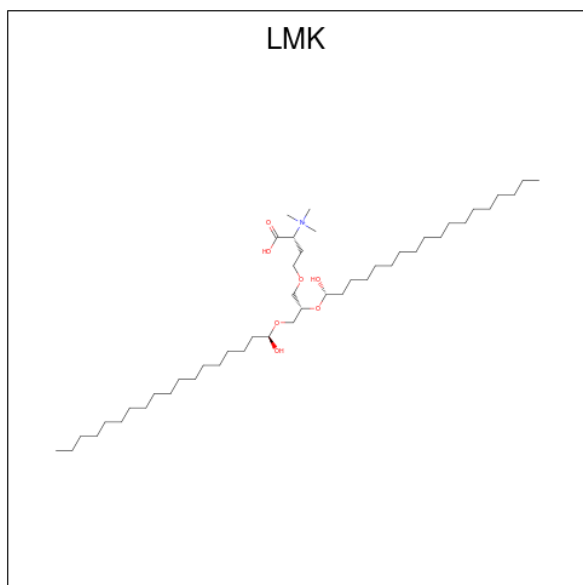
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 30 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: C₄₆H₉₄NO₇) (labeled as "Ligand of Interest" by depositor).

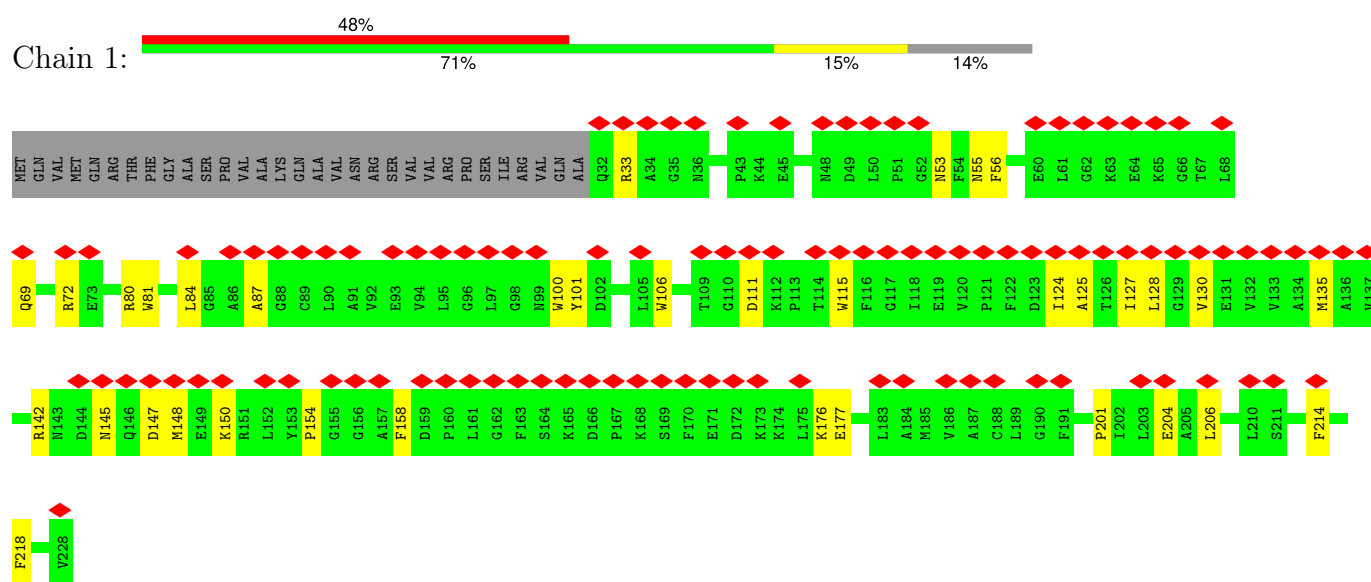


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	J	1	35	27	1	7	0

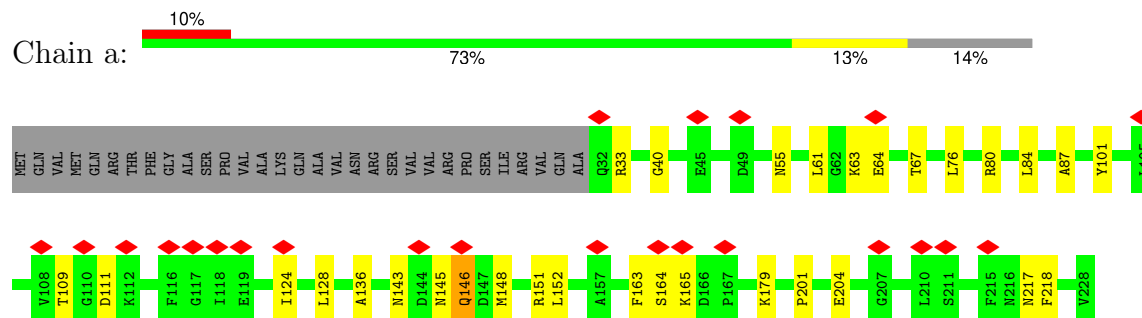
3 Residue-property plots

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

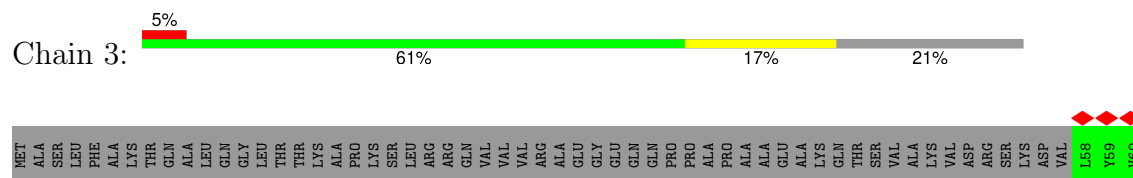
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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

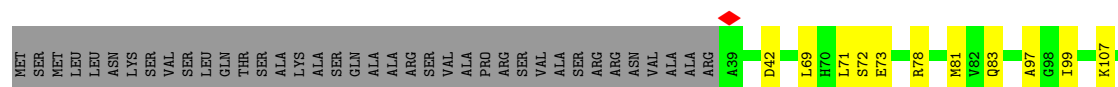


- Molecule 2: LHCA3

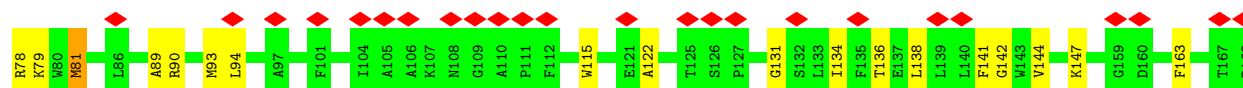
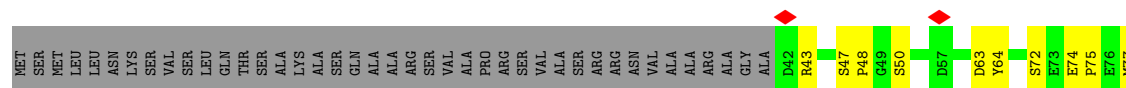




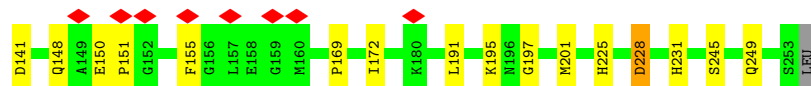
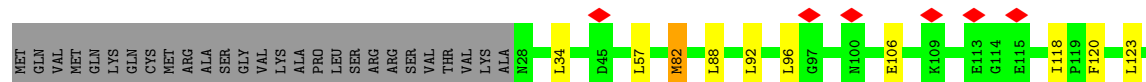
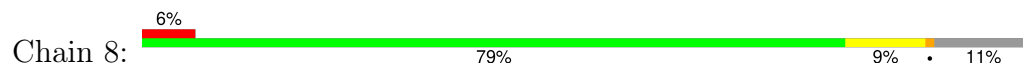
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



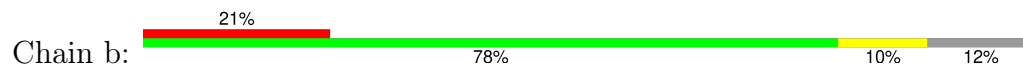
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

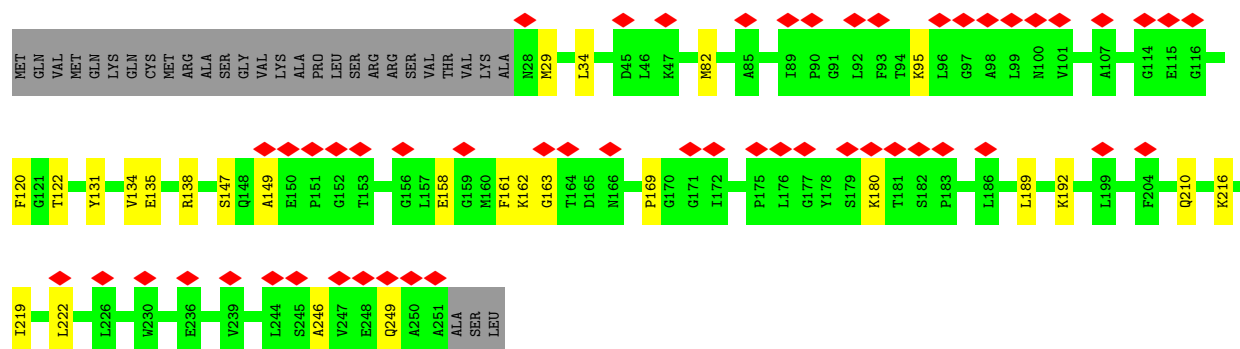


- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



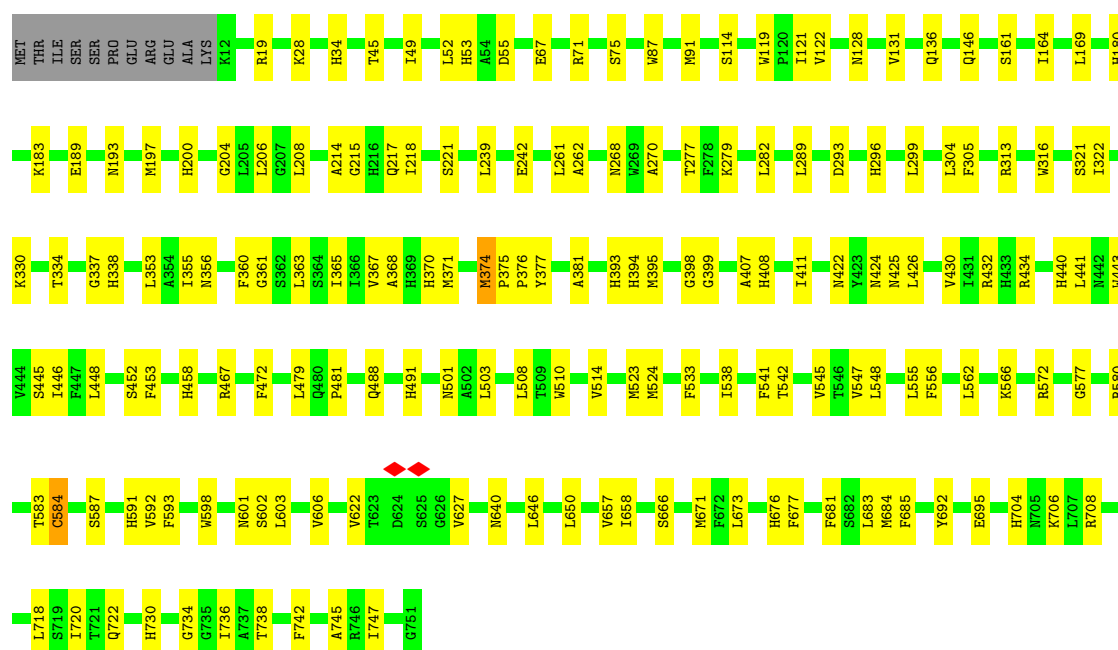
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic





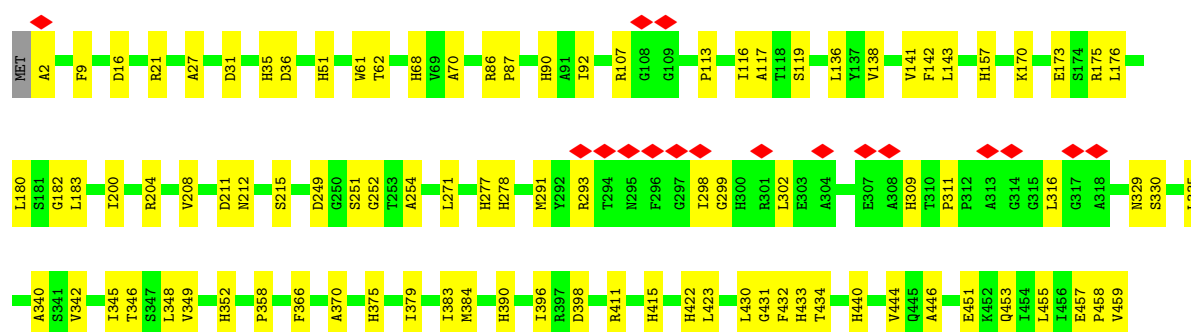
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

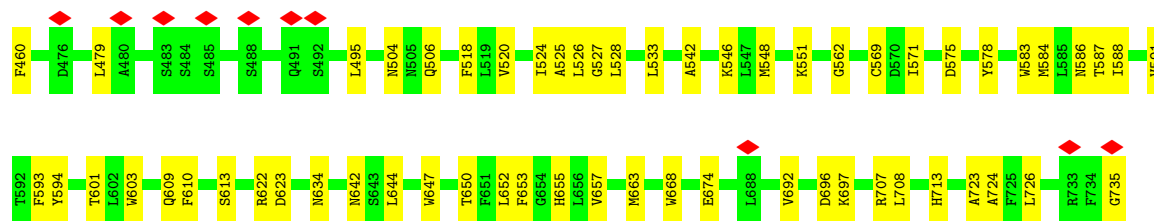
Chain A: 76% 23%



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 79% 21%





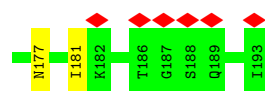
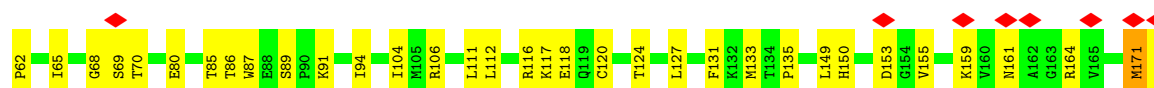
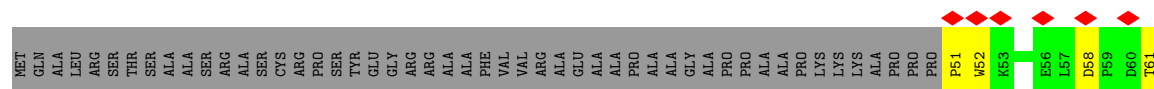
• Molecule 7: Photosystem I iron-sulfur center

Chain C: 80% 19%



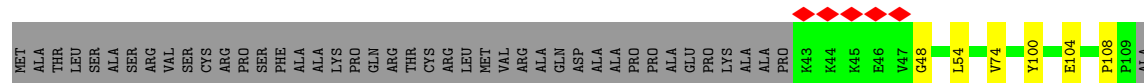
• Molecule 8: Photosystem I reaction center subunit II, chloroplastic

Chain D: 10% 53% 20% 26%



• Molecule 9: Photosystem I reaction center subunit IV

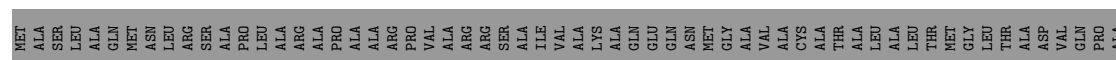
Chain E: 5% 55% 5% 40%



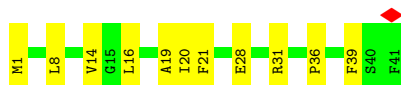
LYS

• Molecule 10: PSAF1

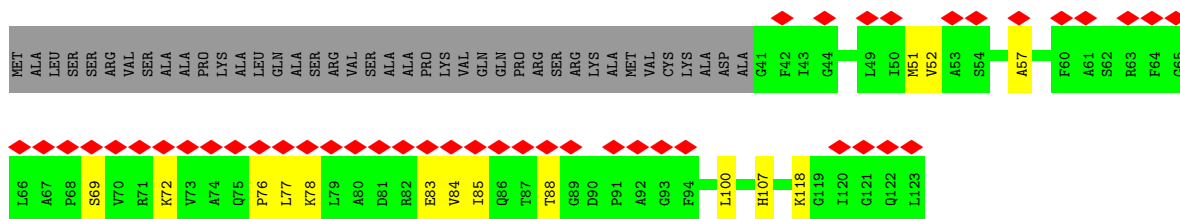
Chain F: 57% 16% 27%



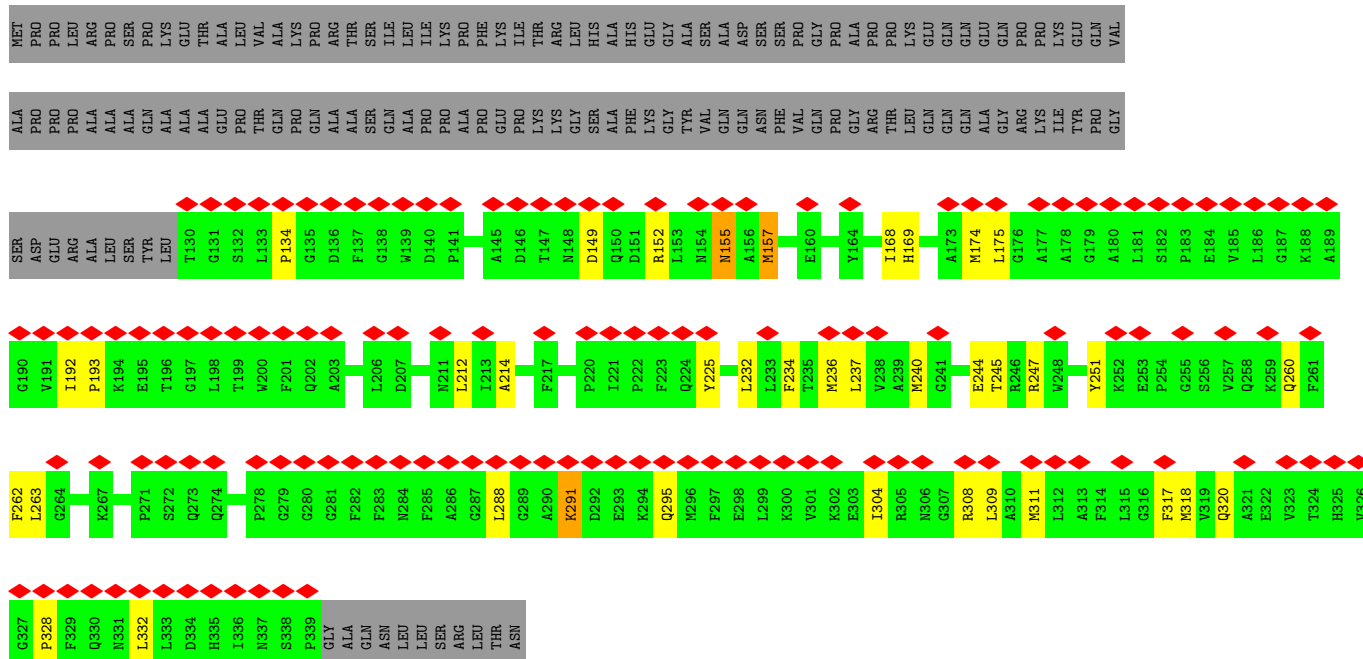
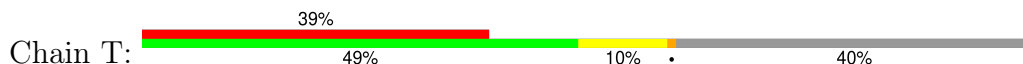
- Molecule 11: Photosystem I reaction center subunit IX



- Molecule 12: PSI-K



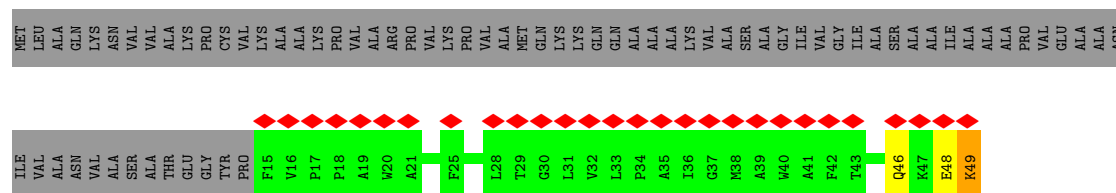
- Molecule 13: TIDI1



- Molecule 14: PSAL1



- Molecule 15: Photosystem I reaction center subunit VIII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0151	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.19	0/1544	0.40	0/2093
1	a	0.16	0/1544	0.43	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.14	0/1722	0.36	0/2339
3	c	0.16	0/1657	0.41	1/2251 (0.0%)
4	8	0.15	0/1770	0.38	1/2401 (0.0%)
4	b	0.14	0/1759	0.33	0/2386
5	A	0.14	0/6004	0.30	0/8190
6	B	0.14	0/6026	0.33	0/8235
7	C	0.11	0/610	0.30	0/828
8	D	0.13	0/1163	0.41	1/1571 (0.1%)
9	E	0.19	0/547	0.37	0/743
10	F	0.16	0/1329	0.36	0/1797
11	J	0.18	0/338	0.46	0/461
12	K	0.19	0/587	0.52	0/795
13	T	0.18	0/1688	0.47	0/2292
14	L	0.18	0/914	0.39	0/1248
15	I	0.19	0/286	0.41	0/394
All	All	0.15	0/31256	0.37	3/42519 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8	82	MET	CB-CG-SD	5.25	128.45	112.70
3	c	81	MET	CB-CG-SD	5.23	128.40	112.70
8	D	171	MET	CB-CG-SD	5.06	127.89	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1470	31	0
1	a	1505	0	1469	35	0
2	3	1719	0	1671	48	0
3	7	1669	0	1615	35	0
3	c	1607	0	1563	49	0
4	8	1721	0	1662	22	0
4	b	1710	0	1652	21	0
5	A	5808	0	5637	148	0
6	B	5814	0	5560	132	0
7	C	600	0	582	15	0
8	D	1133	0	1138	31	0
9	E	535	0	534	3	0
10	F	1300	0	1322	26	0
11	J	327	0	328	12	0
12	K	579	0	608	14	0
13	T	1639	0	1590	29	0
14	L	894	0	908	27	0
15	I	274	0	282	3	0
16	1	98	0	68	4	0
16	3	123	0	114	16	0
16	7	141	0	95	10	0
16	8	144	0	99	10	0
16	T	97	0	68	11	0
16	a	94	0	62	3	0
16	b	145	0	99	12	0
16	c	144	0	101	22	0
17	1	614	0	522	23	0
17	3	773	0	655	27	0
17	7	510	0	423	18	0
17	8	546	0	431	18	0
17	A	2453	0	2473	140	0
17	B	2252	0	2113	107	0
17	F	263	0	230	8	0
17	J	49	0	39	3	0
17	K	181	0	132	7	0
17	L	110	0	101	4	0
17	T	531	0	401	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	578	0	441	15	0
17	b	551	0	440	14	0
17	c	526	0	457	27	0
18	1	42	0	56	6	0
18	3	42	0	56	3	0
18	7	42	0	56	3	0
18	8	42	0	56	1	0
18	T	42	0	47	4	0
18	a	42	0	56	4	0
18	b	42	0	56	1	0
18	c	42	0	56	0	0
19	1	44	0	56	1	0
19	3	44	0	56	4	0
19	7	44	0	56	6	0
19	8	44	0	56	1	0
19	T	44	0	56	2	0
19	a	44	0	56	1	0
19	b	44	0	56	0	0
19	c	44	0	55	1	0
20	1	40	0	54	8	0
20	3	120	0	163	9	0
20	7	40	0	56	3	0
20	8	40	0	56	5	0
20	A	240	0	336	24	0
20	B	280	0	391	21	0
20	F	80	0	112	9	0
20	I	40	0	53	2	0
20	J	80	0	112	6	0
20	K	40	0	55	5	0
20	L	80	0	110	6	0
20	T	40	0	56	3	0
20	a	40	0	56	4	0
20	b	40	0	56	6	0
20	c	40	0	56	2	0
21	1	58	0	56	2	0
21	7	34	0	37	0	0
21	8	30	0	30	2	0
21	A	115	0	143	9	0
21	F	31	0	31	0	0
21	a	46	0	29	2	0
21	b	21	0	12	0	0
21	c	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3	35	0	33	5	0
23	3	50	0	56	1	0
23	8	39	0	36	2	0
23	B	61	0	83	8	0
24	7	50	0	73	5	0
24	A	32	0	27	2	0
24	F	29	0	28	1	0
25	7	35	0	46	3	0
25	A	35	0	46	1	0
26	8	42	0	30	0	0
26	F	51	0	49	0	0
27	A	65	0	72	8	0
28	A	33	0	46	2	0
28	B	33	0	46	3	0
29	A	8	0	0	0	0
29	C	16	0	0	1	0
30	J	35	0	0	0	0
All	All	44202	0	42797	957	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 11.

The worst 5 of 957 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)
14:L:81:VAL:CG1	14:L:85:LEU:HD12	1.67	1.23
1:a:76:LEU:HD12	1:a:152:LEU:CD2	1.71	1.20
5:A:646:LEU:HD22	6:B:652:LEU:HD21	1.24	1.18
1:a:76:LEU:CD1	1:a:152:LEU:HD22	1.73	1.17
1:1:201:PRO:HD2	1:1:204:GLU:OE1	1.43	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	195/228 (86%)	187 (96%)	7 (4%)	1 (0%)	24	55
1	a	195/228 (86%)	184 (94%)	9 (5%)	2 (1%)	12	38
2	3	224/286 (78%)	213 (95%)	11 (5%)	0	100	100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100	100
3	c	207/255 (81%)	201 (97%)	6 (3%)	0	100	100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100	100
4	b	222/254 (87%)	217 (98%)	5 (2%)	0	100	100
5	A	738/751 (98%)	715 (97%)	23 (3%)	0	100	100
6	B	732/735 (100%)	711 (97%)	21 (3%)	0	100	100
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	141/193 (73%)	131 (93%)	10 (7%)	0	100	100
9	E	65/111 (59%)	62 (95%)	3 (5%)	0	100	100
10	F	163/227 (72%)	154 (94%)	9 (6%)	0	100	100
11	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
12	K	81/123 (66%)	72 (89%)	9 (11%)	0	100	100
13	T	208/350 (59%)	200 (96%)	8 (4%)	0	100	100
14	L	120/198 (61%)	118 (98%)	2 (2%)	0	100	100
15	I	33/108 (31%)	33 (100%)	0	0	100	100
All	All	3880/4678 (83%)	3738 (96%)	139 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	146	GLN
1	a	64	GLU
1	1	55	ASN

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	153/179 (86%)	153 (100%)	0	100	100
1	a	153/179 (86%)	153 (100%)	0	100	100
2	3	170/217 (78%)	169 (99%)	1 (1%)	78	92
3	7	171/201 (85%)	168 (98%)	3 (2%)	51	82
3	c	166/201 (83%)	165 (99%)	1 (1%)	78	92
4	8	173/197 (88%)	172 (99%)	1 (1%)	78	92
4	b	172/197 (87%)	168 (98%)	4 (2%)	44	78
5	A	599/609 (98%)	596 (100%)	3 (0%)	81	93
6	B	595/596 (100%)	592 (100%)	3 (0%)	81	93
7	C	68/69 (99%)	68 (100%)	0	100	100
8	D	123/156 (79%)	123 (100%)	0	100	100
9	E	60/93 (64%)	60 (100%)	0	100	100
10	F	136/177 (77%)	135 (99%)	1 (1%)	76	91
11	J	36/36 (100%)	36 (100%)	0	100	100
12	K	58/88 (66%)	58 (100%)	0	100	100
13	T	169/280 (60%)	161 (95%)	8 (5%)	23	57
14	L	91/150 (61%)	90 (99%)	1 (1%)	65	87
15	I	28/76 (37%)	27 (96%)	1 (4%)	31	66
All	All	3121/3701 (84%)	3094 (99%)	27 (1%)	68	89

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	T	174	MET
13	T	291	LYS
3	c	187	MET
13	T	240	MET
13	T	317	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	30	ASN
14	L	69	ASN

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Mol	Chain	Res	Type
4	b	140	GLN
3	c	154	ASN
15	I	46	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

284 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	CLA	A	5039	5	59,63,73	1.23	7 (11%)	70,101,113	1.21	6 (8%)
17	CLA	B	830	6,21	69,73,73	1.17	7 (10%)	82,113,113	1.21	6 (7%)
17	CLA	A	5027	-	61,65,73	1.31	8 (13%)	72,103,113	1.19	6 (8%)
17	CLA	A	5016	5	69,73,73	1.18	9 (13%)	82,113,113	1.25	8 (9%)
17	CLA	A	5036	5	68,72,73	1.19	8 (11%)	80,111,113	1.20	4 (5%)
21	LHG	A	5002	24	35,35,48	0.35	0	38,41,54	0.37	0
17	CLA	8	314	4	50,54,73	1.33	7 (14%)	59,90,113	1.29	4 (6%)
17	CLA	c	312	3	54,58,73	1.32	7 (12%)	64,95,113	1.24	6 (9%)
17	CLA	8	315	4	49,53,73	1.37	7 (14%)	58,89,113	1.27	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5022	-	69,73,73	1.15	7 (10%)	82,113,113	1.16	4 (4%)
17	CLA	L	201	14	69,73,73	1.14	7 (10%)	82,113,113	1.08	5 (6%)
16	CHL	8	306	-	50,54,74	1.62	3 (6%)	55,90,114	1.80	10 (18%)
17	CLA	T	407	13	54,58,73	1.27	8 (14%)	64,95,113	1.22	6 (9%)
17	CLA	A	5013	17,24,5	69,73,73	1.12	7 (10%)	82,113,113	1.12	7 (8%)
17	CLA	A	5043	21	49,53,73	1.35	8 (16%)	58,89,113	1.30	5 (8%)
17	CLA	8	312	4	54,58,73	1.37	10 (18%)	64,95,113	1.40	7 (10%)
17	CLA	8	310	4	64,68,73	1.18	7 (10%)	76,107,113	1.10	4 (5%)
17	CLA	T	402	13,17	54,58,73	1.30	8 (14%)	64,95,113	1.31	6 (9%)
17	CLA	b	608	-	49,53,73	1.37	6 (12%)	58,89,113	1.31	5 (8%)
17	CLA	B	815	-	54,58,73	1.31	7 (12%)	64,95,113	1.34	6 (9%)
17	CLA	b	603	4	54,58,73	1.33	9 (16%)	64,95,113	1.40	5 (7%)
17	CLA	c	313	3	49,53,73	1.35	7 (14%)	58,89,113	1.33	4 (6%)
17	CLA	B	826	6	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
24	LMG	F	5011	-	29,29,55	0.20	0	37,37,63	0.15	0
16	CHL	1	601	-	55,59,74	1.33	3 (5%)	61,96,114	1.80	12 (19%)
25	LMU	A	5054	-	36,36,36	0.13	0	47,47,47	0.19	0
17	CLA	c	307	3	54,58,73	1.31	8 (14%)	64,95,113	1.58	10 (15%)
17	CLA	A	5008	5	69,73,73	1.11	7 (10%)	82,113,113	1.11	7 (8%)
17	CLA	3	307	2	69,73,73	1.15	7 (10%)	82,113,113	1.11	6 (7%)
29	SF4	A	5046	6,5	0,12,12	-	-	-	-	-
20	BCR	A	5052	-	41,41,41	0.17	0	56,56,56	0.36	0
17	CLA	a	610	21	50,54,73	1.35	6 (12%)	59,90,113	1.25	4 (6%)
23	DGD	3	321	2	51,51,67	0.17	0	65,65,81	0.16	0
17	CLA	a	605	-	49,53,73	1.37	8 (16%)	58,89,113	1.28	4 (6%)
19	XAT	1	616	-	41,47,47	0.15	0	54,74,74	0.97	3 (5%)
17	CLA	K	201	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	4 (6%)
17	CLA	c	310	3	49,53,73	1.41	9 (18%)	58,89,113	1.47	5 (8%)
17	CLA	A	5024	5	64,68,73	1.18	7 (10%)	76,107,113	1.09	4 (5%)
17	CLA	B	832	6	59,63,73	1.26	8 (13%)	70,101,113	1.15	7 (10%)
17	CLA	T	412	-	46,50,73	1.38	7 (15%)	53,85,113	1.18	4 (7%)
18	LUT	a	615	-	42,43,43	0.17	0	51,60,60	1.17	6 (11%)
21	LHG	a	619	1,16,17	22,22,48	0.40	0	25,28,54	0.38	0
17	CLA	K	203	12	49,53,73	1.37	8 (16%)	58,89,113	1.23	4 (6%)
17	CLA	B	805	-	69,73,73	1.13	6 (8%)	82,113,113	1.24	7 (8%)
17	CLA	A	5042	5	64,68,73	1.24	8 (12%)	76,107,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	7	317	-	41,41,41	0.16	0	56,56,56	0.43	0
16	CHL	T	401	13	55,59,74	1.26	3 (5%)	61,96,114	2.41	14 (22%)
18	LUT	1	615	-	42,43,43	0.20	0	51,60,60	1.47	8 (15%)
17	CLA	B	804	6	52,56,73	1.31	8 (15%)	61,92,113	1.15	5 (8%)
17	CLA	3	311	2	59,63,73	1.26	7 (11%)	70,101,113	1.28	5 (7%)
20	BCR	J	103	-	41,41,41	0.15	0	56,56,56	0.27	0
17	CLA	7	304	17	54,58,73	1.35	8 (14%)	64,95,113	1.39	6 (9%)
19	XAT	a	616	-	41,47,47	0.15	0	54,74,74	0.77	2 (3%)
20	BCR	T	415	-	41,41,41	0.12	0	56,56,56	0.28	0
17	CLA	A	5033	5	59,63,73	1.26	8 (13%)	70,101,113	1.18	5 (7%)
17	CLA	B	806	6	69,73,73	1.15	9 (13%)	82,113,113	1.11	4 (4%)
17	CLA	c	309	3,21	64,68,73	1.20	7 (10%)	76,107,113	1.27	6 (7%)
20	BCR	B	849	-	41,41,41	0.22	0	56,56,56	1.03	4 (7%)
17	CLA	K	202	-	50,54,73	1.34	7 (14%)	59,90,113	1.22	5 (8%)
17	CLA	1	602	1	59,63,73	1.25	7 (11%)	70,101,113	1.32	7 (10%)
19	XAT	b	616	-	41,47,47	0.14	0	54,74,74	0.79	2 (3%)
20	BCR	B	846	-	41,41,41	0.15	0	56,56,56	0.21	0
17	CLA	B	835	6	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
19	XAT	8	317	-	41,47,47	0.15	0	54,74,74	0.88	1 (1%)
20	BCR	A	5049	-	41,41,41	0.29	0	56,56,56	0.83	2 (3%)
17	CLA	T	409	18	56,60,73	1.31	6 (10%)	65,97,113	1.49	8 (12%)
17	CLA	c	311	-	54,58,73	1.30	6 (11%)	64,95,113	1.32	5 (7%)
17	CLA	L	202	14	49,53,73	1.46	9 (18%)	58,89,113	1.34	3 (5%)
17	CLA	B	816	6	54,58,73	1.30	8 (14%)	64,95,113	1.33	6 (9%)
18	LUT	T	413	17,13	42,43,43	0.37	0	51,60,60	0.63	2 (3%)
21	LHG	c	317	17	27,27,48	0.37	0	30,33,54	0.35	0
17	CLA	B	839	6	69,73,73	1.18	9 (13%)	82,113,113	1.11	6 (7%)
17	CLA	A	5021	5	54,58,73	1.29	8 (14%)	64,95,113	1.28	6 (9%)
17	CLA	1	610	21	50,54,73	1.34	6 (12%)	59,90,113	1.25	4 (6%)
18	LUT	b	615	-	42,43,43	0.23	0	51,60,60	0.42	0
20	BCR	B	844	-	41,41,41	0.21	0	56,56,56	0.44	0
17	CLA	B	833	6	64,68,73	1.19	7 (10%)	76,107,113	1.21	5 (6%)
19	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.78	2 (3%)
18	LUT	7	315	-	42,43,43	0.38	1 (2%)	51,60,60	0.52	1 (1%)
17	CLA	8	304	4	55,59,73	1.33	8 (14%)	64,96,113	1.41	6 (9%)
17	CLA	a	607	-	50,54,73	1.38	9 (18%)	59,90,113	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PQN	B	842	-	34,34,34	0.29	0	43,45,45	0.51	1 (2%)
17	CLA	A	5015	5	59,63,73	1.23	6 (10%)	70,101,113	1.37	6 (8%)
17	CLA	A	5018	5	64,68,73	1.18	8 (12%)	76,107,113	1.18	4 (5%)
17	CLA	A	5017	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	5 (7%)
22	SQD	3	320	2	33,35,54	0.27	0	43,46,65	0.52	0
17	CLA	a	608	1,17	49,53,73	1.36	7 (14%)	57,88,113	1.42	5 (8%)
17	CLA	B	824	-	54,58,73	1.33	8 (14%)	64,95,113	1.48	6 (9%)
17	CLA	A	5025	5	64,68,73	1.19	8 (12%)	76,107,113	1.22	5 (6%)
17	CLA	B	802	6	69,73,73	1.17	9 (13%)	82,113,113	1.02	5 (6%)
17	CLA	F	5004	6,10	69,73,73	1.27	11 (15%)	82,113,113	1.36	6 (7%)
17	CLA	B	808	6	69,73,73	1.14	9 (13%)	82,113,113	1.12	5 (6%)
20	BCR	J	104	-	41,41,41	0.16	0	56,56,56	0.33	0
17	CLA	B	837	6	54,58,73	1.27	7 (12%)	64,95,113	1.26	6 (9%)
17	CLA	A	5030	-	69,73,73	1.16	8 (11%)	82,113,113	1.19	5 (6%)
17	CLA	1	607	-	69,73,73	1.16	6 (8%)	82,113,113	1.12	5 (6%)
17	CLA	3	310	2	50,54,73	1.34	8 (16%)	59,90,113	1.39	4 (6%)
17	CLA	7	303	3	59,63,73	1.28	9 (15%)	70,101,113	1.23	5 (7%)
17	CLA	7	311	3	50,54,73	1.37	8 (16%)	59,90,113	1.43	6 (10%)
17	CLA	T	405	13	49,53,73	1.37	7 (14%)	58,89,113	1.26	5 (8%)
19	XAT	c	315	3	41,47,47	0.16	0	54,74,74	0.76	2 (3%)
20	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.37	0
20	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.32	0
26	PTY	F	5002	10	32,32,49	0.56	0	35,37,54	0.45	0
20	BCR	I	4001	20	41,41,41	0.17	0	56,56,56	0.26	0
17	CLA	3	309	17,2	50,54,73	1.34	7 (14%)	59,90,113	1.14	4 (6%)
17	CLA	8	309	4	50,54,73	1.38	7 (14%)	59,90,113	1.30	4 (6%)
17	CLA	3	324	5,2	59,63,73	1.26	8 (13%)	70,101,113	1.21	4 (5%)
17	CLA	1	609	1	69,73,73	1.14	8 (11%)	82,113,113	1.20	4 (4%)
17	CLA	B	823	6	54,58,73	1.27	6 (11%)	64,95,113	1.19	5 (7%)
17	CLA	B	825	-	54,58,73	1.34	8 (14%)	64,95,113	1.18	7 (10%)
29	SF4	C	101	7	0,12,12	-	-	-	-	-
17	CLA	1	605	-	49,53,73	1.41	7 (14%)	58,89,113	1.45	4 (6%)
17	CLA	8	303	4	54,58,73	1.29	7 (12%)	64,95,113	1.18	5 (7%)
20	BCR	L	204	20	41,41,41	0.14	0	56,56,56	0.24	0
16	CHL	c	304	17	50,54,74	1.16	3 (6%)	55,90,114	2.16	8 (14%)
17	CLA	7	310	21	50,54,73	1.35	5 (10%)	59,90,113	1.22	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SF4	C	102	7	0,12,12	-	-	-		
17	CLA	3	312	2	50,54,73	1.32	7 (14%)	59,90,113	1.15	4 (6%)
17	CLA	B	820	-	59,63,73	1.26	7 (11%)	70,101,113	1.30	5 (7%)
16	CHL	7	305	-	50,54,74	1.44	3 (6%)	55,90,114	1.49	11 (20%)
17	CLA	A	5006	5	69,73,73	1.14	8 (11%)	82,113,113	1.20	6 (7%)
16	CHL	T	416	-	50,54,74	1.25	4 (8%)	55,90,114	2.21	11 (20%)
17	CLA	B	810	6	59,63,73	1.26	7 (11%)	70,101,113	1.29	4 (5%)
20	BCR	a	617	-	41,41,41	0.18	0	56,56,56	0.34	0
23	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.23	0
20	BCR	A	5047	-	41,41,41	0.17	0	56,56,56	0.32	0
17	CLA	B	836	6	64,68,73	1.17	7 (10%)	76,107,113	1.23	5 (6%)
17	CLA	8	311	21,17	59,63,73	1.26	8 (13%)	70,101,113	1.22	5 (7%)
17	CLA	F	5009	10	50,54,73	1.37	7 (14%)	59,90,113	1.43	4 (6%)
17	CLA	3	305	2	54,58,73	1.31	9 (16%)	64,95,113	1.27	6 (9%)
17	CLA	A	5035	5	69,73,73	1.13	8 (11%)	82,113,113	1.16	5 (6%)
17	CLA	a	612	-	54,58,73	1.30	8 (14%)	64,95,113	1.25	5 (7%)
20	BCR	F	5005	-	41,41,41	0.15	0	56,56,56	0.26	0
20	BCR	F	5010	-	41,41,41	0.15	0	56,56,56	0.33	0
17	CLA	3	303	-	50,54,73	1.33	7 (14%)	59,90,113	1.33	4 (6%)
17	CLA	B	814	-	54,58,73	1.30	8 (14%)	64,95,113	1.36	6 (9%)
17	CLA	B	827	-	64,68,73	1.18	7 (10%)	76,107,113	1.13	4 (5%)
17	CLA	c	302	3	50,54,73	1.32	8 (16%)	59,90,113	1.21	4 (6%)
21	LHG	a	618	1	22,22,48	0.45	0	25,27,54	0.46	0
25	LMU	7	319	-	36,36,36	0.12	0	47,47,47	0.15	0
16	CHL	3	301	2	66,70,74	1.12	3 (4%)	74,109,114	1.88	11 (14%)
20	BCR	3	319	2	41,41,41	0.19	0	56,56,56	0.29	0
16	CHL	b	607	-	55,59,74	1.16	4 (7%)	61,96,114	2.17	12 (19%)
17	CLA	A	5010	-	54,58,73	1.35	10 (18%)	64,95,113	1.35	6 (9%)
17	CLA	A	5004	-	69,73,73	1.14	8 (11%)	82,113,113	1.08	4 (4%)
17	CLA	1	612	-	64,68,73	1.21	6 (9%)	76,107,113	1.20	6 (7%)
17	CLA	B	818	6	69,73,73	1.14	8 (11%)	82,113,113	1.14	6 (7%)
16	CHL	8	308	-	55,59,74	1.14	3 (5%)	61,96,114	2.43	11 (18%)
17	CLA	B	829	6	69,73,73	1.15	6 (8%)	82,113,113	1.13	5 (6%)
20	BCR	K	205	-	41,41,41	0.27	0	56,56,56	0.76	2 (3%)
20	BCR	c	316	-	41,41,41	0.14	0	56,56,56	0.58	2 (3%)
21	LHG	1	618	17	26,26,48	0.40	0	29,32,54	0.43	0
18	LUT	c	314	-	42,43,43	0.40	1 (2%)	51,60,60	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5044	-	69,73,73	1.15	7 (10%)	82,113,113	1.11	7 (8%)
17	CLA	A	5041	5	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
16	CHL	c	306	-	52,56,74	1.38	3 (5%)	57,92,114	1.96	10 (17%)
17	CLA	3	323	5,2	59,63,73	1.22	7 (11%)	70,101,113	1.23	5 (7%)
17	CLA	T	403	-	54,58,73	1.44	10 (18%)	64,95,113	1.28	11 (17%)
16	CHL	c	305	-	54,58,74	1.04	4 (7%)	58,94,114	2.15	11 (18%)
17	CLA	7	309	3	50,54,73	1.30	8 (16%)	59,90,113	1.14	3 (5%)
17	CLA	B	817	6	59,63,73	1.24	7 (11%)	70,101,113	1.18	5 (7%)
17	CLA	B	831	6	59,63,73	1.26	8 (13%)	70,101,113	1.22	6 (8%)
17	CLA	a	614	1,17	50,54,73	1.36	7 (14%)	59,90,113	1.36	4 (6%)
17	CLA	b	602	4	64,68,73	1.19	7 (10%)	76,107,113	1.10	5 (6%)
17	CLA	c	308	3	69,73,73	1.14	8 (11%)	82,113,113	1.17	5 (6%)
17	CLA	F	5008	10	49,53,73	1.37	7 (14%)	58,89,113	1.29	4 (6%)
17	CLA	3	313	-	46,50,73	1.38	7 (15%)	53,85,113	1.23	4 (7%)
21	LHG	F	5001	17	30,30,48	0.37	0	33,36,54	0.32	0
26	PTY	8	319	26	20,20,49	0.69	0	23,25,54	0.51	0
17	CLA	A	5019	5	65,69,73	1.25	10 (15%)	77,108,113	1.28	4 (5%)
26	PTY	F	5003	26	17,17,49	0.70	0	18,21,54	0.60	0
30	LMK	J	101	-	34,34,53	0.44	0	34,41,60	0.56	1 (2%)
17	CLA	B	807	6	59,63,73	1.22	7 (11%)	70,101,113	1.20	5 (7%)
17	CLA	7	308	3	50,54,73	1.33	6 (12%)	59,90,113	1.34	4 (6%)
17	CLA	8	302	4	50,54,73	1.34	6 (12%)	59,90,113	1.40	5 (8%)
17	CLA	7	312	3	69,73,73	1.23	8 (11%)	82,113,113	1.25	6 (7%)
17	CLA	A	5023	5	50,54,73	1.34	7 (14%)	59,90,113	1.35	4 (6%)
17	CLA	b	604	-	54,58,73	1.32	8 (14%)	64,95,113	1.42	5 (7%)
17	CLA	B	819	-	64,68,73	1.23	8 (12%)	76,107,113	1.27	4 (5%)
17	CLA	c	301	3	69,73,73	1.17	7 (10%)	82,113,113	1.10	6 (7%)
17	CLA	1	604	-	54,58,73	1.28	7 (12%)	64,95,113	1.32	5 (7%)
17	CLA	a	603	-	49,53,73	1.38	7 (14%)	58,89,113	1.40	4 (6%)
21	LHG	7	318	17	33,33,48	0.35	0	36,39,54	0.34	0
20	BCR	3	317	2	41,41,41	0.14	0	56,56,56	0.32	0
24	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
17	CLA	a	602	1	59,63,73	1.25	8 (13%)	70,101,113	1.19	5 (7%)
17	CLA	7	314	3	50,54,73	1.33	7 (14%)	59,90,113	1.29	4 (6%)
20	BCR	B	843	6	41,41,41	0.16	0	56,56,56	0.31	0
17	CLA	A	5012	5	59,63,73	1.27	9 (15%)	70,101,113	1.36	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5014	-	69,73,73	1.14	7 (10%)	82,113,113	1.25	5 (6%)
17	CLA	B	834	-	54,58,73	1.30	7 (12%)	64,95,113	1.31	6 (9%)
16	CHL	a	606	-	51,55,74	1.24	4 (7%)	56,91,114	2.21	14 (25%)
20	BCR	8	318	-	41,41,41	0.17	0	56,56,56	0.53	0
21	LHG	1	619	-	30,30,48	0.36	0	33,36,54	0.34	0
17	CLA	1	608	-	49,53,73	1.36	6 (12%)	58,89,113	1.32	4 (6%)
17	CLA	A	5026	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	4 (4%)
17	CLA	c	303	16	54,58,73	1.31	7 (12%)	64,95,113	1.32	5 (7%)
17	CLA	T	410	13	54,58,73	1.30	7 (12%)	64,95,113	1.29	6 (9%)
24	LMG	A	5001	17,21,5	32,32,55	0.23	0	40,40,63	0.25	0
17	CLA	T	404	-	50,54,73	1.41	7 (14%)	59,90,113	1.17	5 (8%)
17	CLA	F	5006	-	64,68,73	1.18	7 (10%)	76,107,113	1.11	5 (6%)
17	CLA	3	304	-	50,54,73	1.35	7 (14%)	59,90,113	1.28	4 (6%)
17	CLA	a	604	-	53,56,73	1.36	8 (15%)	62,92,113	1.29	6 (9%)
20	BCR	L	203	-	41,41,41	0.14	0	56,56,56	0.36	0
17	CLA	7	313	3	54,58,73	1.31	7 (12%)	64,95,113	1.29	6 (9%)
17	CLA	a	609	1	64,68,73	1.18	7 (10%)	76,107,113	1.09	5 (6%)
20	BCR	A	5048	-	41,41,41	0.29	0	56,56,56	0.58	0
17	CLA	A	5020	5	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
17	CLA	J	102	11	53,57,73	1.30	6 (11%)	61,93,113	1.36	5 (8%)
19	XAT	7	316	-	41,47,47	0.18	0	54,74,74	0.85	3 (5%)
17	CLA	B	822	6	49,53,73	1.36	7 (14%)	58,89,113	1.35	4 (6%)
26	PTY	8	320	-	20,20,49	0.66	0	21,24,54	0.55	0
16	CHL	3	322	-	65,69,74	1.31	3 (4%)	73,108,114	1.89	10 (13%)
17	CLA	B	803	-	69,73,73	1.14	8 (11%)	82,113,113	1.14	4 (4%)
20	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.35	0
17	CLA	3	308	2	59,63,73	1.24	7 (11%)	70,101,113	1.12	6 (8%)
16	CHL	7	306	-	51,55,74	1.05	4 (7%)	56,91,114	2.37	12 (21%)
16	CHL	7	307	-	52,56,74	1.32	3 (5%)	57,92,114	1.96	10 (17%)
17	CLA	8	305	-	50,54,73	1.38	9 (18%)	59,90,113	1.43	4 (6%)
17	CLA	b	613	4	50,54,73	1.32	7 (14%)	59,90,113	1.18	5 (8%)
17	CLA	a	613	1	50,54,73	1.34	7 (14%)	59,90,113	1.19	4 (6%)
28	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.57	1 (2%)
17	CLA	A	5031	5	69,73,73	1.14	7 (10%)	82,113,113	1.20	5 (6%)
21	LHG	8	321	17	29,29,48	0.37	0	32,35,54	0.35	0
21	LHG	A	5055	17	29,29,48	0.37	0	33,35,54	0.33	0
18	LUT	8	316	-	42,43,43	0.26	0	51,60,60	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CL0	A	5003	5	69,73,73	1.09	4 (5%)	82,113,113	1.85	10 (12%)
17	CLA	T	411	-	50,54,73	1.33	7 (14%)	59,90,113	1.20	4 (6%)
17	CLA	3	306	-	59,63,73	1.24	8 (13%)	70,101,113	1.24	6 (8%)
17	CLA	b	601	4	50,54,73	1.36	6 (12%)	59,90,113	1.27	4 (6%)
17	CLA	A	5028	5	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
18	LUT	3	315	-	42,43,43	0.20	0	51,60,60	0.35	0
17	CLA	3	314	2	50,54,73	1.33	8 (16%)	59,90,113	1.28	4 (6%)
21	LHG	A	5053	5	48,48,48	0.29	0	51,54,54	0.29	0
16	CHL	1	606	-	51,55,74	1.29	4 (7%)	56,91,114	2.17	11 (19%)
17	CLA	8	313	4	55,59,73	1.41	8 (14%)	64,96,113	1.22	5 (7%)
17	CLA	F	5007	-	51,55,73	1.31	8 (15%)	60,91,113	1.17	5 (8%)
17	CLA	B	840	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	4 (4%)
20	BCR	B	845	-	41,41,41	0.28	0	56,56,56	0.91	3 (5%)
16	CHL	8	307	-	51,55,74	1.07	4 (7%)	56,91,114	2.10	11 (19%)
16	CHL	a	601	21	51,55,74	1.33	4 (7%)	56,91,114	1.99	12 (21%)
17	CLA	K	204	-	49,53,73	1.36	7 (14%)	58,89,113	1.23	4 (6%)
17	CLA	A	5040	-	64,68,73	1.21	8 (12%)	76,107,113	1.15	4 (5%)
17	CLA	A	5011	5	69,73,73	1.17	8 (11%)	82,113,113	1.12	6 (7%)
20	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
17	CLA	1	614	1	50,54,73	1.35	6 (12%)	59,90,113	1.35	4 (6%)
17	CLA	1	611	1	50,54,73	1.39	10 (20%)	59,90,113	1.41	6 (10%)
17	CLA	B	812	6	50,54,73	1.34	7 (14%)	59,90,113	1.28	4 (6%)
17	CLA	b	609	4	64,68,73	1.17	8 (12%)	76,107,113	1.08	4 (5%)
20	BCR	B	801	-	41,41,41	0.15	0	56,56,56	0.35	0
23	DGD	8	301	-	40,40,67	0.27	0	54,54,81	0.47	0
17	CLA	B	838	-	59,63,73	1.30	9 (15%)	70,101,113	1.27	5 (7%)
17	CLA	b	612	4	52,56,73	1.40	8 (15%)	61,92,113	1.27	5 (8%)
17	CLA	T	406	-	54,58,73	1.32	7 (12%)	64,95,113	1.33	6 (9%)
17	CLA	A	5038	5	54,58,73	1.34	8 (14%)	64,95,113	1.39	5 (7%)
19	XAT	T	414	-	41,47,47	0.15	0	54,74,74	0.72	1 (1%)
17	CLA	3	302	2	69,73,73	1.16	9 (13%)	82,113,113	1.21	4 (4%)
17	CLA	1	613	1	50,54,73	1.34	7 (14%)	59,90,113	1.33	4 (6%)
21	LHG	b	618	17	20,20,48	0.39	0	23,26,54	0.39	0
20	BCR	A	5050	-	41,41,41	0.17	0	56,56,56	0.29	0
16	CHL	b	606	-	51,55,74	1.08	4 (7%)	56,91,114	2.17	12 (21%)
17	CLA	A	5007	17	64,68,73	1.17	5 (7%)	76,107,113	1.12	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	5032	5	49,53,73	1.40	8 (16%)	58,89,113	1.34	4 (6%)
17	CLA	B	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.16	5 (6%)
17	CLA	B	809	6	64,68,73	1.21	7 (10%)	76,107,113	1.19	5 (6%)
17	CLA	T	408	18,13	54,58,73	1.28	8 (14%)	64,95,113	1.24	6 (9%)
17	CLA	a	611	1	50,54,73	1.37	8 (16%)	59,90,113	1.42	6 (10%)
17	CLA	B	821	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	4 (7%)
17	CLA	1	603	1	49,53,73	1.39	8 (16%)	58,89,113	1.37	4 (6%)
17	CLA	A	5005	-	69,73,73	1.13	8 (11%)	82,113,113	1.10	5 (6%)
17	CLA	A	5009	5	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
17	CLA	b	610	21	54,58,73	1.29	6 (11%)	64,95,113	1.24	5 (7%)
17	CLA	7	302	3	64,68,73	1.20	8 (12%)	76,107,113	1.08	3 (3%)
20	BCR	1	617	1	41,41,41	0.24	0	56,56,56	0.46	0
17	CLA	A	5034	5	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
17	CLA	A	5037	5	54,58,73	1.31	8 (14%)	64,95,113	1.30	6 (9%)
17	CLA	B	811	6	54,58,73	1.31	7 (12%)	64,95,113	1.28	5 (7%)
17	CLA	A	5029	5	69,73,73	1.11	6 (8%)	82,113,113	1.24	6 (7%)
17	CLA	B	813	6	54,58,73	1.31	5 (9%)	64,95,113	1.35	6 (9%)
17	CLA	B	828	-	59,63,73	1.35	8 (13%)	70,101,113	1.29	5 (7%)
17	CLA	b	611	4	54,58,73	1.35	8 (14%)	64,95,113	1.41	7 (10%)
17	CLA	b	614	4	50,54,73	1.33	7 (14%)	59,90,113	1.25	4 (6%)
16	CHL	b	605	-	51,55,74	1.19	3 (5%)	56,91,114	2.21	11 (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
17	CLA	A	5039	5	-	5/27/103/115	-
17	CLA	B	830	6,21	-	12/39/115/115	-
17	CLA	A	5027	-	-	9/30/106/115	-
17	CLA	A	5016	5	-	16/39/115/115	-
17	CLA	A	5036	5	-	9/39/115/115	-
21	LHG	A	5002	24	-	8/40/40/53	-
17	CLA	8	314	4	-	9/17/93/115	-
17	CLA	c	312	3	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	315	4	-	8/15/91/115	-
17	CLA	A	5022	-	-	14/39/115/115	-
17	CLA	L	201	14	-	10/39/115/115	-
16	CHL	8	306	-	-	9/17/93/117	-
17	CLA	T	407	13	-	11/21/97/115	-
17	CLA	A	5013	17,24,5	-	15/39/115/115	-
17	CLA	A	5043	21	-	8/15/91/115	-
17	CLA	8	312	4	-	8/21/97/115	-
17	CLA	8	310	4	-	11/33/109/115	-
17	CLA	T	402	13,17	-	6/21/97/115	-
17	CLA	b	608	-	-	6/15/91/115	-
17	CLA	B	815	-	-	6/21/97/115	-
17	CLA	b	603	4	-	10/21/97/115	-
17	CLA	c	313	3	-	6/15/91/115	-
17	CLA	B	826	6	-	9/39/115/115	-
24	LMG	F	5011	-	-	3/24/44/70	0/1/1/1
16	CHL	1	601	-	-	9/23/99/117	-
25	LMU	A	5054	-	-	5/21/61/61	0/2/2/2
17	CLA	c	307	3	-	6/21/97/115	-
17	CLA	A	5008	5	-	13/39/115/115	-
17	CLA	3	307	2	-	13/39/115/115	-
29	SF4	A	5046	6,5	-	-	0/6/5/5
20	BCR	A	5052	-	-	5/29/63/63	0/2/2/2
17	CLA	a	610	21	-	8/17/93/115	-
23	DGD	3	321	2	-	10/39/79/95	0/2/2/2
17	CLA	a	605	-	-	6/15/91/115	-
19	XAT	1	616	-	-	2/31/93/93	0/4/4/4
17	CLA	K	201	-	-	7/15/91/115	-
17	CLA	c	310	3	-	7/15/91/115	-
17	CLA	A	5024	5	-	16/33/109/115	-
17	CLA	B	832	6	-	8/27/103/115	-
18	LUT	a	615	-	3/3/12/27	9/29/67/67	0/2/2/2
17	CLA	T	412	-	-	4/12/88/115	-
21	LHG	a	619	1,16,17	-	6/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	K	203	12	-	10/15/91/115	-
17	CLA	B	805	-	-	9/39/115/115	-
17	CLA	A	5042	5	-	8/33/109/115	-
20	BCR	7	317	-	-	4/29/63/63	0/2/2/2
16	CHL	T	401	13	-	10/23/99/117	-
18	LUT	1	615	-	3/3/12/27	10/29/67/67	0/2/2/2
17	CLA	B	804	6	-	9/19/95/115	-
17	CLA	3	311	2	-	10/27/103/115	-
20	BCR	J	103	-	-	4/29/63/63	0/2/2/2
17	CLA	7	304	17	-	7/21/97/115	-
19	XAT	a	616	-	-	3/31/93/93	0/4/4/4
20	BCR	T	415	-	-	4/29/63/63	0/2/2/2
17	CLA	A	5033	5	-	5/27/103/115	-
17	CLA	B	806	6	-	17/39/115/115	-
17	CLA	c	309	3,21	-	11/33/109/115	-
20	BCR	B	849	-	-	6/29/63/63	0/2/2/2
17	CLA	K	202	-	-	7/17/93/115	-
17	CLA	1	602	1	-	15/27/103/115	-
19	XAT	b	616	-	-	0/31/93/93	0/4/4/4
20	BCR	B	846	-	-	2/29/63/63	0/2/2/2
17	CLA	B	835	6	-	9/21/97/115	-
19	XAT	8	317	-	-	0/31/93/93	0/4/4/4
20	BCR	A	5049	-	-	3/29/63/63	0/2/2/2
17	CLA	T	409	18	-	13/24/100/115	-
18	LUT	T	413	17,13	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	c	311	-	-	6/21/97/115	-
17	CLA	B	816	6	-	6/21/97/115	-
17	CLA	L	202	14	-	6/15/91/115	-
21	LHG	c	317	17	-	3/32/32/53	-
17	CLA	B	839	6	-	10/39/115/115	-
17	CLA	A	5021	5	-	5/21/97/115	-
18	LUT	b	615	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	1	610	21	-	9/17/93/115	-
20	BCR	B	844	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	833	6	-	11/33/109/115	-
19	XAT	3	316	-	-	3/31/93/93	0/4/4/4
18	LUT	7	315	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	8	304	4	-	10/23/99/115	-
17	CLA	a	607	-	-	4/17/93/115	-
28	PQN	B	842	-	-	1/23/43/43	0/2/2/2
17	CLA	A	5015	5	-	6/27/103/115	-
17	CLA	A	5018	5	-	13/33/109/115	-
17	CLA	A	5017	-	-	12/27/103/115	-
22	SQD	3	320	2	-	11/30/50/69	0/1/1/1
17	CLA	a	608	1,17	-	7/15/91/115	-
17	CLA	B	824	-	-	11/21/97/115	-
17	CLA	A	5025	5	-	9/33/109/115	-
17	CLA	B	802	6	-	15/39/115/115	-
17	CLA	F	5004	6,10	-	12/39/115/115	-
17	CLA	B	808	6	-	20/39/115/115	-
20	BCR	J	104	-	-	2/29/63/63	0/2/2/2
17	CLA	B	837	6	-	8/21/97/115	-
17	CLA	A	5030	-	-	10/39/115/115	-
17	CLA	1	607	-	-	13/39/115/115	-
17	CLA	3	310	2	-	8/17/93/115	-
17	CLA	7	303	3	-	4/27/103/115	-
17	CLA	7	311	3	-	7/17/93/115	-
17	CLA	T	405	13	-	6/15/91/115	-
19	XAT	c	315	3	-	3/31/93/93	0/4/4/4
20	BCR	b	617	-	-	4/29/63/63	0/2/2/2
20	BCR	3	318	-	-	4/29/63/63	0/2/2/2
26	PTY	F	5002	10	-	6/36/36/53	-
20	BCR	I	4001	20	-	2/29/63/63	0/2/2/2
17	CLA	3	309	17,2	-	9/17/93/115	-
17	CLA	8	309	4	-	5/17/93/115	-
17	CLA	3	324	5,2	-	6/27/103/115	-
17	CLA	1	609	1	-	11/39/115/115	-
17	CLA	B	823	6	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	825	-	-	4/21/97/115	-
29	SF4	C	101	7	-	-	0/6/5/5
17	CLA	1	605	-	-	6/15/91/115	-
17	CLA	8	303	4	-	8/21/97/115	-
20	BCR	L	204	20	-	4/29/63/63	0/2/2/2
16	CHL	c	304	17	-	7/17/93/117	-
17	CLA	7	310	21	-	7/17/93/115	-
29	SF4	C	102	7	-	-	0/6/5/5
17	CLA	3	312	2	-	8/17/93/115	-
17	CLA	B	820	-	-	10/27/103/115	-
16	CHL	7	305	-	-	5/17/93/117	-
17	CLA	A	5006	5	-	17/39/115/115	-
16	CHL	T	416	-	-	8/17/93/117	-
17	CLA	B	810	6	-	13/27/103/115	-
20	BCR	a	617	-	-	5/29/63/63	0/2/2/2
23	DGD	B	848	-	-	4/50/90/95	0/2/2/2
20	BCR	A	5047	-	-	4/29/63/63	0/2/2/2
17	CLA	B	836	6	-	7/33/109/115	-
17	CLA	8	311	21,17	-	6/27/103/115	-
17	CLA	F	5009	10	-	5/17/93/115	-
17	CLA	3	305	2	-	6/21/97/115	-
17	CLA	A	5035	5	-	15/39/115/115	-
17	CLA	a	612	-	-	8/21/97/115	-
20	BCR	F	5005	-	-	0/29/63/63	0/2/2/2
20	BCR	F	5010	-	-	4/29/63/63	0/2/2/2
17	CLA	3	303	-	-	8/17/93/115	-
17	CLA	B	814	-	-	12/21/97/115	-
17	CLA	B	827	-	-	10/33/109/115	-
17	CLA	c	302	3	-	4/17/93/115	-
21	LHG	a	618	1	-	14/26/26/53	-
25	LMU	7	319	-	-	9/21/61/61	0/2/2/2
16	CHL	3	301	2	1/1/14/21	21/37/113/117	-
20	BCR	3	319	2	-	4/29/63/63	0/2/2/2
16	CHL	b	607	-	-	8/23/99/117	-
17	CLA	A	5010	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	5004	-	-	15/39/115/115	-
17	CLA	1	612	-	-	11/33/109/115	-
17	CLA	B	818	6	-	14/39/115/115	-
16	CHL	8	308	-	-	10/23/99/117	-
17	CLA	B	829	6	-	16/39/115/115	-
20	BCR	K	205	-	-	10/29/63/63	0/2/2/2
20	BCR	c	316	-	-	9/29/63/63	0/2/2/2
21	LHG	1	618	17	-	11/31/31/53	-
18	LUT	c	314	-	3/3/12/27	5/29/67/67	0/2/2/2
17	CLA	A	5044	-	-	12/39/115/115	-
17	CLA	A	5041	5	-	8/39/115/115	-
16	CHL	c	306	-	-	6/20/96/117	-
18	LUT	8	316	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	3	323	5,2	-	10/27/103/115	-
16	CHL	c	305	-	-	14/22/98/117	-
17	CLA	7	309	3	-	7/17/93/115	-
17	CLA	B	817	6	-	9/27/103/115	-
17	CLA	B	831	6	-	10/27/103/115	-
17	CLA	T	403	-	-	10/21/97/115	-
17	CLA	a	614	1,17	-	8/17/93/115	-
17	CLA	b	602	4	-	11/33/109/115	-
17	CLA	F	5008	10	-	5/15/91/115	-
17	CLA	3	313	-	-	5/12/88/115	-
17	CLA	c	308	3	-	16/39/115/115	-
21	LHG	F	5001	17	-	11/35/35/53	-
26	PTY	8	319	26	-	9/23/23/53	-
17	CLA	A	5019	5	-	10/35/111/115	-
26	PTY	F	5003	26	-	10/19/19/53	-
30	LMK	J	101	-	-	3/41/41/60	-
17	CLA	B	807	6	-	11/27/103/115	-
17	CLA	7	308	3	-	6/17/93/115	-
17	CLA	8	302	4	-	5/17/93/115	-
17	CLA	7	312	3	-	13/39/115/115	-
17	CLA	A	5023	5	-	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	604	-	-	8/21/97/115	-
17	CLA	B	819	-	-	9/33/109/115	-
17	CLA	c	301	3	-	14/39/115/115	-
17	CLA	1	604	-	-	9/21/97/115	-
17	CLA	a	603	-	-	8/15/91/115	-
21	LHG	7	318	17	-	2/38/38/53	-
20	BCR	3	317	2	-	4/29/63/63	0/2/2/2
24	LMG	7	301	-	-	12/45/65/70	0/1/1/1
17	CLA	a	602	1	-	6/27/103/115	-
17	CLA	7	314	3	-	7/17/93/115	-
20	BCR	B	843	6	-	5/29/63/63	0/2/2/2
17	CLA	A	5012	5	-	7/27/103/115	-
17	CLA	A	5014	-	-	14/39/115/115	-
17	CLA	B	834	-	-	13/21/97/115	-
16	CHL	a	606	-	-	6/19/95/117	-
20	BCR	8	318	-	-	6/29/63/63	0/2/2/2
21	LHG	1	619	-	-	7/35/35/53	-
17	CLA	1	608	-	-	8/15/91/115	-
17	CLA	A	5026	-	-	11/39/115/115	-
17	CLA	c	303	16	-	6/21/97/115	-
17	CLA	T	410	13	-	7/21/97/115	-
24	LMG	A	5001	17,21,5	-	4/26/46/70	0/1/1/1
17	CLA	T	404	-	-	9/17/93/115	-
17	CLA	F	5006	-	-	8/33/109/115	-
17	CLA	3	304	-	-	8/17/93/115	-
17	CLA	a	604	-	-	10/19/95/115	-
20	BCR	L	203	-	-	4/29/63/63	0/2/2/2
17	CLA	7	313	3	-	5/21/97/115	-
17	CLA	a	609	1	-	11/33/109/115	-
20	BCR	A	5048	-	-	7/29/63/63	0/2/2/2
17	CLA	A	5020	5	-	13/39/115/115	-
17	CLA	J	102	11	-	7/20/96/115	-
19	XAT	7	316	-	-	4/31/93/93	0/4/4/4
17	CLA	B	822	6	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PTY	8	320	-	-	8/23/23/53	-
16	CHL	3	322	-	1/1/14/21	19/35/111/117	-
17	CLA	B	803	-	-	18/39/115/115	-
20	BCR	B	847	-	-	2/29/63/63	0/2/2/2
17	CLA	3	308	2	-	10/27/103/115	-
16	CHL	7	306	-	-	9/19/95/117	-
16	CHL	7	307	-	-	6/20/96/117	-
17	CLA	8	305	-	-	9/17/93/115	-
17	CLA	b	613	4	-	7/17/93/115	-
17	CLA	a	613	1	-	6/17/93/115	-
28	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
17	CLA	A	5031	5	-	9/39/115/115	-
21	LHG	8	321	17	-	9/34/34/53	-
21	LHG	A	5055	17	-	3/33/33/53	-
27	CL0	A	5003	5	-	16/39/115/115	-
17	CLA	T	411	-	-	10/17/93/115	-
17	CLA	3	306	-	-	8/27/103/115	-
18	LUT	3	315	-	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	A	5028	5	-	16/39/115/115	-
17	CLA	b	601	4	-	9/17/93/115	-
17	CLA	3	314	2	-	8/17/93/115	-
21	LHG	A	5053	5	-	11/53/53/53	-
16	CHL	1	606	-	-	4/19/95/117	-
17	CLA	8	313	4	-	8/23/99/115	-
17	CLA	F	5007	-	-	9/18/94/115	-
17	CLA	B	840	-	-	11/39/115/115	-
20	BCR	B	845	-	-	9/29/63/63	0/2/2/2
16	CHL	8	307	-	-	9/19/95/117	-
16	CHL	a	601	21	-	7/19/95/117	-
17	CLA	K	204	-	-	9/15/91/115	-
17	CLA	A	5040	-	-	10/33/109/115	-
17	CLA	A	5011	5	-	14/39/115/115	-
20	BCR	A	5051	-	-	2/29/63/63	0/2/2/2
17	CLA	1	614	1	-	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	611	1	-	8/17/93/115	-
17	CLA	B	812	6	-	6/17/93/115	-
17	CLA	b	609	4	-	11/33/109/115	-
20	BCR	B	801	-	-	2/29/63/63	0/2/2/2
23	DGD	8	301	-	-	14/28/68/95	0/2/2/2
17	CLA	B	838	-	-	9/27/103/115	-
17	CLA	b	612	4	-	8/19/95/115	-
17	CLA	T	406	-	-	10/21/97/115	-
17	CLA	A	5038	5	-	7/21/97/115	-
19	XAT	T	414	-	-	1/31/93/93	0/4/4/4
17	CLA	3	302	2	-	7/39/115/115	-
17	CLA	1	613	1	-	7/17/93/115	-
21	LHG	b	618	17	-	7/23/23/53	-
20	BCR	A	5050	-	-	2/29/63/63	0/2/2/2
16	CHL	b	606	-	-	8/19/95/117	-
17	CLA	A	5007	17	-	11/33/109/115	-
17	CLA	A	5032	5	-	6/15/91/115	-
17	CLA	B	841	-	-	13/39/115/115	-
17	CLA	B	809	6	-	12/33/109/115	-
17	CLA	T	408	18,13	-	7/21/97/115	-
17	CLA	a	611	1	-	8/17/93/115	-
17	CLA	B	821	-	-	8/13/89/115	-
17	CLA	1	603	1	-	6/15/91/115	-
17	CLA	A	5005	-	-	3/39/115/115	-
17	CLA	A	5009	5	-	15/39/115/115	-
17	CLA	b	610	21	-	8/21/97/115	-
17	CLA	7	302	3	-	13/33/109/115	-
20	BCR	1	617	1	-	5/29/63/63	0/2/2/2
17	CLA	A	5034	5	-	8/39/115/115	-
17	CLA	A	5037	5	-	9/21/97/115	-
17	CLA	B	811	6	-	8/21/97/115	-
17	CLA	A	5029	5	-	11/39/115/115	-
17	CLA	B	813	6	-	9/21/97/115	-
17	CLA	B	828	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	611	4	-	10/21/97/115	-
17	CLA	b	614	4	-	7/17/93/115	-
16	CHL	b	605	-	-	8/19/95/117	-

The worst 5 of 1460 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	8	306	CHL	MG-NA	7.52	2.24	2.06
16	3	322	CHL	MG-NA	7.12	2.23	2.06
16	8	306	CHL	MG-NC	7.00	2.22	2.06
16	7	305	CHL	MG-NA	6.62	2.22	2.06
16	1	606	CHL	MG-NA	6.60	2.21	2.06

The worst 5 of 1224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	8	308	CHL	C4A-NA-C1A	15.65	113.82	106.68
16	T	401	CHL	C4A-NA-C1A	15.40	113.71	106.68
16	7	306	CHL	C4A-NA-C1A	14.52	113.31	106.68
16	b	607	CHL	C4A-NA-C1A	13.23	112.72	106.68
27	A	5003	CL0	C4A-NA-C1A	13.04	112.63	106.68

5 of 26 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	3	301	CHL	C8
16	3	322	CHL	C8
18	1	615	LUT	C3
18	1	615	LUT	C26
18	1	615	LUT	C23

5 of 2283 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CHL	C1A-C2A-CAA-CBA
16	1	601	CHL	C3A-C2A-CAA-CBA
16	1	601	CHL	C1C-C2C-CMC-OMC
16	1	601	CHL	C3C-C2C-CMC-OMC
16	1	601	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

247 monomers are involved in 585 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	830	CLA	3	0
17	A	5027	CLA	1	0
17	A	5016	CLA	7	0
17	A	5036	CLA	5	0
21	A	5002	LHG	2	0
17	8	314	CLA	1	0
17	c	312	CLA	2	0
17	8	315	CLA	1	0
17	A	5022	CLA	4	0
17	L	201	CLA	4	0
16	8	306	CHL	4	0
17	A	5013	CLA	6	0
17	A	5043	CLA	1	0
17	8	312	CLA	1	0
17	8	310	CLA	2	0
17	T	402	CLA	1	0
17	c	313	CLA	3	0
17	B	826	CLA	5	0
24	F	5011	LMG	1	0
16	1	601	CHL	2	0
25	A	5054	LMU	1	0
17	c	307	CLA	5	0
17	A	5008	CLA	5	0
17	3	307	CLA	7	0
20	A	5052	BCR	7	0
23	3	321	DGD	1	0
17	a	605	CLA	1	0
19	1	616	XAT	1	0
17	K	201	CLA	1	0
17	A	5024	CLA	1	0
17	B	832	CLA	4	0
17	T	412	CLA	2	0
18	a	615	LUT	4	0
21	a	619	LHG	1	0
17	K	203	CLA	3	0
17	B	805	CLA	2	0
17	A	5042	CLA	4	0
20	7	317	BCR	3	0
16	T	401	CHL	4	0
18	1	615	LUT	6	0
17	B	804	CLA	1	0
17	3	311	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	BCR	2	0
17	7	304	CLA	1	0
19	a	616	XAT	1	0
20	T	415	BCR	3	0
17	A	5033	CLA	4	0
17	B	806	CLA	5	0
17	c	309	CLA	1	0
20	B	849	BCR	5	0
17	K	202	CLA	1	0
20	B	846	BCR	4	0
19	8	317	XAT	1	0
20	A	5049	BCR	4	0
17	T	409	CLA	1	0
17	c	311	CLA	1	0
17	B	816	CLA	1	0
18	T	413	LUT	4	0
21	c	317	LHG	1	0
17	B	839	CLA	6	0
17	A	5021	CLA	1	0
17	1	610	CLA	1	0
18	b	615	LUT	1	0
20	B	844	BCR	2	0
17	B	833	CLA	1	0
19	3	316	XAT	4	0
18	7	315	LUT	3	0
17	8	304	CLA	1	0
17	a	607	CLA	1	0
28	B	842	PQN	3	0
17	A	5015	CLA	2	0
17	A	5018	CLA	6	0
17	A	5017	CLA	7	0
22	3	320	SQD	5	0
17	a	608	CLA	2	0
17	A	5025	CLA	6	0
17	B	802	CLA	7	0
17	F	5004	CLA	4	0
17	B	808	CLA	3	0
20	J	104	BCR	4	0
17	B	837	CLA	2	0
17	A	5030	CLA	5	0
17	1	607	CLA	3	0
17	7	303	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	405	CLA	1	0
19	c	315	XAT	1	0
20	b	617	BCR	6	0
20	3	318	BCR	4	0
20	I	4001	BCR	2	0
17	3	309	CLA	1	0
17	8	309	CLA	1	0
17	3	324	CLA	3	0
17	1	609	CLA	3	0
17	B	823	CLA	1	0
17	B	825	CLA	3	0
17	1	605	CLA	5	0
17	8	303	CLA	3	0
20	L	204	BCR	4	0
16	c	304	CHL	7	0
29	C	102	SF4	1	0
17	3	312	CLA	1	0
17	B	820	CLA	2	0
16	7	305	CHL	4	0
17	A	5006	CLA	2	0
16	T	416	CHL	7	0
17	B	810	CLA	2	0
20	a	617	BCR	4	0
23	B	848	DGD	8	0
20	A	5047	BCR	2	0
17	B	836	CLA	4	0
17	8	311	CLA	2	0
17	F	5009	CLA	1	0
17	3	305	CLA	4	0
17	A	5035	CLA	5	0
17	a	612	CLA	2	0
20	F	5005	BCR	5	0
20	F	5010	BCR	4	0
17	B	814	CLA	1	0
17	B	827	CLA	5	0
17	c	302	CLA	1	0
21	a	618	LHG	1	0
25	7	319	LMU	3	0
16	3	301	CHL	10	0
20	3	319	BCR	2	0
16	b	607	CHL	4	0
17	A	5010	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5004	CLA	11	0
17	1	612	CLA	2	0
17	B	818	CLA	9	0
16	8	308	CHL	4	0
17	B	829	CLA	7	0
20	K	205	BCR	5	0
20	c	316	BCR	2	0
21	1	618	LHG	1	0
17	A	5044	CLA	7	0
17	A	5041	CLA	2	0
16	c	306	CHL	14	0
17	3	323	CLA	3	0
17	T	403	CLA	2	0
16	c	305	CHL	4	0
17	7	309	CLA	1	0
17	B	817	CLA	4	0
17	B	831	CLA	1	0
17	b	602	CLA	3	0
17	c	308	CLA	4	0
17	A	5019	CLA	8	0
17	B	807	CLA	4	0
17	7	308	CLA	2	0
17	8	302	CLA	3	0
17	7	312	CLA	6	0
17	b	604	CLA	2	0
17	B	819	CLA	3	0
17	c	301	CLA	7	0
17	1	604	CLA	6	0
20	3	317	BCR	3	0
24	7	301	LMG	5	0
17	a	602	CLA	1	0
20	B	843	BCR	2	0
17	A	5012	CLA	2	0
17	A	5014	CLA	8	0
16	a	606	CHL	1	0
20	8	318	BCR	5	0
21	1	619	LHG	1	0
17	1	608	CLA	2	0
17	A	5026	CLA	3	0
17	c	303	CLA	3	0
17	T	410	CLA	1	0
24	A	5001	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	404	CLA	3	0
17	F	5006	CLA	1	0
17	3	304	CLA	1	0
17	a	604	CLA	4	0
20	L	203	BCR	2	0
17	7	313	CLA	2	0
17	a	609	CLA	2	0
20	A	5048	BCR	6	0
17	A	5020	CLA	4	0
17	J	102	CLA	3	0
19	7	316	XAT	6	0
17	B	822	CLA	2	0
16	3	322	CHL	6	0
17	B	803	CLA	8	0
20	B	847	BCR	2	0
17	3	308	CLA	1	0
16	7	306	CHL	4	0
16	7	307	CHL	4	0
17	8	305	CLA	3	0
17	b	613	CLA	1	0
17	a	613	CLA	1	0
28	A	5045	PQN	2	0
17	A	5031	CLA	2	0
21	8	321	LHG	2	0
21	A	5055	LHG	2	0
18	8	316	LUT	1	0
27	A	5003	CL0	8	0
17	3	306	CLA	2	0
17	b	601	CLA	3	0
17	A	5028	CLA	6	0
18	3	315	LUT	3	0
17	3	314	CLA	1	0
21	A	5053	LHG	5	0
16	1	606	CHL	2	0
17	8	313	CLA	2	0
17	F	5007	CLA	2	0
17	B	840	CLA	2	0
20	B	845	BCR	3	0
16	8	307	CHL	2	0
16	a	601	CHL	2	0
17	K	204	CLA	2	0
17	A	5040	CLA	1	0

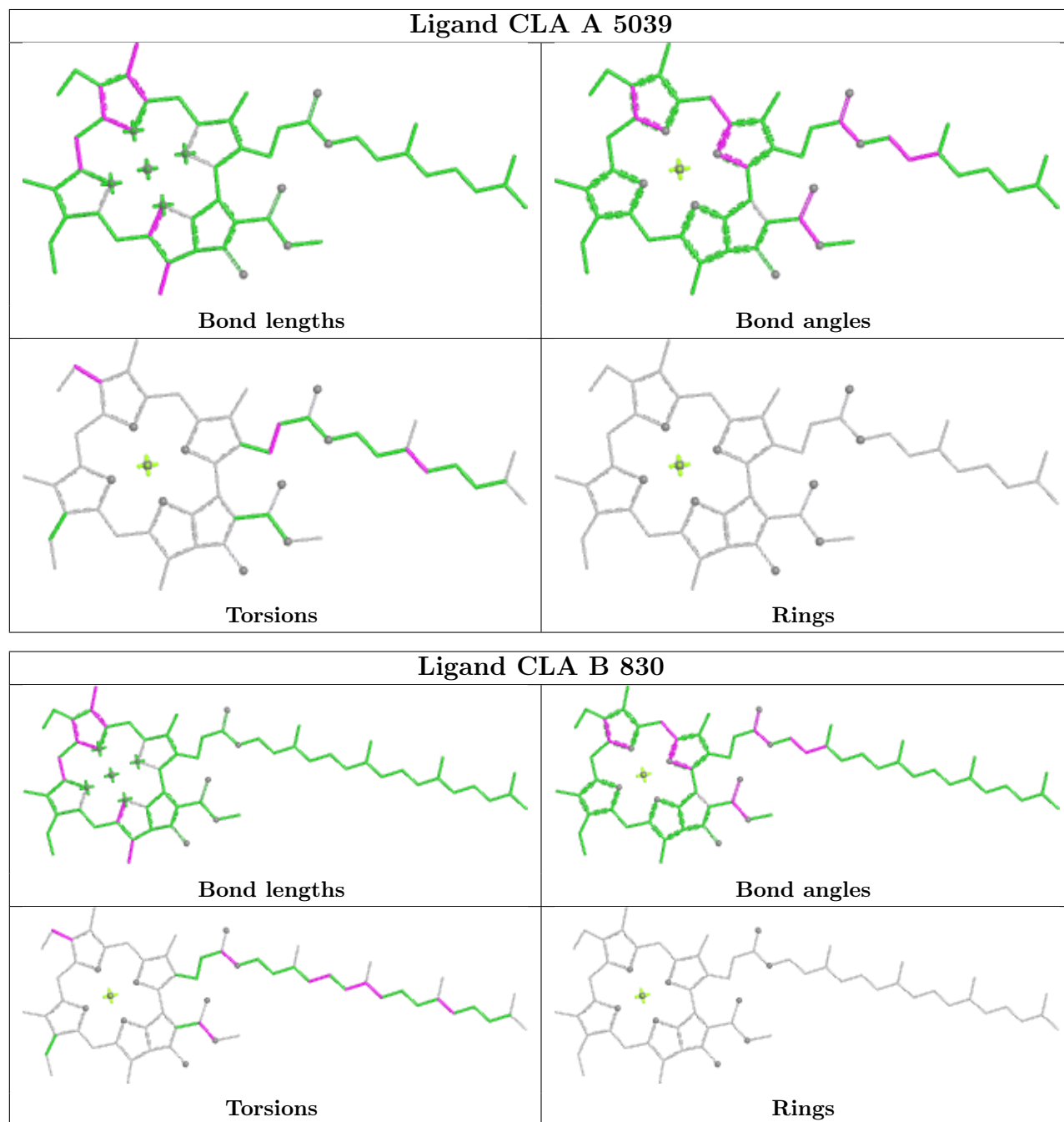
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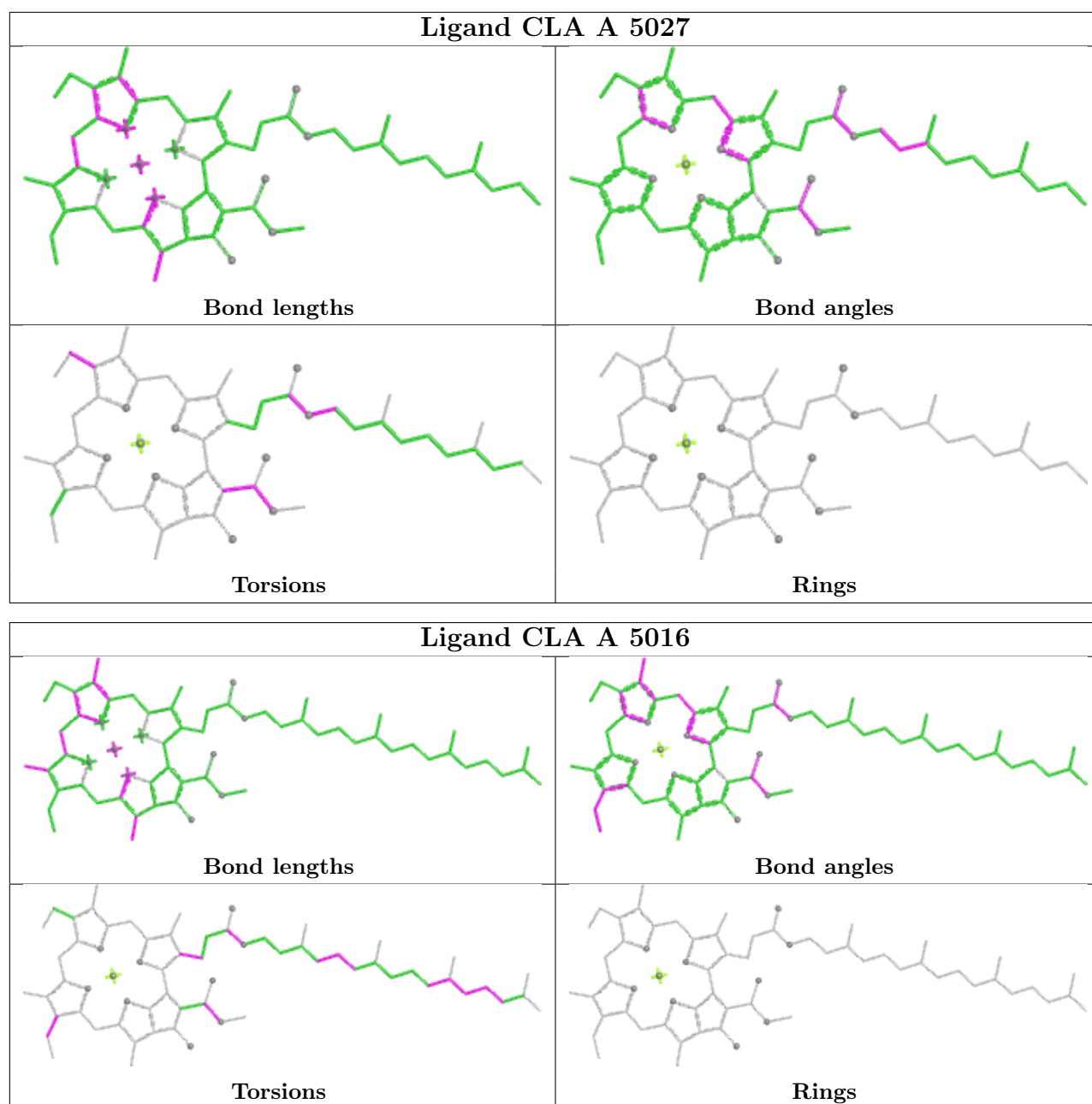
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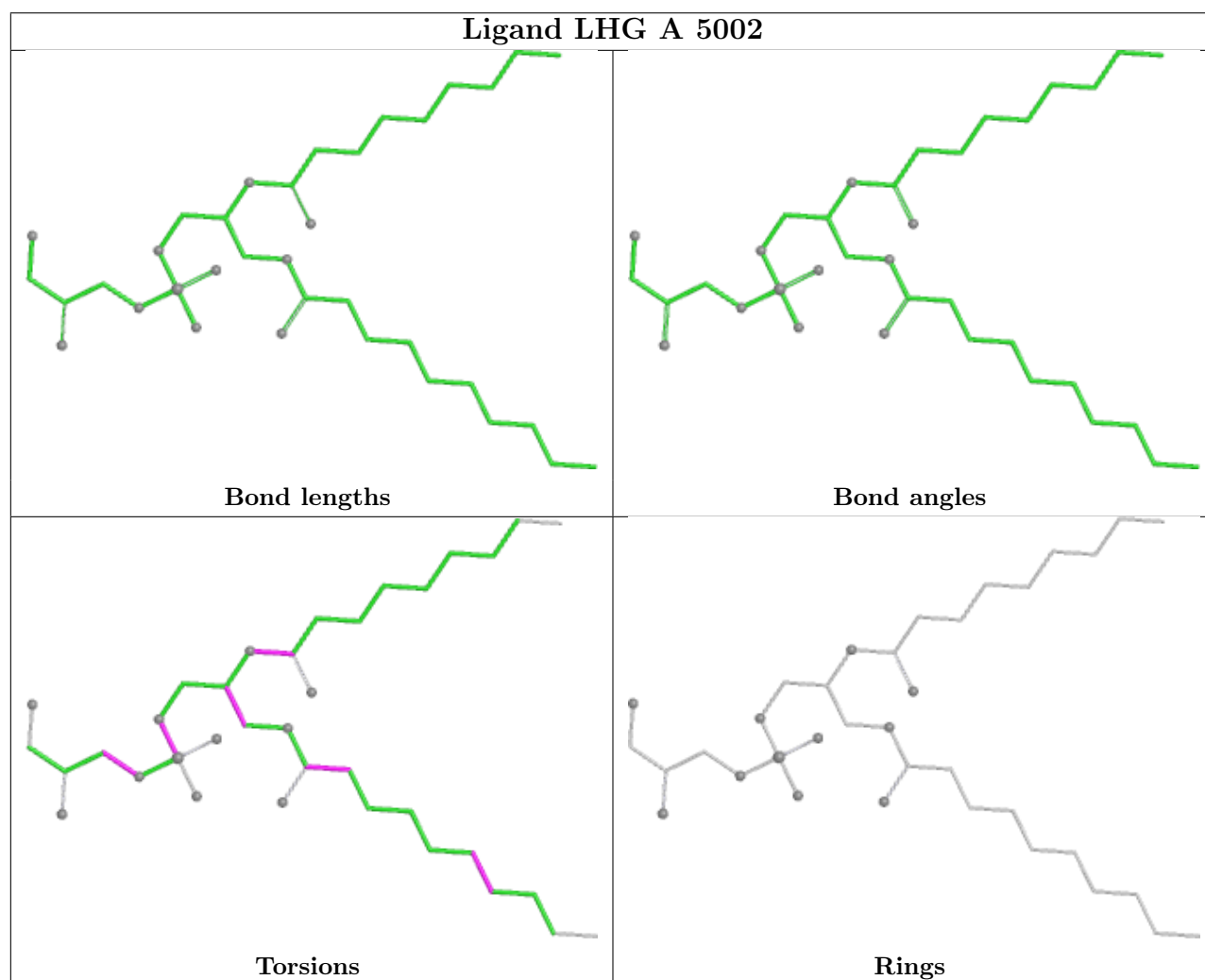
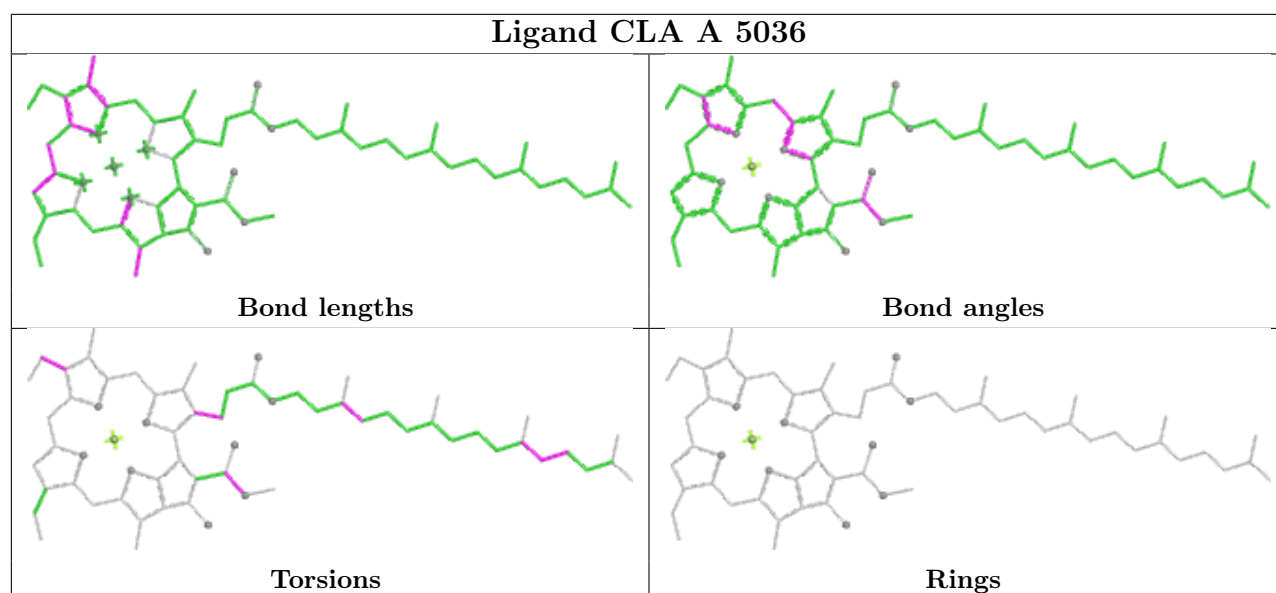
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5011	CLA	6	0
20	A	5051	BCR	3	0
17	1	614	CLA	1	0
17	1	611	CLA	1	0
17	B	812	CLA	1	0
17	b	609	CLA	2	0
20	B	801	BCR	3	0
23	8	301	DGD	2	0
17	B	838	CLA	2	0
17	b	612	CLA	1	0
17	T	406	CLA	2	0
19	T	414	XAT	2	0
17	3	302	CLA	4	0
17	1	613	CLA	1	0
20	A	5050	BCR	5	0
16	b	606	CHL	3	0
17	A	5007	CLA	3	0
17	A	5032	CLA	3	0
17	B	841	CLA	3	0
17	B	809	CLA	5	0
17	T	408	CLA	1	0
17	a	611	CLA	1	0
17	B	821	CLA	2	0
17	A	5005	CLA	6	0
17	A	5009	CLA	3	0
17	b	610	CLA	1	0
17	7	302	CLA	4	0
20	1	617	BCR	8	0
17	A	5034	CLA	2	0
17	A	5037	CLA	2	0
17	B	811	CLA	2	0
17	A	5029	CLA	9	0
17	B	813	CLA	4	0
17	B	828	CLA	5	0
17	b	611	CLA	2	0
17	b	614	CLA	1	0
16	b	605	CHL	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

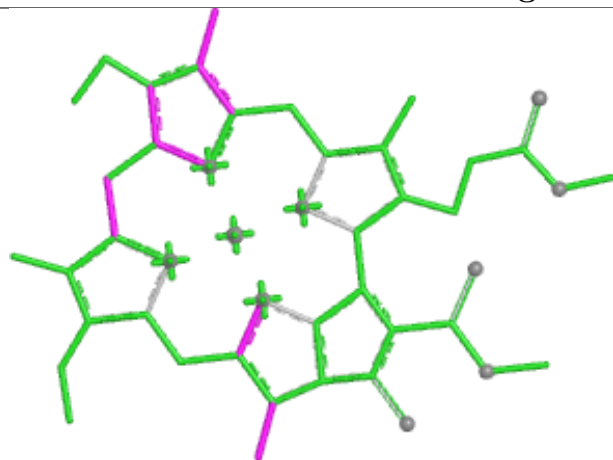
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



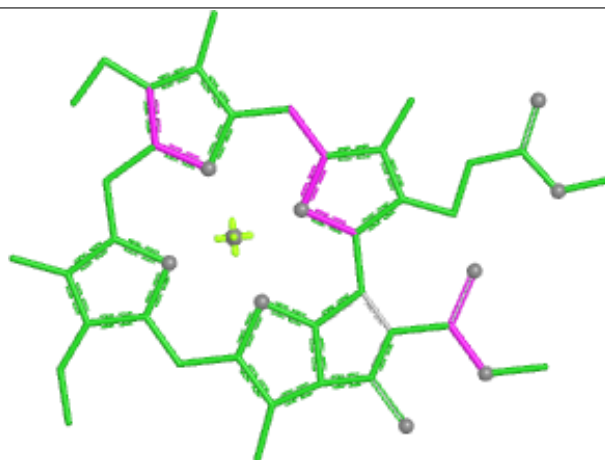




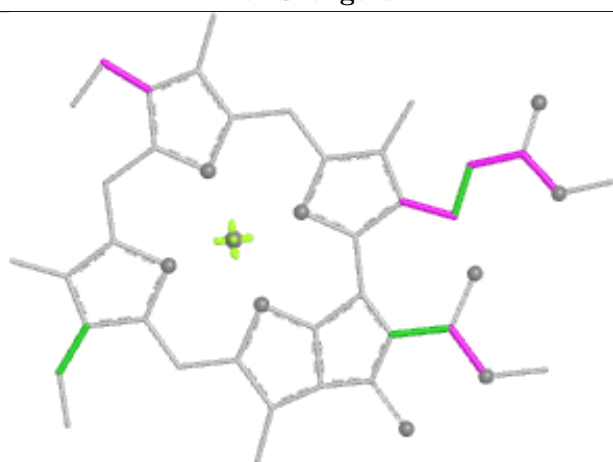
Ligand CLA 8 314



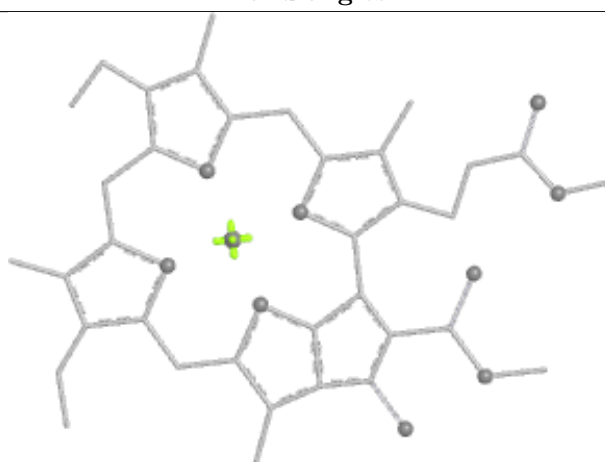
Bond lengths



Bond angles

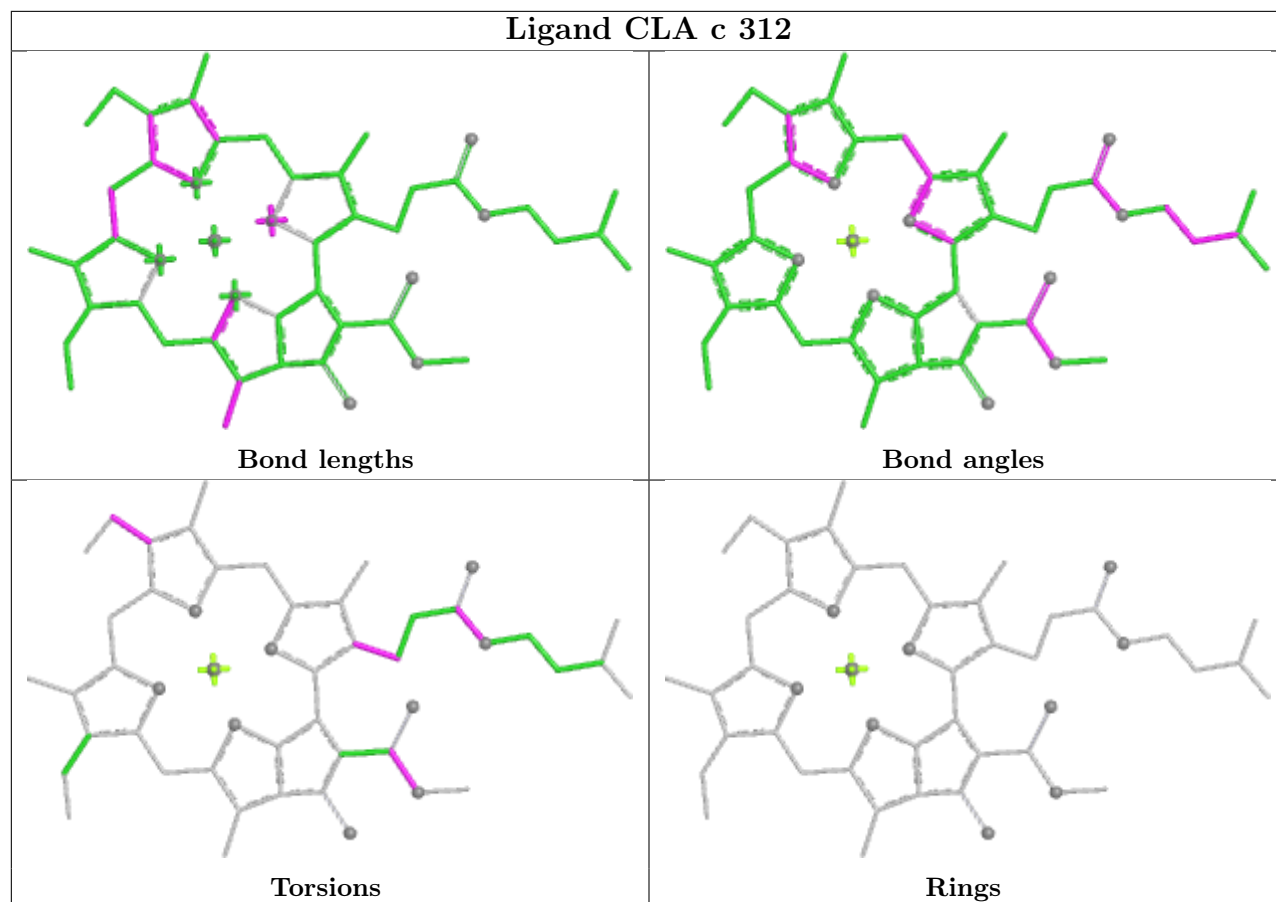


Torsions

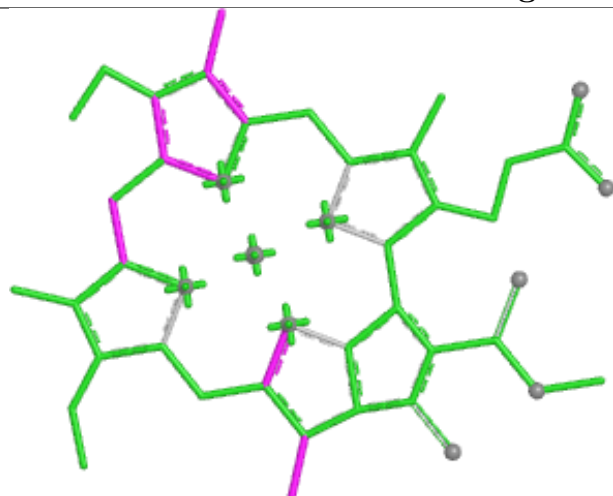


Rings

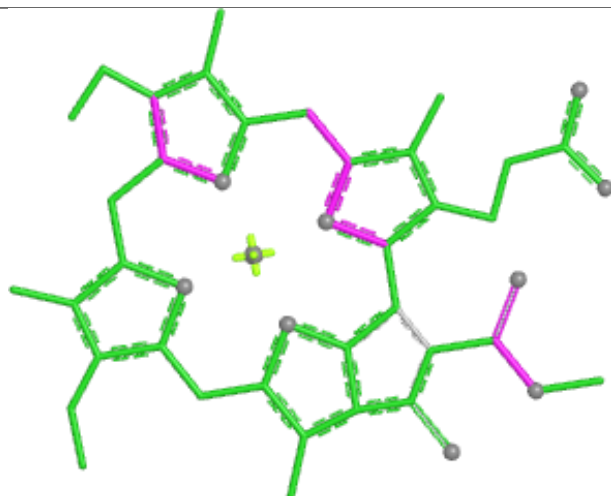
Ligand CLA c 312



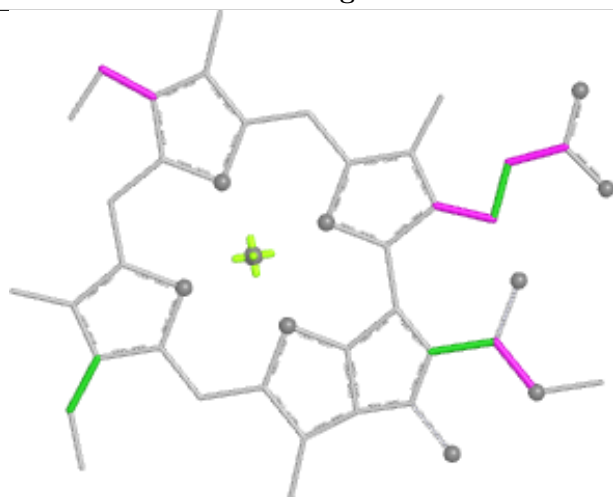
Ligand CLA 8 315



Bond lengths



Bond angles

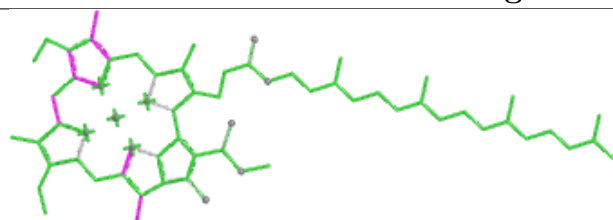


Torsions

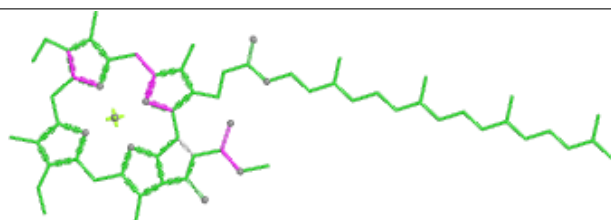


Rings

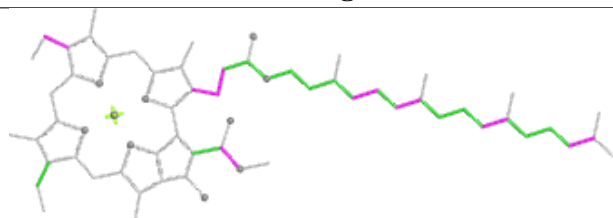
Ligand CLA A 5022



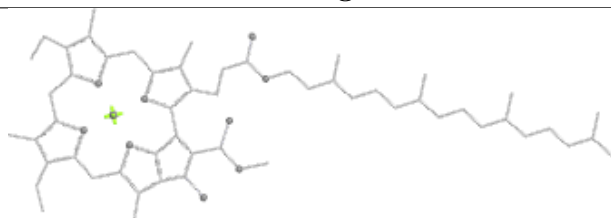
Bond lengths



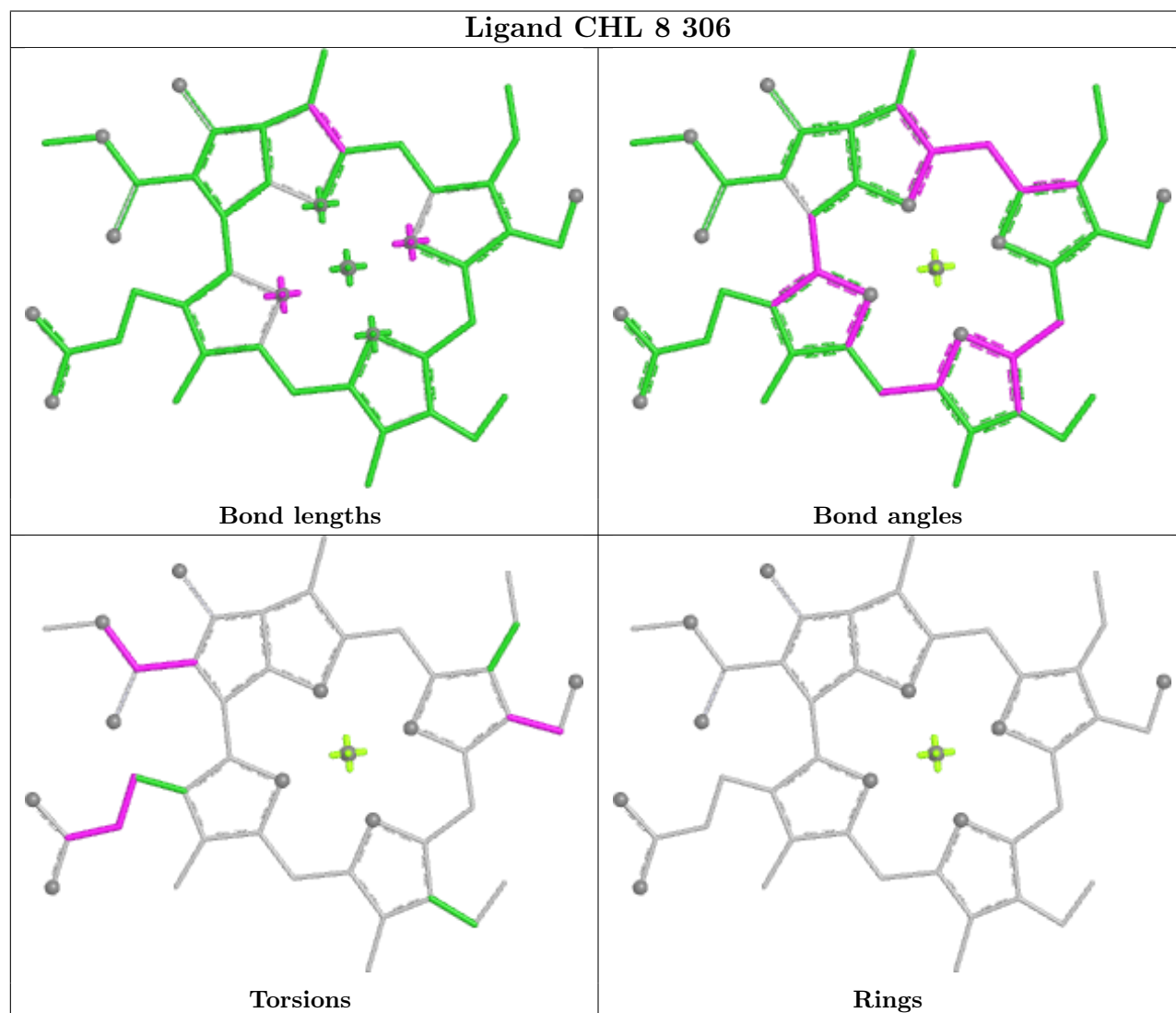
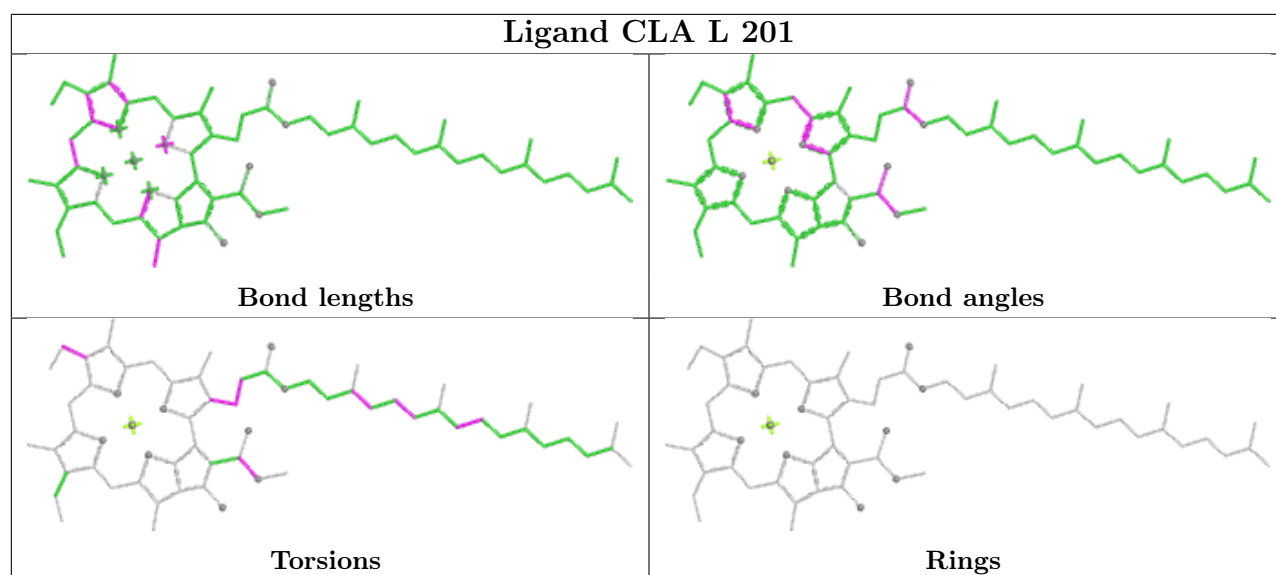
Bond angles



