



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 11:08 AM JST

PDB ID : 9JZR / pdb_00009jzr
EMDB ID : EMD-61940
Title : Structure of PSI-LHCI-LHCII supercomplex from Bryopsis corticulans
Authors : Liu, X.Y.; Wang, W.D.
Deposited on : 2024-10-14
Resolution : 2.73 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

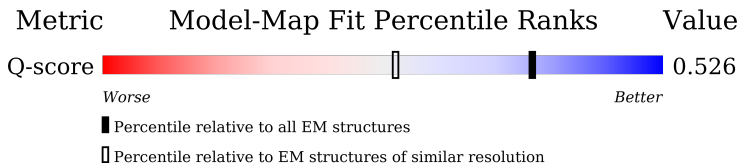
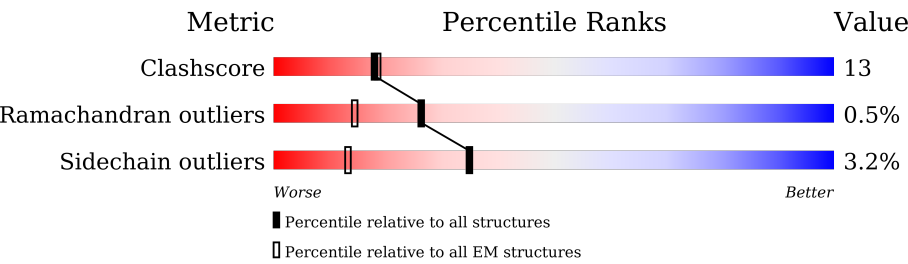
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.73 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.



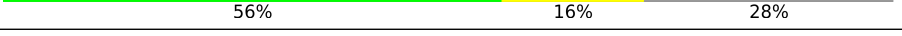
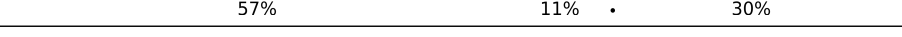
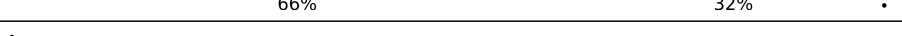
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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	0	245	61% 25% 13%
2	1	226	55% 29% 14%
2	5	226	8% 61% 23% 14%
3	2	256	70% 13% 16%

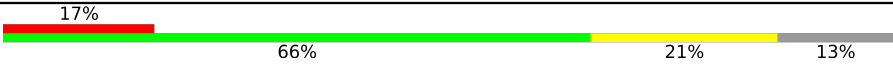
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Mol	Chain	Length	Quality of chain
4	3	281	
5	6	267	
6	7	264	
7	4	248	
7	8	248	
8	9	222	
9	A	751	
10	B	734	
11	D	198	
12	E	91	
13	F	236	
14	G	167	
15	I	36	
16	J	41	
17	L	204	
18	C	81	
19	K	123	
20	M	32	
21	O	137	
22	a	250	
22	h	250	
23	c	254	
24	b	251	
25	d	280	
25	g	280	

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Mol	Chain	Length	Quality of chain
26	f	259	
27	H	133	
28	i	282	
29	e	250	

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
30	CHL	i	606	-	-	X	-
31	CLA	i	604	-	-	X	-
42	NEX	f	523	-	-	X	-
42	NEX	i	523	-	-	X	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 77090 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	0	213	Total	C	N	O	S	0	0
			1640	1063	270	296	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	195	Total	C	N	O	S	0	0
			1478	950	243	273	12		
2	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1667	1082	269	304	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	228	Total	C	N	O	S	0	0
			1768	1141	288	329	10		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		
7	4	207	Total	C	N	O	S	0	0
			1569	1030	257	273	9		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	189	Total	C	N	O	S	0	0
			1453	932	245	267	9		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	746	Total	C	N	O	S	0	0
			5872	3836	998	1016	22		

- Molecule 10 is a protein called photosystem I.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	733	Total	C	N	O	S	0	0
			5824	3824	979	1002	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	142	Total	C	N	O	S	0	0
			1109	709	193	202	5		

- Molecule 12 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	64	Total	C	N	O	S	0	0
			509	323	90	95	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	165	Total	C	N	O	S	0	0
			1273	810	224	235	4		

- Molecule 14 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	93	Total	C	N	O	S	0	0
			726	471	119	136			

- 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
			262	180	37	43	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	162	Total	C	N	O	S	0	0
			1195	773	192	226	4		

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	80	Total	C	N	O	S	0	0
			602	370	105	116	11		

- Molecule 19 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	31	Total	C	N	O	0	0
			238	158	37	43		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			728	488	116	120	4		

- Molecule 22 is a protein called Lhcb-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	198	Total	C	N	O	S	0	0
			1511	978	243	279	11		
22	h	201	Total	C	N	O	S	0	0
			1520	985	245	280	10		

- Molecule 23 is a protein called Lhcb-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	219	Total	C	N	O	S	0	0
			1680	1083	271	317	9		

- Molecule 24 is a protein called Lhcb-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	209	Total	C	N	O	S	0	0
			1609	1038	265	295	11		

- Molecule 25 is a protein called Lhcb-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	217	Total	C	N	O	S	0	0
			1634	1059	260	305	10		
25	g	199	Total	C	N	O	S	0	0
			1502	971	238	283	10		

- Molecule 26 is a protein called Lhcb-f.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	f	225	Total	C	N	O	P	S	0	0
			1727	1107	282	330	1	7		

- Molecule 27 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	94	Total	C	N	O	S	0	0
			717	451	126	139	1		

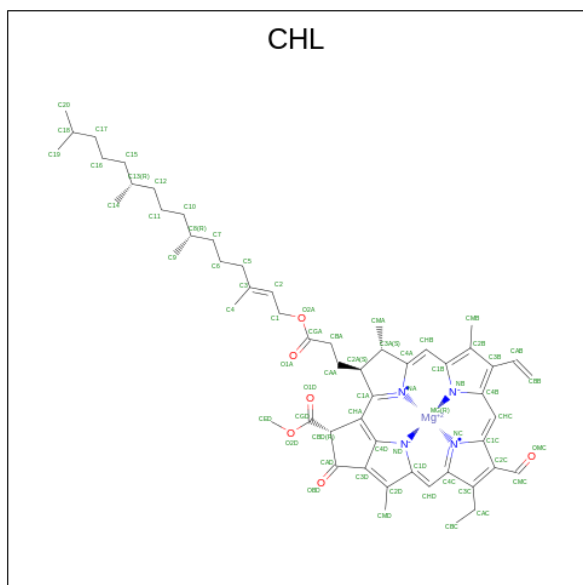
- Molecule 28 is a protein called Lhcb-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	237	Total	C	N	O	P S	0	0
			1834	1179	305	342	1 7		

- Molecule 29 is a protein called Lhcb-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	216	Total	C	N	O	S	0	0
			1647	1066	261	310	10		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
30	0	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	1	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	1	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	1	1	Total 62	C 51	Mg 1	N 4	O 6	0
30	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	2	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	2	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	3	1	Total 62	C 51	Mg 1	N 4	O 6	0
30	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	5	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	5	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	5	1	Total 48	C 37	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	5	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	6	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	6	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	6	1	Total 60	C 49	Mg 1	N 4	O 6	0
30	6	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	7	1	Total 63	C 52	Mg 1	N 4	O 6	0
30	7	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	7	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	7	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	8	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	8	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	8	1	Total 51	C 40	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	9	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	9	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	9	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	a	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	a	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	a	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	a	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	a	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	a	1	Total 49	C 38	Mg 1	N 4	O 6	0
30	a	1	Total 59	C 48	Mg 1	N 4	O 6	0
30	a	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	c	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	c	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	c	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	c	1	Total 44	C 35	Mg 1	N 4	O 4	0
30	c	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	c	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	c	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
30	b	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	d	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
30	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
30	f	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	f	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	f	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	f	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	f	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	g	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	g	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	g	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	g	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	g	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	g	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	h	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	h	1	Total 64	C 53	Mg 1	N 4	O 6	0
30	h	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	h	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	h	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	h	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	h	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	h	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	i	1	Total 47	C 36	Mg 1	N 4	O 6	0

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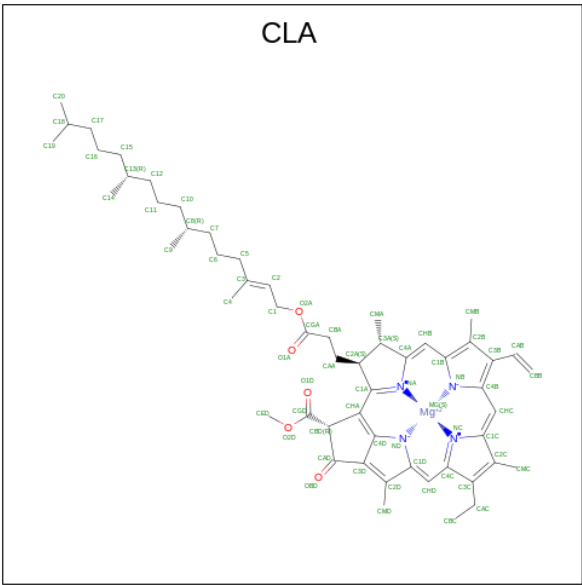
Mol	Chain	Residues	Atoms					AltConf
30	i	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	i	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	i	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	i	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	i	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	i	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	i	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	e	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	e	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	e	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	e	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	e	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	e	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	e	1	Total 42	C 33	Mg 1	N 4	O 4	0
30	4	1	Total 53	C 42	Mg 1	N 4	O 6	0
30	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	4	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	4	1	Total 51	C 40	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	4	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	6	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	6	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	7	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	9	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	9	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	L	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	L	1	Total 63	C 53	Mg 1	N 4	O 5	0
31	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	K	1	Total 53	C 43	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	M	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	a	1	Total 53	C 43	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	d	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	g	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	h	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	h	1	Total 46	C 36	Mg 1	N 4	O 5	0

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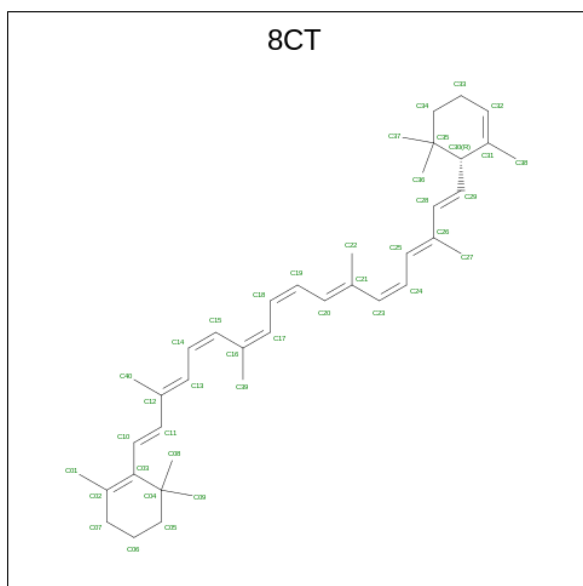
Mol	Chain	Residues	Atoms					AltConf
31	h	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	h	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	h	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	i	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	e	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 32 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
32	0	1	Total	C	0
			40	40	
32	1	1	Total	C	0
			40	40	
32	2	1	Total	C	0
			40	40	
32	3	1	Total	C	0
			40	40	
32	3	1	Total	C	0
			40	40	

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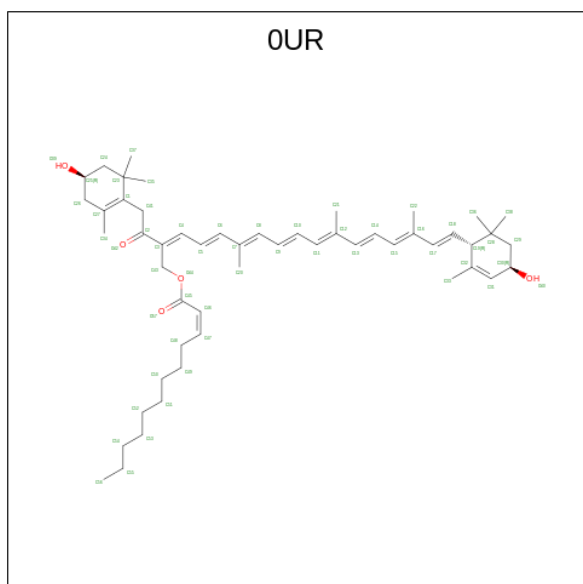
Mol	Chain	Residues	Atoms	AltConf
32	6	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	7	1	Total C 40 40	0
32	8	1	Total C 40 40	0
32	8	1	Total C 40 40	0
32	9	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	A	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0
32	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
32	F	1	Total C 40 40	0
32	G	1	Total C 40 40	0
32	I	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	J	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	L	1	Total C 40 40	0
32	K	1	Total C 40 40	0
32	M	1	Total C 40 40	0
32	O	1	Total C 40 40	0
32	4	1	Total C 40 40	0

- Molecule 33 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



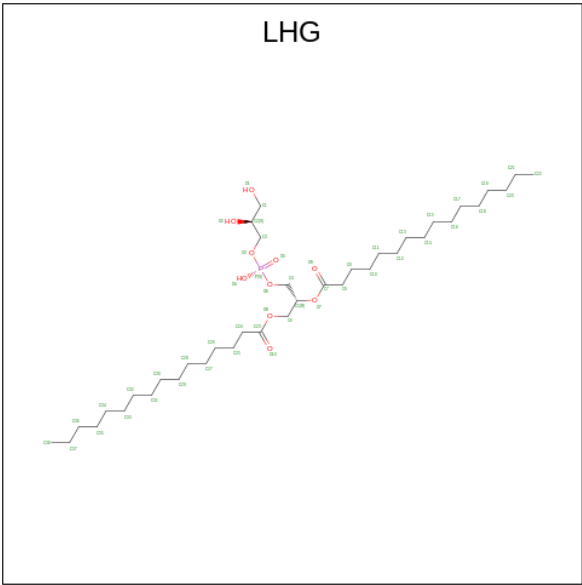
Mol	Chain	Residues	Atoms			AltConf
33	0	1	Total	C	O	0
			52	47	5	
33	0	1	Total	C	O	0
			52	47	5	
33	1	1	Total	C	O	0
			52	47	5	
33	1	1	Total	C	O	0
			52	47	5	
33	2	1	Total	C	O	0
			51	46	5	
33	2	1	Total	C	O	0
			50	45	5	
33	3	1	Total	C	O	0
			51	46	5	
33	5	1	Total	C	O	0
			51	46	5	
33	5	1	Total	C	O	0
			52	47	5	
33	6	1	Total	C	O	0
			51	46	5	
33	6	1	Total	C	O	0
			52	47	5	
33	7	1	Total	C	O	0
			51	46	5	
33	8	1	Total	C	O	0
			51	46	5	
33	8	1	Total	C	O	0
			52	47	5	
33	9	1	Total	C	O	0
			52	47	5	
33	9	1	Total	C	O	0
			52	47	5	
33	O	1	Total	C	O	0
			52	47	5	
33	a	1	Total	C	O	0
			47	42	5	
33	c	1	Total	C	O	0
			52	47	5	
33	b	1	Total	C	O	0
			52	47	5	
33	d	1	Total	C	O	0
			49	44	5	
33	f	1	Total	C	O	0
			49	44	5	

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Mol	Chain	Residues	Atoms			AltConf
33	g	1	Total	C	O	0
			52	47	5	
33	h	1	Total	C	O	0
			52	47	5	
33	i	1	Total	C	O	0
			50	45	5	
33	e	1	Total	C	O	0
			52	47	5	
33	4	1	Total	C	O	0
			51	46	5	
33	4	1	Total	C	O	0
			50	45	5	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
34	0	1	Total	C	O	P	0
			49	38	10	1	
34	1	1	Total	C	O	P	0
			49	38	10	1	
34	2	1	Total	C	O	P	0
			32	21	10	1	
34	3	1	Total	C	O	P	0
			36	25	10	1	
34	3	1	Total	C	O	P	0
			37	26	10	1	

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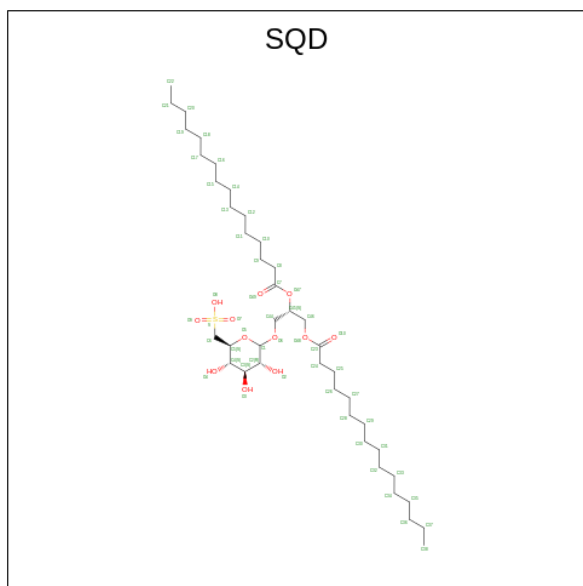
Mol	Chain	Residues	Atoms				AltConf
34	5	1	Total	C	O	P	0
			37	26	10	1	
34	6	1	Total	C	O	P	0
			37	26	10	1	
34	6	1	Total	C	O	P	0
			31	20	10	1	
34	7	1	Total	C	O	P	0
			30	19	10	1	
34	7	1	Total	C	O	P	0
			38	27	10	1	
34	7	1	Total	C	O	P	0
			39	28	10	1	
34	8	1	Total	C	O	P	0
			44	33	10	1	
34	9	1	Total	C	O	P	0
			47	36	10	1	
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			27	16	10	1	
34	A	1	Total	C	O	P	0
			42	31	10	1	
34	B	1	Total	C	O	P	0
			23	12	10	1	
34	B	1	Total	C	O	P	0
			43	32	10	1	
34	G	1	Total	C	O	P	0
			38	27	10	1	
34	K	1	Total	C	O	P	0
			43	34	8	1	
34	M	1	Total	C	O	P	0
			46	35	10	1	
34	a	1	Total	C	O	P	0
			43	32	10	1	
34	c	1	Total	C	O	P	0
			40	29	10	1	
34	b	1	Total	C	O	P	0
			41	30	10	1	
34	d	1	Total	C	O	P	0
			36	25	10	1	
34	f	1	Total	C	O	P	0
			40	29	10	1	

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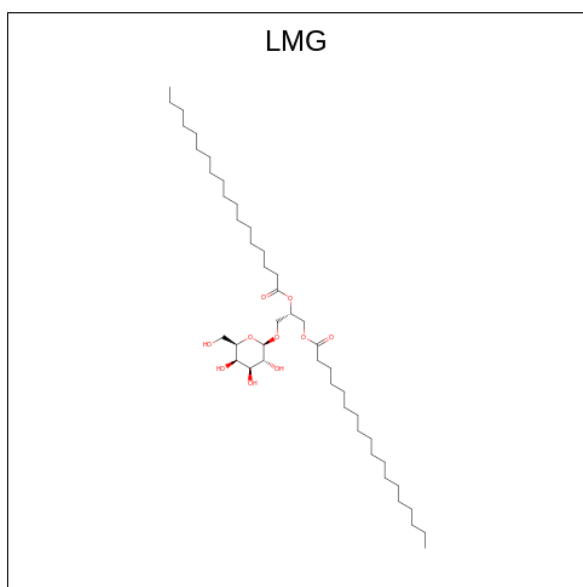
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
34	g	1	Total 30	19	10	1	0
34	h	1	Total 39	28	10	1	0
34	H	1	Total 31	20	10	1	0
34	i	1	Total 30	19	10	1	0
34	e	1	Total 43	32	10	1	0
34	4	1	Total 32	21	10	1	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



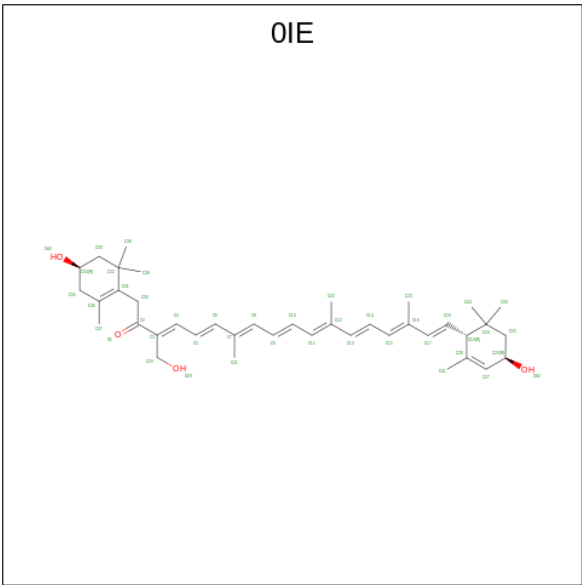
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
35	0	1	Total 36	26	9	1	0

- Molecule 36 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
36	2	1	Total	C	O	0
			36	26	10	
36	3	1	Total	C	O	0
			36	26	10	
36	9	1	Total	C	O	0
			55	45	10	
36	A	1	Total	C	O	0
			36	26	10	
36	B	1	Total	C	O	0
			42	32	10	
36	J	1	Total	C	O	0
			29	19	10	
36	J	1	Total	C	O	0
			46	36	10	
36	L	1	Total	C	O	0
			31	21	10	
36	L	1	Total	C	O	0
			37	27	10	
36	O	1	Total	C	O	0
			39	29	10	

- Molecule 37 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



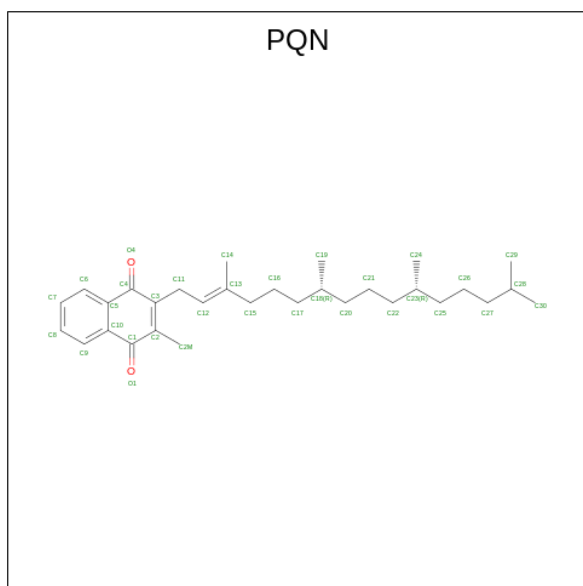
Mol	Chain	Residues	Atoms			AltConf
37	3	1	Total	C	O	0
			44	40	4	
37	7	1	Total	C	O	0
			44	40	4	
37	a	1	Total	C	O	0
			44	40	4	
37	a	1	Total	C	O	0
			44	40	4	
37	c	1	Total	C	O	0
			44	40	4	
37	c	1	Total	C	O	0
			44	40	4	
37	b	1	Total	C	O	0
			44	40	4	
37	b	1	Total	C	O	0
			44	40	4	
37	d	1	Total	C	O	0
			44	40	4	
37	d	1	Total	C	O	0
			44	40	4	
37	f	1	Total	C	O	0
			44	40	4	
37	f	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	

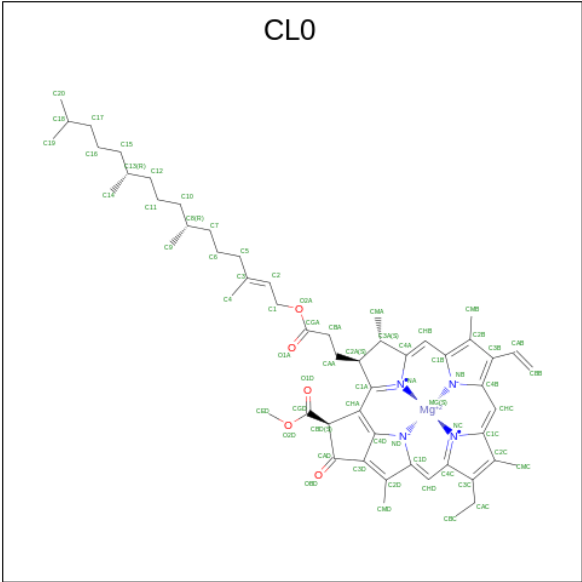
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Mol	Chain	Residues	Atoms			AltConf
37	h	1	Total	C	O	0
			44	40	4	
37	h	1	Total	C	O	0
			44	40	4	
37	i	1	Total	C	O	0
			44	40	4	
37	i	1	Total	C	O	0
			44	40	4	
37	e	1	Total	C	O	0
			44	40	4	
37	e	1	Total	C	O	0
			44	40	4	

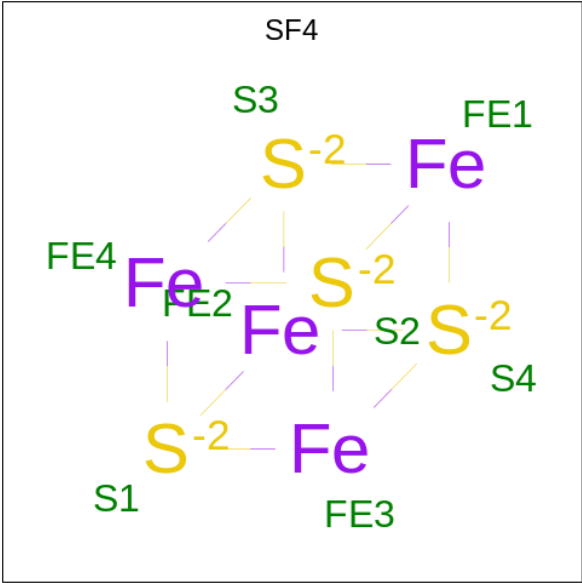
- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



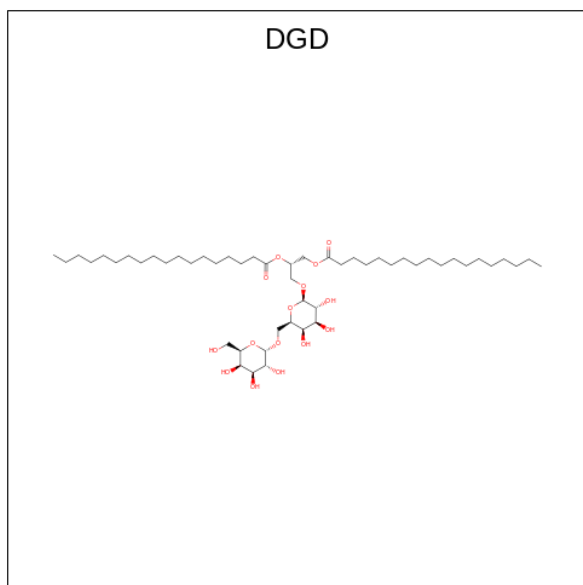
Mol	Chain	Residues	Atoms			AltConf
40	B	1	Total	Fe	S	0
			8	4	4	
40	C	1	Total	Fe	S	0
			8	4	4	

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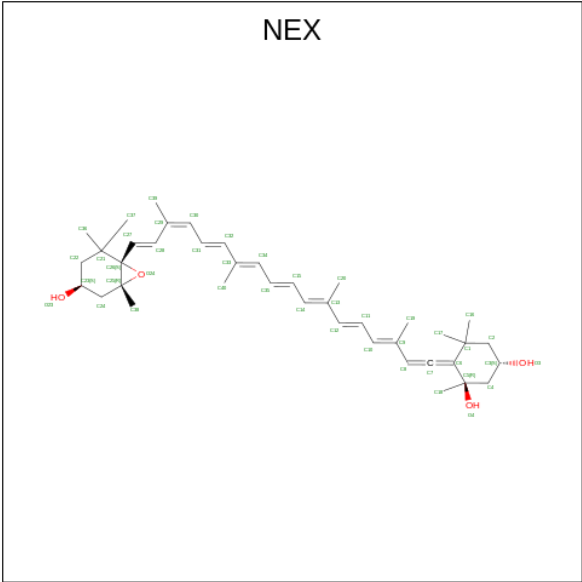
Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 41 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
41	B	1	Total	C	O	0
			56	41	15	

- Molecule 42 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



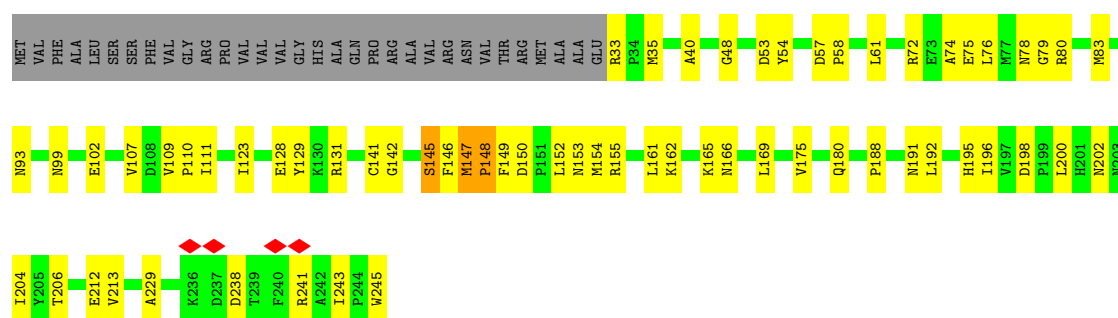
Mol	Chain	Residues	Atoms			AltConf
42	a	1	Total	C	O	0
			44	40	4	
42	c	1	Total	C	O	0
			44	40	4	
42	b	1	Total	C	O	0
			44	40	4	
42	d	1	Total	C	O	0
			44	40	4	
42	f	1	Total	C	O	0
			44	40	4	
42	g	1	Total	C	O	0
			44	40	4	
42	h	1	Total	C	O	0
			44	40	4	
42	i	1	Total	C	O	0
			44	40	4	
42	e	1	Total	C	O	0
			44	40	4	

3 Residue-property plots [i](#)

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

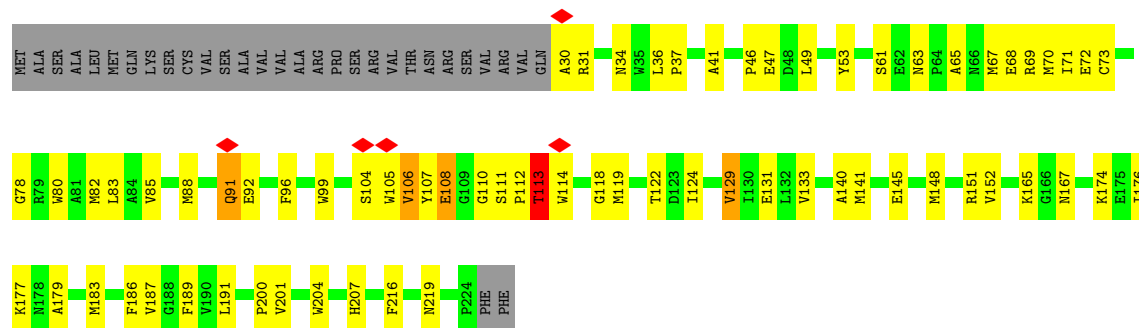
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 0: 



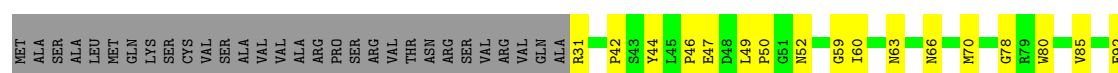
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

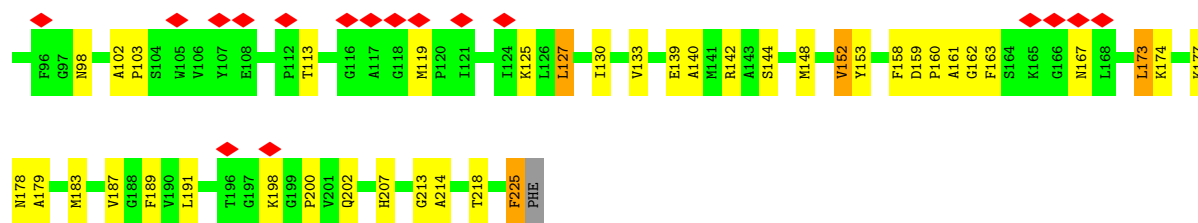
Chain 1: 



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

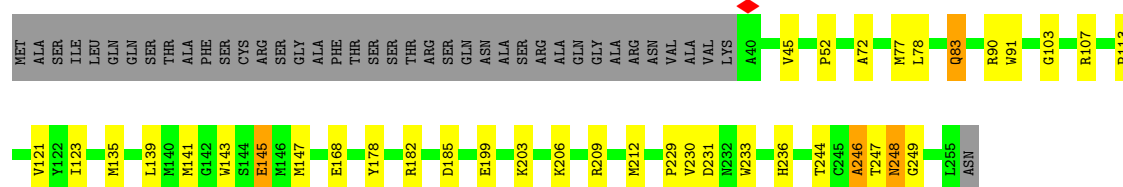
Chain 5: 





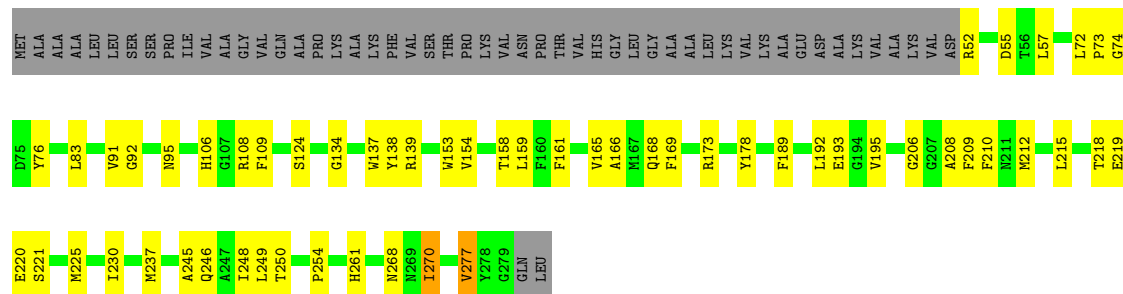
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 70% 13% 16%



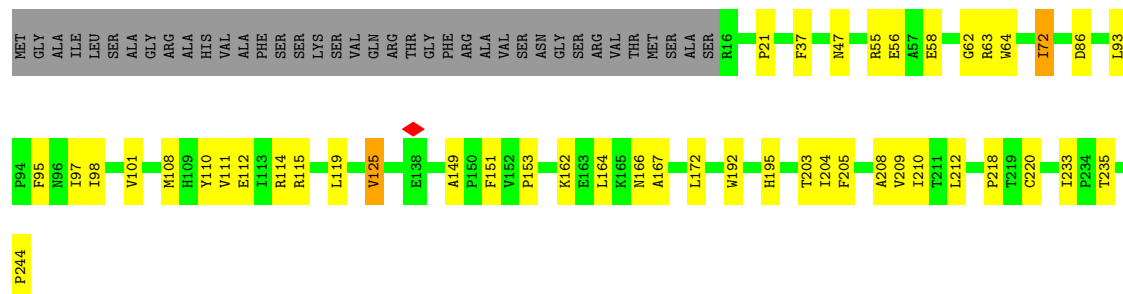
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 61% 20% 19%



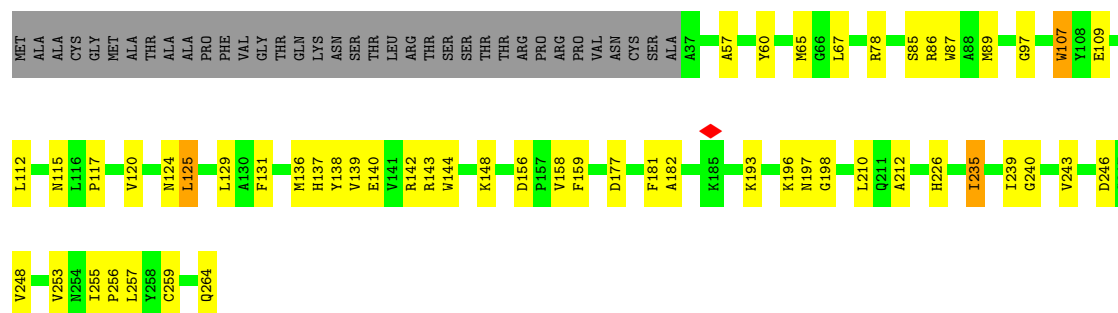
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 69% 16% 14%

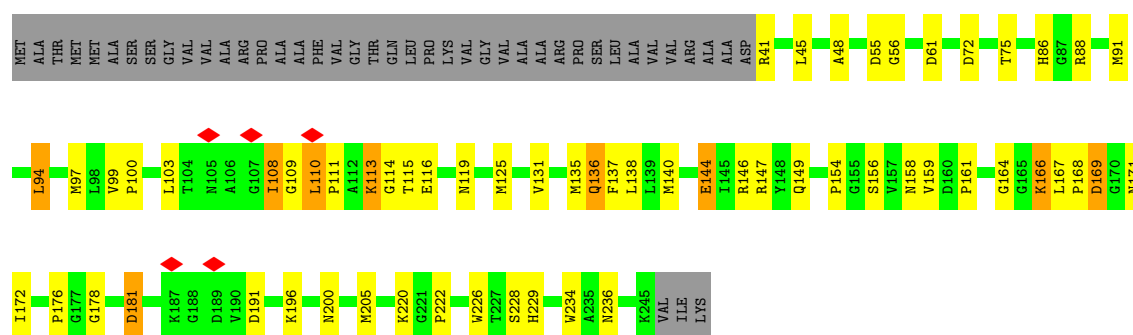


- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

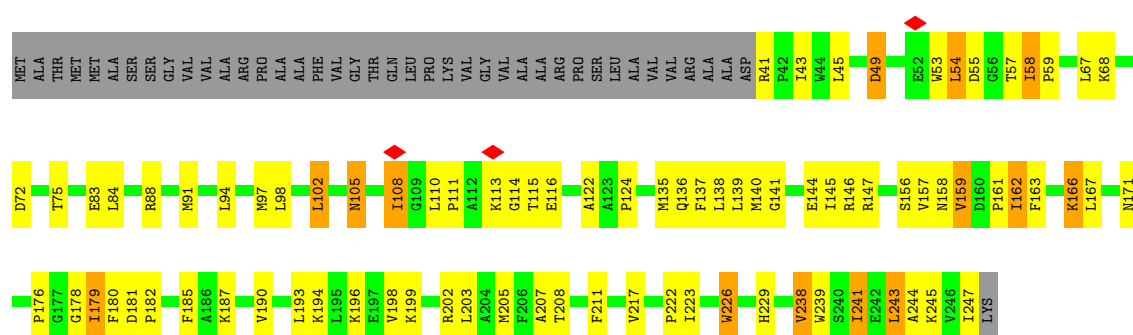
Chain 7: 66% 19% 14%



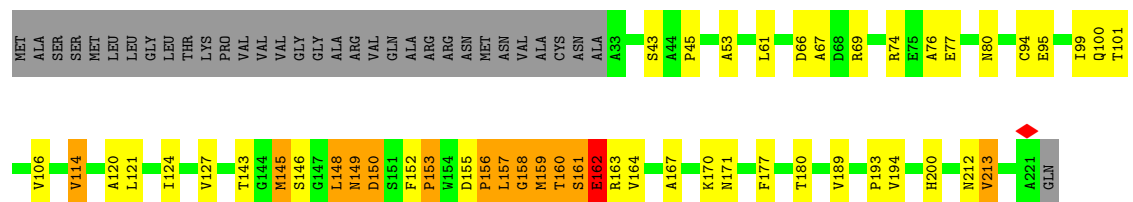
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

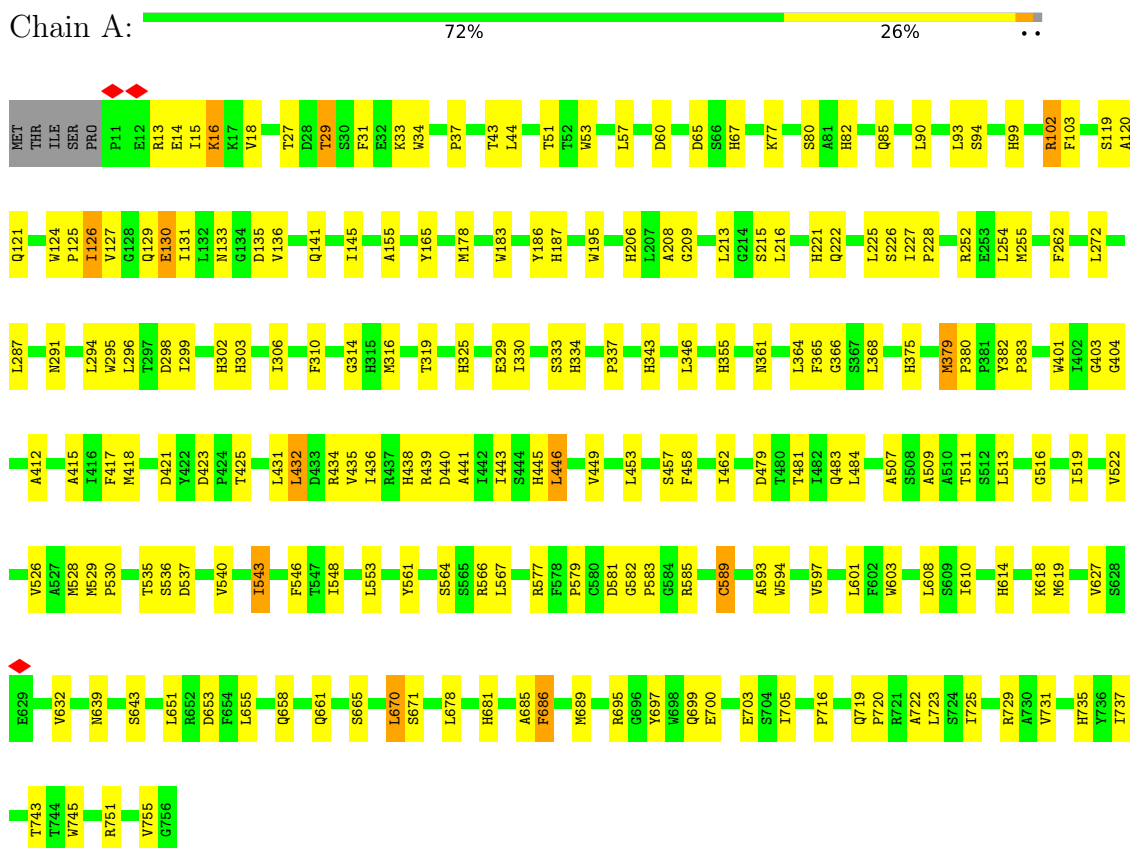


- Molecule 8: Chlorophyll a-b binding protein, chloroplastic



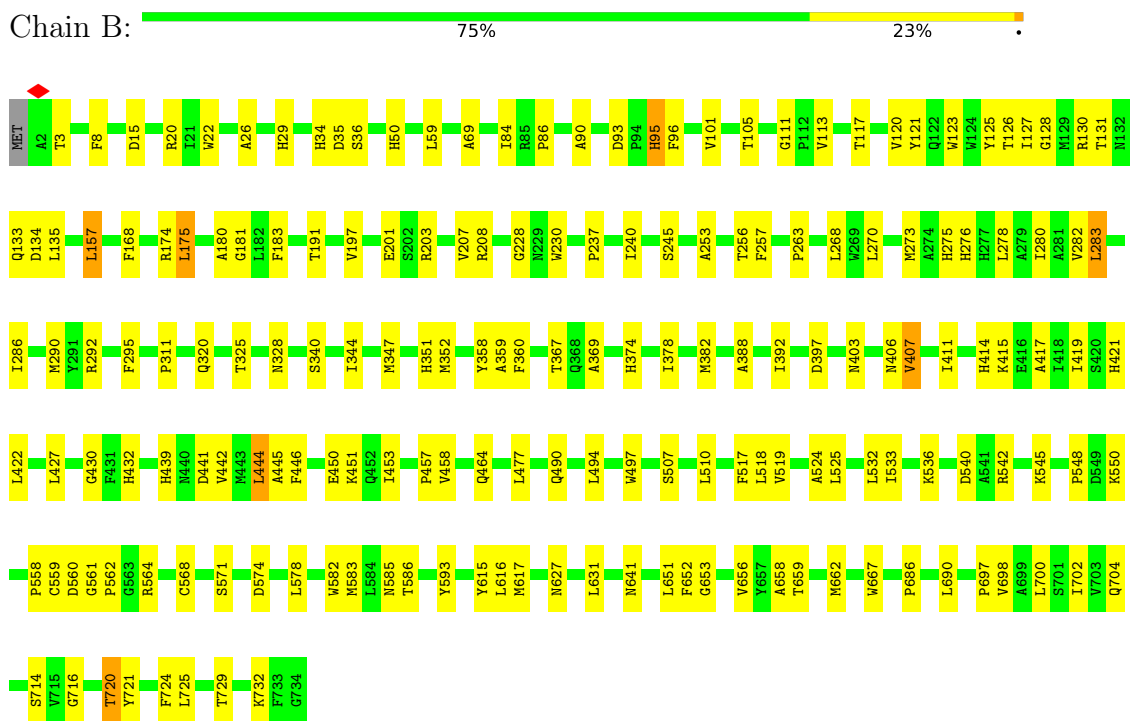
- Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



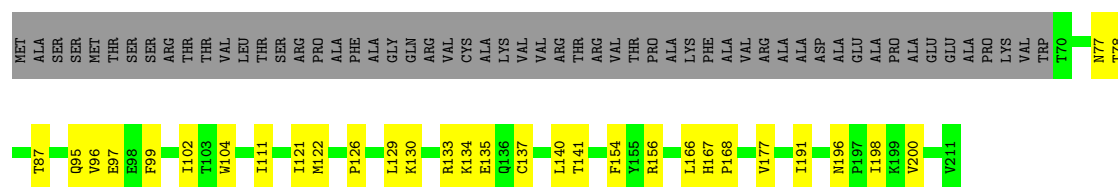
• Molecule 10: photosystem I

Chain B:



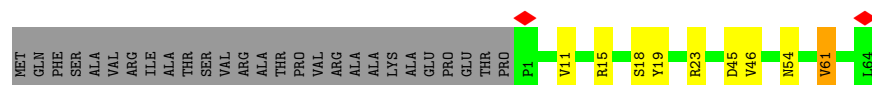
• Molecule 11: Photosystem I reaction center subunit II, chloroplastic

Chain D: 



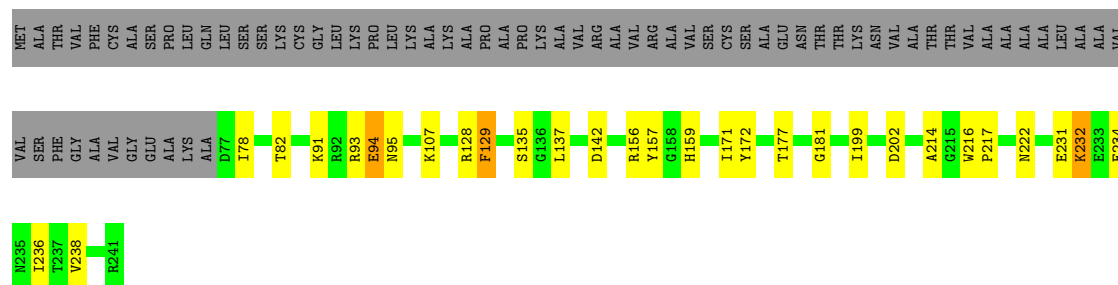
• Molecule 12: PsaE

Chain E: 



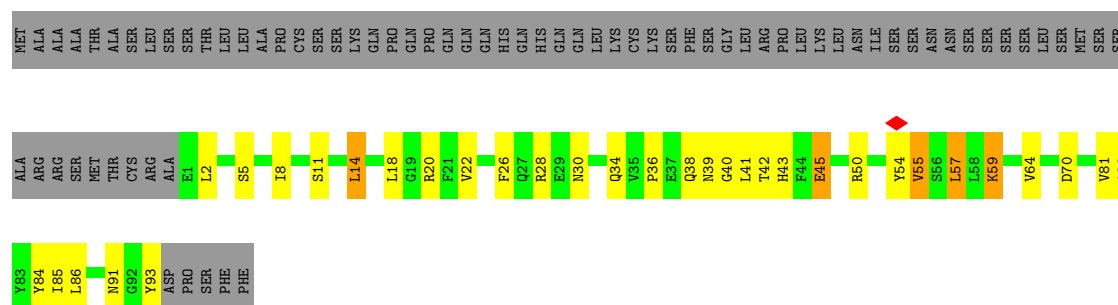
• Molecule 13: Photosystem I reaction center subunit III

Chain F: 



• Molecule 14: PsaG

Chain G: 



• Molecule 15: Photosystem I reaction center subunit VIII

Chain I: 



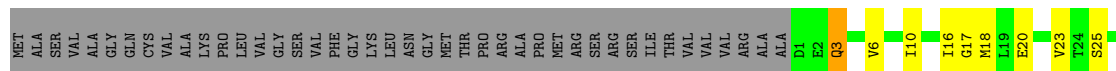
• Molecule 16: Photosystem I reaction center subunit IX

Chain J:  66% 32% .



• Molecule 17: PSI subunit V

Chain L:  64% 15% 21%



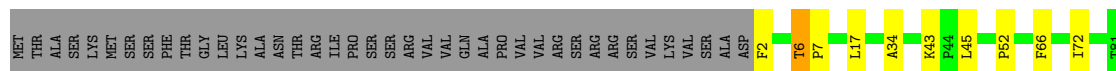
• Molecule 18: Photosystem I iron-sulfur center

Chain C:  74% 25% .



• Molecule 19: PsaK

Chain K:  57% 7% 35%



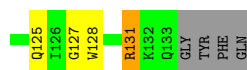
• Molecule 20: Photosystem I reaction center subunit XII

Chain M:  84% 12% .

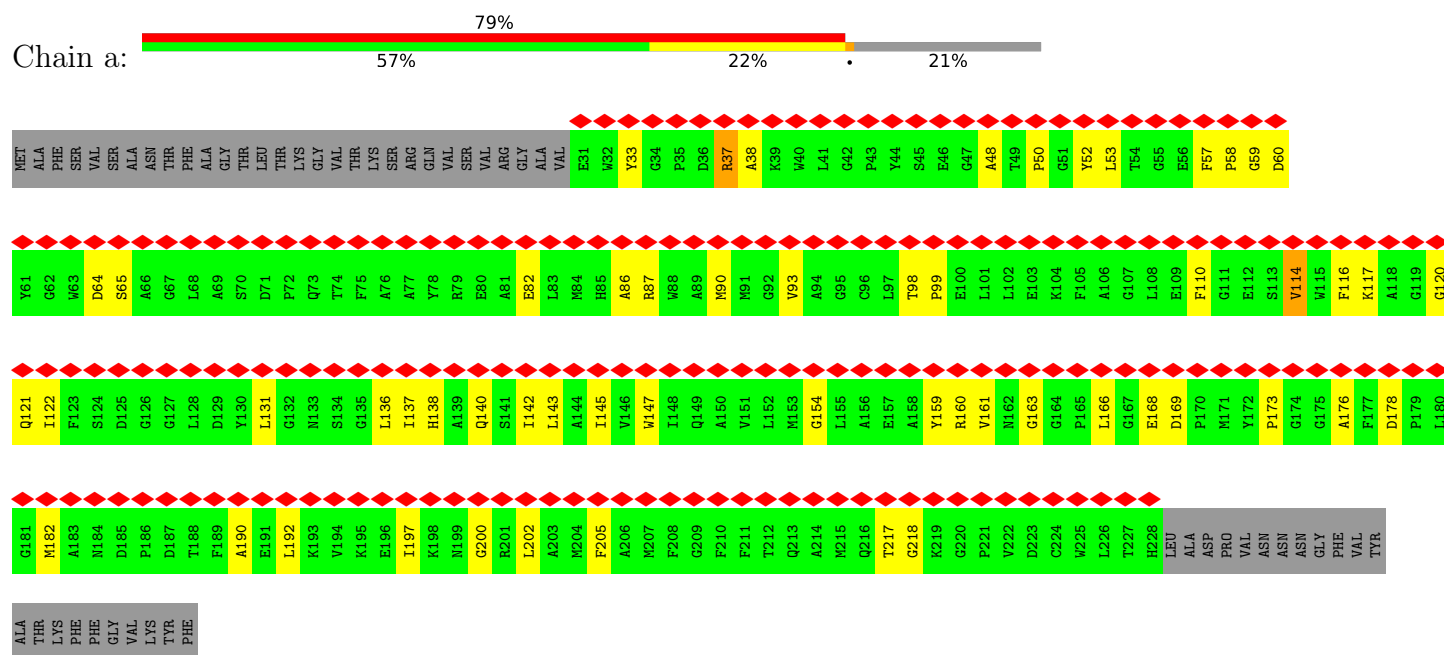


• Molecule 21: PsaO

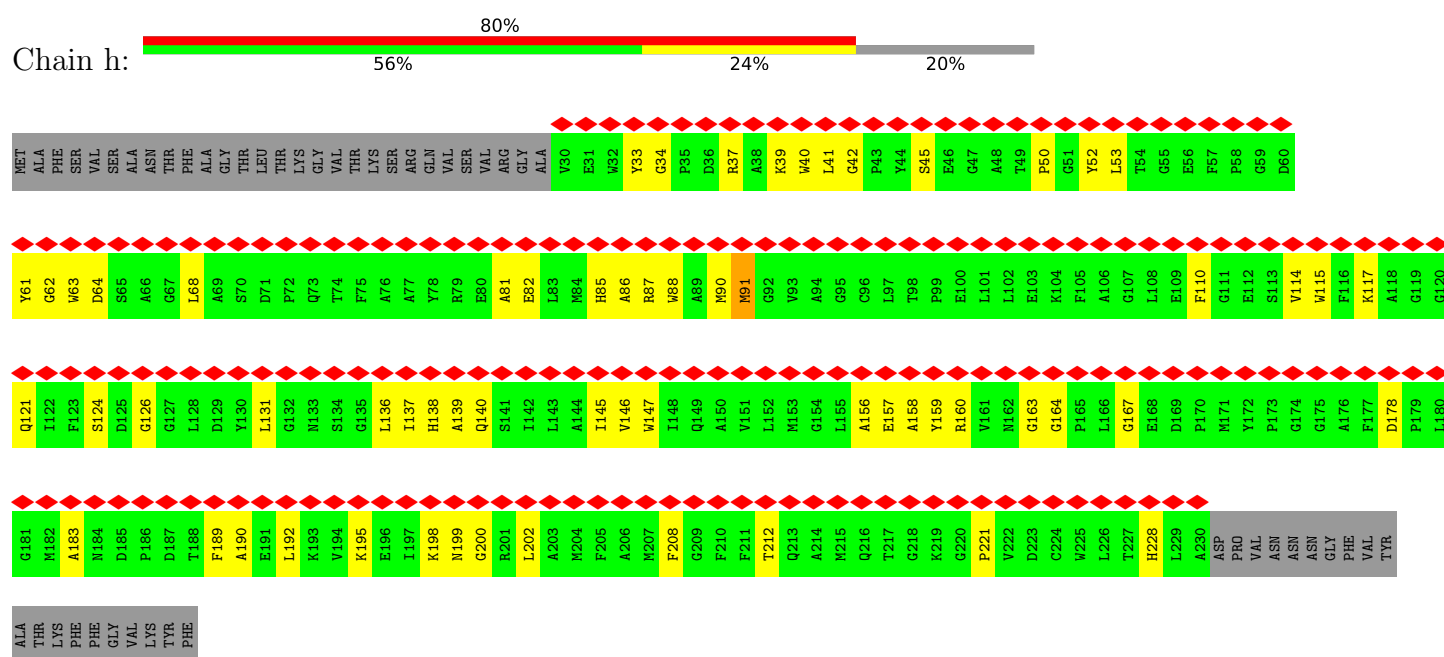
Chain O:  57% 9% 33%



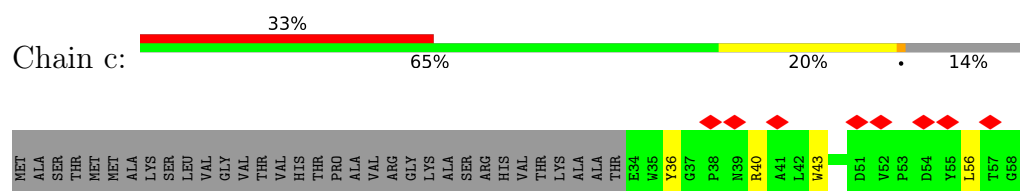
- Molecule 22: Lhcb-a

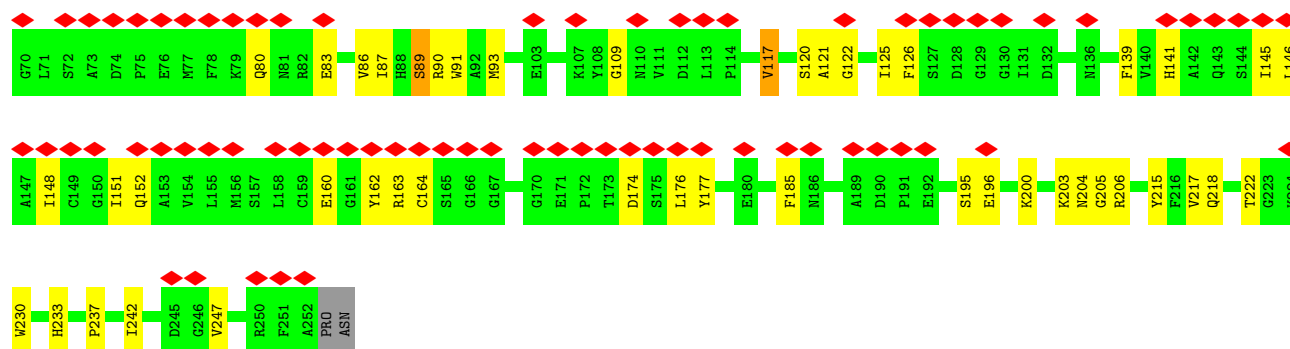


- Molecule 22: Lhcb-a

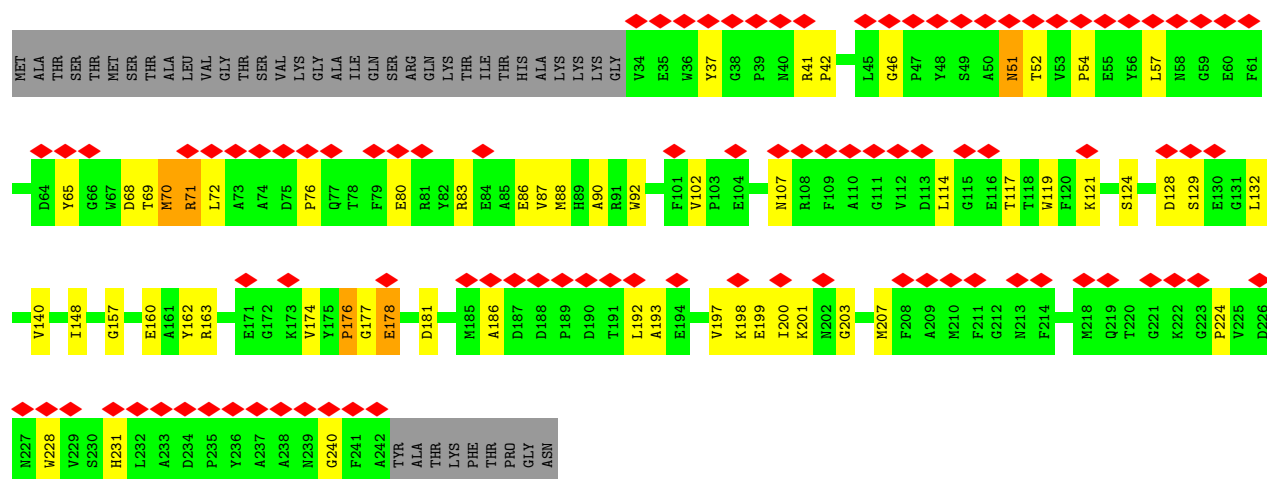


- Molecule 23: Lhcb-c

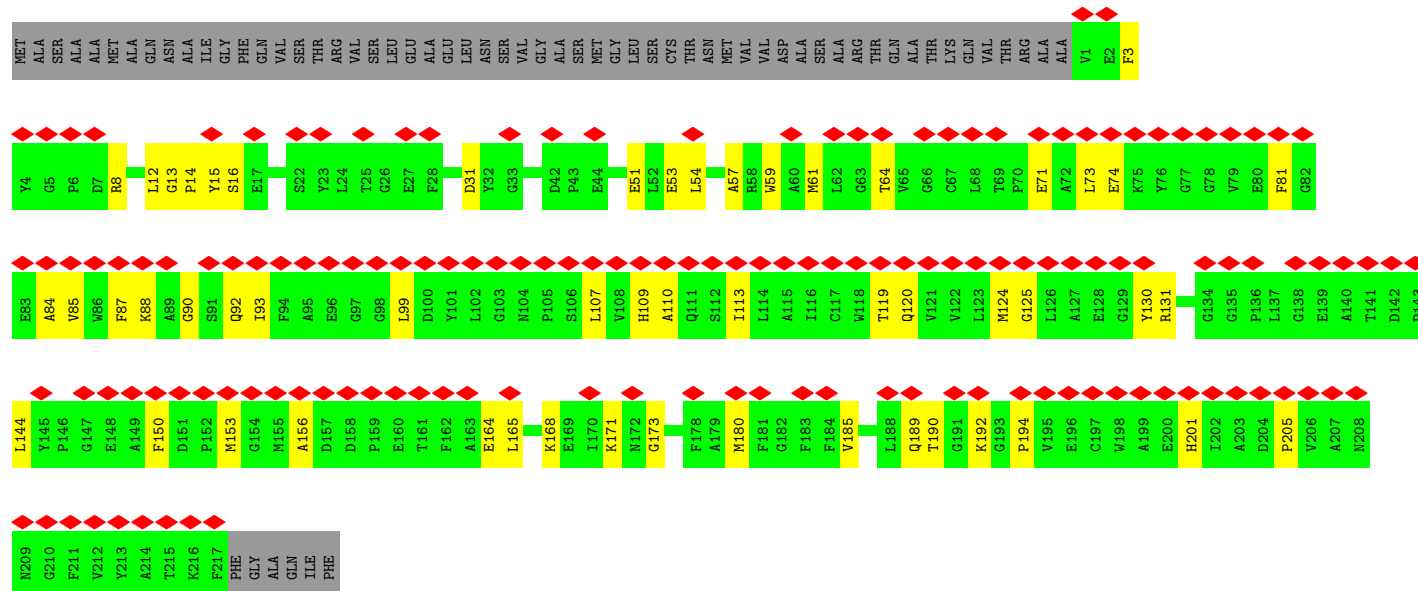




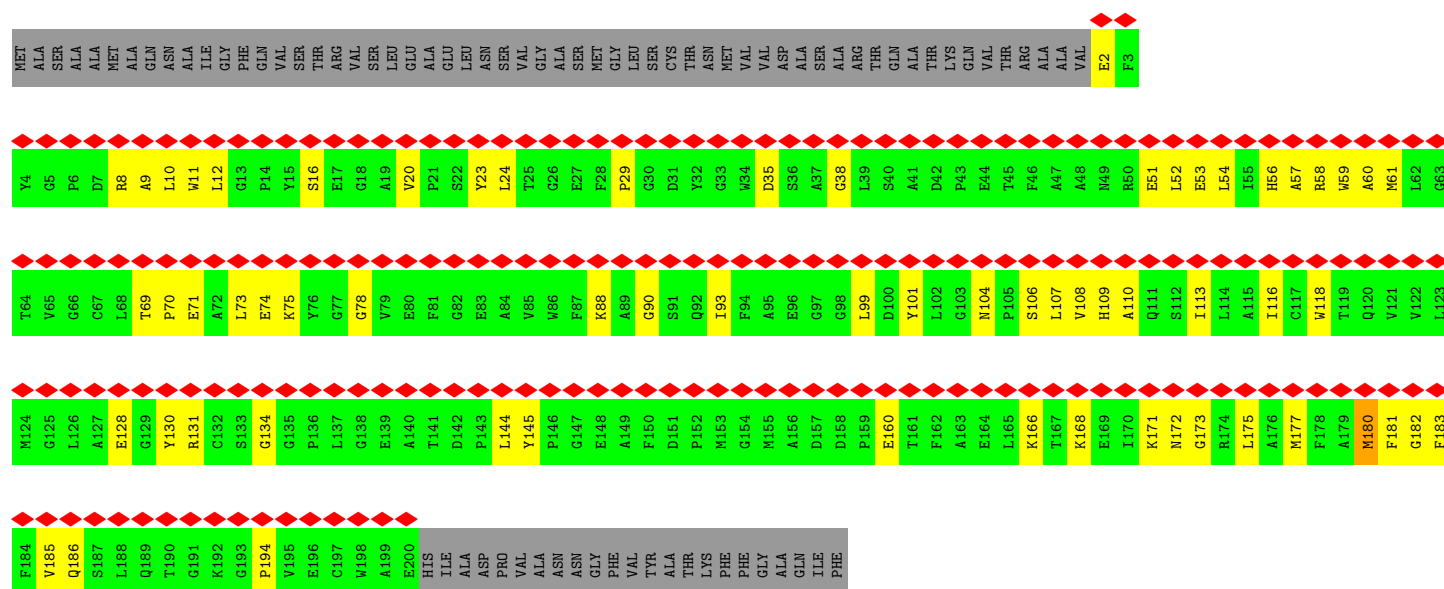
• Molecule 24: Lhcb-b



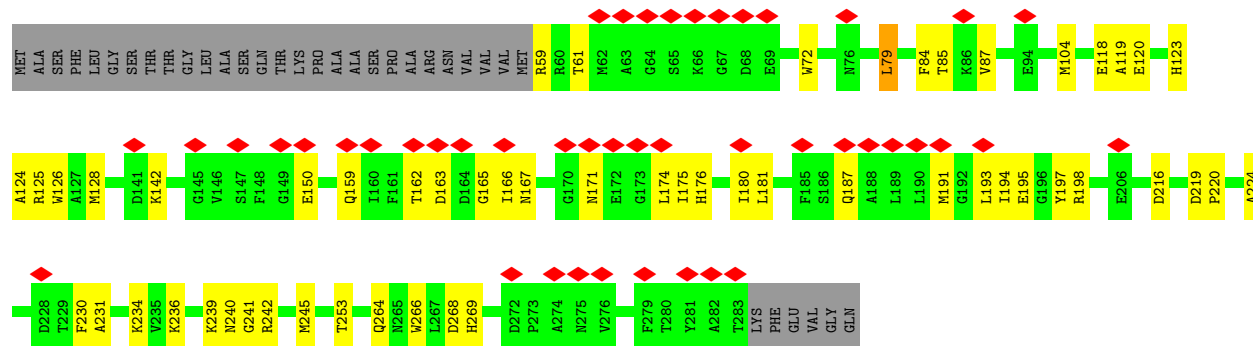
• Molecule 25: Lhcb-d



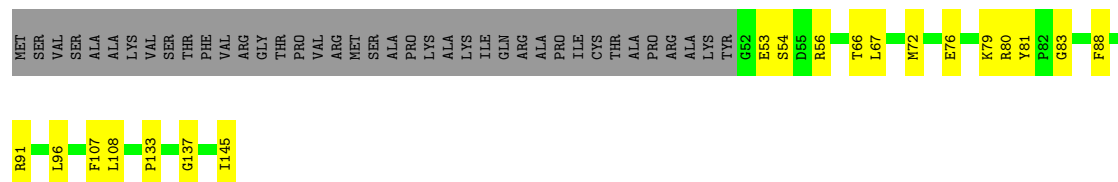
- Molecule 25: Lhcb-d



- Molecule 26: Lhcb-f

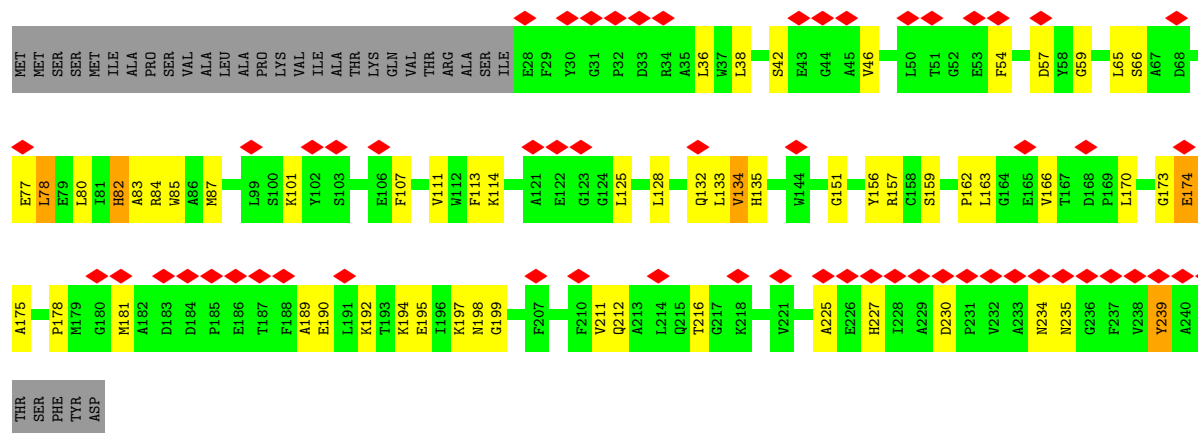


- Molecule 27: PsaH



- Molecule 28: Lhcb-i





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPHERA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.557	Depositor
Minimum map value	-0.337	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.217	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0UR, 8CT, CHL, TPO, SQD, PQN, LHG, LMG, SF4, CLA, CL0, 0IE, NEX, DGD

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	0	0.27	0/1685	0.38	0/2285
2	1	0.41	1/1523 (0.1%)	0.45	1/2073 (0.0%)
2	5	0.21	0/1530	0.41	0/2082
3	2	0.47	2/1727 (0.1%)	0.42	2/2351 (0.1%)
4	3	0.25	0/1818	0.32	0/2466
5	6	0.22	0/1862	0.29	0/2542
6	7	0.22	0/1812	0.31	0/2468
7	4	0.34	0/1619	0.62	1/2206 (0.0%)
7	8	0.20	0/1627	0.41	2/2217 (0.1%)
8	9	0.53	0/1492	0.48	1/2036 (0.0%)
9	A	0.42	1/6069 (0.0%)	0.35	1/8267 (0.0%)
10	B	0.37	0/6034	0.35	0/8239
11	D	0.21	0/1135	0.34	0/1533
12	E	0.19	0/521	0.26	0/706
13	F	0.21	0/1298	0.31	0/1748
14	G	0.25	0/743	0.41	0/1010
15	I	0.60	0/269	0.45	0/367
16	J	0.25	0/346	0.37	0/472
17	L	0.22	0/1224	0.34	0/1673
18	C	0.25	0/612	0.37	0/830
19	K	0.20	0/567	0.27	0/769
20	M	0.66	0/241	0.34	0/325
21	O	0.22	0/760	0.32	0/1042
22	a	0.12	0/1559	0.32	1/2116 (0.0%)
22	h	0.10	0/1568	0.28	0/2132
23	c	0.13	0/1733	0.30	0/2363
24	b	0.17	0/1658	0.34	0/2254
25	d	0.12	0/1685	0.29	0/2296
25	g	0.11	0/1548	0.26	0/2106
26	f	0.13	0/1765	0.27	0/2399
27	H	0.18	0/729	0.34	0/979
28	i	0.10	0/1881	0.30	0/2561

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	e	0.11	0/1697	0.29	0/2311
All	All	0.29	4/52337 (0.0%)	0.36	9/71224 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	246	ALA	CA-C	-5.28	1.46	1.52
9	A	689	MET	CA-C	-5.24	1.45	1.52
2	1	113	THR	CA-C	-5.19	1.45	1.53
3	2	247	THR	N-CA	-5.09	1.39	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	180	PHE	N-CA-C	-13.97	96.79	112.72
8	9	163	ARG	N-CA-C	-8.39	102.09	111.07
7	8	109	GLY	CA-C-N	6.66	129.49	123.10
7	8	109	GLY	C-N-CA	6.66	129.49	123.10
2	1	108	GLU	N-CA-C	-6.25	104.35	112.23

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	0	1640	0	1609	50	0
2	1	1478	0	1423	56	0
2	5	1484	0	1427	42	0
3	2	1667	0	1562	27	0
4	3	1768	0	1702	49	0
5	6	1797	0	1752	37	0
6	7	1758	0	1701	48	0
7	4	1569	0	1551	65	0
7	8	1574	0	1550	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	9	1453	0	1404	42	0
9	A	5872	0	5715	162	0
10	B	5824	0	5603	149	0
11	D	1109	0	1124	26	0
12	E	509	0	506	9	0
13	F	1273	0	1290	23	0
14	G	726	0	717	32	0
15	I	262	0	279	9	0
16	J	336	0	355	13	0
17	L	1195	0	1187	25	0
18	C	602	0	591	22	0
19	K	558	0	591	7	0
20	M	238	0	248	4	0
21	O	728	0	699	16	0
22	a	1511	0	1426	44	0
22	h	1520	0	1429	56	0
23	c	1680	0	1582	47	0
24	b	1609	0	1531	51	0
25	d	1634	0	1535	49	0
25	g	1502	0	1412	51	0
26	f	1727	0	1634	62	0
27	H	717	0	684	22	0
28	i	1834	0	1741	91	0
29	e	1647	0	1559	48	0
30	0	215	0	172	13	0
30	1	291	0	262	19	0
30	2	426	0	344	21	0
30	3	179	0	166	9	0
30	4	347	0	251	22	0
30	5	304	0	228	16	0
30	6	425	0	344	22	0
30	7	334	0	280	20	0
30	8	420	0	332	20	0
30	9	193	0	132	4	0
30	a	405	0	307	21	0
30	b	390	0	341	25	0
30	c	425	0	362	32	0
30	d	415	0	331	24	0
30	e	422	0	345	24	0
30	f	430	0	364	24	0
30	g	381	0	266	15	0
30	h	386	0	280	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	i	389	0	282	32	0
31	0	478	0	426	26	0
31	1	434	0	386	18	0
31	2	389	0	356	9	0
31	3	603	0	554	23	0
31	4	371	0	324	13	0
31	5	409	0	340	13	0
31	6	527	0	456	15	0
31	7	569	0	496	26	0
31	8	364	0	314	6	0
31	9	496	0	458	19	0
31	A	2599	0	2656	135	0
31	B	2357	0	2336	146	0
31	F	45	0	33	3	0
31	G	141	0	105	2	0
31	H	200	0	160	4	0
31	J	42	0	31	2	0
31	K	209	0	176	9	0
31	L	260	0	221	11	0
31	M	46	0	33	0	0
31	O	168	0	108	7	0
31	a	315	0	266	10	0
31	b	320	0	276	11	0
31	c	303	0	244	9	0
31	d	306	0	250	11	0
31	e	317	0	270	13	0
31	f	315	0	266	12	0
31	g	280	0	208	19	0
31	h	273	0	200	11	0
31	i	292	0	228	38	0
32	0	40	0	0	0	0
32	1	40	0	0	0	0
32	2	40	0	0	0	0
32	3	80	0	0	1	0
32	4	40	0	0	1	0
32	6	40	0	0	0	0
32	7	120	0	0	1	0
32	8	80	0	0	1	0
32	9	40	0	0	0	0
32	A	240	0	0	1	0
32	B	320	0	0	2	0
32	F	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	G	40	0	0	0	0
32	I	40	0	0	0	0
32	J	80	0	0	1	0
32	K	40	0	0	0	0
32	L	120	0	0	1	0
32	M	40	0	0	0	0
32	O	40	0	0	0	0
33	0	104	0	0	1	0
33	1	104	0	0	1	0
33	2	101	0	0	3	0
33	3	51	0	0	1	0
33	4	101	0	0	3	0
33	5	103	0	0	4	0
33	6	103	0	0	1	0
33	7	51	0	0	2	0
33	8	103	0	0	3	0
33	9	104	0	0	3	0
33	O	52	0	0	1	0
33	a	47	0	0	2	0
33	b	52	0	0	3	0
33	c	52	0	0	1	0
33	d	49	0	0	1	0
33	e	52	0	0	0	0
33	f	49	0	0	0	0
33	g	52	0	0	0	0
33	h	52	0	0	1	0
33	i	50	0	0	2	0
34	0	49	0	74	4	0
34	1	49	0	74	6	0
34	2	32	0	34	3	0
34	3	73	0	84	4	0
34	4	32	0	34	0	0
34	5	37	0	44	1	0
34	6	68	0	76	5	0
34	7	107	0	127	4	0
34	8	44	0	58	0	0
34	9	47	0	63	5	0
34	A	118	0	152	8	0
34	B	66	0	75	4	0
34	G	38	0	46	2	0
34	H	31	0	32	0	0
34	K	43	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	46	0	65	4	0
34	a	43	0	56	4	0
34	b	41	0	52	2	0
34	c	40	0	50	5	0
34	d	36	0	42	5	0
34	e	43	0	56	5	0
34	f	40	0	50	5	0
34	g	30	0	30	3	0
34	h	39	0	48	4	0
34	i	30	0	30	4	0
35	0	36	0	41	2	0
36	2	36	0	42	0	0
36	3	36	0	42	1	0
36	9	55	0	86	4	0
36	A	36	0	42	3	0
36	B	42	0	54	1	0
36	J	75	0	93	3	0
36	L	68	0	76	3	0
36	O	39	0	48	1	0
37	3	44	0	0	0	0
37	7	44	0	0	0	0
37	a	88	0	0	0	0
37	b	88	0	0	2	0
37	c	88	0	0	1	0
37	d	88	0	0	0	0
37	e	88	0	0	0	0
37	f	88	0	0	0	0
37	g	88	0	0	0	0
37	h	88	0	0	2	0
37	i	88	0	0	4	0
38	A	33	0	46	5	0
38	B	33	0	46	1	0
39	A	65	0	72	7	0
40	B	8	0	0	1	0
40	C	16	0	0	0	0
41	B	56	0	70	3	0
42	a	44	0	56	7	0
42	b	44	0	56	3	0
42	c	44	0	56	5	0
42	d	44	0	56	10	0
42	e	44	0	56	3	0
42	f	44	0	56	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	g	44	0	56	8	0
42	h	44	0	56	15	0
42	i	44	0	56	35	0
All	All	77090	0	69459	1948	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 13.

The worst 5 of 1948 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)
28:i:179:VAL:HG11	30:i:606:CHL:HED2	1.28	1.16
42:i:523:NEX:H362	31:i:604:CLA:C4B	1.79	1.11
42:a:523:NEX:H241	31:a:604:CLA:H2	1.36	1.05
1:0:147:MET:HB3	1:0:148:PRO:HD2	1.42	1.00
2:5:160:PRO:HD2	33:5:501:OUR:C30	1.90	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	211/245 (86%)	192 (91%)	17 (8%)	2 (1%)	14	26
2	1	193/226 (85%)	186 (96%)	6 (3%)	1 (0%)	24	40
2	5	193/226 (85%)	177 (92%)	15 (8%)	1 (0%)	24	40
3	2	214/256 (84%)	205 (96%)	9 (4%)	0	100	100
4	3	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
5	6	227/267 (85%)	222 (98%)	5 (2%)	0	100	100
6	7	226/264 (86%)	211 (93%)	13 (6%)	2 (1%)	14	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	4	205/248 (83%)	176 (86%)	28 (14%)	1 (0%)	24	40
7	8	203/248 (82%)	187 (92%)	14 (7%)	2 (1%)	12	22
8	9	187/222 (84%)	168 (90%)	12 (6%)	7 (4%)	2	4
9	A	744/751 (99%)	711 (96%)	32 (4%)	1 (0%)	48	69
10	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
11	D	140/198 (71%)	134 (96%)	6 (4%)	0	100	100
12	E	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
13	F	163/236 (69%)	155 (95%)	8 (5%)	0	100	100
14	G	91/167 (54%)	85 (93%)	6 (7%)	0	100	100
15	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
16	J	39/41 (95%)	39 (100%)	0	0	100	100
17	L	160/204 (78%)	157 (98%)	3 (2%)	0	100	100
18	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
19	K	78/123 (63%)	78 (100%)	0	0	100	100
20	M	29/32 (91%)	29 (100%)	0	0	100	100
21	O	90/137 (66%)	84 (93%)	6 (7%)	0	100	100
22	a	196/250 (78%)	173 (88%)	21 (11%)	2 (1%)	12	22
22	h	199/250 (80%)	181 (91%)	17 (8%)	1 (0%)	24	40
23	c	217/254 (85%)	208 (96%)	8 (4%)	1 (0%)	24	40
24	b	207/251 (82%)	189 (91%)	15 (7%)	3 (1%)	9	15
25	d	215/280 (77%)	194 (90%)	21 (10%)	0	100	100
25	g	197/280 (70%)	187 (95%)	9 (5%)	1 (0%)	24	40
26	f	222/259 (86%)	209 (94%)	12 (5%)	1 (0%)	24	40
27	H	92/133 (69%)	82 (89%)	10 (11%)	0	100	100
28	i	234/282 (83%)	204 (87%)	26 (11%)	4 (2%)	7	12
29	e	214/250 (86%)	201 (94%)	11 (5%)	2 (1%)	14	26
All	All	6516/7803 (84%)	6116 (94%)	368 (6%)	32 (0%)	26	40

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	148	PRO
6	7	125	LEU

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Mol	Chain	Res	Type
7	8	108	ILE
8	9	153	PRO
22	a	121	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	167/194 (86%)	162 (97%)	5 (3%)	36	58
2	1	148/175 (85%)	139 (94%)	9 (6%)	17	30
2	5	149/175 (85%)	144 (97%)	5 (3%)	32	55
3	2	166/197 (84%)	163 (98%)	3 (2%)	51	69
4	3	186/225 (83%)	183 (98%)	3 (2%)	55	72
5	6	188/216 (87%)	181 (96%)	7 (4%)	30	52
6	7	181/209 (87%)	176 (97%)	5 (3%)	38	60
7	4	158/189 (84%)	133 (84%)	25 (16%)	2	3
7	8	159/189 (84%)	150 (94%)	9 (6%)	18	34
8	9	147/173 (85%)	136 (92%)	11 (8%)	12	23
9	A	609/614 (99%)	591 (97%)	18 (3%)	36	58
10	B	600/601 (100%)	586 (98%)	14 (2%)	44	65
11	D	119/162 (74%)	117 (98%)	2 (2%)	53	71
12	E	56/77 (73%)	54 (96%)	2 (4%)	31	53
13	F	129/180 (72%)	123 (95%)	6 (5%)	23	43
14	G	79/145 (54%)	71 (90%)	8 (10%)	7	14
15	I	27/28 (96%)	26 (96%)	1 (4%)	30	52
16	J	38/38 (100%)	36 (95%)	2 (5%)	20	37
17	L	124/157 (79%)	119 (96%)	5 (4%)	28	49
18	C	68/69 (99%)	66 (97%)	2 (3%)	37	59
19	K	58/94 (62%)	55 (95%)	3 (5%)	21	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	M	26/27 (96%)	26 (100%)	0	100	100
21	O	76/111 (68%)	75 (99%)	1 (1%)	61	75
22	a	146/187 (78%)	145 (99%)	1 (1%)	76	85
22	h	145/187 (78%)	144 (99%)	1 (1%)	76	85
23	c	174/202 (86%)	172 (99%)	2 (1%)	65	79
24	b	159/193 (82%)	157 (99%)	2 (1%)	61	75
25	d	159/210 (76%)	159 (100%)	0	100	100
25	g	147/210 (70%)	145 (99%)	2 (1%)	59	74
26	f	172/198 (87%)	169 (98%)	3 (2%)	53	71
27	H	69/103 (67%)	69 (100%)	0	100	100
28	i	181/218 (83%)	177 (98%)	4 (2%)	45	65
29	e	164/193 (85%)	159 (97%)	5 (3%)	36	58
All	All	5174/6146 (84%)	5008 (97%)	166 (3%)	35	56

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	C	11	CYS
7	4	54	LEU
19	K	45	LEU
25	g	181	PHE
7	4	113	LYS

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

Mol	Chain	Res	Type
22	a	213	GLN
22	h	228	HIS
23	c	81	ASN
23	c	241	ASN
28	i	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
28	TPO	i	46	28	8,10,11	1.07	0	10,14,16	1.86	2 (20%)
26	TPO	f	61	26	8,10,11	1.06	0	10,14,16	1.83	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	TPO	i	46	28	-	3/9/11/13	-
26	TPO	f	61	26	-	1/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	61	TPO	P-OG1-CB	-5.17	107.59	123.21
28	i	46	TPO	P-OG1-CB	-5.09	107.83	123.21
28	i	46	TPO	CG2-CB-CA	-2.16	108.90	113.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	i	46	TPO	N-CA-CB-CG2
28	i	46	TPO	N-CA-CB-OG1
28	i	46	TPO	C-CA-CB-CG2
26	f	61	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

522 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	$\# Z > 2$
31	CLA	3	311	4	50,54,73	1.45	10 (20%)	60,90,113	1.48	5 (8%)
31	CLA	f	603	-	59,63,73	1.35	9 (15%)	71,101,113	1.34	7 (9%)
37	OIE	e	521	-	42,45,45	1.42	6 (14%)	49,63,63	1.55	10 (20%)
30	CHL	5	302	2	68,72,74	1.83	18 (26%)	77,111,114	2.90	31 (40%)
36	LMG	A	856	-	36,36,55	0.91	0	44,44,63	1.30	4 (9%)
30	CHL	h	601	22	51,55,74	2.29	19 (37%)	57,91,114	3.22	24 (42%)
31	CLA	8	311	7	50,54,73	1.46	10 (20%)	60,90,113	1.41	5 (8%)
31	CLA	a	611	-	61,65,73	1.35	8 (13%)	73,103,113	1.31	5 (6%)
32	8CT	A	846	-	40,41,41	4.62	23 (57%)	50,56,56	2.80	20 (40%)
31	CLA	g	610	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	5 (8%)
31	CLA	5	314	2	50,54,73	1.46	9 (18%)	60,90,113	1.37	4 (6%)
30	CHL	h	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.21	24 (42%)
31	CLA	6	314	-	49,53,73	1.46	8 (16%)	59,89,113	1.47	6 (10%)
31	CLA	B	816	10	64,68,73	1.28	10 (15%)	77,107,113	1.37	8 (10%)
33	OUR	h	520	-	50,53,58	0.95	1 (2%)	58,72,77	1.83	11 (18%)
31	CLA	d	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	5 (7%)
31	CLA	a	603	-	57,61,73	1.38	8 (14%)	68,98,113	1.39	5 (7%)
34	LHG	d	630	-	35,35,48	1.26	6 (17%)	38,41,54	1.05	3 (7%)
30	CHL	2	305	-	47,51,74	2.13	18 (38%)	52,86,114	3.48	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	4	312	7	57,61,73	1.36	10 (17%)	68,98,113	1.38	7 (10%)
32	8CT	B	851	-	40,41,41	4.62	23 (57%)	50,56,56	2.48	14 (28%)
37	0IE	g	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.59	10 (20%)
31	CLA	a	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.39	8 (12%)
31	CLA	9	302	-	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
30	CHL	4	305	-	47,51,74	2.14	18 (38%)	52,86,114	3.39	25 (48%)
30	CHL	3	302	4	66,70,74	1.89	19 (28%)	75,109,114	2.95	30 (40%)
31	CLA	B	841	34	69,73,73	1.25	9 (13%)	83,113,113	1.33	8 (9%)
31	CLA	0	321	1	49,53,73	1.49	9 (18%)	59,89,113	1.48	5 (8%)
31	CLA	i	611	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
31	CLA	O	206	-	55,59,73	1.40	9 (16%)	66,96,113	1.33	6 (9%)
34	LHG	A	845	31	26,26,48	1.28	4 (15%)	29,32,54	1.22	2 (6%)
30	CHL	g	606	-	55,59,74	2.20	19 (34%)	62,96,114	3.12	29 (46%)
31	CLA	B	831	10	54,58,73	1.39	9 (16%)	65,95,113	1.42	6 (9%)
30	CHL	c	609	-	70,74,74	1.94	19 (27%)	80,114,114	2.75	26 (32%)
31	CLA	h	604	-	50,54,73	1.46	8 (16%)	60,90,113	1.44	6 (10%)
31	CLA	F	301	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
30	CHL	2	302	3	68,72,74	1.84	18 (26%)	77,111,114	2.94	32 (41%)
31	CLA	B	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.26	6 (7%)
31	CLA	i	603	-	50,54,73	1.46	9 (18%)	60,90,113	1.40	4 (6%)
30	CHL	0	301	1	56,60,74	2.05	19 (33%)	63,97,114	3.17	28 (44%)
31	CLA	A	826	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	8 (9%)
32	8CT	O	205	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	17 (34%)
30	CHL	b	606	-	55,59,74	2.12	20 (36%)	62,96,114	3.17	27 (43%)
36	LMG	J	105	-	46,46,55	0.87	2 (4%)	54,54,63	1.36	8 (14%)
31	CLA	A	816	-	49,53,73	1.49	9 (18%)	59,89,113	1.48	5 (8%)
31	CLA	9	309	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	9 (11%)
34	LHG	f	630	31	39,39,48	1.20	5 (12%)	42,45,54	1.08	3 (7%)
34	LHG	6	601	31	36,36,48	1.25	5 (13%)	39,42,54	1.05	2 (5%)
31	CLA	B	829	-	69,73,73	1.25	10 (14%)	83,113,113	1.23	5 (6%)
31	CLA	B	817	10	64,68,73	1.27	9 (14%)	77,107,113	1.45	9 (11%)
30	CHL	3	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.23	28 (45%)
31	CLA	3	303	-	59,63,73	1.33	10 (16%)	71,101,113	1.37	7 (9%)
37	0IE	d	521	-	42,45,45	1.43	6 (14%)	49,63,63	1.57	10 (20%)
36	LMG	L	211	-	37,37,55	0.89	1 (2%)	45,45,63	1.26	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	603	24	59,63,73	1.35	9 (15%)	71,101,113	1.33	5 (7%)
30	CHL	e	609	-	65,69,74	1.97	18 (27%)	74,108,114	2.89	27 (36%)
31	CLA	1	311	2	56,60,73	1.38	10 (17%)	67,97,113	1.41	5 (7%)
30	CHL	6	313	5	56,60,74	2.06	17 (30%)	63,97,114	3.22	32 (50%)
32	8CT	B	804	-	40,41,41	4.63	23 (57%)	50,56,56	2.57	19 (38%)
36	LMG	3	602	-	36,36,55	0.87	0	44,44,63	1.26	5 (11%)
34	LHG	0	601	-	48,48,48	1.09	5 (10%)	51,54,54	0.93	2 (3%)
31	CLA	B	827	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	7 (8%)
32	8CT	3	403	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	16 (32%)
31	CLA	A	843	34	56,60,73	1.37	10 (17%)	67,97,113	1.42	8 (11%)
33	OUR	0	501	-	50,53,58	0.94	1 (2%)	58,72,77	1.67	12 (20%)
32	8CT	7	402	-	40,41,41	4.58	23 (57%)	50,56,56	2.59	17 (34%)
31	CLA	B	832	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	8 (9%)
34	LHG	3	601	-	35,35,48	1.27	6 (17%)	38,41,54	1.12	2 (5%)
36	LMG	B	853	-	42,42,55	0.80	0	50,50,63	1.30	6 (12%)
31	CLA	5	308	-	50,54,73	1.46	9 (18%)	60,90,113	1.38	4 (6%)
37	OIE	c	521	-	42,45,45	1.40	6 (14%)	49,63,63	1.60	10 (20%)
31	CLA	7	304	-	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
31	CLA	6	309	5	62,66,73	1.31	10 (16%)	74,104,113	1.34	9 (12%)
31	CLA	3	313	4	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
32	8CT	B	844	-	40,41,41	4.72	25 (62%)	50,56,56	2.70	20 (40%)
30	CHL	8	302	7	68,72,74	1.85	19 (27%)	77,111,114	2.91	30 (38%)
31	CLA	e	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
30	CHL	5	307	-	51,55,74	2.23	18 (35%)	57,91,114	3.21	26 (45%)
31	CLA	9	310	34	45,49,73	1.51	10 (22%)	54,84,113	1.49	7 (12%)
31	CLA	7	310	34	42,45,73	1.53	9 (21%)	50,78,113	1.44	5 (10%)
32	8CT	B	843	-	40,41,41	4.74	24 (60%)	50,56,56	2.76	18 (36%)
32	8CT	B	848	-	40,41,41	4.67	24 (60%)	50,56,56	2.54	19 (38%)
42	NEX	d	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
30	CHL	e	606	-	55,59,74	2.15	19 (34%)	62,96,114	3.16	27 (43%)
31	CLA	L	203	17	67,71,73	1.26	10 (14%)	80,110,113	1.34	7 (8%)
31	CLA	A	822	-	53,57,73	1.40	9 (16%)	62,93,113	1.41	6 (9%)
31	CLA	A	829	9	69,73,73	1.24	10 (14%)	83,113,113	1.32	6 (7%)
32	8CT	L	209	-	40,41,41	4.65	23 (57%)	50,56,56	2.54	18 (36%)
31	CLA	7	311	6	56,60,73	1.38	10 (17%)	67,97,113	1.40	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	OUR	6	502	-	50,53,58	1.01	2 (4%)	58,72,77	1.82	15 (25%)
31	CLA	0	312	1	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
30	CHL	c	605	23	47,51,74	2.34	18 (38%)	52,86,114	3.35	24 (46%)
31	CLA	e	610	-	59,63,73	1.35	9 (15%)	71,101,113	1.35	10 (14%)
31	CLA	c	610	-	59,63,73	1.34	9 (15%)	71,101,113	1.35	7 (9%)
30	CHL	2	308	-	51,55,74	2.13	19 (37%)	57,91,114	3.18	24 (42%)
31	CLA	B	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
31	CLA	A	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	3 (3%)
31	CLA	O	203	-	41,46,73	1.67	9 (21%)	52,81,113	1.59	8 (15%)
32	8CT	A	849	-	40,41,41	4.57	23 (57%)	50,56,56	3.04	20 (40%)
30	CHL	1	302	-	68,72,74	1.85	18 (26%)	77,111,114	2.93	30 (38%)
30	CHL	8	313	7	60,64,74	1.98	18 (30%)	68,102,114	3.08	31 (45%)
31	CLA	i	610	-	59,63,73	1.35	8 (13%)	71,101,113	1.34	7 (9%)
31	CLA	A	852	10	69,73,73	1.23	10 (14%)	83,113,113	1.29	8 (9%)
37	OIE	g	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.68	10 (20%)
31	CLA	B	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	5 (6%)
32	8CT	0	401	-	40,41,41	4.66	24 (60%)	50,56,56	2.78	18 (36%)
40	SF4	B	802	-	0,12,12	-	-	-	-	-
30	CHL	i	606	28	55,59,74	2.21	19 (34%)	62,96,114	3.14	29 (46%)
30	CHL	c	607	-	51,55,74	2.26	19 (37%)	57,91,114	3.16	26 (45%)
31	CLA	B	823	-	56,60,73	1.38	10 (17%)	67,97,113	3.52	9 (13%)
31	CLA	9	304	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	5 (7%)
34	LHG	G	105	-	37,37,48	1.24	6 (16%)	40,43,54	1.14	4 (10%)
31	CLA	h	603	-	53,57,73	1.43	8 (15%)	62,93,113	1.43	4 (6%)
31	CLA	M	101	-	50,54,73	1.44	9 (18%)	60,90,113	1.42	4 (6%)
31	CLA	B	801	-	69,73,73	1.23	9 (13%)	83,113,113	1.37	8 (9%)
31	CLA	2	314	3	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
33	OUR	4	502	-	48,51,58	0.97	1 (2%)	56,70,77	1.68	14 (25%)
31	CLA	6	303	5	56,60,73	1.39	9 (16%)	67,97,113	1.40	7 (10%)
32	8CT	7	405	-	40,41,41	4.60	23 (57%)	50,56,56	2.69	19 (38%)
30	CHL	6	306	-	55,59,74	2.06	18 (32%)	62,96,114	3.21	28 (45%)
31	CLA	6	310	34	64,68,73	1.30	9 (14%)	77,107,113	1.32	6 (7%)
30	CHL	g	602	-	56,60,74	2.18	19 (33%)	63,97,114	3.06	26 (41%)
42	NEX	g	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	A	810	9	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	1	307	-	70,74,74	1.87	19 (27%)	80,114,114	2.84	27 (33%)
31	CLA	H	201	10	59,63,73	1.34	9 (15%)	71,101,113	1.37	6 (8%)
30	CHL	e	614	-	46,50,74	2.38	18 (39%)	51,85,114	3.38	27 (52%)
31	CLA	J	103	16	46,50,73	1.49	9 (19%)	55,85,113	1.47	5 (9%)
30	CHL	4	307	-	55,59,74	2.05	18 (32%)	62,96,114	3.22	30 (48%)
31	CLA	B	809	10	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
42	NEX	b	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	8	314	7	49,53,73	1.47	9 (18%)	59,89,113	1.44	6 (10%)
35	SQD	0	603	-	36,36,54	1.21	5 (13%)	44,44,65	1.48	6 (13%)
31	CLA	c	612	23	49,53,73	1.48	9 (18%)	59,89,113	1.47	4 (6%)
30	CHL	5	313	2	51,55,74	2.29	18 (35%)	57,91,114	3.20	26 (45%)
31	CLA	O	202	21	40,46,73	1.60	9 (22%)	48,80,113	1.51	7 (14%)
32	8CT	6	402	-	40,41,41	4.66	24 (60%)	50,56,56	3.43	21 (42%)
31	CLA	6	304	-	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
31	CLA	G	101	14	54,58,73	1.40	10 (18%)	65,95,113	1.43	6 (9%)
31	CLA	K	102	19	57,61,73	1.36	10 (17%)	68,98,113	1.40	8 (11%)
31	CLA	h	612	-	49,53,73	1.50	7 (14%)	59,89,113	1.43	5 (8%)
31	CLA	i	612	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
32	8CT	I	101	-	40,41,41	4.58	23 (57%)	50,56,56	2.76	15 (30%)
33	OUR	7	501	-	49,52,58	0.99	1 (2%)	57,71,77	2.07	16 (28%)
32	8CT	G	104	-	40,41,41	4.66	24 (60%)	50,56,56	3.08	19 (38%)
34	LHG	h	630	-	38,38,48	1.23	6 (15%)	41,44,54	0.99	2 (4%)
31	CLA	H	205	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
30	CHL	6	302	5	68,72,74	1.84	18 (26%)	77,111,114	2.93	31 (40%)
31	CLA	8	310	34	50,54,73	1.44	10 (20%)	60,90,113	1.38	4 (6%)
31	CLA	0	308	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	7 (9%)
30	CHL	1	313	2	66,70,74	1.91	18 (27%)	75,109,114	2.92	27 (36%)
34	LHG	H	203	-	30,30,48	1.32	6 (20%)	33,36,54	1.14	3 (9%)
30	CHL	h	605	22	47,51,74	2.37	18 (38%)	52,86,114	3.29	25 (48%)
31	CLA	6	311	5	52,56,73	1.44	10 (19%)	62,92,113	1.39	6 (9%)
36	LMG	J	102	-	29,29,55	0.98	1 (3%)	37,37,63	1.27	4 (10%)
30	CHL	g	608	-	47,51,74	2.31	18 (38%)	52,86,114	3.32	24 (46%)
30	CHL	9	301	8	51,55,74	2.14	19 (37%)	57,91,114	3.25	26 (45%)
31	CLA	3	318	4	50,54,73	1.44	10 (20%)	60,90,113	1.43	6 (10%)
34	LHG	A	844	-	48,48,48	1.07	5 (10%)	51,54,54	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	OUR	d	520	-	47,50,58	0.98	1 (2%)	55,69,77	1.75	13 (23%)
32	8CT	F	302	-	40,41,41	4.63	23 (57%)	50,56,56	2.71	18 (36%)
32	8CT	A	847	-	40,41,41	4.59	23 (57%)	50,56,56	2.97	18 (36%)
31	CLA	3	306	4	51,55,73	1.43	9 (17%)	61,91,113	1.42	6 (9%)
30	CHL	f	609	-	70,74,74	1.95	19 (27%)	80,114,114	2.74	27 (33%)
30	CHL	c	606	-	48,52,74	2.19	18 (37%)	53,87,114	3.30	23 (43%)
30	CHL	0	306	-	52,56,74	2.20	19 (36%)	58,92,114	3.28	24 (41%)
31	CLA	A	809	9	69,73,73	1.23	10 (14%)	83,113,113	1.34	8 (9%)
34	LHG	A	855	-	41,41,48	1.19	6 (14%)	44,47,54	1.03	3 (6%)
32	8CT	A	848	-	40,41,41	4.58	23 (57%)	50,56,56	2.70	22 (44%)
31	CLA	A	827	9	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
31	CLA	A	832	9	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
42	NEX	a	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
32	8CT	8	402	-	40,41,41	4.66	23 (57%)	50,56,56	2.66	19 (38%)
31	CLA	A	808	9	69,73,73	1.22	9 (13%)	83,113,113	1.31	6 (7%)
34	LHG	M	104	-	45,45,48	1.12	5 (11%)	48,51,54	0.96	3 (6%)
36	LMG	9	602	-	55,55,55	0.70	1 (1%)	63,63,63	1.39	9 (14%)
30	CHL	a	609	-	63,67,74	2.08	18 (28%)	71,105,114	2.93	27 (38%)
31	CLA	B	814	10	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
32	8CT	L	205	-	40,41,41	4.62	23 (57%)	50,56,56	2.95	19 (38%)
33	OUR	f	520	-	47,50,58	1.01	2 (4%)	55,69,77	1.92	16 (29%)
30	CHL	f	608	-	55,59,74	2.07	18 (32%)	62,96,114	3.23	29 (46%)
42	NEX	h	523	-	38,46,46	0.95	2 (5%)	50,70,70	4.90	19 (38%)
30	CHL	0	302	1	68,72,74	1.85	19 (27%)	77,111,114	2.91	29 (37%)
33	OUR	a	520	-	45,48,58	0.78	1 (2%)	54,67,77	1.67	16 (29%)
30	CHL	a	608	-	53,57,74	2.19	19 (35%)	59,93,114	3.18	26 (44%)
31	CLA	B	824	10	64,68,73	1.30	10 (15%)	77,107,113	1.30	6 (7%)
33	OUR	9	501	-	50,53,58	0.96	1 (2%)	58,72,77	1.69	17 (29%)
31	CLA	A	818	9	69,73,73	1.23	9 (13%)	83,113,113	1.35	9 (10%)
37	OIE	a	521	-	42,45,45	1.42	6 (14%)	49,63,63	1.57	10 (20%)
31	CLA	1	314	-	50,54,73	1.45	9 (18%)	60,90,113	1.44	6 (10%)
34	LHG	g	630	-	29,29,48	1.34	6 (20%)	32,35,54	1.15	3 (9%)
30	CHL	5	306	-	52,56,74	2.27	19 (36%)	58,92,114	3.12	25 (43%)
30	CHL	8	306	-	55,59,74	2.10	19 (34%)	62,96,114	3.19	29 (46%)
31	CLA	B	850	13	51,55,73	1.43	10 (19%)	61,91,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	6	301	5	65,69,74	1.92	18 (27%)	74,108,114	2.91	30 (40%)
30	CHL	d	605	25	47,51,74	2.37	18 (38%)	52,86,114	3.37	24 (46%)
32	8CT	1	402	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	20 (40%)
32	8CT	J	104	-	40,41,41	4.66	23 (57%)	50,56,56	3.42	22 (44%)
31	CLA	A	836	-	55,59,73	1.38	10 (18%)	66,96,113	1.43	9 (13%)
31	CLA	c	611	-	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
31	CLA	3	320	-	56,60,73	1.37	9 (16%)	67,97,113	1.49	7 (10%)
31	CLA	e	613	-	59,63,73	1.35	7 (11%)	70,100,113	1.37	7 (10%)
31	CLA	B	819	10	64,68,73	1.28	10 (15%)	77,107,113	1.33	9 (11%)
30	CHL	3	307	-	70,74,74	1.78	18 (25%)	80,114,114	2.85	31 (38%)
31	CLA	1	310	34	67,71,73	1.25	9 (13%)	80,110,113	1.30	4 (5%)
34	LHG	b	630	-	40,40,48	1.19	5 (12%)	43,46,54	0.98	2 (4%)
30	CHL	g	607	-	55,59,74	2.23	18 (32%)	62,96,114	3.14	28 (45%)
31	CLA	g	612	-	49,53,73	1.49	7 (14%)	59,89,113	1.45	4 (6%)
37	OIE	f	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.57	9 (18%)
33	OUR	g	520	-	50,53,58	0.93	1 (2%)	58,72,77	1.98	14 (24%)
33	OUR	2	502	-	48,51,58	0.98	1 (2%)	56,70,77	1.95	14 (25%)
31	CLA	h	611	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
40	SF4	C	102	18	0,12,12	-	-	-	-	-
31	CLA	8	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
31	CLA	H	204	-	51,55,73	1.43	10 (19%)	61,91,113	1.45	5 (8%)
30	CHL	a	606	-	55,59,74	2.19	19 (34%)	62,96,114	3.10	29 (46%)
33	OUR	6	501	-	49,52,58	0.99	1 (2%)	57,71,77	1.92	18 (31%)
34	LHG	4	601	31	31,31,48	1.31	5 (16%)	34,37,54	1.14	3 (8%)
31	CLA	4	314	7	49,53,73	1.46	9 (18%)	59,89,113	1.44	8 (13%)
31	CLA	A	839	9	69,73,73	1.24	10 (14%)	83,113,113	1.33	7 (8%)
30	CHL	f	607	-	51,55,74	2.28	18 (35%)	57,91,114	3.18	25 (43%)
37	OIE	b	521	-	42,45,45	1.44	6 (14%)	49,63,63	1.56	10 (20%)
30	CHL	d	608	-	55,59,74	2.16	18 (32%)	62,96,114	3.15	30 (48%)
31	CLA	i	613	-	55,59,73	1.41	7 (12%)	66,96,113	1.37	6 (9%)
37	OIE	d	522	-	42,45,45	1.48	6 (14%)	49,63,63	1.74	10 (20%)
31	CLA	6	317	5	69,73,73	1.24	9 (13%)	83,113,113	1.34	9 (10%)
30	CHL	d	602	-	68,72,74	1.89	20 (29%)	77,111,114	2.86	29 (37%)
31	CLA	1	304	-	56,60,73	1.38	9 (16%)	67,97,113	1.36	7 (10%)
31	CLA	G	102	14	49,53,73	1.47	8 (16%)	59,89,113	1.47	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	OUR	9	502	-	50,53,58	0.98	1 (2%)	58,72,77	1.69	16 (27%)
34	LHG	7	602	-	37,37,48	1.18	6 (16%)	40,43,54	1.04	2 (5%)
33	OUR	O	204	-	50,53,58	0.99	1 (2%)	58,72,77	1.92	16 (27%)
33	OUR	3	501	-	49,52,58	1.01	1 (2%)	57,71,77	2.10	17 (29%)
31	CLA	K	101	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	7 (9%)
33	OUR	c	520	-	50,53,58	1.00	2 (4%)	58,72,77	1.91	17 (29%)
31	CLA	9	312	8	60,64,73	1.33	10 (16%)	72,102,113	1.35	7 (9%)
31	CLA	A	823	9	55,59,73	1.41	10 (18%)	66,96,113	1.40	5 (7%)
31	CLA	d	612	25	49,53,73	1.50	9 (18%)	59,89,113	1.44	5 (8%)
31	CLA	A	813	9	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
31	CLA	a	610	-	59,63,73	1.36	8 (13%)	71,101,113	1.37	7 (9%)
31	CLA	1	309	2	59,63,73	1.34	10 (16%)	71,101,113	1.33	6 (8%)
31	CLA	6	318	-	50,54,73	1.45	9 (18%)	60,90,113	1.42	5 (8%)
33	OUR	2	501	-	49,52,58	1.00	1 (2%)	57,71,77	2.13	17 (29%)
31	CLA	7	316	6	52,56,73	1.41	10 (19%)	62,92,113	1.44	5 (8%)
33	OUR	8	501	-	49,52,58	0.96	1 (2%)	57,71,77	1.74	16 (28%)
31	CLA	0	313	1	50,54,73	1.45	8 (16%)	60,90,113	1.37	4 (6%)
31	CLA	5	303	2	63,67,73	1.30	9 (14%)	75,105,113	1.37	6 (8%)
31	CLA	A	834	9	50,54,73	1.42	9 (18%)	60,90,113	1.45	5 (8%)
31	CLA	1	308	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
31	CLA	c	613	-	59,63,73	1.34	9 (15%)	70,100,113	1.37	7 (10%)
30	CHL	f	614	26	46,50,74	2.34	18 (39%)	51,85,114	3.43	26 (50%)
31	CLA	A	833	9	69,73,73	1.23	10 (14%)	83,113,113	1.31	7 (8%)
31	CLA	A	811	9	69,73,73	1.23	9 (13%)	83,113,113	1.29	5 (6%)
34	LHG	e	630	31	42,42,48	1.18	6 (14%)	45,48,54	0.96	2 (4%)
34	LHG	c	630	-	39,39,48	1.20	5 (12%)	42,45,54	0.97	2 (4%)
30	CHL	h	602	-	68,72,74	2.00	19 (27%)	77,111,114	2.78	27 (35%)
30	CHL	2	307	-	55,59,74	2.02	18 (32%)	62,96,114	3.24	31 (50%)
31	CLA	4	304	-	64,68,73	1.28	9 (14%)	77,107,113	1.30	6 (7%)
31	CLA	B	836	10	64,68,73	1.29	10 (15%)	77,107,113	1.35	10 (12%)
34	LHG	6	603	-	30,30,48	1.33	6 (20%)	33,36,54	1.11	2 (6%)
31	CLA	3	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	7 (8%)
31	CLA	A	828	9	69,73,73	1.23	10 (14%)	83,113,113	1.29	7 (8%)
31	CLA	8	312	7	60,64,73	1.34	10 (16%)	72,102,113	1.35	6 (8%)
31	CLA	B	812	10	56,60,73	1.38	9 (16%)	67,97,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	i	630	-	29,29,48	1.34	6 (20%)	32,35,54	1.12	2 (6%)
30	CHL	d	606	-	55,59,74	2.18	19 (34%)	62,96,114	3.11	27 (43%)
31	CLA	A	815	9	69,73,73	1.24	9 (13%)	83,113,113	1.34	8 (9%)
31	CLA	c	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	6 (9%)
30	CHL	2	306	-	52,56,74	2.15	19 (36%)	58,92,114	3.26	27 (46%)
30	CHL	9	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.19	28 (45%)
30	CHL	4	308	-	51,55,74	2.18	18 (35%)	57,91,114	3.17	24 (42%)
30	CHL	7	307	-	55,59,74	2.09	19 (34%)	62,96,114	3.14	26 (41%)
30	CHL	7	305	-	52,56,74	2.12	19 (36%)	58,92,114	3.27	26 (44%)
32	8CT	M	102	-	40,41,41	4.61	23 (57%)	50,56,56	2.83	18 (36%)
31	CLA	O	201	-	45,49,73	1.50	9 (20%)	54,84,113	1.55	6 (11%)
31	CLA	A	803	9	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
31	CLA	7	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.26	6 (7%)
30	CHL	7	306	-	65,69,74	1.95	19 (29%)	73,107,114	2.91	30 (41%)
31	CLA	B	840	10	69,73,73	1.25	8 (11%)	83,113,113	1.32	5 (6%)
31	CLA	g	613	25	51,55,73	1.46	7 (13%)	61,91,113	1.47	6 (9%)
30	CHL	a	607	-	53,57,74	2.24	19 (35%)	57,92,114	3.19	25 (43%)
30	CHL	f	606	-	55,59,74	2.16	18 (32%)	62,96,114	3.22	30 (48%)
32	8CT	B	845	-	40,41,41	4.62	23 (57%)	50,56,56	3.23	22 (44%)
31	CLA	K	104	19	50,54,73	1.45	10 (20%)	60,90,113	1.46	6 (10%)
31	CLA	B	806	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	8 (9%)
32	8CT	A	854	-	40,41,41	4.64	23 (57%)	50,56,56	2.90	20 (40%)
31	CLA	8	309	-	64,68,73	1.29	10 (15%)	77,107,113	1.33	8 (10%)
30	CHL	i	614	-	46,50,74	2.39	19 (41%)	51,85,114	3.38	25 (49%)
42	NEX	i	523	-	38,46,46	0.97	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	B	834	10	65,69,73	1.29	10 (15%)	78,108,113	1.29	6 (7%)
36	LMG	O	207	-	39,39,55	0.82	1 (2%)	47,47,63	1.26	5 (10%)
31	CLA	K	105	19	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
31	CLA	g	604	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
30	CHL	d	609	-	70,74,74	1.95	18 (25%)	80,114,114	2.75	27 (33%)
31	CLA	A	837	9	65,69,73	1.27	10 (15%)	78,108,113	1.37	7 (8%)
31	CLA	A	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	9 (10%)
36	LMG	L	210	-	31,31,55	0.92	0	39,39,63	1.25	5 (12%)
31	CLA	9	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
30	CHL	h	606	-	55,59,74	2.17	18 (32%)	62,96,114	3.13	27 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	e	608	-	70,74,74	1.87	19 (27%)	80,114,114	2.80	27 (33%)
31	CLA	g	611	-	50,54,73	1.45	8 (16%)	60,90,113	1.42	6 (10%)
30	CHL	e	601	29	55,59,74	2.12	18 (32%)	62,96,114	3.24	30 (48%)
33	OUR	1	501	-	50,53,58	0.95	1 (2%)	58,72,77	1.71	16 (27%)
32	8CT	L	206	-	40,41,41	4.65	23 (57%)	50,56,56	2.78	19 (38%)
31	CLA	7	312	6	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)
37	OIE	i	521	-	42,45,45	1.46	6 (14%)	49,63,63	1.57	9 (18%)
31	CLA	h	613	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
31	CLA	A	820	9	59,63,73	1.33	10 (16%)	71,101,113	1.38	7 (9%)
30	CHL	5	305	-	50,54,74	2.24	19 (38%)	56,90,114	3.28	25 (44%)
31	CLA	A	821	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
31	CLA	B	833	10	59,63,73	1.35	10 (16%)	71,101,113	1.37	9 (12%)
30	CHL	4	306	-	52,56,74	2.15	19 (36%)	58,92,114	3.24	27 (46%)
31	CLA	A	841	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
31	CLA	B	811	10	69,73,73	1.23	10 (14%)	83,113,113	1.36	9 (10%)
30	CHL	b	602	-	68,72,74	1.90	18 (26%)	77,111,114	2.86	28 (36%)
31	CLA	b	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	6 (9%)
31	CLA	7	303	6	49,53,73	1.48	10 (20%)	59,89,113	1.45	5 (8%)
31	CLA	A	831	9	54,58,73	1.39	10 (18%)	65,95,113	1.46	7 (10%)
31	CLA	1	312	2	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
31	CLA	B	807	10	49,53,73	1.46	10 (20%)	59,89,113	1.53	9 (15%)
30	CHL	b	607	-	51,55,74	2.23	18 (35%)	57,91,114	3.16	26 (45%)
31	CLA	f	611	34	59,63,73	1.35	9 (15%)	71,101,113	1.36	6 (8%)
40	SF4	C	101	-	0,12,12	-	-	-	-	-
42	NEX	c	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.91	19 (38%)
31	CLA	0	304	-	56,60,73	1.39	9 (16%)	67,97,113	1.39	7 (10%)
42	NEX	e	523	-	38,46,46	1.06	2 (5%)	50,70,70	2.82	17 (34%)
30	CHL	i	601	28	51,55,74	2.29	19 (37%)	57,91,114	3.19	24 (42%)
32	8CT	2	402	-	40,41,41	4.66	24 (60%)	50,56,56	3.05	20 (40%)
30	CHL	2	319	7	65,69,74	1.91	18 (27%)	74,108,114	2.94	31 (41%)
31	CLA	5	311	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	7 (11%)
31	CLA	2	304	-	64,68,73	1.29	9 (14%)	77,107,113	1.31	6 (7%)
31	CLA	5	309	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	10 (12%)
33	OUR	5	502	-	50,53,58	0.96	1 (2%)	58,72,77	2.05	15 (25%)
37	OIE	f	522	-	42,45,45	1.44	6 (14%)	49,63,63	1.65	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	812	9	58,62,73	1.37	10 (17%)	69,99,113	1.34	7 (10%)
32	8CT	7	404	-	40,41,41	4.62	24 (60%)	50,56,56	3.57	23 (46%)
31	CLA	2	310	34	64,68,73	1.29	10 (15%)	77,107,113	1.30	6 (7%)
31	CLA	0	311	-	51,55,73	1.43	10 (19%)	61,91,113	1.49	6 (9%)
31	CLA	0	309	-	64,68,73	1.29	8 (12%)	77,107,113	1.33	7 (9%)
33	0UR	0	502	-	50,53,58	0.97	1 (2%)	58,72,77	1.89	16 (27%)
31	CLA	A	853	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
30	CHL	6	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.24	31 (50%)
31	CLA	2	309	3	64,68,73	1.29	10 (15%)	77,107,113	1.32	10 (12%)
37	0IE	a	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.58	8 (16%)
30	CHL	7	313	6	51,55,74	2.19	19 (37%)	57,91,114	3.22	24 (42%)
30	CHL	a	614	-	46,50,74	2.41	18 (39%)	51,85,114	3.42	25 (49%)
31	CLA	4	309	-	64,68,73	1.30	8 (12%)	77,107,113	1.25	8 (10%)
30	CHL	f	601	26	70,74,74	1.89	20 (28%)	80,114,114	2.80	27 (33%)
31	CLA	B	830	10	60,64,73	1.37	10 (16%)	72,102,113	1.47	10 (13%)
34	LHG	B	852	31	22,22,48	1.30	3 (13%)	25,28,54	1.07	1 (4%)
33	0UR	b	520	-	50,53,58	0.94	1 (2%)	58,72,77	1.74	15 (25%)
30	CHL	b	608	-	70,74,74	1.85	18 (25%)	80,114,114	2.81	30 (37%)
37	0IE	h	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.59	8 (16%)
31	CLA	g	603	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	4 (6%)
30	CHL	h	614	-	46,50,74	2.41	19 (41%)	51,85,114	3.37	25 (49%)
30	CHL	8	315	-	47,51,74	2.27	18 (38%)	52,86,114	3.31	24 (46%)
31	CLA	L	207	-	51,55,73	1.45	9 (17%)	61,91,113	1.39	6 (9%)
30	CHL	c	608	-	70,74,74	1.88	19 (27%)	80,114,114	2.80	26 (32%)
30	CHL	4	313	7	55,59,74	2.05	18 (32%)	62,96,114	3.22	31 (50%)
31	CLA	B	826	-	53,56,73	1.45	11 (20%)	61,89,113	2.06	11 (18%)
31	CLA	A	835	9	61,65,73	1.32	9 (14%)	73,103,113	1.39	7 (9%)
30	CHL	d	607	-	51,55,74	2.31	19 (37%)	57,91,114	3.19	24 (42%)
32	8CT	K	107	-	40,41,41	4.61	23 (57%)	50,56,56	3.28	24 (48%)
33	0UR	i	520	-	48,51,58	0.96	1 (2%)	56,70,77	1.83	13 (23%)
30	CHL	i	608	-	54,58,74	2.18	18 (33%)	59,94,114	3.15	26 (44%)
31	CLA	L	204	-	50,54,73	1.44	10 (20%)	60,90,113	1.40	5 (8%)
31	CLA	f	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
30	CHL	8	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.17	28 (45%)
31	CLA	B	820	-	60,64,73	1.34	9 (15%)	72,102,113	1.39	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	e	611	34	59,63,73	1.36	8 (13%)	71,101,113	1.33	6 (8%)
31	CLA	b	610	-	59,63,73	1.36	9 (15%)	71,101,113	1.31	9 (12%)
30	CHL	9	313	8	51,55,74	2.17	17 (33%)	57,91,114	3.27	28 (49%)
31	CLA	A	806	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
31	CLA	B	822	10	64,68,73	1.30	9 (14%)	77,107,113	1.35	6 (7%)
31	CLA	L	202	17	50,54,73	1.44	10 (20%)	60,90,113	1.45	5 (8%)
38	PQN	B	842	-	34,34,34	1.54	2 (5%)	42,45,45	1.11	2 (4%)
32	8CT	8	406	-	40,41,41	4.70	24 (60%)	50,56,56	2.49	18 (36%)
39	CL0	A	857	9	69,73,73	1.31	8 (11%)	83,113,113	1.40	11 (13%)
34	LHG	B	854	-	42,42,48	1.17	6 (14%)	45,48,54	0.97	2 (4%)
37	0IE	3	502	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
31	CLA	A	814	9	61,65,73	1.32	9 (14%)	73,103,113	1.36	5 (6%)
31	CLA	B	808	10	69,73,73	1.23	10 (14%)	83,113,113	1.35	8 (9%)
31	CLA	f	613	26	59,63,73	1.36	9 (15%)	70,100,113	1.36	6 (8%)
31	CLA	d	610	-	59,63,73	1.35	8 (13%)	71,101,113	1.34	10 (14%)
31	CLA	f	610	-	59,63,73	1.35	9 (15%)	71,101,113	1.34	7 (9%)
30	CHL	g	605	-	47,51,74	2.37	18 (38%)	52,86,114	3.34	24 (46%)
30	CHL	c	601	23	60,64,74	2.00	19 (31%)	68,102,114	3.07	30 (44%)
30	CHL	d	614	-	46,50,74	2.41	19 (41%)	51,85,114	3.44	25 (49%)
33	0UR	5	501	-	49,52,58	0.95	1 (2%)	57,71,77	1.75	12 (21%)
30	CHL	1	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.24	30 (48%)
31	CLA	a	613	22	59,63,73	1.37	8 (13%)	70,100,113	1.38	6 (8%)
30	CHL	7	301	6	67,71,74	1.91	18 (26%)	76,110,114	2.90	28 (36%)
31	CLA	B	818	10	63,67,73	1.30	10 (15%)	75,105,113	1.39	7 (9%)
30	CHL	f	602	-	68,72,74	1.88	19 (27%)	77,111,114	2.90	29 (37%)
36	LMG	2	602	-	36,36,55	0.89	1 (2%)	44,44,63	1.24	5 (11%)
32	8CT	9	401	-	40,41,41	4.66	23 (57%)	50,56,56	2.71	17 (34%)
31	CLA	d	611	-	50,54,73	1.46	7 (14%)	60,90,113	1.40	4 (6%)
31	CLA	b	612	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
32	8CT	4	402	-	40,41,41	4.64	24 (60%)	50,56,56	3.01	20 (40%)
34	LHG	9	601	31	45,45,48	1.13	6 (13%)	47,50,54	0.95	2 (4%)
31	CLA	A	838	9	60,64,73	1.34	10 (16%)	72,102,113	1.34	7 (9%)
41	DGD	B	849	-	57,57,67	0.88	2 (3%)	71,71,81	1.17	5 (7%)
31	CLA	4	310	34	64,68,73	1.29	10 (15%)	77,107,113	1.31	6 (7%)
34	LHG	1	601	31	48,48,48	1.09	5 (10%)	51,54,54	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	613	-	59,63,73	1.36	8 (13%)	70,100,113	1.37	6 (8%)
31	CLA	A	804	9	59,63,73	1.32	10 (16%)	71,101,113	1.41	6 (8%)
34	LHG	a	630	-	42,42,48	1.17	6 (14%)	45,48,54	0.96	2 (4%)
31	CLA	i	604	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	5 (7%)
30	CHL	i	607	-	51,55,74	2.29	18 (35%)	57,91,114	3.21	26 (45%)
31	CLA	6	320	-	55,59,73	1.40	9 (16%)	66,96,113	1.34	5 (7%)
32	8CT	B	847	-	40,41,41	4.61	23 (57%)	50,56,56	3.09	22 (44%)
30	CHL	a	605	22	47,51,74	2.35	18 (38%)	52,86,114	3.33	24 (46%)
30	CHL	b	614	-	46,50,74	2.37	19 (41%)	51,85,114	3.38	25 (49%)
33	OUR	1	502	-	50,53,58	0.99	2 (4%)	58,72,77	1.90	15 (25%)
30	CHL	6	305	-	47,51,74	2.15	19 (40%)	52,86,114	3.38	25 (48%)
31	CLA	7	309	-	63,67,73	1.29	10 (15%)	75,105,113	1.35	7 (9%)
31	CLA	A	807	9	57,61,73	1.36	10 (17%)	66,97,113	1.44	10 (15%)
30	CHL	e	607	-	51,55,74	2.25	19 (37%)	57,91,114	3.18	26 (45%)
32	8CT	A	850	-	40,41,41	4.55	23 (57%)	50,56,56	3.10	22 (44%)
31	CLA	8	303	7	50,54,73	1.46	10 (20%)	60,90,113	1.40	5 (8%)
32	8CT	B	846	-	40,41,41	4.76	24 (60%)	50,56,56	3.25	20 (40%)
31	CLA	2	312	3	64,68,73	1.28	9 (14%)	77,107,113	1.37	7 (9%)
30	CHL	h	609	-	51,55,74	2.28	19 (37%)	57,91,114	3.19	26 (45%)
31	CLA	e	603	29	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
31	CLA	c	603	-	56,60,73	1.39	9 (16%)	67,97,113	1.41	6 (8%)
34	LHG	7	601	31	29,29,48	1.35	5 (17%)	32,35,54	1.09	2 (6%)
37	OIE	b	522	-	42,45,45	1.46	6 (14%)	49,63,63	1.56	8 (16%)
30	CHL	g	614	-	46,50,74	2.42	19 (41%)	51,85,114	3.42	26 (50%)
31	CLA	9	311	8	56,60,73	1.40	10 (17%)	67,97,113	1.38	7 (10%)
37	OIE	h	521	-	42,45,45	1.46	6 (14%)	49,63,63	1.58	8 (16%)
34	LHG	5	601	31	36,36,48	1.24	5 (13%)	39,42,54	1.08	3 (7%)
34	LHG	8	601	31	43,43,48	1.16	5 (11%)	46,49,54	0.92	2 (4%)
30	CHL	e	605	29	47,51,74	2.30	18 (38%)	52,86,114	3.32	24 (46%)
30	CHL	4	319	2	58,62,74	2.02	19 (32%)	65,99,114	3.12	31 (47%)
31	CLA	B	837	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	8 (9%)
30	CHL	c	602	-	65,69,74	1.93	19 (29%)	74,108,114	2.93	30 (40%)
31	CLA	3	309	4	69,73,73	1.24	10 (14%)	83,113,113	1.31	9 (10%)
31	CLA	1	303	2	60,64,73	1.34	10 (16%)	72,102,113	1.41	6 (8%)
34	LHG	3	603	-	35,35,48	1.26	6 (17%)	38,41,54	1.05	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	813	10	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
30	CHL	i	605	28	47,51,74	2.35	18 (38%)	52,86,114	3.35	24 (46%)
34	LHG	K	106	-	42,42,48	1.15	6 (14%)	45,47,54	1.05	3 (6%)
30	CHL	1	306	-	52,56,74	2.17	18 (34%)	58,92,114	3.21	25 (43%)
30	CHL	b	601	24	70,74,74	1.95	18 (25%)	80,114,114	2.80	27 (33%)
30	CHL	8	305	-	51,55,74	2.16	18 (35%)	57,91,114	3.25	27 (47%)
31	CLA	7	318	6	64,68,73	1.28	9 (14%)	77,107,113	1.33	6 (7%)
30	CHL	6	308	5	64,68,74	1.96	18 (28%)	72,106,114	2.90	28 (38%)
31	CLA	4	311	-	52,56,73	1.42	10 (19%)	62,92,113	1.44	6 (9%)
31	CLA	A	830	9	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
42	NEX	f	523	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
31	CLA	B	810	10	66,70,73	1.26	10 (15%)	79,109,113	1.34	7 (8%)
37	OIE	7	502	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
31	CLA	B	828	-	64,68,73	1.28	10 (15%)	77,107,113	1.29	6 (7%)
31	CLA	B	838	10	51,55,73	1.41	10 (19%)	61,91,113	1.42	6 (9%)
31	CLA	0	303	1	66,70,73	1.27	9 (13%)	79,109,113	1.28	5 (6%)
30	CHL	c	614	-	46,50,74	2.35	19 (41%)	51,85,114	3.38	26 (50%)
31	CLA	5	310	34	49,53,73	1.47	9 (18%)	59,89,113	1.43	4 (6%)
31	CLA	L	201	9	62,66,73	1.30	10 (16%)	74,104,113	1.38	8 (10%)
31	CLA	2	303	3	60,64,73	1.35	10 (16%)	72,102,113	1.38	6 (8%)
34	LHG	7	603	-	38,38,48	1.22	6 (15%)	41,44,54	0.99	2 (4%)
30	CHL	5	301	2	56,60,74	2.15	19 (33%)	63,97,114	3.08	29 (46%)
31	CLA	A	824	9	59,63,73	1.34	10 (16%)	71,101,113	1.35	7 (9%)
38	PQN	A	842	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	5 (11%)
37	OIE	i	522	-	42,45,45	1.45	6 (14%)	49,63,63	1.61	9 (18%)
31	CLA	B	805	10	69,73,73	1.23	10 (14%)	83,113,113	1.27	7 (8%)
31	CLA	0	310	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	7 (12%)
31	CLA	4	303	7	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
30	CHL	b	609	-	58,62,74	2.12	18 (31%)	65,99,114	3.02	26 (40%)
37	OIE	e	522	-	42,45,45	1.42	6 (14%)	49,63,63	1.67	9 (18%)
31	CLA	f	612	26	49,53,73	1.47	10 (20%)	59,89,113	1.48	4 (6%)
31	CLA	e	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	5 (7%)
31	CLA	5	312	2	60,64,73	1.33	10 (16%)	72,102,113	1.37	5 (6%)
33	OUR	e	520	-	50,53,58	0.96	1 (2%)	58,72,77	1.99	17 (29%)
30	CHL	a	602	-	68,72,74	1.95	19 (27%)	77,111,114	2.80	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	9	306	-	52,56,74	2.15	18 (34%)	58,92,114	3.24	25 (43%)
30	CHL	6	315	5	47,51,74	2.21	17 (36%)	52,86,114	3.32	23 (44%)
31	CLA	3	310	-	66,70,73	1.28	9 (13%)	79,109,113	1.30	6 (7%)
30	CHL	i	602	-	65,69,74	1.98	18 (27%)	74,108,114	2.91	28 (37%)
31	CLA	H	202	27	51,55,73	1.43	10 (19%)	61,91,113	1.41	5 (8%)
31	CLA	a	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.47	4 (6%)
30	CHL	f	605	26	47,51,74	2.34	18 (38%)	52,86,114	3.33	24 (46%)
31	CLA	h	610	-	50,54,73	1.46	7 (14%)	60,90,113	1.43	6 (10%)
30	CHL	0	305	-	55,59,74	2.14	18 (32%)	62,96,114	3.13	29 (46%)
30	CHL	2	313	3	55,59,74	2.07	18 (32%)	62,96,114	3.22	28 (45%)
33	OUR	8	502	-	50,53,58	0.95	1 (2%)	58,72,77	1.86	15 (25%)
30	CHL	d	601	25	55,59,74	2.23	19 (34%)	62,96,114	3.10	28 (45%)
31	CLA	7	317	-	49,53,73	1.48	8 (16%)	59,89,113	1.48	5 (8%)
30	CHL	7	302	6	68,72,74	1.84	18 (26%)	77,111,114	2.93	30 (38%)
30	CHL	2	301	-	65,69,74	1.91	19 (29%)	74,108,114	2.93	28 (37%)
31	CLA	3	308	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	7 (8%)
31	CLA	3	312	4	59,63,73	1.33	10 (16%)	71,101,113	1.35	6 (8%)
31	CLA	5	304	-	56,60,73	1.38	8 (14%)	67,97,113	1.35	4 (5%)
31	CLA	A	817	9	65,69,73	1.26	10 (15%)	78,108,113	1.37	7 (8%)
30	CHL	8	301	7	65,69,74	1.95	19 (29%)	74,108,114	2.99	29 (39%)
30	CHL	g	601	25	56,60,74	2.24	18 (32%)	63,97,114	3.12	27 (42%)
30	CHL	g	609	25	50,54,74	2.34	20 (40%)	53,88,114	3.22	24 (45%)
30	CHL	h	607	-	50,54,74	2.36	19 (38%)	56,90,114	3.16	24 (42%)
37	OIE	c	522	-	42,45,45	1.43	6 (14%)	49,63,63	1.67	10 (20%)
31	CLA	7	315	6	51,55,73	1.44	10 (19%)	61,91,113	1.43	5 (8%)
31	CLA	b	611	-	64,68,73	1.30	8 (12%)	77,107,113	1.30	4 (5%)
31	CLA	A	805	9	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
31	CLA	A	819	9	69,73,73	1.25	10 (14%)	83,113,113	1.32	11 (13%)
32	8CT	3	402	-	40,41,41	4.64	23 (57%)	50,56,56	3.05	16 (32%)
31	CLA	6	312	5	60,64,73	1.32	10 (16%)	72,102,113	1.35	7 (9%)
31	CLA	B	835	-	49,53,73	1.47	10 (20%)	59,89,113	1.48	5 (8%)
31	CLA	G	103	14	50,54,73	1.45	9 (18%)	60,90,113	1.41	5 (8%)
31	CLA	d	603	25	59,63,73	1.35	8 (13%)	71,101,113	1.35	5 (7%)
30	CHL	4	302	7	57,61,74	2.02	18 (31%)	64,98,114	3.20	33 (51%)
31	CLA	2	311	3	52,56,73	1.42	9 (17%)	62,92,113	1.47	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	9	300	10	62,66,73	1.29	9 (14%)	74,104,113	1.39	7 (9%)
31	CLA	B	815	10	59,63,73	1.33	10 (16%)	71,101,113	1.37	8 (11%)
30	CHL	a	601	22	51,55,74	2.26	18 (35%)	57,91,114	3.22	25 (43%)
30	CHL	e	602	-	65,69,74	1.96	19 (29%)	74,108,114	2.92	27 (36%)
33	OUR	4	501	-	49,52,58	0.98	1 (2%)	57,71,77	2.10	19 (33%)
30	CHL	i	609	-	52,56,74	2.30	19 (36%)	58,92,114	3.14	25 (43%)
31	CLA	9	303	8	52,56,73	1.42	9 (17%)	62,92,113	1.44	6 (9%)
32	8CT	J	101	-	40,41,41	4.61	23 (57%)	50,56,56	2.81	17 (34%)
30	CHL	8	308	-	51,55,74	2.17	18 (35%)	57,91,114	3.19	24 (42%)
34	LHG	2	601	31	31,31,48	1.32	5 (16%)	34,37,54	1.12	3 (8%)
31	CLA	d	613	-	59,63,73	1.36	8 (13%)	70,100,113	1.34	5 (7%)
31	CLA	B	821	10	54,58,73	1.39	7 (12%)	65,95,113	1.47	7 (10%)
31	CLA	A	840	9	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)

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
31	CLA	3	311	4	-	3/17/93/115	-
31	CLA	f	603	-	-	8/27/103/115	-
37	OIE	e	521	-	-	2/33/72/72	0/2/2/2
30	CHL	5	302	2	-	21/39/115/117	-
36	LMG	A	856	-	-	14/31/51/70	0/1/1/1
30	CHL	h	601	22	-	10/19/95/117	-
31	CLA	8	311	7	-	8/17/93/115	-
31	CLA	a	611	-	-	8/30/106/115	-
32	8CT	A	846	-	-	4/29/63/63	0/2/2/2
31	CLA	g	610	-	-	6/17/93/115	-
31	CLA	5	314	2	-	11/17/93/115	-
30	CHL	h	608	-	-	7/17/93/117	-
31	CLA	6	314	-	-	3/15/91/115	-
31	CLA	B	816	10	-	9/33/109/115	-
33	OUR	h	520	-	-	9/42/81/86	0/2/2/2
31	CLA	d	604	-	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	a	603	-	-	4/25/101/115	-
34	LHG	d	630	-	-	17/40/40/53	-
30	CHL	2	305	-	-	0/14/90/117	-
31	CLA	4	312	7	-	9/25/101/115	-
32	8CT	B	851	-	-	13/29/63/63	0/2/2/2
37	0IE	g	521	-	-	3/33/72/72	0/2/2/2
31	CLA	a	604	-	-	3/21/97/115	-
31	CLA	9	302	-	-	15/39/115/115	-
30	CHL	4	305	-	-	0/14/90/117	-
30	CHL	3	302	4	-	22/37/113/117	-
31	CLA	B	841	34	-	8/39/115/115	-
31	CLA	0	321	1	-	11/15/91/115	-
31	CLA	i	611	-	-	8/15/91/115	-
31	CLA	O	206	-	-	11/23/99/115	-
34	LHG	A	845	31	-	17/31/31/53	-
30	CHL	g	606	-	-	7/23/99/117	-
31	CLA	B	831	10	-	11/21/97/115	-
30	CHL	c	609	-	-	21/41/117/117	-
31	CLA	h	604	-	-	6/17/93/115	-
31	CLA	F	301	-	-	8/15/91/115	-
30	CHL	2	302	3	-	29/39/115/117	-
31	CLA	B	803	-	-	15/39/115/115	-
31	CLA	i	603	-	-	6/17/93/115	-
30	CHL	0	301	1	-	11/25/101/117	-
31	CLA	A	826	-	-	11/39/115/115	-
32	8CT	O	205	-	-	6/29/63/63	0/2/2/2
30	CHL	b	606	-	-	3/23/99/117	-
36	LMG	J	105	-	-	15/41/61/70	0/1/1/1
31	CLA	A	816	-	-	5/15/91/115	-
31	CLA	9	309	-	-	7/33/109/115	-
34	LHG	f	630	31	-	27/44/44/53	-
34	LHG	6	601	31	-	17/41/41/53	-
31	CLA	B	829	-	-	9/39/115/115	-
31	CLA	B	817	10	-	21/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	3	305	-	-	8/23/99/117	-
31	CLA	3	303	-	-	8/27/103/115	-
37	0IE	d	521	-	-	2/33/72/72	0/2/2/2
36	LMG	L	211	-	-	15/32/52/70	0/1/1/1
31	CLA	b	603	24	-	7/27/103/115	-
30	CHL	e	609	-	-	13/35/111/117	-
31	CLA	1	311	2	-	6/24/100/115	-
30	CHL	6	313	5	-	7/25/101/117	-
32	8CT	B	804	-	-	14/29/63/63	0/2/2/2
36	LMG	3	602	-	-	16/31/51/70	0/1/1/1
34	LHG	0	601	-	-	33/53/53/53	-
31	CLA	B	827	-	-	12/39/115/115	-
32	8CT	3	403	-	-	9/29/63/63	0/2/2/2
31	CLA	A	843	34	-	8/24/100/115	-
33	0UR	0	501	-	-	3/42/81/86	0/2/2/2
32	8CT	7	402	-	-	15/29/63/63	0/2/2/2
31	CLA	B	832	-	-	9/39/115/115	-
34	LHG	3	601	-	-	16/40/40/53	-
36	LMG	B	853	-	-	22/37/57/70	0/1/1/1
31	CLA	5	308	-	-	7/17/93/115	-
37	0IE	c	521	-	-	2/33/72/72	0/2/2/2
31	CLA	7	304	-	-	7/27/103/115	-
31	CLA	6	309	5	-	2/31/107/115	-
31	CLA	3	313	4	-	7/15/91/115	-
32	8CT	B	844	-	-	11/29/63/63	0/2/2/2
30	CHL	8	302	7	-	19/39/115/117	-
31	CLA	e	612	-	-	4/15/91/115	-
30	CHL	5	307	-	-	8/19/95/117	-
31	CLA	9	310	34	-	5/10/86/115	-
31	CLA	7	310	34	-	2/4/76/115	-
32	8CT	B	843	-	-	14/29/63/63	0/2/2/2
32	8CT	B	848	-	-	9/29/63/63	0/2/2/2
42	NEX	d	523	-	-	5/27/83/83	0/3/3/3
30	CHL	e	606	-	-	8/23/99/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	L	203	17	-	21/37/113/115	-
31	CLA	A	822	-	-	5/20/96/115	-
31	CLA	A	829	9	-	13/39/115/115	-
32	8CT	L	209	-	-	9/29/63/63	0/2/2/2
31	CLA	7	311	6	-	8/24/100/115	-
33	0UR	6	502	-	-	11/42/81/86	0/2/2/2
31	CLA	0	312	1	-	14/39/115/115	-
30	CHL	c	605	23	-	2/14/90/117	-
31	CLA	e	610	-	-	4/27/103/115	-
31	CLA	c	610	-	-	4/27/103/115	-
30	CHL	2	308	-	-	4/19/95/117	-
31	CLA	B	839	-	-	12/39/115/115	-
31	CLA	A	802	-	-	5/39/115/115	-
31	CLA	O	203	-	-	0/4/80/115	-
32	8CT	A	849	-	-	8/29/63/63	0/2/2/2
30	CHL	1	302	-	-	16/39/115/117	-
30	CHL	8	313	7	-	9/29/105/117	-
31	CLA	i	610	-	-	4/27/103/115	-
31	CLA	A	852	10	-	13/39/115/115	-
37	0IE	g	522	-	-	1/33/72/72	0/2/2/2
31	CLA	B	825	-	-	5/39/115/115	-
32	8CT	0	401	-	-	5/29/63/63	0/2/2/2
40	SF4	B	802	-	-	-	0/6/5/5
30	CHL	i	606	28	-	7/23/99/117	-
30	CHL	c	607	-	-	8/19/95/117	-
31	CLA	B	823	-	-	10/24/100/115	-
31	CLA	9	304	-	-	0/23/99/115	-
34	LHG	G	105	-	-	27/42/42/53	-
31	CLA	h	603	-	-	5/20/96/115	-
31	CLA	M	101	-	-	3/17/93/115	-
31	CLA	B	801	-	-	11/39/115/115	-
31	CLA	2	314	3	-	5/15/91/115	-
33	0UR	4	502	-	-	14/40/79/86	0/2/2/2
31	CLA	6	303	5	-	7/24/100/115	-
32	8CT	7	405	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	6	306	-	-	6/23/99/117	-
31	CLA	6	310	34	-	11/33/109/115	-
30	CHL	g	602	-	-	13/25/101/117	-
42	NEX	g	523	-	-	5/27/83/83	0/3/3/3
31	CLA	A	810	9	-	3/39/115/115	-
30	CHL	1	307	-	-	23/41/117/117	-
31	CLA	H	201	10	-	8/27/103/115	-
30	CHL	e	614	-	-	5/12/88/117	-
31	CLA	J	103	16	-	2/12/88/115	-
30	CHL	4	307	-	-	8/23/99/117	-
31	CLA	B	809	10	-	12/39/115/115	-
42	NEX	b	523	-	-	5/27/83/83	0/3/3/3
31	CLA	8	314	7	-	10/15/91/115	-
35	SQD	0	603	-	-	17/31/51/69	0/1/1/1
31	CLA	c	612	23	-	4/15/91/115	-
30	CHL	5	313	2	-	8/19/95/117	-
31	CLA	O	202	21	-	1/6/78/115	-
32	8CT	6	402	-	-	8/29/63/63	0/2/2/2
31	CLA	6	304	-	-	5/17/93/115	-
31	CLA	G	101	14	-	7/21/97/115	-
31	CLA	K	102	19	-	13/25/101/115	-
31	CLA	h	612	-	-	7/15/91/115	-
31	CLA	i	612	-	-	3/15/91/115	-
32	8CT	I	101	-	-	9/29/63/63	0/2/2/2
33	0UR	7	501	-	-	9/41/80/86	0/2/2/2
32	8CT	G	104	-	-	13/29/63/63	0/2/2/2
34	LHG	h	630	-	-	18/43/43/53	-
31	CLA	H	205	-	-	9/23/99/115	-
30	CHL	6	302	5	-	20/39/115/117	-
31	CLA	8	310	34	-	4/17/93/115	-
31	CLA	0	308	-	-	12/33/109/115	-
30	CHL	1	313	2	-	19/37/113/117	-
34	LHG	H	203	-	-	13/35/35/53	-
30	CHL	h	605	22	-	2/14/90/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	6	311	5	-	4/19/95/115	-
36	LMG	J	102	-	-	12/24/44/70	0/1/1/1
30	CHL	g	608	-	-	5/14/90/117	-
30	CHL	9	301	8	-	6/19/95/117	-
31	CLA	3	318	4	-	0/17/93/115	-
34	LHG	A	844	-	-	20/53/53/53	-
33	OUR	d	520	-	-	10/39/78/86	0/2/2/2
32	8CT	F	302	-	-	9/29/63/63	0/2/2/2
32	8CT	A	847	-	-	10/29/63/63	0/2/2/2
31	CLA	3	306	4	-	5/18/94/115	-
30	CHL	f	609	-	-	19/41/117/117	-
30	CHL	c	606	-	-	3/15/91/117	-
30	CHL	0	306	-	-	9/20/96/117	-
31	CLA	A	809	9	-	11/39/115/115	-
34	LHG	A	855	-	-	27/46/46/53	-
32	8CT	A	848	-	-	7/29/63/63	0/2/2/2
31	CLA	A	827	9	-	4/39/115/115	-
31	CLA	A	832	9	-	14/39/115/115	-
42	NEX	a	523	-	-	5/27/83/83	0/3/3/3
32	8CT	8	402	-	-	10/29/63/63	0/2/2/2
31	CLA	A	808	9	-	20/39/115/115	-
34	LHG	M	104	-	-	19/50/50/53	-
36	LMG	9	602	-	-	31/50/70/70	0/1/1/1
30	CHL	a	609	-	-	10/33/109/117	-
31	CLA	B	814	10	-	16/39/115/115	-
32	8CT	L	205	-	-	6/29/63/63	0/2/2/2
33	OUR	f	520	-	-	9/39/78/86	0/2/2/2
30	CHL	f	608	-	-	8/23/99/117	-
42	NEX	h	523	-	-	5/27/83/83	0/3/3/3
30	CHL	0	302	1	-	14/39/115/117	-
33	OUR	a	520	-	-	7/36/75/86	0/2/2/2
30	CHL	a	608	-	-	9/21/97/117	-
31	CLA	B	824	10	-	10/33/109/115	-
33	OUR	9	501	-	-	3/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	818	9	-	12/39/115/115	-
37	0IE	a	521	-	-	2/33/72/72	0/2/2/2
31	CLA	1	314	-	-	5/17/93/115	-
34	LHG	g	630	-	-	15/34/34/53	-
30	CHL	5	306	-	-	9/20/96/117	-
30	CHL	8	306	-	-	16/23/99/117	-
31	CLA	B	850	13	-	5/18/94/115	-
30	CHL	6	301	5	-	15/35/111/117	-
30	CHL	d	605	25	-	4/14/90/117	-
32	8CT	1	402	-	-	8/29/63/63	0/2/2/2
32	8CT	J	104	-	-	9/29/63/63	0/2/2/2
31	CLA	A	836	-	-	9/23/99/115	-
31	CLA	c	611	-	-	4/17/93/115	-
31	CLA	3	320	-	-	7/24/100/115	-
31	CLA	e	613	-	-	11/27/103/115	-
31	CLA	B	819	10	-	15/33/109/115	-
30	CHL	3	307	-	-	27/41/117/117	-
31	CLA	1	310	34	-	11/37/113/115	-
34	LHG	b	630	-	-	31/45/45/53	-
30	CHL	g	607	-	-	9/23/99/117	-
31	CLA	g	612	-	-	7/15/91/115	-
37	0IE	f	521	-	-	2/33/72/72	0/2/2/2
33	0UR	g	520	-	-	9/42/81/86	0/2/2/2
33	0UR	2	502	-	-	11/40/79/86	0/2/2/2
31	CLA	h	611	-	-	4/10/86/115	-
40	SF4	C	102	18	-	-	0/6/5/5
31	CLA	8	304	-	-	11/39/115/115	-
31	CLA	H	204	-	-	3/18/94/115	-
30	CHL	a	606	-	-	7/23/99/117	-
33	0UR	6	501	-	-	11/41/80/86	0/2/2/2
34	LHG	4	601	31	-	12/36/36/53	-
31	CLA	4	314	7	-	5/15/91/115	-
31	CLA	A	839	9	-	13/39/115/115	-
30	CHL	f	607	-	-	5/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OIE	b	521	-	-	2/33/72/72	0/2/2/2
30	CHL	d	608	-	-	5/23/99/117	-
31	CLA	i	613	-	-	5/23/99/115	-
37	OIE	d	522	-	-	4/33/72/72	0/2/2/2
31	CLA	6	317	5	-	17/39/115/115	-
30	CHL	d	602	-	-	18/39/115/117	-
31	CLA	1	304	-	-	4/24/100/115	-
31	CLA	G	102	14	-	4/15/91/115	-
33	OUR	9	502	-	-	8/42/81/86	0/2/2/2
34	LHG	7	602	-	-	21/42/42/53	-
33	OUR	O	204	-	-	5/42/81/86	0/2/2/2
33	OUR	3	501	-	-	9/41/80/86	0/2/2/2
31	CLA	K	101	-	-	12/33/109/115	-
33	OUR	c	520	-	-	9/42/81/86	0/2/2/2
31	CLA	9	312	8	-	6/29/105/115	-
31	CLA	A	823	9	-	4/23/99/115	-
31	CLA	d	612	25	-	7/15/91/115	-
31	CLA	A	813	9	-	8/39/115/115	-
31	CLA	a	610	-	-	5/27/103/115	-
31	CLA	1	309	2	-	6/27/103/115	-
31	CLA	6	318	-	-	14/17/93/115	-
33	OUR	2	501	-	-	7/41/80/86	0/2/2/2
31	CLA	7	316	6	-	3/15/91/115	-
33	OUR	8	501	-	-	7/41/80/86	0/2/2/2
31	CLA	0	313	1	-	11/17/93/115	-
31	CLA	5	303	2	-	11/32/108/115	-
31	CLA	A	834	9	-	2/17/93/115	-
31	CLA	1	308	-	-	7/15/91/115	-
31	CLA	c	613	-	-	8/27/103/115	-
30	CHL	f	614	26	-	8/12/88/117	-
31	CLA	A	833	9	-	12/39/115/115	-
31	CLA	A	811	9	-	13/39/115/115	-
34	LHG	e	630	31	-	22/47/47/53	-
34	LHG	c	630	-	-	20/44/44/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	h	602	-	-	17/39/115/117	-
30	CHL	2	307	-	-	5/23/99/117	-
31	CLA	4	304	-	-	8/33/109/115	-
31	CLA	B	836	10	-	11/33/109/115	-
34	LHG	6	603	-	-	13/35/35/53	-
31	CLA	3	304	-	-	6/39/115/115	-
31	CLA	A	828	9	-	19/39/115/115	-
31	CLA	8	312	7	-	10/29/105/115	-
31	CLA	B	812	10	-	6/24/100/115	-
34	LHG	i	630	-	-	9/34/34/53	-
30	CHL	d	606	-	-	8/23/99/117	-
31	CLA	A	815	9	-	11/39/115/115	-
31	CLA	c	604	-	-	5/21/97/115	-
30	CHL	2	306	-	-	5/20/96/117	-
30	CHL	9	305	-	-	8/23/99/117	-
30	CHL	4	308	-	-	5/19/95/117	-
30	CHL	7	307	-	-	6/23/99/117	-
30	CHL	7	305	-	-	9/20/96/117	-
32	8CT	M	102	-	-	7/29/63/63	0/2/2/2
31	CLA	O	201	-	-	7/10/86/115	-
31	CLA	A	803	9	-	10/39/115/115	-
31	CLA	7	308	-	-	16/39/115/115	-
30	CHL	7	306	-	-	17/35/111/117	-
31	CLA	B	840	10	-	11/39/115/115	-
31	CLA	g	613	25	-	5/18/94/115	-
30	CHL	a	607	-	-	7/19/95/117	-
30	CHL	f	606	-	-	8/23/99/117	-
32	8CT	B	845	-	-	10/29/63/63	0/2/2/2
31	CLA	K	104	19	-	6/17/93/115	-
31	CLA	B	806	-	-	11/39/115/115	-
32	8CT	A	854	-	-	10/29/63/63	0/2/2/2
31	CLA	8	309	-	-	7/33/109/115	-
30	CHL	i	614	-	-	6/12/88/117	-
42	NEX	i	523	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	834	10	-	16/35/111/115	-
36	LMG	O	207	-	-	10/34/54/70	0/1/1/1
31	CLA	K	105	19	-	12/21/97/115	-
31	CLA	g	604	-	-	7/15/91/115	-
30	CHL	d	609	-	-	18/41/117/117	-
31	CLA	A	837	9	-	12/35/111/115	-
31	CLA	A	825	-	-	8/39/115/115	-
36	LMG	L	210	-	-	12/26/46/70	0/1/1/1
31	CLA	9	308	-	-	13/39/115/115	-
30	CHL	h	606	-	-	6/23/99/117	-
30	CHL	e	608	-	-	18/41/117/117	-
31	CLA	g	611	-	-	2/17/93/115	-
30	CHL	e	601	29	-	5/23/99/117	-
33	OUR	1	501	-	-	3/42/81/86	0/2/2/2
32	8CT	L	206	-	-	8/29/63/63	0/2/2/2
31	CLA	7	312	6	-	13/27/103/115	-
37	OIE	i	521	-	-	4/33/72/72	0/2/2/2
31	CLA	h	613	-	-	5/15/91/115	-
31	CLA	A	820	9	-	9/27/103/115	-
30	CHL	5	305	-	-	7/17/93/117	-
31	CLA	A	821	-	-	10/39/115/115	-
31	CLA	B	833	10	-	9/27/103/115	-
30	CHL	4	306	-	-	6/20/96/117	-
31	CLA	A	841	-	-	11/39/115/115	-
31	CLA	B	811	10	-	10/39/115/115	-
30	CHL	b	602	-	-	21/39/115/117	-
31	CLA	b	604	-	-	7/21/97/115	-
31	CLA	7	303	6	-	7/15/91/115	-
31	CLA	A	831	9	-	4/21/97/115	-
31	CLA	1	312	2	-	14/39/115/115	-
31	CLA	B	807	10	-	5/15/91/115	-
30	CHL	b	607	-	-	5/19/95/117	-
31	CLA	f	611	34	-	5/27/103/115	-
42	NEX	c	523	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	e	523	-	-	4/27/83/83	0/3/3/3
31	CLA	0	304	-	-	5/24/100/115	-
40	SF4	C	101	-	-	-	0/6/5/5
30	CHL	i	601	28	-	5/19/95/117	-
32	8CT	2	402	-	-	12/29/63/63	0/2/2/2
30	CHL	2	319	7	-	18/35/111/117	-
31	CLA	5	311	-	-	9/15/91/115	-
31	CLA	2	304	-	-	11/33/109/115	-
31	CLA	5	309	-	-	9/33/109/115	-
33	0UR	5	502	-	-	10/42/81/86	0/2/2/2
37	0IE	f	522	-	-	0/33/72/72	0/2/2/2
31	CLA	A	812	9	-	3/26/102/115	-
32	8CT	7	404	-	-	7/29/63/63	0/2/2/2
31	CLA	2	310	34	-	12/33/109/115	-
31	CLA	0	311	-	-	9/18/94/115	-
31	CLA	0	309	-	-	11/33/109/115	-
33	0UR	0	502	-	-	12/42/81/86	0/2/2/2
31	CLA	A	853	-	-	15/39/115/115	-
30	CHL	6	307	-	-	12/23/99/117	-
31	CLA	2	309	3	-	3/33/109/115	-
37	0IE	a	522	-	-	0/33/72/72	0/2/2/2
30	CHL	7	313	6	-	7/19/95/117	-
30	CHL	a	614	-	-	0/12/88/117	-
31	CLA	4	309	-	-	5/33/109/115	-
30	CHL	f	601	26	-	14/41/117/117	-
31	CLA	B	830	10	-	8/29/105/115	-
34	LHG	B	852	31	-	17/26/26/53	-
33	0UR	b	520	-	-	11/42/81/86	0/2/2/2
30	CHL	b	608	-	-	20/41/117/117	-
37	0IE	h	522	-	-	0/33/72/72	0/2/2/2
31	CLA	g	603	-	-	5/23/99/115	-
30	CHL	h	614	-	-	5/12/88/117	-
30	CHL	8	315	-	-	4/14/90/117	-
31	CLA	L	207	-	-	7/18/94/115	-
30	CHL	c	608	-	-	20/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	4	313	7	-	5/23/99/117	-
31	CLA	B	826	-	-	2/23/87/115	-
31	CLA	A	835	9	-	14/30/106/115	-
30	CHL	d	607	-	-	9/19/95/117	-
32	8CT	K	107	-	-	12/29/63/63	0/2/2/2
33	0UR	i	520	-	-	5/40/79/86	0/2/2/2
30	CHL	i	608	-	-	9/22/98/117	-
31	CLA	L	204	-	-	7/17/93/115	-
31	CLA	f	604	-	-	7/21/97/115	-
30	CHL	8	307	-	-	11/23/99/117	-
31	CLA	B	820	-	-	10/29/105/115	-
31	CLA	e	611	34	-	7/27/103/115	-
31	CLA	b	610	-	-	4/27/103/115	-
30	CHL	9	313	8	-	9/19/95/117	-
31	CLA	A	806	-	-	19/39/115/115	-
31	CLA	B	822	10	-	13/33/109/115	-
31	CLA	L	202	17	-	6/17/93/115	-
38	PQN	B	842	-	-	6/23/43/43	0/2/2/2
32	8CT	8	406	-	-	12/29/63/63	0/2/2/2
39	CL0	A	857	9	-	10/39/115/115	-
34	LHG	B	854	-	-	17/47/47/53	-
37	0IE	3	502	-	-	2/33/72/72	0/2/2/2
31	CLA	A	814	9	-	10/30/106/115	-
31	CLA	B	808	10	-	11/39/115/115	-
31	CLA	f	613	26	-	9/27/103/115	-
31	CLA	d	610	-	-	5/27/103/115	-
31	CLA	f	610	-	-	4/27/103/115	-
30	CHL	g	605	-	-	2/14/90/117	-
30	CHL	c	601	23	-	11/29/105/117	-
30	CHL	d	614	-	-	1/12/88/117	-
33	0UR	5	501	-	-	11/41/80/86	0/2/2/2
30	CHL	1	305	-	-	9/23/99/117	-
31	CLA	a	613	22	-	12/27/103/115	-
30	CHL	7	301	6	-	14/38/114/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	818	10	-	9/32/108/115	-
30	CHL	f	602	-	-	21/39/115/117	-
36	LMG	2	602	-	-	13/31/51/70	0/1/1/1
32	8CT	9	401	-	-	11/29/63/63	0/2/2/2
31	CLA	d	611	-	-	7/17/93/115	-
31	CLA	b	612	-	-	3/15/91/115	-
32	8CT	4	402	-	-	8/29/63/63	0/2/2/2
34	LHG	9	601	31	-	19/48/48/53	-
31	CLA	A	838	9	-	5/29/105/115	-
41	DGD	B	849	-	-	28/45/85/95	0/2/2/2
31	CLA	4	310	34	-	13/33/109/115	-
34	LHG	1	601	31	-	21/53/53/53	-
31	CLA	b	613	-	-	8/27/103/115	-
31	CLA	A	804	9	-	8/27/103/115	-
34	LHG	a	630	-	-	29/47/47/53	-
31	CLA	i	604	-	-	8/21/97/115	-
30	CHL	i	607	-	-	11/19/95/117	-
31	CLA	6	320	-	-	11/23/99/115	-
32	8CT	B	847	-	-	9/29/63/63	0/2/2/2
30	CHL	a	605	22	-	2/14/90/117	-
30	CHL	b	614	-	-	4/12/88/117	-
33	OUR	1	502	-	-	10/42/81/86	0/2/2/2
30	CHL	6	305	-	-	0/14/90/117	-
31	CLA	7	309	-	-	11/32/108/115	-
31	CLA	A	807	9	-	5/23/99/115	-
30	CHL	e	607	-	-	4/19/95/117	-
32	8CT	A	850	-	-	10/29/63/63	0/2/2/2
31	CLA	8	303	7	-	7/17/93/115	-
32	8CT	B	846	-	-	12/29/63/63	0/2/2/2
31	CLA	2	312	3	-	12/33/109/115	-
30	CHL	h	609	-	-	3/19/95/117	-
31	CLA	e	603	29	-	6/30/106/115	-
31	CLA	c	603	-	-	5/24/100/115	-
34	LHG	7	601	31	-	10/34/34/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OIE	b	522	-	-	3/33/72/72	0/2/2/2
30	CHL	g	614	-	-	2/12/88/117	-
31	CLA	9	311	8	-	6/24/100/115	-
37	OIE	h	521	-	-	4/33/72/72	0/2/2/2
34	LHG	5	601	31	-	13/41/41/53	-
34	LHG	8	601	31	-	30/48/48/53	-
30	CHL	e	605	29	-	4/14/90/117	-
30	CHL	4	319	2	-	9/27/103/117	-
31	CLA	B	837	-	-	4/39/115/115	-
30	CHL	c	602	-	-	20/35/111/117	-
31	CLA	3	309	4	-	12/39/115/115	-
31	CLA	1	303	2	-	14/29/105/115	-
34	LHG	3	603	-	-	18/40/40/53	-
31	CLA	B	813	10	-	9/27/103/115	-
30	CHL	i	605	28	-	2/14/90/117	-
34	LHG	K	106	-	-	23/46/46/53	-
30	CHL	1	306	-	-	7/20/96/117	-
30	CHL	b	601	24	-	19/41/117/117	-
30	CHL	8	305	-	-	8/19/95/117	-
31	CLA	7	318	6	-	9/33/109/115	-
30	CHL	6	308	5	-	10/34/110/117	-
31	CLA	4	311	-	-	6/19/95/115	-
31	CLA	A	830	9	-	14/39/115/115	-
42	NEX	f	523	-	-	5/27/83/83	0/3/3/3
31	CLA	B	810	10	-	8/36/112/115	-
37	OIE	7	502	-	-	2/33/72/72	0/2/2/2
31	CLA	B	828	-	-	8/33/109/115	-
31	CLA	B	838	10	-	3/18/94/115	-
31	CLA	0	303	1	-	11/36/112/115	-
30	CHL	c	614	-	-	7/12/88/117	-
31	CLA	5	310	34	-	6/15/91/115	-
31	CLA	L	201	9	-	8/31/107/115	-
31	CLA	2	303	3	-	10/29/105/115	-
34	LHG	7	603	-	-	21/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	5	301	2	-	12/25/101/117	-
31	CLA	A	824	9	-	10/27/103/115	-
38	PQN	A	842	-	-	7/23/43/43	0/2/2/2
37	OIE	i	522	-	-	1/33/72/72	0/2/2/2
31	CLA	B	805	10	-	11/39/115/115	-
31	CLA	0	310	-	-	3/10/86/115	-
31	CLA	4	303	7	-	4/15/91/115	-
30	CHL	b	609	-	-	11/27/103/117	-
37	OIE	e	522	-	-	0/33/72/72	0/2/2/2
31	CLA	f	612	26	-	6/15/91/115	-
31	CLA	e	604	-	-	7/21/97/115	-
31	CLA	5	312	2	-	11/29/105/115	-
33	OUR	e	520	-	-	10/42/81/86	0/2/2/2
30	CHL	a	602	-	-	20/39/115/117	-
30	CHL	9	306	-	-	6/20/96/117	-
30	CHL	6	315	5	-	4/14/90/117	-
31	CLA	3	310	-	-	15/36/112/115	-
30	CHL	i	602	-	-	22/35/111/117	-
31	CLA	H	202	27	-	8/18/94/115	-
31	CLA	a	612	-	-	2/15/91/115	-
30	CHL	f	605	26	-	2/14/90/117	-
31	CLA	h	610	-	-	5/17/93/115	-
30	CHL	0	305	-	-	7/23/99/117	-
30	CHL	2	313	3	-	5/23/99/117	-
33	OUR	8	502	-	-	8/42/81/86	0/2/2/2
30	CHL	d	601	25	-	3/23/99/117	-
31	CLA	7	317	-	-	13/15/91/115	-
30	CHL	7	302	6	-	18/39/115/117	-
30	CHL	2	301	-	-	10/35/111/117	-
31	CLA	3	308	-	-	18/39/115/115	-
31	CLA	3	312	4	-	8/27/103/115	-
31	CLA	5	304	-	-	12/24/100/115	-
31	CLA	A	817	9	-	16/35/111/115	-
30	CHL	8	301	7	-	6/35/111/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	g	601	25	-	6/25/101/117	-
30	CHL	g	609	25	-	3/14/90/117	-
30	CHL	h	607	-	-	3/17/93/117	-
37	OIE	c	522	-	-	12/33/72/72	0/2/2/2
31	CLA	7	315	6	-	9/18/94/115	-
31	CLA	b	611	-	-	4/33/109/115	-
31	CLA	A	805	9	-	14/39/115/115	-
31	CLA	A	819	9	-	18/39/115/115	-
32	8CT	3	402	-	-	9/29/63/63	0/2/2/2
31	CLA	6	312	5	-	10/29/105/115	-
31	CLA	B	835	-	-	0/15/91/115	-
31	CLA	G	103	14	-	5/17/93/115	-
31	CLA	d	603	25	-	9/27/103/115	-
30	CHL	4	302	7	-	15/26/102/117	-
31	CLA	2	311	3	-	5/19/95/115	-
31	CLA	9	300	10	-	13/31/107/115	-
31	CLA	B	815	10	-	4/27/103/115	-
30	CHL	a	601	22	-	6/19/95/117	-
30	CHL	e	602	-	-	19/35/111/117	-
33	OUR	4	501	-	-	9/41/80/86	0/2/2/2
30	CHL	i	609	-	-	3/20/96/117	-
31	CLA	9	303	8	-	4/19/95/115	-
32	8CT	J	101	-	-	11/29/63/63	0/2/2/2
30	CHL	8	308	-	-	2/19/95/117	-
34	LHG	2	601	31	-	18/36/36/53	-
31	CLA	d	613	-	-	8/27/103/115	-
31	CLA	B	821	10	-	2/21/97/115	-
31	CLA	A	840	9	-	17/39/115/115	-

The worst 5 of 5939 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	844	8CT	C02-C03	14.48	1.59	1.34
32	J	104	8CT	C02-C03	14.47	1.59	1.34
32	8	406	8CT	C02-C03	14.39	1.59	1.34
32	B	848	8CT	C02-C03	14.35	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	846	8CT	C02-C03	14.35	1.59	1.34

The worst 5 of 6775 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	823	CLA	O2A-CGA-O1A	-19.76	73.72	123.59
42	a	523	NEX	O24-C25-C24	19.75	128.22	113.38
42	i	523	NEX	O24-C25-C24	19.71	128.19	113.38
42	c	523	NEX	O24-C25-C24	19.70	128.18	113.38
42	f	523	NEX	O24-C25-C24	19.70	128.18	113.38

There are no chirality outliers.

5 of 4828 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	301	CHL	C1A-C2A-CAA-CBA
30	0	301	CHL	C3A-C2A-CAA-CBA
30	0	301	CHL	C1C-C2C-CMC-OMC
30	0	301	CHL	C3C-C2C-CMC-OMC
30	0	301	CHL	C2-C3-C5-C6

There are no ring outliers.

411 monomers are involved in 1119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	311	CLA	1	0
30	5	302	CHL	4	0
36	A	856	LMG	3	0
30	h	601	CHL	1	0
31	8	311	CLA	2	0
31	a	611	CLA	1	0
31	g	610	CLA	5	0
31	5	314	CLA	1	0
30	h	608	CHL	5	0
31	B	816	CLA	1	0
33	h	520	OUR	1	0
31	d	604	CLA	1	0
31	a	603	CLA	2	0
34	d	630	LHG	5	0
31	4	312	CLA	2	0
31	a	604	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	9	302	CLA	5	0
30	4	305	CHL	3	0
30	3	302	CHL	3	0
31	B	841	CLA	4	0
31	0	321	CLA	4	0
31	i	611	CLA	4	0
31	O	206	CLA	3	0
34	A	845	LHG	3	0
30	g	606	CHL	2	0
31	B	831	CLA	3	0
30	c	609	CHL	5	0
31	h	604	CLA	2	0
31	F	301	CLA	3	0
30	2	302	CHL	2	0
31	B	803	CLA	7	0
31	i	603	CLA	2	0
30	0	301	CHL	6	0
31	A	826	CLA	3	0
30	b	606	CHL	2	0
36	J	105	LMG	2	0
31	A	816	CLA	1	0
31	9	309	CLA	4	0
34	f	630	LHG	5	0
34	6	601	LHG	5	0
31	B	829	CLA	4	0
31	B	817	CLA	8	0
30	3	305	CHL	1	0
31	3	303	CLA	2	0
36	L	211	LMG	3	0
31	b	603	CLA	2	0
30	e	609	CHL	6	0
31	1	311	CLA	2	0
30	6	313	CHL	2	0
32	B	804	8CT	1	0
36	3	602	LMG	1	0
34	0	601	LHG	4	0
31	B	827	CLA	3	0
31	A	843	CLA	4	0
33	0	501	0UR	1	0
31	B	832	CLA	3	0
34	3	601	LHG	1	0
36	B	853	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	308	CLA	2	0
31	7	304	CLA	4	0
31	6	309	CLA	1	0
31	3	313	CLA	1	0
30	8	302	CHL	1	0
31	e	612	CLA	3	0
30	5	307	CHL	2	0
42	d	523	NEX	10	0
30	e	606	CHL	1	0
31	L	203	CLA	5	0
31	A	822	CLA	3	0
31	A	829	CLA	4	0
33	6	502	OUR	1	0
31	0	312	CLA	8	0
30	c	605	CHL	1	0
31	e	610	CLA	2	0
31	c	610	CLA	2	0
30	2	308	CHL	1	0
31	B	839	CLA	5	0
31	A	802	CLA	2	0
31	O	203	CLA	4	0
30	1	302	CHL	4	0
30	8	313	CHL	3	0
31	i	610	CLA	2	0
31	A	852	CLA	3	0
31	B	825	CLA	5	0
40	B	802	SF4	1	0
30	i	606	CHL	21	0
30	c	607	CHL	3	0
31	B	823	CLA	4	0
34	G	105	LHG	2	0
31	B	801	CLA	8	0
31	2	314	CLA	1	0
31	6	303	CLA	1	0
30	6	306	CHL	2	0
31	6	310	CLA	2	0
30	g	602	CHL	2	0
42	g	523	NEX	8	0
31	A	810	CLA	3	0
30	1	307	CHL	5	0
31	H	201	CLA	3	0
31	J	103	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	4	307	CHL	2	0
31	B	809	CLA	9	0
42	b	523	NEX	3	0
35	0	603	SQD	2	0
30	5	313	CHL	1	0
31	6	304	CLA	2	0
31	K	102	CLA	3	0
31	h	612	CLA	3	0
31	i	612	CLA	1	0
33	7	501	0UR	2	0
34	h	630	LHG	4	0
30	6	302	CHL	3	0
31	0	308	CLA	1	0
30	1	313	CHL	3	0
31	6	311	CLA	1	0
36	J	102	LMG	1	0
30	g	608	CHL	3	0
30	9	301	CHL	1	0
31	3	318	CLA	3	0
34	A	844	LHG	4	0
33	d	520	0UR	1	0
31	3	306	CLA	2	0
30	f	609	CHL	6	0
30	c	606	CHL	3	0
30	0	306	CHL	4	0
31	A	809	CLA	8	0
34	A	855	LHG	1	0
31	A	827	CLA	2	0
31	A	832	CLA	6	0
42	a	523	NEX	7	0
32	8	402	8CT	1	0
31	A	808	CLA	7	0
34	M	104	LHG	4	0
36	9	602	LMG	4	0
30	a	609	CHL	5	0
31	B	814	CLA	5	0
32	L	205	8CT	1	0
30	f	608	CHL	3	0
42	h	523	NEX	15	0
30	0	302	CHL	3	0
33	a	520	0UR	2	0
30	a	608	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	824	CLA	5	0
33	9	501	0UR	2	0
31	A	818	CLA	10	0
34	g	630	LHG	3	0
30	5	306	CHL	1	0
30	8	306	CHL	1	0
31	B	850	CLA	1	0
30	6	301	CHL	5	0
30	d	605	CHL	2	0
32	J	104	8CT	1	0
31	A	836	CLA	1	0
31	3	320	CLA	1	0
31	e	613	CLA	3	0
31	B	819	CLA	5	0
30	3	307	CHL	5	0
34	b	630	LHG	2	0
30	g	607	CHL	2	0
31	g	612	CLA	1	0
31	h	611	CLA	1	0
31	8	304	CLA	2	0
31	H	204	CLA	1	0
30	a	606	CHL	4	0
31	4	314	CLA	1	0
31	A	839	CLA	5	0
30	f	607	CHL	2	0
37	b	521	0IE	1	0
30	d	608	CHL	5	0
31	i	613	CLA	1	0
31	6	317	CLA	4	0
30	d	602	CHL	2	0
31	1	304	CLA	1	0
31	G	102	CLA	1	0
33	9	502	0UR	1	0
34	7	602	LHG	2	0
33	O	204	0UR	1	0
33	3	501	0UR	1	0
31	K	101	CLA	1	0
33	c	520	0UR	1	0
31	9	312	CLA	2	0
31	A	823	CLA	1	0
31	d	612	CLA	4	0
31	A	813	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	610	CLA	4	0
31	1	309	CLA	2	0
31	6	318	CLA	1	0
33	2	501	0UR	3	0
33	8	501	0UR	3	0
31	0	313	CLA	2	0
31	5	303	CLA	3	0
31	1	308	CLA	2	0
31	c	613	CLA	4	0
30	f	614	CHL	2	0
31	A	811	CLA	6	0
34	e	630	LHG	5	0
34	c	630	LHG	5	0
30	h	602	CHL	5	0
30	2	307	CHL	3	0
31	4	304	CLA	1	0
31	B	836	CLA	3	0
31	3	304	CLA	3	0
31	A	828	CLA	8	0
31	8	312	CLA	1	0
31	B	812	CLA	1	0
34	i	630	LHG	4	0
30	d	606	CHL	8	0
31	A	815	CLA	3	0
31	c	604	CLA	1	0
30	2	306	CHL	1	0
30	9	305	CHL	1	0
30	4	308	CHL	3	0
30	7	307	CHL	7	0
30	7	305	CHL	3	0
31	A	803	CLA	5	0
31	7	308	CLA	7	0
30	7	306	CHL	4	0
31	B	840	CLA	1	0
31	g	613	CLA	3	0
30	a	607	CHL	3	0
30	f	606	CHL	5	0
31	K	104	CLA	3	0
31	B	806	CLA	8	0
31	8	309	CLA	1	0
30	i	614	CHL	2	0
42	i	523	NEX	35	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	834	CLA	7	0
36	O	207	LMG	1	0
31	K	105	CLA	2	0
31	g	604	CLA	6	0
30	d	609	CHL	4	0
31	A	837	CLA	3	0
31	A	825	CLA	6	0
31	9	308	CLA	5	0
30	h	606	CHL	5	0
30	e	608	CHL	7	0
31	g	611	CLA	1	0
30	e	601	CHL	2	0
33	1	501	OUR	1	0
31	7	312	CLA	5	0
37	i	521	OIE	4	0
31	h	613	CLA	3	0
31	A	820	CLA	1	0
30	5	305	CHL	4	0
31	A	821	CLA	9	0
31	B	833	CLA	6	0
30	4	306	CHL	2	0
31	A	841	CLA	5	0
31	B	811	CLA	7	0
30	b	602	CHL	7	0
31	b	604	CLA	3	0
31	A	831	CLA	3	0
31	1	312	CLA	9	0
30	b	607	CHL	3	0
31	f	611	CLA	3	0
42	c	523	NEX	5	0
31	0	304	CLA	1	0
42	e	523	NEX	3	0
30	2	319	CHL	6	0
31	5	311	CLA	2	0
31	2	304	CLA	1	0
31	5	309	CLA	4	0
32	7	404	8CT	1	0
31	2	310	CLA	3	0
31	0	311	CLA	2	0
31	0	309	CLA	3	0
31	A	853	CLA	5	0
30	6	307	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	309	CLA	2	0
31	4	309	CLA	5	0
30	f	601	CHL	6	0
31	B	830	CLA	6	0
34	B	852	LHG	2	0
33	b	520	0UR	3	0
30	b	608	CHL	5	0
37	h	522	0IE	1	0
31	g	603	CLA	3	0
30	h	614	CHL	1	0
30	8	315	CHL	3	0
30	c	608	CHL	7	0
30	4	313	CHL	3	0
31	B	826	CLA	3	0
30	d	607	CHL	3	0
33	i	520	0UR	2	0
30	i	608	CHL	2	0
31	L	204	CLA	3	0
31	f	604	CLA	4	0
30	8	307	CHL	4	0
31	B	820	CLA	4	0
31	b	610	CLA	3	0
31	A	806	CLA	3	0
31	B	822	CLA	4	0
31	L	202	CLA	2	0
38	B	842	PQN	1	0
39	A	857	CL0	7	0
34	B	854	LHG	2	0
31	A	814	CLA	2	0
31	B	808	CLA	6	0
31	f	613	CLA	4	0
31	d	610	CLA	1	0
31	f	610	CLA	1	0
30	g	605	CHL	3	0
30	c	601	CHL	8	0
33	5	501	0UR	4	0
30	1	305	CHL	4	0
31	a	613	CLA	1	0
30	7	301	CHL	3	0
31	B	818	CLA	12	0
30	f	602	CHL	1	0
31	d	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	612	CLA	1	0
32	4	402	8CT	1	0
34	9	601	LHG	5	0
31	A	838	CLA	3	0
41	B	849	DGD	3	0
31	4	310	CLA	3	0
34	1	601	LHG	6	0
31	b	613	CLA	2	0
31	A	804	CLA	1	0
34	a	630	LHG	4	0
31	i	604	CLA	28	0
30	i	607	CHL	1	0
32	B	847	8CT	1	0
30	a	605	CHL	2	0
30	b	614	CHL	2	0
30	6	305	CHL	2	0
31	7	309	CLA	4	0
31	A	807	CLA	2	0
30	e	607	CHL	2	0
32	A	850	8CT	1	0
31	2	312	CLA	2	0
30	h	609	CHL	1	0
31	e	603	CLA	5	0
31	c	603	CLA	2	0
34	7	601	LHG	2	0
37	b	522	0IE	1	0
31	9	311	CLA	2	0
37	h	521	0IE	1	0
34	5	601	LHG	1	0
30	e	605	CHL	2	0
30	4	319	CHL	8	0
31	B	837	CLA	1	0
30	c	602	CHL	2	0
31	3	309	CLA	4	0
31	1	303	CLA	2	0
34	3	603	LHG	3	0
31	B	813	CLA	3	0
30	i	605	CHL	1	0
34	K	106	LHG	4	0
30	1	306	CHL	3	0
30	b	601	CHL	4	0
30	8	305	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	318	CLA	1	0
30	6	308	CHL	4	0
31	4	311	CLA	4	0
31	A	830	CLA	5	0
42	f	523	NEX	26	0
31	B	810	CLA	5	0
31	B	828	CLA	3	0
31	B	838	CLA	3	0
31	0	303	CLA	4	0
30	c	614	CHL	3	0
31	L	201	CLA	2	0
30	5	301	CHL	5	0
31	A	824	CLA	1	0
38	A	842	PQN	5	0
31	B	805	CLA	4	0
31	0	310	CLA	2	0
30	b	609	CHL	3	0
31	e	604	CLA	1	0
31	5	312	CLA	2	0
30	a	602	CHL	3	0
30	9	306	CHL	2	0
30	6	315	CHL	1	0
30	i	602	CHL	3	0
31	h	610	CLA	2	0
30	0	305	CHL	4	0
30	2	313	CHL	6	0
30	d	601	CHL	2	0
31	7	317	CLA	5	0
30	7	302	CHL	3	0
30	2	301	CHL	2	0
31	3	308	CLA	4	0
31	3	312	CLA	2	0
31	5	304	CLA	2	0
31	A	817	CLA	1	0
30	8	301	CHL	4	0
30	g	601	CHL	1	0
30	g	609	CHL	2	0
30	h	607	CHL	1	0
37	c	522	OIE	1	0
31	7	315	CLA	2	0
31	A	805	CLA	2	0
31	A	819	CLA	4	0

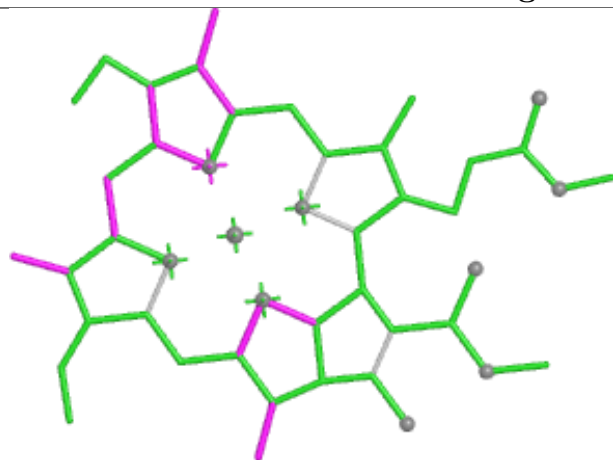
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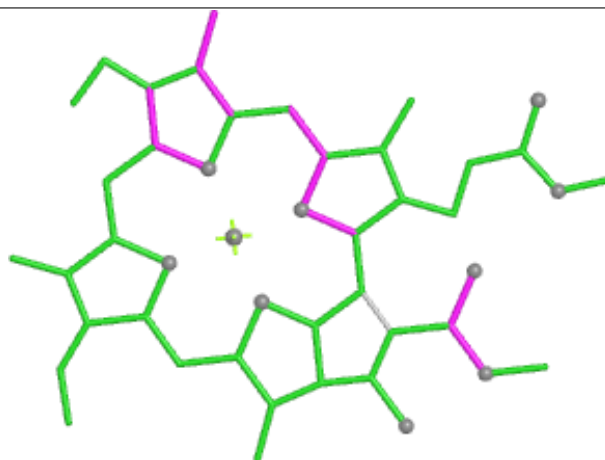
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	3	402	8CT	1	0
31	6	312	CLA	3	0
31	B	835	CLA	1	0
31	G	103	CLA	1	0
31	d	603	CLA	3	0
30	4	302	CHL	2	0
31	9	300	CLA	1	0
30	a	601	CHL	1	0
30	e	602	CHL	5	0
33	4	501	0UR	3	0
30	i	609	CHL	4	0
31	9	303	CLA	1	0
30	8	308	CHL	3	0
34	2	601	LHG	3	0
31	d	613	CLA	2	0
31	B	821	CLA	1	0
31	A	840	CLA	7	0

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

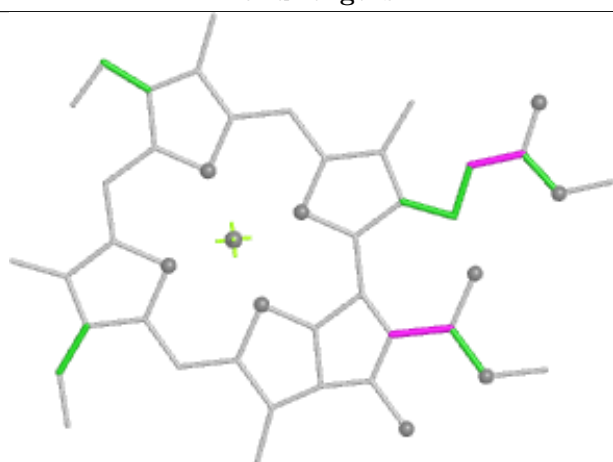
Ligand CLA 3 311



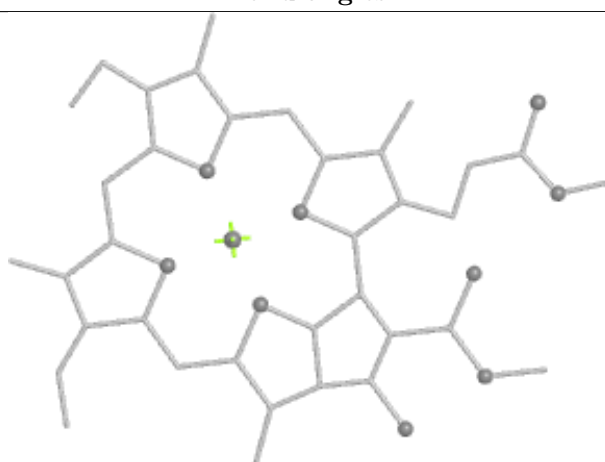
Bond lengths



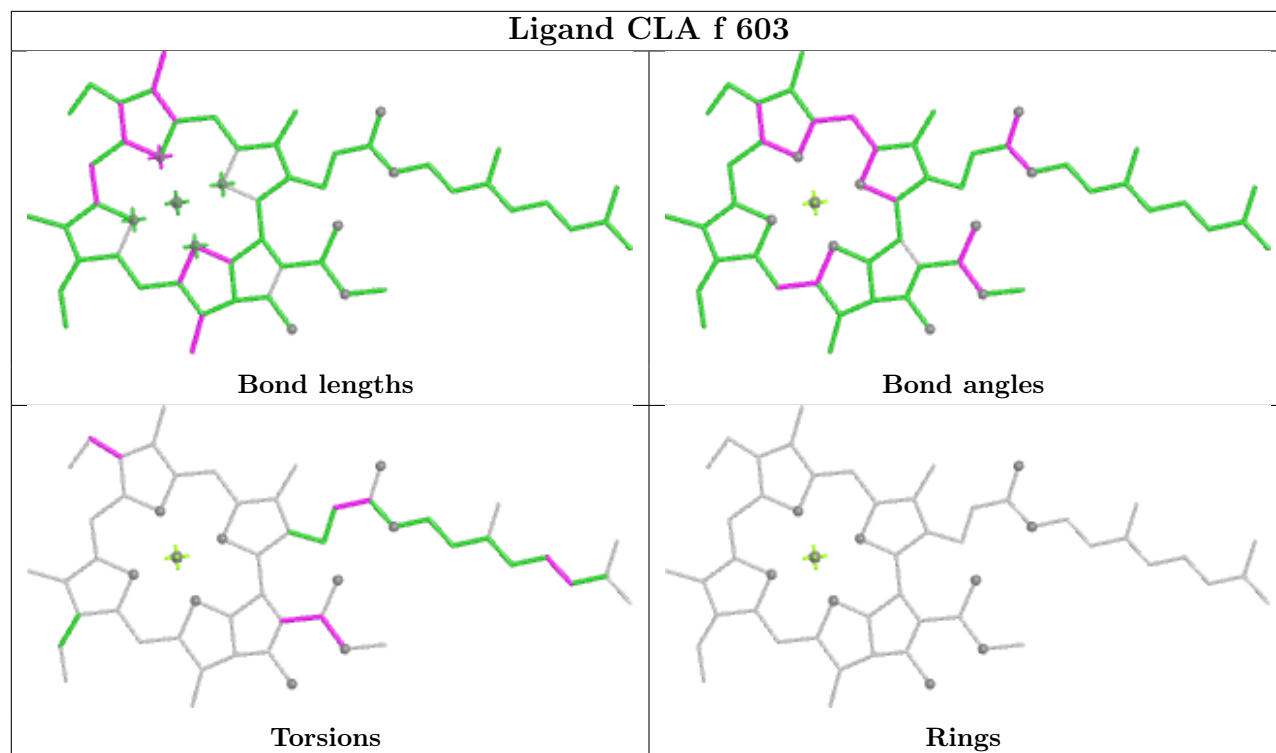
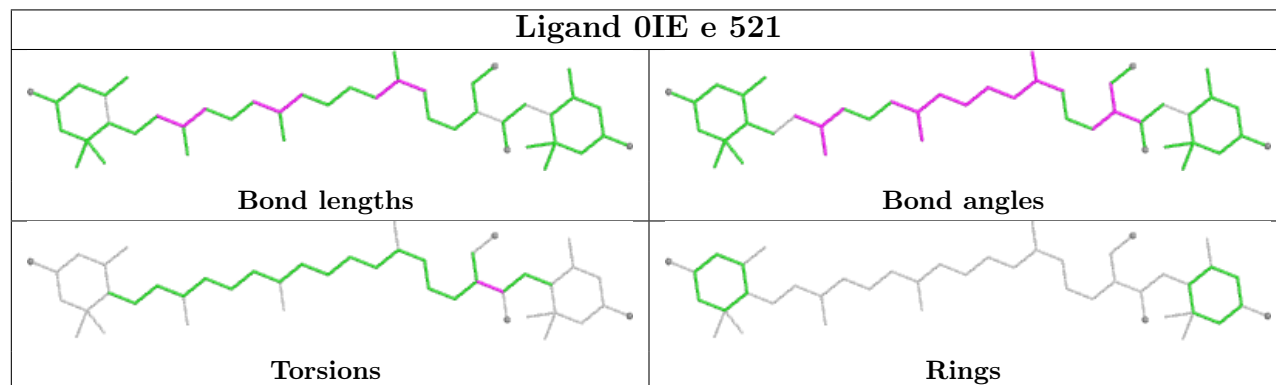
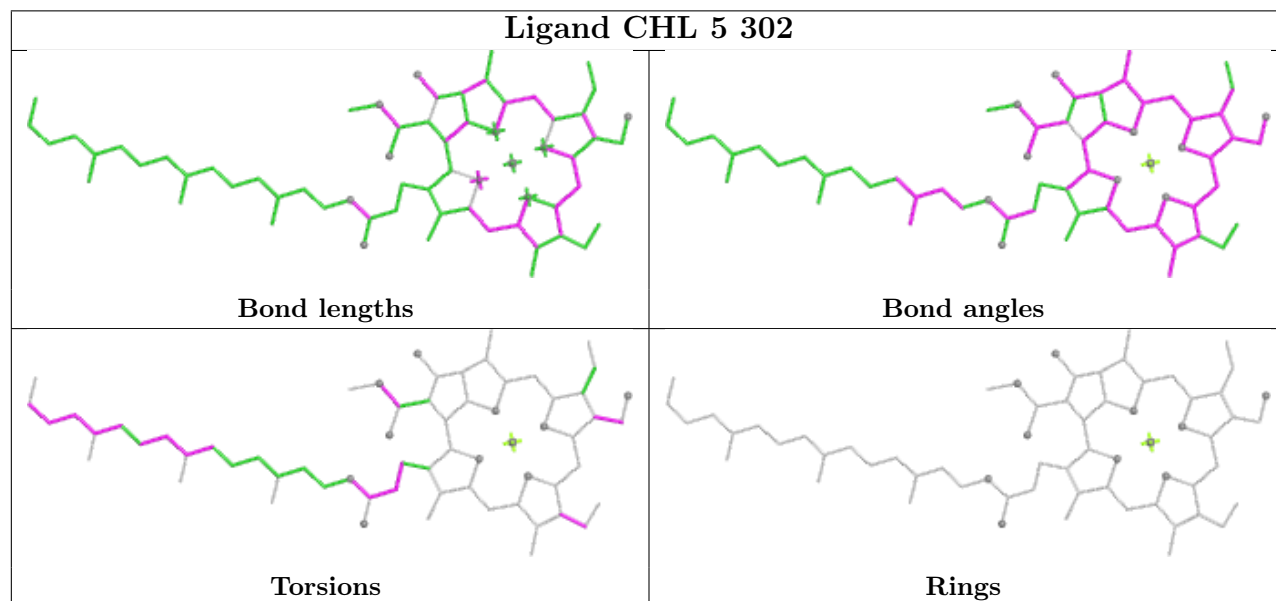
Bond angles

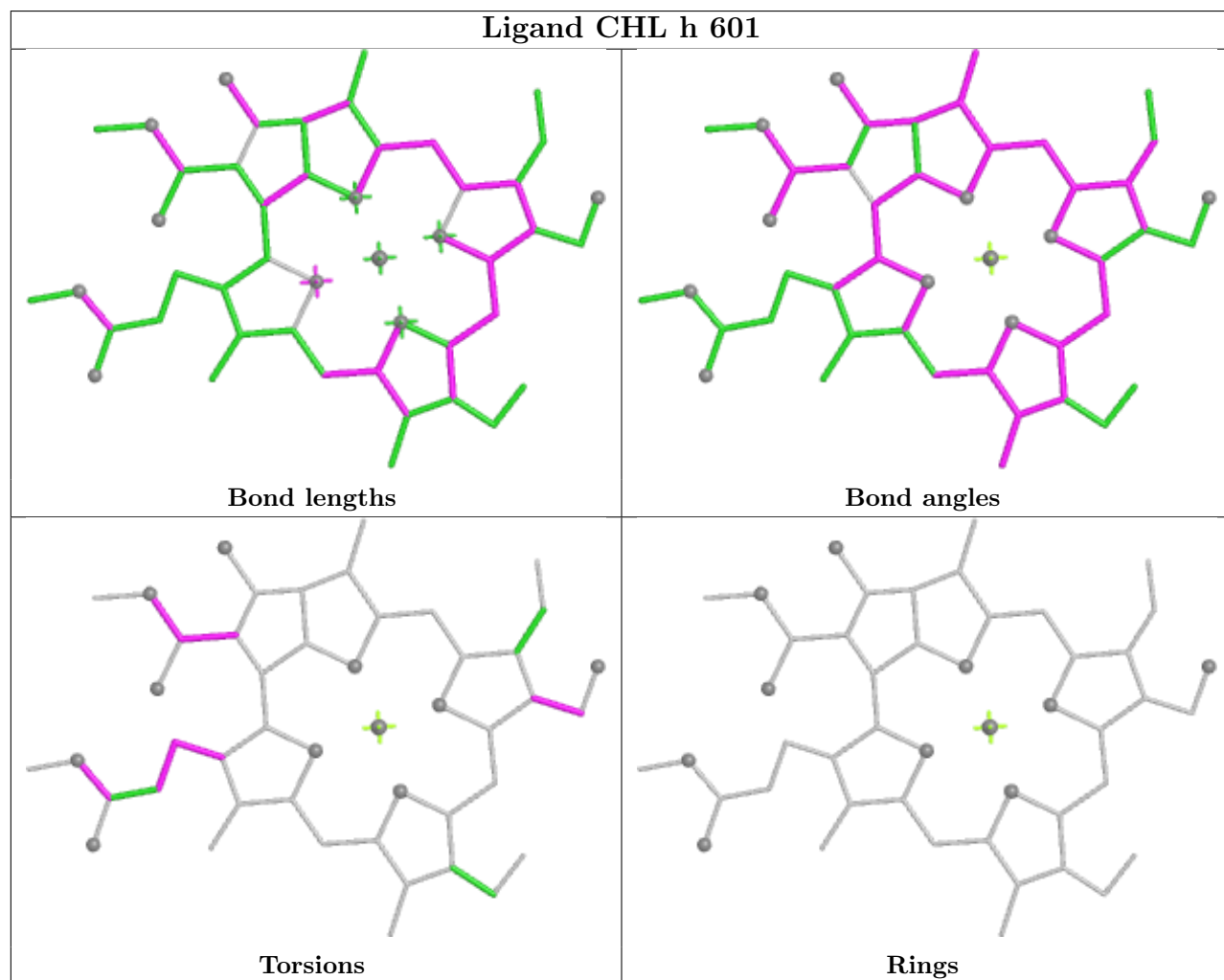
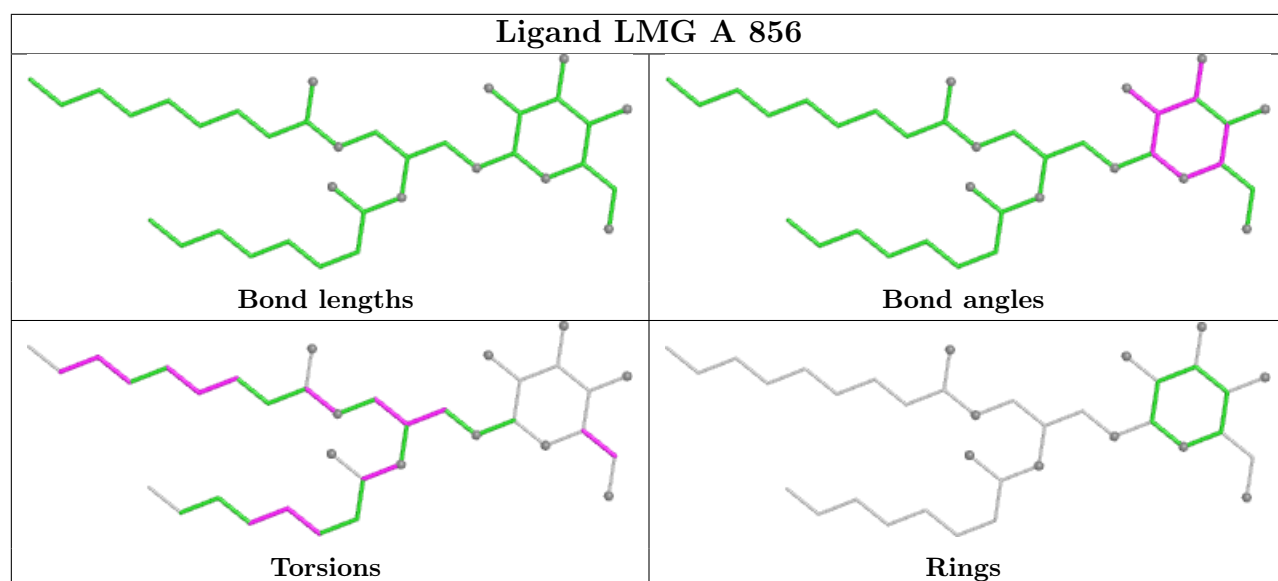


Torsions

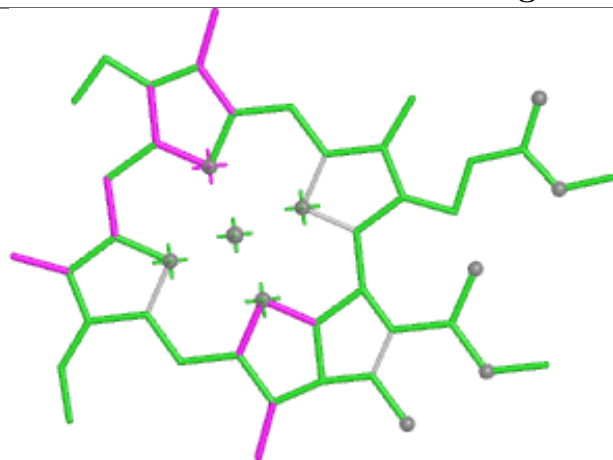


Rings

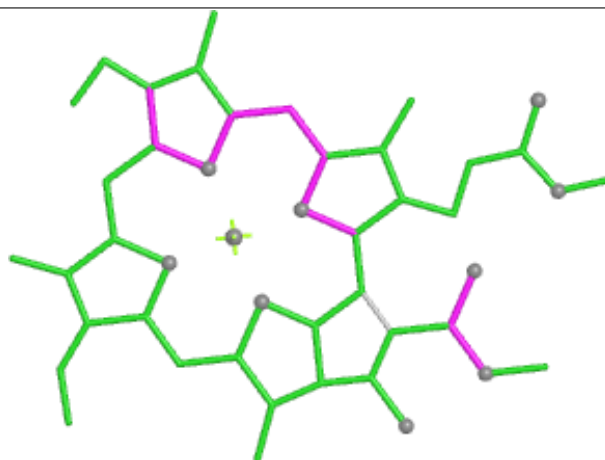
Ligand CLA f 603**Ligand OIE e 521****Ligand CHL 5 302**



