



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 01:28 AM JST

PDB ID : 8WB4 / pdb_00008wb4
EMDB ID : EMD-37414
Title : Structure of PSII-ACPII supercomplex from cryptophyte algae
Authors : Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on : 2023-09-08
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

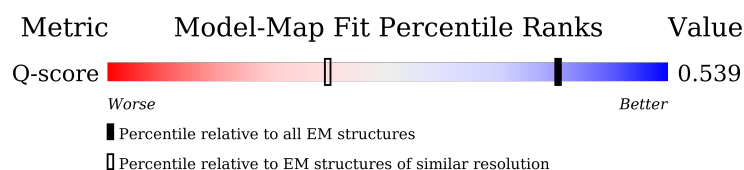
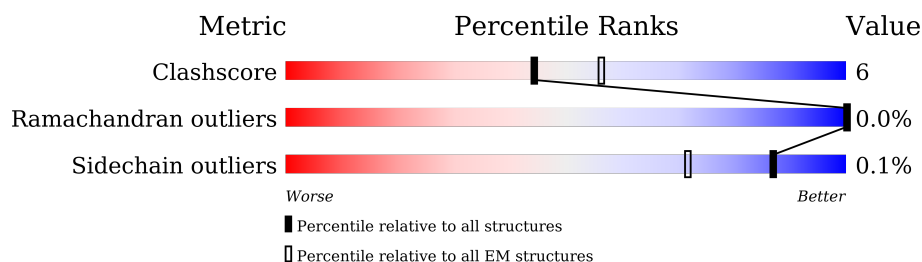
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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	6086 (1.98 - 2.97)

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	M	115	
1	m	115	
2	1	235	
2	7	235	

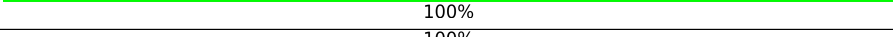
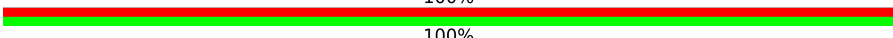
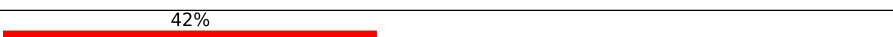
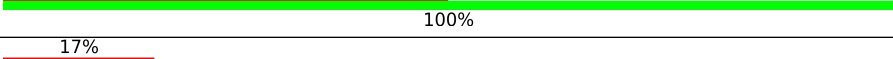
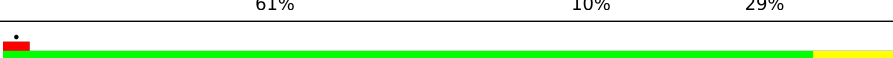
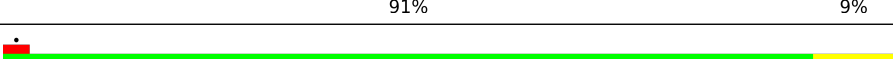
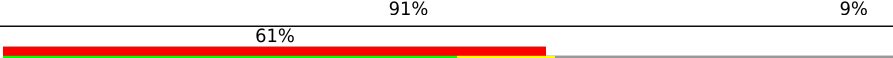
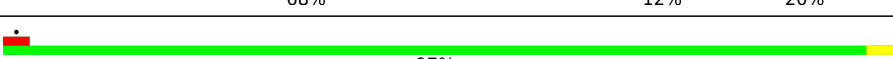
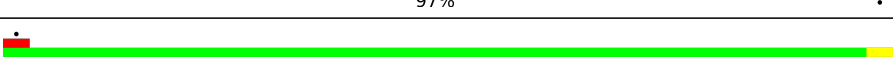
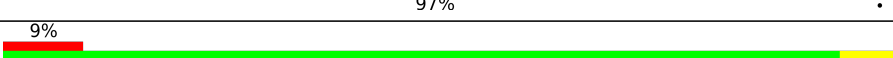
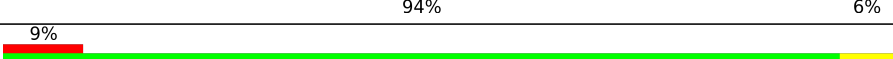
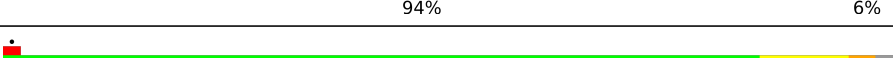
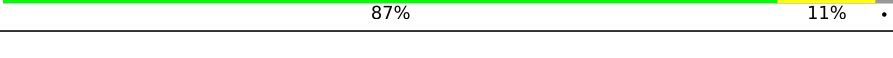
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Mol	Chain	Length	Quality of chain
3	2	217	
3	8	217	
4	3	222	
4	9	222	
5	0	226	
5	4	226	
6	5	218	
6	p	218	
7	6	220	
7	P	220	
8	A	360	
8	a	360	
9	D	351	
9	d	351	
10	E	84	
10	e	84	
11	F	42	
11	f	42	
12	H	67	
12	h	67	
13	I	38	
13	i	38	
14	J	39	
14	j	39	
15	K	45	

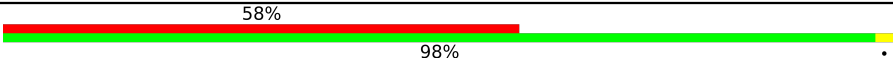
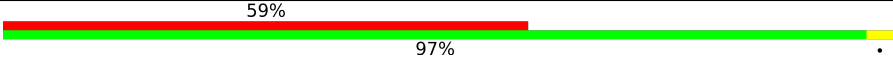
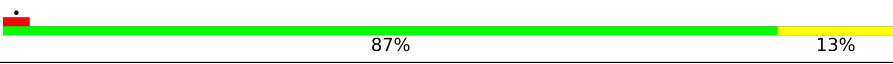
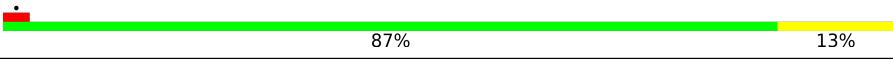
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Mol	Chain	Length	Quality of chain
15	k	45	
16	O	330	
16	o	330	
17	Q	21	
17	q	21	
18	R	26	
18	r	26	
19	S	285	
19	s	285	
20	T	32	
20	t	32	
21	U	150	
21	u	150	
22	V	163	
22	v	163	
23	X	39	
23	x	39	
24	Y	34	
24	y	34	
25	Z	62	
25	z	62	
26	B	509	
26	b	509	
27	C	461	
27	c	461	

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Mol	Chain	Length	Quality of chain
28	G	64	
28	g	64	
29	L	38	
29	l	38	
30	W	114	
30	w	114	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 80246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II reaction center M.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	m	36	Total	C	N	O	0	0
			265	175	42	48		
1	M	36	Total	C	N	O	0	0
			265	175	42	48		

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		
2	7	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		
3	8	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		
4	9	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		

- Molecule 5 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		
5	0	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		
6	p	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		
7	P	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		

- Molecule 8 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		
8	a	334	Total	C	N	O	S	0	0
			2618	1712	430	464	12		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		
9	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	77	Total	C	N	O	0	0
			629	409	104	116		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	77	Total	C	N	O	0	0
			629	409	104	116		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	30	Total	C	N	O	S	0	0
			247	168	41	37	1		
11	f	30	Total	C	N	O	S	0	0
			247	168	41	37	1		

- Molecule 12 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	65	Total	C	N	O	S	0	0
			515	344	81	88	2		
12	h	65	Total	C	N	O	S	0	0
			515	344	81	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	35	Total	C	N	O	S	0	0
			287	191	46	49	1		
13	i	35	Total	C	N	O	S	0	0
			287	191	46	49	1		

- Molecule 14 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	28	Total	C	N	O	0	0
			214	147	32	35		
14	j	28	Total	C	N	O	0	0
			214	147	32	35		

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	37	Total	C	N	O	0	0
			297	209	44	44		
15	k	37	Total	C	N	O	0	0
			297	209	44	44		

- Molecule 16 is a protein called Photosystem II reaction center protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		
16	o	231	Total	C	N	O	S	0	0
			1749	1103	282	358	6		

- Molecule 17 is a protein called Photosystem II reaction center protein Q.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	21	Total	C	N	O	0	0
			105	63	21	21		
17	q	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 18 is a protein called Photosystem II reaction center protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	26	Total	C	N	O	0	0
			130	78	26	26		
18	r	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 19 is a protein called CCPH-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		
19	s	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	32	Total	C	N	O	S	0	0
			260	179	40	40	1		
20	t	32	Total	C	N	O	S	0	0
			260	179	40	40	1		

- Molecule 21 is a protein called Photosystem II reaction center protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	93	Total	C	N	O	S	0	0
			742	476	122	142	2		
21	u	93	Total	C	N	O	S	0	0
			742	476	122	142	2		

- Molecule 22 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	131	Total	C	N	O	S	0	0
			996	626	170	196	4		
22	v	131	Total	C	N	O	S	0	0
			996	626	170	196	4		

- Molecule 23 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	39	Total	C	N	O	S	0	0
			292	192	47	52	1		
23	x	39	Total	C	N	O	S	0	0
			292	192	47	52	1		

- Molecule 24 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		
24	y	34	Total	C	N	O	S	0	0
			266	180	43	42	1		

- Molecule 25 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
25	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 26 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	504	Total	C	N	O	S	0	0
			3962	2587	676	688	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	504	Total	C	N	O	S	0	0
			3962	2587	676	688	11		

- Molecule 27 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	451	Total	C	N	O	S	0	0
			3504	2290	589	615	10		
27	C	451	Total	C	N	O	S	0	0
			3504	2290	589	615	10		

- Molecule 28 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	64	Total	C	N	O	0	0
			320	192	64	64		
28	G	64	Total	C	N	O	0	0
			320	192	64	64		

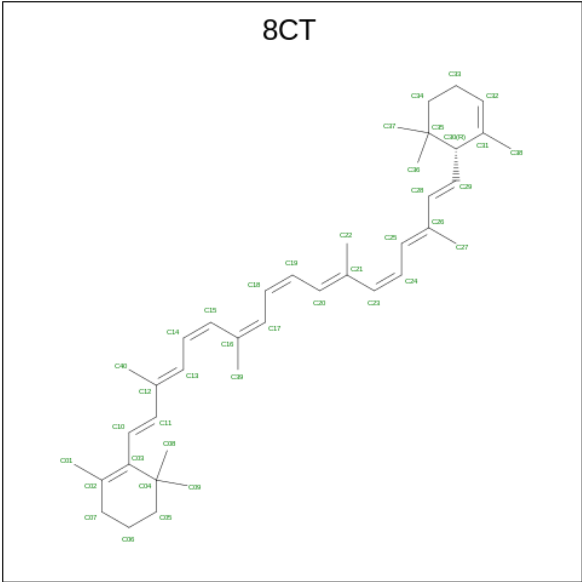
- Molecule 29 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	38	Total	C	N	O	S	0	0
			310	209	48	52	1		
29	L	38	Total	C	N	O	S	0	0
			310	209	48	52	1		

- Molecule 30 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	w	45	Total	C	N	O	0	0
			367	238	57	72		
30	W	45	Total	C	N	O	0	0
			367	238	57	72		

- Molecule 31 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).



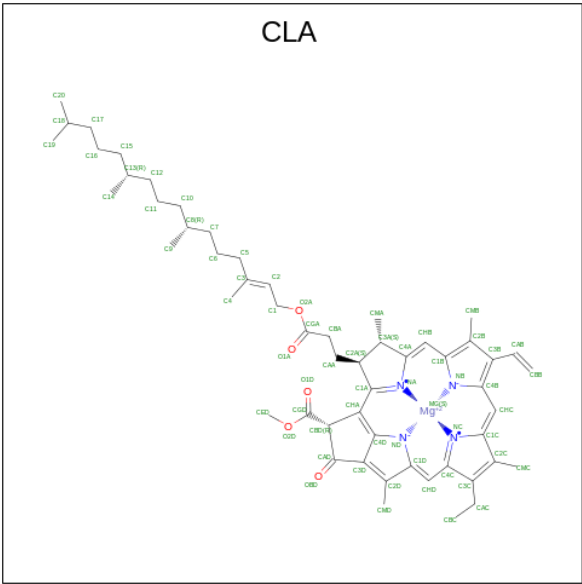
Mol	Chain	Residues	Atoms	AltConf
31	M	1	Total C 40 40	0
31	3	1	Total C 40 40	0
31	6	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	Z	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	k	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
31	k	1	Total	C	0
			40	40	
31	z	1	Total	C	0
			40	40	
31	9	1	Total	C	0
			40	40	
31	C	1	Total	C	0
			40	40	
31	P	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	h	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			40	40	

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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

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Mol	Chain	Residues	Atoms					AltConf
32	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	3	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	4	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	6	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	d	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	0	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	8	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	9	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	P	1	Total 59	C 49	Mg 1	N 4	O 5	0

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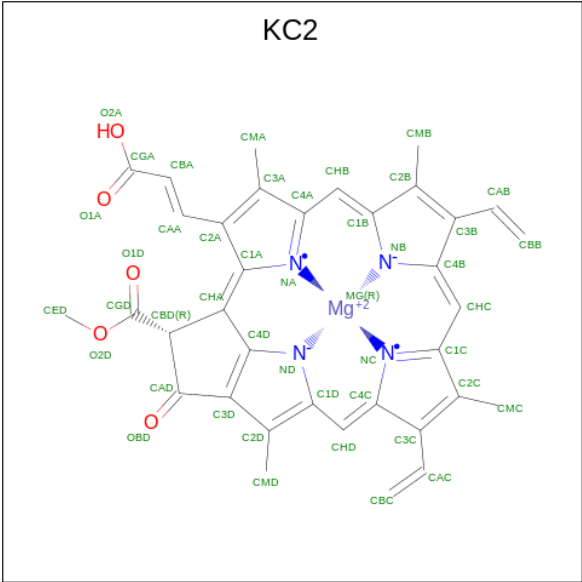
Mol	Chain	Residues	Atoms					AltConf
32	P	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	p	1	Total 59	C 49	Mg 1	N 4	O 5	0
32	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂)

The chemical structure shows a long, zig-zagging carbon chain with alternating double bonds. At each end of the chain, there is a terminal group consisting of a carbon atom bonded to two methyl groups and a hydroxyl group (OH). The carbon atoms are labeled with IDs: C005, C006, C007, C008, C009, C010, C011, C012, C013, C014, C015, C016, C017, C018, C019, C020, C021, C022, C023, C024, C025, C026, C027, C028, C029, C030, C031, C032, C033, C034, C035, C036, C037, C038, C039, C040, C041, C042, C043, C044, C045, C046, C047, C048, C049, C050, C051, C052, C053, C054, C055, C056, C057, C058, C059, C060, C061, C062, C063, C064, C065, C066, C067, C068, C069, C070, C071, C072, C073, C074, C075, C076, C077, C078, C079, C080, C081, C082, C083, C084, C085, C086, C087, C088, C089, C090, C091, C092, C093, C094, C095, C096, C097, C098, C099, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C8

Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0



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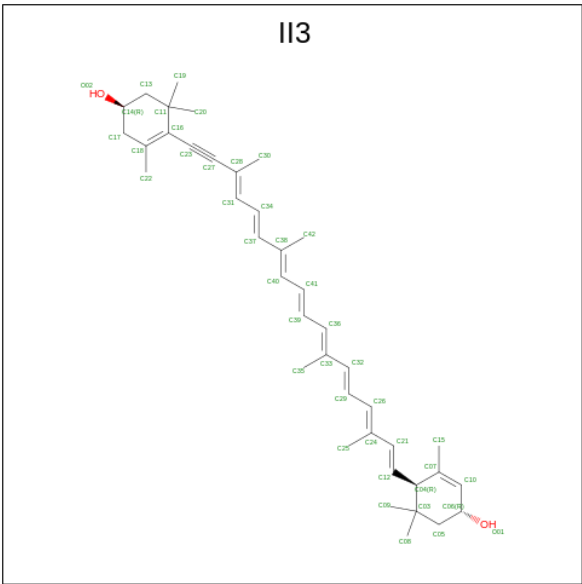
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34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	0	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	9	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
34	9	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	P	1	Total	C	O	0
			42	40	2	
34	P	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	
34	p	1	Total	C	O	0
			42	40	2	

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).



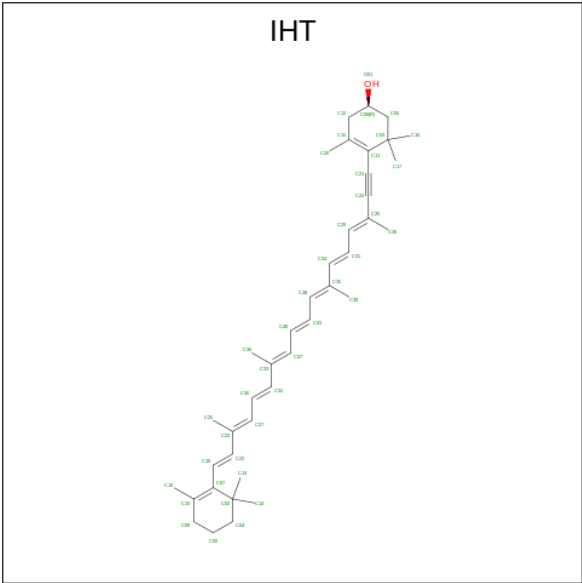
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			42	40	2	
35	6	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
35	7	1	Total	C	O	0
			42	40	2	
35	P	1	Total	C	O	0
			42	40	2	

- Molecule 36 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



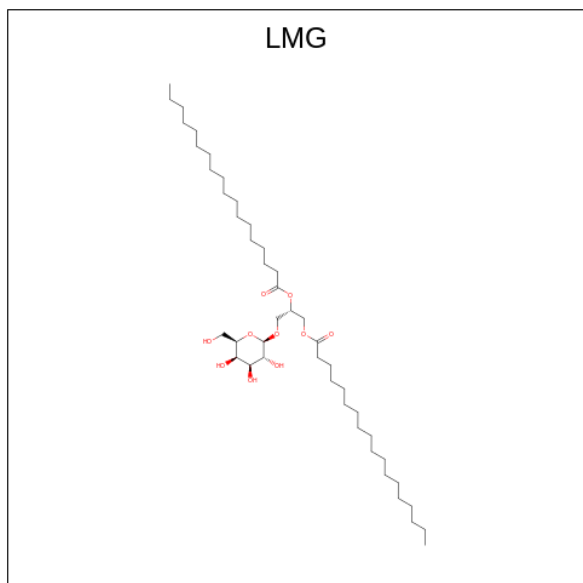
Mol	Chain	Residues	Atoms			AltConf
36	1	1	Total	C	O	0
			41	40	1	
36	2	1	Total	C	O	0
			41	40	1	
36	4	1	Total	C	O	0
			41	40	1	
36	4	1	Total	C	O	0
			41	40	1	
36	5	1	Total	C	O	0
			41	40	1	
36	0	1	Total	C	O	0
			41	40	1	
36	0	1	Total	C	O	0
			41	40	1	
36	7	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
36	8	1	Total	C	O	0
			41	40	1	
36	p	1	Total	C	O	0
			41	40	1	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



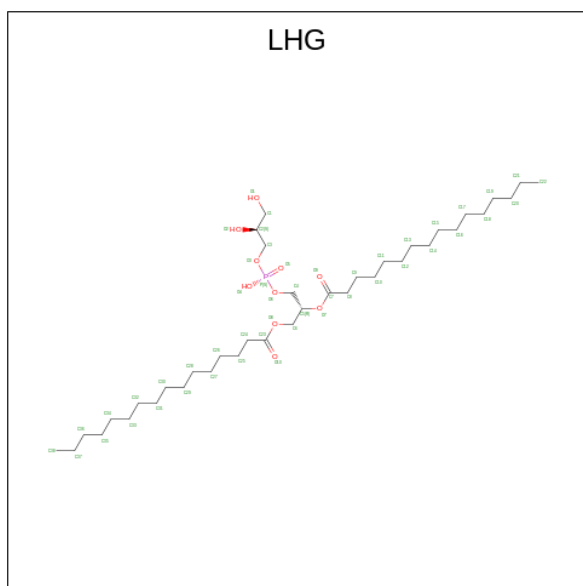
Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	O	0
			36	26	10	
37	4	1	Total	C	O	0
			36	26	10	
37	6	1	Total	C	O	0
			28	18	10	
37	A	1	Total	C	O	0
			48	38	10	
37	D	1	Total	C	O	0
			46	36	10	
37	D	1	Total	C	O	0
			40	30	10	
37	b	1	Total	C	O	0
			51	41	10	
37	c	1	Total	C	O	0
			46	36	10	
37	d	1	Total	C	O	0
			40	30	10	

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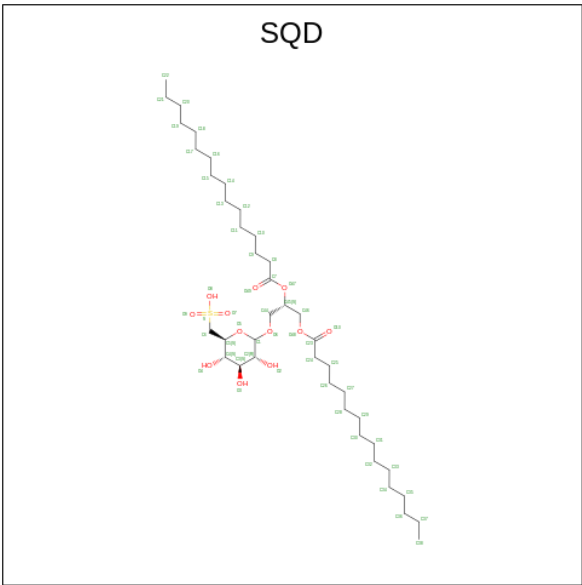
Mol	Chain	Residues	Atoms			AltConf
37	d	1	Total	C	O	0
			46	36	10	
37	g	1	Total	C	O	0
			28	18	10	
37	l	1	Total	C	O	0
			40	30	10	
37	o	1	Total	C	O	0
			36	26	10	
37	8	1	Total	C	O	0
			36	26	10	
37	C	1	Total	C	O	0
			46	36	10	
37	G	1	Total	C	O	0
			28	18	10	
37	L	1	Total	C	O	0
			40	30	10	
37	P	1	Total	C	O	0
			28	18	10	
37	a	1	Total	C	O	0
			48	38	10	
37	B	1	Total	C	O	0
			51	41	10	

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



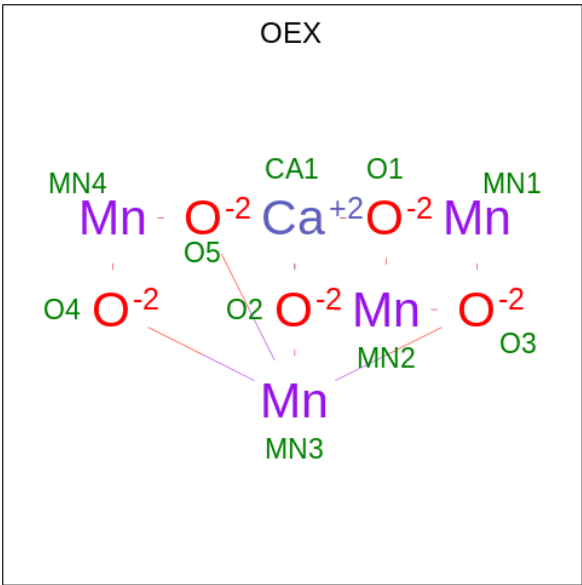
Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	O	P	0
			22	12	9	1	
38	A	1	Total	C	O	P	0
			43	32	10	1	
38	A	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			48	38	9	1	
38	D	1	Total	C	O	P	0
			32	21	10	1	
38	S	1	Total	C	O	P	0
			37	26	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	b	1	Total	C	O	P	0
			39	28	10	1	
38	d	1	Total	C	O	P	0
			48	38	9	1	
38	d	1	Total	C	O	P	0
			32	21	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	8	1	Total	C	O	P	0
			22	12	9	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	a	1	Total	C	O	P	0
			43	32	10	1	
38	a	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			37	26	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	
38	B	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



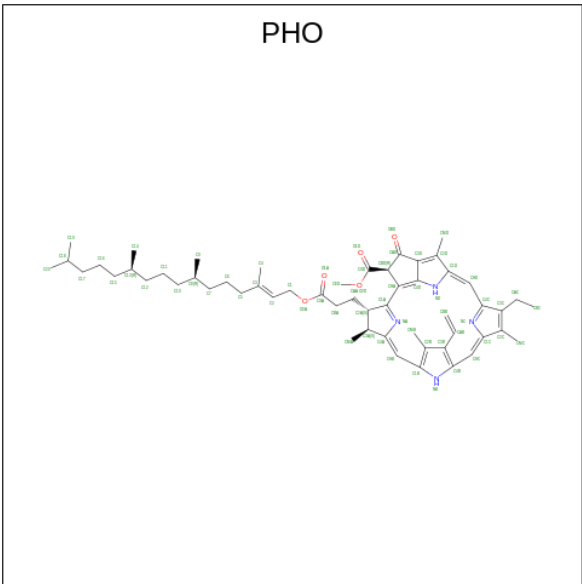
Mol	Chain	Residues	Atoms				AltConf
39	5	1	Total	C	O	S	0
			35	22	12	1	
39	A	1	Total	C	O	S	0
			54	41	12	1	
39	b	1	Total	C	O	S	0
			48	35	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	a	1	Total	C	O	S	0
			54	41	12	1	
39	p	1	Total	C	O	S	0
			35	22	12	1	
39	B	1	Total	C	O	S	0
			48	35	12	1	
39	B	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 40 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
40	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 41 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	A	1	Total	C	N	O	0
			64	55	4	5	

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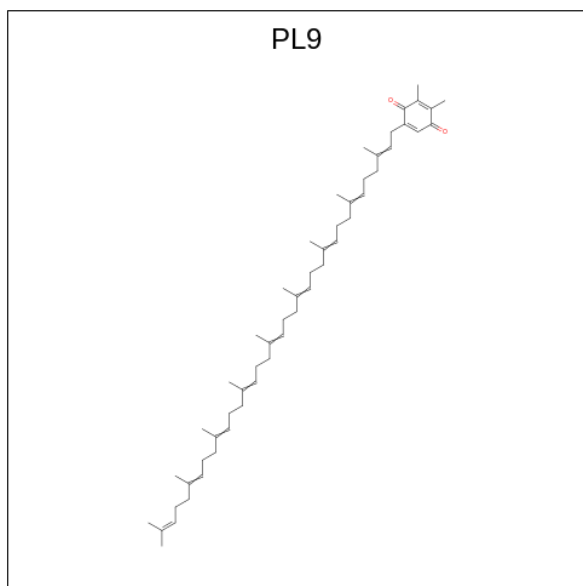
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Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	N	O	0
			64	55	4	5	
41	d	1	Total	C	N	O	0
			64	55	4	5	
41	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 42 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
42	A	1	Total	Cl	0
			1	1	
42	a	1	Total	Cl	0
			1	1	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



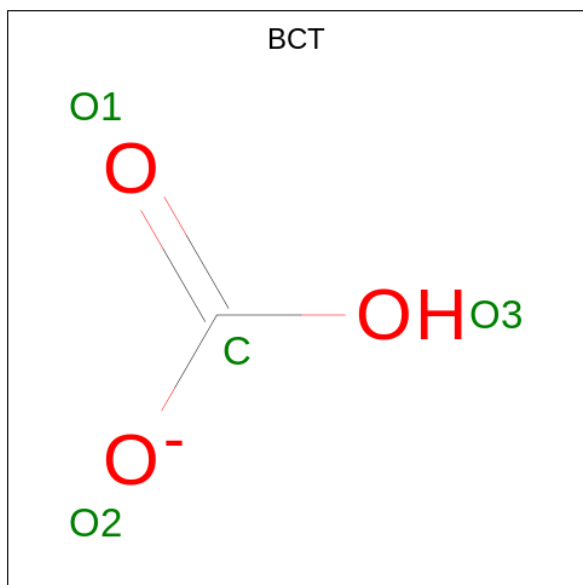
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			13	11	2	
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	

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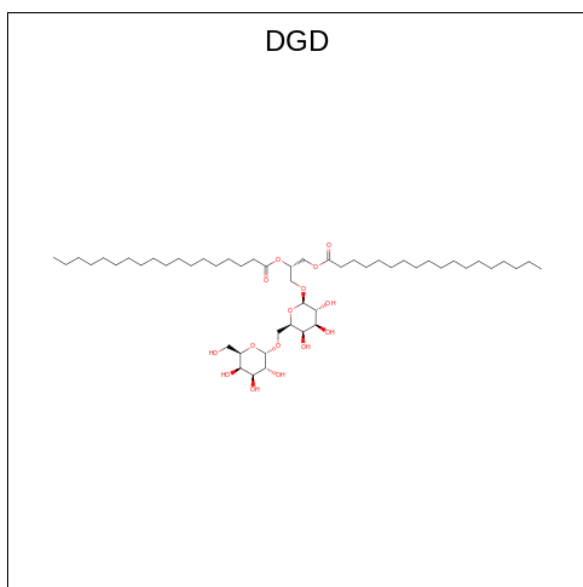
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			13	11	2	

- Molecule 44 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	C	O	0
			4	1	3	
44	a	1	Total	C	O	0
			4	1	3	

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).

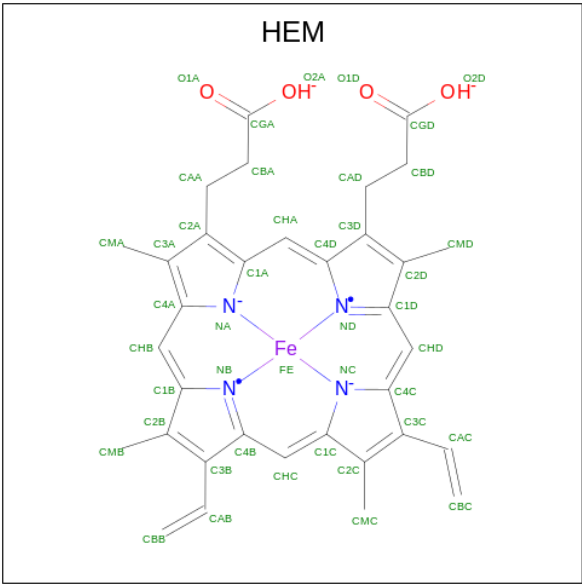


Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			53	39	14	
45	H	1	Total	C	O	0
			62	47	15	
45	c	1	Total	C	O	0
			55	40	15	
45	c	1	Total	C	O	0
			56	41	15	
45	c	1	Total	C	O	0
			55	40	15	
45	C	1	Total	C	O	0
			55	40	15	
45	C	1	Total	C	O	0
			56	41	15	
45	C	1	Total	C	O	0
			55	40	15	
45	a	1	Total	C	O	0
			53	39	14	
45	h	1	Total	C	O	0
			62	47	15	

- Molecule 46 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
46	D	1	Total	Fe	0
			1	1	
46	d	1	Total	Fe	0
			1	1	

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

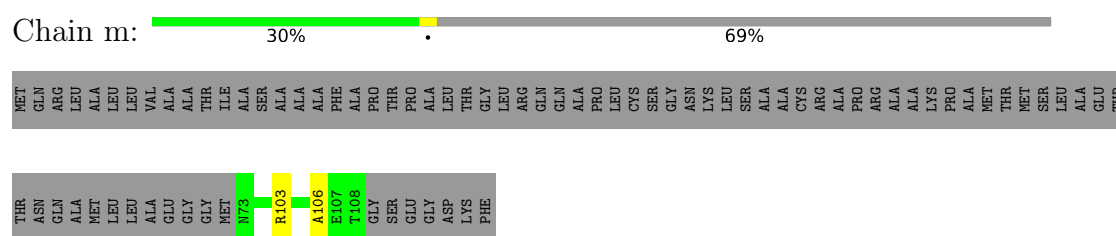


Mol	Chain	Residues	Atoms					AltConf
47	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

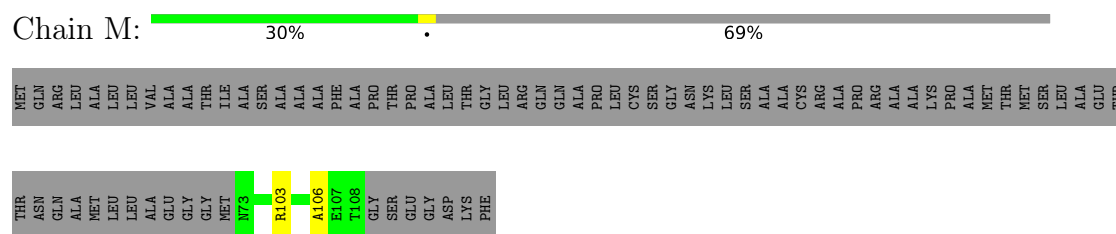
3 Residue-property plots

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

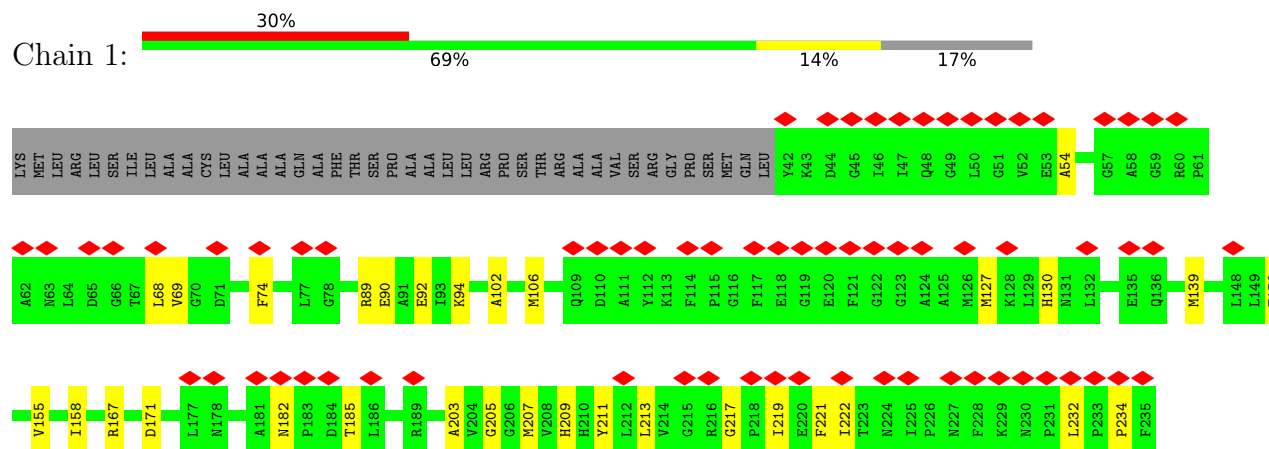
• Molecule 1: Photosystem II reaction center M



• Molecule 1: Photosystem II reaction center M

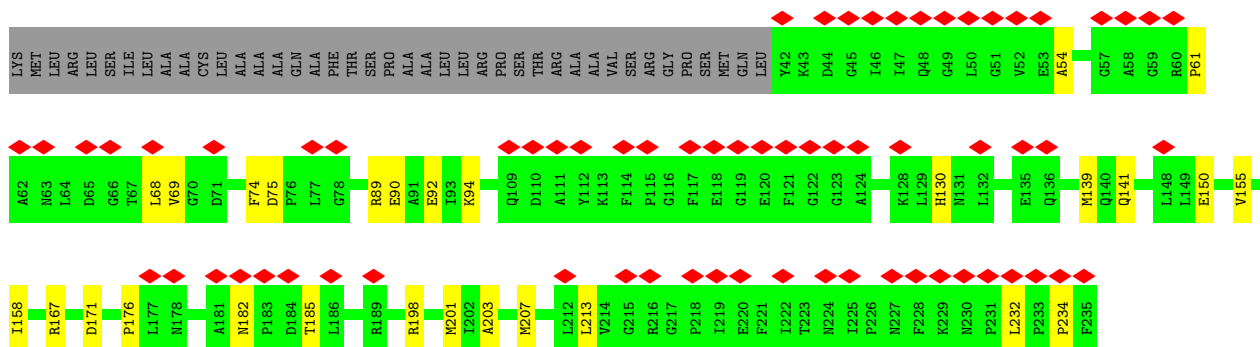


• Molecule 2: ACPII-1

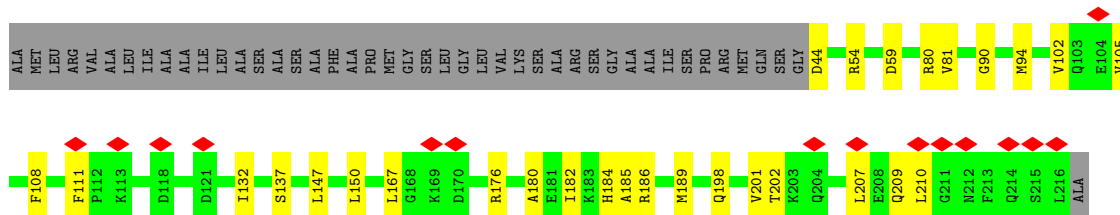


• Molecule 2: ACPII-1

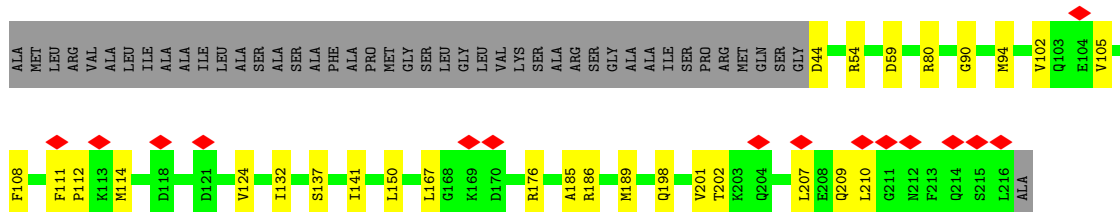




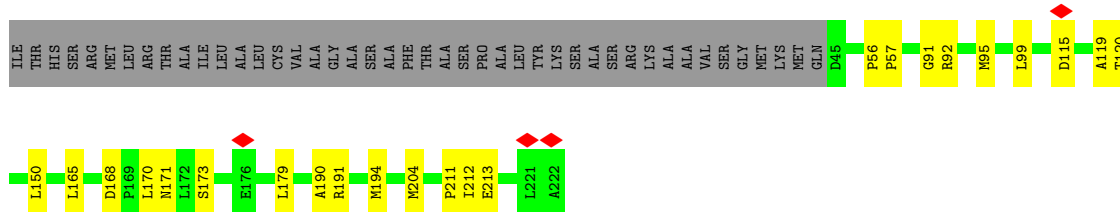
• Molecule 3: ACPII-2



• Molecule 3: ACPII-2

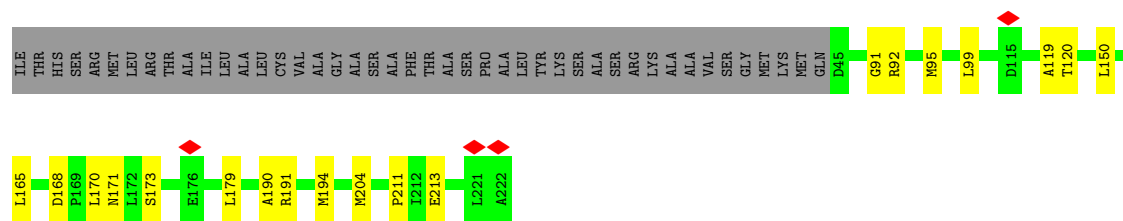


• Molecule 4: ACPII-3

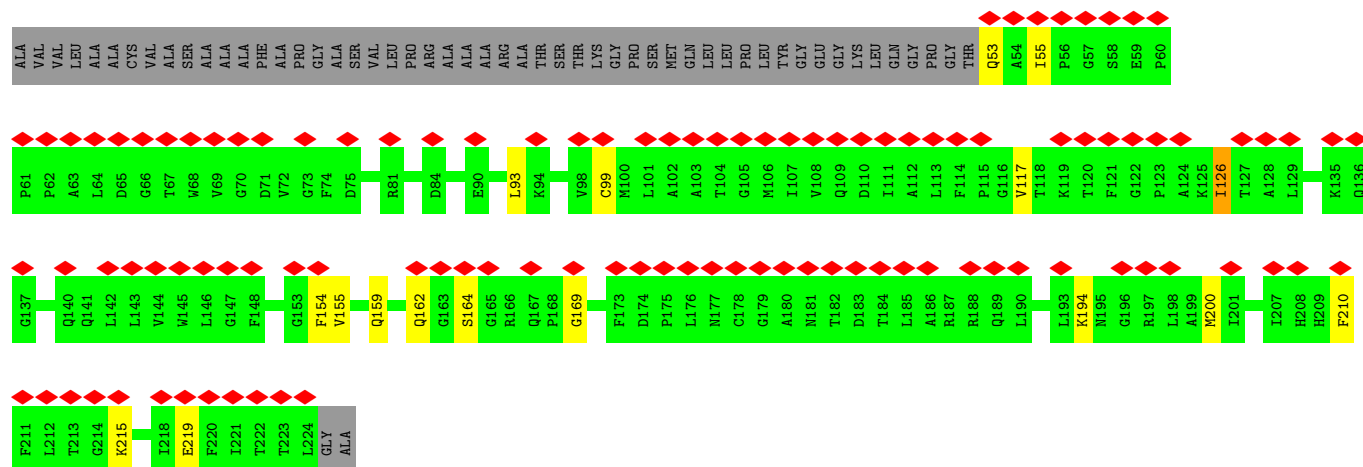


• Molecule 4: ACPII-3

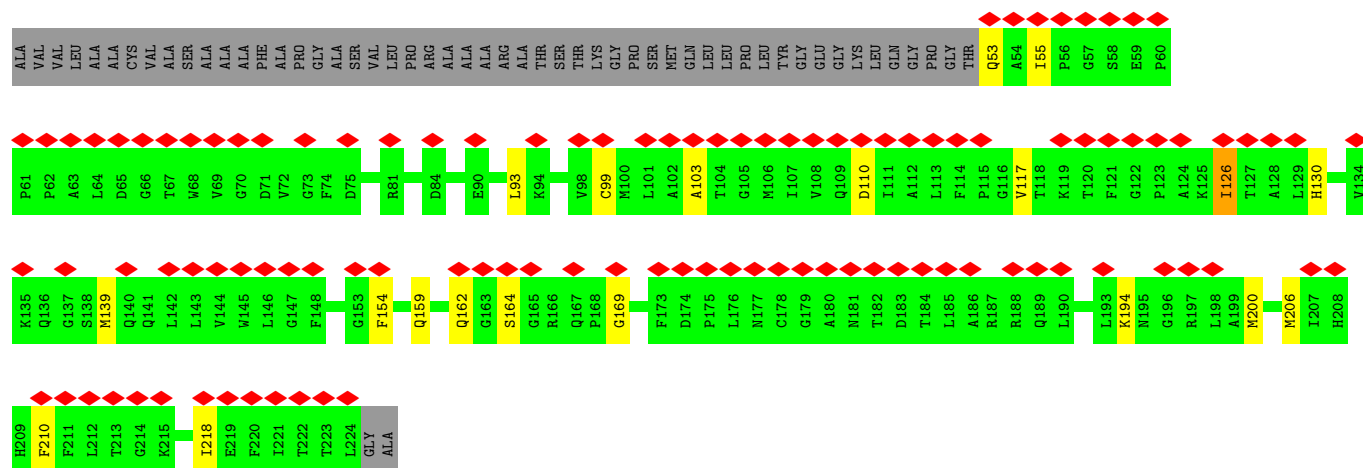




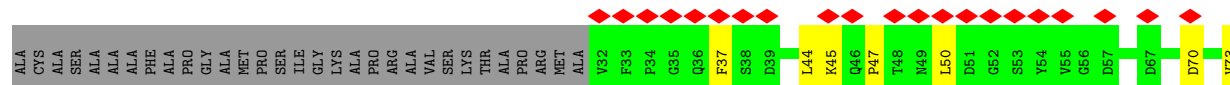
• Molecule 5: ACPII-4

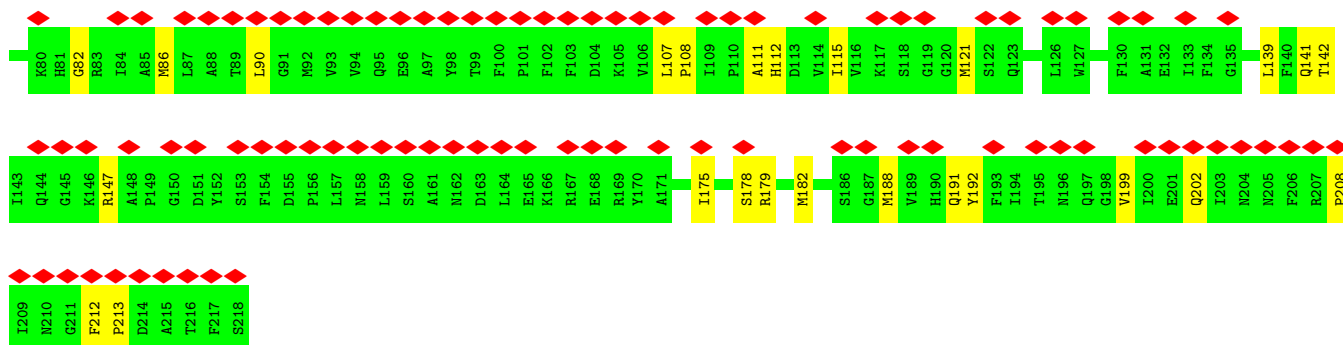


• Molecule 5: ACPII-4

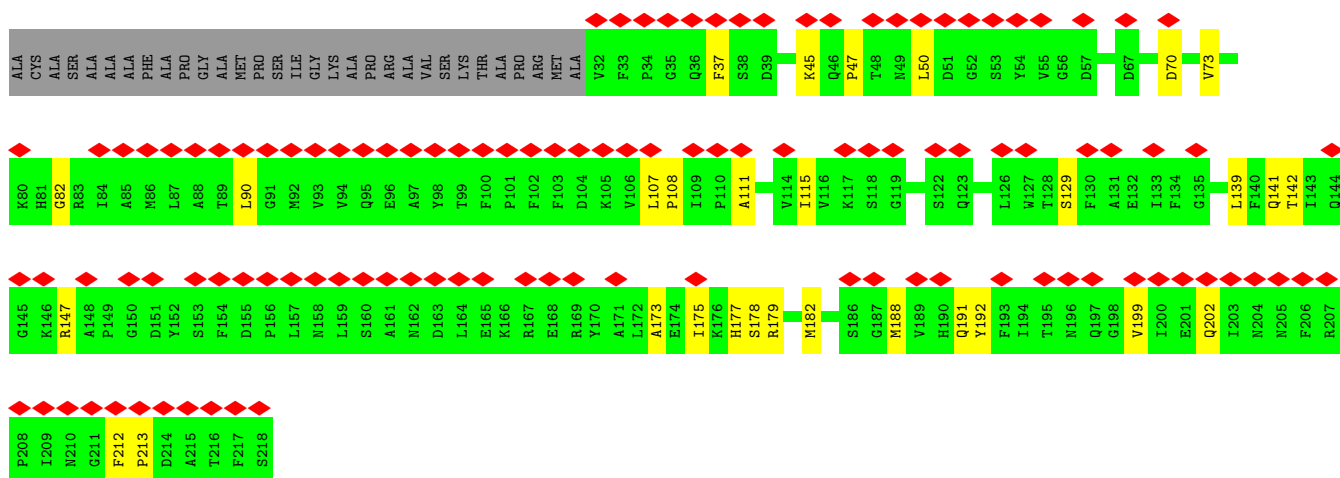
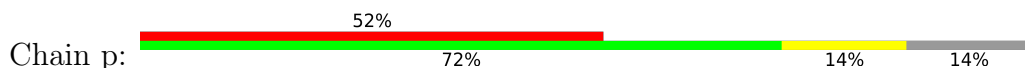


• Molecule 6: ACPII-5

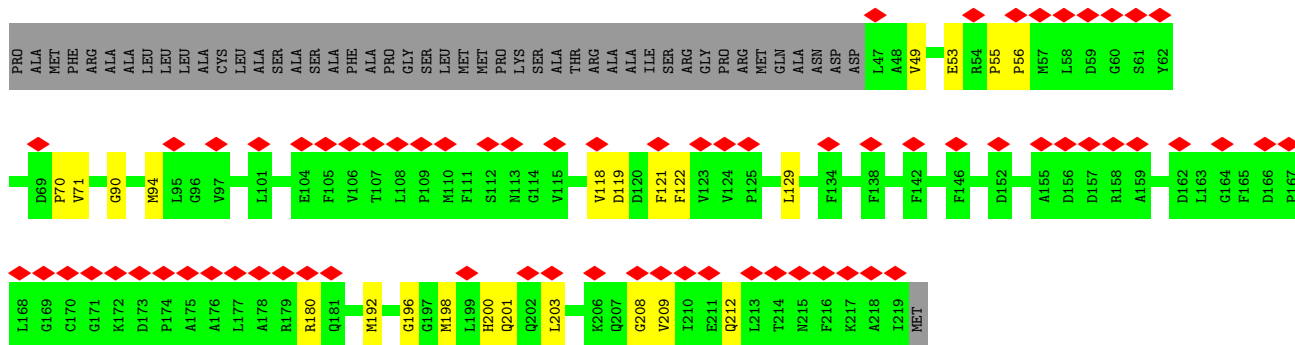




• Molecule 6: ACPII-5

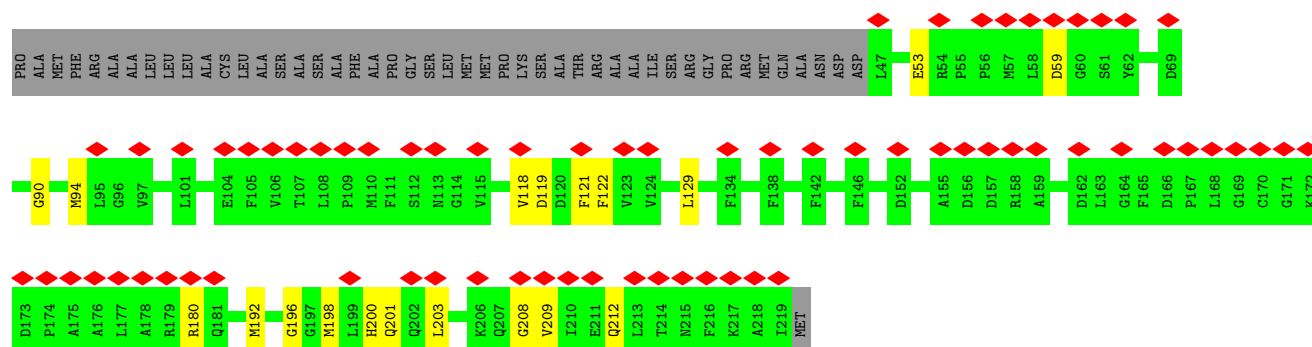


• Molecule 7: ACPII-6



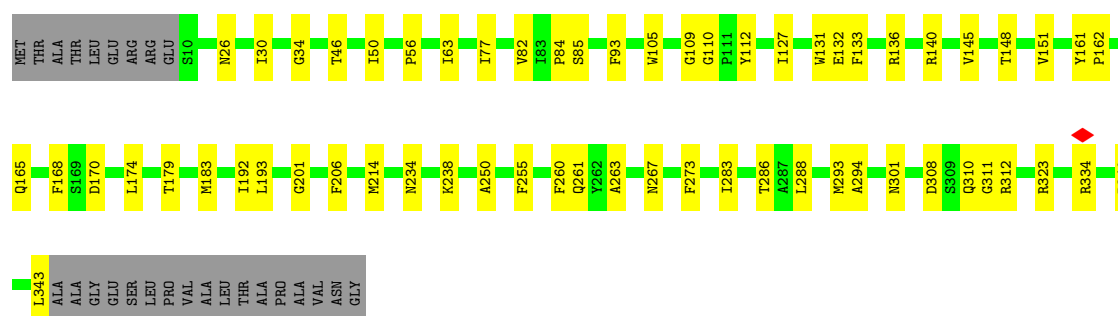
• Molecule 7: ACPII-6





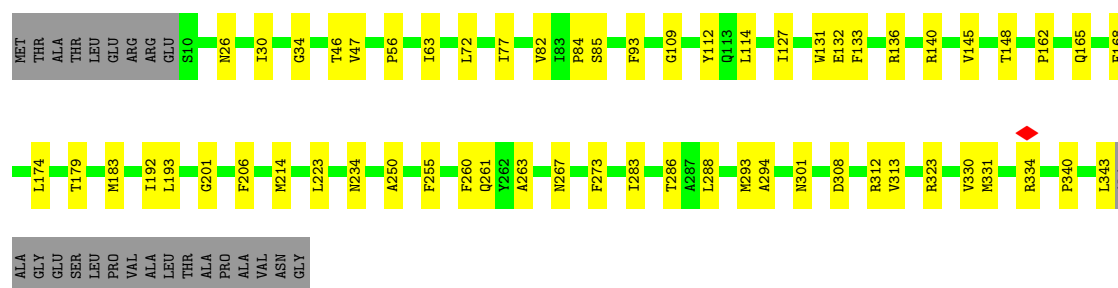
• Molecule 8: Photosystem II protein D1

Chain A: 76% 17% 7%



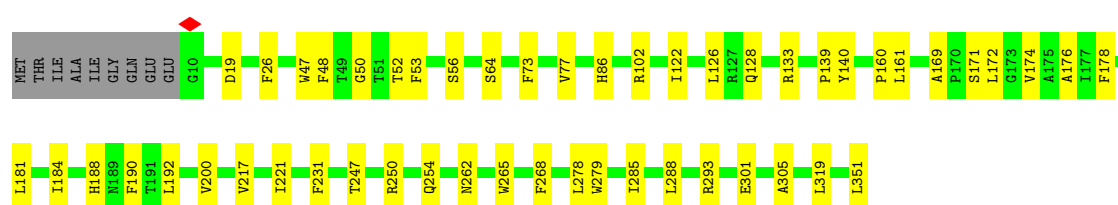
• Molecule 8: Photosystem II protein D1

Chain a: 76% 16% 7%



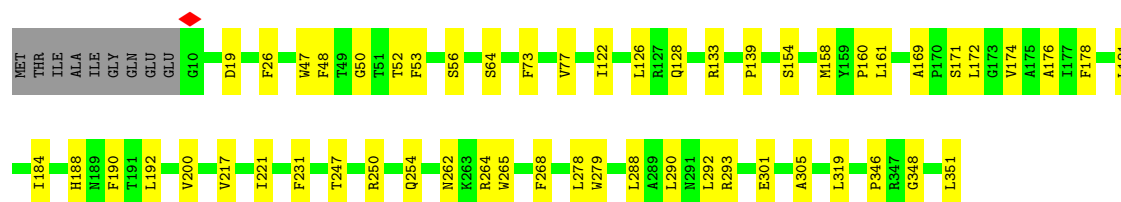
• Molecule 9: Photosystem II D2 protein

Chain D: 83% 15% 2%



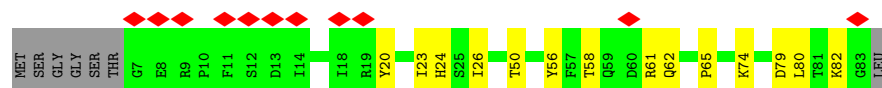
• Molecule 9: Photosystem II D2 protein

Chain d:  82% 15% .



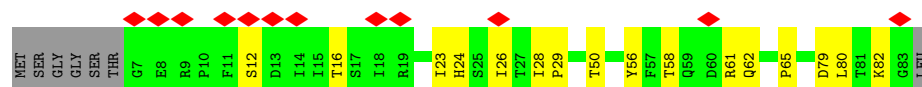
- Molecule 10: Cytochrome b559 subunit alpha

Chain E:  13% 75% 17% 8%



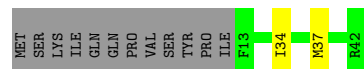
- Molecule 10: Cytochrome b559 subunit alpha

Chain e:  14% 73% 19% 8%



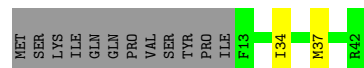
- Molecule 11: Cytochrome b559 subunit beta

Chain F:  67% 5% 29%



- Molecule 11: Cytochrome b559 subunit beta

Chain f:  67% 5% 29%



- Molecule 12: Photosystem II reaction center protein H

Chain H:  85% 12% .

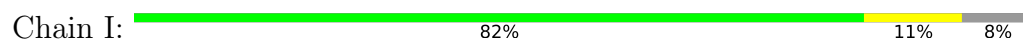


- Molecule 12: Photosystem II reaction center protein H

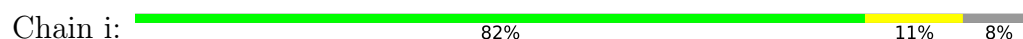
Chain h:  85% 12% .



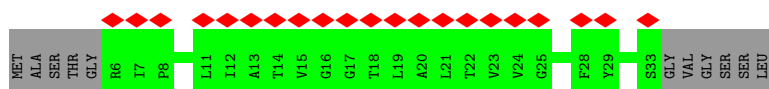
- Molecule 13: Photosystem II reaction center protein I



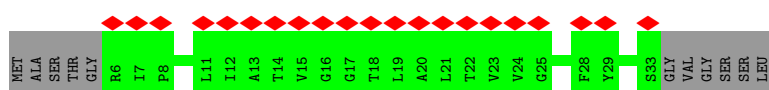
- Molecule 13: Photosystem II reaction center protein I



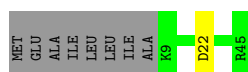
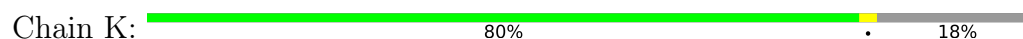
- Molecule 14: Photosystem II reaction center protein J



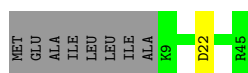
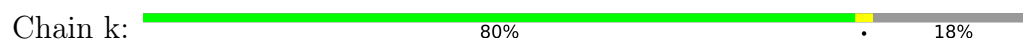
- Molecule 14: Photosystem II reaction center protein J



- Molecule 15: Photosystem II reaction center protein K

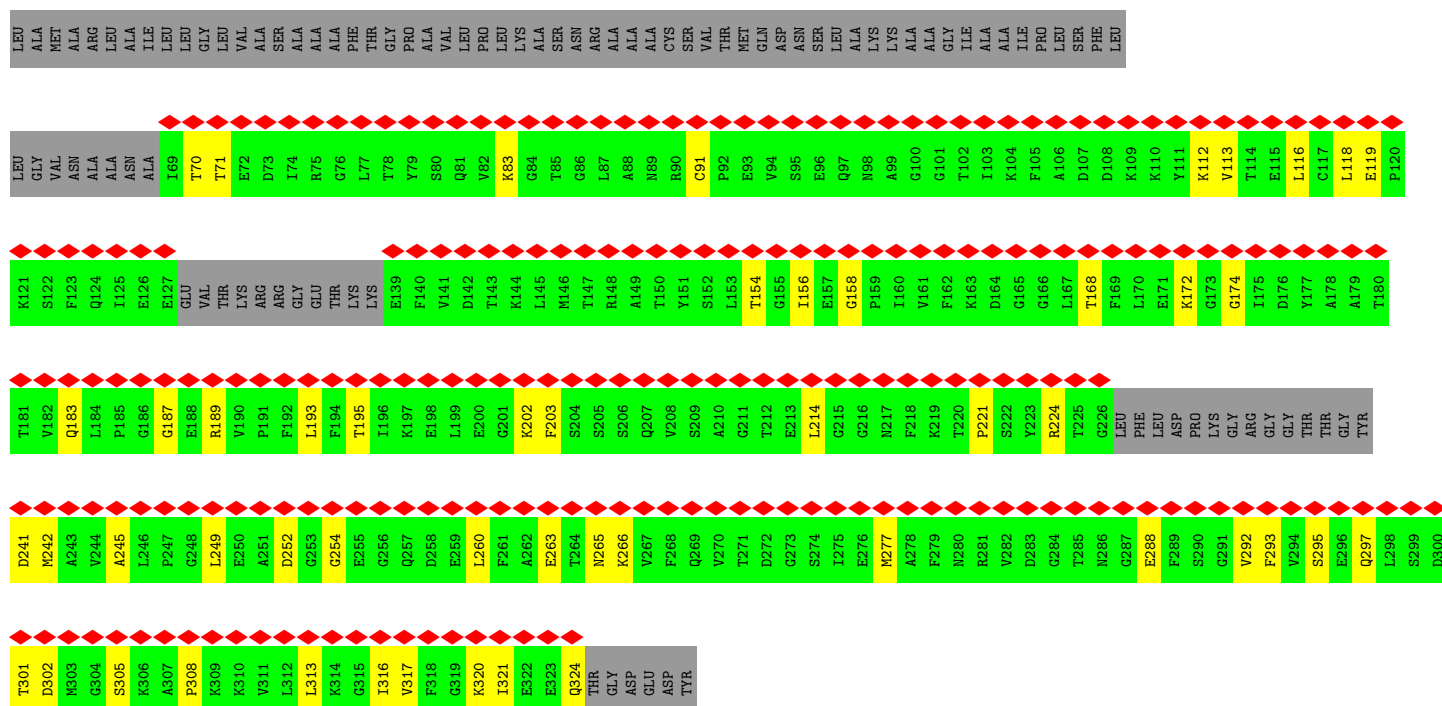


- Molecule 15: Photosystem II reaction center protein K

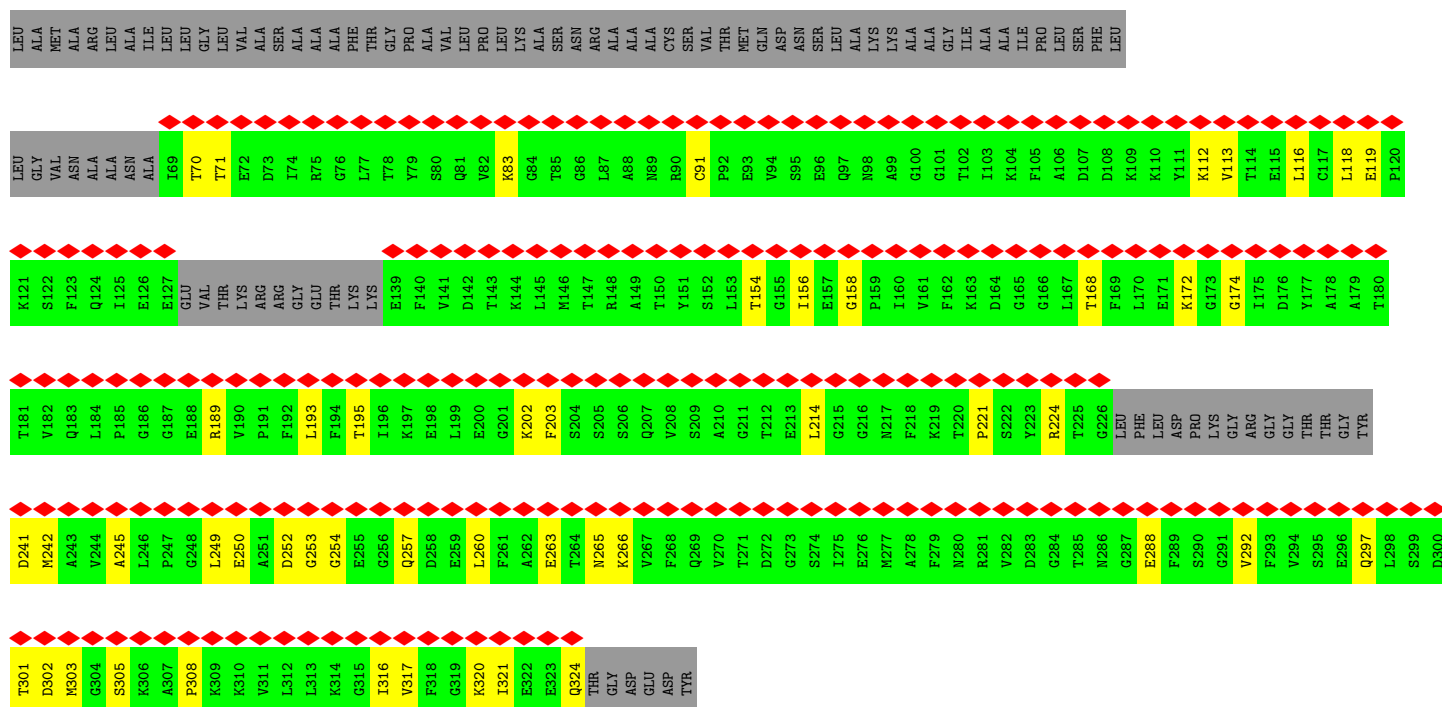


- Molecule 16: Photosystem II reaction center protein O



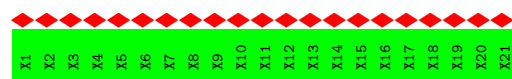


• Molecule 16: Photosystem II reaction center protein O

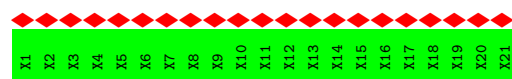


• Molecule 17: Photosystem II reaction center protein Q

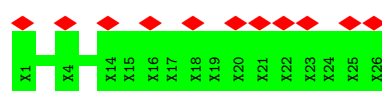
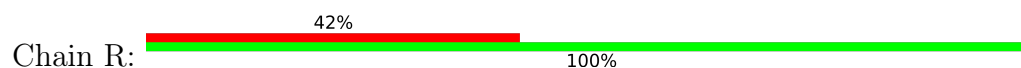




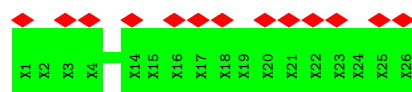
- Molecule 17: Photosystem II reaction center protein Q



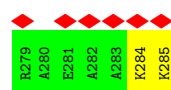
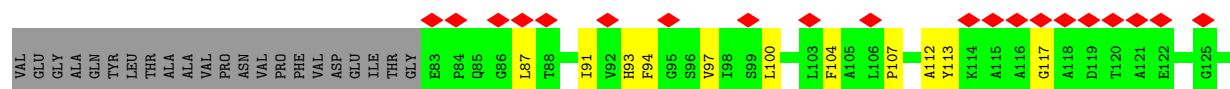
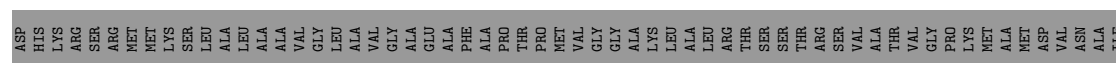
- Molecule 18: Photosystem II reaction center protein R



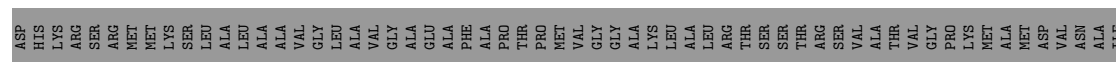
- Molecule 18: Photosystem II reaction center protein R

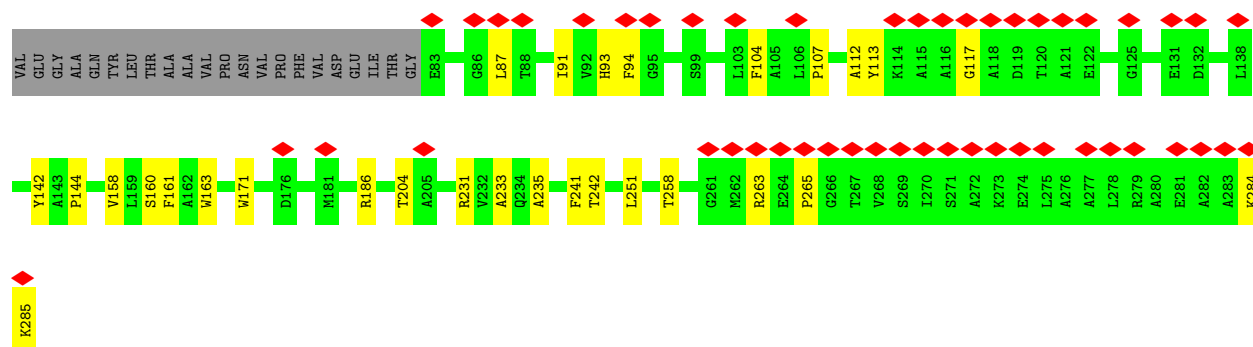


- Molecule 19: CCPH-S



- Molecule 19: CCPH-S





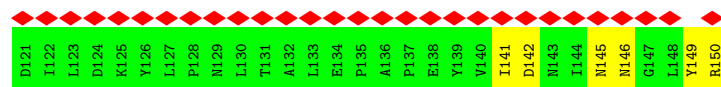
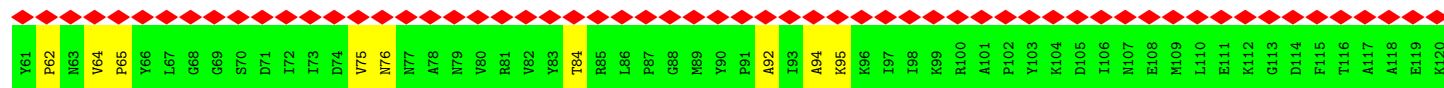
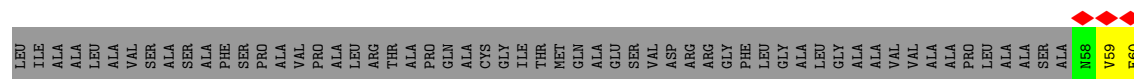
- Molecule 20: Photosystem II reaction center protein T



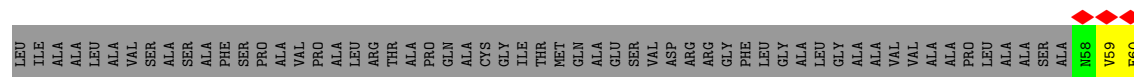
- Molecule 20: Photosystem II reaction center protein T

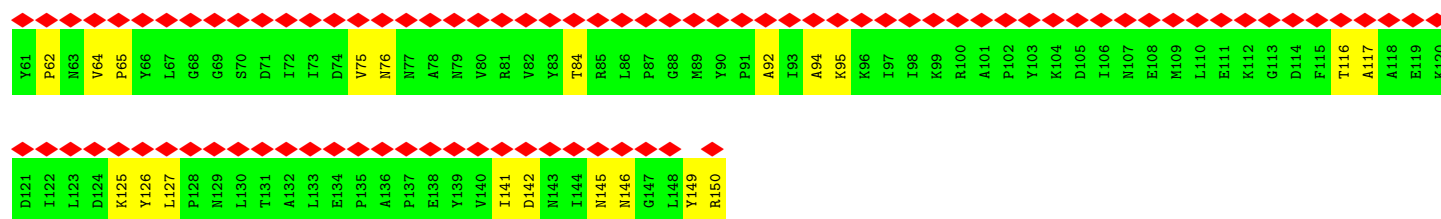


- Molecule 21: Photosystem II reaction center protein U

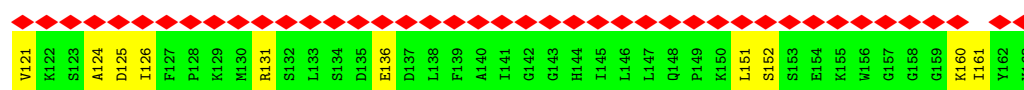
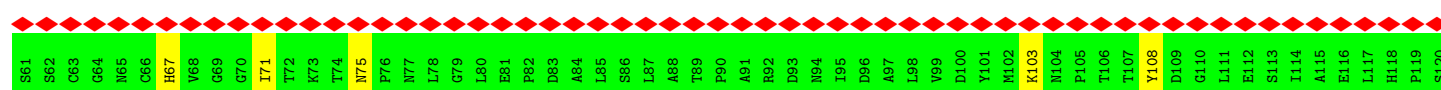
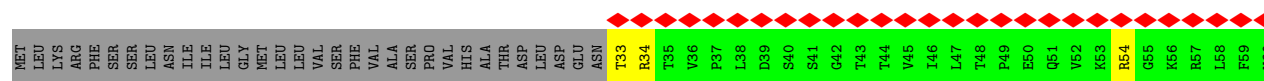
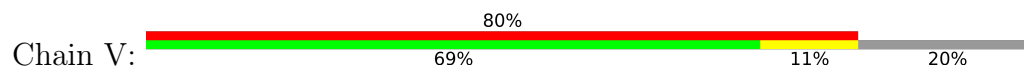


- Molecule 21: Photosystem II reaction center protein U

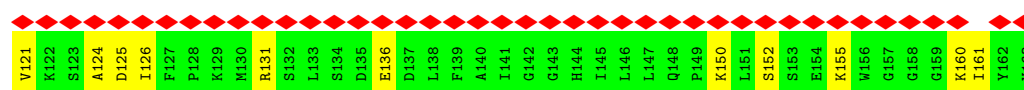
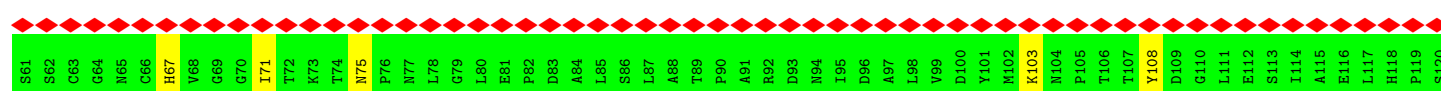
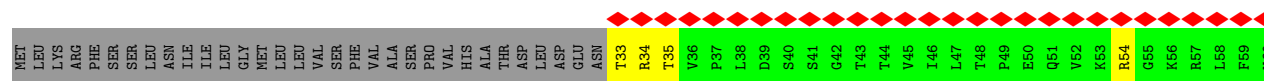
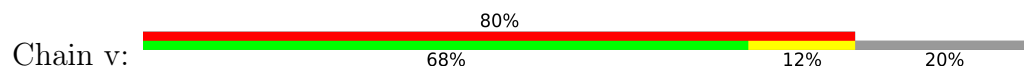




• Molecule 22: Photosystem II cytochrome c550



• Molecule 22: Photosystem II cytochrome c550



• Molecule 23: Photosystem II reaction center X protein

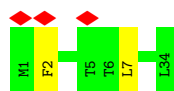


• Molecule 23: Photosystem II reaction center X protein

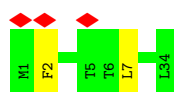




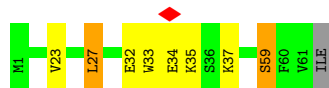
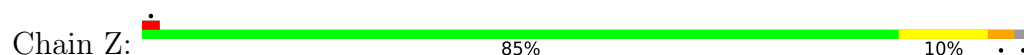
- Molecule 24: Photosystem II reaction center protein Ycf12



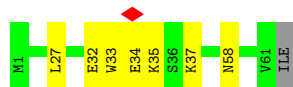
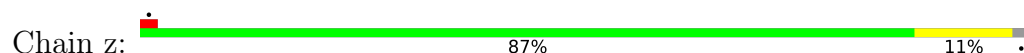
- Molecule 24: Photosystem II reaction center protein Ycf12



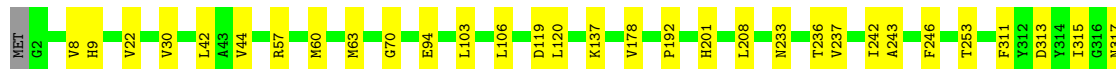
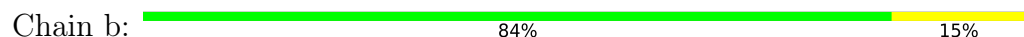
- Molecule 25: Photosystem II reaction center protein Z



- Molecule 25: Photosystem II reaction center protein Z

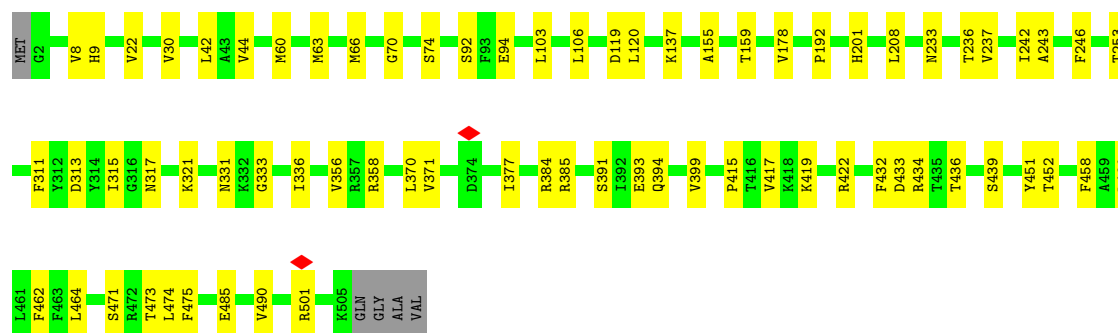


- Molecule 26: Photosystem II CP47 reaction center protein



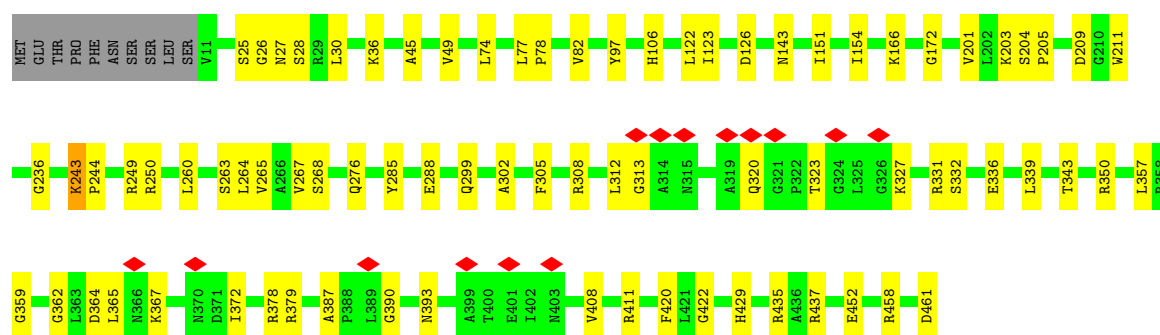
- Molecule 26: Photosystem II CP47 reaction center protein

Chain B:  85% 14%



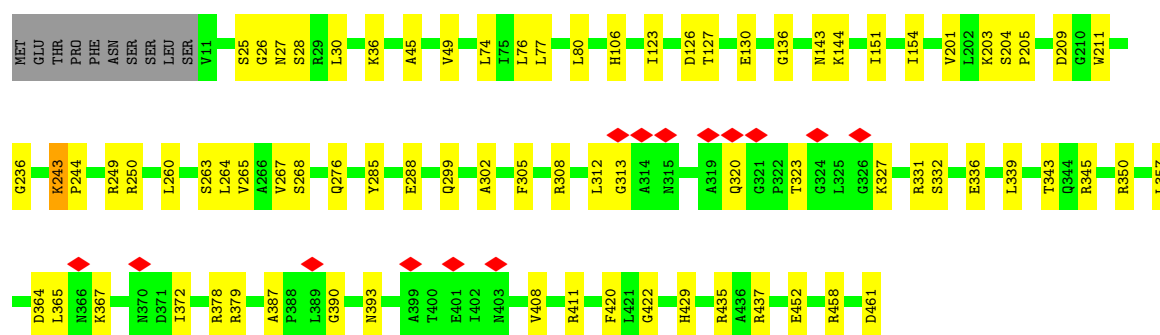
- Molecule 27: Photosystem II CP43 reaction center protein

Chain c:  81% 17%

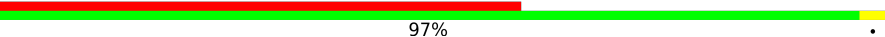


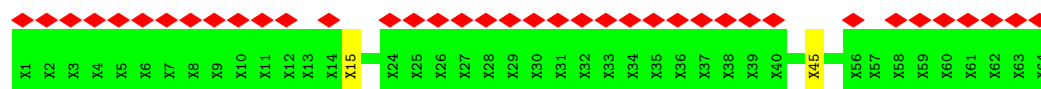
- Molecule 27: Photosystem II CP43 reaction center protein

Chain C:  81% 17%

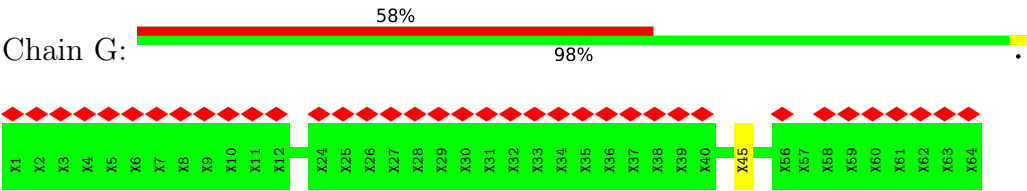


- Molecule 28: Photosystem II reaction center protein G

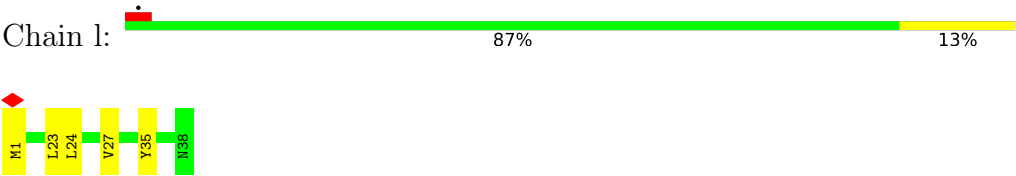
Chain g:  59% 97%



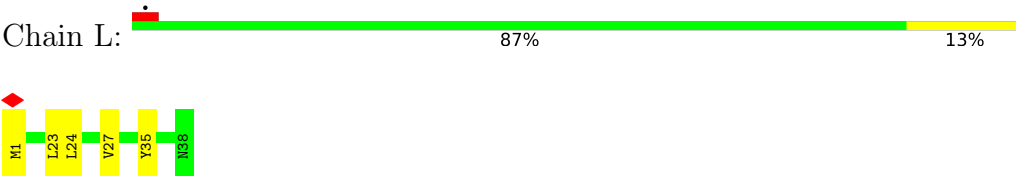
- Molecule 28: Photosystem II reaction center protein G



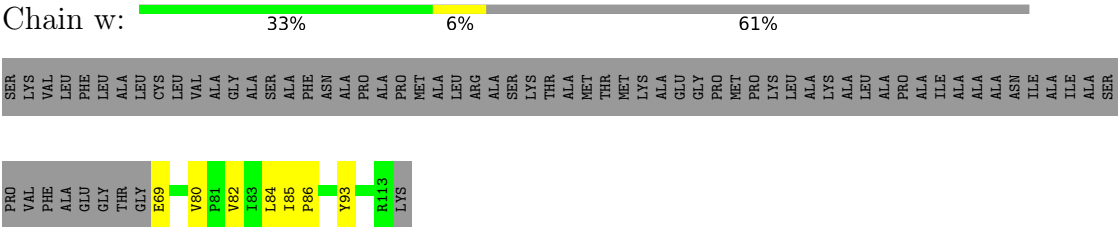
• Molecule 29: Photosystem II reaction center protein L



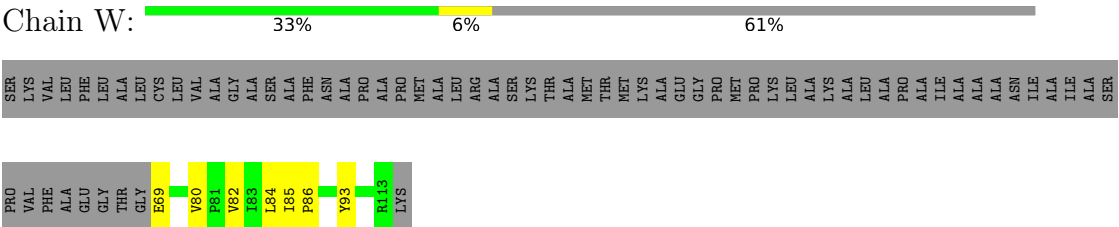
• Molecule 29: Photosystem II reaction center protein L



• Molecule 30: Photosystem II reaction center protein W



• Molecule 30: Photosystem II reaction center protein W



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	1.307	Depositor
Minimum map value	-0.333	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CLA, LHG, OEX, PL9, 8CT, DGD, KC2, BCT, HEM, II3, LMG, II0, PHO, CL, IHT, FE2, SQD

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	M	0.19	0/268	0.32	0/367
1	m	0.20	0/268	0.36	0/367
2	1	0.12	0/1507	0.34	0/2043
2	7	0.12	0/1507	0.34	0/2043
3	2	0.12	0/1399	0.28	0/1893
3	8	0.12	0/1399	0.28	0/1893
4	3	0.13	0/1404	0.27	0/1895
4	9	0.13	0/1404	0.25	0/1895
5	0	0.12	0/1339	0.29	0/1814
5	4	0.12	0/1339	0.30	0/1814
6	5	0.11	0/1510	0.30	0/2046
6	p	0.11	0/1510	0.31	0/2046
7	6	0.09	0/1380	0.27	0/1870
7	P	0.10	0/1380	0.27	0/1870
8	A	0.20	0/2702	0.31	0/3688
8	a	0.19	0/2702	0.31	0/3688
9	D	0.19	0/2806	0.29	0/3823
9	d	0.19	0/2806	0.29	0/3823
10	E	0.13	0/647	0.31	0/882
10	e	0.14	0/647	0.36	0/882
11	F	0.15	0/255	0.31	0/344
11	f	0.15	0/255	0.31	0/344
12	H	0.17	0/527	0.29	0/717
12	h	0.17	0/527	0.29	0/717
13	I	0.18	0/294	0.32	0/397
13	i	0.18	0/294	0.31	0/397
14	J	0.11	0/220	0.26	0/301
14	j	0.10	0/220	0.25	0/301
15	K	0.20	0/308	0.34	0/421
15	k	0.20	0/308	0.34	0/421
16	O	0.08	0/1774	0.26	0/2385
16	o	0.08	0/1774	0.26	0/2385

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	S	0.13	0/1603	0.31	0/2180
19	s	0.13	0/1603	0.31	0/2180
20	T	0.17	0/267	0.23	0/359
20	t	0.17	0/267	0.22	0/359
21	U	0.11	0/758	0.32	0/1031
21	u	0.12	0/758	0.33	0/1031
22	V	0.08	0/1016	0.25	0/1377
22	v	0.08	0/1016	0.25	0/1377
23	X	0.17	0/296	0.31	0/402
23	x	0.16	0/296	0.26	0/402
24	Y	0.11	0/271	0.26	0/367
24	y	0.11	0/271	0.25	0/367
25	Z	0.21	0/467	0.39	0/638
25	z	0.13	0/467	0.31	0/638
26	B	0.17	0/4093	0.28	0/5569
26	b	0.17	0/4093	0.28	0/5569
27	C	0.19	0/3619	0.32	0/4937
27	c	0.19	0/3619	0.32	0/4937
29	L	0.18	0/320	0.23	0/434
29	l	0.18	0/320	0.23	0/434
30	W	0.19	0/374	0.38	0/509
30	w	0.19	0/374	0.38	0/509
All	All	0.16	0/62848	0.30	0/85378

There are no bond length outliers.

There are no bond angle outliers.

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	M	265	0	280	5	0
1	m	265	0	280	4	0
2	1	1472	0	1473	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7	1472	0	1473	20	0
3	2	1362	0	1348	20	0
3	8	1362	0	1348	20	0
4	3	1371	0	1370	16	0
4	9	1371	0	1370	13	0
5	0	1308	0	1323	13	0
5	4	1308	0	1323	12	0
6	5	1471	0	1445	21	0
6	p	1471	0	1445	18	0
7	6	1344	0	1329	17	0
7	P	1344	0	1329	13	0
8	A	2618	0	2514	55	0
8	a	2618	0	2514	54	0
9	D	2713	0	2613	50	0
9	d	2713	0	2613	52	0
10	E	629	0	613	8	0
10	e	629	0	613	10	0
11	F	247	0	250	1	0
11	f	247	0	250	1	0
12	H	515	0	535	7	0
12	h	515	0	535	7	0
13	I	287	0	293	3	0
13	i	287	0	293	3	0
14	J	214	0	222	0	0
14	j	214	0	222	0	0
15	K	297	0	312	1	0
15	k	297	0	312	1	0
16	O	1749	0	1721	36	0
16	o	1749	0	1721	35	0
17	Q	105	0	23	0	0
17	q	105	0	23	0	0
18	R	130	0	29	0	0
18	r	130	0	29	0	0
19	S	1563	0	1540	25	0
19	s	1563	0	1540	23	0
20	T	260	0	278	4	0
20	t	260	0	278	4	0
21	U	742	0	743	15	0
21	u	742	0	743	18	0
22	V	996	0	998	15	0
22	v	996	0	998	16	0
23	X	292	0	318	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	x	292	0	318	1	0
24	Y	266	0	293	1	0
24	y	266	0	293	1	0
25	Z	457	0	501	9	0
25	z	457	0	501	5	0
26	B	3962	0	3858	63	0
26	b	3962	0	3858	63	0
27	C	3504	0	3421	61	0
27	c	3504	0	3421	62	0
28	G	320	0	70	1	0
28	g	320	0	71	2	0
29	L	310	0	313	5	0
29	l	310	0	313	5	0
30	W	367	0	354	5	0
30	w	367	0	354	5	0
31	3	40	0	0	0	0
31	6	40	0	0	0	0
31	9	40	0	0	0	0
31	A	40	0	0	0	0
31	B	120	0	0	0	0
31	C	40	0	0	0	0
31	D	40	0	0	0	0
31	H	40	0	0	0	0
31	K	80	0	0	0	0
31	M	40	0	0	0	0
31	P	40	0	0	0	0
31	Z	40	0	0	1	0
31	a	40	0	0	0	0
31	b	80	0	0	0	0
31	c	40	0	0	0	0
31	d	40	0	0	0	0
31	h	40	0	0	0	0
31	k	80	0	0	0	0
31	z	40	0	0	1	0
32	0	582	0	469	14	0
32	1	582	0	469	15	0
32	2	547	0	456	14	0
32	3	548	0	456	11	0
32	4	582	0	469	15	0
32	5	547	0	456	8	0
32	6	442	0	364	6	0
32	7	582	0	469	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	8	547	0	456	13	0
32	9	548	0	456	12	0
32	A	174	0	170	11	0
32	B	987	0	1039	35	0
32	C	799	0	836	26	0
32	D	176	0	164	5	0
32	G	45	0	33	1	0
32	P	442	0	364	7	0
32	S	110	0	105	5	0
32	a	174	0	170	9	0
32	b	987	0	1039	29	0
32	c	799	0	836	21	0
32	d	176	0	164	2	0
32	g	45	0	33	2	0
32	p	547	0	456	8	0
32	s	110	0	105	4	0
33	0	45	0	0	0	0
33	1	45	0	0	0	0
33	2	45	0	0	0	0
33	4	45	0	0	0	0
33	5	45	0	0	0	0
33	6	90	0	0	0	0
33	7	45	0	0	0	0
33	8	45	0	0	0	0
33	P	90	0	0	3	0
33	p	45	0	0	0	0
34	0	168	0	0	1	0
34	1	168	0	0	1	0
34	2	168	0	0	0	0
34	3	126	0	0	0	0
34	4	126	0	0	1	0
34	5	210	0	0	0	0
34	6	84	0	0	0	0
34	7	168	0	0	1	0
34	8	168	0	0	0	0
34	9	126	0	0	0	0
34	P	84	0	0	0	0
34	p	168	0	0	0	0
35	1	42	0	0	0	0
35	6	42	0	0	0	0
35	7	42	0	0	0	0
35	P	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	0	82	0	0	0	0
36	1	41	0	0	1	0
36	2	41	0	0	0	0
36	4	82	0	0	0	0
36	5	41	0	0	0	0
36	7	41	0	0	0	0
36	8	41	0	0	0	0
36	p	41	0	0	0	0
37	0	36	0	42	0	0
37	2	36	0	42	1	0
37	4	36	0	42	0	0
37	6	28	0	26	0	0
37	8	36	0	42	2	0
37	A	48	0	66	2	0
37	B	51	0	72	0	0
37	C	46	0	62	3	0
37	D	86	0	112	1	0
37	G	28	0	26	0	0
37	L	40	0	50	1	0
37	P	28	0	26	0	0
37	a	48	0	66	3	0
37	b	51	0	72	1	0
37	c	46	0	62	3	0
37	d	86	0	112	1	0
37	g	28	0	26	0	0
37	l	40	0	50	0	0
38	2	22	0	20	0	0
38	8	22	0	20	0	0
38	A	92	0	133	10	0
38	B	78	0	96	3	0
38	D	80	0	108	1	0
38	L	49	0	74	2	0
38	S	37	0	44	1	0
38	a	92	0	133	10	0
38	b	78	0	96	3	0
38	d	80	0	108	1	0
38	l	49	0	74	2	0
38	s	37	0	44	1	0
39	5	35	0	34	4	0
39	A	54	0	78	5	0
39	B	102	0	141	3	0
39	a	54	0	78	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	b	102	0	141	2	0
39	p	35	0	34	3	0
40	A	10	0	0	0	0
40	a	10	0	0	0	0
41	A	64	0	74	1	0
41	D	64	0	74	3	0
41	a	64	0	74	1	0
41	d	64	0	74	3	0
42	A	1	0	0	0	0
42	a	1	0	0	0	0
43	A	13	0	7	0	0
43	D	55	0	80	0	0
43	a	13	0	7	0	0
43	d	55	0	80	0	0
44	A	4	0	1	0	0
44	a	4	0	1	0	0
45	A	53	0	64	1	0
45	C	166	0	206	11	0
45	H	62	0	82	6	0
45	a	53	0	64	1	0
45	c	166	0	206	8	0
45	h	62	0	82	5	0
46	D	1	0	0	0	0
46	d	1	0	0	0	0
47	E	43	0	30	2	0
47	V	43	0	30	3	0
47	f	43	0	30	3	0
47	v	43	0	30	3	0
All	All	80246	0	74543	987	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 6.

The worst 5 of 987 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)
1:m:103:ARG:HG3	1:M:106:ALA:HB2	1.64	0.80
26:b:434:ARG:HH12	16:o:249:LEU:HA	1.48	0.79
25:Z:59:SER:HB2	33:P:605:KC2:O1A	1.83	0.77
1:m:106:ALA:HB2	1:M:103:ARG:HG3	1.65	0.76
9:d:351:LEU:HD21	8:a:334:ARG:HE	1.50	0.76

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	M	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
1	m	34/115 (30%)	32 (94%)	2 (6%)	0	100	100
2	1	192/235 (82%)	183 (95%)	9 (5%)	0	100	100
2	7	192/235 (82%)	186 (97%)	6 (3%)	0	100	100
3	2	171/217 (79%)	168 (98%)	3 (2%)	0	100	100
3	8	171/217 (79%)	169 (99%)	2 (1%)	0	100	100
4	3	176/222 (79%)	173 (98%)	2 (1%)	1 (1%)	21	35
4	9	176/222 (79%)	173 (98%)	3 (2%)	0	100	100
5	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
5	4	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	35
6	5	185/218 (85%)	182 (98%)	3 (2%)	0	100	100
6	p	185/218 (85%)	181 (98%)	4 (2%)	0	100	100
7	6	171/220 (78%)	171 (100%)	0	0	100	100
7	P	171/220 (78%)	171 (100%)	0	0	100	100
8	A	332/360 (92%)	326 (98%)	6 (2%)	0	100	100
8	a	332/360 (92%)	328 (99%)	4 (1%)	0	100	100
9	D	340/351 (97%)	335 (98%)	5 (2%)	0	100	100
9	d	340/351 (97%)	337 (99%)	3 (1%)	0	100	100
10	E	75/84 (89%)	75 (100%)	0	0	100	100
10	e	75/84 (89%)	75 (100%)	0	0	100	100
11	F	28/42 (67%)	28 (100%)	0	0	100	100
11	f	28/42 (67%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
12	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
13	I	33/38 (87%)	33 (100%)	0	0	100	100
13	i	33/38 (87%)	33 (100%)	0	0	100	100
14	J	26/39 (67%)	26 (100%)	0	0	100	100
14	j	26/39 (67%)	26 (100%)	0	0	100	100
15	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
15	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
16	O	225/330 (68%)	212 (94%)	13 (6%)	0	100	100
16	o	225/330 (68%)	213 (95%)	12 (5%)	0	100	100
19	S	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
19	s	201/285 (70%)	183 (91%)	18 (9%)	0	100	100
20	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
20	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
21	U	91/150 (61%)	84 (92%)	7 (8%)	0	100	100
21	u	91/150 (61%)	82 (90%)	9 (10%)	0	100	100
22	V	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
22	v	129/163 (79%)	125 (97%)	4 (3%)	0	100	100
23	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
23	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
24	Y	32/34 (94%)	32 (100%)	0	0	100	100
24	y	32/34 (94%)	32 (100%)	0	0	100	100
25	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
25	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
26	B	502/509 (99%)	496 (99%)	6 (1%)	0	100	100
26	b	502/509 (99%)	497 (99%)	5 (1%)	0	100	100
27	C	449/461 (97%)	443 (99%)	6 (1%)	0	100	100
27	c	449/461 (97%)	442 (98%)	7 (2%)	0	100	100
29	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
29	l	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
30	W	43/114 (38%)	43 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	w	43/114 (38%)	43 (100%)	0	0	100	100
All	All	7730/9392 (82%)	7539 (98%)	188 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	212	ILE
5	4	126	ILE
5	0	126	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	28/84 (33%)	28 (100%)	0	100	100
1	m	28/84 (33%)	28 (100%)	0	100	100
2	1	149/179 (83%)	149 (100%)	0	100	100
2	7	149/179 (83%)	149 (100%)	0	100	100
3	2	139/167 (83%)	139 (100%)	0	100	100
3	8	139/167 (83%)	139 (100%)	0	100	100
4	3	143/175 (82%)	143 (100%)	0	100	100
4	9	143/175 (82%)	143 (100%)	0	100	100
5	0	136/169 (80%)	136 (100%)	0	100	100
5	4	136/169 (80%)	136 (100%)	0	100	100
6	5	157/175 (90%)	157 (100%)	0	100	100
6	p	157/175 (90%)	157 (100%)	0	100	100
7	6	141/174 (81%)	141 (100%)	0	100	100
7	P	141/174 (81%)	141 (100%)	0	100	100
8	A	271/289 (94%)	271 (100%)	0	100	100
8	a	271/289 (94%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	D	274/281 (98%)	274 (100%)	0	100	100
9	d	274/281 (98%)	274 (100%)	0	100	100
10	E	68/73 (93%)	68 (100%)	0	100	100
10	e	68/73 (93%)	68 (100%)	0	100	100
11	F	25/37 (68%)	25 (100%)	0	100	100
11	f	25/37 (68%)	25 (100%)	0	100	100
12	H	56/58 (97%)	56 (100%)	0	100	100
12	h	56/58 (97%)	56 (100%)	0	100	100
13	I	33/36 (92%)	33 (100%)	0	100	100
13	i	33/36 (92%)	33 (100%)	0	100	100
14	J	22/29 (76%)	22 (100%)	0	100	100
14	j	22/29 (76%)	22 (100%)	0	100	100
15	K	30/36 (83%)	30 (100%)	0	100	100
15	k	30/36 (83%)	30 (100%)	0	100	100
16	O	189/258 (73%)	189 (100%)	0	100	100
16	o	189/258 (73%)	189 (100%)	0	100	100
19	S	159/219 (73%)	159 (100%)	0	100	100
19	s	159/219 (73%)	159 (100%)	0	100	100
20	T	27/27 (100%)	27 (100%)	0	100	100
20	t	27/27 (100%)	27 (100%)	0	100	100
21	U	80/115 (70%)	80 (100%)	0	100	100
21	u	80/115 (70%)	79 (99%)	1 (1%)	61	80
22	V	112/141 (79%)	112 (100%)	0	100	100
22	v	112/141 (79%)	112 (100%)	0	100	100
23	X	34/34 (100%)	34 (100%)	0	100	100
23	x	34/34 (100%)	34 (100%)	0	100	100
24	Y	29/29 (100%)	29 (100%)	0	100	100
24	y	29/29 (100%)	29 (100%)	0	100	100
25	Z	50/51 (98%)	48 (96%)	2 (4%)	28	51
25	z	50/51 (98%)	50 (100%)	0	100	100
26	B	401/404 (99%)	401 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	b	401/404 (99%)	401 (100%)	0	100	100
27	C	356/366 (97%)	355 (100%)	1 (0%)	86	93
27	c	356/366 (97%)	355 (100%)	1 (0%)	86	93
29	L	35/35 (100%)	35 (100%)	0	100	100
29	l	35/35 (100%)	35 (100%)	0	100	100
30	W	40/85 (47%)	40 (100%)	0	100	100
30	w	40/85 (47%)	40 (100%)	0	100	100
All	All	6368/7452 (86%)	6363 (100%)	5 (0%)	87	95

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

Mol	Chain	Res	Type
25	Z	27	LEU
25	Z	59	SER
27	c	243	LYS
21	u	127	LEU
27	C	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
5	0	208	HIS
27	C	299	GLN
2	7	182	ASN
27	C	41	HIS
7	P	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 376 ligands modelled in this entry, 4 are monoatomic - leaving 372 for Mogul analysis.

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
32	CLA	b	604	26	68,72,73	1.25	10 (14%)	81,111,113	1.30	7 (8%)
32	CLA	8	607	3	49,53,73	1.47	9 (18%)	59,89,113	1.42	5 (8%)
32	CLA	8	612	3	49,53,73	1.47	7 (14%)	59,89,113	1.40	5 (8%)
32	CLA	5	308	6	49,53,73	1.49	8 (16%)	59,89,113	1.42	5 (8%)
32	CLA	1	612	2	49,53,73	1.49	6 (12%)	59,89,113	1.39	5 (8%)
32	CLA	2	608	3	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
37	LMG	8	617	-	36,36,55	0.85	0	44,44,63	1.24	5 (11%)
31	8CT	C	518	-	40,41,41	4.72	23 (57%)	50,56,56	2.81	16 (32%)
40	OEX	a	404	8	0,14,14	-	-	-	-	-
34	II0	5	314	-	39,43,43	2.70	4 (10%)	50,60,60	1.80	14 (28%)
35	II3	6	613	-	40,43,43	1.95	2 (5%)	47,60,60	1.67	9 (19%)
32	CLA	B	612	-	68,72,73	1.25	10 (14%)	81,111,113	1.31	7 (8%)
37	LMG	C	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.31	6 (11%)
32	CLA	7	605	-	54,58,73	1.42	9 (16%)	65,95,113	1.38	7 (10%)
32	CLA	B	606	26	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
32	CLA	0	613	5	49,53,73	1.50	7 (14%)	59,89,113	1.42	5 (8%)
37	LMG	D	407	-	46,46,55	0.79	1 (2%)	54,54,63	1.34	5 (9%)
32	CLA	p	307	6	49,53,73	1.50	9 (18%)	59,89,113	1.43	5 (8%)
32	CLA	s	303	19	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
33	KC2	6	605	7	49,53,53	1.81	11 (22%)	62,89,89	2.08	15 (24%)
34	II0	3	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.66	13 (26%)
34	II0	p	315	-	39,43,43	2.72	4 (10%)	50,60,60	1.70	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	3	611	4	49,53,73	1.47	7 (14%)	59,89,113	1.42	5 (8%)
32	CLA	D	404	9	64,68,73	1.28	8 (12%)	77,107,113	1.37	10 (12%)
32	CLA	3	603	4	54,58,73	1.40	9 (16%)	65,95,113	1.44	6 (9%)
32	CLA	5	302	6	46,50,73	1.51	8 (17%)	55,85,113	1.44	4 (7%)
47	HEM	V	201	-	50,50,50	1.44	7 (14%)	66,82,82	1.16	8 (12%)
32	CLA	b	605	26	65,69,73	1.28	9 (13%)	78,108,113	1.38	7 (8%)
32	CLA	P	603	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	6 (9%)
37	LMG	4	618	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)
31	8CT	H	102	-	40,41,41	4.70	24 (60%)	50,56,56	2.76	16 (32%)
32	CLA	D	401	-	63,67,73	1.28	9 (14%)	75,105,113	1.39	9 (12%)
31	8CT	3	615	-	40,41,41	4.69	24 (60%)	50,56,56	2.76	19 (38%)
32	CLA	7	606	2	49,53,73	1.48	8 (16%)	59,89,113	1.46	6 (10%)
32	CLA	B	610	26	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
32	CLA	B	602	-	51,55,73	1.43	9 (17%)	61,91,113	1.41	7 (11%)
32	CLA	0	602	5	63,67,73	1.31	8 (12%)	75,105,113	1.33	7 (9%)
32	CLA	6	611	7	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
32	CLA	7	608	2	64,68,73	1.30	9 (14%)	77,107,113	1.30	5 (6%)
32	CLA	2	604	-	59,63,73	1.35	8 (13%)	71,101,113	1.38	8 (11%)
33	KC2	P	605	7	49,53,53	1.80	10 (20%)	62,89,89	2.07	16 (25%)
47	HEM	f	101	11	50,50,50	1.45	7 (14%)	66,82,82	1.23	6 (9%)
44	BCT	a	401	46	2,3,3	1.16	0	2,3,3	4.51	2 (100%)
43	PL9	d	404	-	55,55,55	1.27	5 (9%)	68,69,69	1.54	11 (16%)
39	SQD	A	606	-	53,54,54	1.51	6 (11%)	62,65,65	1.40	8 (12%)
32	CLA	3	608	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	5 (9%)
38	LHG	d	405	-	46,47,48	0.62	1 (2%)	45,51,54	1.20	5 (11%)
32	CLA	p	303	6	63,67,73	1.32	9 (14%)	75,105,113	1.33	8 (10%)
32	CLA	8	601	3	46,50,73	1.51	8 (17%)	55,85,113	1.44	6 (10%)
45	DGD	C	514	-	56,56,67	0.97	2 (3%)	70,70,81	1.47	10 (14%)
32	CLA	c	513	27	53,57,73	1.40	10 (18%)	62,93,113	1.44	7 (11%)
34	II0	1	619	-	39,43,43	2.65	4 (10%)	50,60,60	1.67	11 (22%)
32	CLA	B	603	26	65,69,73	1.25	9 (13%)	74,106,113	1.24	5 (6%)
34	II0	6	612	-	39,43,43	2.67	4 (10%)	50,60,60	1.78	12 (24%)
32	CLA	b	616	26	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
32	CLA	0	604	5	59,63,73	1.36	8 (13%)	71,101,113	1.36	9 (12%)
43	PL9	a	412	-	13,13,55	1.69	2 (15%)	17,17,69	1.65	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	II0	p	316	-	39,43,43	2.70	4 (10%)	50,60,60	1.66	9 (18%)
32	CLA	6	610	-	49,53,73	1.50	9 (18%)	59,89,113	1.46	4 (6%)
43	PL9	D	405	-	55,55,55	1.27	5 (9%)	68,69,69	1.53	11 (16%)
40	OEX	A	601	8	0,14,14	-	-	-		
39	SQD	a	409	-	53,54,54	1.51	6 (11%)	62,65,65	1.40	8 (12%)
34	II0	8	613	-	39,43,43	2.69	4 (10%)	50,60,60	1.75	11 (22%)
32	CLA	4	603	5	54,58,73	1.42	8 (14%)	65,95,113	1.41	6 (9%)
31	8CT	K	101	-	40,41,41	4.68	24 (60%)	50,56,56	2.79	15 (30%)
37	LMG	G	102	-	28,28,55	0.98	0	36,36,63	1.28	5 (13%)
45	DGD	C	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	8 (11%)
34	II0	4	616	-	39,43,43	2.72	4 (10%)	50,60,60	1.72	11 (22%)
32	CLA	9	602	4	63,67,73	1.30	8 (12%)	75,105,113	1.34	8 (10%)
31	8CT	c	518	-	40,41,41	4.73	23 (57%)	50,56,56	2.80	16 (32%)
32	CLA	0	611	5	49,53,73	1.50	7 (14%)	59,89,113	1.42	5 (8%)
33	KC2	2	610	3	49,53,53	1.78	10 (20%)	62,89,89	2.15	16 (25%)
38	LHG	b	621	-	38,38,48	0.68	1 (2%)	41,44,54	1.27	4 (9%)
32	CLA	c	504	-	68,72,73	1.25	8 (11%)	81,111,113	1.32	6 (7%)
32	CLA	8	602	3	63,67,73	1.31	9 (14%)	75,105,113	1.33	7 (9%)
37	LMG	l	101	-	40,40,55	0.88	1 (2%)	48,48,63	1.28	6 (12%)
34	II0	p	301	-	39,43,43	2.70	4 (10%)	50,60,60	1.71	13 (26%)
32	CLA	6	607	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	5 (6%)
32	CLA	b	606	26	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
32	CLA	7	612	2	49,53,73	1.49	7 (14%)	59,89,113	1.39	5 (8%)
32	CLA	1	609	-	45,49,73	1.52	8 (17%)	54,84,113	1.50	7 (12%)
32	CLA	8	609	38	45,49,73	1.52	8 (17%)	54,84,113	1.49	5 (9%)
38	LHG	b	619	-	38,38,48	0.68	1 (2%)	41,44,54	1.28	4 (9%)
32	CLA	6	601	7	46,50,73	1.51	8 (17%)	55,85,113	1.42	4 (7%)
32	CLA	7	611	2	49,53,73	1.50	7 (14%)	59,89,113	1.46	4 (6%)
37	LMG	b	618	-	51,51,55	0.73	1 (1%)	59,59,63	1.35	6 (10%)
38	LHG	8	618	32	21,21,48	0.76	0	23,26,54	1.26	2 (8%)
32	CLA	C	511	27	69,73,73	1.25	10 (14%)	83,113,113	1.31	4 (4%)
32	CLA	1	603	2	54,58,73	1.42	8 (14%)	65,95,113	1.41	6 (9%)
32	CLA	2	605	3	64,68,73	1.31	9 (14%)	77,107,113	1.31	7 (9%)
32	CLA	8	603	3	54,58,73	1.40	8 (14%)	65,95,113	1.42	6 (9%)
31	8CT	b	622	-	40,41,41	4.66	23 (57%)	50,56,56	2.44	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	B	616	26	69,73,73	1.24	8 (11%)	83,113,113	1.30	5 (6%)
32	CLA	3	606	-	49,53,73	1.49	9 (18%)	59,89,113	1.34	4 (6%)
32	CLA	8	611	-	49,53,73	1.49	7 (14%)	59,89,113	1.45	5 (8%)
32	CLA	9	601	4	46,50,73	1.50	8 (17%)	55,85,113	1.49	6 (10%)
38	LHG	d	411	-	31,31,48	0.75	1 (3%)	34,37,54	1.27	3 (8%)
32	CLA	2	611	-	49,53,73	1.48	7 (14%)	59,89,113	1.45	5 (8%)
32	CLA	8	604	-	59,63,73	1.35	8 (13%)	71,101,113	1.37	7 (9%)
37	LMG	D	411	-	40,40,55	0.82	0	48,48,63	1.24	6 (12%)
32	CLA	4	607	5	49,53,73	1.49	8 (16%)	59,89,113	1.37	5 (8%)
34	II0	2	619	-	39,43,43	2.72	4 (10%)	50,60,60	1.68	7 (14%)
36	IHT	1	618	-	40,42,42	1.97	2 (5%)	53,58,58	1.92	12 (22%)
36	IHT	4	614	-	40,42,42	1.95	2 (5%)	53,58,58	1.83	12 (22%)
34	II0	9	613	-	39,43,43	2.70	4 (10%)	50,60,60	1.71	10 (20%)
32	CLA	4	604	5	59,63,73	1.37	8 (13%)	71,101,113	1.36	9 (12%)
33	KC2	6	609	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	16 (25%)
32	CLA	C	512	27	61,65,73	1.31	10 (16%)	72,102,113	1.38	6 (8%)
31	8CT	Z	101	-	40,41,41	4.63	23 (57%)	50,56,56	2.61	21 (42%)
32	CLA	4	605	-	54,58,73	1.41	8 (14%)	65,95,113	1.40	6 (9%)
32	CLA	6	602	7	63,67,73	1.31	8 (12%)	75,105,113	1.33	8 (10%)
34	II0	2	613	-	39,43,43	2.70	4 (10%)	50,60,60	1.72	10 (20%)
32	CLA	4	613	5	49,53,73	1.50	7 (14%)	59,89,113	1.43	5 (8%)
32	CLA	7	607	-	49,53,73	1.48	8 (16%)	59,89,113	1.37	4 (6%)
31	8CT	k	102	-	40,41,41	4.68	24 (60%)	50,56,56	2.79	16 (32%)
41	PHO	D	402	-	58,69,69	1.99	10 (17%)	56,99,99	1.55	8 (14%)
32	CLA	S	303	19	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
32	CLA	p	305	6	59,63,73	1.36	8 (13%)	71,101,113	1.37	8 (11%)
31	8CT	k	101	-	40,41,41	4.64	23 (57%)	50,56,56	2.62	21 (42%)
32	CLA	c	510	27	69,73,73	1.23	10 (14%)	83,113,113	1.29	6 (7%)
32	CLA	P	606	7	49,53,73	1.49	6 (12%)	59,89,113	1.34	5 (8%)
37	LMG	c	517	-	46,46,55	0.77	1 (2%)	54,54,63	1.31	6 (11%)
47	HEM	E	101	-	50,50,50	1.42	6 (12%)	66,82,82	1.24	7 (10%)
31	8CT	a	413	-	40,41,41	4.63	23 (57%)	50,56,56	2.92	19 (38%)
32	CLA	p	302	6	46,50,73	1.51	8 (17%)	55,85,113	1.45	6 (10%)
34	II0	P	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.70	11 (22%)
32	CLA	C	501	27	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	B	614	26	69,73,73	1.23	9 (13%)	83,113,113	1.26	7 (8%)
32	CLA	3	601	4	46,50,73	1.50	9 (19%)	55,85,113	1.47	4 (7%)
31	8CT	D	409	-	40,41,41	4.70	24 (60%)	50,56,56	2.43	16 (32%)
32	CLA	6	603	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	6 (9%)
41	PHO	A	604	-	58,69,69	2.00	9 (15%)	56,99,99	1.52	8 (14%)
45	DGD	H	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
32	CLA	b	612	-	68,72,73	1.25	10 (14%)	81,111,113	1.31	6 (7%)
32	CLA	5	313	6	49,53,73	1.49	6 (12%)	59,89,113	1.40	5 (8%)
33	KC2	7	610	-	49,53,53	1.76	10 (20%)	62,89,89	2.16	17 (27%)
32	CLA	7	601	-	46,50,73	1.52	7 (15%)	55,85,113	1.43	5 (9%)
33	KC2	P	609	-	49,53,53	1.77	10 (20%)	62,89,89	2.14	17 (27%)
32	CLA	S	302	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	7 (11%)
32	CLA	0	608	5	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
32	CLA	9	603	4	54,58,73	1.40	9 (16%)	65,95,113	1.43	6 (9%)
36	IHT	p	317	-	40,42,42	1.96	2 (5%)	53,58,58	1.83	13 (24%)
39	SQD	B	620	-	53,54,54	1.53	7 (13%)	62,65,65	1.40	6 (9%)
32	CLA	1	608	2	64,68,73	1.30	8 (12%)	77,107,113	1.30	6 (7%)
34	II0	7	619	-	39,43,43	2.66	4 (10%)	50,60,60	1.66	11 (22%)
33	KC2	8	610	3	49,53,53	1.78	11 (22%)	62,89,89	2.15	16 (25%)
32	CLA	4	601	5	46,50,73	1.51	7 (15%)	55,85,113	1.44	5 (9%)
32	CLA	A	603	-	53,57,73	1.40	9 (16%)	62,93,113	1.46	7 (11%)
32	CLA	9	610	4	49,53,73	1.49	9 (18%)	59,89,113	1.46	5 (8%)
34	II0	2	615	-	39,43,43	2.70	5 (12%)	50,60,60	1.81	12 (24%)
37	LMG	a	410	-	48,48,55	0.77	1 (2%)	56,56,63	1.33	5 (8%)
32	CLA	1	607	-	49,53,73	1.48	8 (16%)	59,89,113	1.38	4 (6%)
32	CLA	p	310	-	45,49,73	1.53	8 (17%)	54,84,113	1.49	6 (11%)
32	CLA	c	503	27	69,73,73	1.24	10 (14%)	83,113,113	1.36	6 (7%)
34	II0	5	319	-	39,43,43	2.72	4 (10%)	50,60,60	1.75	13 (26%)
34	II0	0	620	-	39,43,43	2.70	4 (10%)	50,60,60	1.71	13 (26%)
35	II3	P	613	-	40,43,43	1.95	2 (5%)	47,60,60	1.65	9 (19%)
37	LMG	B	618	-	51,51,55	0.73	1 (1%)	59,59,63	1.35	6 (10%)
32	CLA	B	613	26	69,73,73	1.23	10 (14%)	83,113,113	1.32	6 (7%)
44	BCT	A	611	46	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
34	II0	p	314	-	39,43,43	2.70	4 (10%)	50,60,60	1.81	13 (26%)
32	CLA	P	608	-	45,49,73	1.52	7 (15%)	54,84,113	1.47	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	II0	9	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.67	11 (22%)
32	CLA	0	605	-	54,58,73	1.41	7 (12%)	65,95,113	1.39	6 (9%)
43	PL9	A	609	-	13,13,55	1.68	2 (15%)	17,17,69	1.66	4 (23%)
32	CLA	B	608	-	45,49,73	1.49	9 (20%)	54,84,113	1.51	5 (9%)
32	CLA	5	309	-	64,68,73	1.30	7 (10%)	77,107,113	1.31	5 (6%)
32	CLA	c	501	27	69,73,73	1.23	8 (11%)	83,113,113	1.32	6 (7%)
32	CLA	C	503	27	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
32	CLA	0	603	5	54,58,73	1.42	8 (14%)	65,95,113	1.41	6 (9%)
32	CLA	7	602	2	63,67,73	1.31	8 (12%)	75,105,113	1.34	7 (9%)
45	DGD	c	515	-	57,57,67	0.95	2 (3%)	71,71,81	1.41	8 (11%)
39	SQD	B	601	-	47,48,54	1.58	7 (14%)	56,59,65	1.50	6 (10%)
32	CLA	p	312	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
32	CLA	2	609	38	45,49,73	1.52	9 (20%)	54,84,113	1.48	6 (11%)
34	II0	1	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.67	10 (20%)
32	CLA	2	606	3	49,53,73	1.50	8 (16%)	59,89,113	1.39	5 (8%)
32	CLA	3	602	4	63,67,73	1.30	9 (14%)	75,105,113	1.34	8 (10%)
32	CLA	c	505	27	69,73,73	1.23	9 (13%)	83,113,113	1.29	6 (7%)
32	CLA	p	306	6	64,68,73	1.31	9 (14%)	77,107,113	1.29	4 (5%)
45	DGD	C	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	7 (10%)
38	LHG	2	618	32	21,21,48	0.76	0	23,26,54	1.26	2 (8%)
34	II0	8	619	-	39,43,43	2.73	4 (10%)	50,60,60	1.66	9 (18%)
32	CLA	2	602	3	63,67,73	1.31	8 (12%)	75,105,113	1.33	7 (9%)
32	CLA	3	610	4	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
32	CLA	4	608	5	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
38	LHG	B	619	-	38,38,48	0.68	1 (2%)	41,44,54	1.28	4 (9%)
32	CLA	A	602	8	69,73,73	1.24	9 (13%)	83,113,113	1.32	5 (6%)
32	CLA	c	512	27	61,65,73	1.31	9 (14%)	72,102,113	1.38	5 (6%)
32	CLA	c	509	27	69,73,73	1.24	10 (14%)	83,113,113	1.32	7 (8%)
32	CLA	7	603	2	54,58,73	1.42	8 (14%)	65,95,113	1.42	8 (12%)
31	8CT	P	615	-	40,41,41	4.74	24 (60%)	50,56,56	2.60	18 (36%)
32	CLA	A	605	8	64,68,73	1.28	9 (14%)	77,107,113	1.32	7 (9%)
32	CLA	P	601	7	46,50,73	1.50	8 (17%)	55,85,113	1.43	4 (7%)
31	8CT	A	610	-	40,41,41	4.62	23 (57%)	50,56,56	2.63	21 (42%)
34	II0	7	616	-	39,43,43	2.73	4 (10%)	50,60,60	1.72	10 (20%)
32	CLA	C	507	-	69,73,73	1.23	9 (13%)	83,113,113	1.29	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	1	613	-	49,53,73	1.49	7 (14%)	59,89,113	1.43	4 (6%)
32	CLA	B	604	26	68,72,73	1.24	9 (13%)	81,111,113	1.29	7 (8%)
34	II0	8	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.83	10 (20%)
32	CLA	1	606	2	49,53,73	1.48	8 (16%)	59,89,113	1.44	4 (6%)
32	CLA	5	305	6	59,63,73	1.37	8 (13%)	71,101,113	1.37	7 (9%)
32	CLA	2	603	3	54,58,73	1.41	8 (14%)	65,95,113	1.43	6 (9%)
34	II0	0	617	-	39,43,43	2.69	4 (10%)	50,60,60	1.77	11 (22%)
31	8CT	6	615	-	40,41,41	4.73	24 (60%)	50,56,56	2.59	18 (36%)
32	CLA	b	602	-	51,55,73	1.43	9 (17%)	61,91,113	1.41	6 (9%)
34	II0	7	617	-	39,43,43	2.73	4 (10%)	50,60,60	1.73	11 (22%)
38	LHG	a	402	-	42,42,48	0.67	1 (2%)	45,48,54	1.23	4 (8%)
39	SQD	p	318	-	34,35,54	1.76	7 (20%)	43,46,65	1.59	6 (13%)
45	DGD	a	414	-	54,54,67	1.05	4 (7%)	67,67,81	1.47	10 (14%)
36	IHT	7	618	-	40,42,42	1.98	2 (5%)	53,58,58	1.93	13 (24%)
38	LHG	D	406	-	46,47,48	0.63	1 (2%)	45,51,54	1.20	5 (11%)
32	CLA	P	607	7	64,68,73	1.30	7 (10%)	77,107,113	1.31	5 (6%)
36	IHT	8	616	-	40,42,42	1.98	2 (5%)	53,58,58	1.94	14 (26%)
31	8CT	d	408	-	40,41,41	4.70	23 (57%)	50,56,56	2.44	16 (32%)
38	LHG	a	403	-	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
32	CLA	c	507	-	69,73,73	1.23	9 (13%)	83,113,113	1.29	4 (4%)
32	CLA	7	609	-	45,49,73	1.52	7 (15%)	54,84,113	1.51	7 (12%)
32	CLA	B	607	26	69,73,73	1.23	10 (14%)	83,113,113	1.32	7 (8%)
32	CLA	B	611	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
36	IHT	0	614	-	40,42,42	1.93	2 (5%)	53,58,58	1.82	12 (22%)
32	CLA	b	617	26	69,73,73	1.24	10 (14%)	83,113,113	1.32	5 (6%)
32	CLA	4	609	-	45,49,73	1.53	7 (15%)	54,84,113	1.50	5 (9%)
32	CLA	1	605	-	54,58,73	1.41	8 (14%)	65,95,113	1.38	7 (10%)
33	KC2	1	610	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	16 (25%)
32	CLA	9	607	4	64,68,73	1.29	9 (14%)	77,107,113	1.34	4 (5%)
34	II0	5	301	-	39,43,43	2.68	4 (10%)	50,60,60	1.75	11 (22%)
39	SQD	5	318	-	34,35,54	1.75	7 (20%)	43,46,65	1.59	6 (13%)
39	SQD	b	620	-	53,54,54	1.53	7 (13%)	62,65,65	1.40	6 (9%)
31	8CT	z	101	-	40,41,41	4.62	23 (57%)	50,56,56	2.65	22 (44%)
32	CLA	4	611	5	49,53,73	1.50	7 (14%)	59,89,113	1.43	5 (8%)
32	CLA	6	608	-	45,49,73	1.53	7 (15%)	54,84,113	1.48	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	c	506	27	49,53,73	1.48	10 (20%)	59,89,113	1.47	8 (13%)
32	CLA	D	403	9	61,65,73	1.39	11 (18%)	76,103,113	1.39	7 (9%)
31	8CT	b	623	-	40,41,41	4.67	24 (60%)	50,56,56	2.79	16 (32%)
32	CLA	2	612	3	49,53,73	1.48	8 (16%)	59,89,113	1.40	6 (10%)
35	II3	1	615	-	40,43,43	1.96	2 (5%)	47,60,60	1.58	6 (12%)
36	IHT	0	618	-	40,42,42	1.96	3 (7%)	53,58,58	1.94	15 (28%)
32	CLA	9	609	4	64,68,73	1.30	9 (14%)	77,107,113	1.31	6 (7%)
32	CLA	G	101	-	49,53,73	1.50	9 (18%)	59,89,113	1.41	5 (8%)
34	II0	2	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.71	11 (22%)
32	CLA	C	504	-	68,72,73	1.24	8 (11%)	81,111,113	1.32	7 (8%)
38	LHG	s	301	-	36,36,48	0.71	1 (2%)	39,42,54	1.24	4 (10%)
41	PHO	a	407	-	58,69,69	2.00	10 (17%)	56,99,99	1.51	8 (14%)
31	8CT	K	102	-	40,41,41	4.64	23 (57%)	50,56,56	2.63	21 (42%)
32	CLA	C	510	27	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
32	CLA	b	603	26	65,69,73	1.25	9 (13%)	74,106,113	1.24	5 (6%)
38	LHG	l	102	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
32	CLA	5	303	6	63,67,73	1.32	9 (14%)	75,105,113	1.33	8 (10%)
39	SQD	b	601	-	47,48,54	1.58	7 (14%)	56,59,65	1.50	6 (10%)
31	8CT	M	201	-	40,41,41	4.64	23 (57%)	50,56,56	2.96	18 (36%)
32	CLA	d	409	-	63,67,73	1.28	10 (15%)	75,105,113	1.37	7 (9%)
38	LHG	A	612	-	42,42,48	0.67	1 (2%)	45,48,54	1.23	4 (8%)
34	II0	0	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.74	11 (22%)
32	CLA	s	302	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	6 (10%)
32	CLA	0	612	-	49,53,73	1.50	7 (14%)	59,89,113	1.48	5 (8%)
37	LMG	g	101	-	28,28,55	0.98	0	36,36,63	1.27	5 (13%)
32	CLA	4	606	-	49,53,73	1.49	7 (14%)	59,89,113	1.35	4 (6%)
32	CLA	5	310	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	6 (11%)
32	CLA	0	601	5	46,50,73	1.52	7 (15%)	55,85,113	1.45	5 (9%)
32	CLA	1	611	2	49,53,73	1.49	7 (14%)	59,89,113	1.45	4 (6%)
32	CLA	B	605	26	65,69,73	1.28	8 (12%)	78,108,113	1.37	7 (8%)
33	KC2	4	610	5	49,53,53	1.76	9 (18%)	62,89,89	2.15	16 (25%)
37	LMG	6	616	-	28,28,55	0.98	1 (3%)	36,36,63	1.26	5 (13%)
32	CLA	c	508	27	69,73,73	1.23	10 (14%)	83,113,113	1.32	8 (9%)
34	II0	4	619	-	39,43,43	2.70	4 (10%)	50,60,60	1.71	12 (24%)
32	CLA	2	607	3	49,53,73	1.49	9 (18%)	59,89,113	1.39	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	0	619	-	36,36,55	0.87	1 (2%)	44,44,63	1.26	5 (11%)
32	CLA	b	609	26	69,73,73	1.23	9 (13%)	83,113,113	1.31	8 (9%)
32	CLA	B	617	26	69,73,73	1.24	10 (14%)	83,113,113	1.32	5 (6%)
36	IHT	2	616	-	40,42,42	1.99	2 (5%)	53,58,58	1.96	14 (26%)
32	CLA	b	615	26	68,72,73	1.25	10 (14%)	81,111,113	1.29	6 (7%)
32	CLA	6	604	-	59,63,73	1.36	8 (13%)	71,101,113	1.35	7 (9%)
45	DGD	A	614	-	54,54,67	1.05	4 (7%)	67,67,81	1.48	10 (14%)
32	CLA	a	408	8	64,68,73	1.28	9 (14%)	77,107,113	1.33	7 (9%)
32	CLA	3	605	4	50,54,73	1.45	8 (16%)	60,90,113	1.37	5 (8%)
32	CLA	8	605	3	64,68,73	1.31	9 (14%)	77,107,113	1.30	7 (9%)
32	CLA	p	304	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	6 (9%)
33	KC2	5	311	6	49,53,53	1.77	10 (20%)	62,89,89	2.19	17 (27%)
32	CLA	0	606	-	49,53,73	1.50	9 (18%)	59,89,113	1.37	4 (6%)
32	CLA	b	607	26	69,73,73	1.23	10 (14%)	83,113,113	1.33	8 (9%)
32	CLA	d	402	9	61,65,73	1.39	11 (18%)	76,103,113	1.39	7 (9%)
37	LMG	d	406	-	46,46,55	0.79	1 (2%)	54,54,63	1.34	5 (9%)
34	II0	6	614	-	39,43,43	2.72	5 (12%)	50,60,60	1.69	10 (20%)
31	8CT	h	102	-	40,41,41	4.70	24 (60%)	50,56,56	2.78	16 (32%)
32	CLA	9	604	4	59,63,73	1.36	9 (15%)	71,101,113	1.36	8 (11%)
32	CLA	7	604	2	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
34	II0	5	316	-	39,43,43	2.72	4 (10%)	50,60,60	1.68	8 (16%)
33	KC2	p	311	6	49,53,53	1.78	10 (20%)	62,89,89	2.20	17 (27%)
32	CLA	2	601	3	46,50,73	1.51	9 (19%)	55,85,113	1.43	4 (7%)
34	II0	P	612	-	39,43,43	2.65	4 (10%)	50,60,60	1.74	13 (26%)
32	CLA	4	612	-	49,53,73	1.49	6 (12%)	59,89,113	1.48	5 (8%)
32	CLA	9	606	-	49,53,73	1.49	9 (18%)	59,89,113	1.36	4 (6%)
37	LMG	2	617	-	36,36,55	0.86	0	44,44,63	1.25	5 (11%)
32	CLA	P	610	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
32	CLA	P	602	7	63,67,73	1.31	8 (12%)	75,105,113	1.34	8 (10%)
32	CLA	8	606	3	49,53,73	1.50	9 (18%)	59,89,113	1.38	4 (6%)
32	CLA	C	502	27	68,72,73	1.26	10 (14%)	81,111,113	1.31	5 (6%)
32	CLA	C	513	27	53,57,73	1.40	10 (18%)	62,93,113	1.43	6 (9%)
34	II0	8	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.70	12 (24%)
32	CLA	b	608	-	45,49,73	1.49	9 (20%)	54,84,113	1.51	5 (9%)
41	PHO	d	410	-	58,69,69	2.00	9 (15%)	56,99,99	1.55	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	C	506	27	49,53,73	1.47	10 (20%)	59,89,113	1.46	7 (11%)
32	CLA	b	610	26	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
32	CLA	5	304	-	54,58,73	1.43	8 (14%)	65,95,113	1.41	6 (9%)
38	LHG	B	621	-	38,38,48	0.69	1 (2%)	41,44,54	1.27	4 (9%)
34	II0	1	616	-	39,43,43	2.73	4 (10%)	50,60,60	1.70	9 (18%)
32	CLA	p	309	6	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
31	8CT	B	622	-	40,41,41	4.64	23 (57%)	50,56,56	2.96	18 (36%)
33	KC2	0	610	5	49,53,53	1.77	10 (20%)	62,89,89	2.16	16 (25%)
34	II0	4	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.71	11 (22%)
37	LMG	P	616	-	28,28,55	0.99	0	36,36,63	1.26	5 (13%)
32	CLA	P	611	7	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
32	CLA	1	601	-	46,50,73	1.51	7 (15%)	55,85,113	1.42	5 (9%)
32	CLA	g	102	-	49,53,73	1.50	9 (18%)	59,89,113	1.40	5 (8%)
37	LMG	L	102	-	40,40,55	0.88	1 (2%)	48,48,63	1.28	6 (12%)
32	CLA	4	602	5	63,67,73	1.31	8 (12%)	75,105,113	1.32	6 (8%)
37	LMG	A	607	-	48,48,55	0.77	1 (2%)	56,56,63	1.33	5 (8%)
32	CLA	a	406	-	53,57,73	1.41	10 (18%)	62,93,113	1.48	7 (11%)
45	DGD	c	514	-	56,56,67	0.97	2 (3%)	70,70,81	1.48	10 (14%)
32	CLA	5	307	6	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
32	CLA	1	604	2	59,63,73	1.36	8 (13%)	71,101,113	1.38	5 (7%)
34	II0	5	315	-	39,43,43	2.71	4 (10%)	50,60,60	1.69	11 (22%)
38	LHG	S	301	-	36,36,48	0.71	1 (2%)	39,42,54	1.24	4 (10%)
32	CLA	C	505	27	69,73,73	1.23	9 (13%)	83,113,113	1.30	8 (9%)
34	II0	3	613	-	39,43,43	2.71	4 (10%)	50,60,60	1.71	9 (18%)
36	IHT	5	317	-	40,42,42	1.96	2 (5%)	53,58,58	1.80	13 (24%)
32	CLA	C	509	27	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
32	CLA	9	608	-	45,49,73	1.51	9 (20%)	54,84,113	1.50	5 (9%)
32	CLA	0	609	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	5 (9%)
32	CLA	0	607	5	49,53,73	1.48	8 (16%)	59,89,113	1.36	5 (8%)
32	CLA	B	615	26	68,72,73	1.24	9 (13%)	81,111,113	1.30	7 (8%)
34	II0	1	617	-	39,43,43	2.74	4 (10%)	50,60,60	1.75	10 (20%)
32	CLA	b	613	26	69,73,73	1.23	9 (13%)	83,113,113	1.32	6 (7%)
32	CLA	8	608	3	64,68,73	1.30	9 (14%)	77,107,113	1.31	7 (9%)
32	CLA	1	602	2	63,67,73	1.31	8 (12%)	75,105,113	1.33	6 (8%)
32	CLA	p	308	6	49,53,73	1.49	8 (16%)	59,89,113	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	3	604	4	59,63,73	1.35	10 (16%)	71,101,113	1.35	8 (11%)
32	CLA	7	613	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	4 (6%)
45	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	1.37	8 (10%)
32	CLA	c	511	27	69,73,73	1.25	10 (14%)	83,113,113	1.30	4 (4%)
47	HEM	v	201	-	50,50,50	1.43	7 (14%)	66,82,82	1.17	8 (12%)
36	IHT	4	617	-	40,42,42	1.99	3 (7%)	53,58,58	1.97	15 (28%)
32	CLA	9	611	4	49,53,73	1.48	7 (14%)	59,89,113	1.42	5 (8%)
35	II3	7	615	-	40,43,43	1.95	2 (5%)	47,60,60	1.60	8 (17%)
34	II0	9	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.65	13 (26%)
34	II0	7	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.71	9 (18%)
32	CLA	5	306	6	64,68,73	1.31	9 (14%)	77,107,113	1.31	4 (5%)
32	CLA	3	609	4	64,68,73	1.30	9 (14%)	77,107,113	1.31	6 (7%)
32	CLA	3	607	4	64,68,73	1.29	9 (14%)	77,107,113	1.33	4 (5%)
34	II0	0	615	-	39,43,43	2.66	4 (10%)	50,60,60	1.72	13 (26%)
34	II0	3	612	-	39,43,43	2.68	4 (10%)	50,60,60	1.69	11 (22%)
32	CLA	B	609	26	69,73,73	1.24	10 (14%)	83,113,113	1.31	8 (9%)
31	8CT	9	615	-	40,41,41	4.69	24 (60%)	50,56,56	2.77	20 (40%)
32	CLA	c	502	27	68,72,73	1.26	9 (13%)	81,111,113	1.31	5 (6%)
32	CLA	5	312	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
32	CLA	p	313	6	49,53,73	1.49	7 (14%)	59,89,113	1.39	5 (8%)
32	CLA	6	606	7	49,53,73	1.48	6 (12%)	59,89,113	1.34	5 (8%)
38	LHG	A	613	-	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
38	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
32	CLA	9	605	4	50,54,73	1.45	8 (16%)	60,90,113	1.38	5 (8%)
31	8CT	B	624	-	40,41,41	4.67	24 (60%)	50,56,56	2.78	16 (32%)
32	CLA	b	614	26	69,73,73	1.24	10 (14%)	83,113,113	1.26	7 (8%)
32	CLA	P	604	-	59,63,73	1.36	7 (11%)	71,101,113	1.34	6 (8%)
37	LMG	d	401	-	40,40,55	0.81	0	48,48,63	1.24	6 (12%)
32	CLA	C	508	27	69,73,73	1.24	10 (14%)	83,113,113	1.32	8 (9%)
38	LHG	D	410	-	31,31,48	0.76	1 (3%)	34,37,54	1.27	3 (8%)
32	CLA	b	611	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
45	DGD	c	516	-	56,56,67	0.93	2 (3%)	70,70,81	1.41	7 (10%)
32	CLA	a	405	8	69,73,73	1.24	10 (14%)	83,113,113	1.32	5 (6%)
32	CLA	d	403	9	64,68,73	1.28	8 (12%)	77,107,113	1.36	9 (11%)
31	8CT	B	623	-	40,41,41	4.67	23 (57%)	50,56,56	2.44	15 (30%)

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
32	CLA	b	604	26	-	12/37/113/115	-
32	CLA	8	607	3	-	4/15/91/115	-
32	CLA	8	612	3	-	8/15/91/115	-
32	CLA	5	308	6	-	5/15/91/115	-
32	CLA	1	612	2	-	7/15/91/115	-
32	CLA	2	608	3	-	12/33/109/115	-
37	LMG	8	617	-	-	10/31/51/70	0/1/1/1
31	8CT	C	518	-	-	10/29/63/63	0/2/2/2
34	II0	5	314	-	-	2/21/67/67	0/2/2/2
35	II3	6	613	-	-	1/25/67/67	0/2/2/2
32	CLA	B	612	-	-	15/37/113/115	-
37	LMG	C	517	-	-	25/41/61/70	0/1/1/1
32	CLA	7	605	-	-	9/21/97/115	-
32	CLA	B	606	26	-	13/39/115/115	-
32	CLA	0	613	5	-	8/15/91/115	-
37	LMG	D	407	-	-	17/41/61/70	0/1/1/1
32	CLA	p	307	6	-	4/15/91/115	-
32	CLA	s	303	19	-	17/39/115/115	-
33	KC2	6	605	7	-	10/15/71/71	-
34	II0	3	614	-	-	3/21/67/67	0/2/2/2
34	II0	p	315	-	-	4/21/67/67	0/2/2/2
32	CLA	3	611	4	-	6/15/91/115	-
32	CLA	D	404	9	-	11/33/109/115	-
32	CLA	3	603	4	-	6/21/97/115	-
32	CLA	5	302	6	-	6/12/88/115	-
47	HEM	V	201	-	-	1/14/54/54	-
32	CLA	b	605	26	-	11/35/111/115	-
32	CLA	P	603	-	-	3/21/97/115	-
37	LMG	4	618	-	-	11/31/51/70	0/1/1/1
31	8CT	H	102	-	-	9/29/63/63	0/2/2/2
32	CLA	D	401	-	-	5/32/108/115	-
31	8CT	3	615	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	7	606	2	-	10/15/91/115	-
32	CLA	B	610	26	-	10/39/115/115	-
32	CLA	B	602	-	-	8/18/94/115	-
32	CLA	0	602	5	-	13/32/108/115	-
32	CLA	6	611	7	-	7/15/91/115	-
32	CLA	7	608	2	-	12/33/109/115	-
32	CLA	2	604	-	-	3/27/103/115	-
33	KC2	P	605	7	-	10/15/71/71	-
47	HEM	f	101	11	-	4/14/54/54	-
43	PL9	d	404	-	-	3/53/73/73	0/1/1/1
39	SQD	A	606	-	-	26/49/69/69	0/1/1/1
32	CLA	3	608	-	-	3/10/86/115	-
38	LHG	d	405	-	-	17/47/51/53	-
32	CLA	p	303	6	-	14/32/108/115	-
32	CLA	8	601	3	-	5/12/88/115	-
45	DGD	C	514	-	-	18/44/84/95	0/2/2/2
32	CLA	c	513	27	-	11/20/96/115	-
34	II0	1	619	-	-	2/21/67/67	0/2/2/2
32	CLA	B	603	26	-	12/29/107/115	-
34	II0	6	612	-	-	1/21/67/67	0/2/2/2
32	CLA	b	616	26	-	7/39/115/115	-
32	CLA	0	604	5	-	11/27/103/115	-
43	PL9	a	412	-	-	1/5/18/73	0/1/1/1
34	II0	p	316	-	-	3/21/67/67	0/2/2/2
32	CLA	6	610	-	-	8/15/91/115	-
43	PL9	D	405	-	-	3/53/73/73	0/1/1/1
39	SQD	a	409	-	-	26/49/69/69	0/1/1/1
34	II0	8	613	-	-	0/21/67/67	0/2/2/2
32	CLA	4	603	5	-	6/21/97/115	-
31	8CT	K	101	-	-	13/29/63/63	0/2/2/2
37	LMG	G	102	-	-	9/23/43/70	0/1/1/1
45	DGD	C	515	-	-	18/45/85/95	0/2/2/2
34	II0	4	616	-	-	4/21/67/67	0/2/2/2
32	CLA	9	602	4	-	13/32/108/115	-
31	8CT	c	518	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	0	611	5	-	9/15/91/115	-
33	KC2	2	610	3	-	11/15/71/71	-
38	LHG	b	621	-	-	14/43/43/53	-
32	CLA	c	504	-	-	13/37/113/115	-
32	CLA	8	602	3	-	13/32/108/115	-
37	LMG	l	101	-	-	17/35/55/70	0/1/1/1
34	II0	p	301	-	-	2/21/67/67	0/2/2/2
32	CLA	6	607	7	-	9/33/109/115	-
32	CLA	b	606	26	-	13/39/115/115	-
32	CLA	7	612	2	-	8/15/91/115	-
32	CLA	1	609	-	-	5/10/86/115	-
32	CLA	8	609	38	-	4/10/86/115	-
38	LHG	b	619	-	-	19/43/43/53	-
32	CLA	6	601	7	-	2/12/88/115	-
32	CLA	7	611	2	-	8/15/91/115	-
37	LMG	b	618	-	-	17/46/66/70	0/1/1/1
38	LHG	8	618	32	-	11/24/24/53	-
32	CLA	C	511	27	-	9/39/115/115	-
32	CLA	1	603	2	-	7/21/97/115	-
32	CLA	2	605	3	-	13/33/109/115	-
32	CLA	8	603	3	-	7/21/97/115	-
31	8CT	b	622	-	-	8/29/63/63	0/2/2/2
32	CLA	B	616	26	-	8/39/115/115	-
32	CLA	3	606	-	-	1/15/91/115	-
32	CLA	8	611	-	-	7/15/91/115	-
32	CLA	9	601	4	-	5/12/88/115	-
38	LHG	d	411	-	-	18/36/36/53	-
32	CLA	2	611	-	-	7/15/91/115	-
32	CLA	8	604	-	-	3/27/103/115	-
37	LMG	D	411	-	-	26/35/55/70	0/1/1/1
32	CLA	4	607	5	-	4/15/91/115	-
34	II0	2	619	-	-	2/21/67/67	0/2/2/2
36	IHT	1	618	-	-	4/25/65/65	0/2/2/2
36	IHT	4	614	-	-	5/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	II0	9	613	-	-	1/21/67/67	0/2/2/2
32	CLA	4	604	5	-	11/27/103/115	-
33	KC2	6	609	-	-	11/15/71/71	-
32	CLA	C	512	27	-	13/29/105/115	-
31	8CT	Z	101	-	-	12/29/63/63	0/2/2/2
32	CLA	4	605	-	-	9/21/97/115	-
32	CLA	6	602	7	-	17/32/108/115	-
34	II0	2	613	-	-	1/21/67/67	0/2/2/2
32	CLA	4	613	5	-	8/15/91/115	-
32	CLA	7	607	-	-	9/15/91/115	-
31	8CT	k	102	-	-	13/29/63/63	0/2/2/2
41	PHO	D	402	-	-	8/37/103/103	0/5/6/6
32	CLA	S	303	19	-	17/39/115/115	-
32	CLA	p	305	6	-	11/27/103/115	-
31	8CT	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	c	510	27	-	8/39/115/115	-
32	CLA	P	606	7	-	5/15/91/115	-
37	LMG	c	517	-	-	25/41/61/70	0/1/1/1
47	HEM	E	101	-	-	4/14/54/54	-
31	8CT	a	413	-	-	7/29/63/63	0/2/2/2
32	CLA	p	302	6	-	7/12/88/115	-
34	II0	P	614	-	-	2/21/67/67	0/2/2/2
32	CLA	C	501	27	-	18/39/115/115	-
32	CLA	B	614	26	-	14/39/115/115	-
32	CLA	3	601	4	-	5/12/88/115	-
31	8CT	D	409	-	-	13/29/63/63	0/2/2/2
32	CLA	6	603	-	-	3/21/97/115	-
41	PHO	A	604	-	-	8/37/103/103	0/5/6/6
45	DGD	H	101	-	-	20/51/91/95	0/2/2/2
32	CLA	b	612	-	-	15/37/113/115	-
32	CLA	5	313	6	-	9/15/91/115	-
33	KC2	7	610	-	-	12/15/71/71	-
32	CLA	7	601	-	-	5/12/88/115	-
33	KC2	P	609	-	-	11/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	S	302	-	-	7/15/91/115	-
32	CLA	0	608	5	-	10/33/109/115	-
32	CLA	9	603	4	-	6/21/97/115	-
36	IHT	p	317	-	-	0/25/65/65	0/2/2/2
39	SQD	B	620	-	-	24/49/69/69	0/1/1/1
32	CLA	1	608	2	-	12/33/109/115	-
34	II0	7	619	-	-	2/21/67/67	0/2/2/2
33	KC2	8	610	3	-	11/15/71/71	-
32	CLA	4	601	5	-	6/12/88/115	-
32	CLA	A	603	-	-	6/20/96/115	-
32	CLA	9	610	4	-	9/15/91/115	-
34	II0	2	615	-	-	3/21/67/67	0/2/2/2
37	LMG	a	410	-	-	16/43/63/70	0/1/1/1
32	CLA	1	607	-	-	9/15/91/115	-
32	CLA	p	310	-	-	5/10/86/115	-
32	CLA	c	503	27	-	17/39/115/115	-
34	II0	5	319	-	-	2/21/67/67	0/2/2/2
34	II0	0	620	-	-	1/21/67/67	0/2/2/2
35	II3	P	613	-	-	3/25/67/67	0/2/2/2
37	LMG	B	618	-	-	18/46/66/70	0/1/1/1
32	CLA	B	613	26	-	16/39/115/115	-
34	II0	p	314	-	-	0/21/67/67	0/2/2/2
32	CLA	P	608	-	-	4/10/86/115	-
34	II0	9	612	-	-	3/21/67/67	0/2/2/2
32	CLA	0	605	-	-	9/21/97/115	-
43	PL9	A	609	-	-	1/5/18/73	0/1/1/1
32	CLA	B	608	-	-	3/10/86/115	-
32	CLA	5	309	-	-	12/33/109/115	-
32	CLA	c	501	27	-	19/39/115/115	-
32	CLA	C	503	27	-	17/39/115/115	-
32	CLA	0	603	5	-	6/21/97/115	-
32	CLA	7	602	2	-	12/32/108/115	-
45	DGD	c	515	-	-	18/45/85/95	0/2/2/2
39	SQD	B	601	-	-	23/43/63/69	0/1/1/1
32	CLA	p	312	-	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	2	609	38	-	4/10/86/115	-
34	II0	1	614	-	-	0/21/67/67	0/2/2/2
32	CLA	2	606	3	-	3/15/91/115	-
32	CLA	3	602	4	-	13/32/108/115	-
32	CLA	c	505	27	-	13/39/115/115	-
32	CLA	p	306	6	-	16/33/109/115	-
45	DGD	C	516	-	-	19/44/84/95	0/2/2/2
38	LHG	2	618	32	-	12/24/24/53	-
34	II0	8	619	-	-	1/21/67/67	0/2/2/2
32	CLA	2	602	3	-	12/32/108/115	-
32	CLA	3	610	4	-	9/15/91/115	-
32	CLA	4	608	5	-	10/33/109/115	-
38	LHG	B	619	-	-	19/43/43/53	-
32	CLA	A	602	8	-	7/39/115/115	-
32	CLA	c	512	27	-	13/29/105/115	-
32	CLA	c	509	27	-	8/39/115/115	-
32	CLA	7	603	2	-	8/21/97/115	-
31	8CT	P	615	-	-	5/29/63/63	0/2/2/2
32	CLA	A	605	8	-	3/33/109/115	-
32	CLA	P	601	7	-	2/12/88/115	-
31	8CT	A	610	-	-	5/29/63/63	0/2/2/2
34	II0	7	616	-	-	3/21/67/67	0/2/2/2
32	CLA	C	507	-	-	14/39/115/115	-
32	CLA	1	613	-	-	9/15/91/115	-
32	CLA	B	604	26	-	12/37/113/115	-
34	II0	8	615	-	-	2/21/67/67	0/2/2/2
32	CLA	1	606	2	-	11/15/91/115	-
32	CLA	5	305	6	-	11/27/103/115	-
32	CLA	2	603	3	-	7/21/97/115	-
34	II0	0	617	-	-	2/21/67/67	0/2/2/2
31	8CT	6	615	-	-	5/29/63/63	0/2/2/2
32	CLA	b	602	-	-	8/18/94/115	-
34	II0	7	617	-	-	4/21/67/67	0/2/2/2
38	LHG	a	402	-	-	10/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SQD	p	318	-	-	18/30/50/69	0/1/1/1
45	DGD	a	414	-	-	14/43/79/95	0/2/2/2
36	IHT	7	618	-	-	2/25/65/65	0/2/2/2
38	LHG	D	406	-	-	18/47/51/53	-
32	CLA	P	607	7	-	9/33/109/115	-
36	IHT	8	616	-	-	0/25/65/65	0/2/2/2
31	8CT	d	408	-	-	13/29/63/63	0/2/2/2
38	LHG	a	403	-	-	26/53/53/53	-
32	CLA	c	507	-	-	14/39/115/115	-
32	CLA	7	609	-	-	5/10/86/115	-
32	CLA	B	607	26	-	9/39/115/115	-
32	CLA	B	611	-	-	9/39/115/115	-
36	IHT	0	614	-	-	5/25/65/65	0/2/2/2
32	CLA	b	617	26	-	16/39/115/115	-
32	CLA	4	609	-	-	4/10/86/115	-
32	CLA	1	605	-	-	9/21/97/115	-
33	KC2	1	610	-	-	11/15/71/71	-
32	CLA	9	607	4	-	8/33/109/115	-
34	II0	5	301	-	-	3/21/67/67	0/2/2/2
39	SQD	5	318	-	-	19/30/50/69	0/1/1/1
39	SQD	b	620	-	-	24/49/69/69	0/1/1/1
31	8CT	z	101	-	-	13/29/63/63	0/2/2/2
32	CLA	4	611	5	-	9/15/91/115	-
32	CLA	6	608	-	-	4/10/86/115	-
32	CLA	c	506	27	-	5/15/91/115	-
32	CLA	D	403	9	-	9/28/104/115	-
31	8CT	b	623	-	-	7/29/63/63	0/2/2/2
32	CLA	2	612	3	-	8/15/91/115	-
35	II3	1	615	-	-	2/25/67/67	0/2/2/2
36	IHT	0	618	-	-	5/25/65/65	0/2/2/2
32	CLA	9	609	4	-	8/33/109/115	-
32	CLA	G	101	-	-	8/15/91/115	-
34	II0	2	614	-	-	0/21/67/67	0/2/2/2
32	CLA	C	504	-	-	13/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	s	301	-	-	21/41/41/53	-
41	PHO	a	407	-	-	8/37/103/103	0/5/6/6
31	8CT	K	102	-	-	7/29/63/63	0/2/2/2
32	CLA	C	510	27	-	8/39/115/115	-
32	CLA	b	603	26	-	13/29/107/115	-
38	LHG	l	102	-	-	21/53/53/53	-
32	CLA	5	303	6	-	13/32/108/115	-
39	SQD	b	601	-	-	23/43/63/69	0/1/1/1
31	8CT	M	201	-	-	16/29/63/63	0/2/2/2
32	CLA	d	409	-	-	5/32/108/115	-
38	LHG	A	612	-	-	10/47/47/53	-
34	II0	0	616	-	-	4/21/67/67	0/2/2/2
32	CLA	s	302	-	-	6/15/91/115	-
32	CLA	0	612	-	-	7/15/91/115	-
37	LMG	g	101	-	-	9/23/43/70	0/1/1/1
32	CLA	4	606	-	-	7/15/91/115	-
32	CLA	5	310	-	-	5/10/86/115	-
32	CLA	0	601	5	-	6/12/88/115	-
32	CLA	1	611	2	-	8/15/91/115	-
32	CLA	B	605	26	-	11/35/111/115	-
33	KC2	4	610	5	-	11/15/71/71	-
37	LMG	6	616	-	-	9/23/43/70	0/1/1/1
32	CLA	c	508	27	-	9/39/115/115	-
34	II0	4	619	-	-	2/21/67/67	0/2/2/2
32	CLA	2	607	3	-	4/15/91/115	-
37	LMG	0	619	-	-	11/31/51/70	0/1/1/1
32	CLA	b	609	26	-	9/39/115/115	-
32	CLA	B	617	26	-	16/39/115/115	-
36	IHT	2	616	-	-	1/25/65/65	0/2/2/2
32	CLA	b	615	26	-	15/37/113/115	-
32	CLA	6	604	-	-	7/27/103/115	-
45	DGD	A	614	-	-	15/43/79/95	0/2/2/2
32	CLA	a	408	8	-	3/33/109/115	-
32	CLA	3	605	4	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	8	605	3	-	13/33/109/115	-
32	CLA	p	304	-	-	12/21/97/115	-
33	KC2	5	311	6	-	9/15/71/71	-
32	CLA	0	606	-	-	7/15/91/115	-
32	CLA	b	607	26	-	9/39/115/115	-
32	CLA	d	402	9	-	9/28/104/115	-
37	LMG	d	406	-	-	17/41/61/70	0/1/1/1
34	II0	6	614	-	-	3/21/67/67	0/2/2/2
31	8CT	h	102	-	-	9/29/63/63	0/2/2/2
32	CLA	9	604	4	-	7/27/103/115	-
32	CLA	7	604	2	-	6/27/103/115	-
34	II0	5	316	-	-	3/21/67/67	0/2/2/2
33	KC2	p	311	6	-	10/15/71/71	-
32	CLA	2	601	3	-	5/12/88/115	-
34	II0	P	612	-	-	0/21/67/67	0/2/2/2
32	CLA	4	612	-	-	8/15/91/115	-
32	CLA	9	606	-	-	1/15/91/115	-
37	LMG	2	617	-	-	10/31/51/70	0/1/1/1
32	CLA	P	610	-	-	8/15/91/115	-
32	CLA	P	602	7	-	16/32/108/115	-
32	CLA	8	606	3	-	2/15/91/115	-
32	CLA	C	502	27	-	18/37/113/115	-
32	CLA	C	513	27	-	12/20/96/115	-
34	II0	8	614	-	-	0/21/67/67	0/2/2/2
32	CLA	b	608	-	-	3/10/86/115	-
41	PHO	d	410	-	-	8/37/103/103	0/5/6/6
32	CLA	C	506	27	-	5/15/91/115	-
32	CLA	b	610	26	-	10/39/115/115	-
32	CLA	5	304	-	-	12/21/97/115	-
38	LHG	B	621	-	-	14/43/43/53	-
34	II0	1	616	-	-	4/21/67/67	0/2/2/2
32	CLA	p	309	6	-	12/33/109/115	-
31	8CT	B	622	-	-	16/29/63/63	0/2/2/2
33	KC2	0	610	5	-	12/15/71/71	-
34	II0	4	615	-	-	0/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	P	616	-	-	9/23/43/70	0/1/1/1
32	CLA	P	611	7	-	9/15/91/115	-
32	CLA	1	601	-	-	4/12/88/115	-
32	CLA	g	102	-	-	9/15/91/115	-
37	LMG	L	102	-	-	18/35/55/70	0/1/1/1
32	CLA	4	602	5	-	13/32/108/115	-
37	LMG	A	607	-	-	16/43/63/70	0/1/1/1
32	CLA	a	406	-	-	6/20/96/115	-
45	DGD	c	514	-	-	18/44/84/95	0/2/2/2
32	CLA	5	307	6	-	5/15/91/115	-
32	CLA	1	604	2	-	6/27/103/115	-
34	II0	5	315	-	-	3/21/67/67	0/2/2/2
38	LHG	S	301	-	-	21/41/41/53	-
32	CLA	C	505	27	-	13/39/115/115	-
34	II0	3	613	-	-	0/21/67/67	0/2/2/2
36	IHT	5	317	-	-	1/25/65/65	0/2/2/2
32	CLA	C	509	27	-	8/39/115/115	-
32	CLA	9	608	-	-	3/10/86/115	-
32	CLA	0	609	-	-	4/10/86/115	-
32	CLA	0	607	5	-	2/15/91/115	-
32	CLA	B	615	26	-	15/37/113/115	-
34	II0	1	617	-	-	3/21/67/67	0/2/2/2
32	CLA	b	613	26	-	16/39/115/115	-
32	CLA	8	608	3	-	12/33/109/115	-
32	CLA	1	602	2	-	13/32/108/115	-
32	CLA	p	308	6	-	5/15/91/115	-
32	CLA	3	604	4	-	8/27/103/115	-
32	CLA	7	613	-	-	9/15/91/115	-
45	DGD	h	101	-	-	20/51/91/95	0/2/2/2
32	CLA	c	511	27	-	8/39/115/115	-
47	HEM	v	201	-	-	1/14/54/54	-
36	IHT	4	617	-	-	6/25/65/65	0/2/2/2
32	CLA	9	611	4	-	6/15/91/115	-
35	II3	7	615	-	-	2/25/67/67	0/2/2/2
34	II0	9	614	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	II0	7	614	-	-	1/21/67/67	0/2/2/2
32	CLA	5	306	6	-	17/33/109/115	-
32	CLA	3	609	4	-	8/33/109/115	-
32	CLA	3	607	4	-	8/33/109/115	-
34	II0	0	615	-	-	1/21/67/67	0/2/2/2
34	II0	3	612	-	-	1/21/67/67	0/2/2/2
32	CLA	B	609	26	-	9/39/115/115	-
31	8CT	9	615	-	-	10/29/63/63	0/2/2/2
32	CLA	c	502	27	-	18/37/113/115	-
32	CLA	5	312	-	-	9/15/91/115	-
32	CLA	p	313	6	-	8/15/91/115	-
32	CLA	6	606	7	-	5/15/91/115	-
38	LHG	A	613	-	-	25/53/53/53	-
38	LHG	L	101	-	-	20/53/53/53	-
32	CLA	9	605	4	-	8/17/93/115	-
31	8CT	B	624	-	-	7/29/63/63	0/2/2/2
32	CLA	b	614	26	-	14/39/115/115	-
32	CLA	P	604	-	-	7/27/103/115	-
37	LMG	d	401	-	-	26/35/55/70	0/1/1/1
32	CLA	C	508	27	-	9/39/115/115	-
38	LHG	D	410	-	-	18/36/36/53	-
32	CLA	b	611	-	-	9/39/115/115	-
45	DGD	c	516	-	-	19/44/84/95	0/2/2/2
32	CLA	a	405	8	-	7/39/115/115	-
32	CLA	d	403	9	-	10/33/109/115	-
31	8CT	B	623	-	-	8/29/63/63	0/2/2/2

The worst 5 of 2827 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	408	8CT	C02-C03	14.49	1.59	1.34
31	D	409	8CT	C02-C03	14.46	1.59	1.34
31	b	622	8CT	C02-C03	14.40	1.59	1.34
31	h	102	8CT	C02-C03	14.40	1.59	1.34
31	H	102	8CT	C02-C03	14.39	1.59	1.34

The worst 5 of 2885 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	k	102	8CT	C33-C32-C31	-11.05	114.25	124.85
31	B	622	8CT	C33-C32-C31	-11.04	114.27	124.85
31	M	201	8CT	C33-C32-C31	-11.02	114.28	124.85
31	a	413	8CT	C33-C32-C31	-11.01	114.30	124.85
31	K	101	8CT	C33-C32-C31	-10.98	114.32	124.85

There are no chirality outliers.