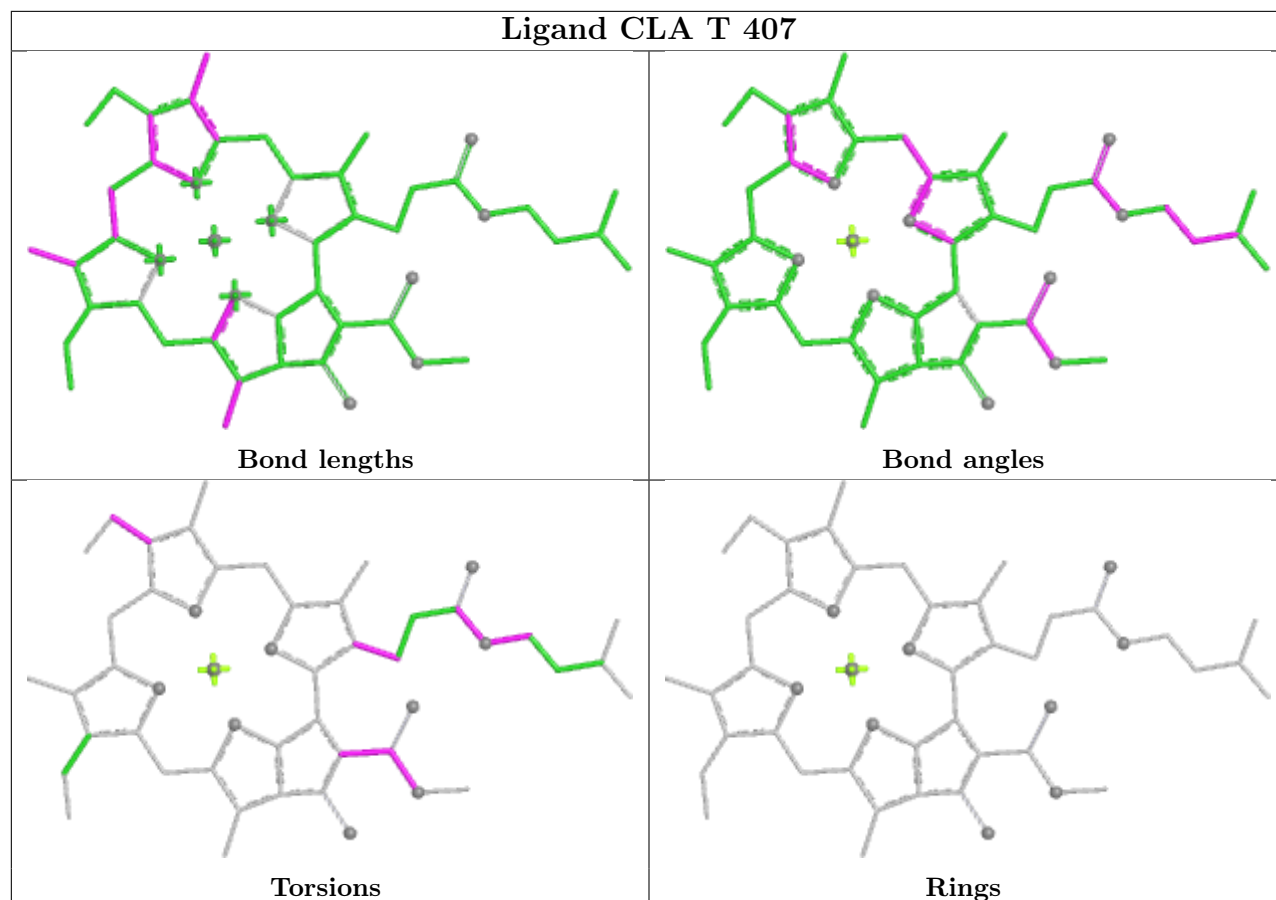
Torsions



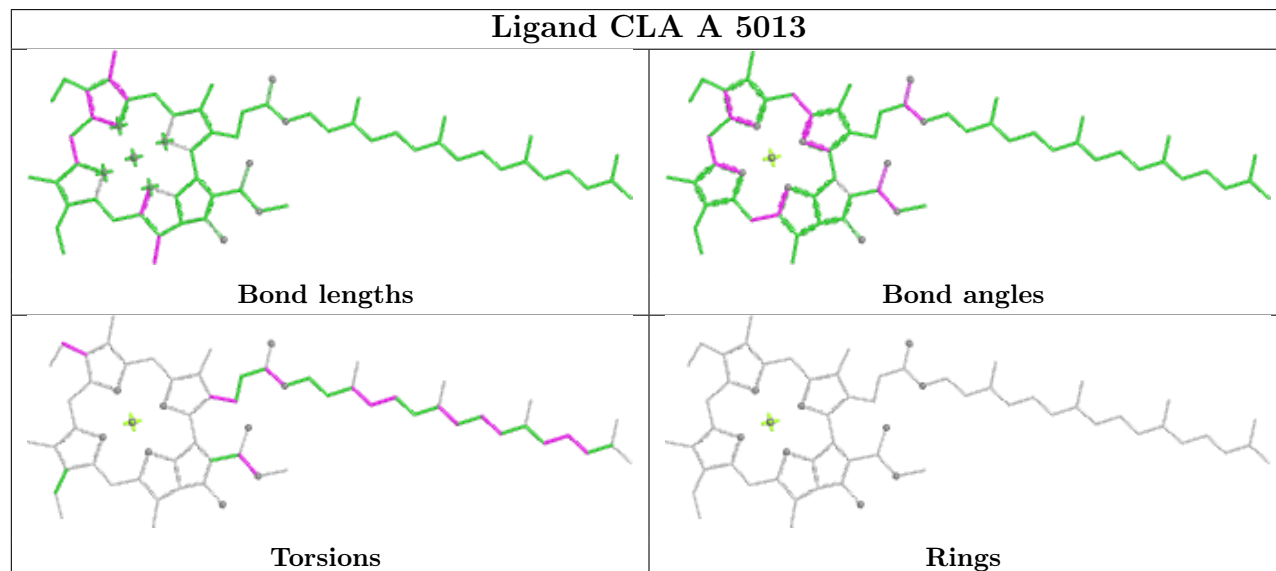
Rings



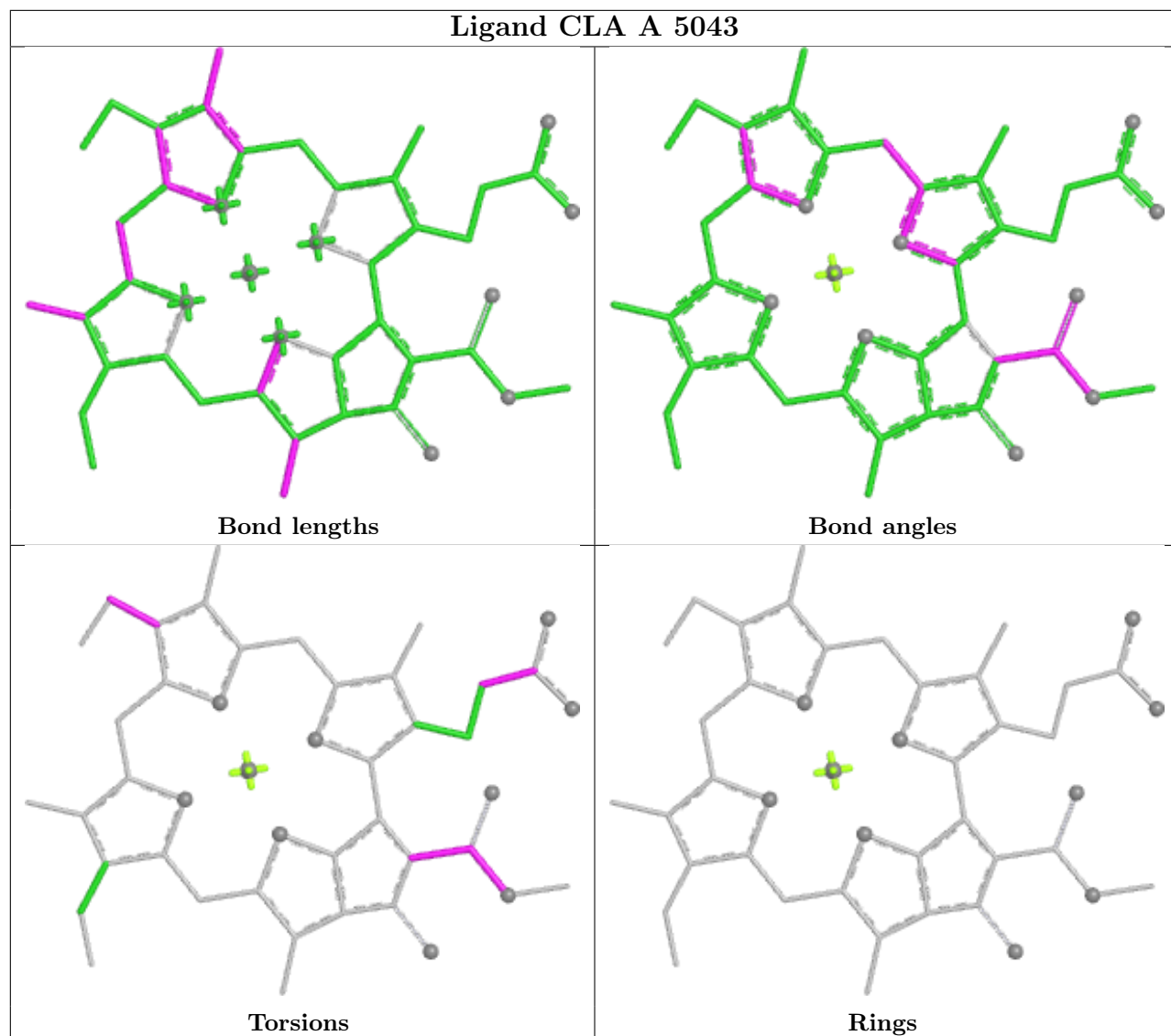
Ligand CLA T 407



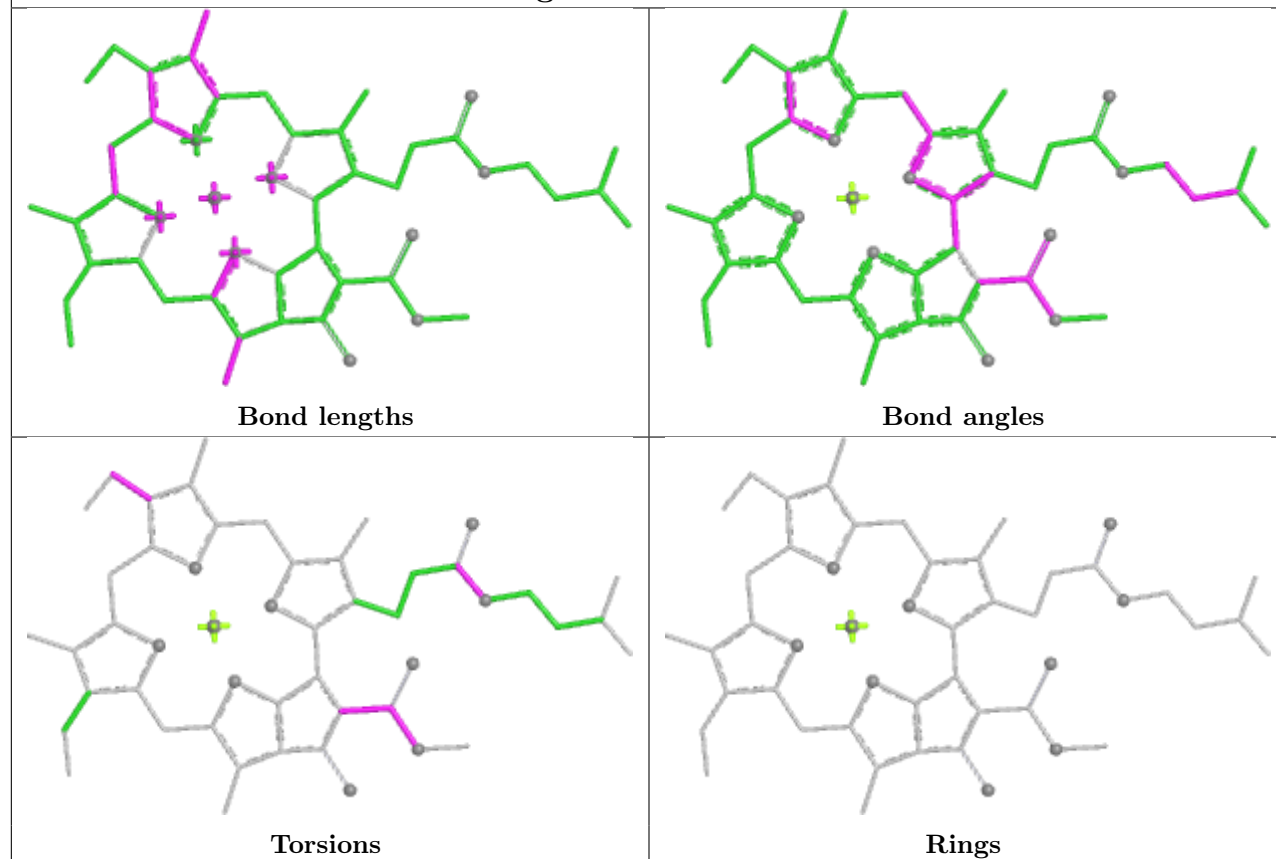
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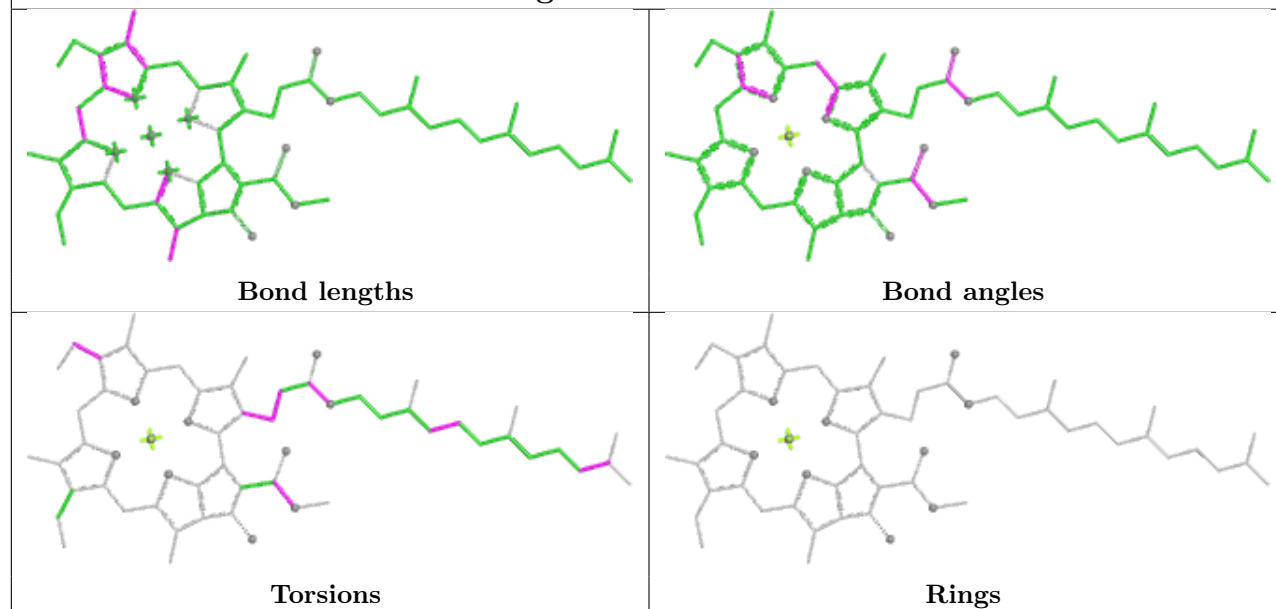
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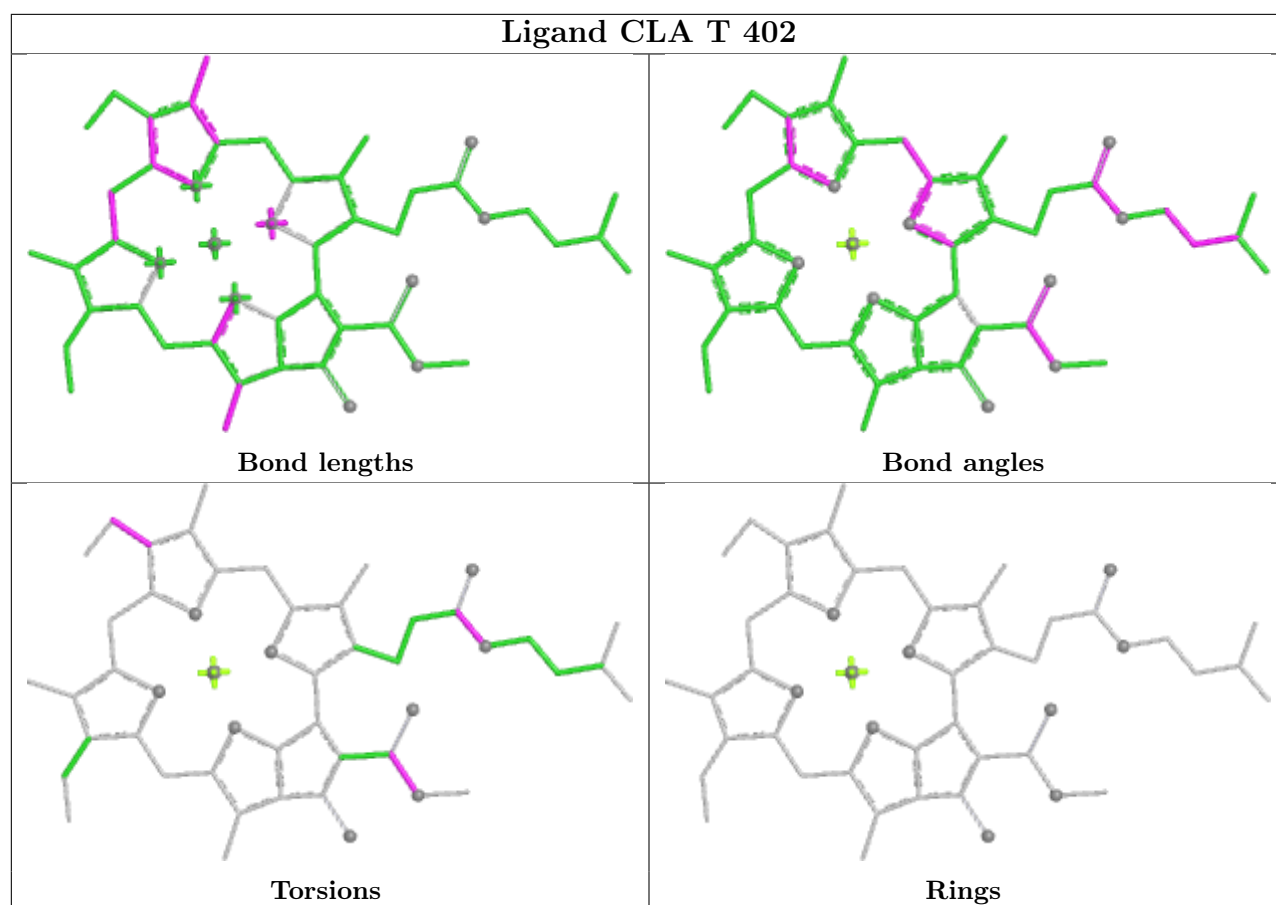


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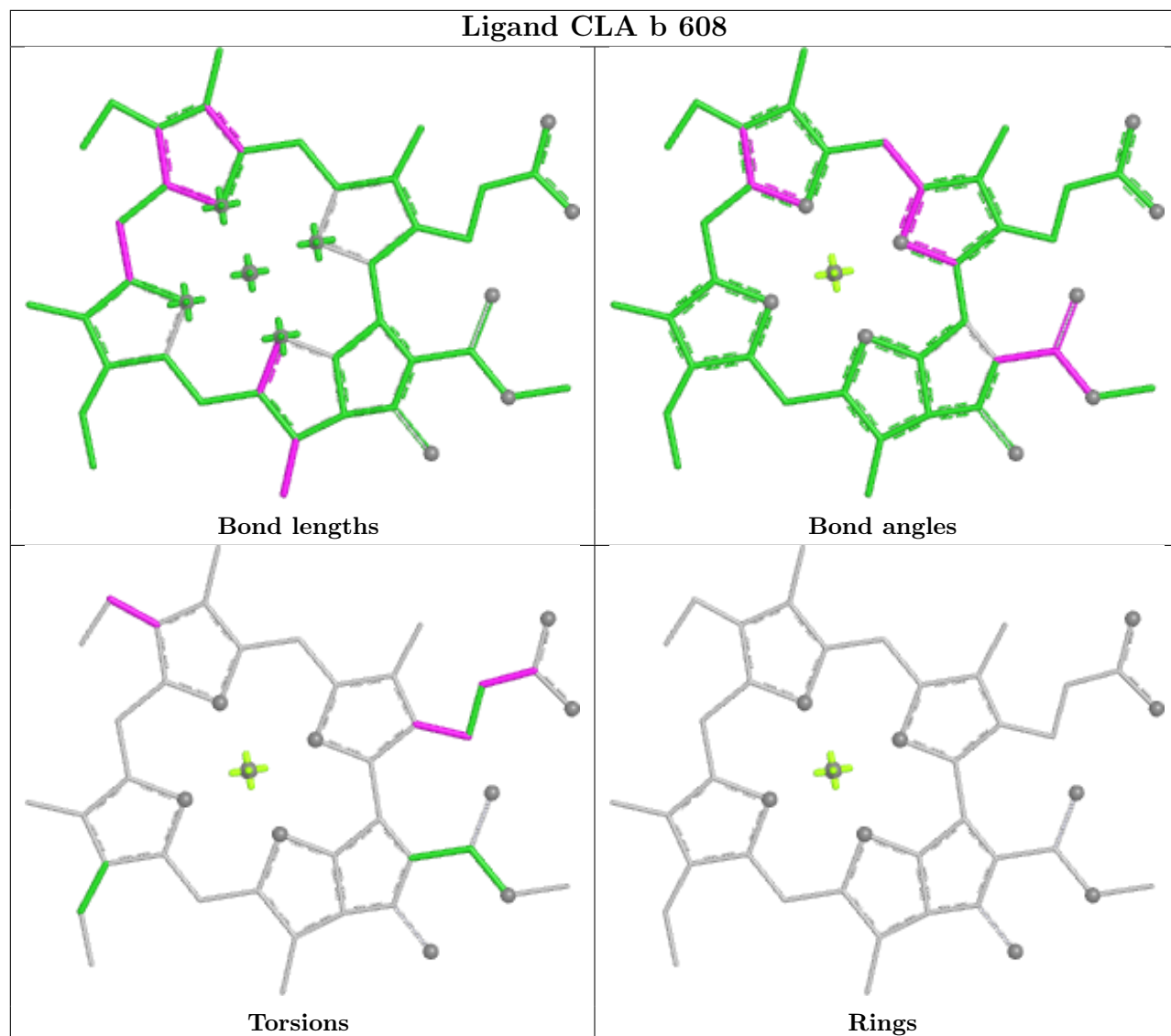


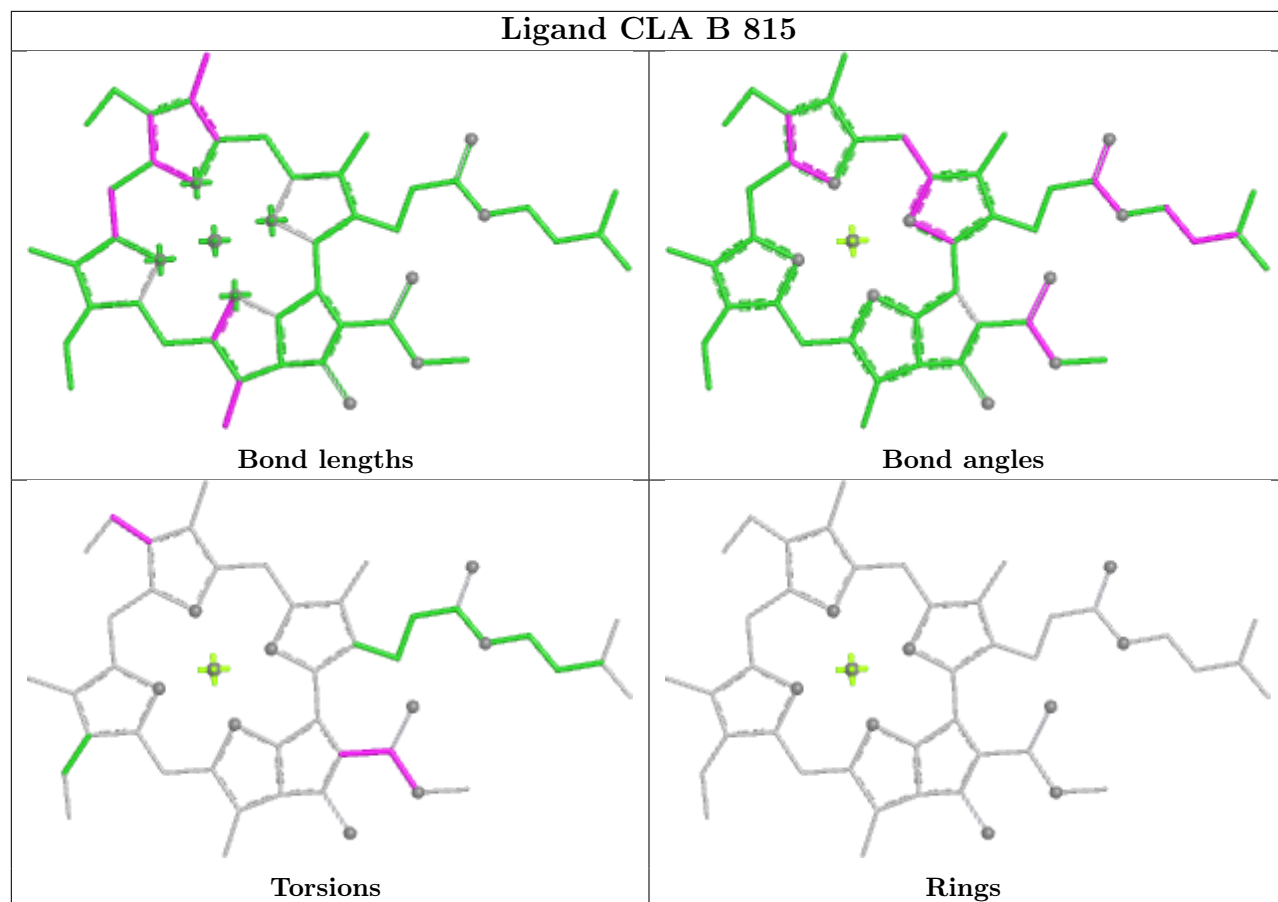
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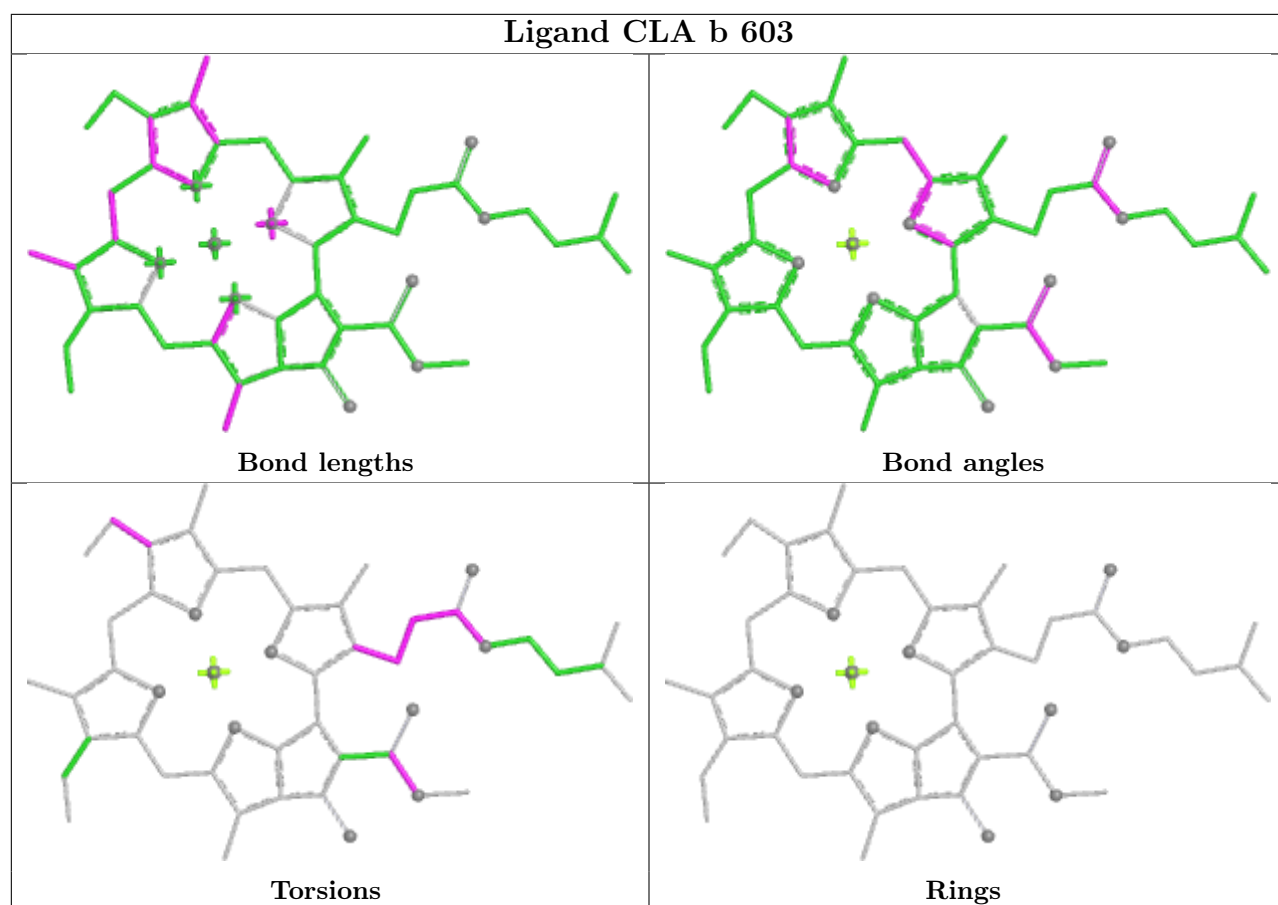




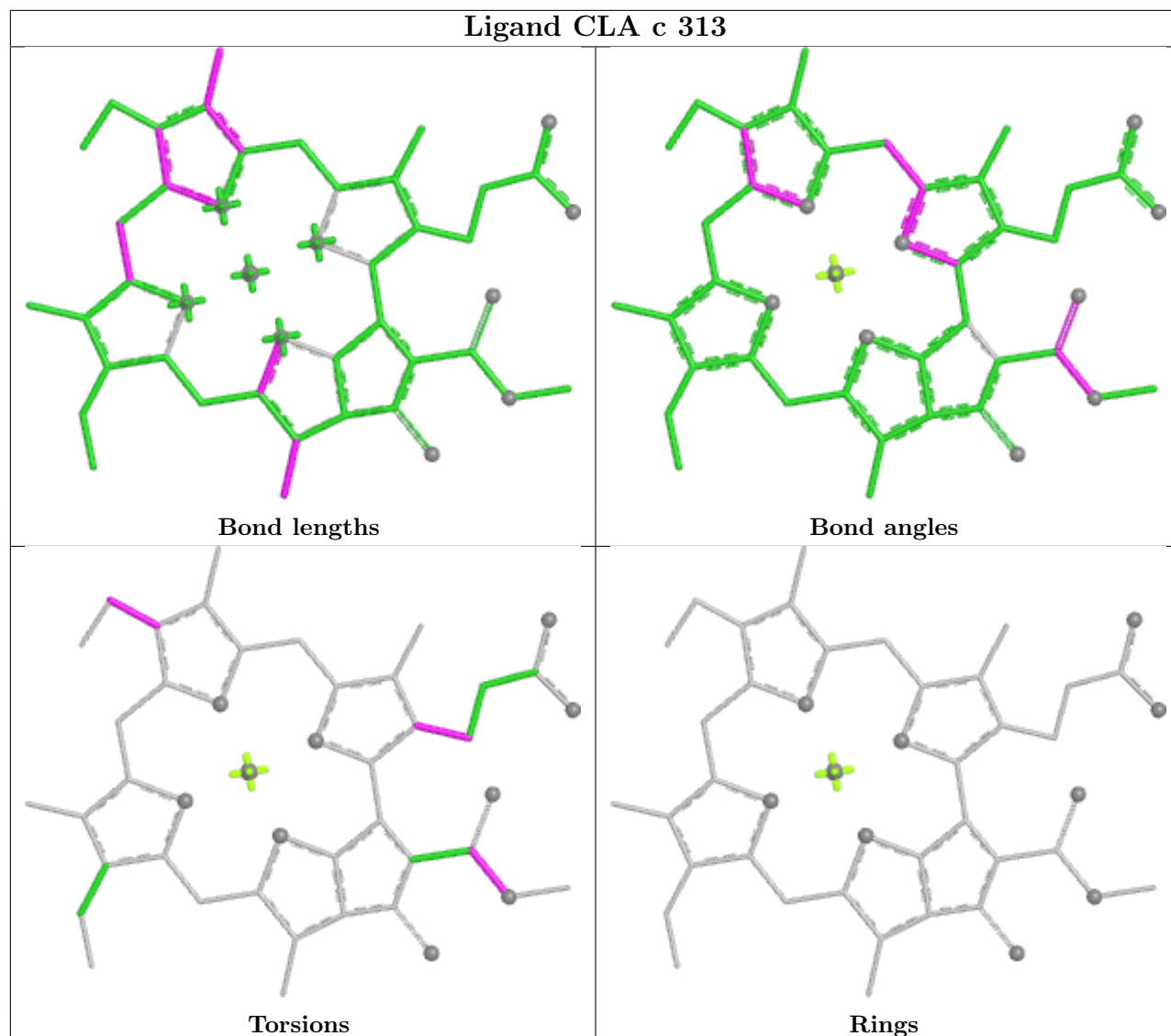
Ligand CLA b 608



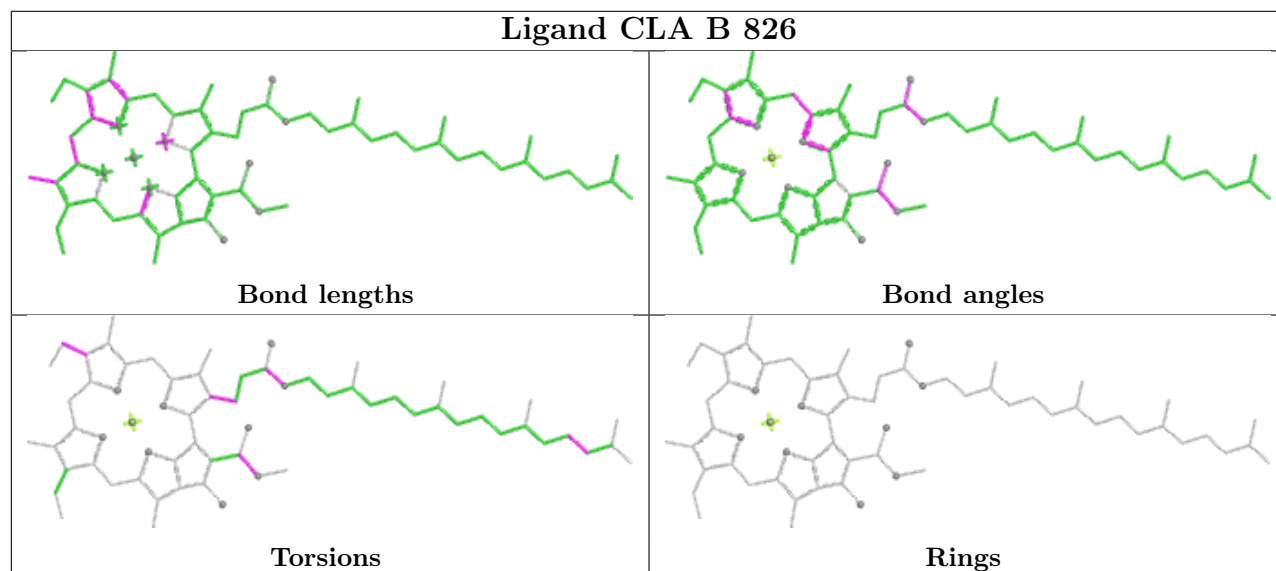


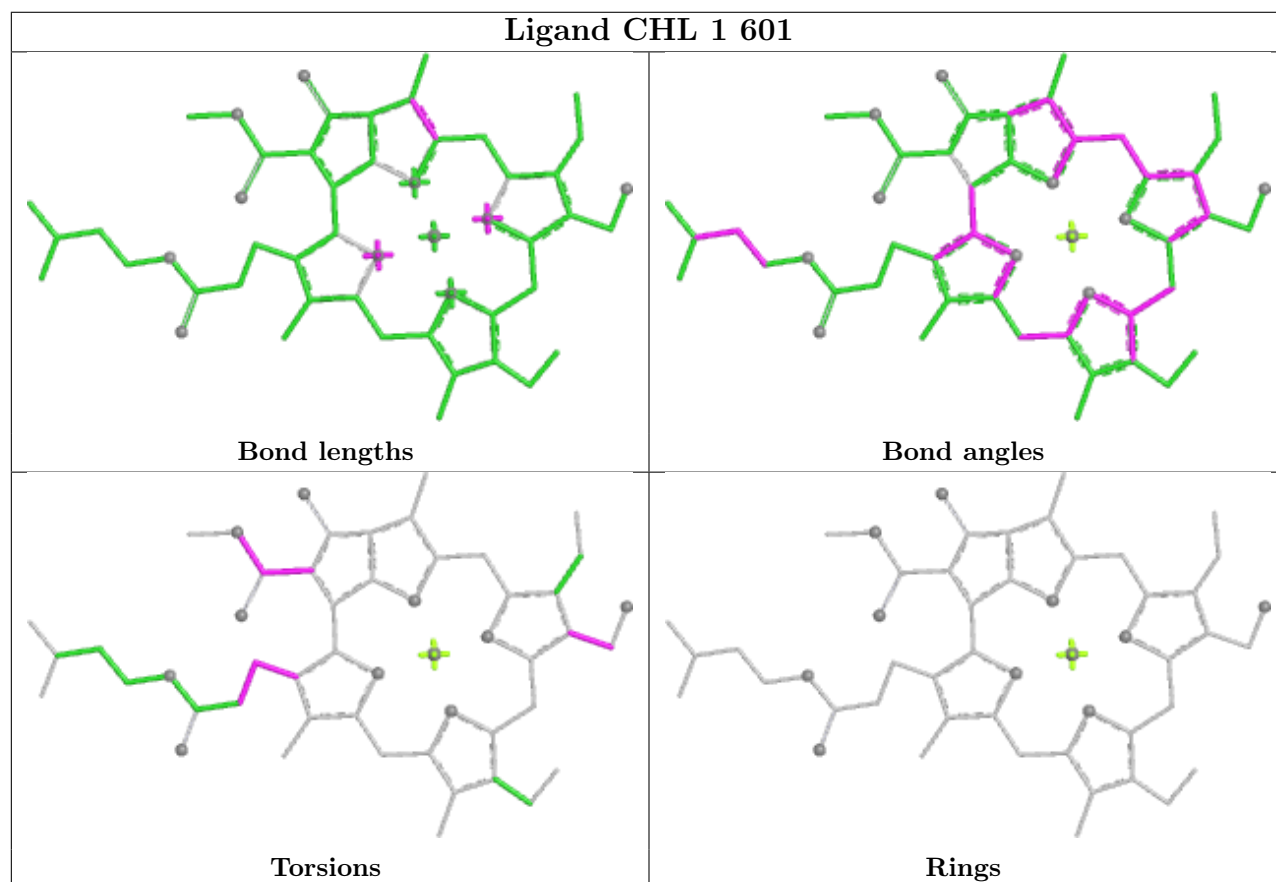
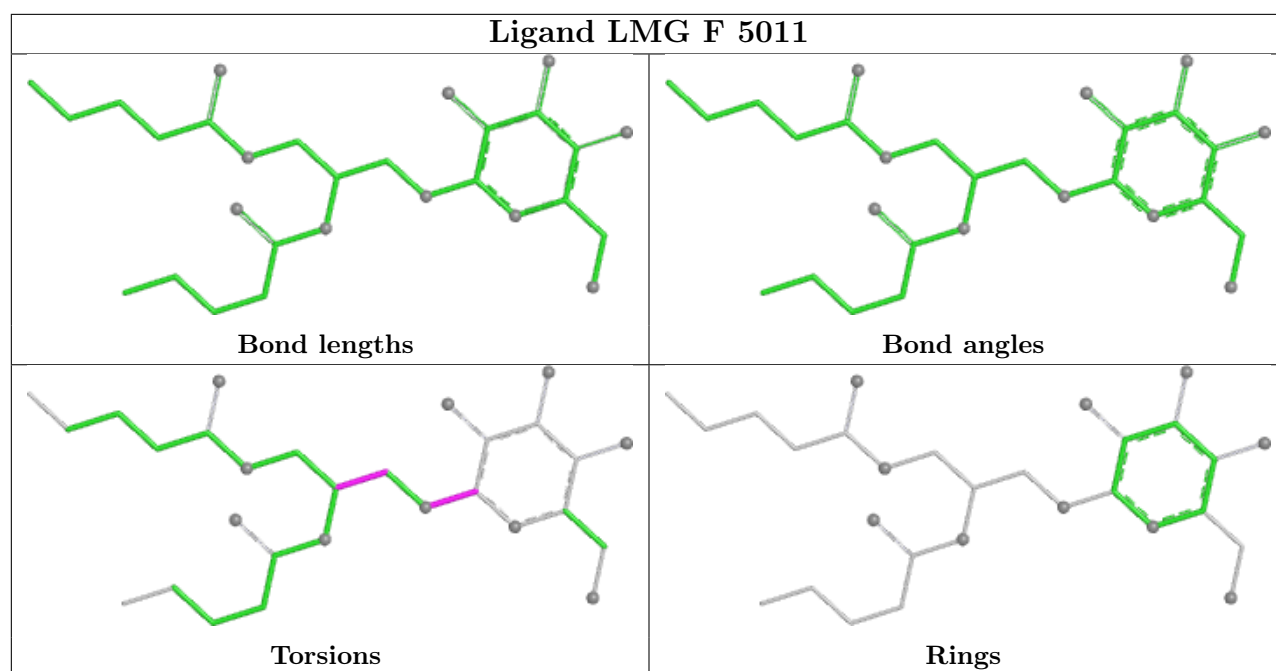


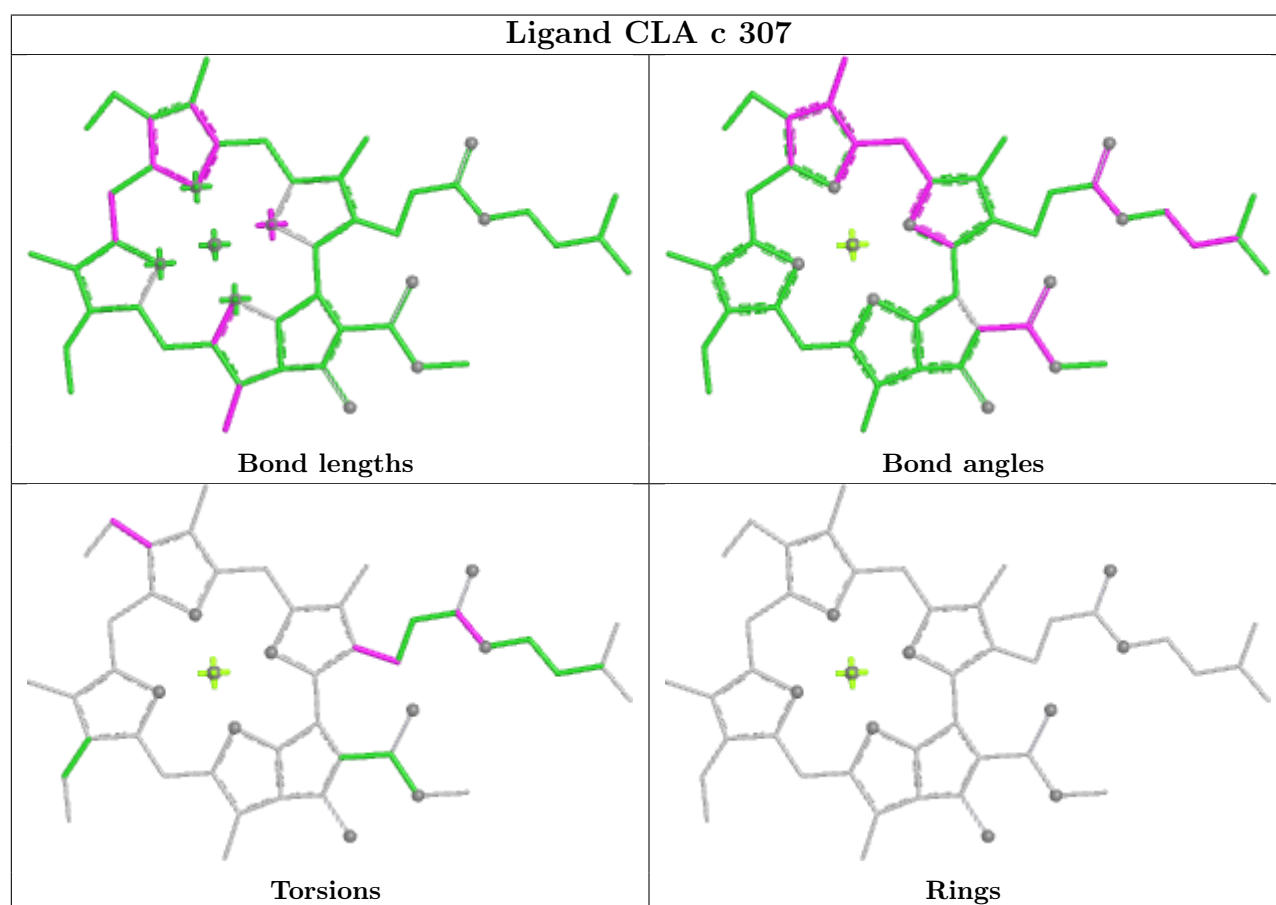
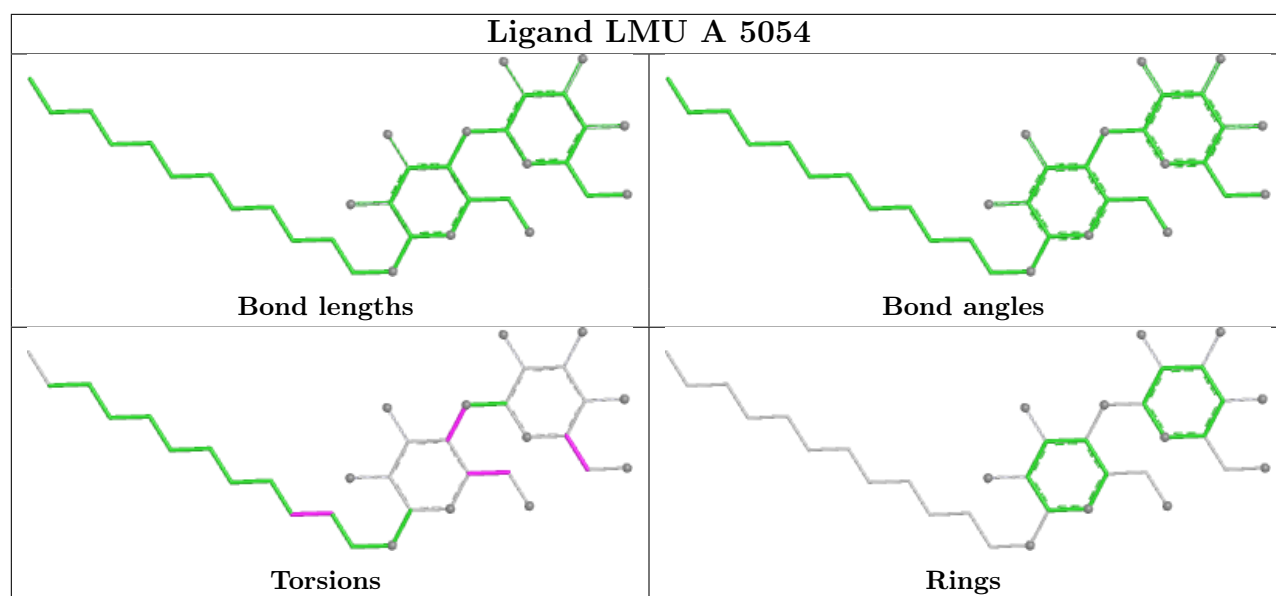
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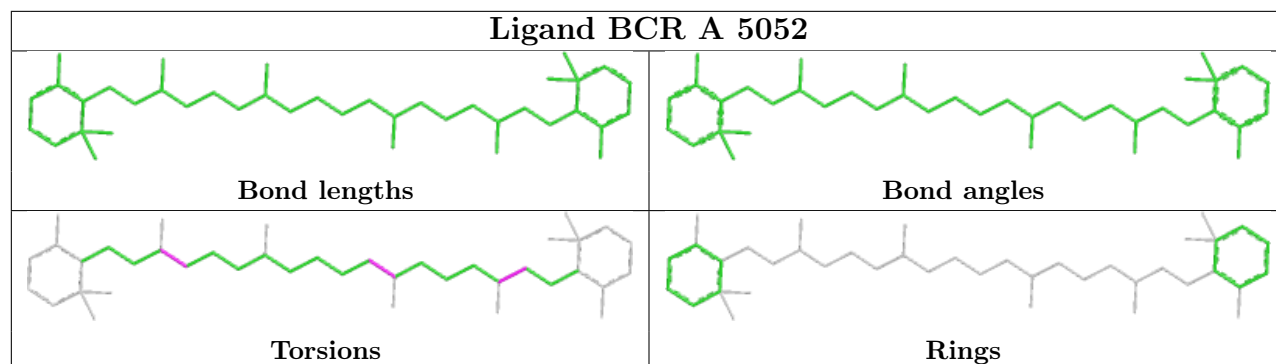
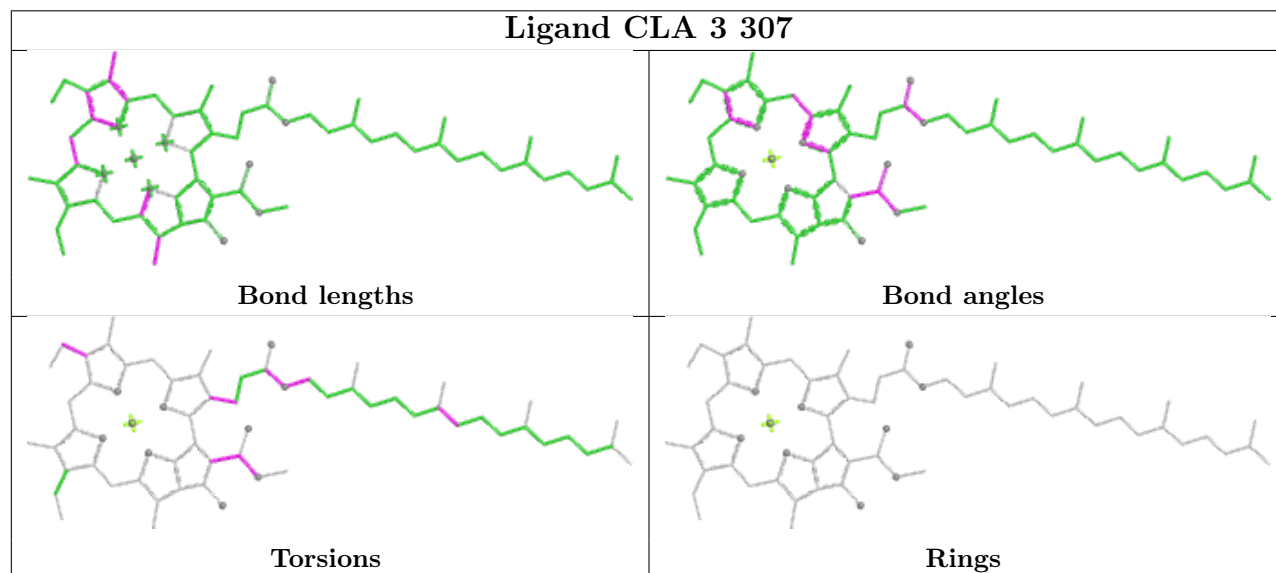
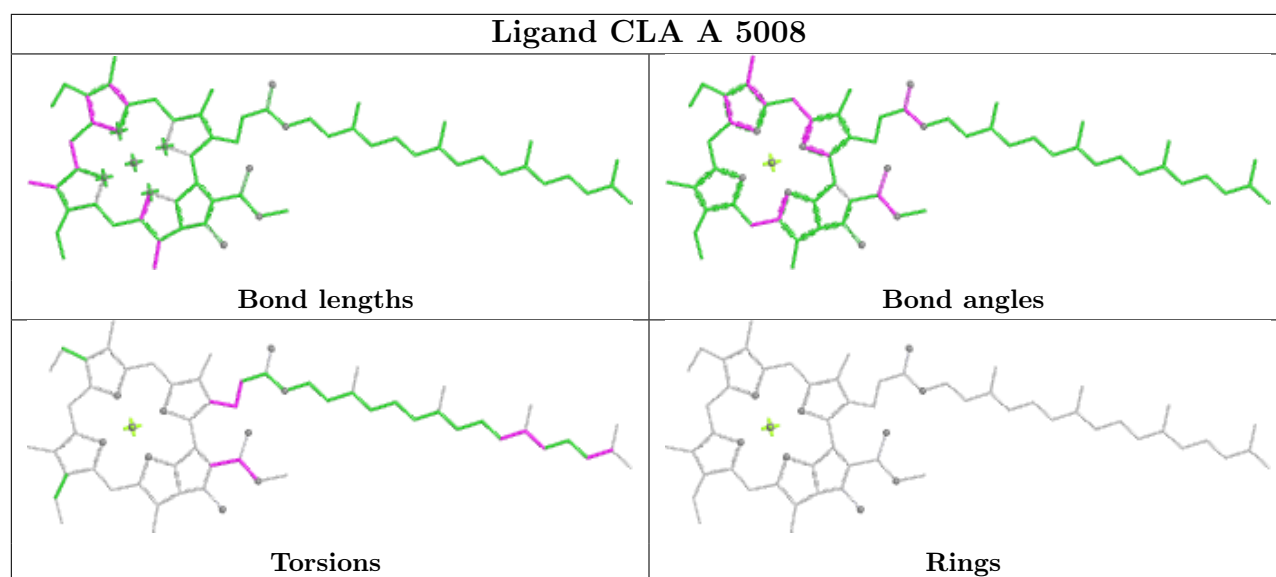


Ligand CLA B 826

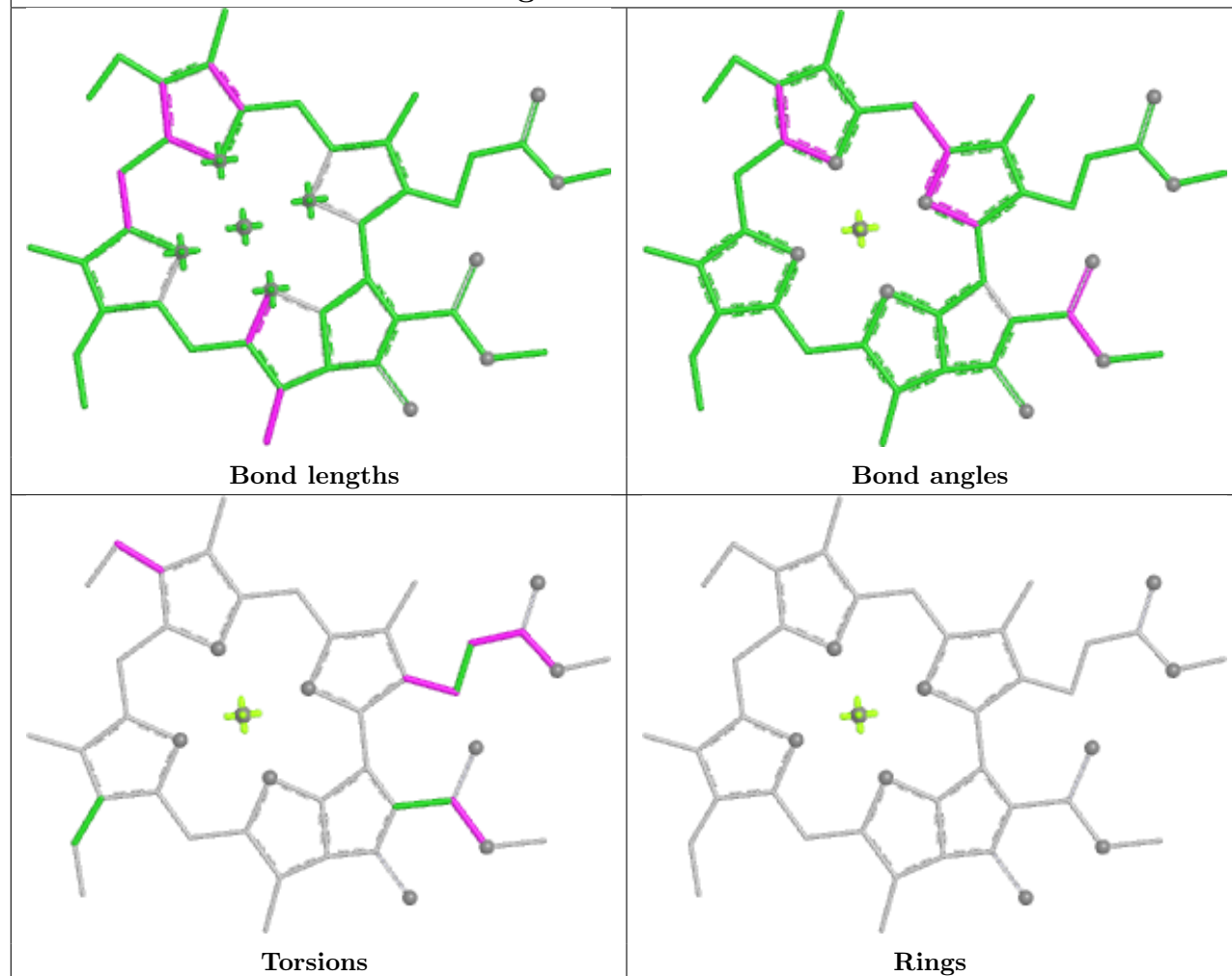




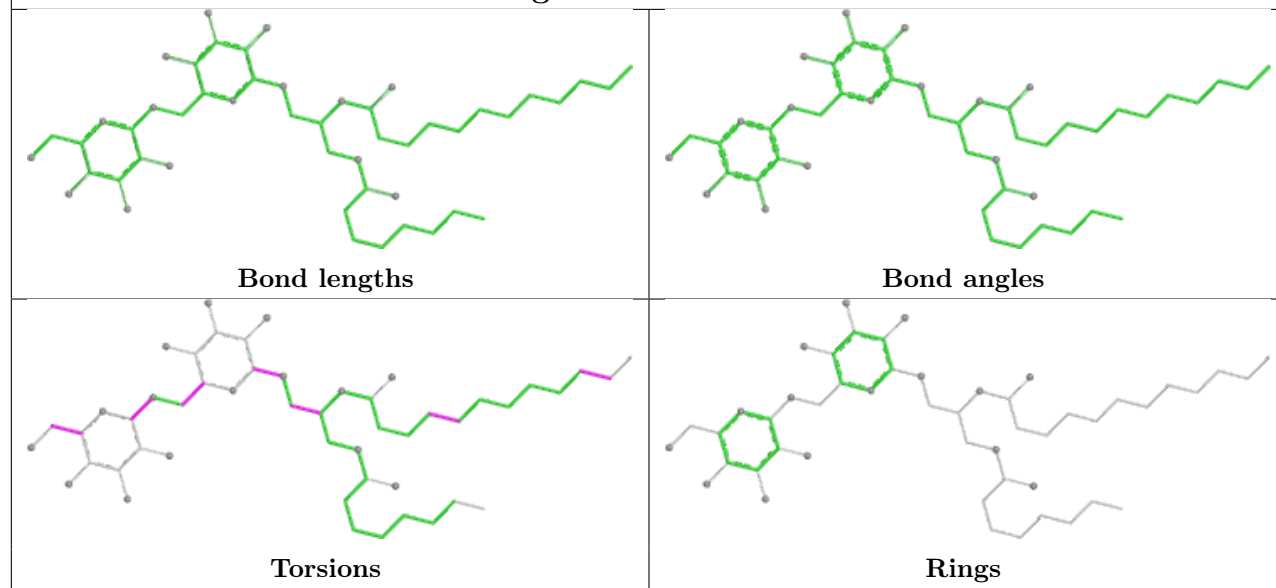




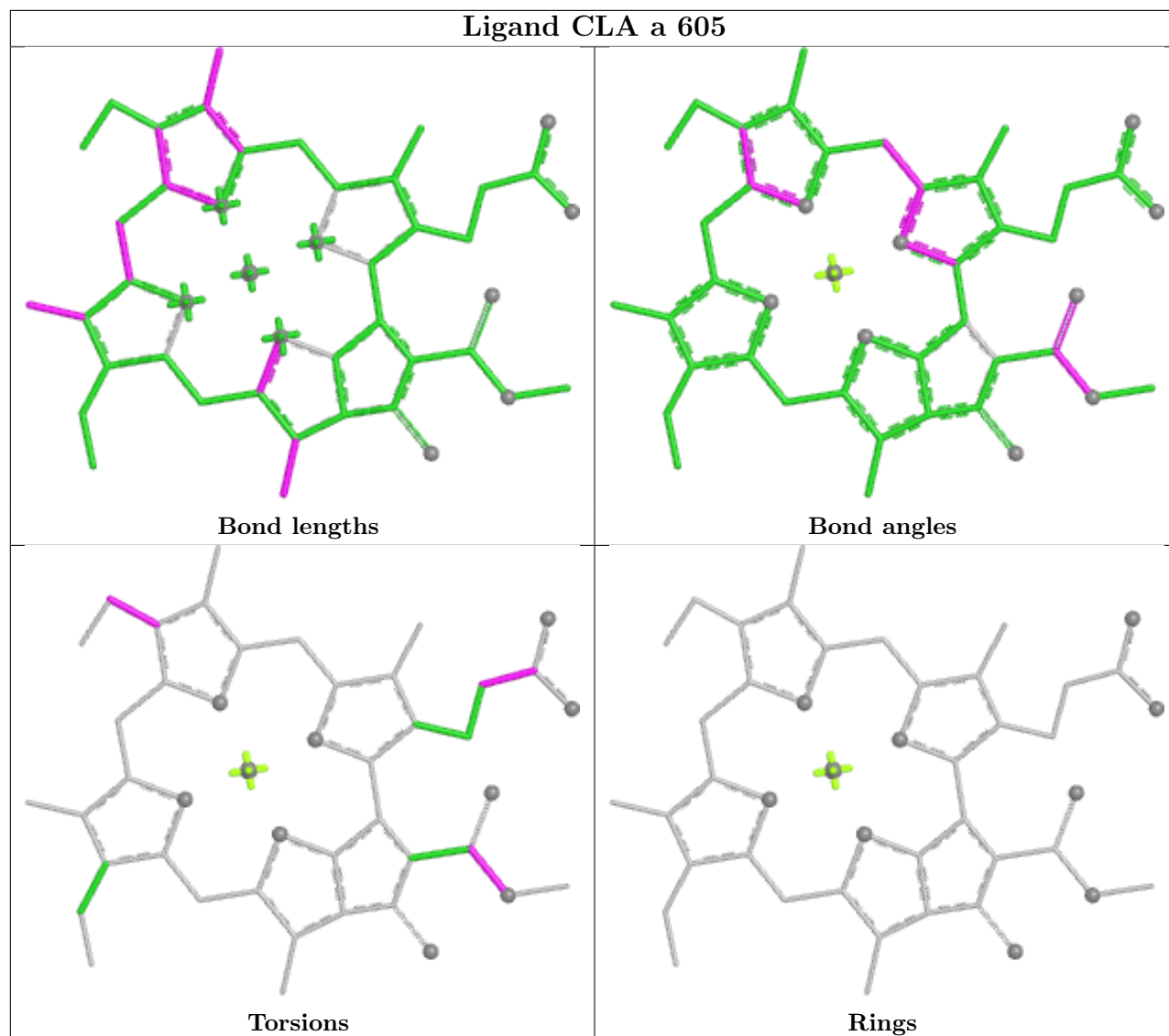
Ligand CLA a 610



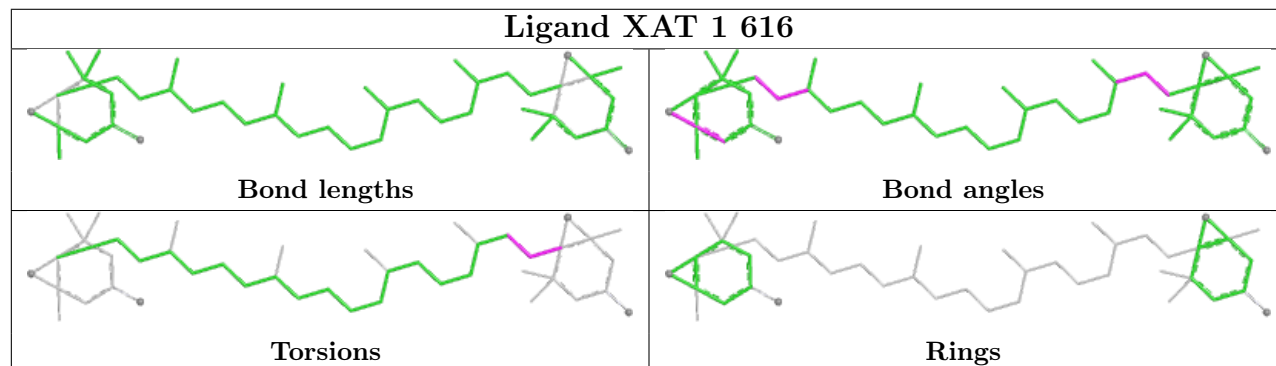
Ligand DGD 3 321



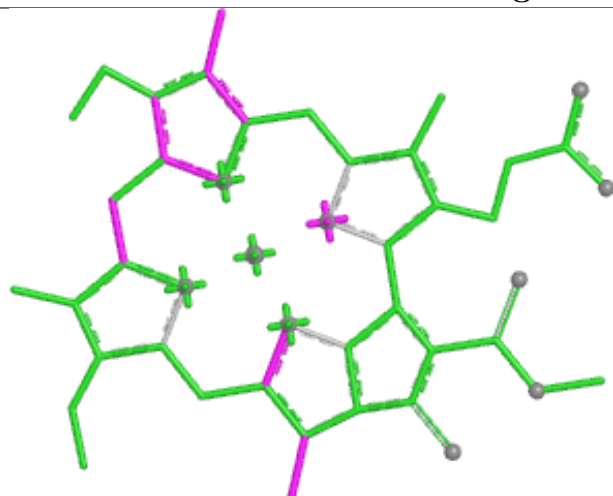
Ligand CLA a 605



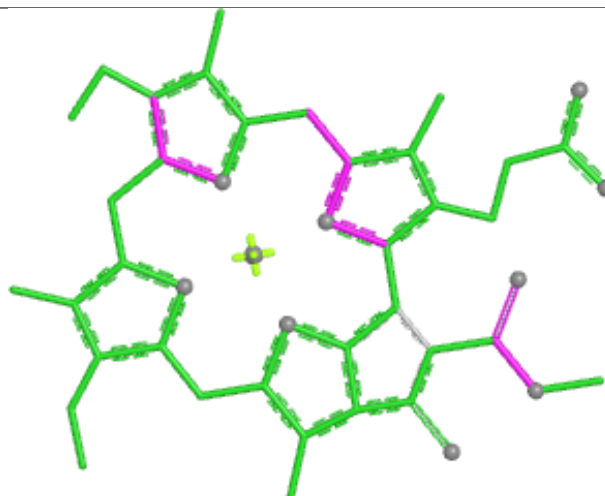
Ligand XAT 1 616



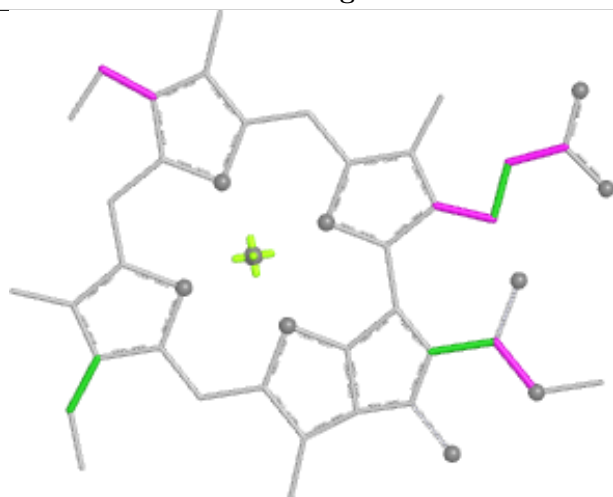
Ligand CLA K 201



Bond lengths



Bond angles

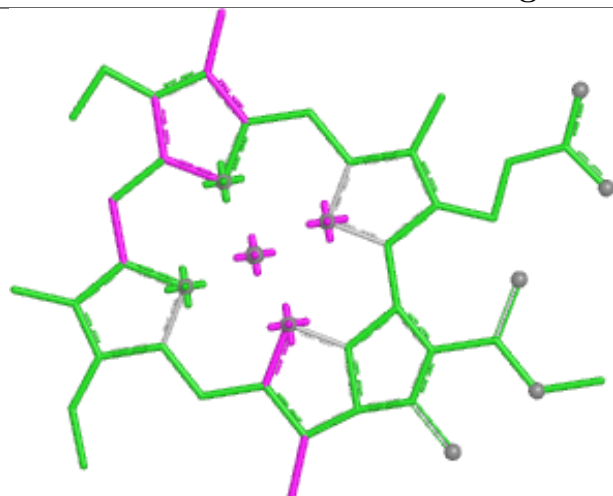


Torsions

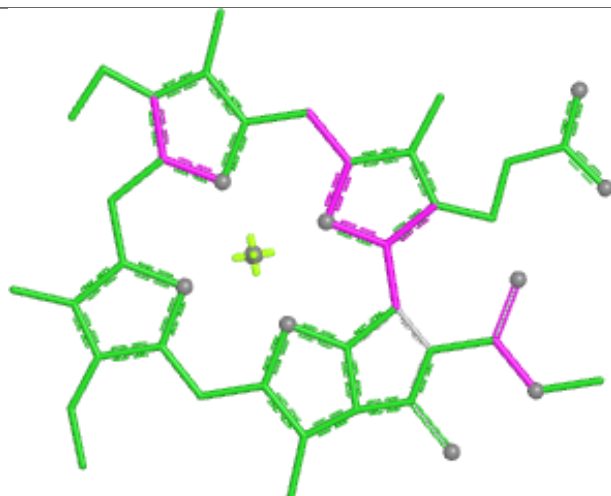


Rings

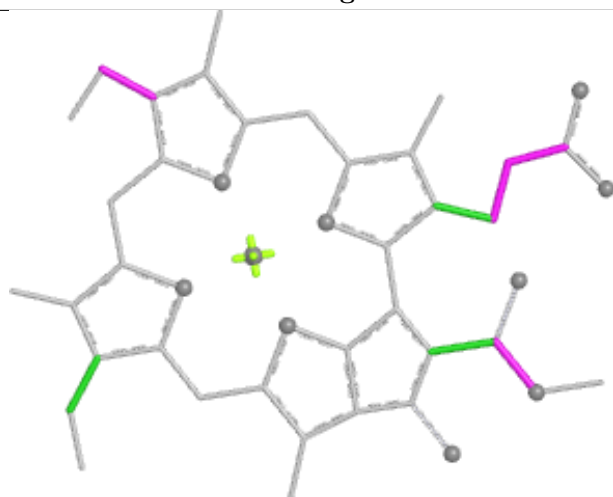
Ligand CLA c 310



Bond lengths



Bond angles

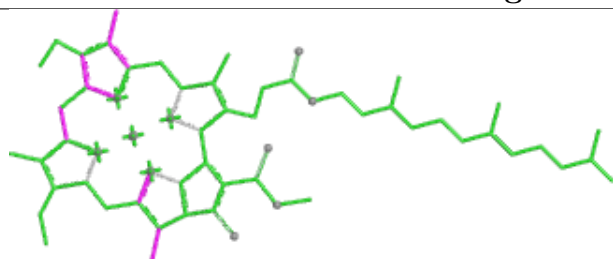


Torsions

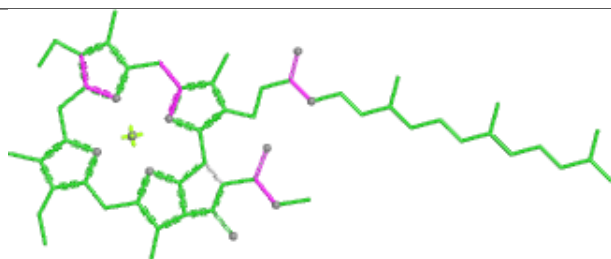


Rings

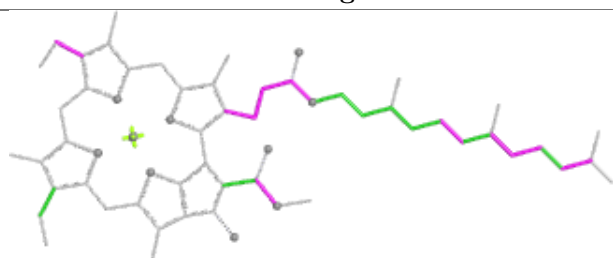
Ligand CLA A 5024



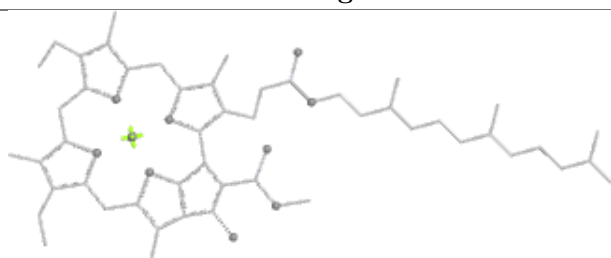
Bond lengths



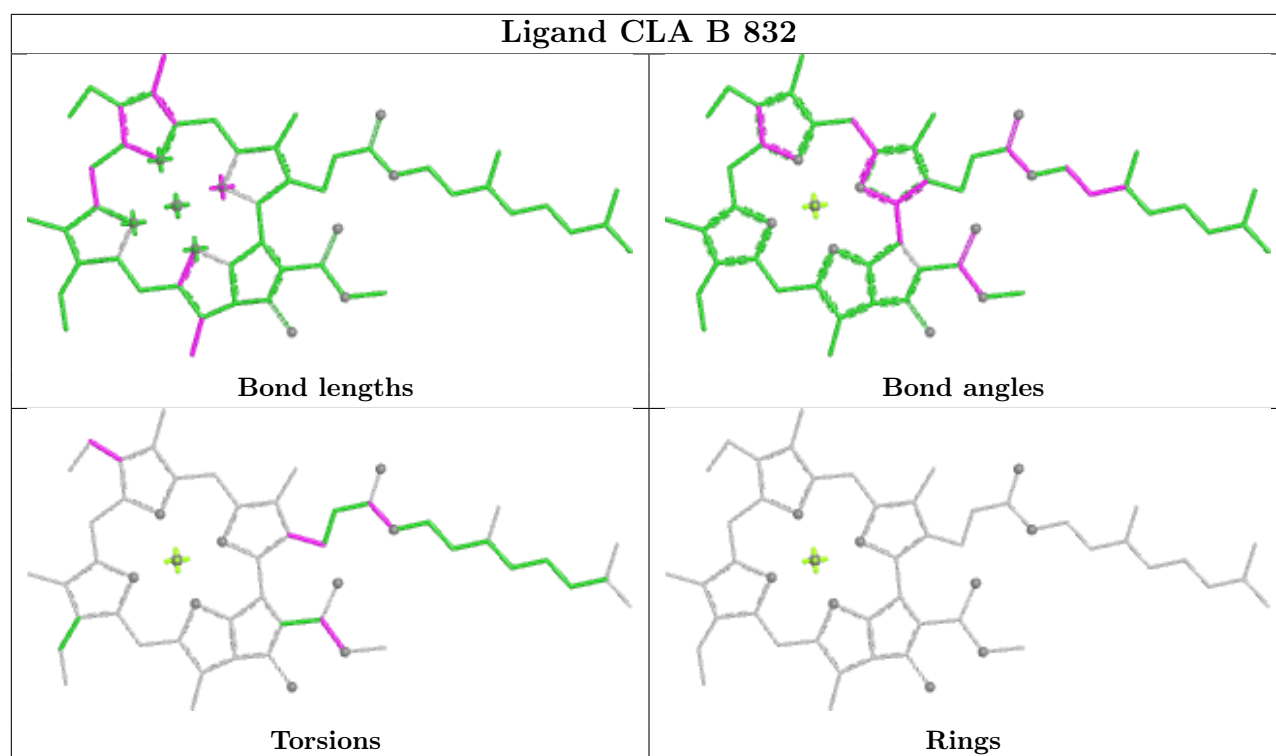
Bond angles



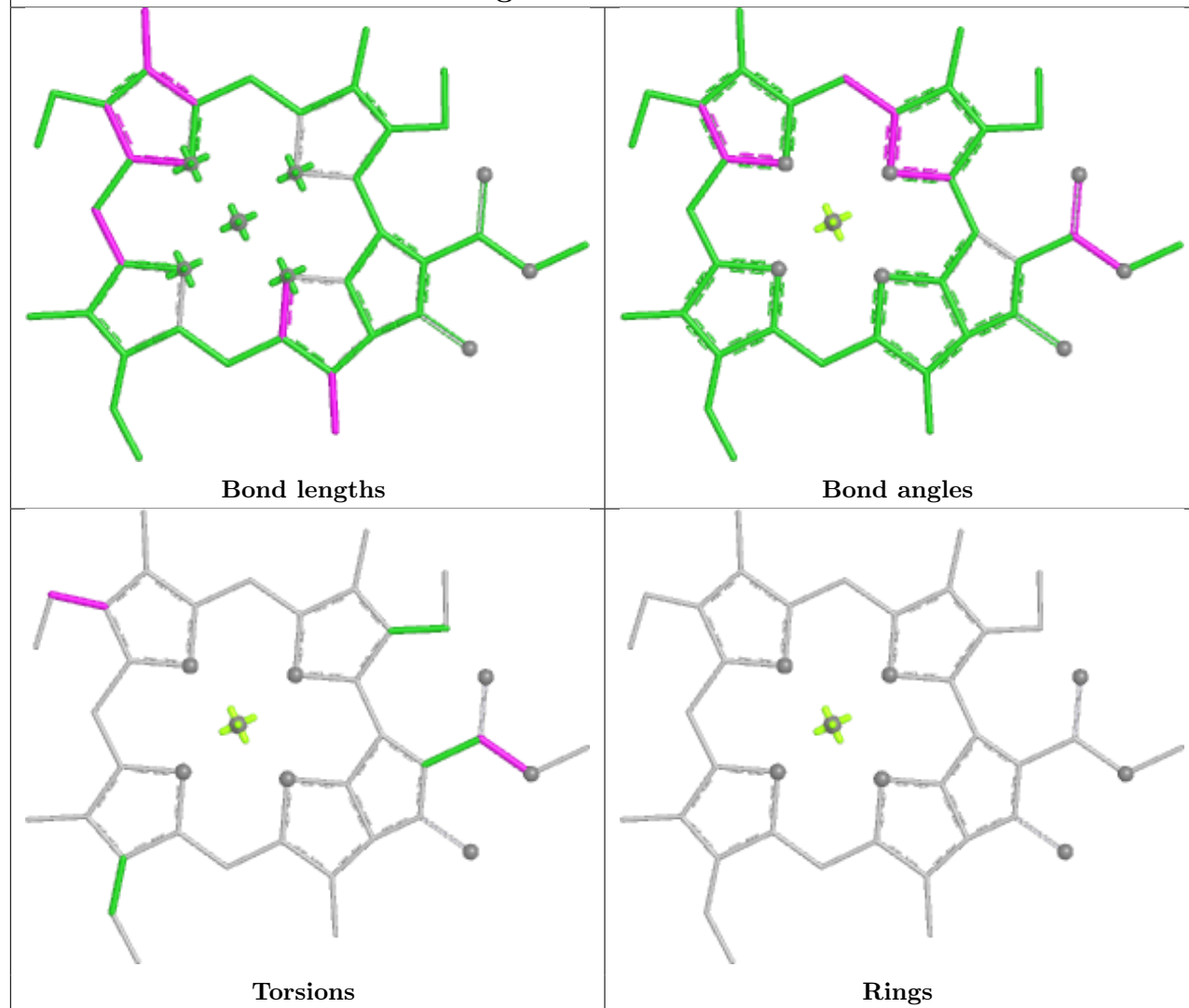
Torsions



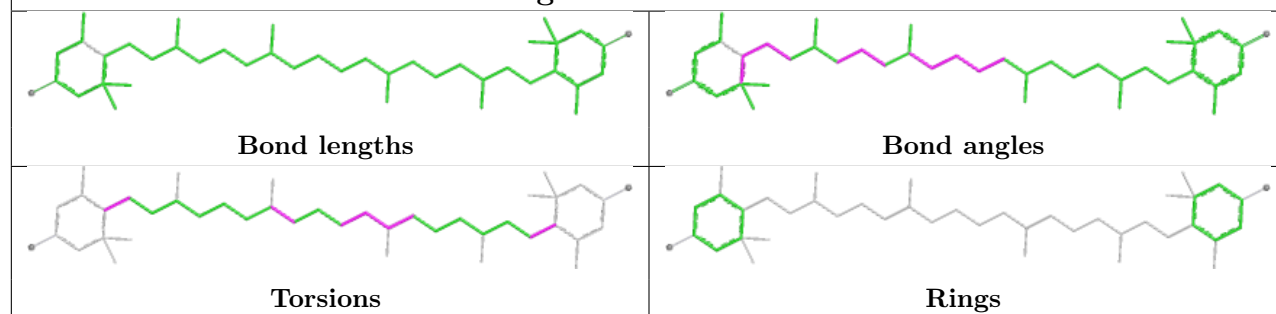
Rings

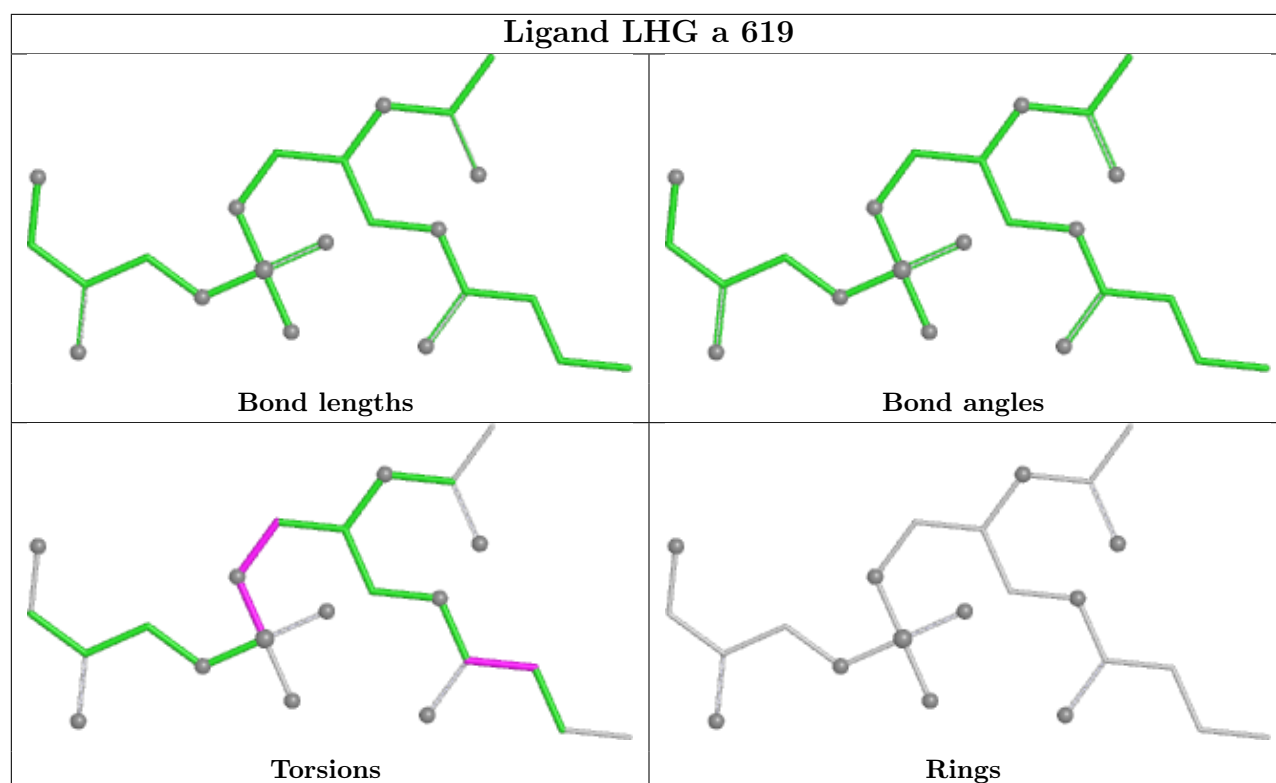


Ligand CLA T 412

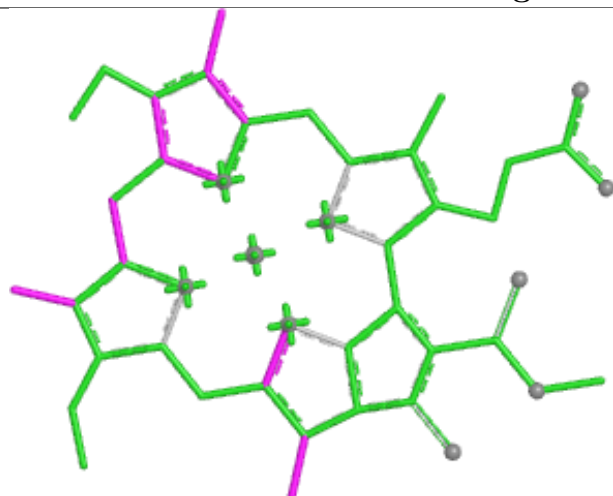


Ligand LUT a 615

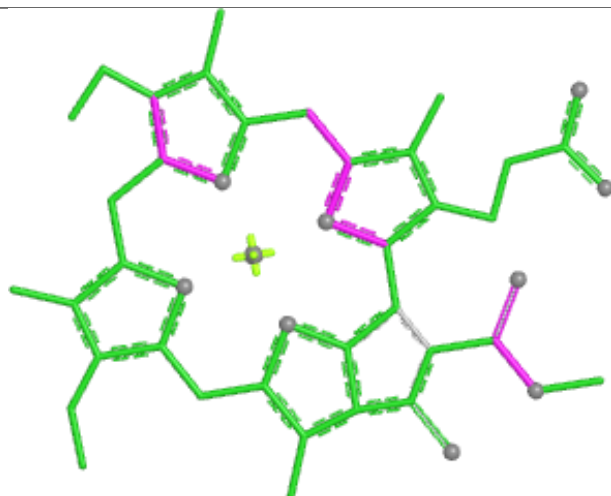




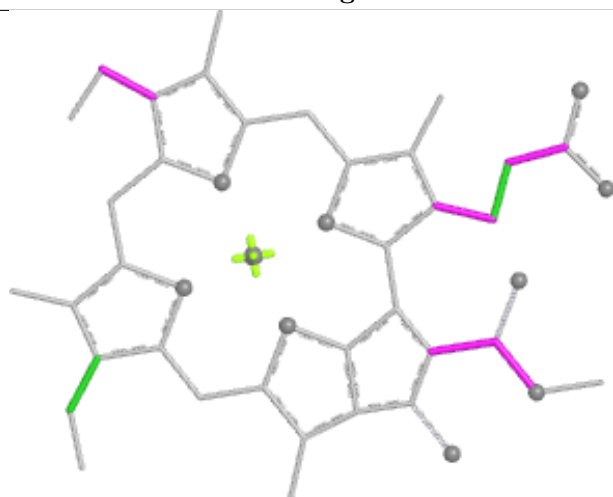
Ligand CLA K 203



Bond lengths



Bond angles

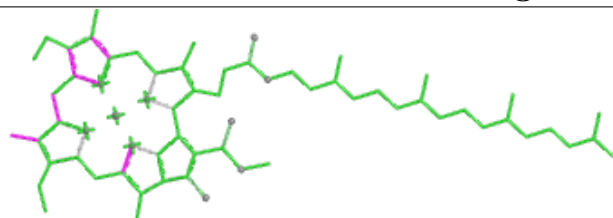


Torsions

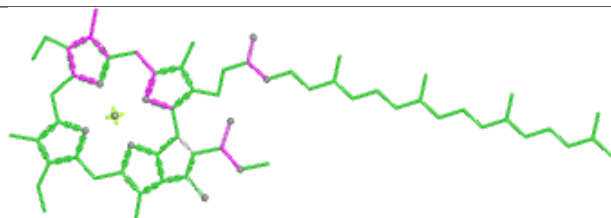


Rings

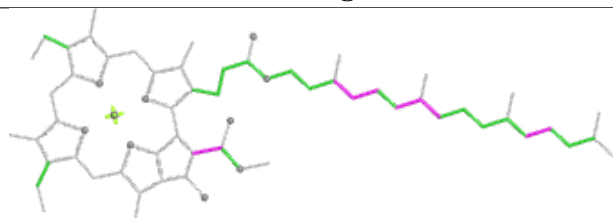
Ligand CLA B 805



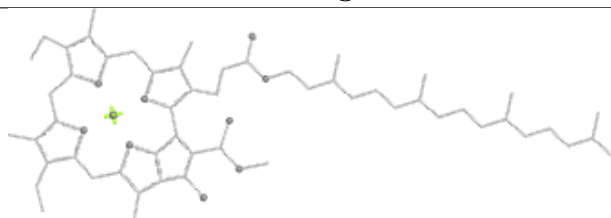
Bond lengths



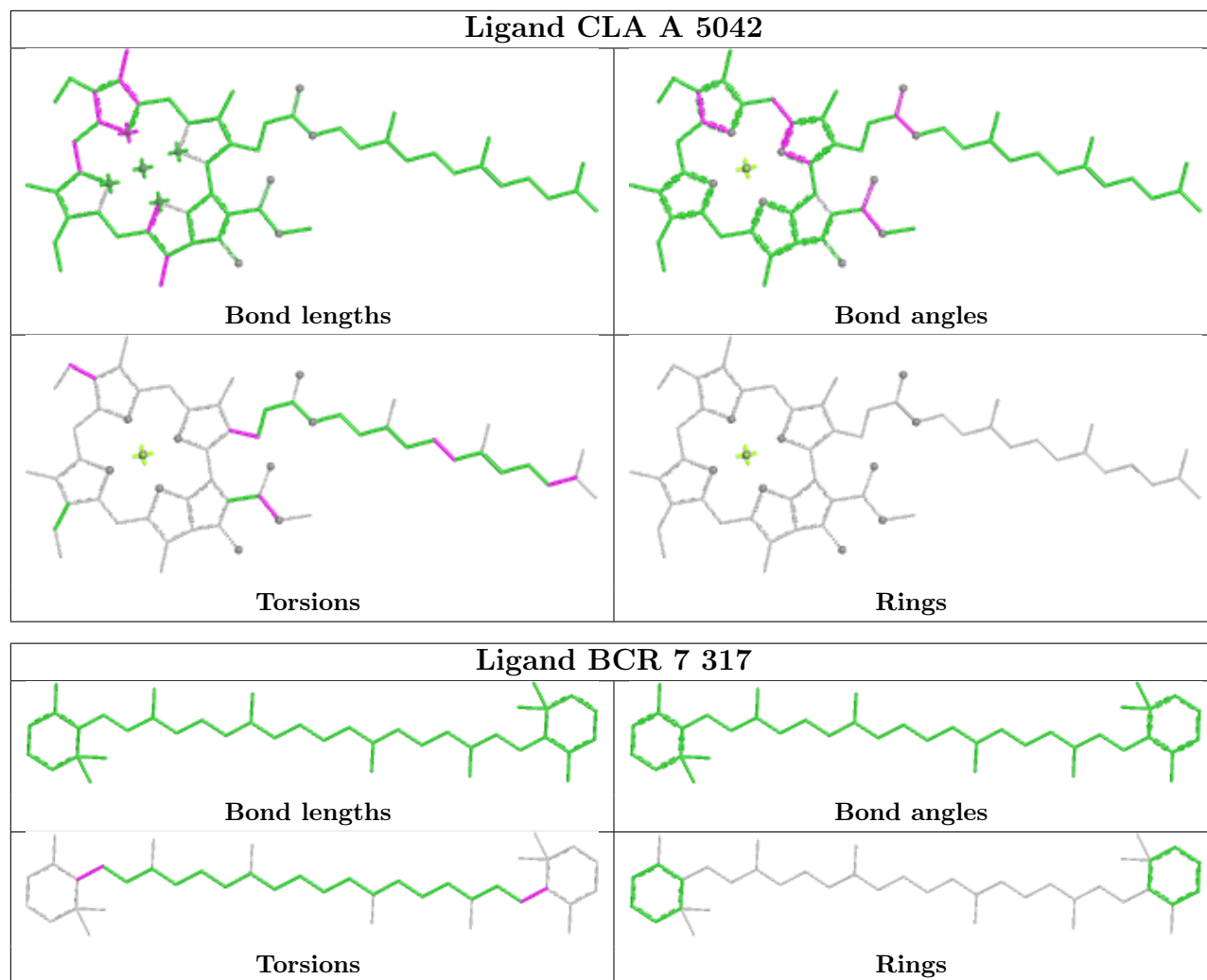
Bond angles

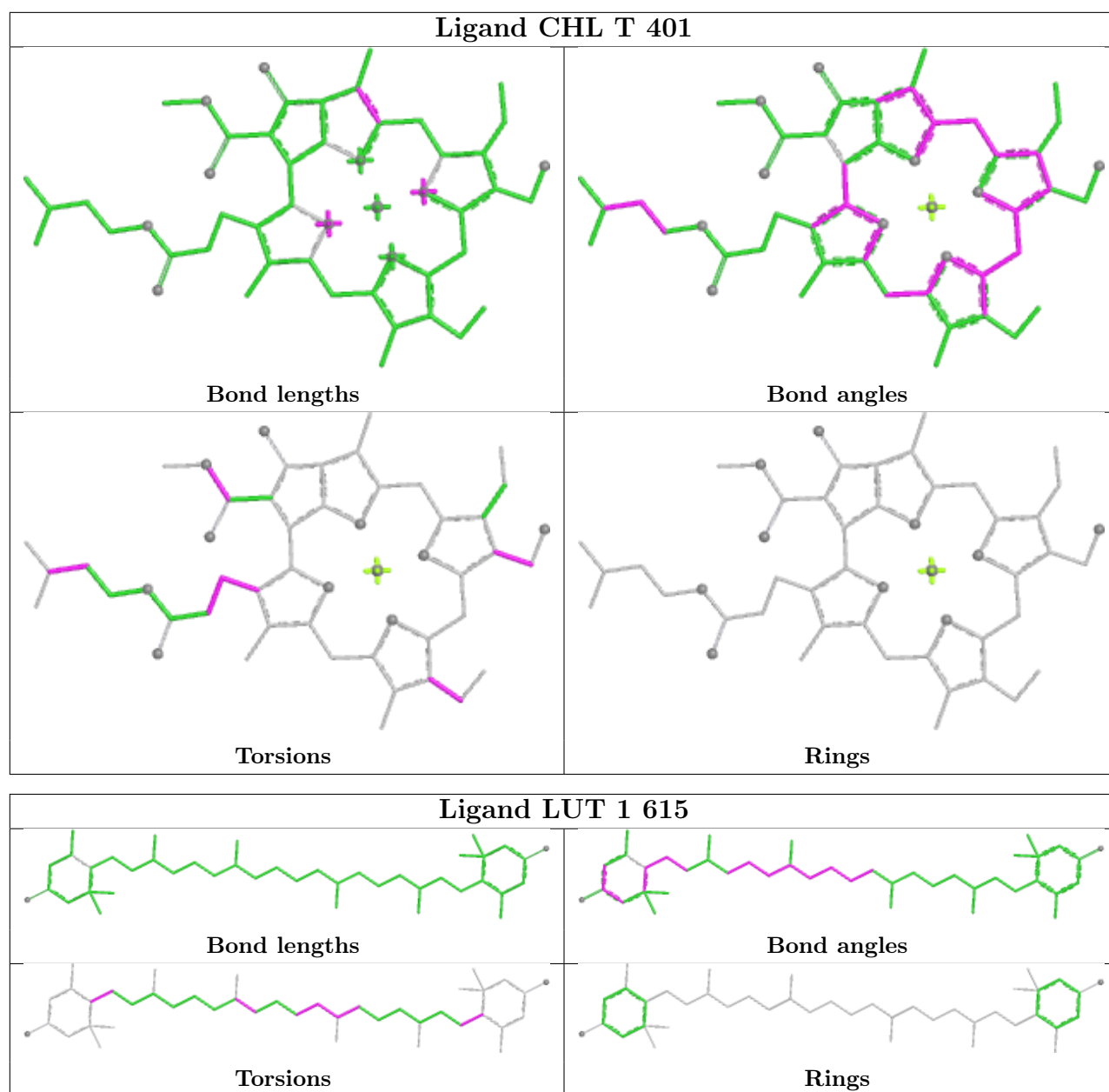


Torsions

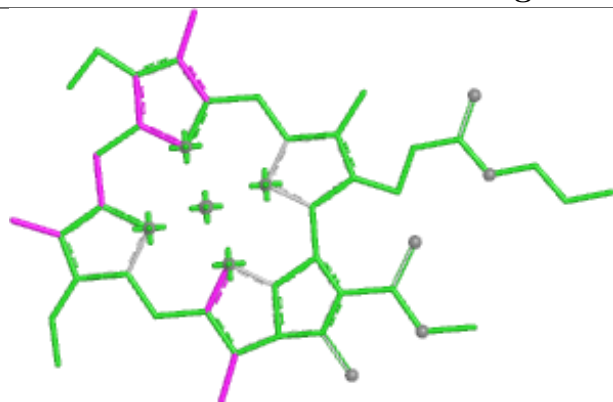


Rings

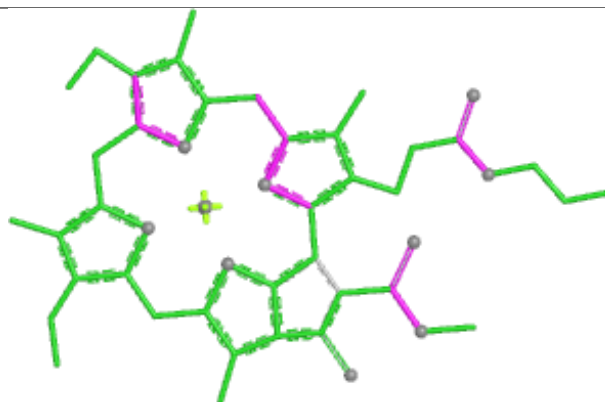




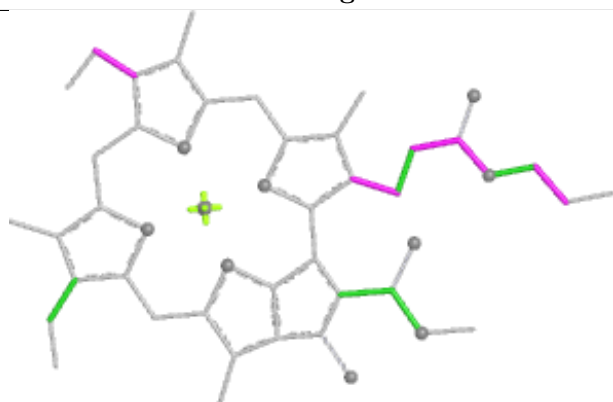
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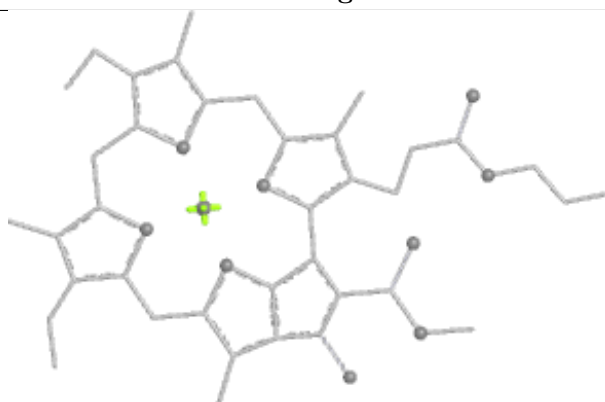
Bond lengths



Bond angles

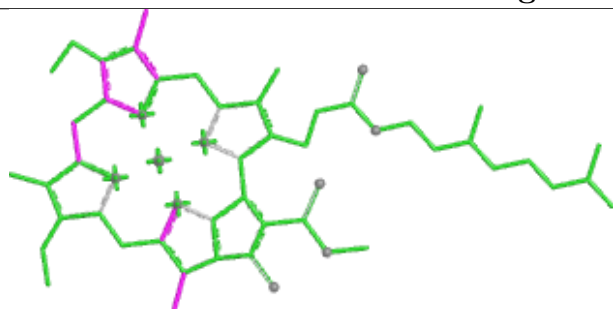


Torsions

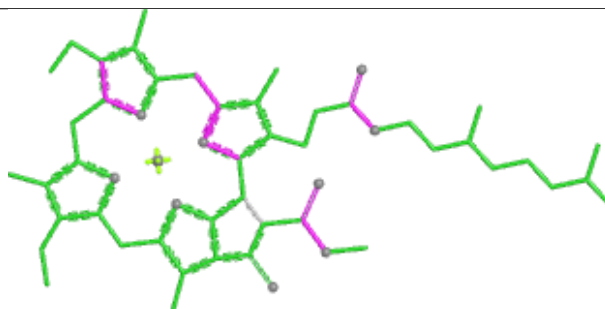


Rings

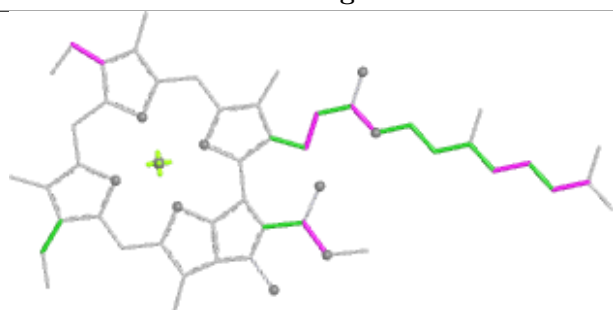
Ligand CLA 3 311



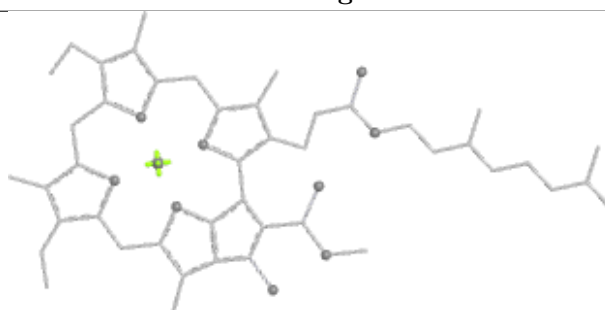
Bond lengths



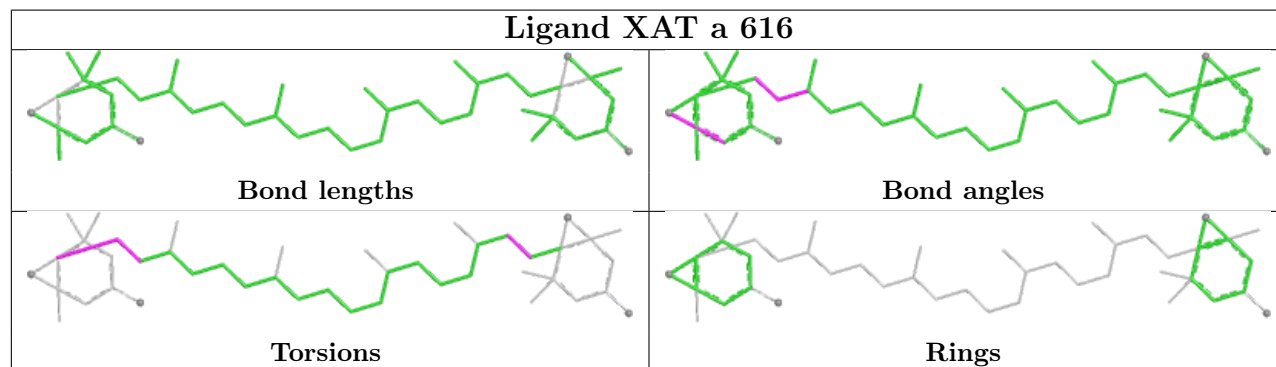
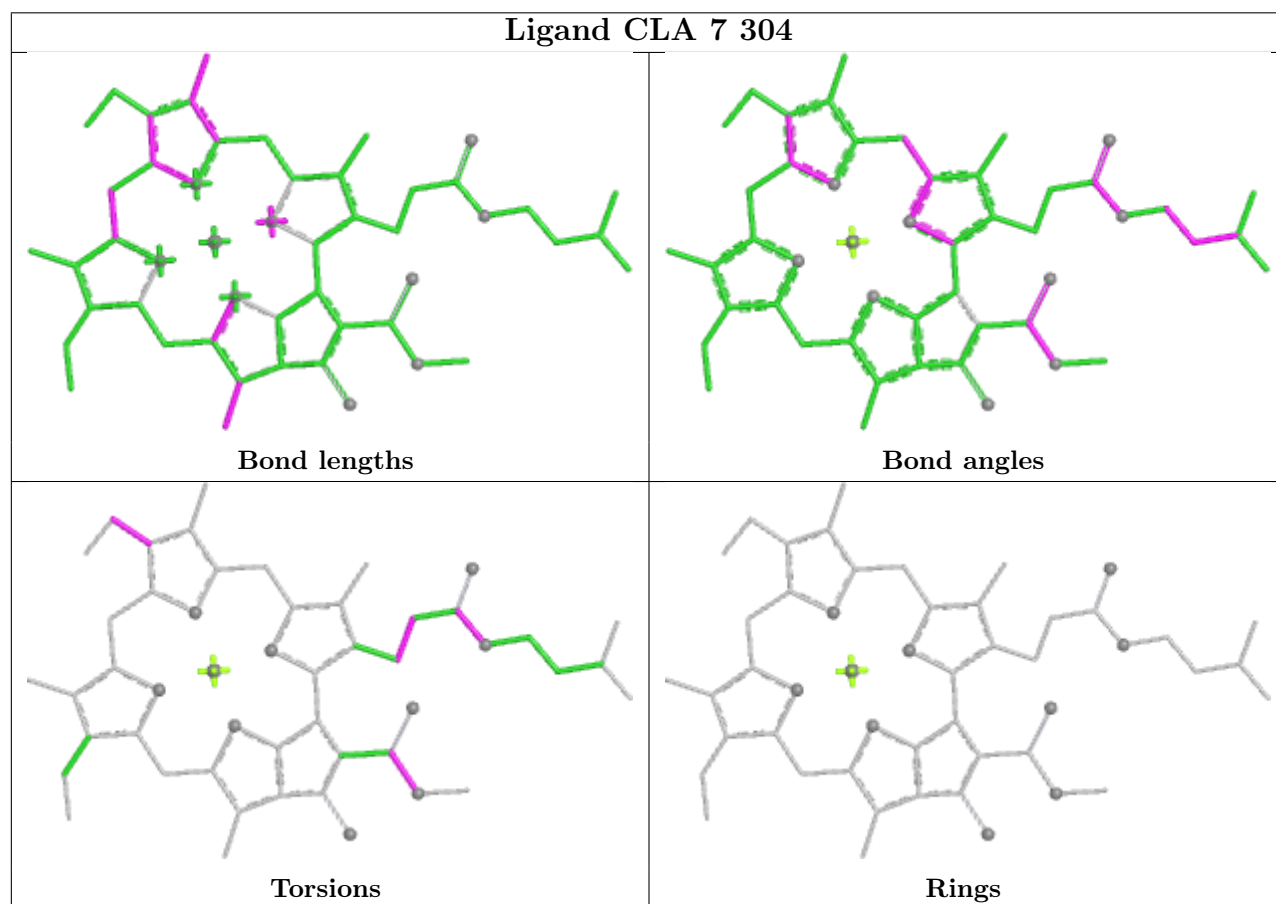
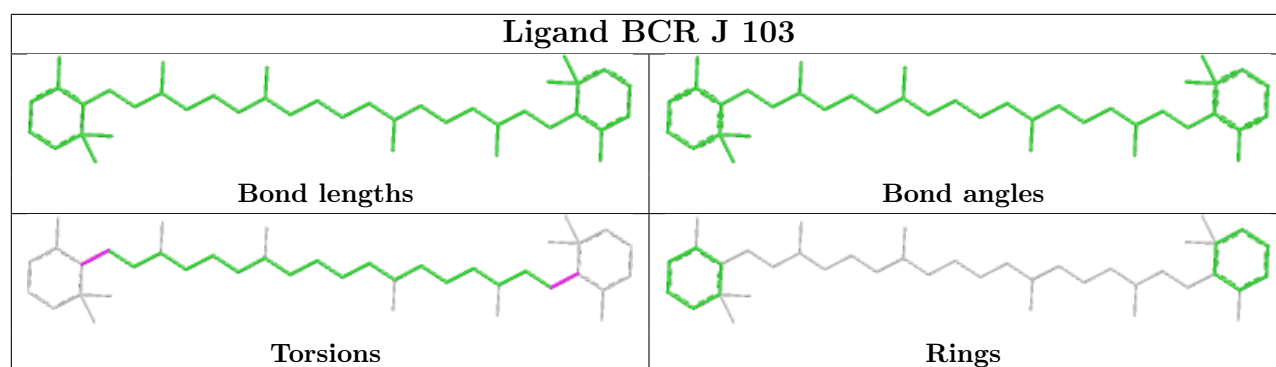
Bond angles