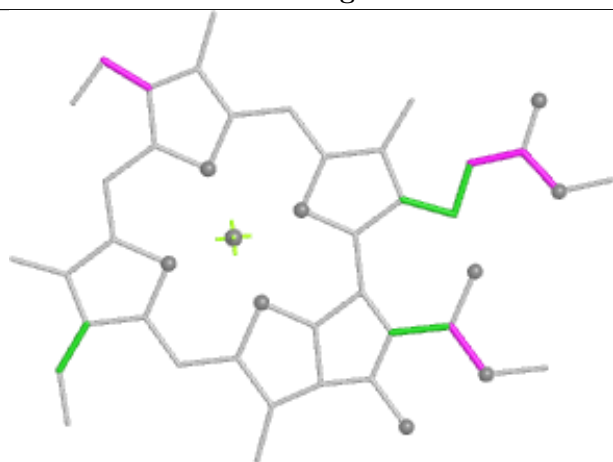
Ligand CLA 8 311



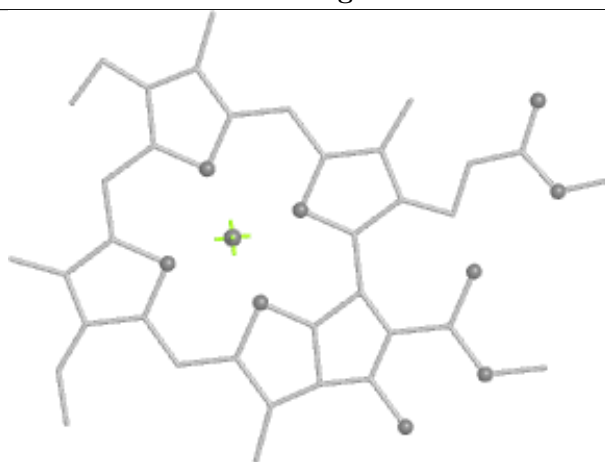
Bond lengths



Bond angles

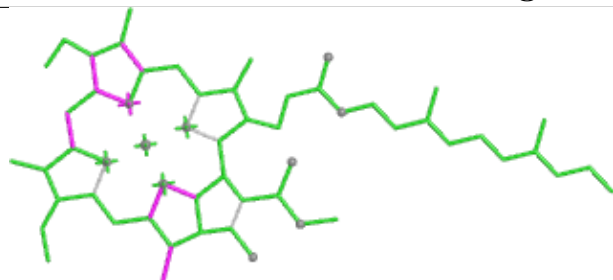


Torsions

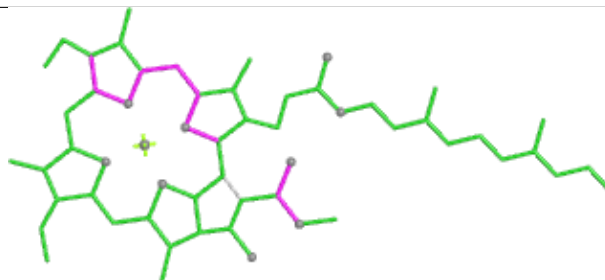


Rings

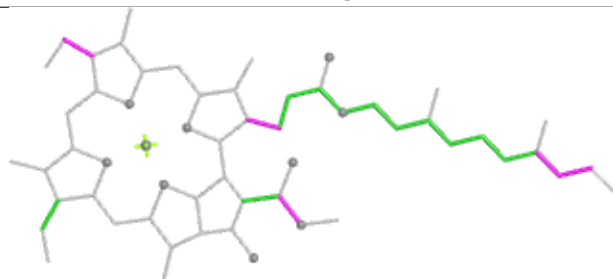
Ligand CLA a 611



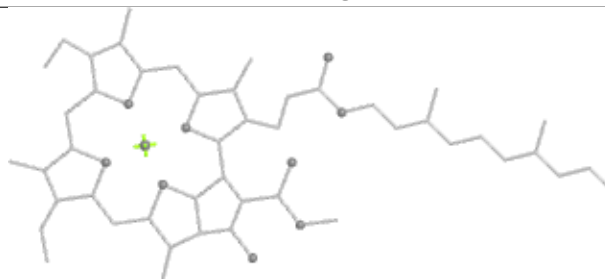
Bond lengths



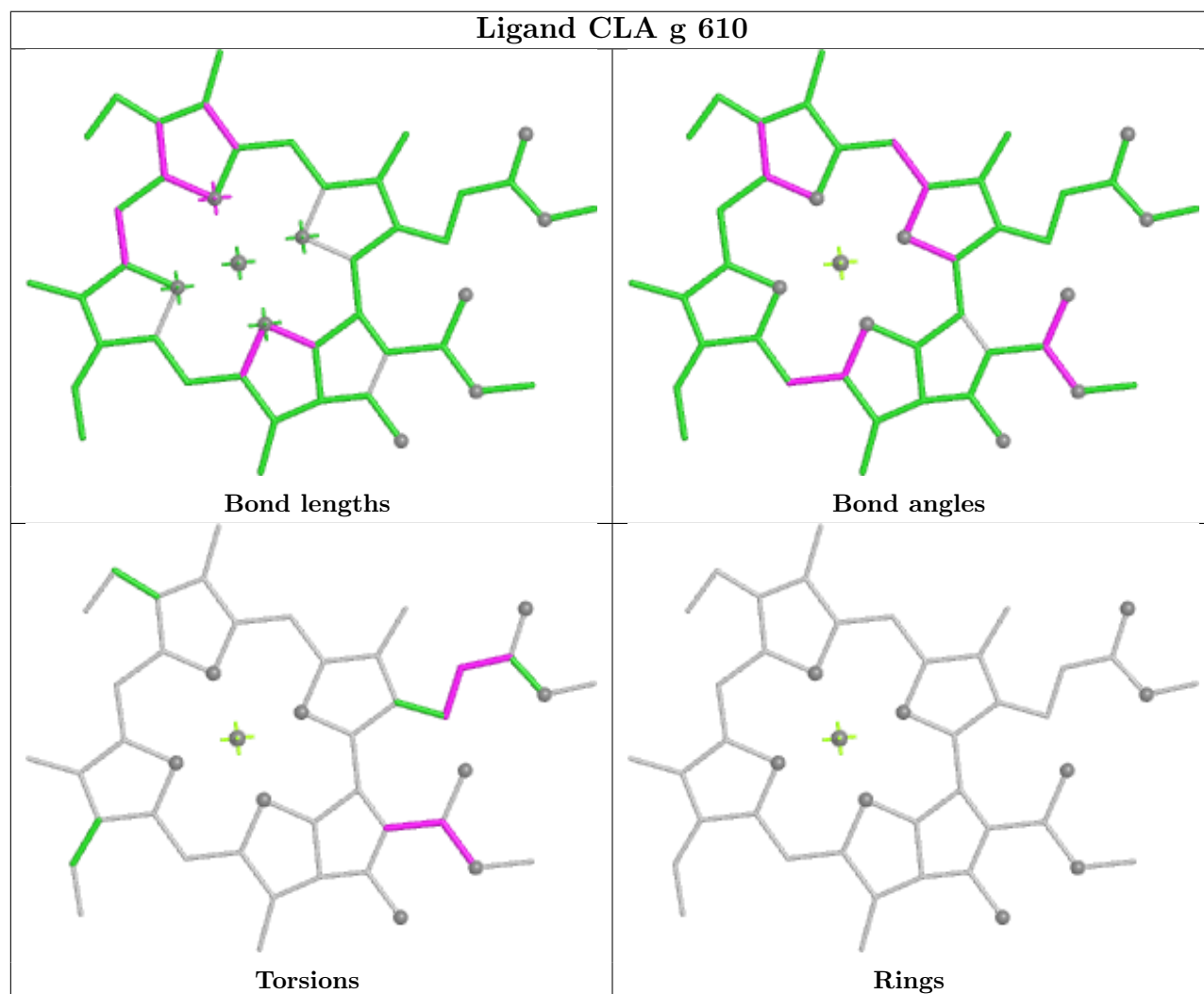
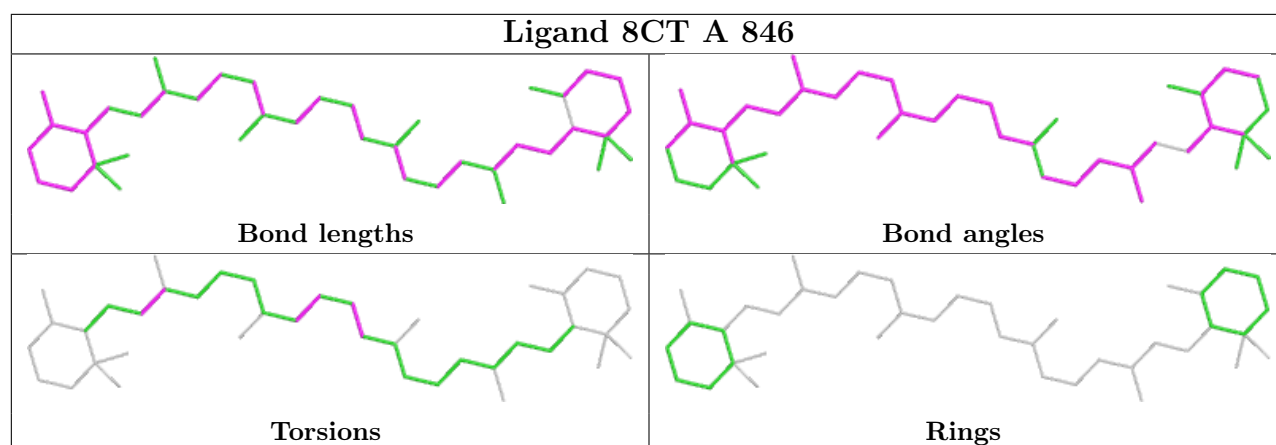
Bond angles



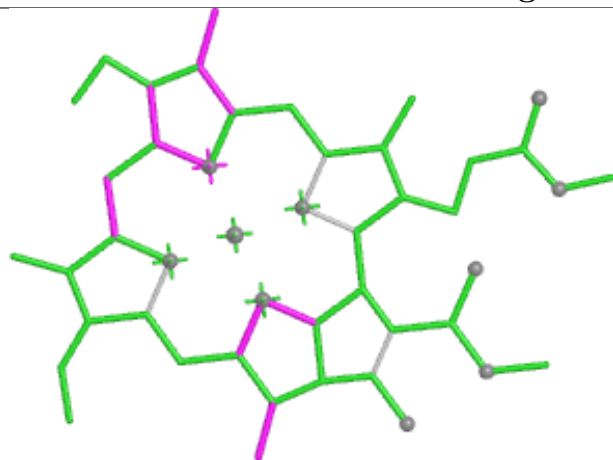
Torsions



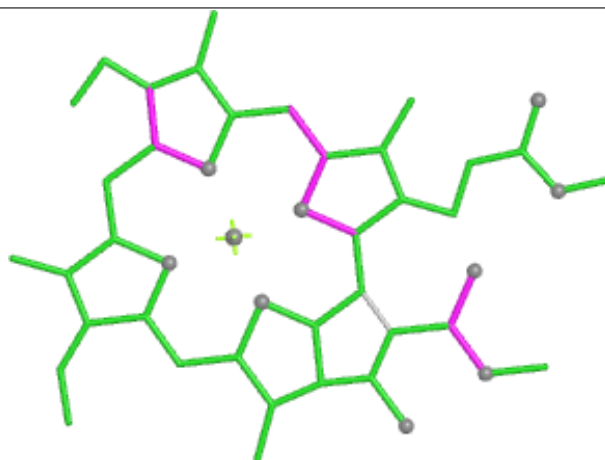
Rings



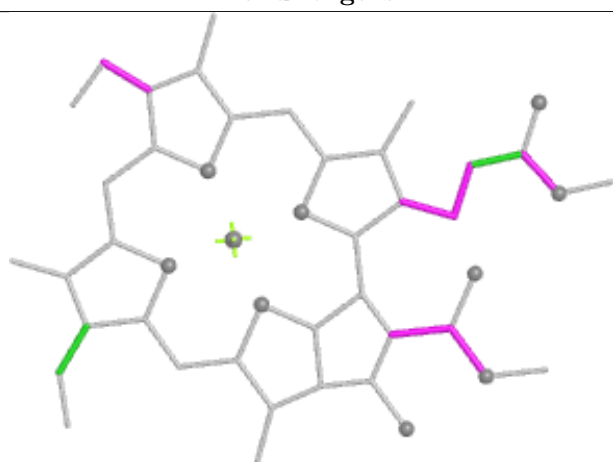
Ligand CLA 5 314



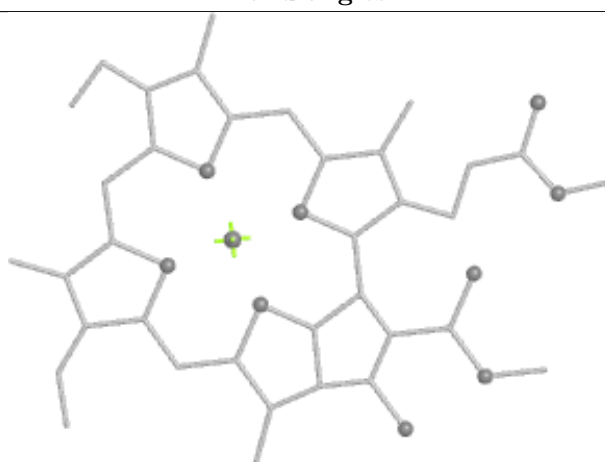
Bond lengths



Bond angles

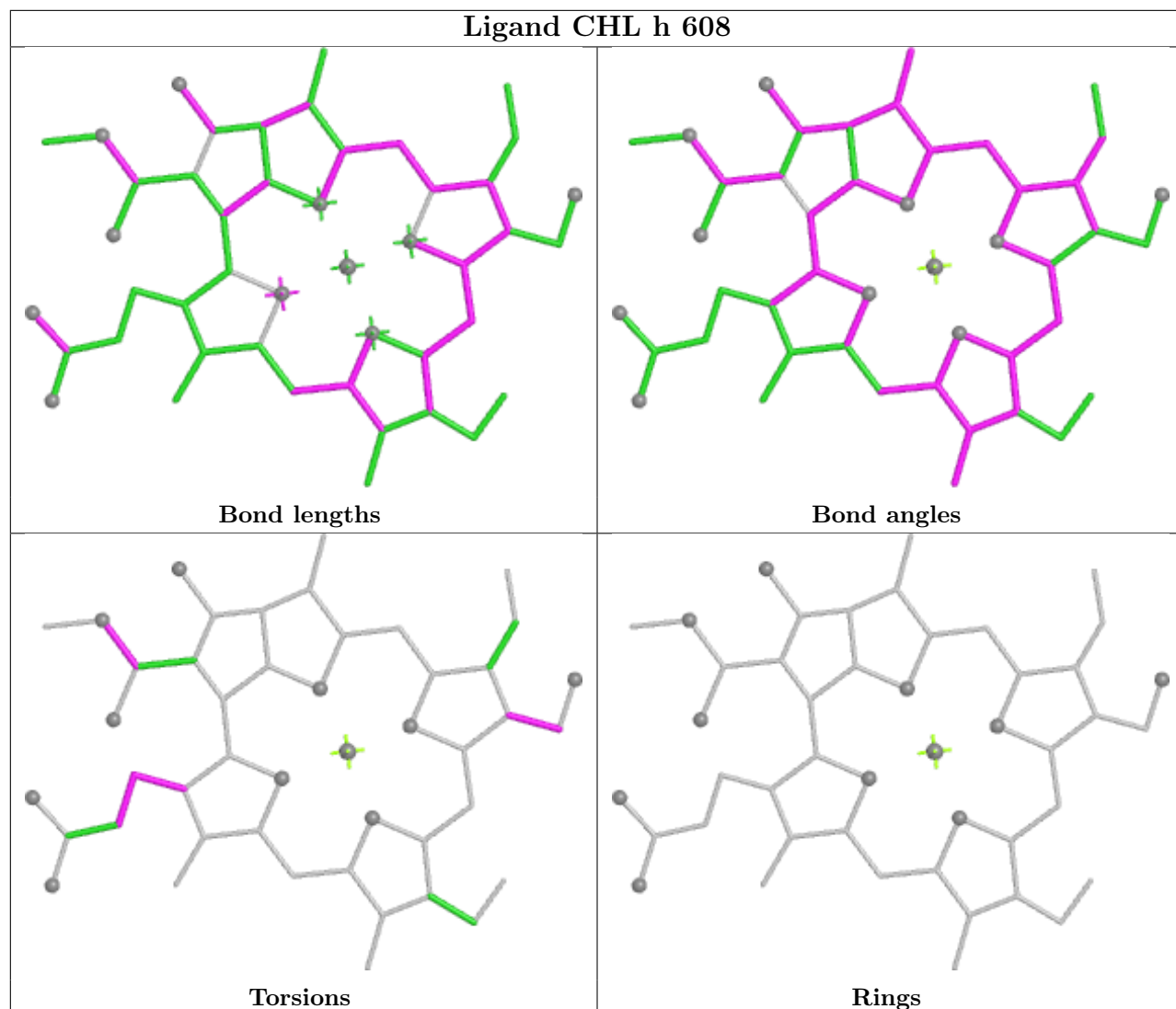


Torsions

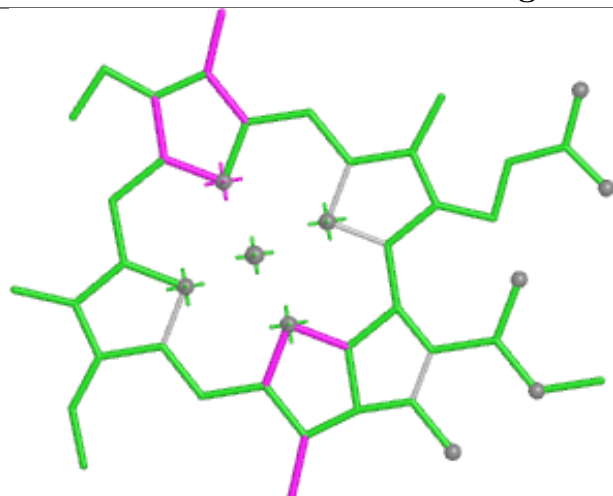


Rings

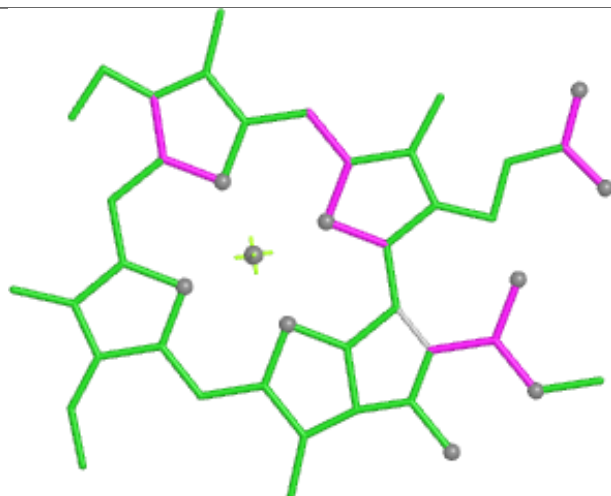
Ligand CHL h 608



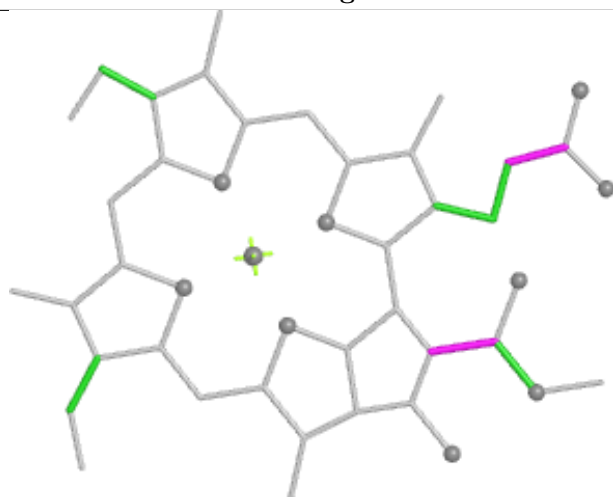
Ligand CLA 6 314



Bond lengths



Bond angles

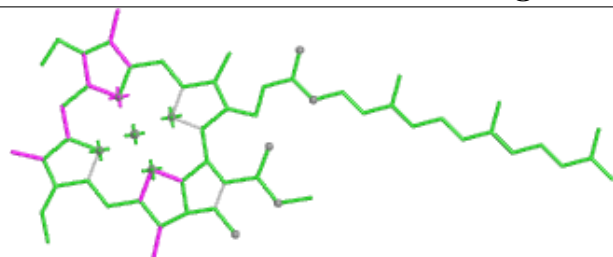


Torsions

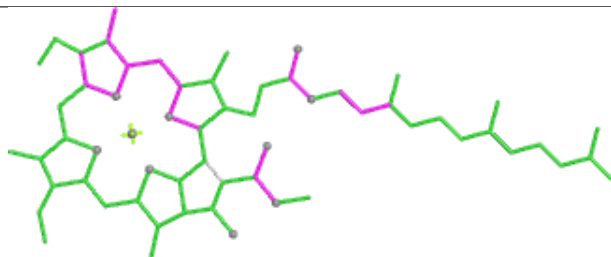


Rings

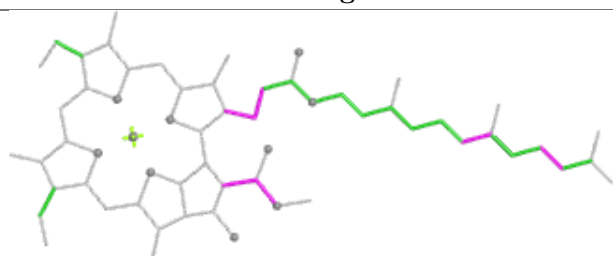
Ligand CLA B 816



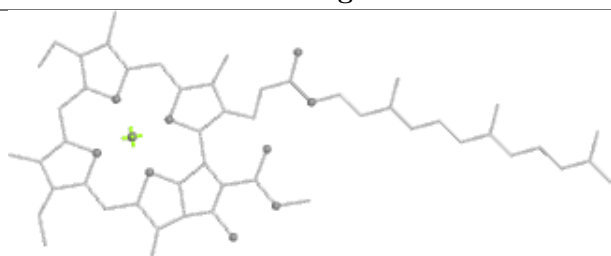
Bond lengths



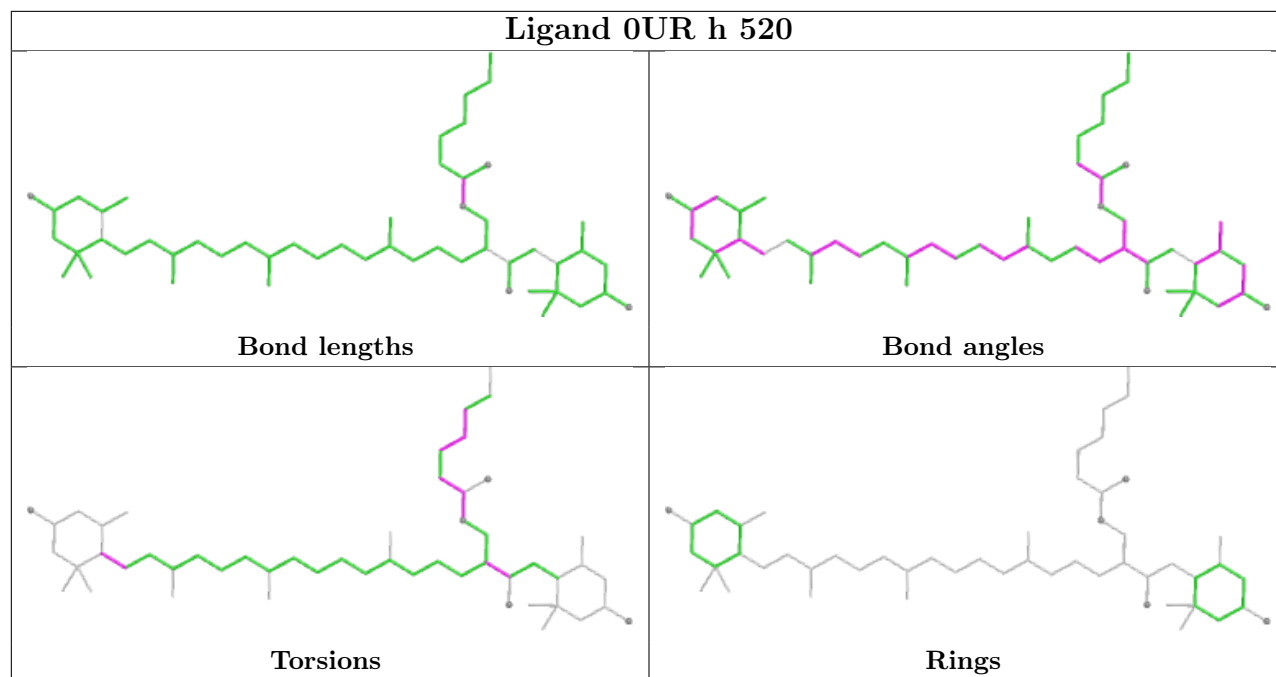
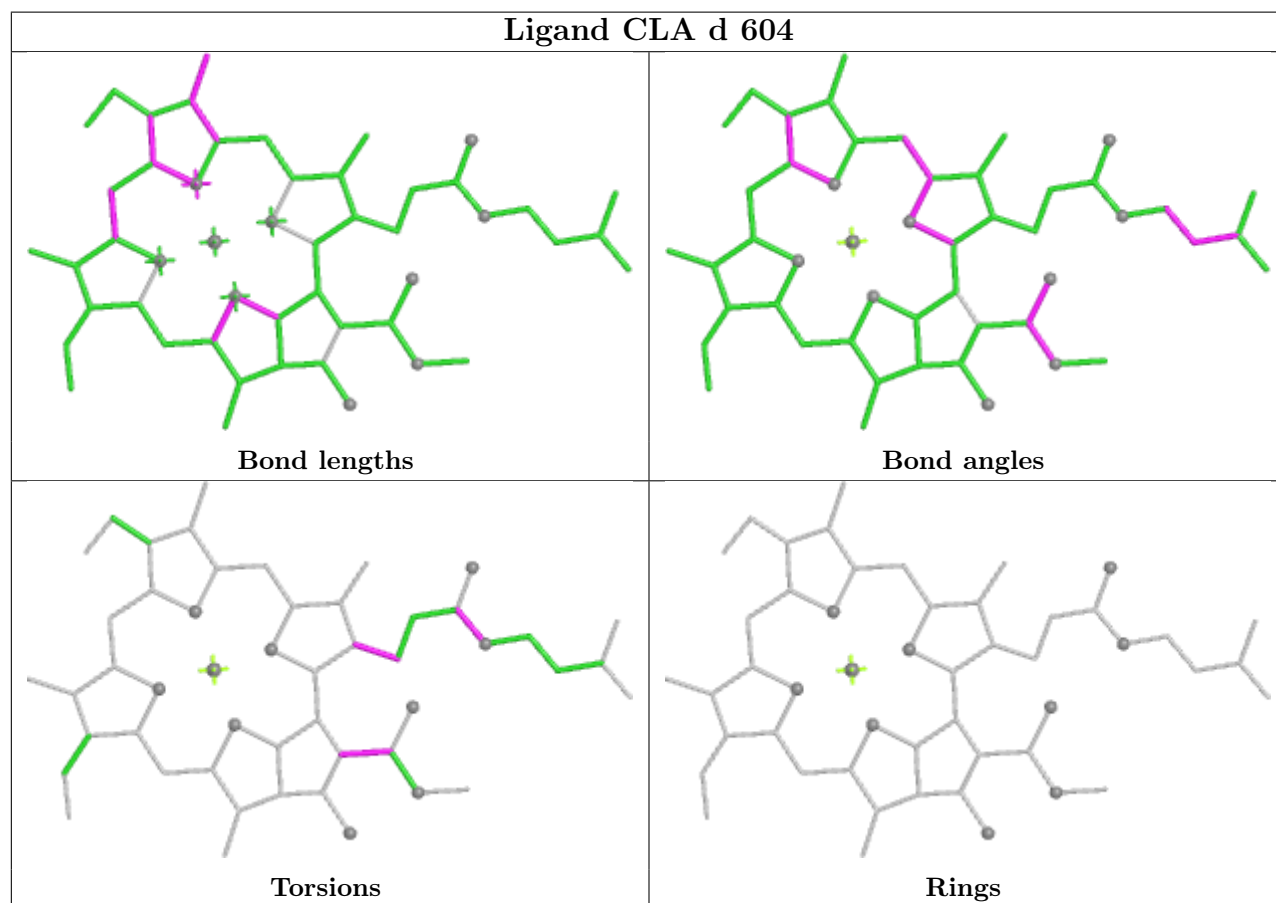
Bond angles

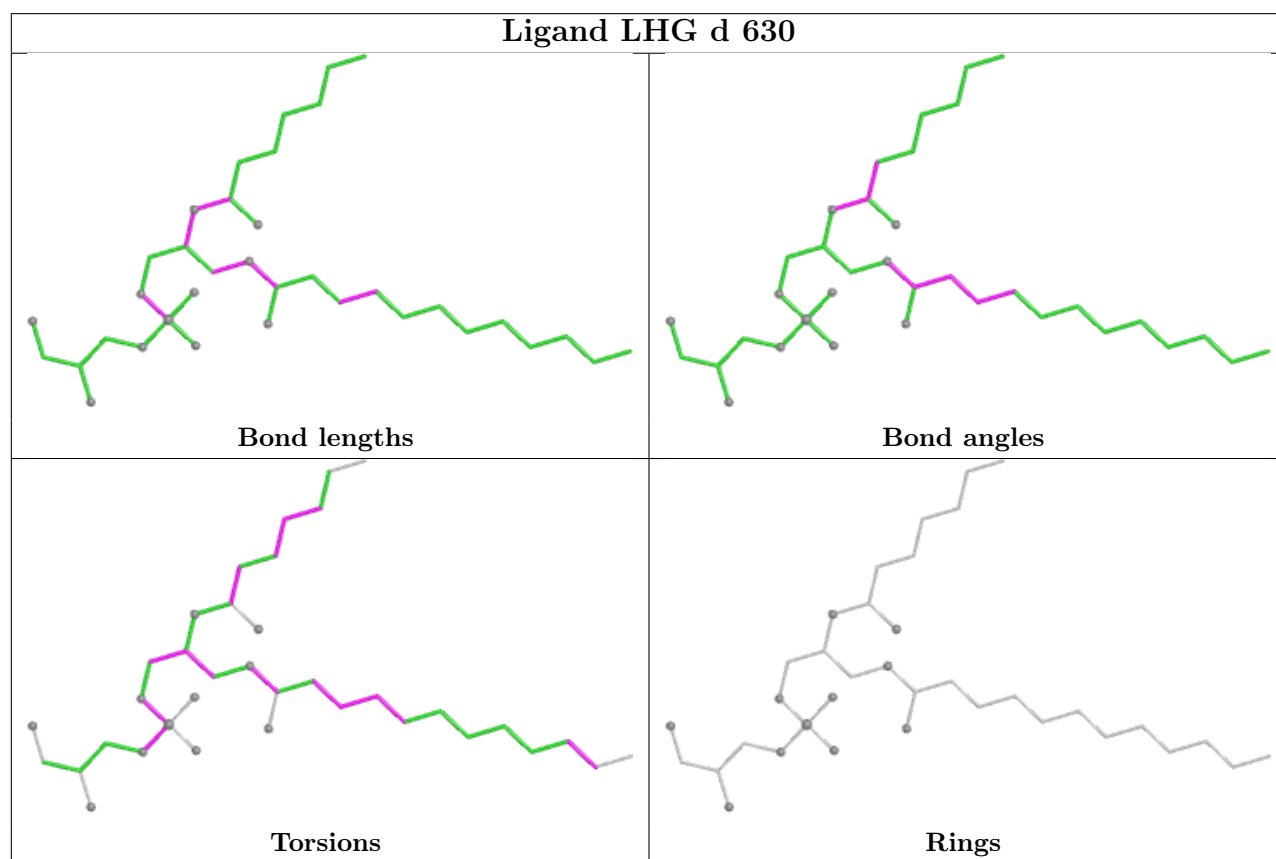
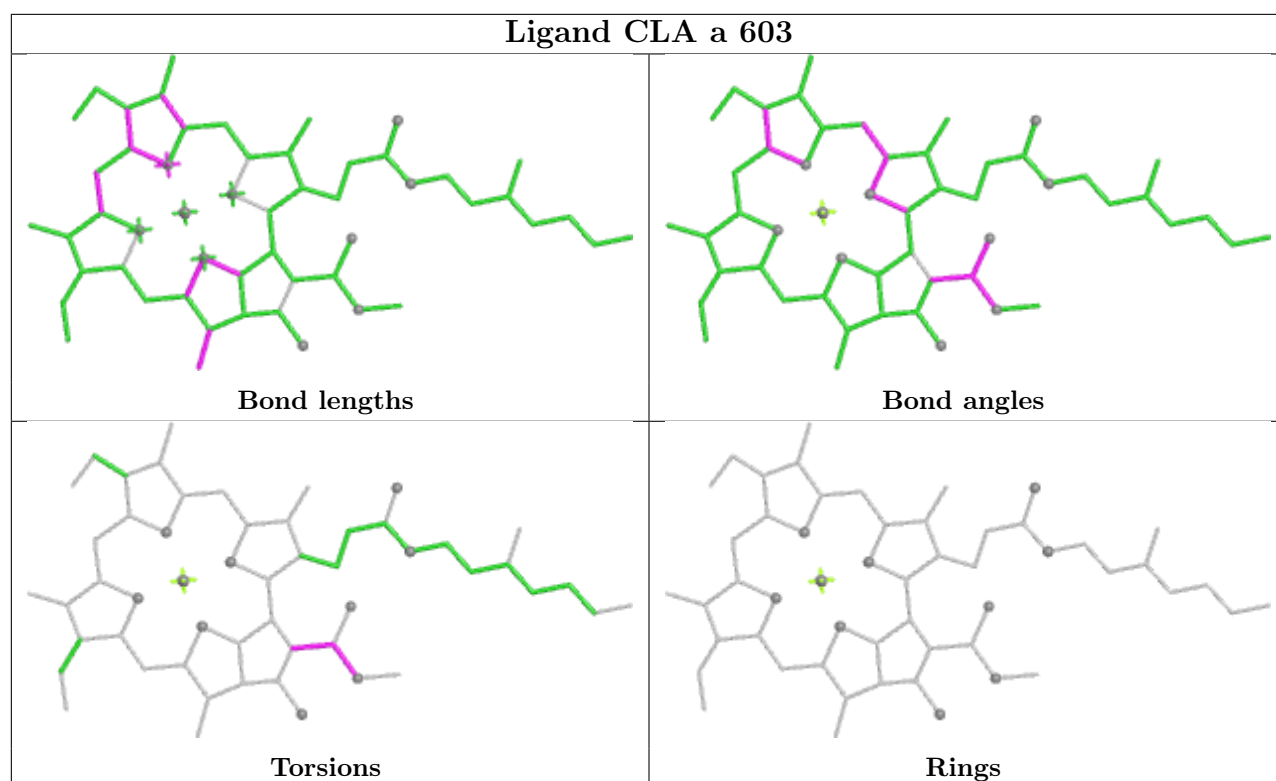


Torsions

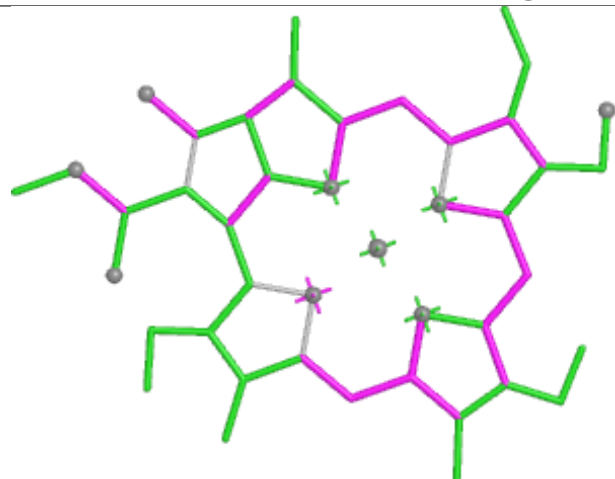


Rings

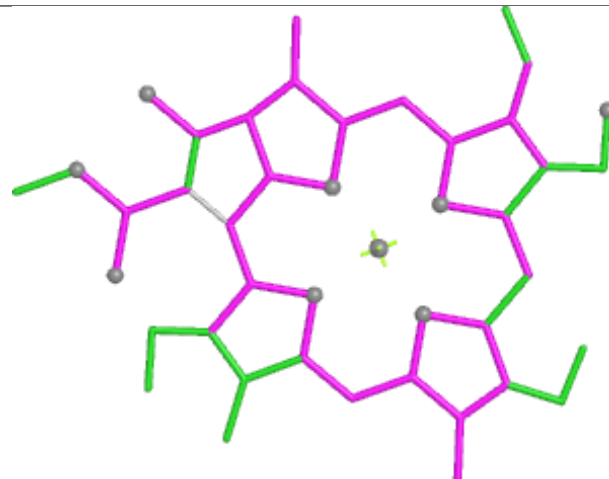
Ligand OUR h 520**Ligand CLA d 604**



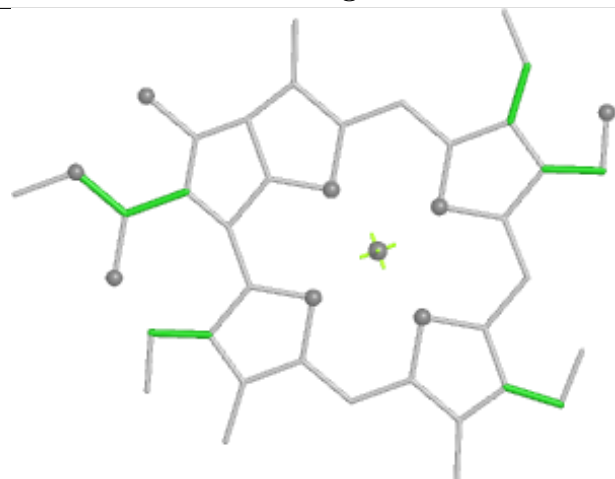
Ligand CHL 2 305



Bond lengths



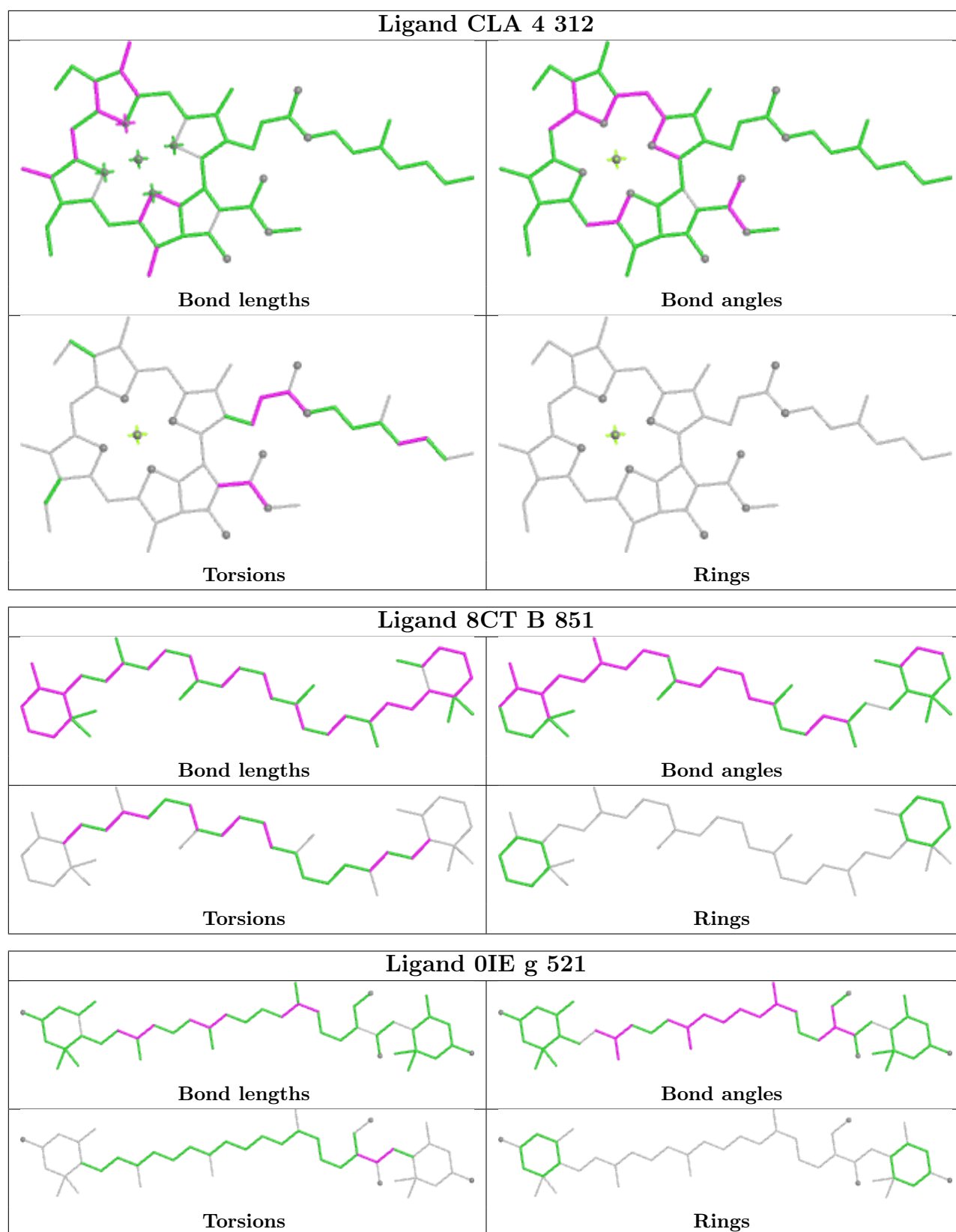
Bond angles



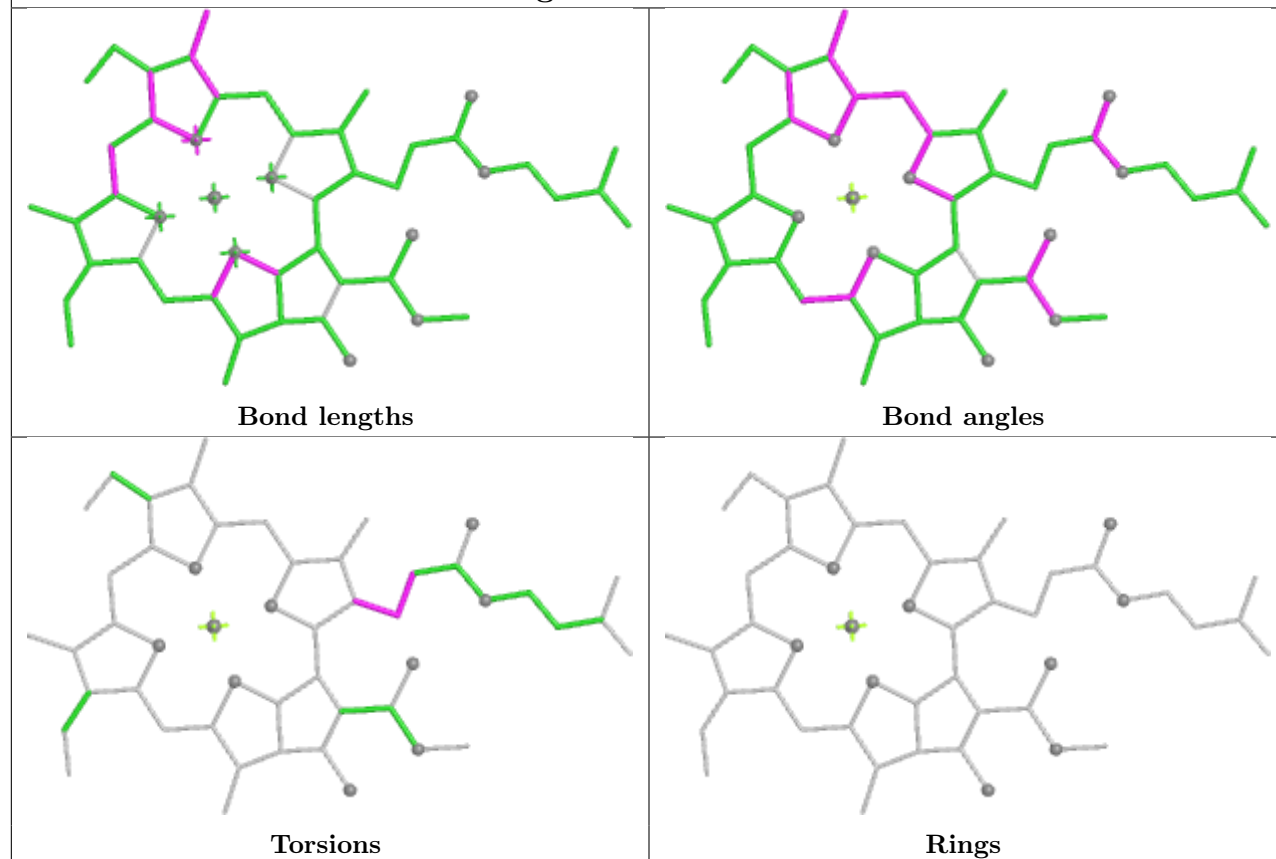
Torsions



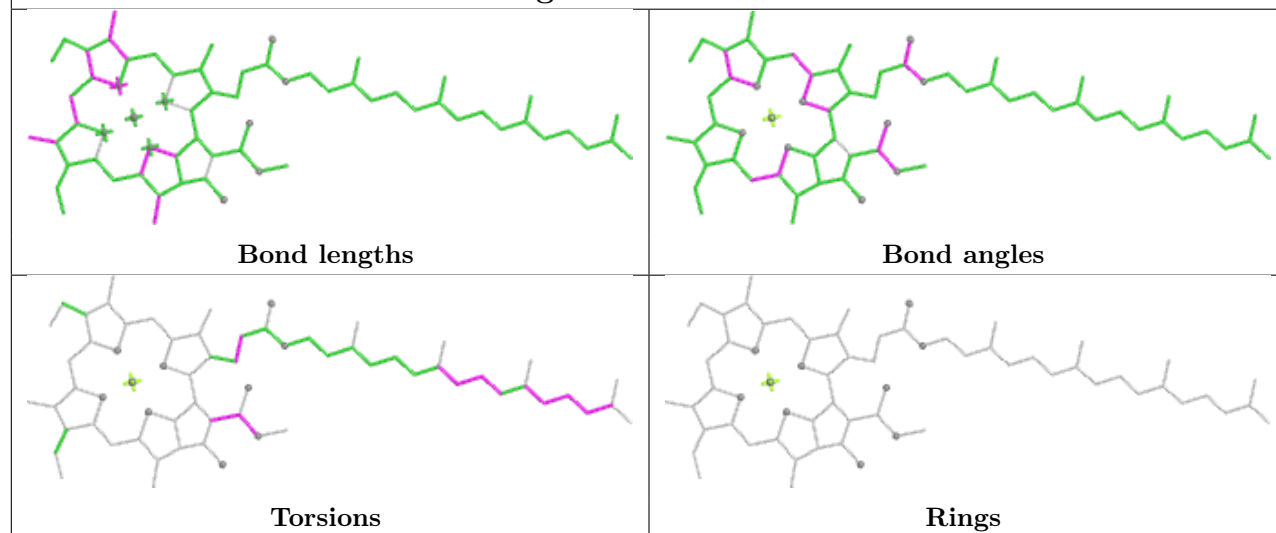
Rings



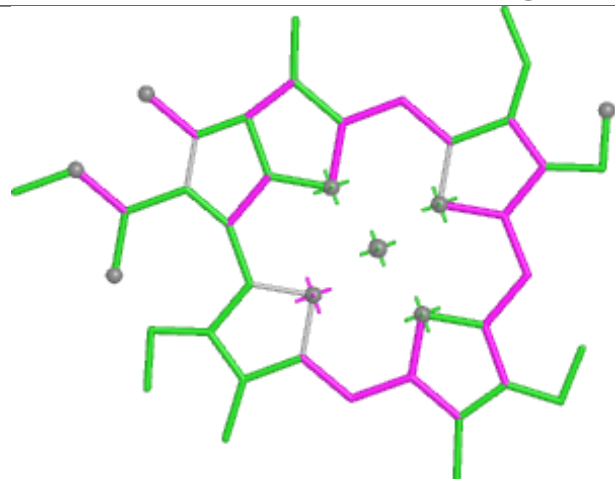
Ligand CLA a 604



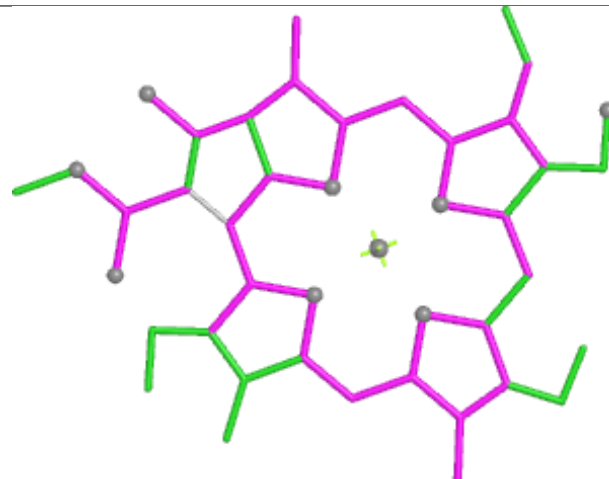
Ligand CLA 9 302



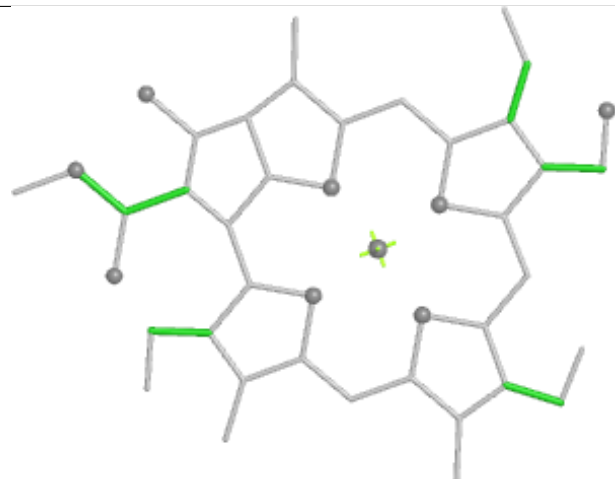
Ligand CHL 4 305



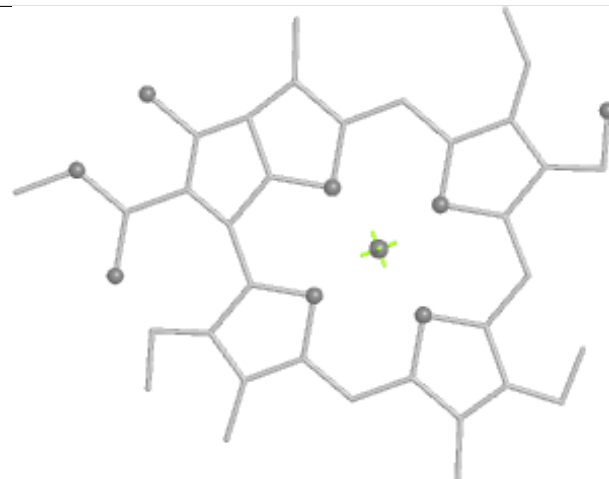
Bond lengths



Bond angles

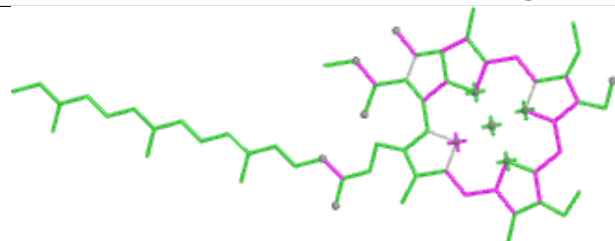


Torsions

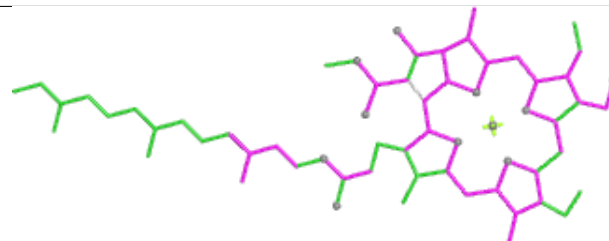


Rings

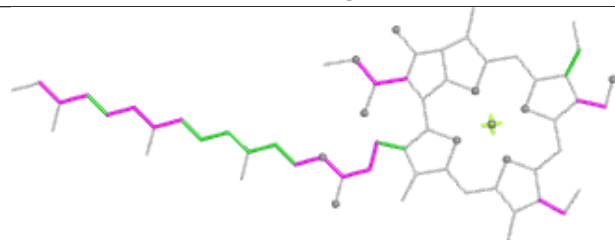
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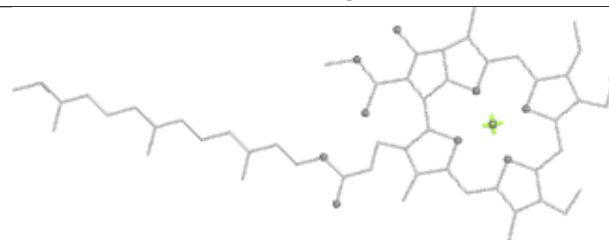
Bond lengths



Bond angles

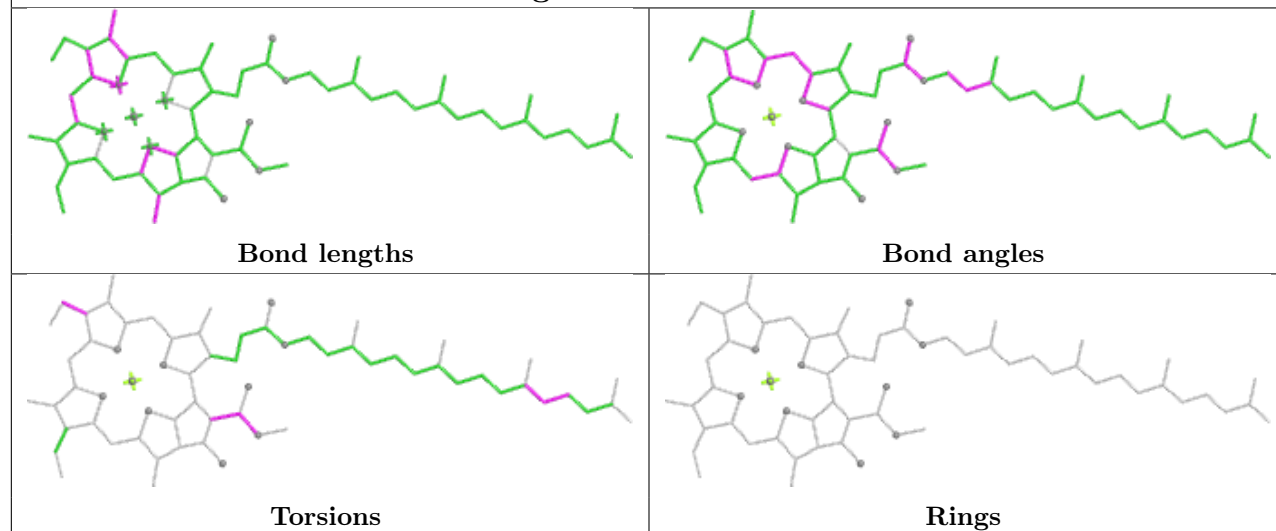


Torsions

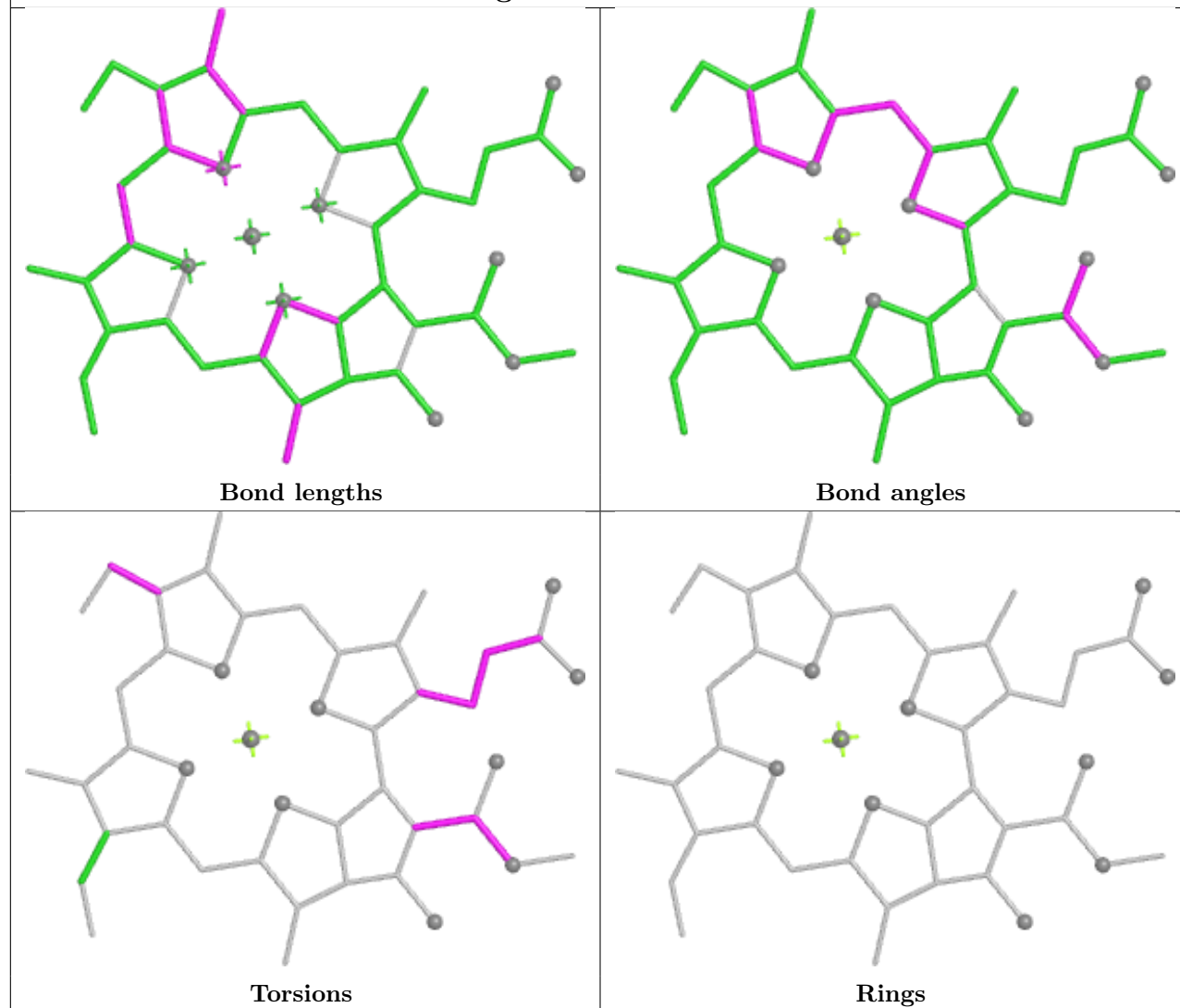


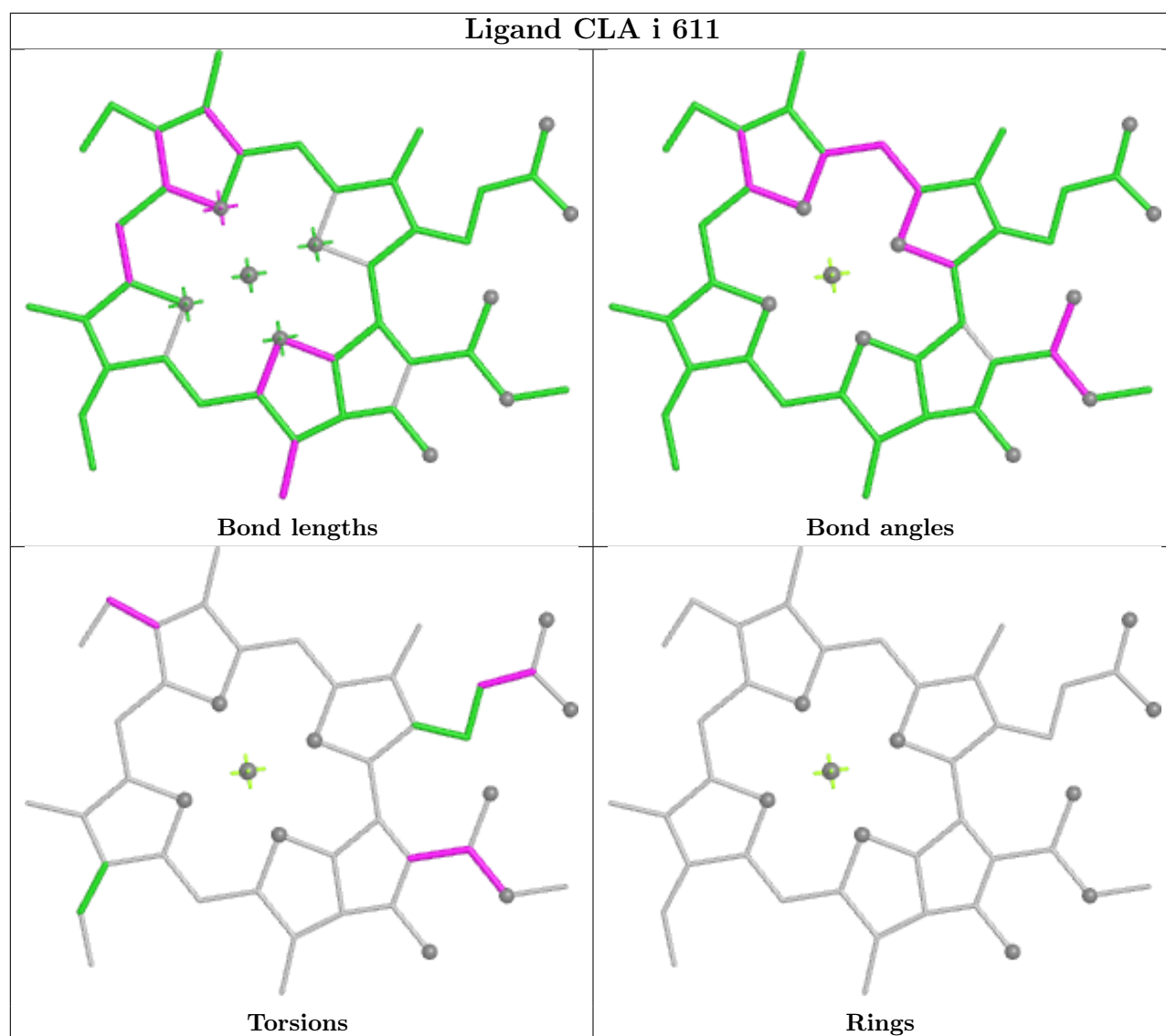
Rings

Ligand CLA B 841

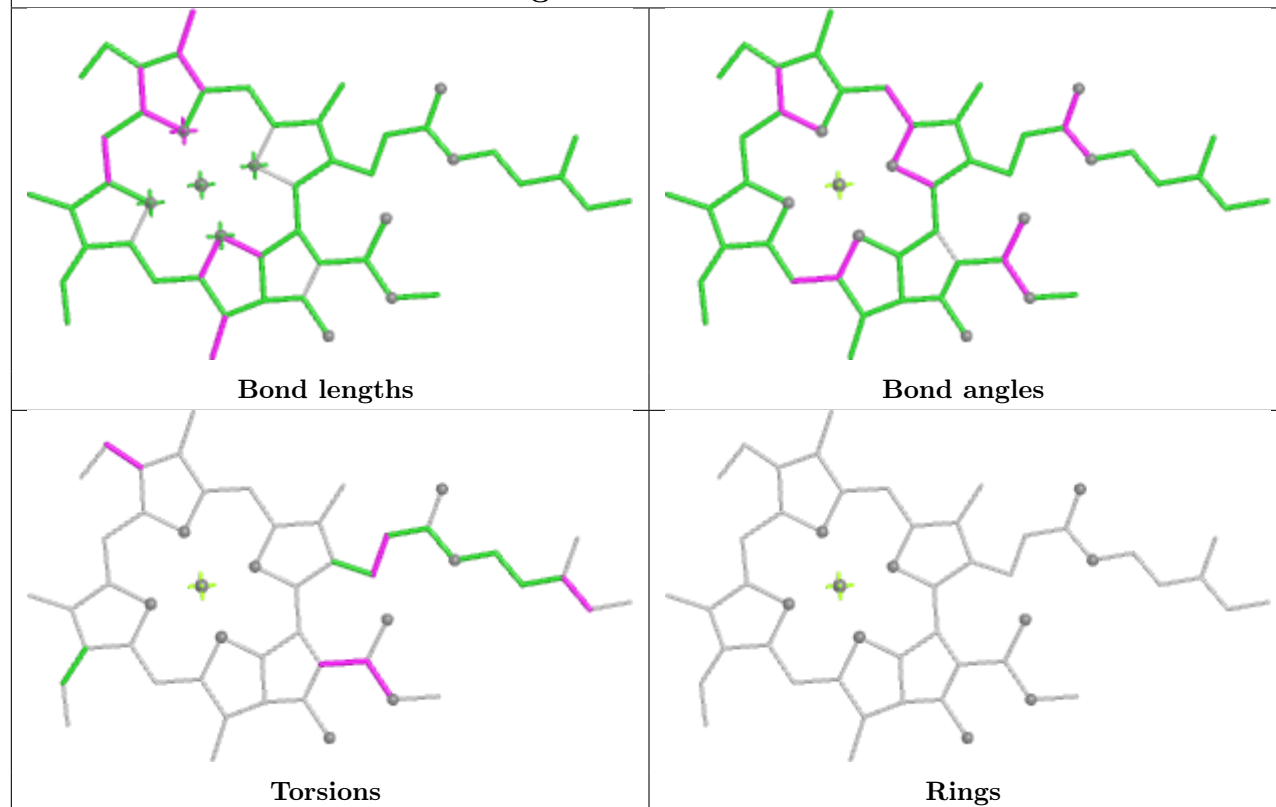


Ligand CLA 0 321

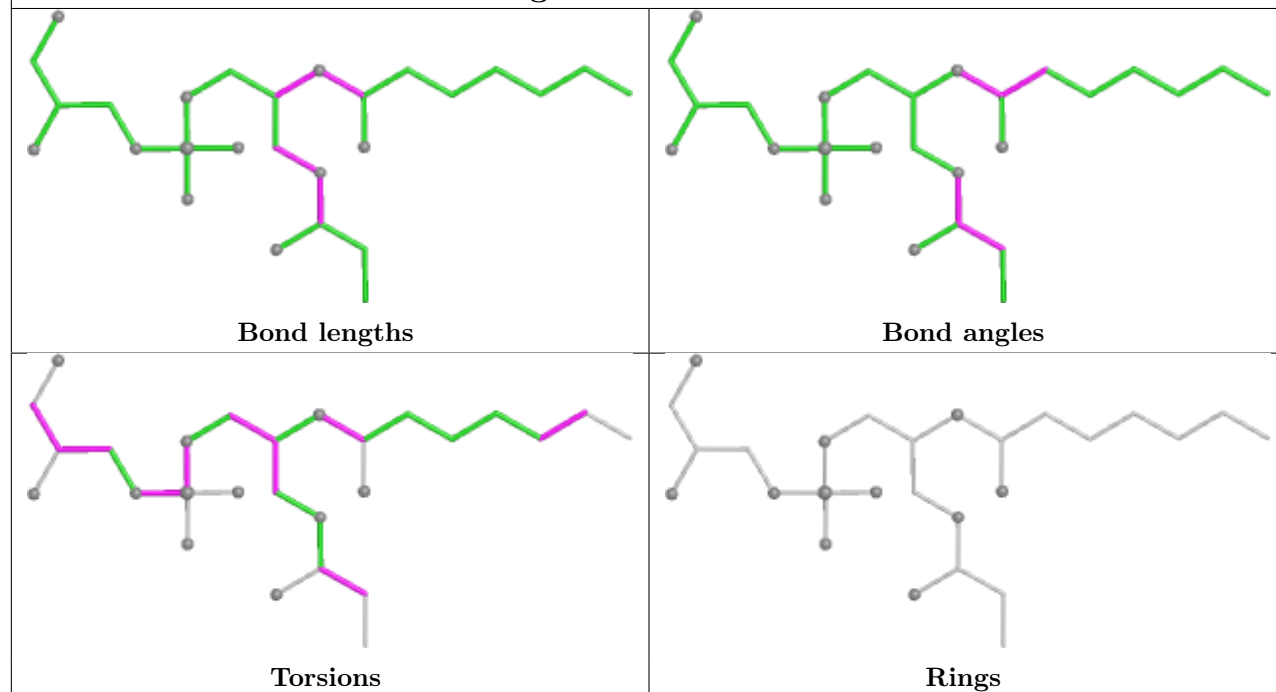




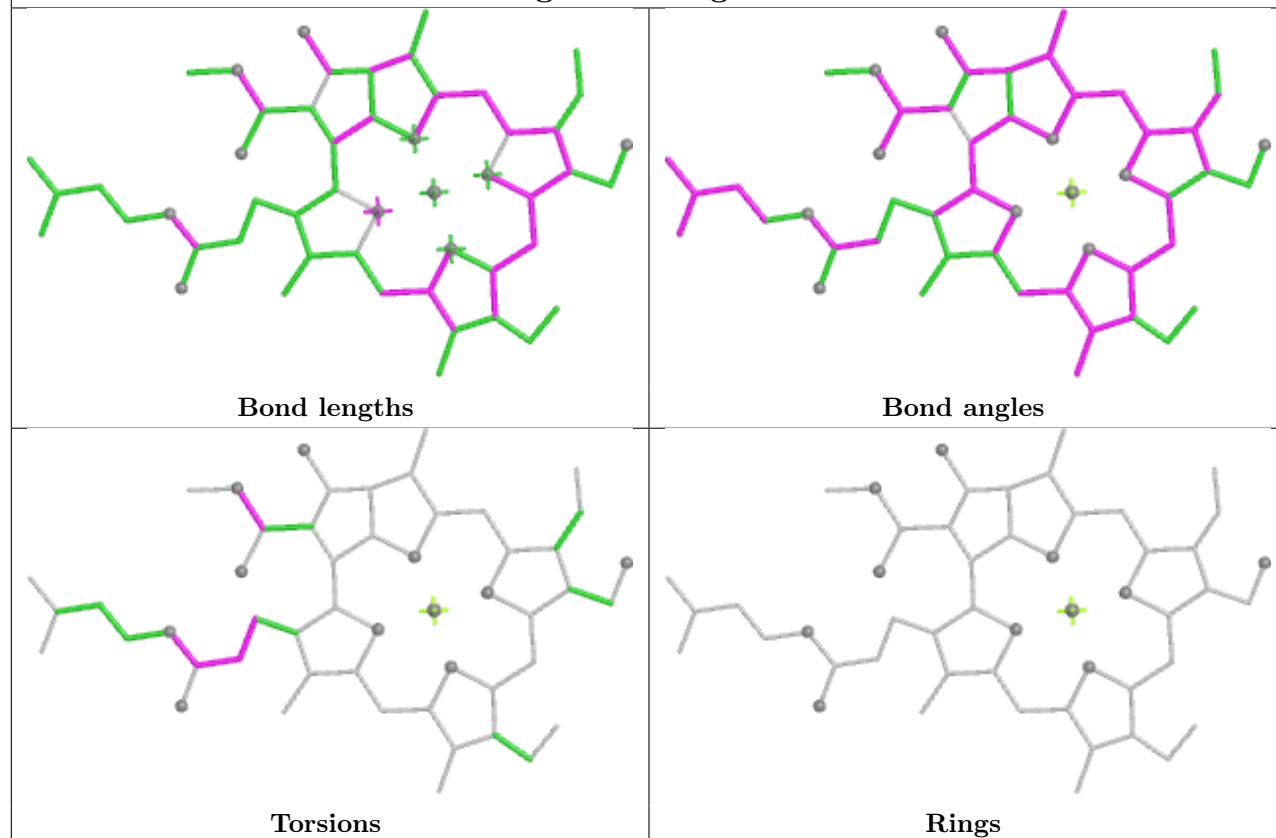
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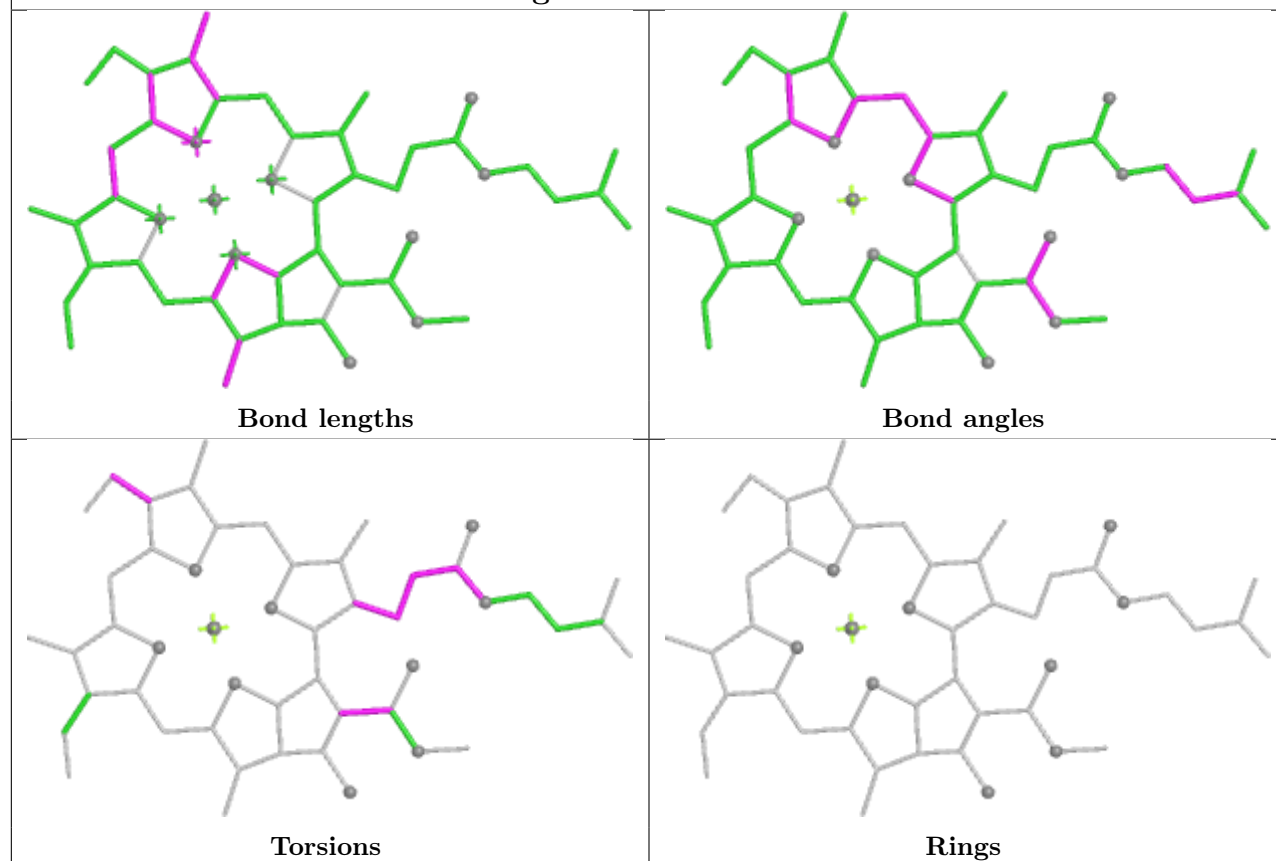
Ligand LHG A 845

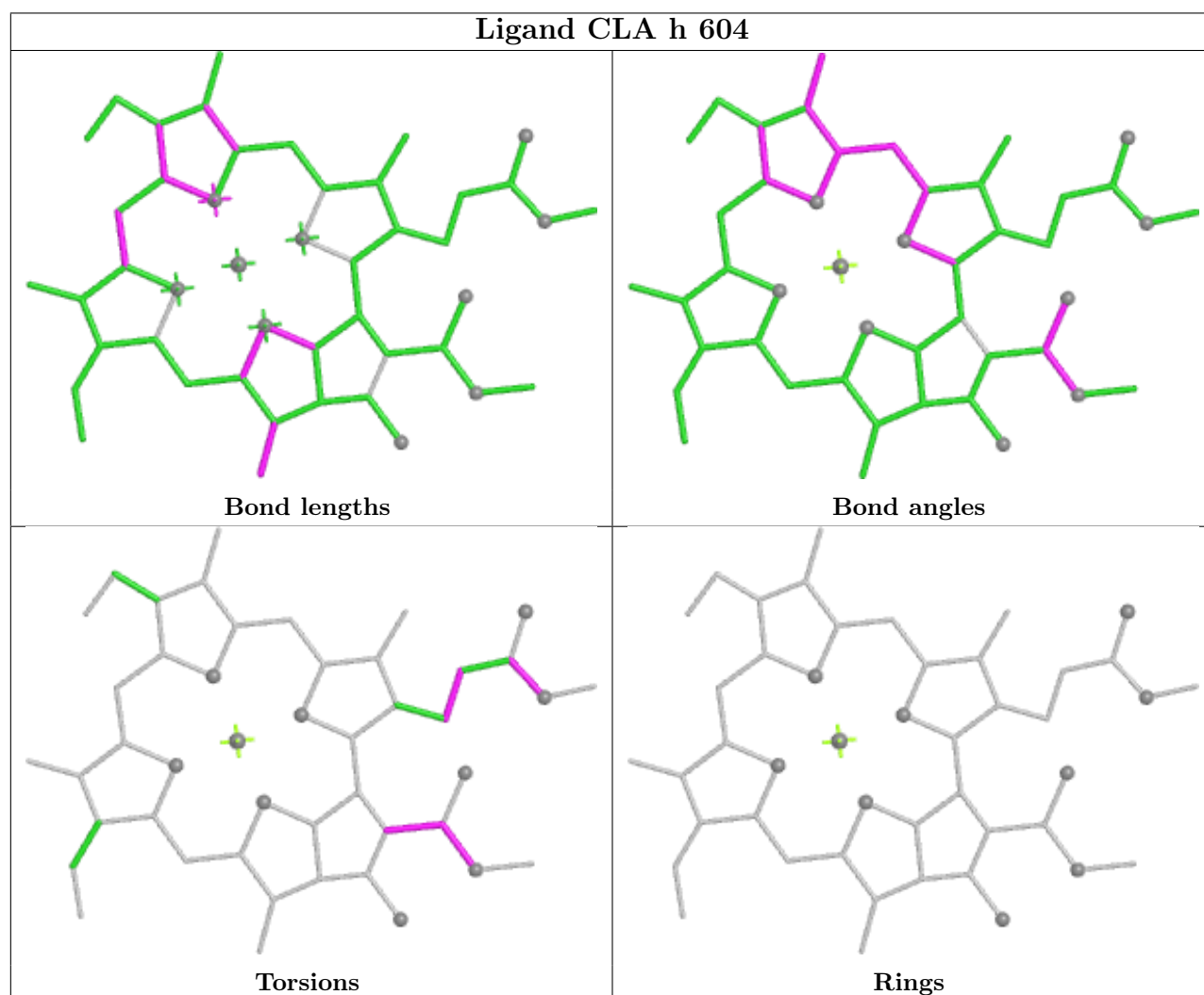
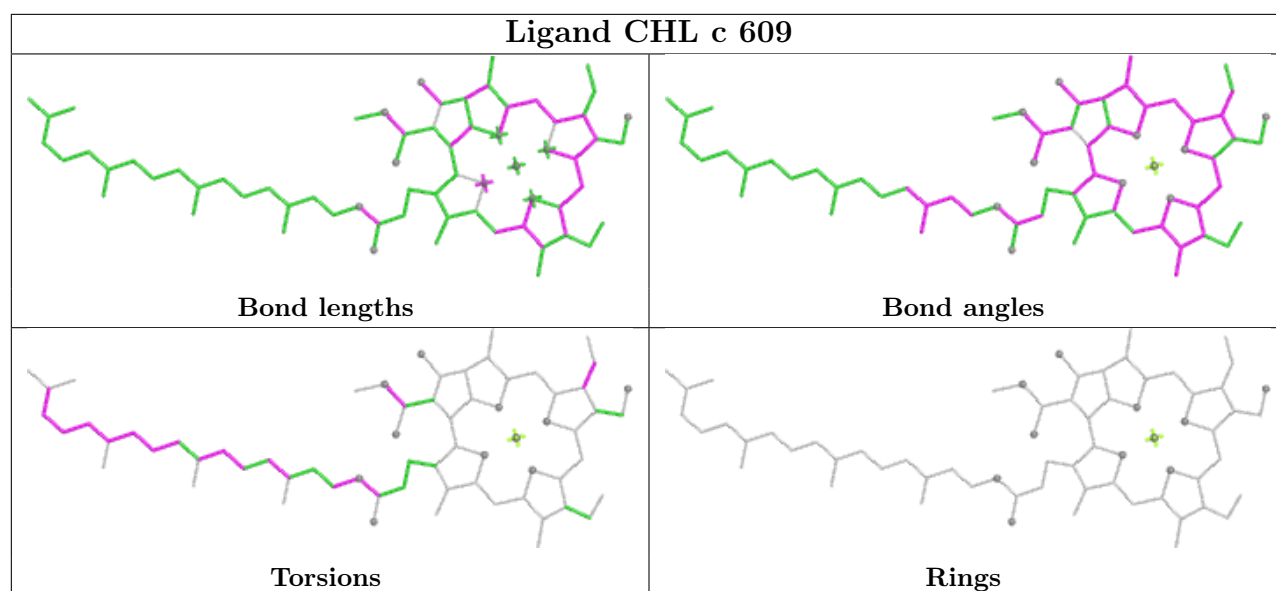


Ligand CHL g 606

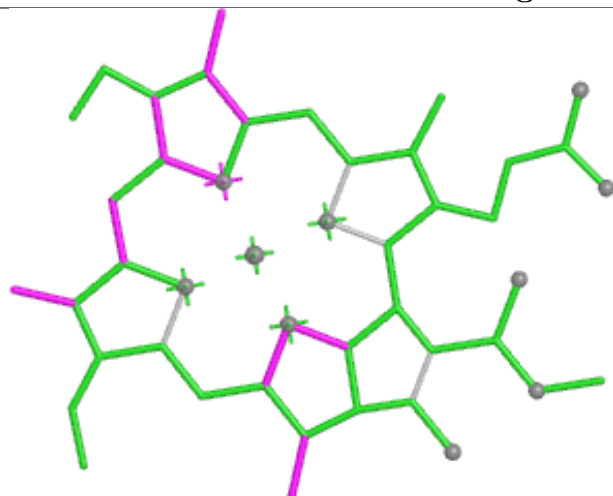


Ligand CLA B 831

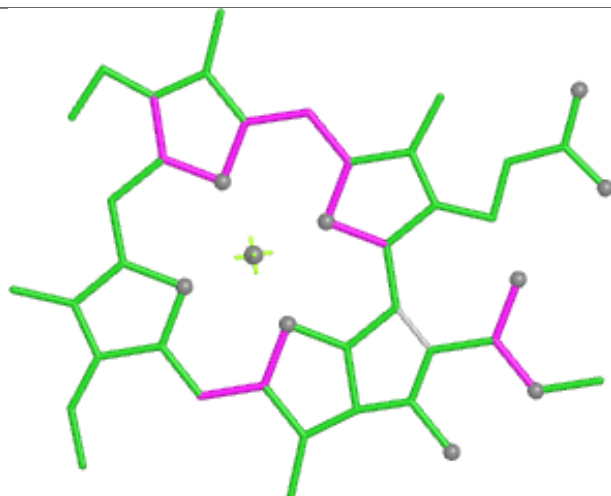




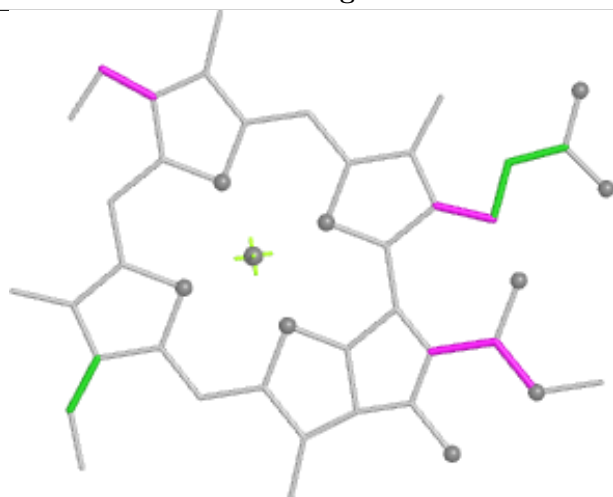
Ligand CLA F 301



Bond lengths



Bond angles

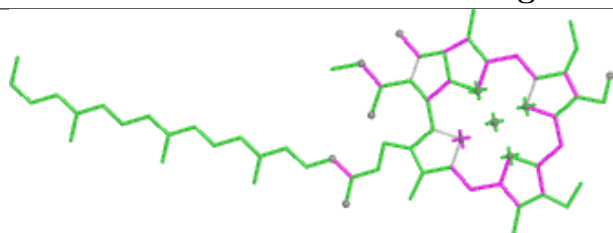


Torsions

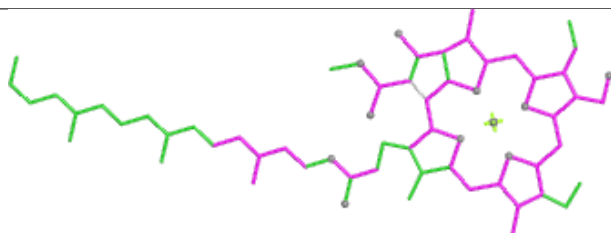


Rings

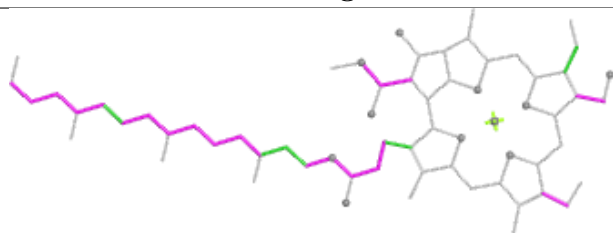
Ligand CHL 2 302



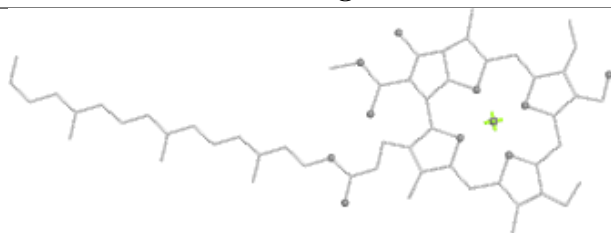
Bond lengths



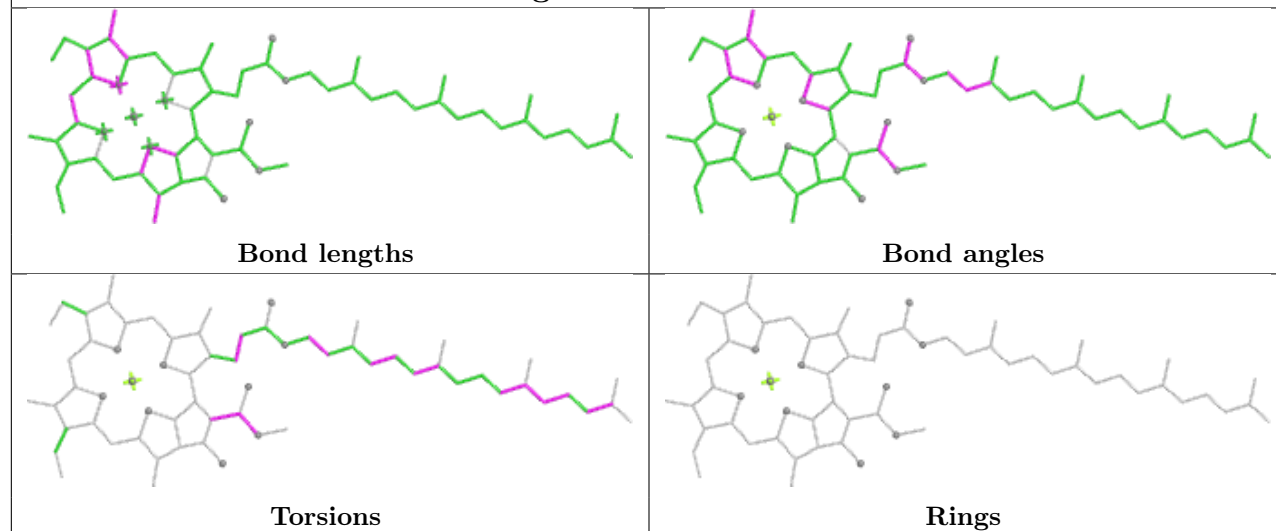
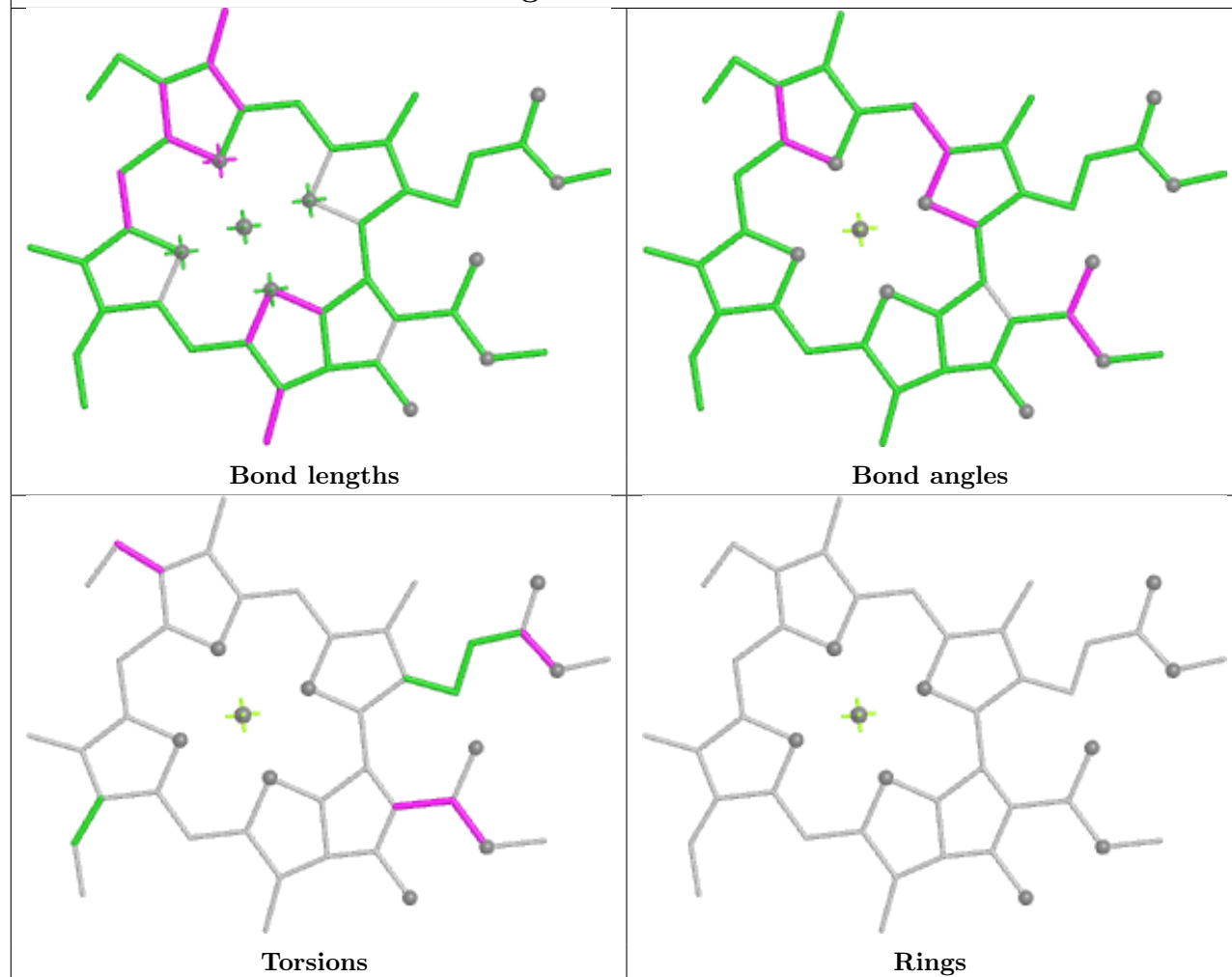
Bond angles

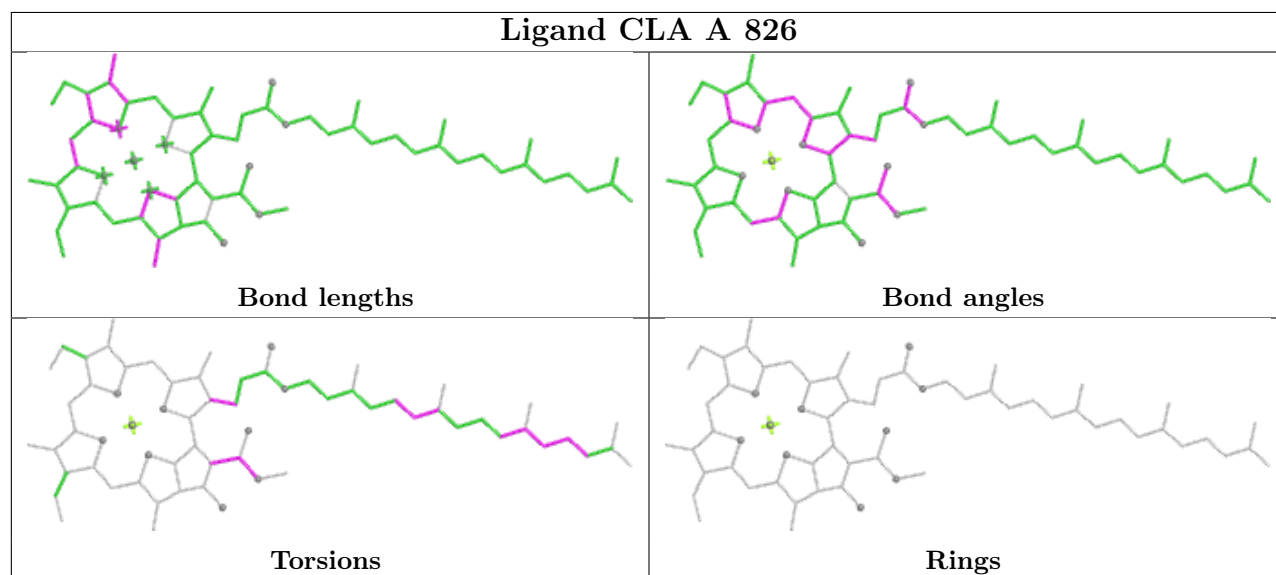
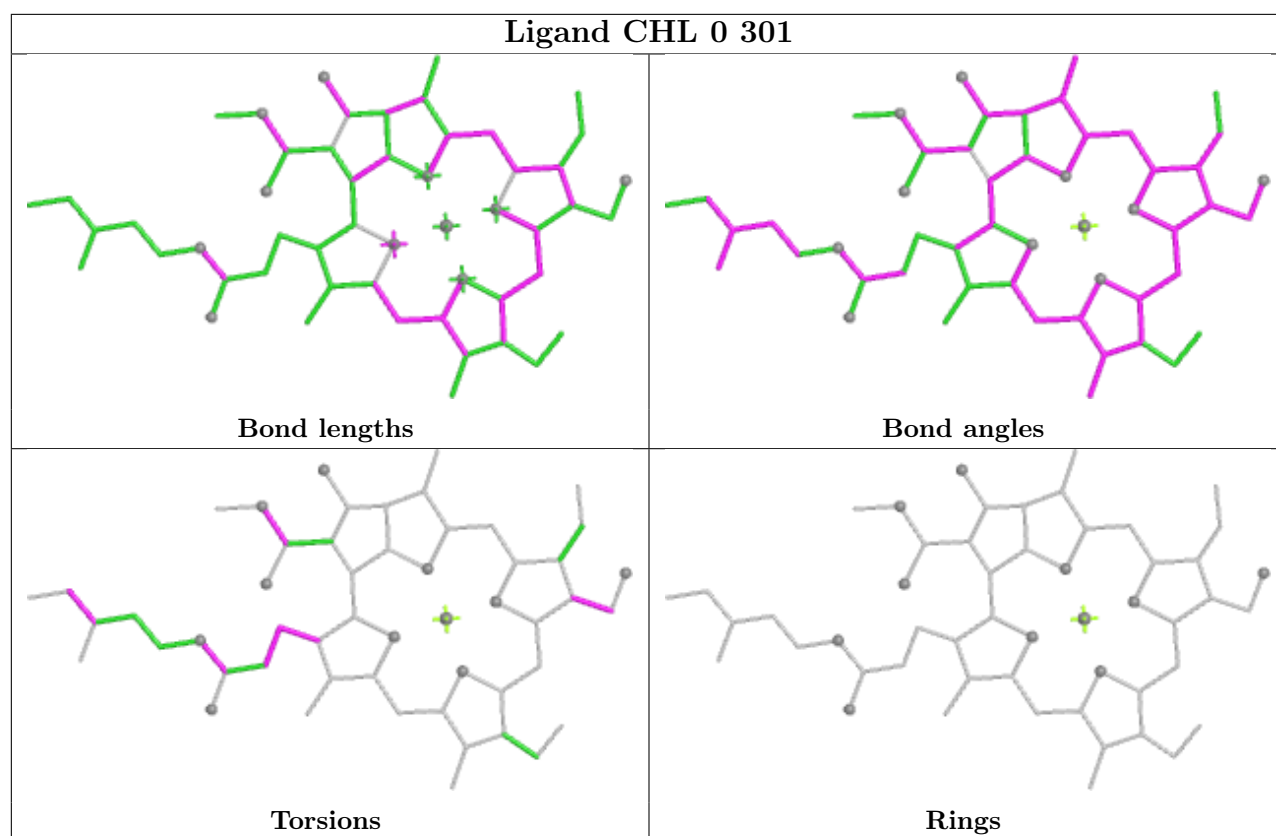


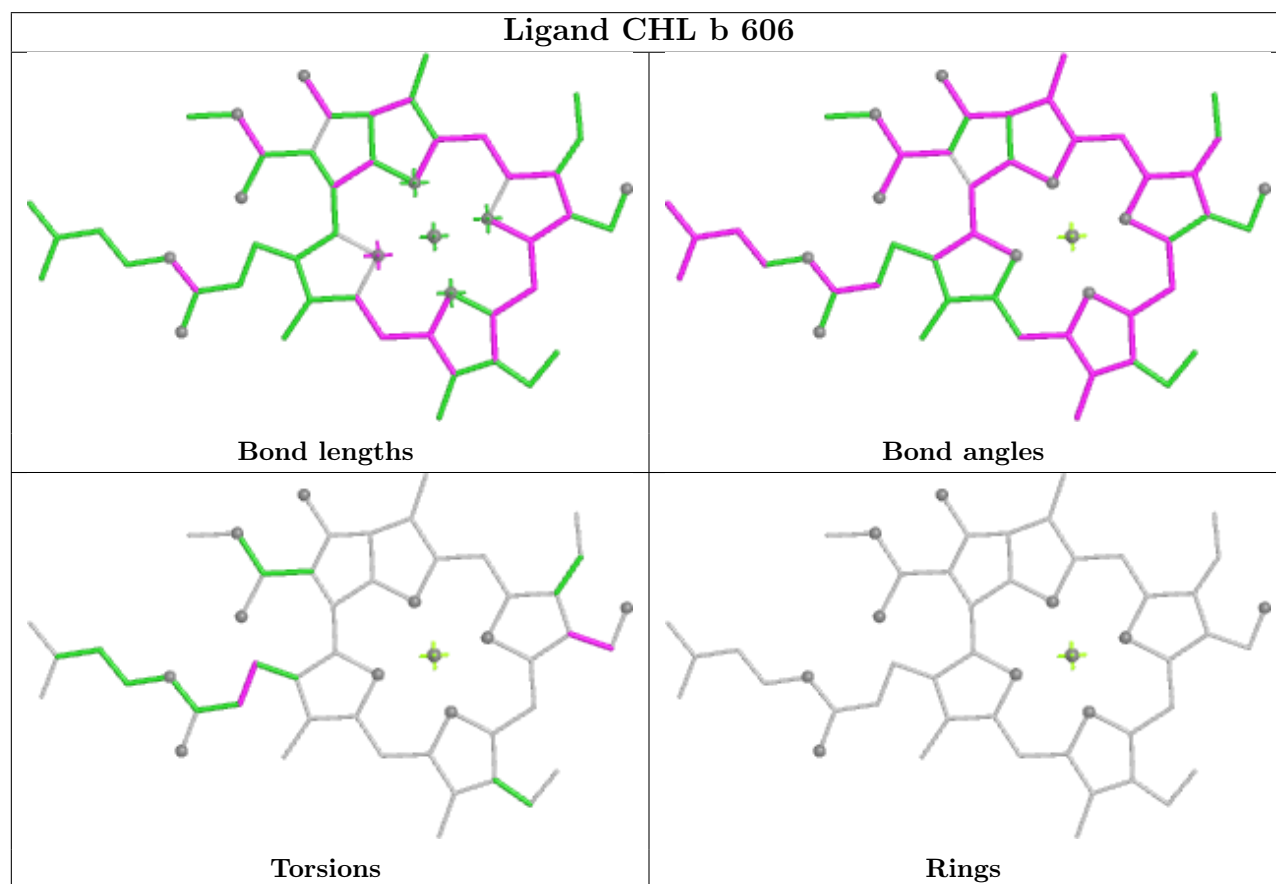
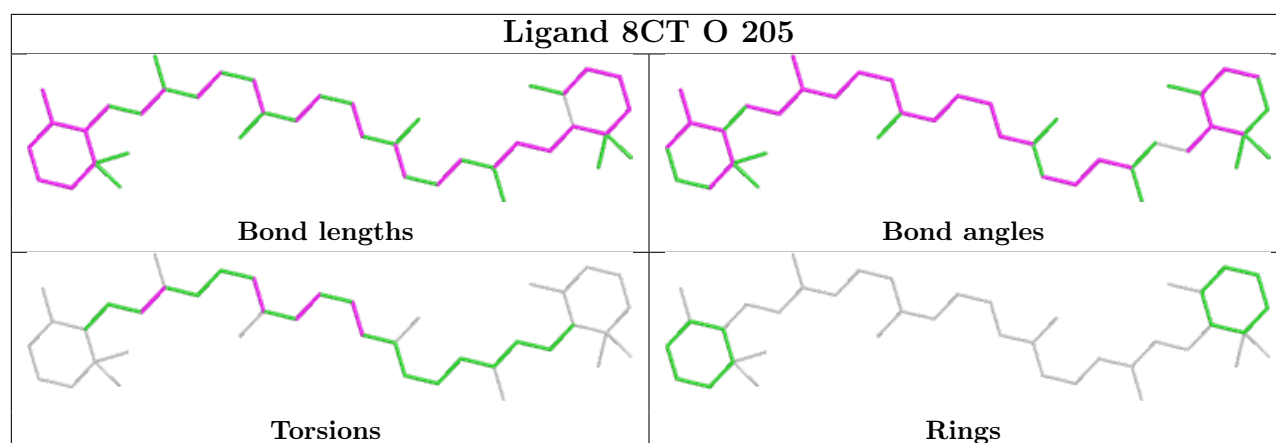
Torsions

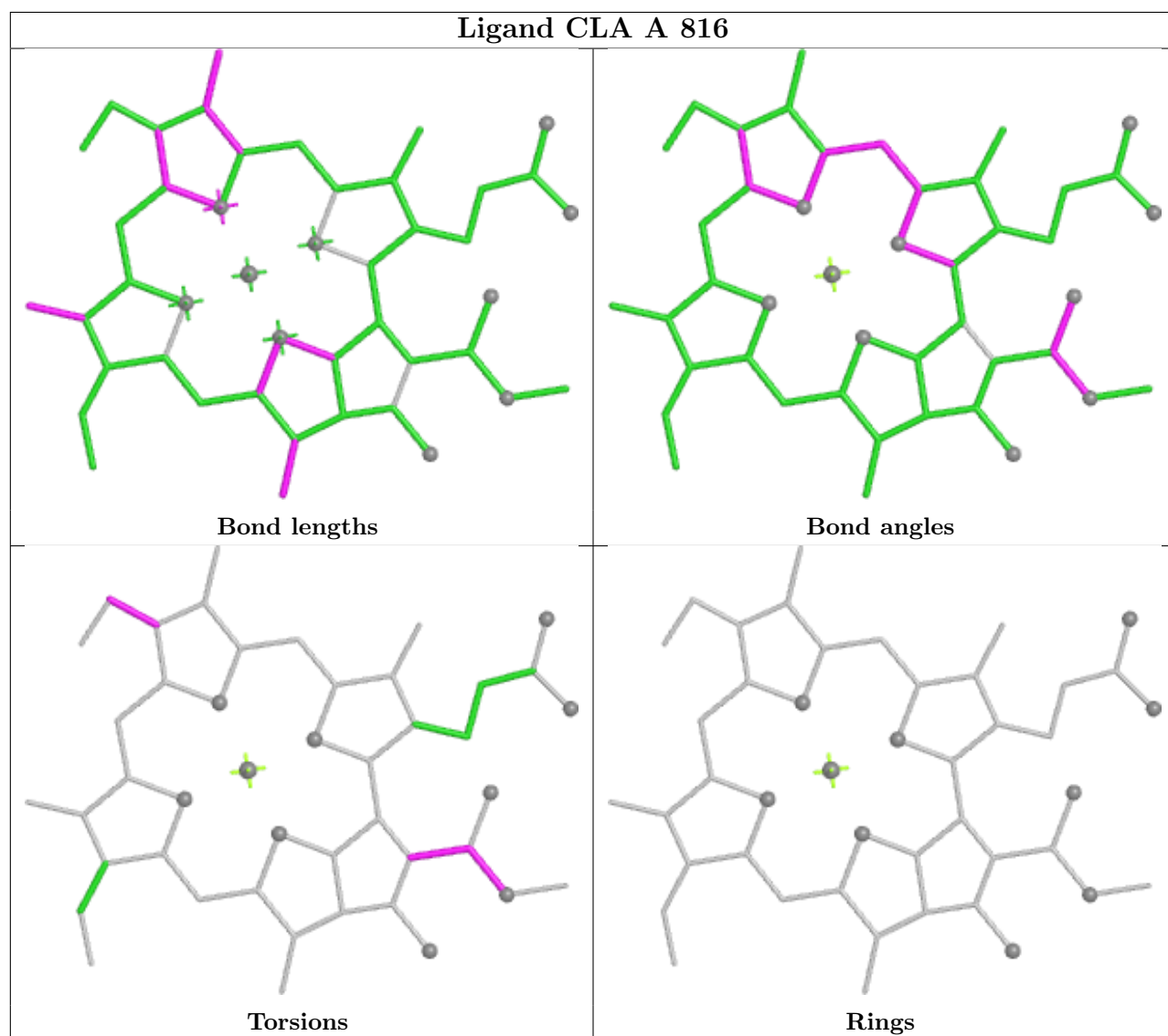
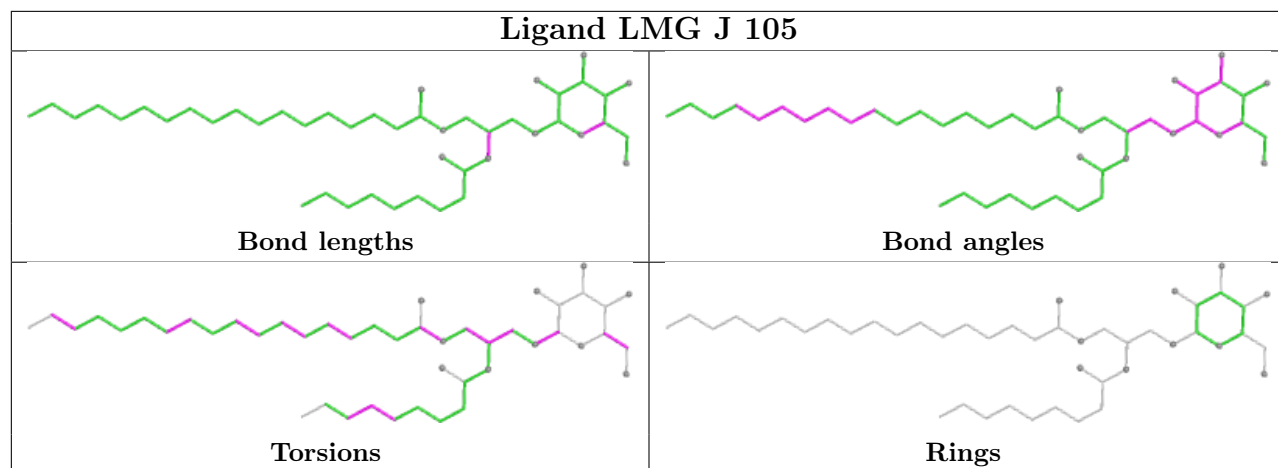


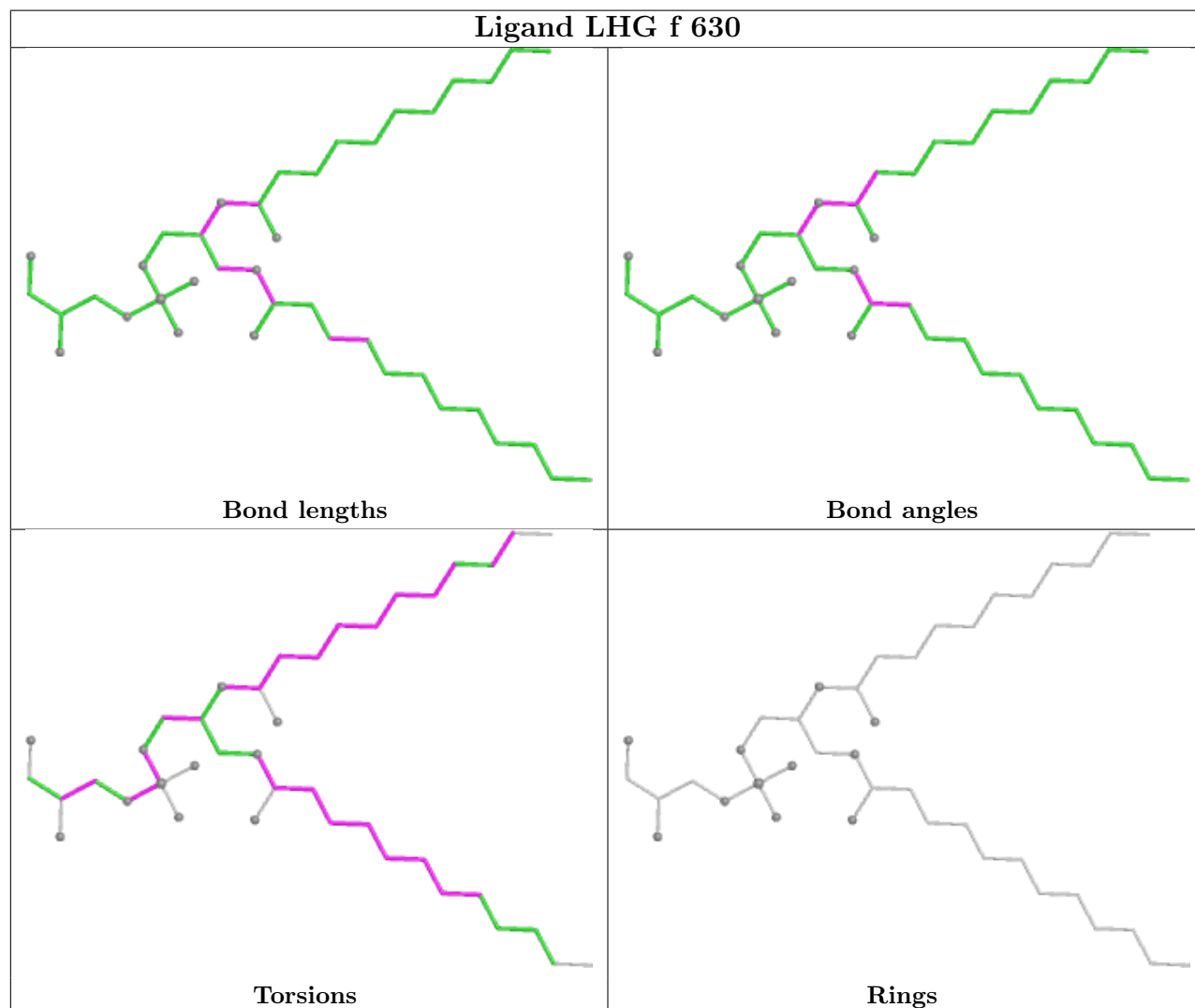
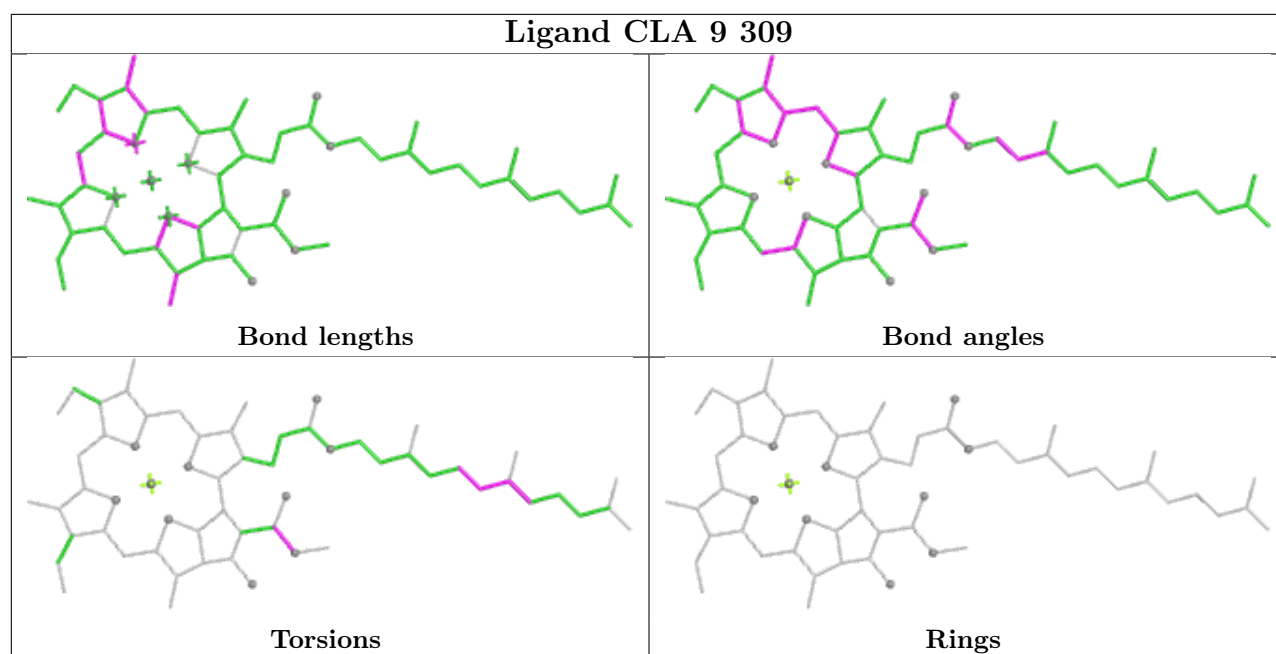
Rings

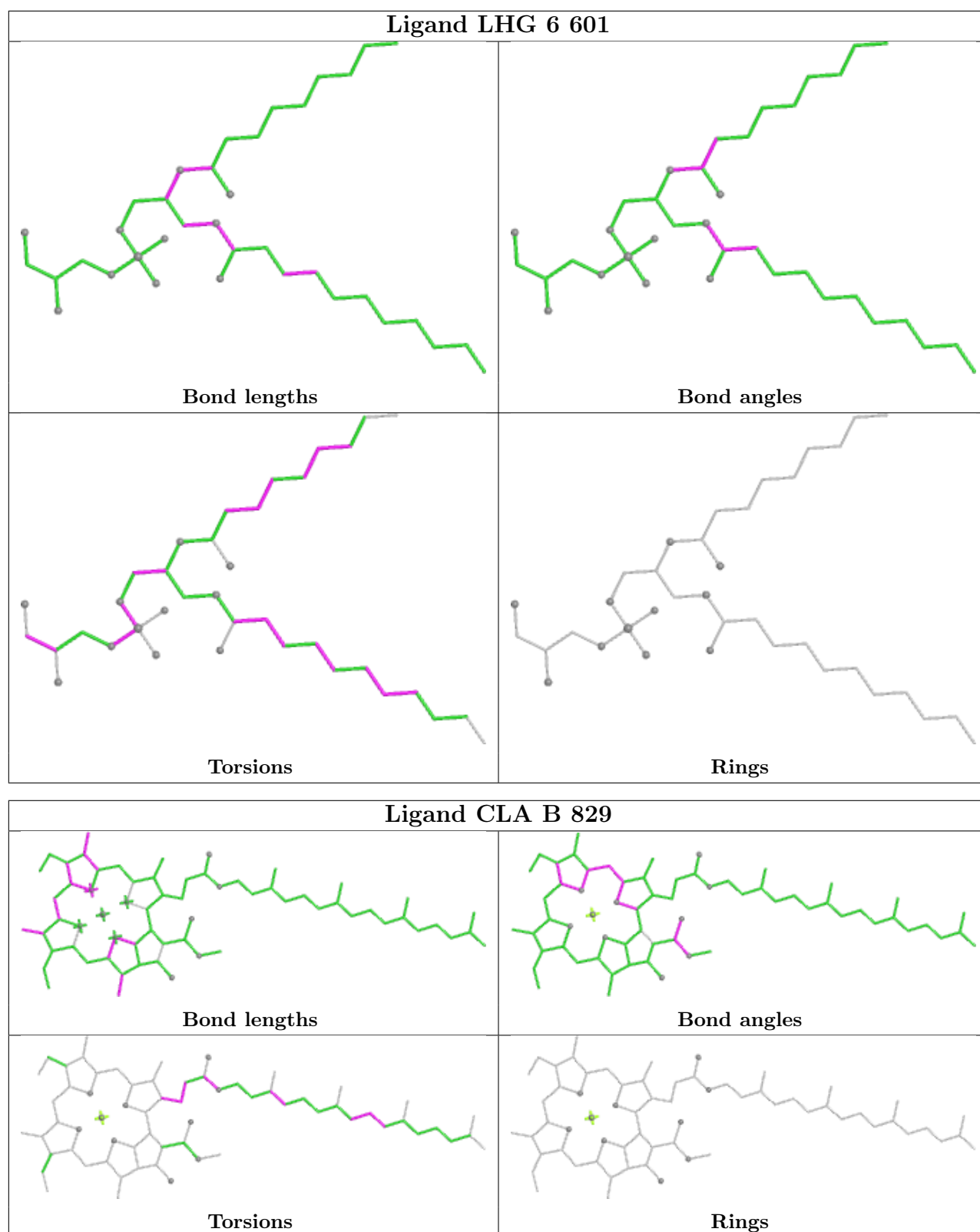
Ligand CLA B 803**Ligand CLA i 603**



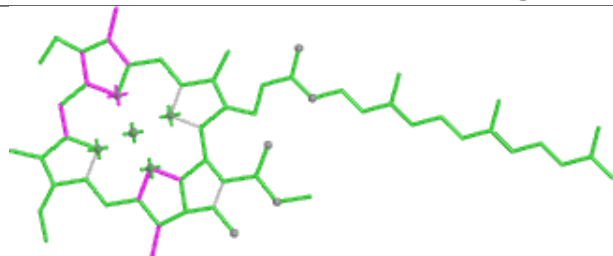




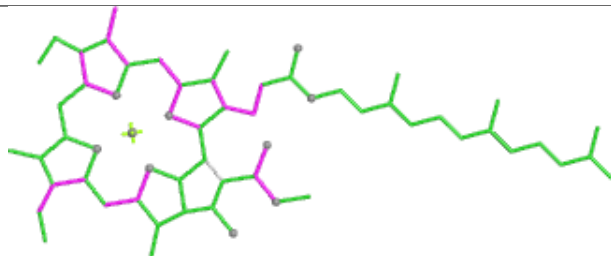




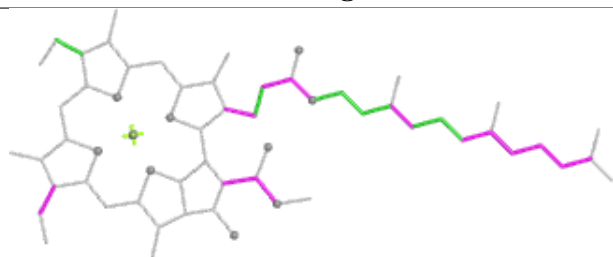
Ligand CLA B 817



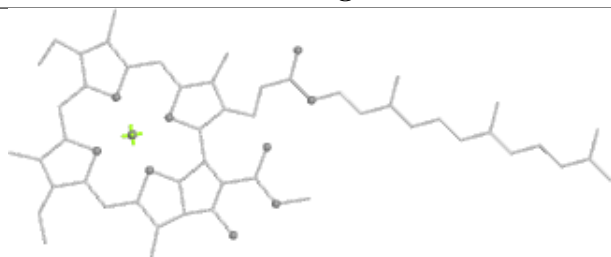
Bond lengths



Bond angles

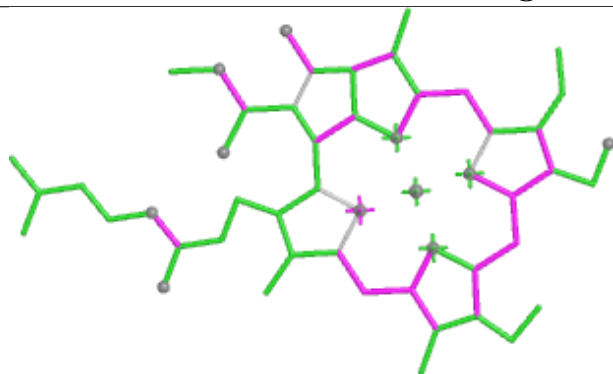


Torsions

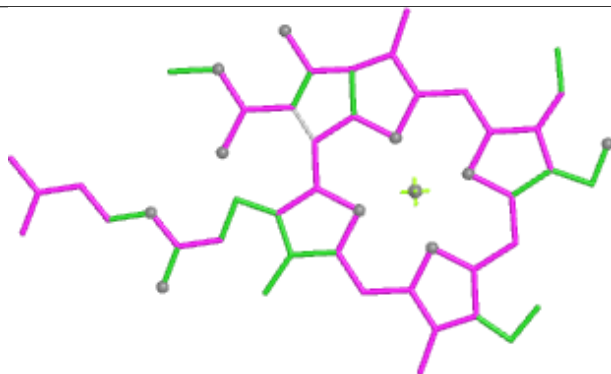


Rings

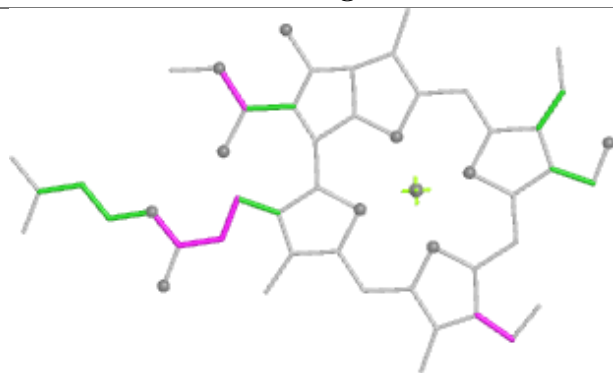
Ligand CHL 3 305



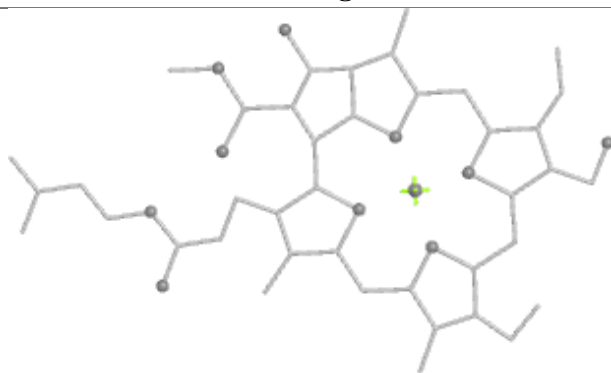
Bond lengths



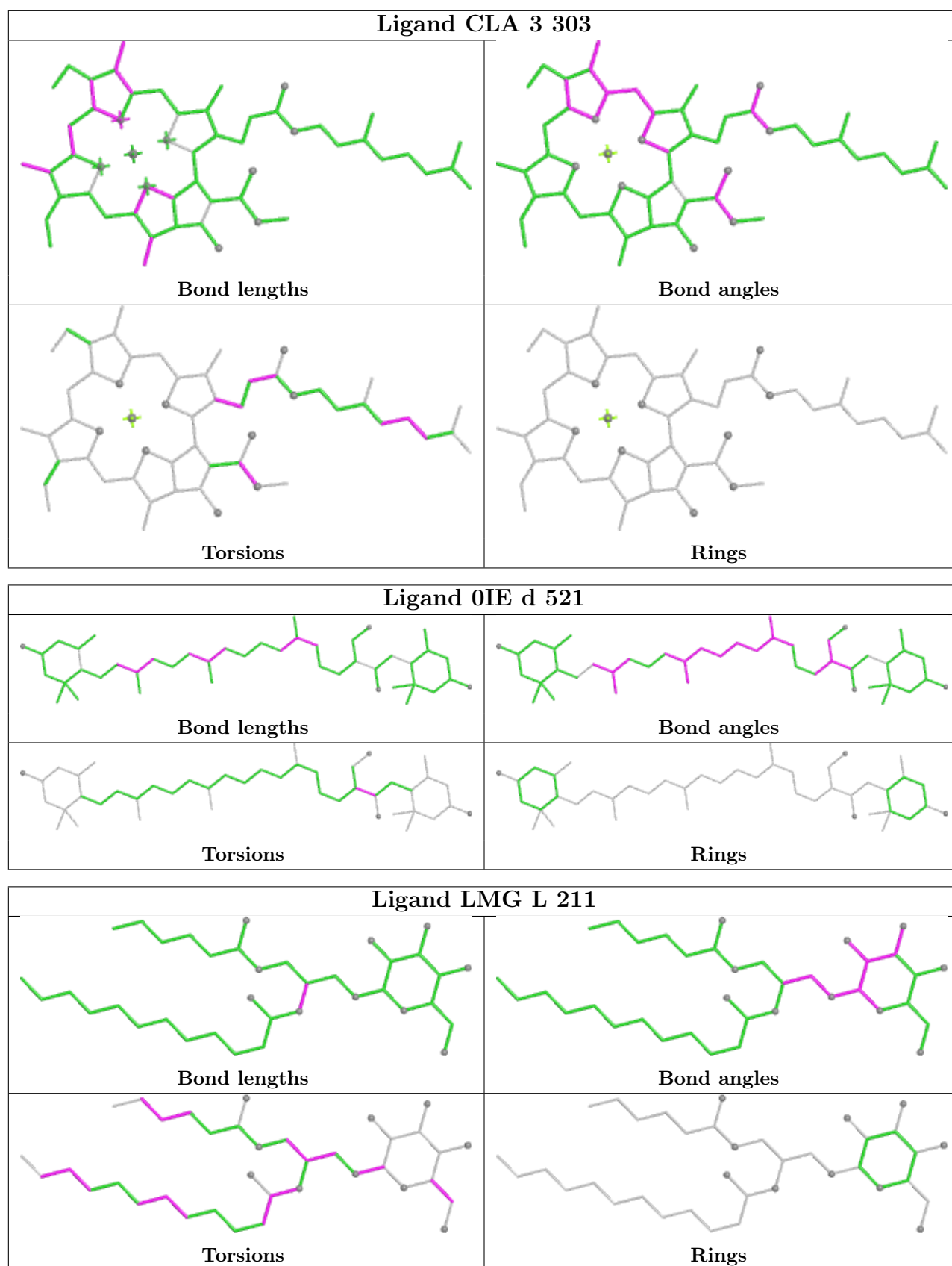
Bond angles

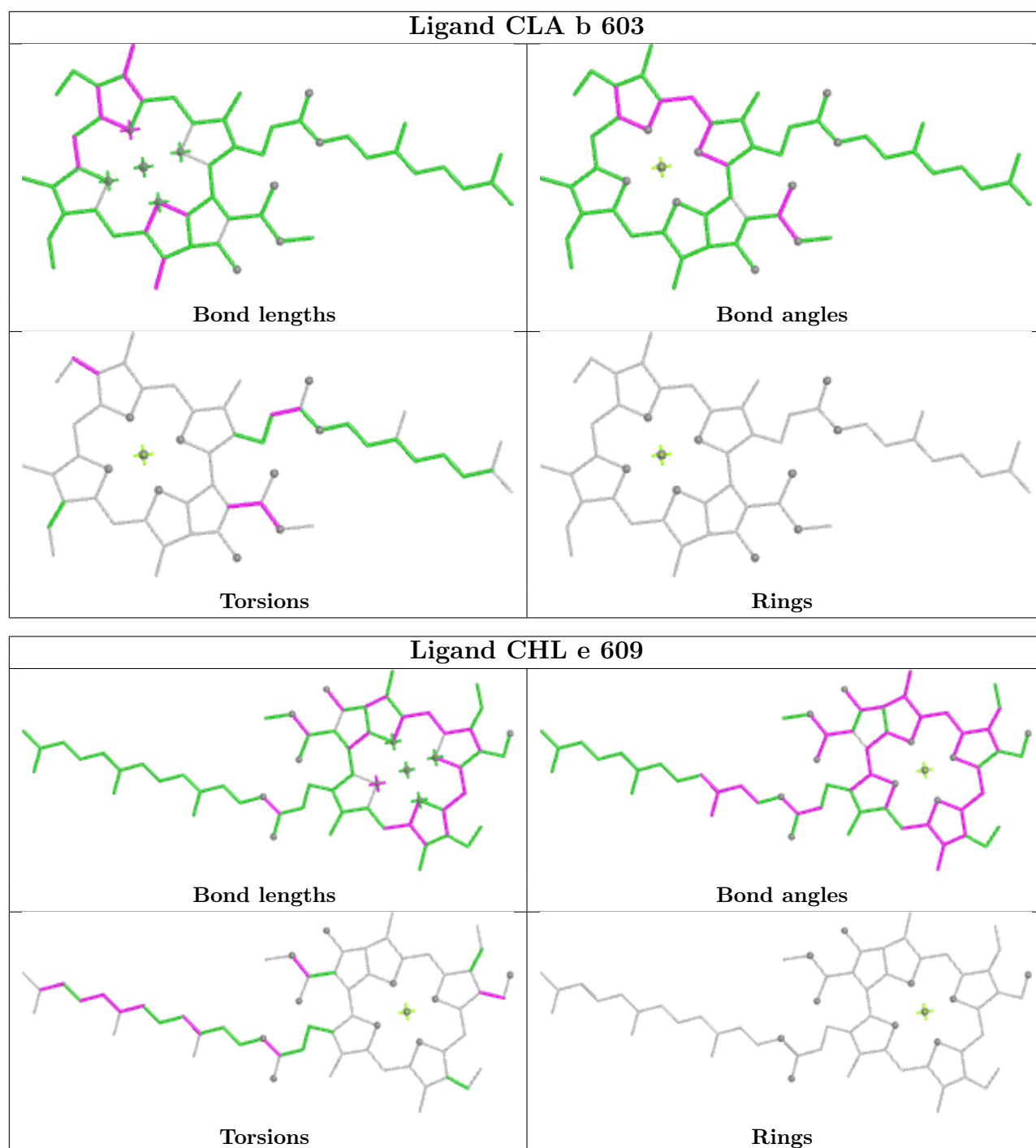


Torsions

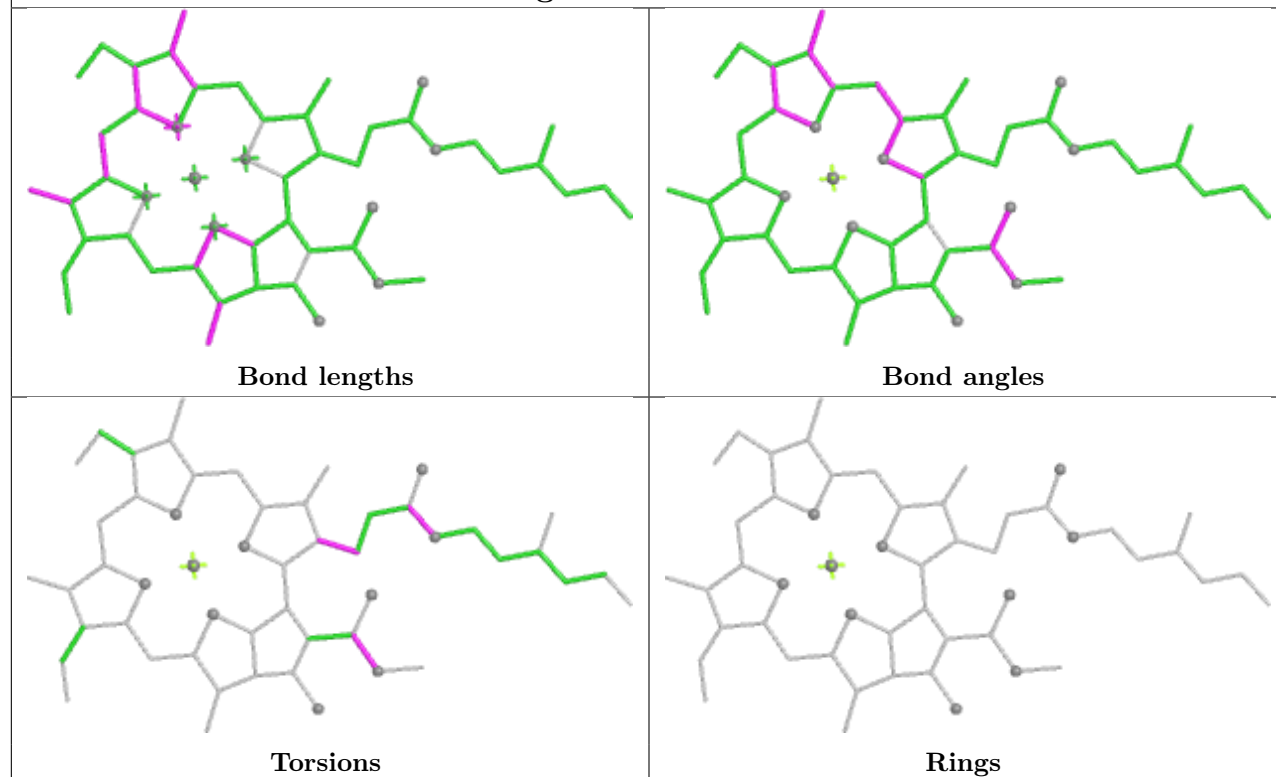


Rings

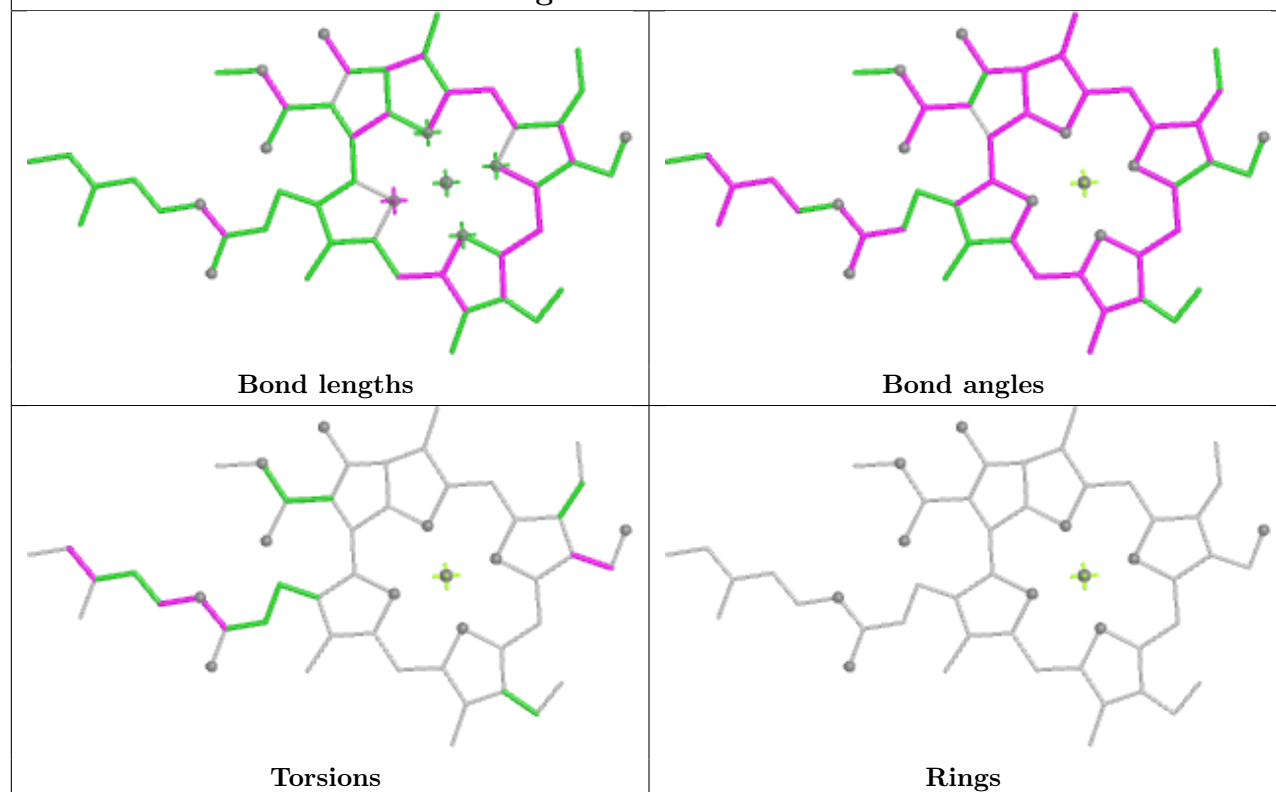


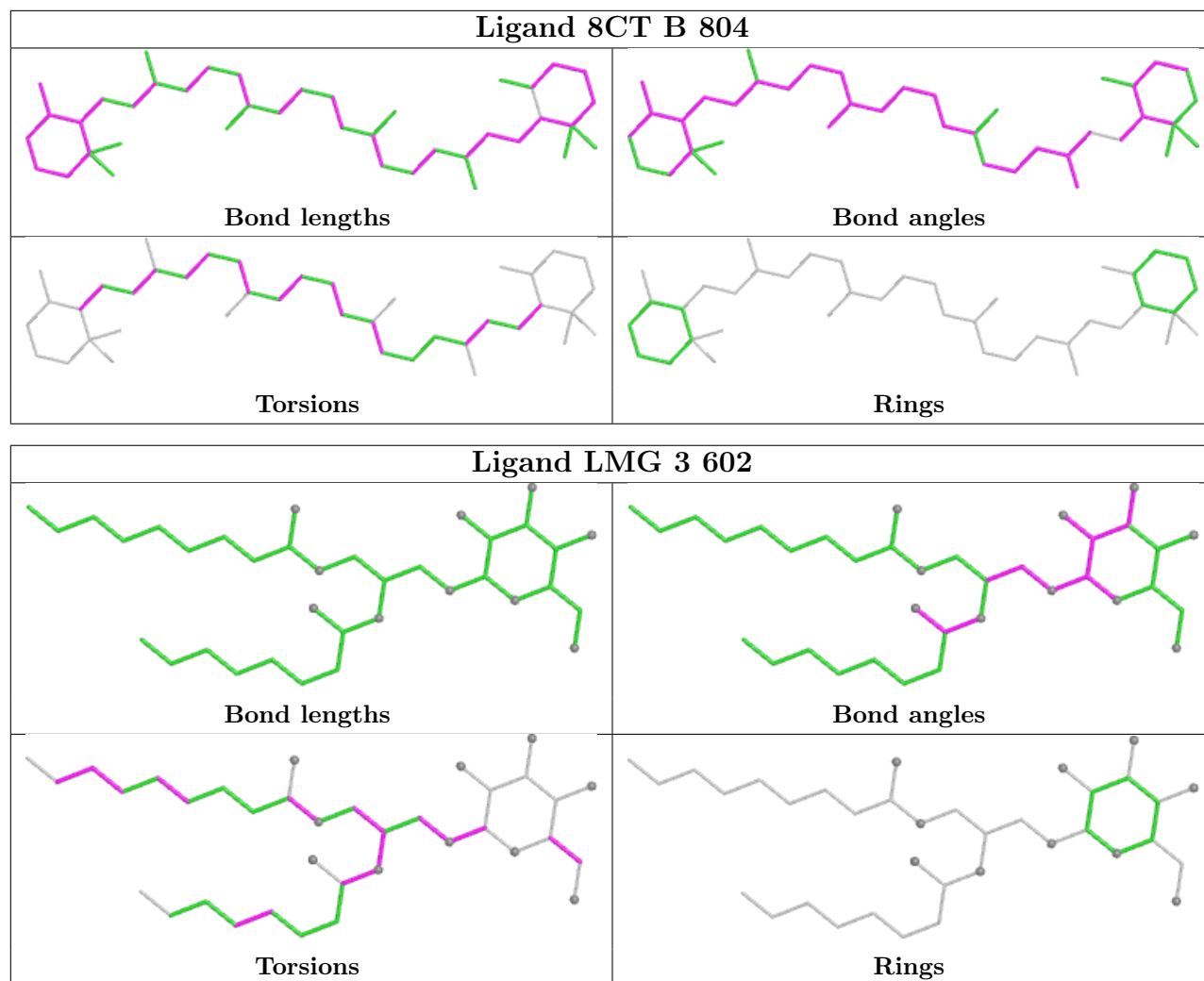


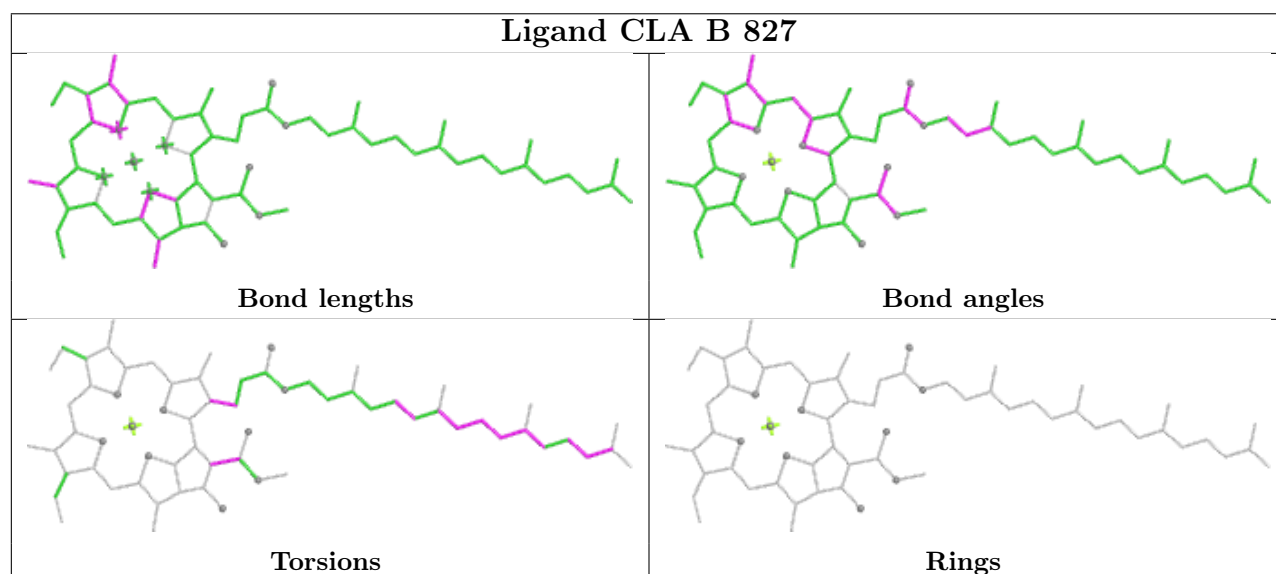
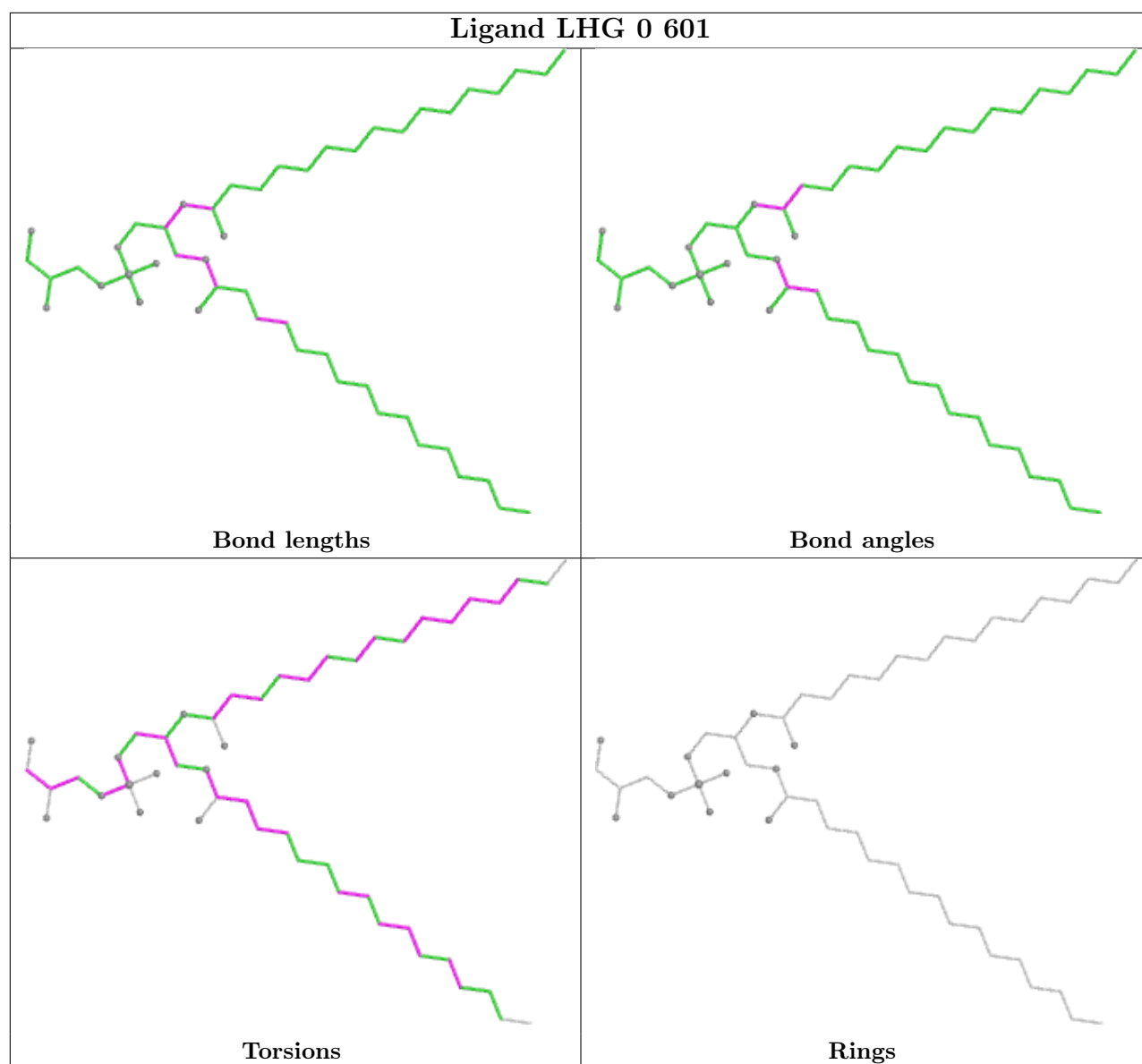
Ligand CLA 1 311

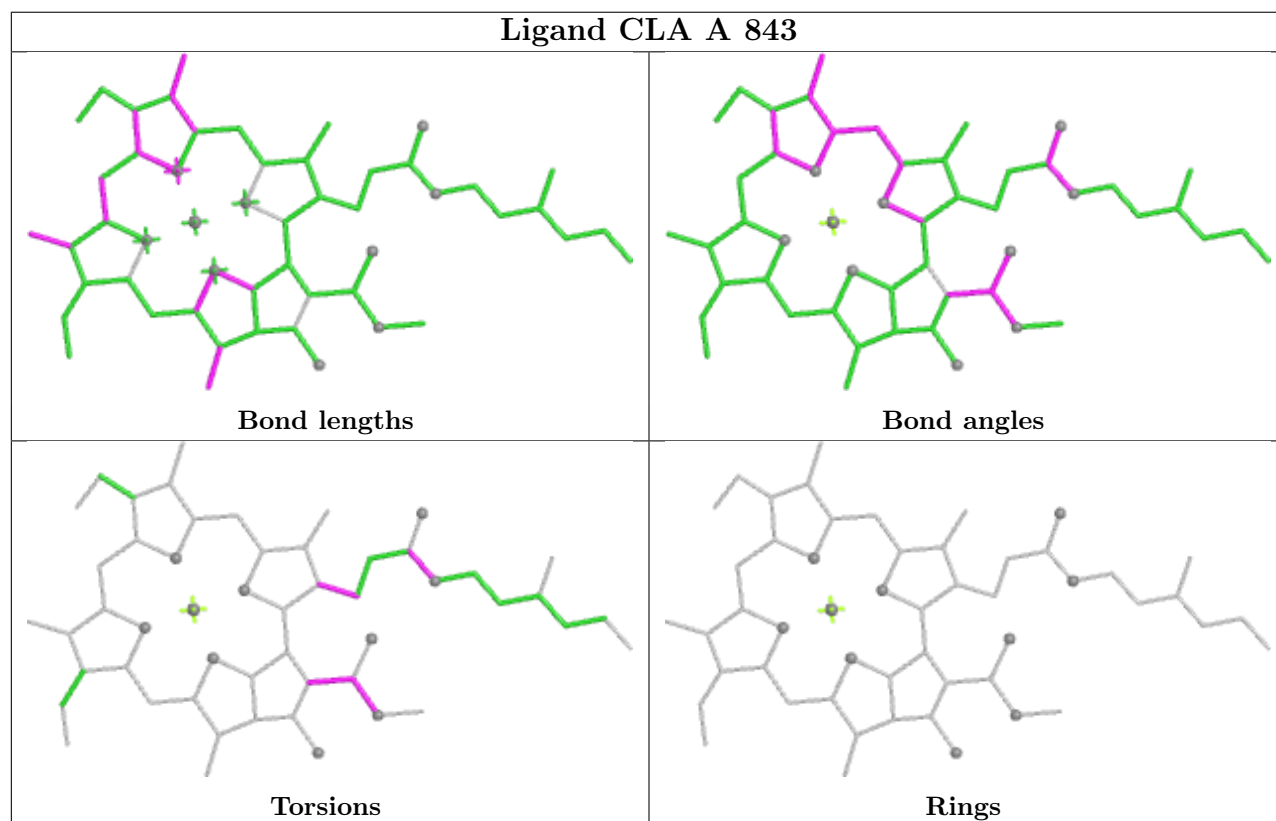
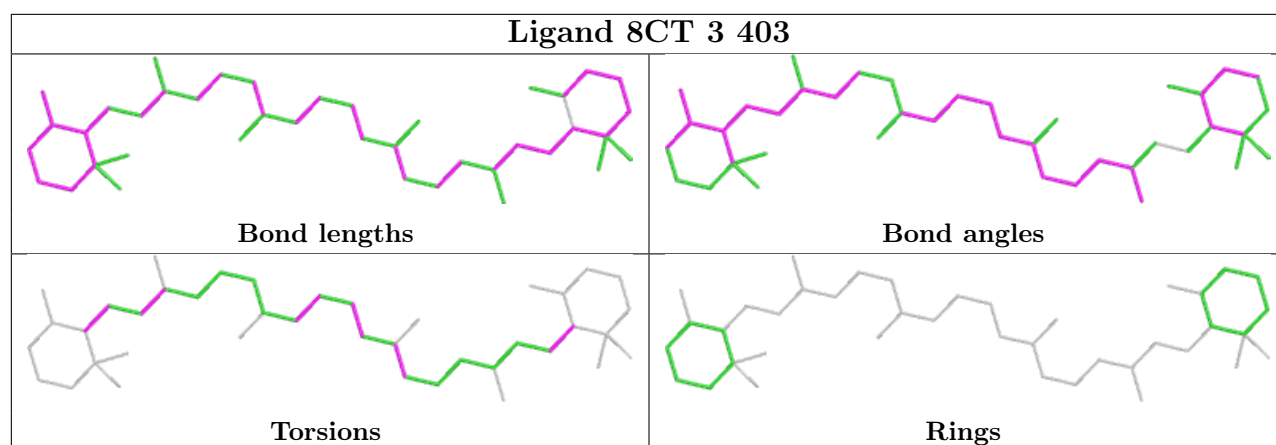


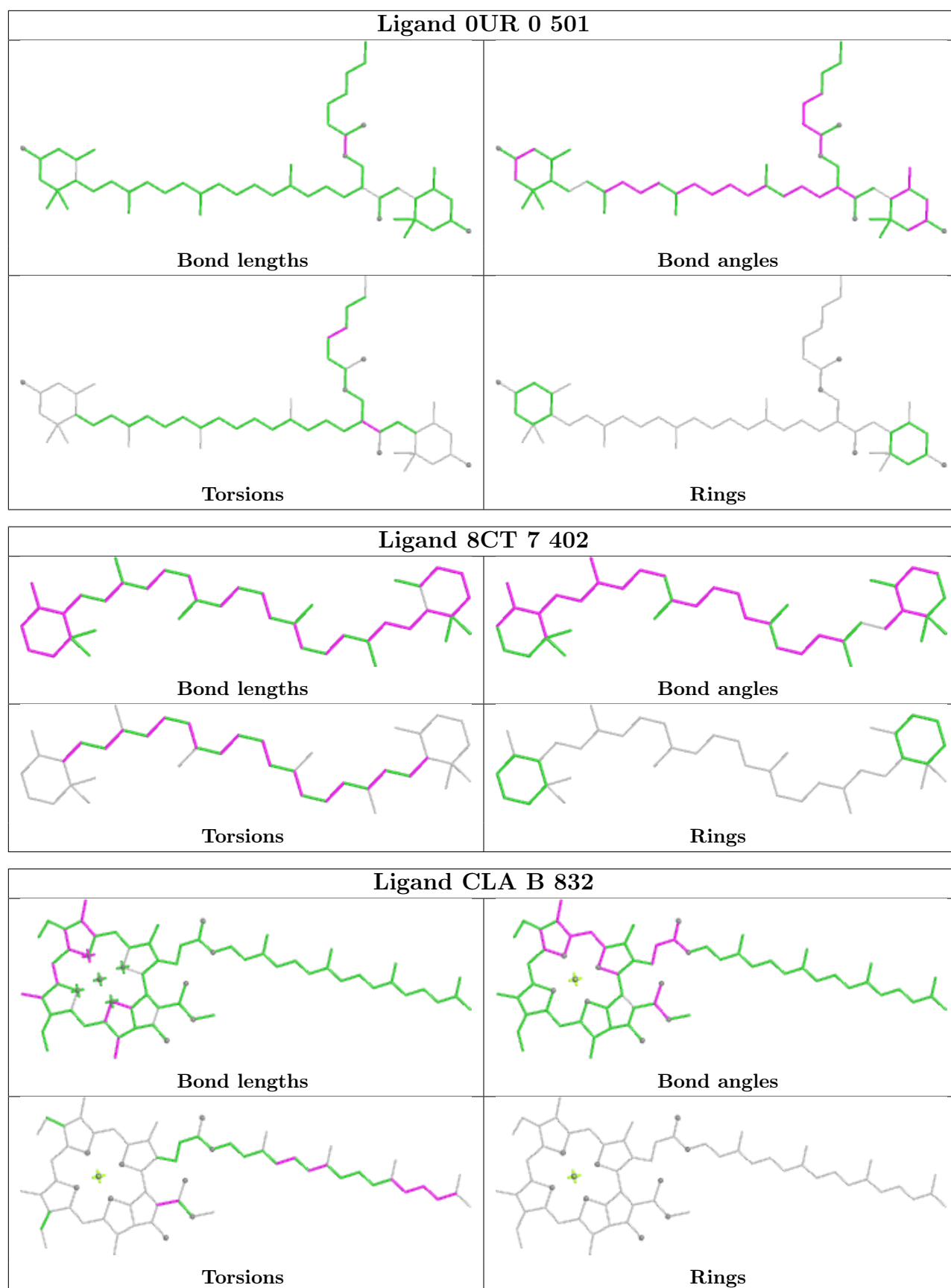
Ligand CHL 6 313

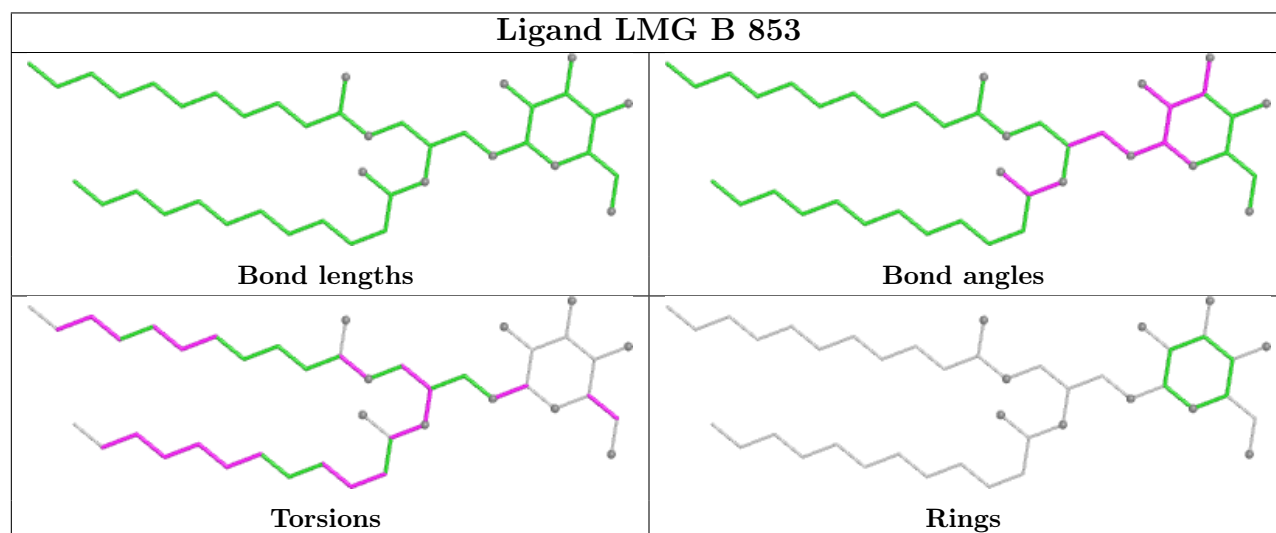
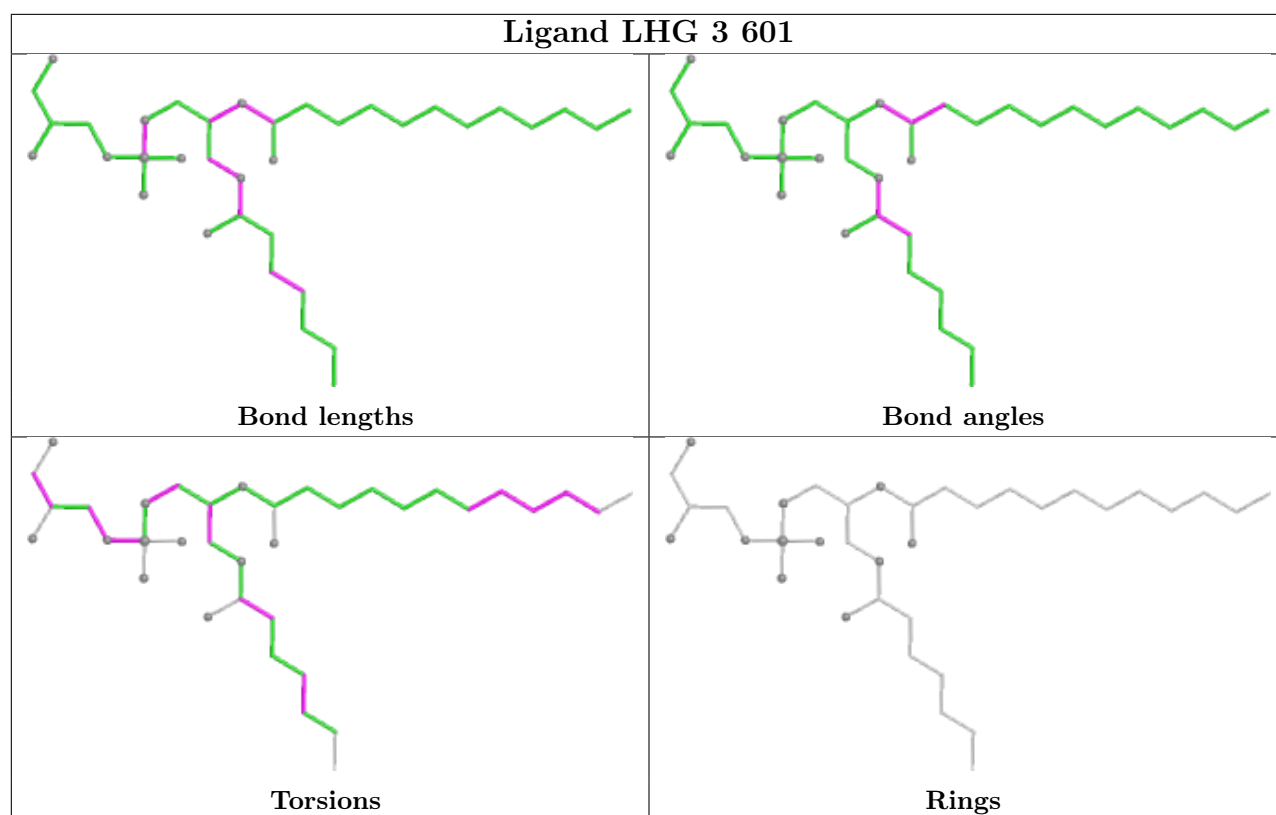




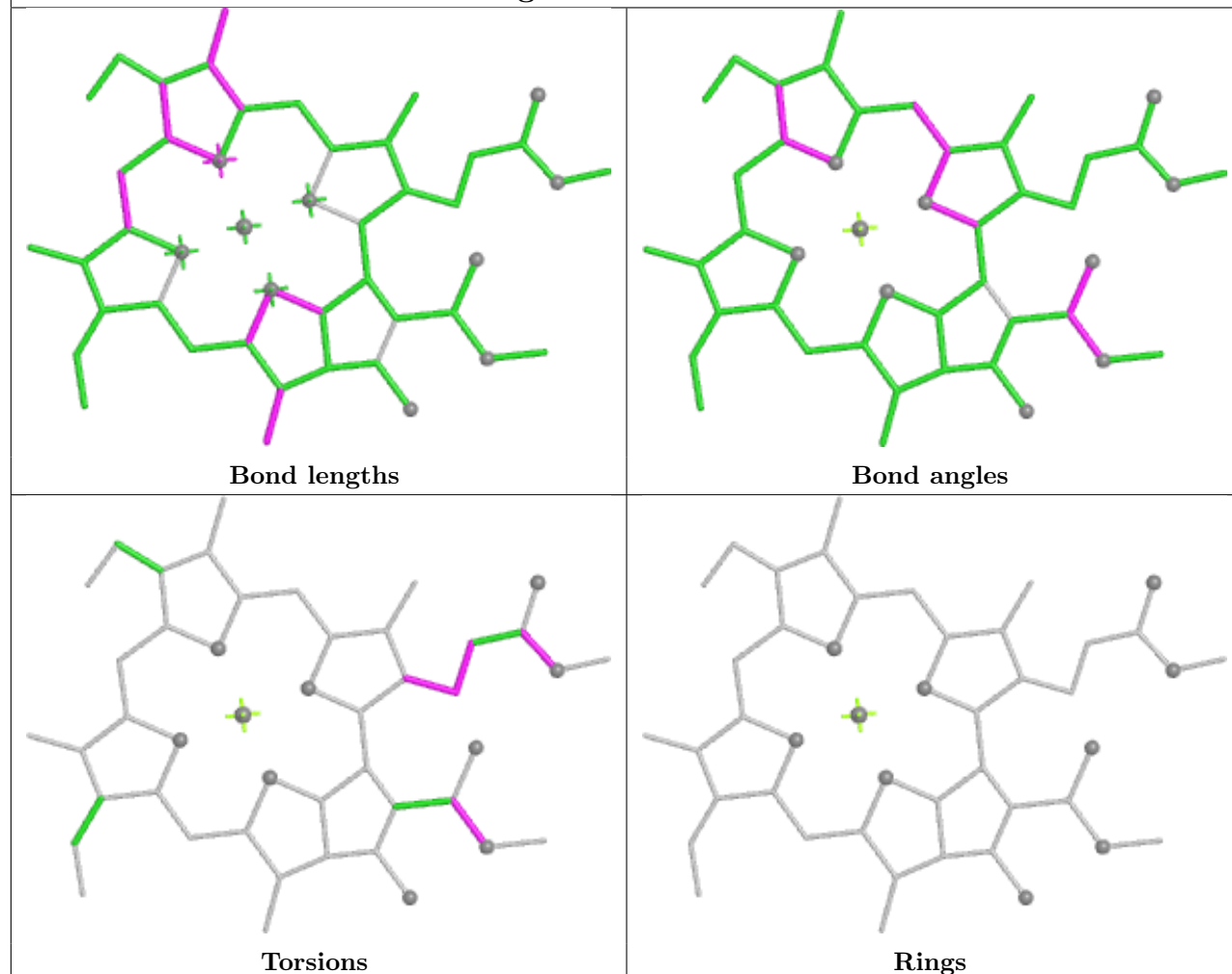




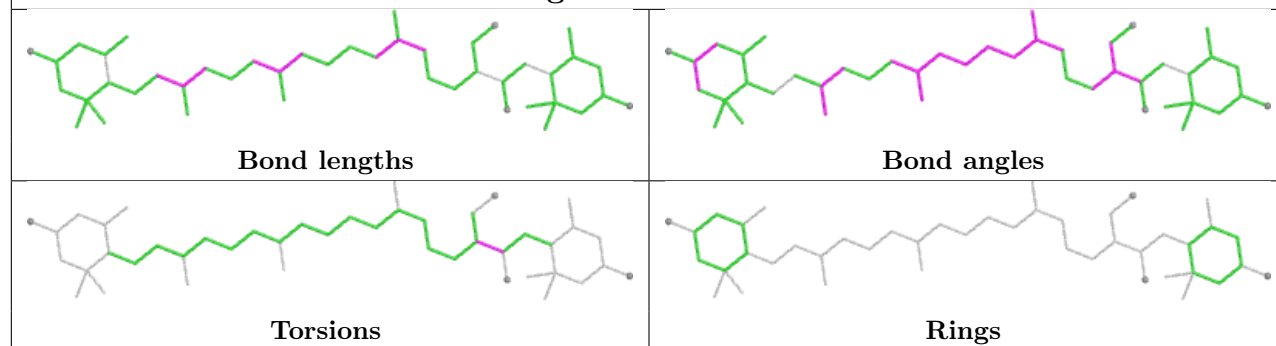




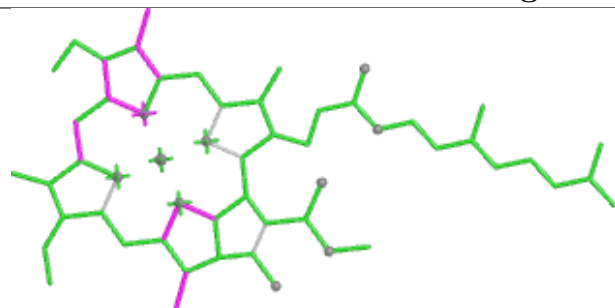
Ligand CLA 5 308



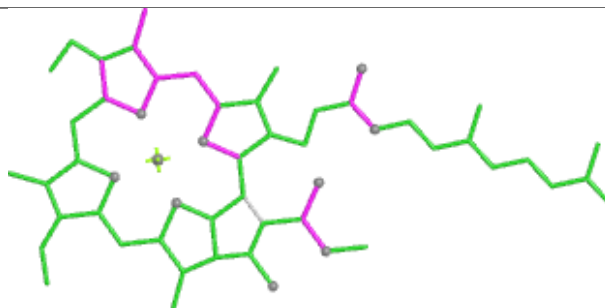
Ligand OIE c 521



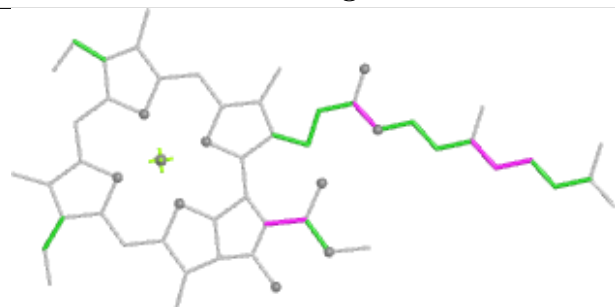
Ligand CLA 7 304



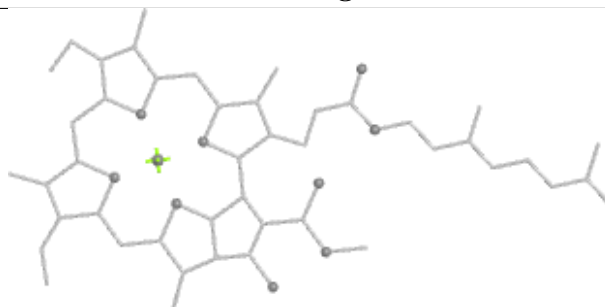
Bond lengths



Bond angles

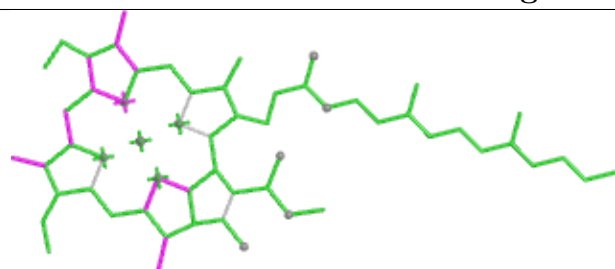


Torsions

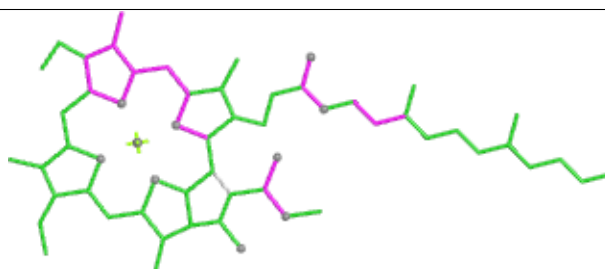


Rings

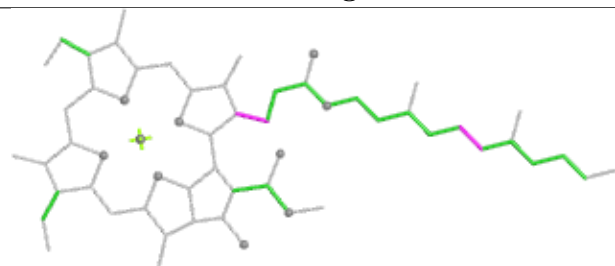
Ligand CLA 6 309



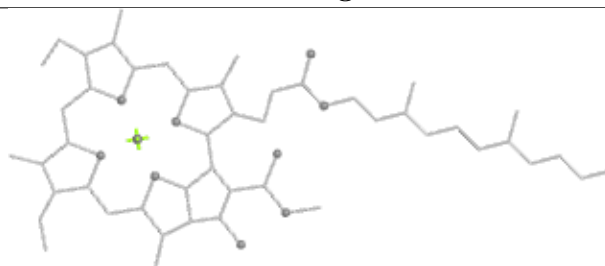
Bond lengths



Bond angles

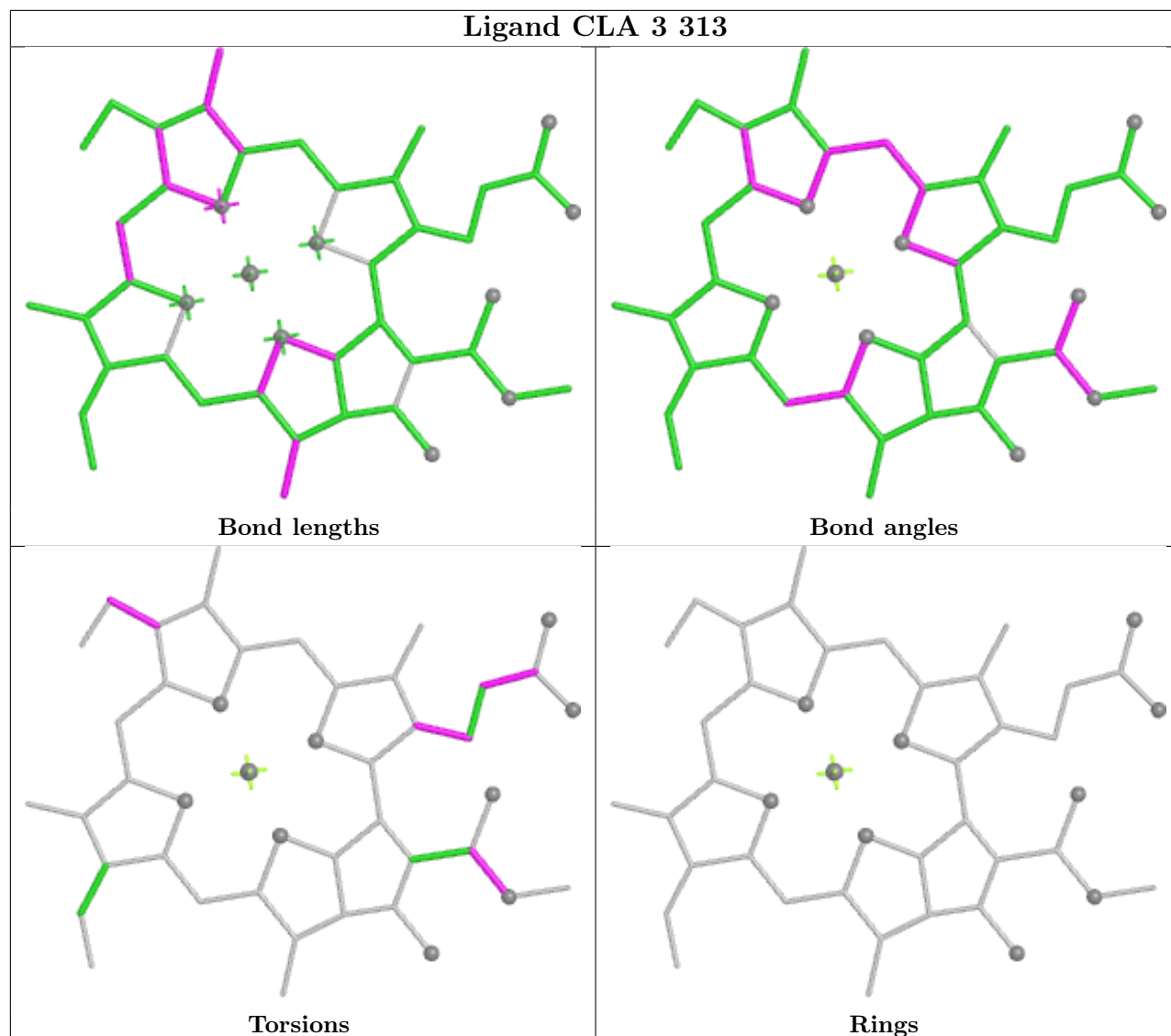


Torsions

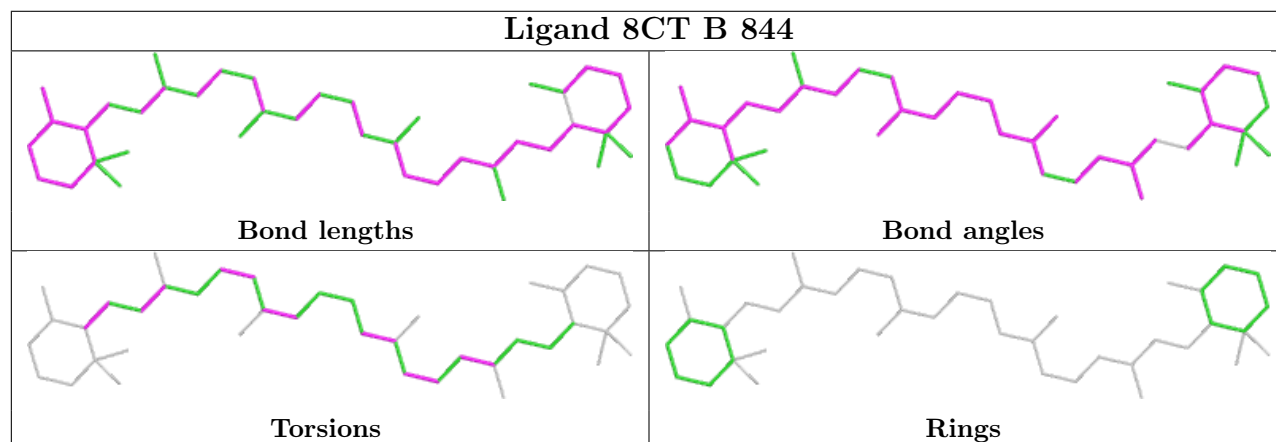


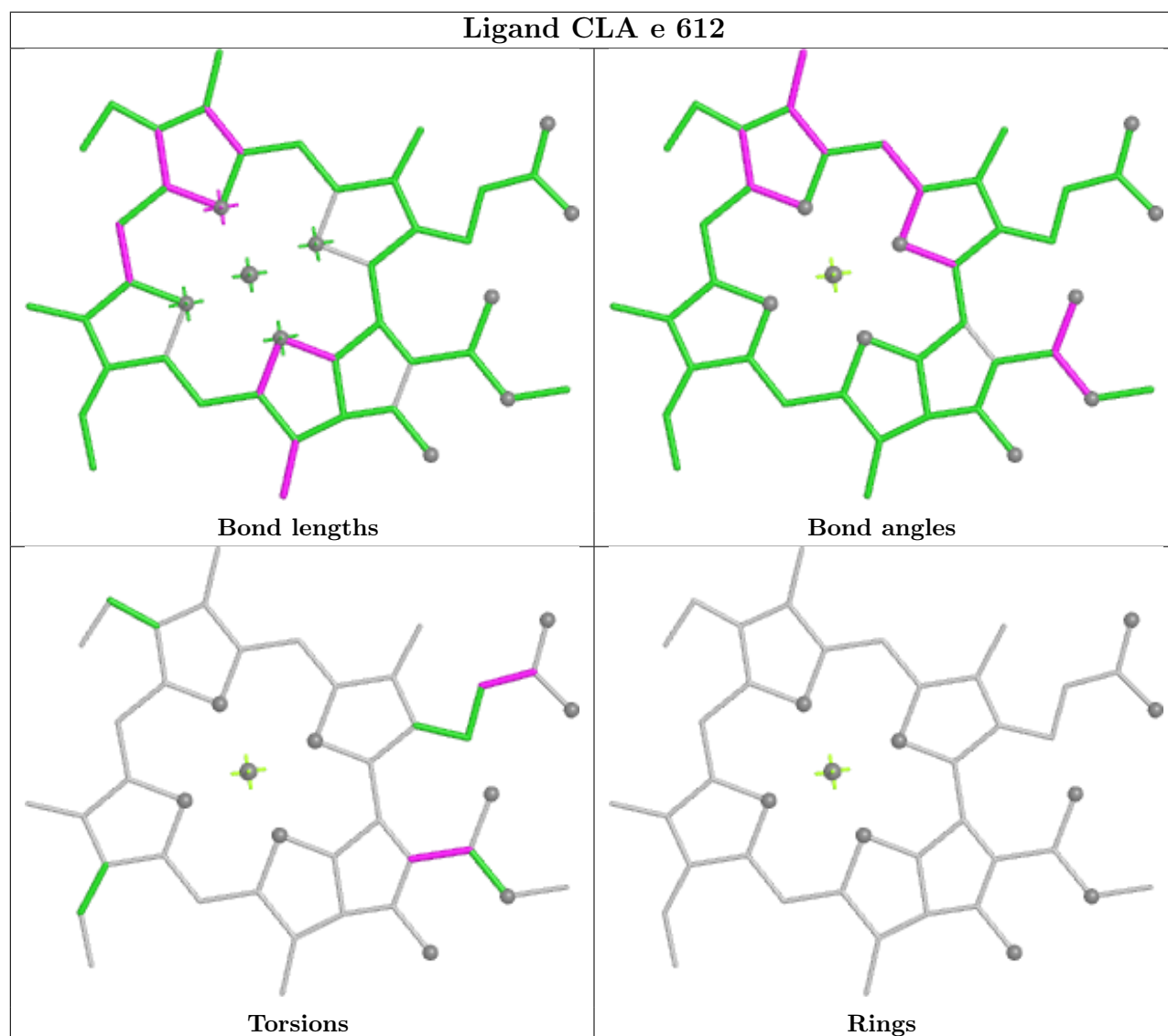
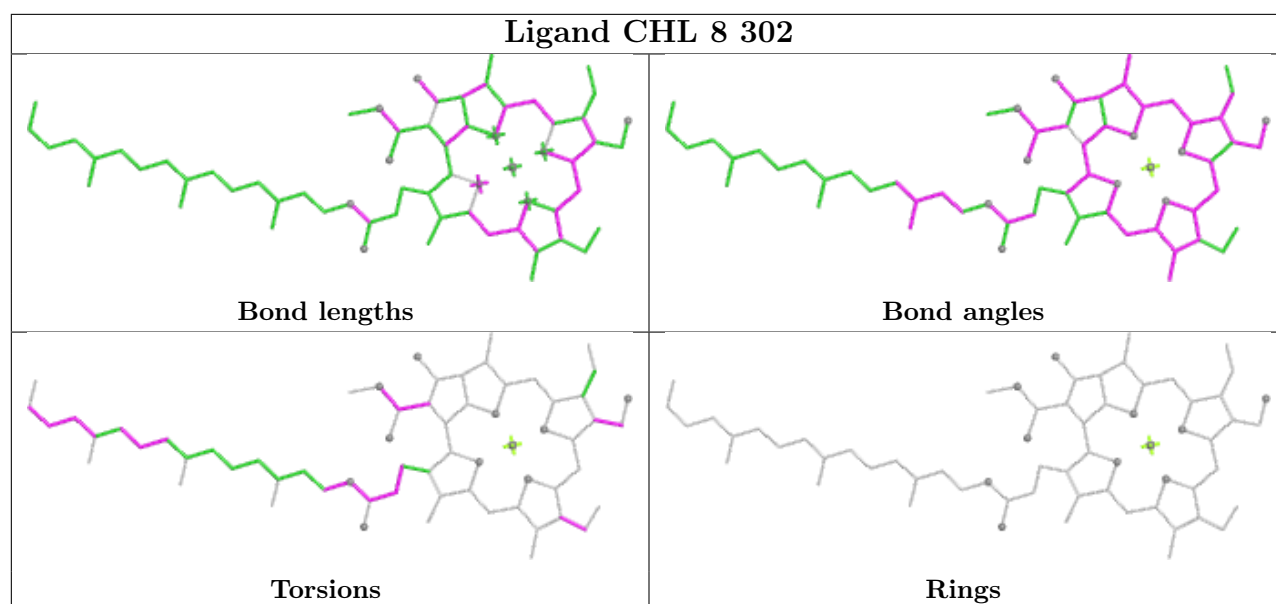
Rings