5 of 3364 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	M	201	8CT	C16-C17-C18-C19
31	M	201	8CT	C20-C21-C23-C24
31	M	201	8CT	C22-C21-C23-C24
31	M	201	8CT	C28-C29-C30-C35
31	3	615	8CT	C12-C13-C14-C15

There are no ring outliers.

202 monomers are involved in 390 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	604	CLA	2	0
32	8	607	CLA	1	0
32	1	612	CLA	2	0
32	2	608	CLA	3	0
37	8	617	LMG	2	0
32	B	612	CLA	3	0
37	C	517	LMG	3	0
32	7	605	CLA	2	0
32	B	606	CLA	6	0
32	0	613	CLA	1	0
32	p	307	CLA	2	0
32	s	303	CLA	1	0
32	D	404	CLA	2	0
47	V	201	HEM	3	0
32	b	605	CLA	3	0
32	7	606	CLA	2	0
32	B	610	CLA	3	0
32	0	602	CLA	3	0
32	6	611	CLA	1	0
32	7	608	CLA	1	0
33	P	605	KC2	3	0
47	f	101	HEM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	A	606	SQD	5	0
38	d	405	LHG	1	0
32	p	303	CLA	2	0
45	C	514	DGD	2	0
32	c	513	CLA	2	0
32	B	603	CLA	4	0
32	b	616	CLA	2	0
32	0	604	CLA	1	0
32	6	610	CLA	1	0
39	a	409	SQD	6	0
32	4	603	CLA	2	0
45	C	515	DGD	4	0
34	4	616	II0	1	0
32	9	602	CLA	1	0
38	b	621	LHG	3	0
32	c	504	CLA	4	0
32	8	602	CLA	1	0
32	6	607	CLA	1	0
32	b	606	CLA	4	0
32	7	612	CLA	2	0
32	8	609	CLA	1	0
37	b	618	LMG	1	0
32	C	511	CLA	3	0
32	1	603	CLA	1	0
32	2	605	CLA	2	0
32	8	603	CLA	2	0
32	B	616	CLA	3	0
32	3	606	CLA	2	0
37	D	411	LMG	1	0
32	4	607	CLA	4	0
36	1	618	IHT	1	0
32	4	604	CLA	1	0
32	C	512	CLA	1	0
31	Z	101	8CT	1	0
32	6	602	CLA	3	0
32	4	613	CLA	1	0
32	7	607	CLA	2	0
41	D	402	PHO	3	0
32	S	303	CLA	1	0
32	p	305	CLA	2	0
32	c	510	CLA	2	0
37	c	517	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	E	101	HEM	2	0
32	C	501	CLA	1	0
32	B	614	CLA	1	0
41	A	604	PHO	1	0
45	H	101	DGD	6	0
32	b	612	CLA	3	0
32	S	302	CLA	4	0
32	0	608	CLA	3	0
39	B	620	SQD	1	0
32	1	608	CLA	1	0
32	4	601	CLA	1	0
32	A	603	CLA	3	0
37	a	410	LMG	3	0
32	1	607	CLA	3	0
32	B	613	CLA	2	0
32	c	501	CLA	1	0
32	C	503	CLA	4	0
32	0	603	CLA	1	0
32	7	602	CLA	4	0
45	c	515	DGD	4	0
39	B	601	SQD	2	0
32	2	609	CLA	1	0
34	1	614	II0	1	0
32	2	606	CLA	5	0
32	3	602	CLA	1	0
32	c	505	CLA	3	0
32	p	306	CLA	1	0
45	C	516	DGD	5	0
32	2	602	CLA	1	0
32	4	608	CLA	3	0
32	A	602	CLA	5	0
32	c	512	CLA	2	0
32	c	509	CLA	1	0
32	7	603	CLA	1	0
32	A	605	CLA	3	0
32	C	507	CLA	3	0
32	1	613	CLA	1	0
32	B	604	CLA	2	0
32	1	606	CLA	3	0
32	5	305	CLA	2	0
32	2	603	CLA	2	0
38	a	402	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	p	318	SQD	3	0
45	a	414	DGD	1	0
38	D	406	LHG	1	0
32	P	607	CLA	1	0
38	a	403	LHG	6	0
32	c	507	CLA	1	0
32	B	607	CLA	3	0
32	B	611	CLA	2	0
32	b	617	CLA	2	0
32	1	605	CLA	1	0
32	9	607	CLA	4	0
39	5	318	SQD	4	0
39	b	620	SQD	1	0
31	z	101	8CT	1	0
32	c	506	CLA	1	0
32	D	403	CLA	3	0
32	9	609	CLA	3	0
32	G	101	CLA	1	0
32	C	504	CLA	4	0
38	s	301	LHG	1	0
41	a	407	PHO	1	0
32	C	510	CLA	2	0
32	b	603	CLA	4	0
38	l	102	LHG	2	0
32	5	303	CLA	2	0
39	b	601	SQD	1	0
38	A	612	LHG	5	0
34	0	616	II0	1	0
32	s	302	CLA	3	0
32	0	612	CLA	1	0
32	4	606	CLA	1	0
32	0	601	CLA	1	0
32	B	605	CLA	3	0
32	2	607	CLA	1	0
32	b	609	CLA	4	0
32	B	617	CLA	4	0
32	b	615	CLA	1	0
45	A	614	DGD	1	0
32	a	408	CLA	2	0
32	3	605	CLA	1	0
32	8	605	CLA	1	0
32	p	304	CLA	1	0

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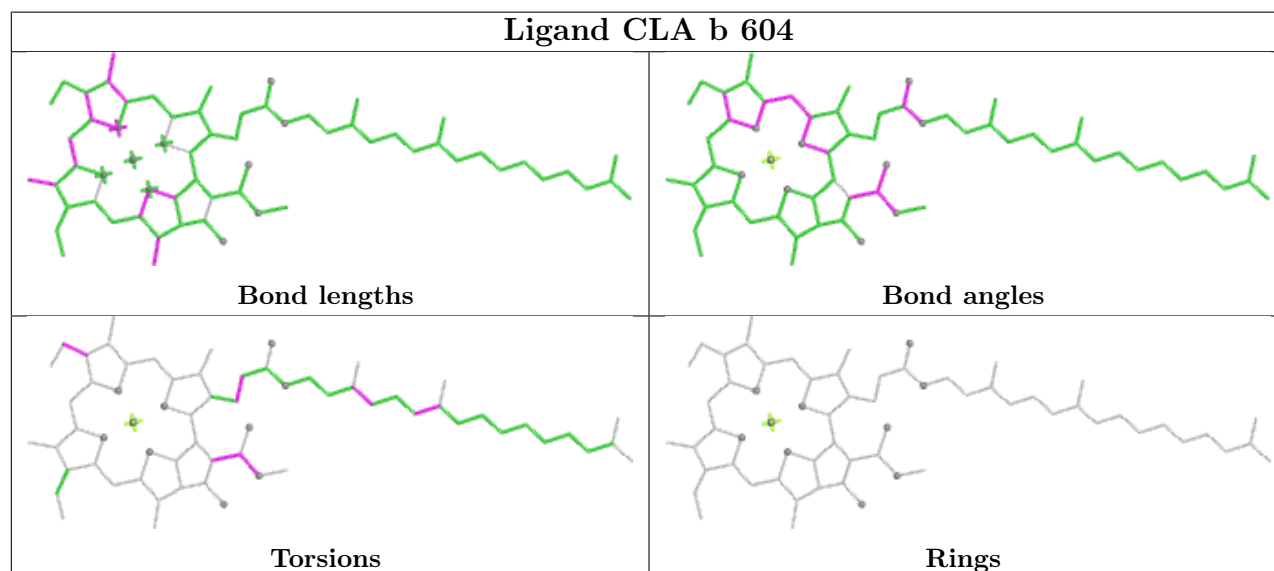
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	607	CLA	2	0
32	d	402	CLA	1	0
32	9	604	CLA	1	0
32	4	612	CLA	1	0
32	9	606	CLA	2	0
37	2	617	LMG	1	0
32	P	610	CLA	1	0
32	P	602	CLA	3	0
32	8	606	CLA	5	0
32	C	502	CLA	2	0
32	C	513	CLA	2	0
41	d	410	PHO	3	0
32	C	506	CLA	1	0
32	b	610	CLA	2	0
32	5	304	CLA	1	0
38	B	621	LHG	3	0
32	P	611	CLA	1	0
32	g	102	CLA	2	0
37	L	102	LMG	1	0
32	4	602	CLA	3	0
37	A	607	LMG	2	0
32	a	406	CLA	3	0
45	c	514	DGD	1	0
32	5	307	CLA	2	0
38	S	301	LHG	1	0
32	C	505	CLA	2	0
32	C	509	CLA	1	0
32	0	607	CLA	4	0
32	B	615	CLA	1	0
32	b	613	CLA	2	0
32	8	608	CLA	3	0
32	1	602	CLA	4	0
32	p	308	CLA	1	0
32	3	604	CLA	1	0
45	h	101	DGD	5	0
32	c	511	CLA	4	0
47	v	201	HEM	3	0
34	7	614	II0	1	0
32	5	306	CLA	2	0
32	3	609	CLA	3	0
32	3	607	CLA	3	0
32	B	609	CLA	4	0

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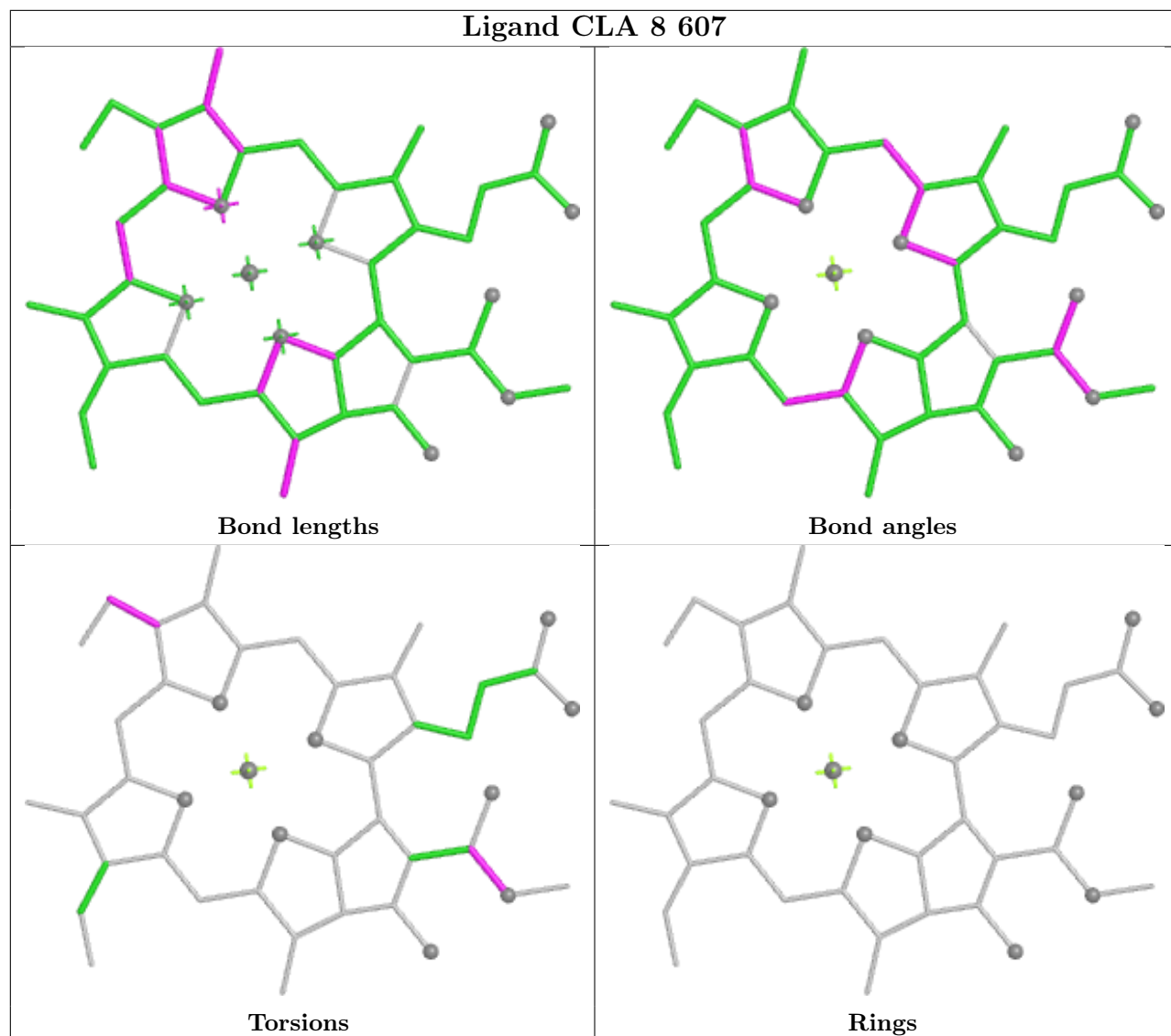
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	502	CLA	1	0
38	A	613	LHG	5	0
38	L	101	LHG	2	0
32	9	605	CLA	1	0
32	b	614	CLA	1	0
32	P	604	CLA	1	0
37	d	401	LMG	1	0
32	C	508	CLA	1	0
32	b	611	CLA	2	0
45	c	516	DGD	3	0
32	a	405	CLA	4	0
32	d	403	CLA	1	0

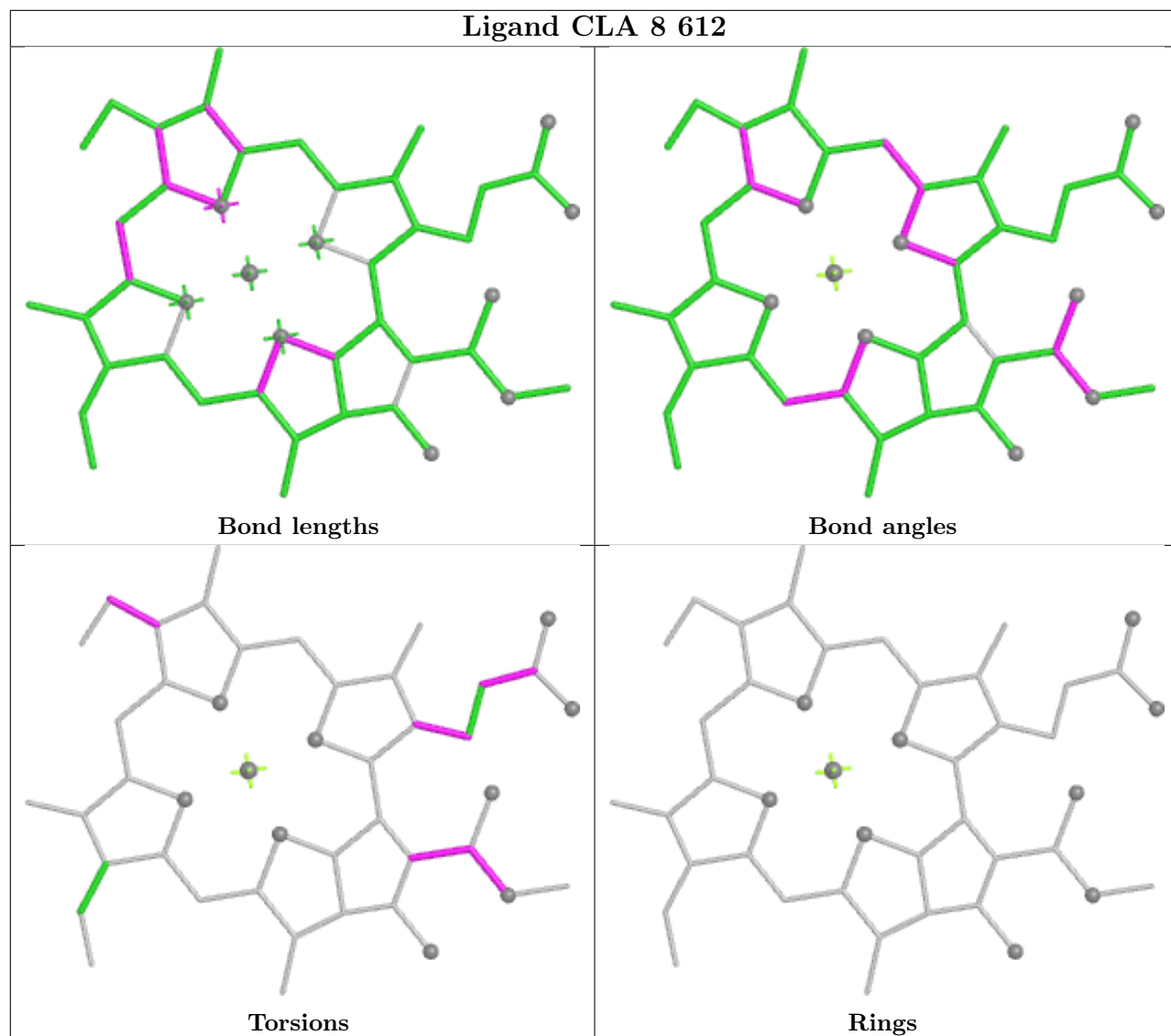
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



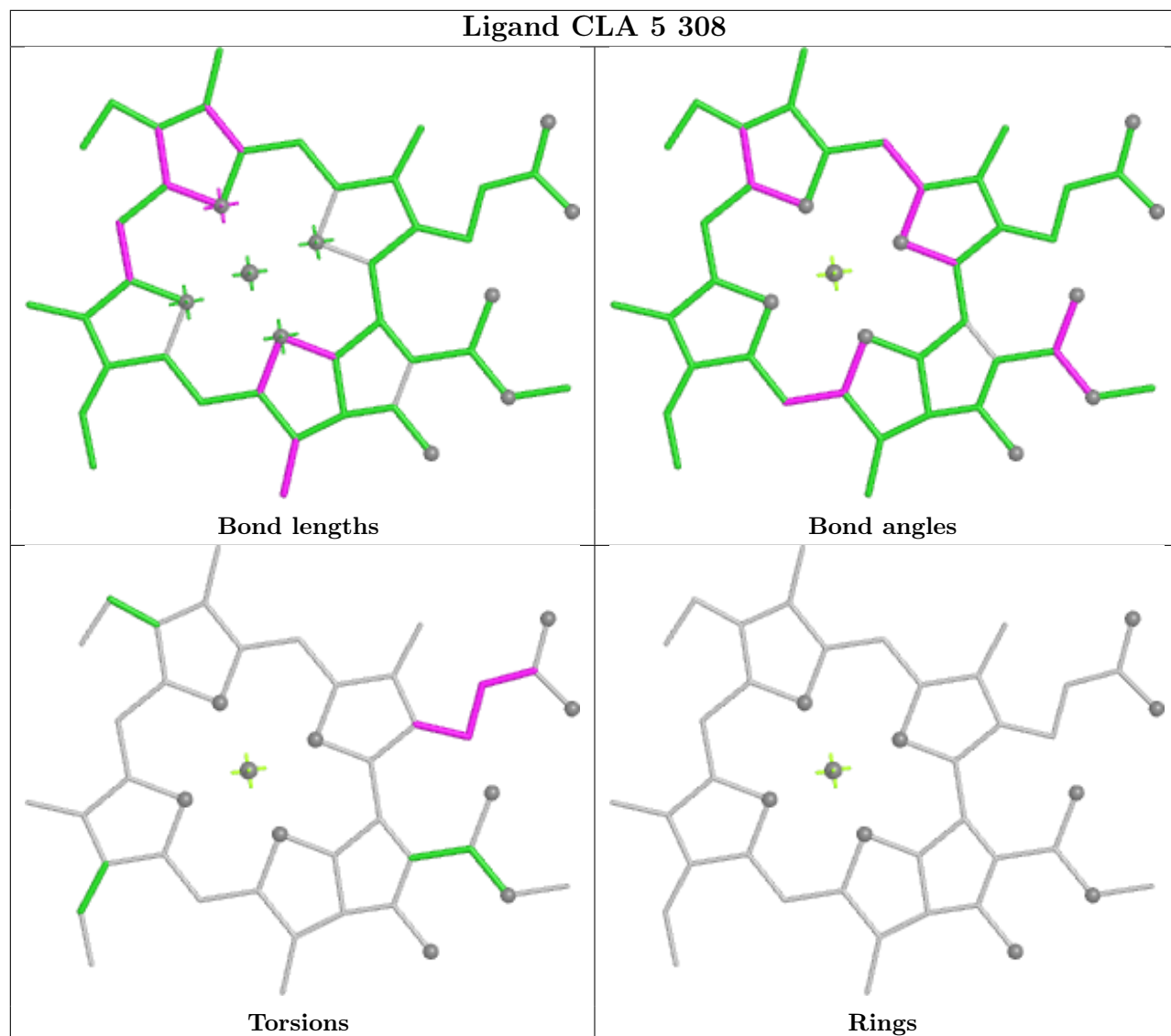
Ligand CLA 8 607



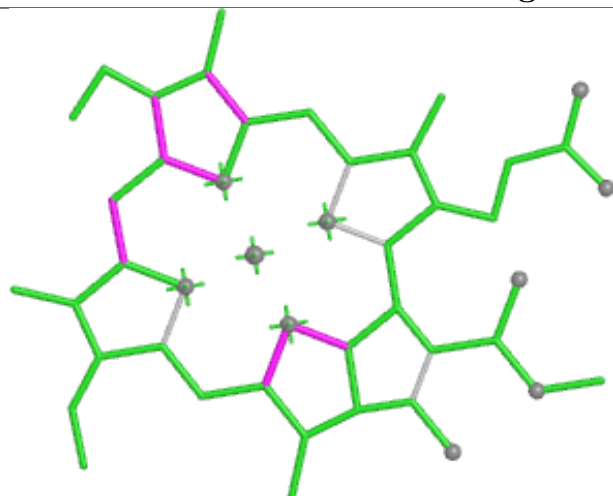
Ligand CLA 8 612



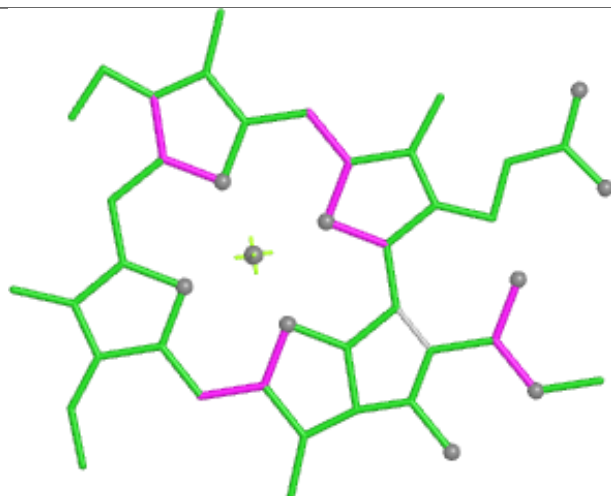
Ligand CLA 5 308



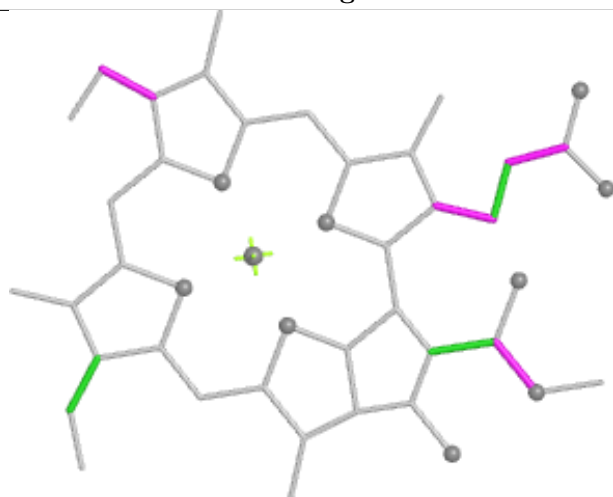
Ligand CLA 1 612



Bond lengths



Bond angles

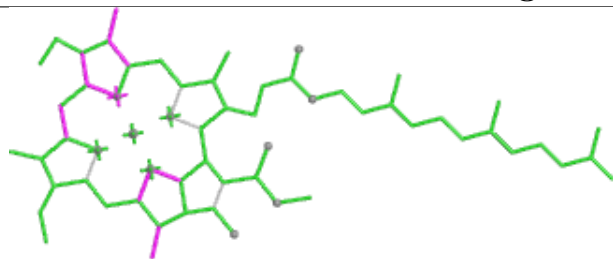


Torsions

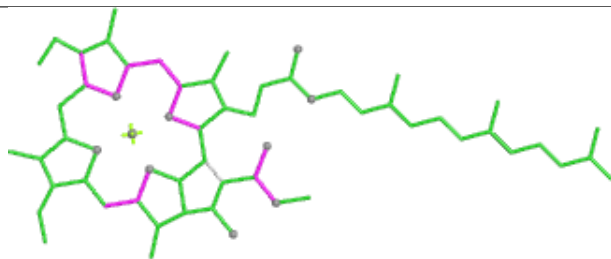


Rings

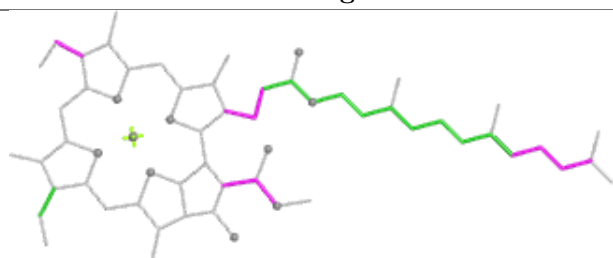
Ligand CLA 2 608



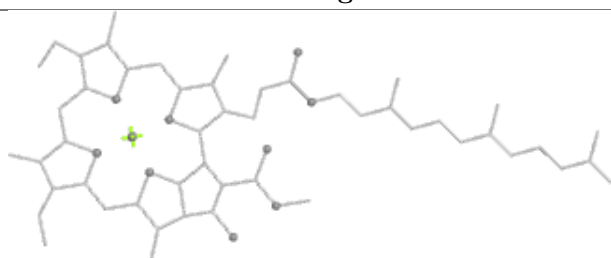
Bond lengths



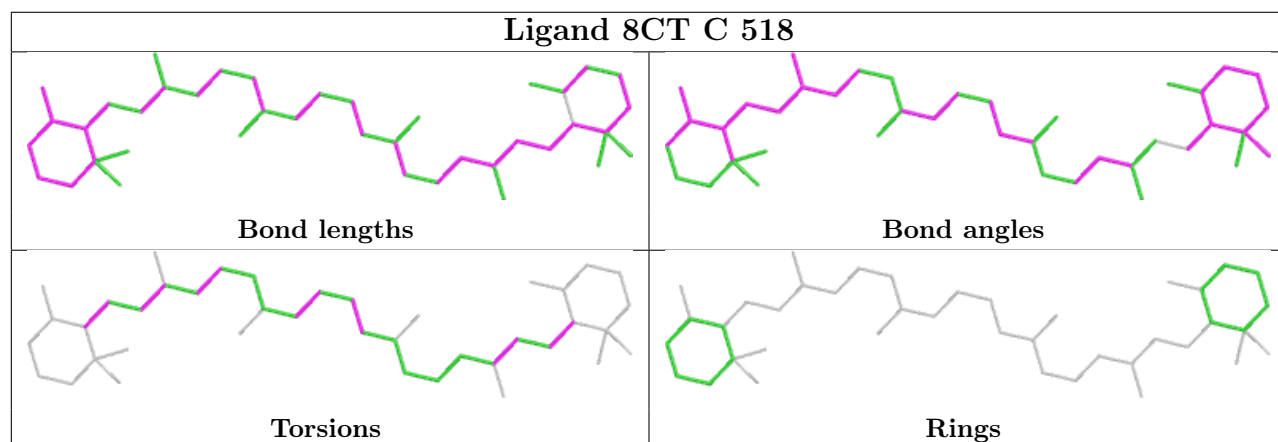
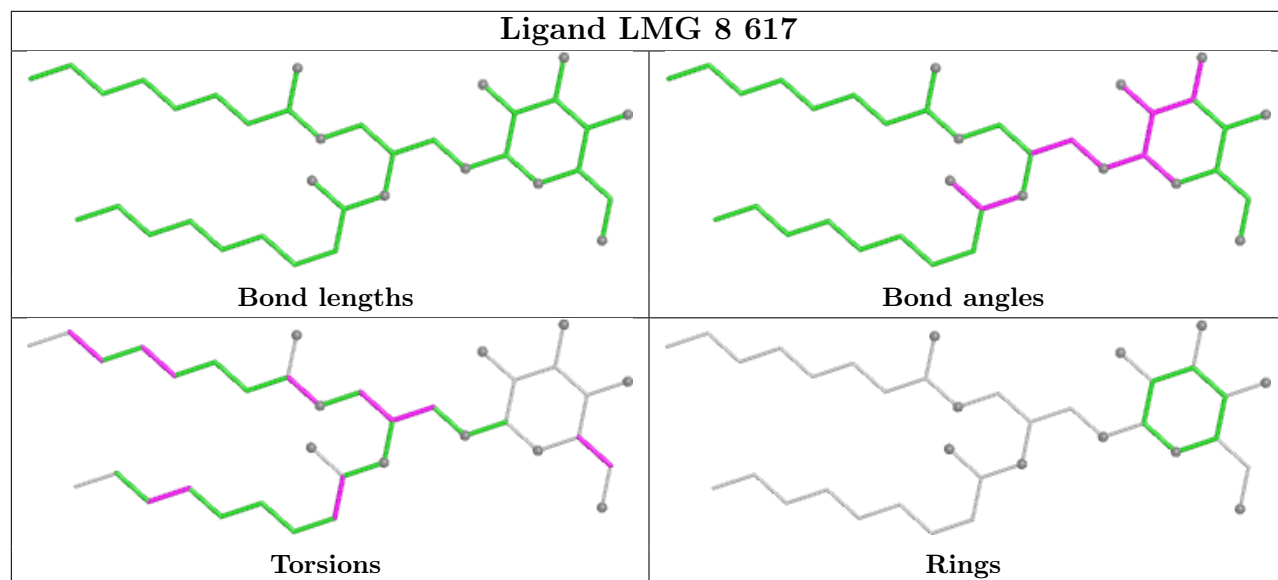
Bond angles

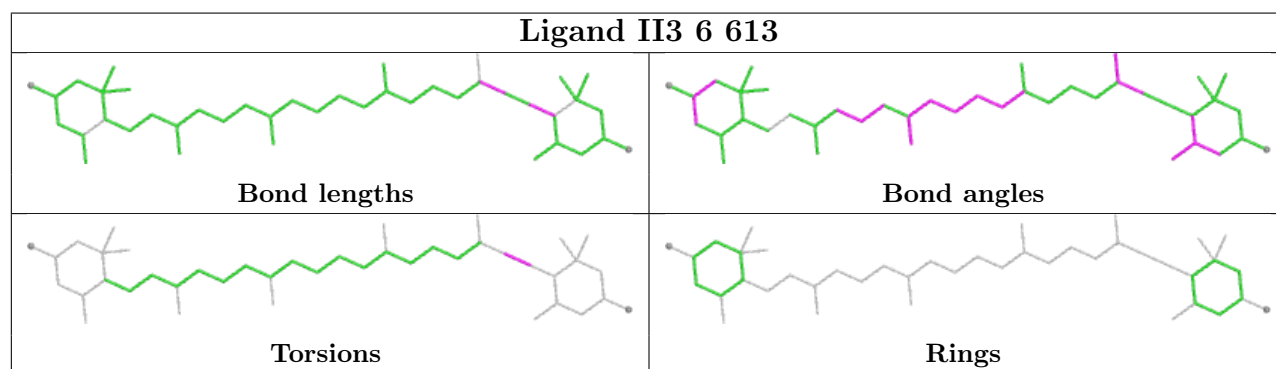
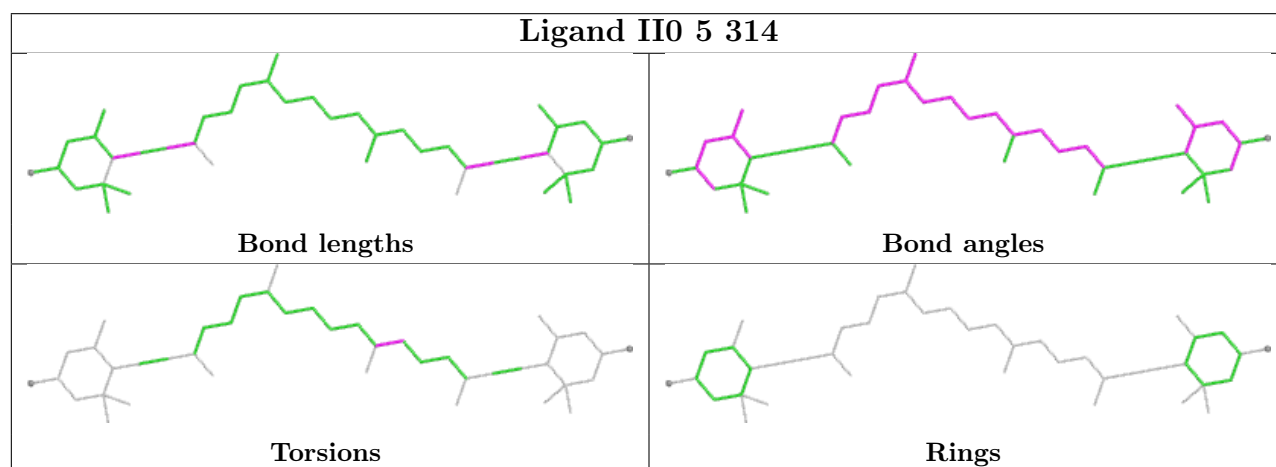
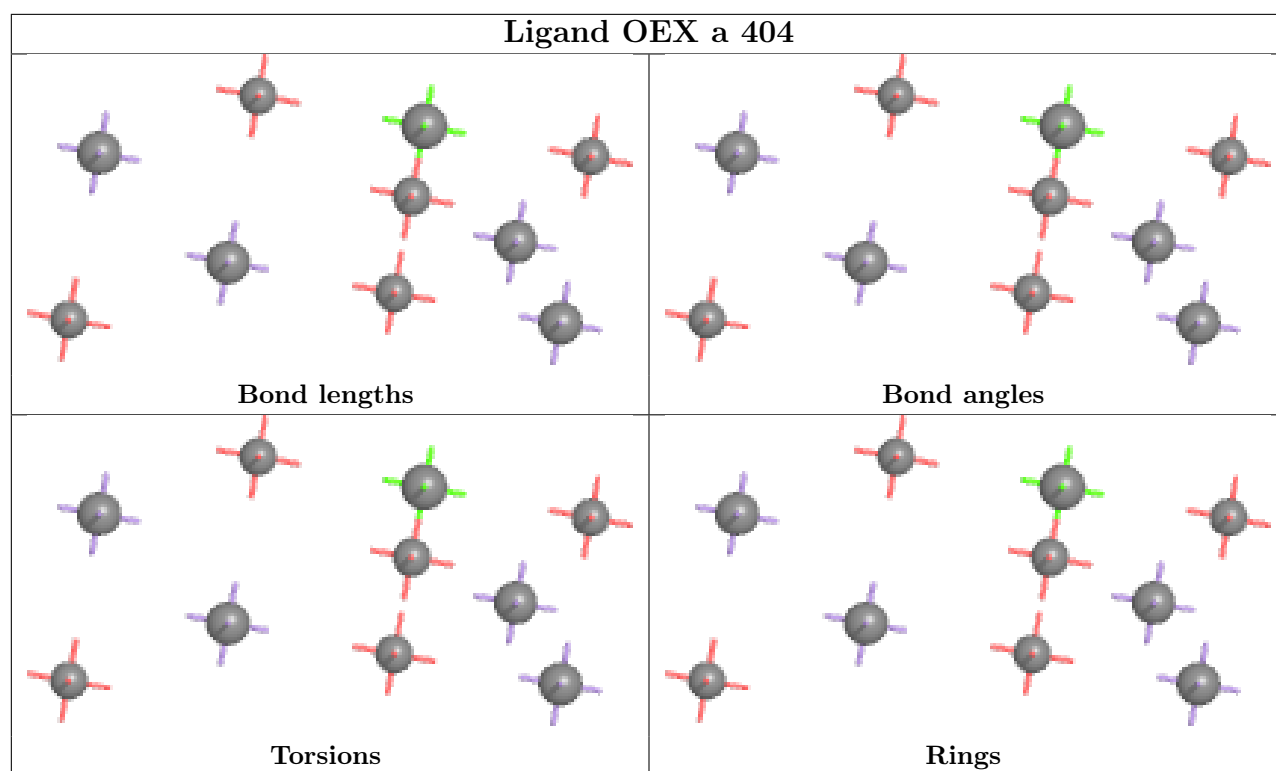


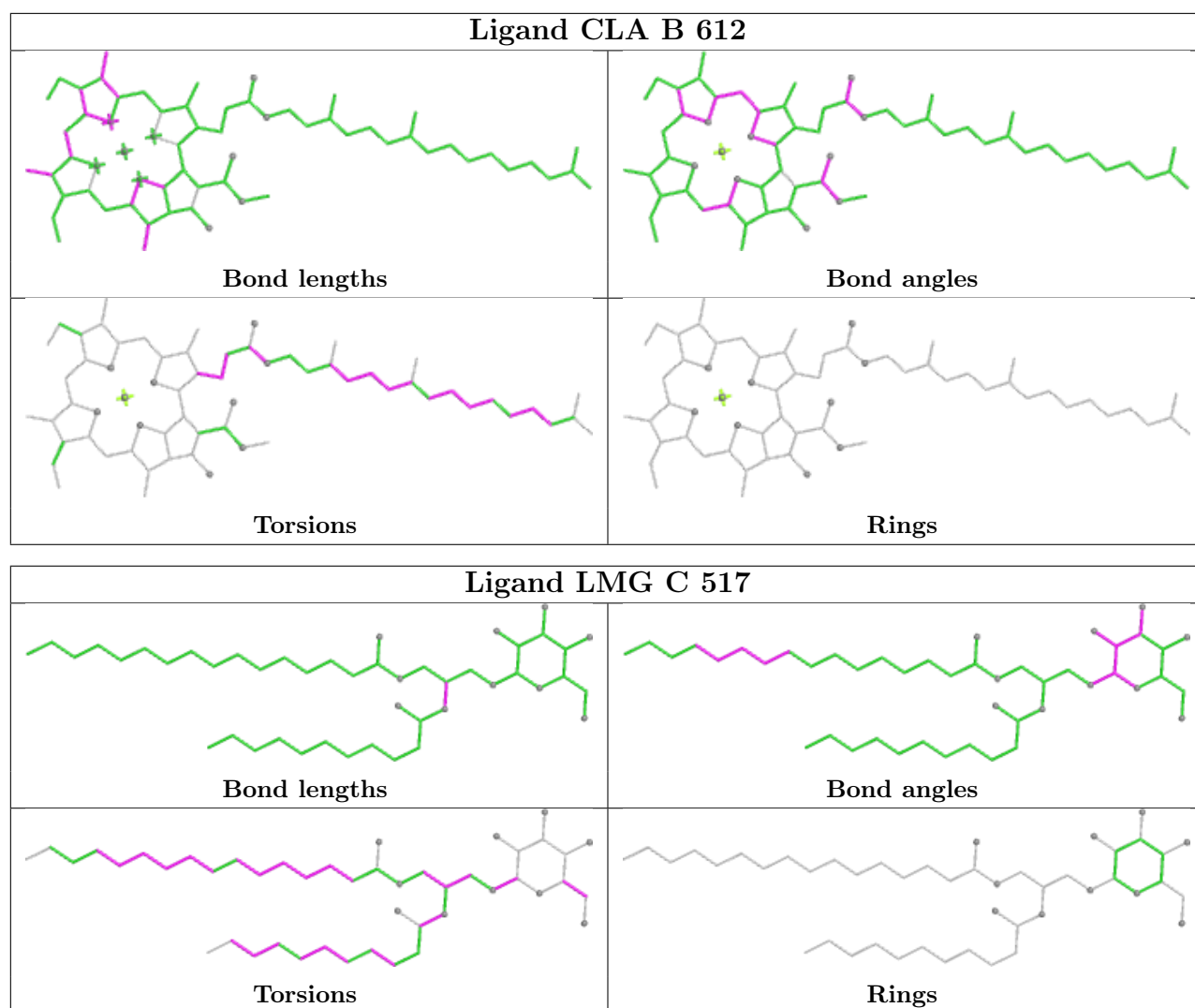
Torsions



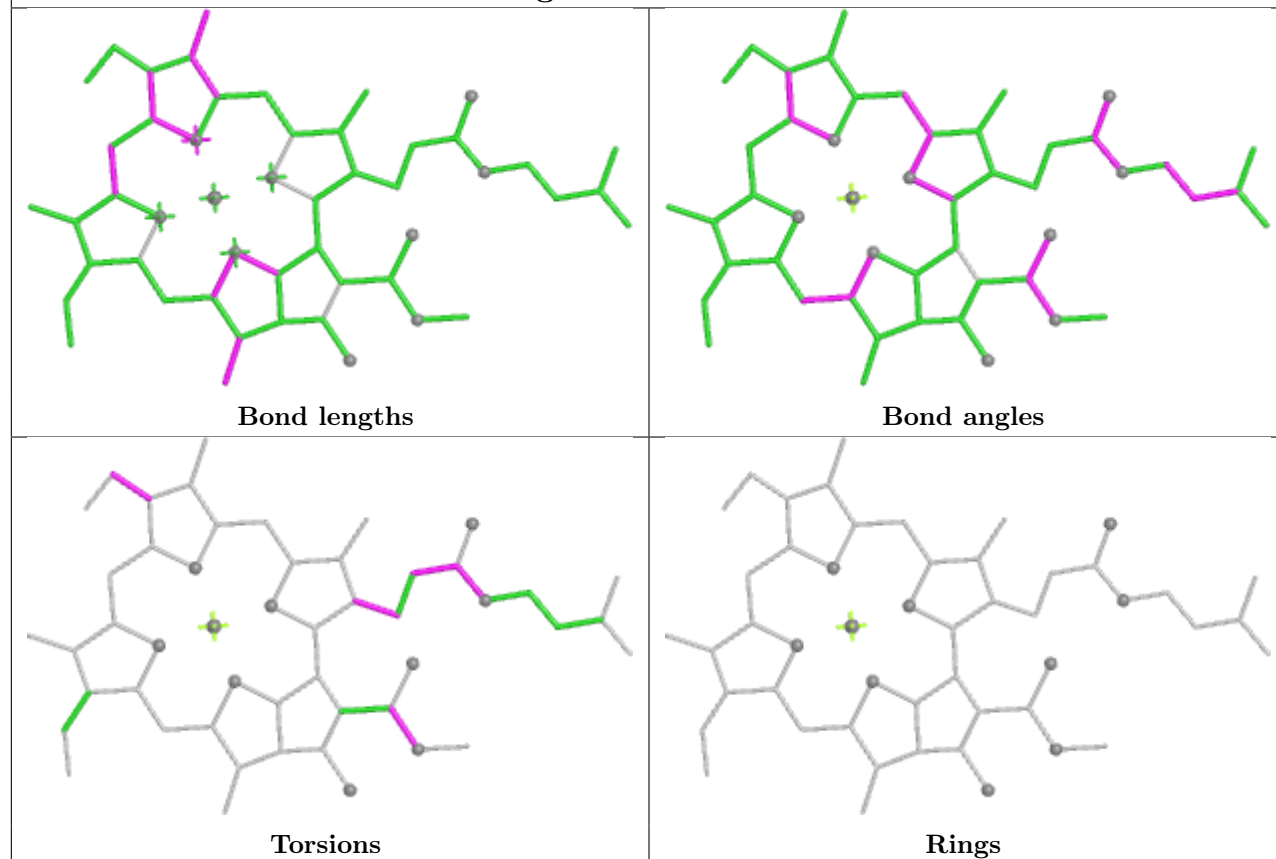
Rings



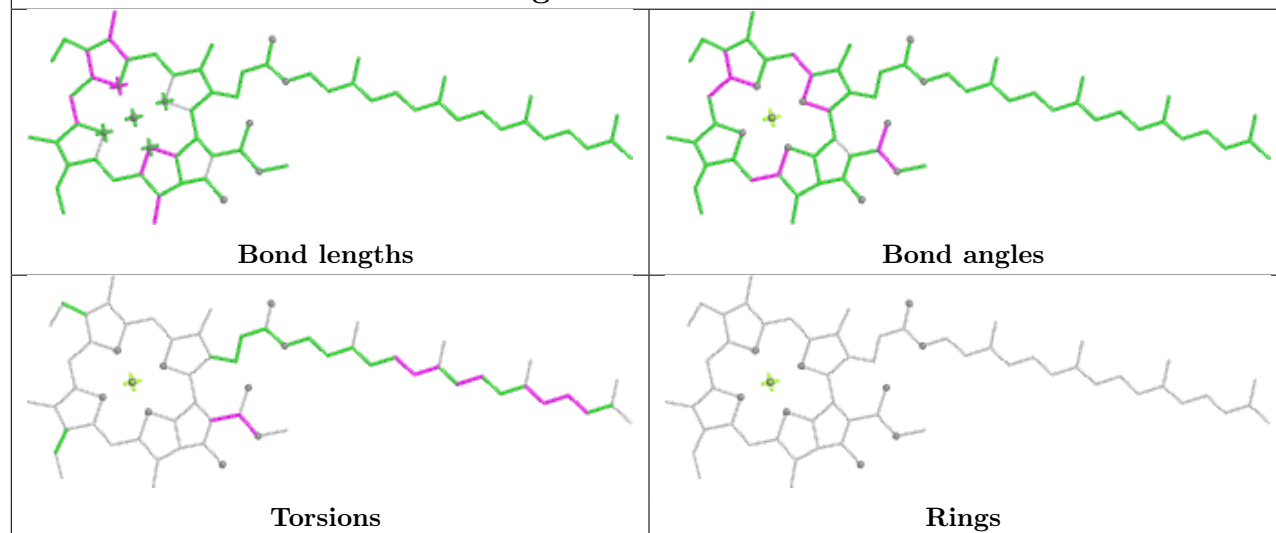




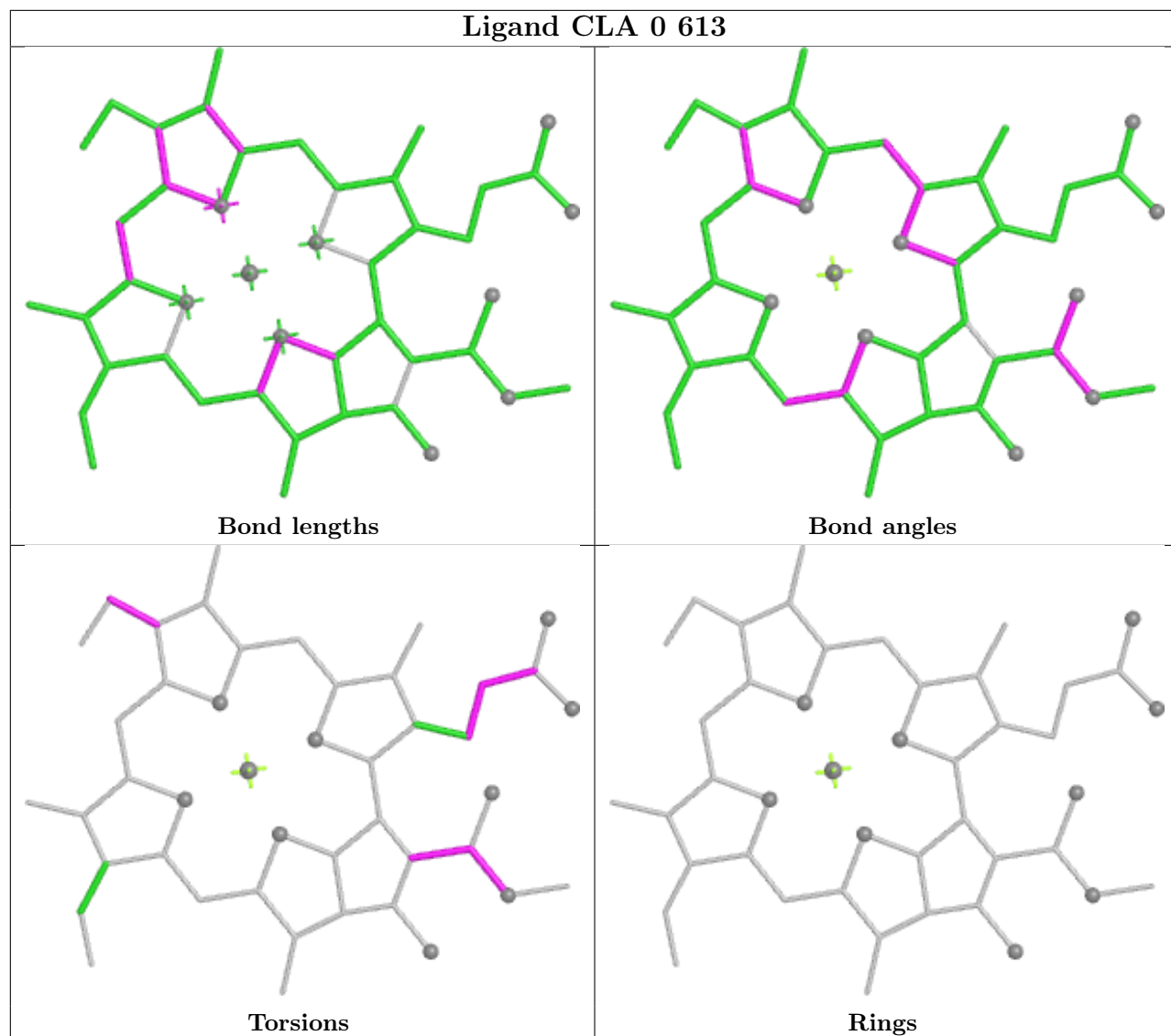
Ligand CLA 7 605



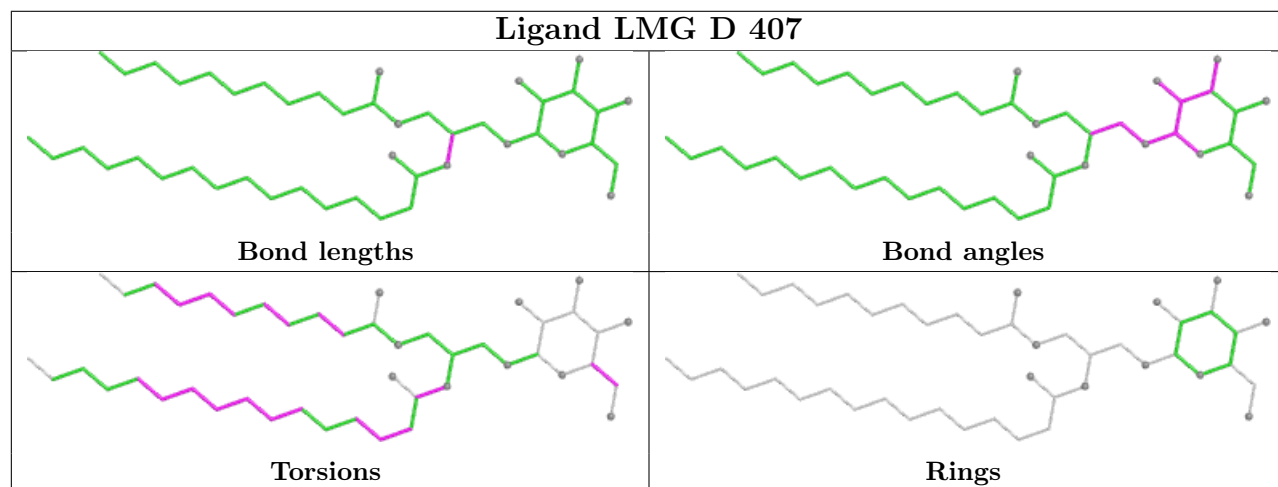
Ligand CLA B 606



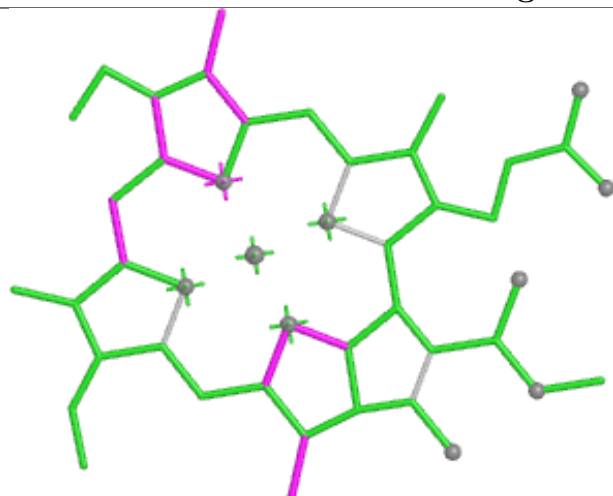
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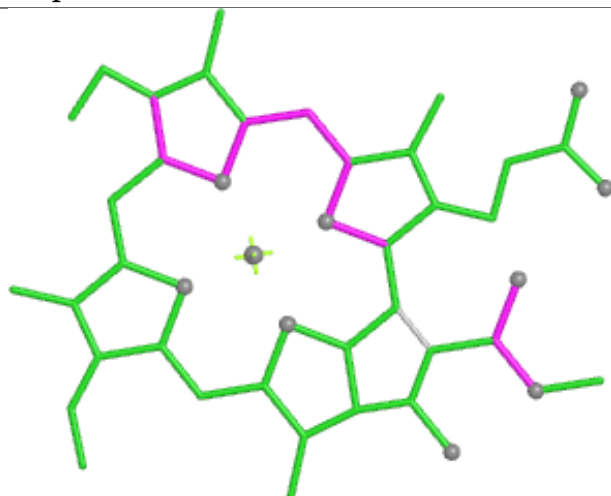
Ligand LMG D 407



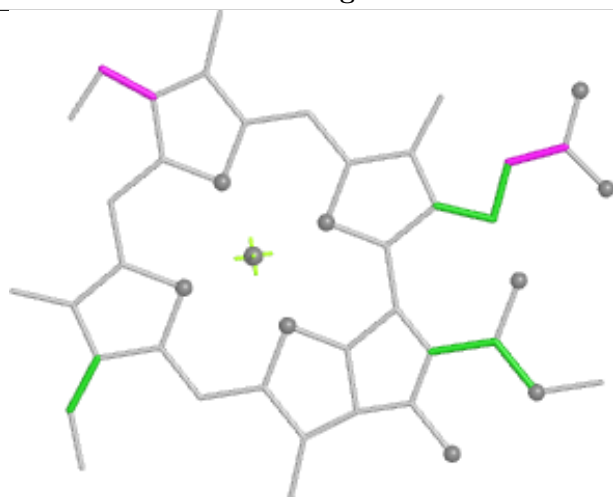
Ligand CLA p 307



Bond lengths



Bond angles

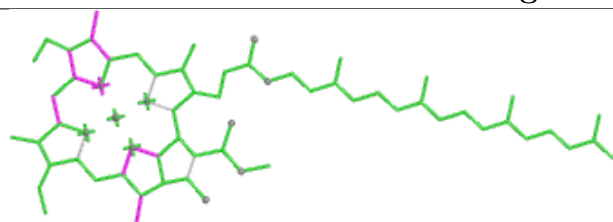


Torsions

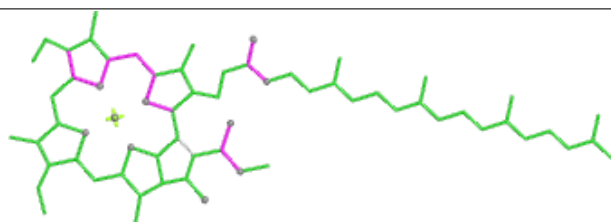


Rings

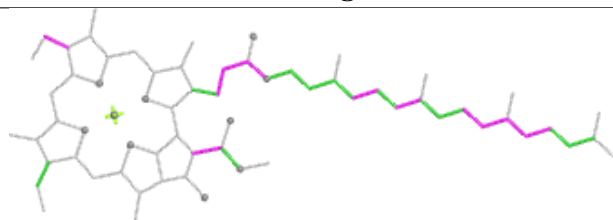
Ligand CLA s 303



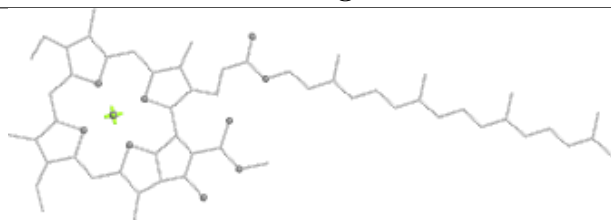
Bond lengths



Bond angles

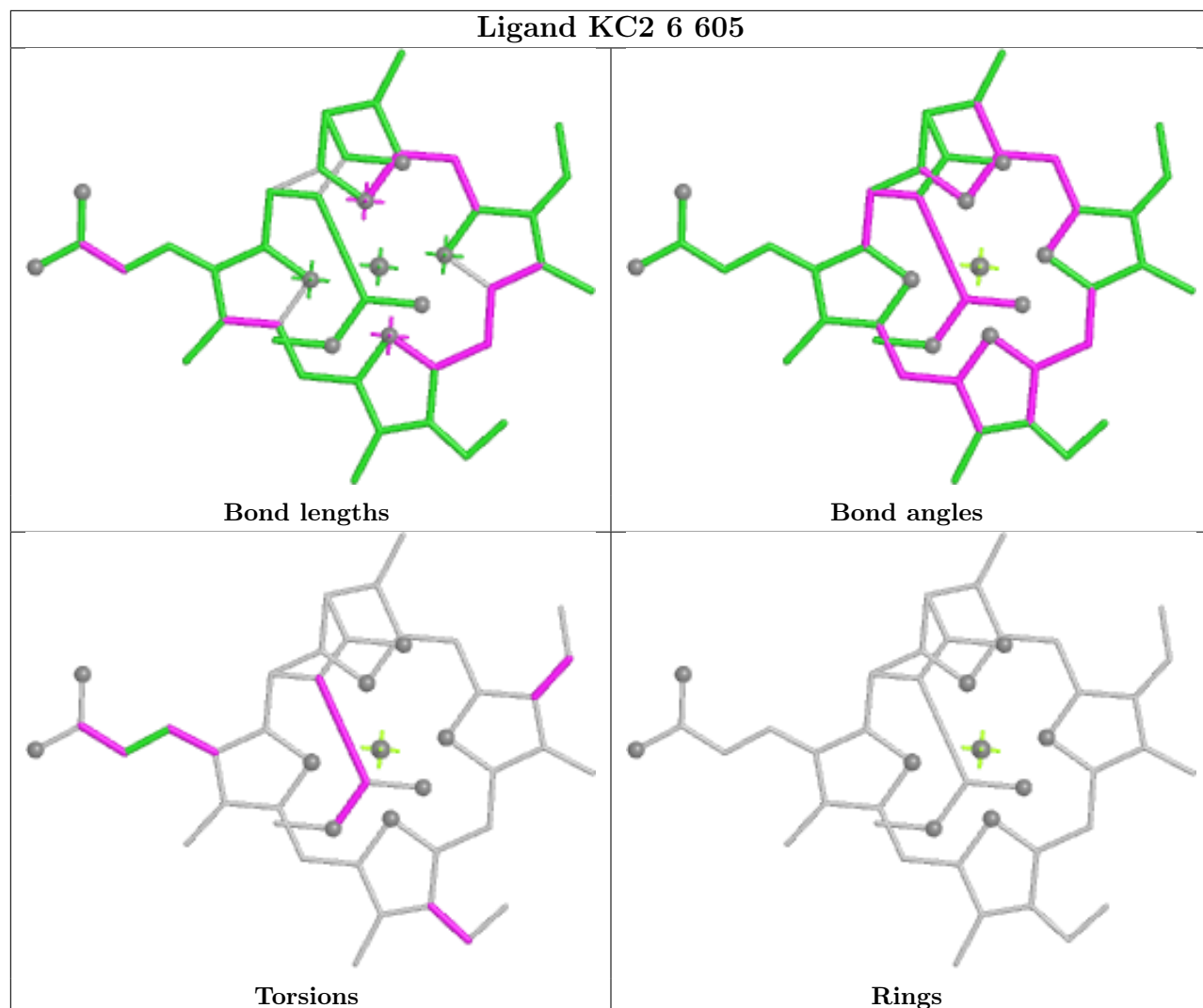


Torsions

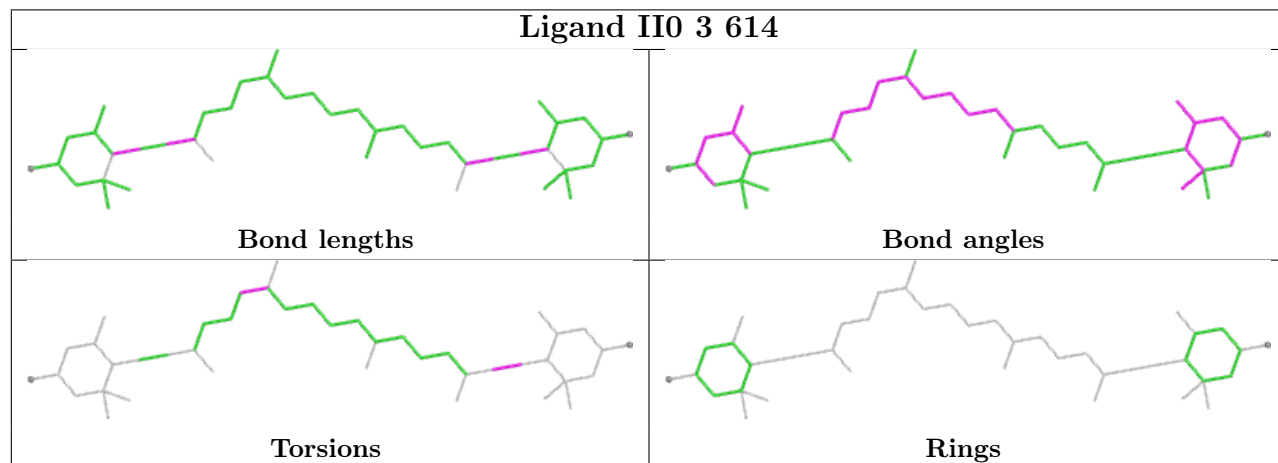


Rings

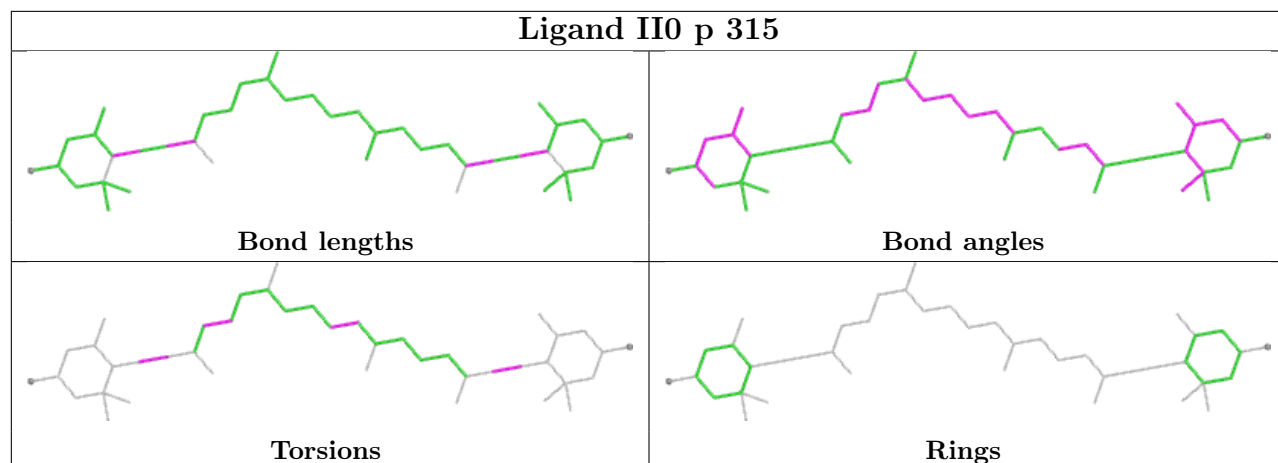
Ligand KC2 6 605



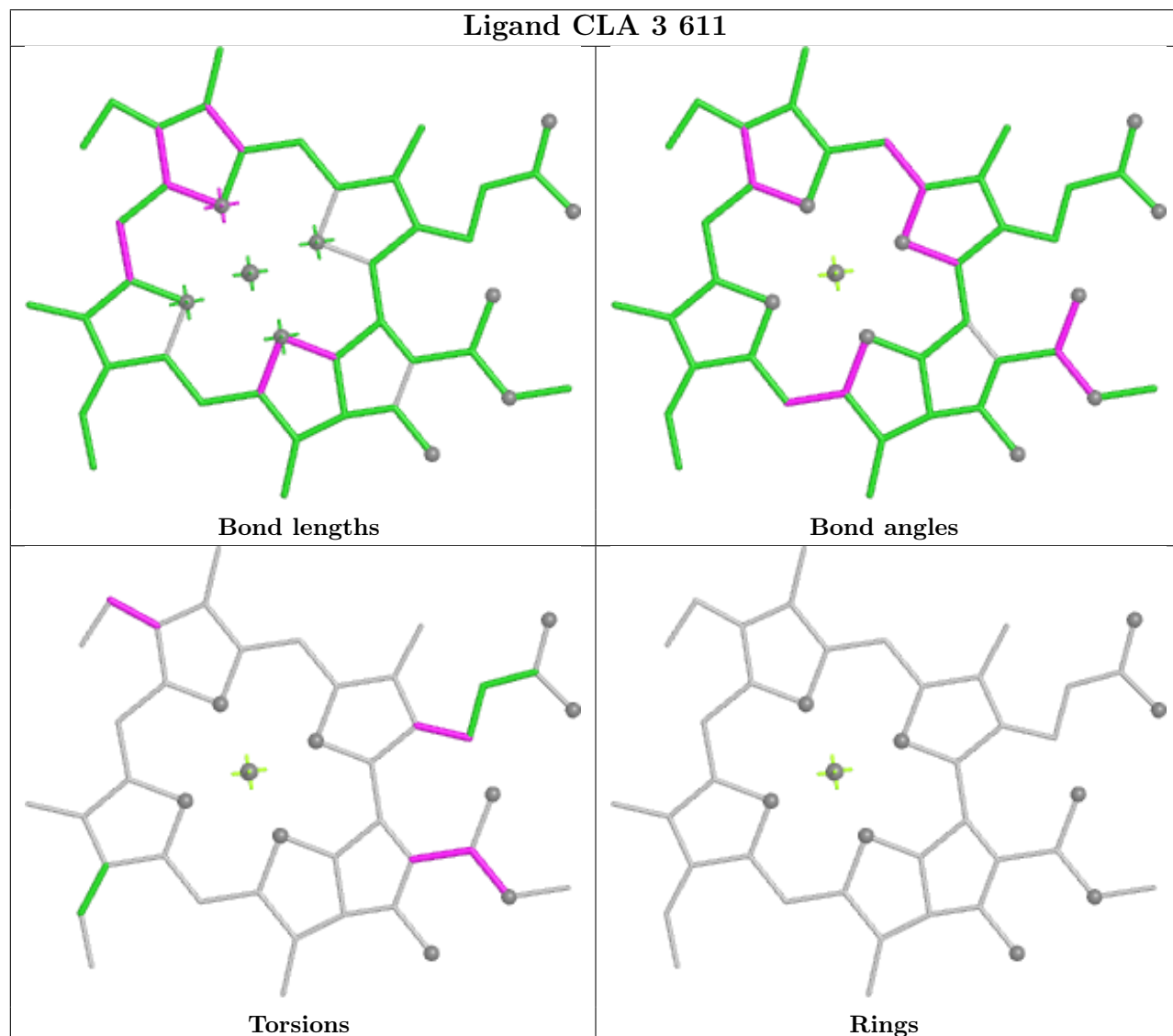
Ligand II0 3 614



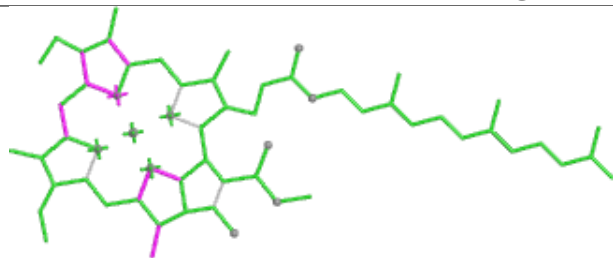
Ligand II0 p 315



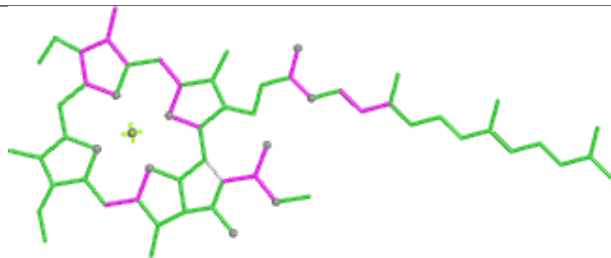
Ligand CLA 3 611



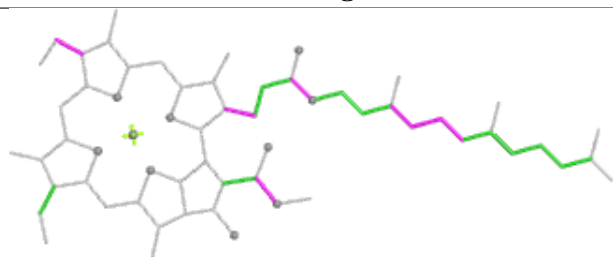
Ligand CLA D 404



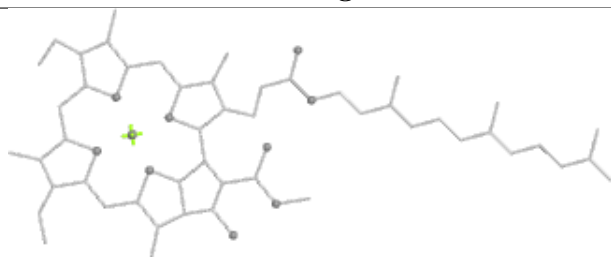
Bond lengths



Bond angles

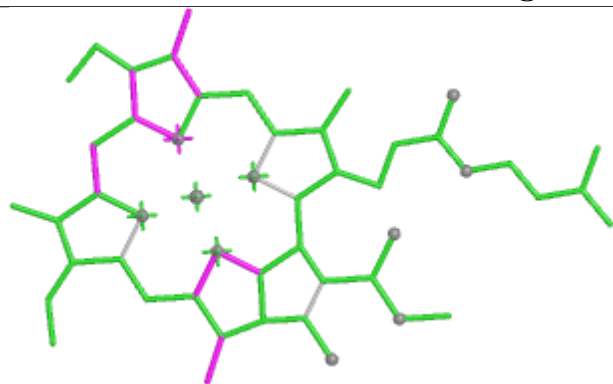


Torsions

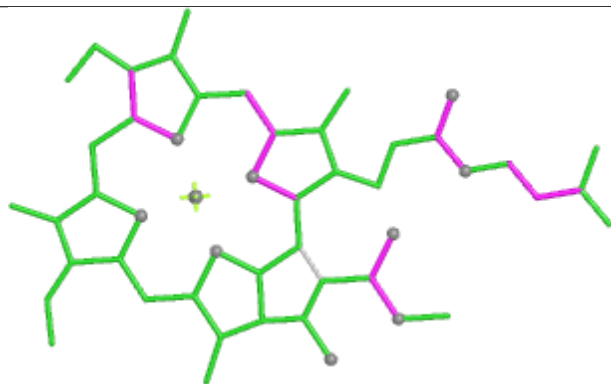


Rings

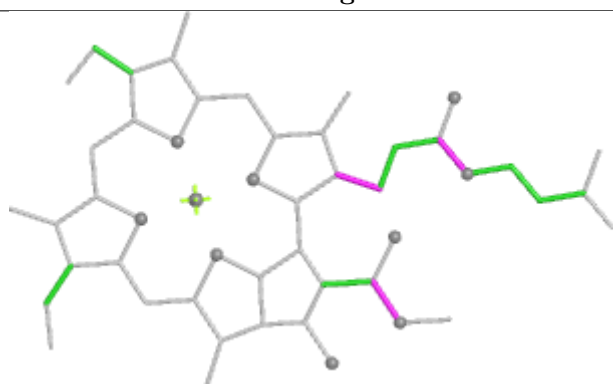
Ligand CLA 3 603



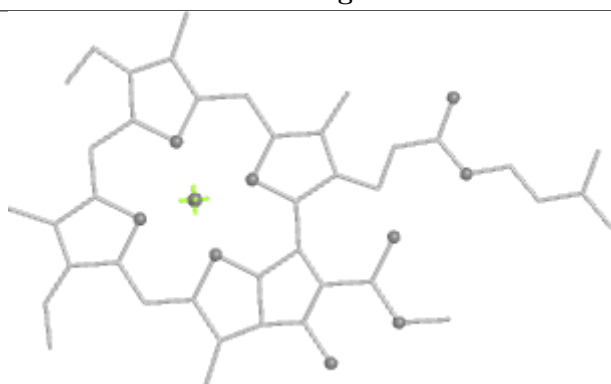
Bond lengths



Bond angles

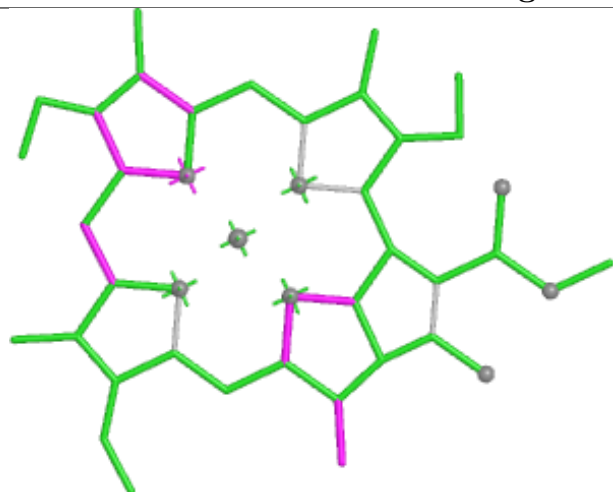


Torsions

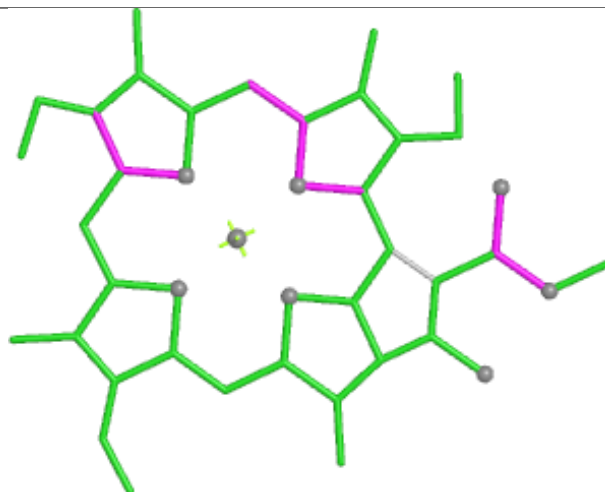


Rings

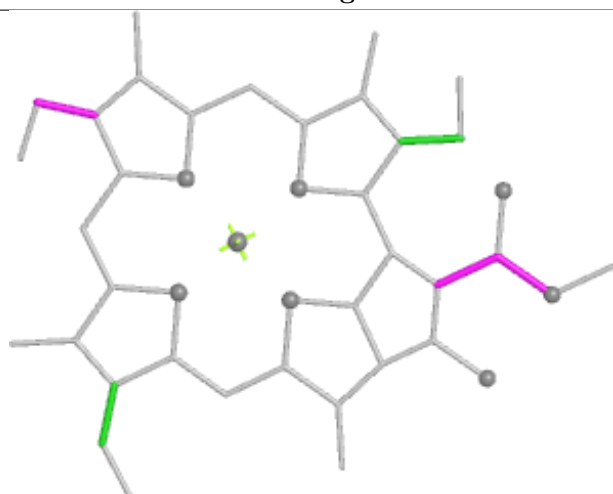
Ligand CLA 5 302



Bond lengths



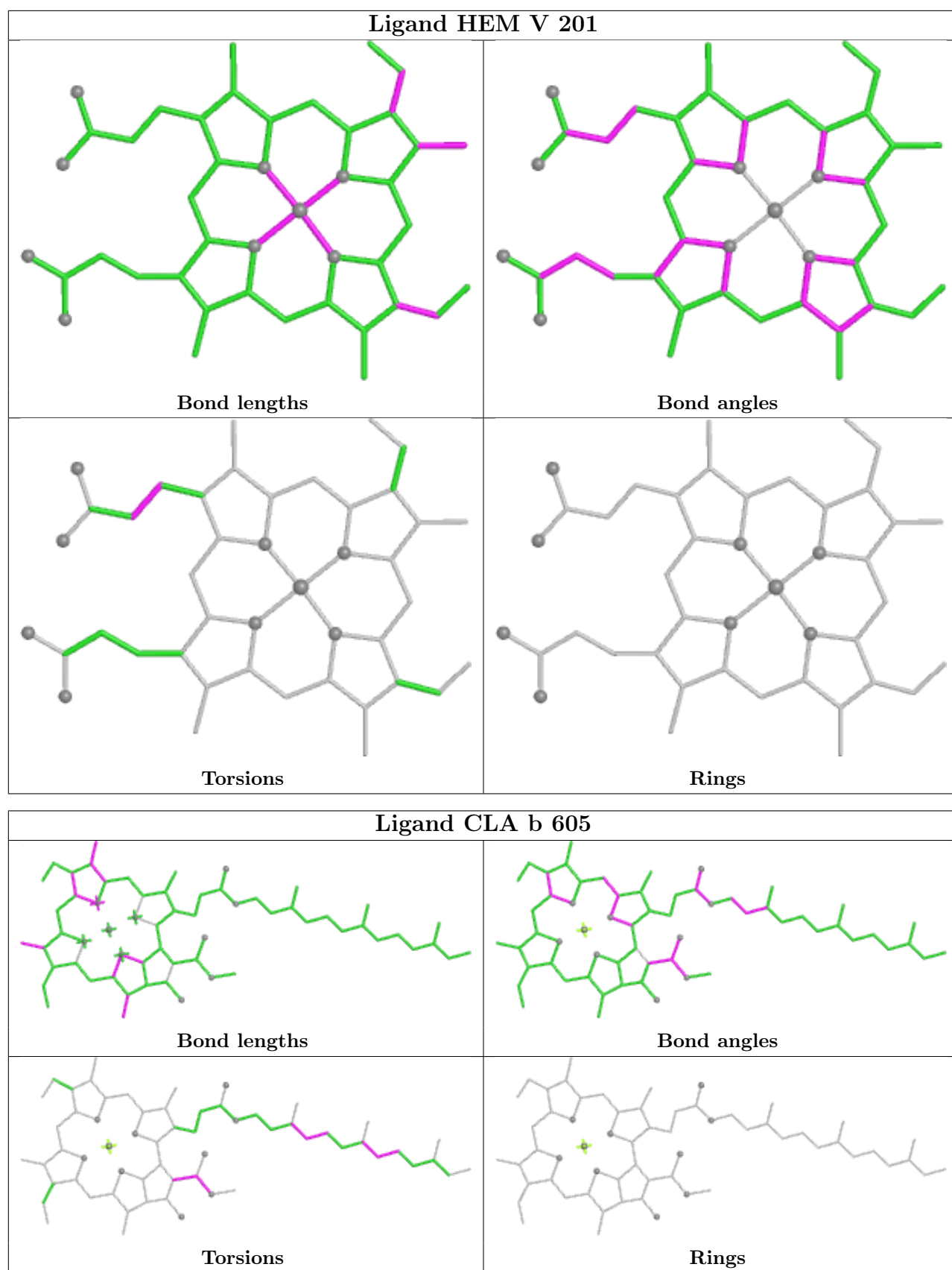
Bond angles



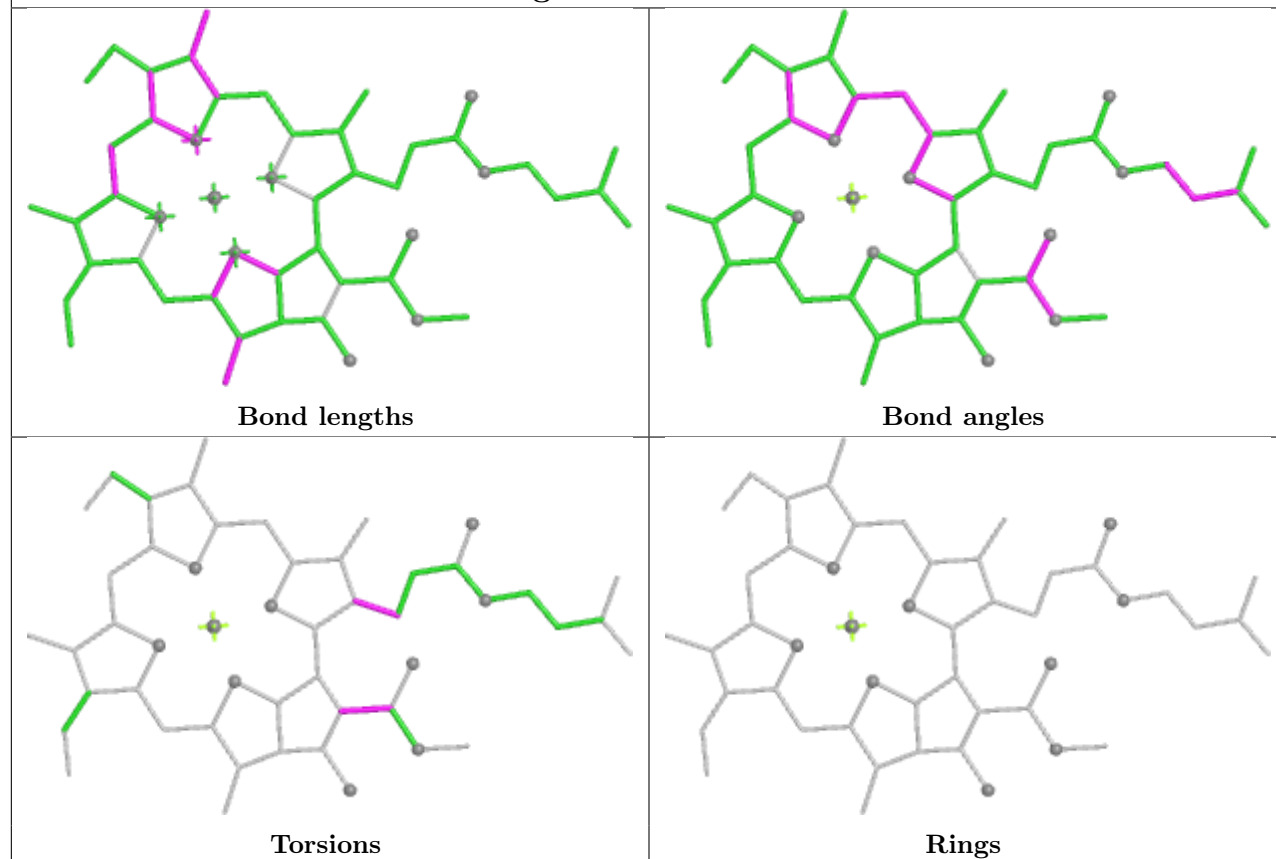
Torsions



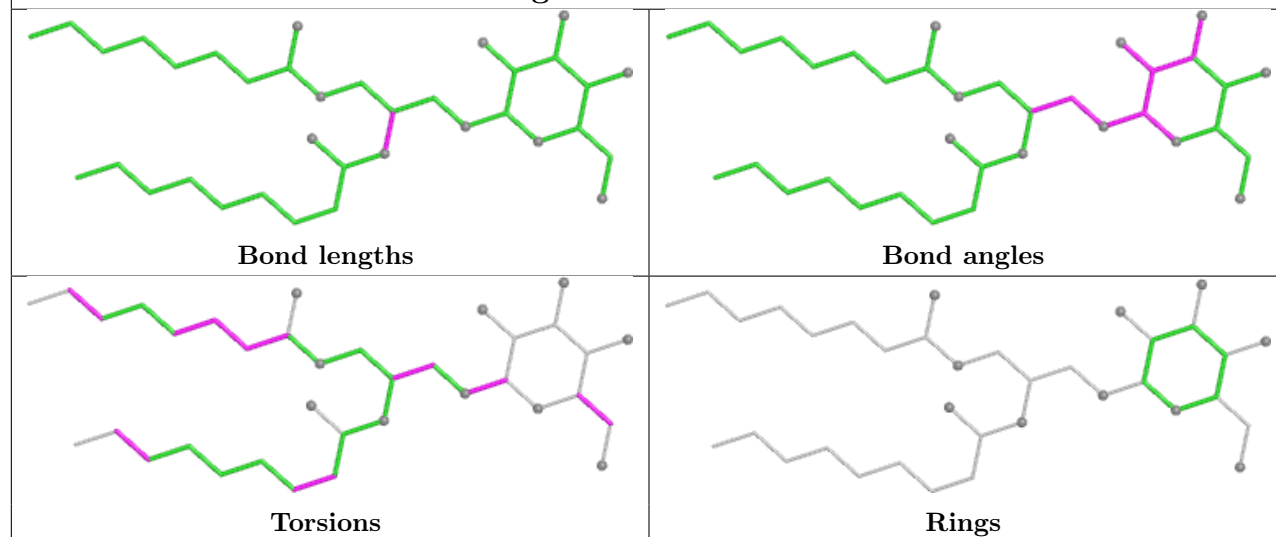
Rings

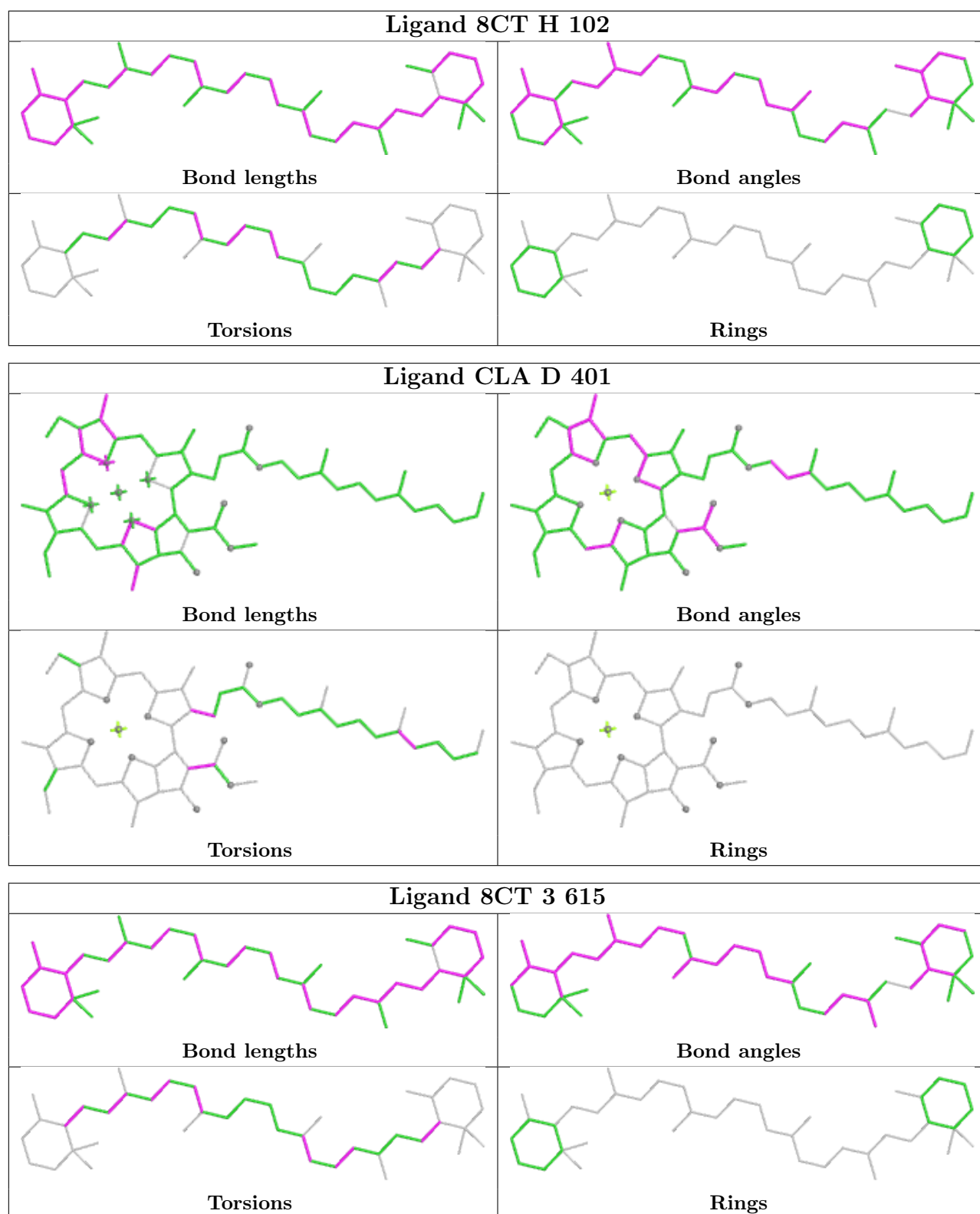


Ligand CLA P 603

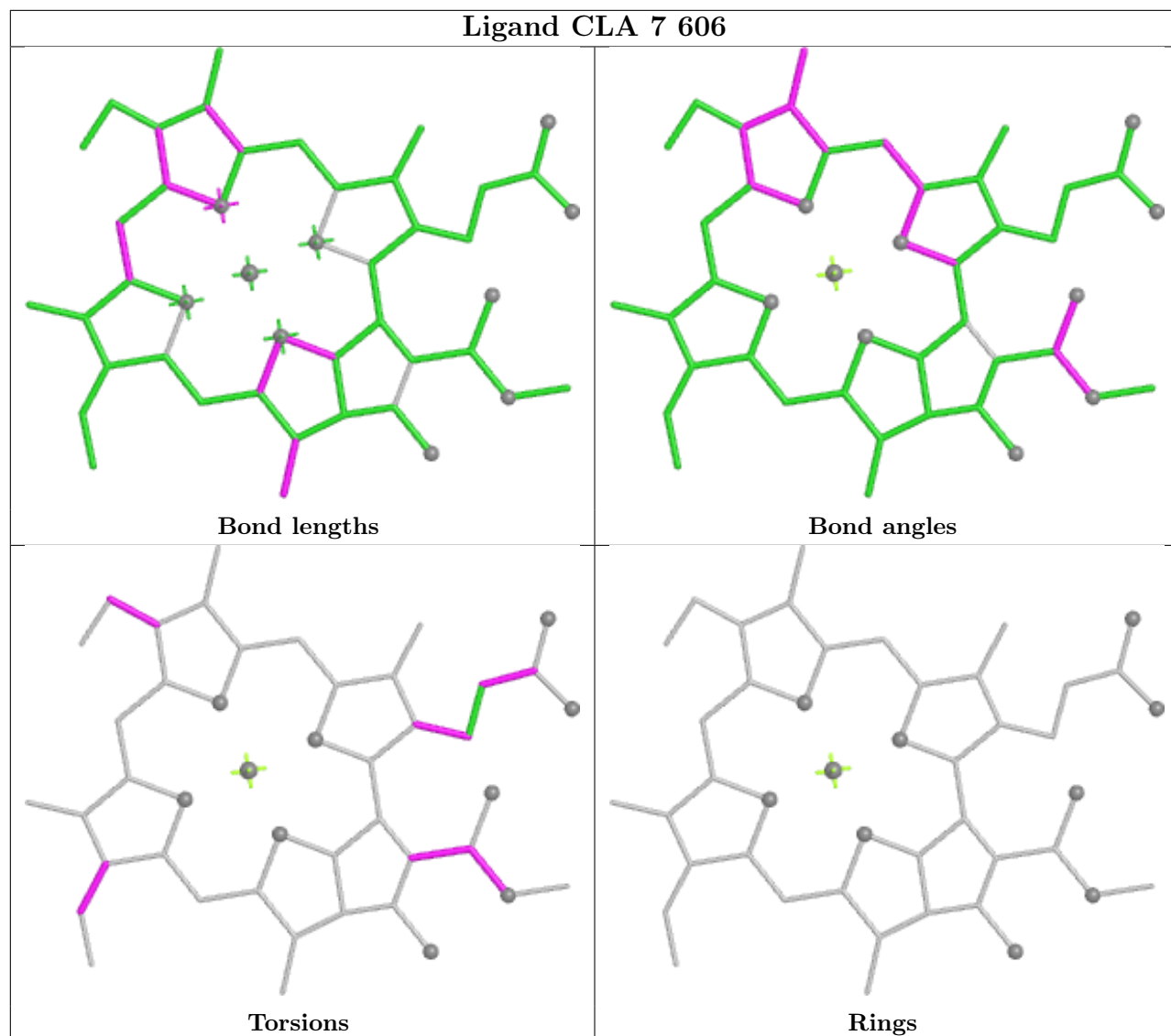


Ligand LMG 4 618

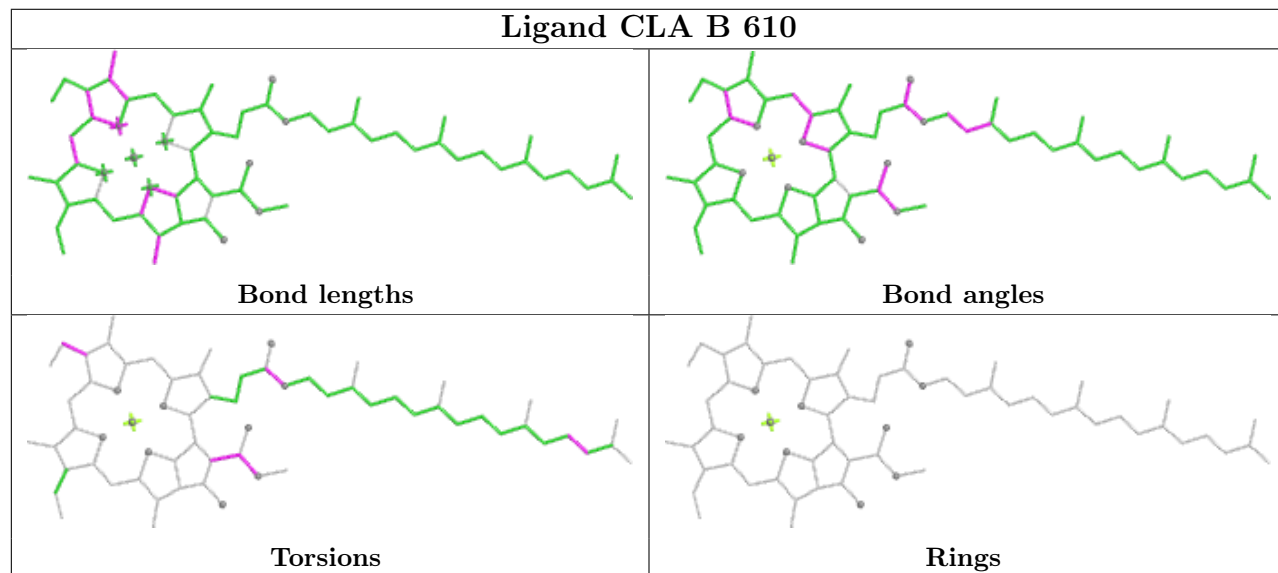




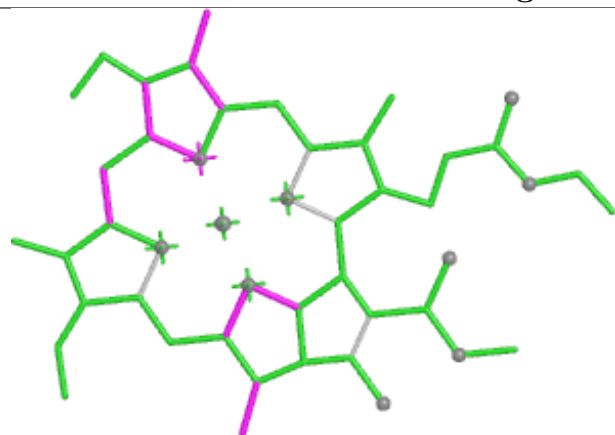
Ligand CLA 7 606



Ligand CLA B 610



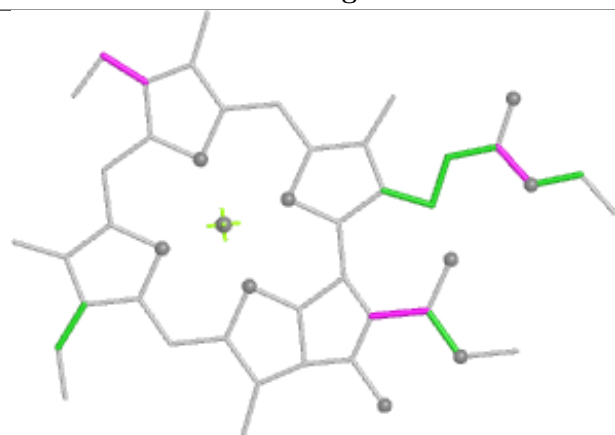
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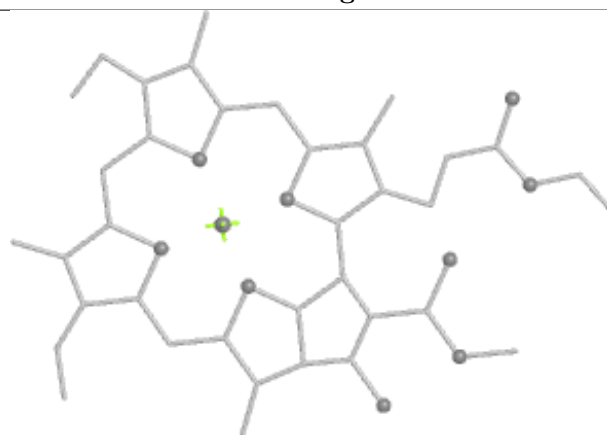
Bond lengths



Bond angles

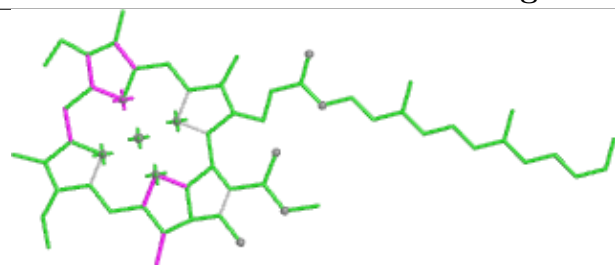


Torsions

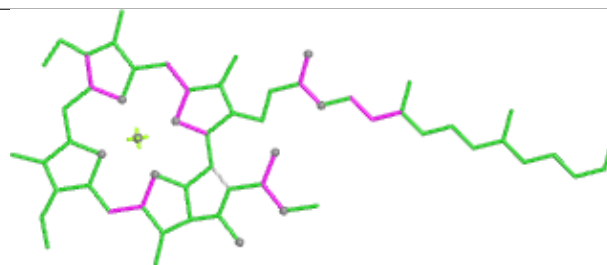


Rings

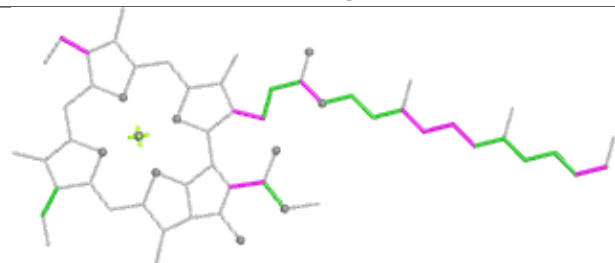
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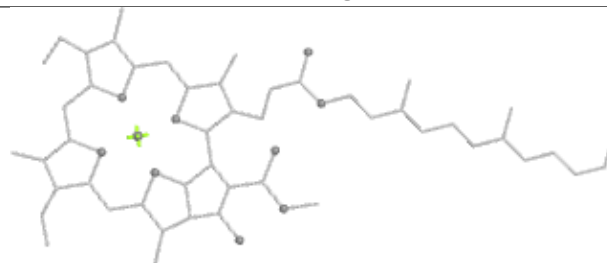
Bond lengths



Bond angles

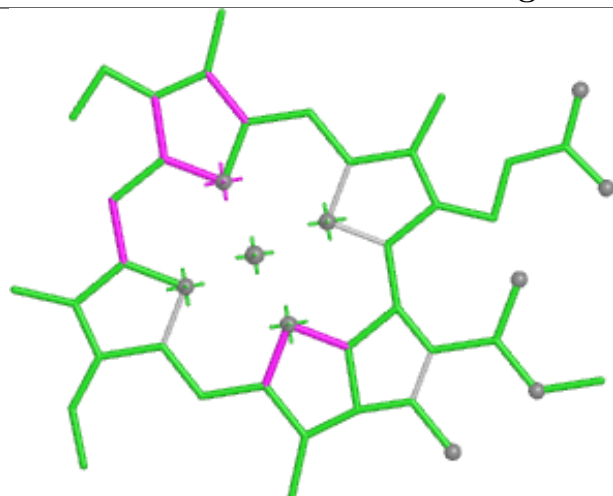


Torsions

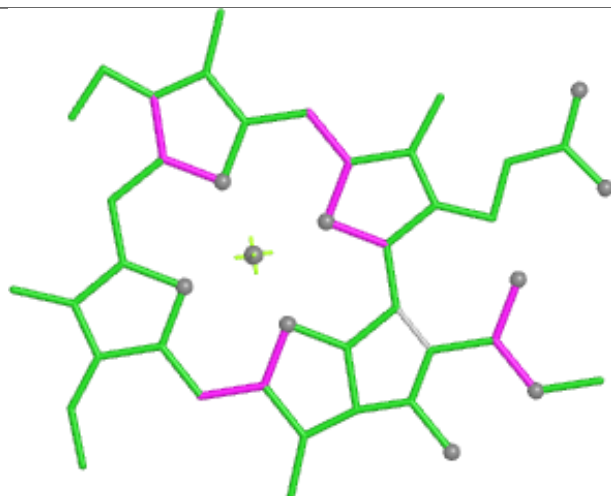


Rings

Ligand CLA 6 611



Bond lengths



Bond angles

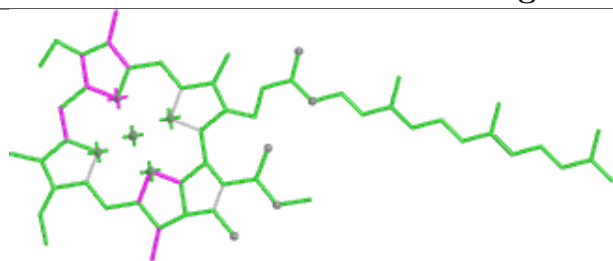


Torsions

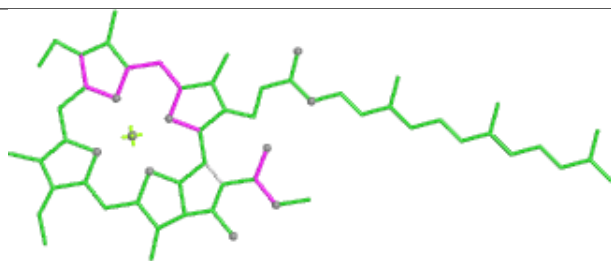


Rings

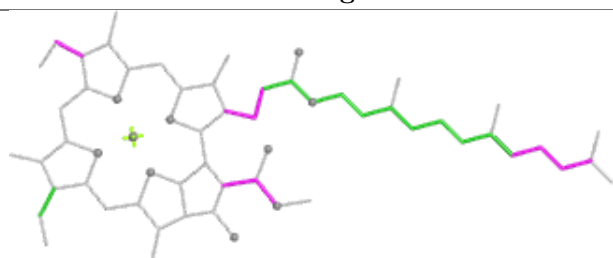
Ligand CLA 7 608



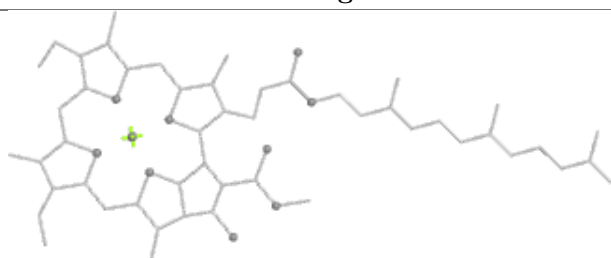
Bond lengths



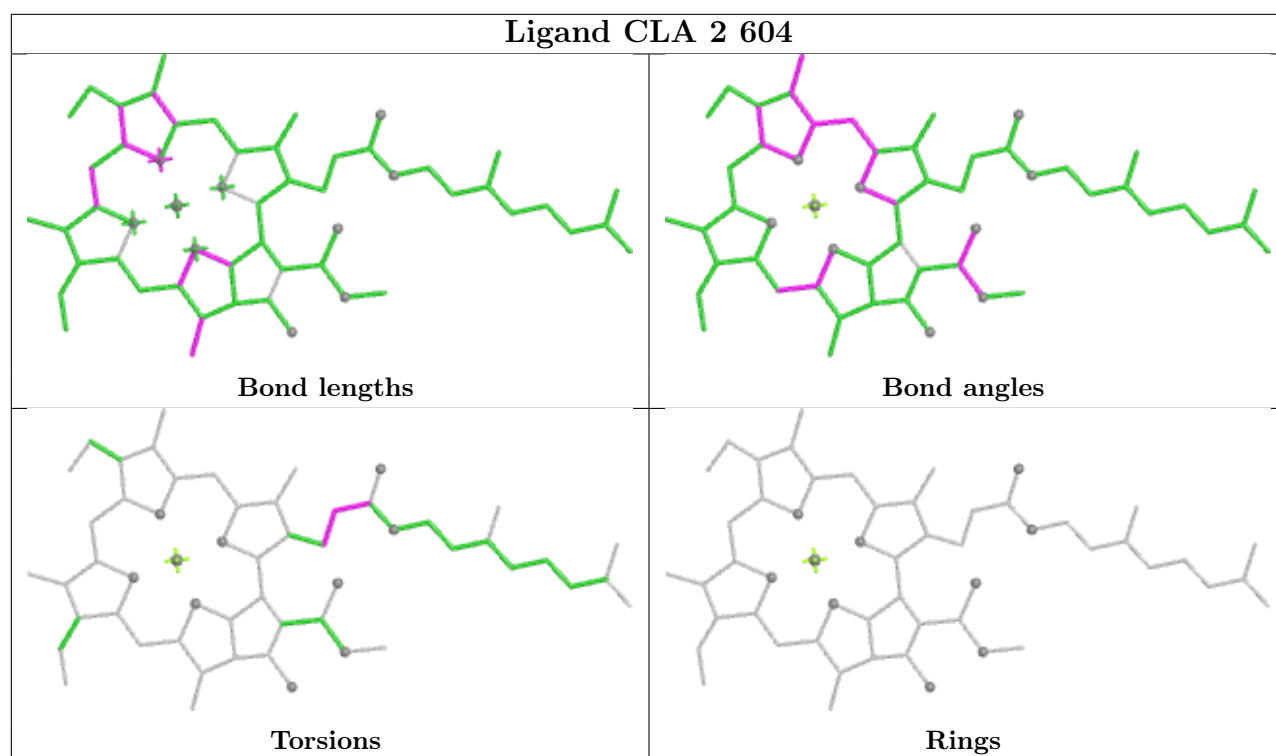
Bond angles



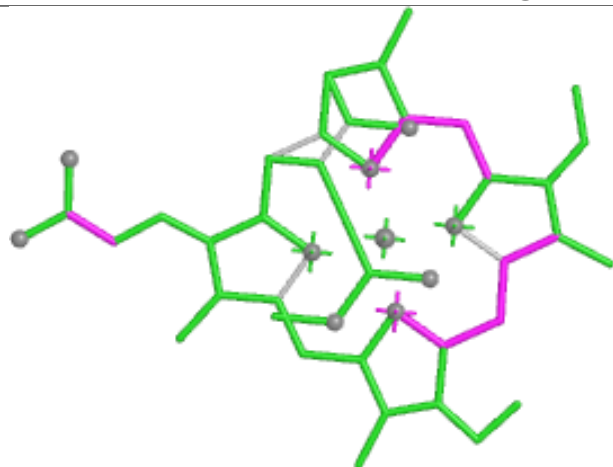
Torsions



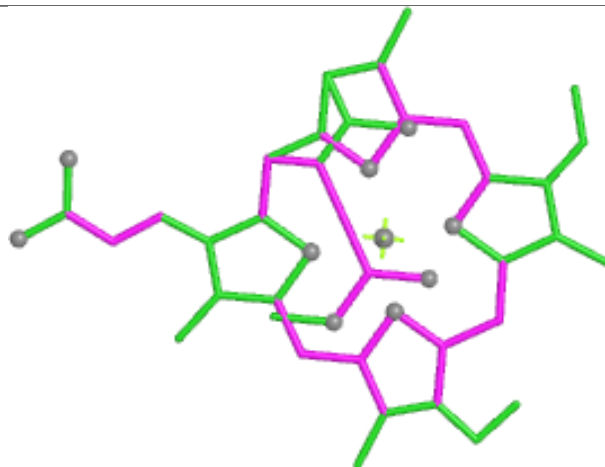
Rings



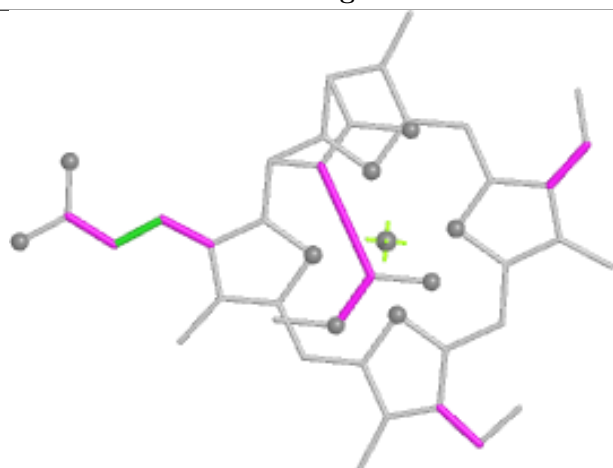
Ligand KC2 P 605



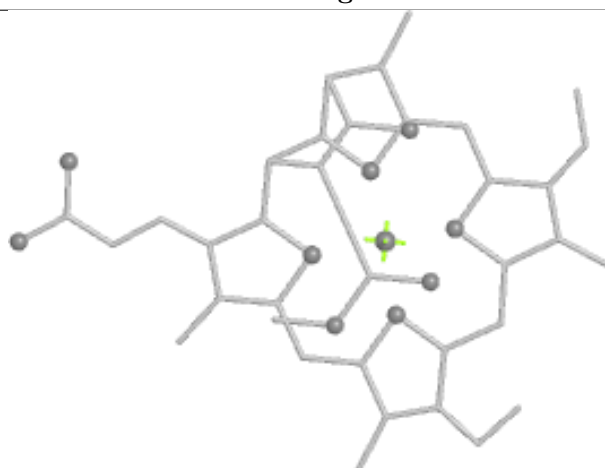
Bond lengths



Bond angles

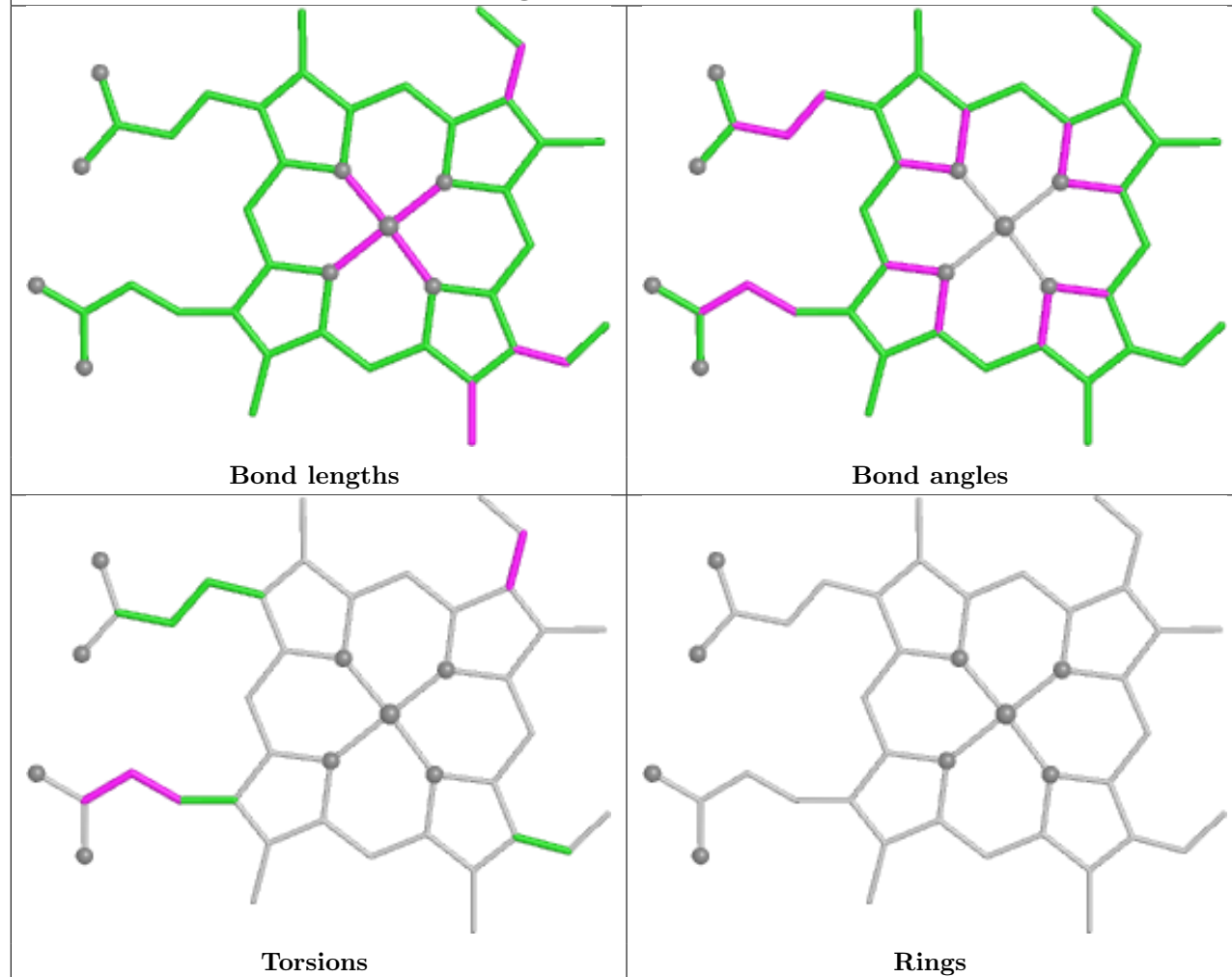


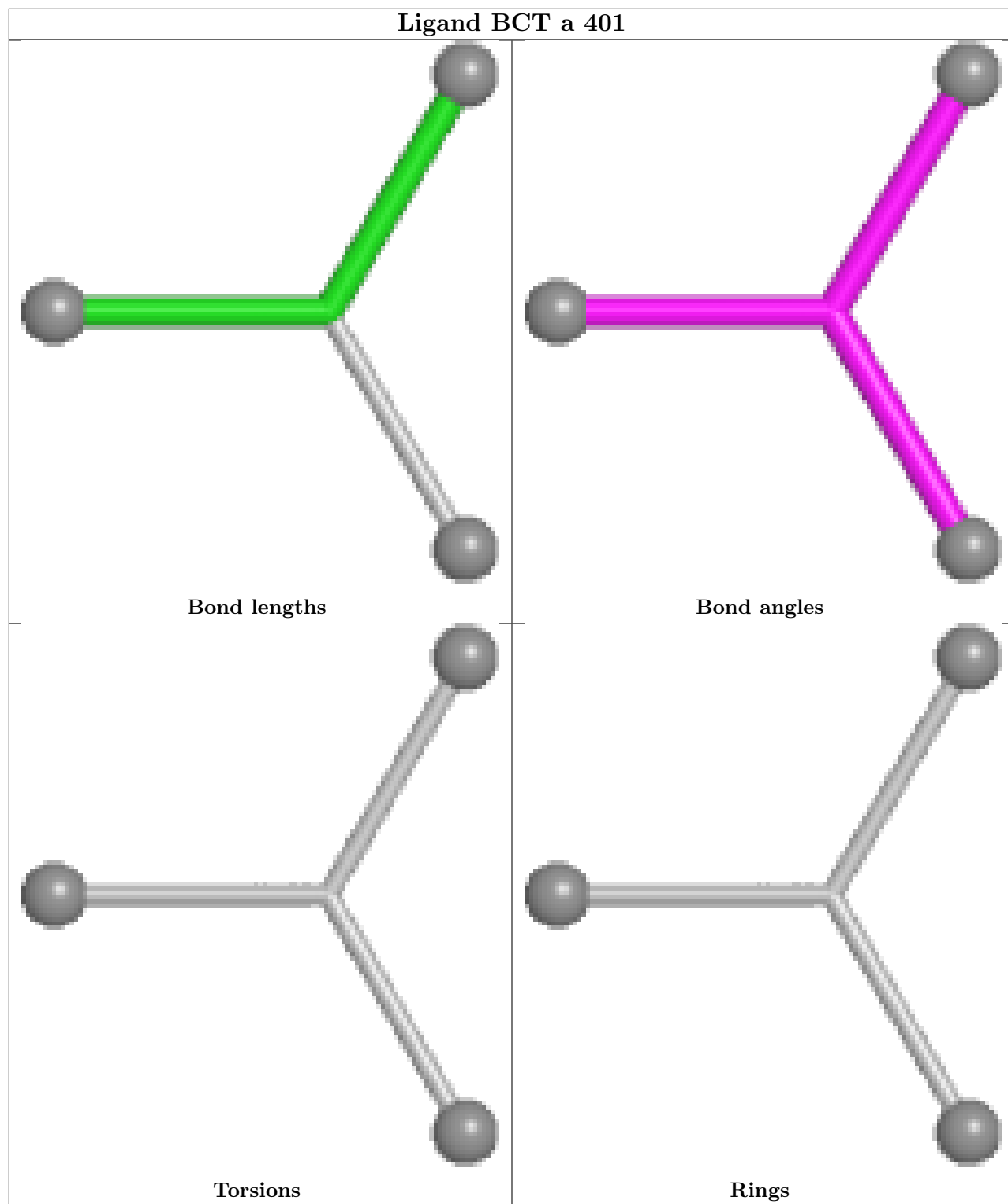
Torsions

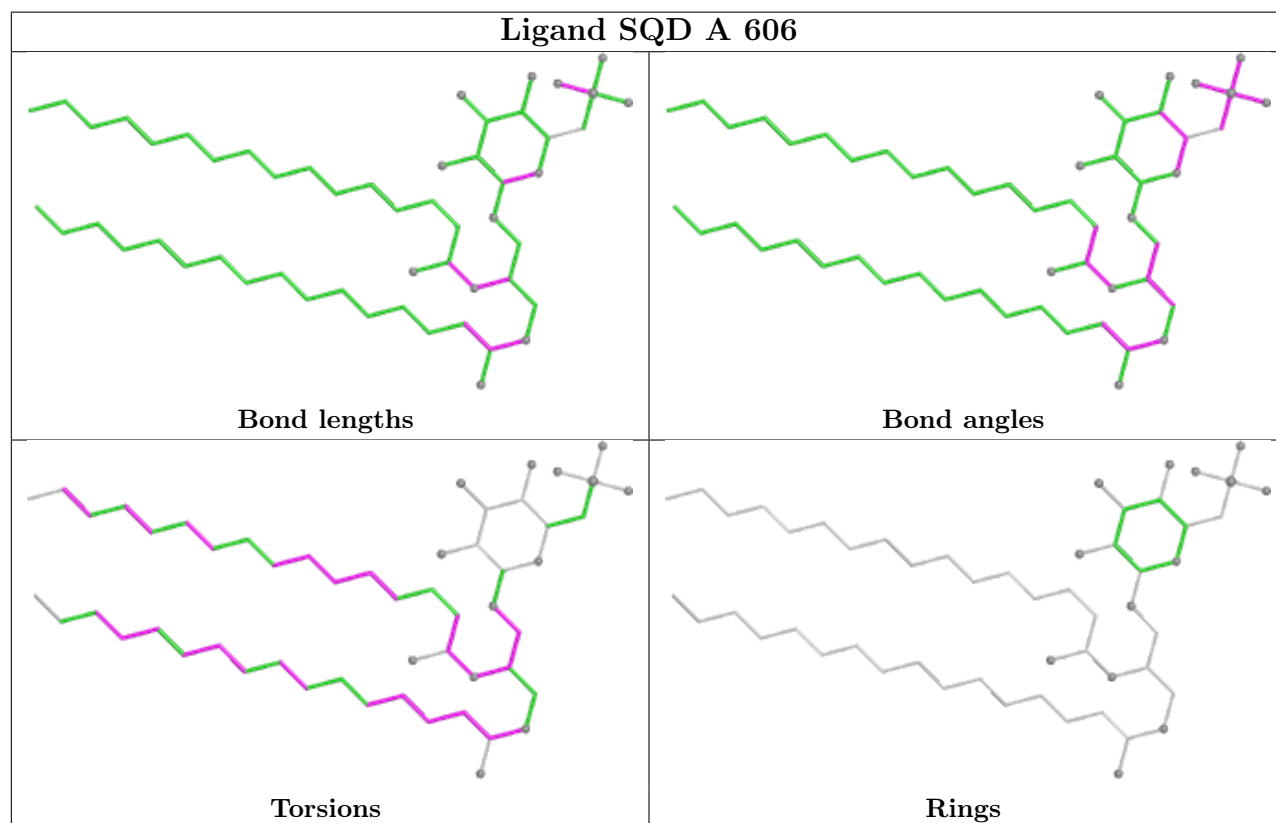
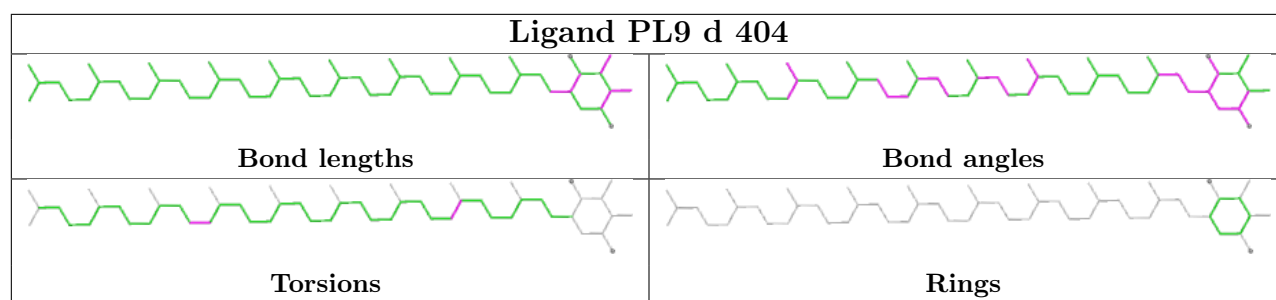