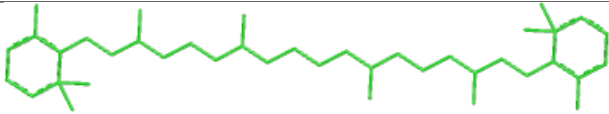
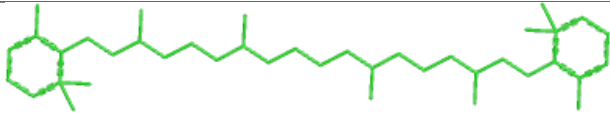
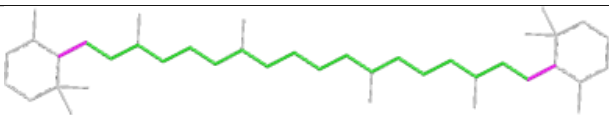
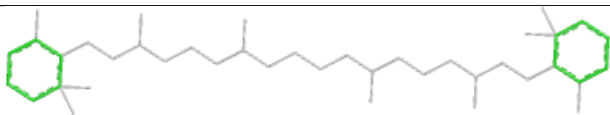


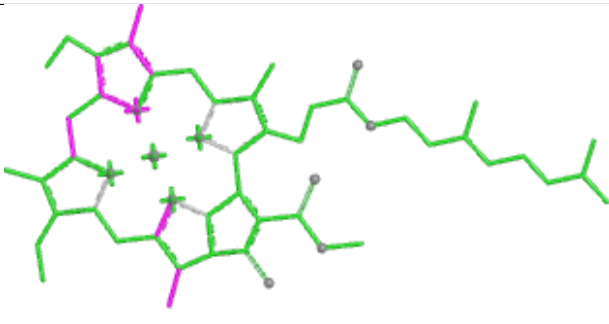
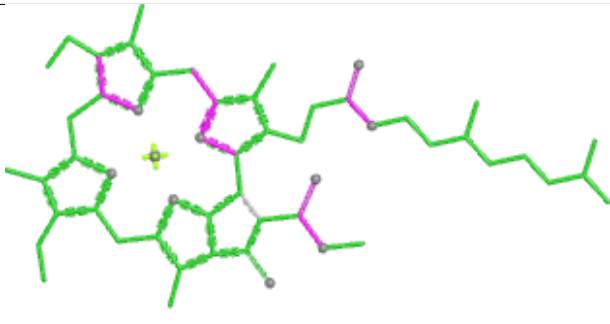
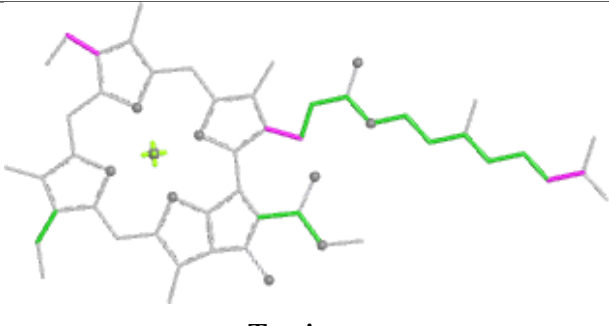
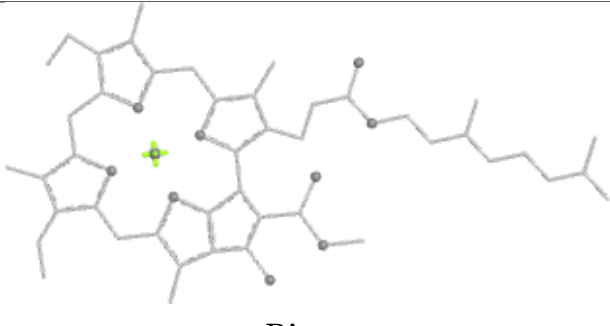
Torsions

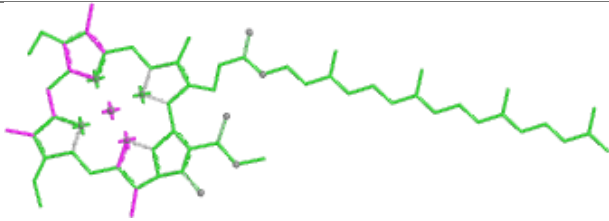
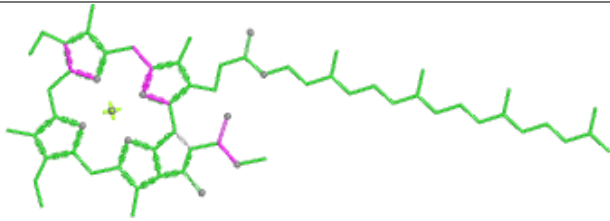
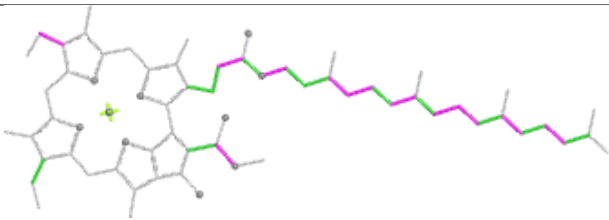
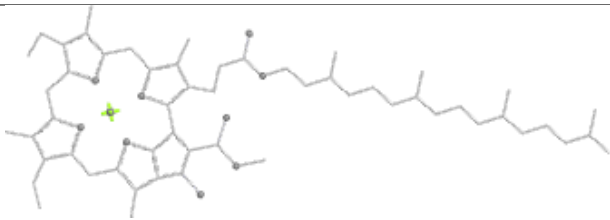


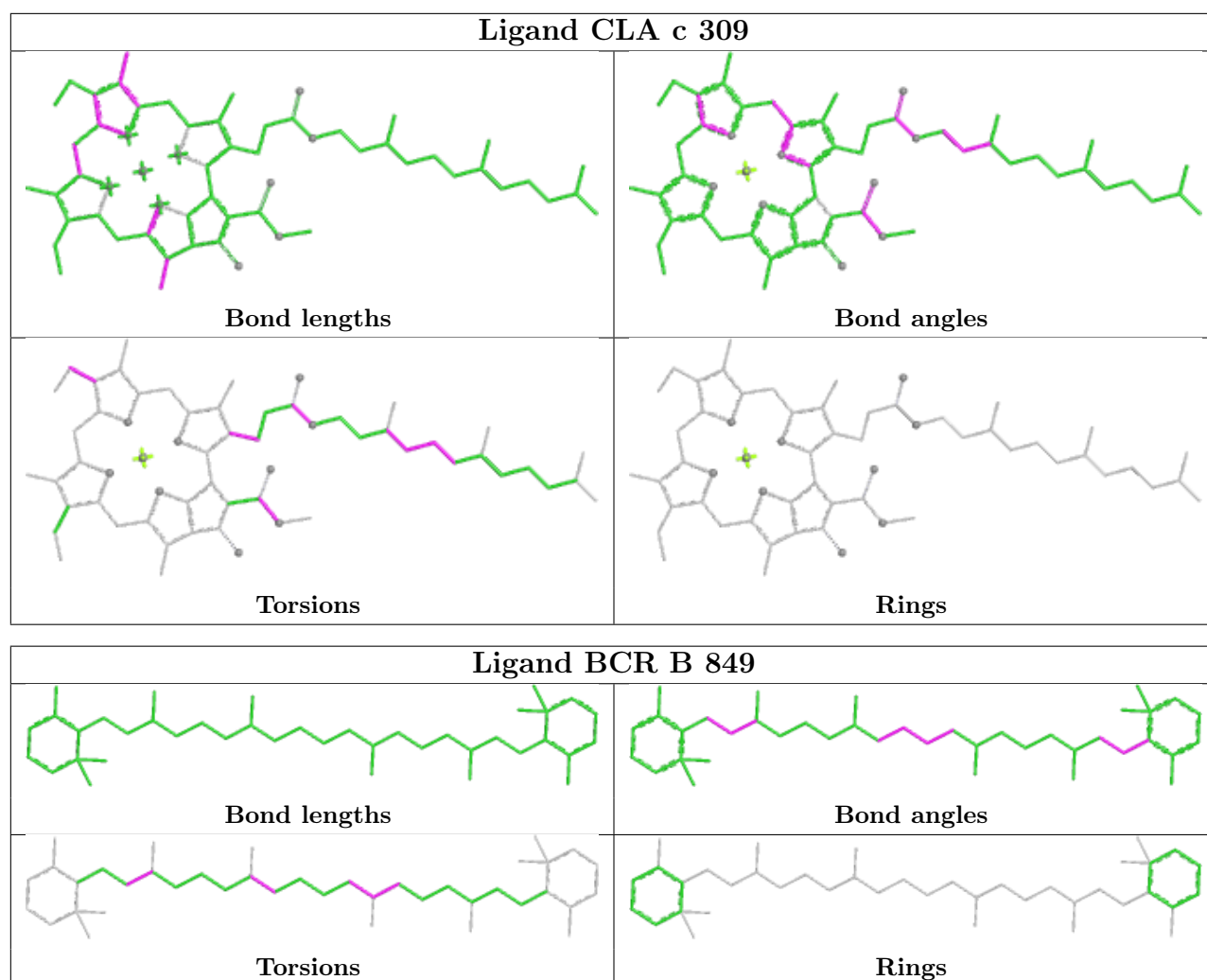
Rings

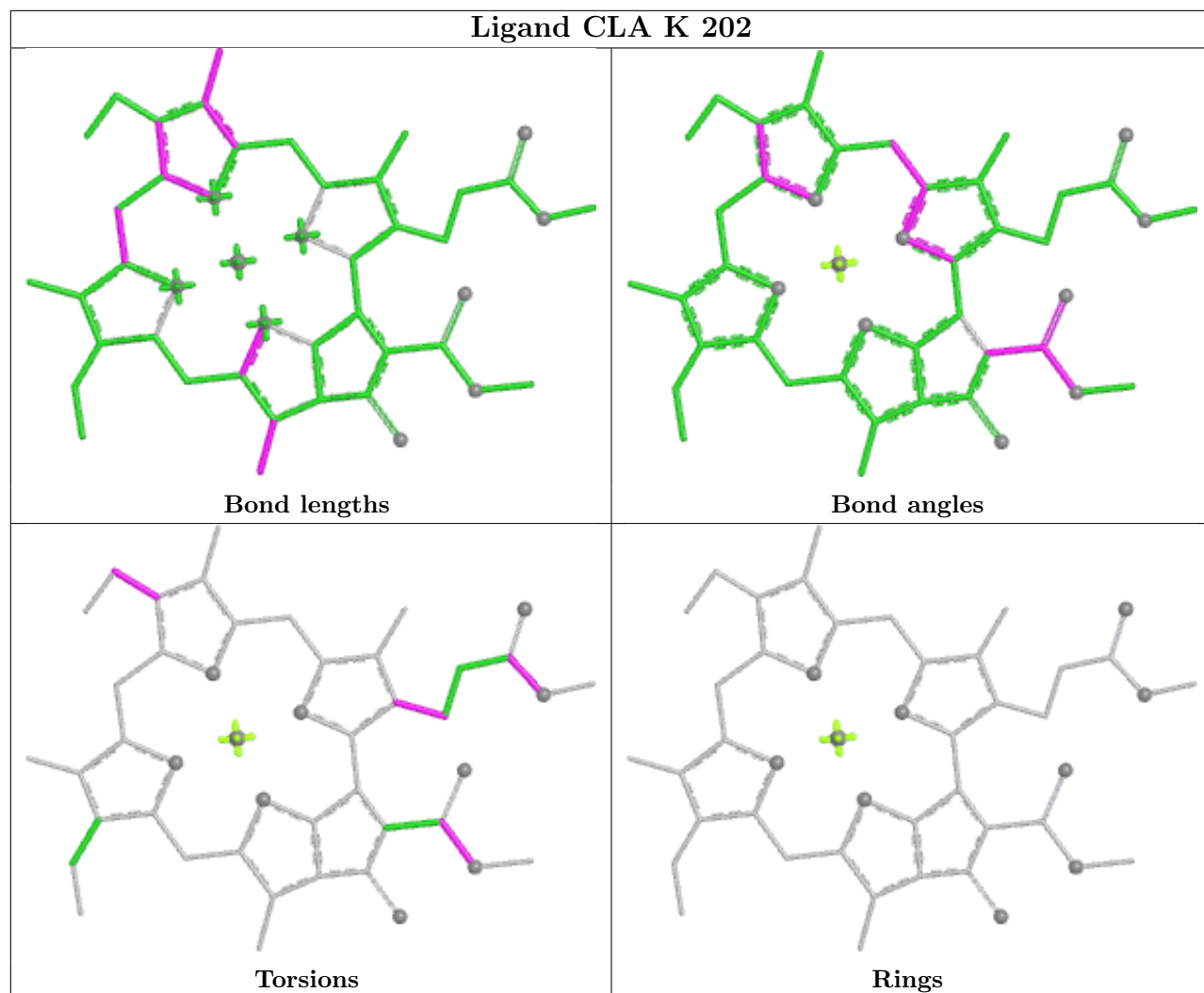


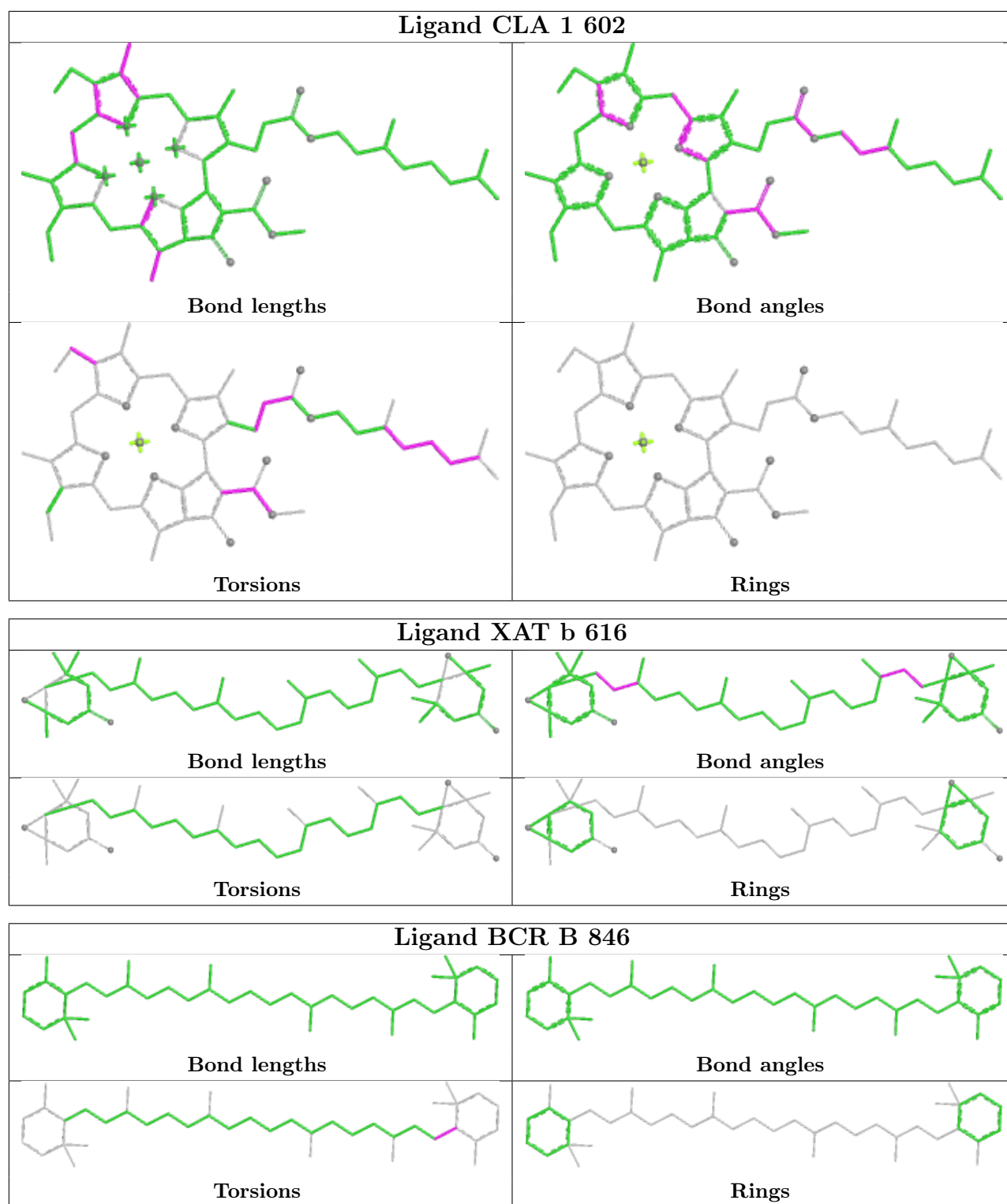
Ligand BCR T 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

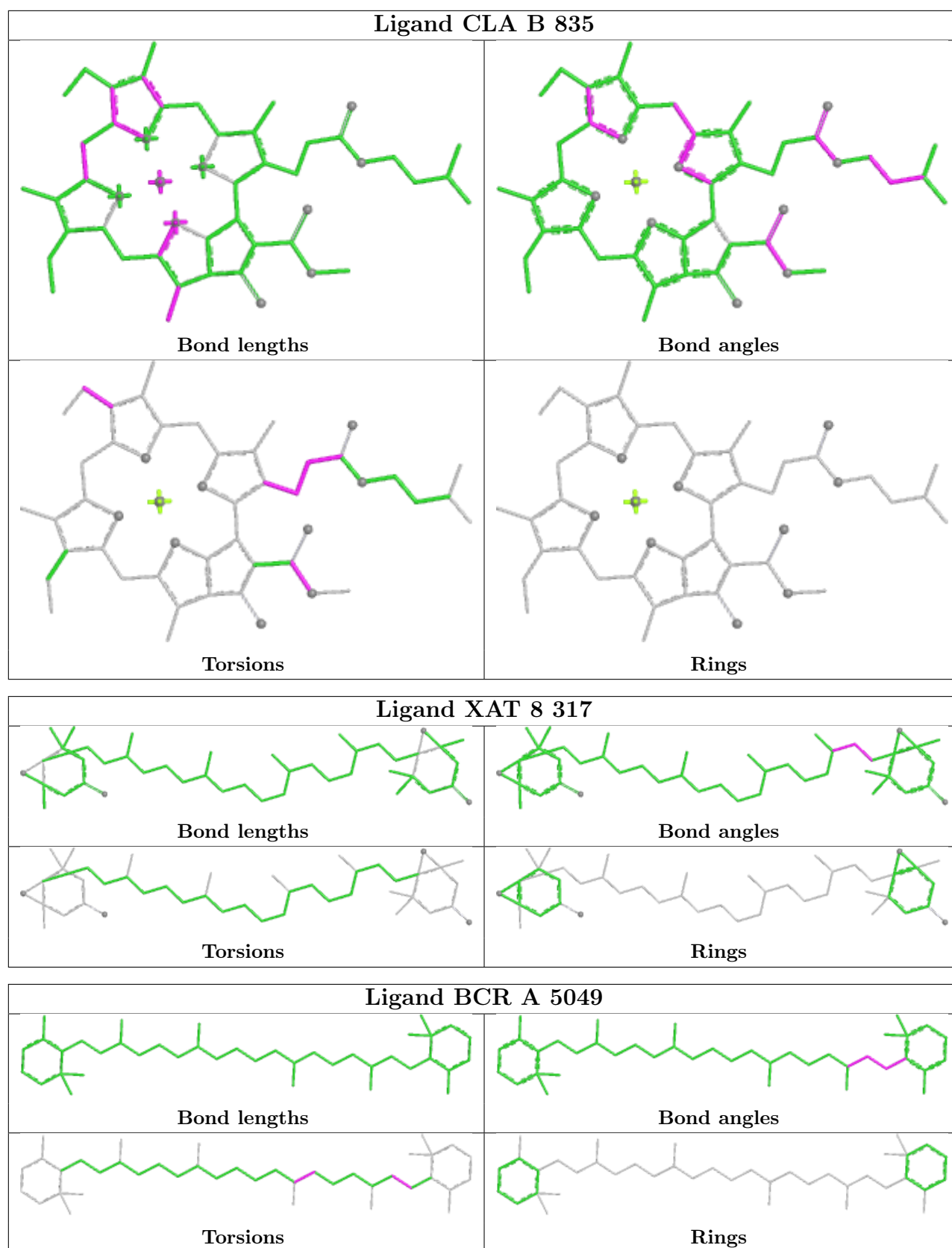
Ligand CLA A 5033	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

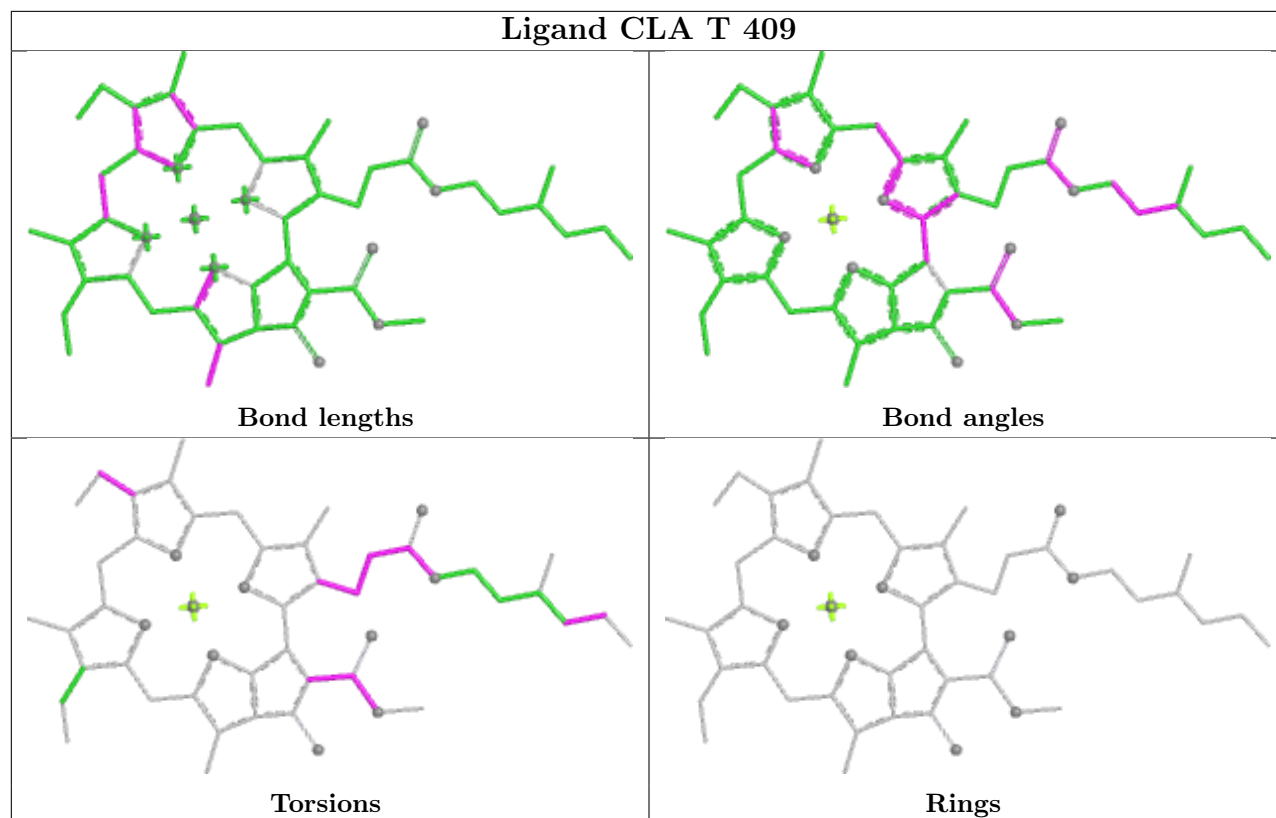




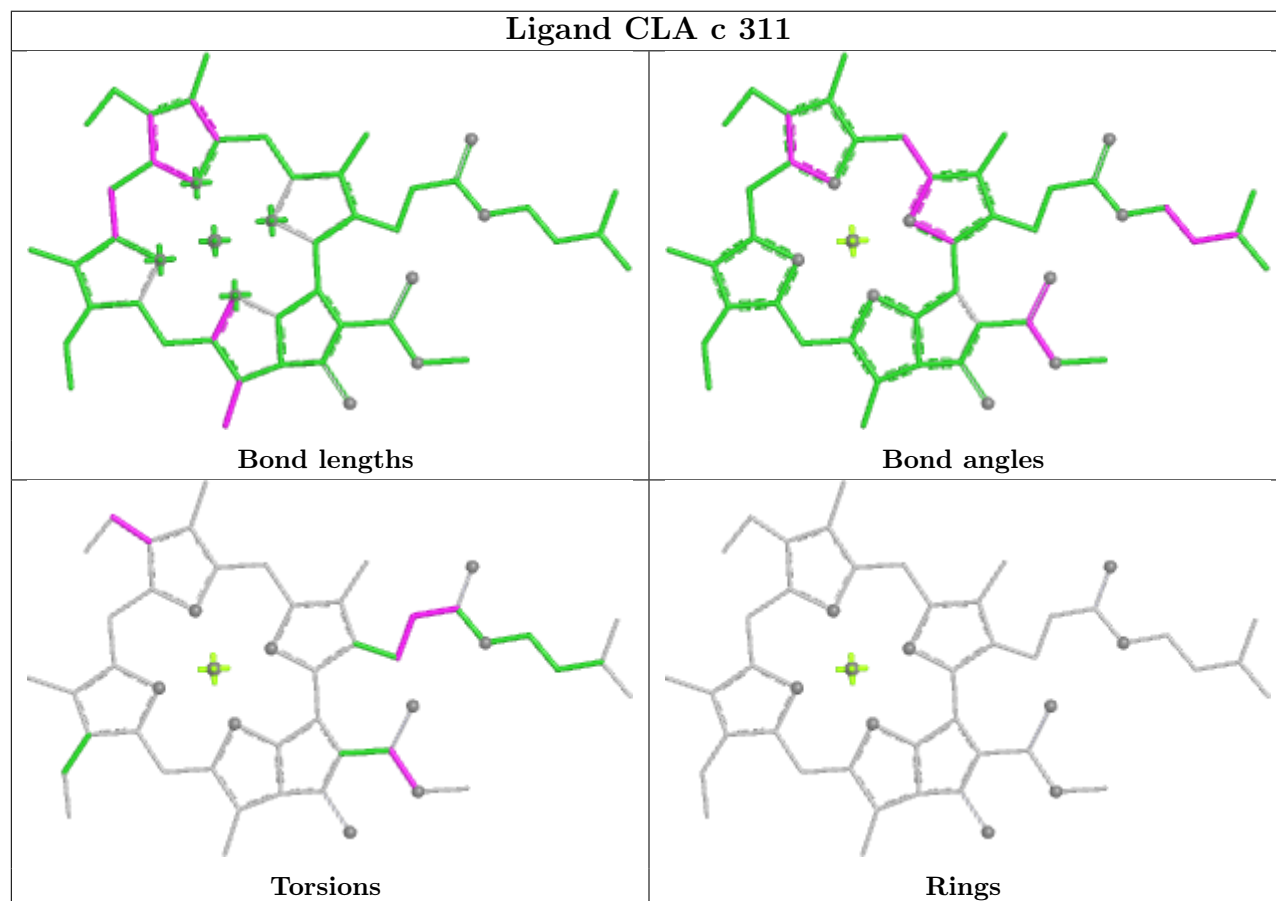




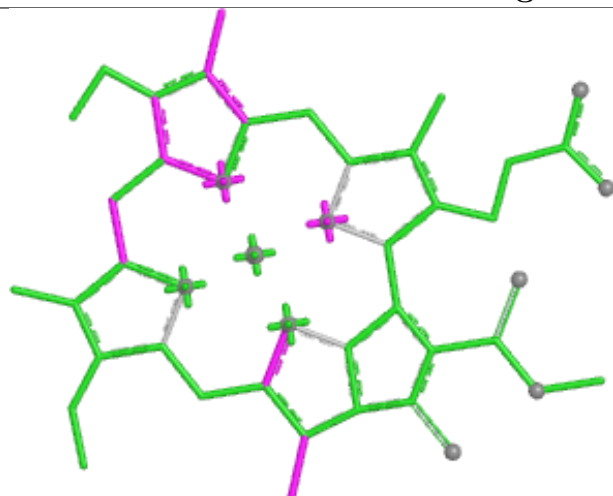
Ligand CLA T 409



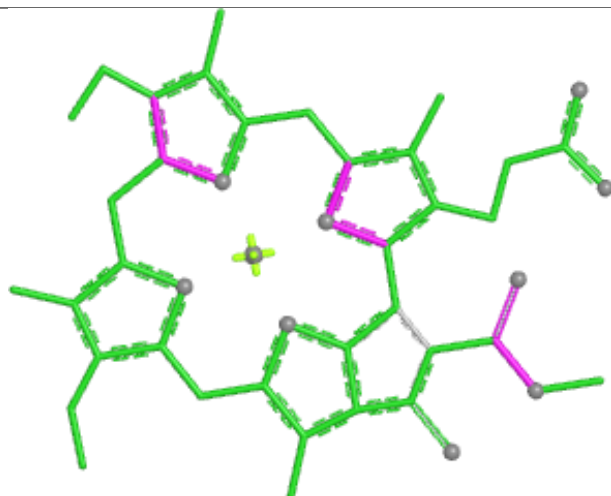
Ligand CLA c 311



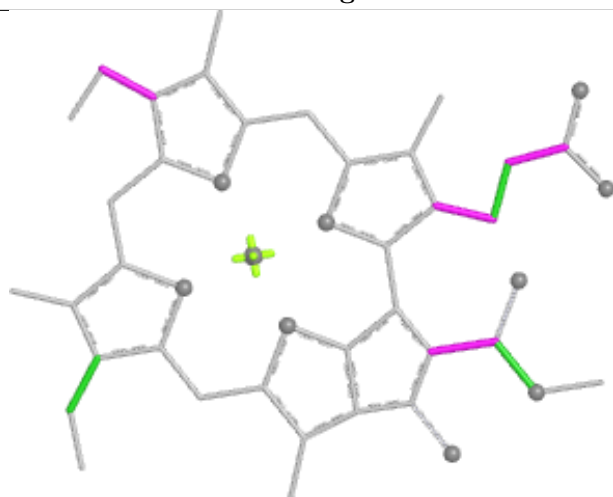
Ligand CLA L 202



Bond lengths



Bond angles

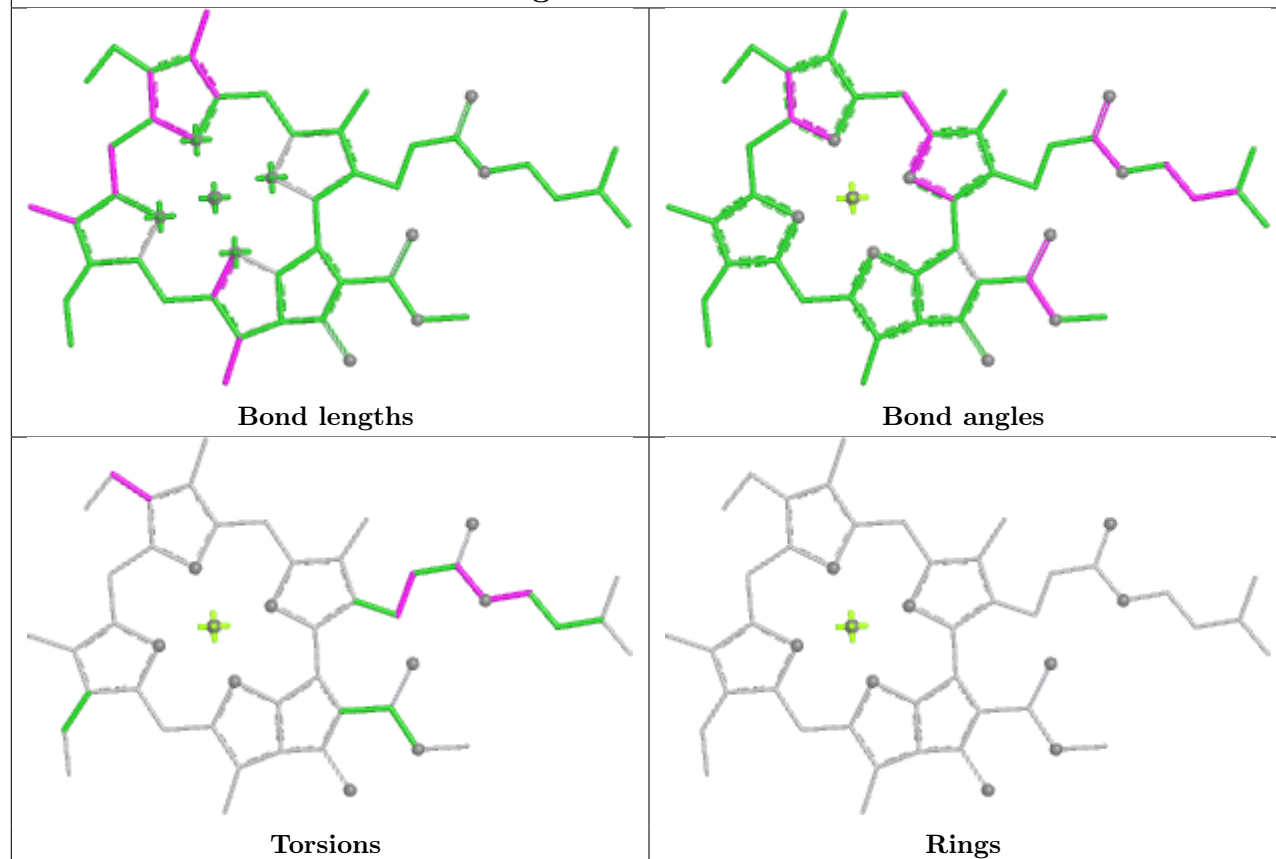


Torsions

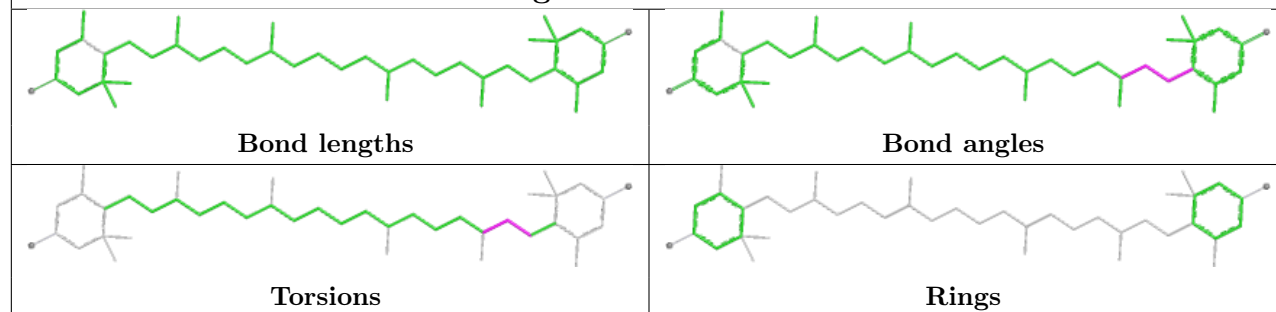


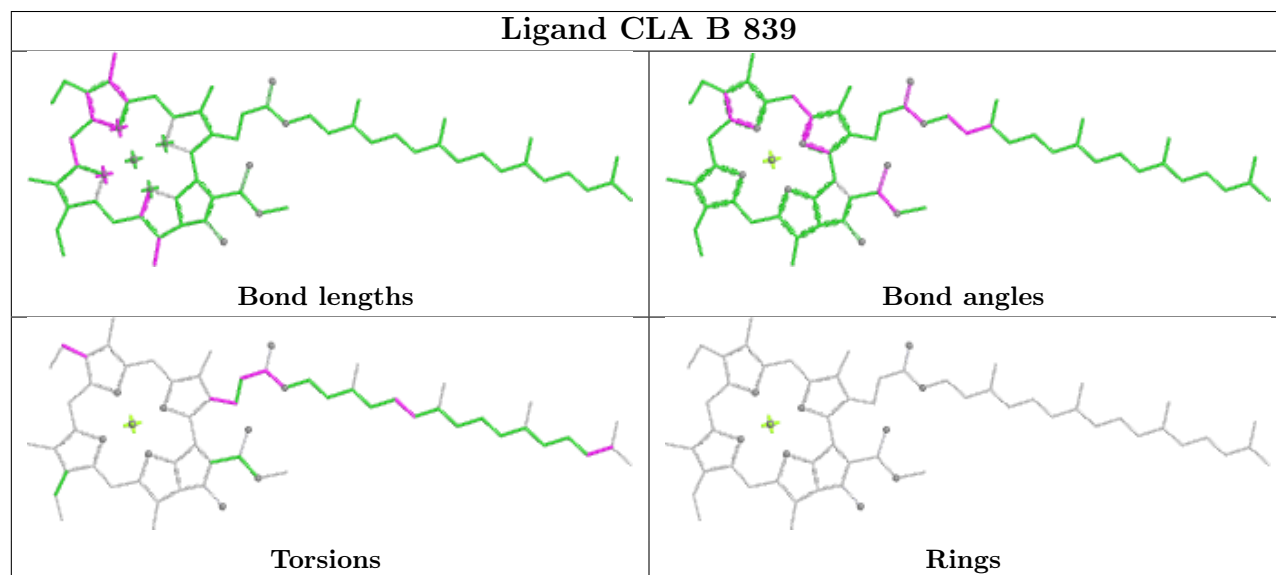
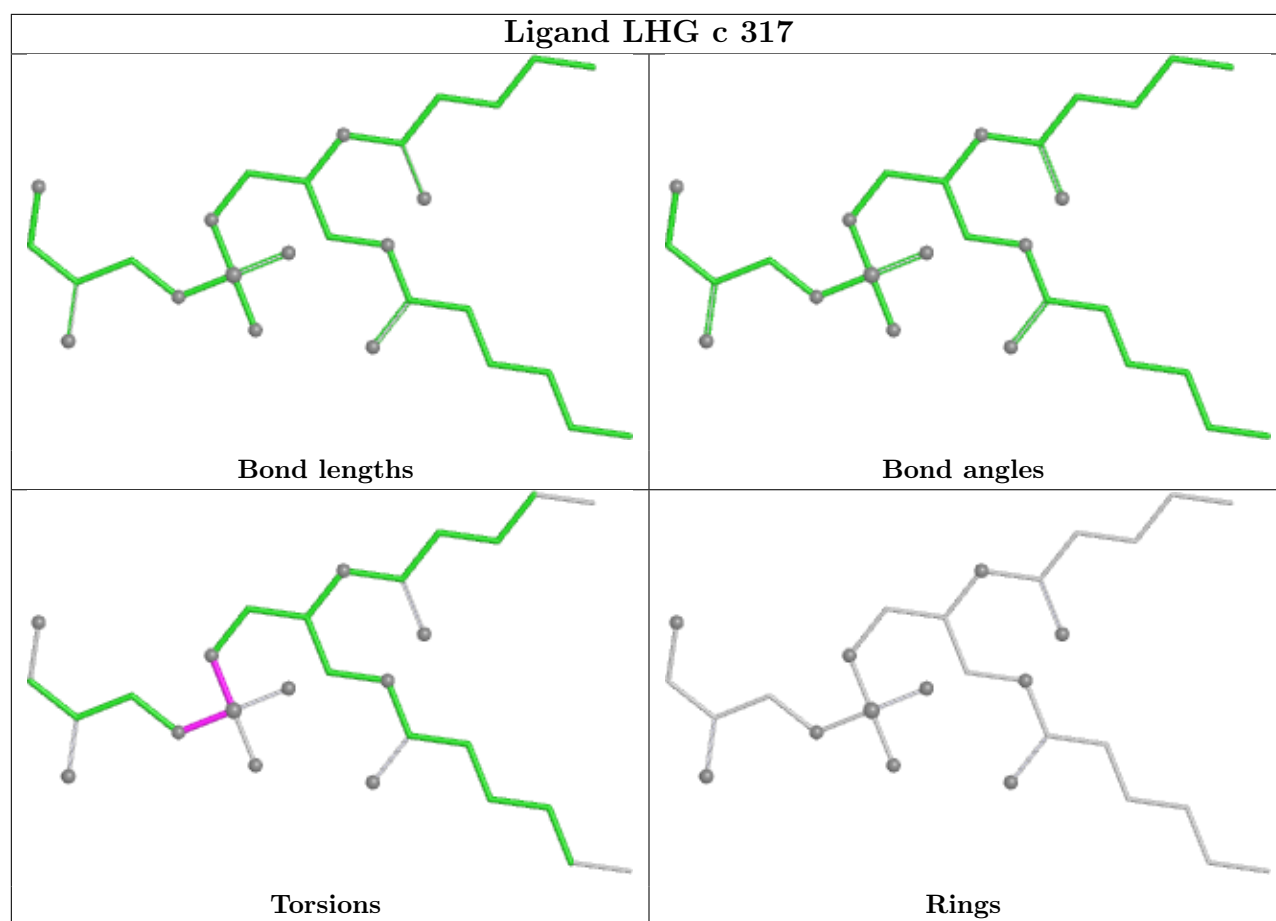
Rings

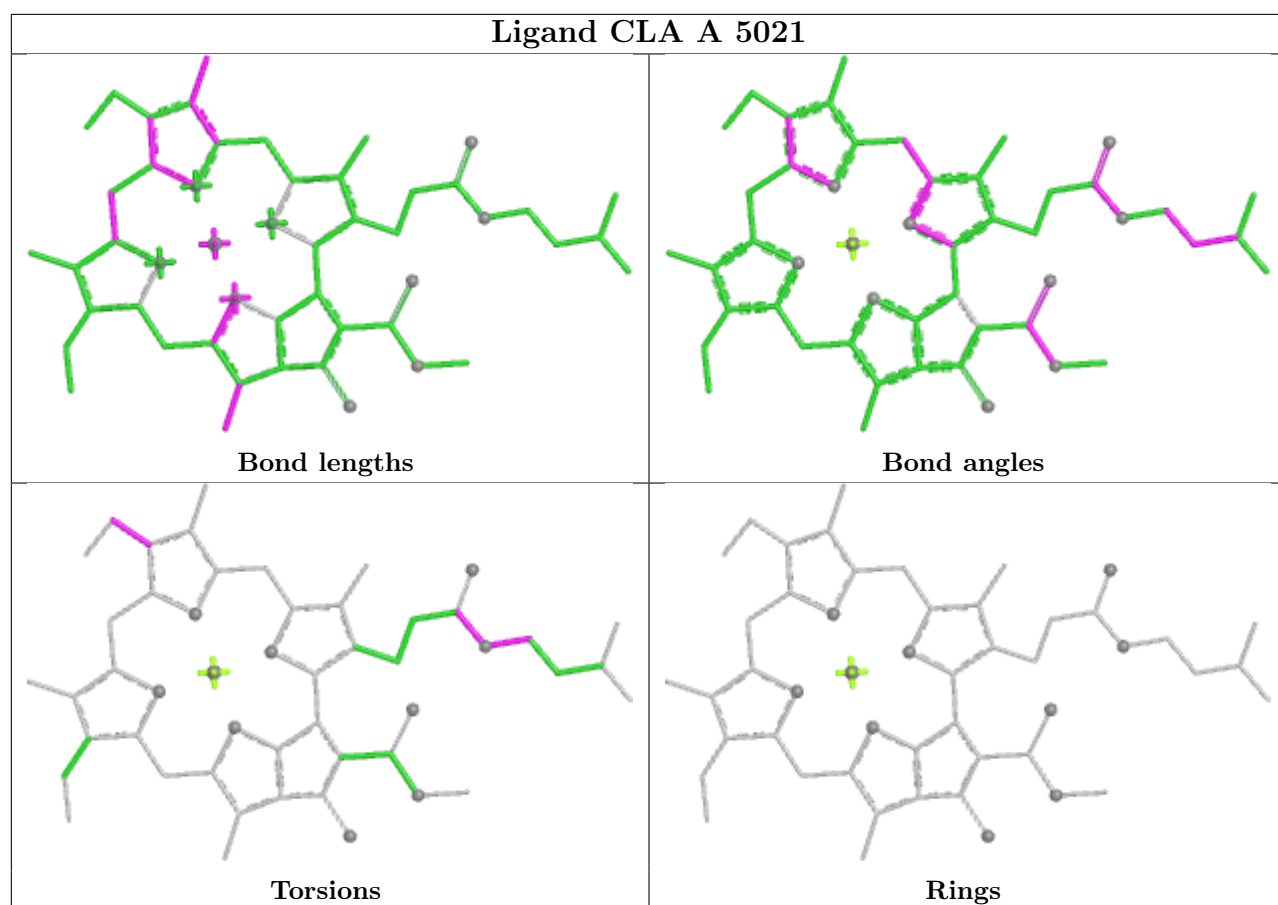
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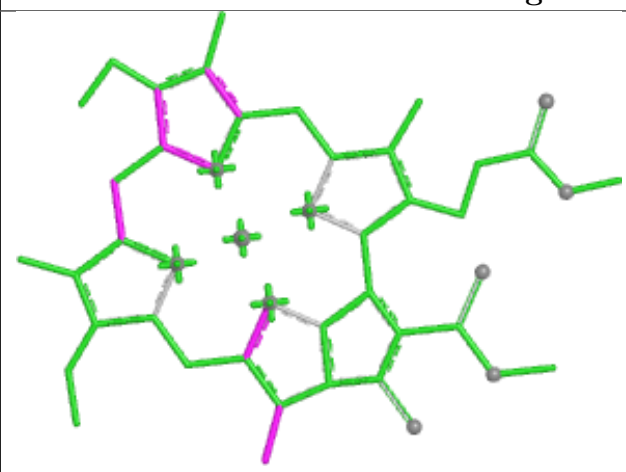
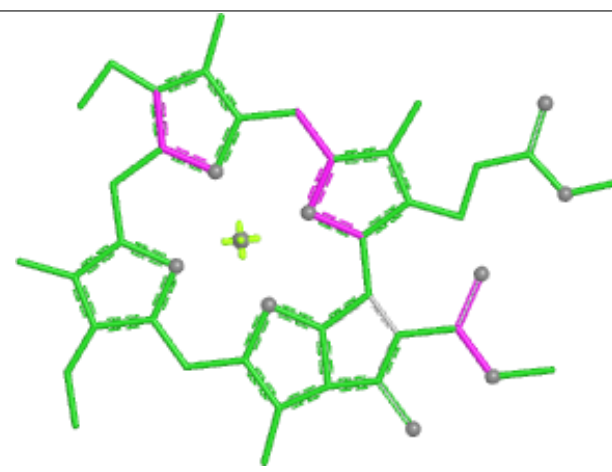
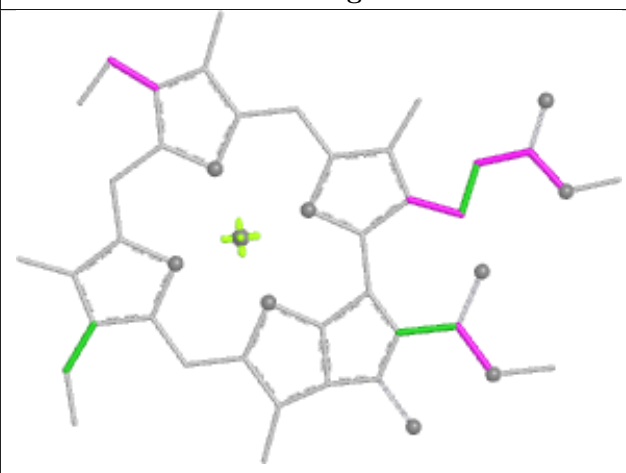
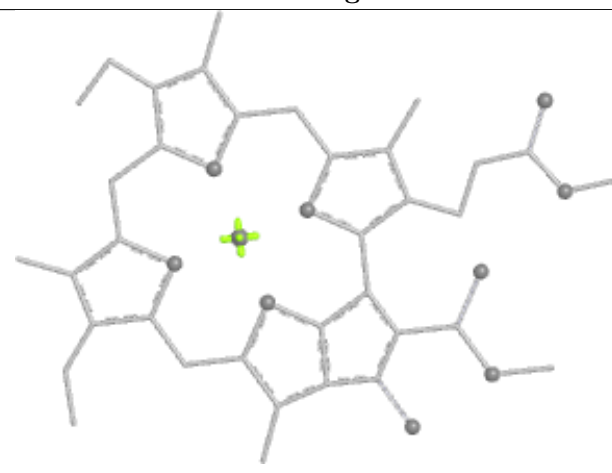


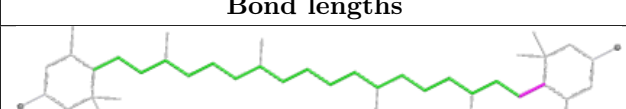
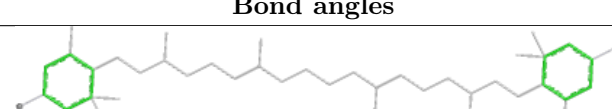
Ligand LUT T 413

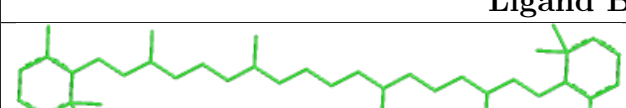
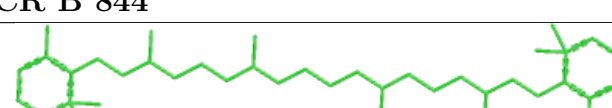
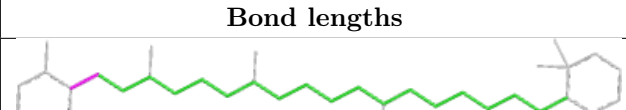
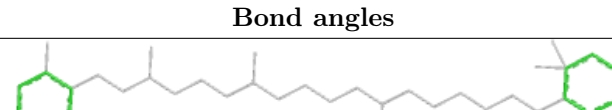


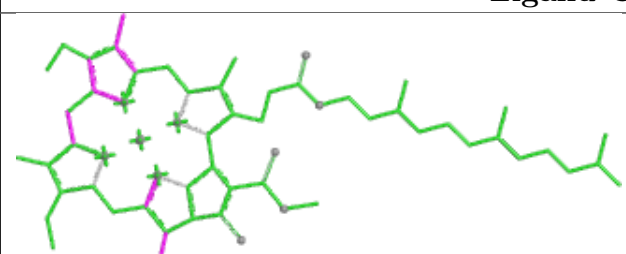
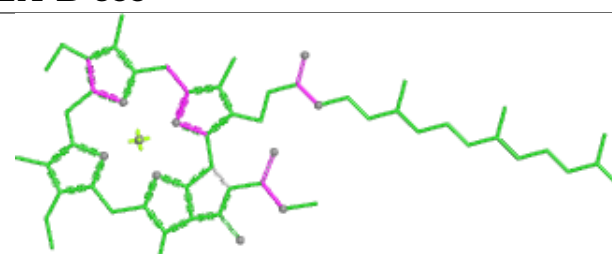
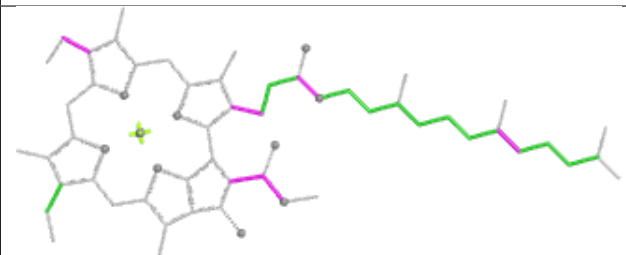
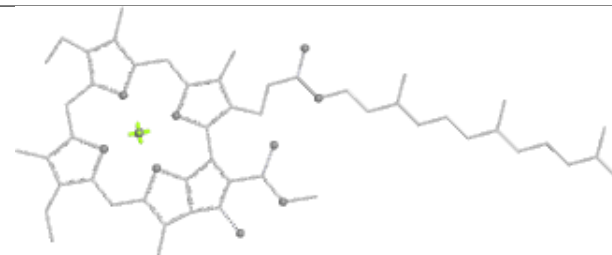


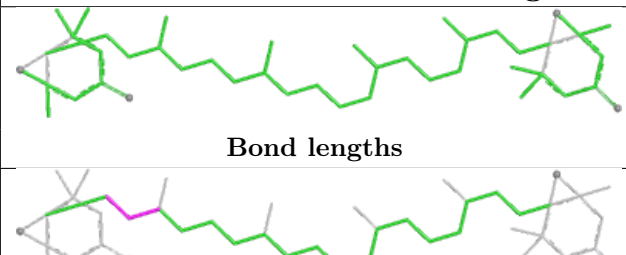
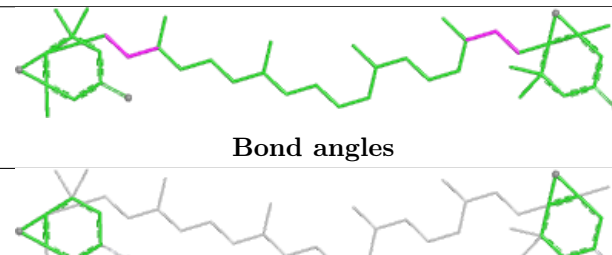
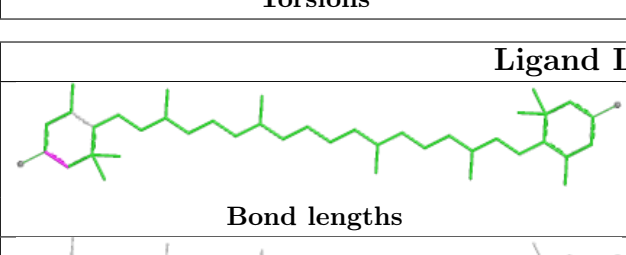
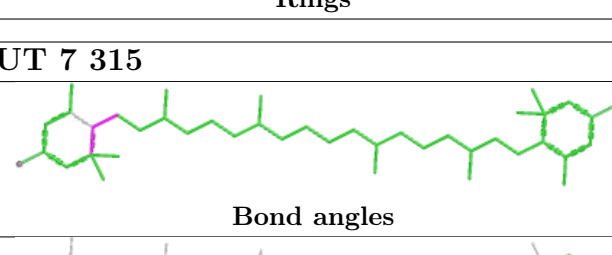


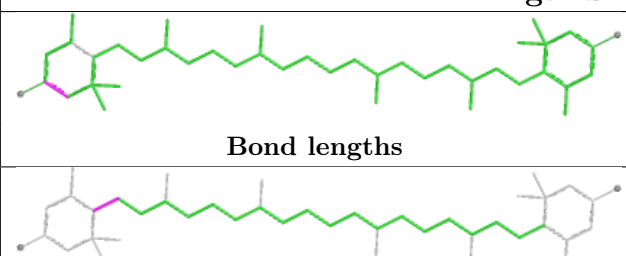
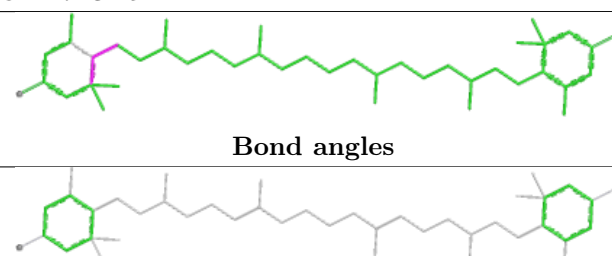
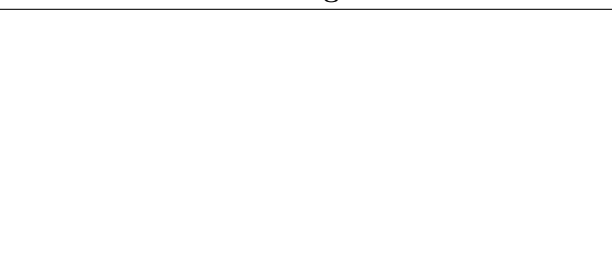
Ligand CLA 1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

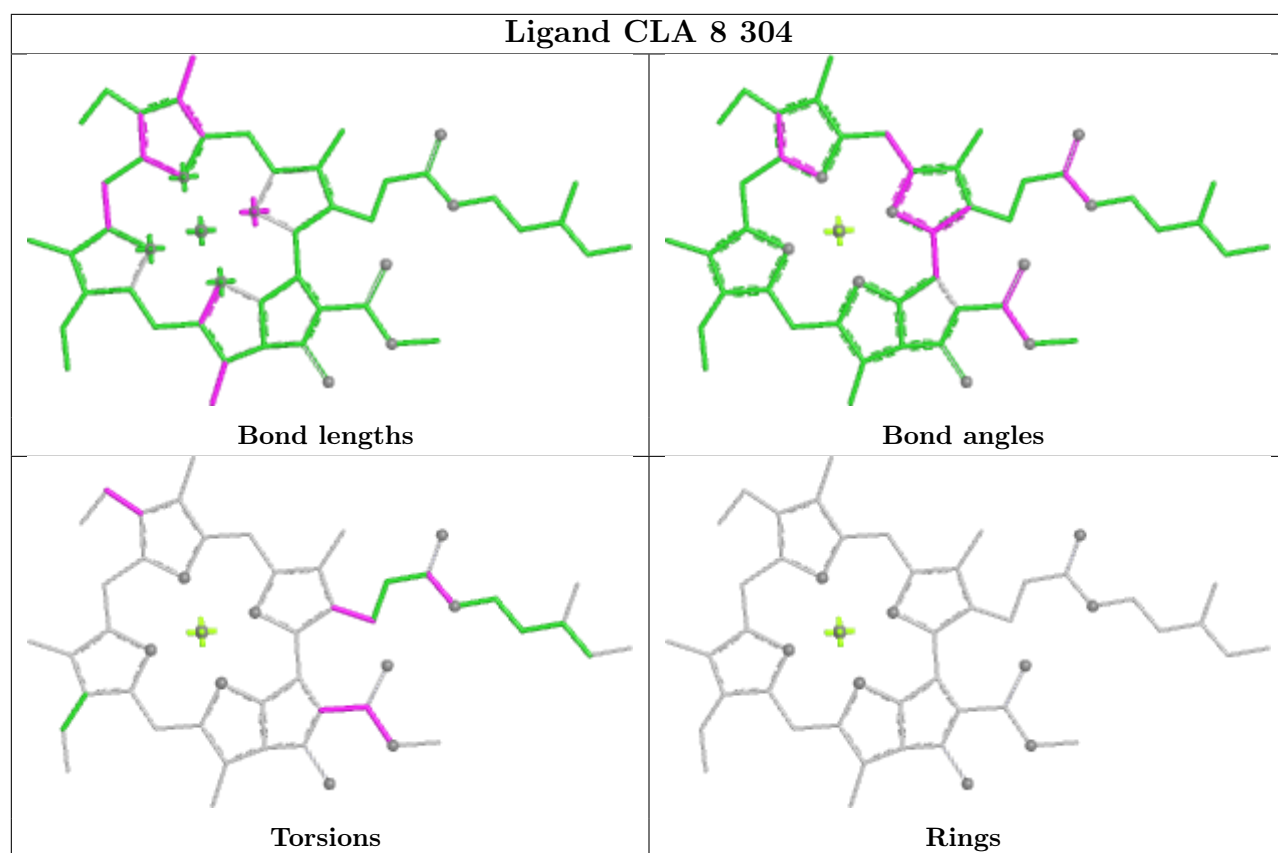
Ligand LUT b 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

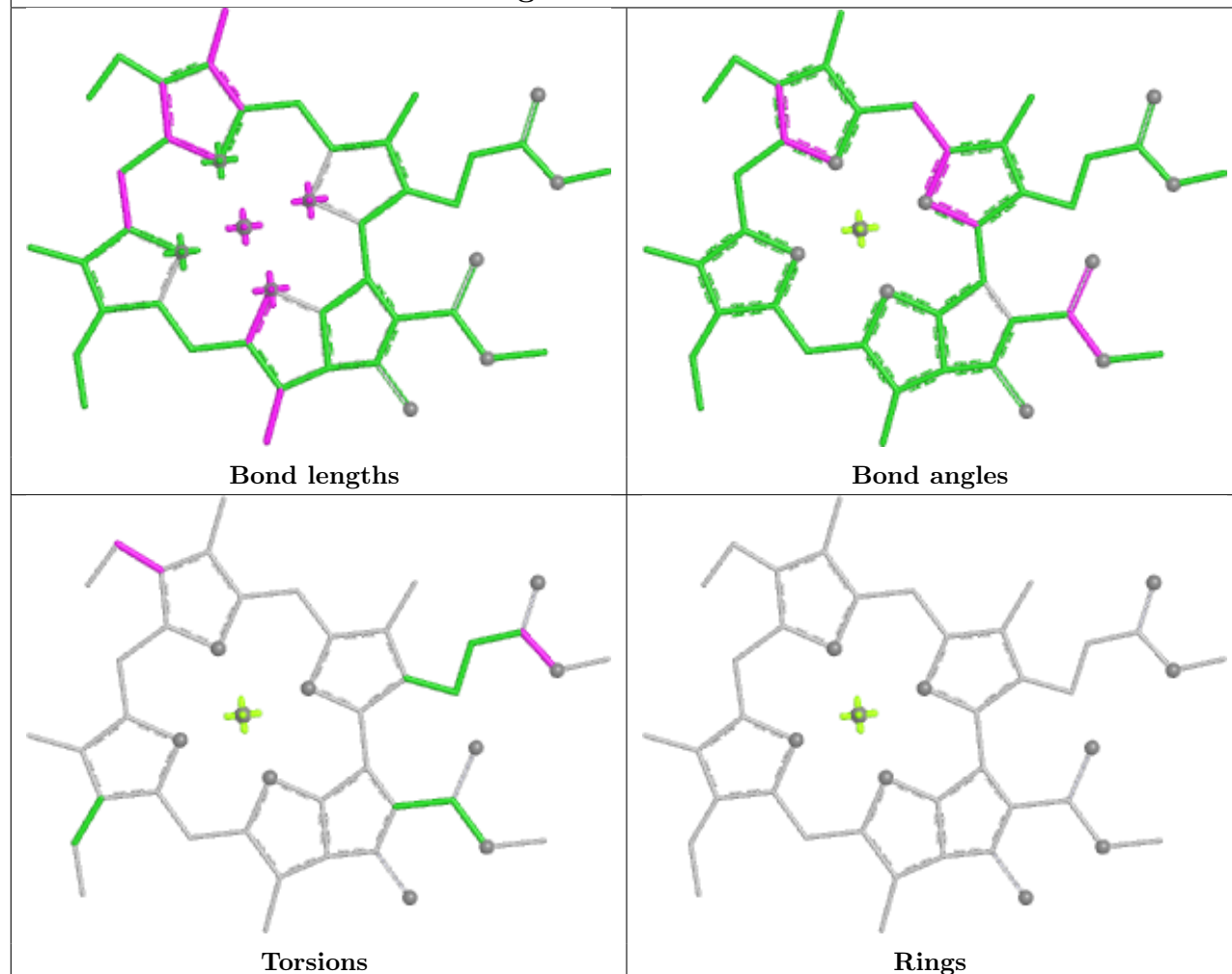
Ligand CLA B 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 3 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

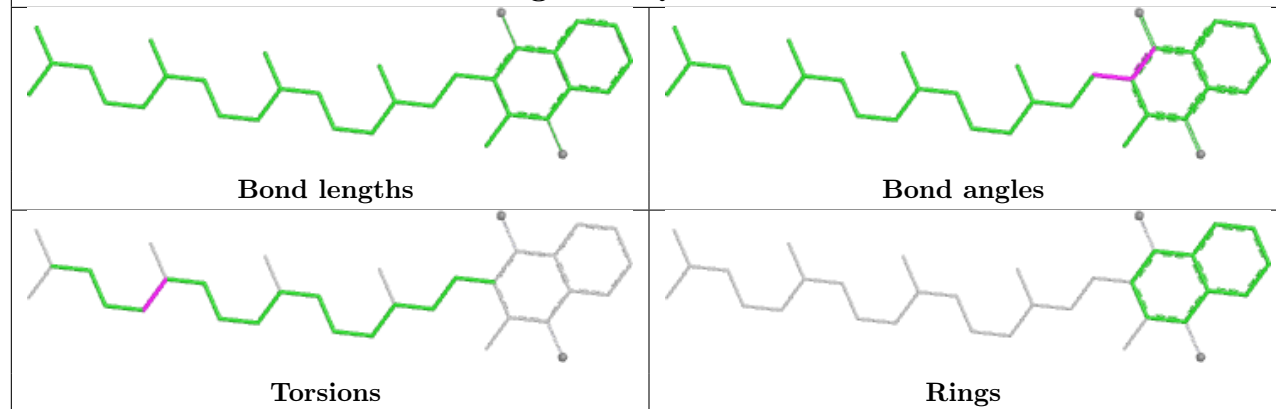
Ligand LUT 7 315	
	
Bond lengths	Bond angles
	
Torsions	Rings



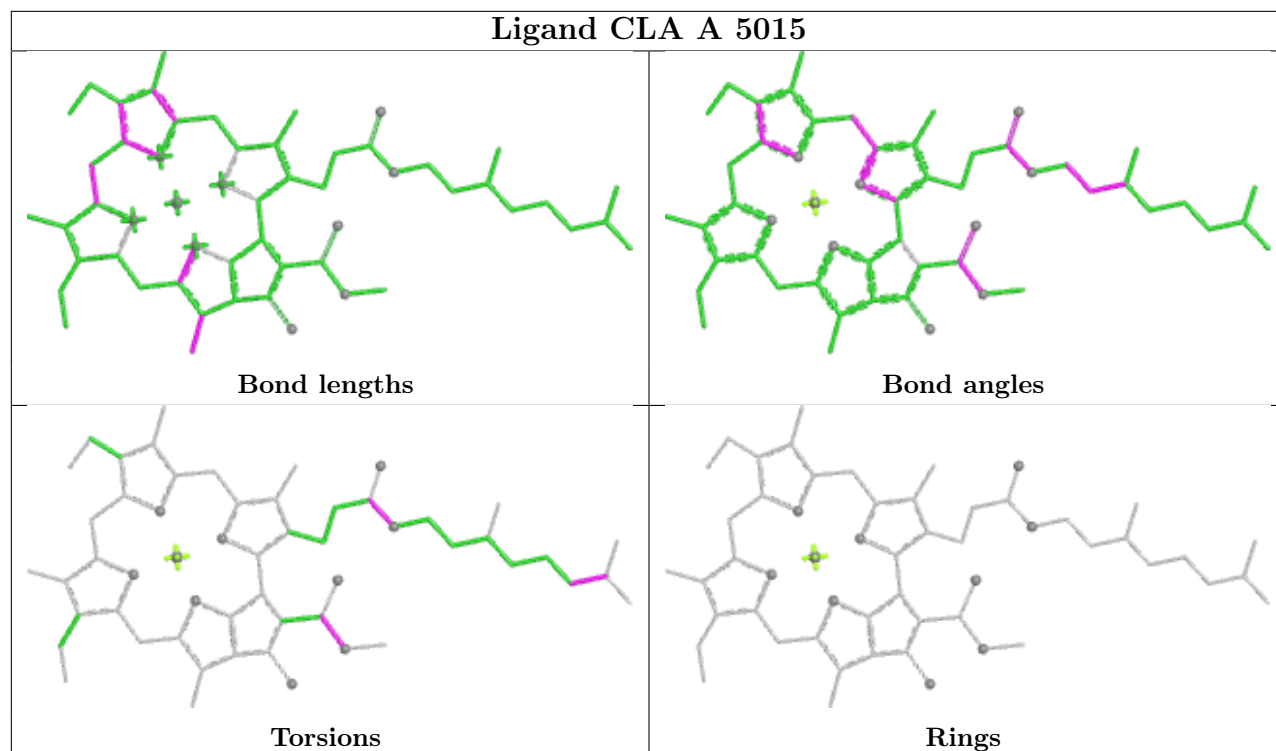
Ligand CLA a 607



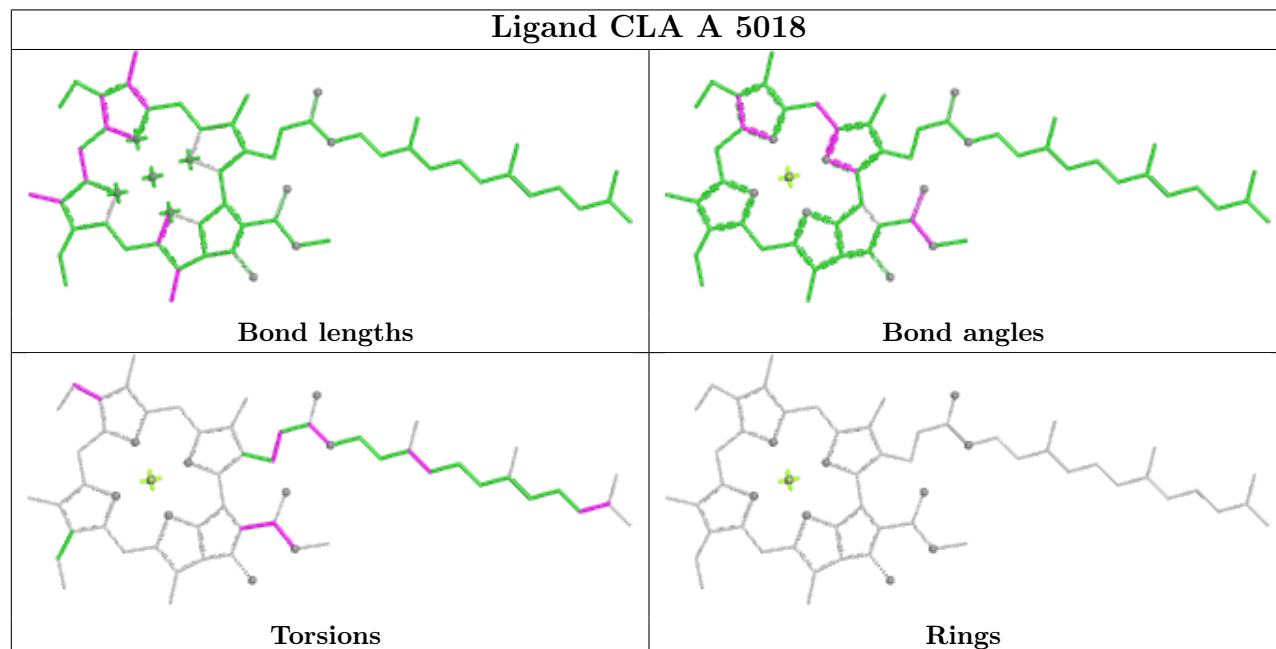
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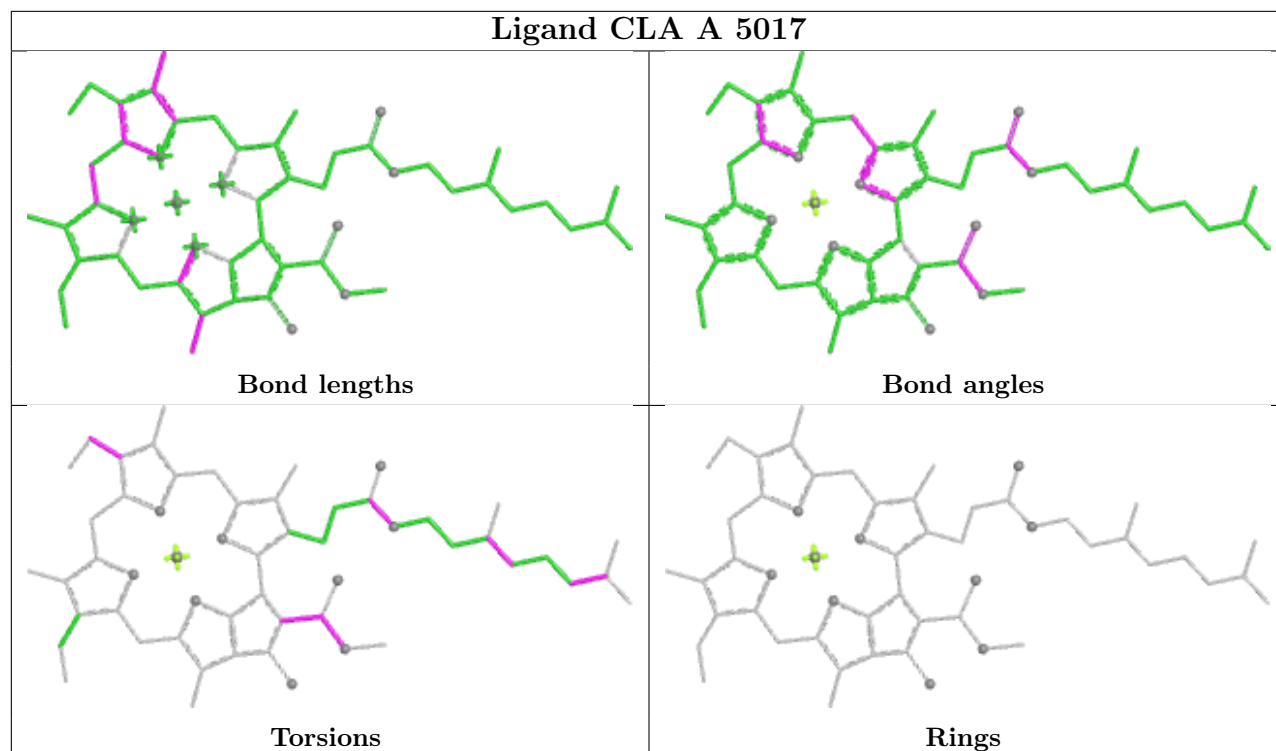
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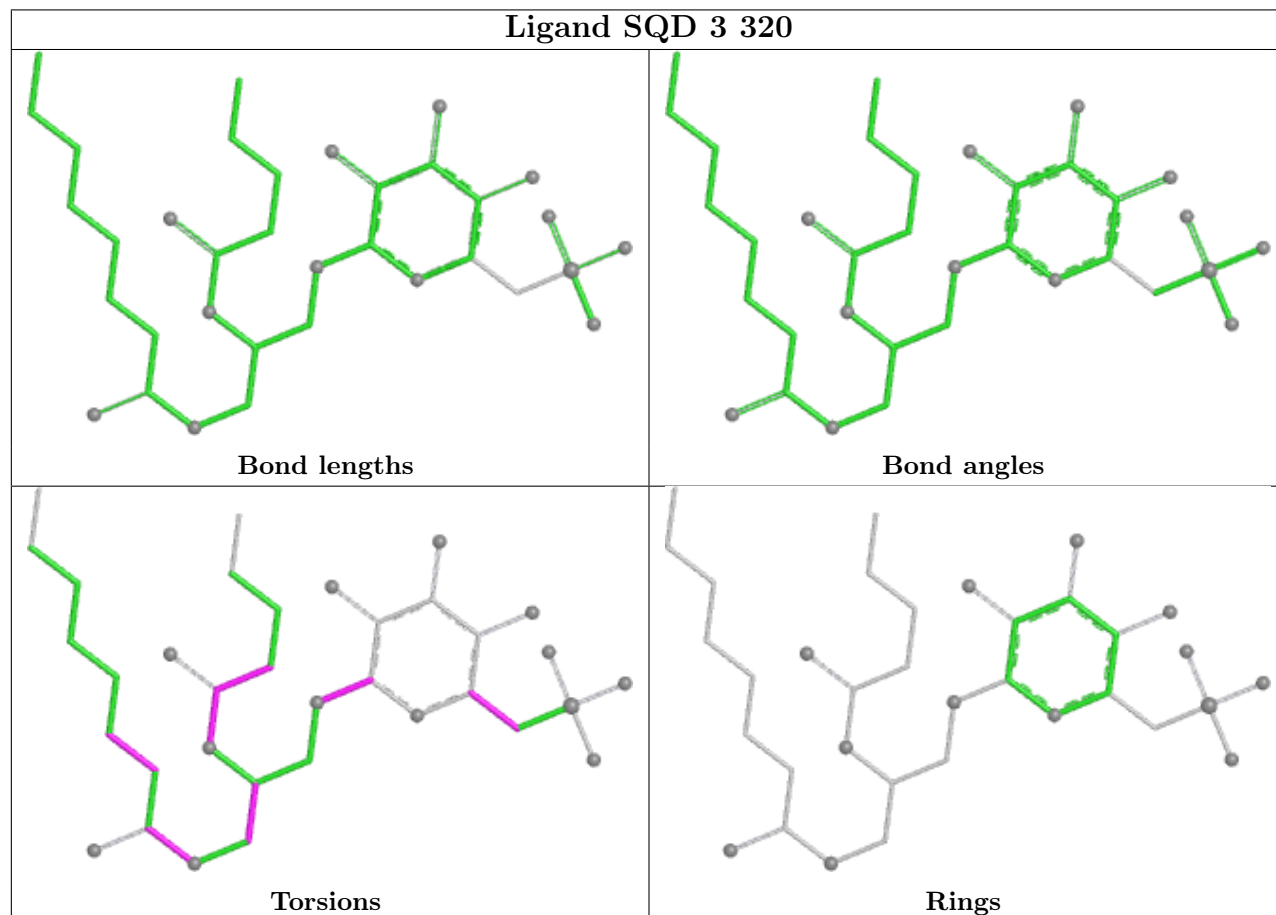
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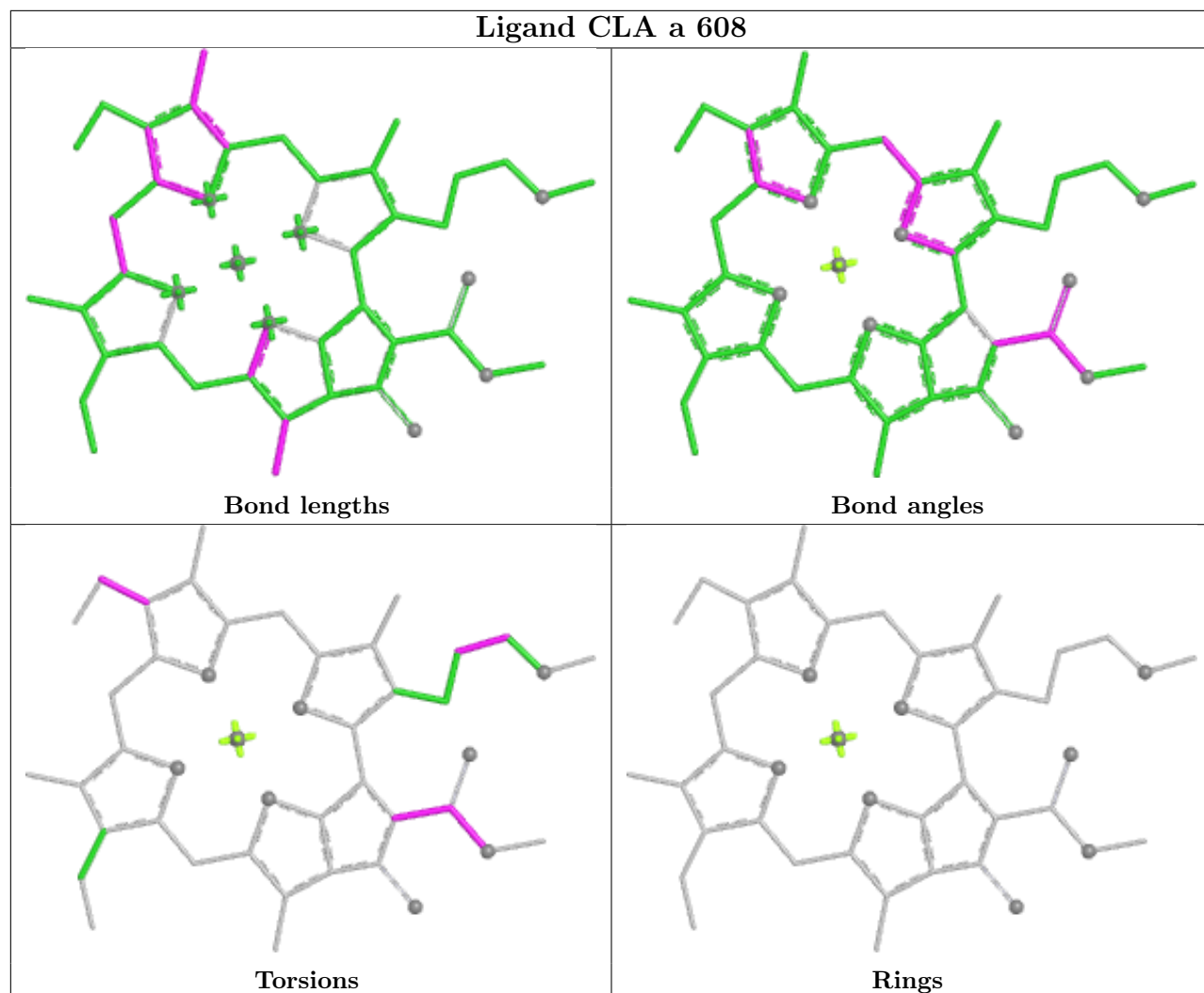
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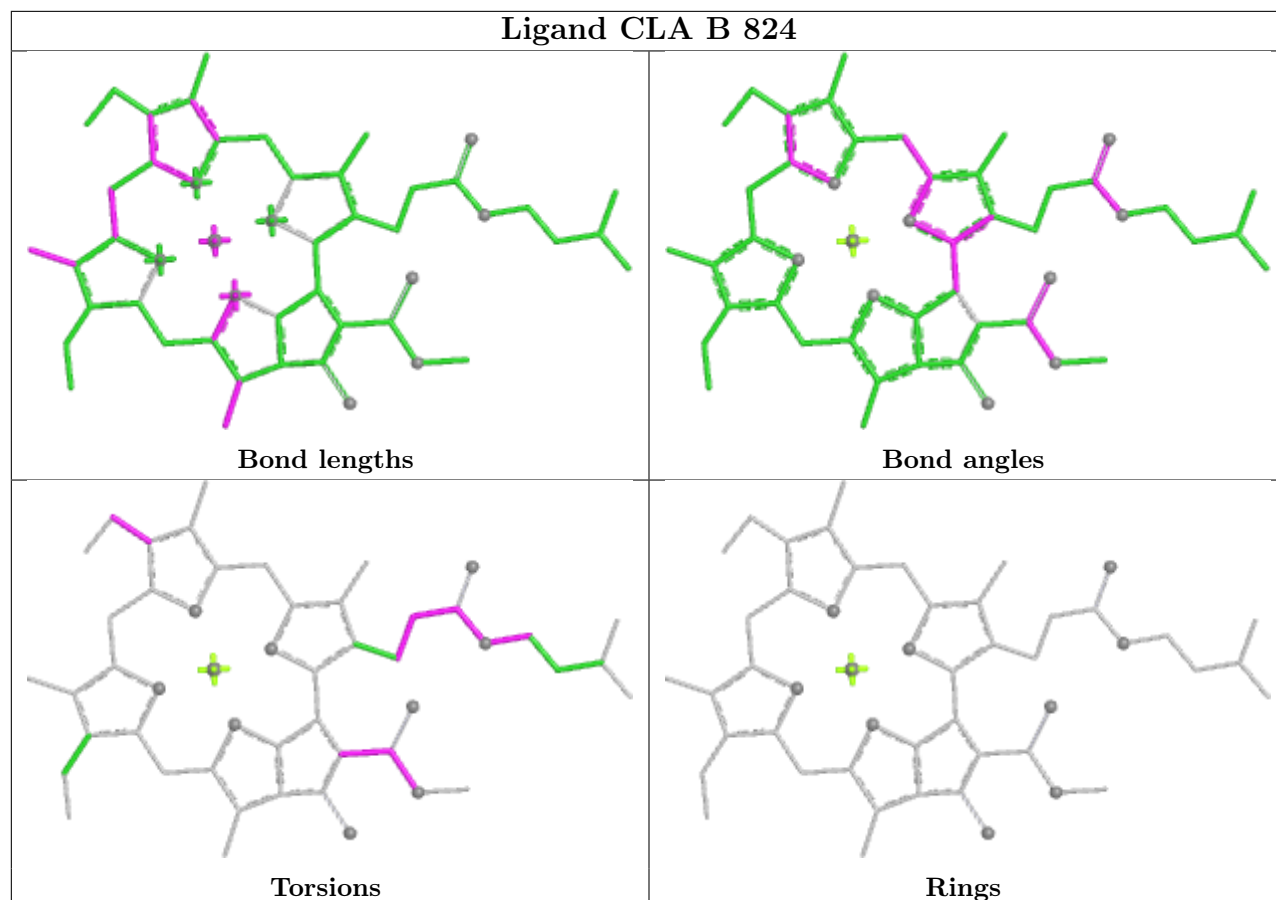
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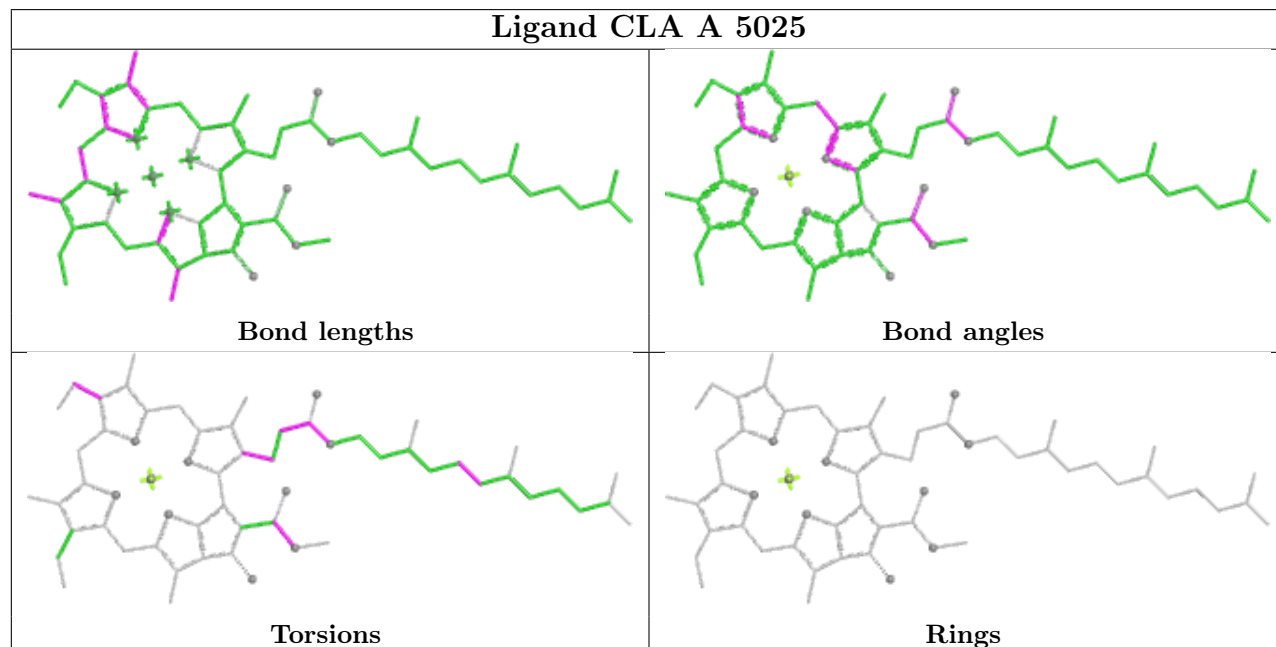
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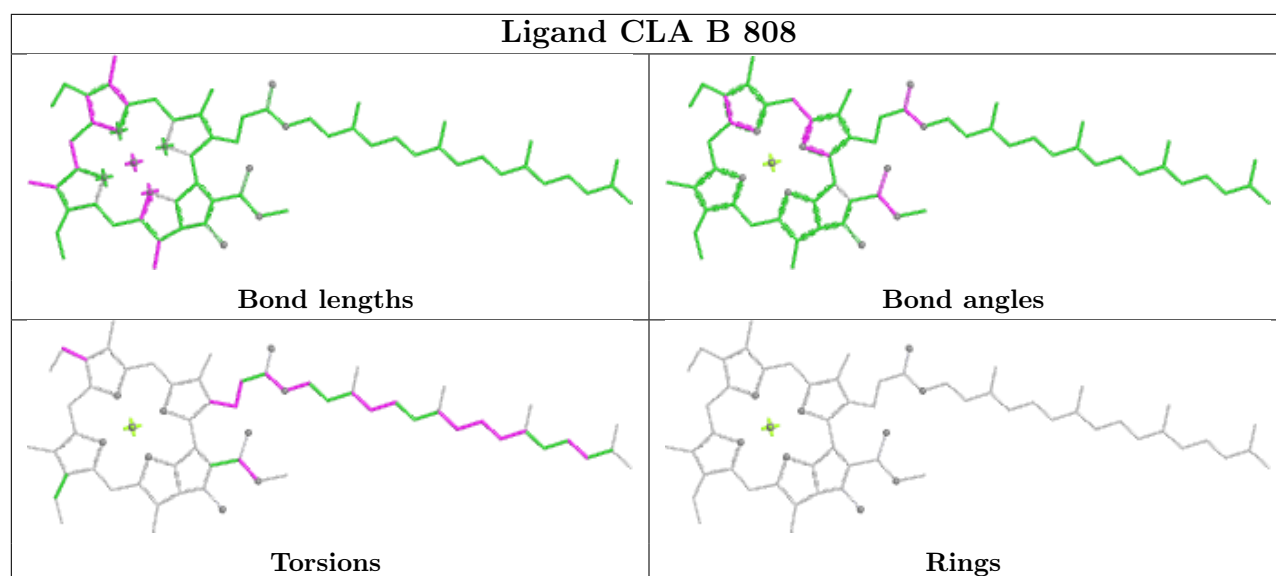
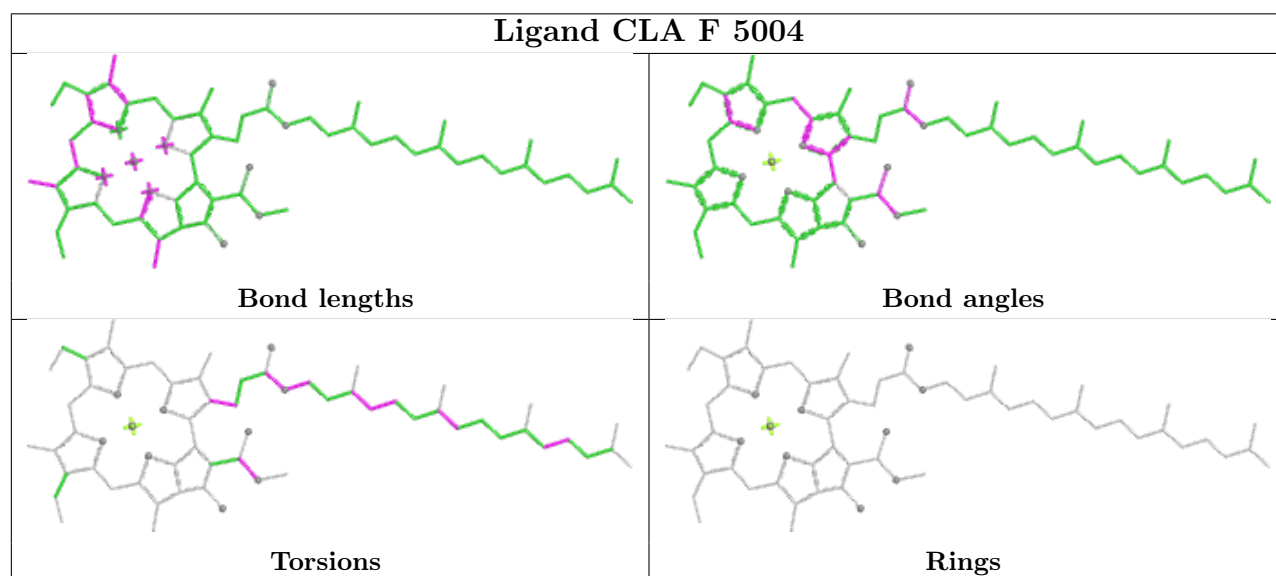
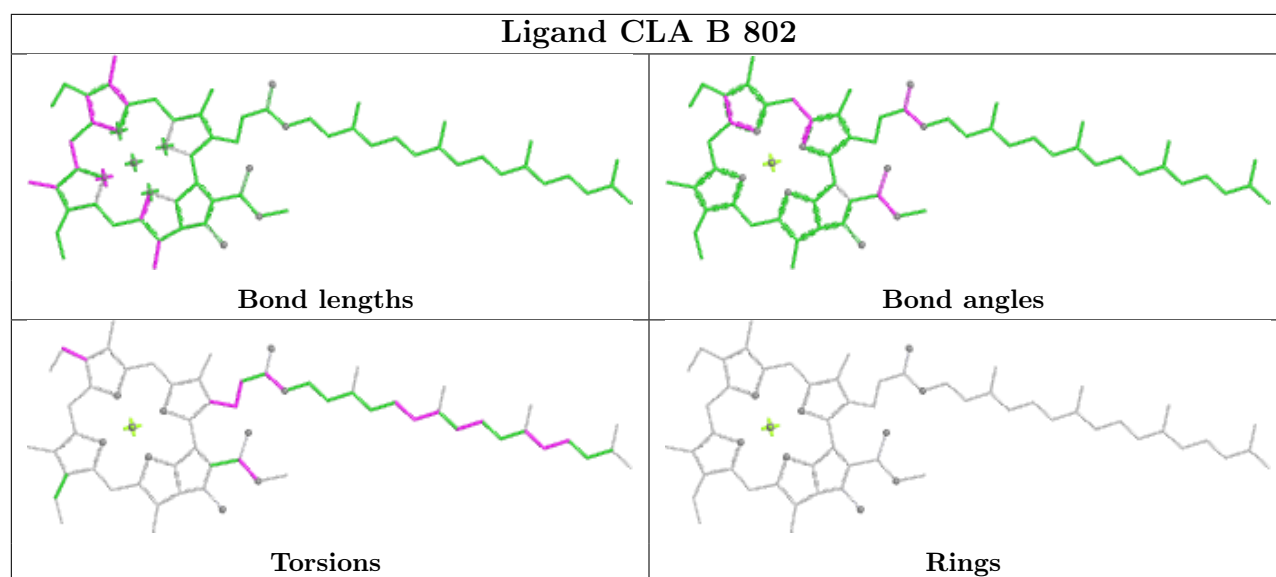


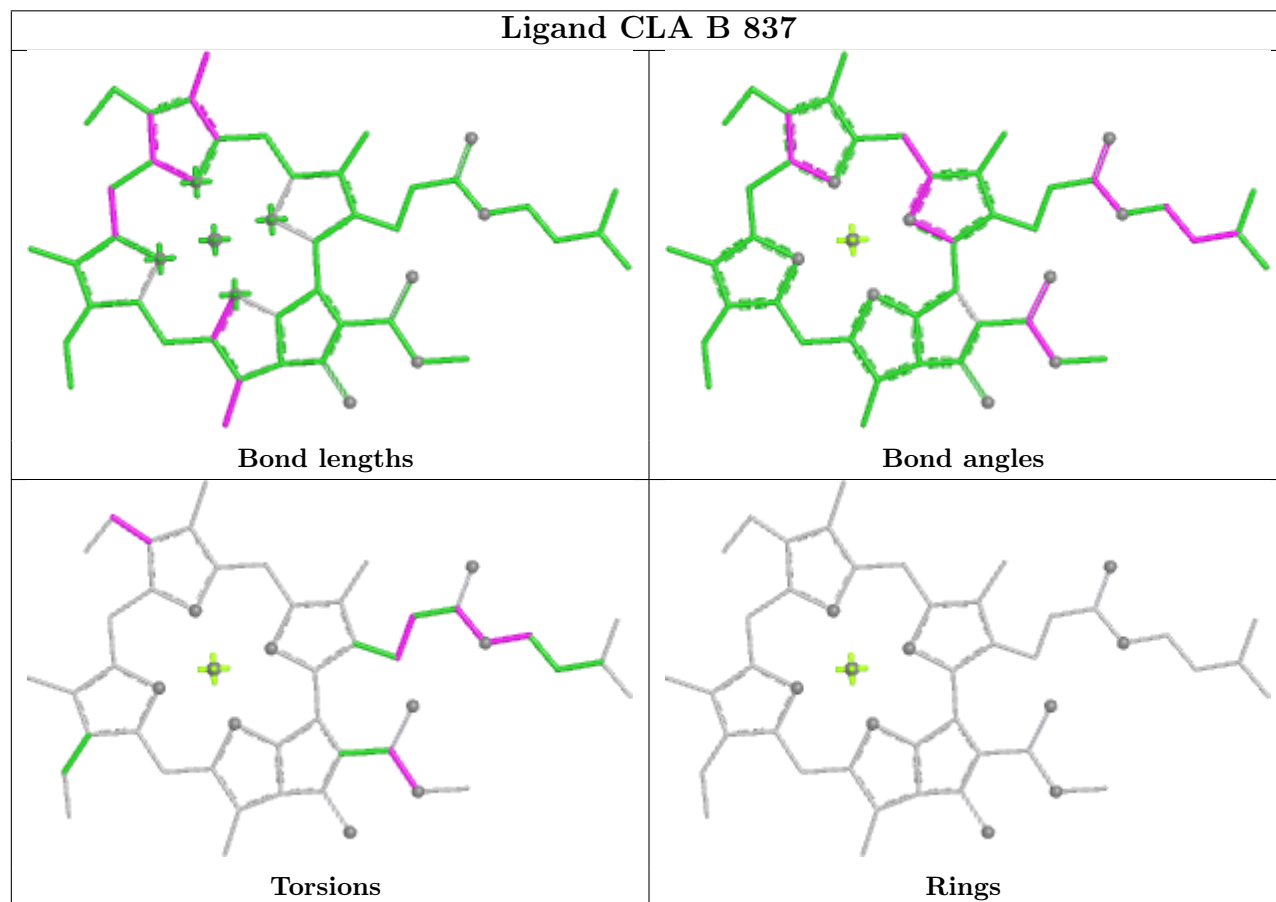
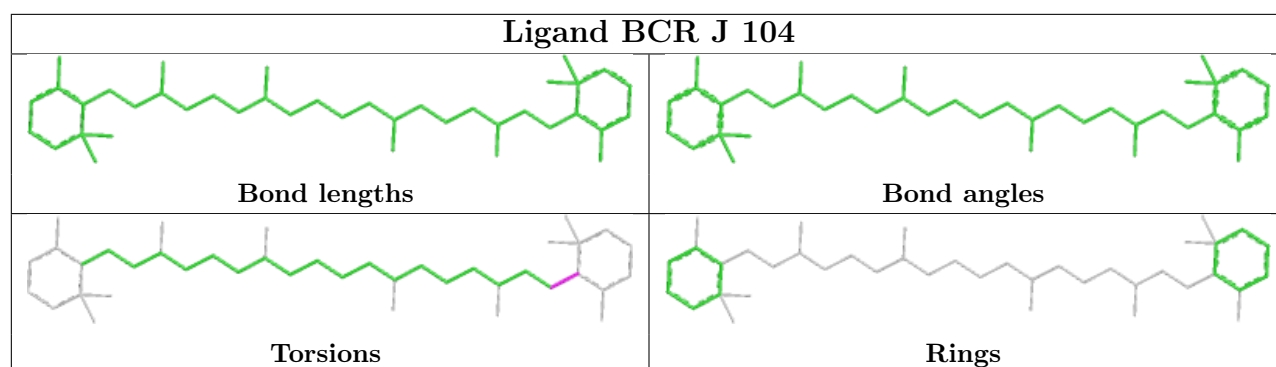
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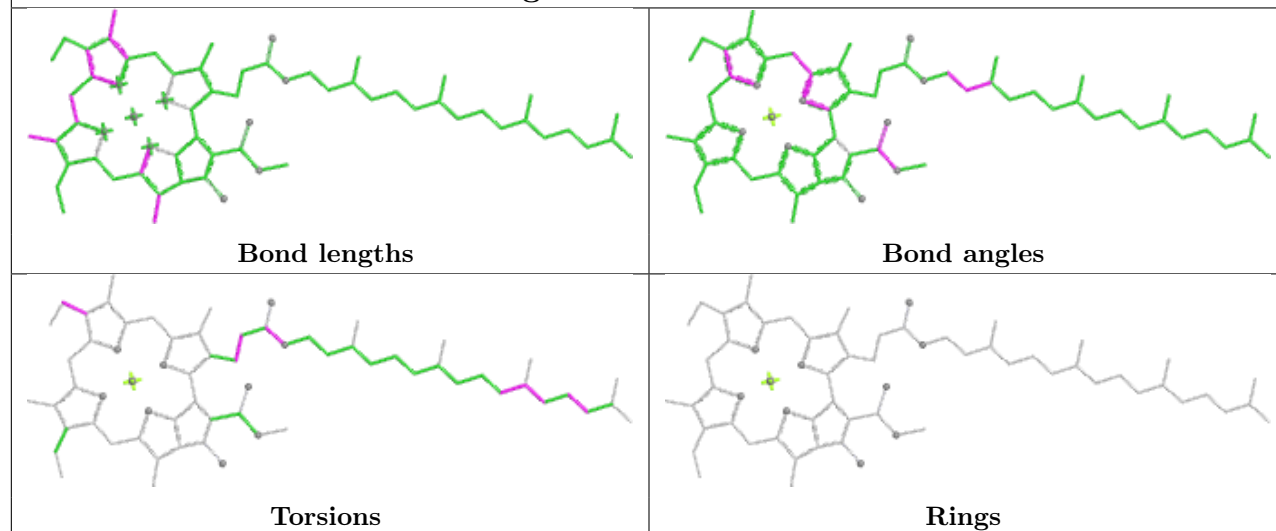
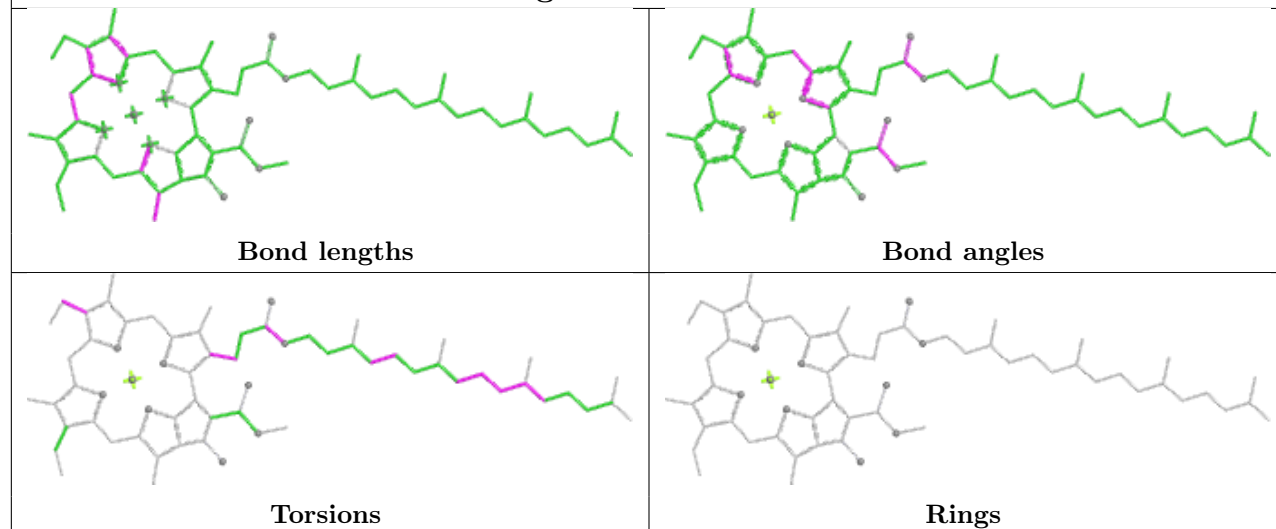


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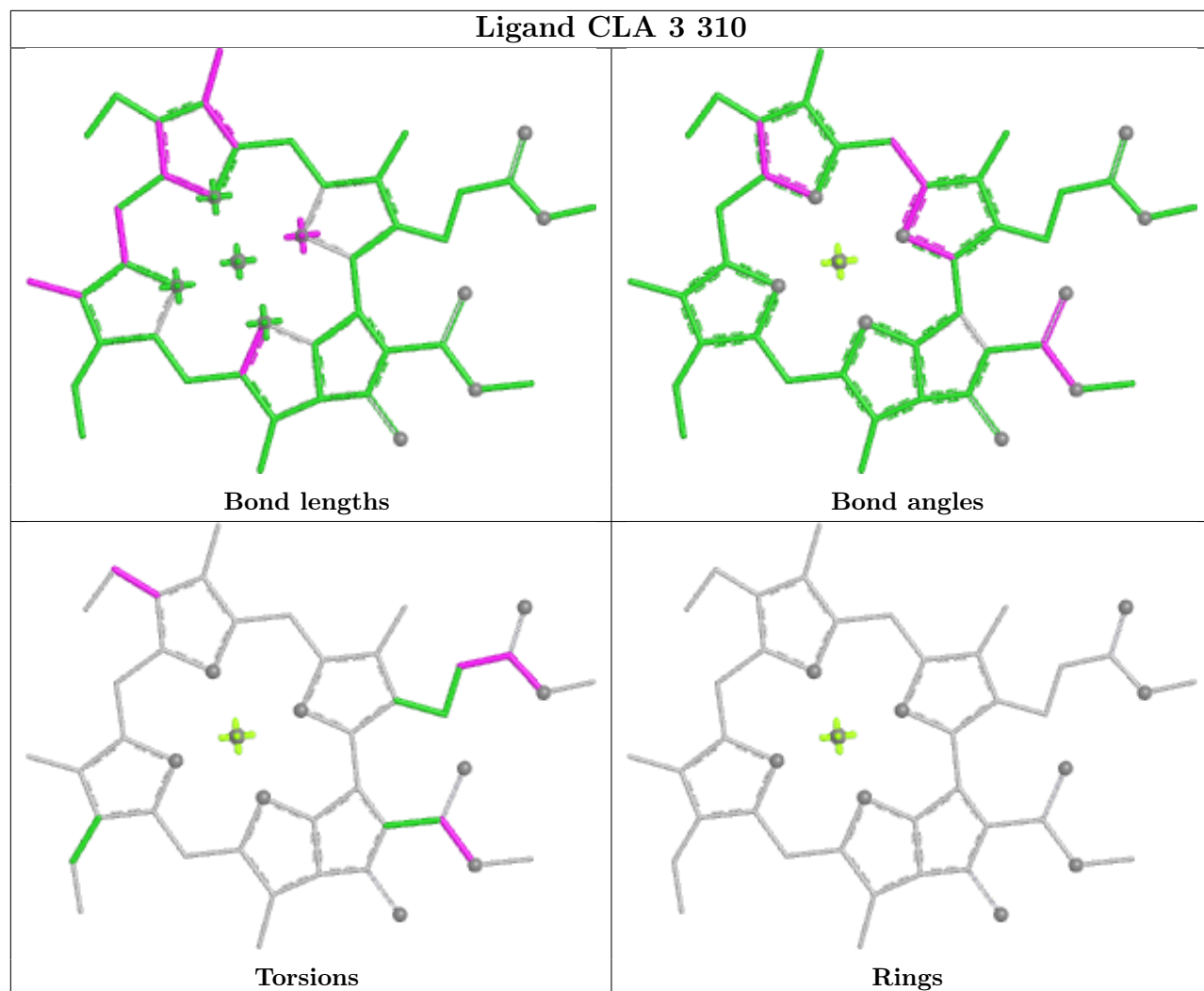