Ligand CLA 3 313

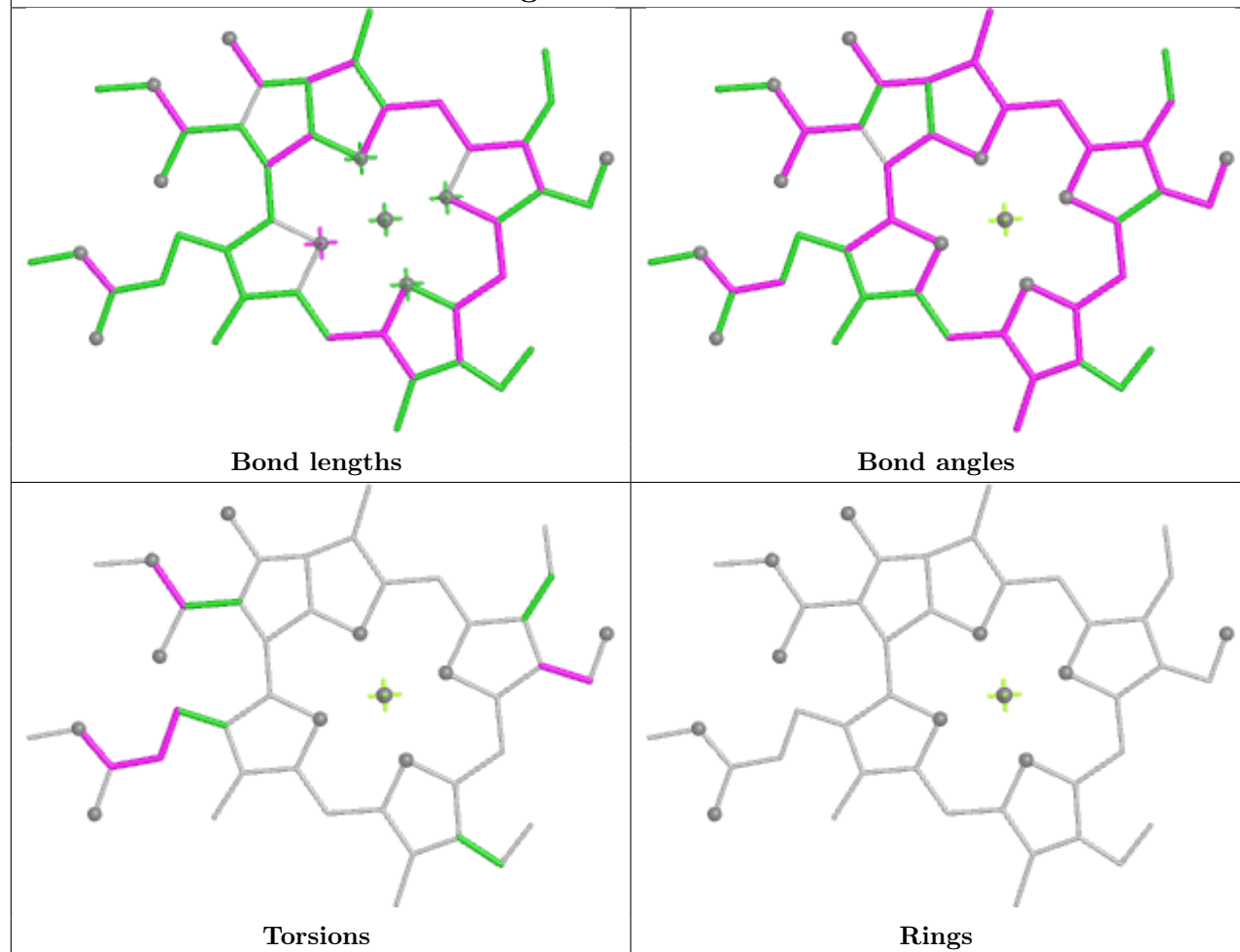


Ligand 8CT B 844

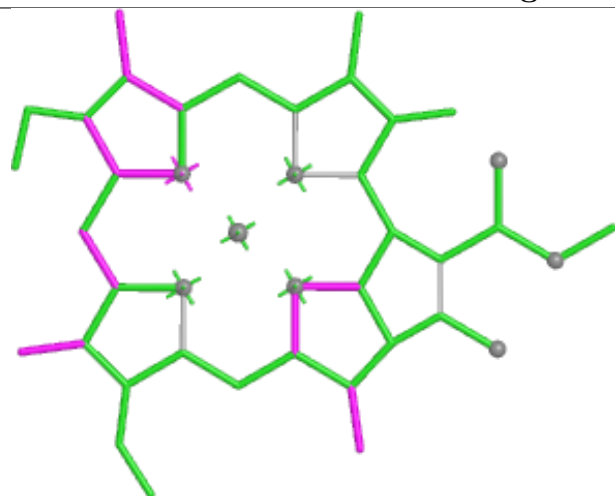




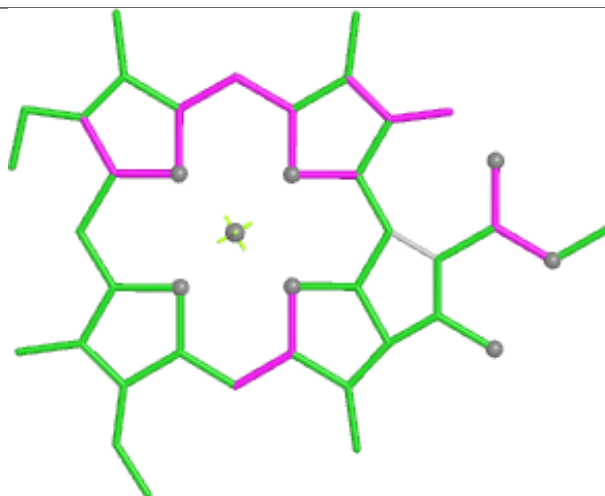
Ligand CHL 5 307



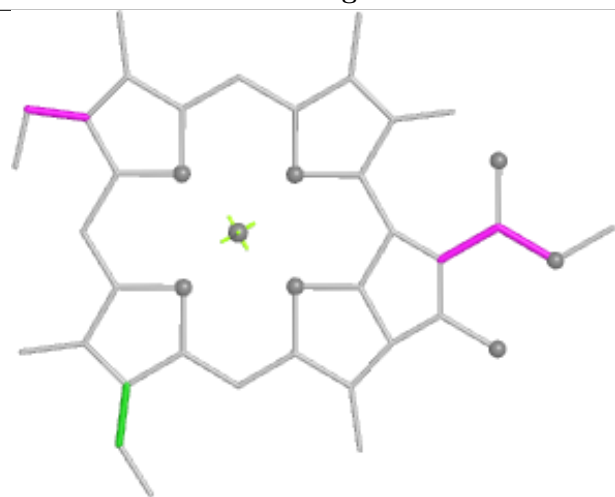
Ligand CLA 9 310



Bond lengths



Bond angles

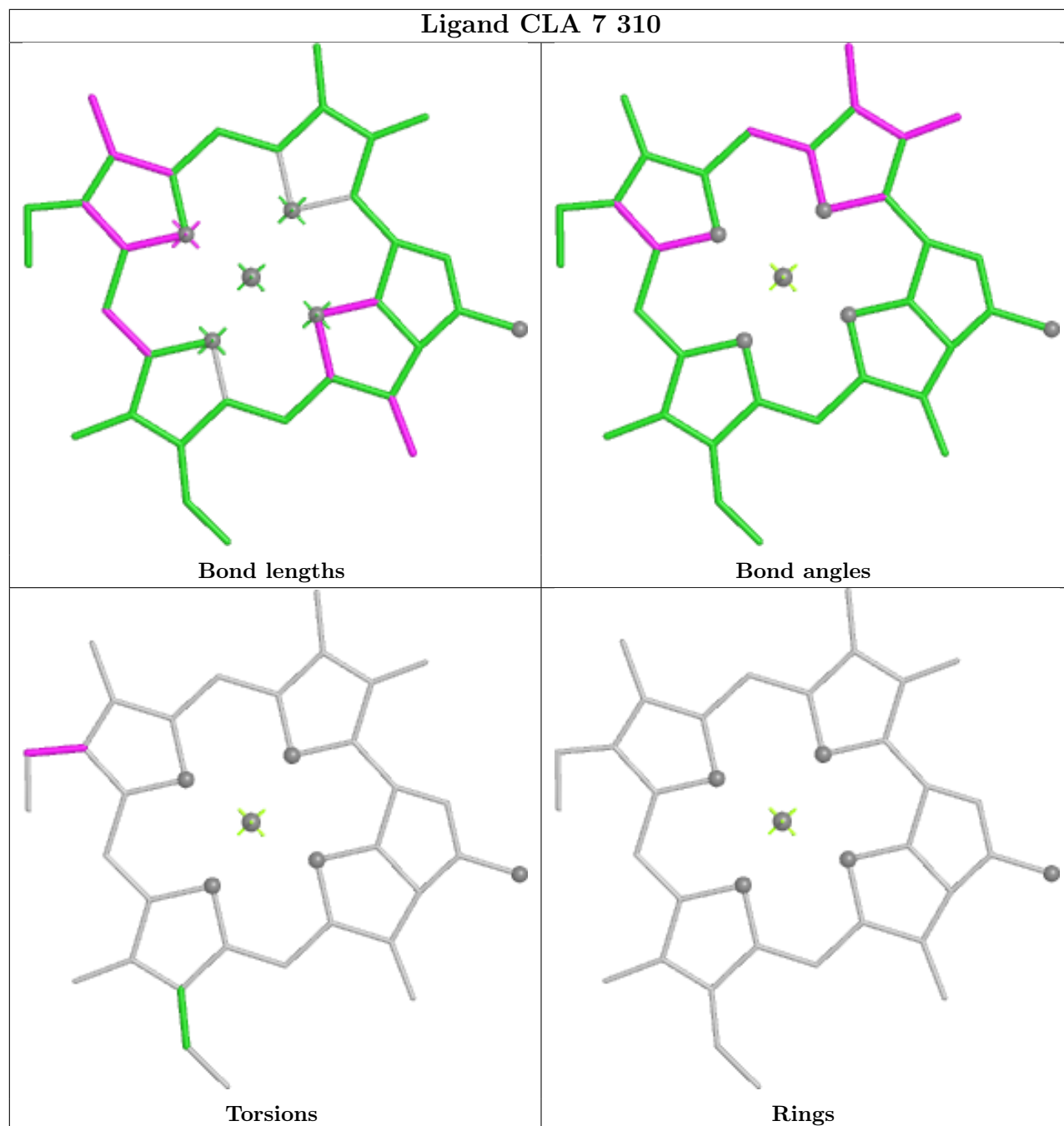


Torsions

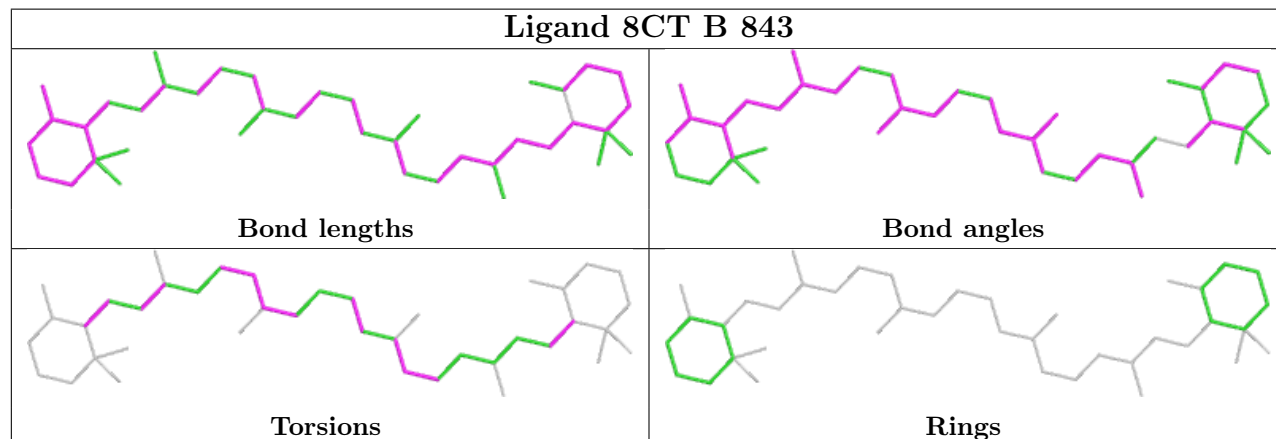


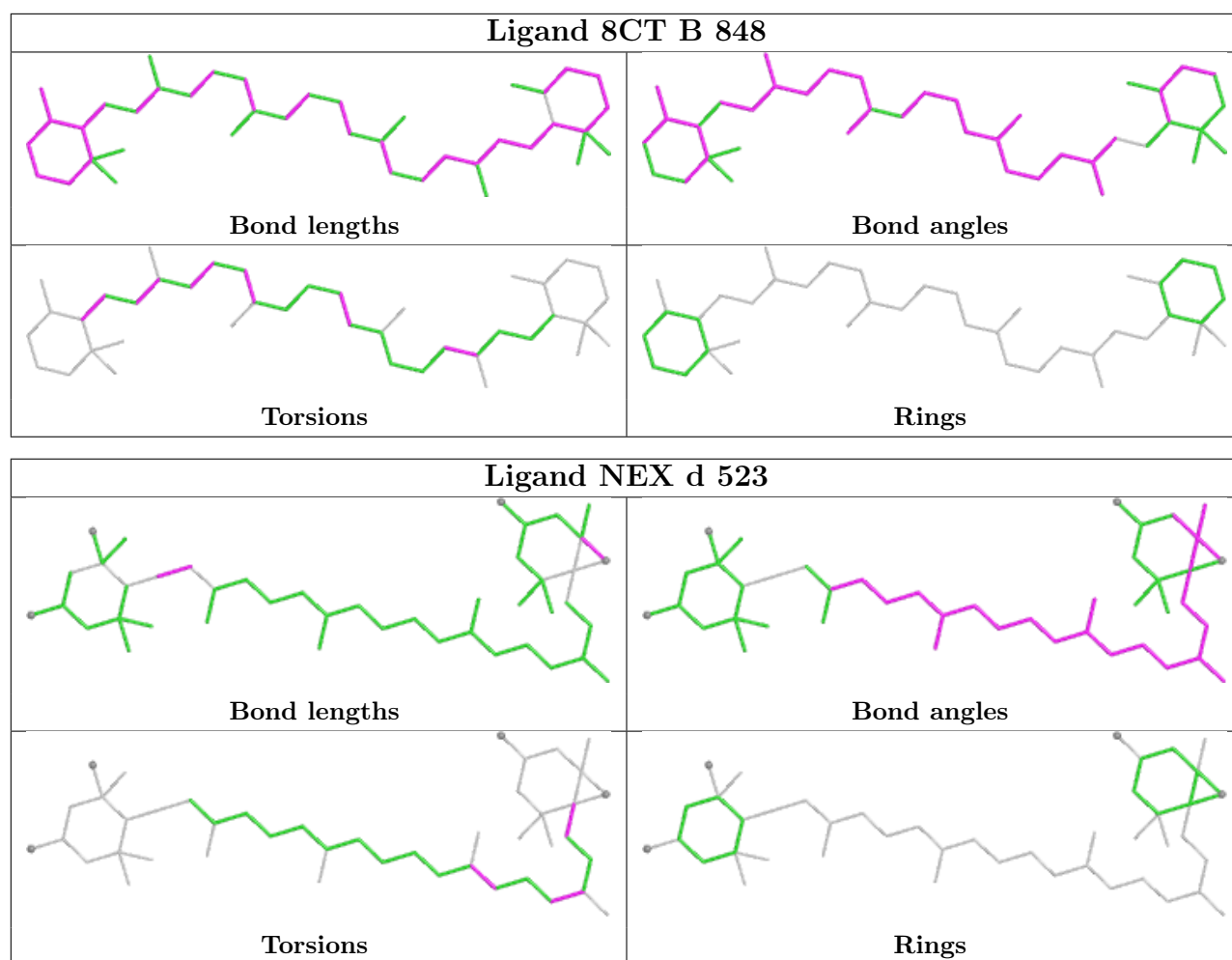
Rings

Ligand CLA 7 310

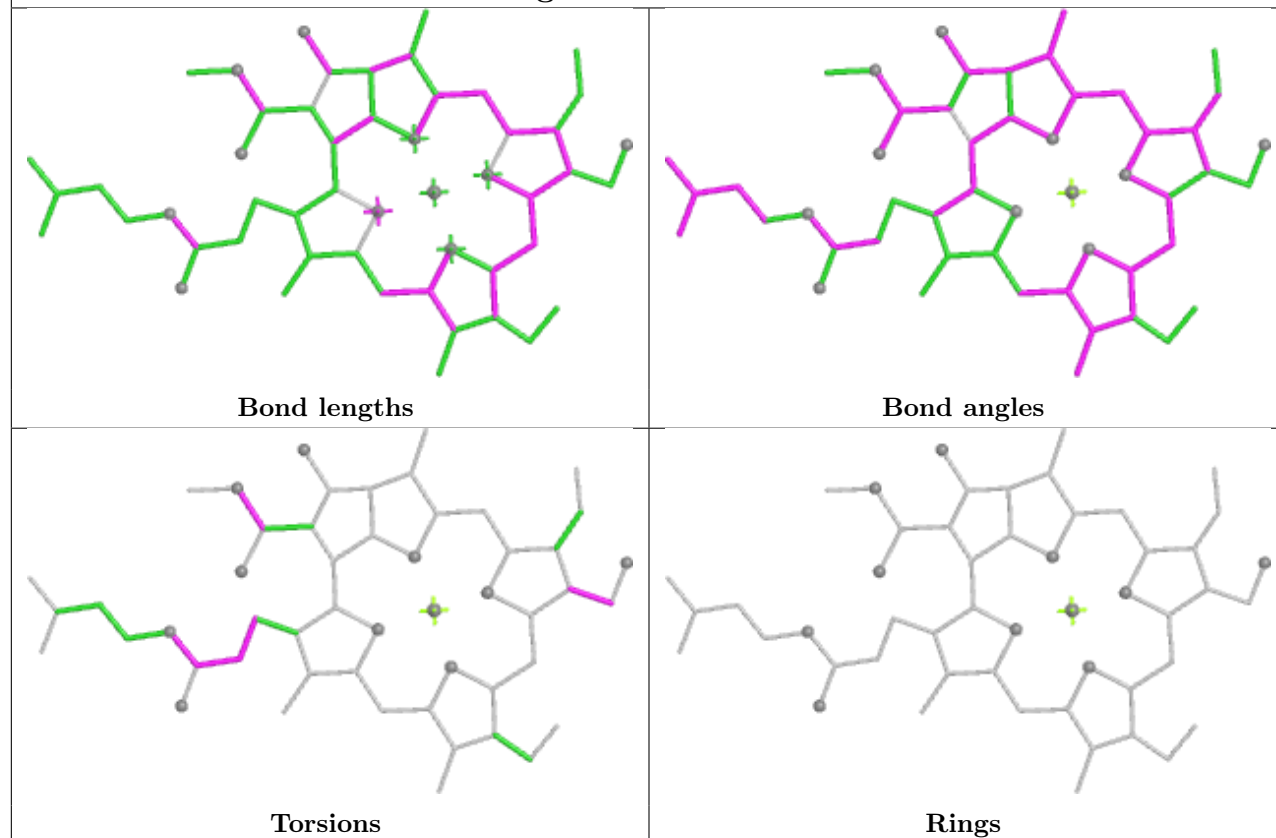


Ligand 8CT B 843

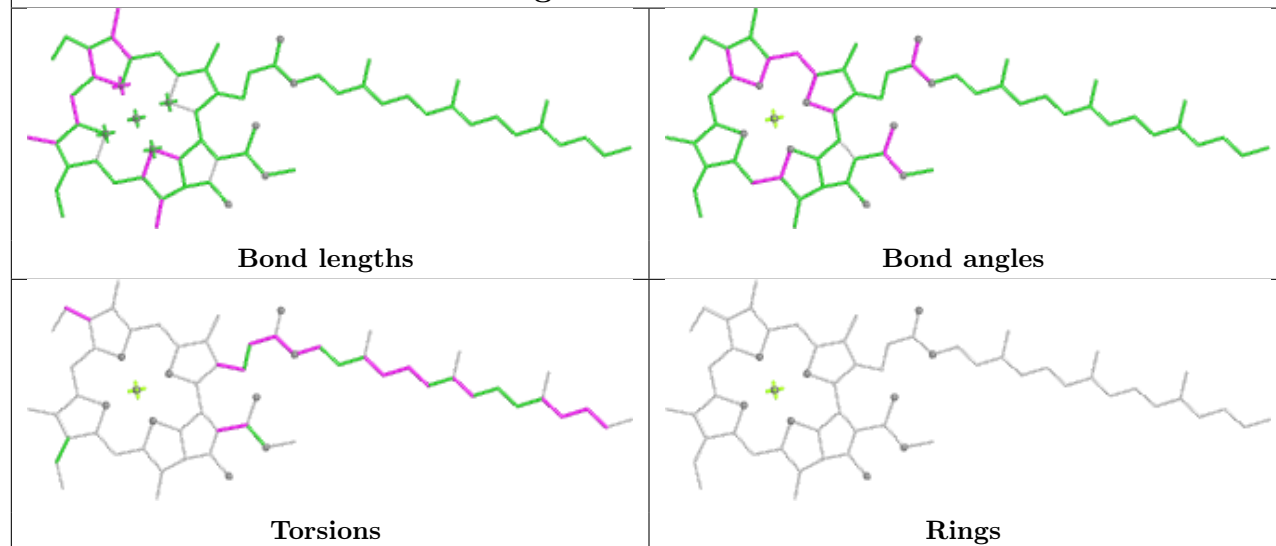




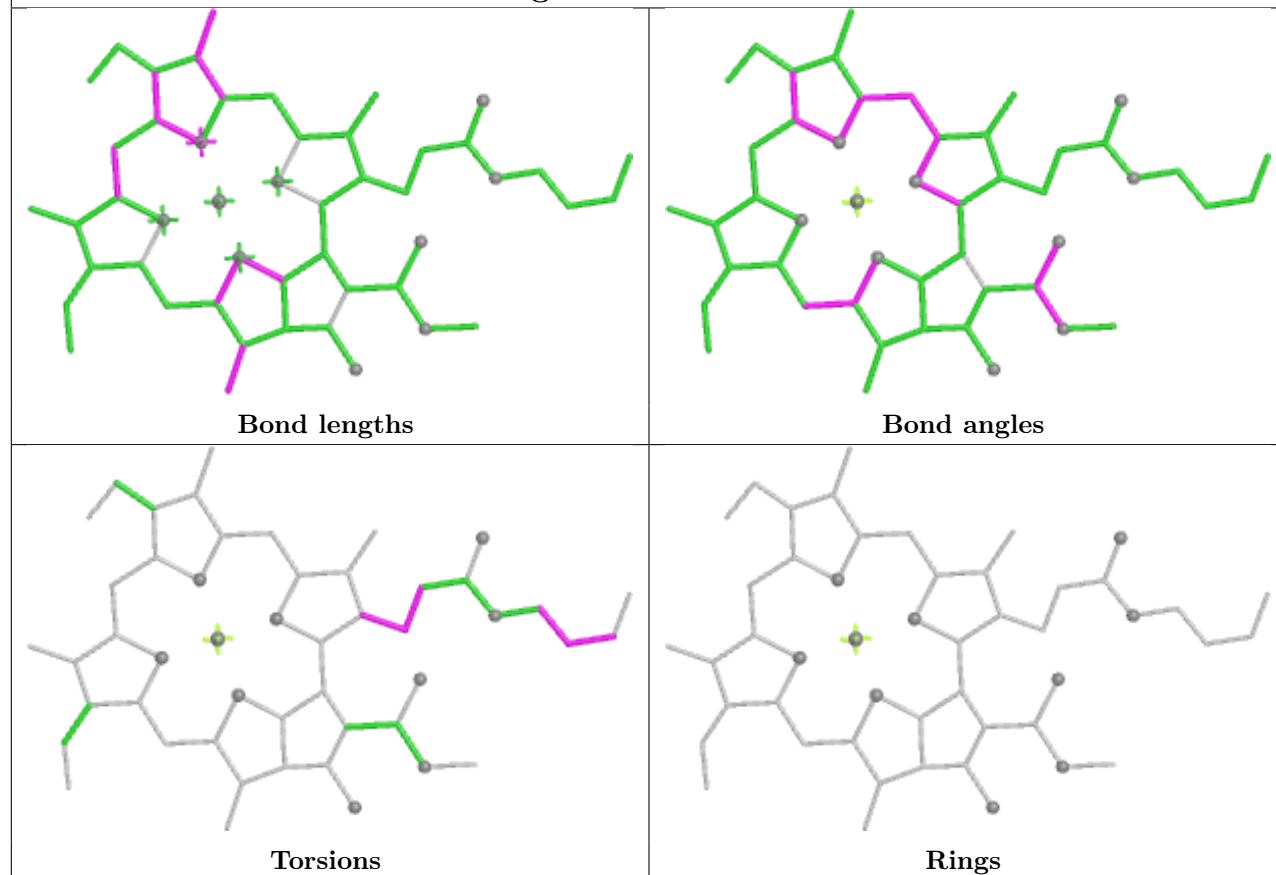
Ligand CHL e 606



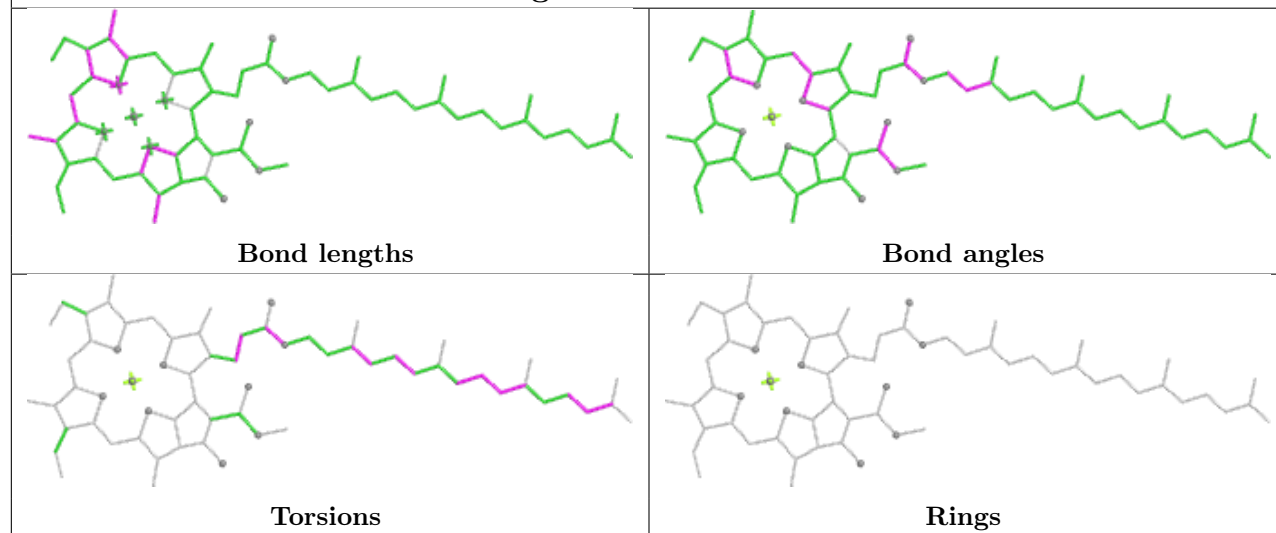
Ligand CLA L 203

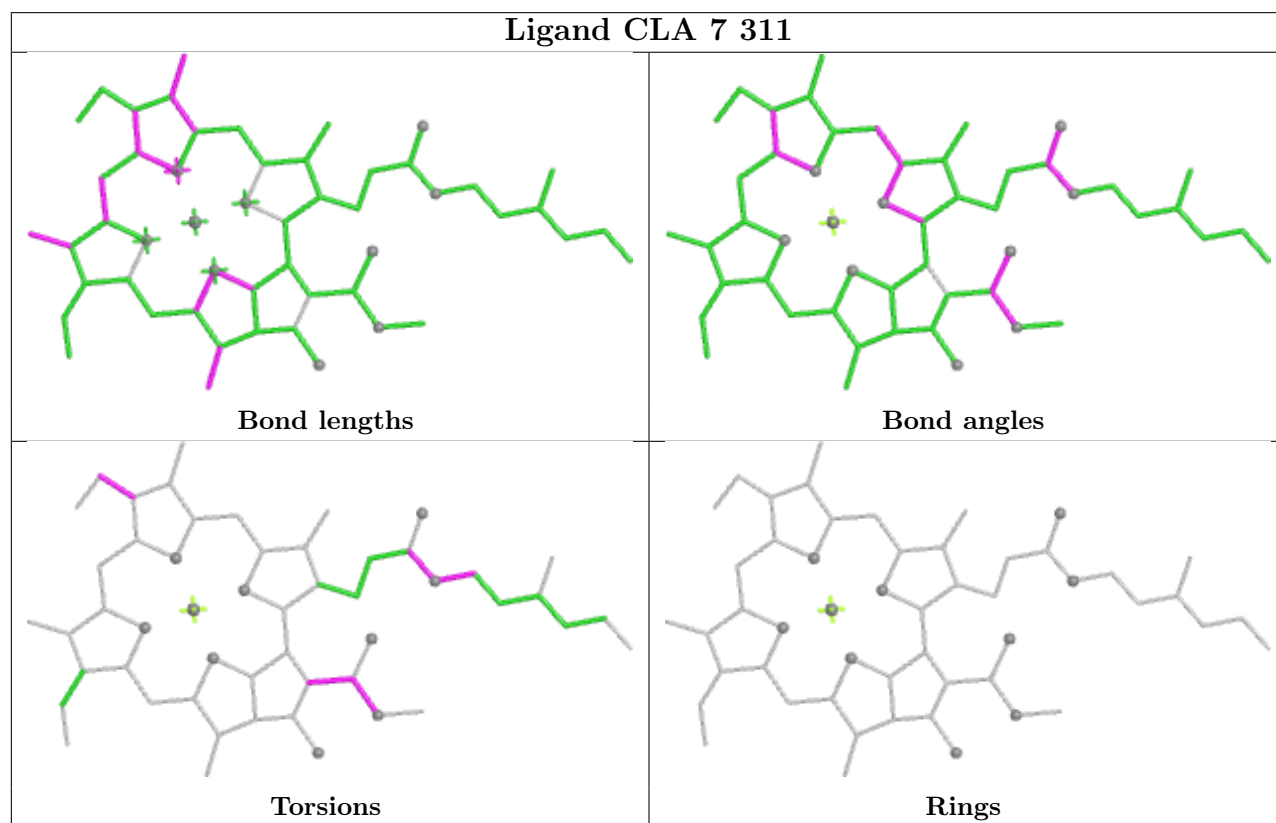
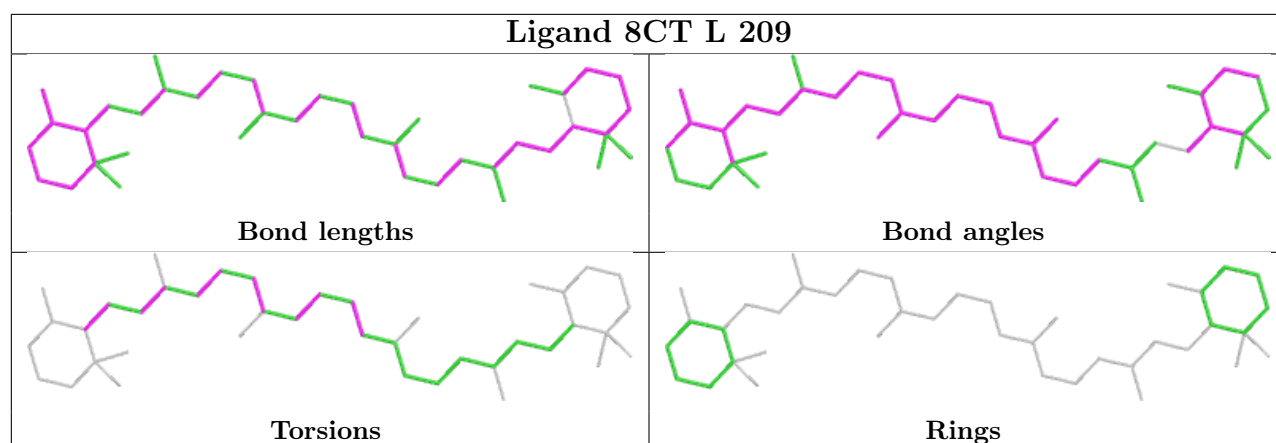


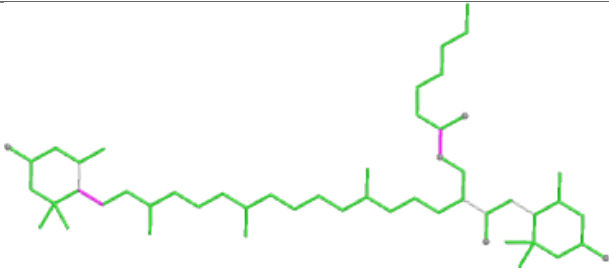
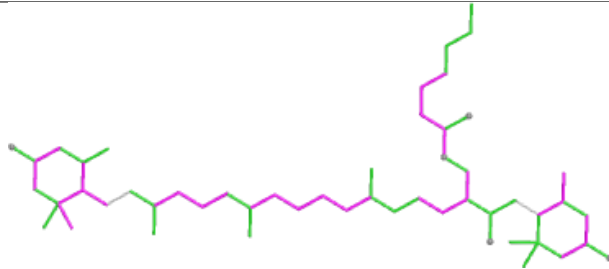
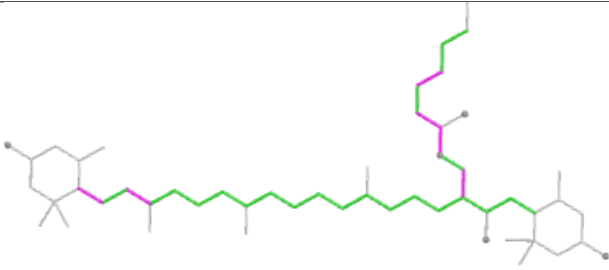
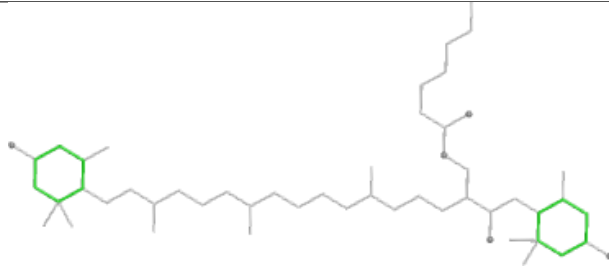
Ligand CLA A 822

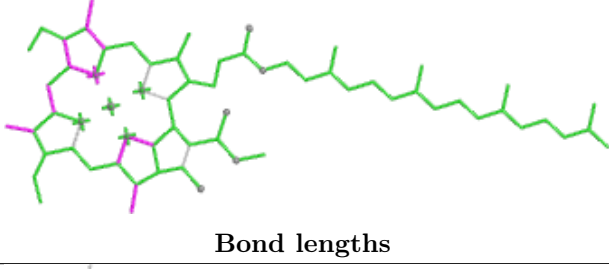
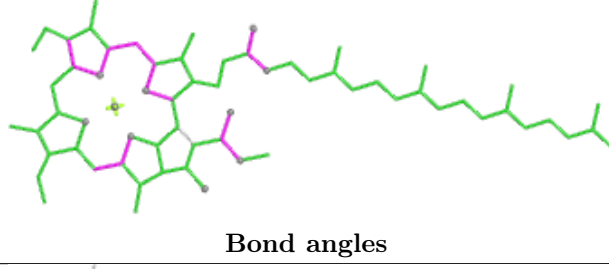
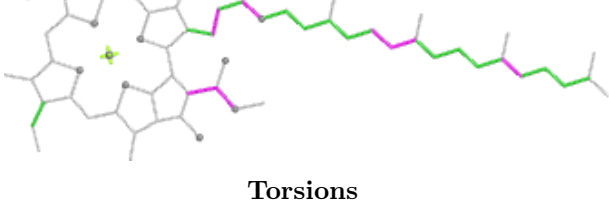


Ligand CLA A 829

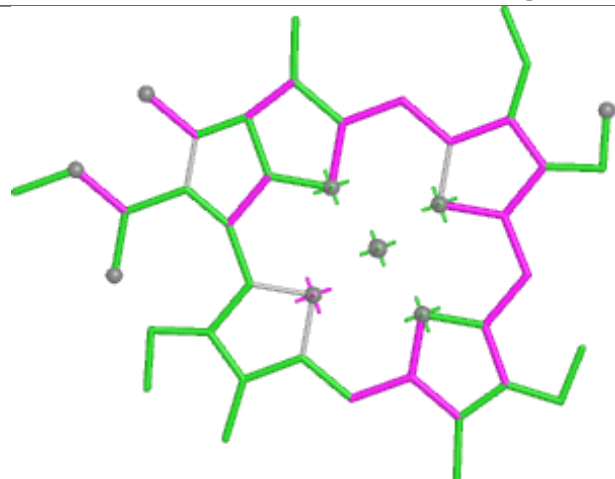




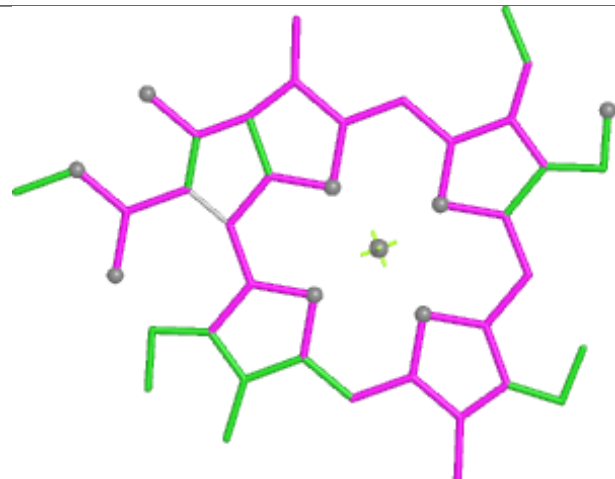
Ligand OUR 6 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 0 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

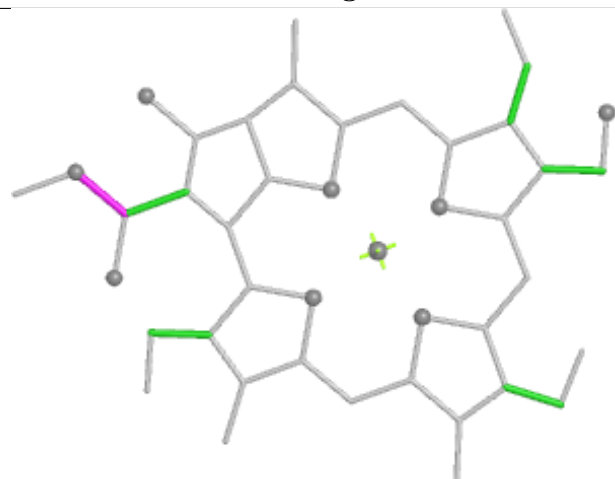
Ligand CHL c 605



Bond lengths



Bond angles

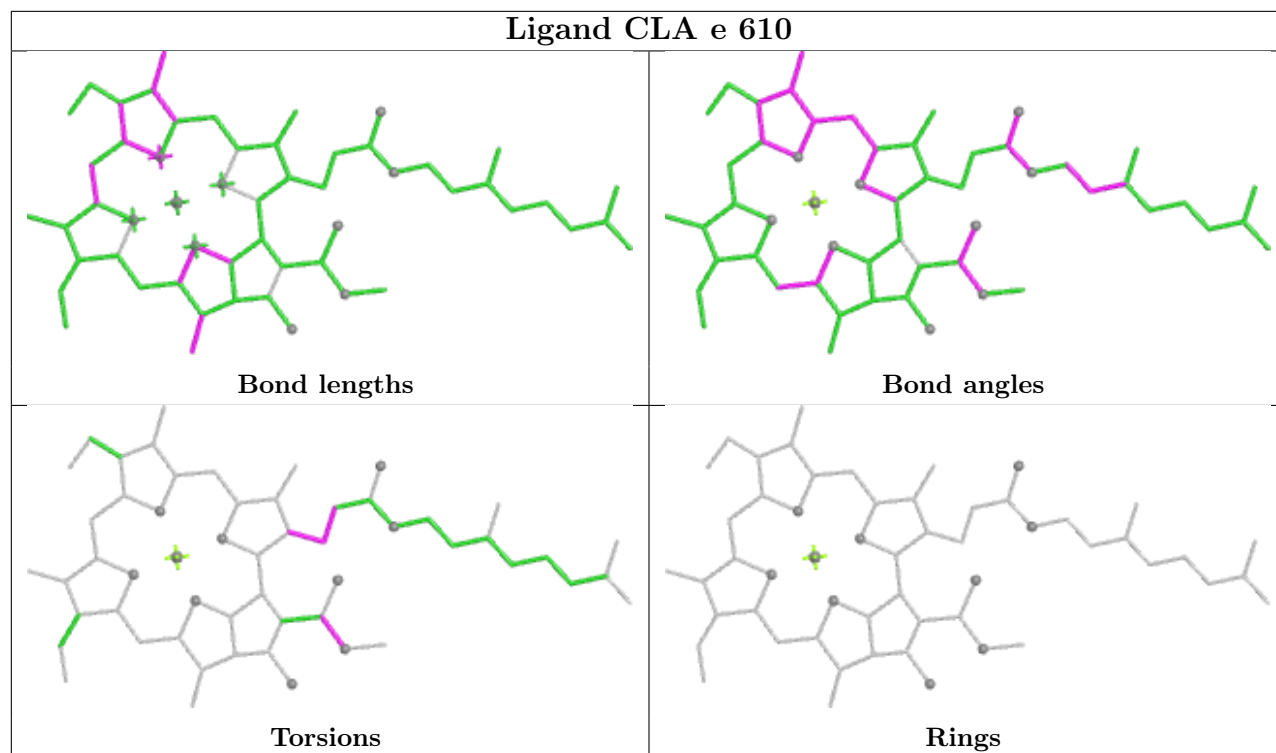


Torsions

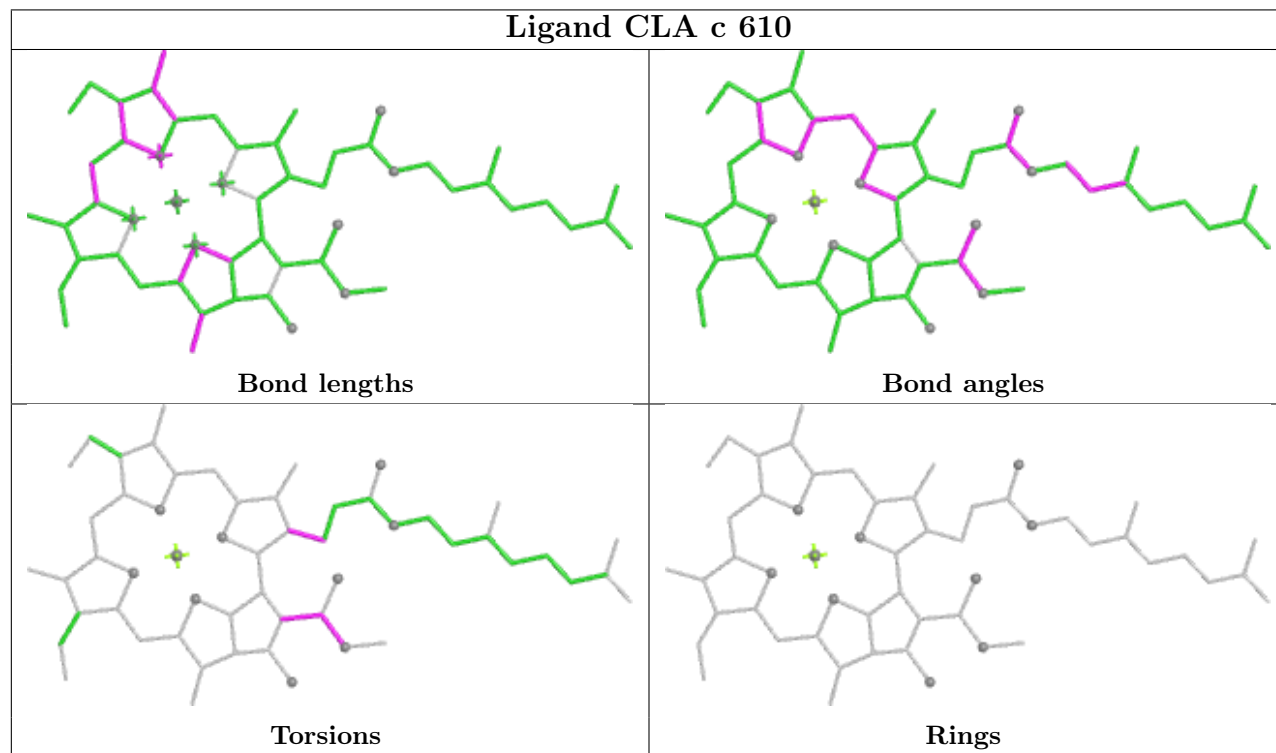


Rings

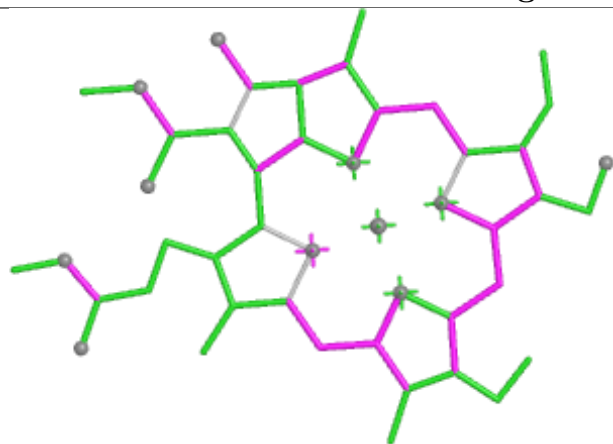
Ligand CLA e 610



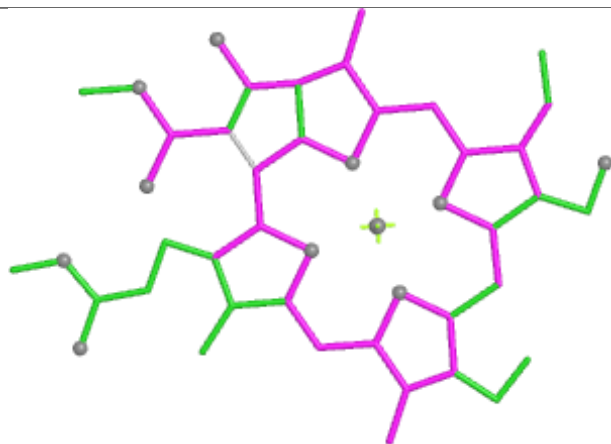
Ligand CLA c 610



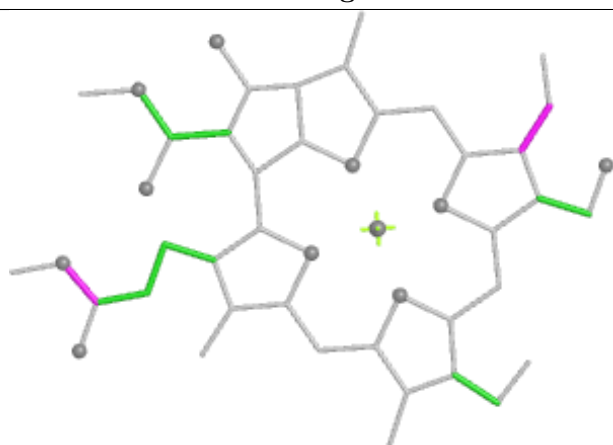
Ligand CHL 2 308



Bond lengths



Bond angles

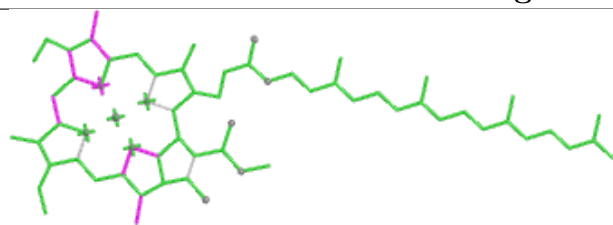


Torsions

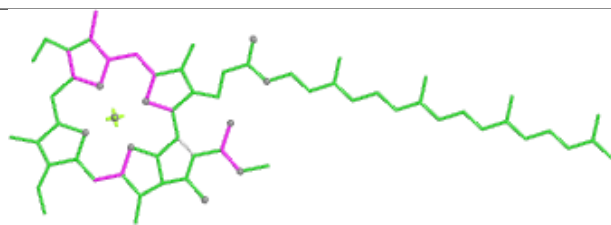


Rings

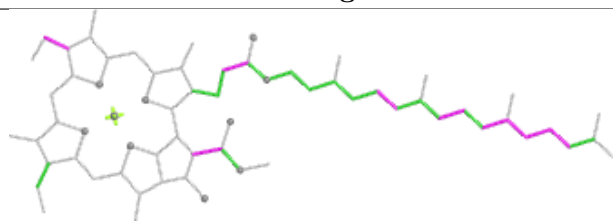
Ligand CLA B 839



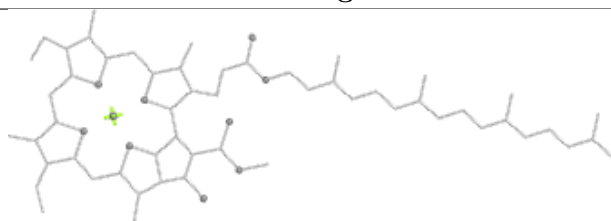
Bond lengths



Bond angles

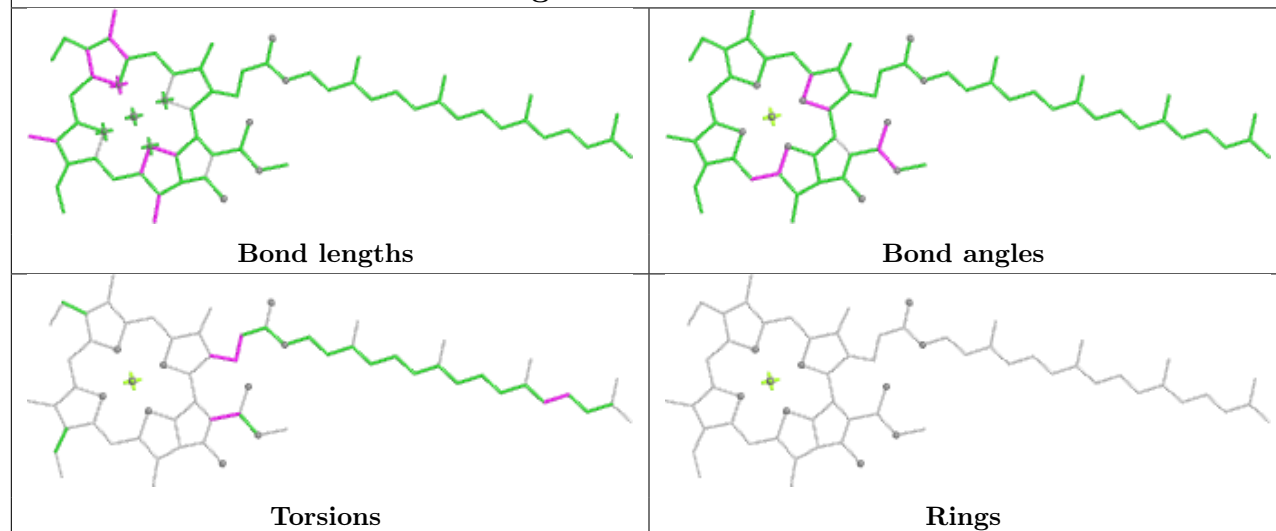


Torsions

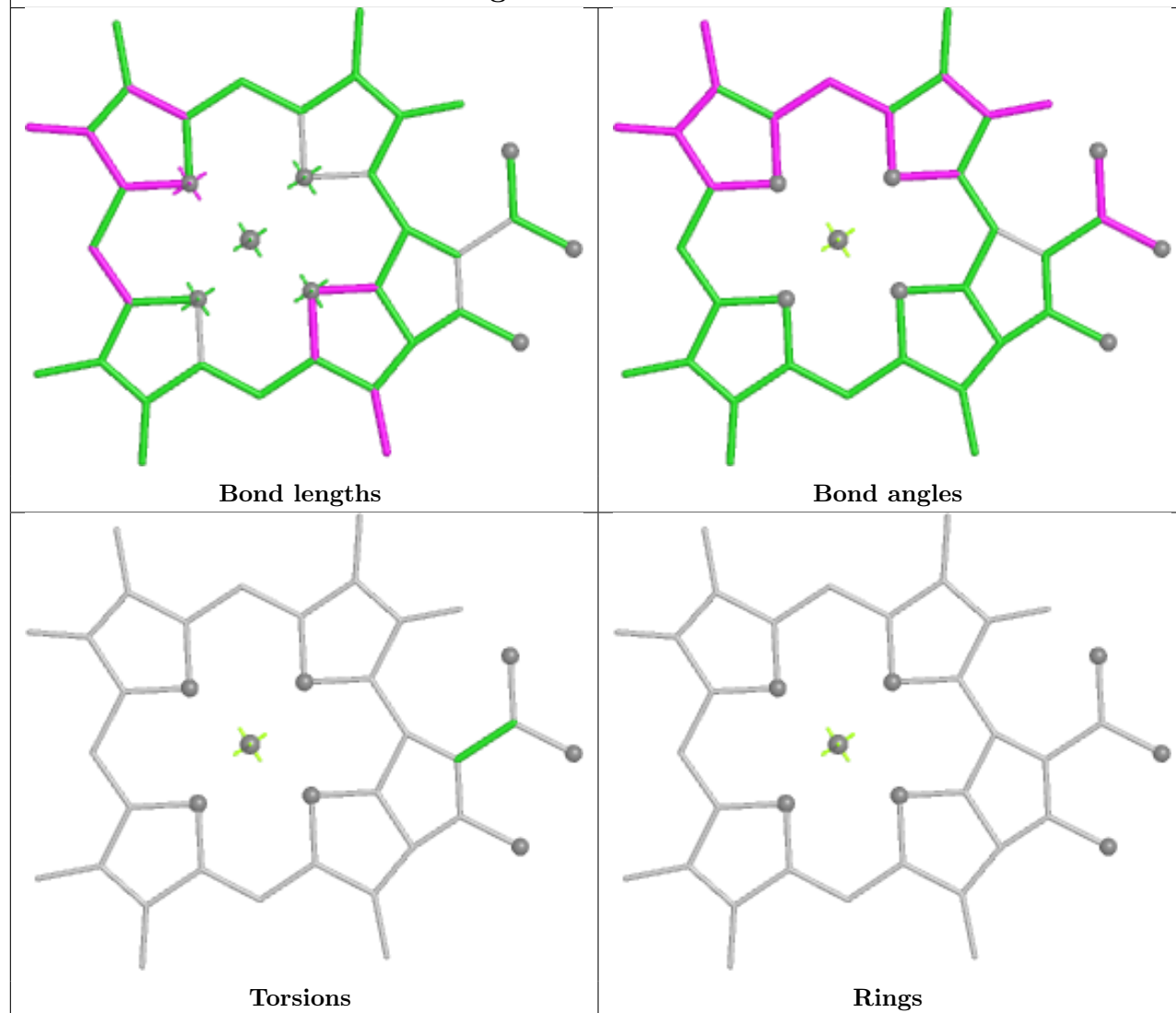


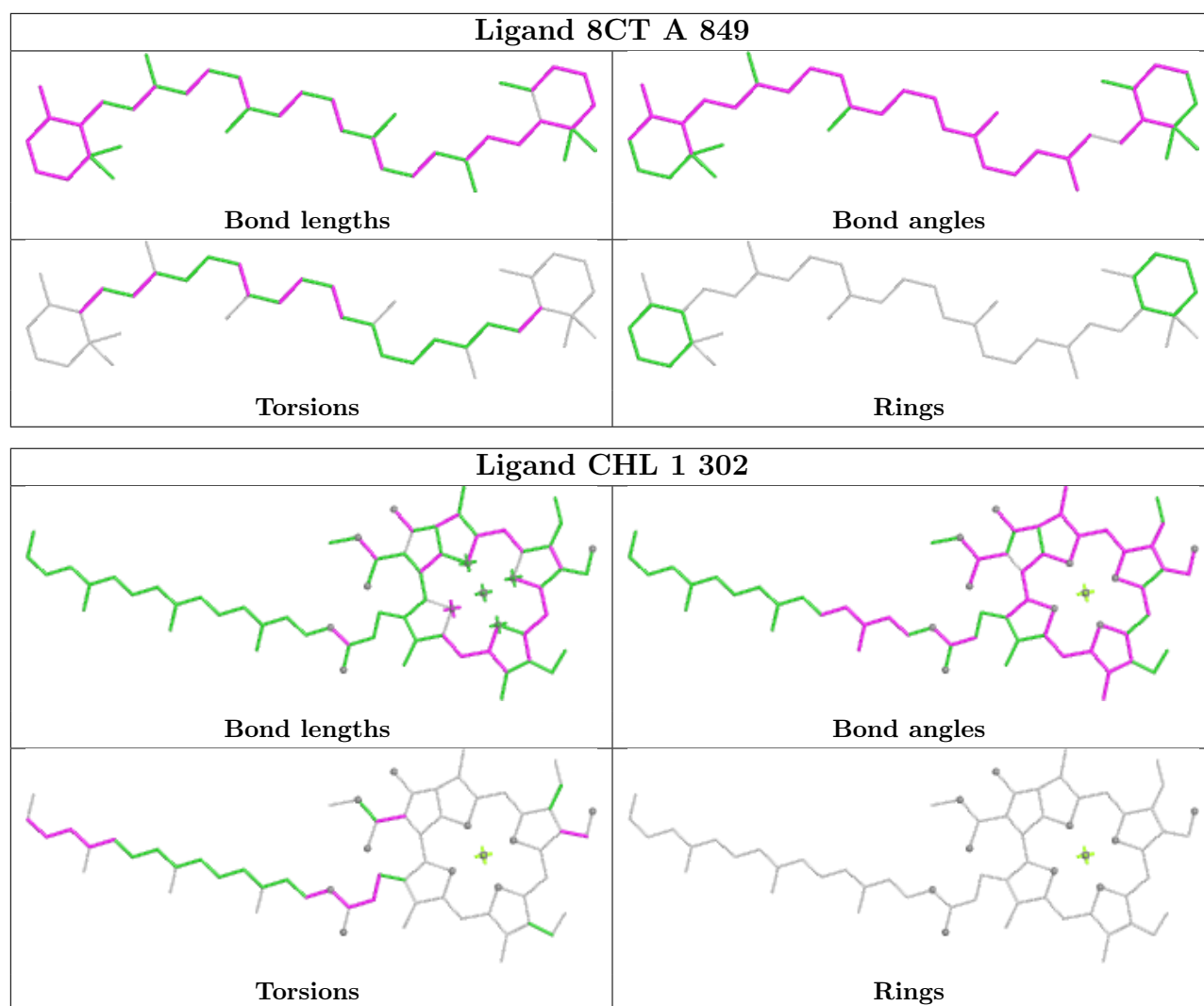
Rings

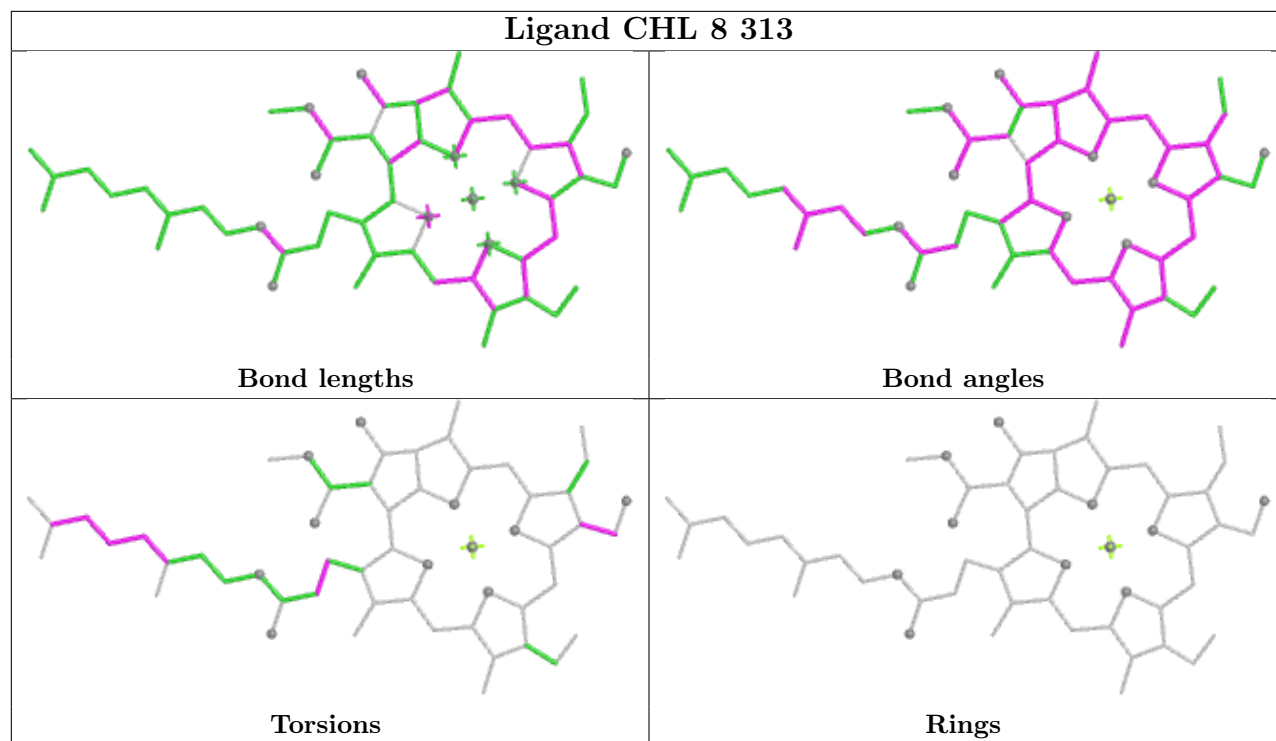
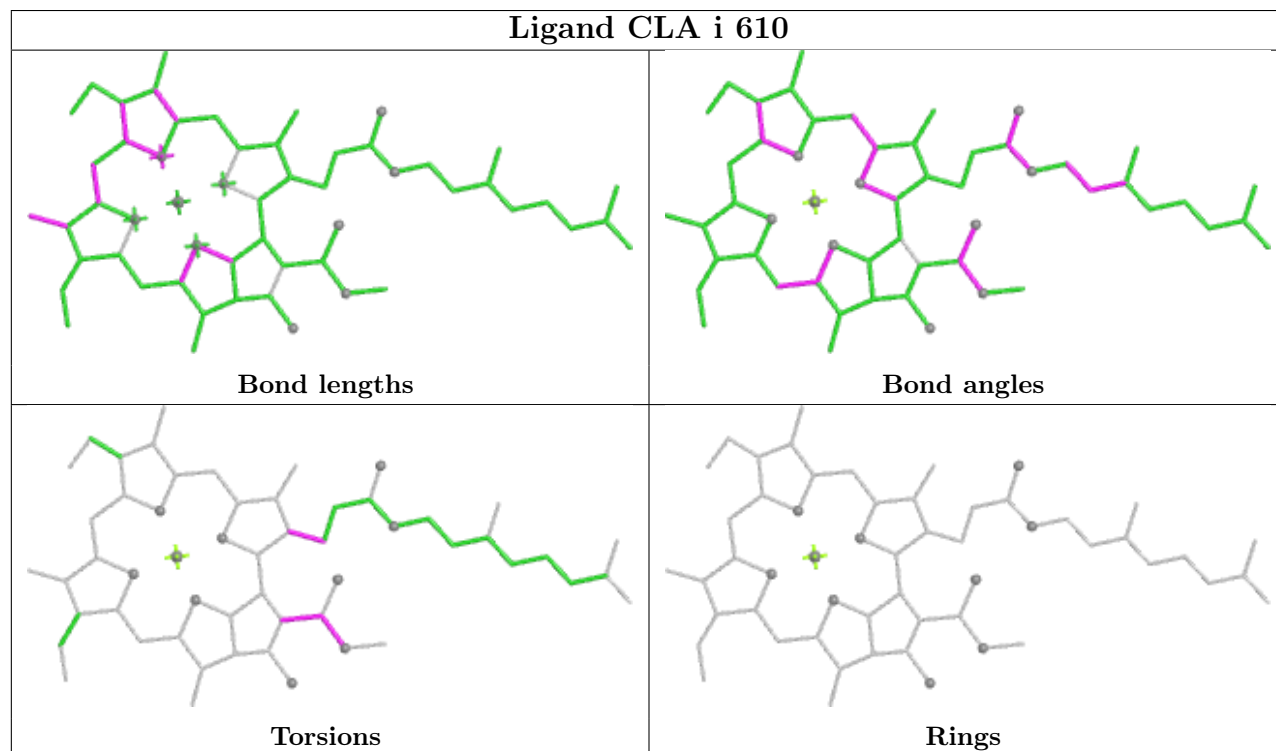
Ligand CLA A 802

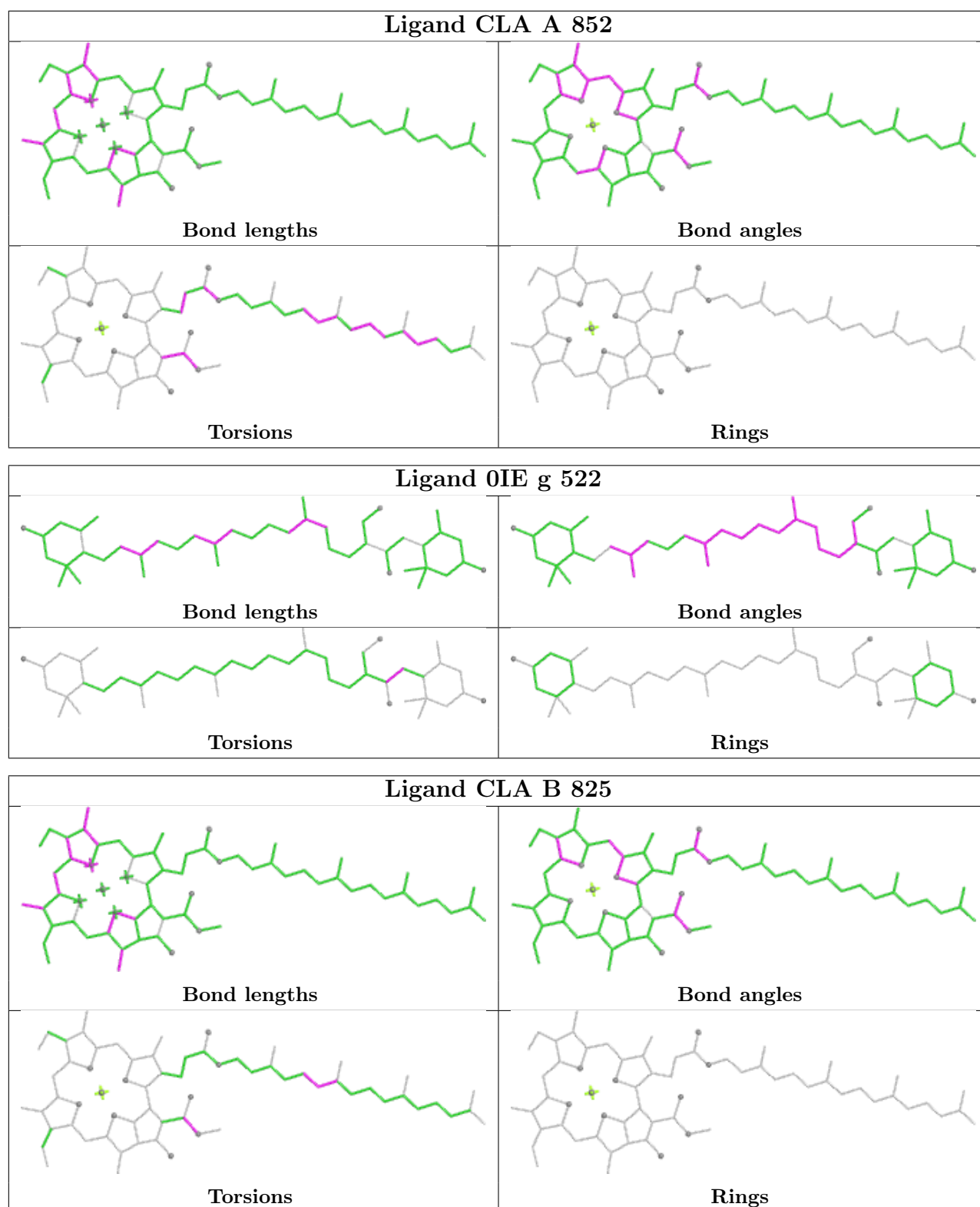


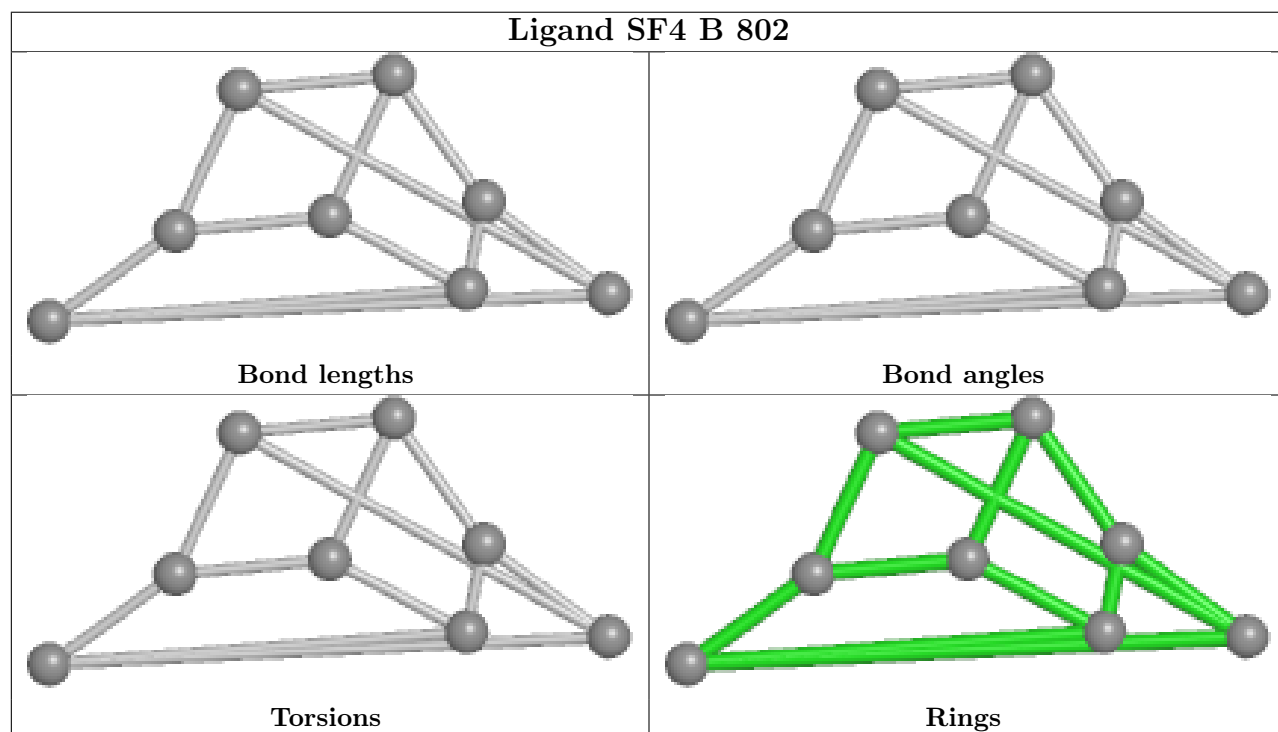
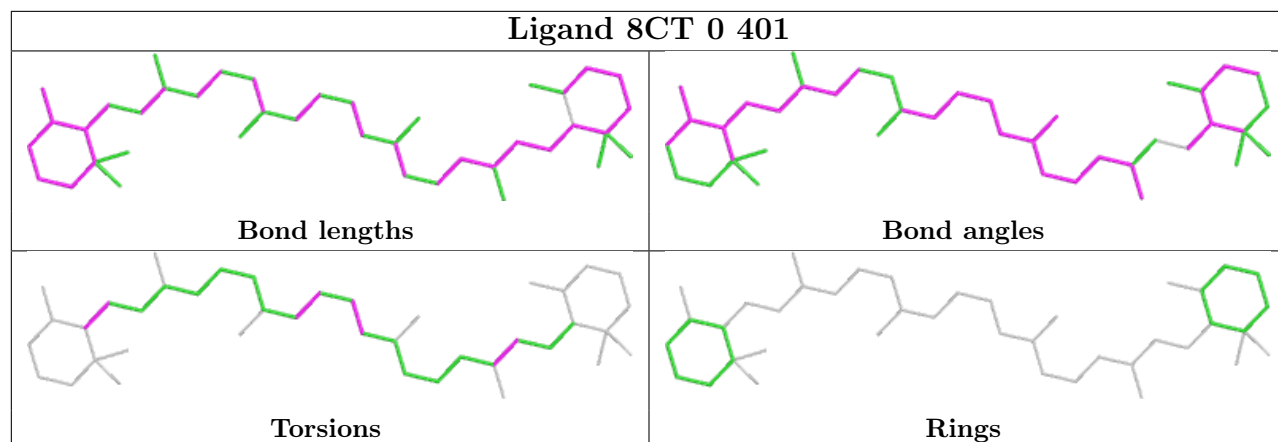
Ligand CLA O 203

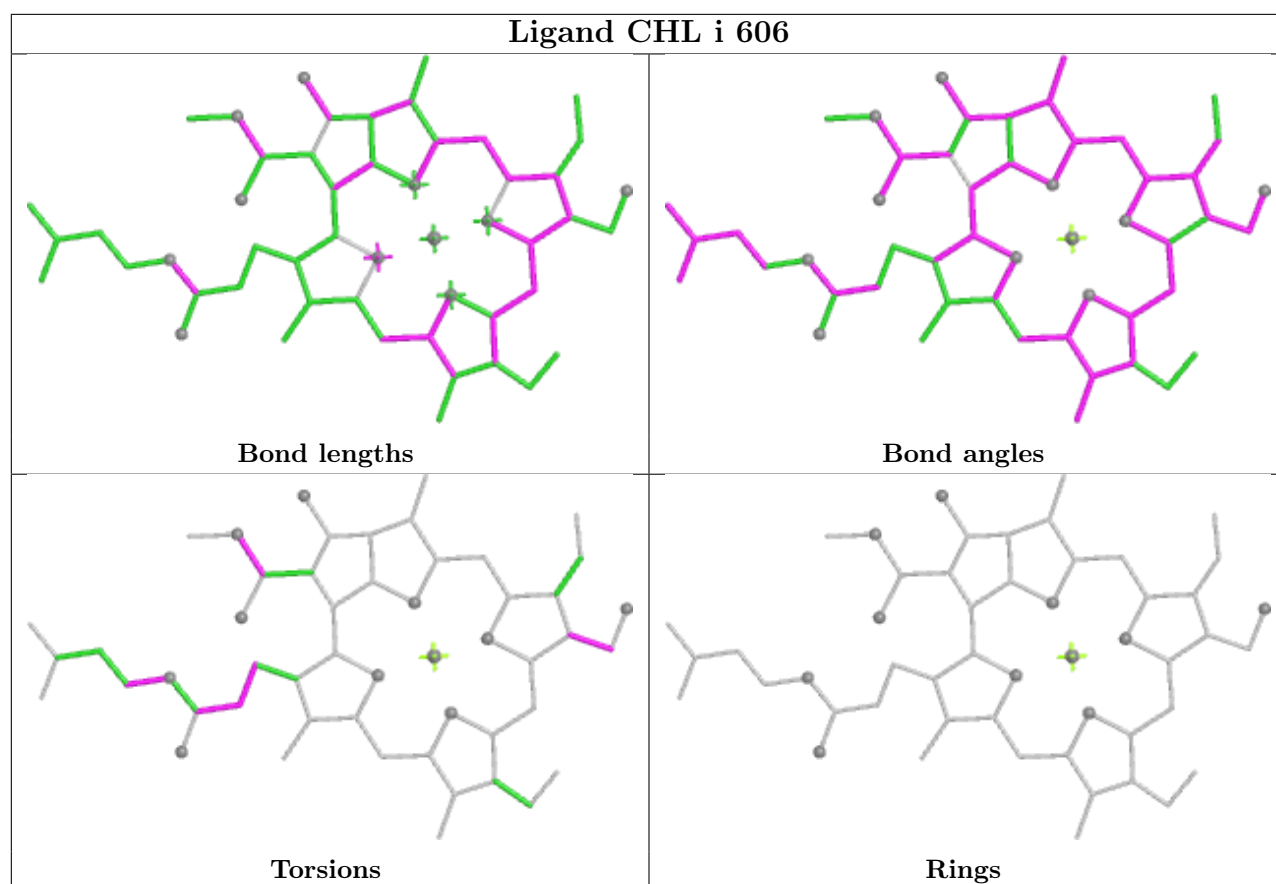


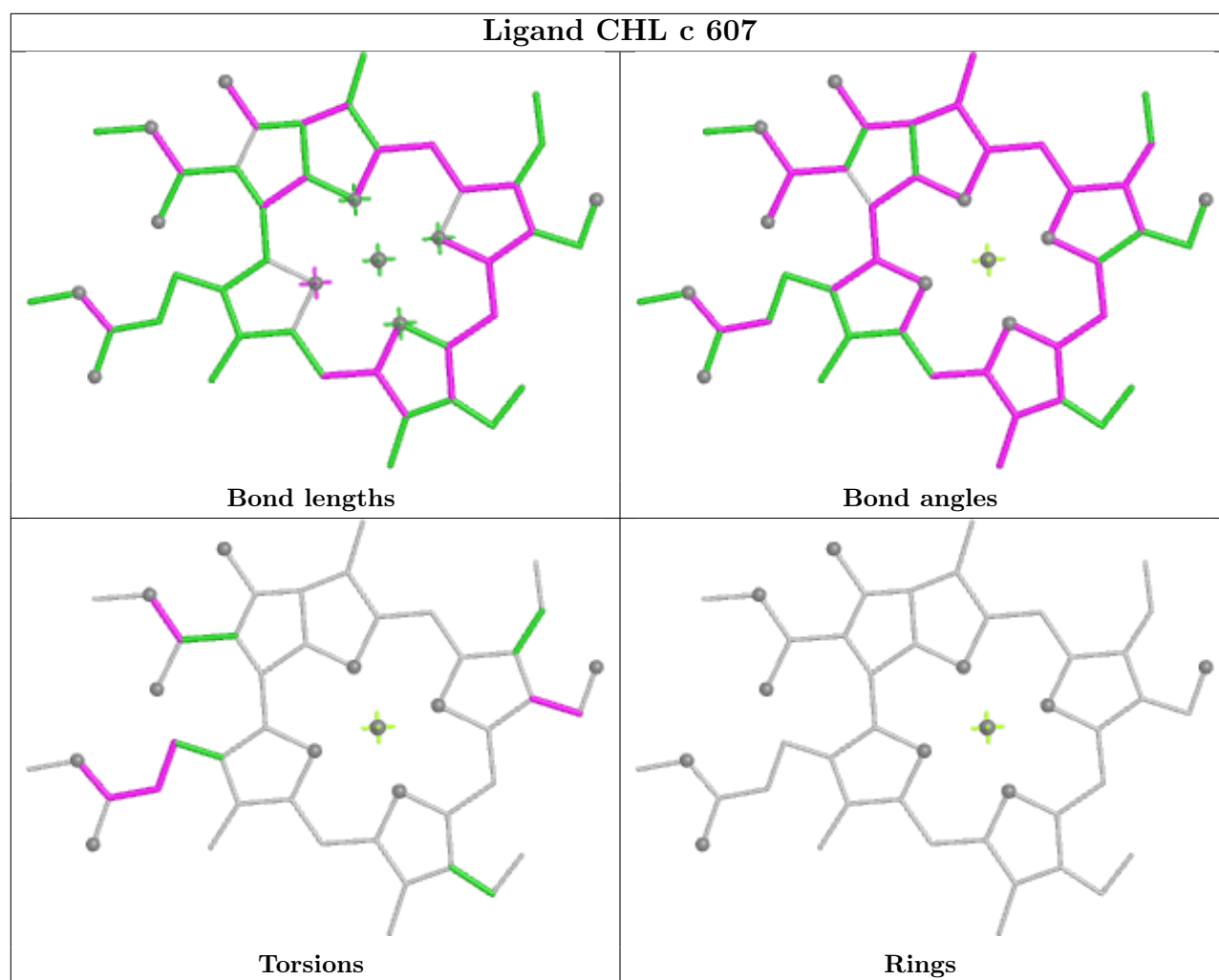


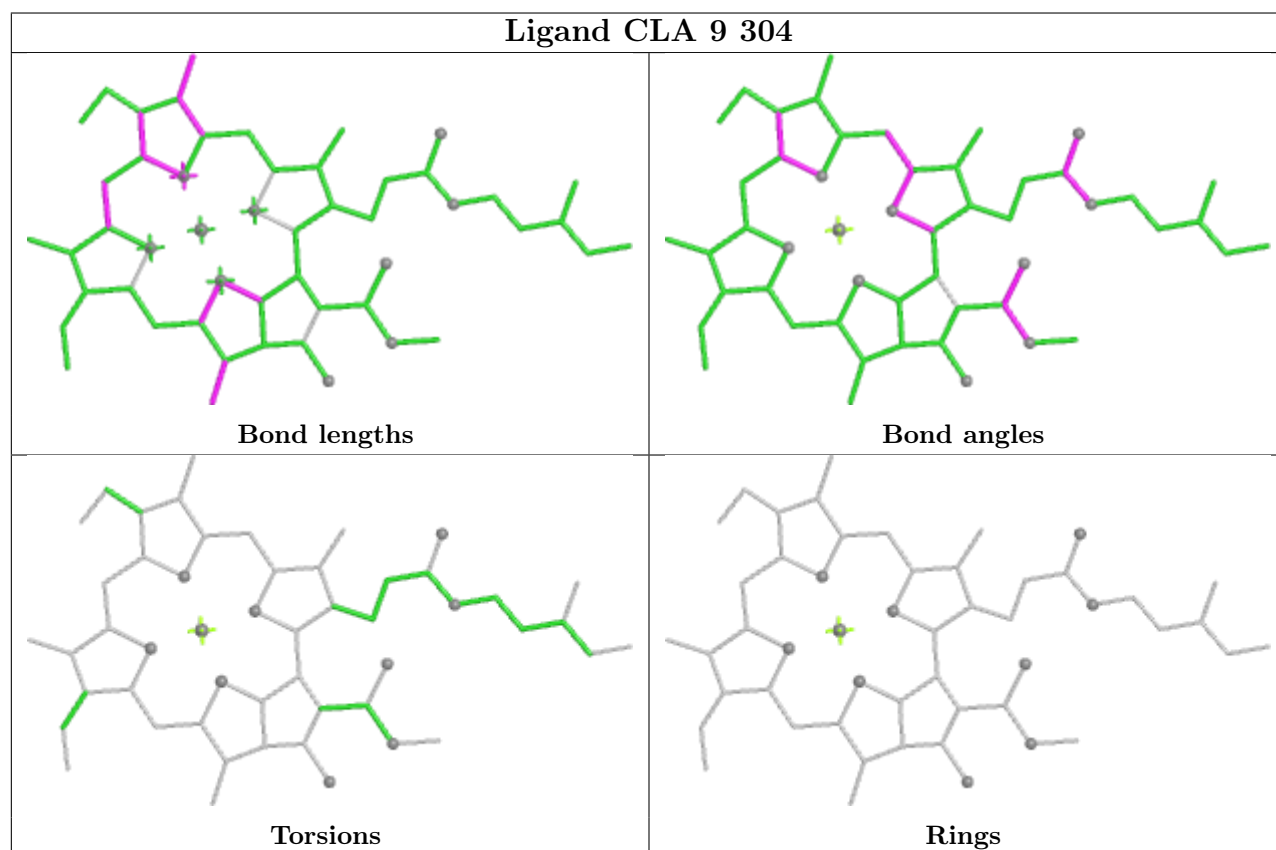
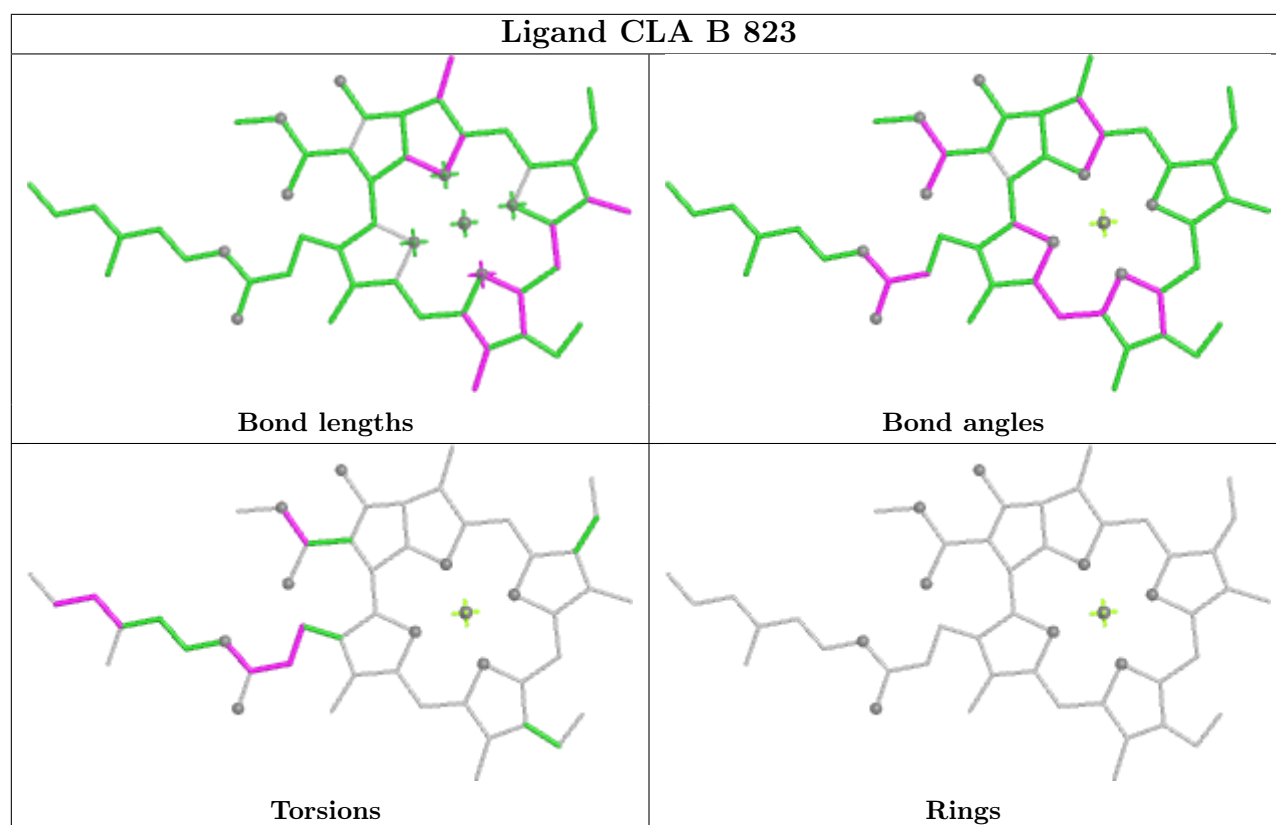
Ligand CHL 8 313**Ligand CLA i 610**

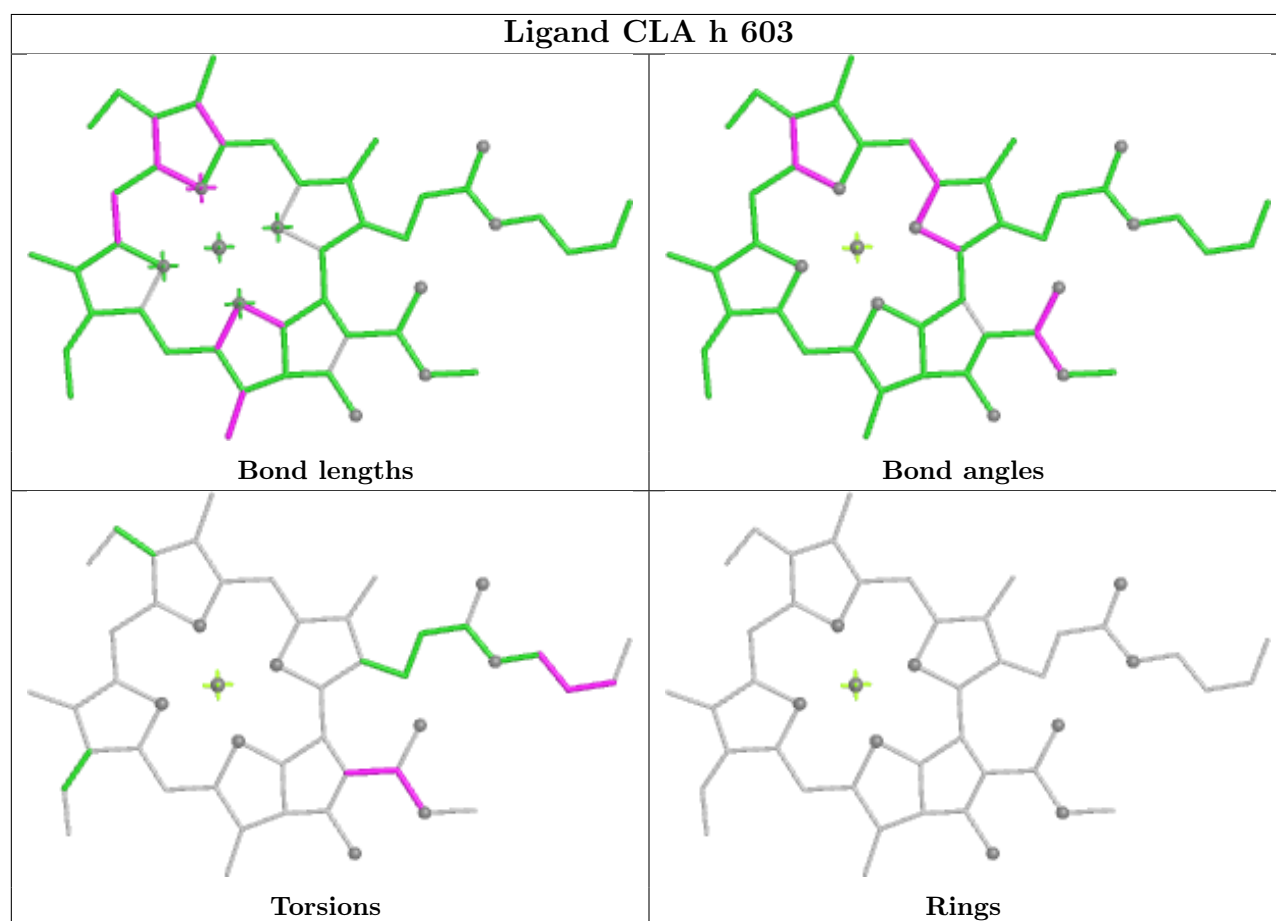
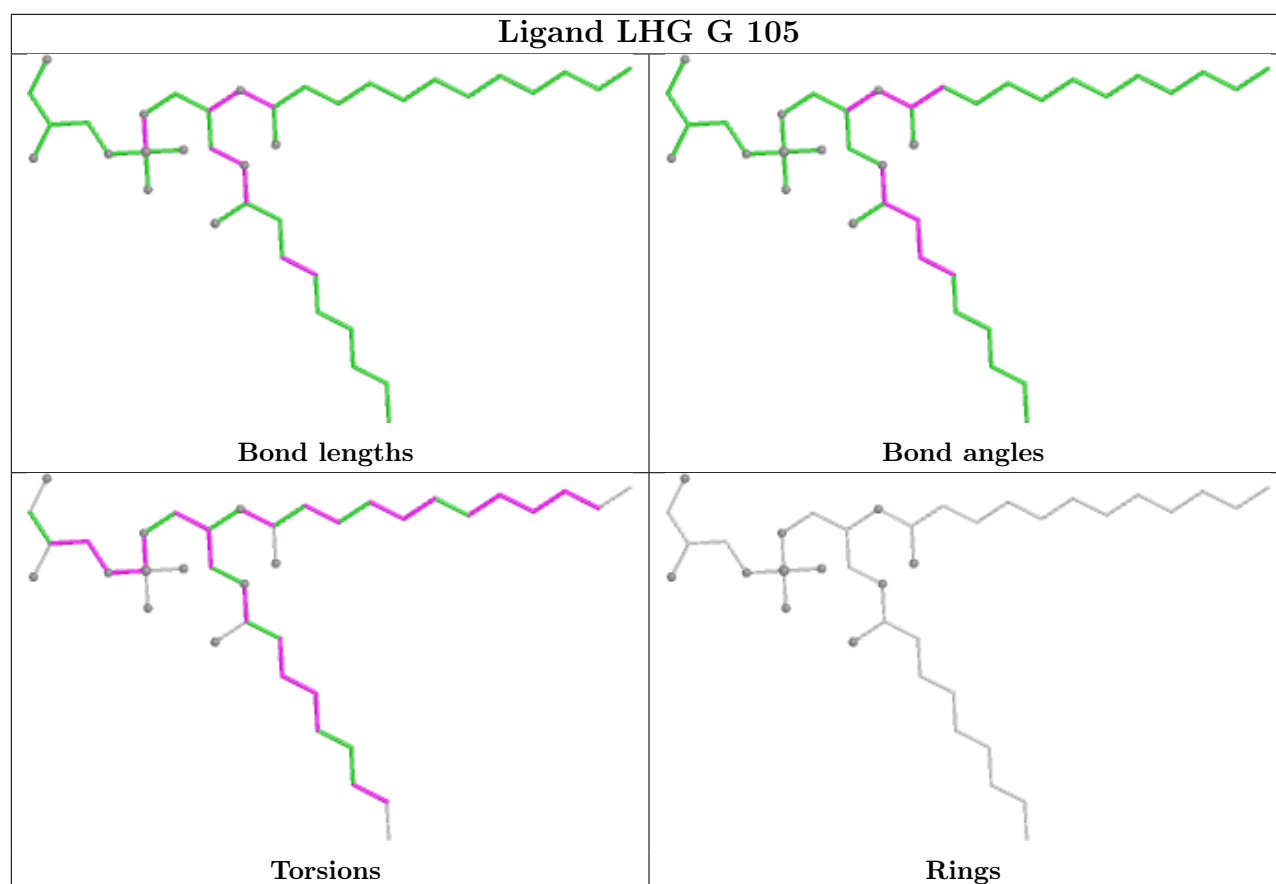


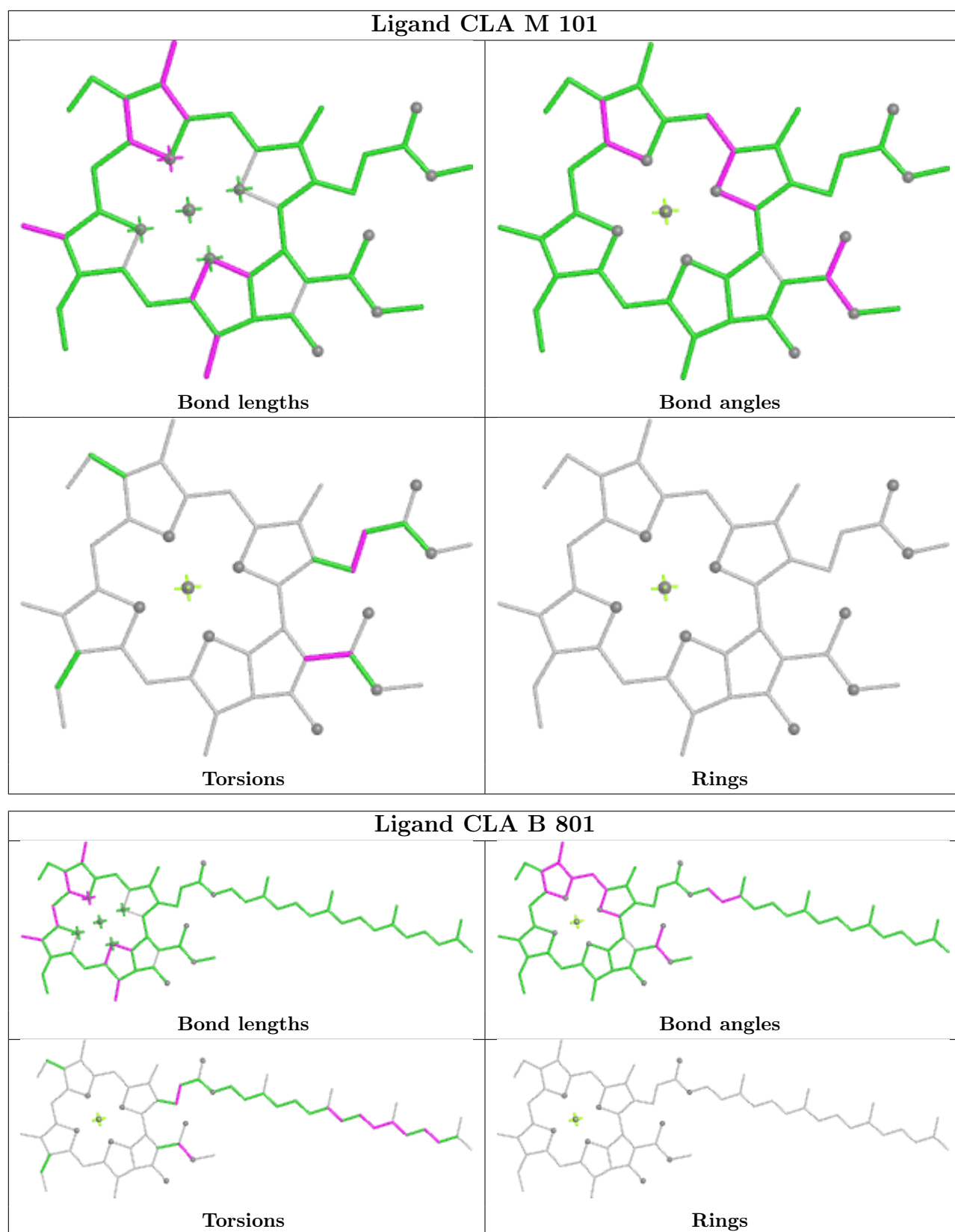




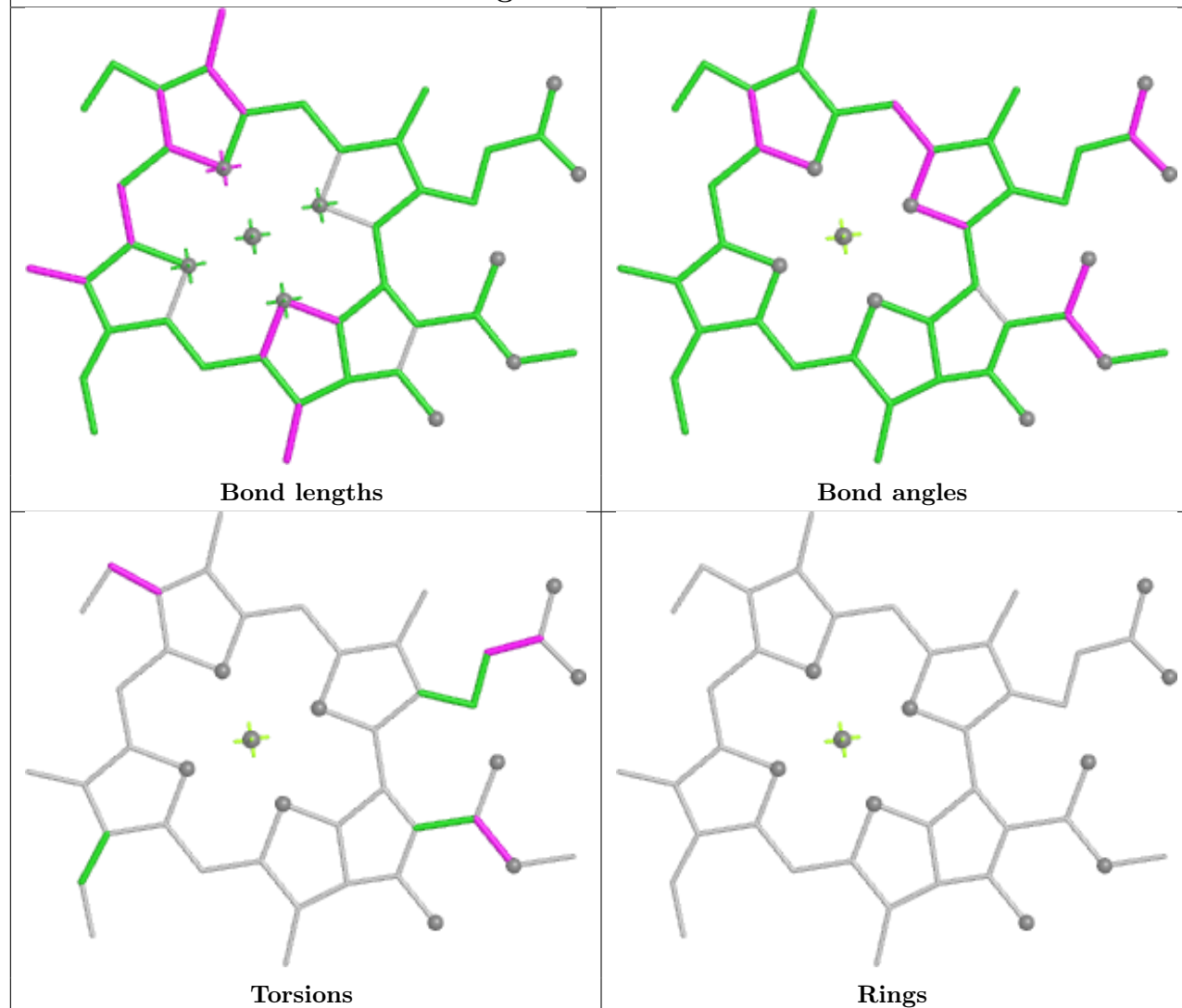




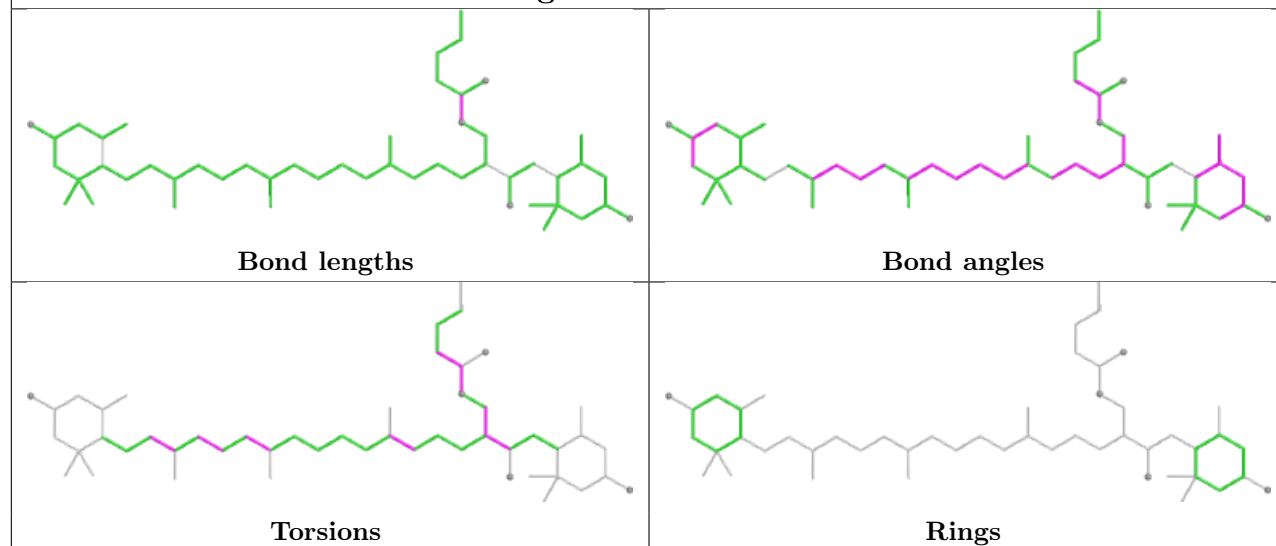


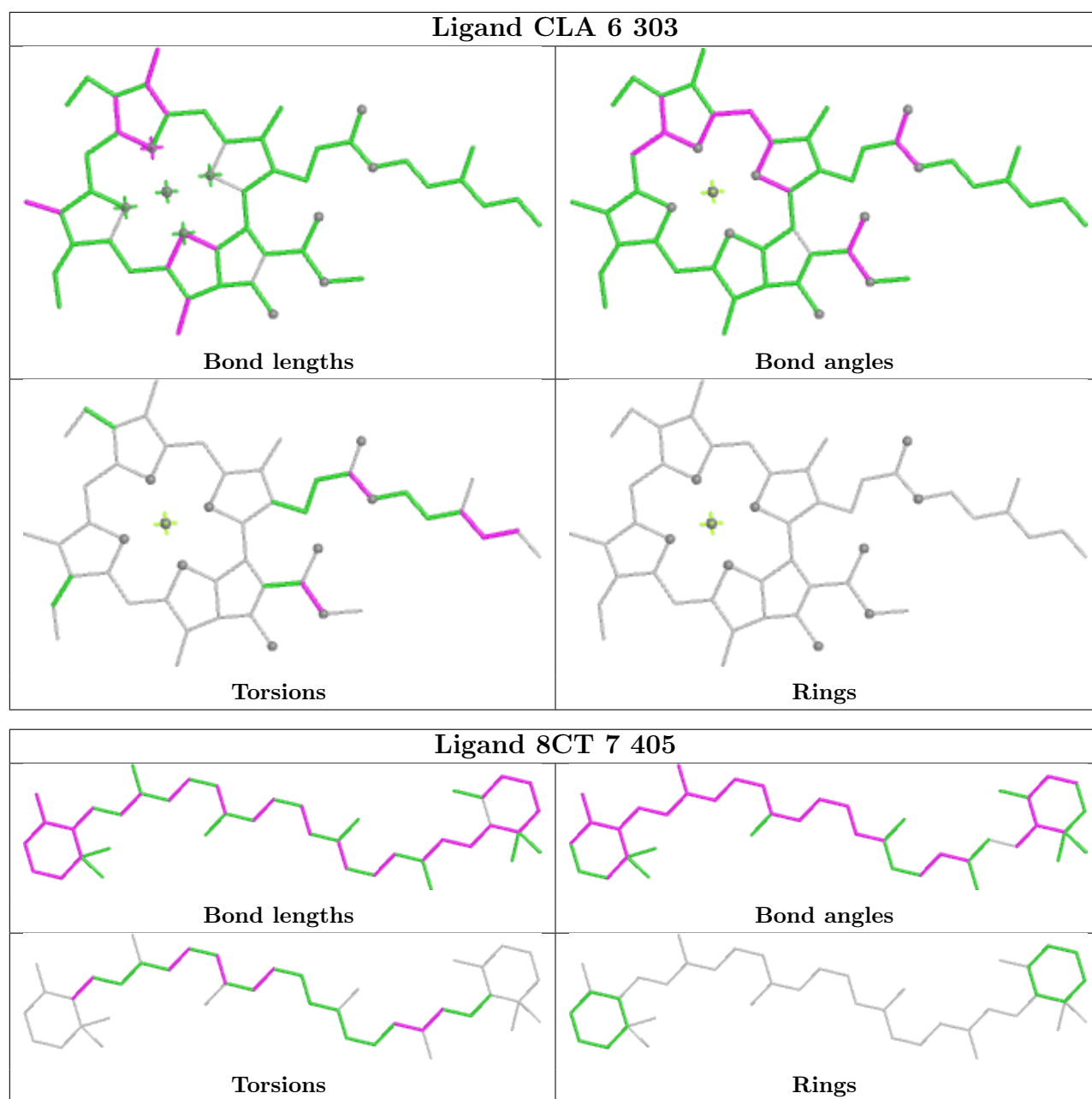


Ligand CLA 2 314

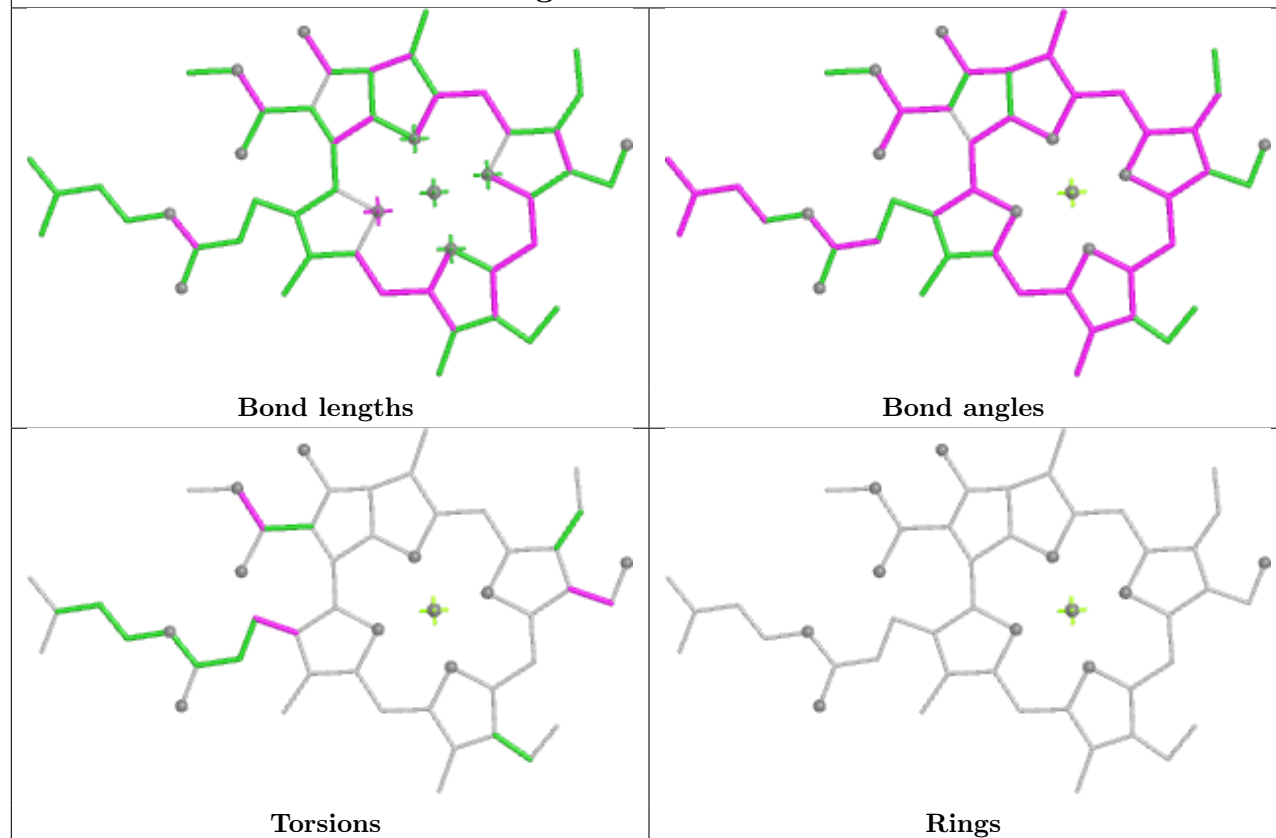


Ligand OUR 4 502

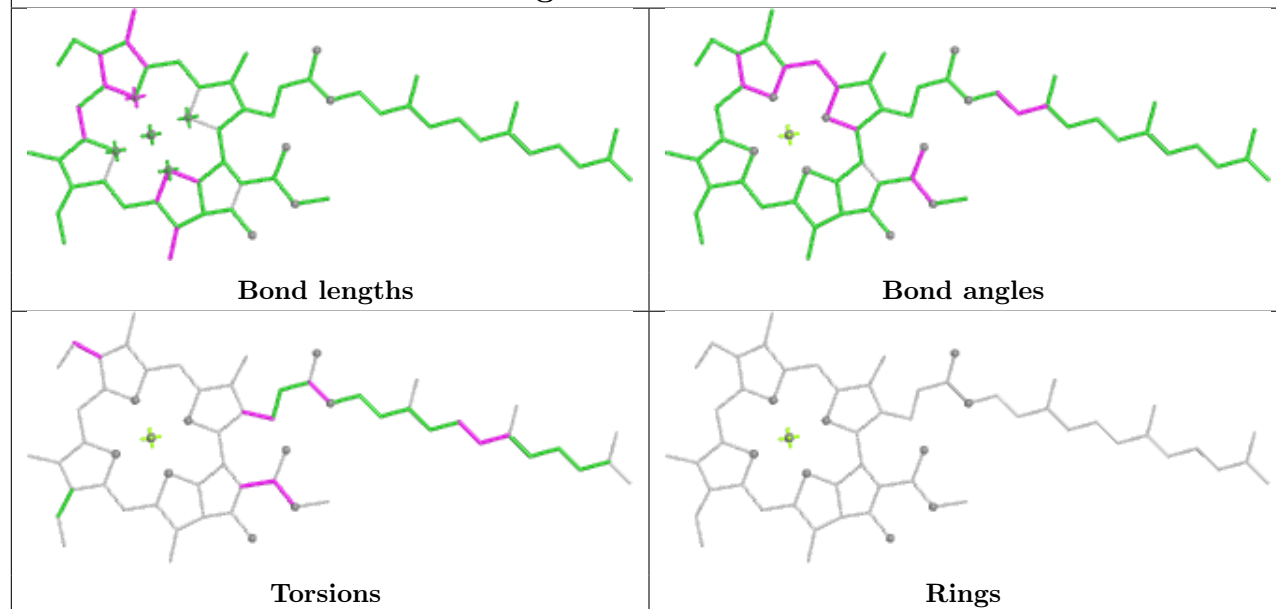


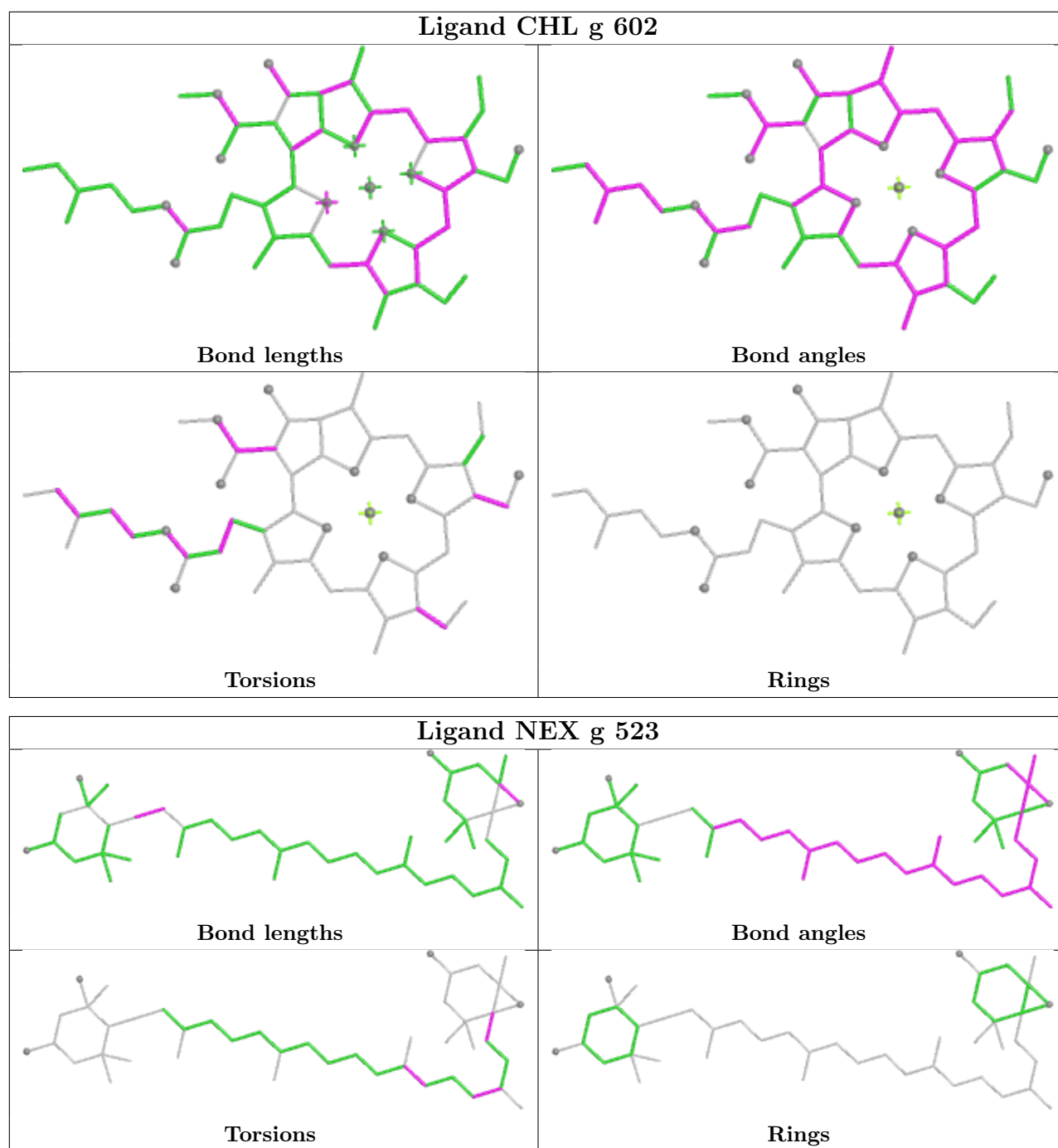


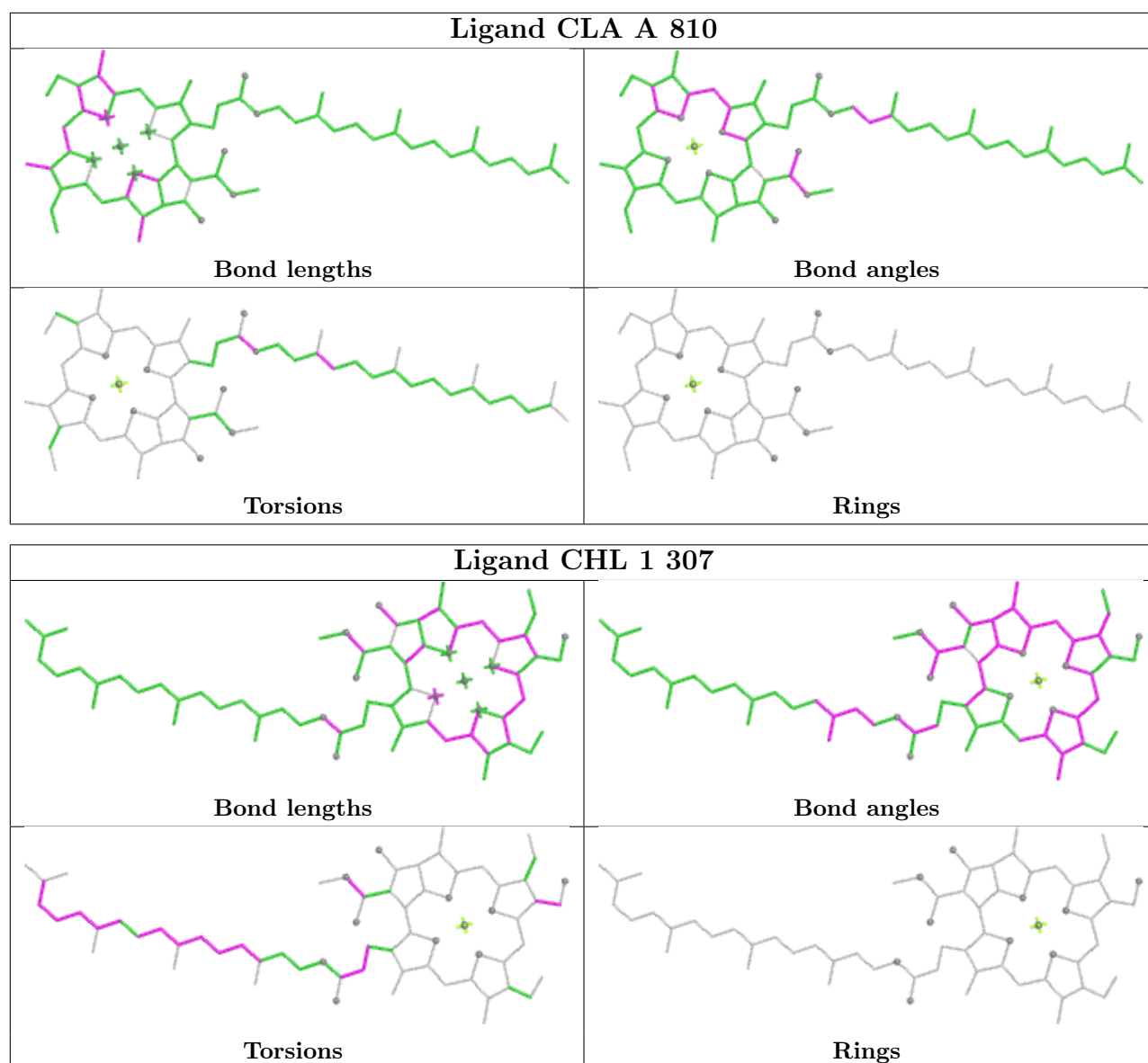
Ligand CHL 6 306

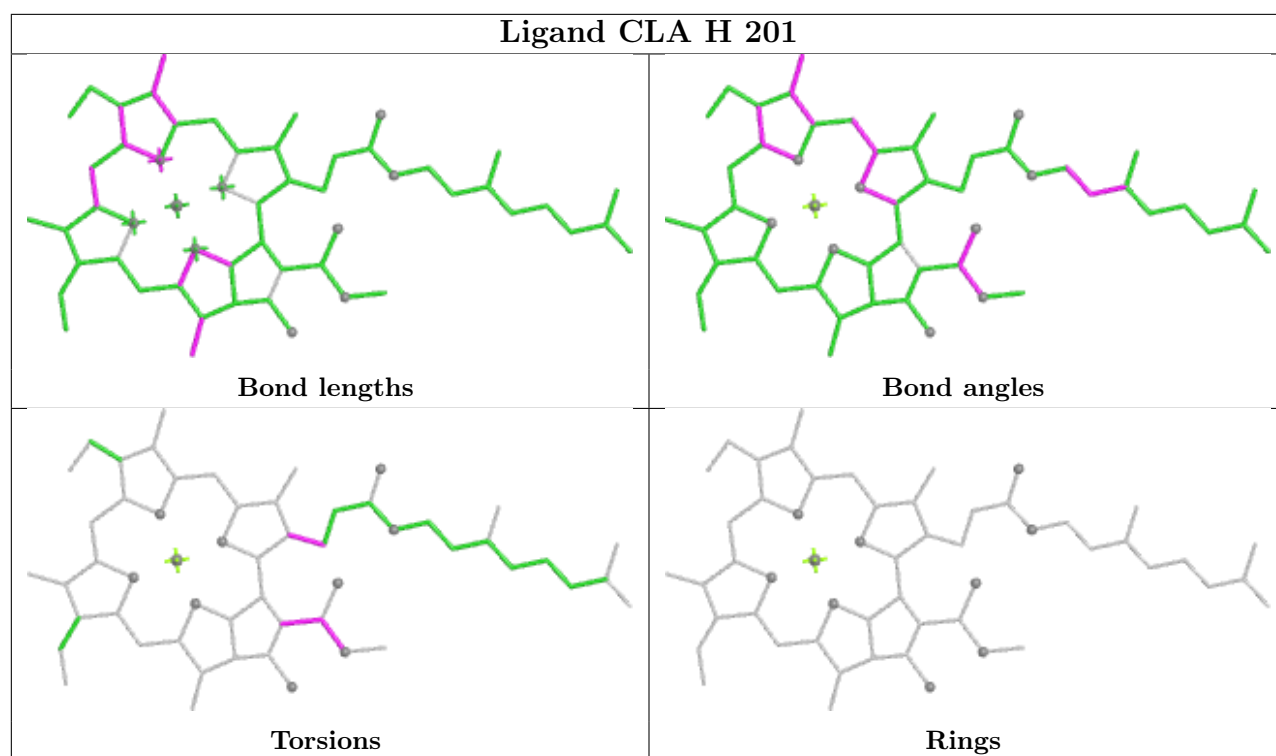


Ligand CLA 6 310

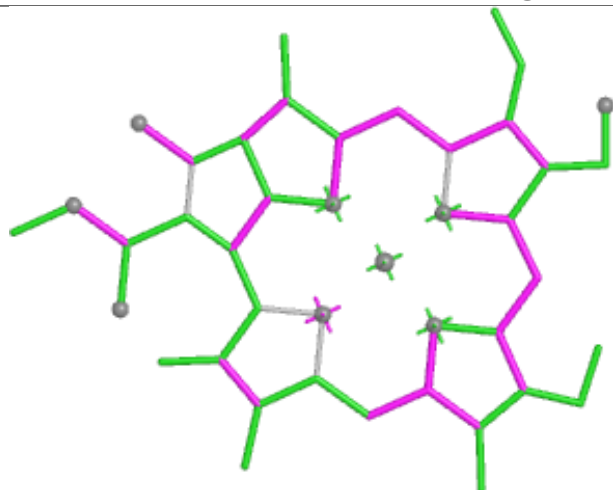




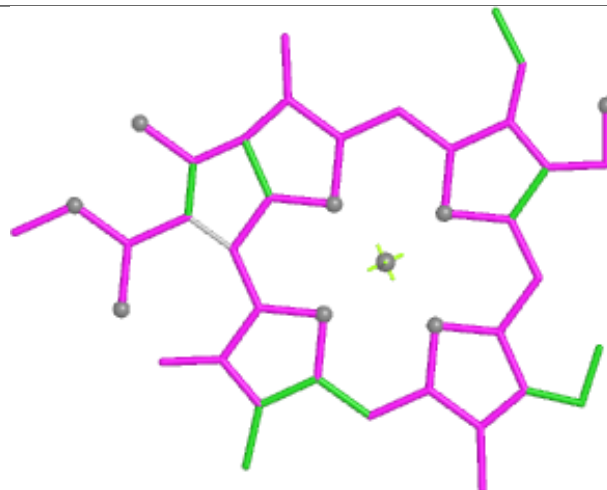




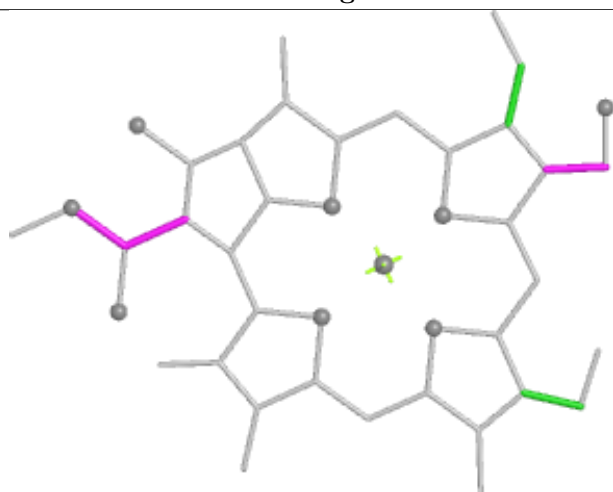
Ligand CHL e 614



Bond lengths



Bond angles

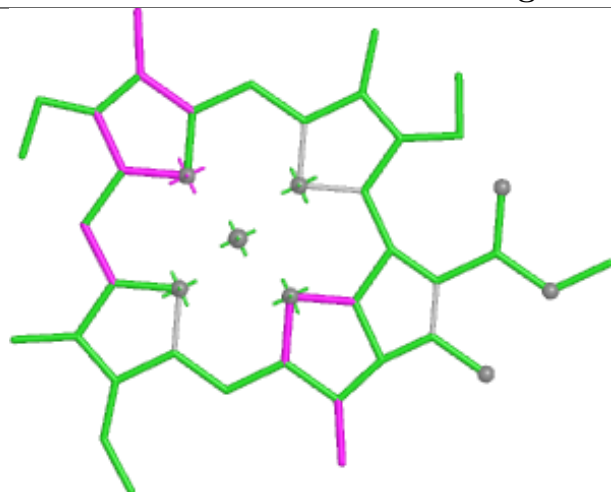


Torsions

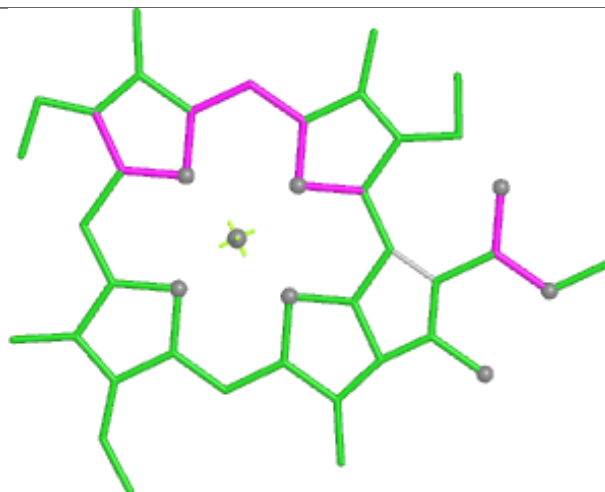


Rings

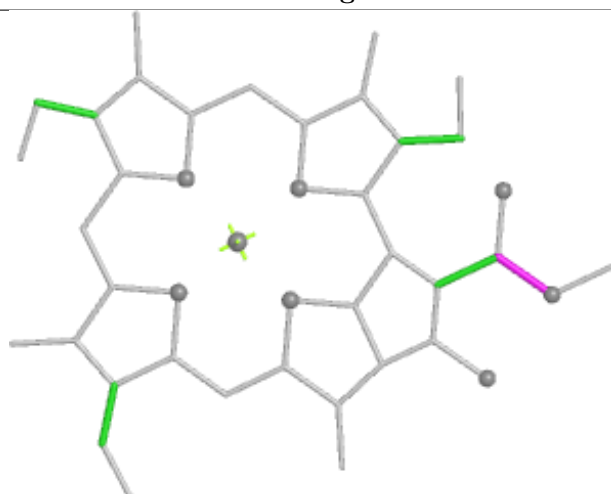
Ligand CLA J 103



Bond lengths



Bond angles

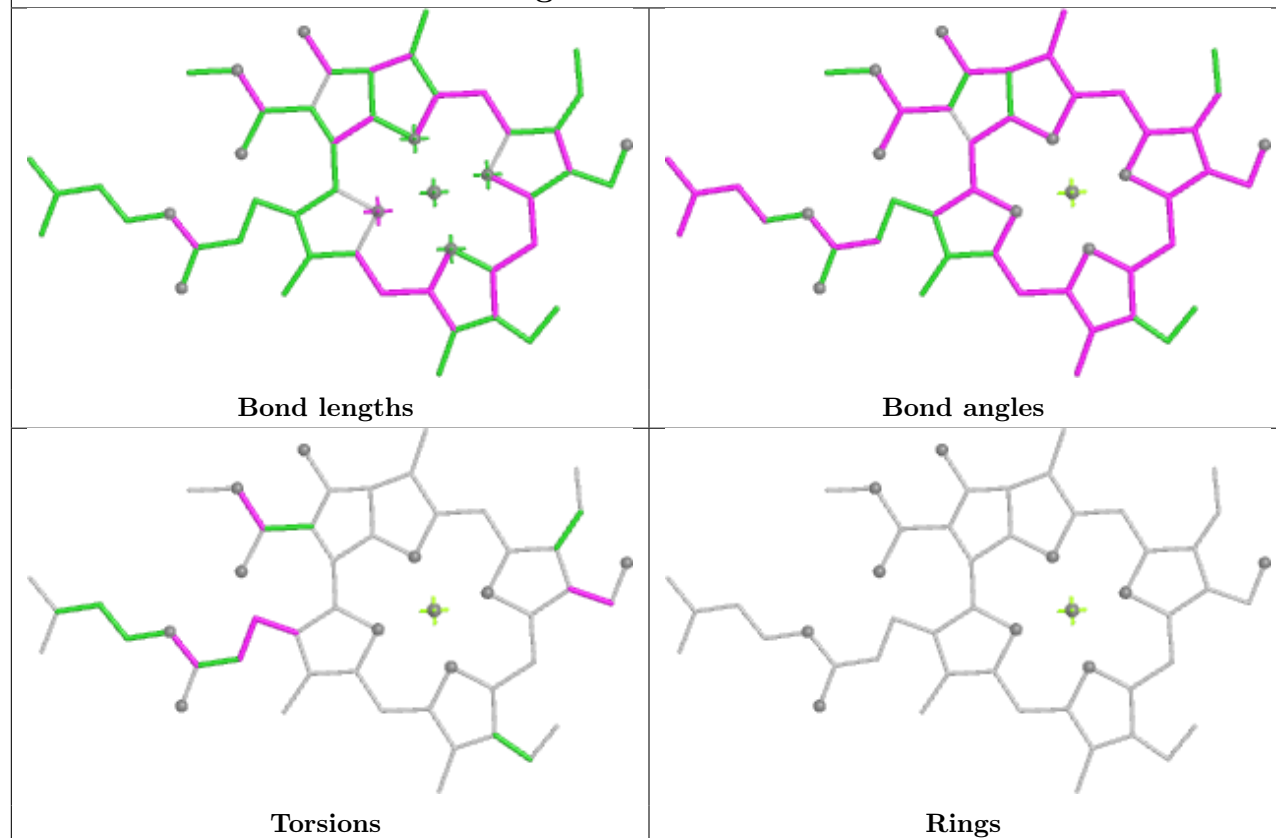


Torsions

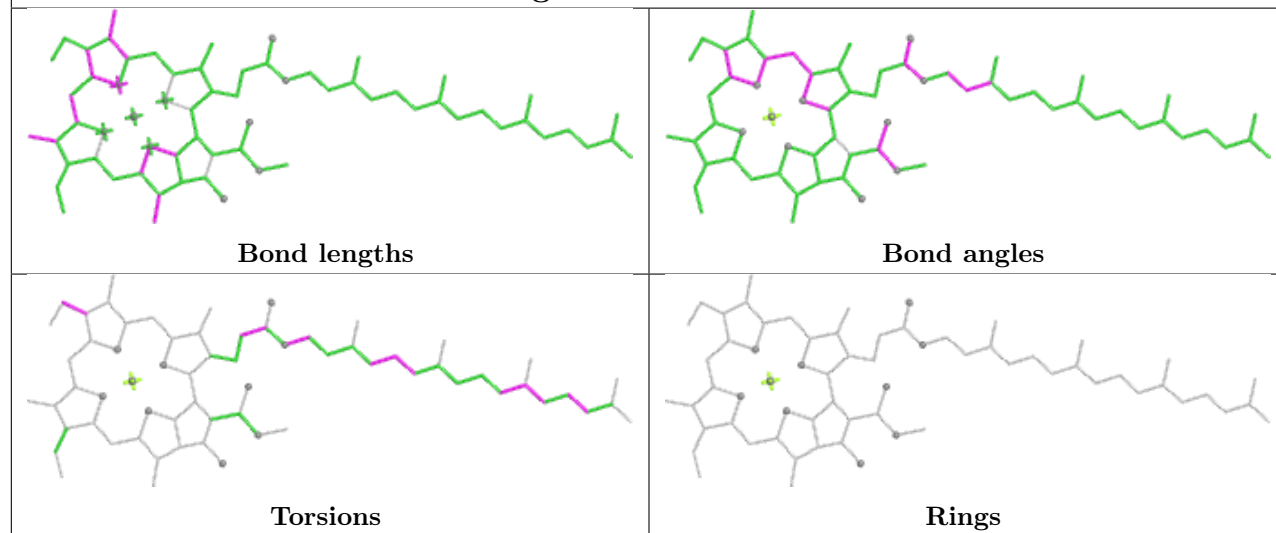


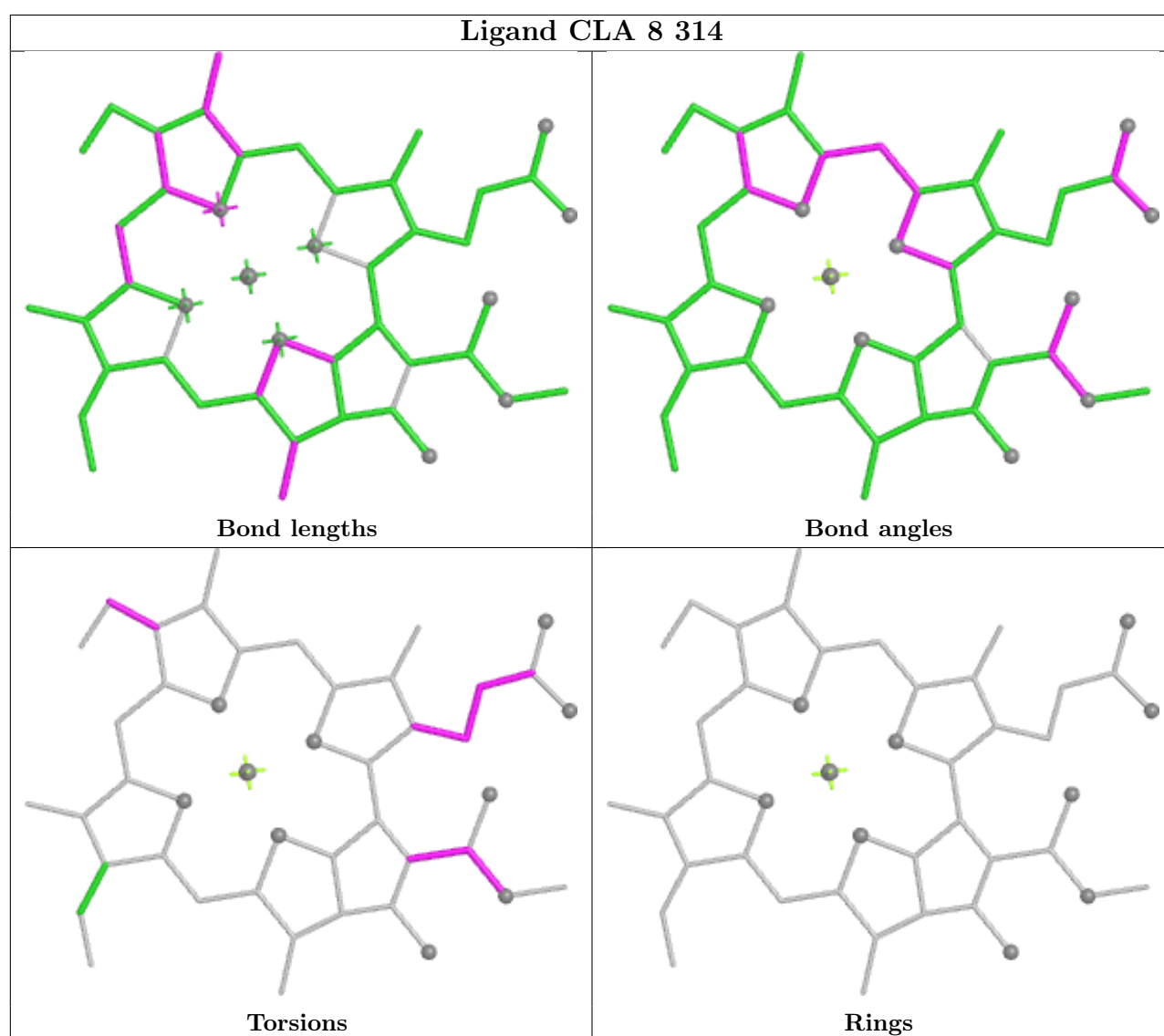
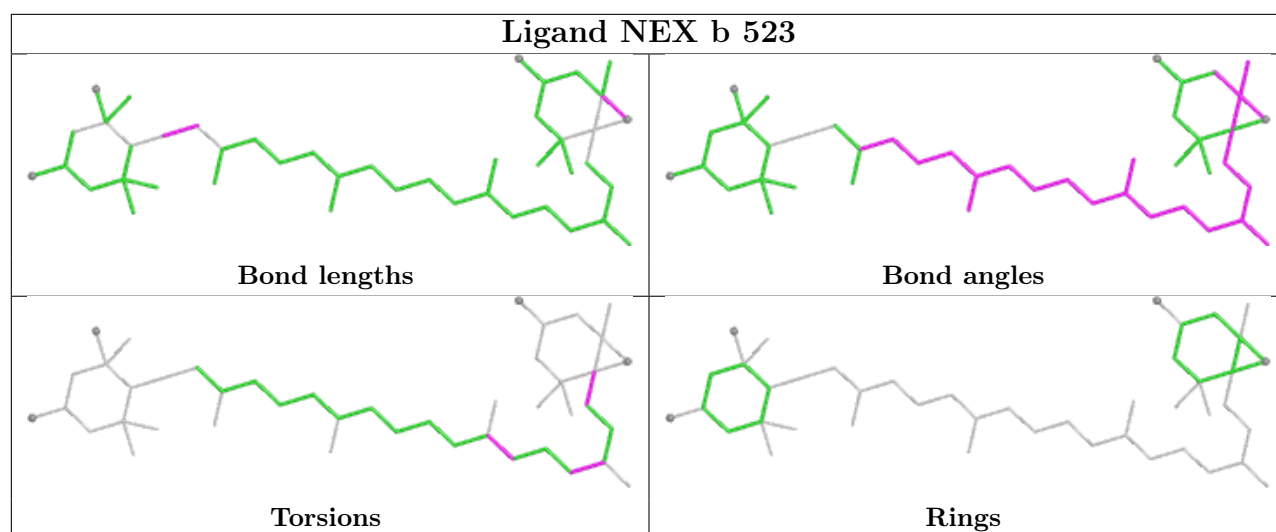
Rings

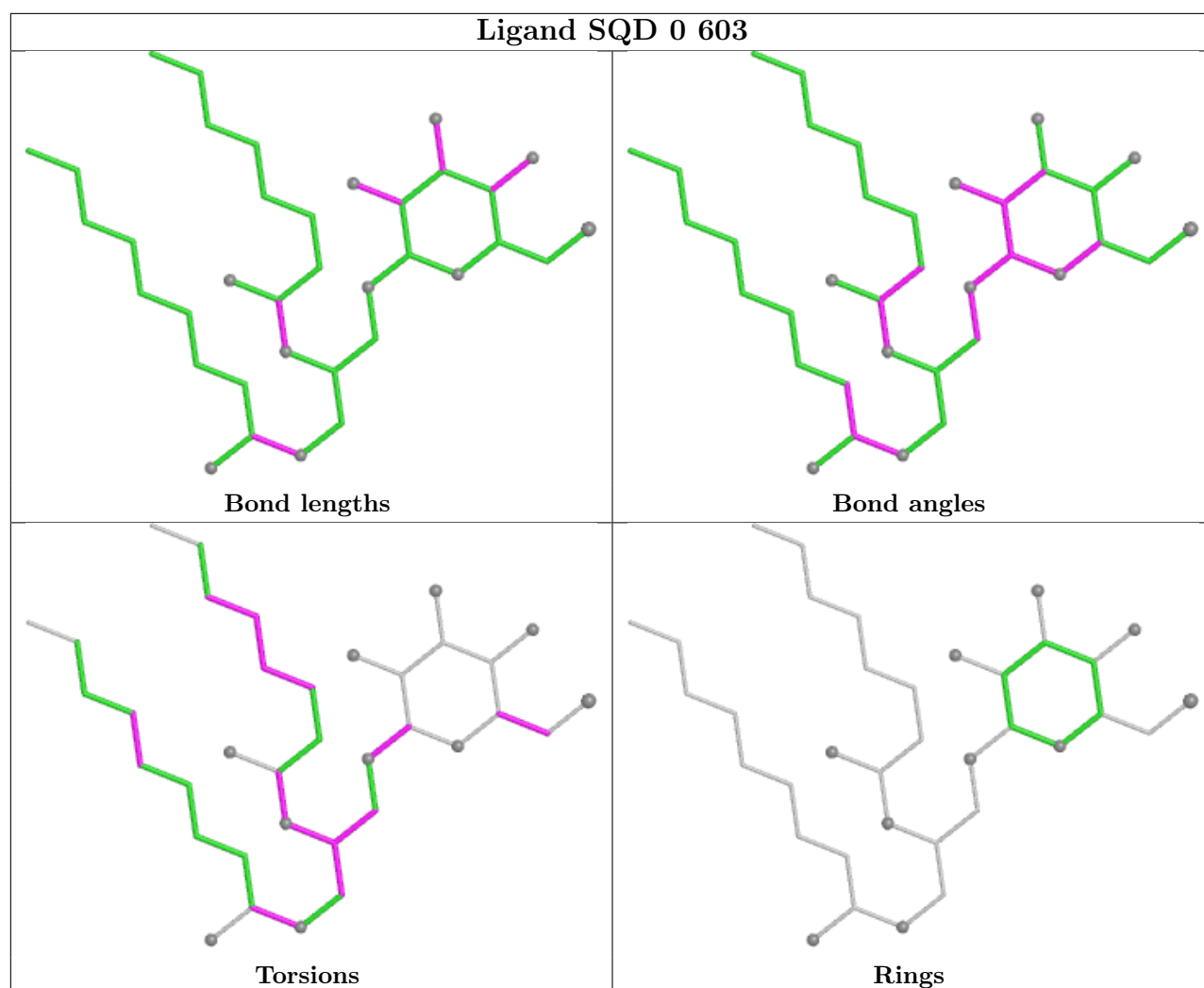
Ligand CHL 4 307



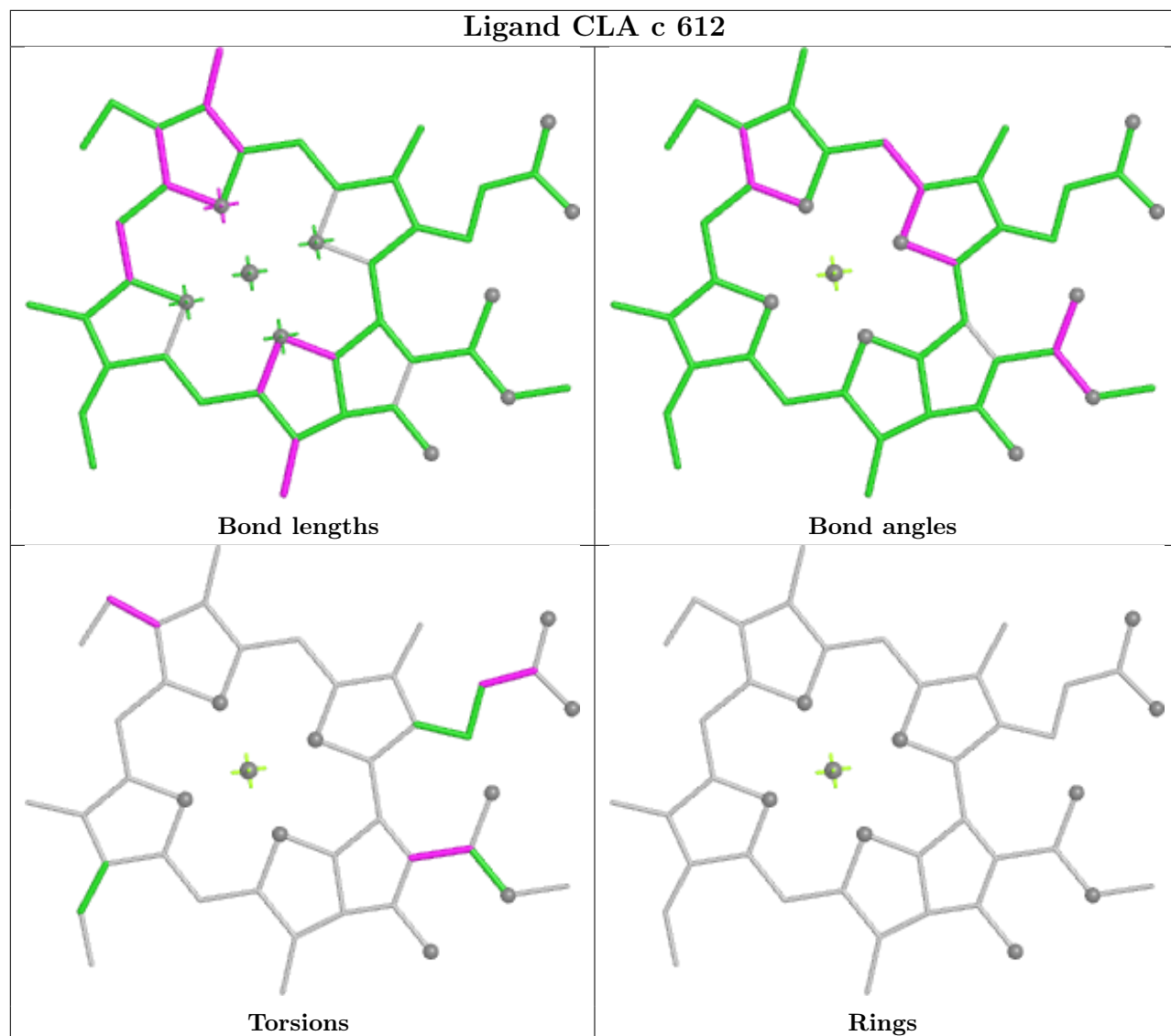
Ligand CLA B 809



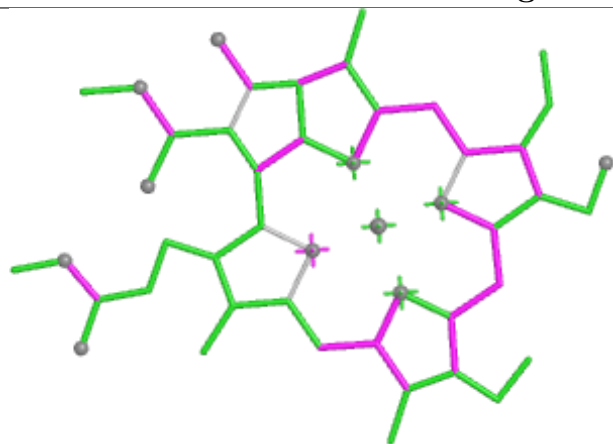




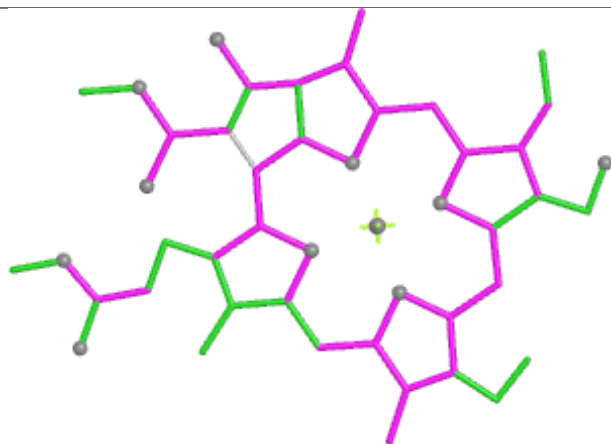
Ligand CLA c 612



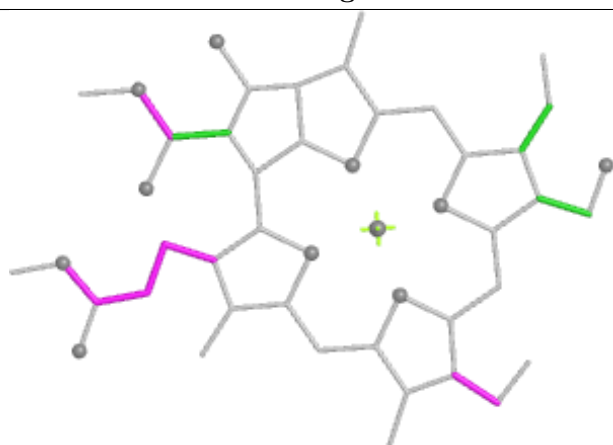
Ligand CHL 5 313



Bond lengths



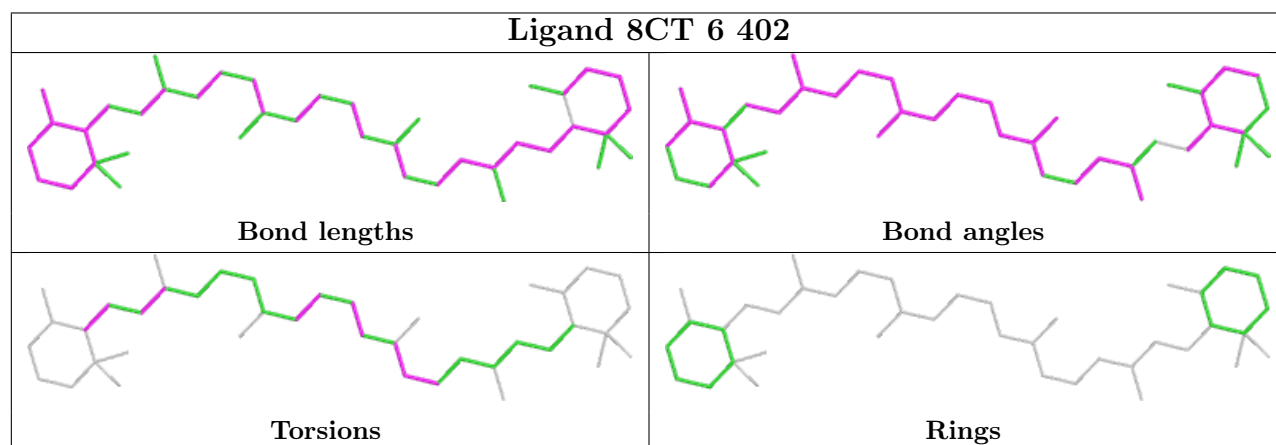
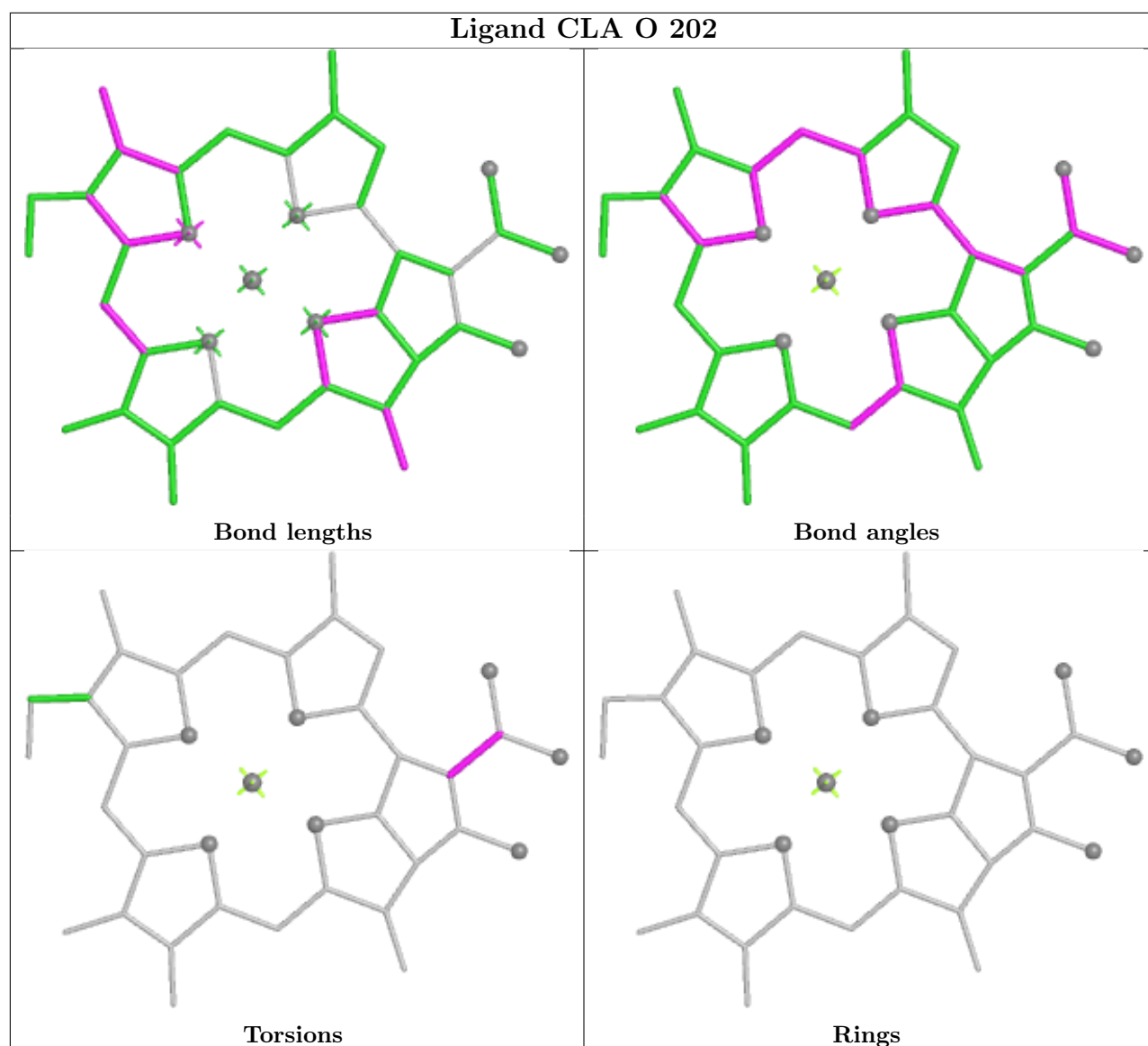
Bond angles



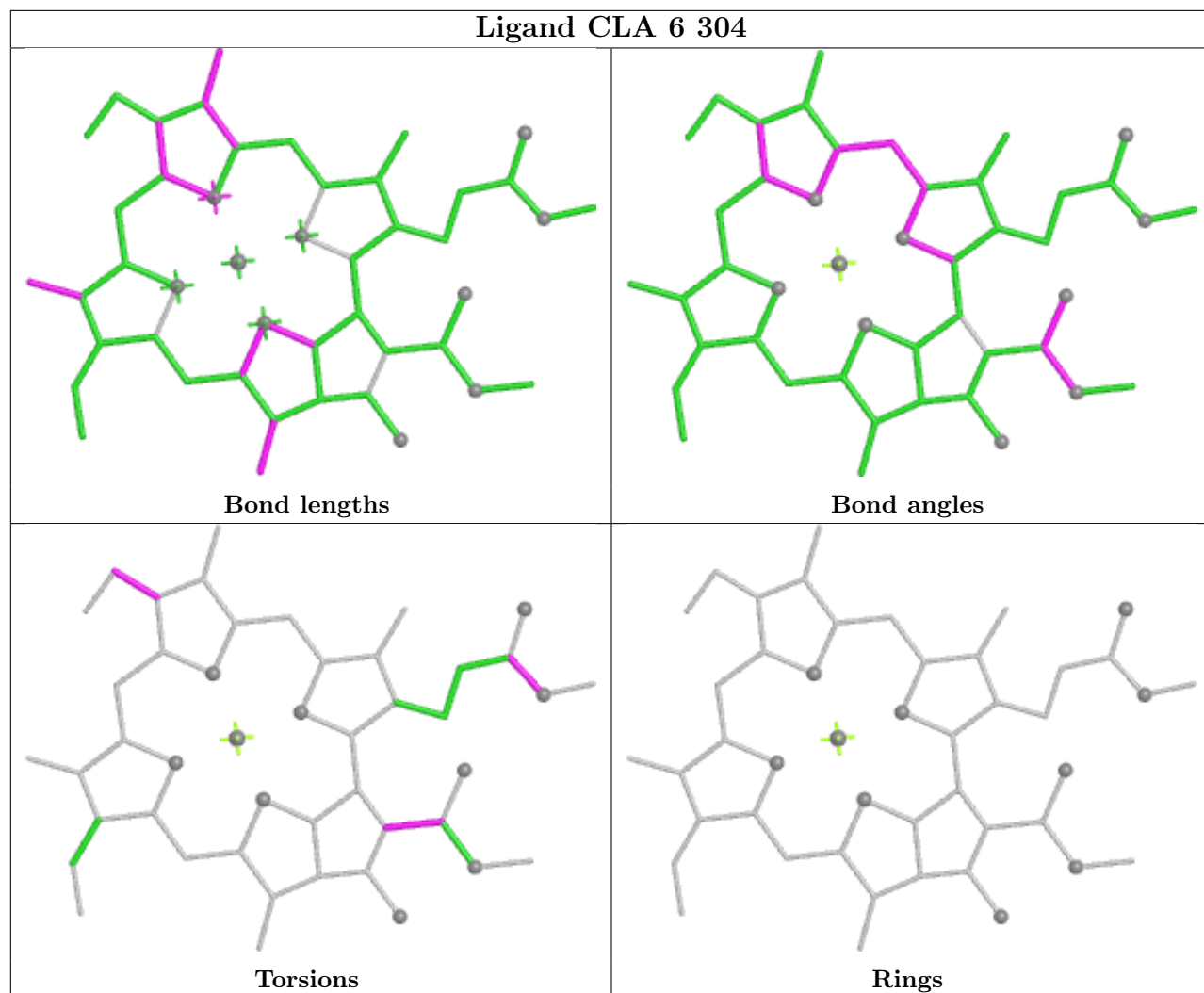
Torsions



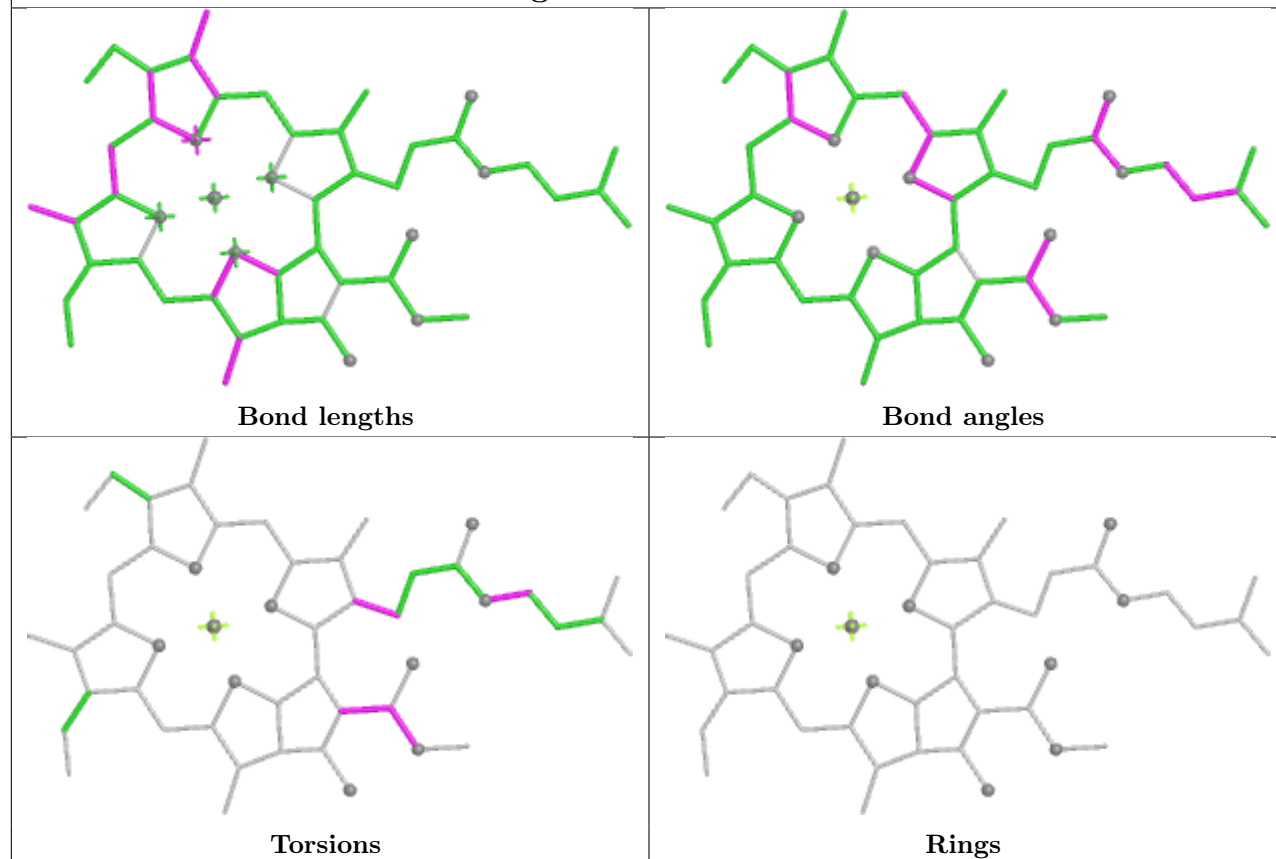
Rings



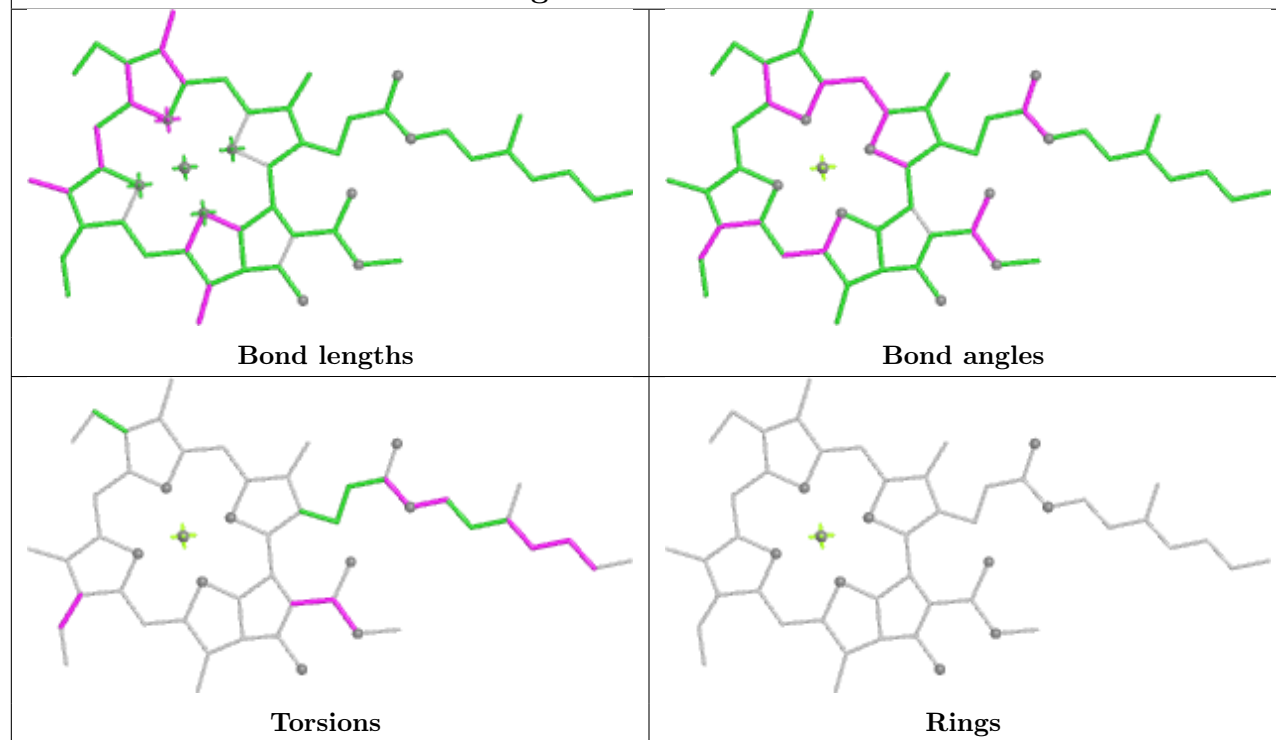
Ligand CLA 6 304



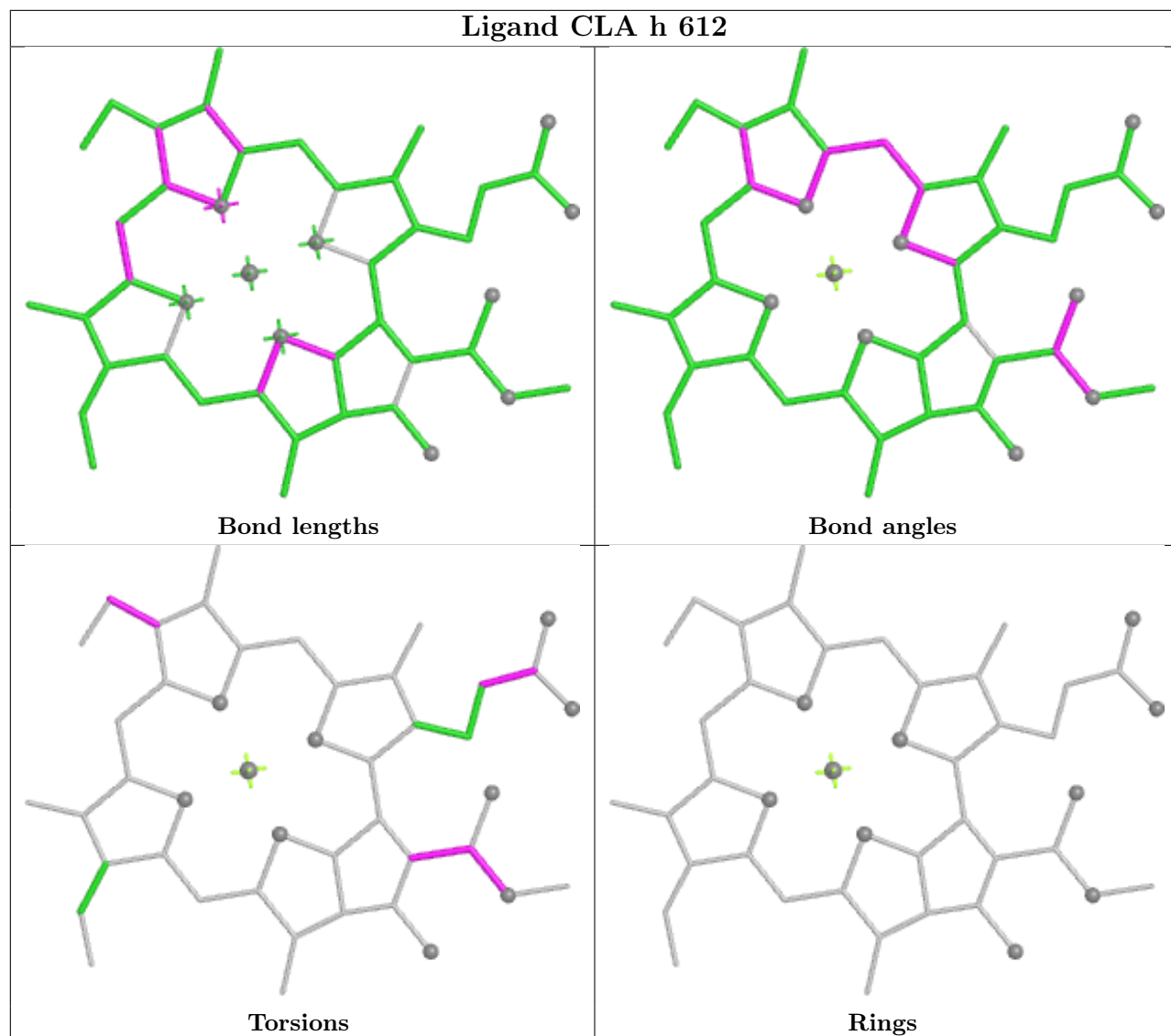
Ligand CLA G 101



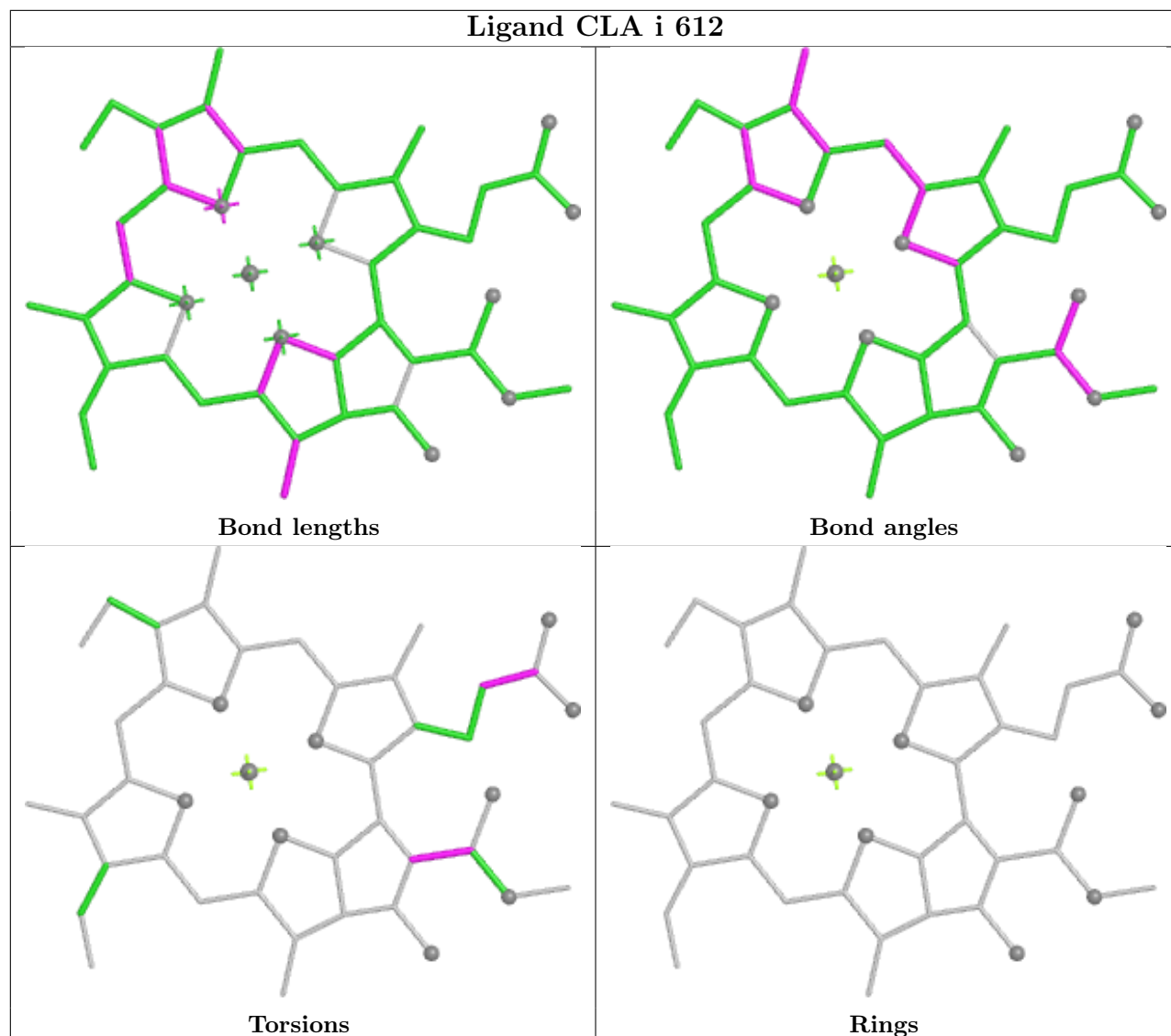
Ligand CLA K 102



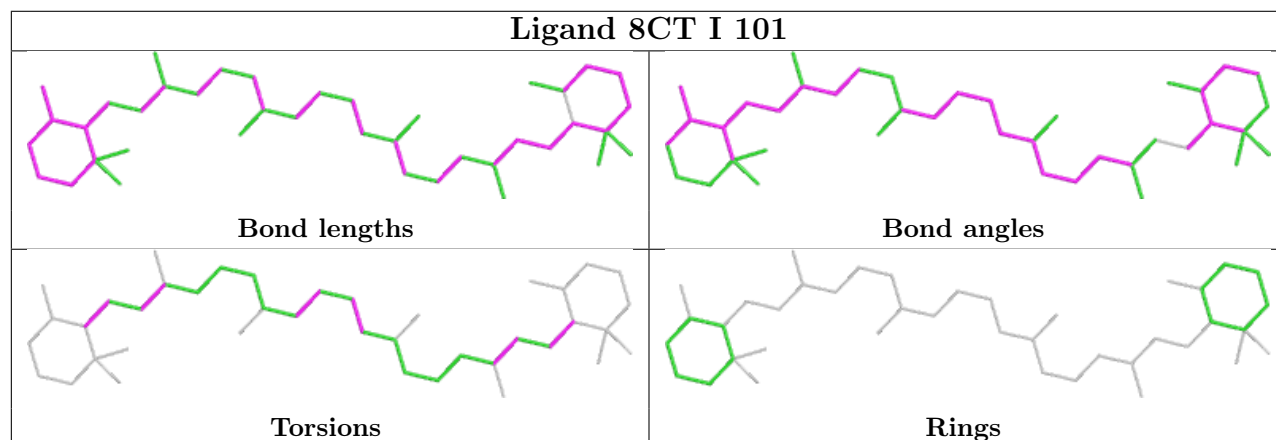
Ligand CLA h 612

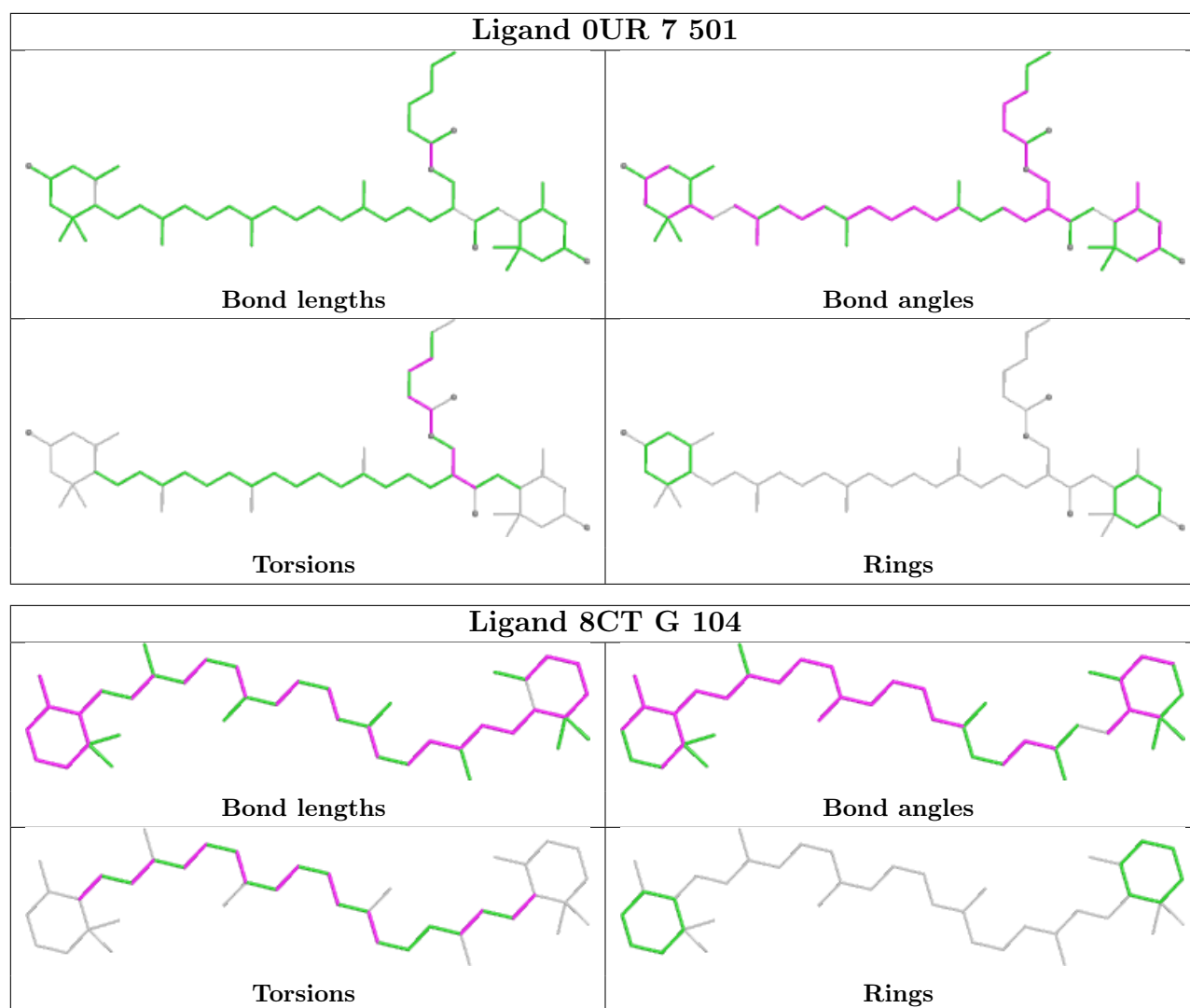


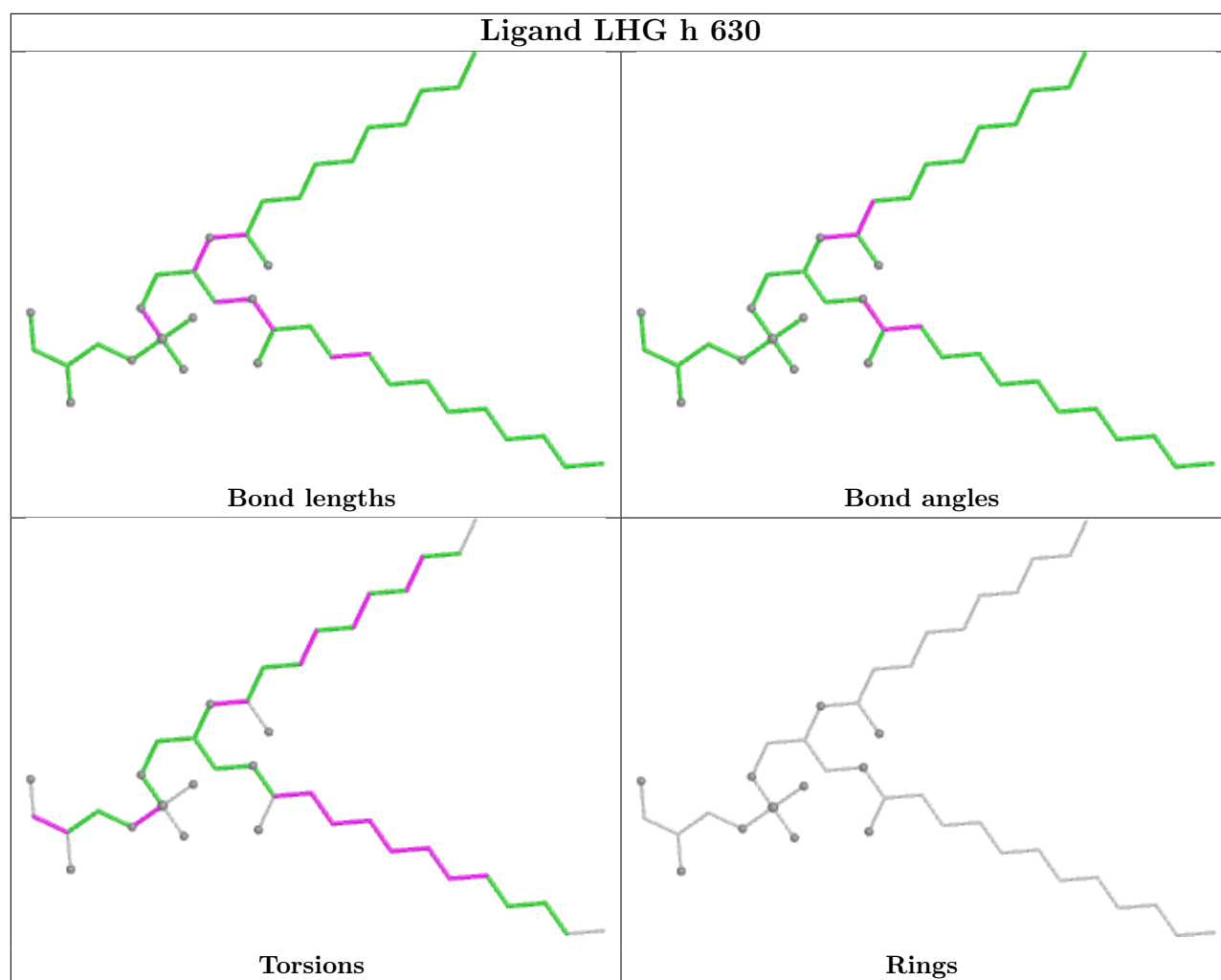
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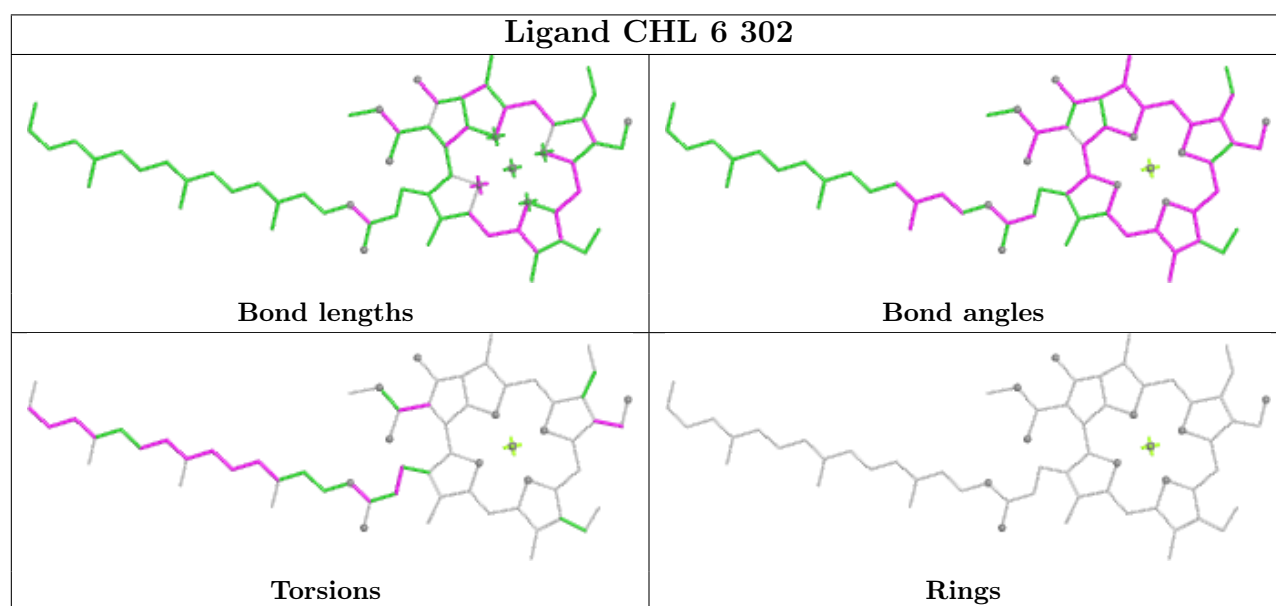
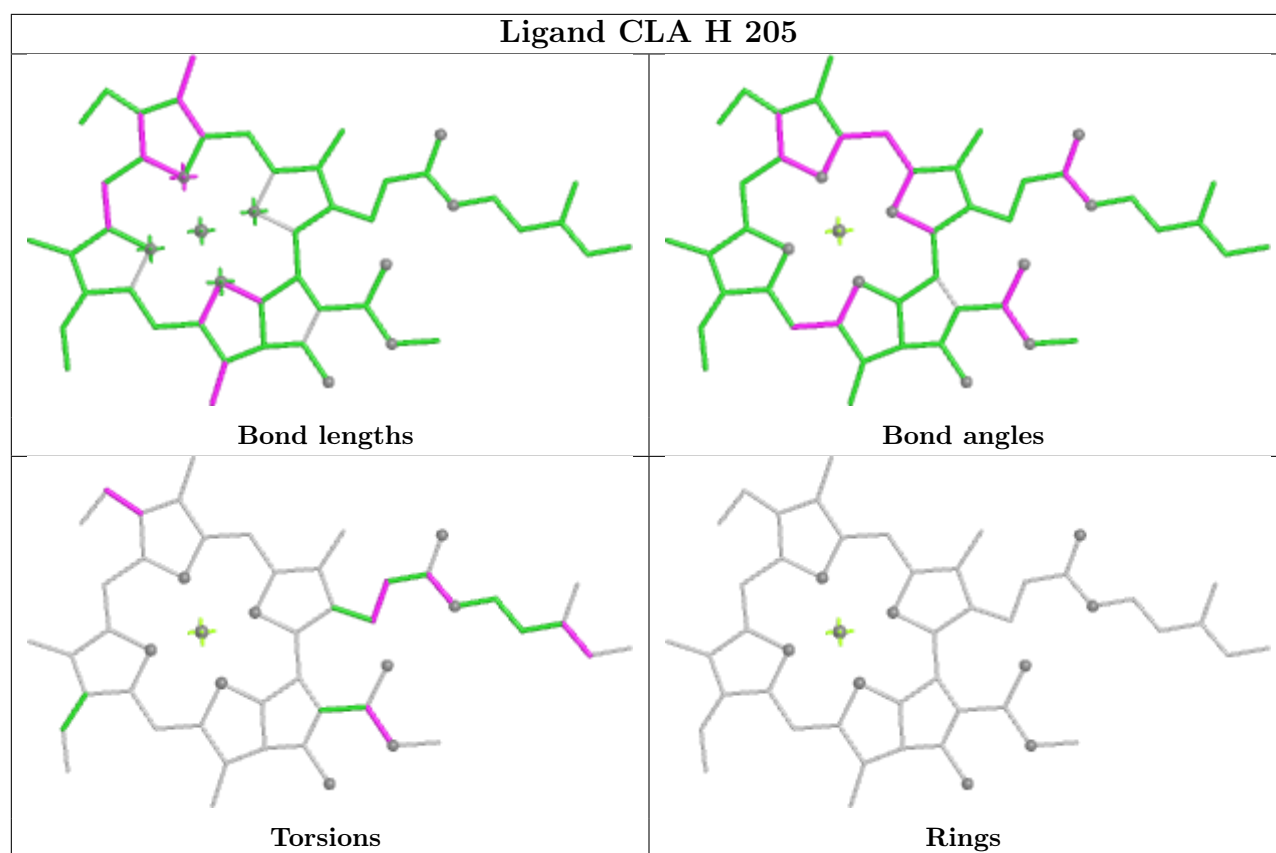


Ligand 8CT I 101

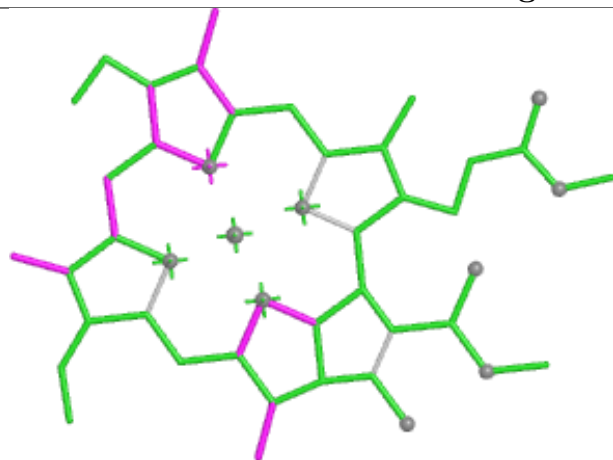




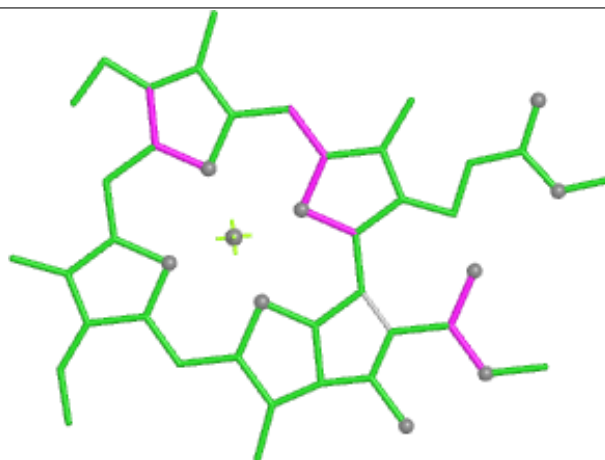




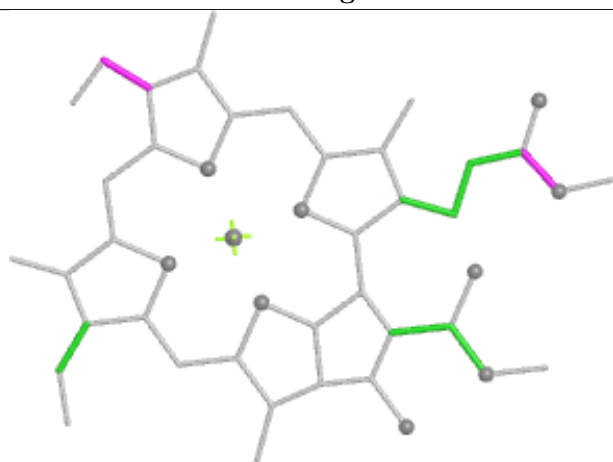
Ligand CLA 8 310



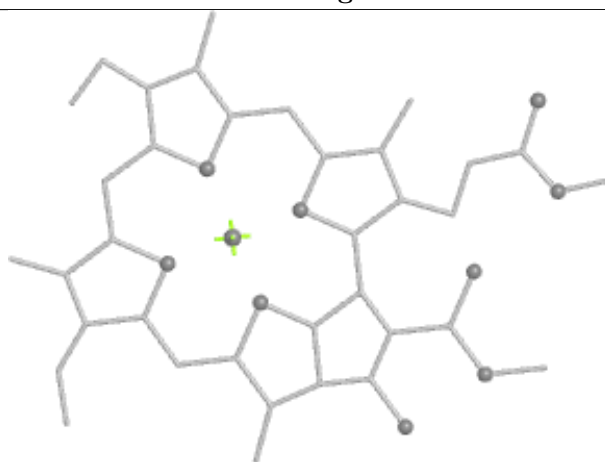
Bond lengths



Bond angles

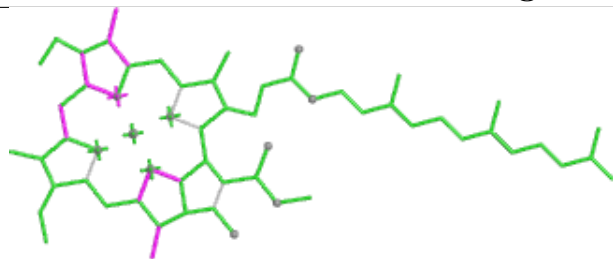


Torsions

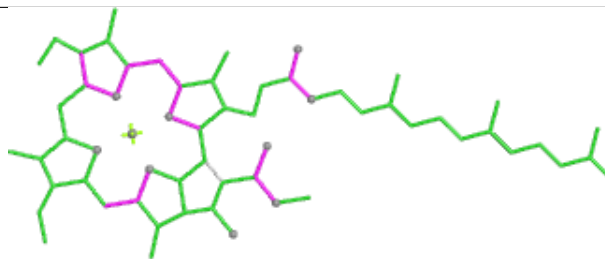


Rings

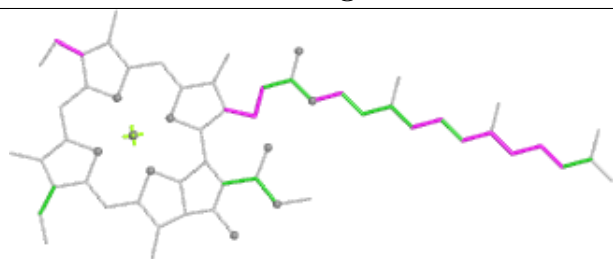
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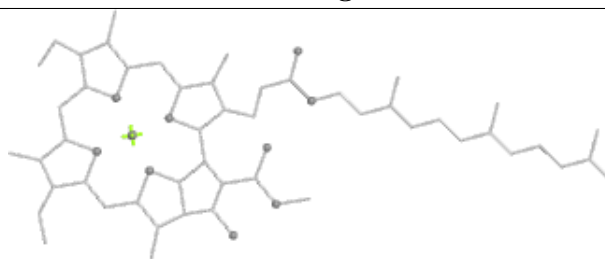
Bond lengths



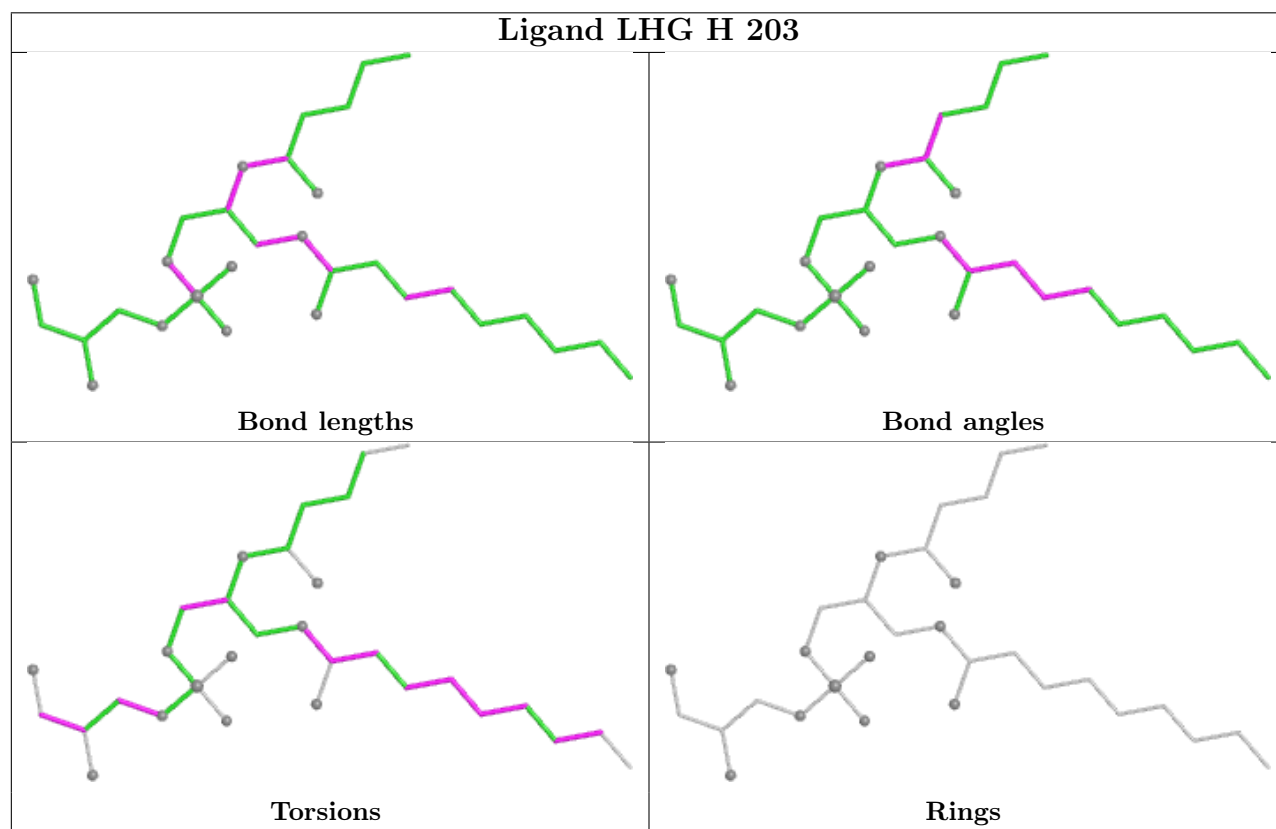
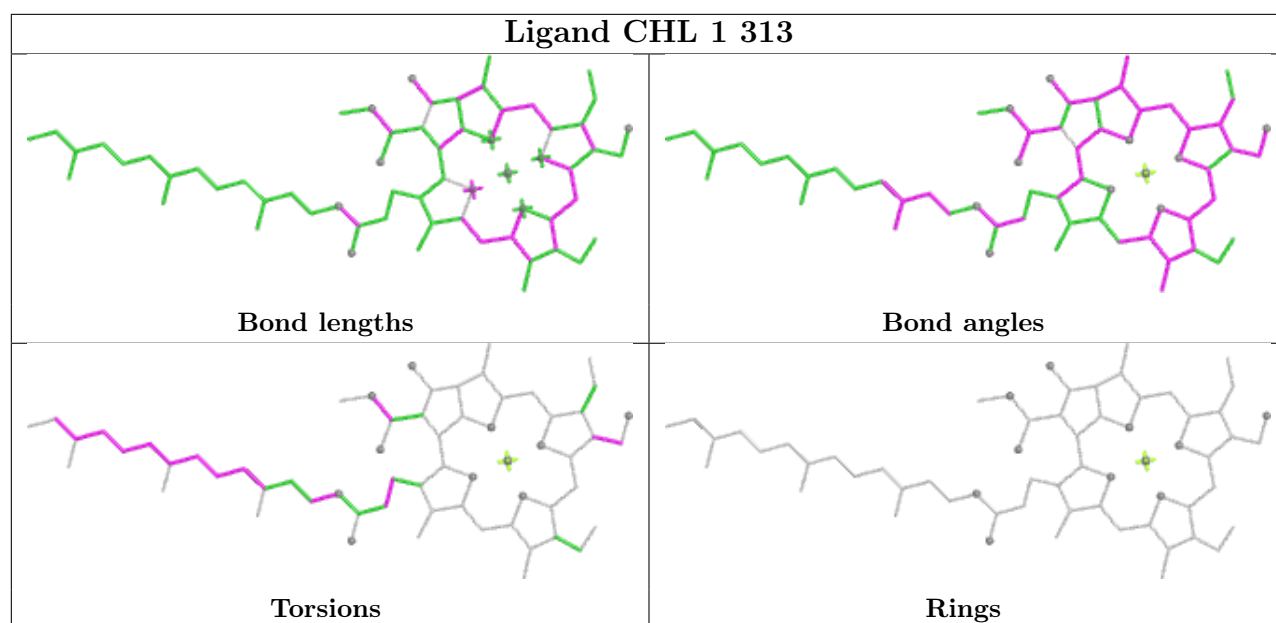
Bond angles



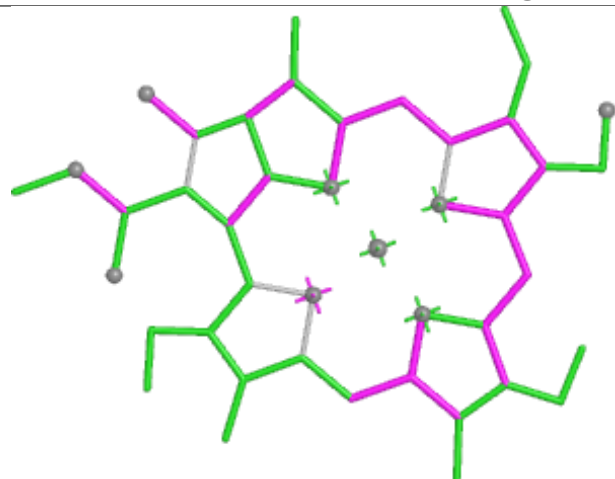
Torsions



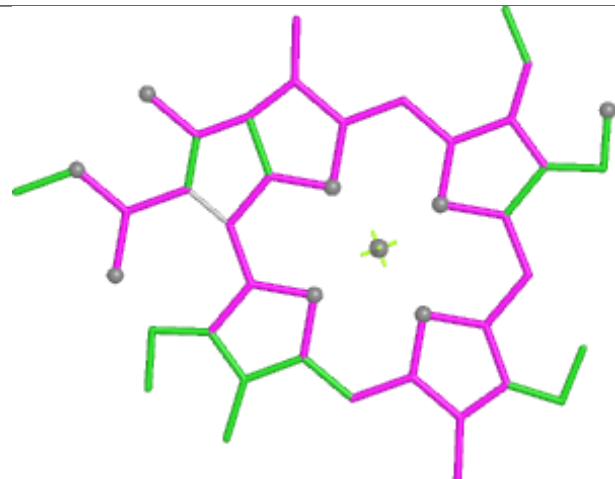
Rings



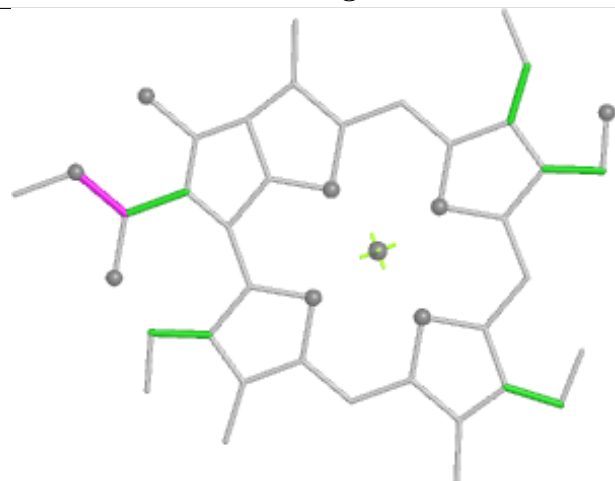
Ligand CHL h 605



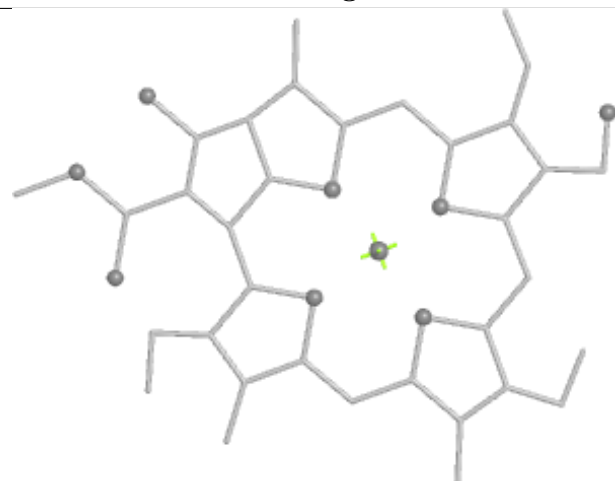
Bond lengths



Bond angles

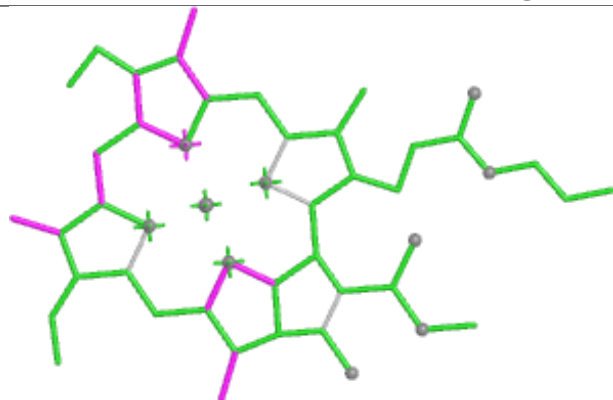


Torsions

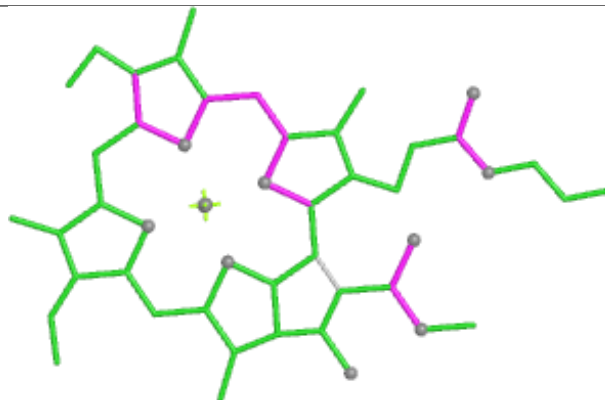


Rings

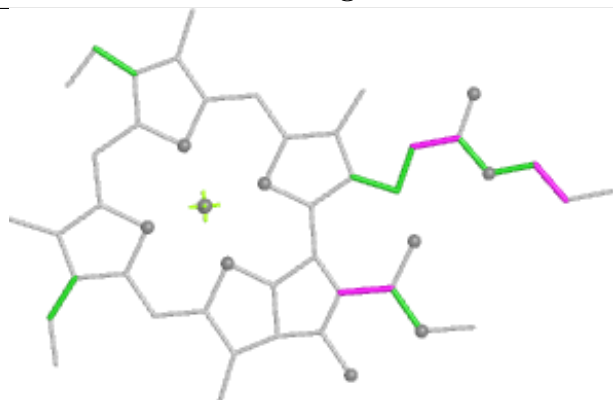
Ligand CLA 6 311



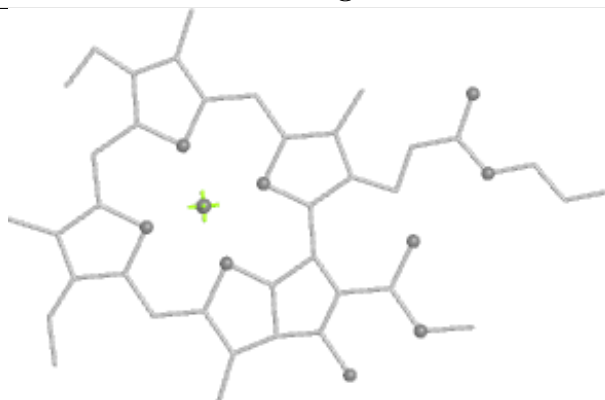
Bond lengths



Bond angles

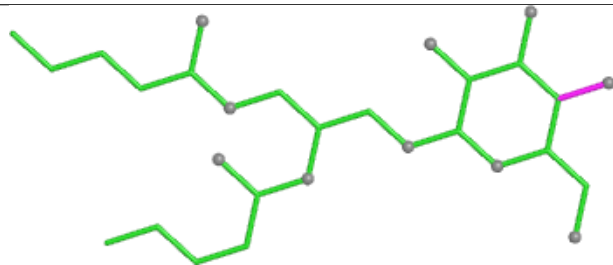


Torsions

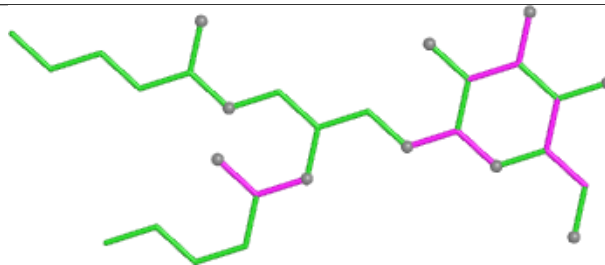


Rings

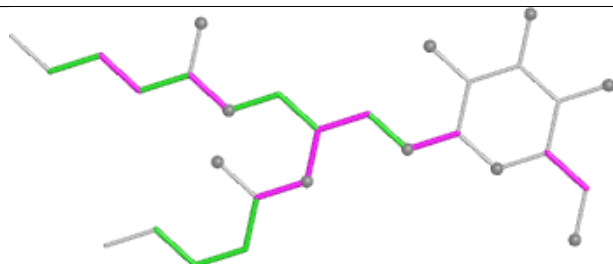
Ligand LMG J 102



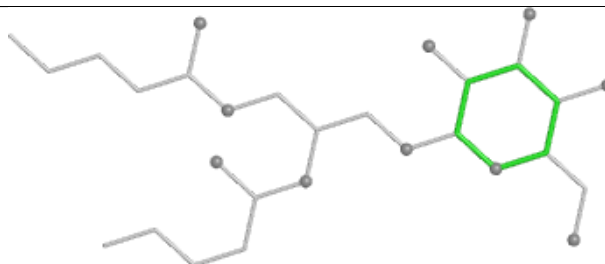
Bond lengths



Bond angles

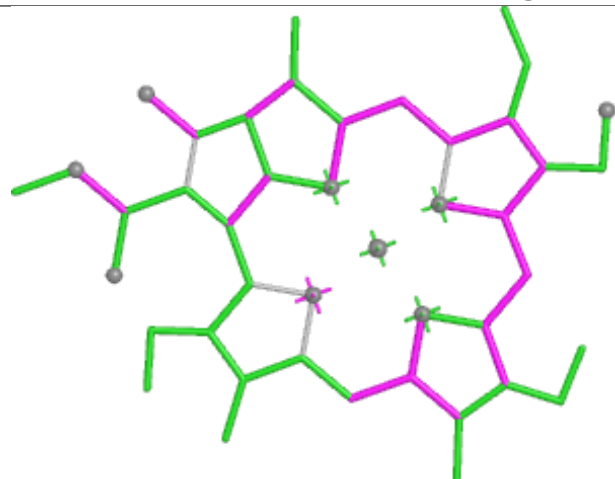


Torsions

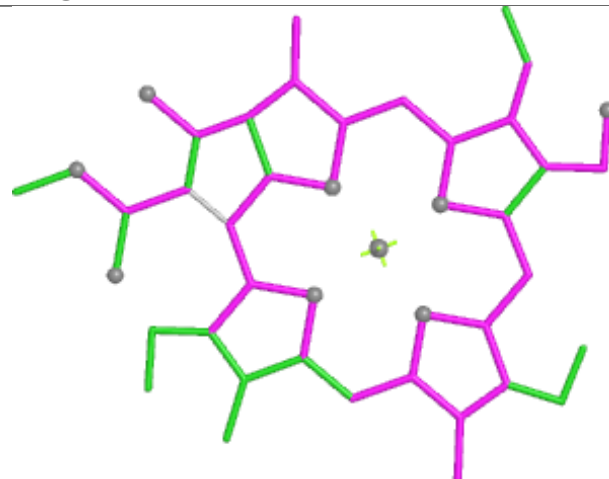


Rings

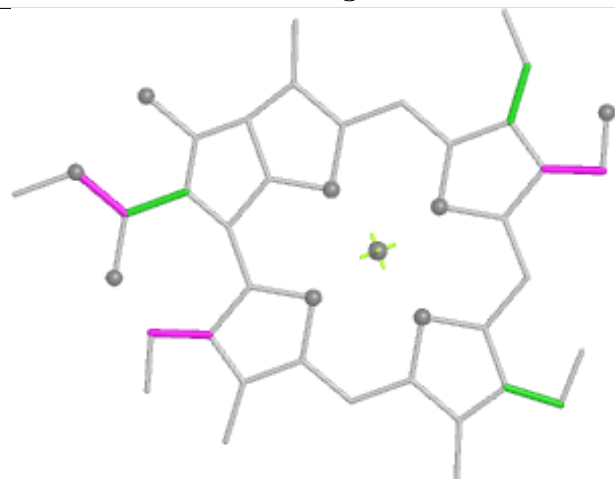
Ligand CHL g 608



Bond lengths



Bond angles

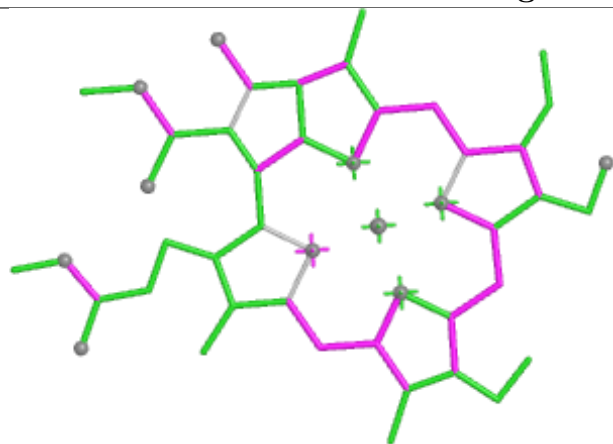


Torsions

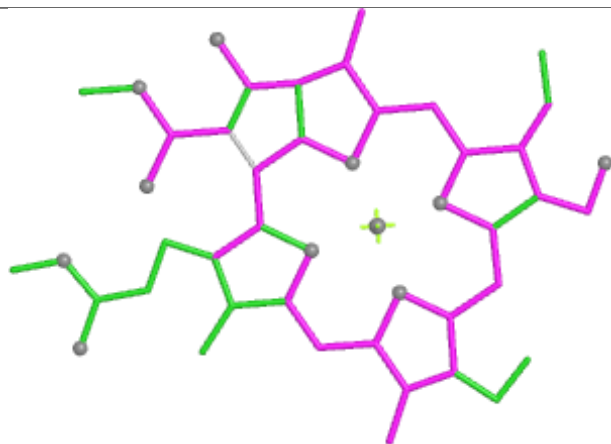


Rings

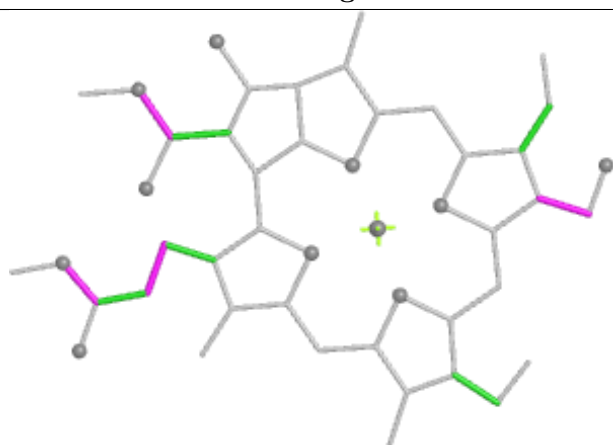
Ligand CHL 9 301



Bond lengths



Bond angles

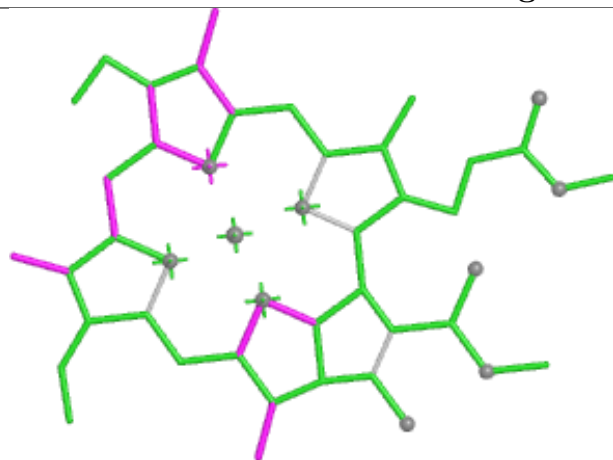


Torsions

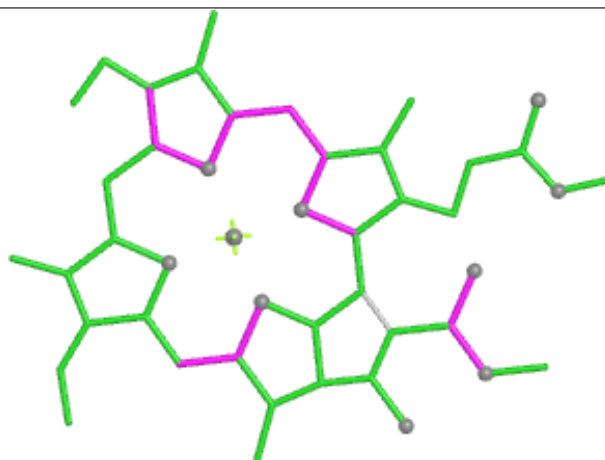


Rings

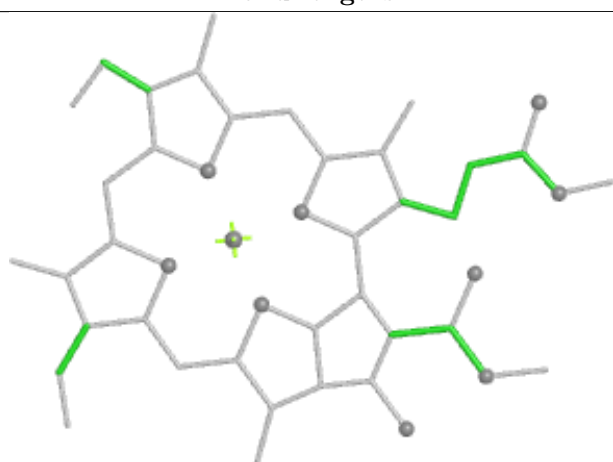
Ligand CLA 3 318



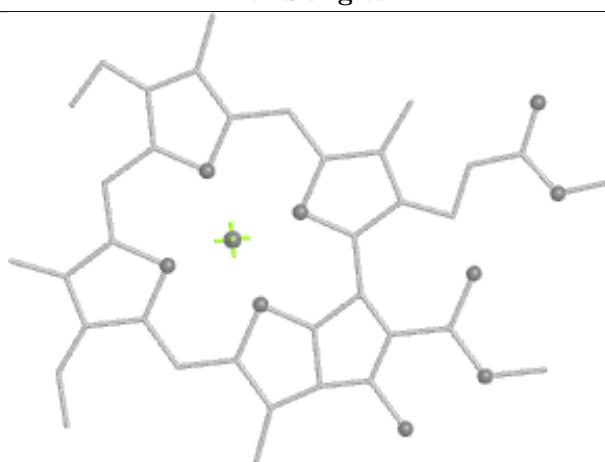
Bond lengths



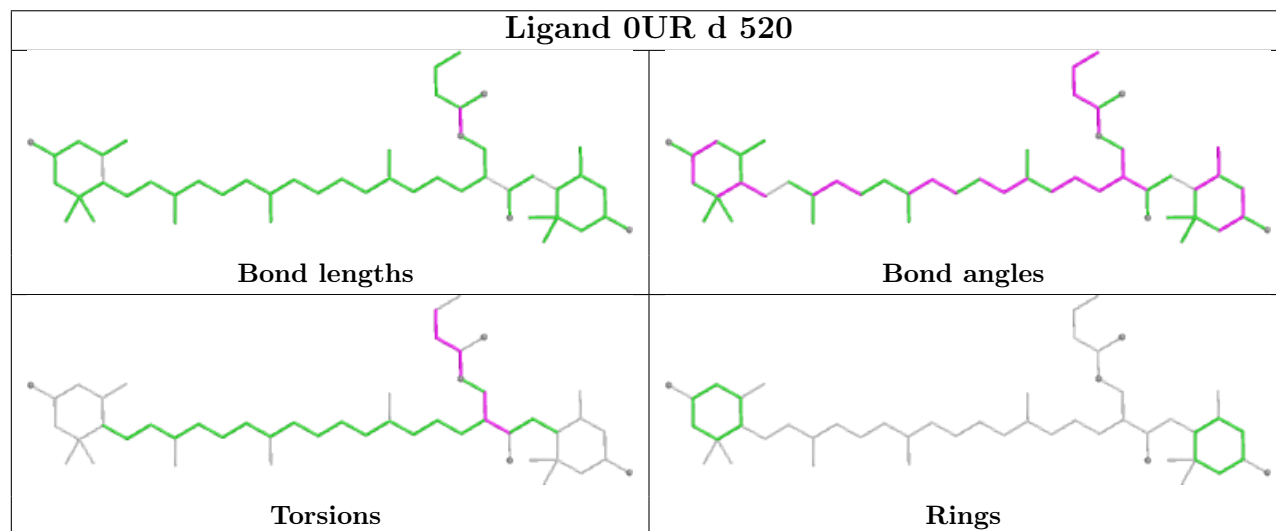
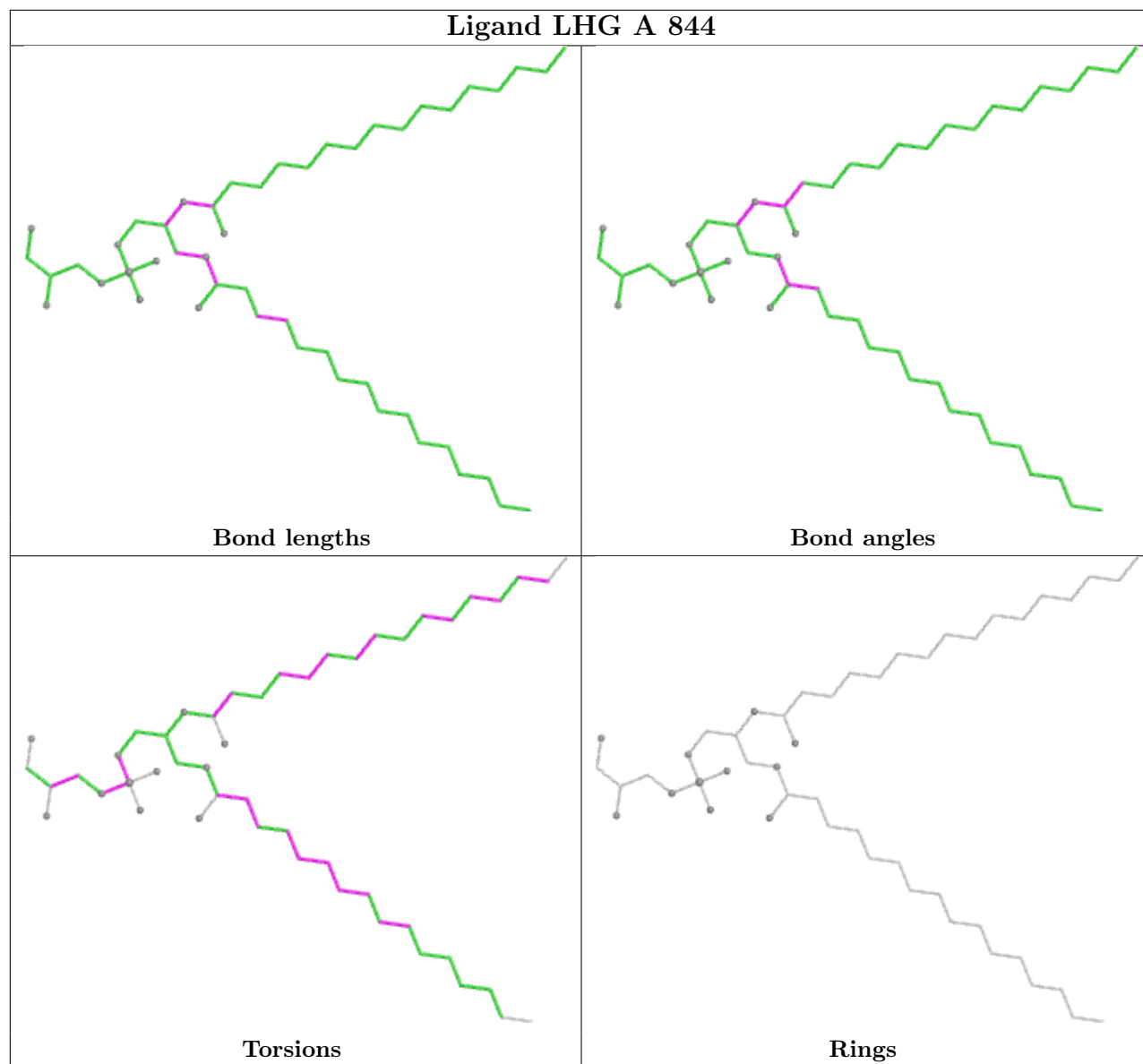
Bond angles