Rings

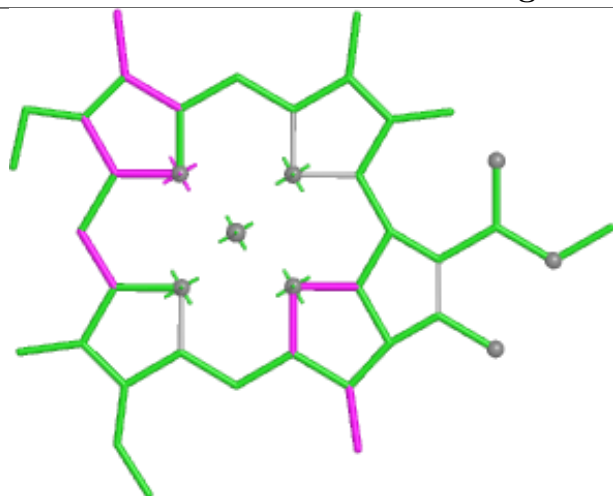
Ligand HEM f 101



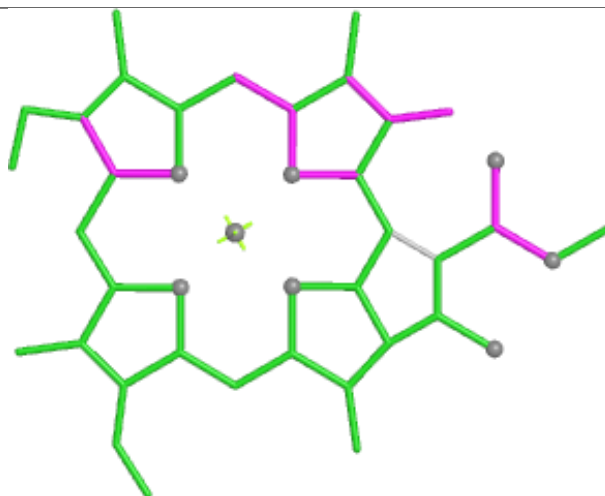




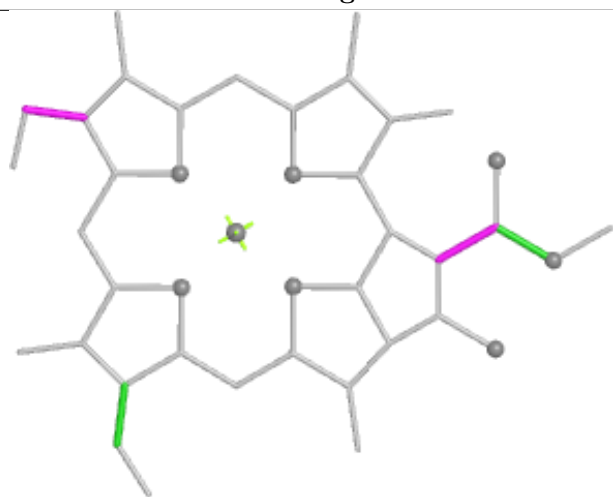
Ligand CLA 3 608



Bond lengths



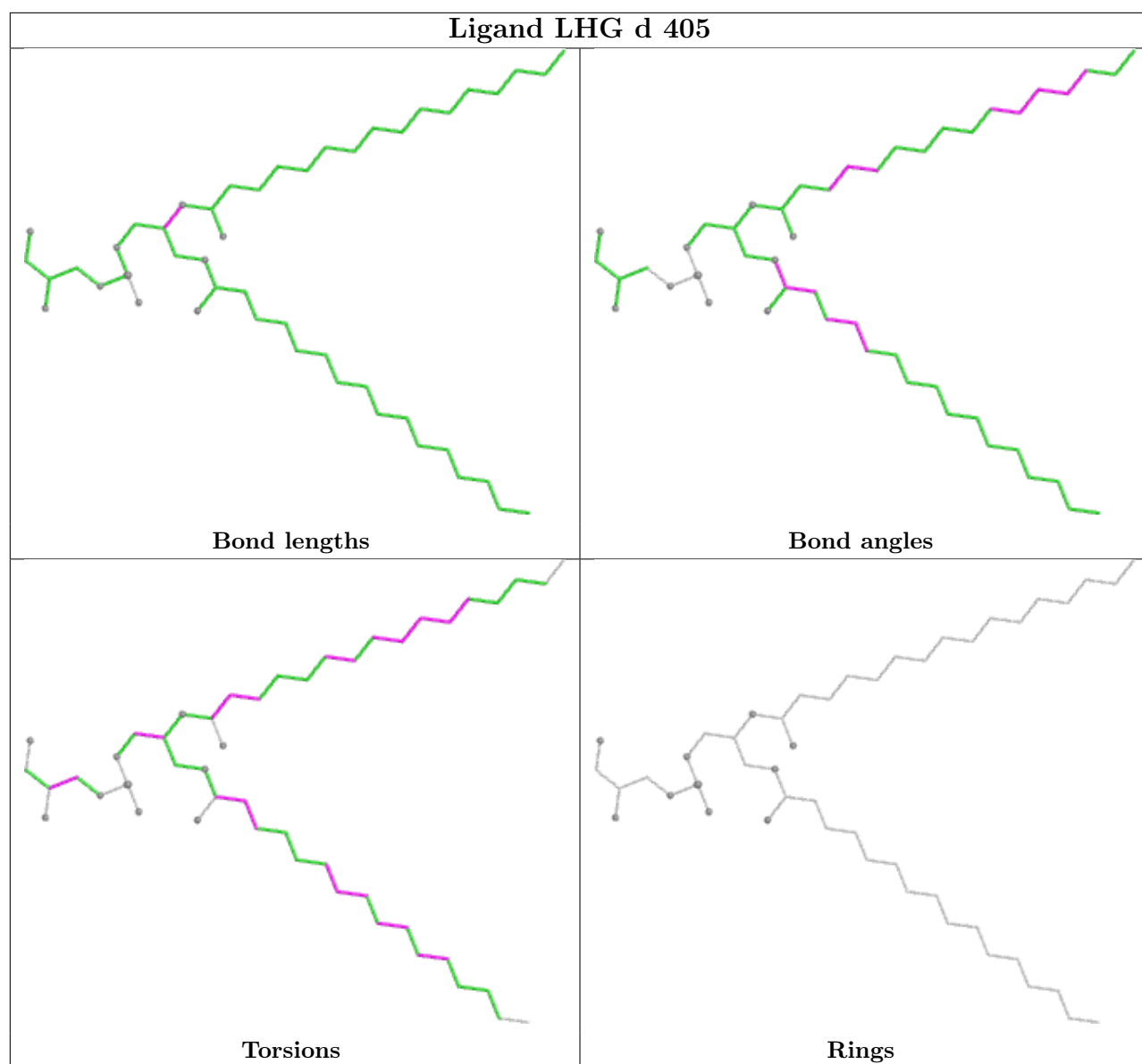
Bond angles



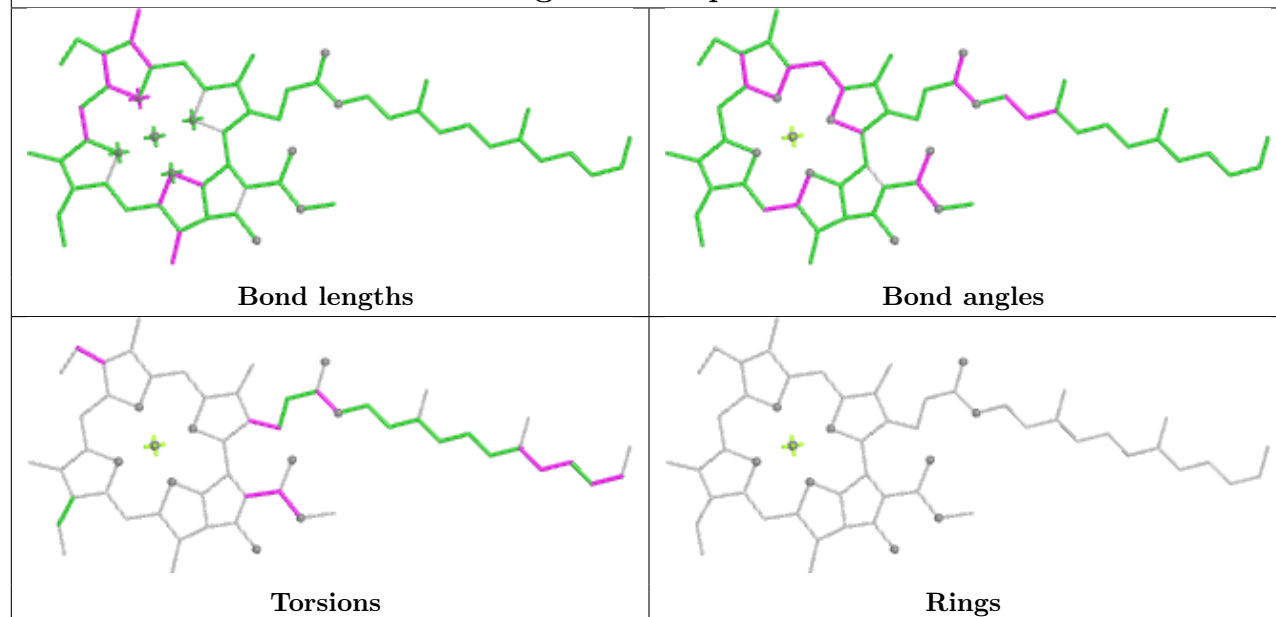
Torsions



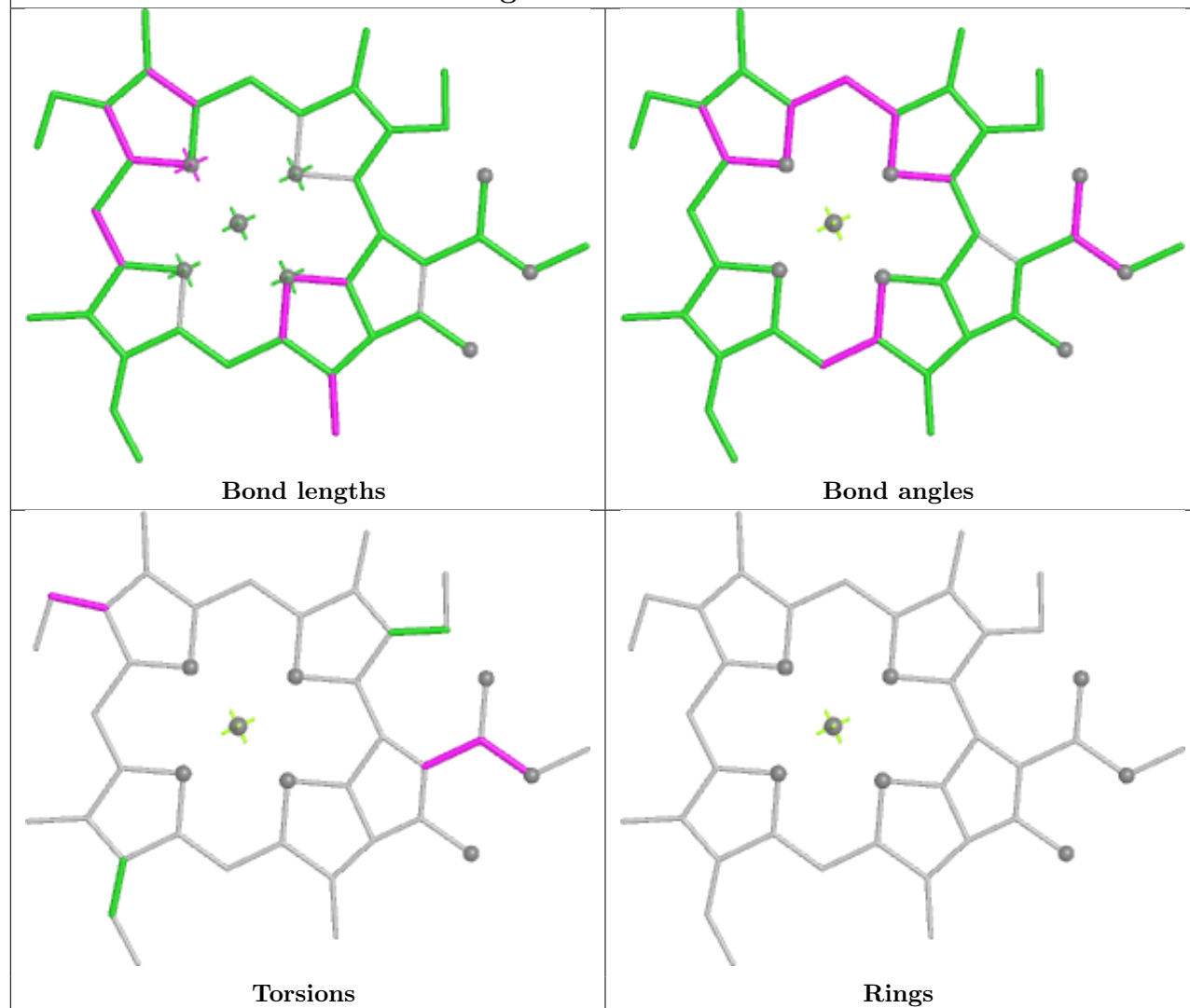
Rings

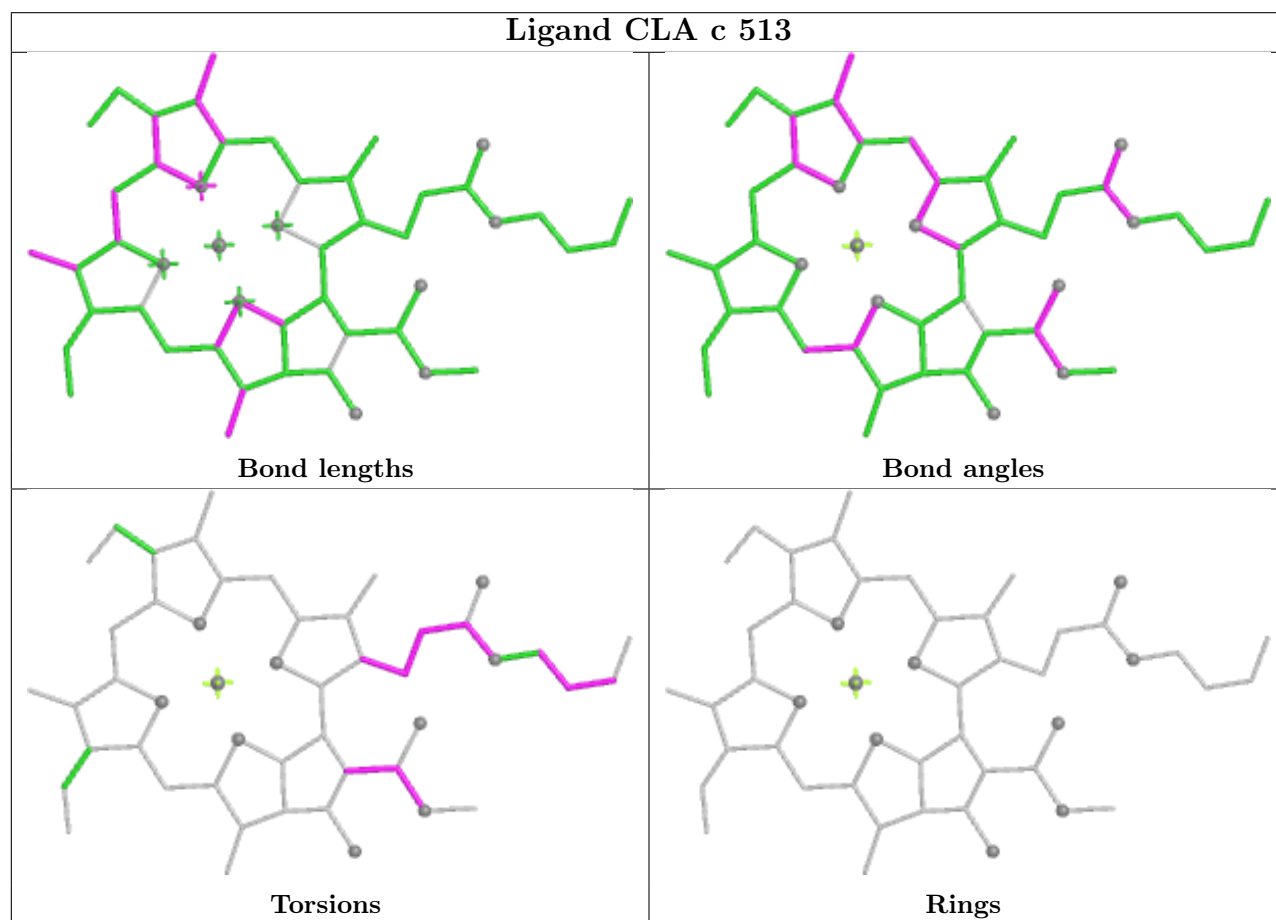
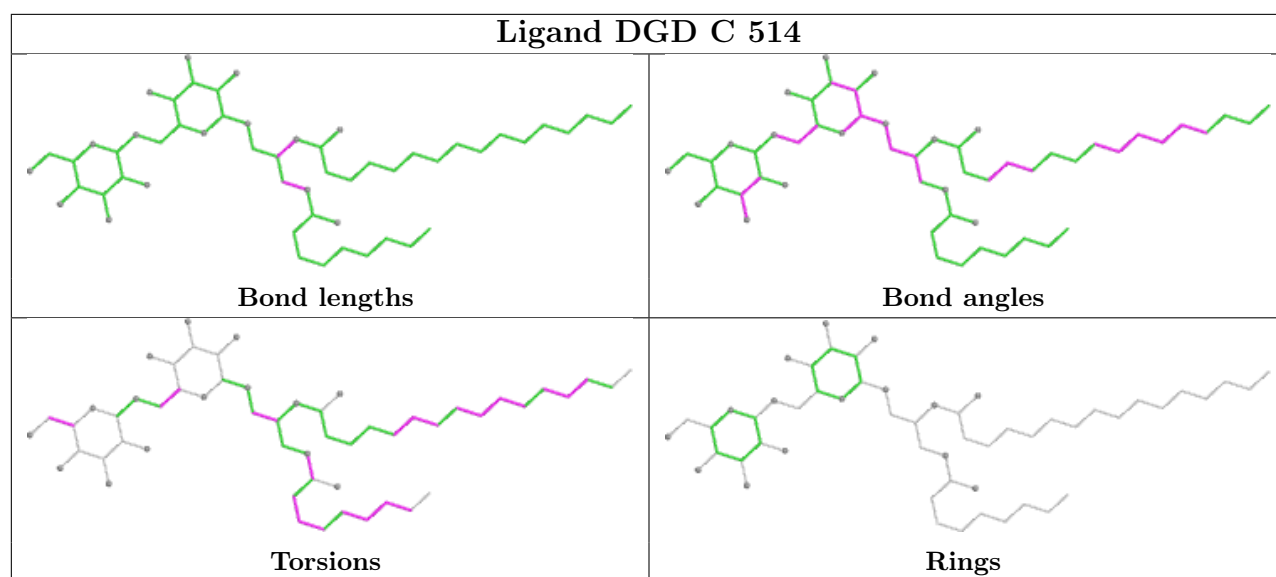


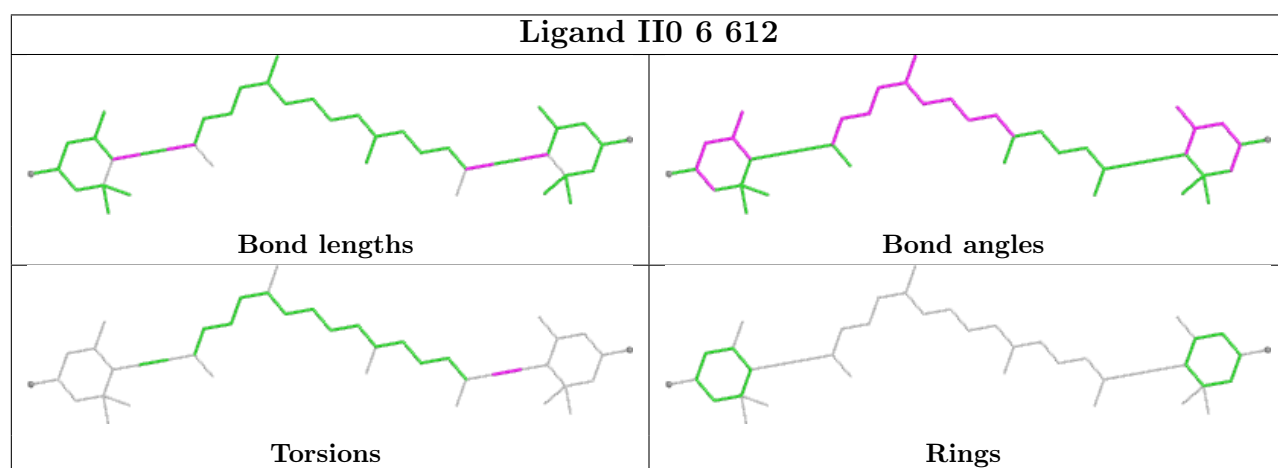
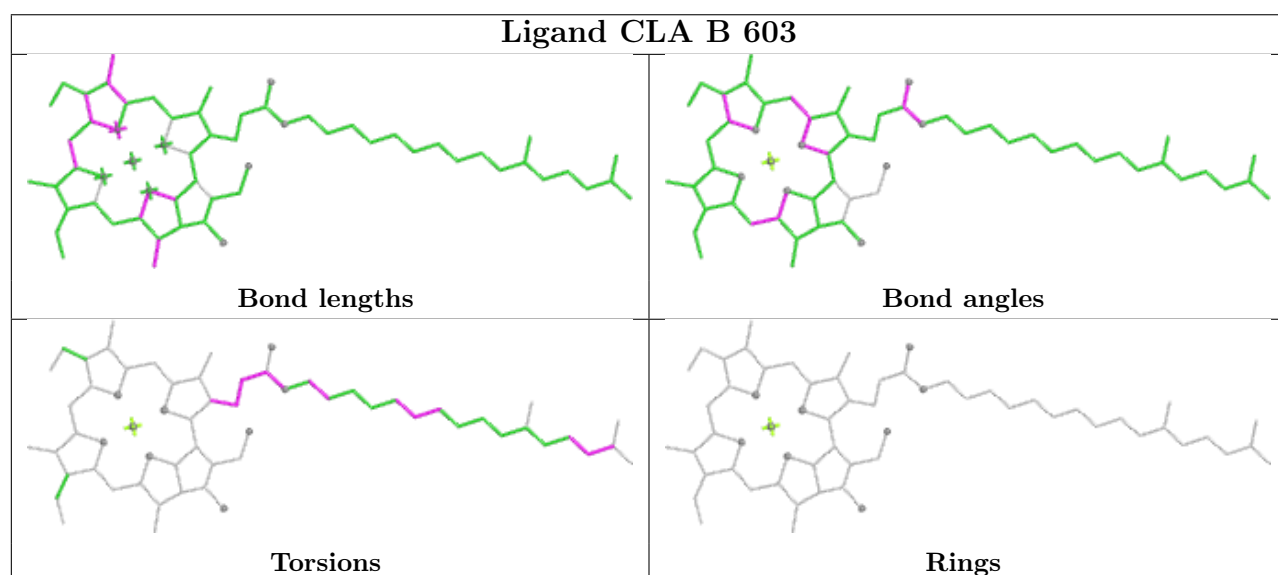
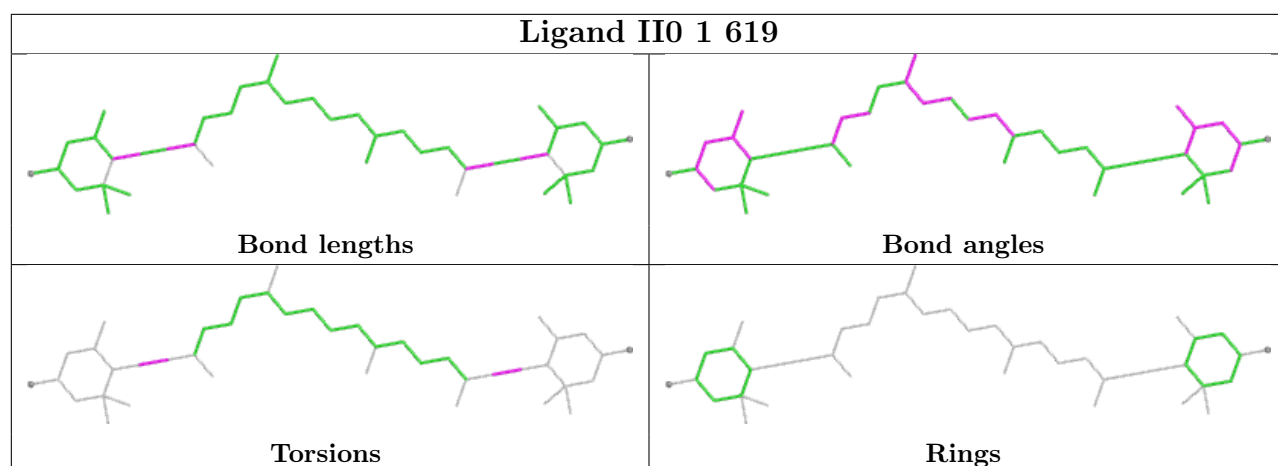
Ligand CLA p 303

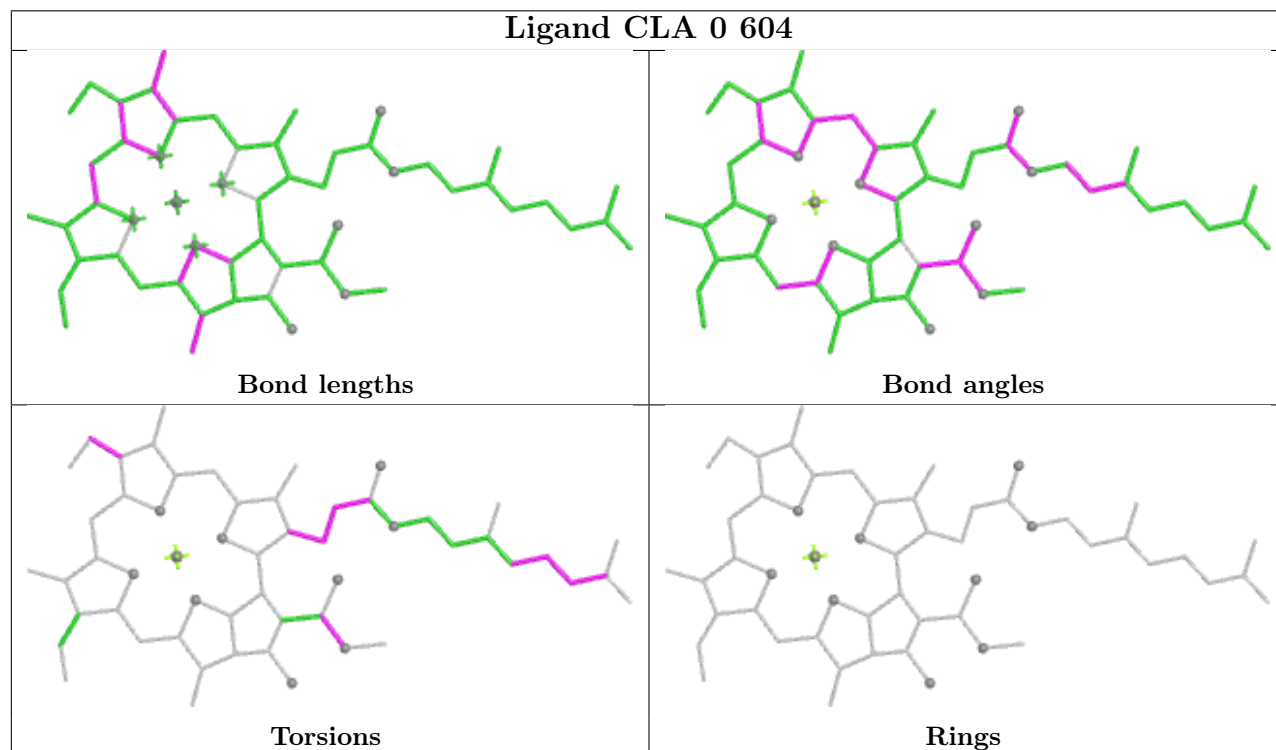
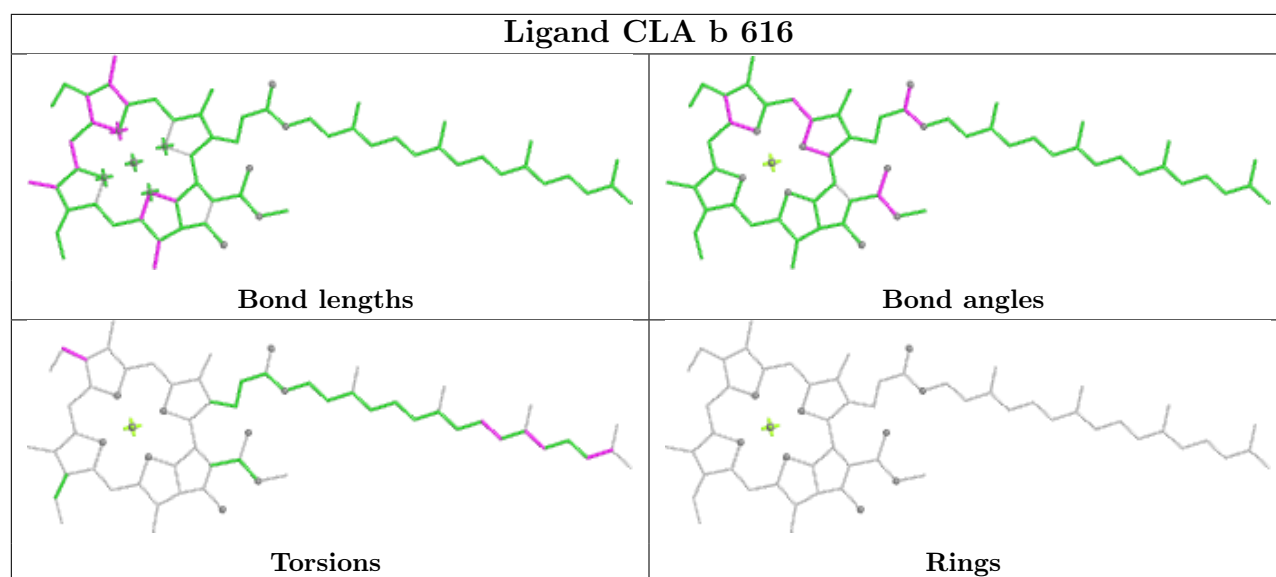


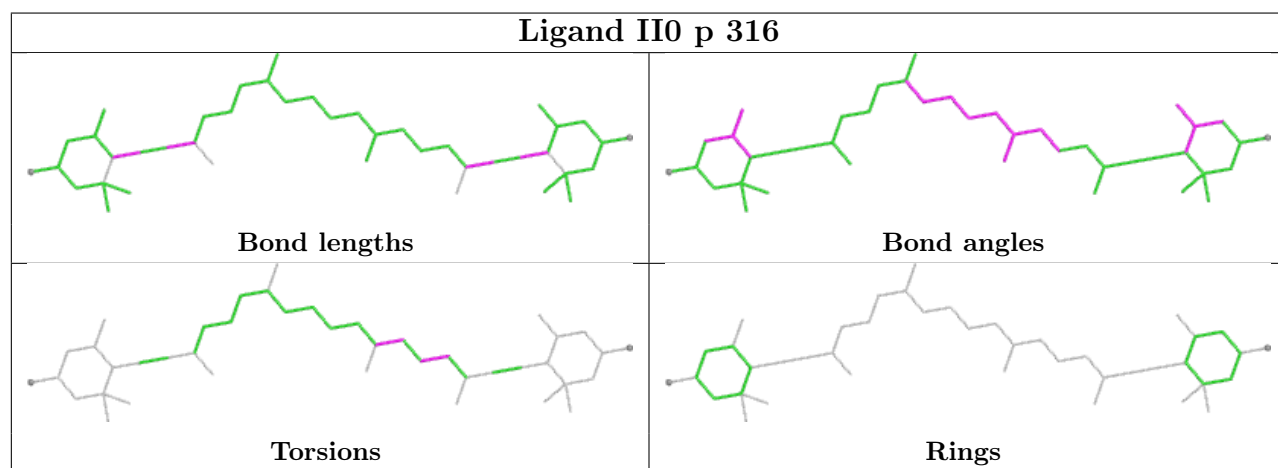
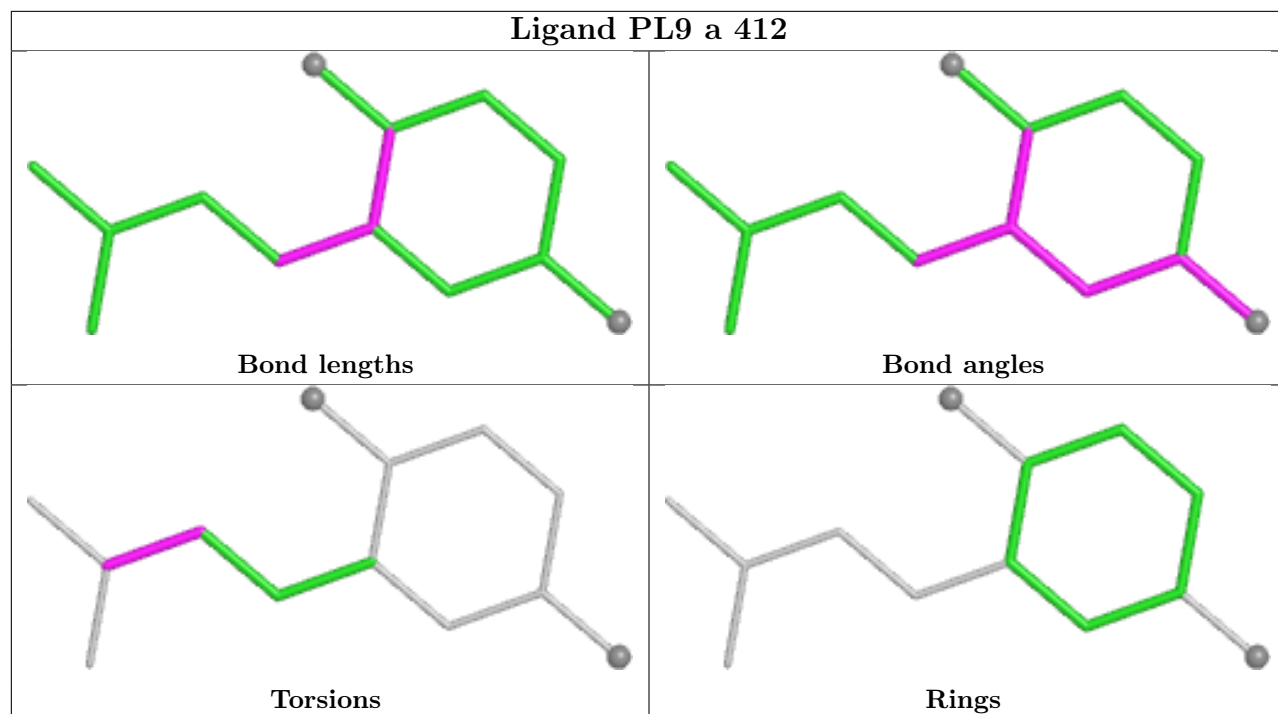
Ligand CLA 8 601

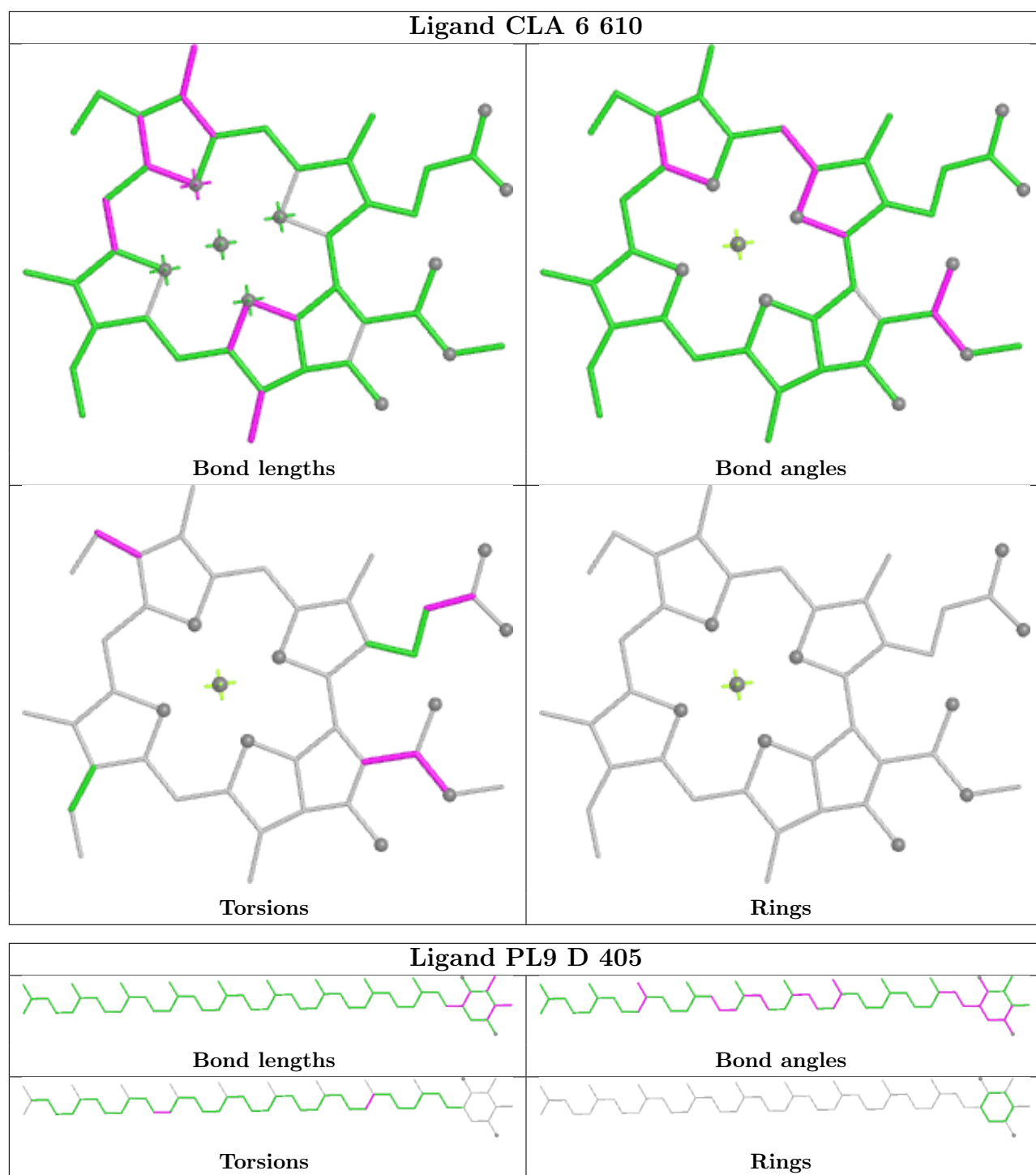


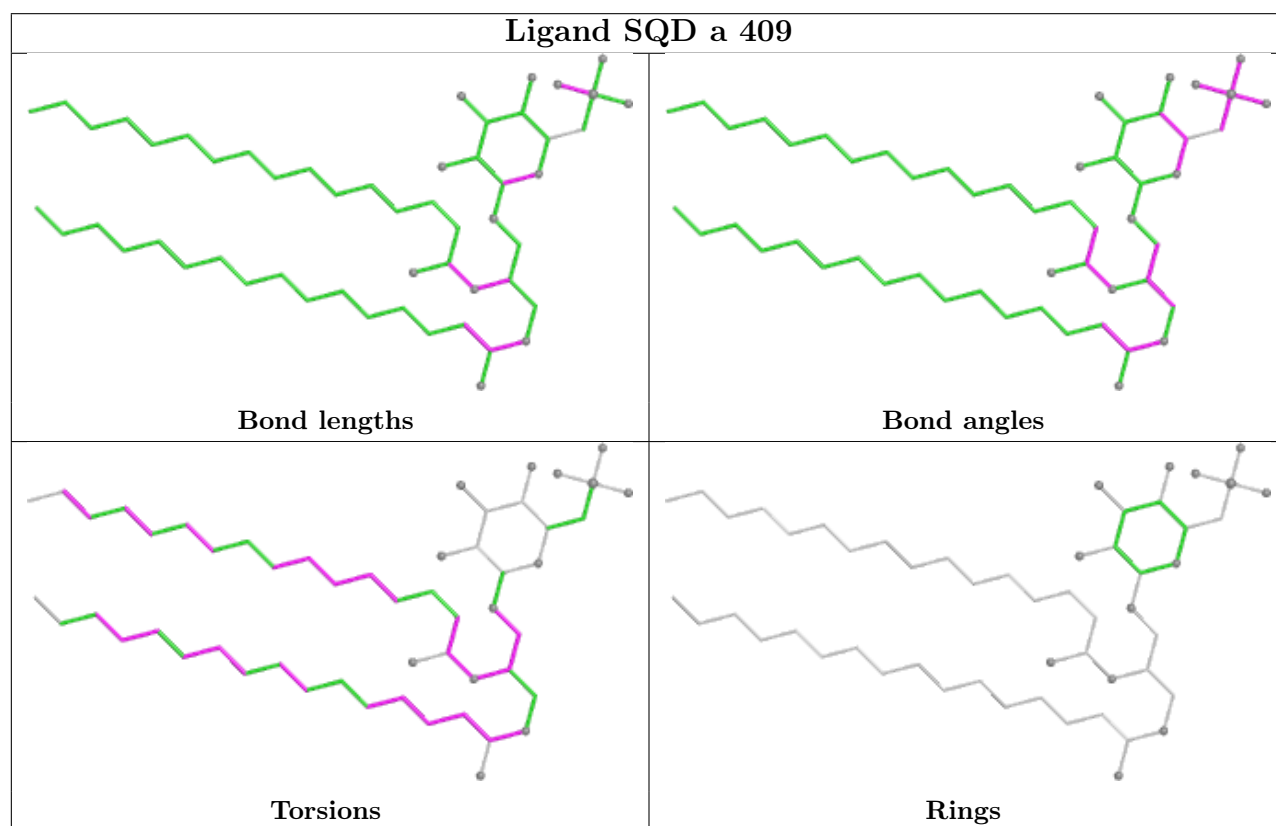
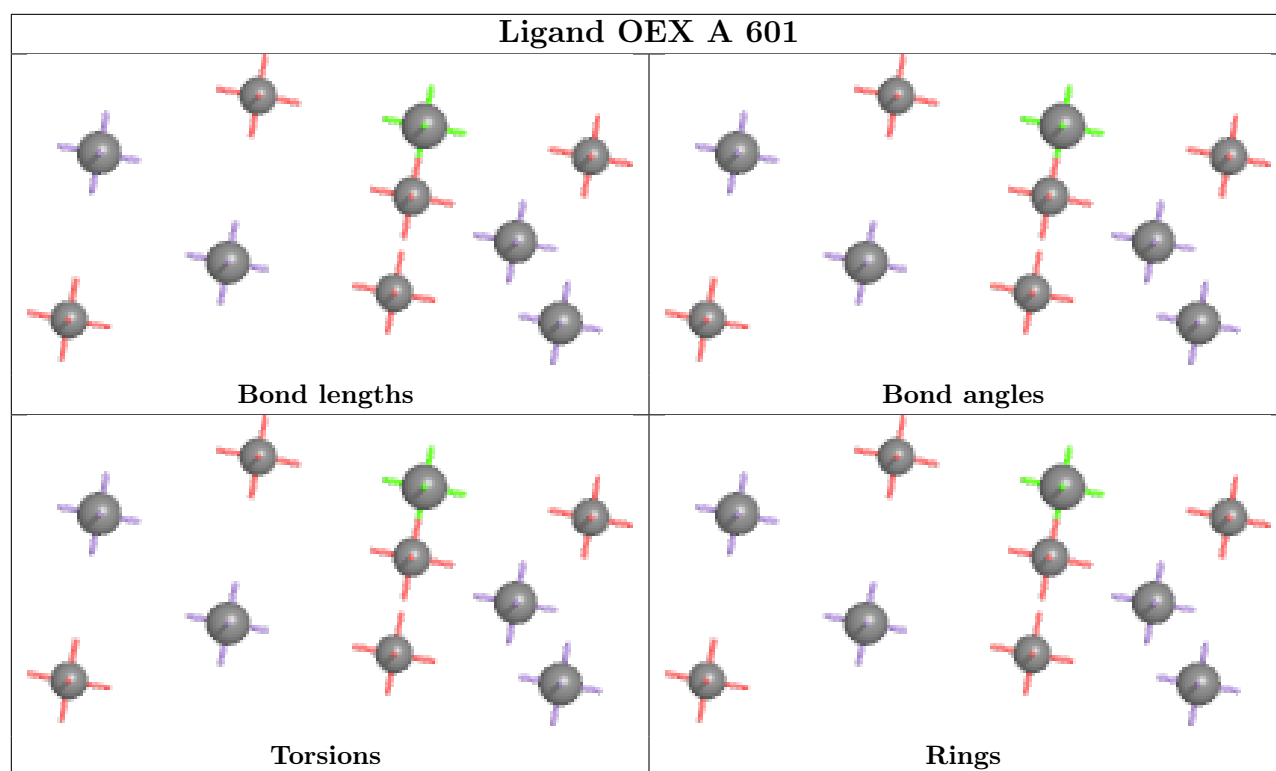


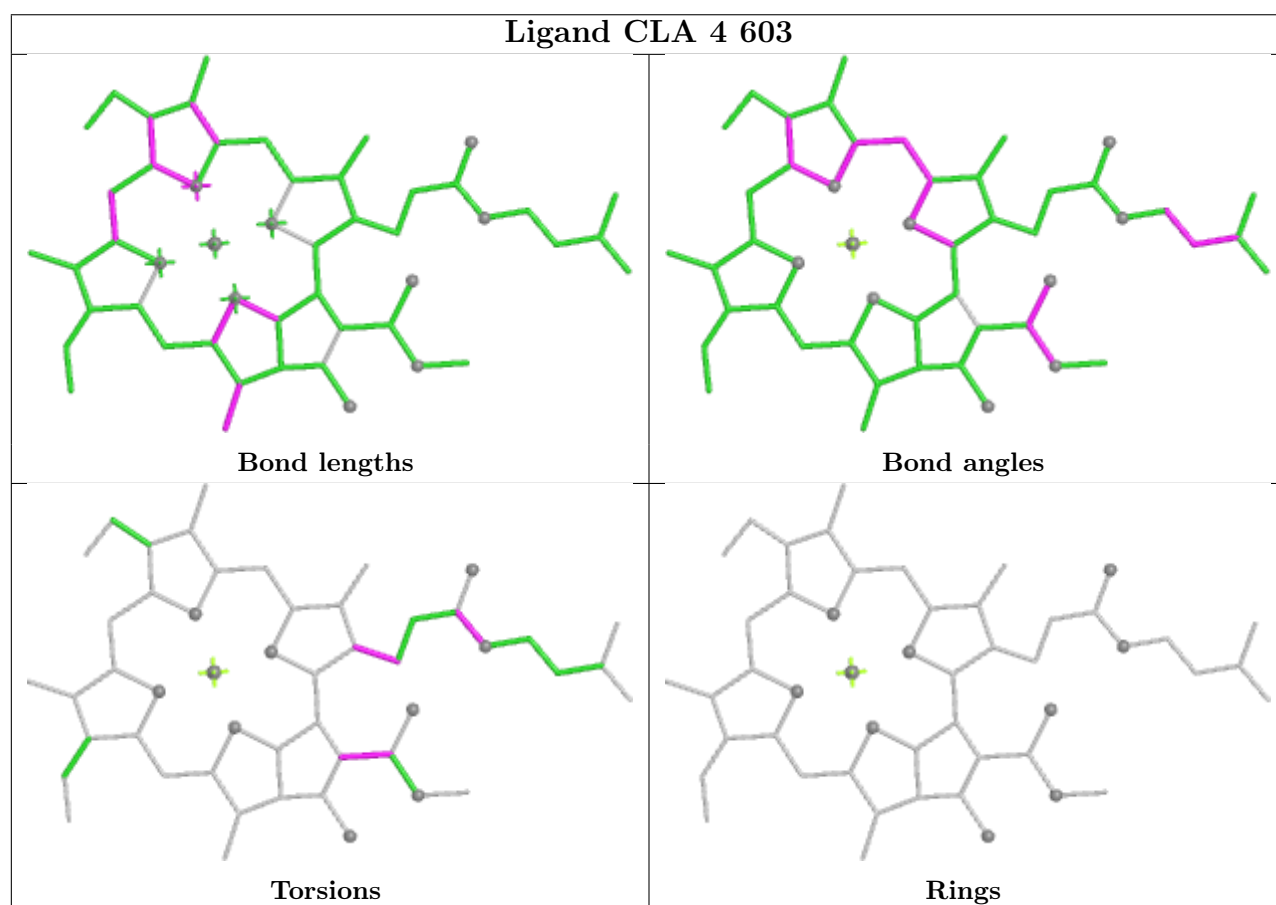
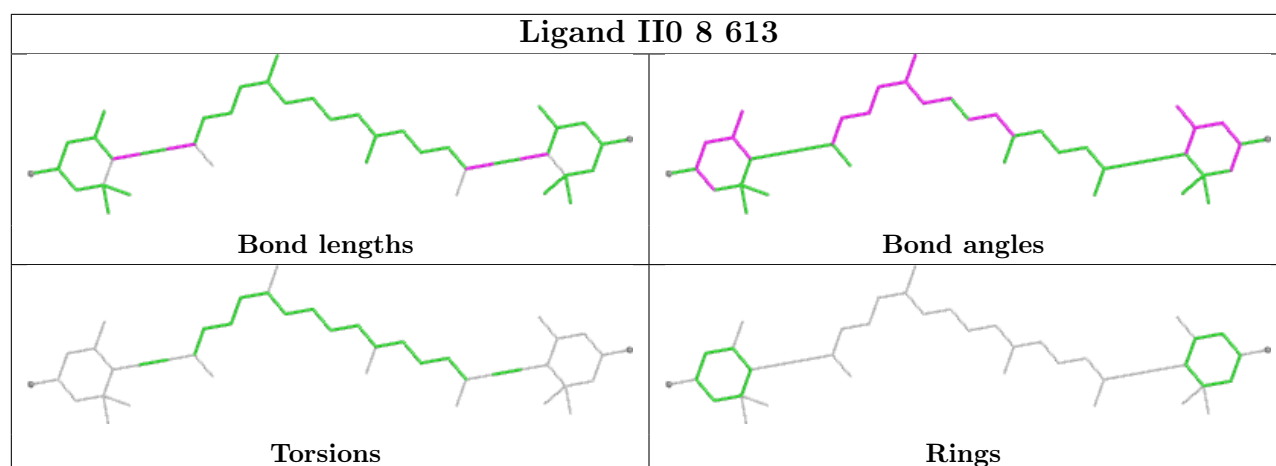


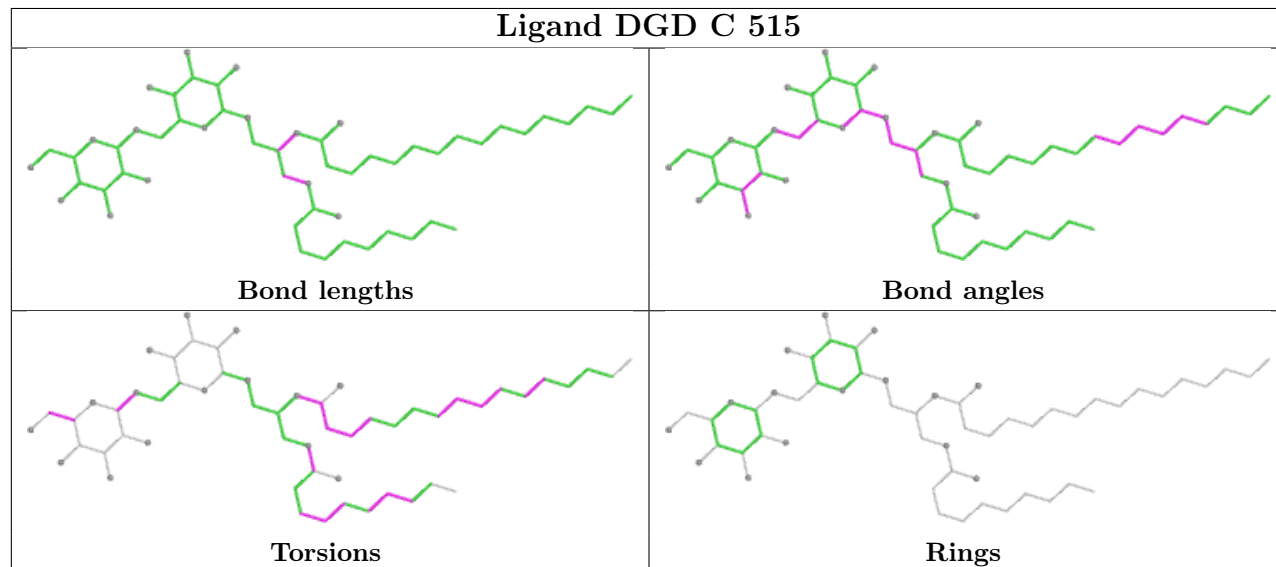
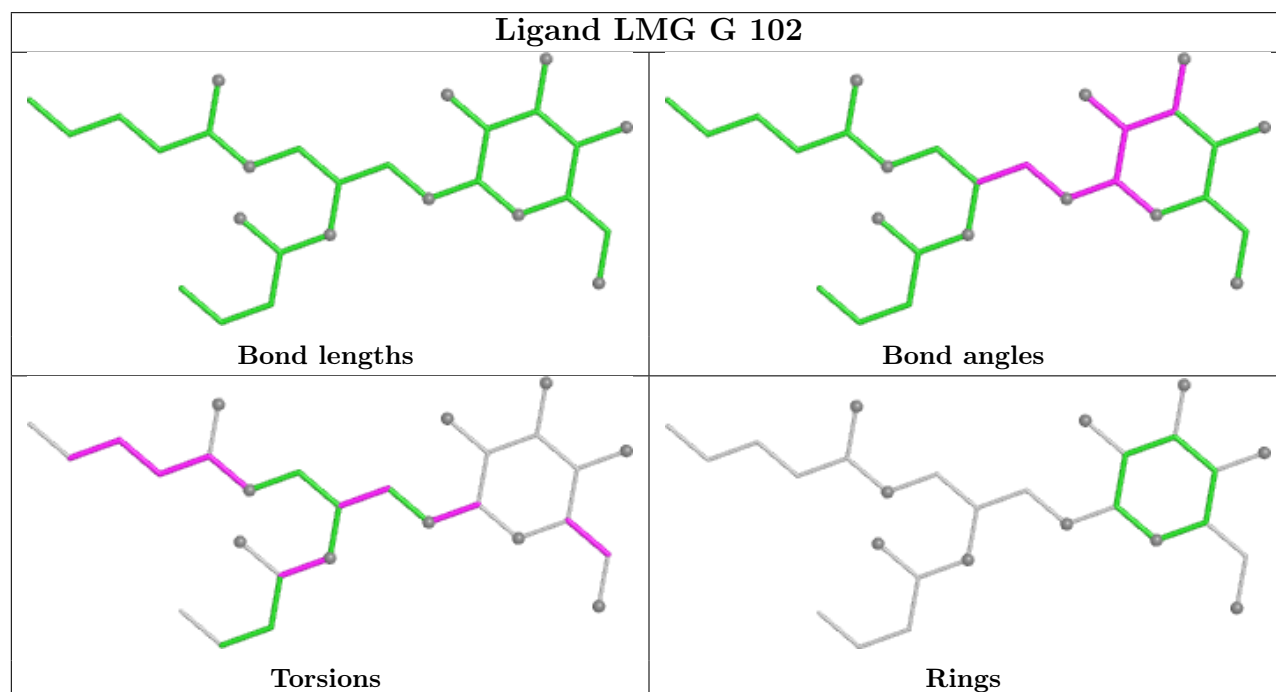
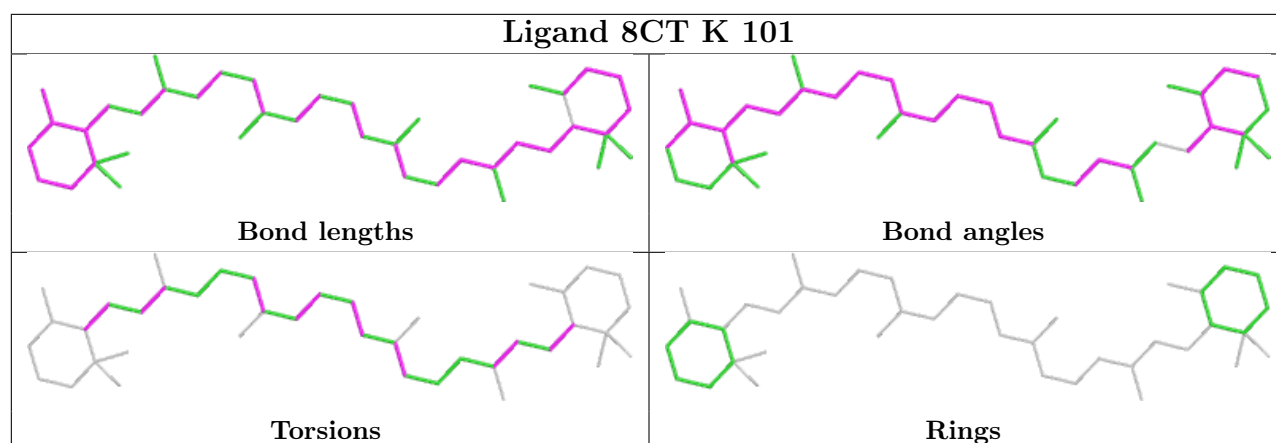




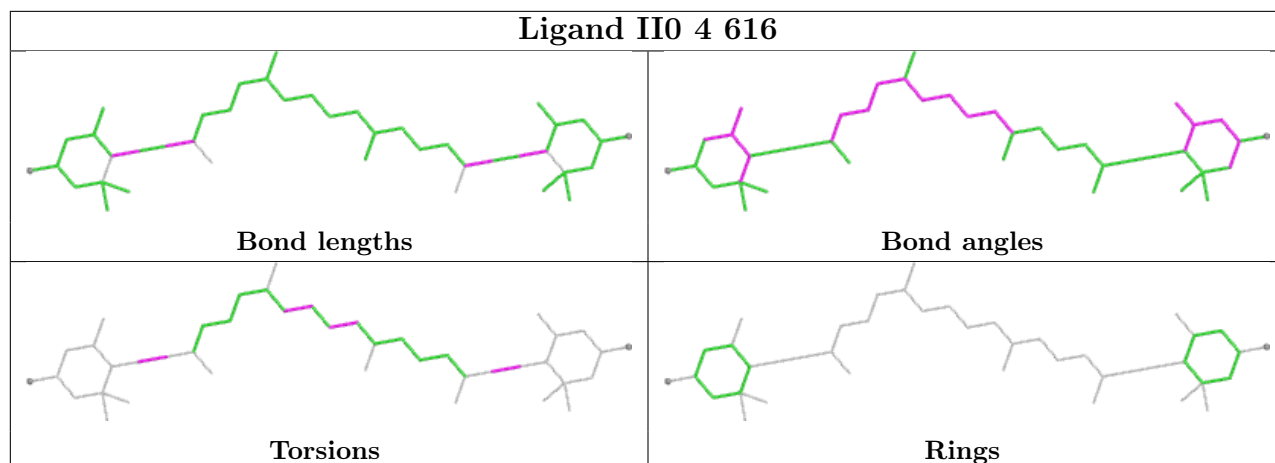




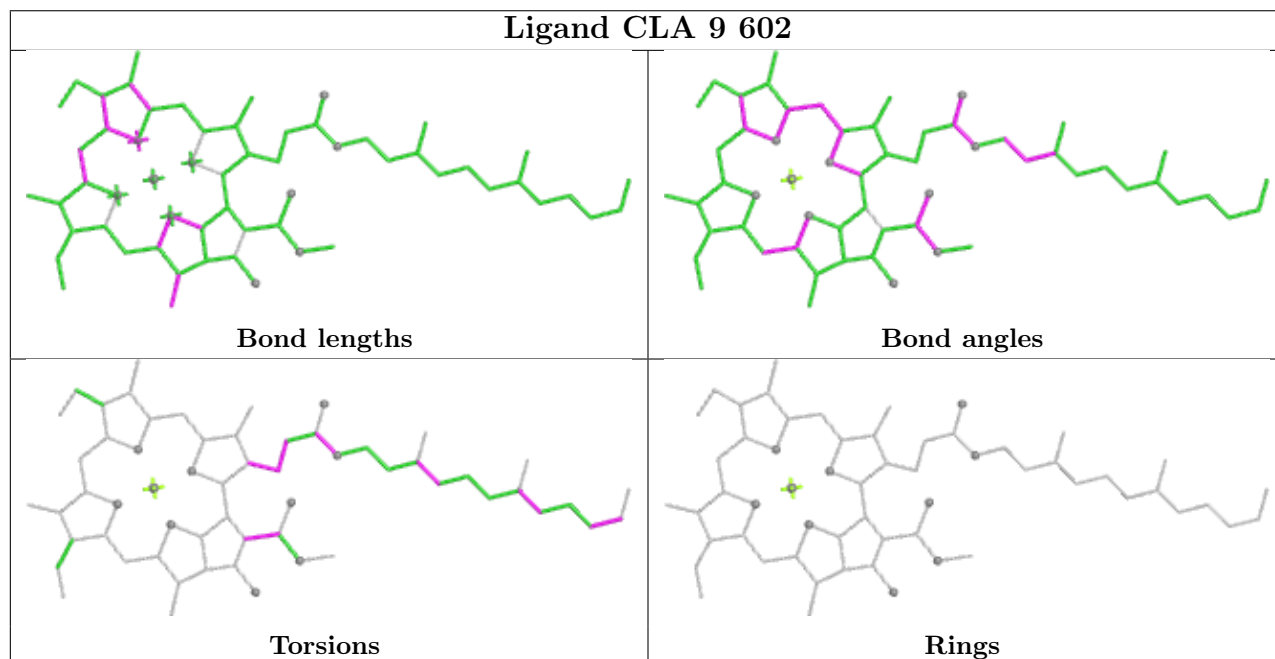




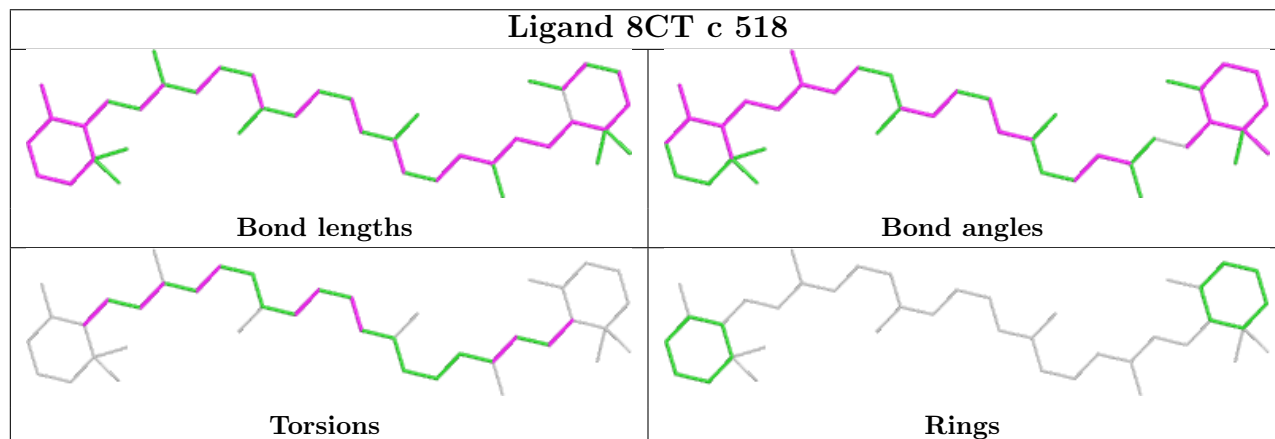
Ligand II0 4 616



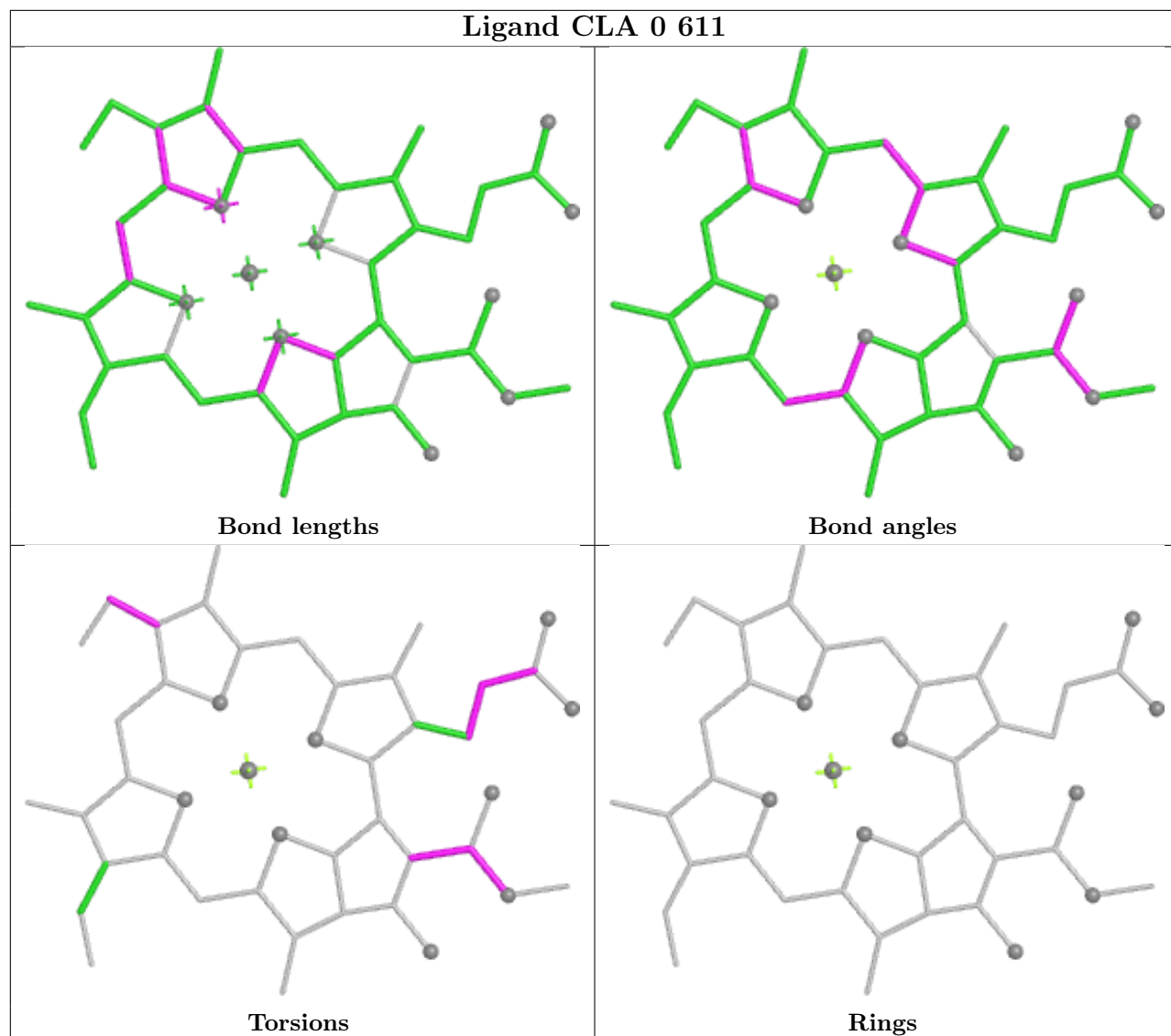
Ligand CLA 9 602



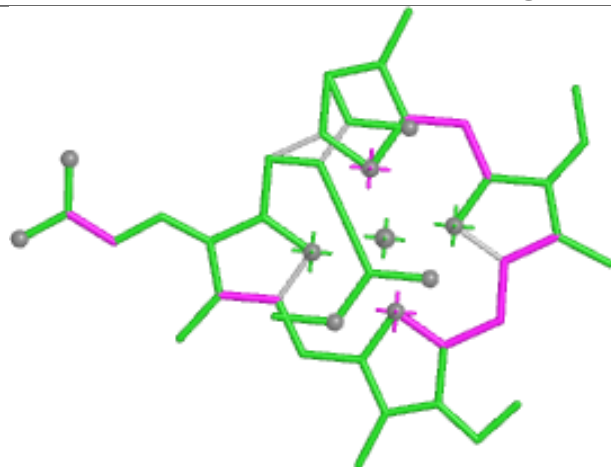
Ligand 8CT c 518



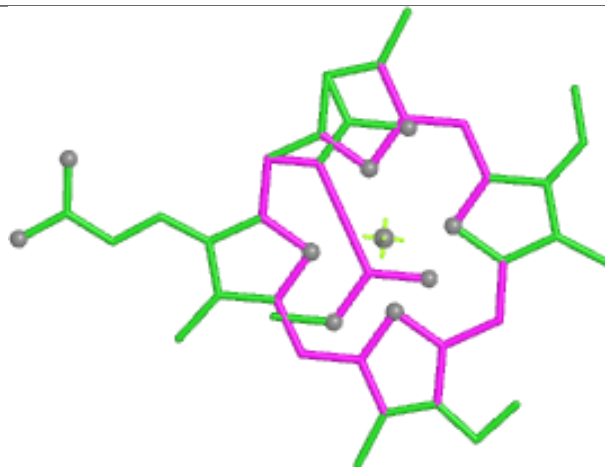
Ligand CLA 0 611



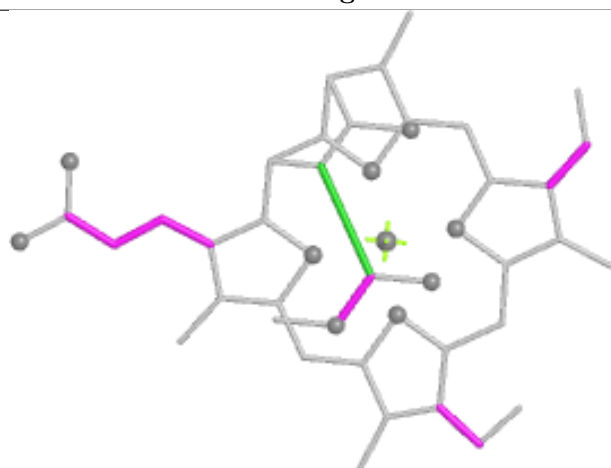
Ligand KC2 2 610



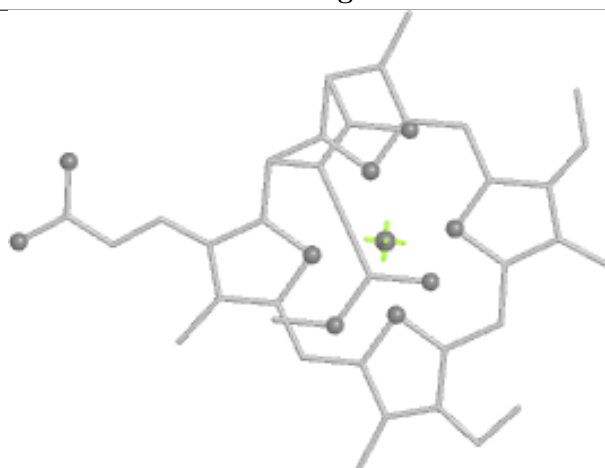
Bond lengths



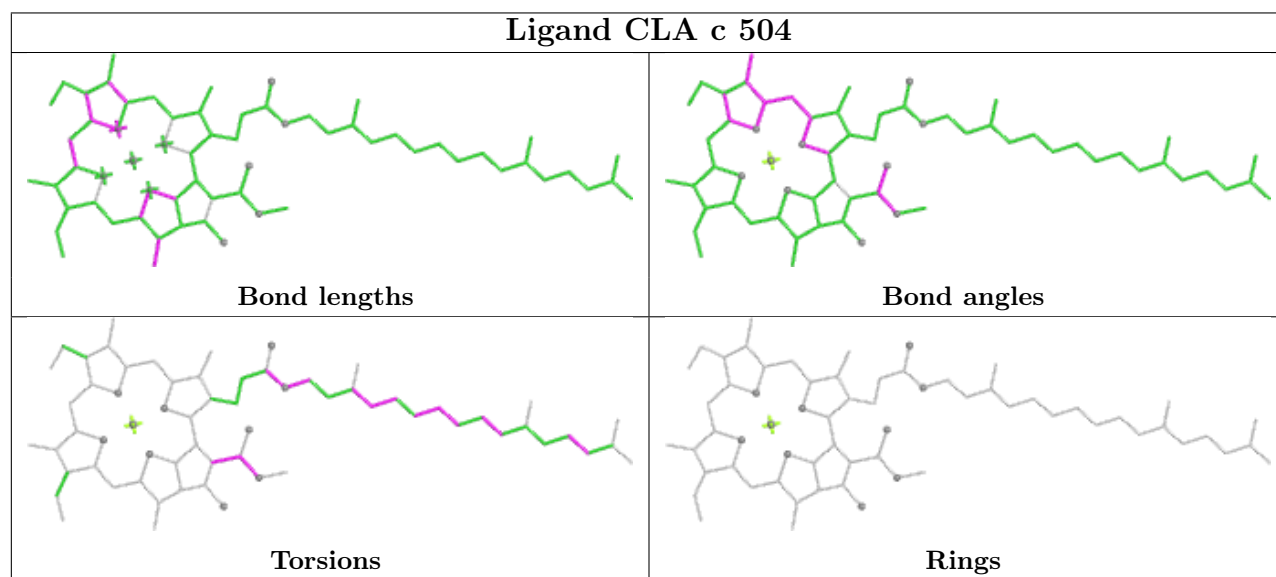
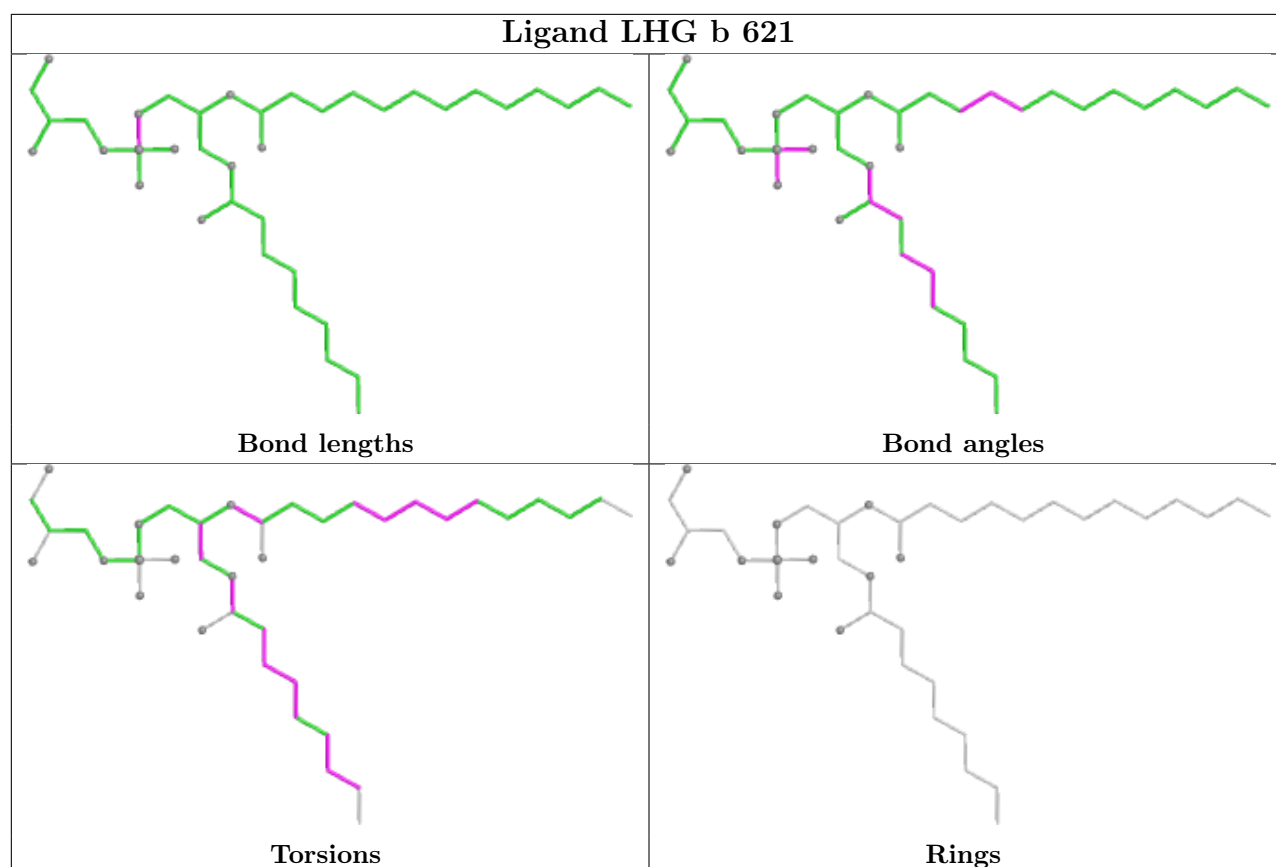
Bond angles

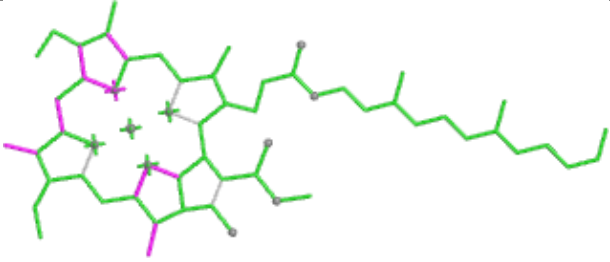
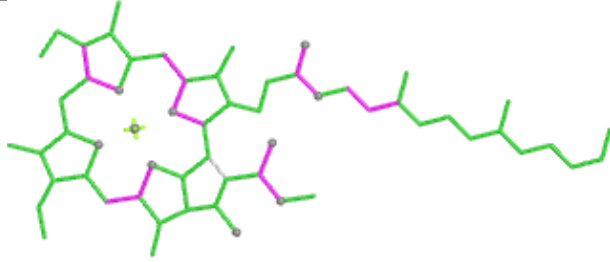
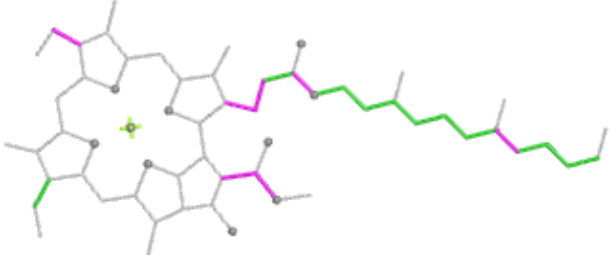
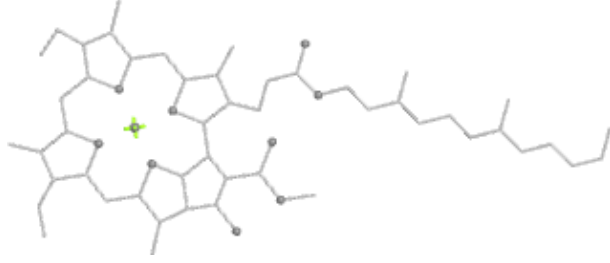
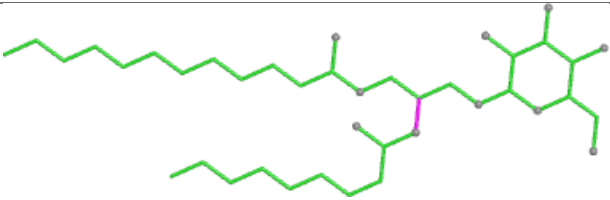
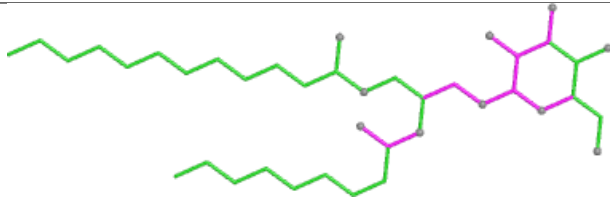
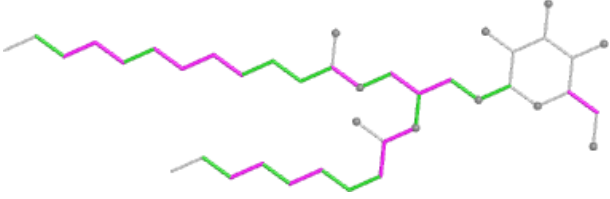
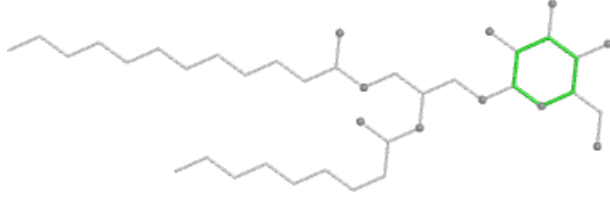
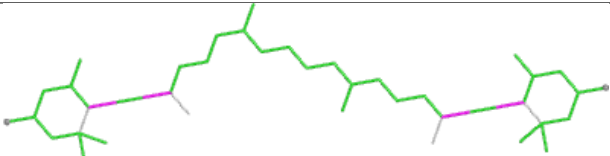
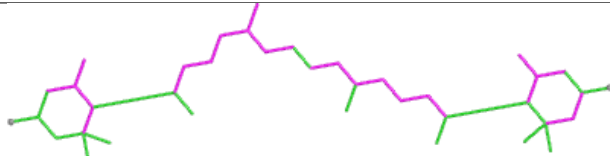
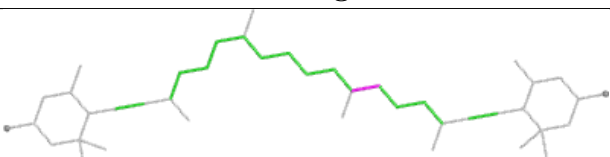
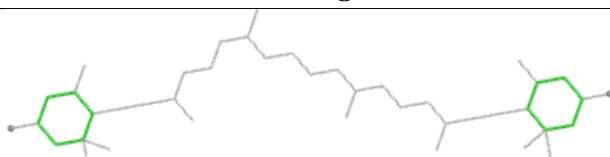


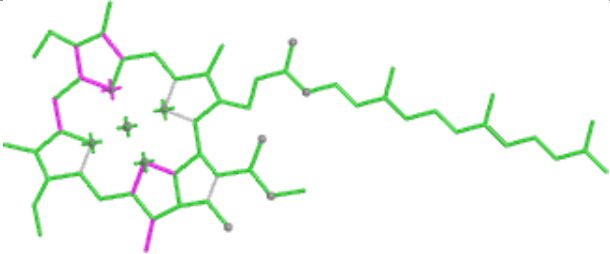
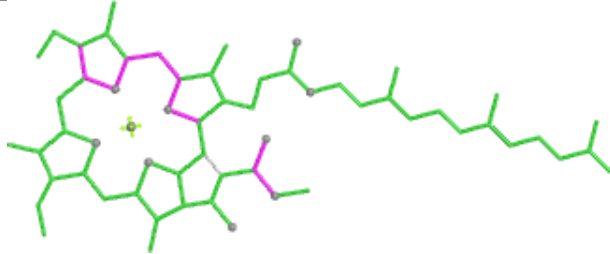
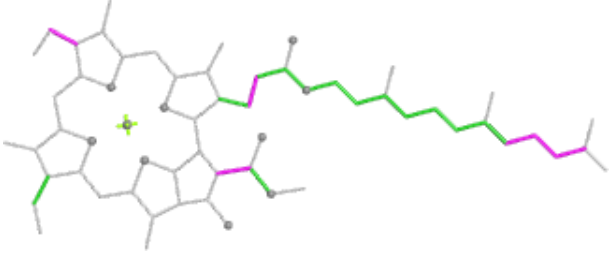
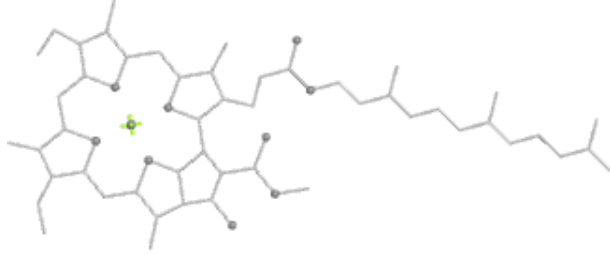
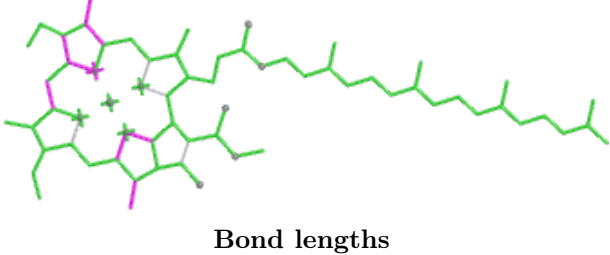
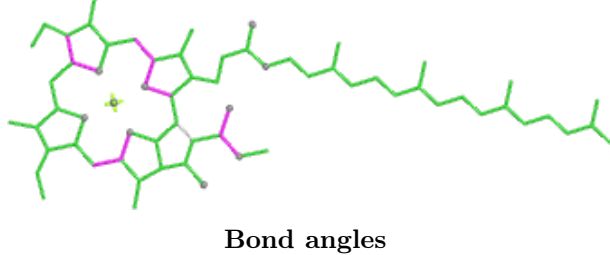
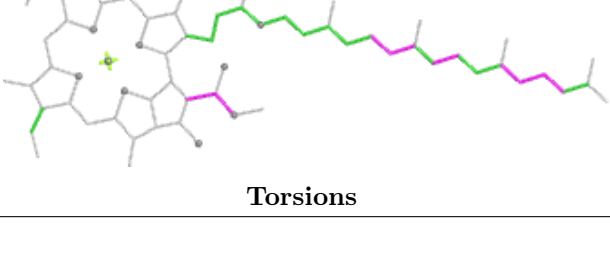
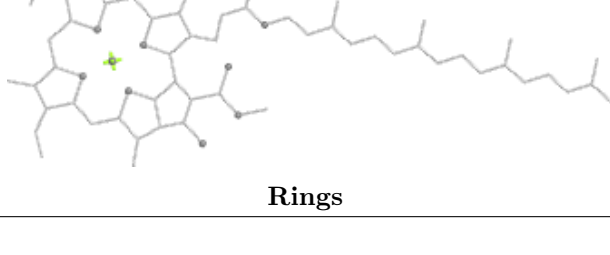
Torsions



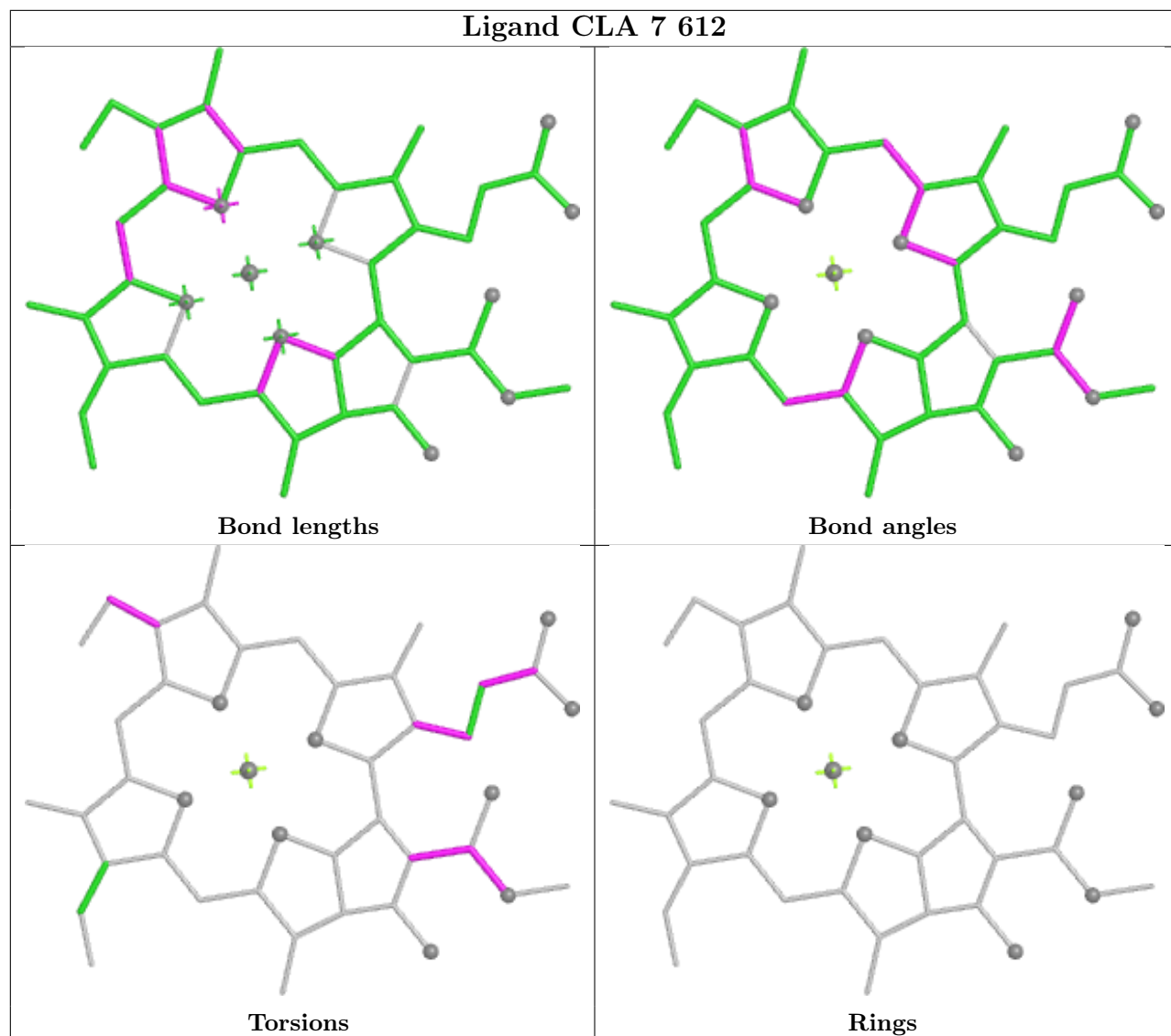
Rings



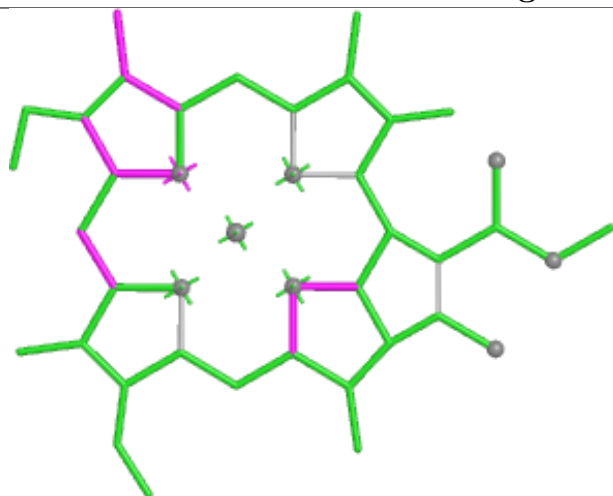
Ligand CLA 8 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 1 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 p 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

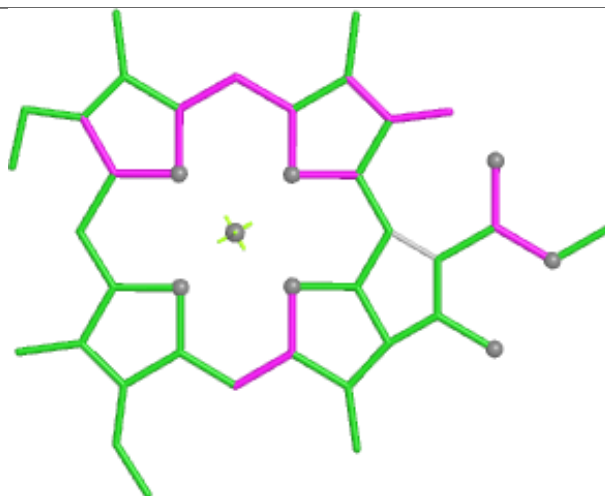
Ligand CLA 7 612



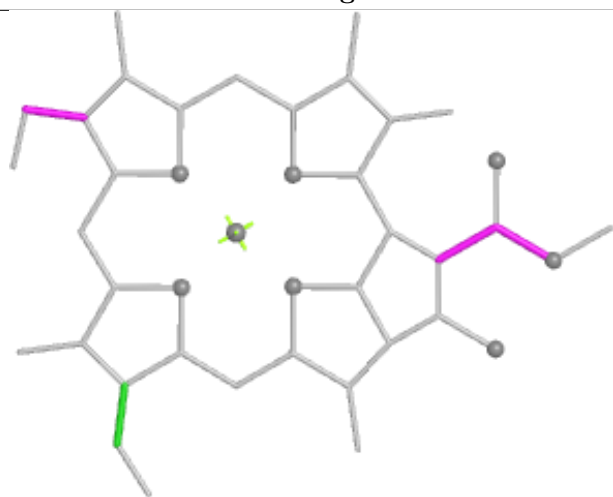
Ligand CLA 1 609



Bond lengths



Bond angles

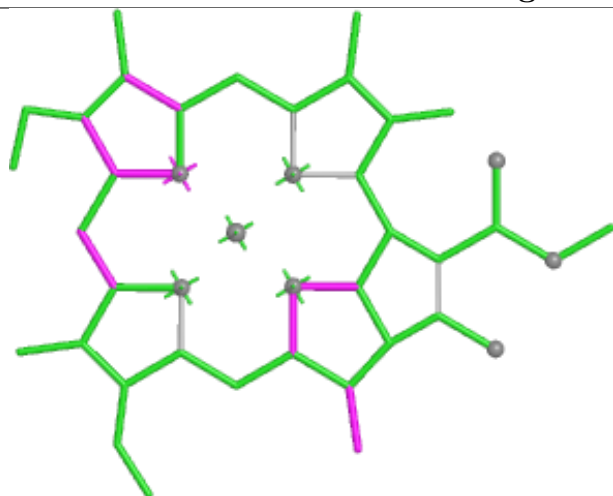


Torsions

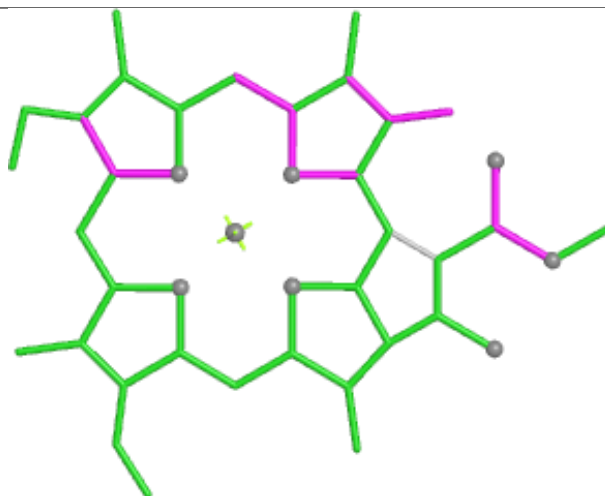


Rings

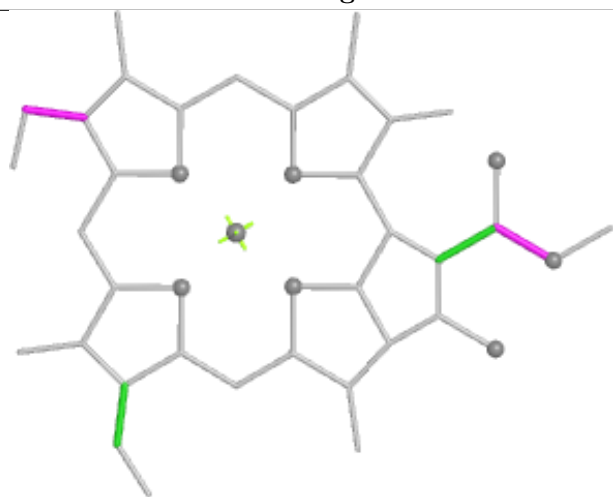
Ligand CLA 8 609



Bond lengths



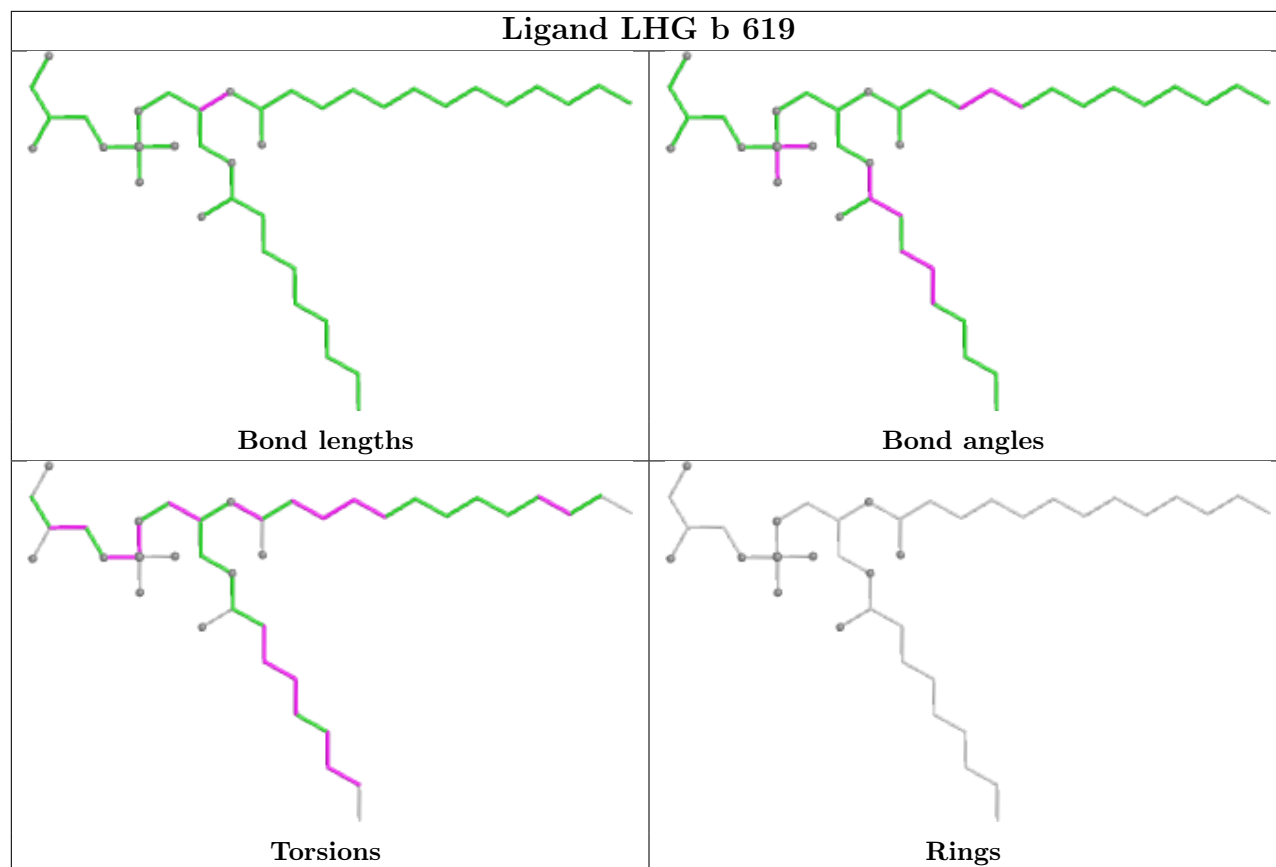
Bond angles



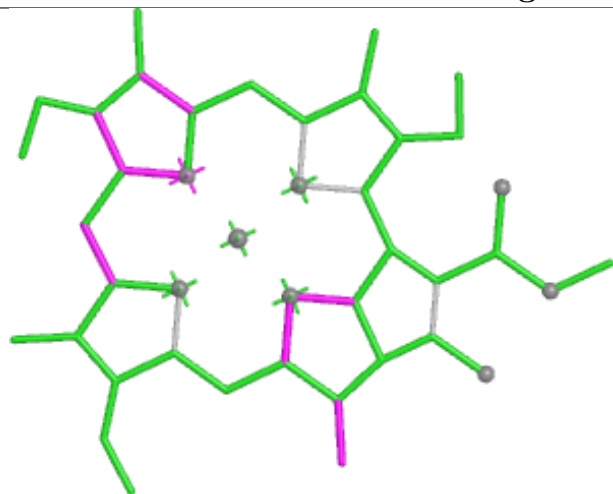
Torsions



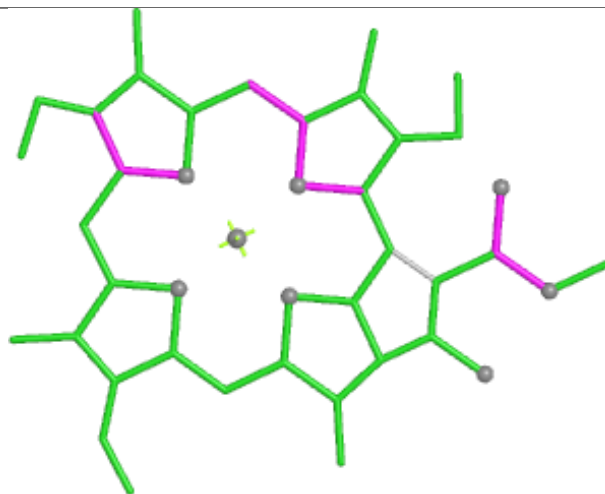
Rings



Ligand CLA 6 601



Bond lengths



Bond angles

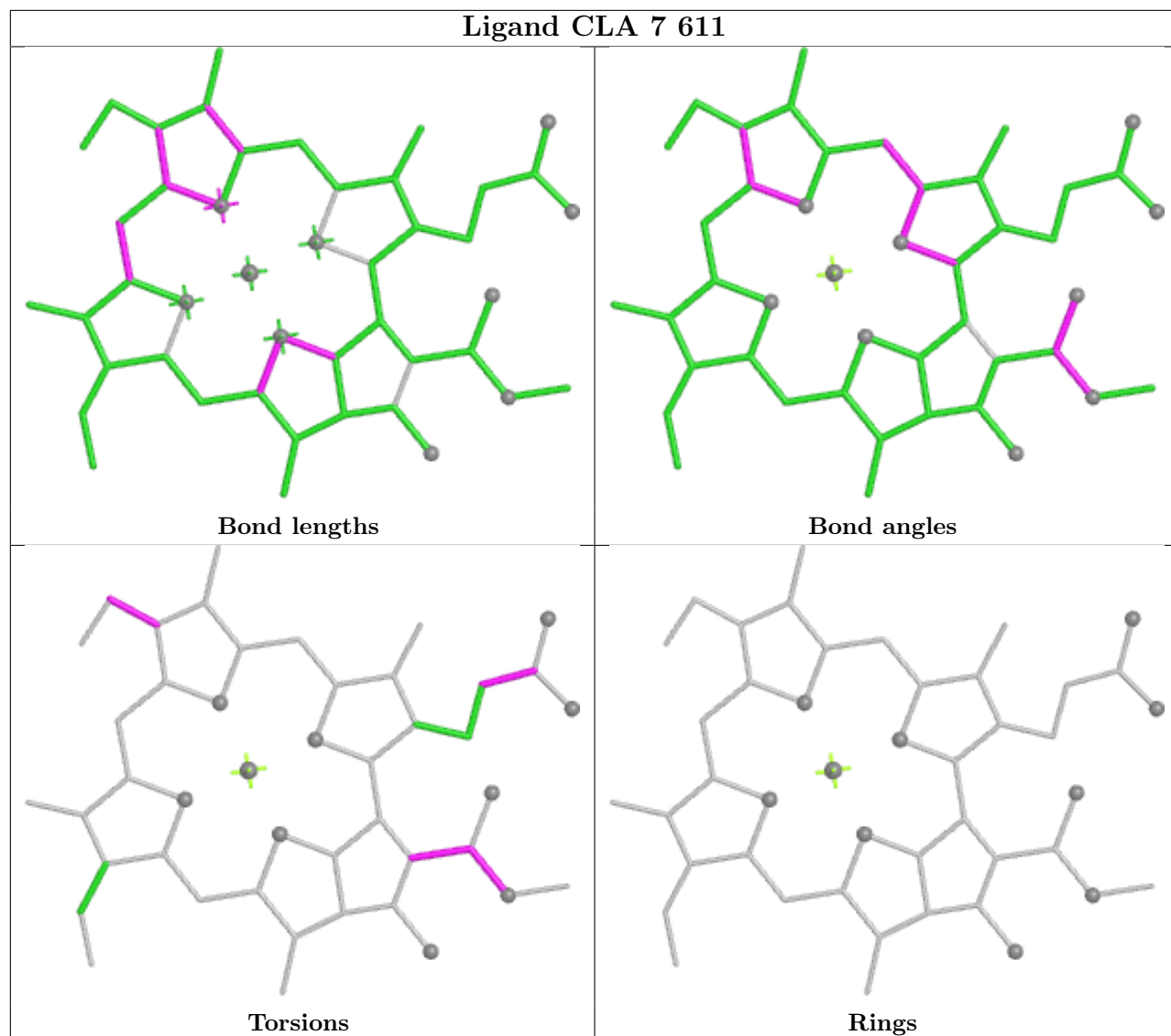


Torsions

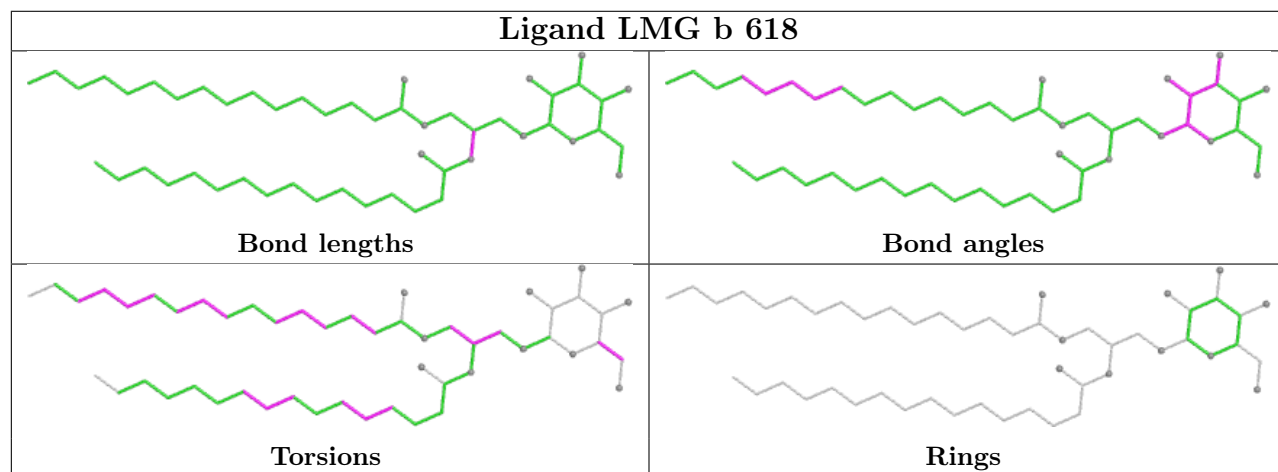


Rings

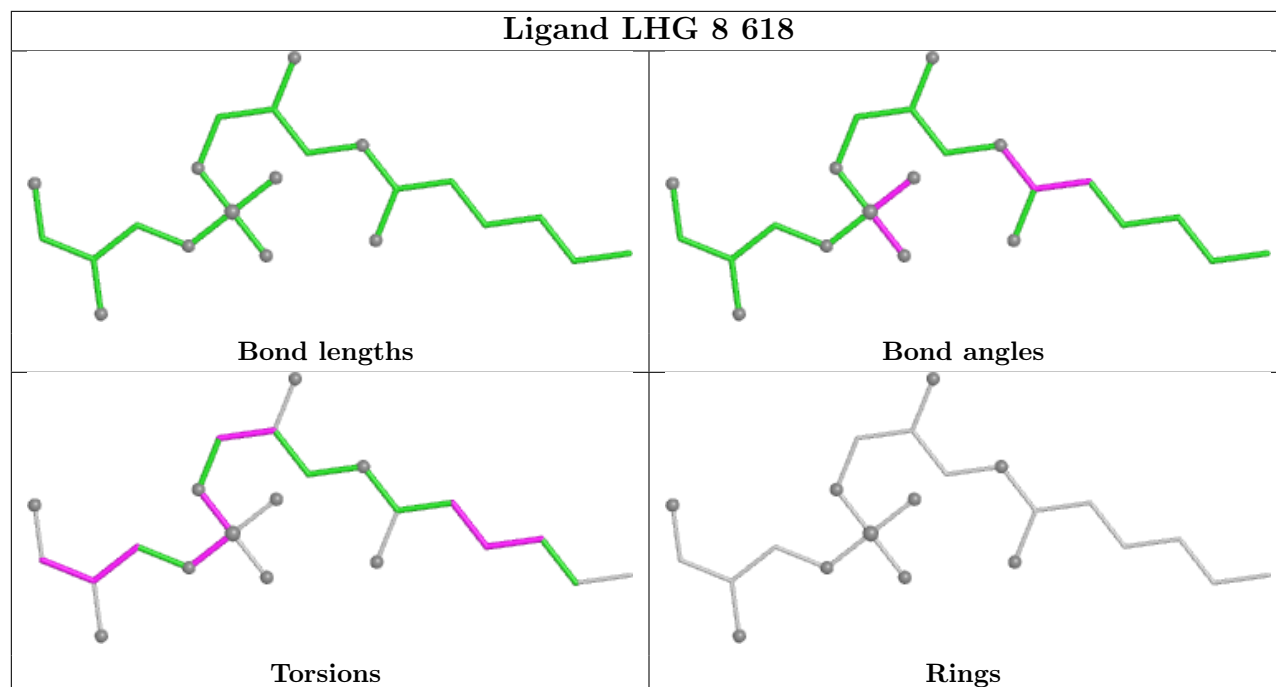
Ligand CLA 7 611



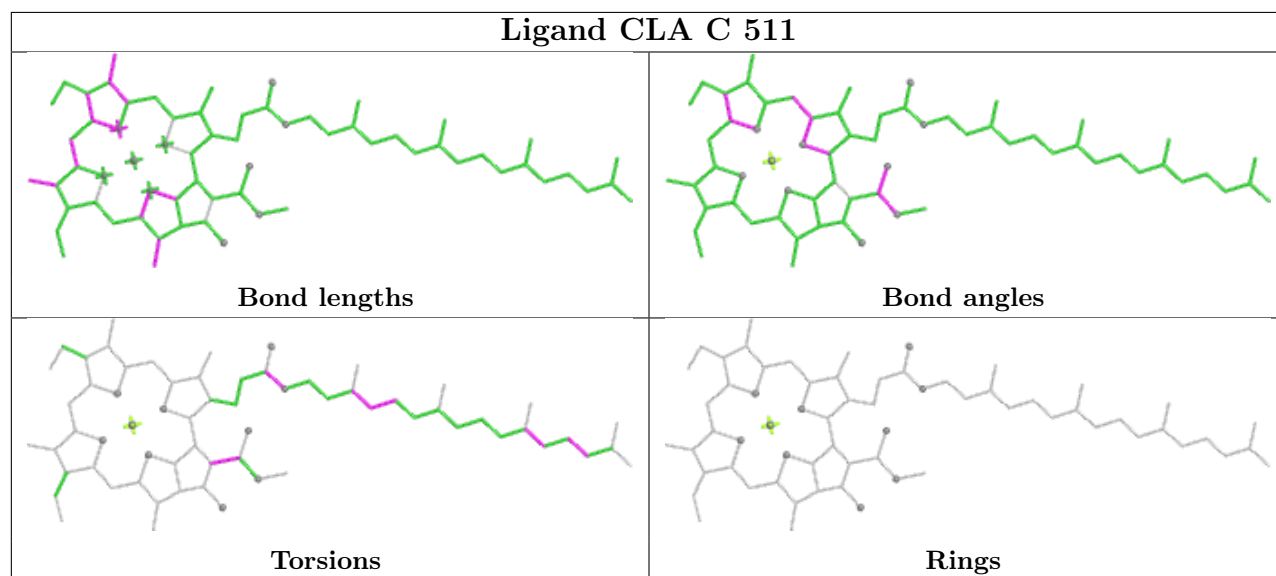
Ligand LMG b 618



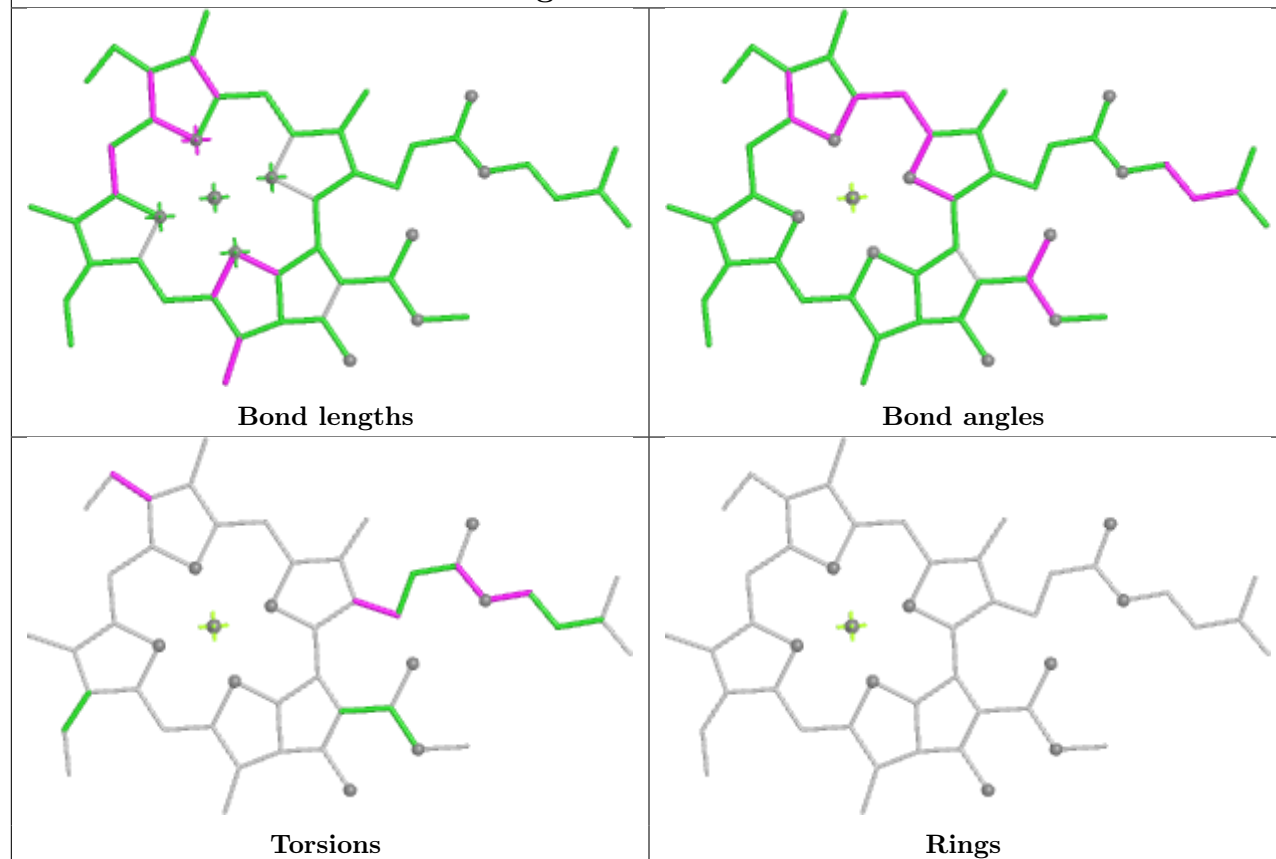
Ligand LHG 8 618



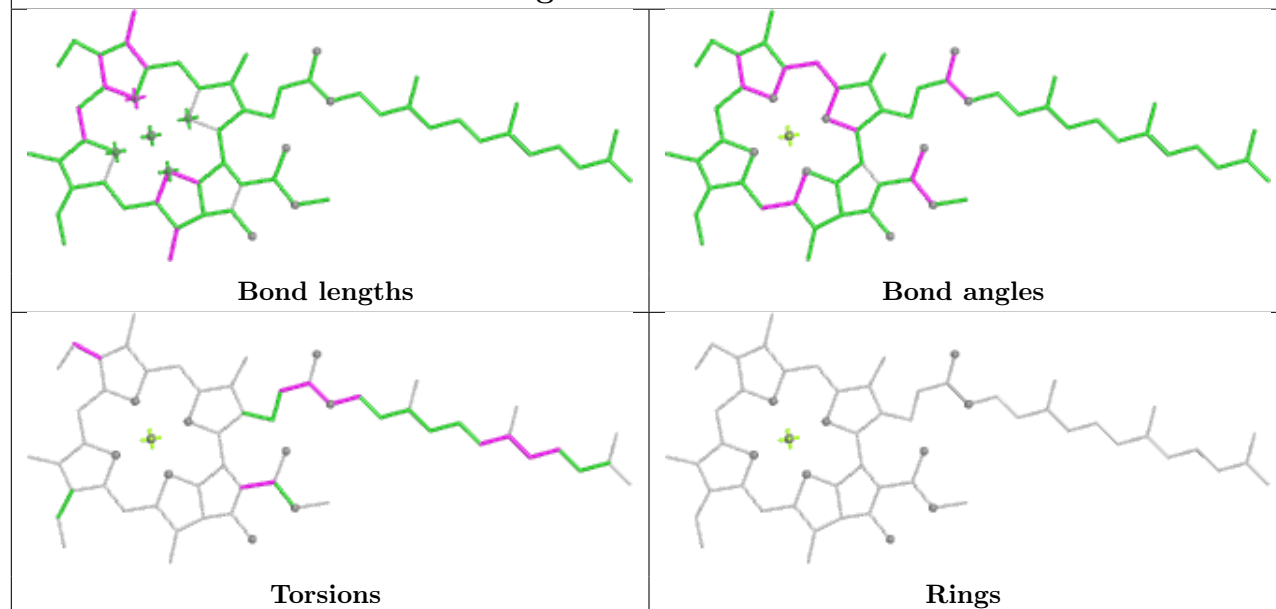
Ligand CLA C 511

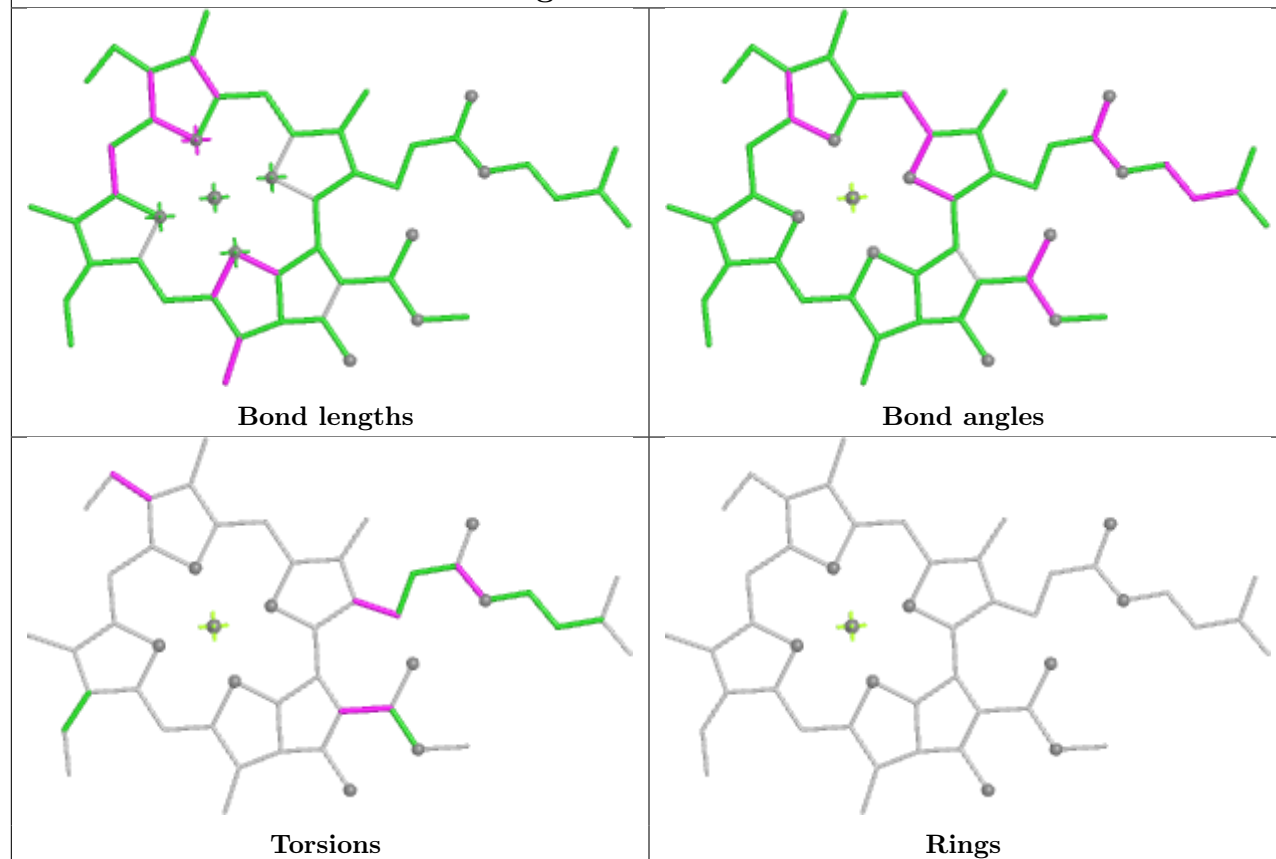
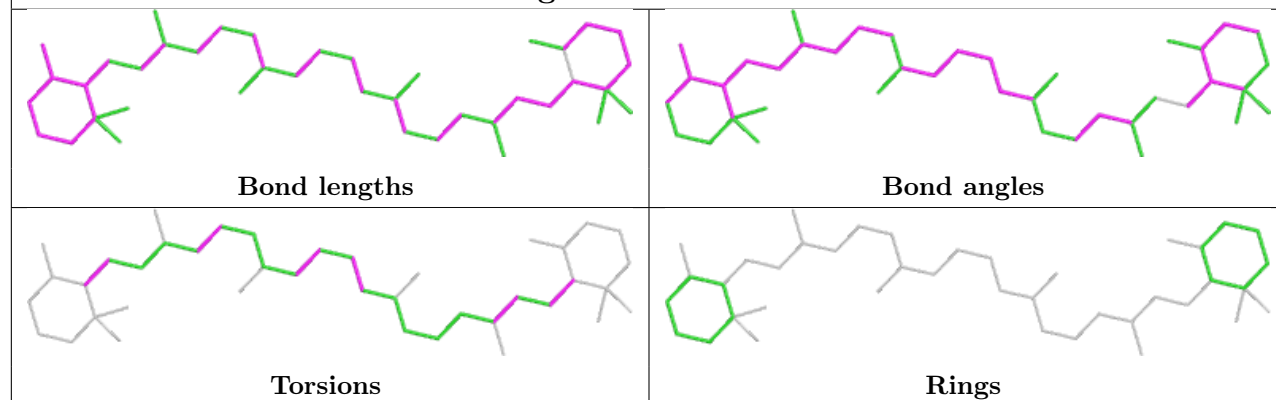


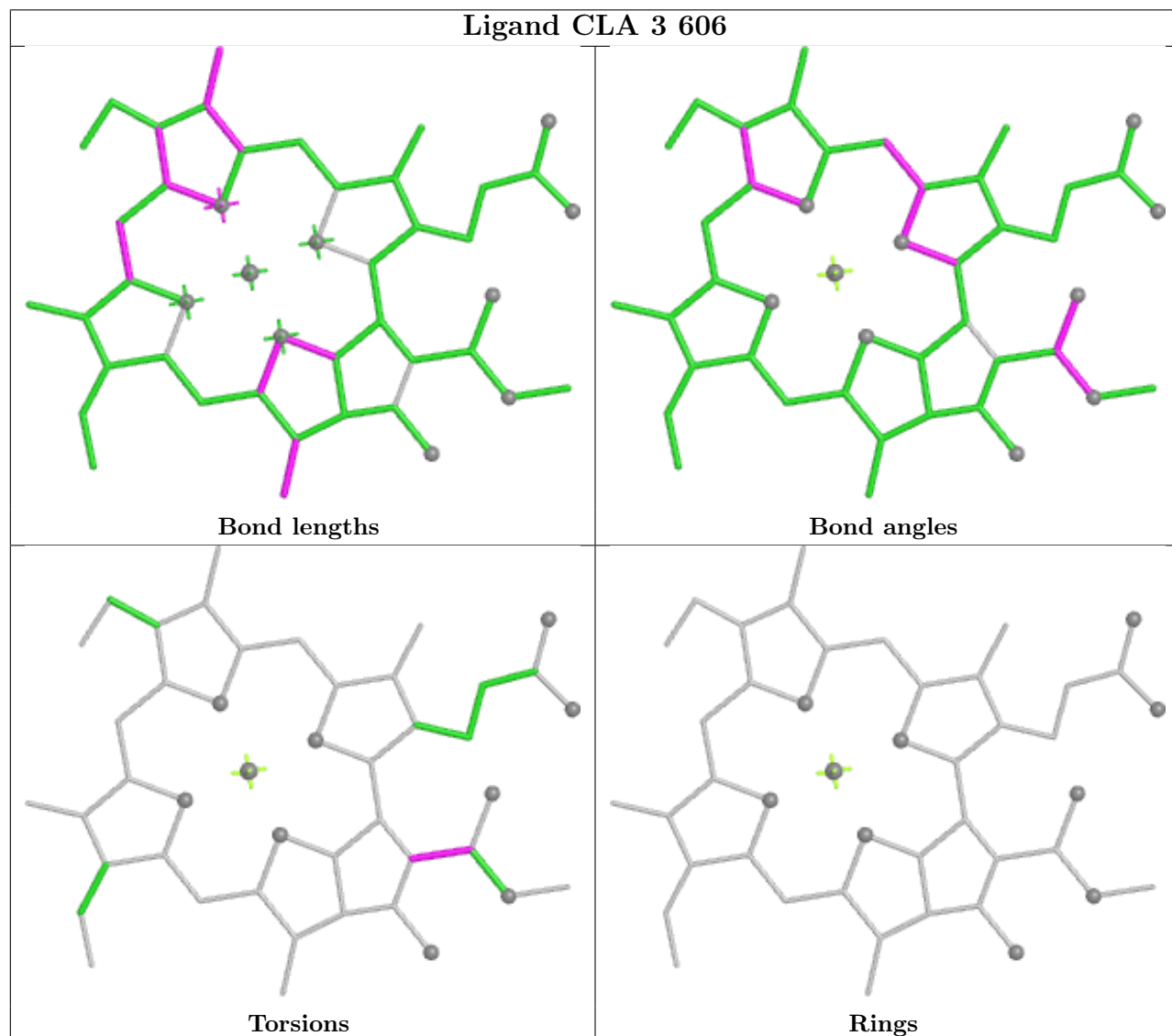
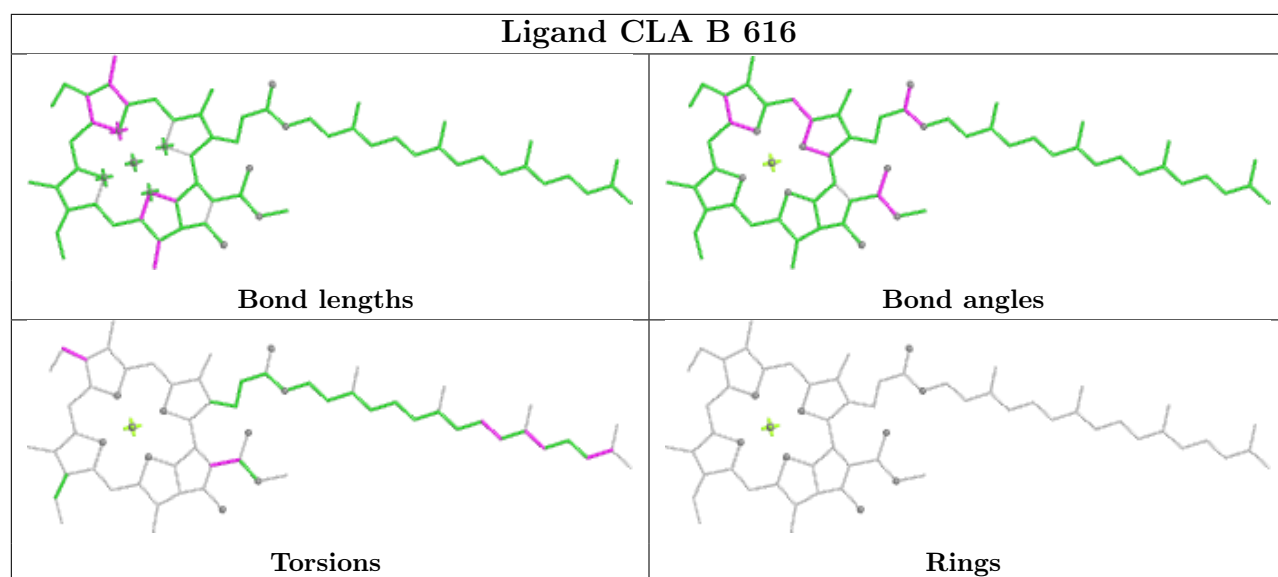
Ligand CLA 1 603