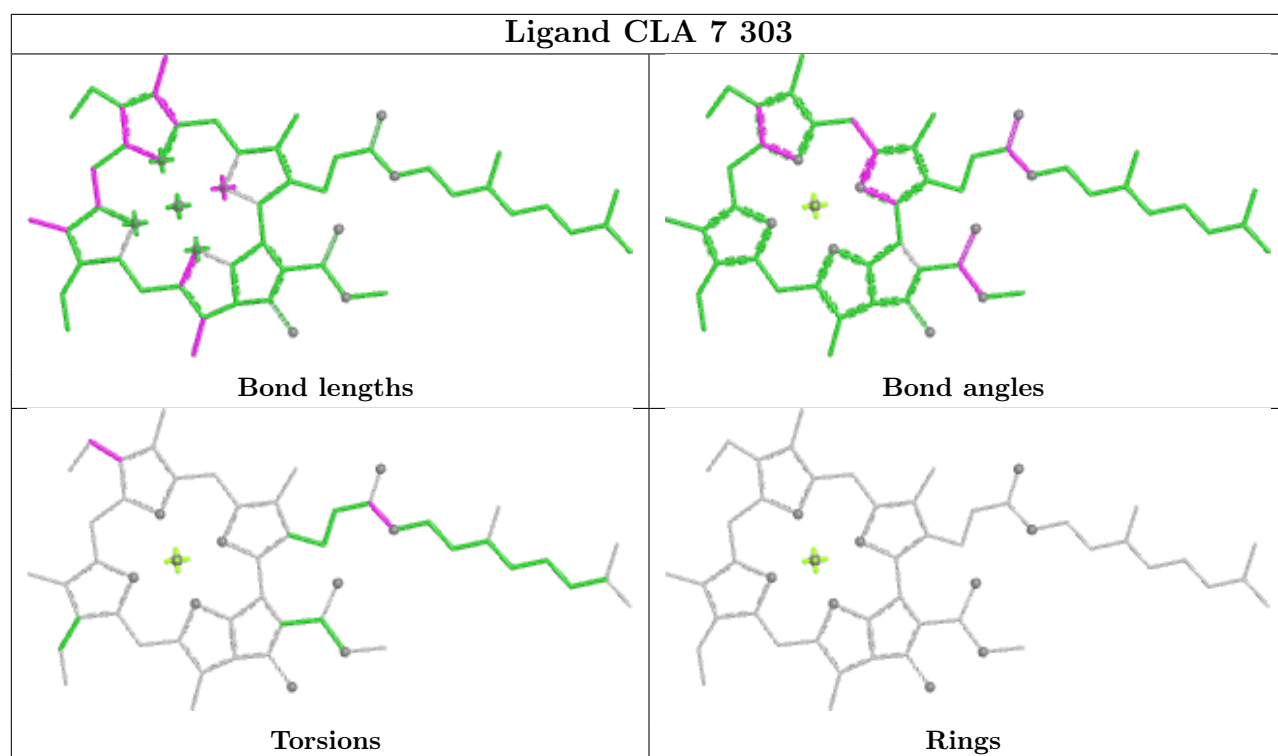




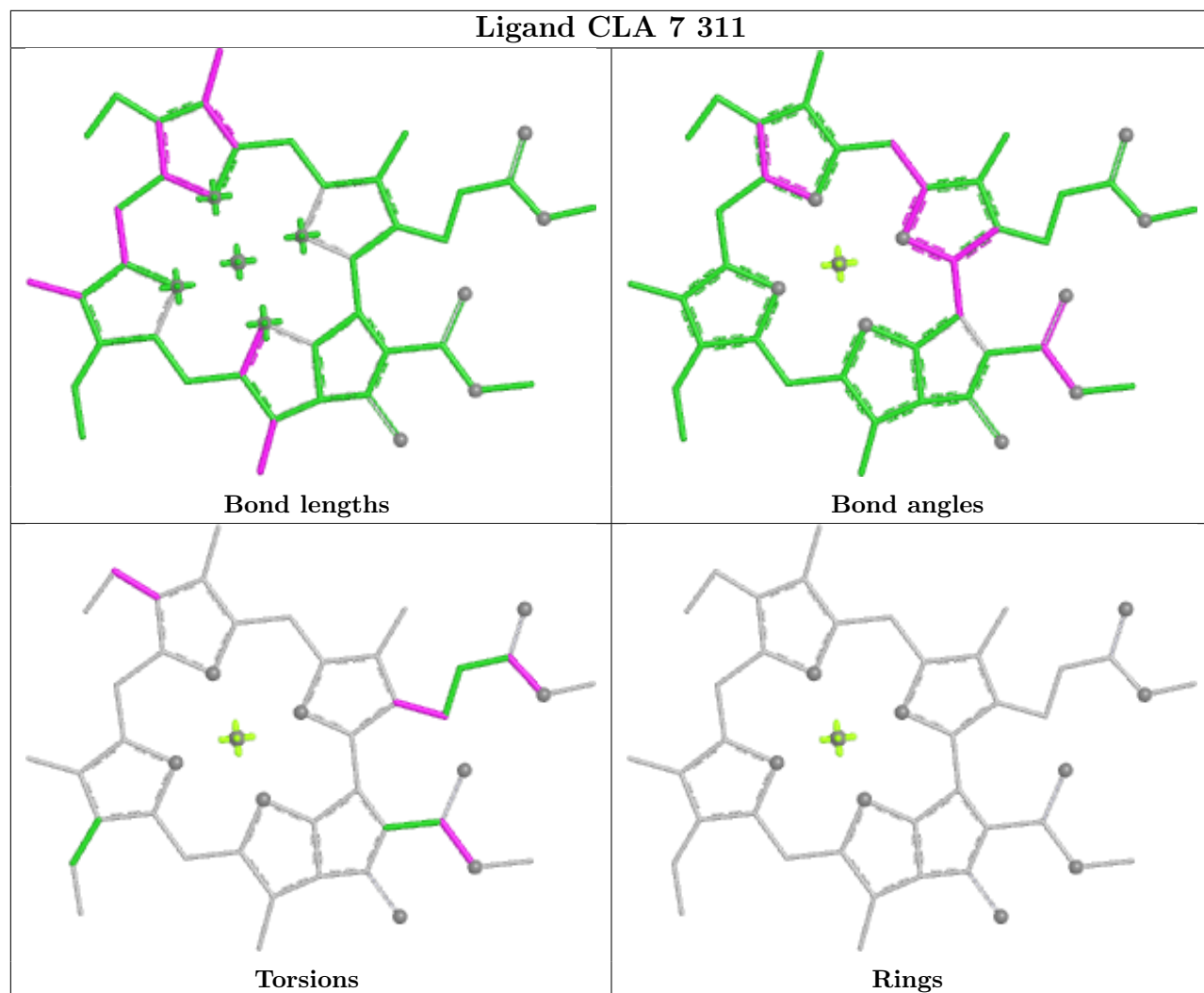
Ligand CLA A 5030**Ligand CLA 1 607**

Ligand CLA 3 310

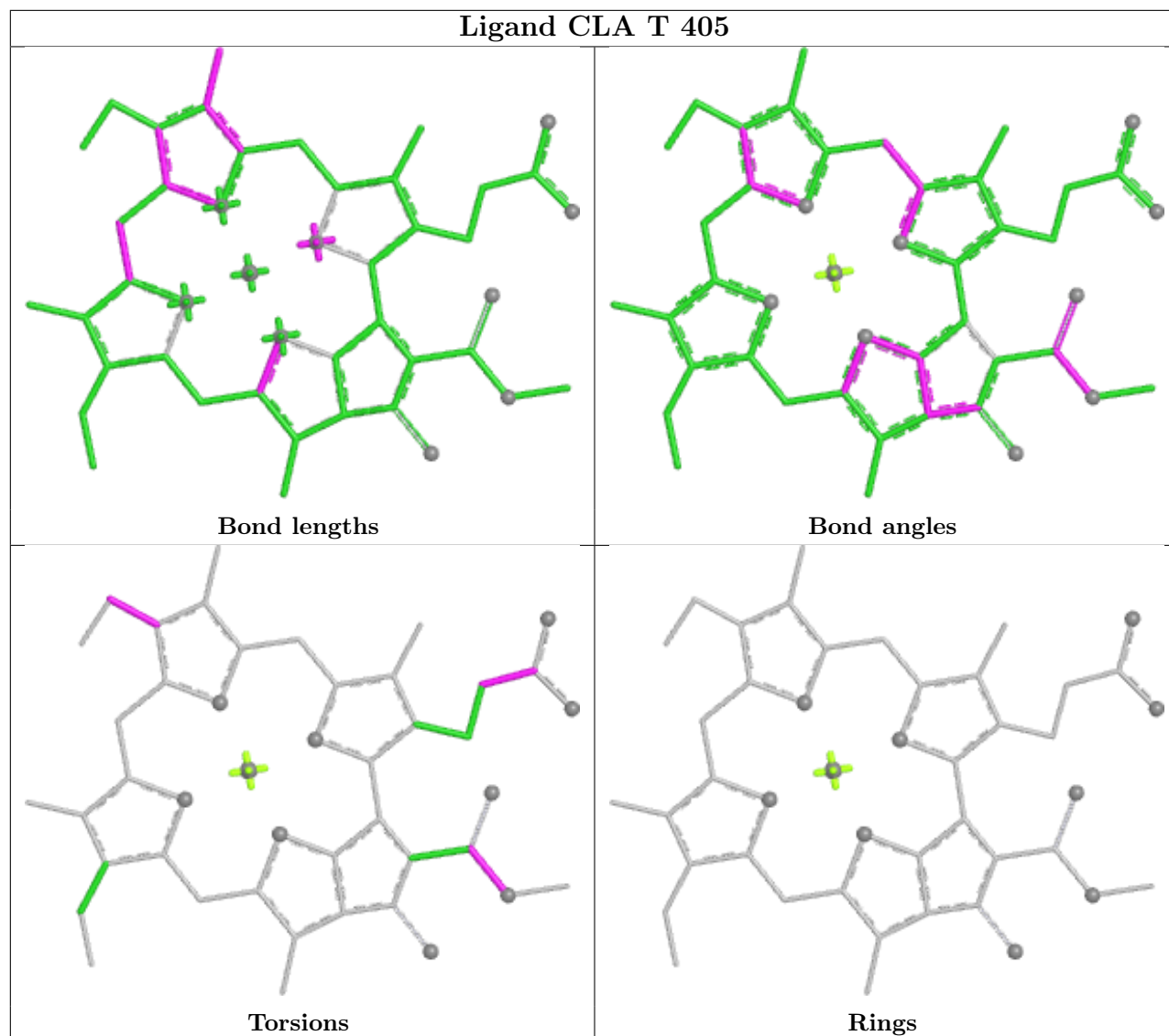




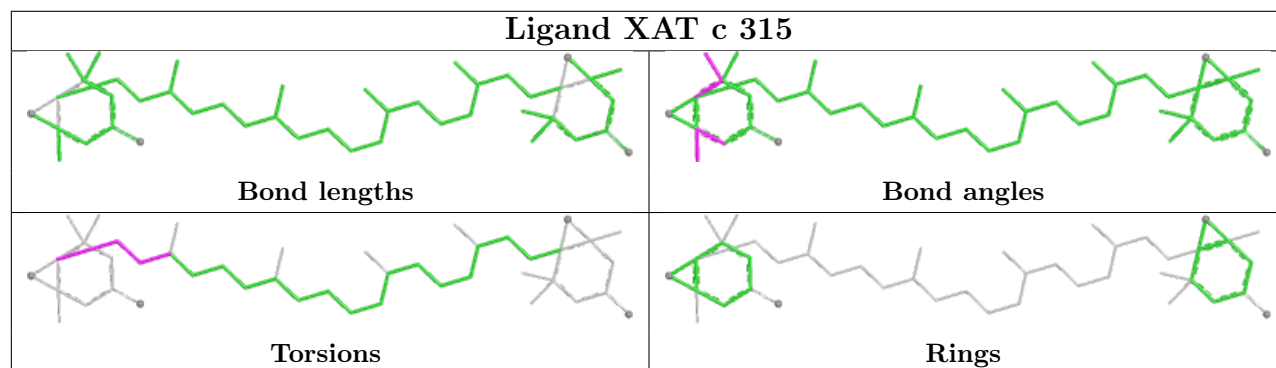
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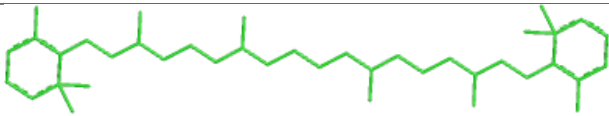
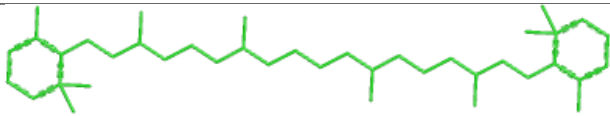
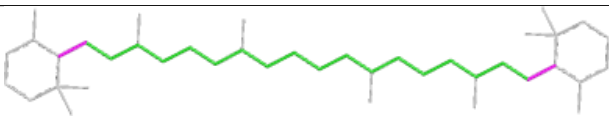
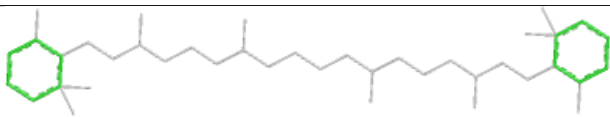


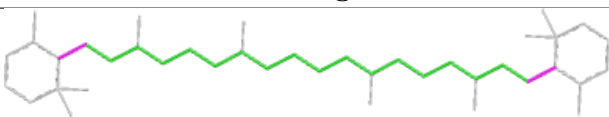
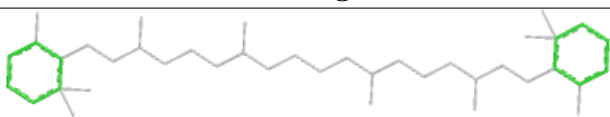
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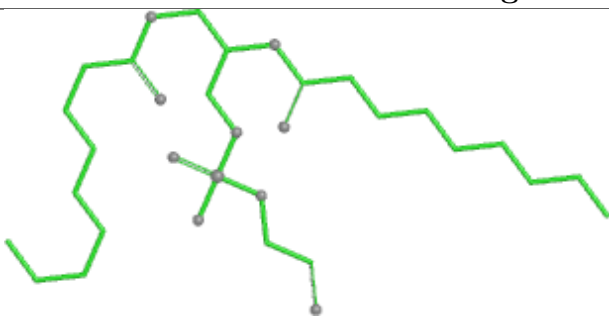
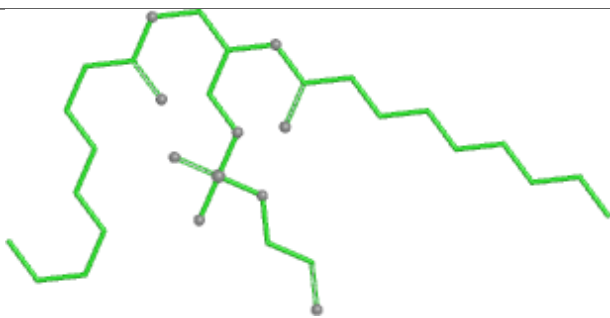
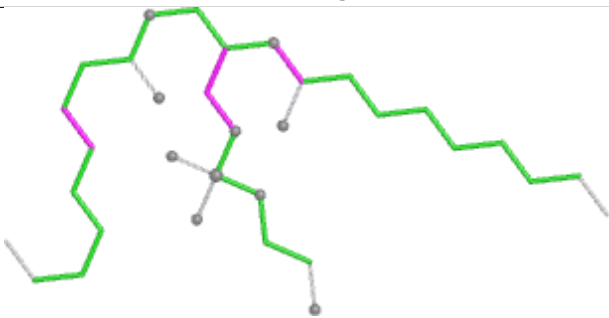
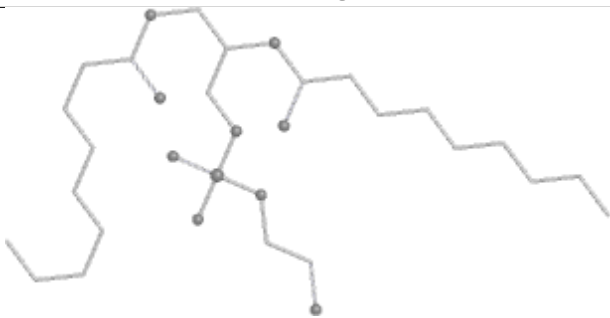


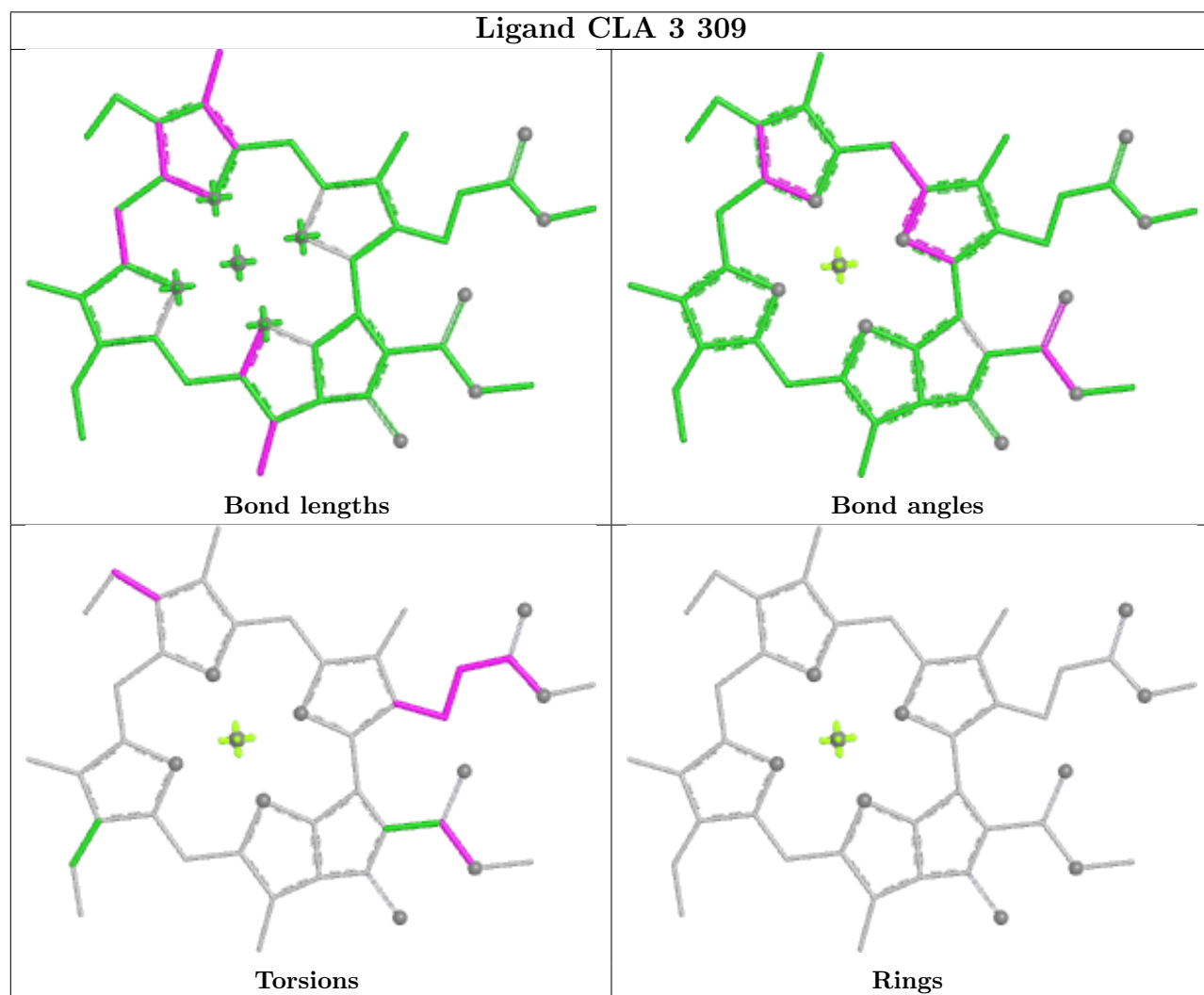
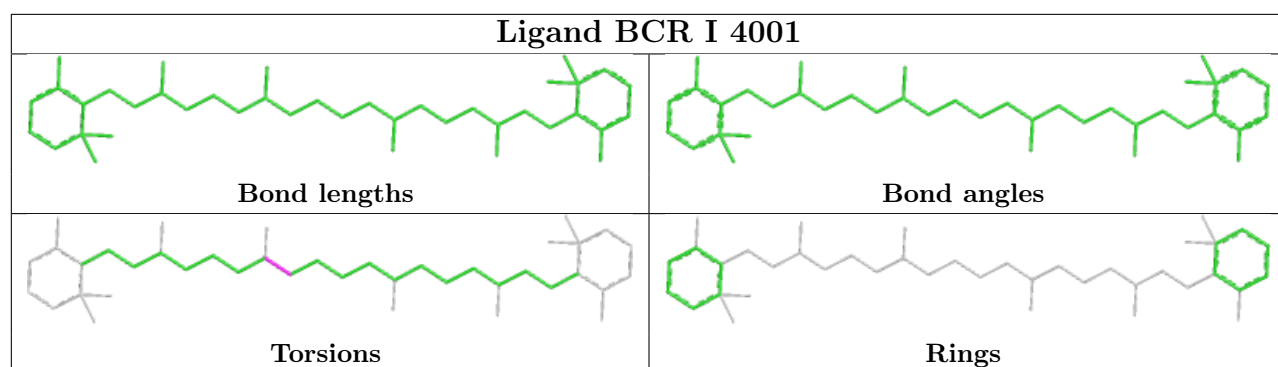
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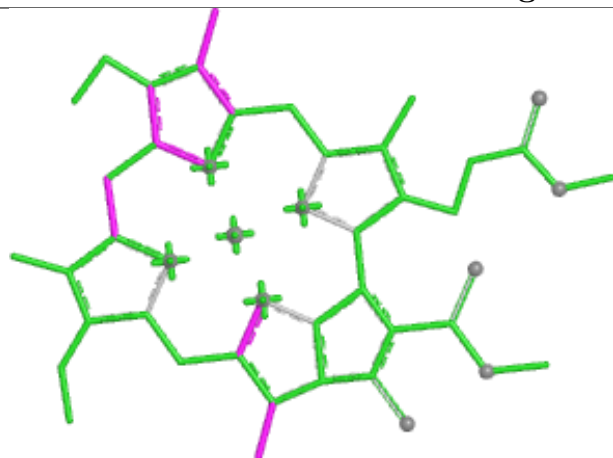
Ligand BCR b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 3 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

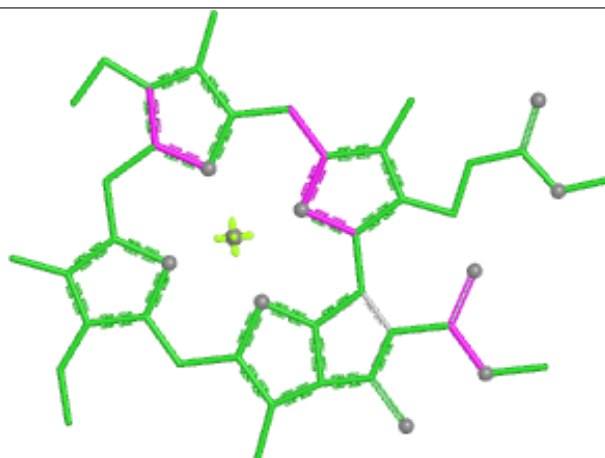
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Bond lengths	Bond angles
	
Torsions	Rings



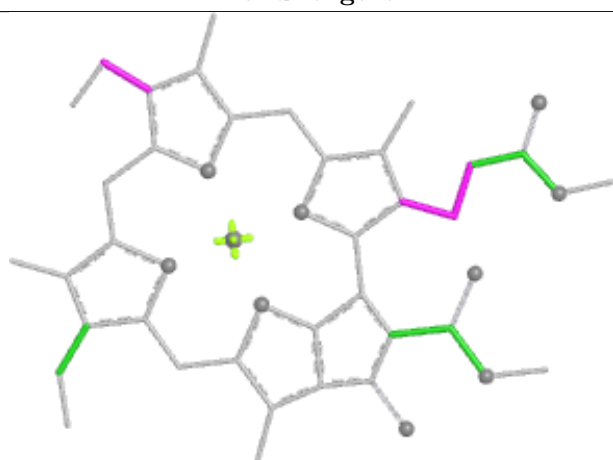
Ligand CLA 8 309



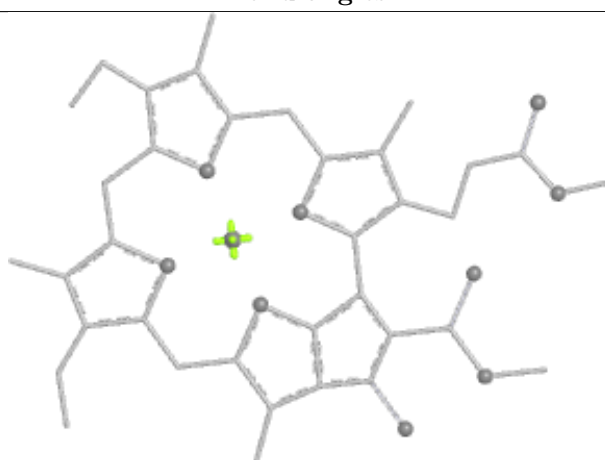
Bond lengths



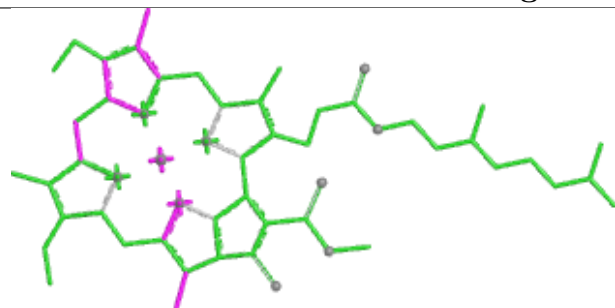
Bond angles



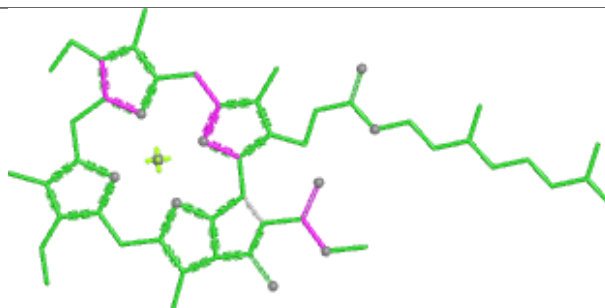
Torsions



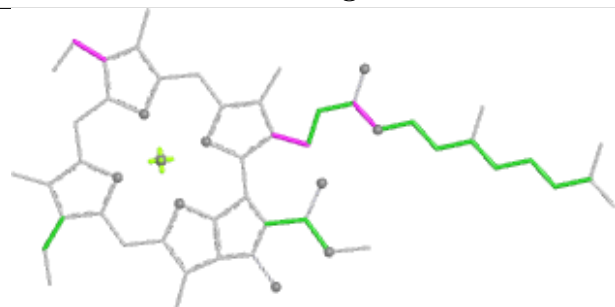
Rings

Ligand CLA 3 324

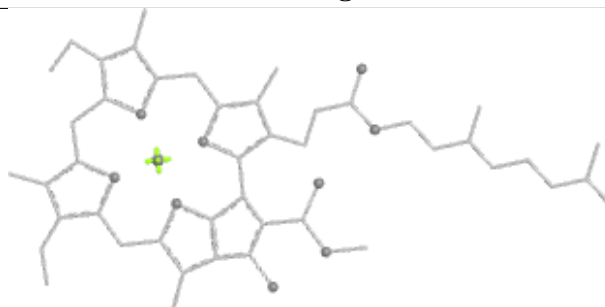
Bond lengths



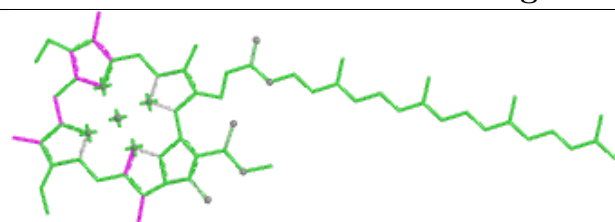
Bond angles



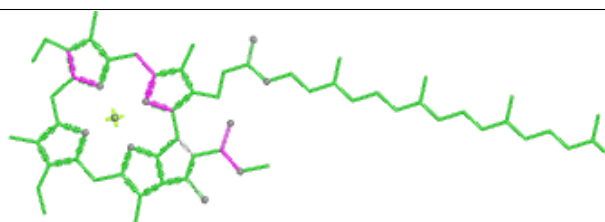
Torsions



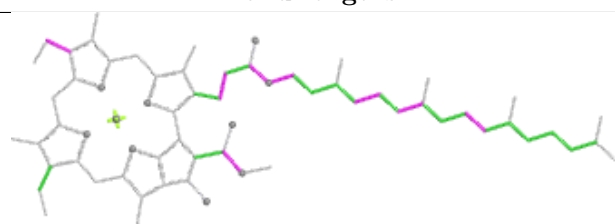
Rings

Ligand CLA 1 609

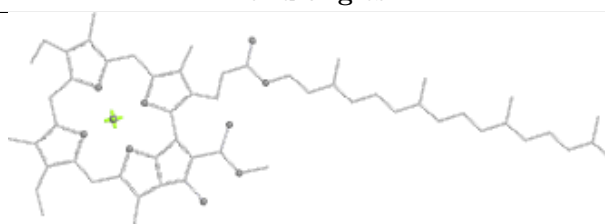
Bond lengths



Bond angles

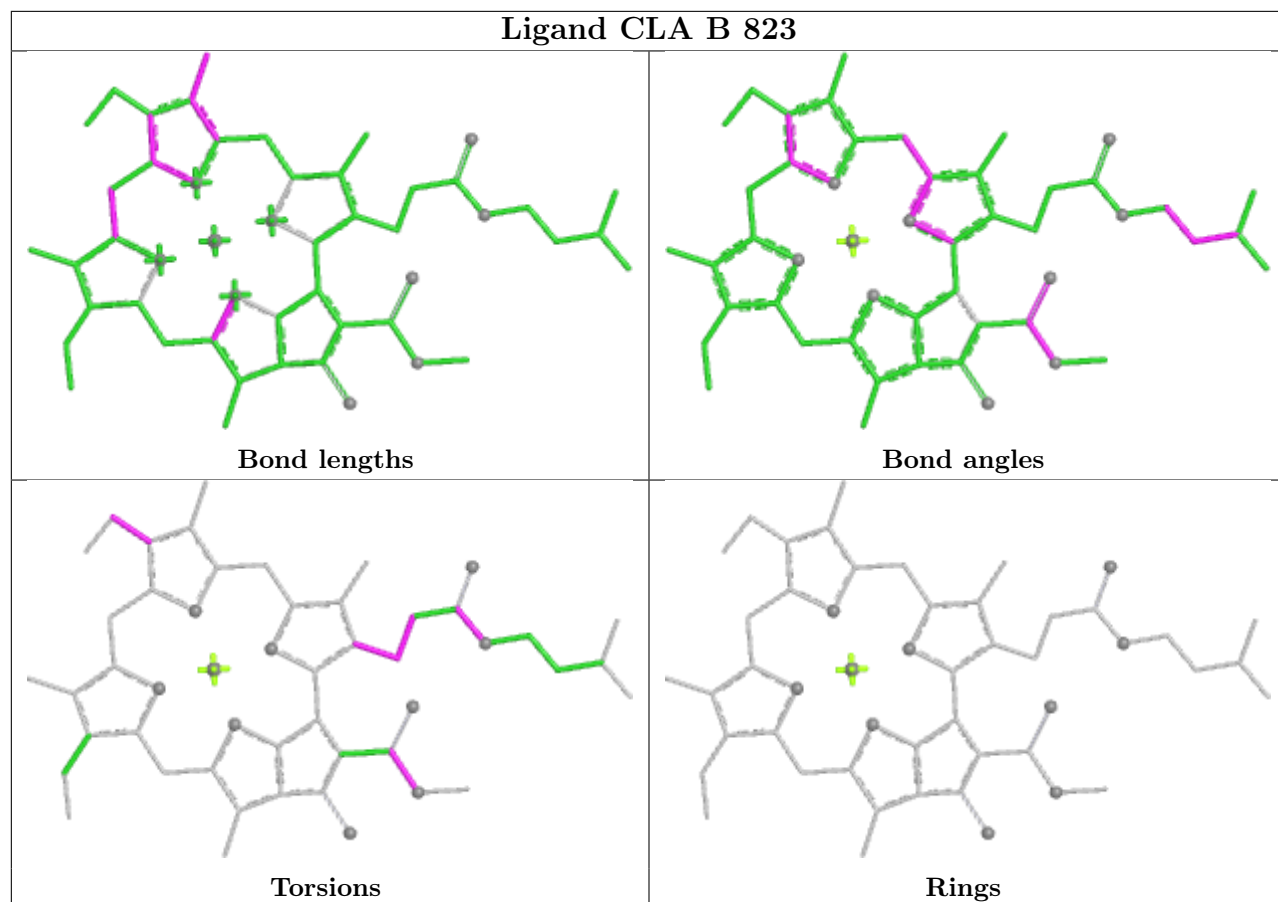


Torsions

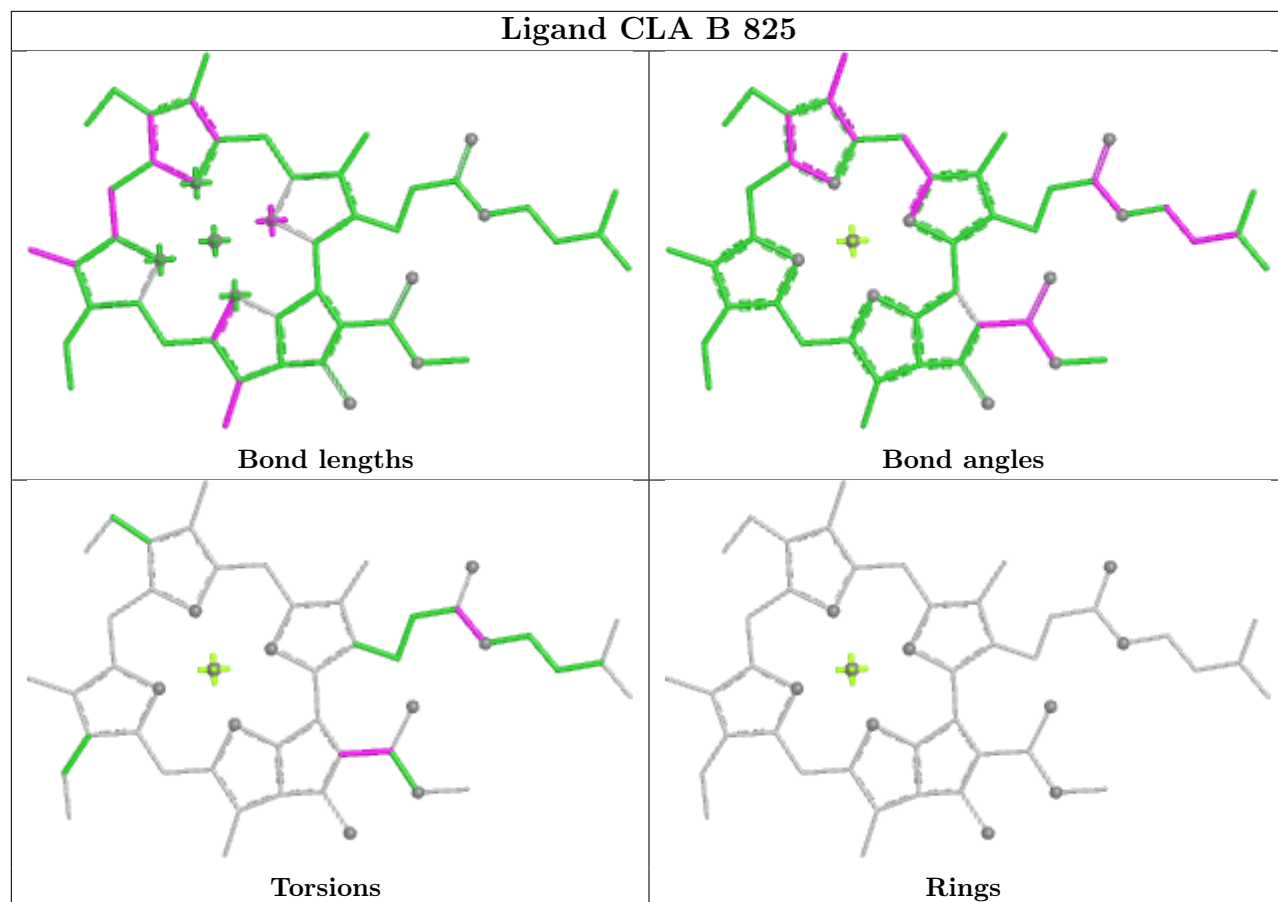


Rings

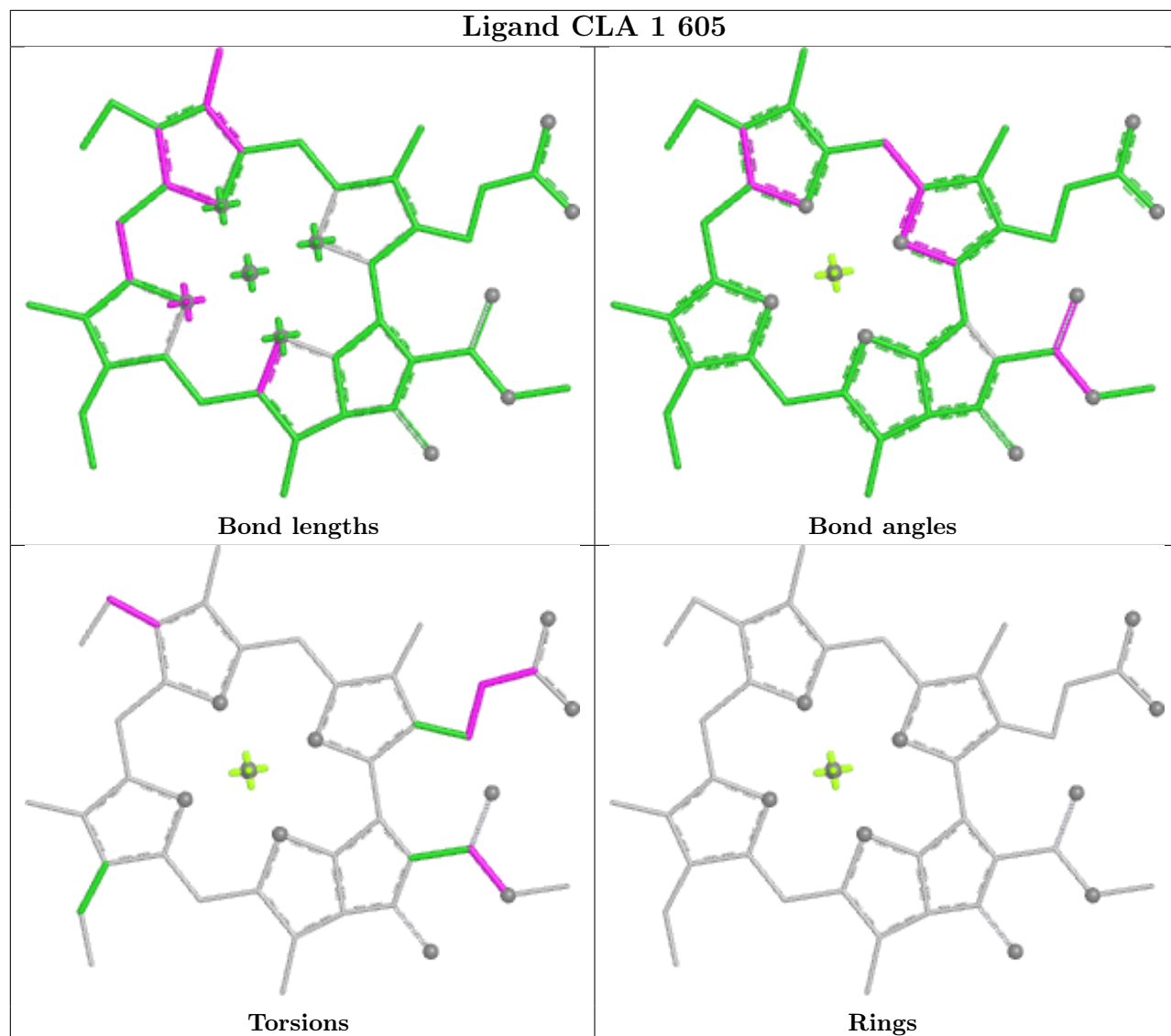
Ligand CLA B 823



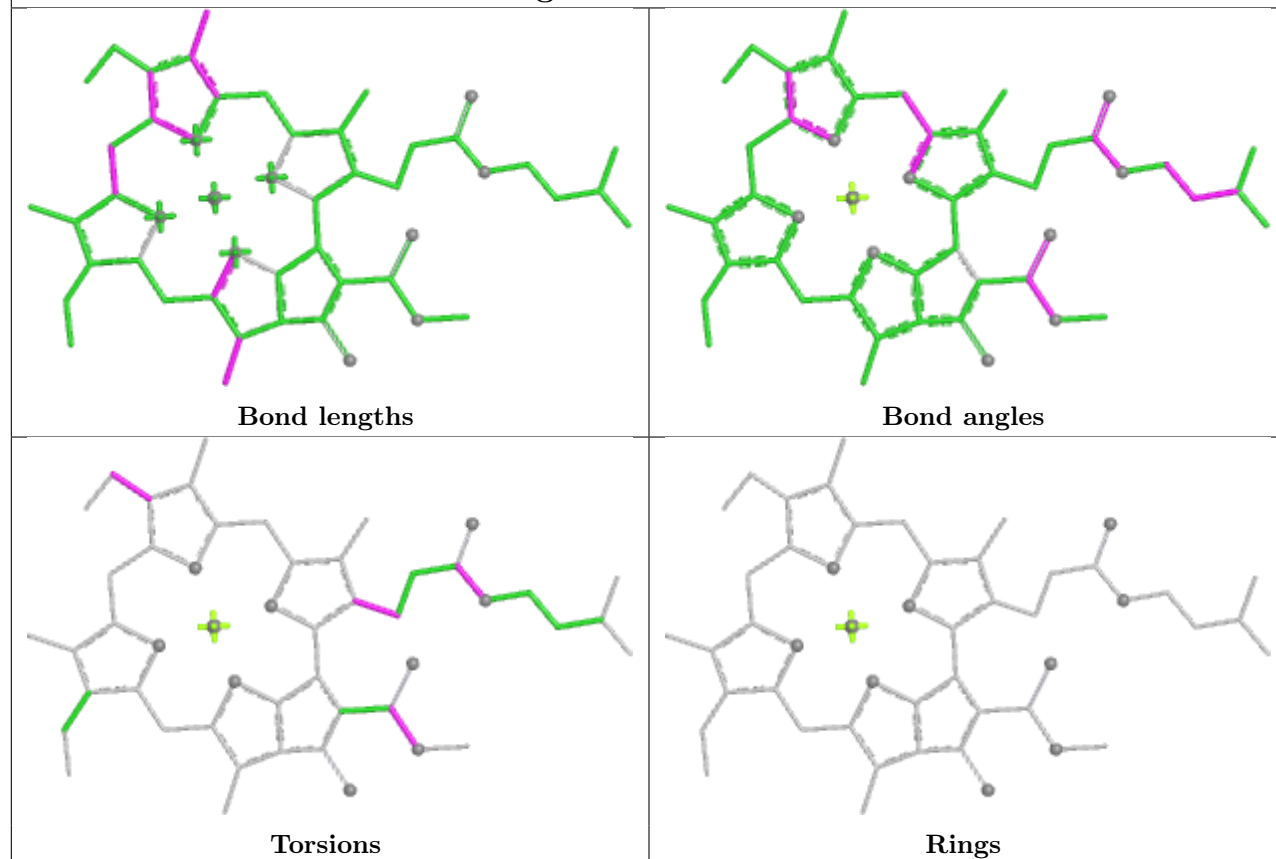
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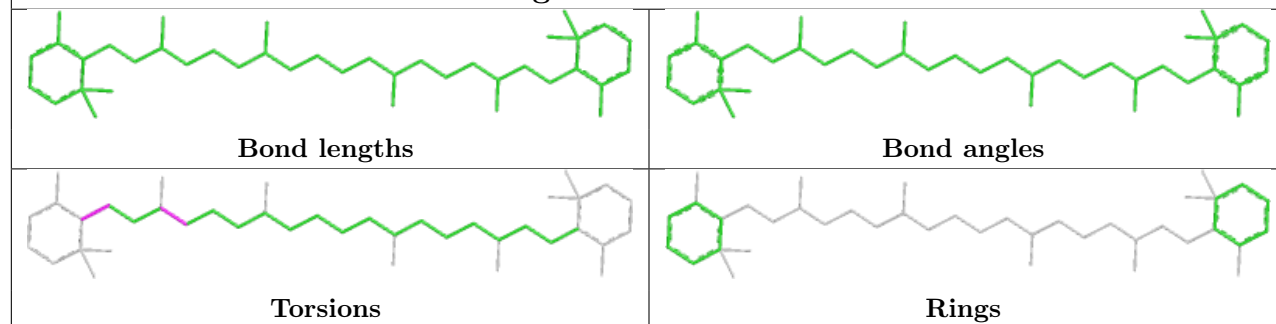
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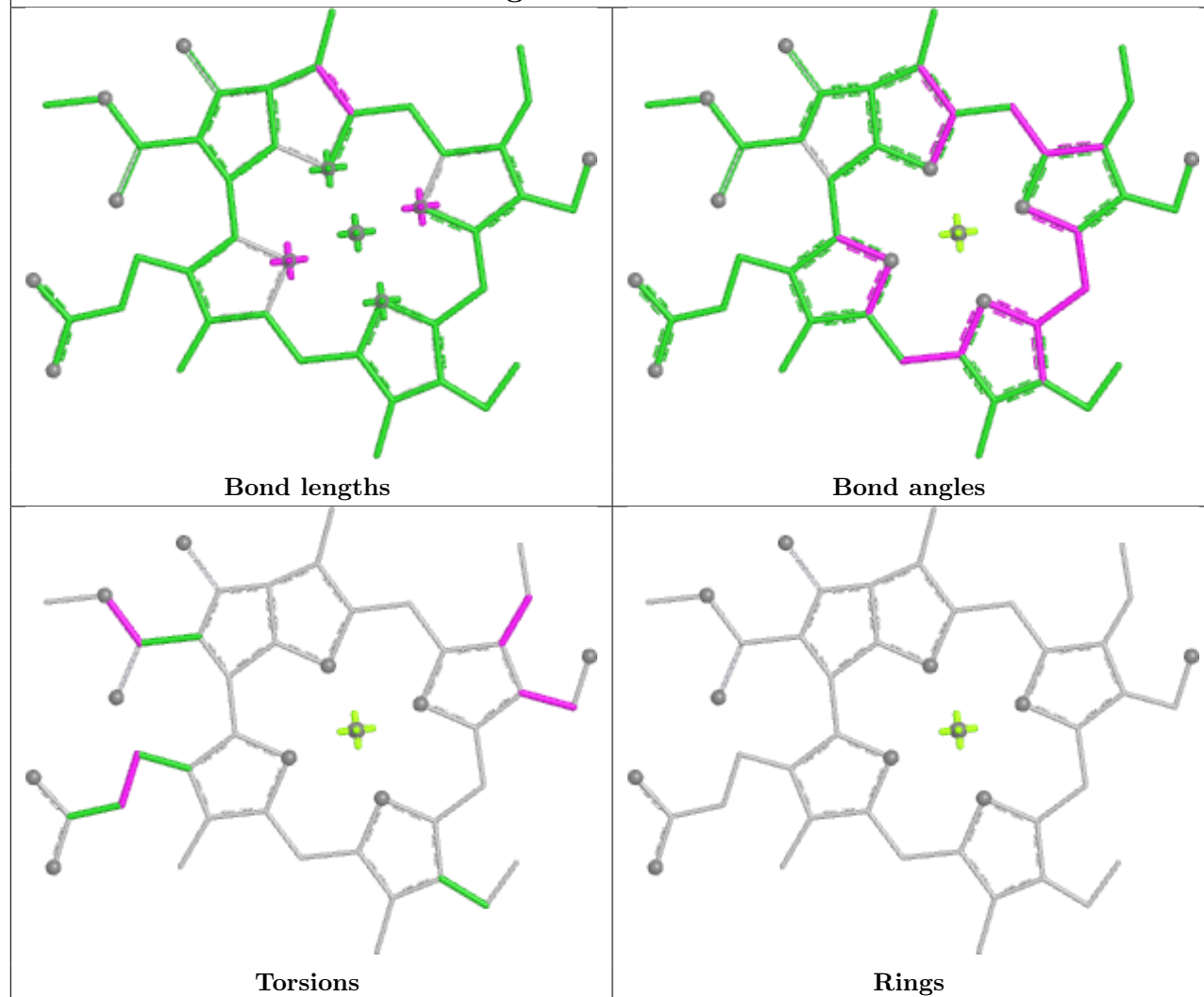
Ligand CLA 8 303



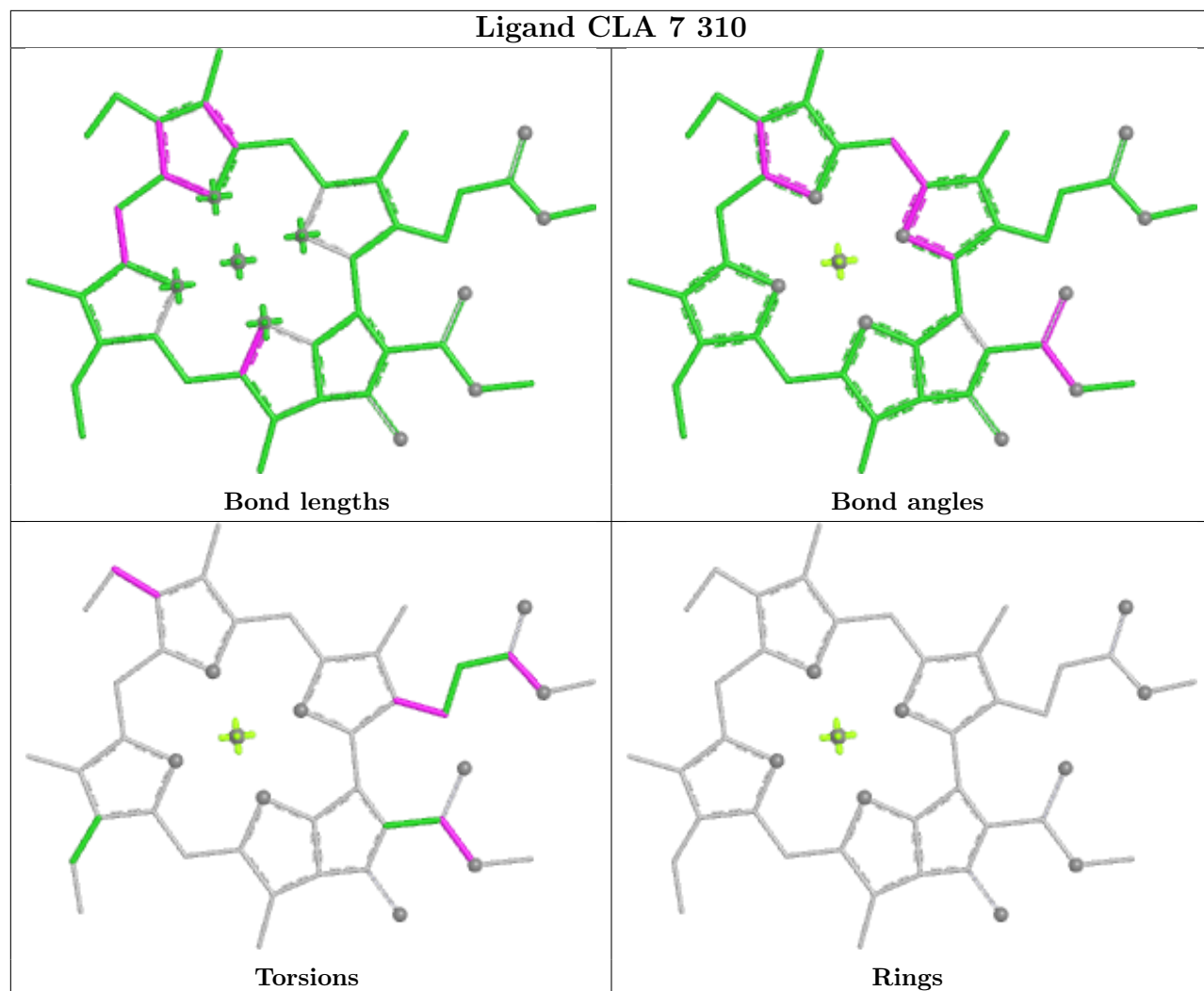
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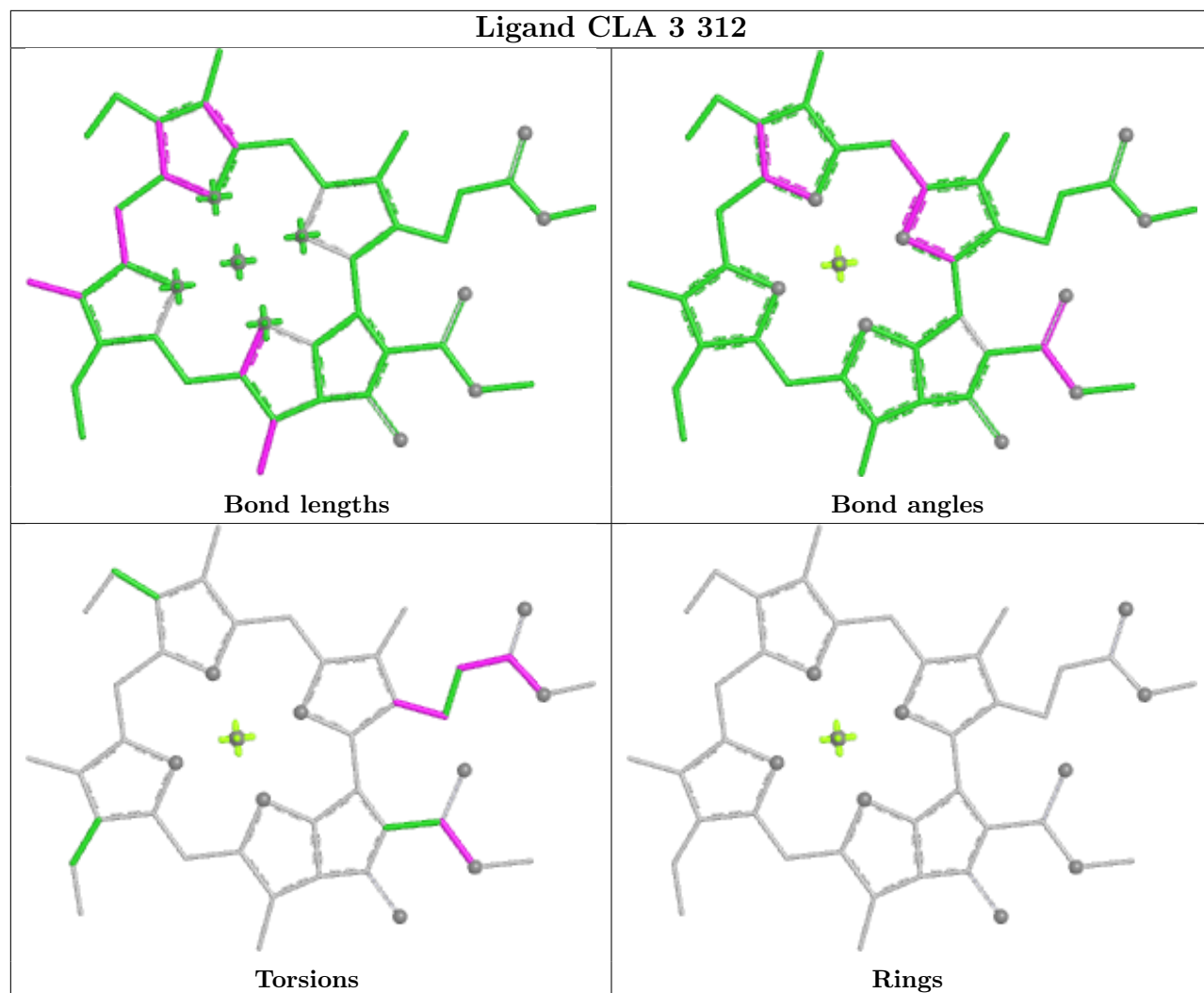
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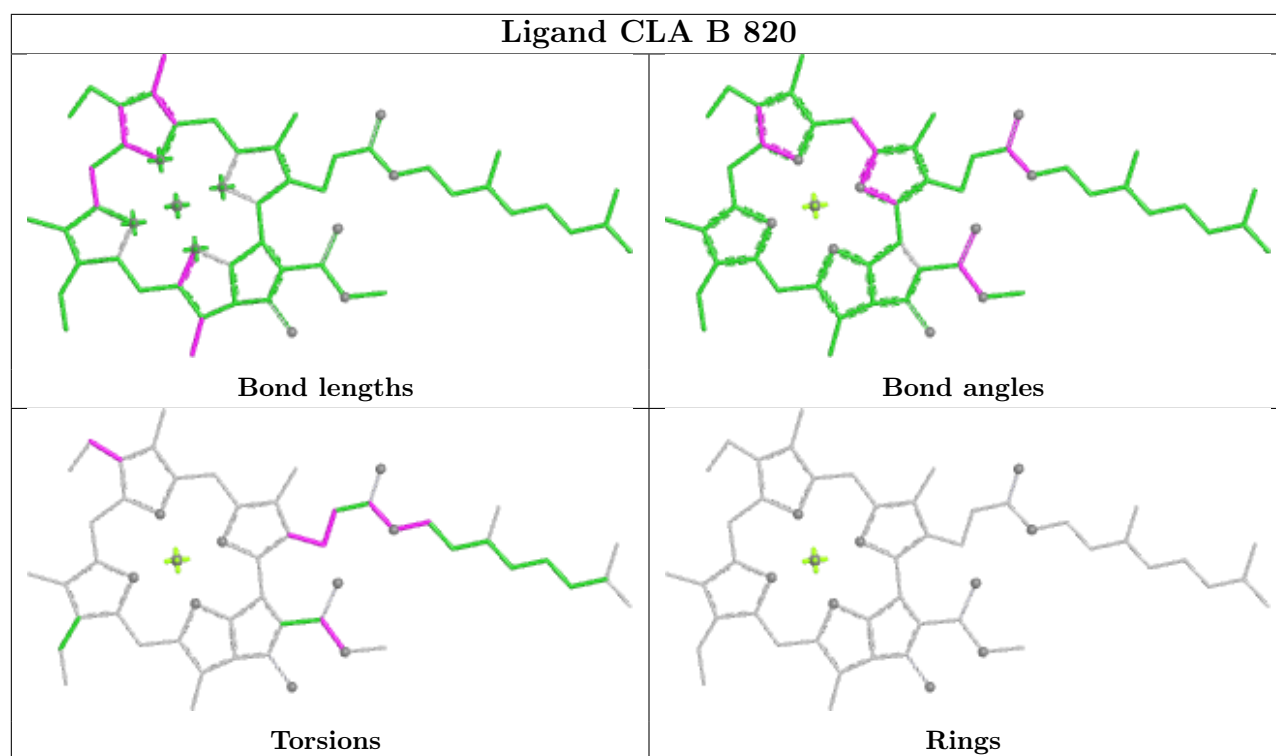


Ligand CLA 7 310

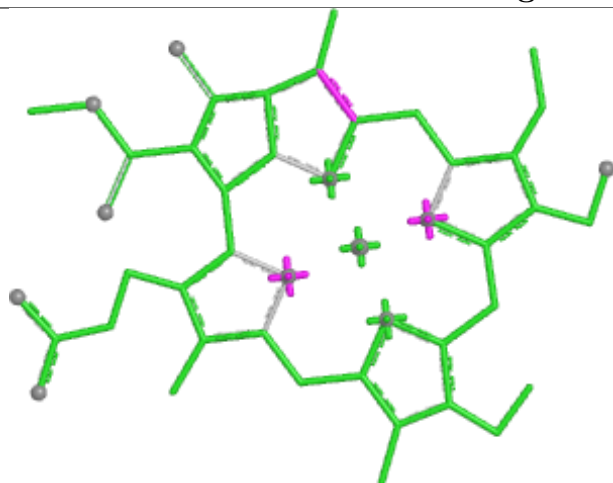


Ligand CLA 3 312

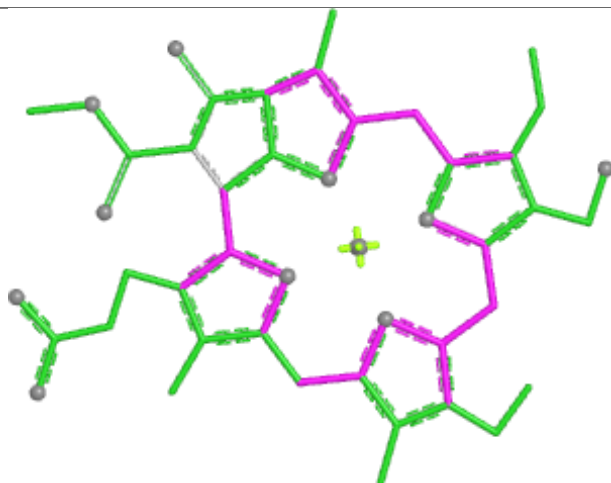




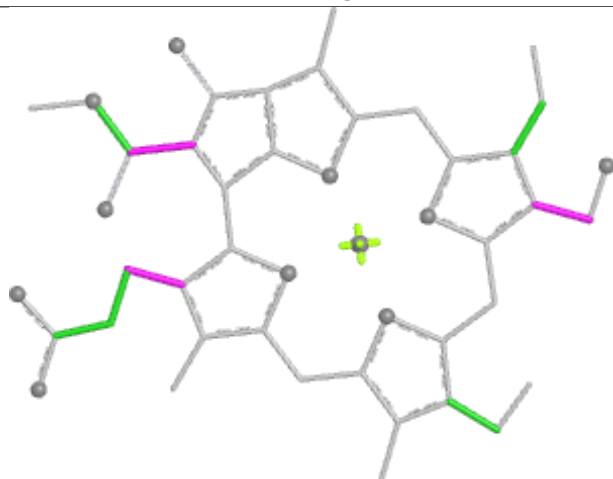
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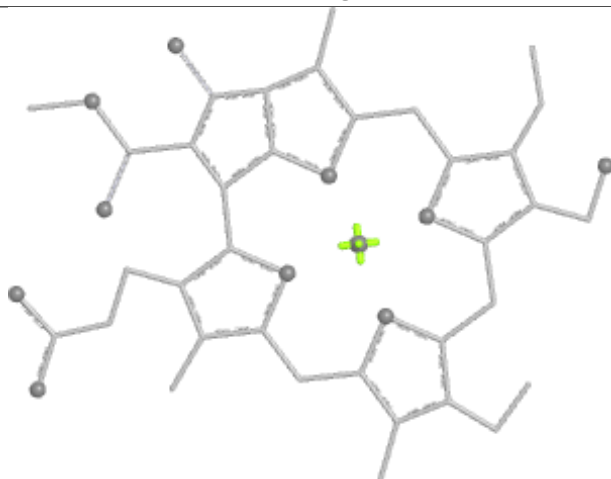
Bond lengths



Bond angles

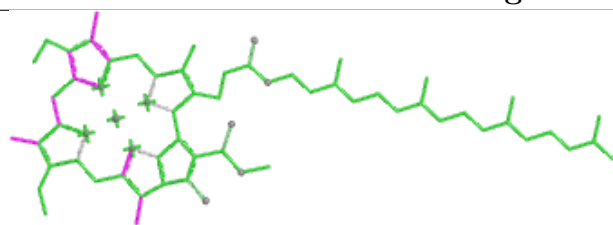


Torsions

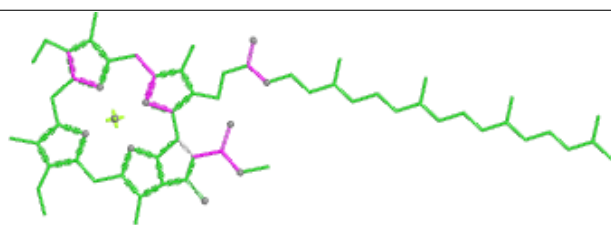


Rings

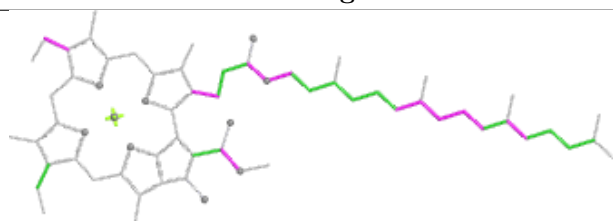
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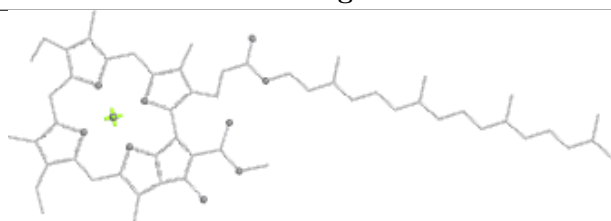
Bond lengths



Bond angles

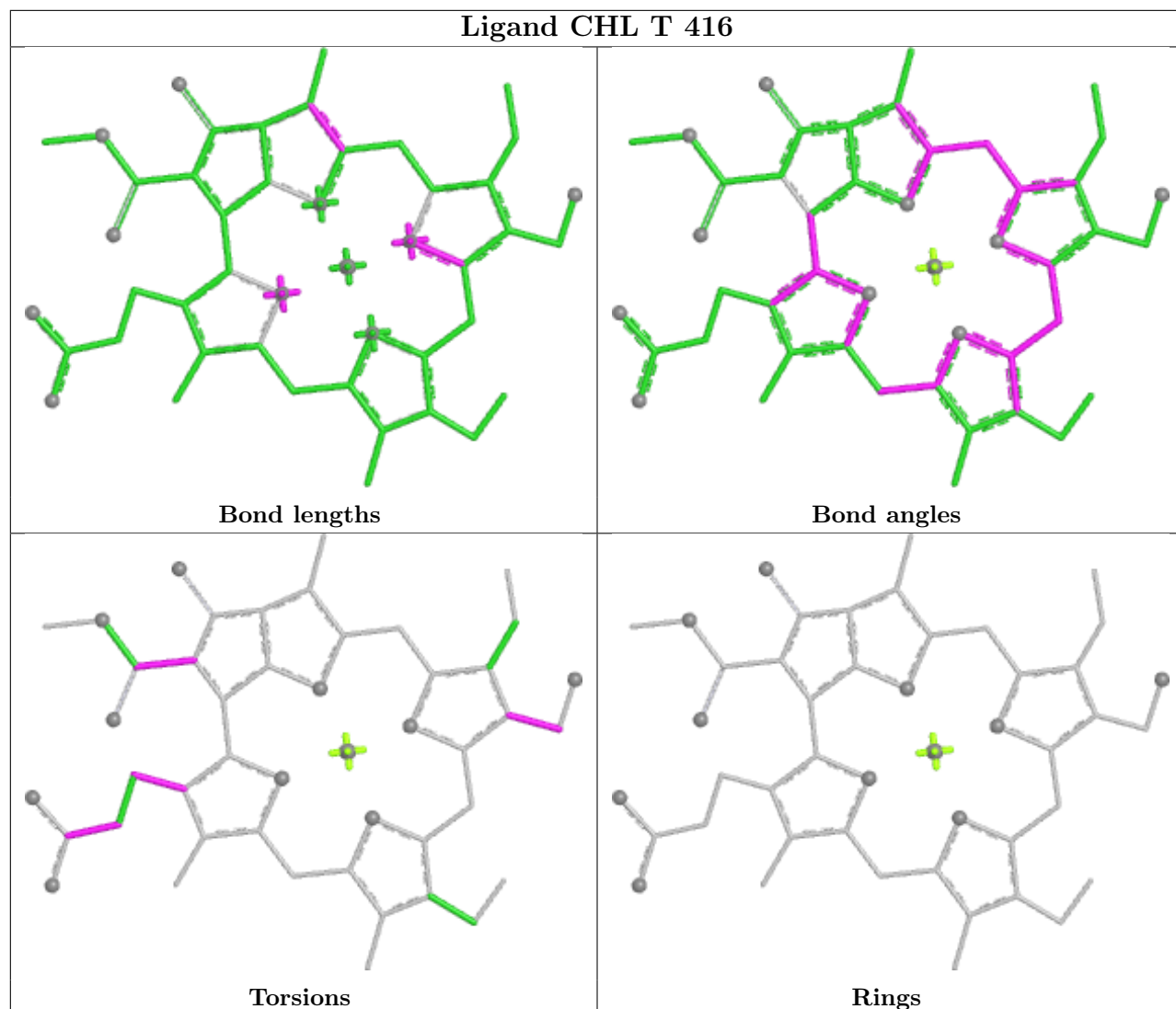


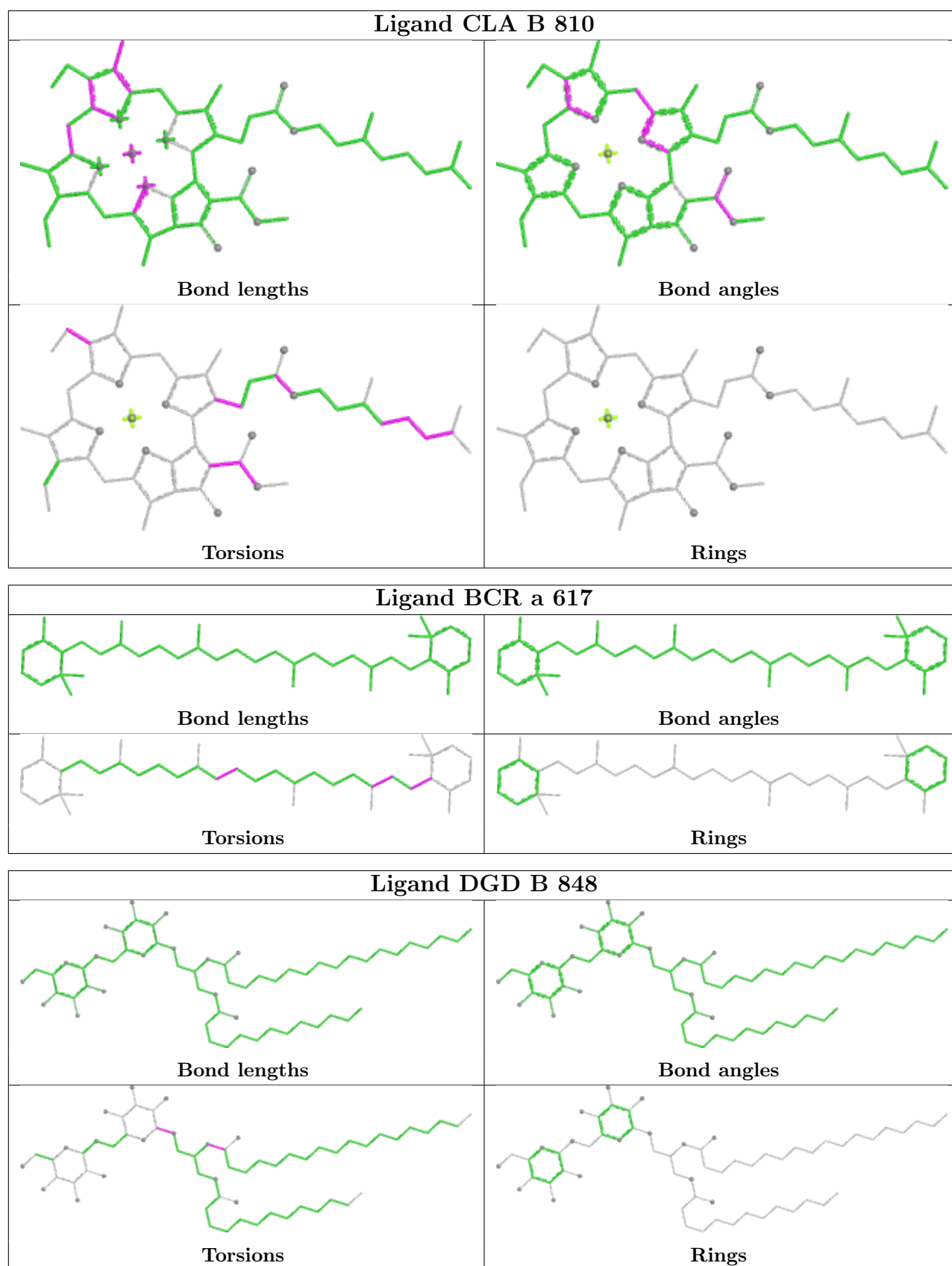
Torsions

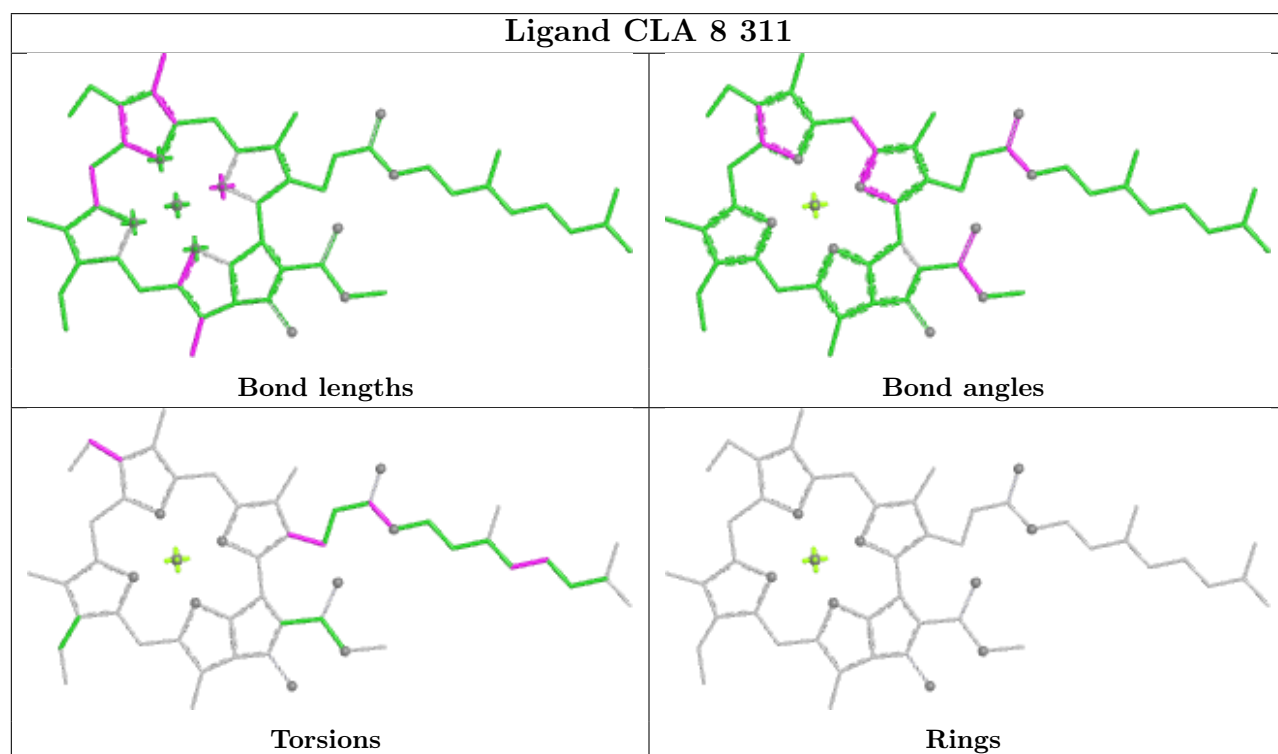
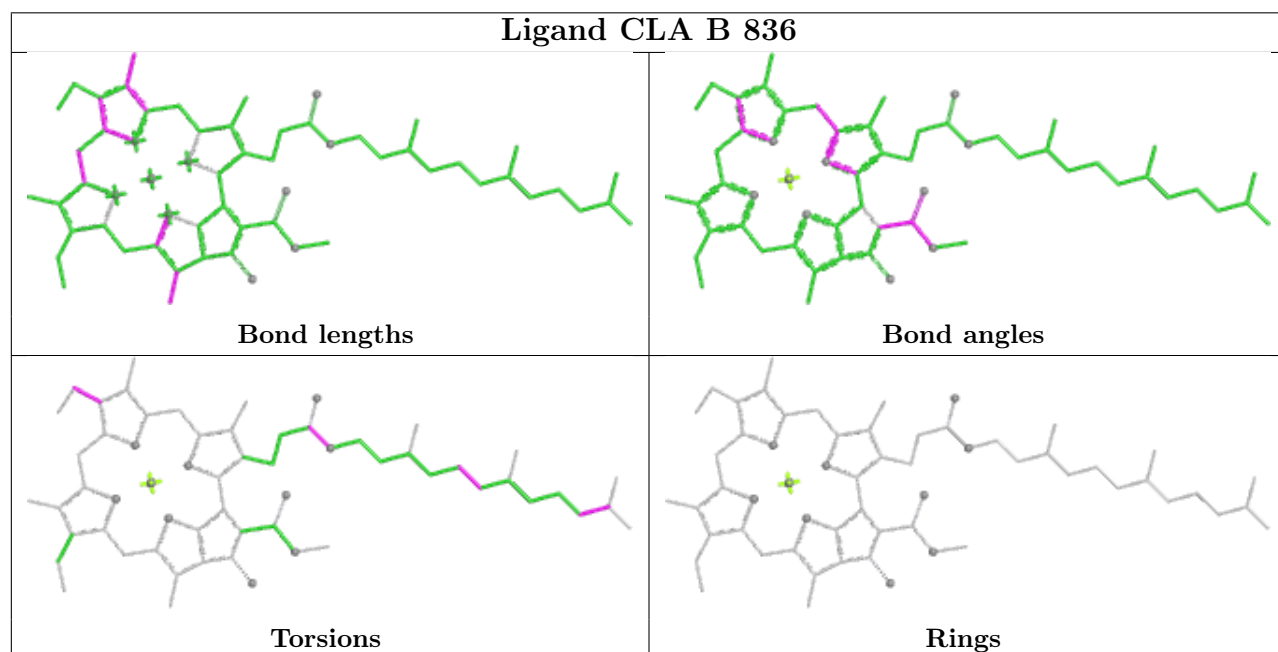
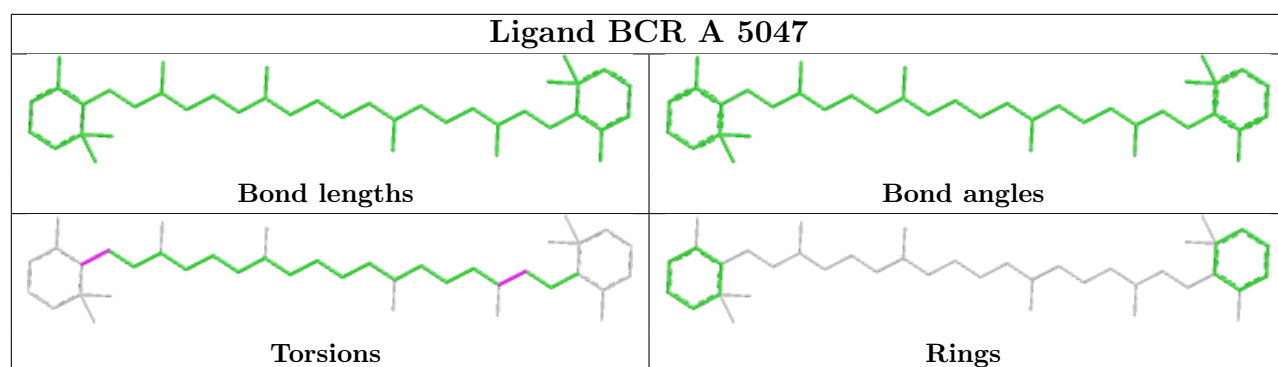


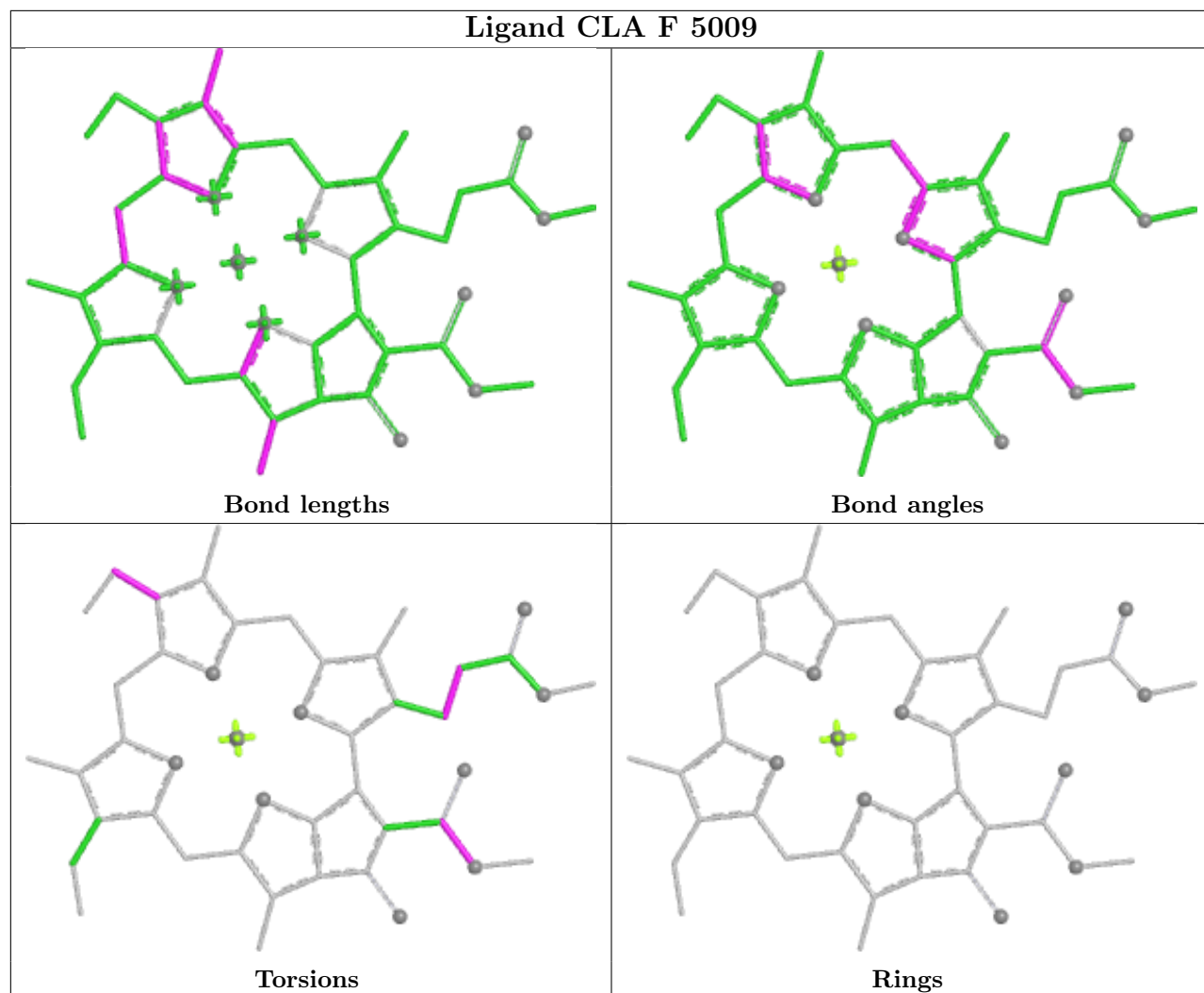
Rings

Ligand CHL T 416

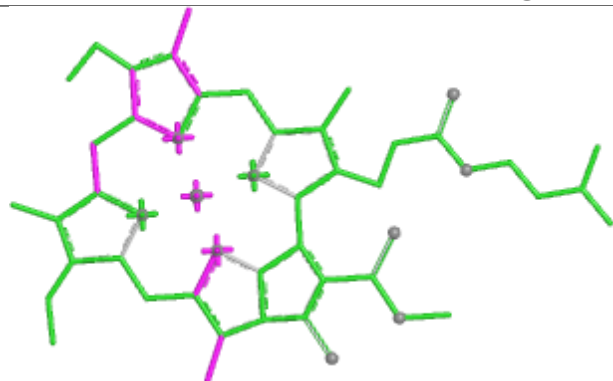




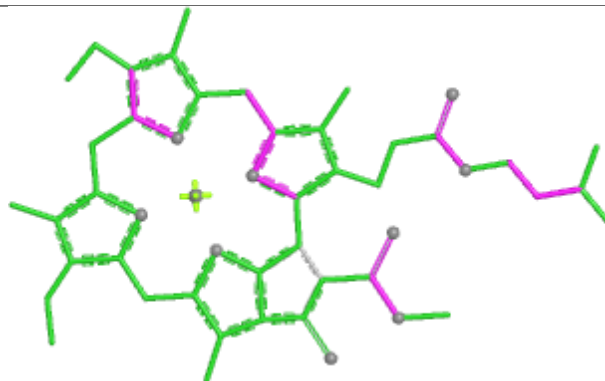




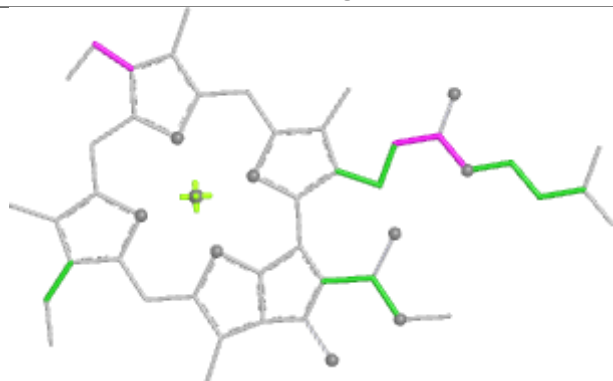
Ligand CLA 3 305



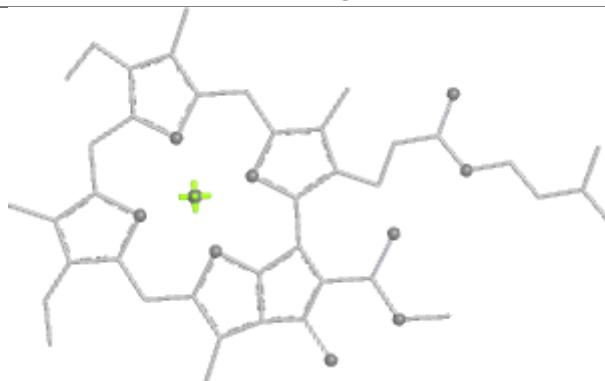
Bond lengths



Bond angles

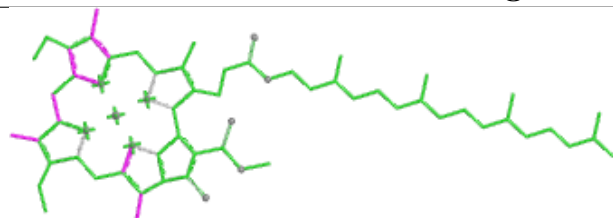


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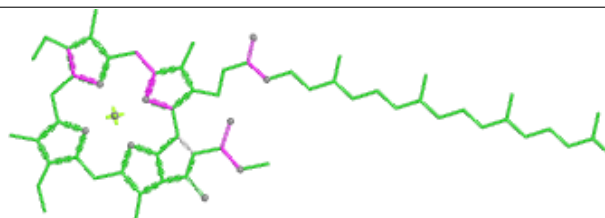


Rings

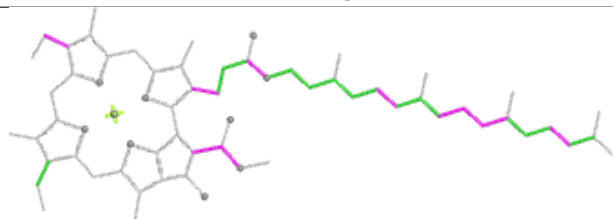
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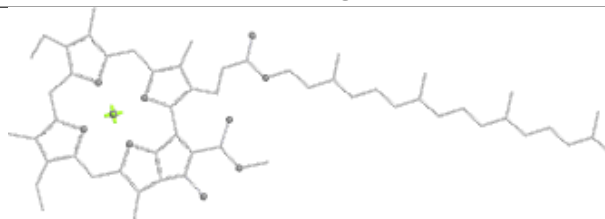
Bond lengths



Bond angles

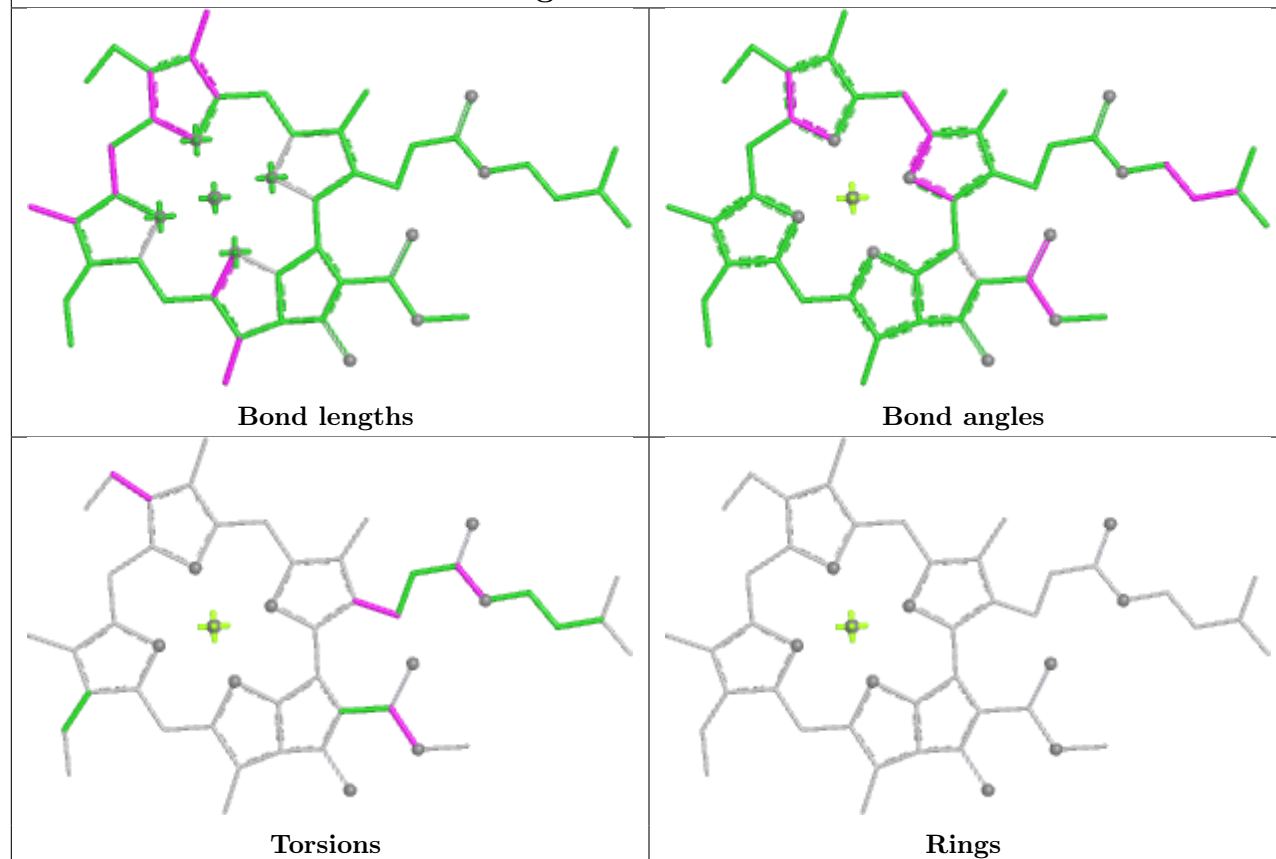


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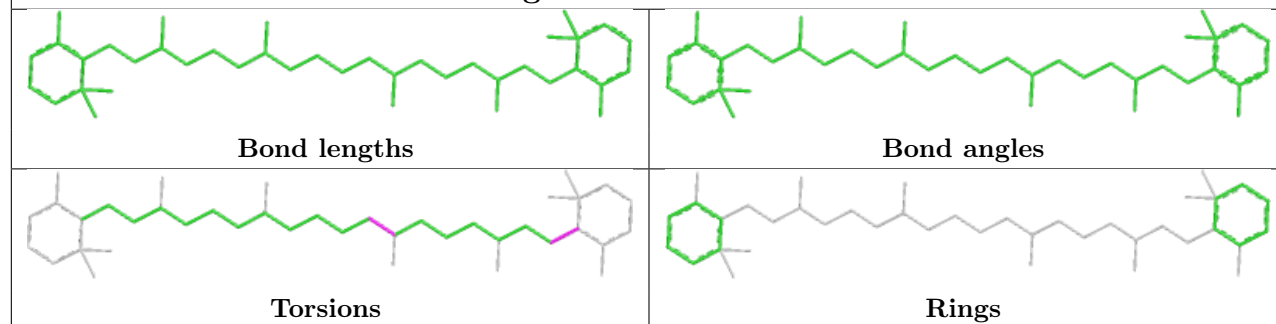


Rings

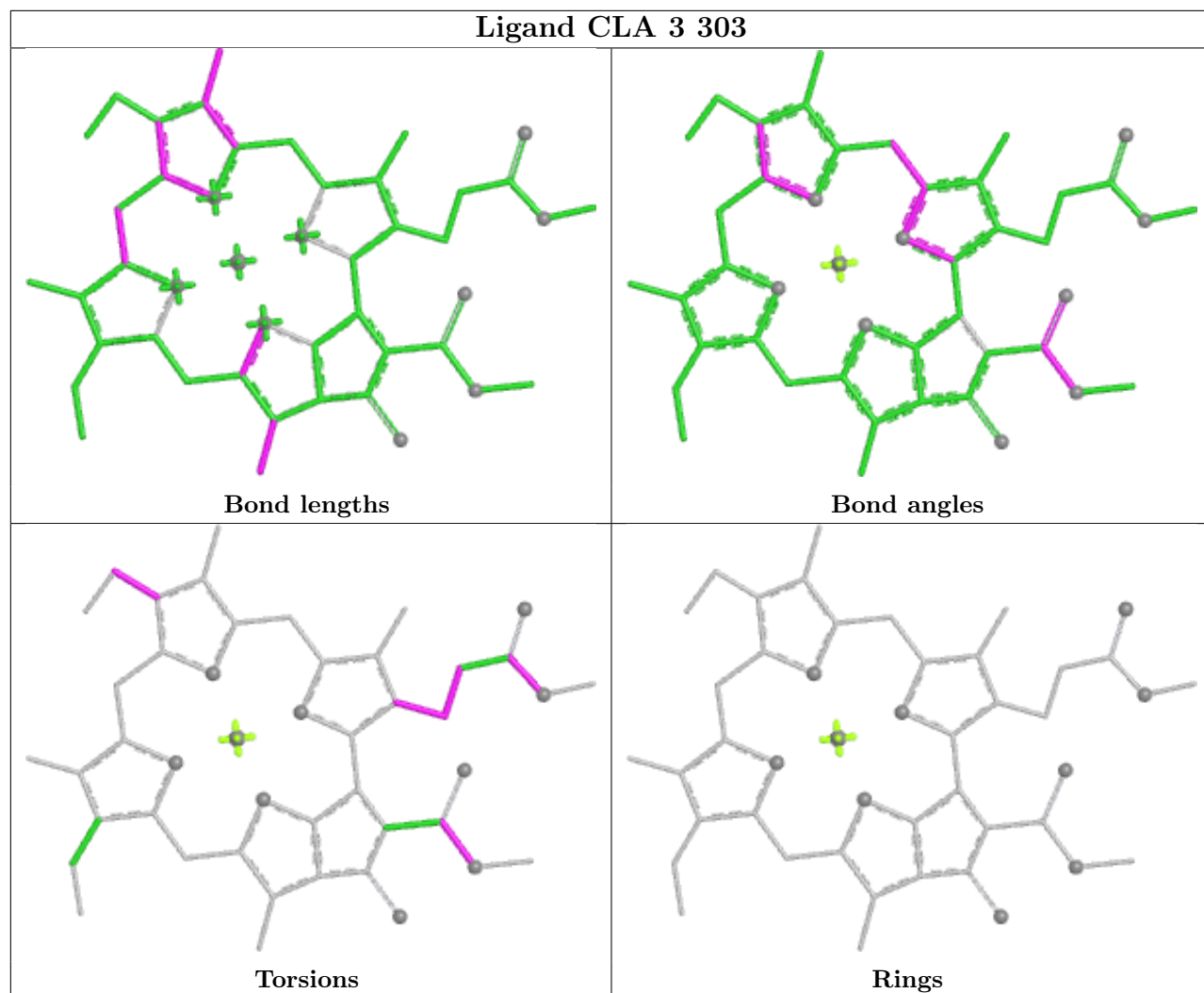
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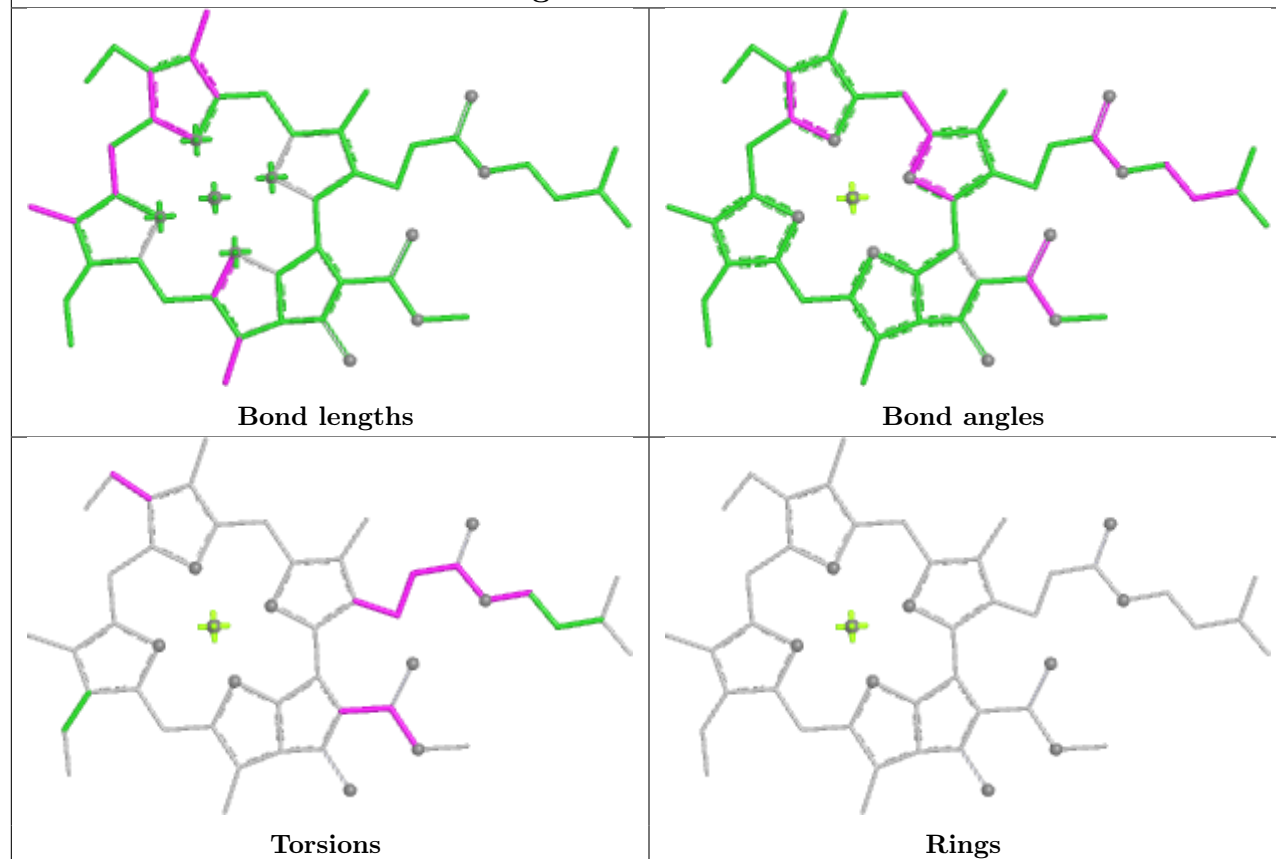
Ligand BCR F 5010



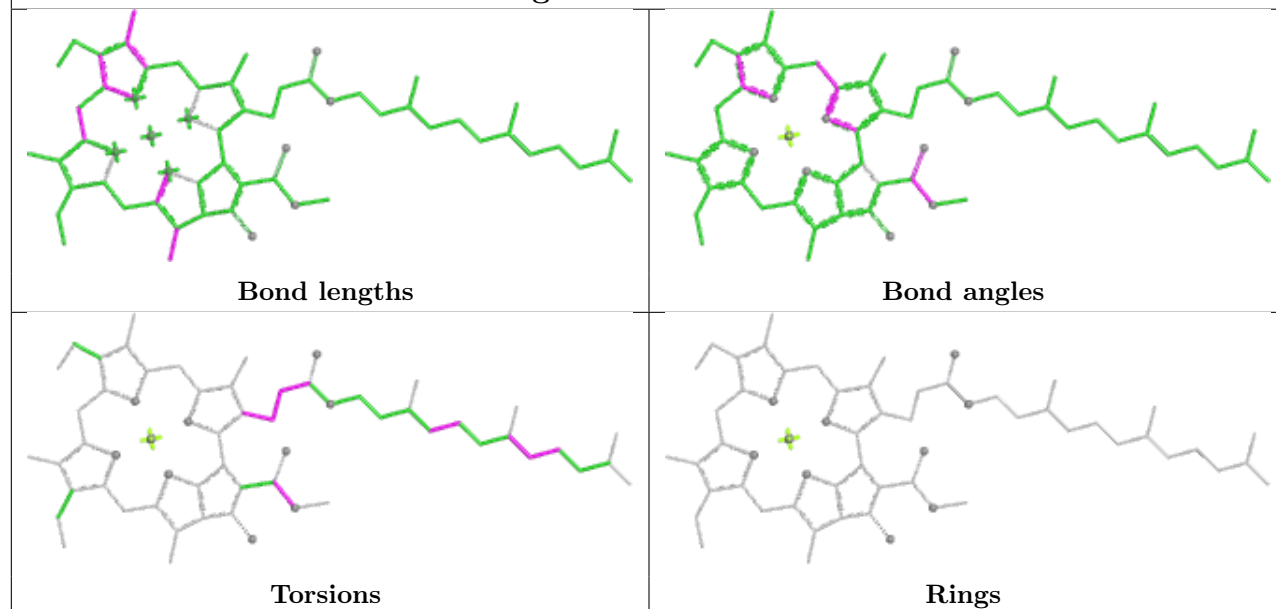
Ligand CLA 3 303



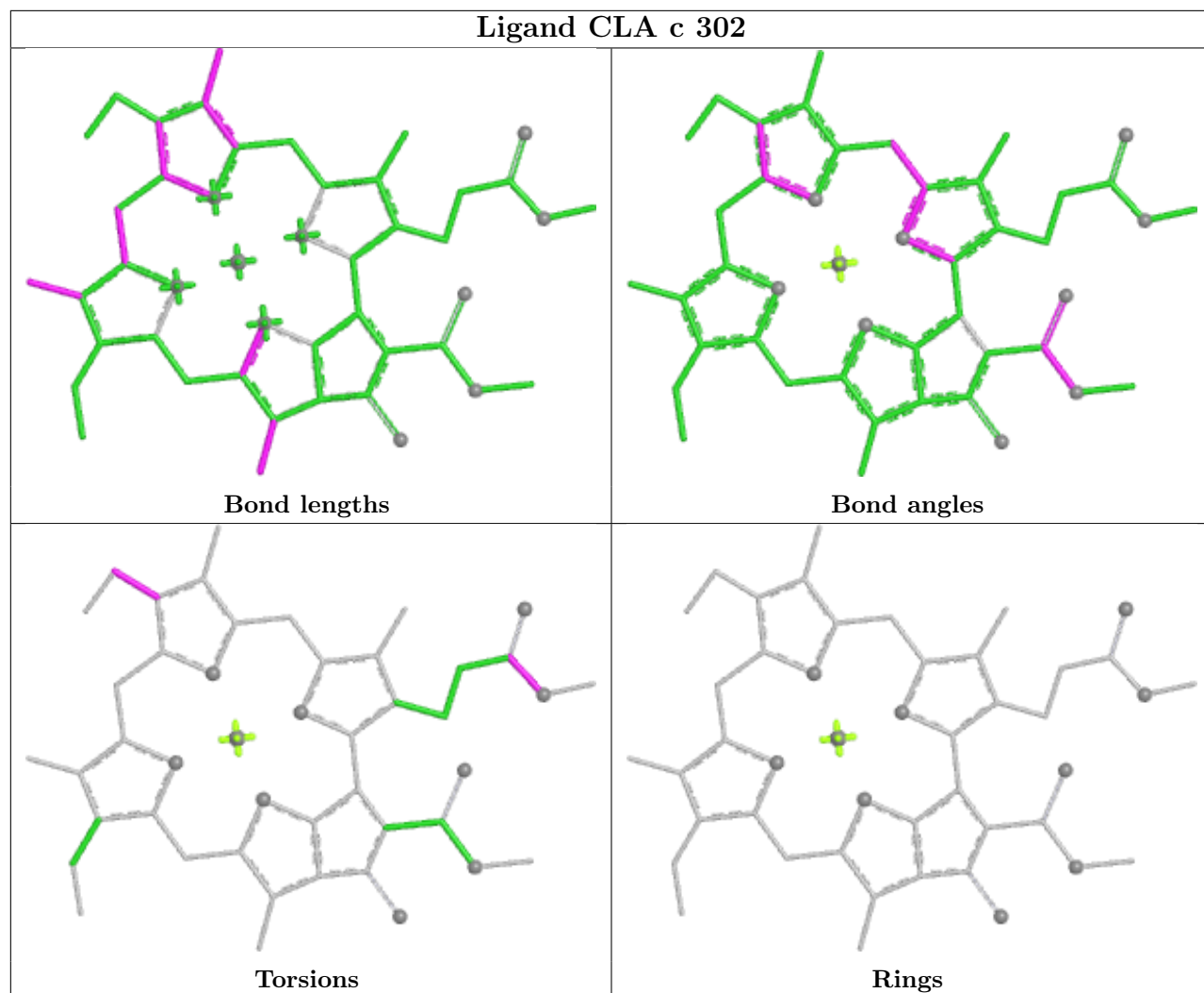
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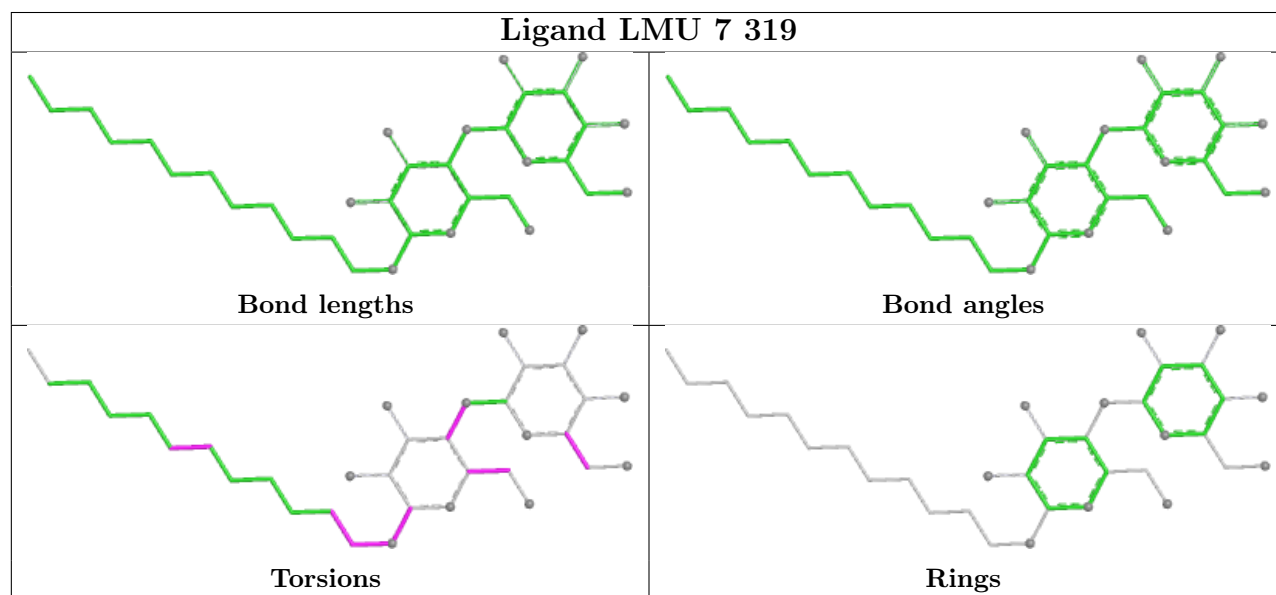
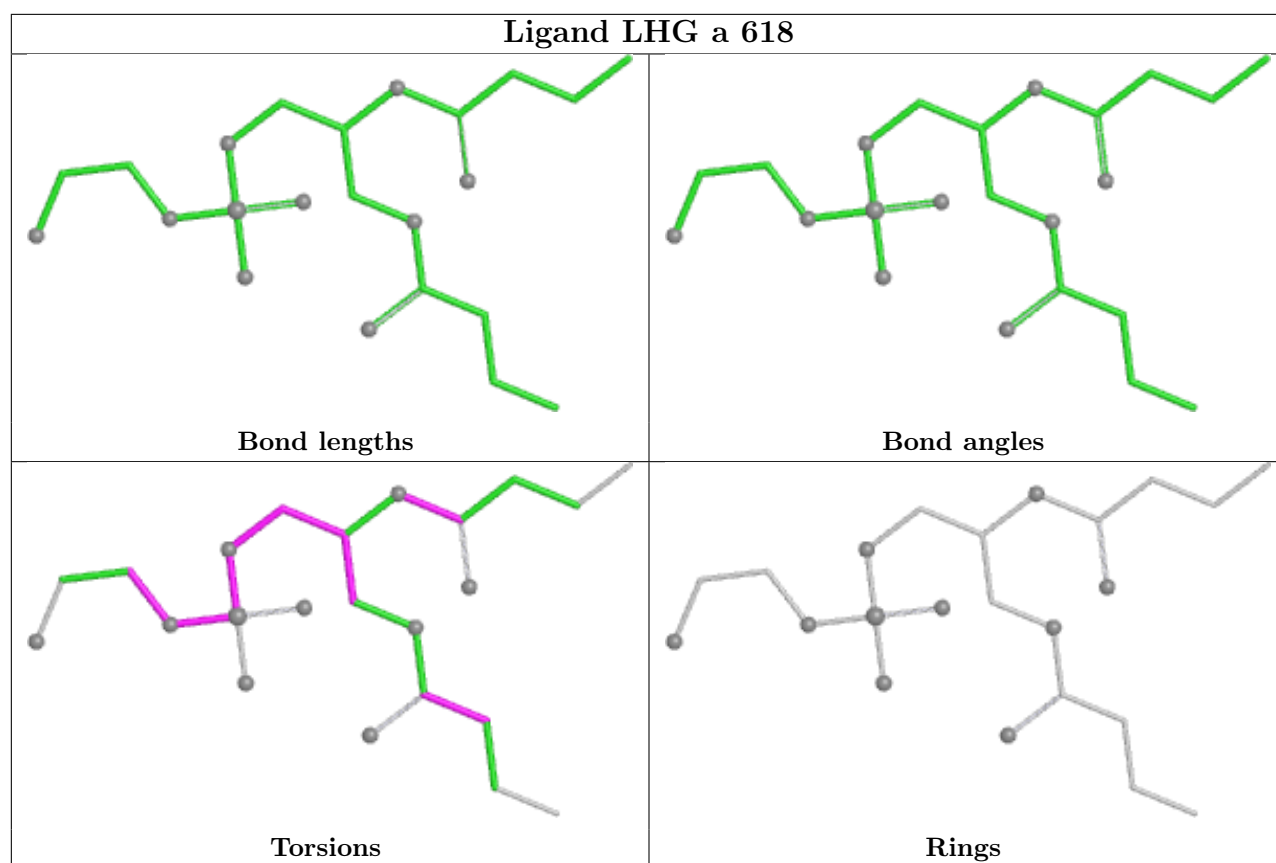