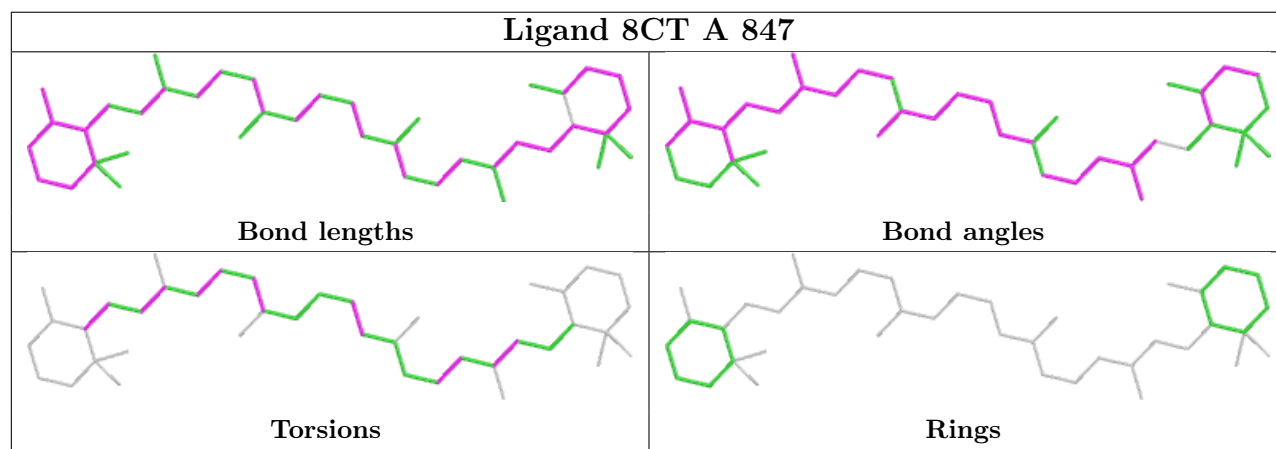
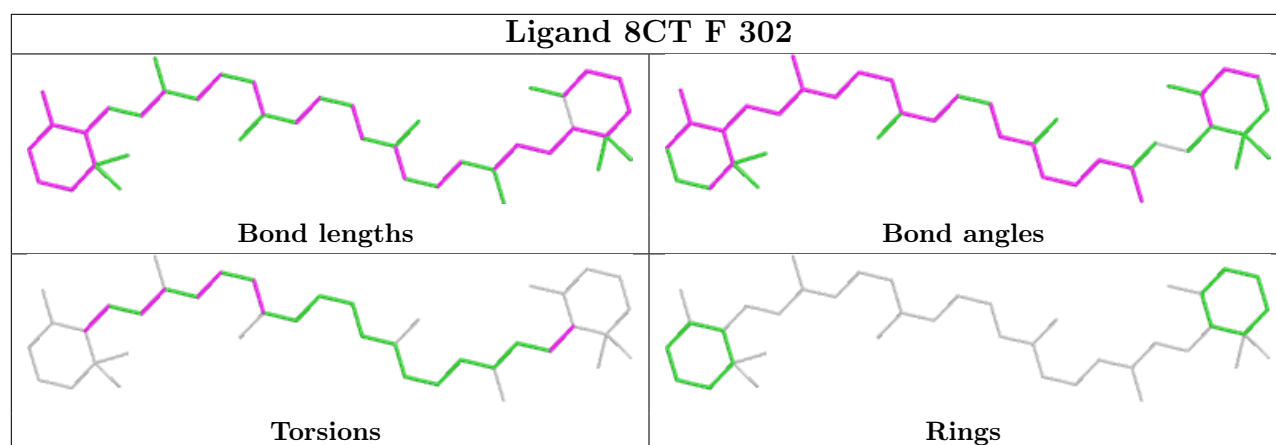


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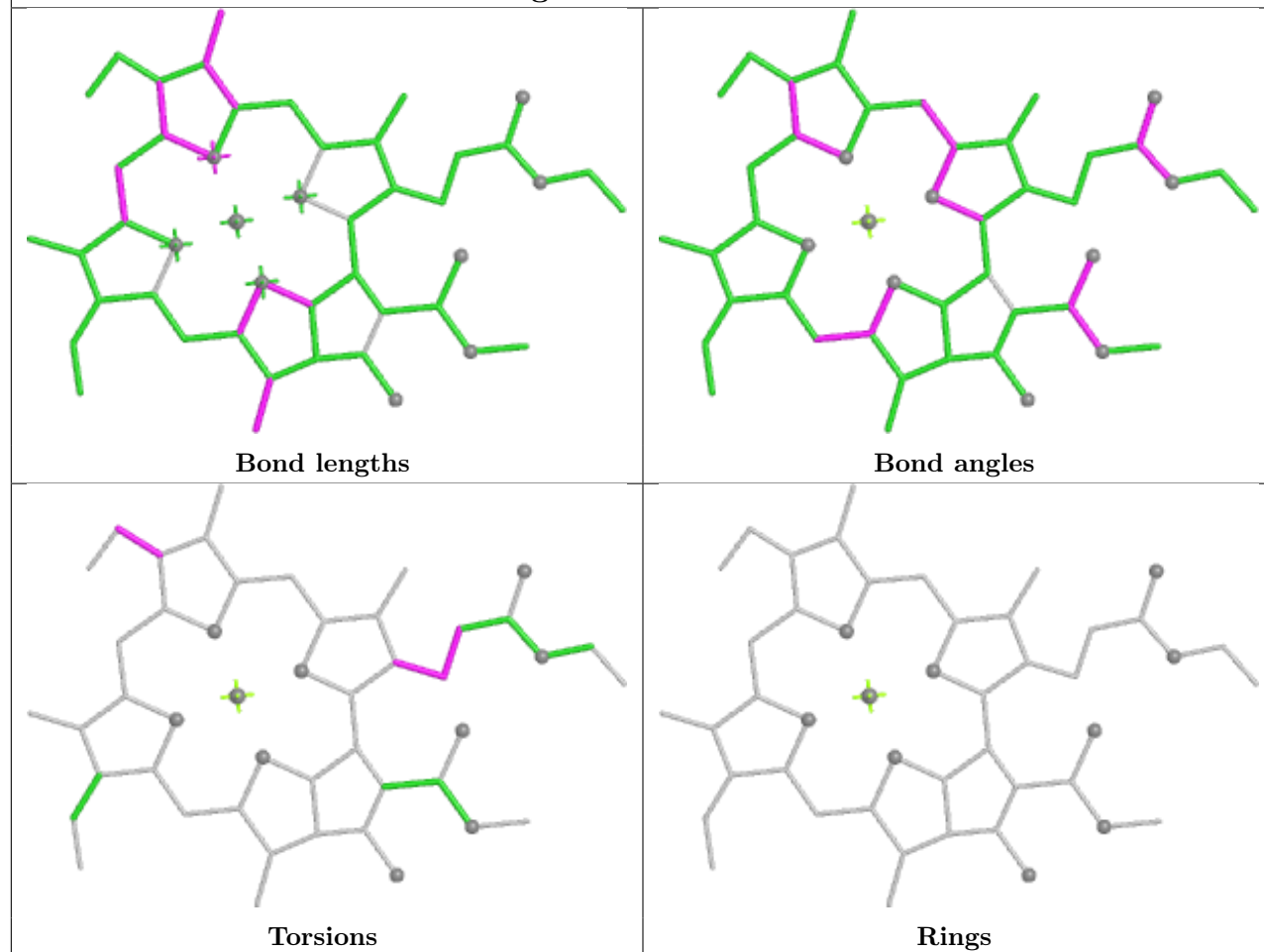


Rings

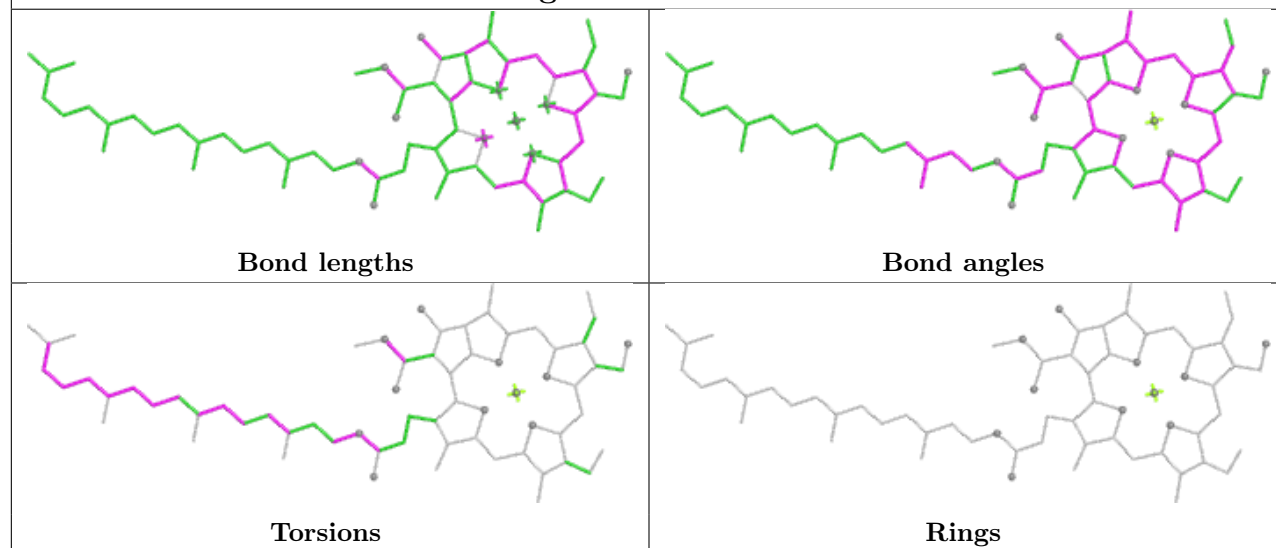




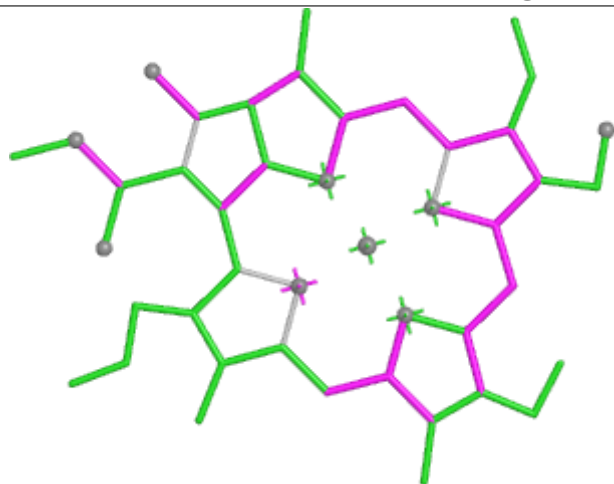
Ligand CLA 3 306



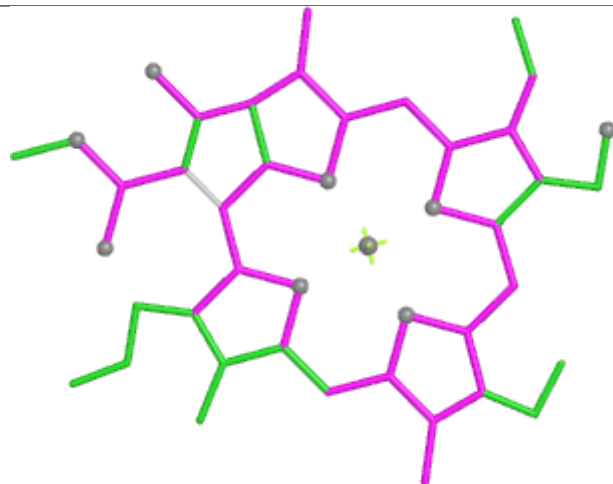
Ligand CHL f 609



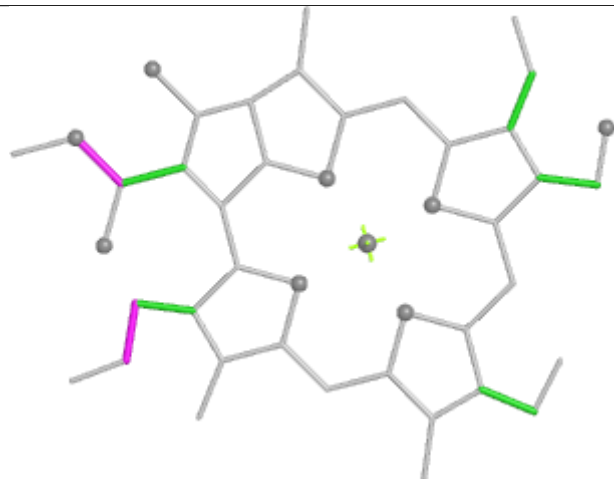
Ligand CHL c 606



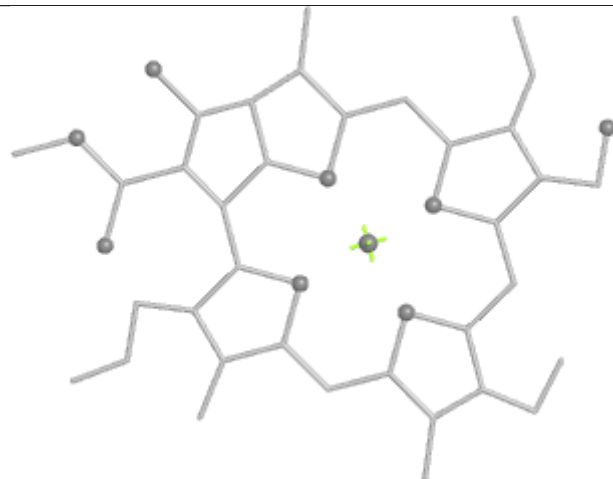
Bond lengths



Bond angles

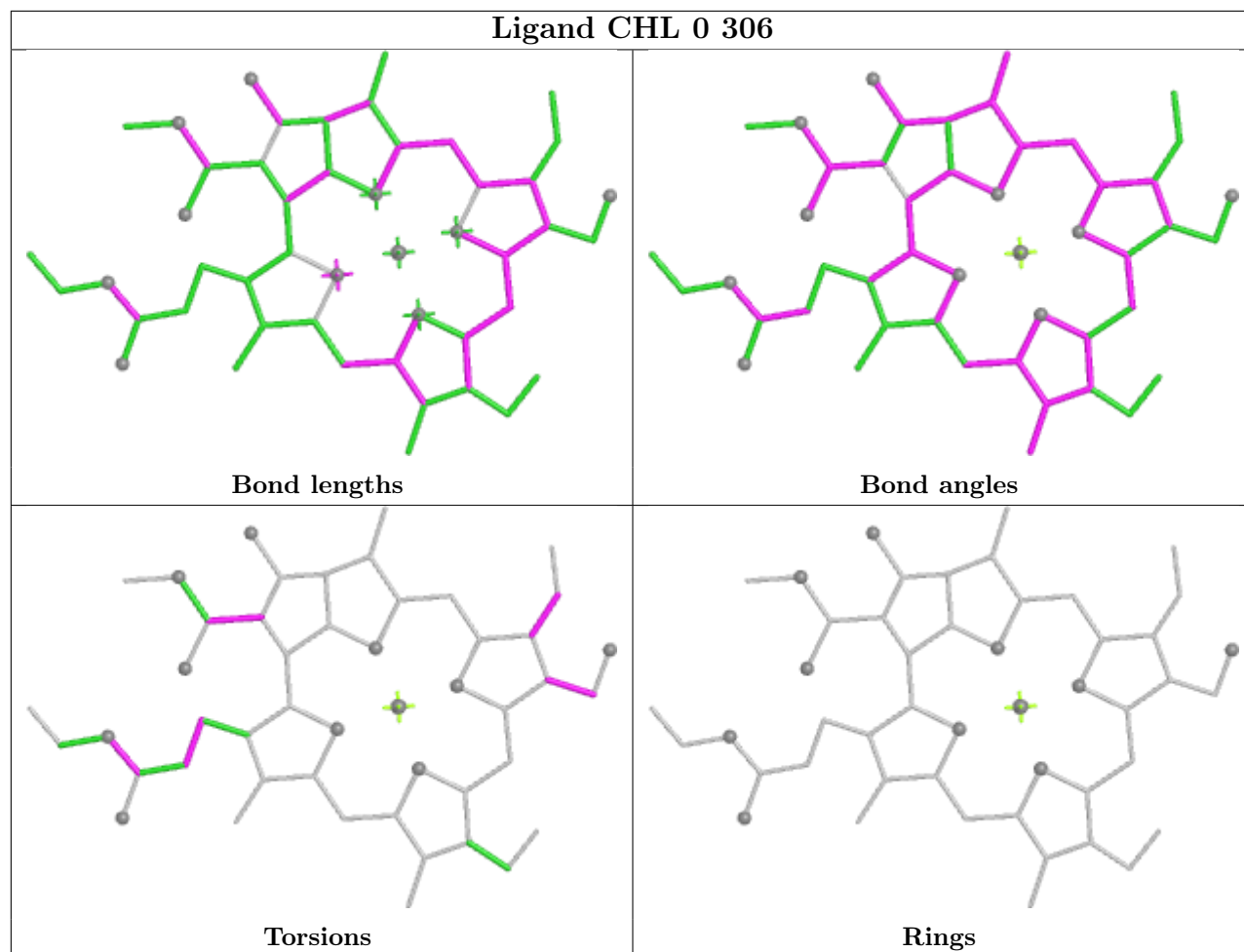


Torsions

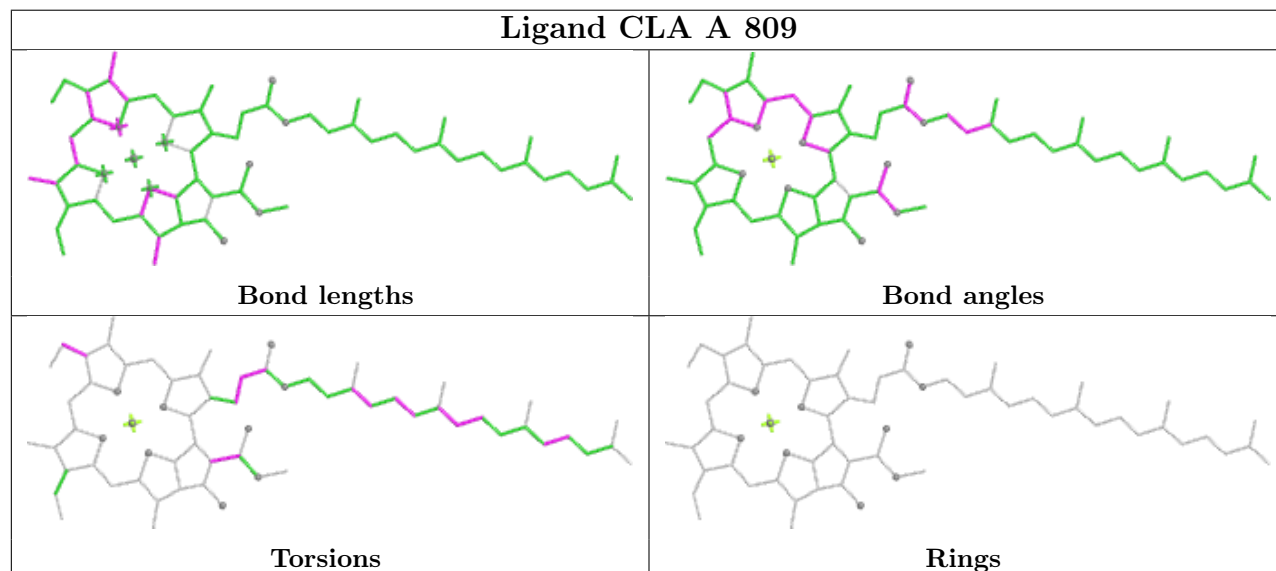


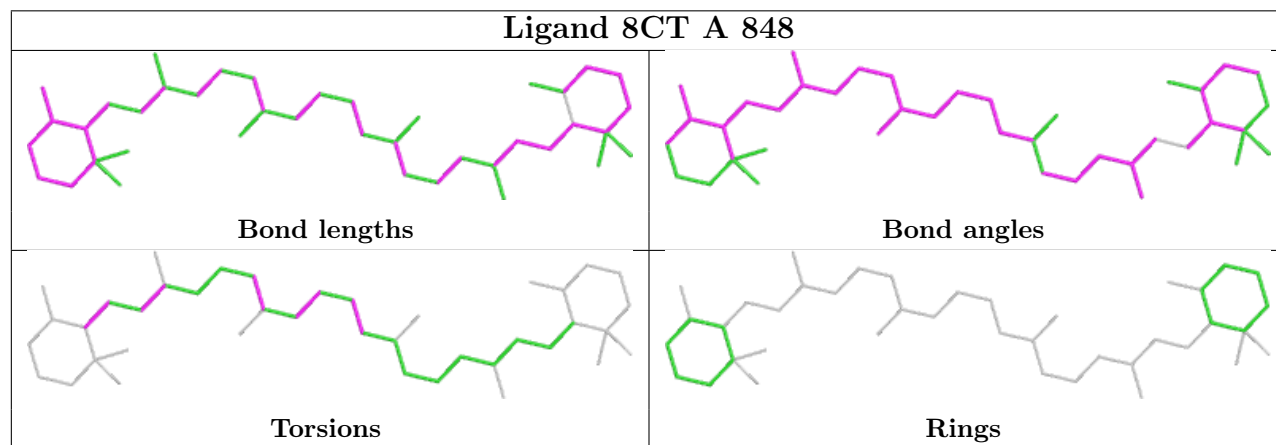
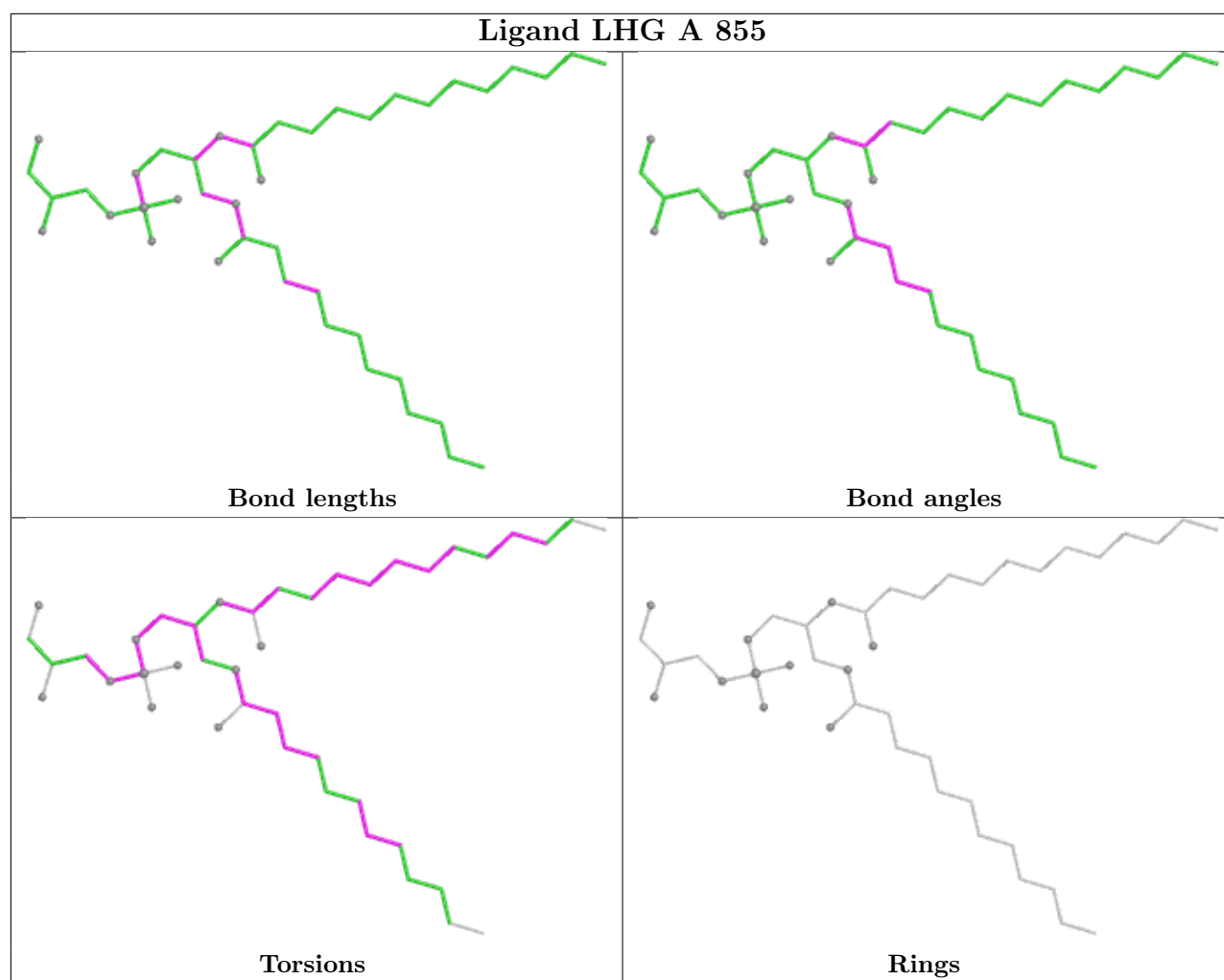
Rings

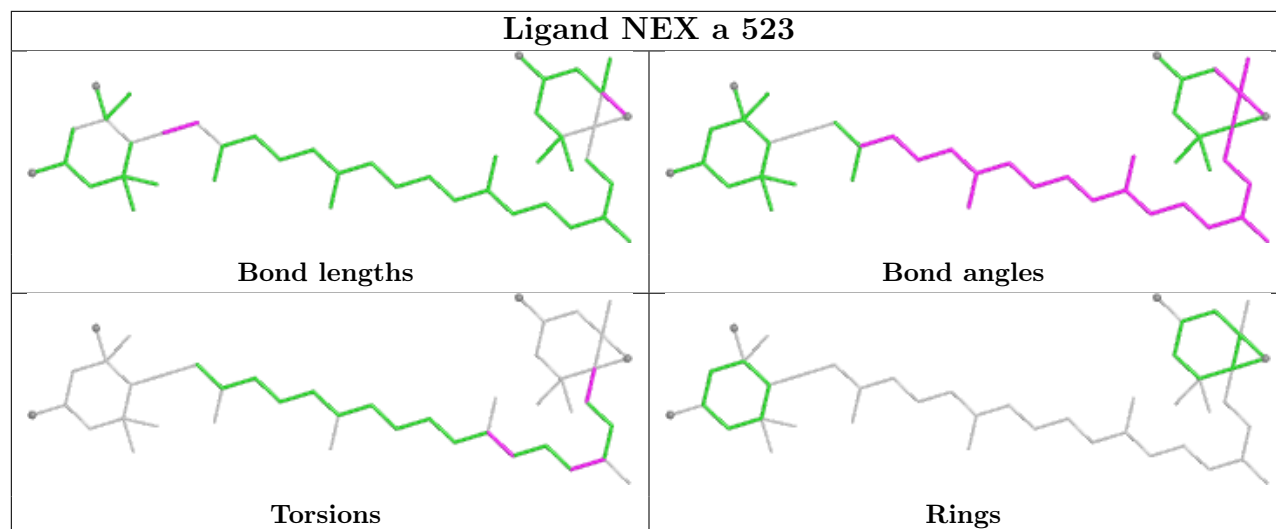
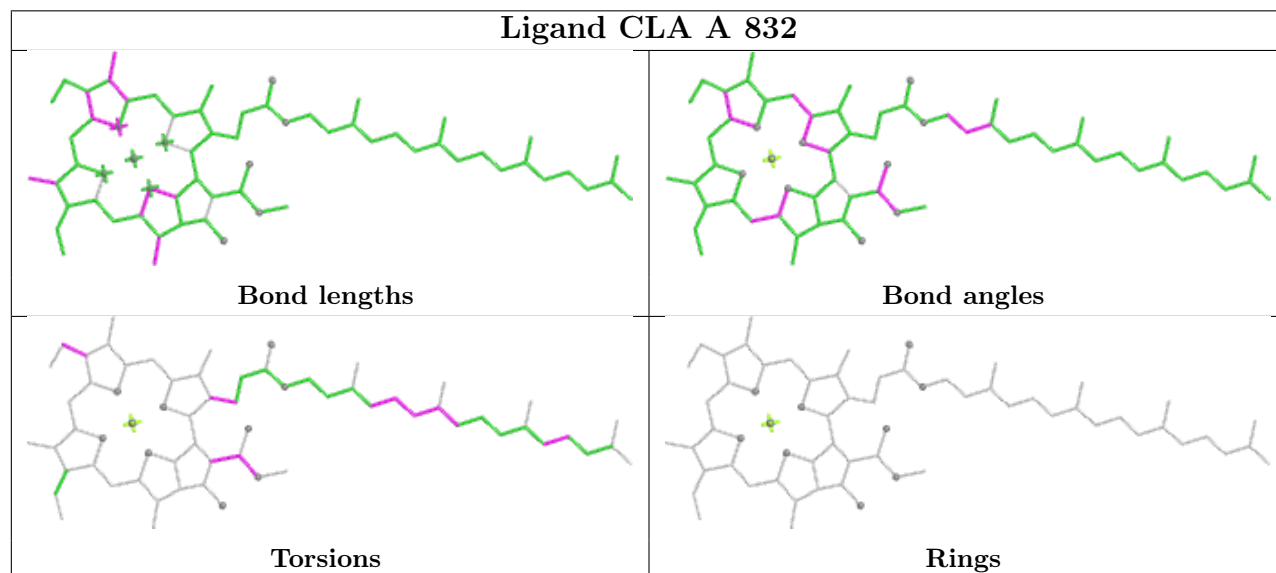
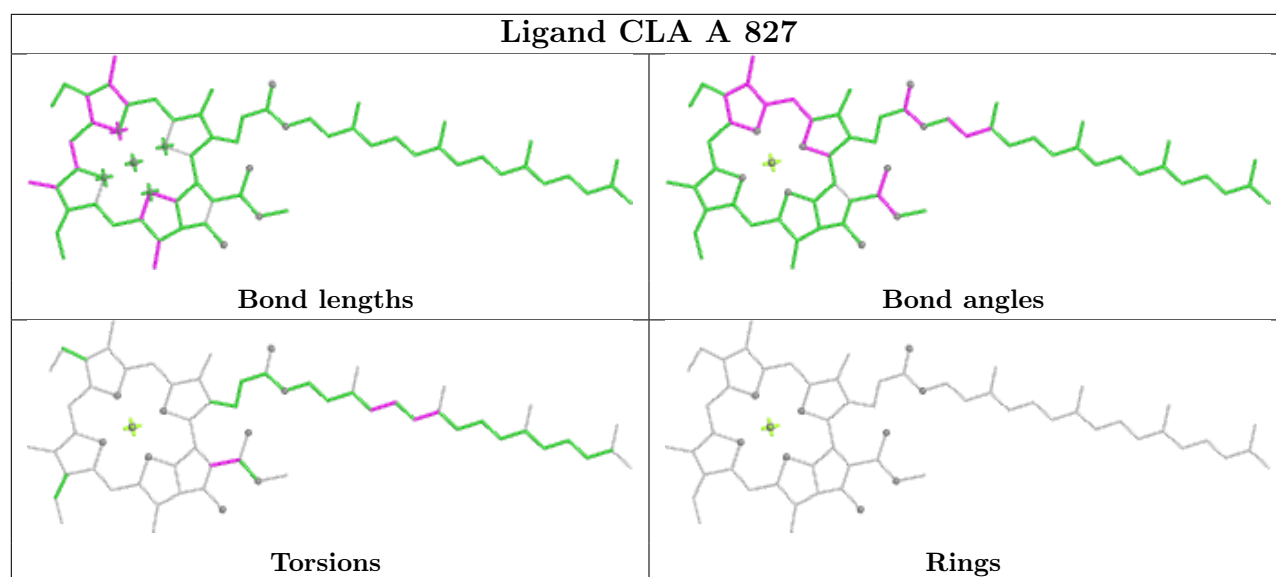
Ligand CHL 0 306

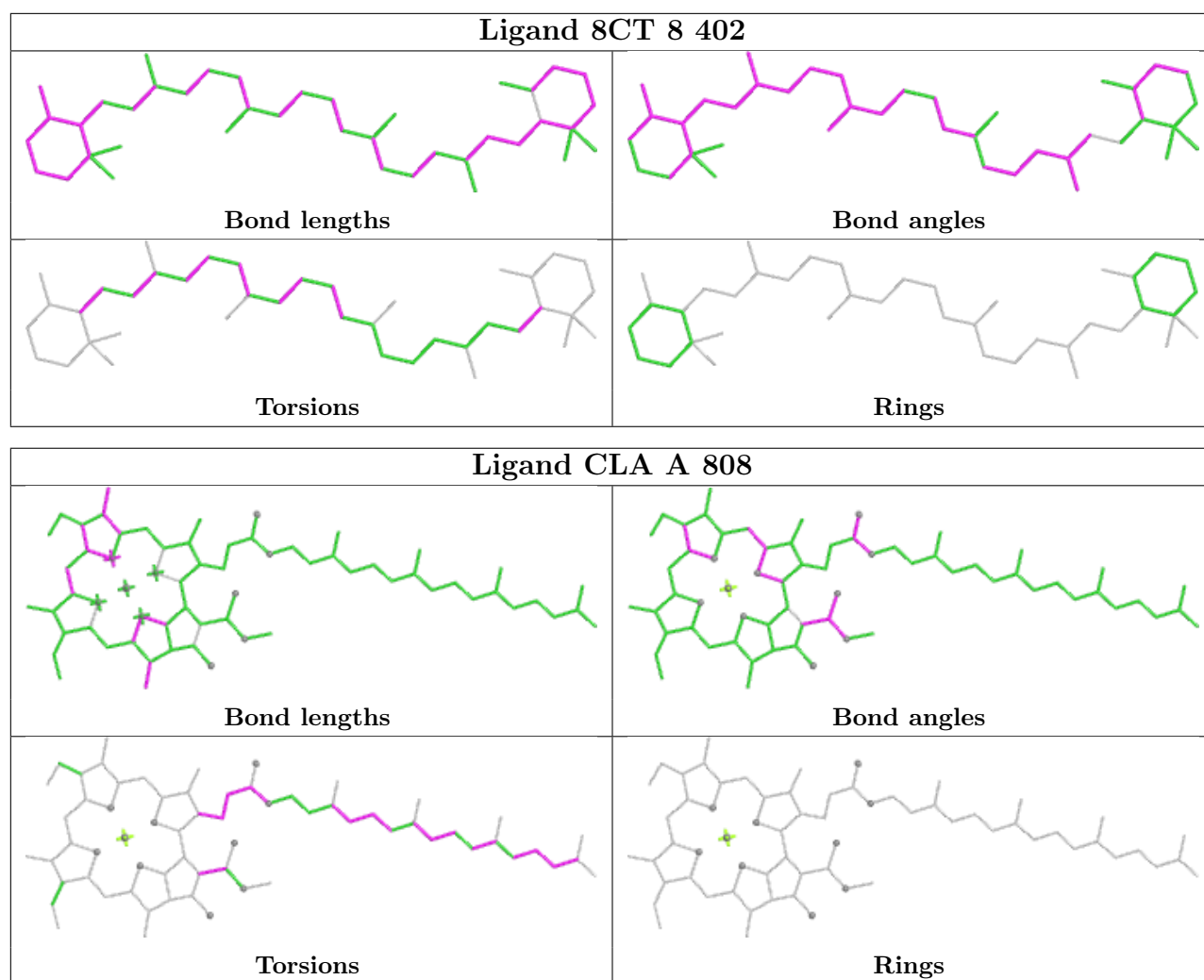


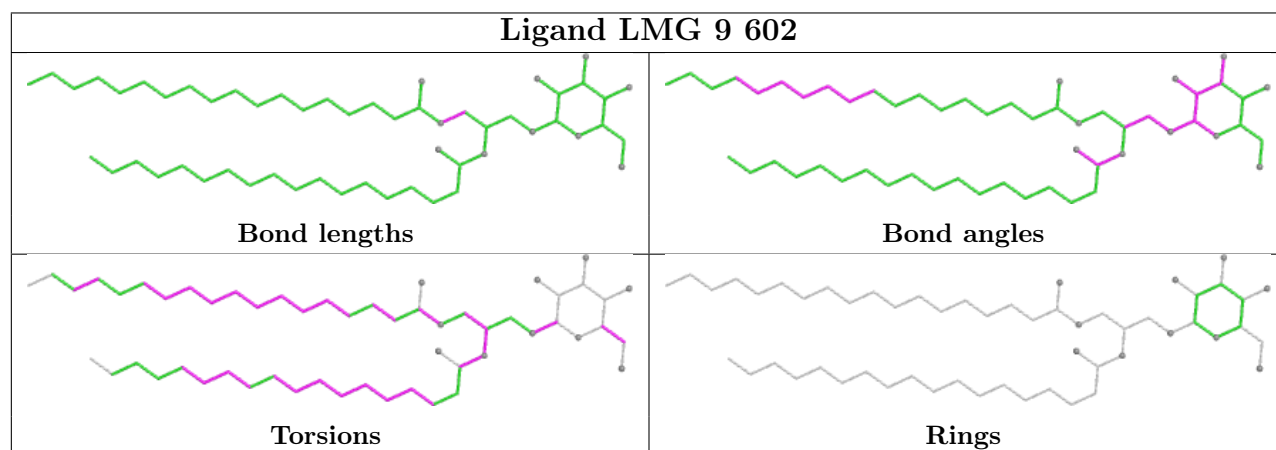
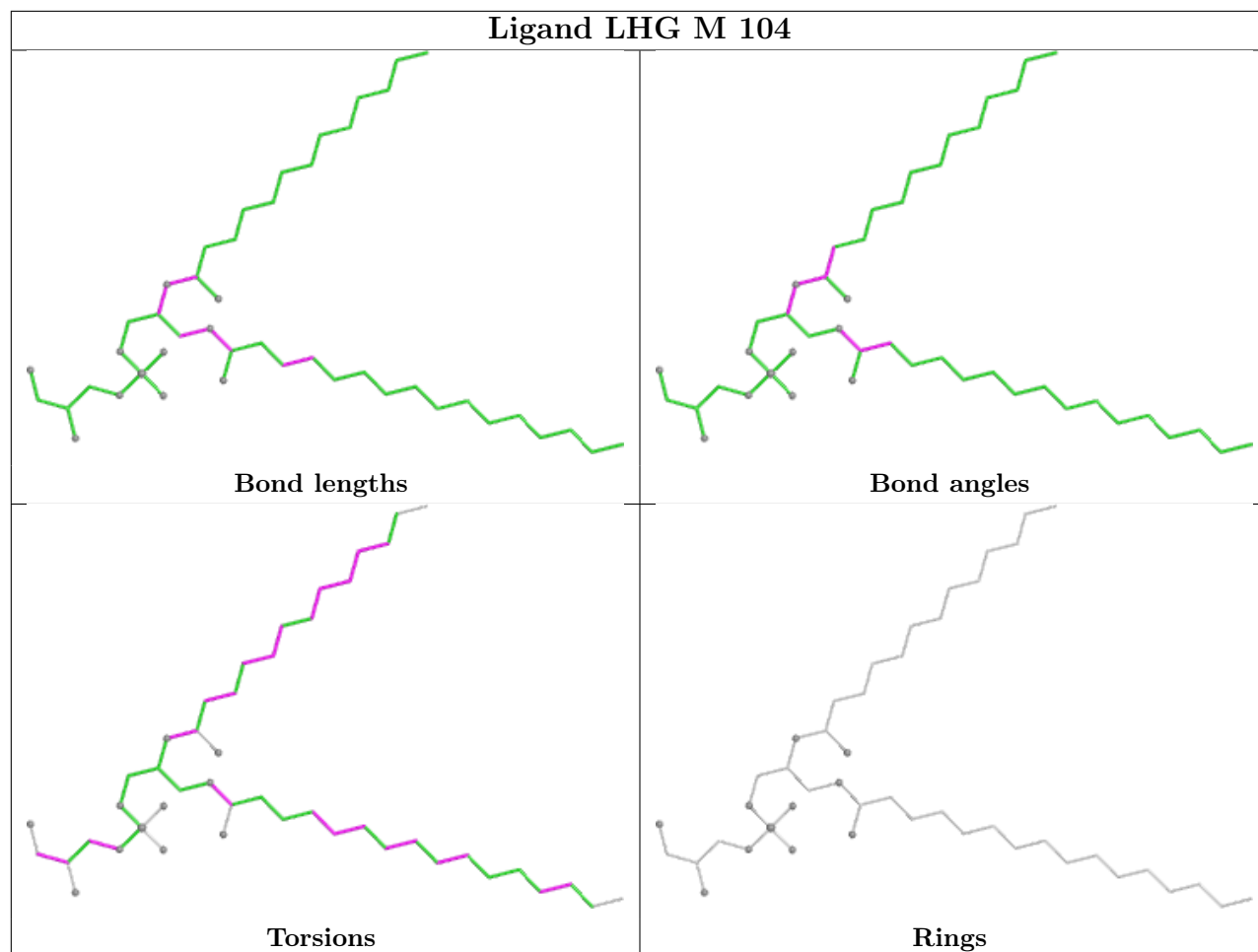
Ligand CLA A 809

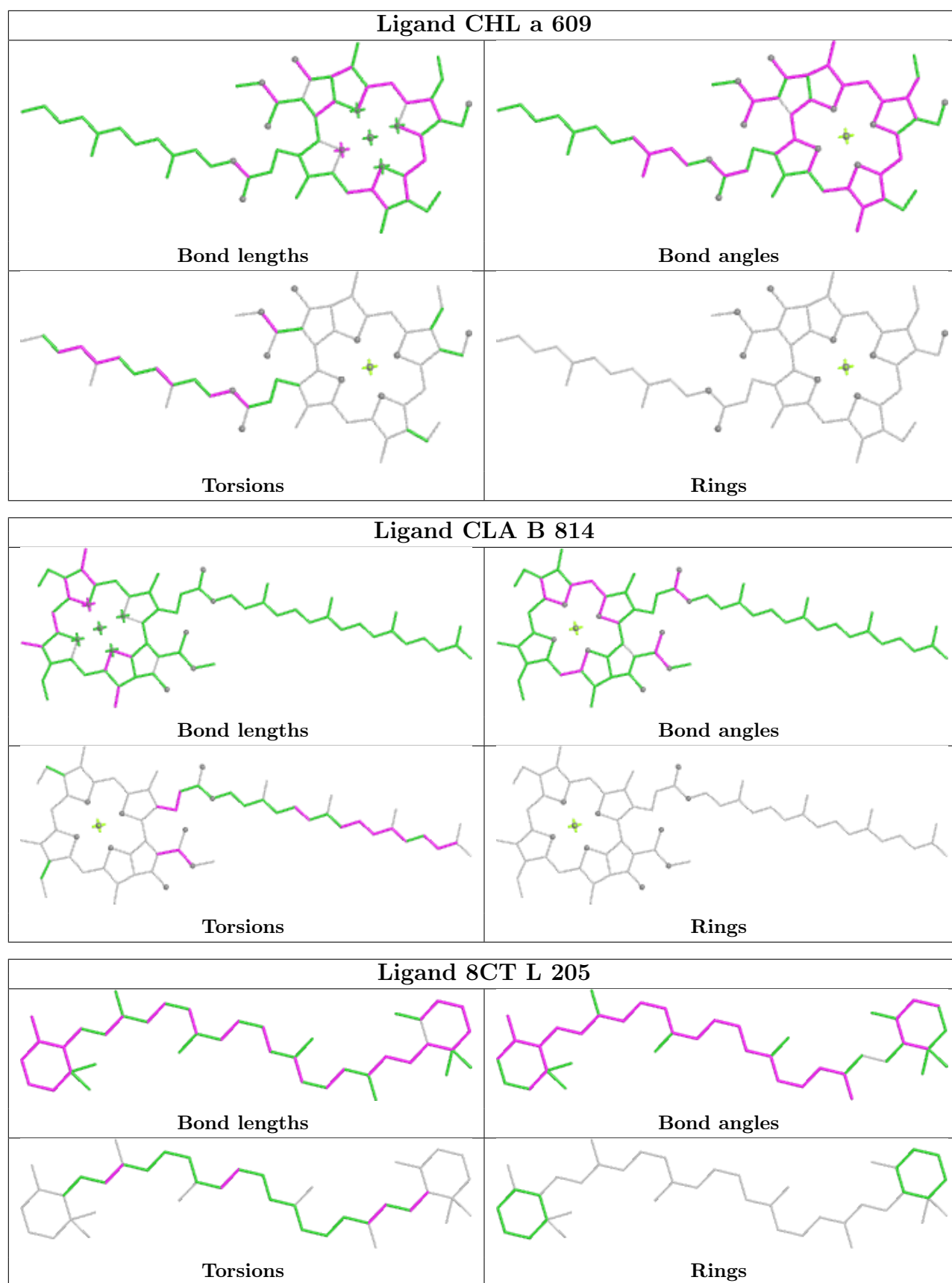


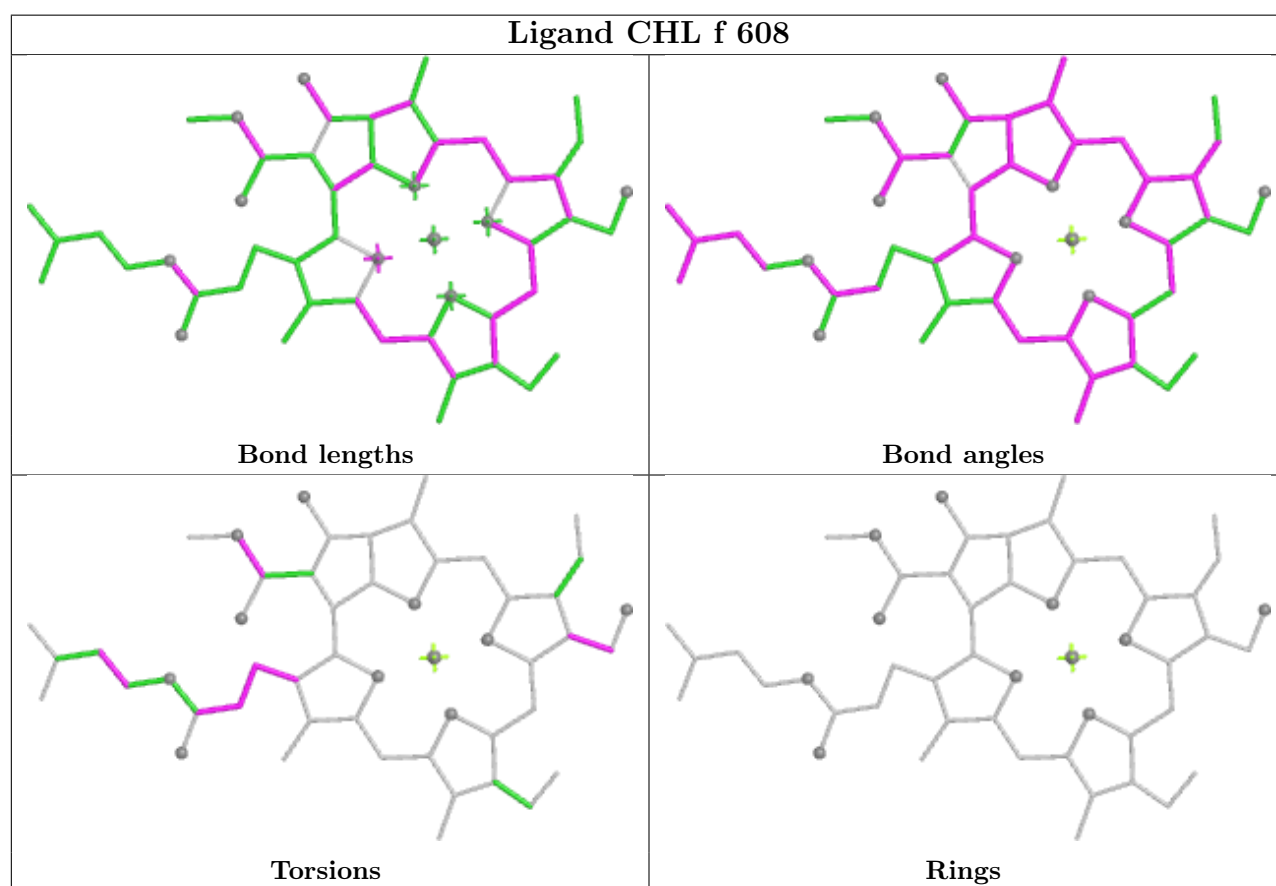
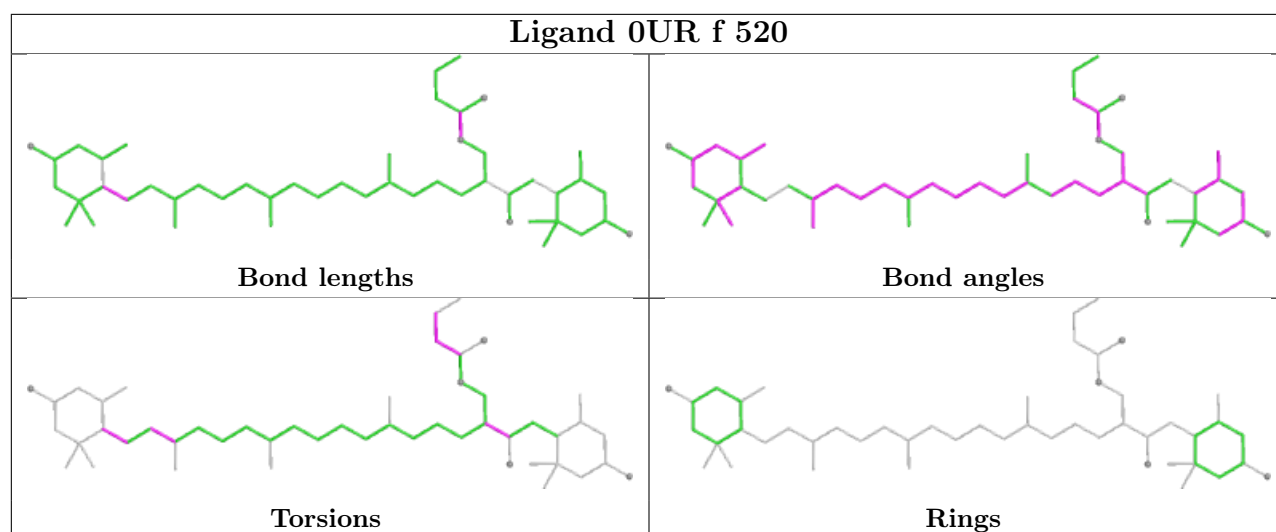


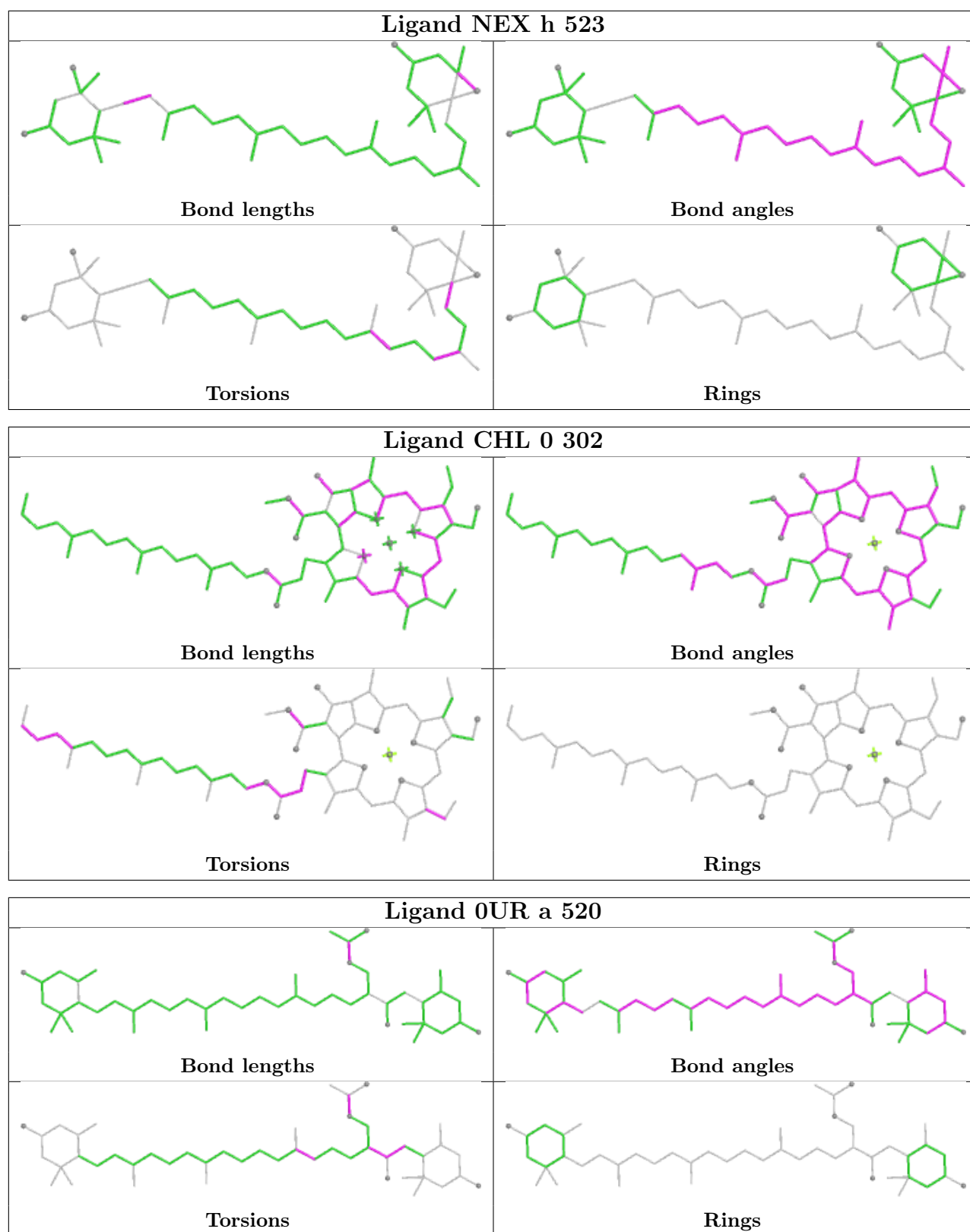




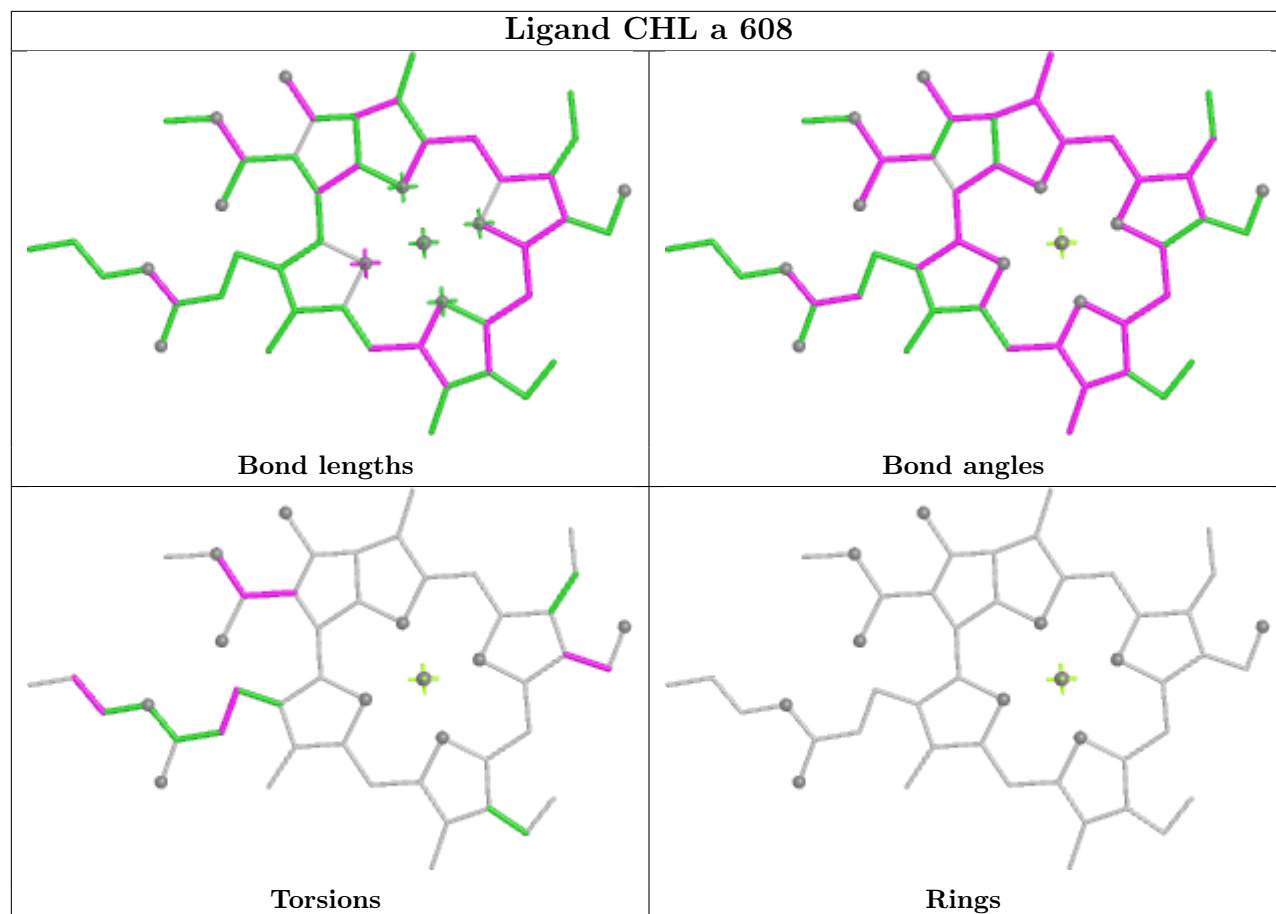




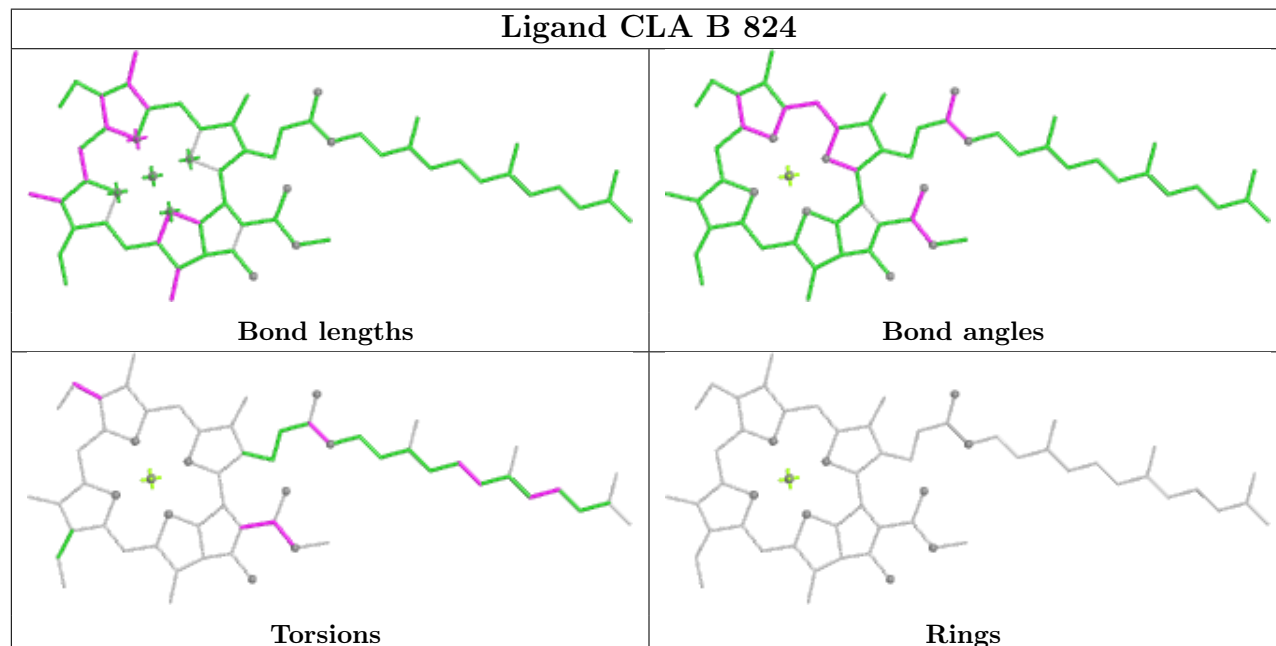


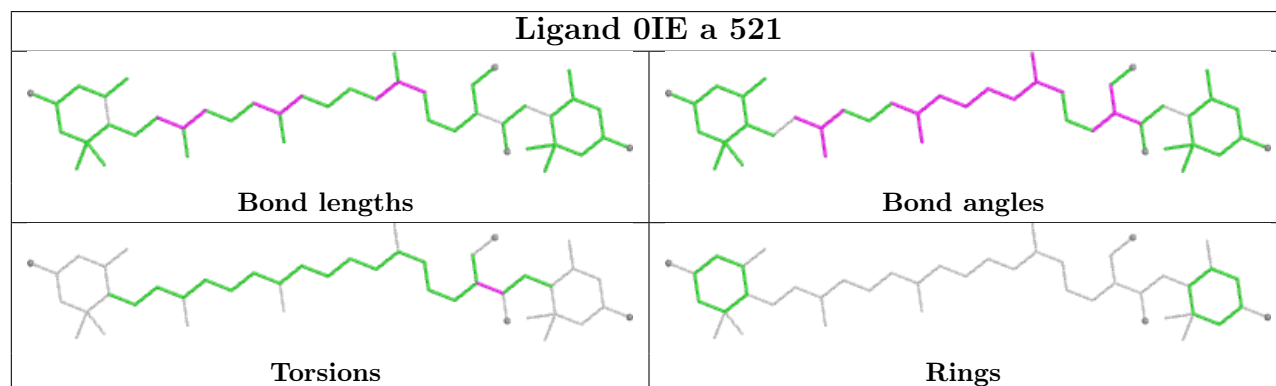
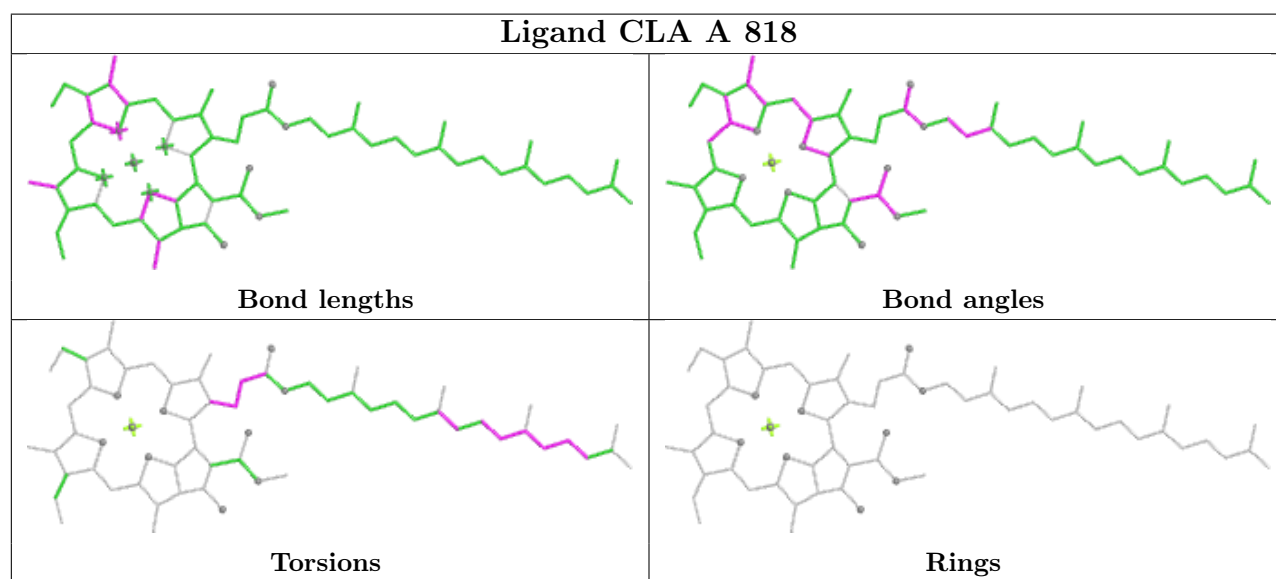
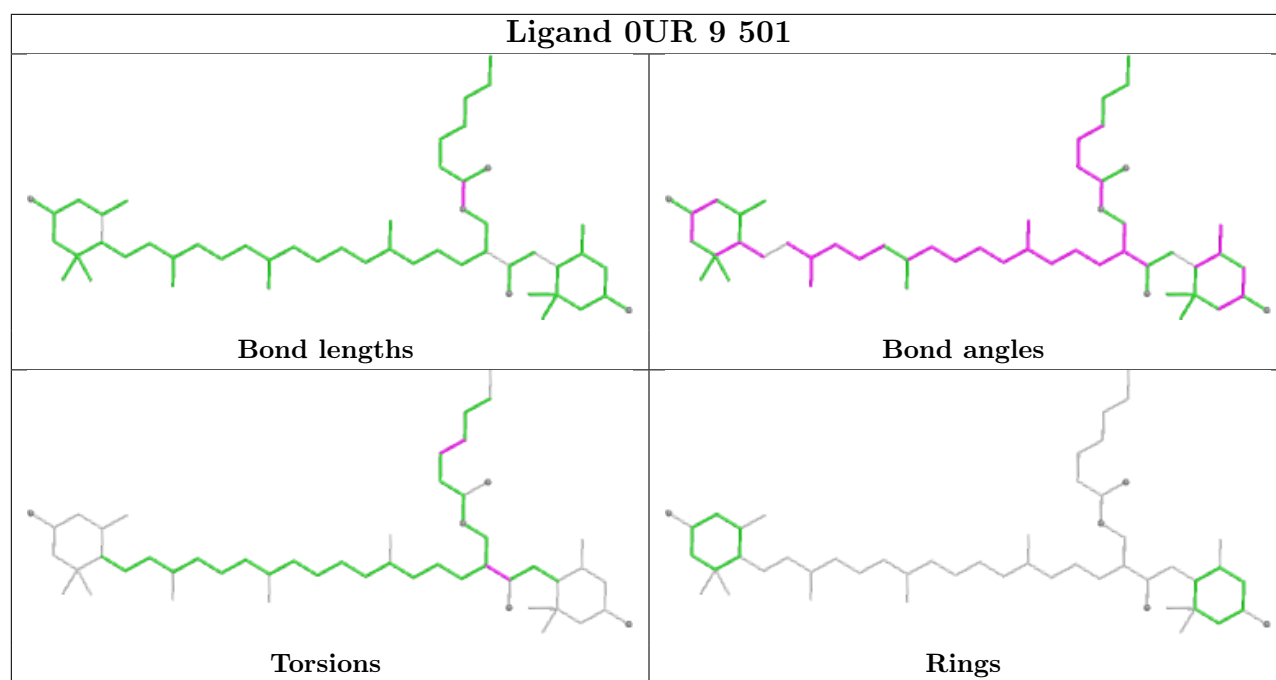


Ligand CHL a 608

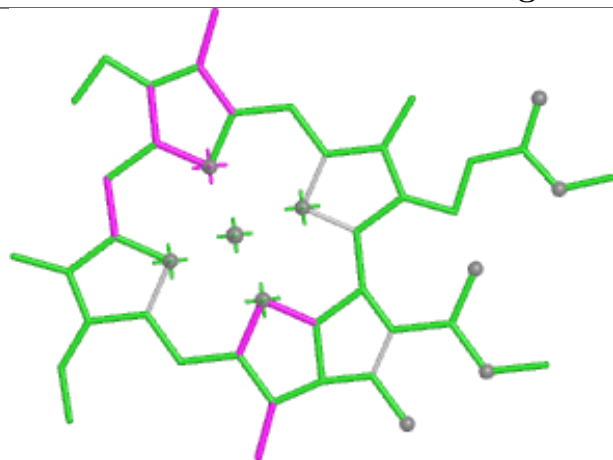


Ligand CLA B 824

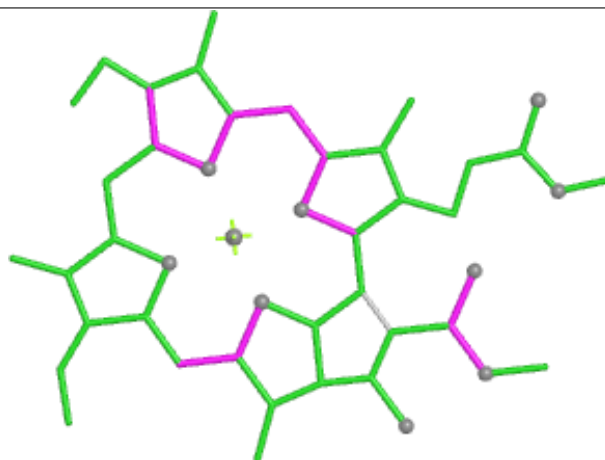




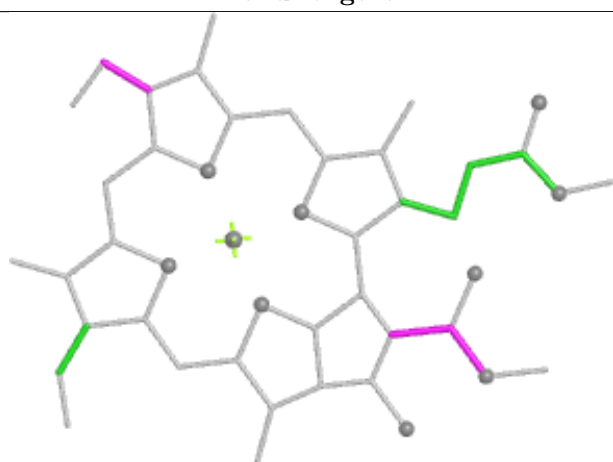
Ligand CLA 1 314



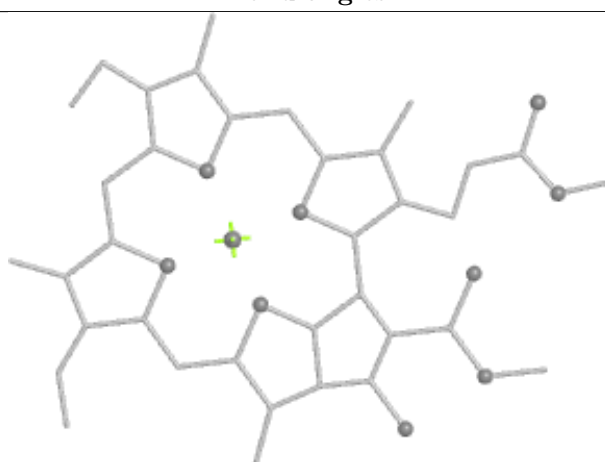
Bond lengths



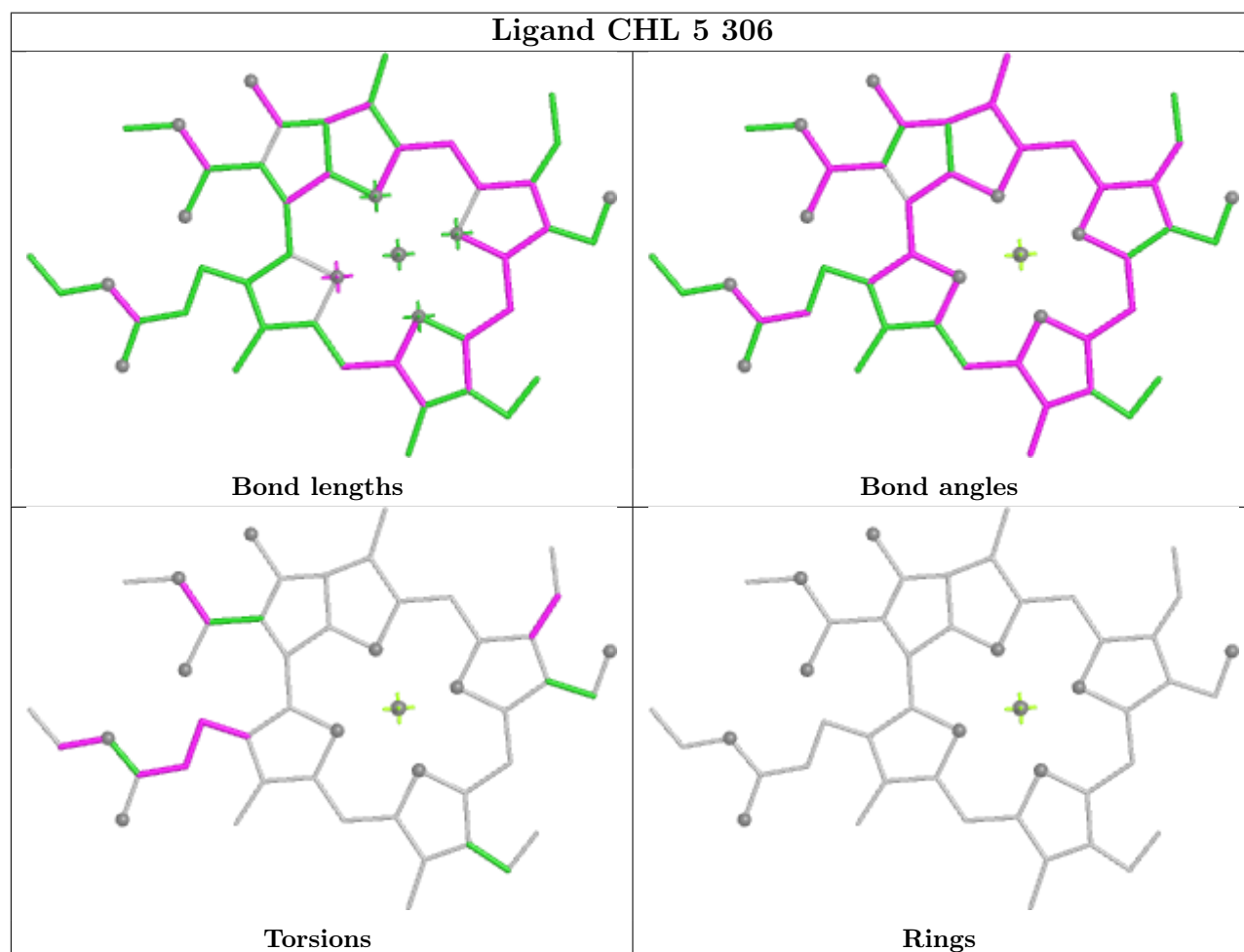
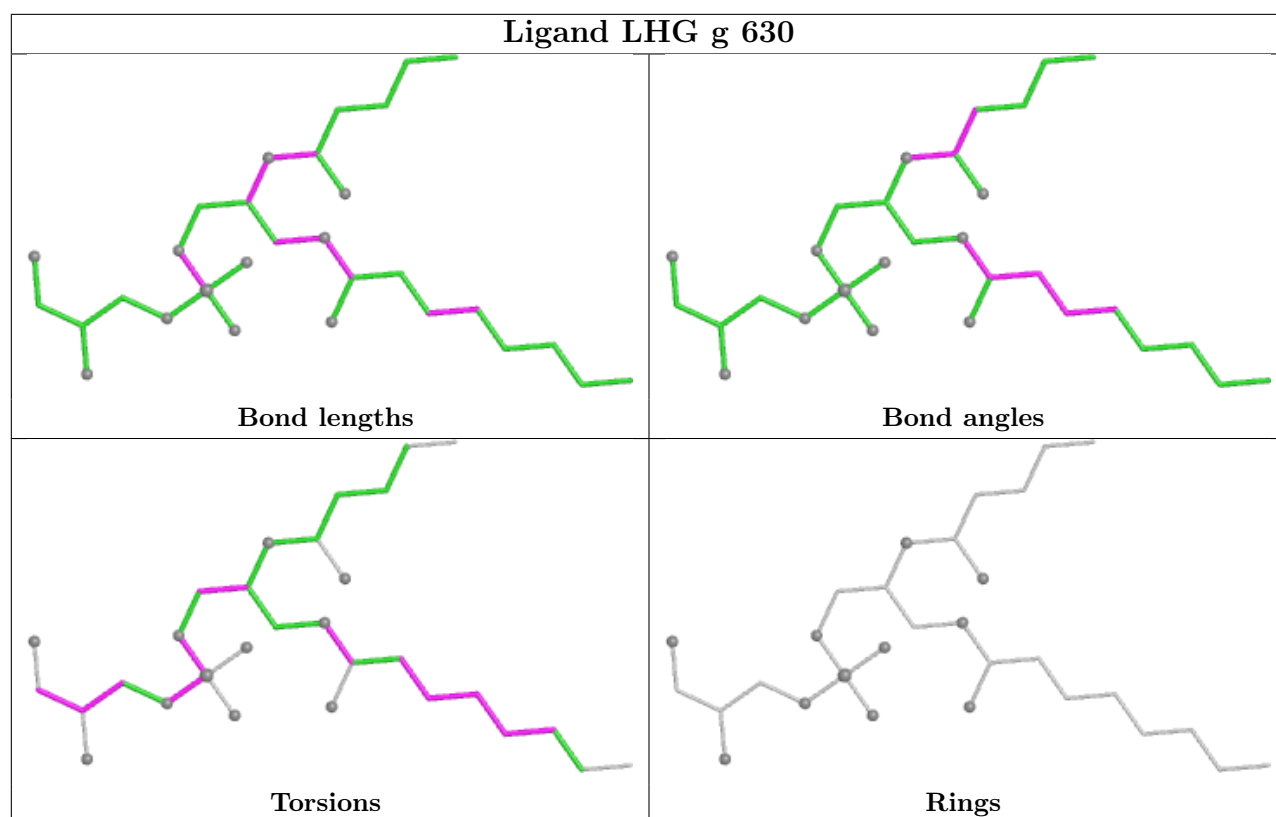
Bond angles

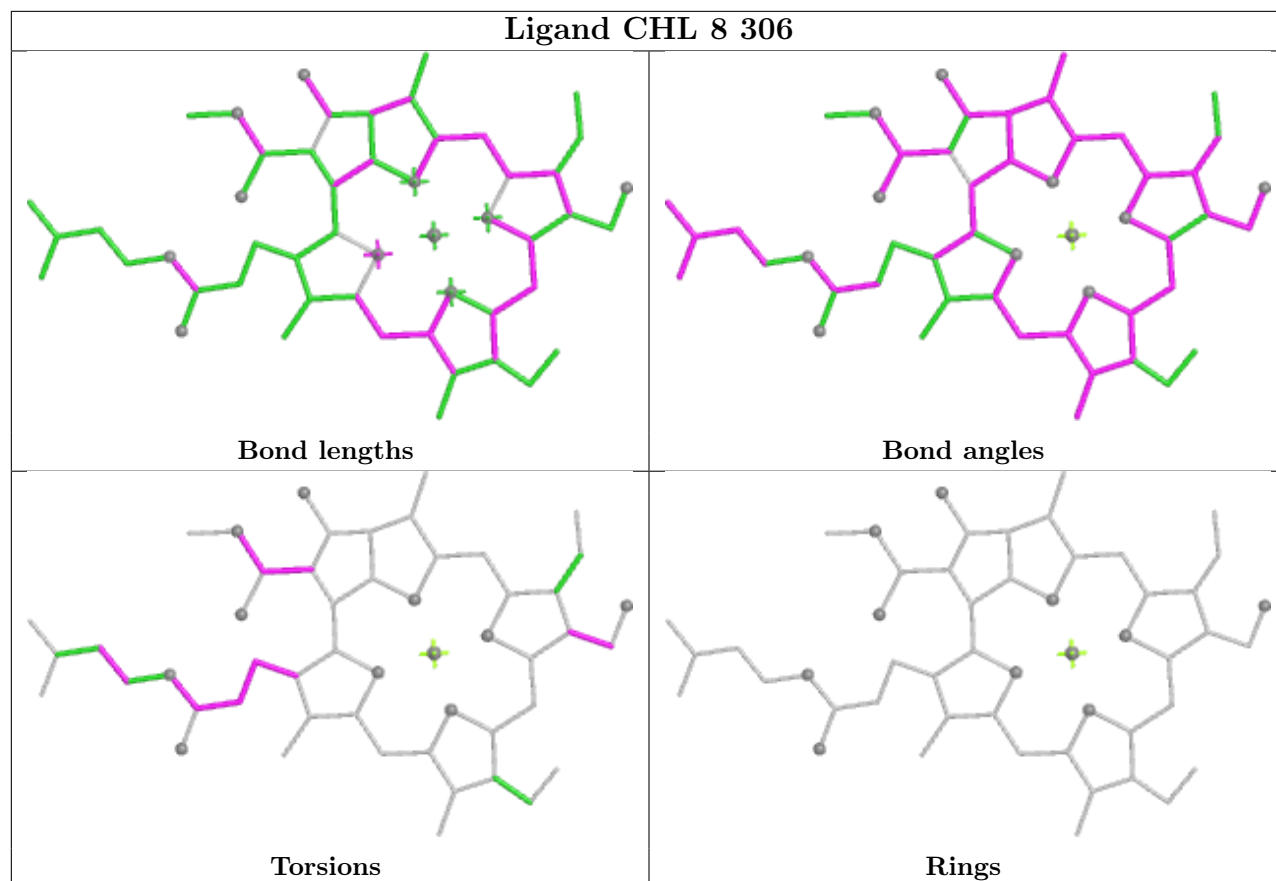


Torsions

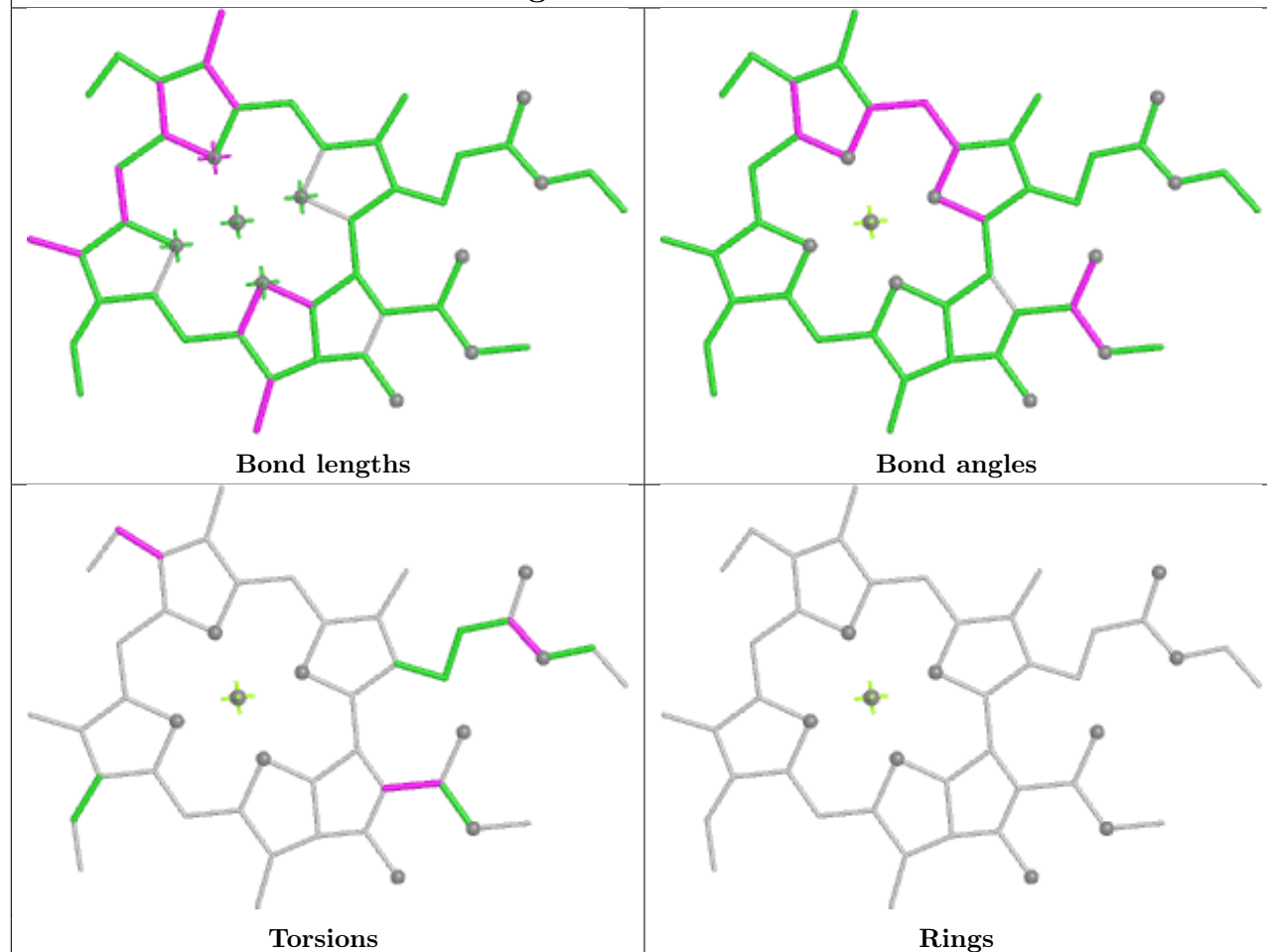


Rings

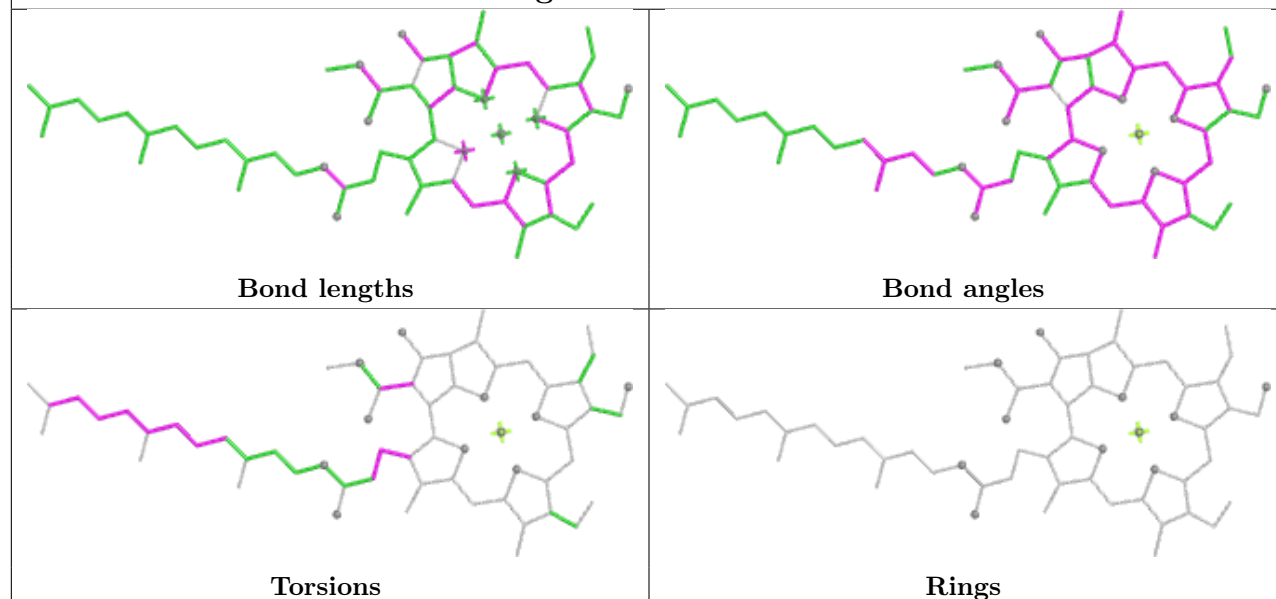




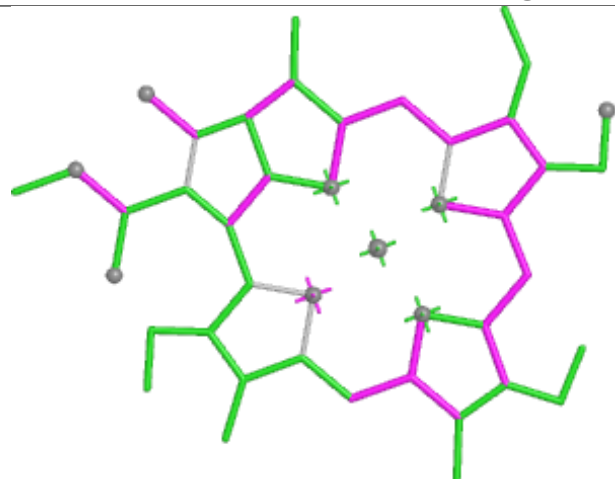
Ligand CLA B 850



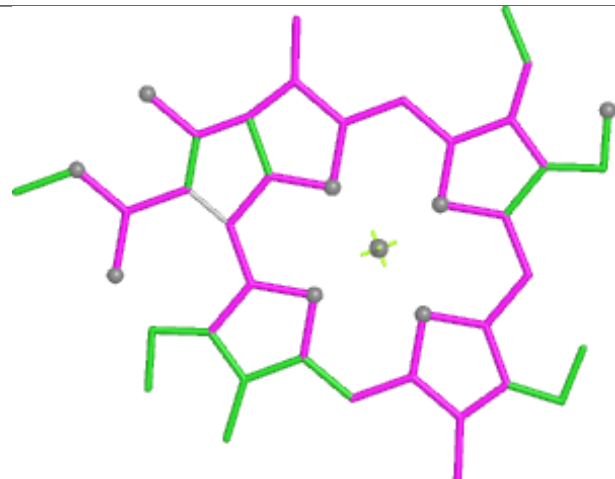
Ligand CHL 6 301



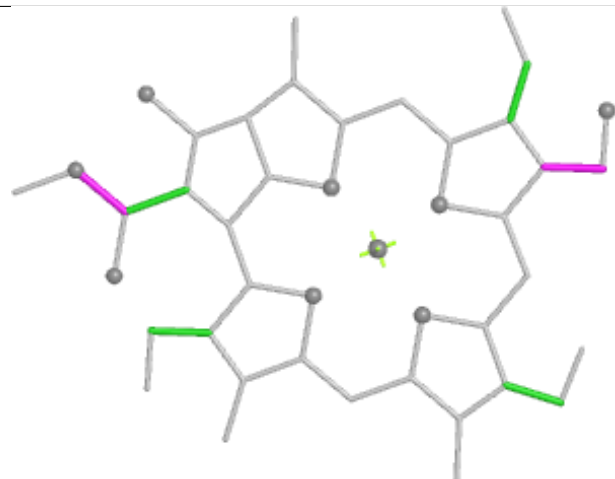
Ligand CHL d 605



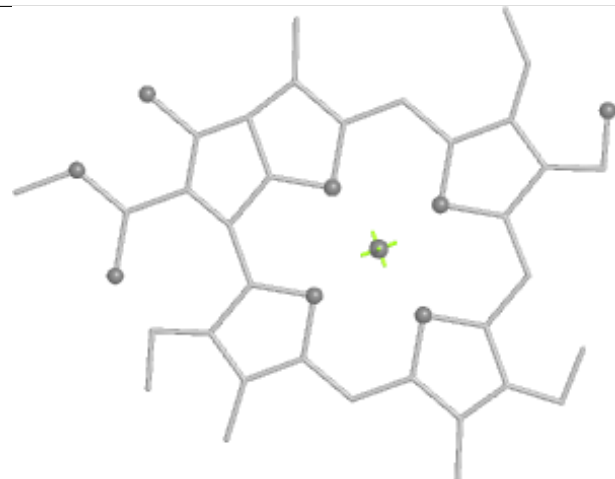
Bond lengths



Bond angles

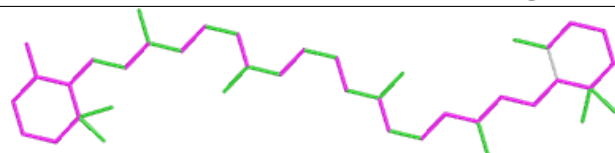


Torsions

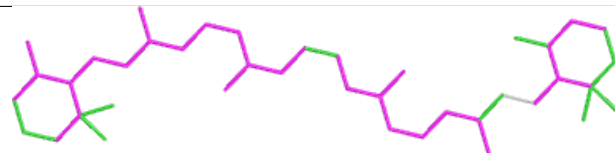


Rings

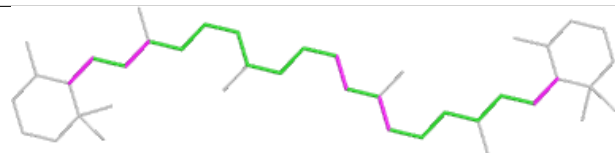
Ligand 8CT 1 402



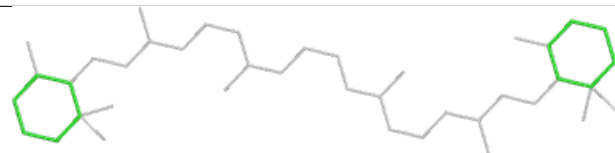
Bond lengths



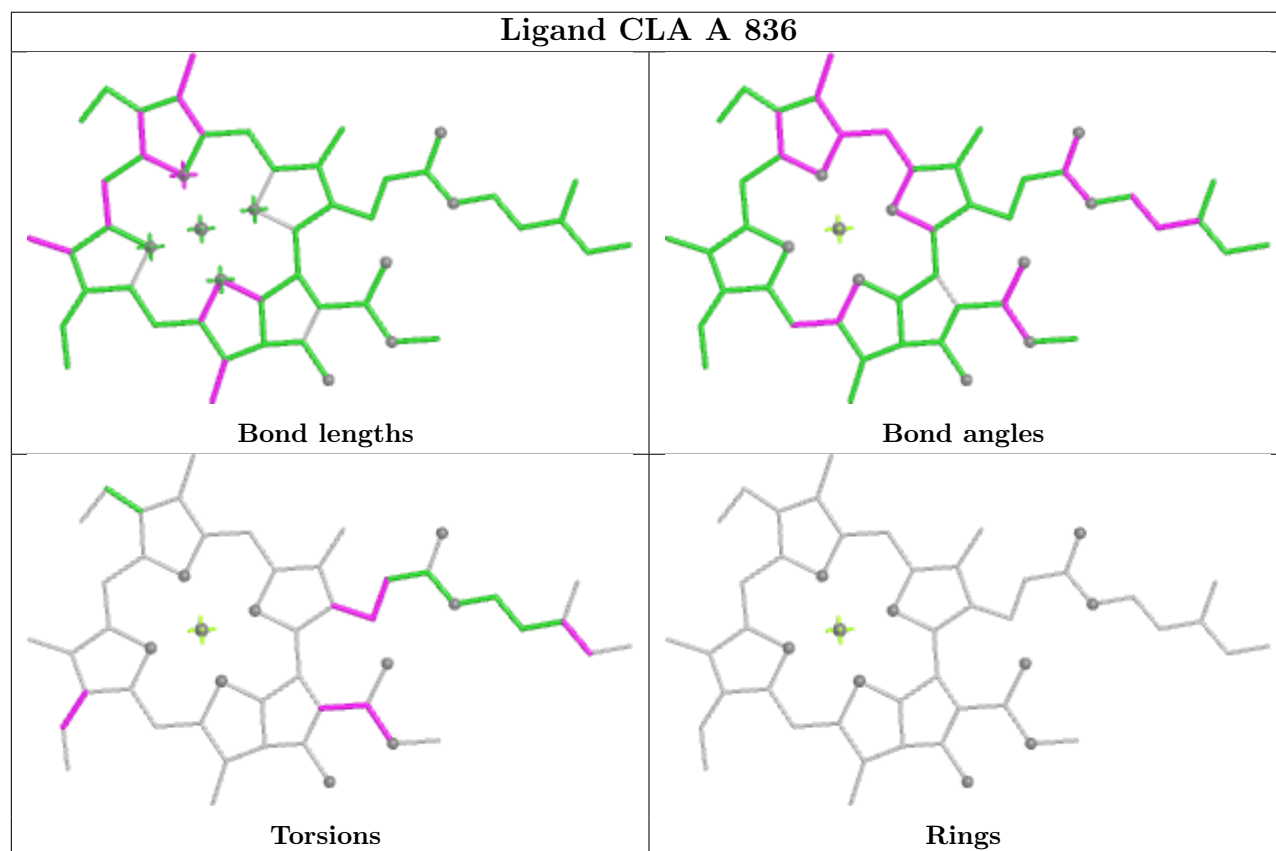
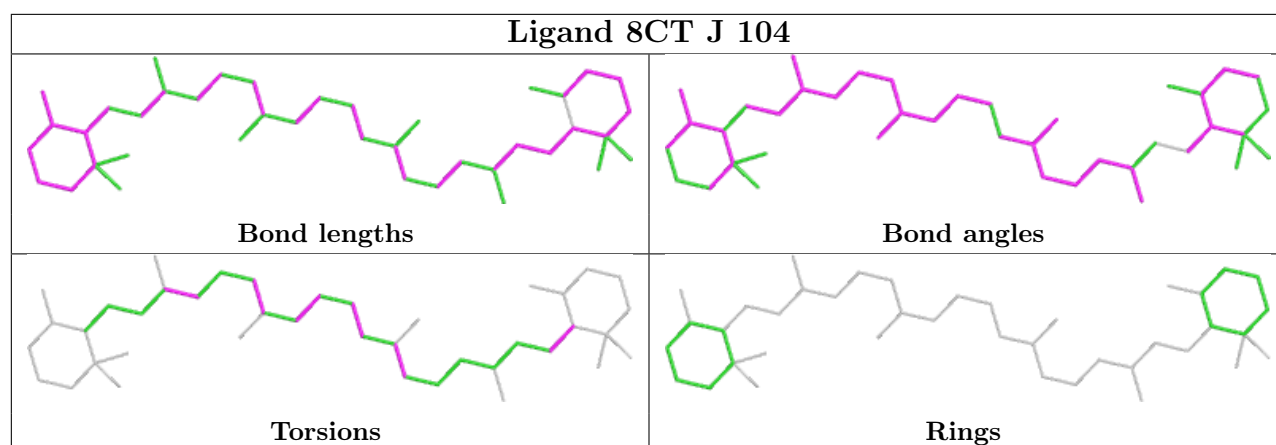
Bond angles



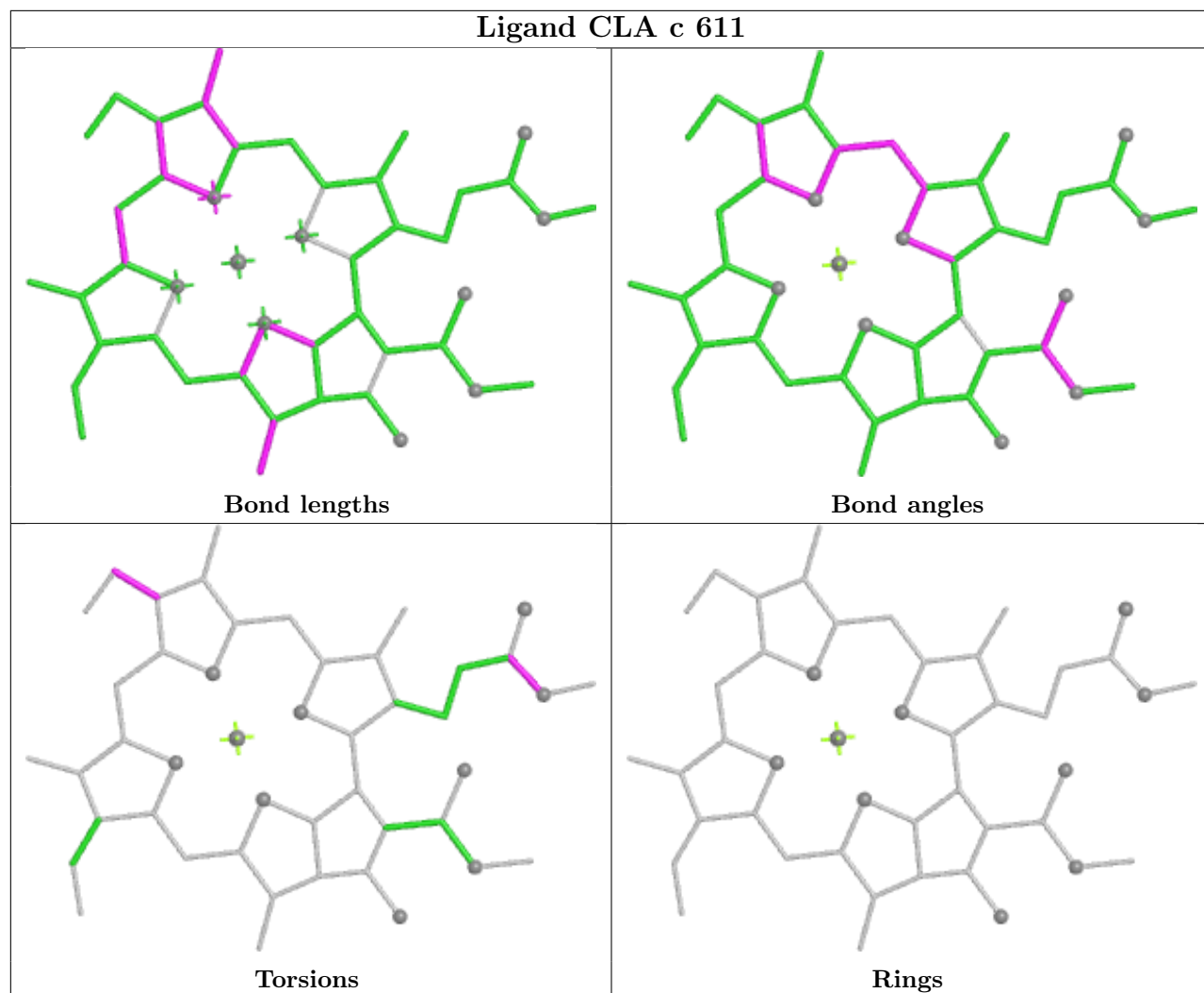
Torsions



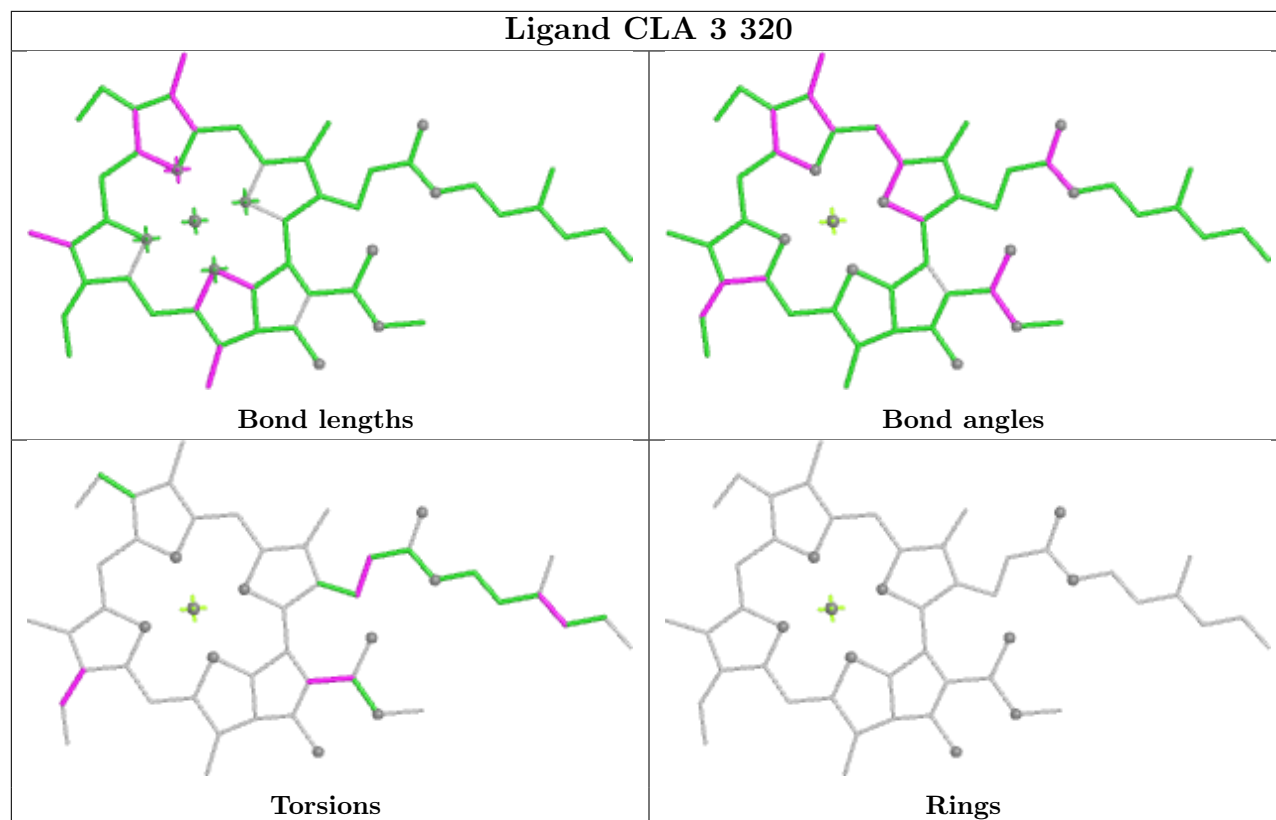
Rings



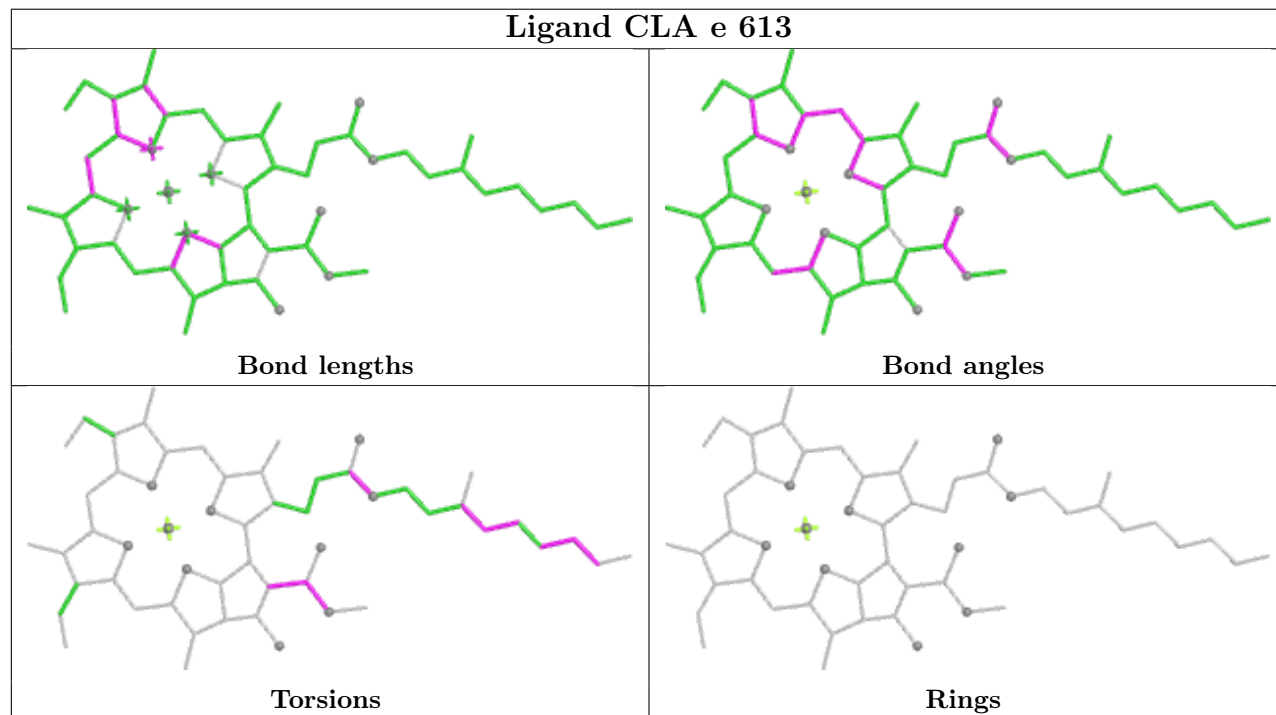
Ligand CLA c 611

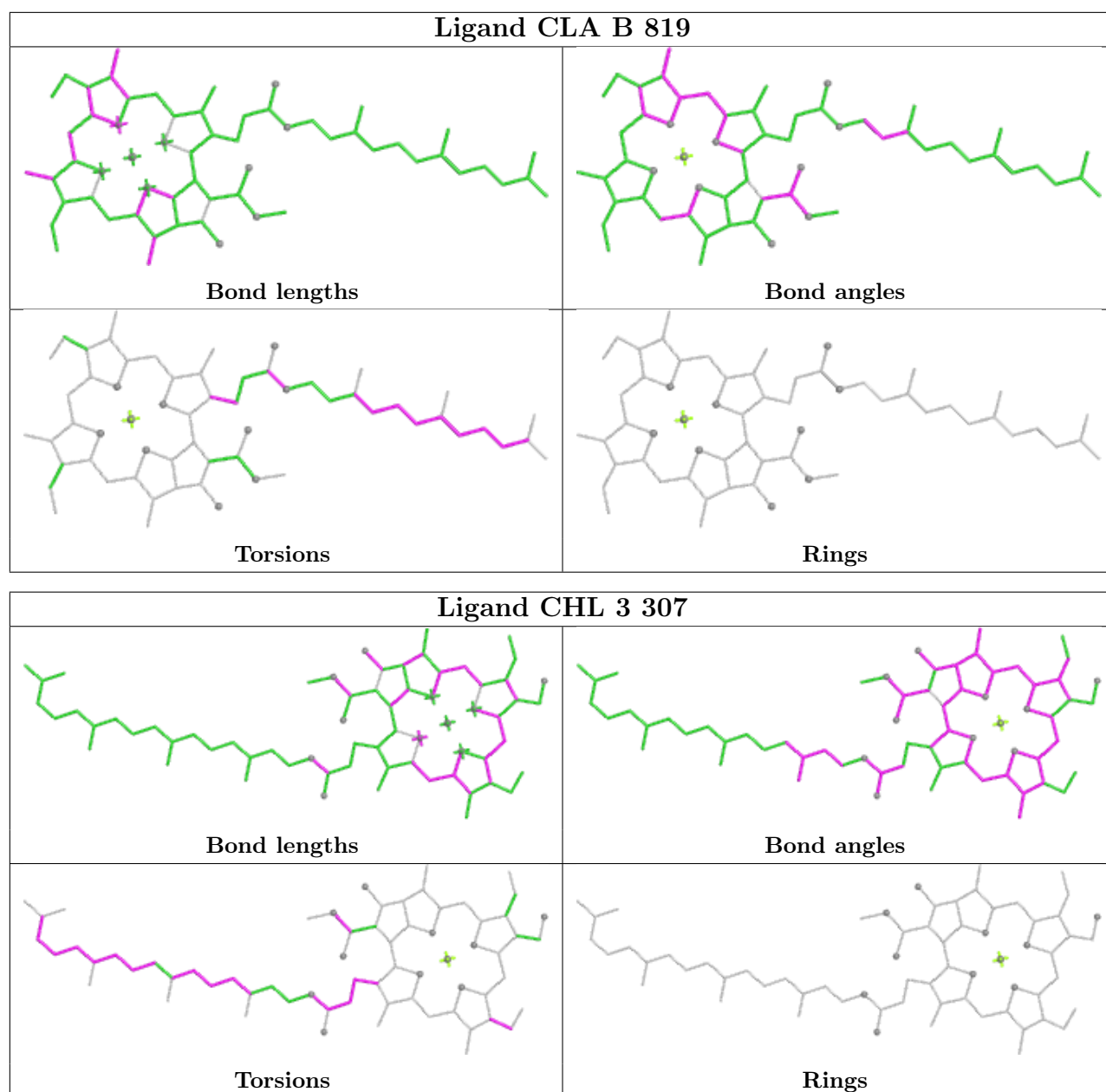


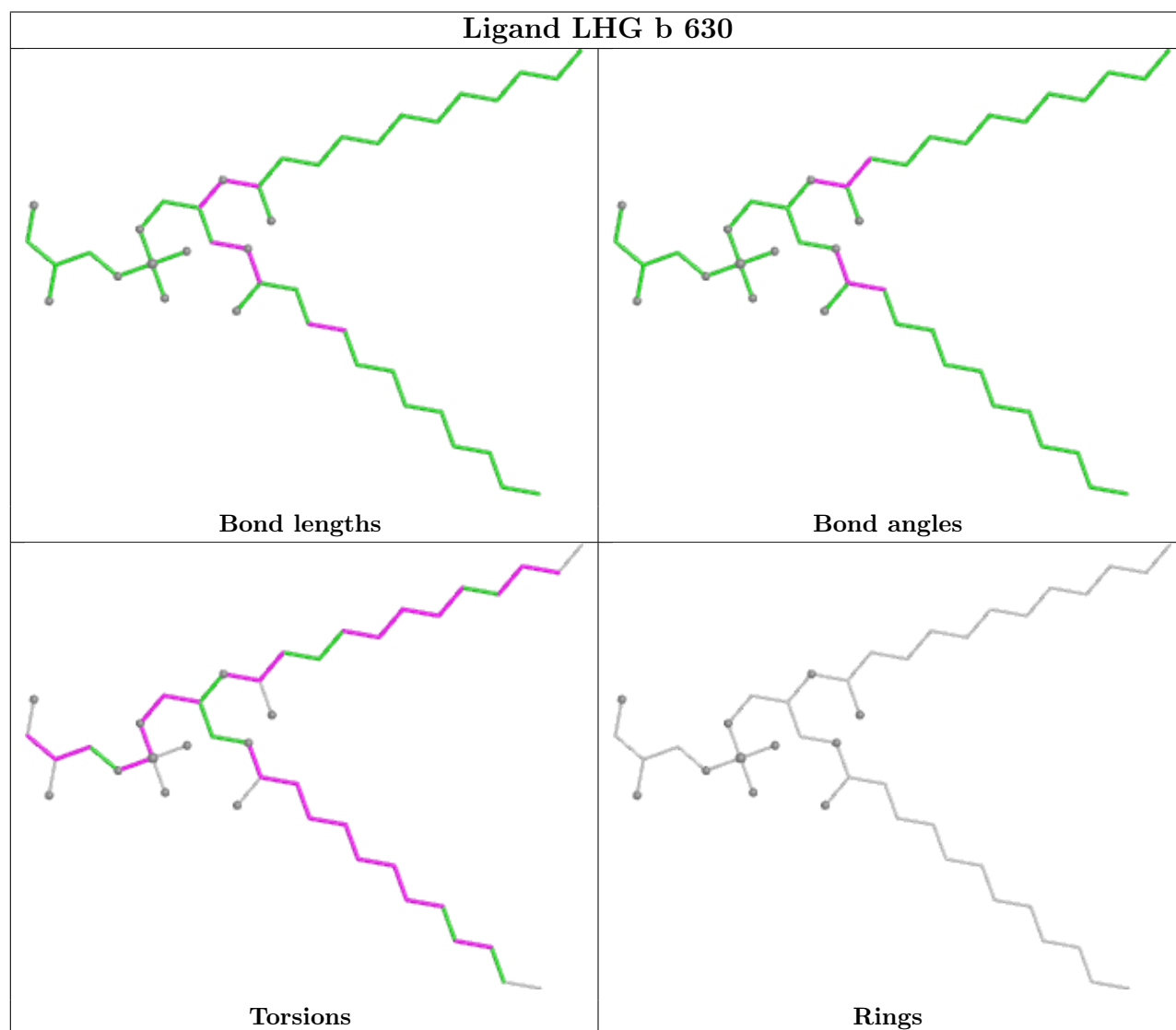
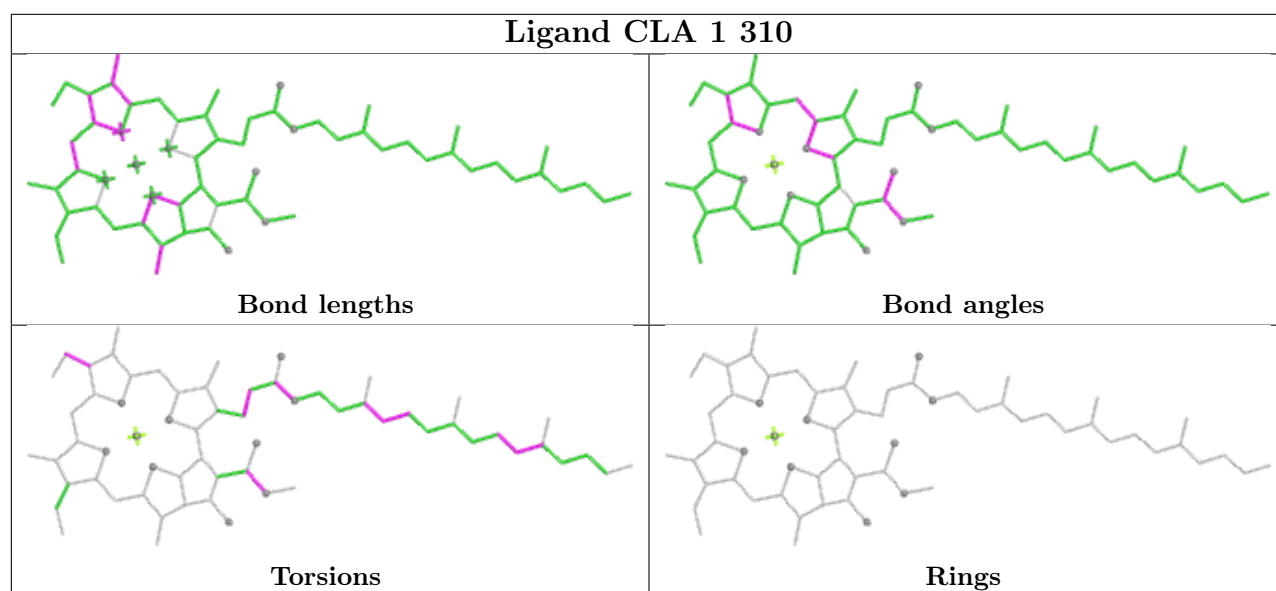
Ligand CLA 3 320

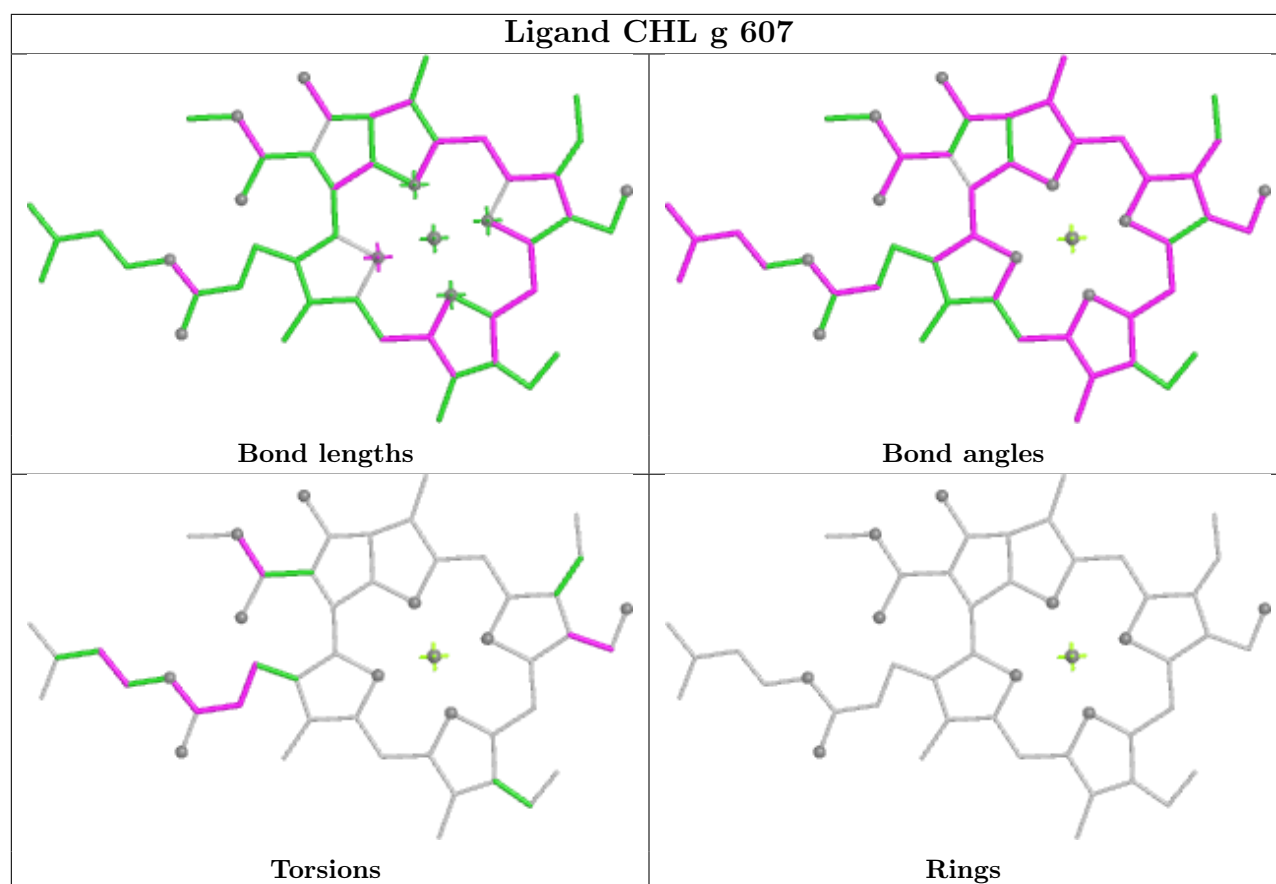


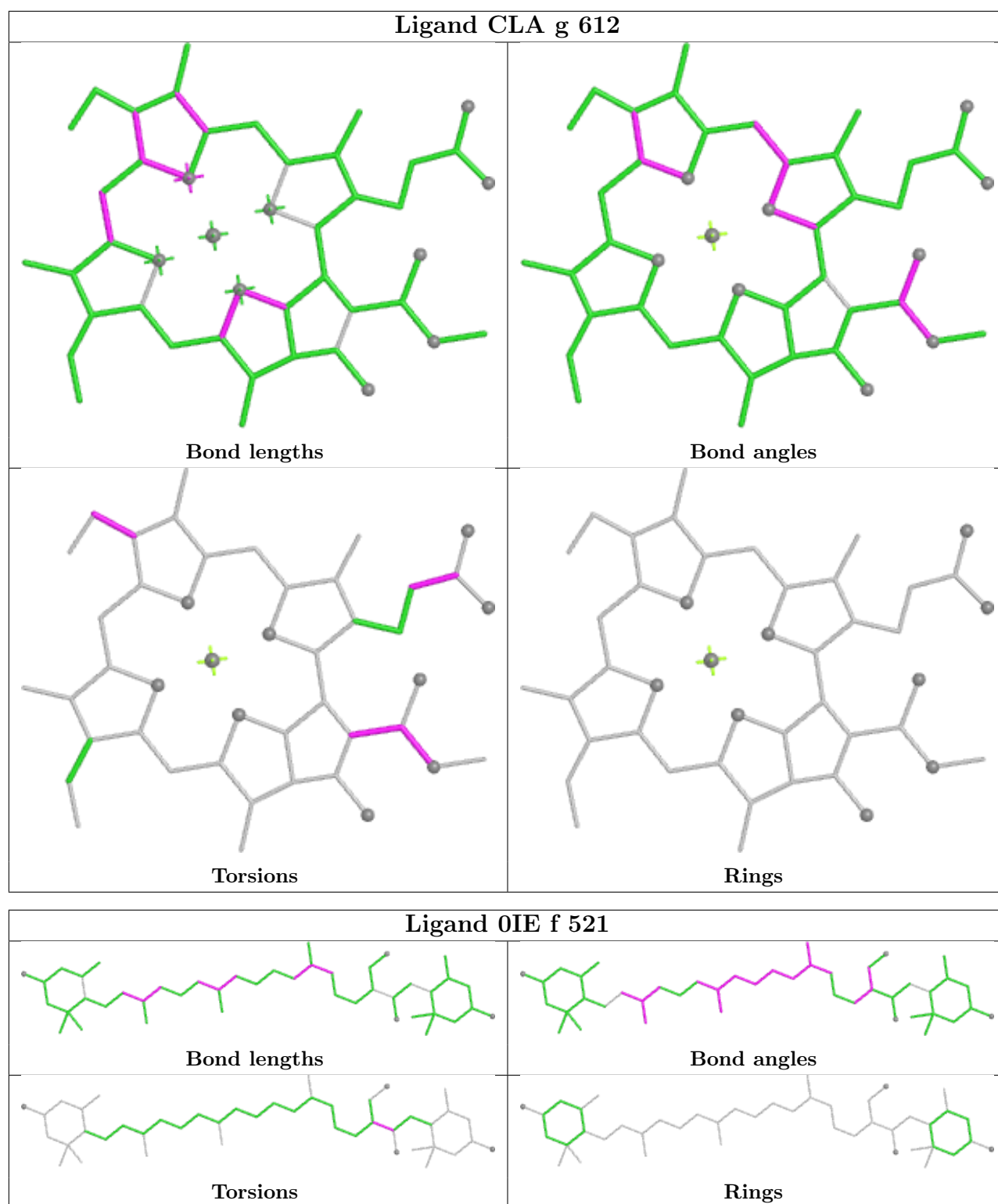
Ligand CLA e 613

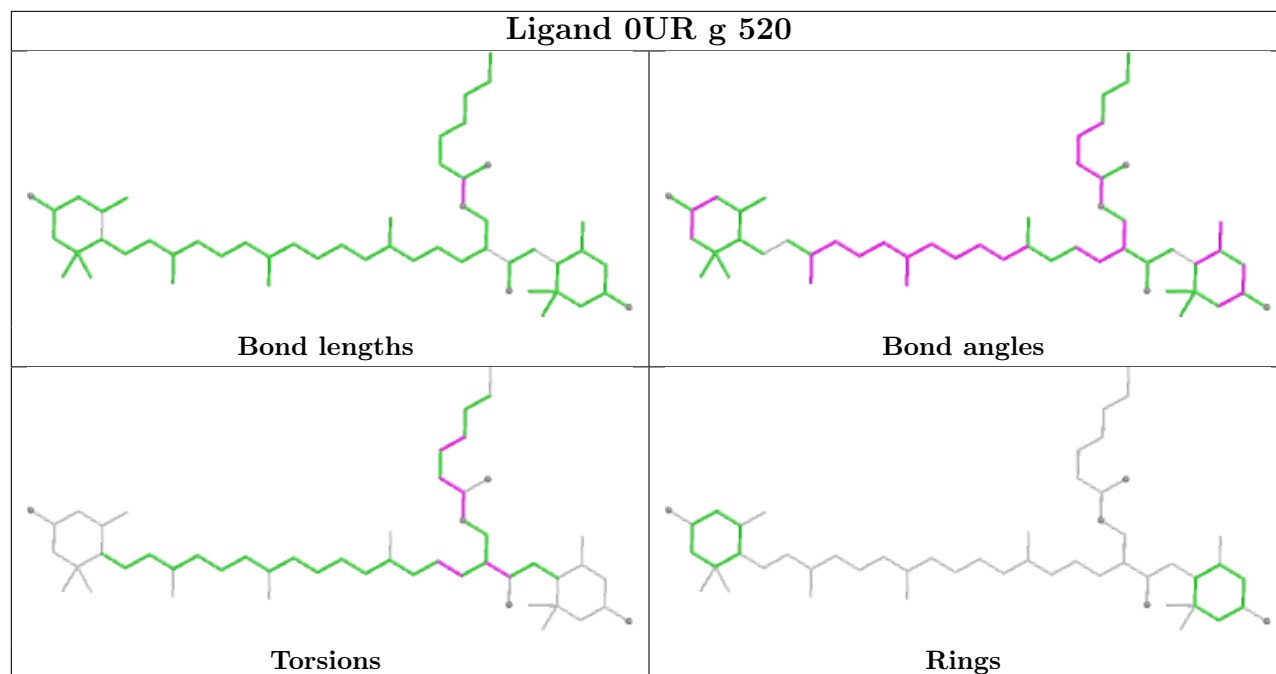
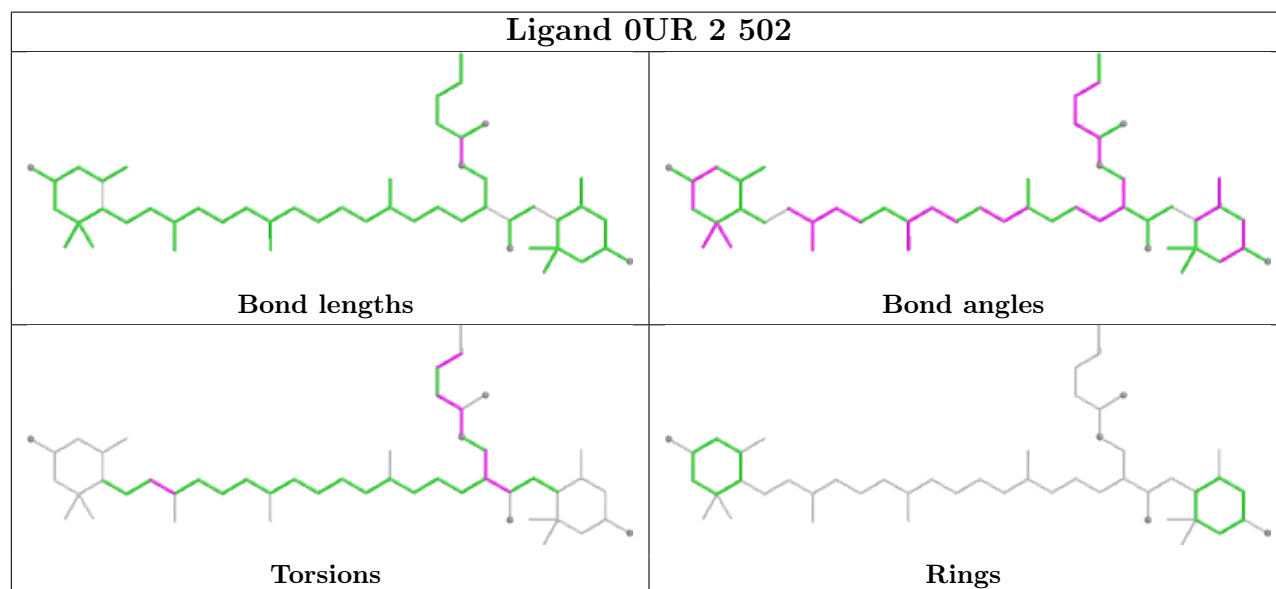




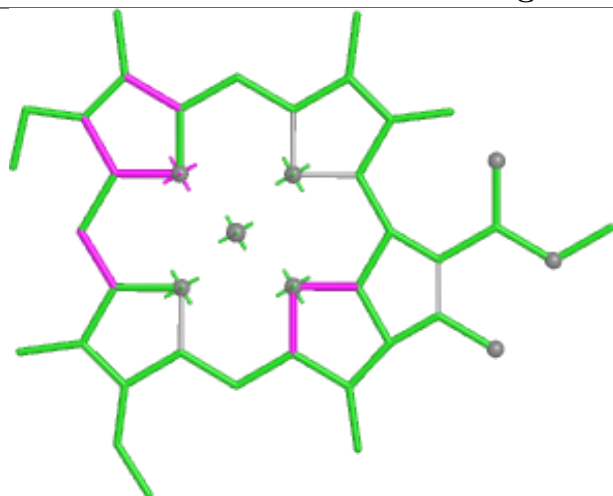




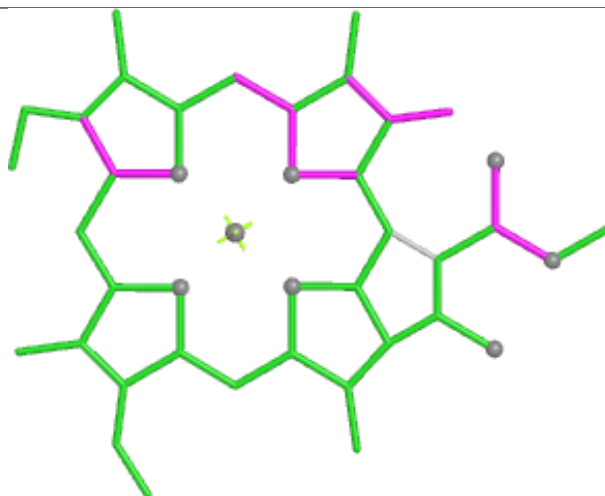


Ligand 0UR g 520**Ligand 0UR 2 502**

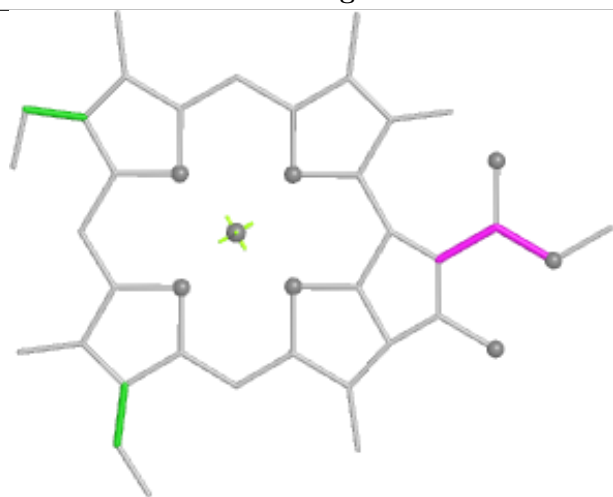
Ligand CLA h 611



Bond lengths



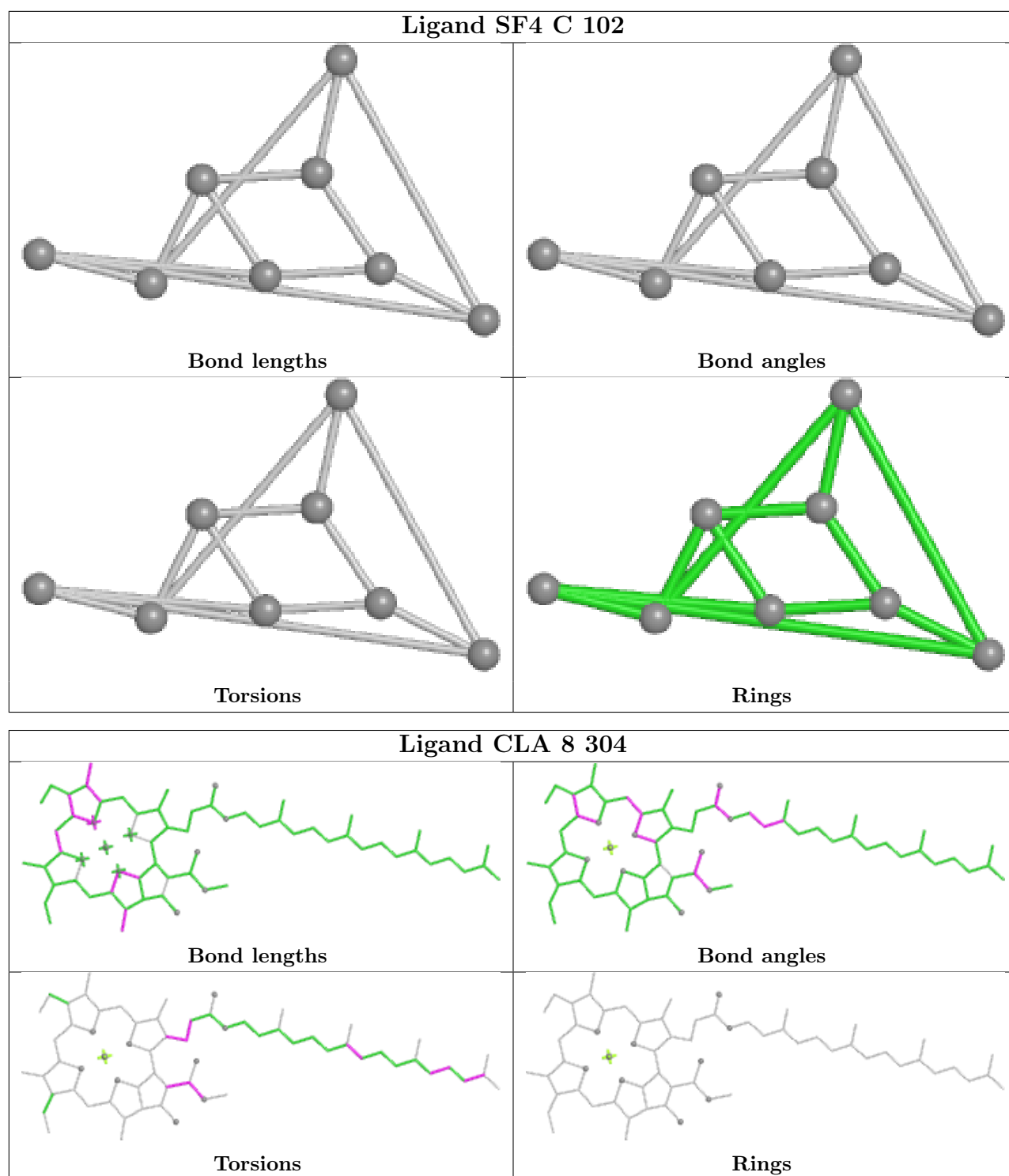
Bond angles



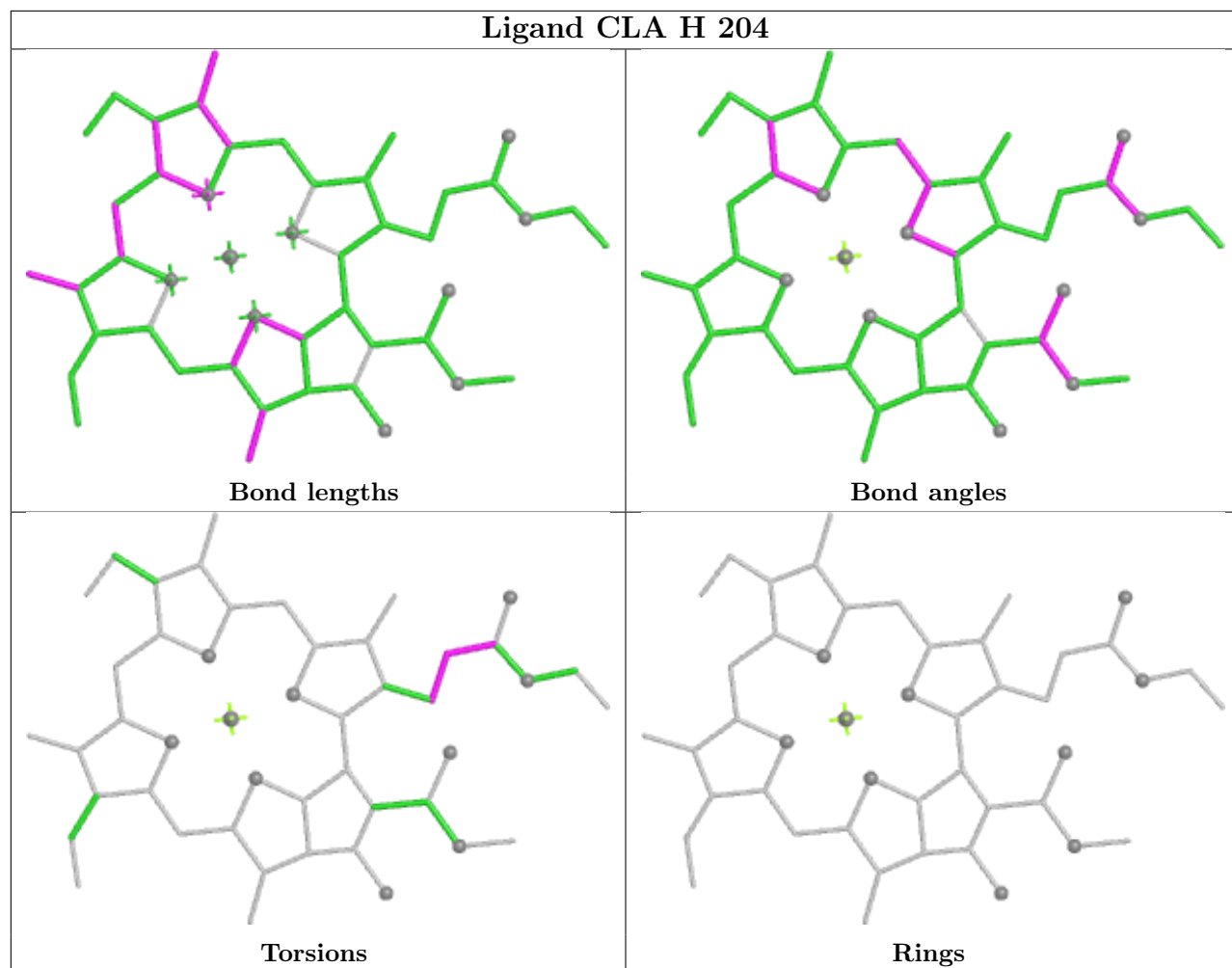
Torsions



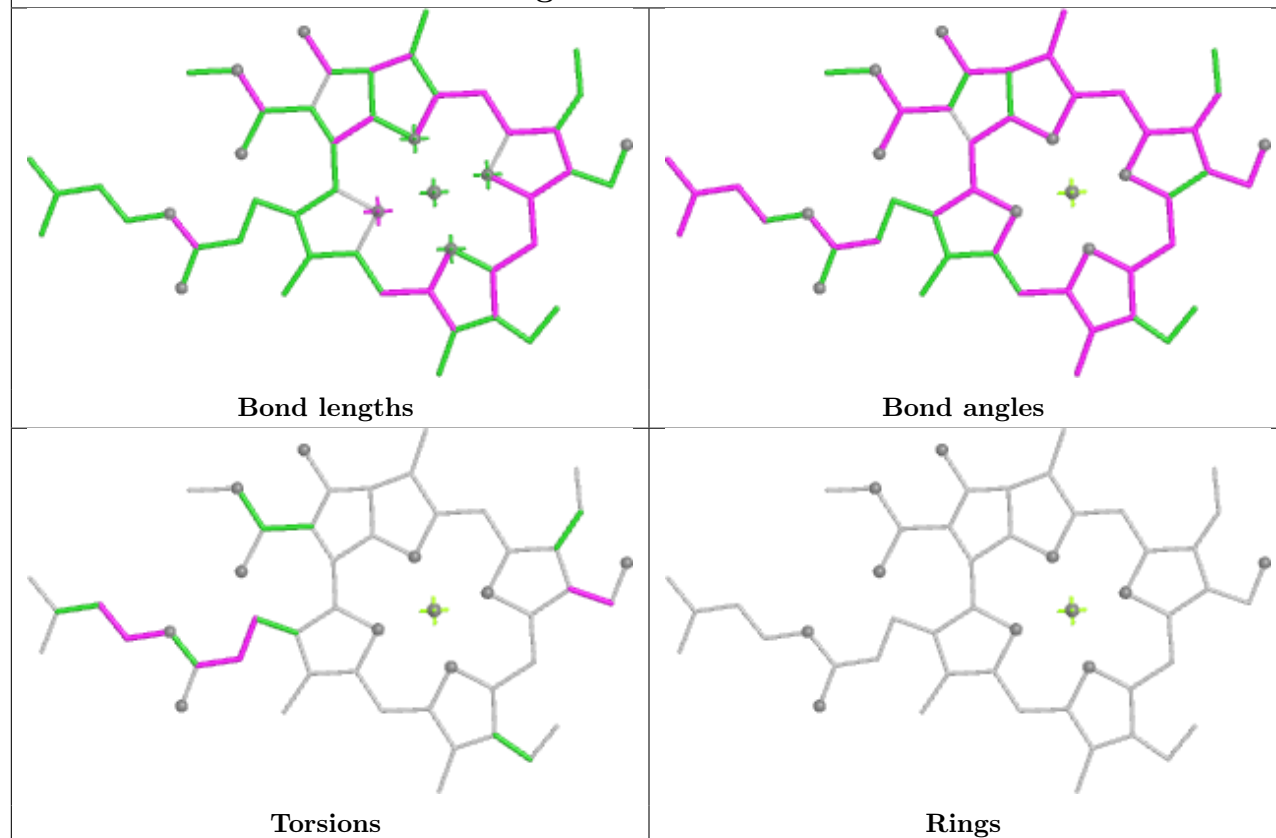
Rings



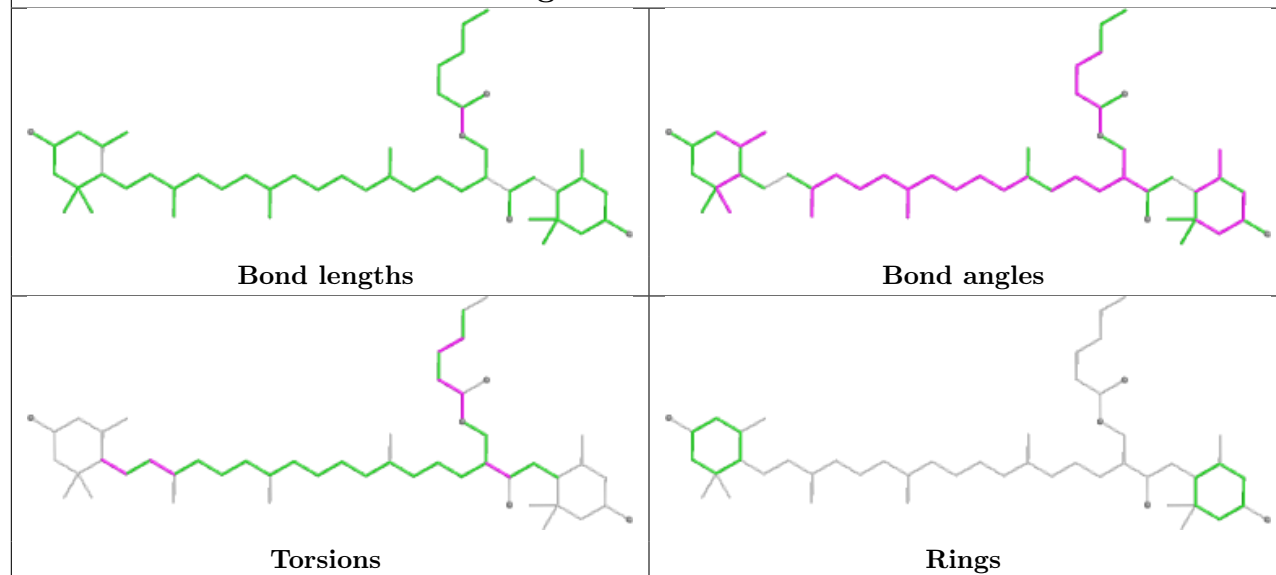
Ligand CLA H 204

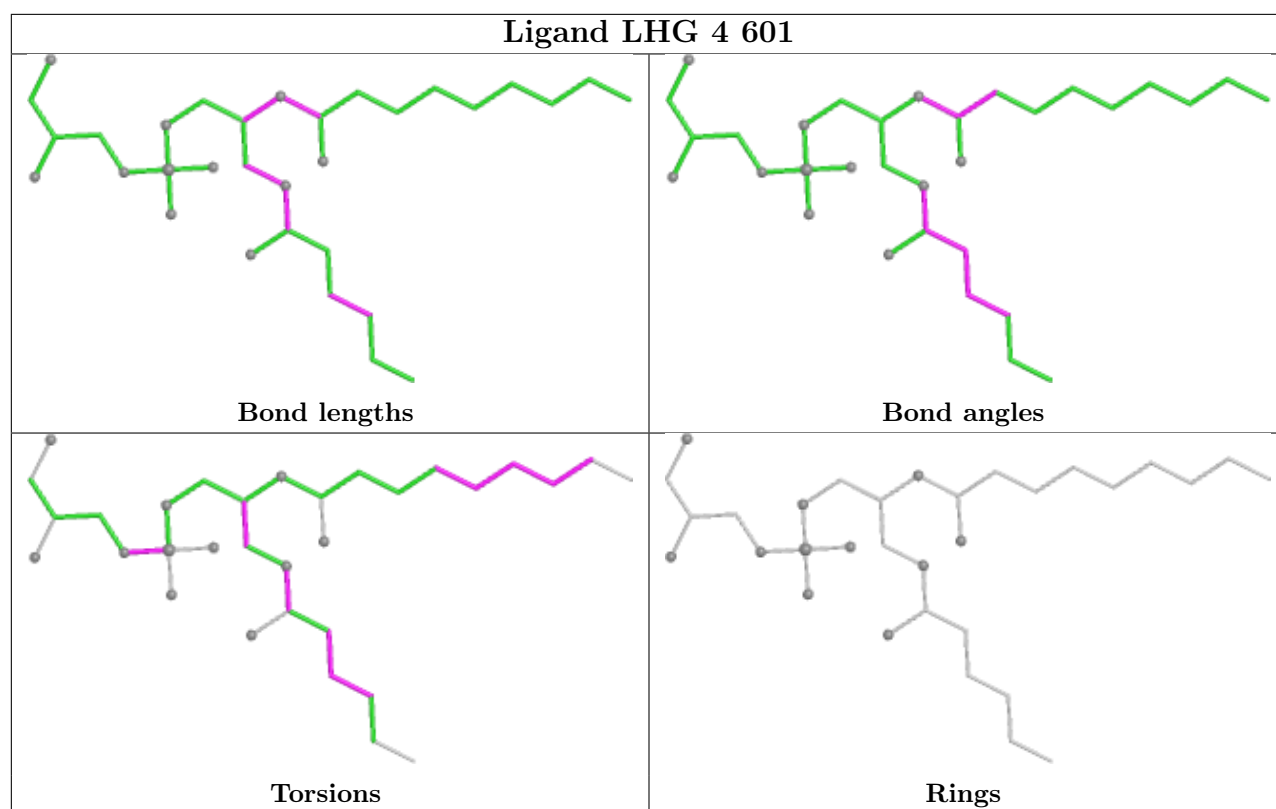


Ligand CHL a 606

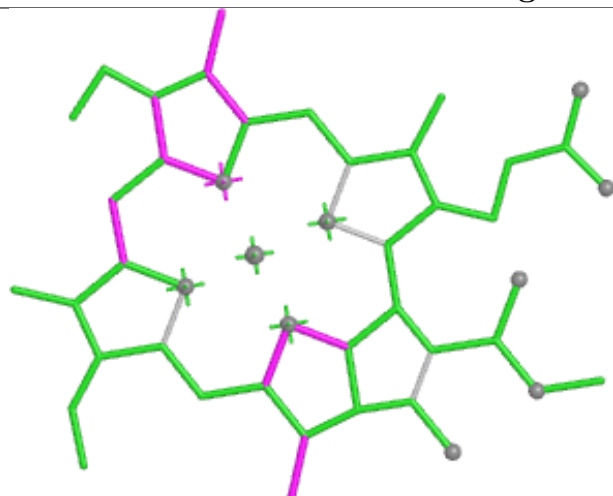


Ligand OUR 6 501

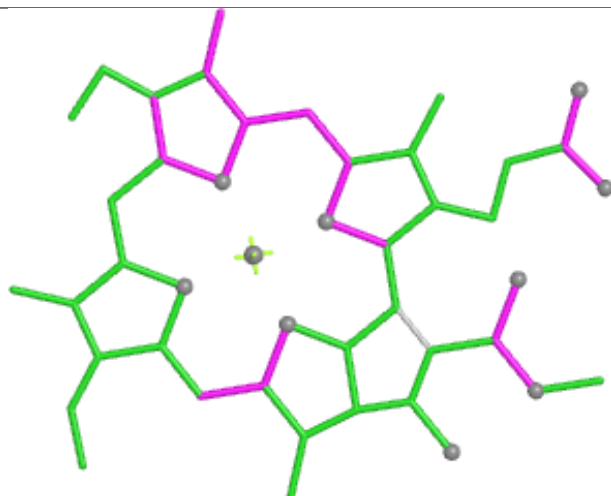




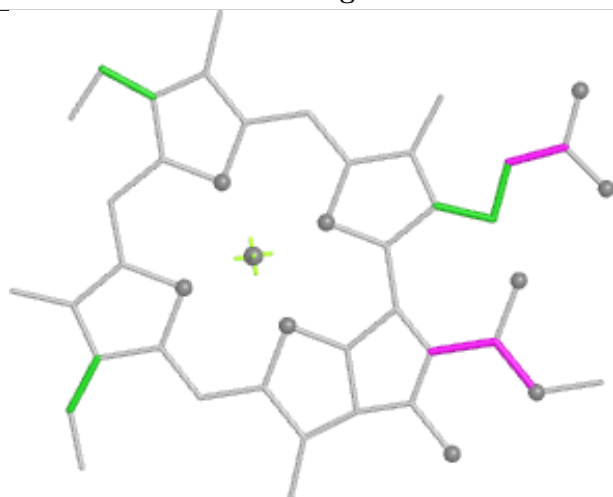
Ligand CLA 4 314



Bond lengths



Bond angles

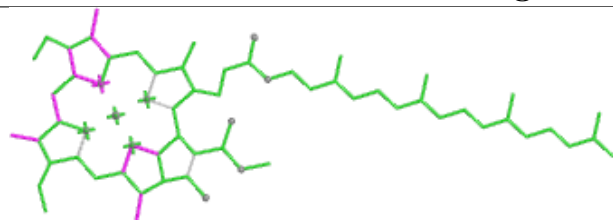


Torsions

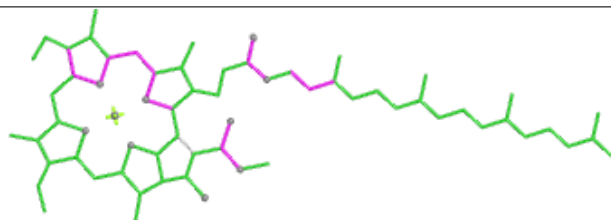


Rings

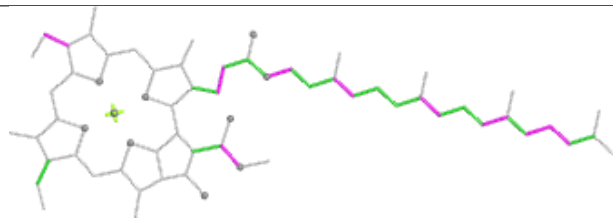
Ligand CLA A 839



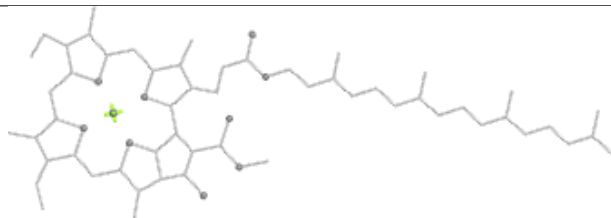
Bond lengths



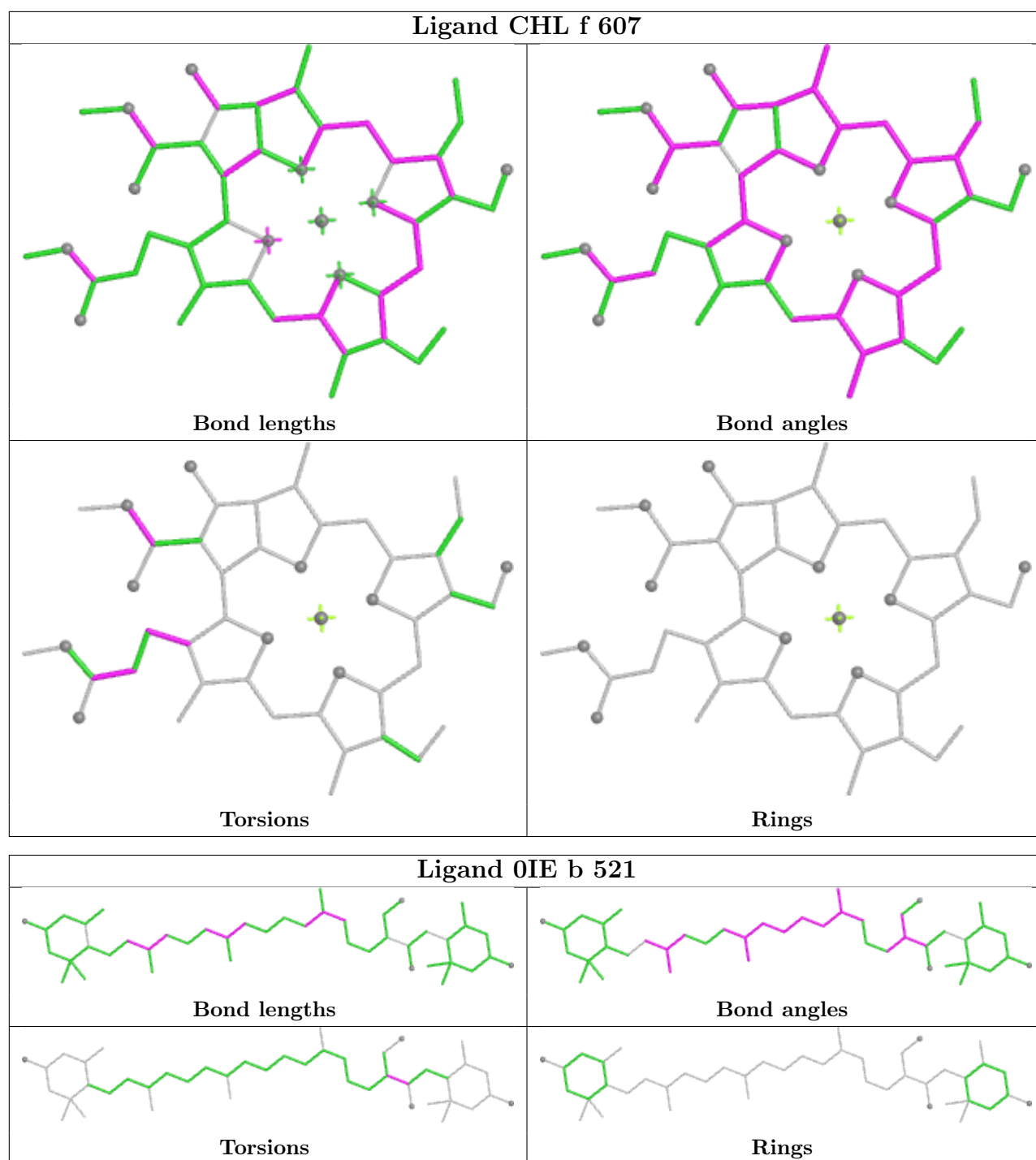
Bond angles



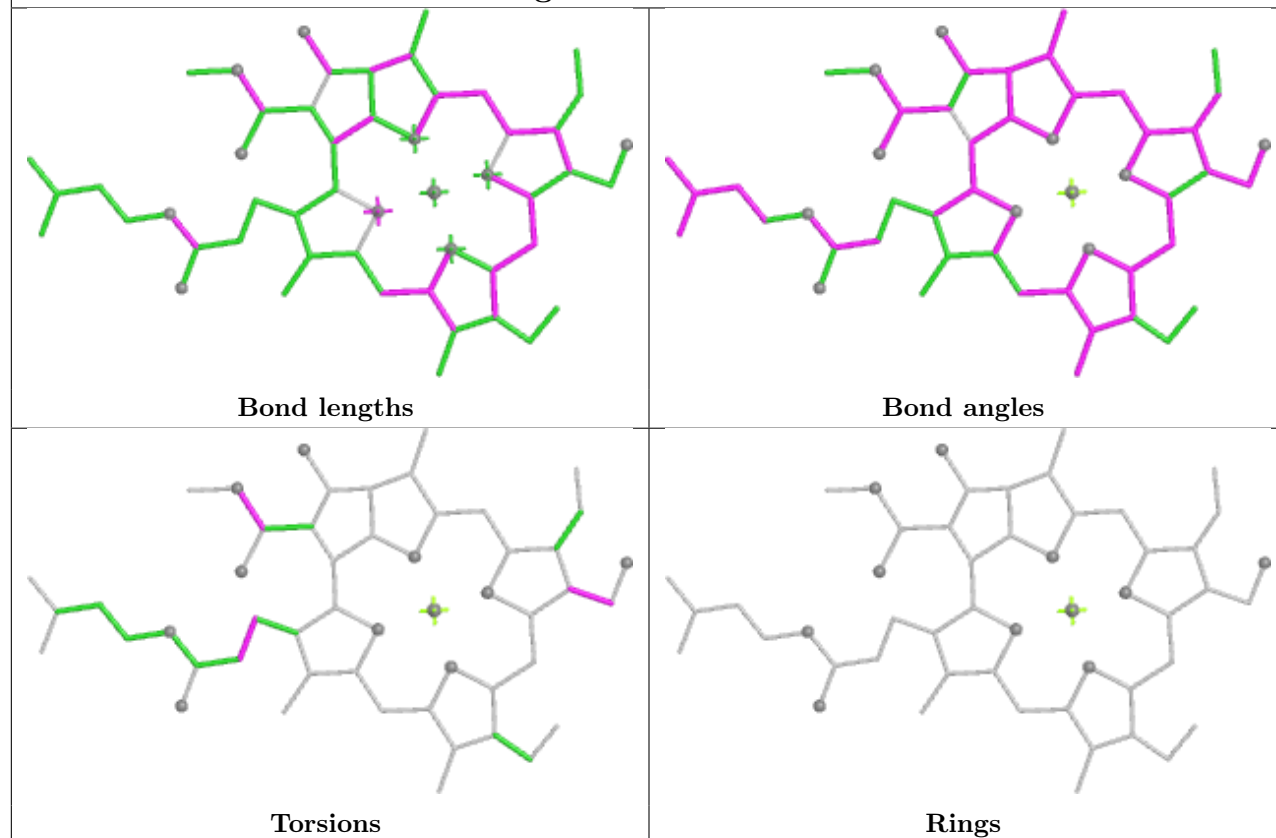
Torsions



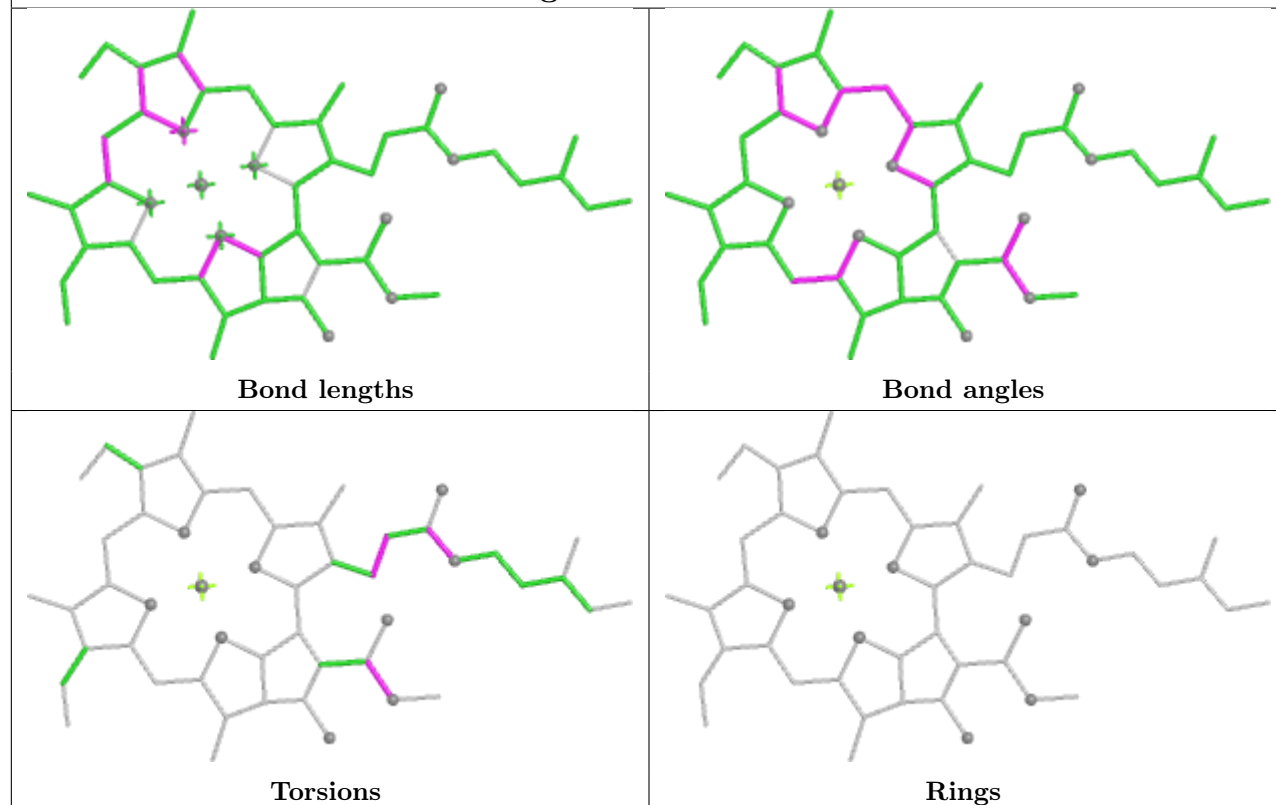
Rings

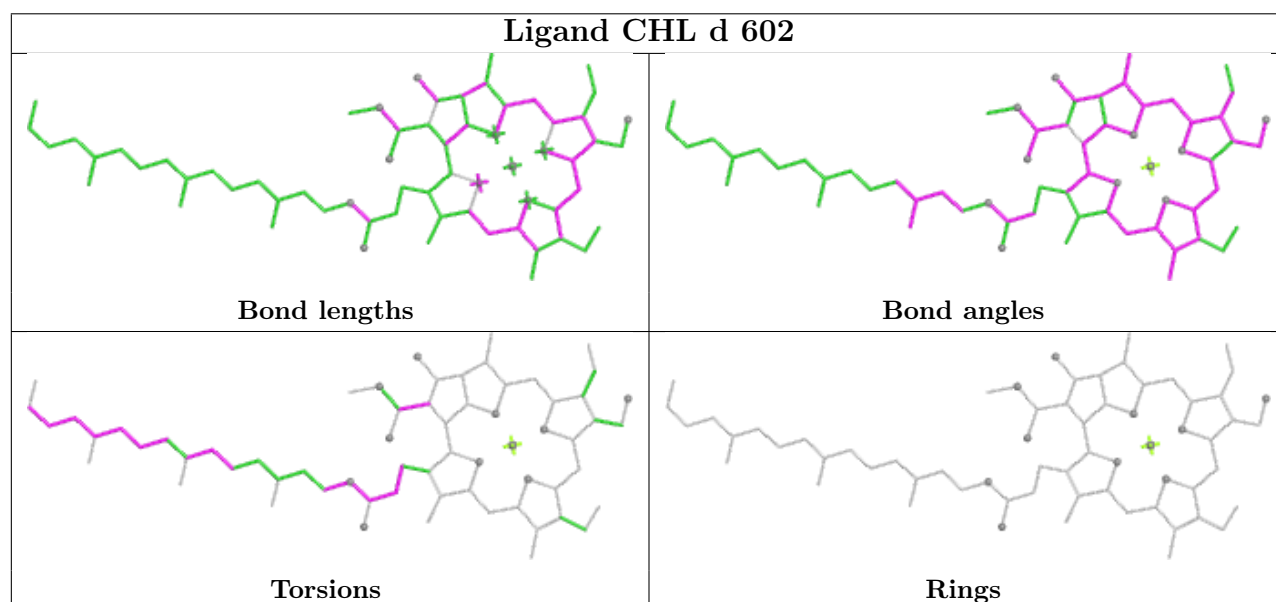
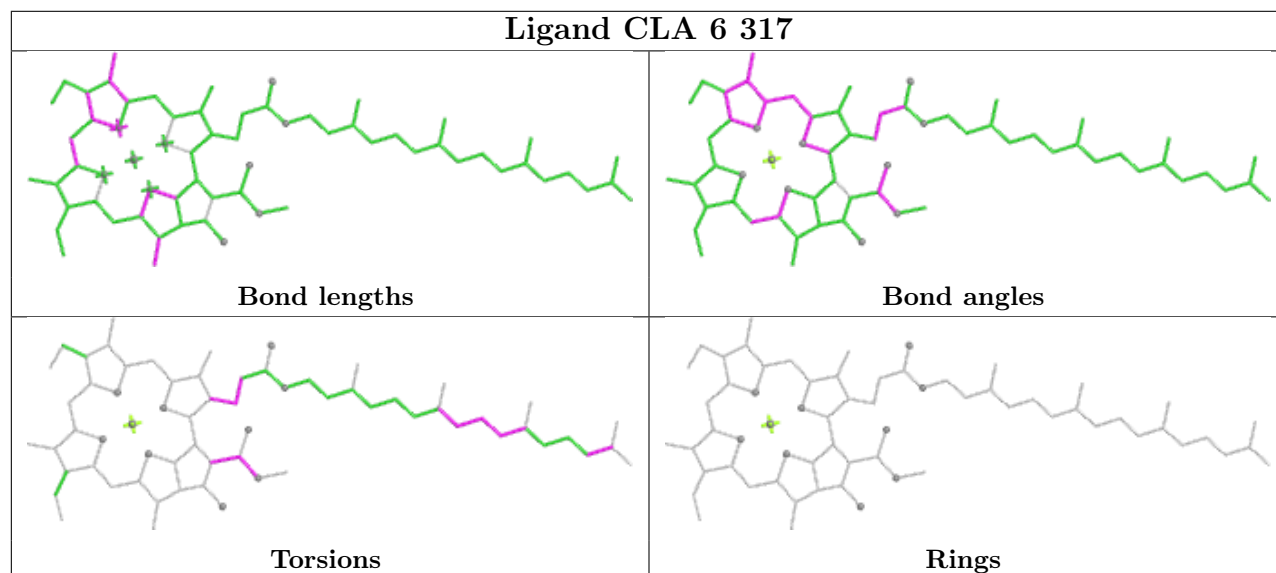
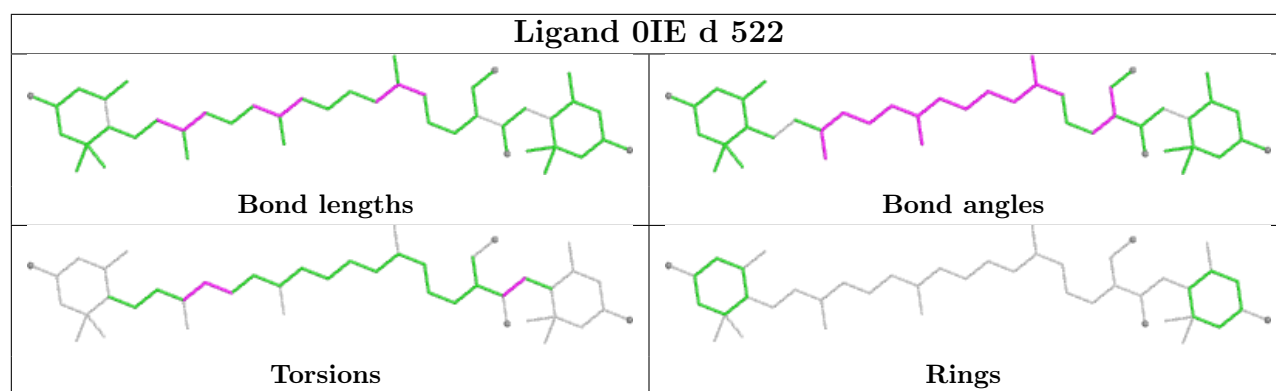


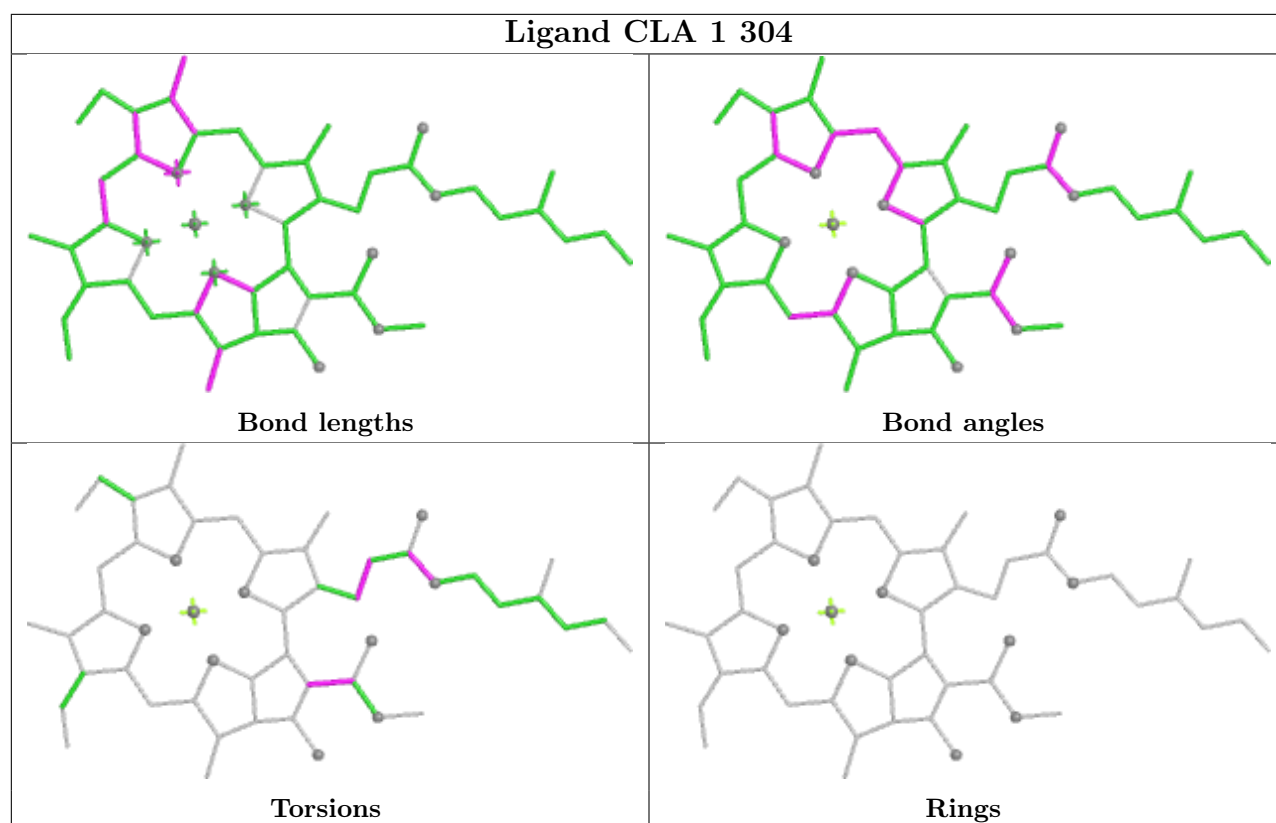
Ligand CHL d 608

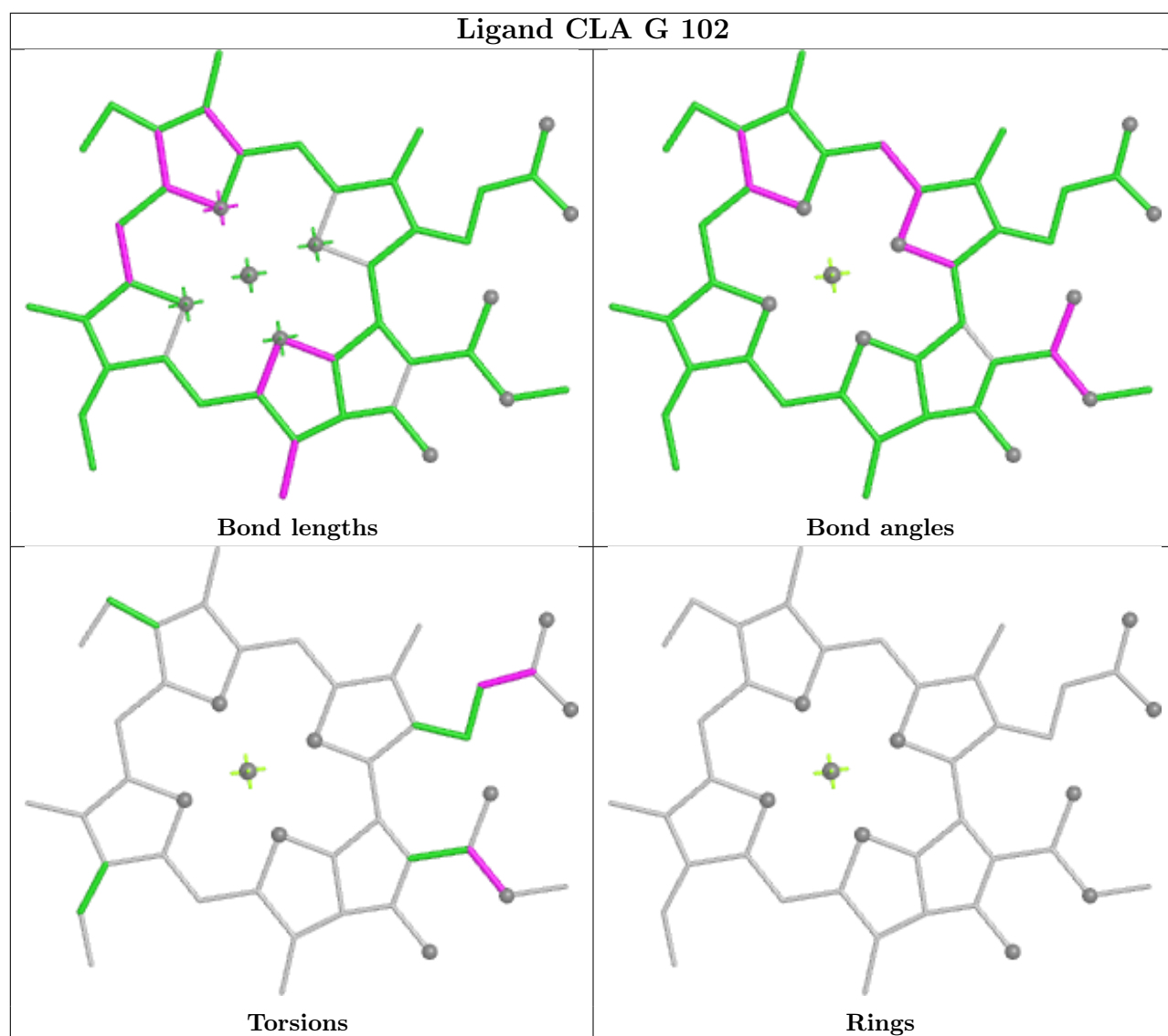


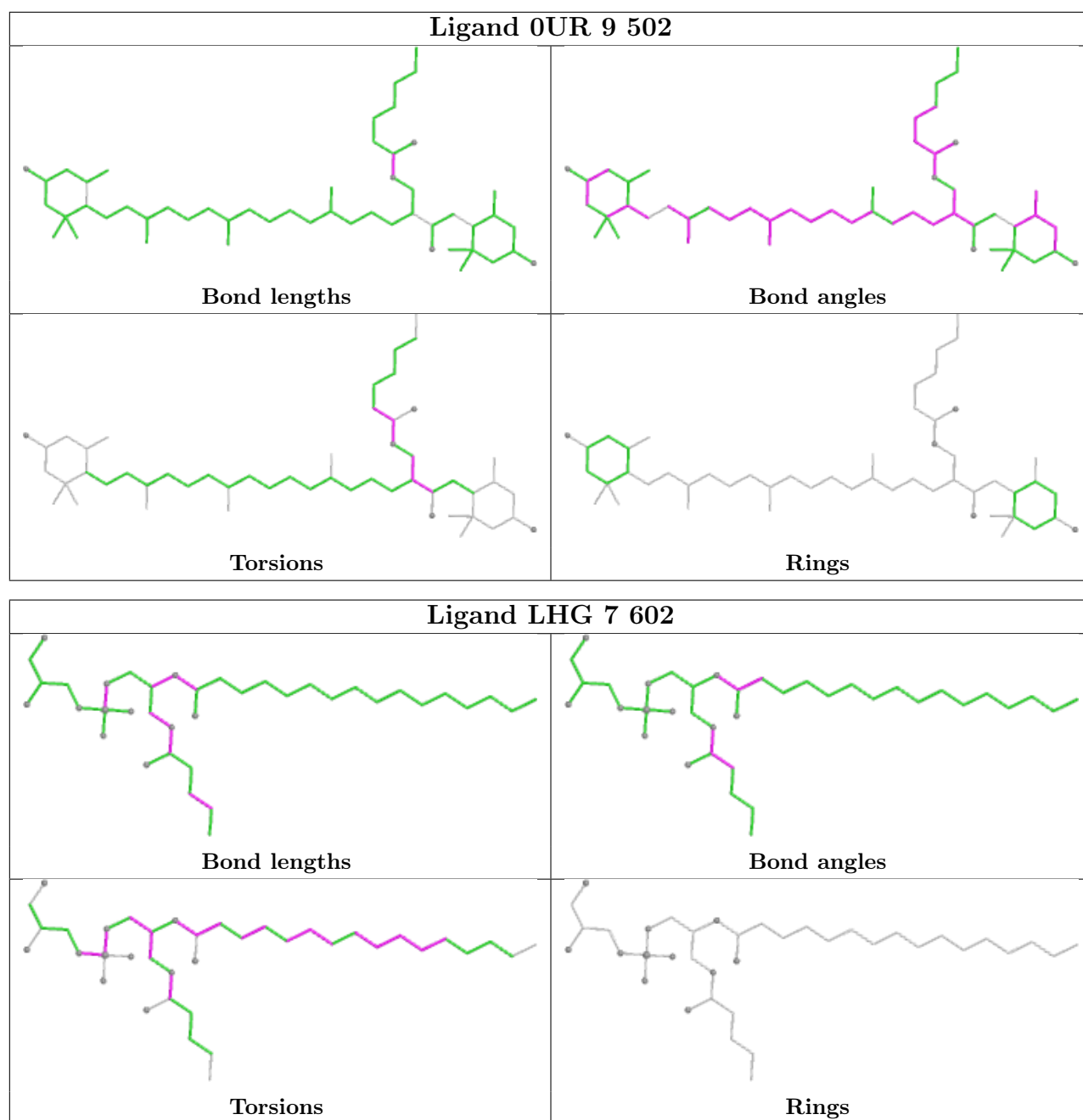
Ligand CLA i 613

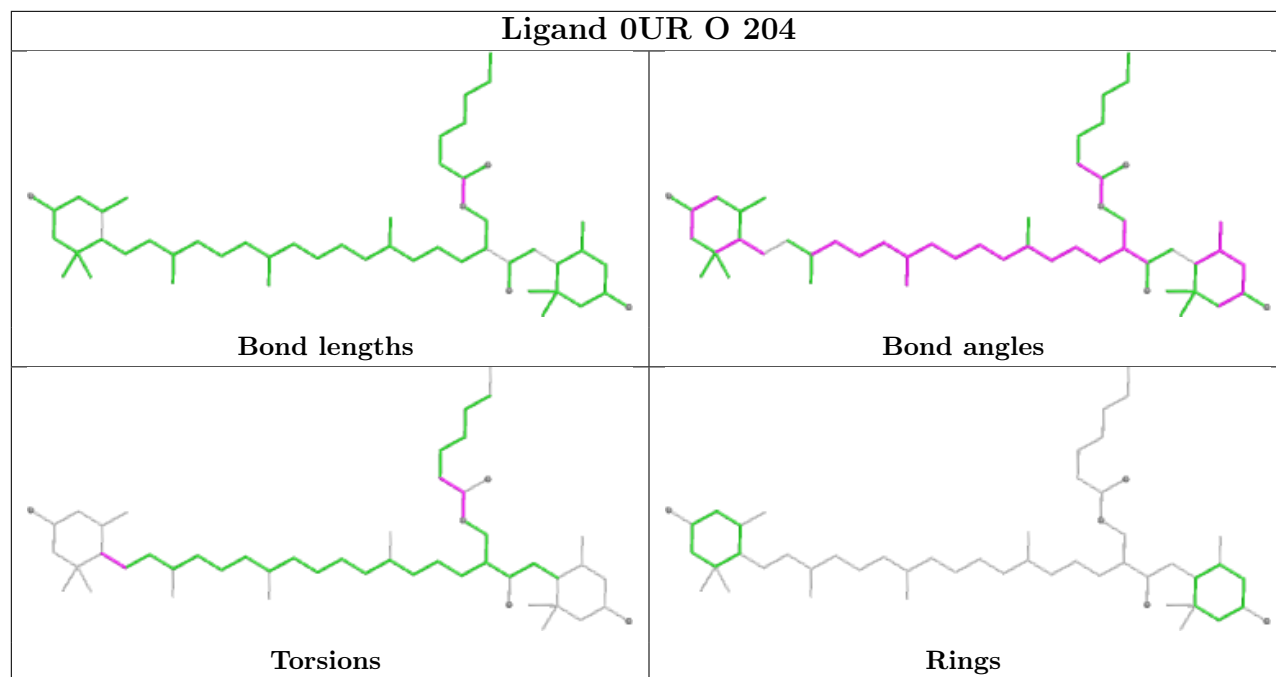
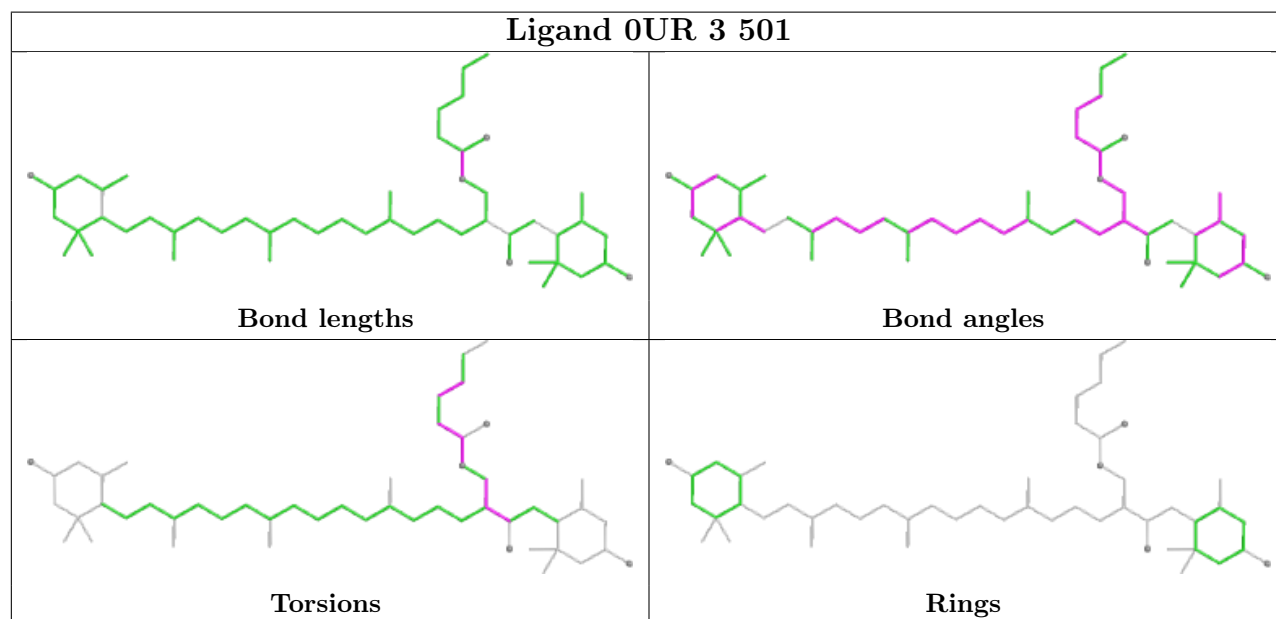