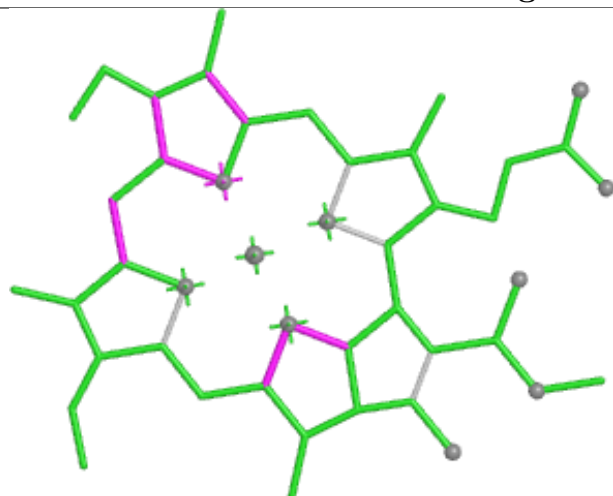
Ligand CLA 2 605



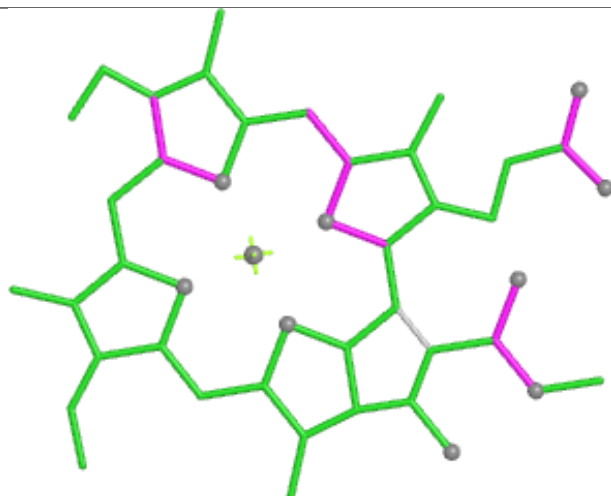
Ligand CLA 8 603**Ligand 8CT b 622**



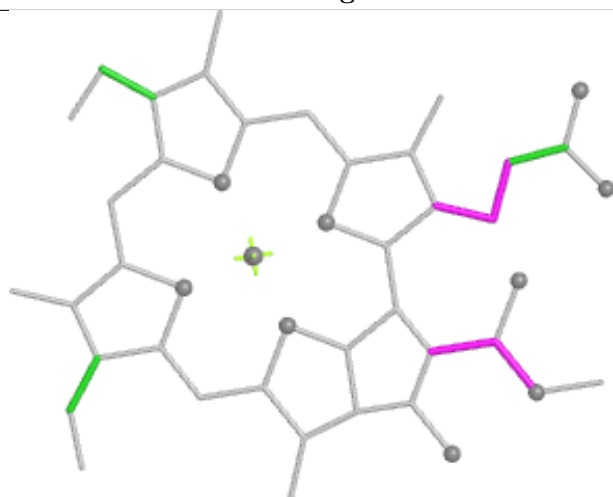
Ligand CLA 8 611



Bond lengths



Bond angles

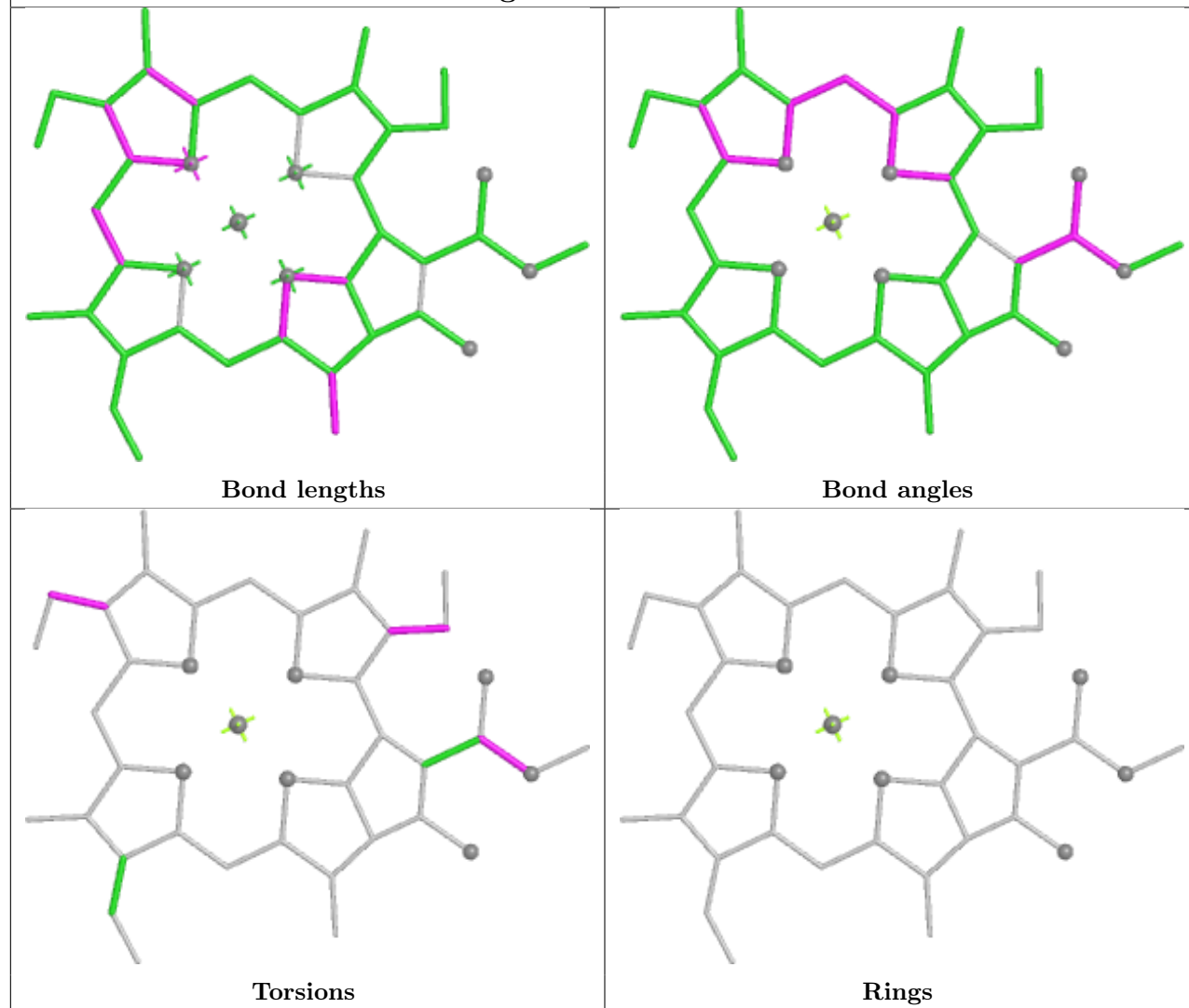


Torsions

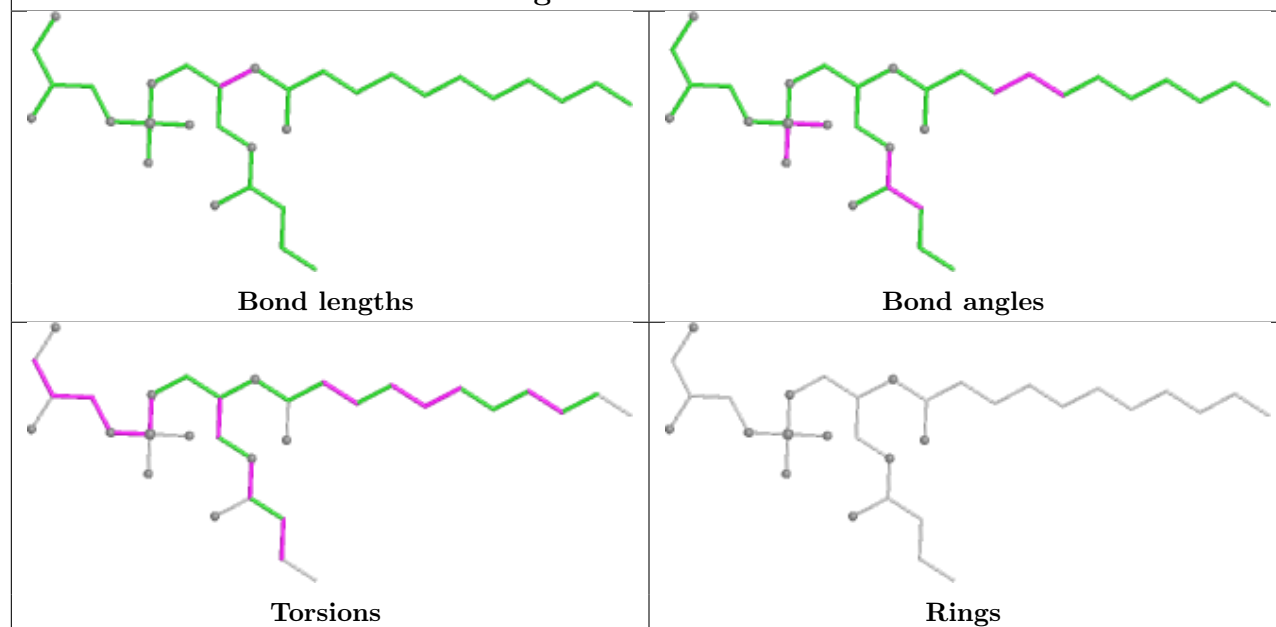


Rings

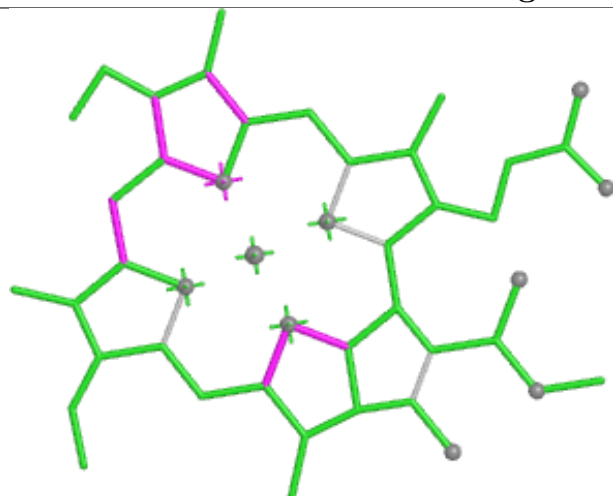
Ligand CLA 9 601



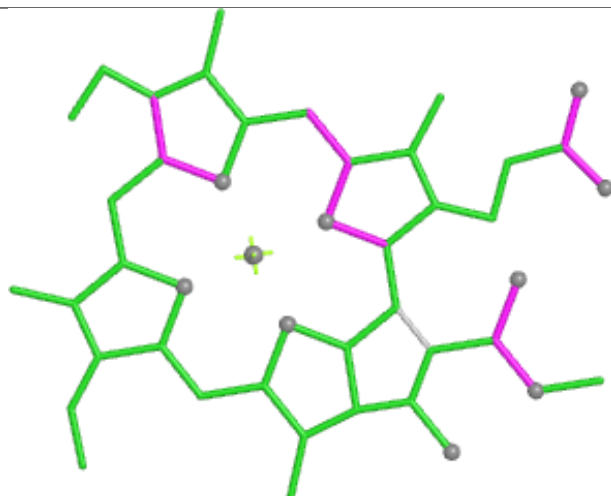
Ligand LHG d 411



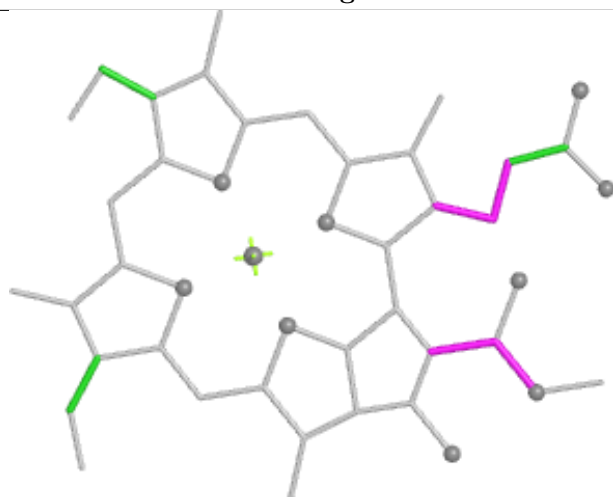
Ligand CLA 2 611



Bond lengths



Bond angles

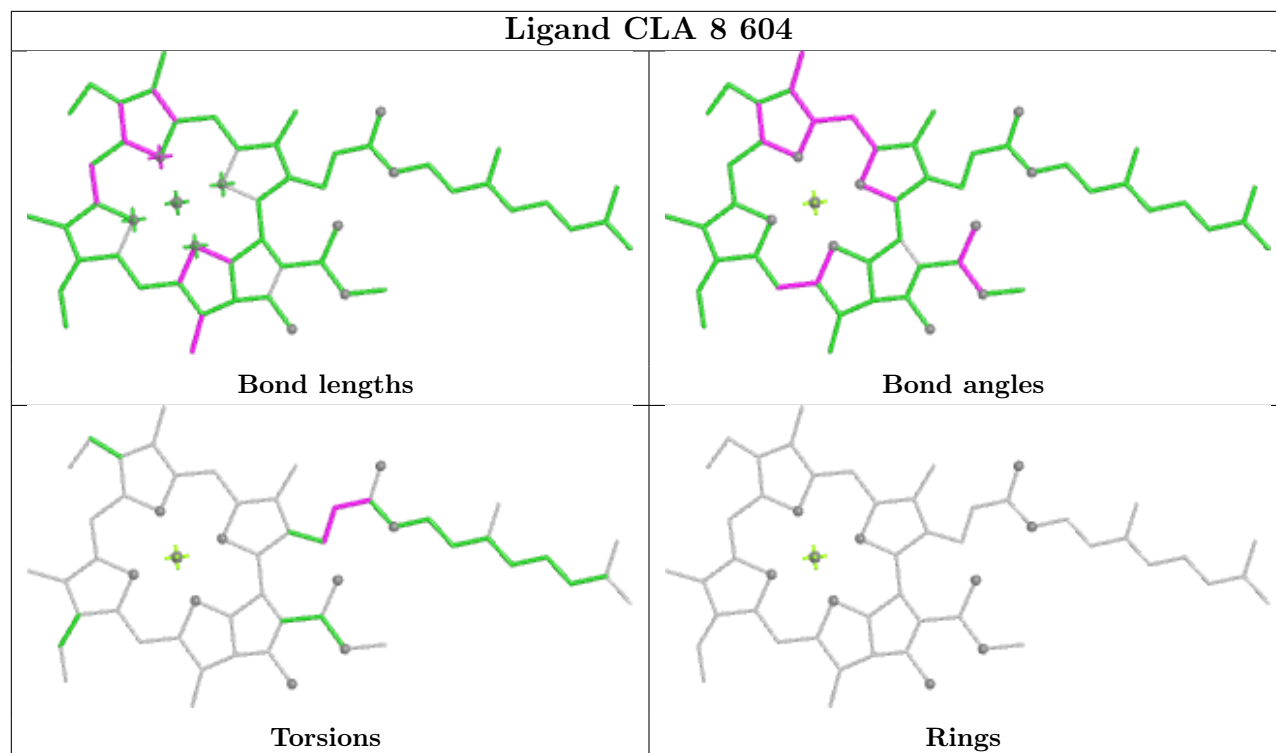


Torsions

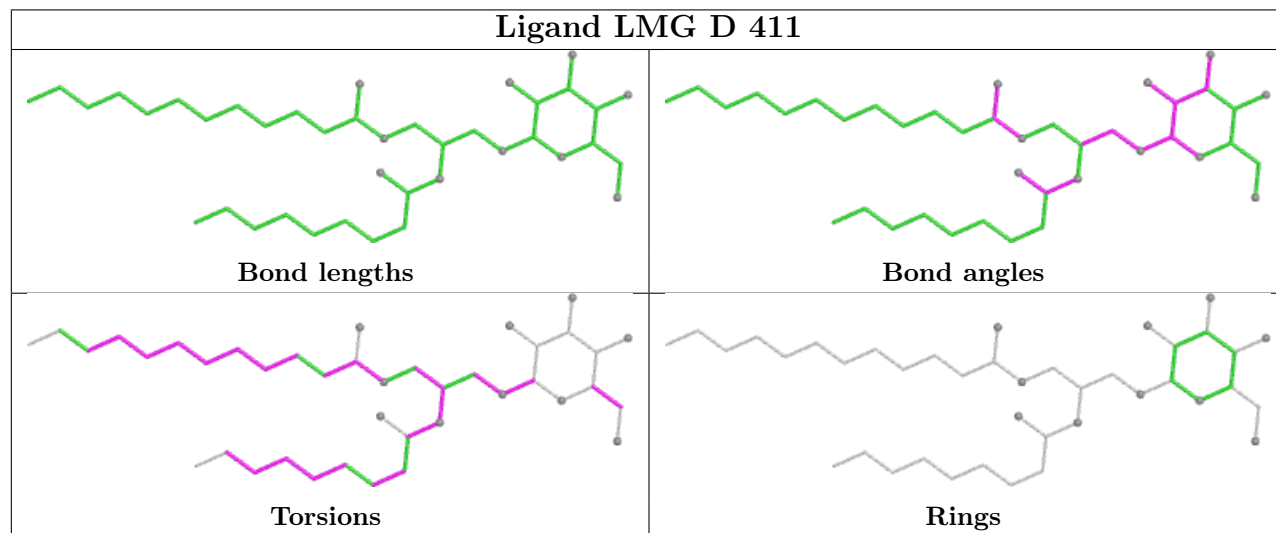


Rings

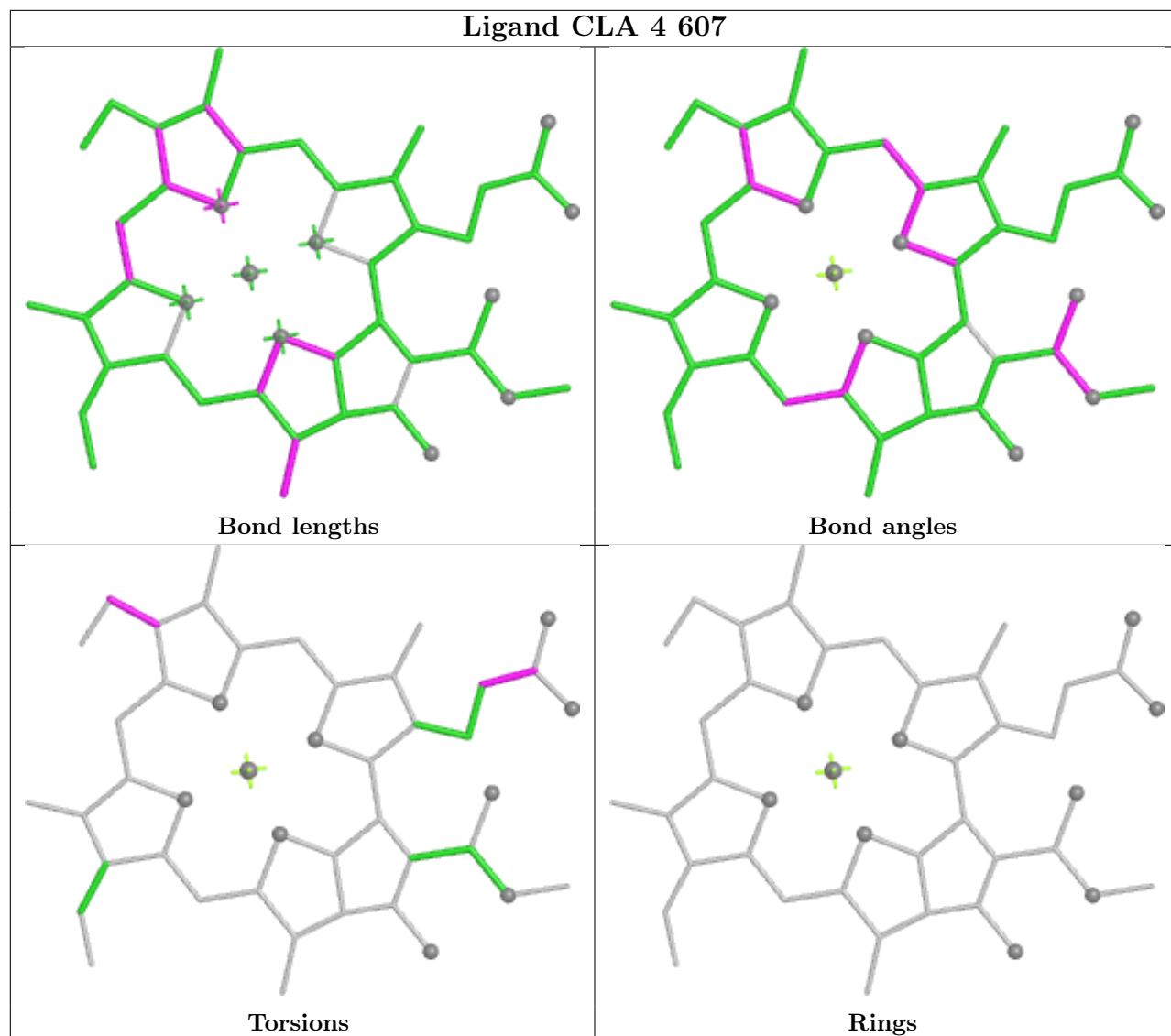
Ligand CLA 8 604



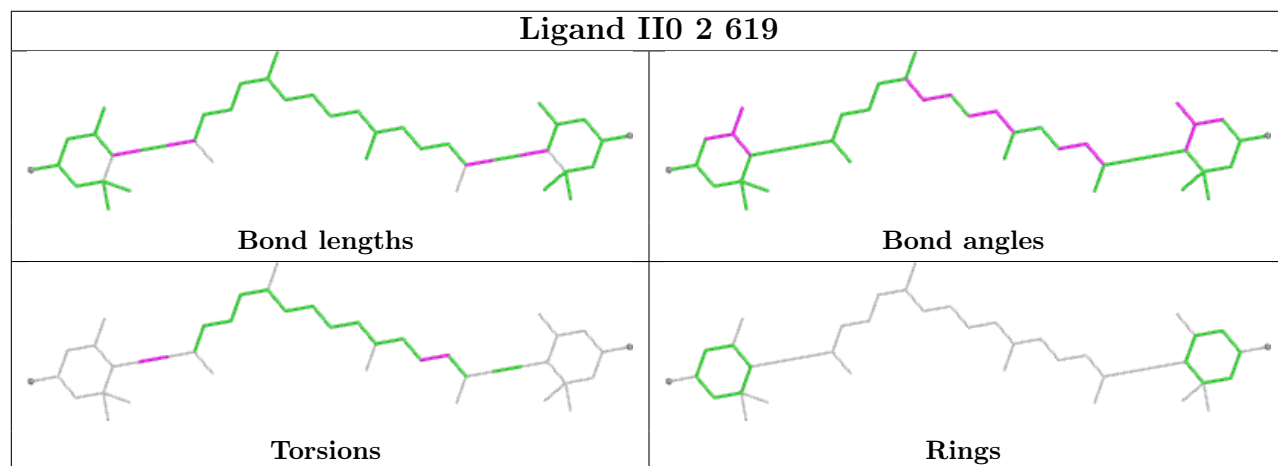
Ligand LMG D 411

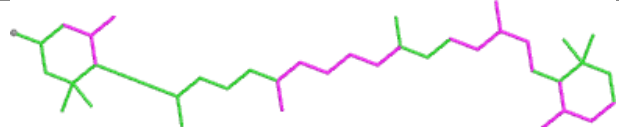
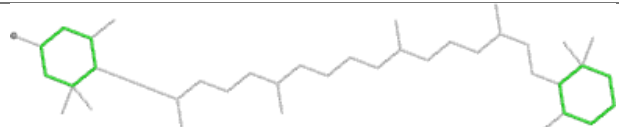


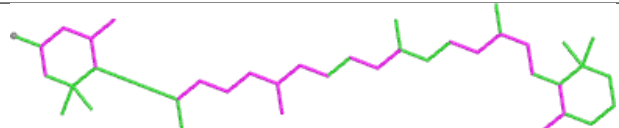
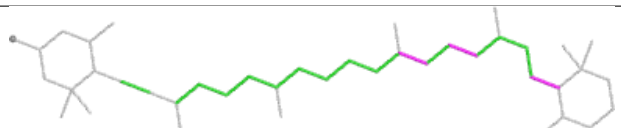
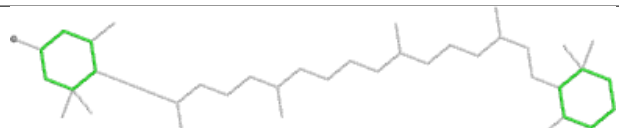
Ligand CLA 4 607

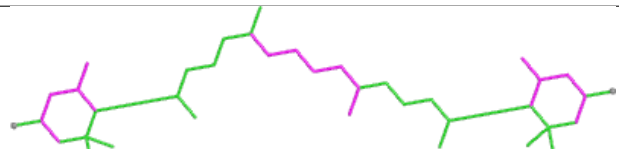
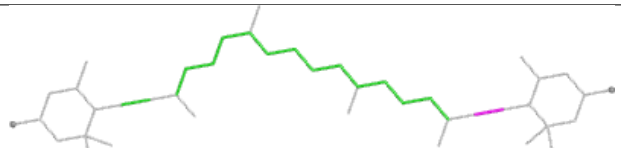
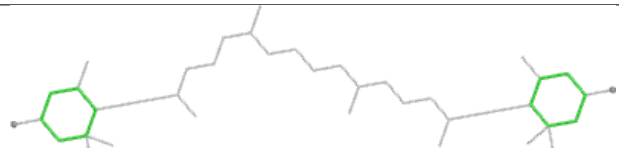


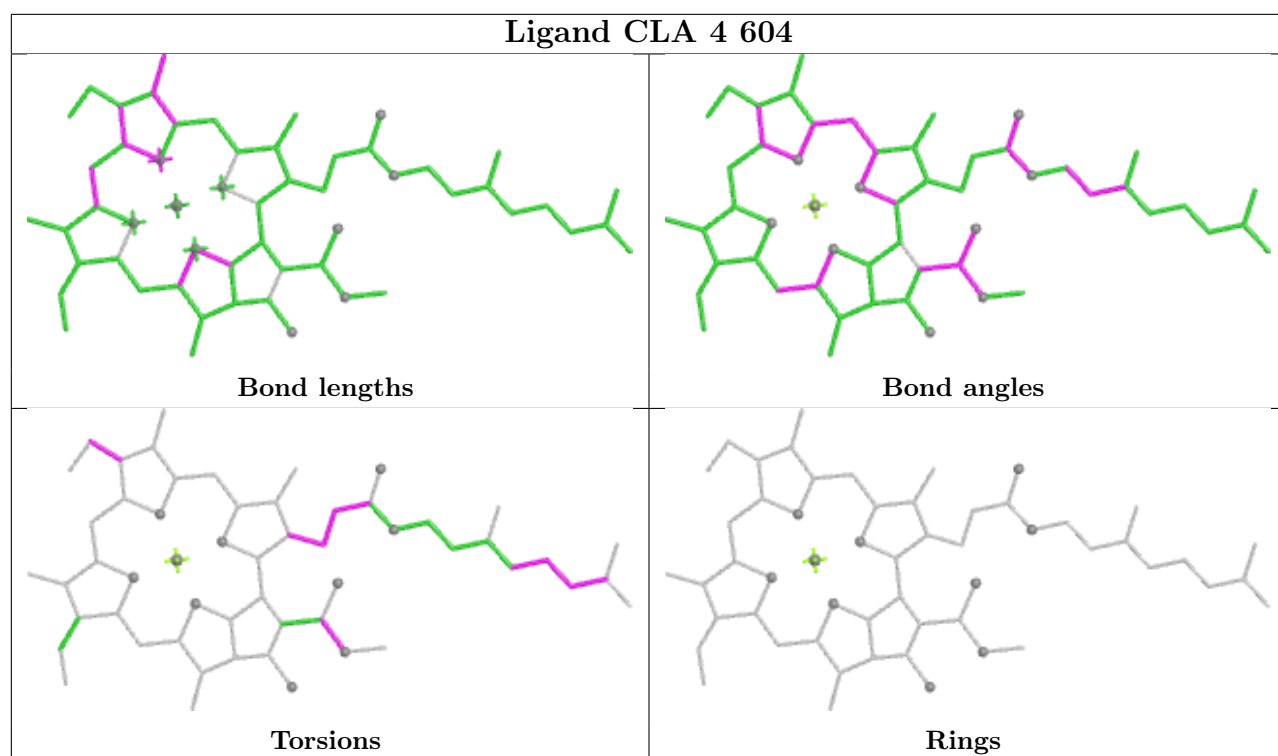
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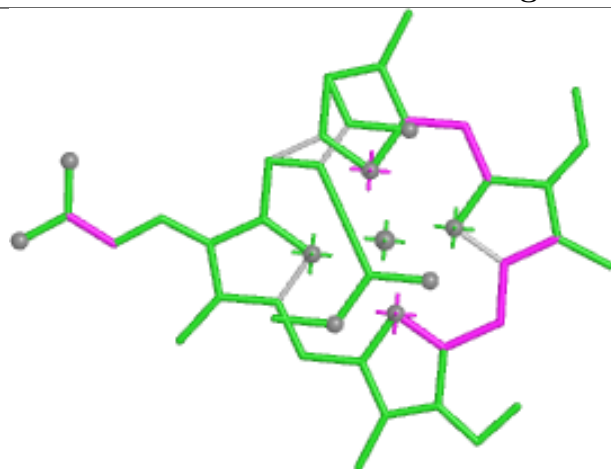
Ligand IHT 1 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand IHT 4 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

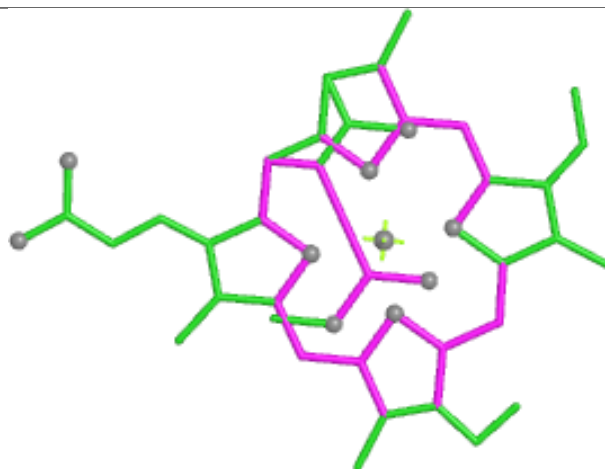
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Bond lengths	Bond angles
	
Torsions	Rings



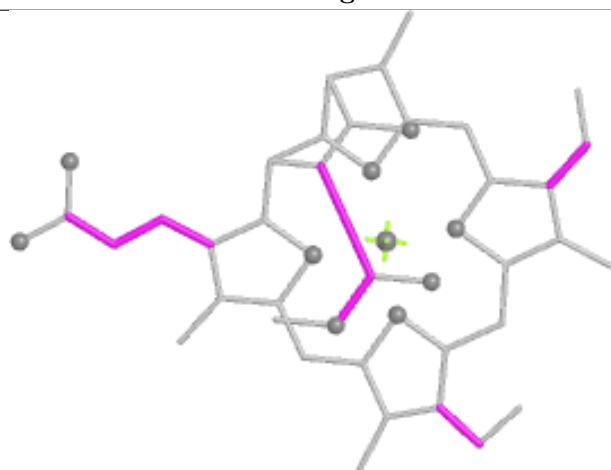
Ligand KC2 6 609



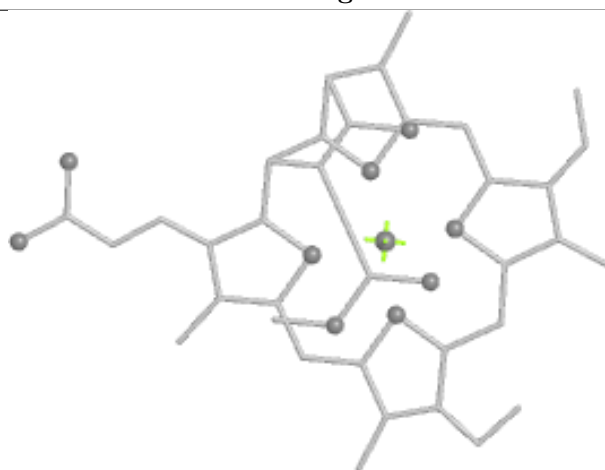
Bond lengths



Bond angles

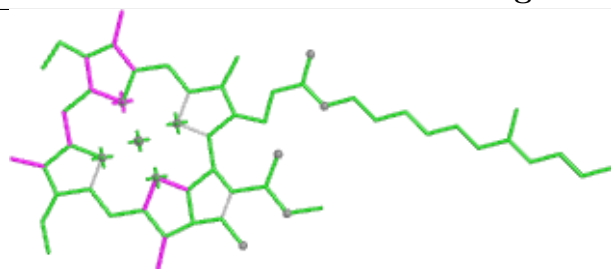


Torsions

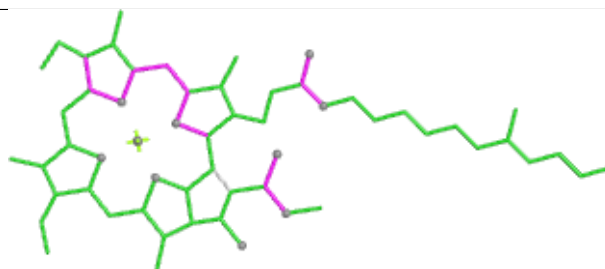


Rings

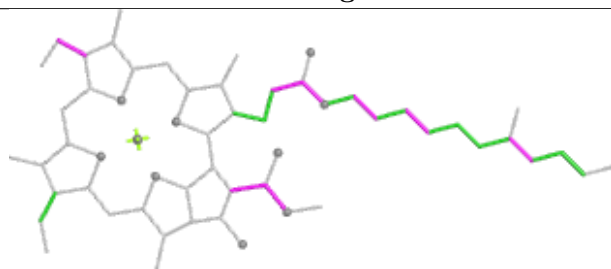
Ligand CLA C 512



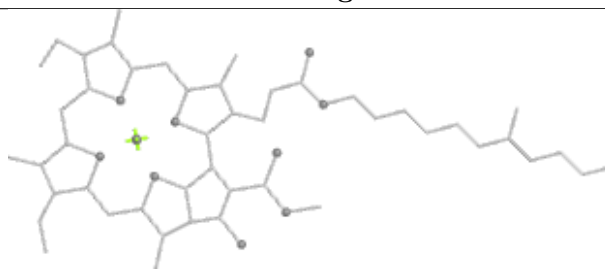
Bond lengths



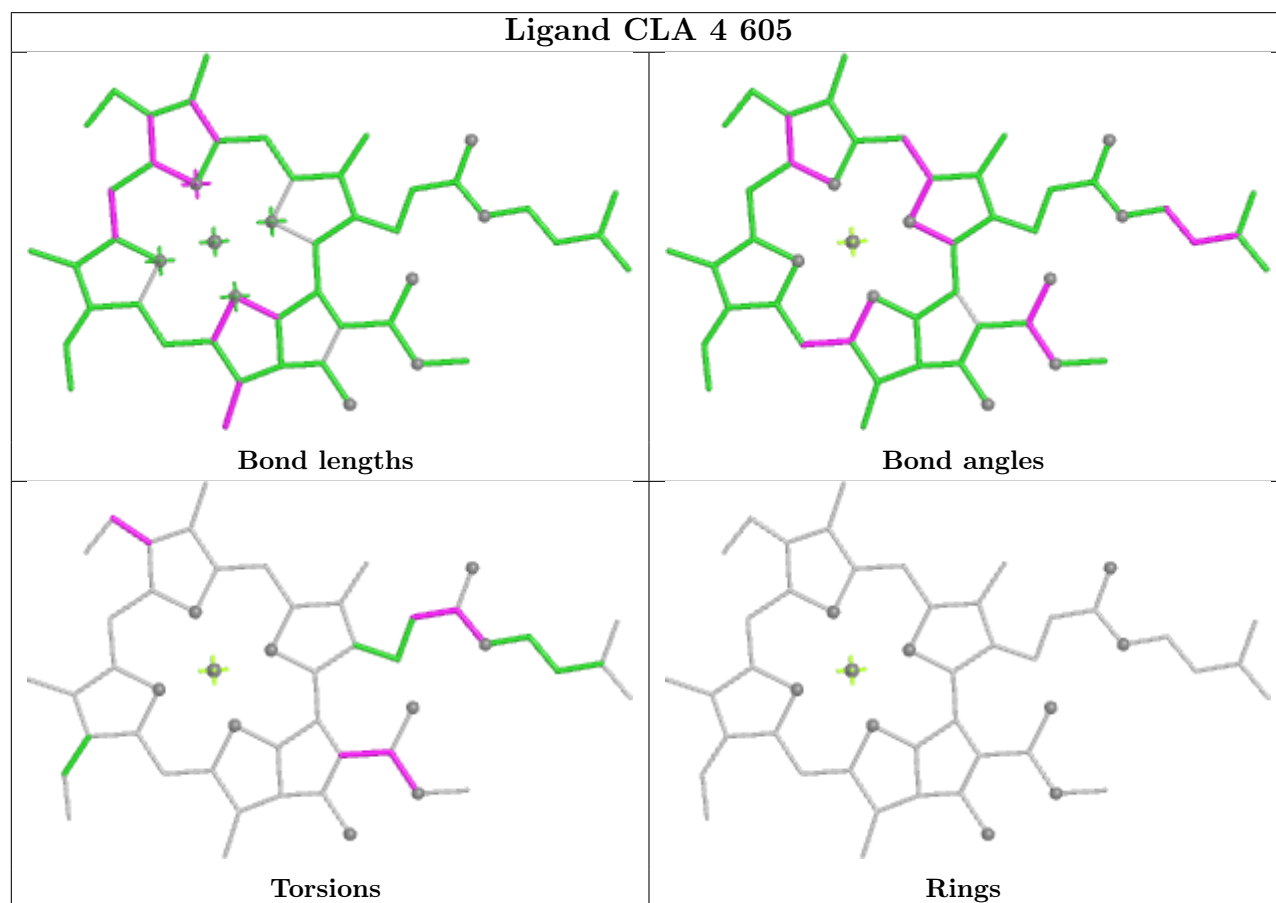
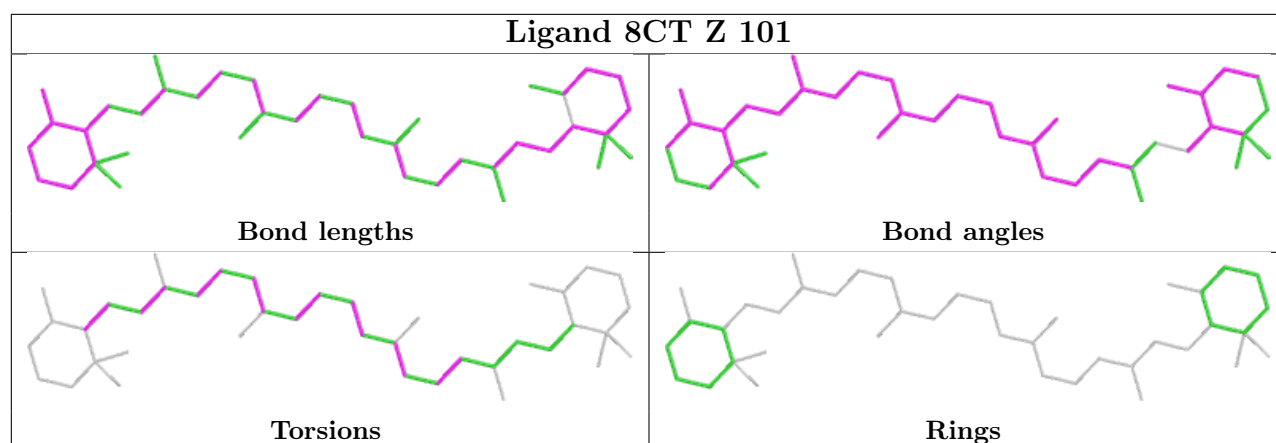
Bond angles

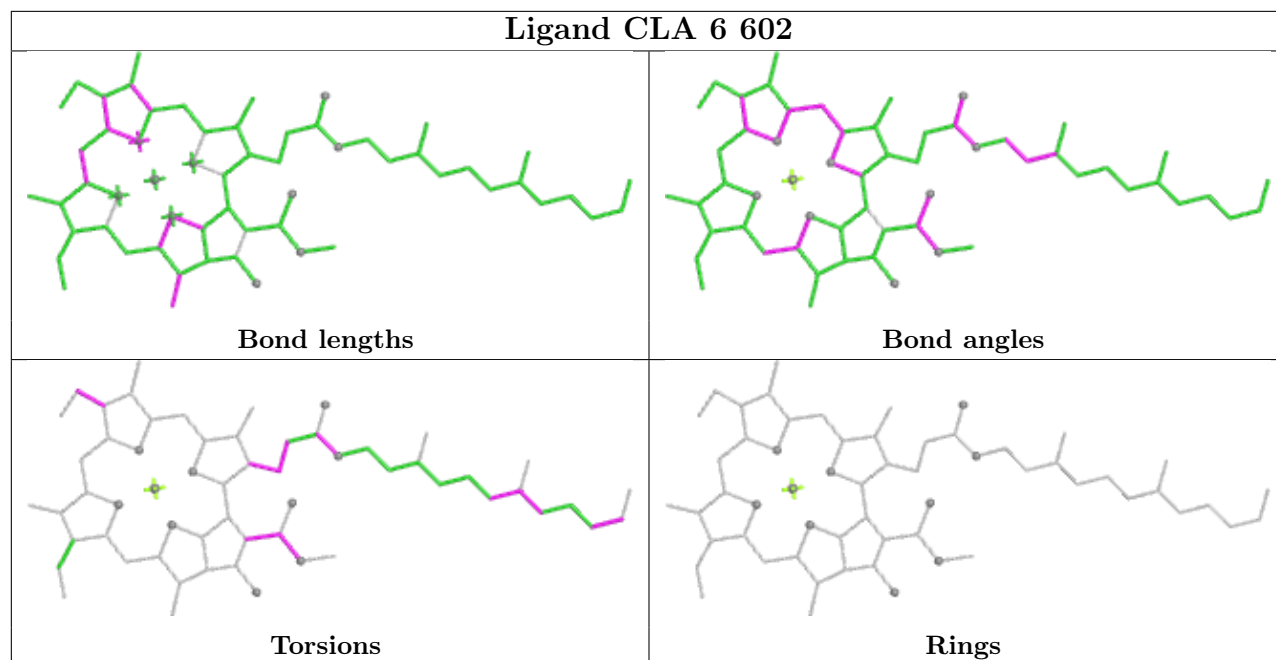
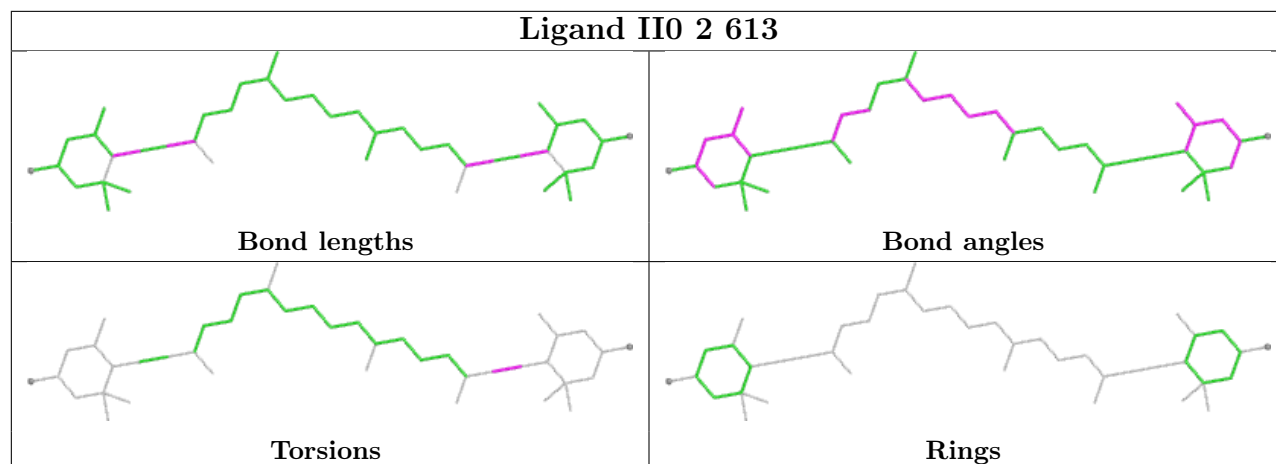


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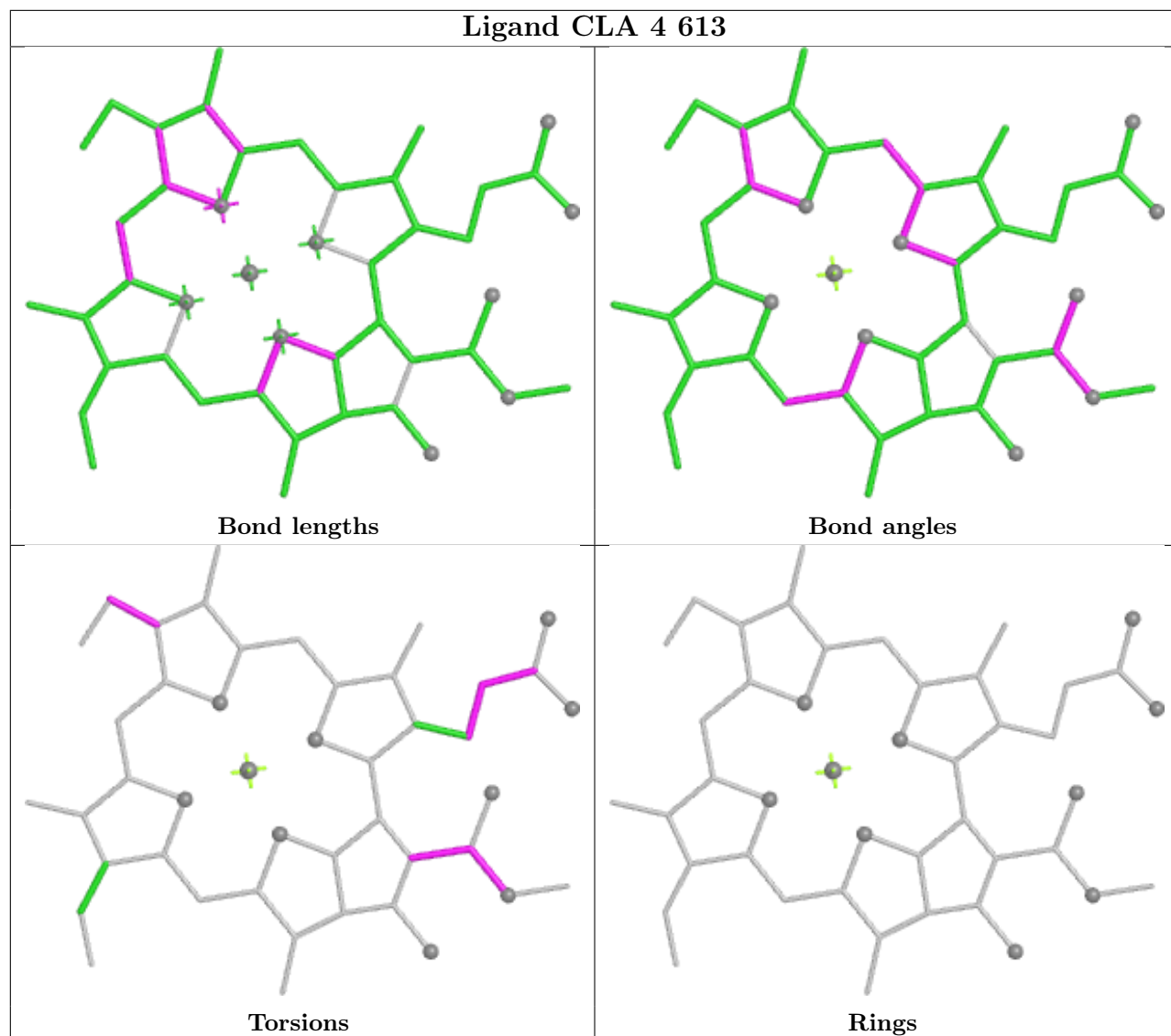


Rings

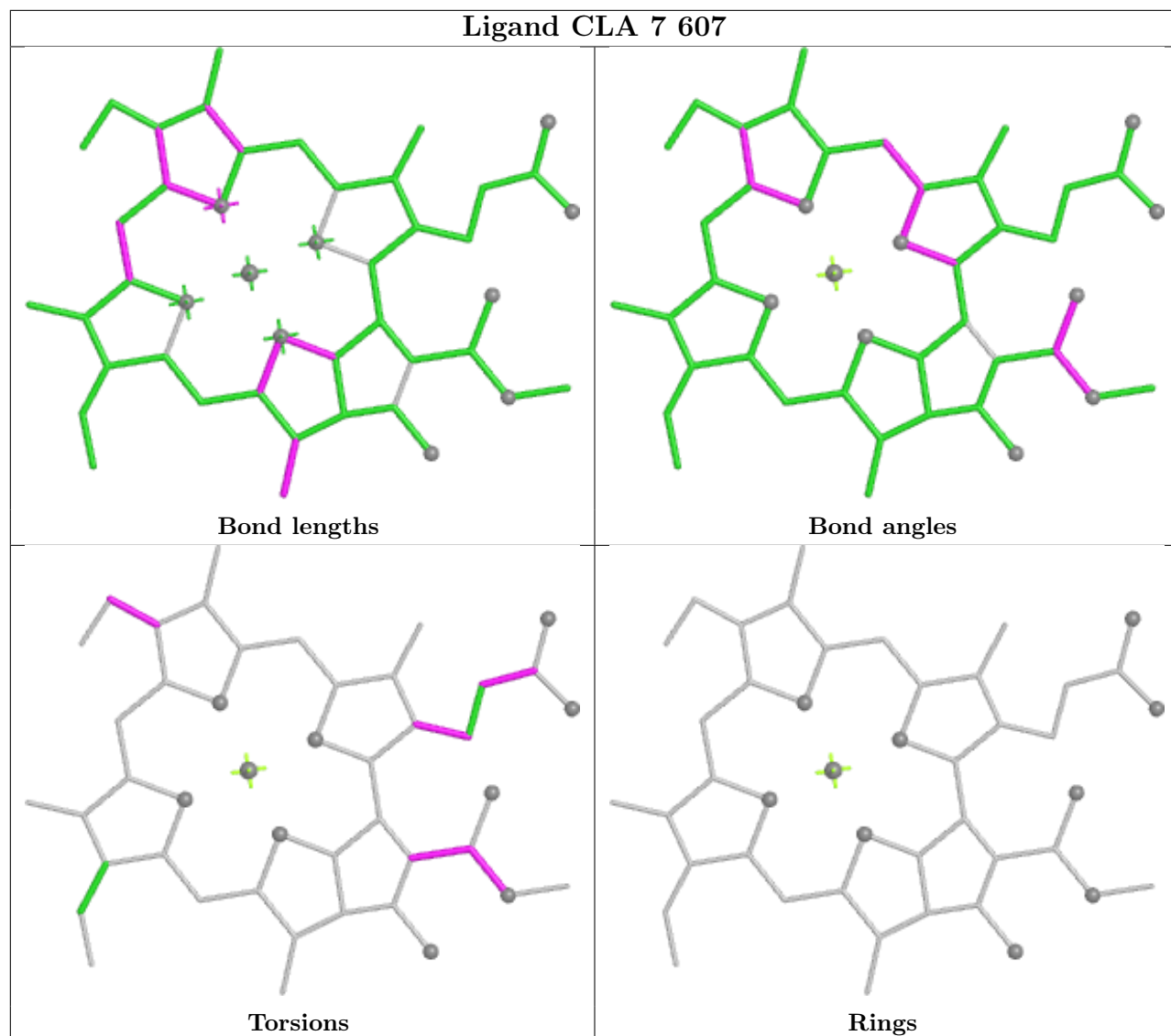


Ligand CLA 6 602**Ligand II0 2 613**

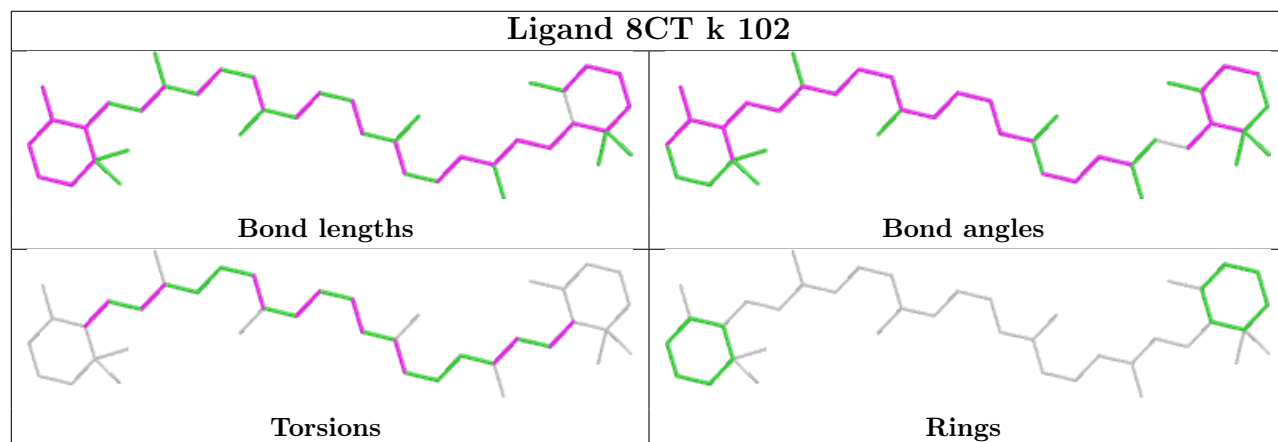
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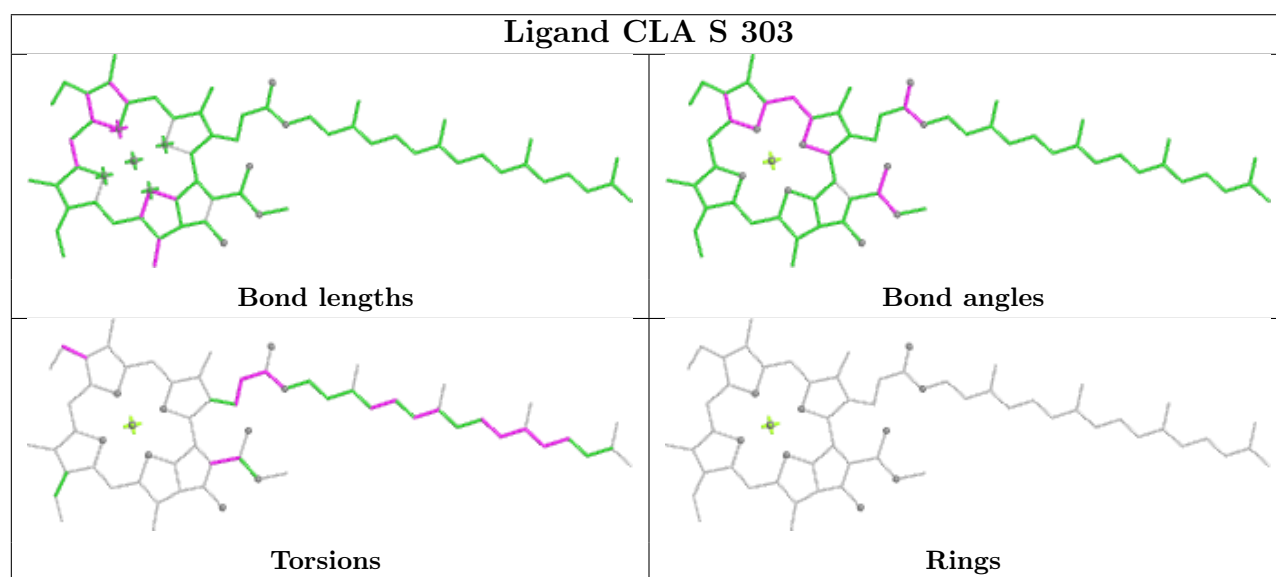
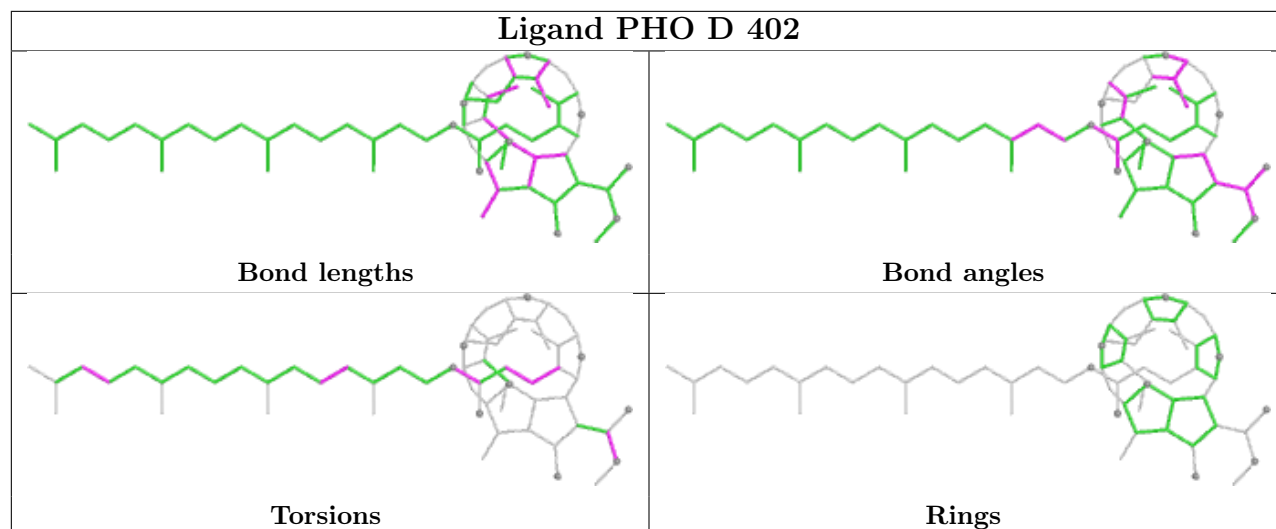


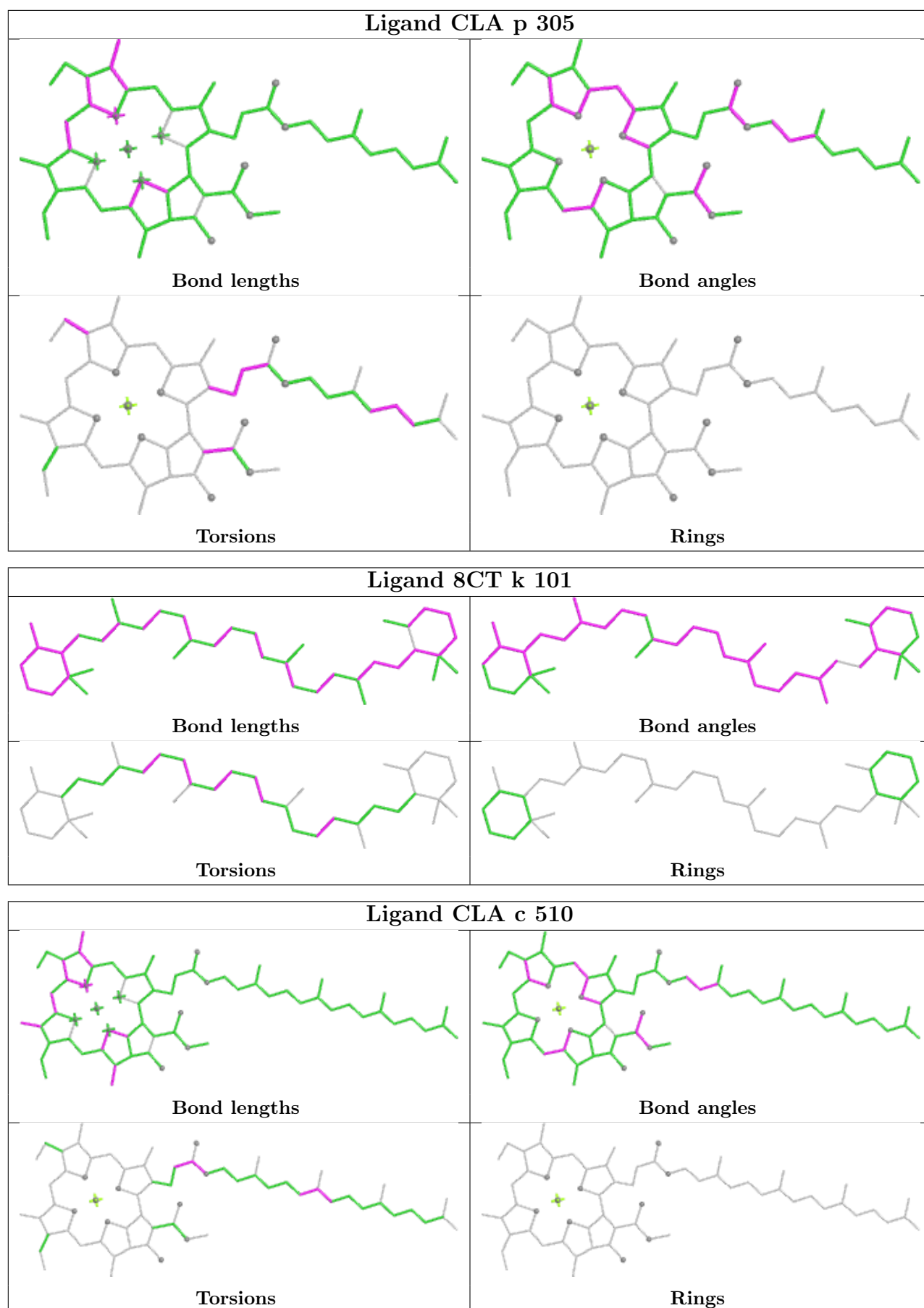
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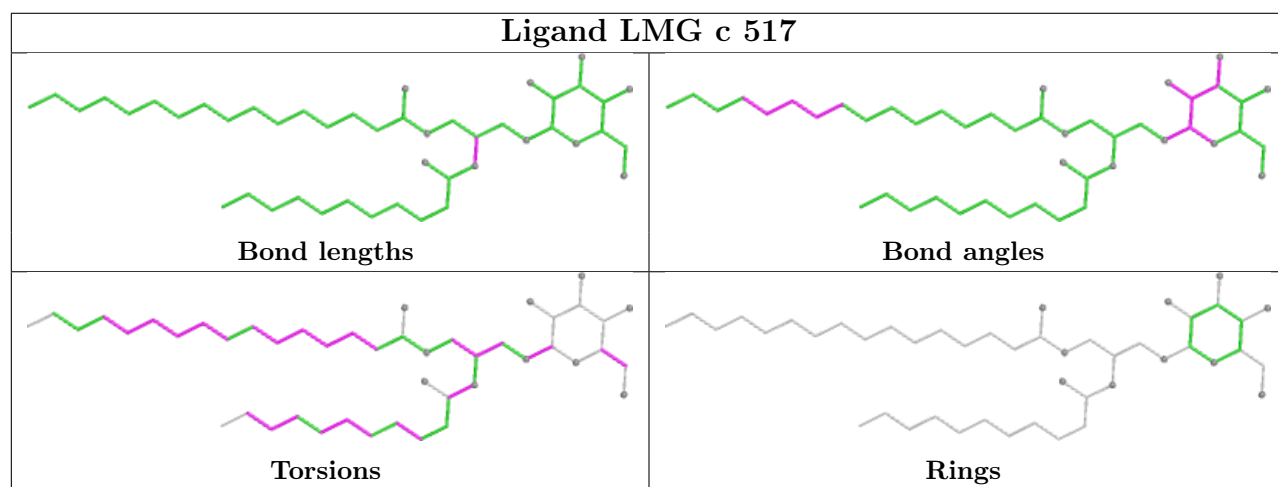
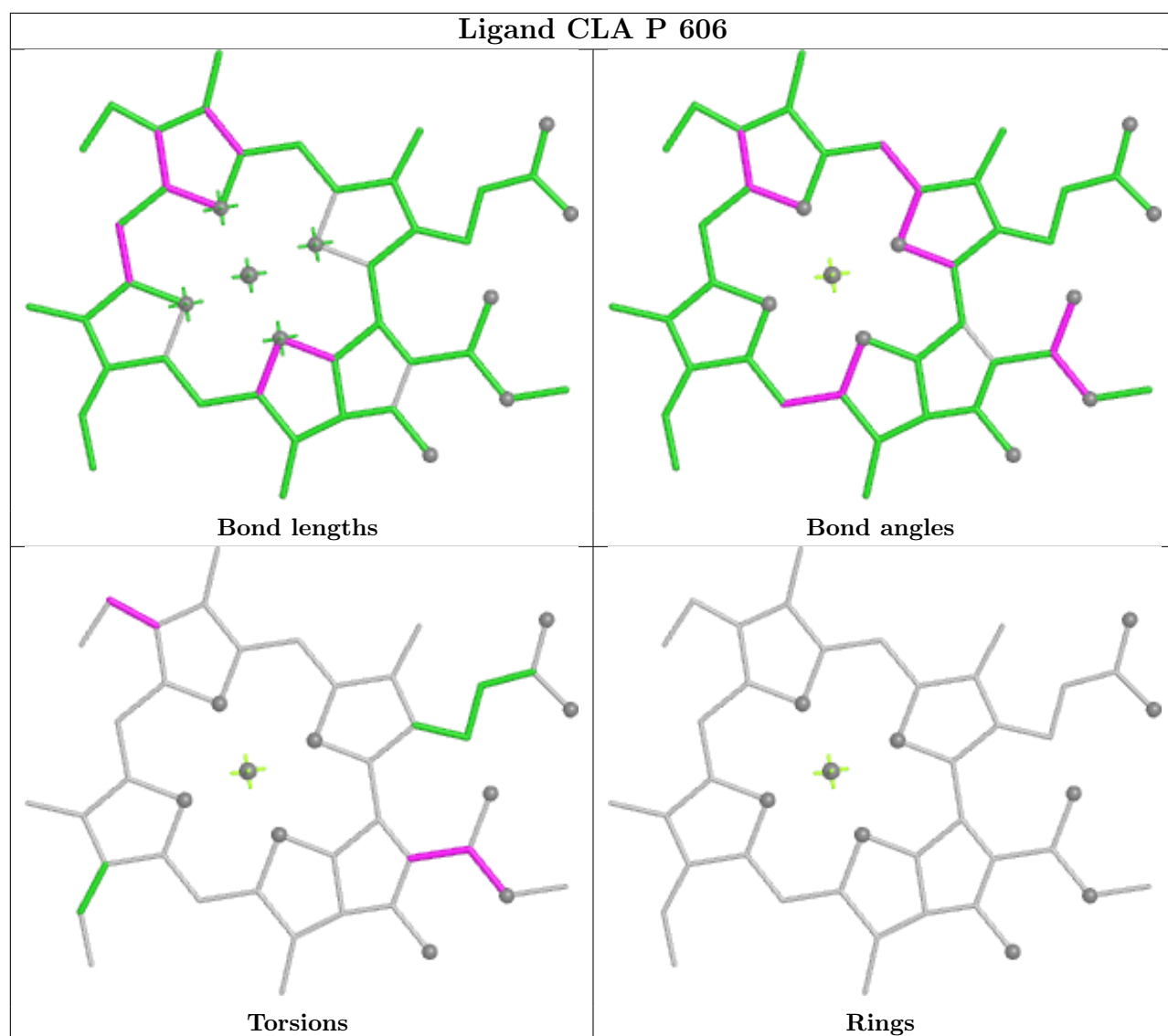


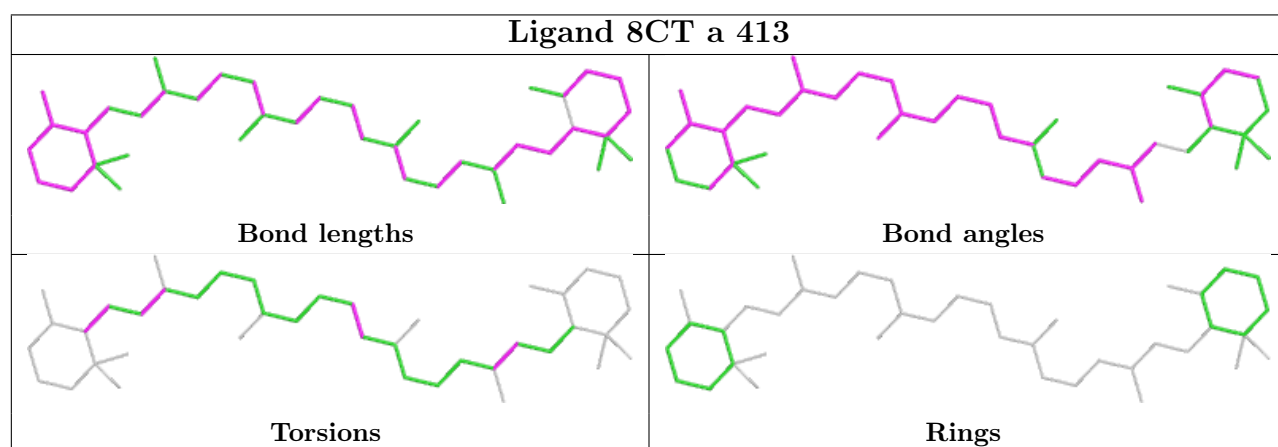
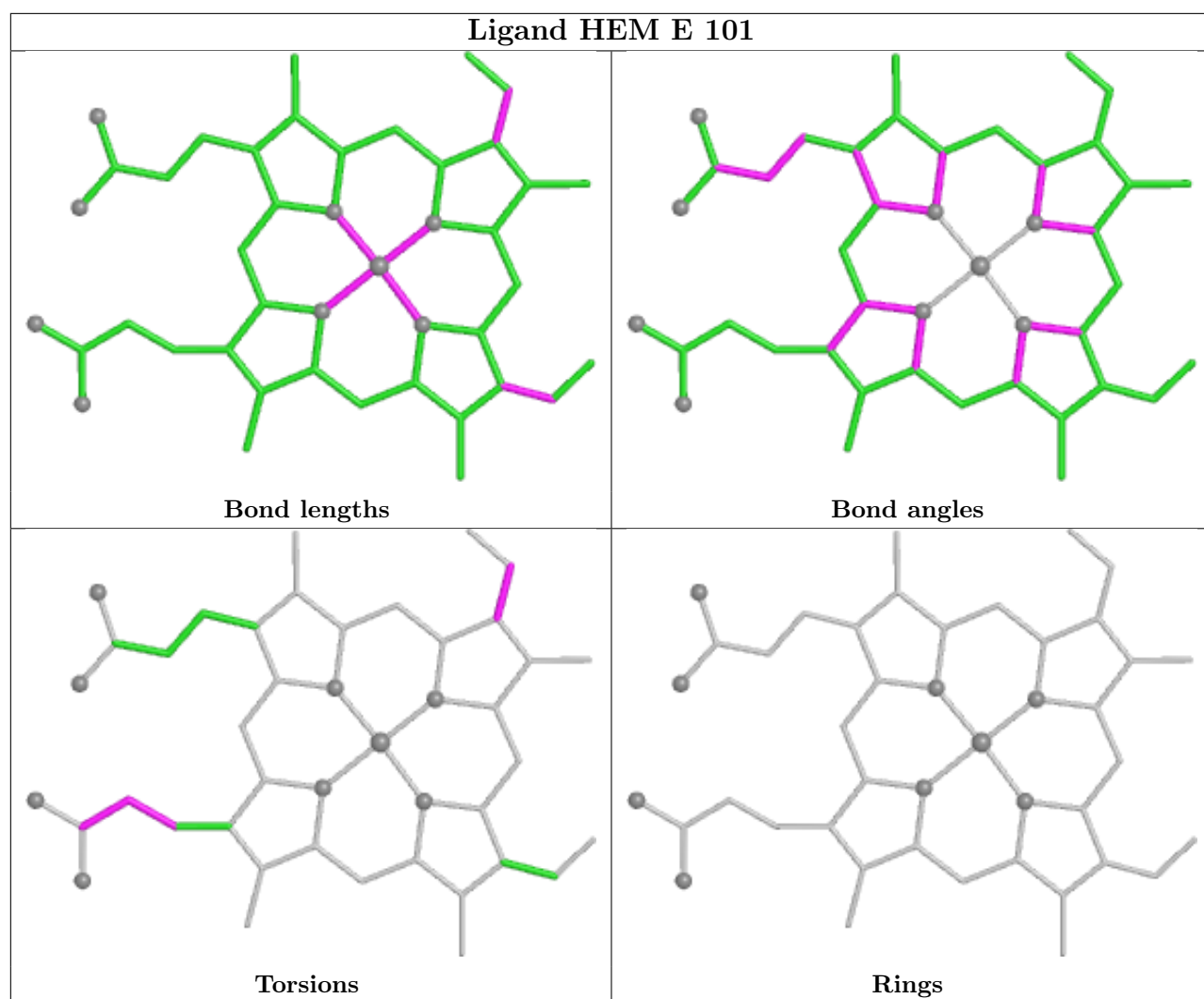
Ligand 8CT k 102



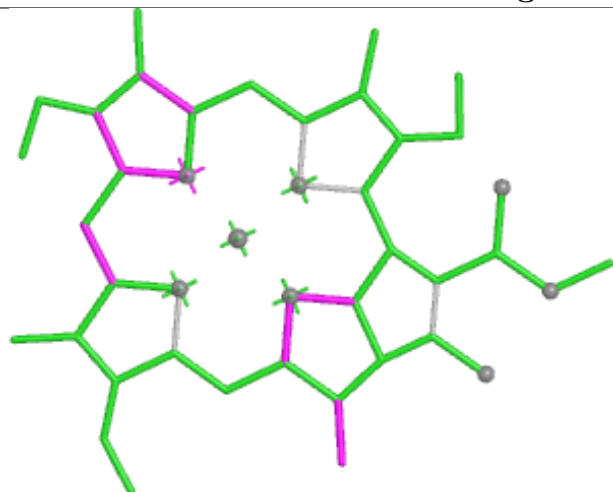




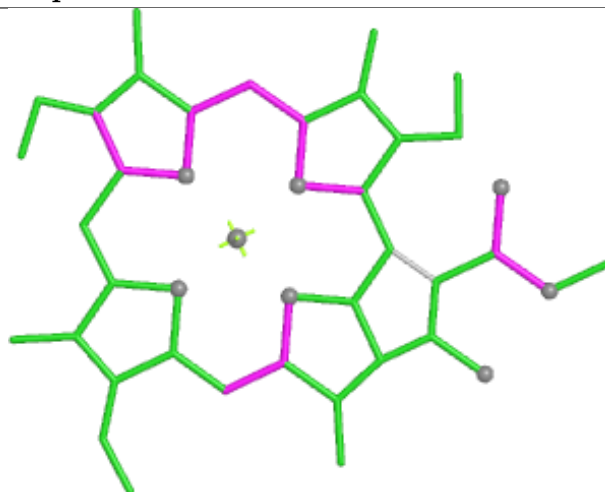




Ligand CLA p 302



Bond lengths



Bond angles

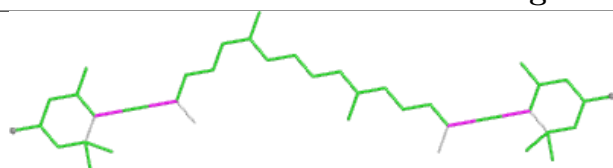


Torsions

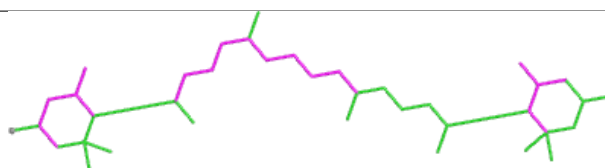


Rings

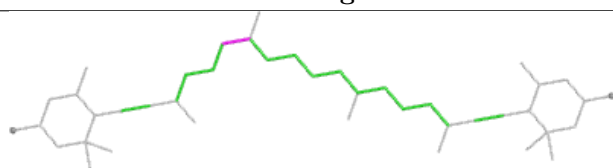
Ligand II0 P 614



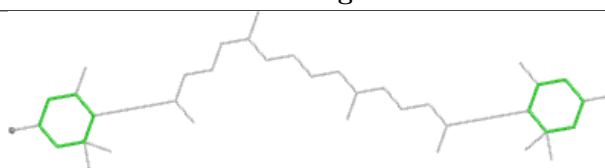
Bond lengths



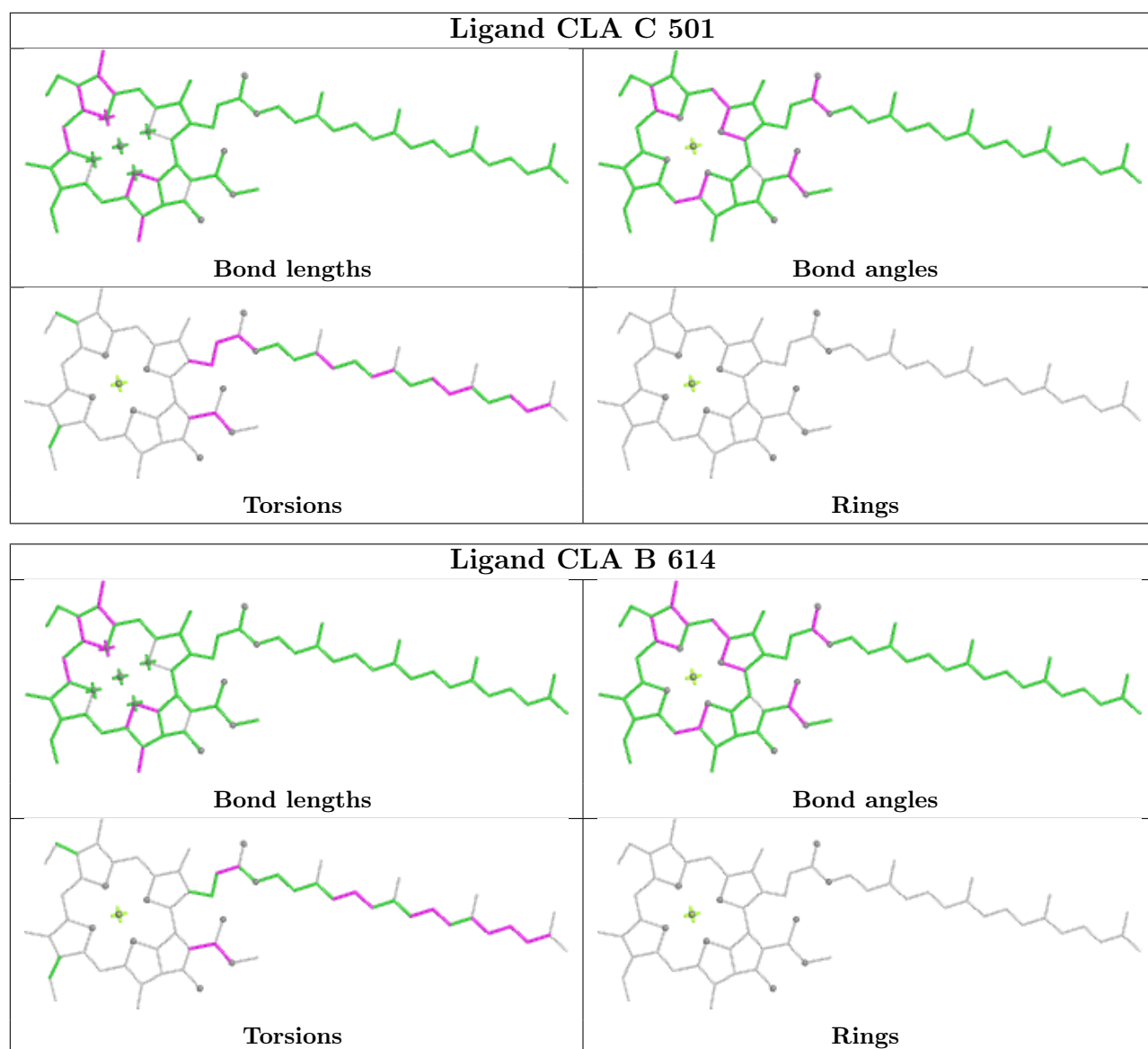
Bond angles



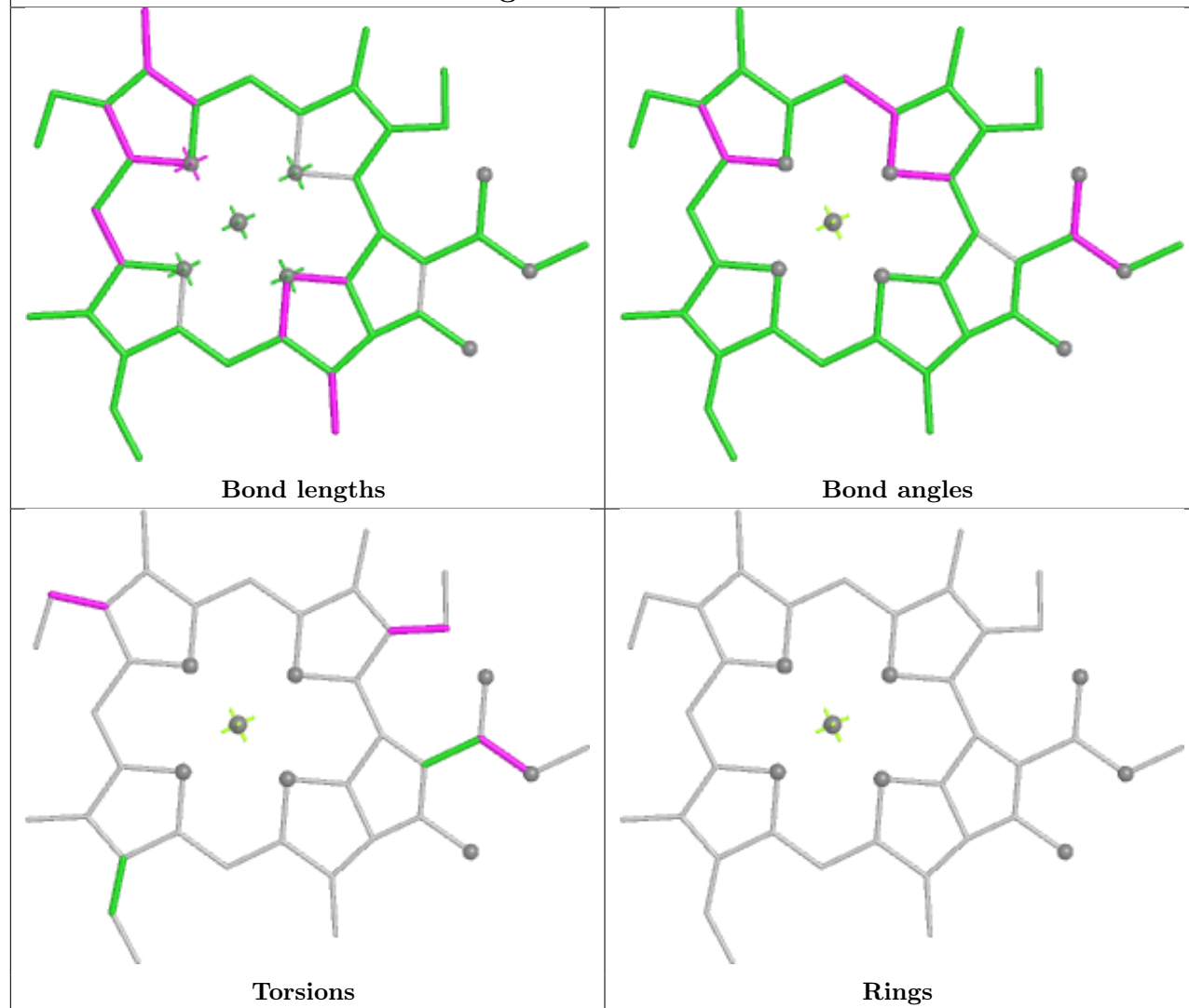
Torsions



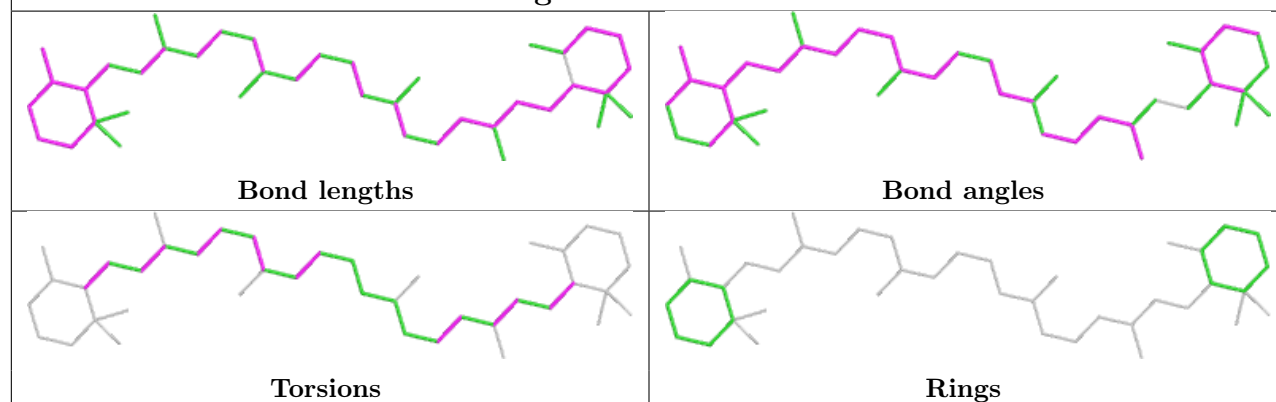
Rings



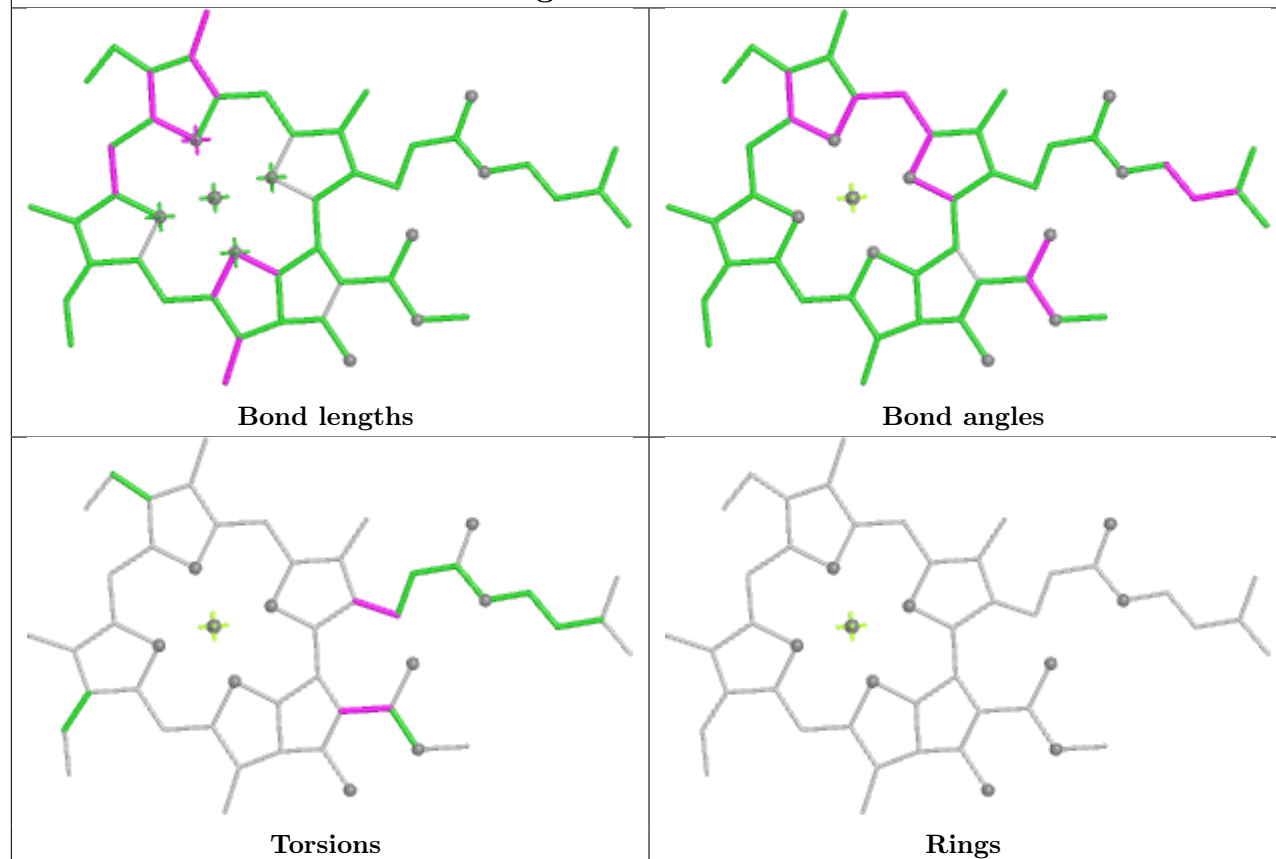
Ligand CLA 3 601



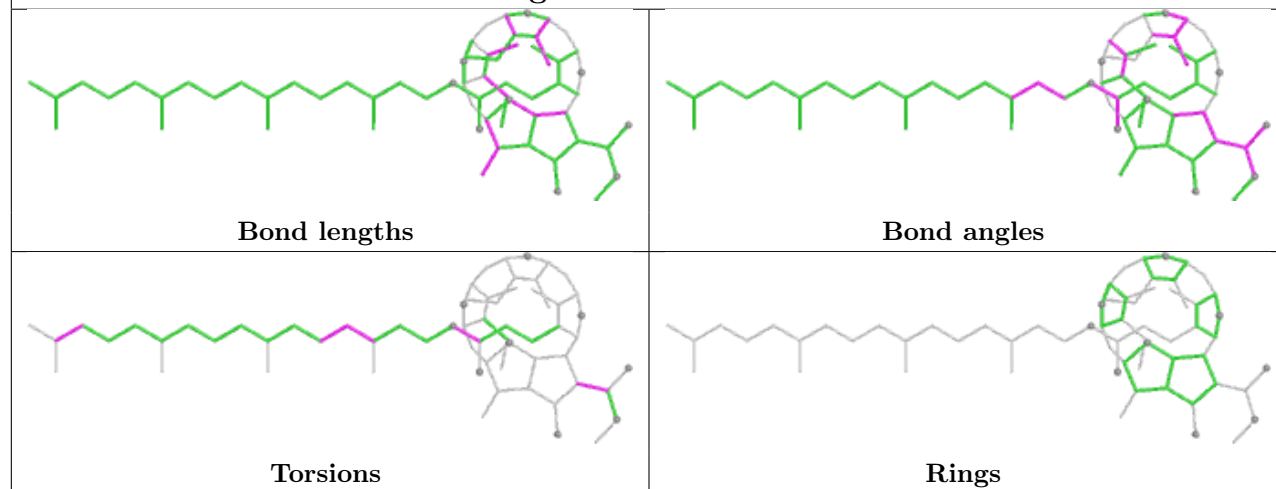
Ligand 8CT D 409

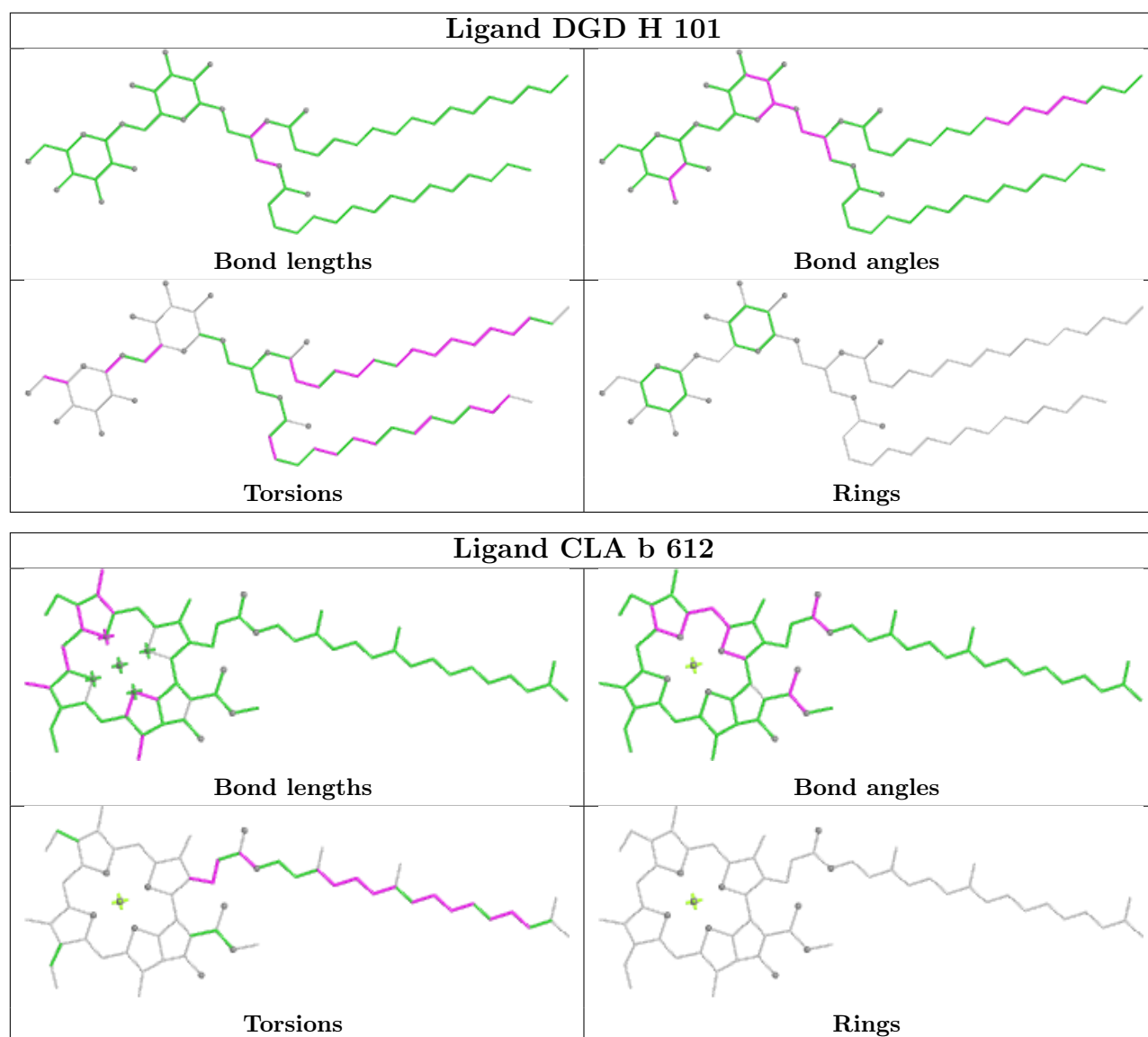


Ligand CLA 6 603

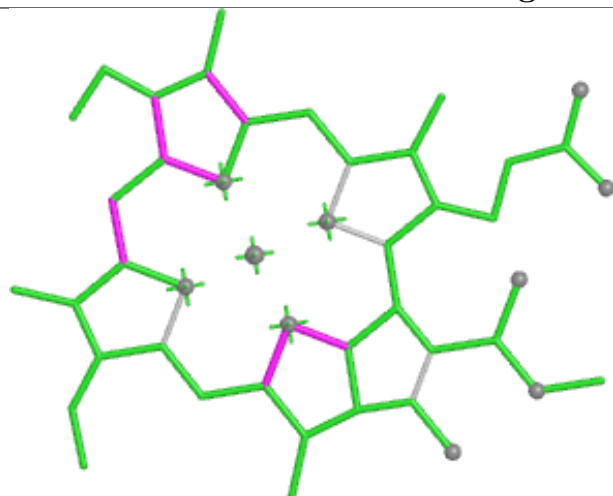


Ligand PHO A 604

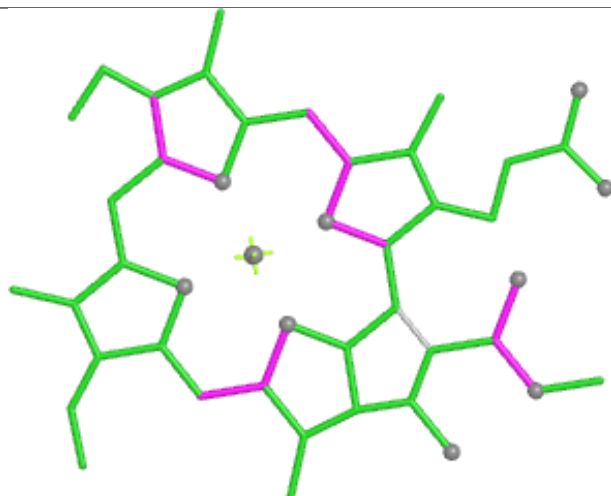




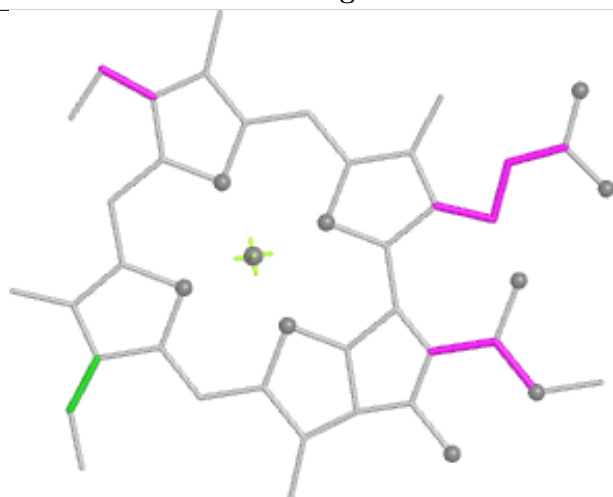
Ligand CLA 5 313



Bond lengths



Bond angles

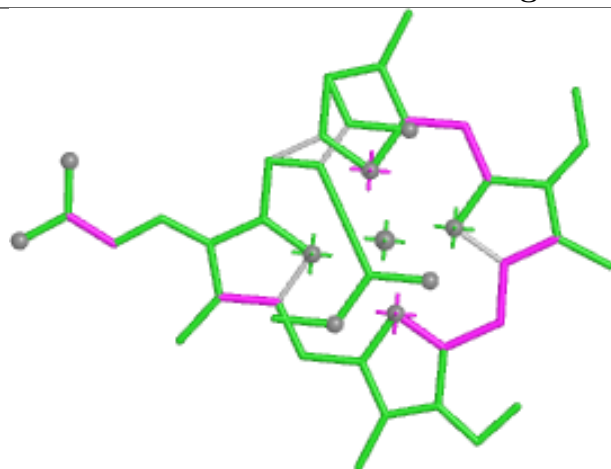


Torsions

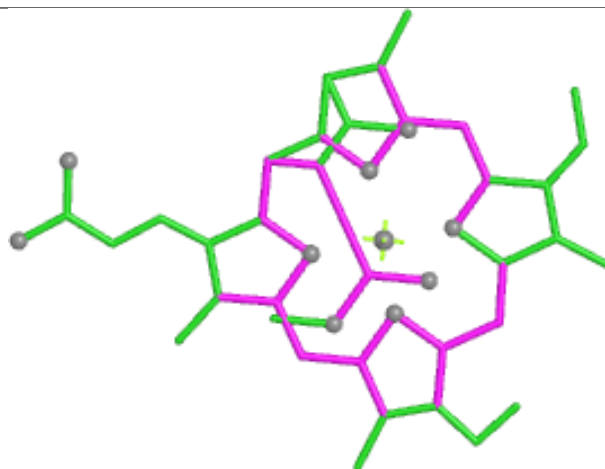


Rings

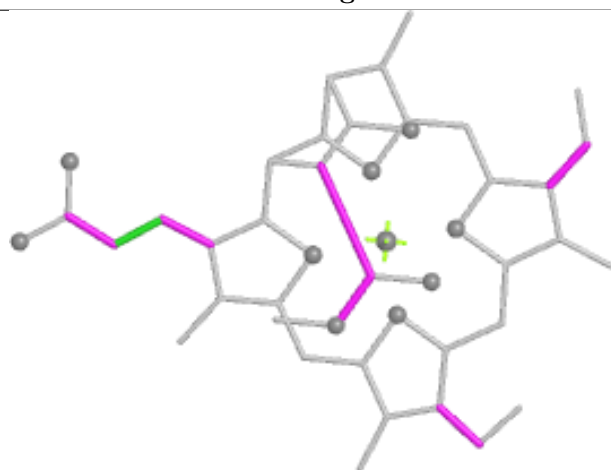
Ligand KC2 7 610



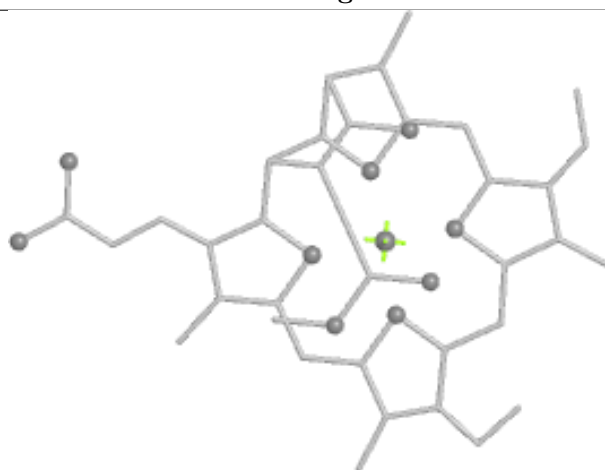
Bond lengths



Bond angles

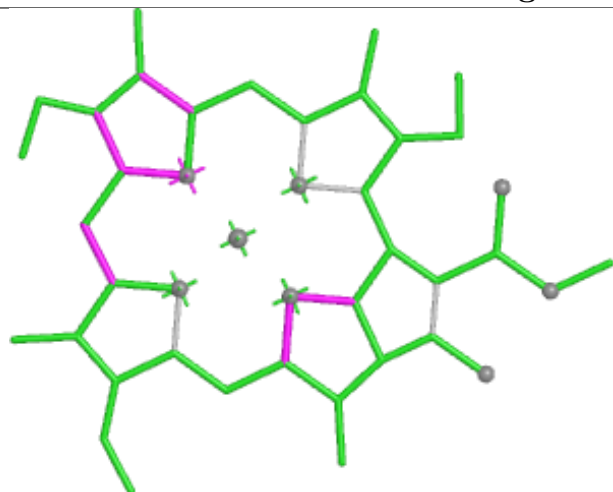


Torsions

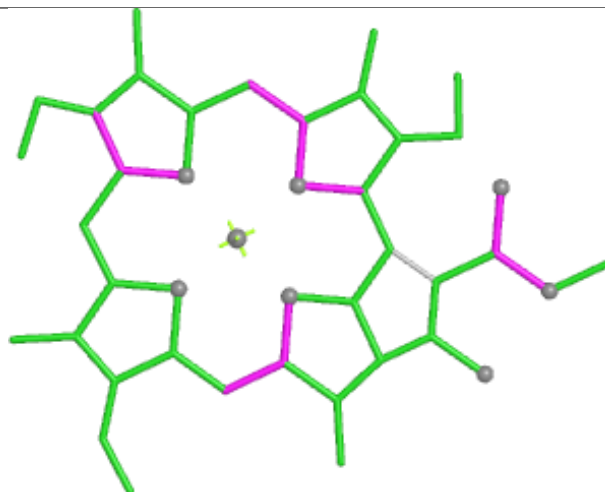


Rings

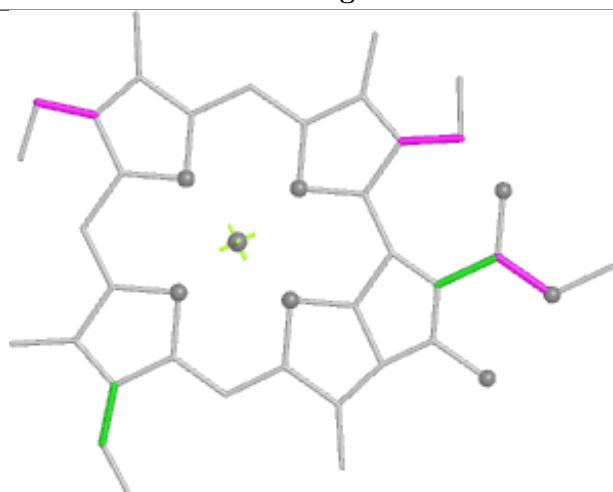
Ligand CLA 7 601



Bond lengths



Bond angles

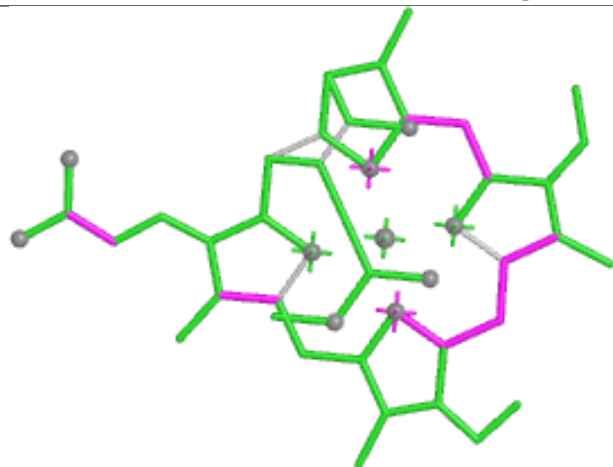


Torsions



Rings

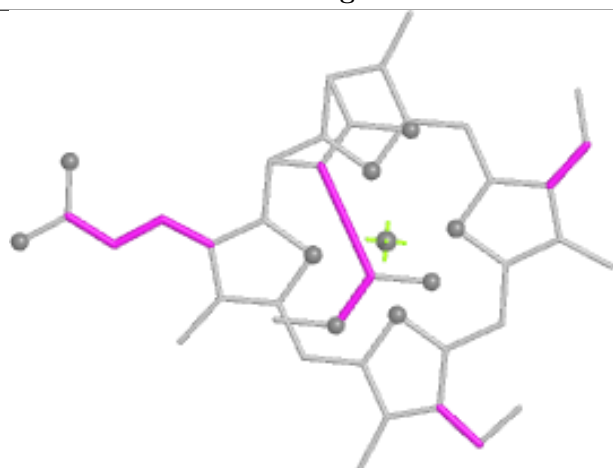
Ligand KC2 P 609



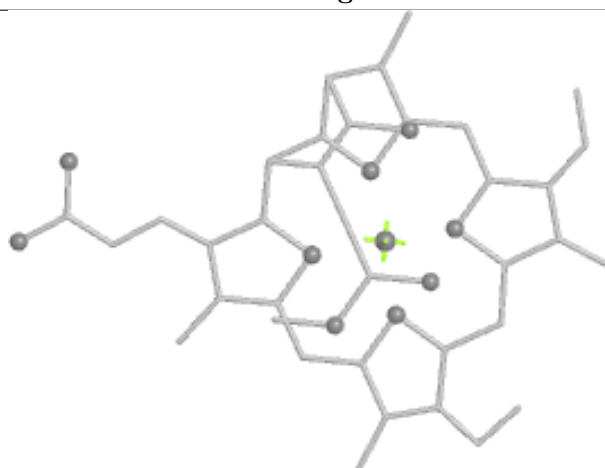
Bond lengths



Bond angles

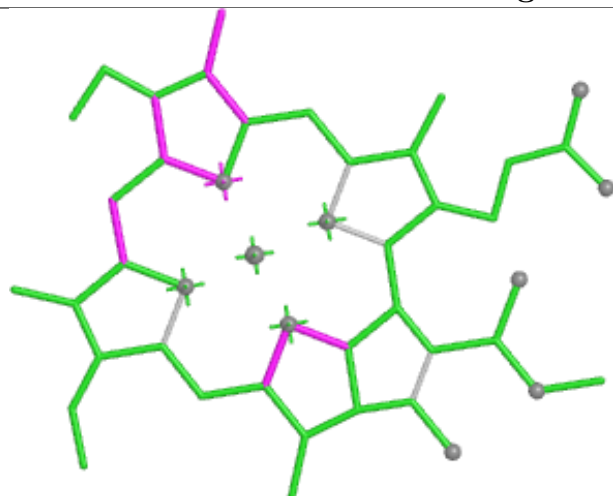


Torsions

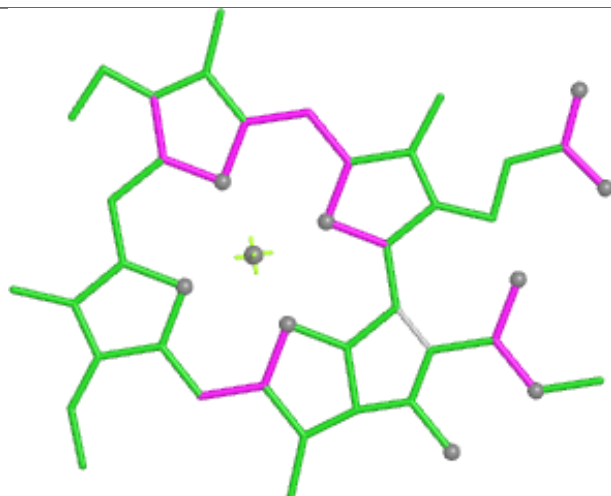


Rings

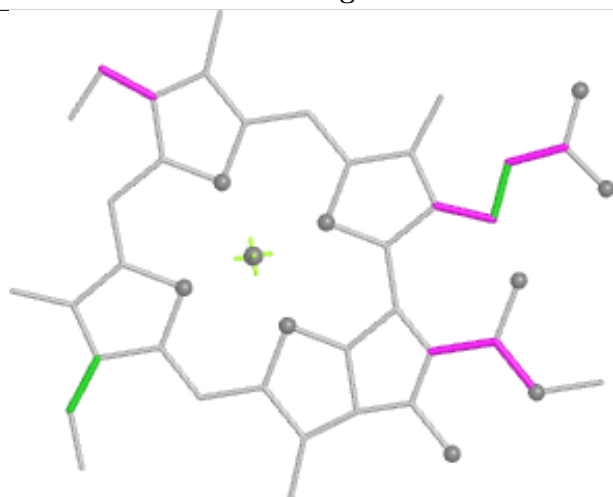
Ligand CLA S 302



Bond lengths



Bond angles

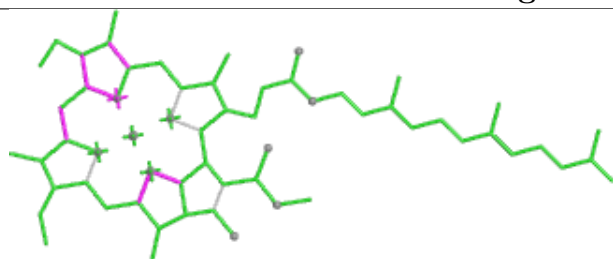


Torsions

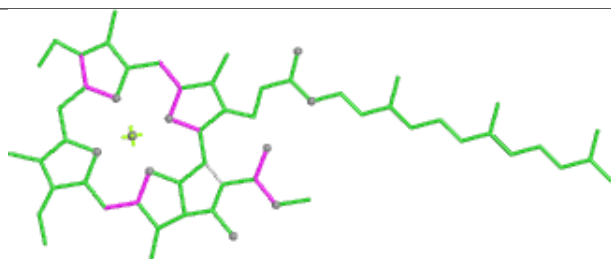


Rings

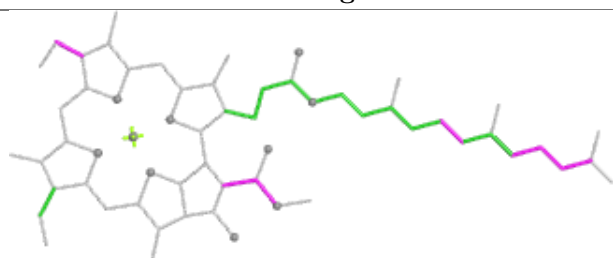
Ligand CLA 0 608



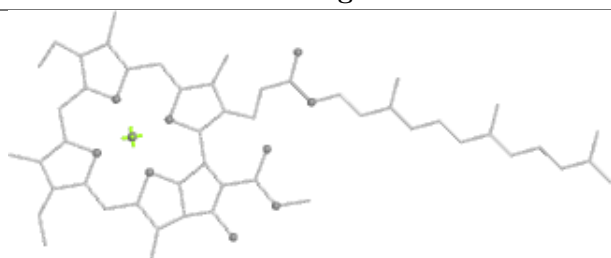
Bond lengths



Bond angles

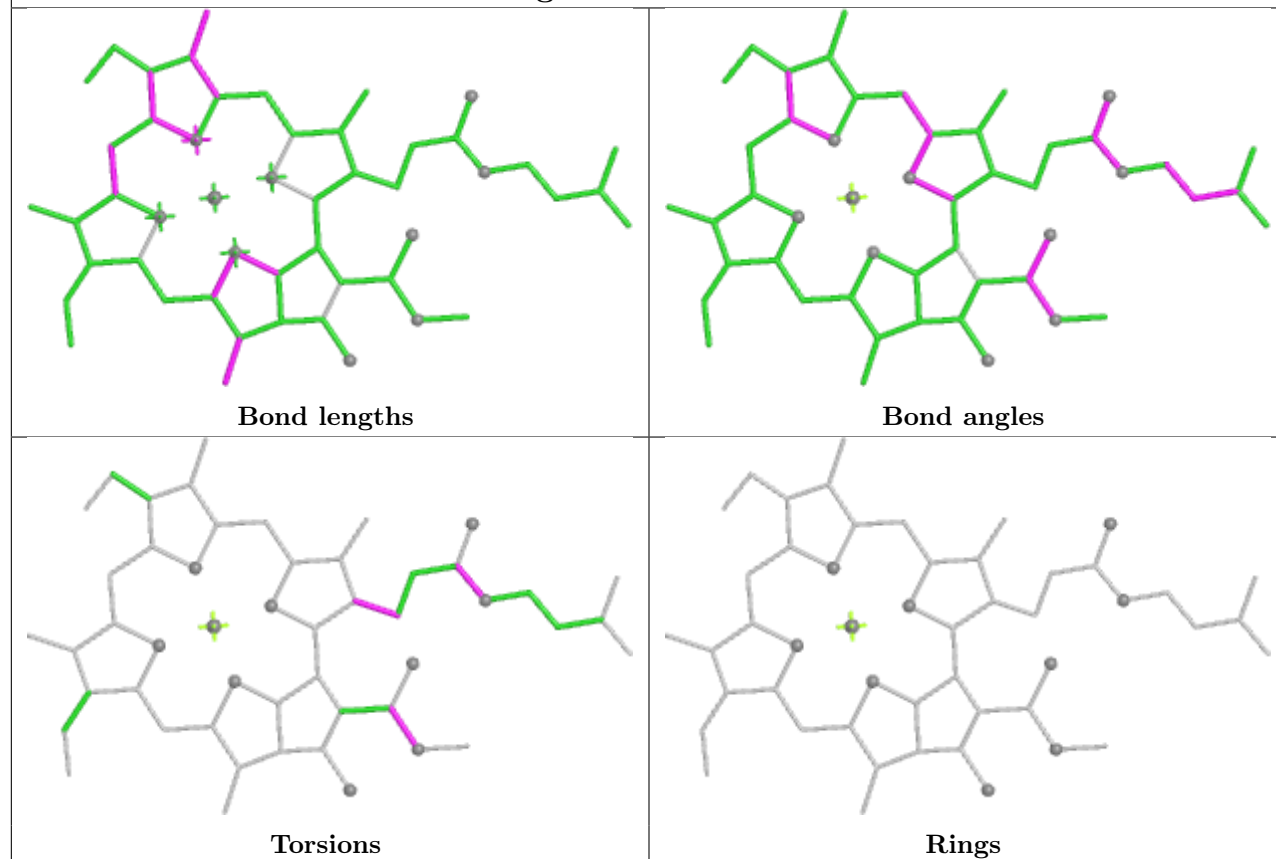


Torsions

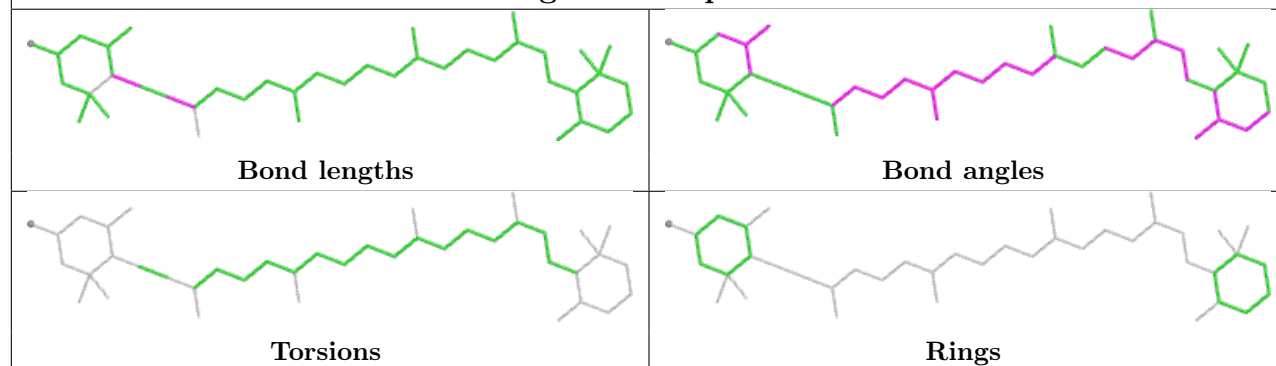


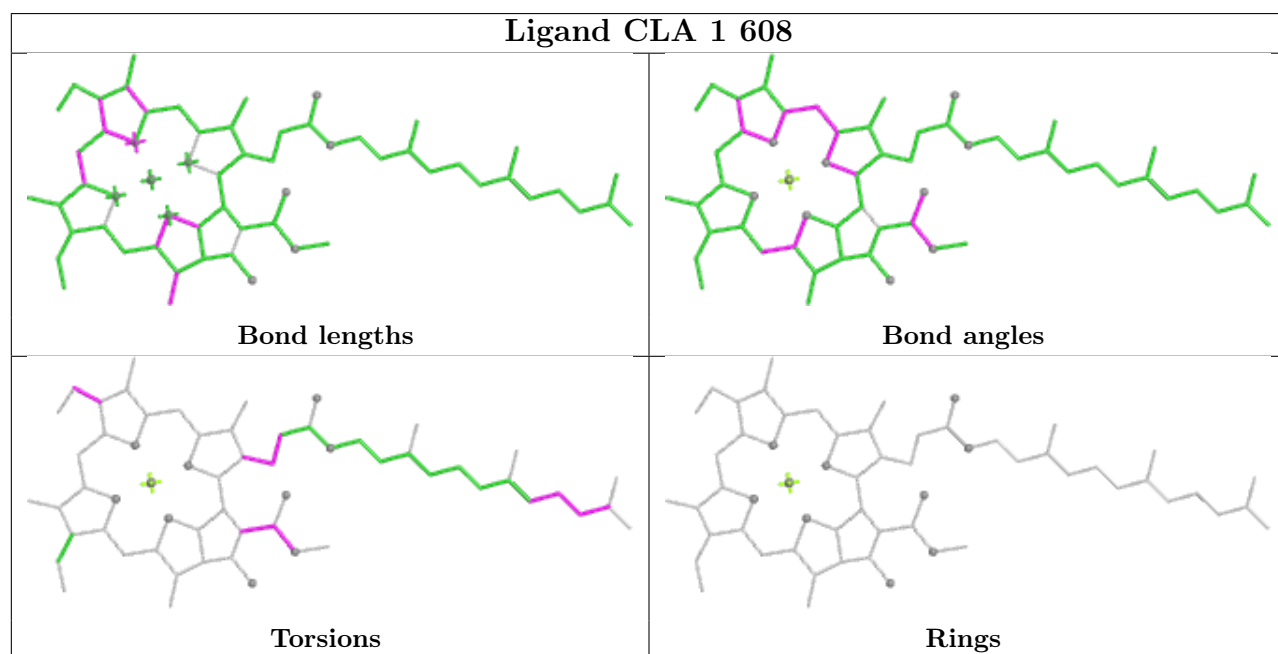
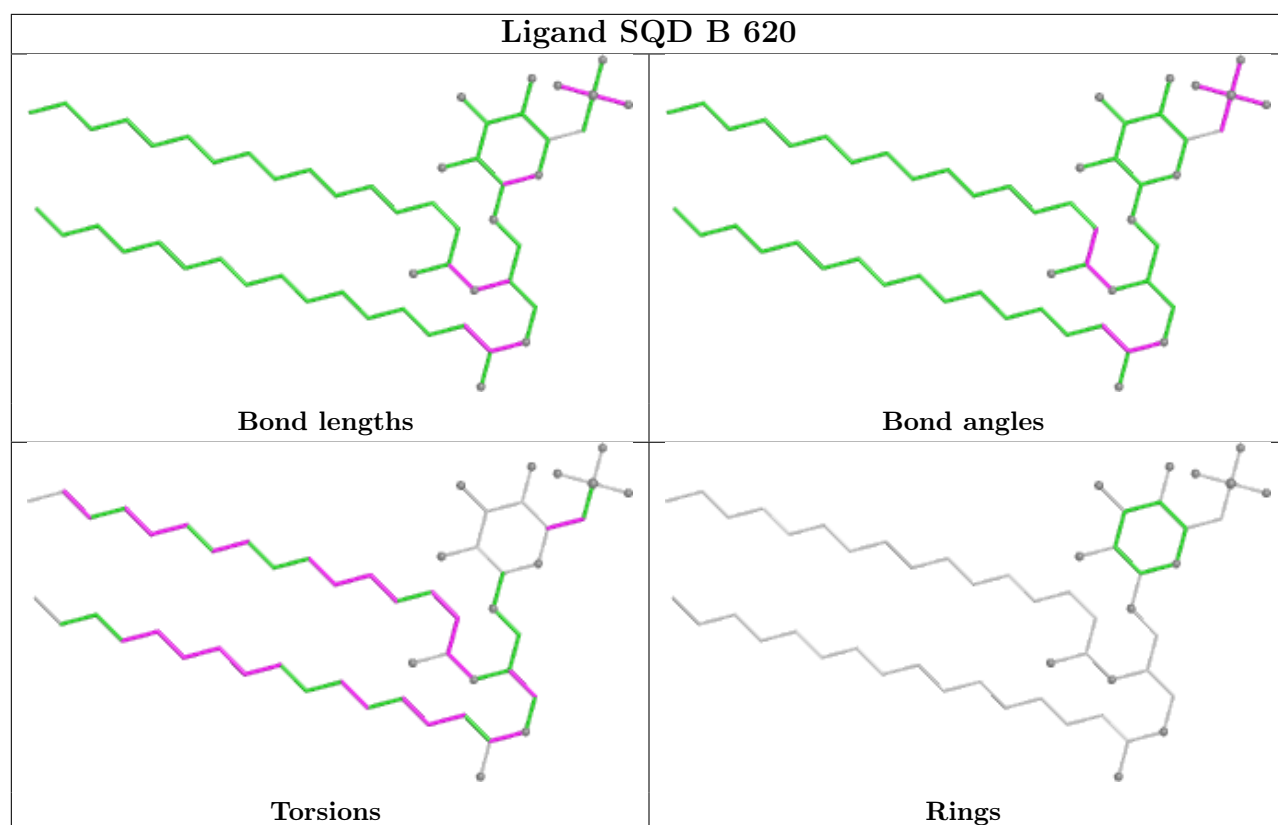
Rings

Ligand CLA 9 603

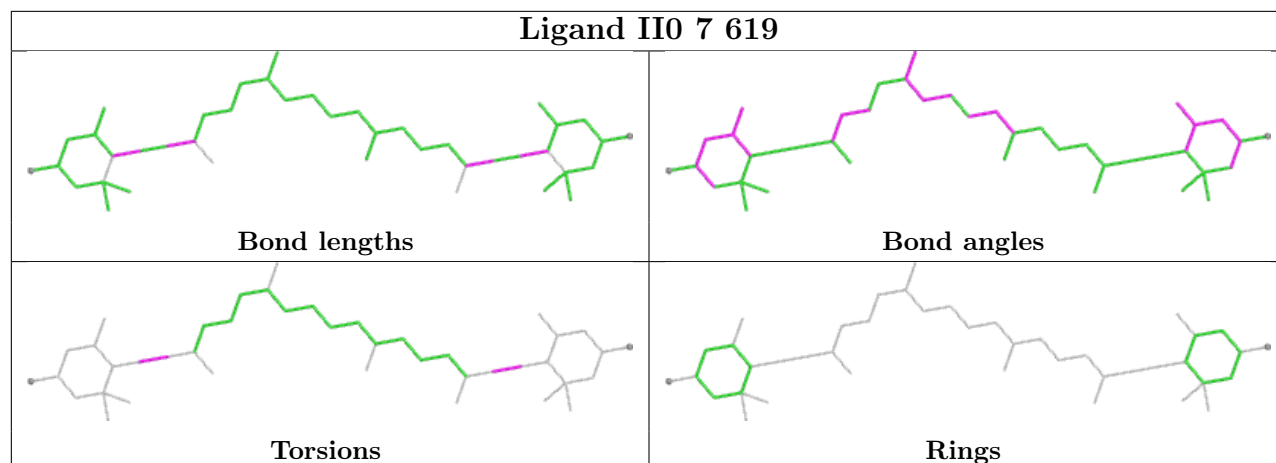


Ligand IHT p 317

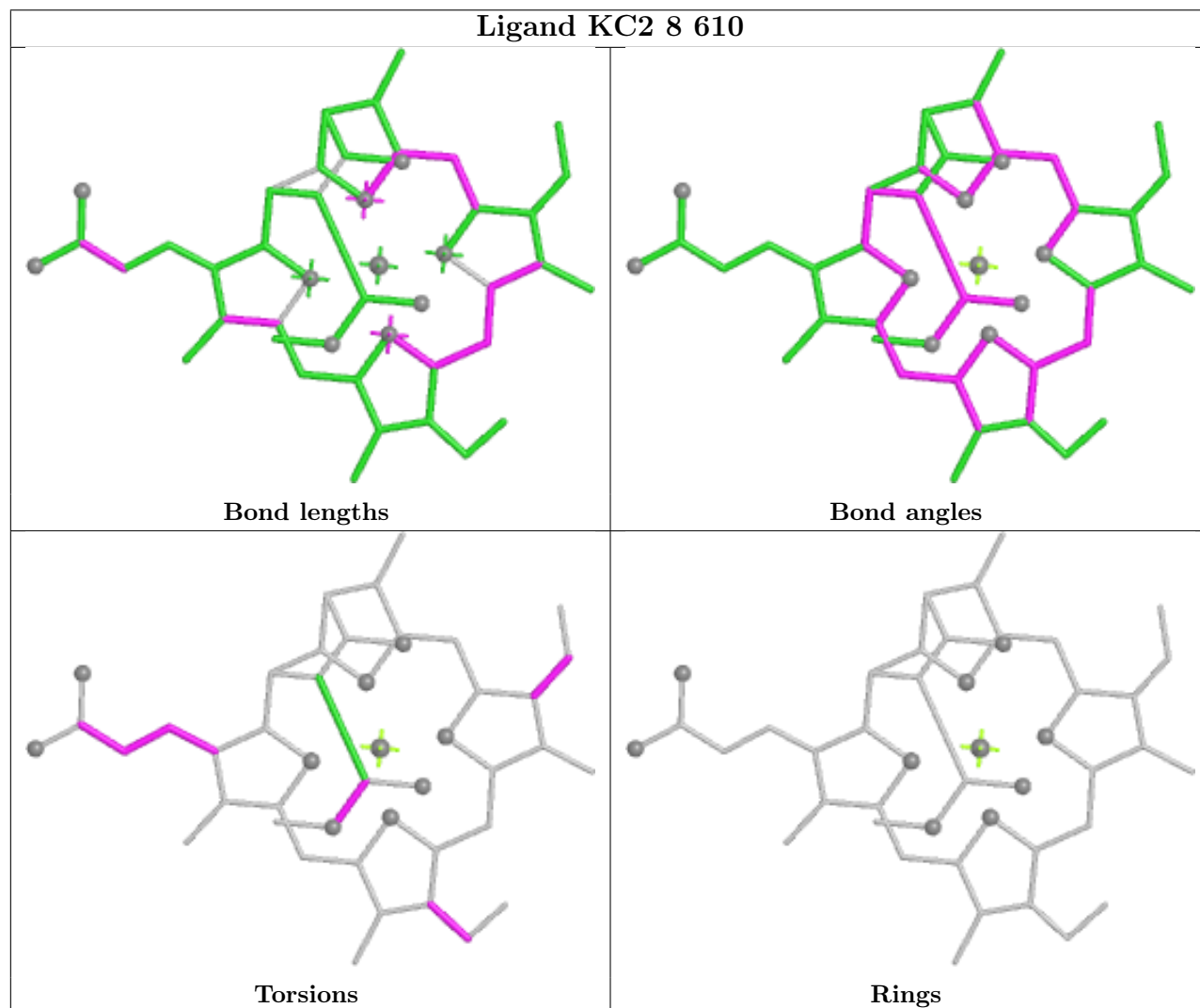




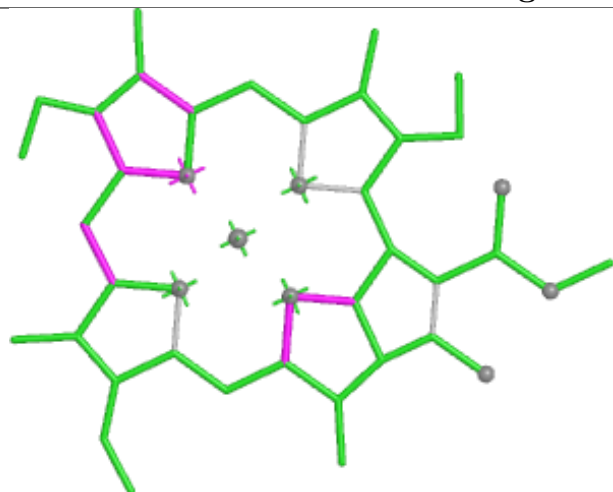
Ligand II0 7 619



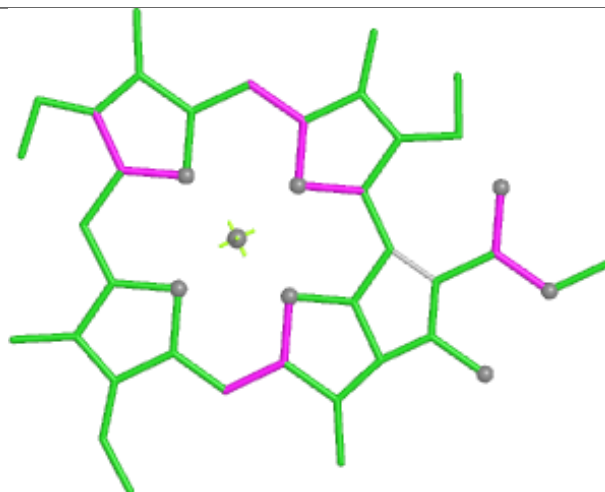
Ligand KC2 8 610



Ligand CLA 4 601



Bond lengths



Bond angles

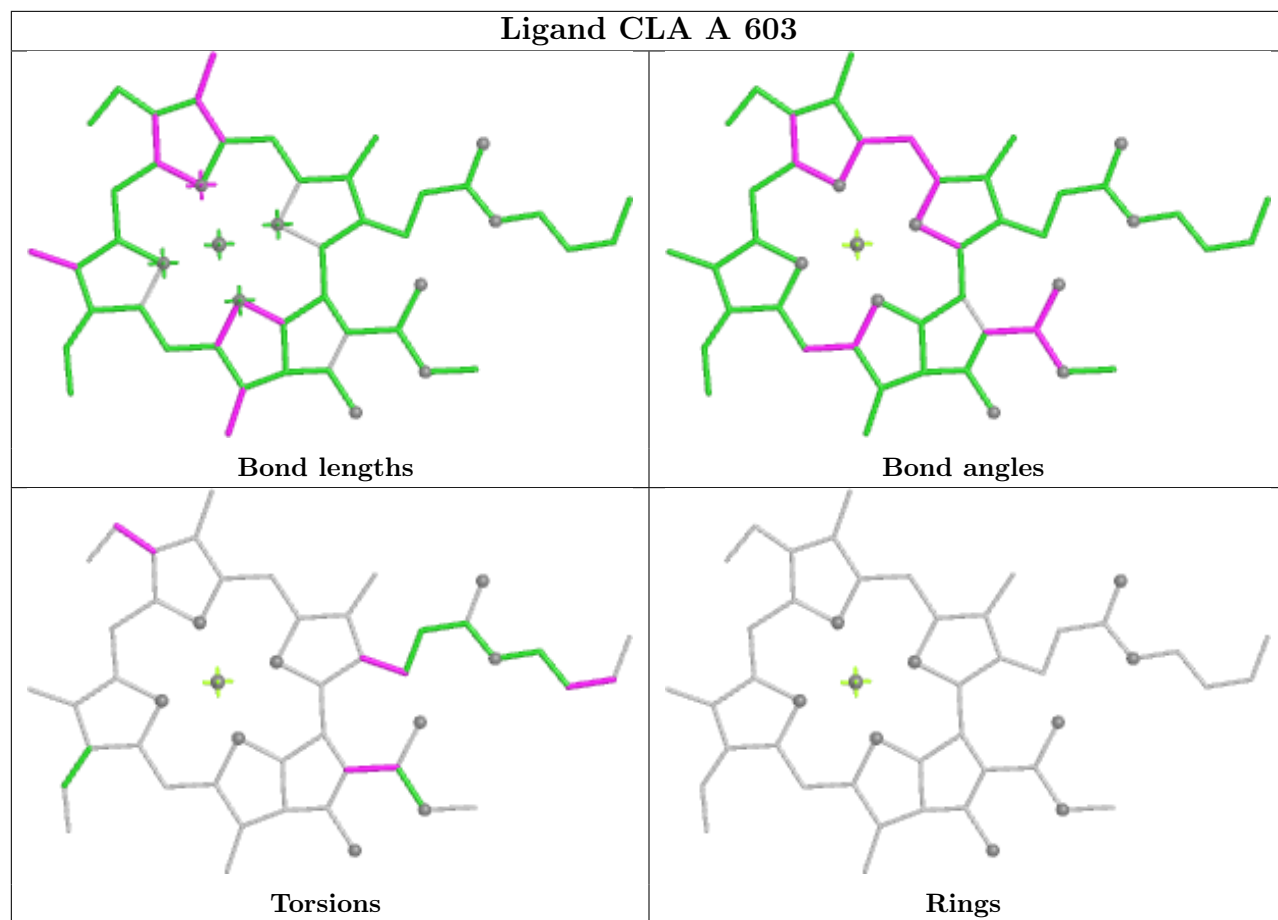


Torsions

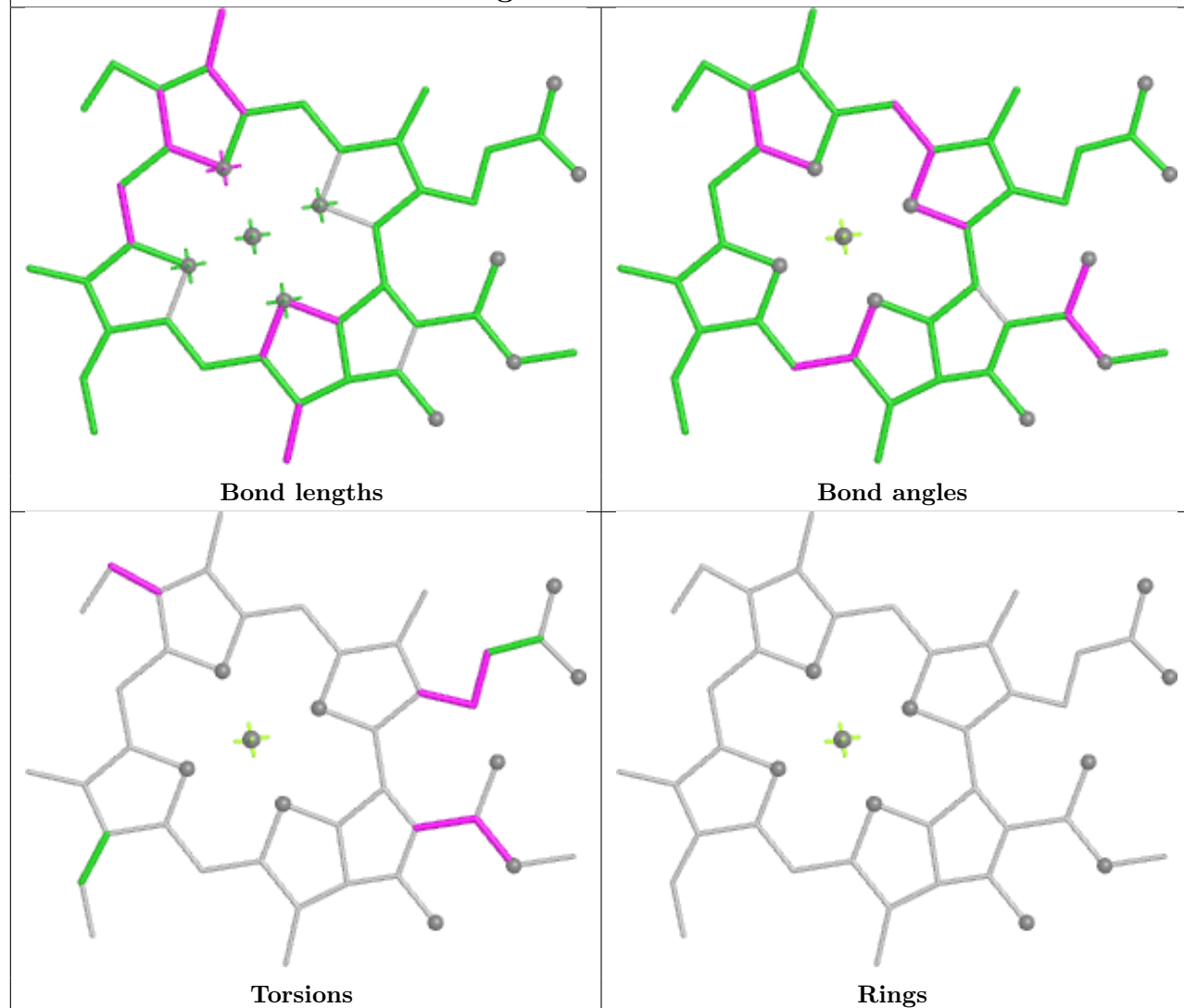


Rings

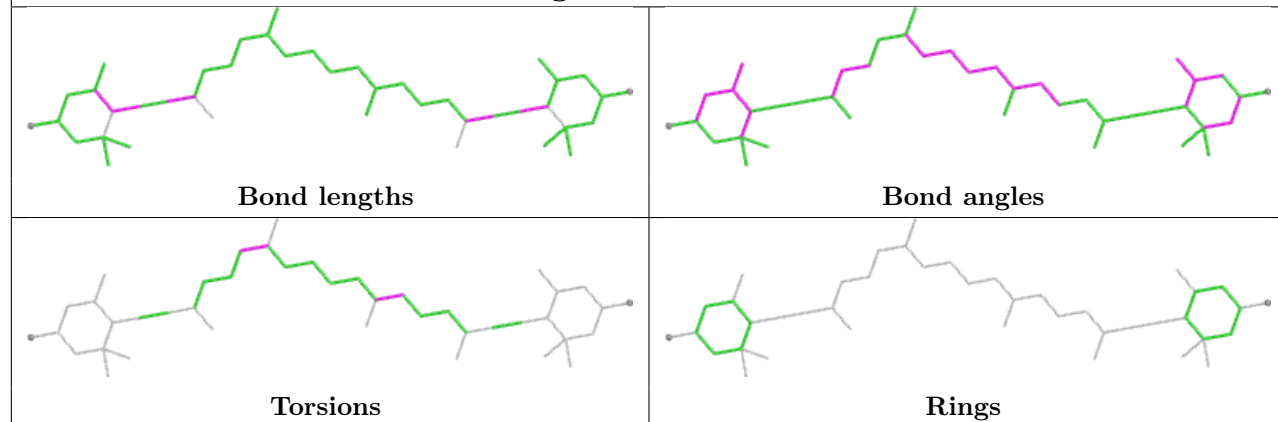
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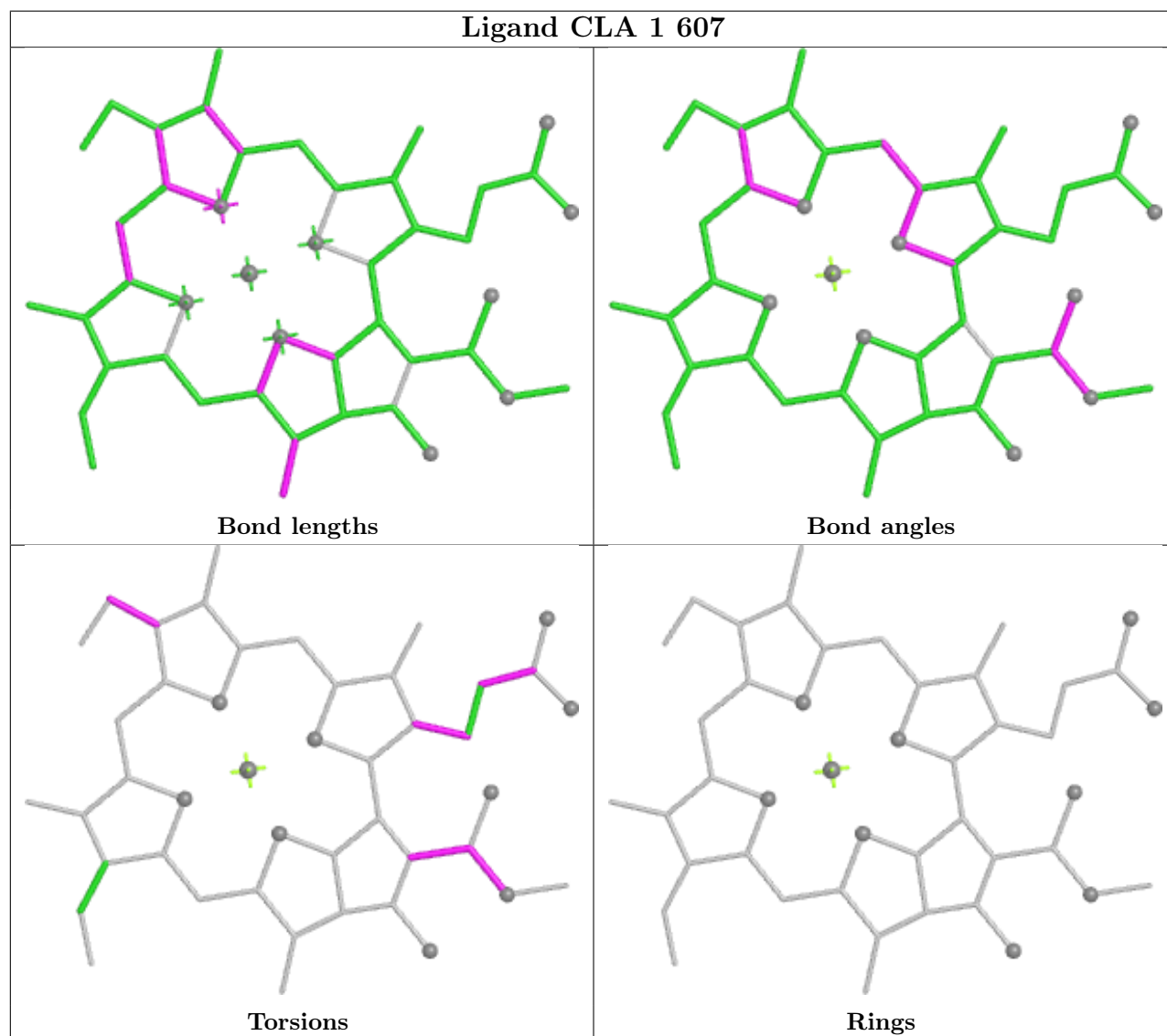
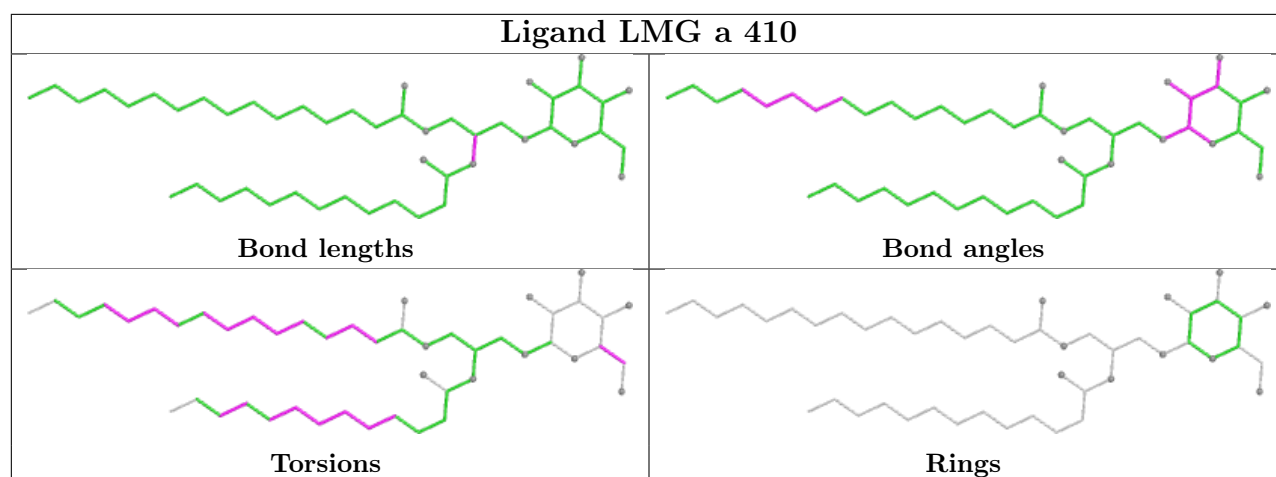


Ligand CLA 9 610

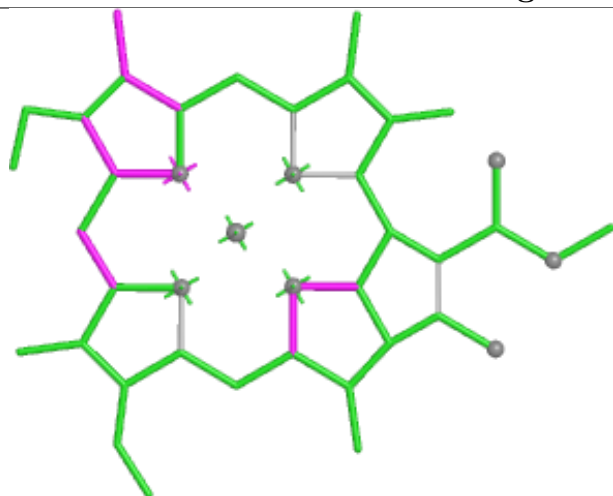


Ligand II0 2 615





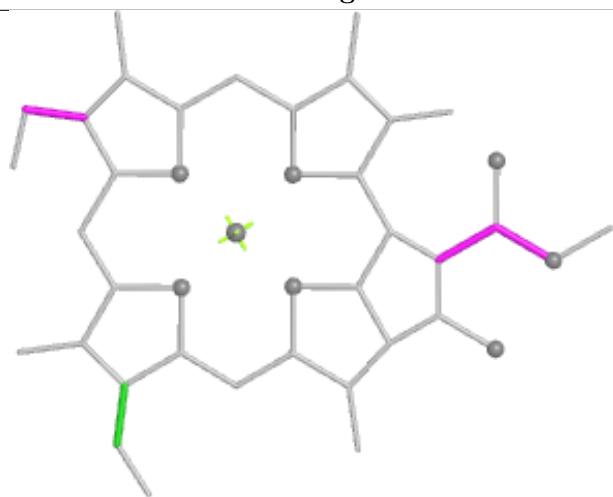
Ligand CLA p 310



Bond lengths



Bond angles

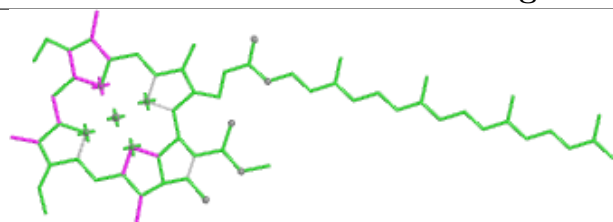


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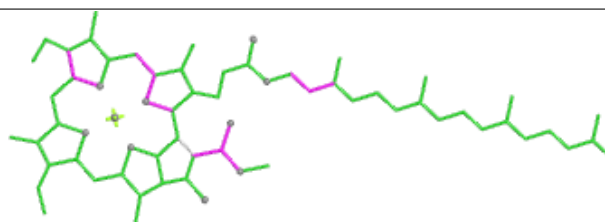