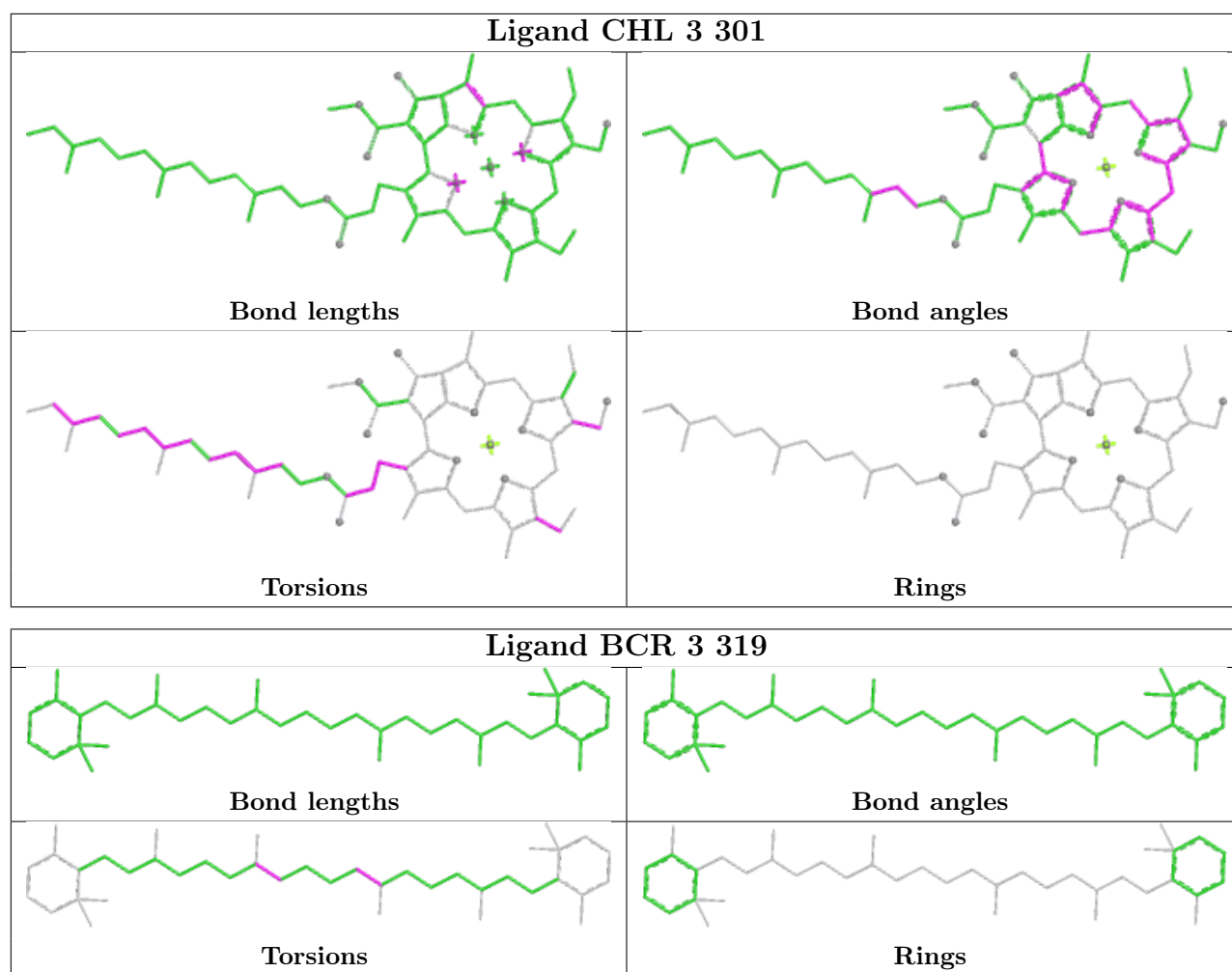
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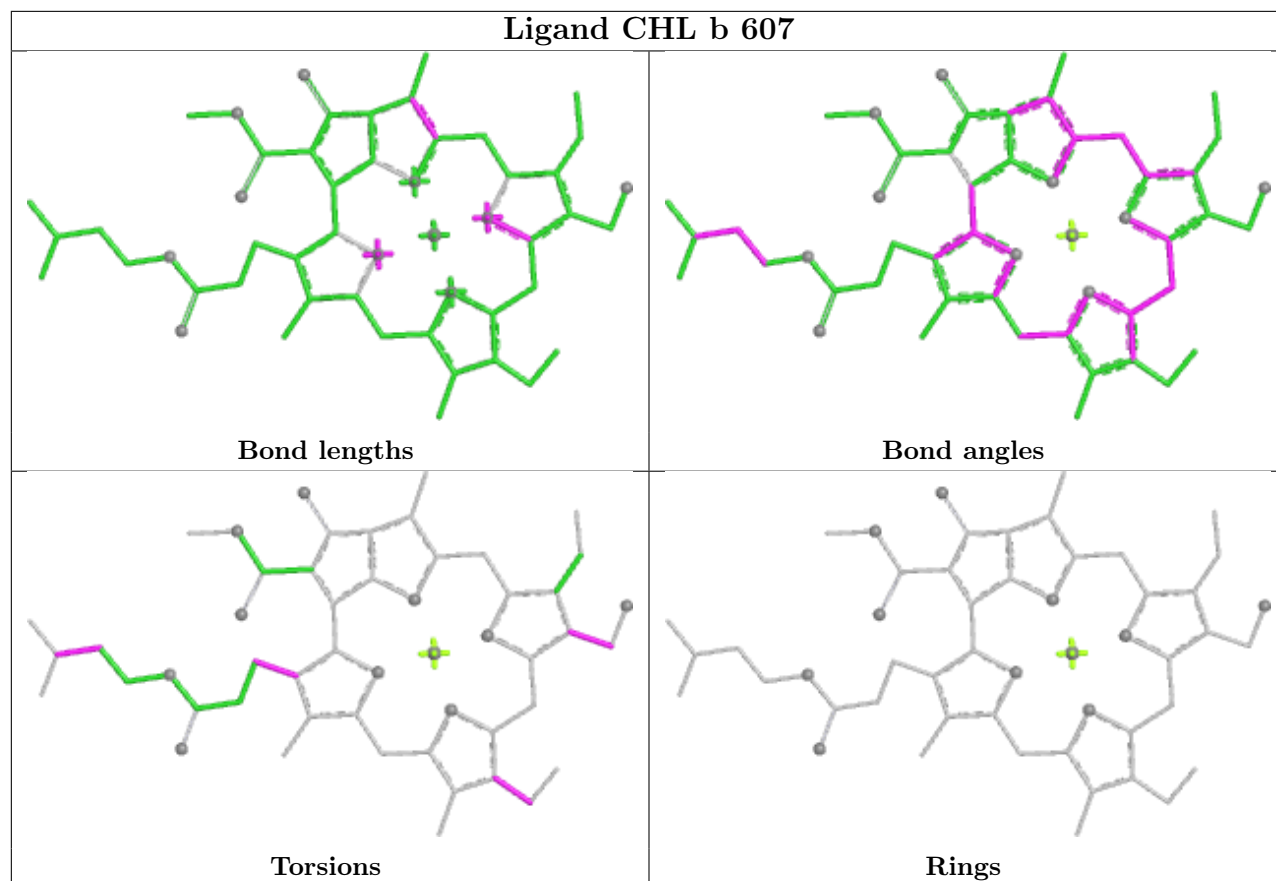
Ligand CLA c 302



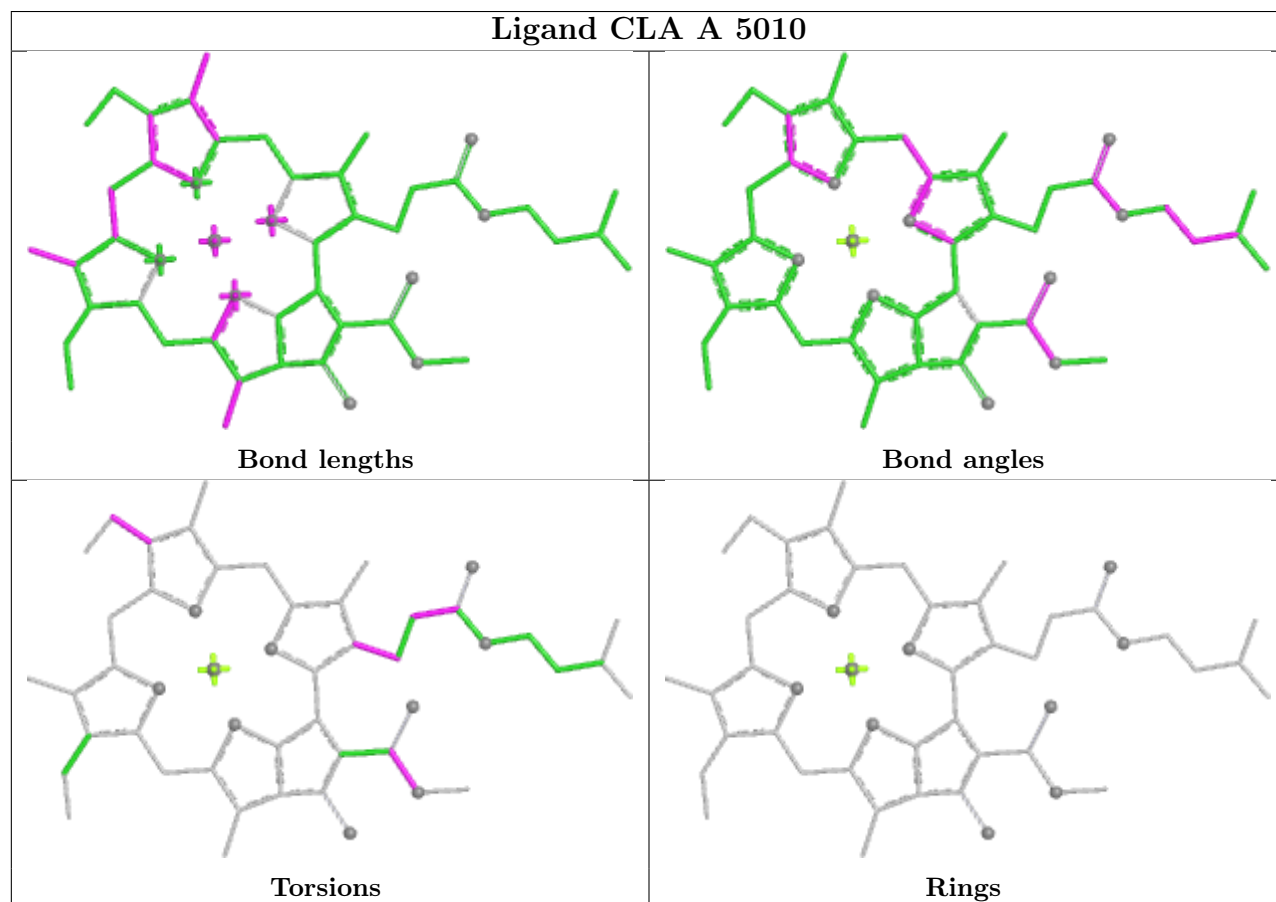


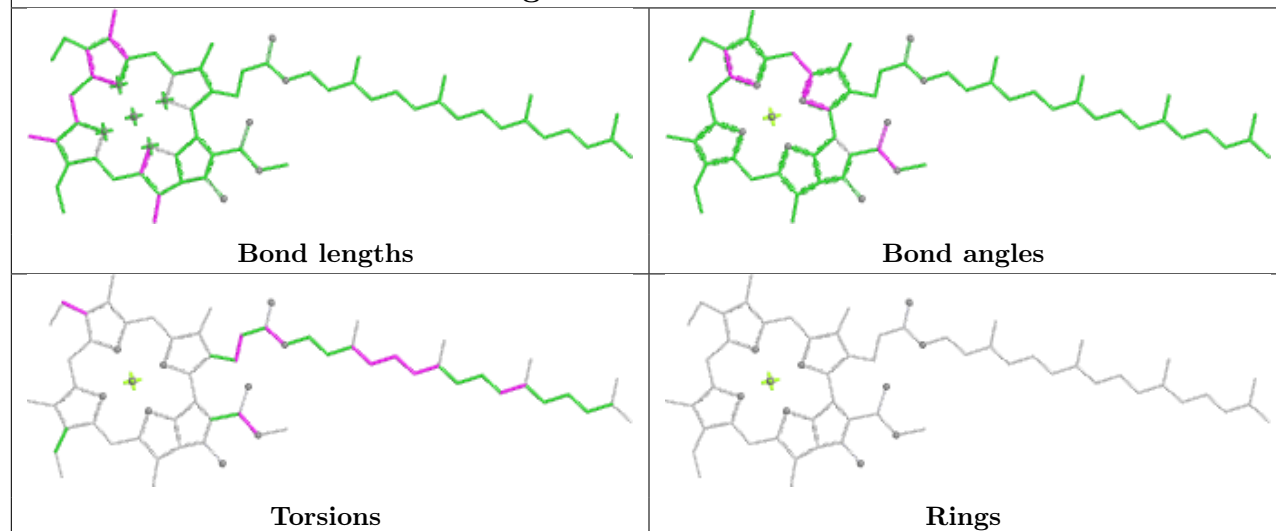
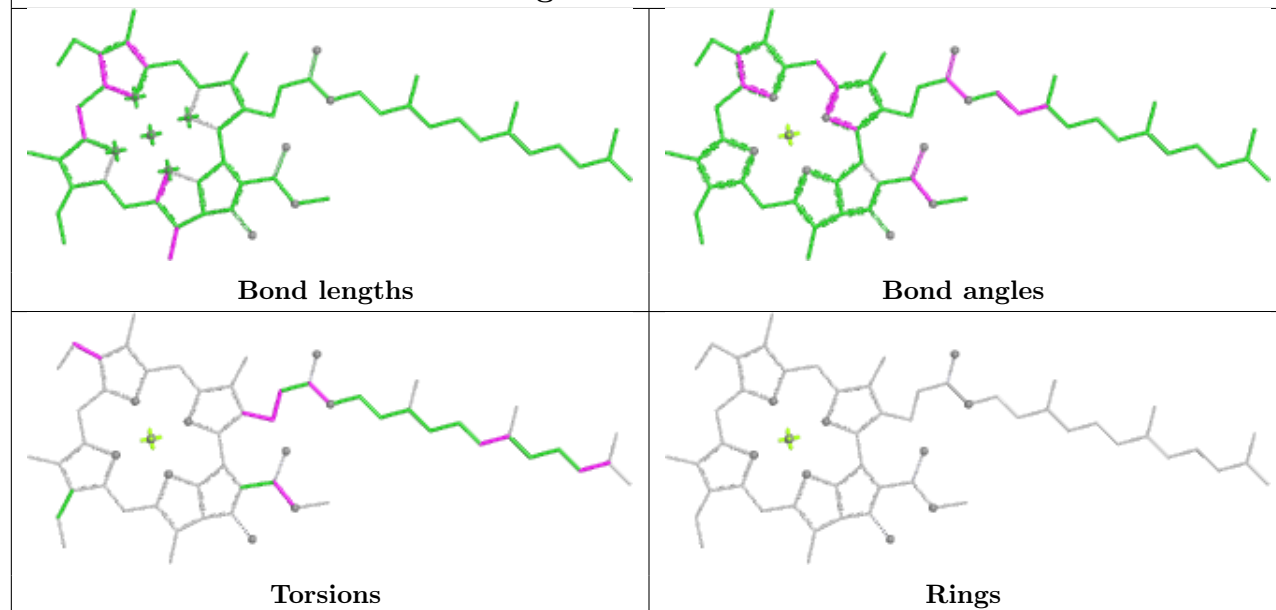


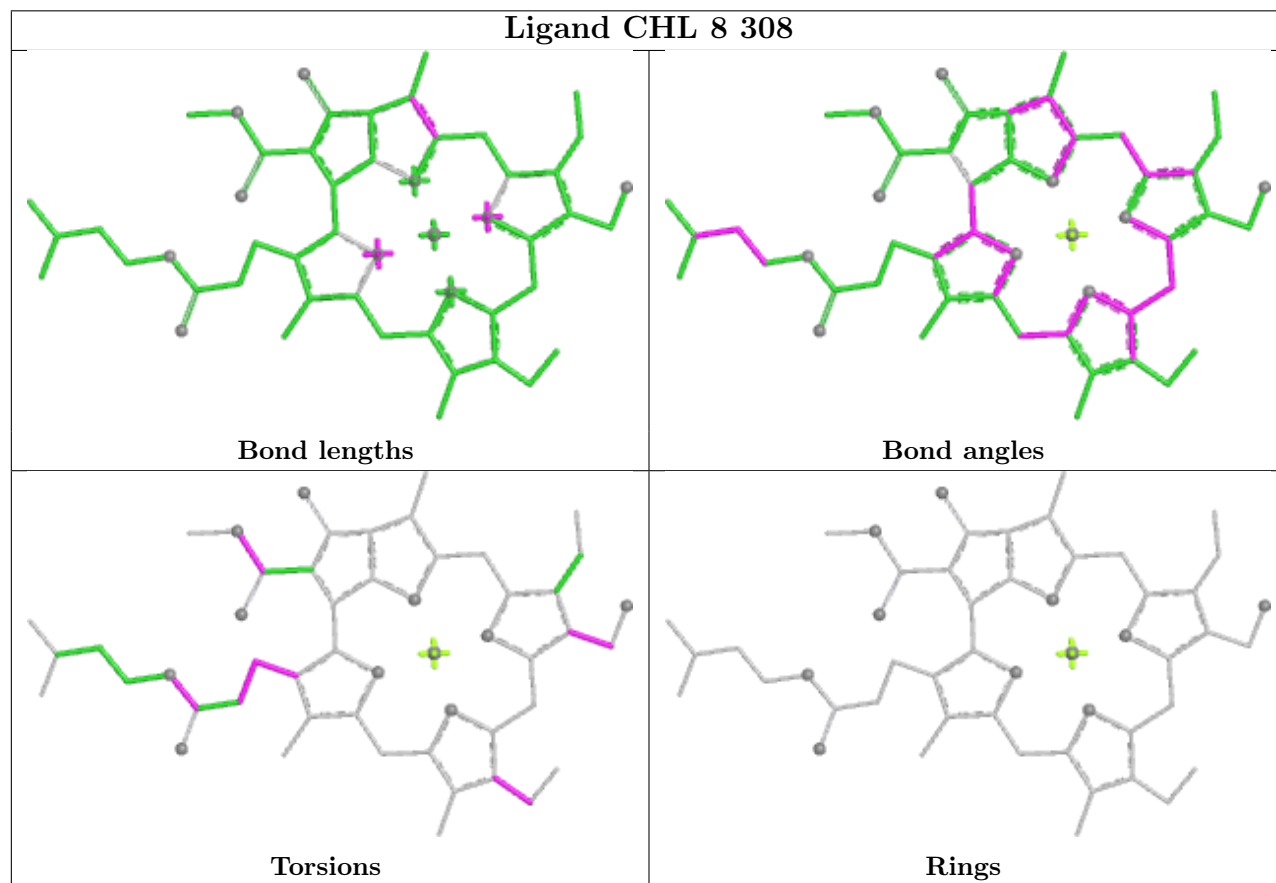
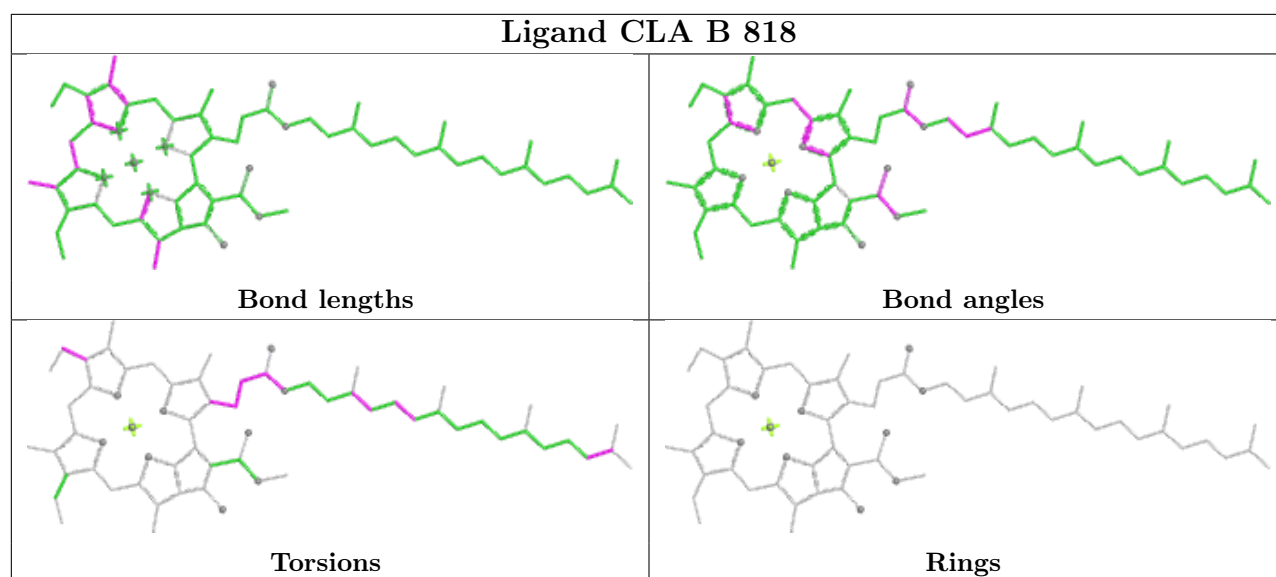
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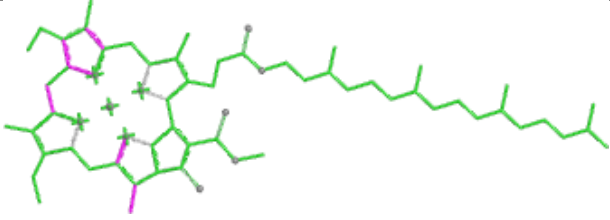
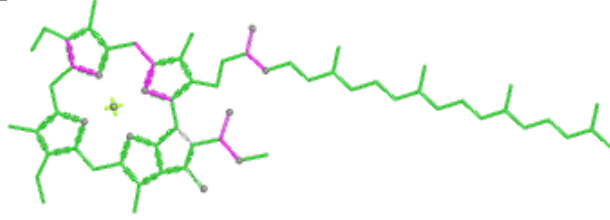
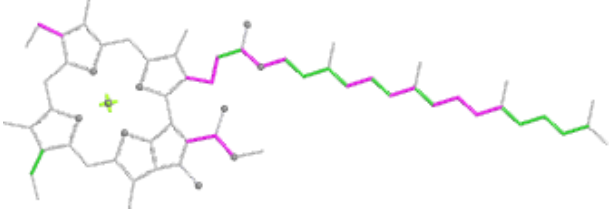
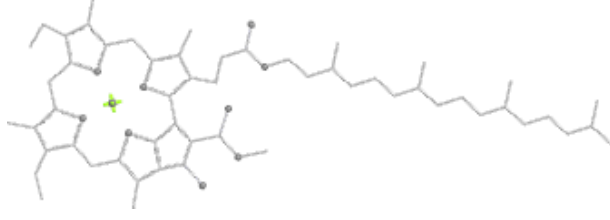
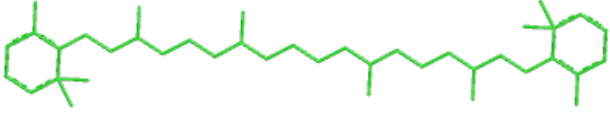
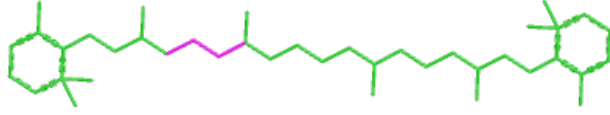
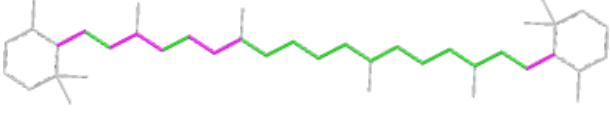
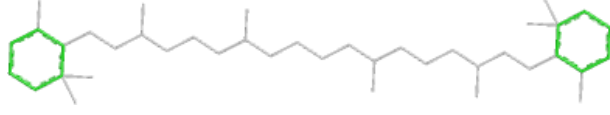
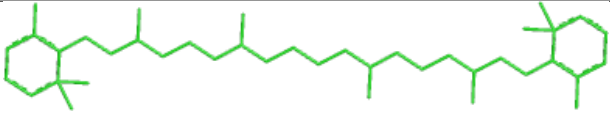
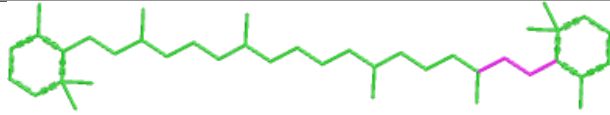
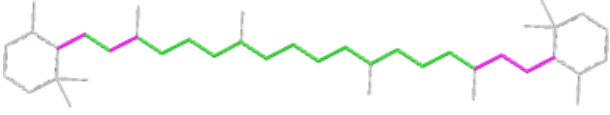
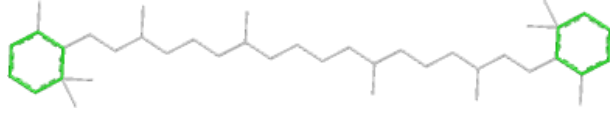


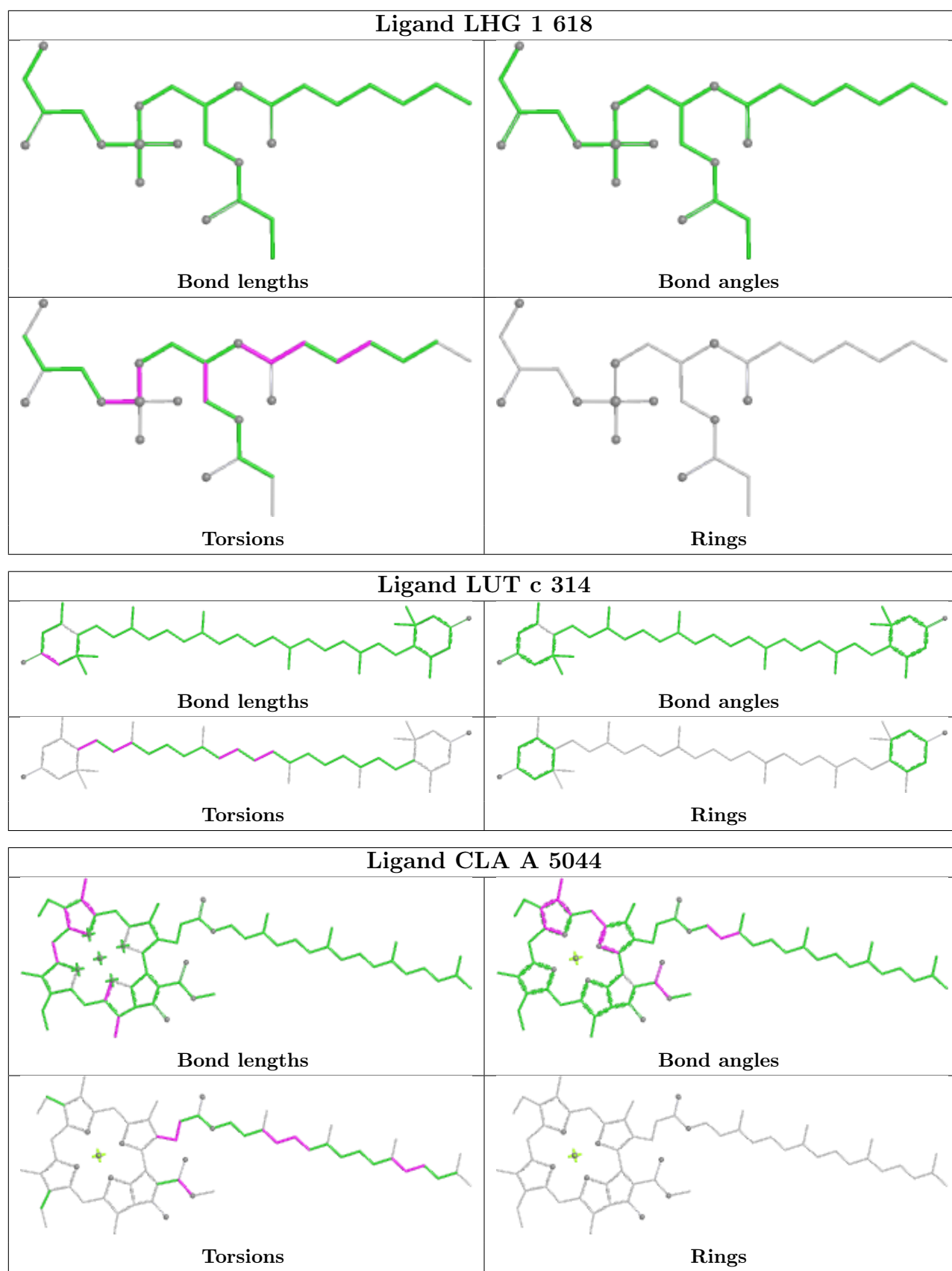
Ligand CLA A 5010

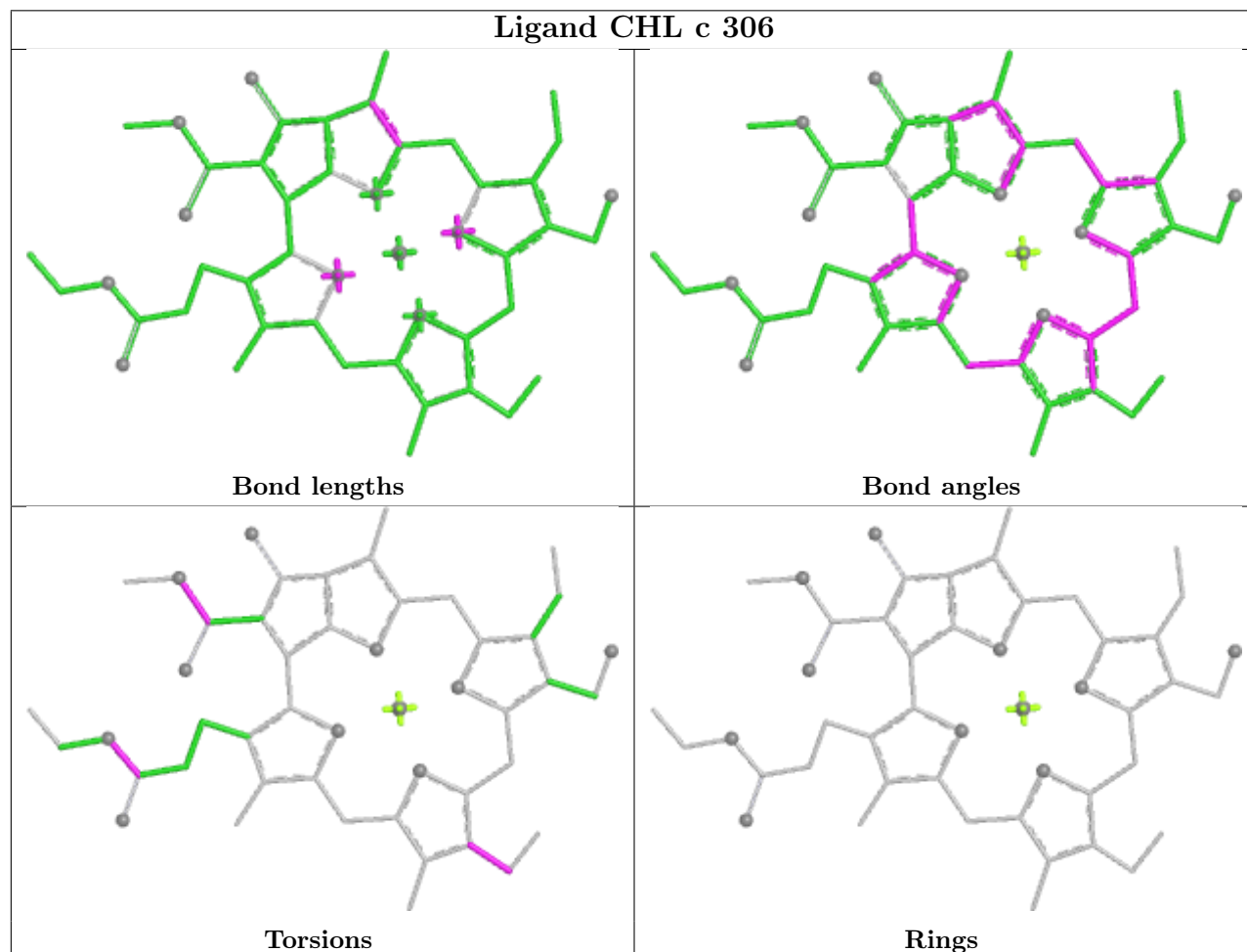
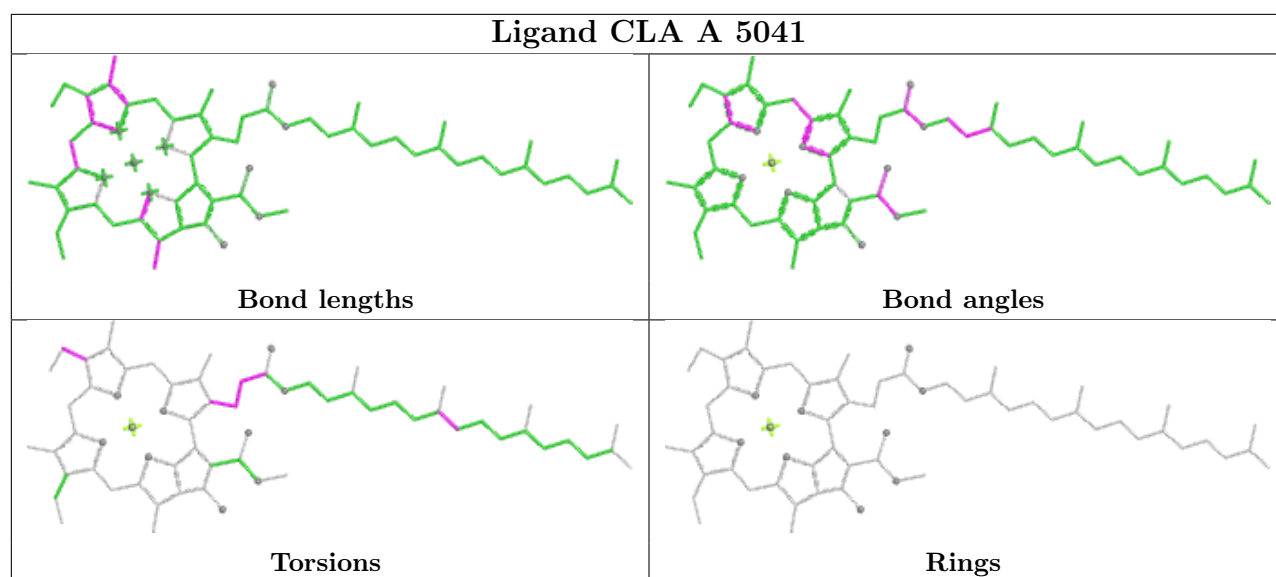


Ligand CLA A 5004**Ligand CLA 1 612**

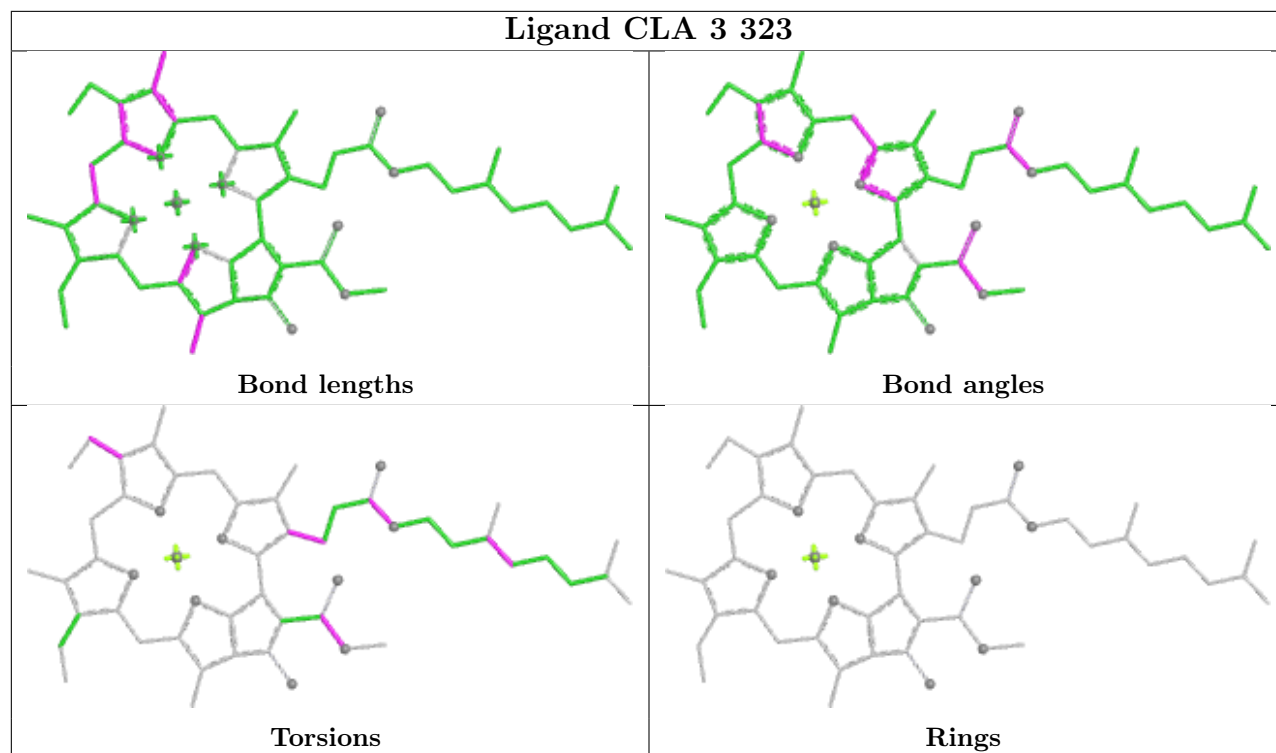


Ligand CLA B 829	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

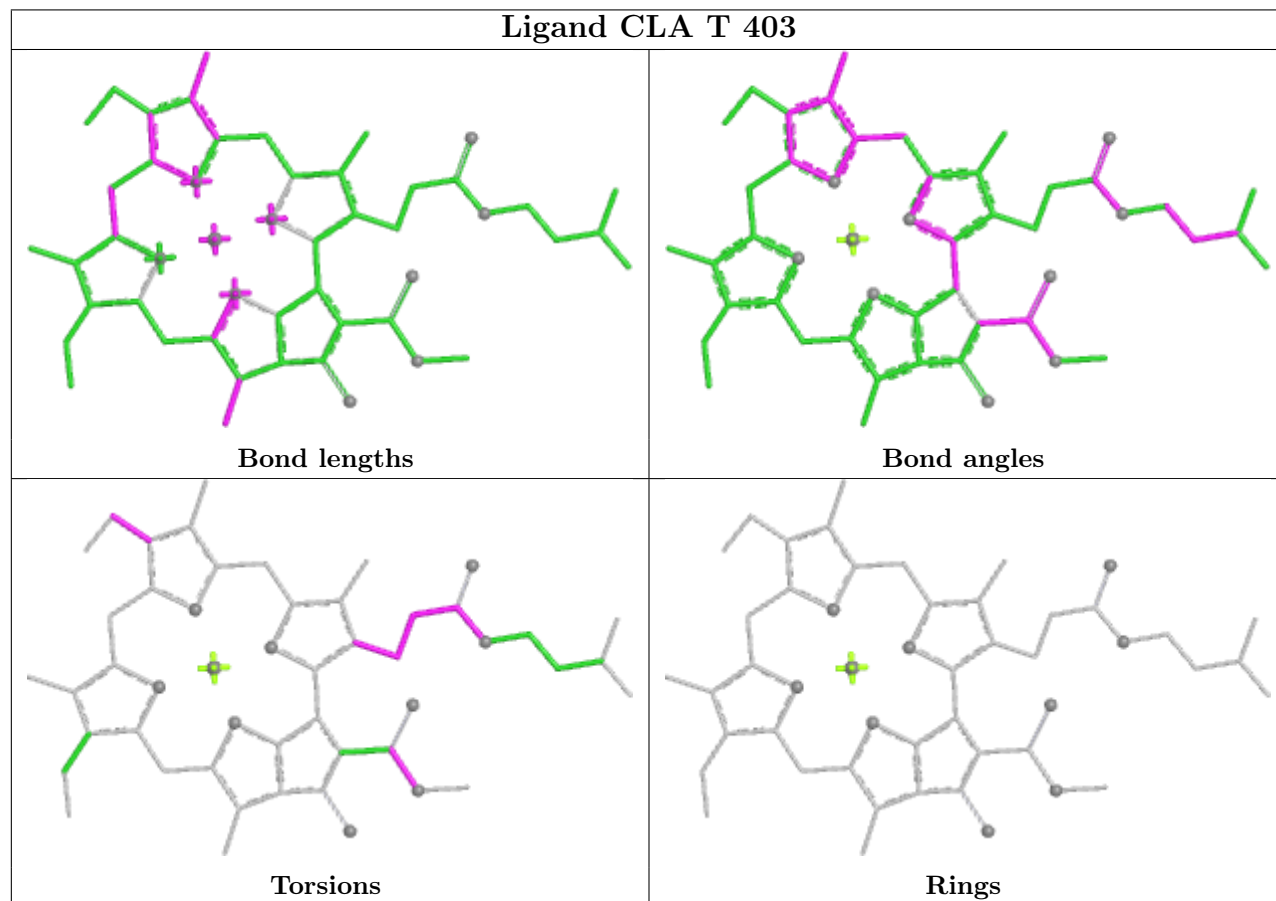


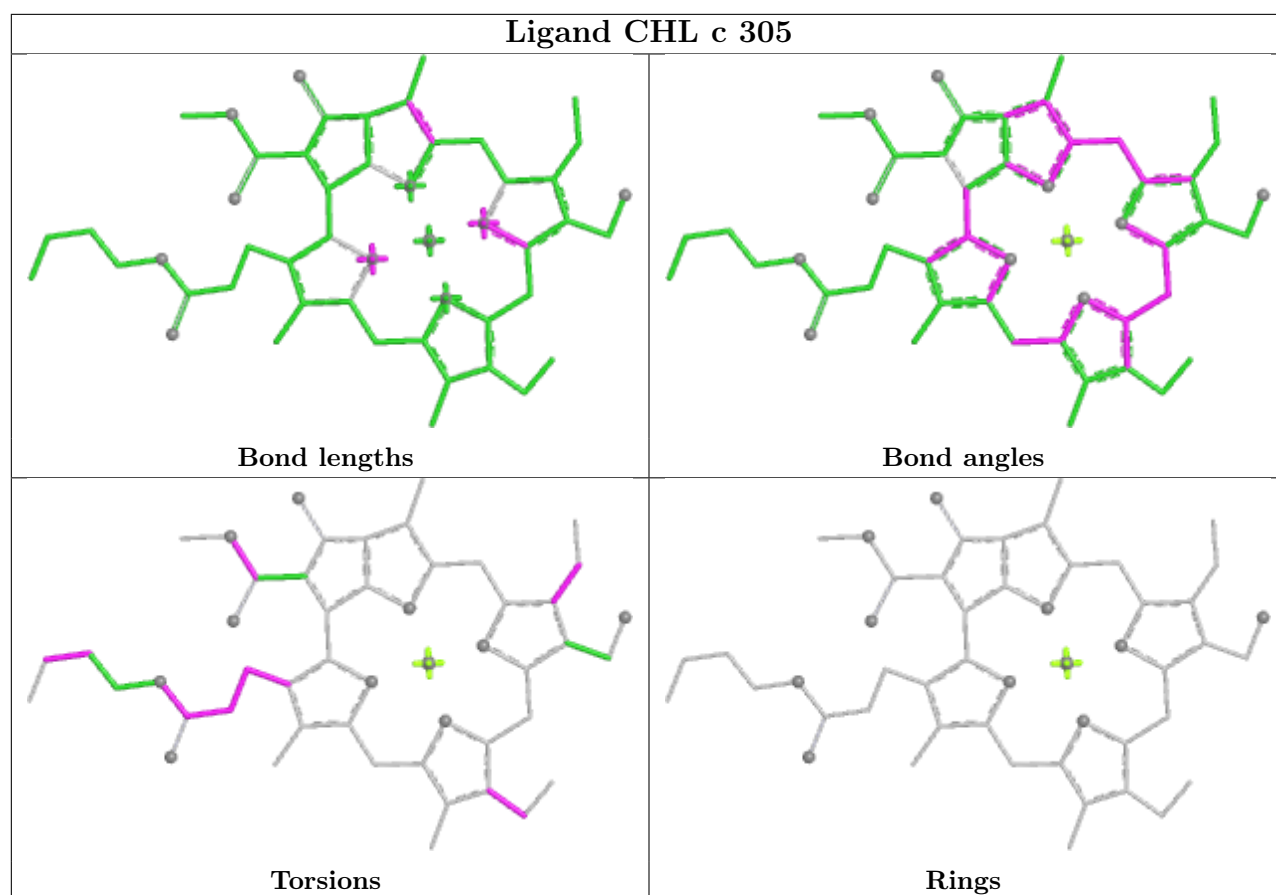


Ligand CLA 3 323

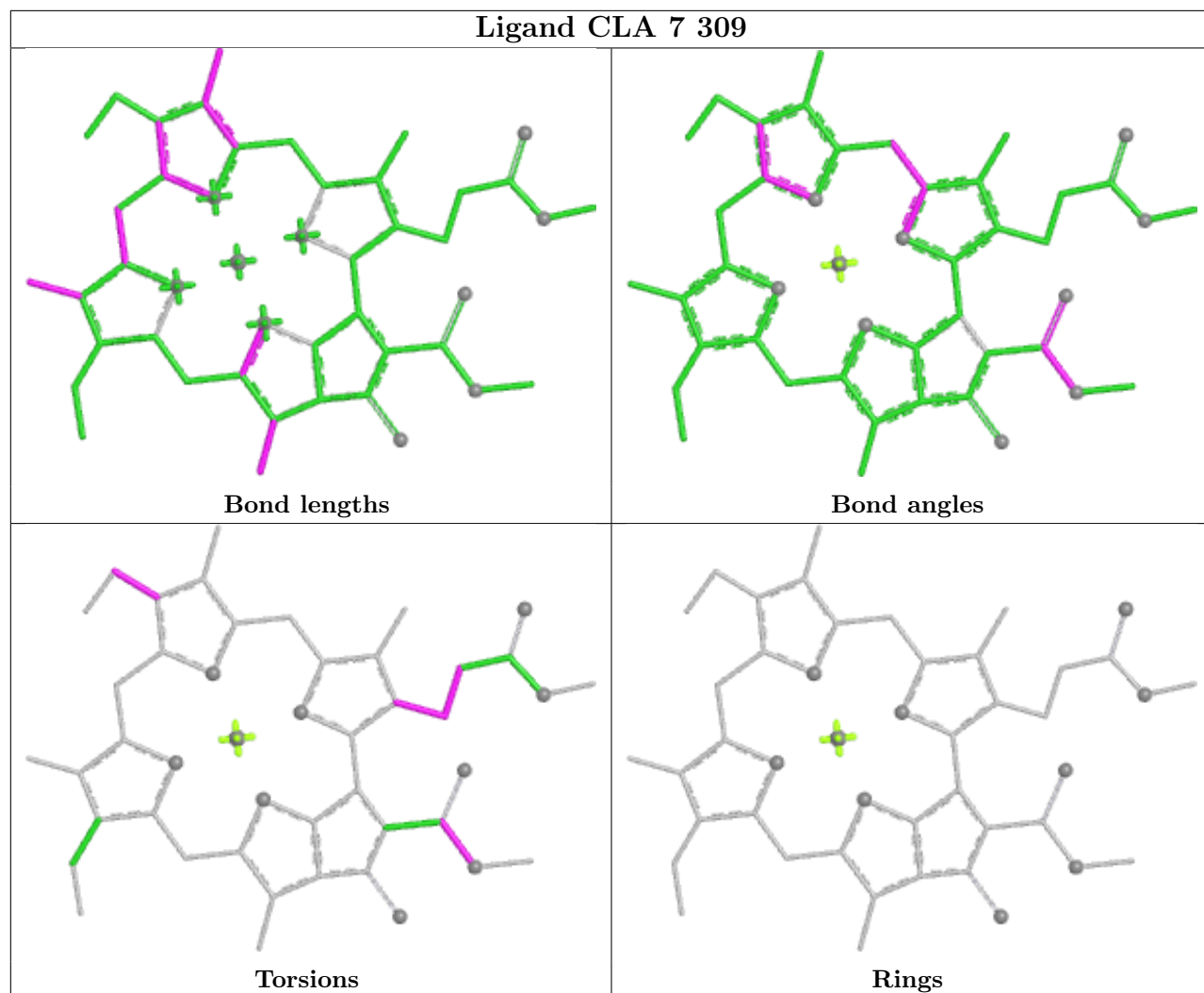


Ligand CLA T 403

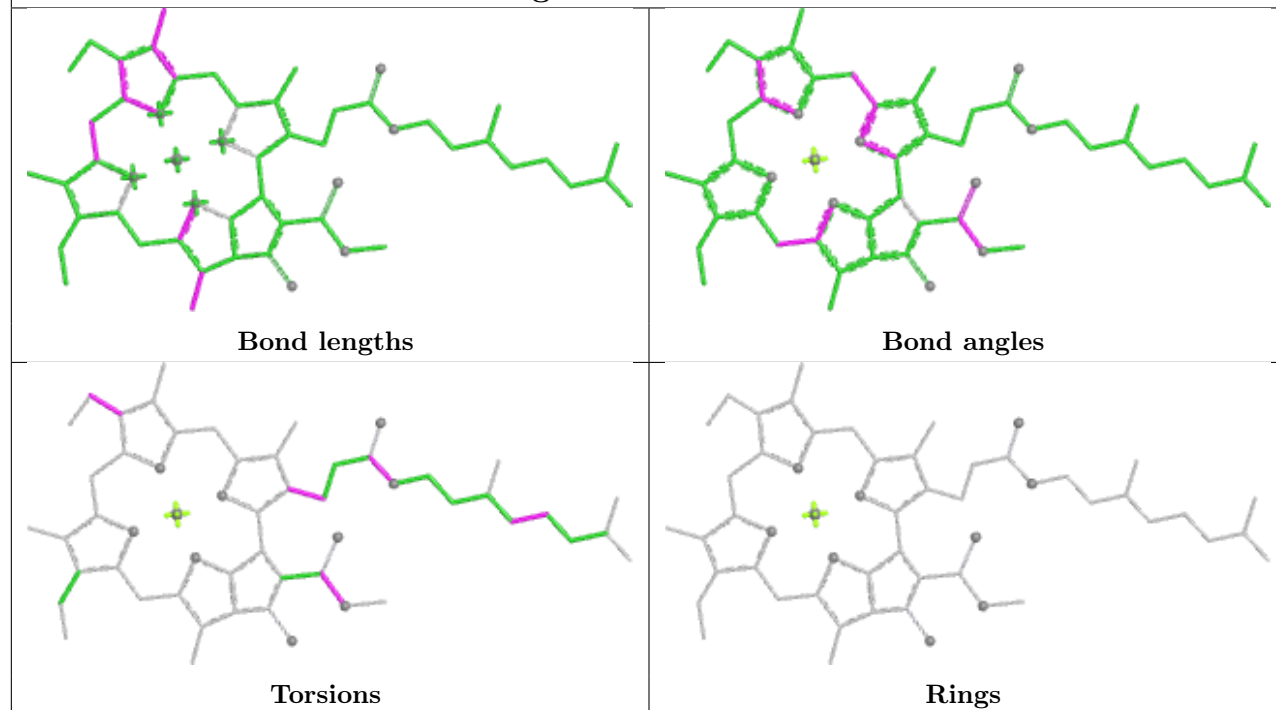




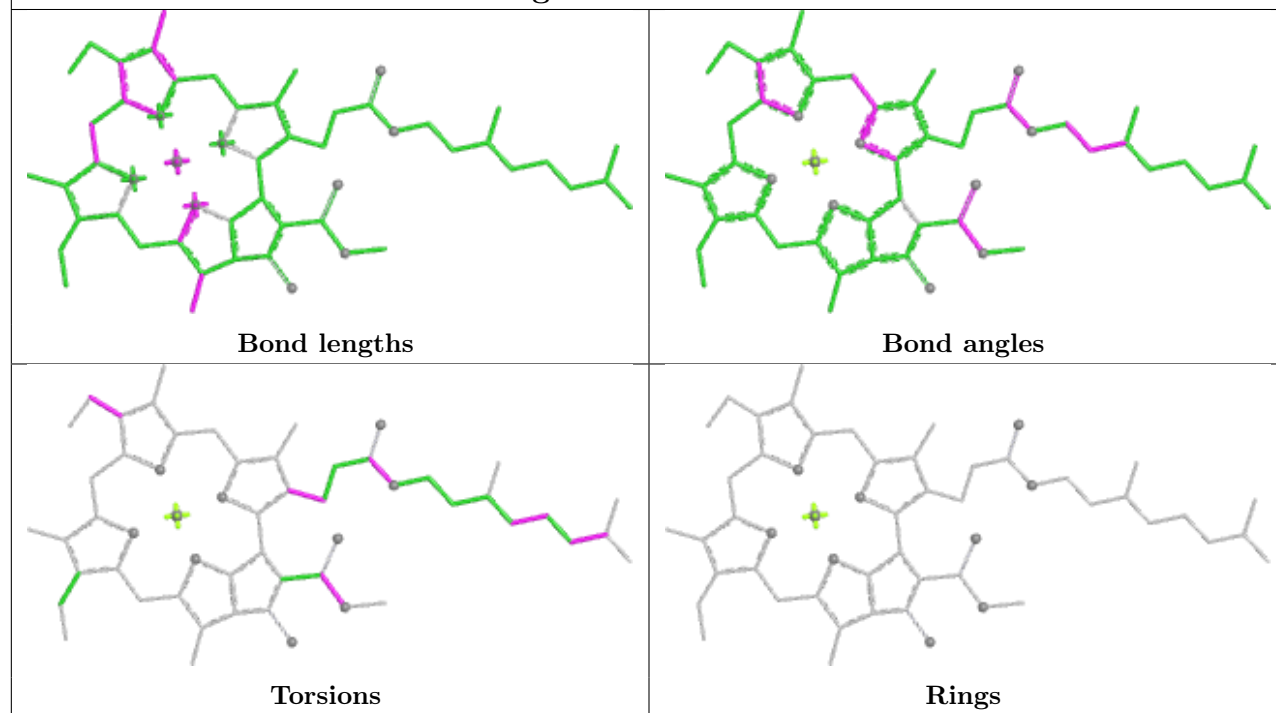
Ligand CLA 7 309



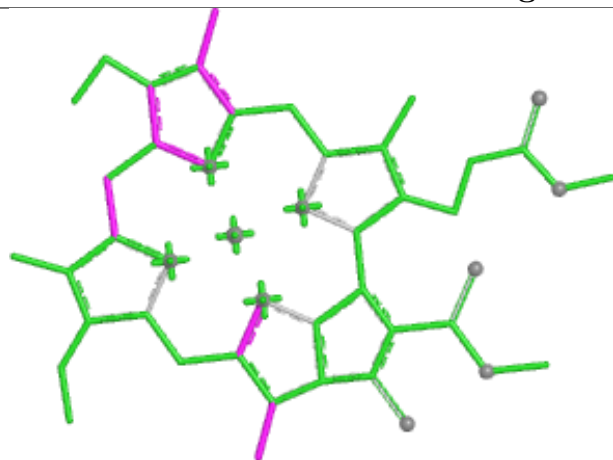
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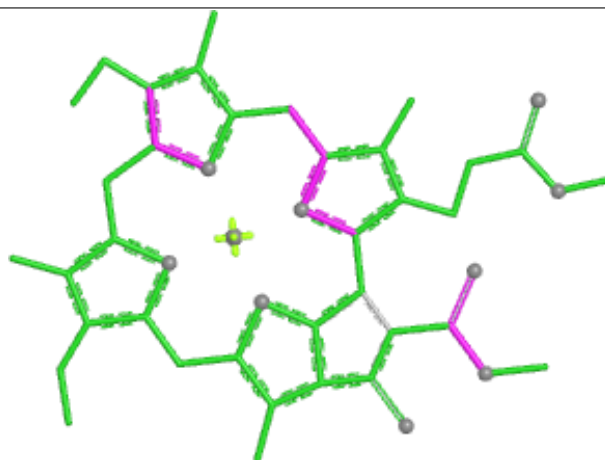
Ligand CLA B 831



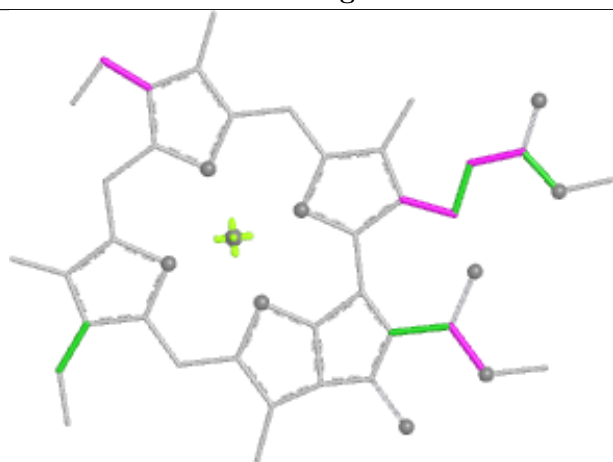
Ligand CLA a 614



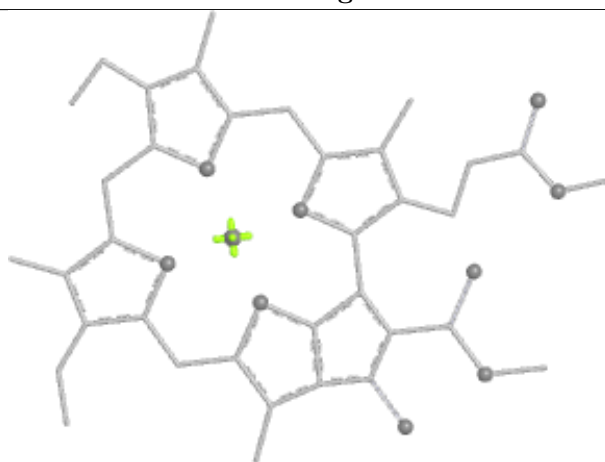
Bond lengths



Bond angles

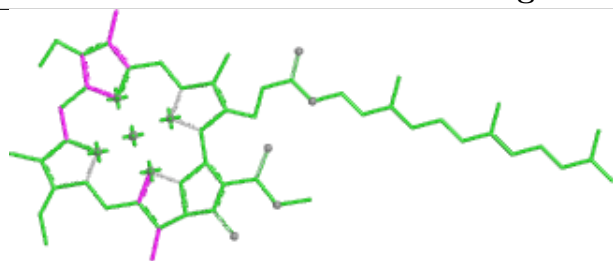


Torsions

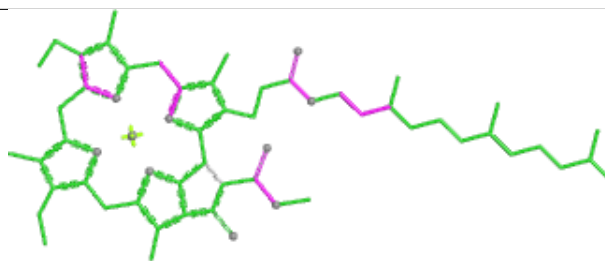


Rings

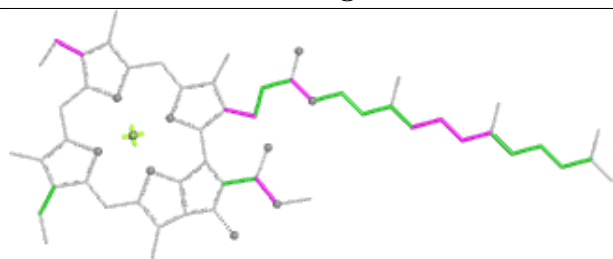
Ligand CLA b 602



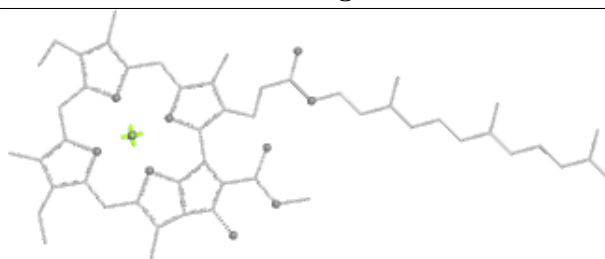
Bond lengths



Bond angles

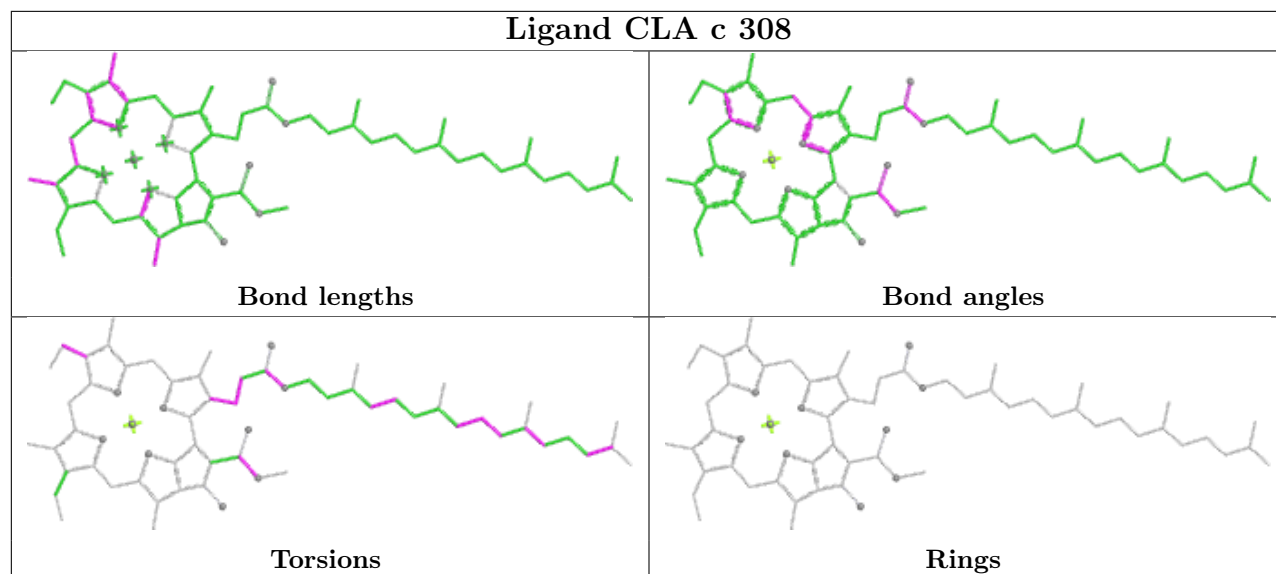


Torsions

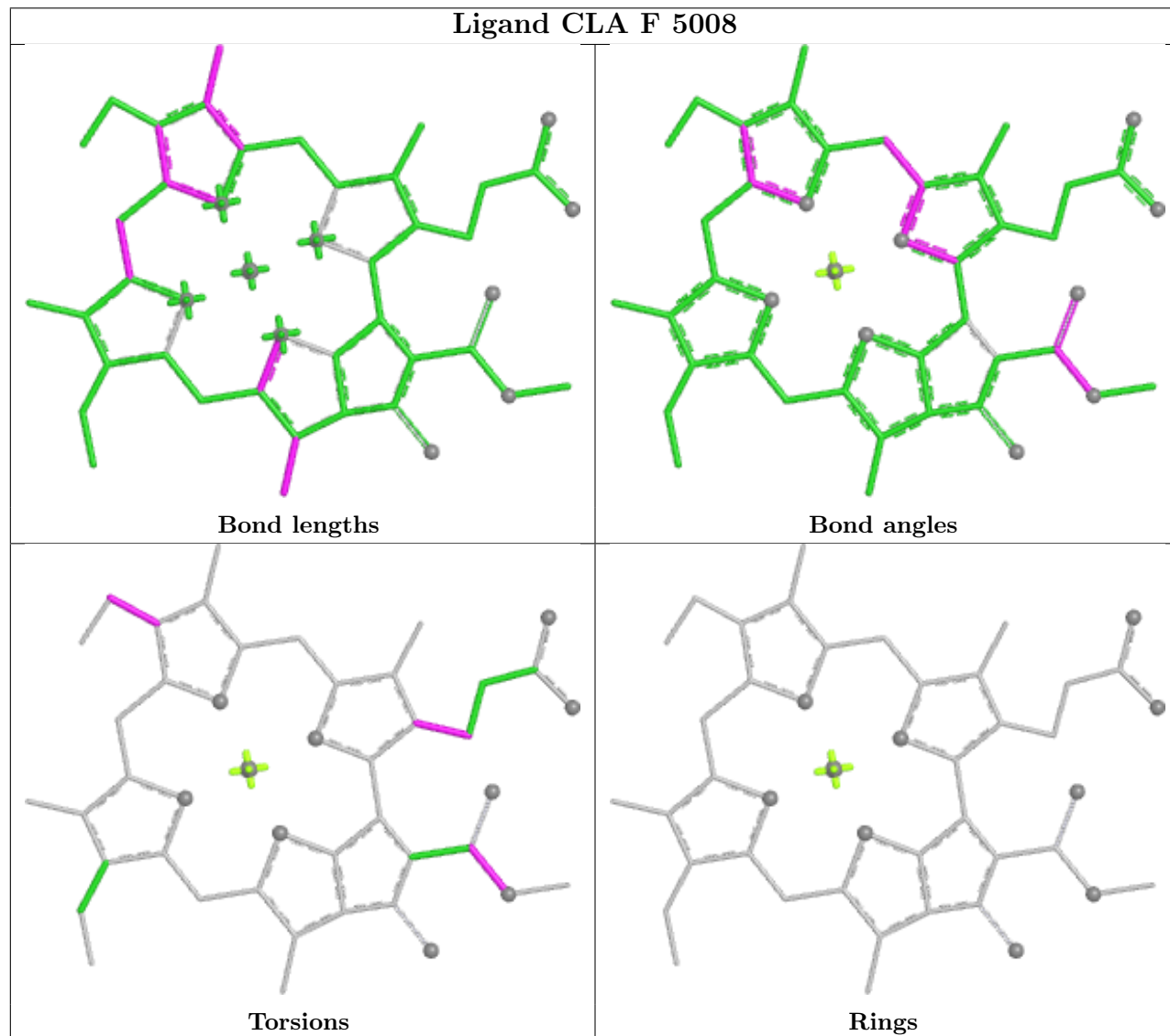


Rings

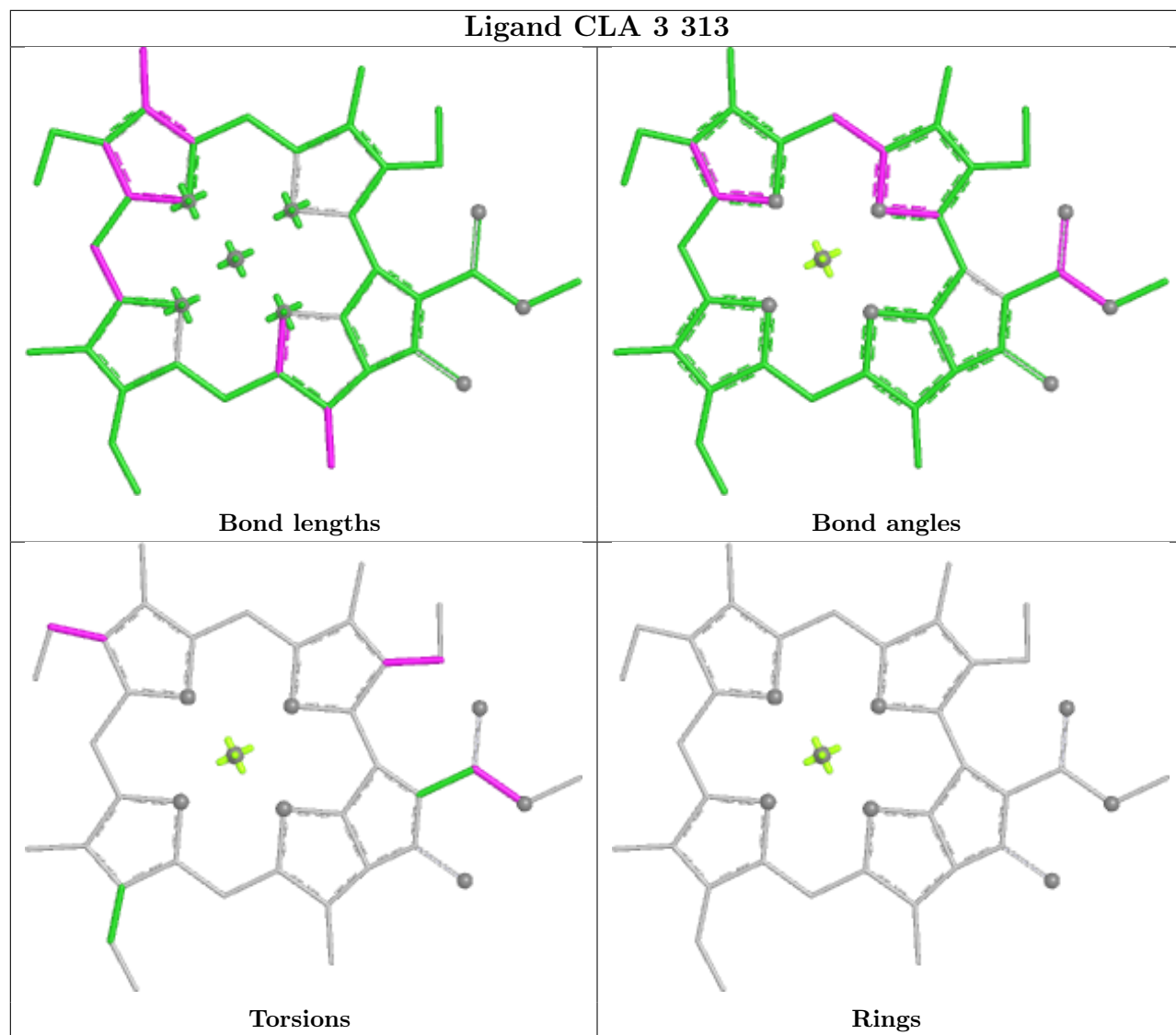
Ligand CLA c 308

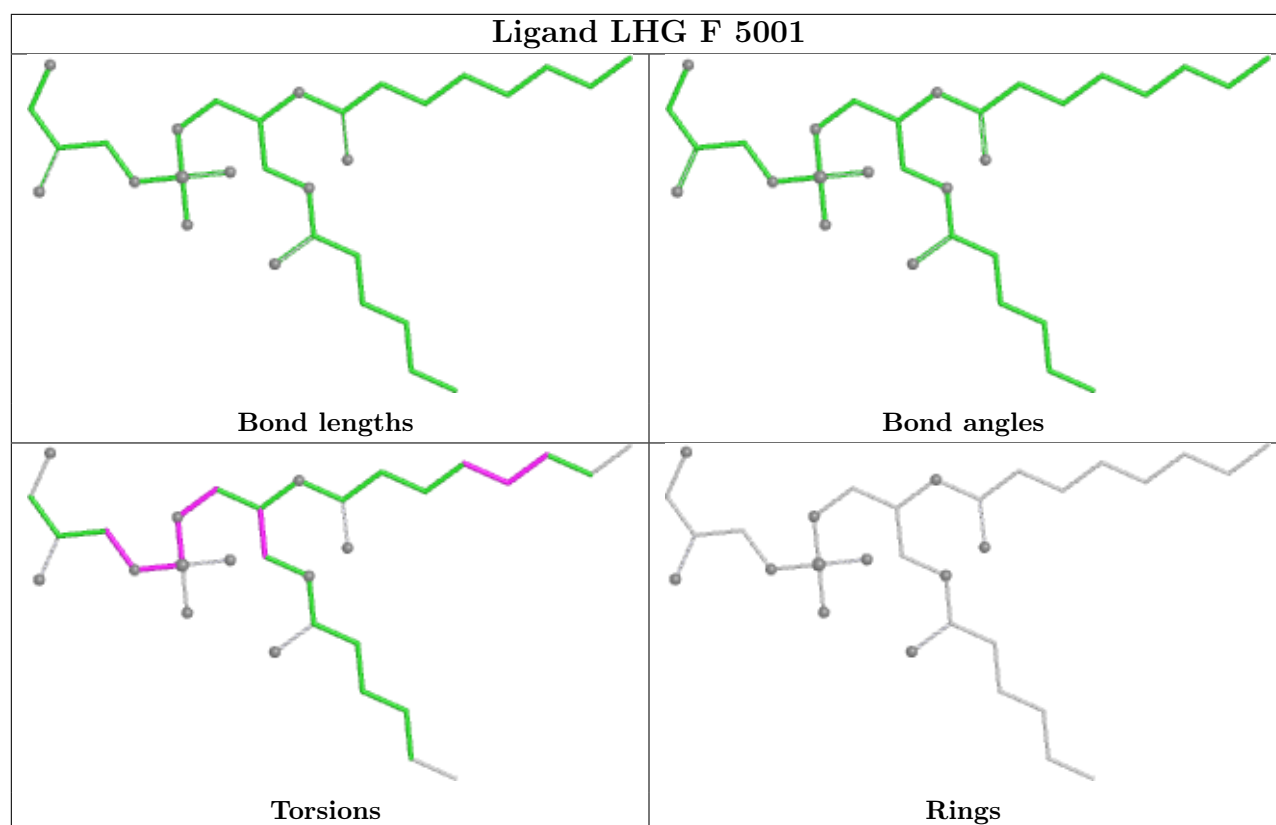


Ligand CLA F 5008

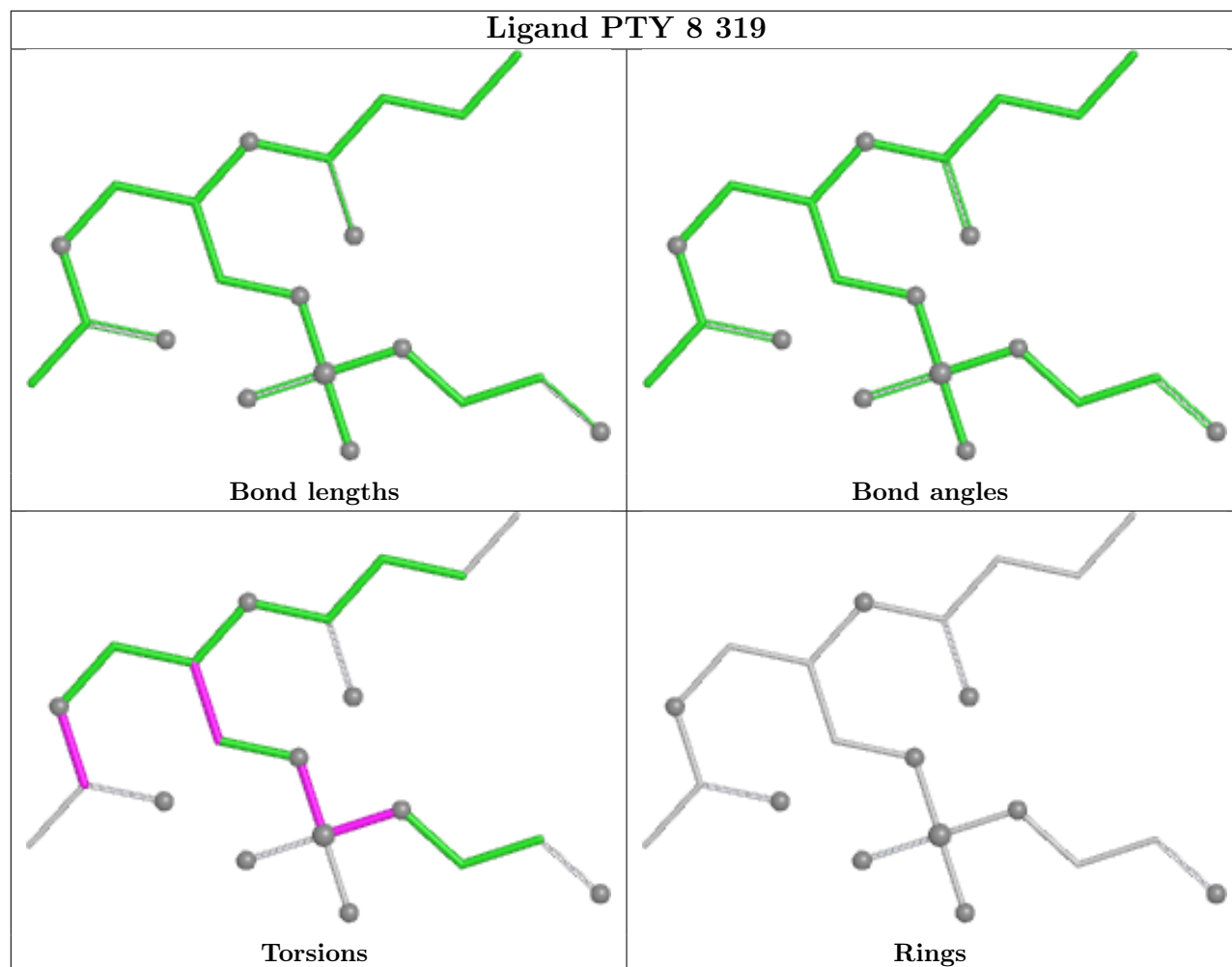


Ligand CLA 3 313

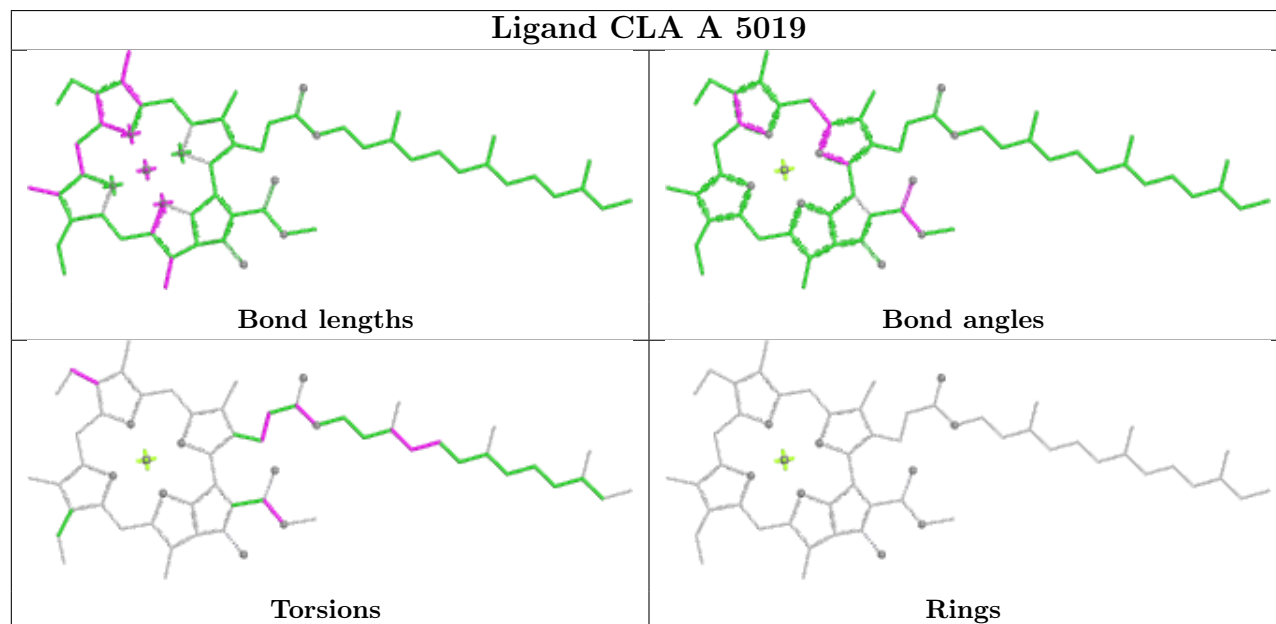


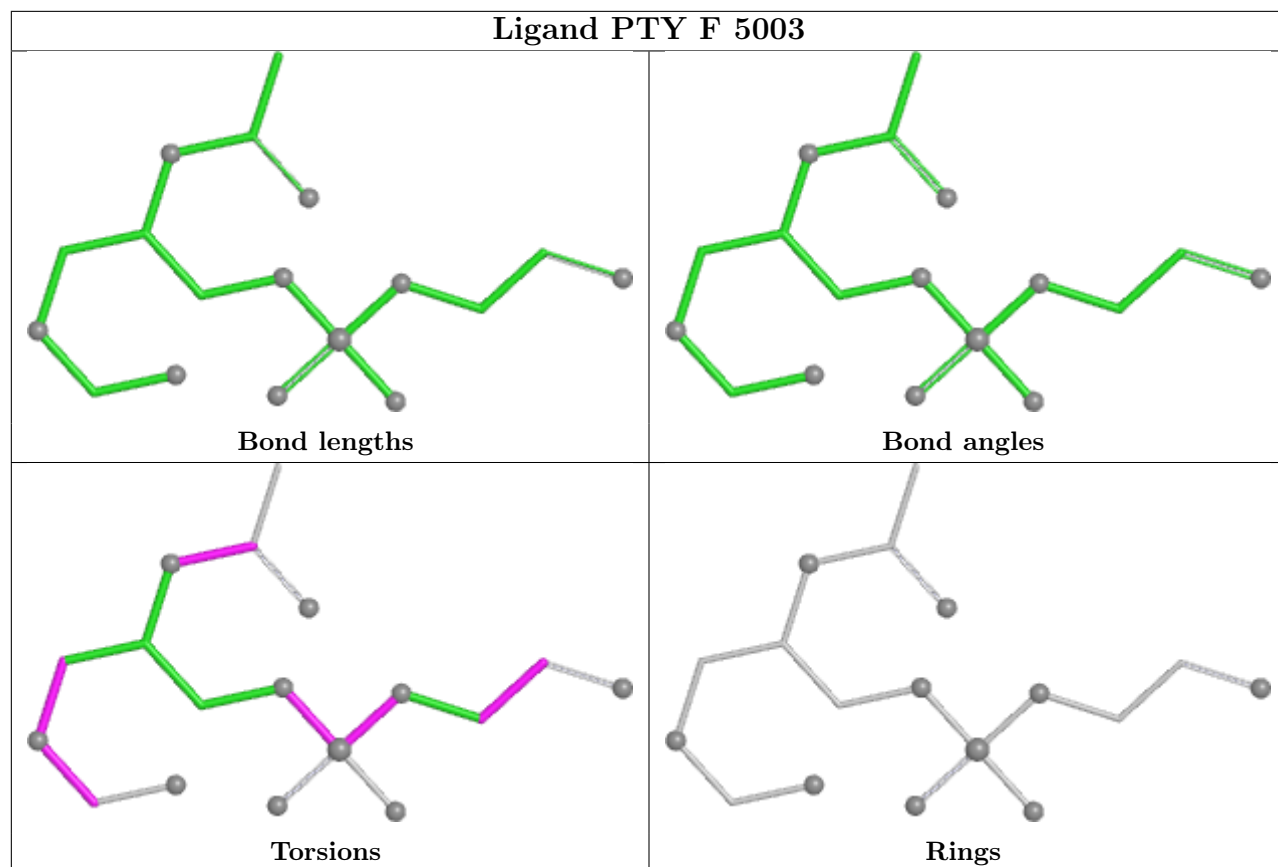


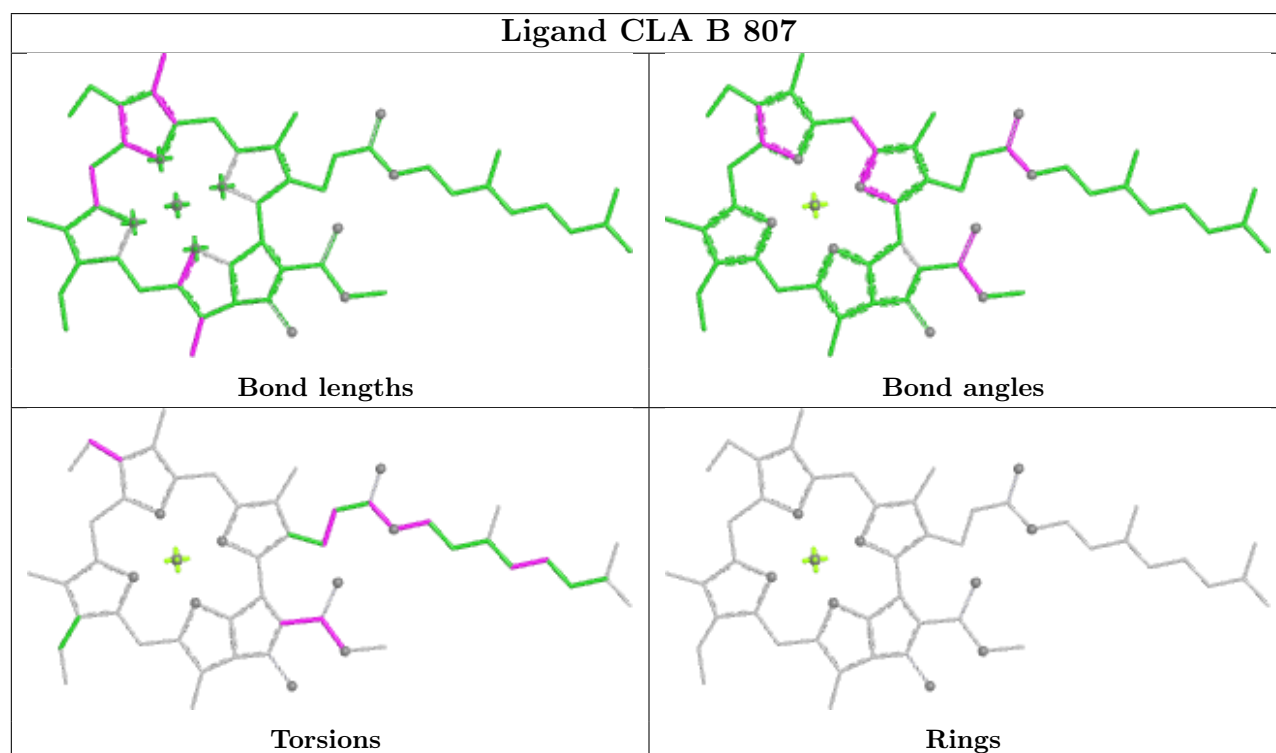
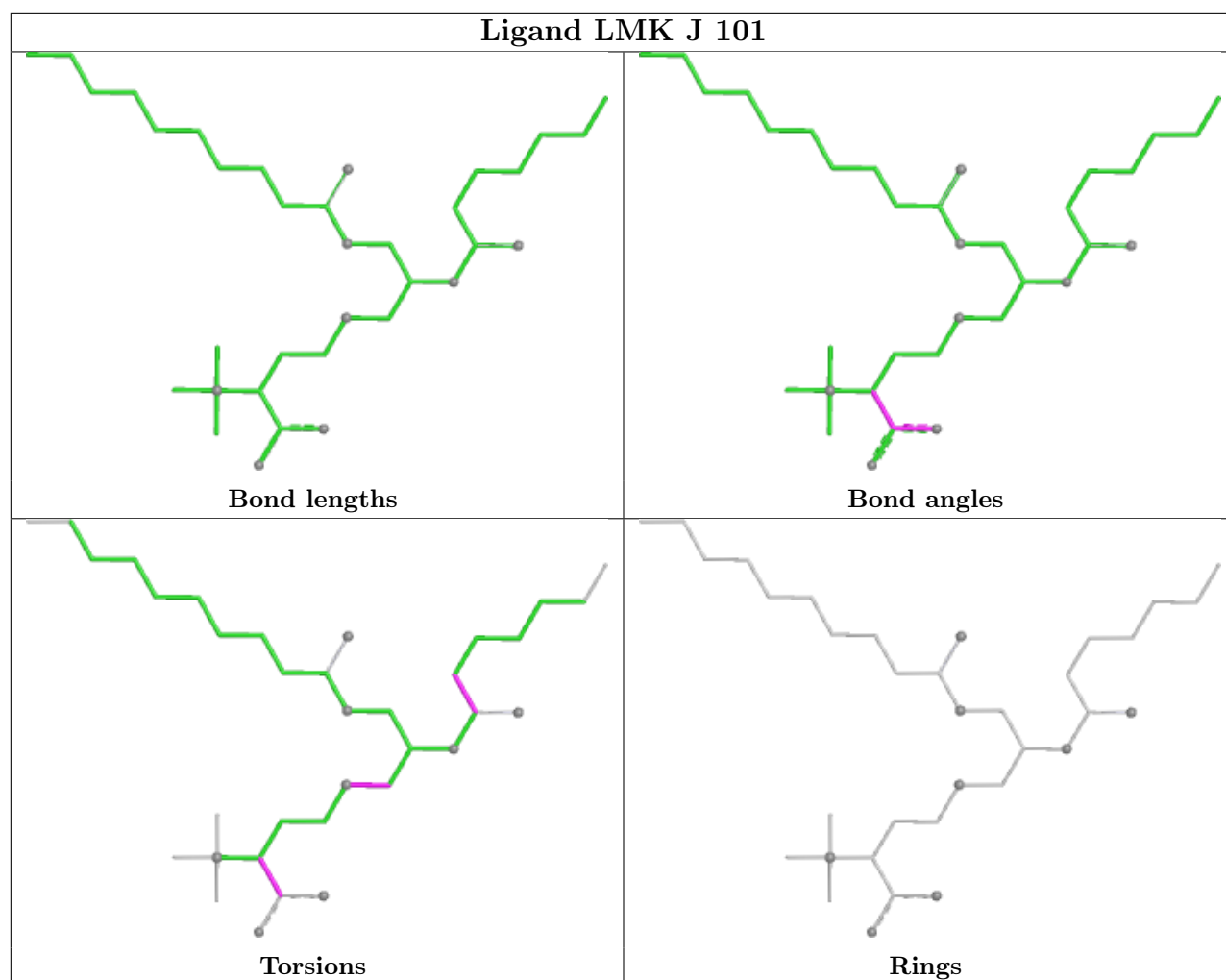
Ligand PTY 8 319