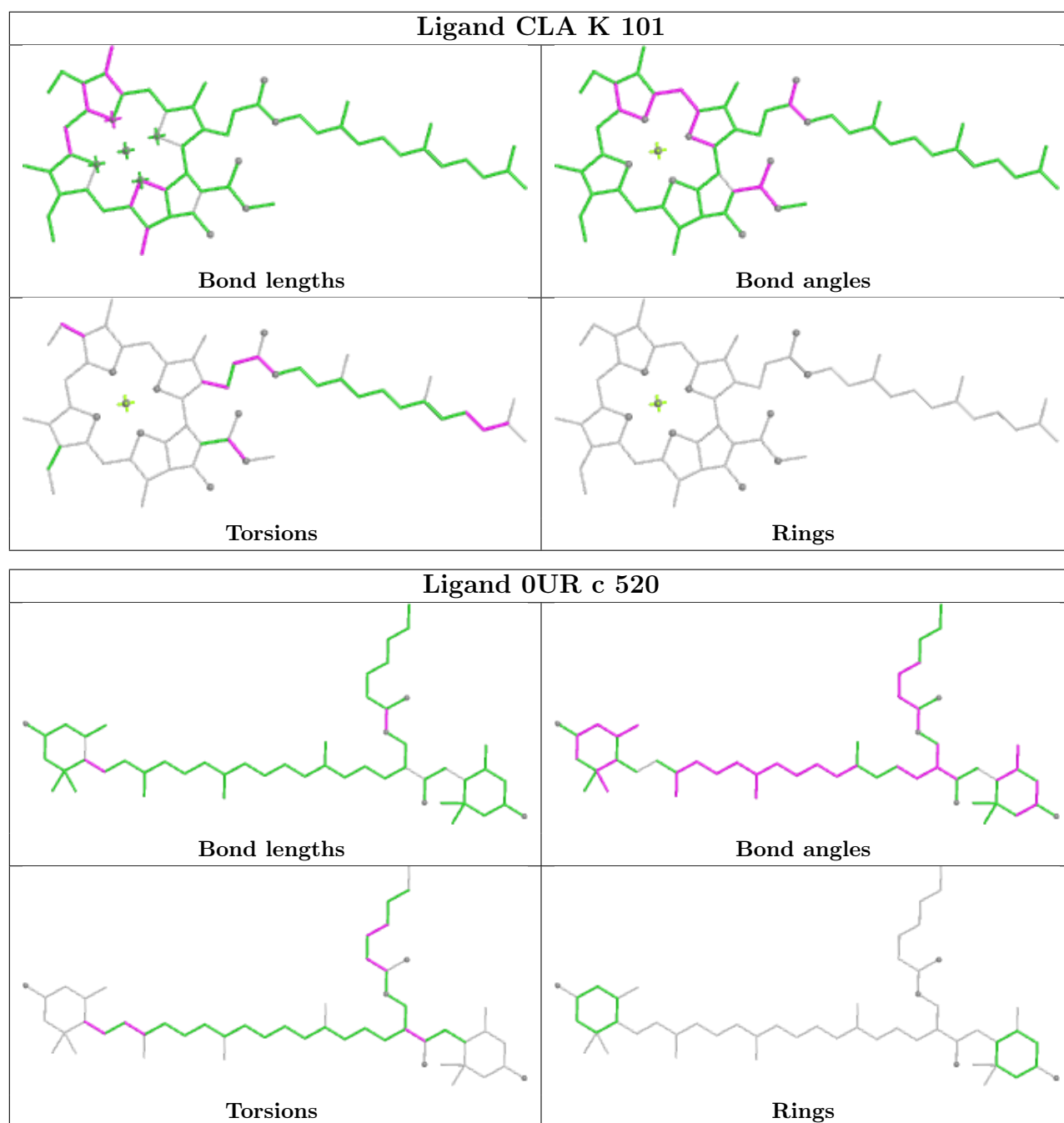




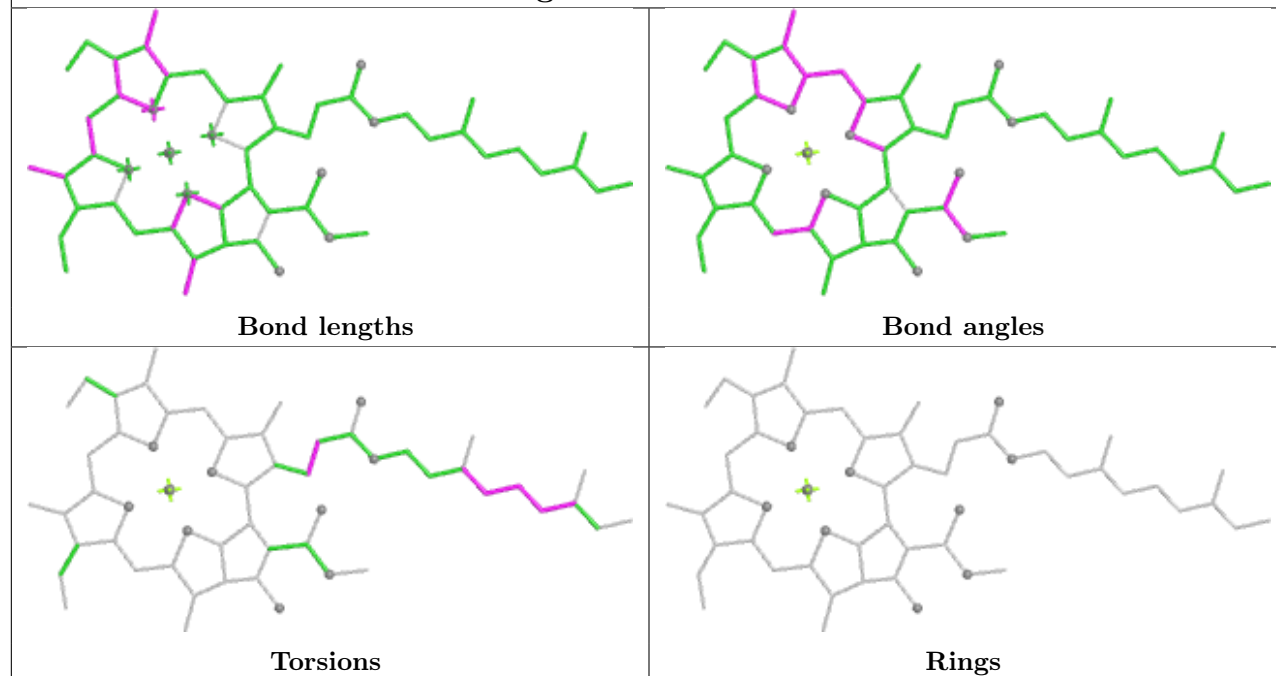




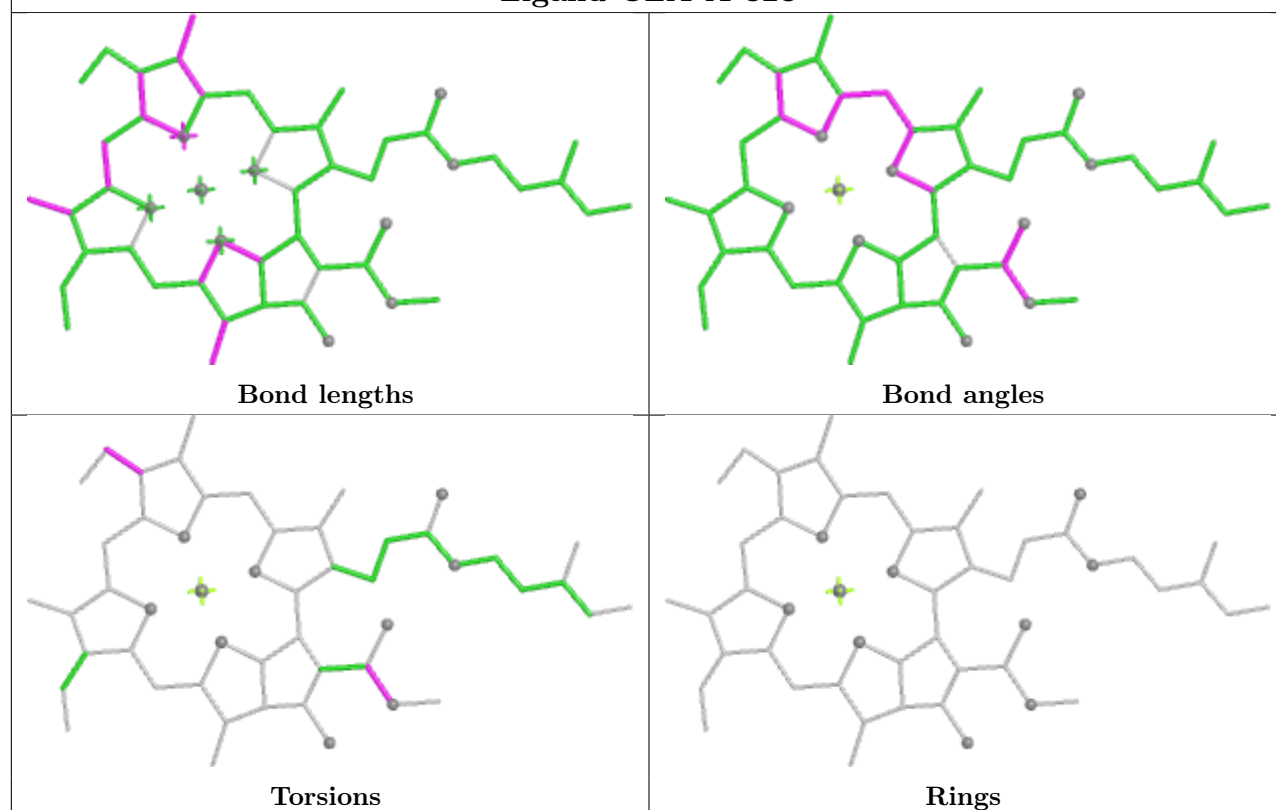
Ligand 0UR O 204**Ligand 0UR 3 501**



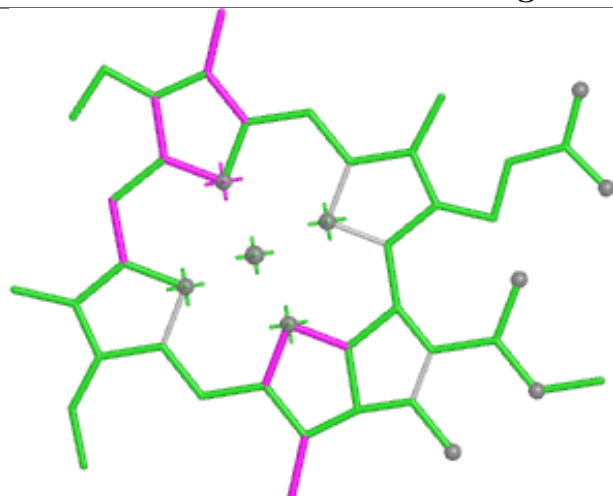
Ligand CLA 9 312



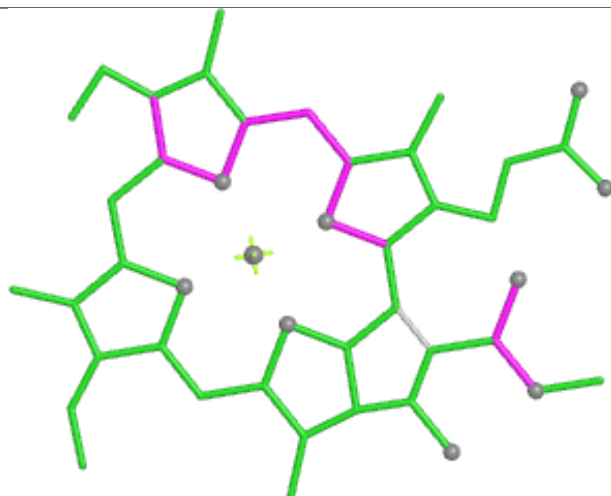
Ligand CLA A 823



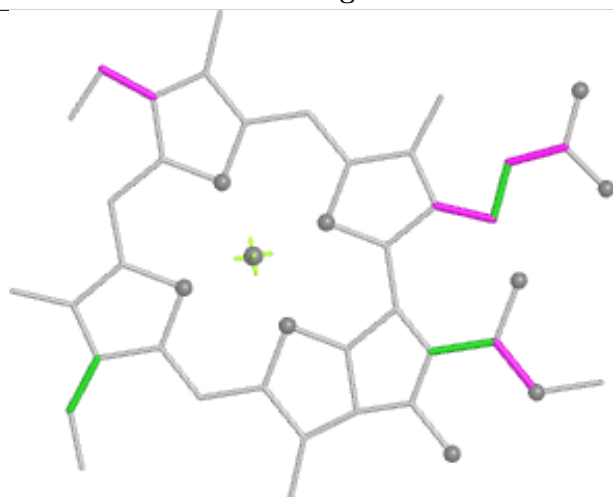
Ligand CLA d 612



Bond lengths



Bond angles

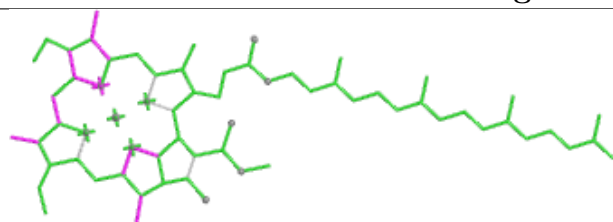


Torsions

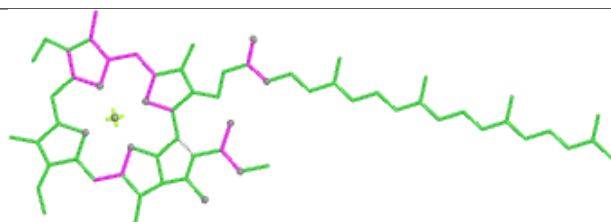


Rings

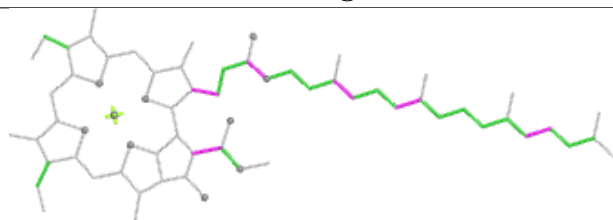
Ligand CLA A 813



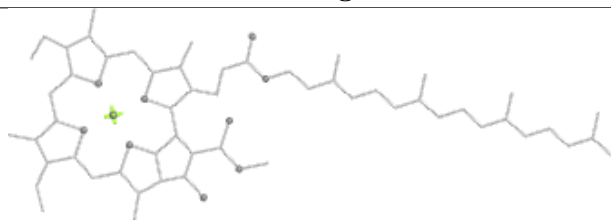
Bond lengths



Bond angles

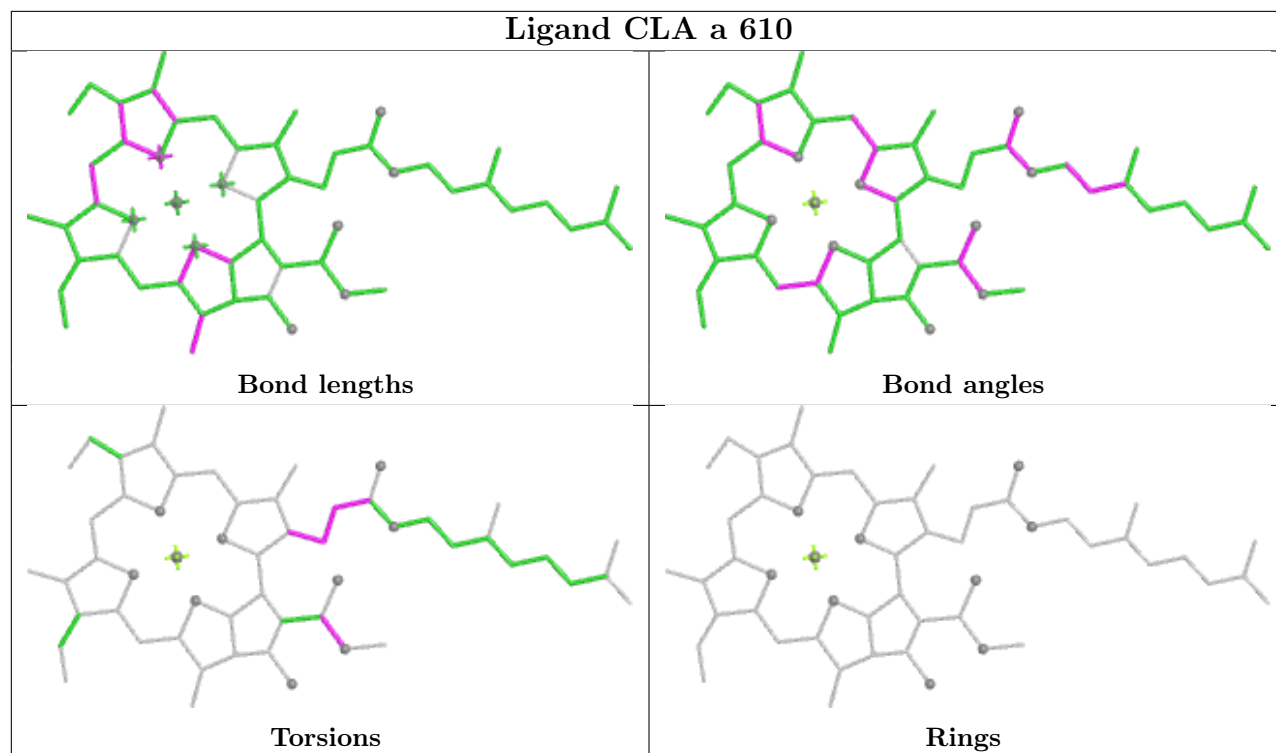


Torsions

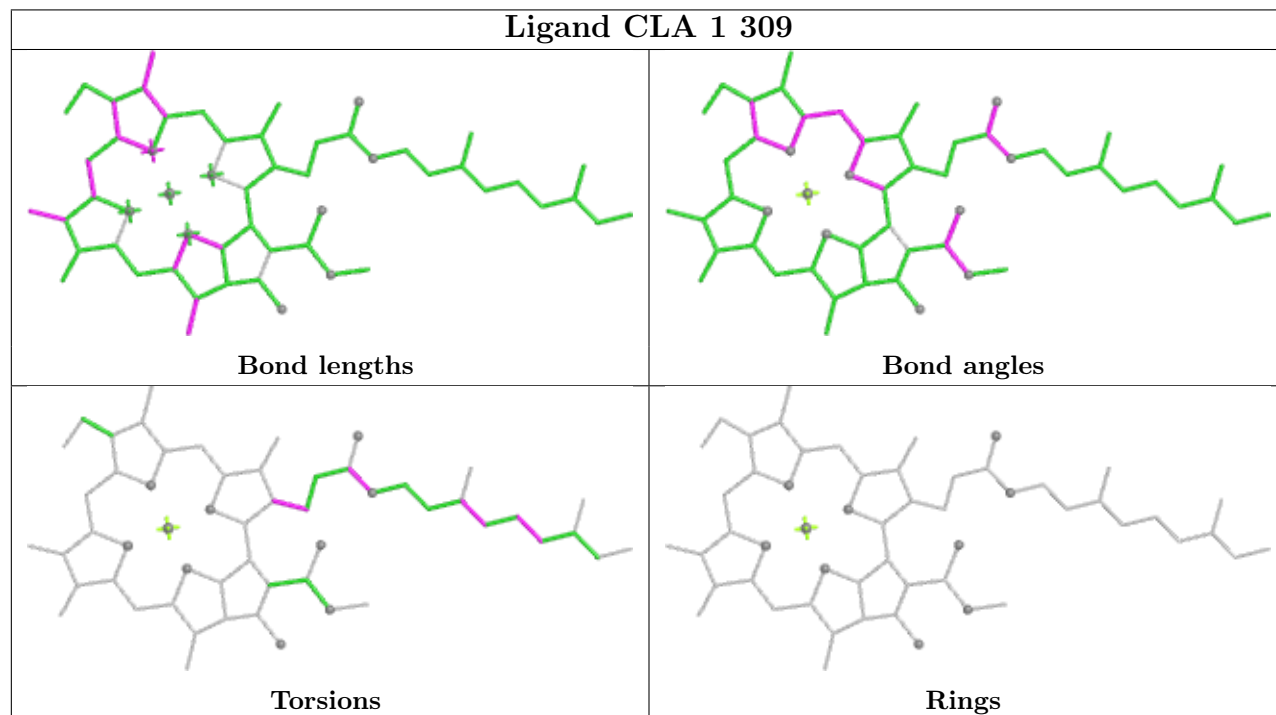


Rings

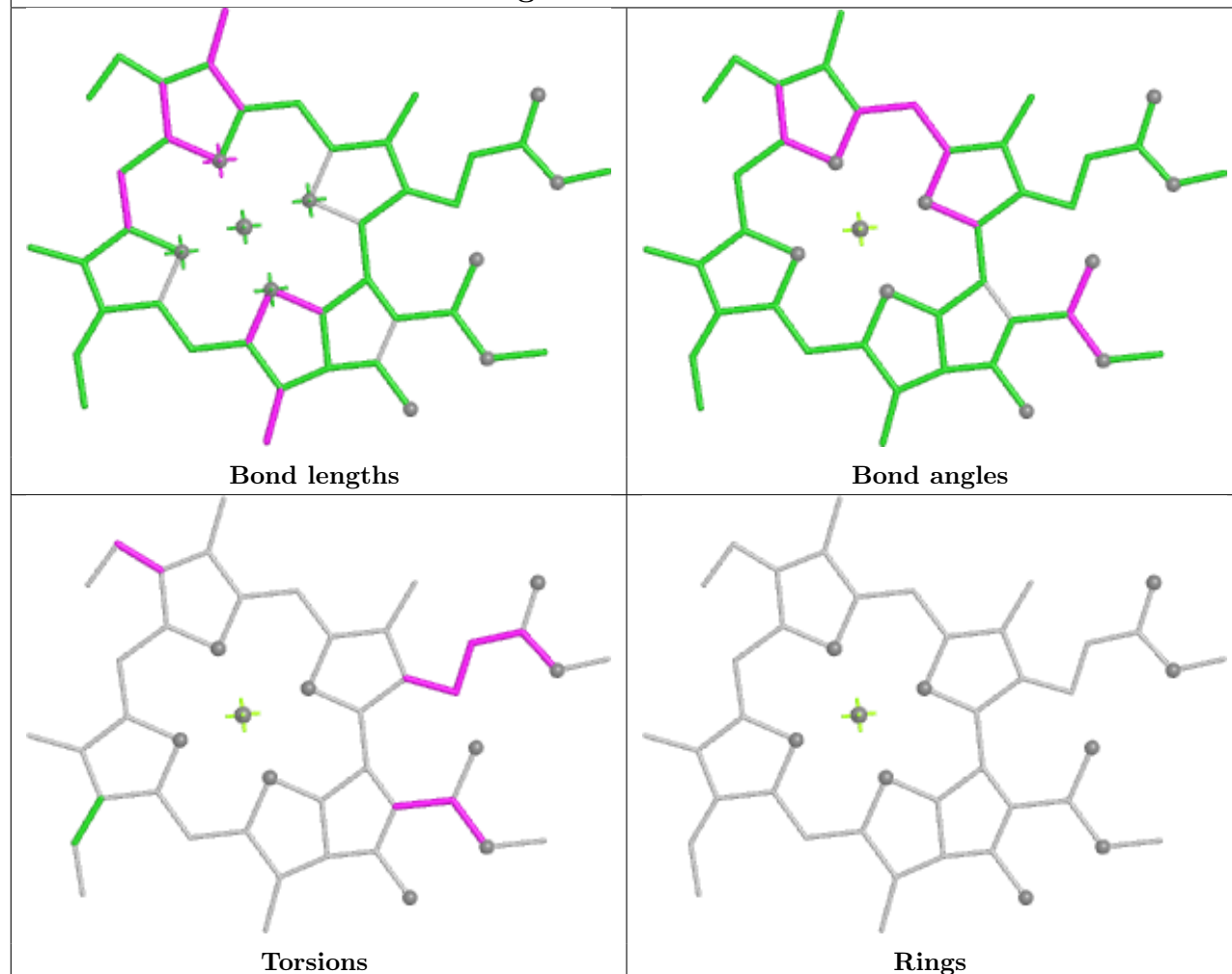
Ligand CLA a 610



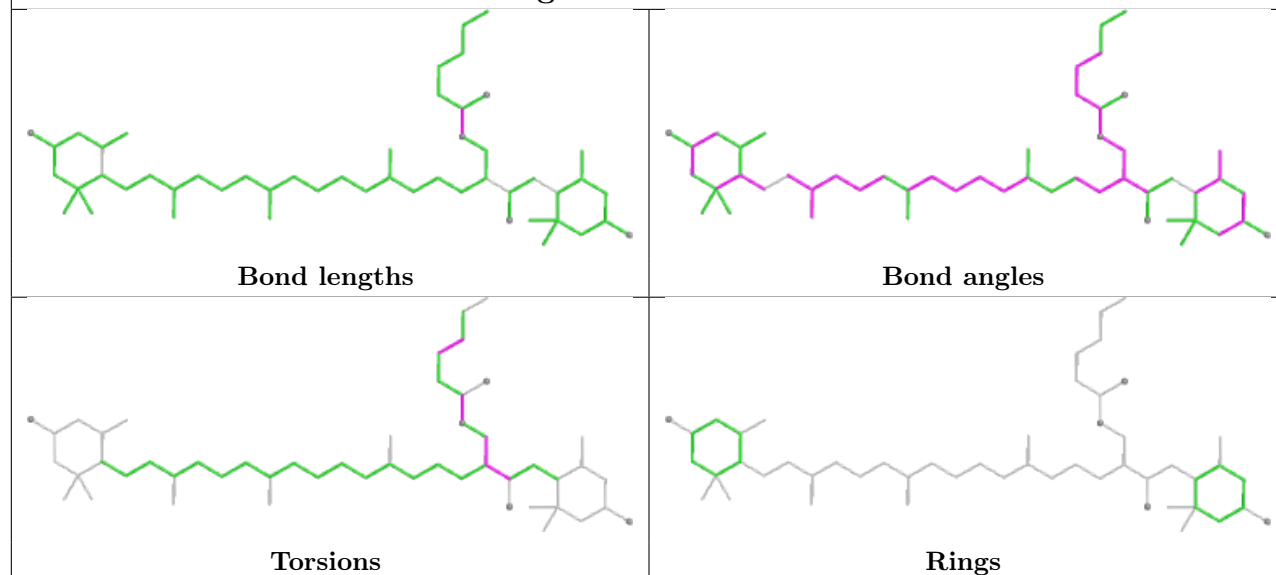
Ligand CLA 1 309

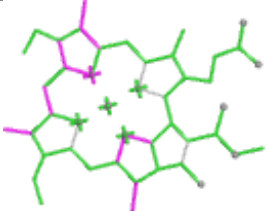
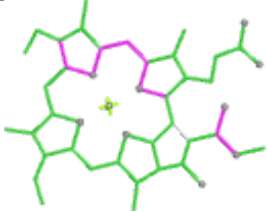
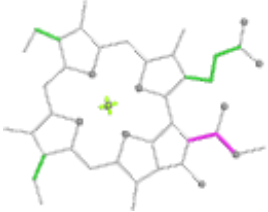
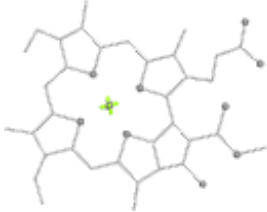


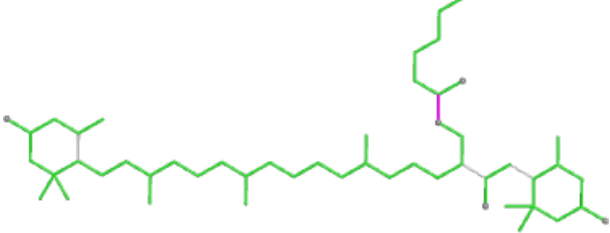
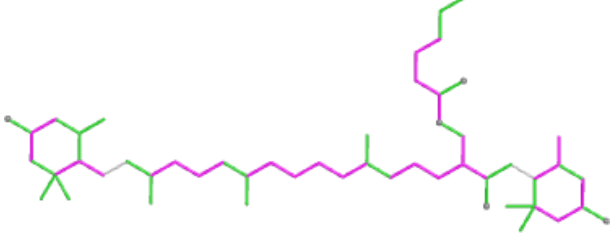
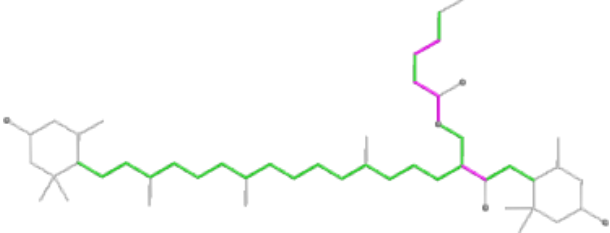
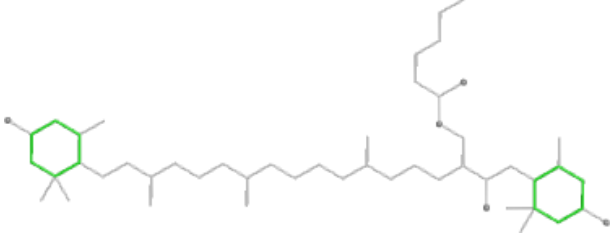
Ligand CLA 6 318



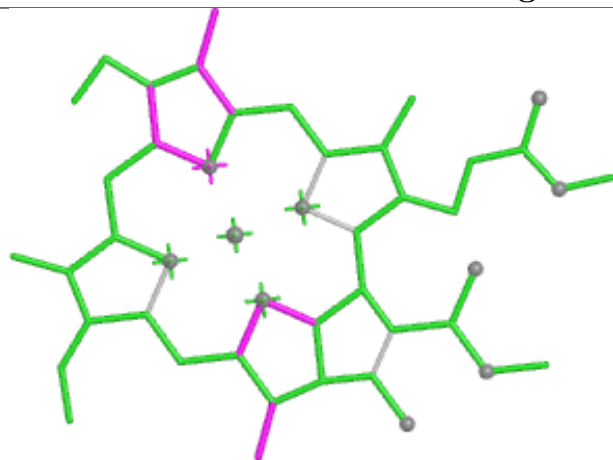
Ligand OUR 2 501



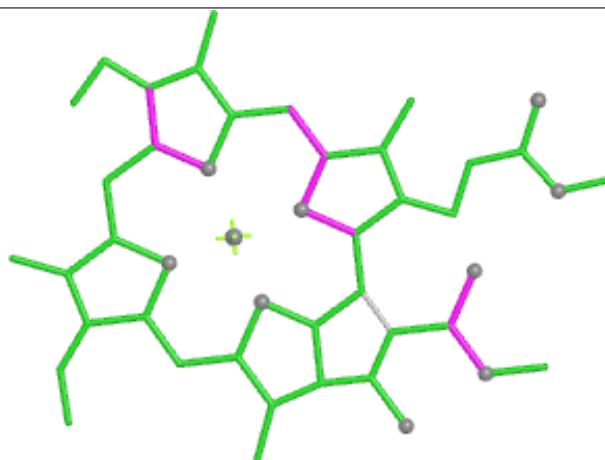
Ligand CLA 7 316			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

Ligand OUR 8 501			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

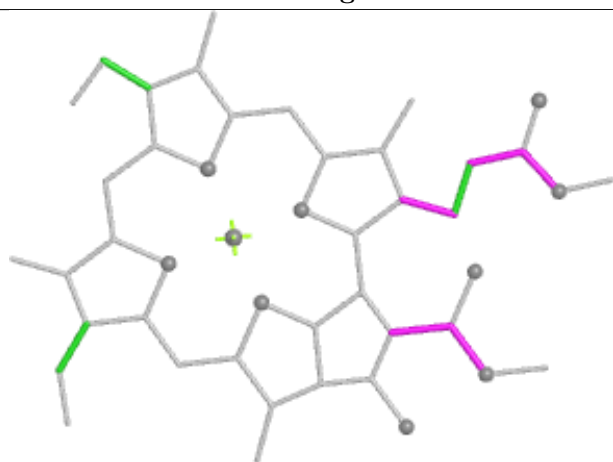
Ligand CLA 0 313



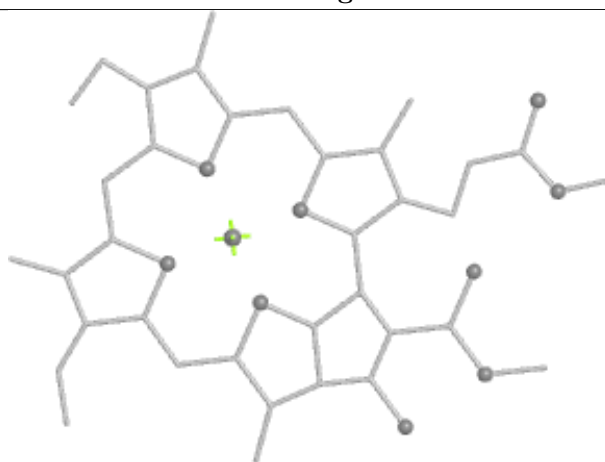
Bond lengths



Bond angles

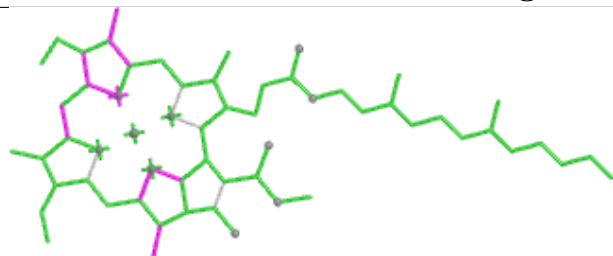


Torsions

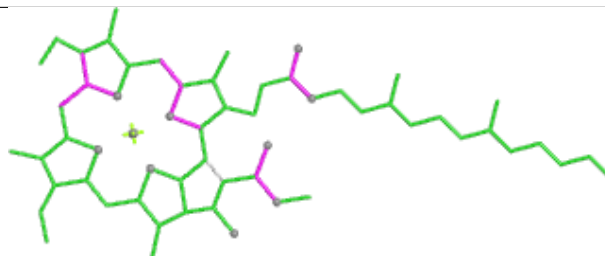


Rings

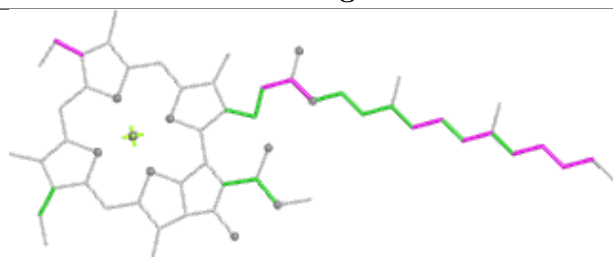
Ligand CLA 5 303



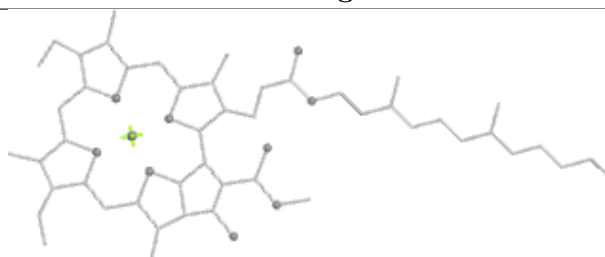
Bond lengths



Bond angles

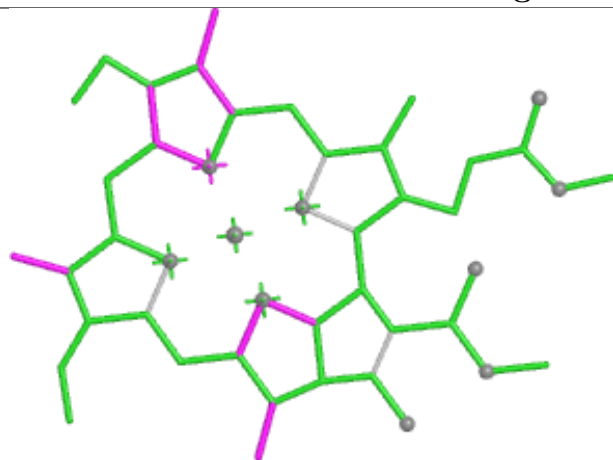


Torsions

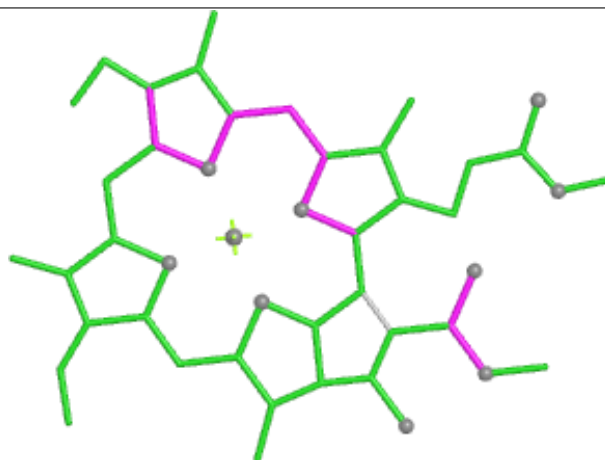


Rings

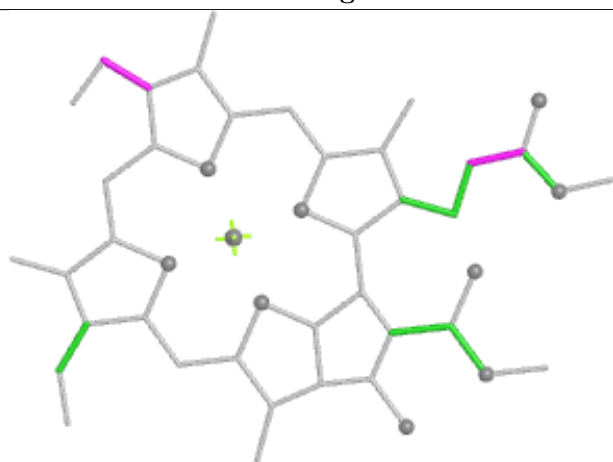
Ligand CLA A 834



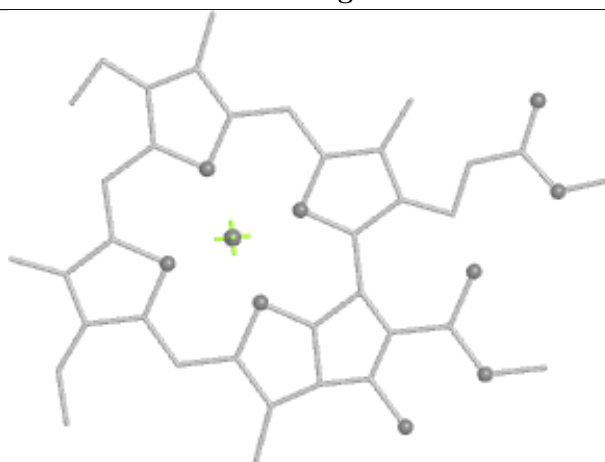
Bond lengths



Bond angles

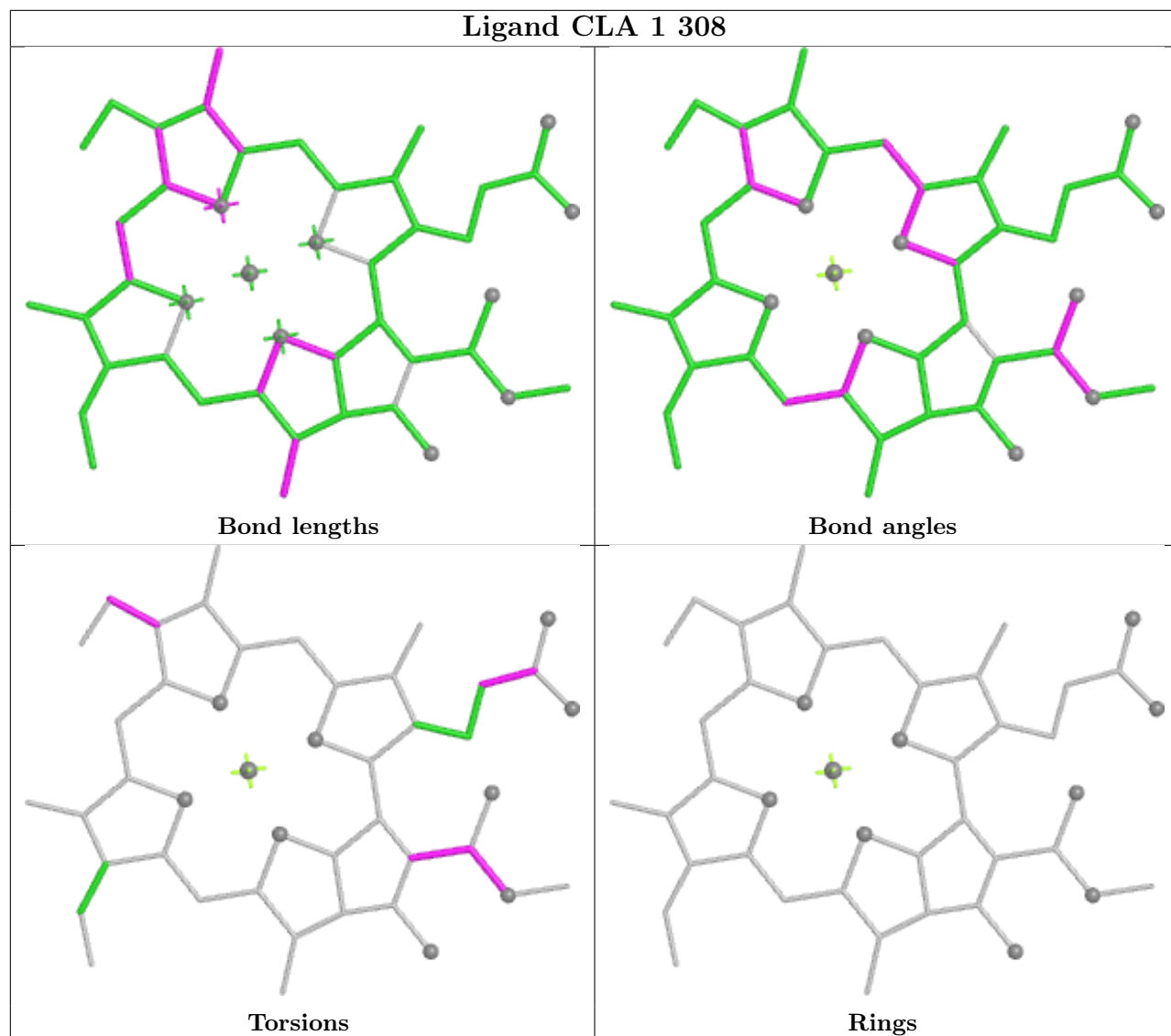


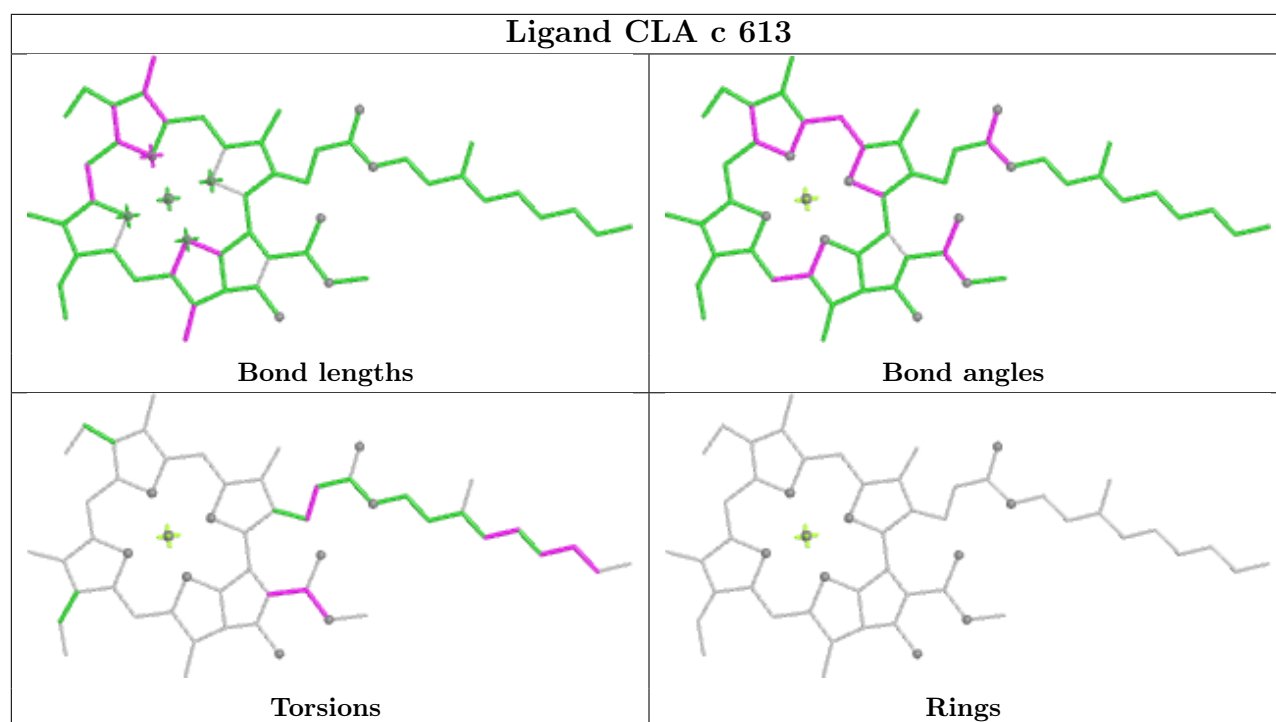
Torsions



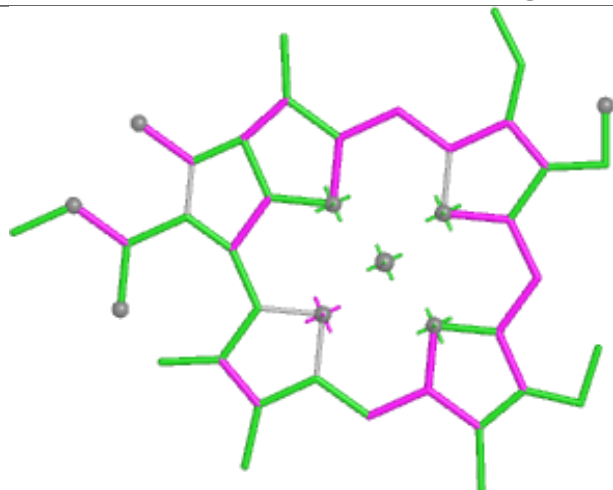
Rings

Ligand CLA 1 308

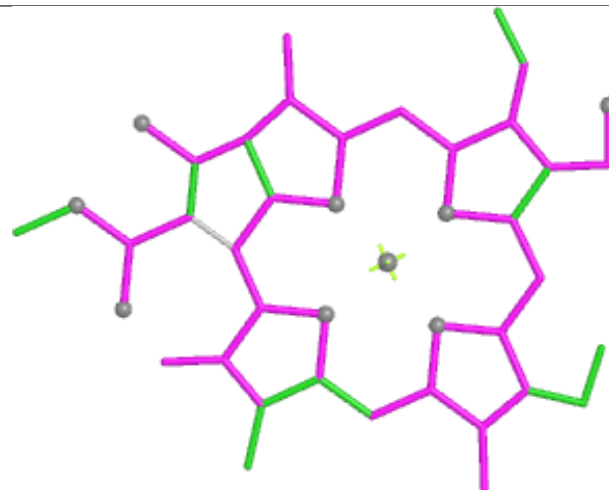




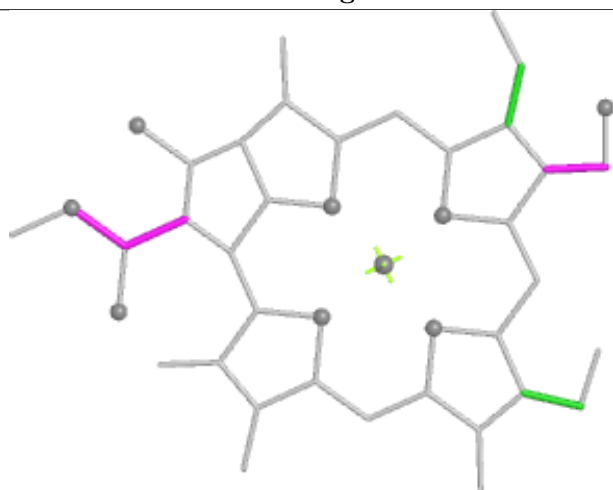
Ligand CHL f 614



Bond lengths



Bond angles

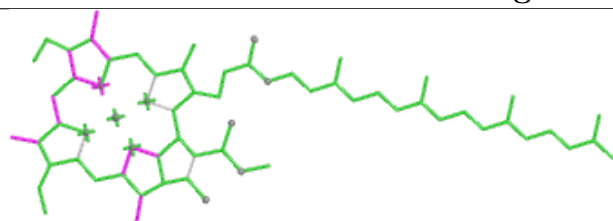


Torsions

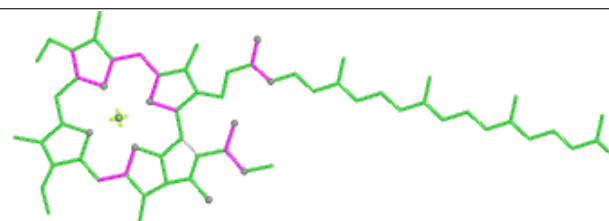


Rings

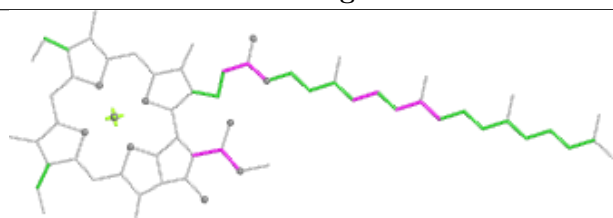
Ligand CLA A 833



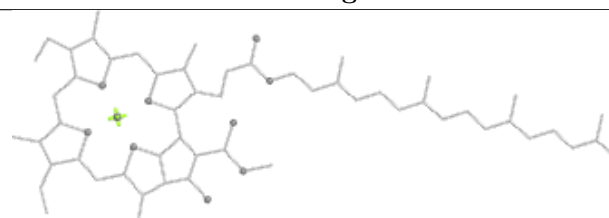
Bond lengths



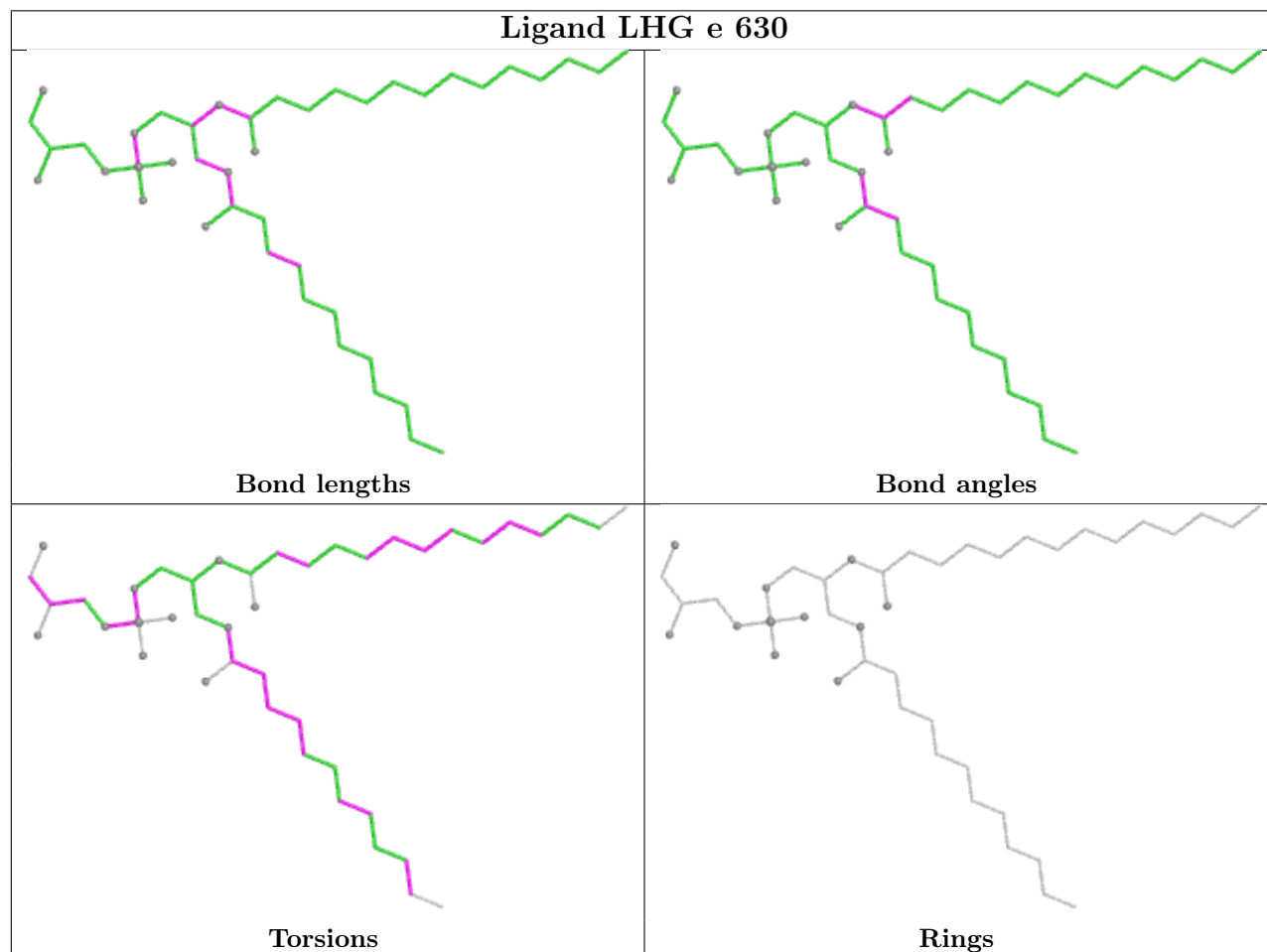
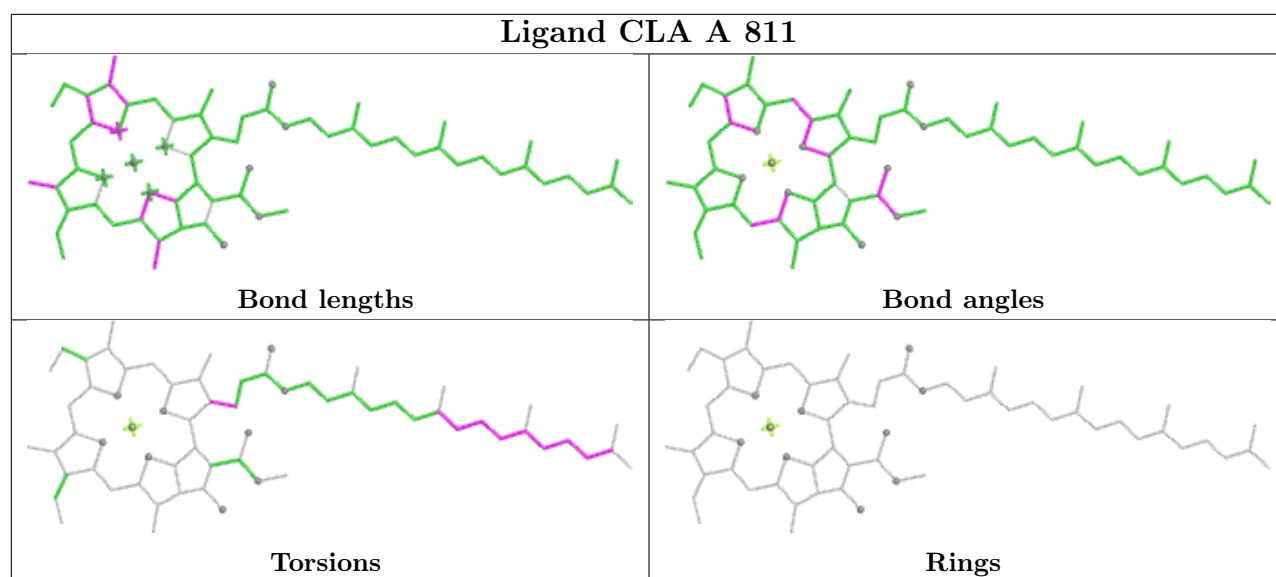
Bond angles

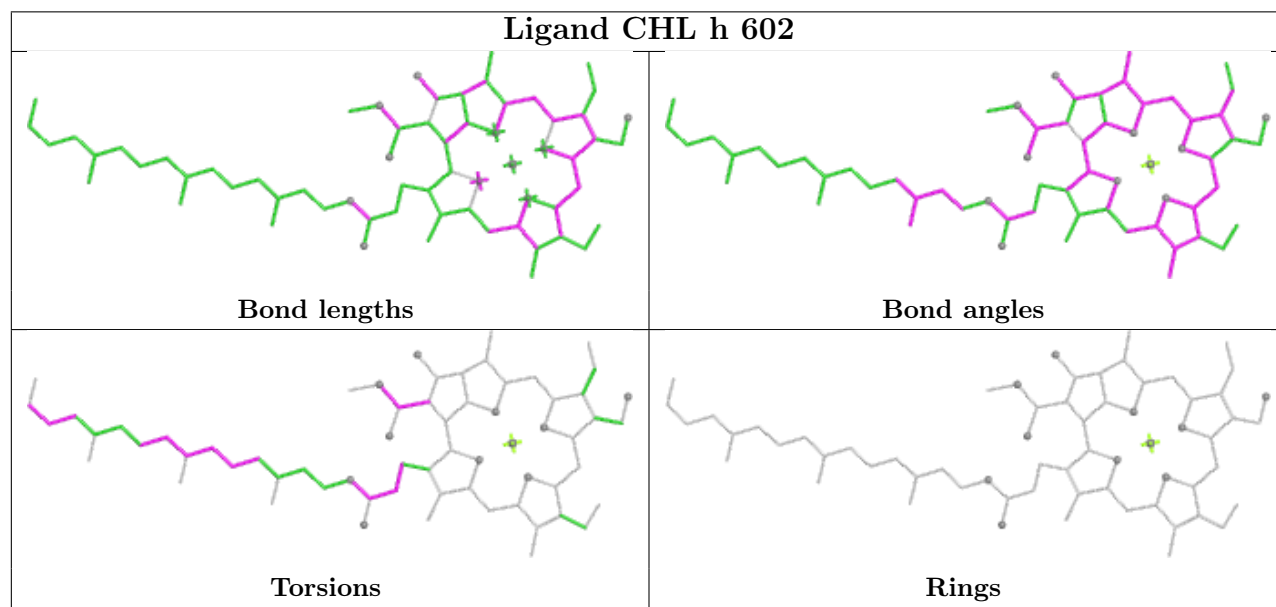
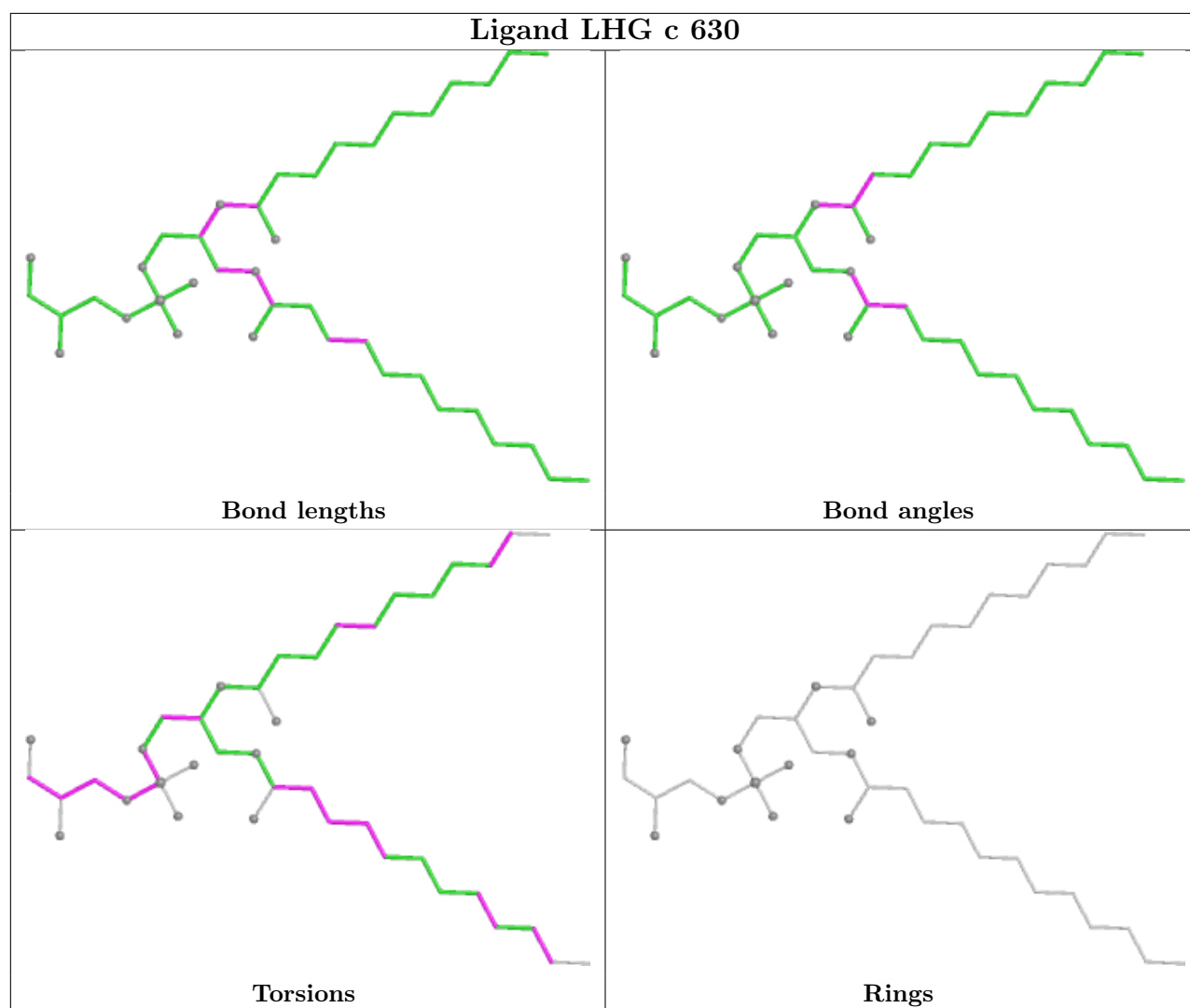


Torsions

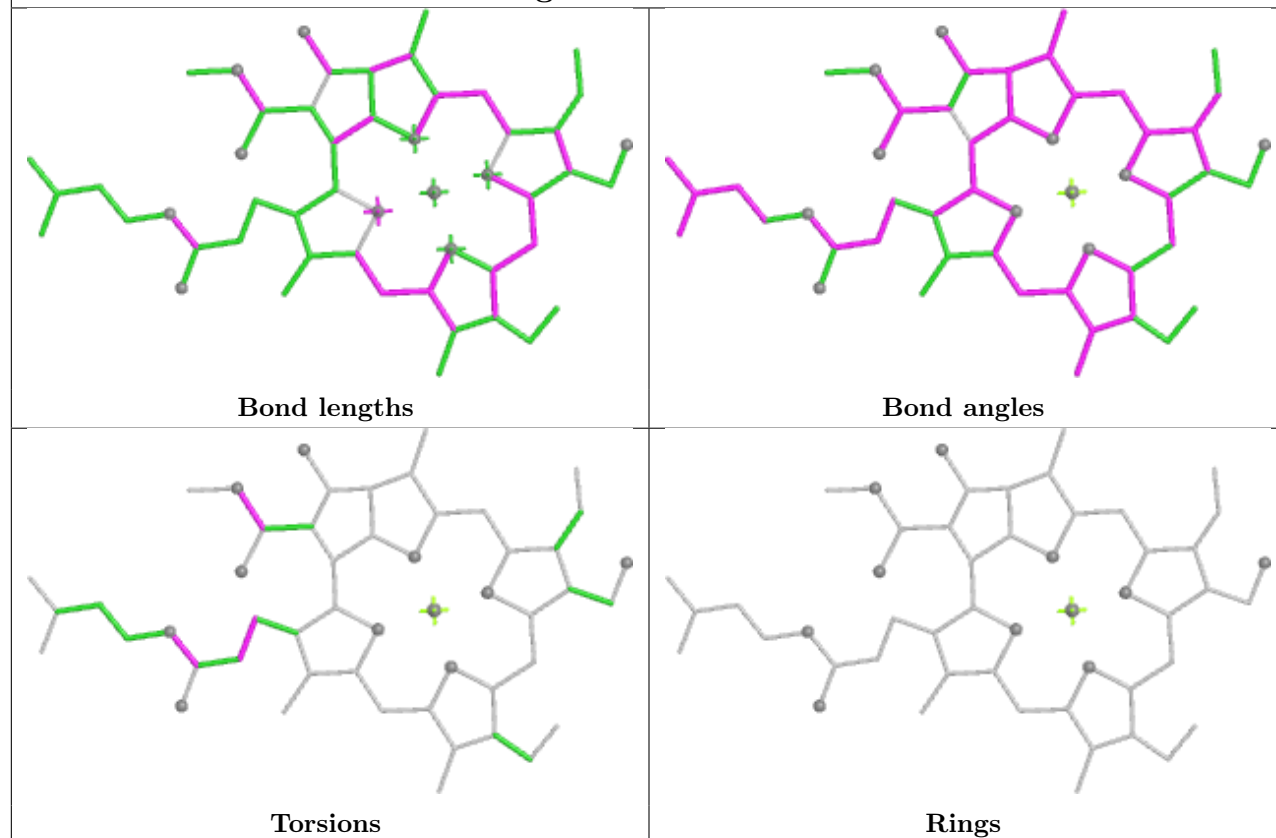


Rings

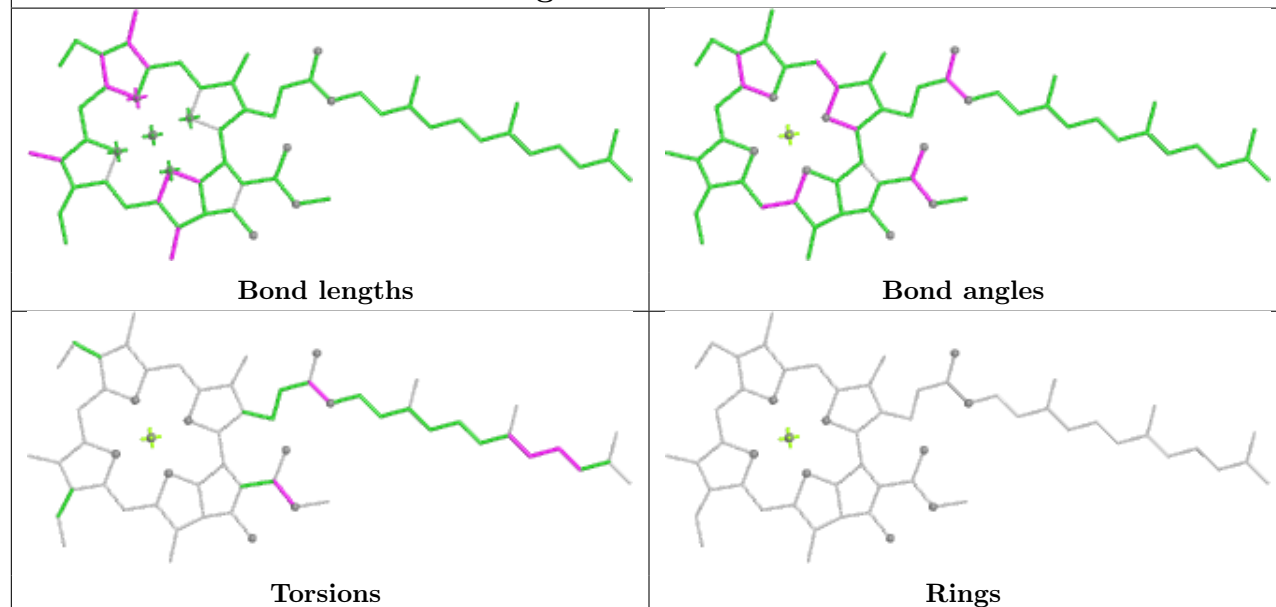


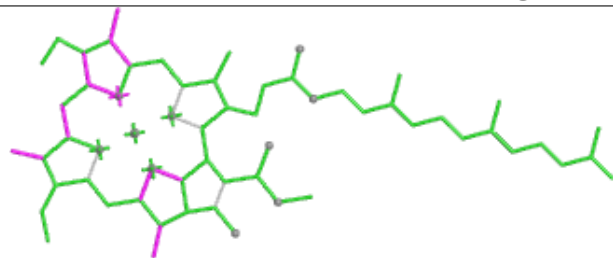
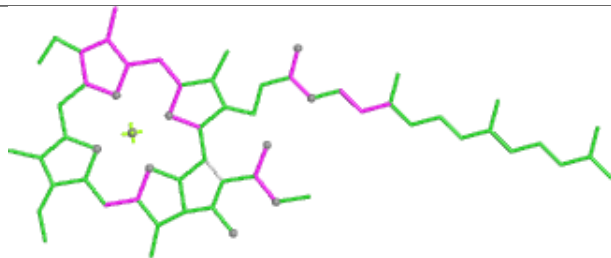
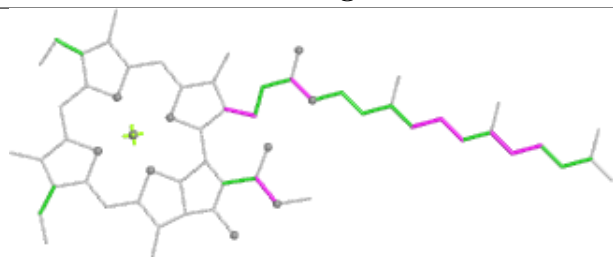
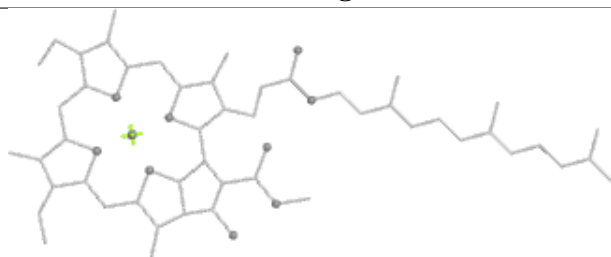
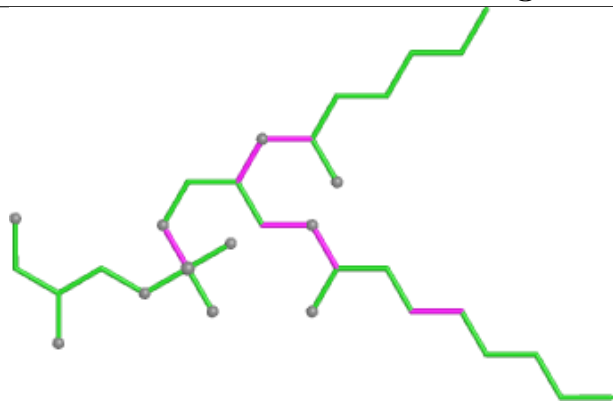
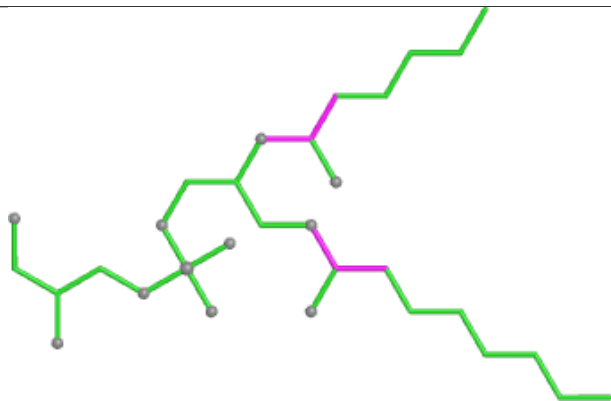
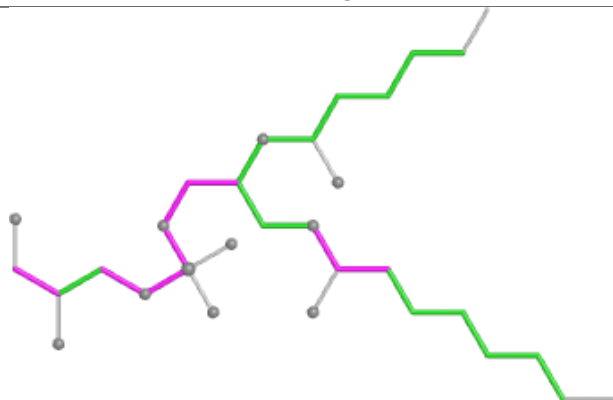
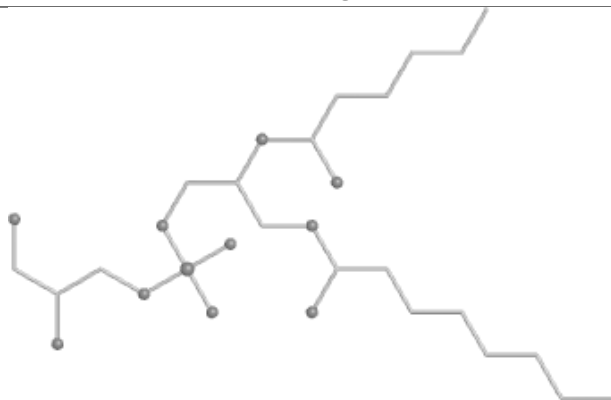


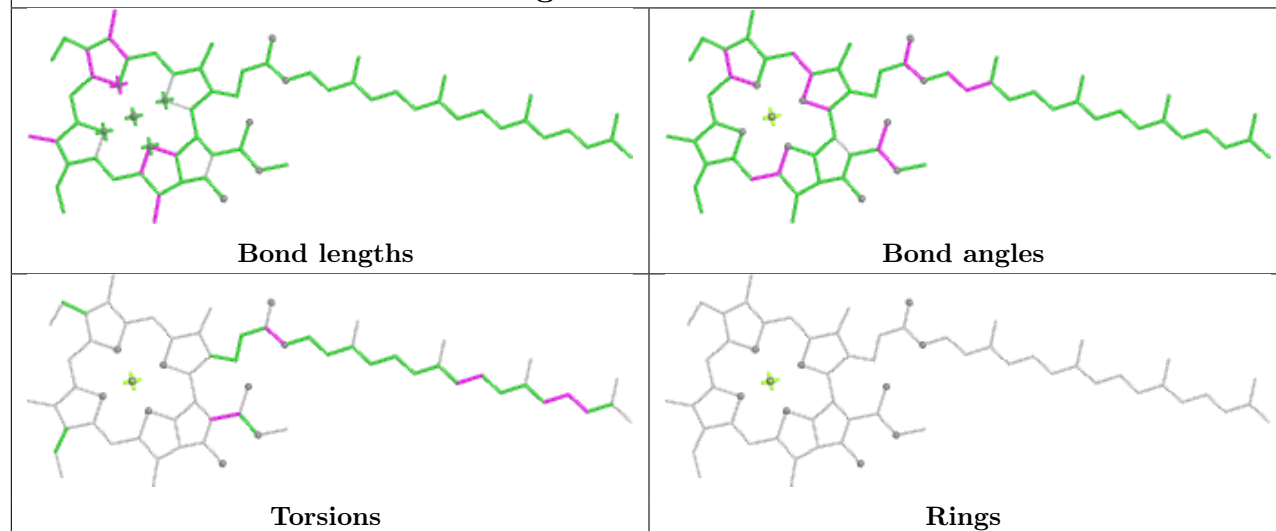
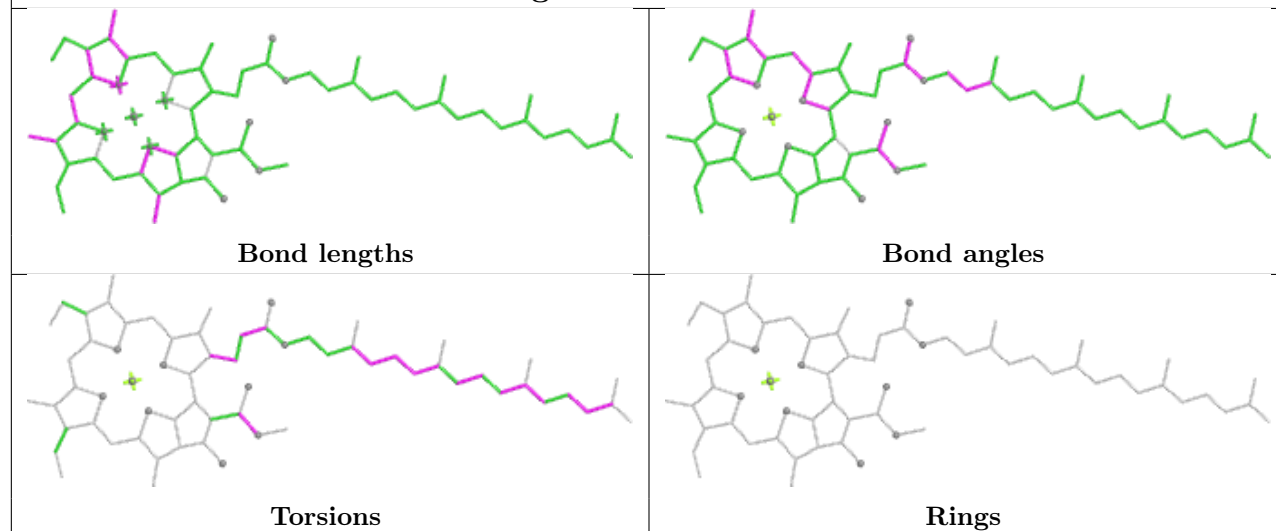
Ligand CHL 2 307



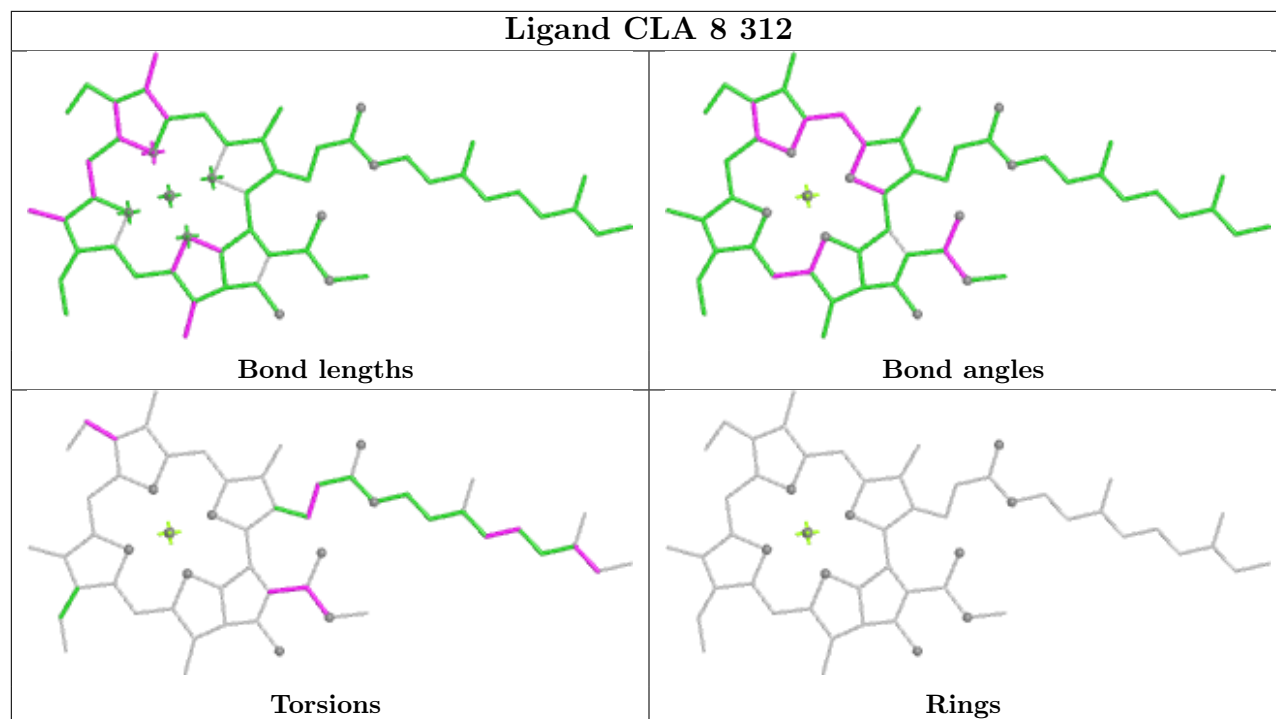
Ligand CLA 4 304



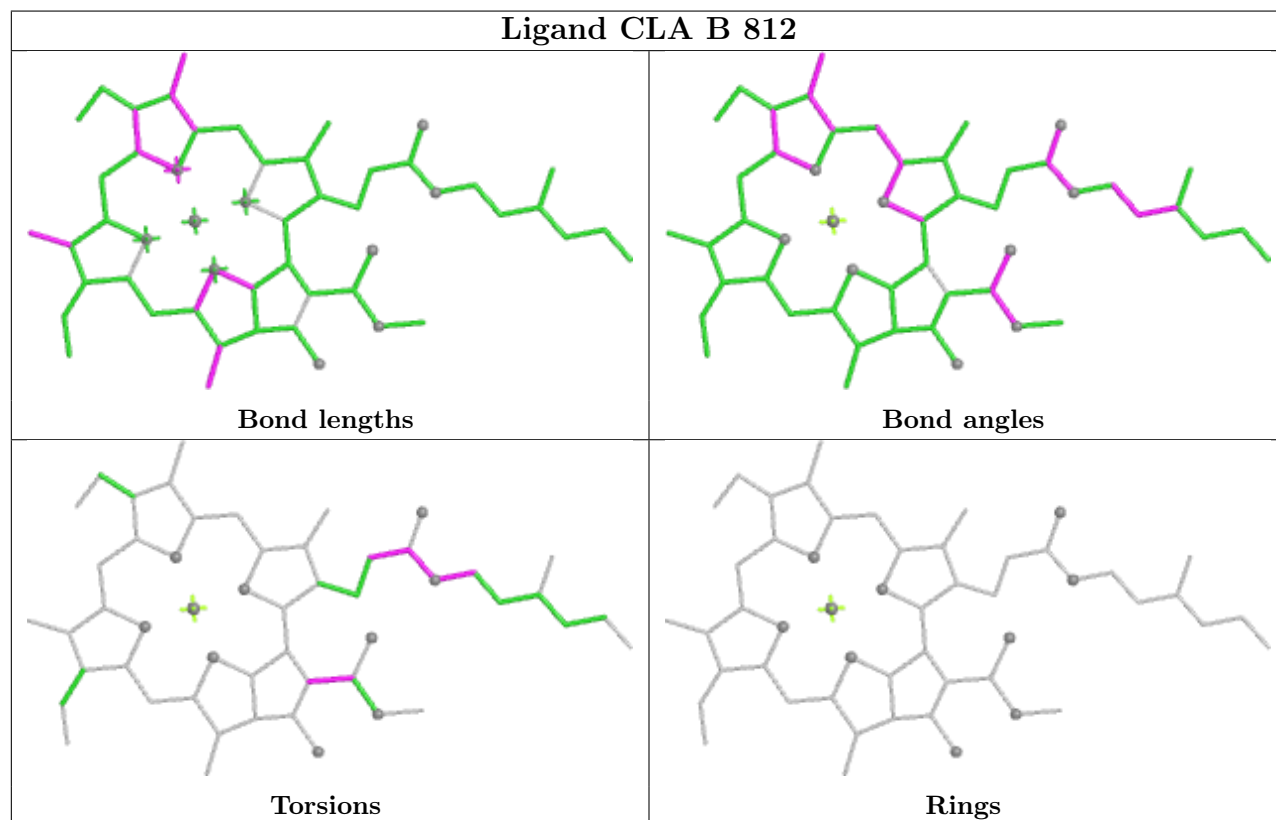
Ligand CLA B 836**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG 6 603****Bond lengths****Bond angles****Torsions****Rings**

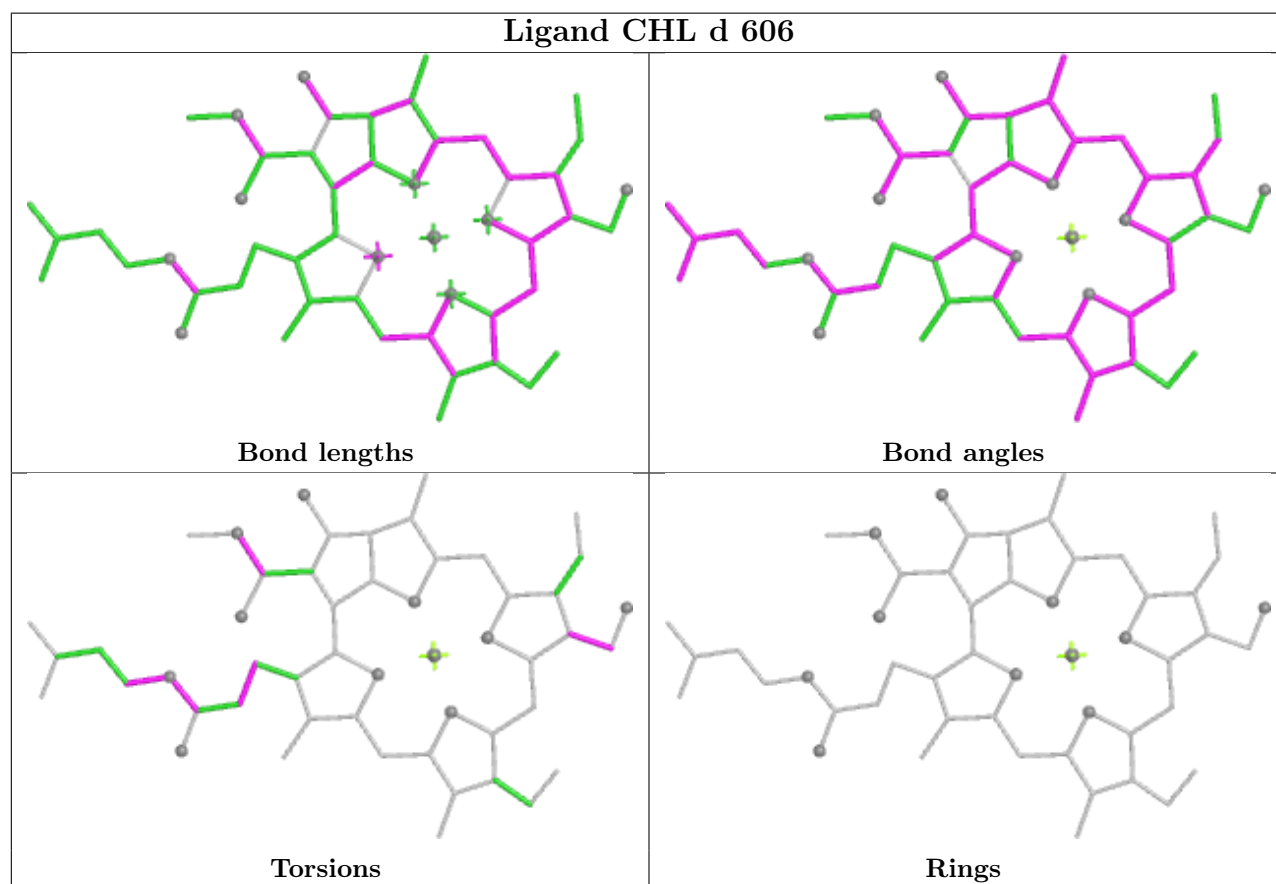
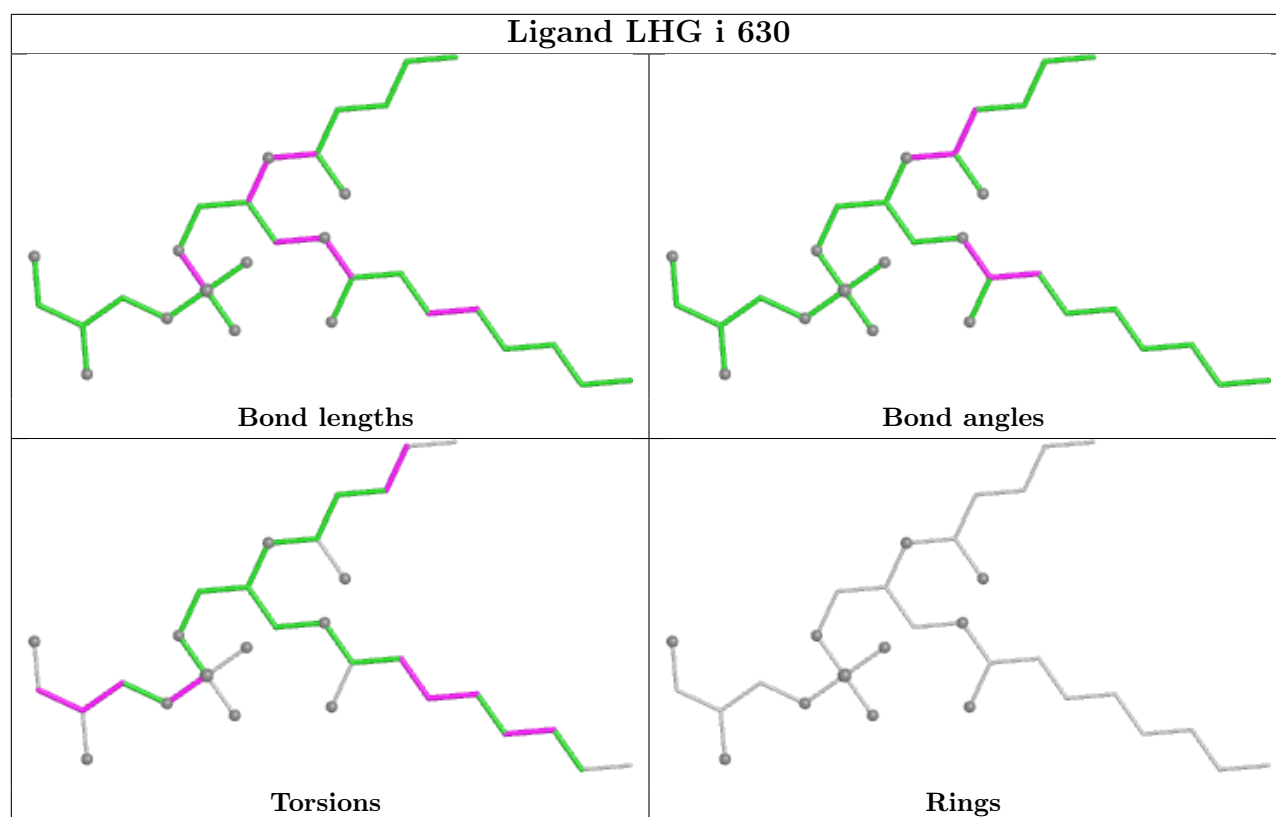
Ligand CLA 3 304**Ligand CLA A 828**

Ligand CLA 8 312

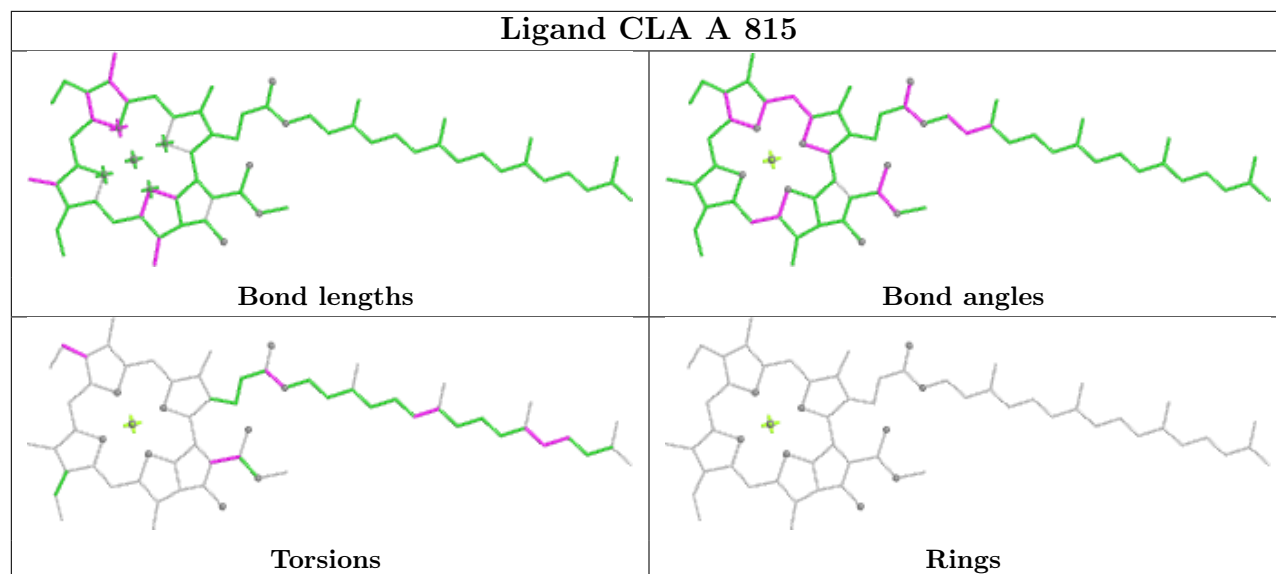


Ligand CLA B 812

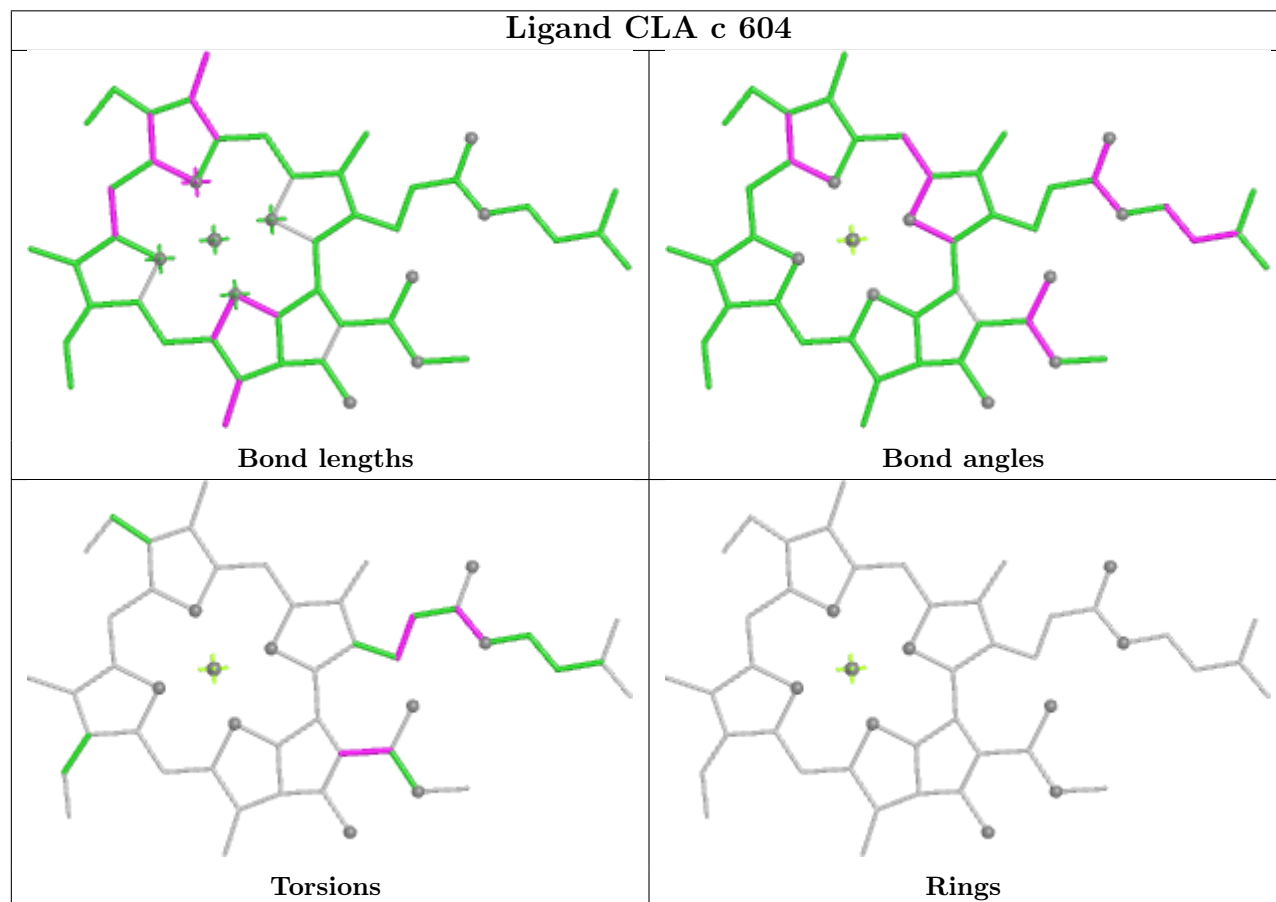




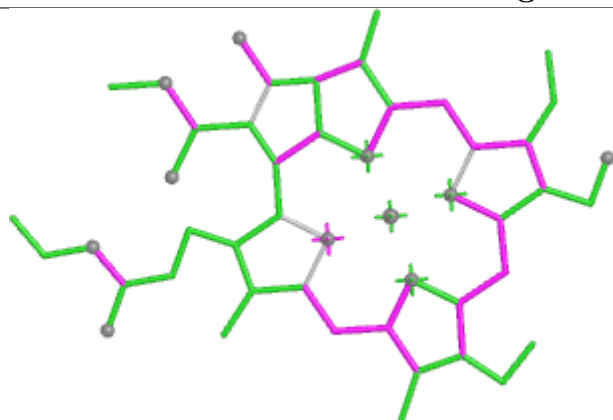
Ligand CLA A 815



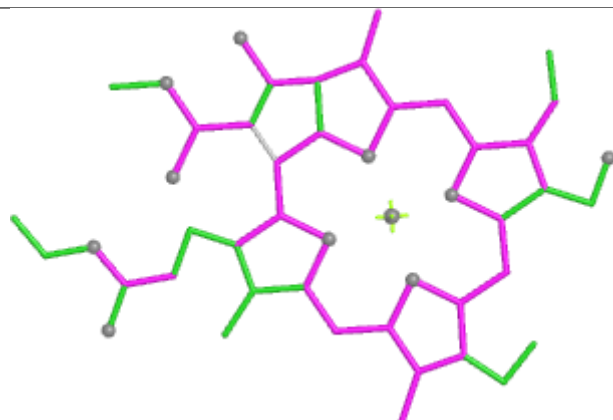
Ligand CLA c 604



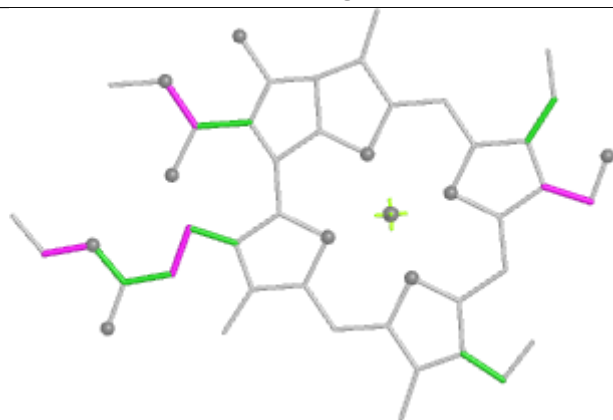
Ligand CHL 2 306



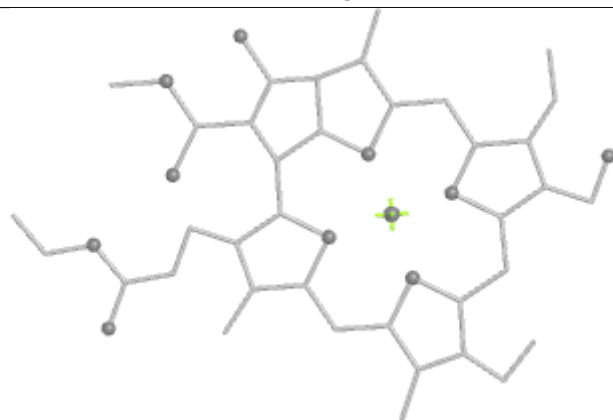
Bond lengths



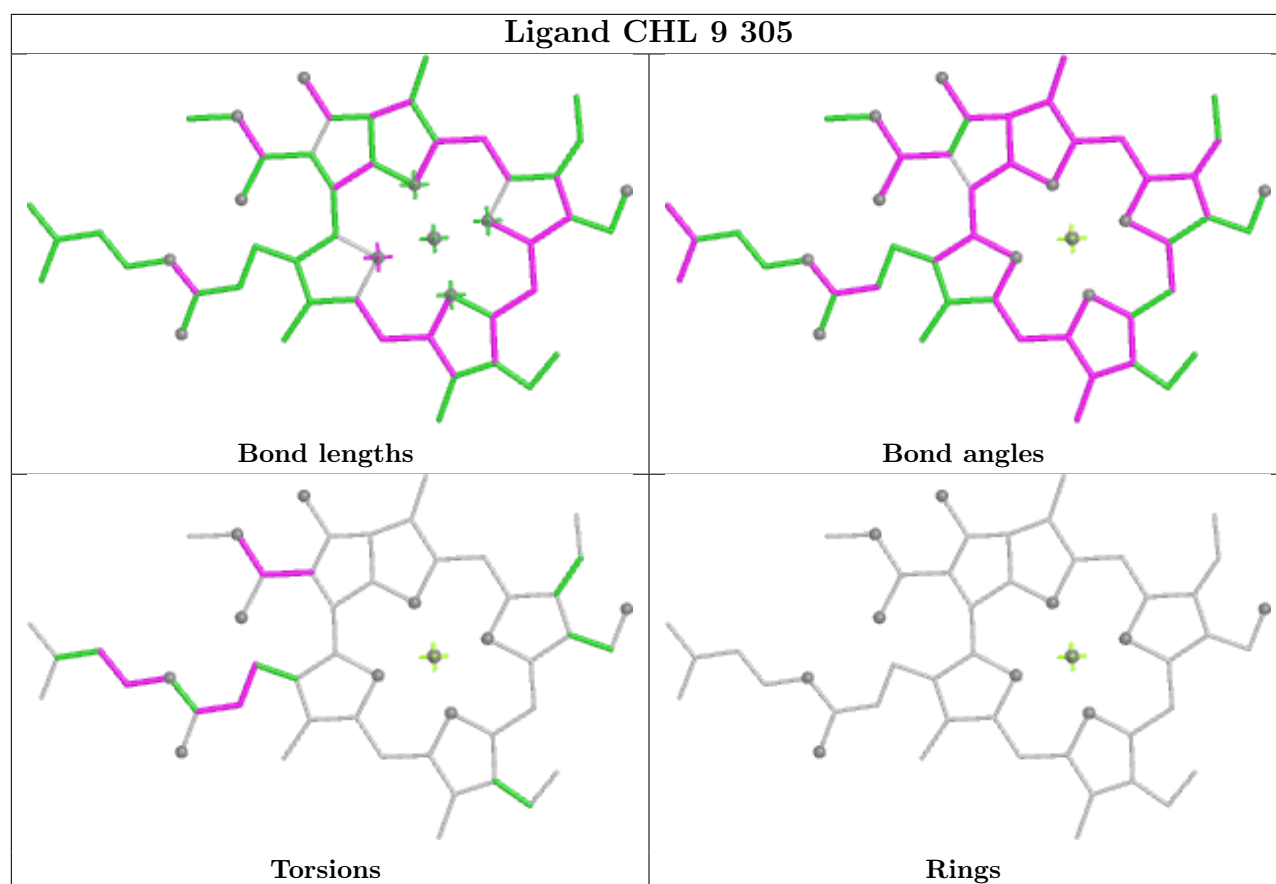
Bond angles



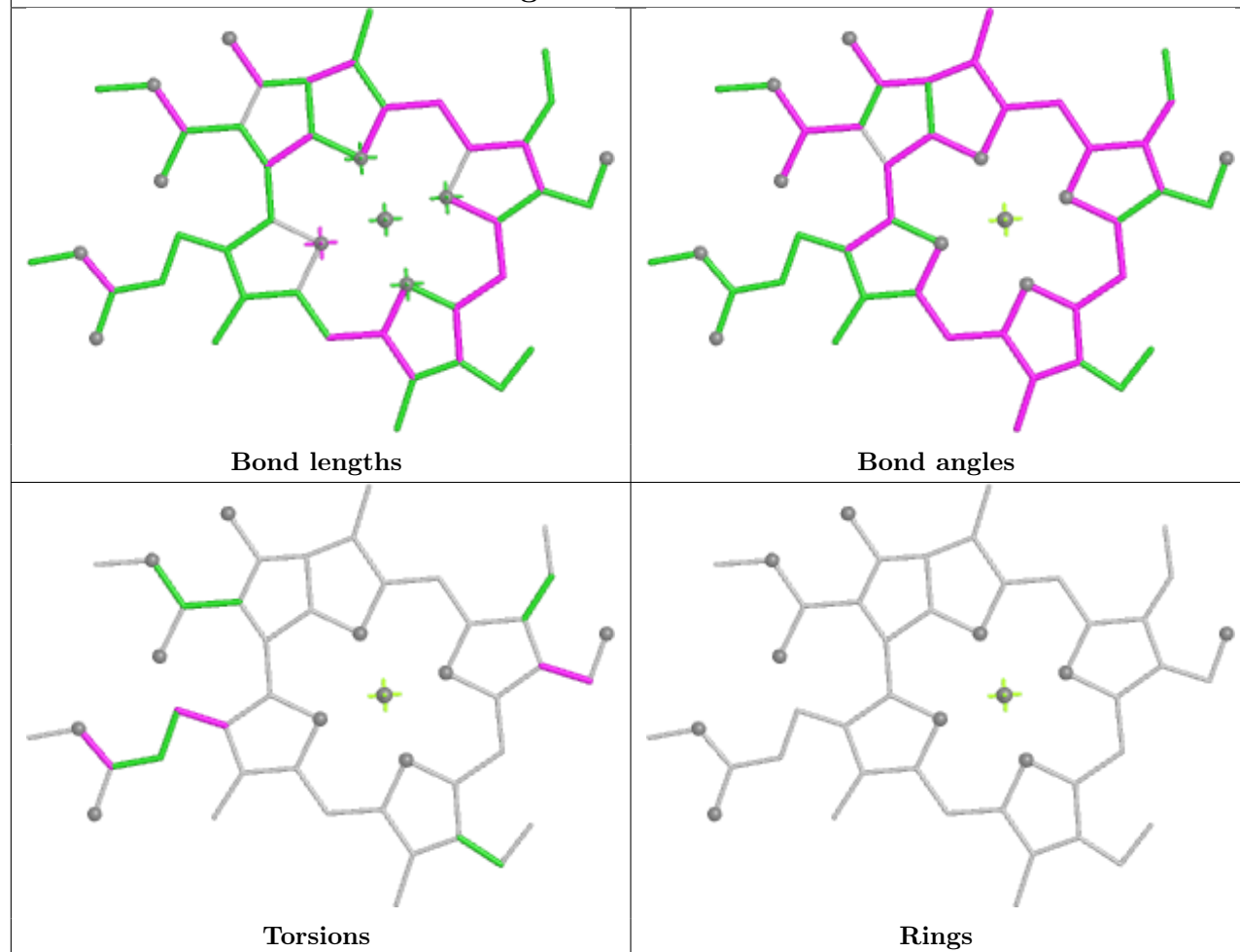
Torsions

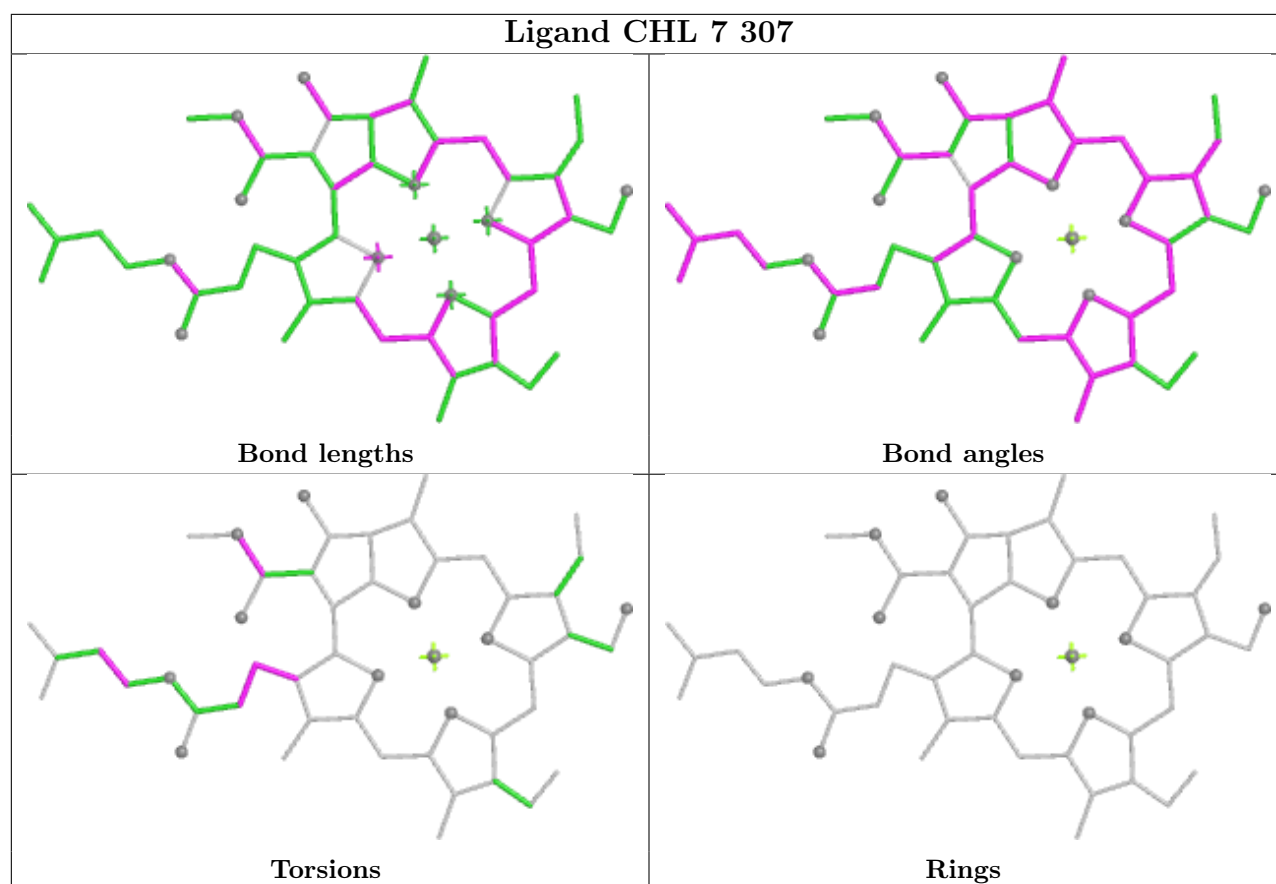


Rings

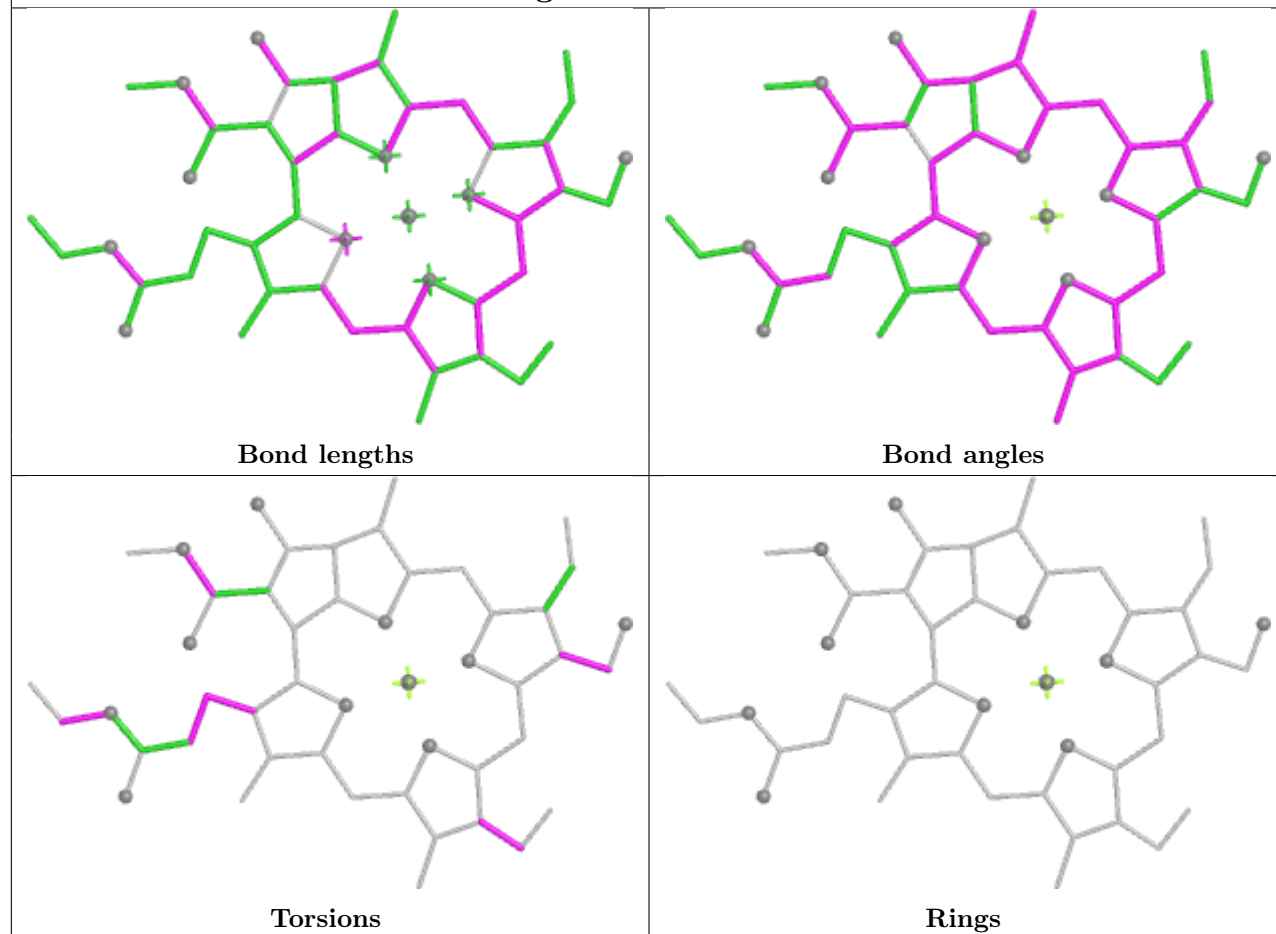


Ligand CHL 4 308

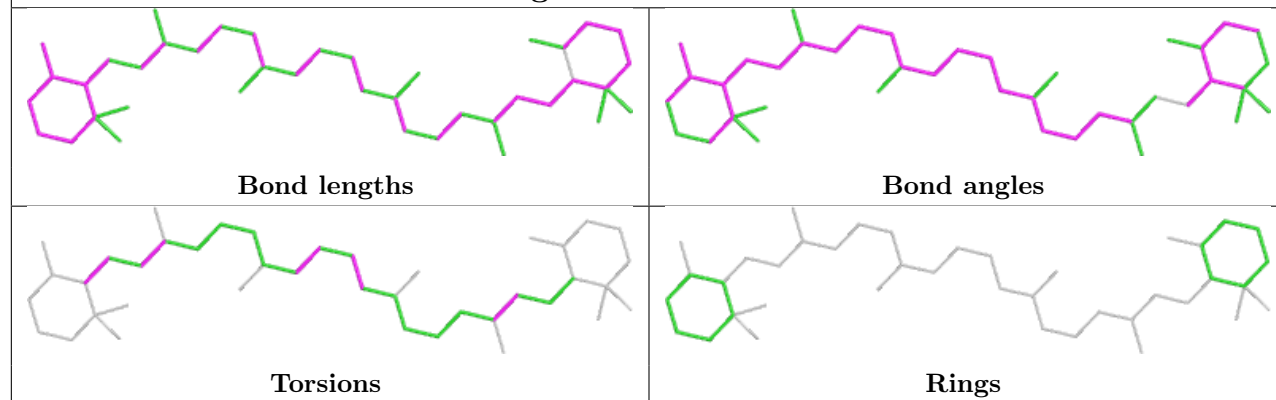




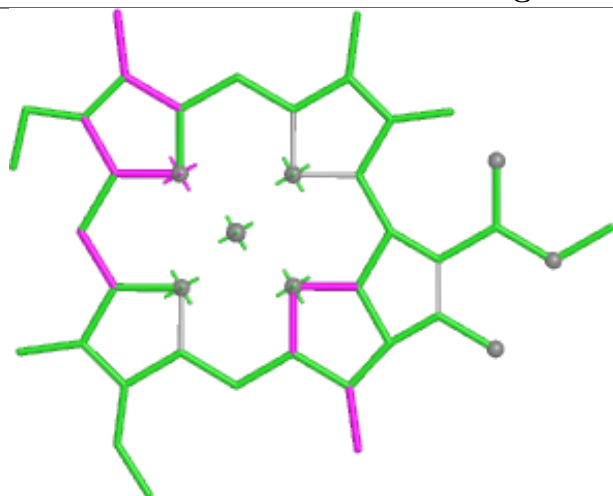
Ligand CHL 7 305



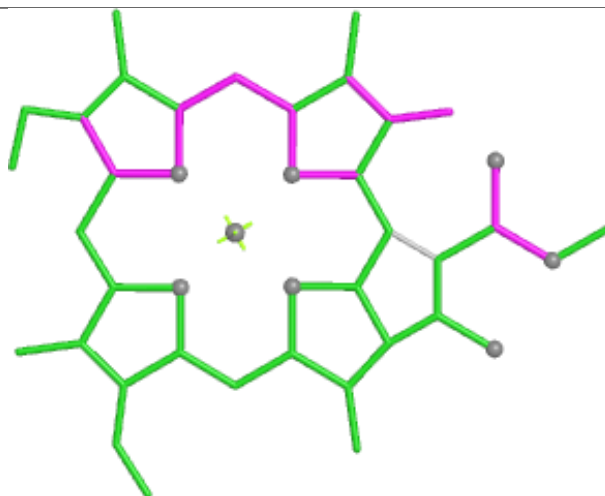
Ligand 8CT M 102



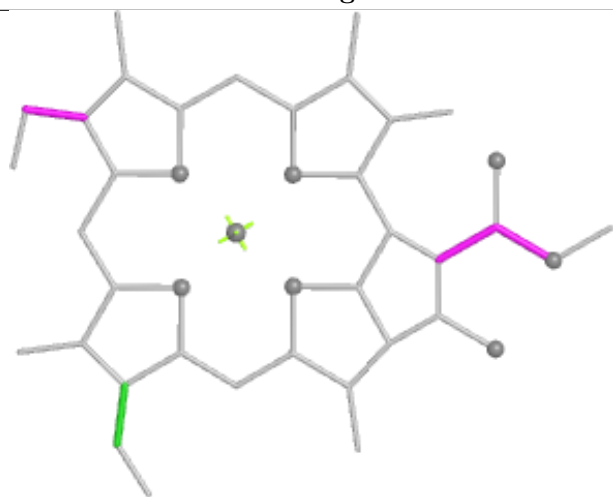
Ligand CLA O 201



Bond lengths



Bond angles

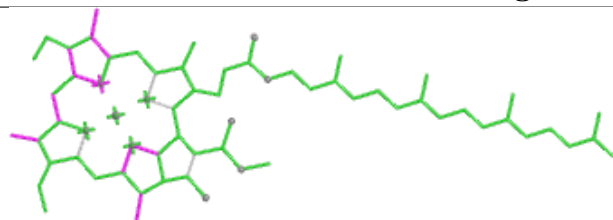


Torsions

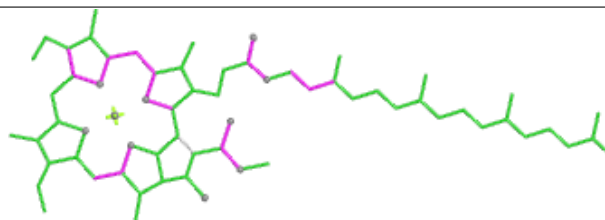


Rings

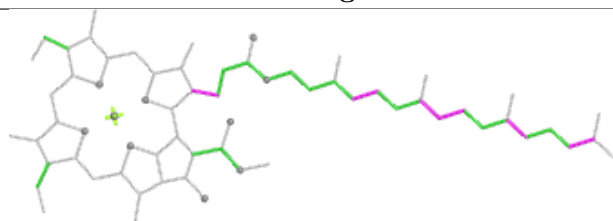
Ligand CLA A 803



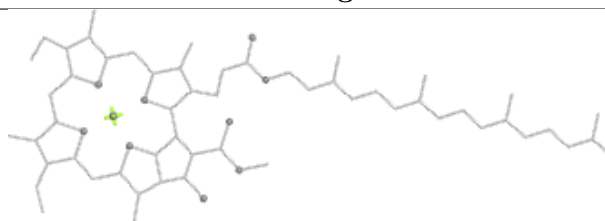
Bond lengths



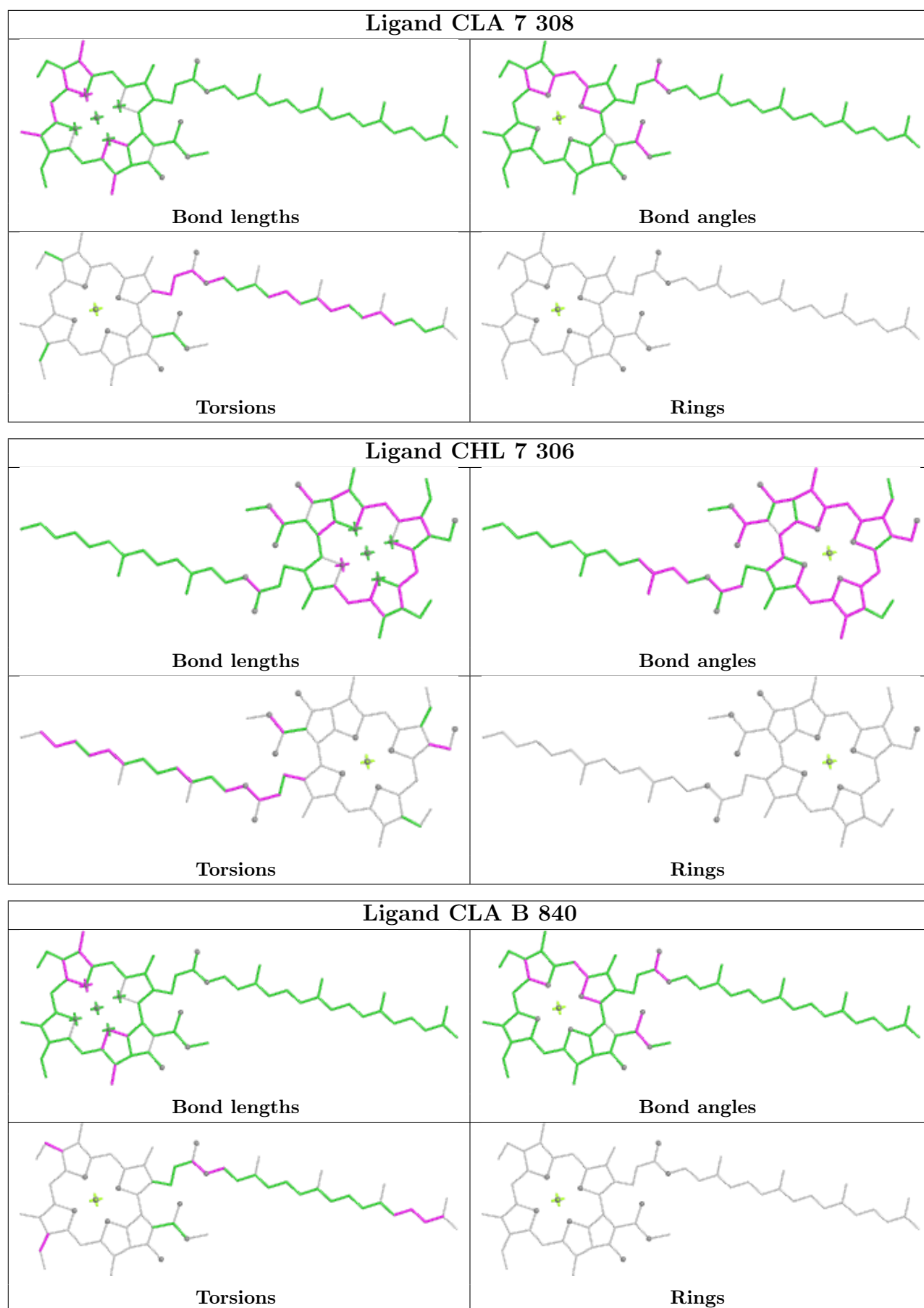
Bond angles



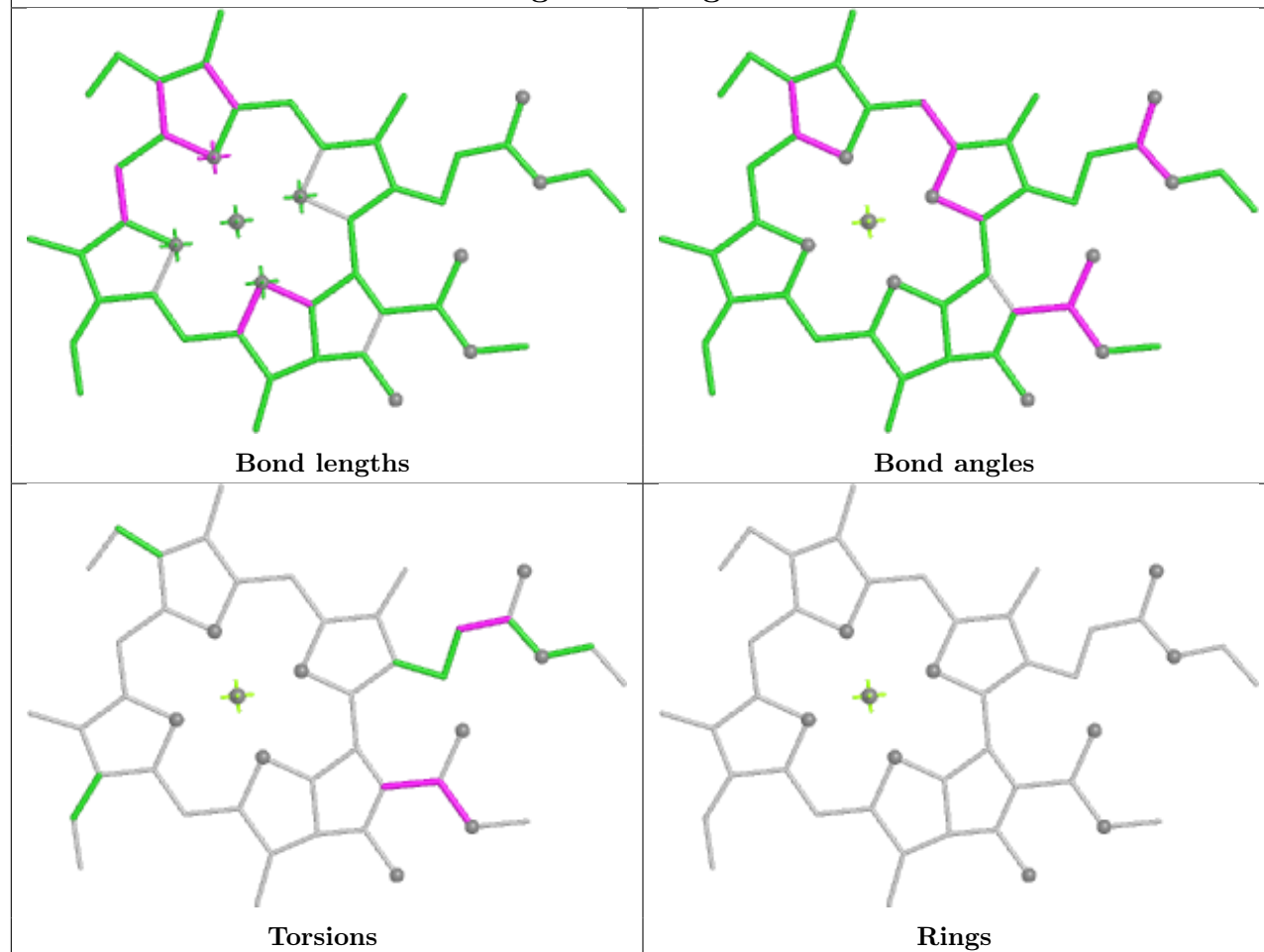
Torsions



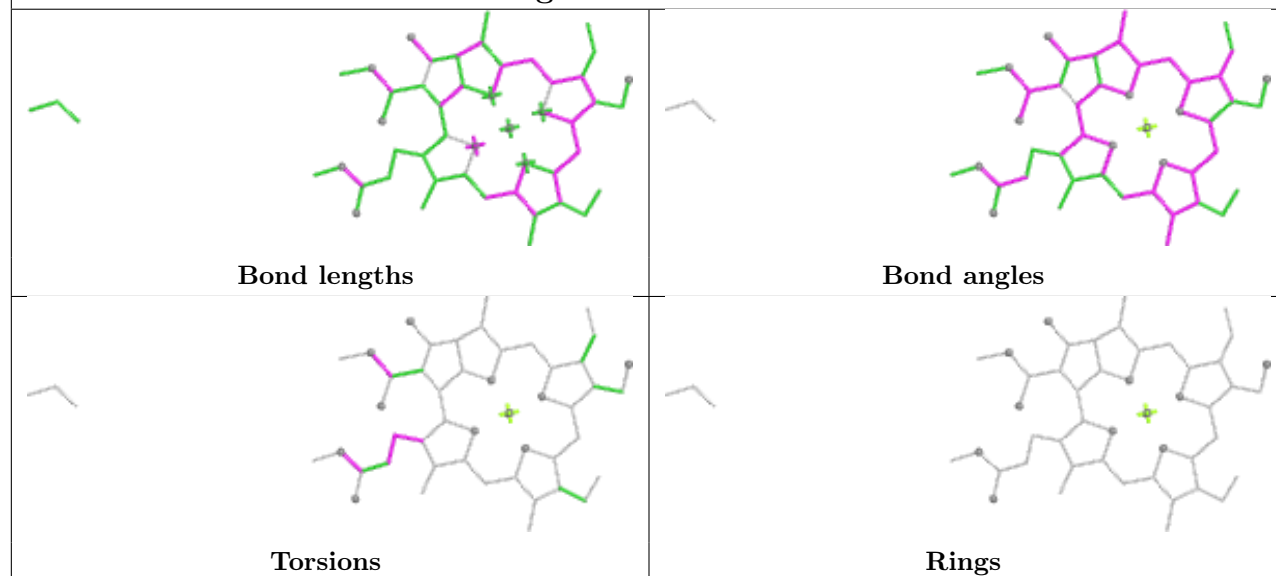
Rings

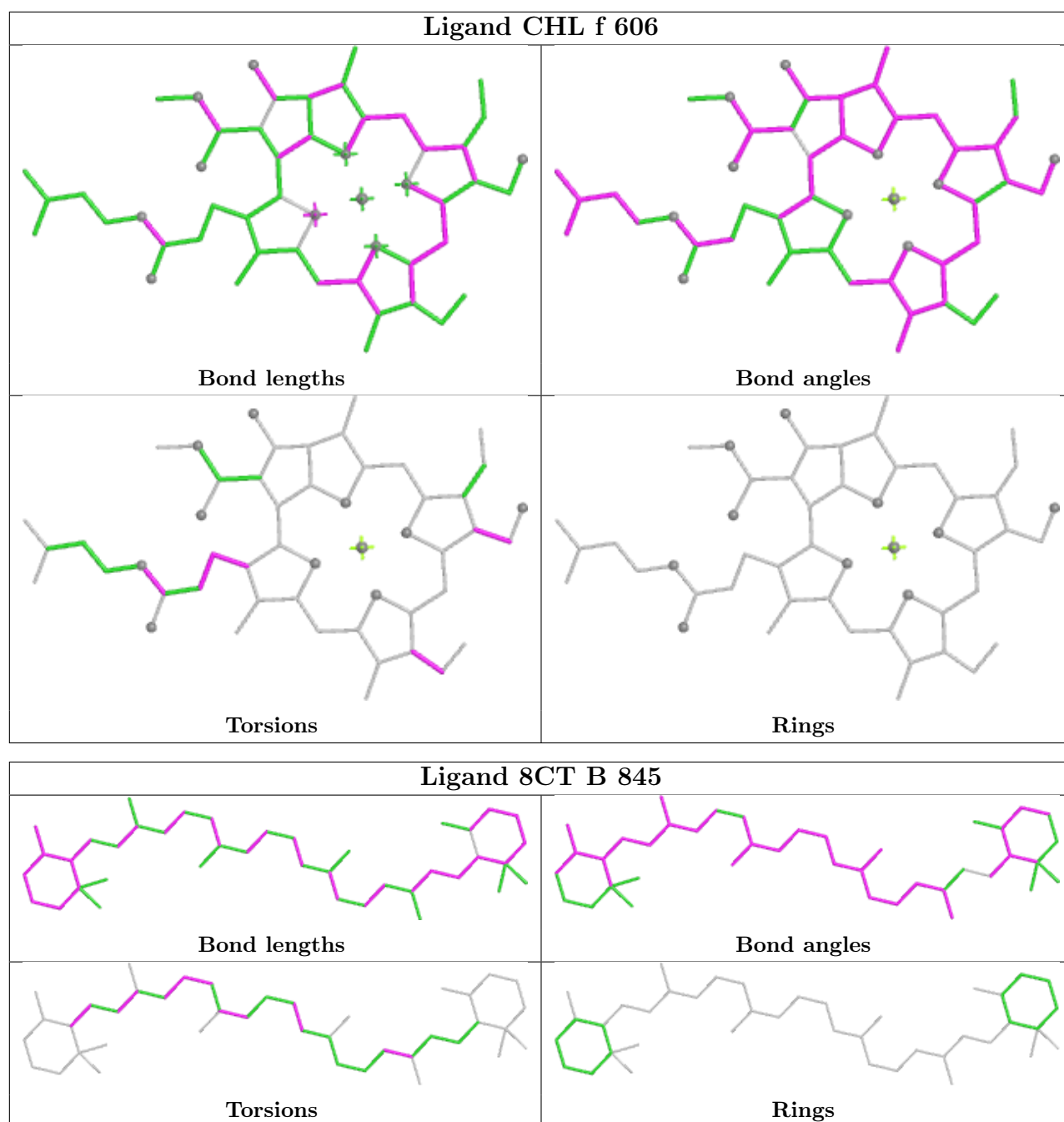


Ligand CLA g 613

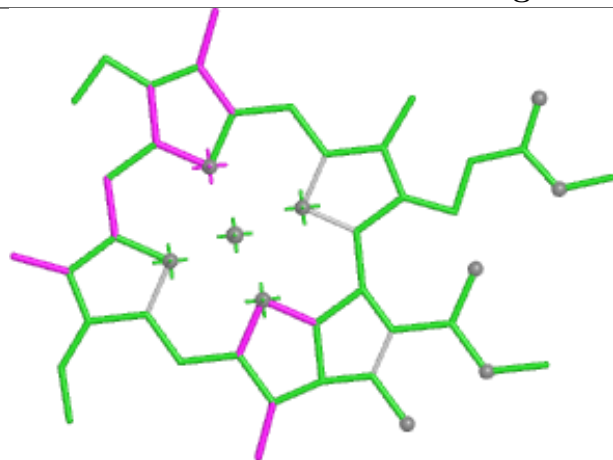


Ligand CHL a 607

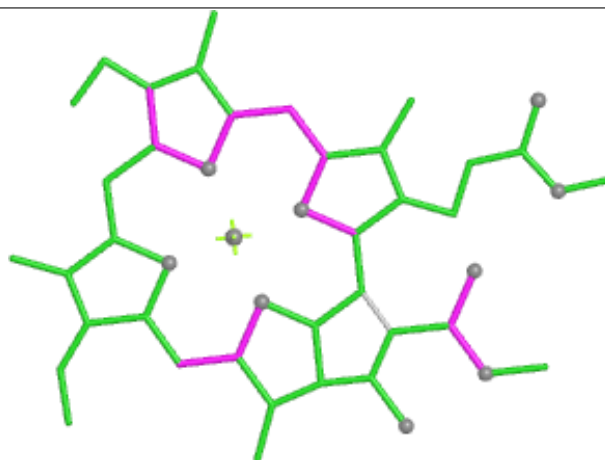




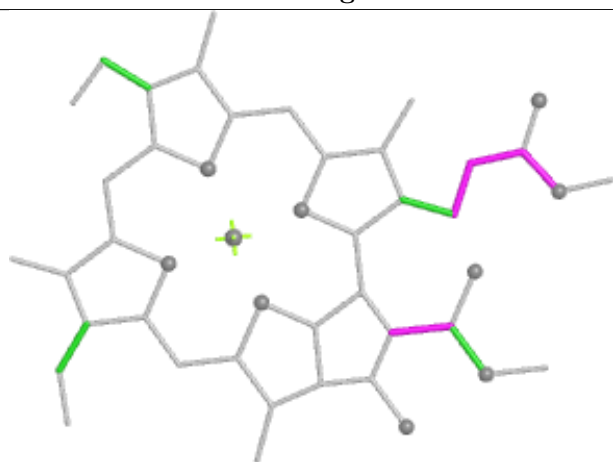
Ligand CLA K 104



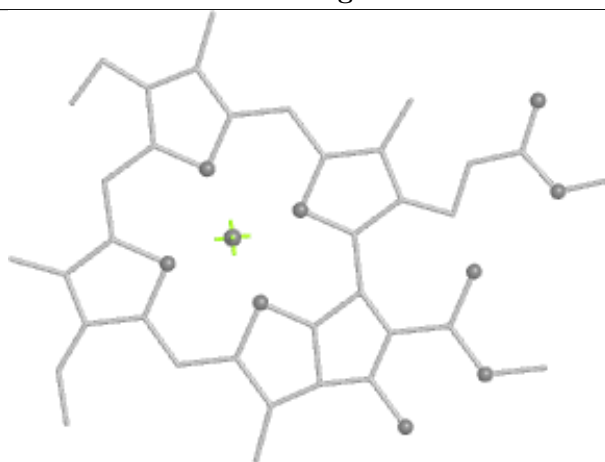
Bond lengths



Bond angles

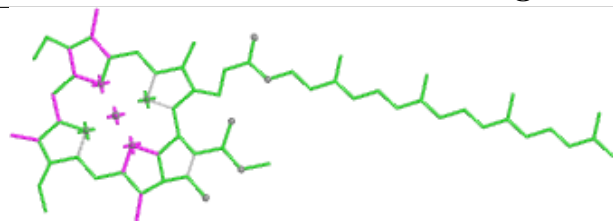


Torsions

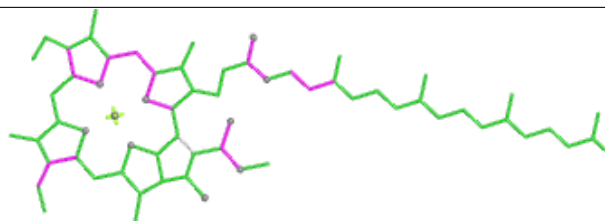


Rings

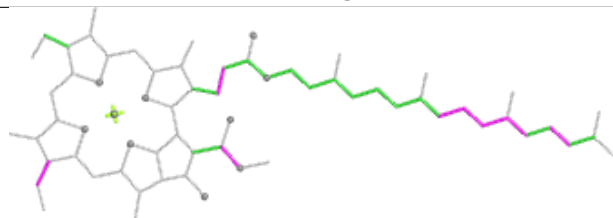
Ligand CLA B 806



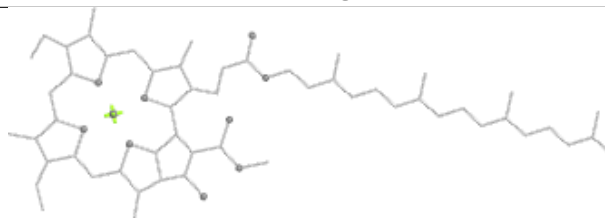
Bond lengths



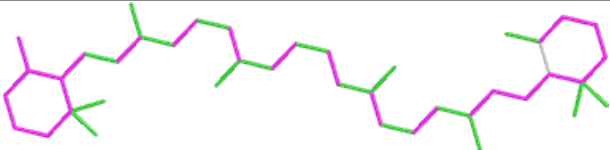
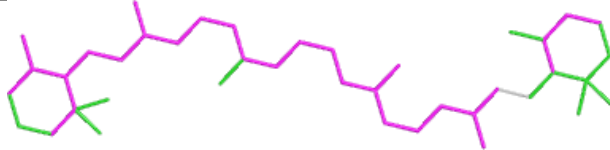
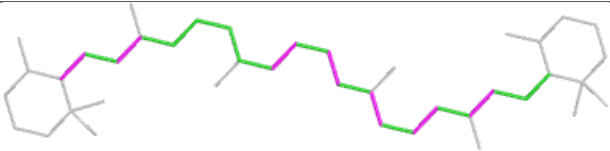
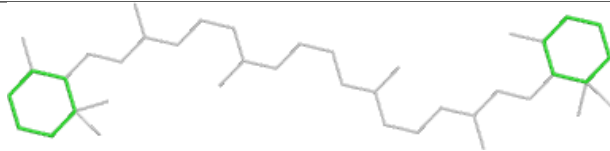
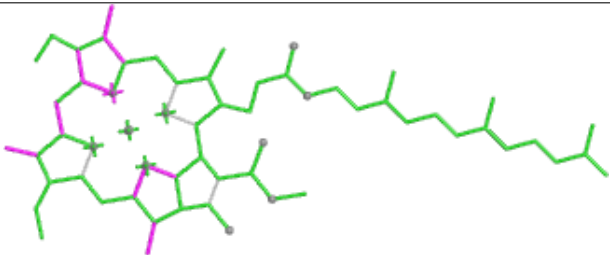
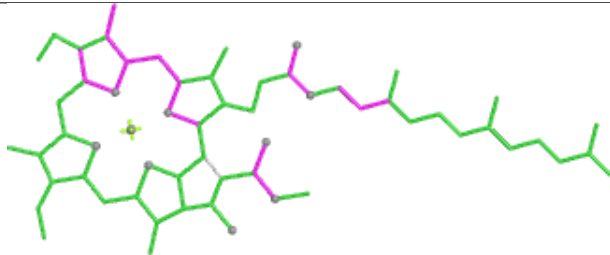
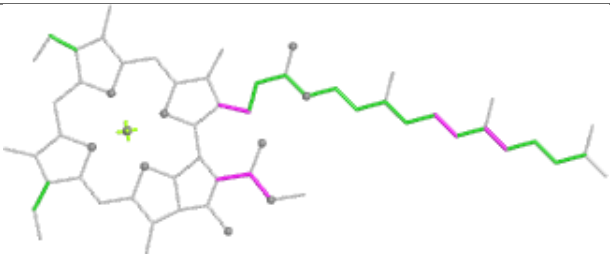
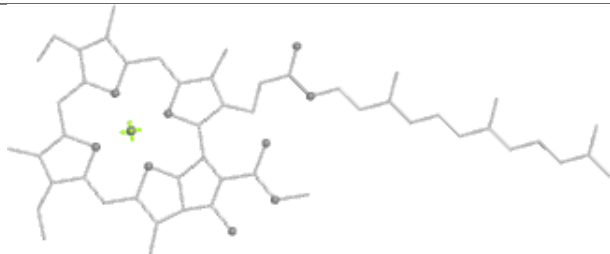
Bond angles

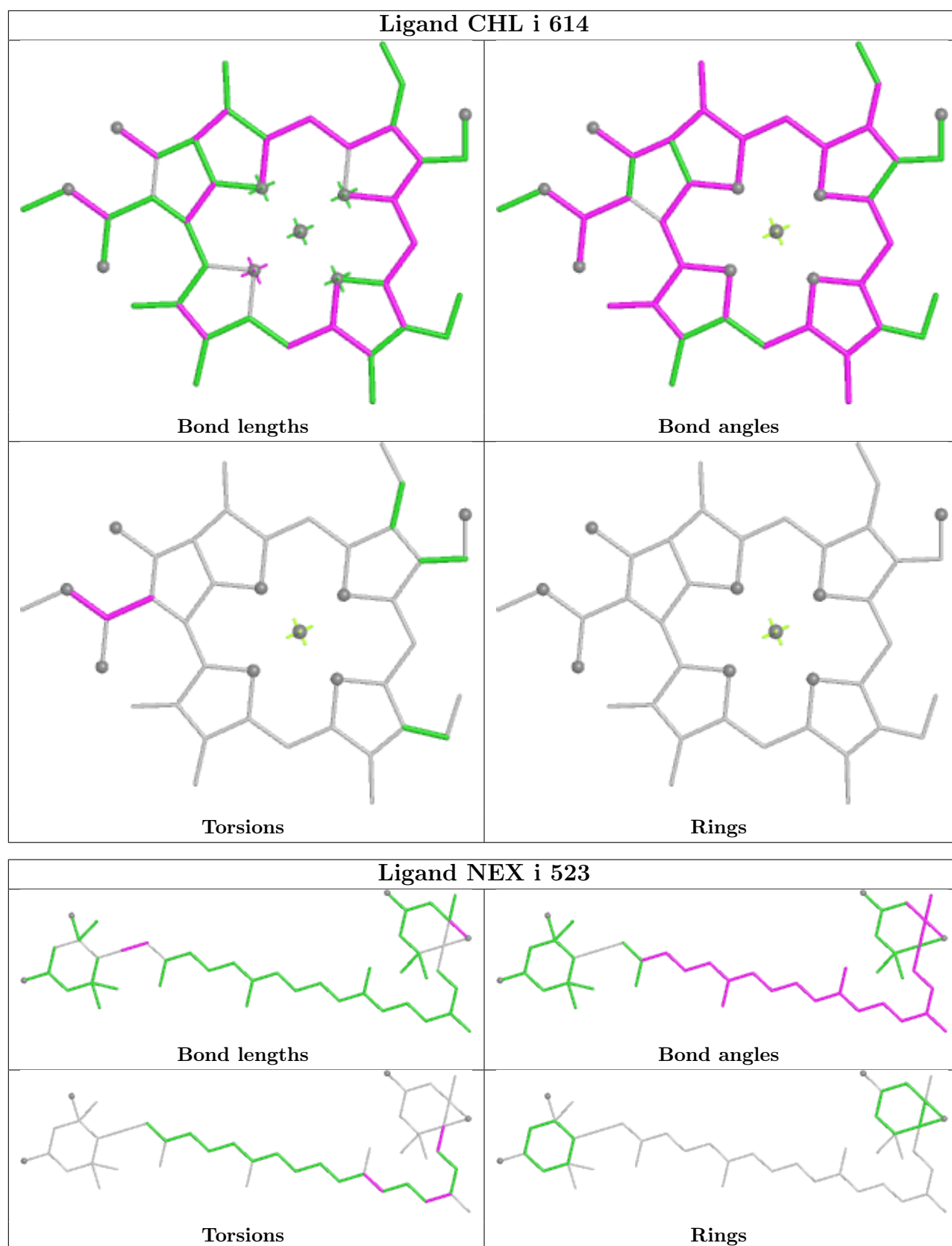


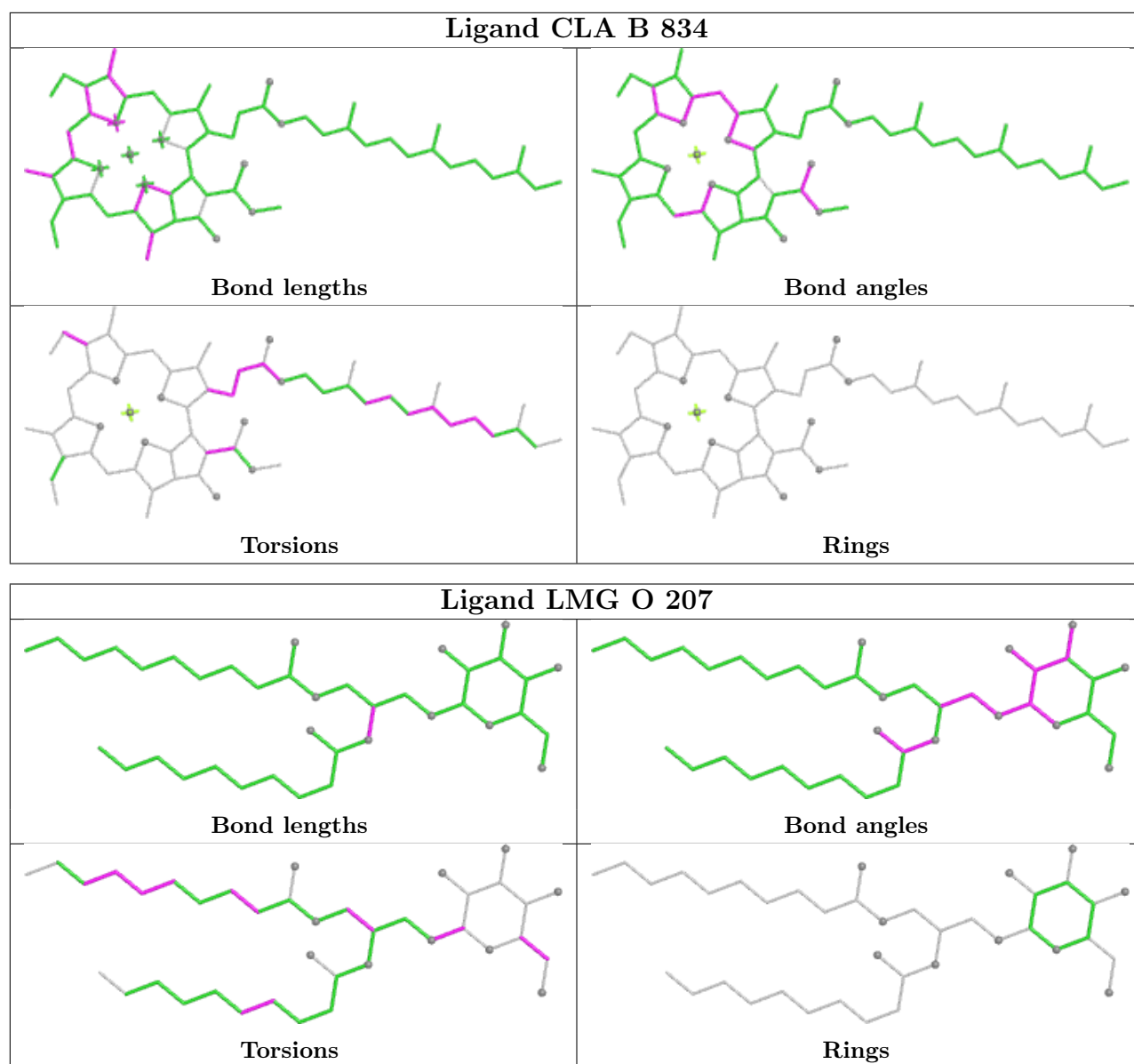
Torsions

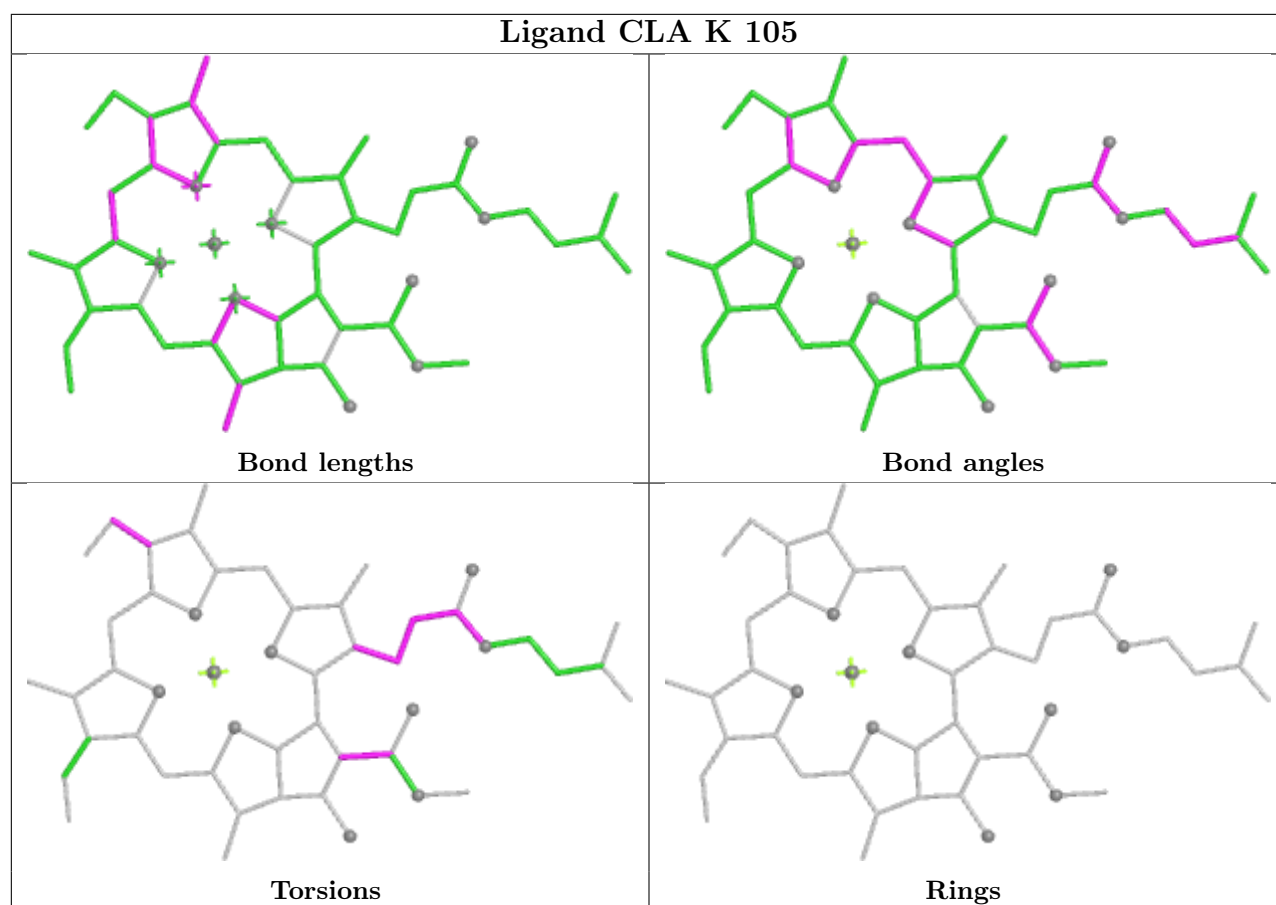


Rings

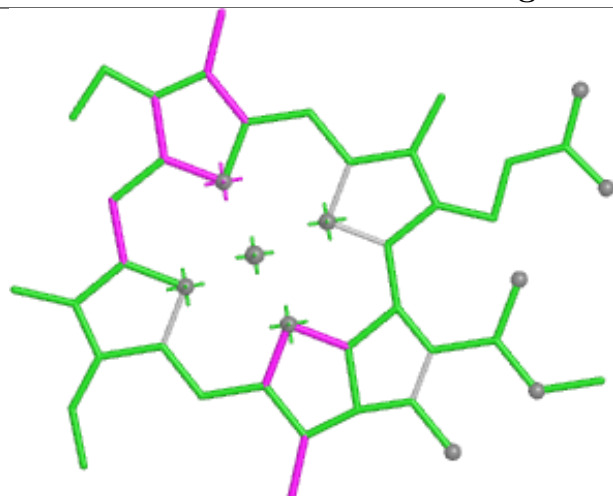
Ligand 8CT A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 8 309	
 Bond lengths	 Bond angles
 Torsions	 Rings



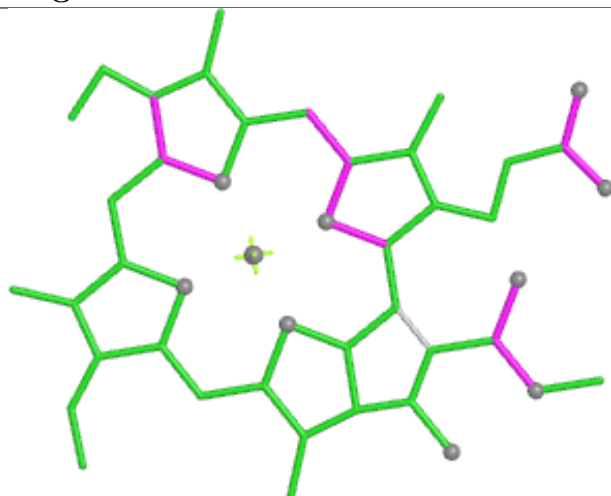




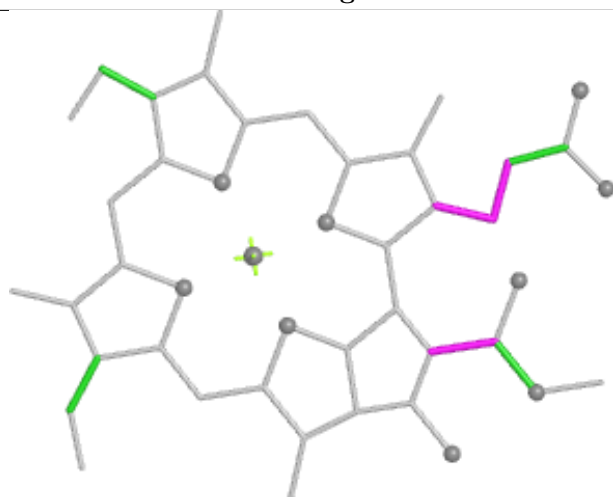
Ligand CLA g 604



Bond lengths



Bond angles

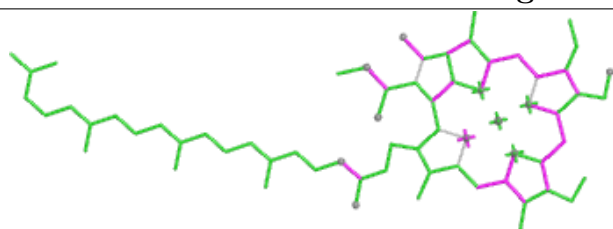


Torsions

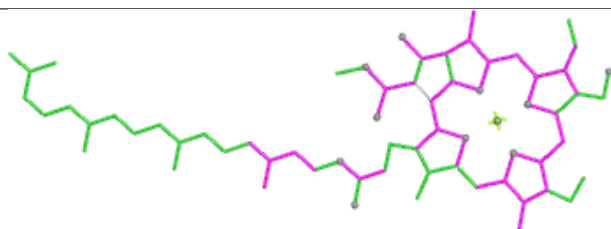


Rings

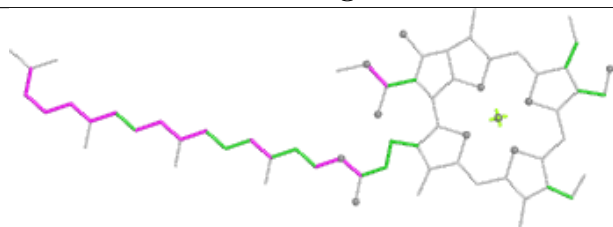
Ligand CHL d 609



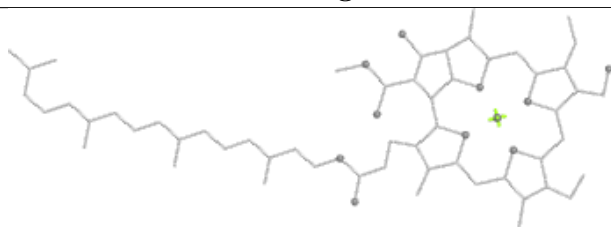
Bond lengths



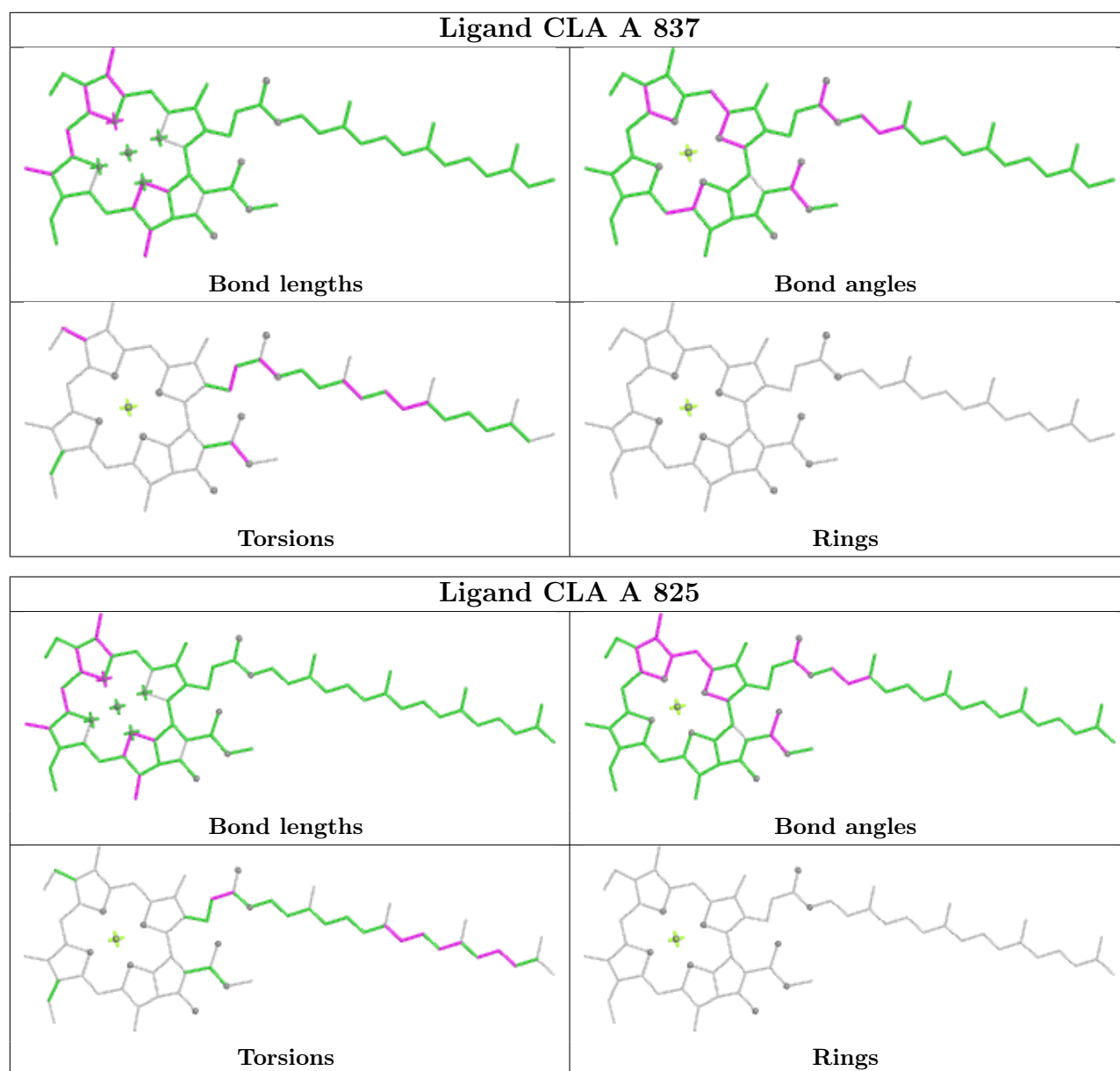
Bond angles

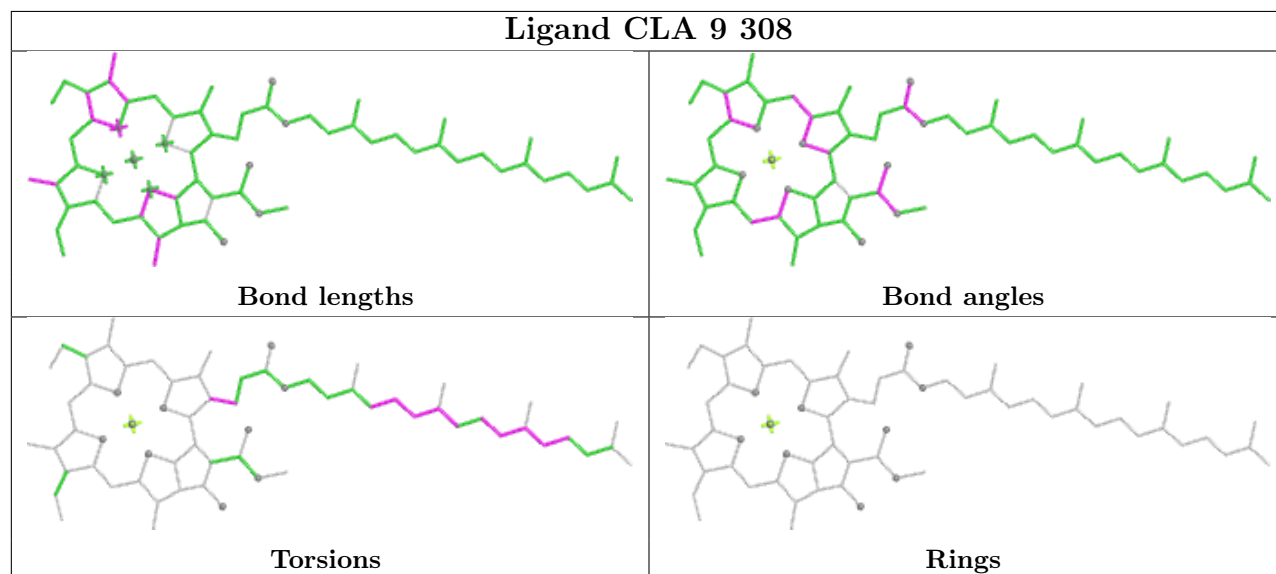
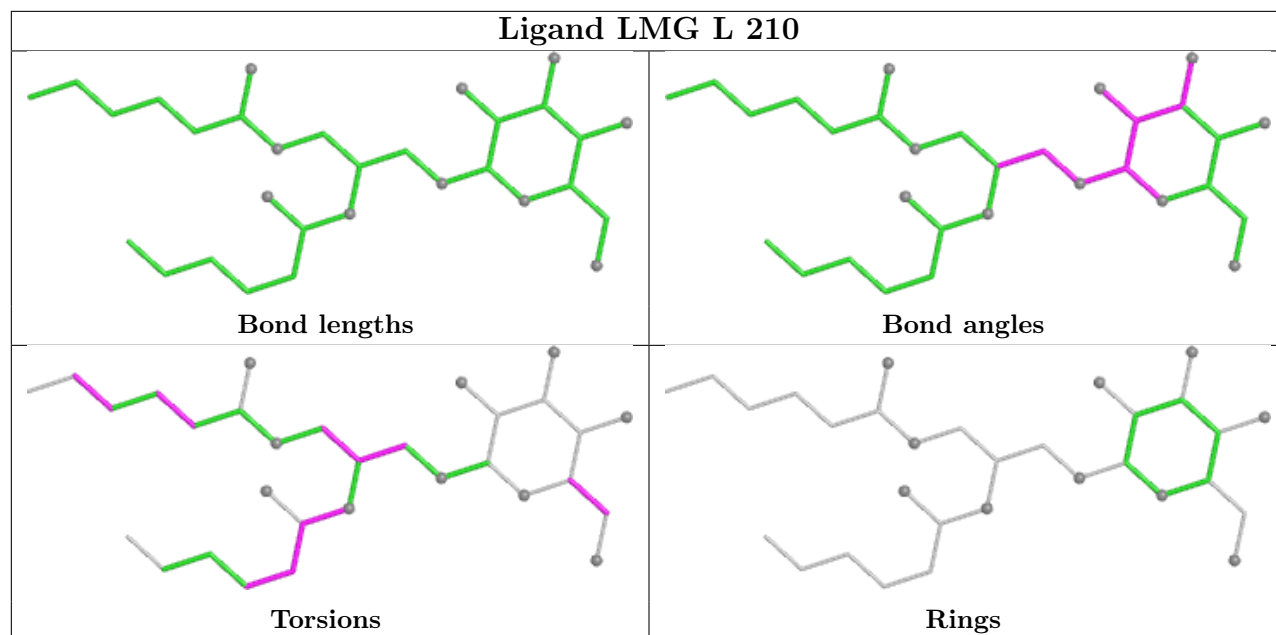


Torsions

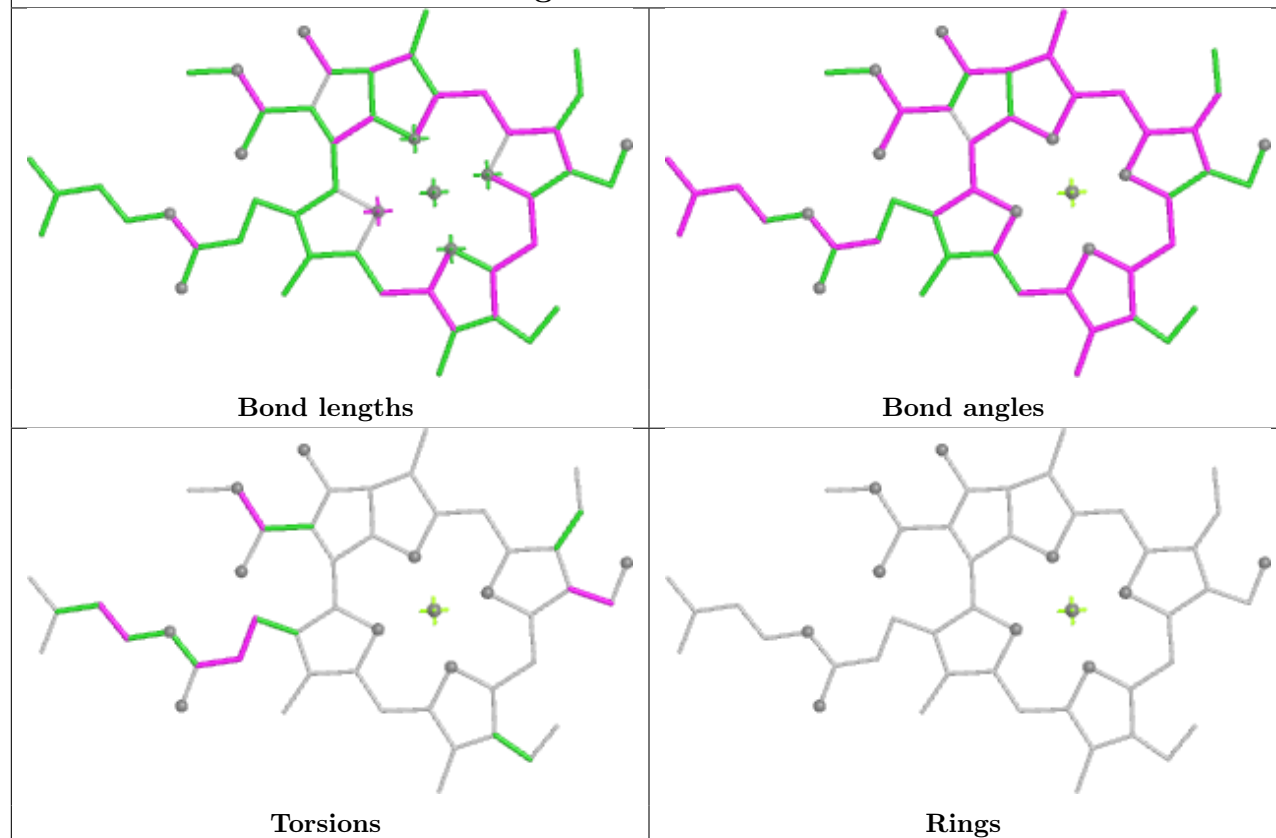


Rings

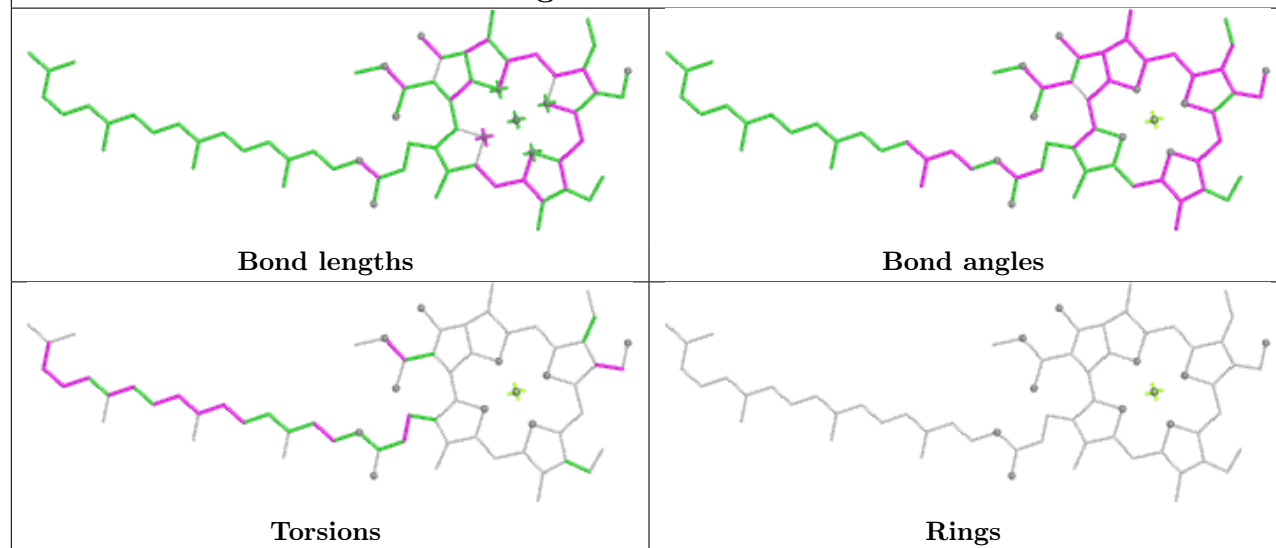




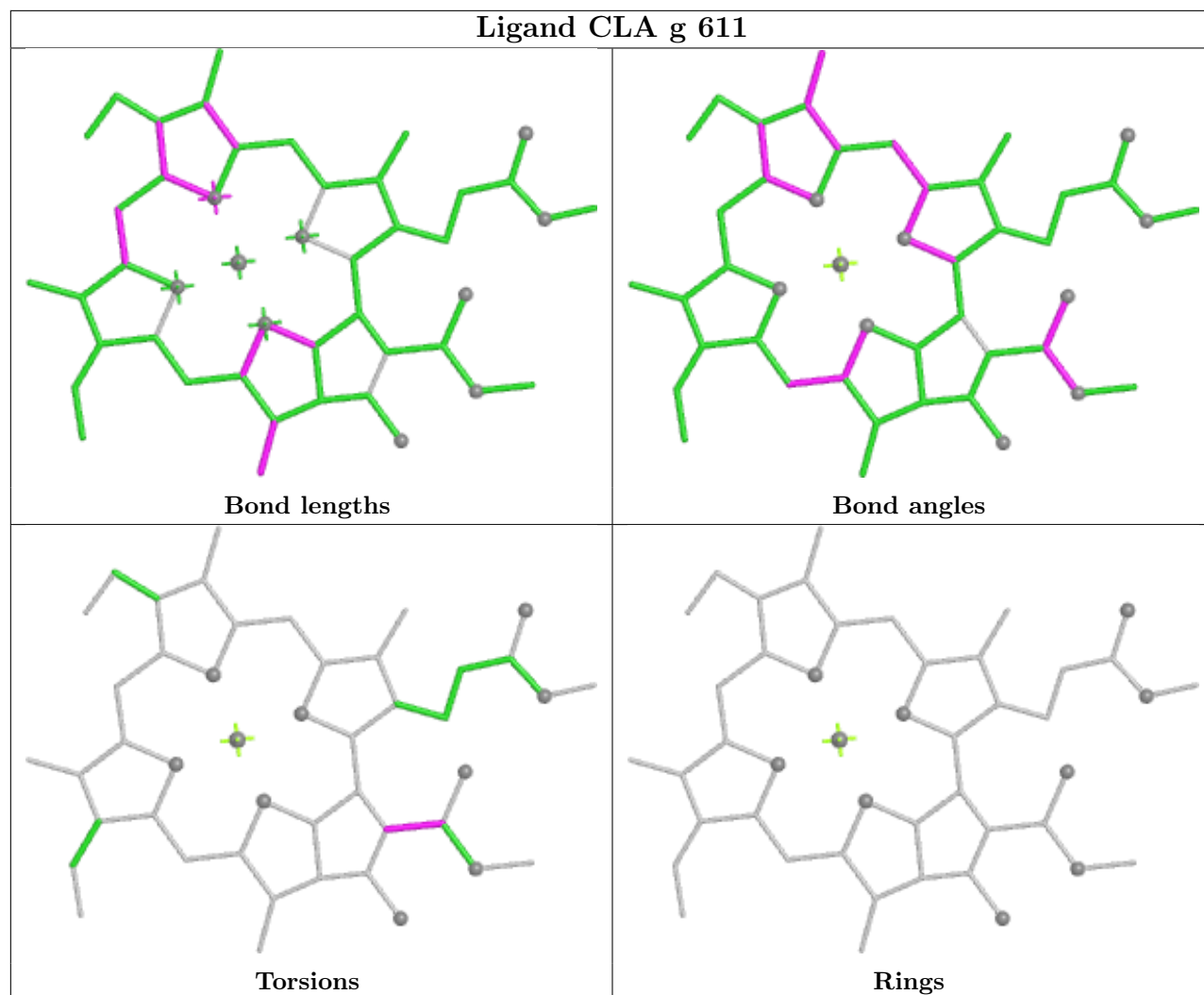
Ligand CHL h 606

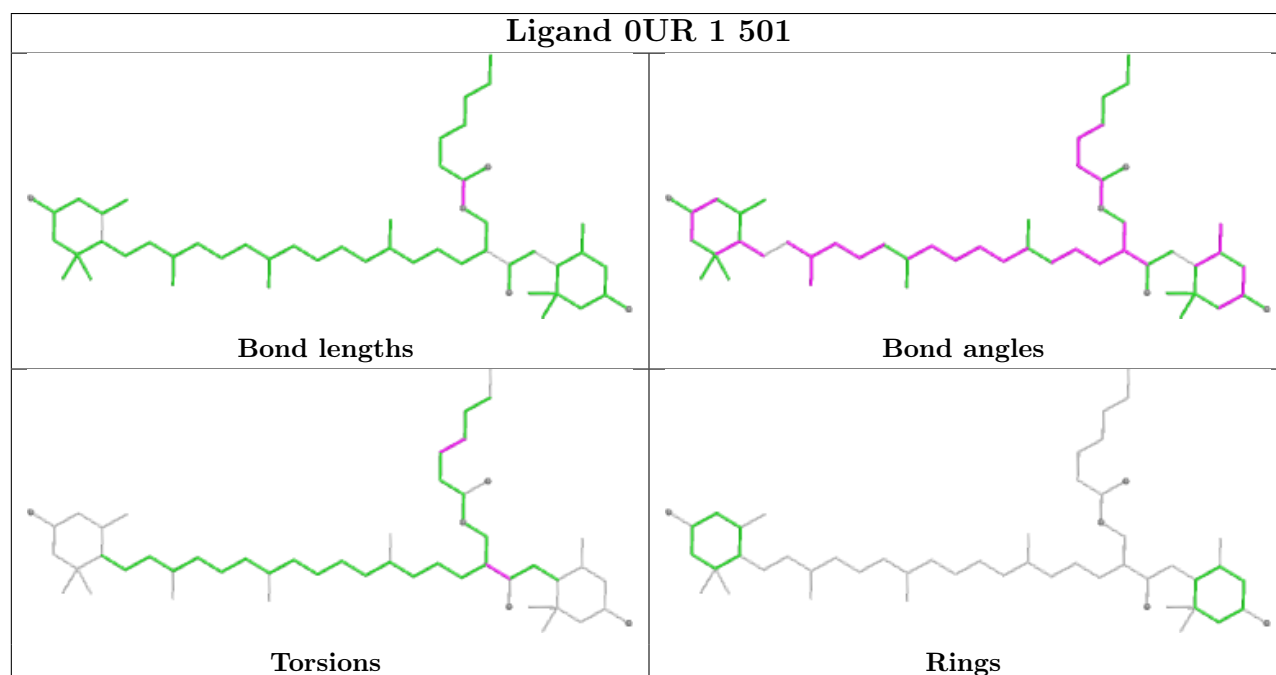
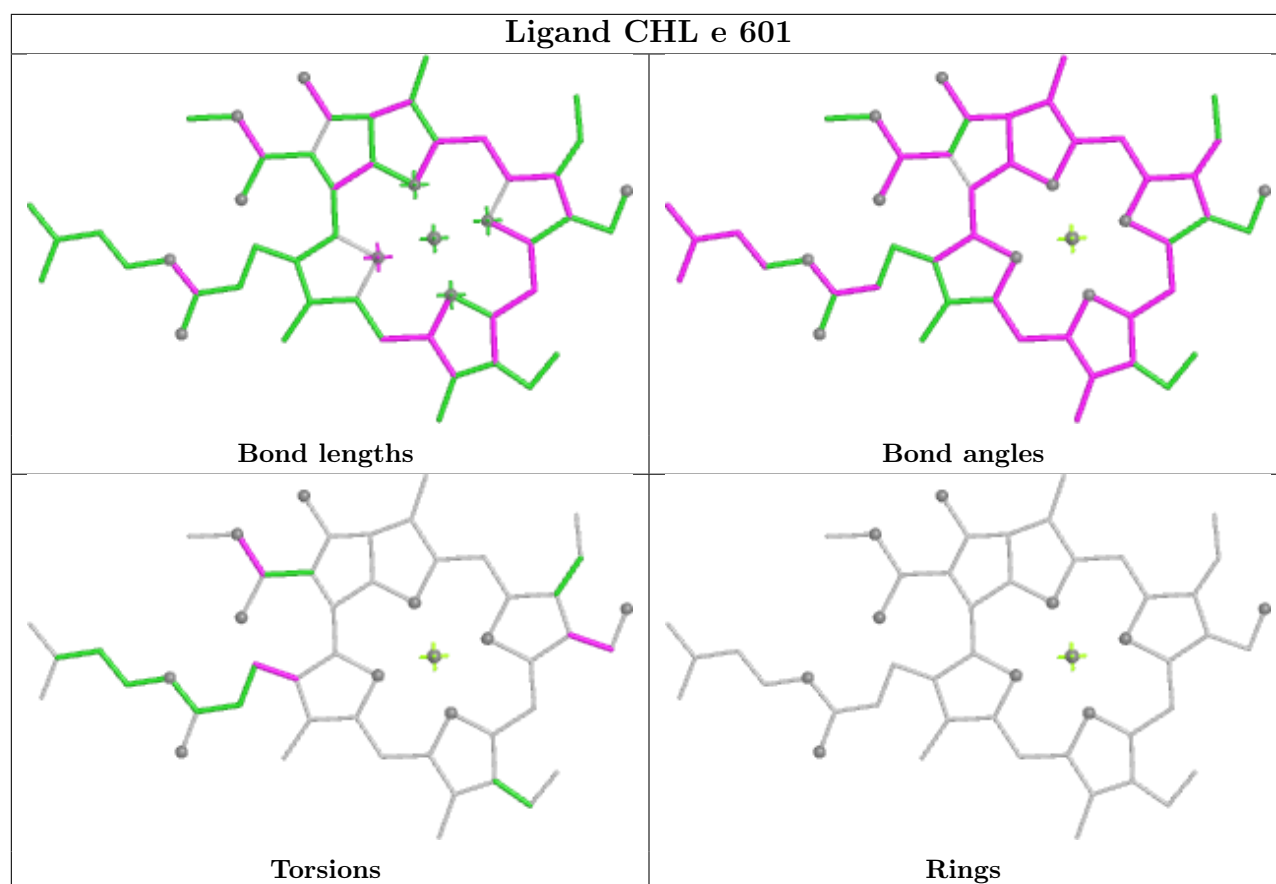


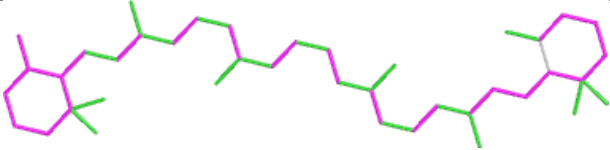
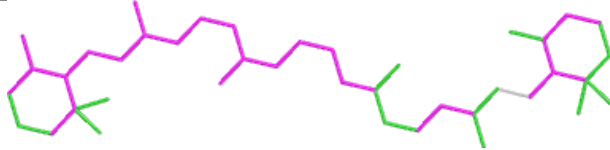
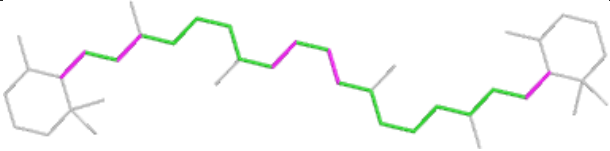
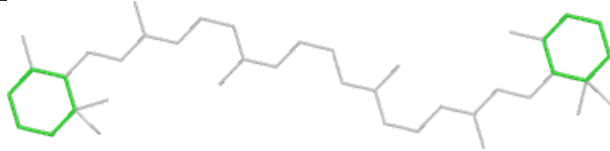
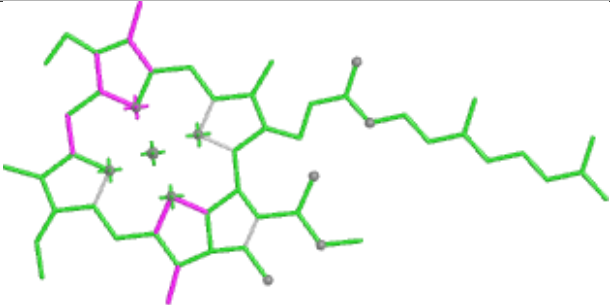
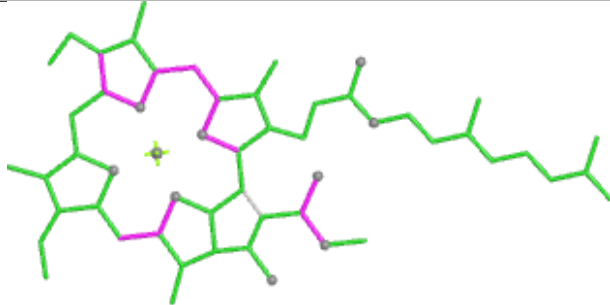
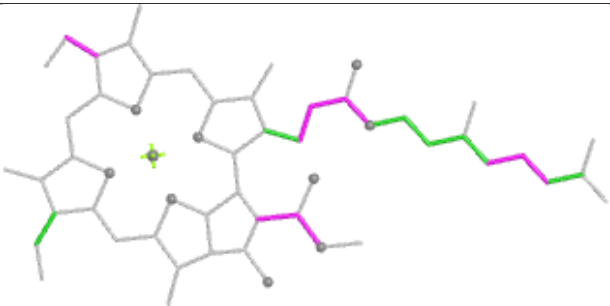
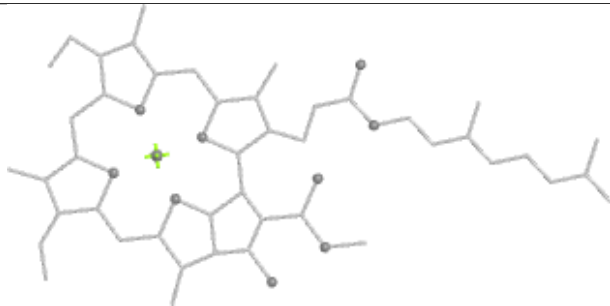
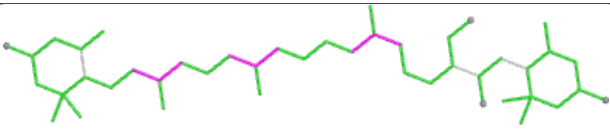
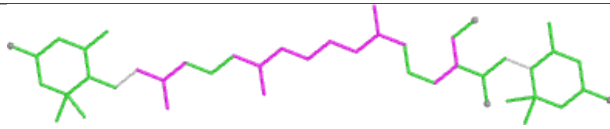
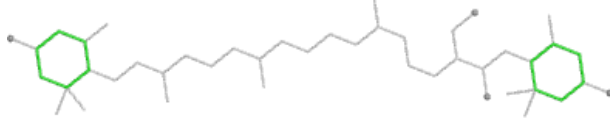
Ligand CHL e 608



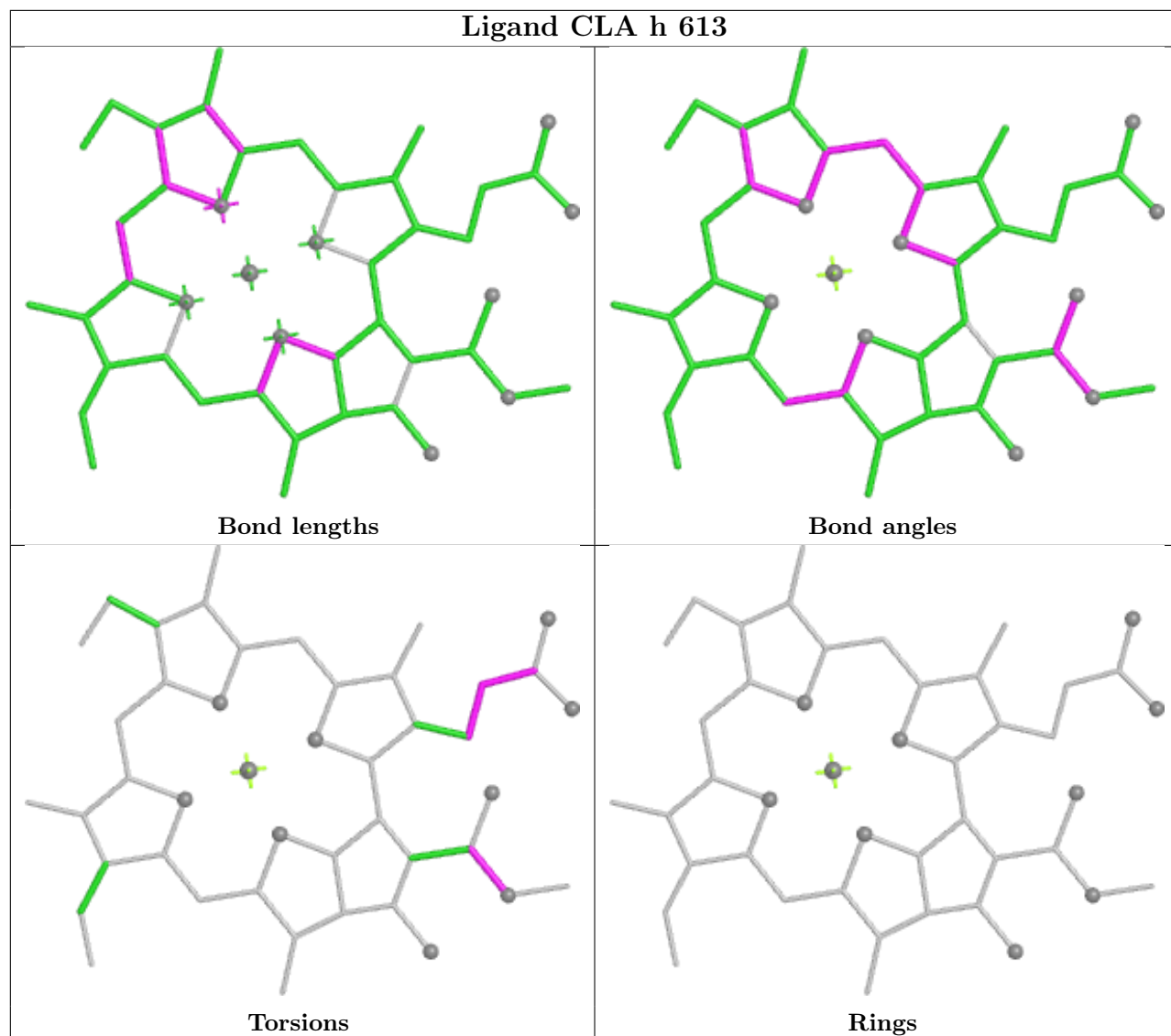
Ligand CLA g 611

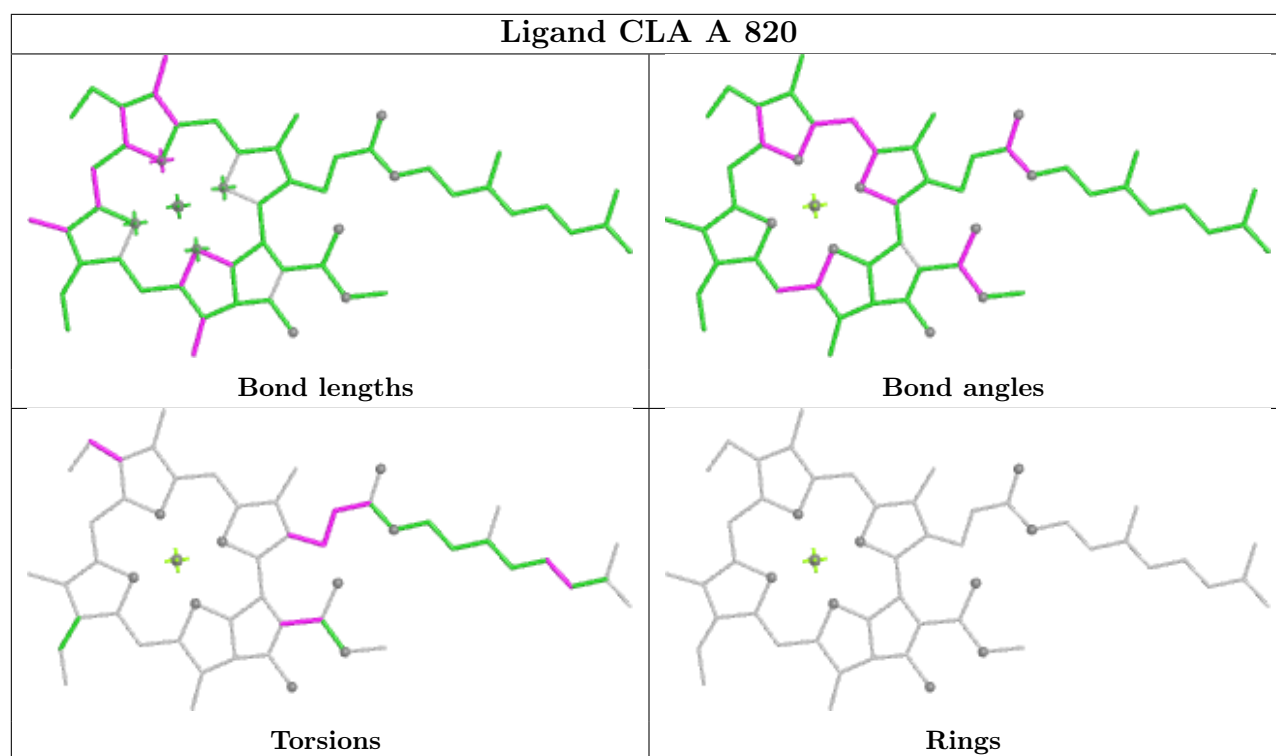




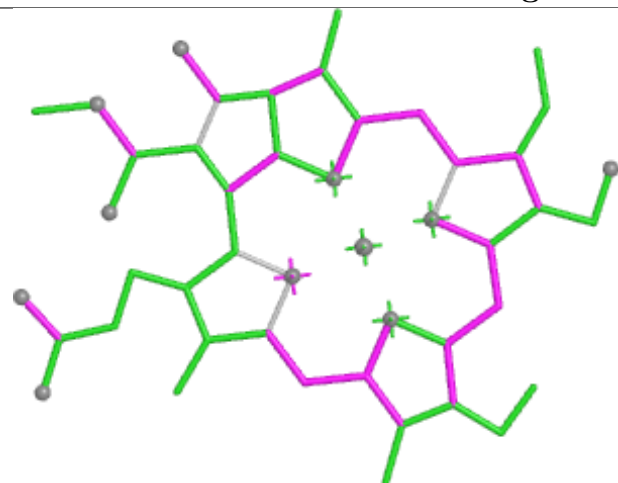
Ligand 8CT L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 7 312	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand OIE i 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 613