Rings

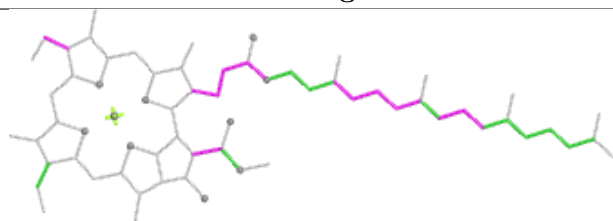
Ligand CLA c 503



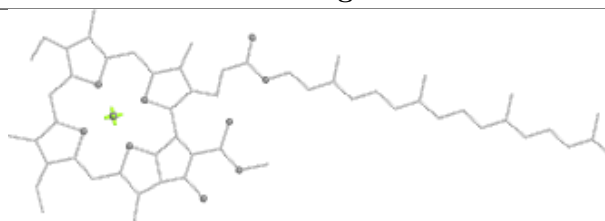
Bond lengths



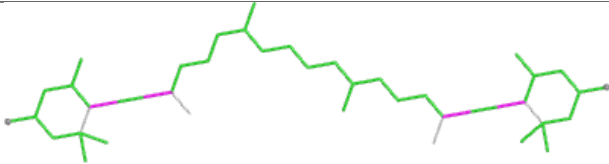
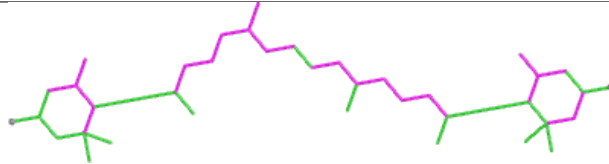
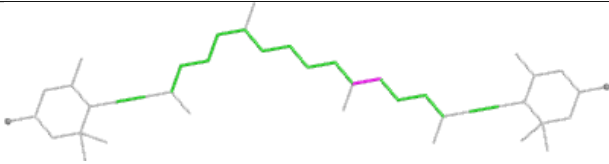
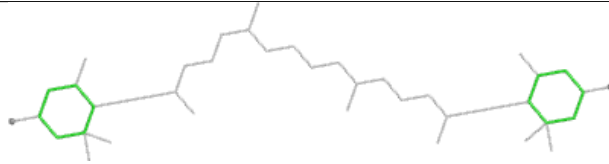
Bond angles

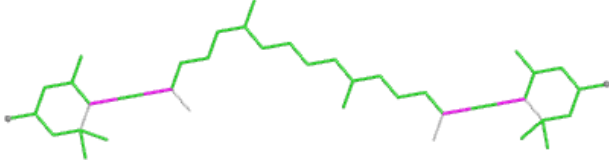
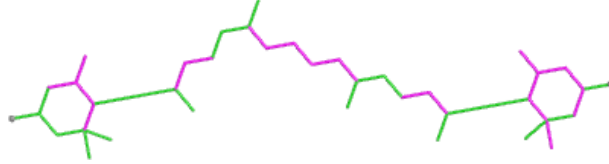
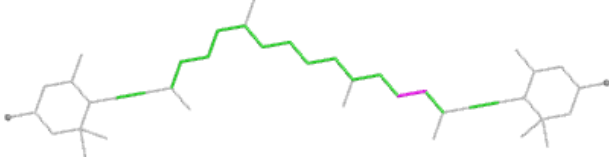
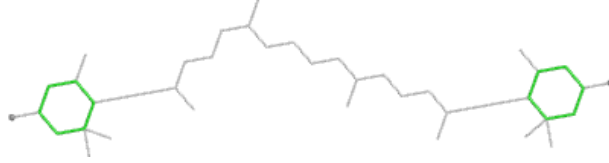


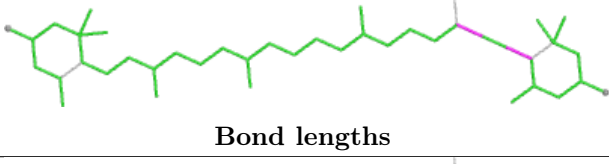
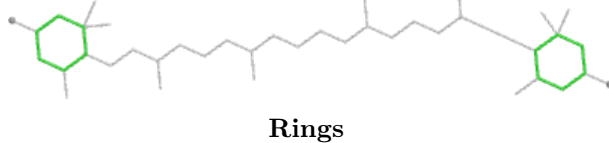
Torsions

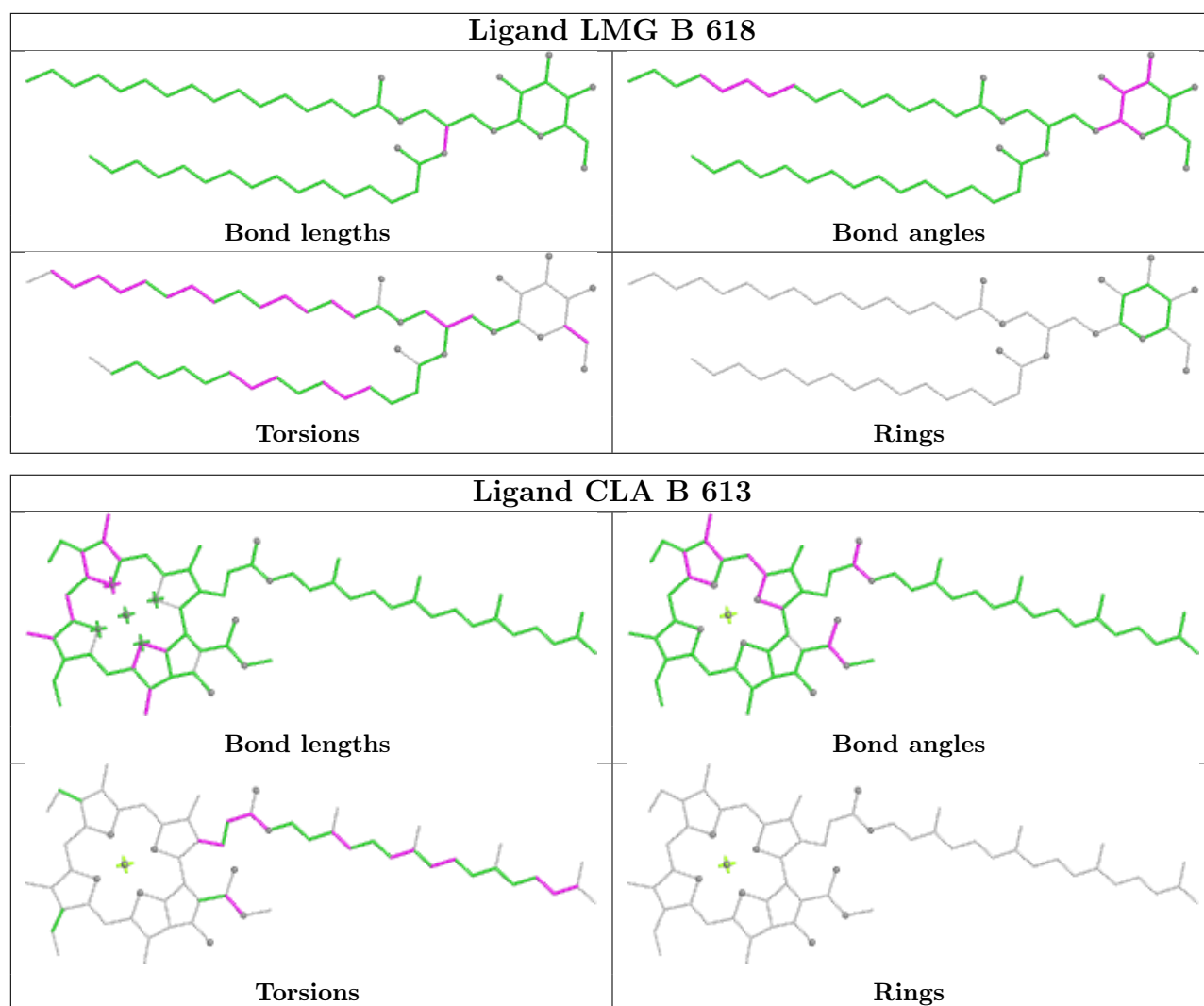


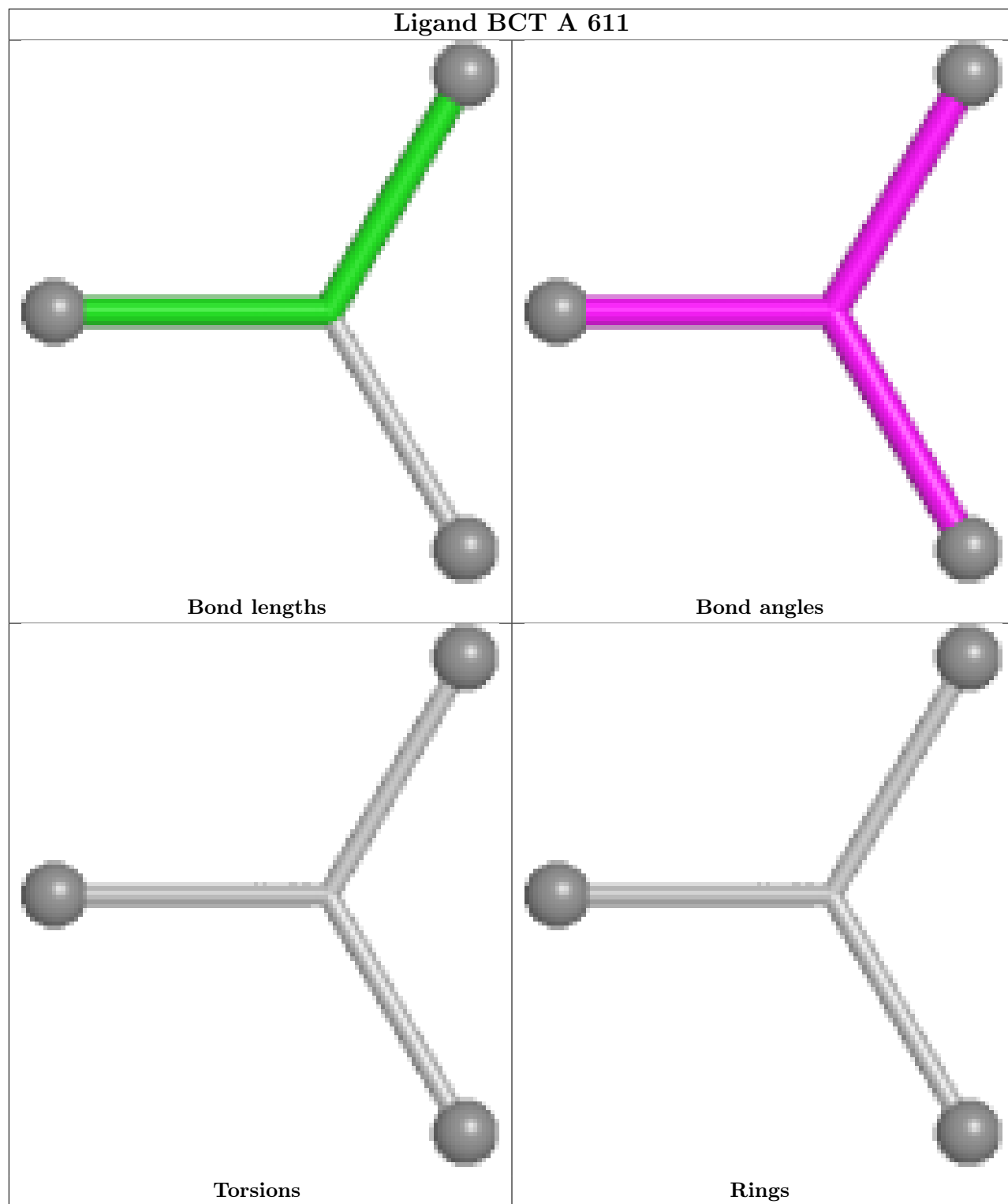
Rings

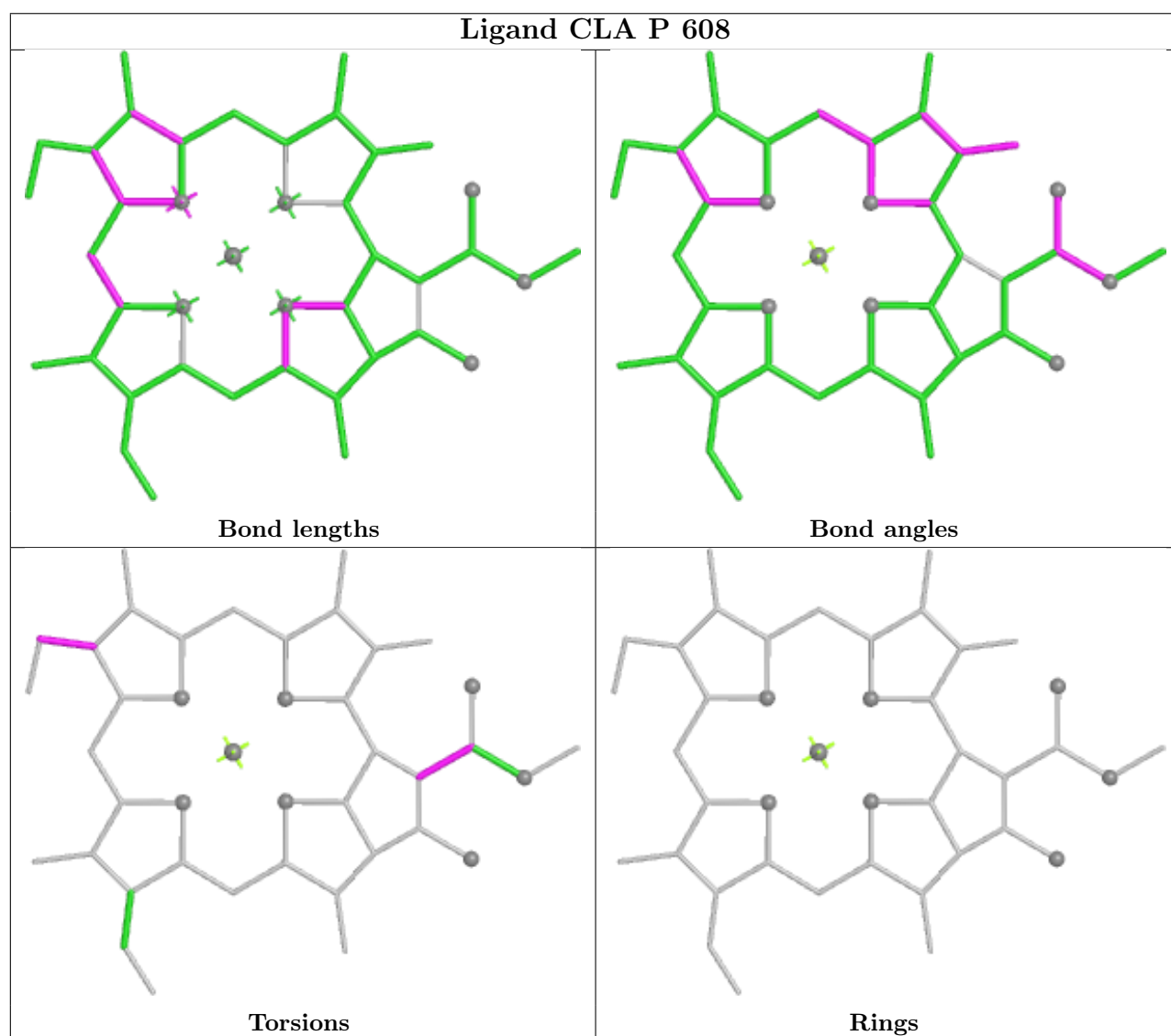
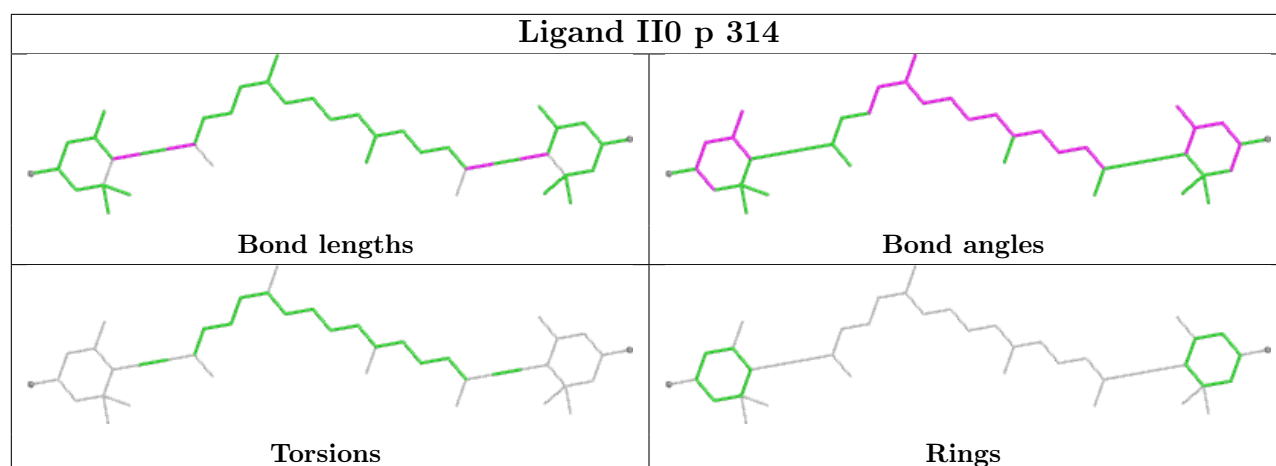
Ligand II0 5 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

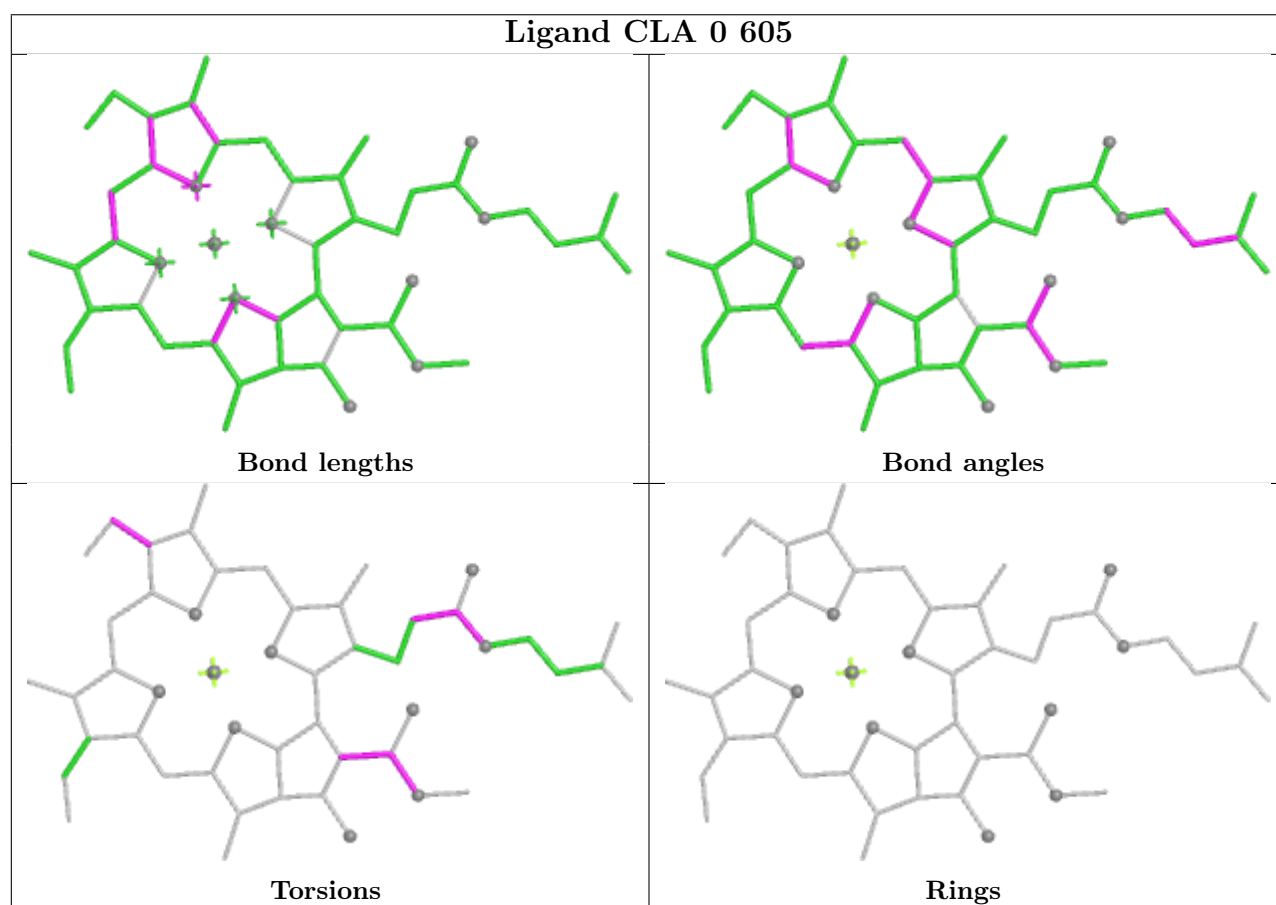
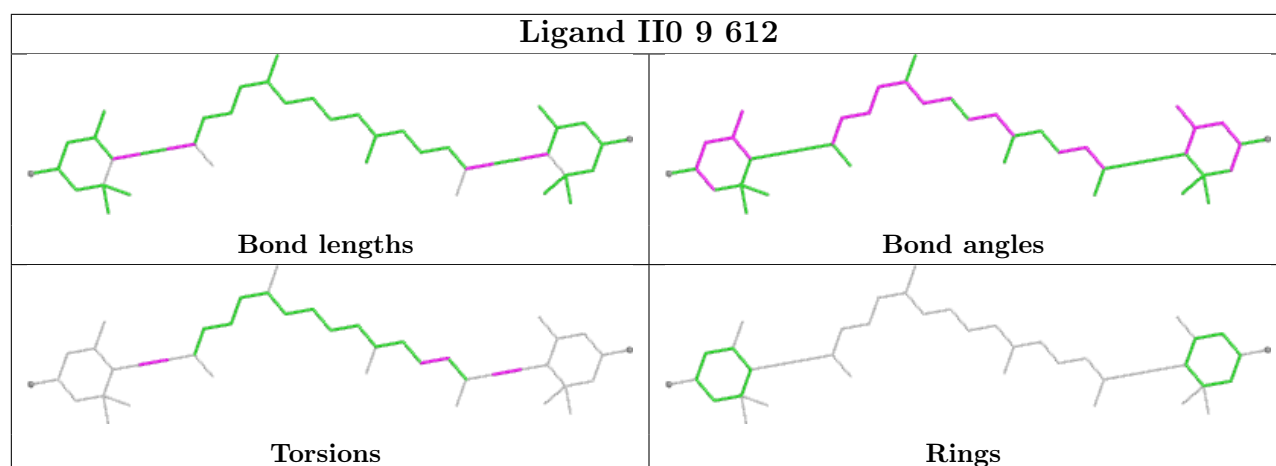
Ligand II0 0 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

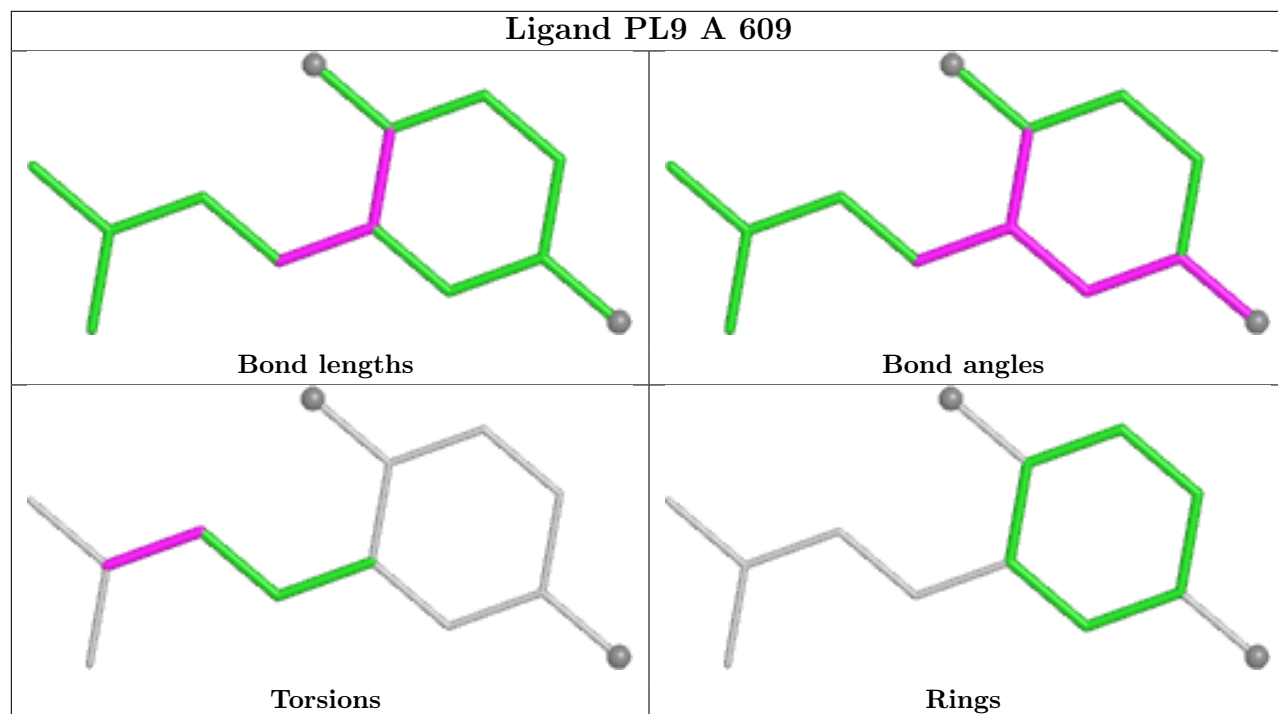
Ligand II3 P 613	
	
Bond lengths	Bond angles
	
Torsions	Rings



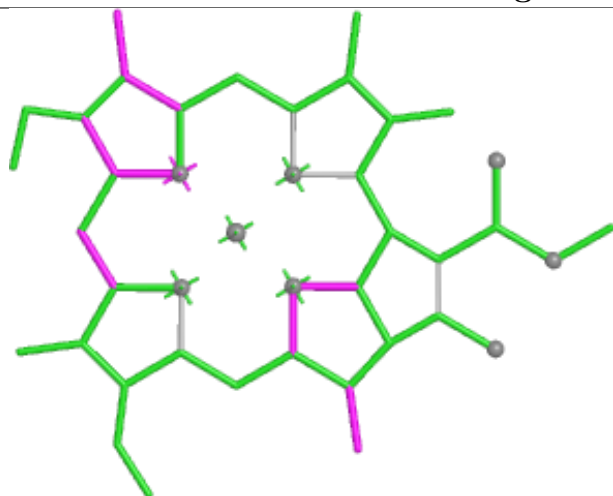




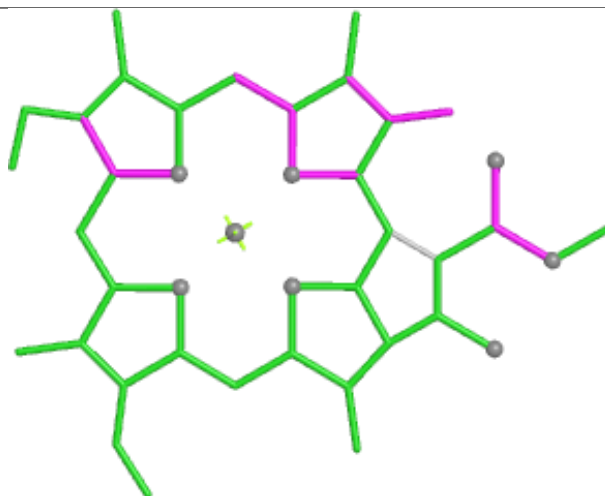




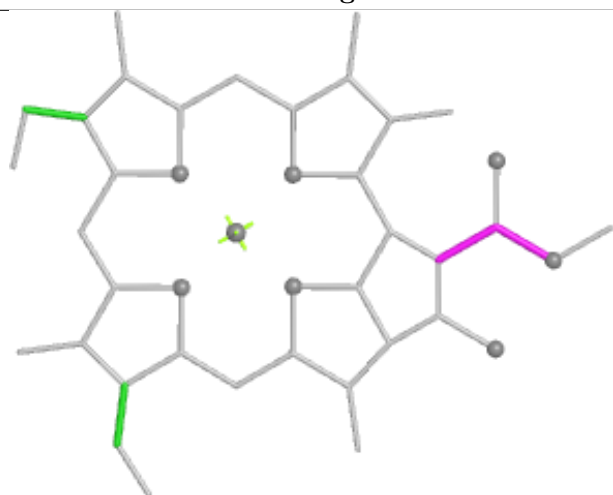
Ligand CLA B 608



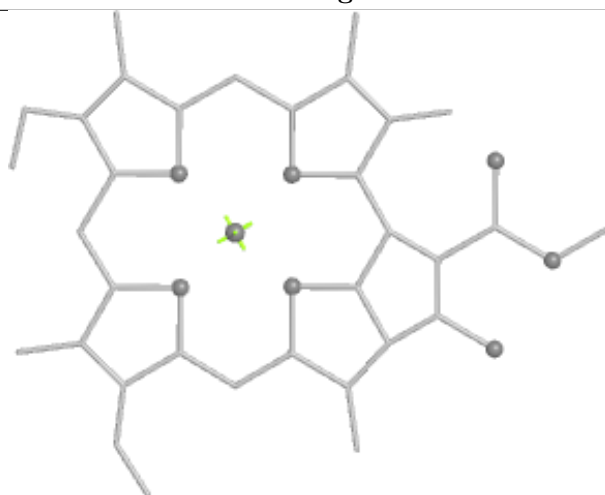
Bond lengths



Bond angles

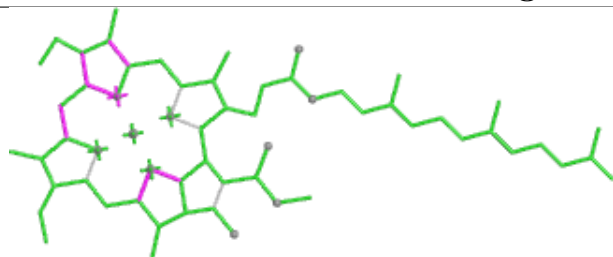


Torsions

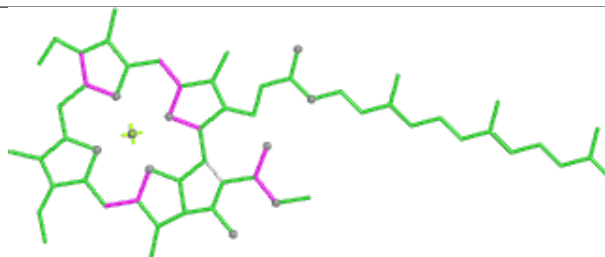


Rings

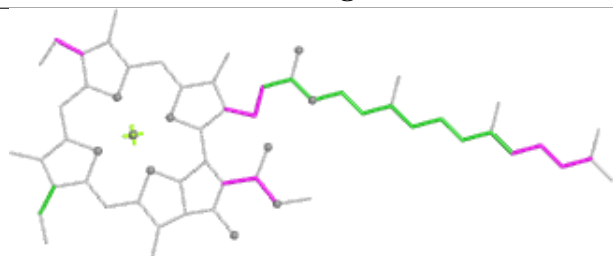
Ligand CLA 5 309



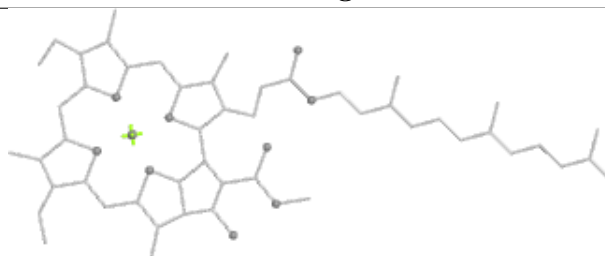
Bond lengths



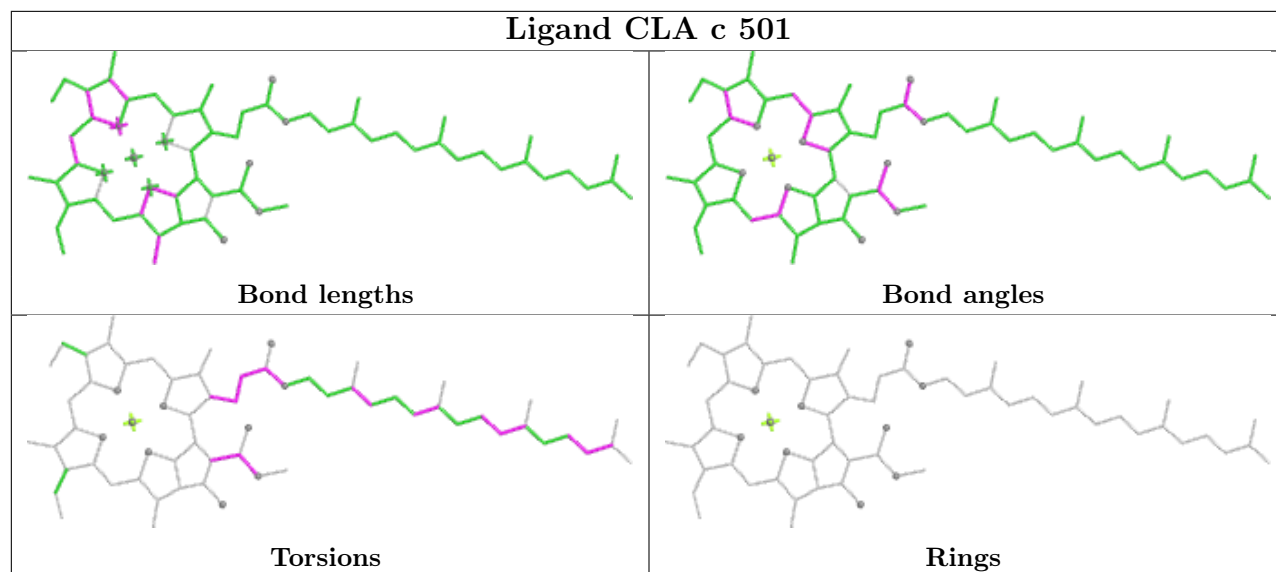
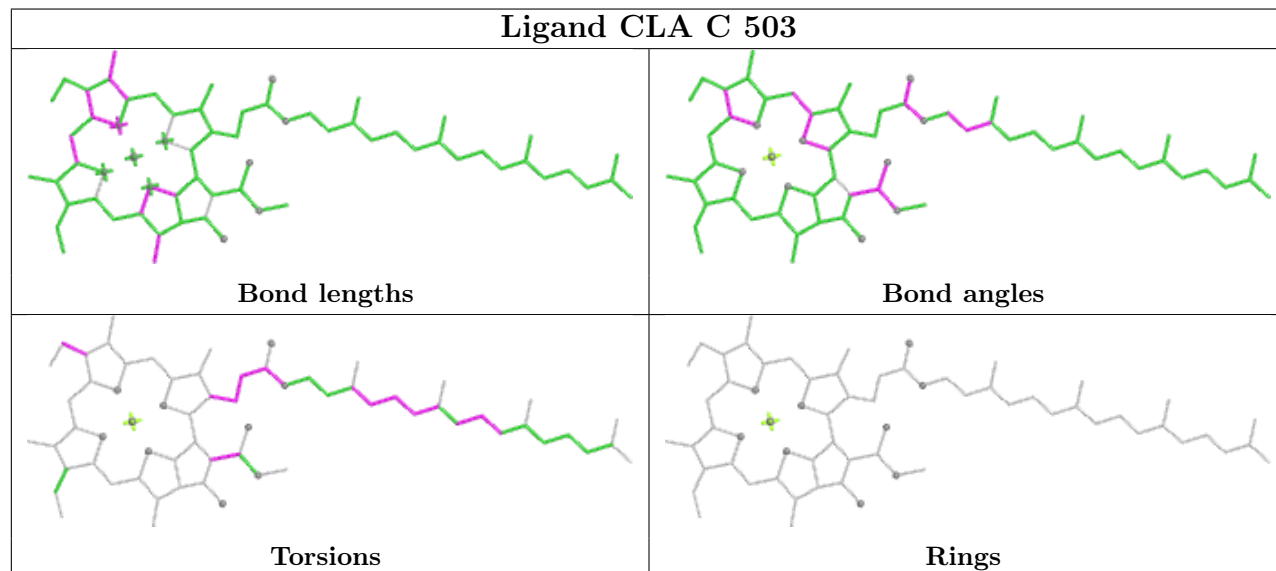
Bond angles



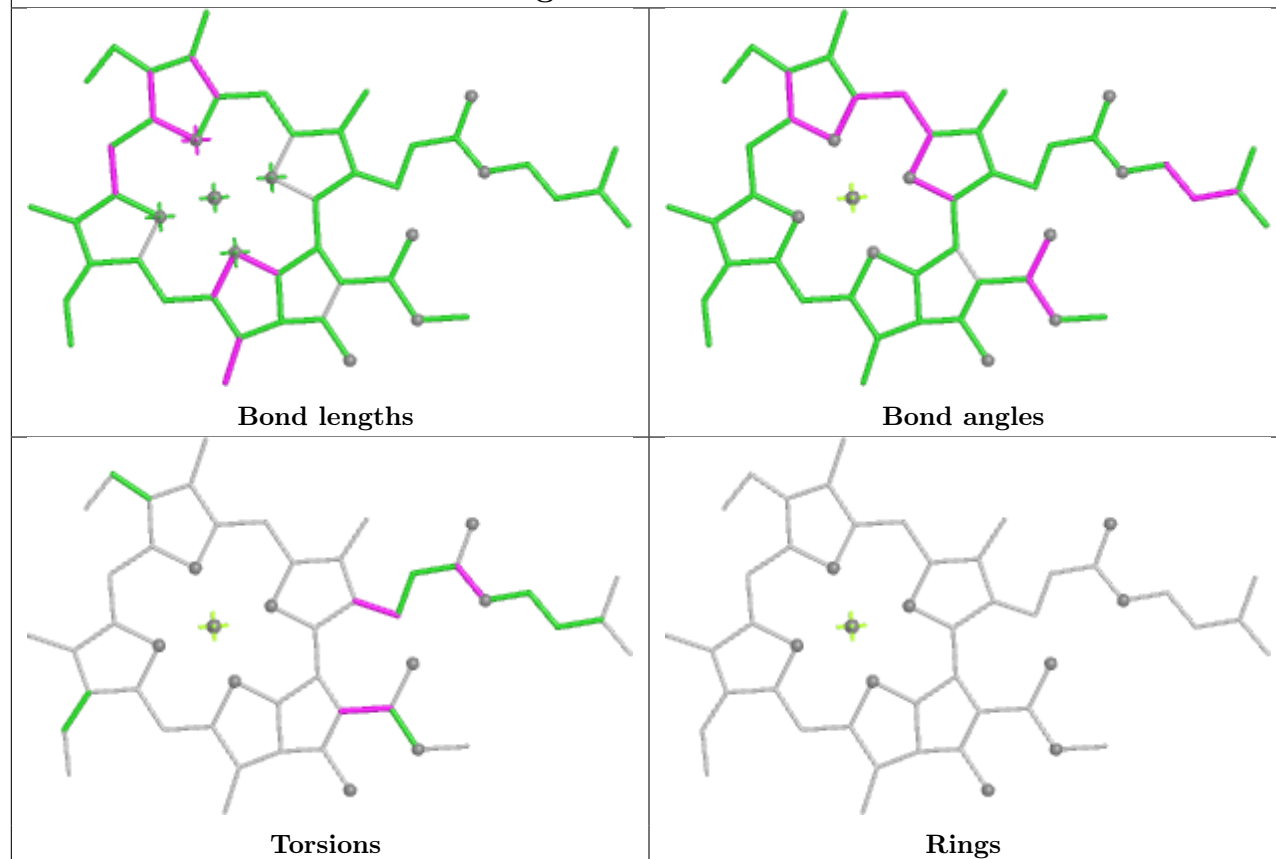
Torsions



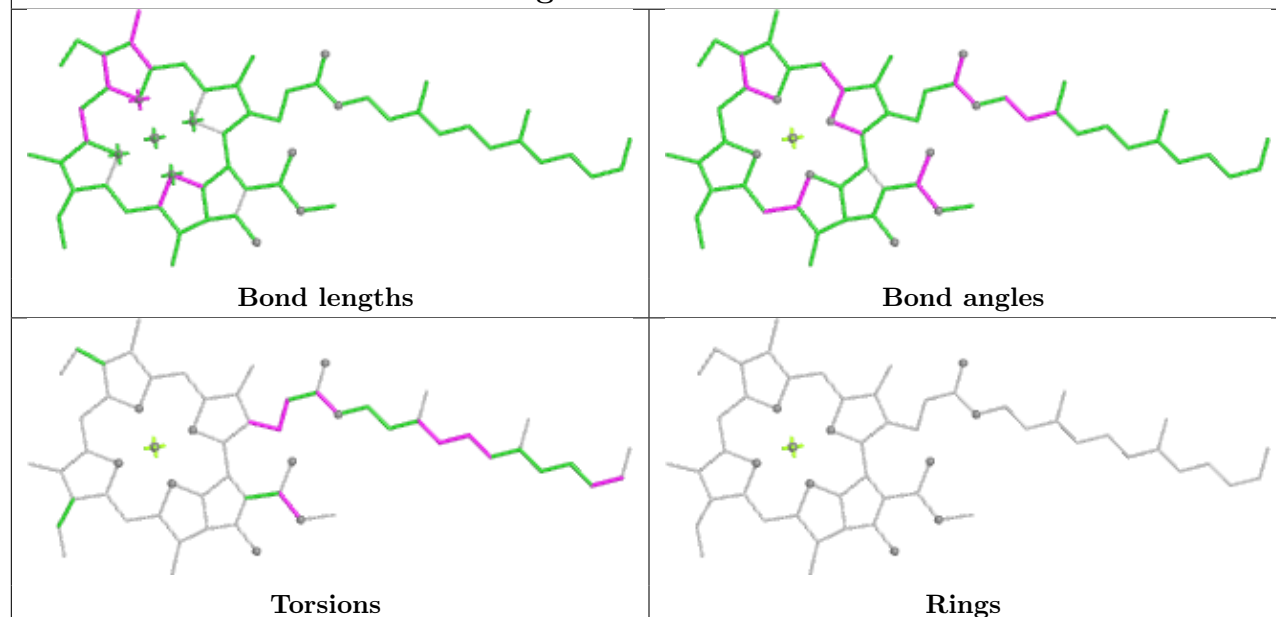
Rings

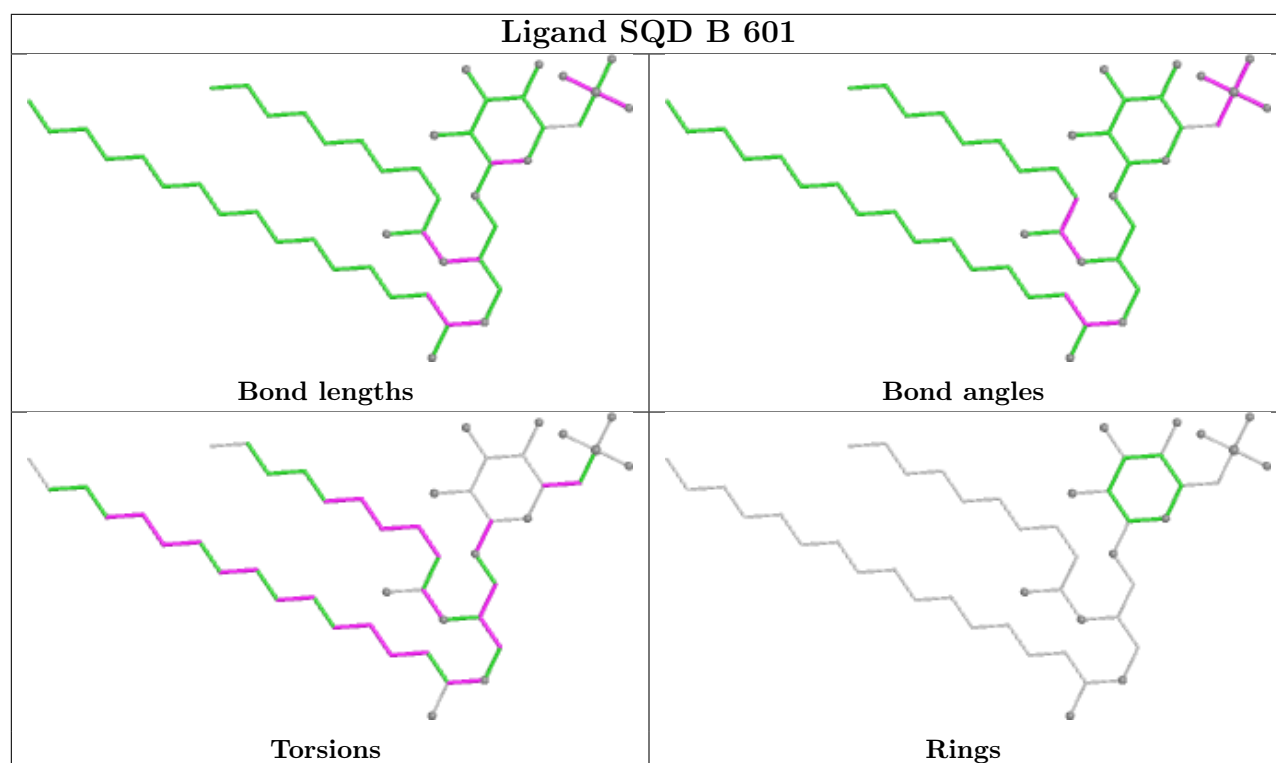
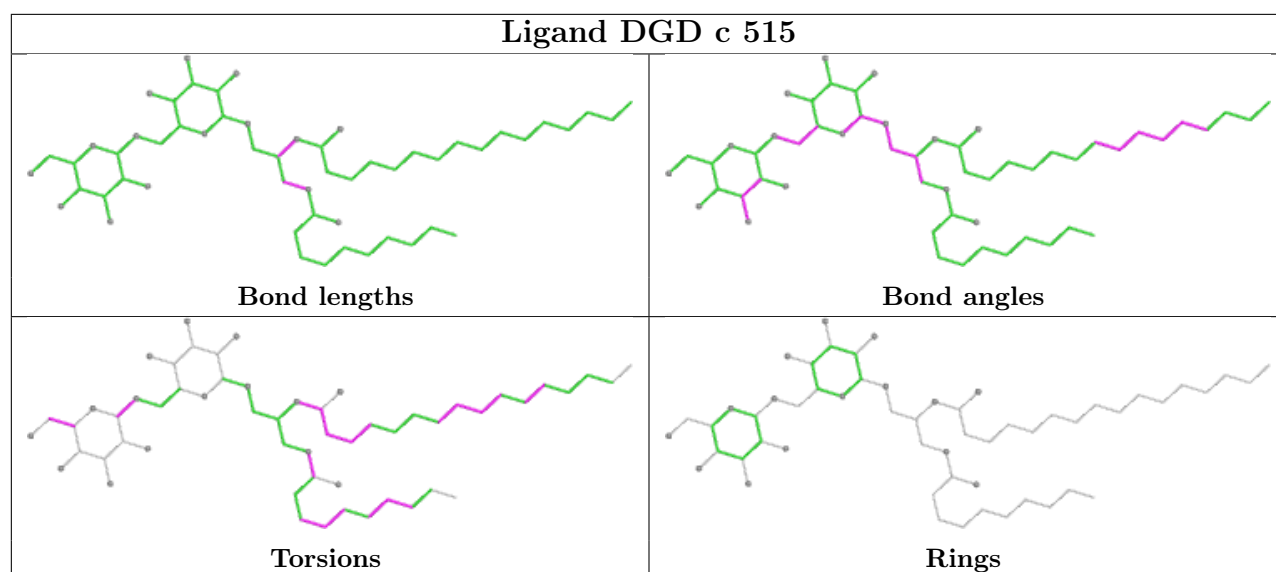
Ligand CLA c 501**Ligand CLA C 503**

Ligand CLA 0 603

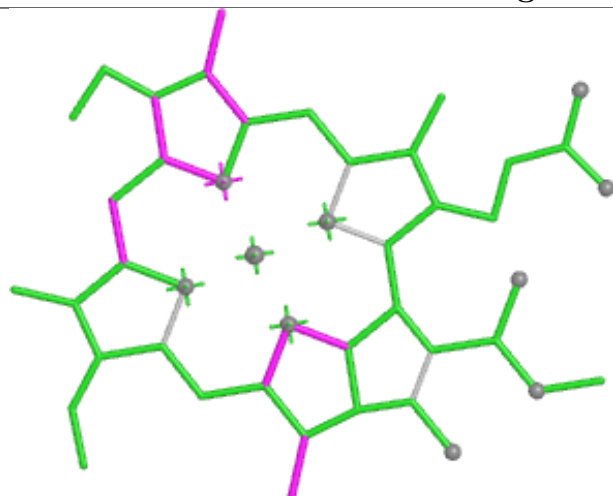


Ligand CLA 7 602

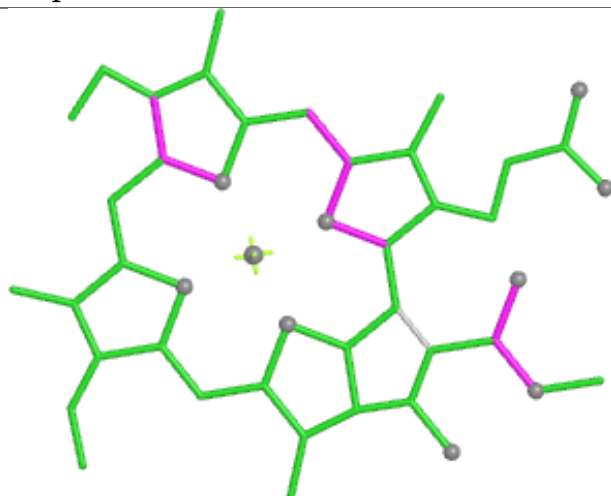




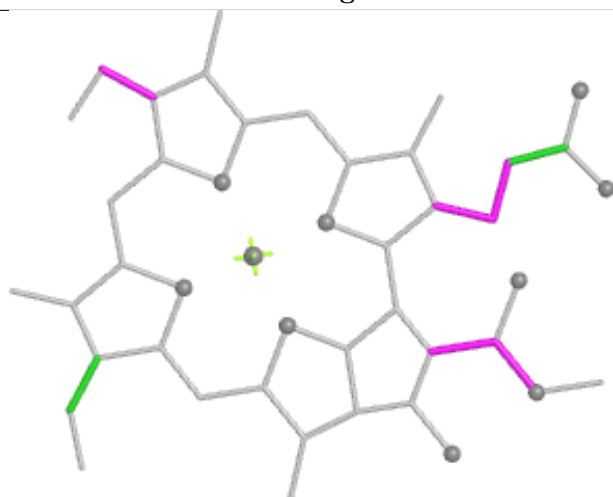
Ligand CLA p 312



Bond lengths



Bond angles

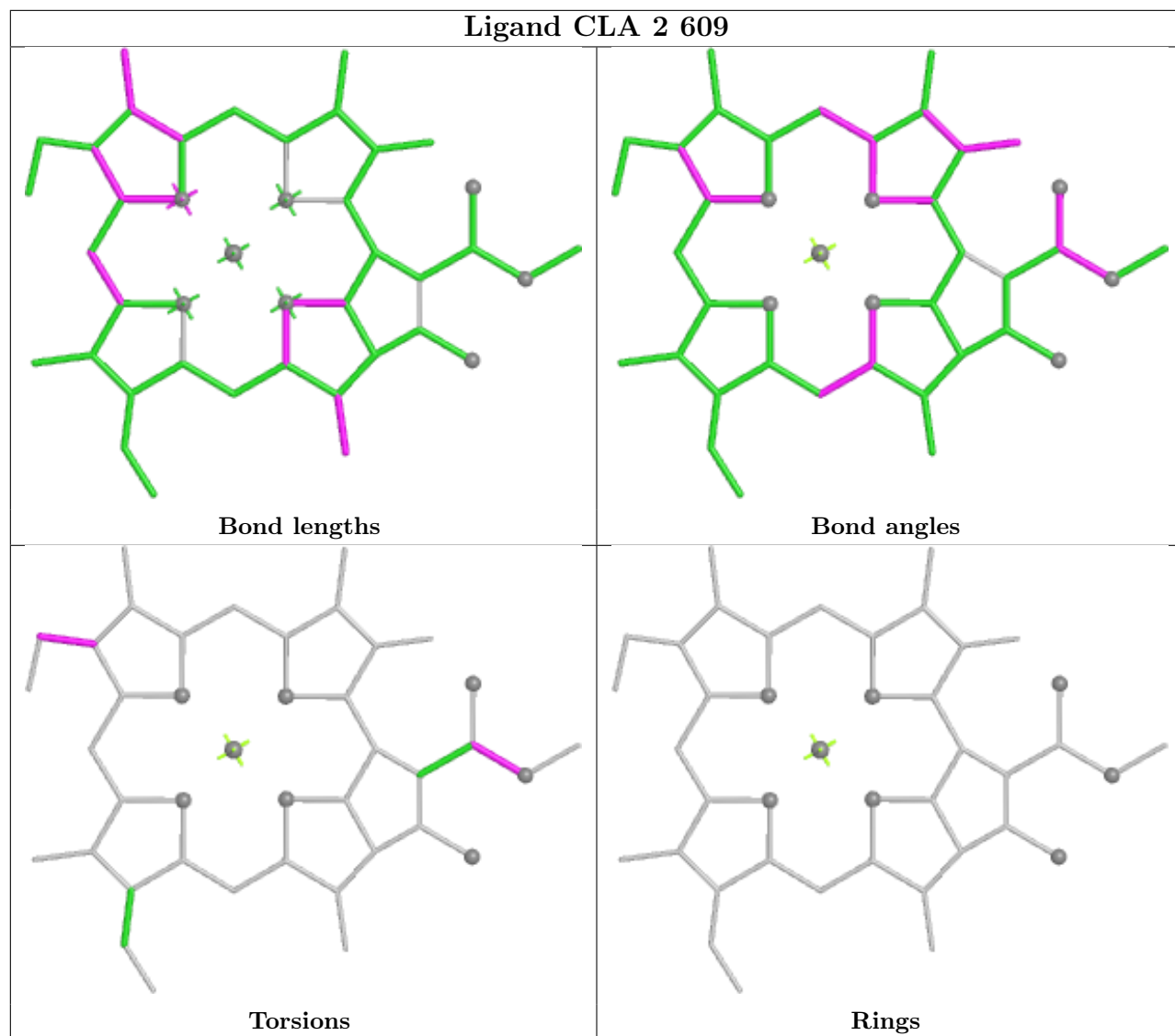


Torsions

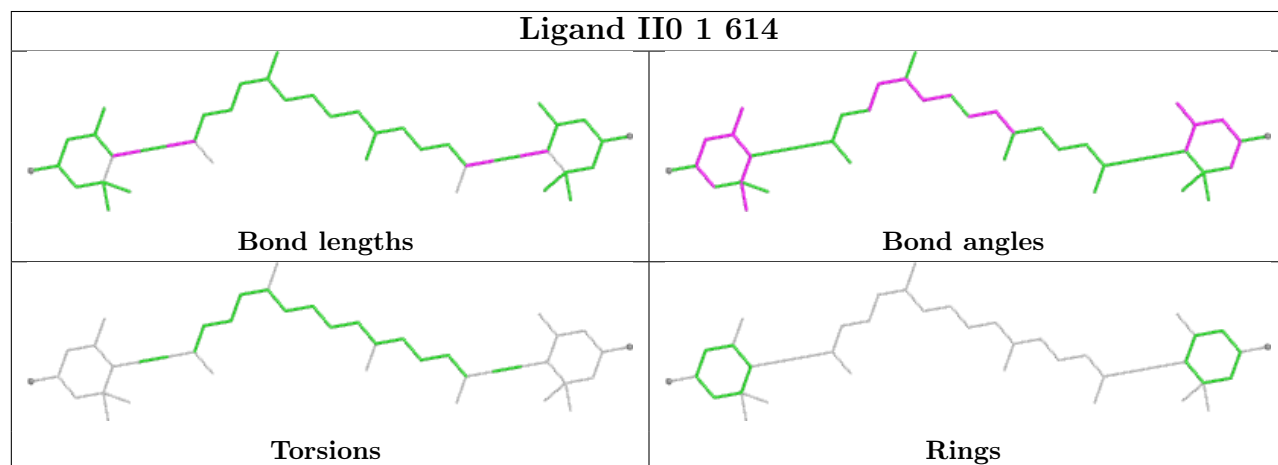


Rings

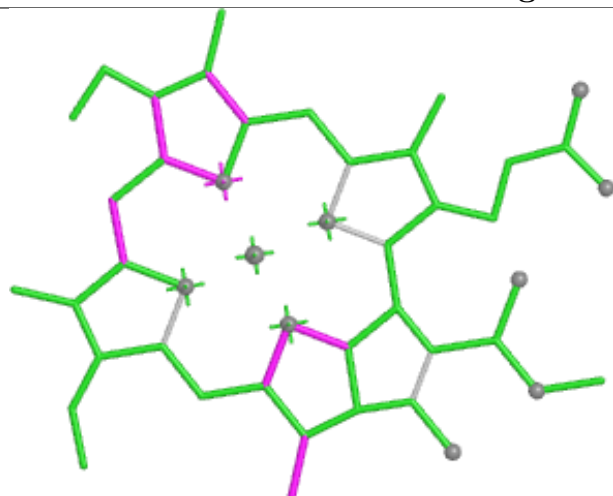
Ligand CLA 2 609



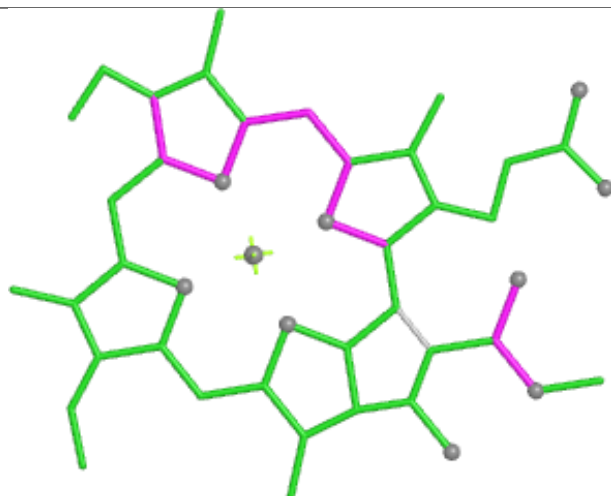
Ligand II0 1 614



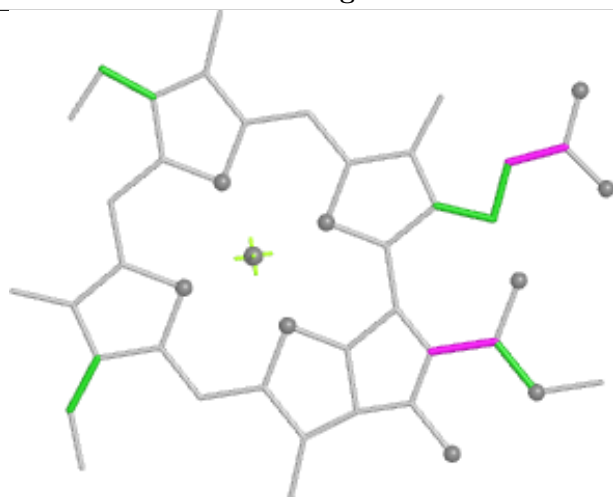
Ligand CLA 2 606



Bond lengths



Bond angles

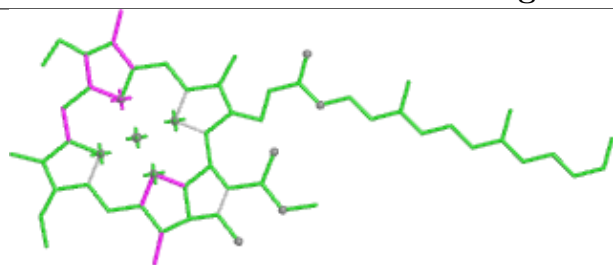


Torsions

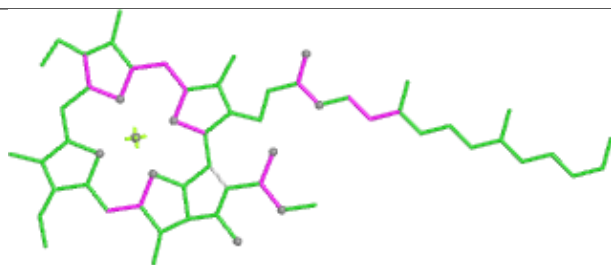


Rings

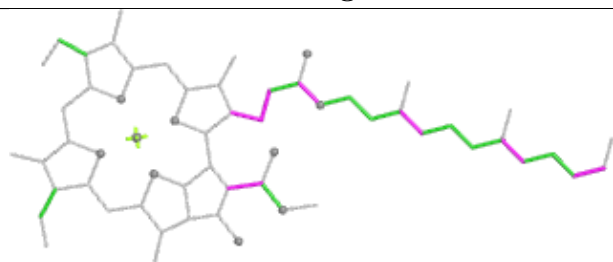
Ligand CLA 3 602



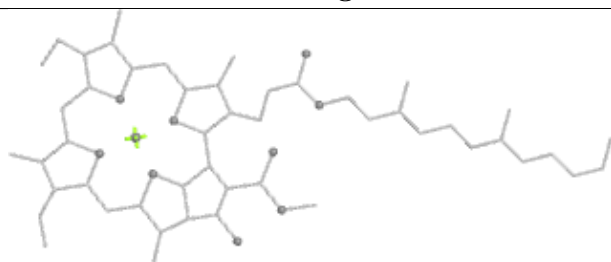
Bond lengths



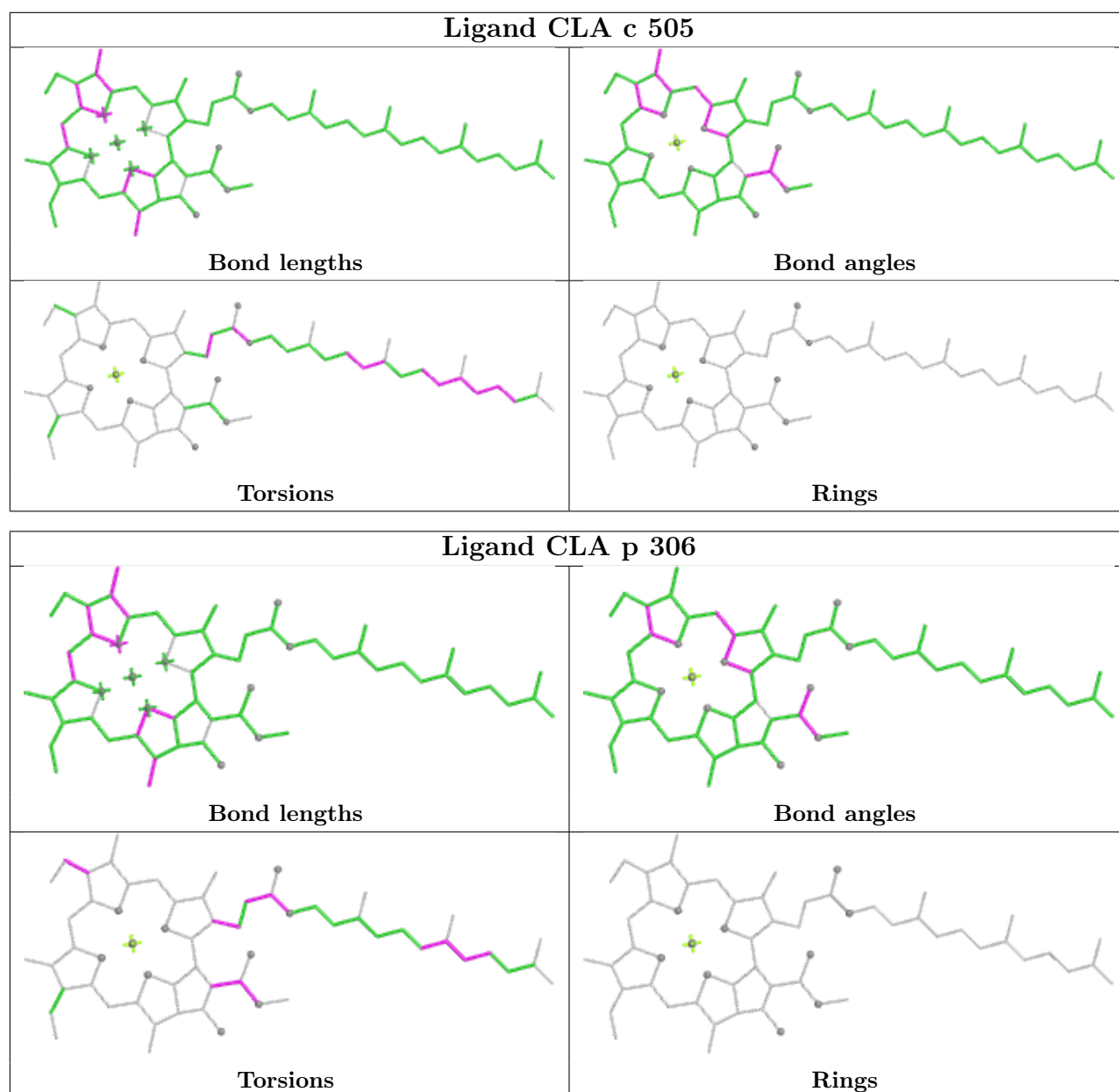
Bond angles

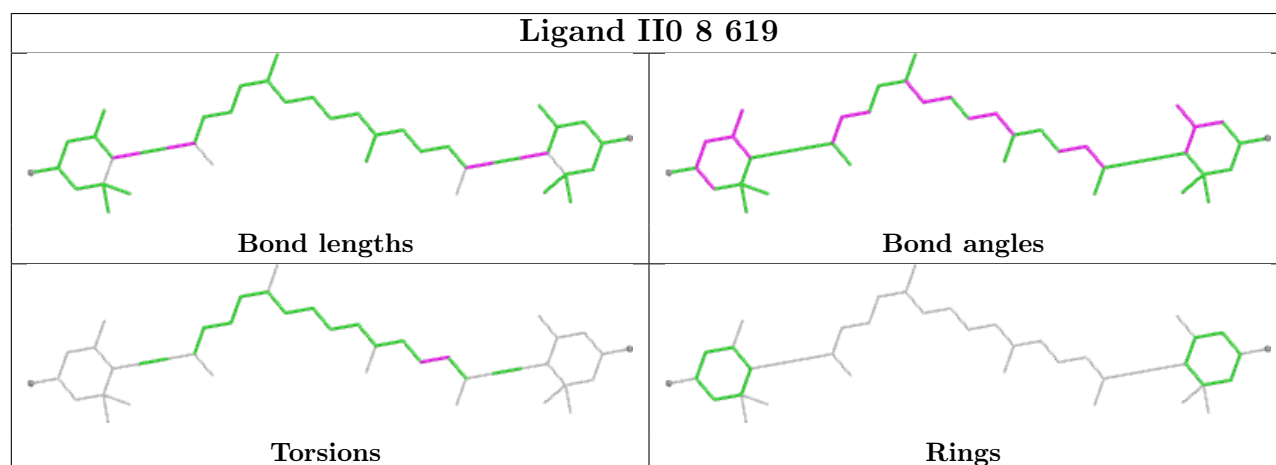
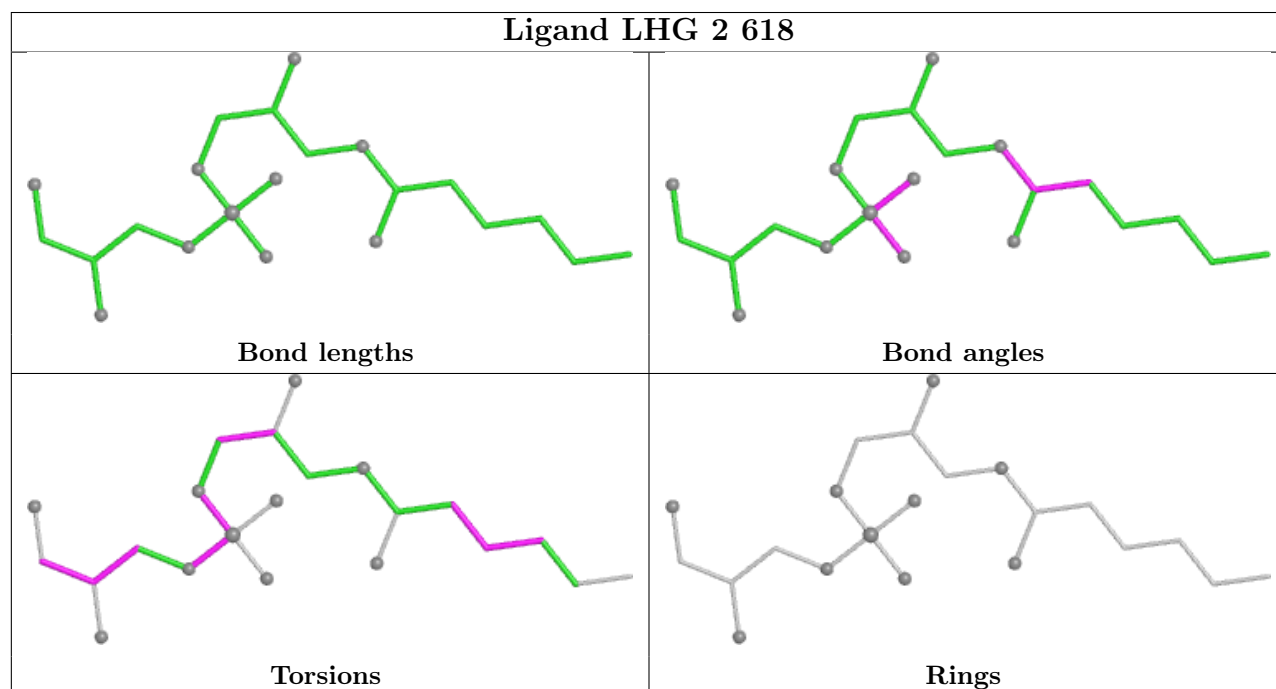
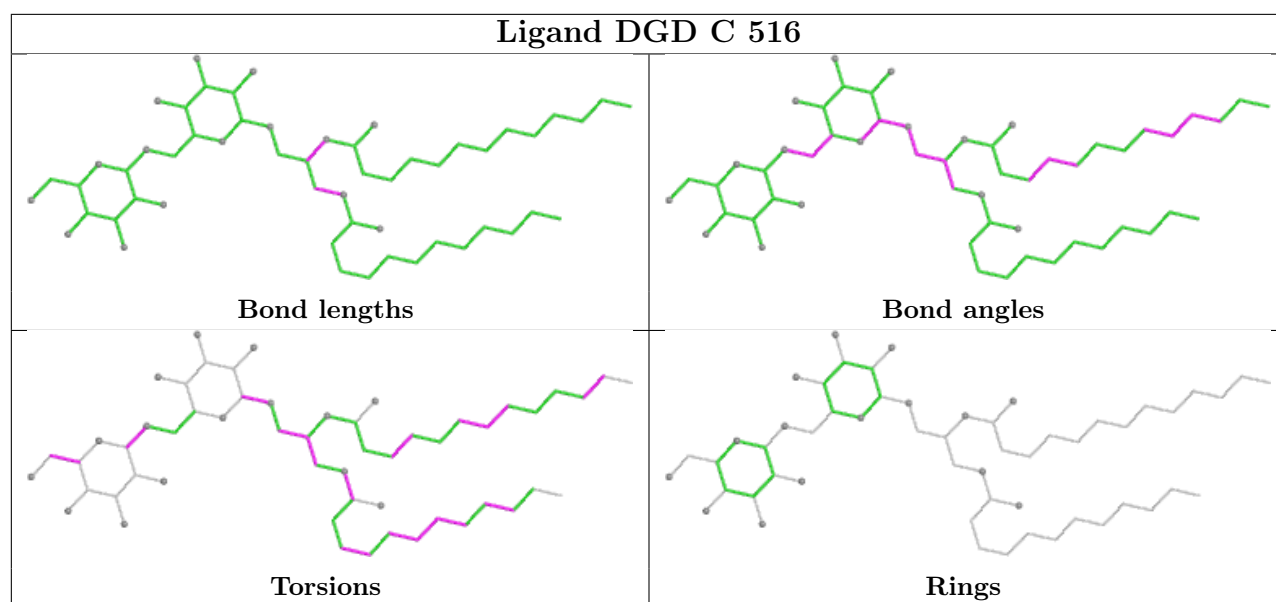


Torsions

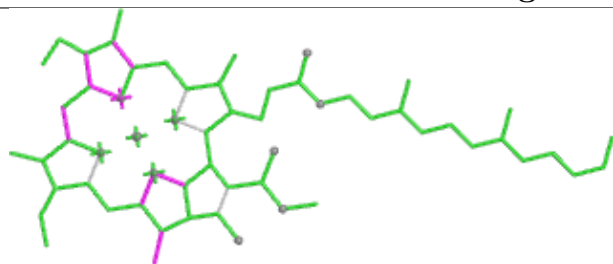


Rings

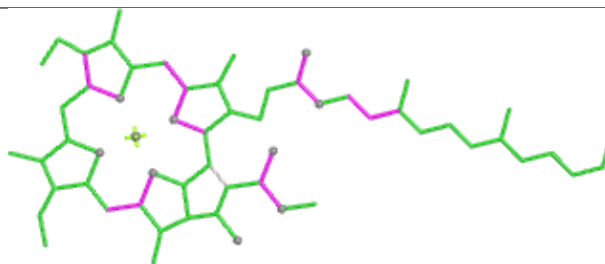




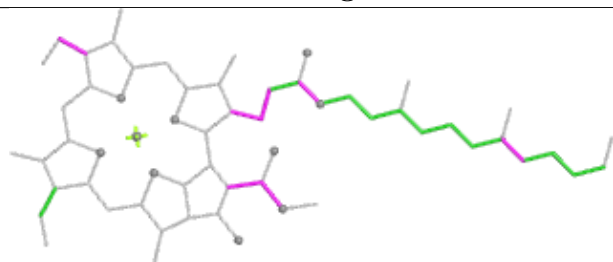
Ligand CLA 2 602



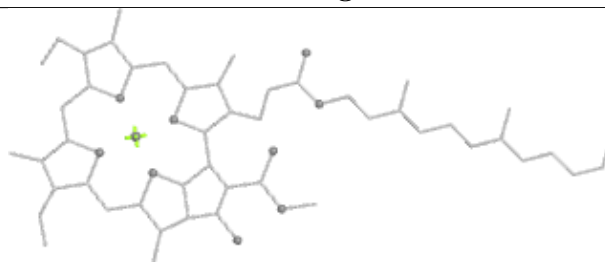
Bond lengths



Bond angles

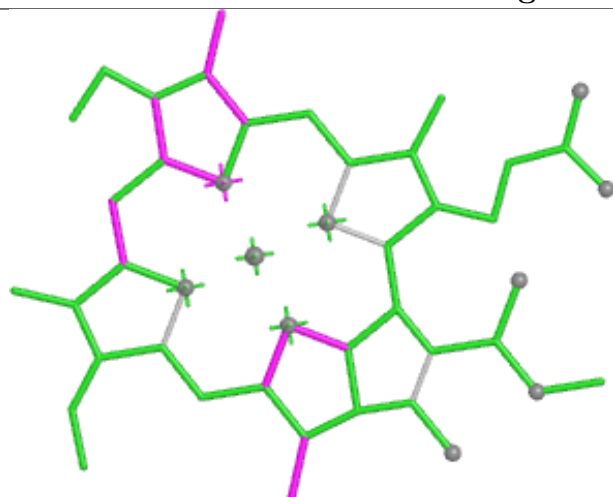


Torsions

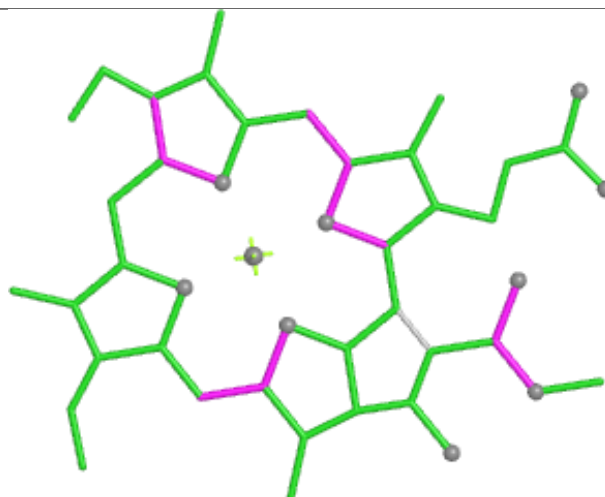


Rings

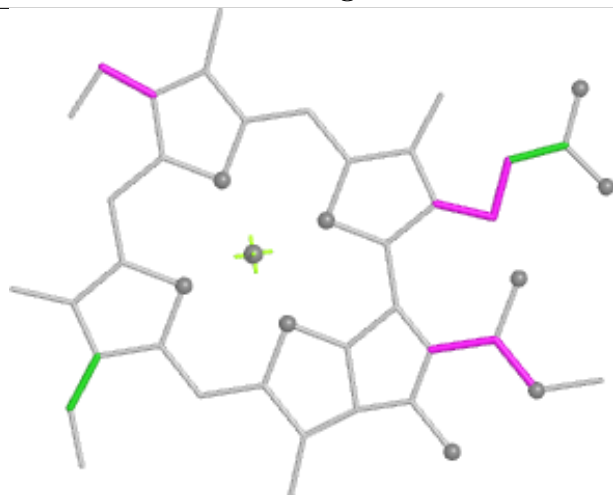
Ligand CLA 3 610



Bond lengths



Bond angles

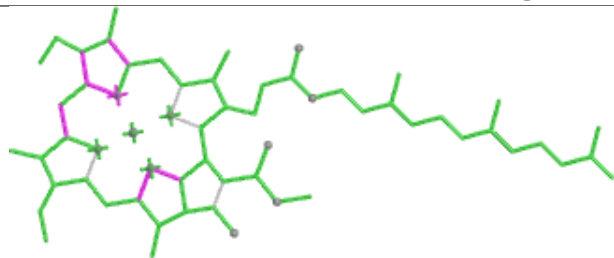


Torsions

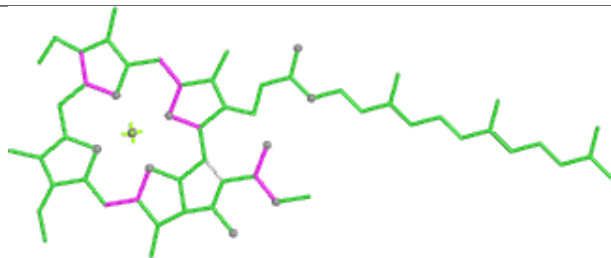


Rings

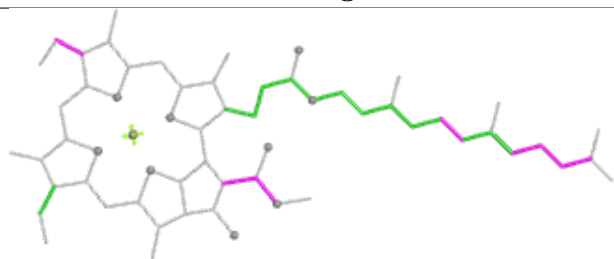
Ligand CLA 4 608



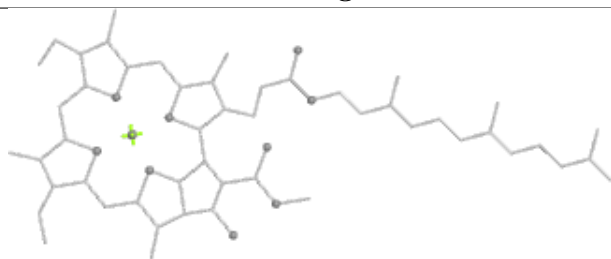
Bond lengths



Bond angles

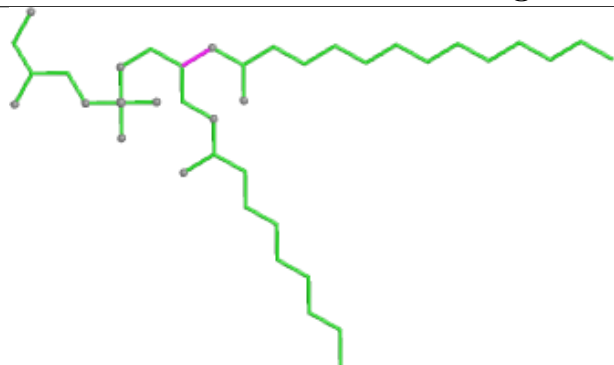


Torsions

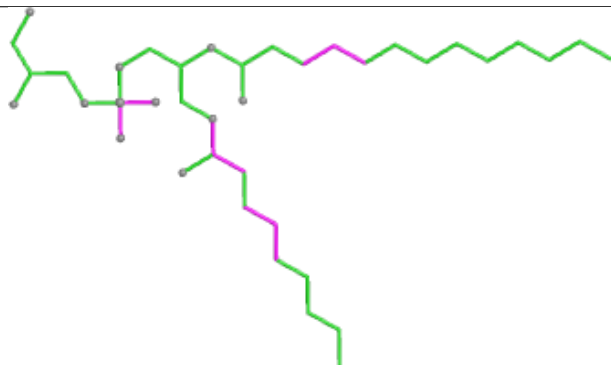


Rings

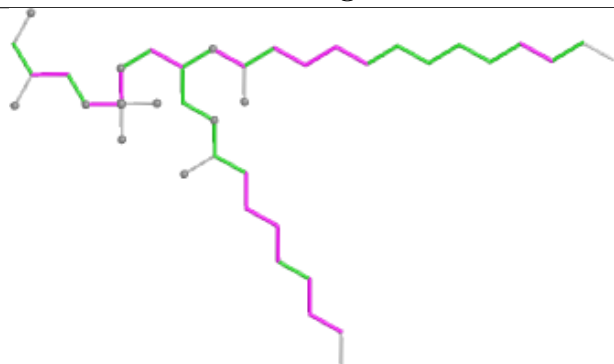
Ligand LHG B 619



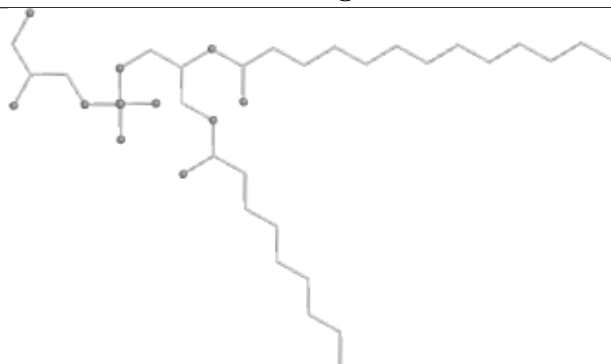
Bond lengths



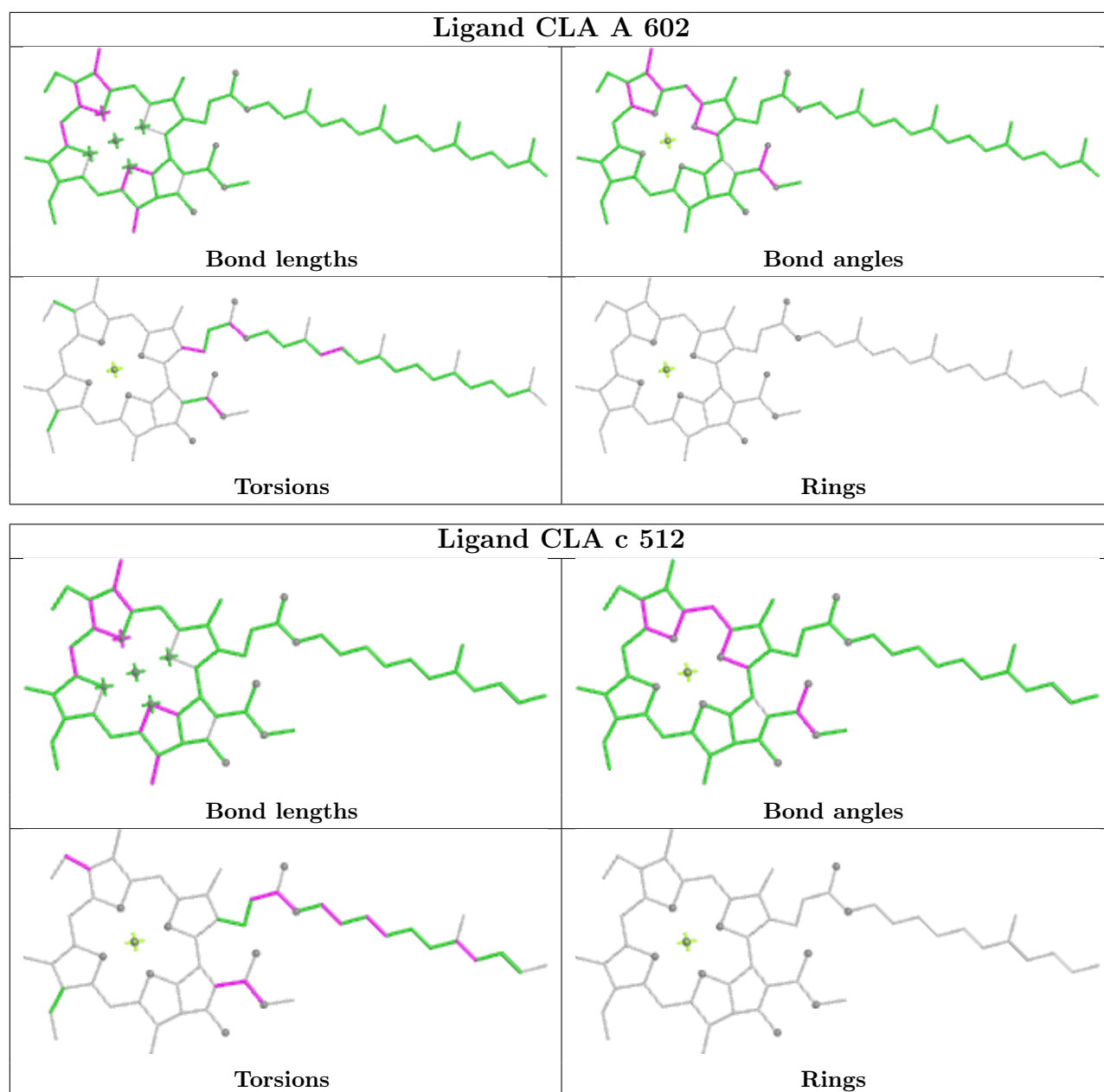
Bond angles



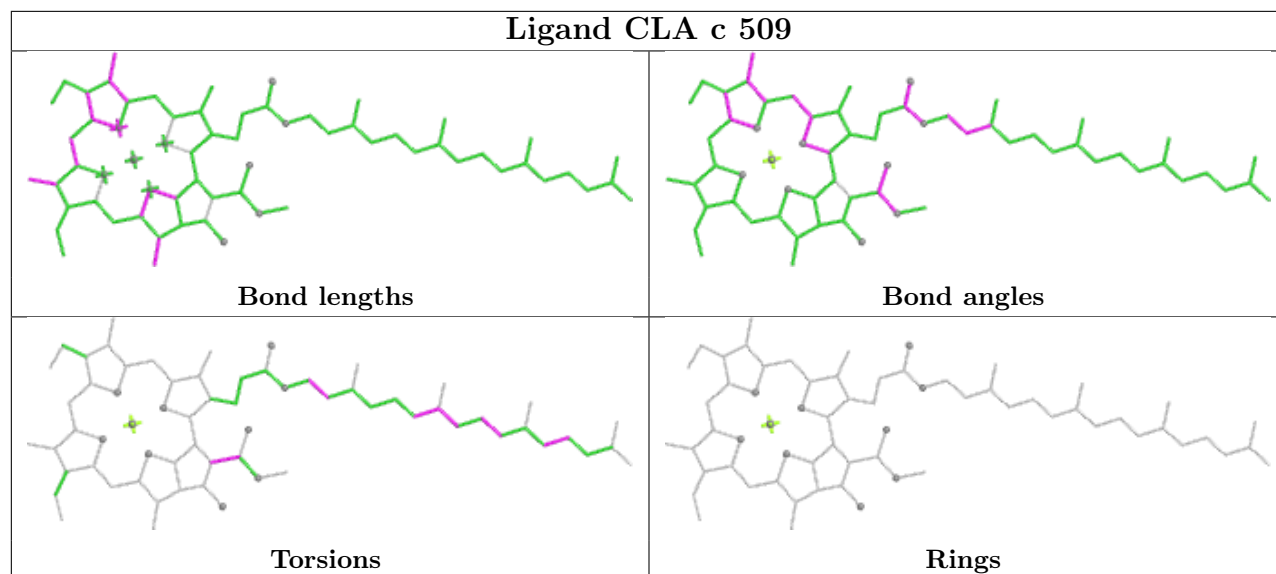
Torsions



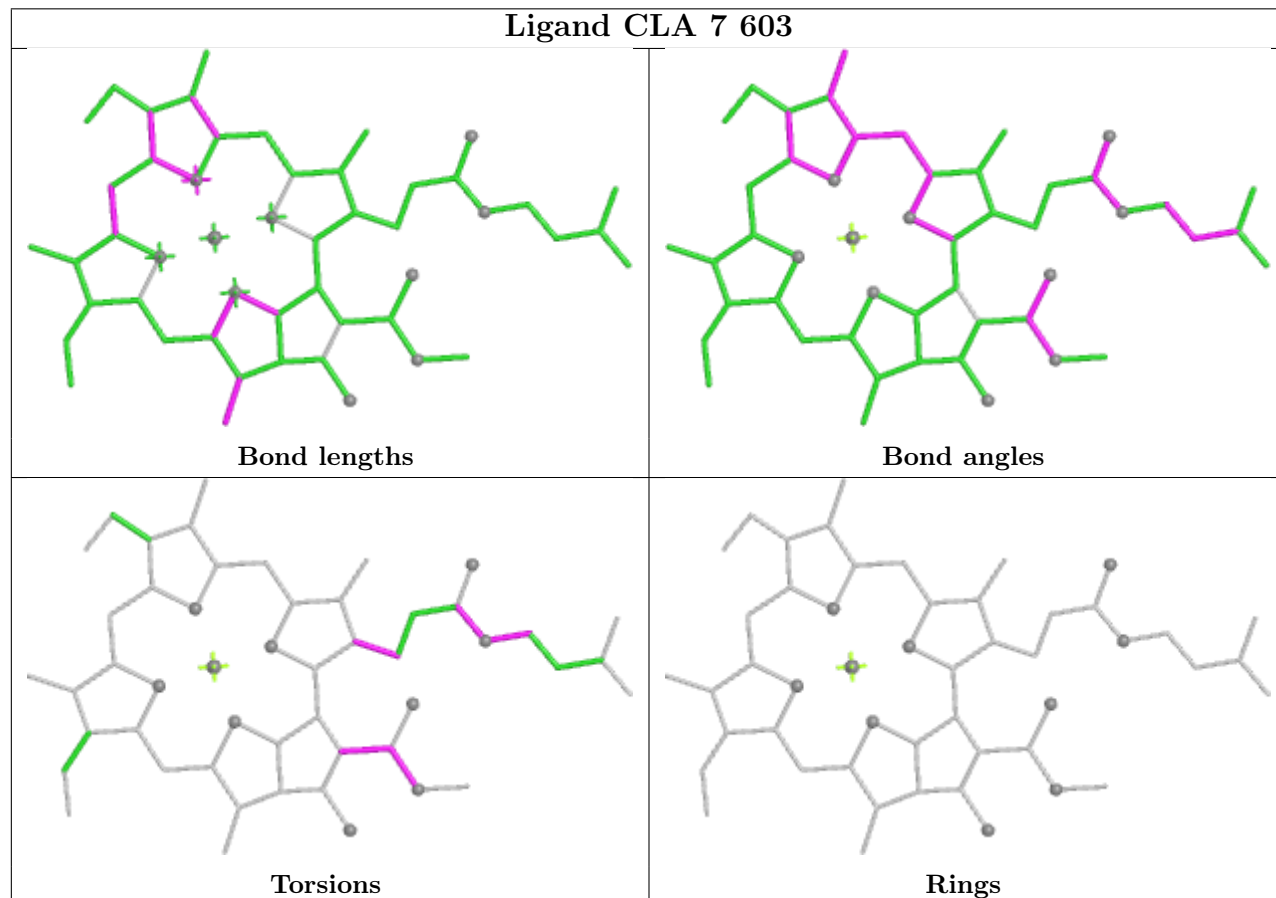
Rings

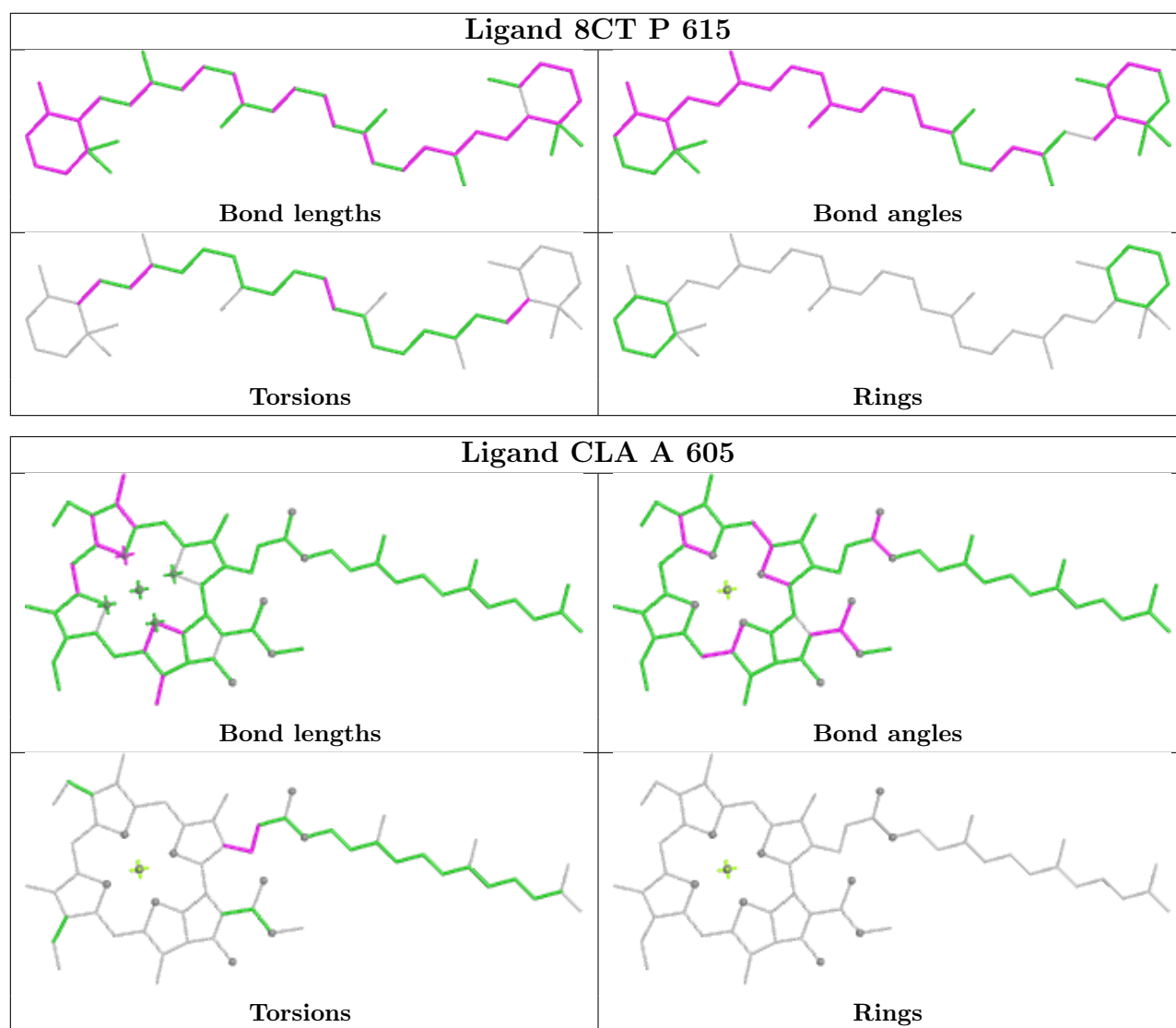


Ligand CLA c 509

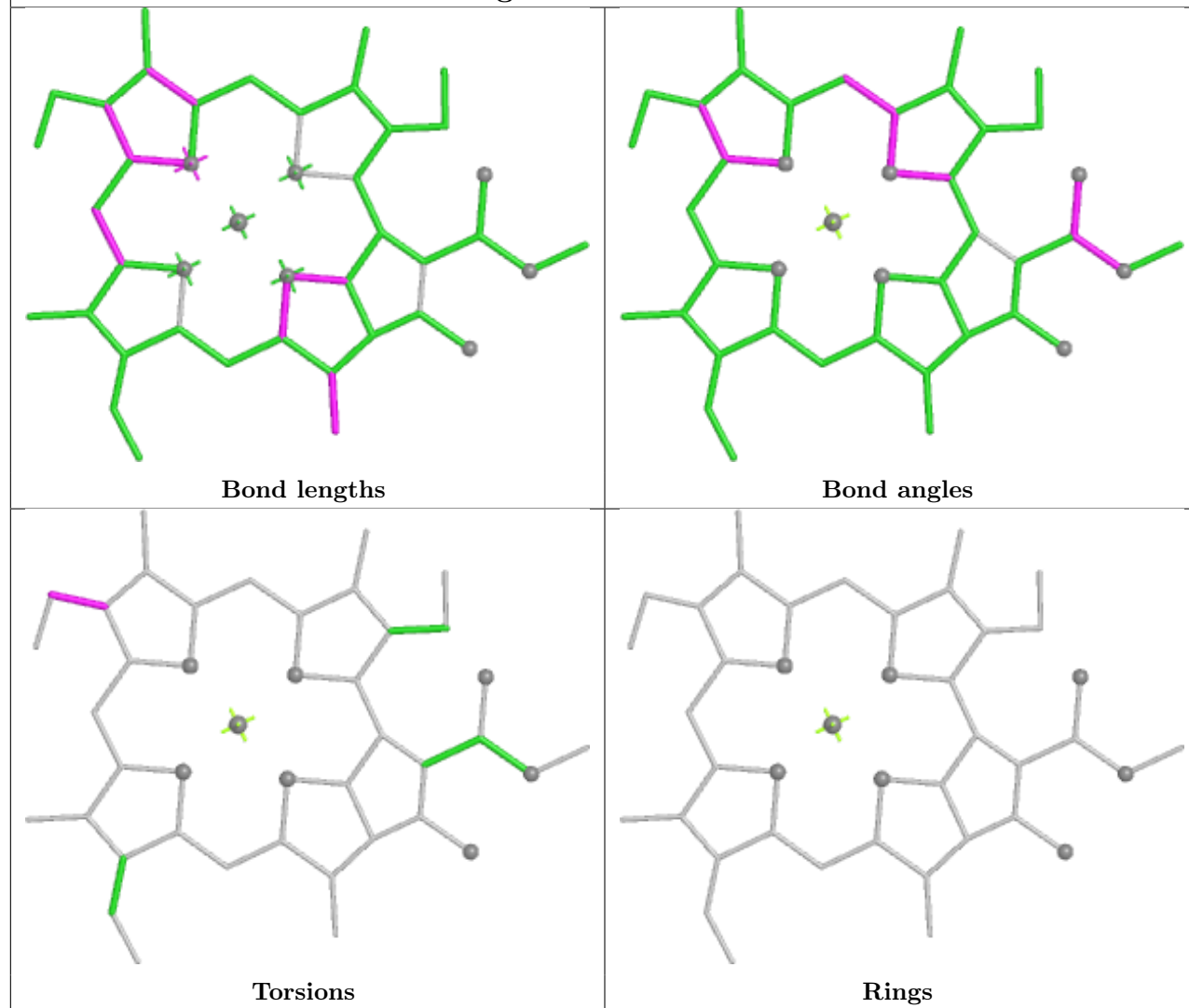


Ligand CLA 7 603

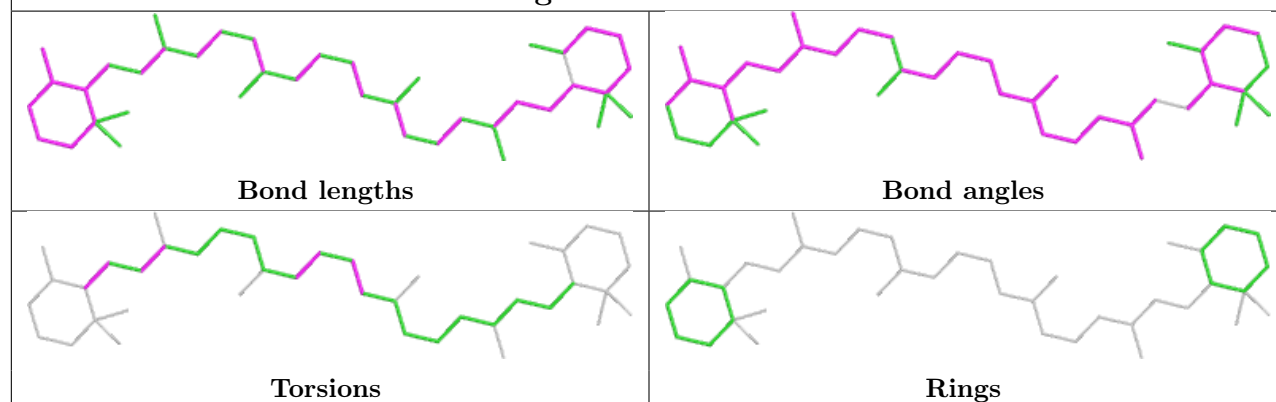


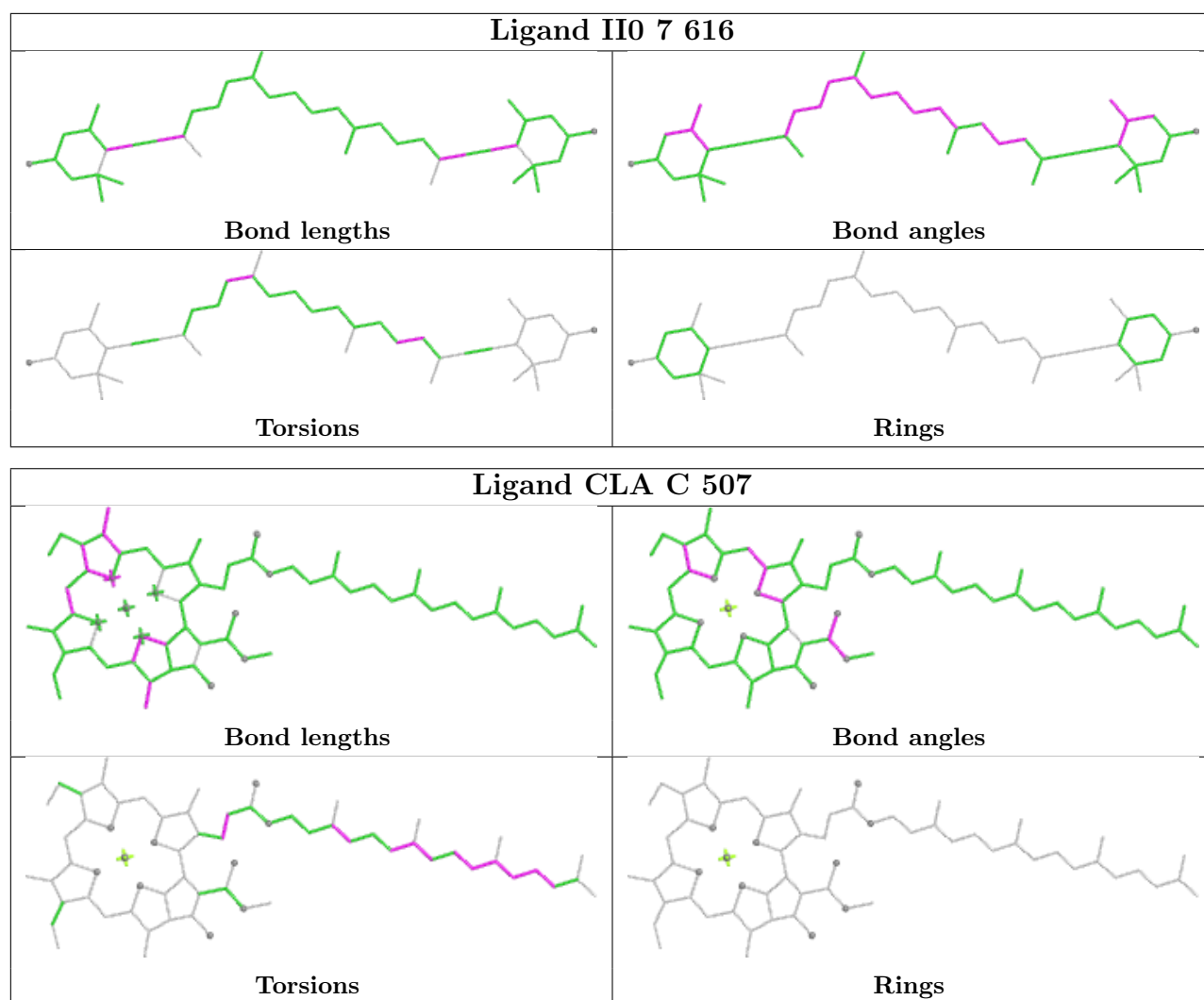


Ligand CLA P 601

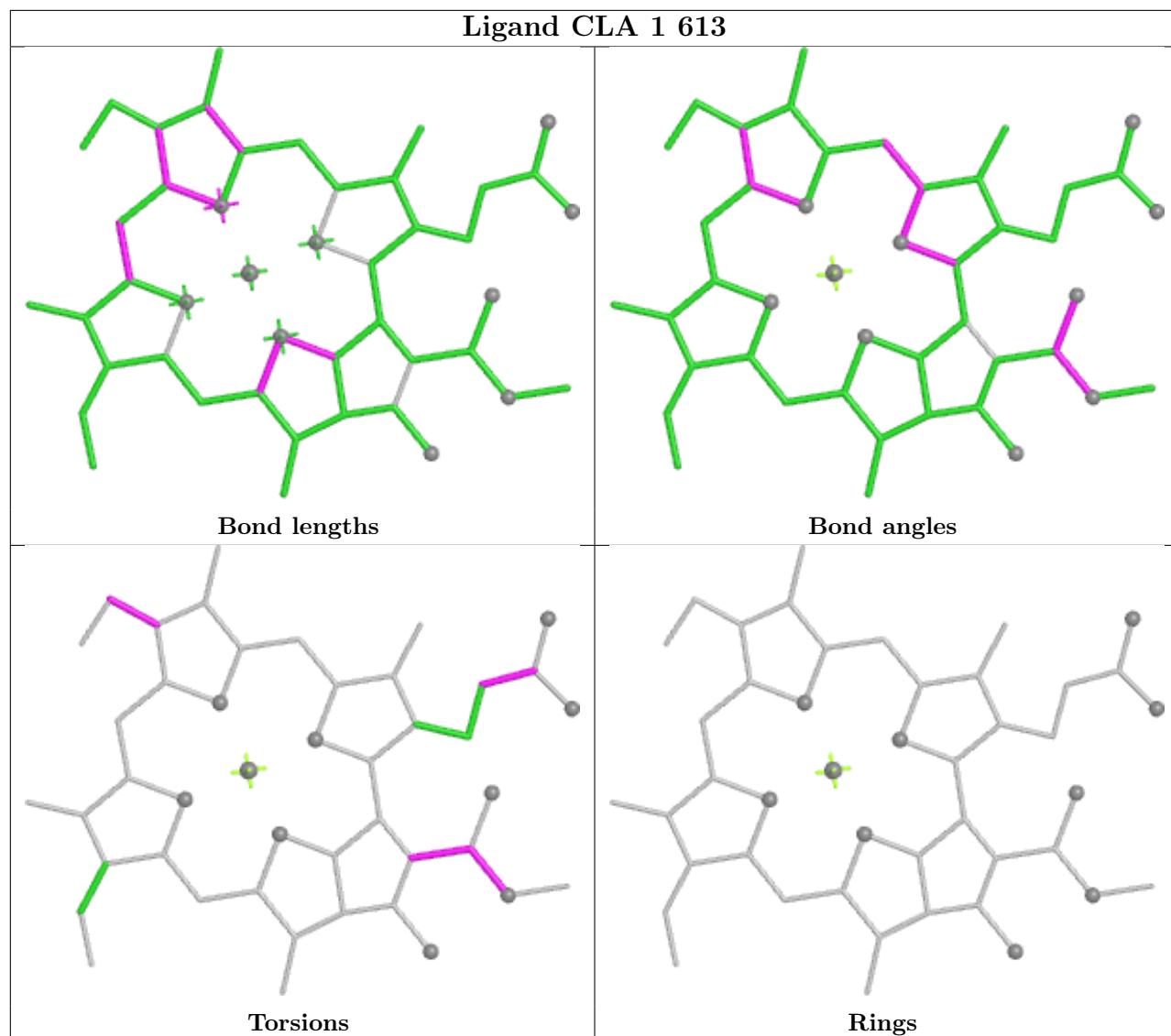


Ligand 8CT A 610

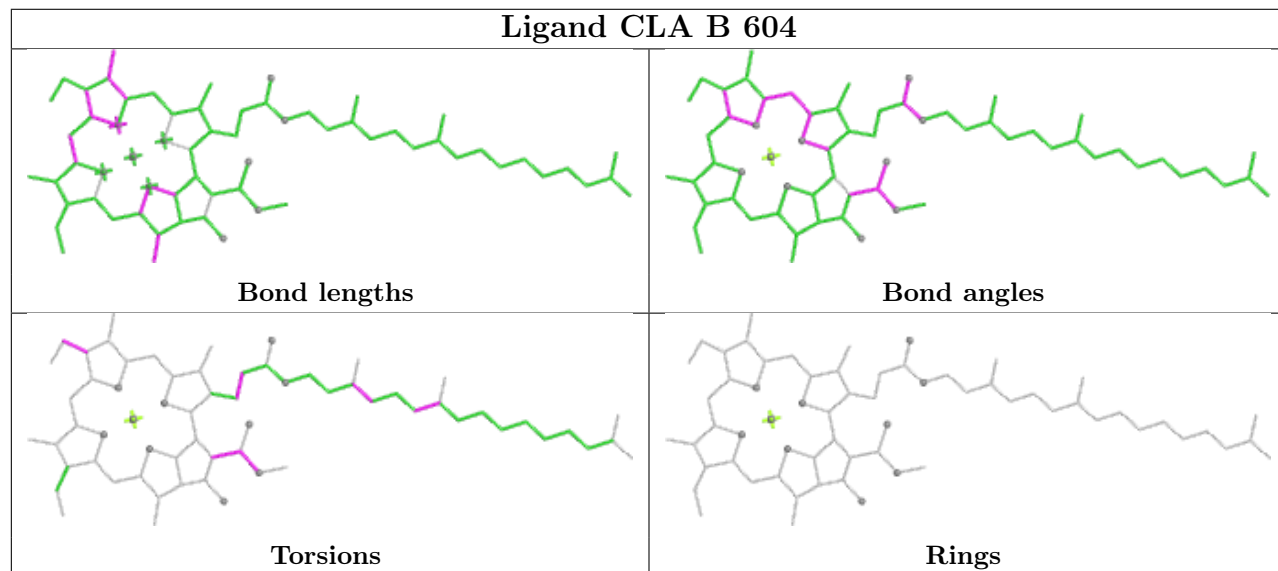


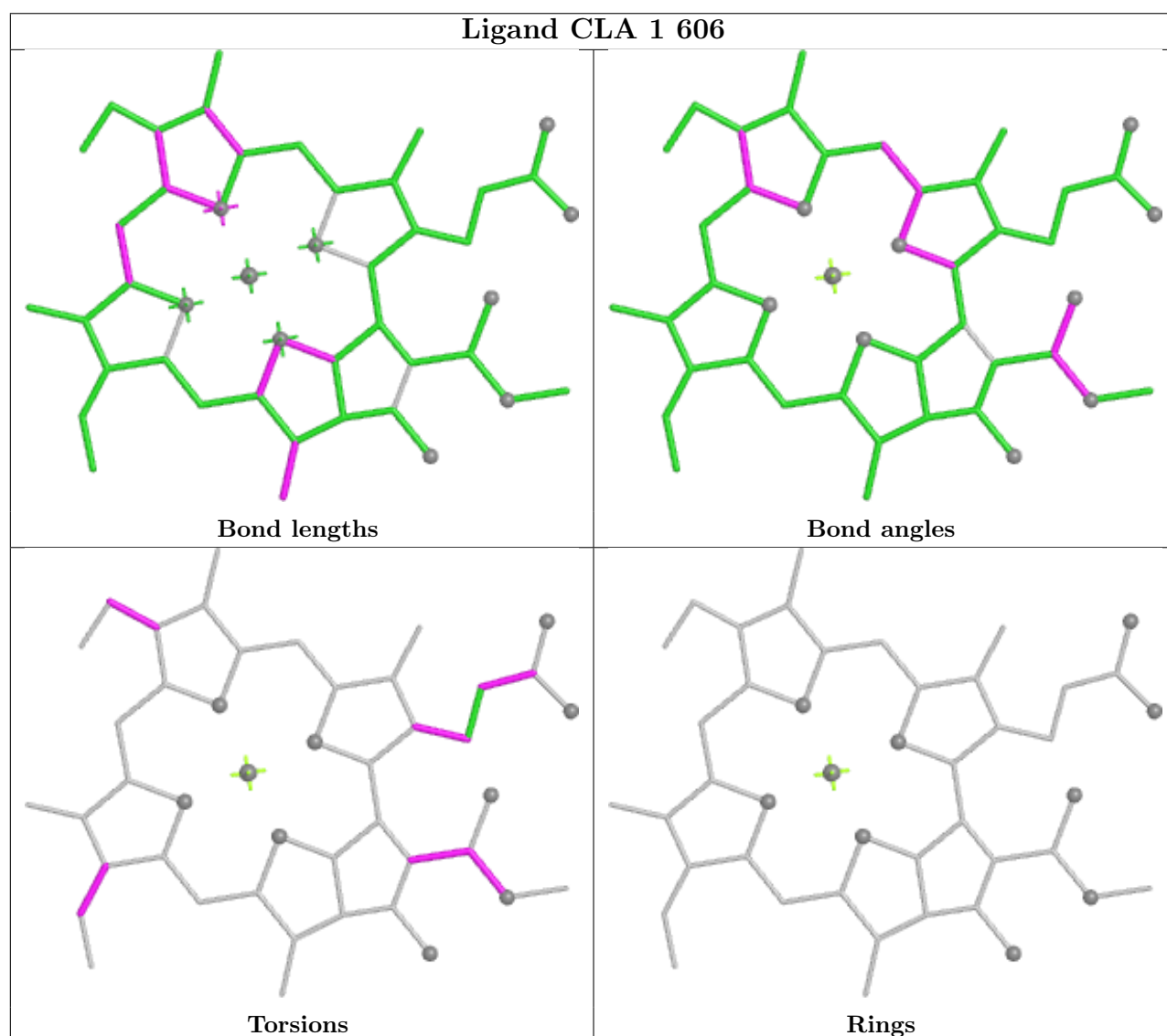
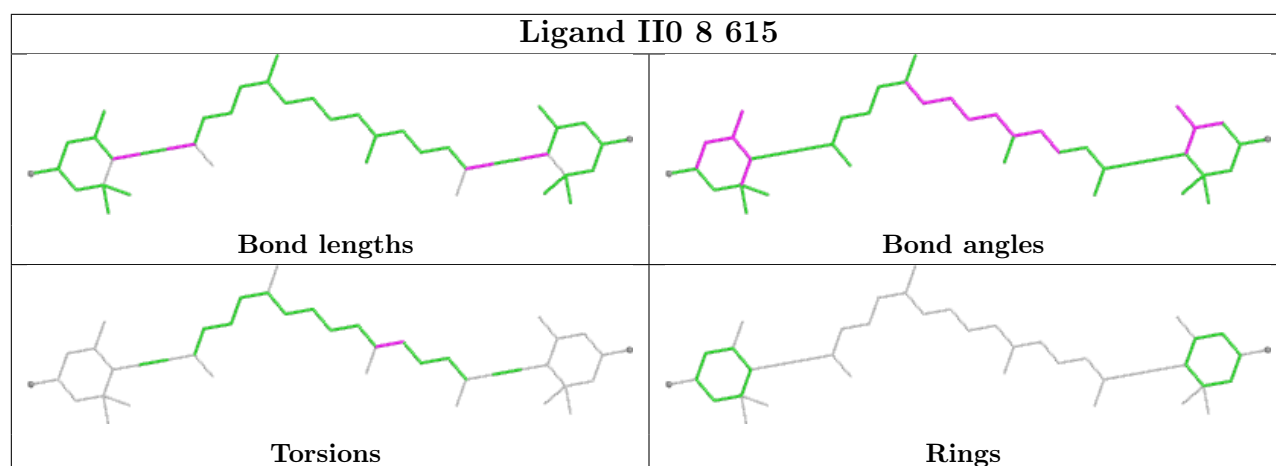


Ligand CLA 1 613

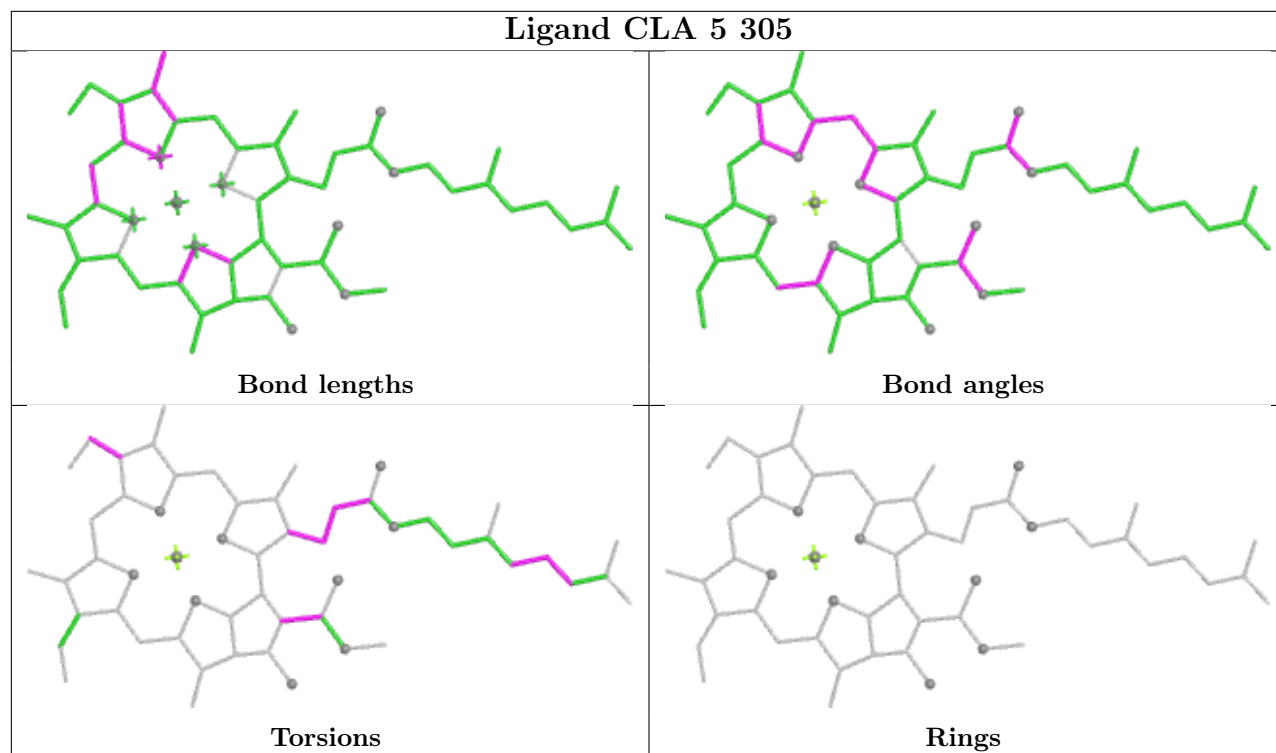


Ligand CLA B 604

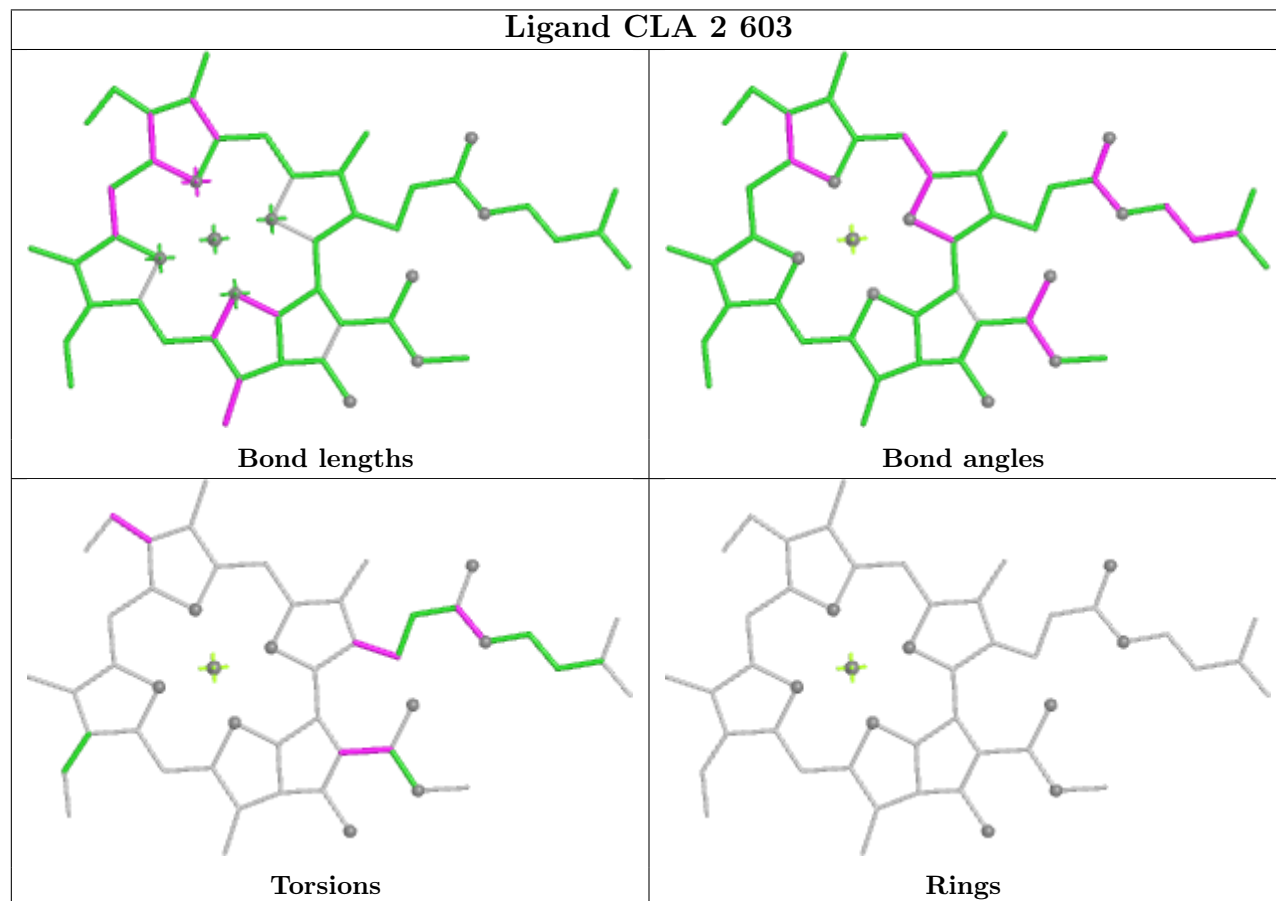


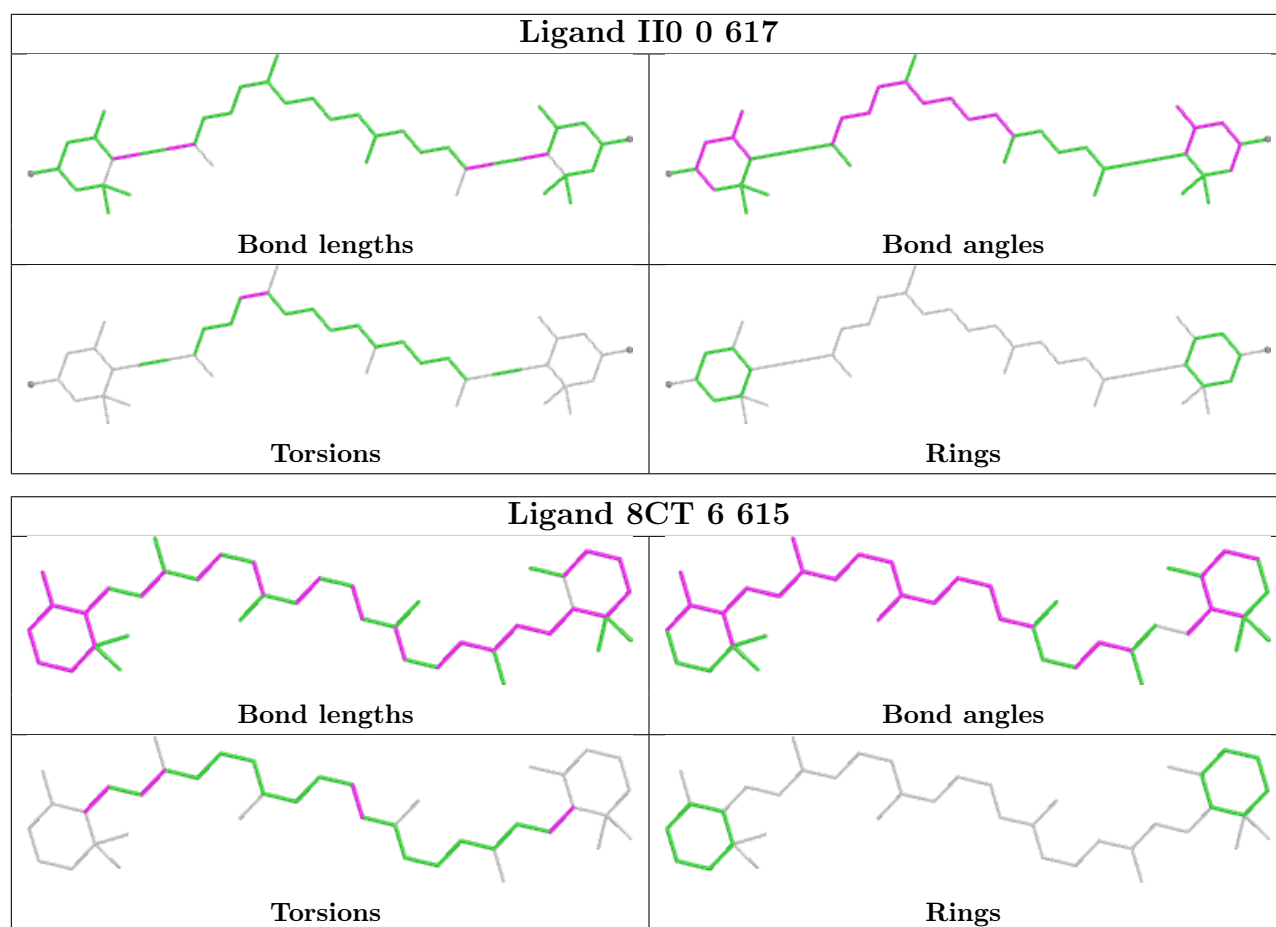


Ligand CLA 5 305

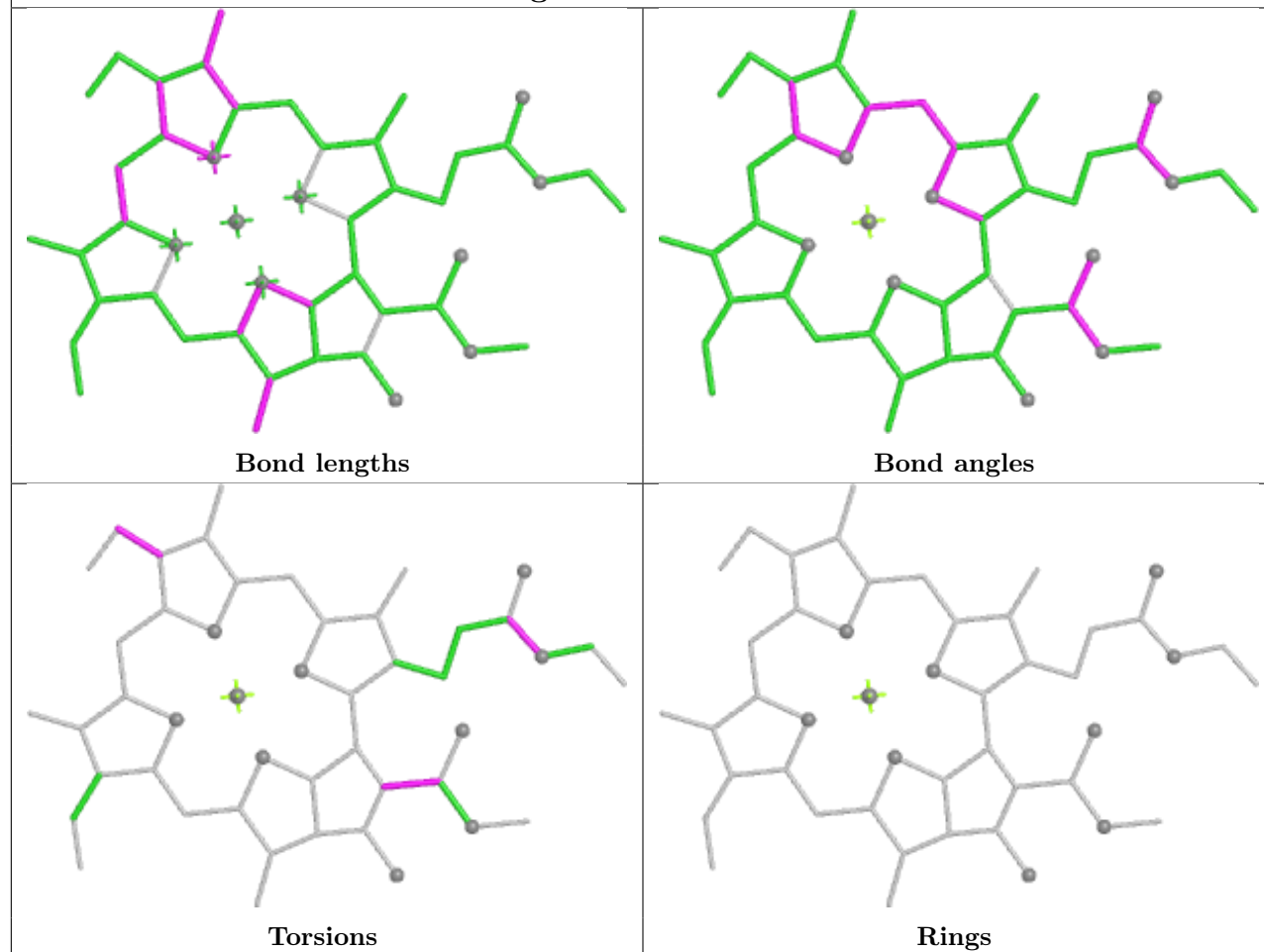


Ligand CLA 2 603

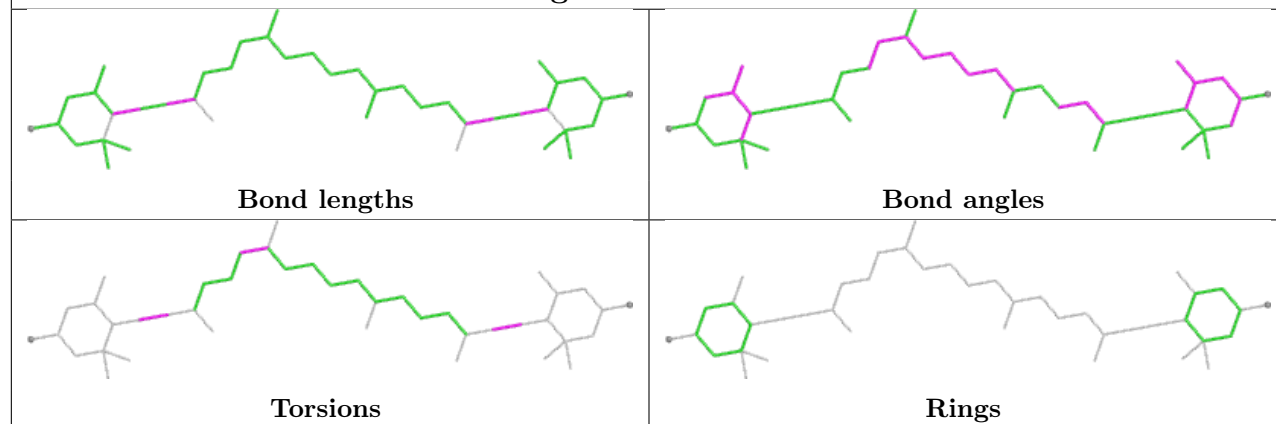


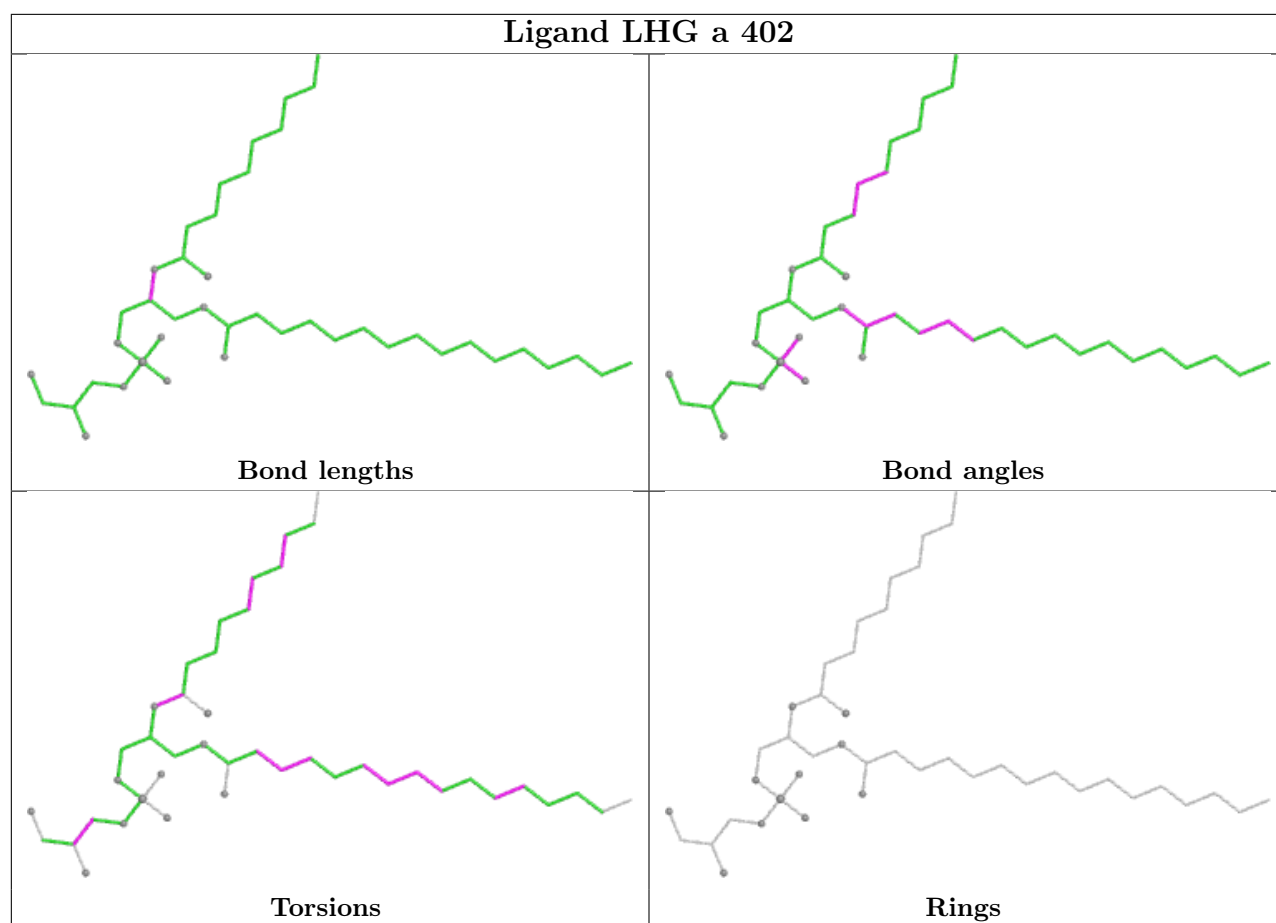


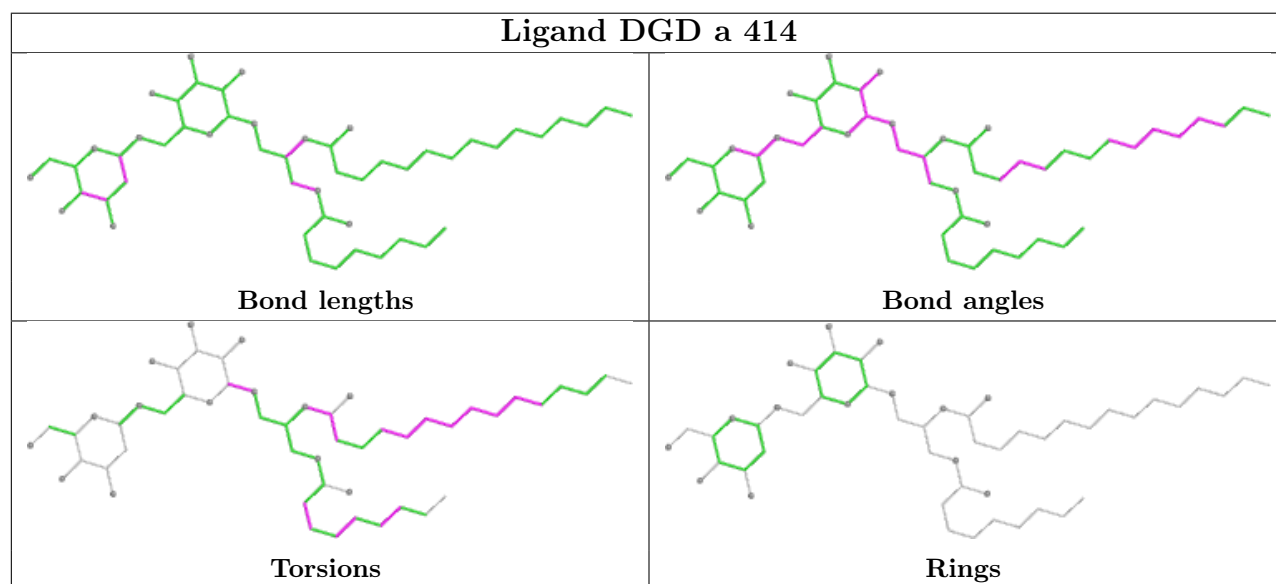
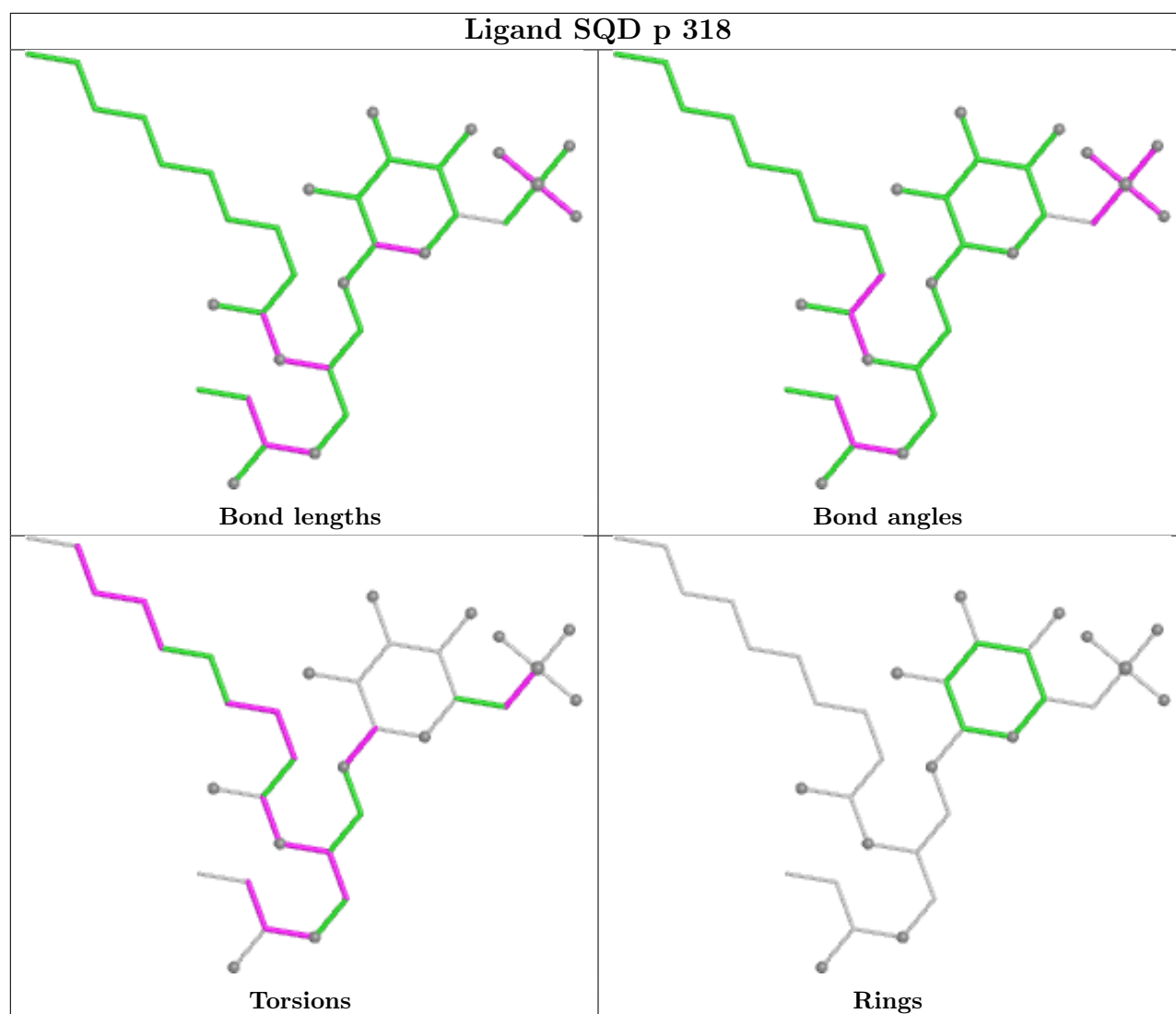
Ligand CLA b 602