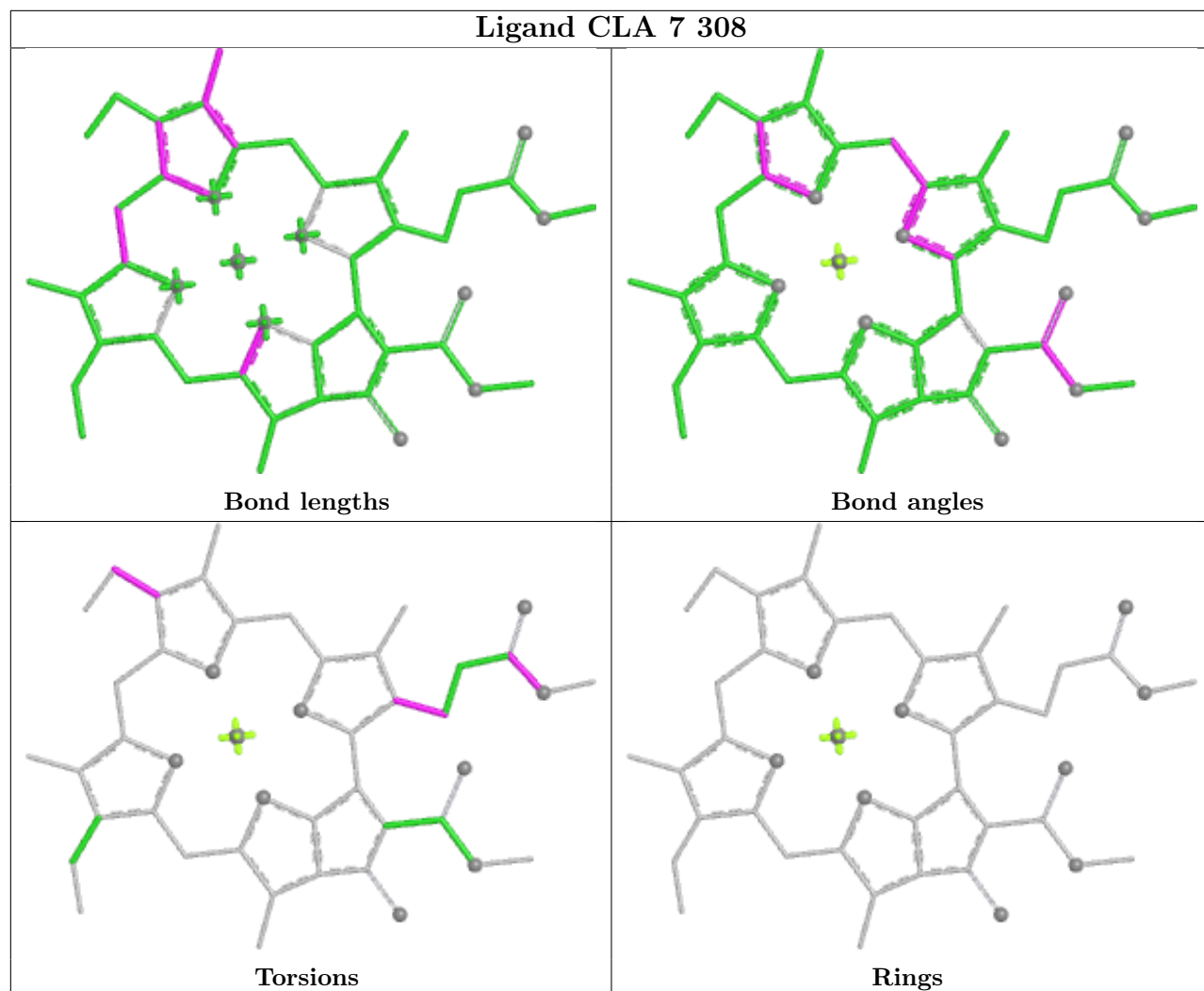
Ligand CLA A 5019



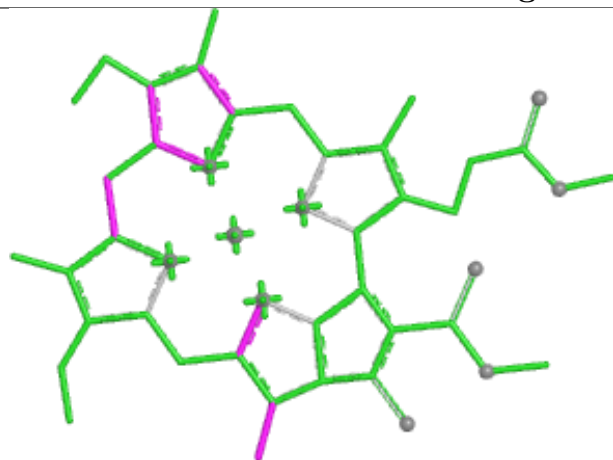




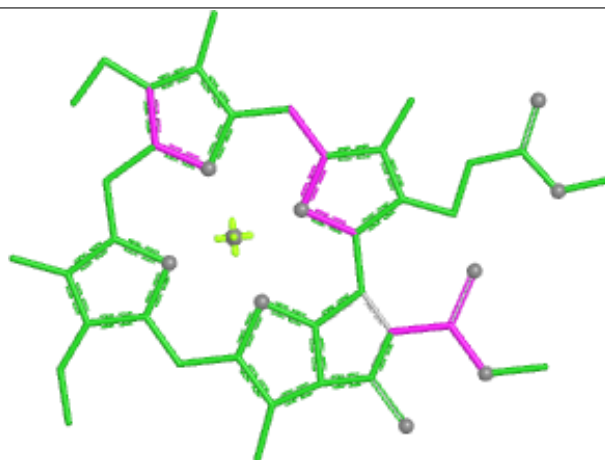
Ligand CLA 7 308



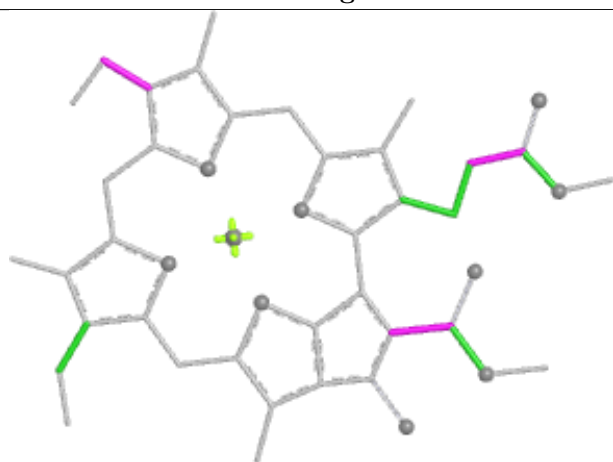
Ligand CLA 8 302



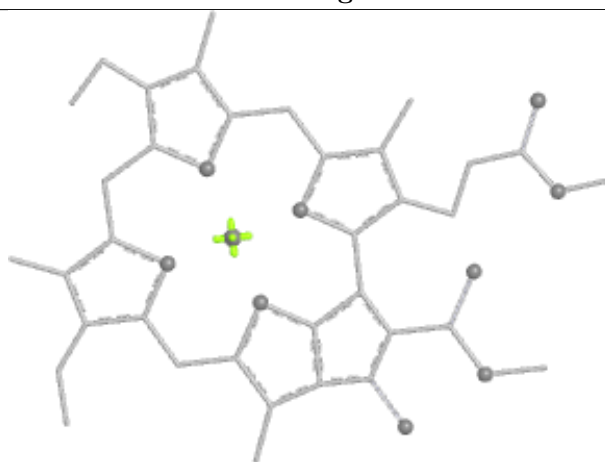
Bond lengths



Bond angles

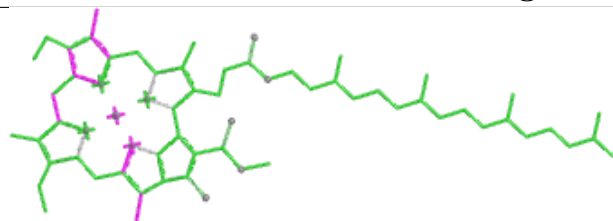


Torsions

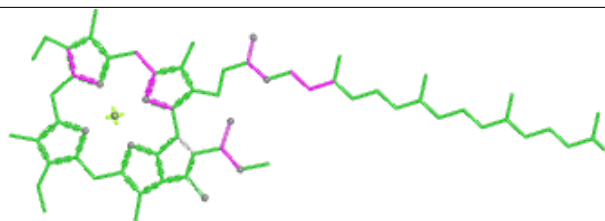


Rings

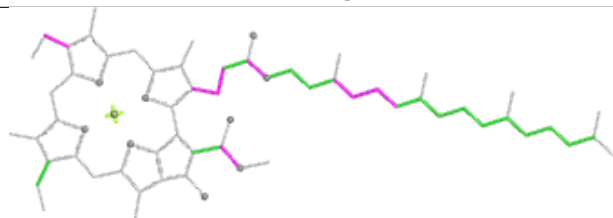
Ligand CLA 7 312



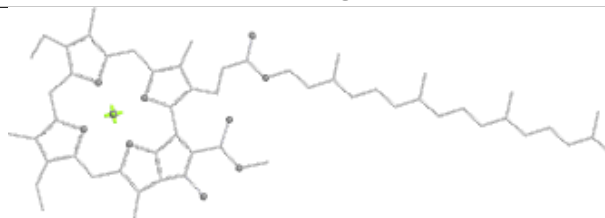
Bond lengths



Bond angles

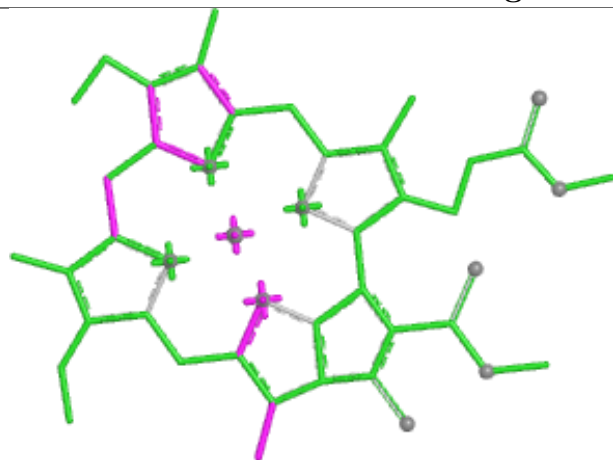


Torsions

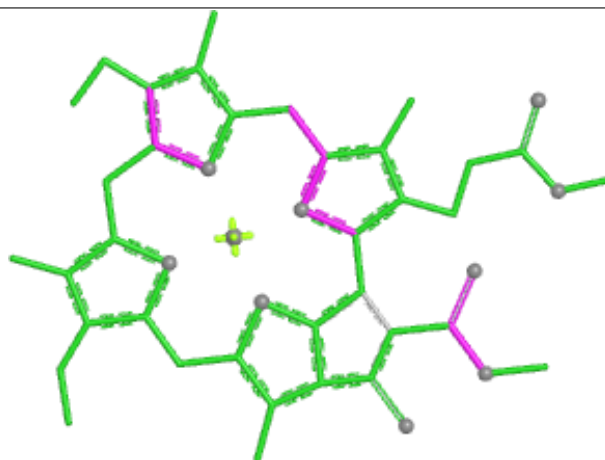


Rings

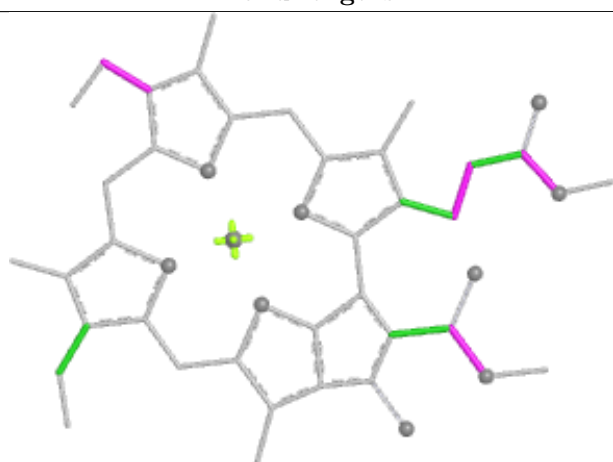
Ligand CLA A 5023



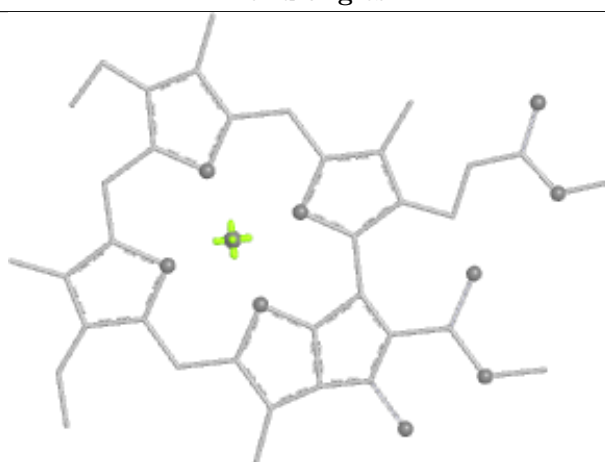
Bond lengths



Bond angles

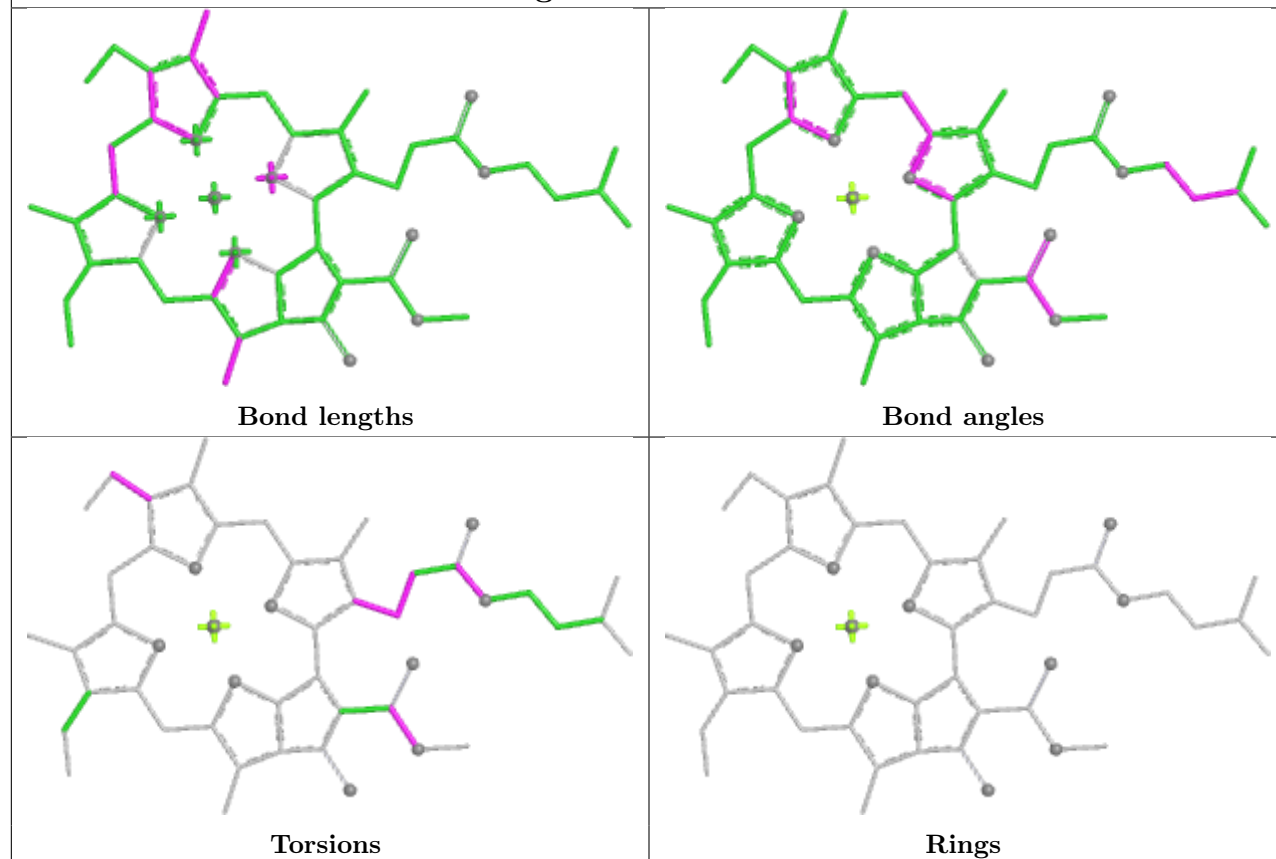


Torsions

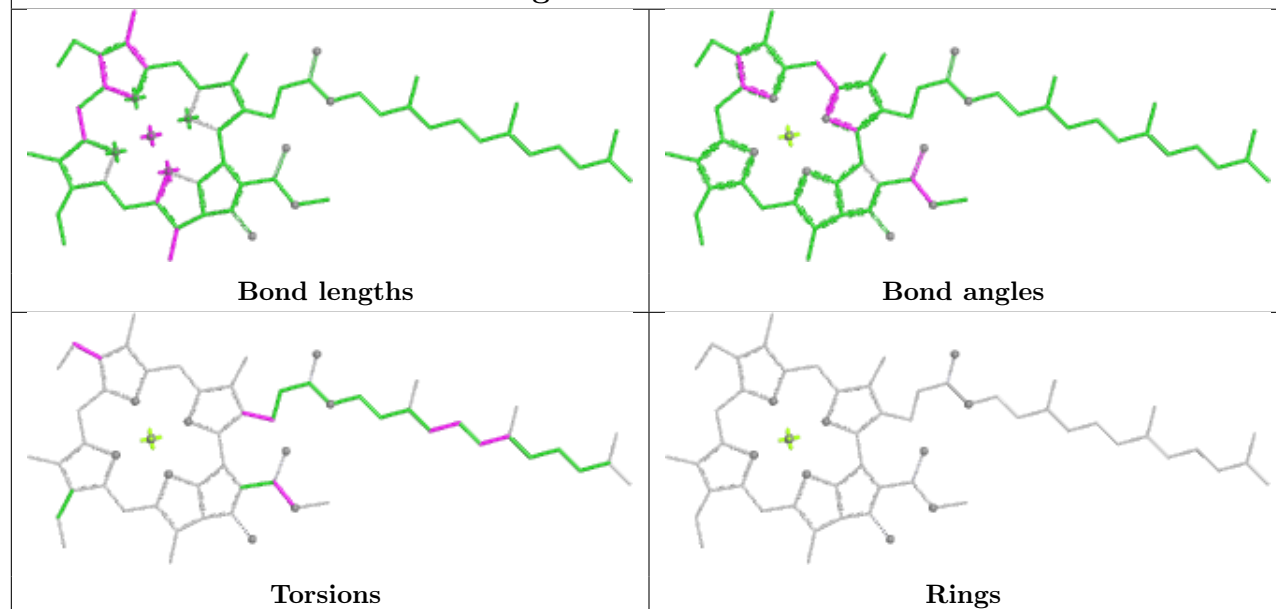


Rings

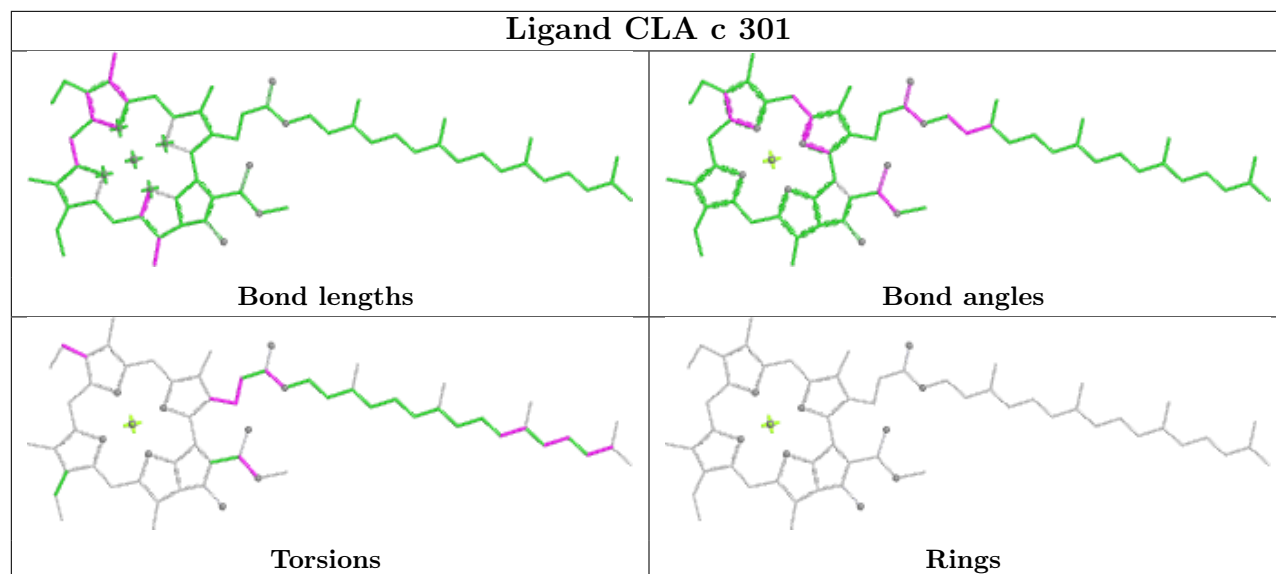
Ligand CLA b 604



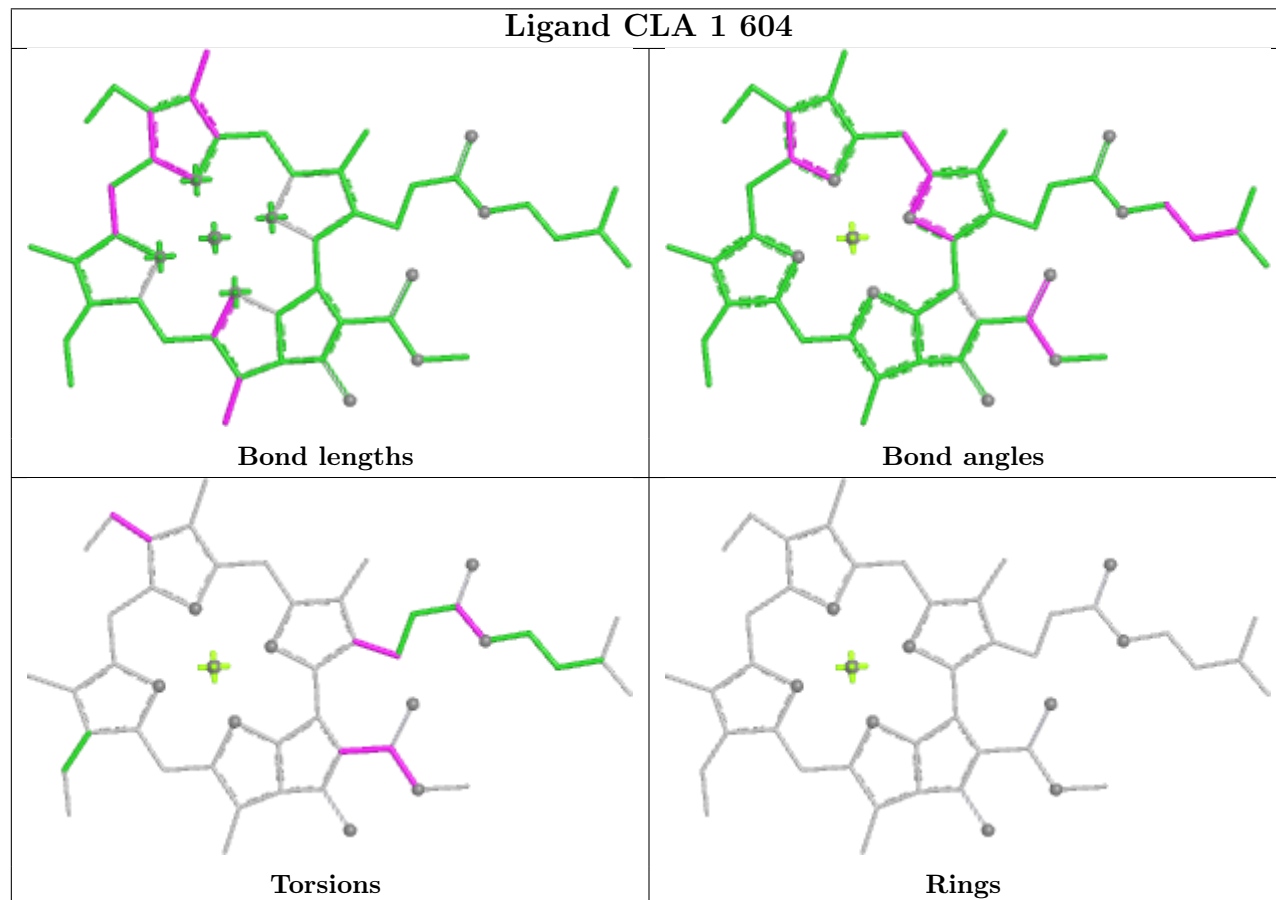
Ligand CLA B 819



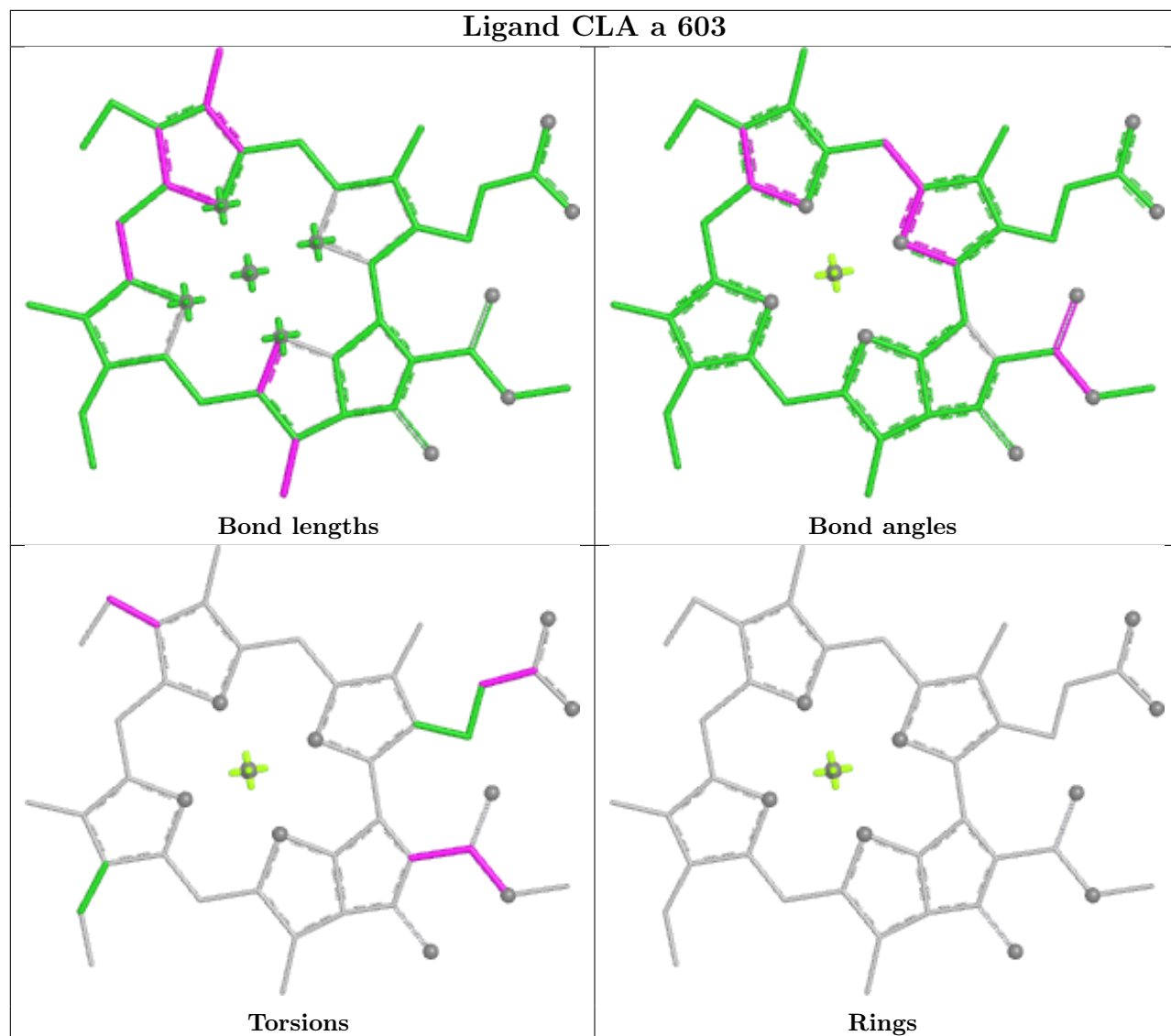
Ligand CLA c 301



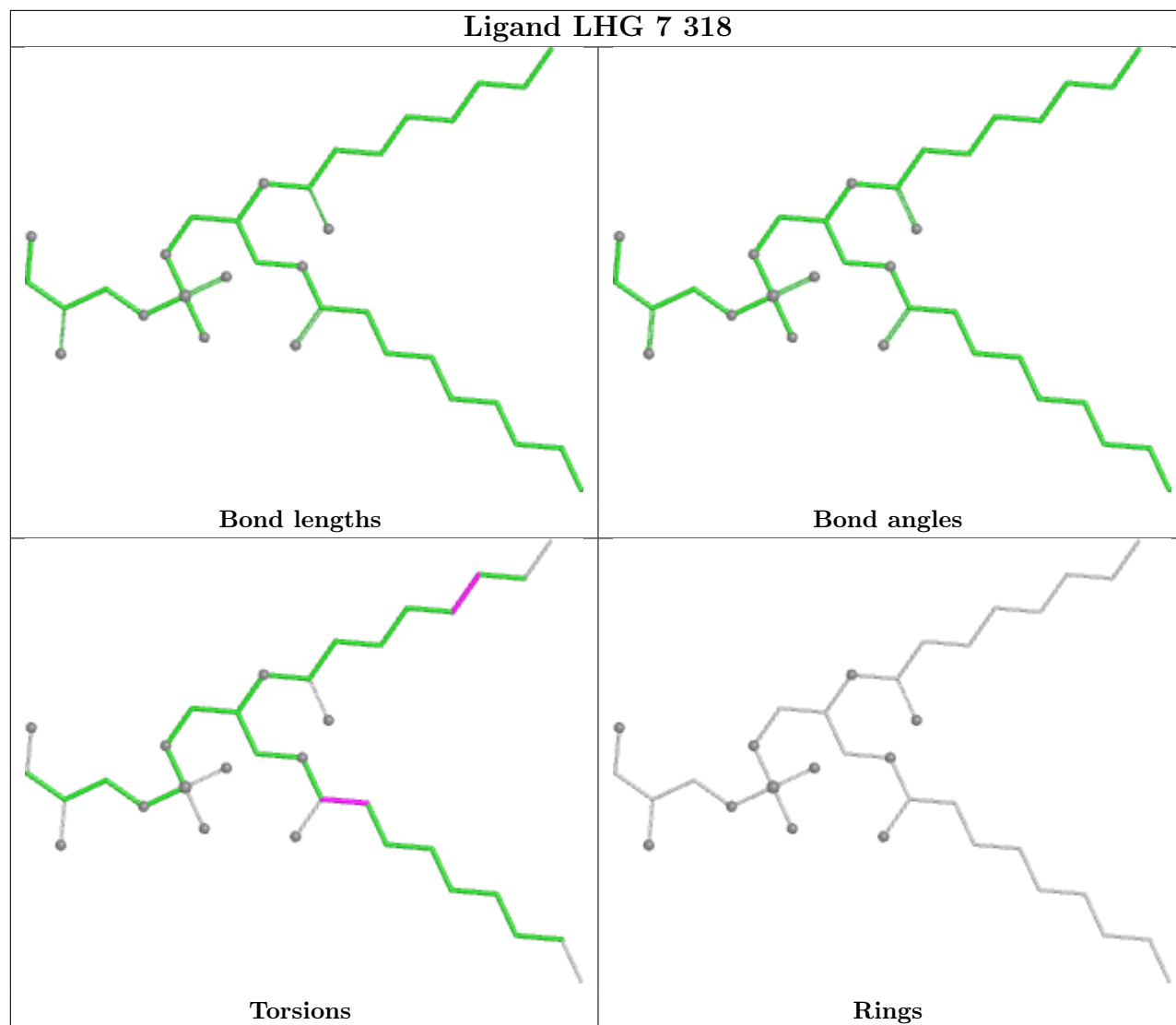
Ligand CLA 1 604



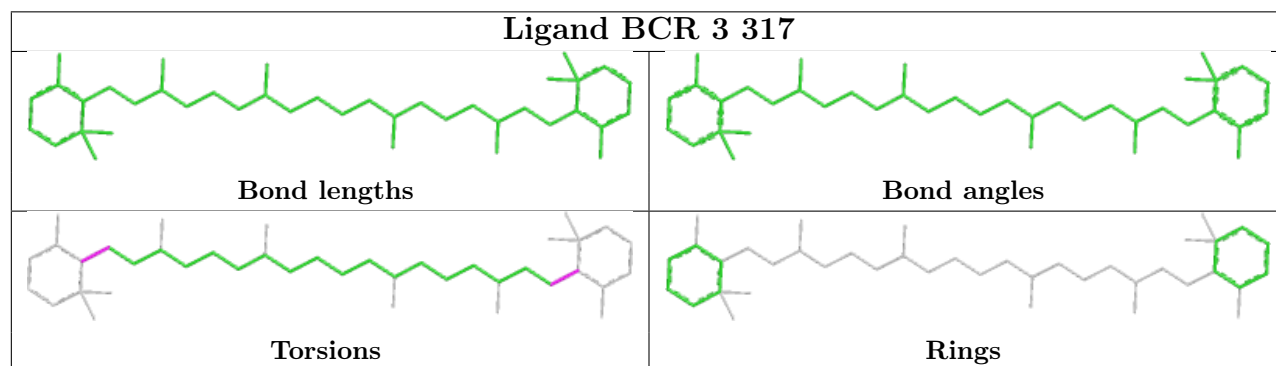
Ligand CLA a 603

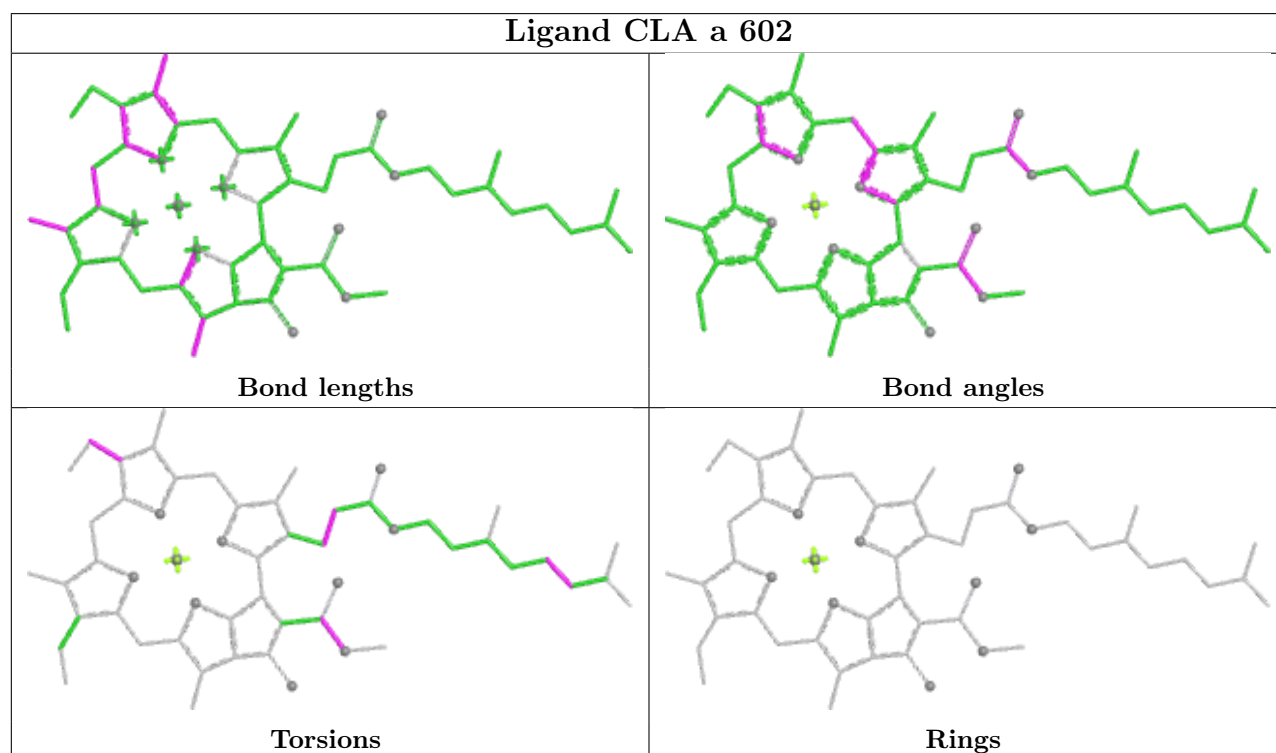
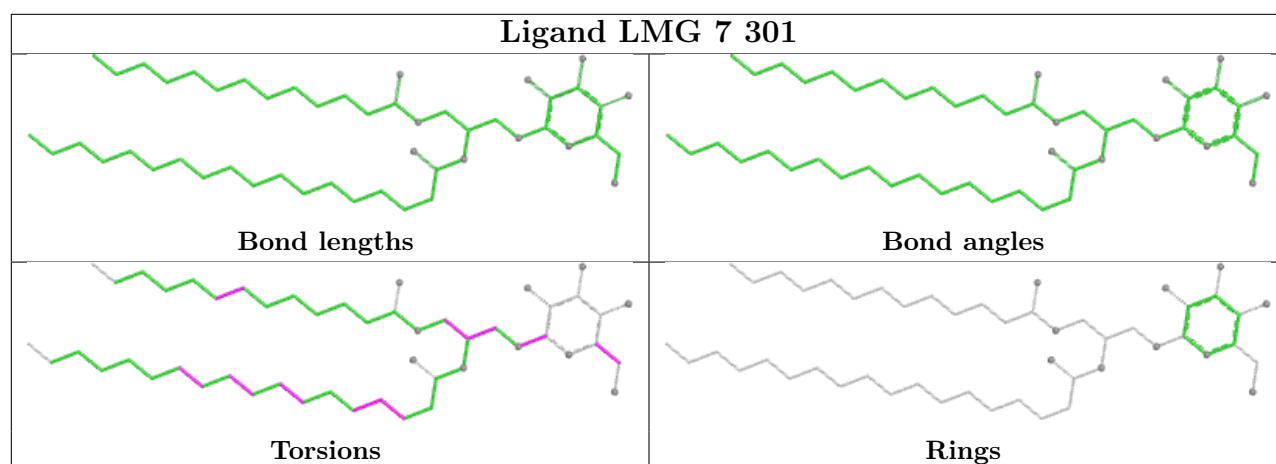


Ligand LHG 7 318

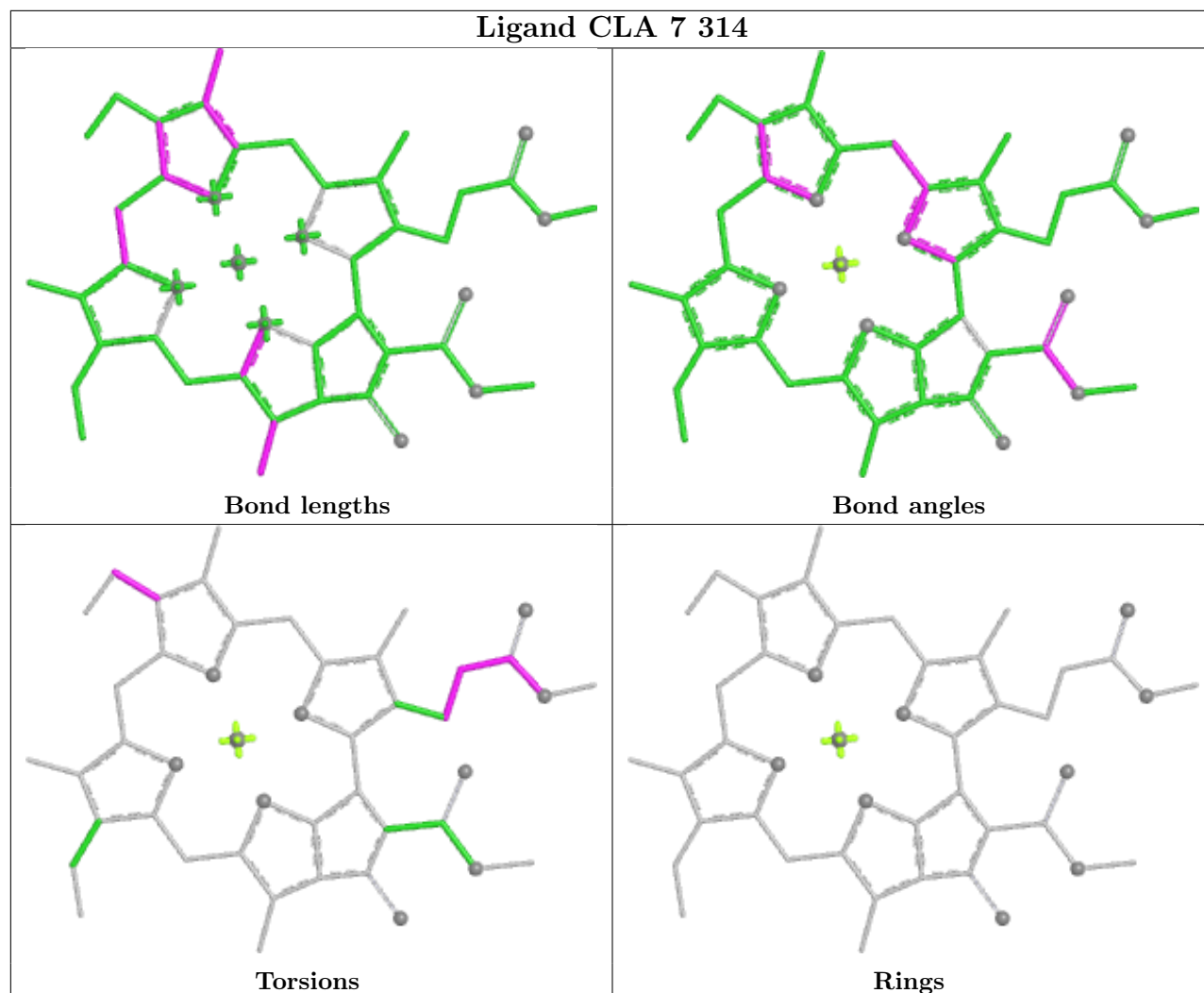


Ligand BCR 3 317

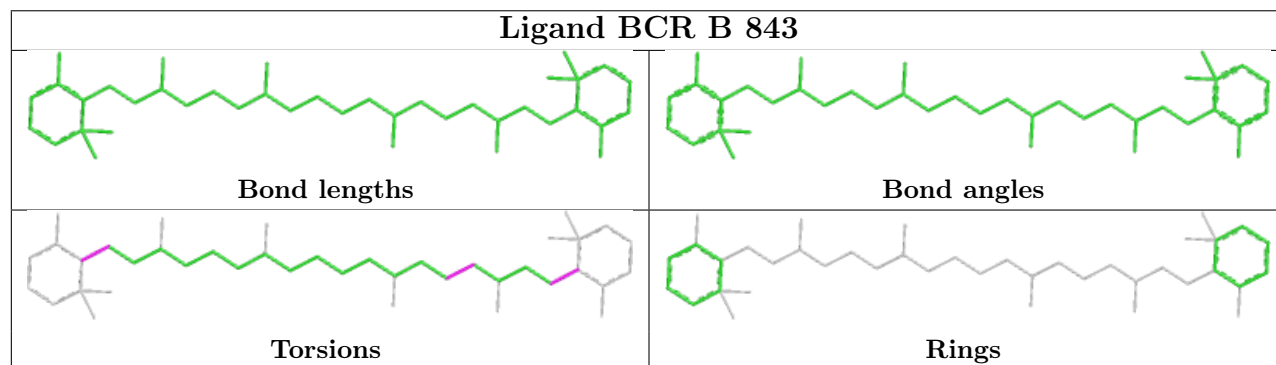




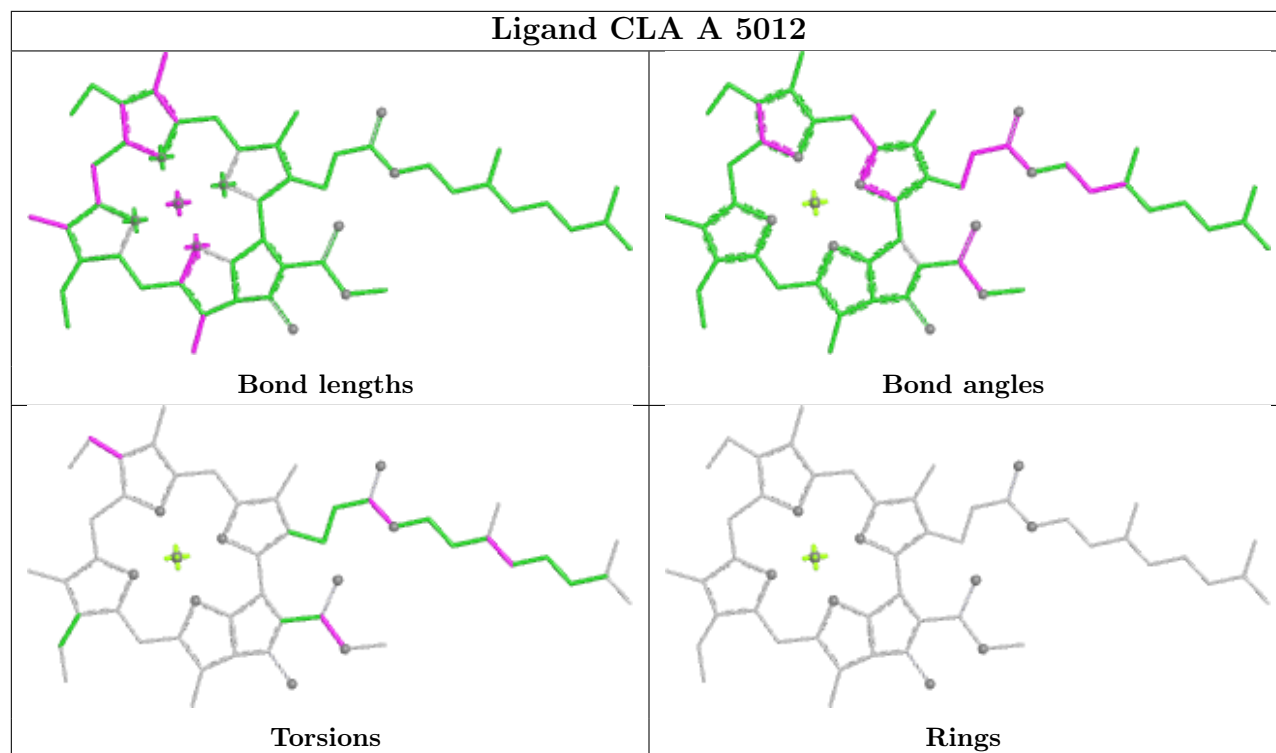
Ligand CLA 7 314



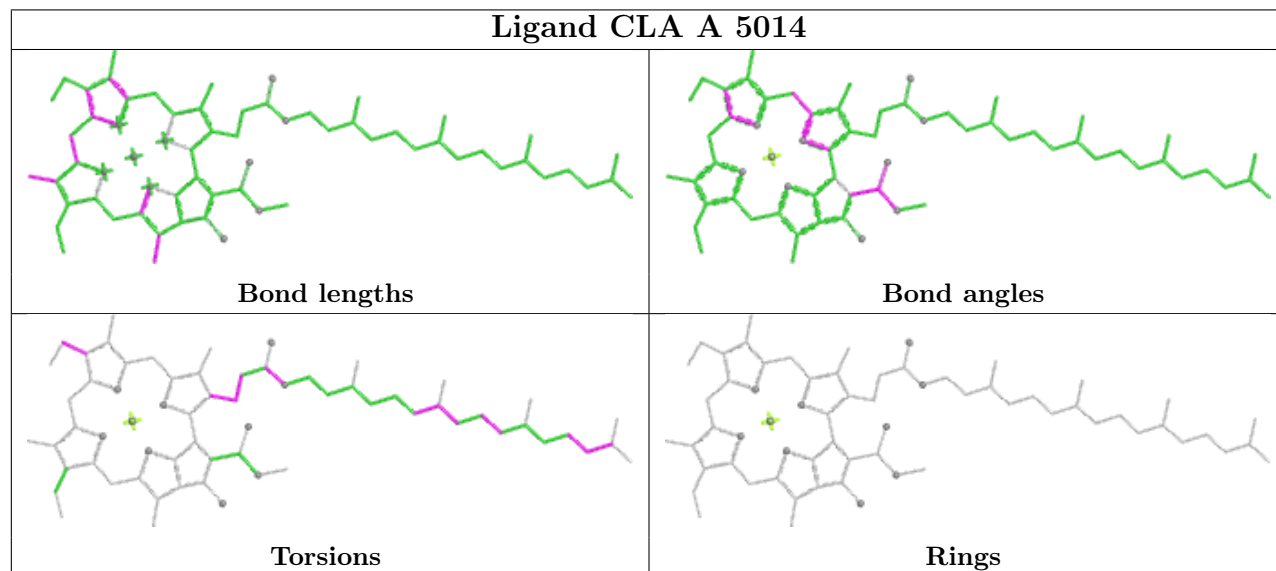
Ligand BCR B 843



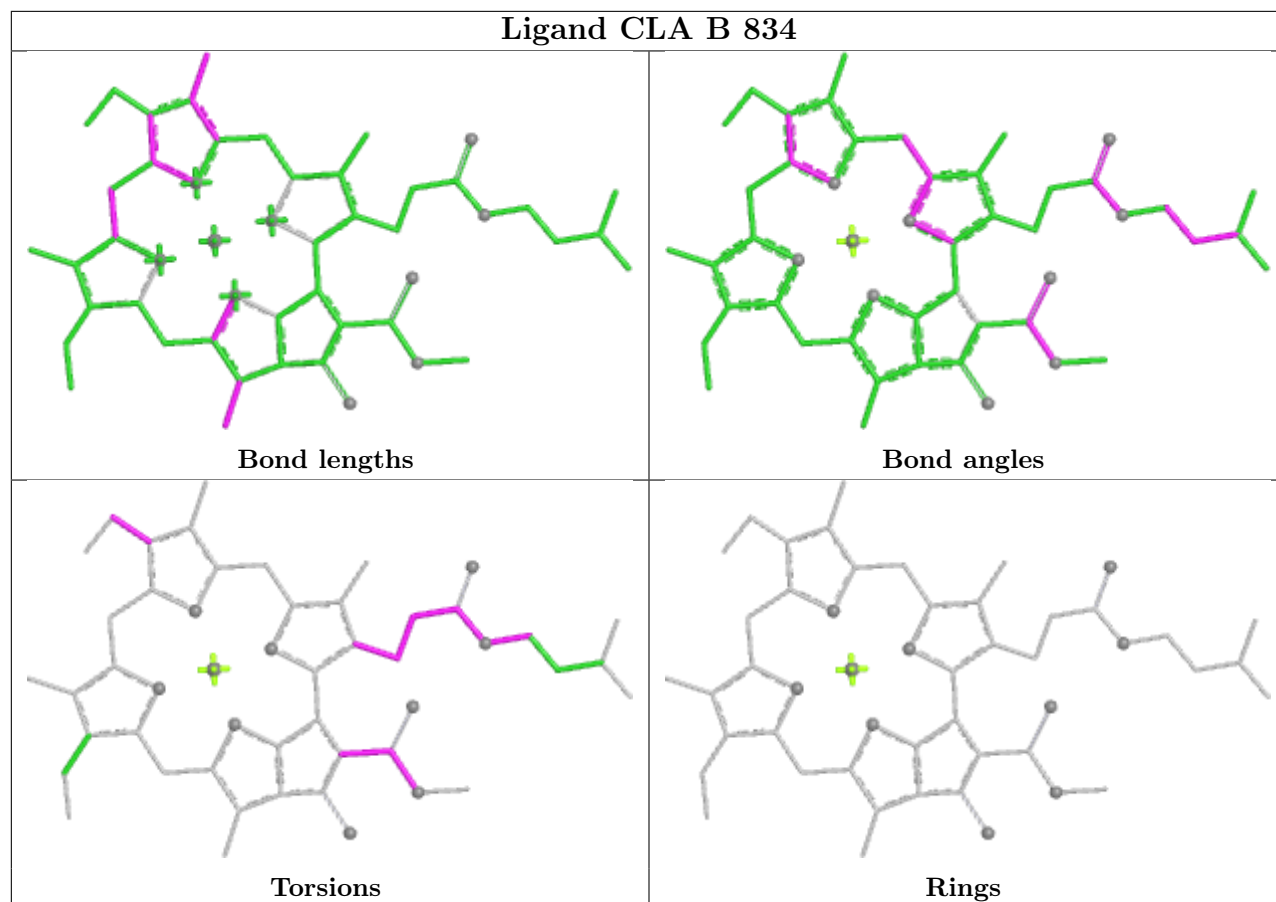
Ligand CLA A 5012

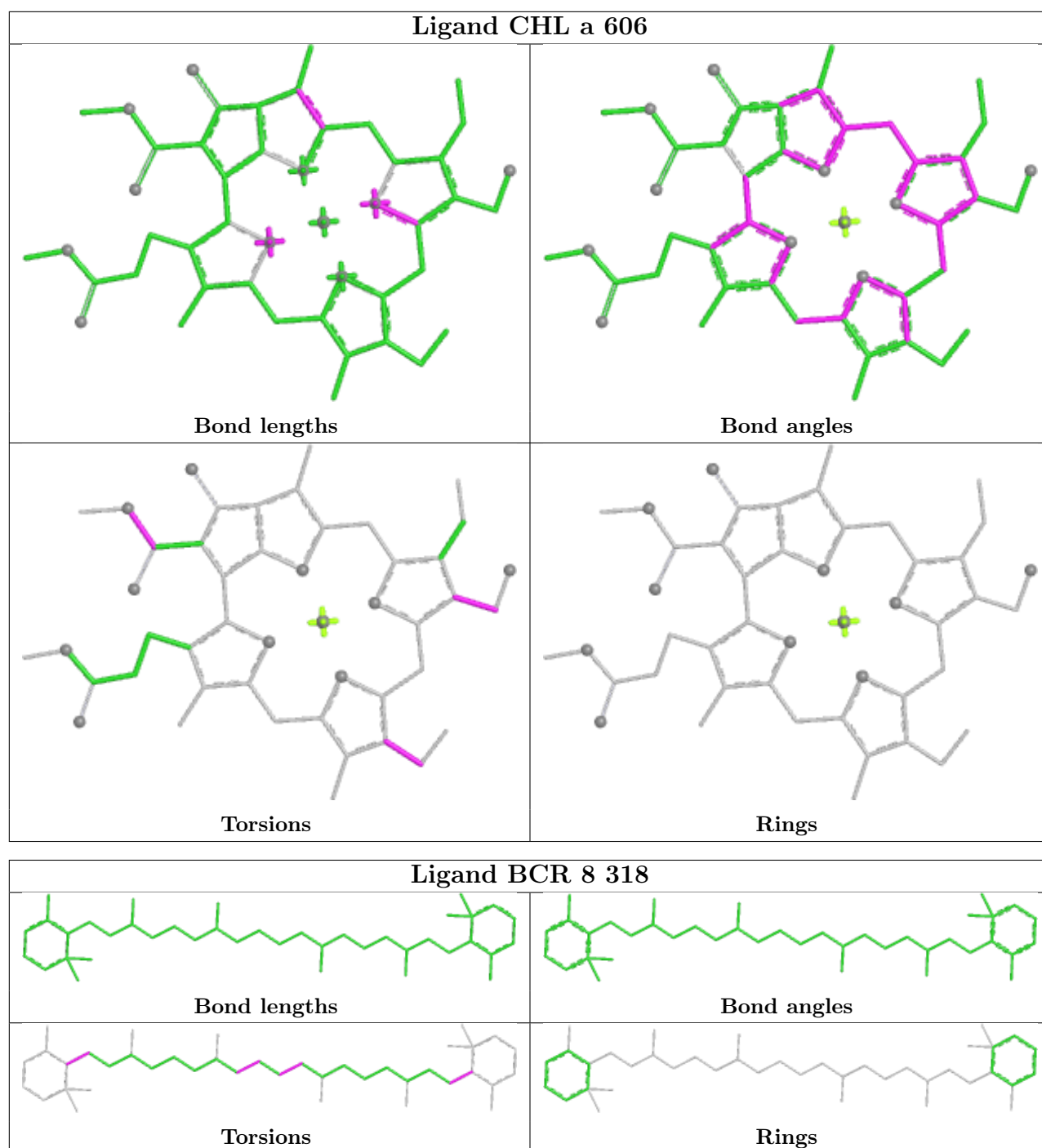


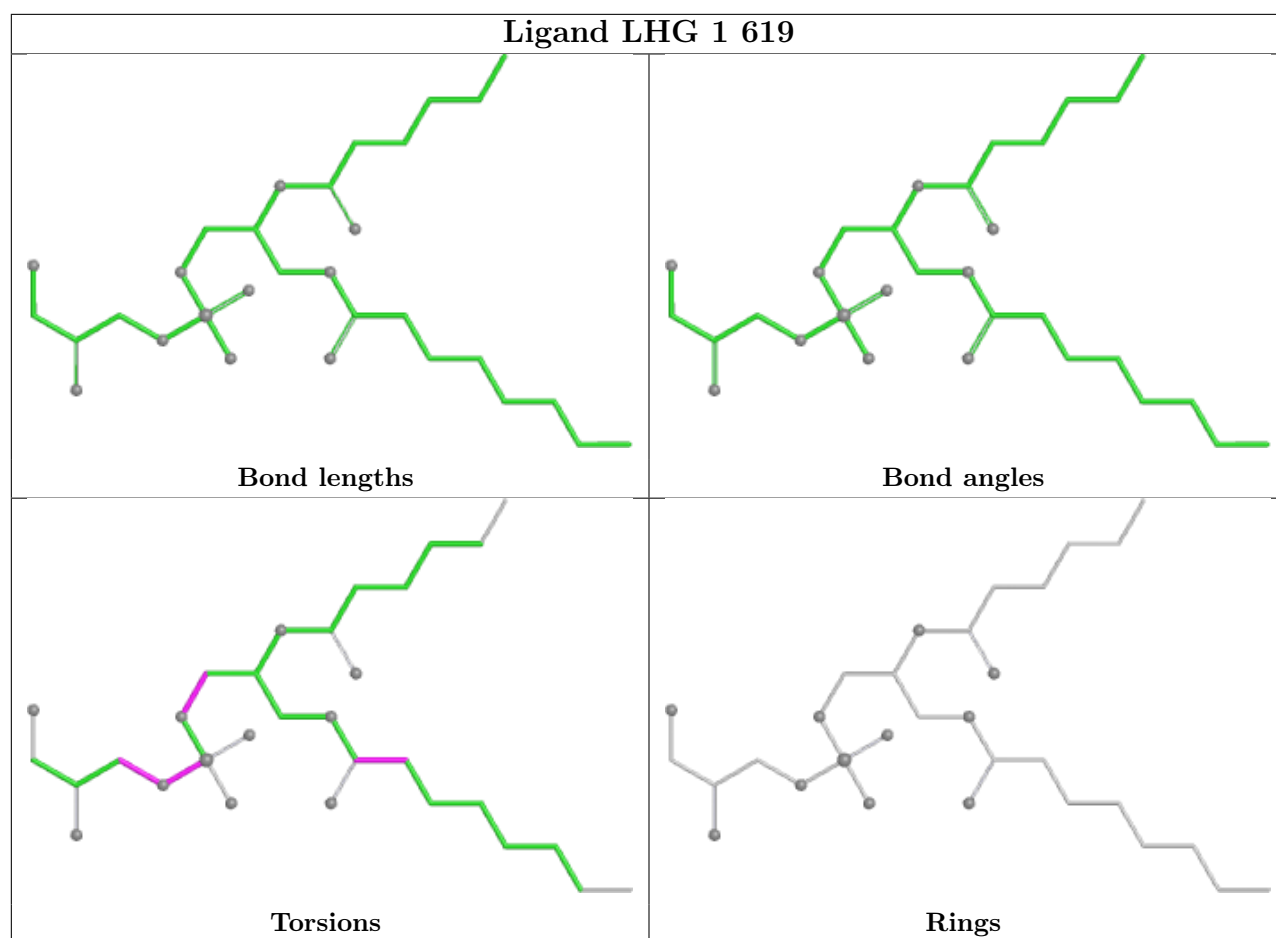
Ligand CLA A 5014



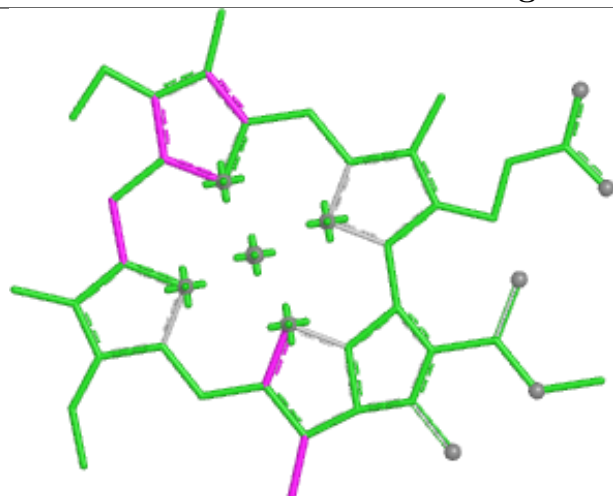
Ligand CLA B 834



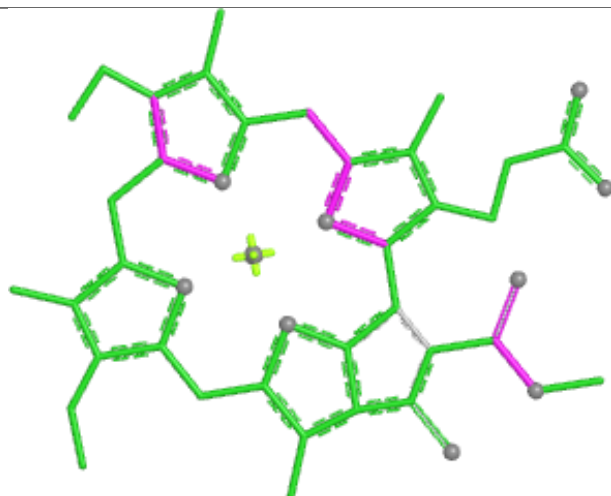




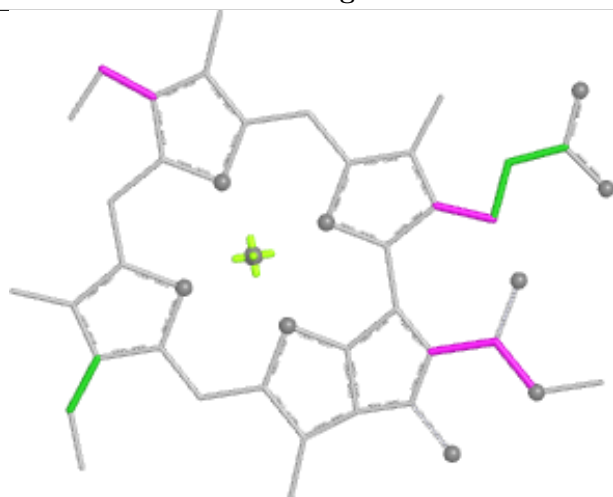
Ligand CLA 1 608



Bond lengths



Bond angles

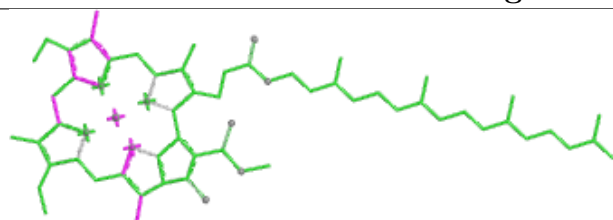


Torsions

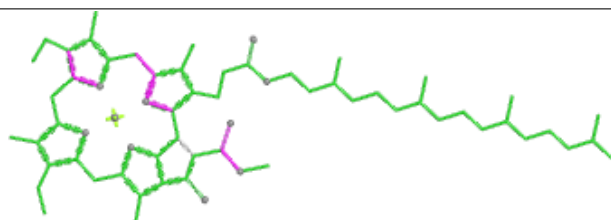


Rings

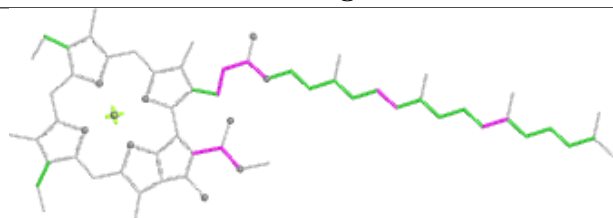
Ligand CLA A 5026



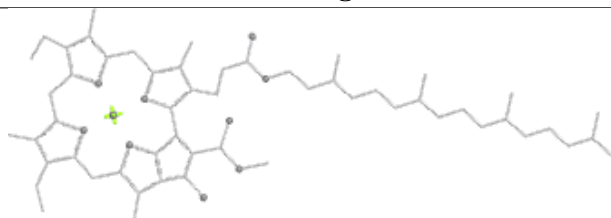
Bond lengths



Bond angles

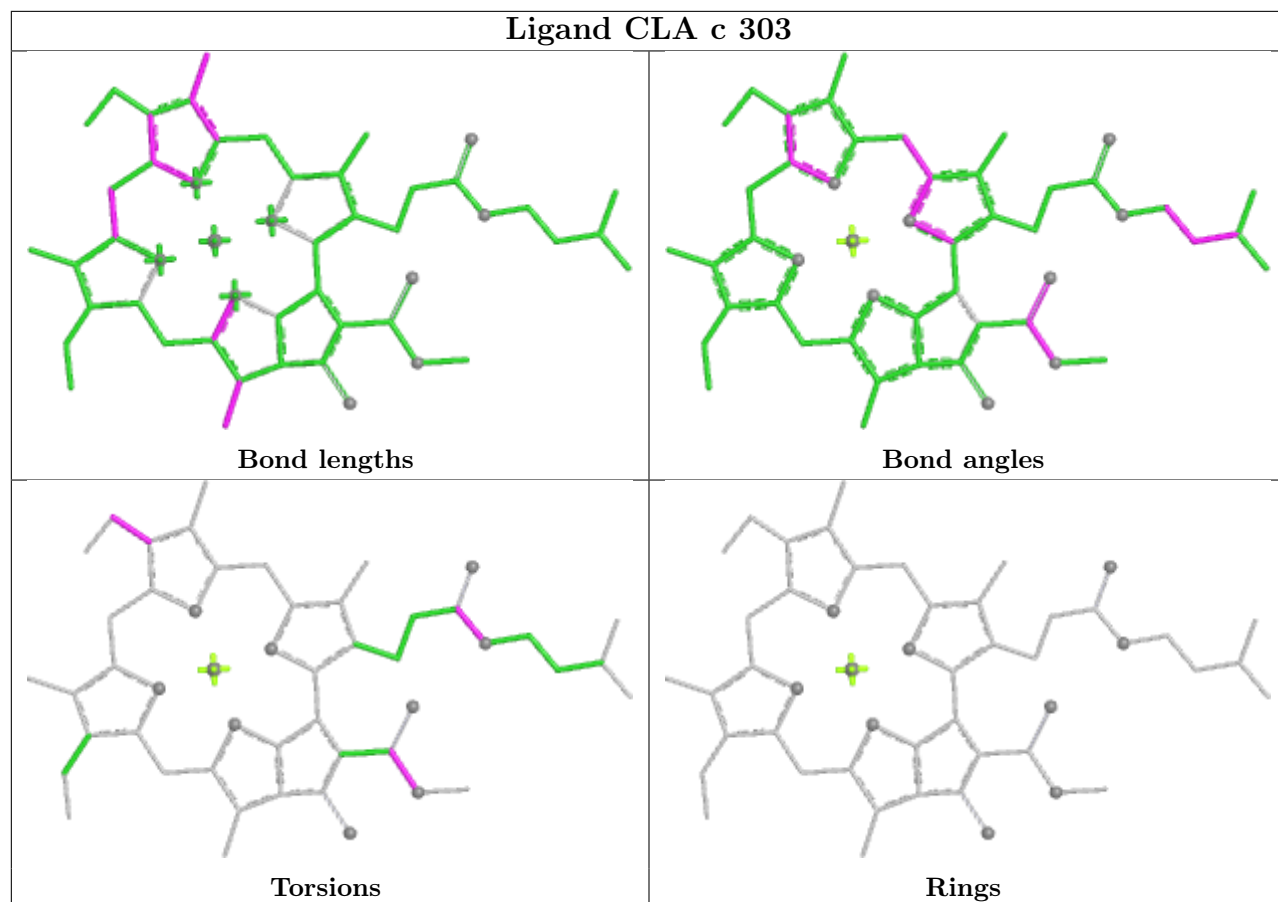


Torsions

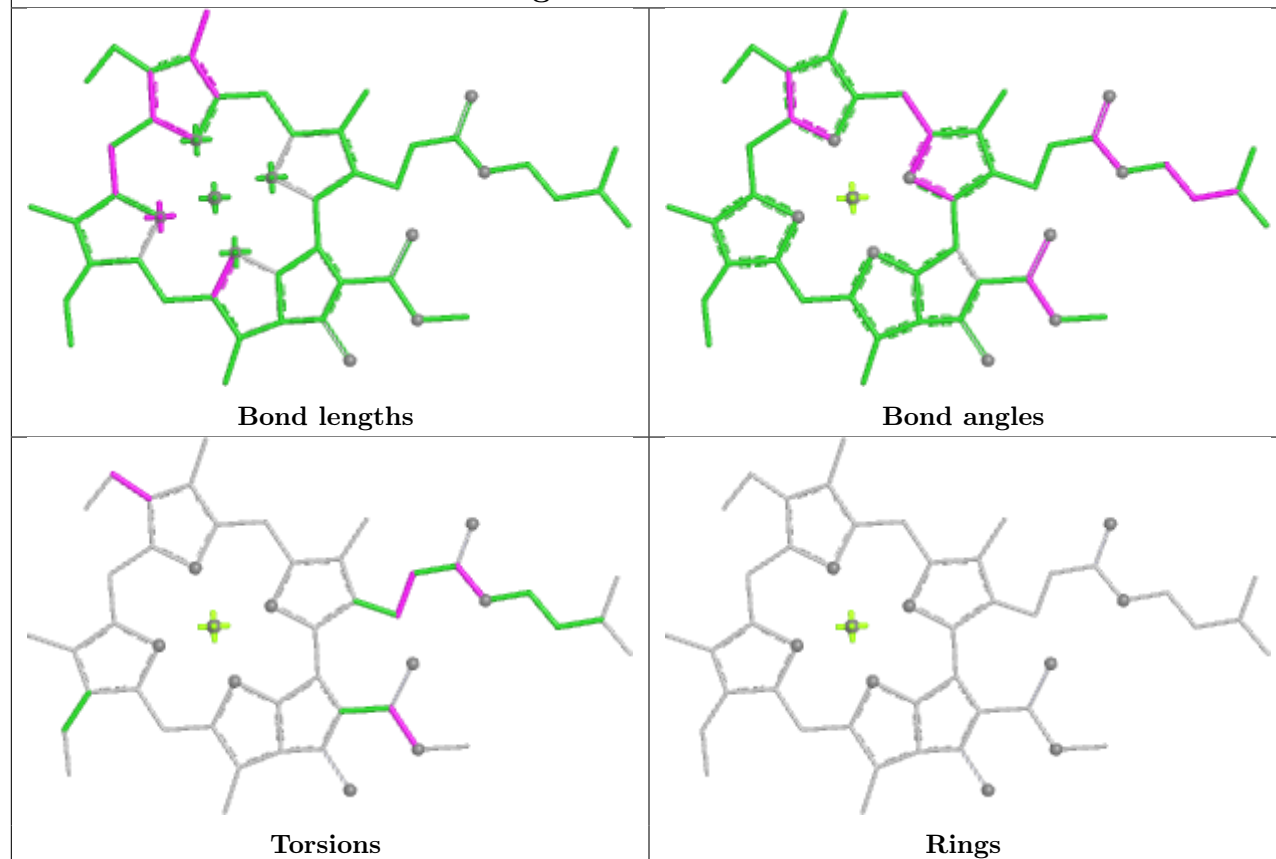


Rings

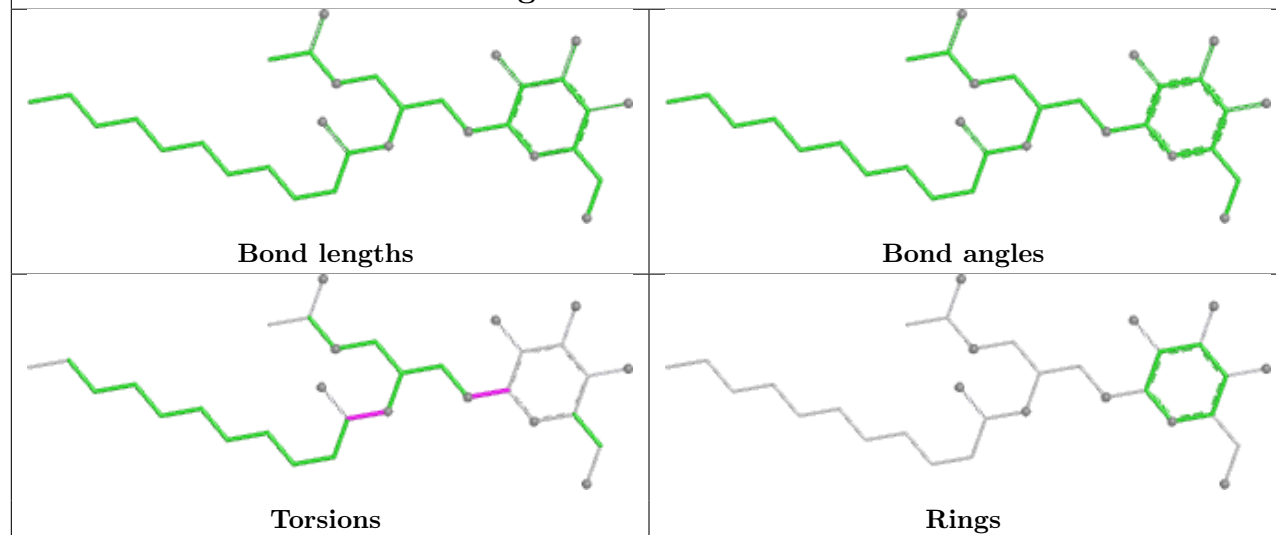
Ligand CLA c 303



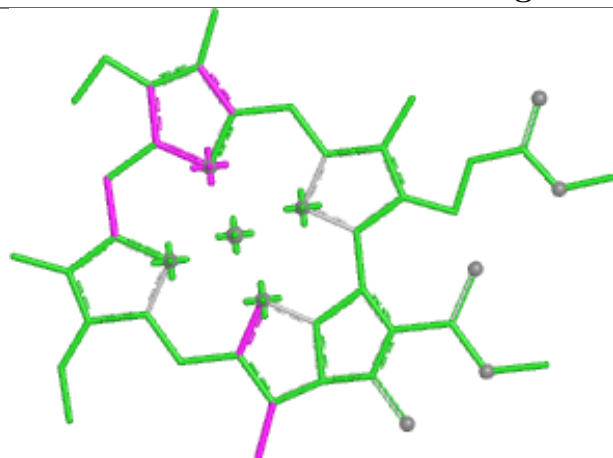
Ligand CLA T 410



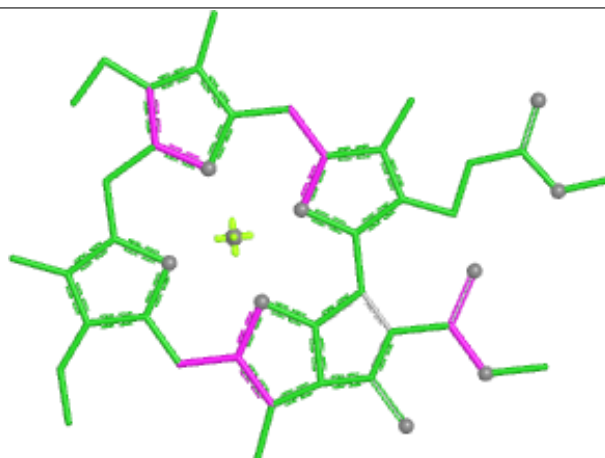
Ligand LMG A 5001



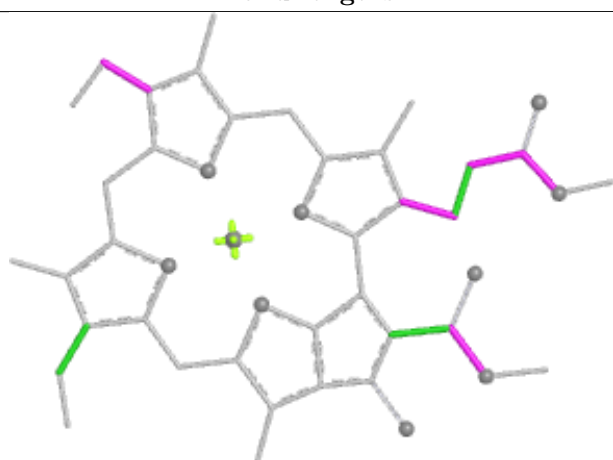
Ligand CLA T 404



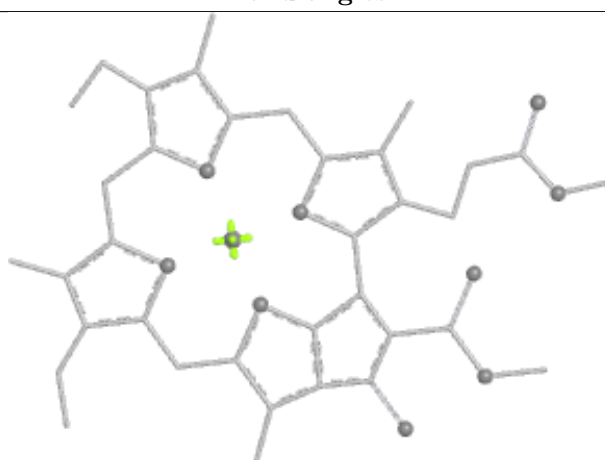
Bond lengths



Bond angles

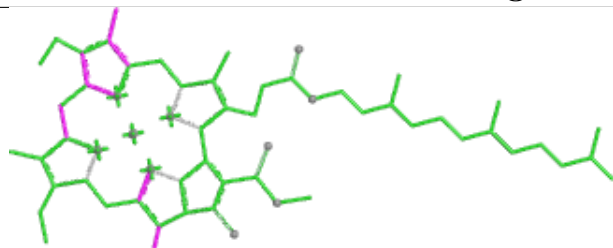


Torsions

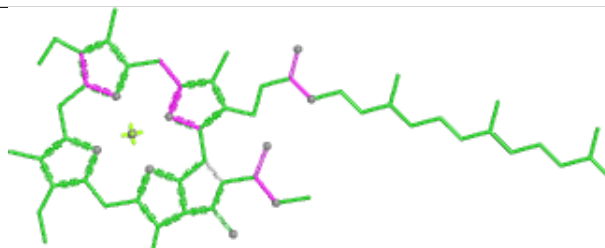


Rings

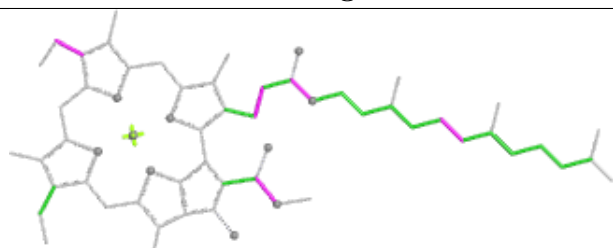
Ligand CLA F 5006



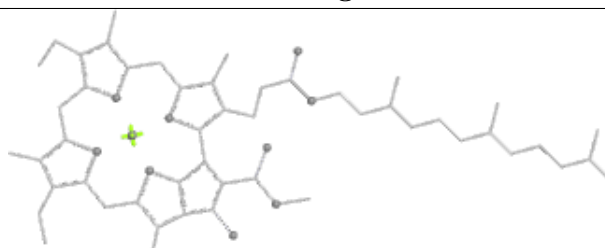
Bond lengths



Bond angles

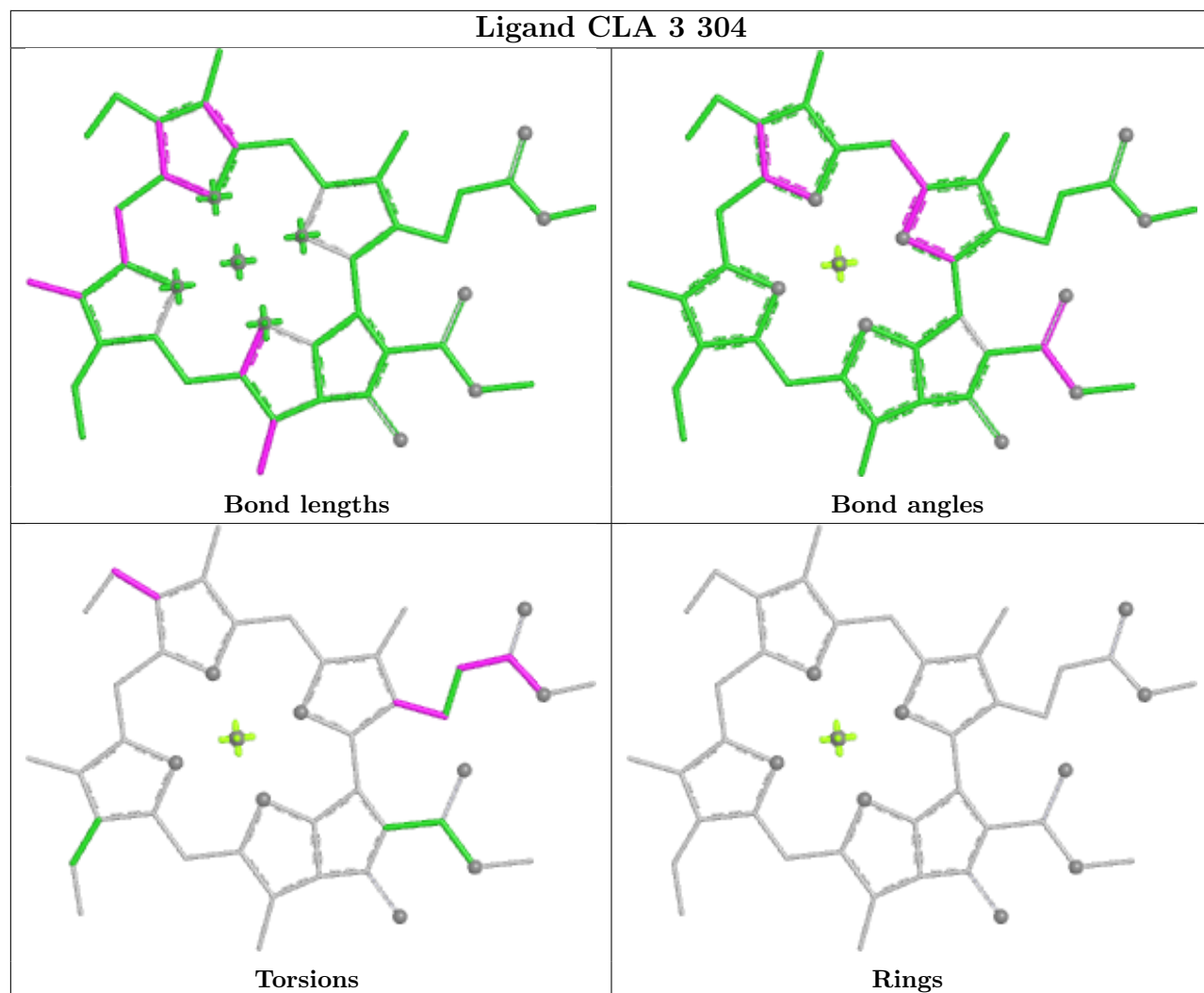


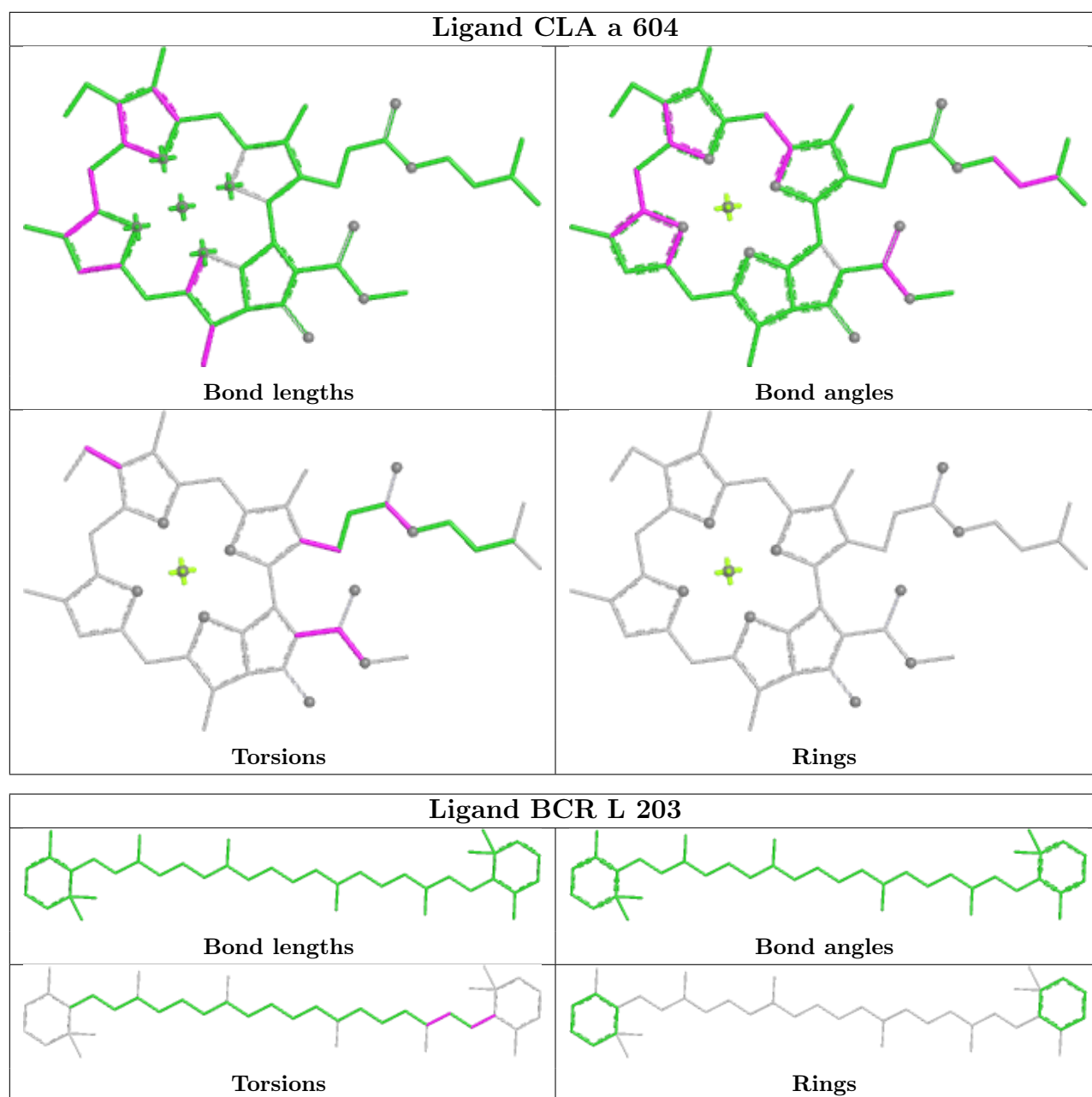
Torsions



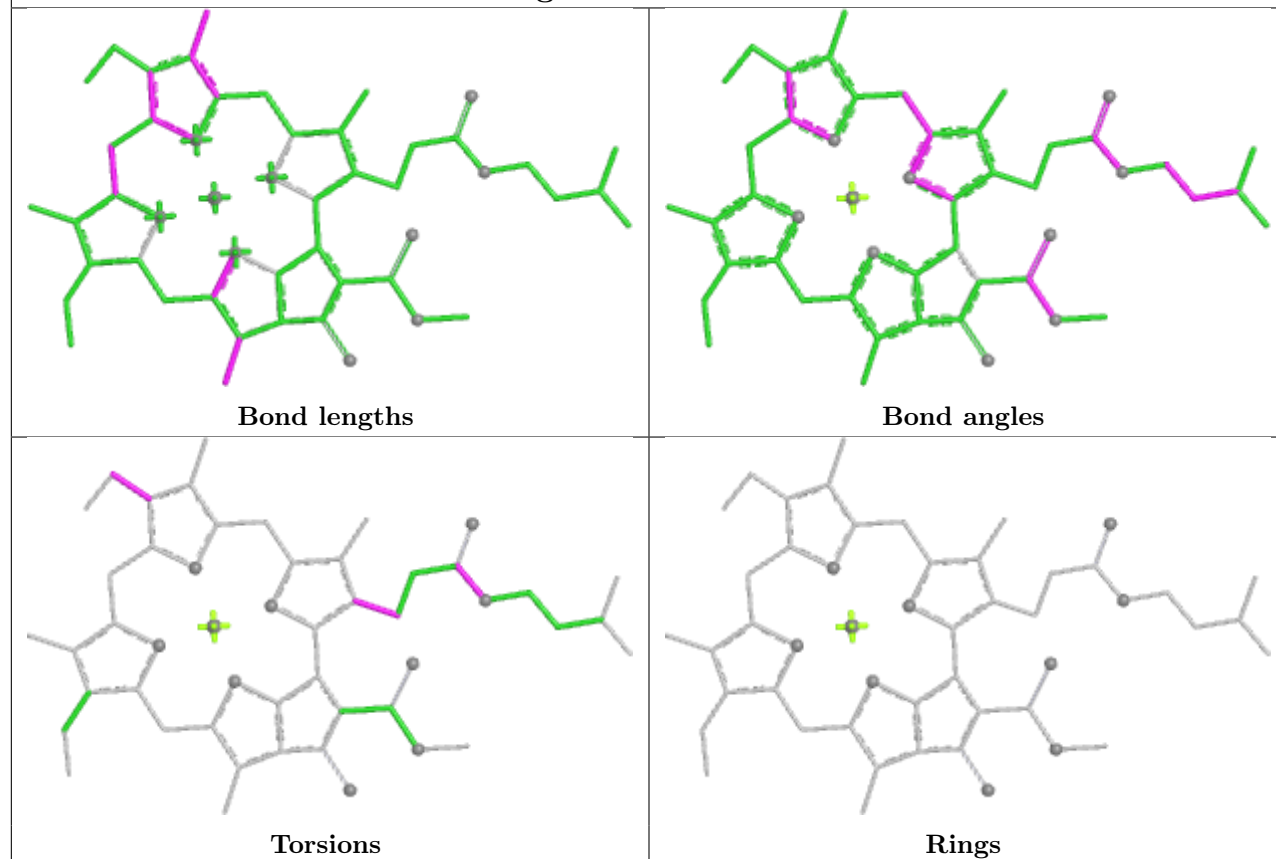
Rings

Ligand CLA 3 304

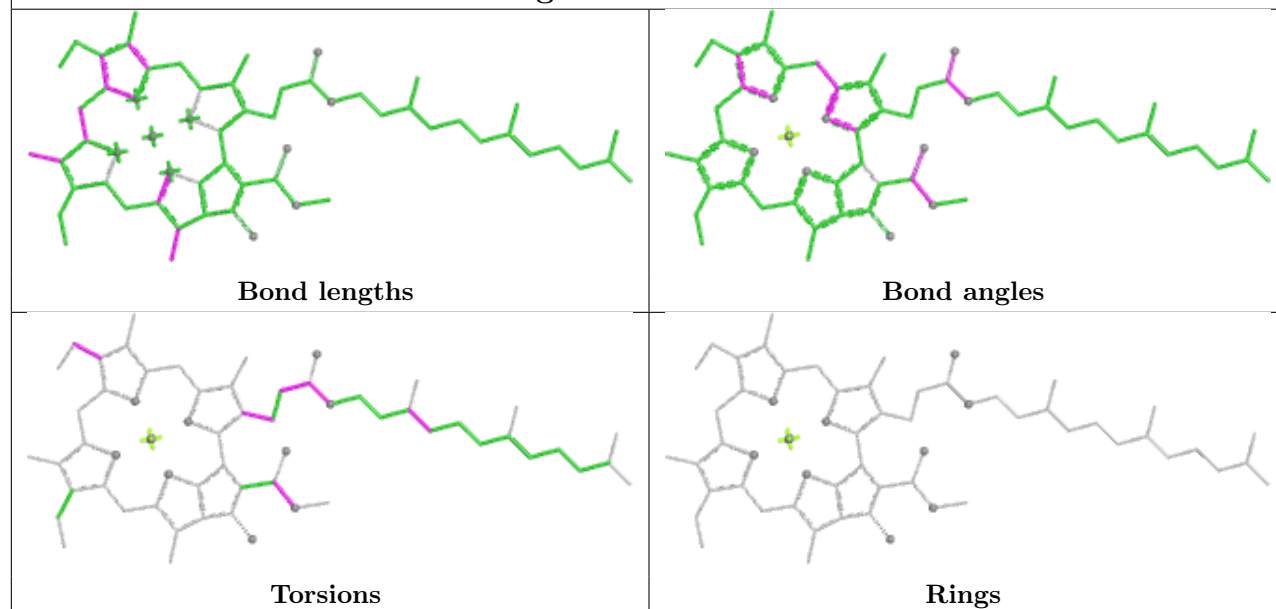


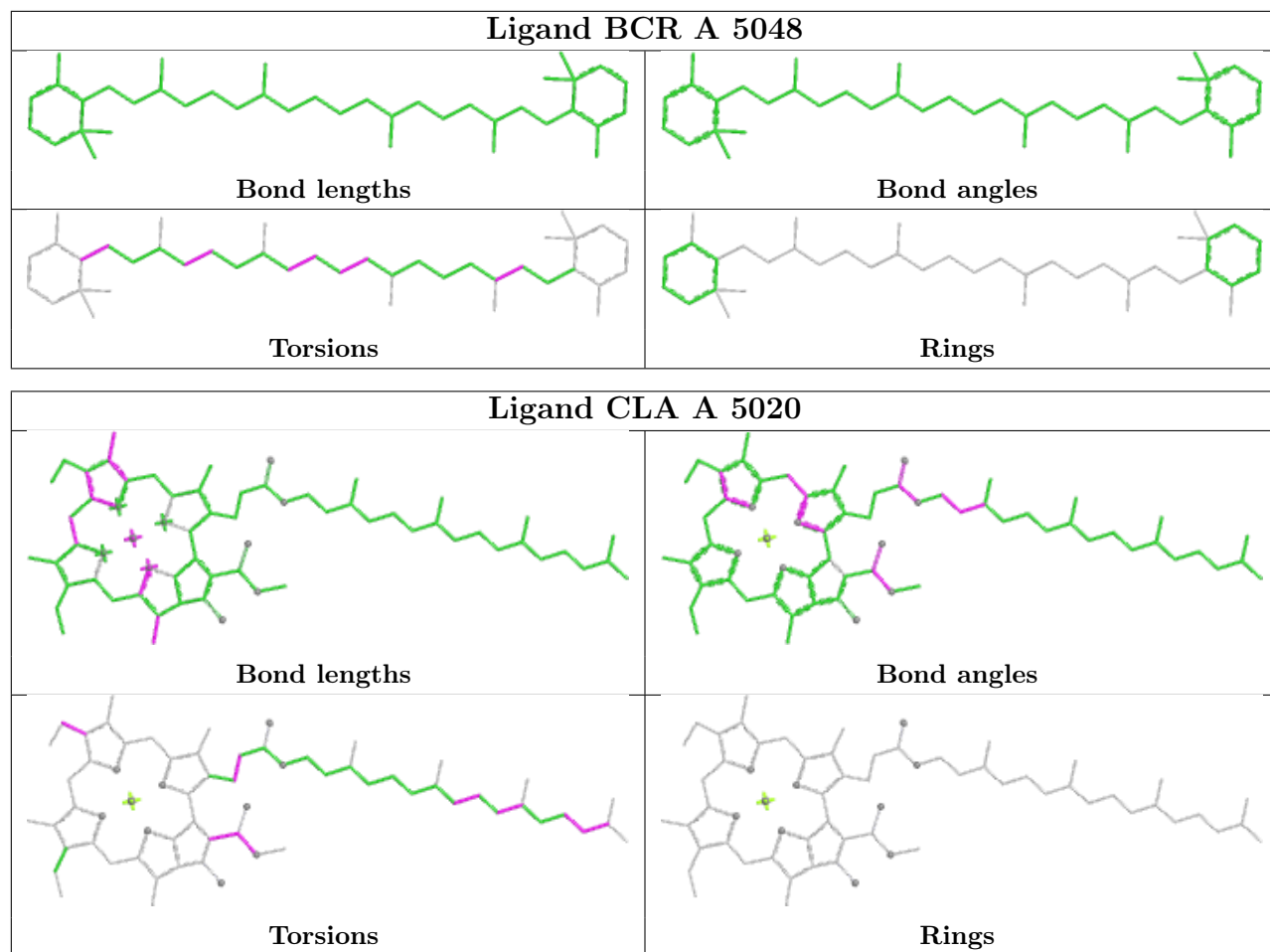


Ligand CLA 7 313

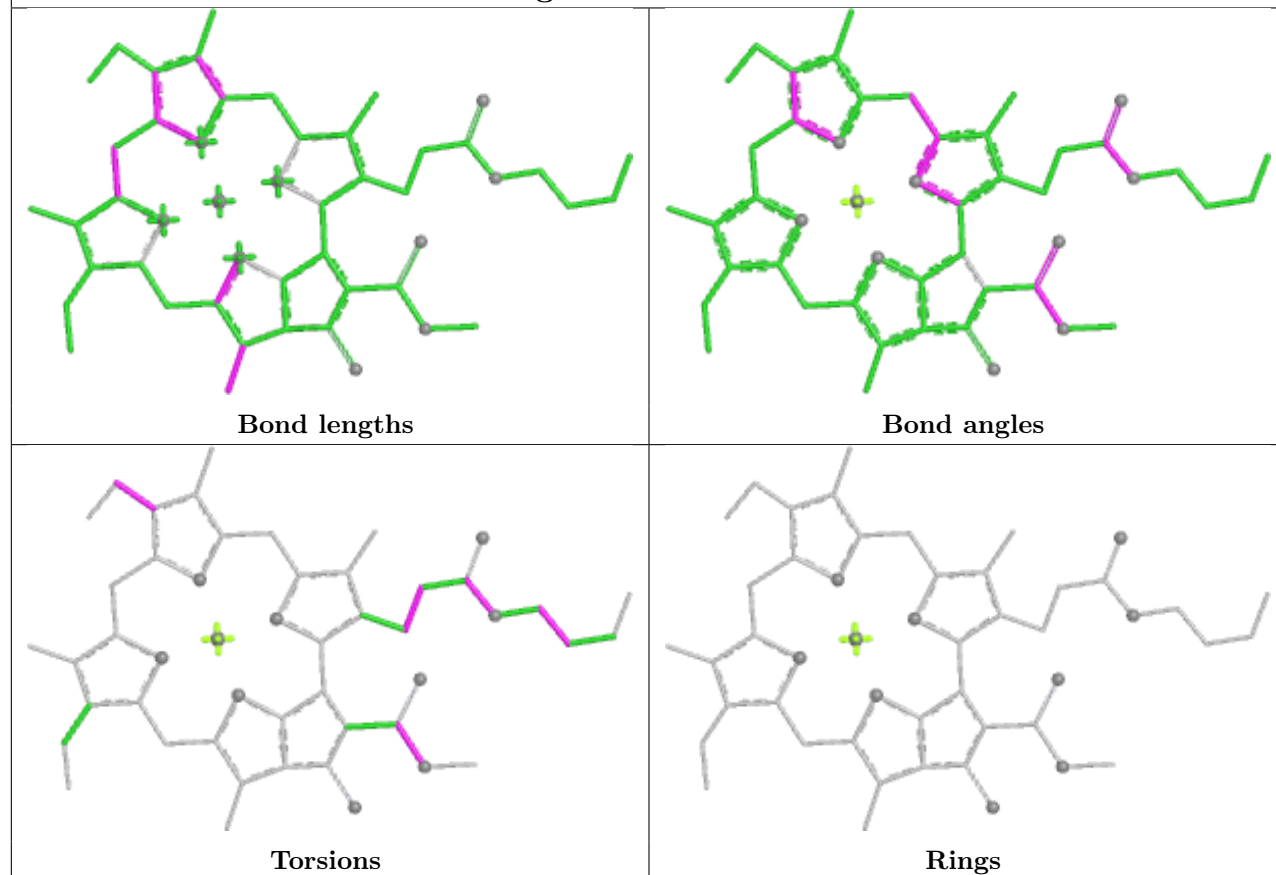


Ligand CLA a 609

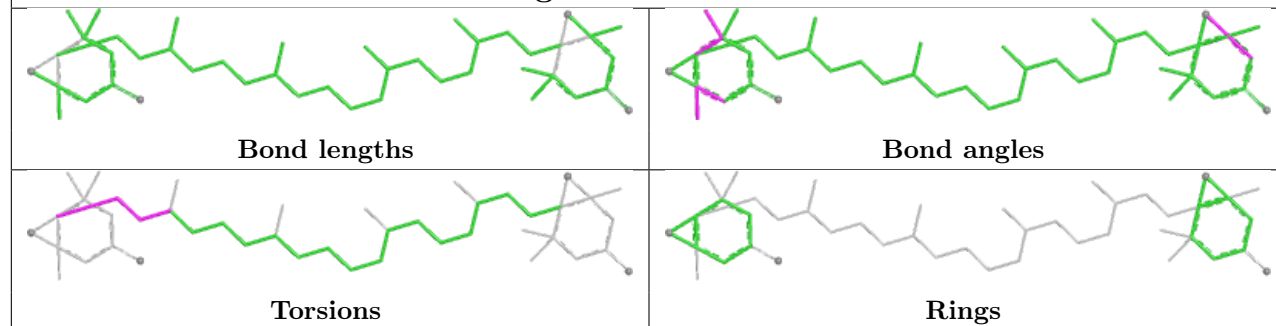




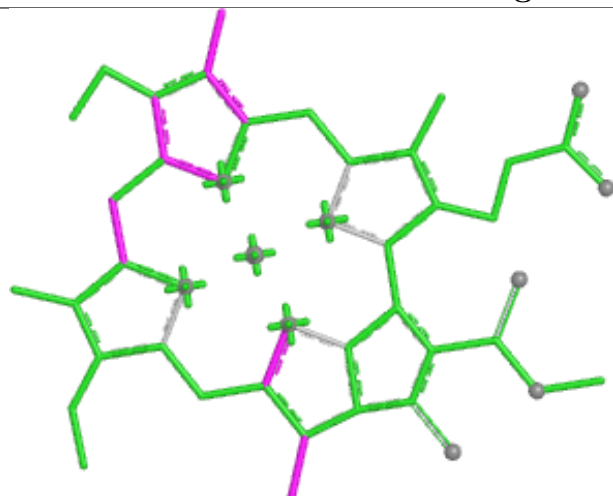
Ligand CLA J 102



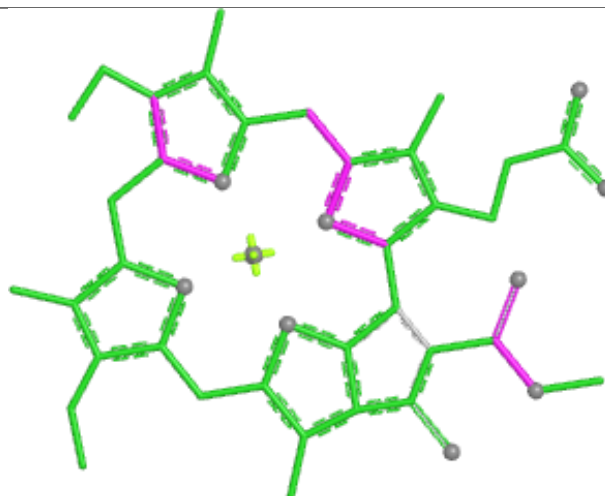
Ligand XAT 7 316



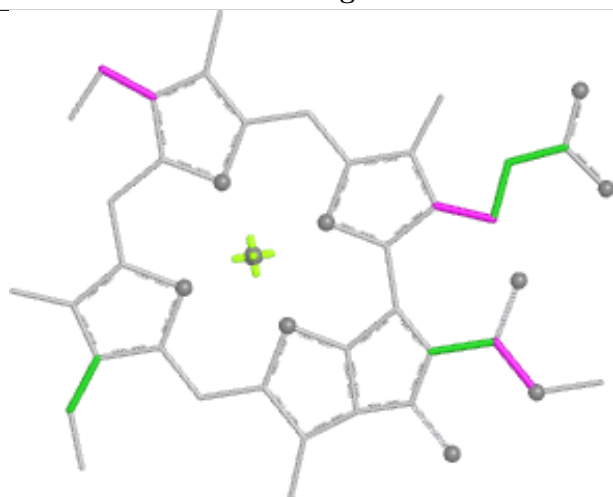
Ligand CLA B 822



Bond lengths



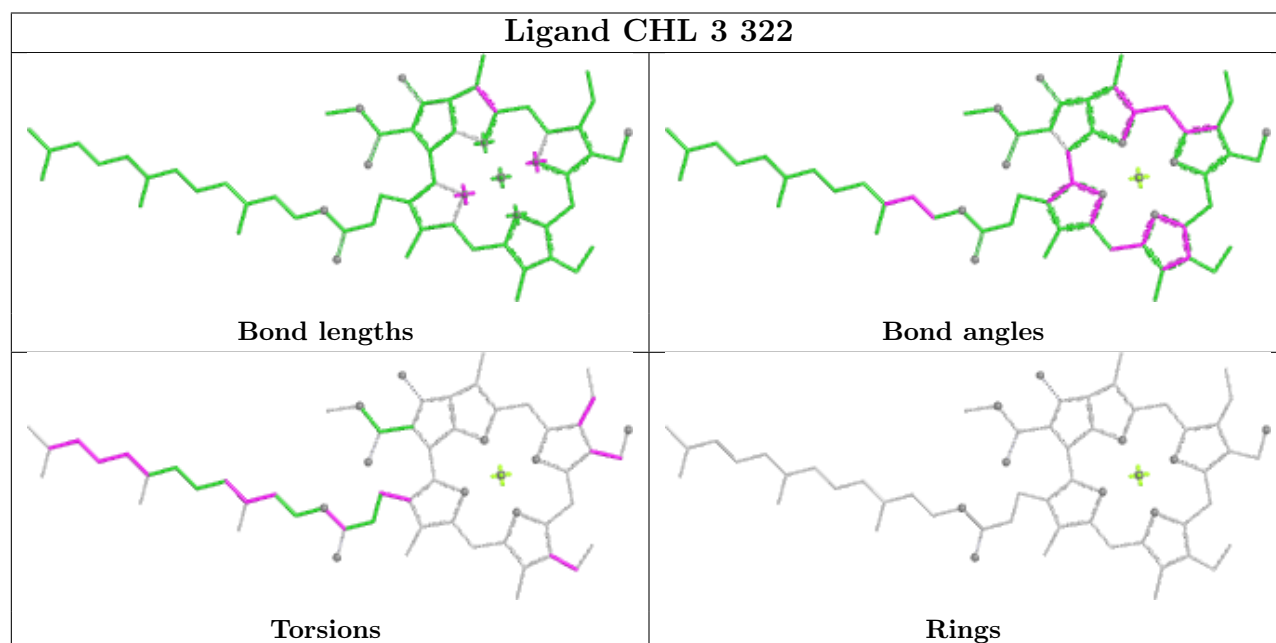
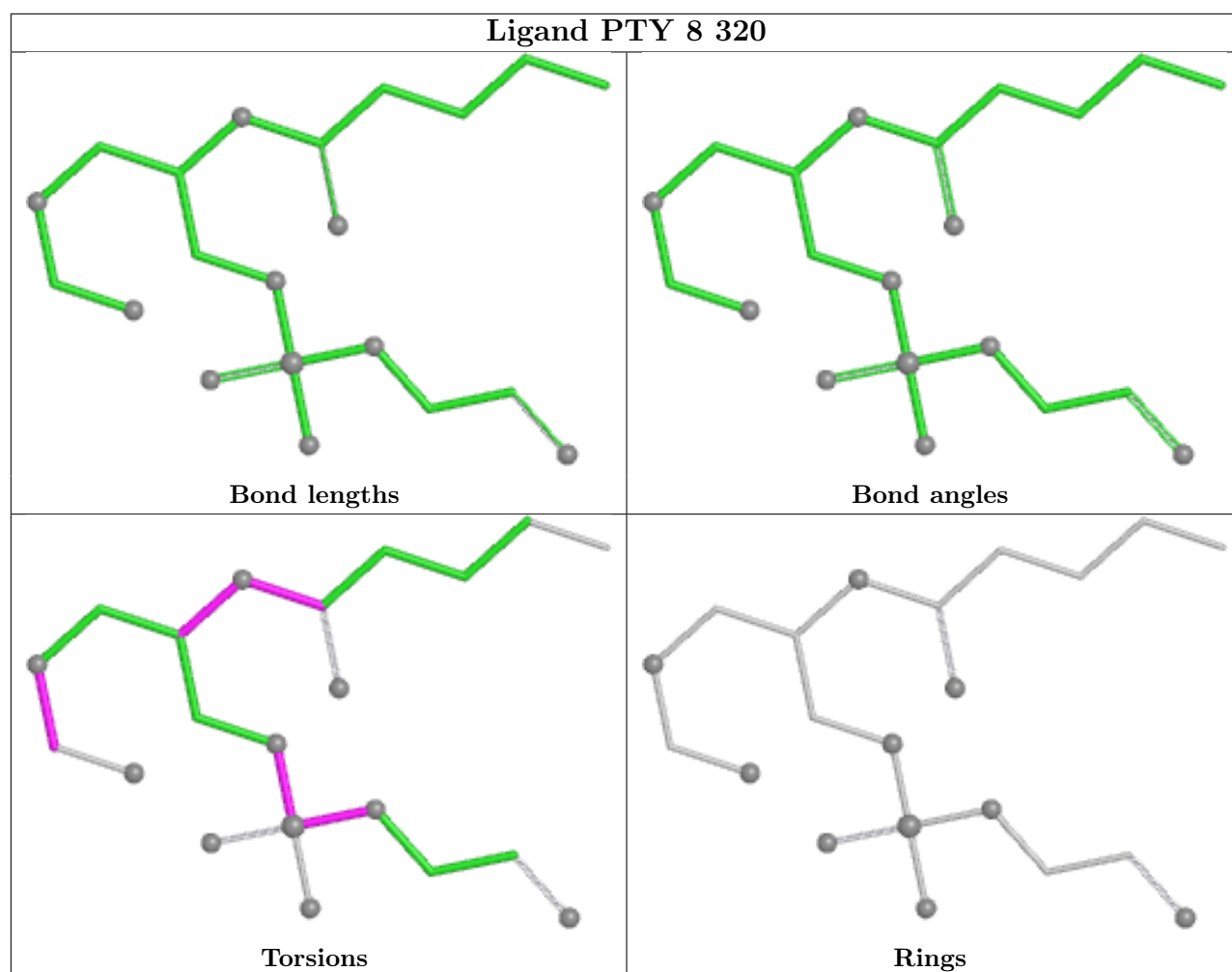
Bond angles

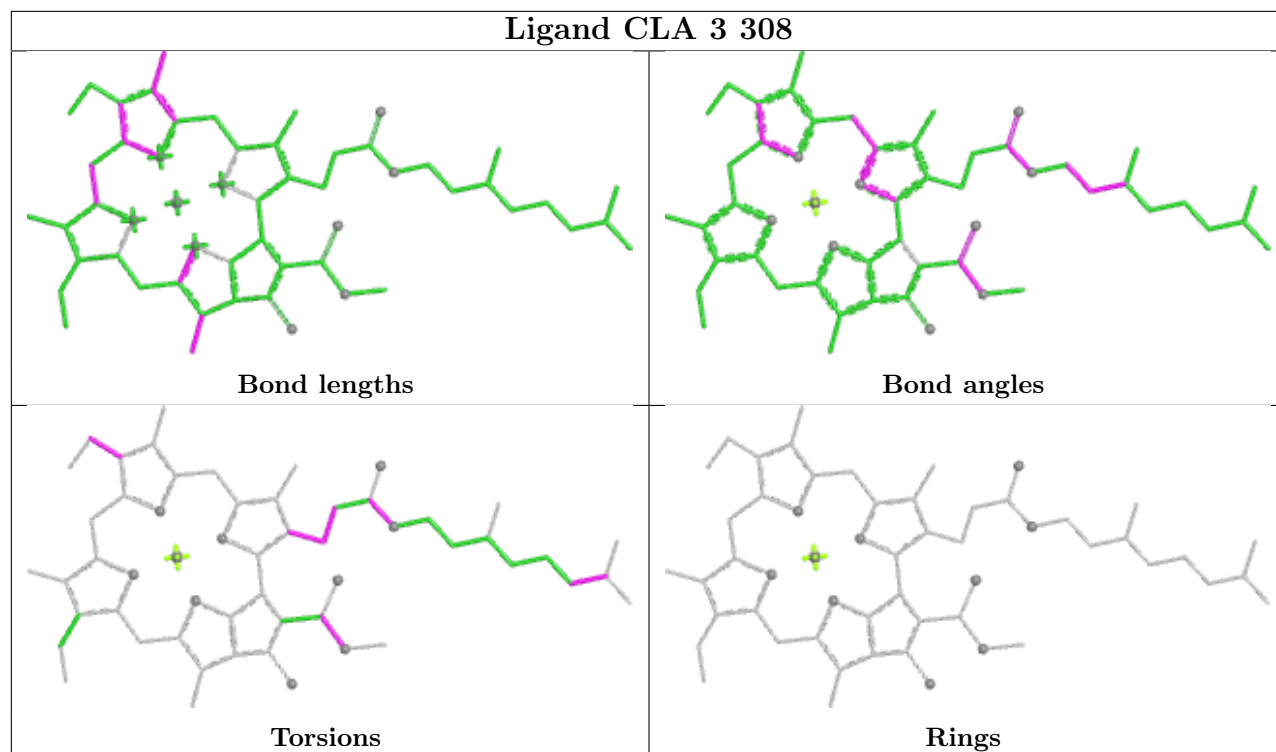
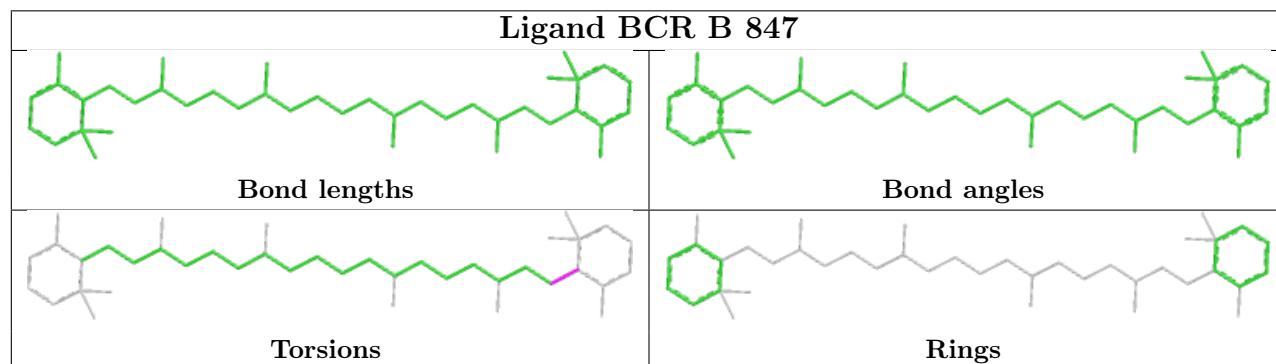
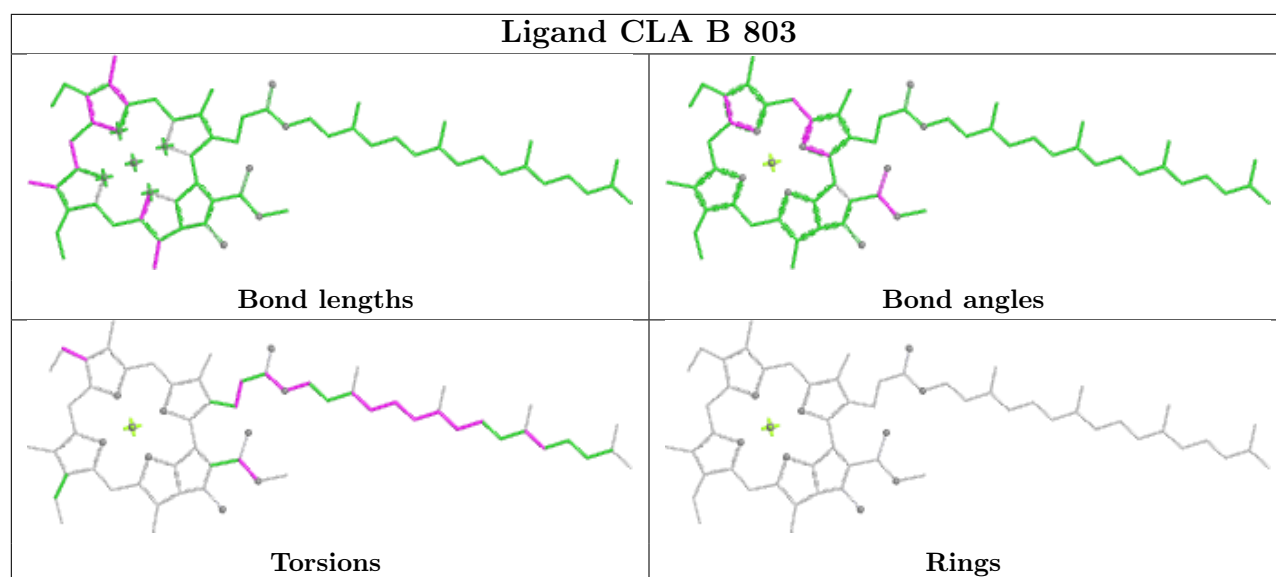