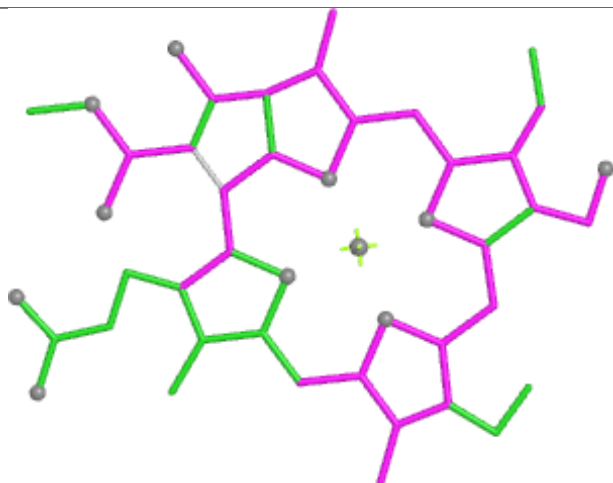




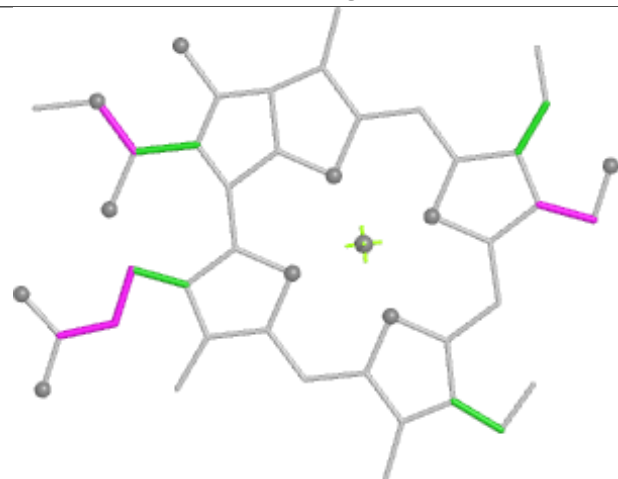
Ligand CHL 5 305



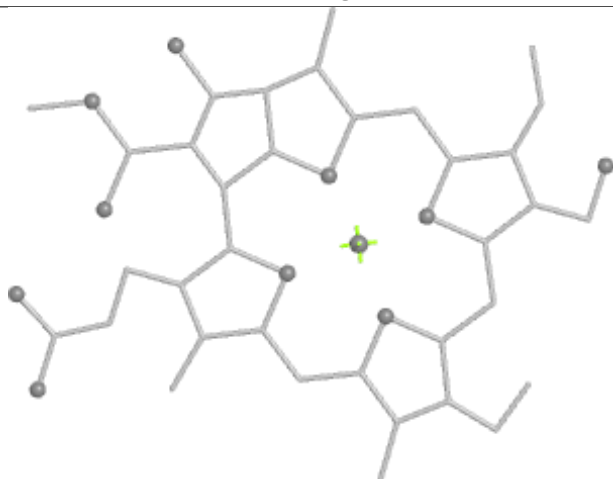
Bond lengths



Bond angles

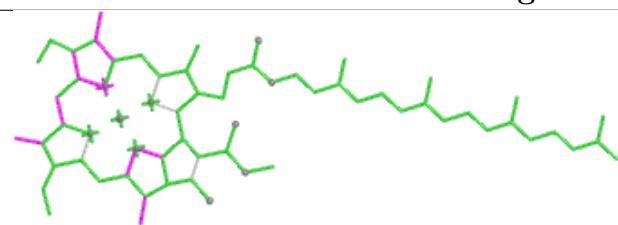


Torsions

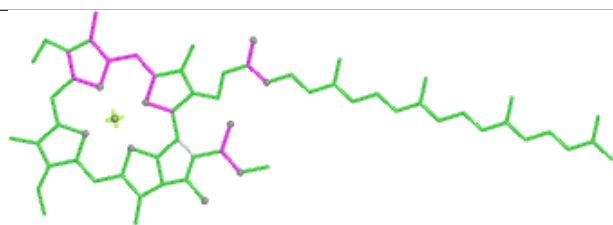


Rings

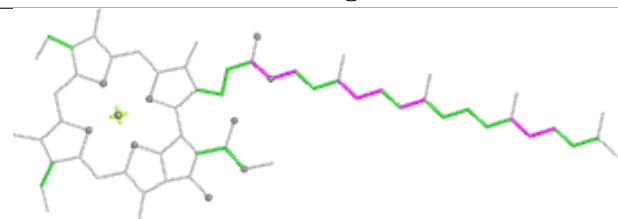
Ligand CLA A 821



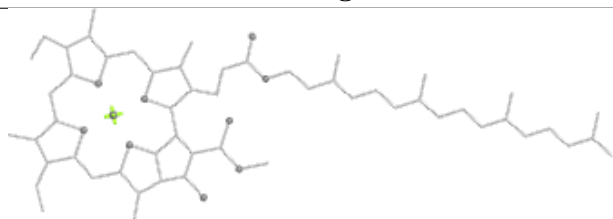
Bond lengths



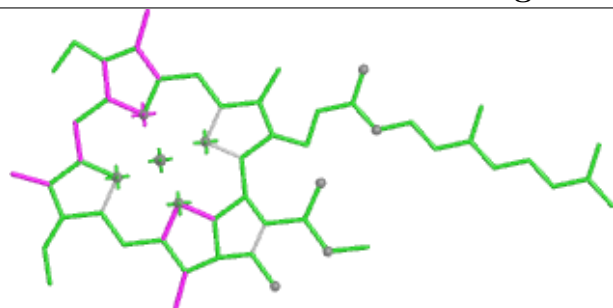
Bond angles



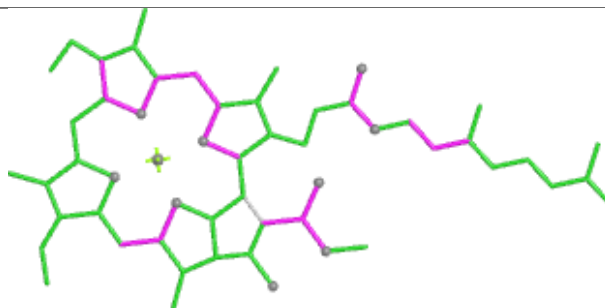
Torsions



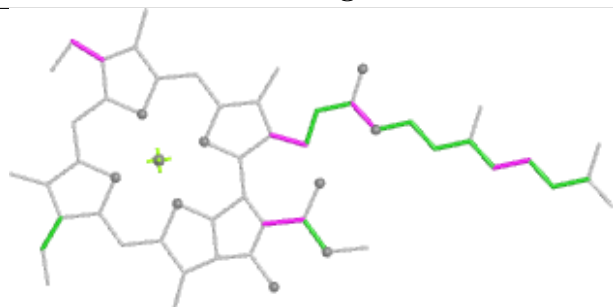
Rings

Ligand CLA B 833

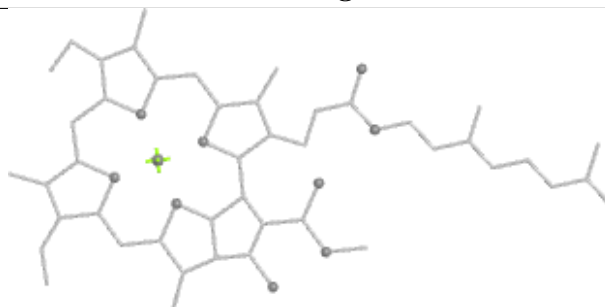
Bond lengths



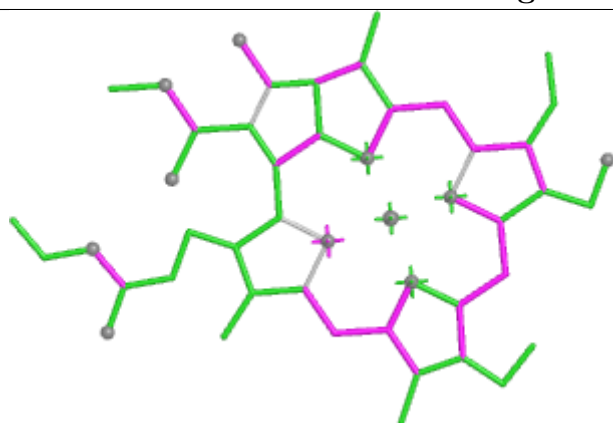
Bond angles



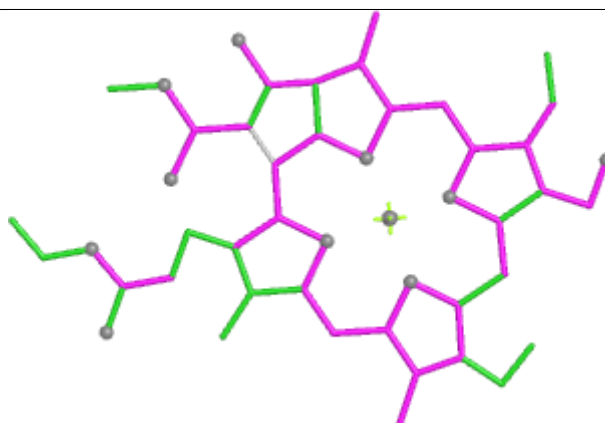
Torsions



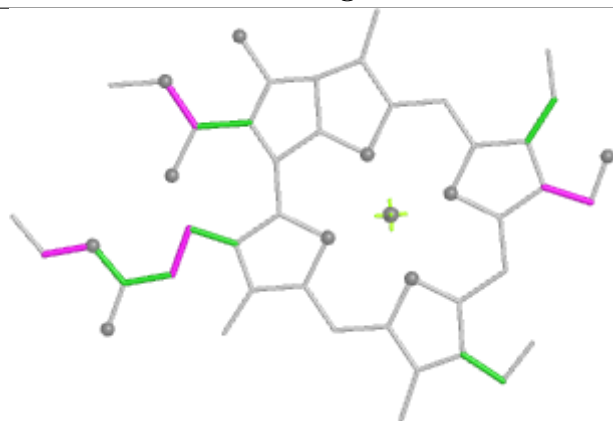
Rings

Ligand CHL 4 306

Bond lengths



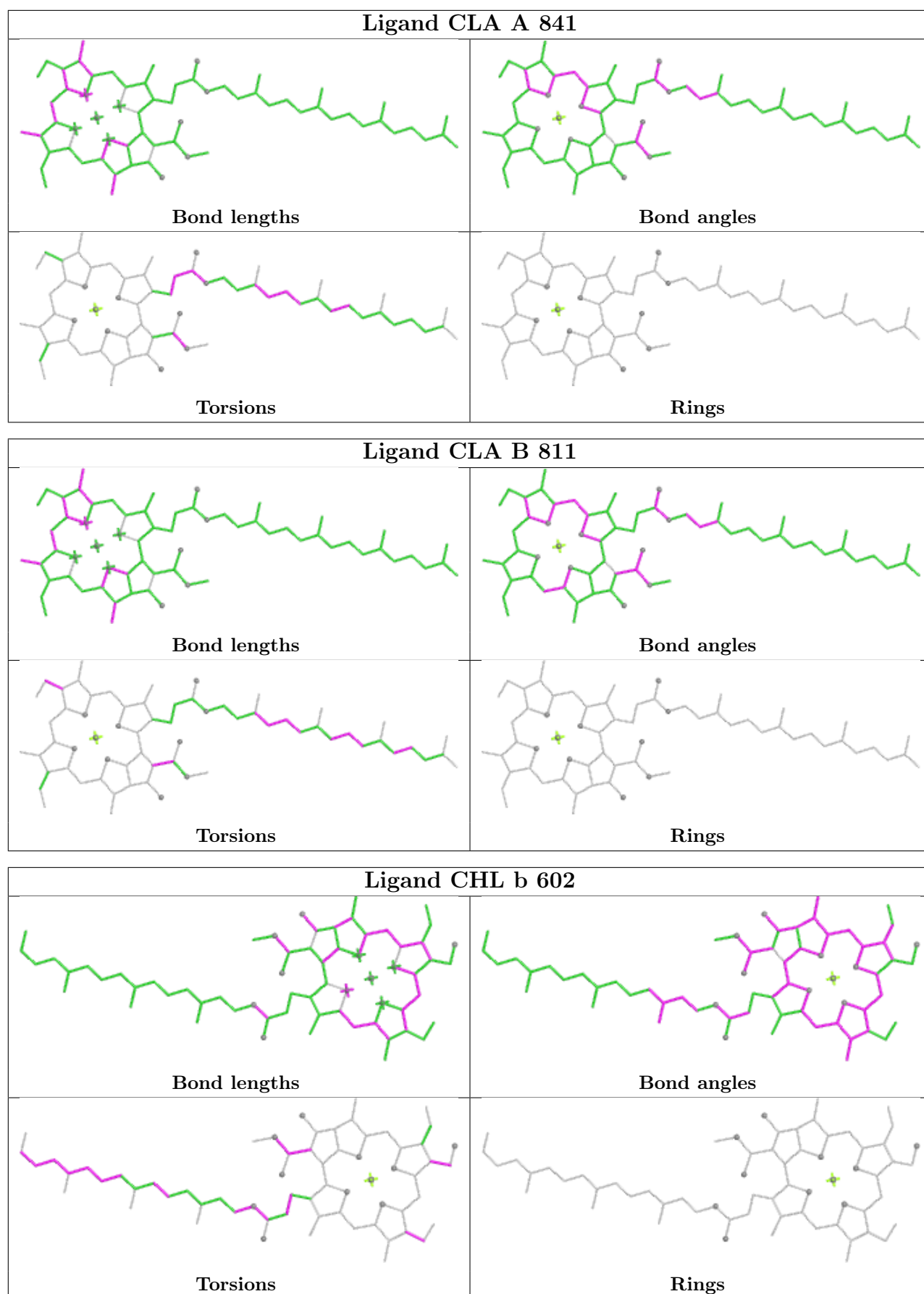
Bond angles



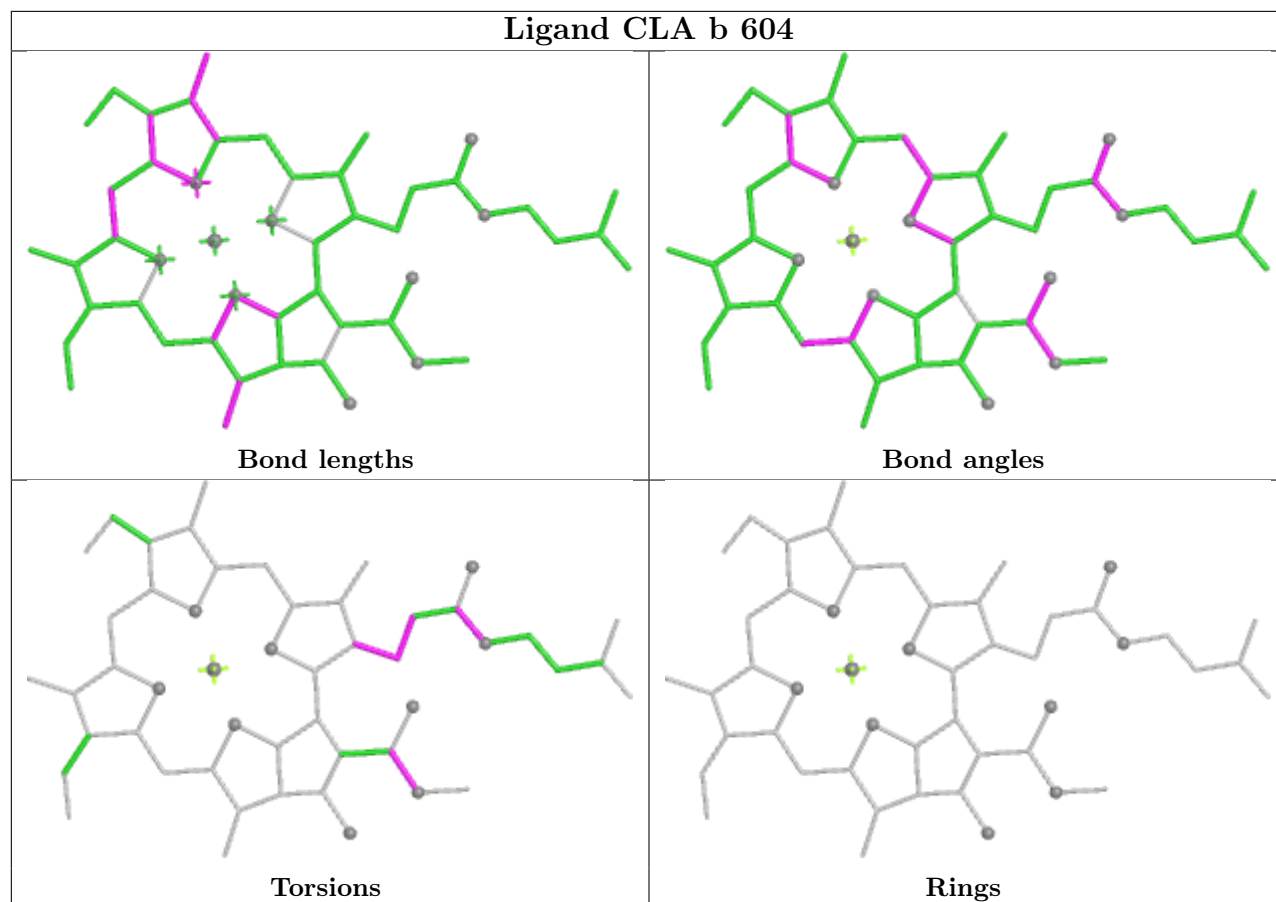
Torsions



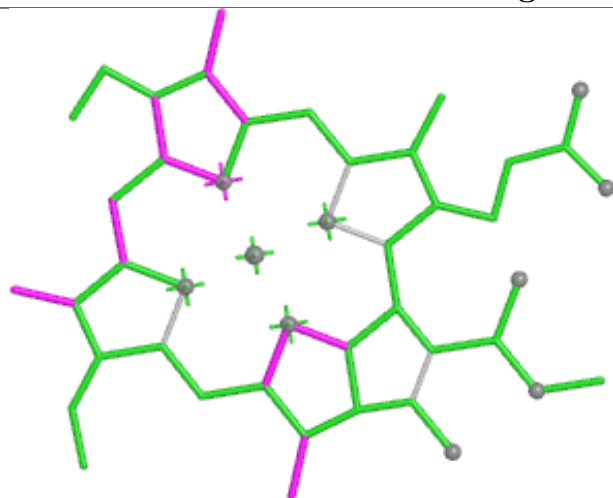
Rings



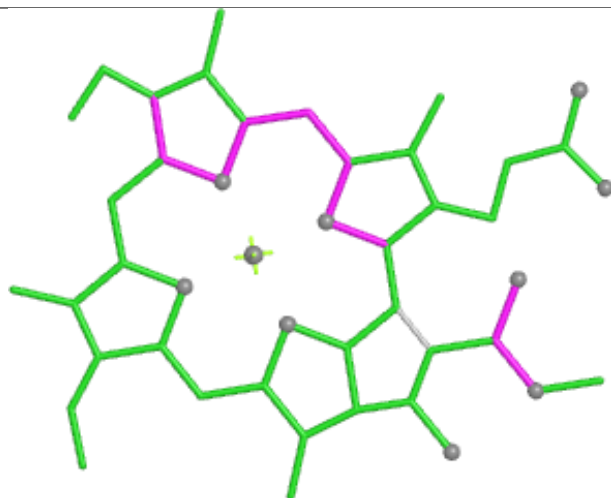
Ligand CLA b 604



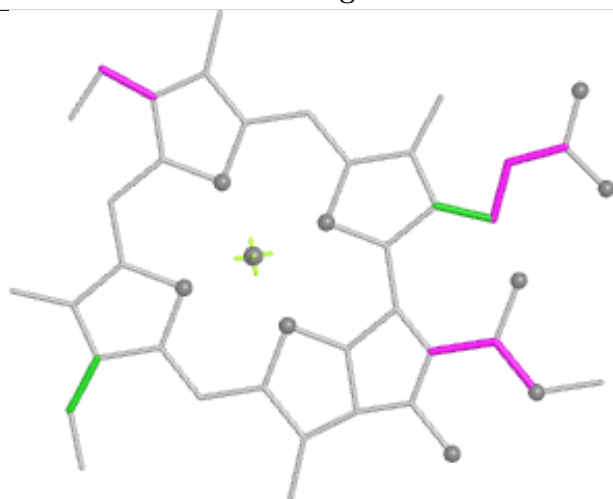
Ligand CLA 7 303



Bond lengths



Bond angles

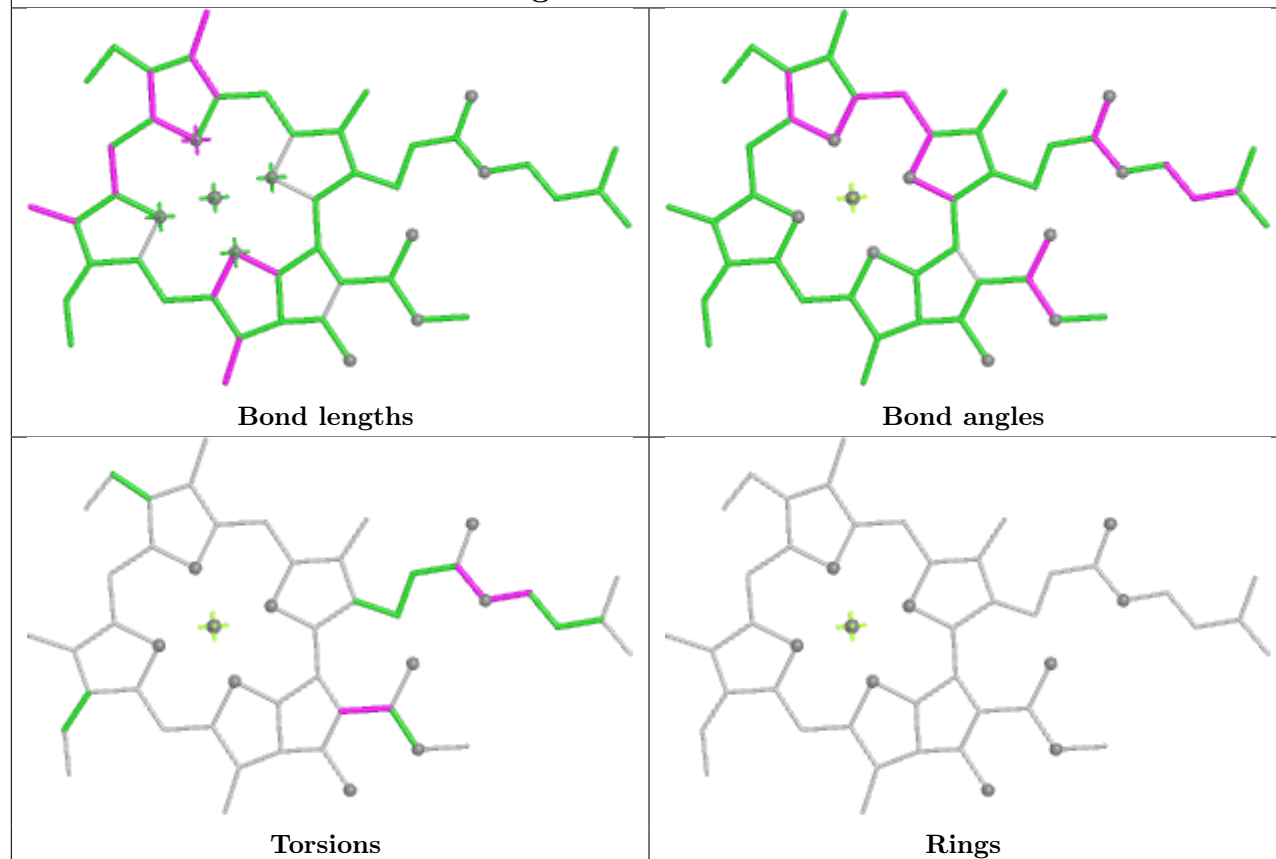


Torsions

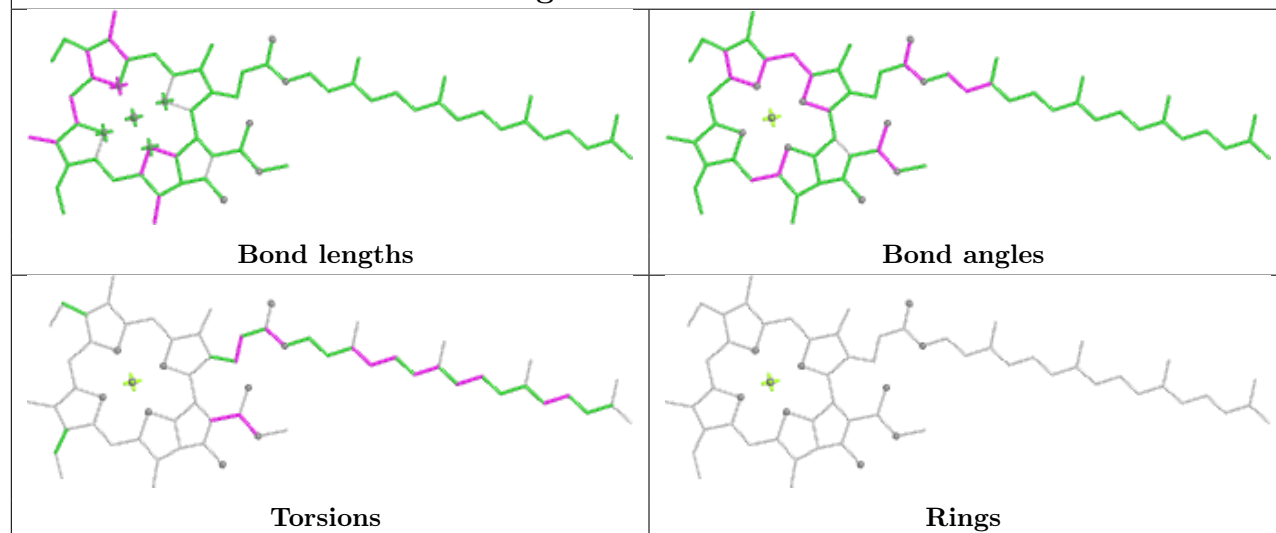


Rings

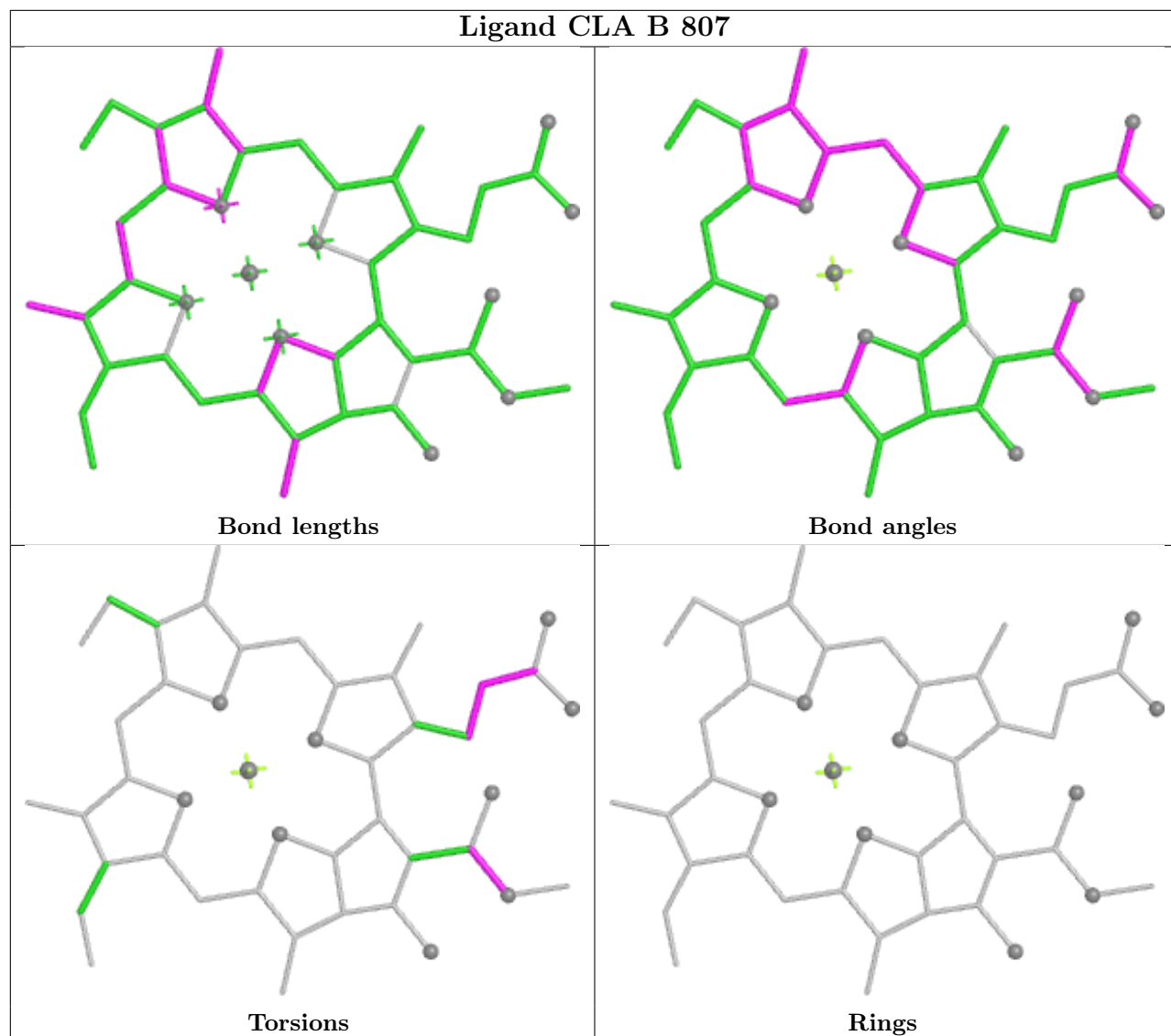
Ligand CLA A 831



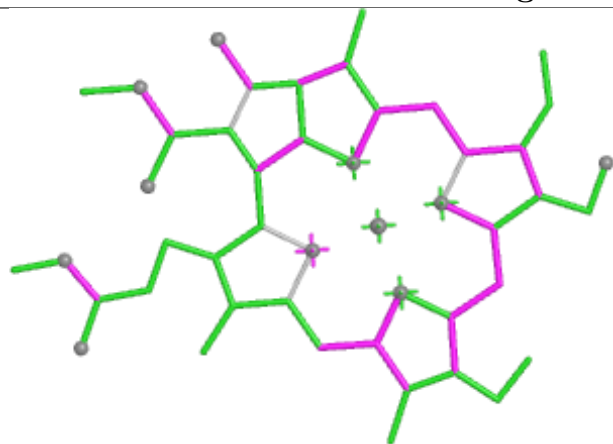
Ligand CLA 1 312



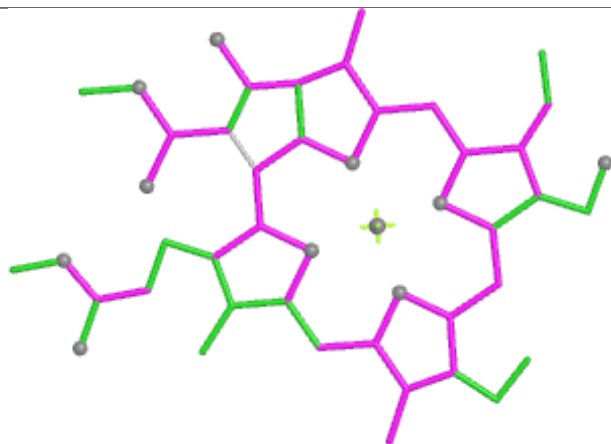
Ligand CLA B 807



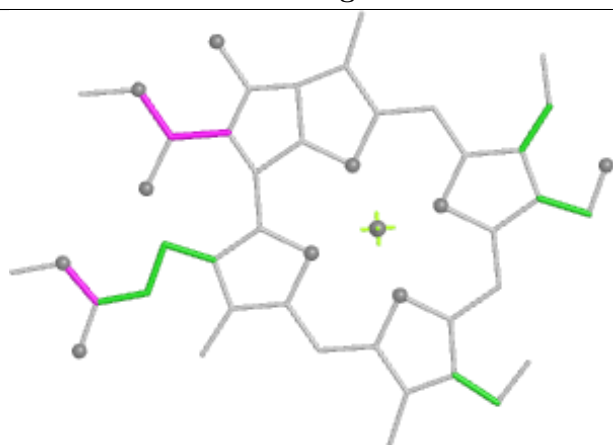
Ligand CHL b 607



Bond lengths



Bond angles

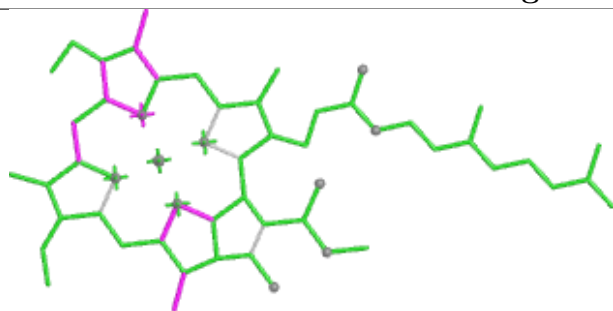


Torsions

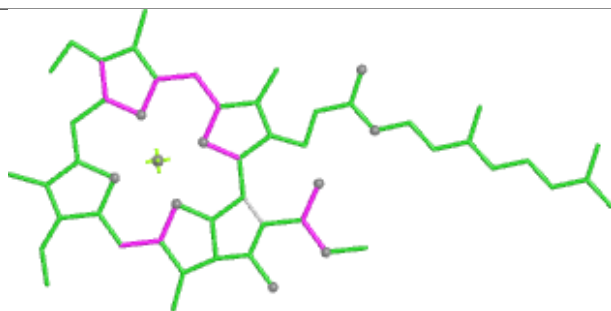


Rings

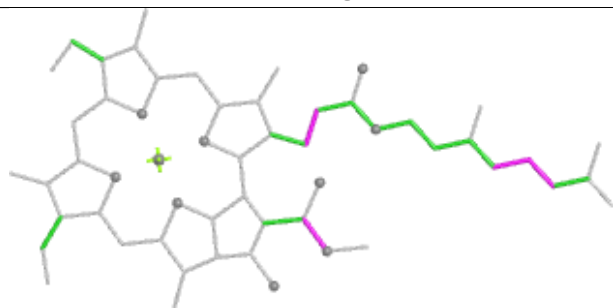
Ligand CLA f 611



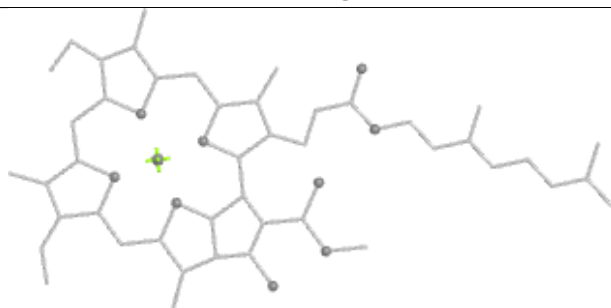
Bond lengths



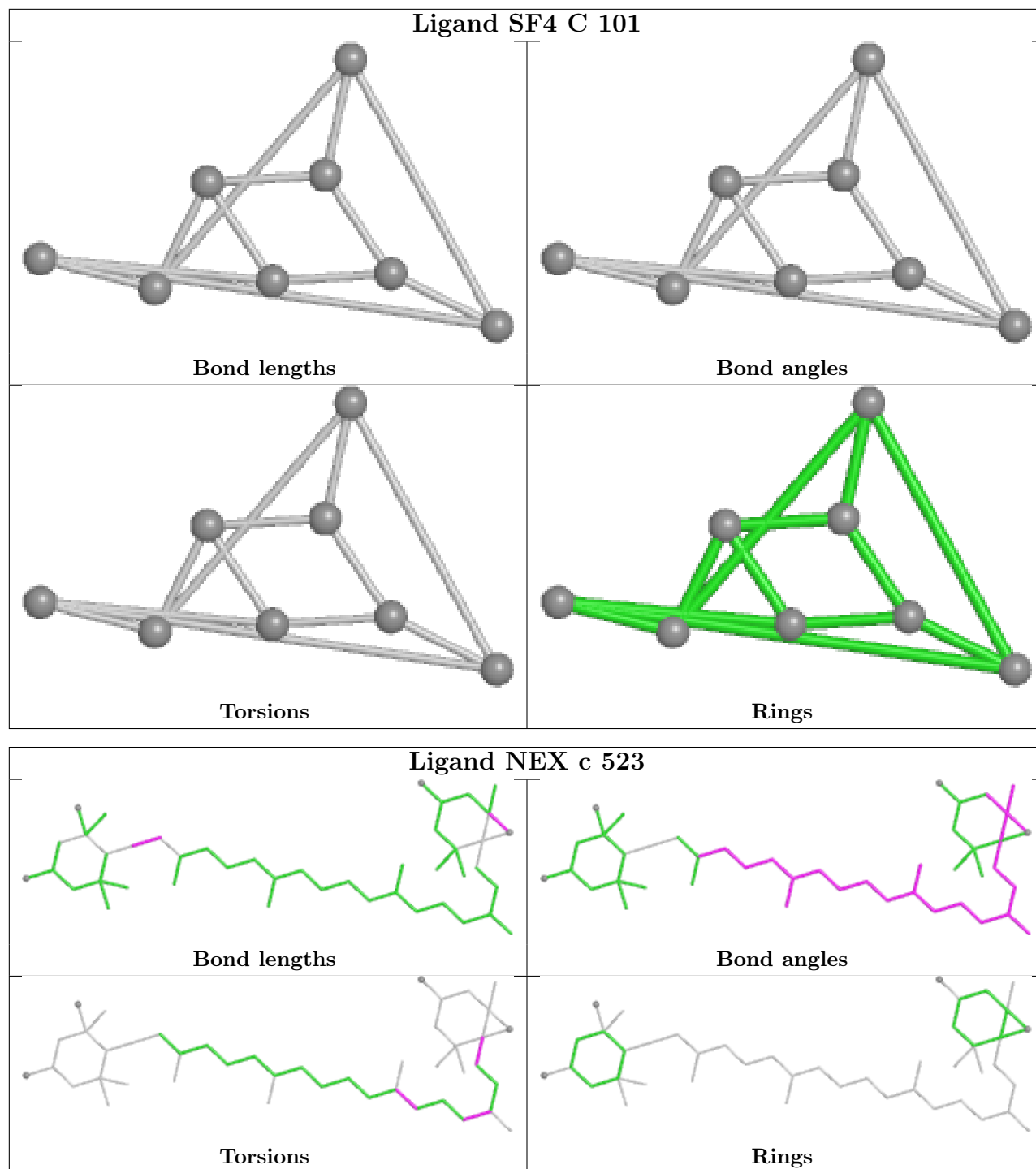
Bond angles



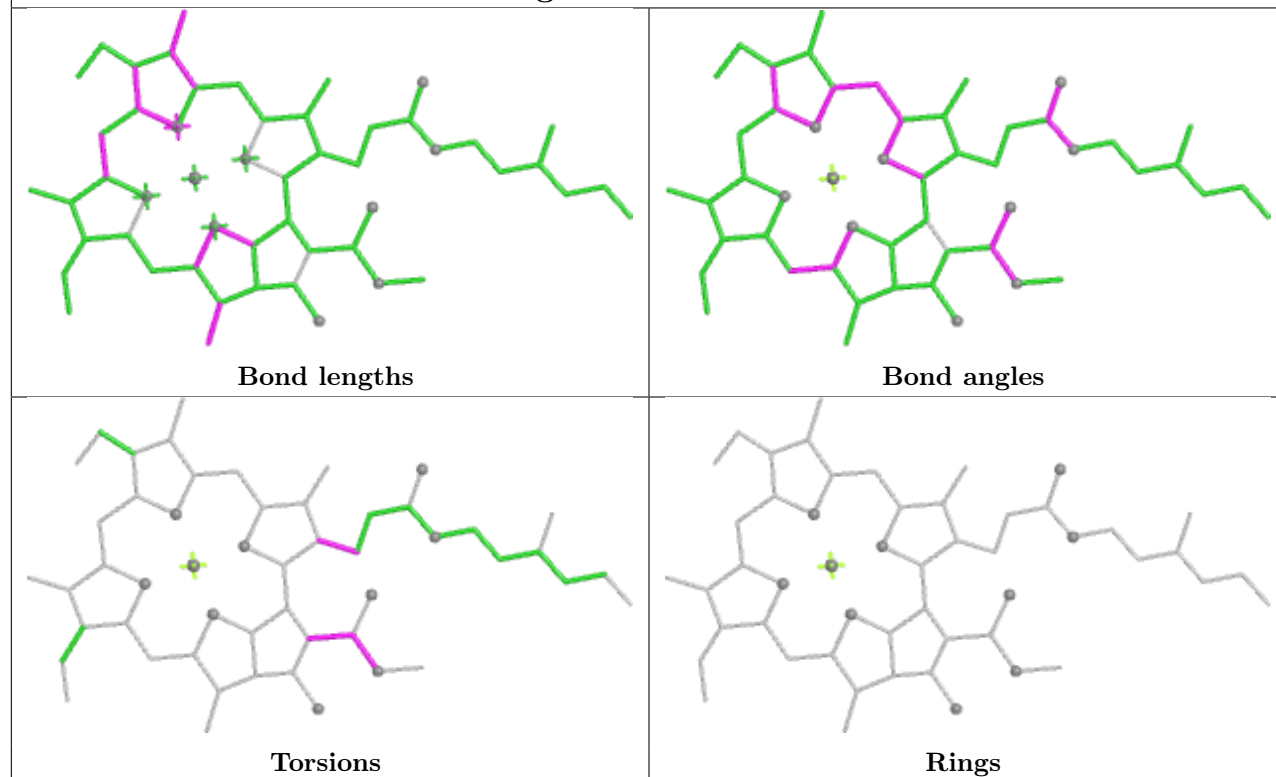
Torsions



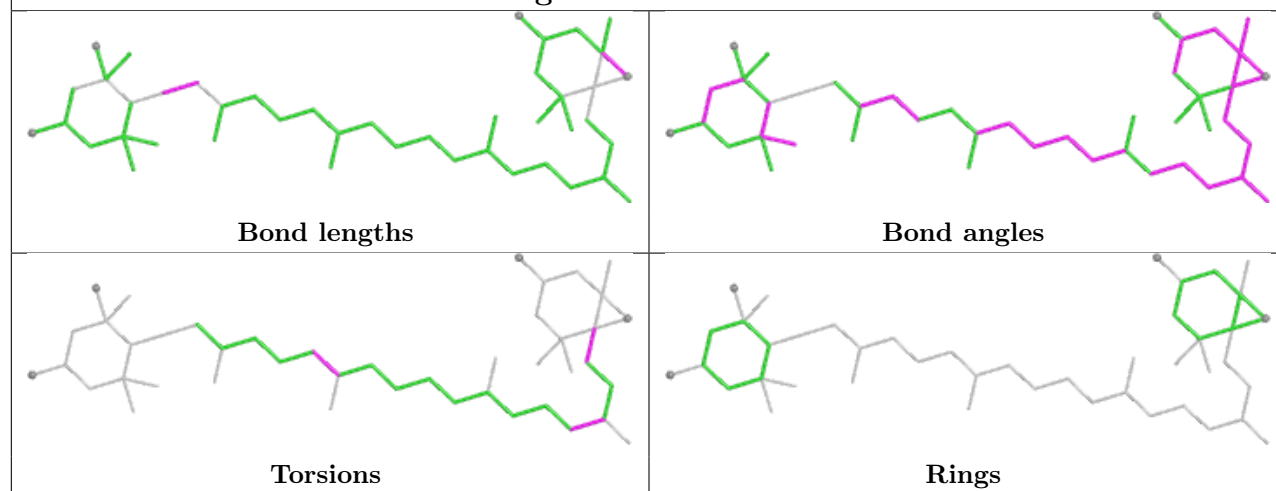
Rings

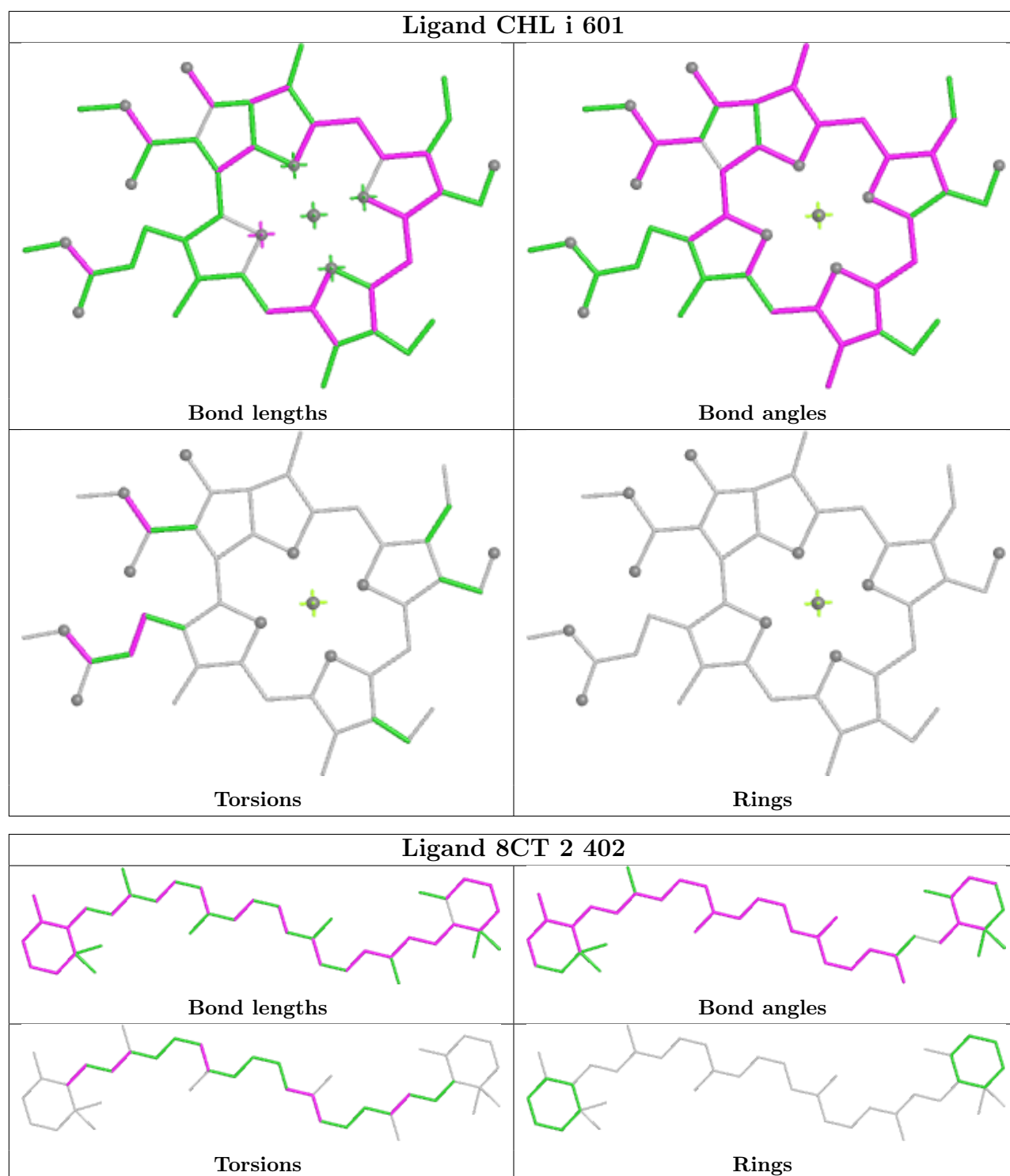


Ligand CLA 0 304

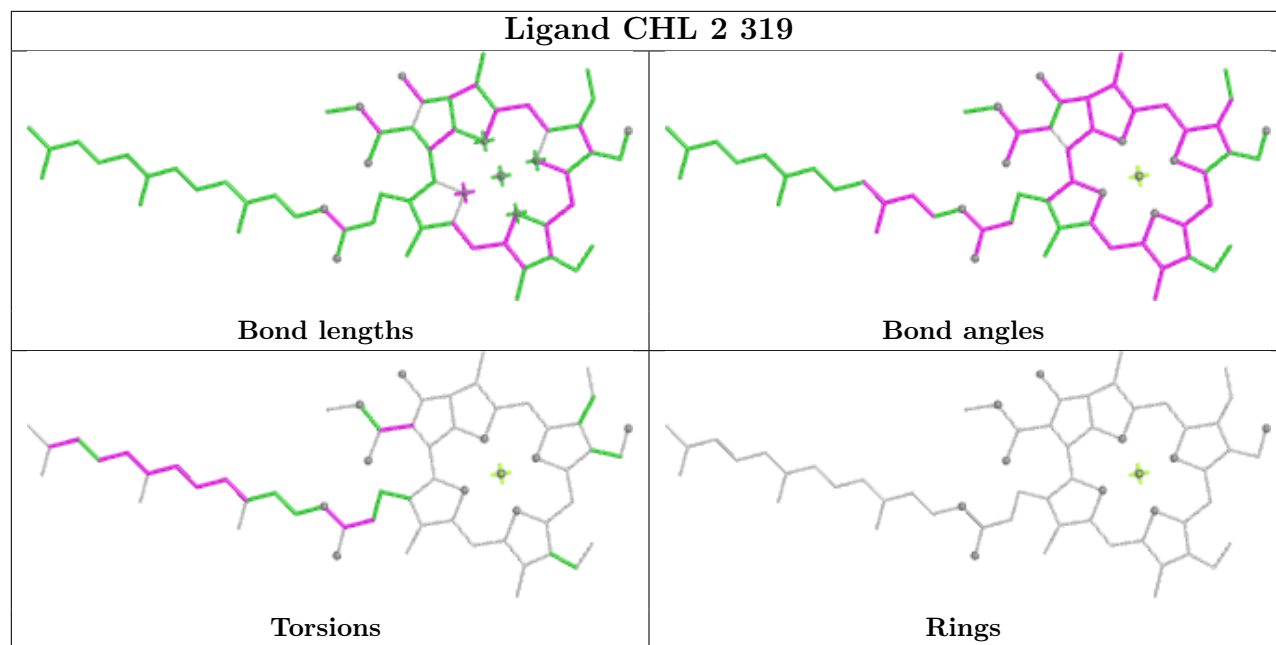


Ligand NEX e 523

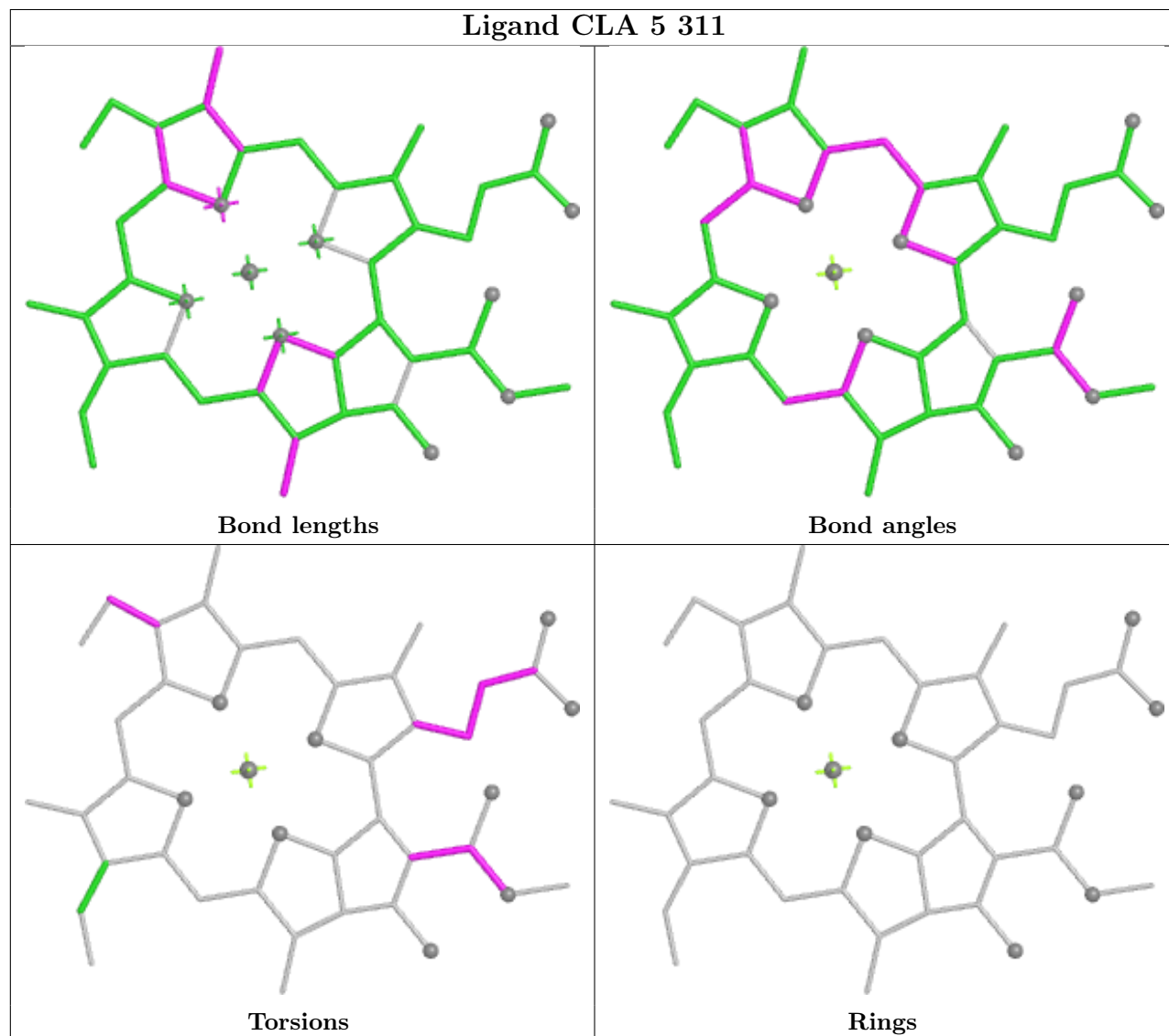


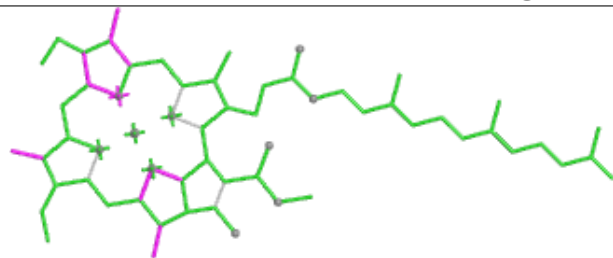
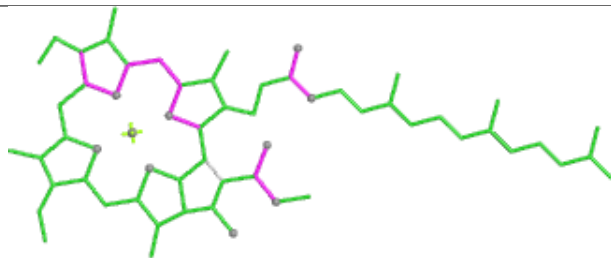
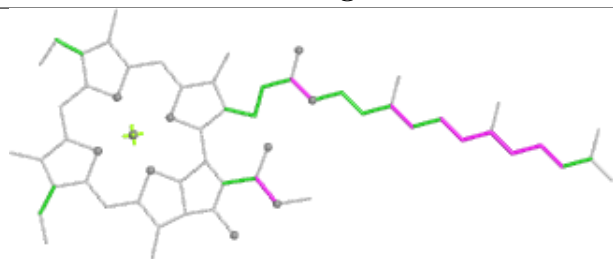
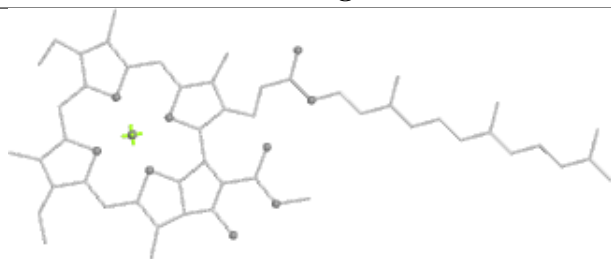
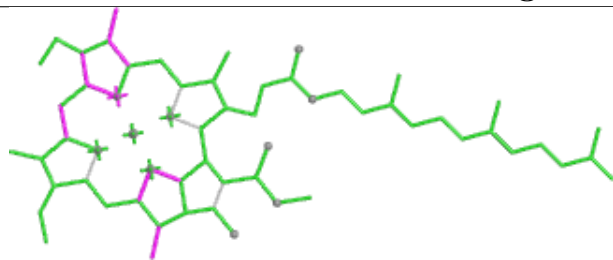
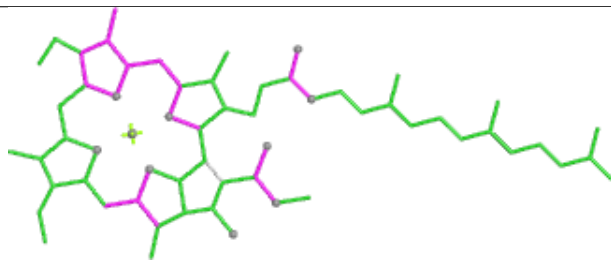
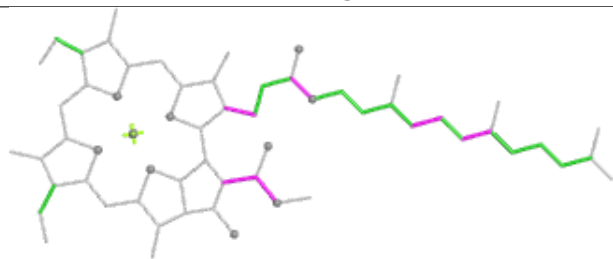
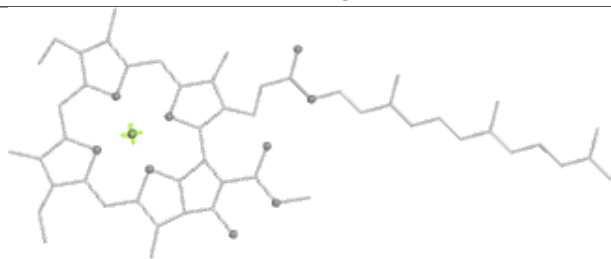


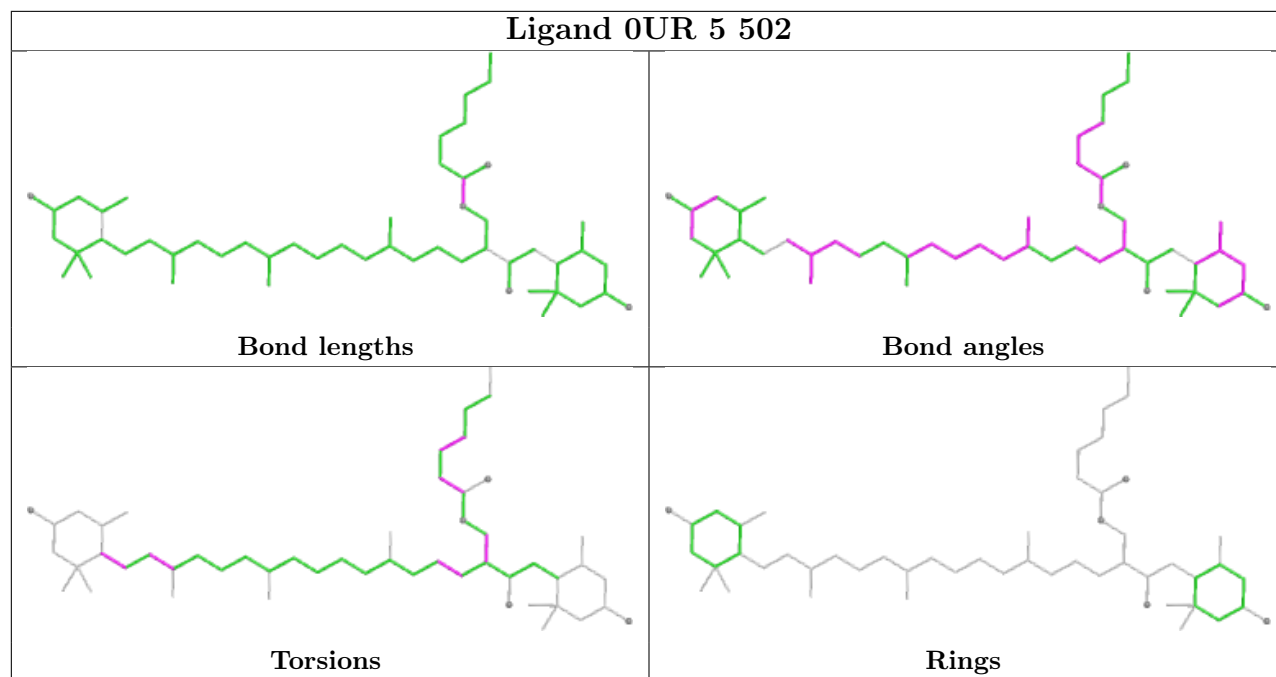
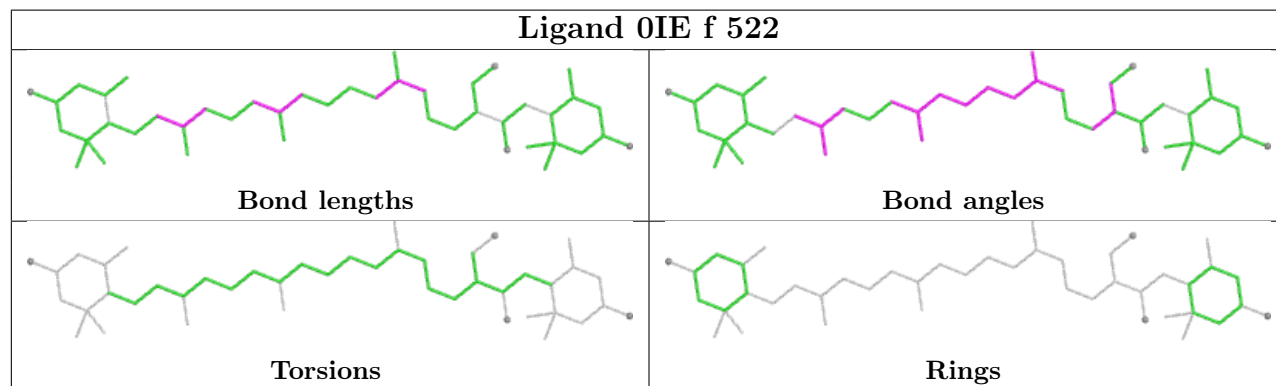
Ligand CHL 2 319

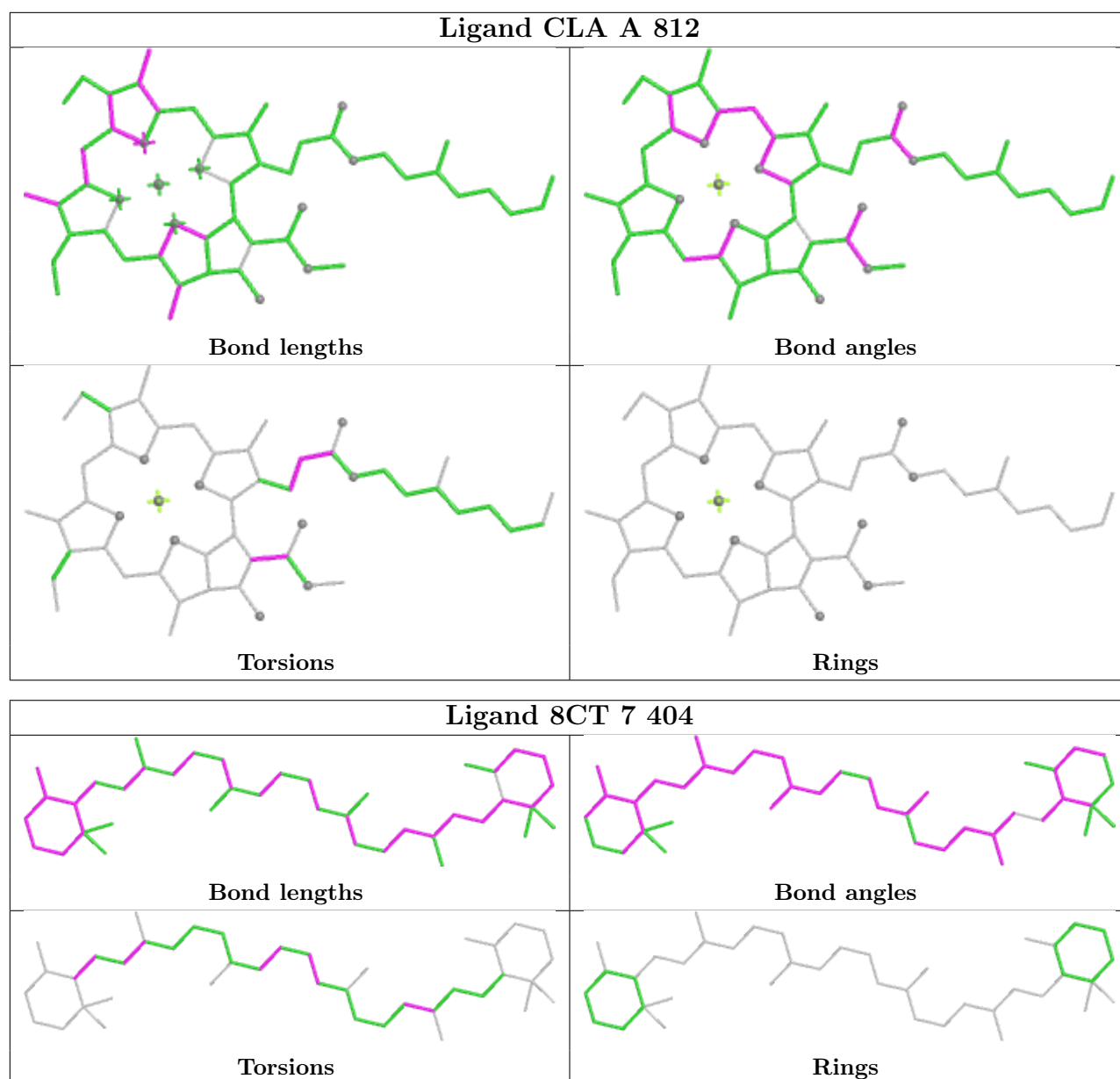


Ligand CLA 5 311

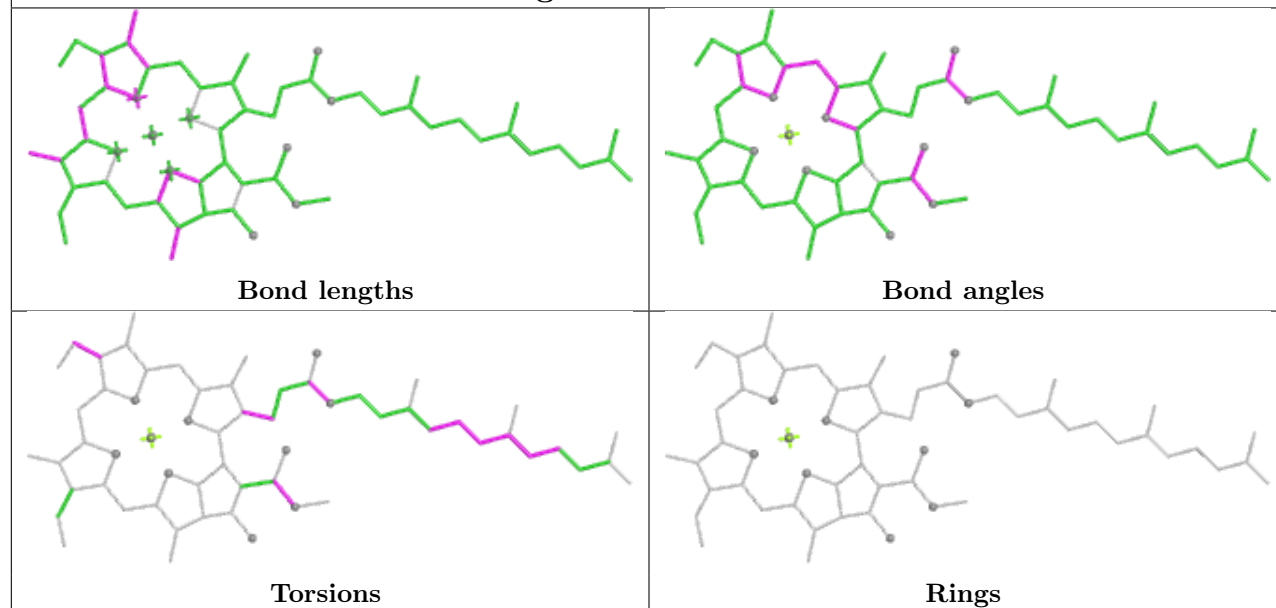


Ligand CLA 2 304**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 309****Bond lengths****Bond angles****Torsions****Rings**

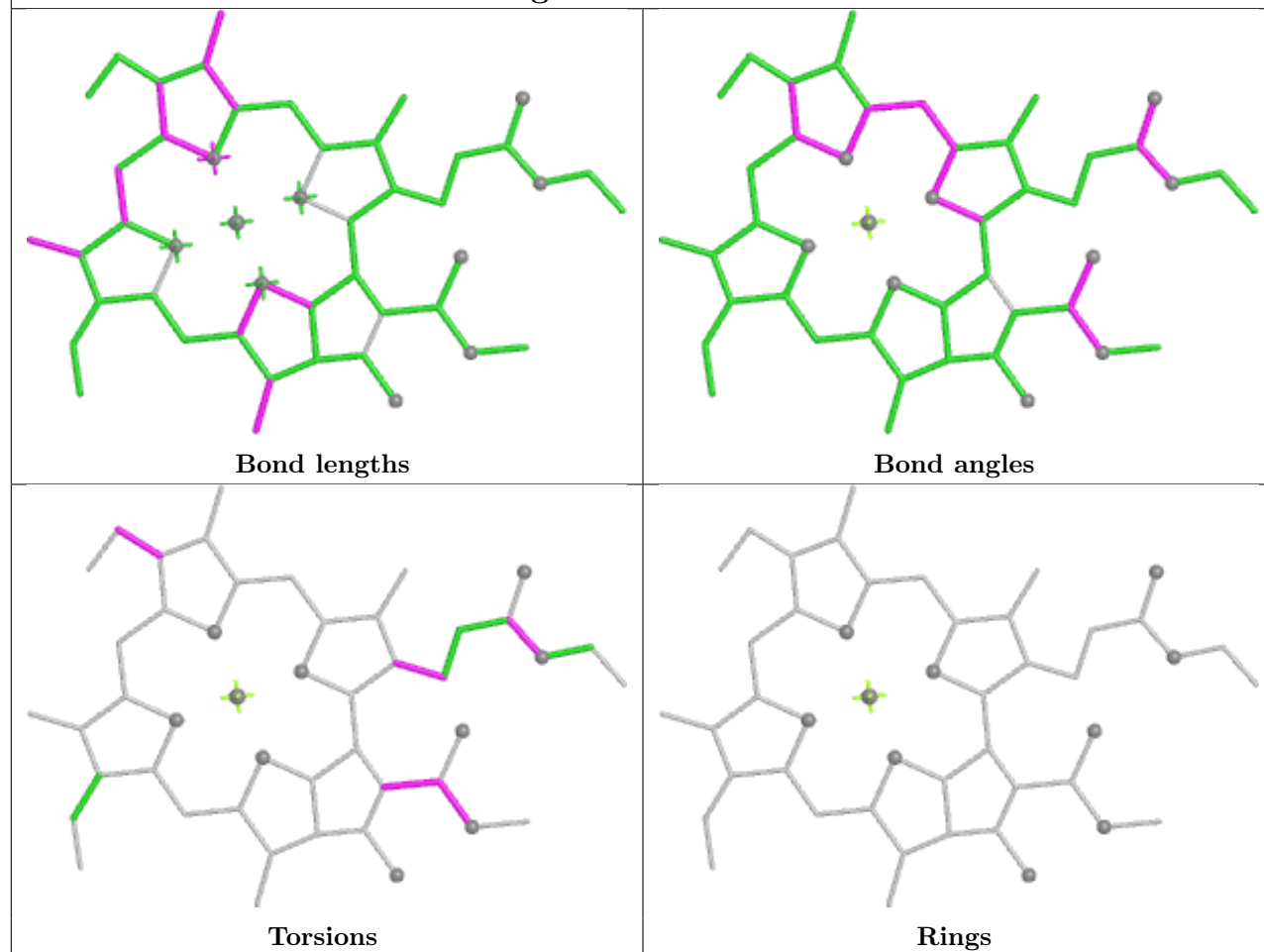
Ligand 0UR 5 502**Ligand 0IE f 522**

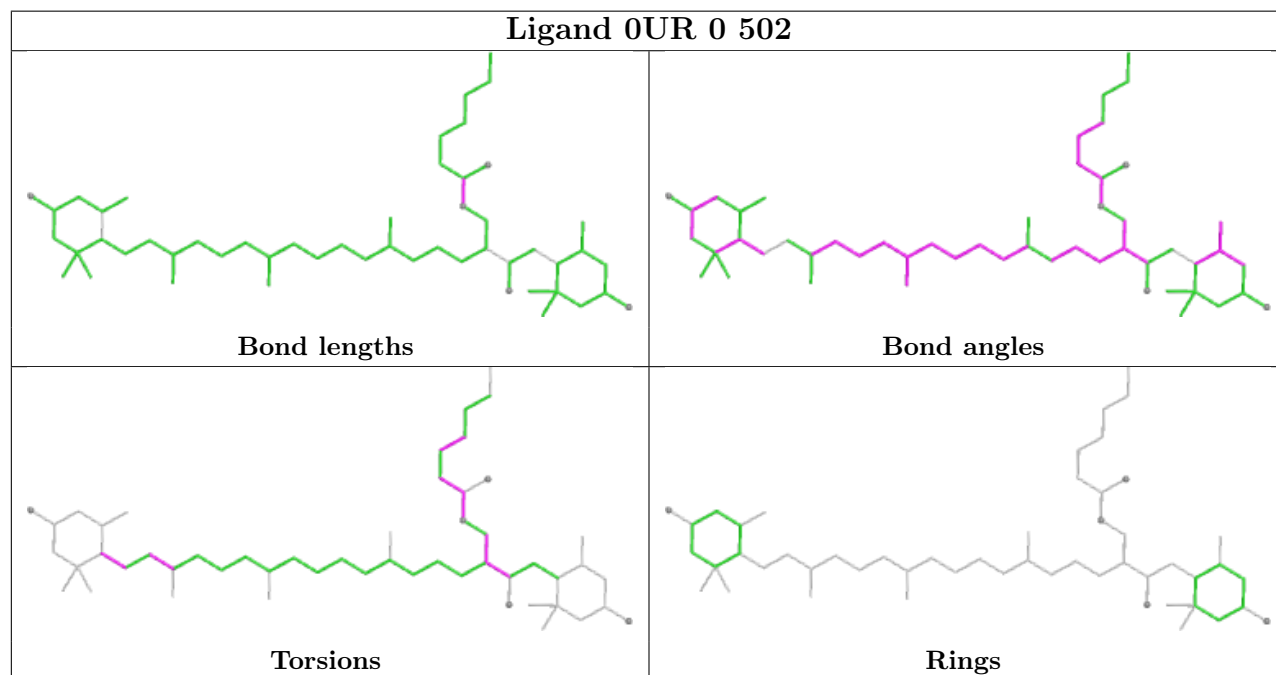
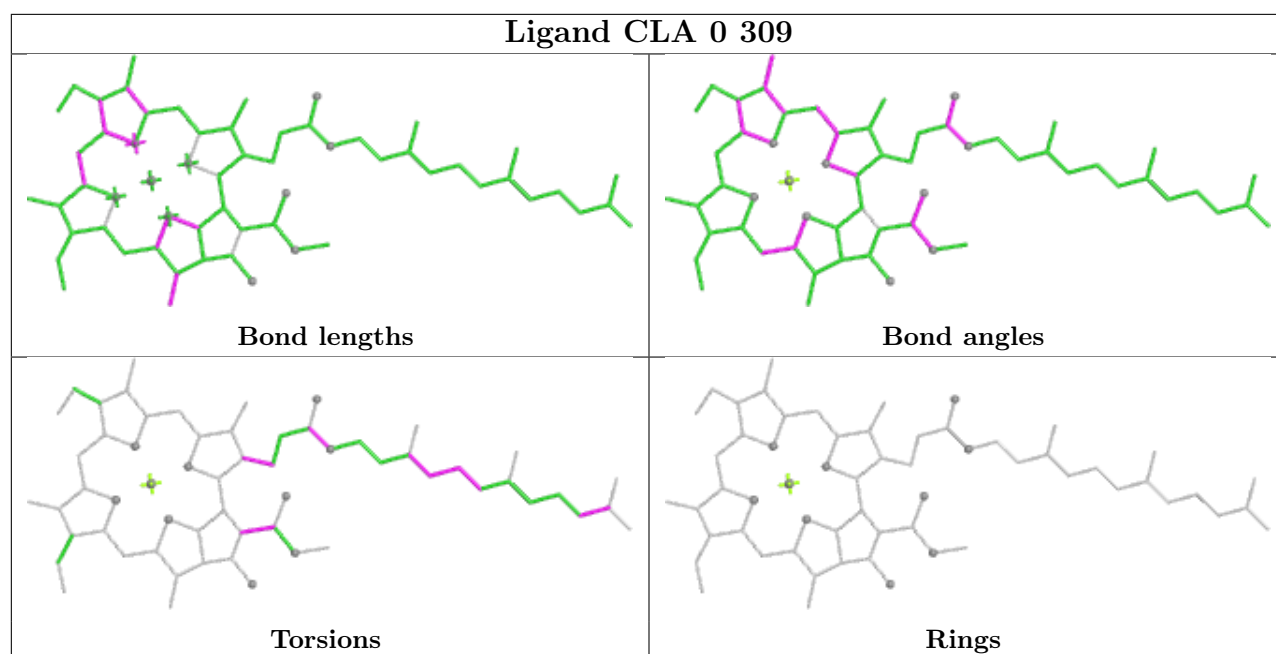


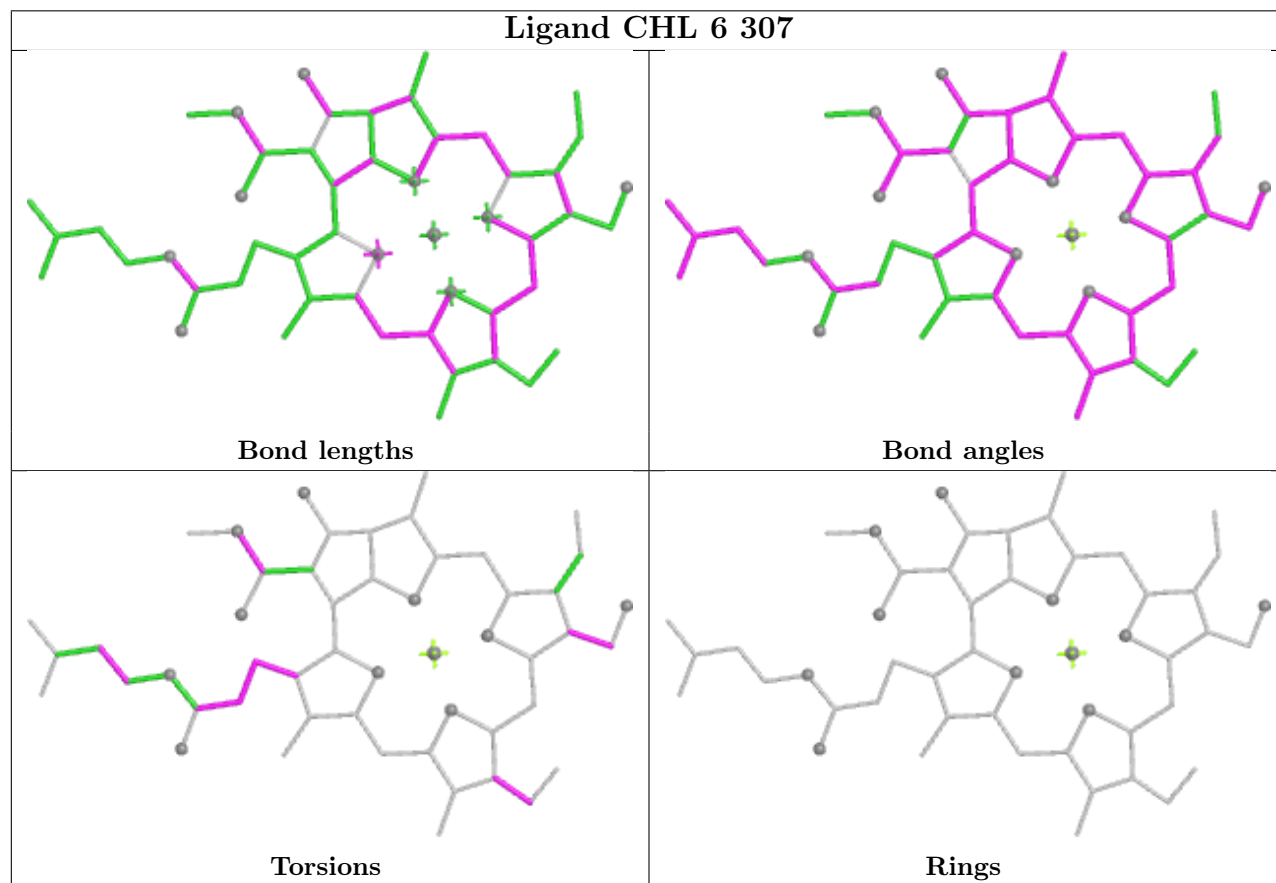
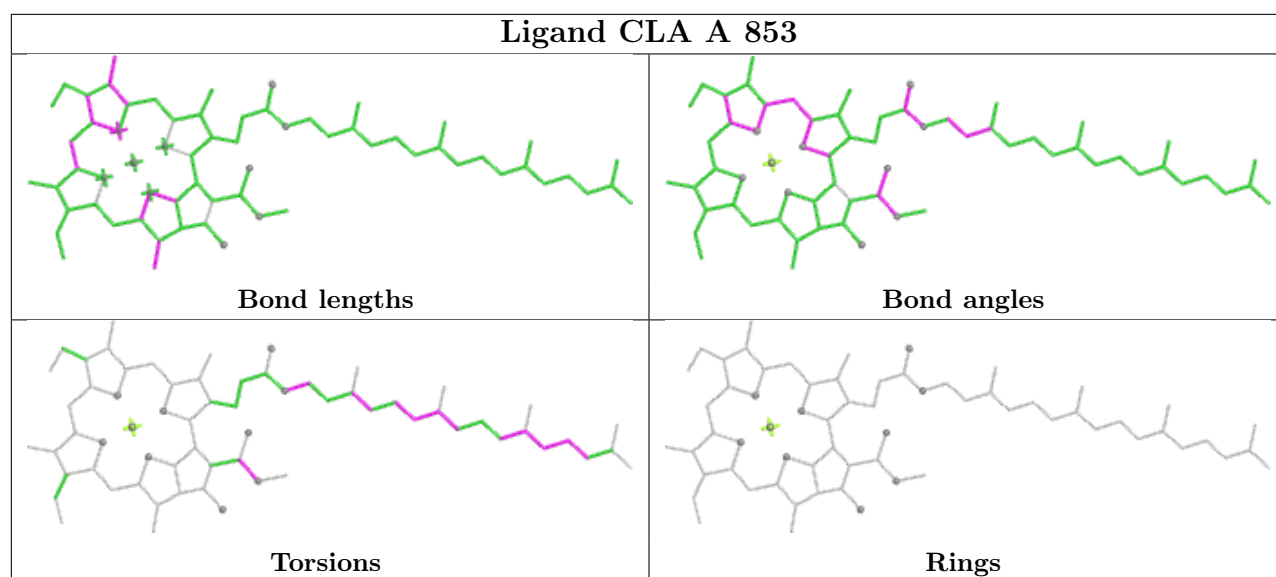
Ligand CLA 2 310

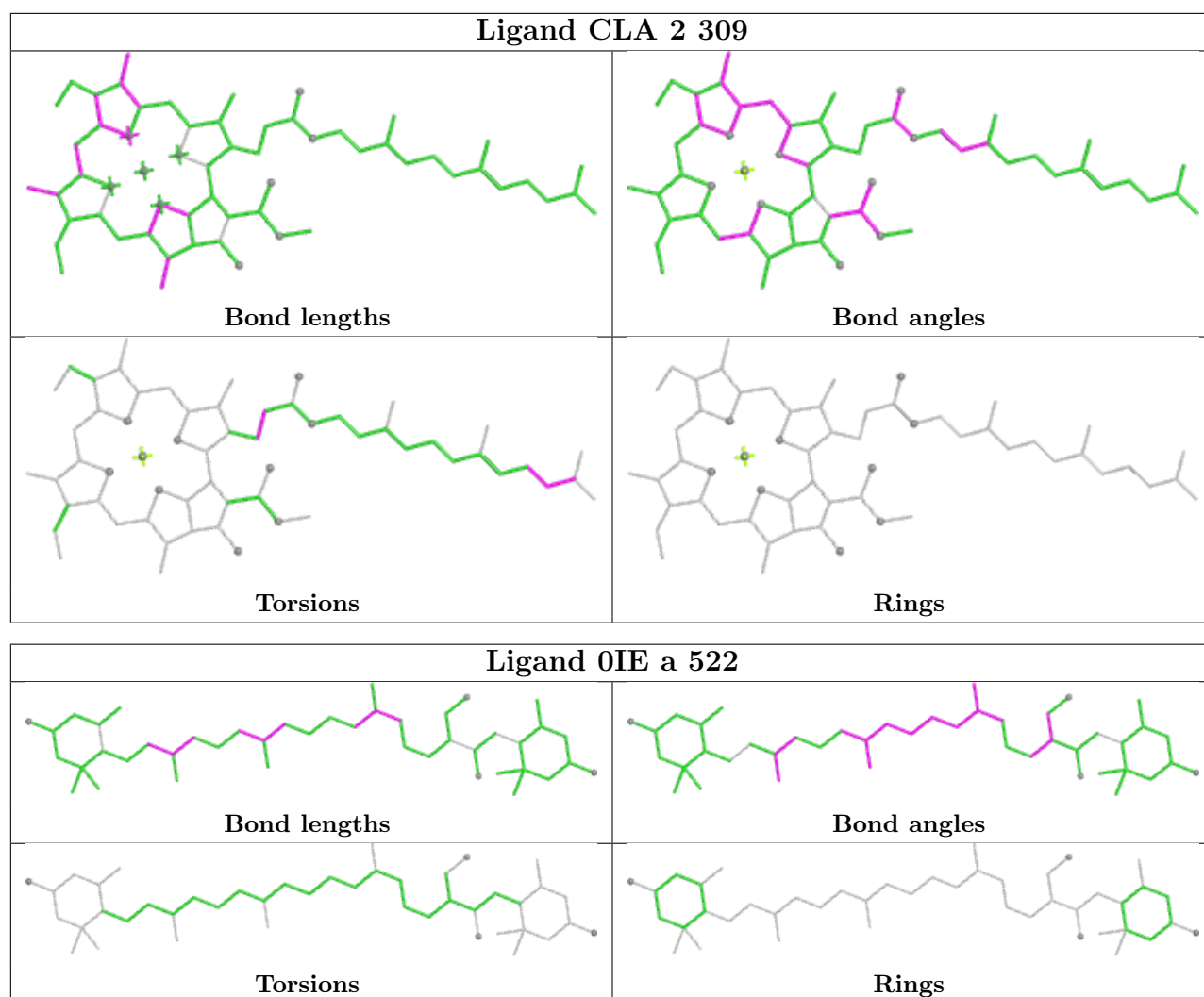


Ligand CLA 0 311

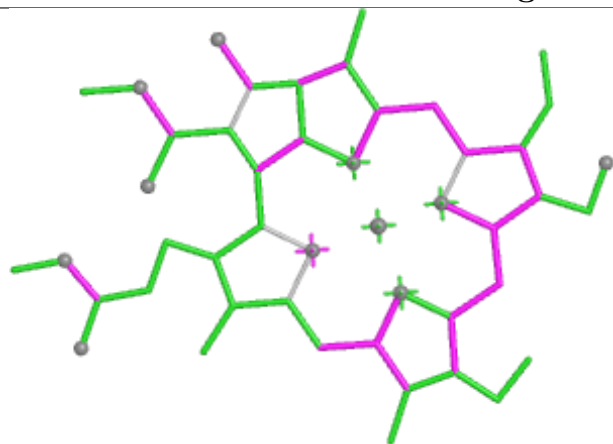




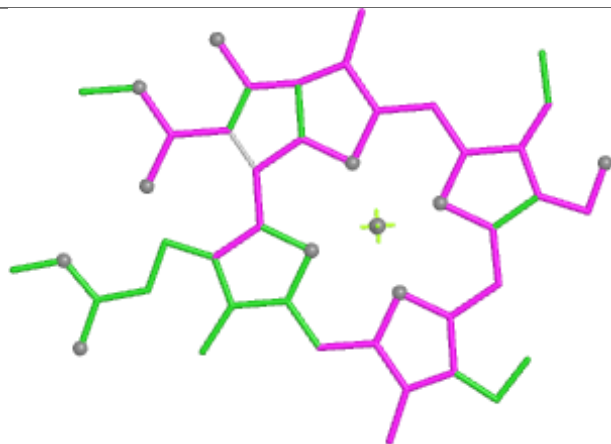




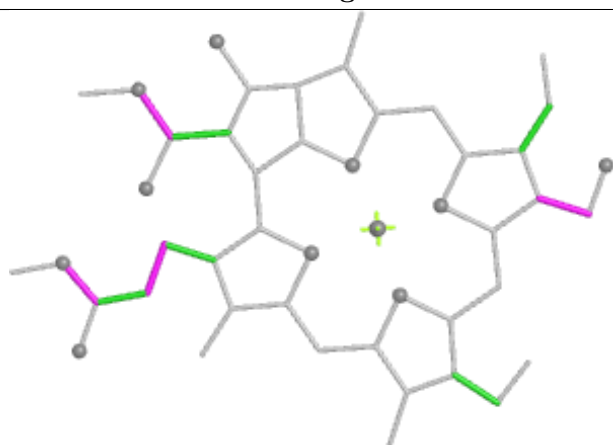
Ligand CHL 7 313



Bond lengths



Bond angles

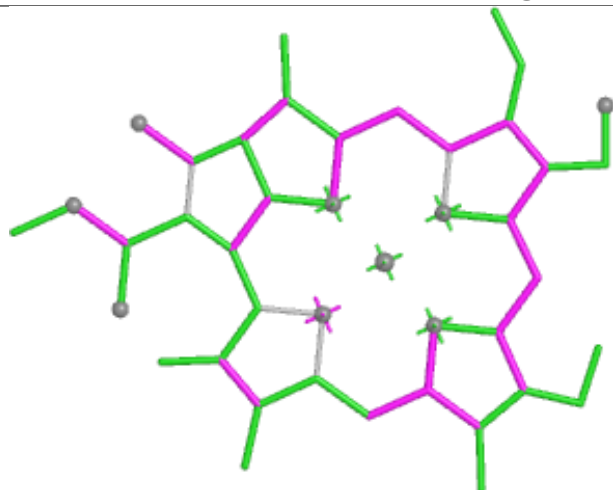


Torsions

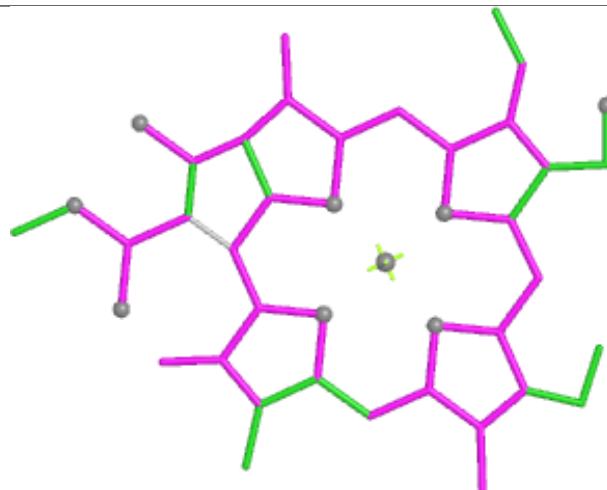


Rings

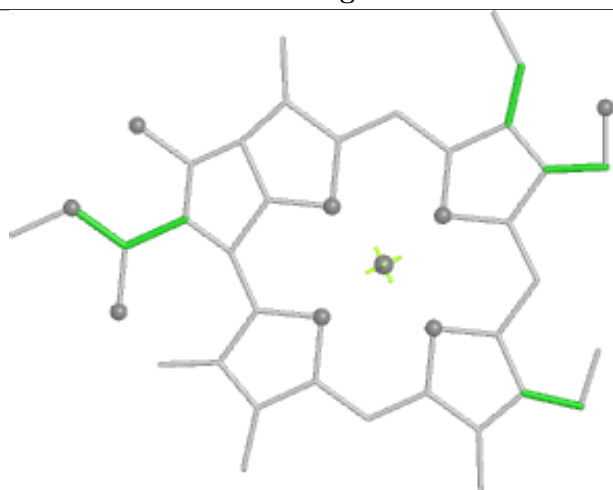
Ligand CHL a 614



Bond lengths



Bond angles

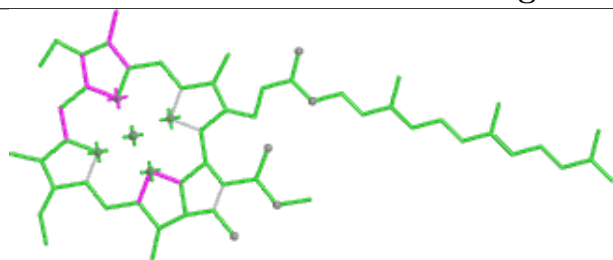


Torsions

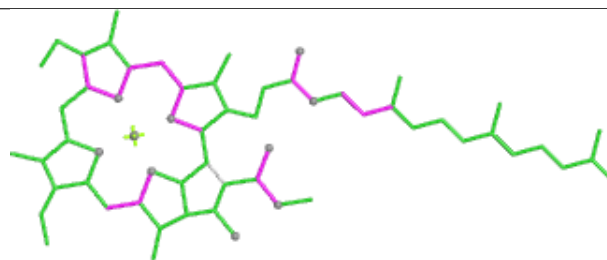


Rings

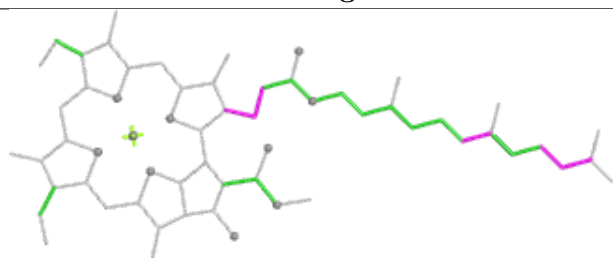
Ligand CLA 4 309



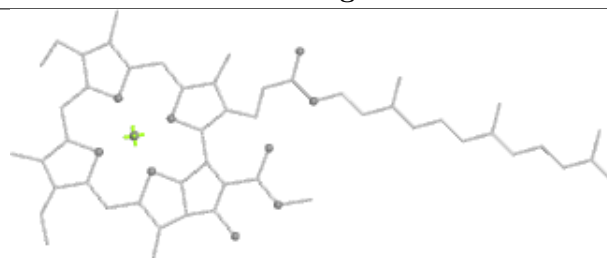
Bond lengths



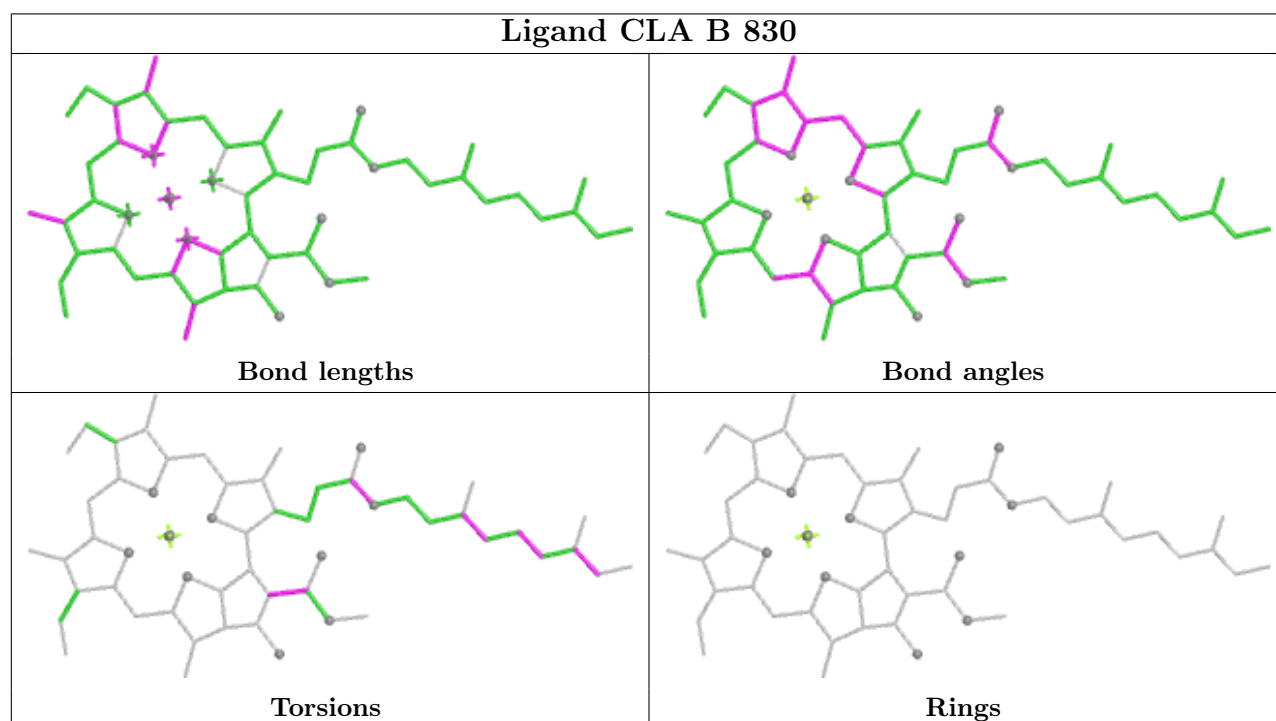
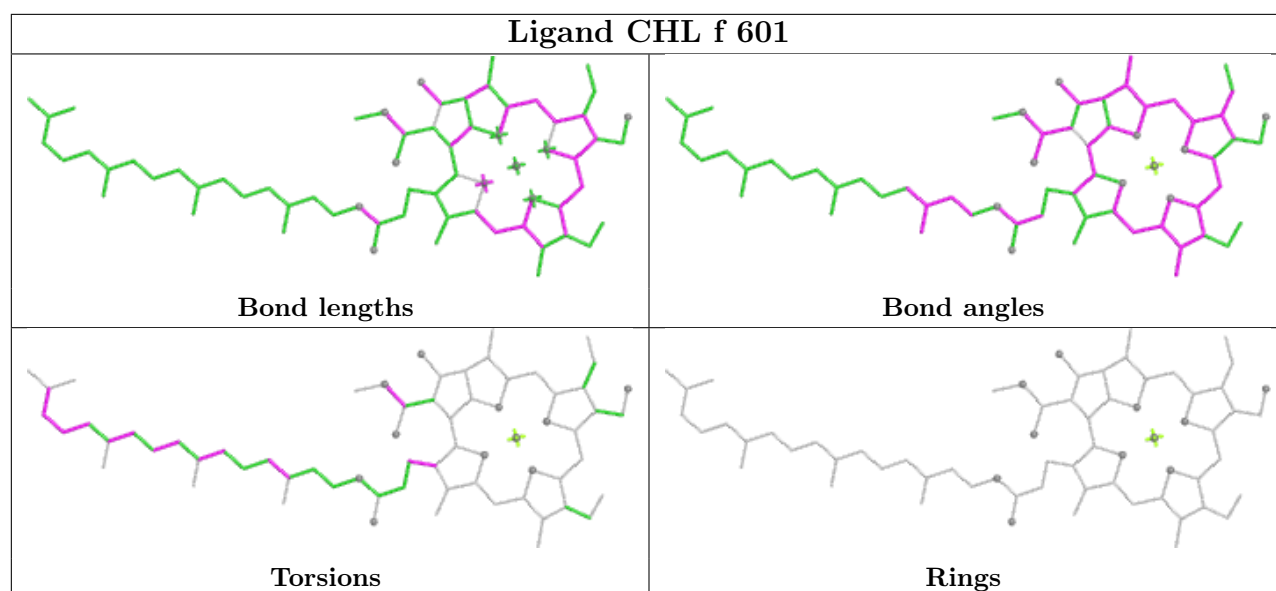
Bond angles

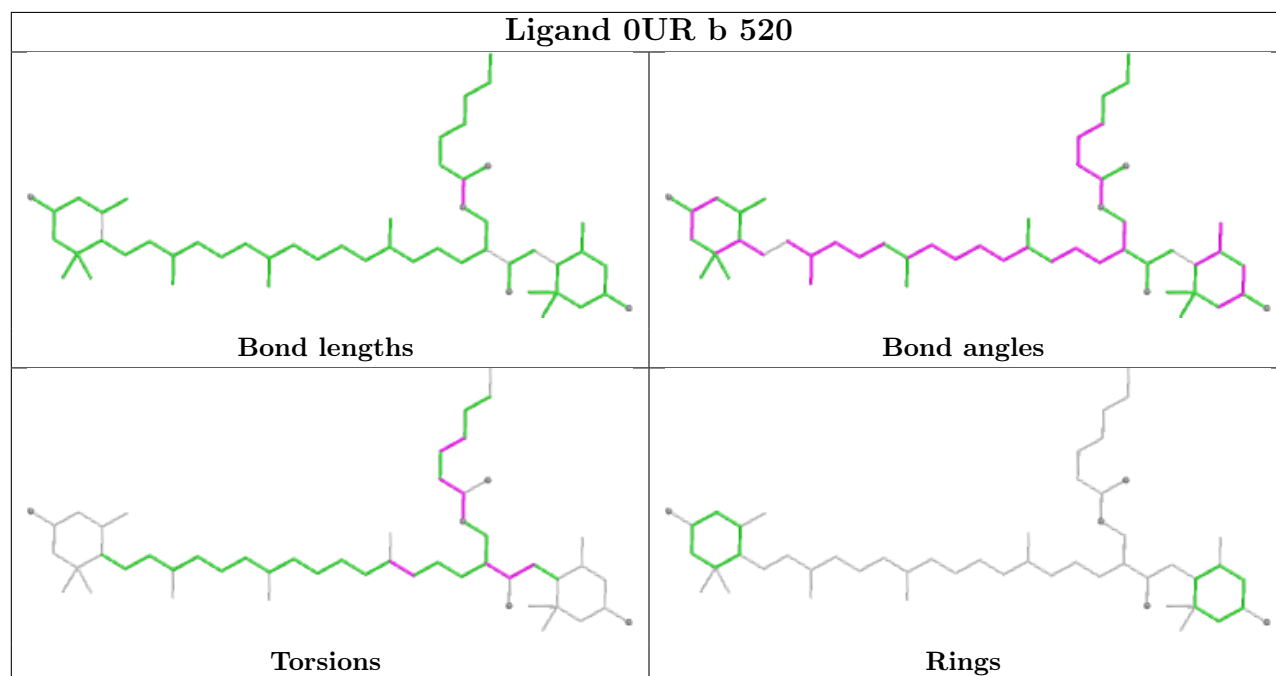
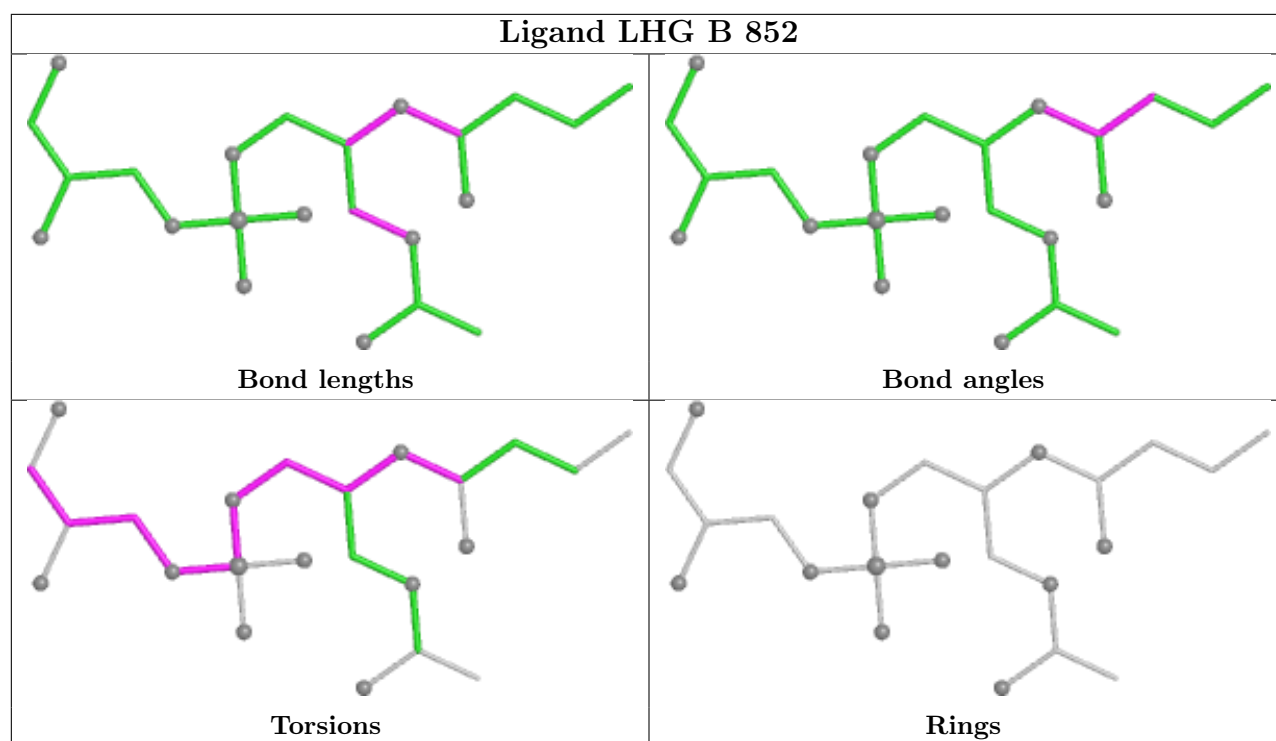


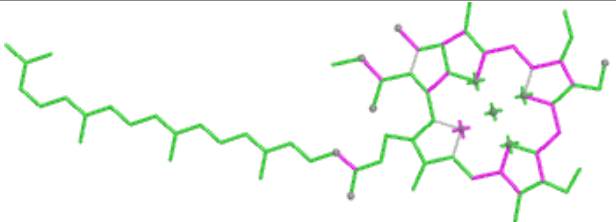
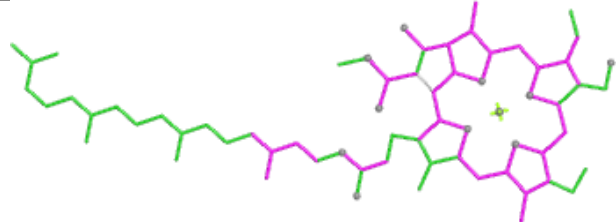
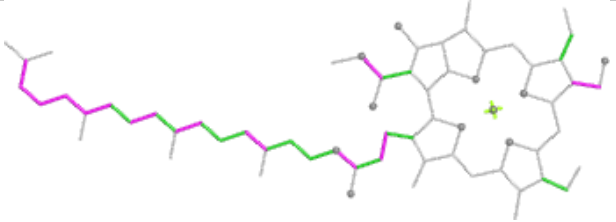
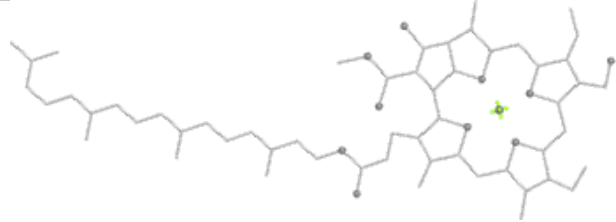
Torsions

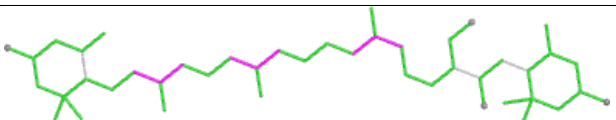
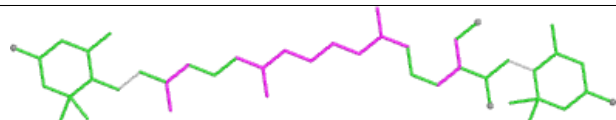
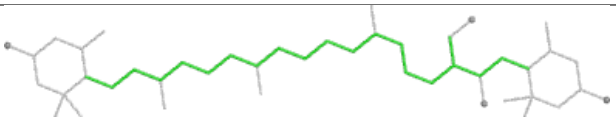
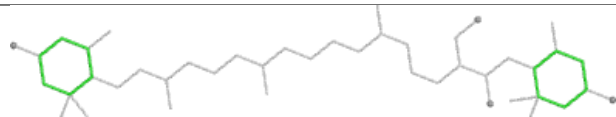


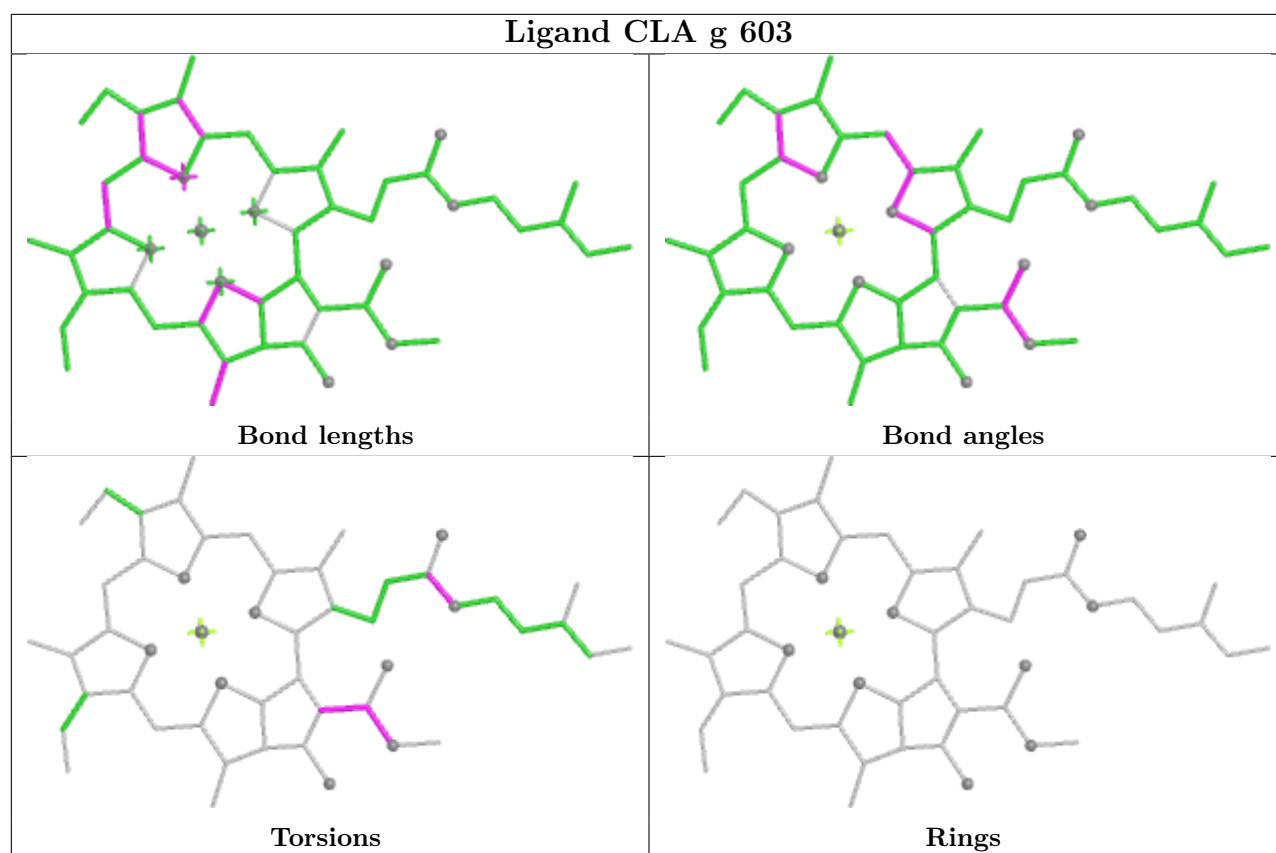
Rings



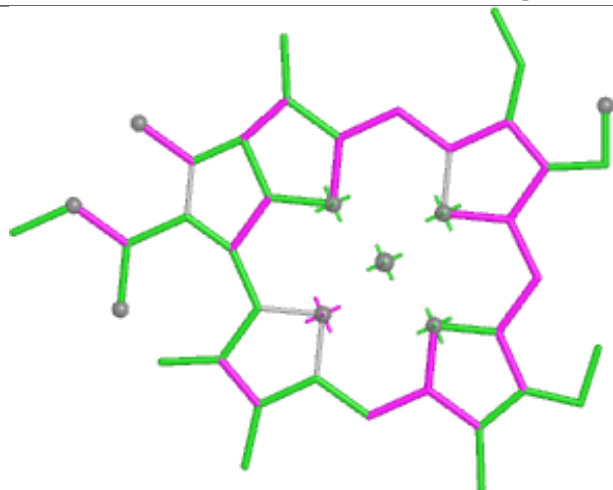


Ligand CHL b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

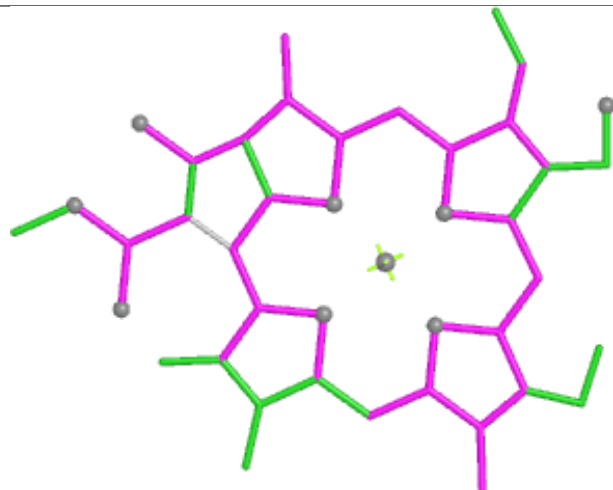
Ligand OIE h 522	
	
Bond lengths	Bond angles
	
Torsions	Rings



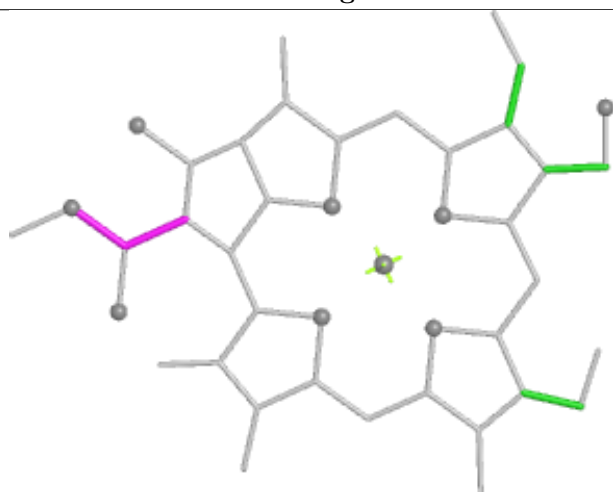
Ligand CHL h 614



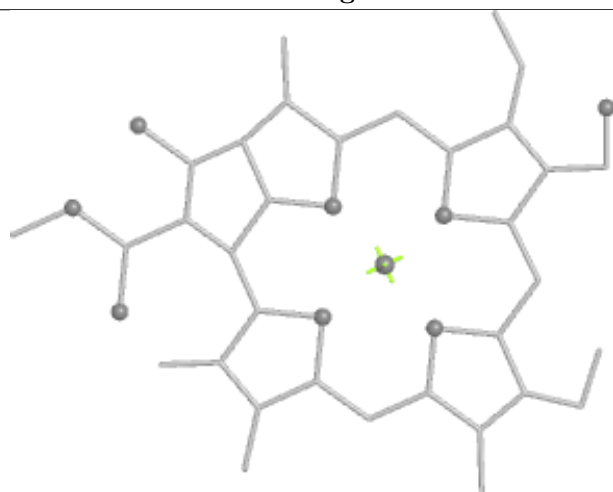
Bond lengths



Bond angles

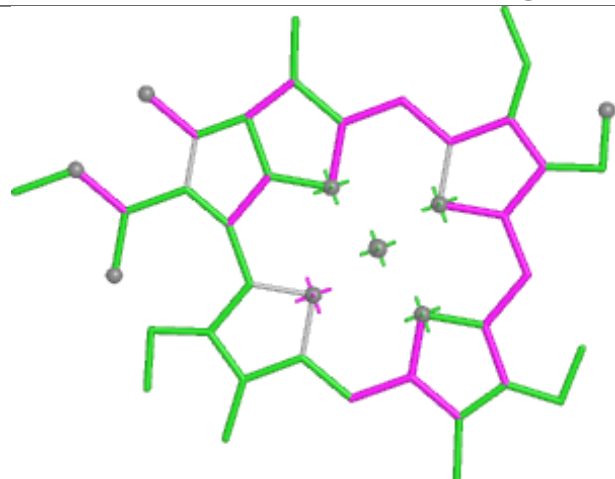


Torsions

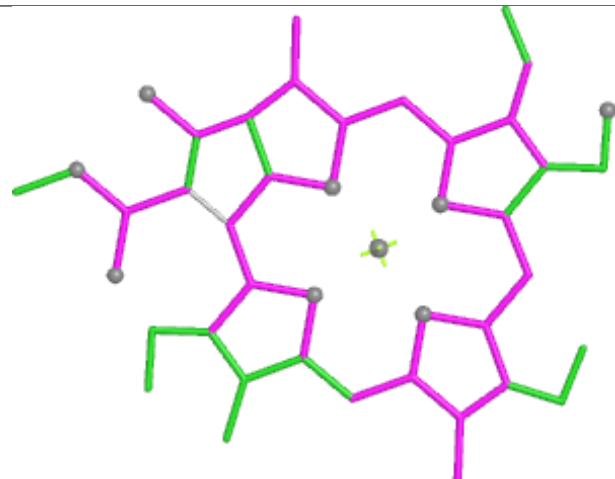


Rings

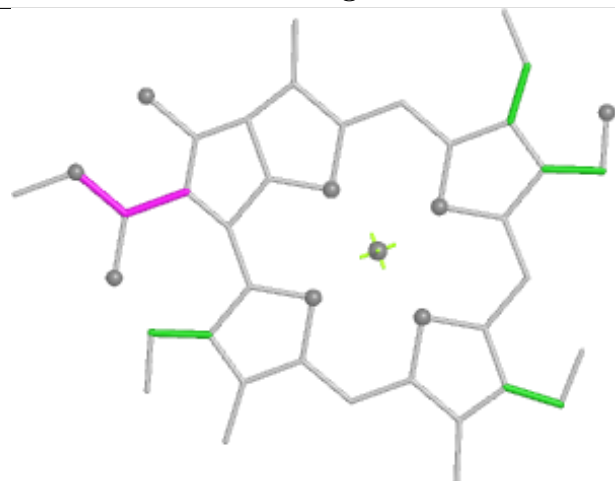
Ligand CHL 8 315



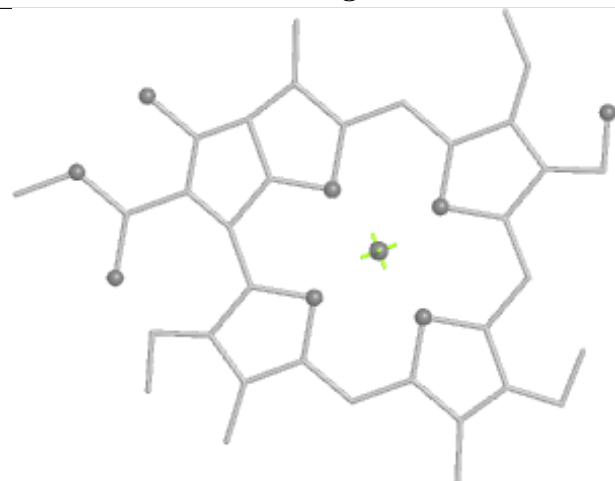
Bond lengths



Bond angles

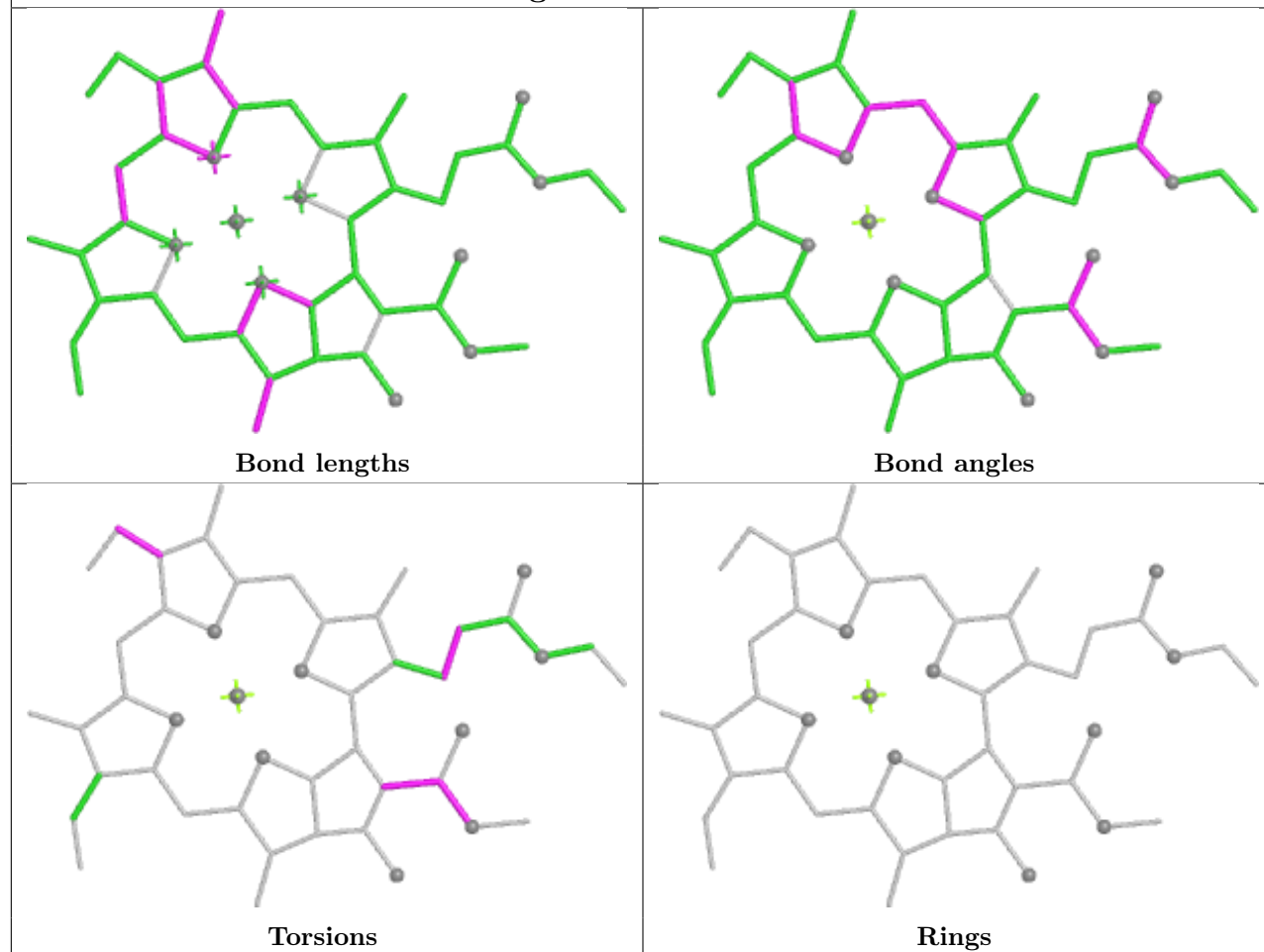


Torsions

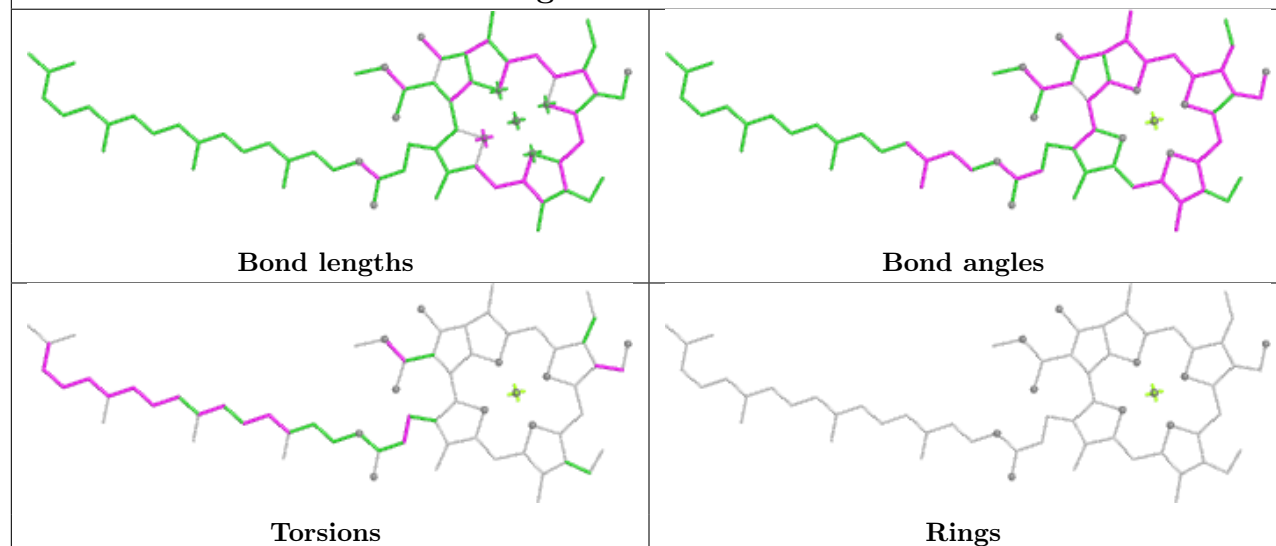


Rings

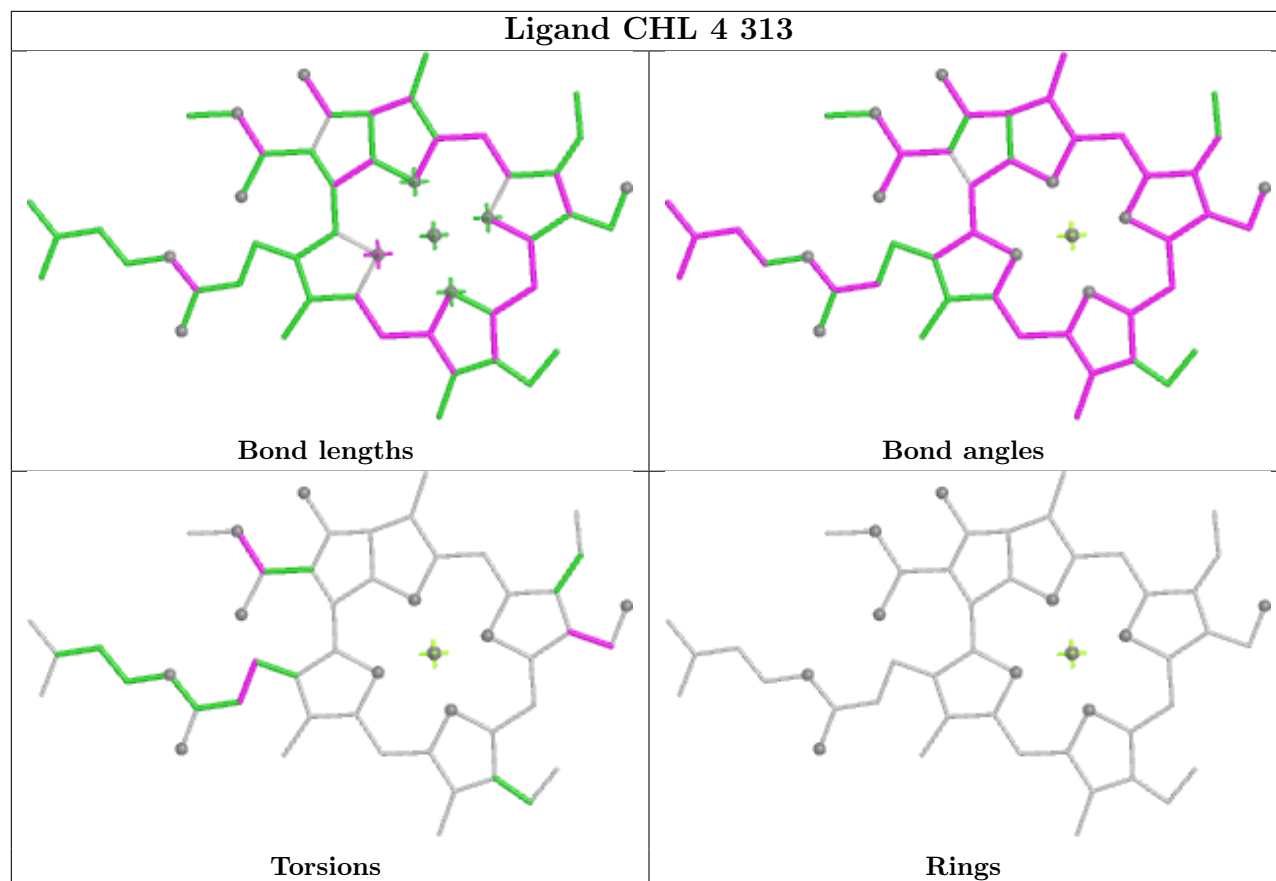
Ligand CLA L 207



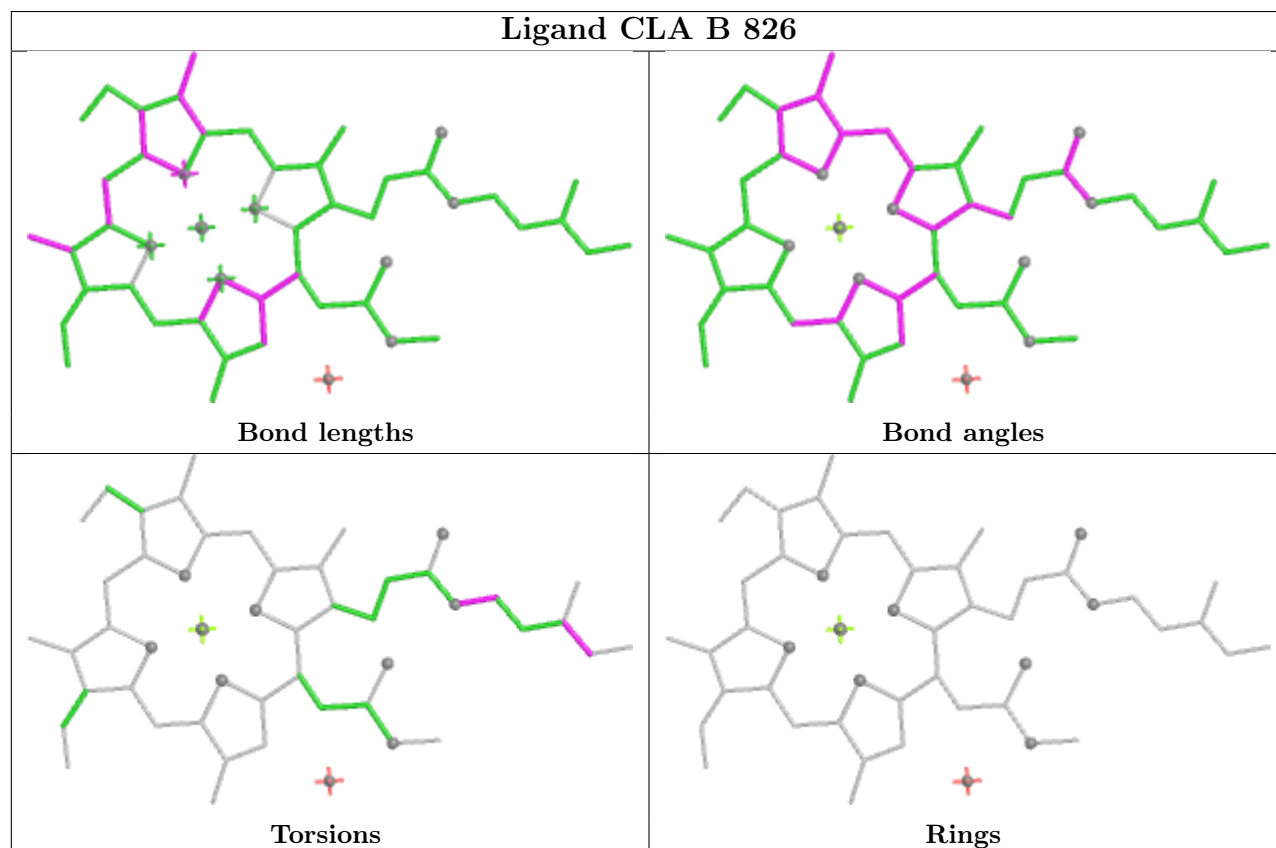
Ligand CHL c 608

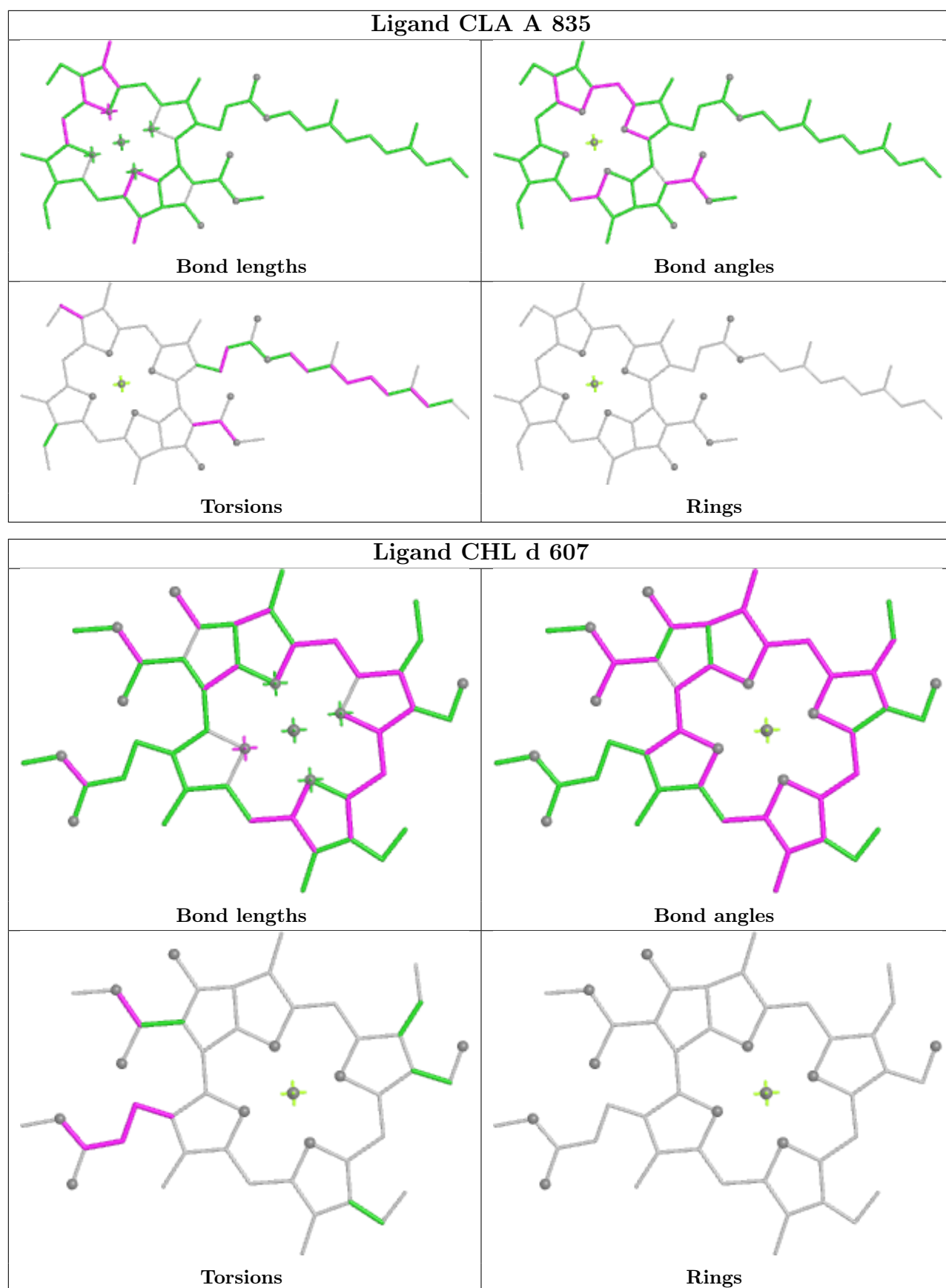


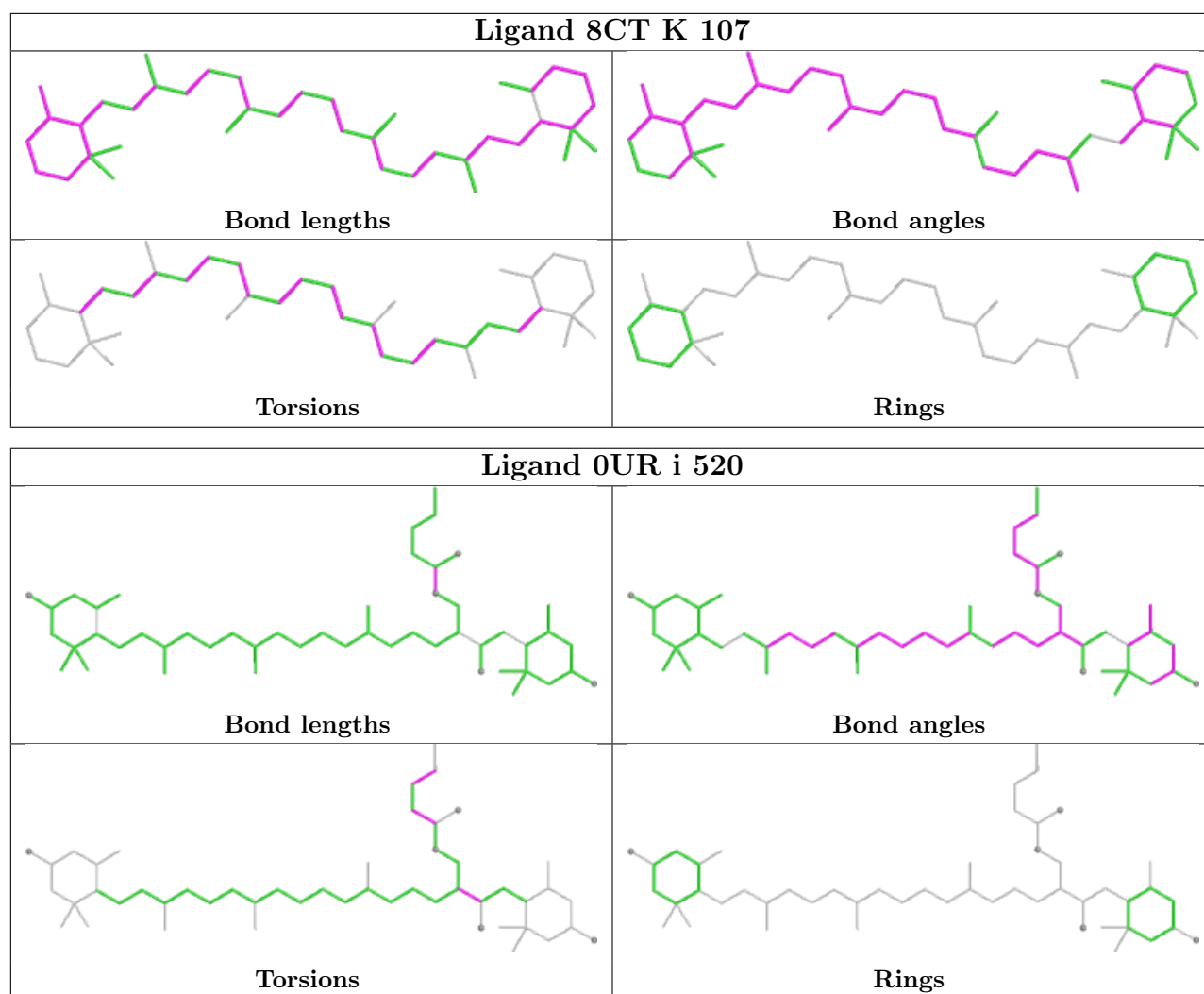
Ligand CHL 4 313

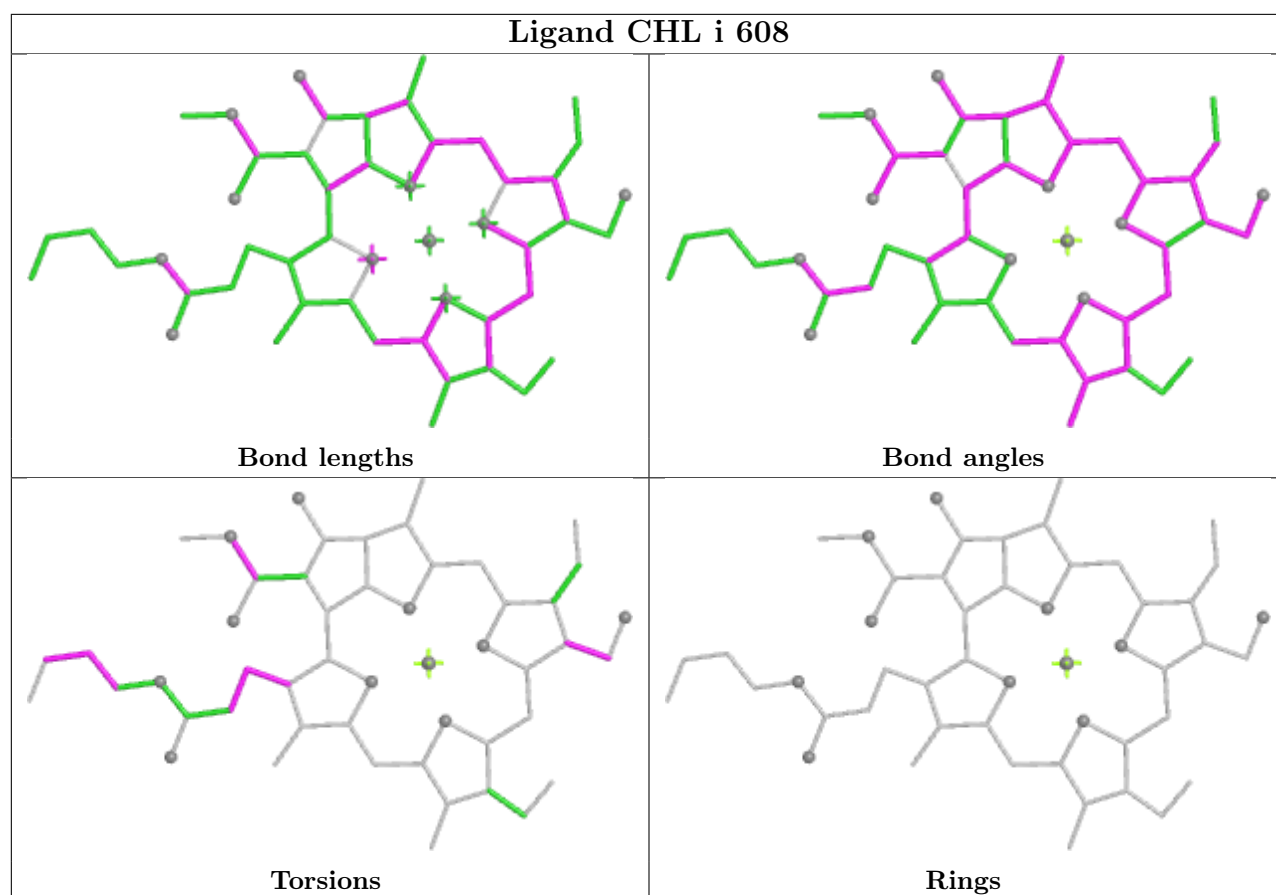


Ligand CLA B 826

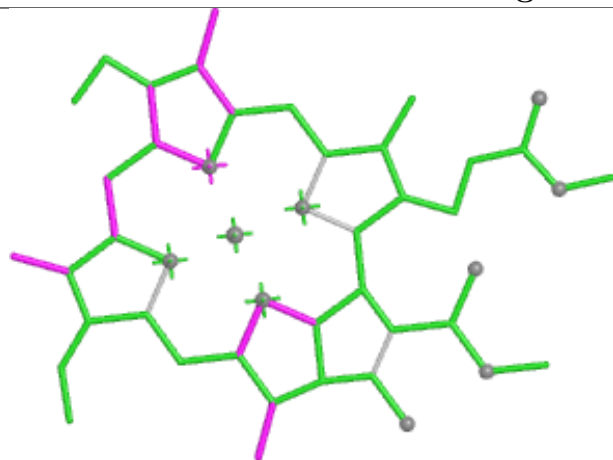




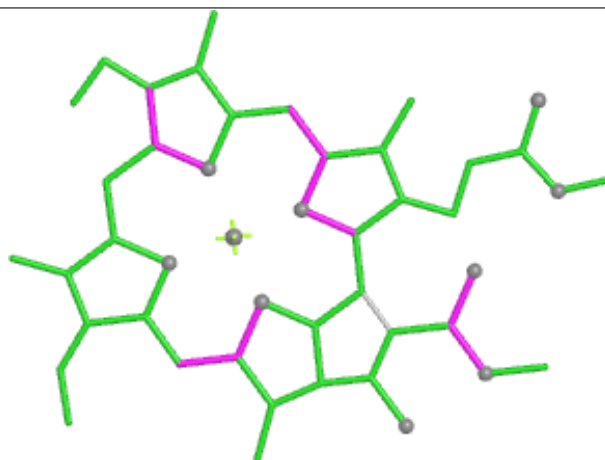




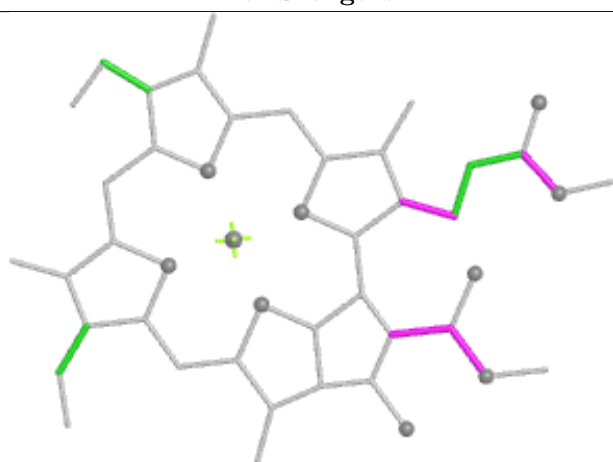
Ligand CLA L 204



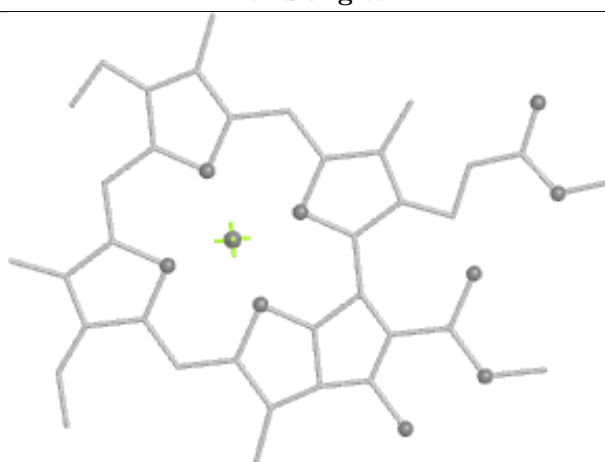
Bond lengths



Bond angles

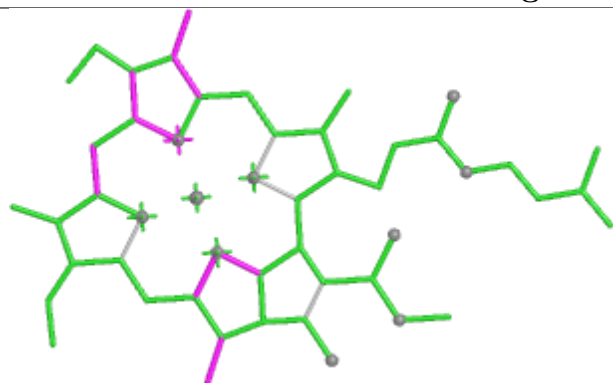


Torsions

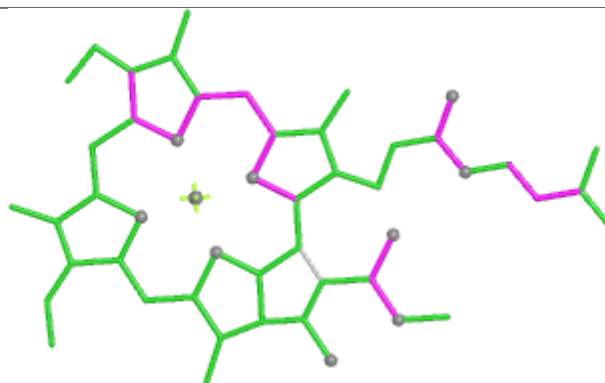


Rings

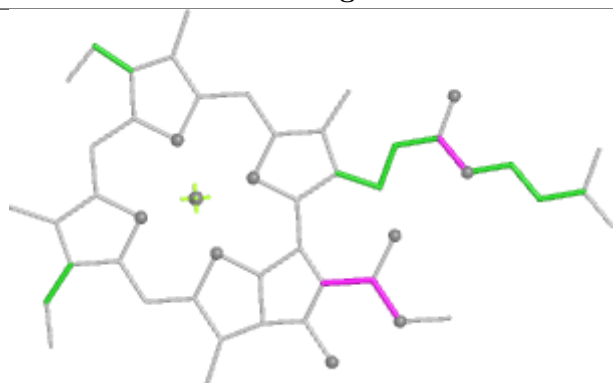
Ligand CLA f 604



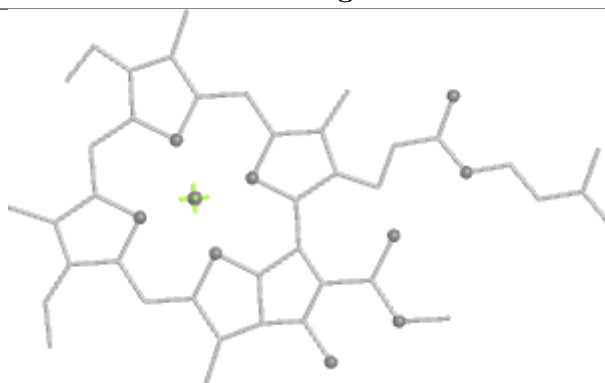
Bond lengths



Bond angles

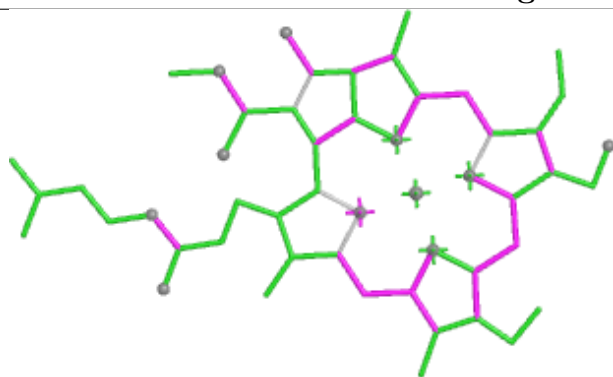


Torsions

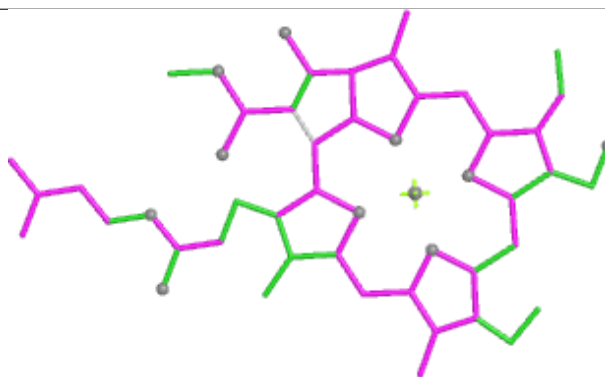


Rings

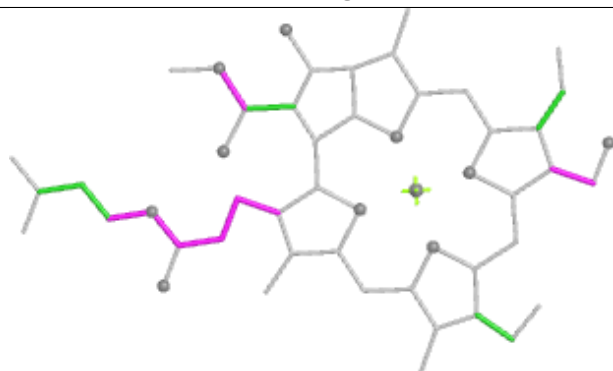
Ligand CHL 8 307



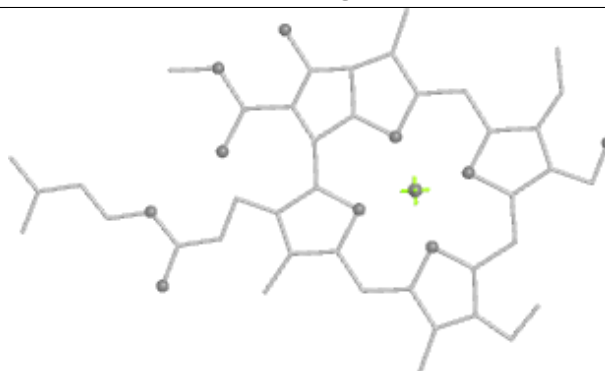
Bond lengths



Bond angles

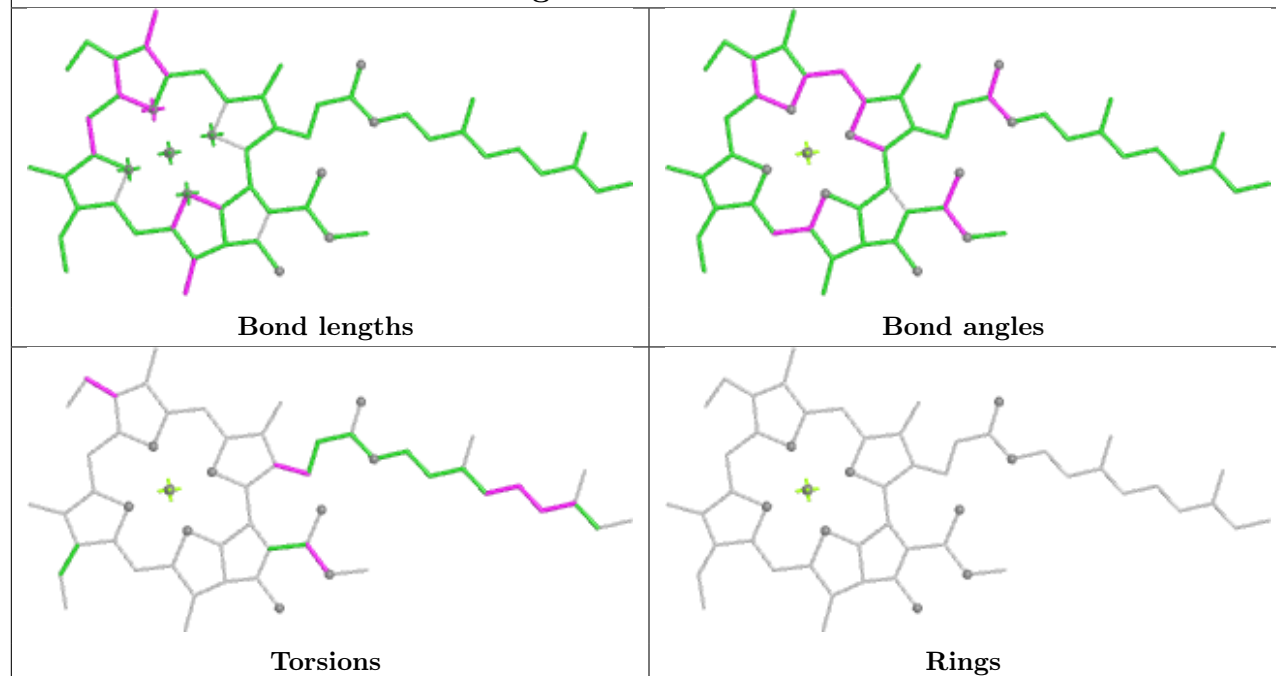


Torsions

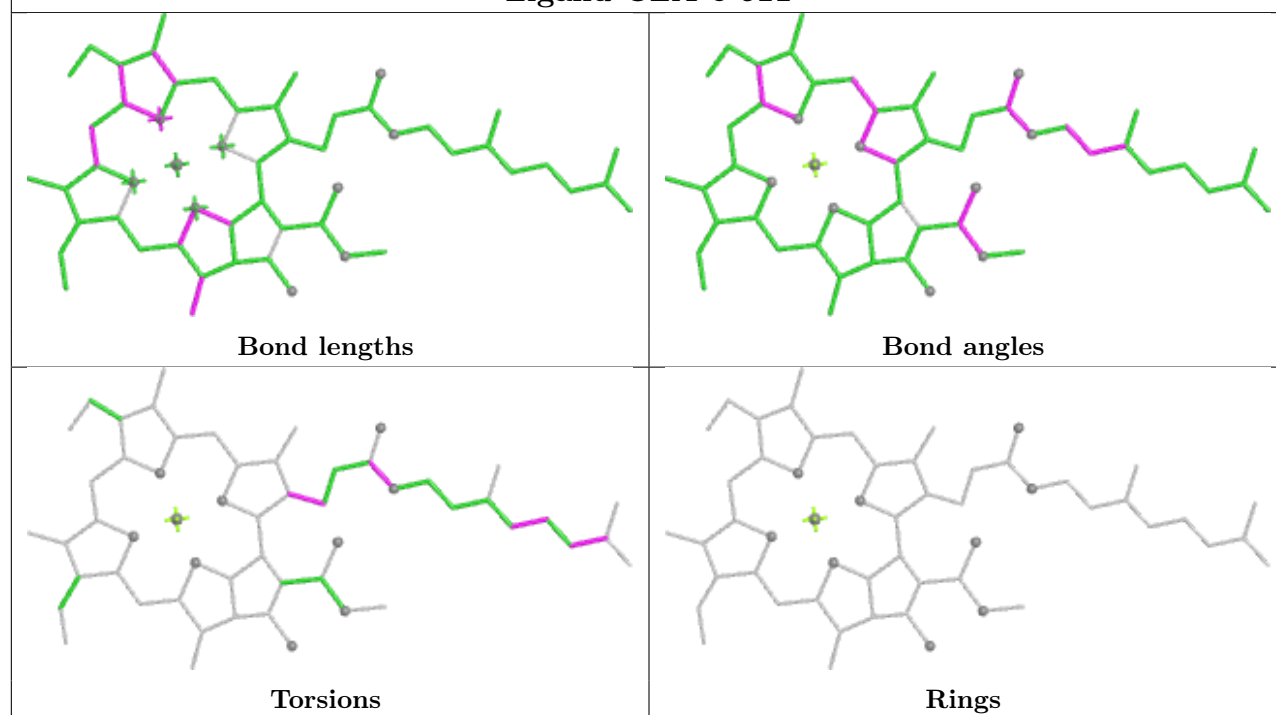


Rings

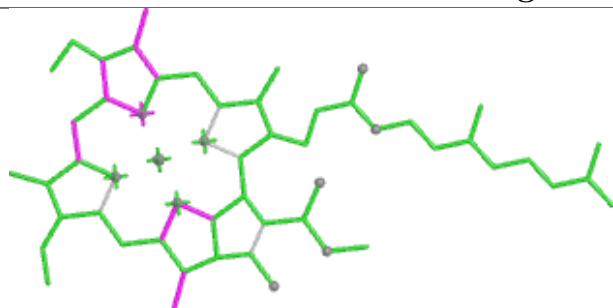
Ligand CLA B 820



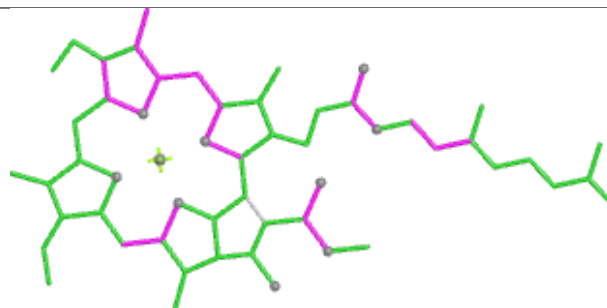
Ligand CLA e 611



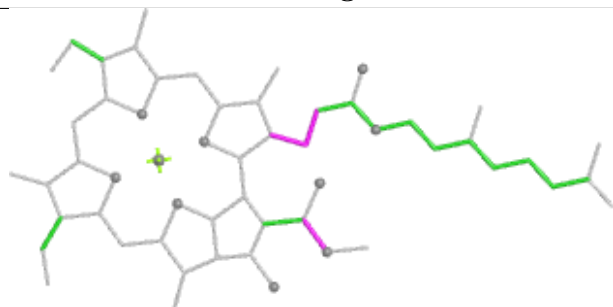
Ligand CLA b 610



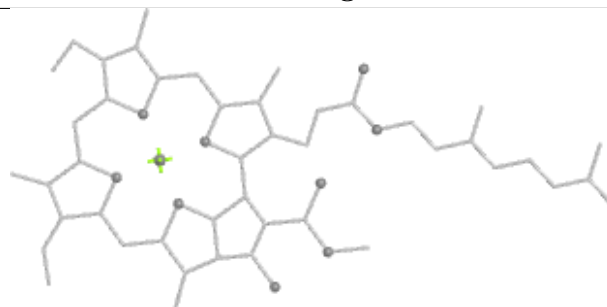
Bond lengths



Bond angles

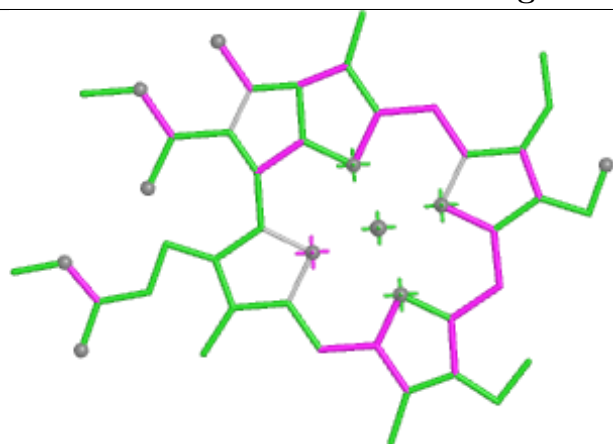


Torsions

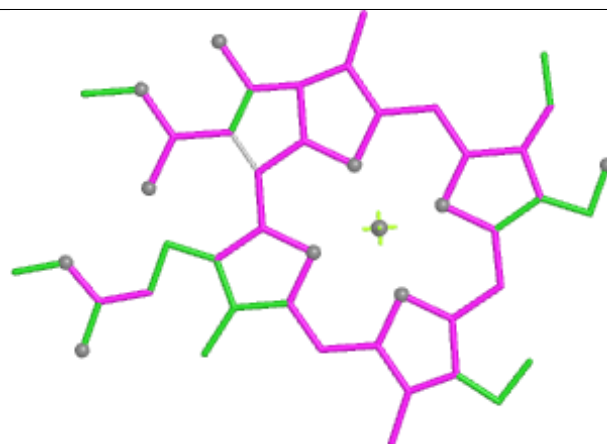


Rings

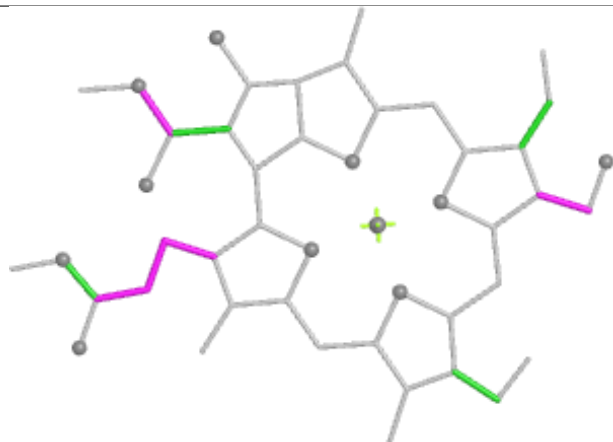
Ligand CHL 9 313



Bond lengths



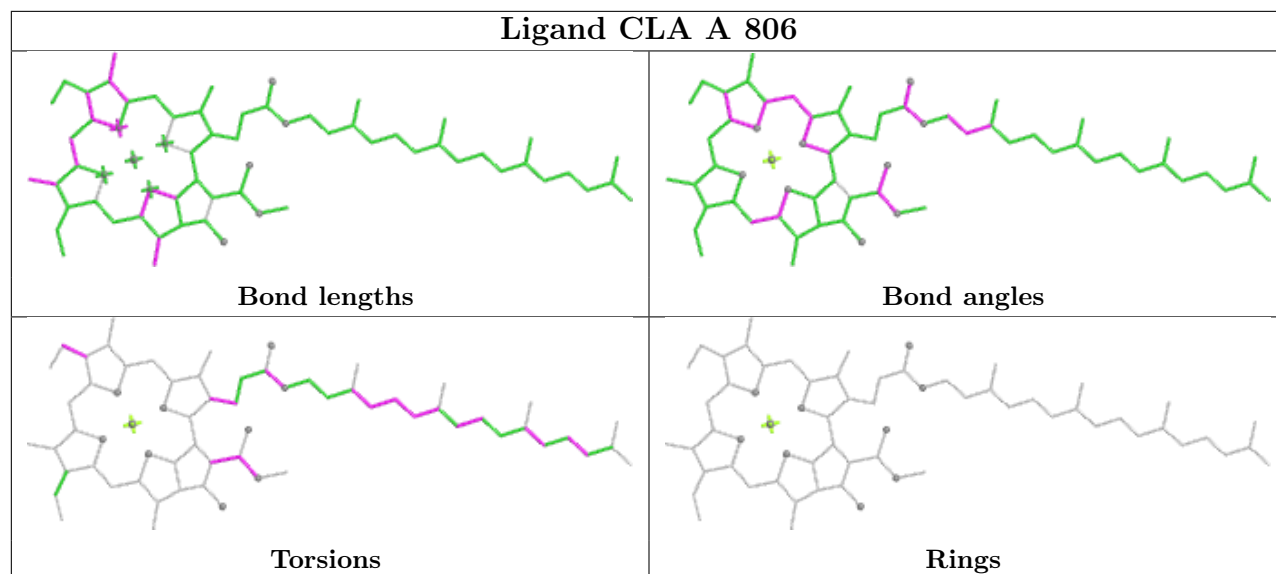
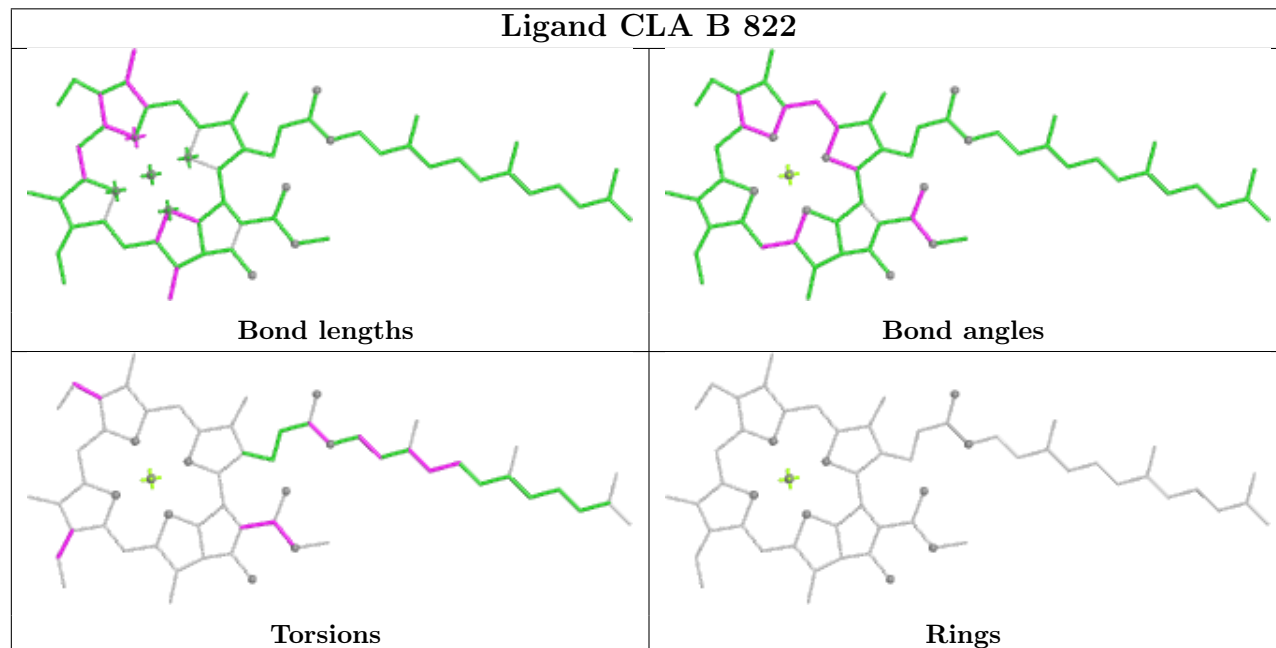
Bond angles



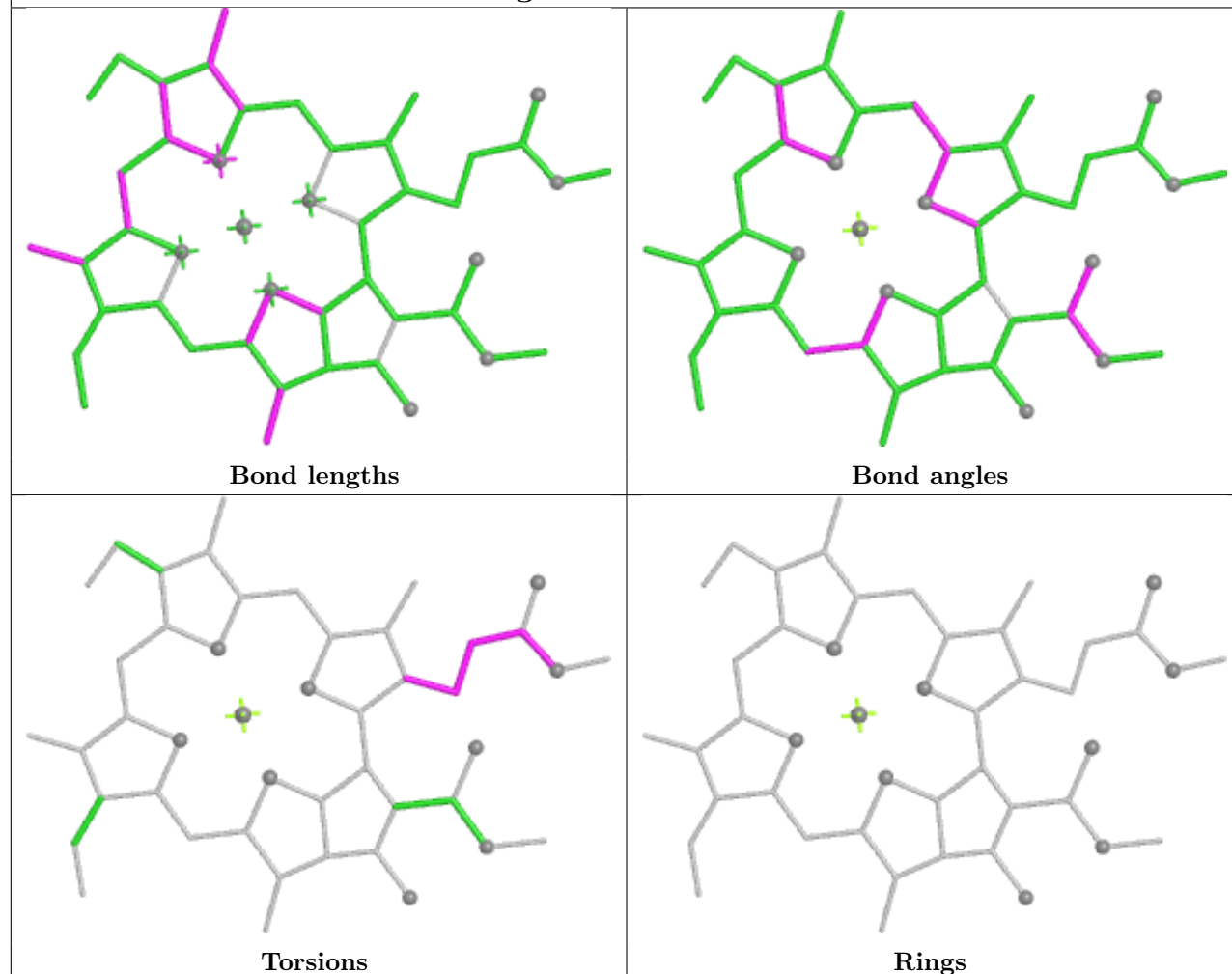
Torsions



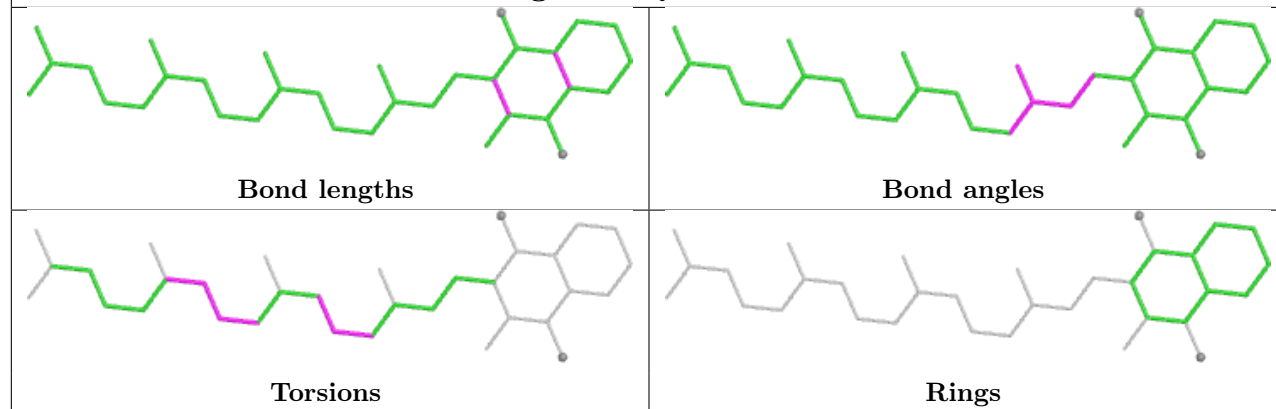
Rings

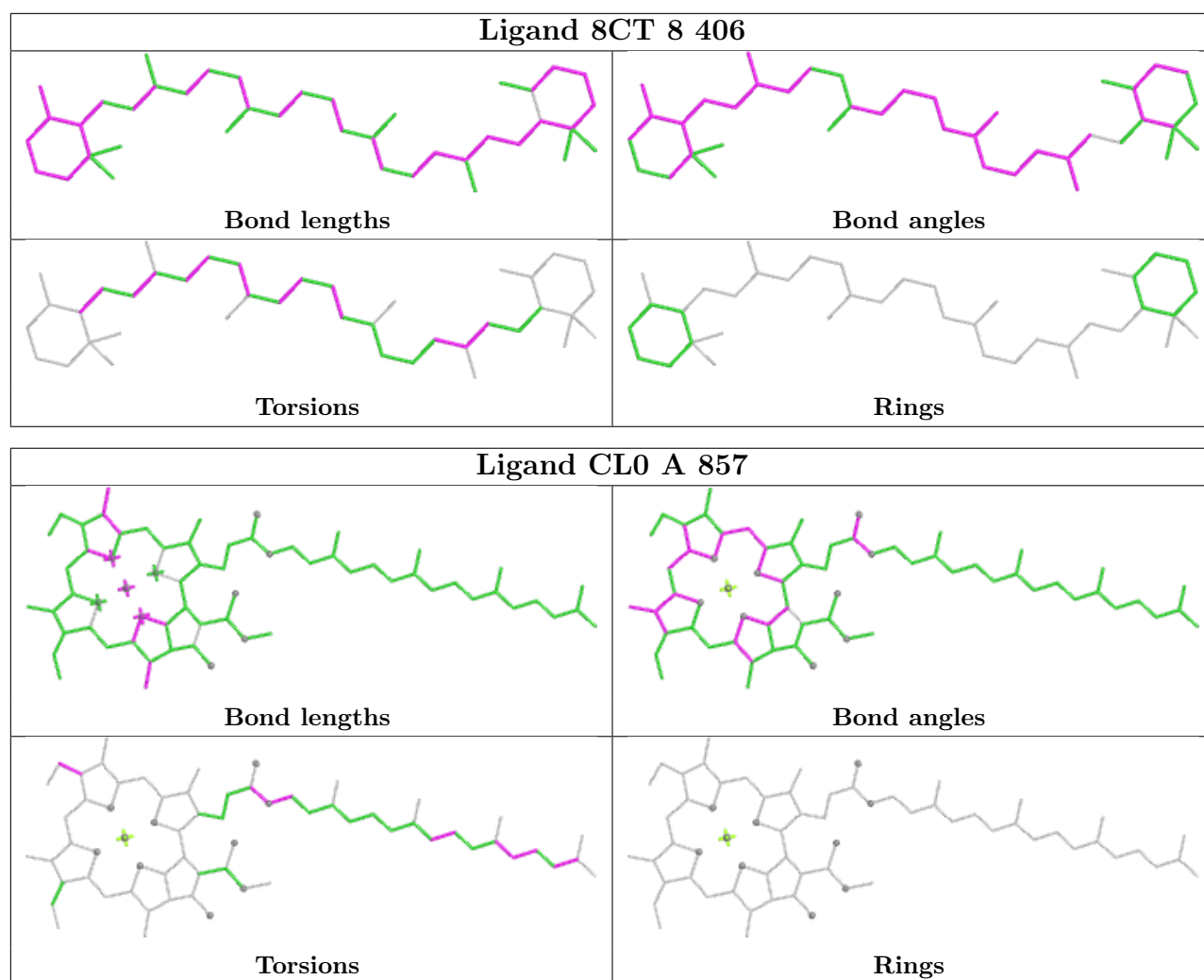
Ligand CLA A 806**Ligand CLA B 822**

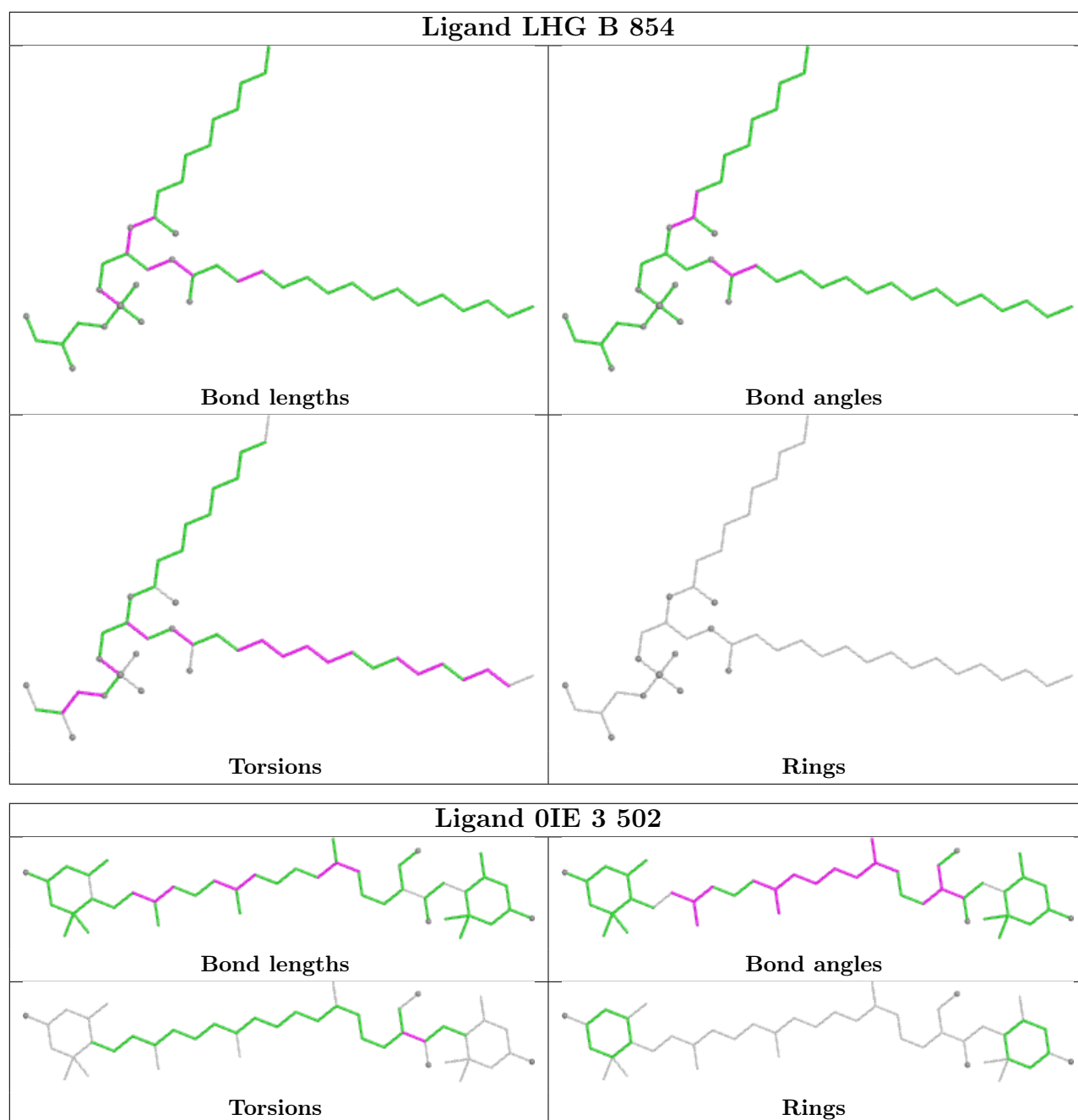
Ligand CLA L 202

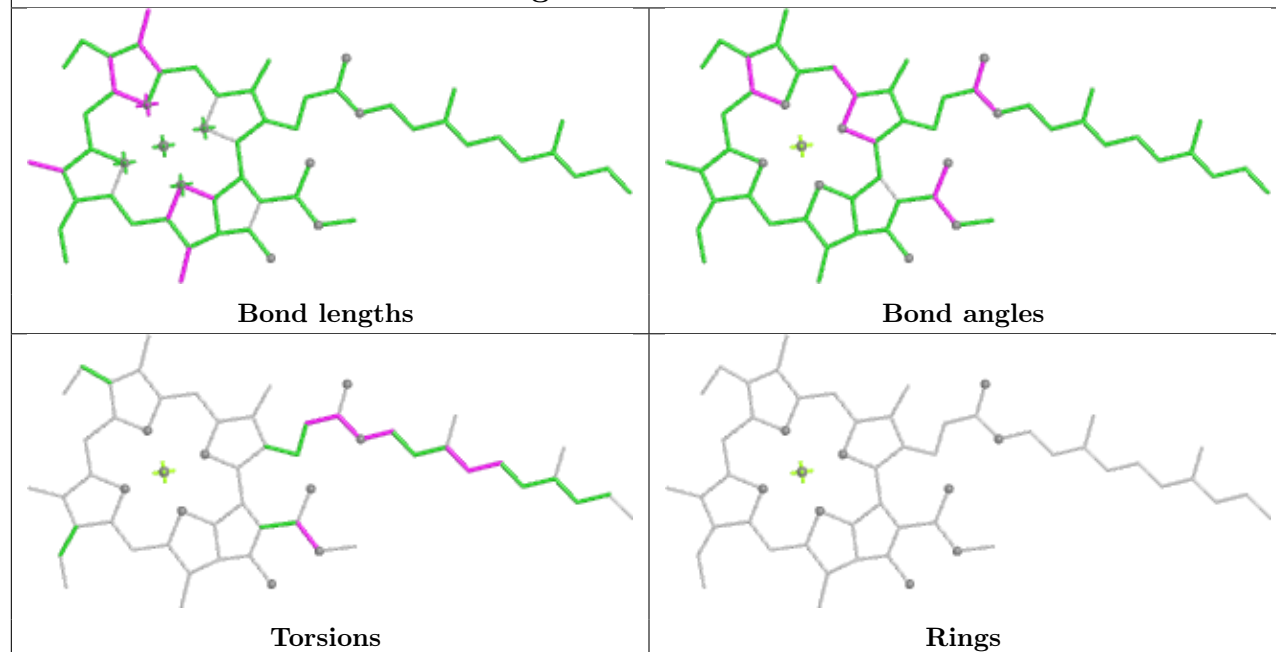
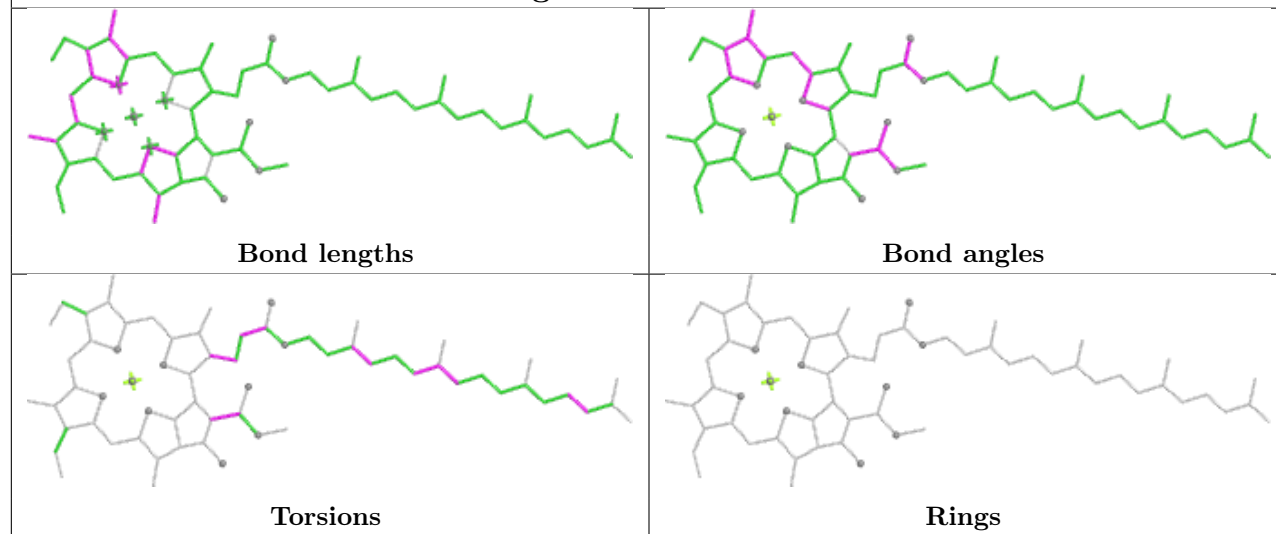