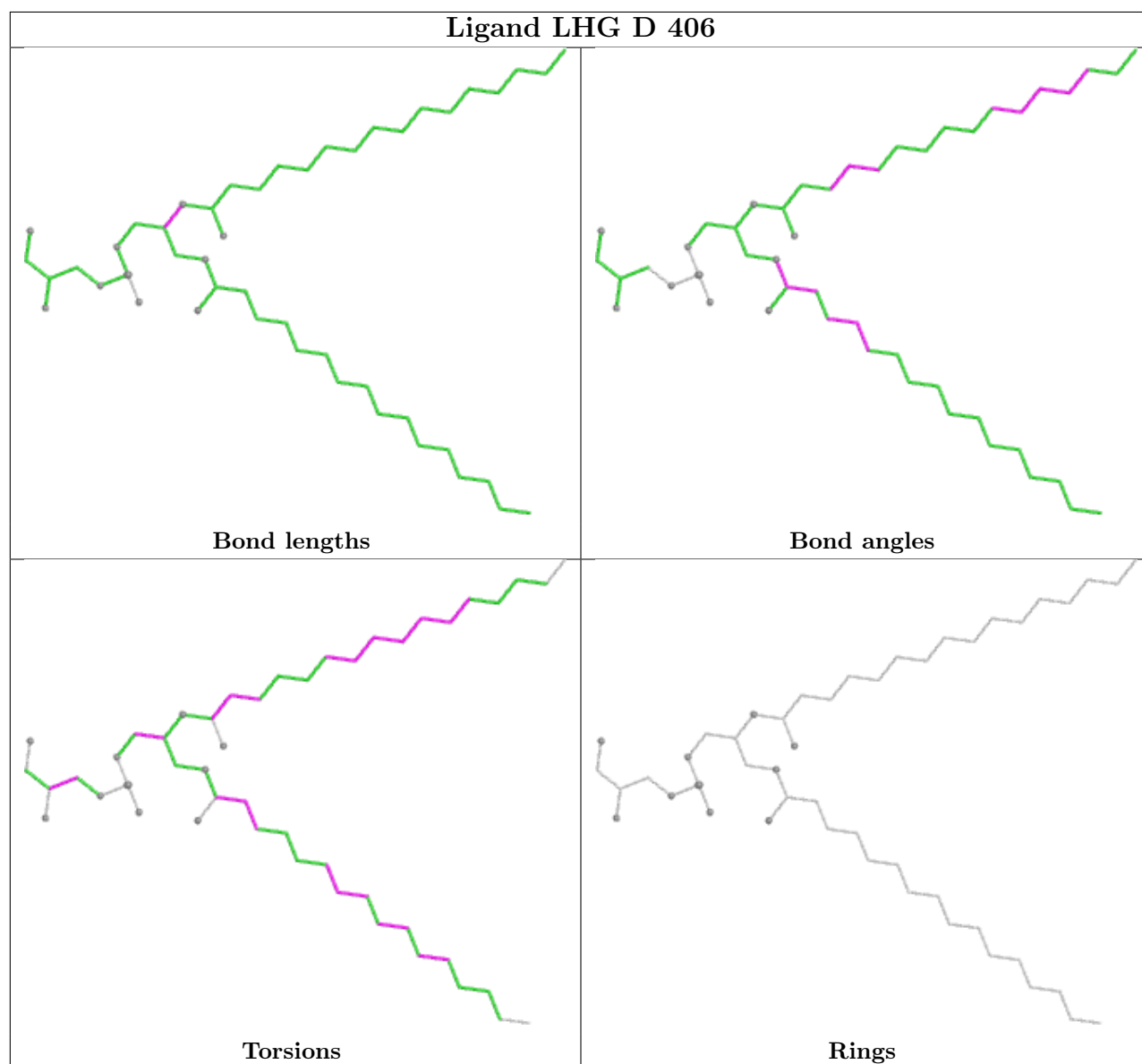
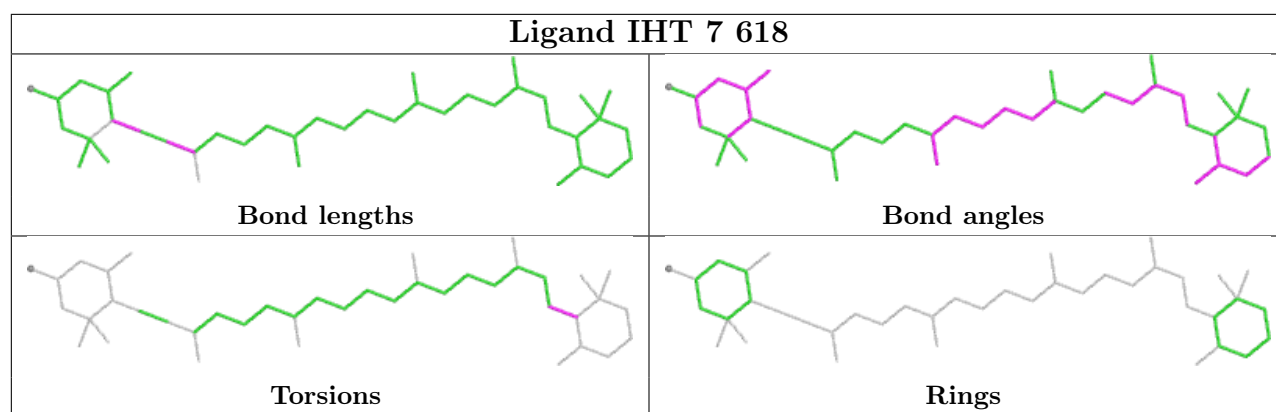


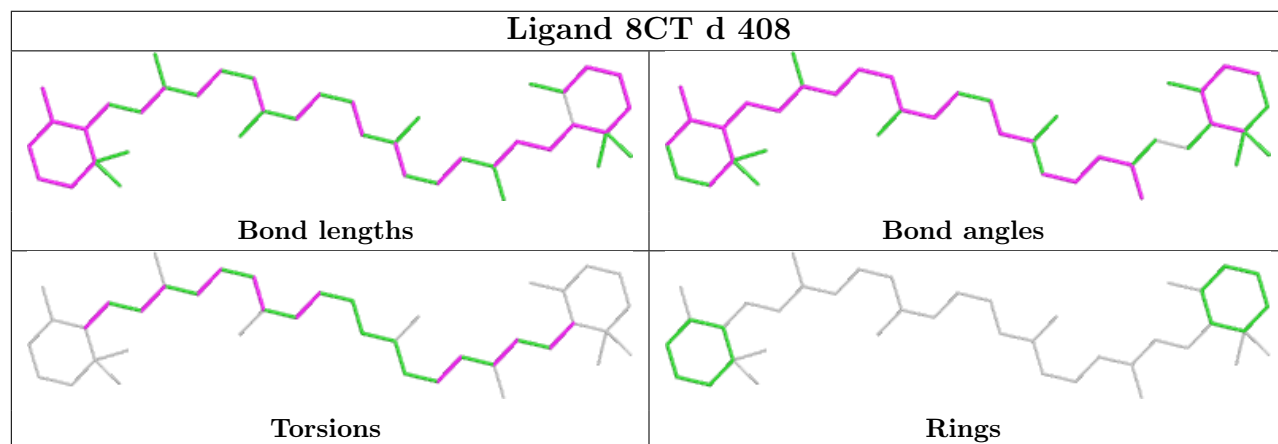
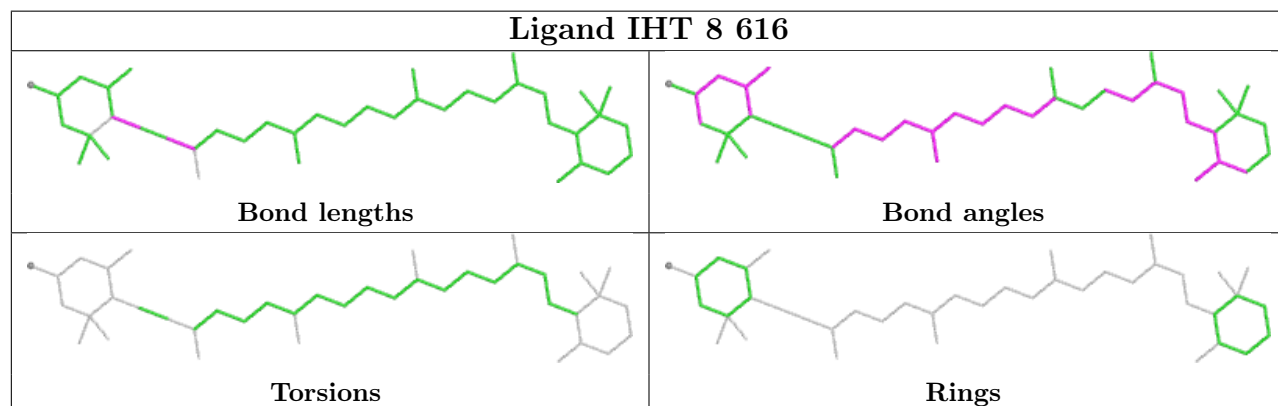
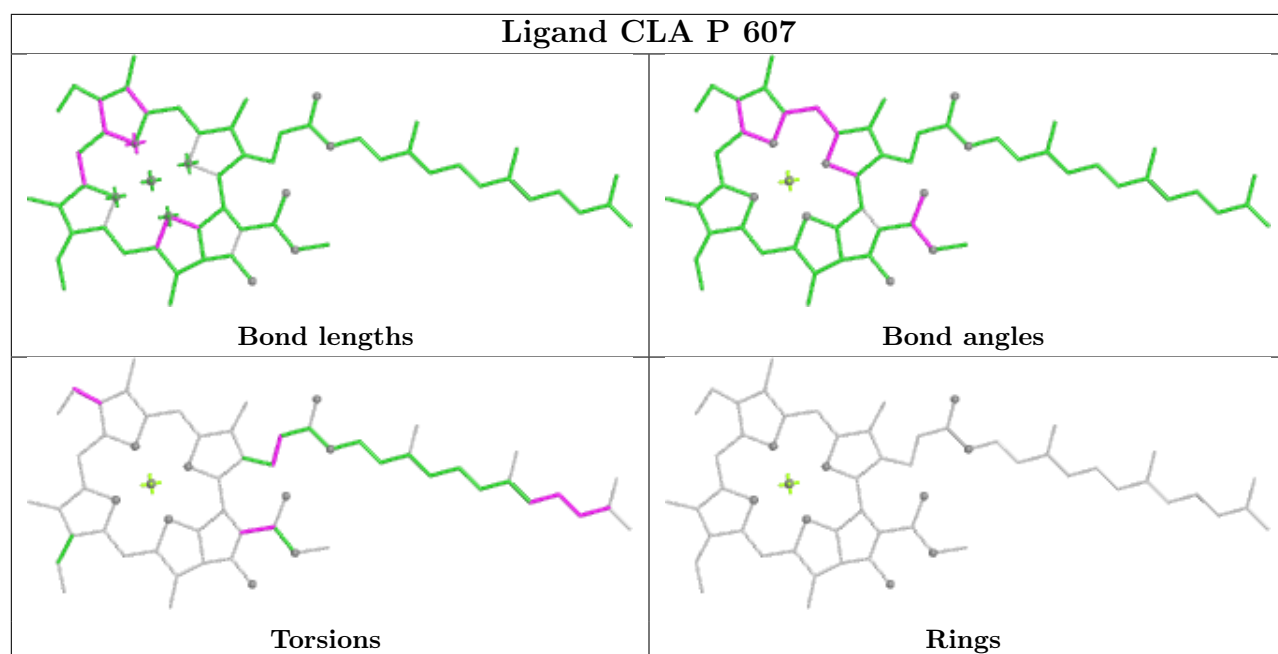
Ligand II0 7 617

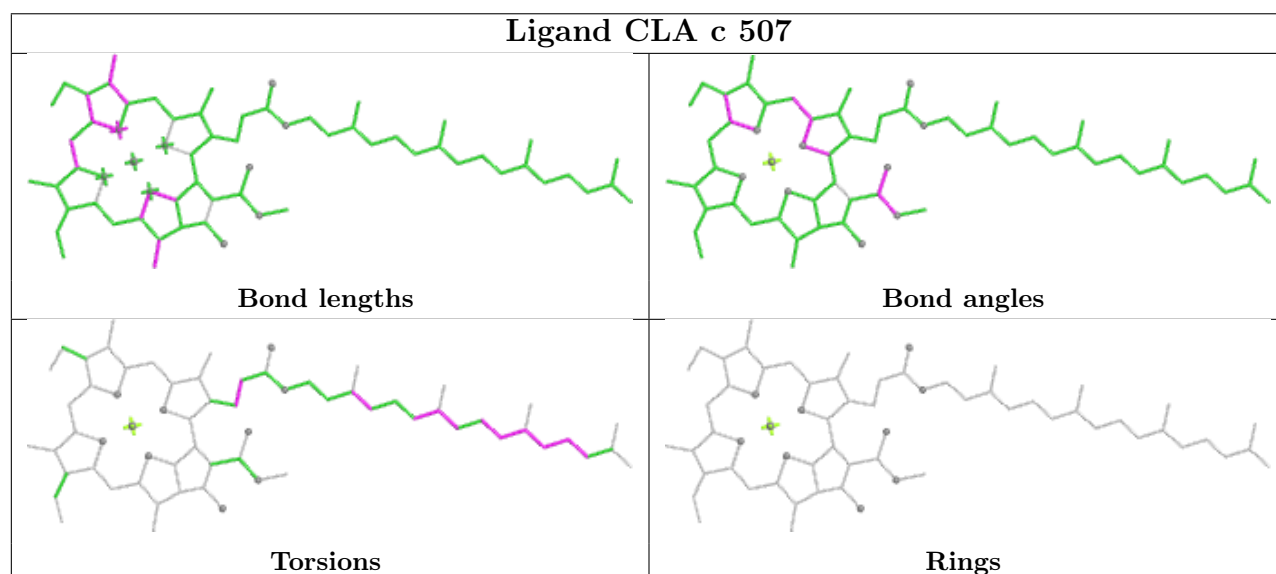
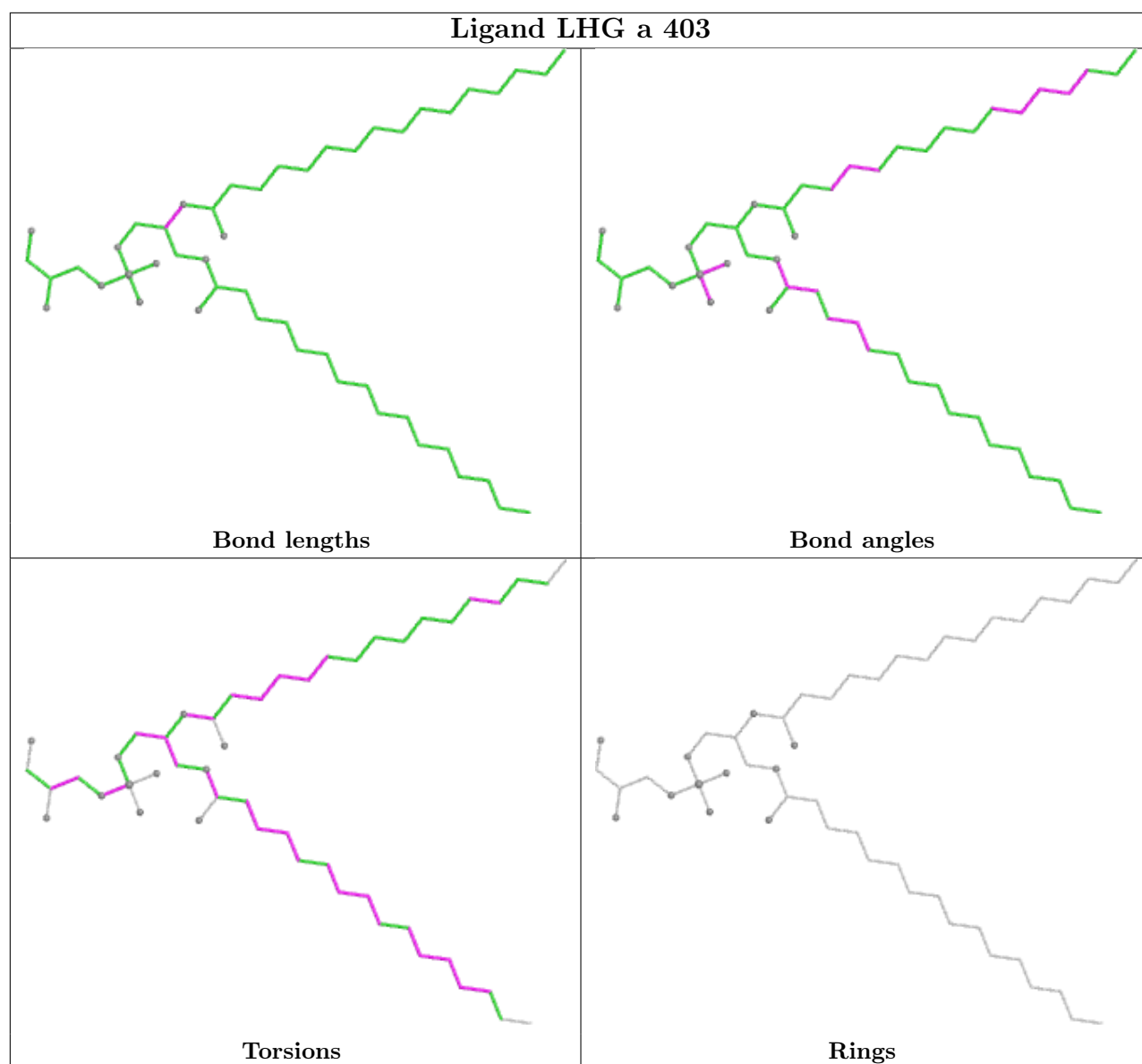




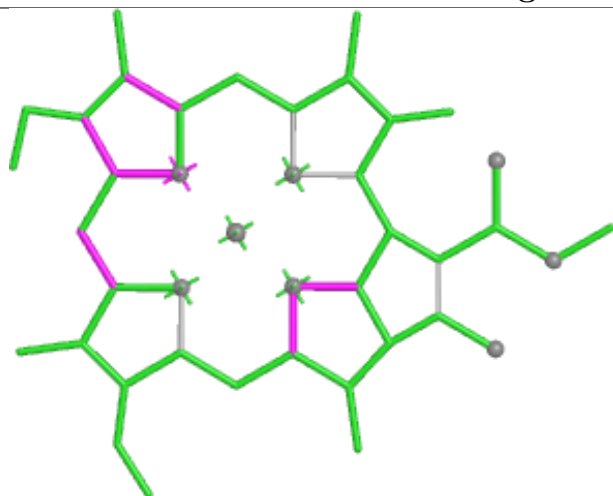




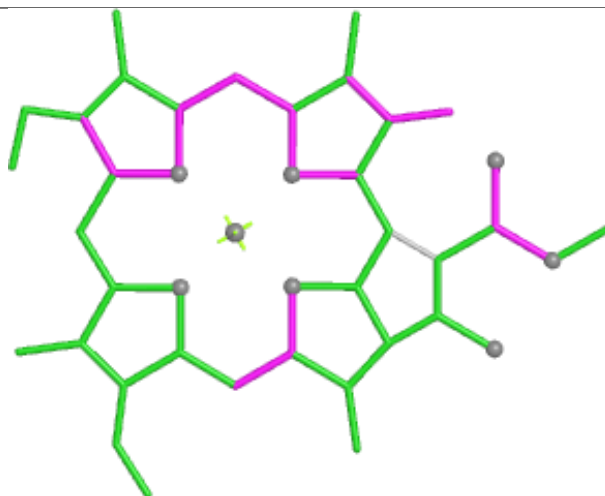




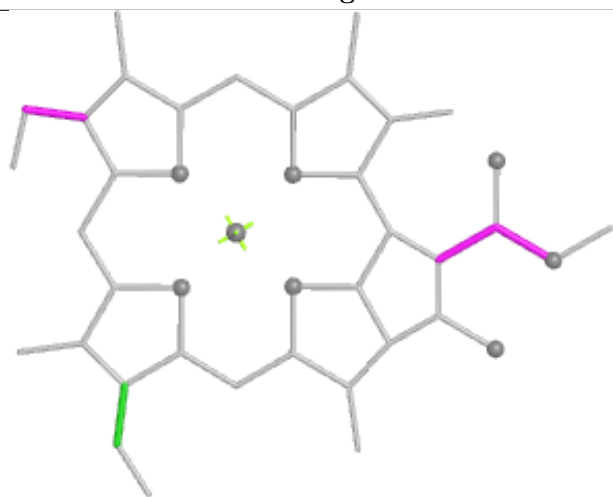
Ligand CLA 7 609



Bond lengths



Bond angles

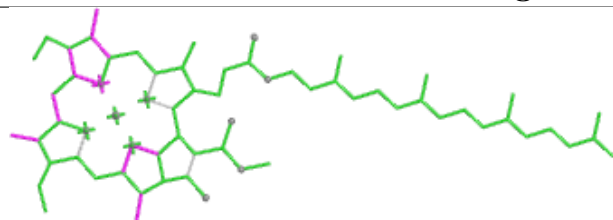


Torsions

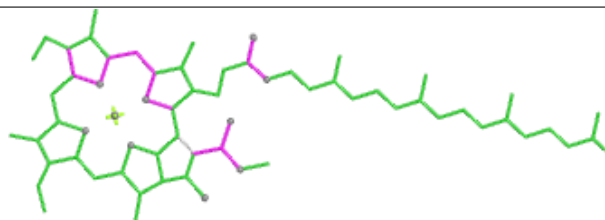


Rings

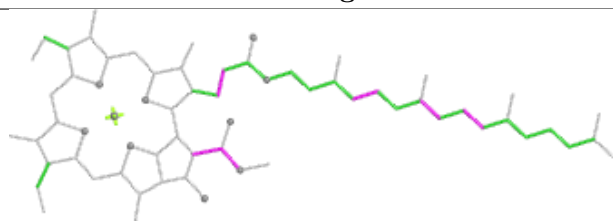
Ligand CLA B 607



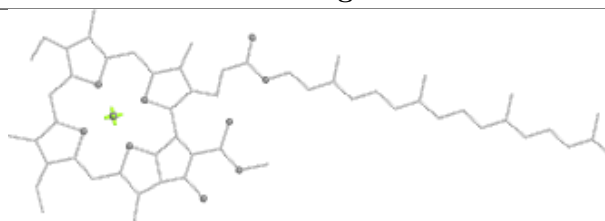
Bond lengths



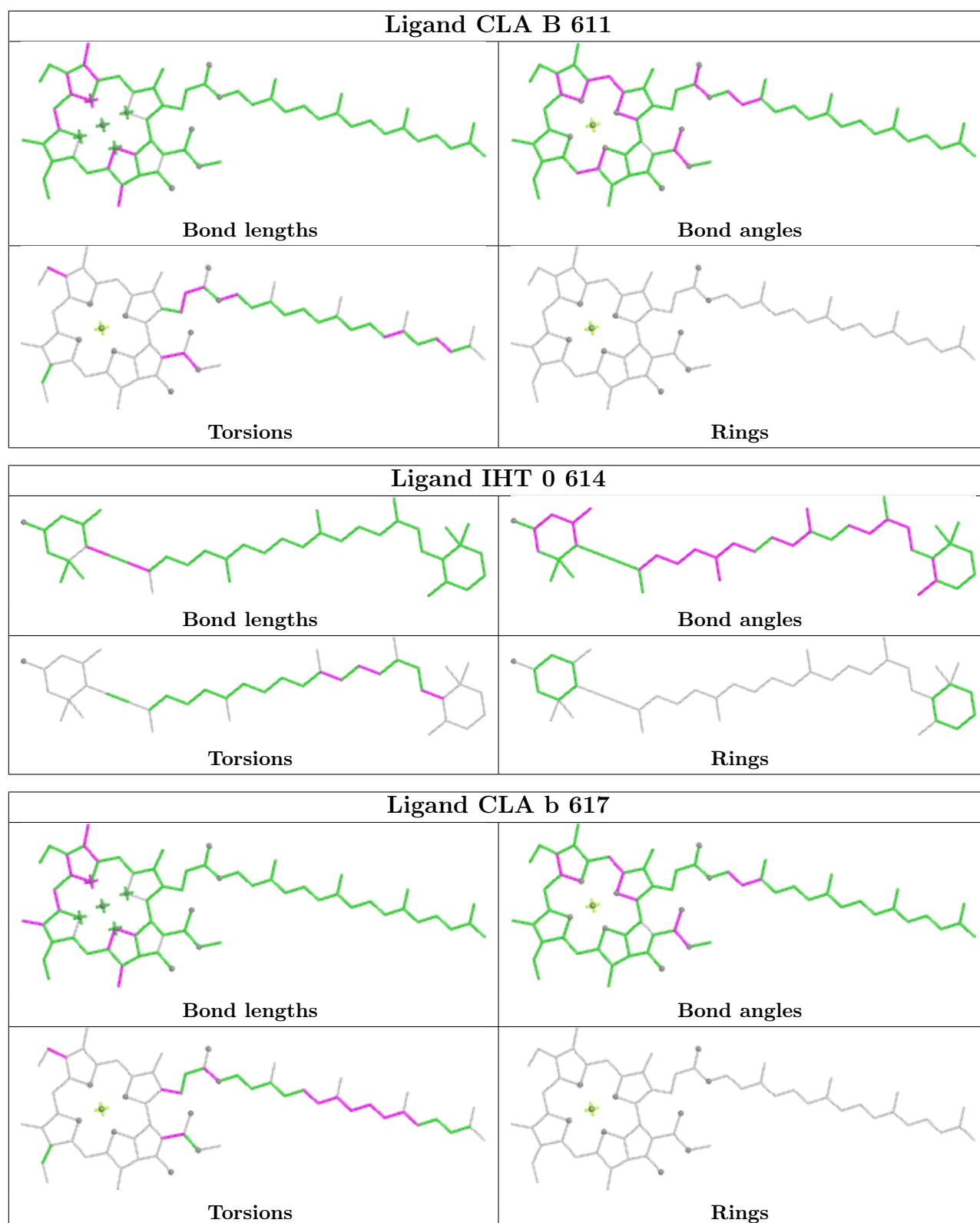
Bond angles



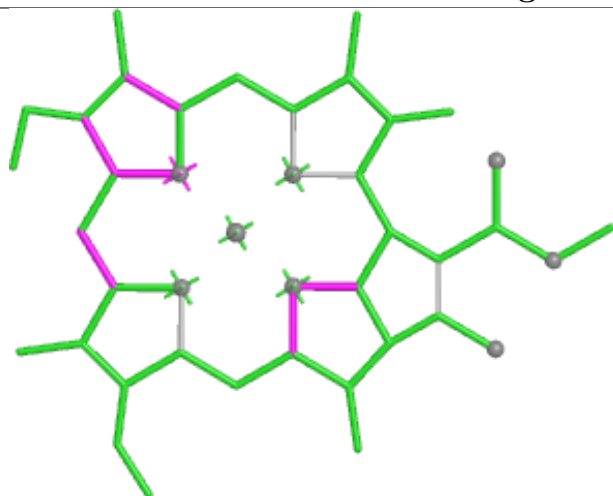
Torsions



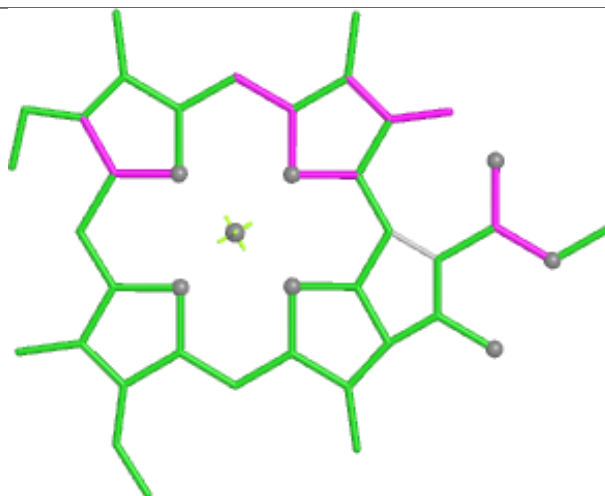
Rings



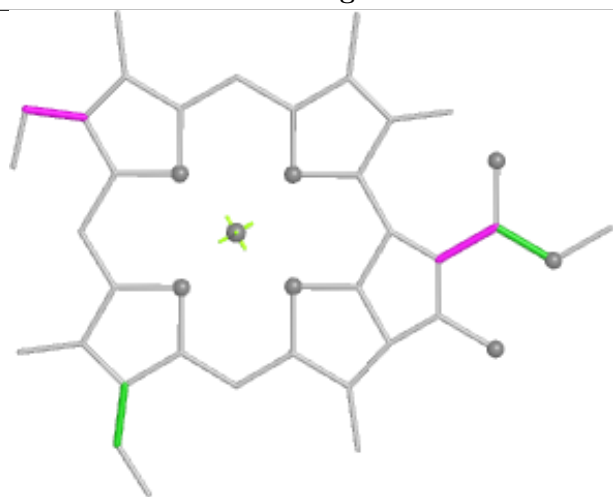
Ligand CLA 4 609



Bond lengths



Bond angles

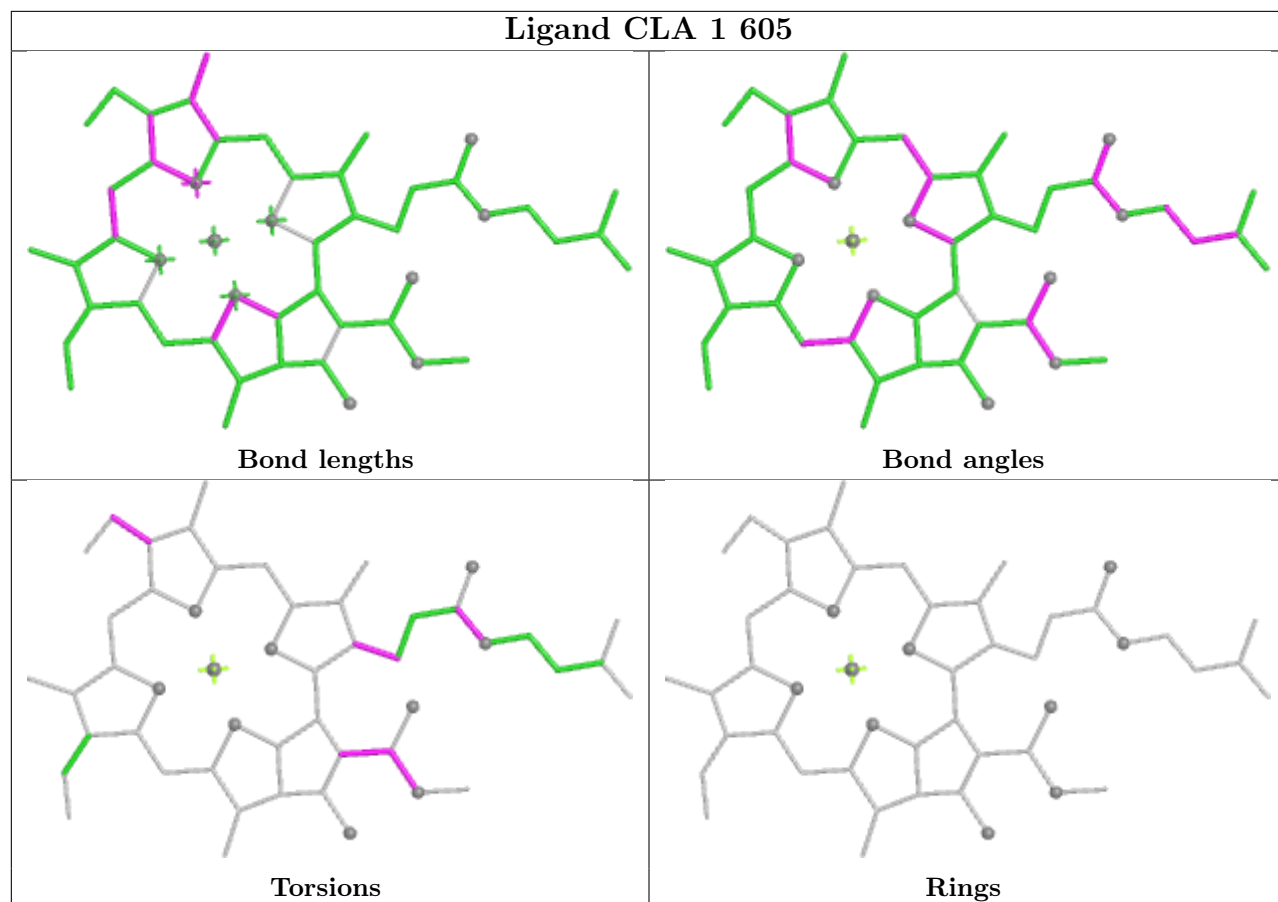


Torsions

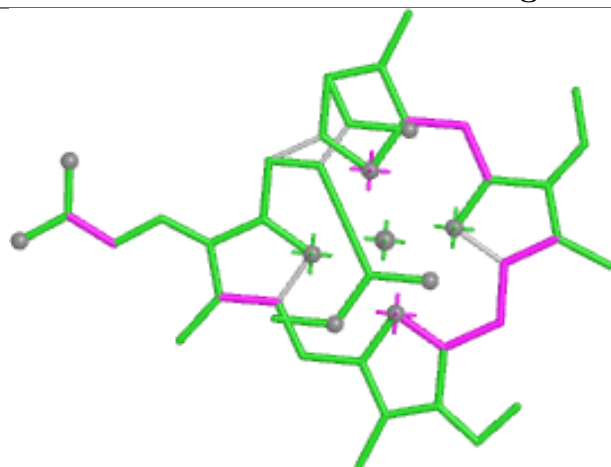


Rings

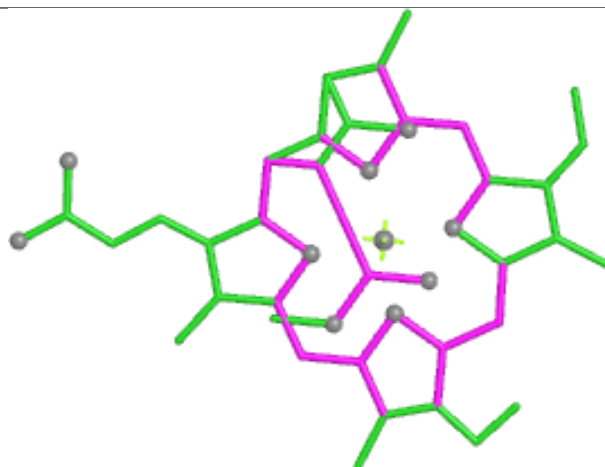
Ligand CLA 1 605



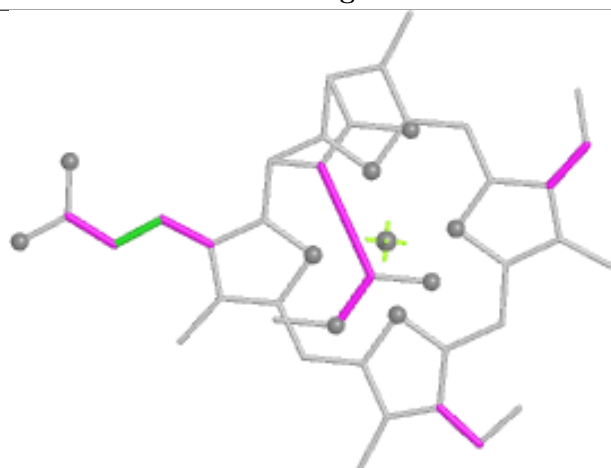
Ligand KC2 1 610



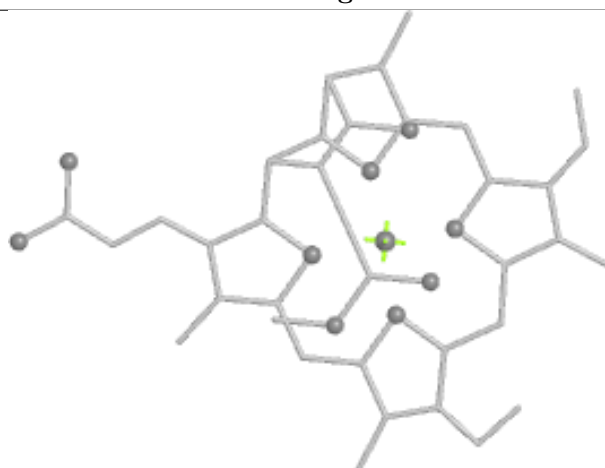
Bond lengths



Bond angles

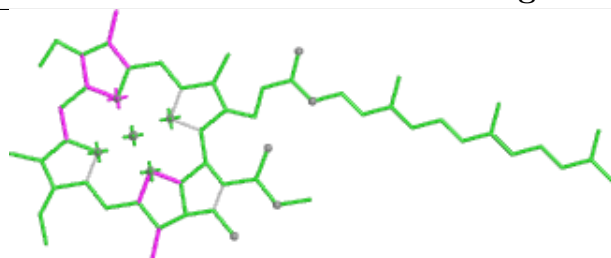


Torsions

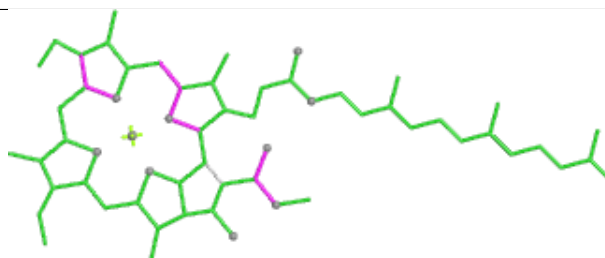


Rings

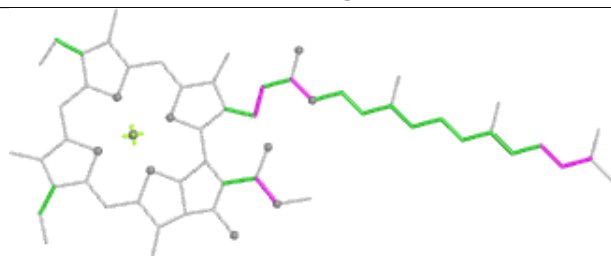
Ligand CLA 9 607



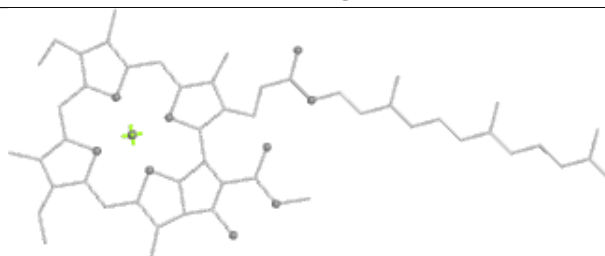
Bond lengths



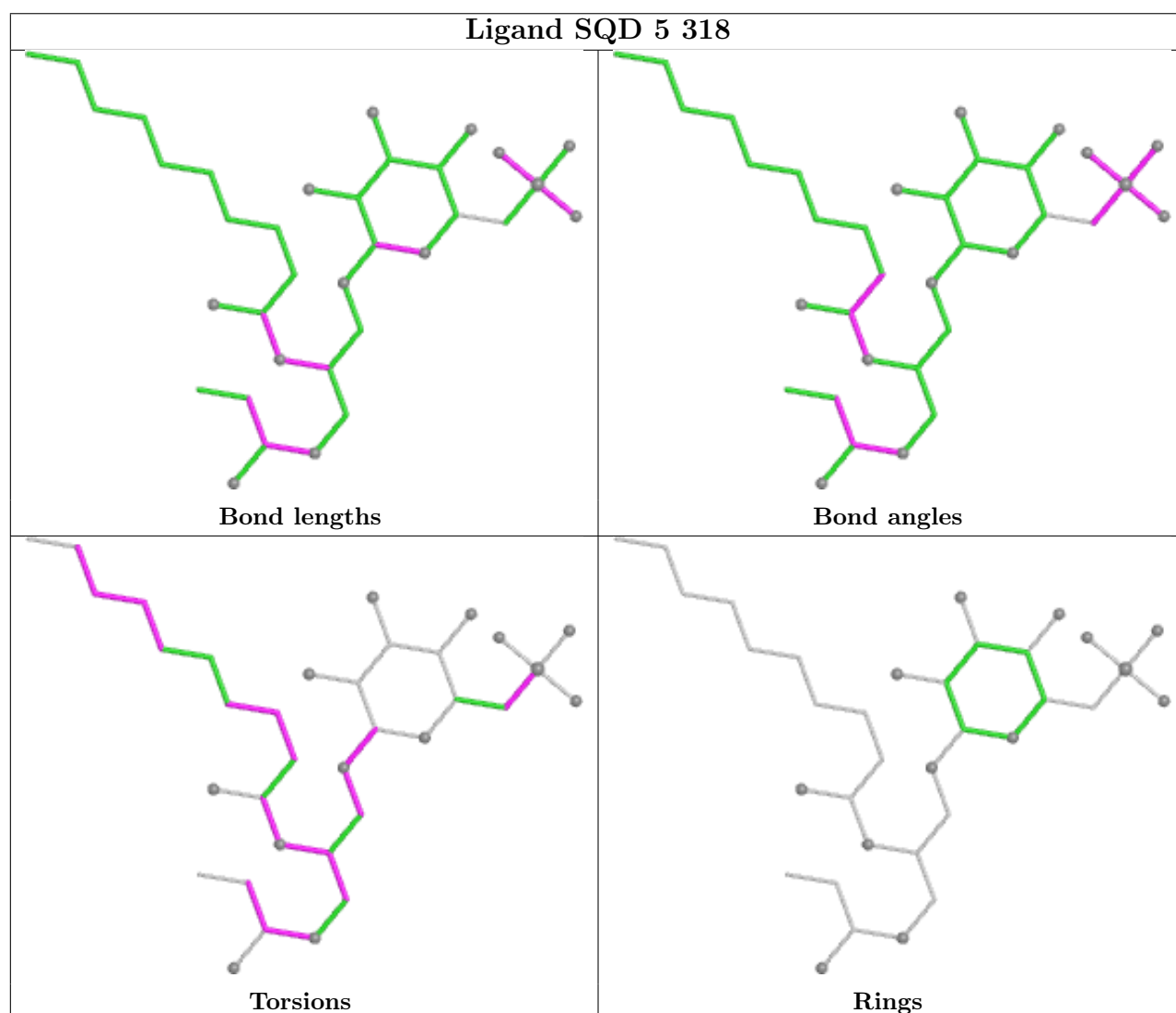
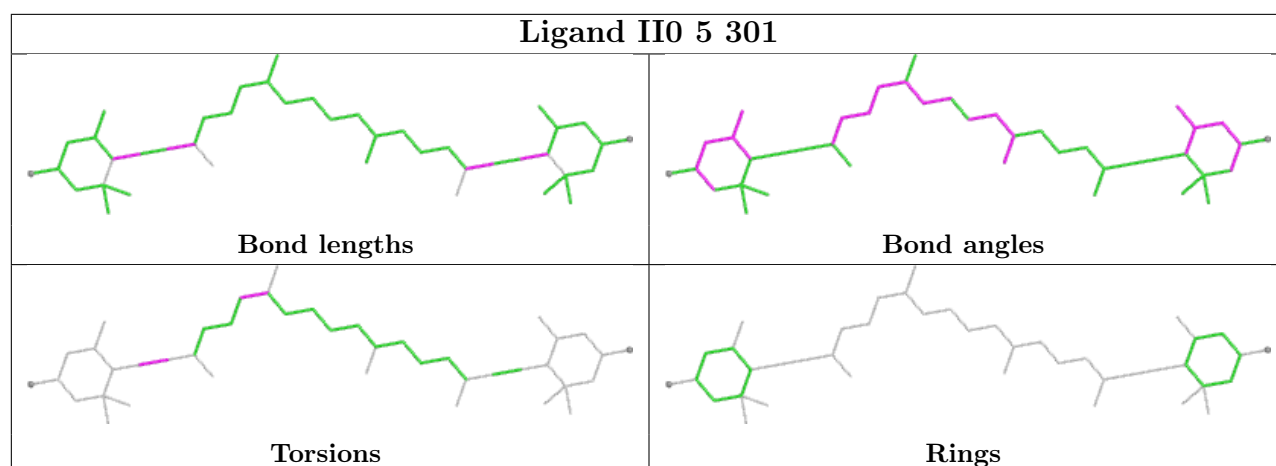
Bond angles

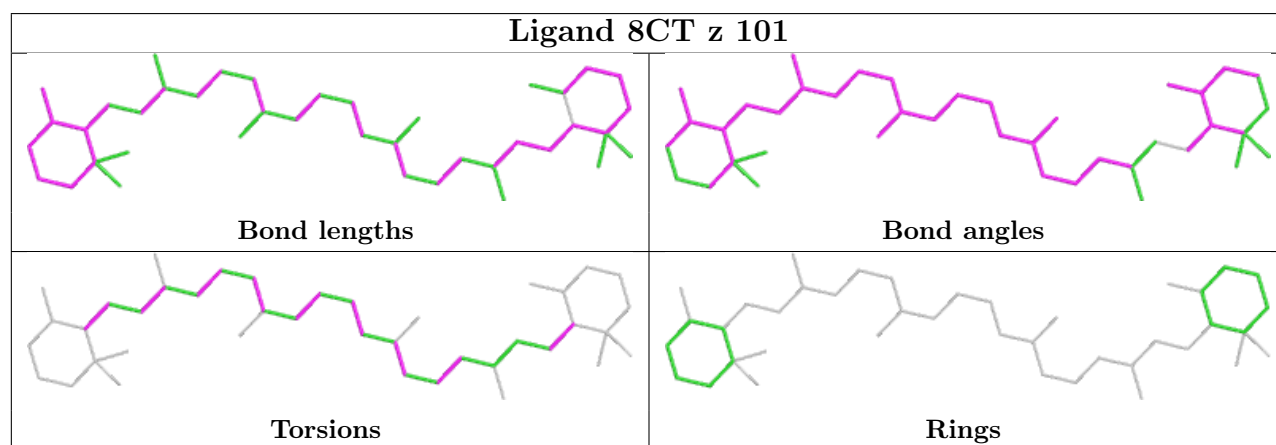
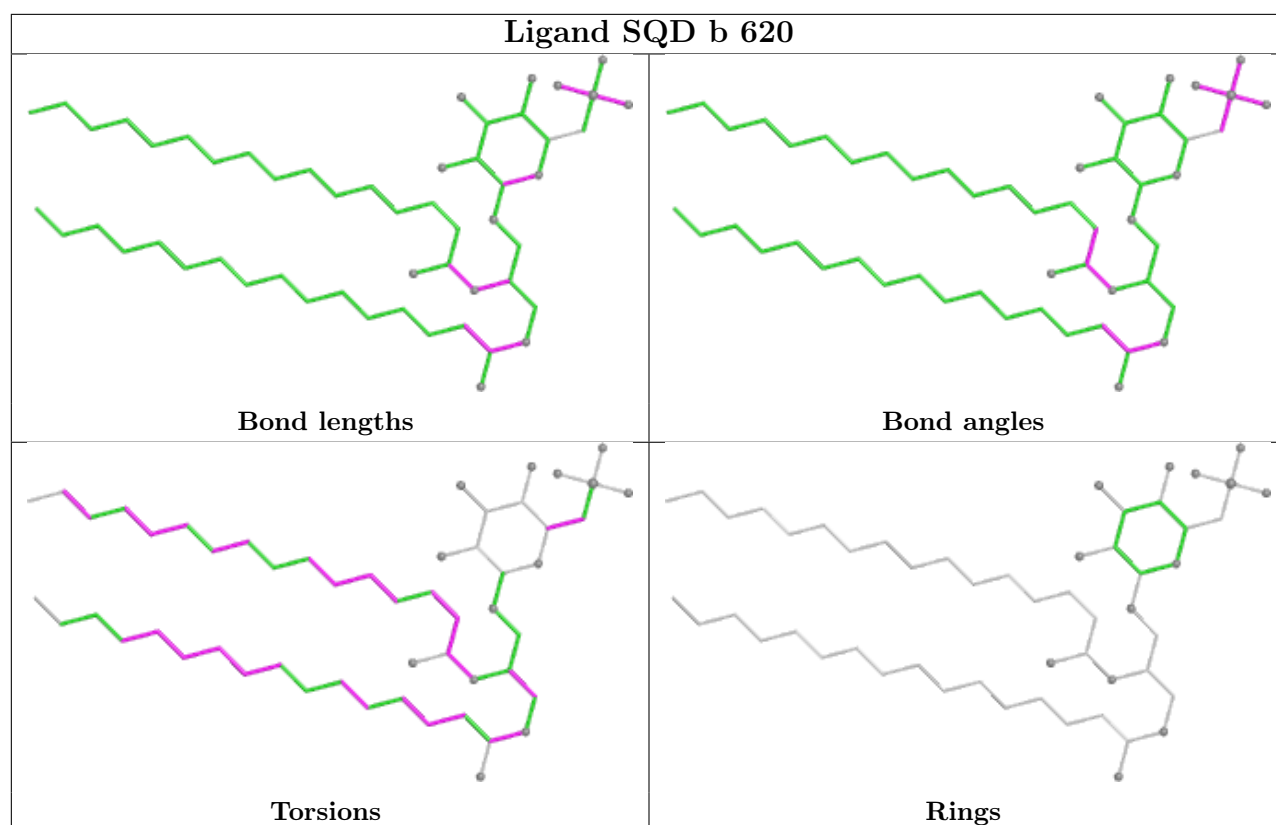


Torsions

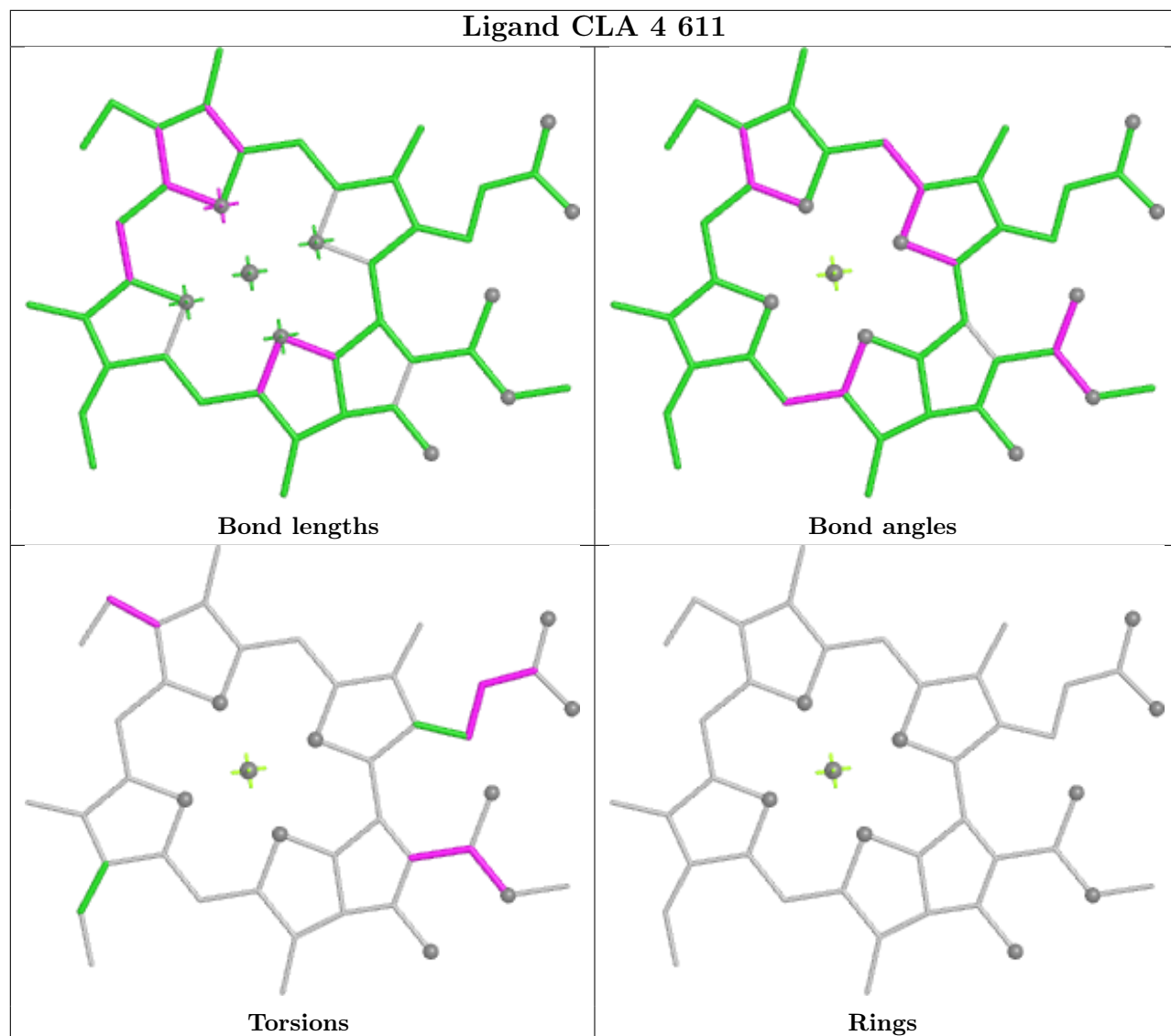


Rings

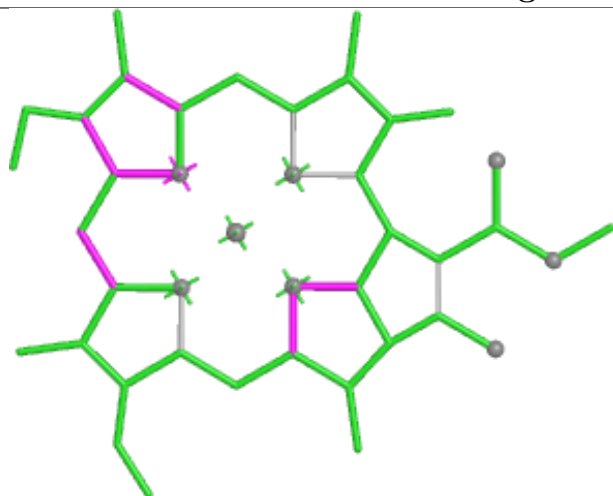




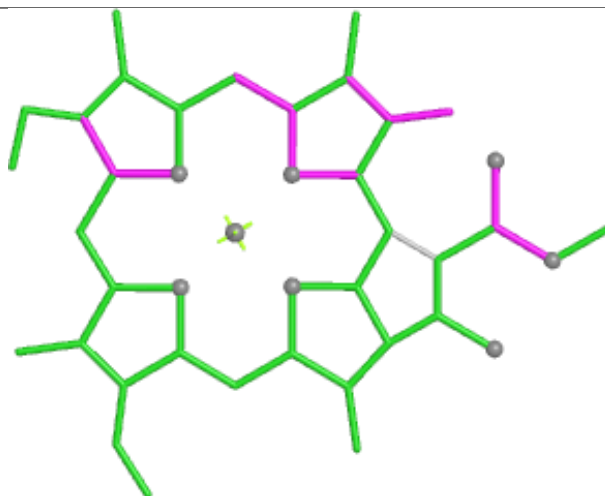
Ligand CLA 4 611



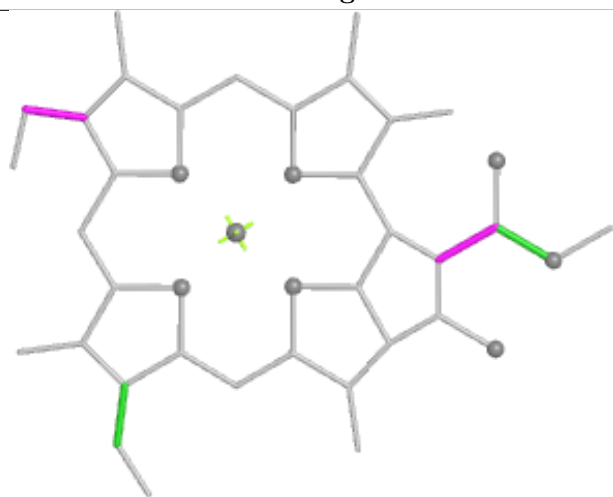
Ligand CLA 6 608



Bond lengths



Bond angles

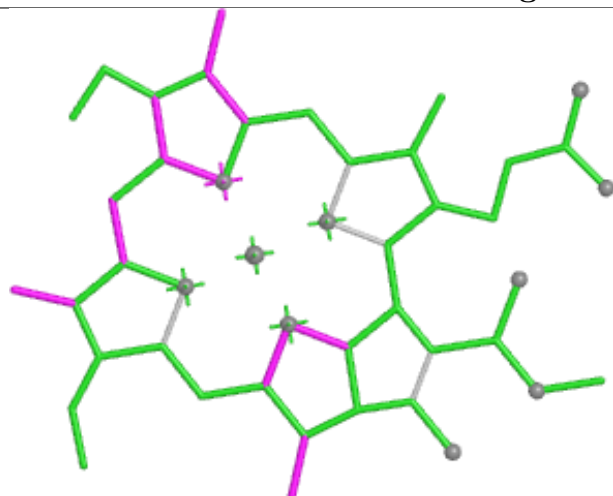


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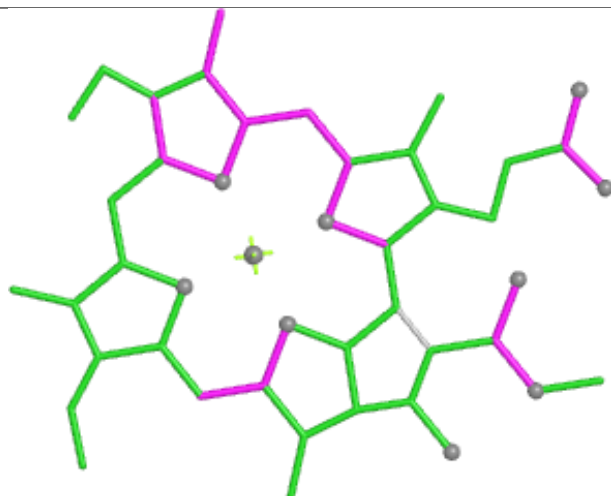


Rings

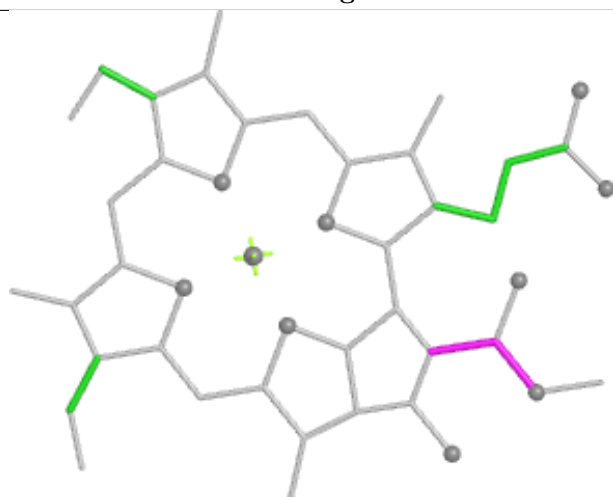
Ligand CLA c 506



Bond lengths



Bond angles

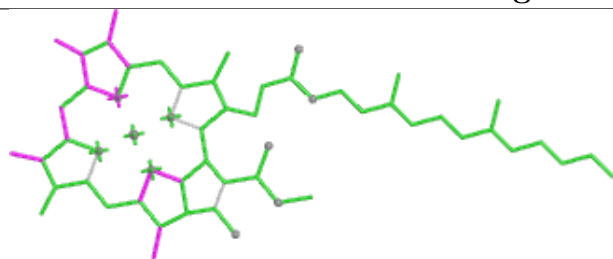


Torsions

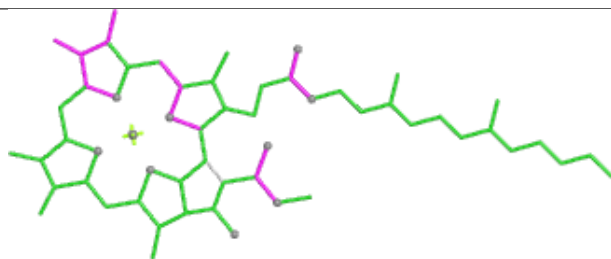


Rings

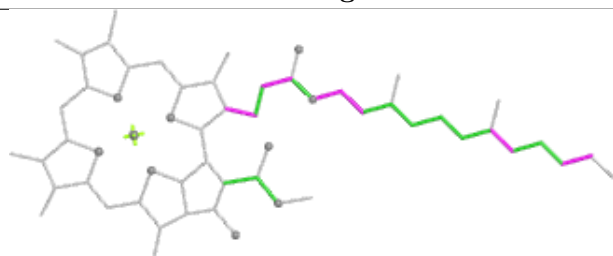
Ligand CLA D 403



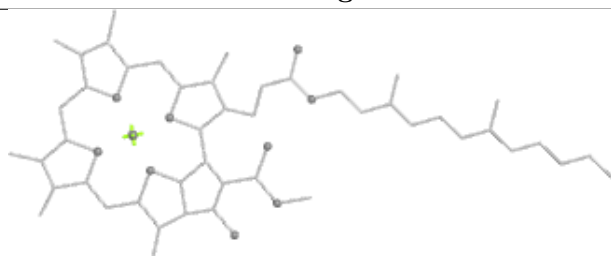
Bond lengths



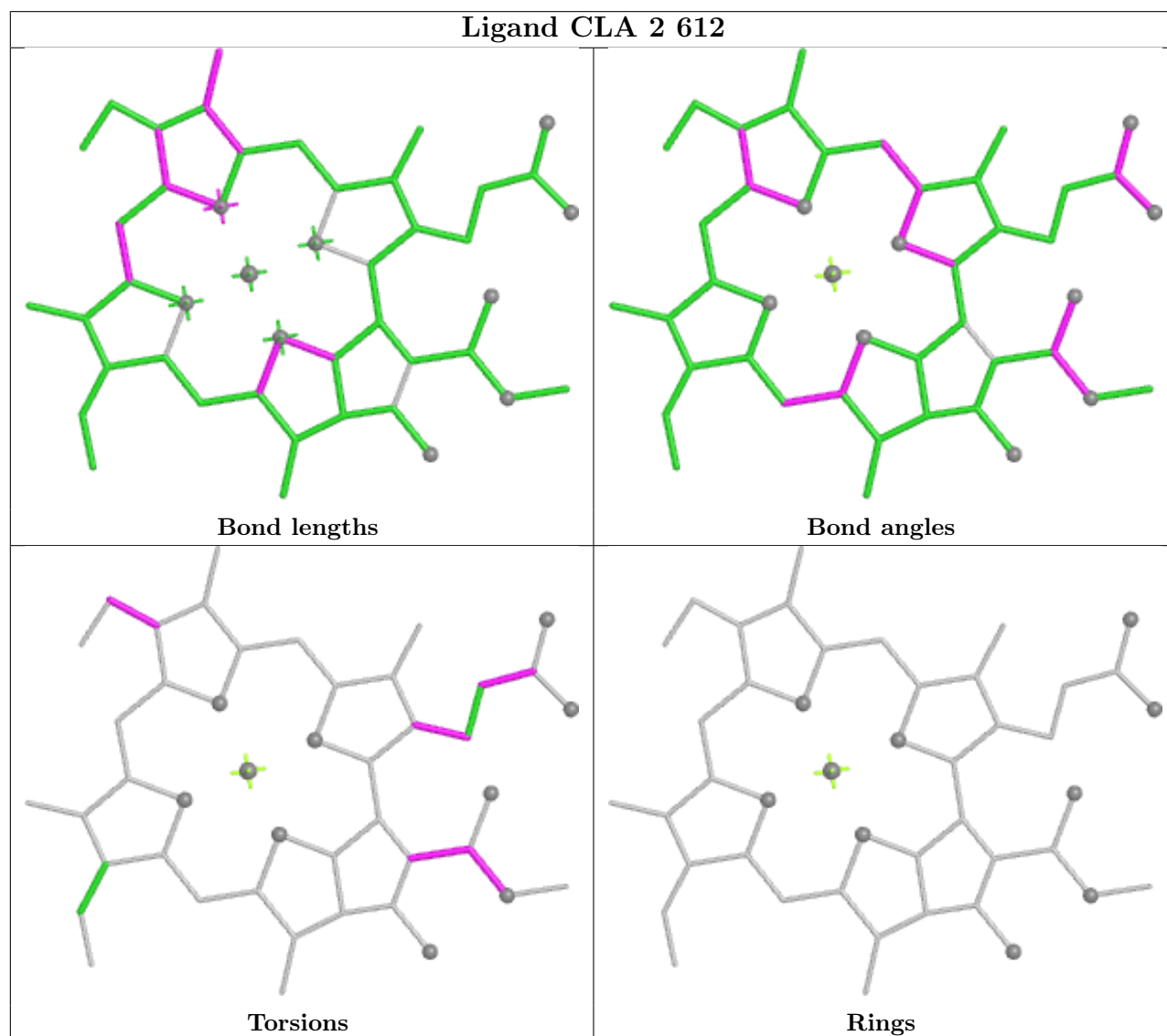
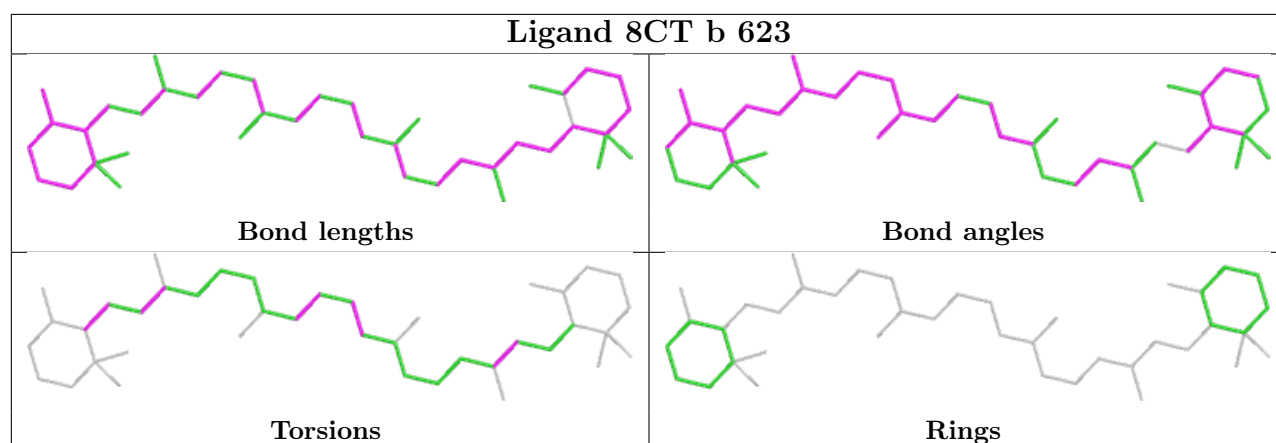
Bond angles

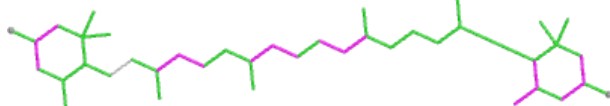
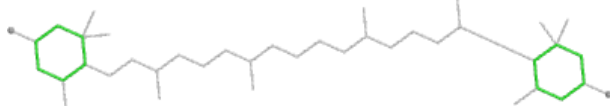
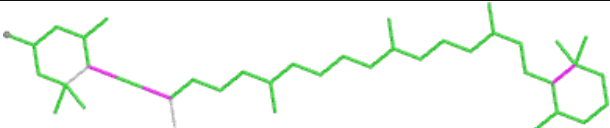
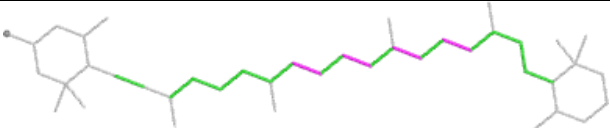
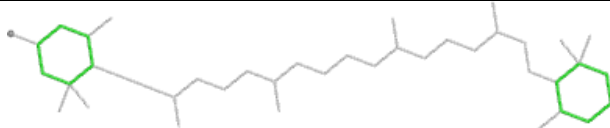
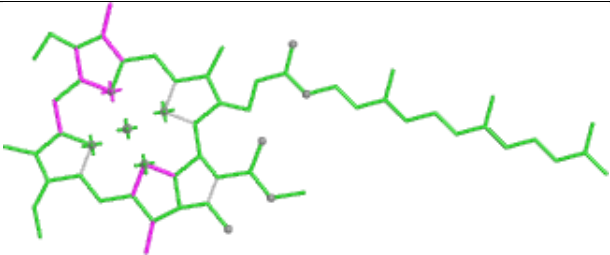
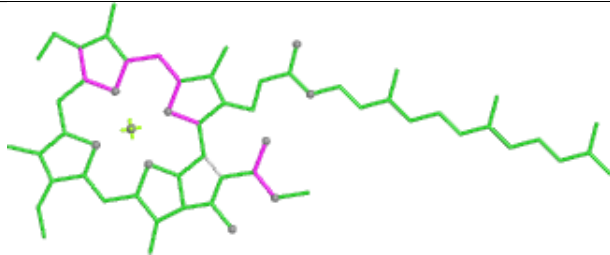
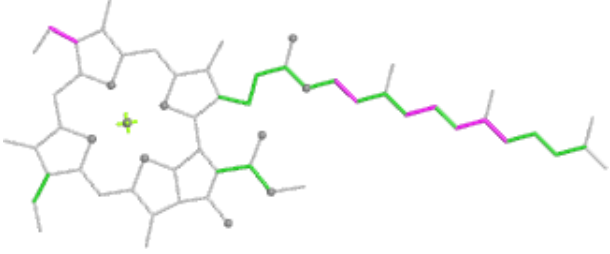
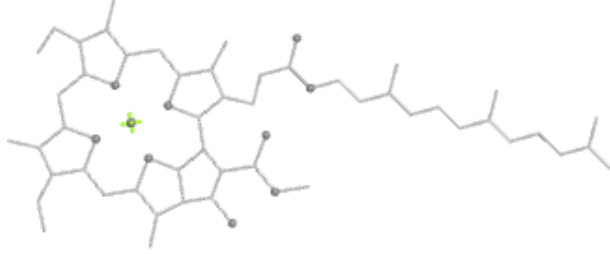


Torsions

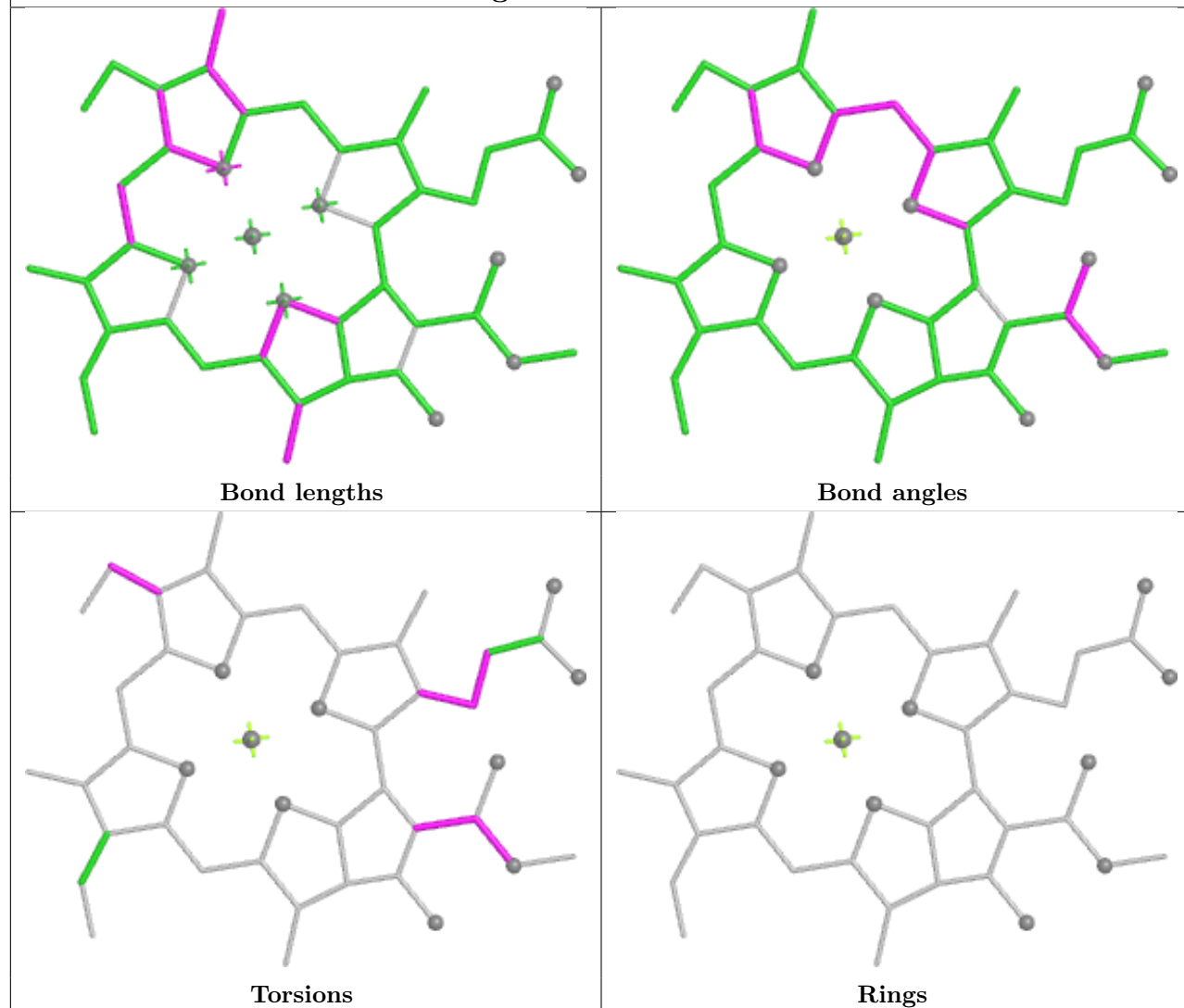


Rings

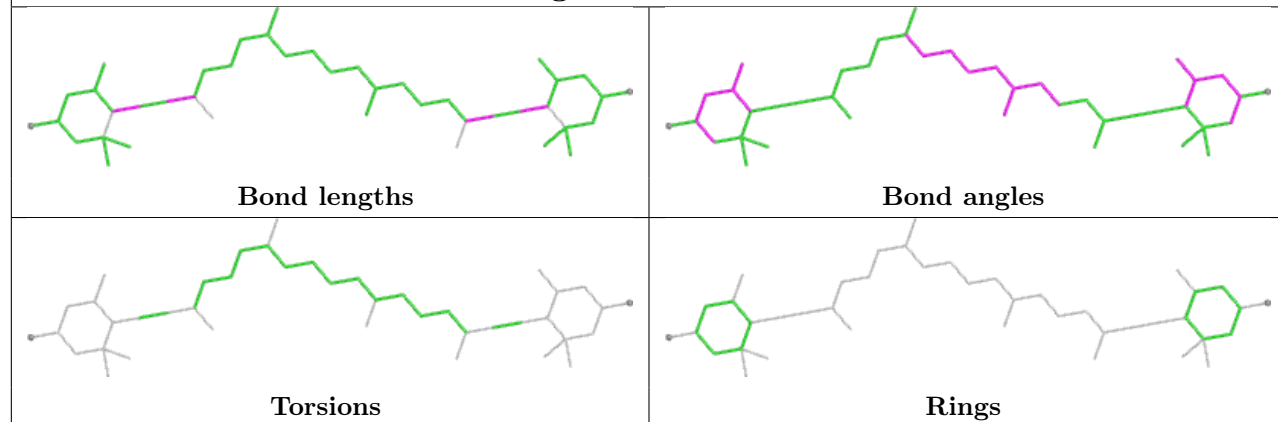


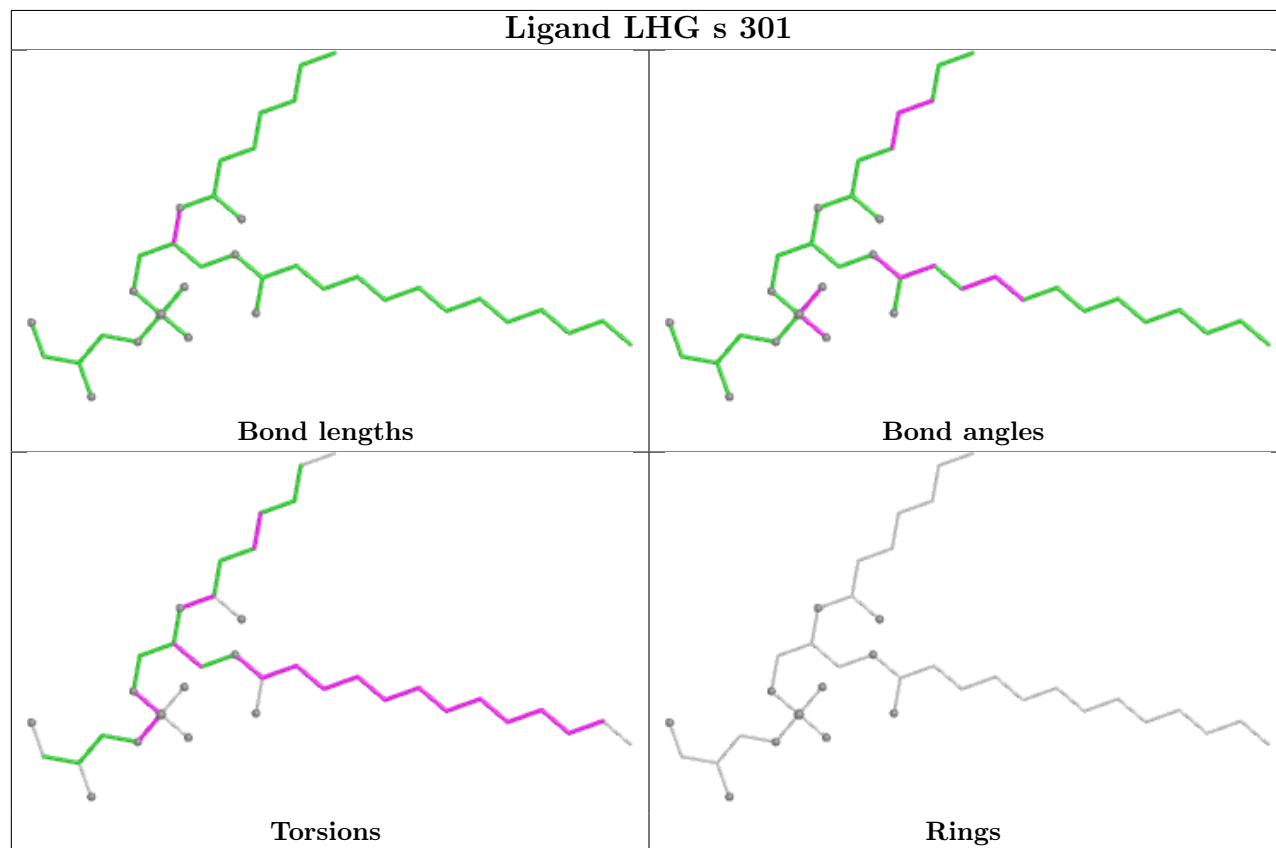
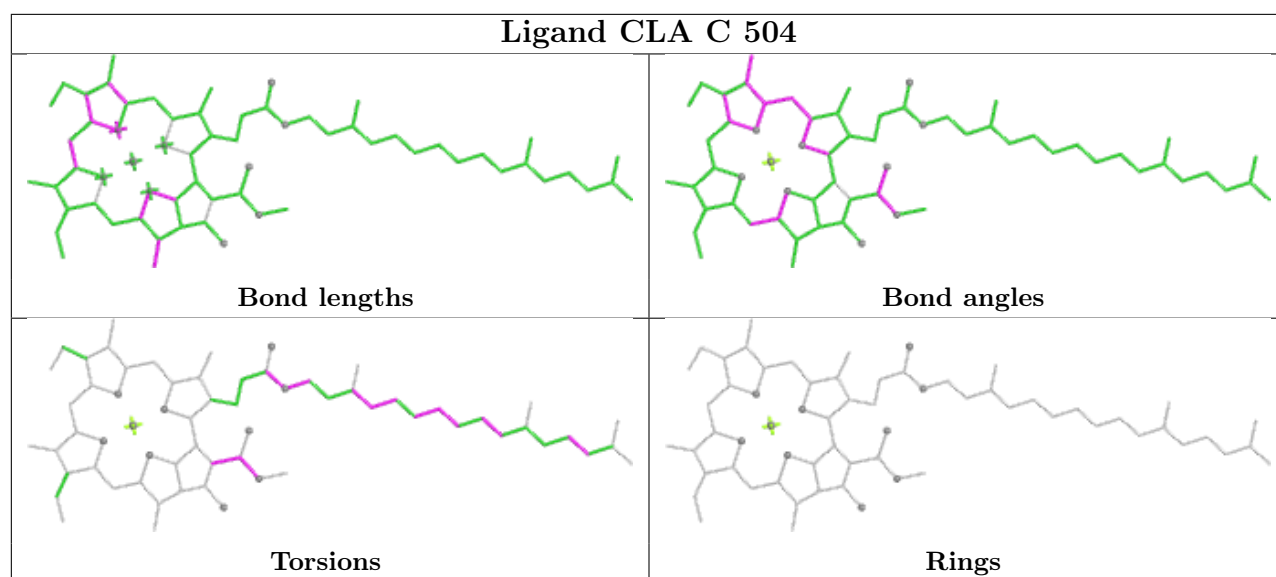
Ligand II3 1 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 9 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

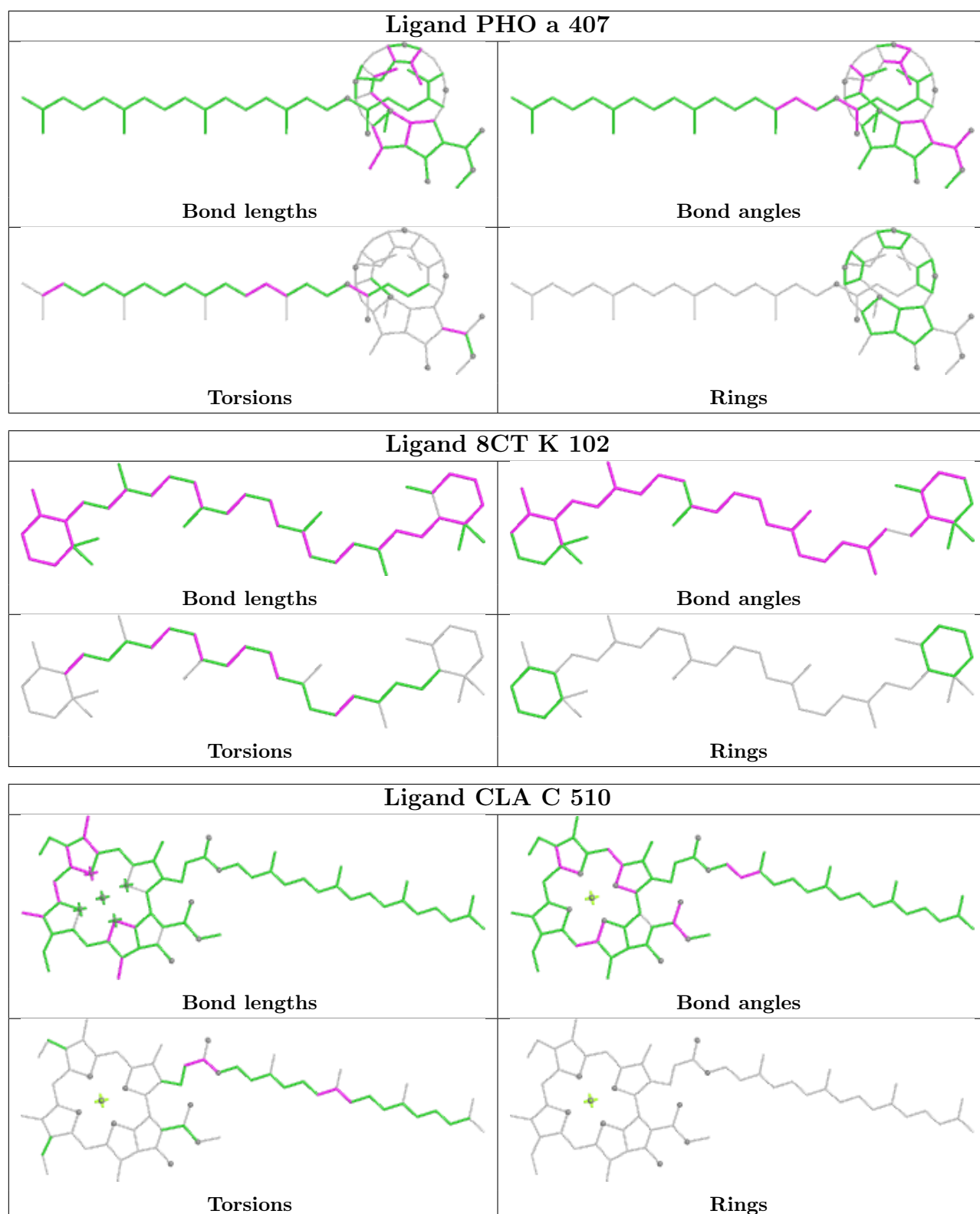
Ligand CLA G 101

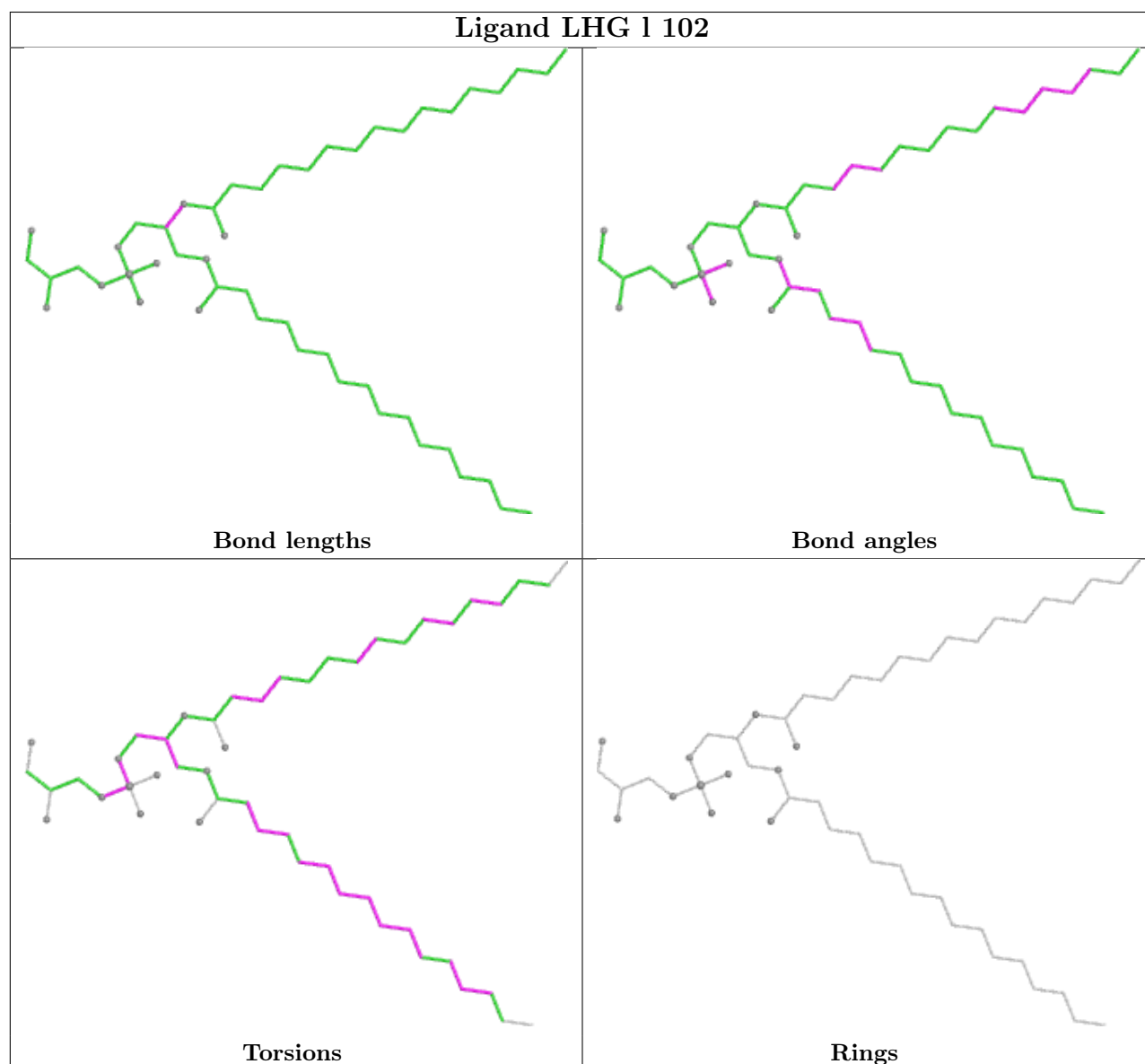
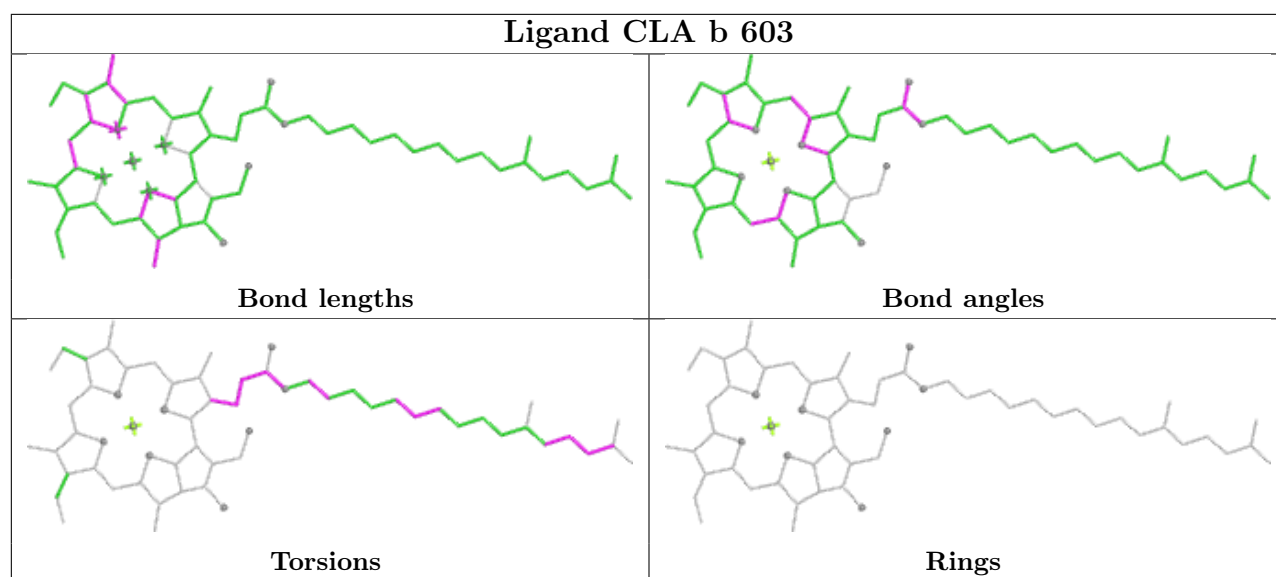


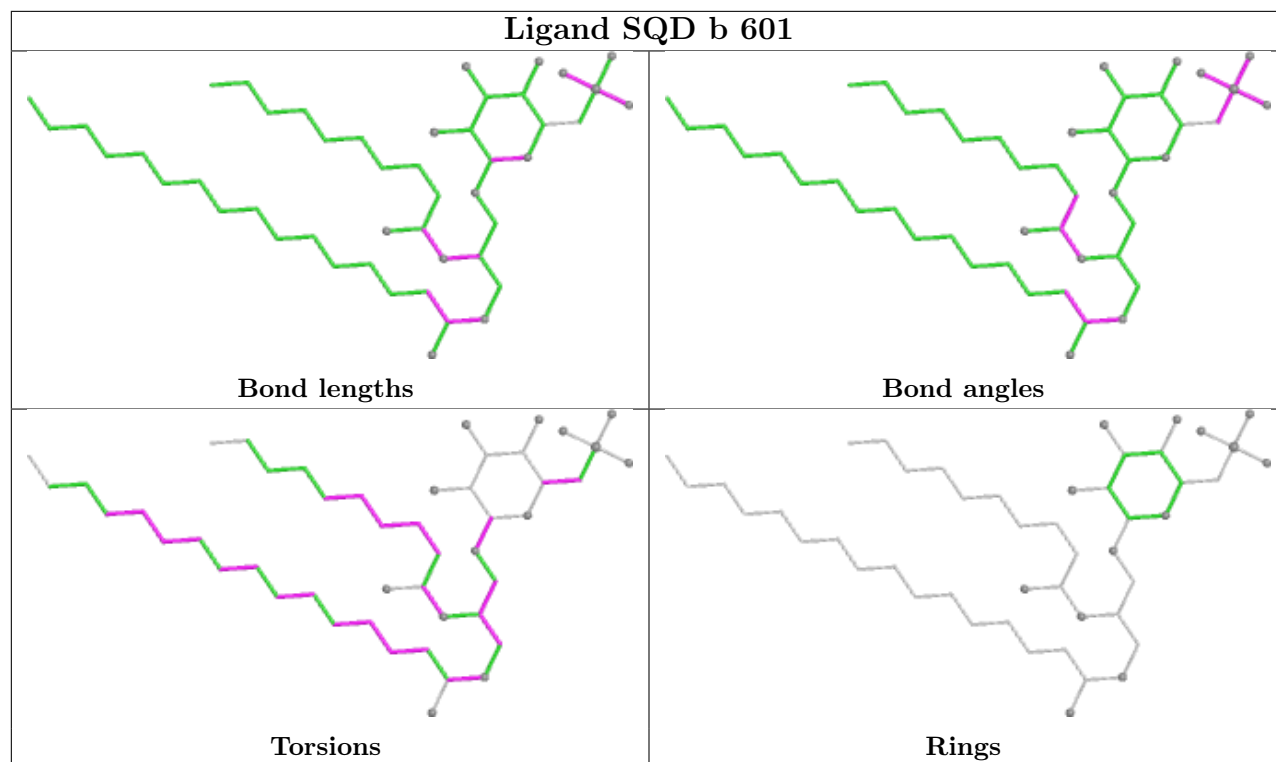
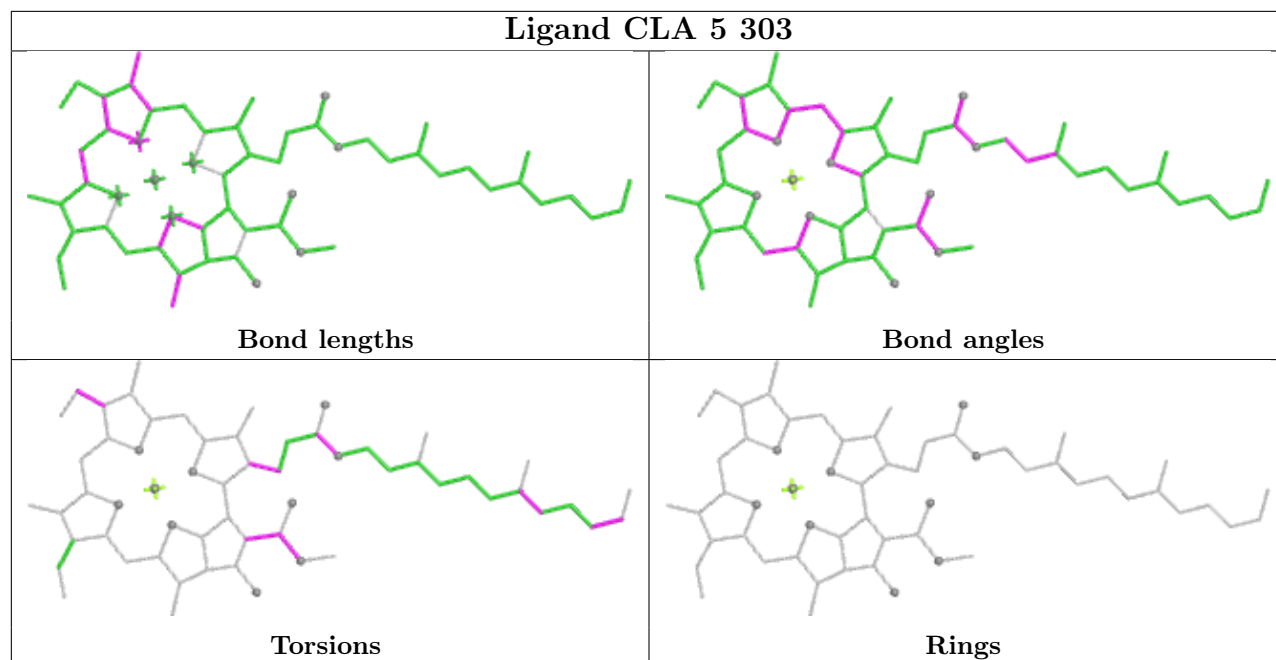
Ligand II0 2 614

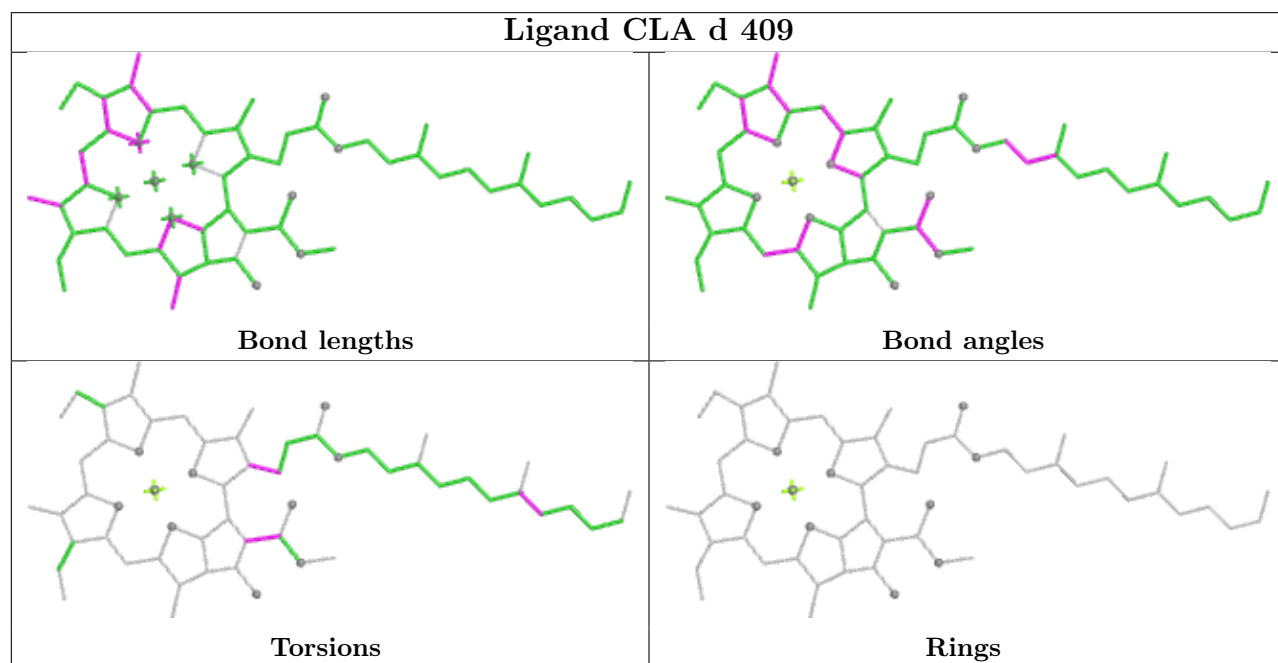
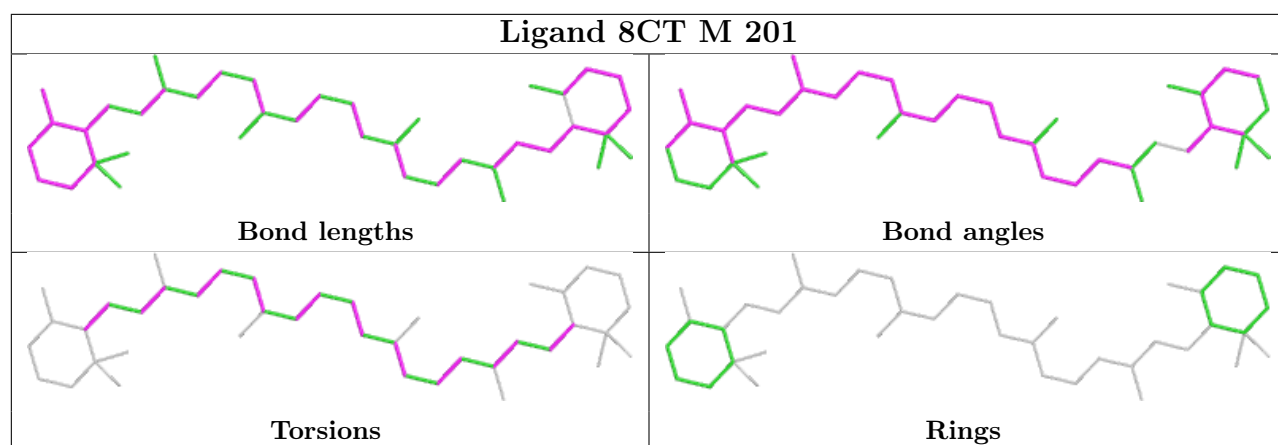


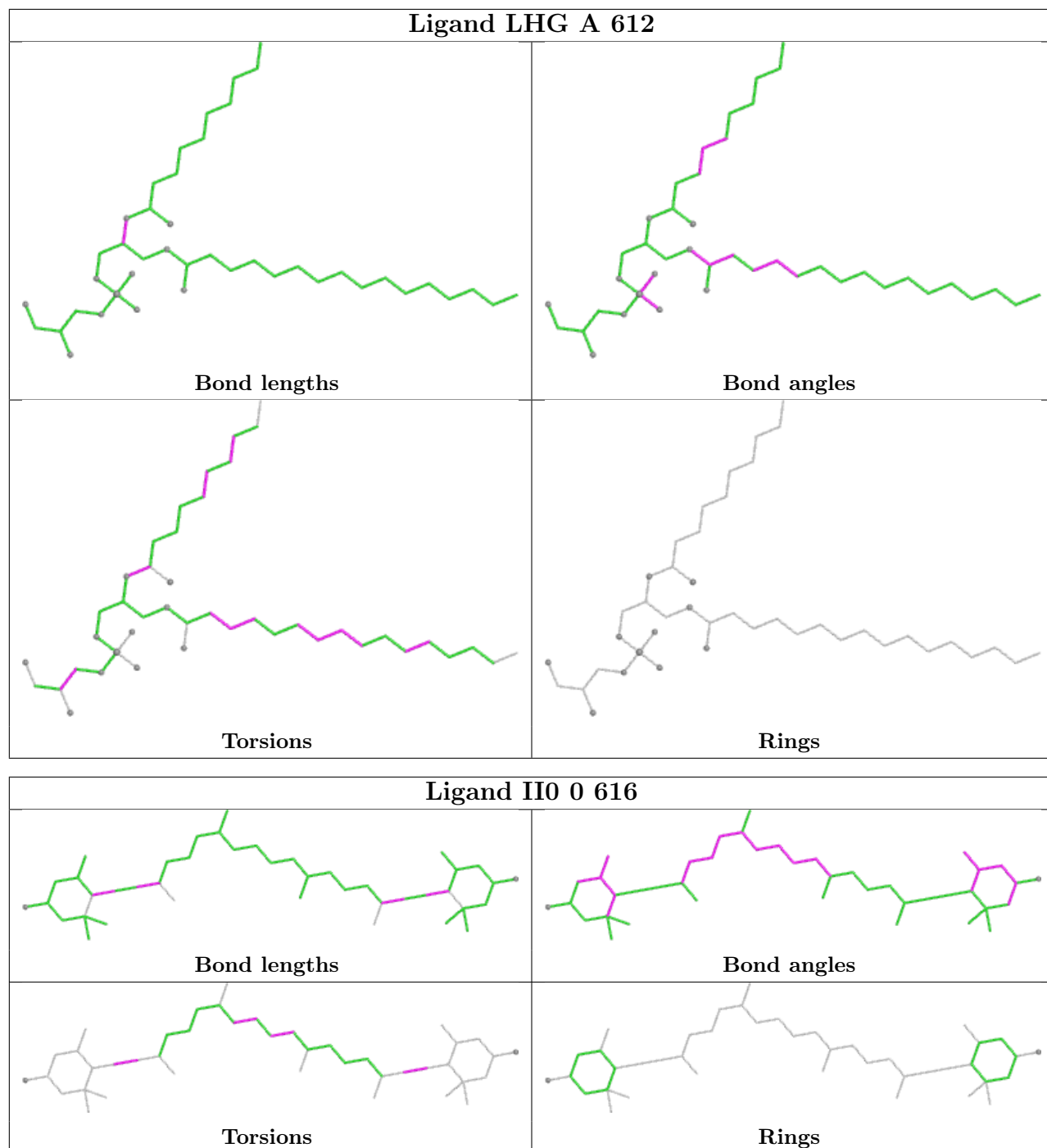




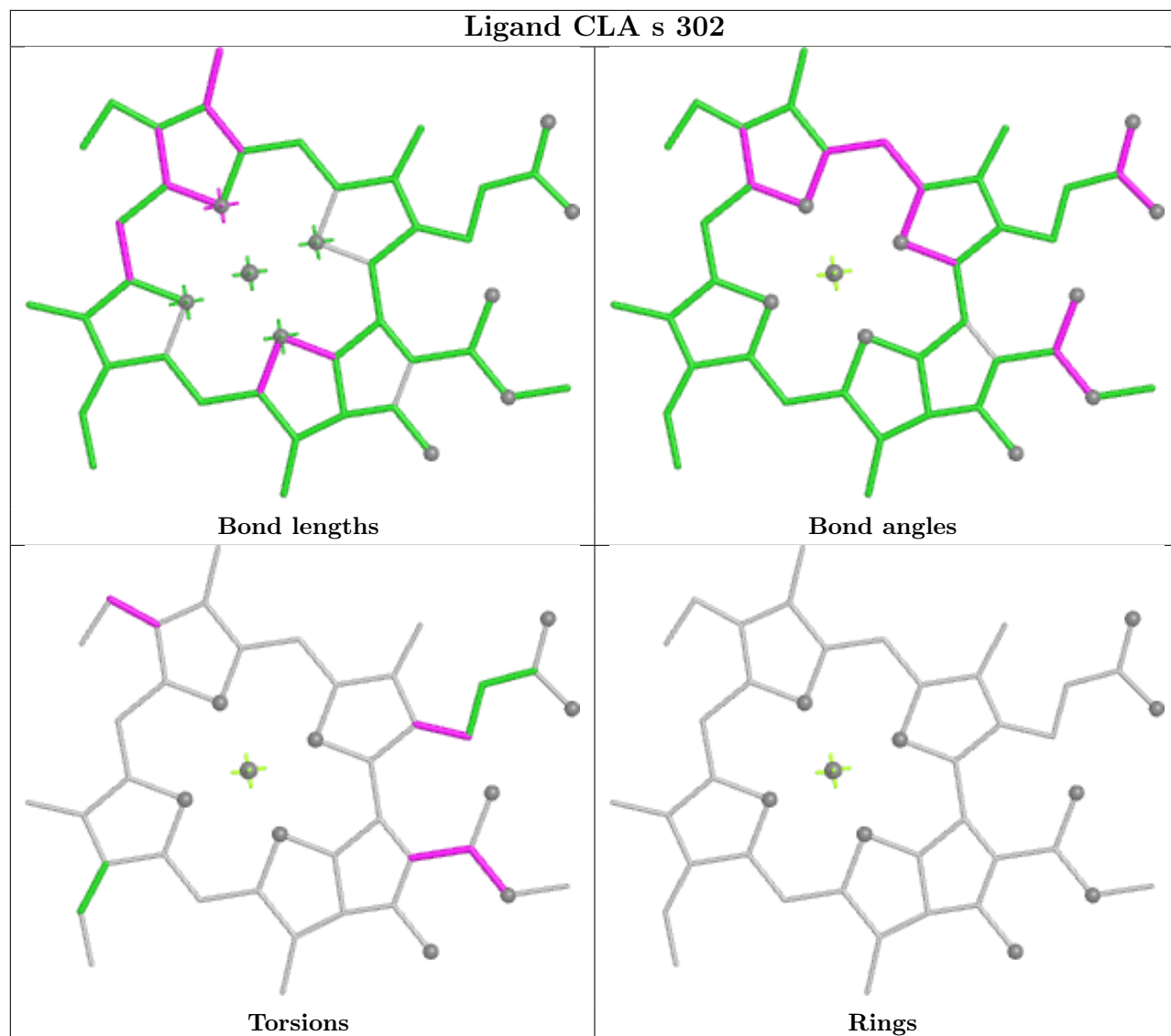




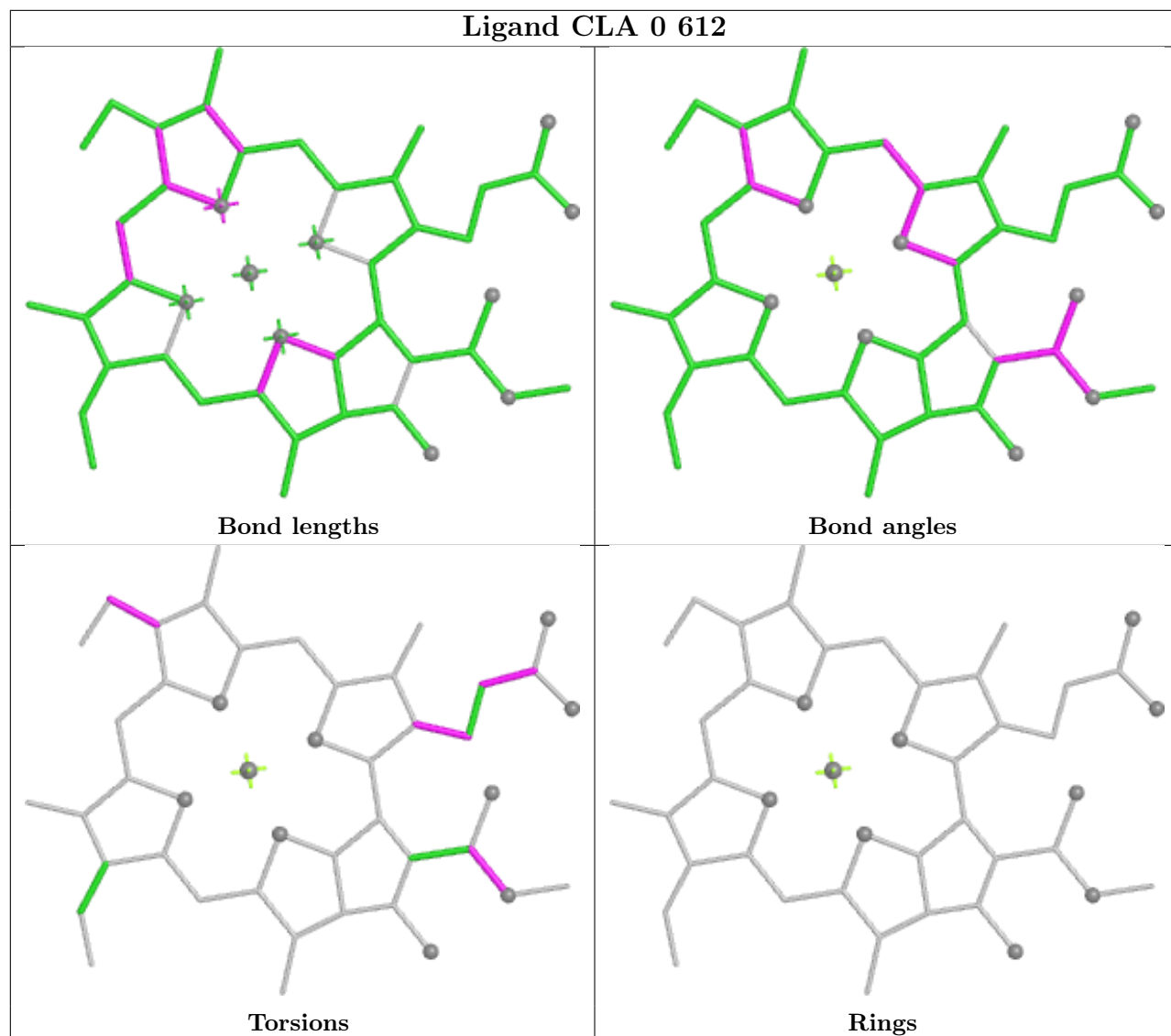


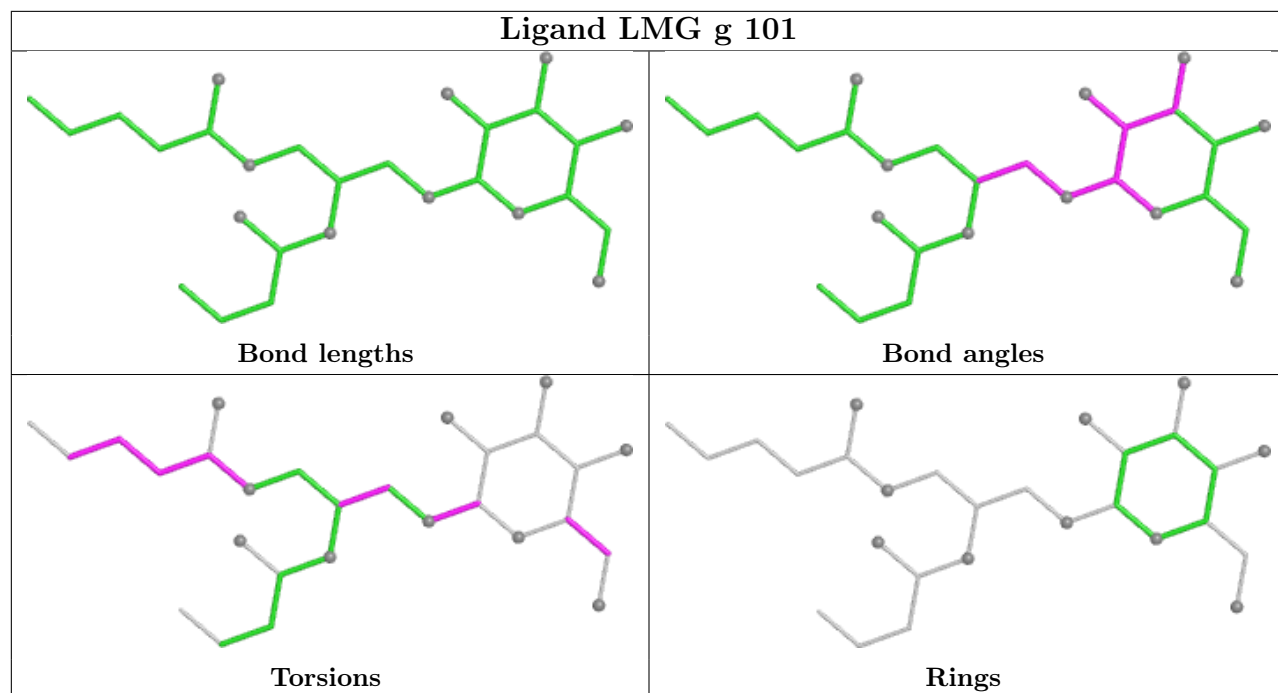


Ligand CLA s 302

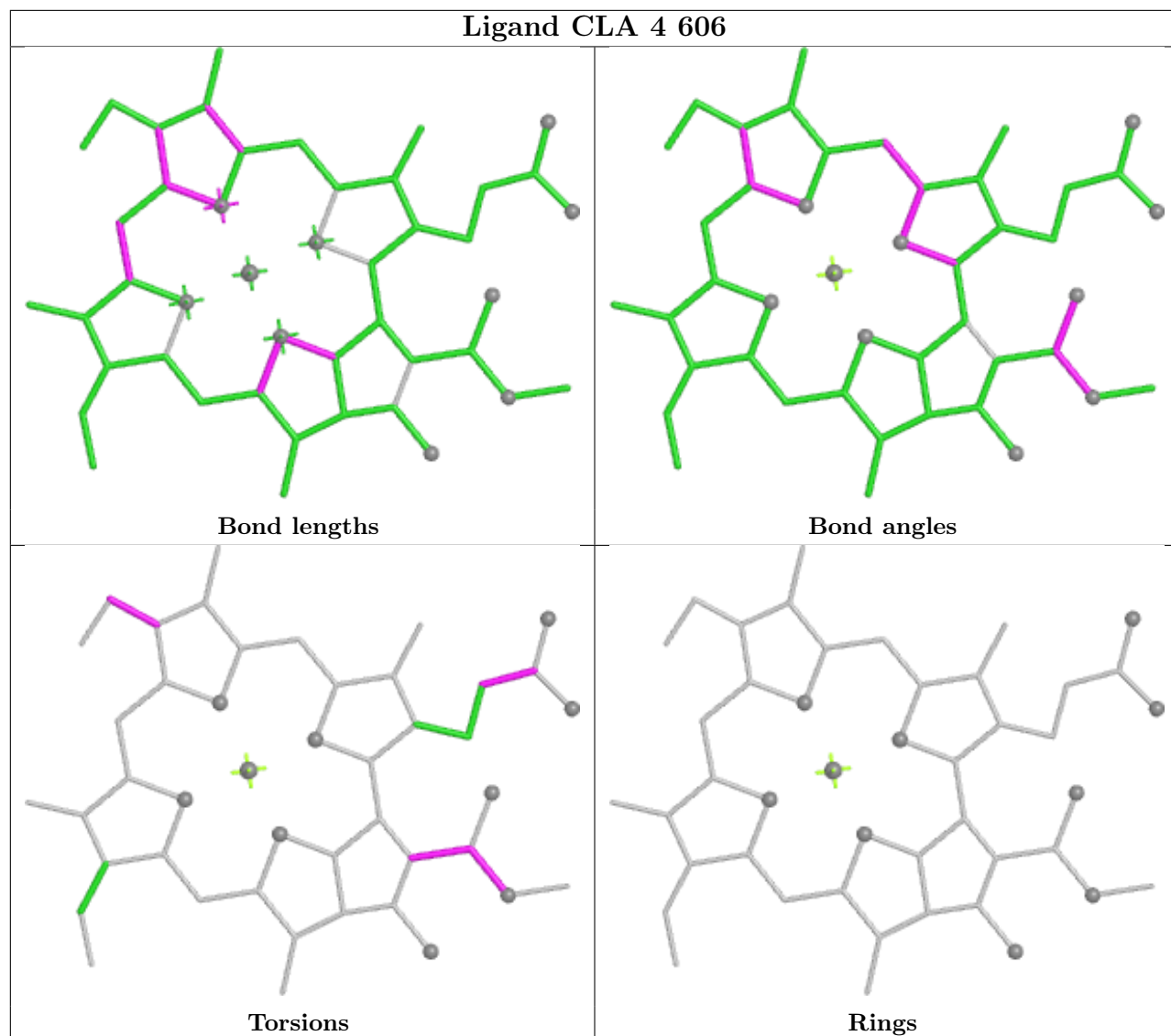


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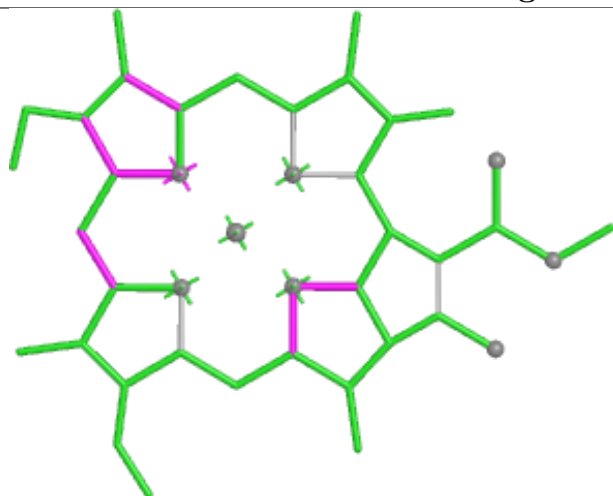




Ligand CLA 4 606



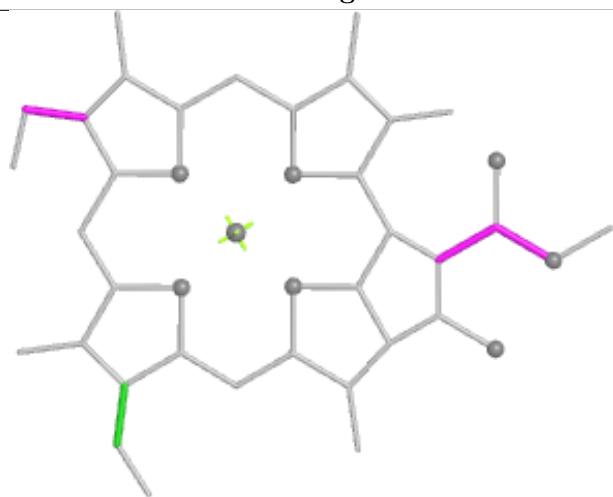
Ligand CLA 5 310



Bond lengths



Bond angles

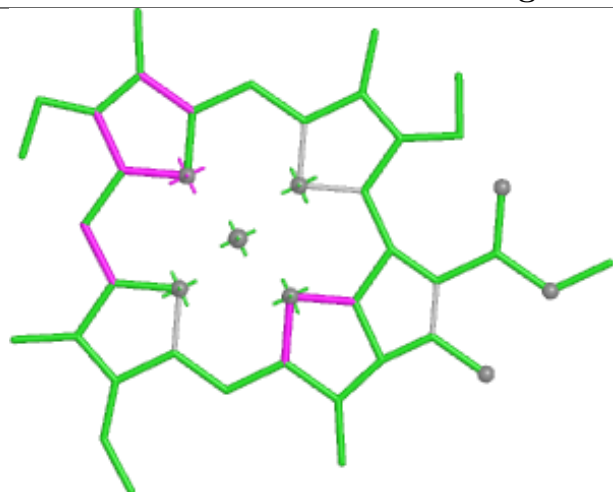


Torsions

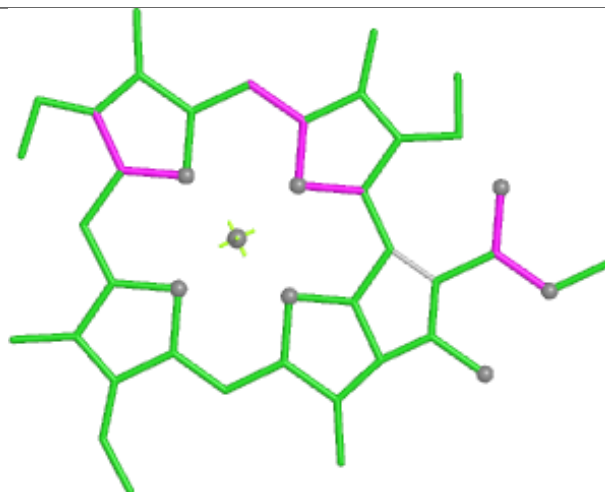


Rings

Ligand CLA 0 601



Bond lengths



Bond angles

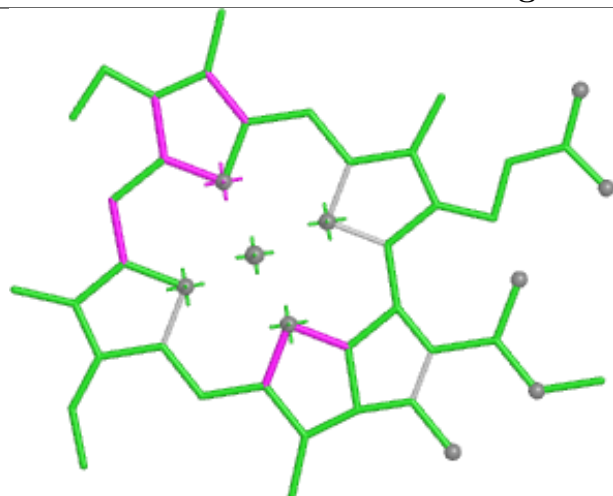


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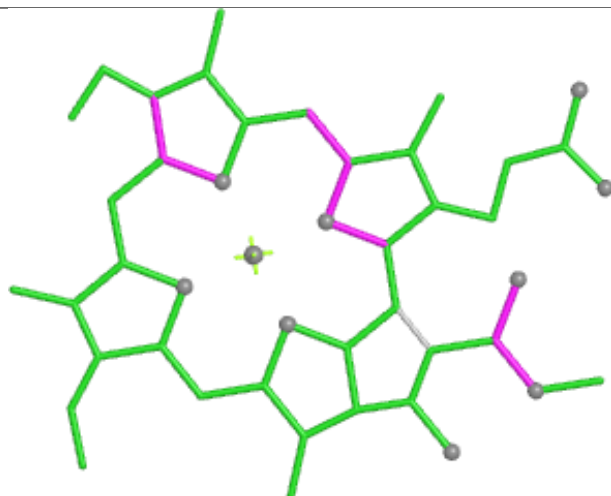


Rings

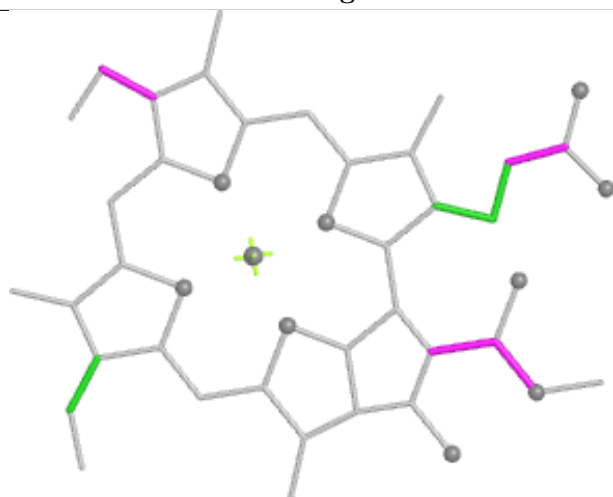
Ligand CLA 1 611



Bond lengths



Bond angles

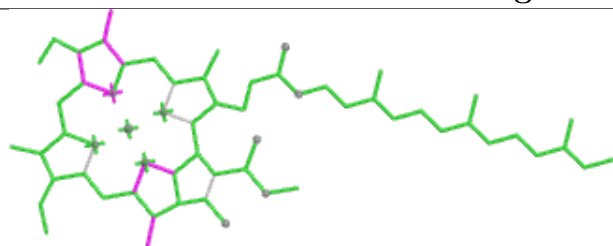


Torsions

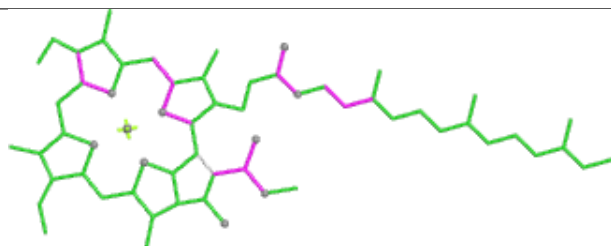


Rings

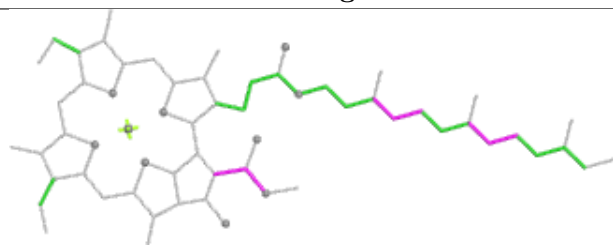
Ligand CLA B 605



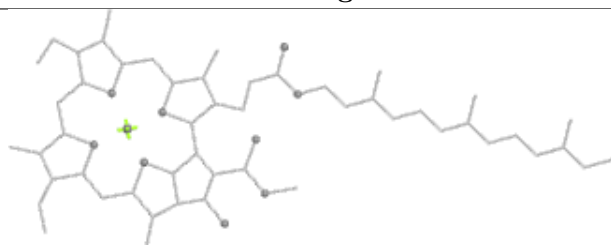
Bond lengths



Bond angles

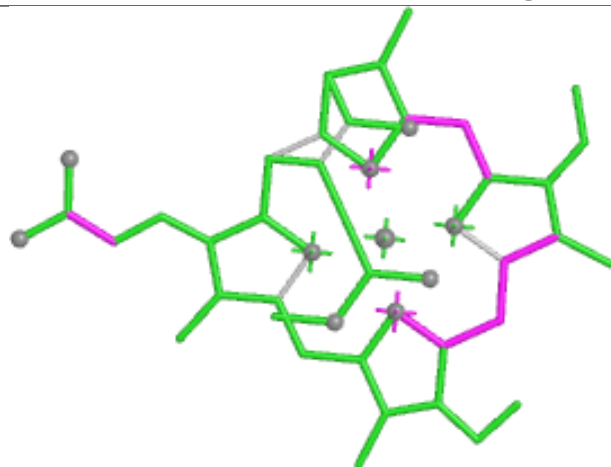


Torsions

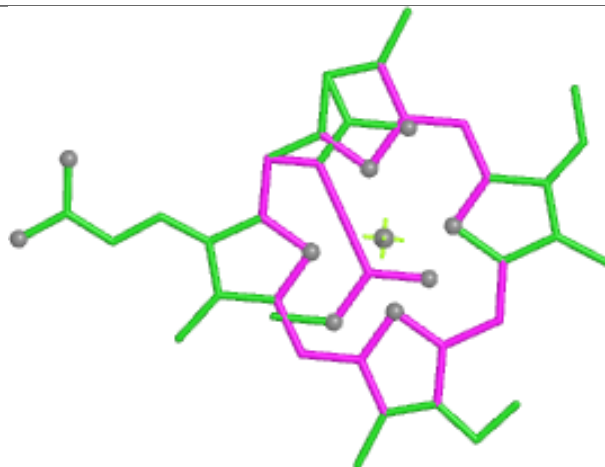


Rings

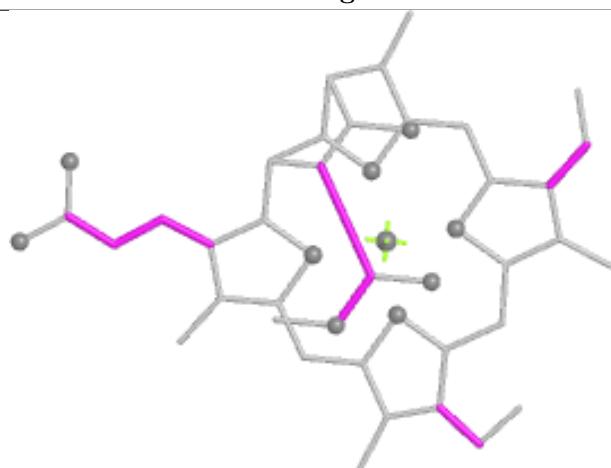
Ligand KC2 4 610



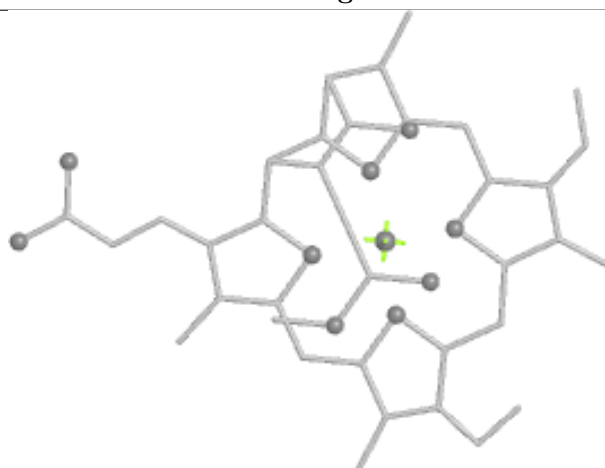
Bond lengths



Bond angles

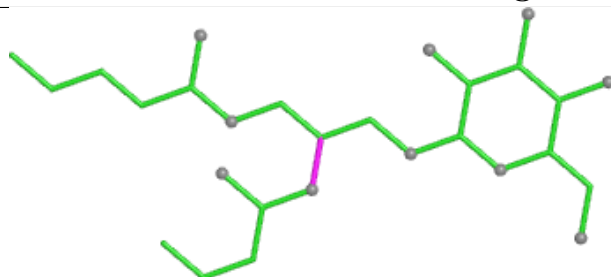


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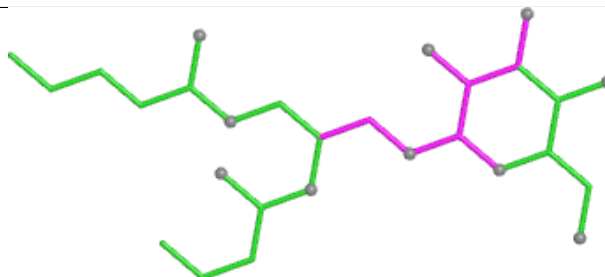