Torsions

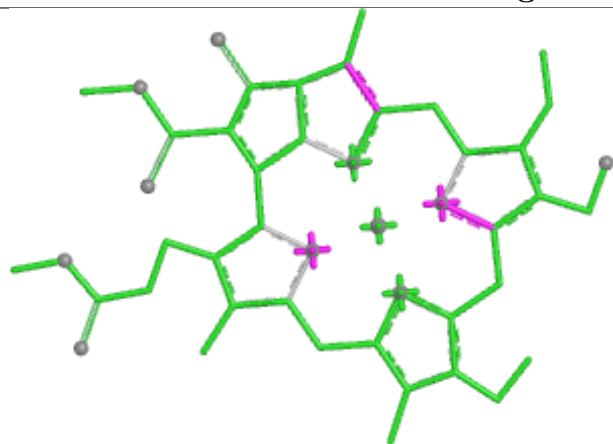


Rings

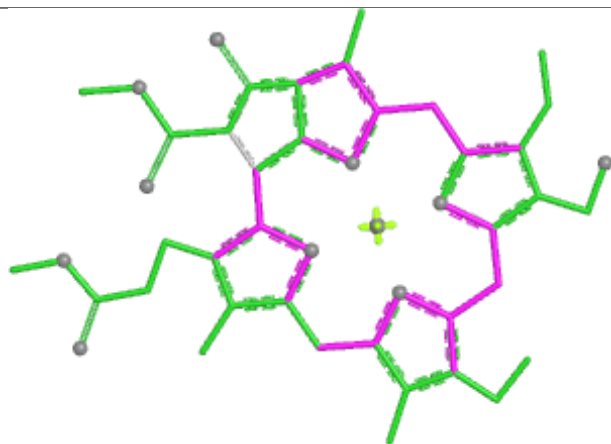




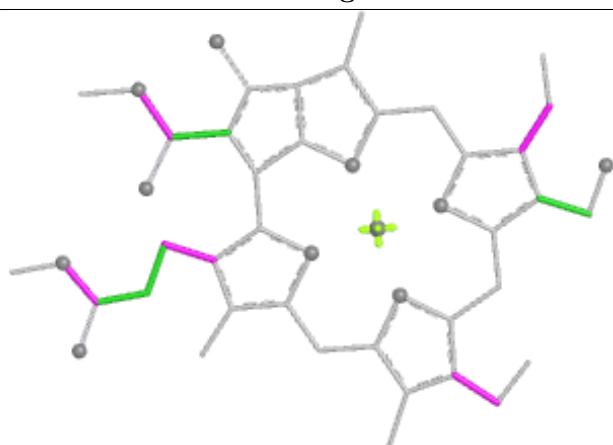
Ligand CHL 7 306



Bond lengths



Bond angles

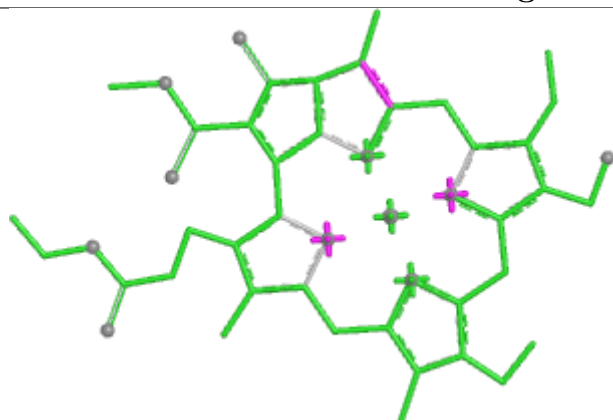


Torsions

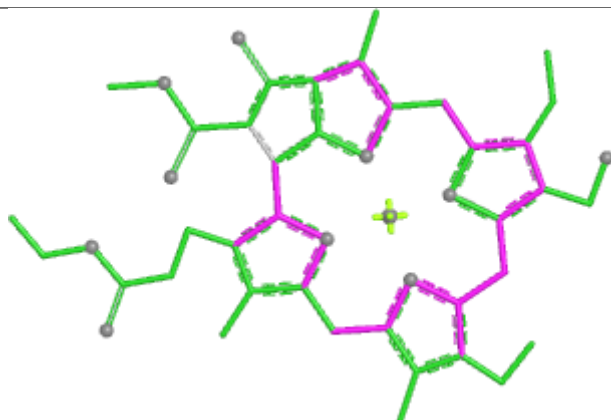


Rings

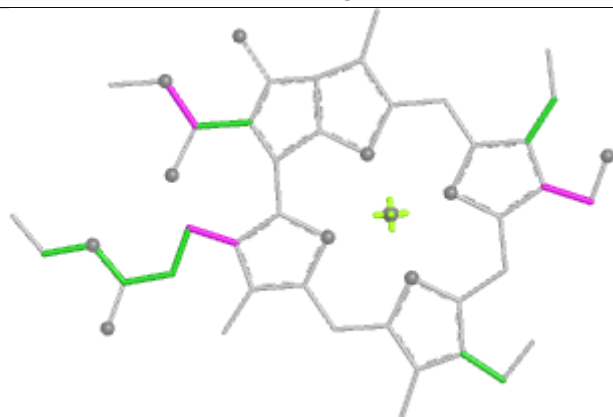
Ligand CHL 7 307



Bond lengths



Bond angles

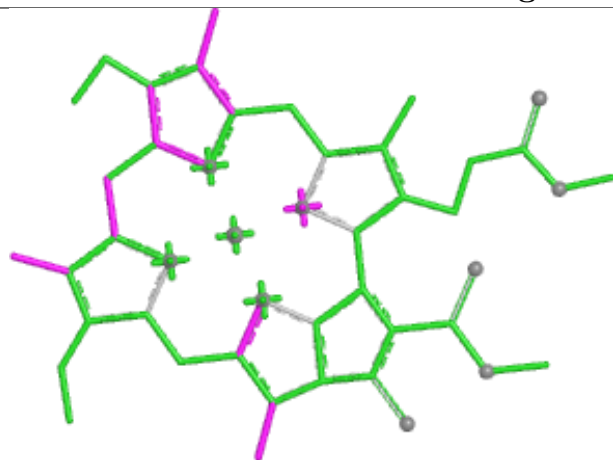


Torsions

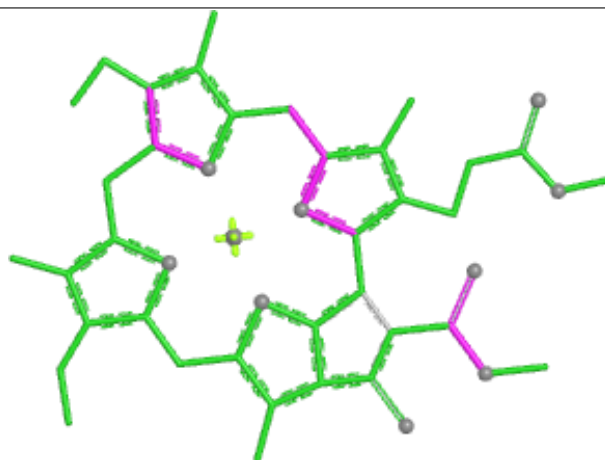


Rings

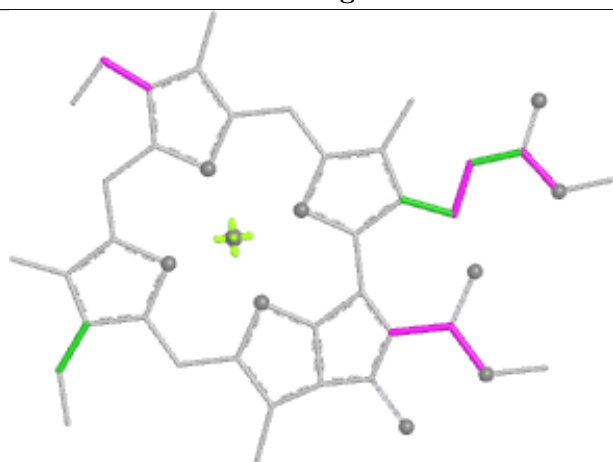
Ligand CLA 8 305



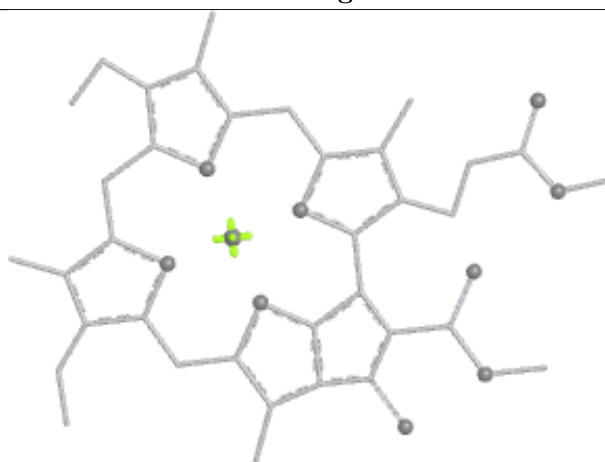
Bond lengths



Bond angles

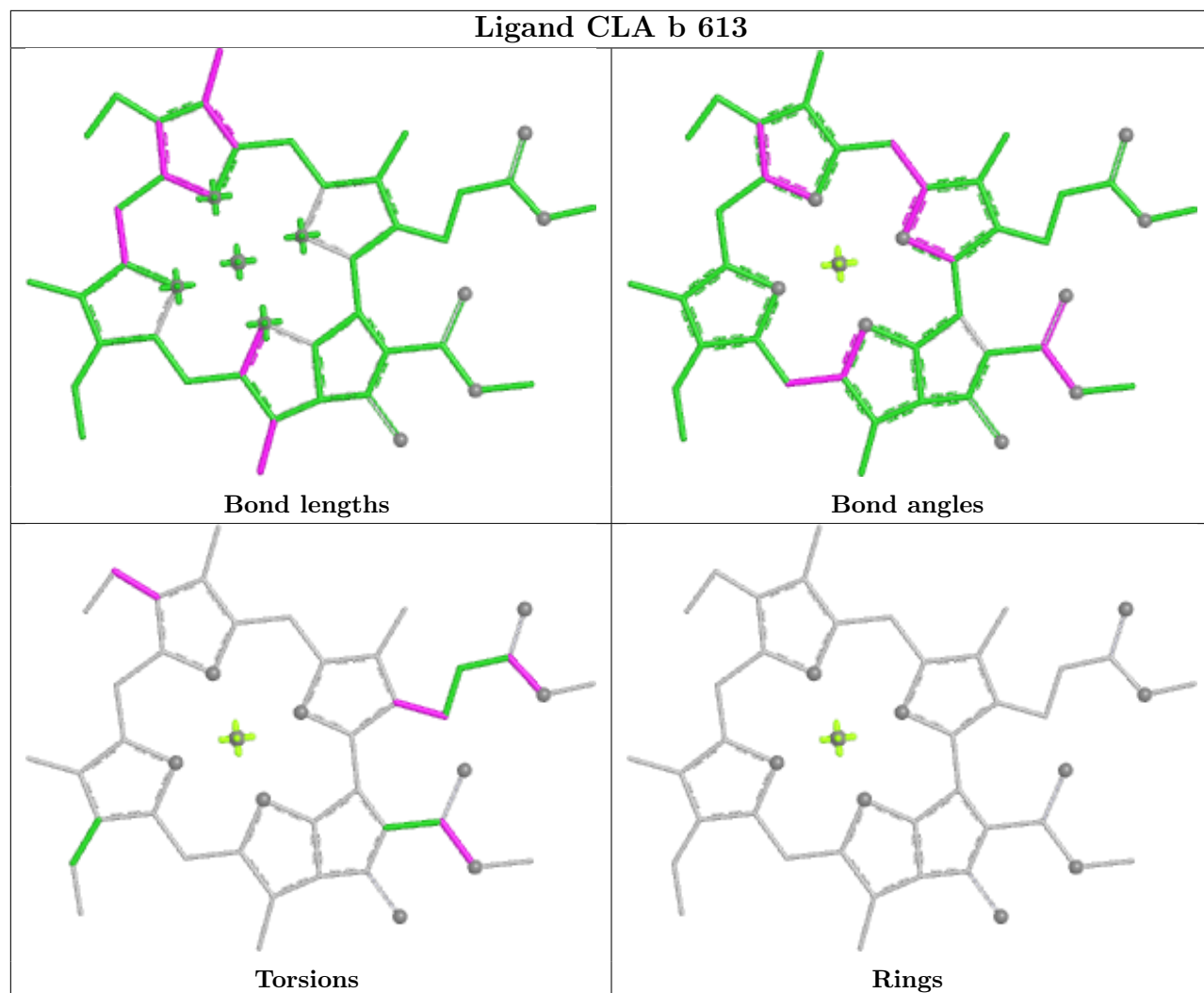


Torsions

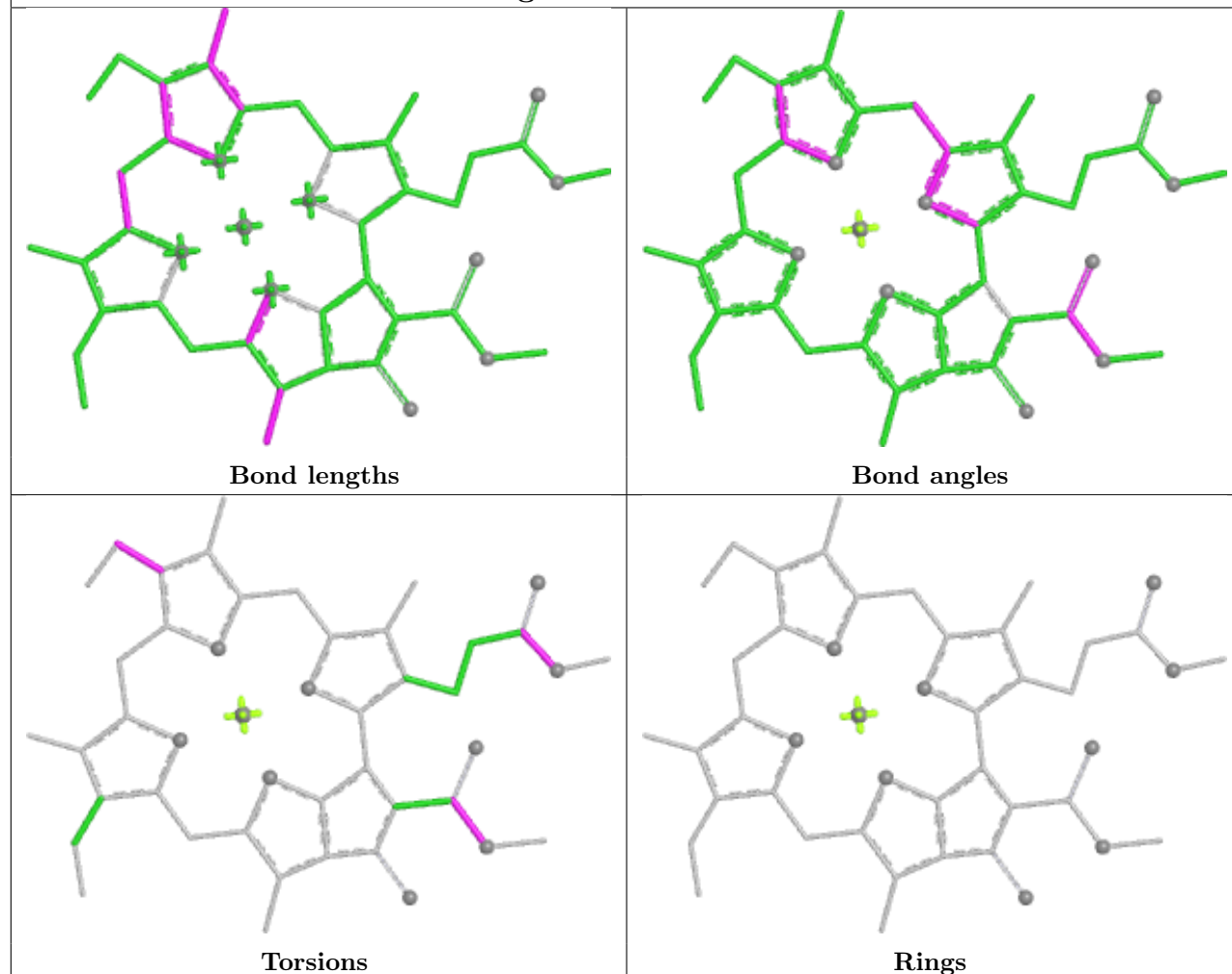


Rings

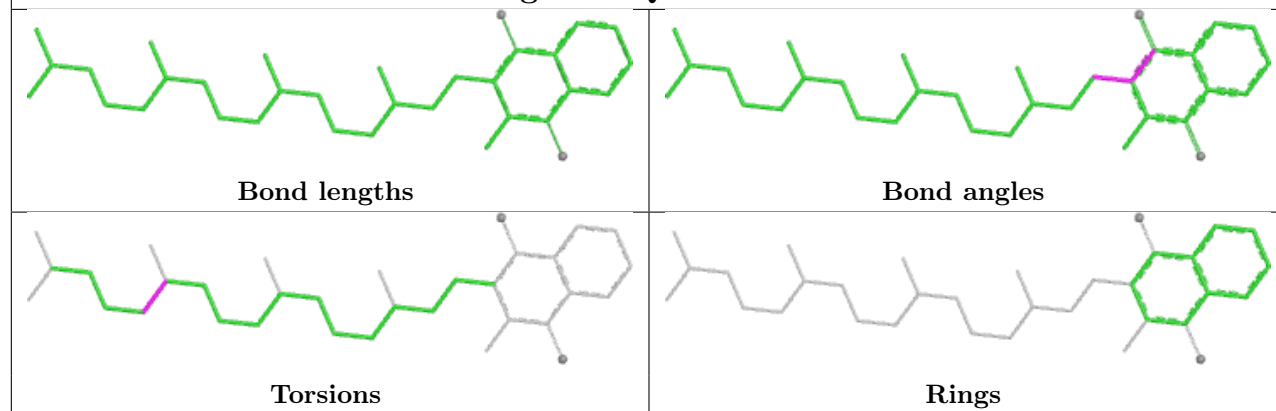
Ligand CLA b 613

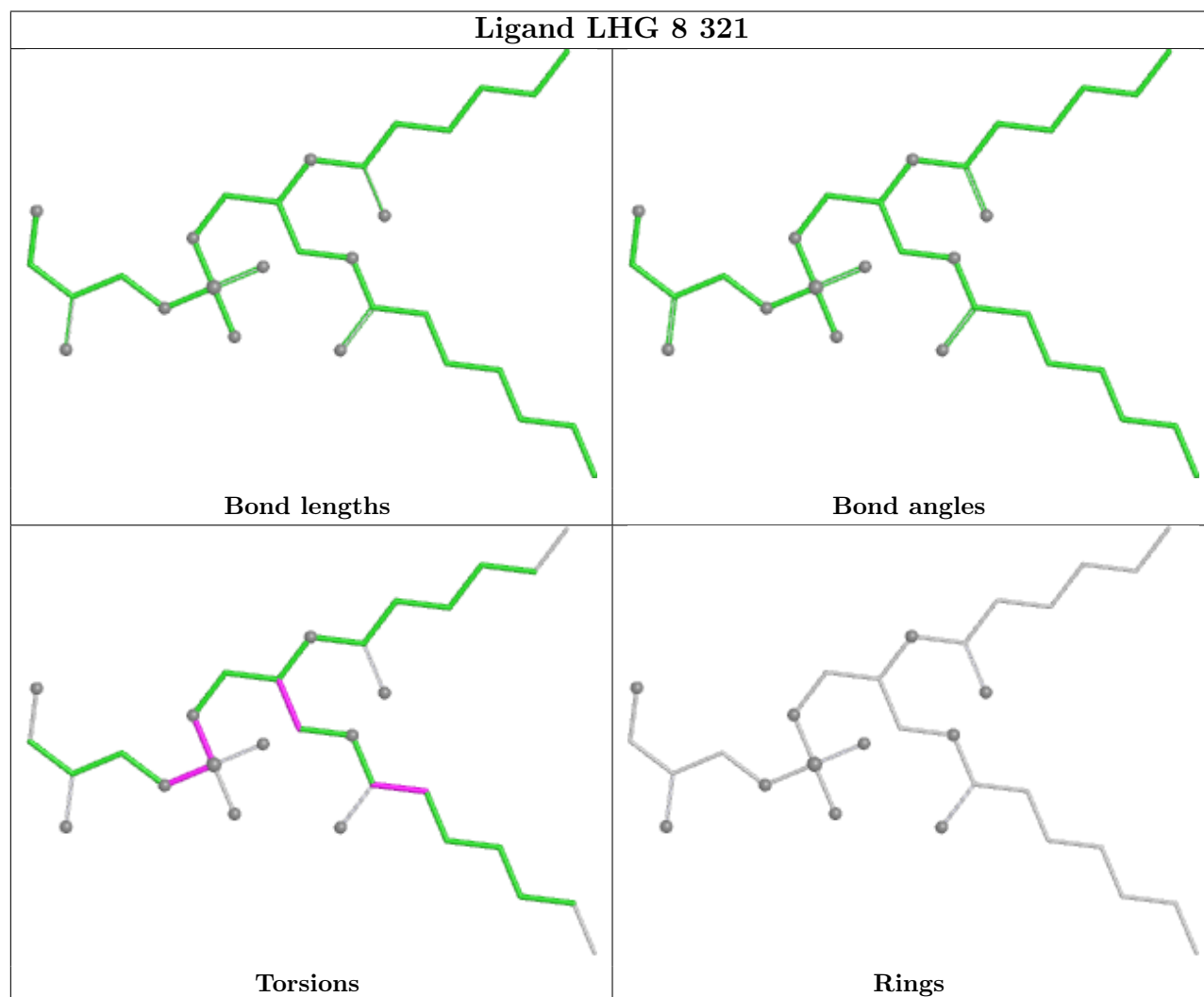
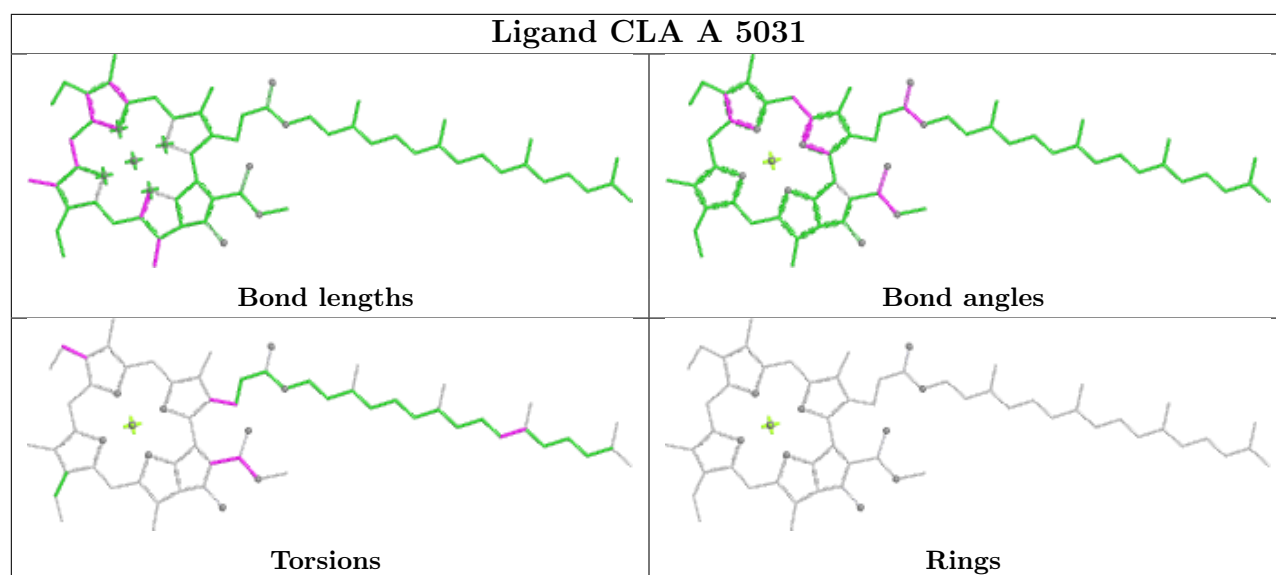


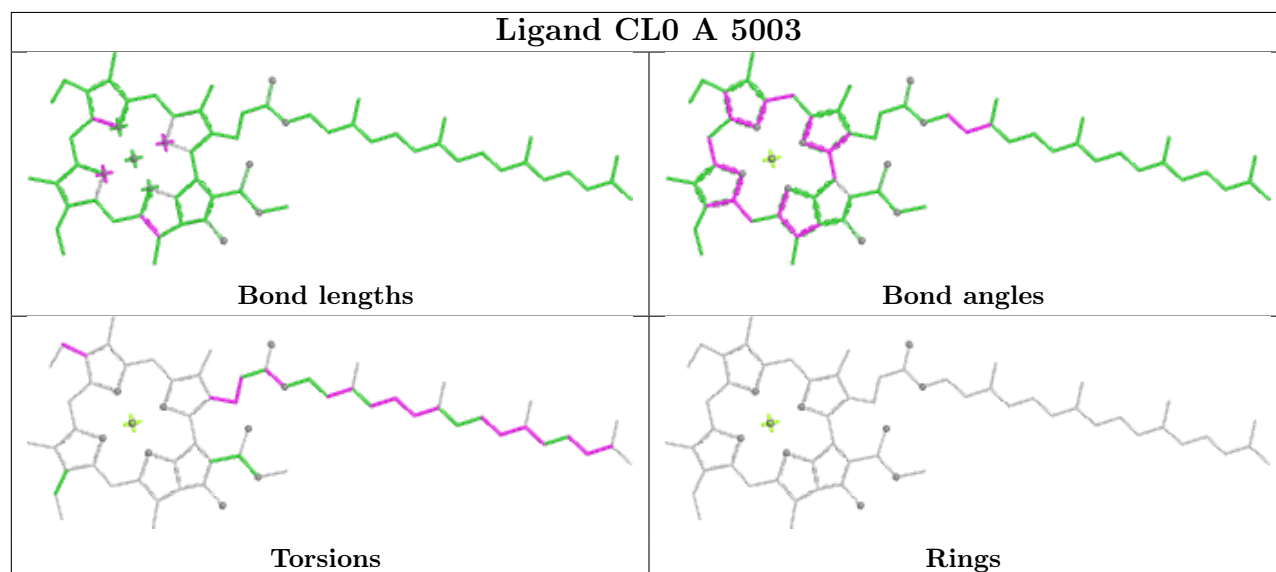
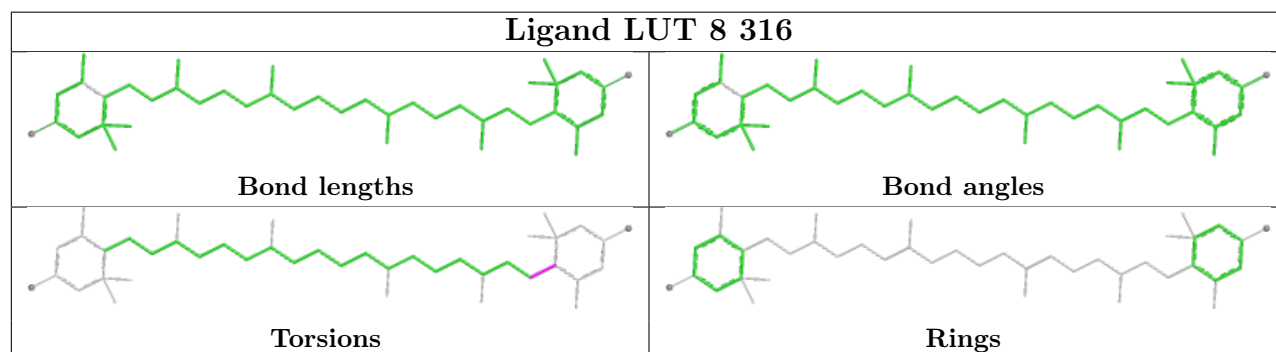
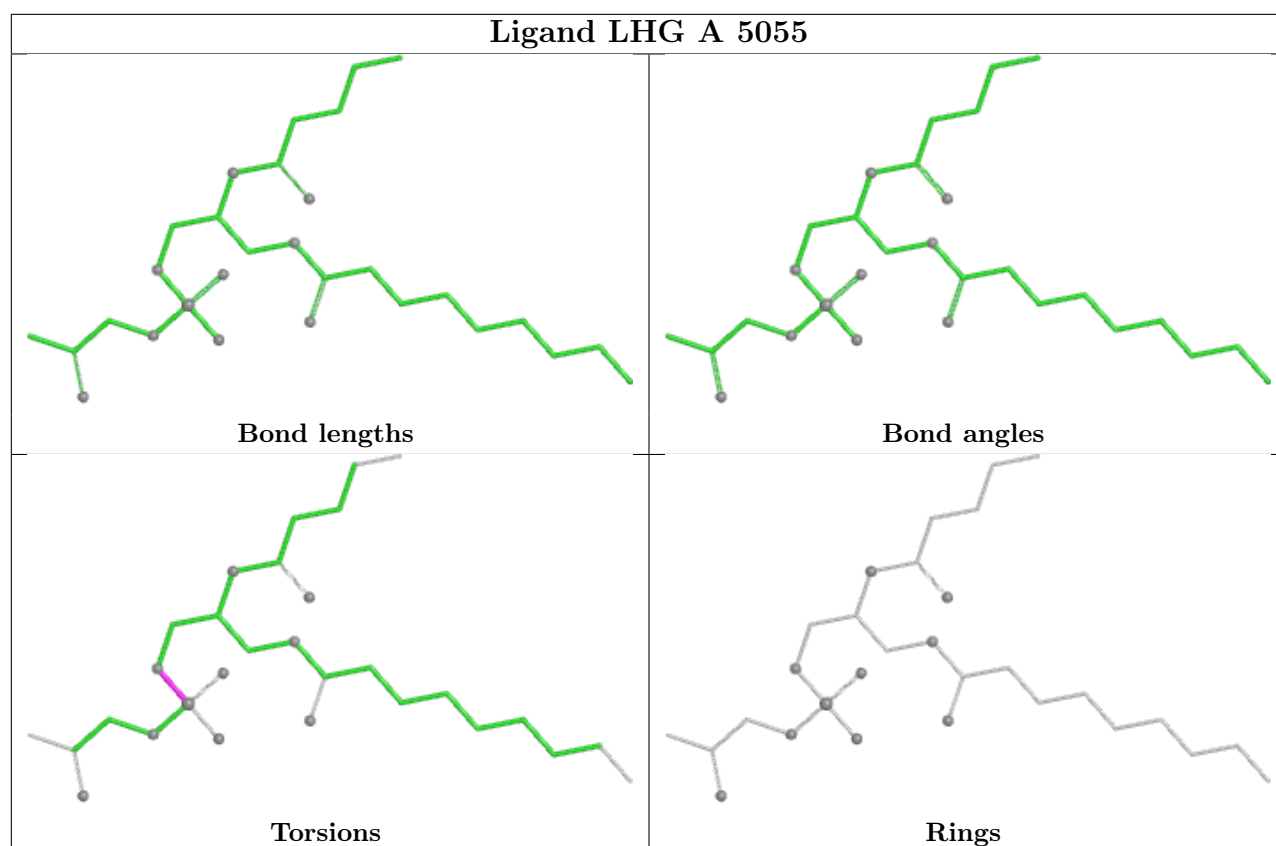
Ligand CLA a 613



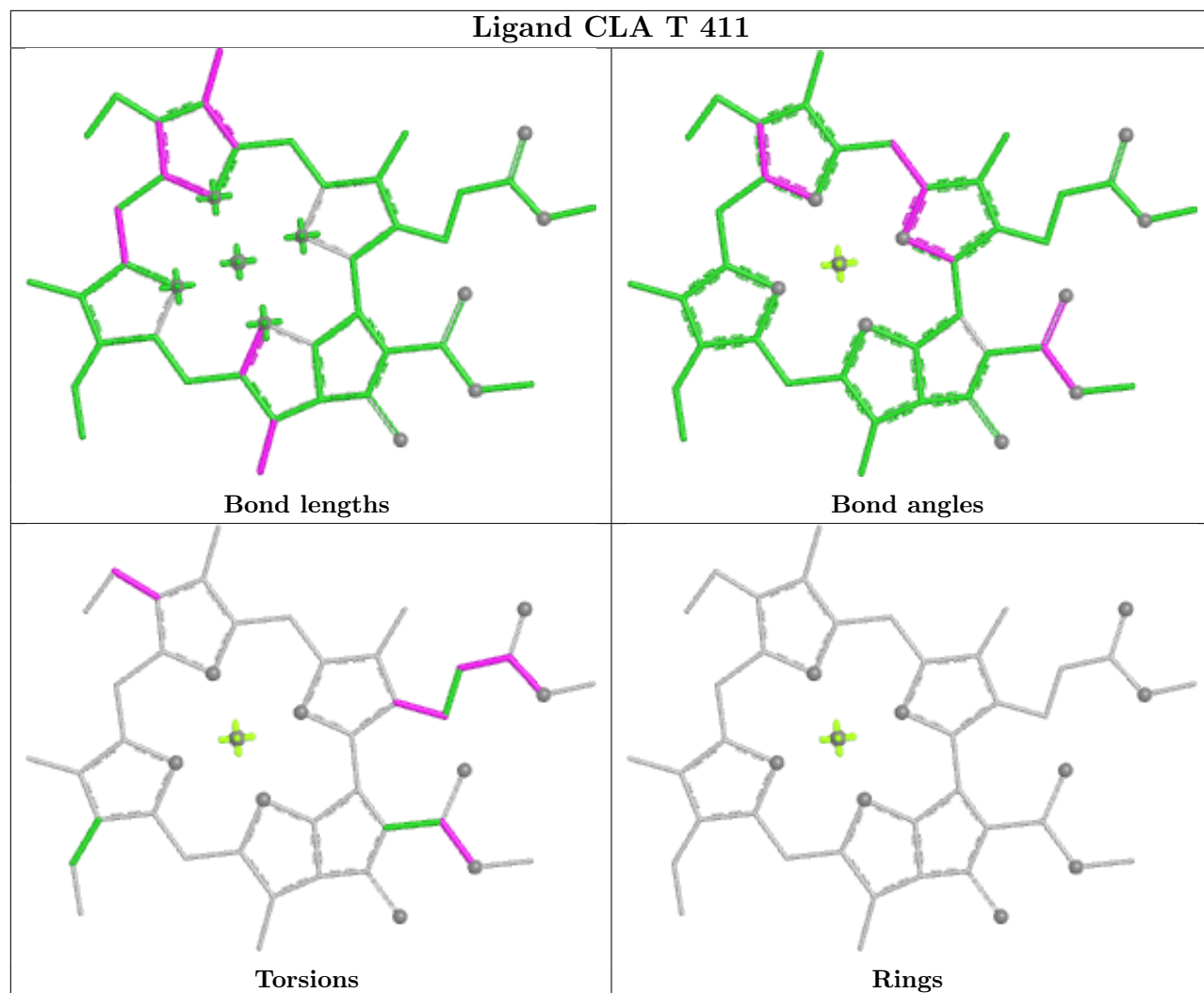
Ligand PQN A 5045

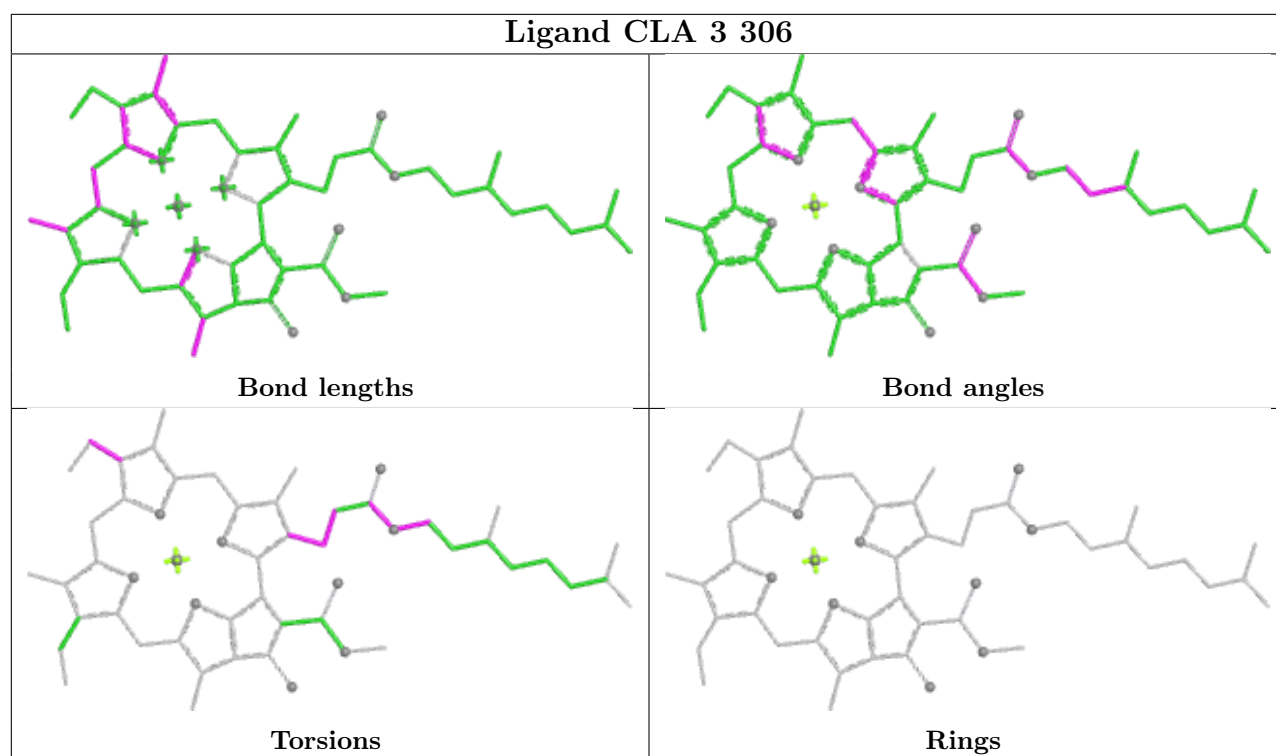




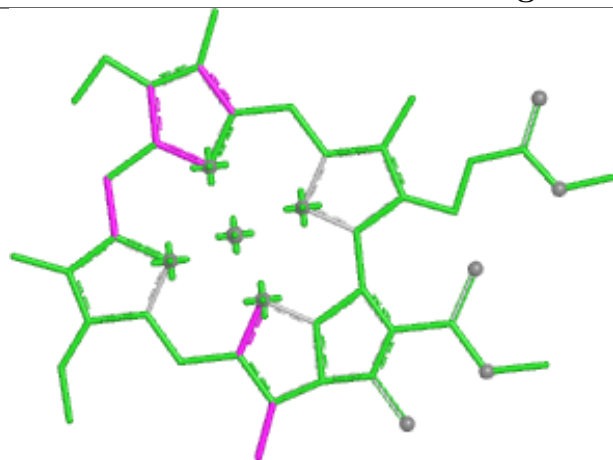


Ligand CLA T 411

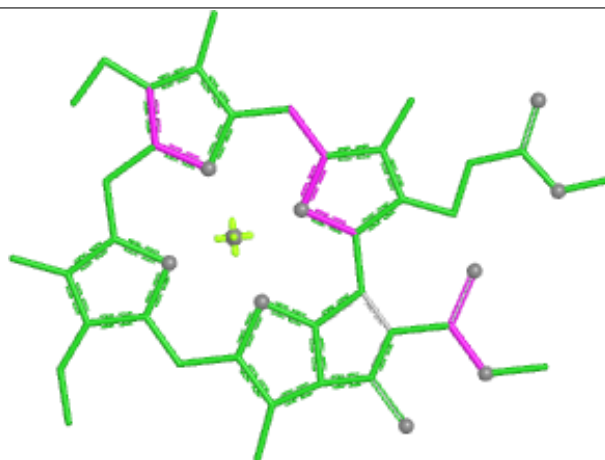




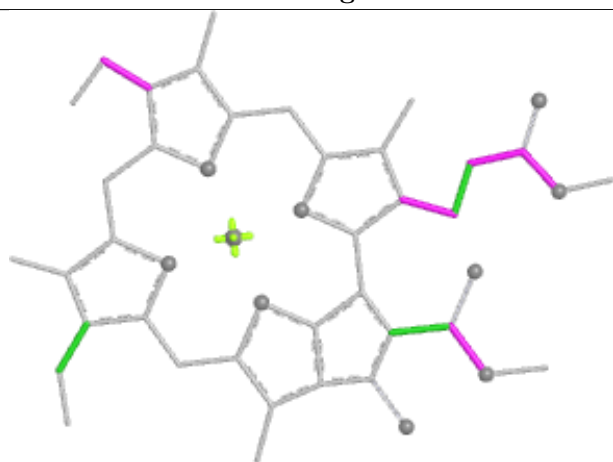
Ligand CLA b 601



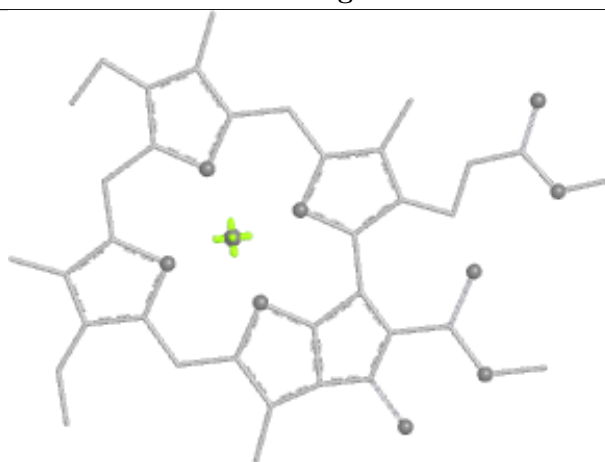
Bond lengths



Bond angles

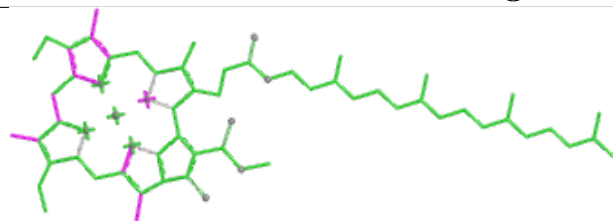


Torsions

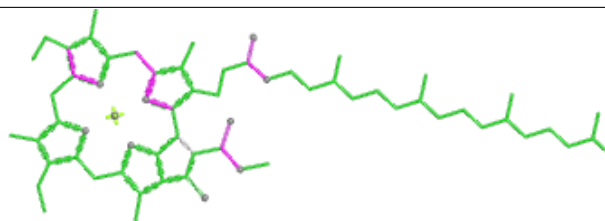


Rings

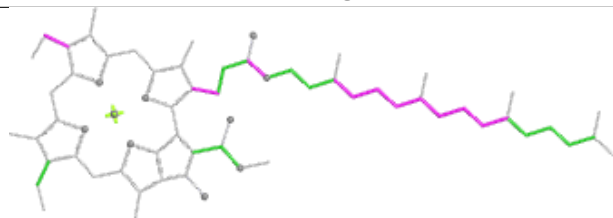
Ligand CLA A 5028



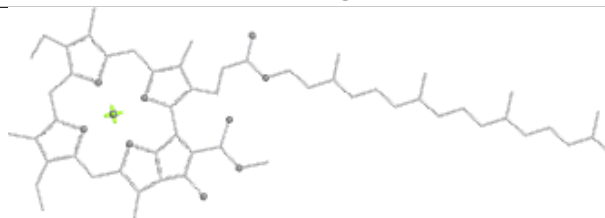
Bond lengths



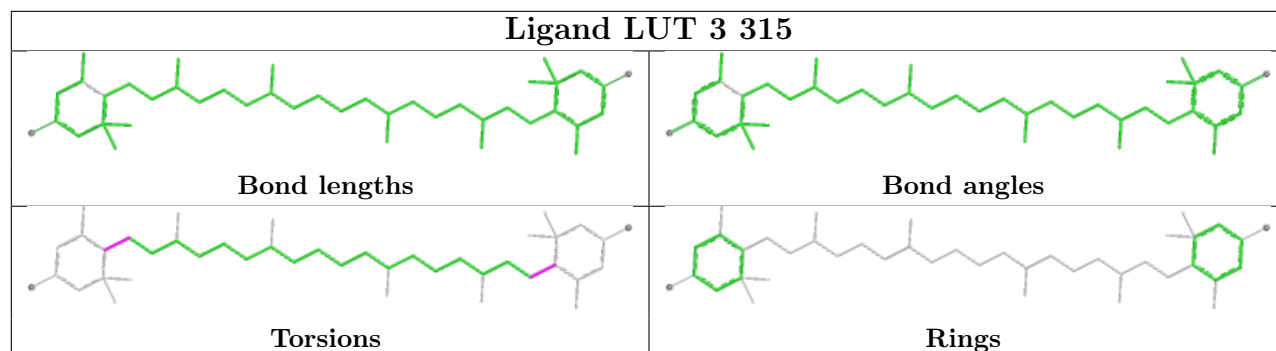
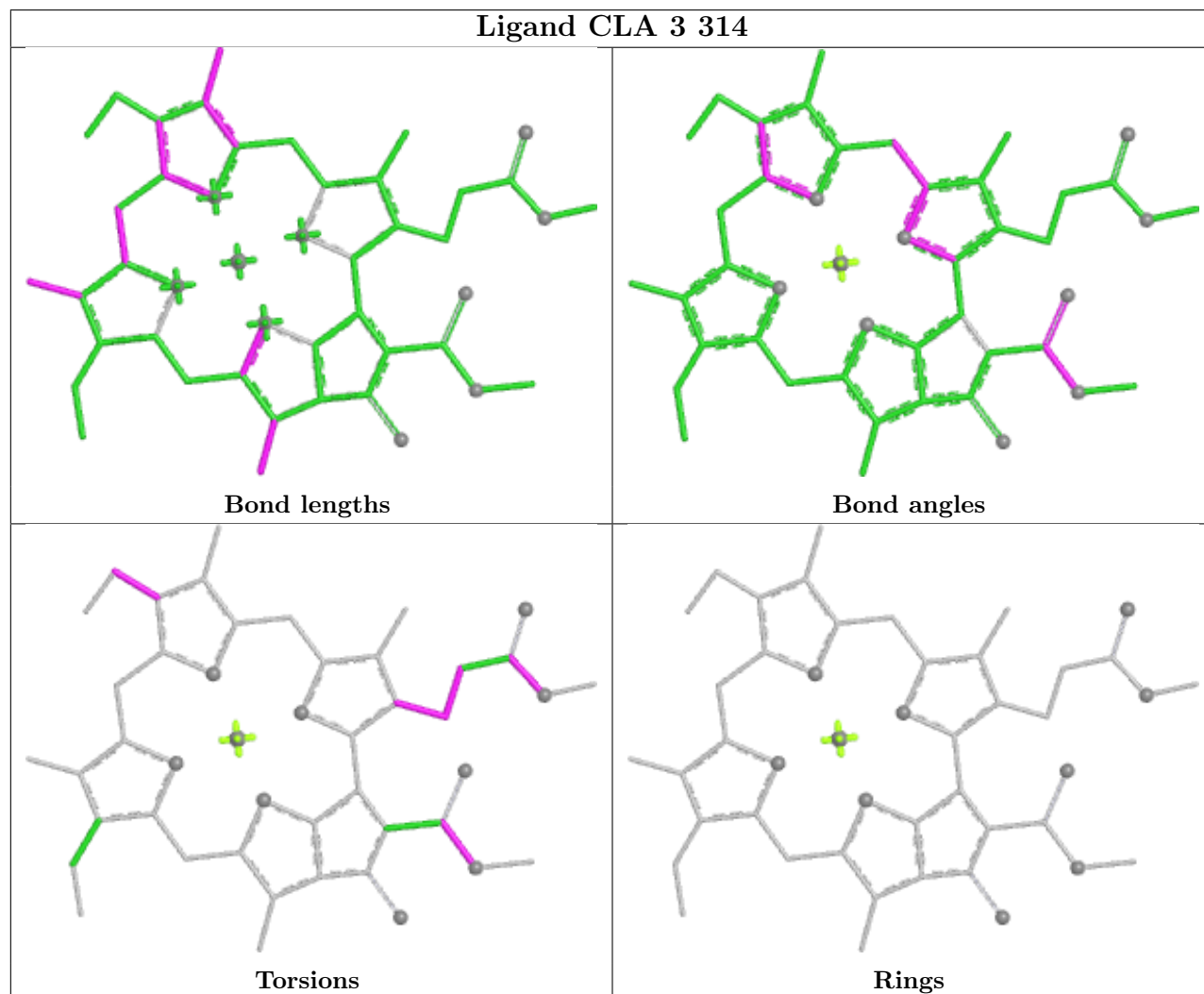
Bond angles

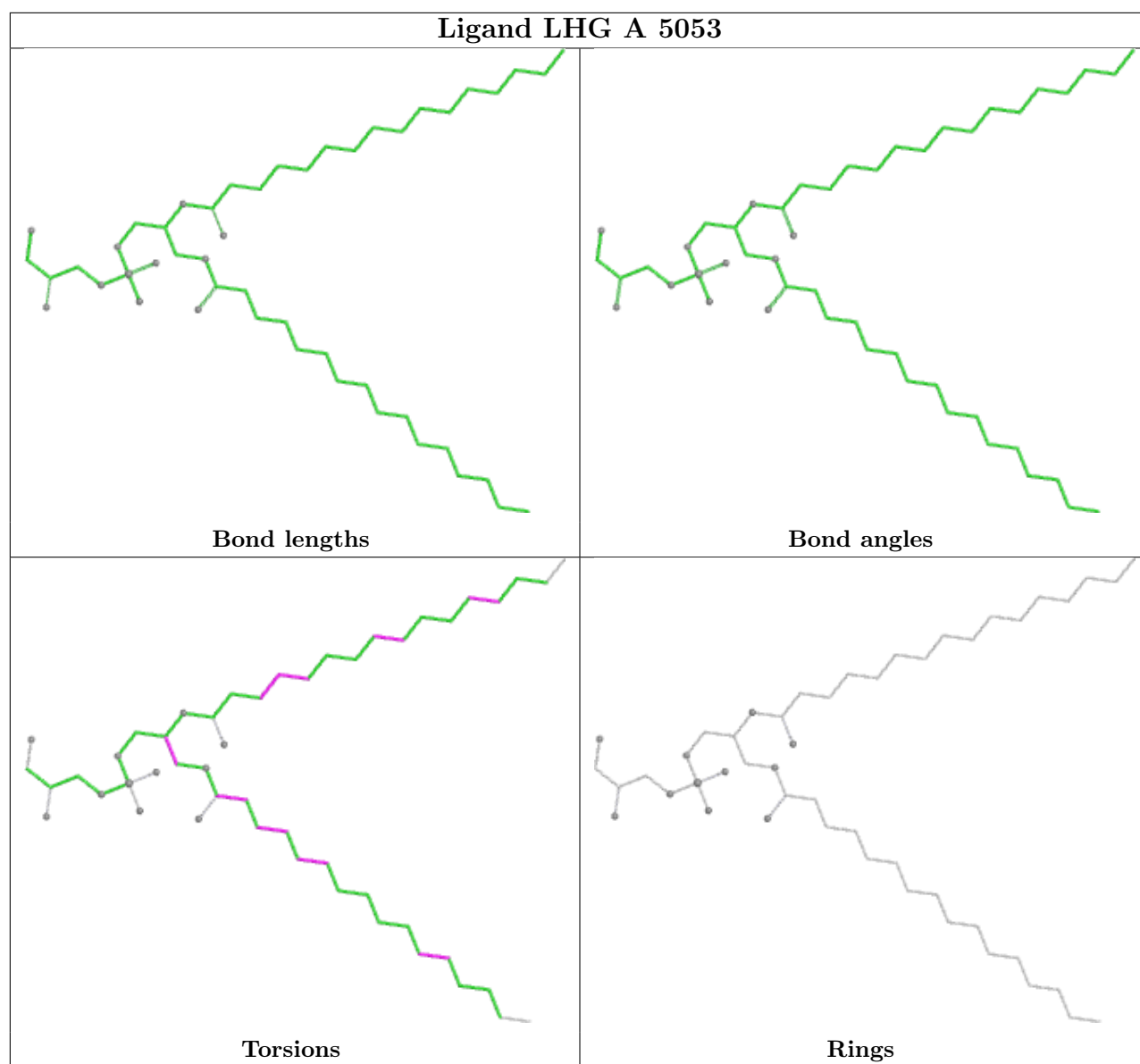


Torsions

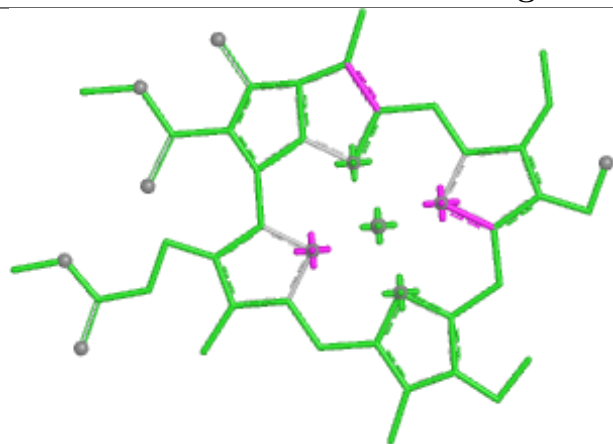


Rings

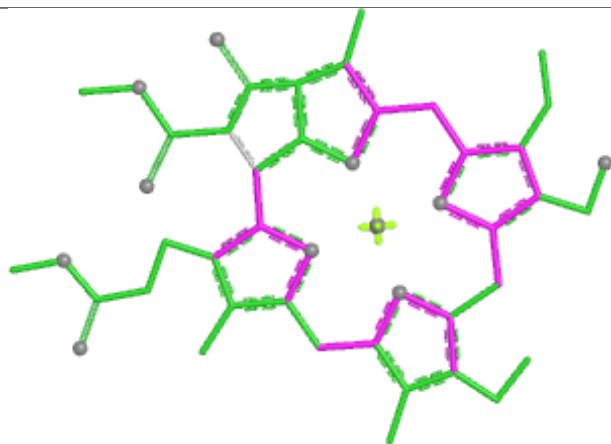
Ligand LUT 3 315**Ligand CLA 3 314**



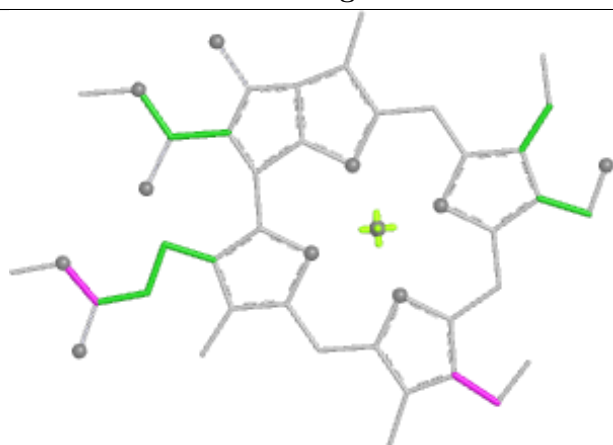
Ligand CHL 1 606



Bond lengths



Bond angles

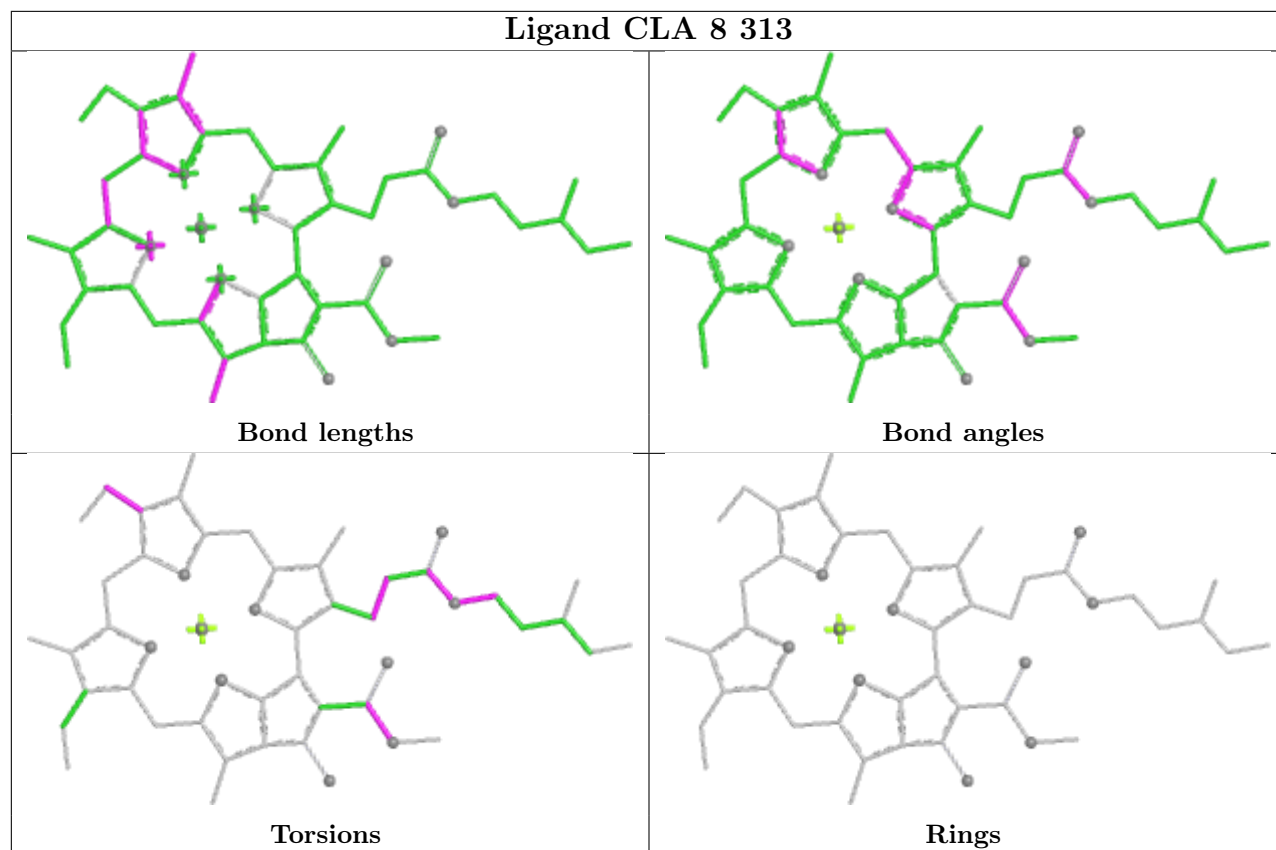


Torsions

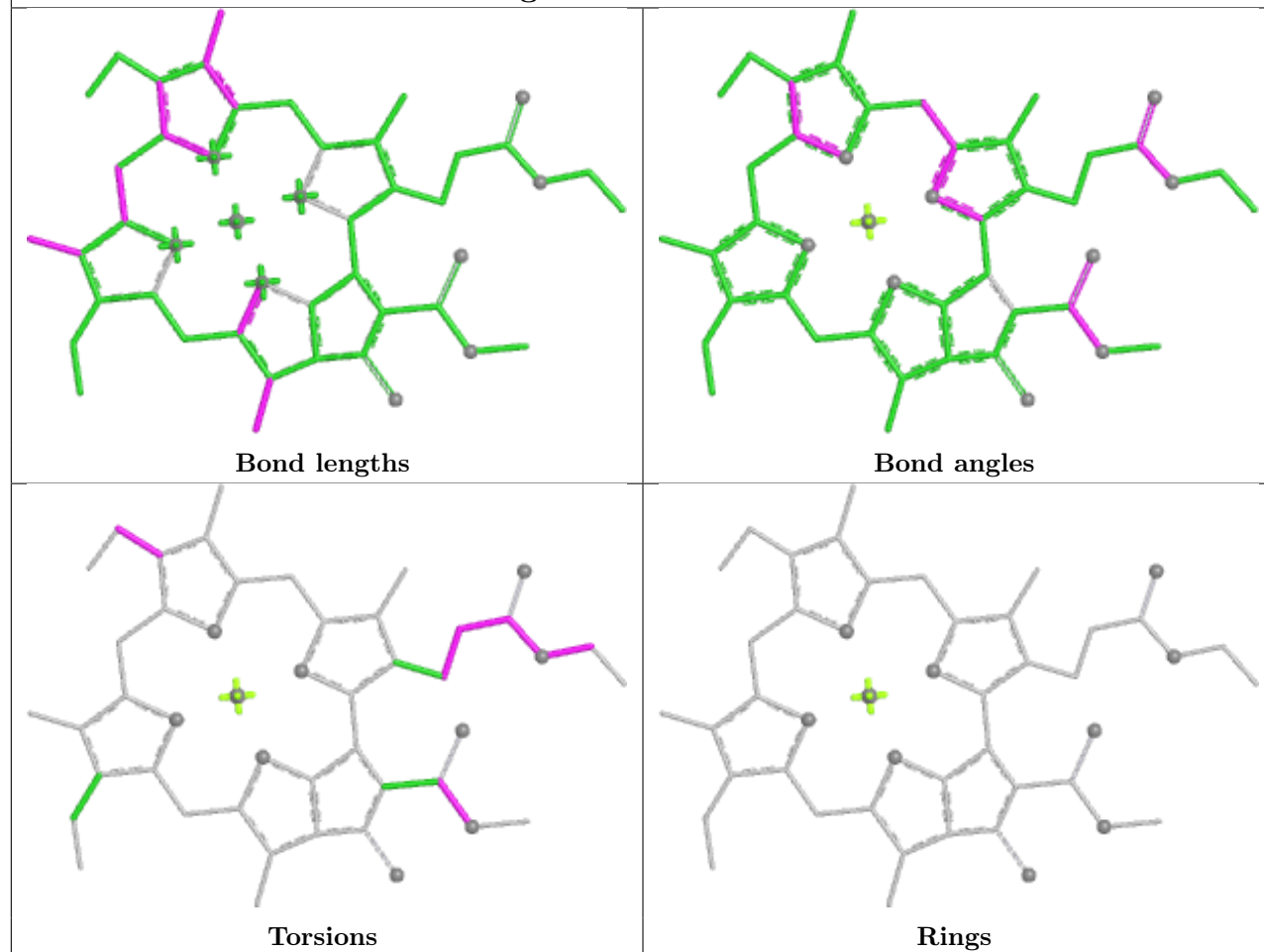


Rings

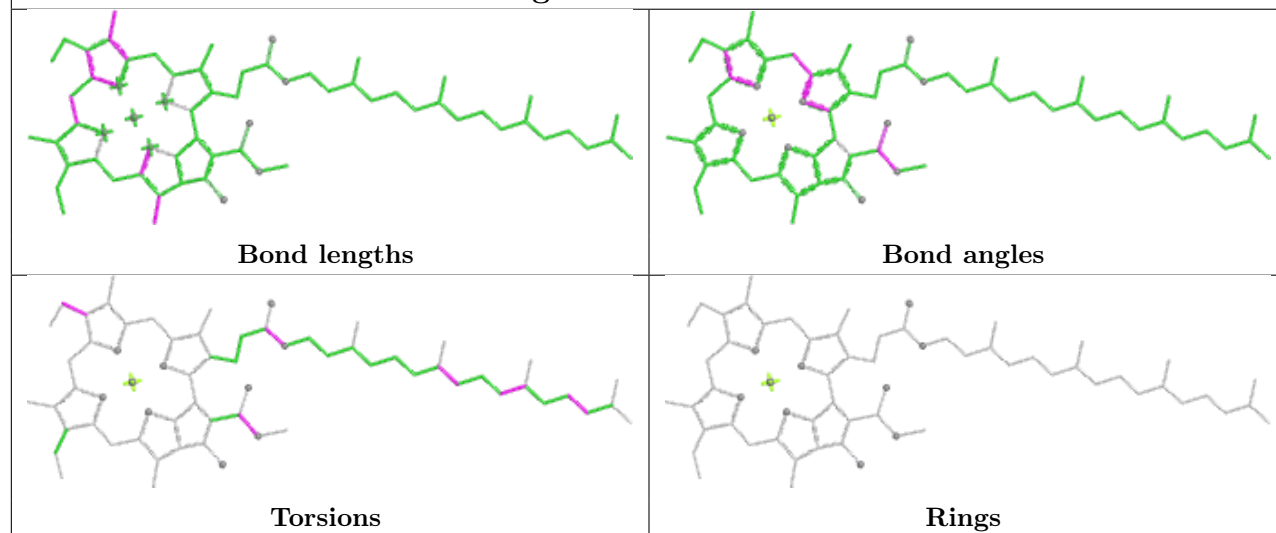
Ligand CLA 8 313

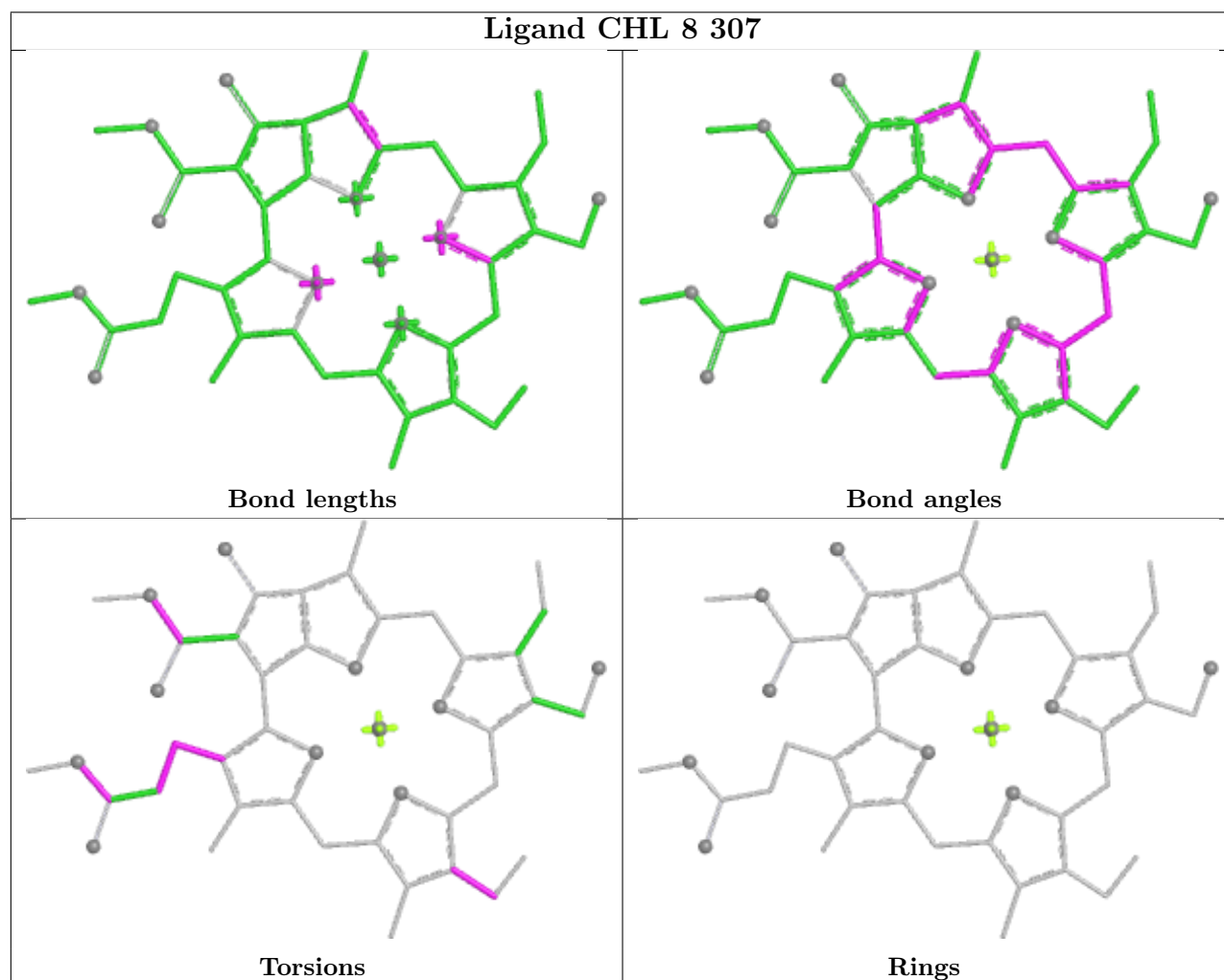
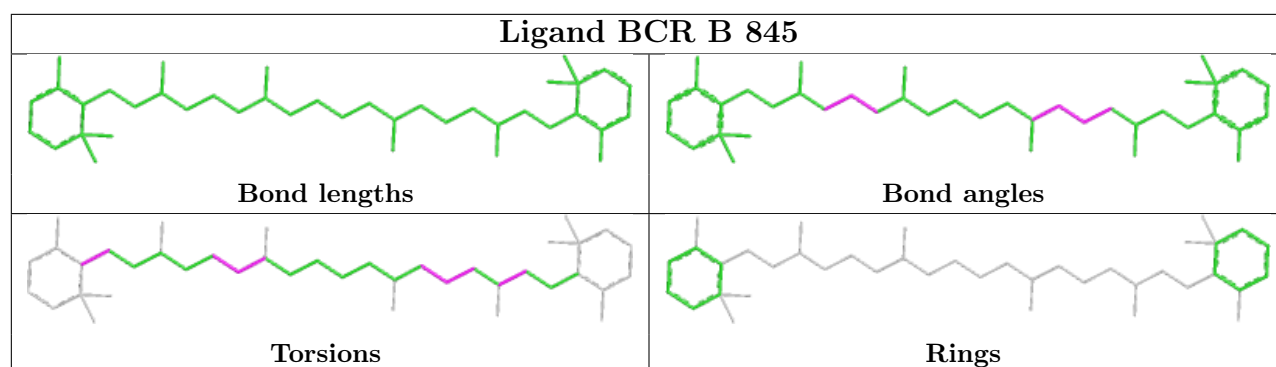


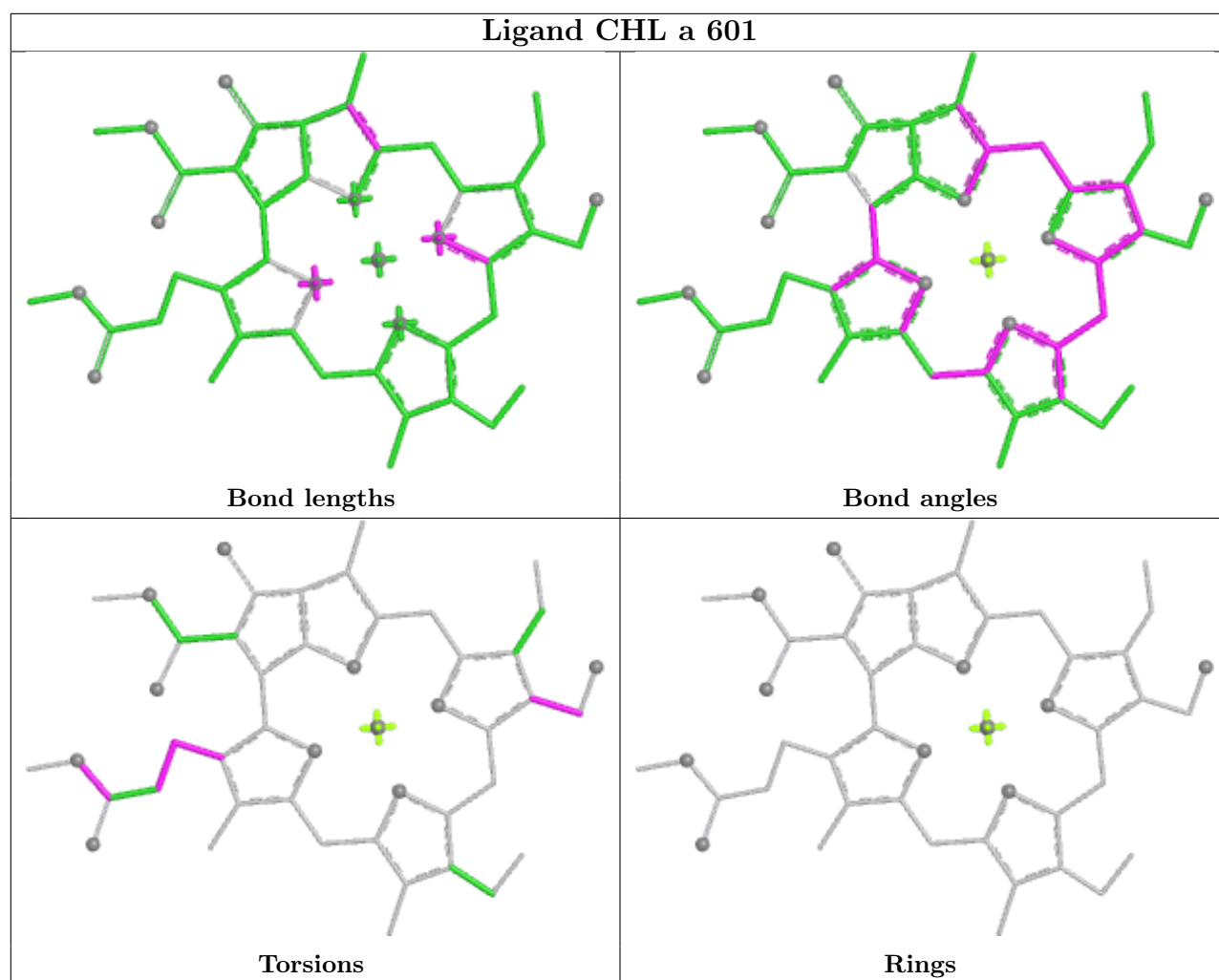
Ligand CLA F 5007



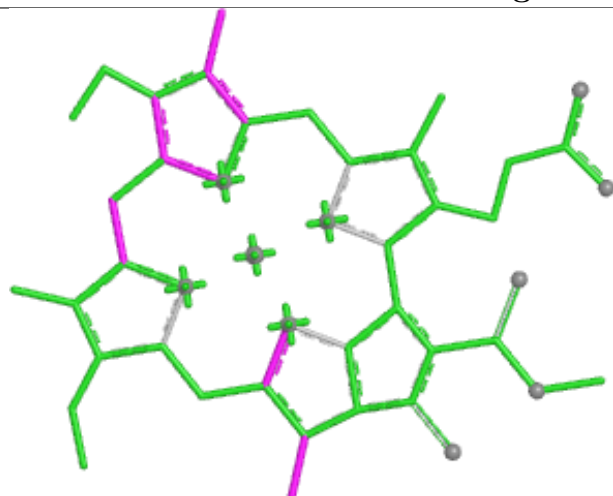
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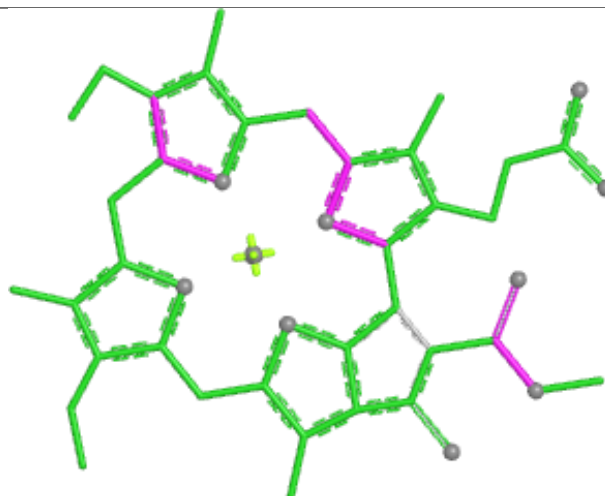




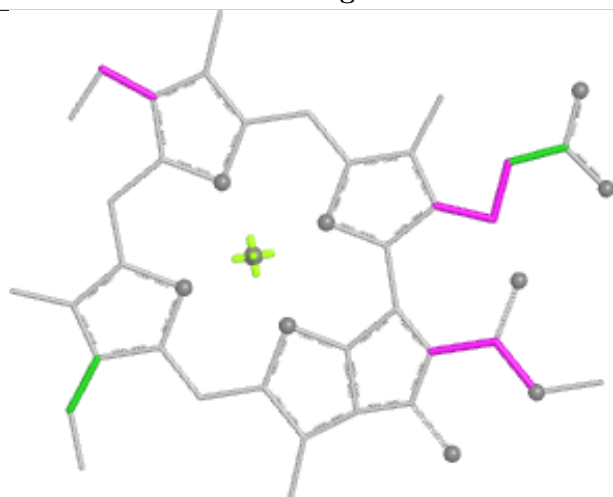
Ligand CLA K 204



Bond lengths



Bond angles

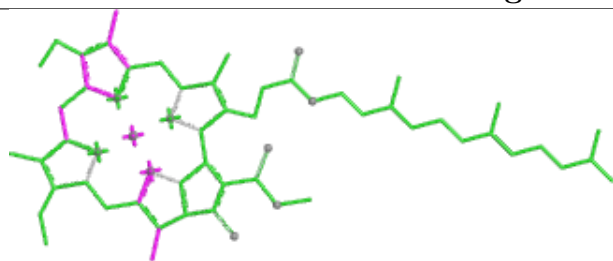


Torsions

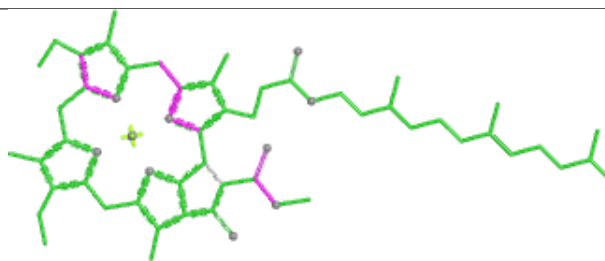


Rings

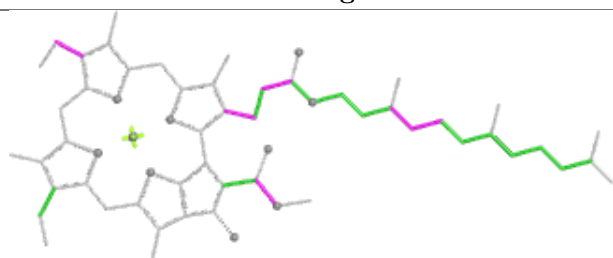
Ligand CLA A 5040



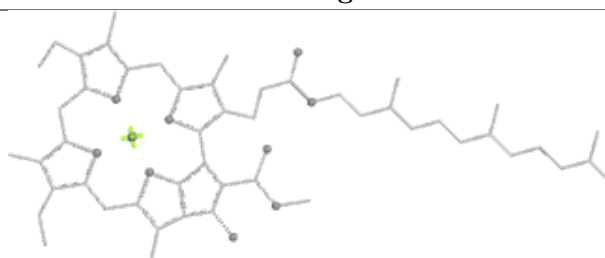
Bond lengths



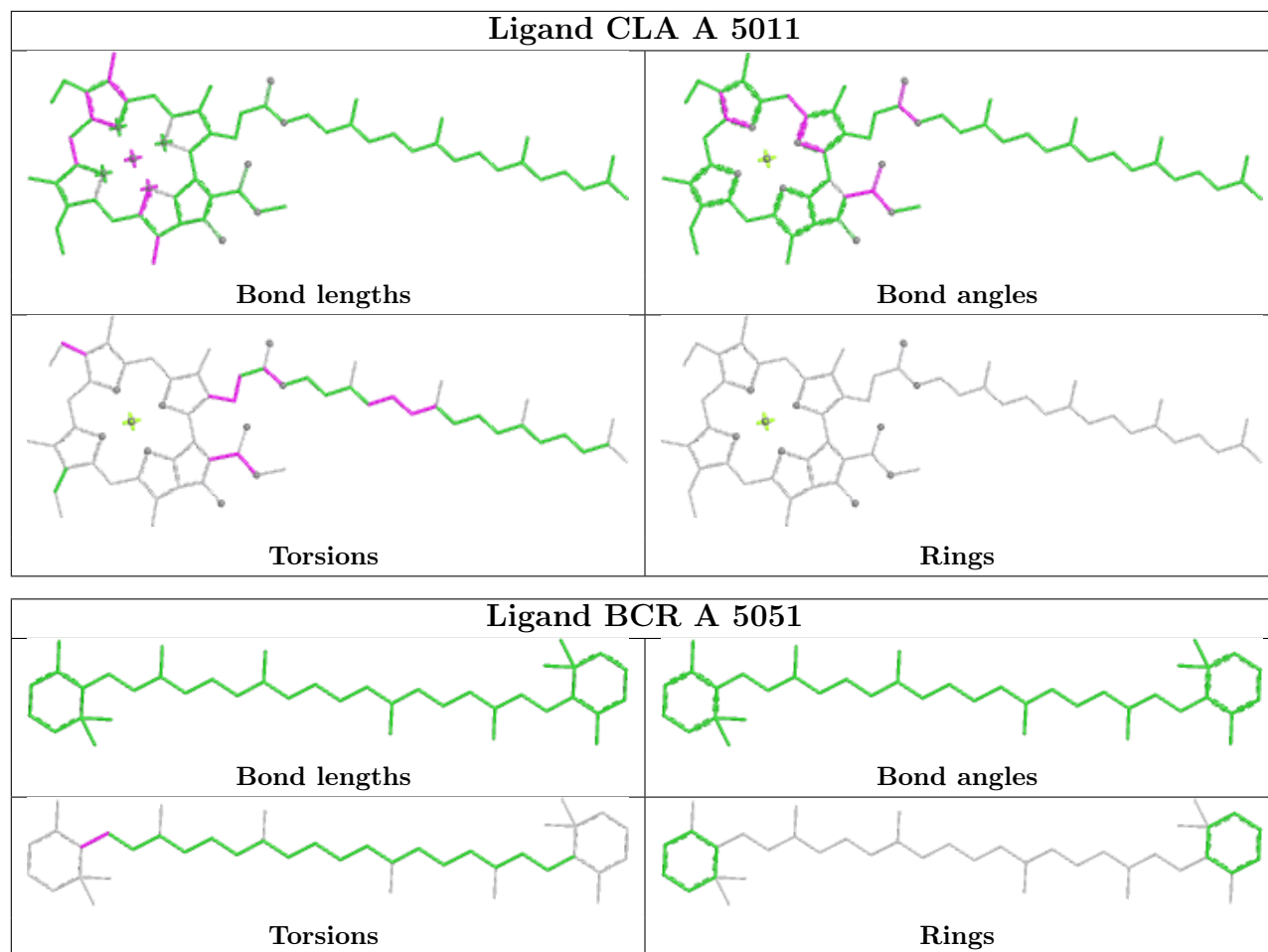
Bond angles



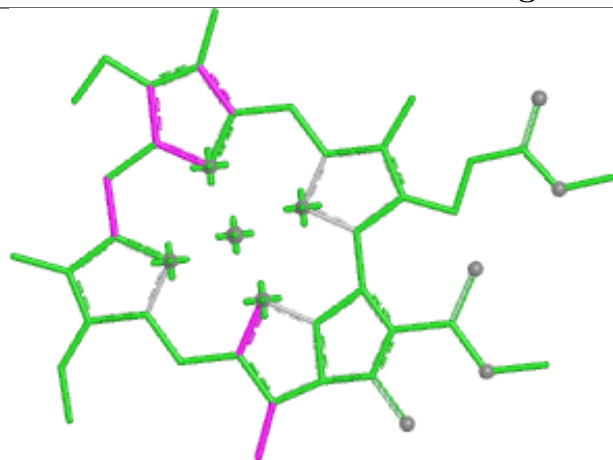
Torsions



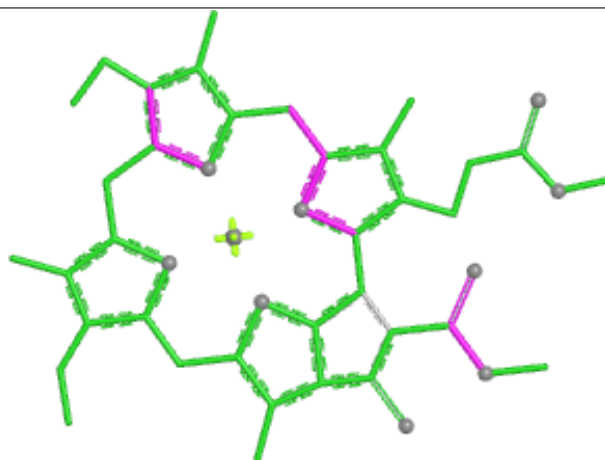
Rings



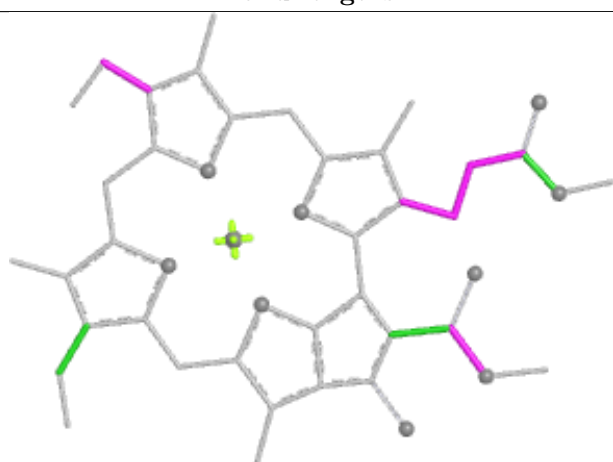
Ligand CLA 1 614



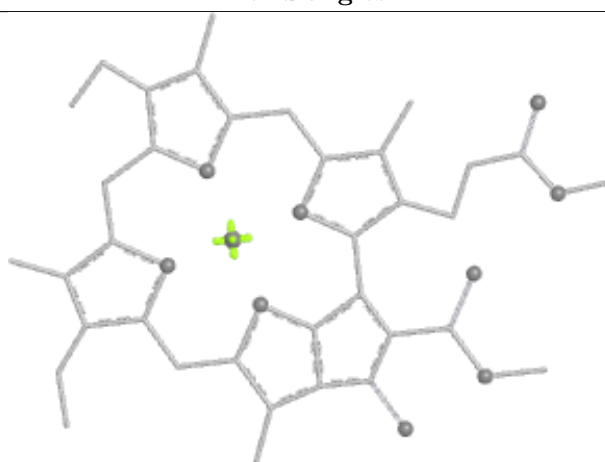
Bond lengths



Bond angles

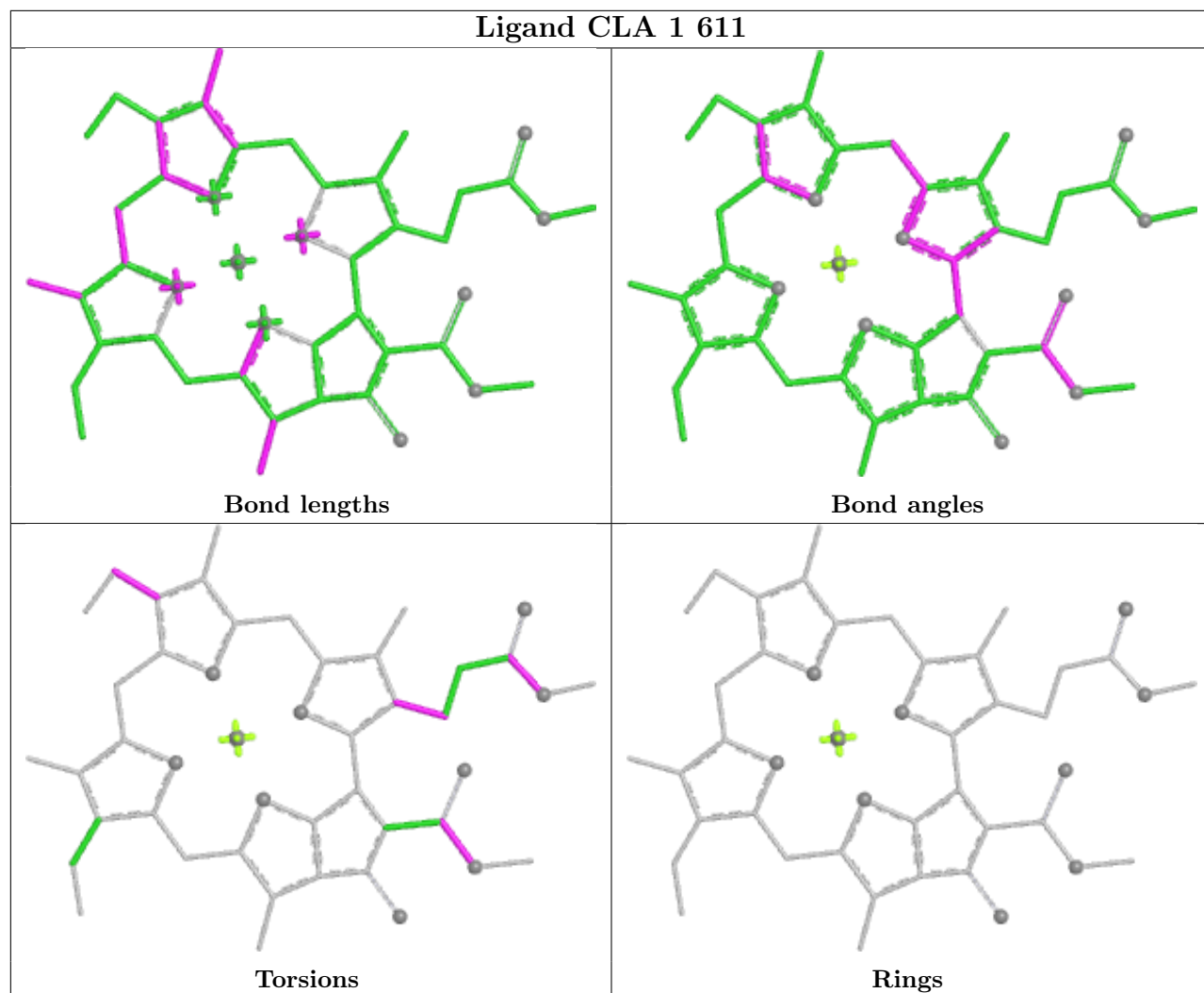


Torsions

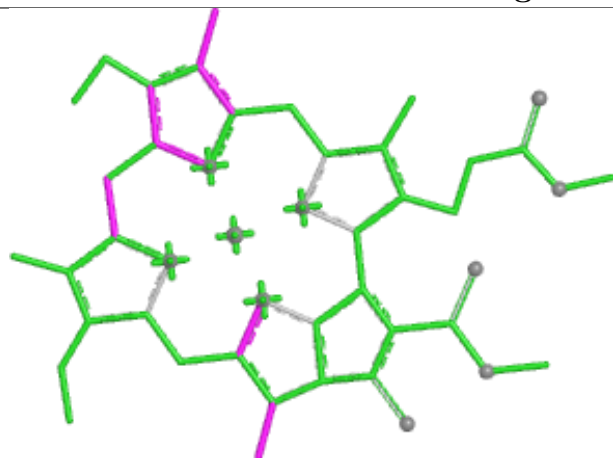


Rings

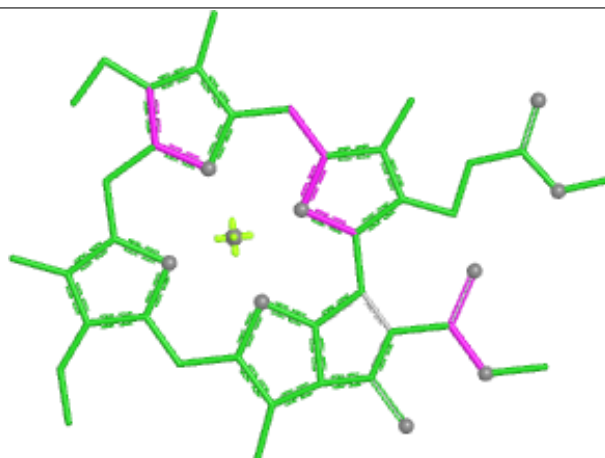
Ligand CLA 1 611



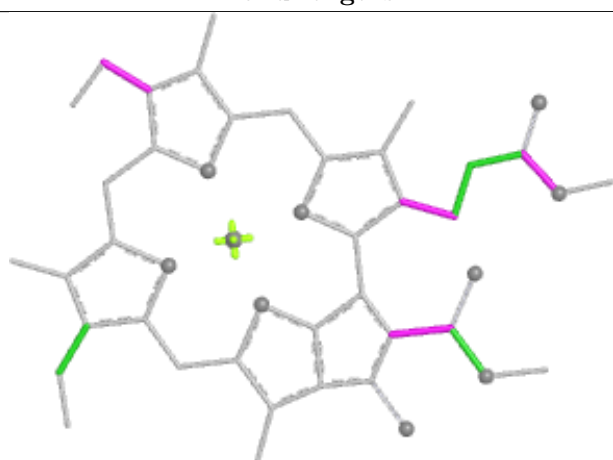
Ligand CLA B 812



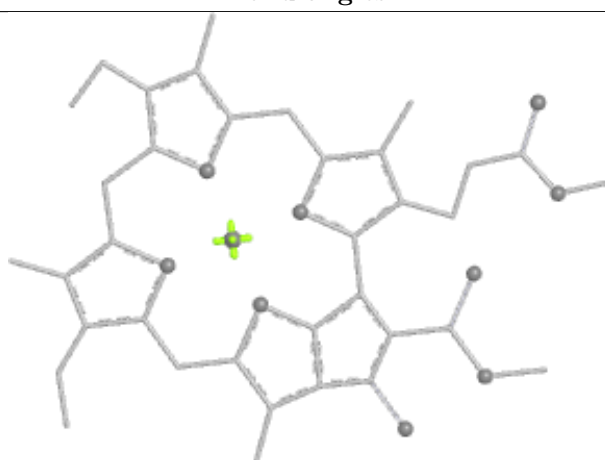
Bond lengths



Bond angles

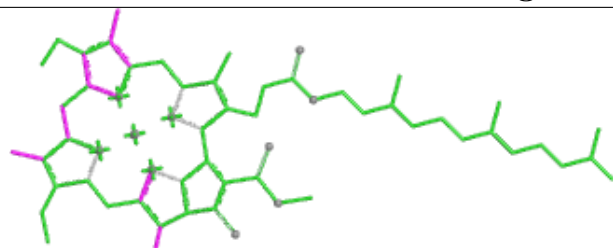


Torsions

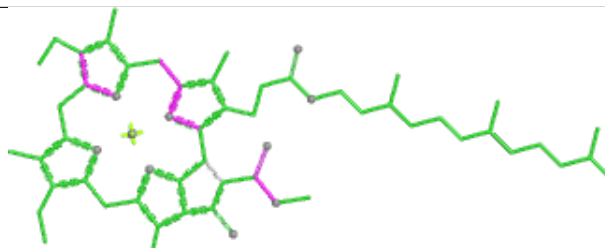


Rings

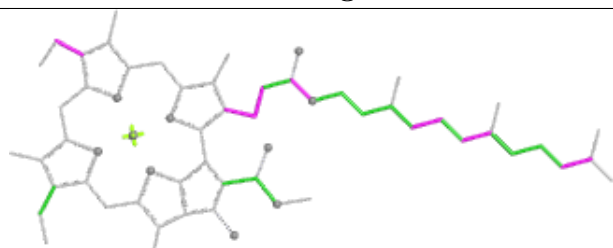
Ligand CLA b 609



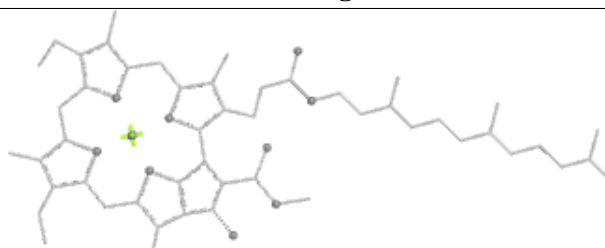
Bond lengths



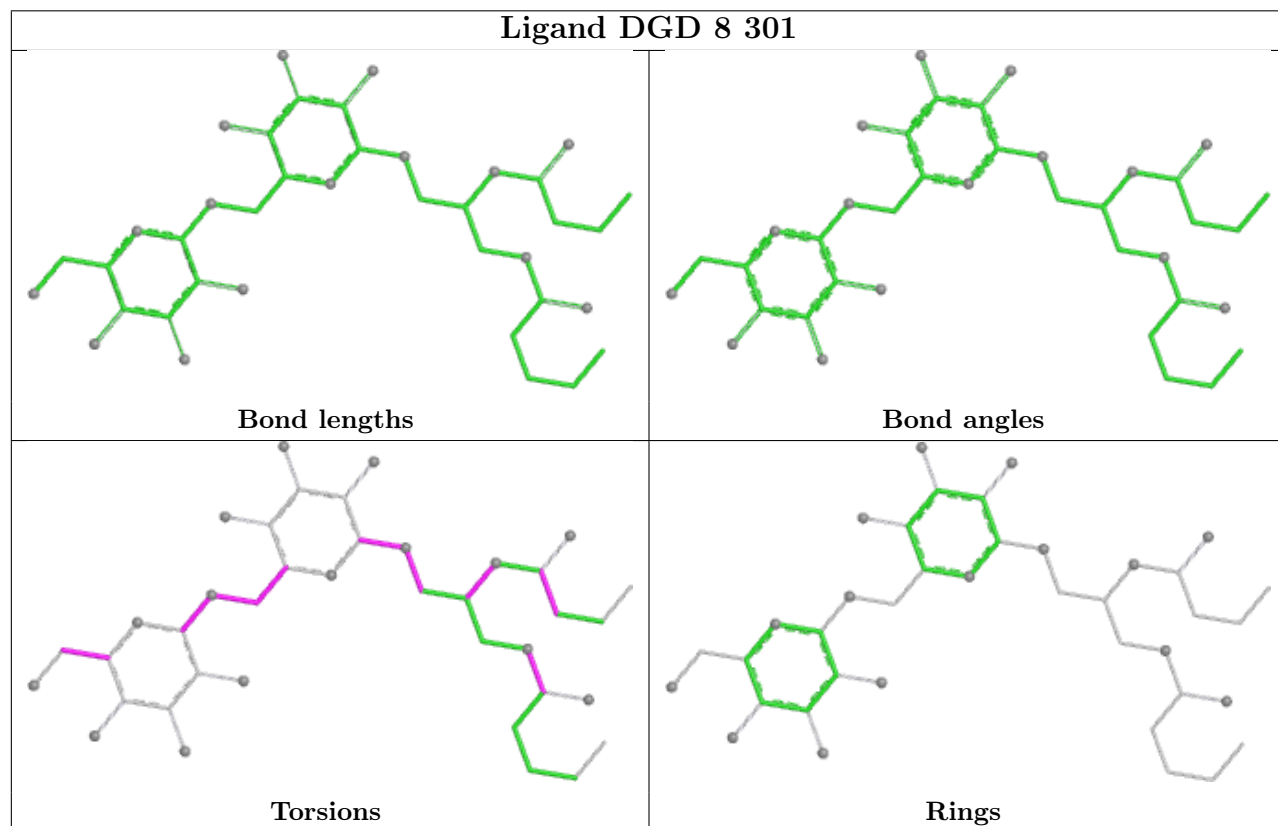
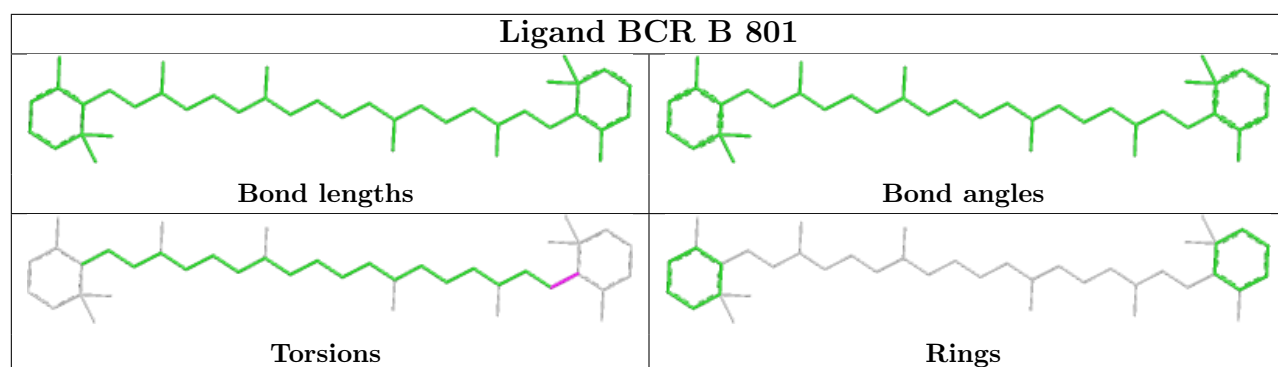
Bond angles



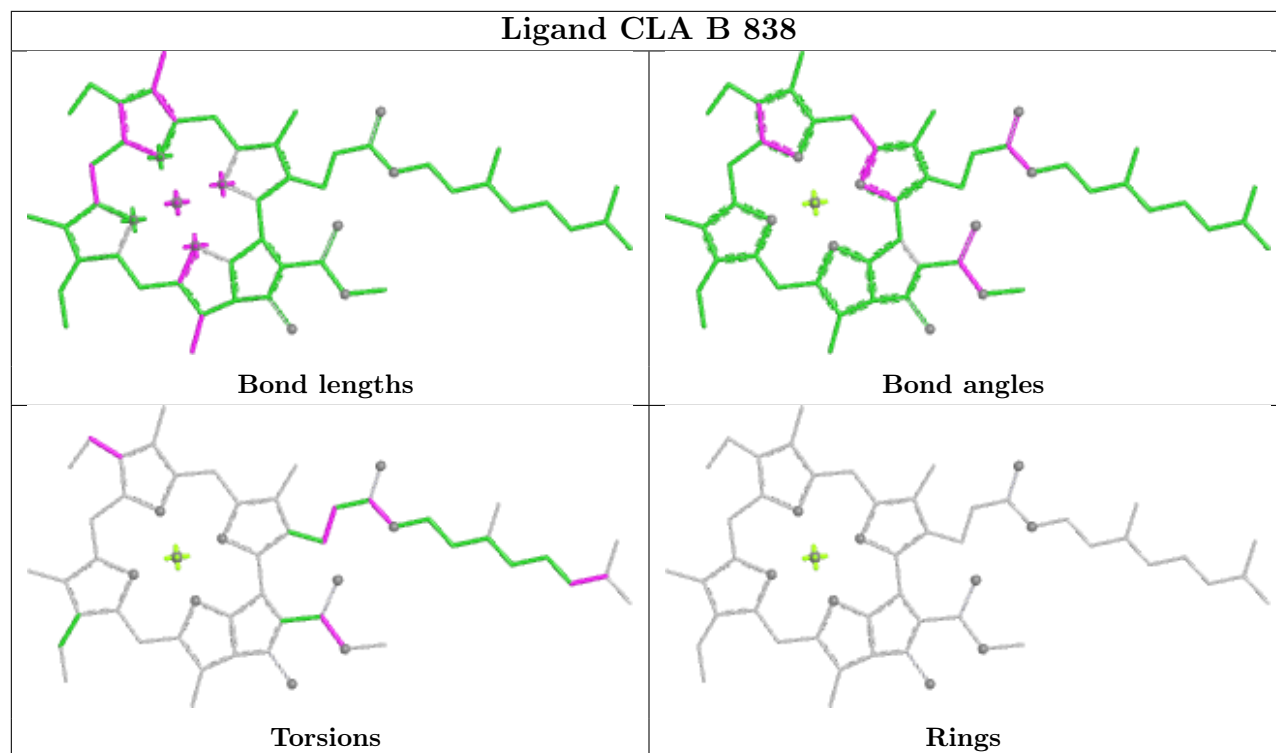
Torsions



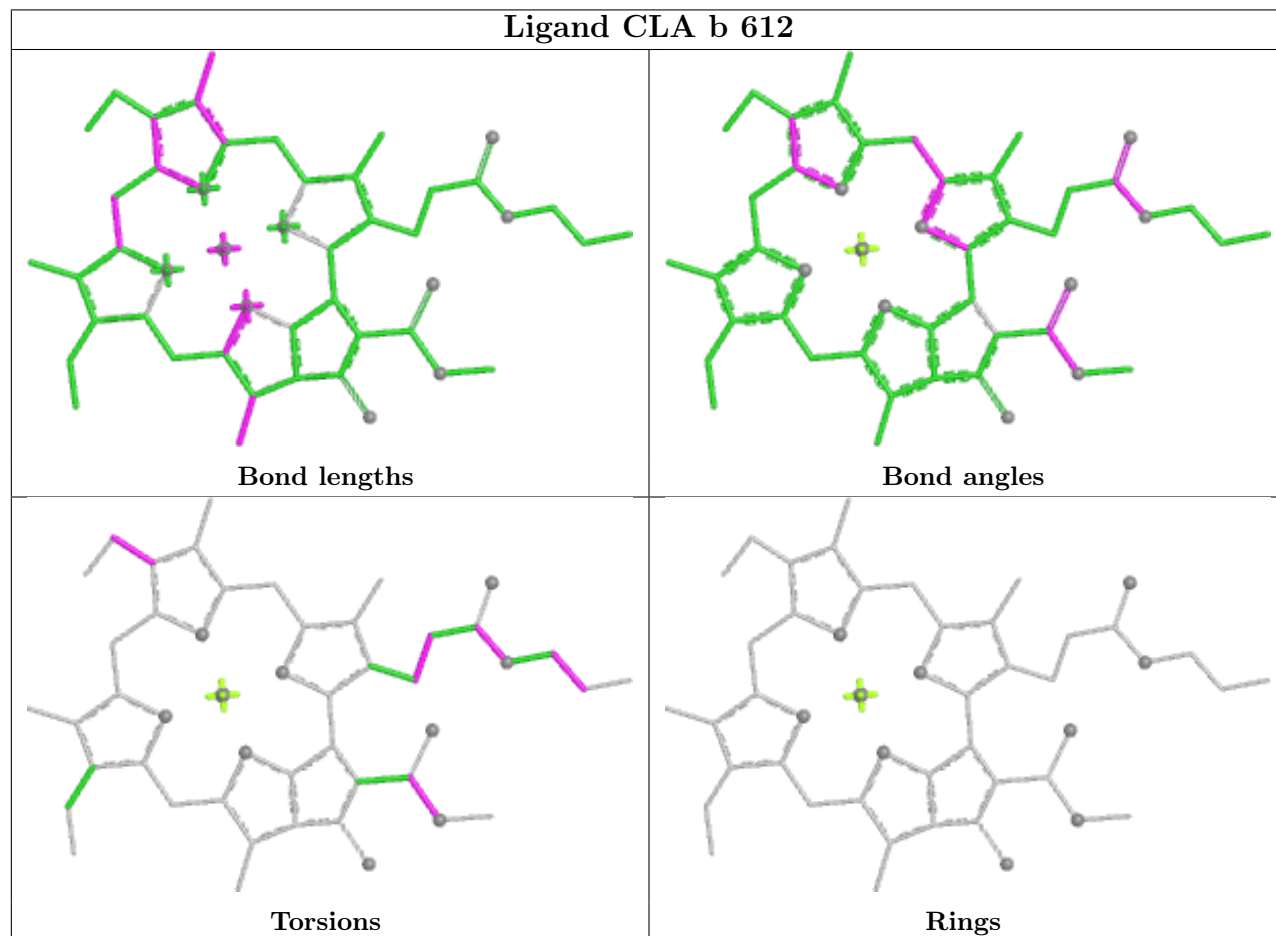
Rings



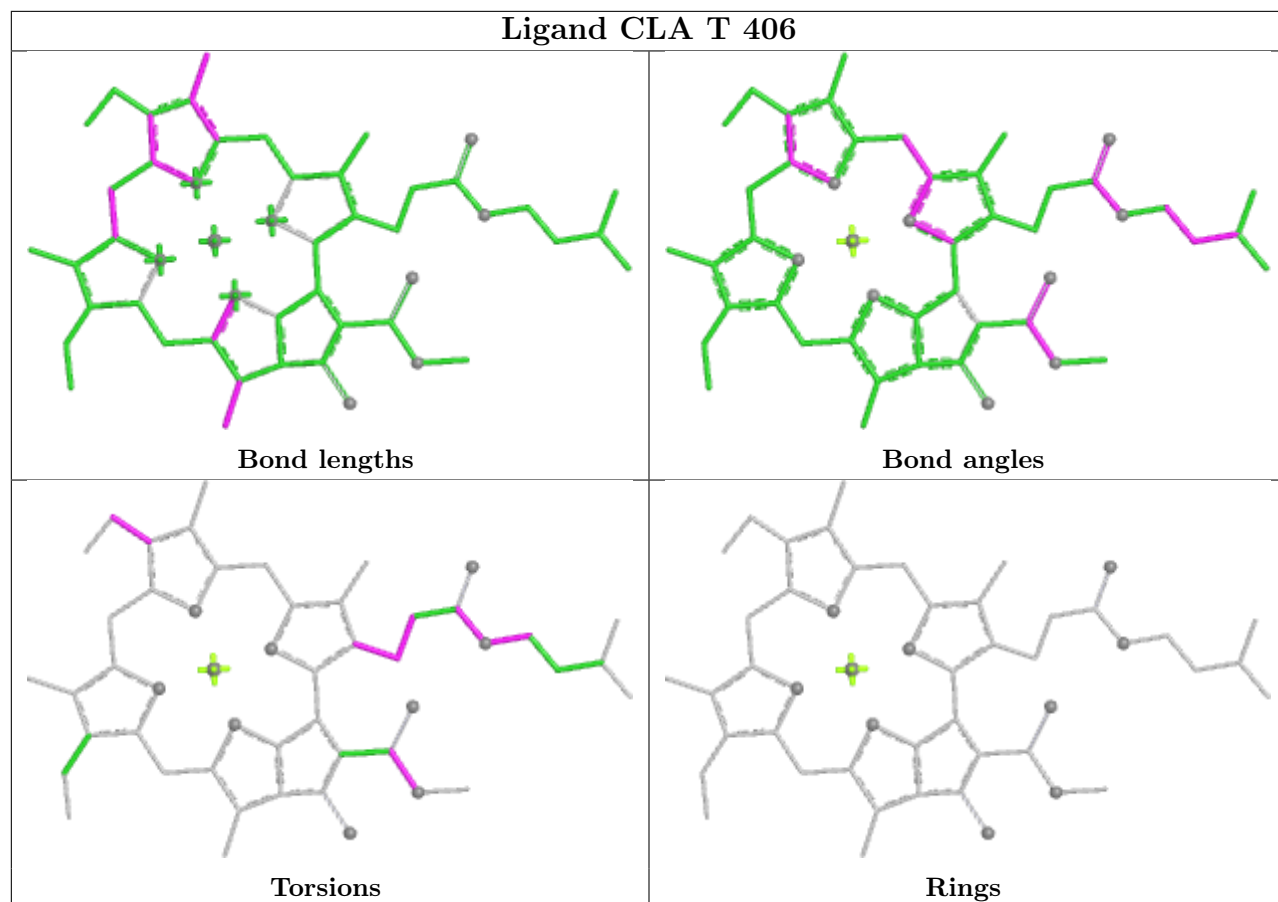
Ligand CLA B 838



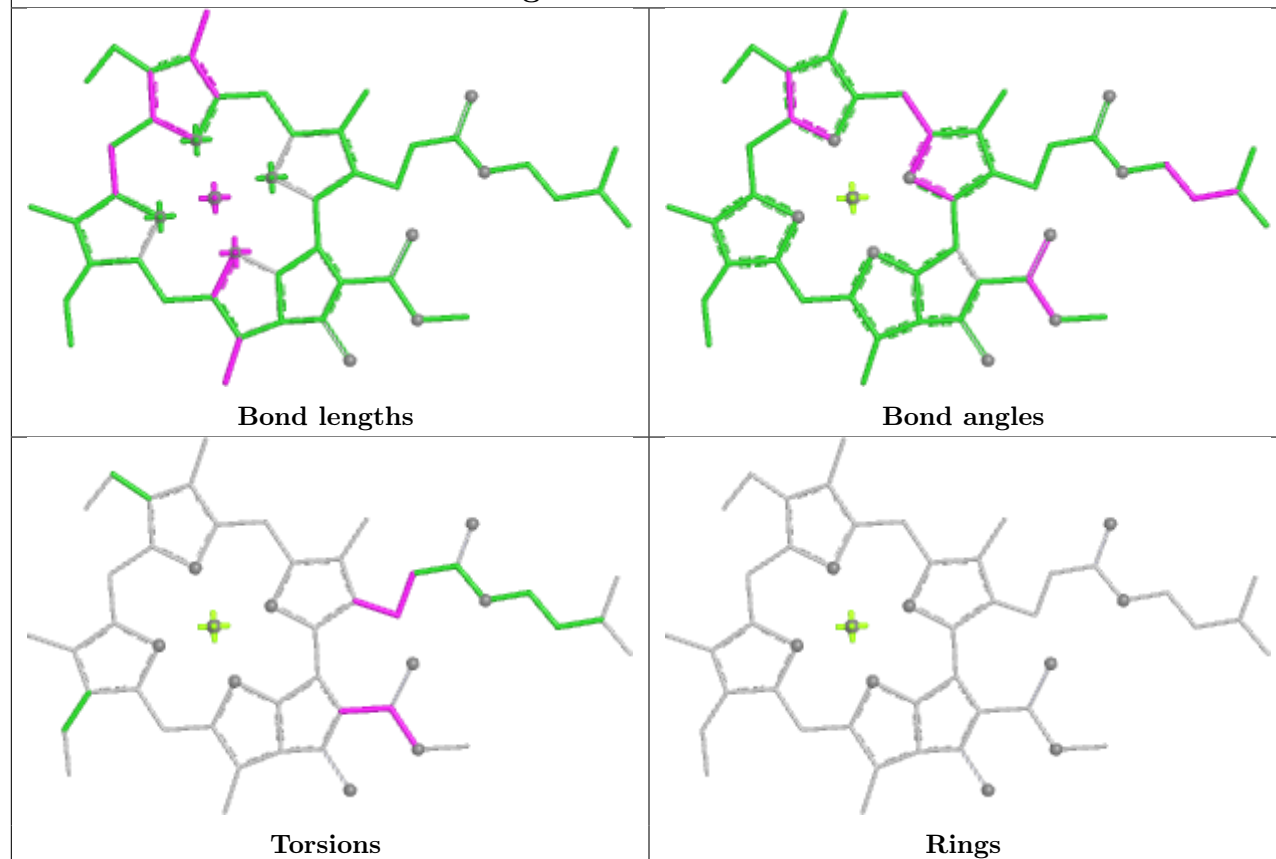
Ligand CLA b 612



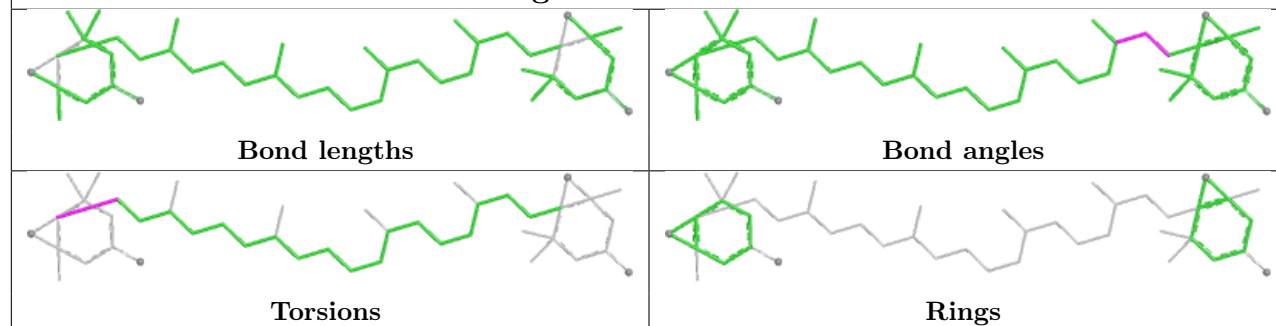
Ligand CLA T 406

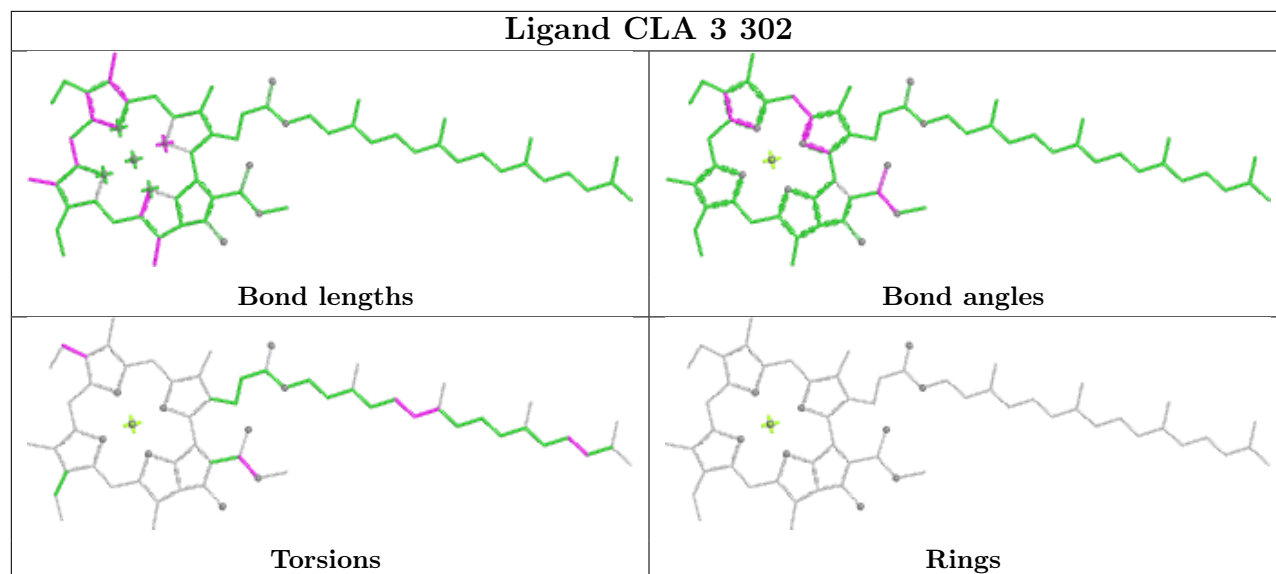
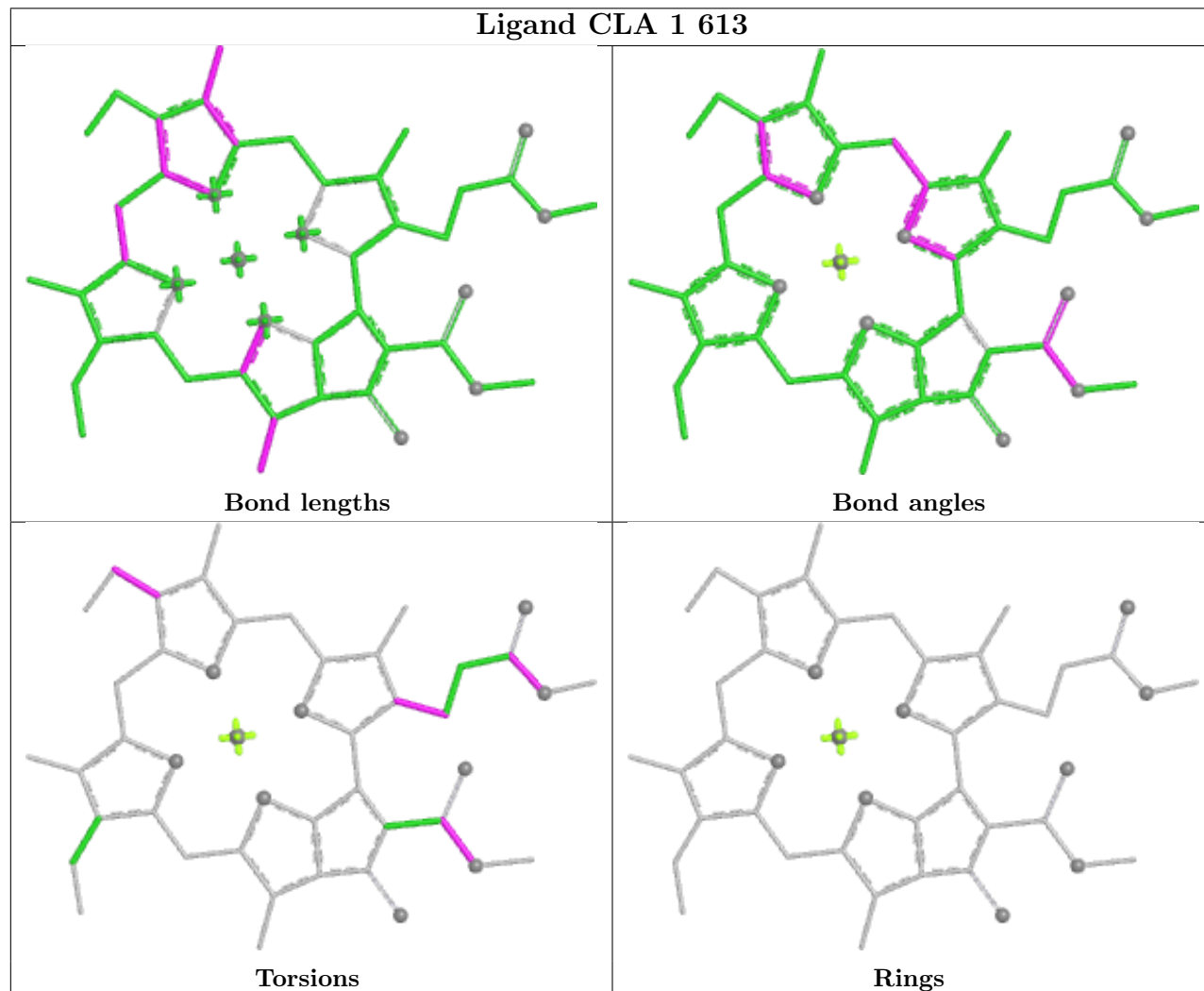