Ligand PQN B 842

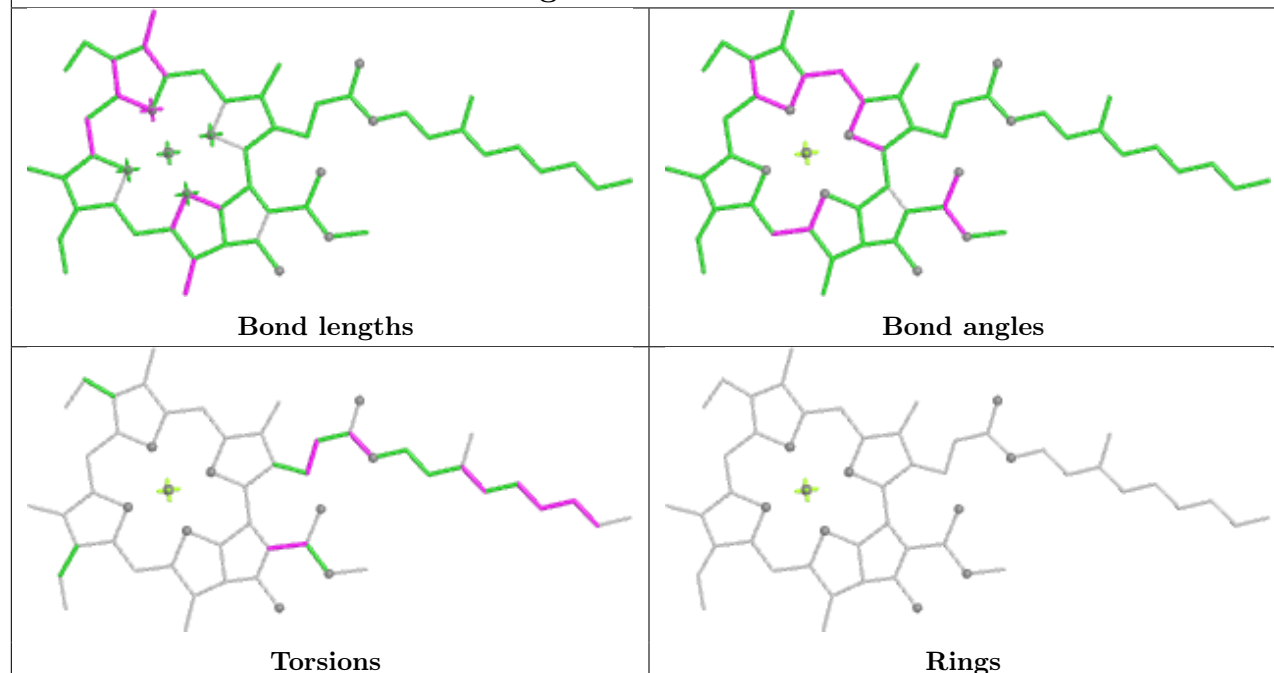




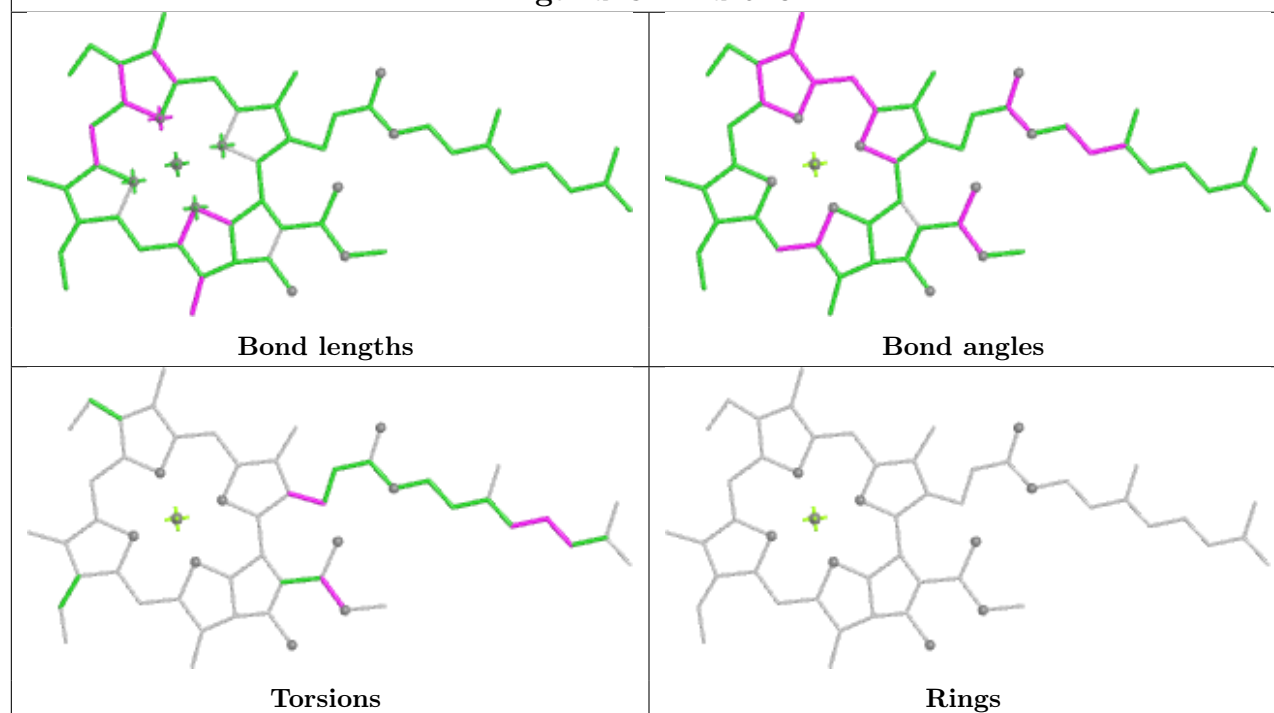


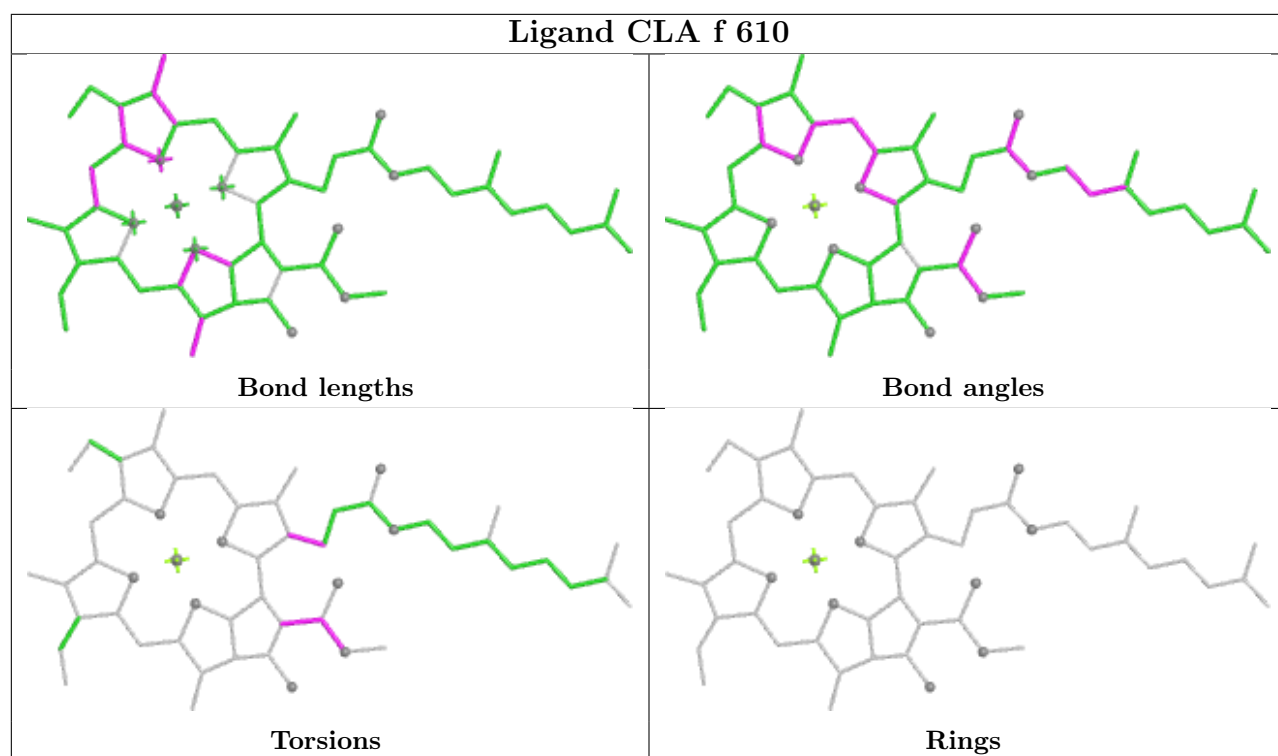
Ligand CLA A 814**Ligand CLA B 808**

Ligand CLA f 613

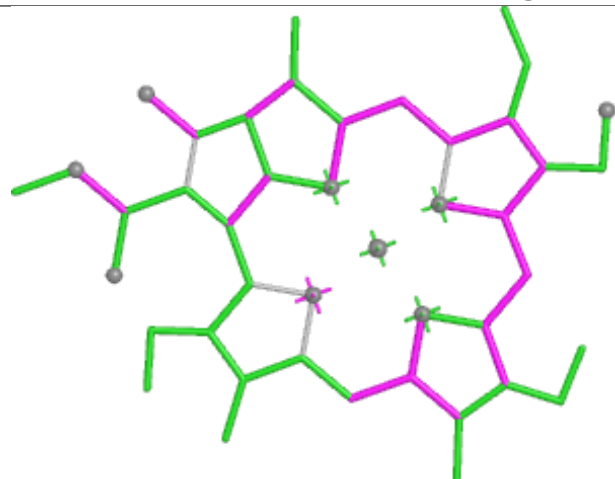


Ligand CLA d 610

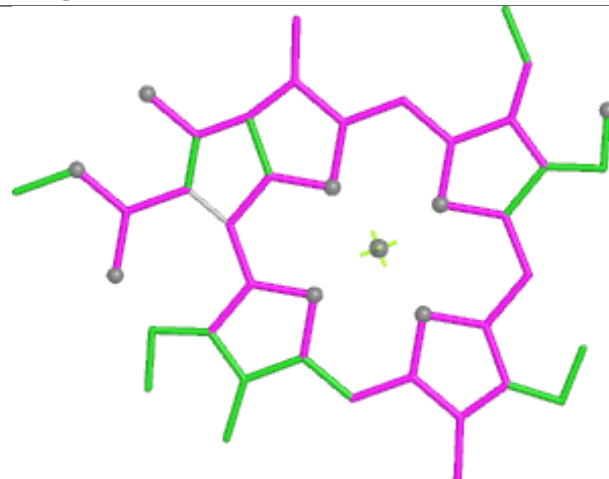




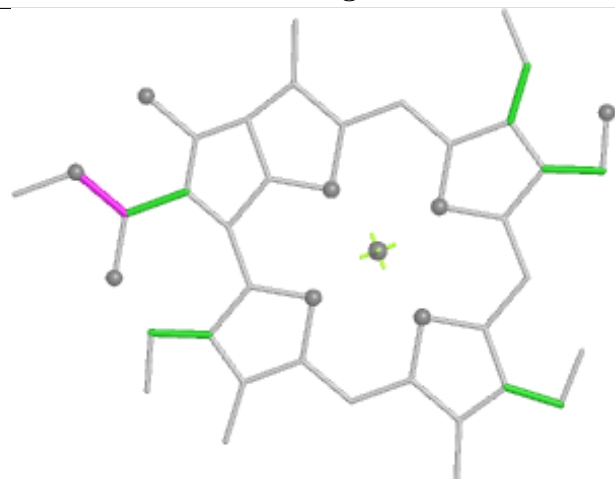
Ligand CHL g 605



Bond lengths



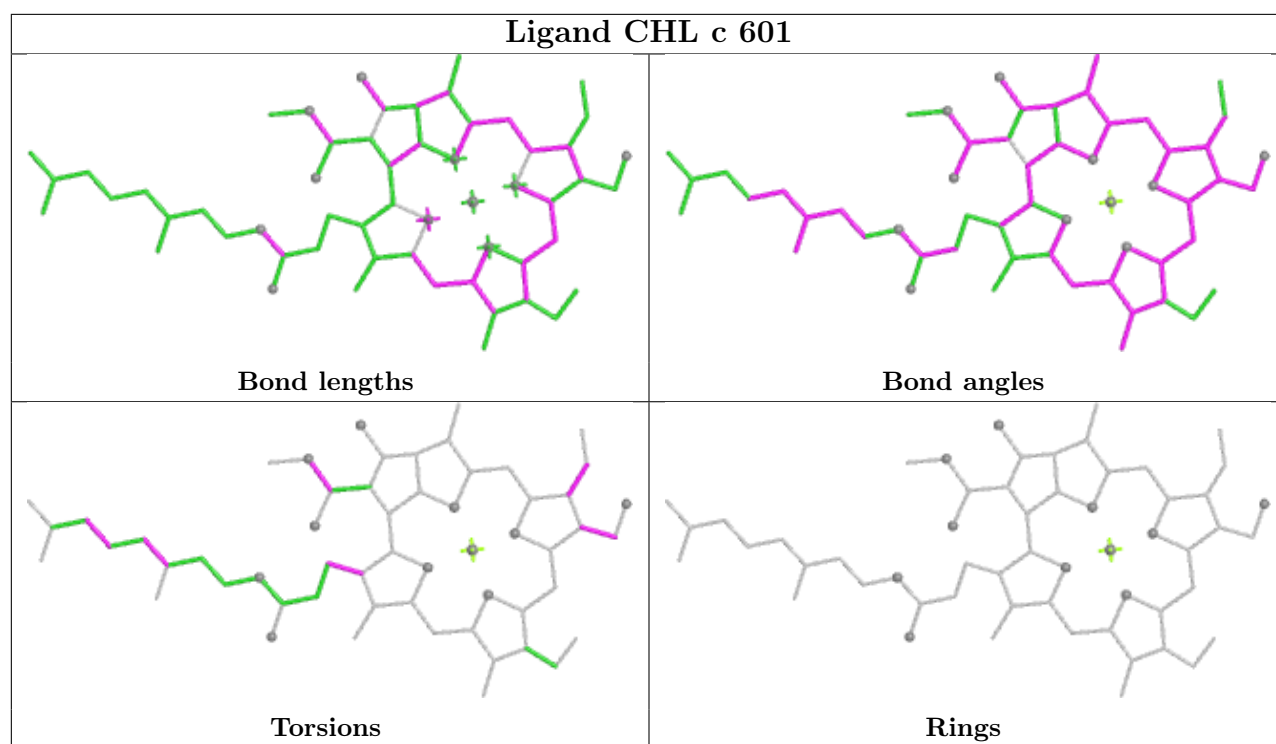
Bond angles



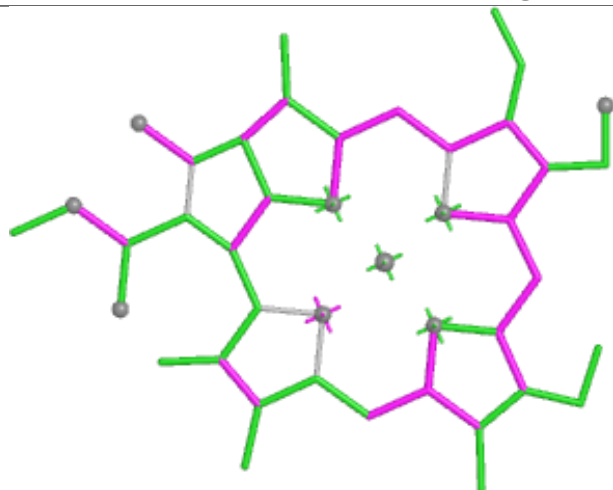
Torsions



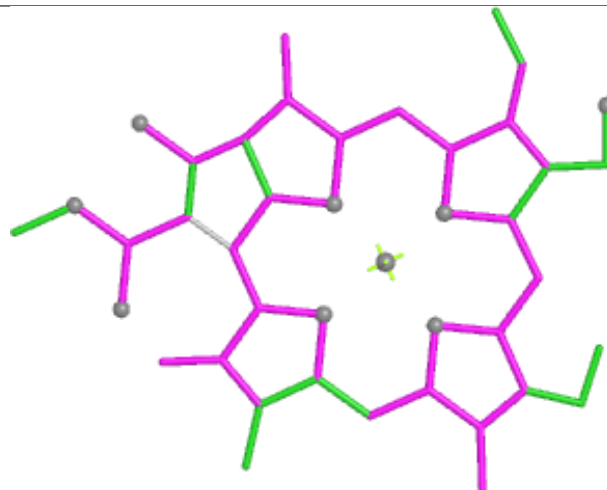
Rings



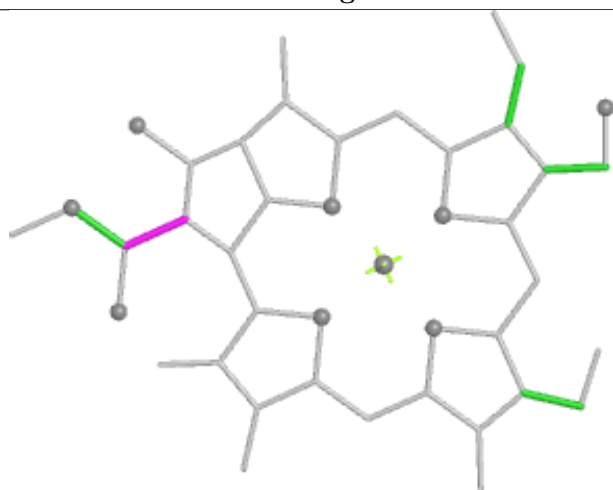
Ligand CHL d 614



Bond lengths



Bond angles

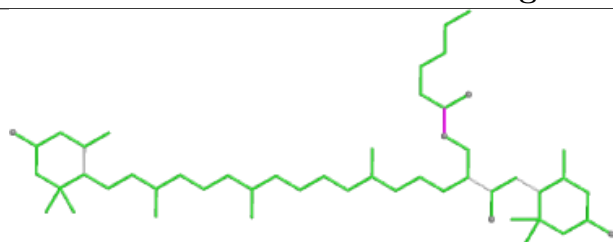


Torsions

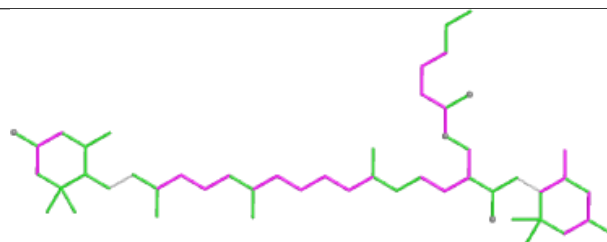


Rings

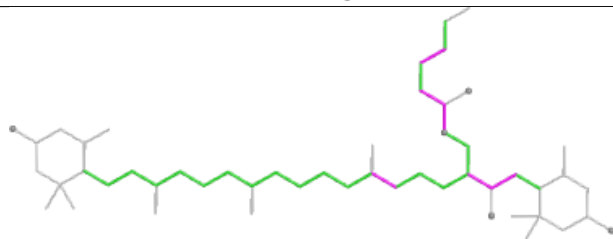
Ligand OUR 5 501



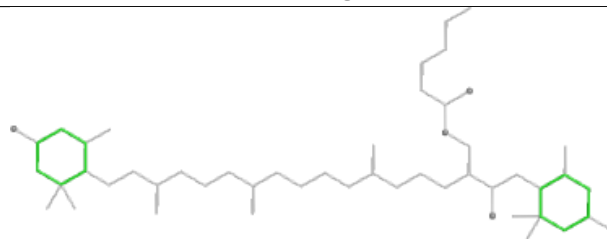
Bond lengths



Bond angles

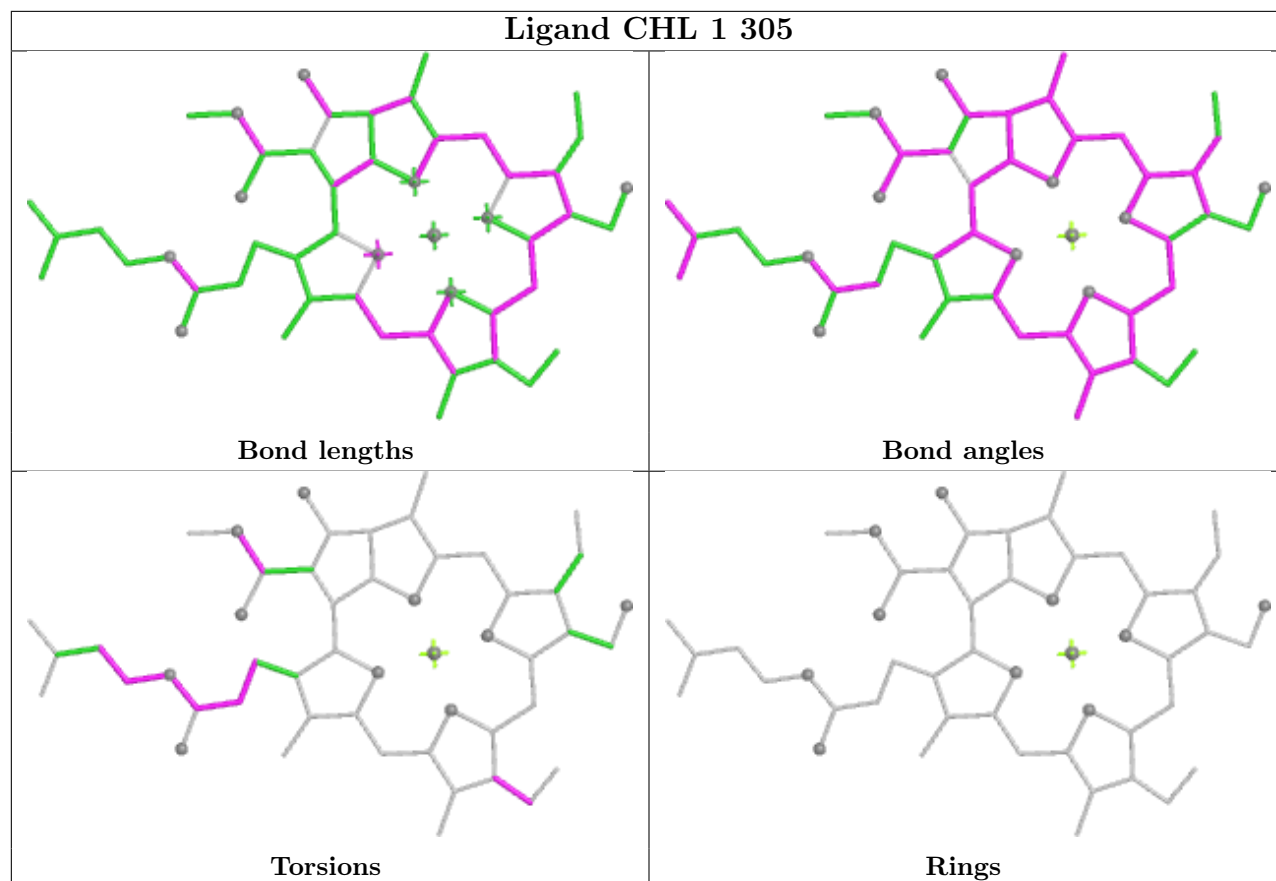


Torsions

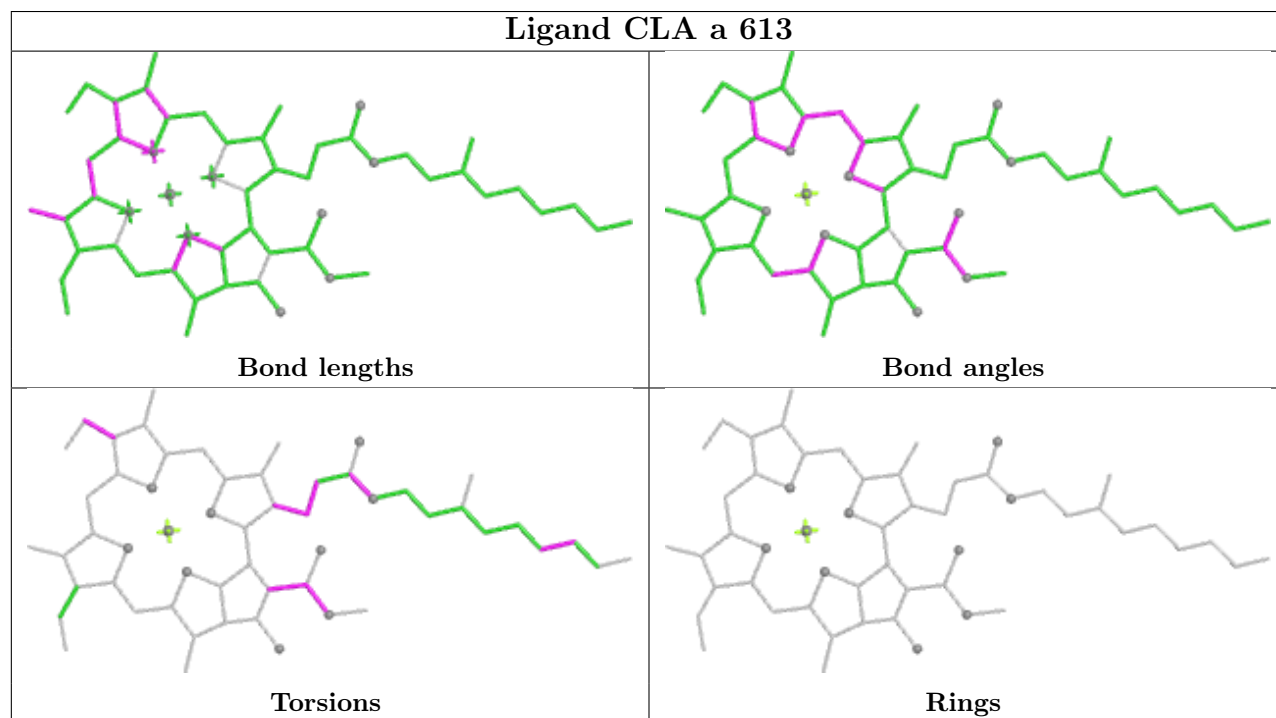


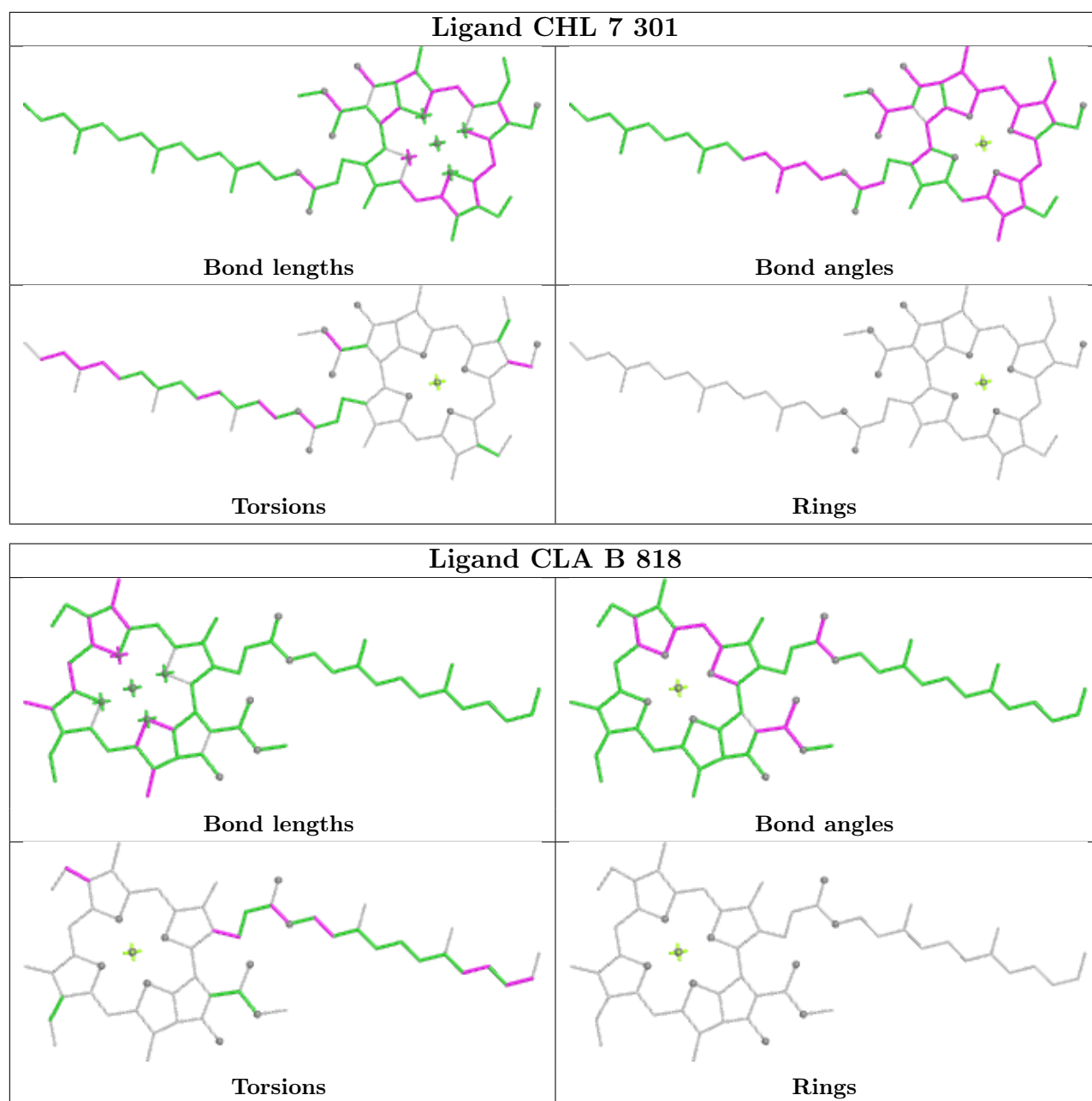
Rings

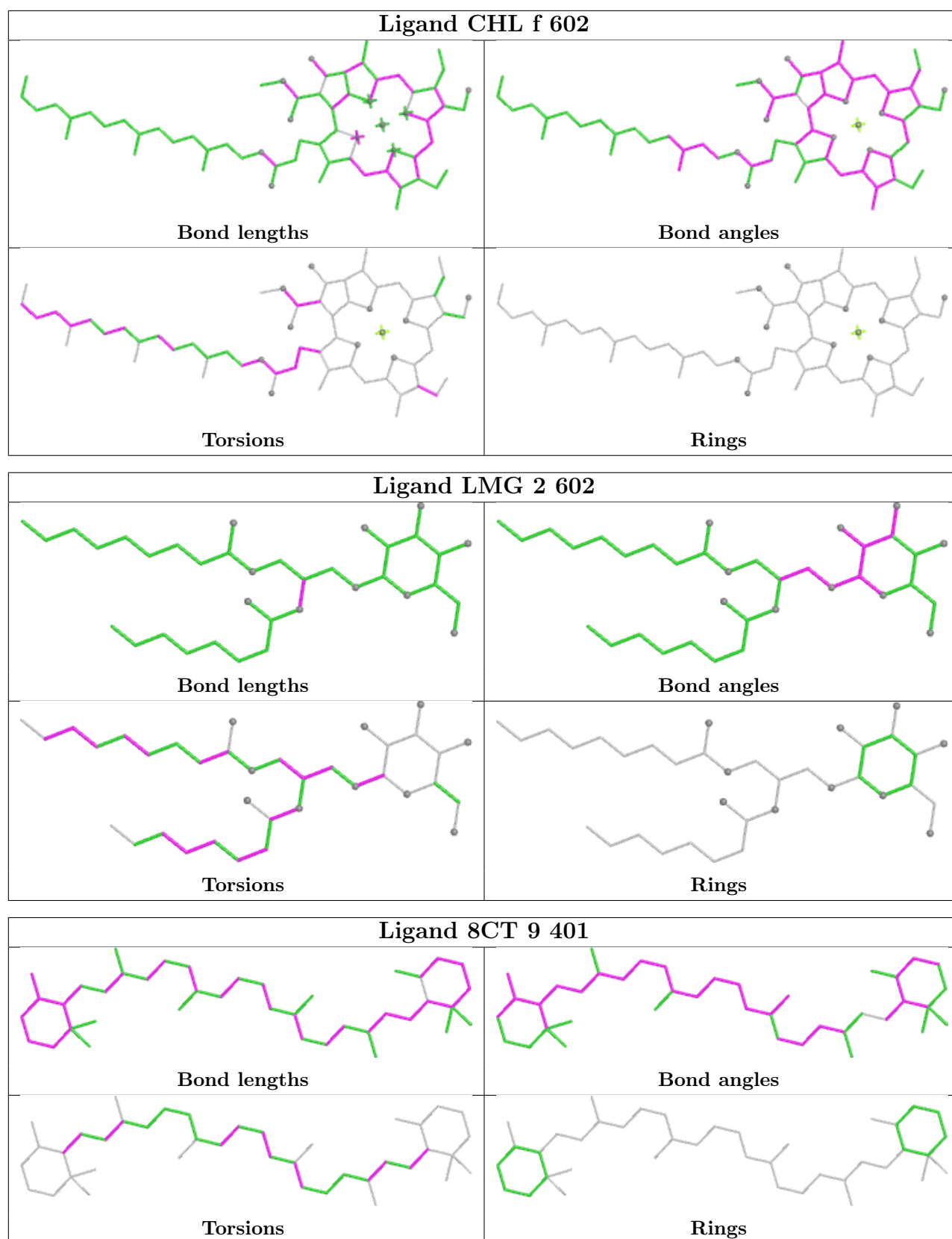
Ligand CHL 1 305



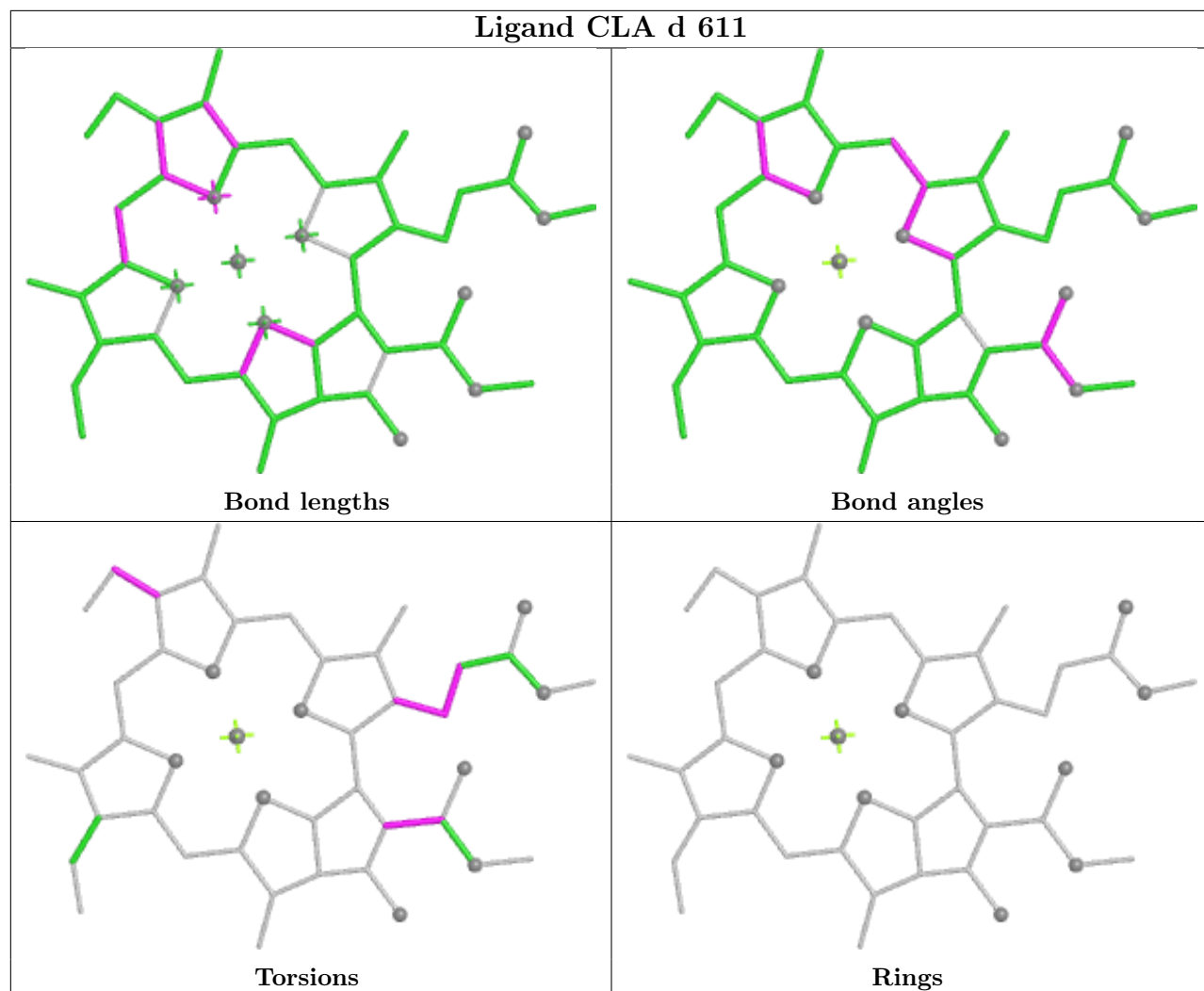
Ligand CLA a 613



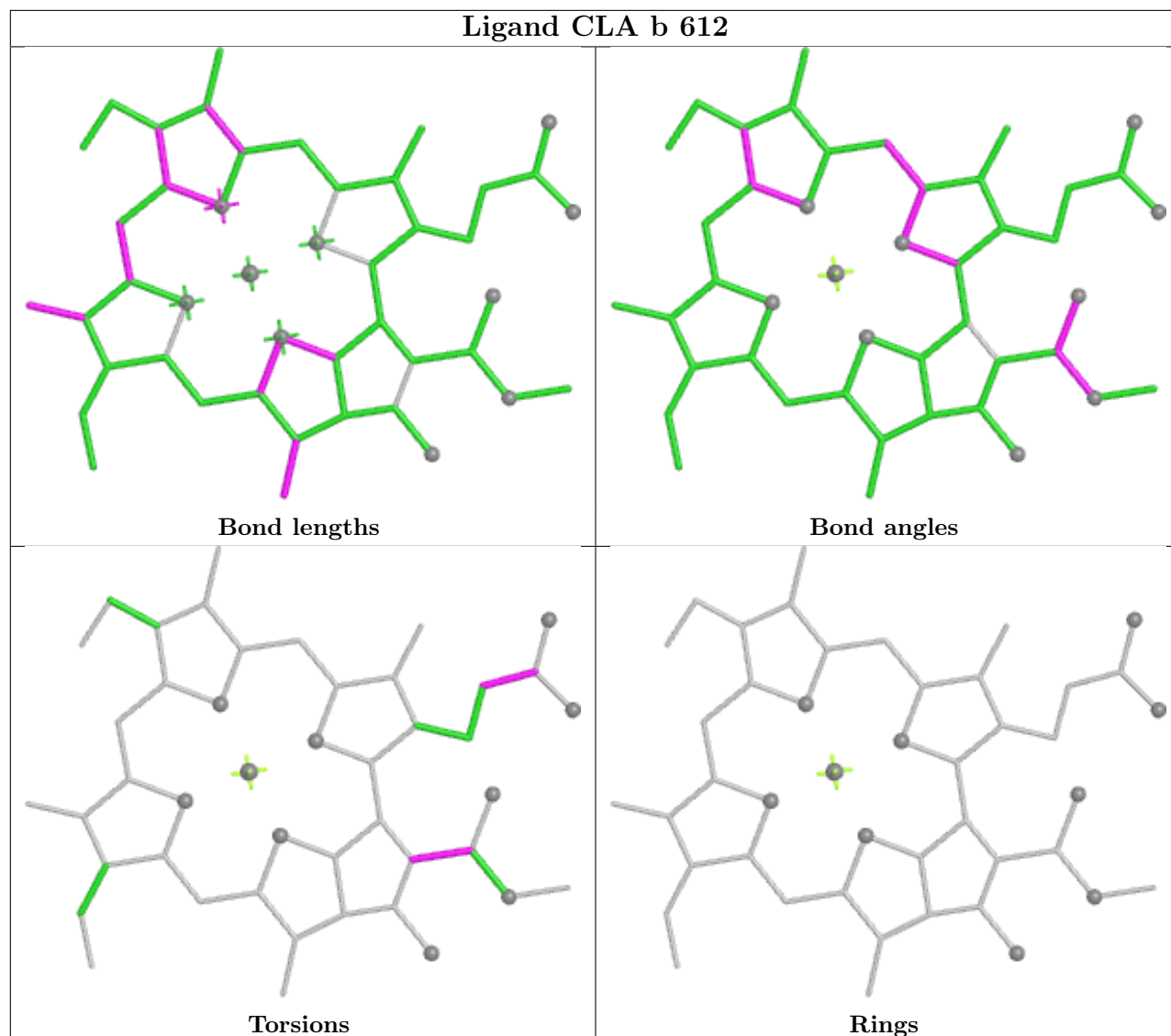




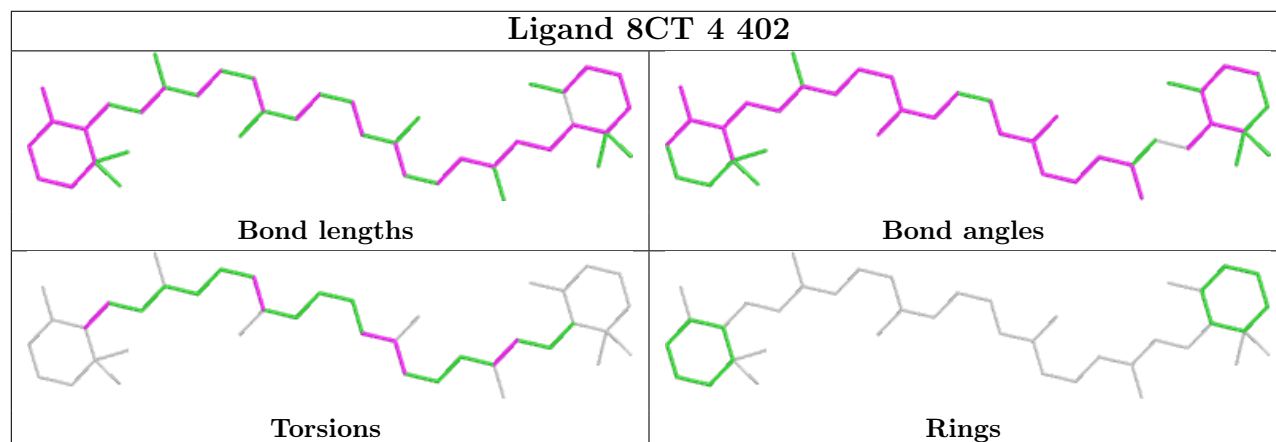
Ligand CLA d 611

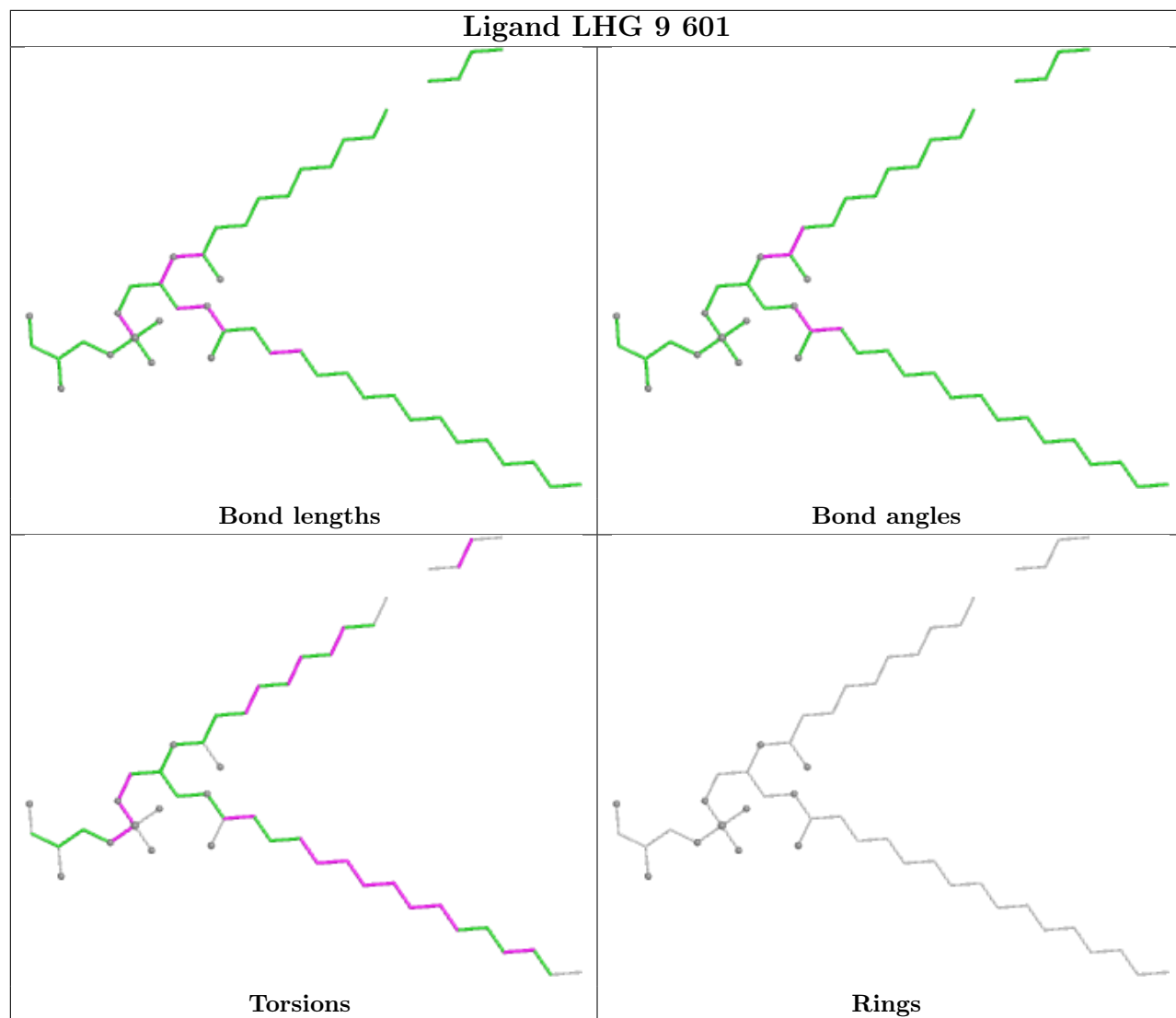


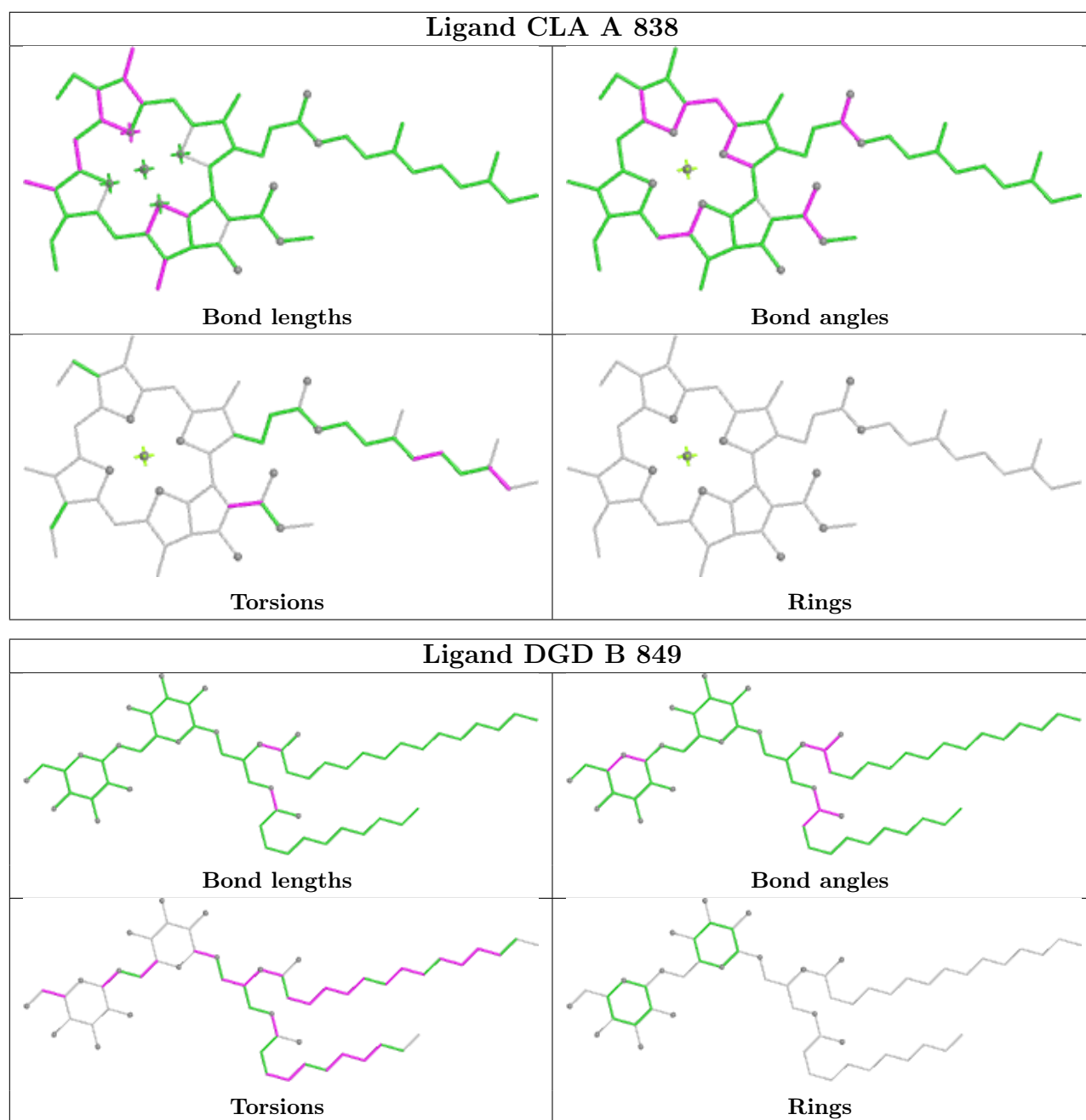
Ligand CLA b 612

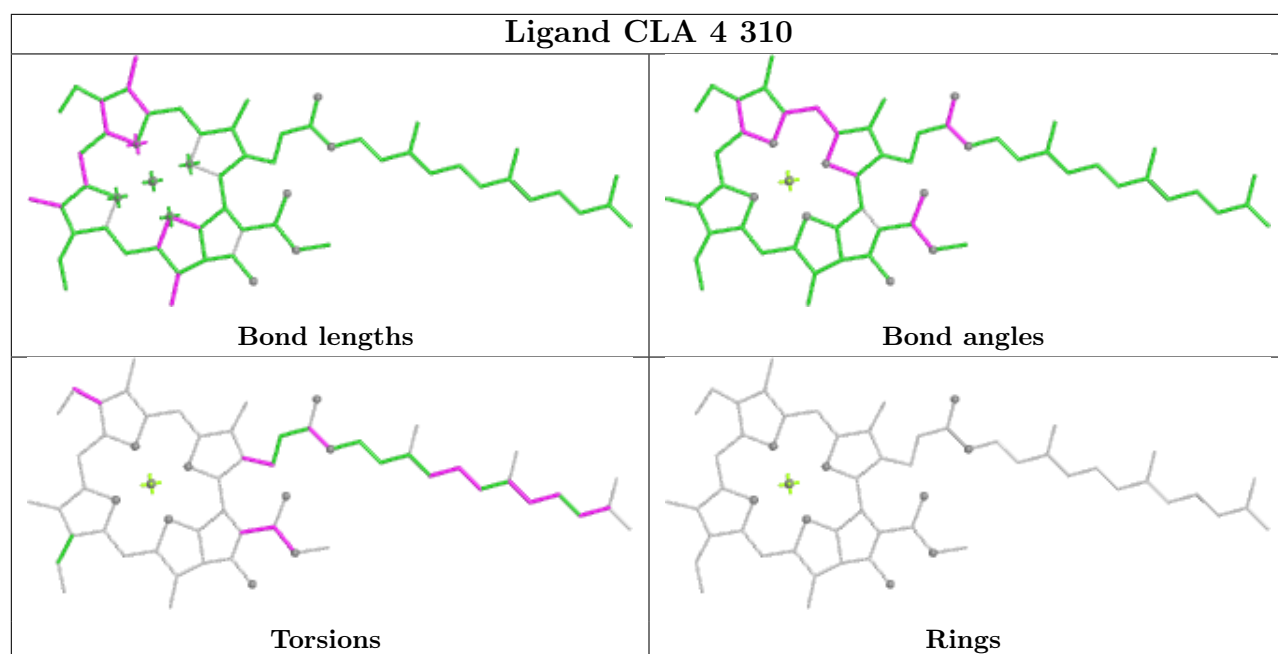


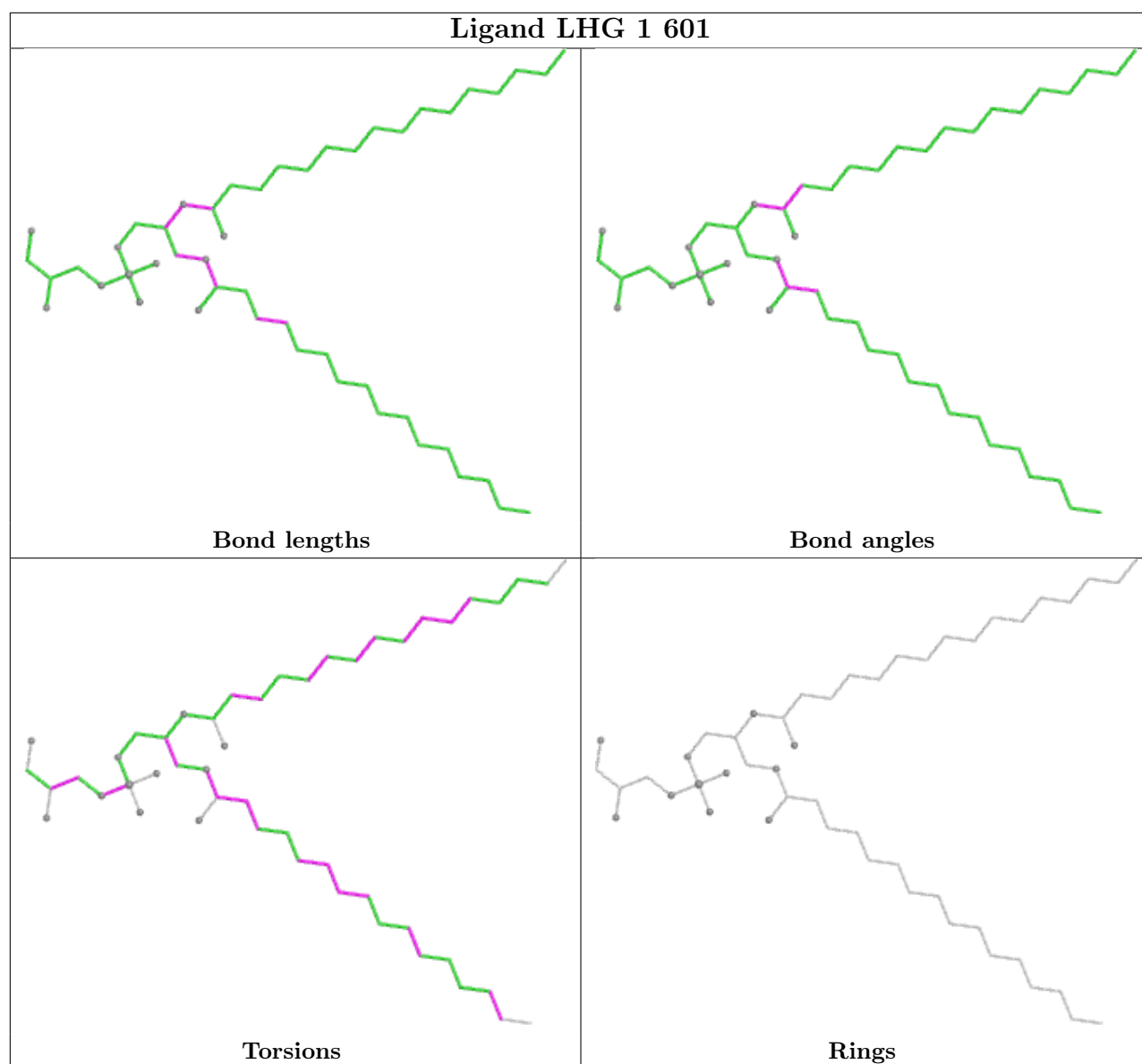
Ligand 8CT 4 402

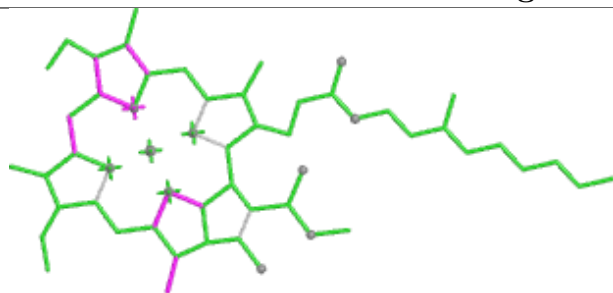




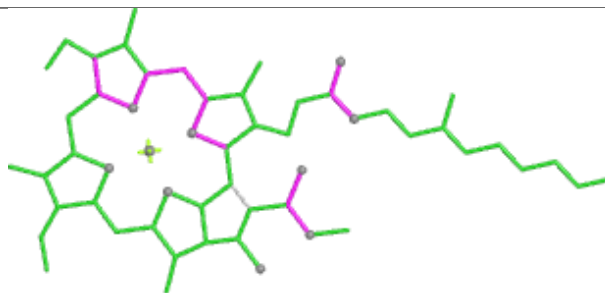




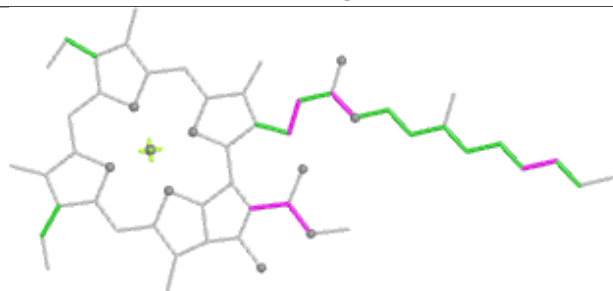


Ligand CLA b 613

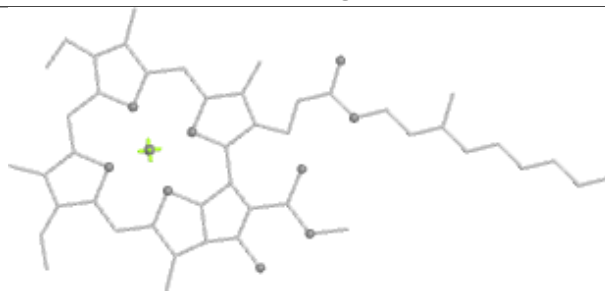
Bond lengths



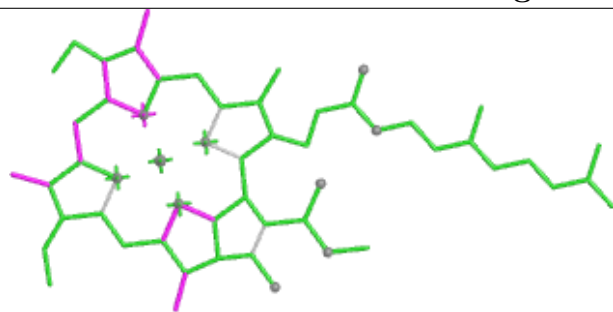
Bond angles



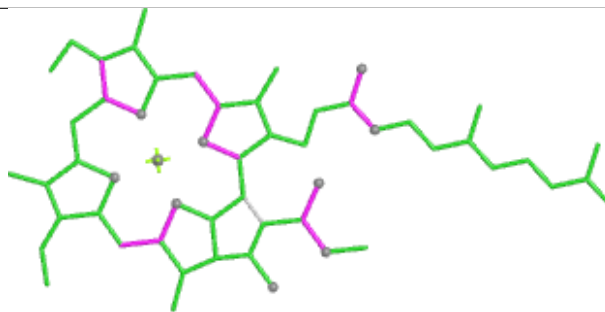
Torsions



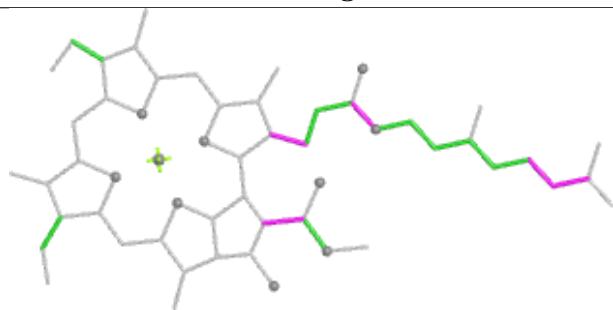
Rings

Ligand CLA A 804

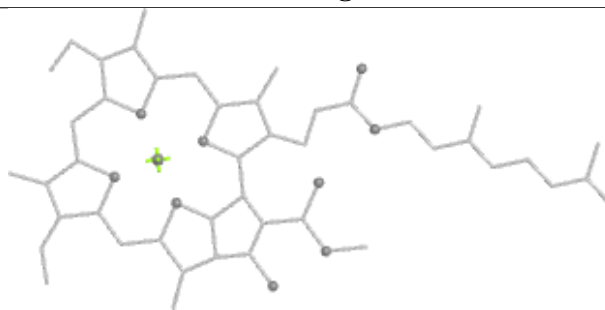
Bond lengths



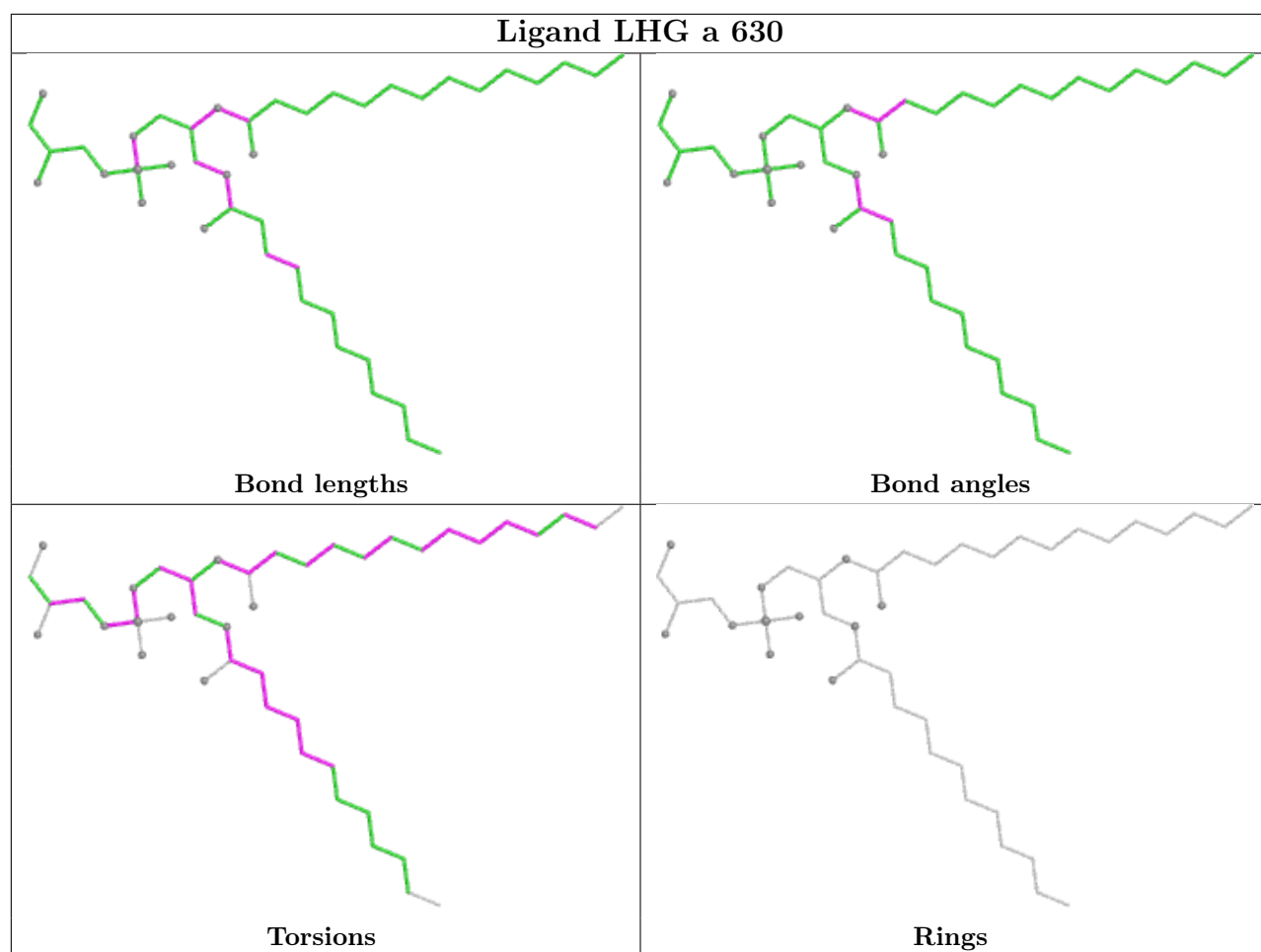
Bond angles



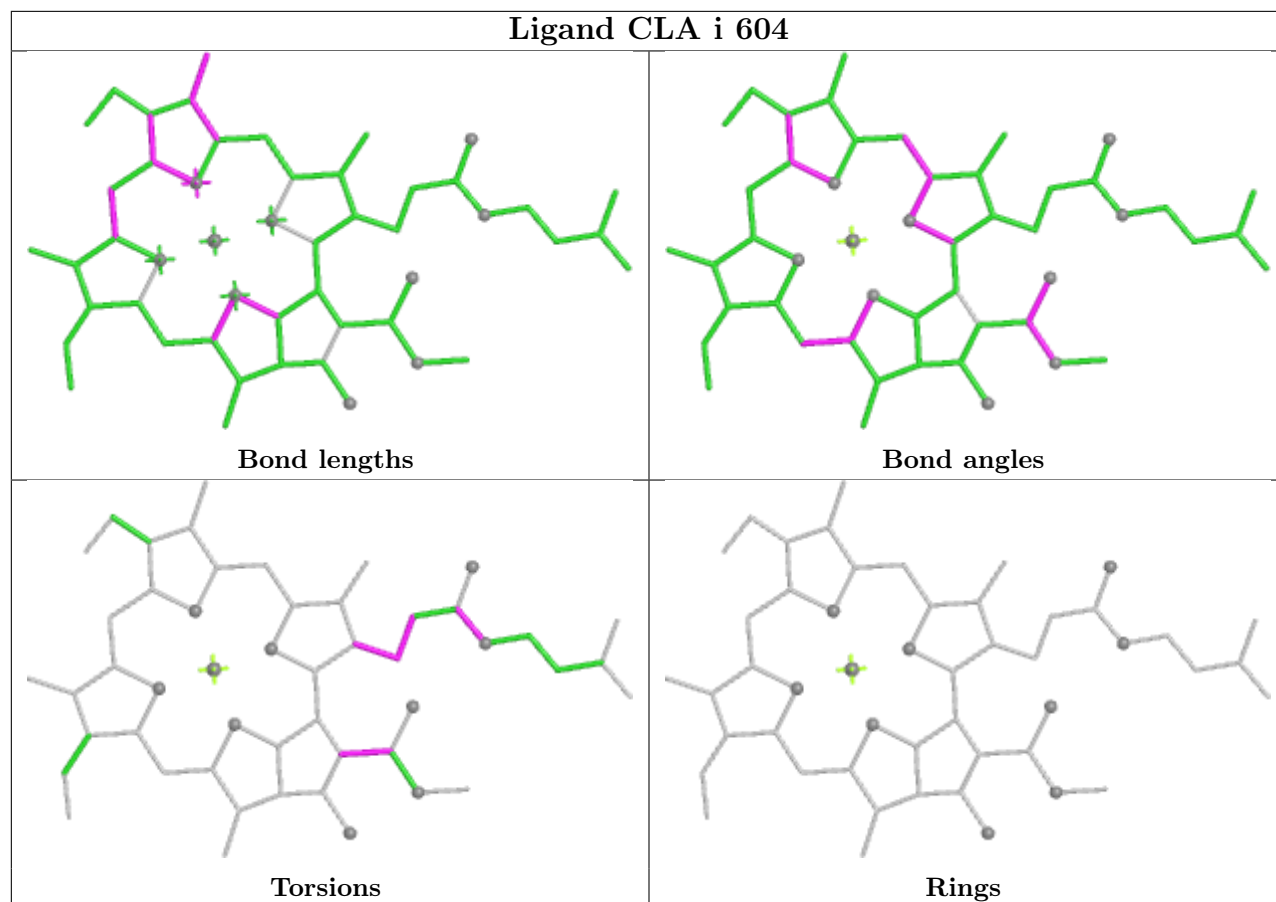
Torsions



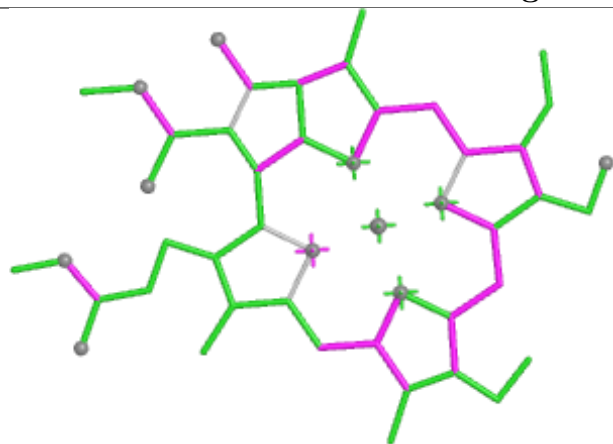
Rings



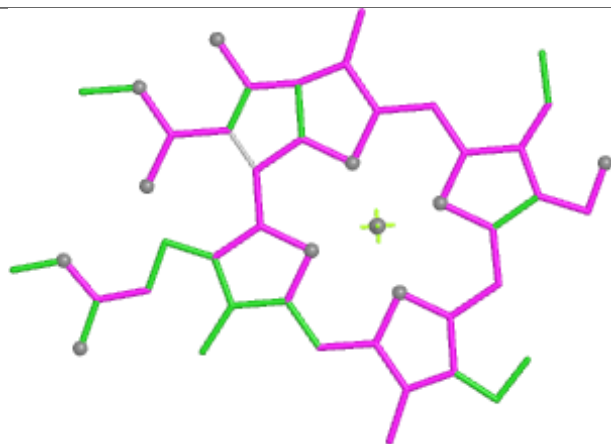
Ligand CLA i 604



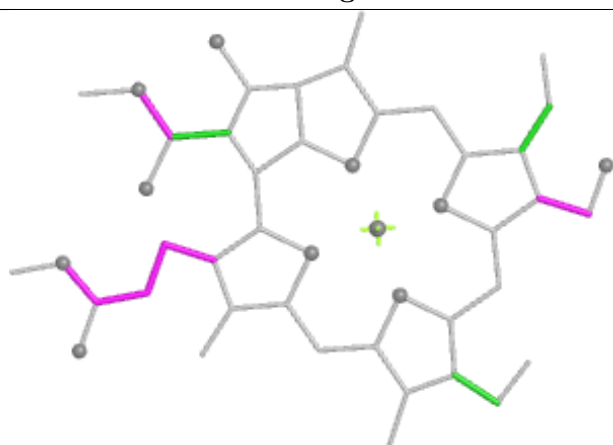
Ligand CHL i 607



Bond lengths



Bond angles

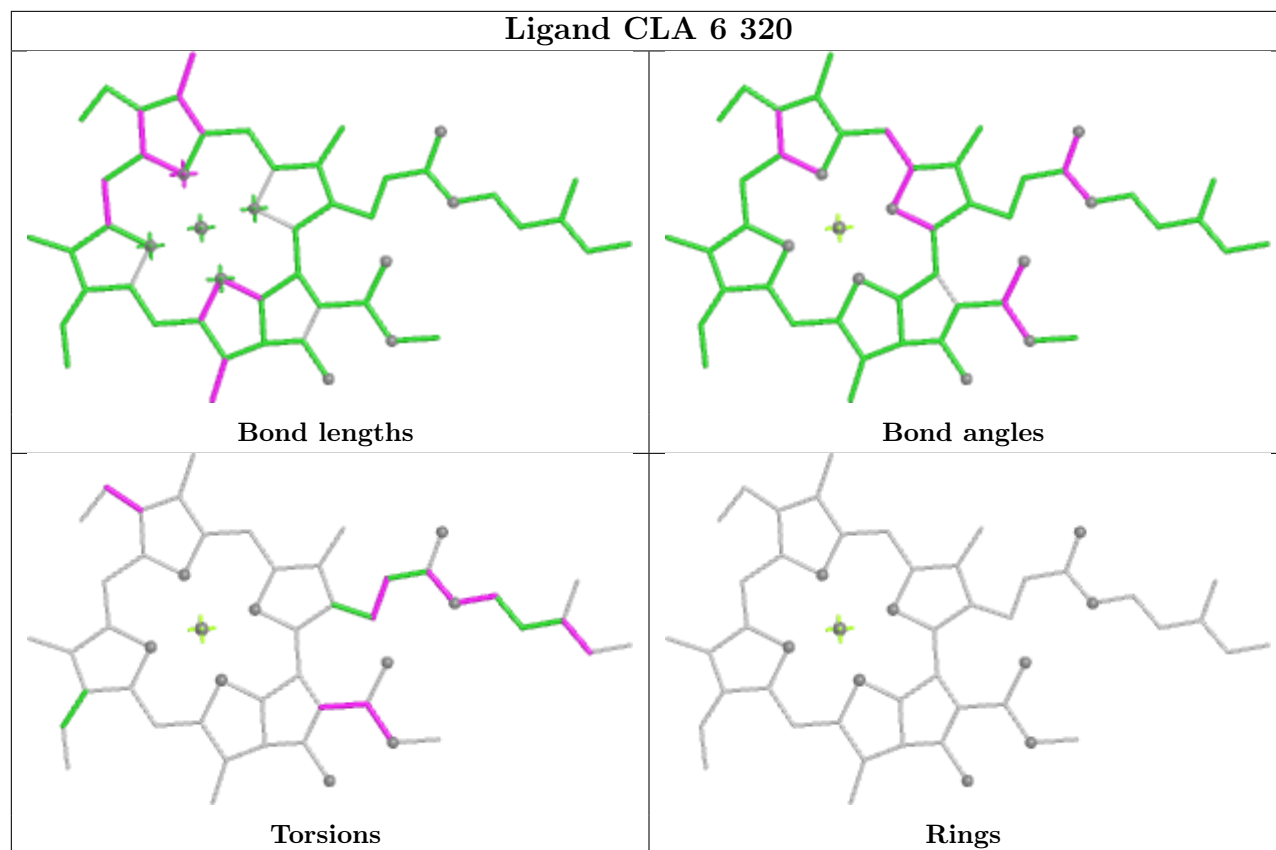


Torsions

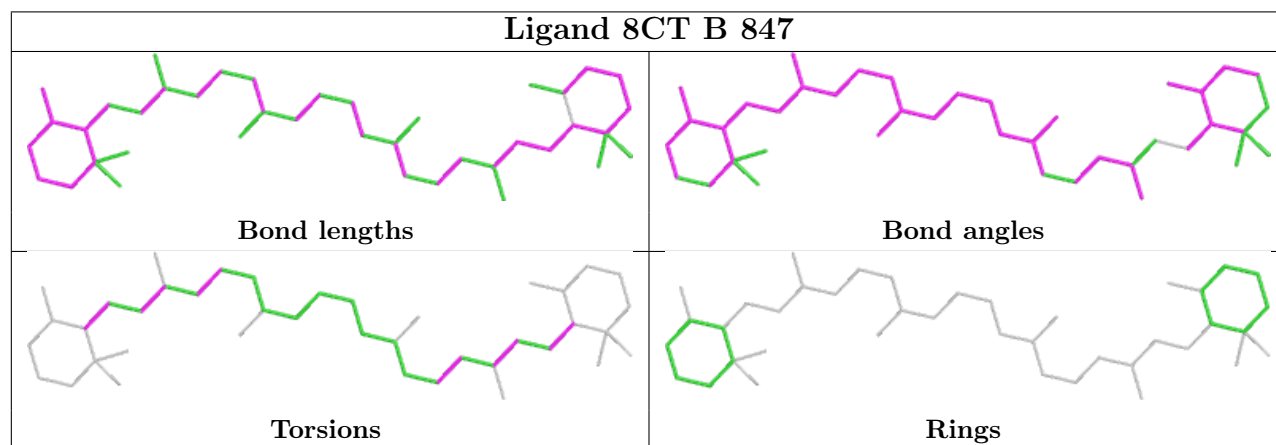


Rings

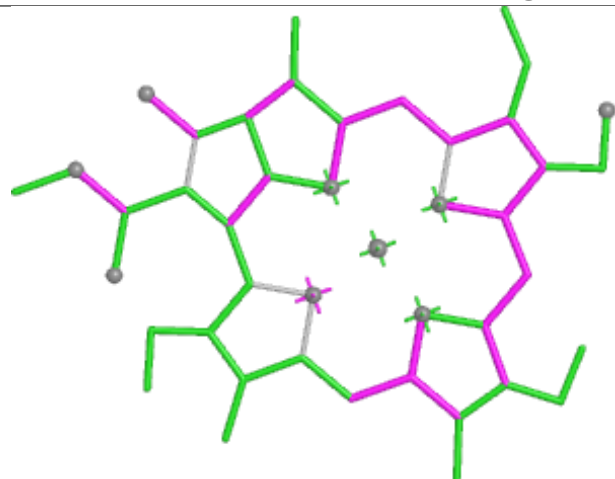
Ligand CLA 6 320



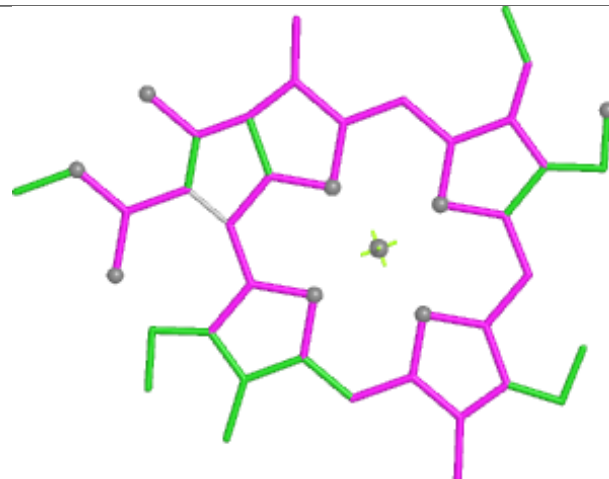
Ligand 8CT B 847



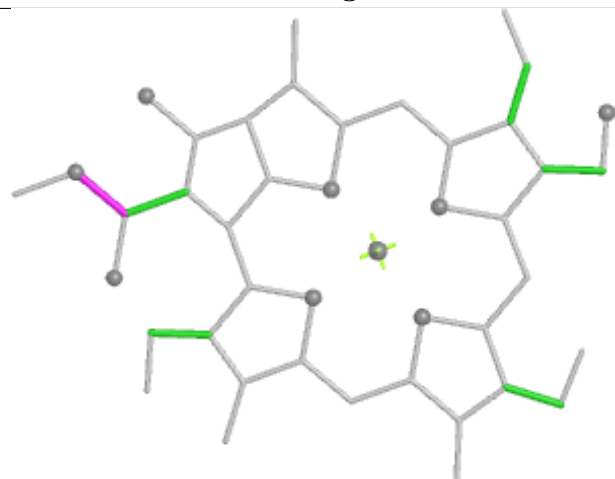
Ligand CHL a 605



Bond lengths



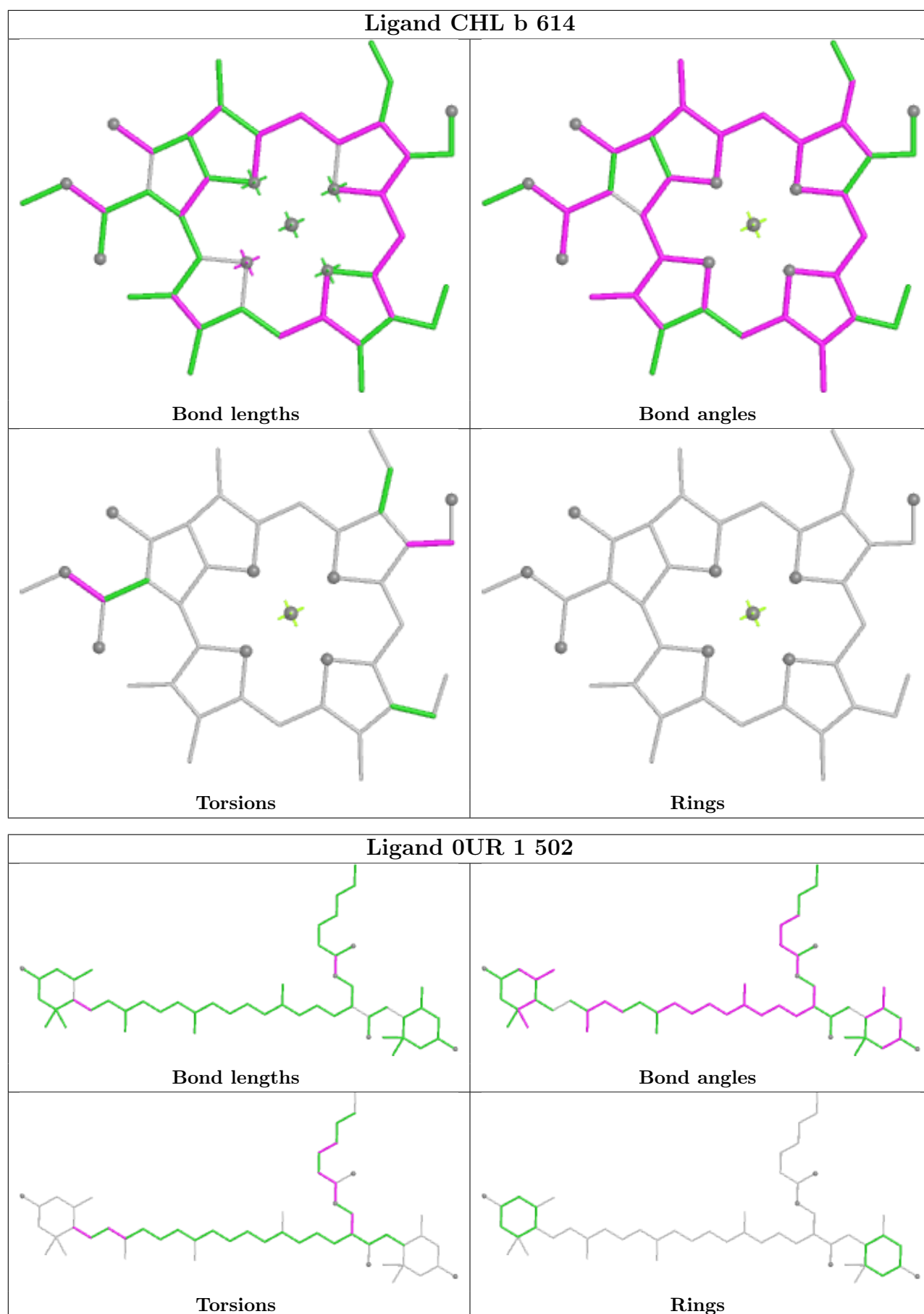
Bond angles



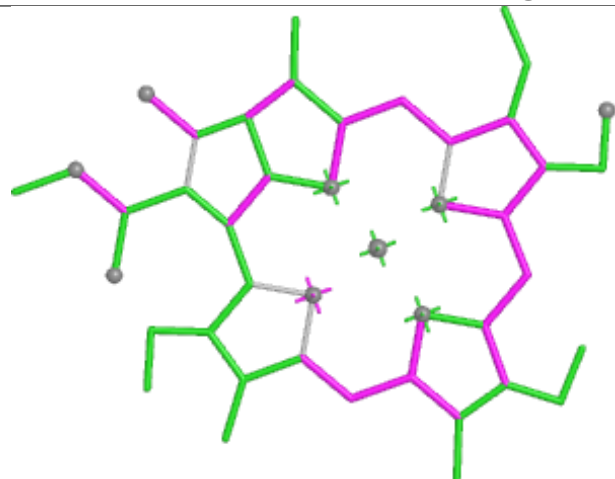
Torsions



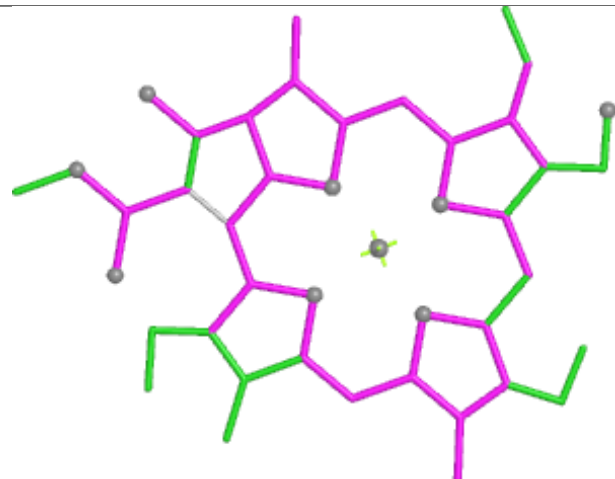
Rings



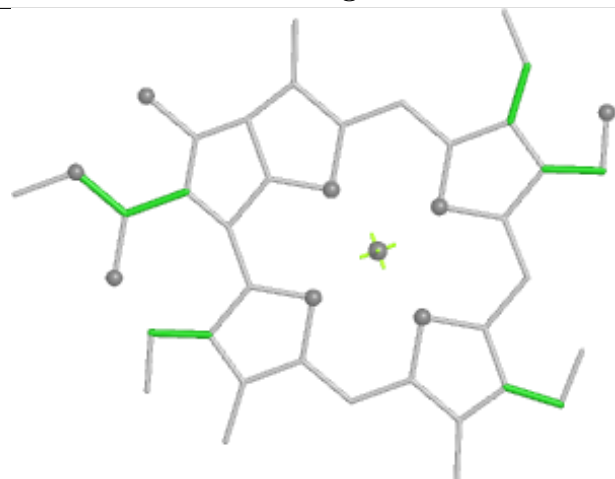
Ligand CHL 6 305



Bond lengths



Bond angles

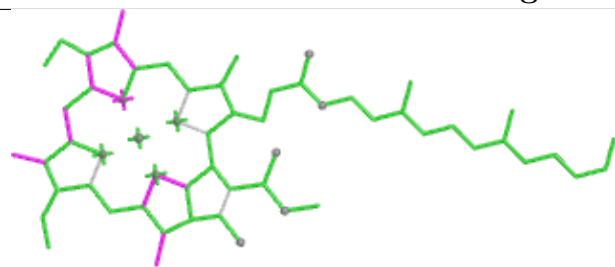


Torsions

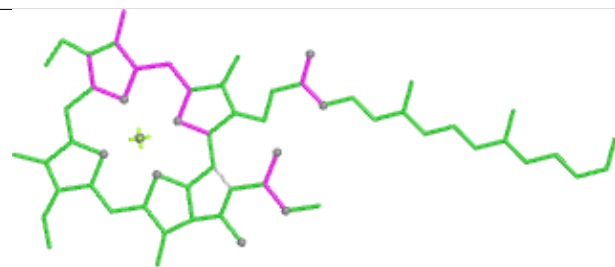


Rings

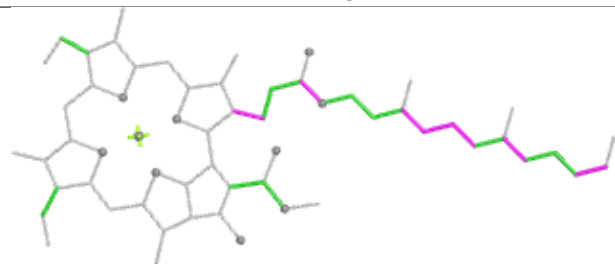
Ligand CLA 7 309



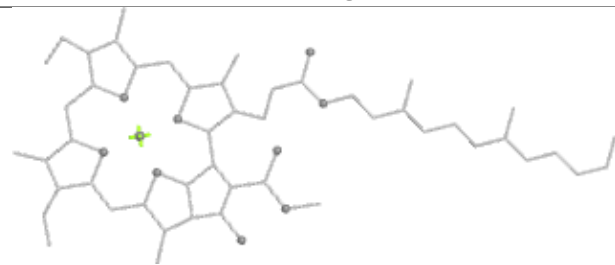
Bond lengths



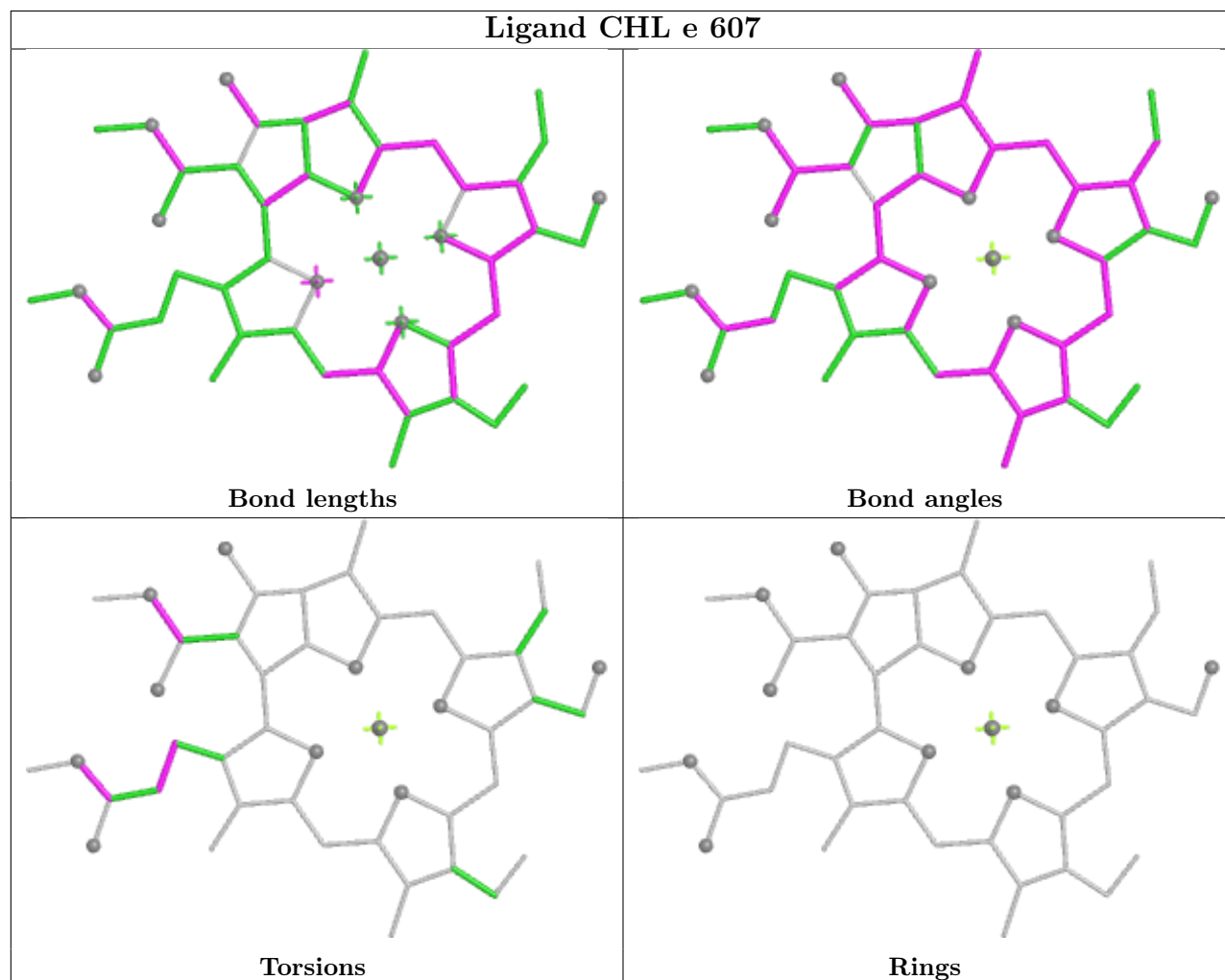
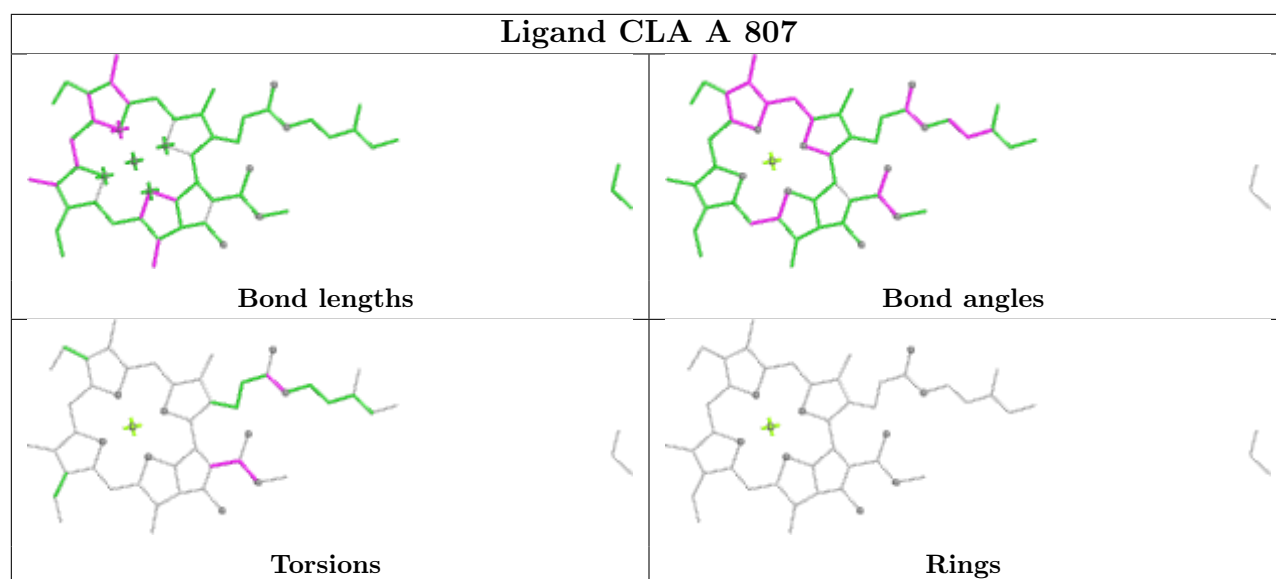
Bond angles

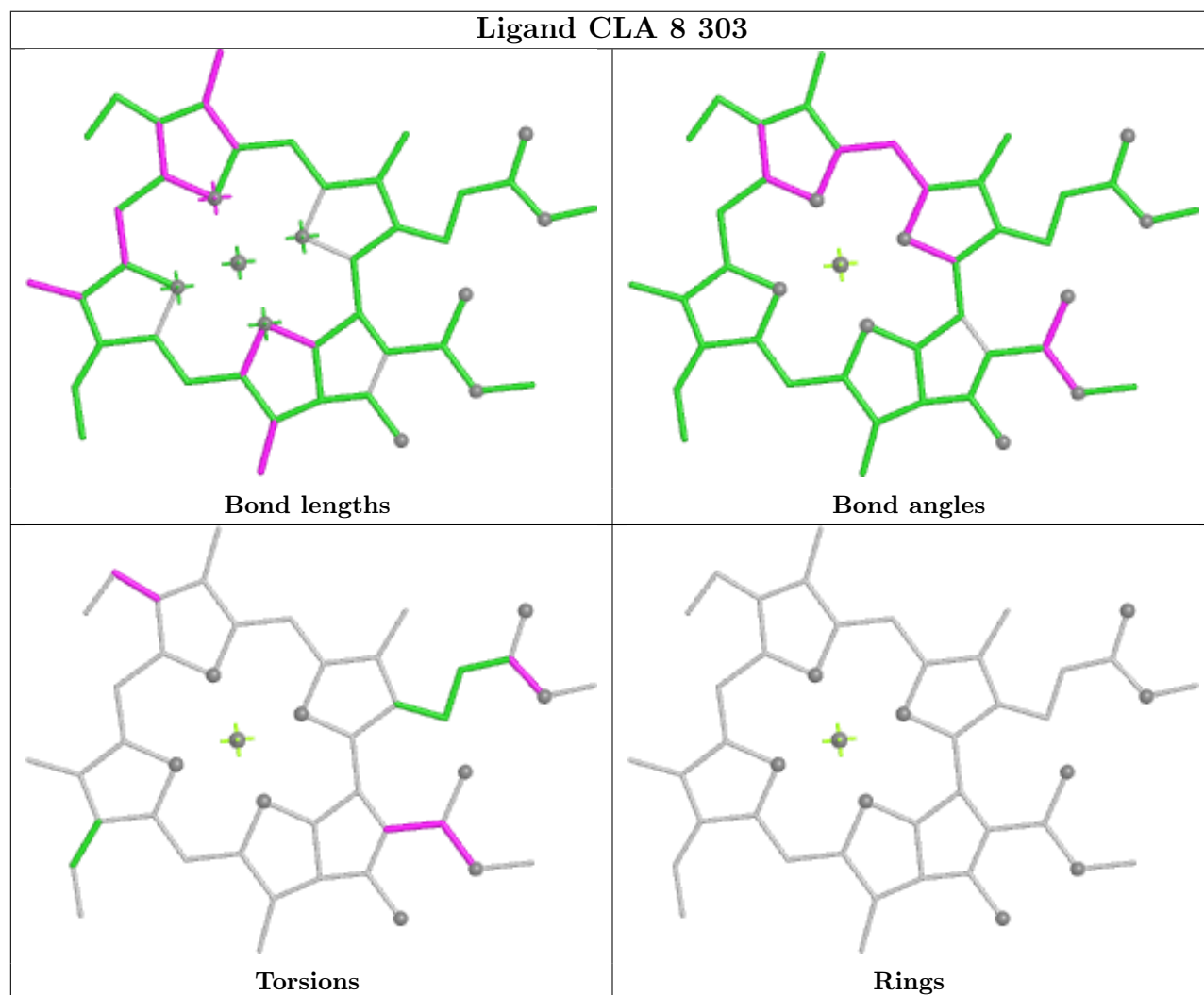
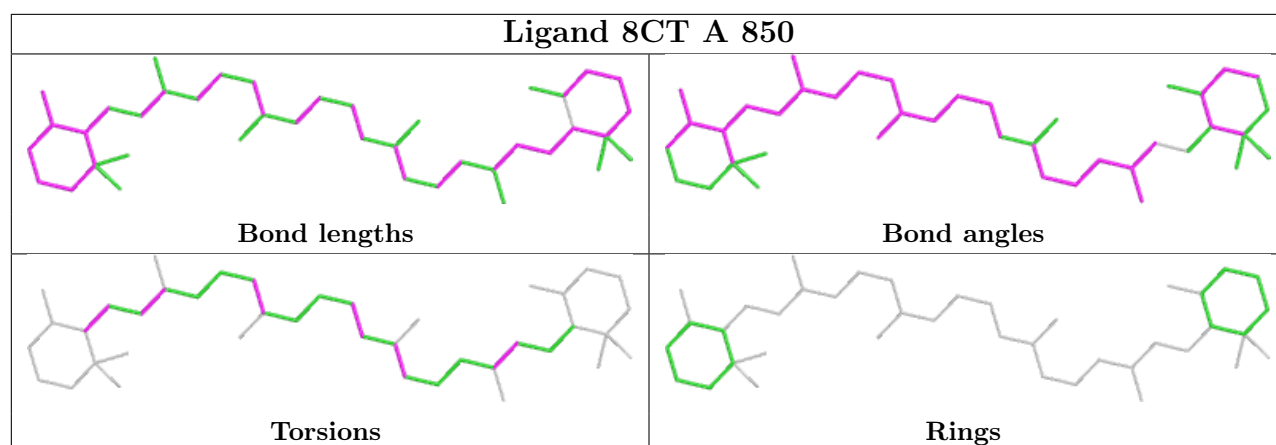


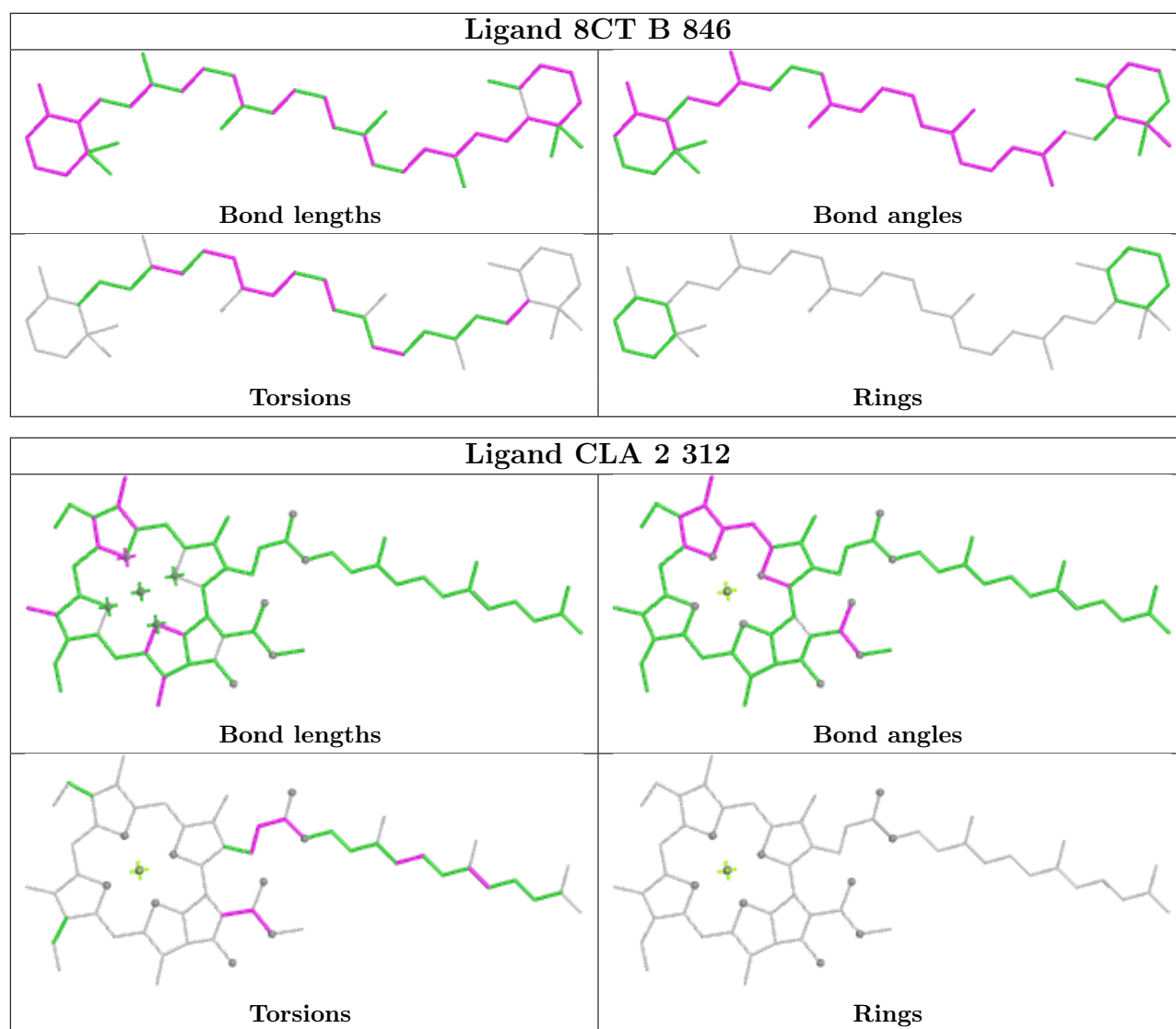
Torsions



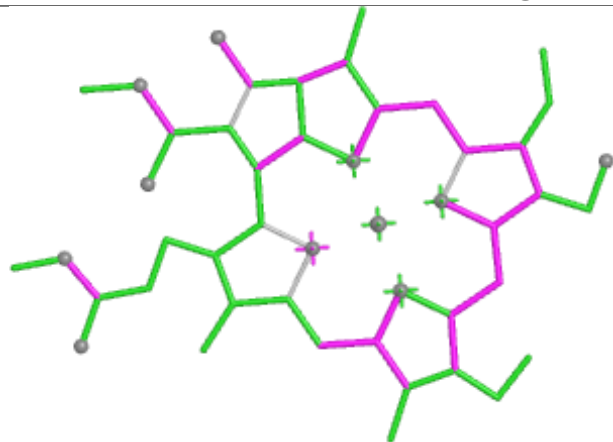
Rings



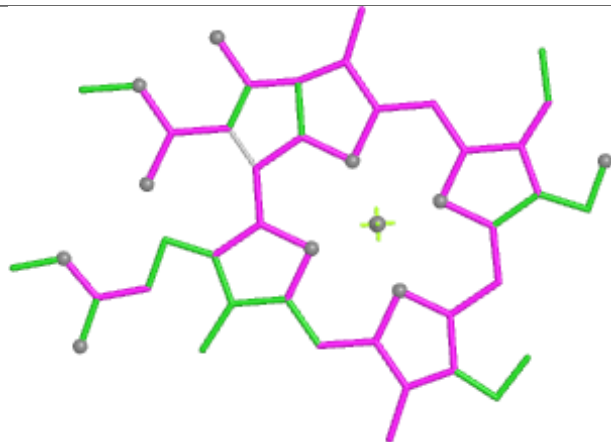




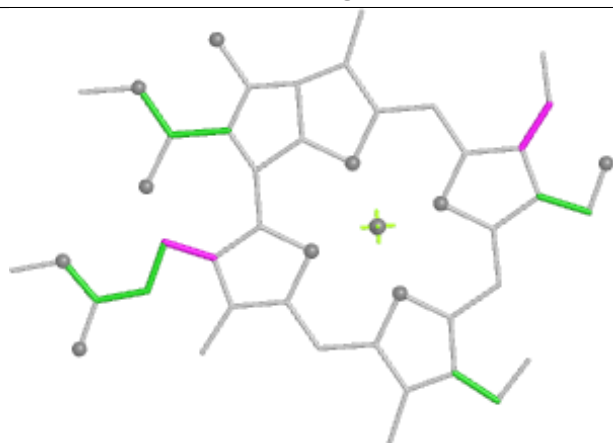
Ligand CHL h 609



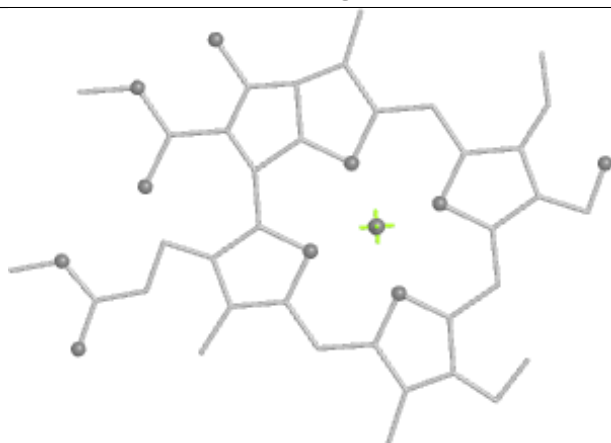
Bond lengths



Bond angles

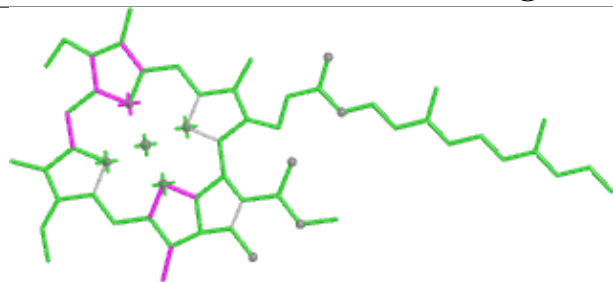


Torsions

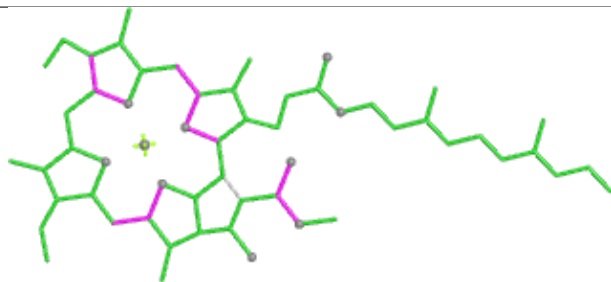


Rings

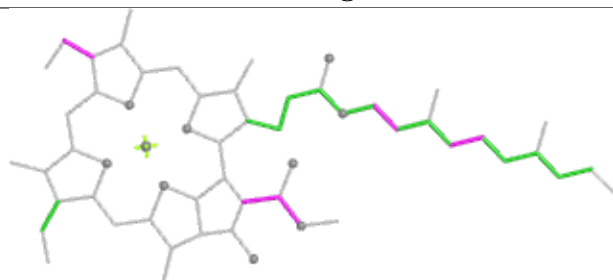
Ligand CLA e 603



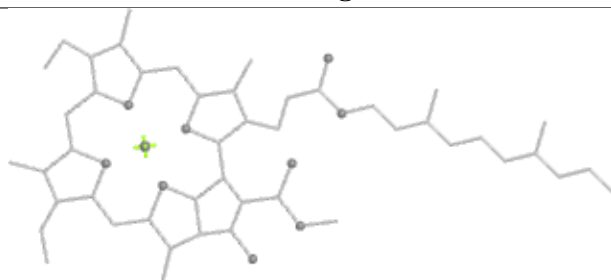
Bond lengths



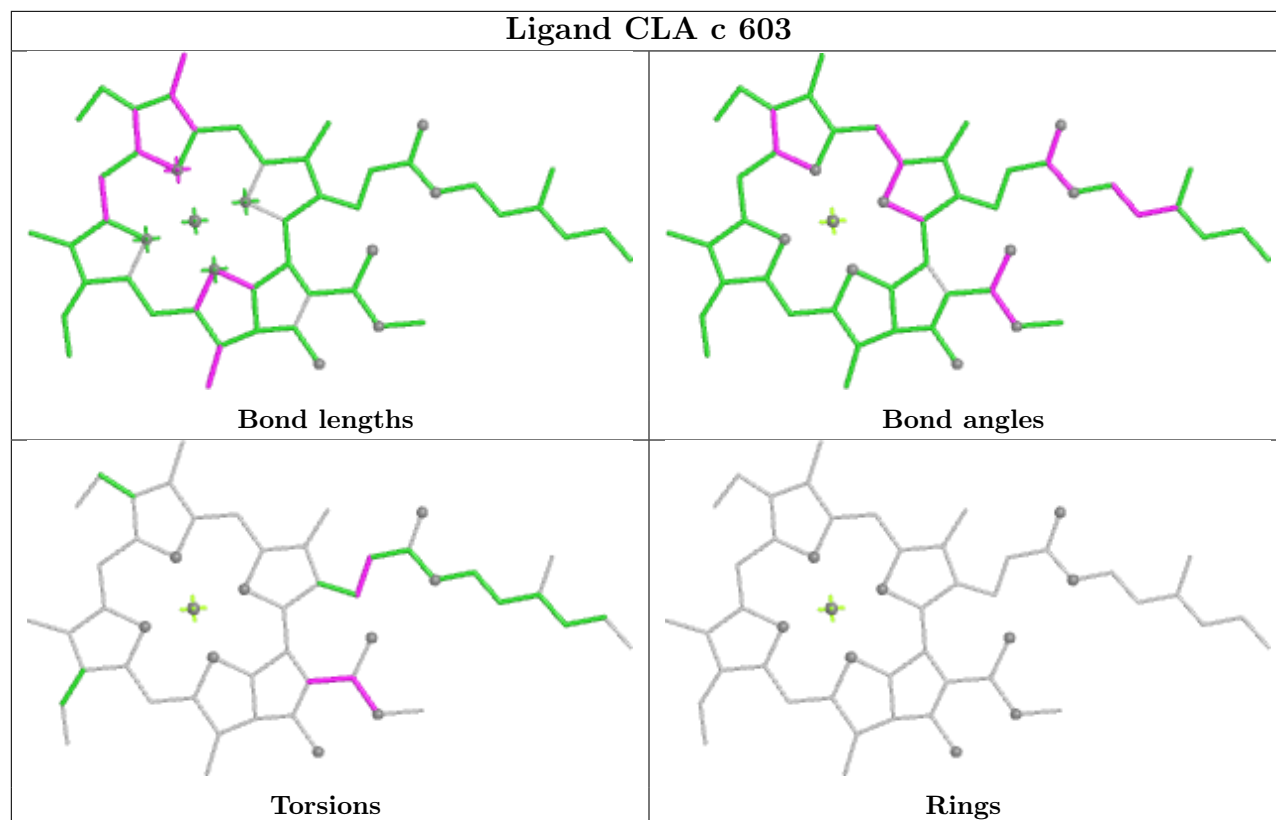
Bond angles



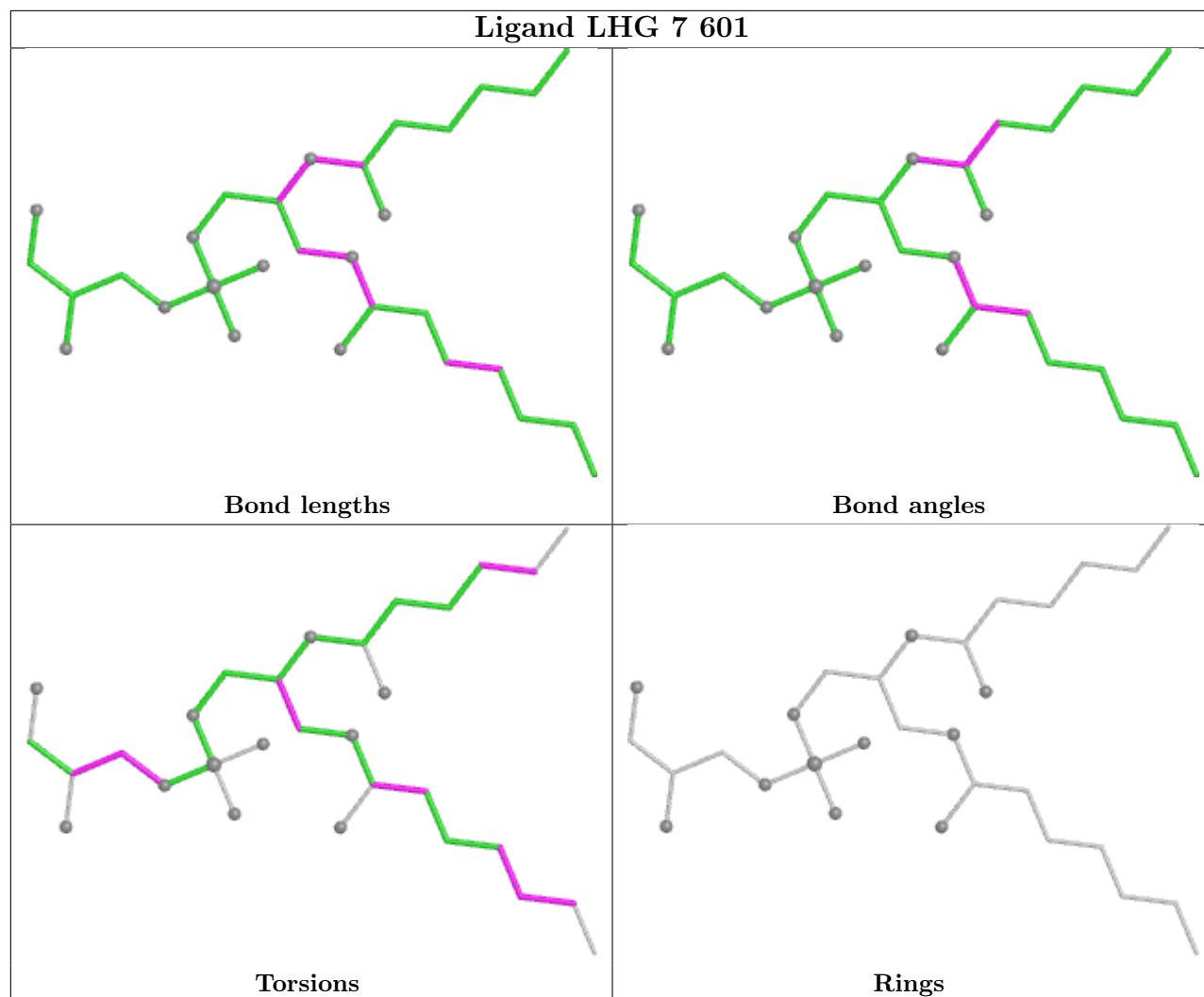
Torsions



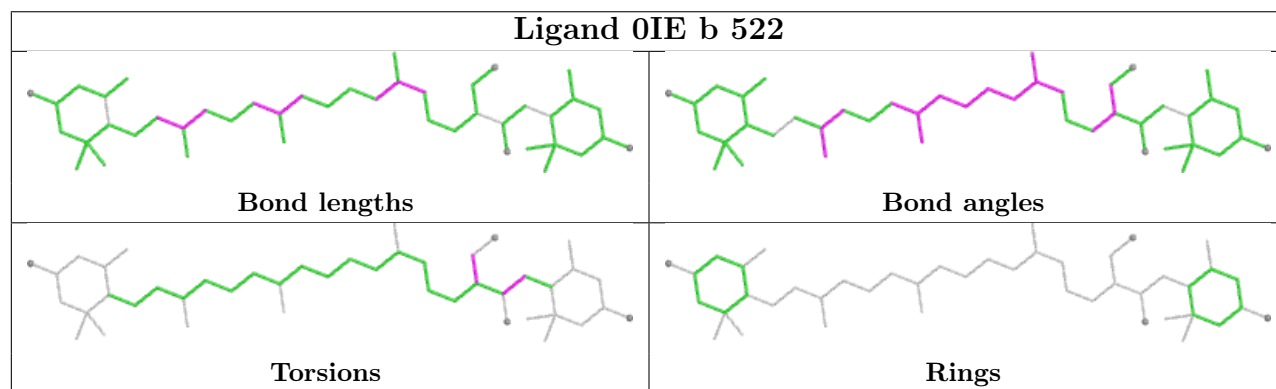
Rings



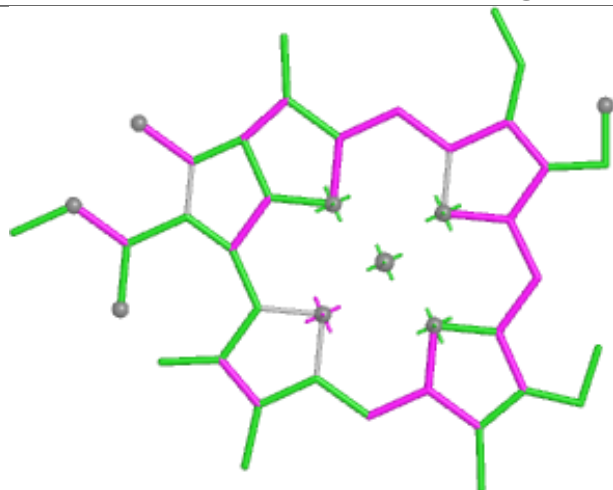
Ligand LHG 7 601



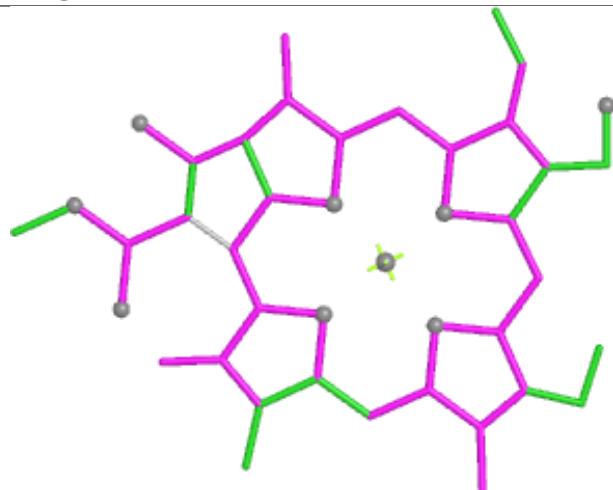
Ligand OIE b 522



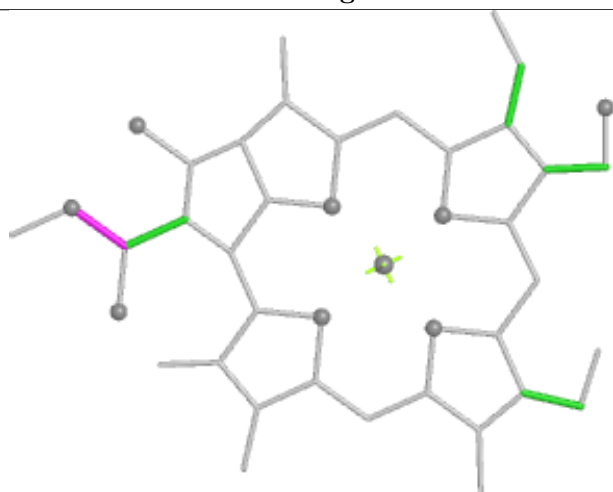
Ligand CHL g 614



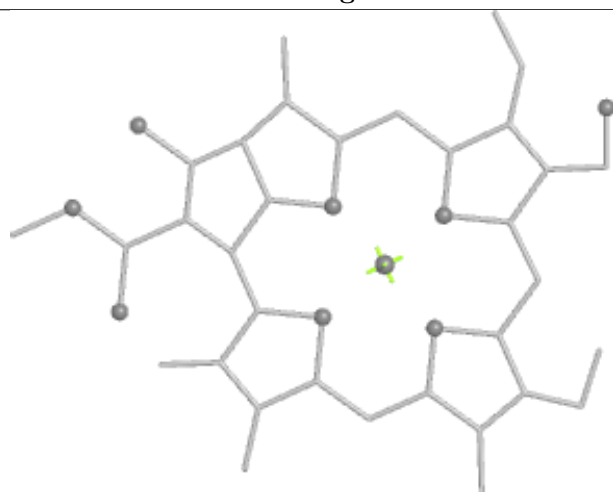
Bond lengths



Bond angles

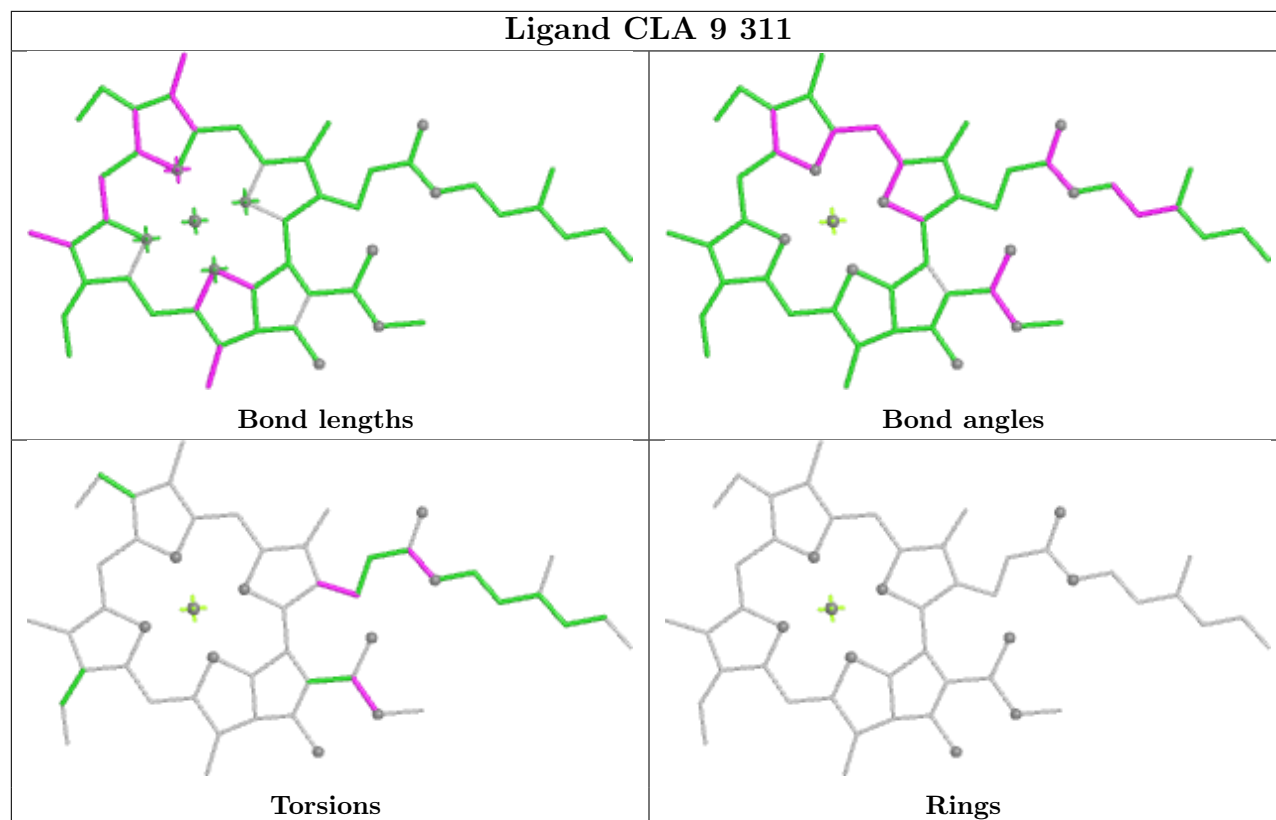


Torsions

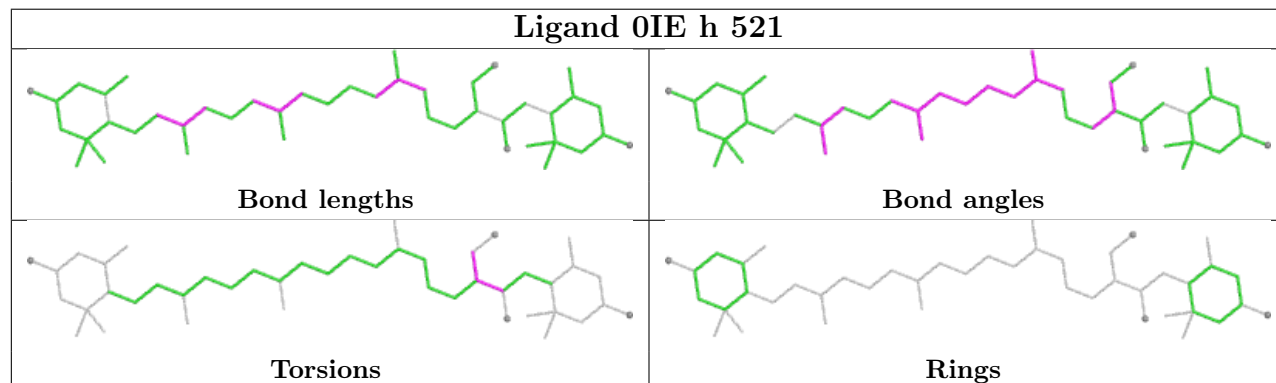


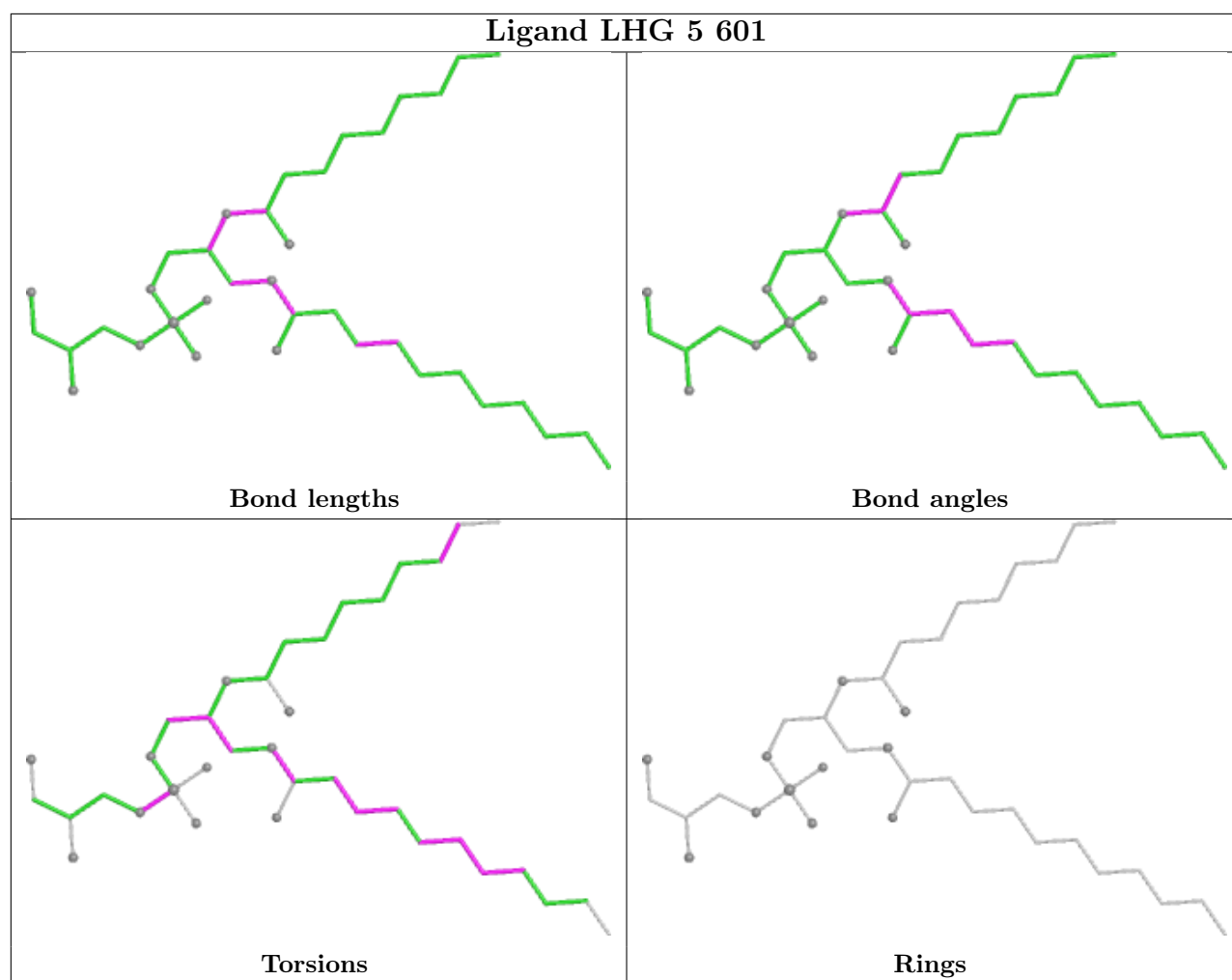
Rings

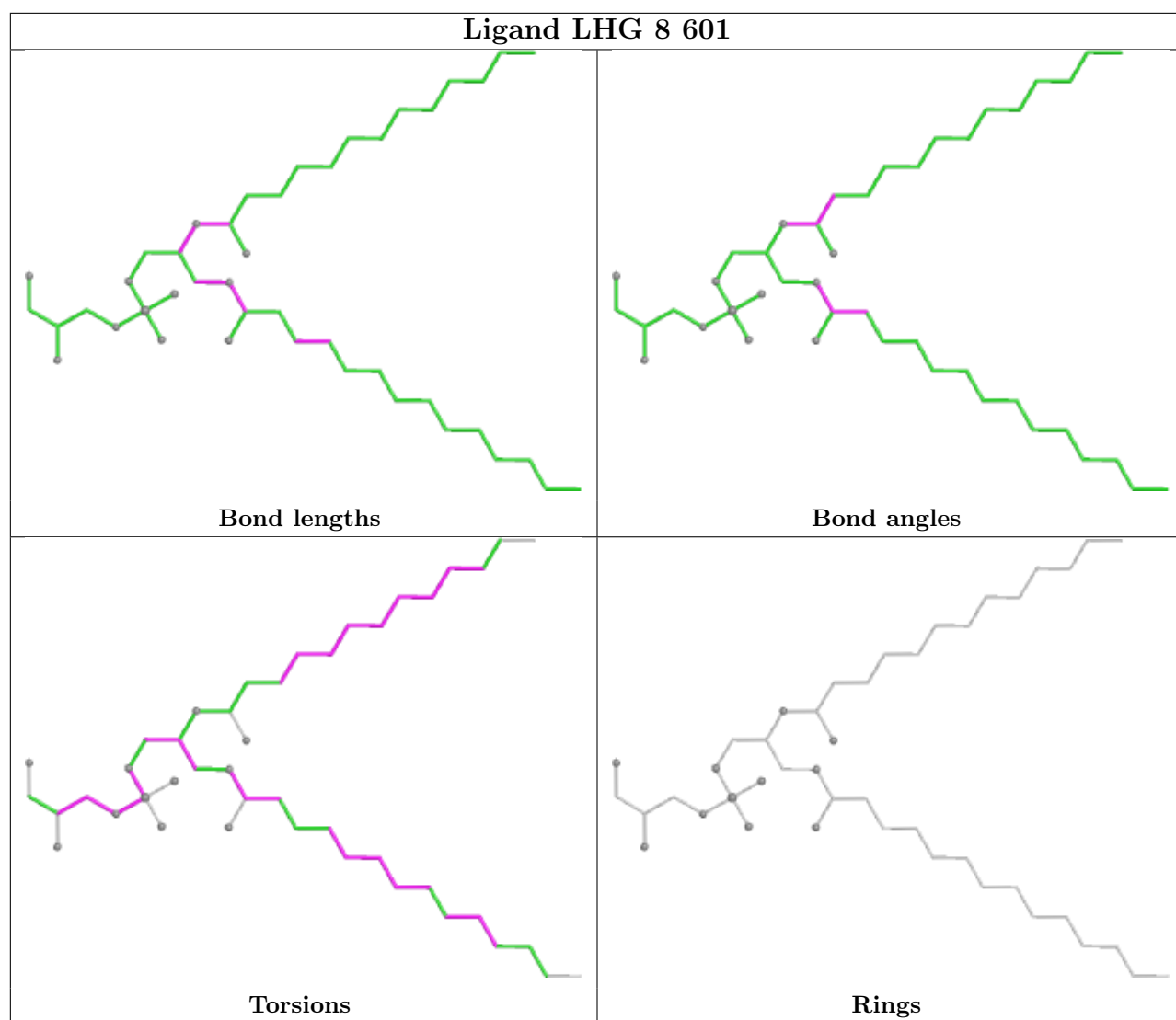
Ligand CLA 9 311



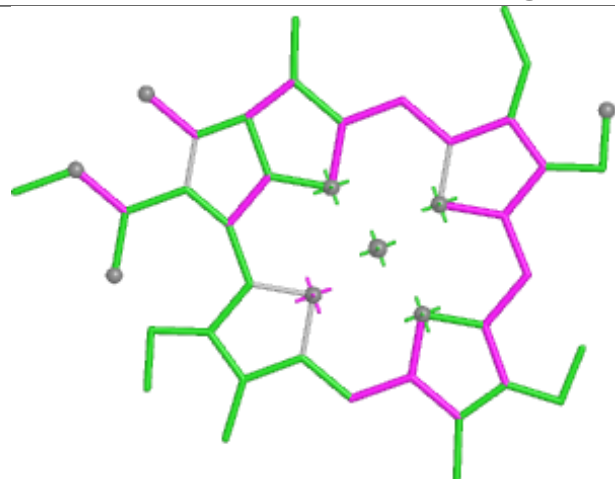
Ligand OIE h 521



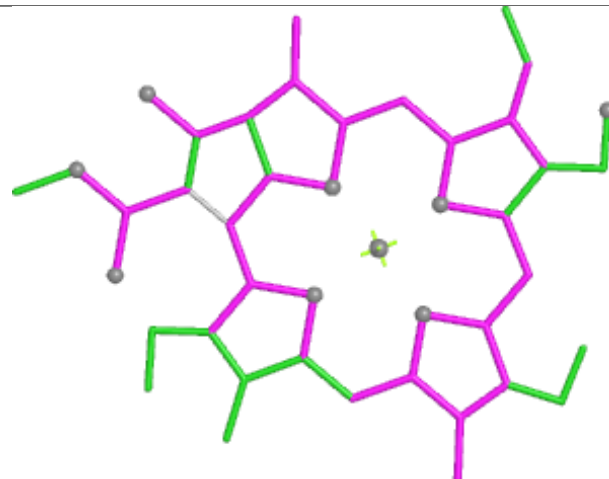




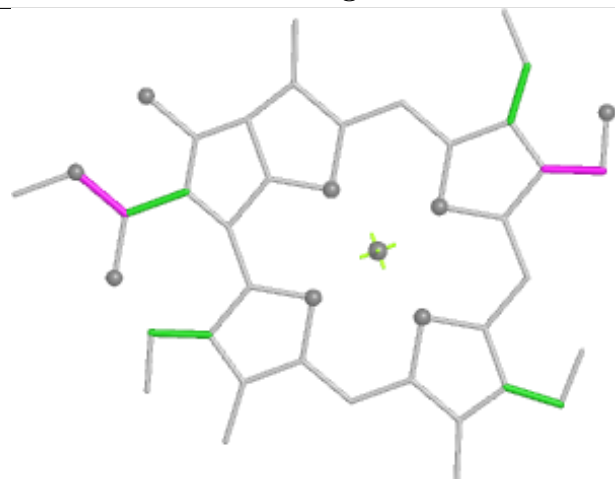
Ligand CHL e 605



Bond lengths



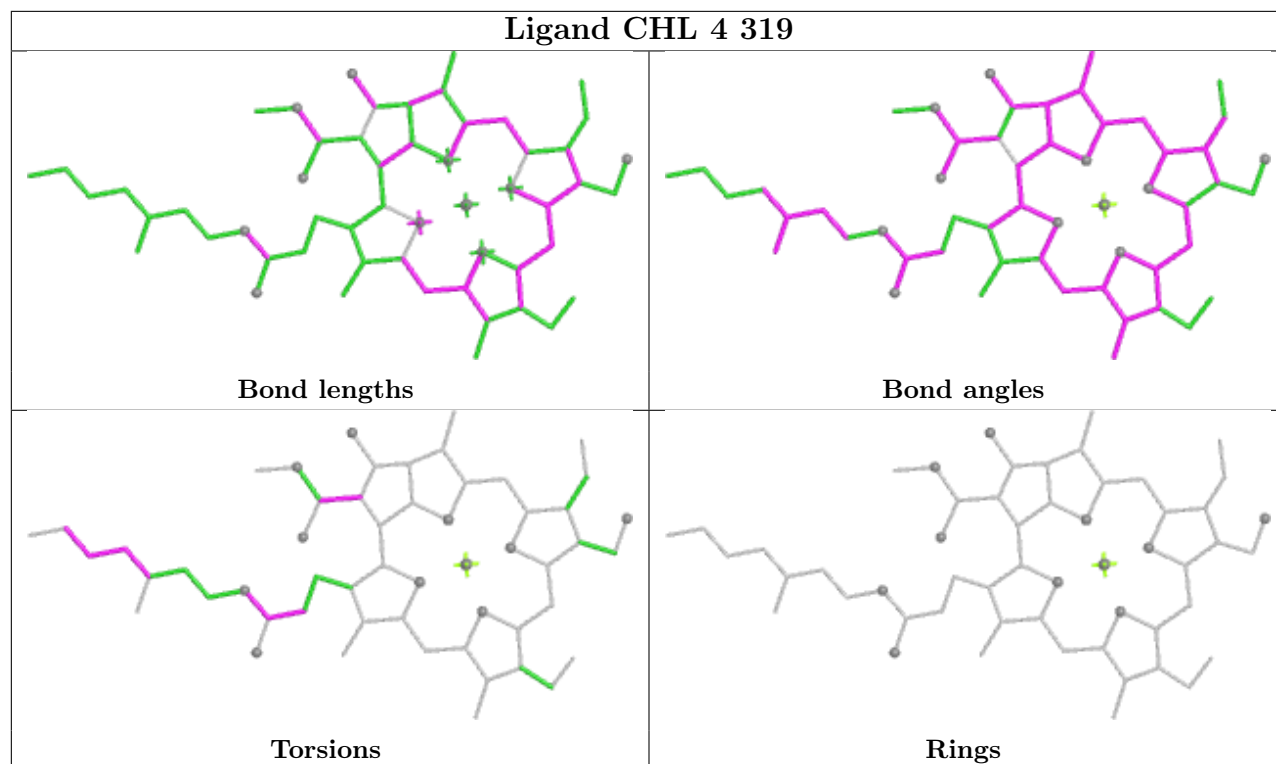
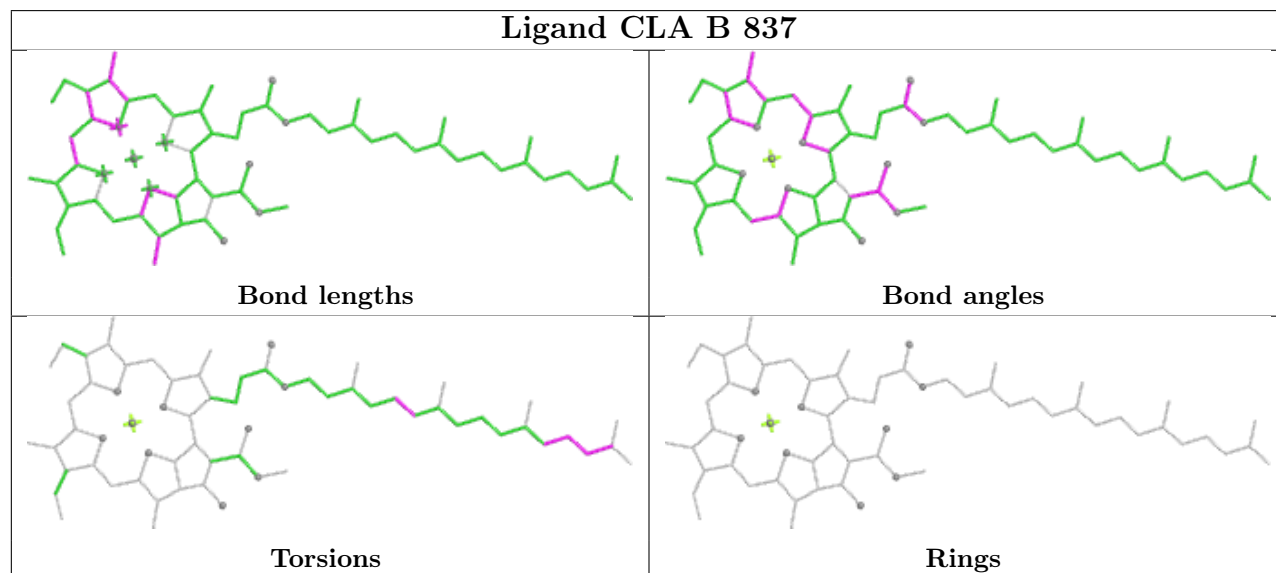
Bond angles

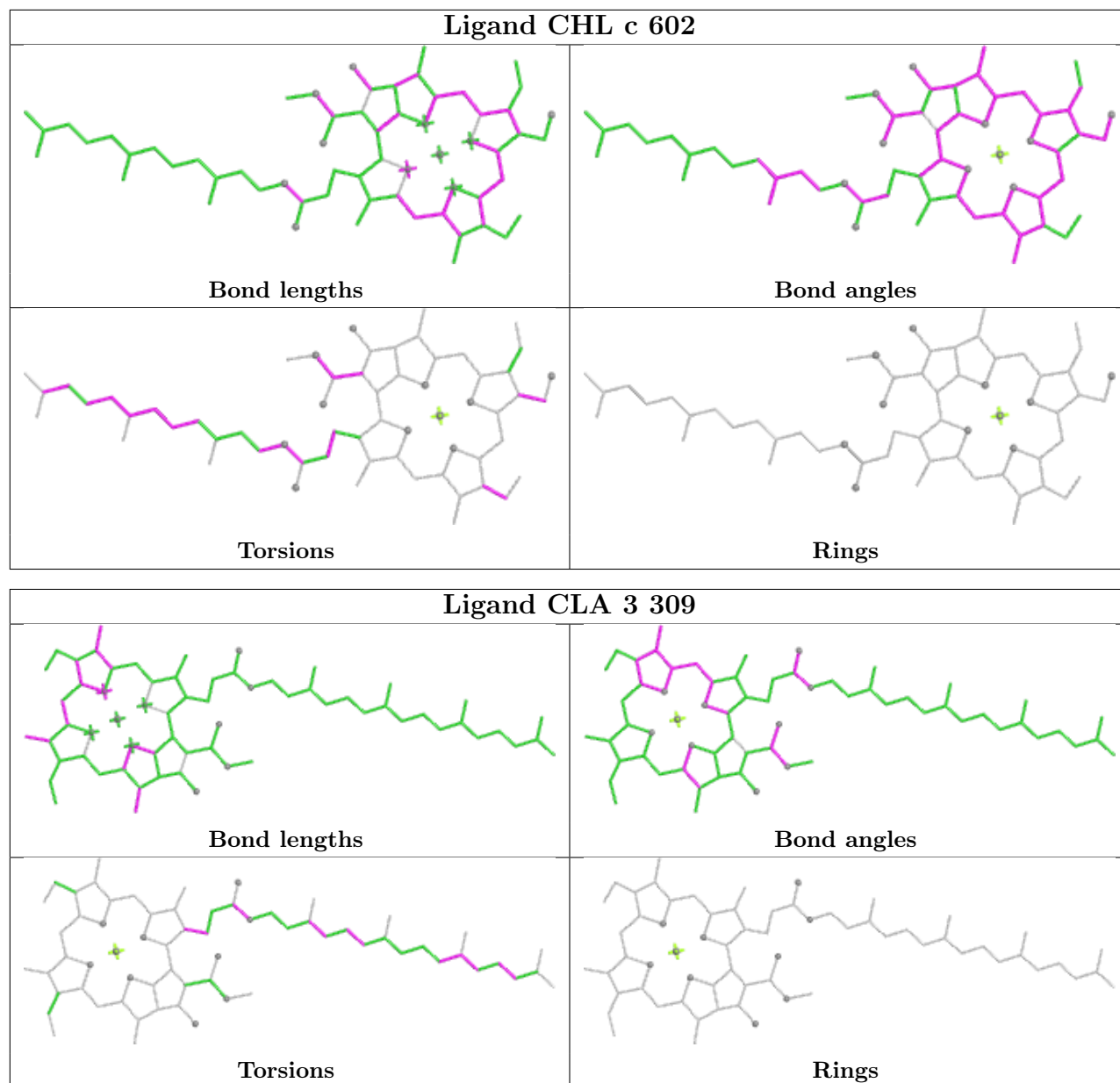


Torsions

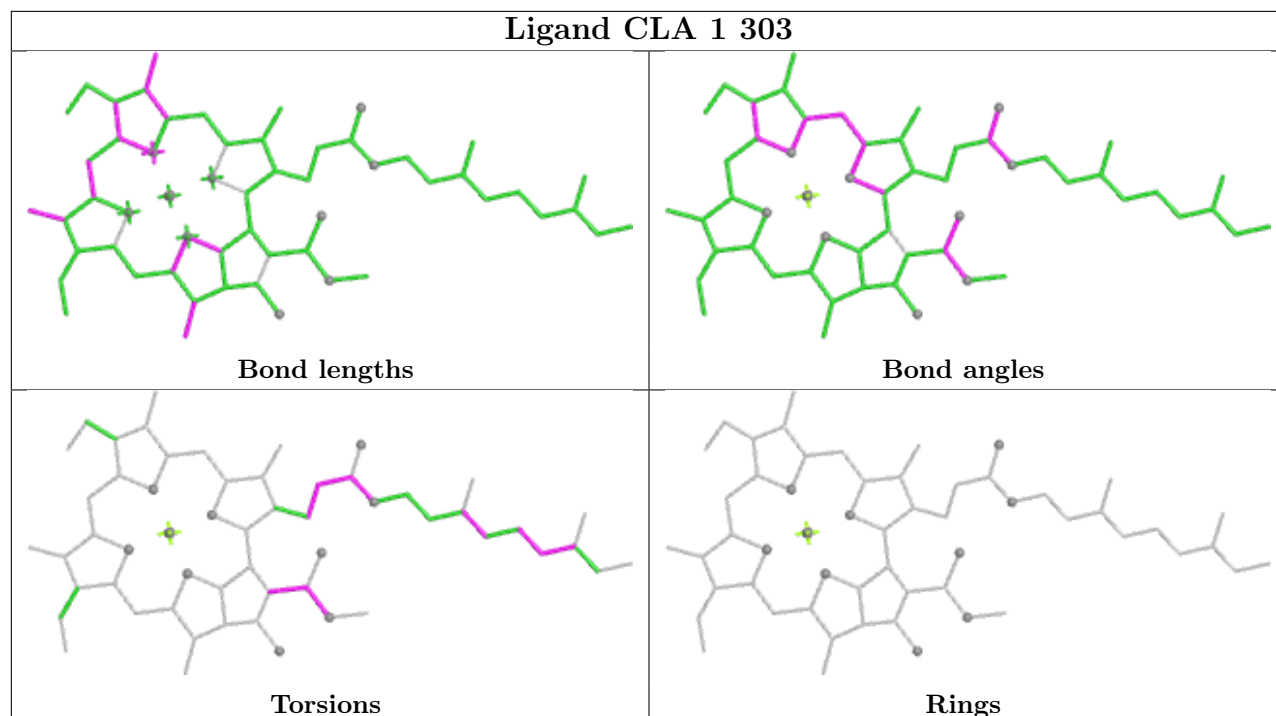


Rings

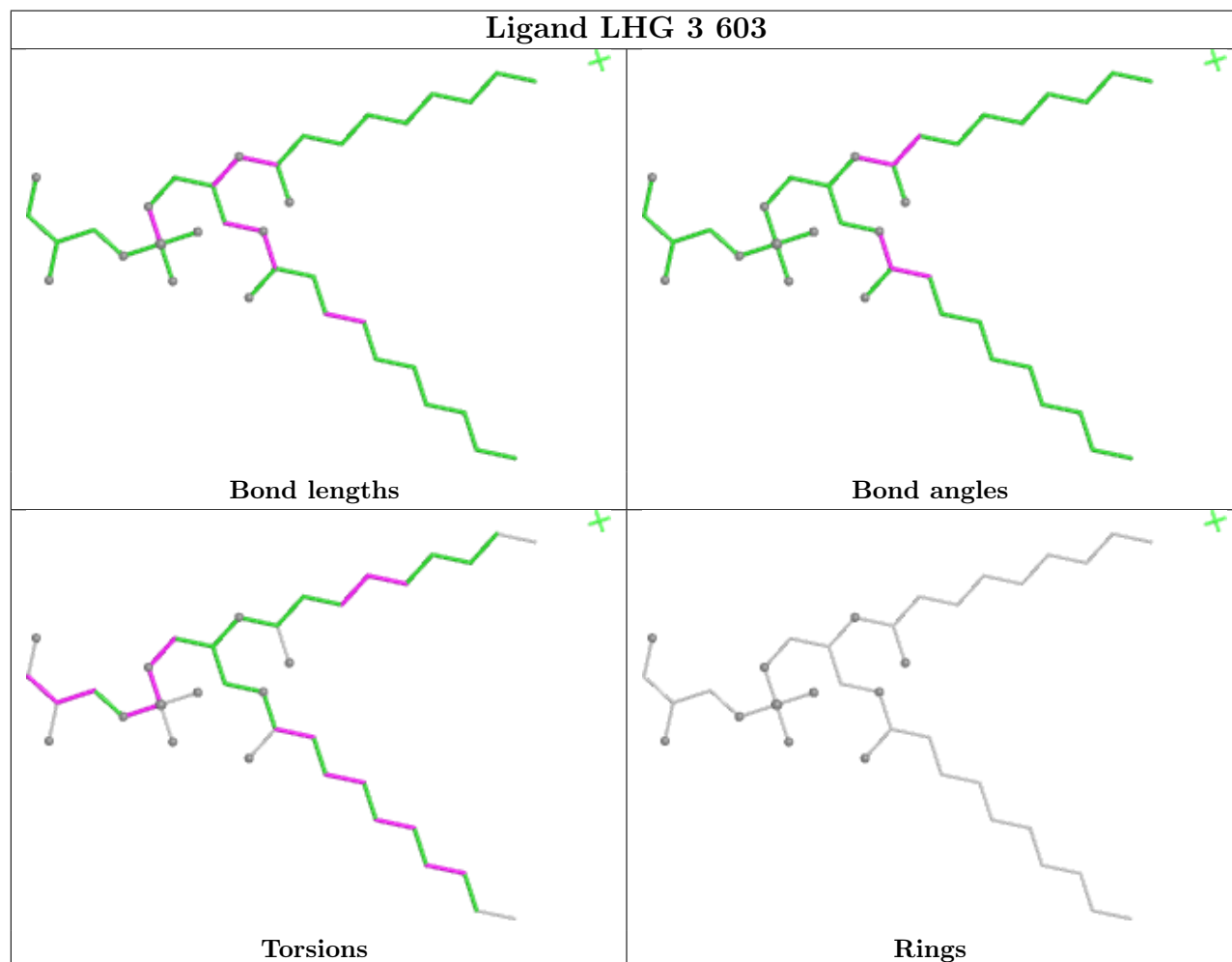
Ligand CHL 4 319**Ligand CLA B 837**

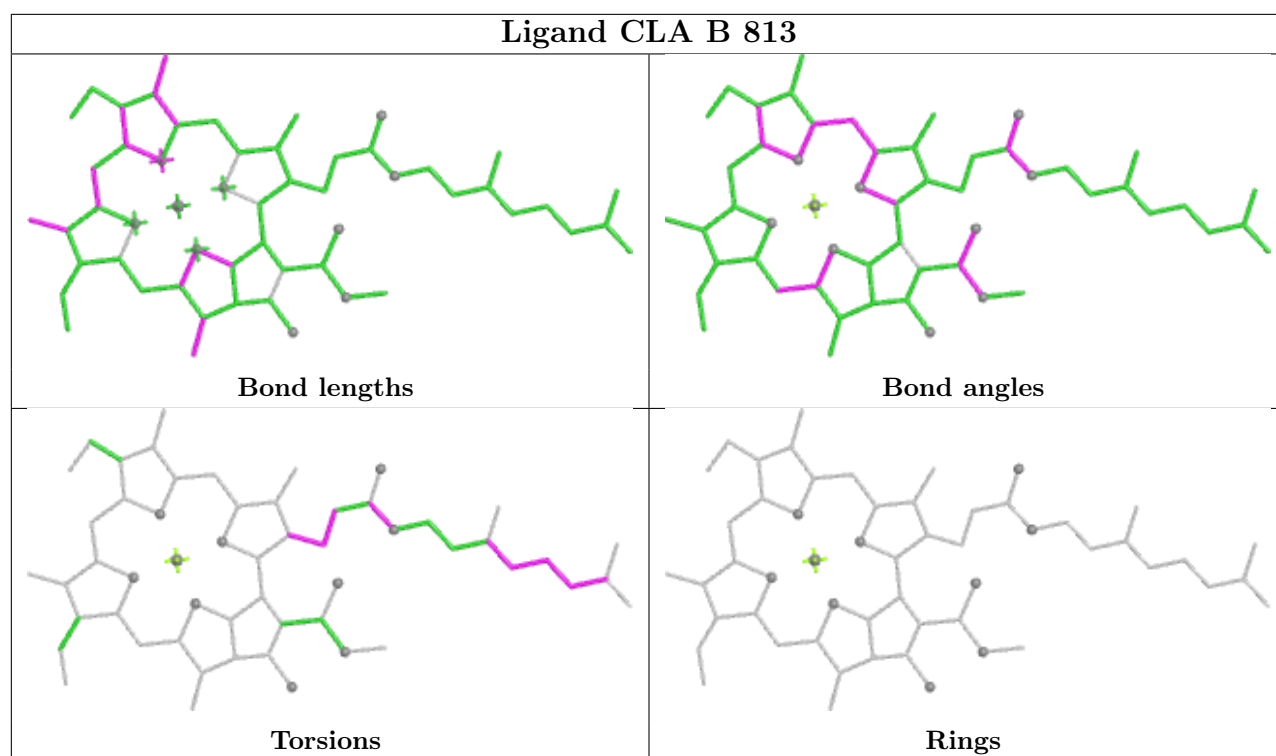


Ligand CLA 1 303

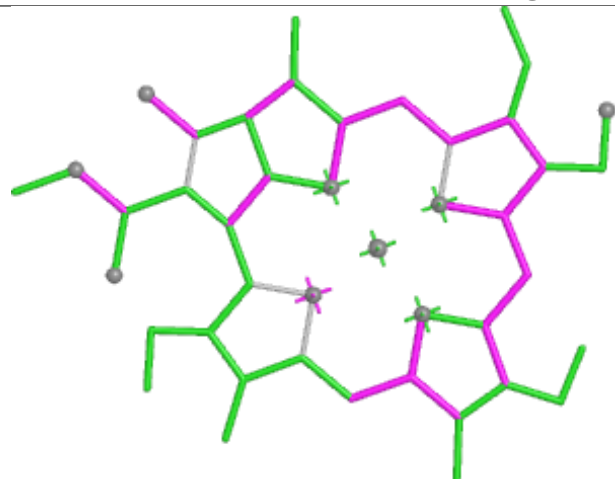


Ligand LHG 3 603

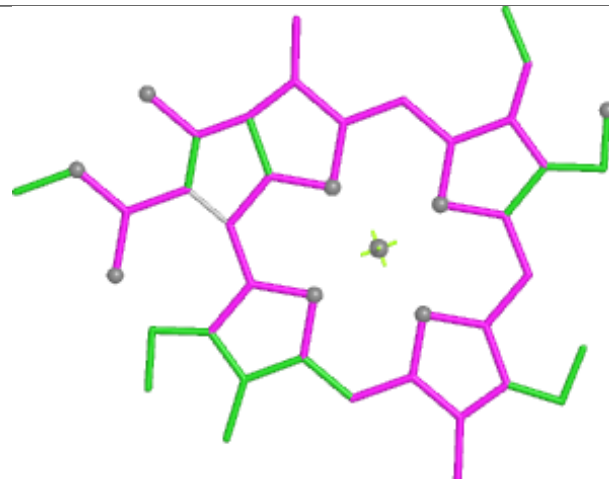




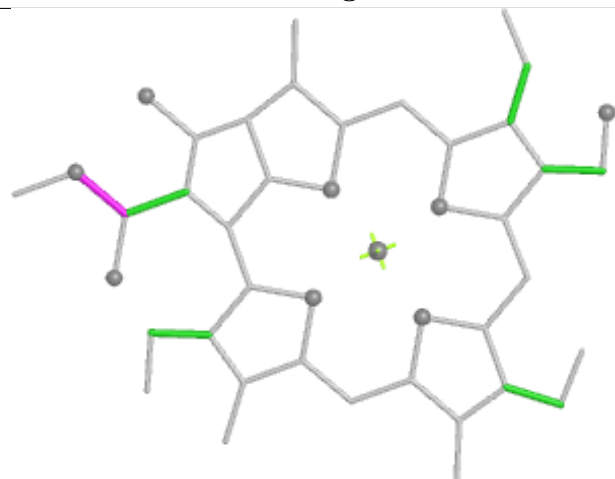
Ligand CHL i 605



Bond lengths



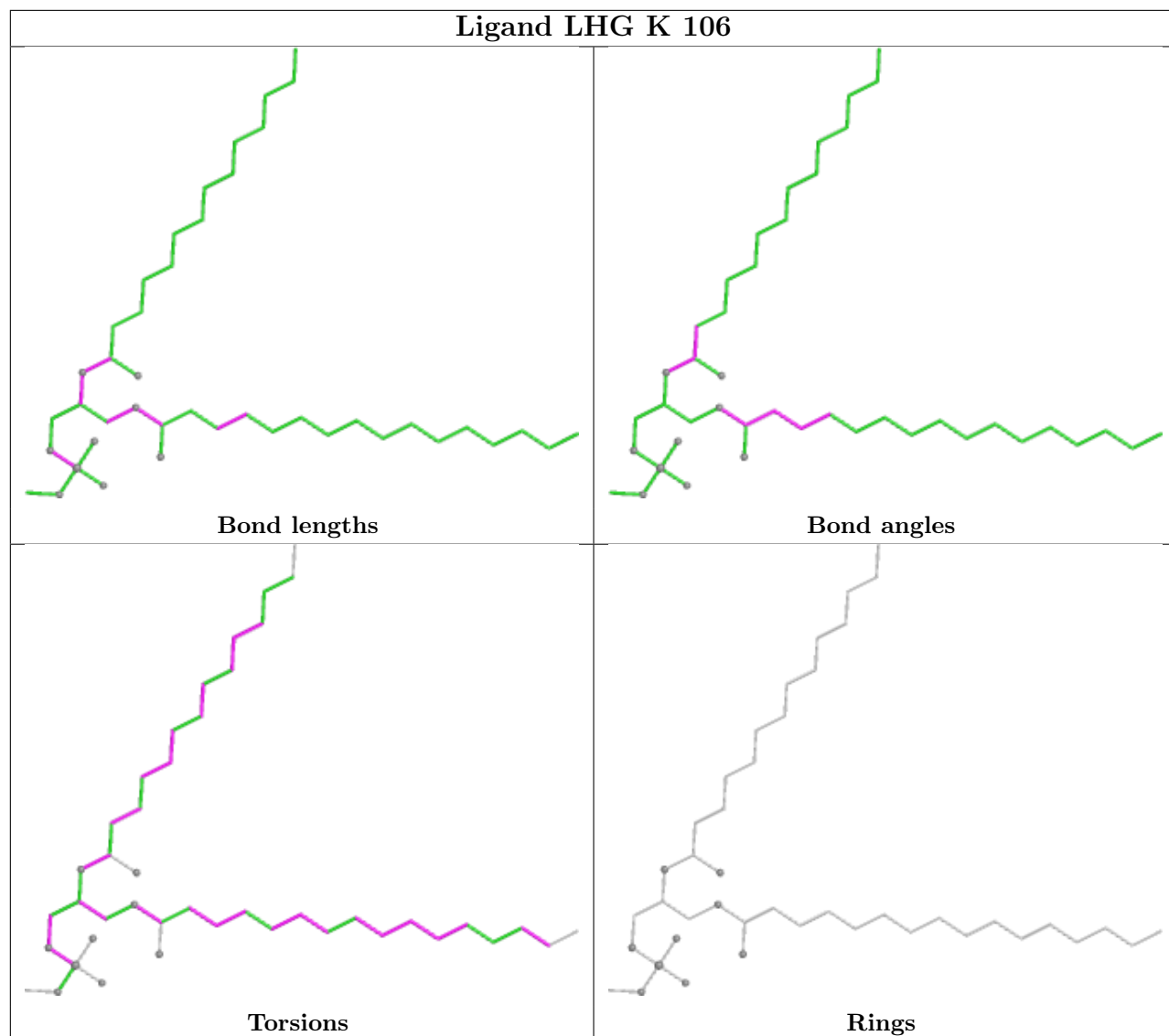
Bond angles



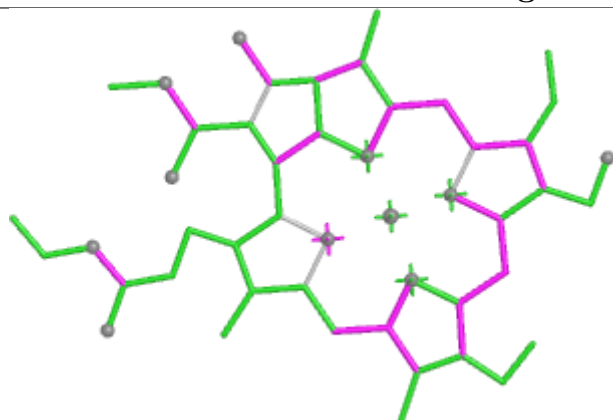
Torsions



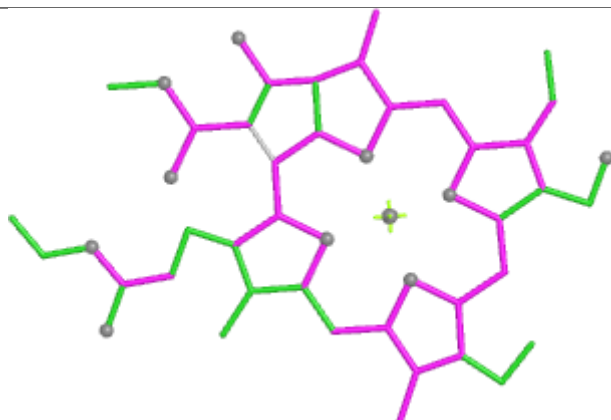
Rings



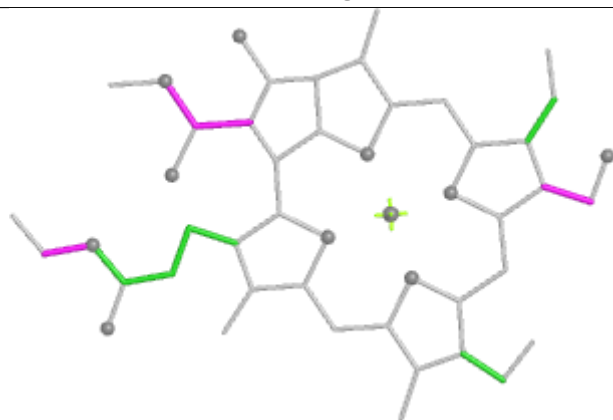
Ligand CHL 1 306



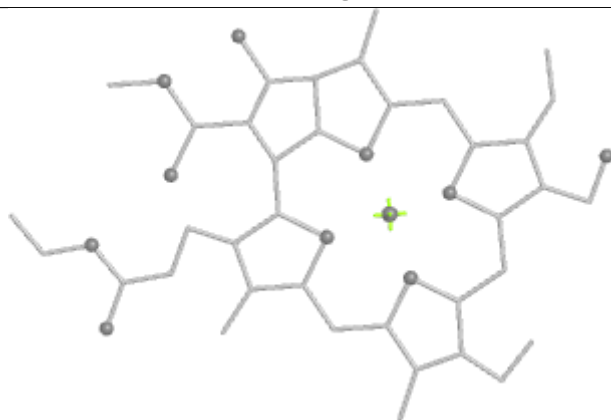
Bond lengths



Bond angles

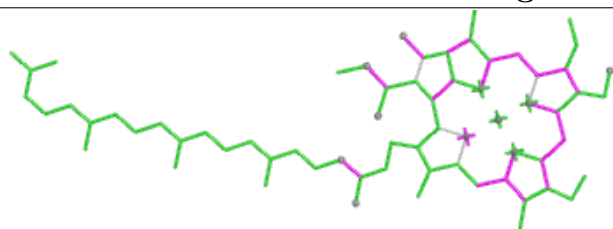


Torsions

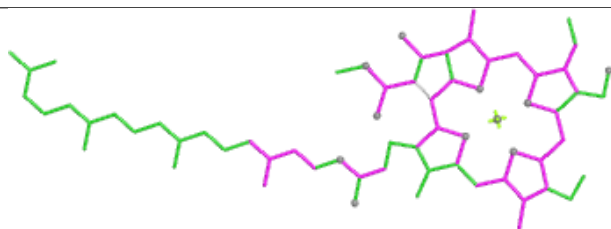


Rings

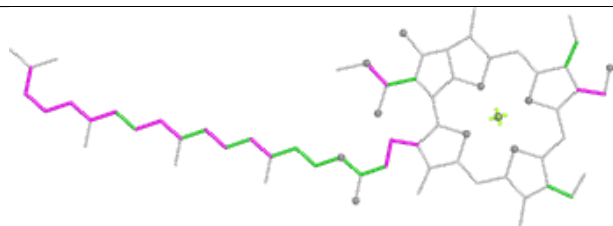
Ligand CHL b 601



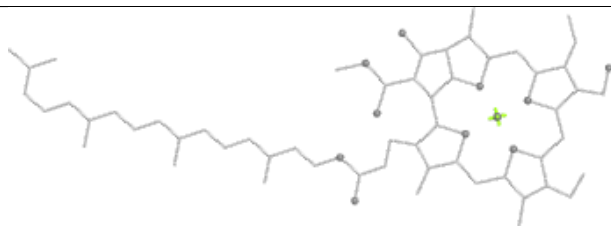
Bond lengths



Bond angles

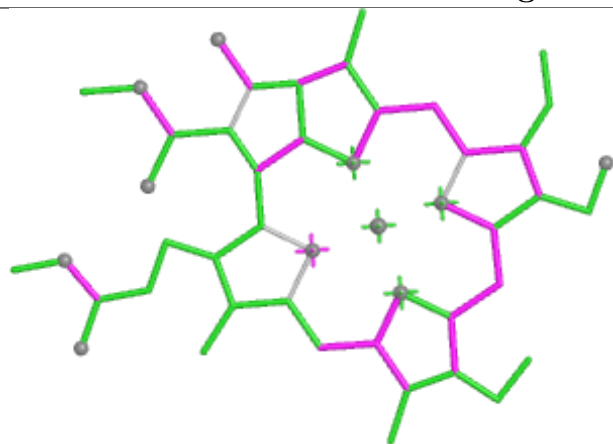


Torsions

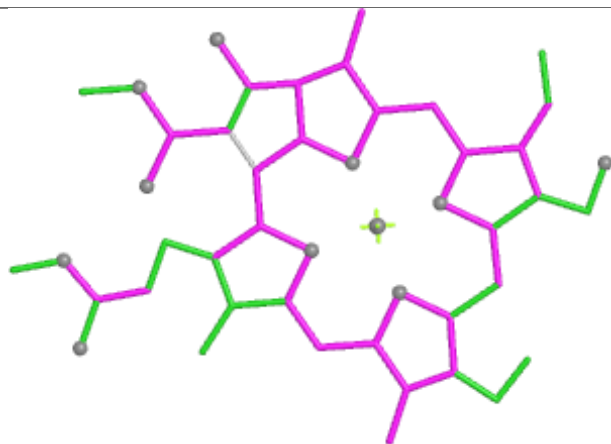


Rings

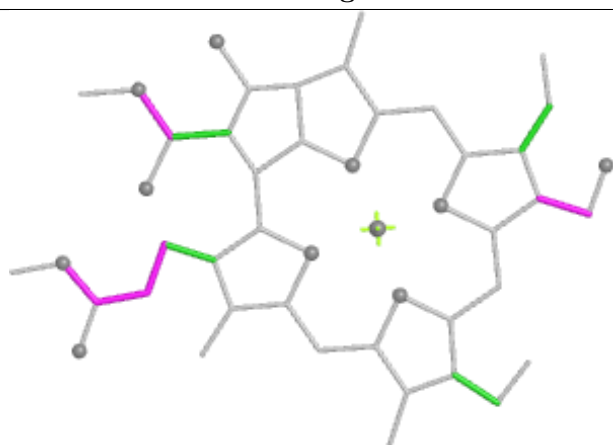
Ligand CHL 8 305



Bond lengths



Bond angles

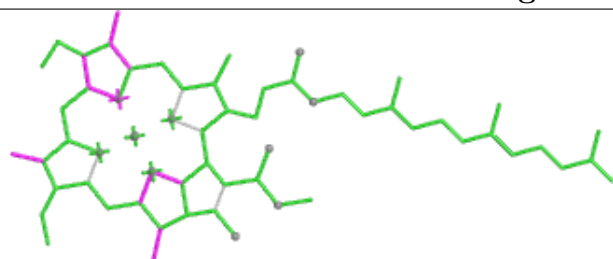


Torsions

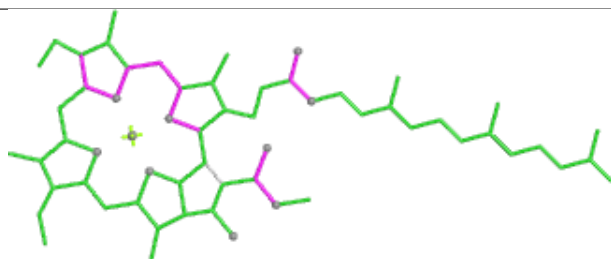


Rings

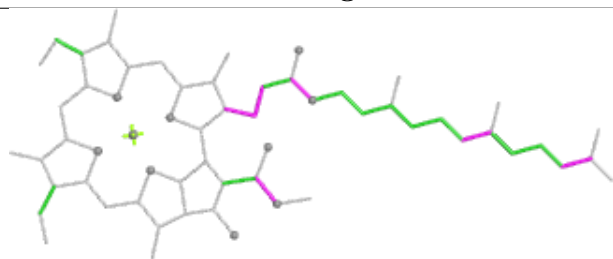
Ligand CLA 7 318



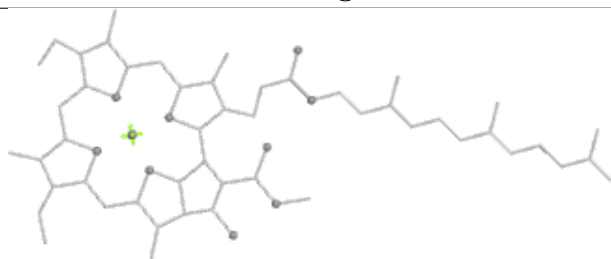
Bond lengths



Bond angles

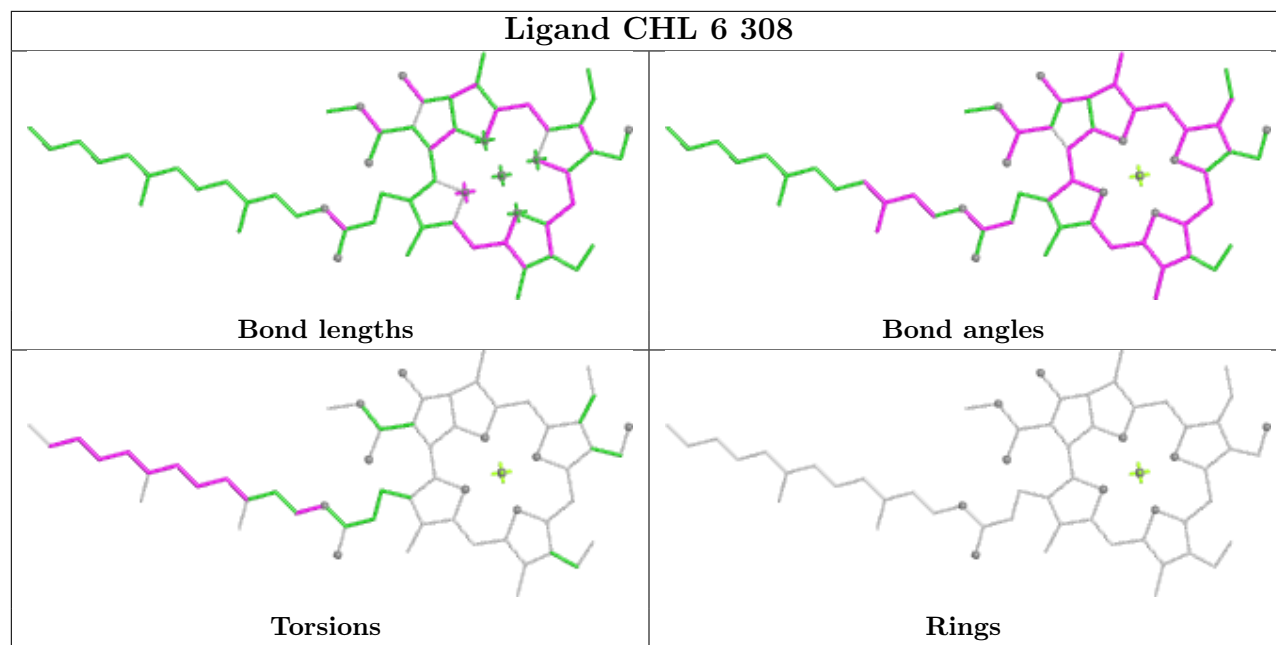


Torsions

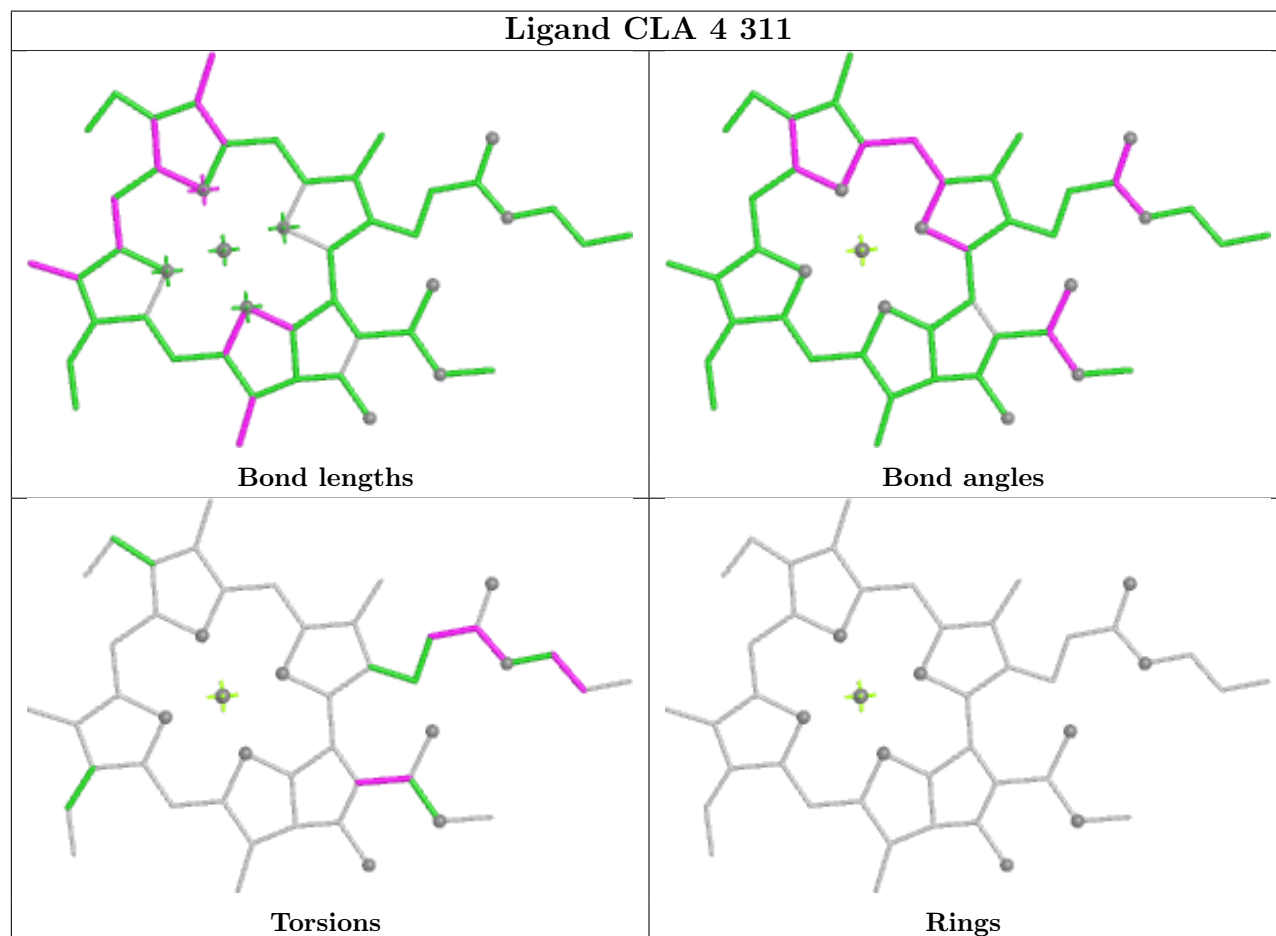


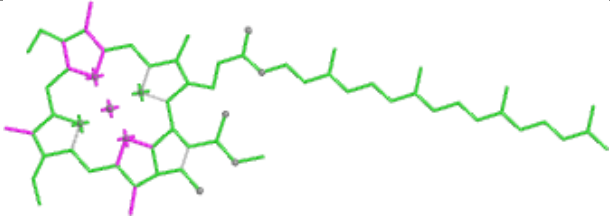
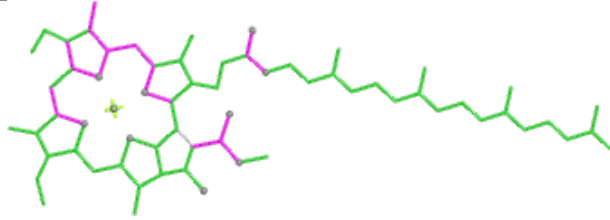
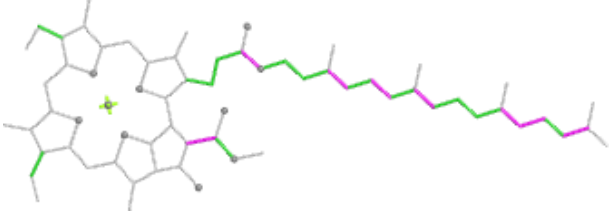
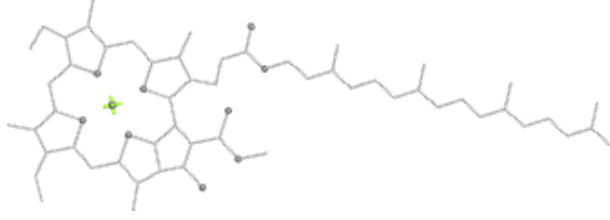
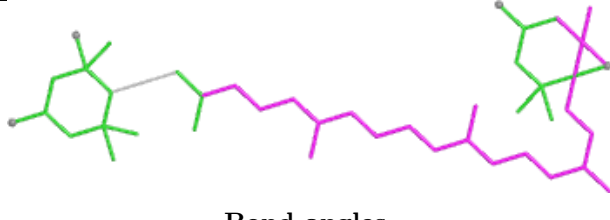
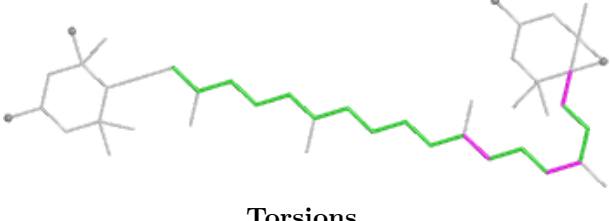
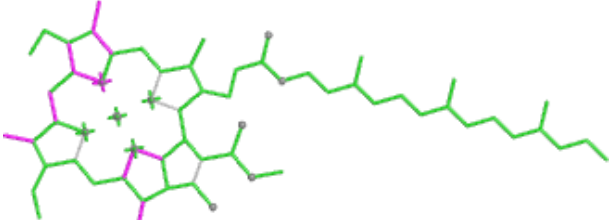
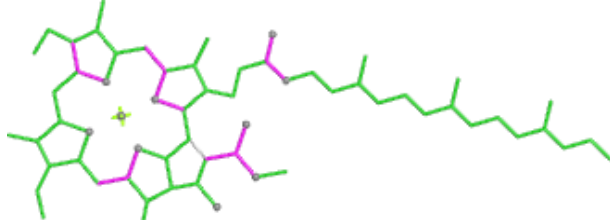
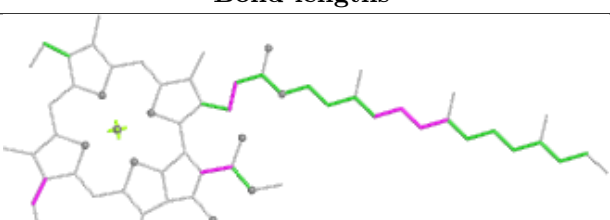
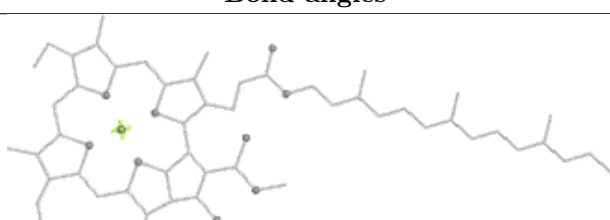
Rings

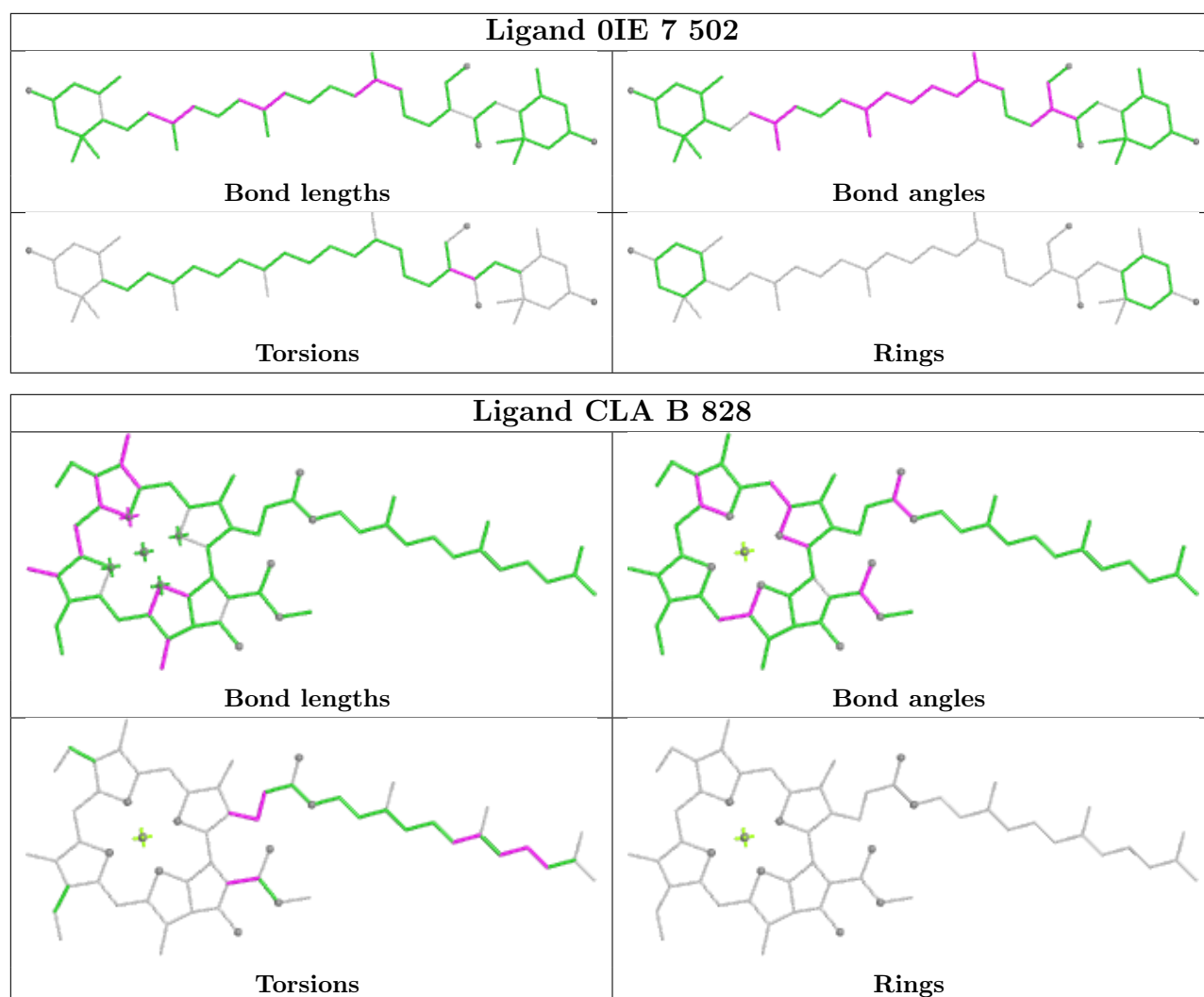
Ligand CHL 6 308



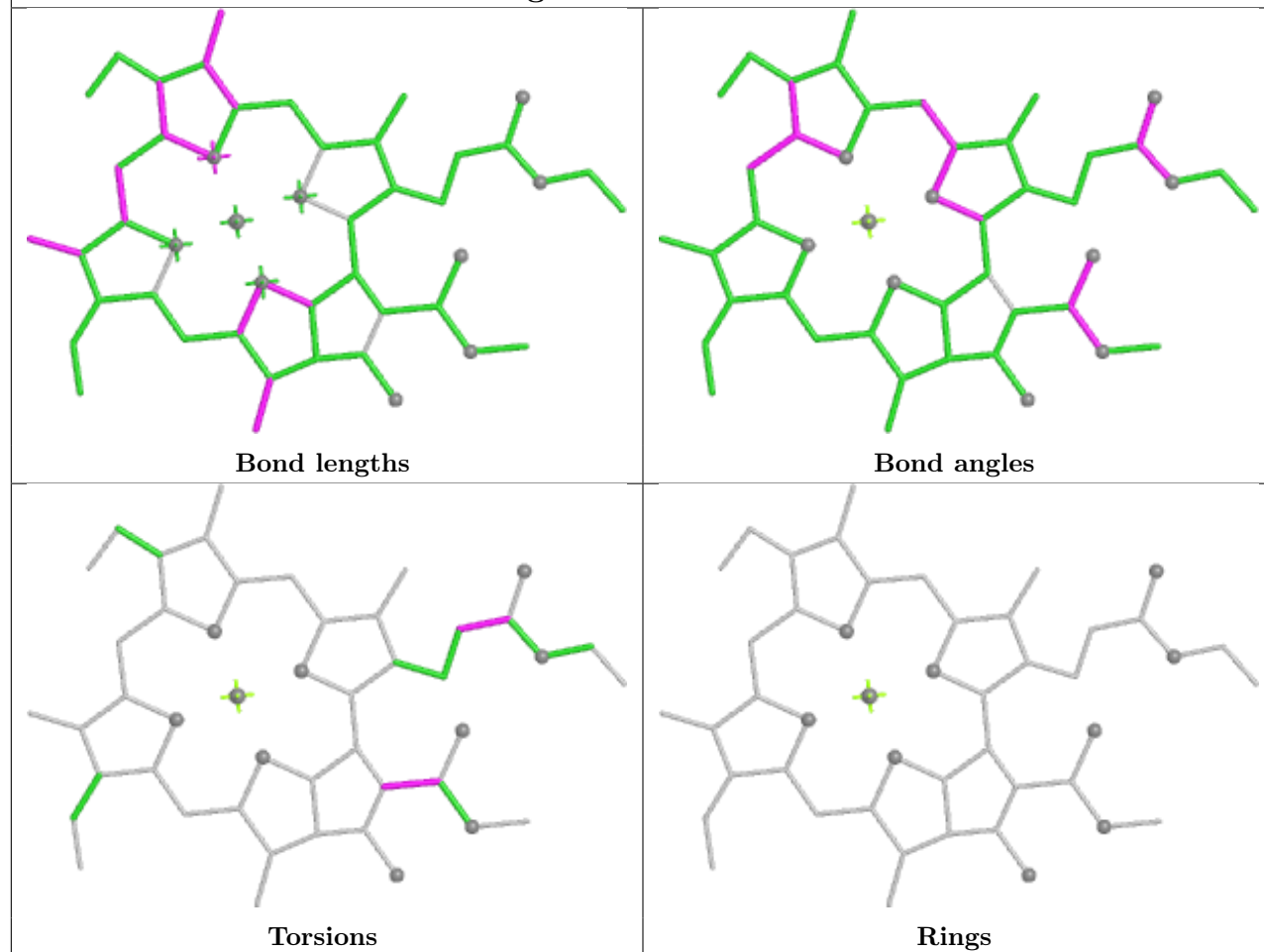
Ligand CLA 4 311



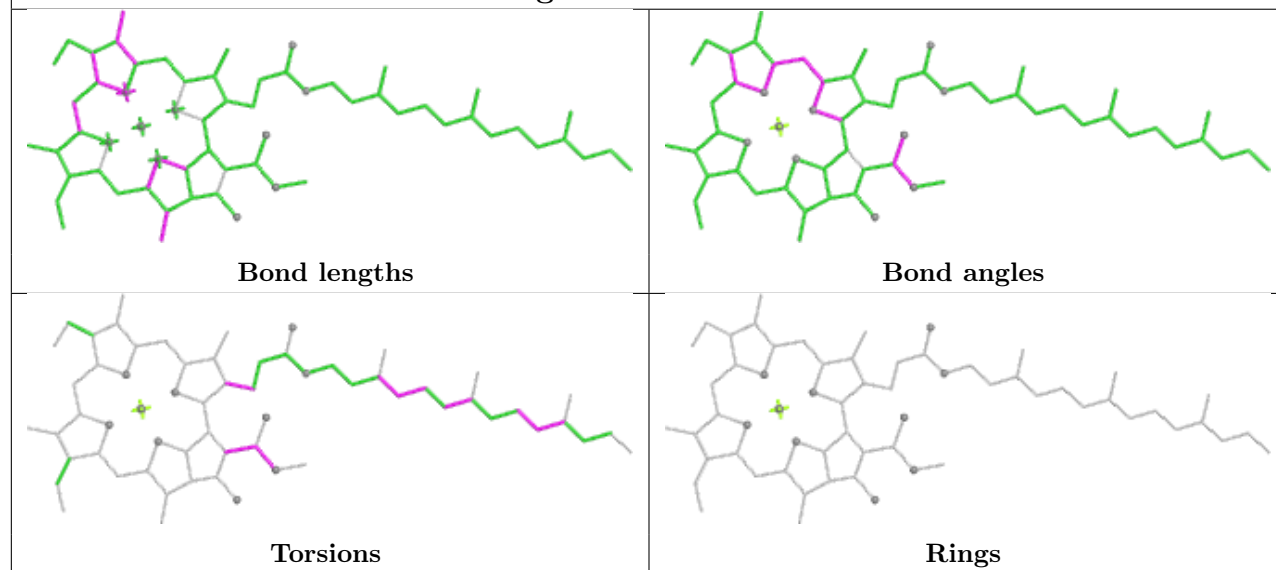
Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NEX f 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 810	
 Bond lengths	 Bond angles
 Torsions	 Rings