Rings

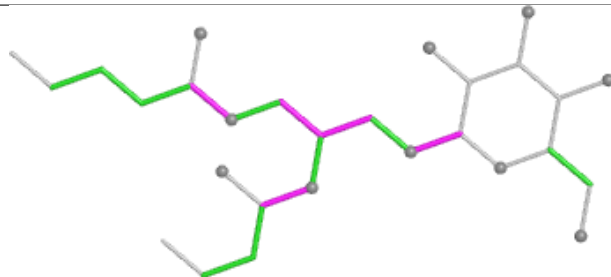
Ligand LMG 6 616



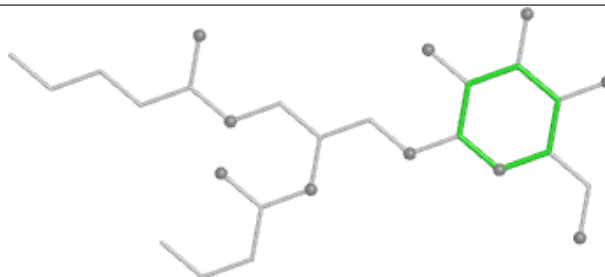
Bond lengths



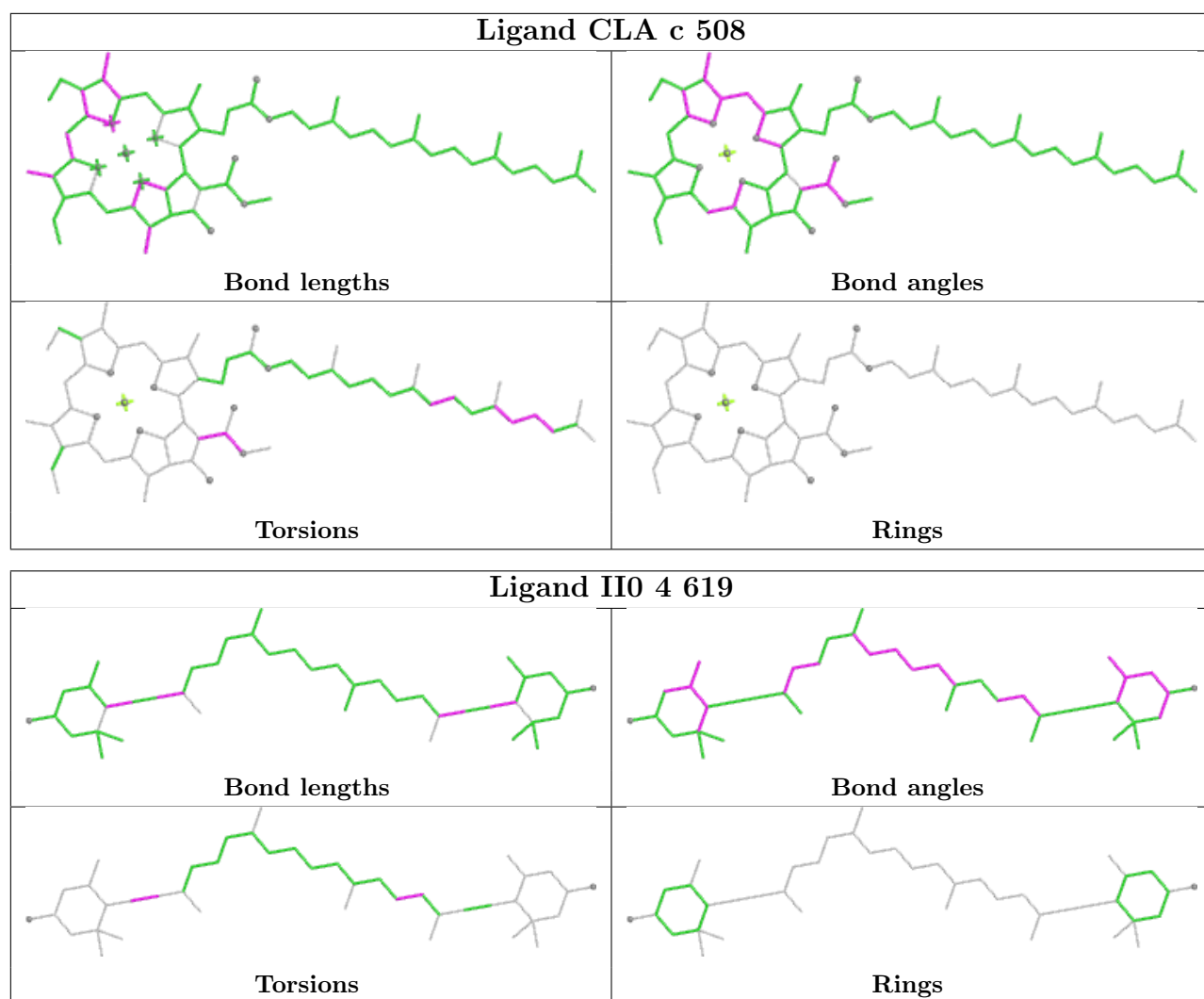
Bond angles



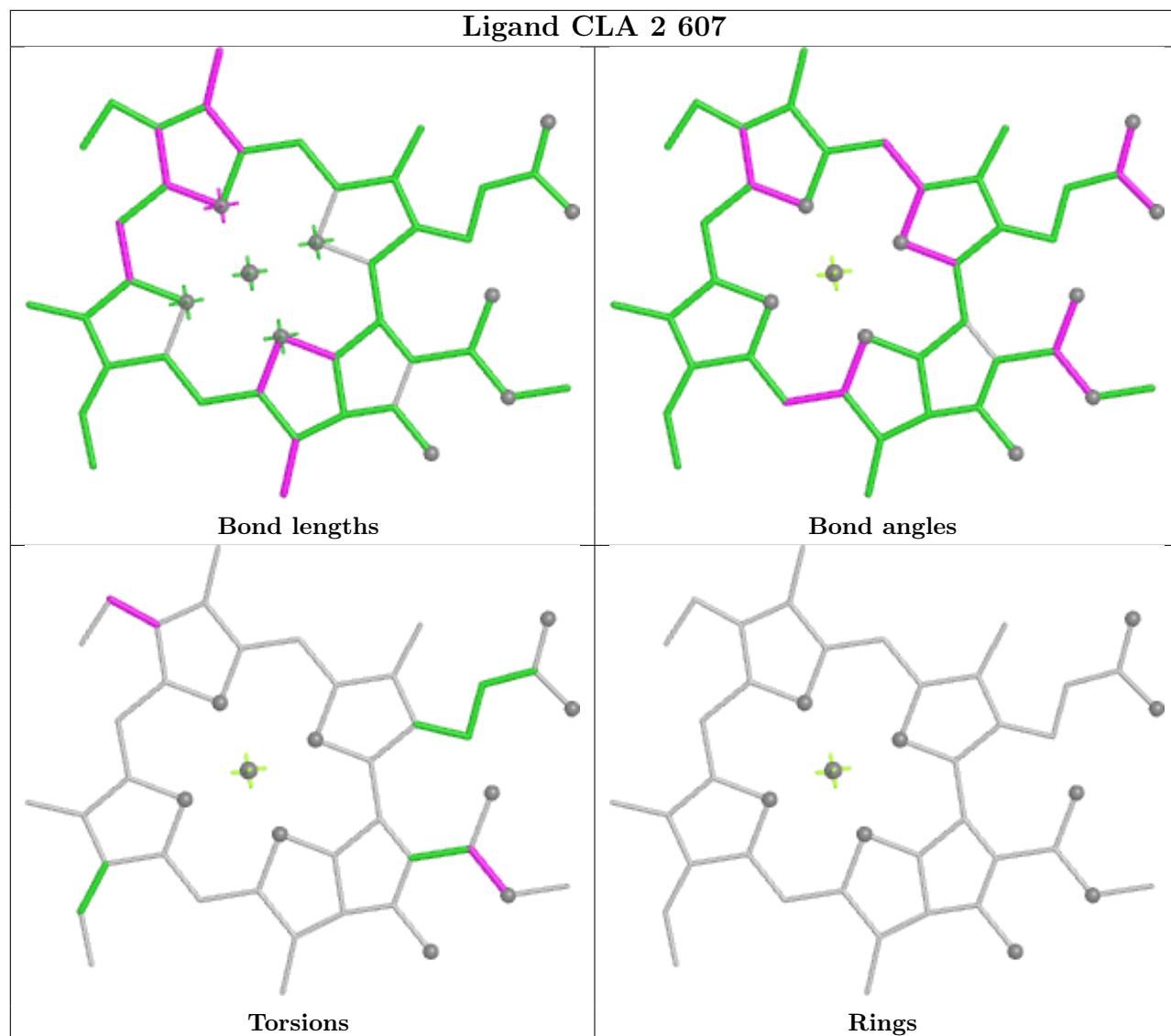
Torsions



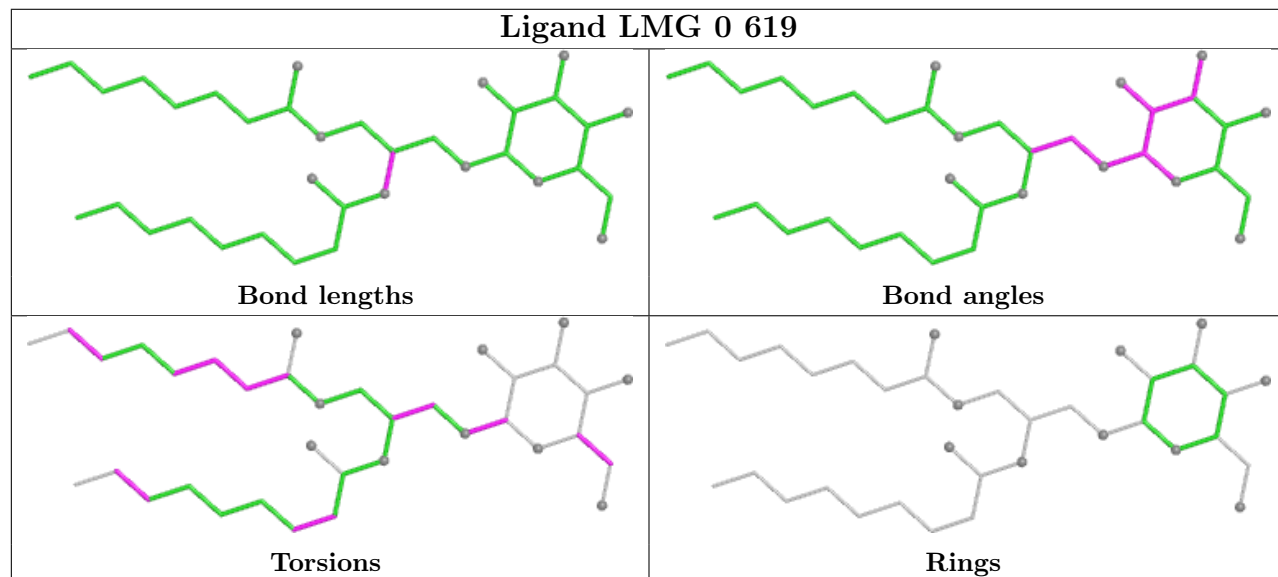
Rings

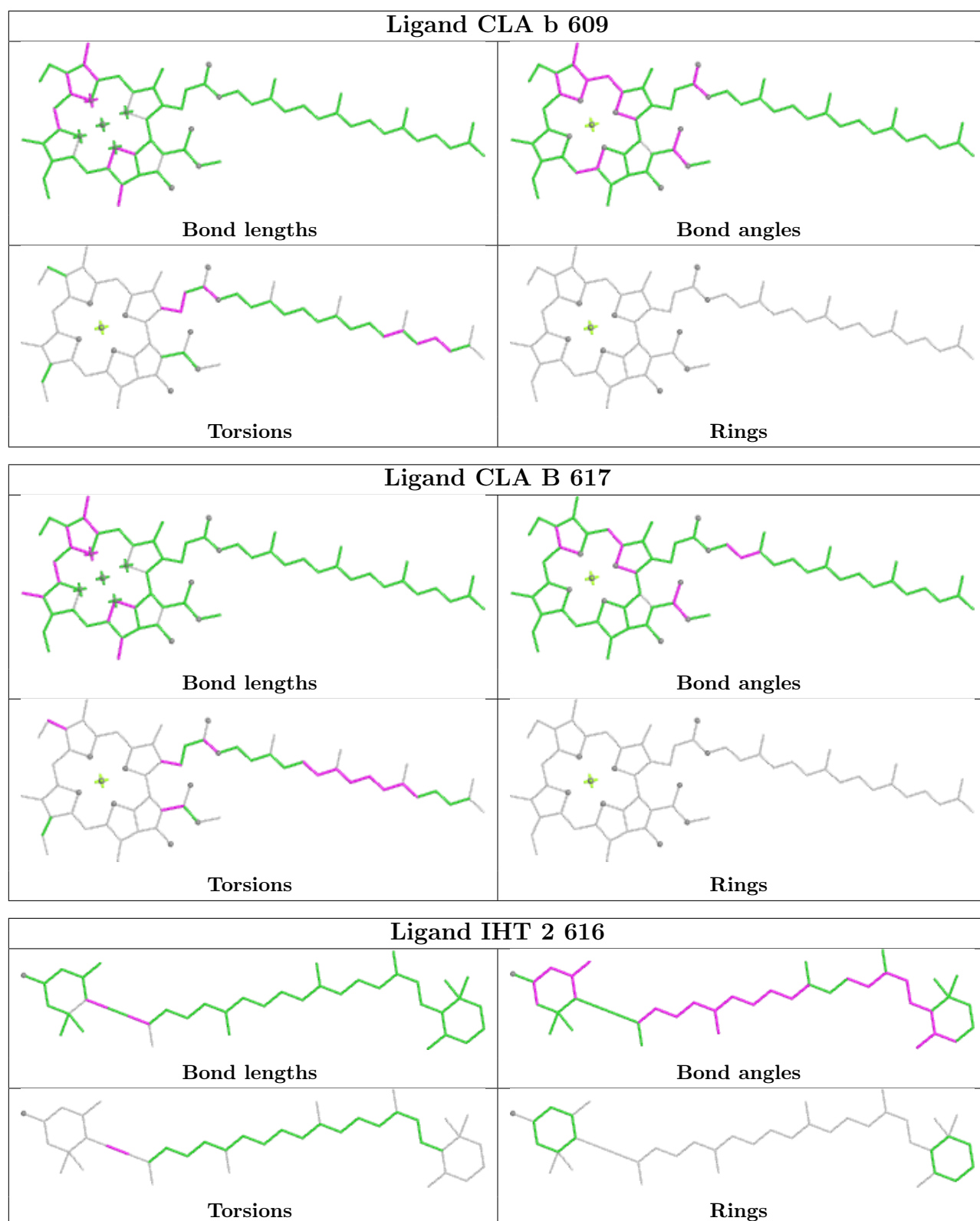


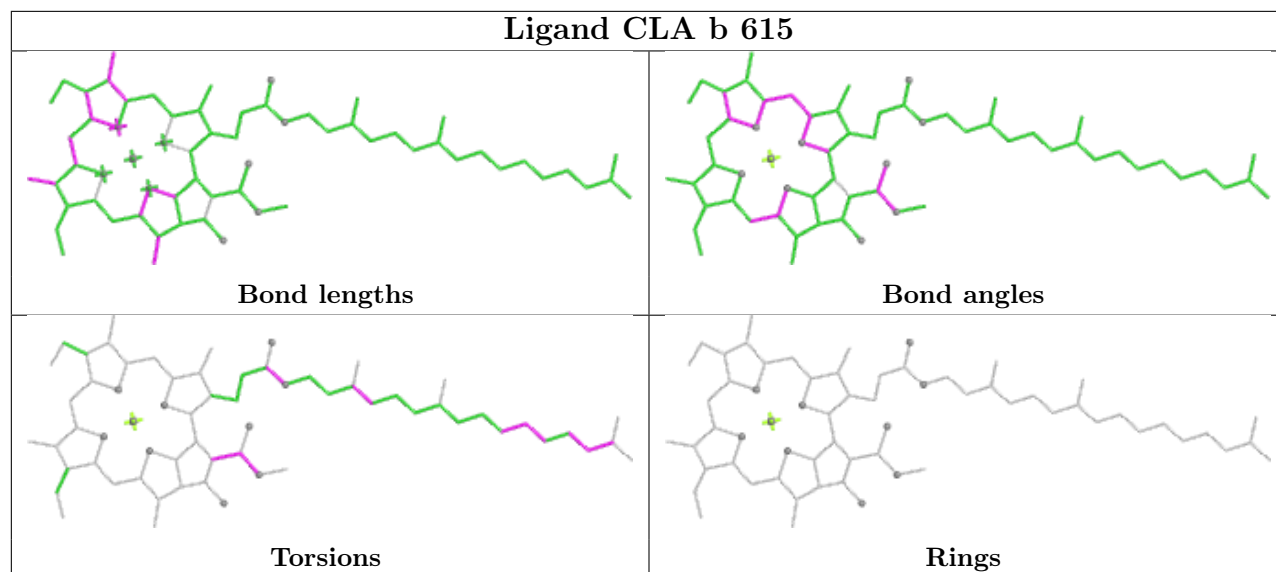
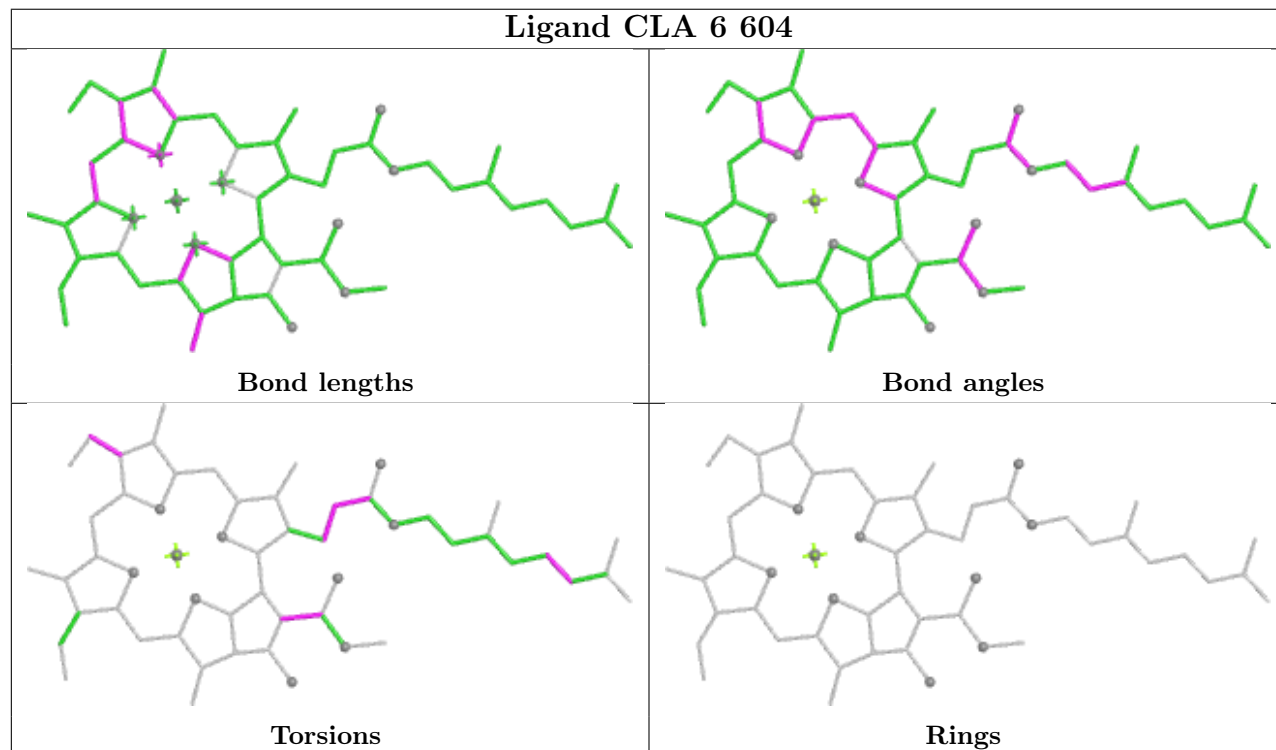
Ligand CLA 2 607

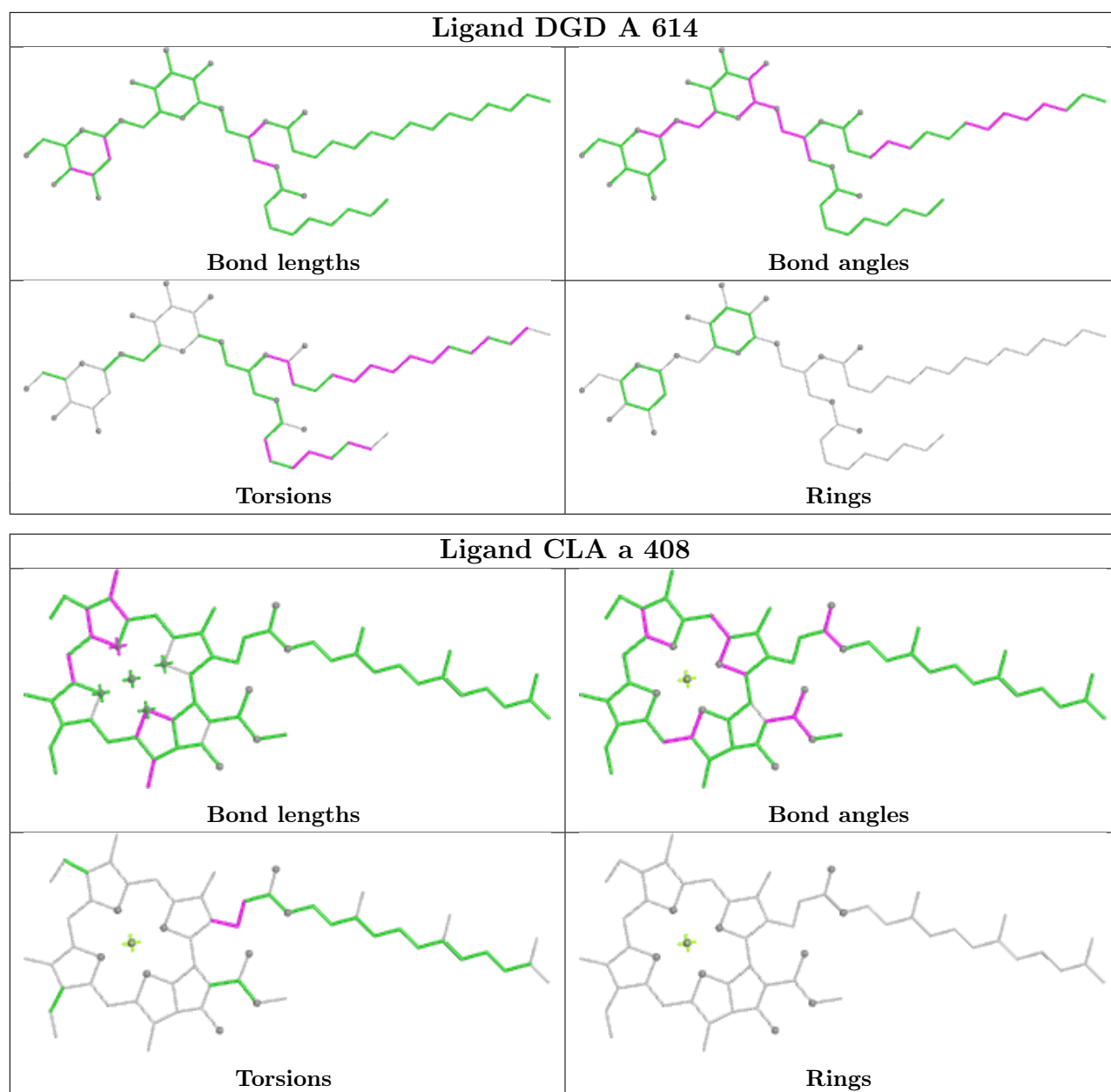


Ligand LMG 0 619

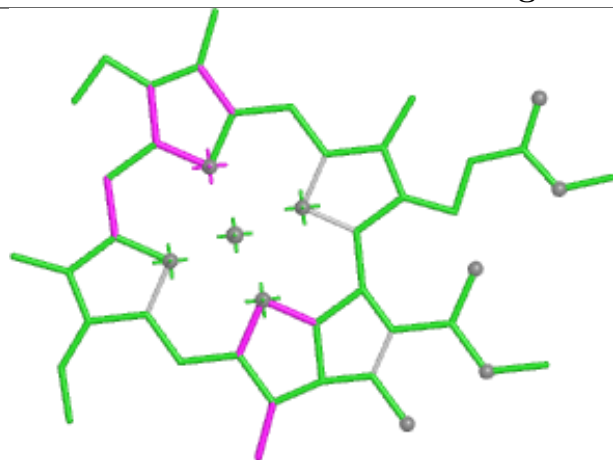




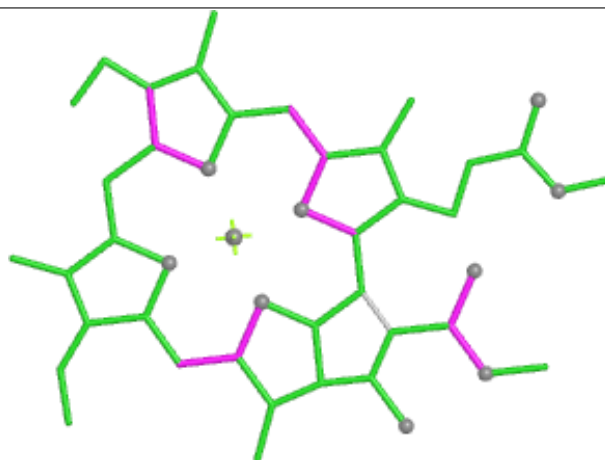
Ligand CLA b 615**Ligand CLA 6 604**



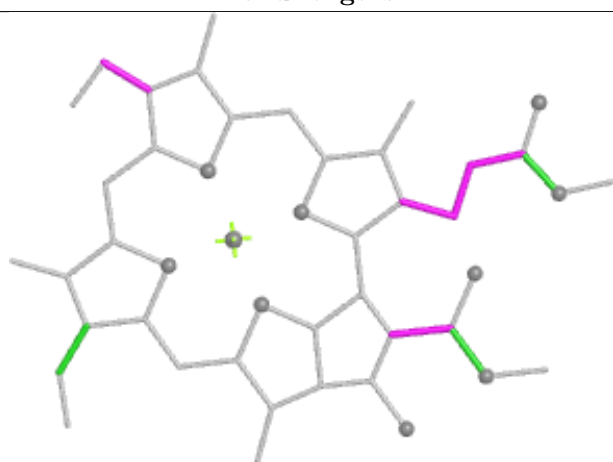
Ligand CLA 3 605



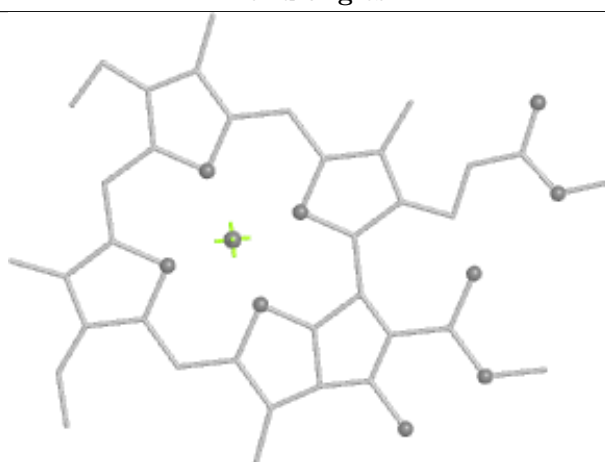
Bond lengths



Bond angles

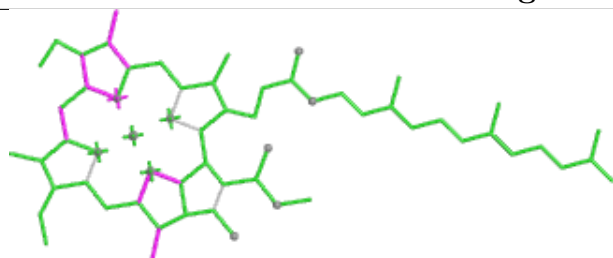


Torsions

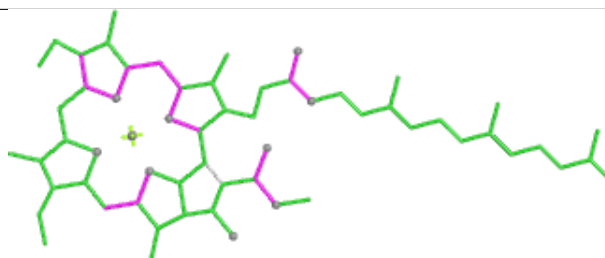


Rings

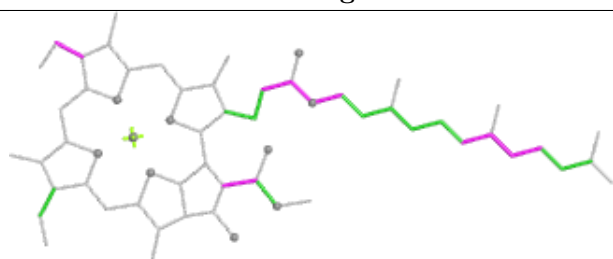
Ligand CLA 8 605



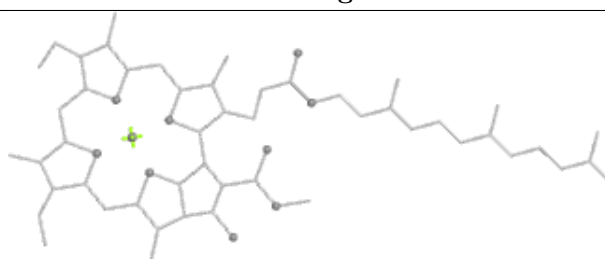
Bond lengths



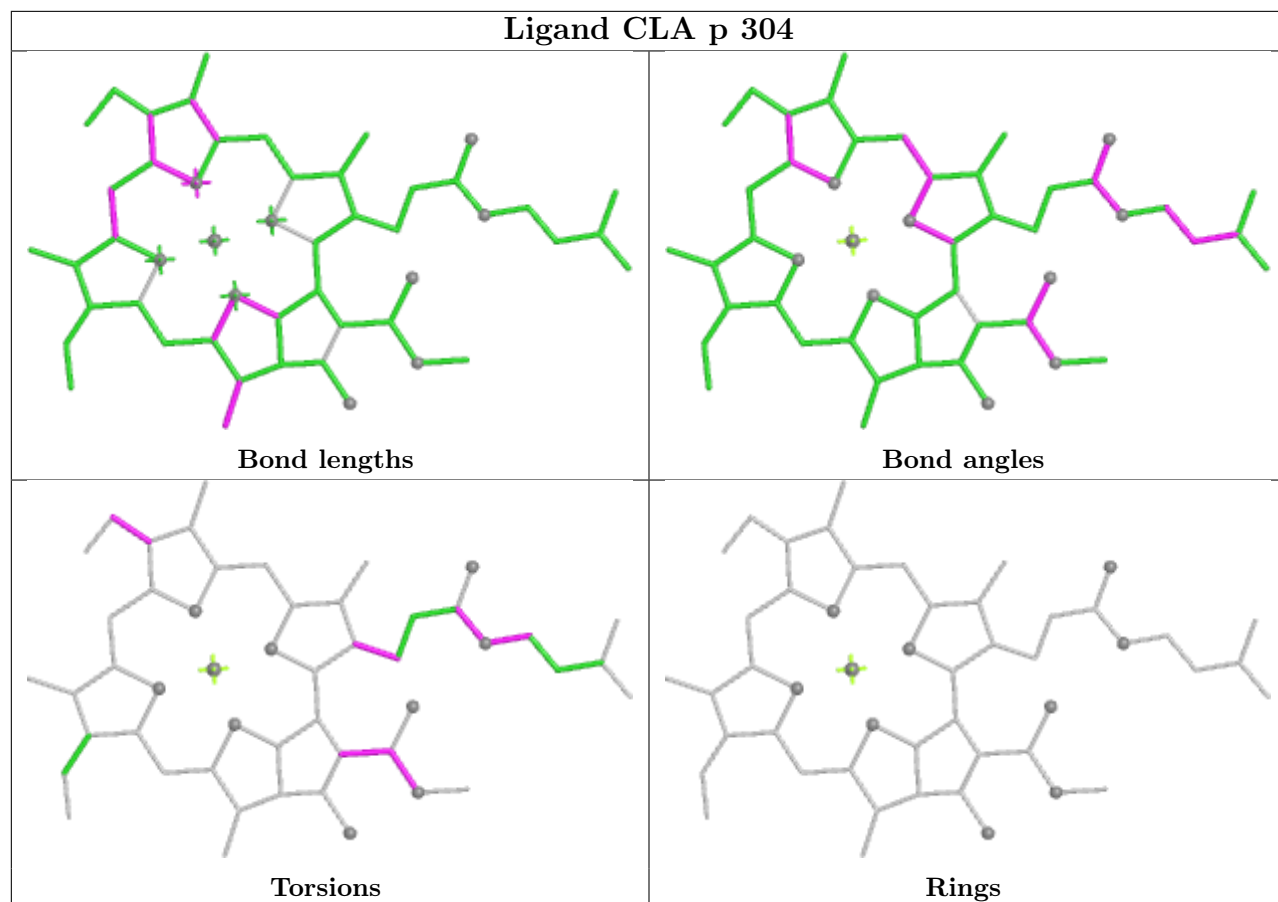
Bond angles



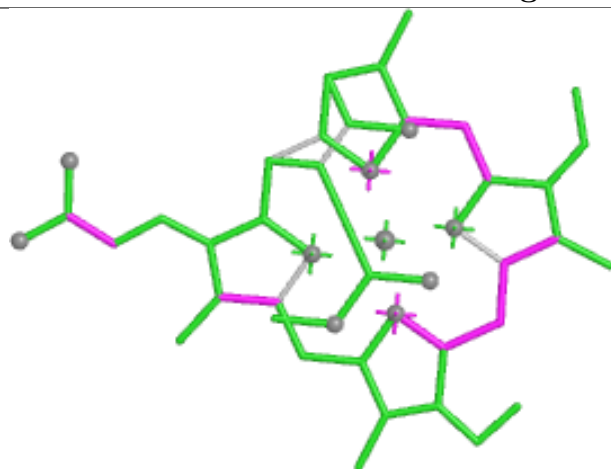
Torsions



Rings



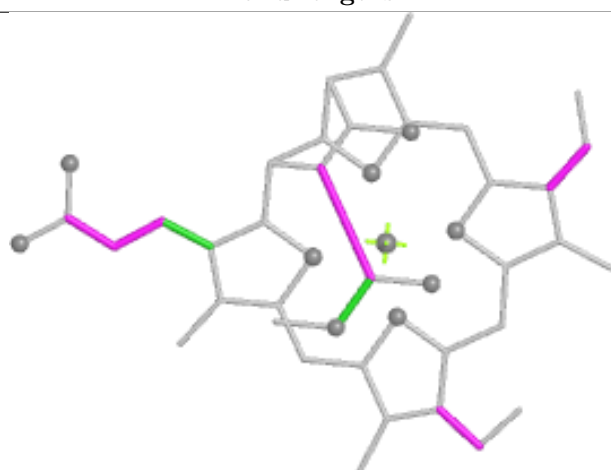
Ligand KC2 5 311



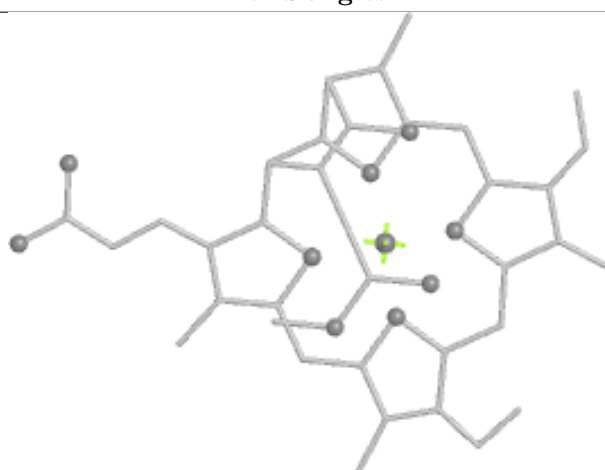
Bond lengths



Bond angles

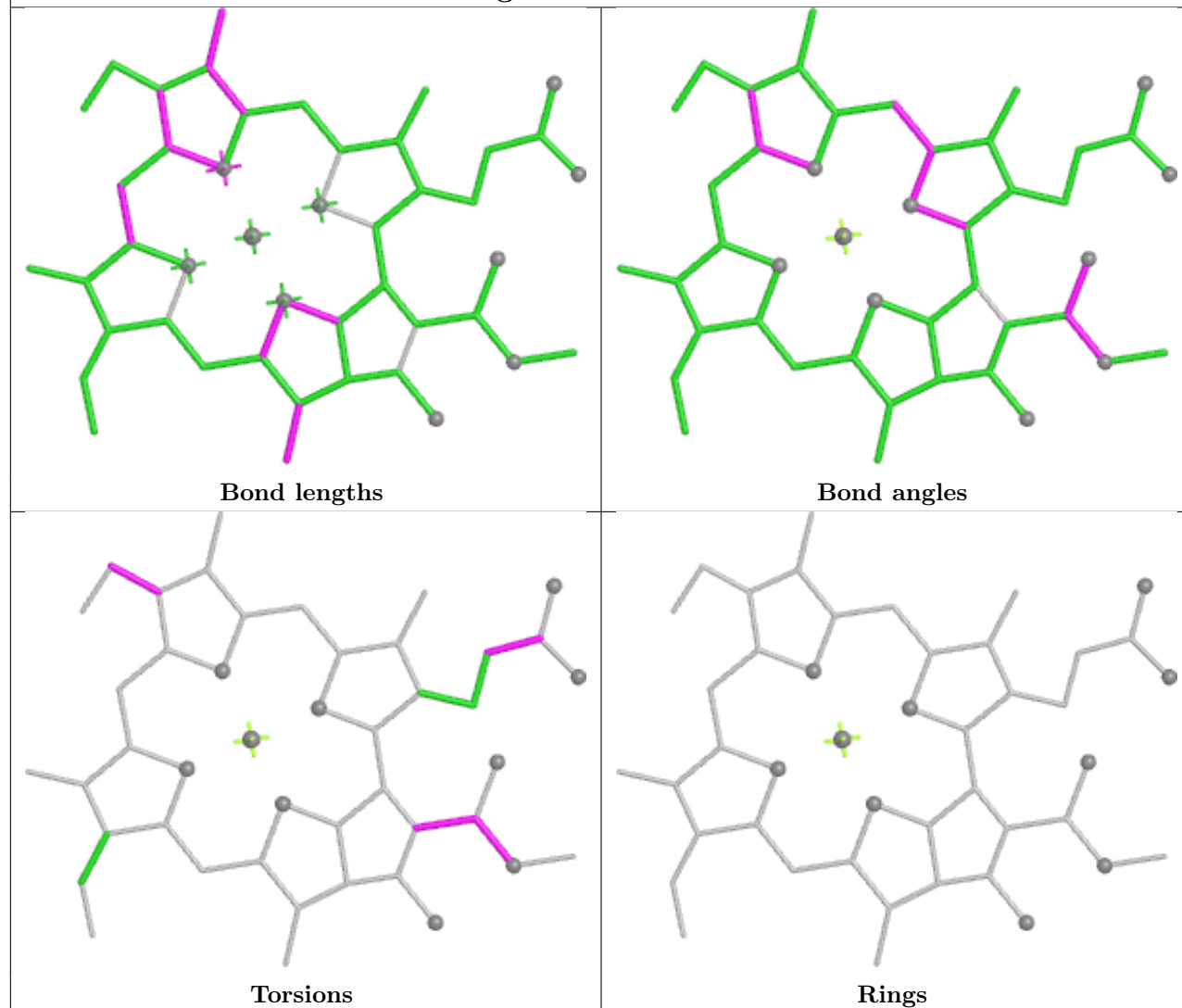


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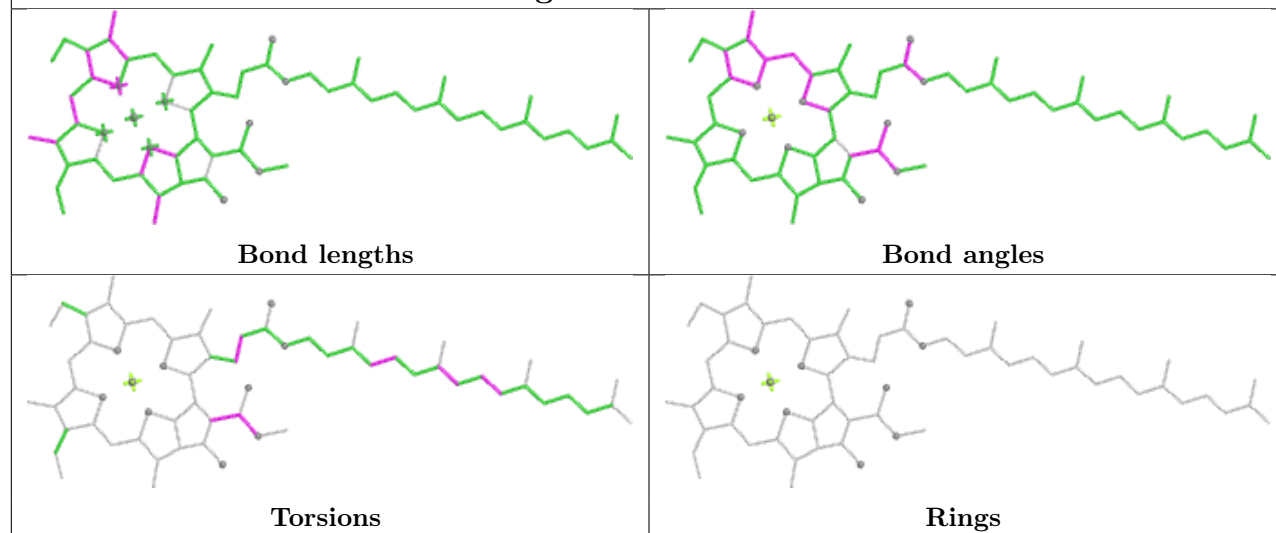


Rings

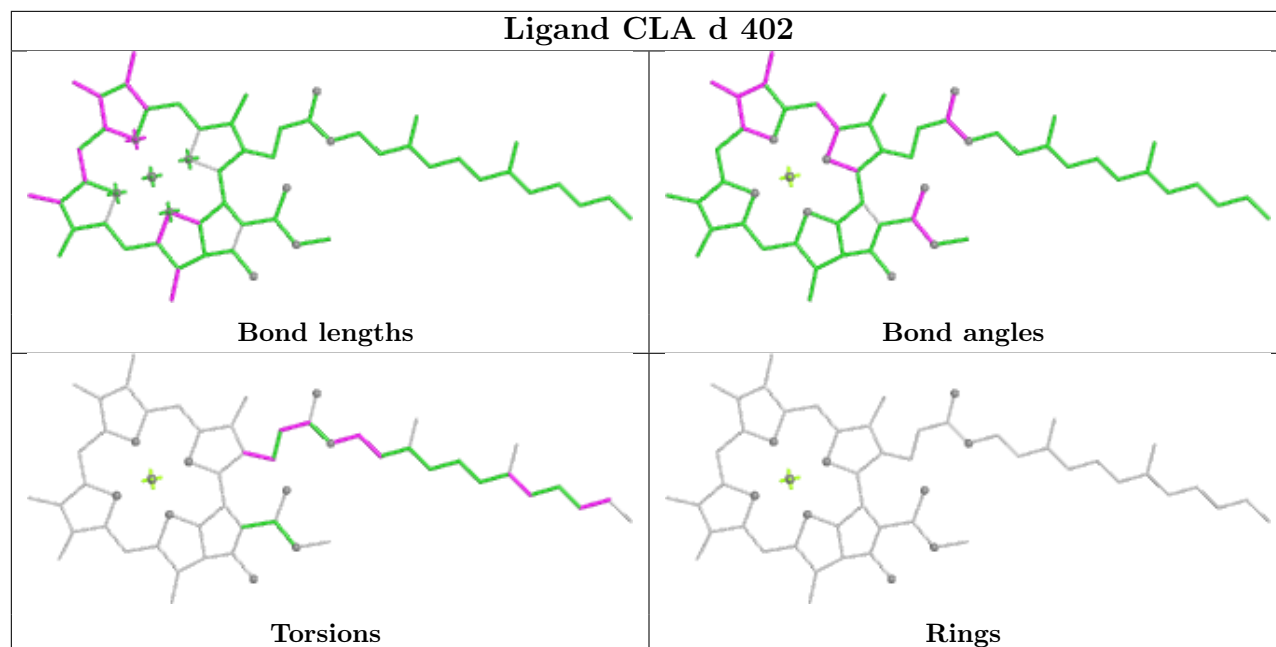
Ligand CLA 0 606



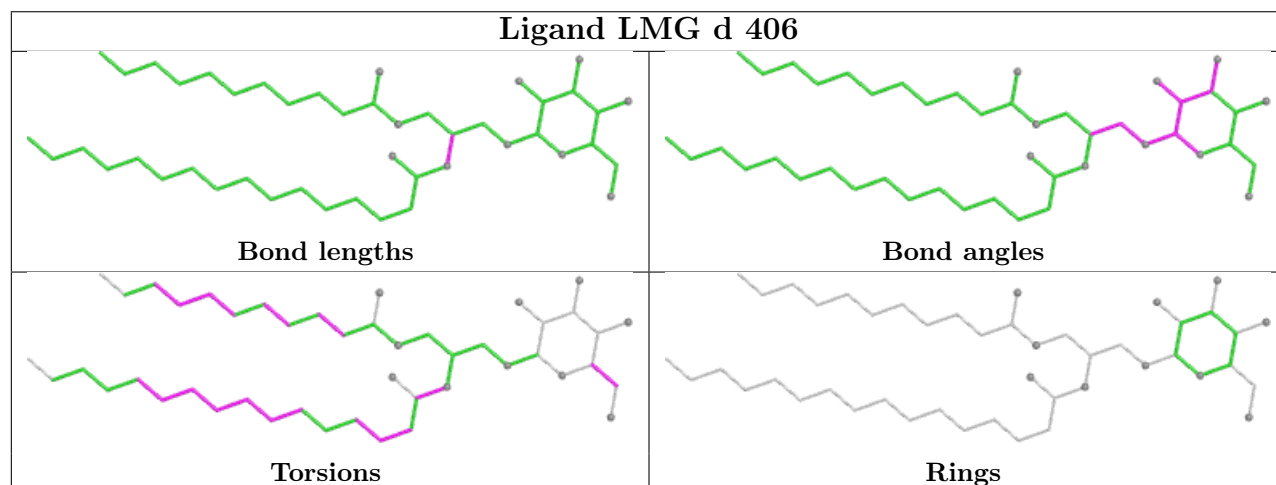
Ligand CLA b 607



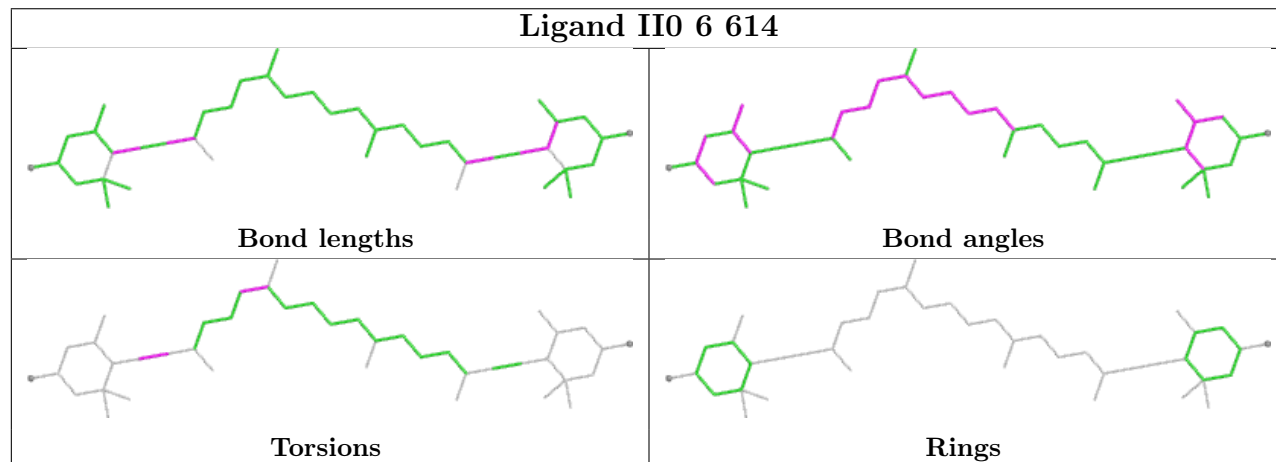
Ligand CLA d 402

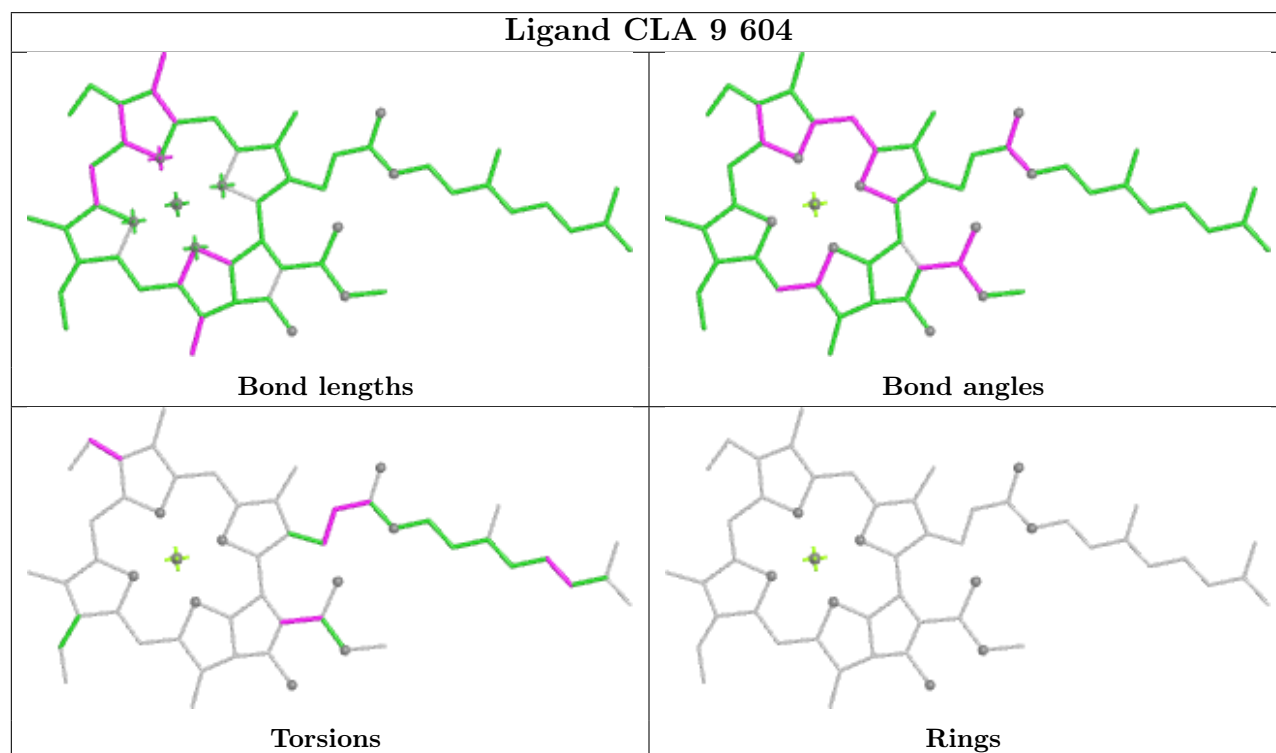
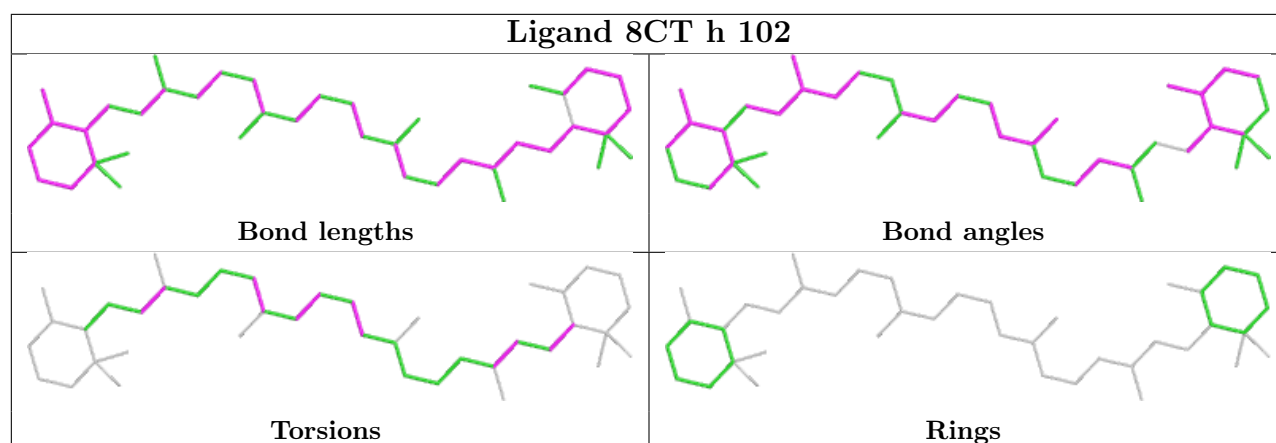


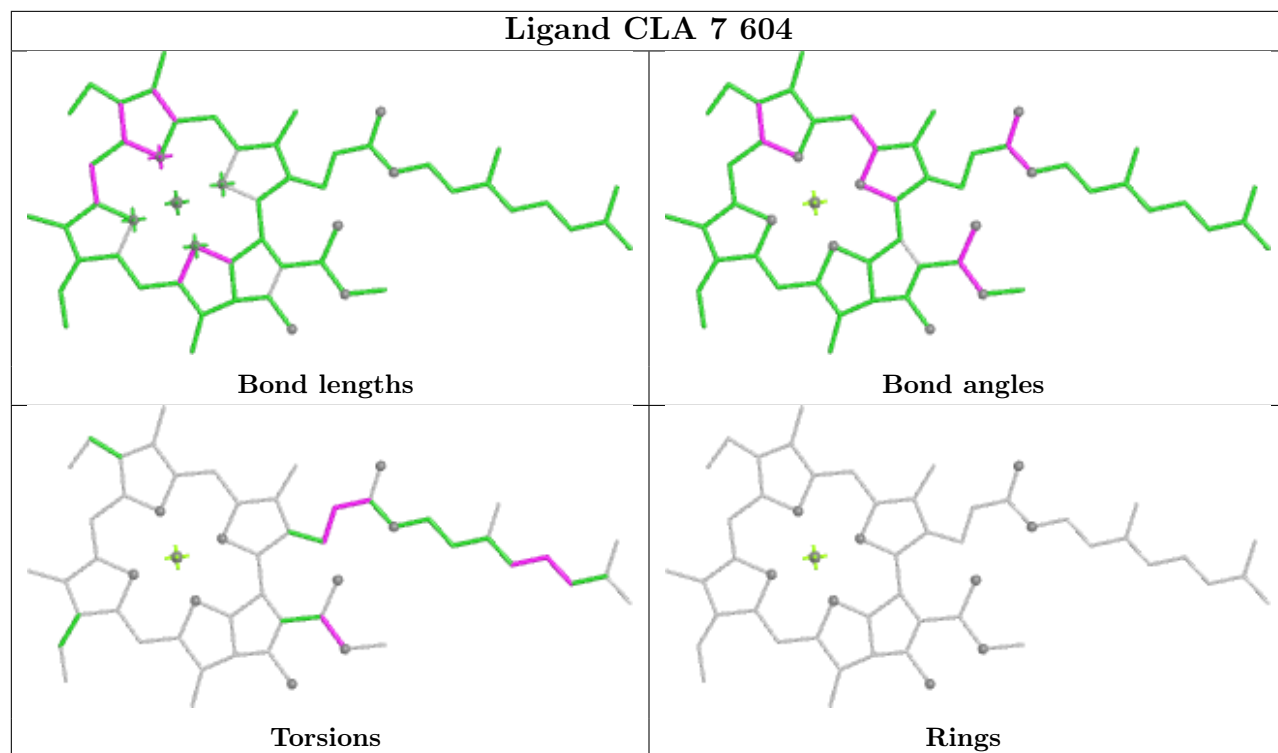
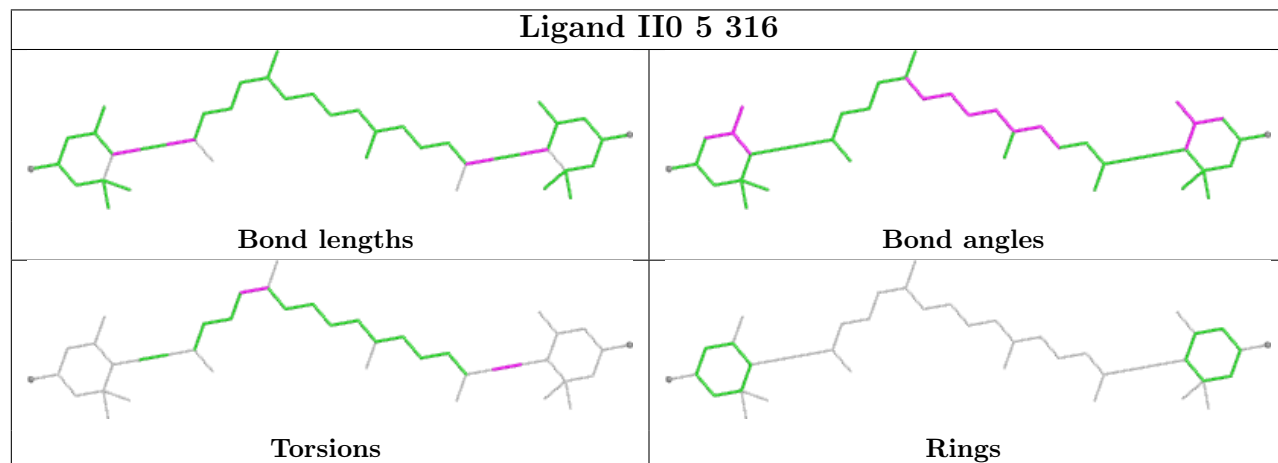
Ligand LMG d 406



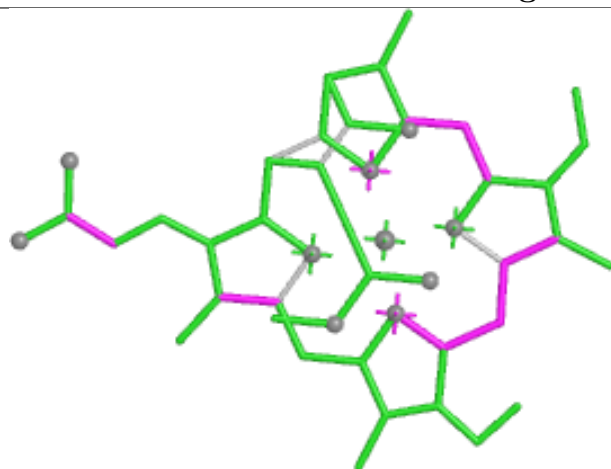
Ligand II0 6 614





Ligand CLA 7 604**Ligand II0 5 316**

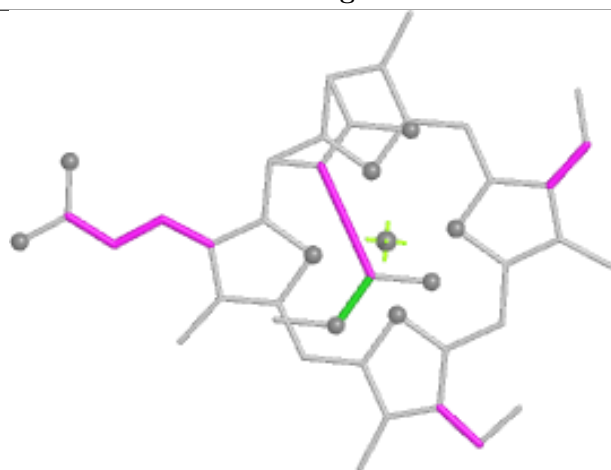
Ligand KC2 p 311



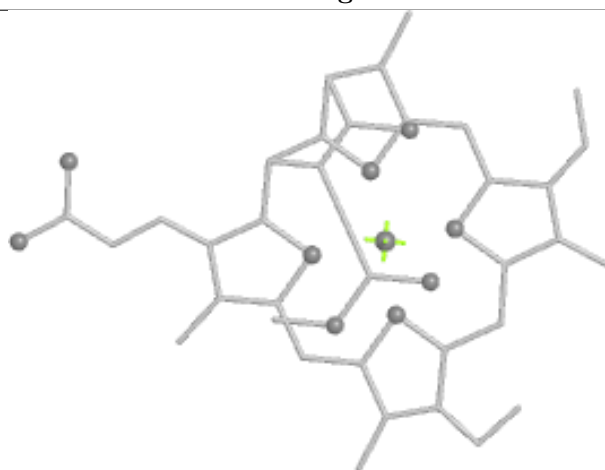
Bond lengths



Bond angles

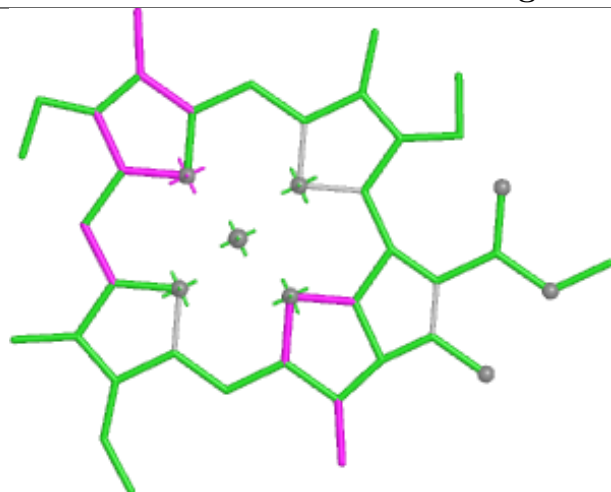


Torsions

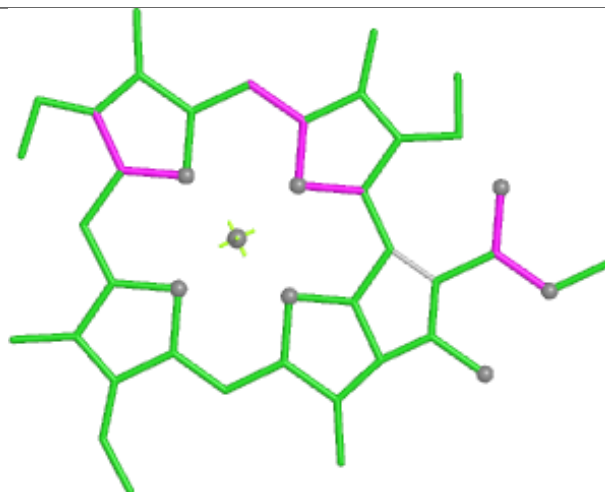


Rings

Ligand CLA 2 601



Bond lengths



Bond angles

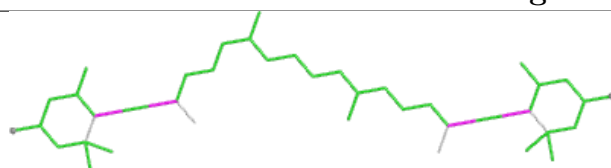


Torsions

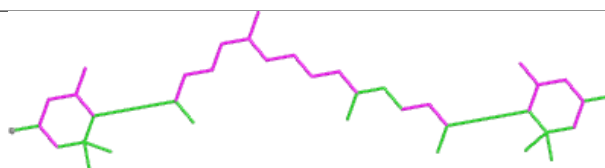


Rings

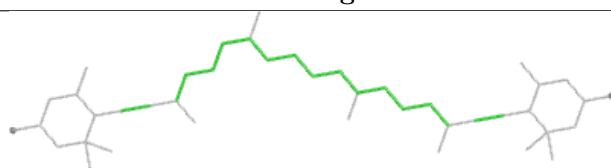
Ligand II0 P 612



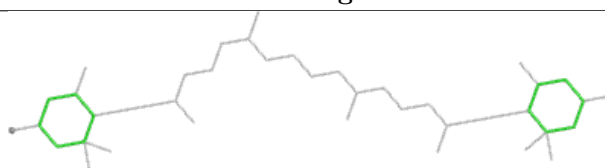
Bond lengths



Bond angles

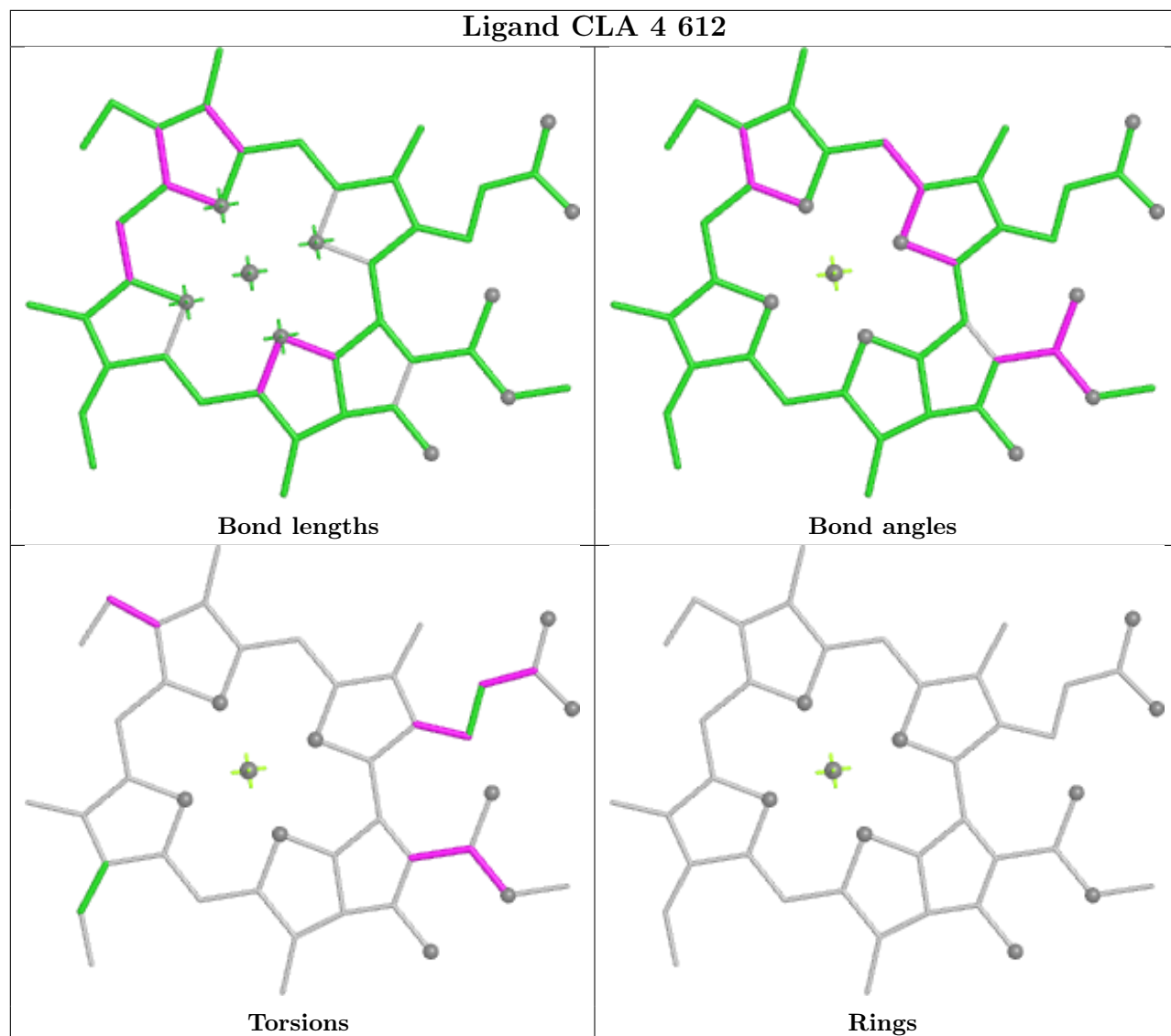


Torsions

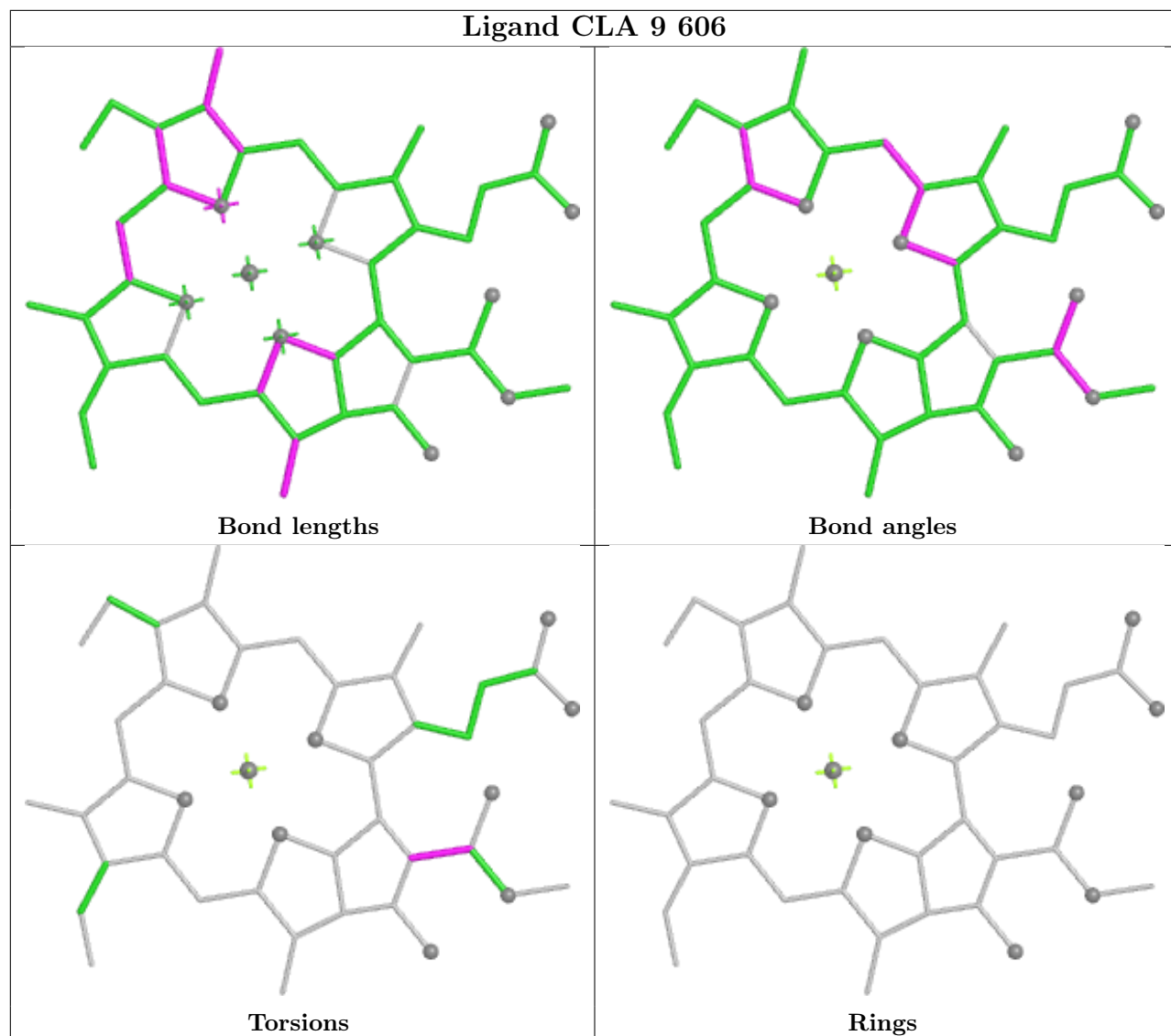


Rings

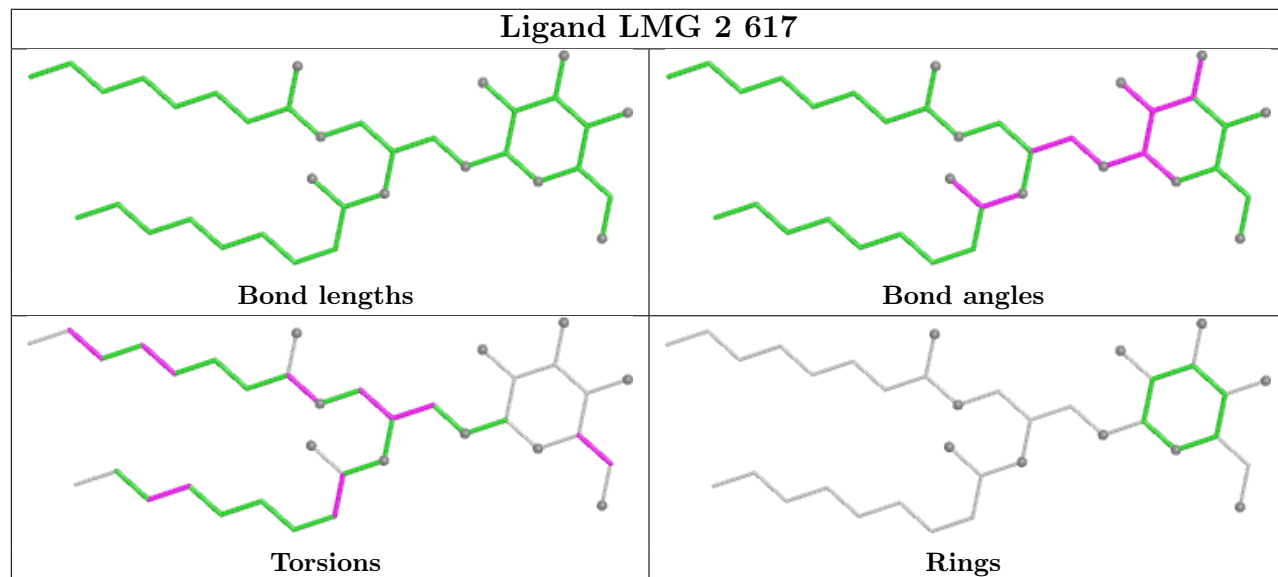
Ligand CLA 4 612



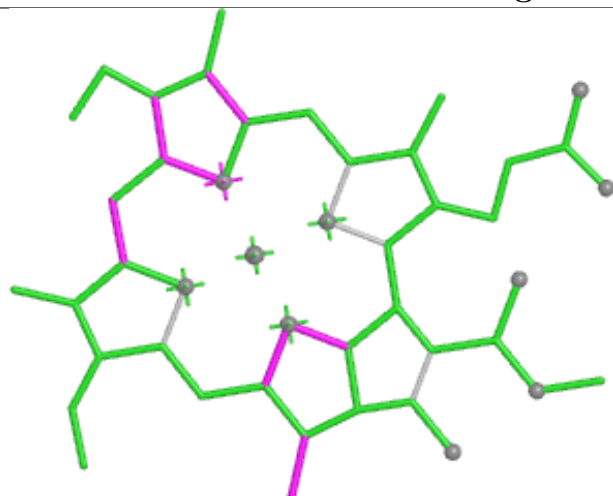
Ligand CLA 9 606



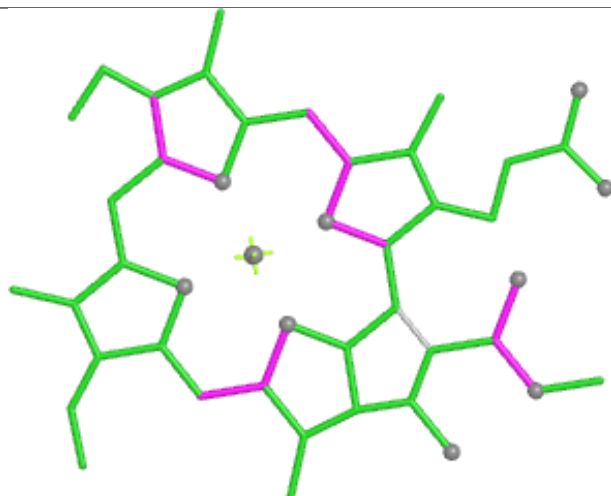
Ligand LMG 2 617



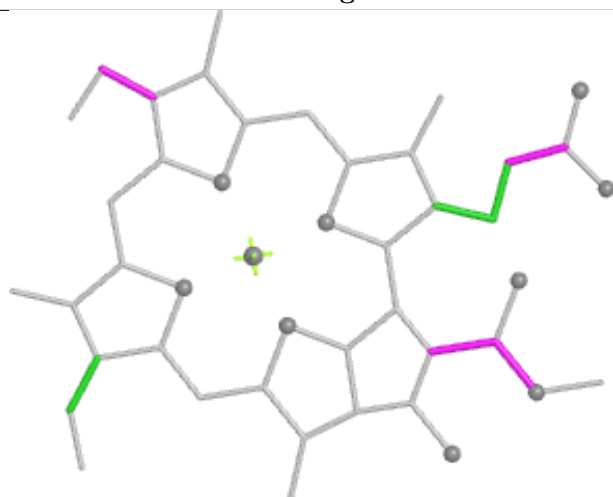
Ligand CLA P 610



Bond lengths



Bond angles

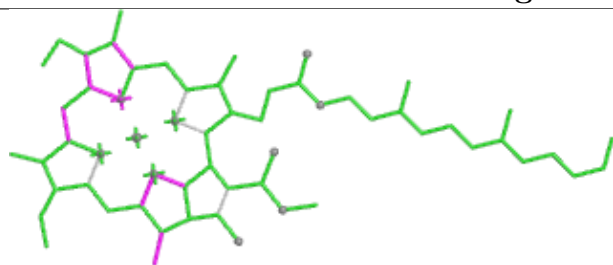


Torsions

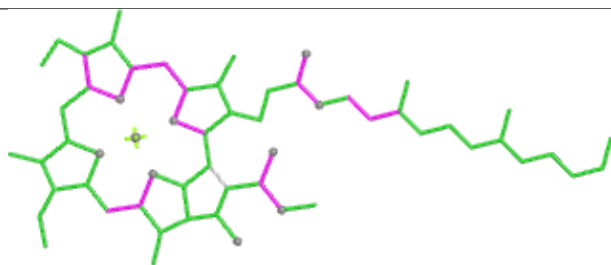


Rings

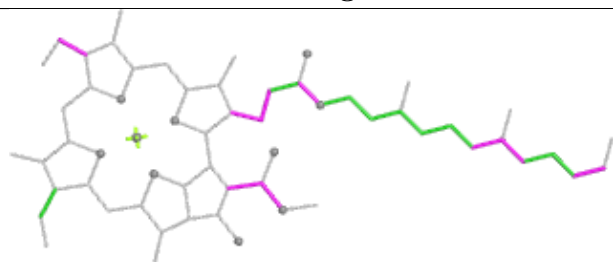
Ligand CLA P 602



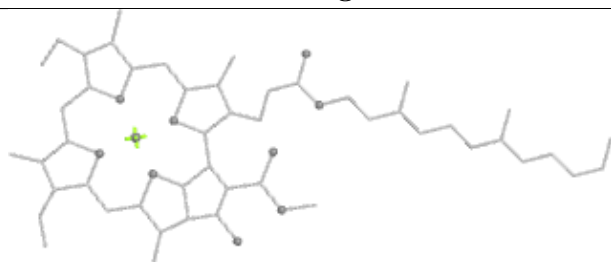
Bond lengths



Bond angles

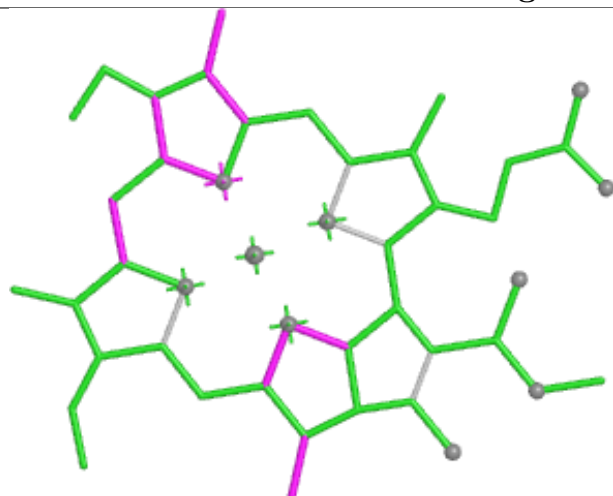


Torsions

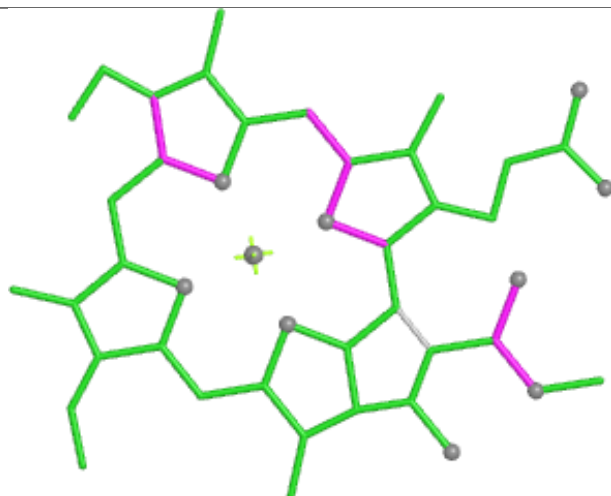


Rings

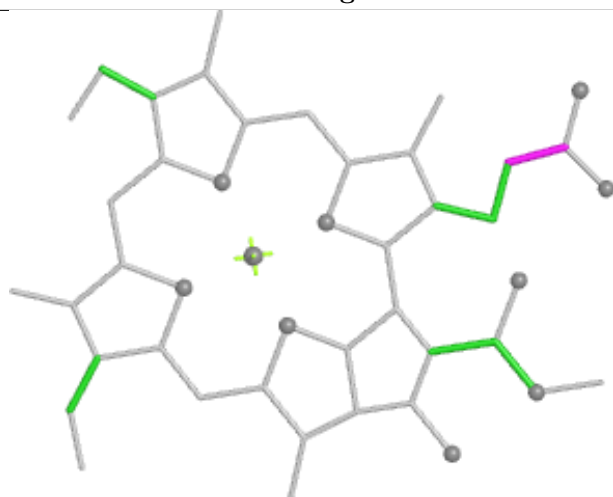
Ligand CLA 8 606



Bond lengths



Bond angles

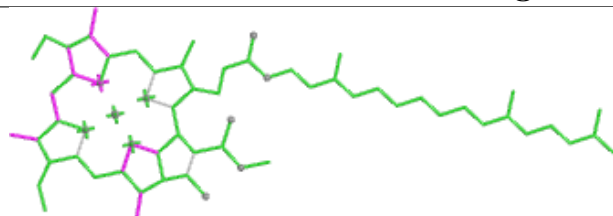


Torsions

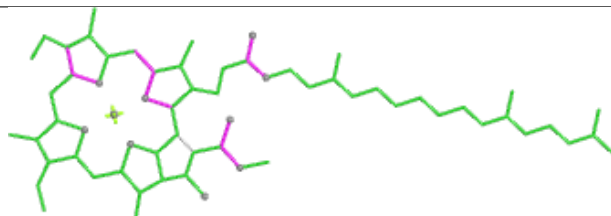


Rings

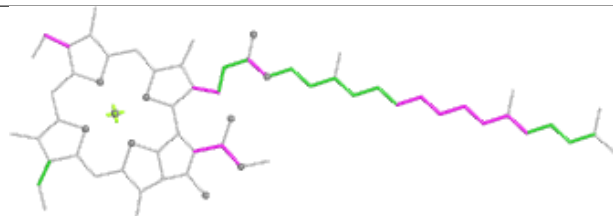
Ligand CLA C 502



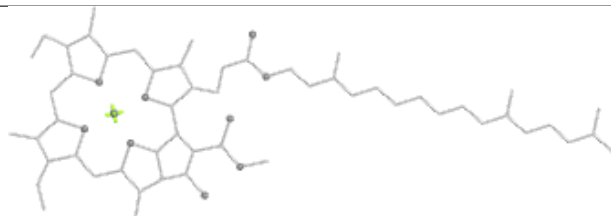
Bond lengths



Bond angles

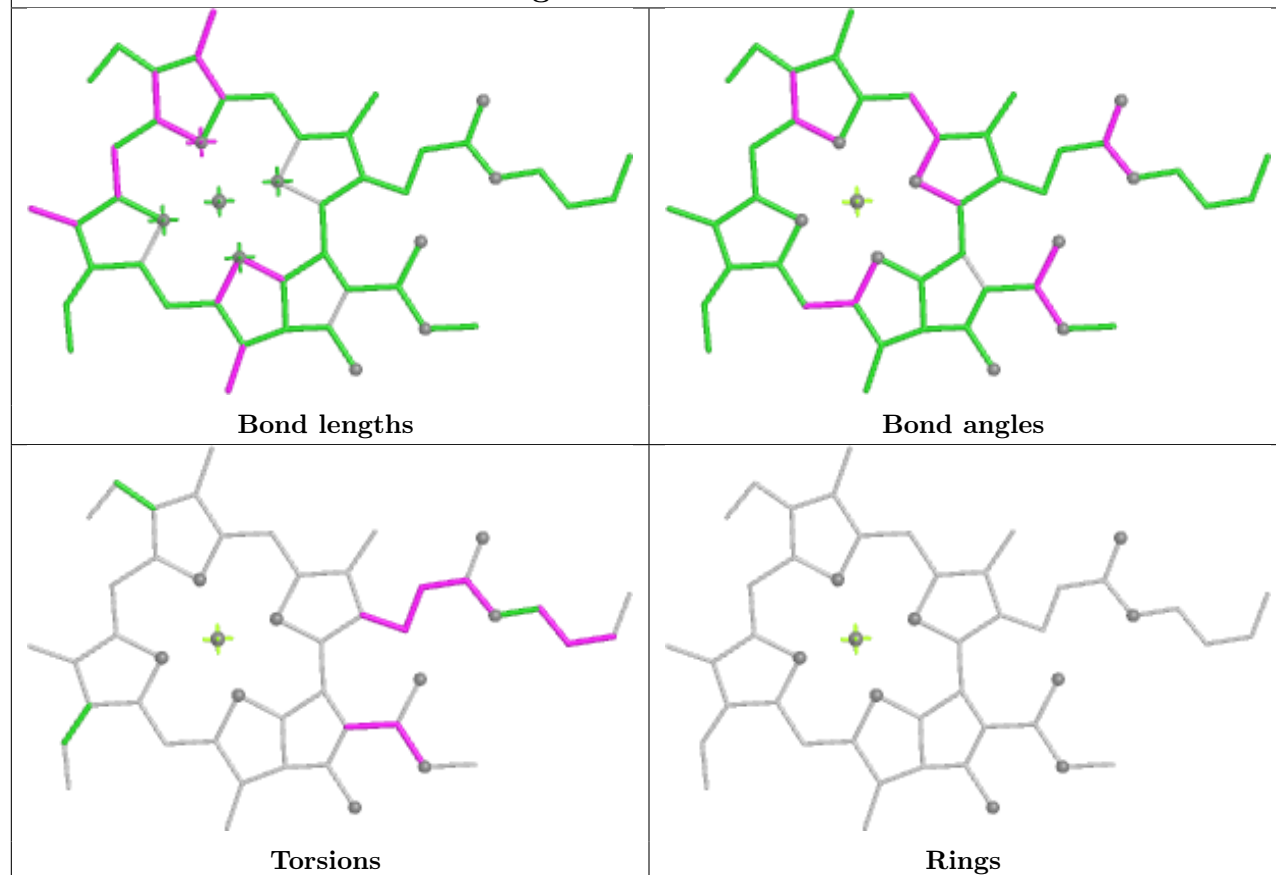


Torsions

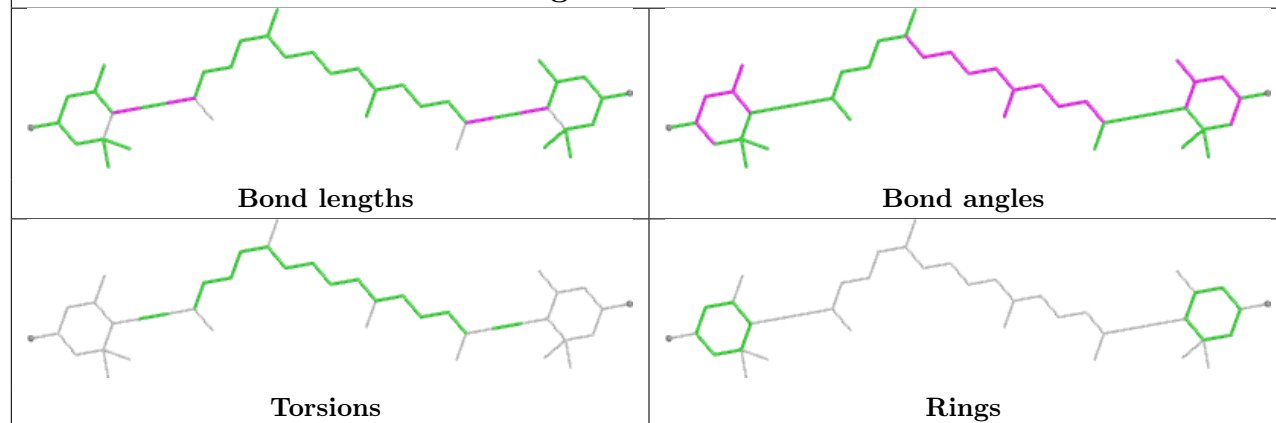


Rings

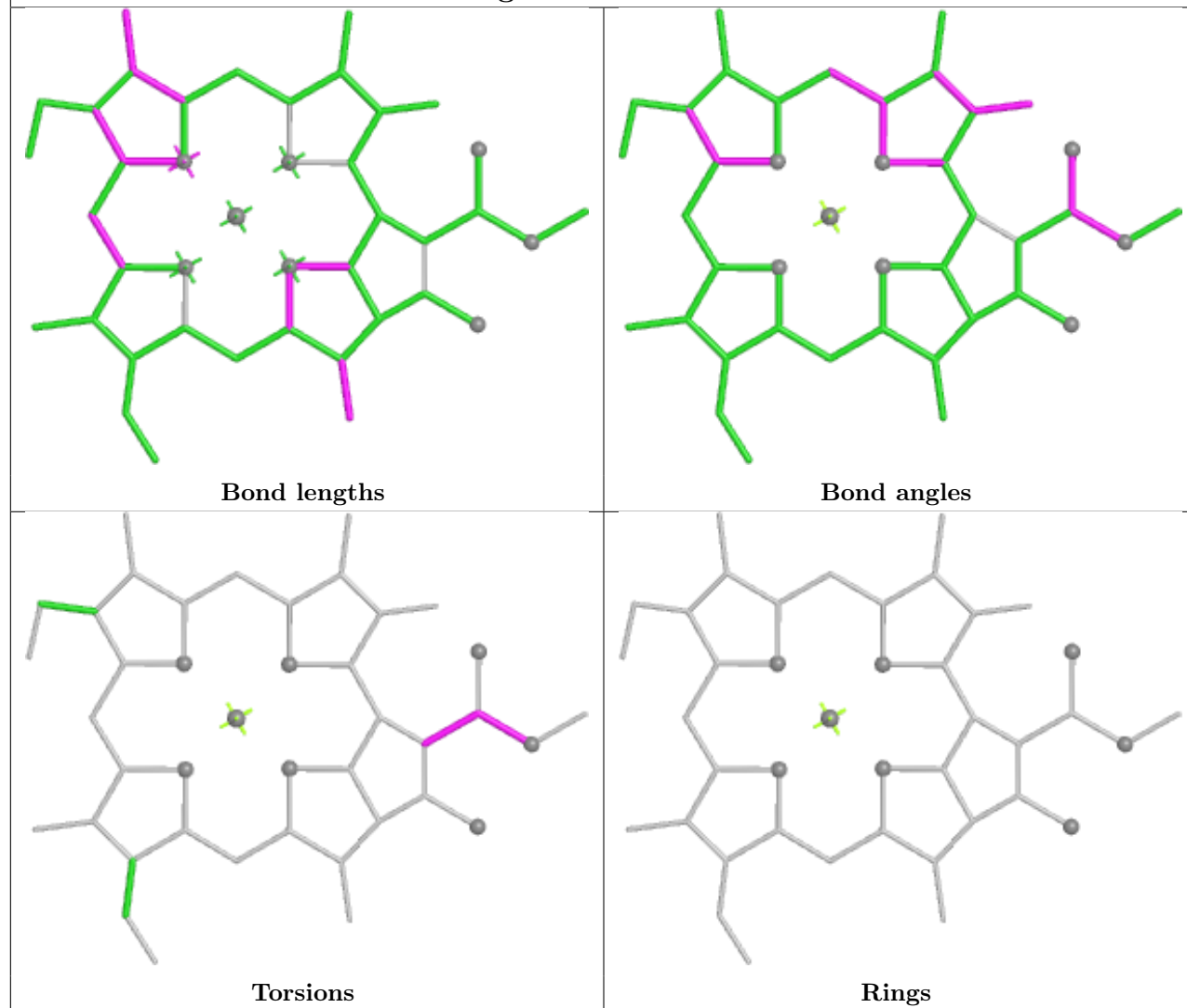
Ligand CLA C 513



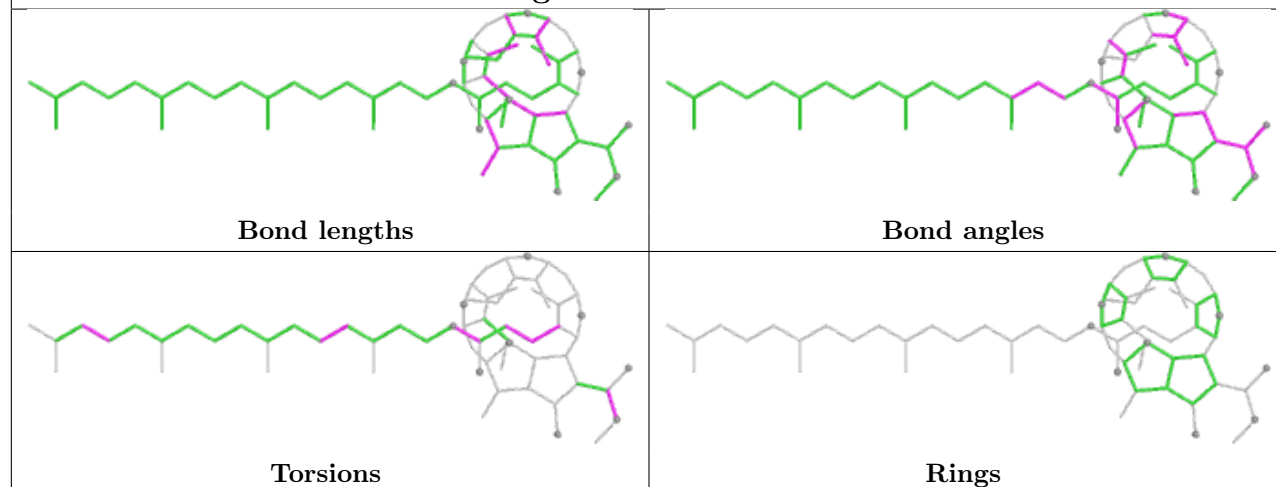
Ligand II0 8 614



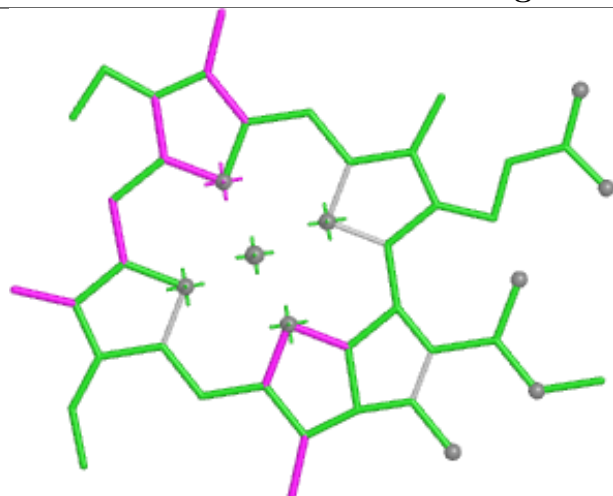
Ligand CLA b 608



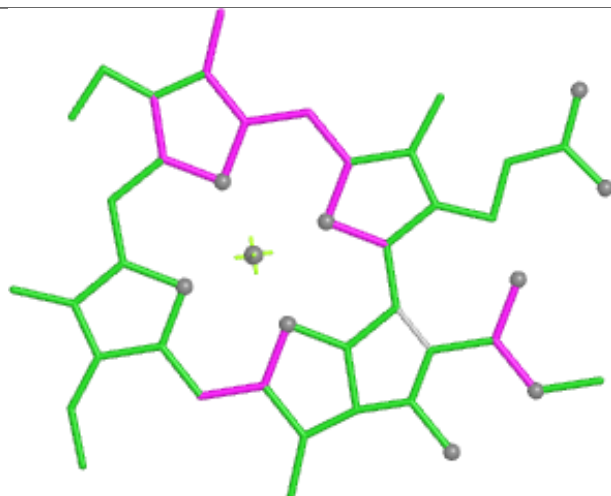
Ligand PHO d 410



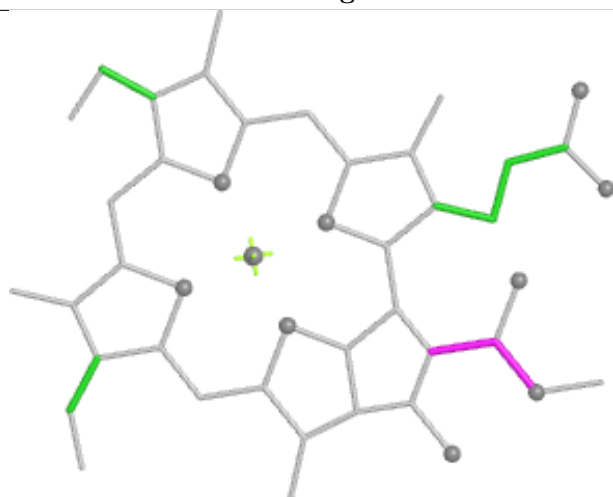
Ligand CLA C 506



Bond lengths



Bond angles

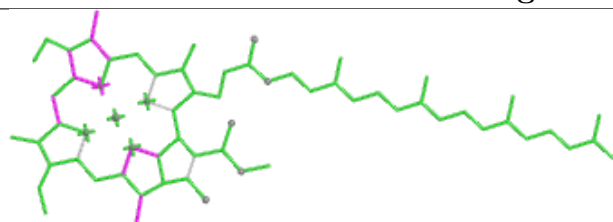


Torsions

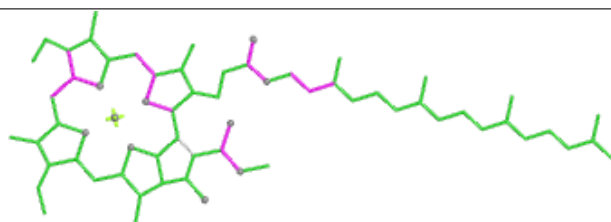


Rings

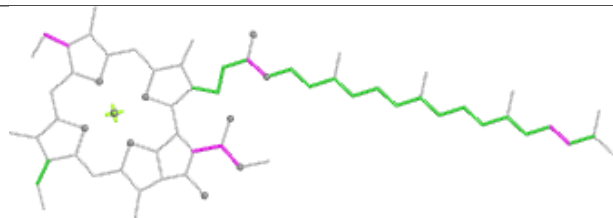
Ligand CLA b 610



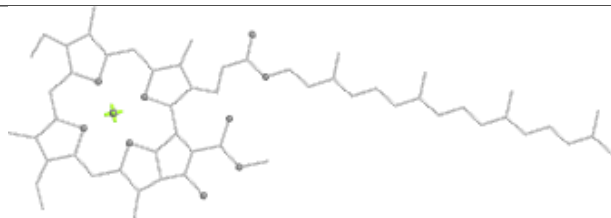
Bond lengths



Bond angles

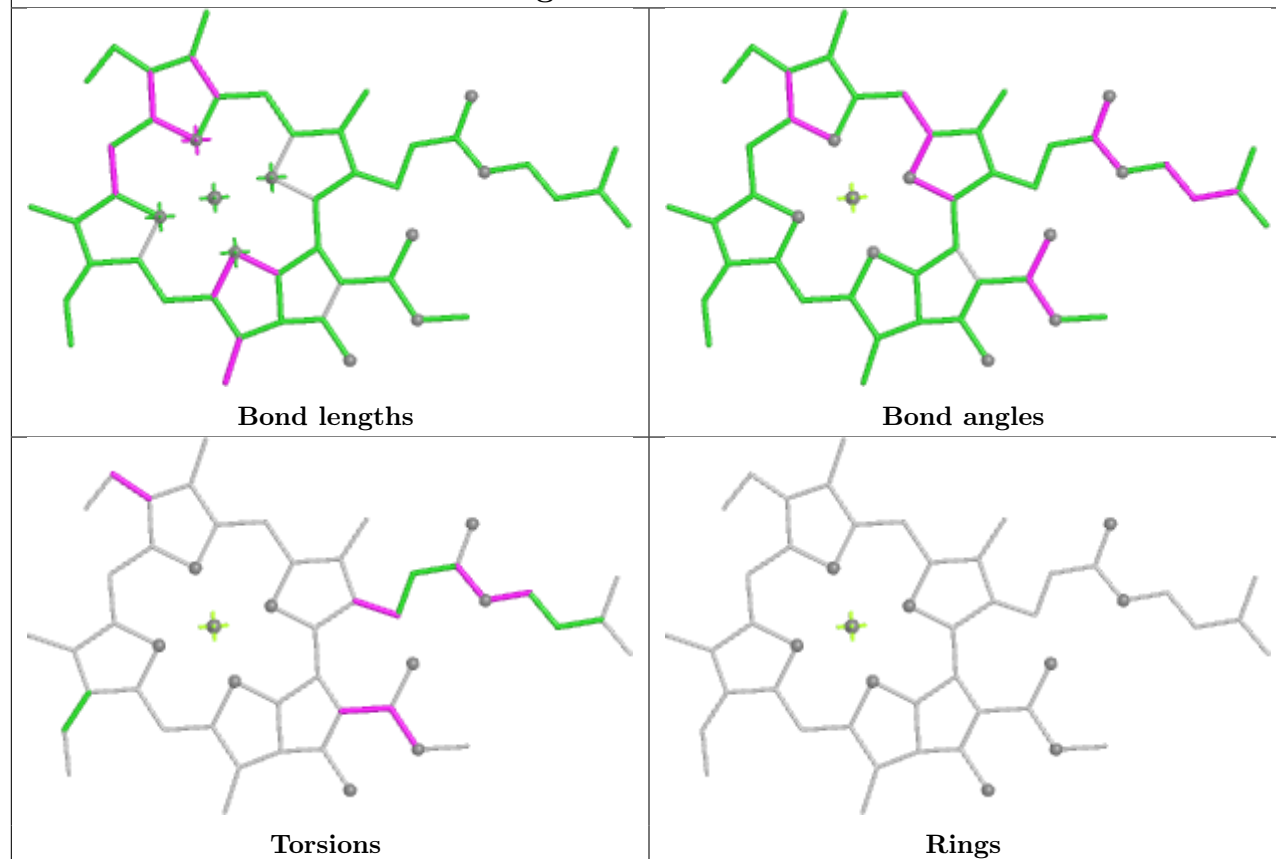


Torsions

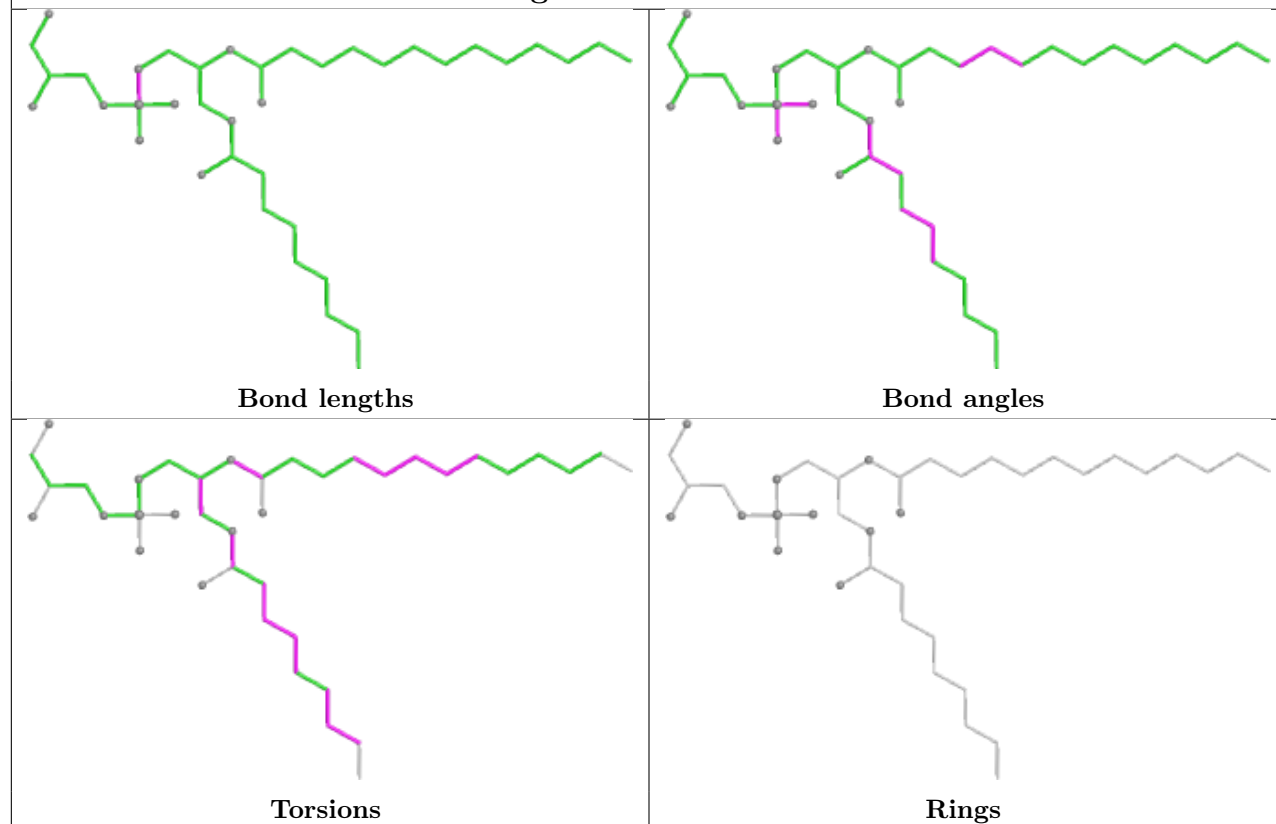


Rings

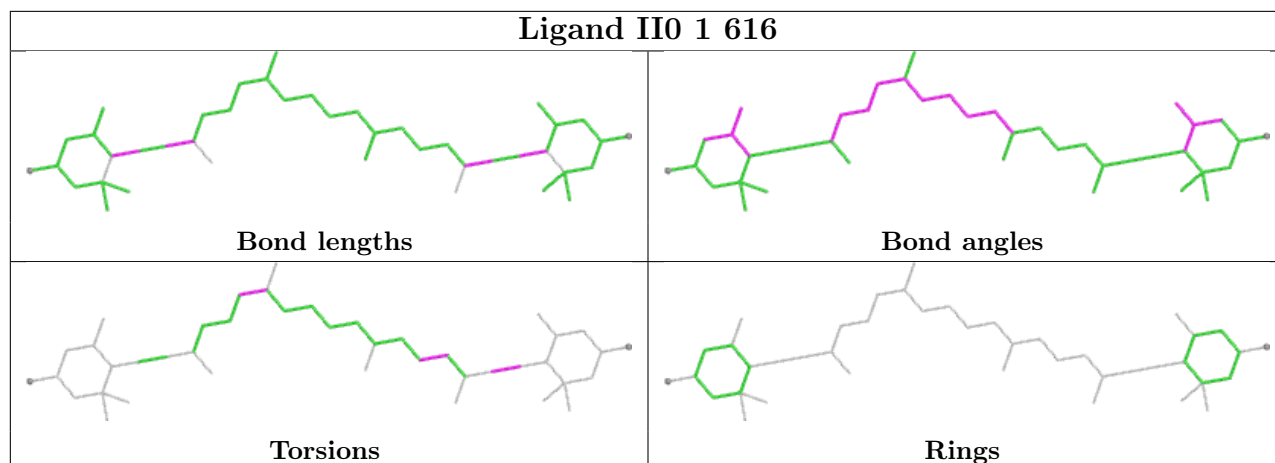
Ligand CLA 5 304



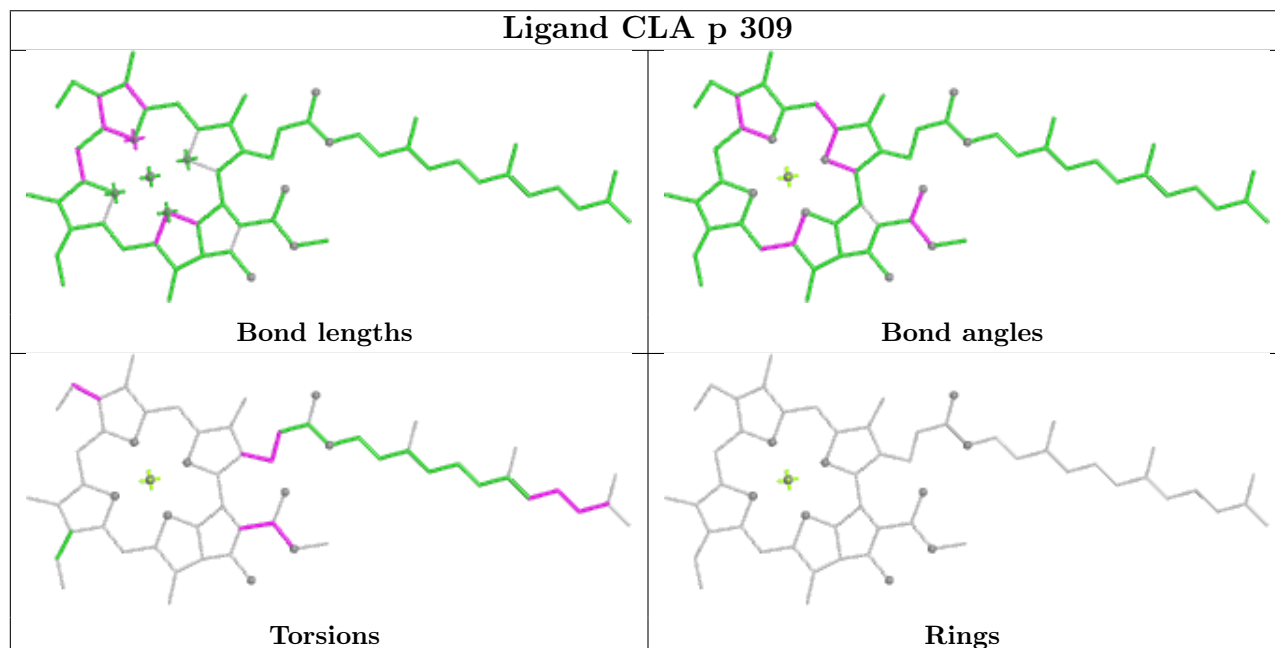
Ligand LHG B 621



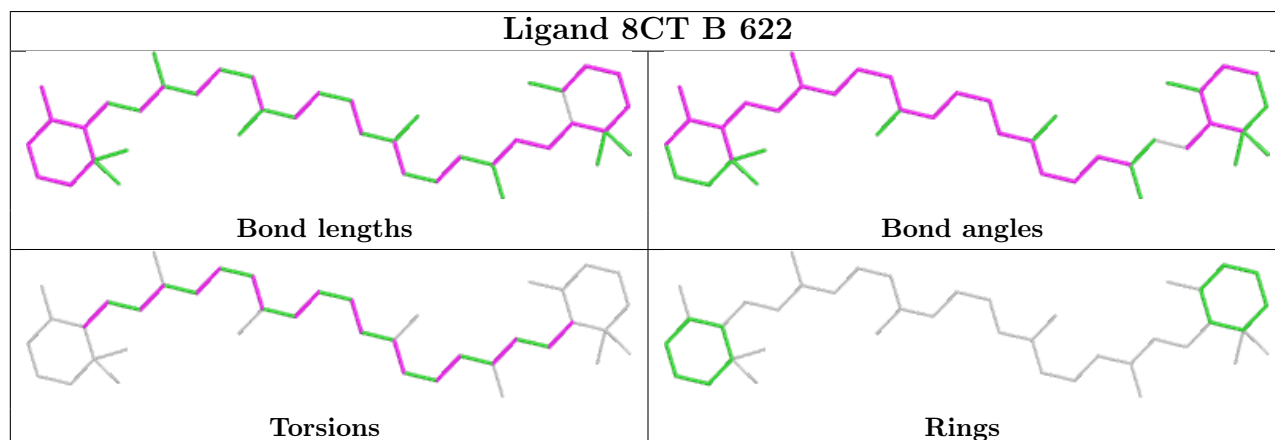
Ligand II0 1 616



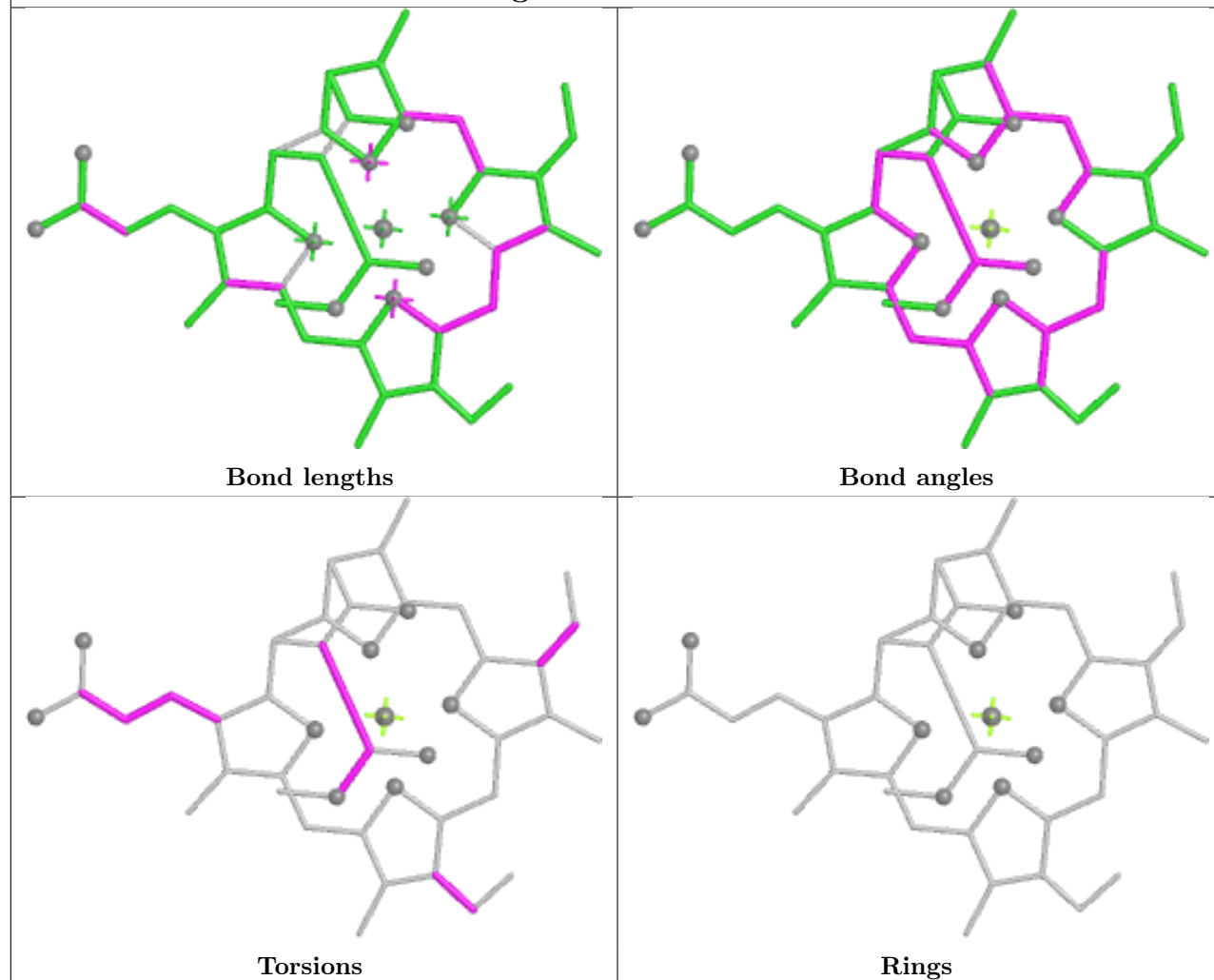
Ligand CLA p 309



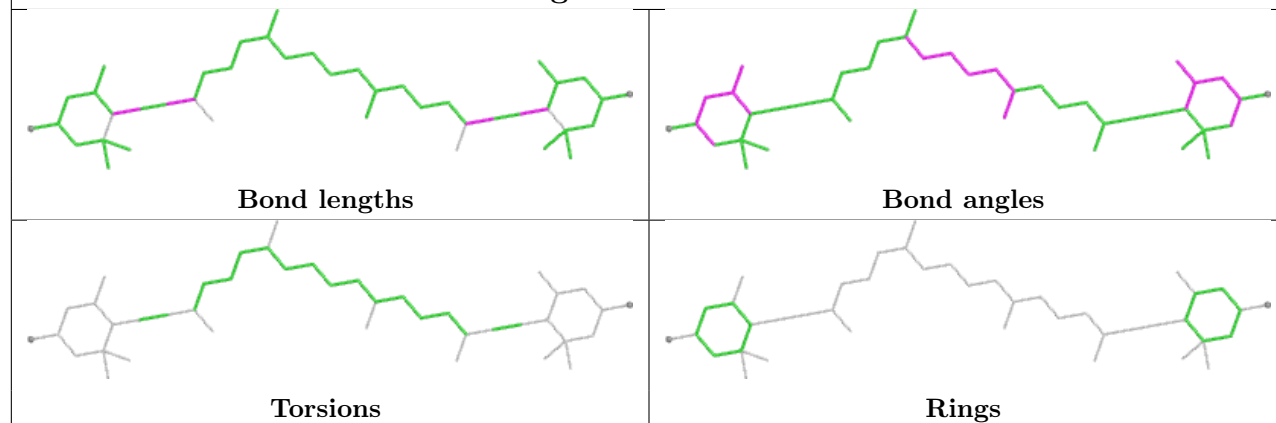
Ligand 8CT B 622

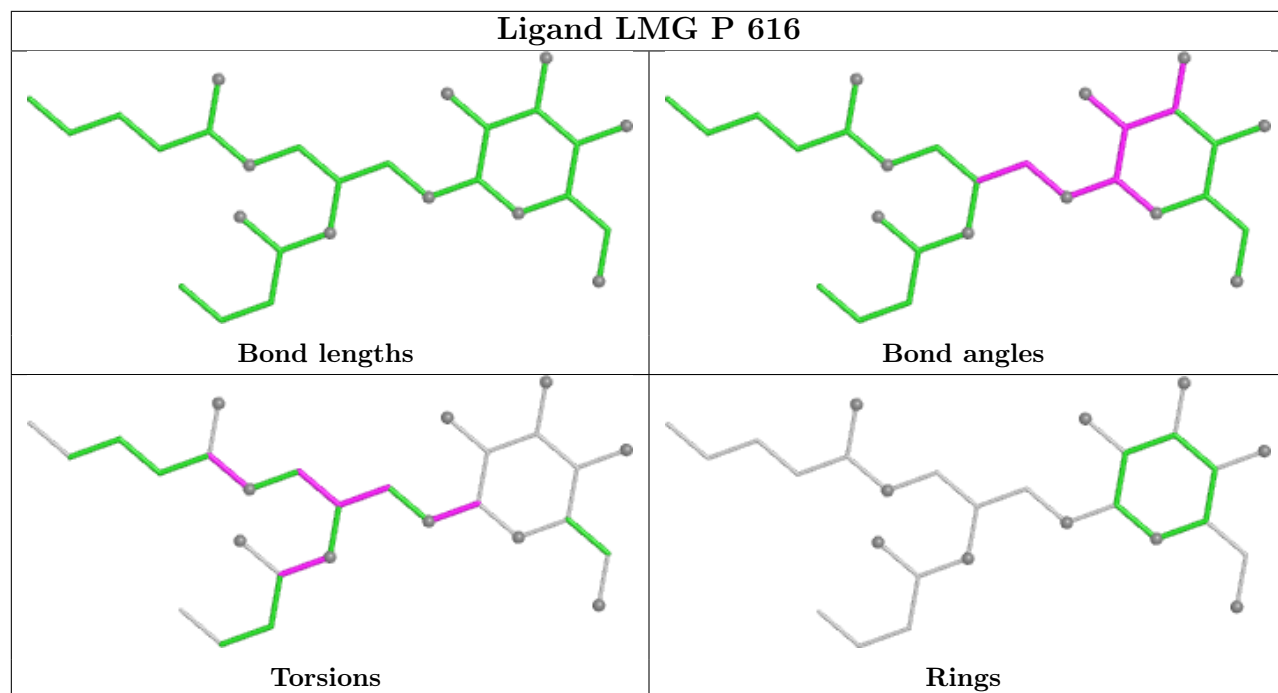


Ligand KC2 0 610

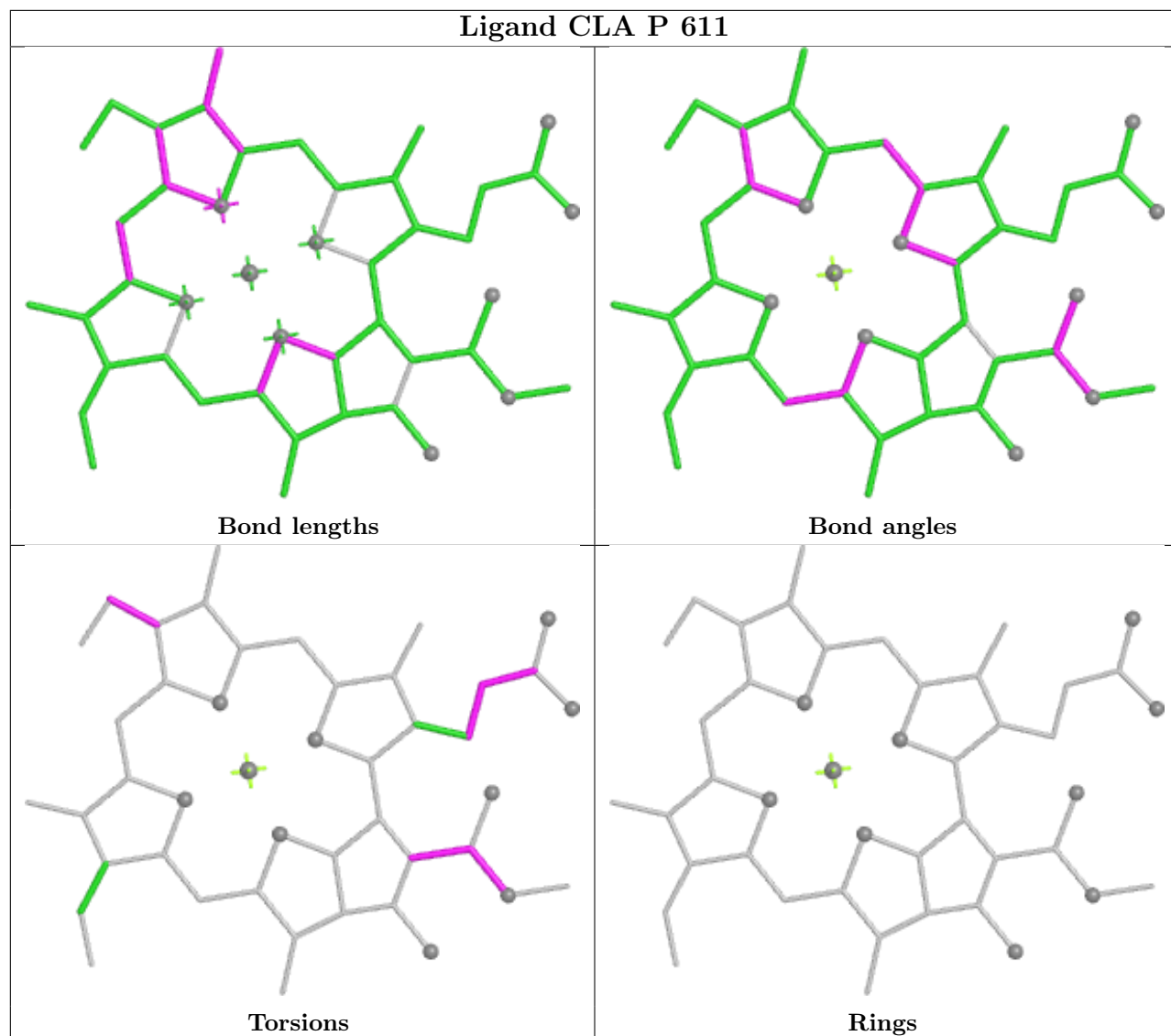


Ligand II0 4 615

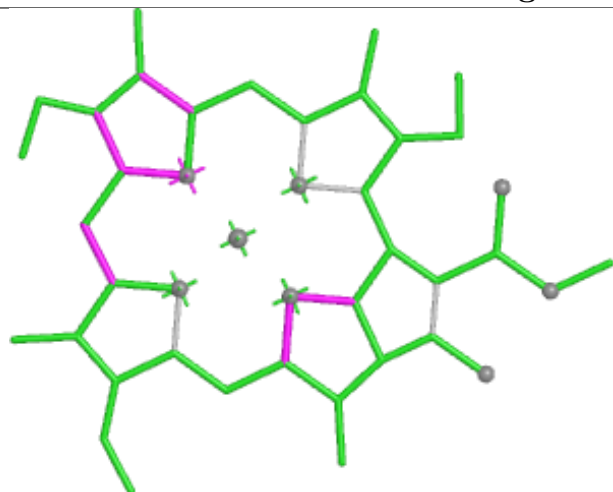




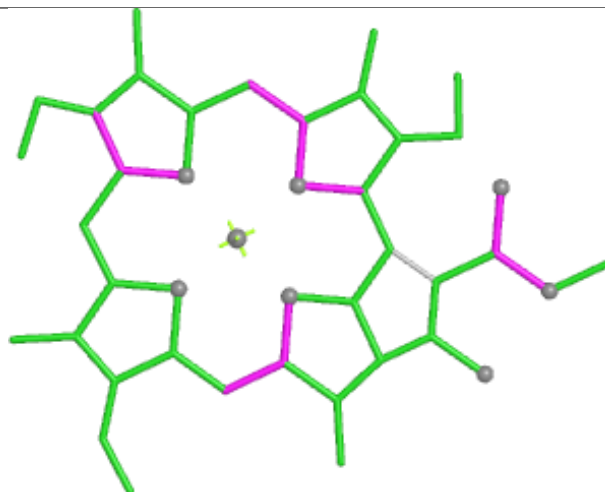
Ligand CLA P 611



Ligand CLA 1 601



Bond lengths



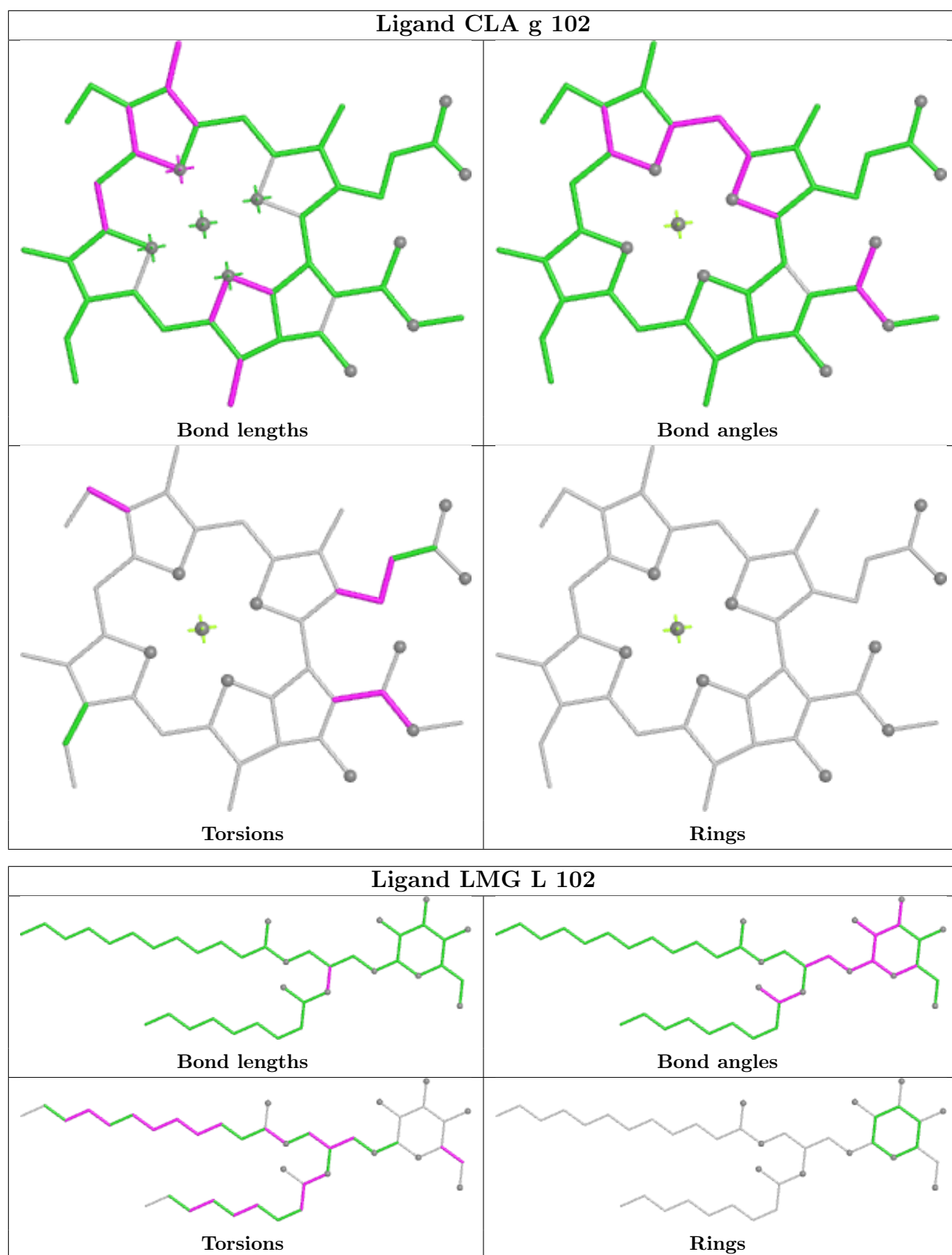
Bond angles

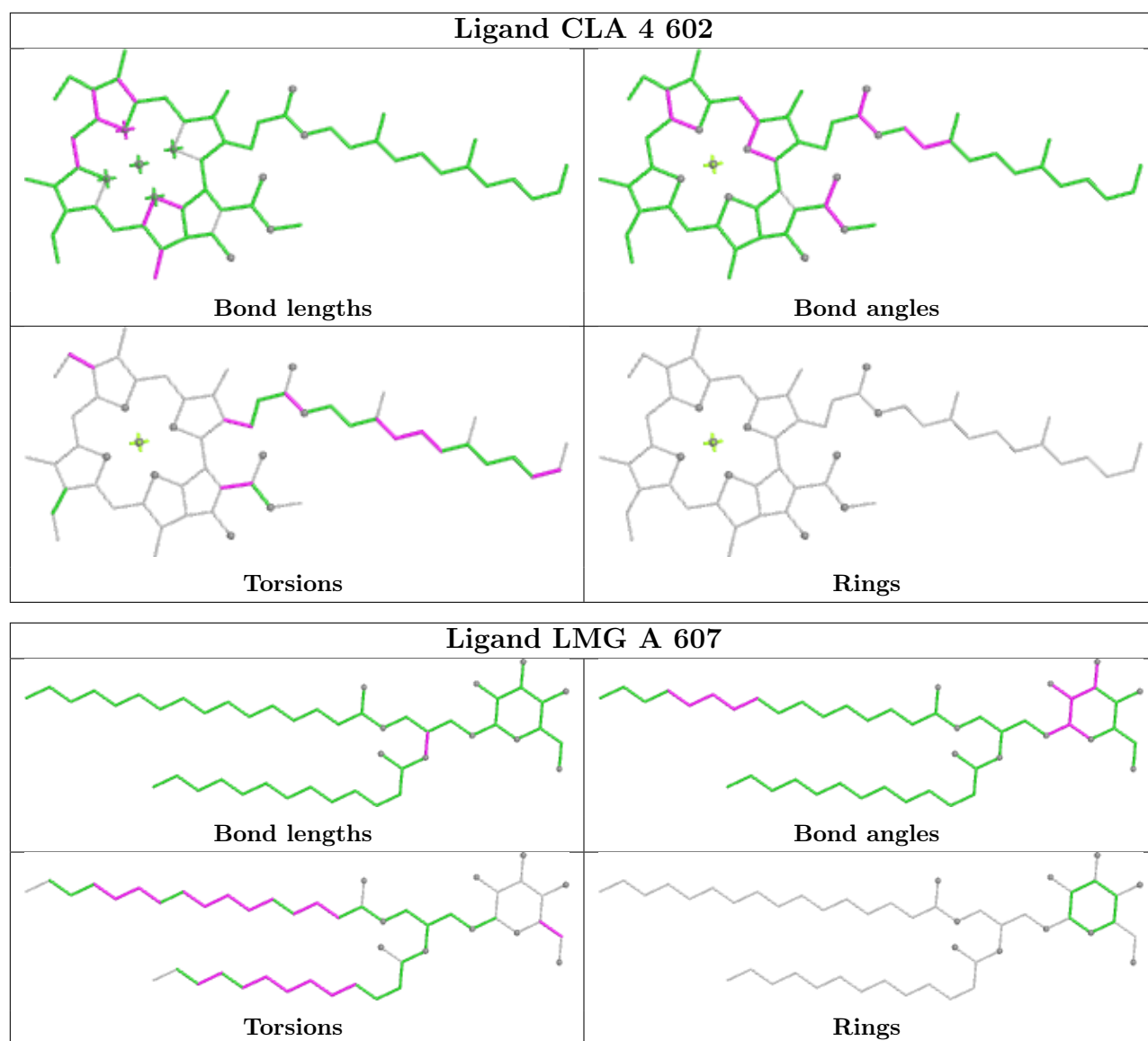


Torsions

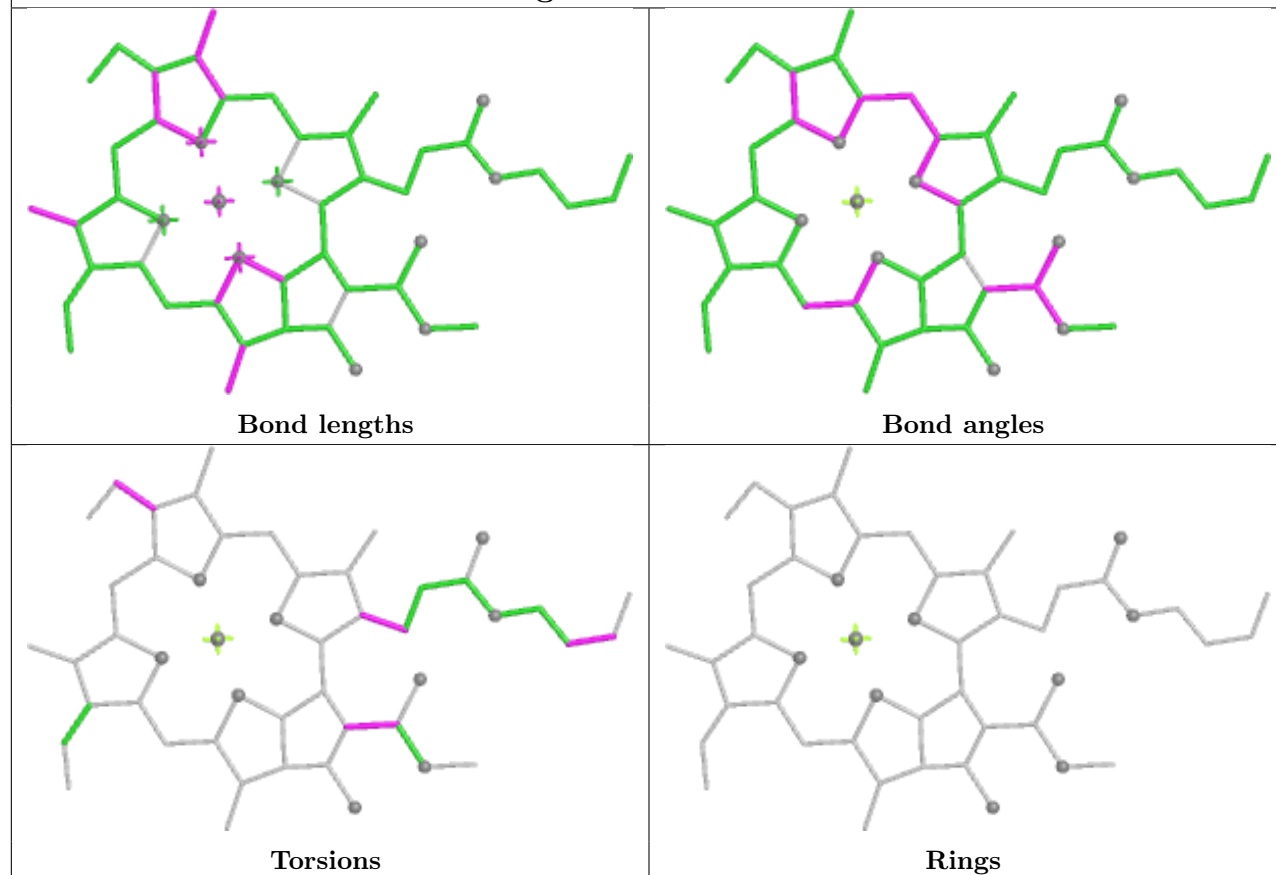


Rings

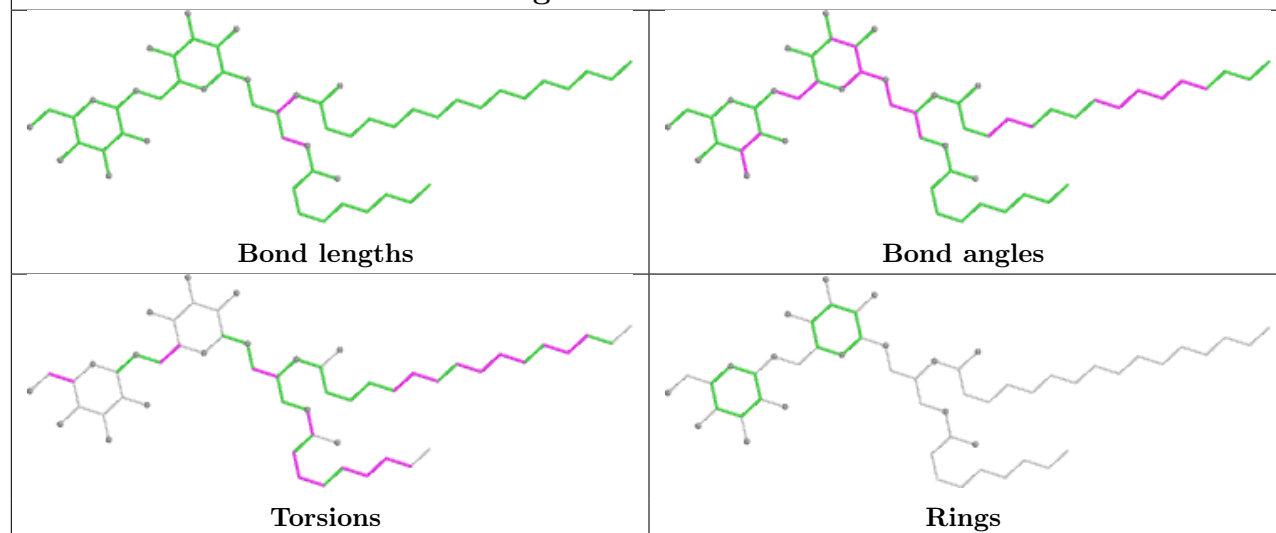




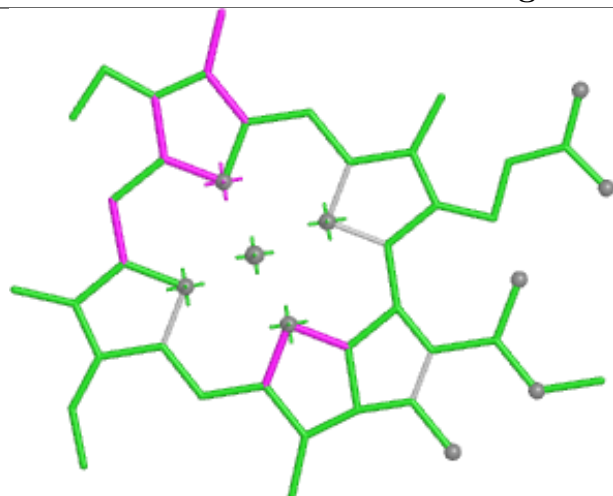
Ligand CLA a 406



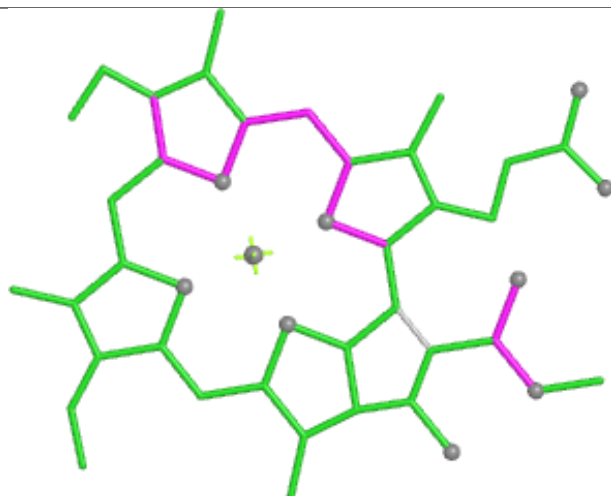
Ligand DGD c 514



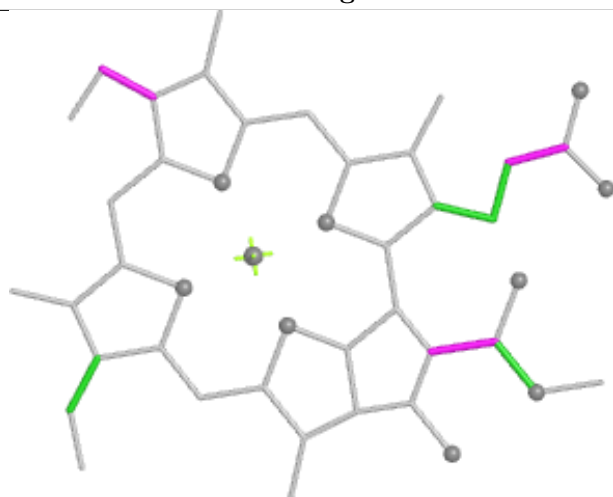
Ligand CLA 5 307



Bond lengths



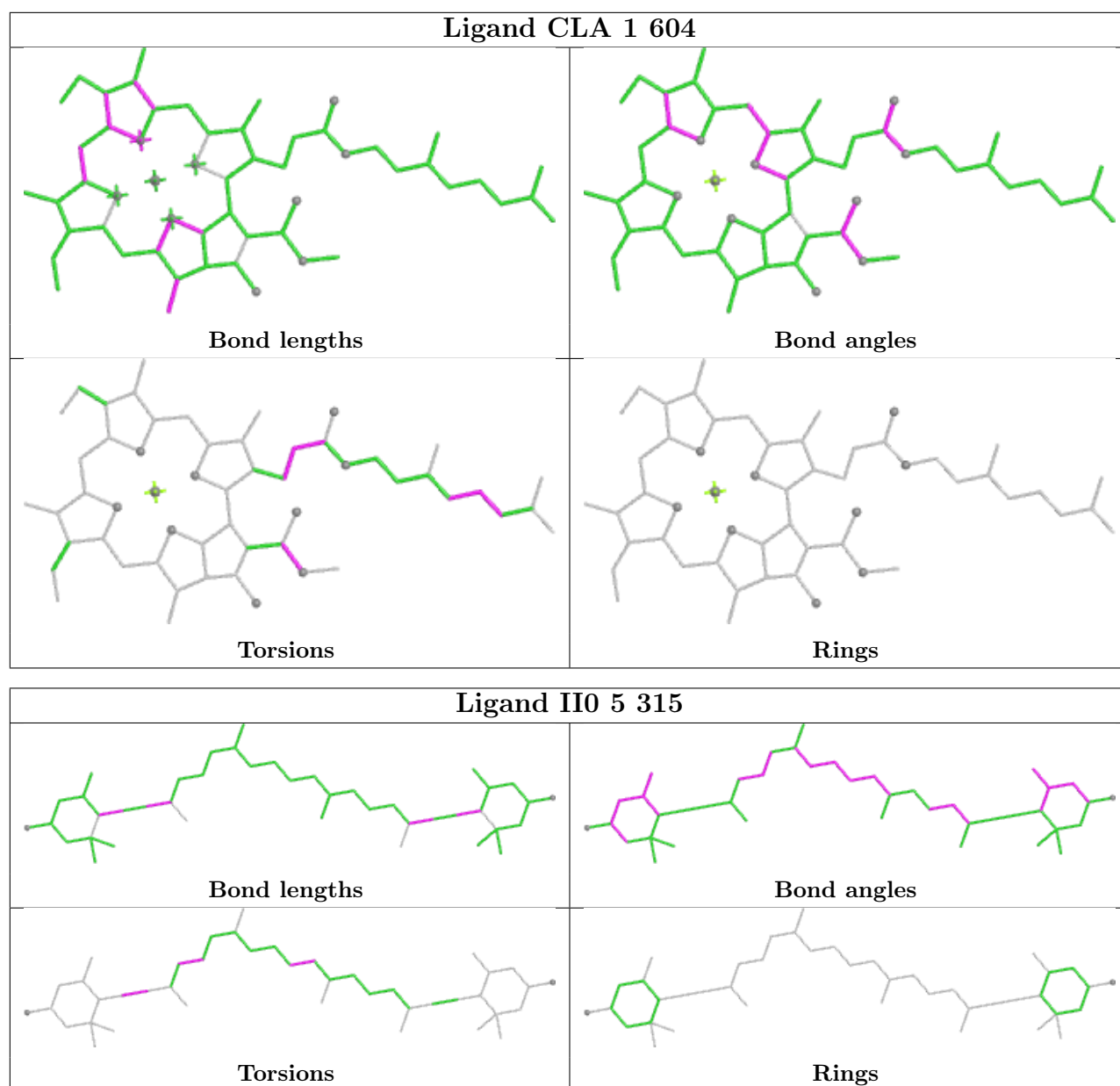
Bond angles

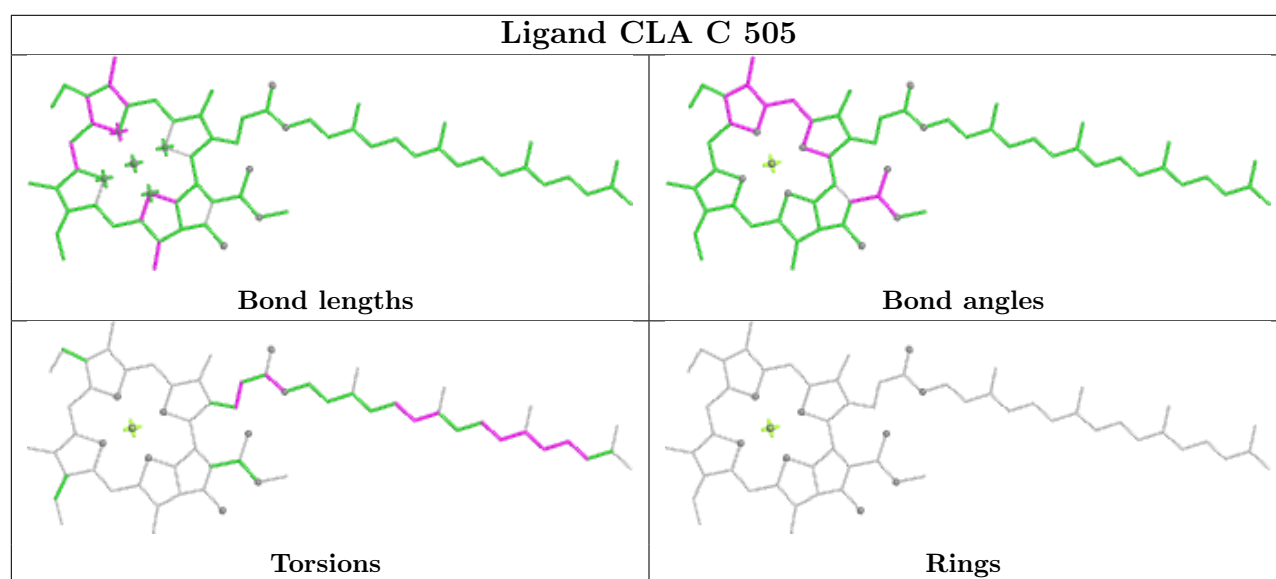
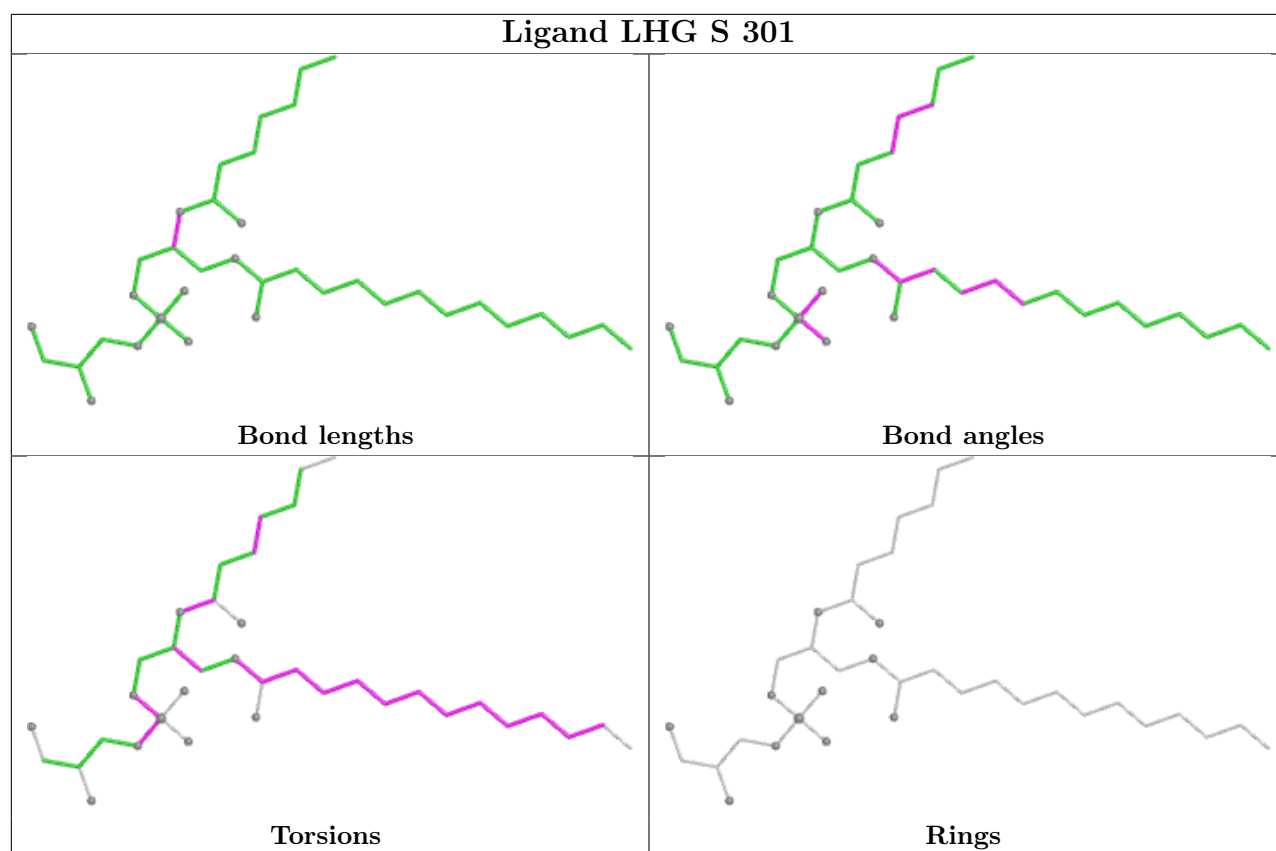