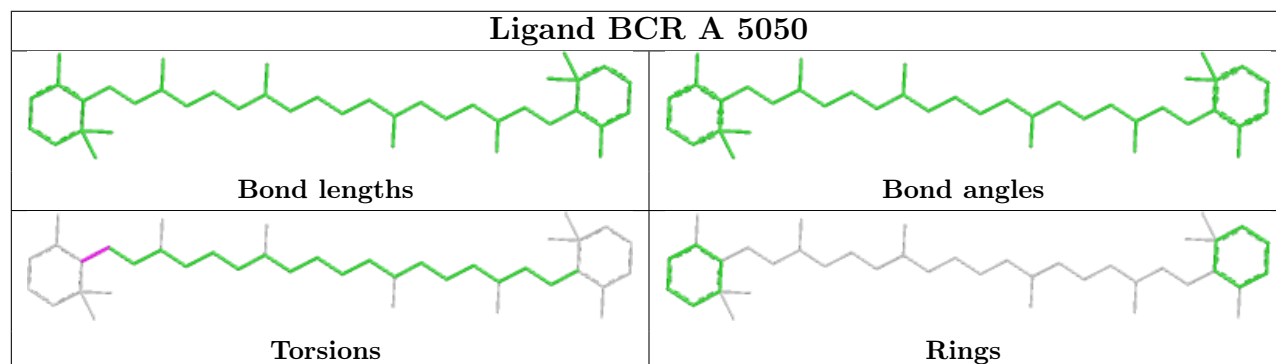
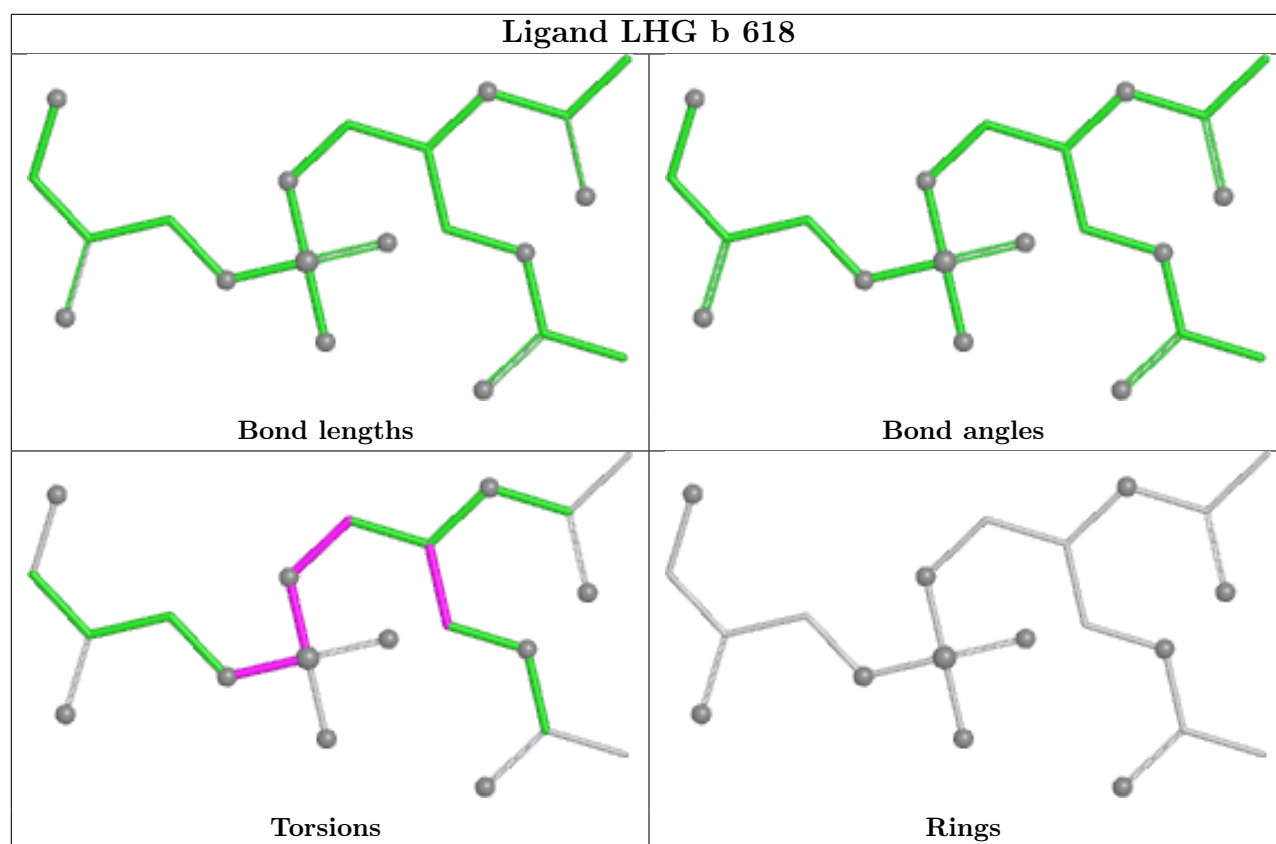
Ligand CLA A 5038



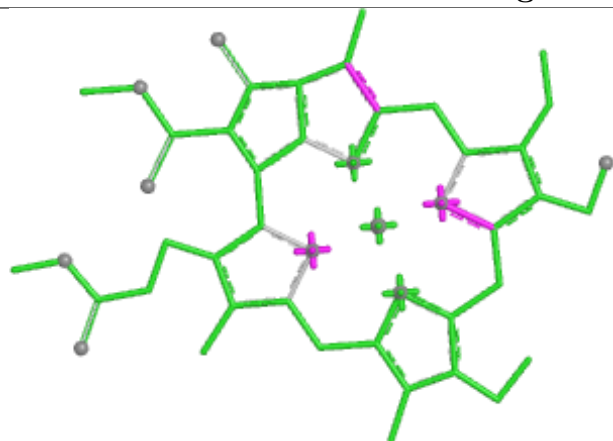
Ligand XAT T 414



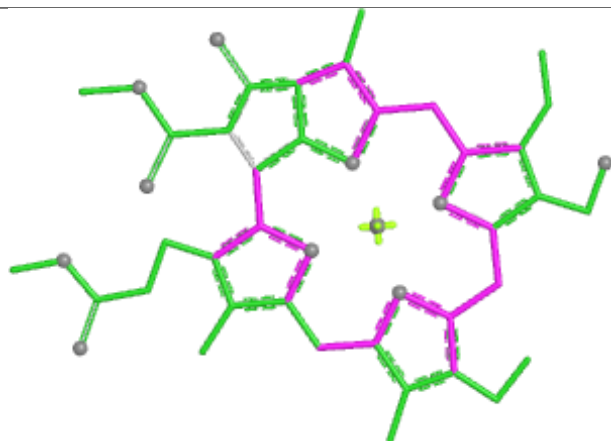
Ligand CLA 3 302**Ligand CLA 1 613**



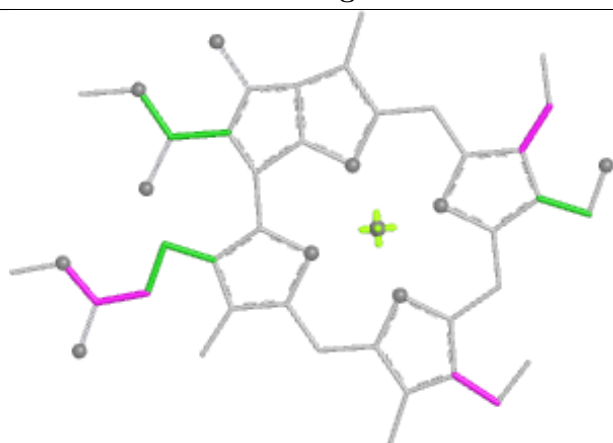
Ligand CHL b 606



Bond lengths



Bond angles

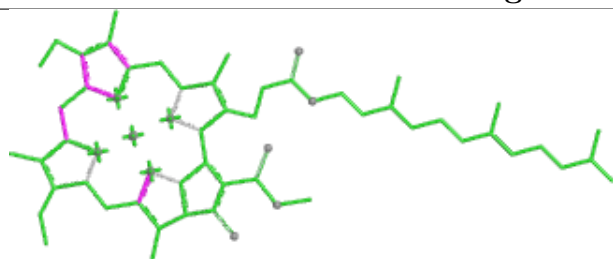


Torsions

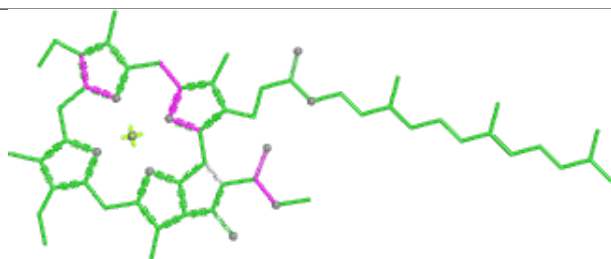


Rings

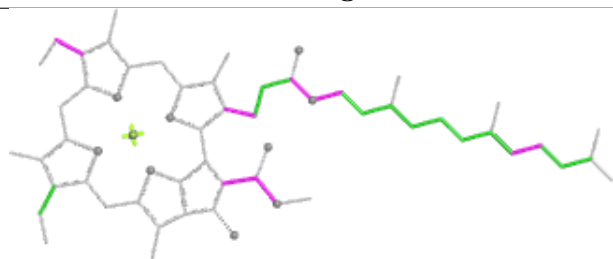
Ligand CLA A 5007



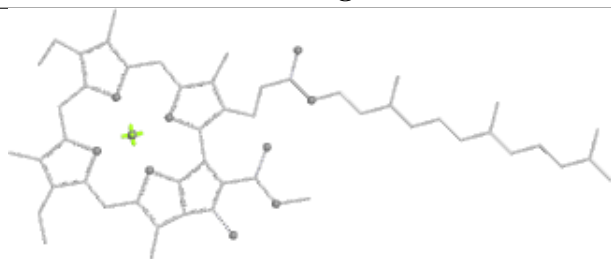
Bond lengths



Bond angles

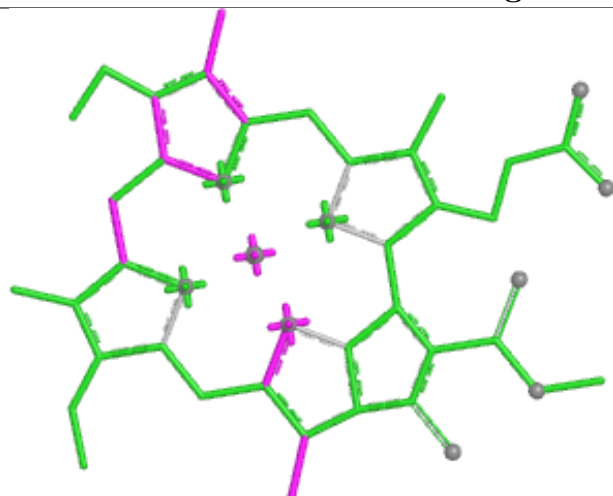


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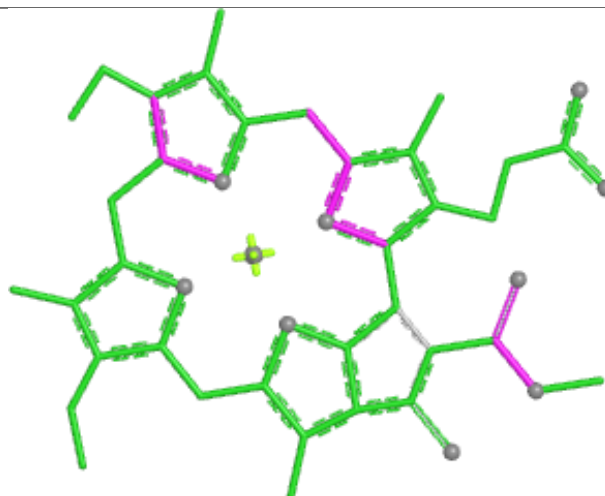


Rings

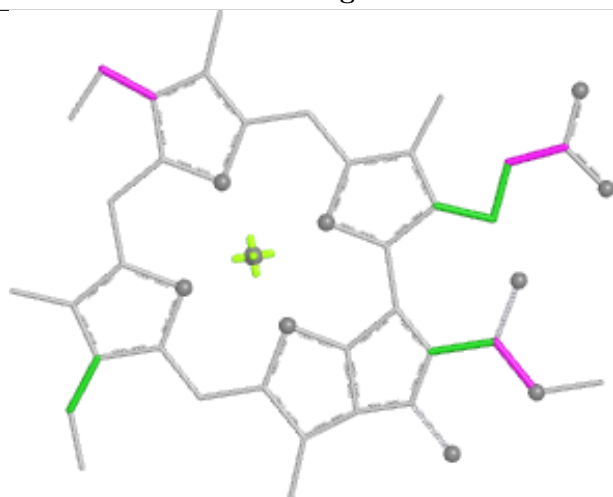
Ligand CLA A 5032



Bond lengths



Bond angles

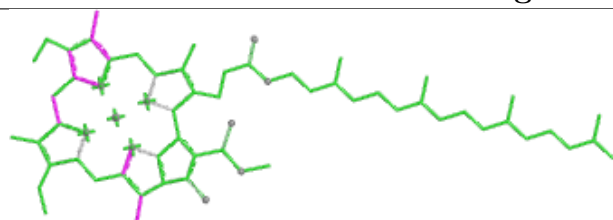


Torsions

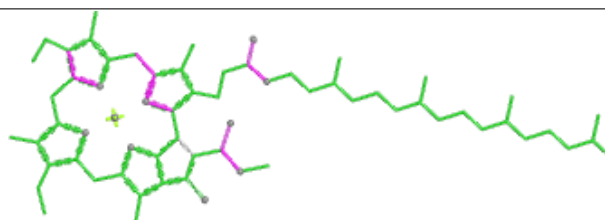


Rings

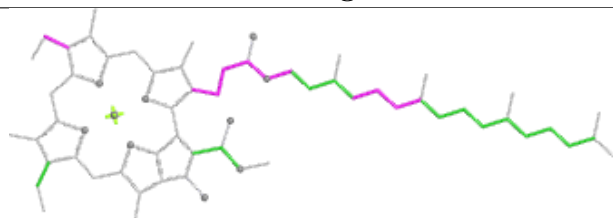
Ligand CLA B 841



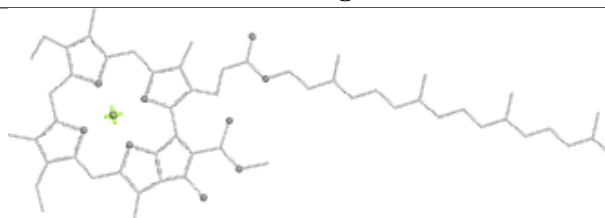
Bond lengths



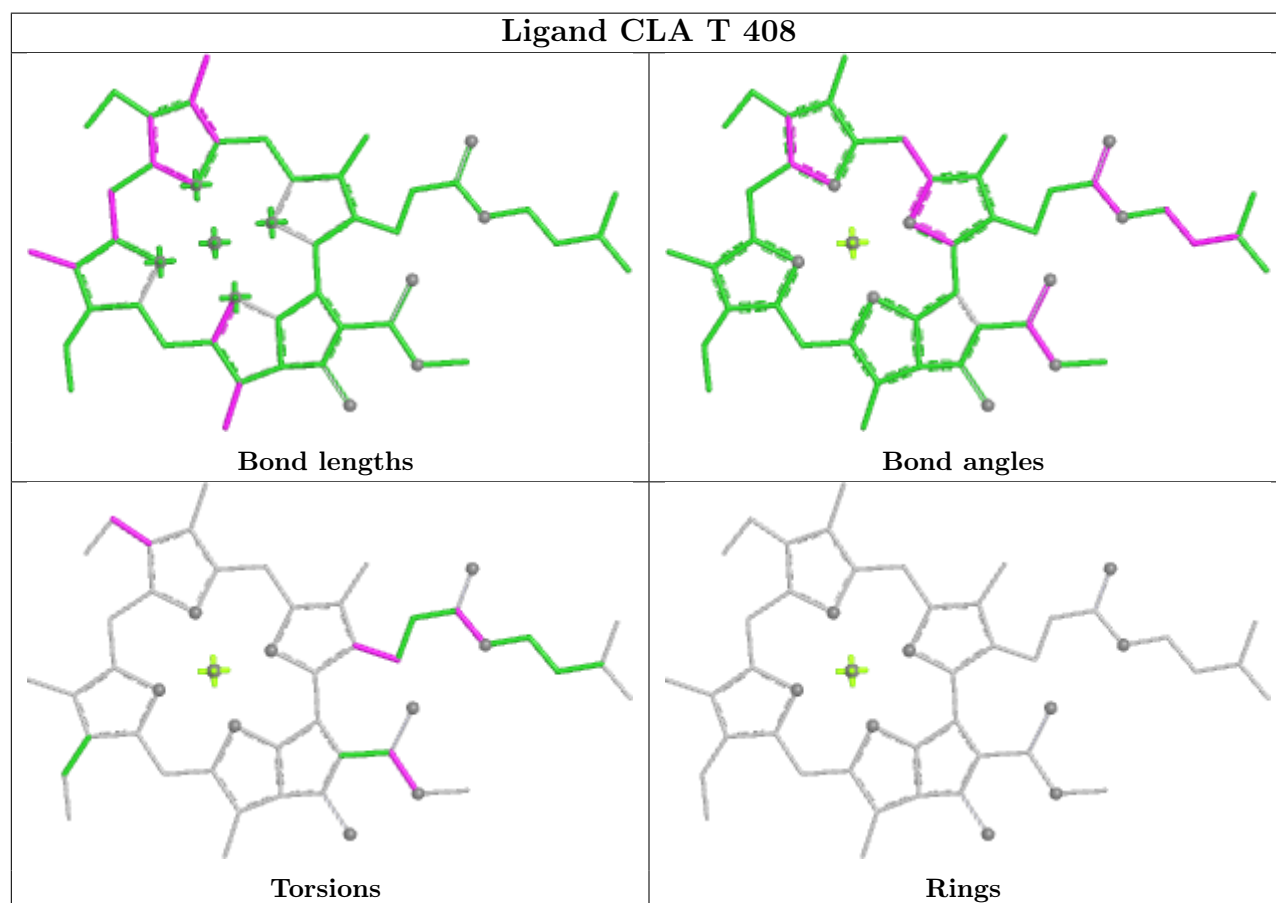
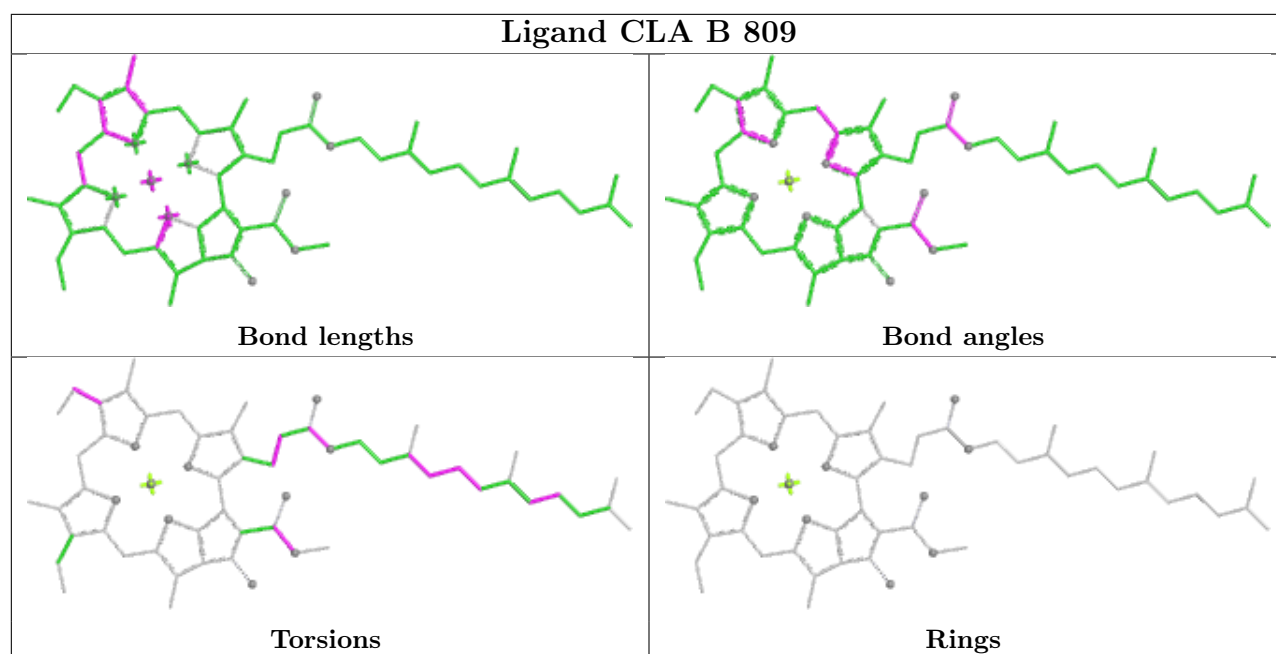
Bond angles



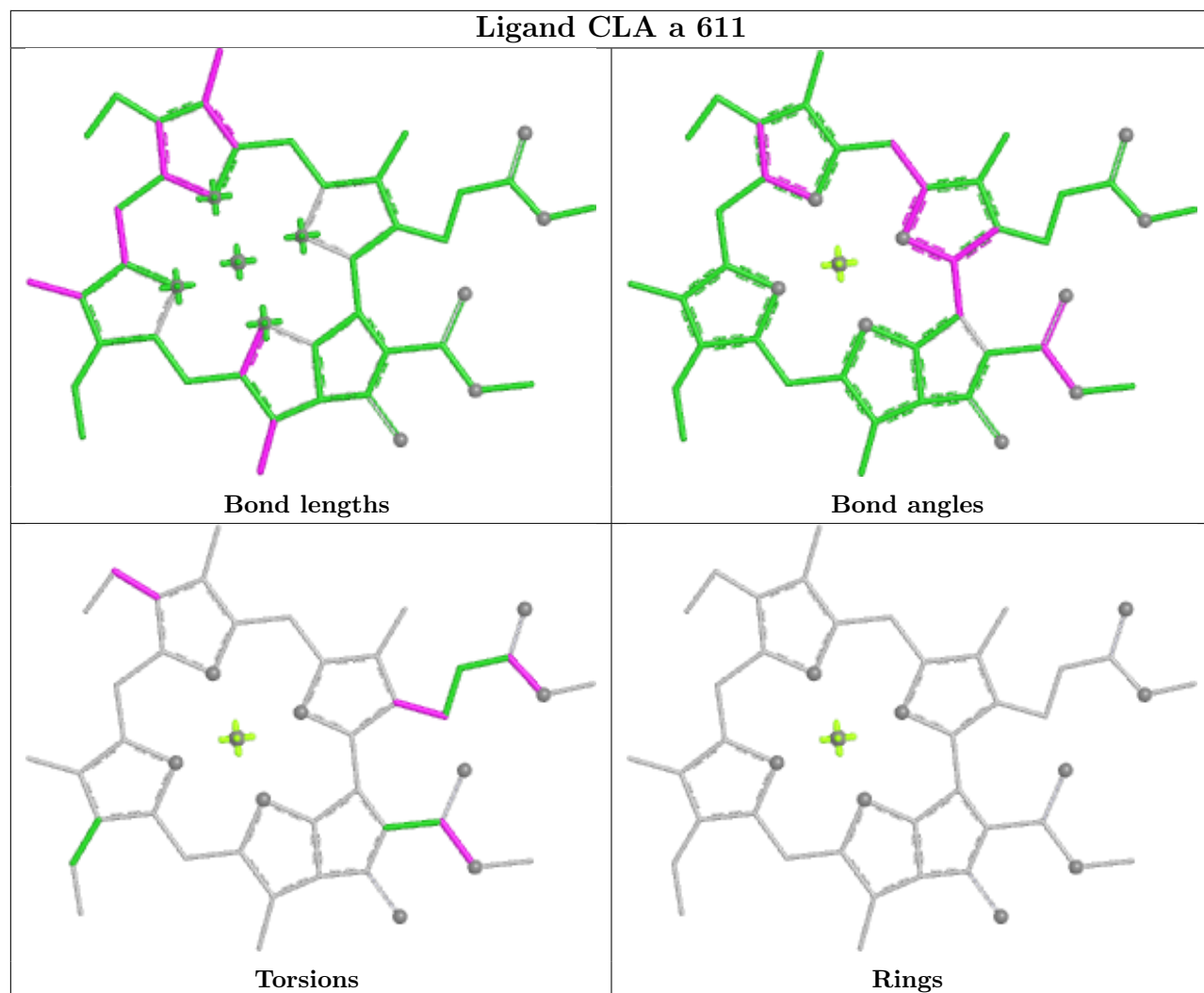
Torsions



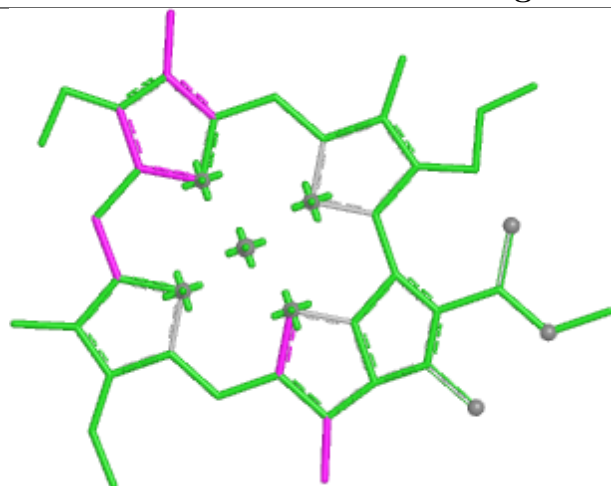
Rings



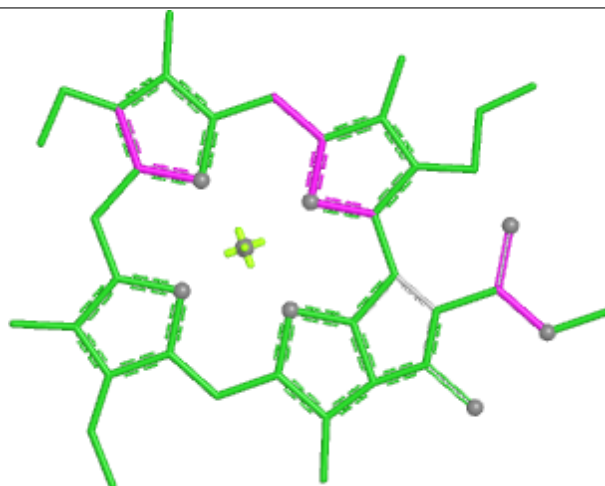
Ligand CLA a 611



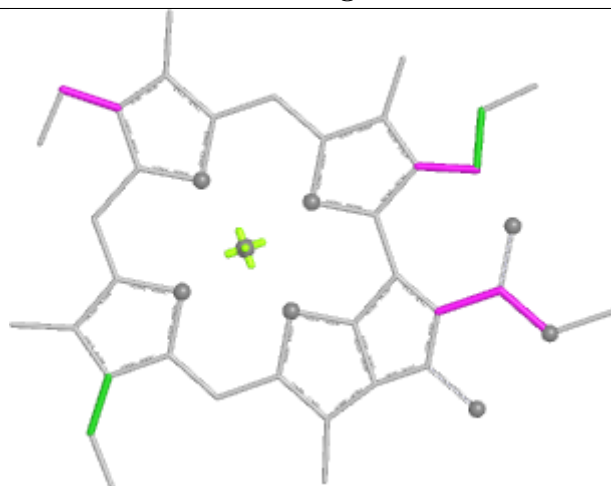
Ligand CLA B 821



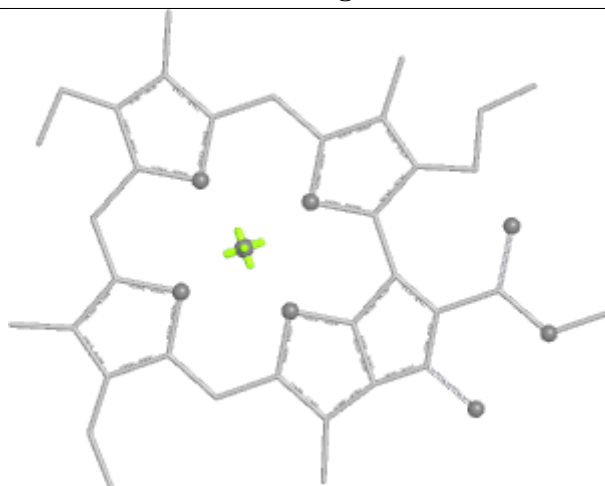
Bond lengths



Bond angles

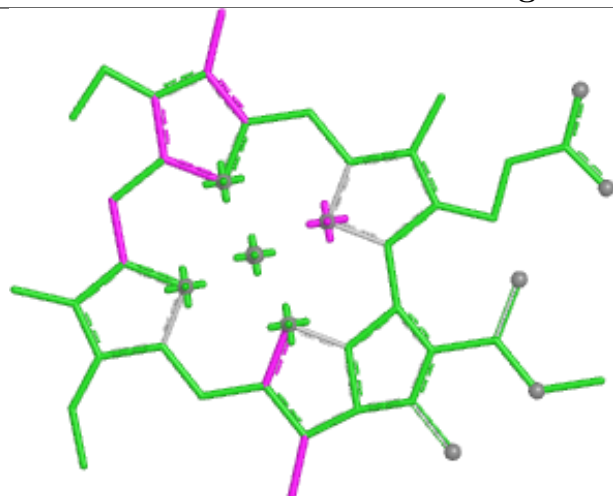


Torsions

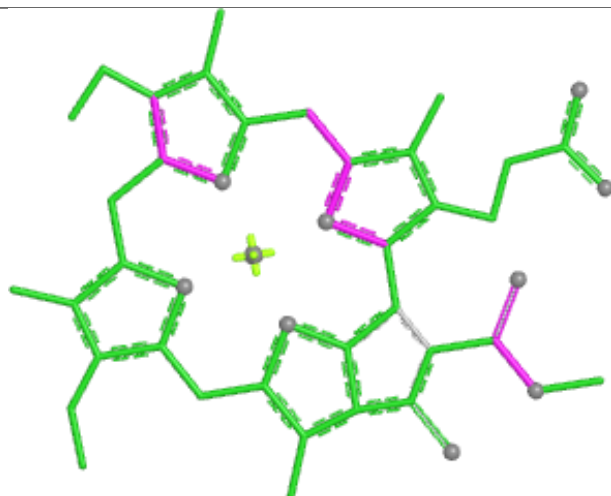


Rings

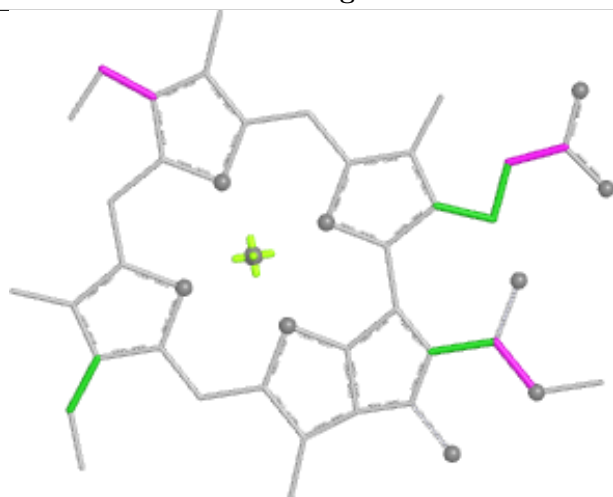
Ligand CLA 1 603



Bond lengths



Bond angles

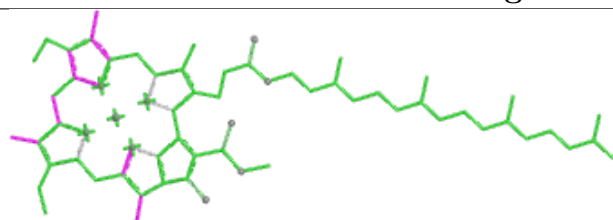


Torsions

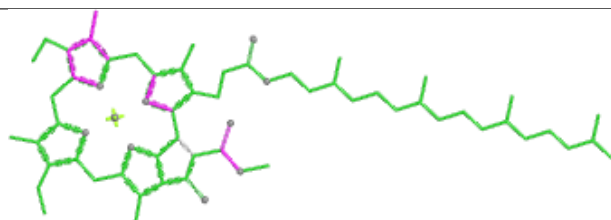


Rings

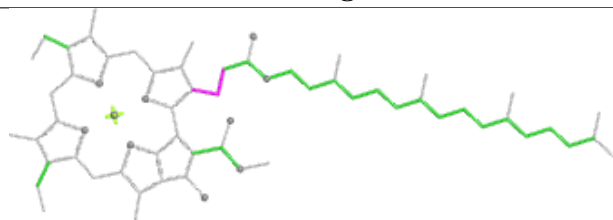
Ligand CLA A 5005



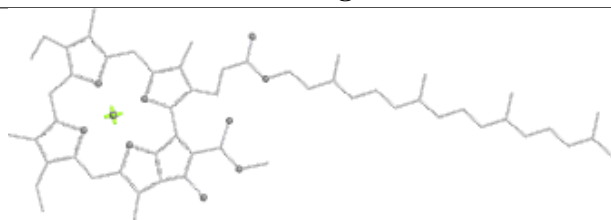
Bond lengths



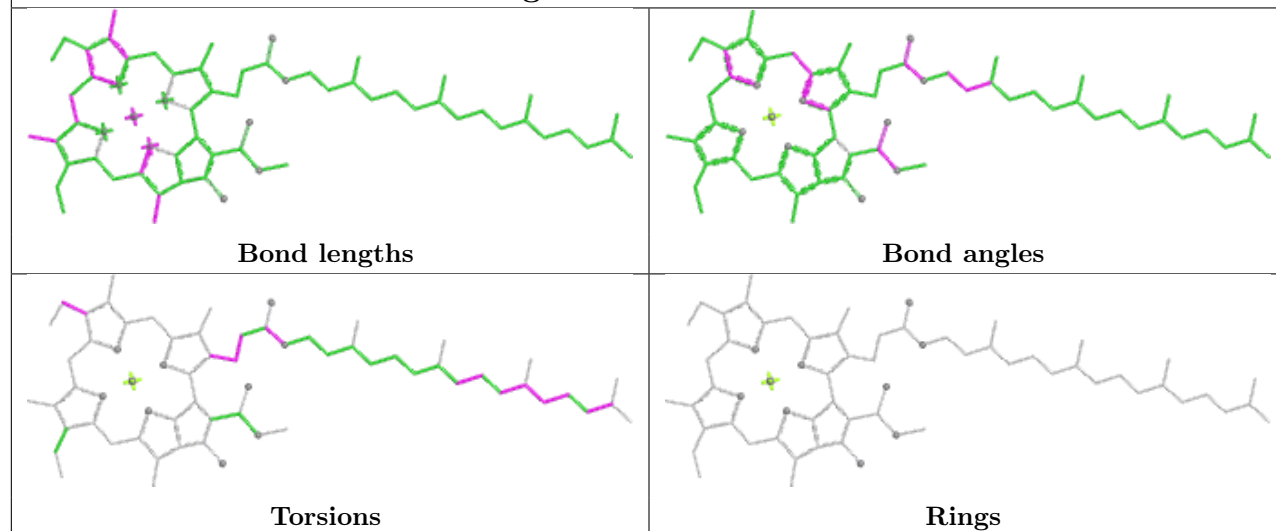
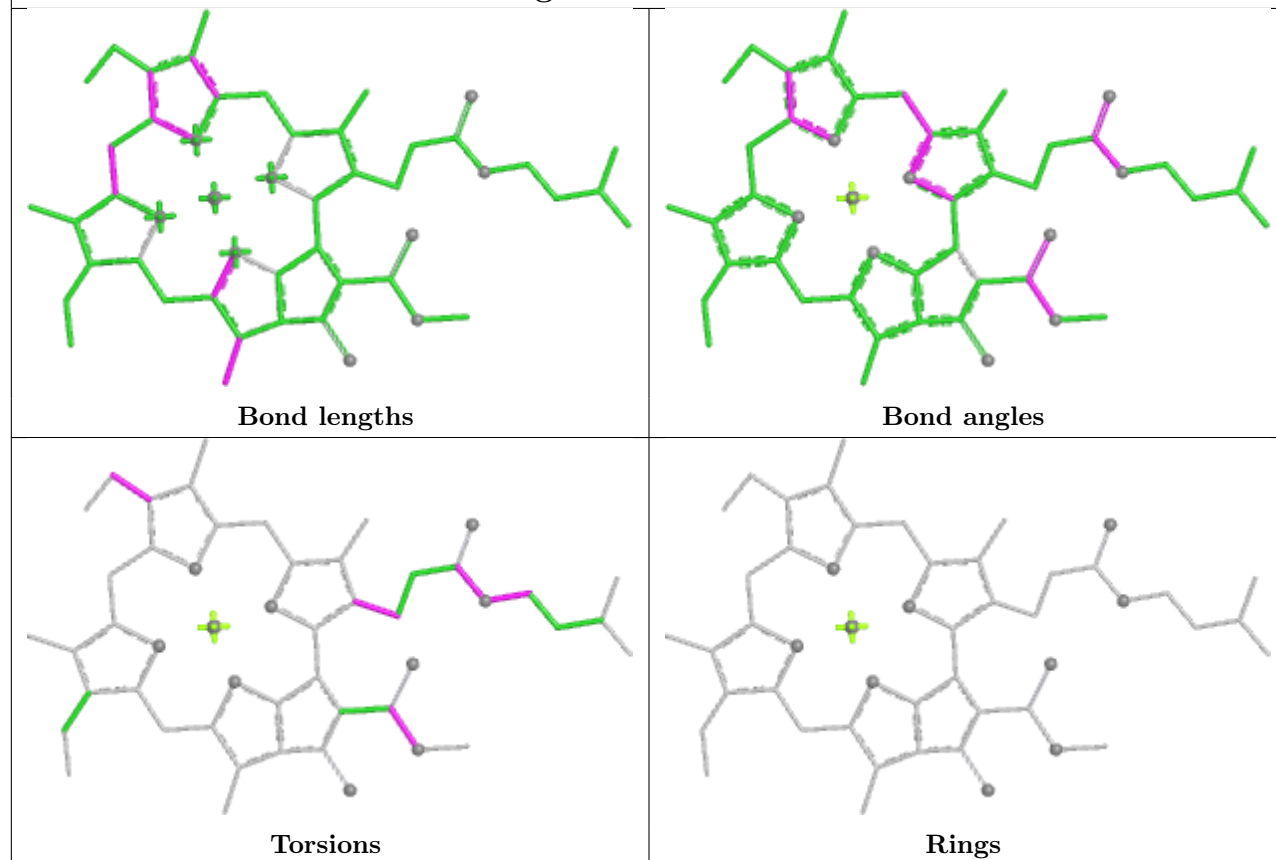
Bond angles

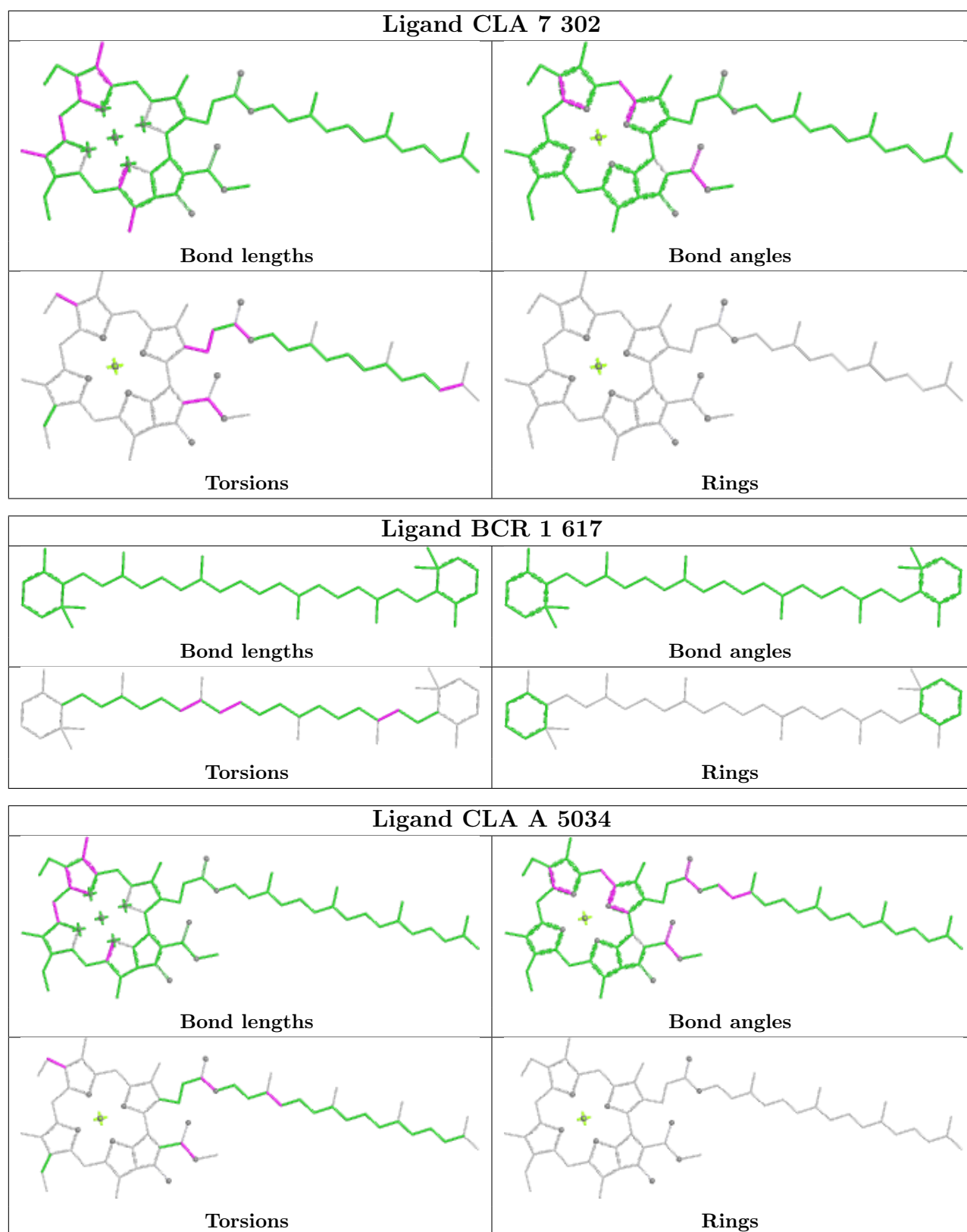


Torsions

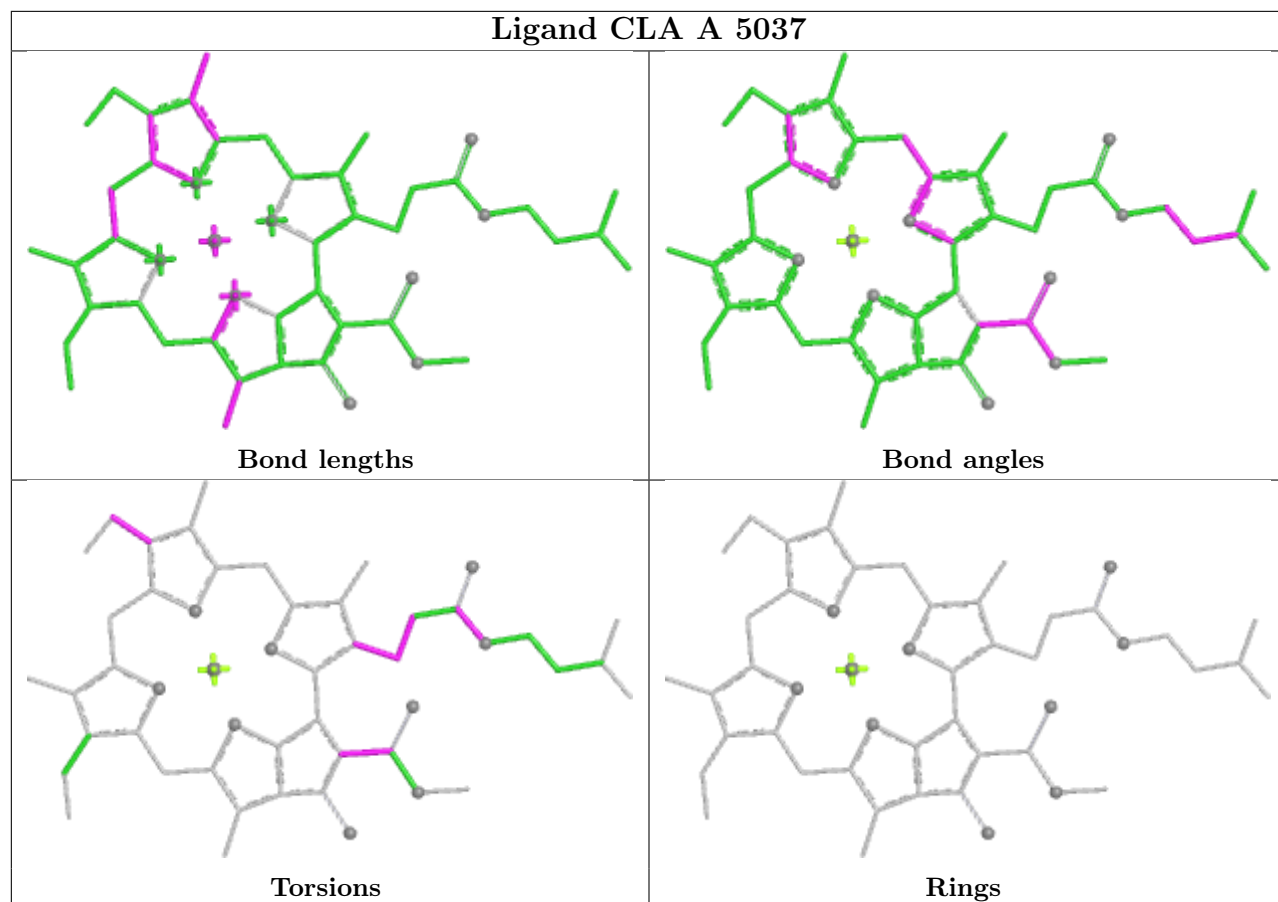


Rings

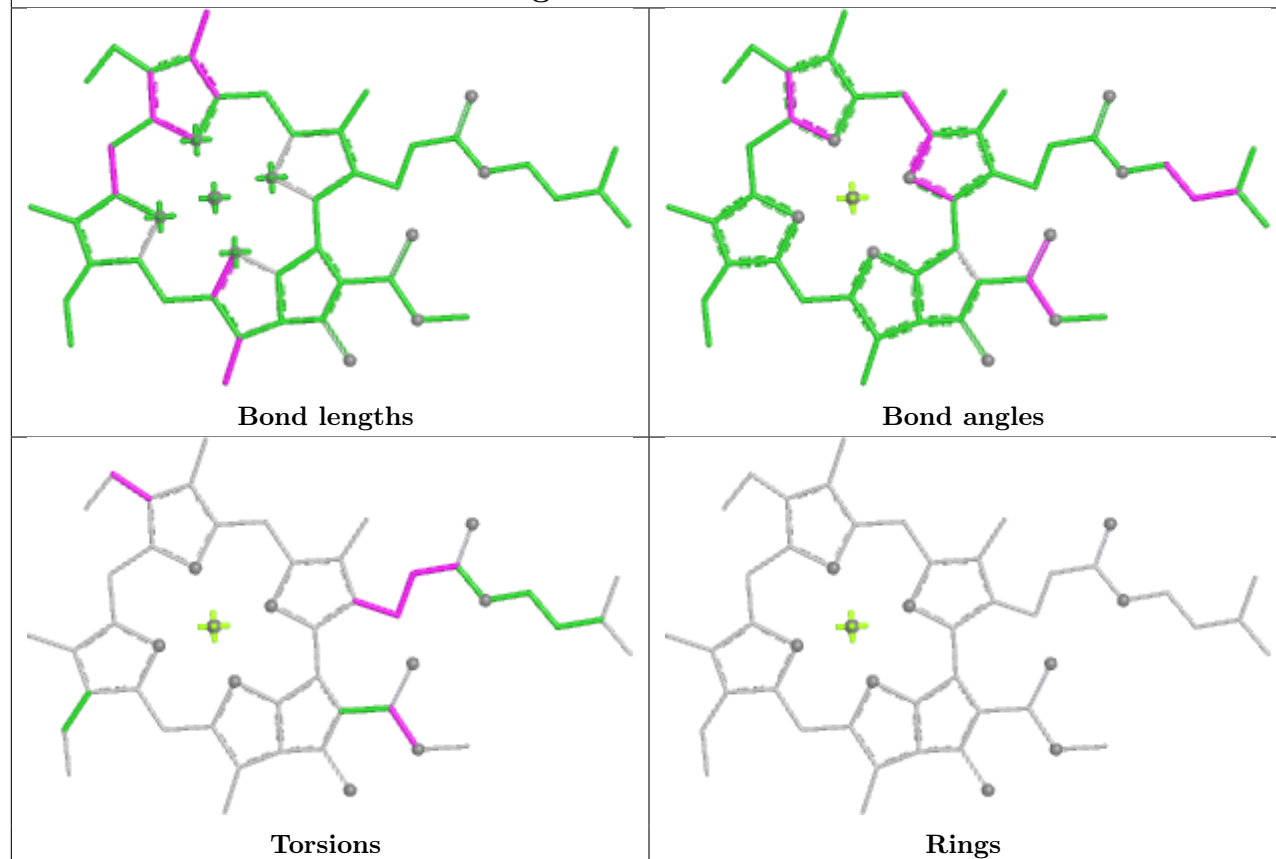
Ligand CLA A 5009**Ligand CLA b 610**



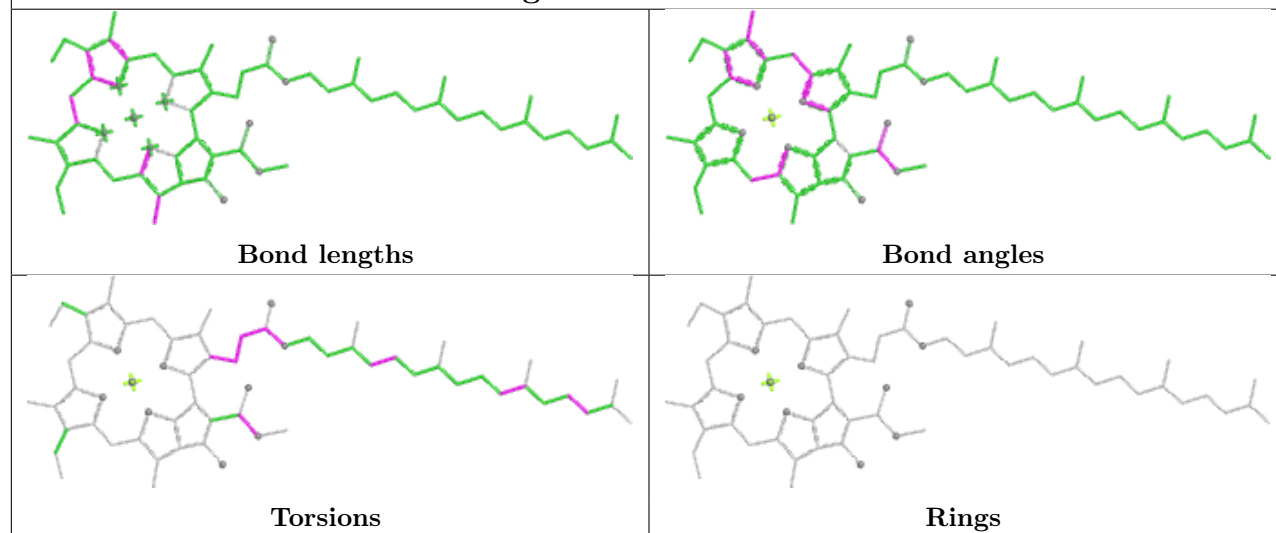
Ligand CLA A 5037



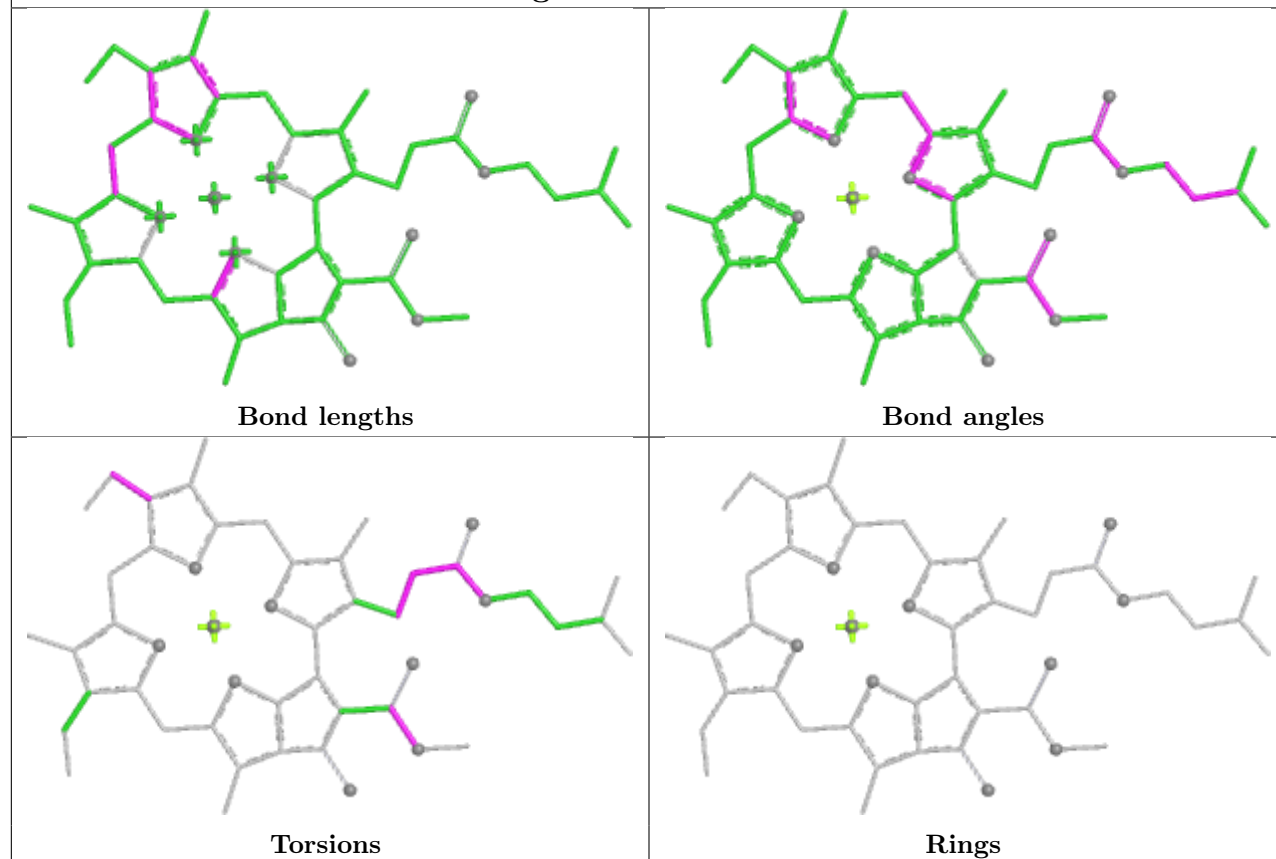
Ligand CLA B 811



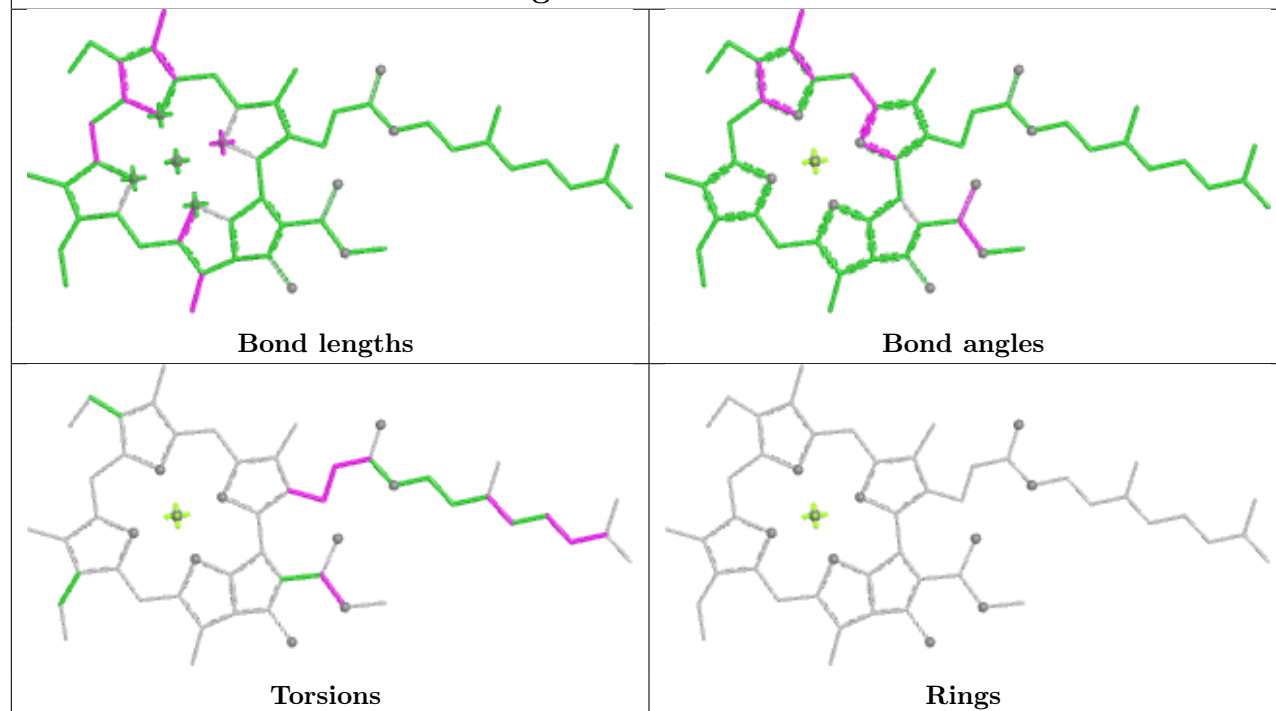
Ligand CLA A 5029



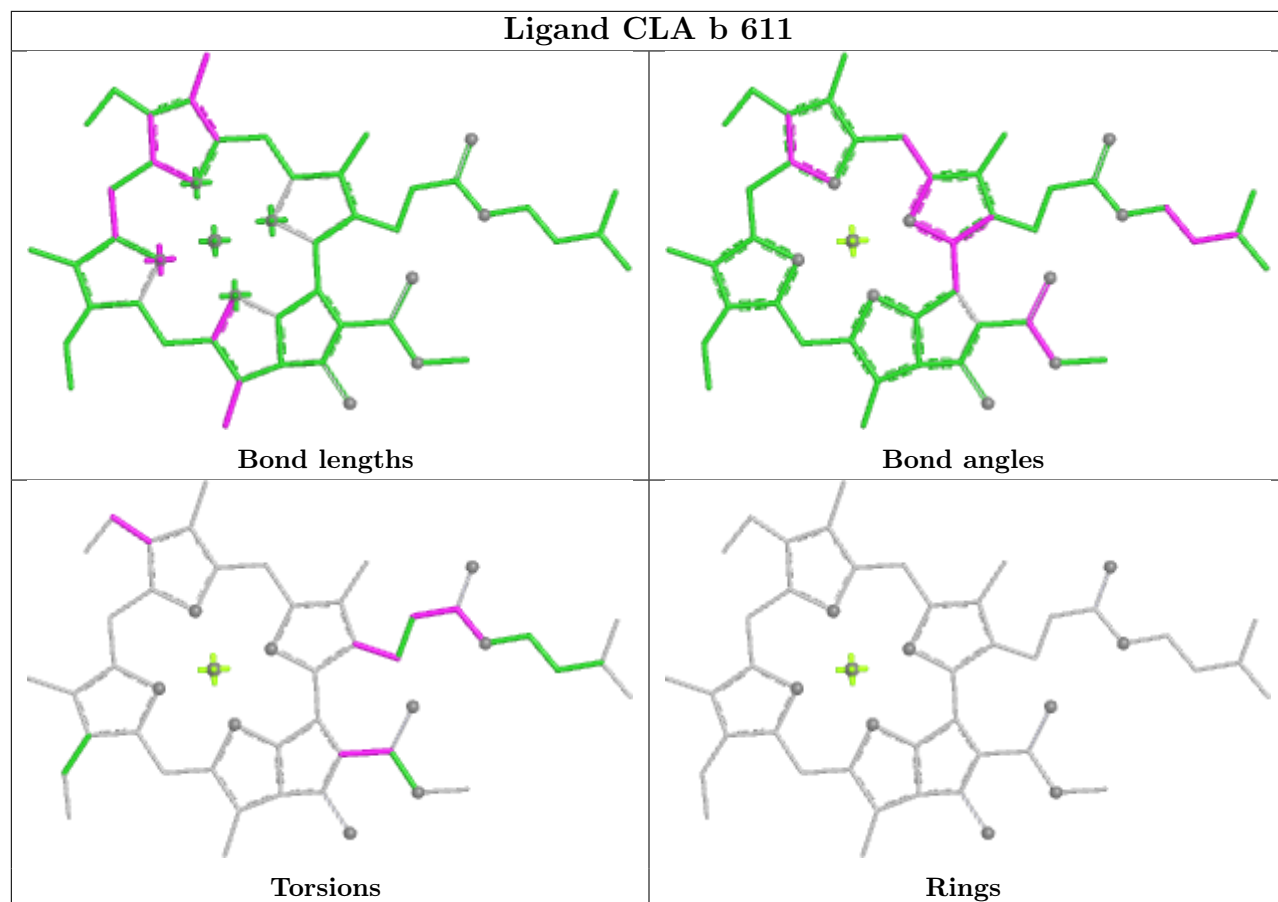
Ligand CLA B 813



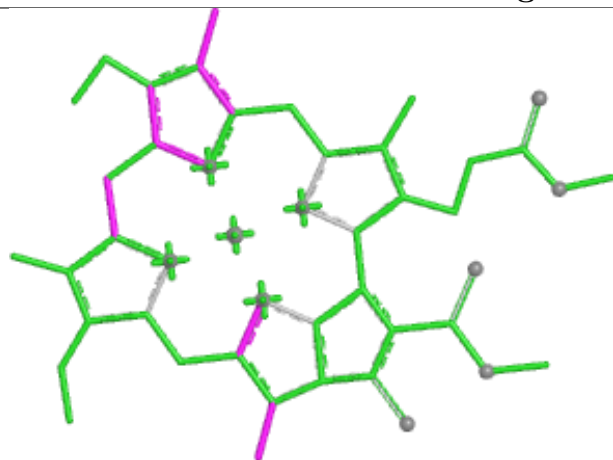
Ligand CLA B 828



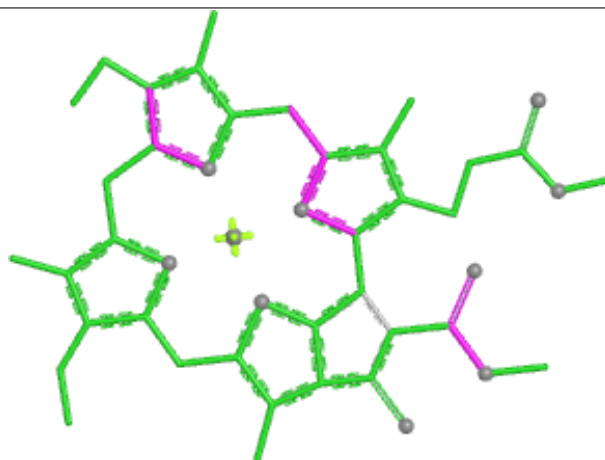
Ligand CLA b 611



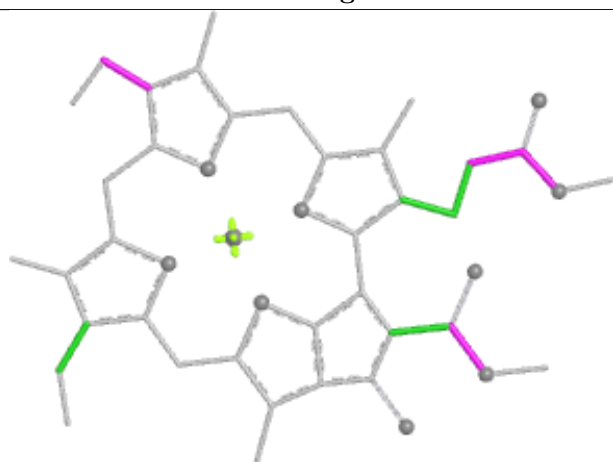
Ligand CLA b 614



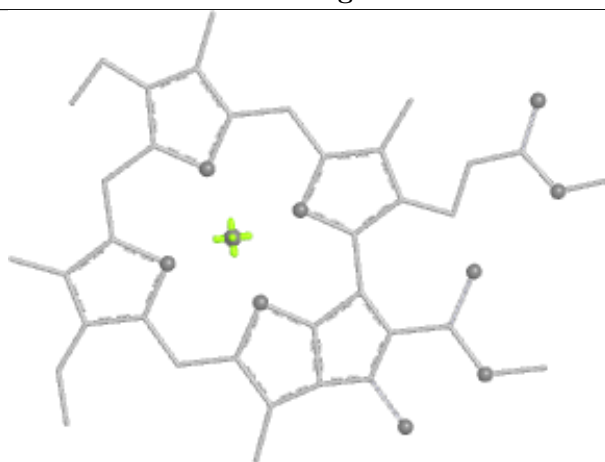
Bond lengths



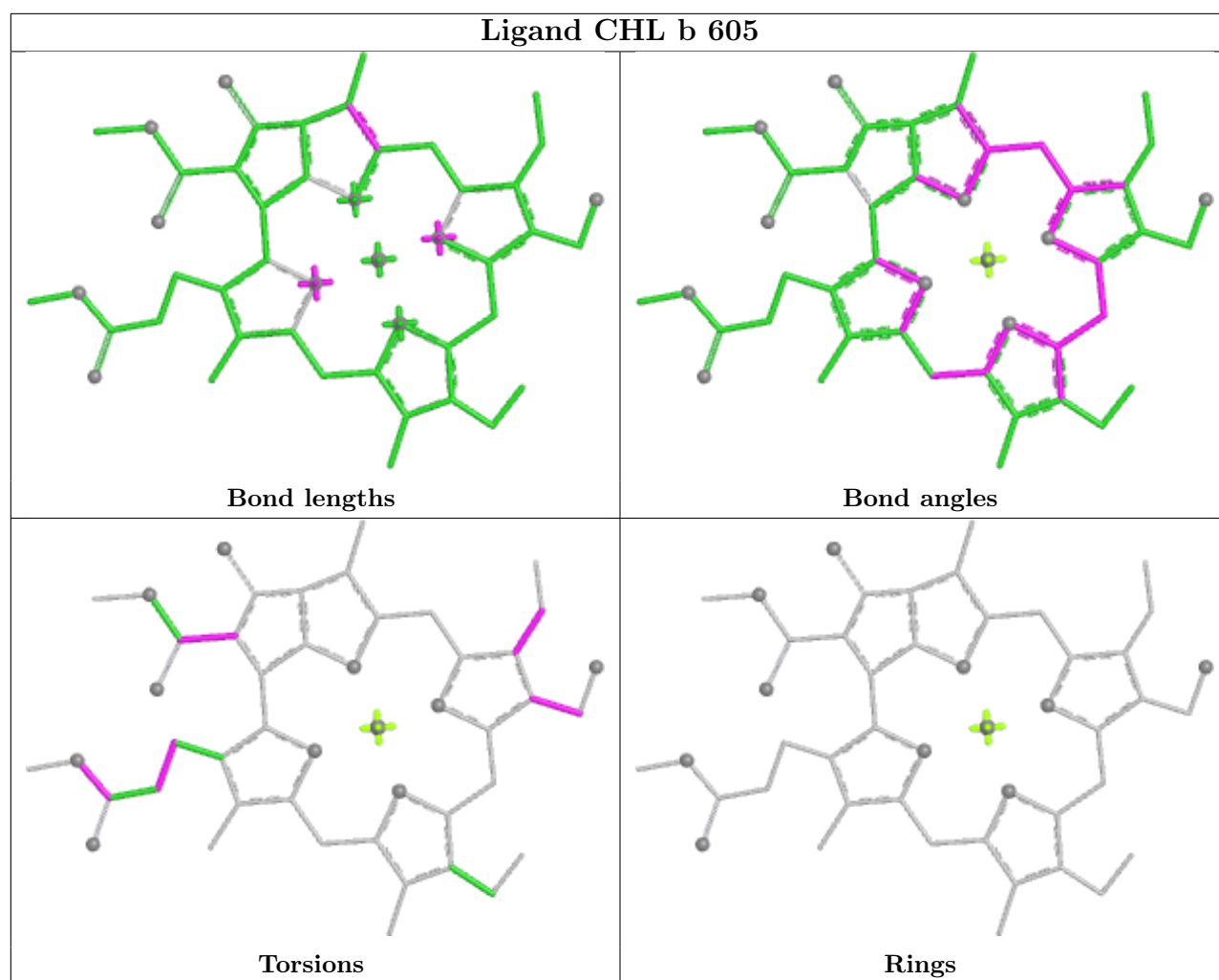
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

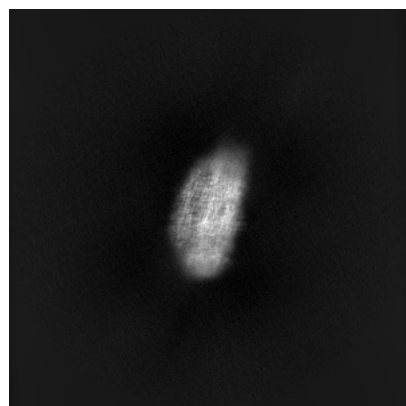
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48264. These allow visual inspection of the internal detail of the map and identification of artifacts.

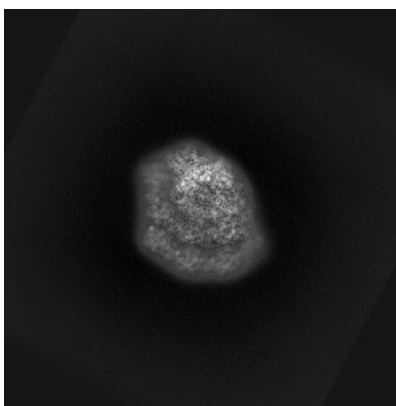
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

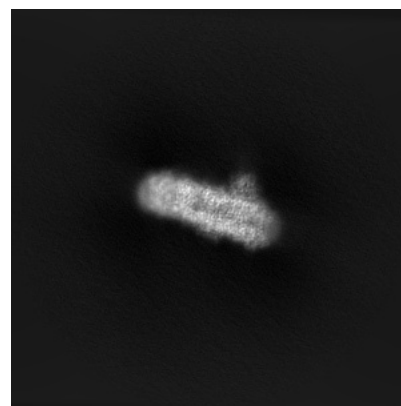
6.1.1 Primary map



X

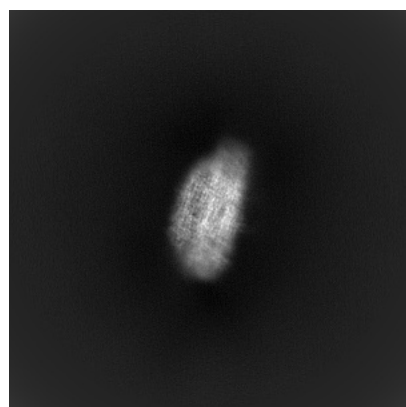


Y

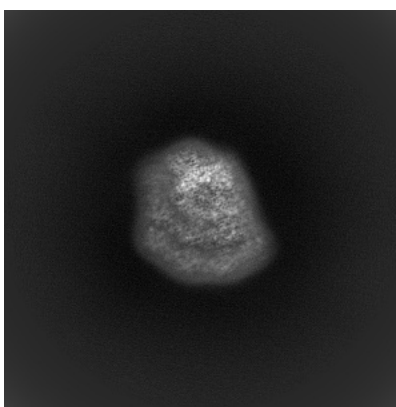


Z

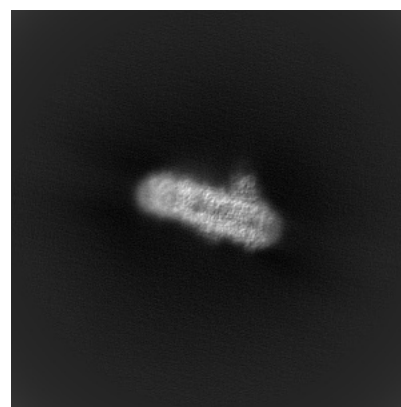
6.1.2 Raw map



X



Y

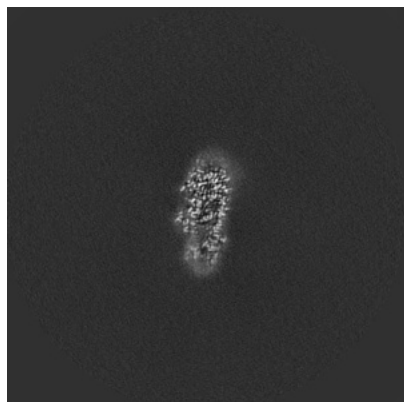


Z

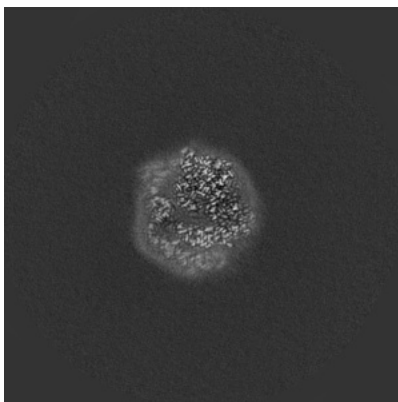
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

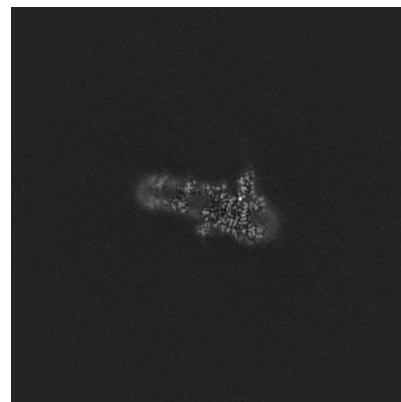
6.2.1 Primary map



X Index: 240

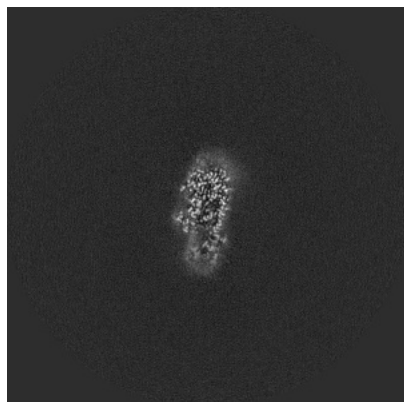


Y Index: 240

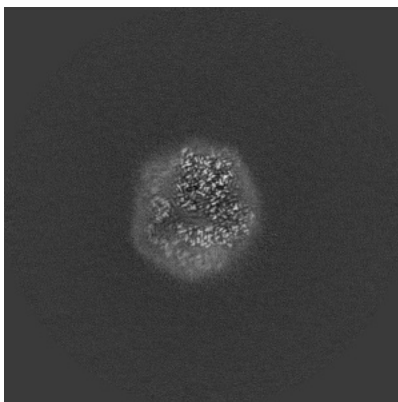


Z Index: 240

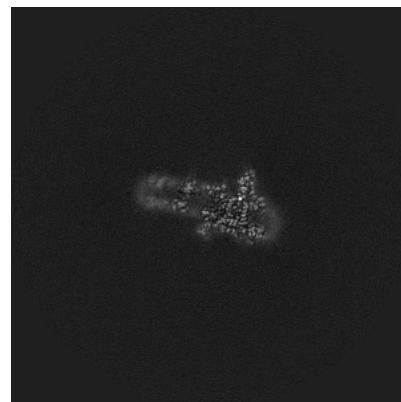
6.2.2 Raw map



X Index: 240



Y Index: 240

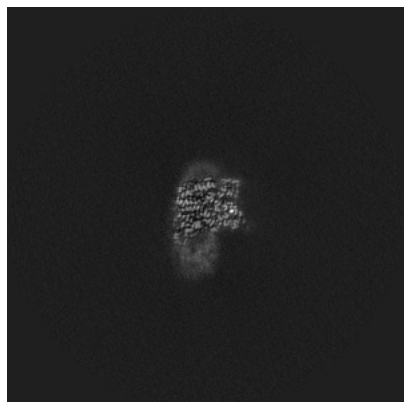


Z Index: 240

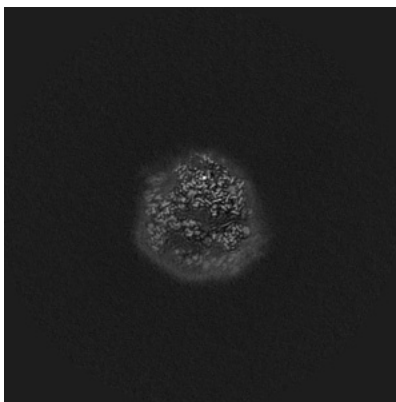
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

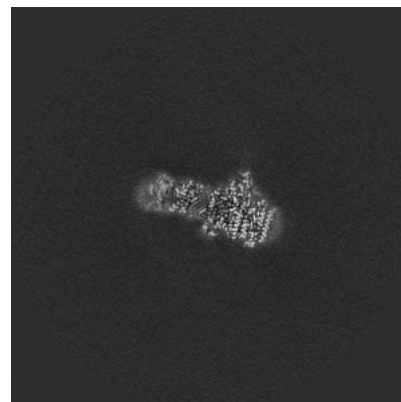
6.3.1 Primary map



X Index: 277

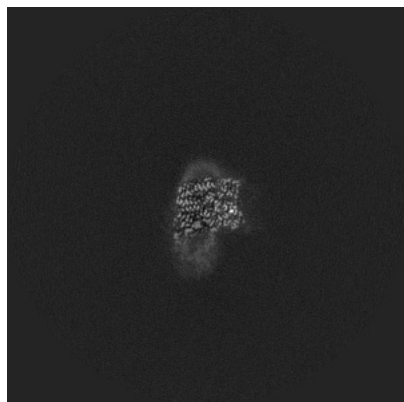


Y Index: 249

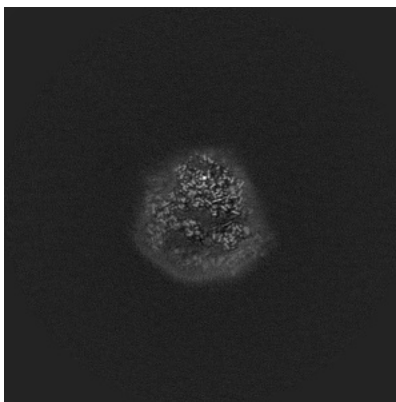


Z Index: 228

6.3.2 Raw map



X Index: 277



Y Index: 249

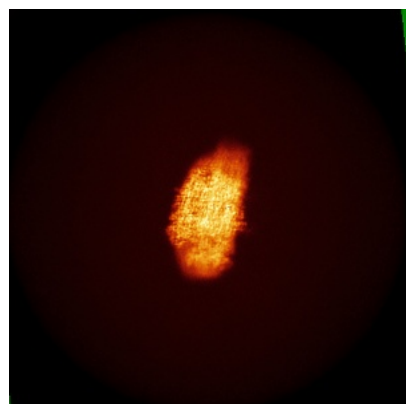


Z Index: 228

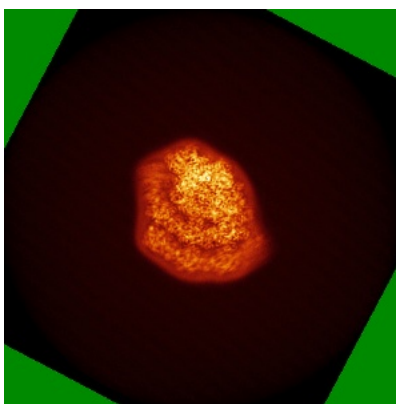
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

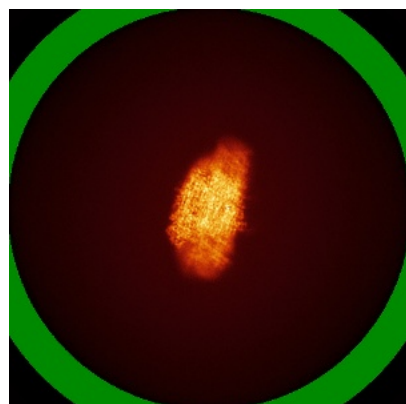


Y

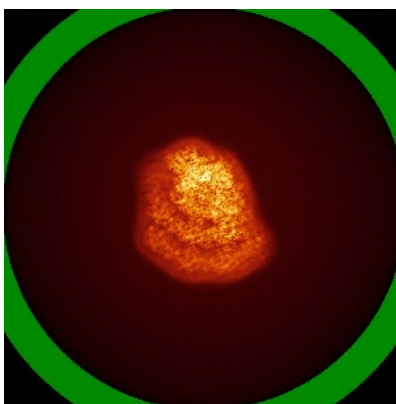


Z

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.

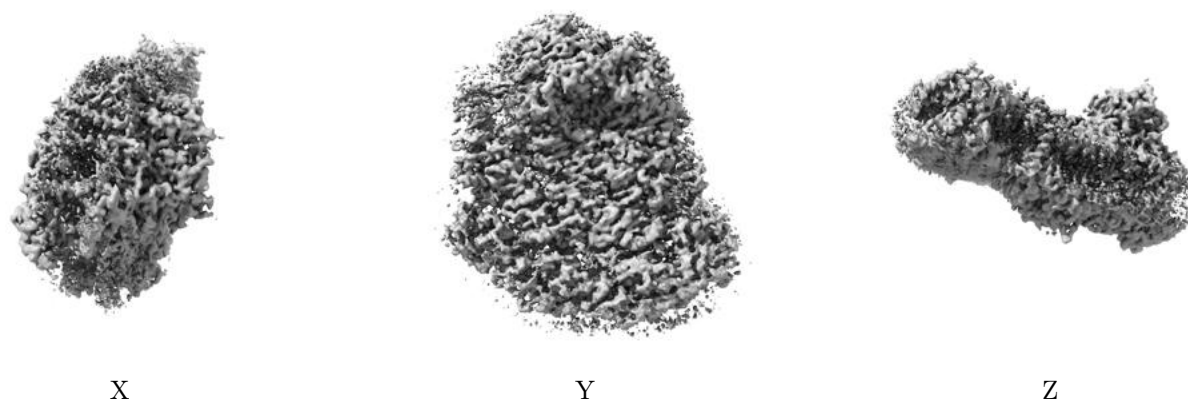
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0151. 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



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.

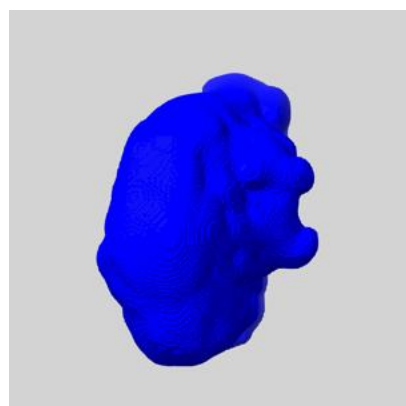
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

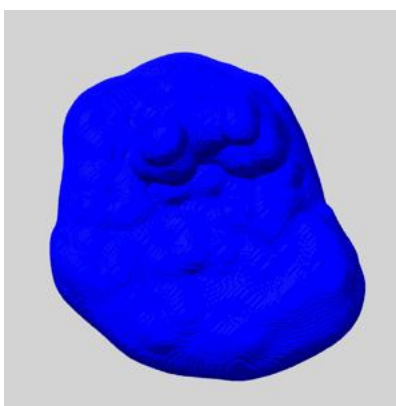
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

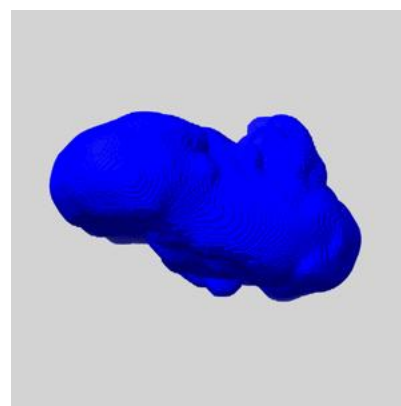
6.6.1 emd_48264_msk_1.map [i](#)



X



Y

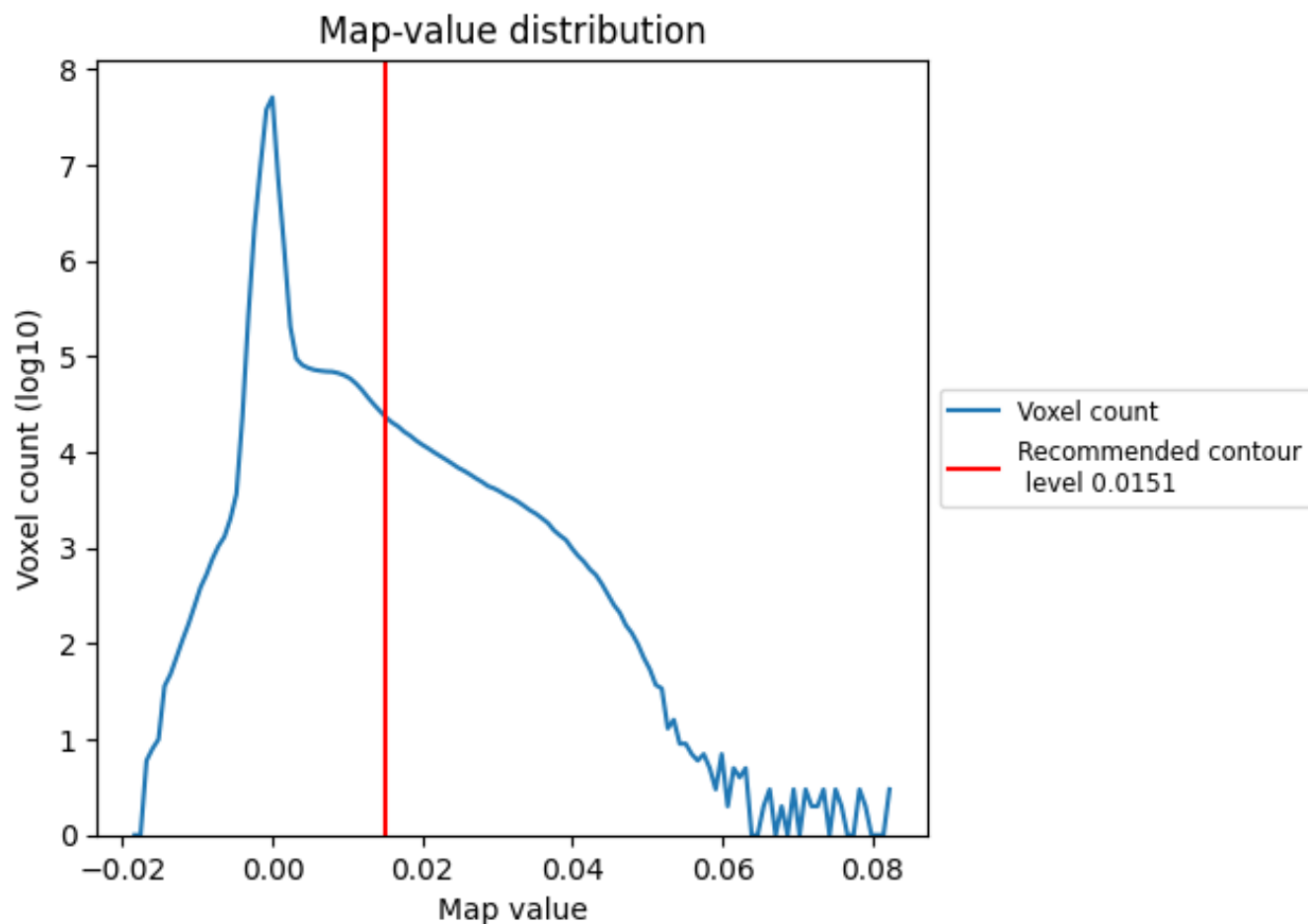


Z

7 Map analysis [i](#)

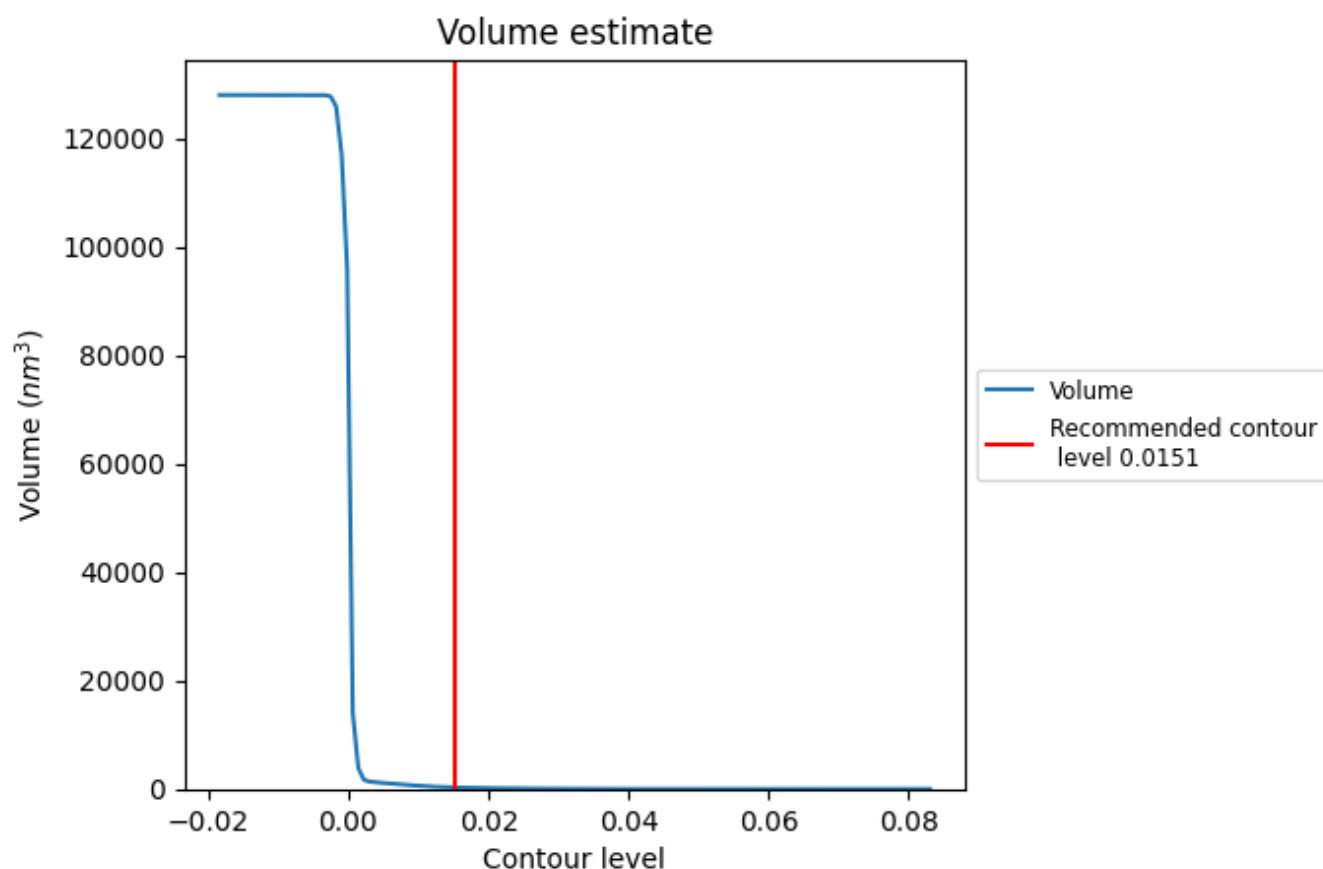
This section contains the results of statistical analysis of the map.

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.

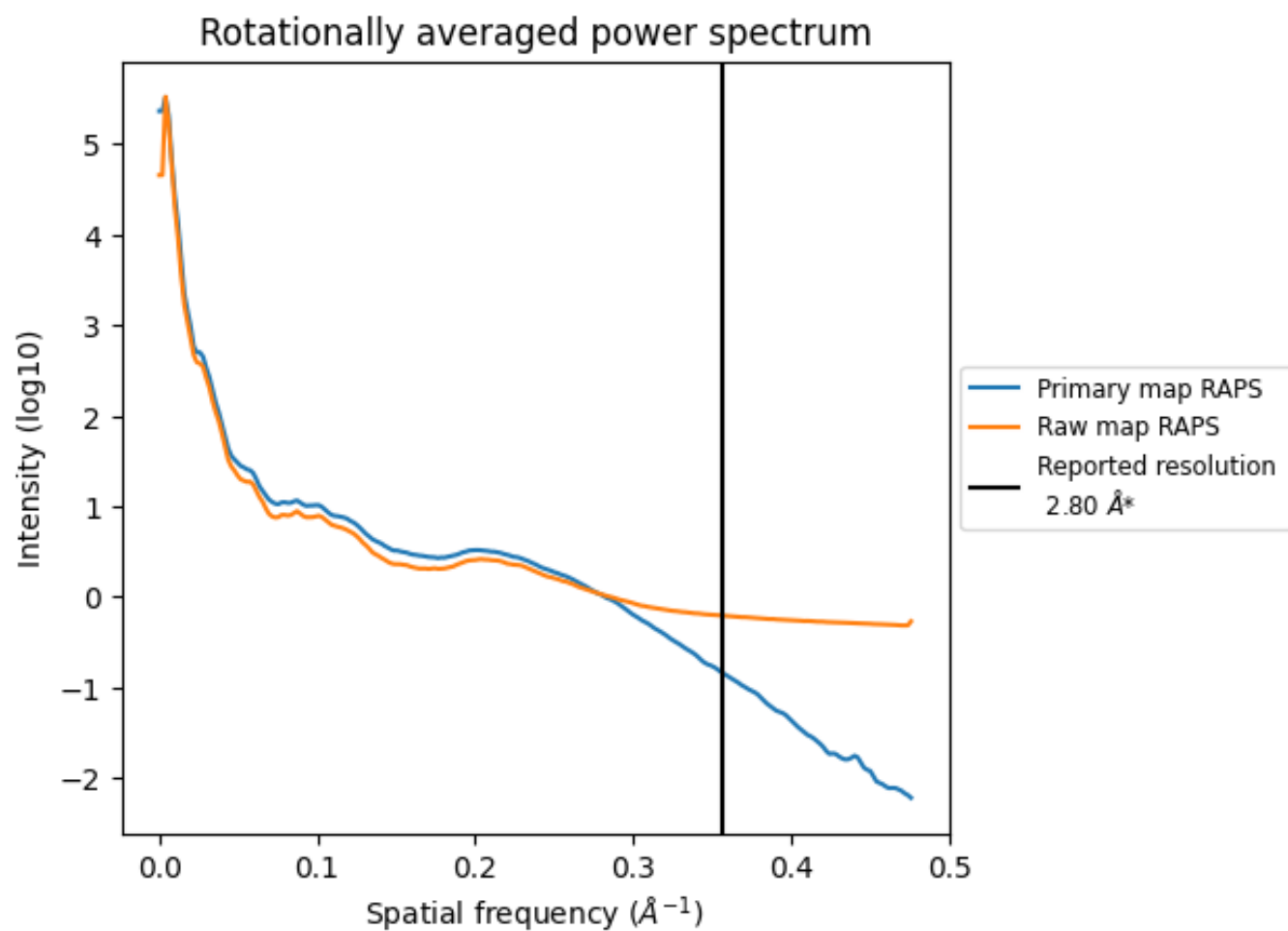
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm^3 ; this corresponds to an approximate mass of 251 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 ⓘ

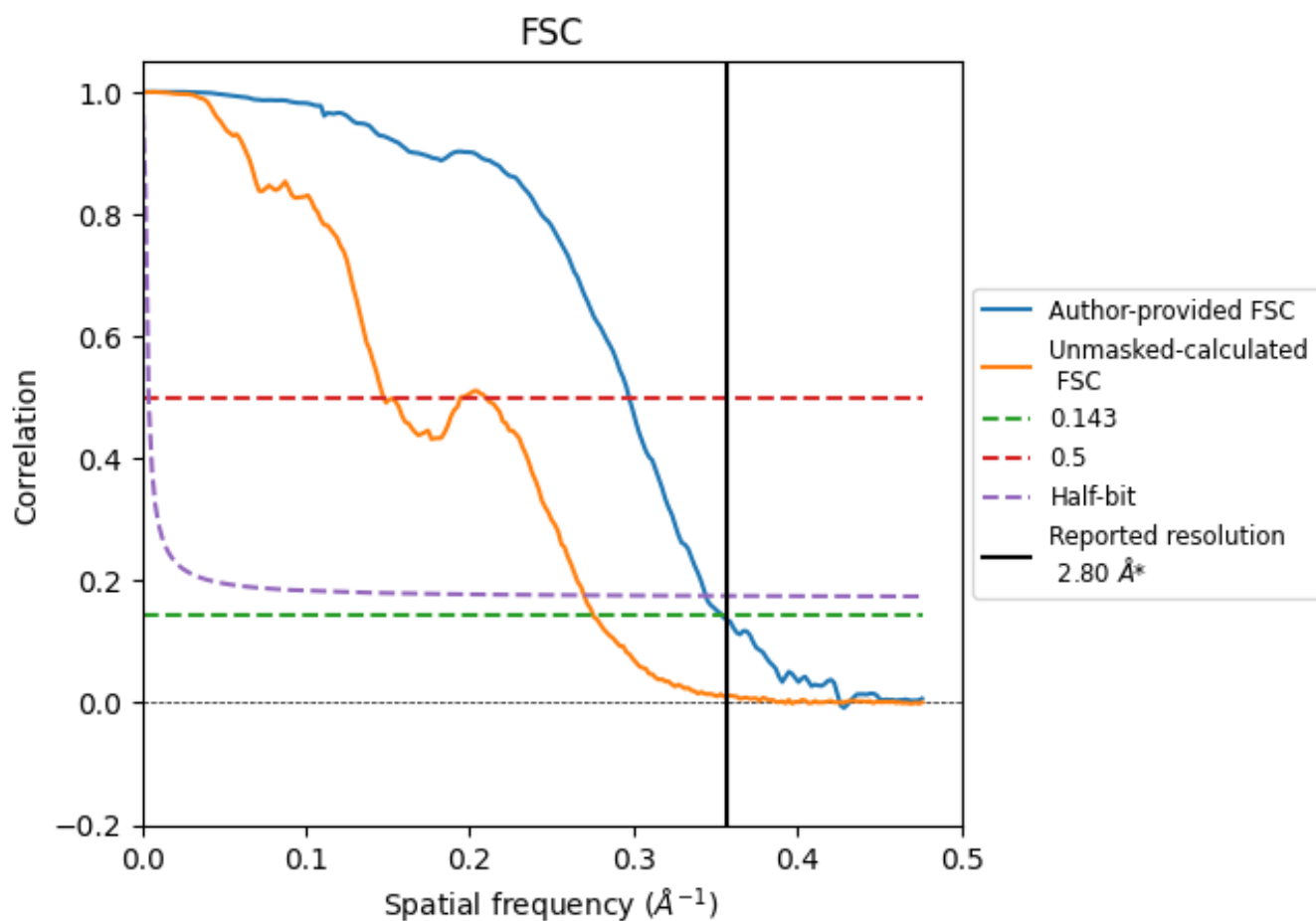


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

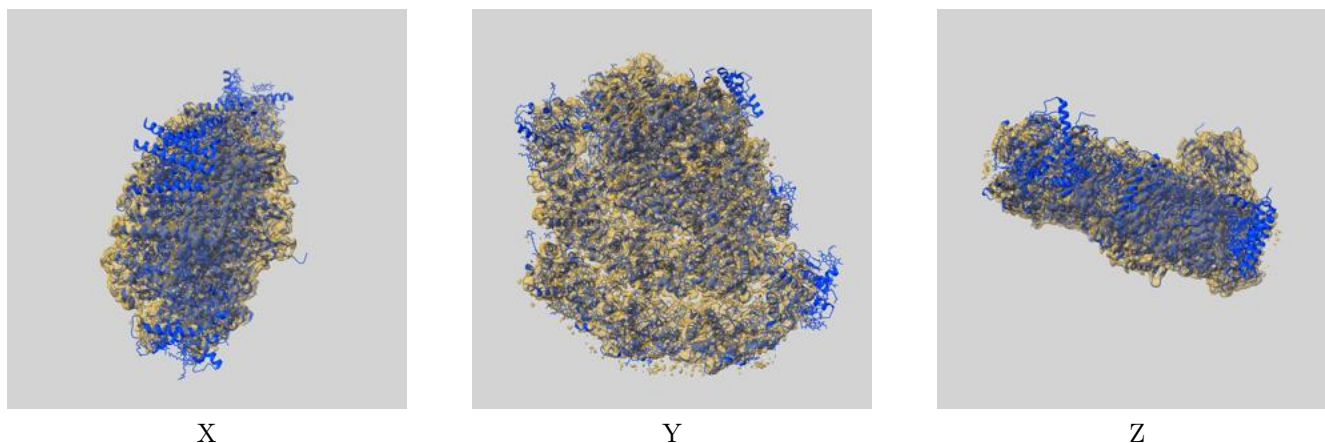
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.36	2.91
Unmasked-calculated*	3.63	6.78	3.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

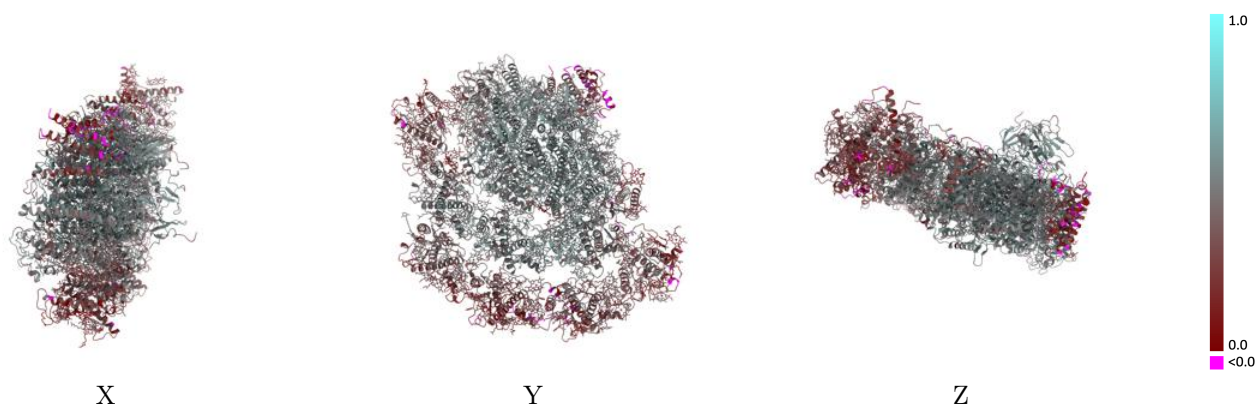
This section contains information regarding the fit between EMDB map EMD-48264 and PDB model 9MGZ. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



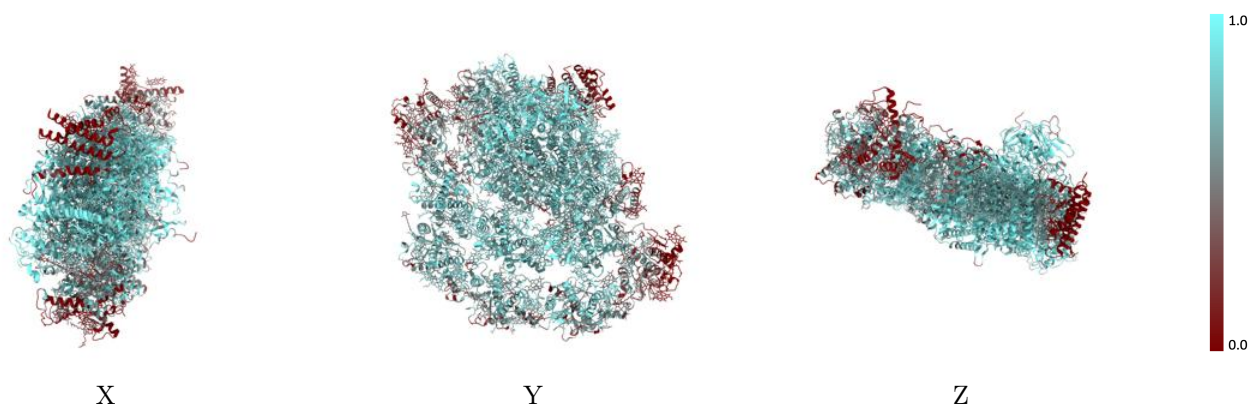
The images above show the 3D surface view of the map at the recommended contour level 0.0151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



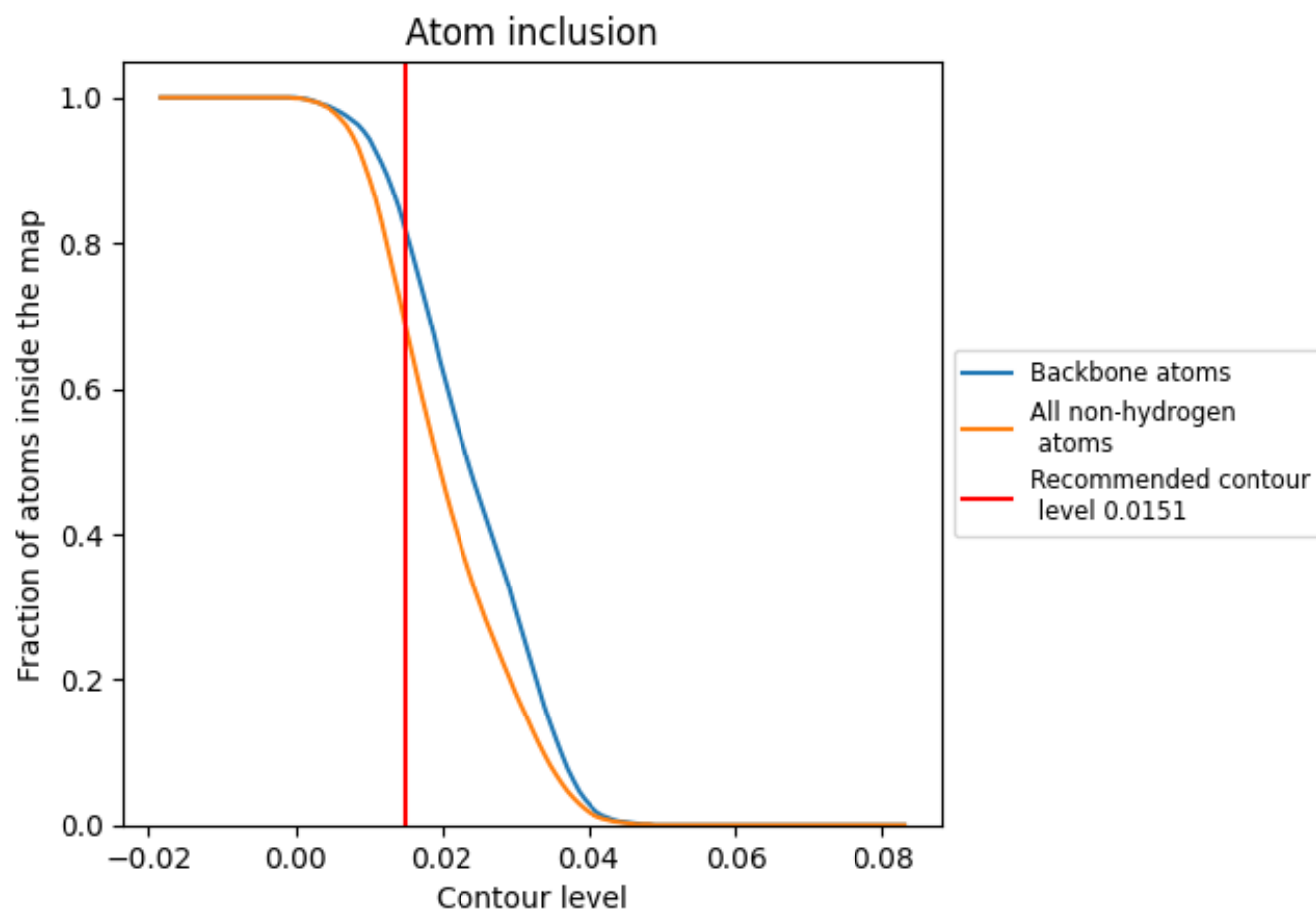
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0151).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.0151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4200
1	0.3730	0.2550
3	0.7700	0.4760
7	0.7960	0.4870
8	0.7280	0.4340
A	0.8310	0.5250
B	0.7930	0.4920
C	0.9220	0.5250
D	0.7140	0.4830
E	0.7810	0.4970
F	0.7440	0.4650
I	0.1160	0.2330
J	0.7660	0.4970
K	0.3510	0.3060
L	0.0170	0.1430
T	0.2980	0.2780
a	0.6690	0.3280
b	0.5940	0.2330
c	0.6130	0.2830