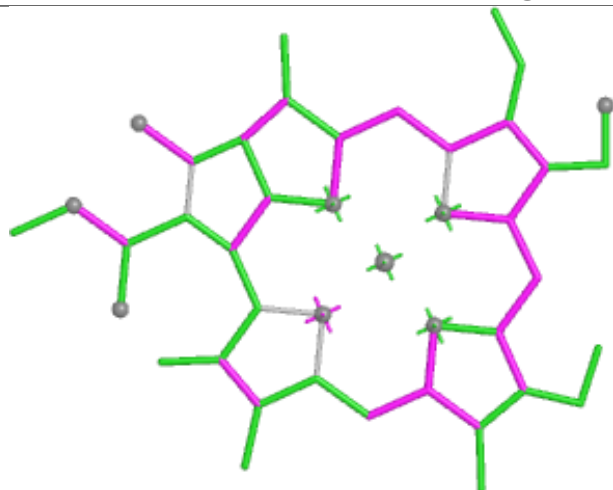
Ligand CLA B 838



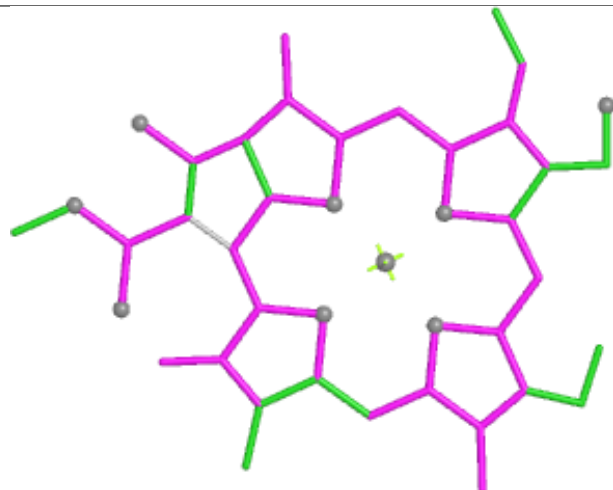
Ligand CLA 0 303



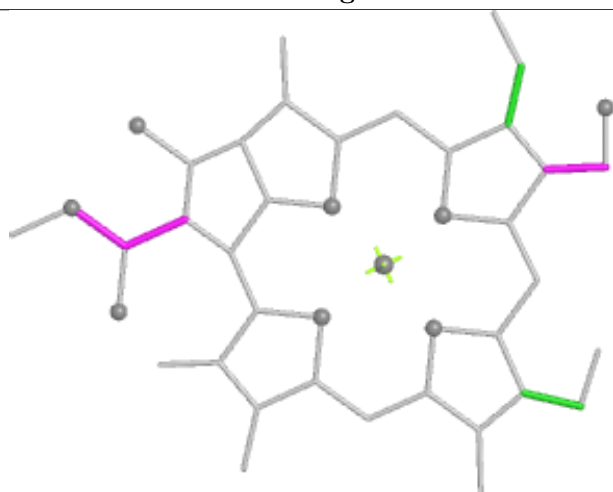
Ligand CHL c 614



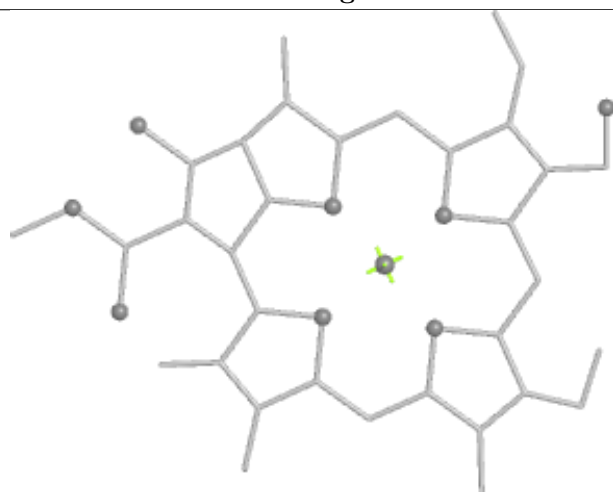
Bond lengths



Bond angles

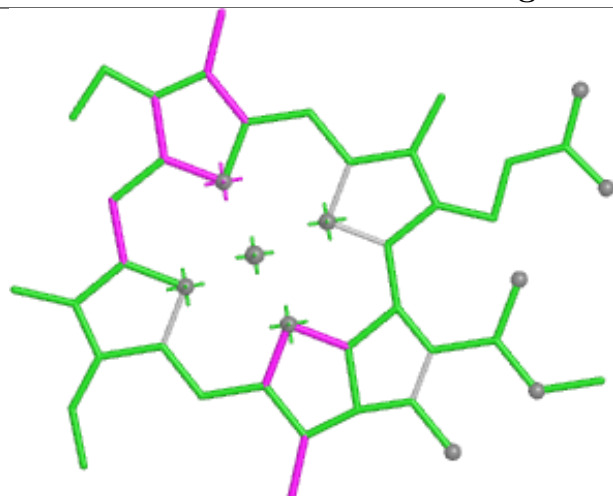


Torsions

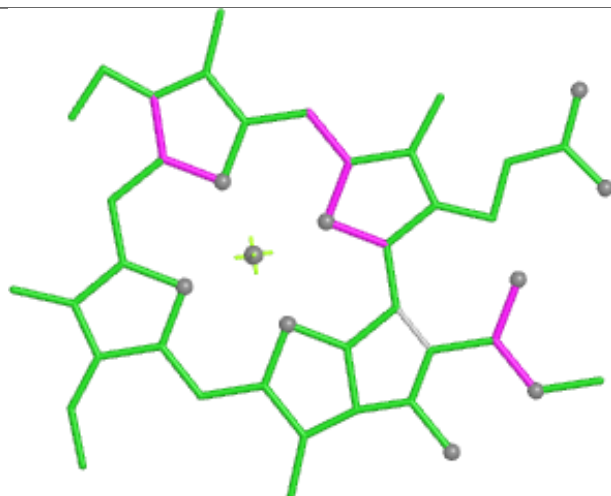


Rings

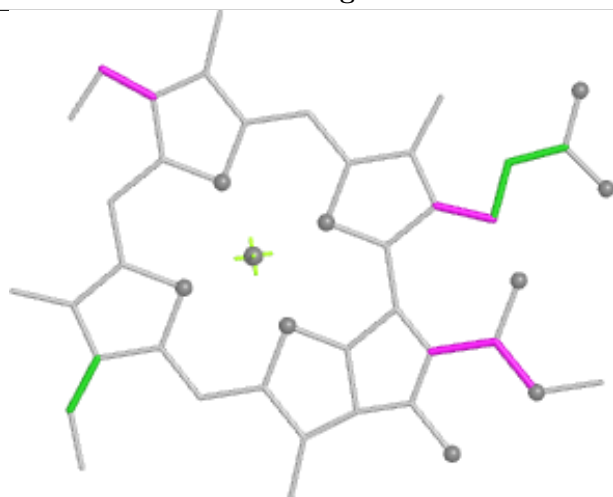
Ligand CLA 5 310



Bond lengths



Bond angles

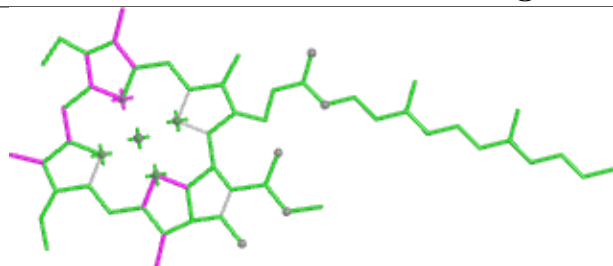


Torsions

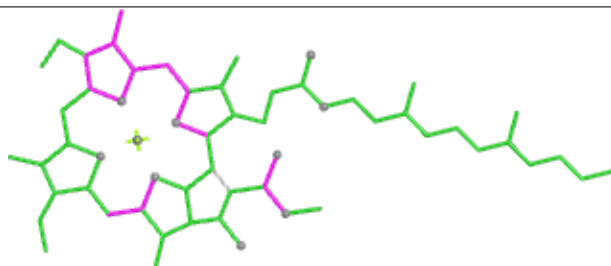


Rings

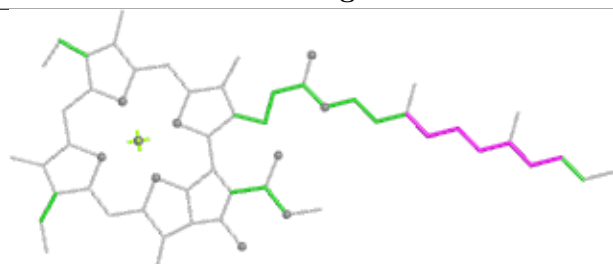
Ligand CLA L 201



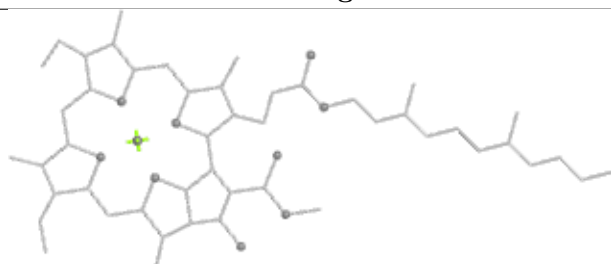
Bond lengths



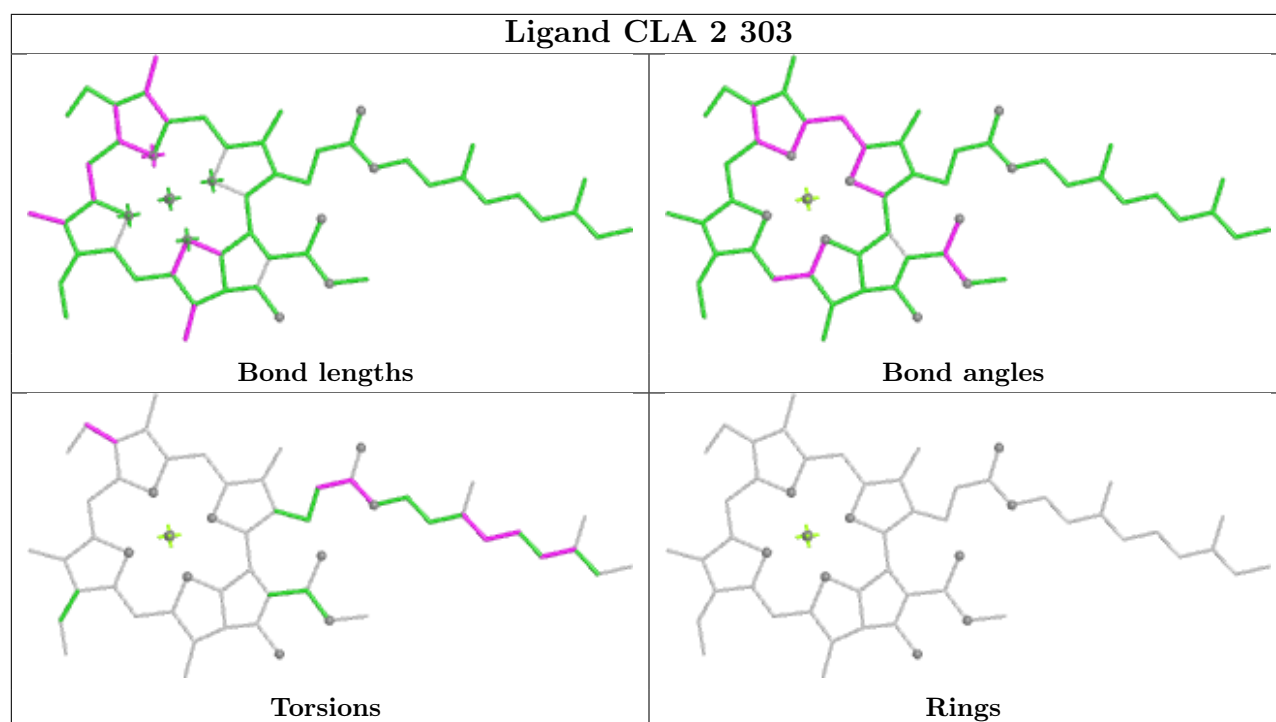
Bond angles

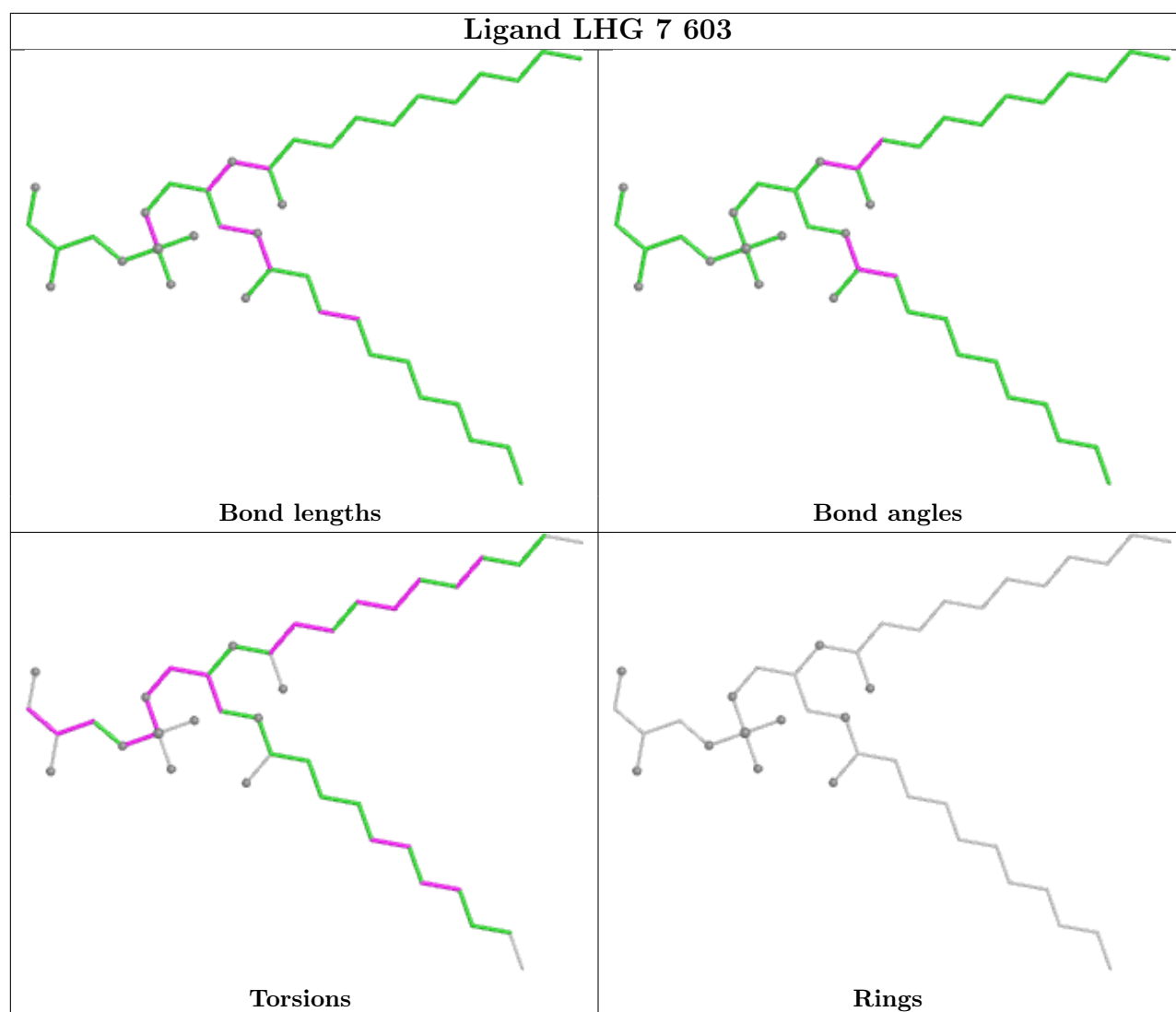


Torsions

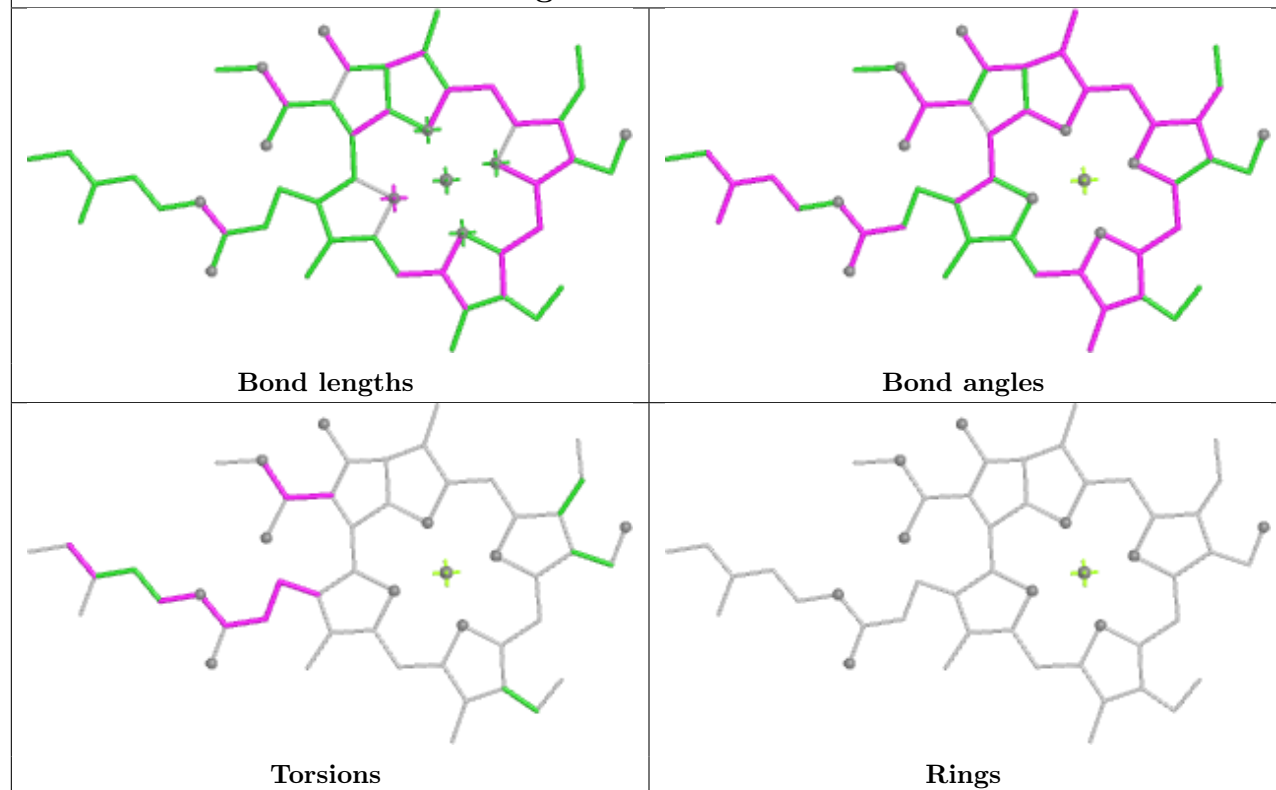


Rings

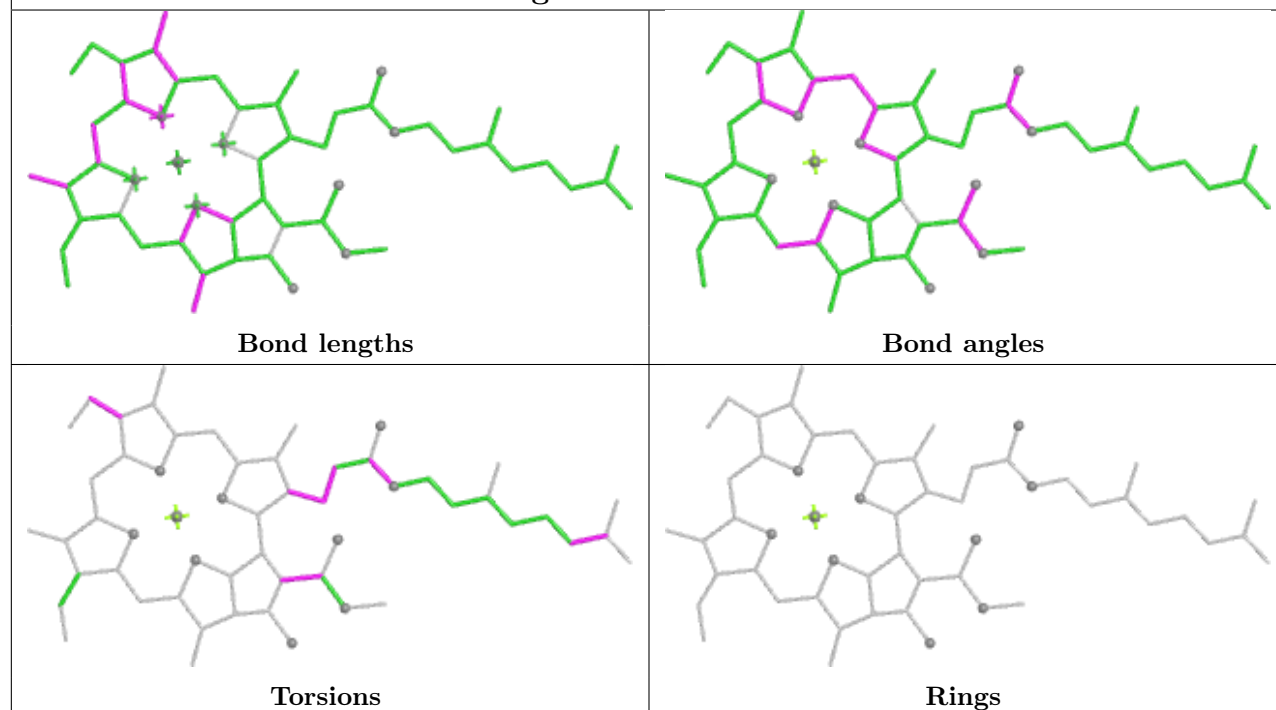


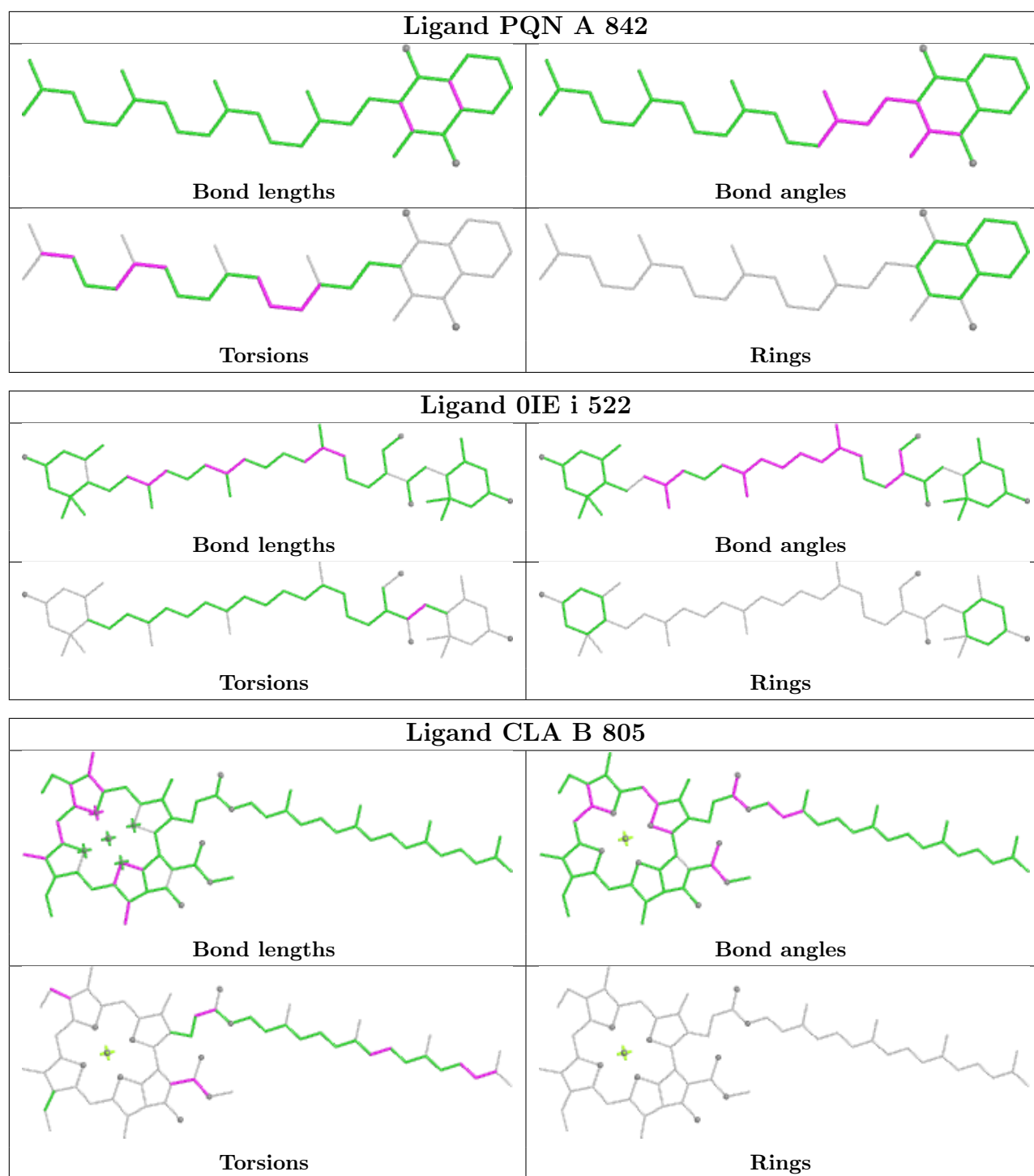


Ligand CHL 5 301

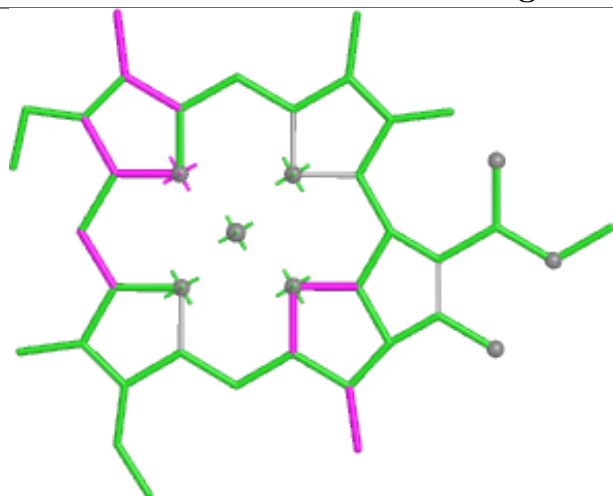


Ligand CLA A 824

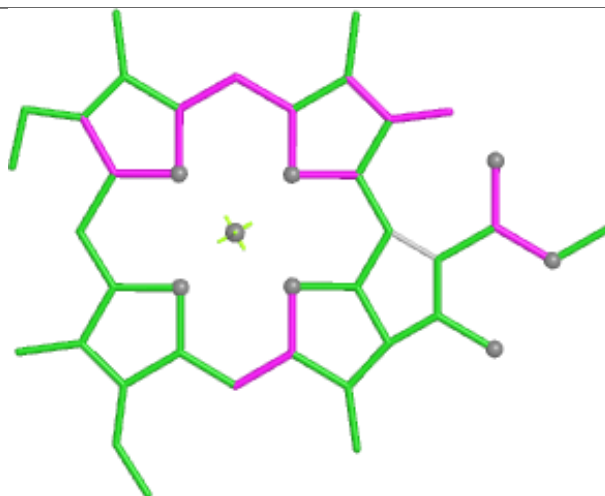




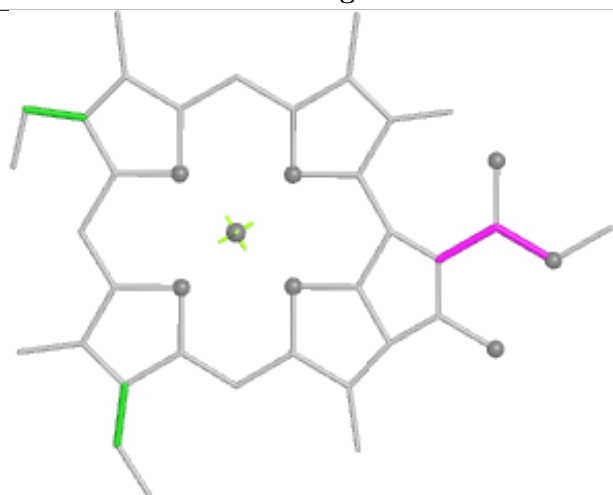
Ligand CLA 0 310



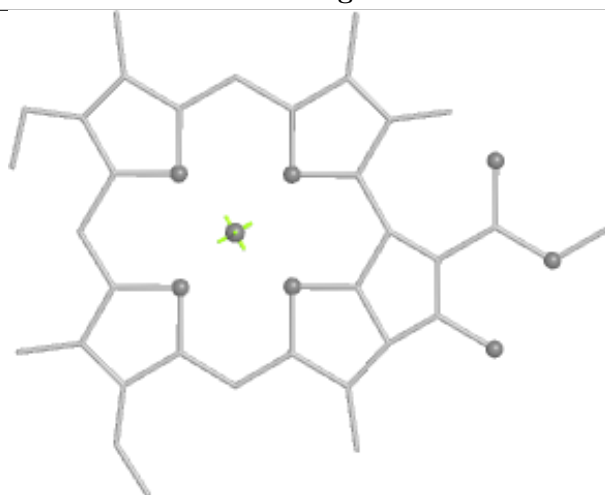
Bond lengths



Bond angles

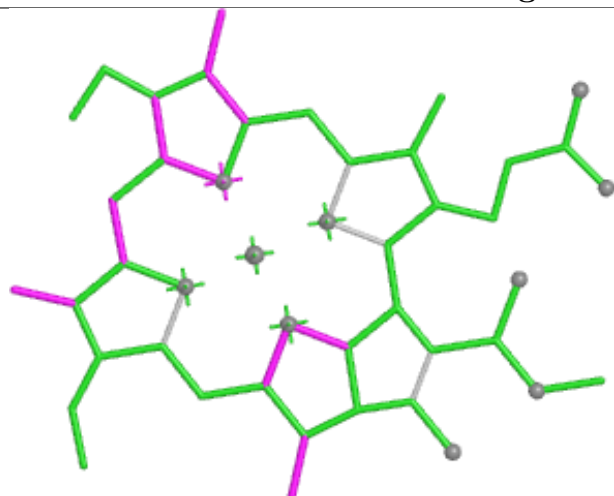


Torsions

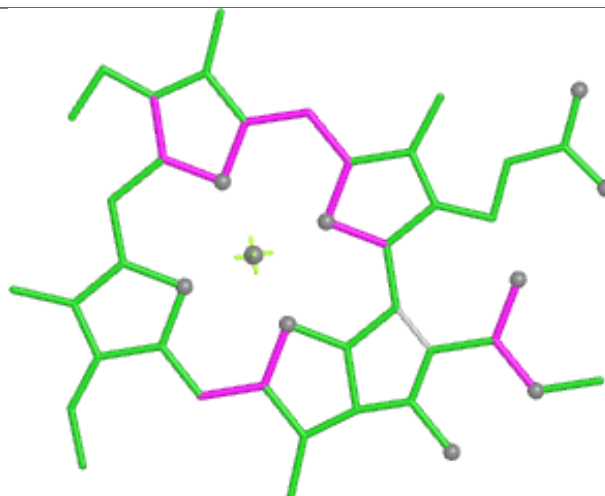


Rings

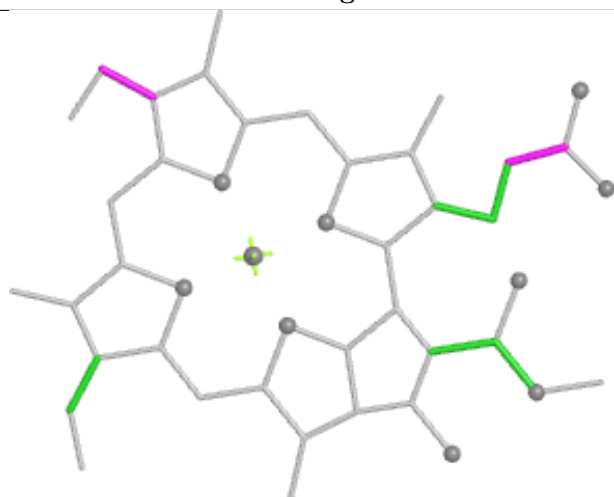
Ligand CLA 4 303



Bond lengths



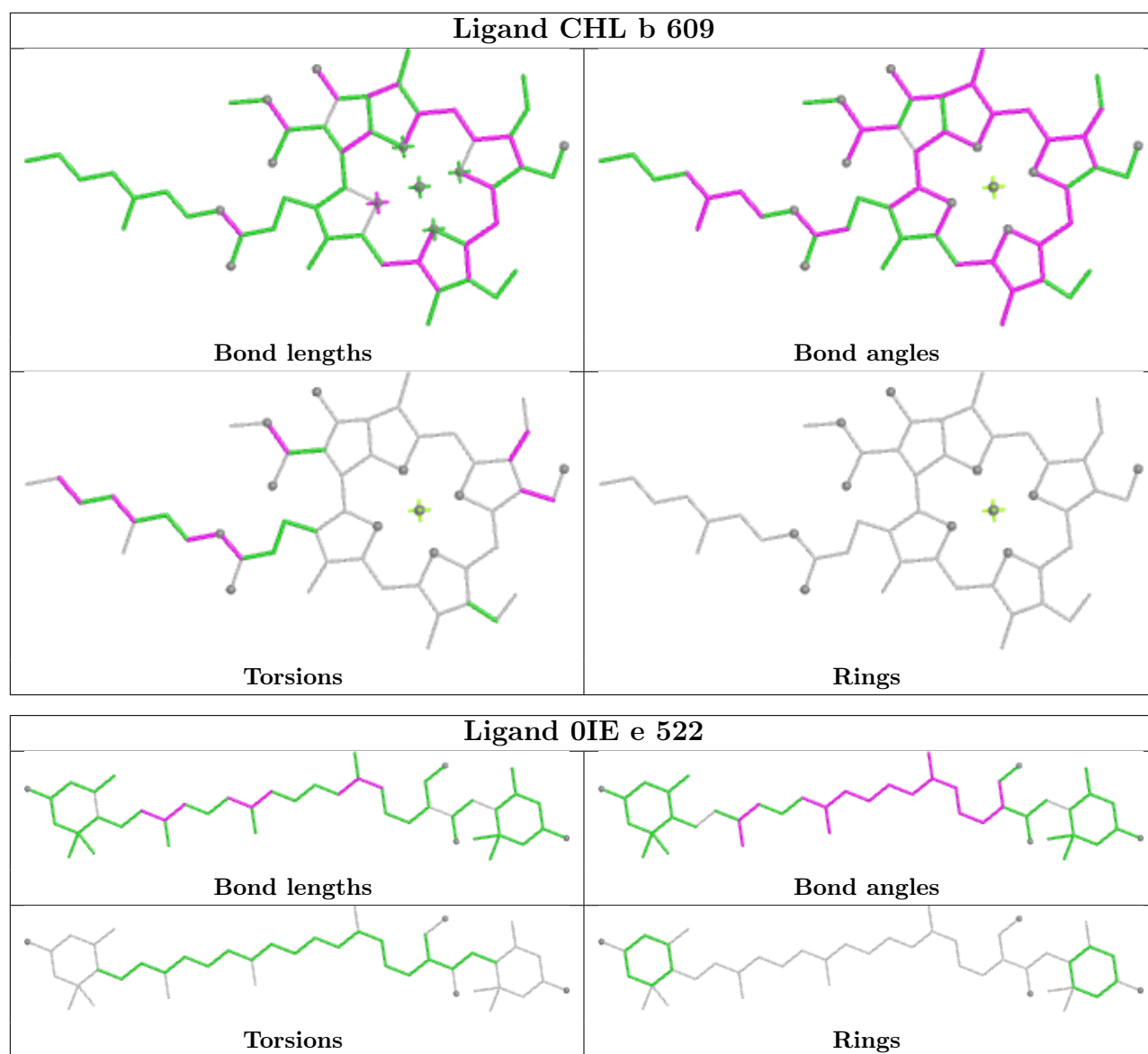
Bond angles



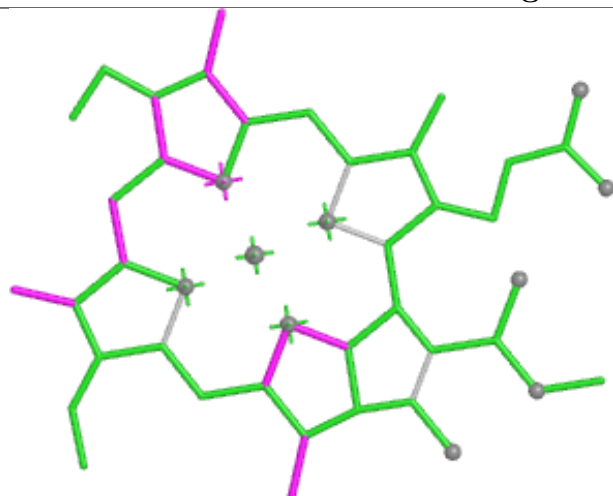
Torsions



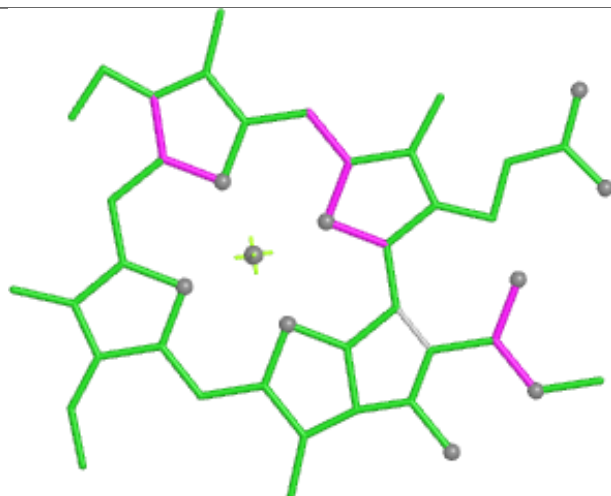
Rings



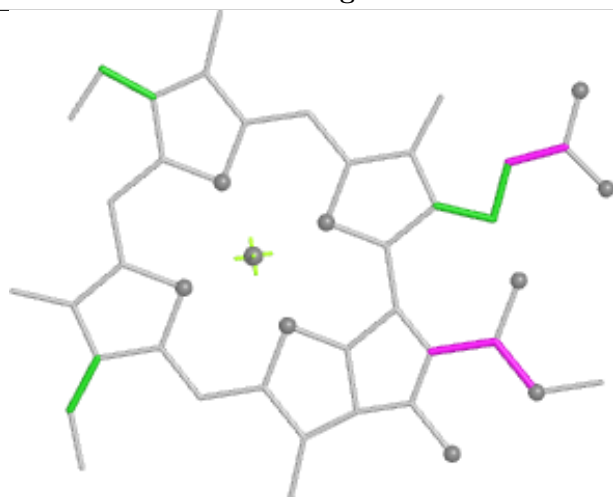
Ligand CLA f 612



Bond lengths



Bond angles

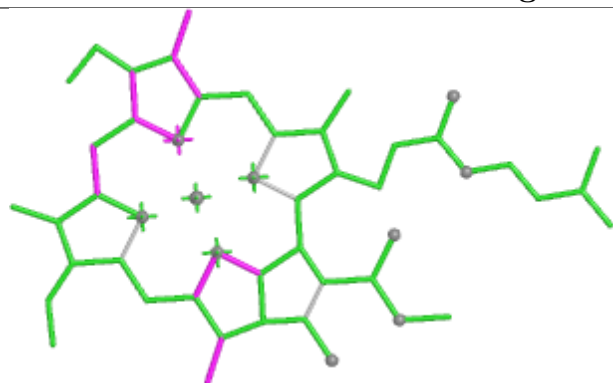


Torsions

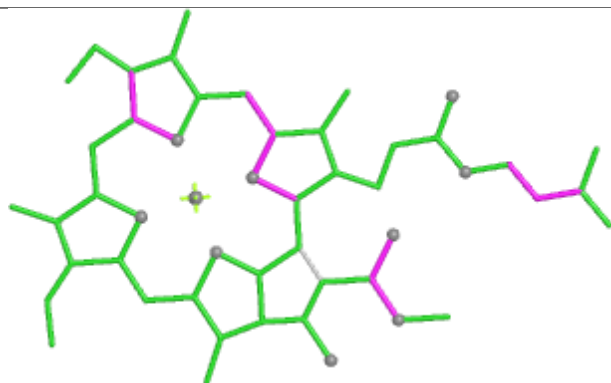


Rings

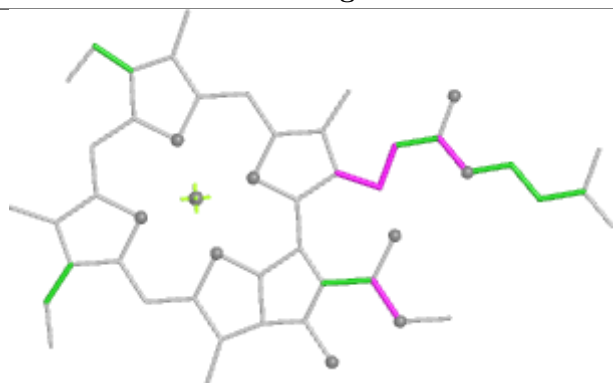
Ligand CLA e 604



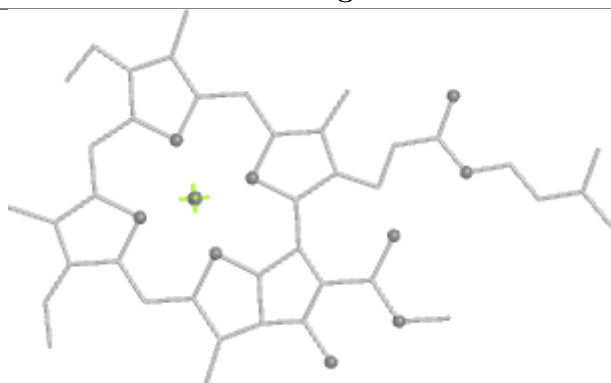
Bond lengths



Bond angles

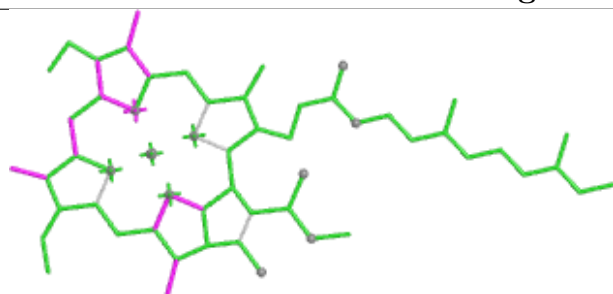


Torsions

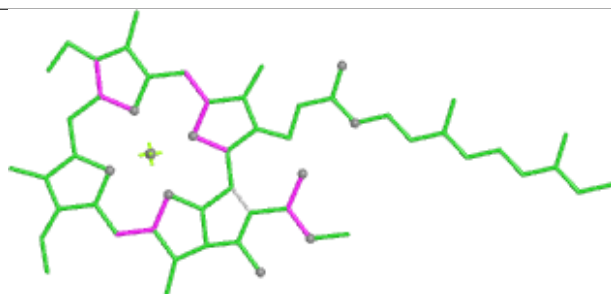


Rings

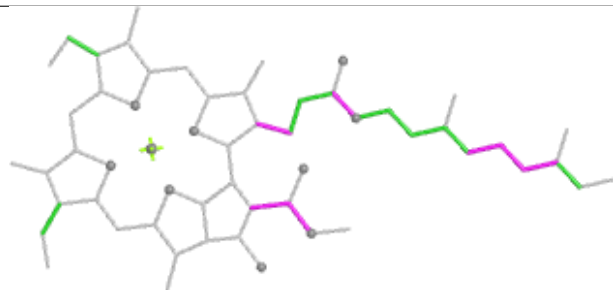
Ligand CLA 5 312



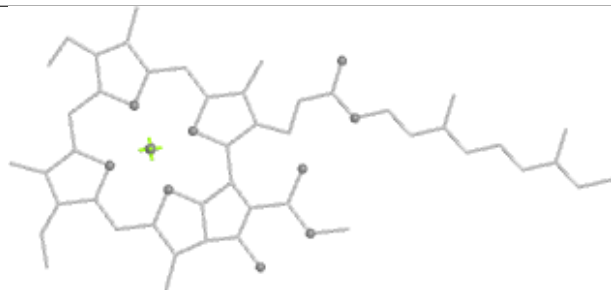
Bond lengths



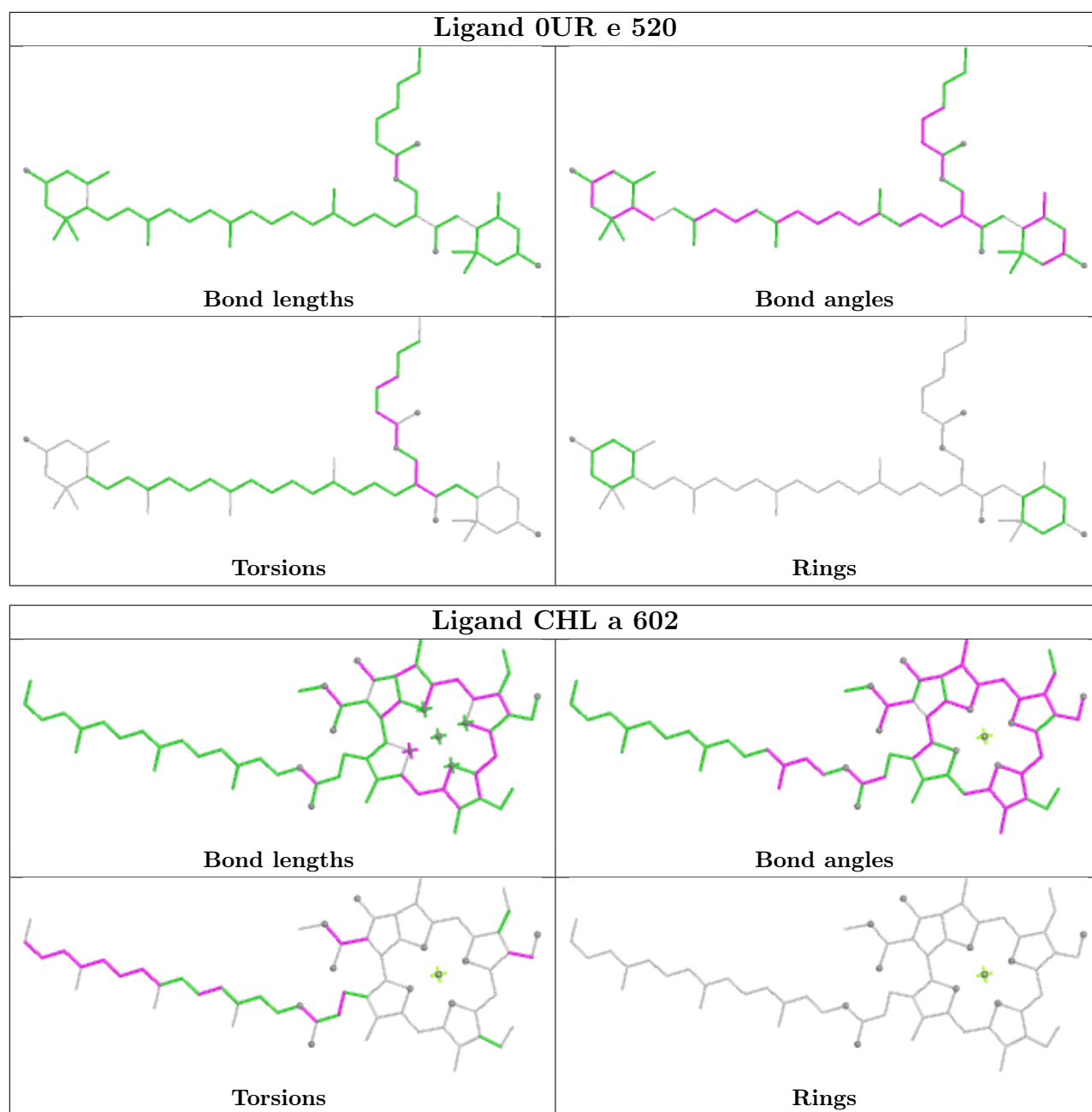
Bond angles



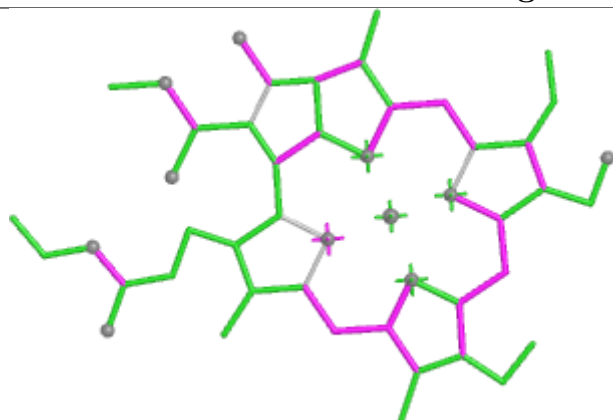
Torsions



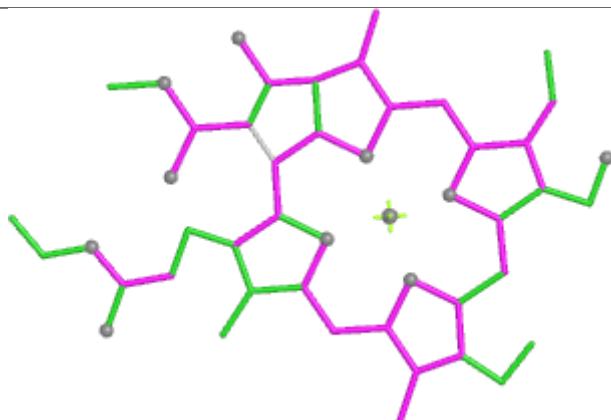
Rings



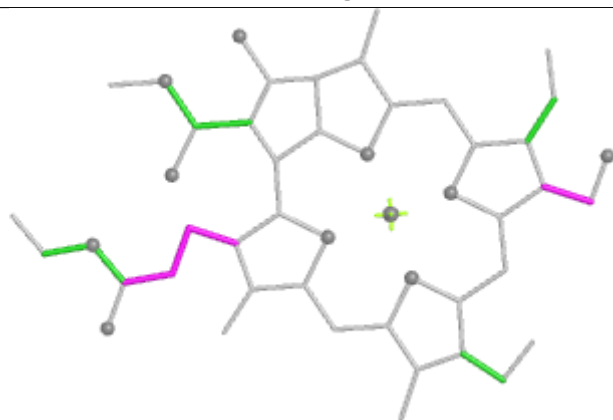
Ligand CHL 9 306



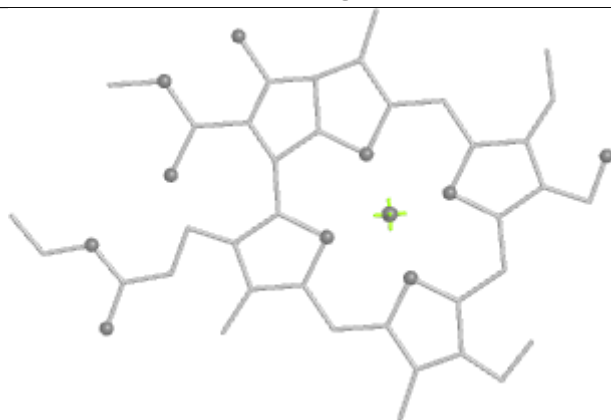
Bond lengths



Bond angles

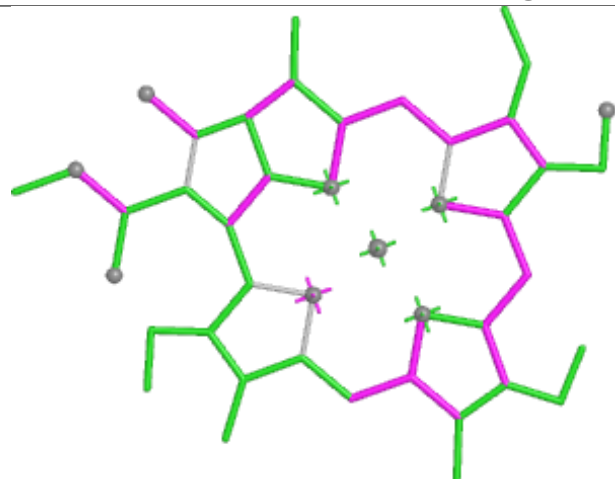


Torsions

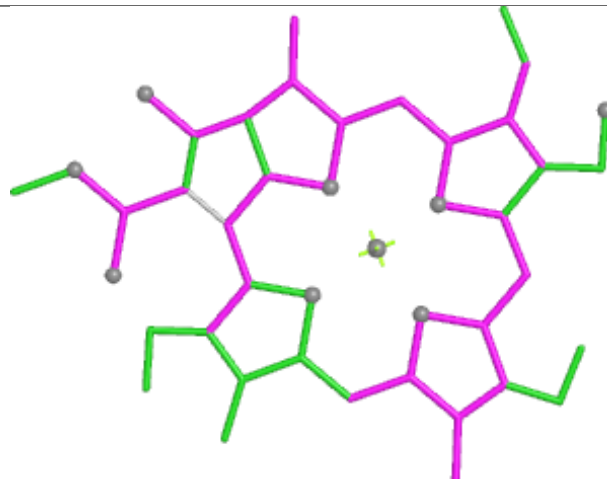


Rings

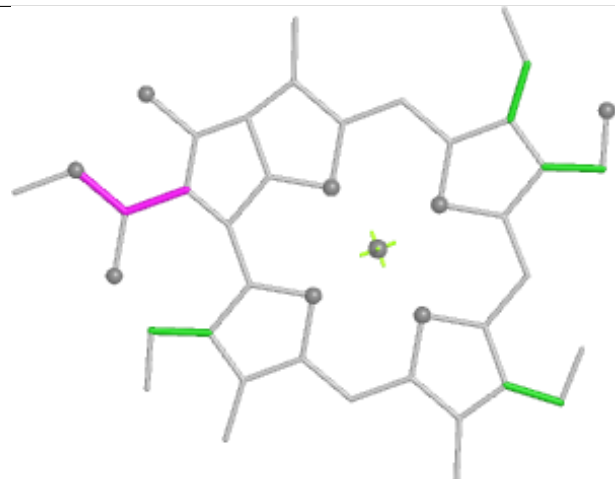
Ligand CHL 6 315



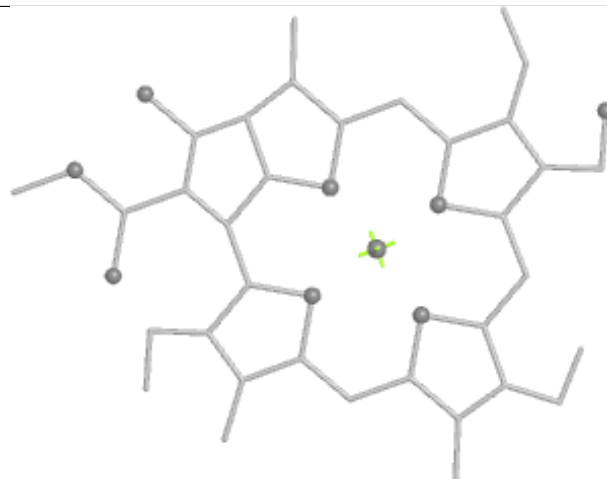
Bond lengths



Bond angles

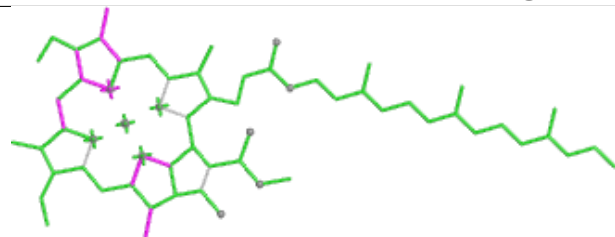


Torsions

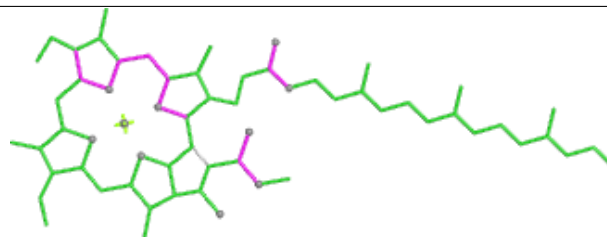


Rings

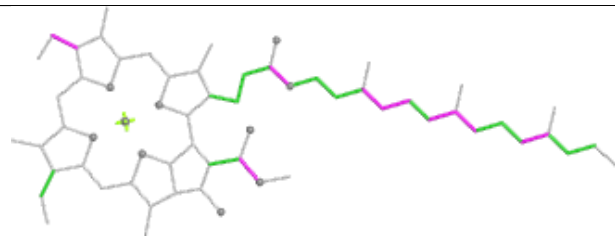
Ligand CLA 3 310



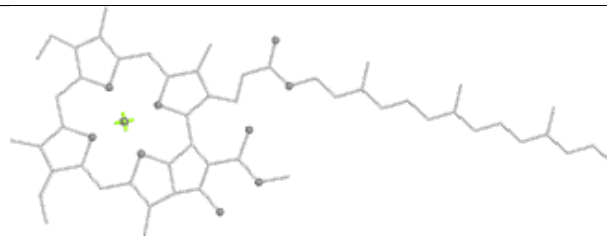
Bond lengths



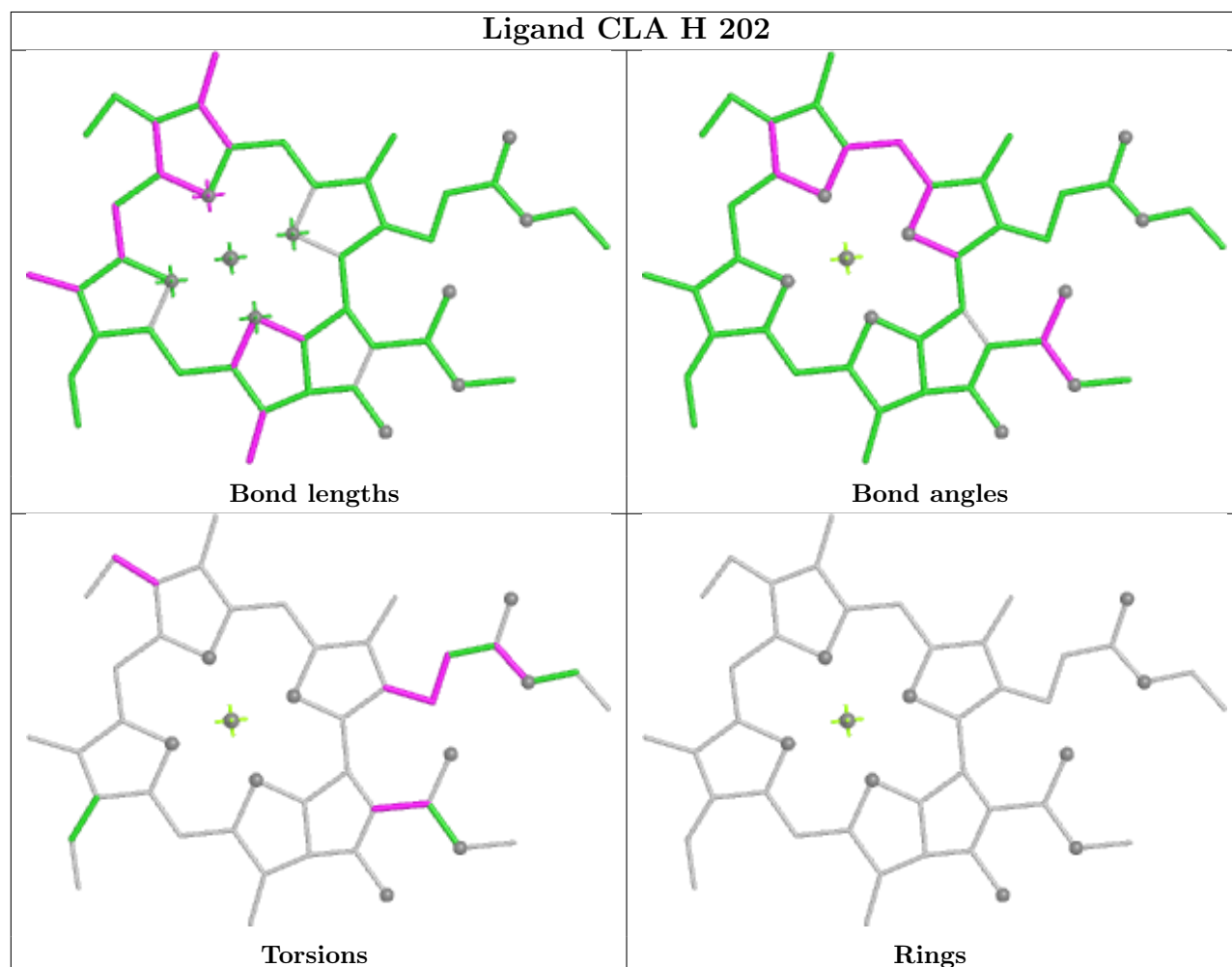
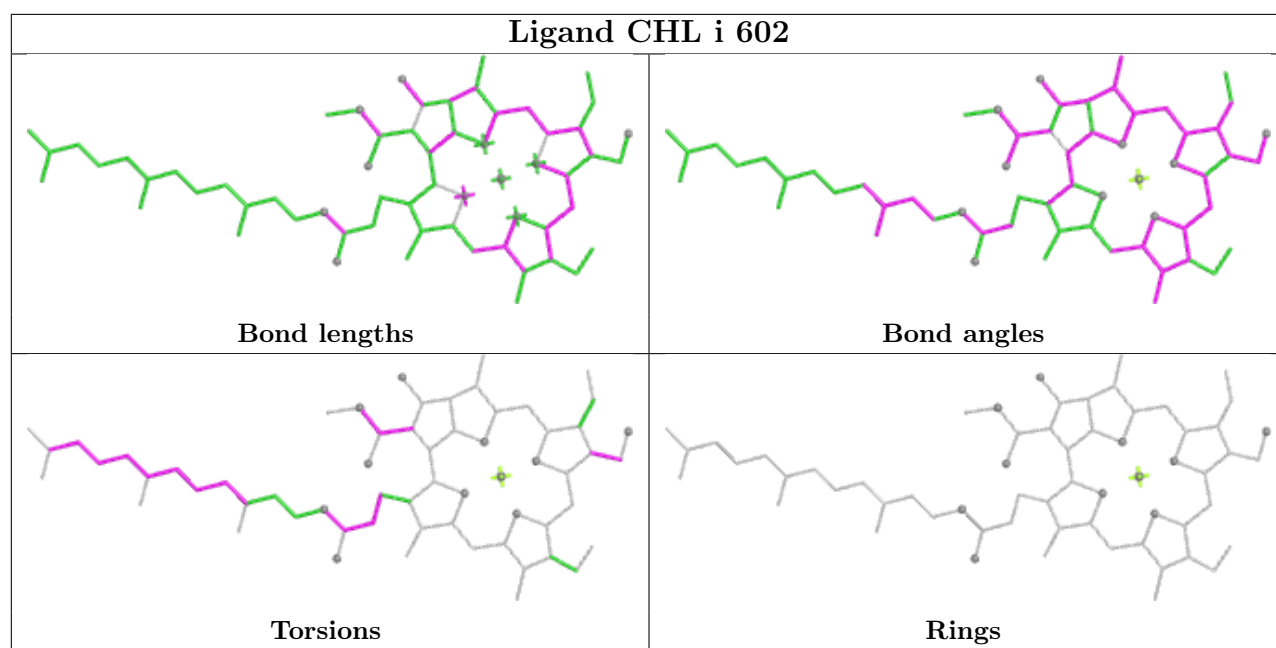
Bond angles



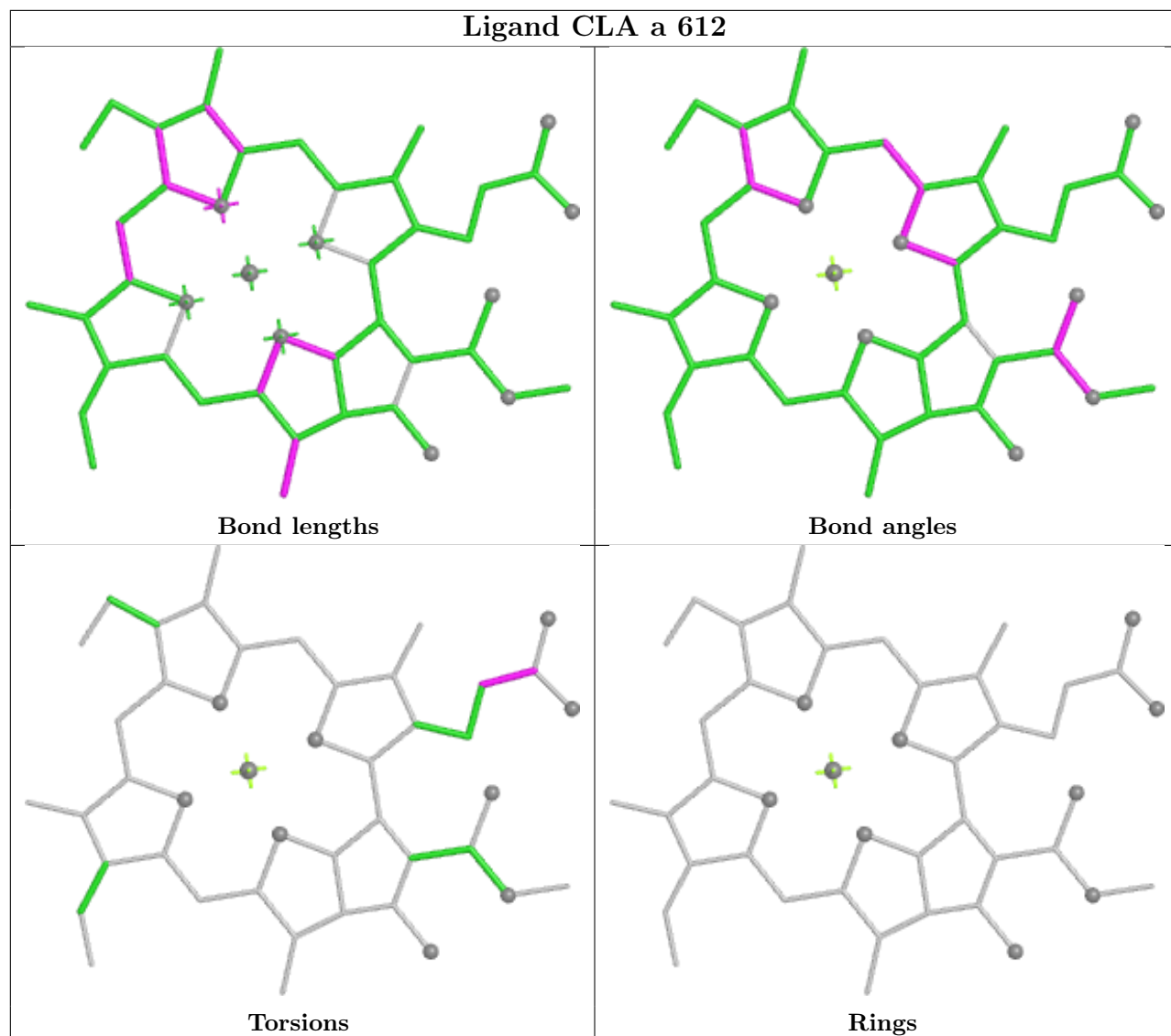
Torsions



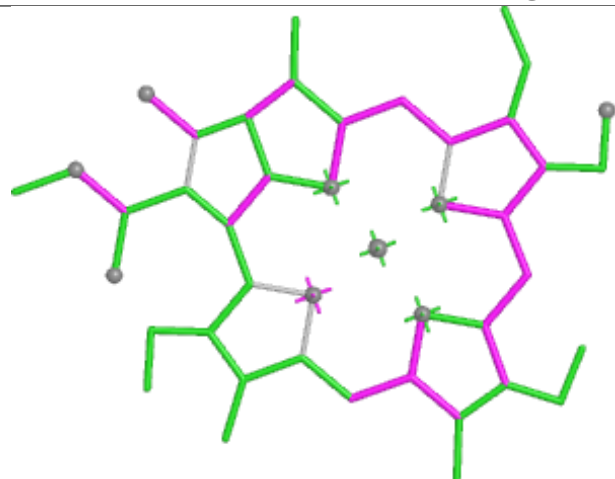
Rings



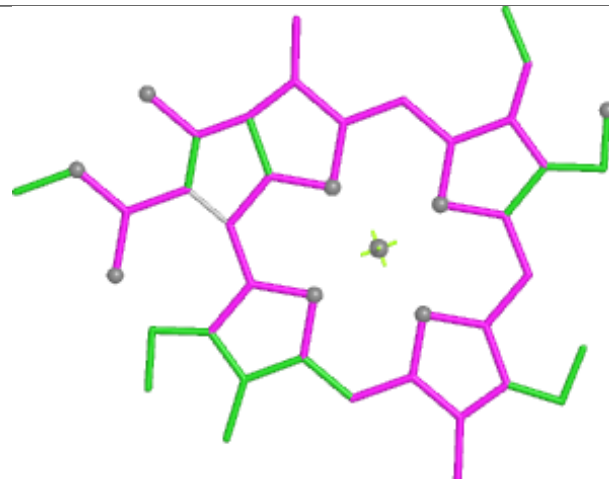
Ligand CLA a 612



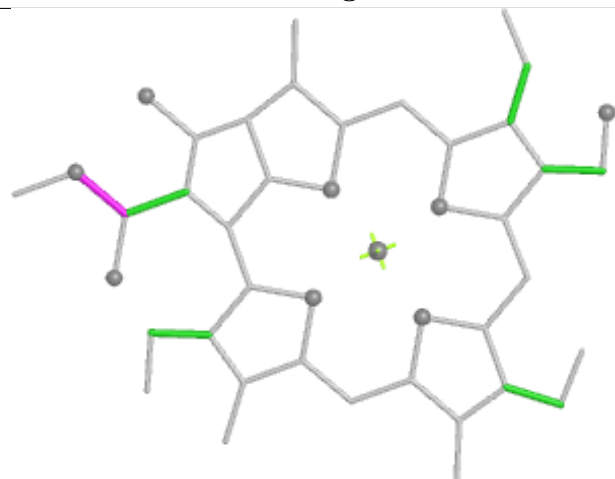
Ligand CHL f 605



Bond lengths



Bond angles

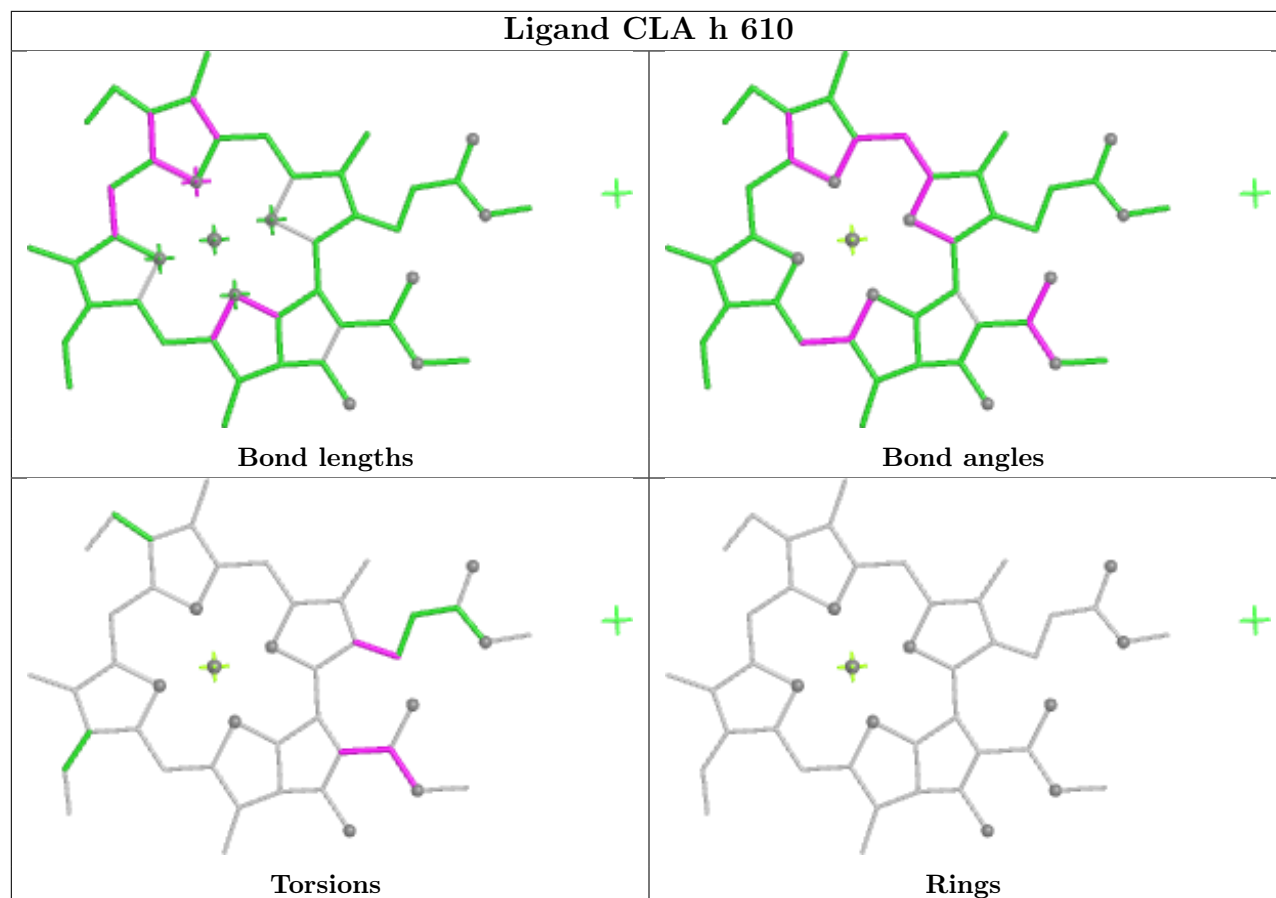


Torsions

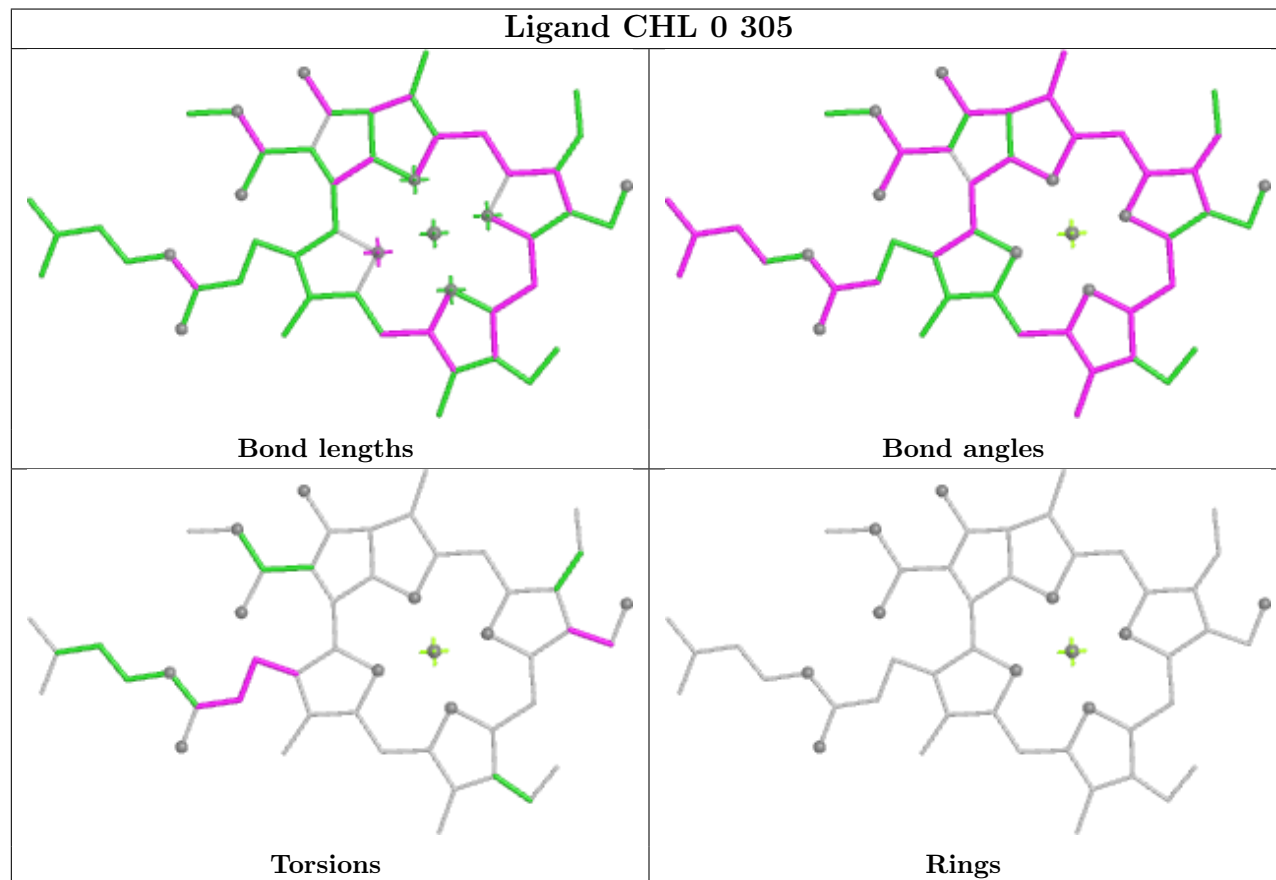


Rings

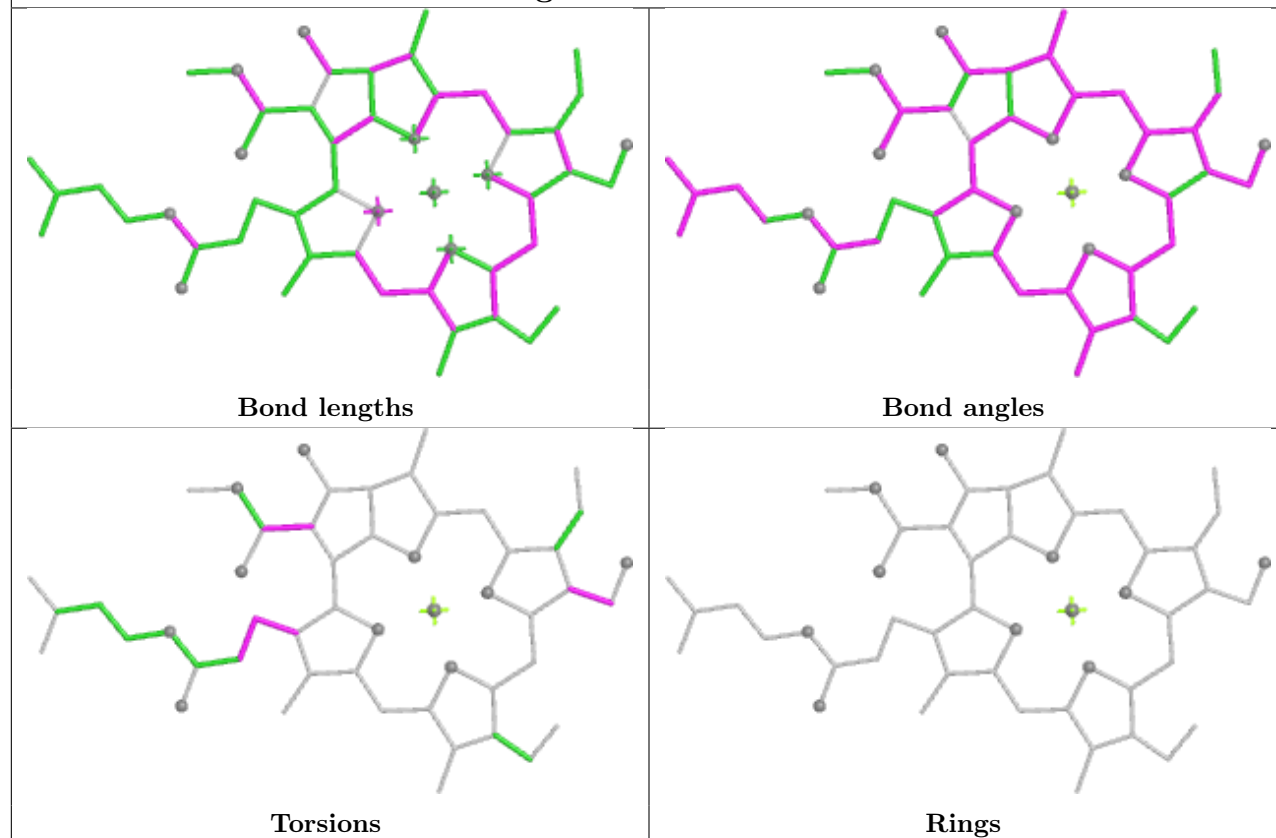
Ligand CLA h 610



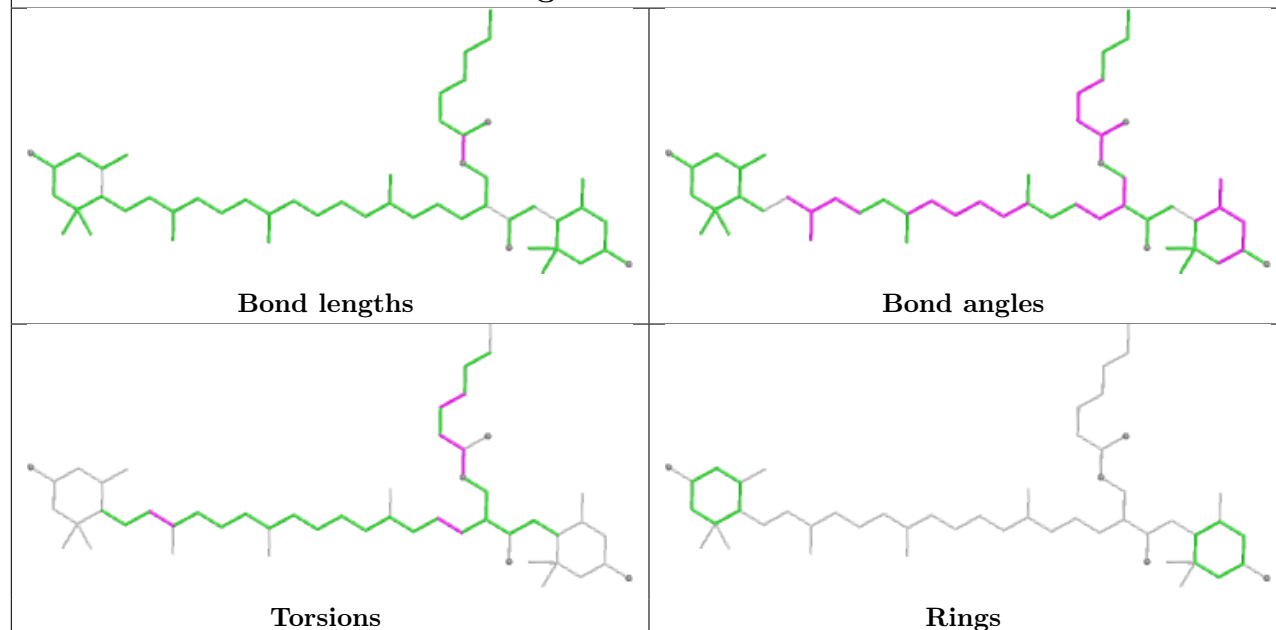
Ligand CHL 0 305

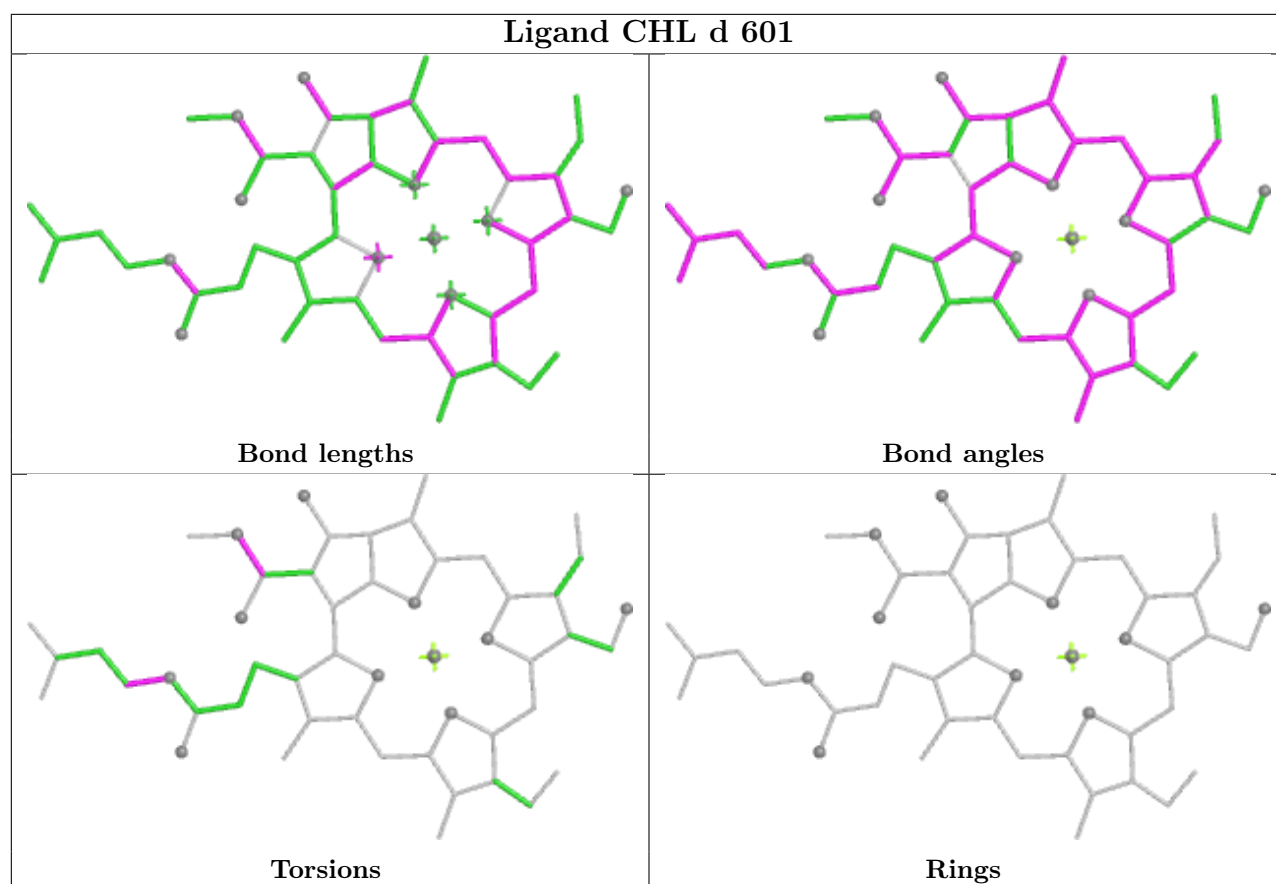


Ligand CHL 2 313

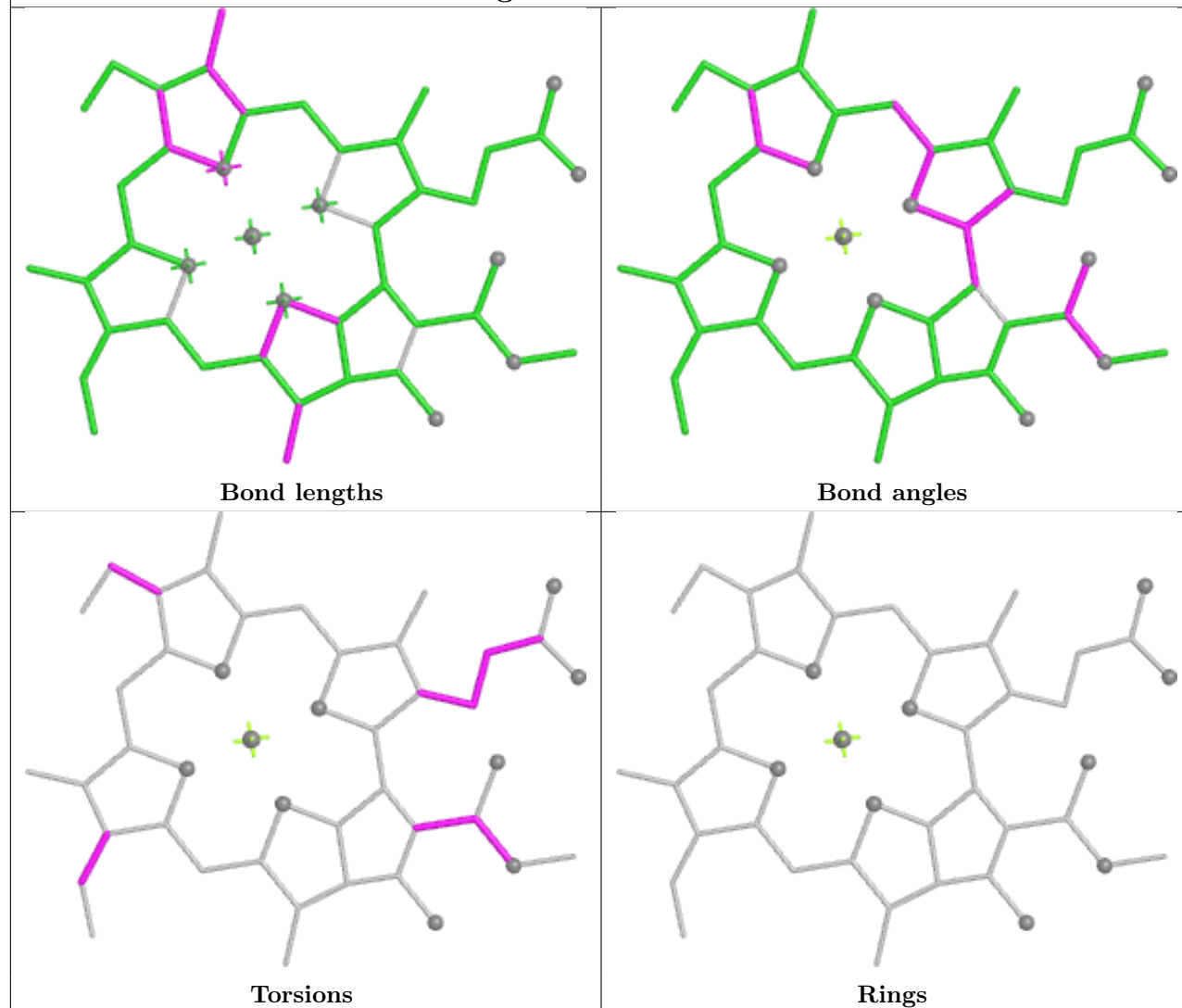


Ligand OUR 8 502

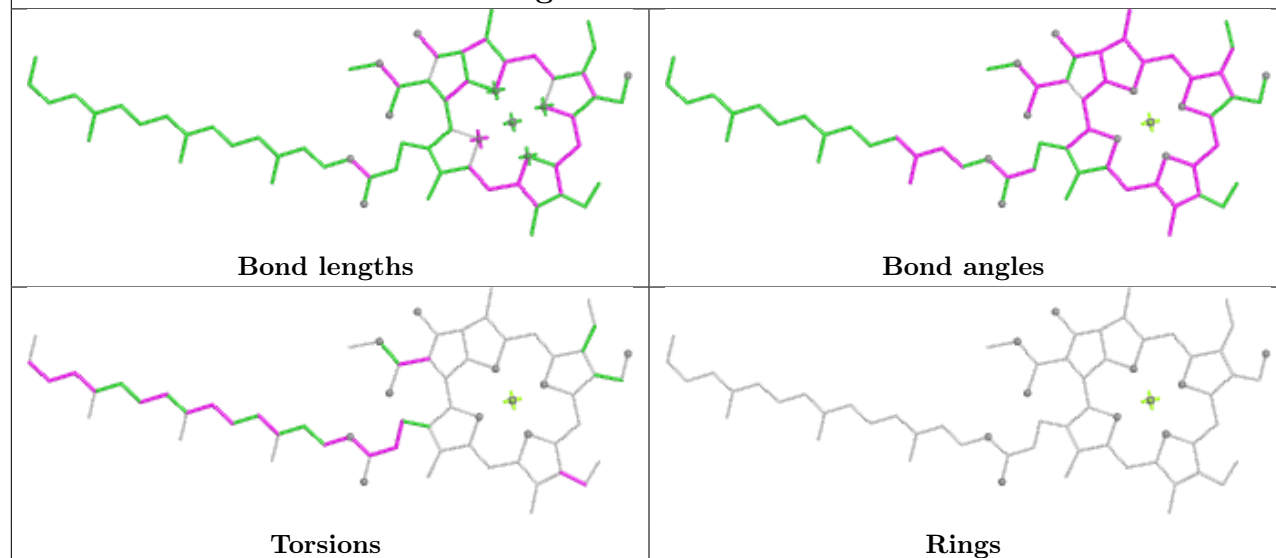


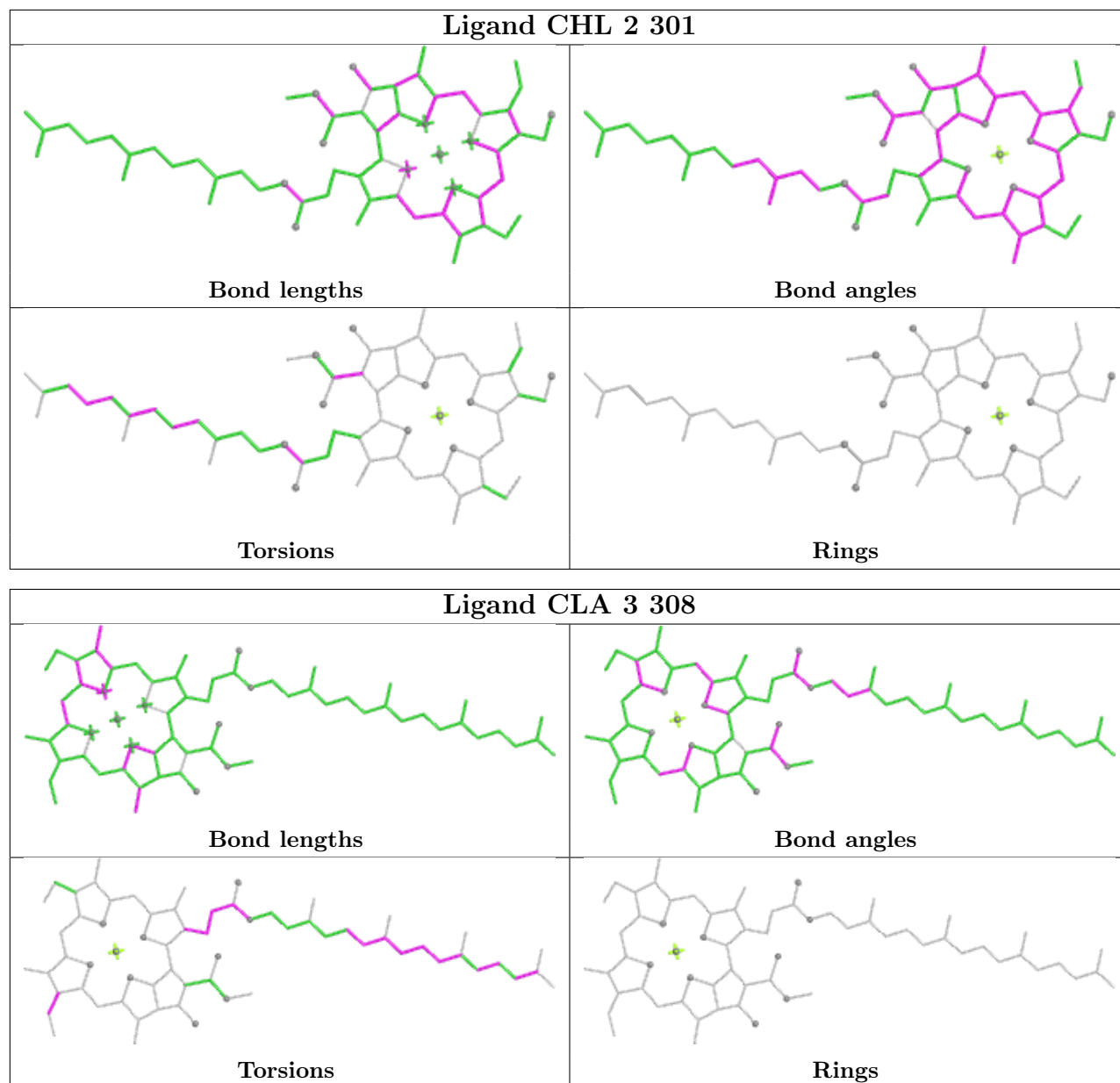


Ligand CLA 7 317

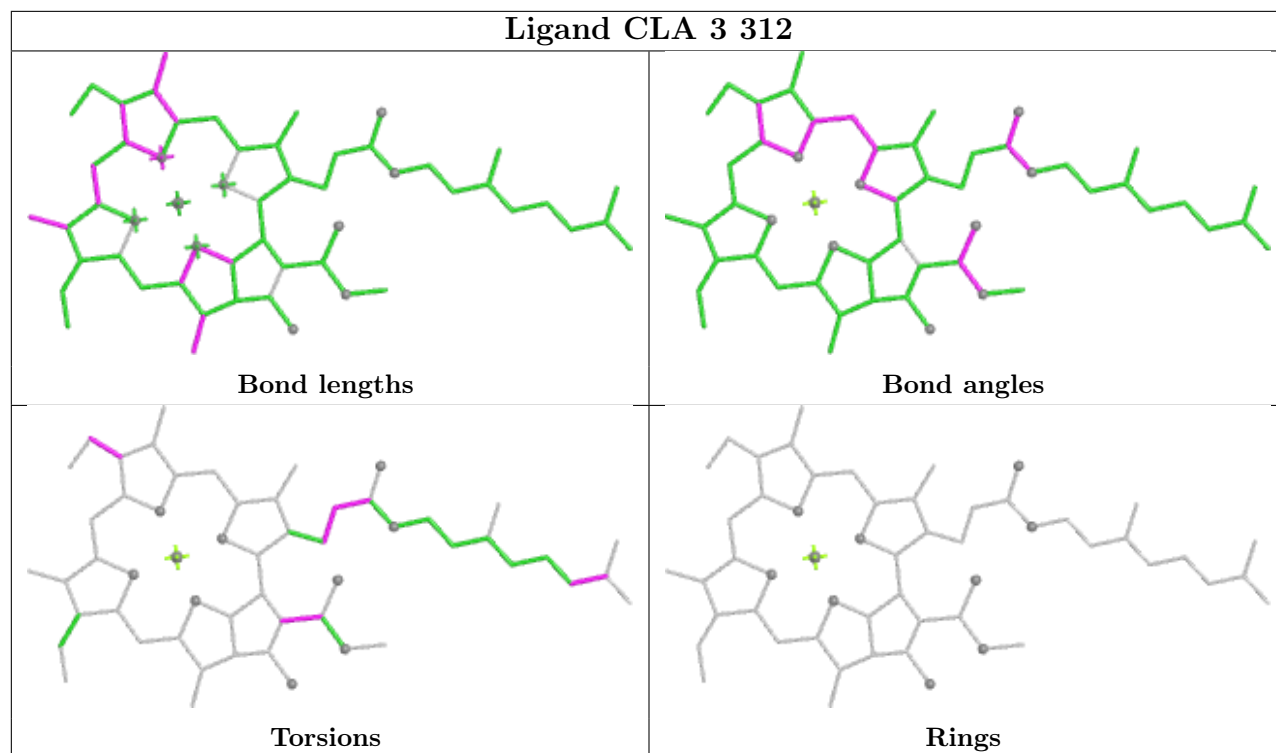


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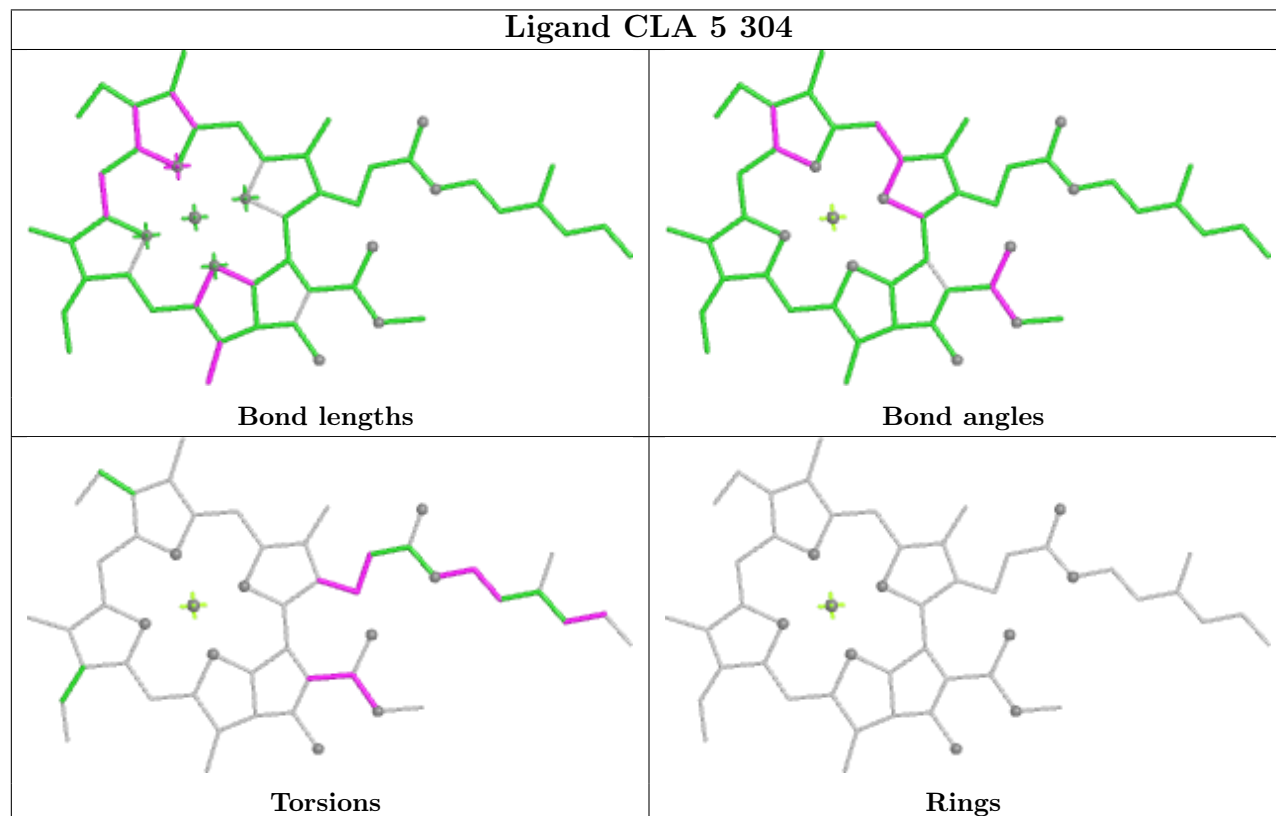


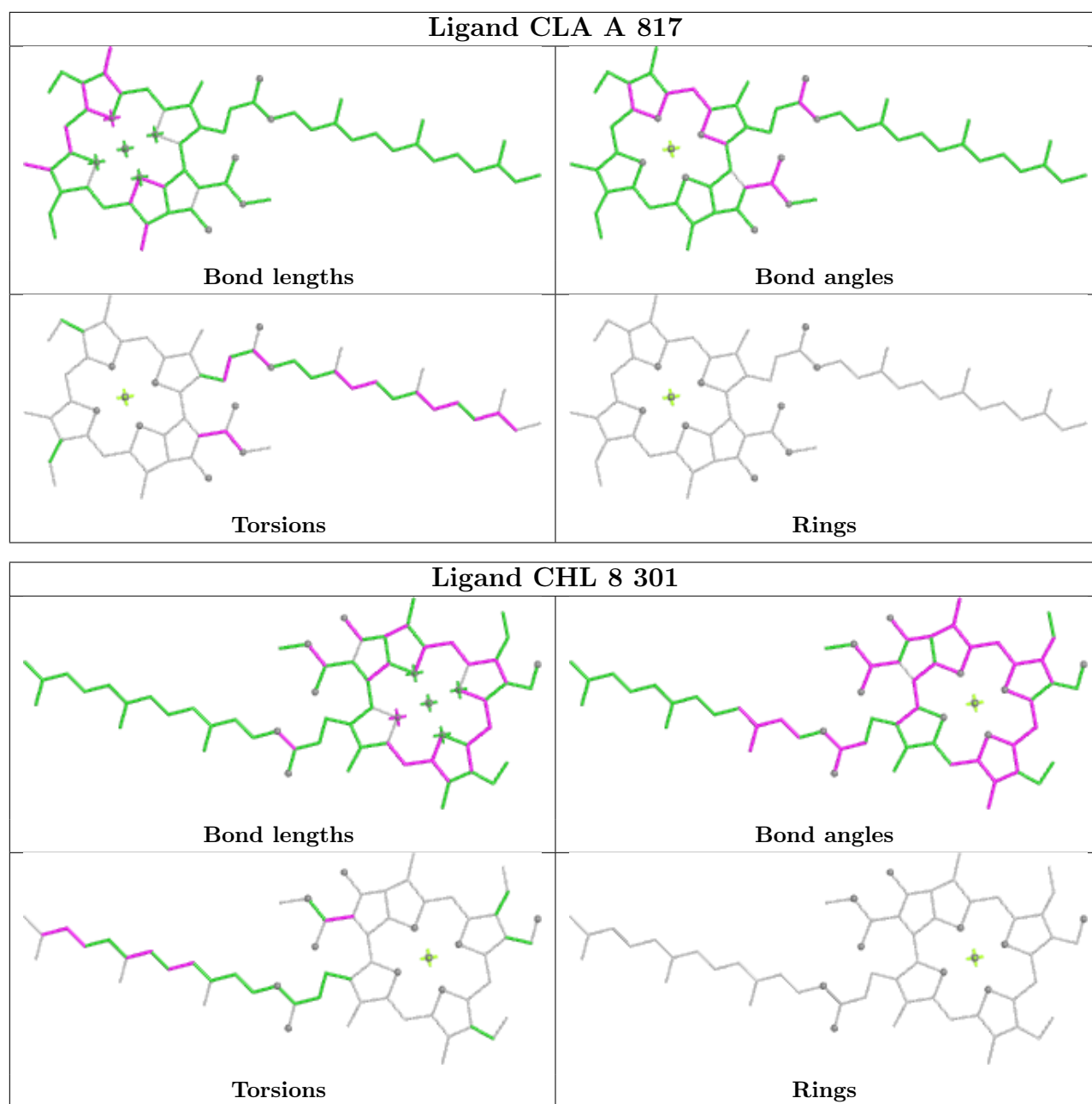


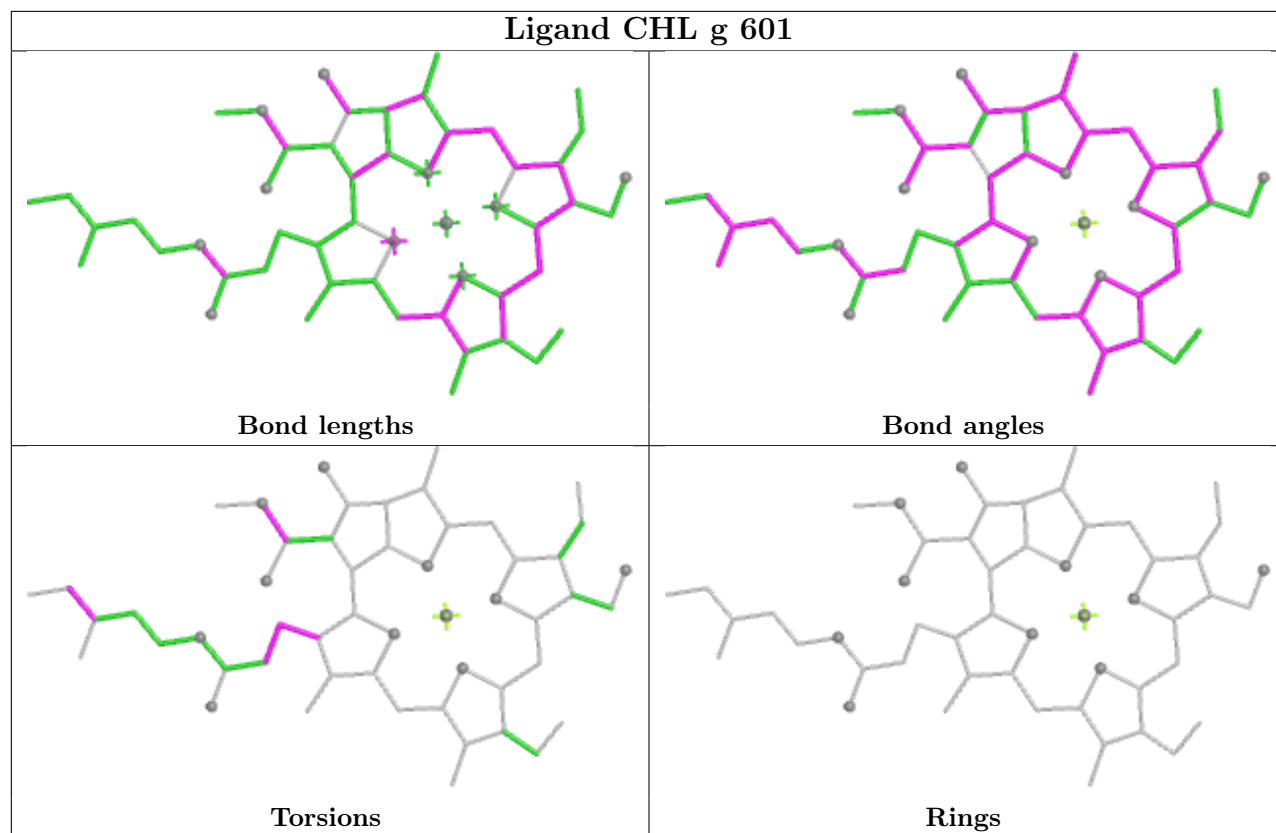
Ligand CLA 3 312

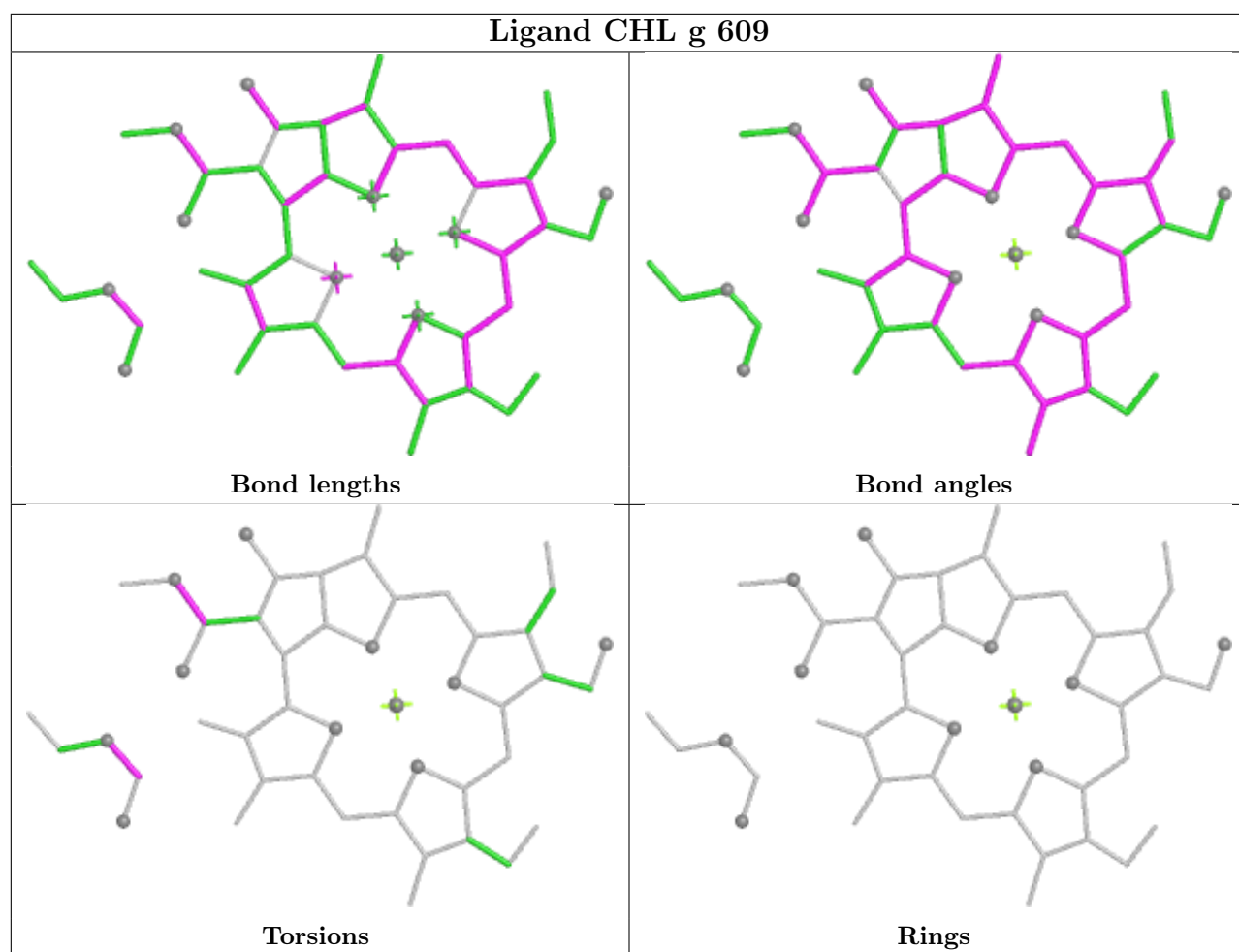


Ligand CLA 5 304

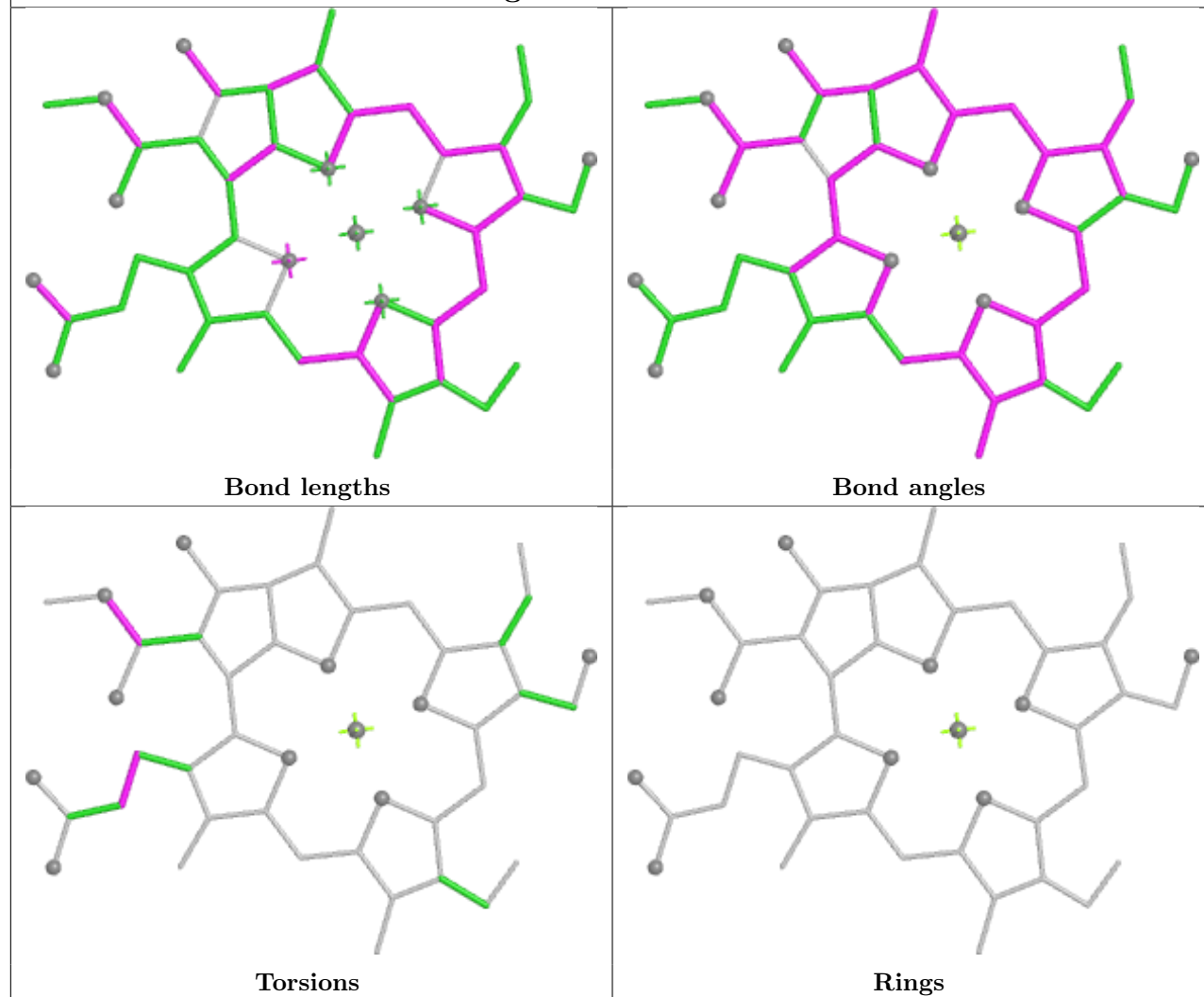




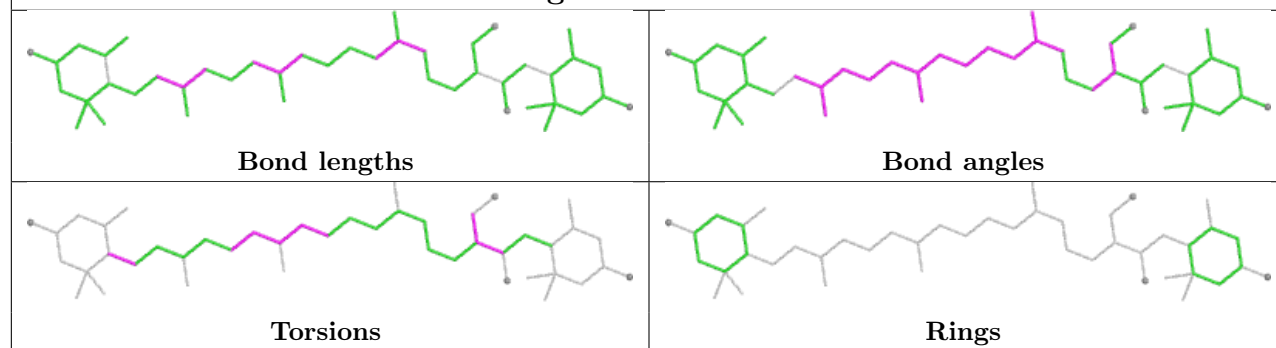




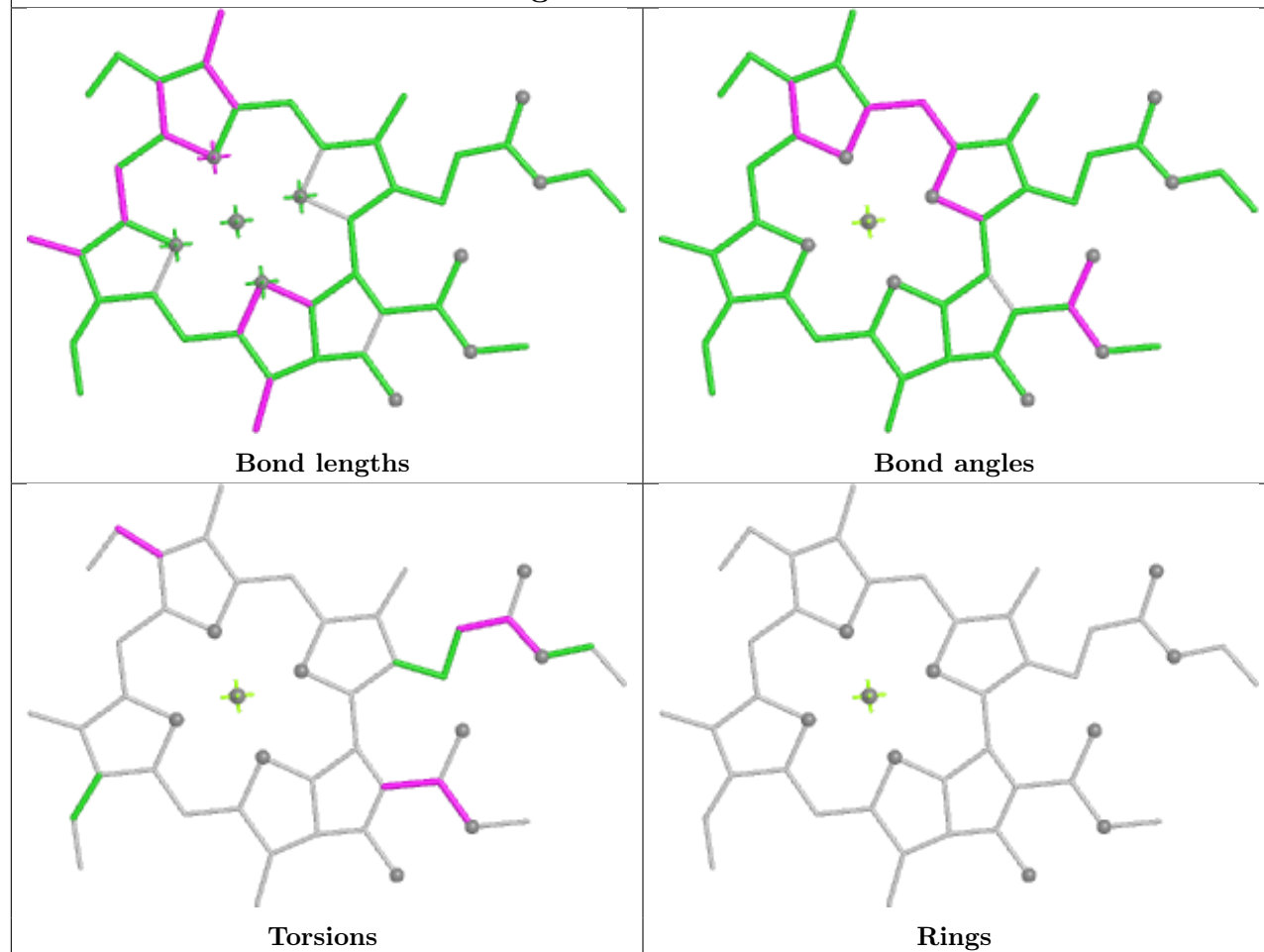
Ligand CHL h 607



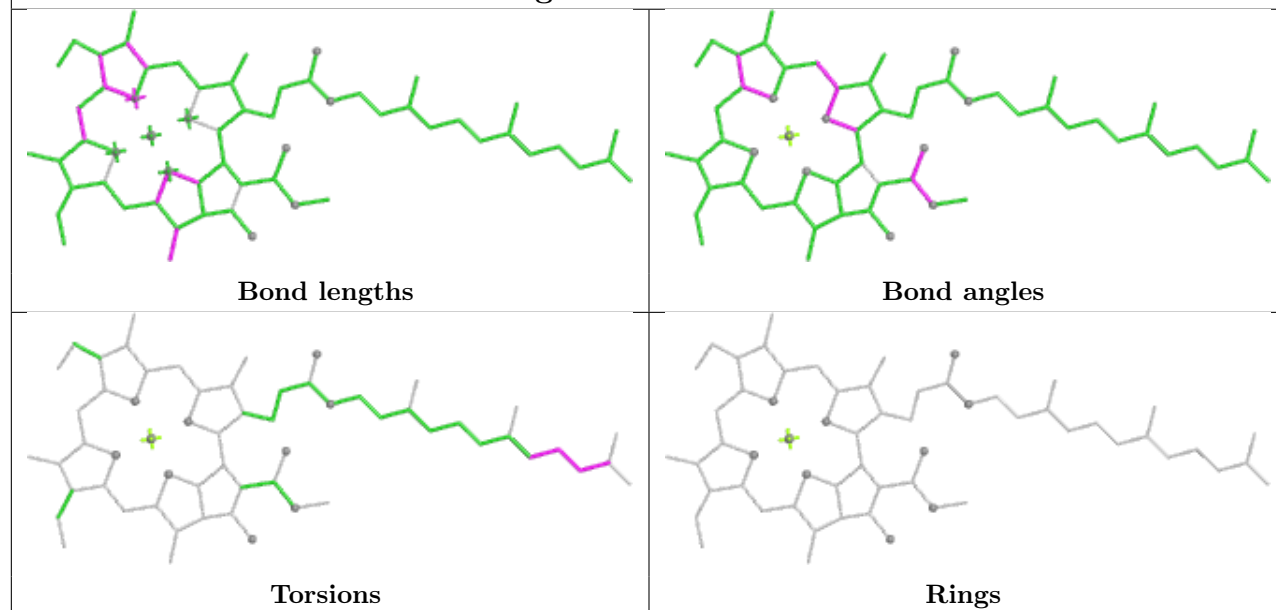
Ligand OIE c 522

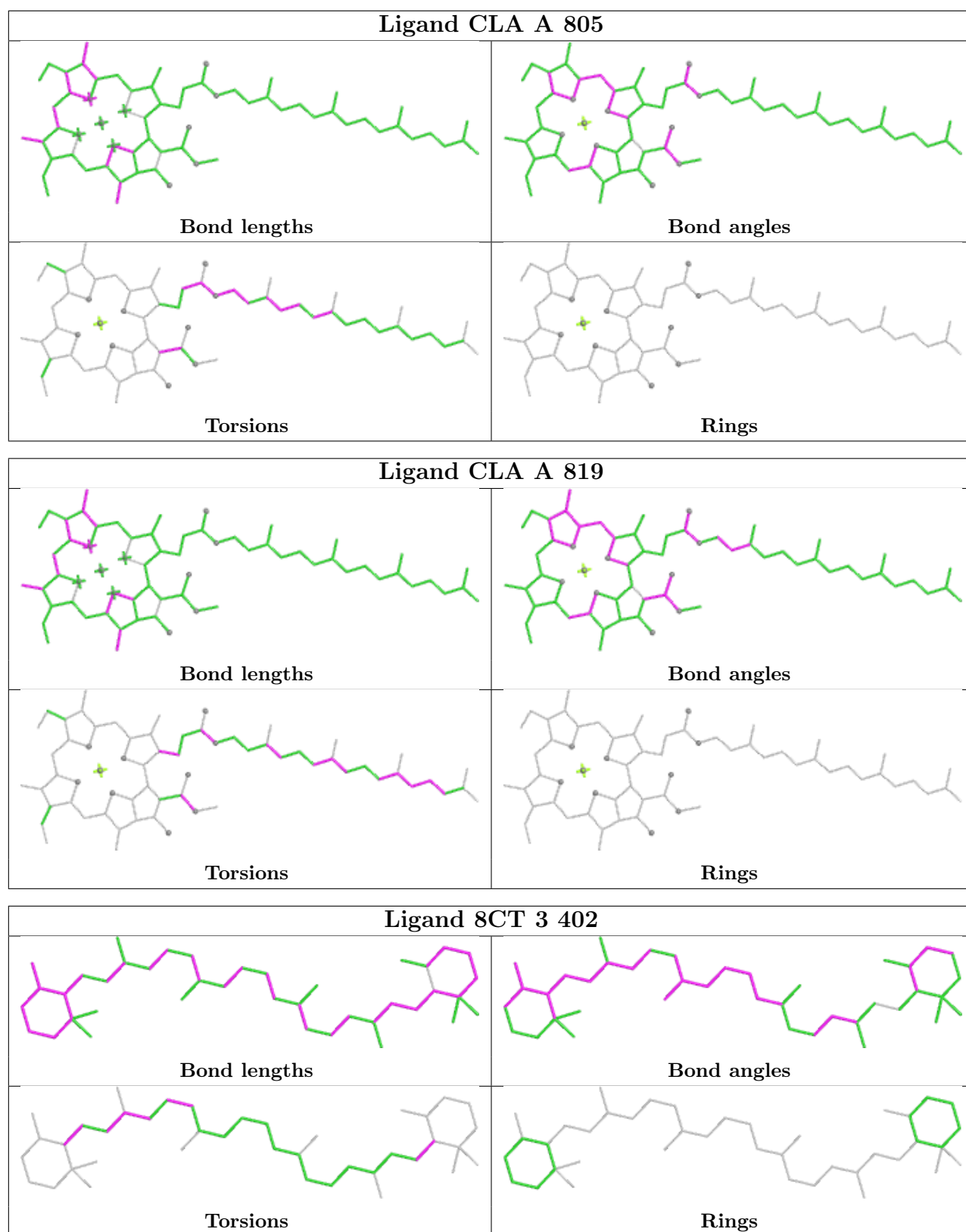


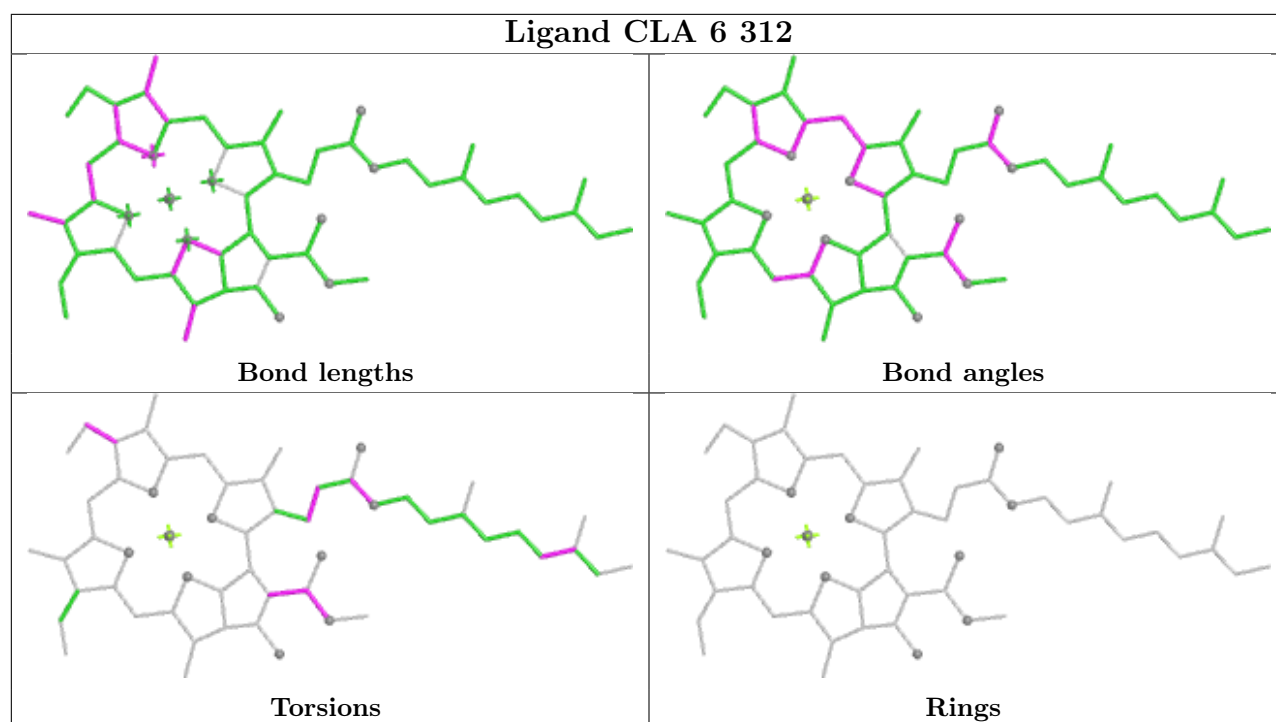
Ligand CLA 7 315



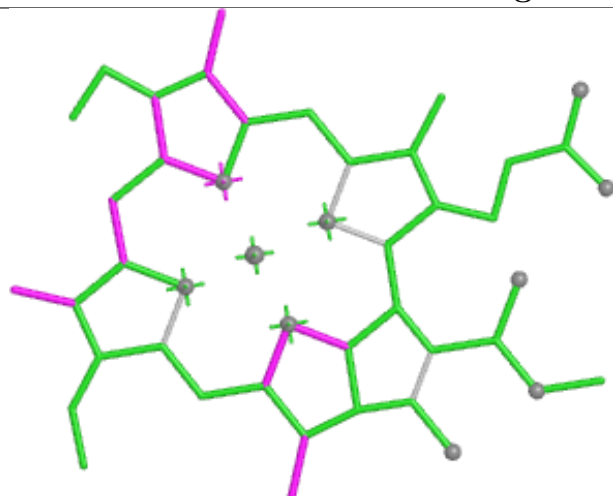
Ligand CLA b 611



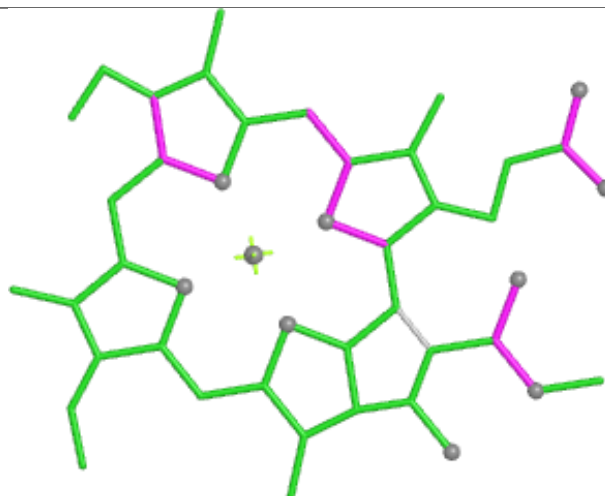




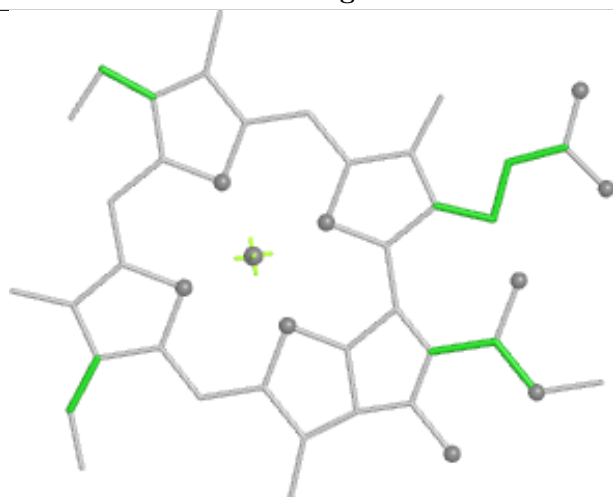
Ligand CLA B 835



Bond lengths



Bond angles

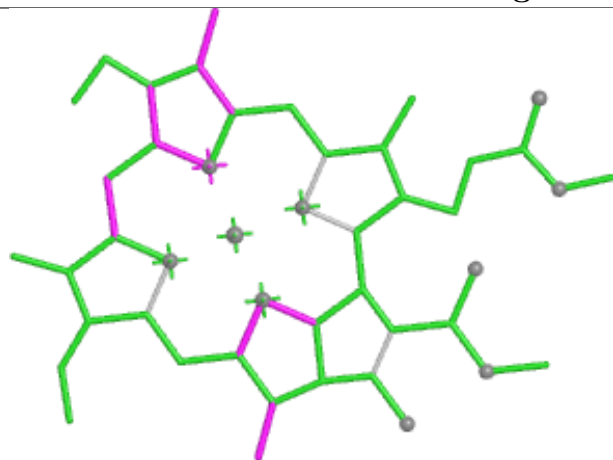


Torsions

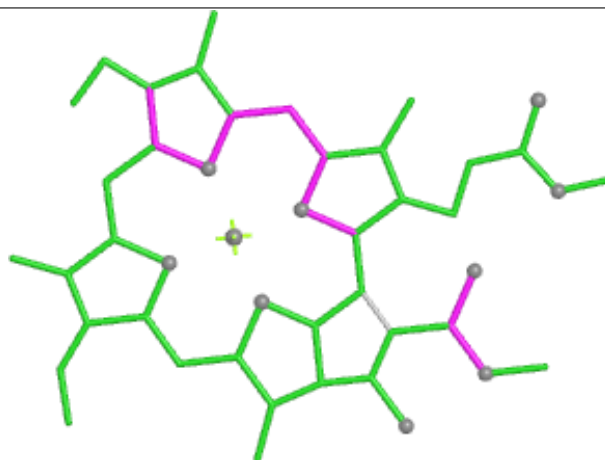


Rings

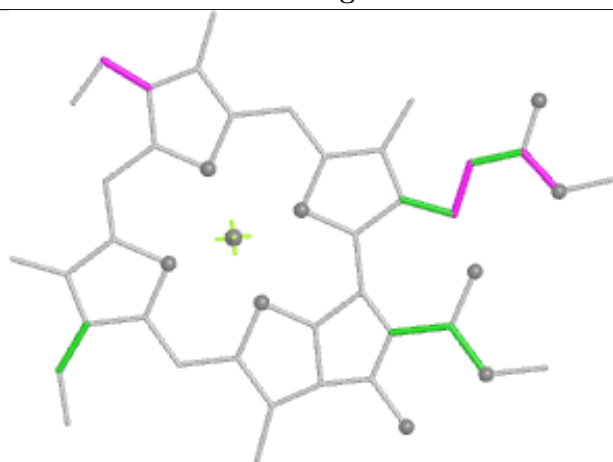
Ligand CLA G 103



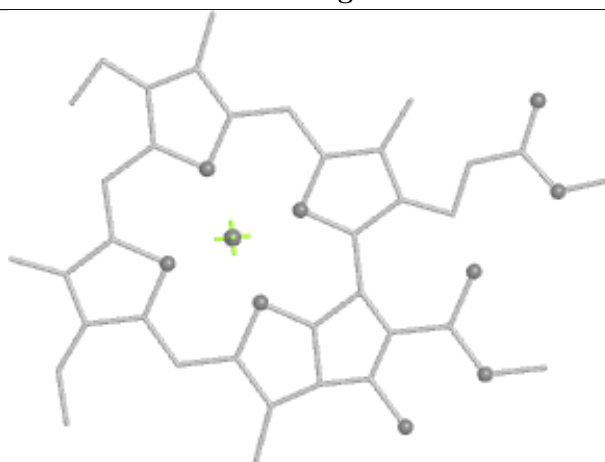
Bond lengths



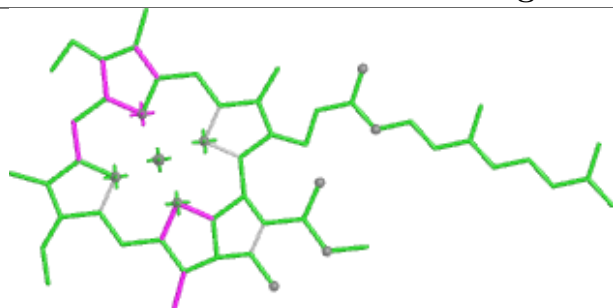
Bond angles



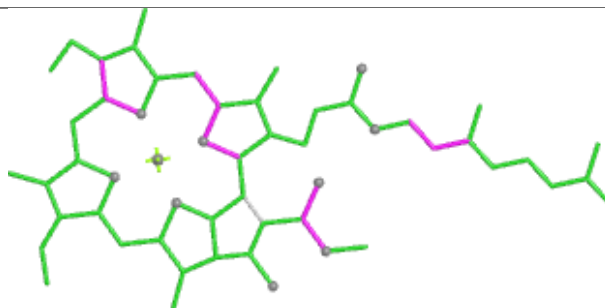
Torsions



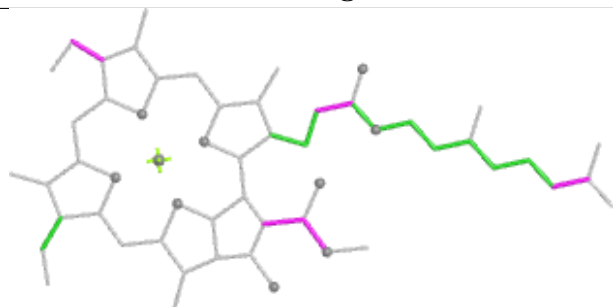
Rings

Ligand CLA d 603

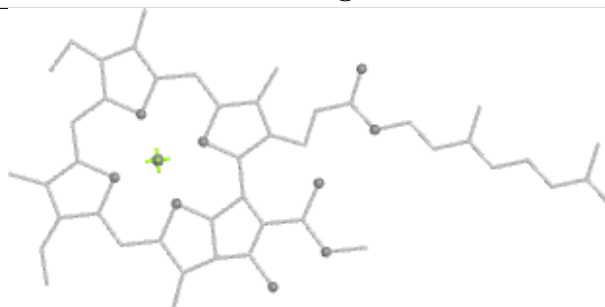
Bond lengths



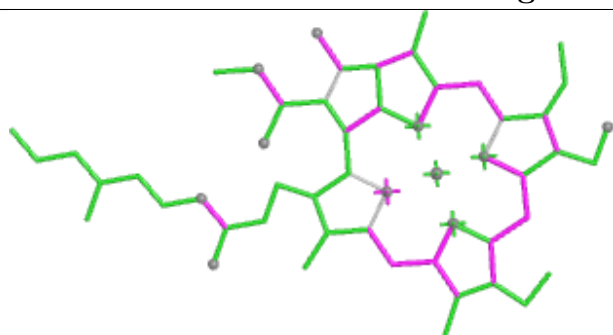
Bond angles



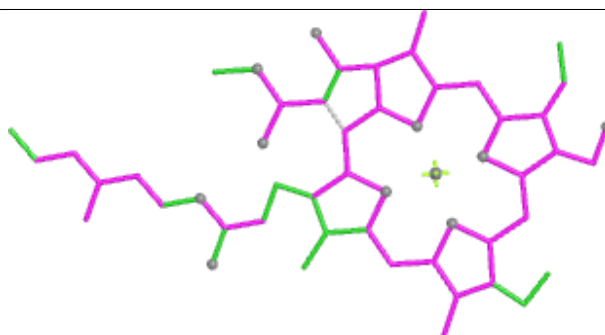
Torsions



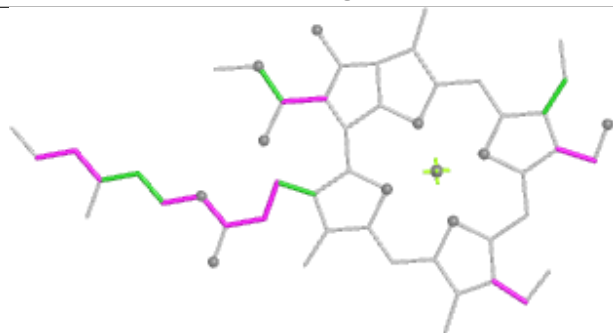
Rings

Ligand CHL 4 302

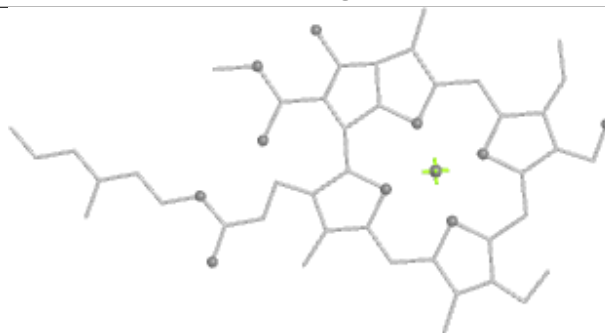
Bond lengths



Bond angles

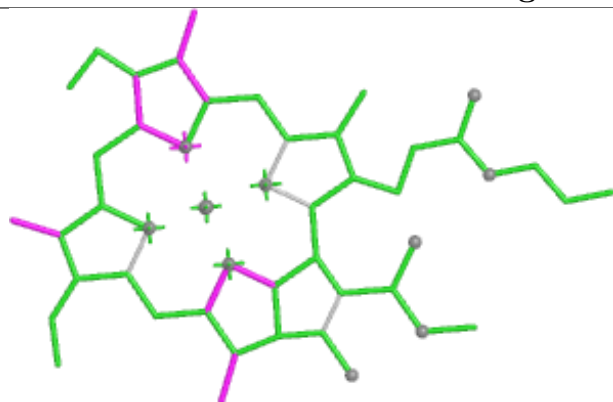


Torsions

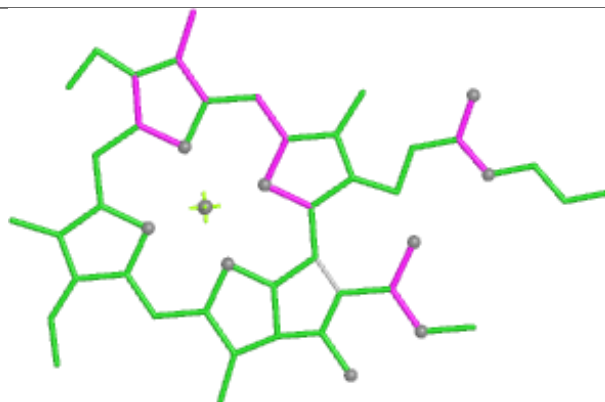


Rings

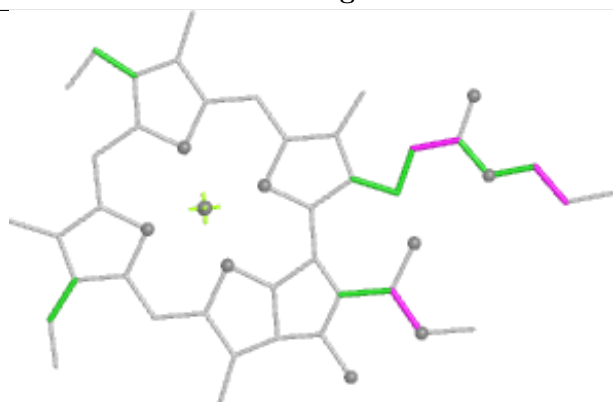
Ligand CLA 2 311



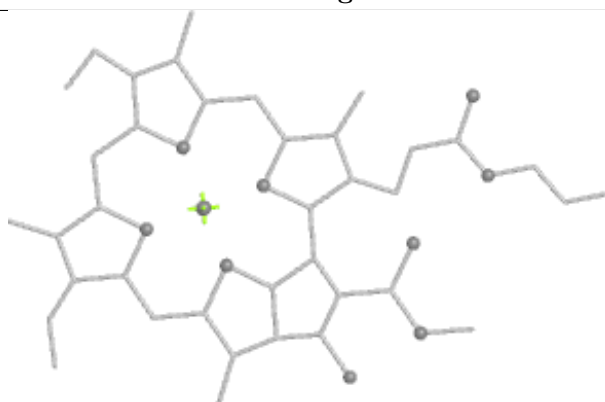
Bond lengths



Bond angles

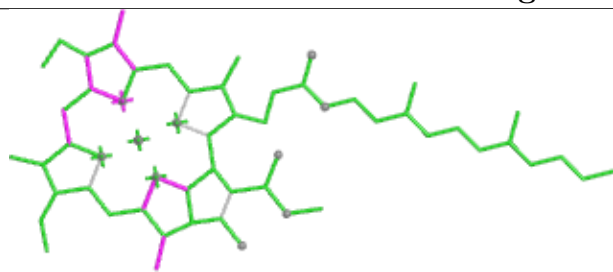


Torsions

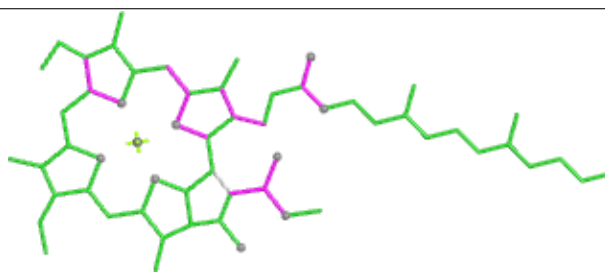


Rings

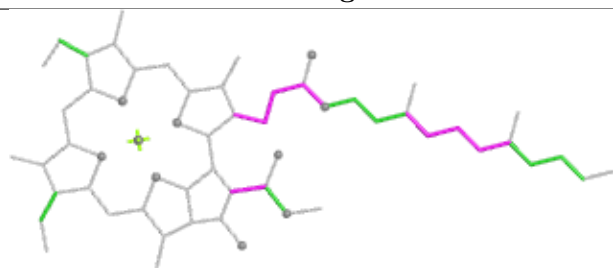
Ligand CLA 9 300



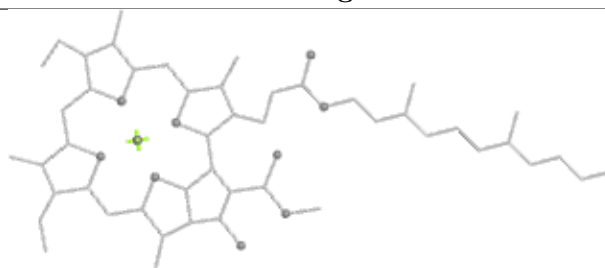
Bond lengths



Bond angles

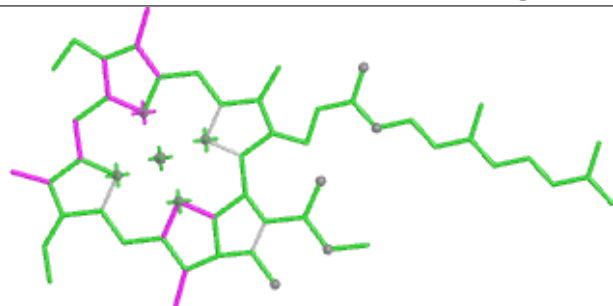


Torsions

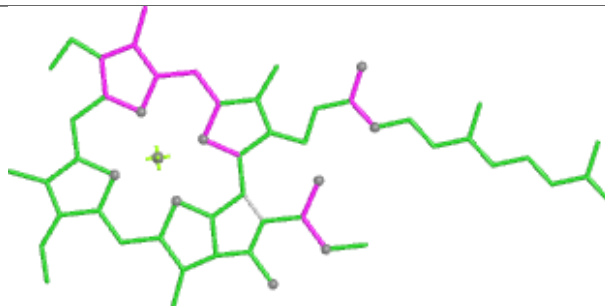


Rings

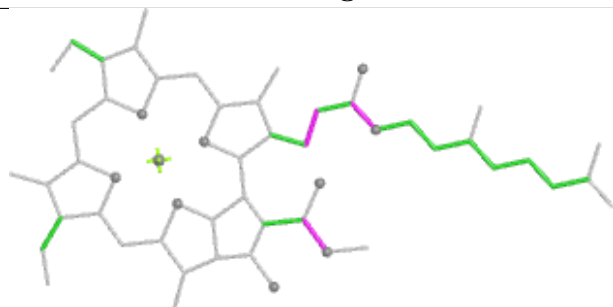
Ligand CLA B 815



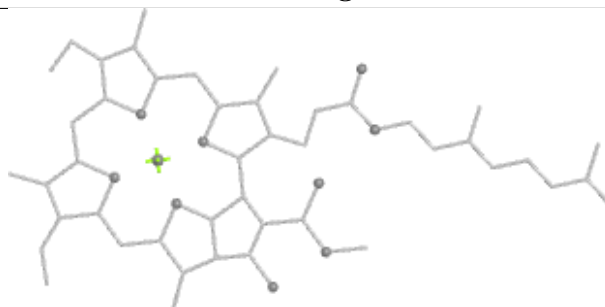
Bond lengths



Bond angles

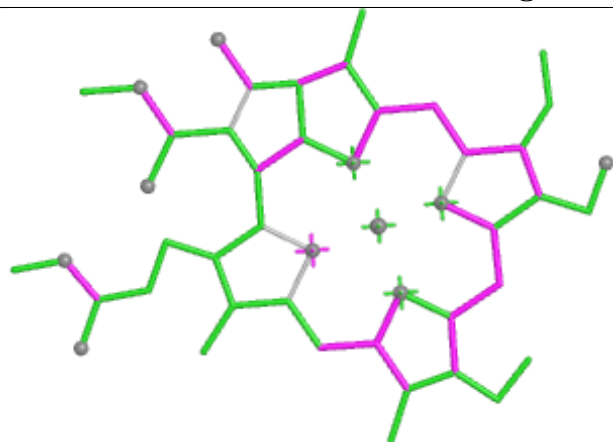


Torsions

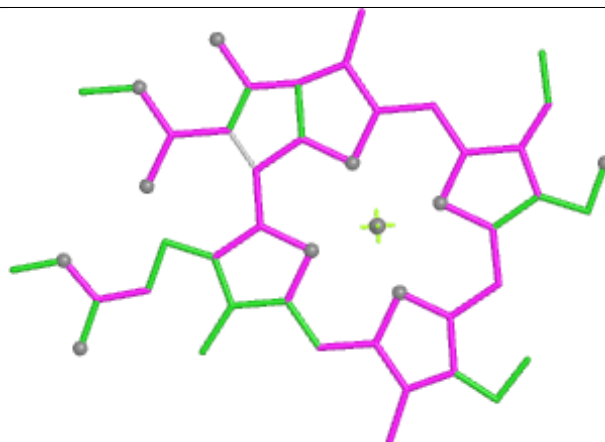


Rings

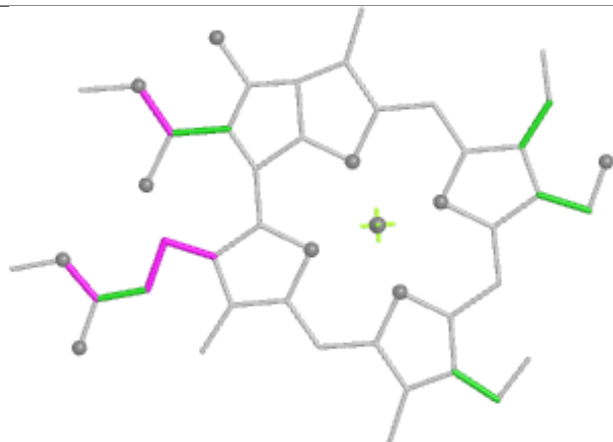
Ligand CHL a 601



Bond lengths



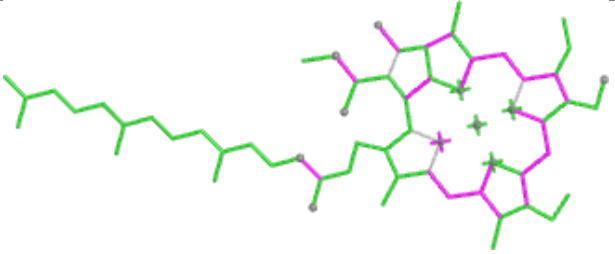
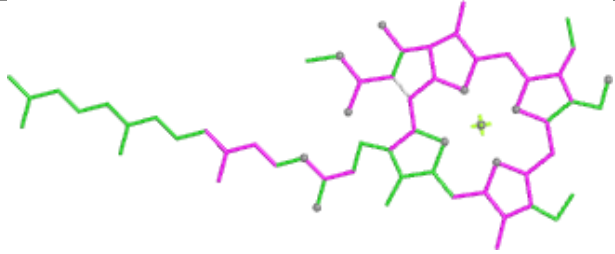
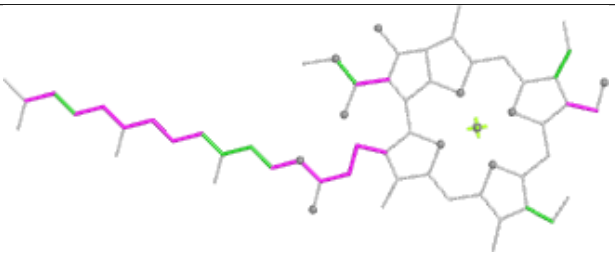
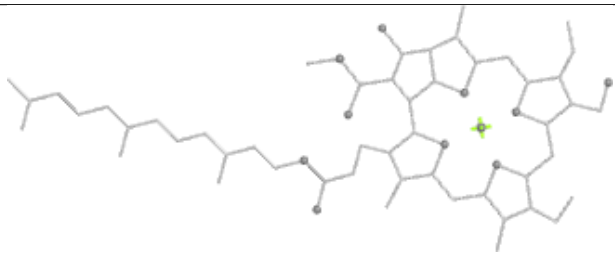
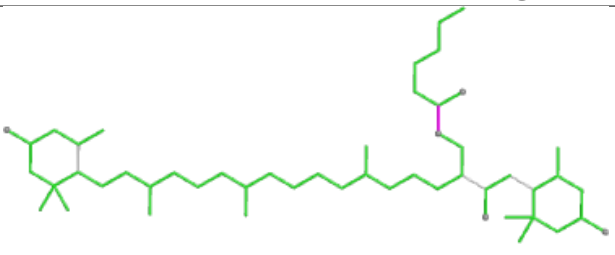
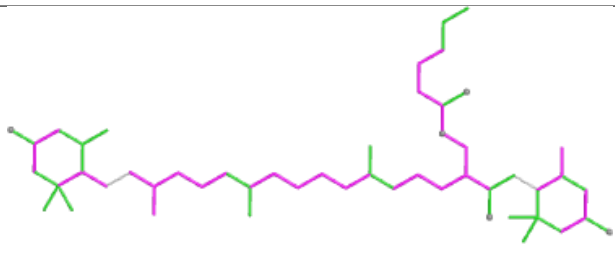
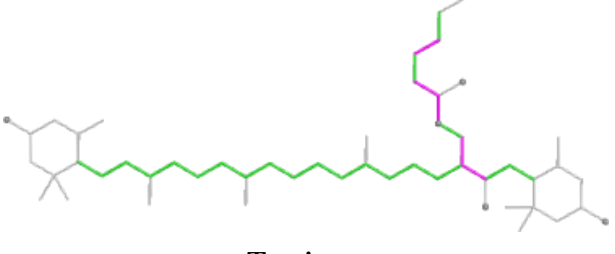
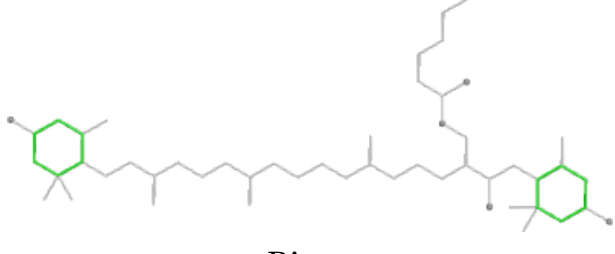
Bond angles



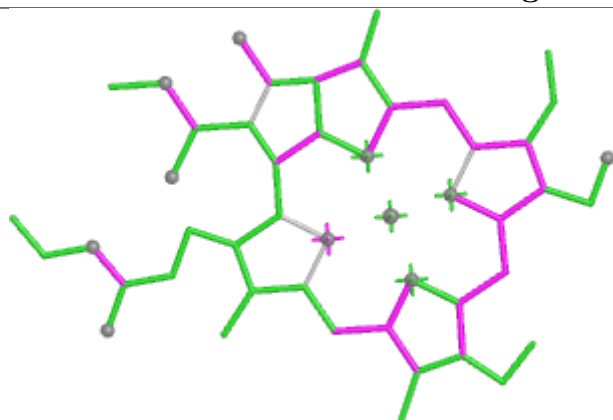
Torsions



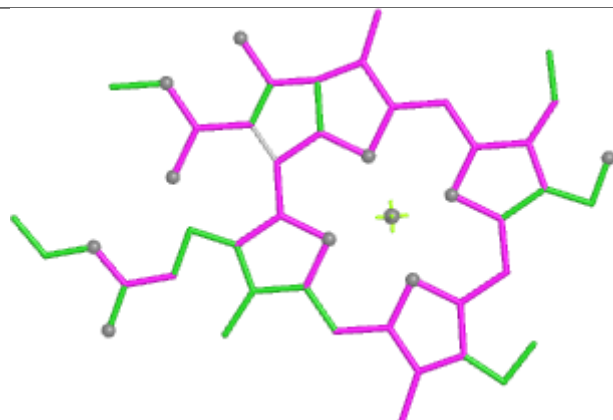
Rings

Ligand CHL e 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand OUR 4 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

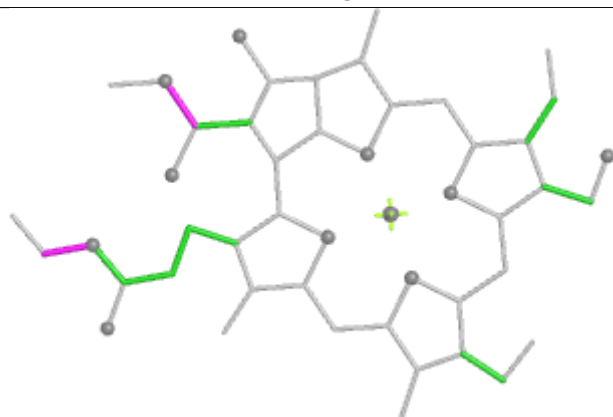
Ligand CHL i 609



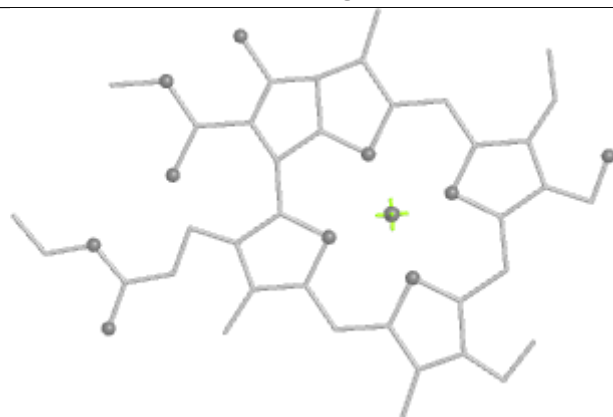
Bond lengths



Bond angles

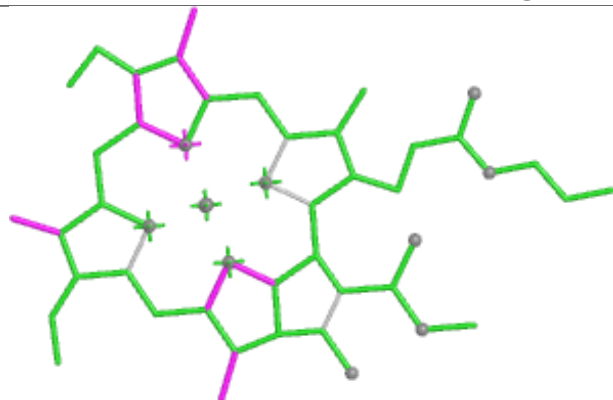


Torsions

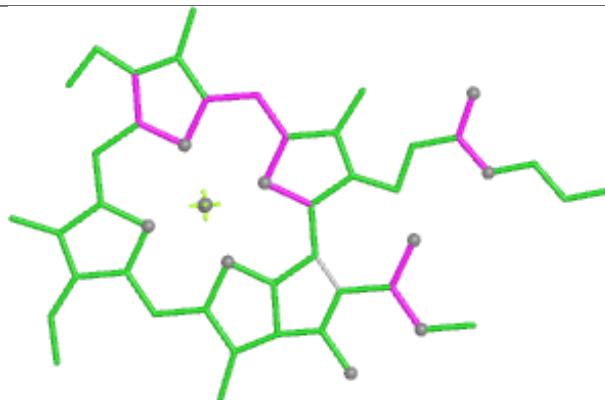


Rings

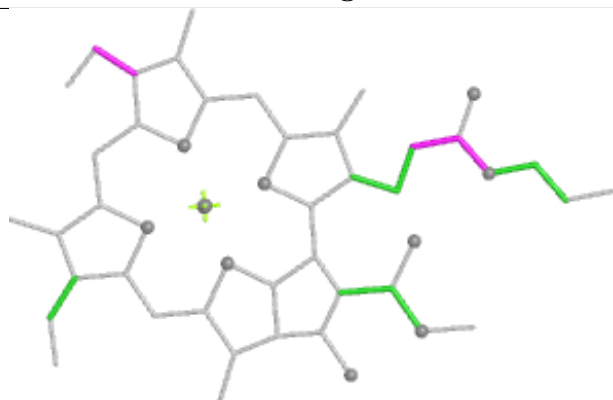
Ligand CLA 9 303



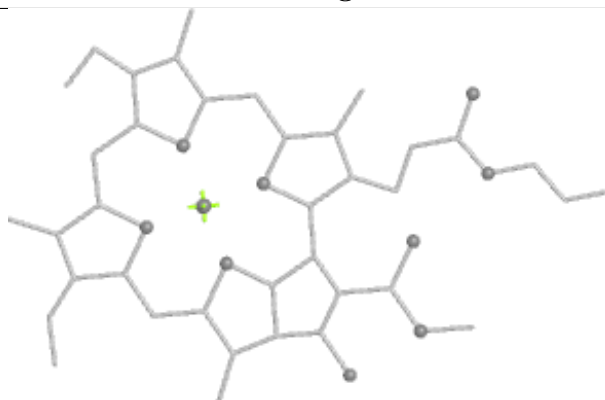
Bond lengths



Bond angles

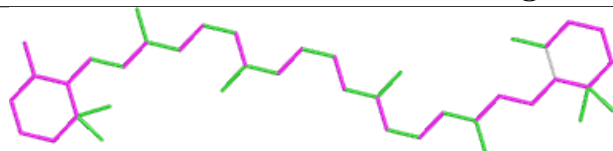


Torsions

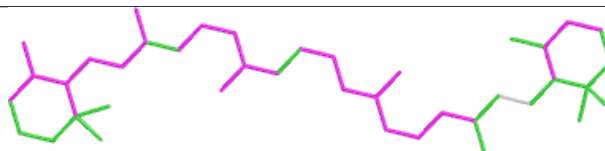


Rings

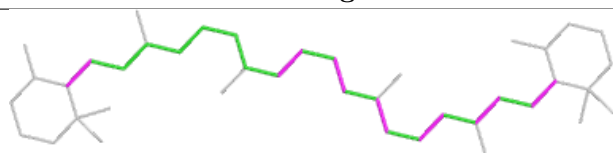
Ligand 8CT J 101



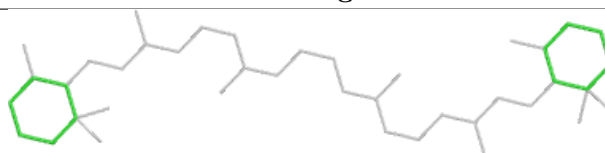
Bond lengths



Bond angles

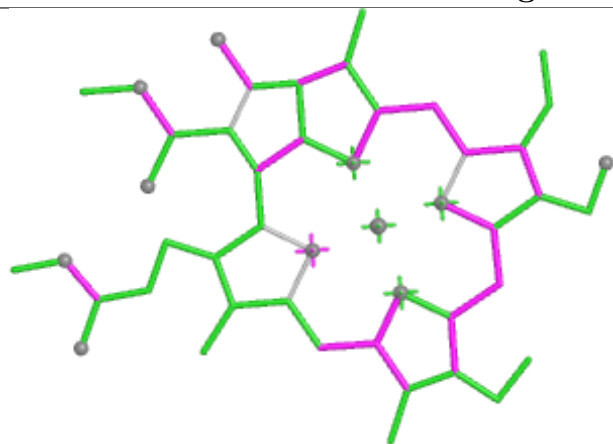


Torsions

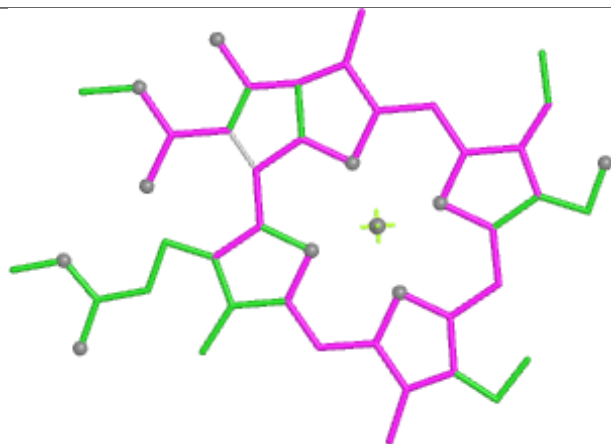


Rings

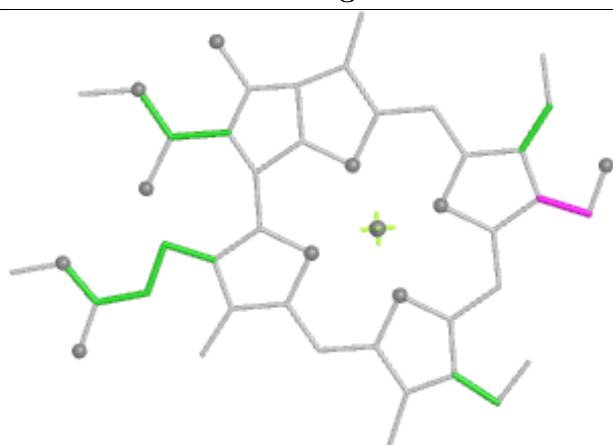
Ligand CHL 8 308



Bond lengths



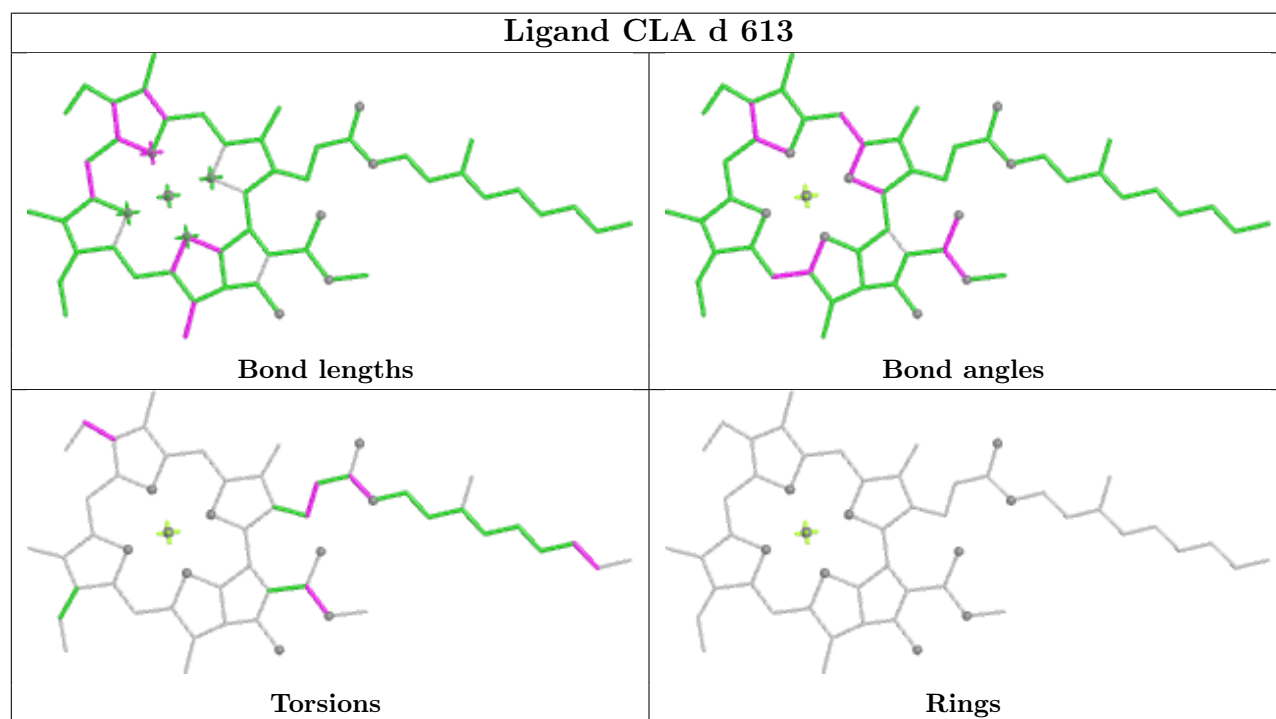
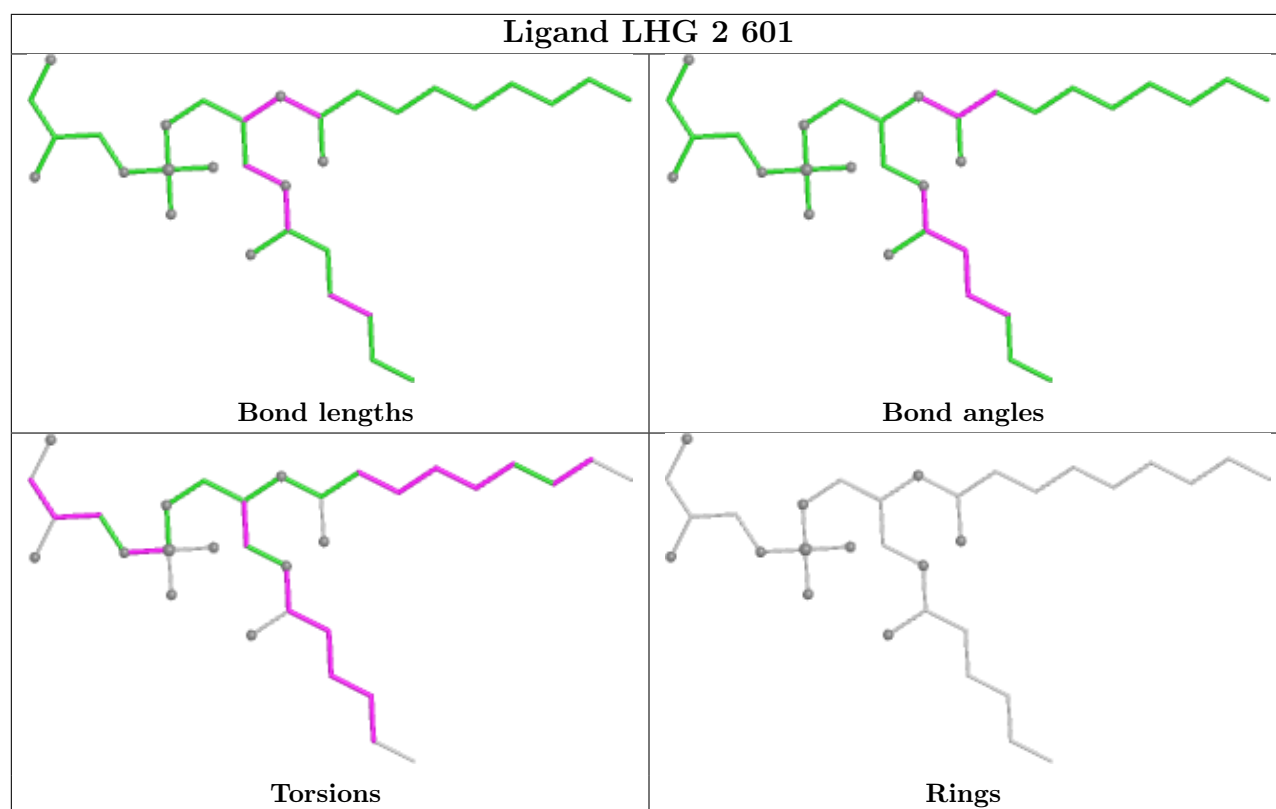
Bond angles

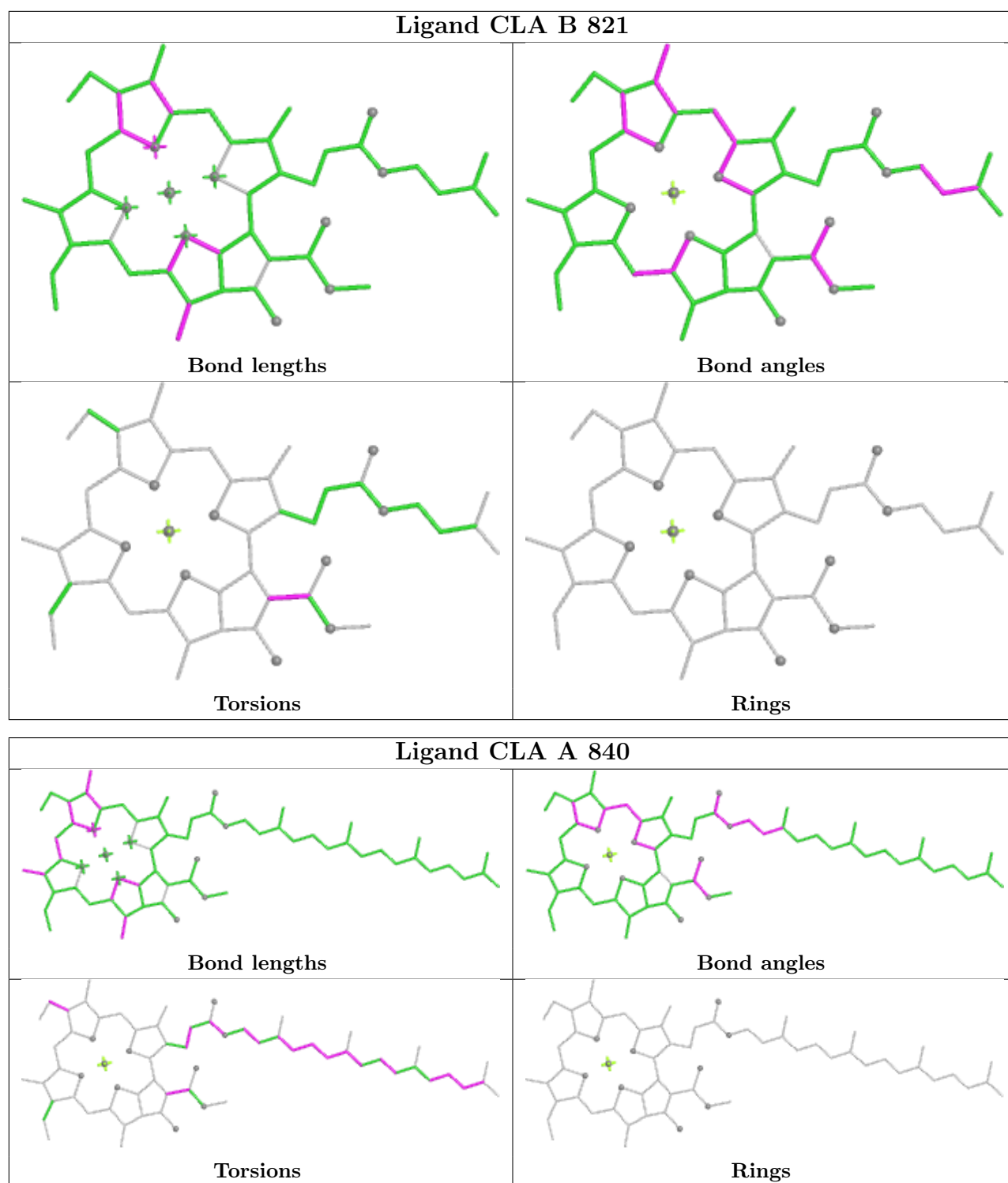


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

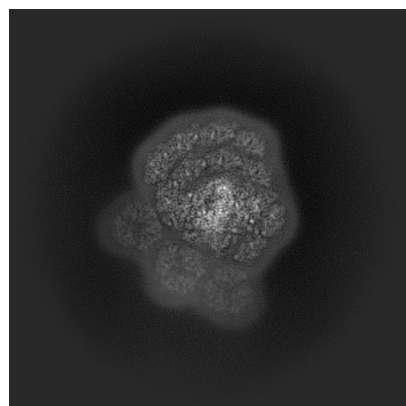
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61940. These allow visual inspection of the internal detail of the map and identification of artifacts.

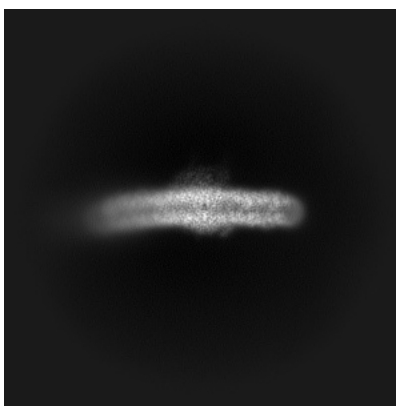
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

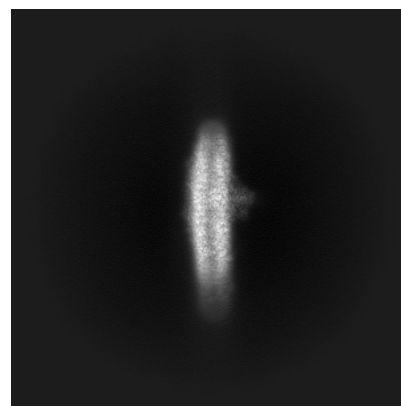
6.1.1 Primary map



X

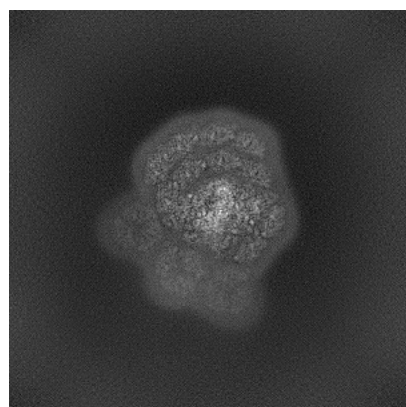


Y

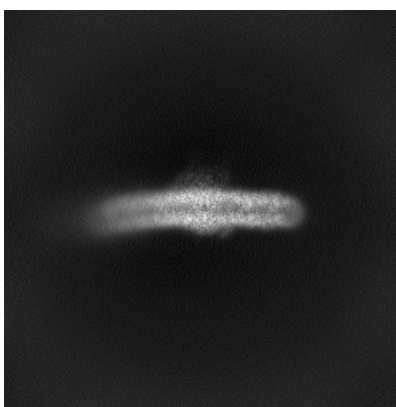


Z

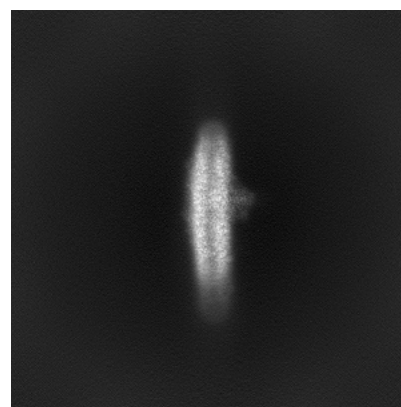
6.1.2 Raw map



X



Y

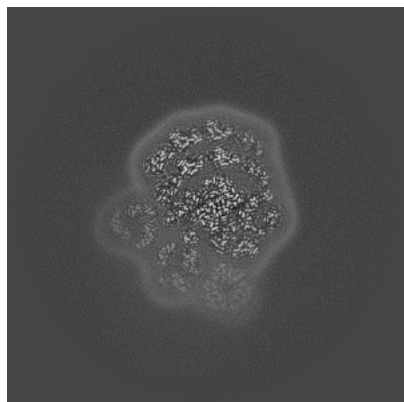


Z

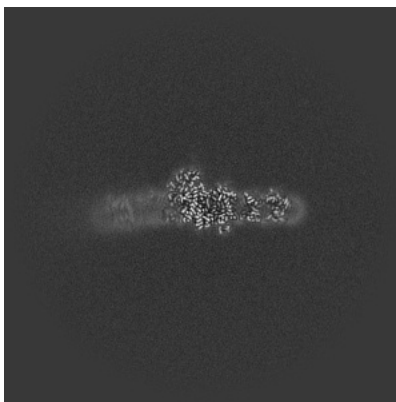
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

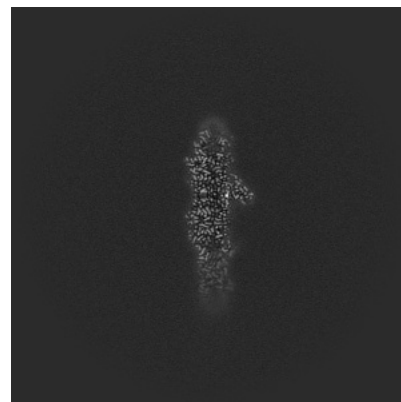
6.2.1 Primary map



X Index: 256

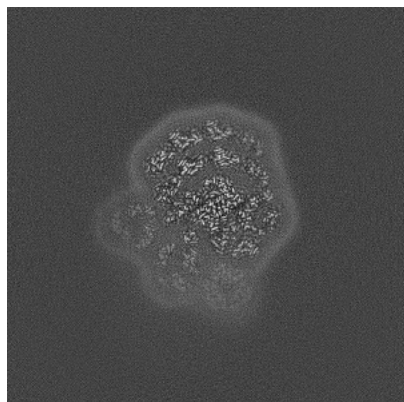


Y Index: 256

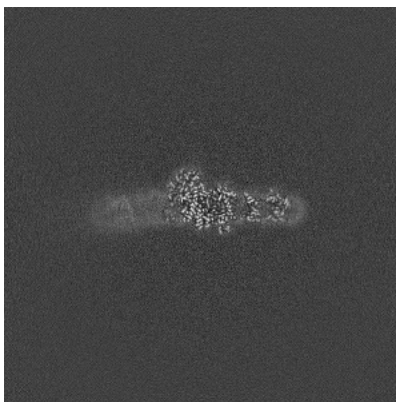


Z Index: 256

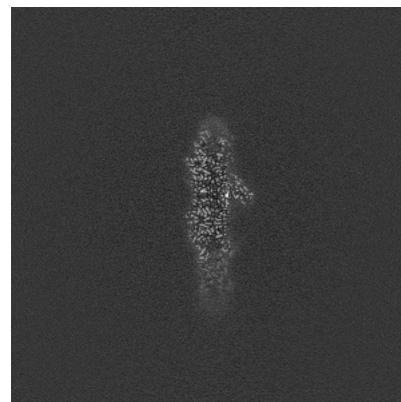
6.2.2 Raw map



X Index: 256



Y Index: 256

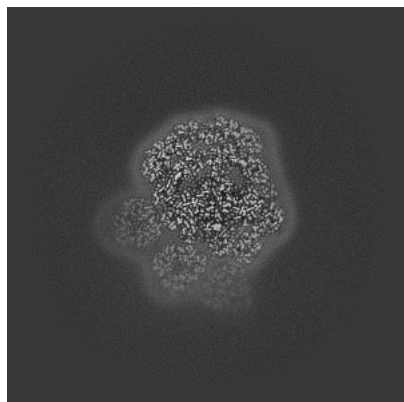


Z Index: 256

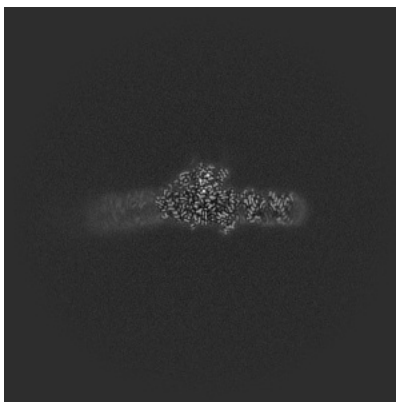
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

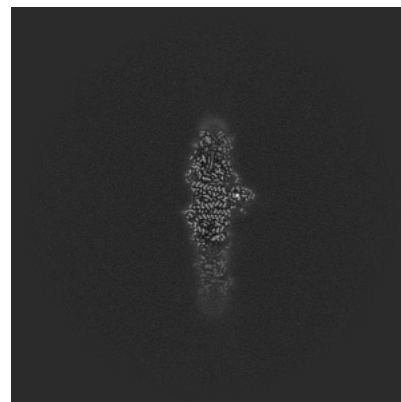
6.3.1 Primary map



X Index: 266

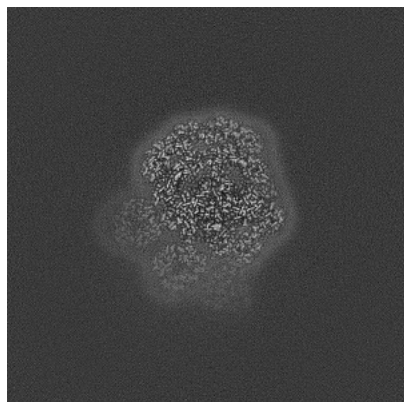


Y Index: 269

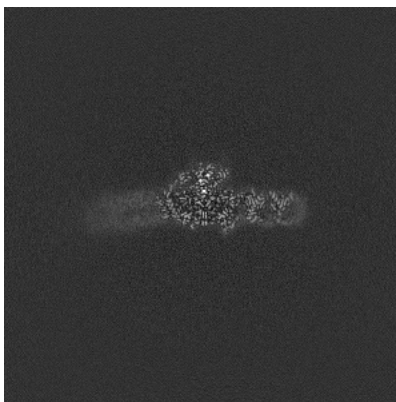


Z Index: 251

6.3.2 Raw map



X Index: 266



Y Index: 270

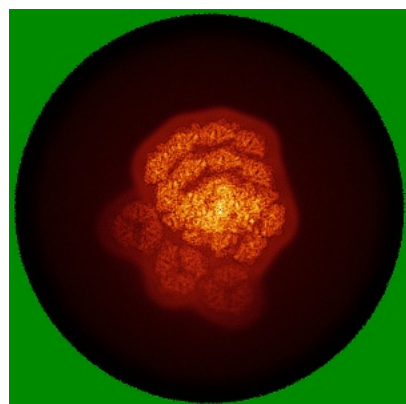


Z Index: 251

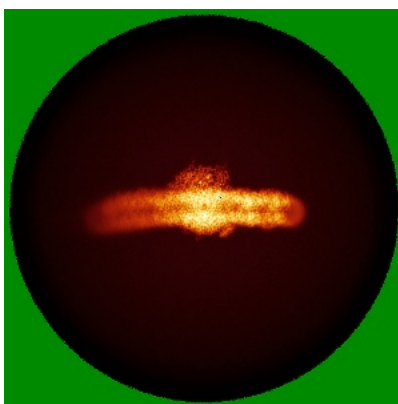
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

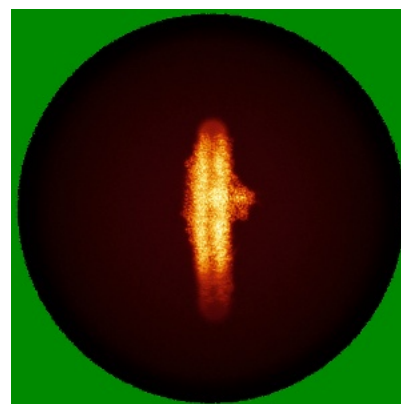
6.4.1 Primary map



X

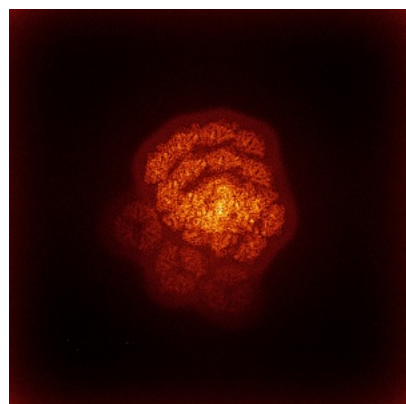


Y

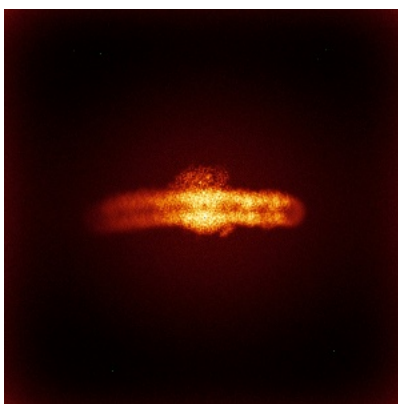


Z

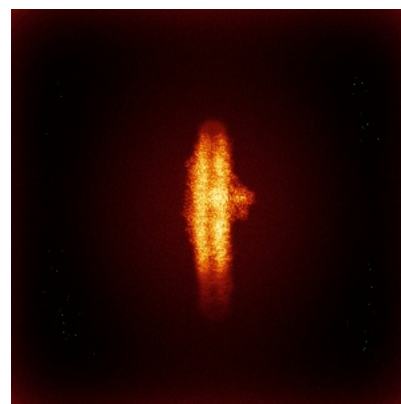
6.4.2 Raw map



X



Y

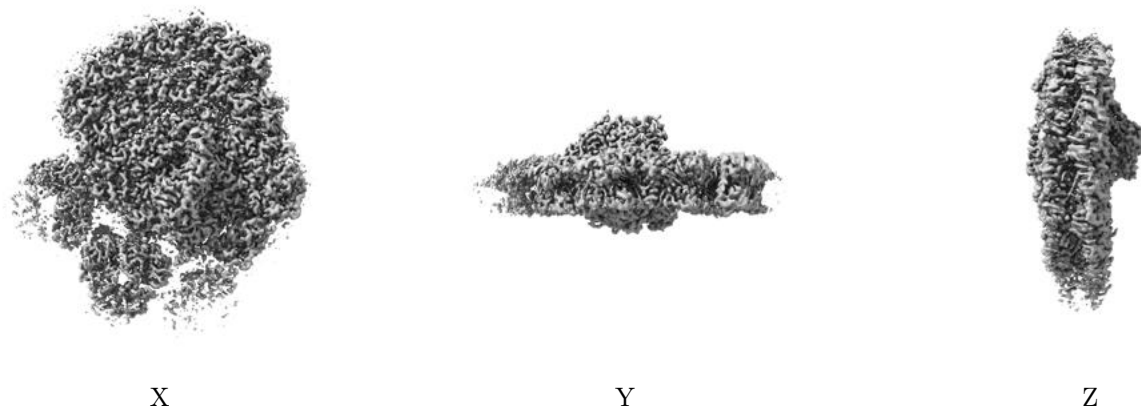


Z

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.

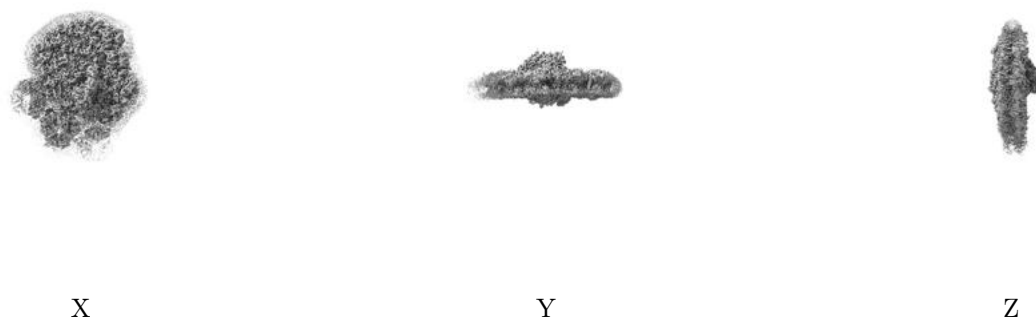
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.217. 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.

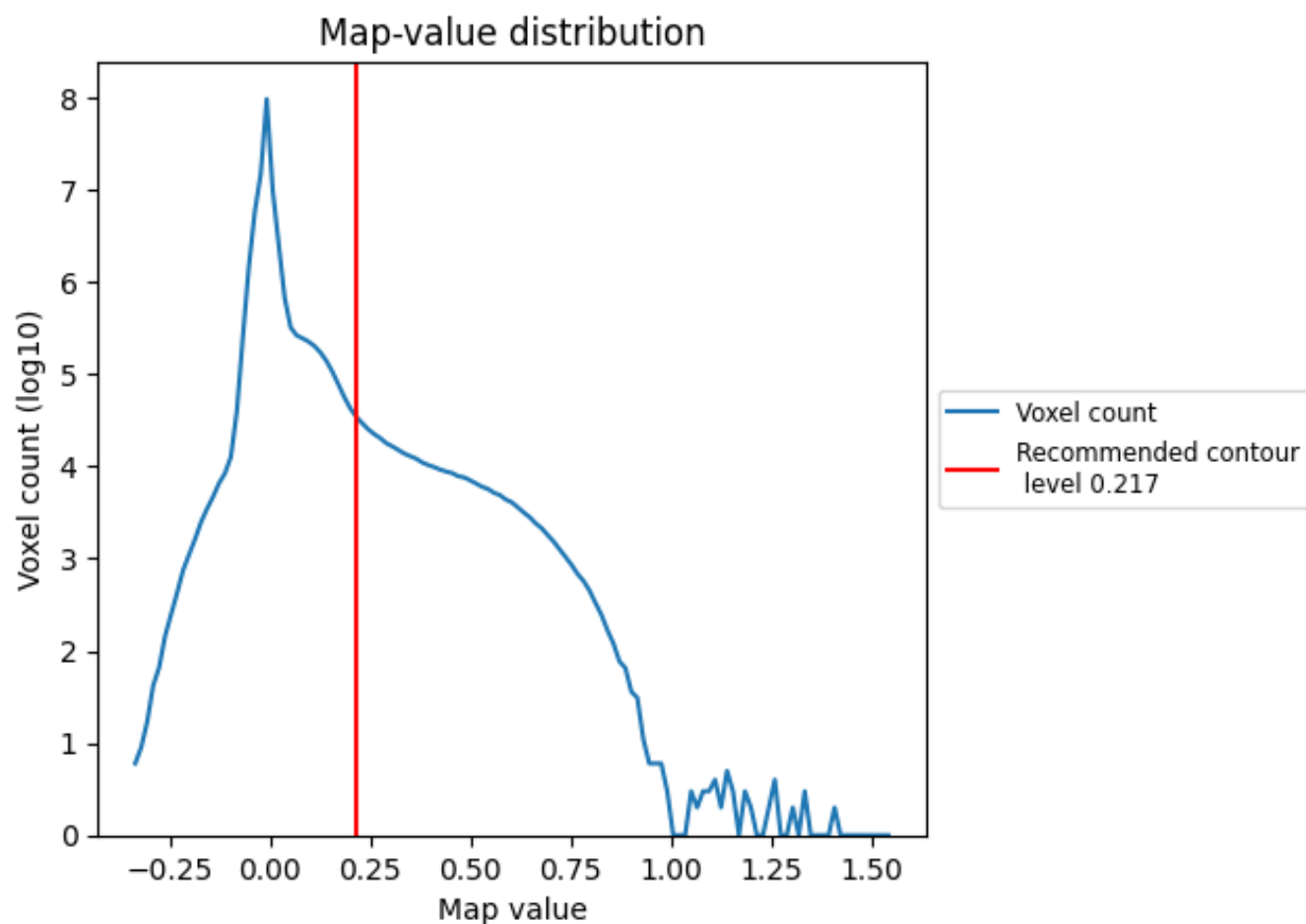
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

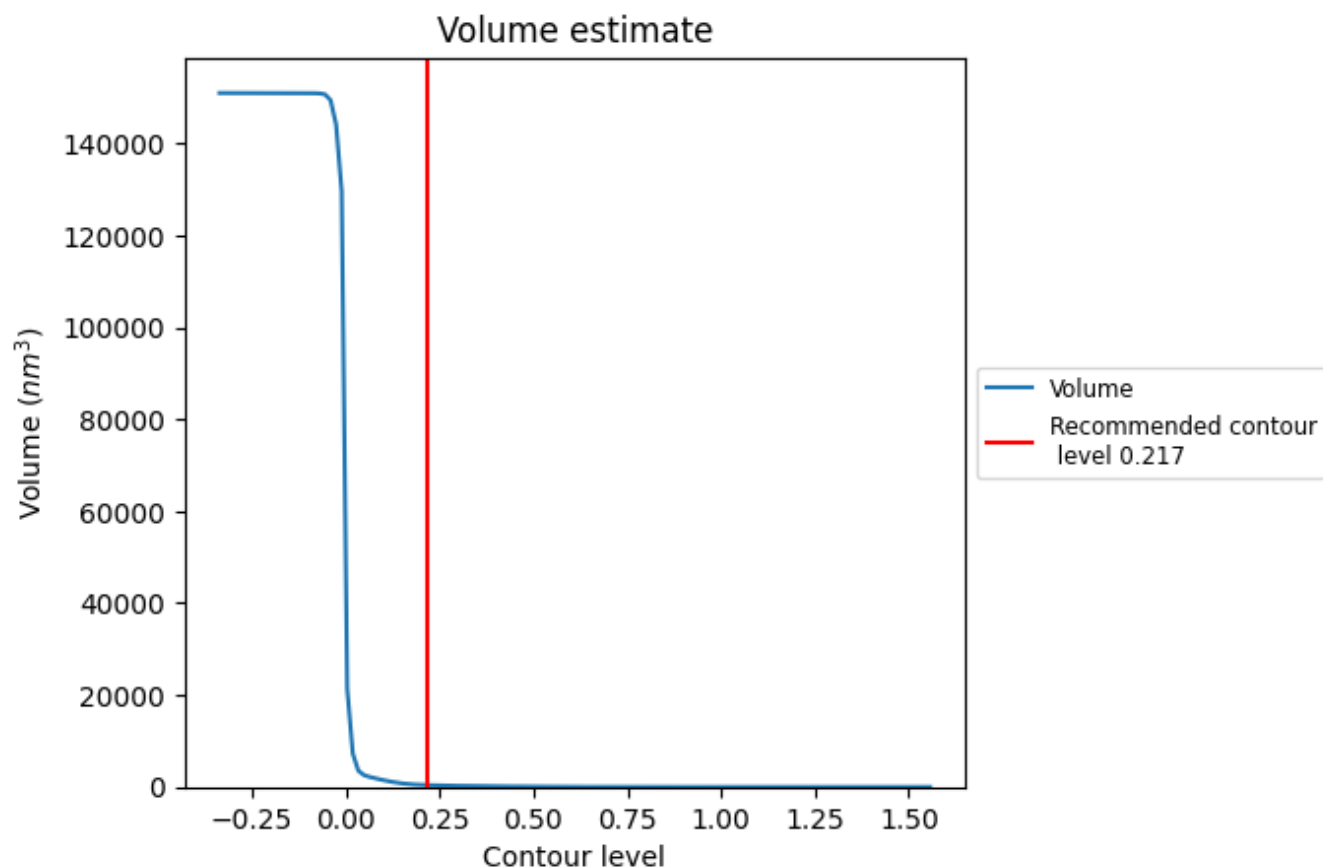
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

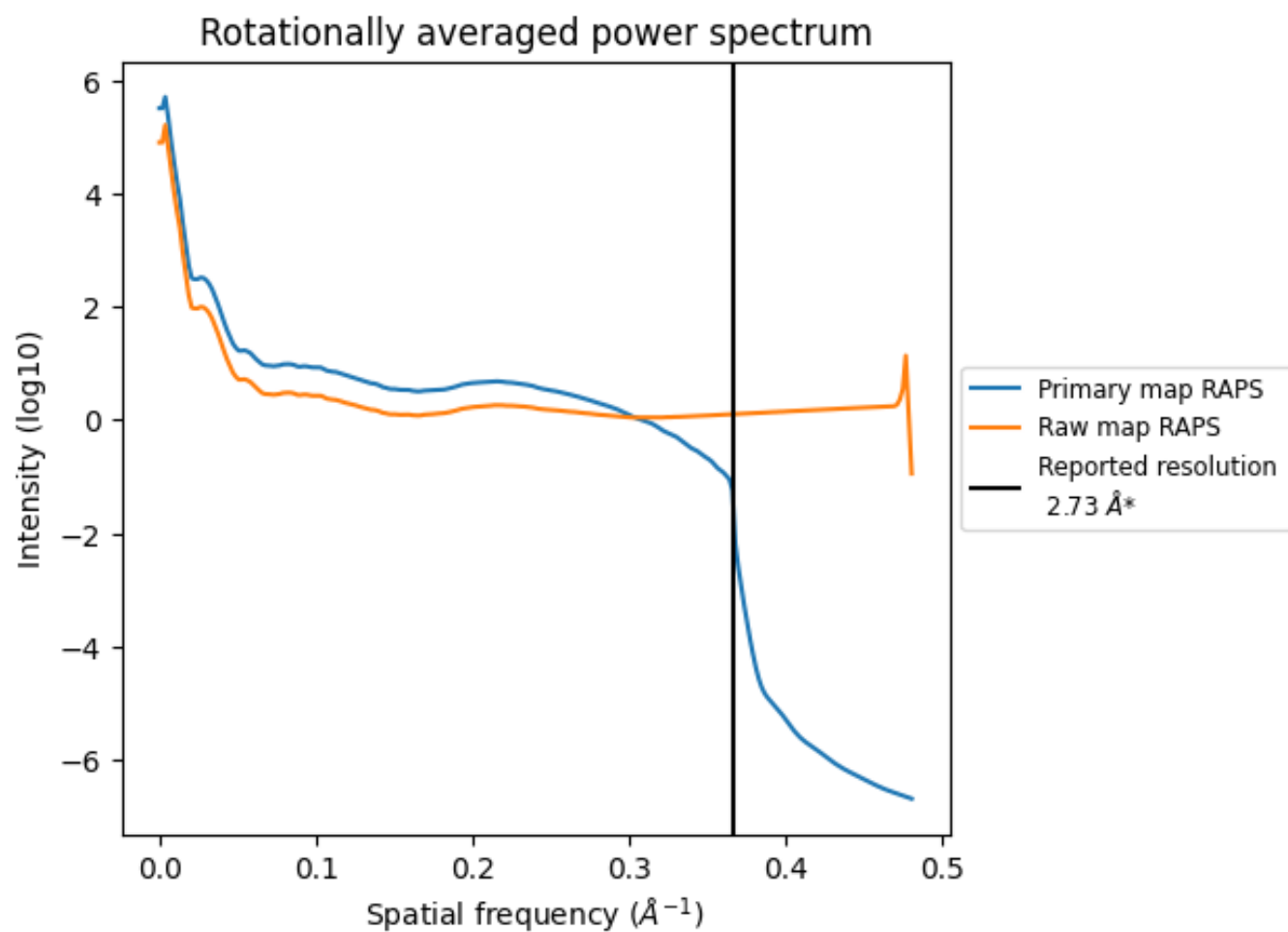
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 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 ⓘ

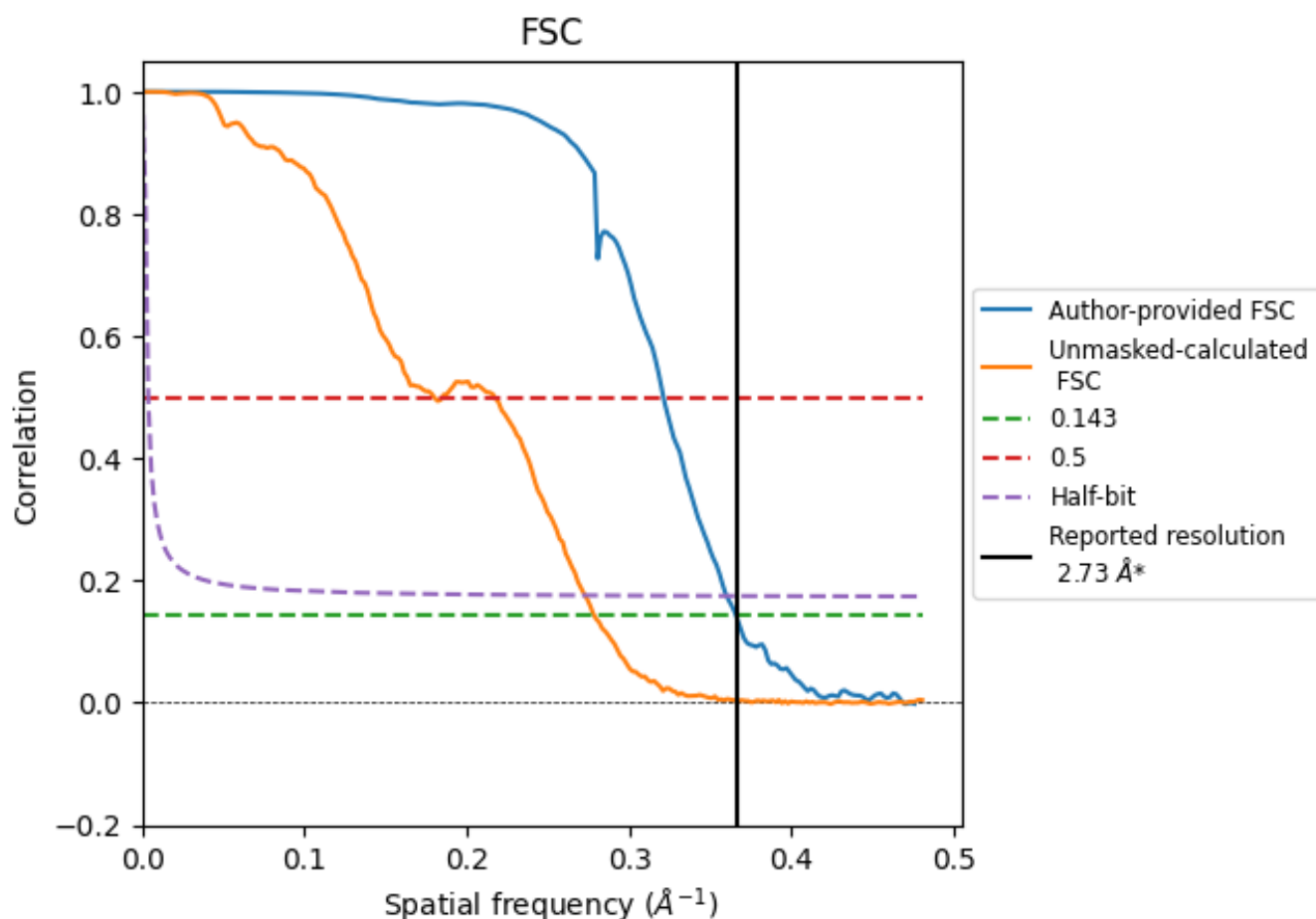


*Reported resolution corresponds to spatial frequency of 0.366 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.366 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

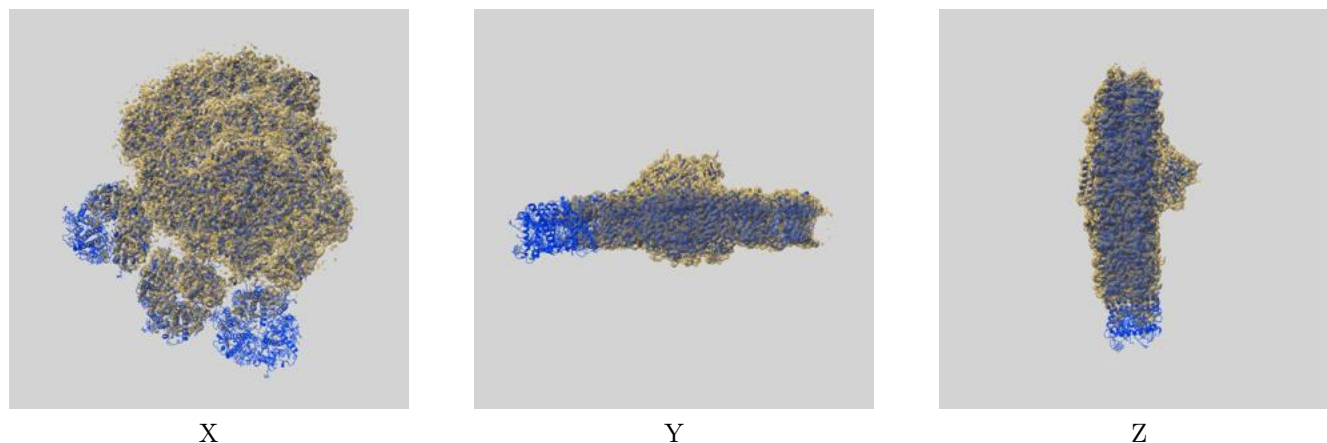
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.11	2.78
Unmasked-calculated*	3.59	5.56	3.66

*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 3.59 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

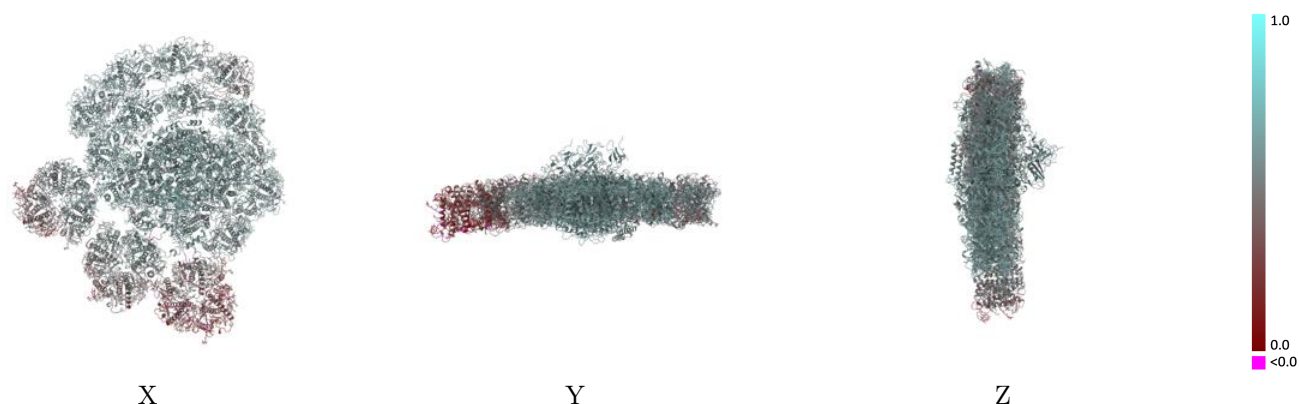
This section contains information regarding the fit between EMDB map EMD-61940 and PDB model 9JZR. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



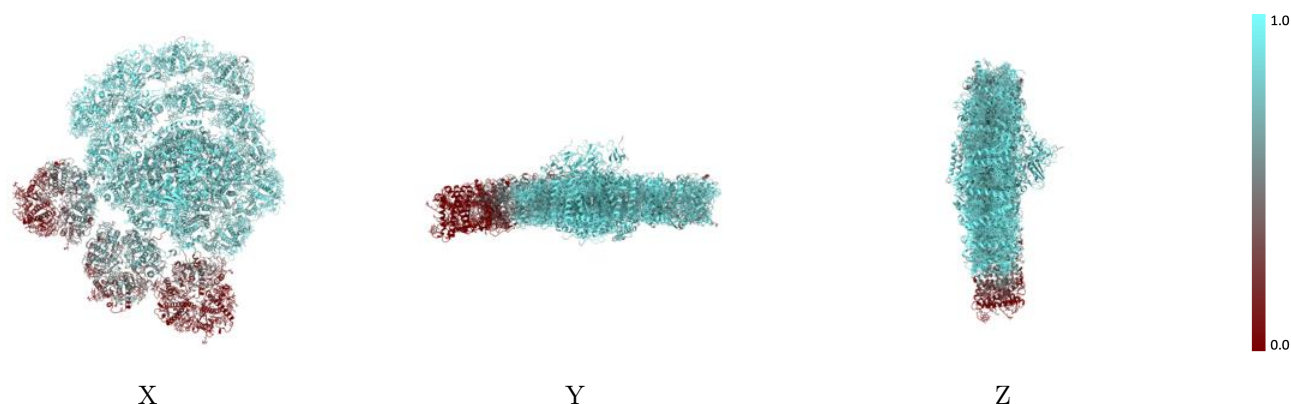
The images above show the 3D surface view of the map at the recommended contour level 0.217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



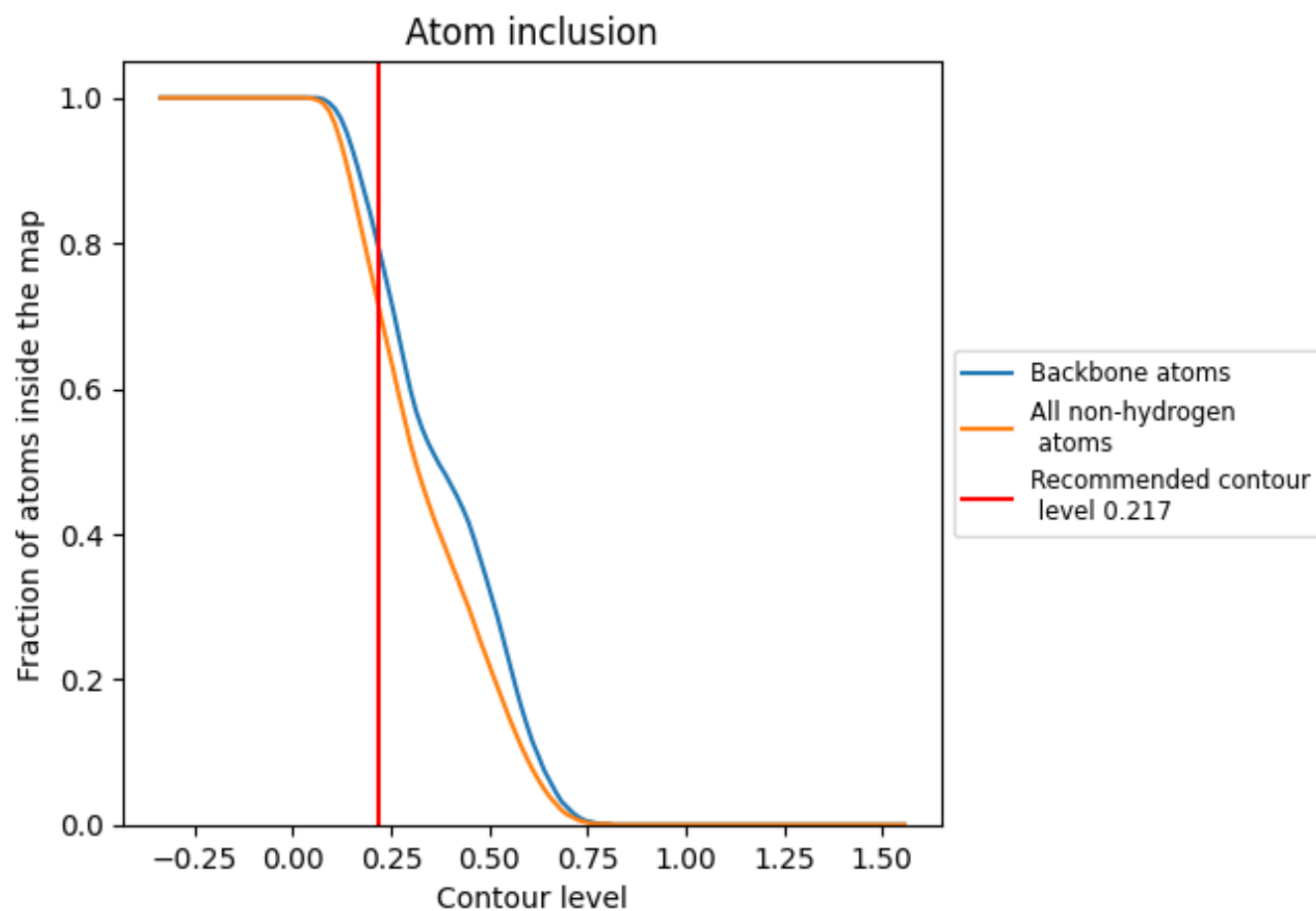
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.217).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.5260
0	 0.8170	 0.5440
1	 0.8570	 0.5600
2	 0.9190	 0.5900
3	 0.9250	 0.5940
4	 0.8710	 0.5490
5	 0.7530	 0.4730
6	 0.9000	 0.5700
7	 0.8930	 0.5770
8	 0.8400	 0.5370
9	 0.8730	 0.5690
A	 0.9360	 0.6060
B	 0.9410	 0.6020
C	 0.9520	 0.5880
D	 0.9270	 0.5990
E	 0.8480	 0.5730
F	 0.8930	 0.5690
G	 0.7920	 0.5390
H	 0.8480	 0.5790
I	 0.9130	 0.5760
J	 0.9030	 0.5870
K	 0.8830	 0.5830
L	 0.8710	 0.5780
M	 0.8950	 0.5860
O	 0.8770	 0.5710
a	 0.0580	 0.3680
b	 0.4230	 0.5140
c	 0.5090	 0.5130
d	 0.2950	 0.3960
e	 0.4980	 0.4730
f	 0.6060	 0.5100
g	 0.0030	 0.2200
h	 0.0250	 0.2680
i	 0.2140	 0.3760