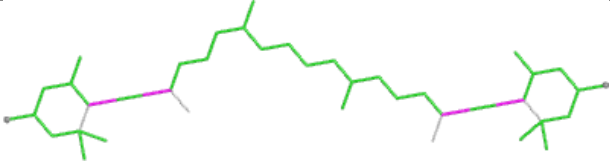
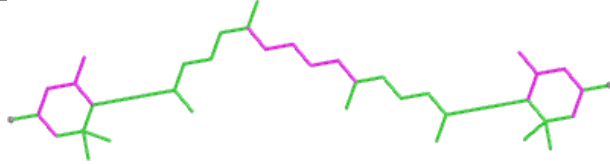
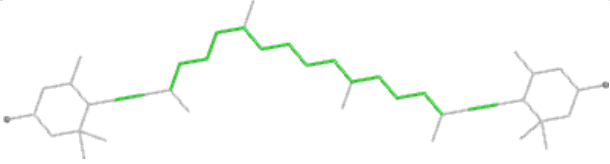
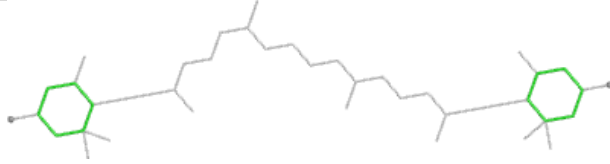
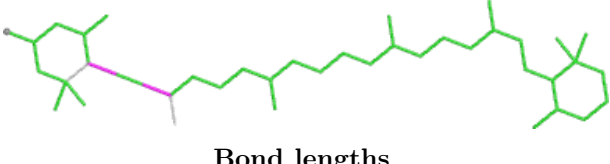
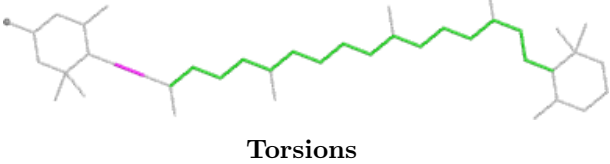
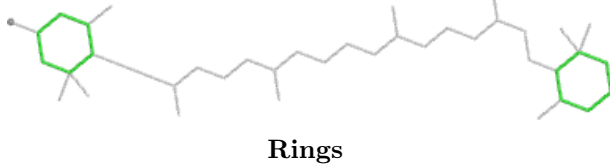
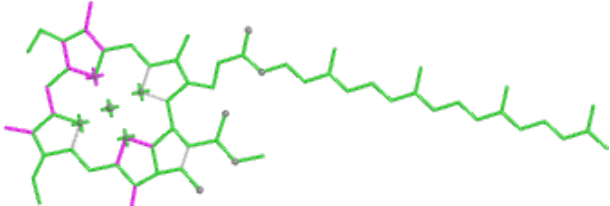
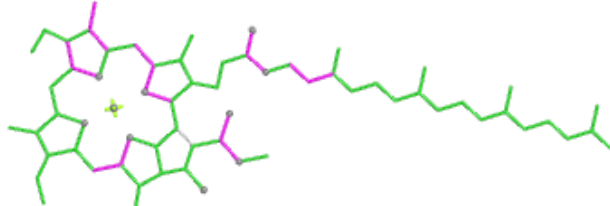
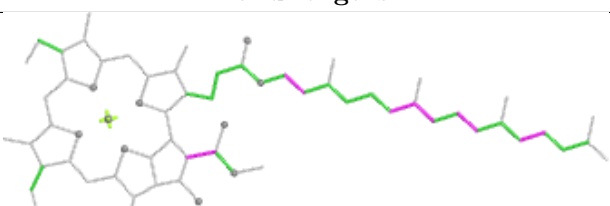
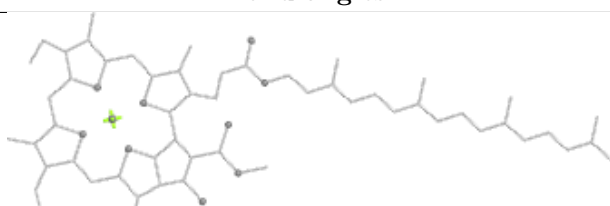
Torsions



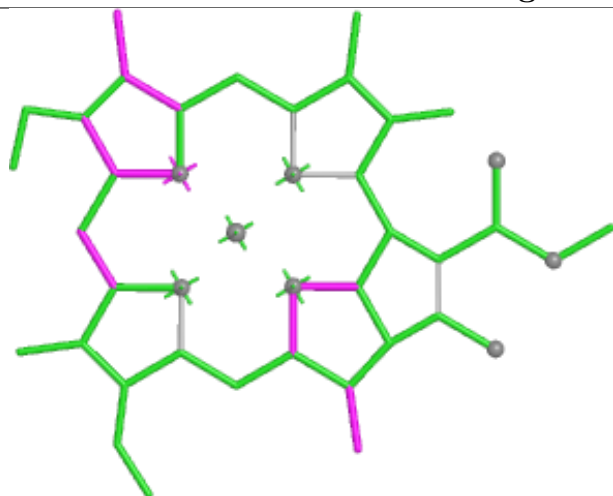
Rings



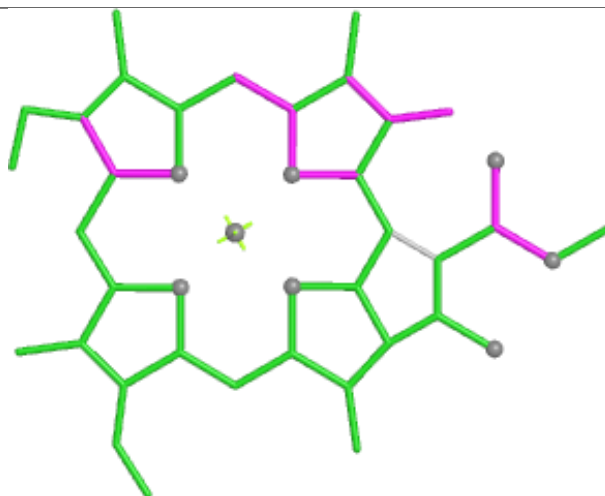


Ligand II0 3 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand IHT 5 317	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

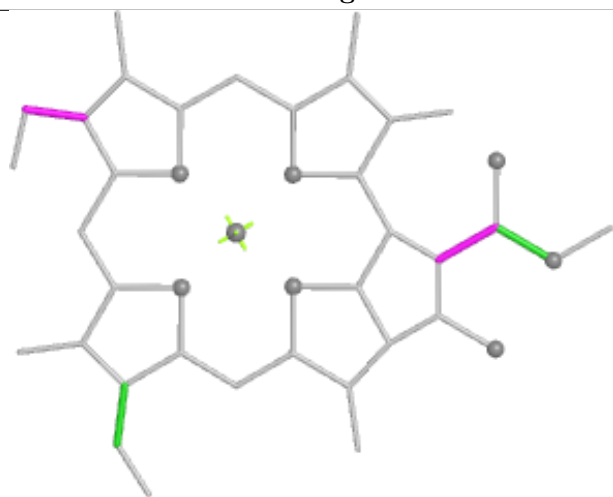
Ligand CLA 9 608



Bond lengths



Bond angles

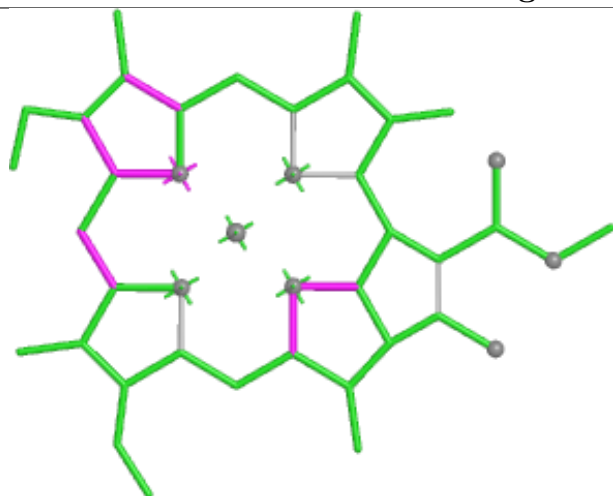


Torsions

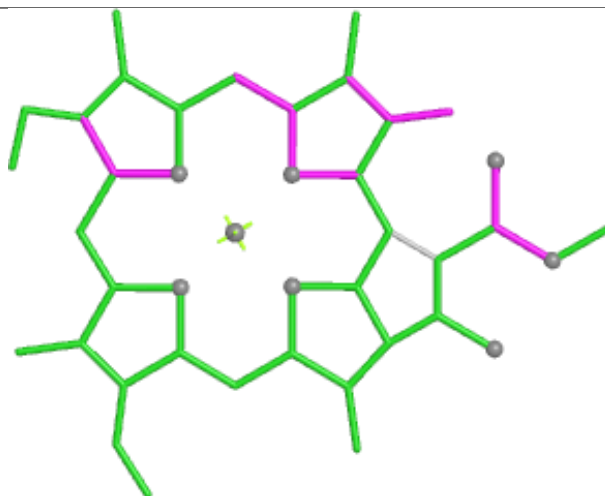


Rings

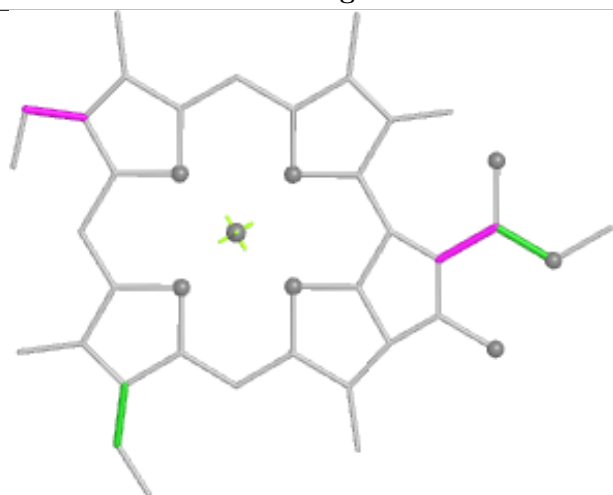
Ligand CLA 0 609



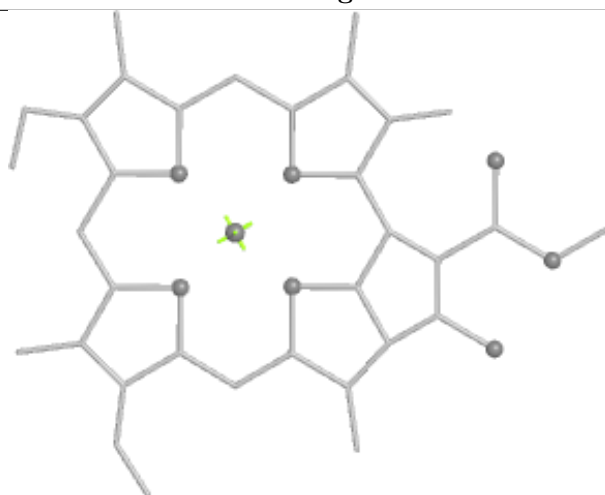
Bond lengths



Bond angles

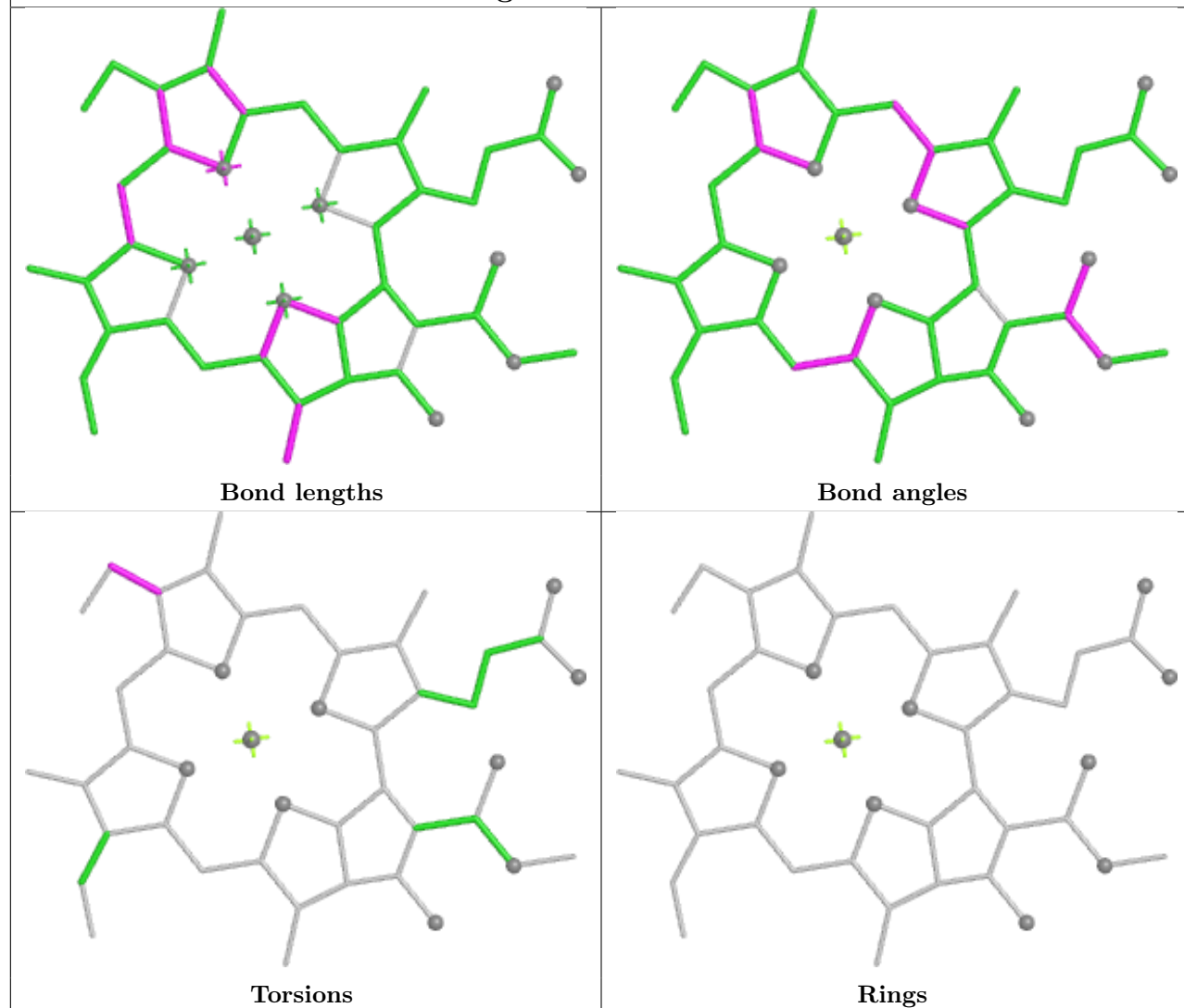


Torsions

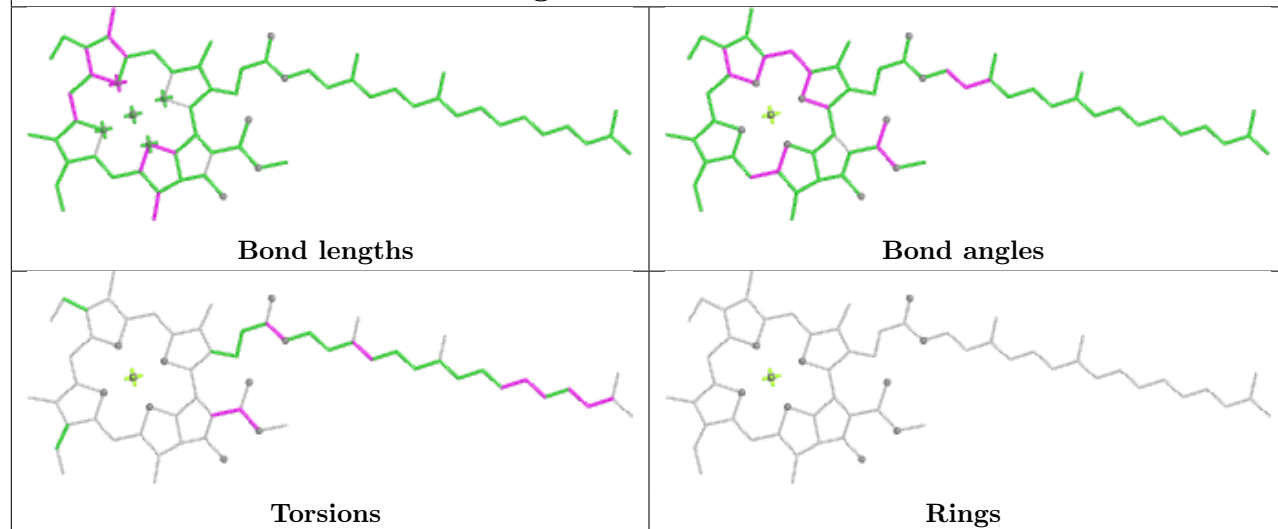


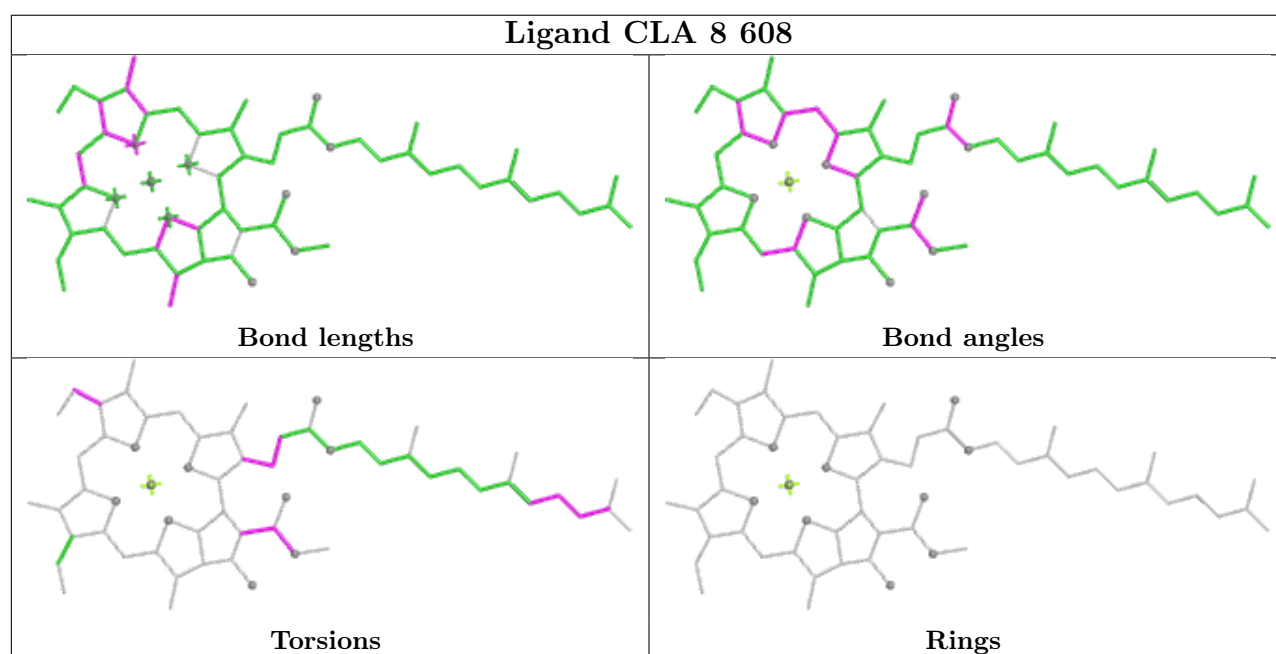
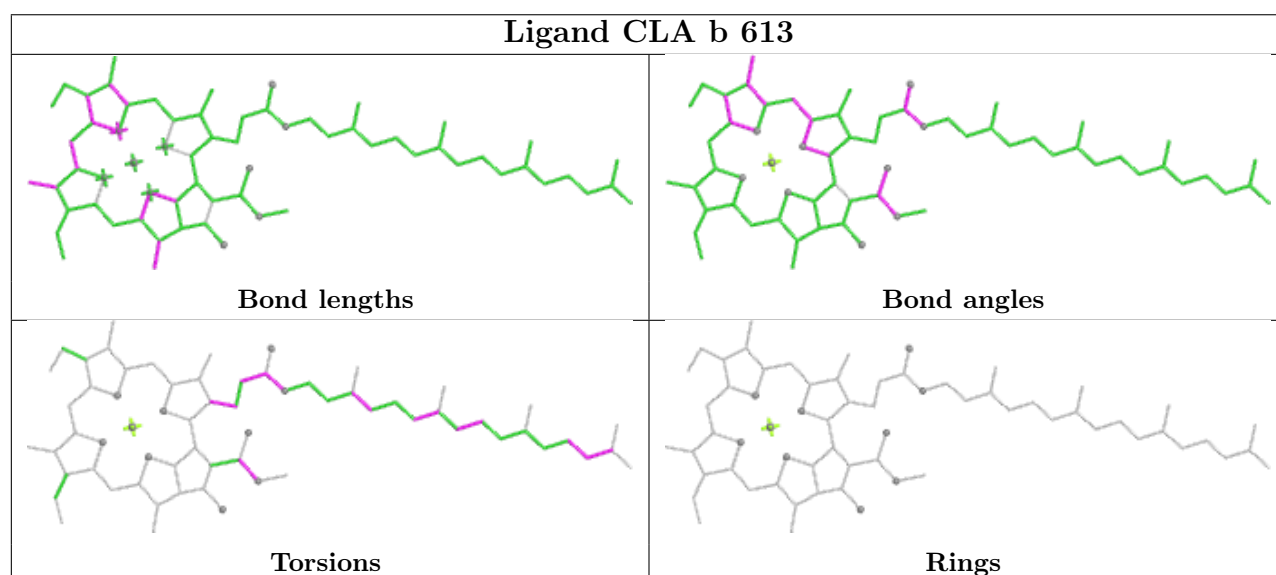
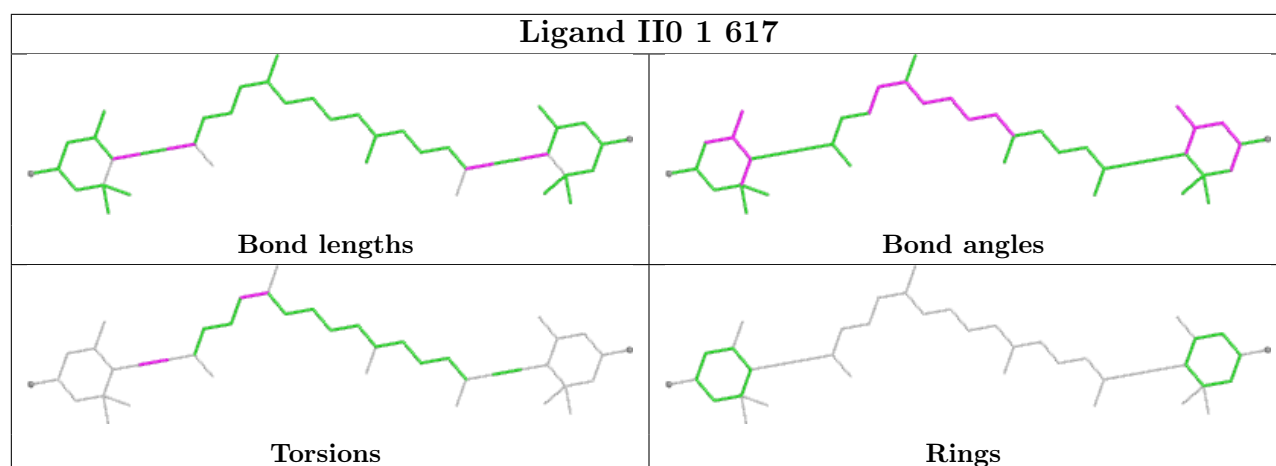
Rings

Ligand CLA 0 607

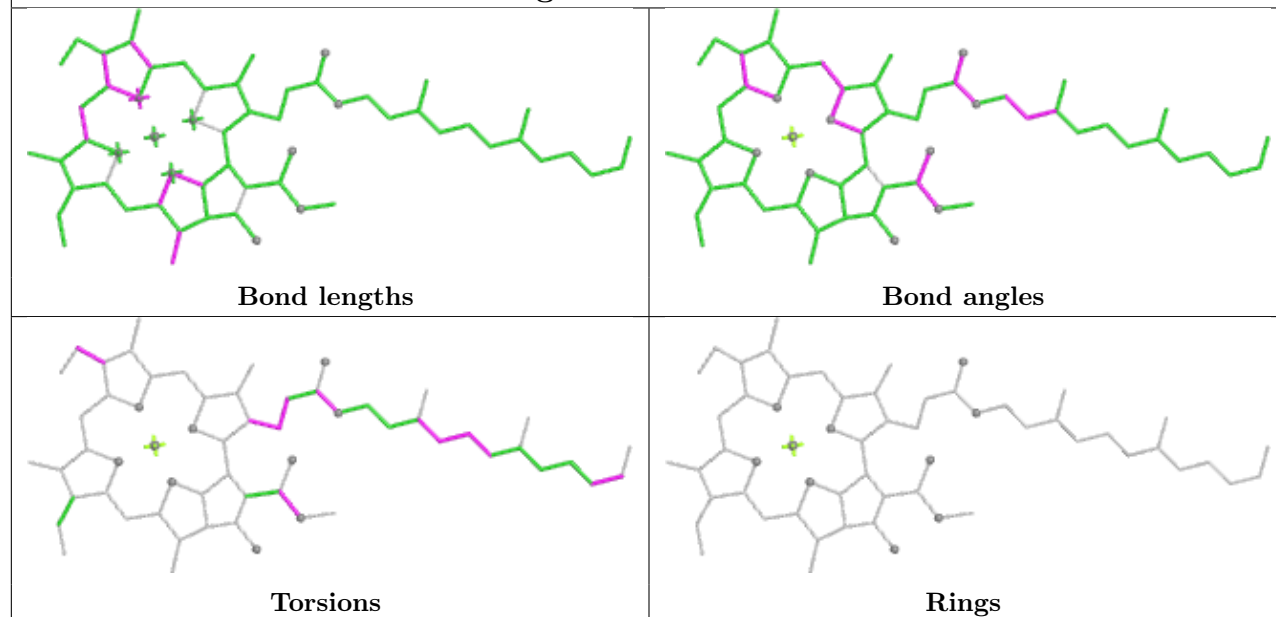


Ligand CLA B 615

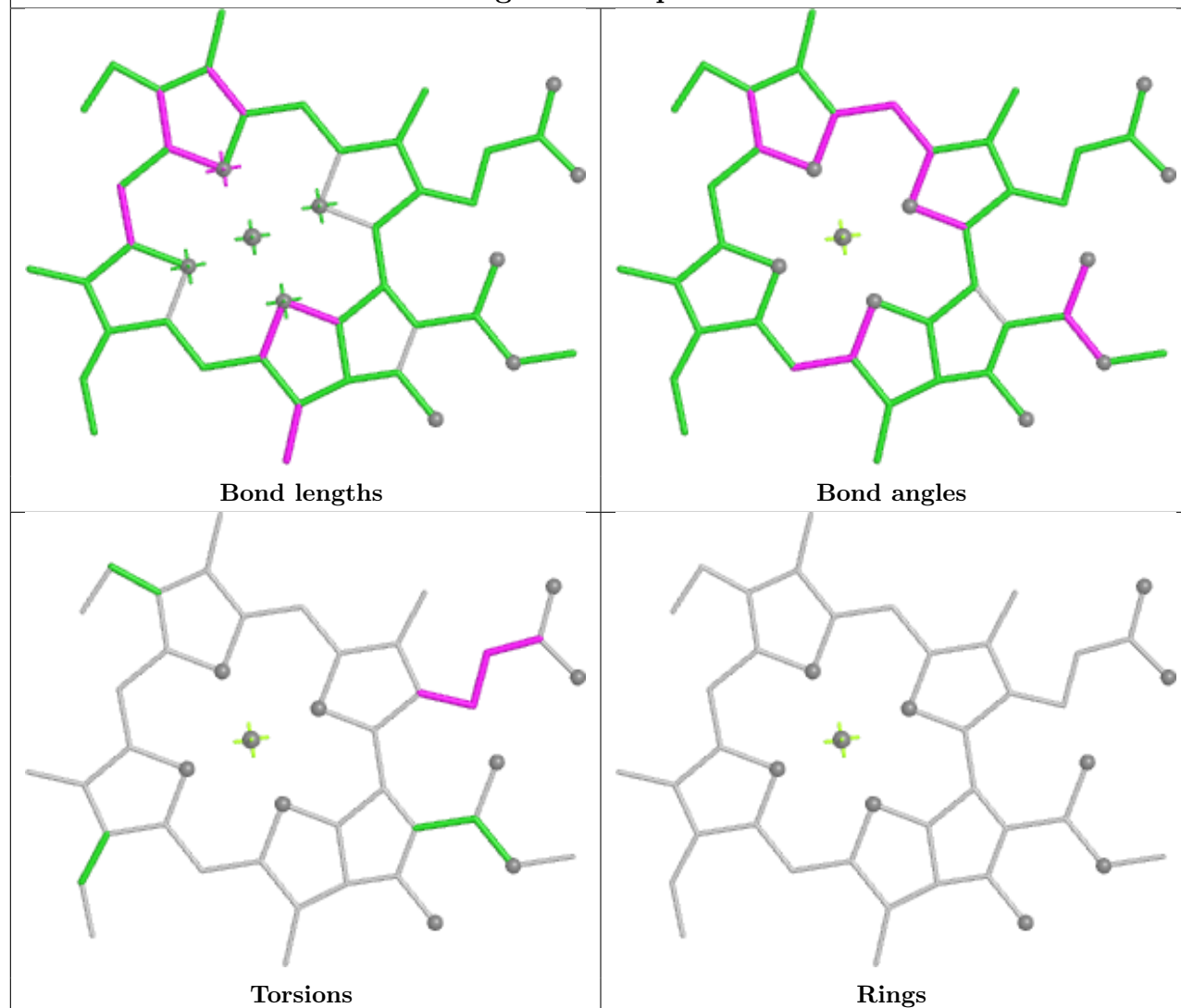


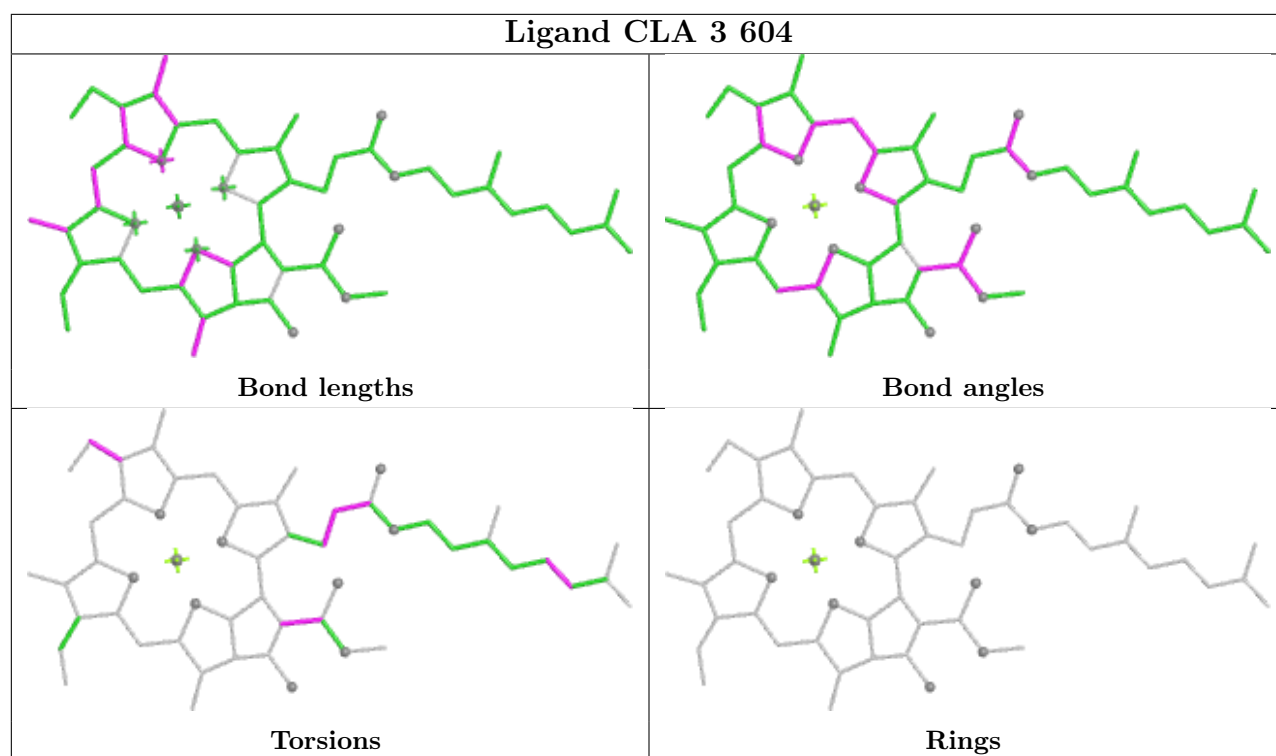


Ligand CLA 1 602

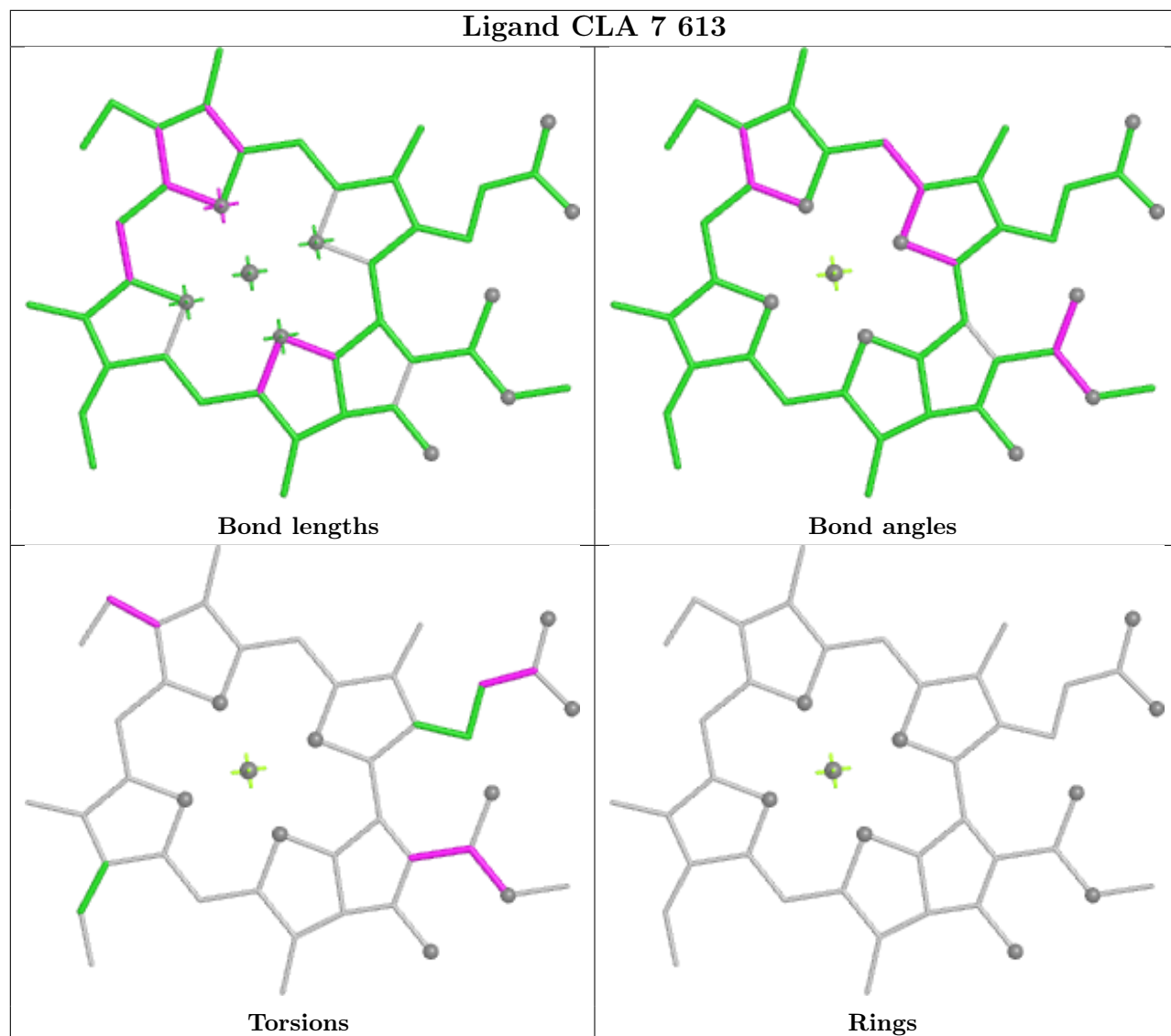


Ligand CLA p 308

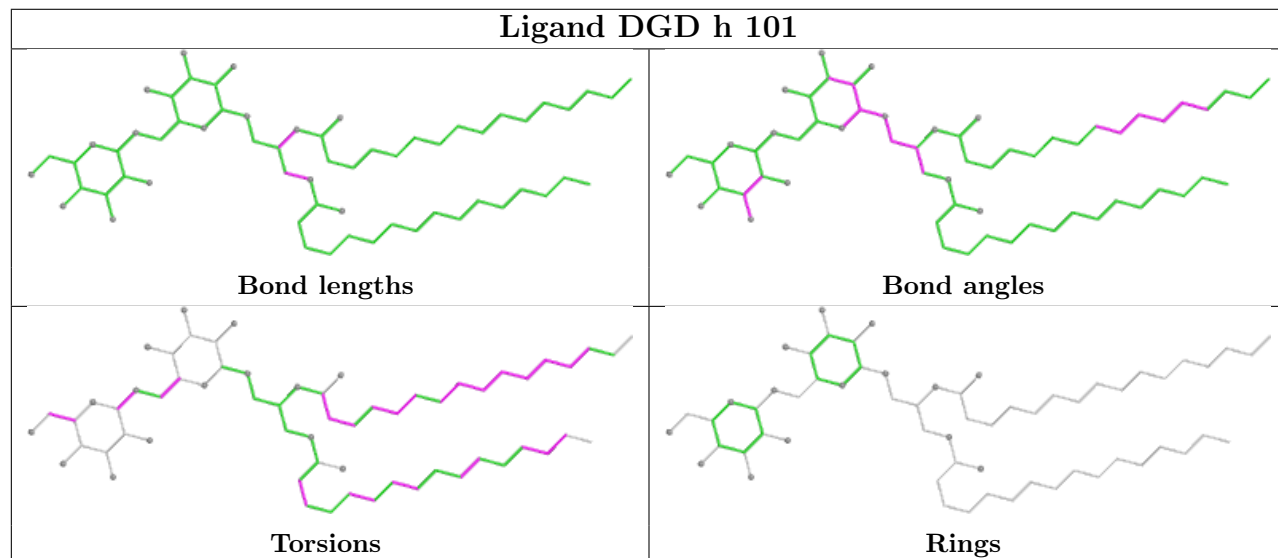




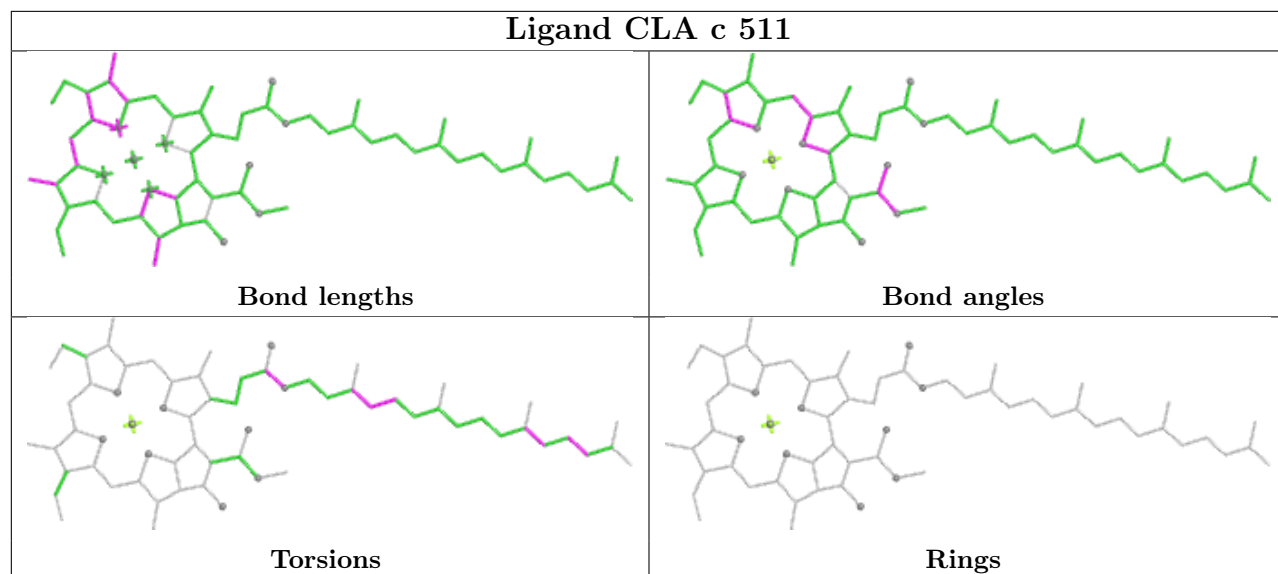
Ligand CLA 7 613



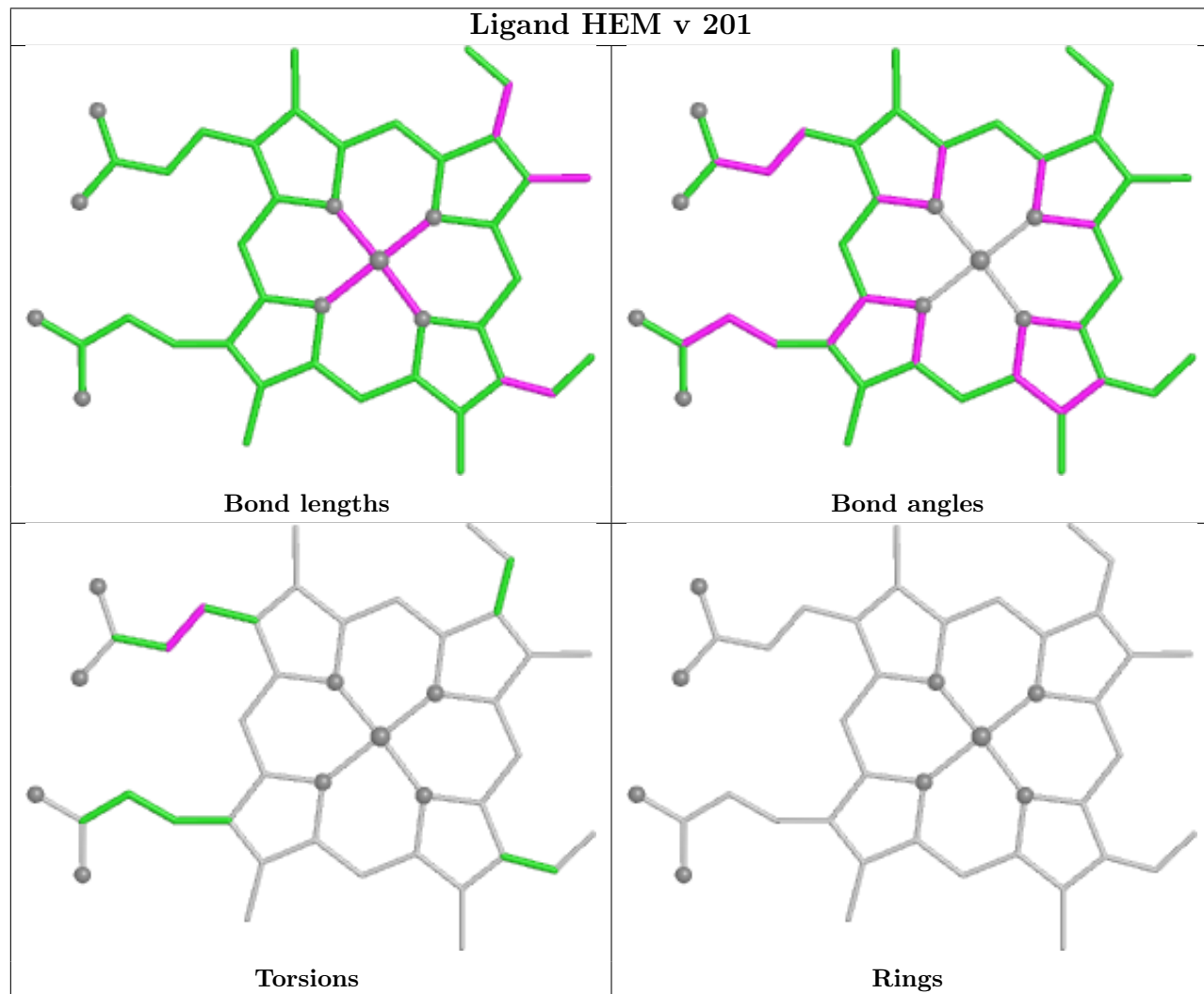
Ligand DGD h 101

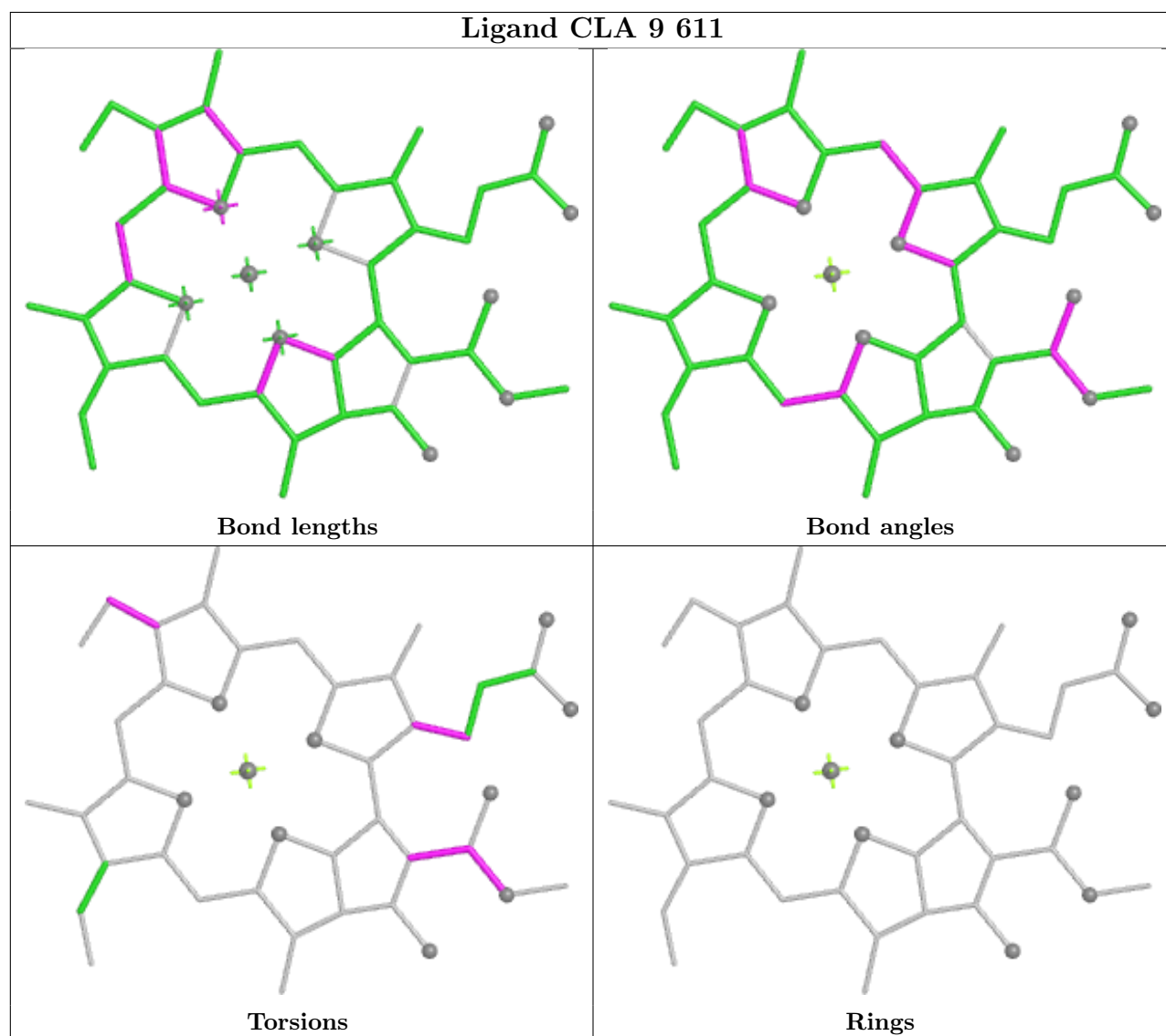
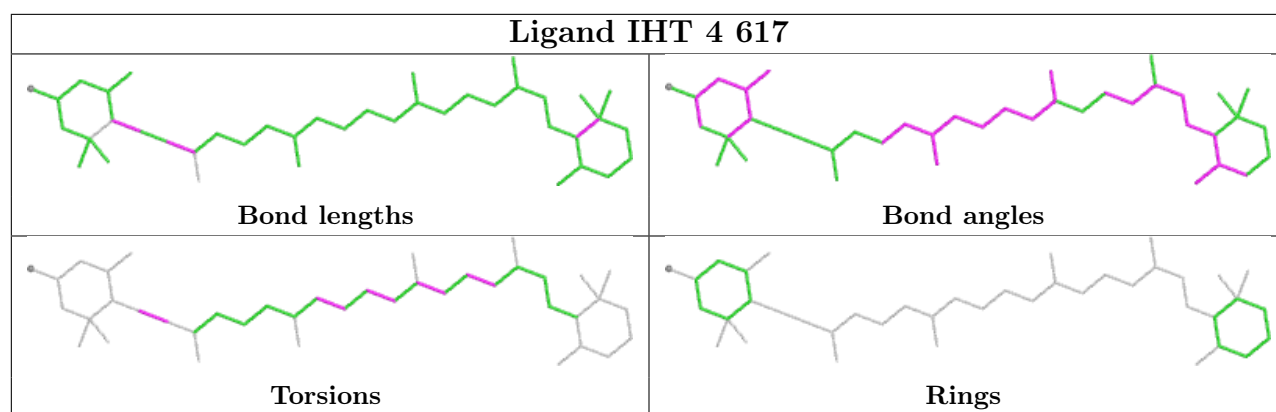


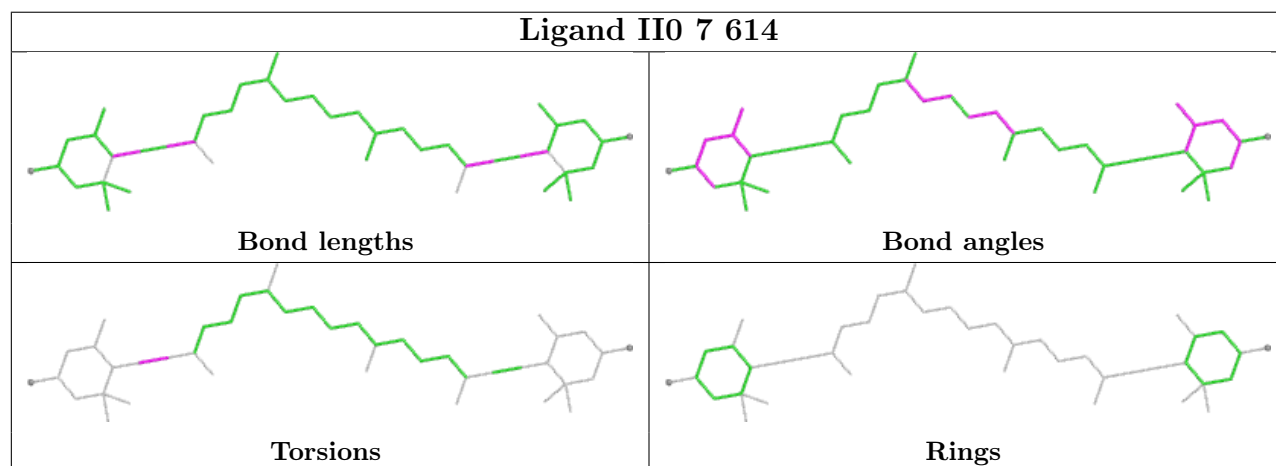
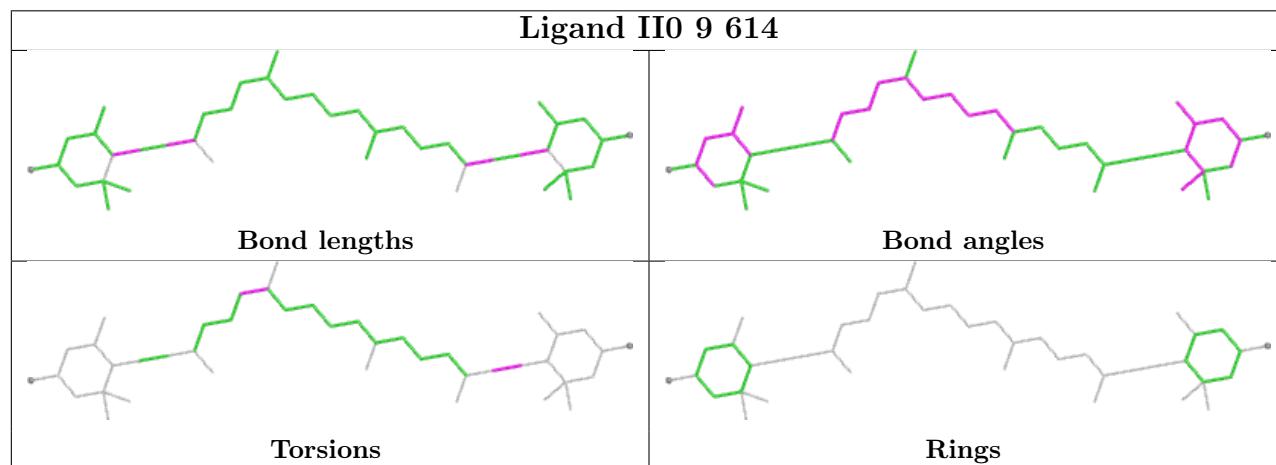
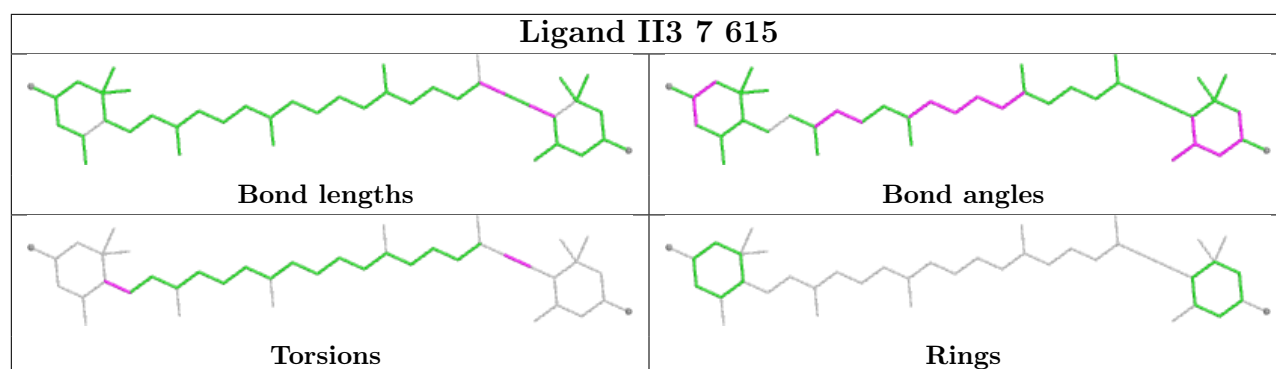
Ligand CLA c 511

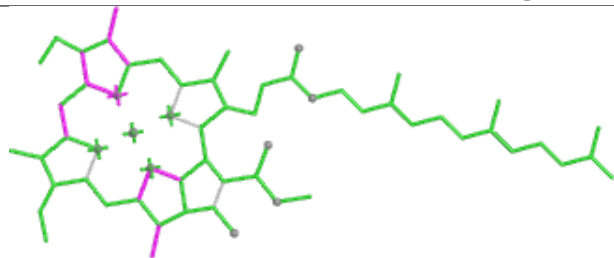
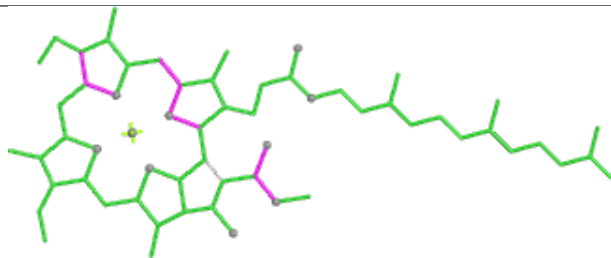
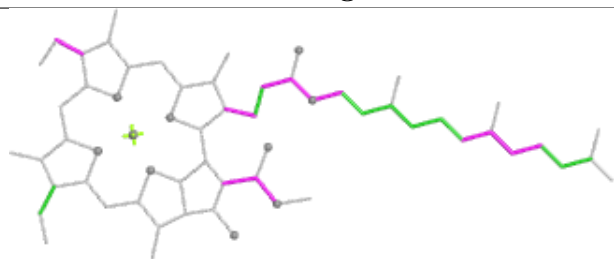
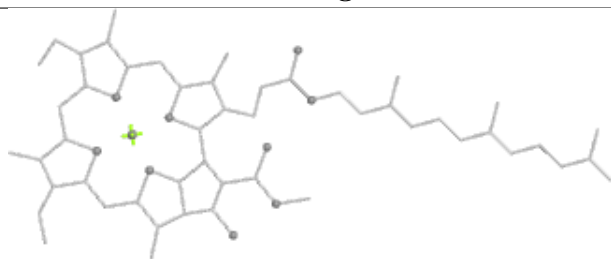
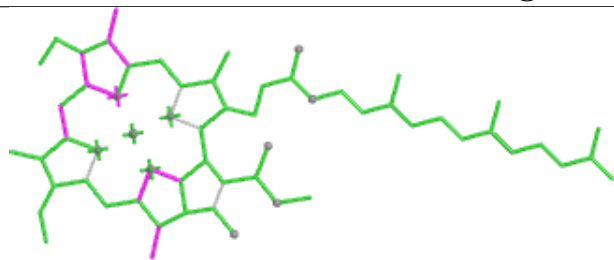
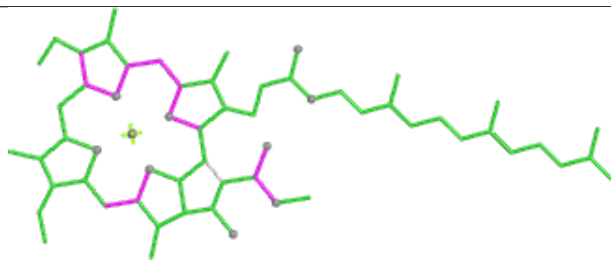
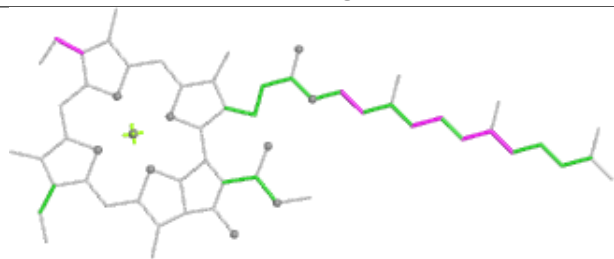
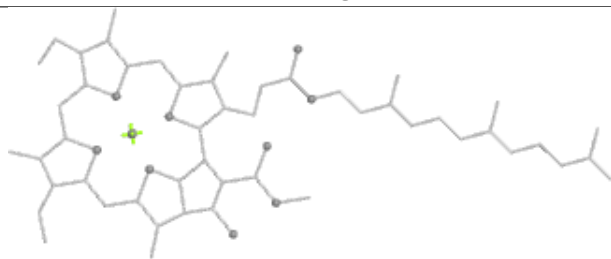


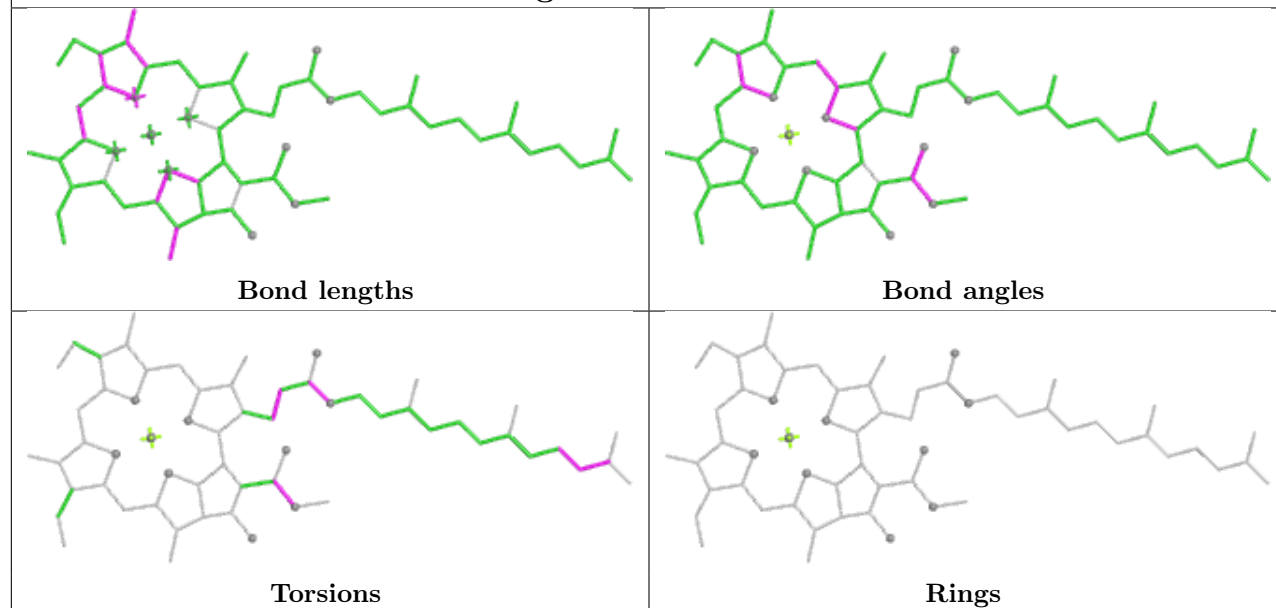
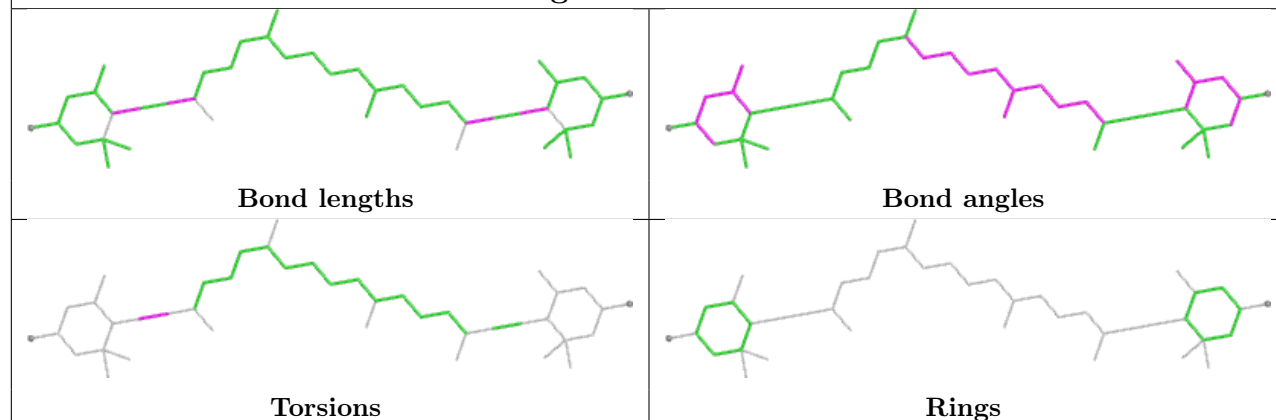
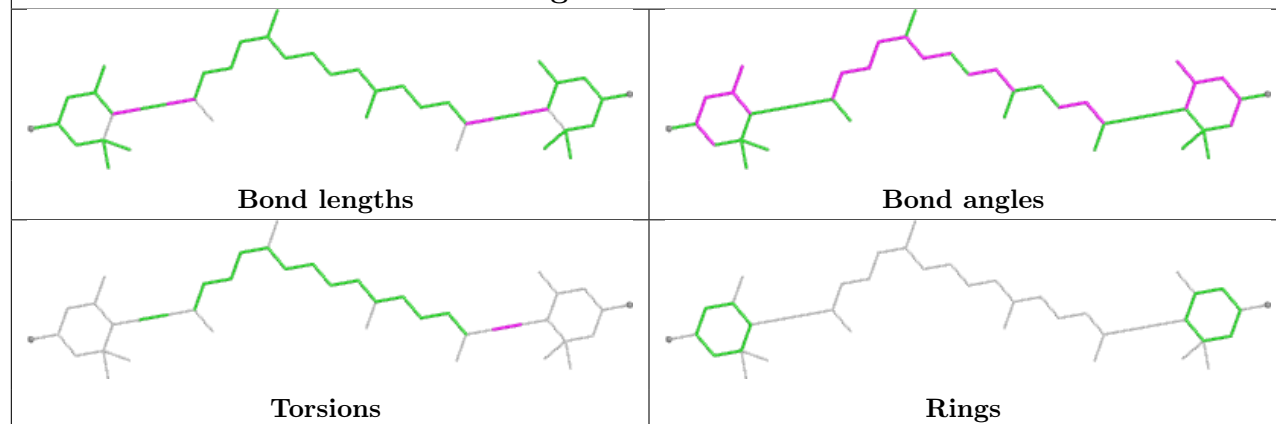
Ligand HEM v 201

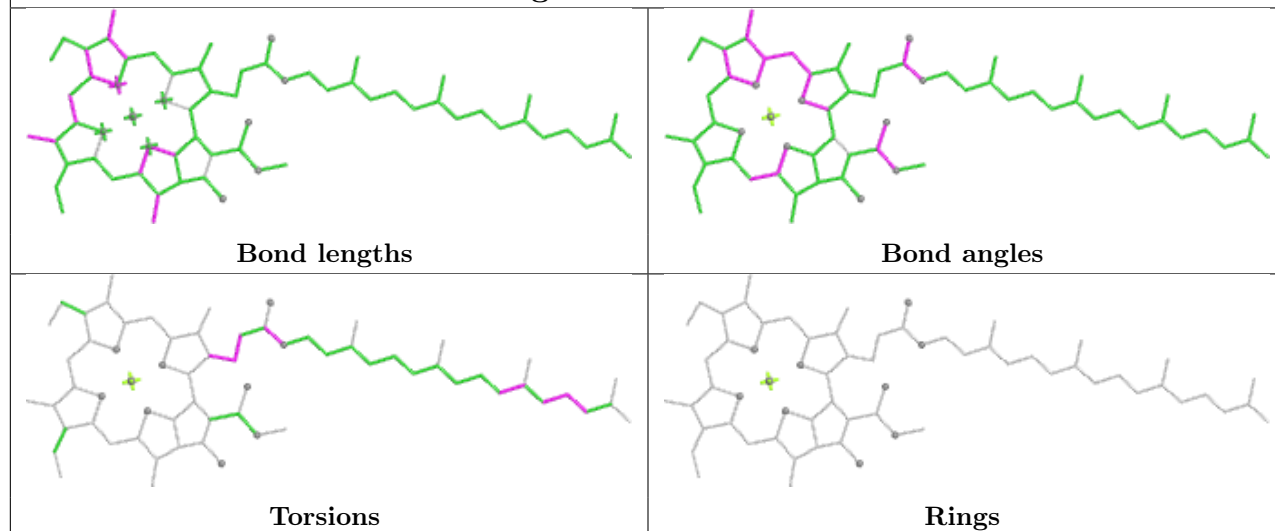
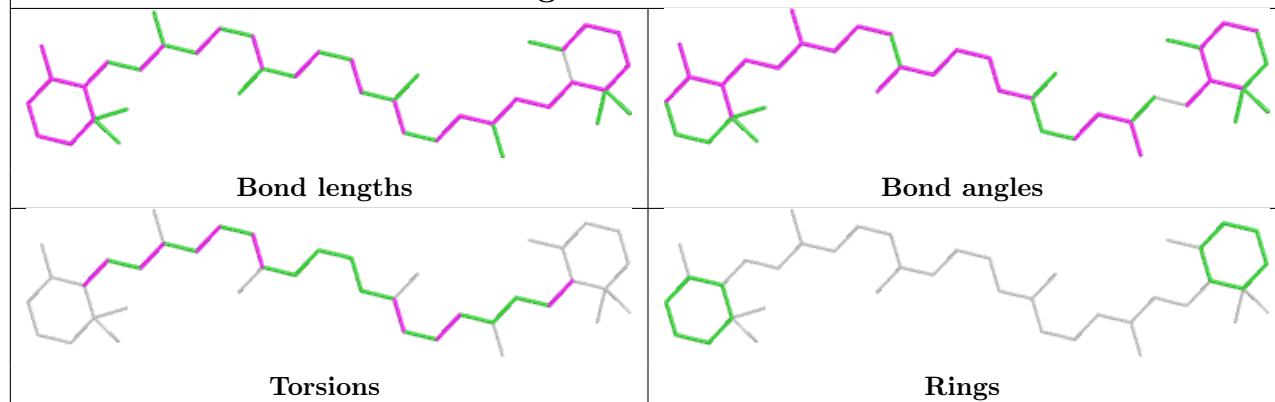
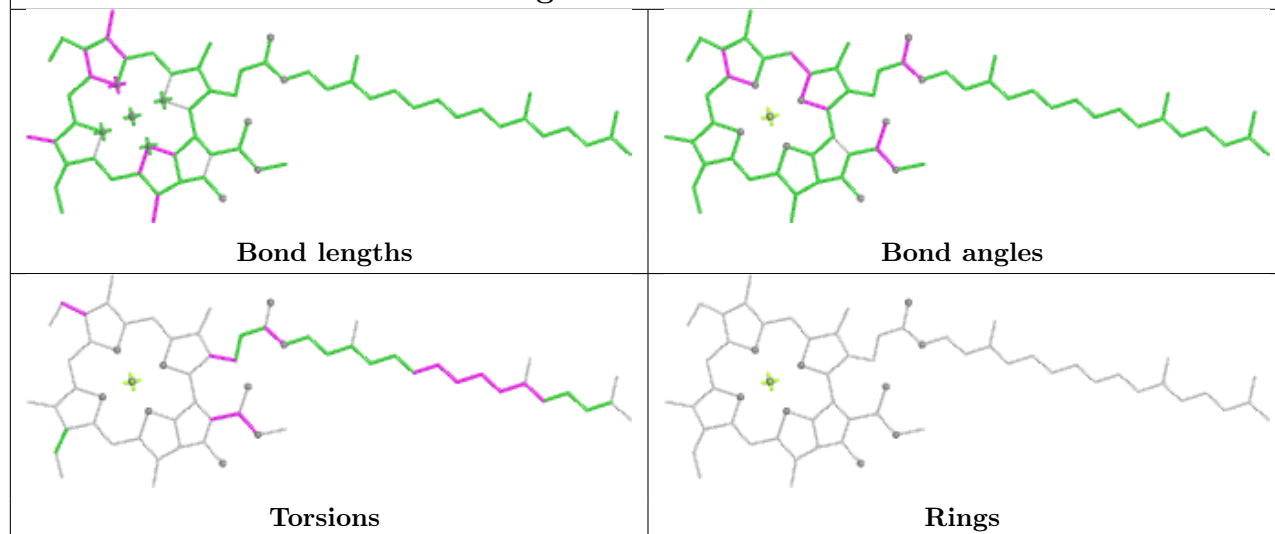




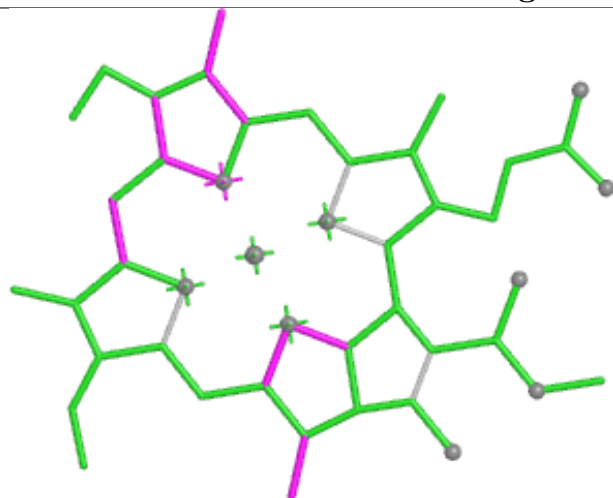


Ligand CLA 5 306**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 3 609****Bond lengths****Bond angles****Torsions****Rings**

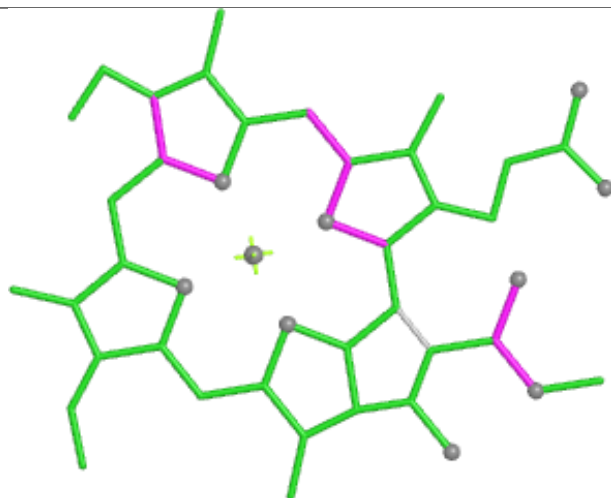
Ligand CLA 3 607**Ligand II0 0 615****Ligand II0 3 612**

Ligand CLA B 609**Ligand 8CT 9 615****Ligand CLA c 502**

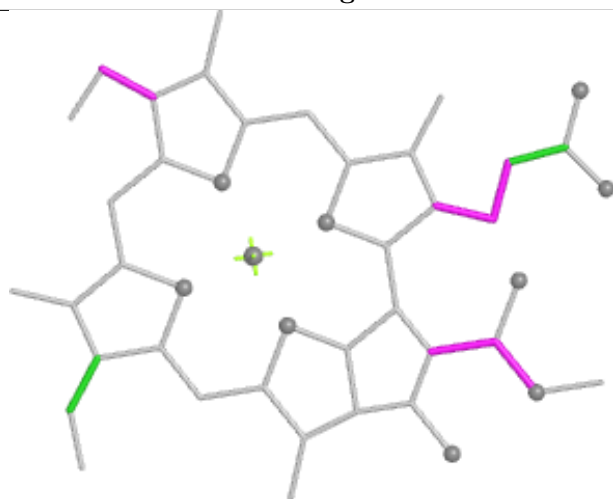
Ligand CLA 5 312



Bond lengths



Bond angles

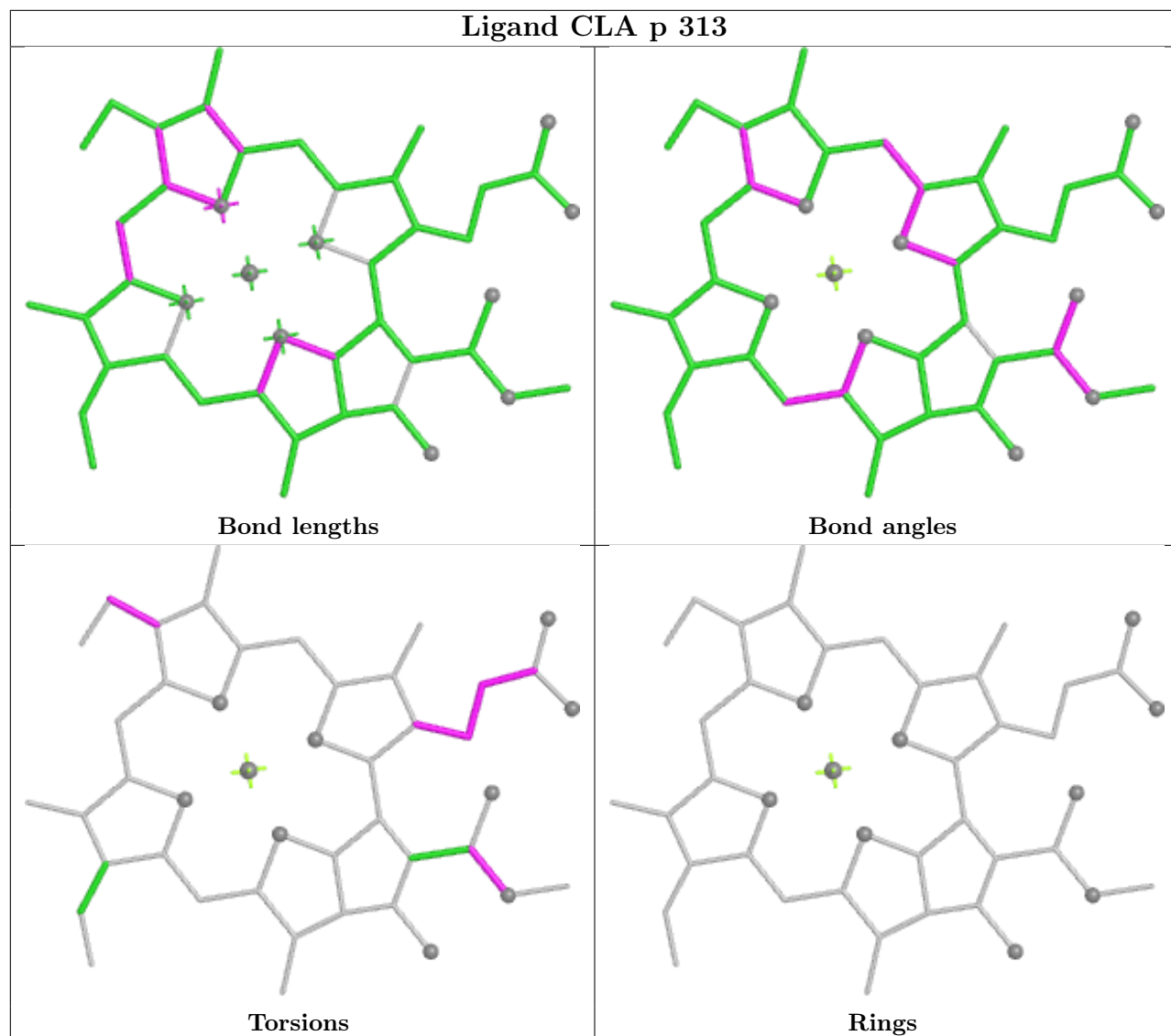


Torsions

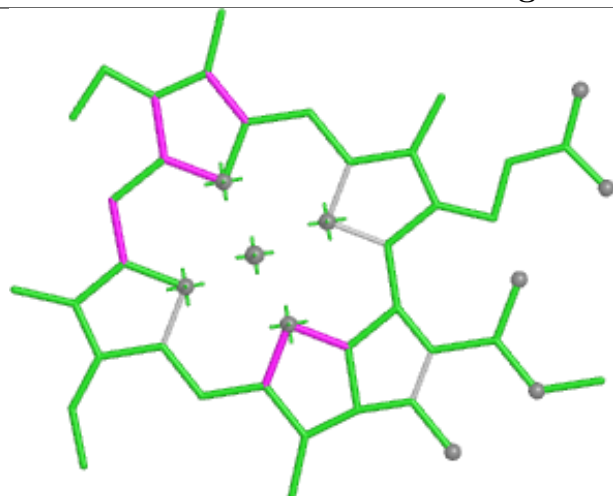


Rings

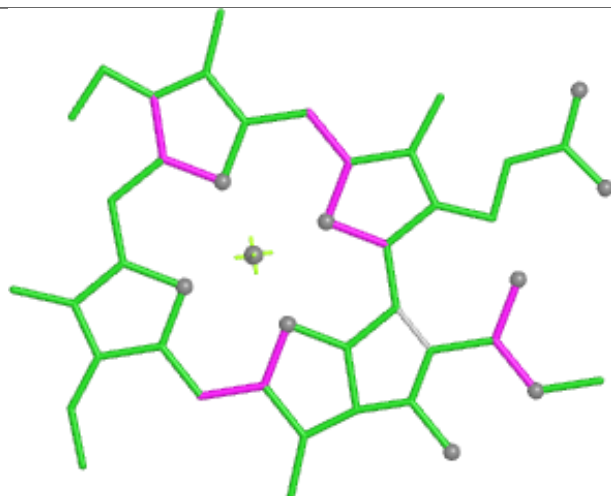
Ligand CLA p 313



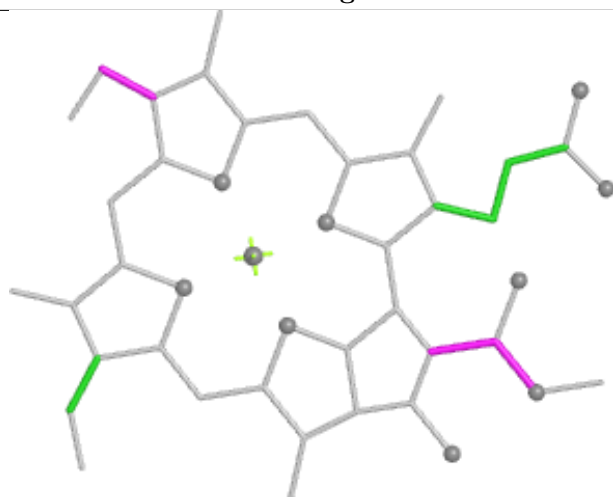
Ligand CLA 6 606



Bond lengths



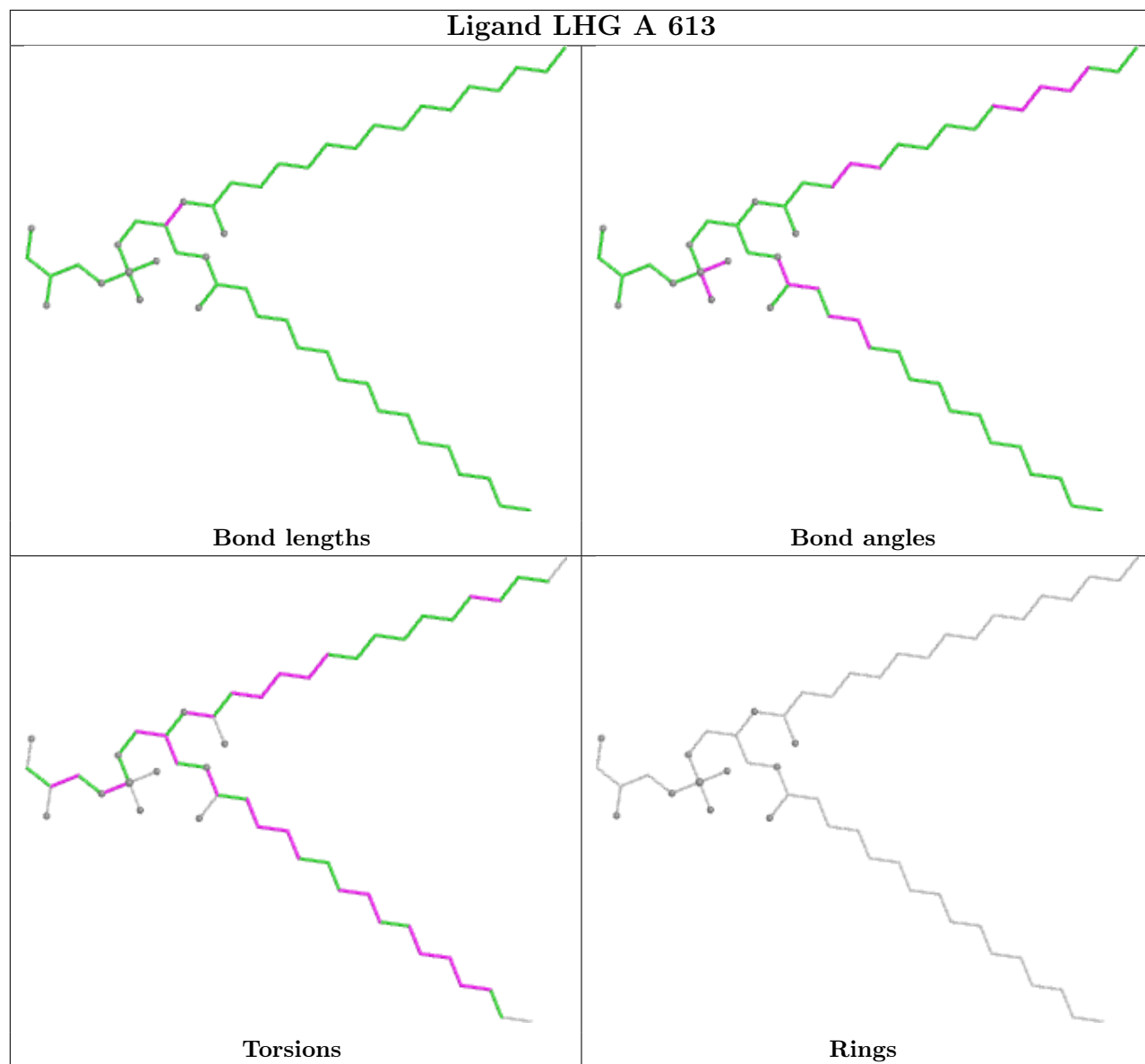
Bond angles

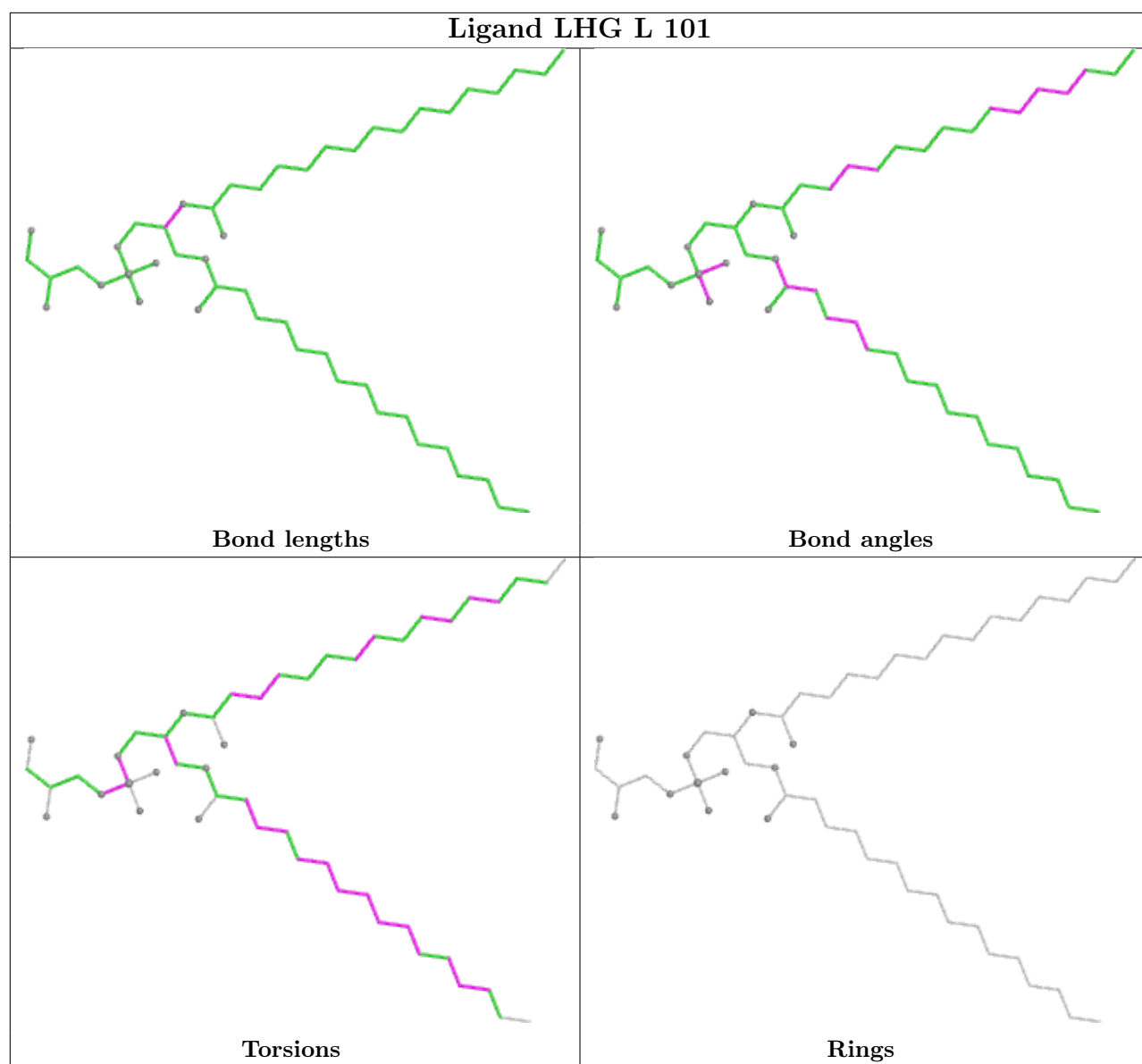


Torsions

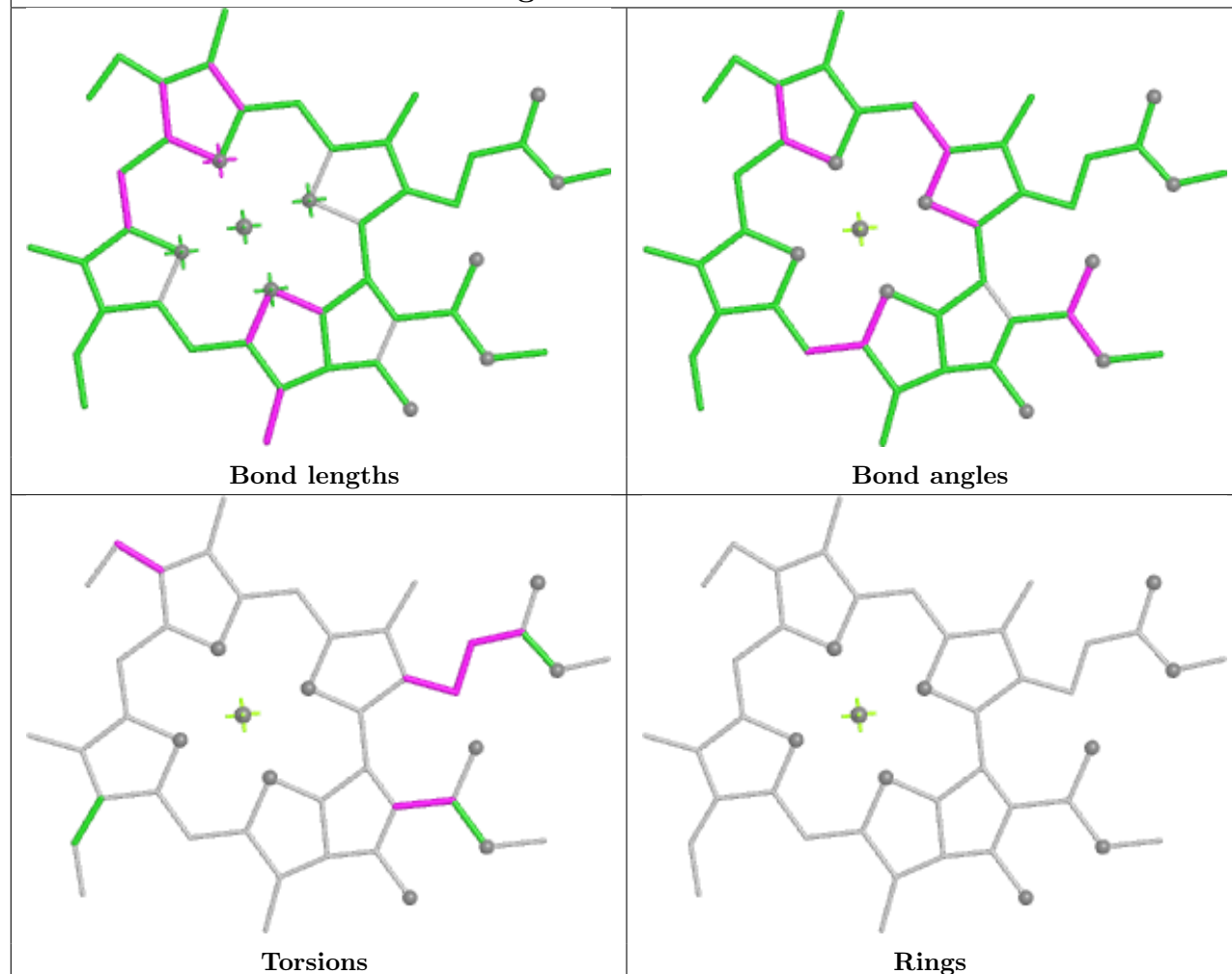


Rings

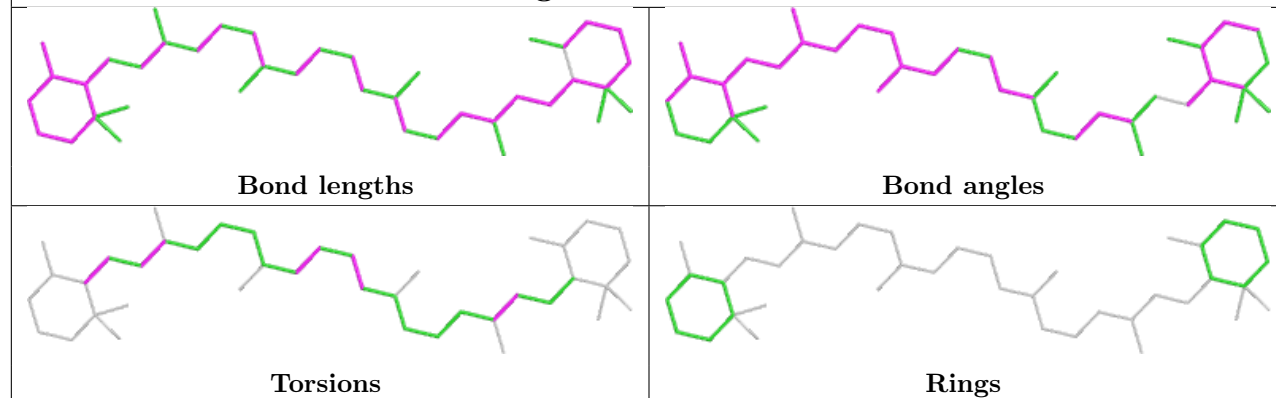




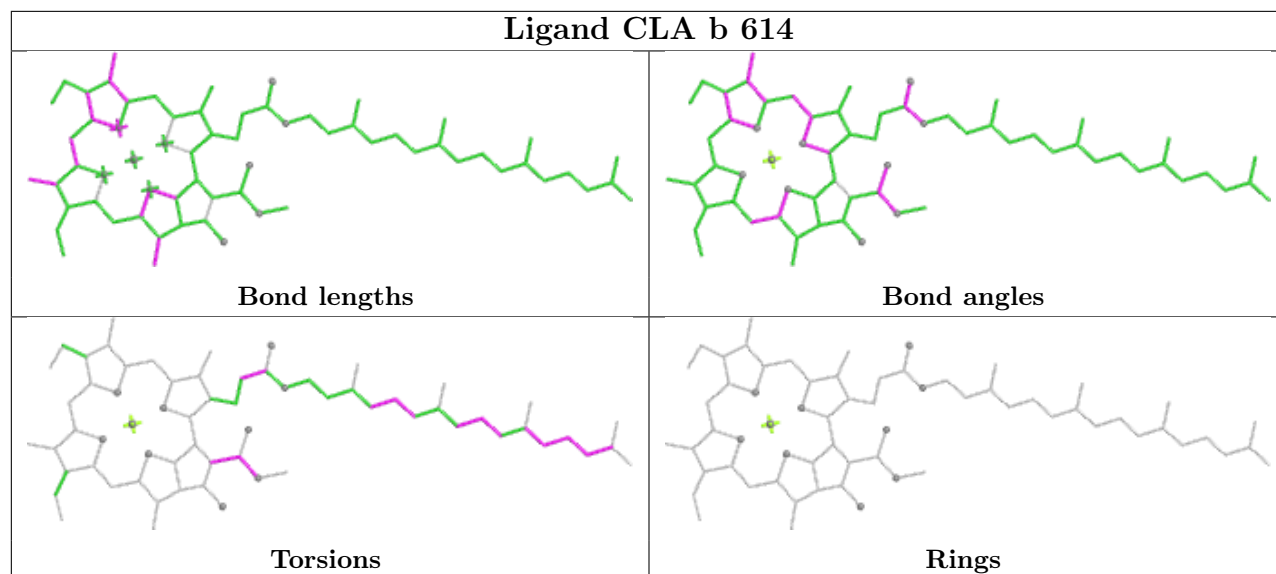
Ligand CLA 9 605



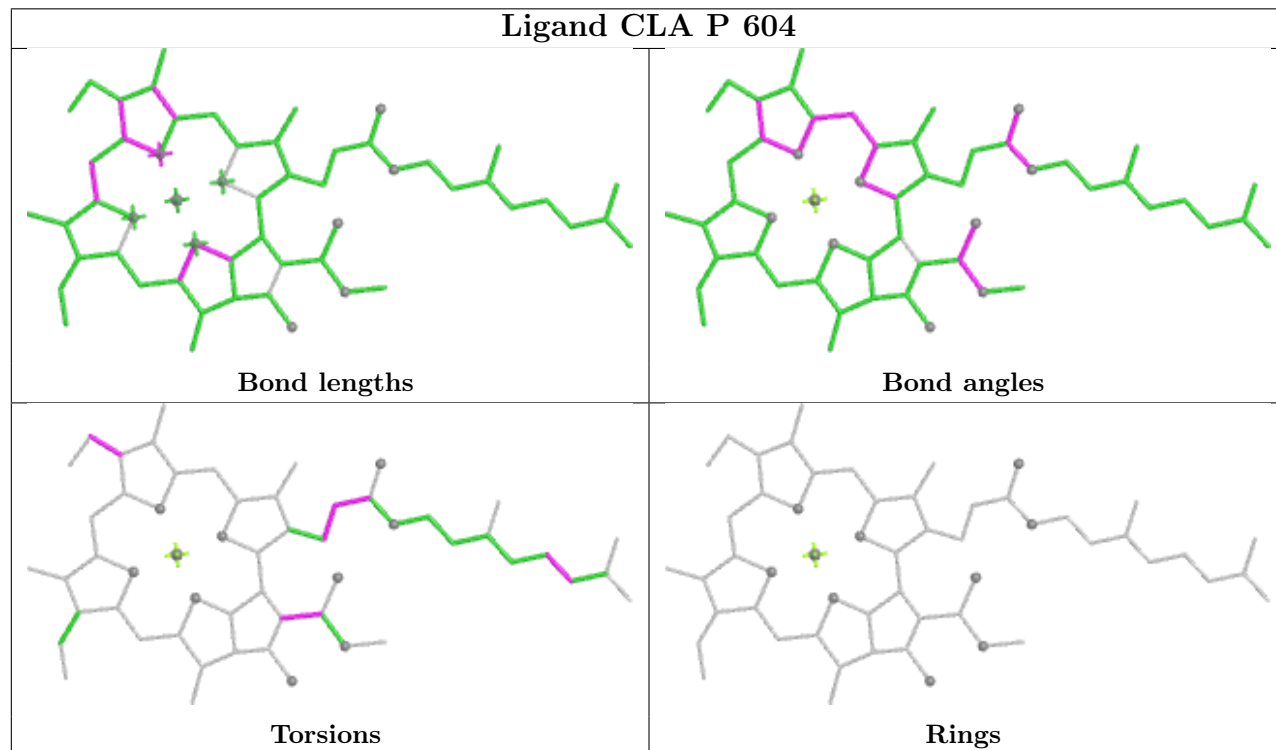
Ligand 8CT B 624

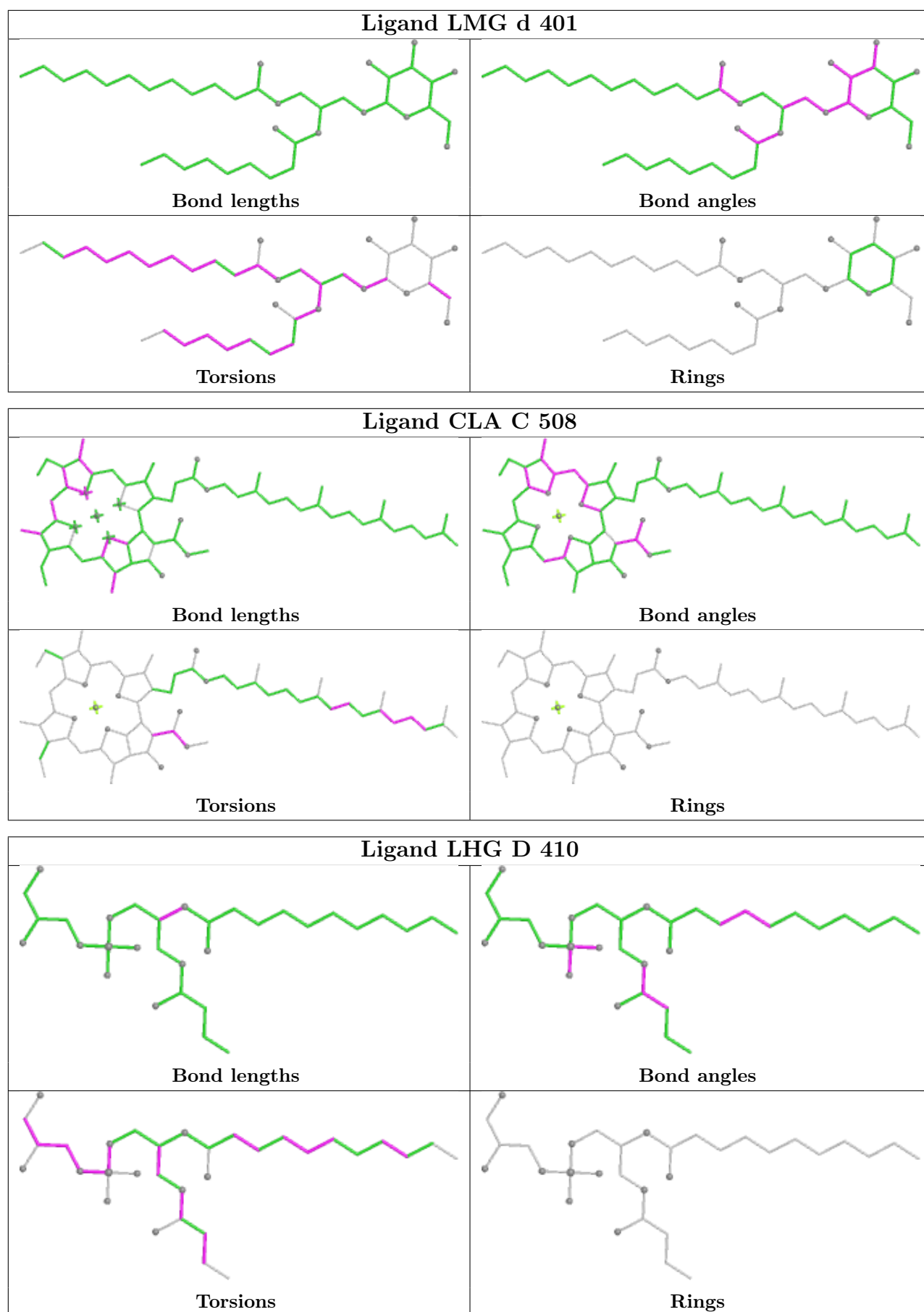


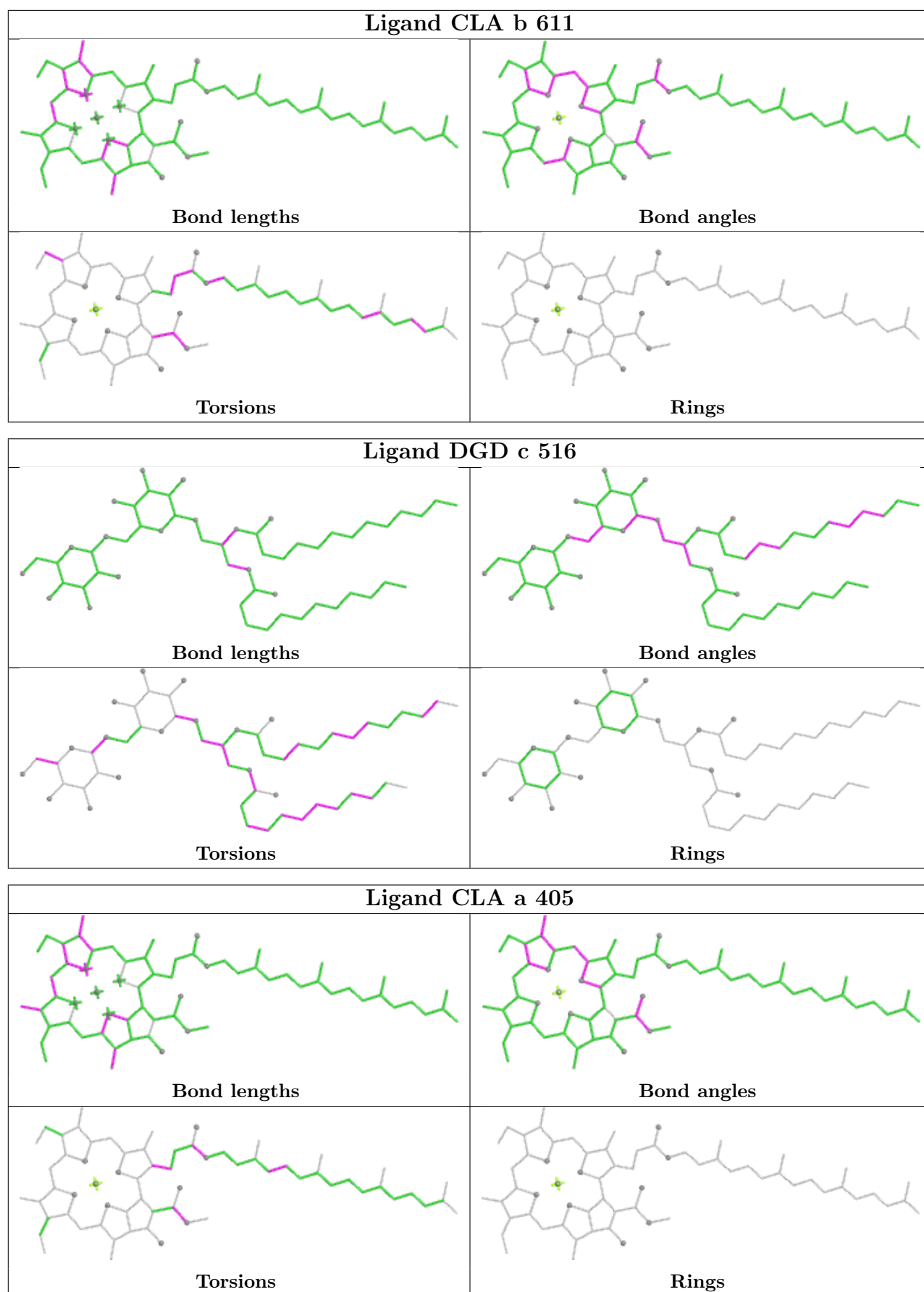
Ligand CLA b 614

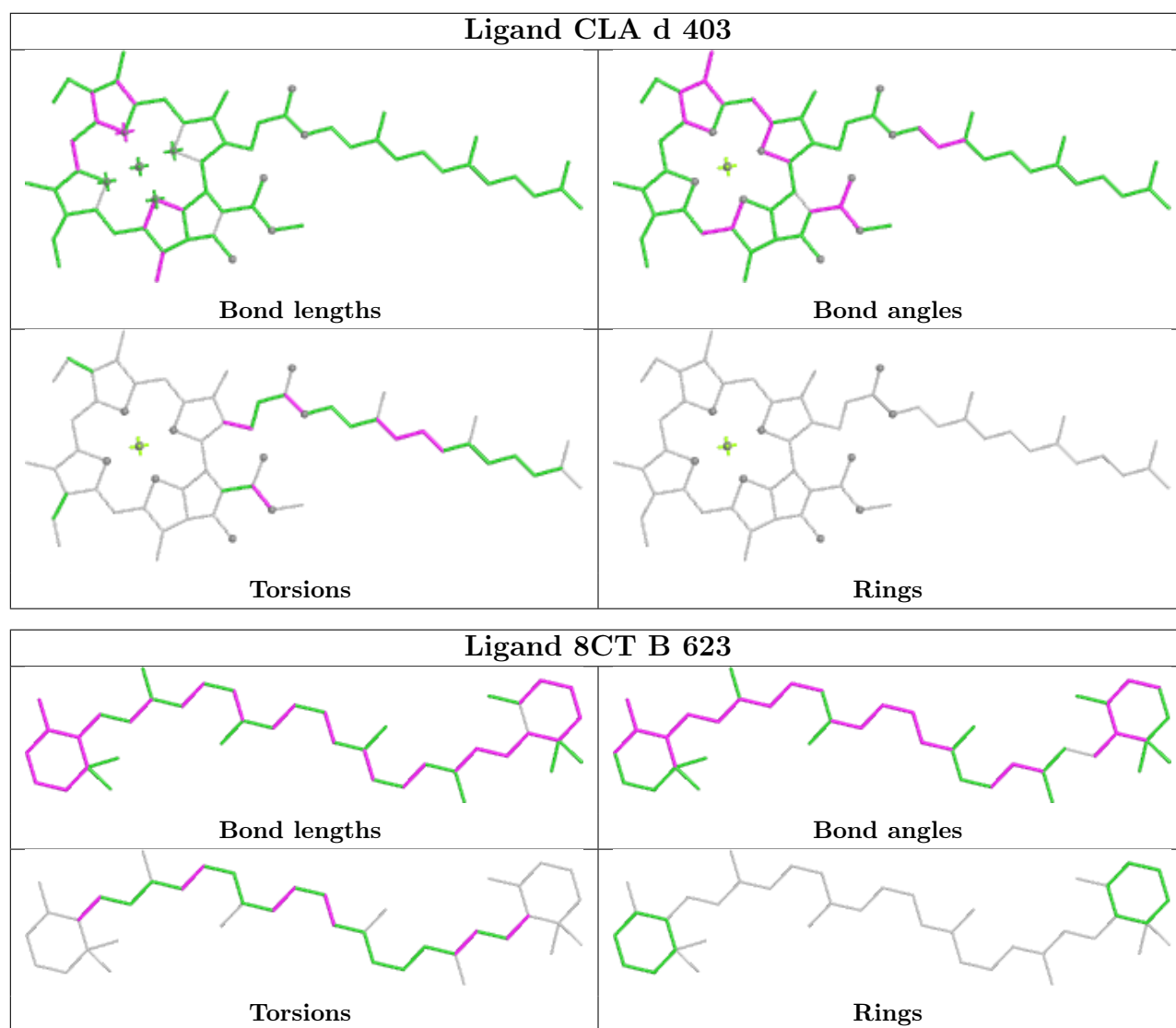


Ligand CLA P 604









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

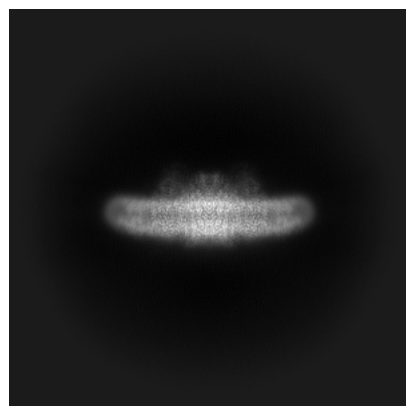
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37414. These allow visual inspection of the internal detail of the map and identification of artifacts.

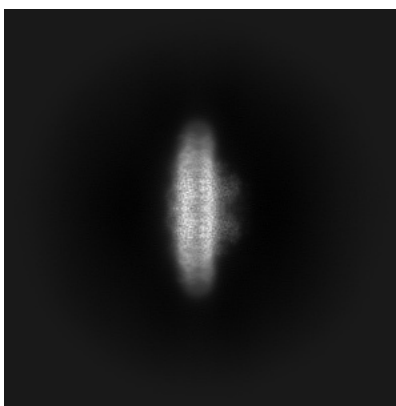
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

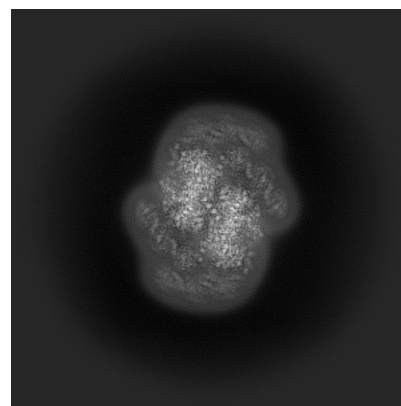
6.1.1 Primary map



X

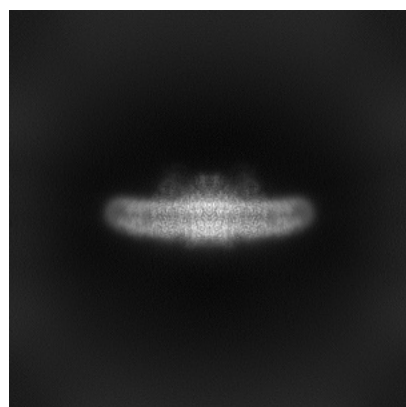


Y

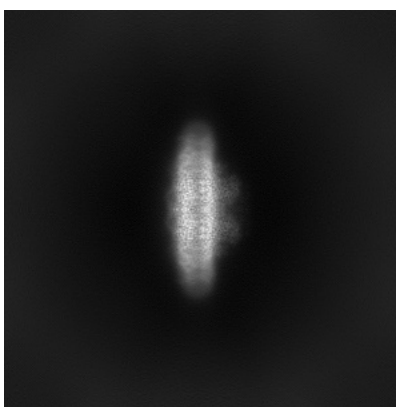


Z

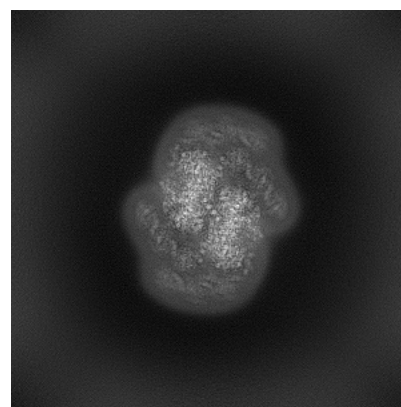
6.1.2 Raw map



X



Y

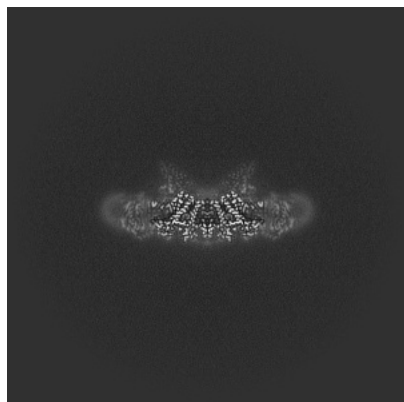


Z

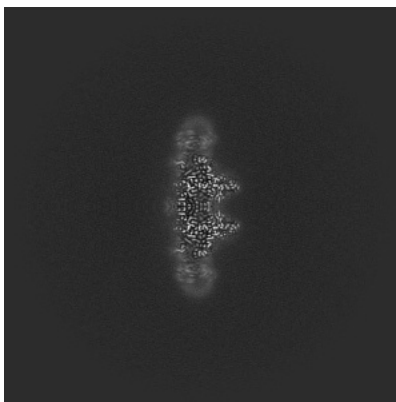
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

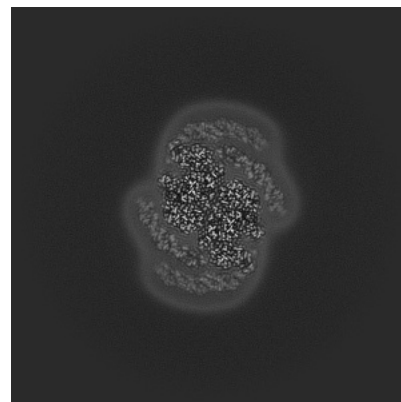
6.2.1 Primary map



X Index: 256

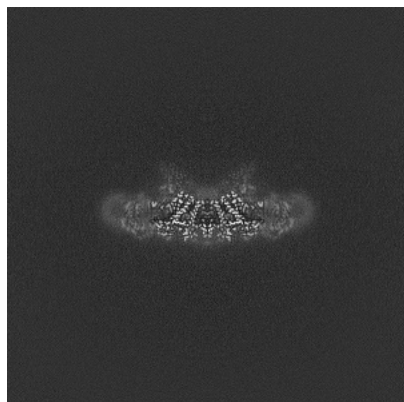


Y Index: 256

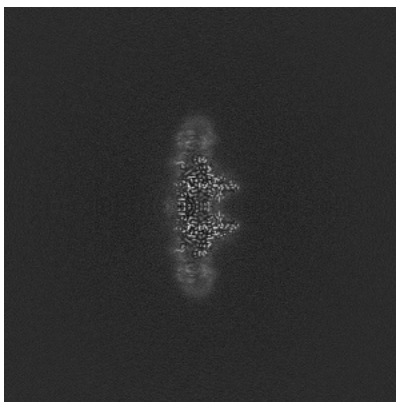


Z Index: 256

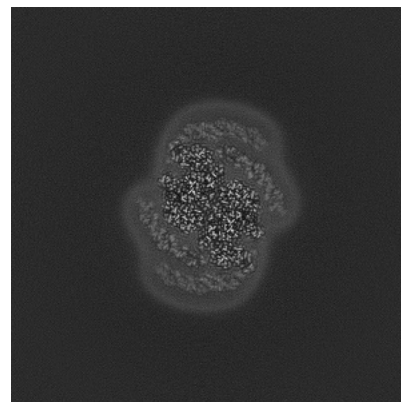
6.2.2 Raw map



X Index: 256



Y Index: 256

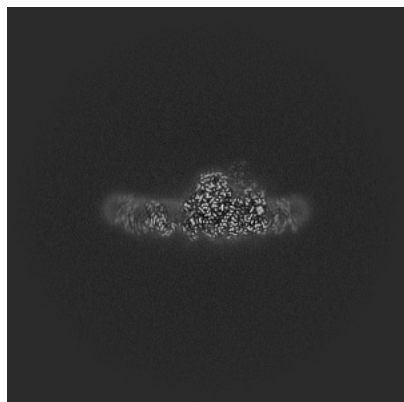


Z Index: 256

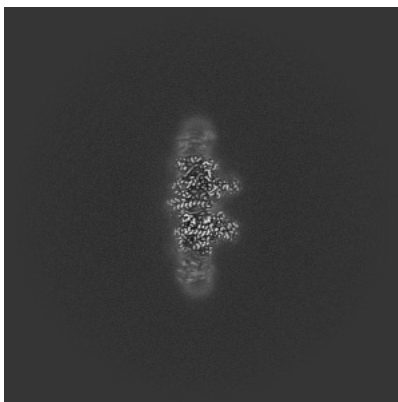
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

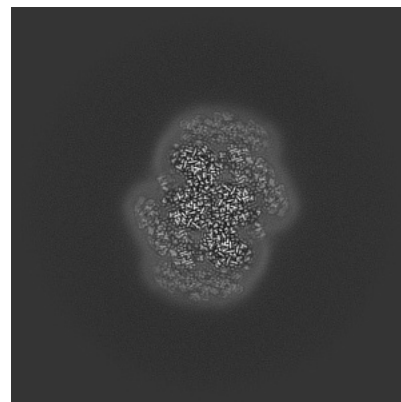
6.3.1 Primary map



X Index: 229

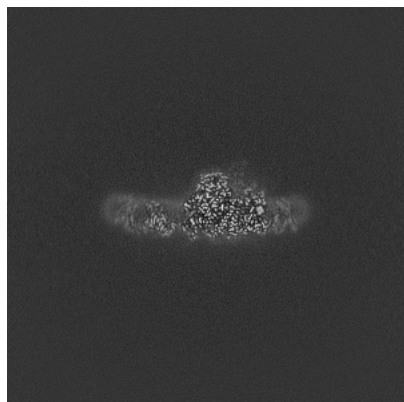


Y Index: 251

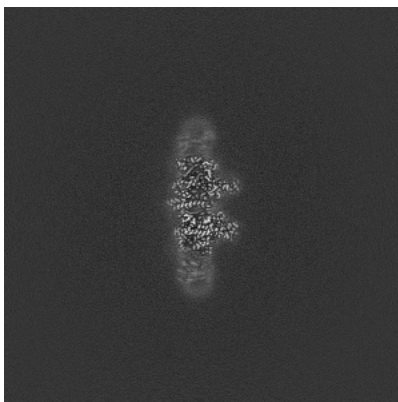


Z Index: 235

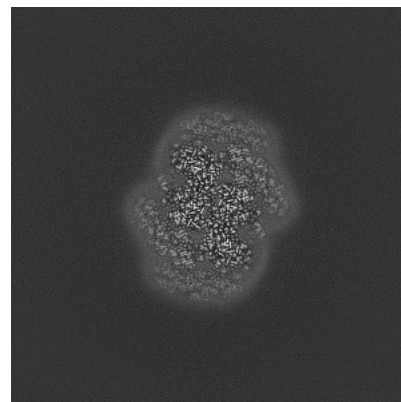
6.3.2 Raw map



X Index: 229



Y Index: 251



Z Index: 235

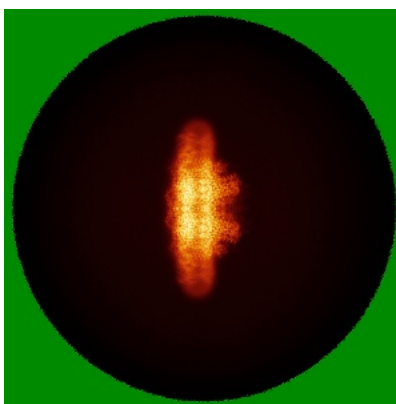
The images above show the largest variance slices of the map in three orthogonal directions.

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

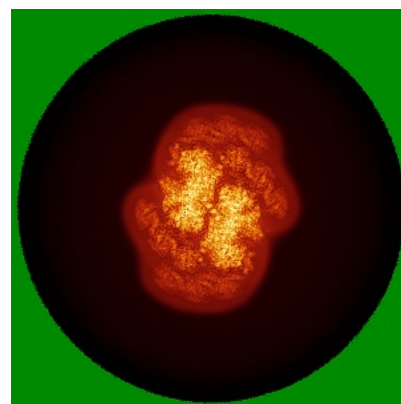
6.4.1 Primary map



X



Y

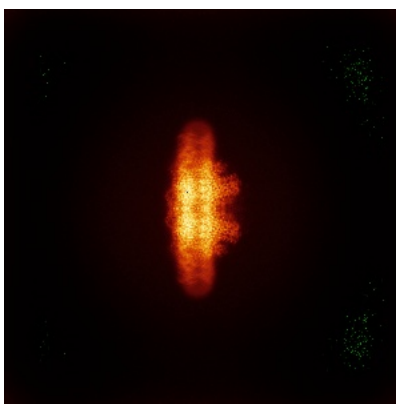


Z

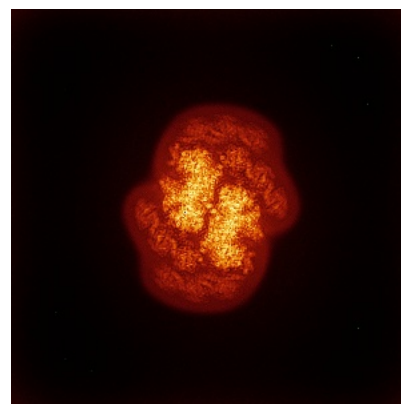
6.4.2 Raw map



X



Y

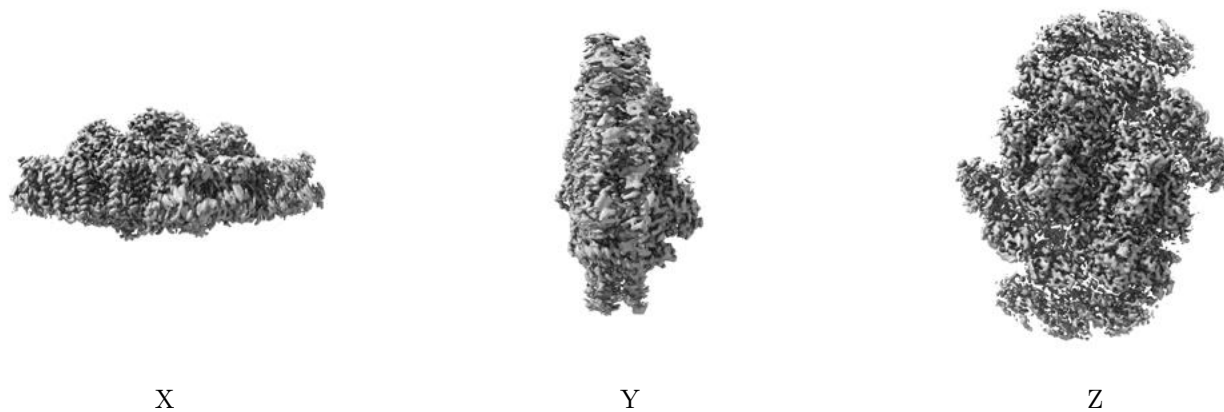


Z

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

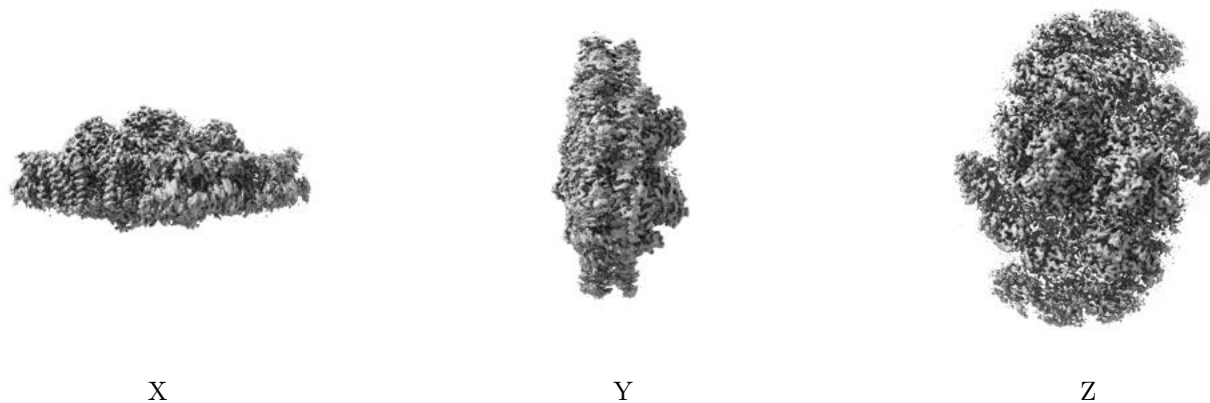
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. 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.

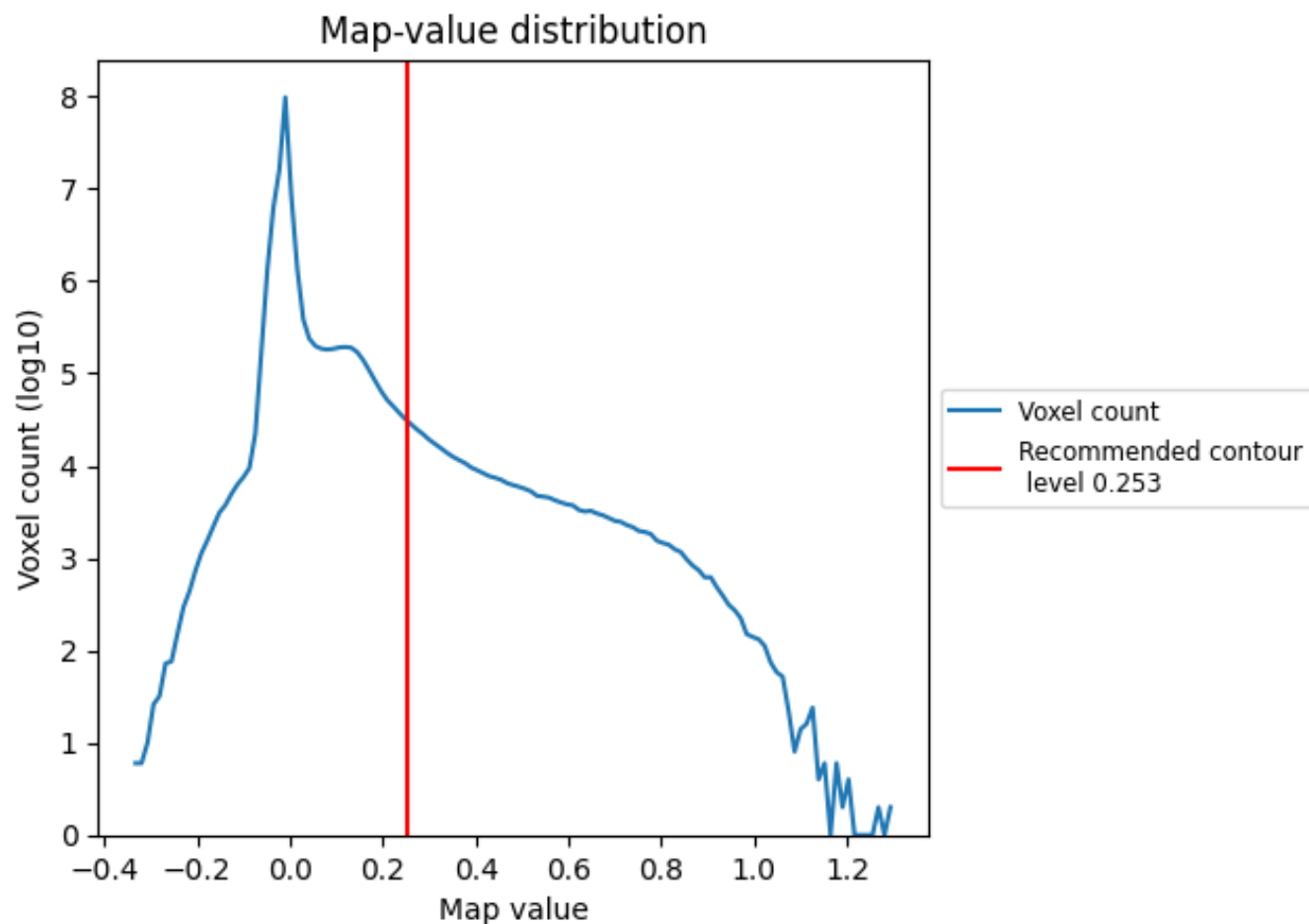
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

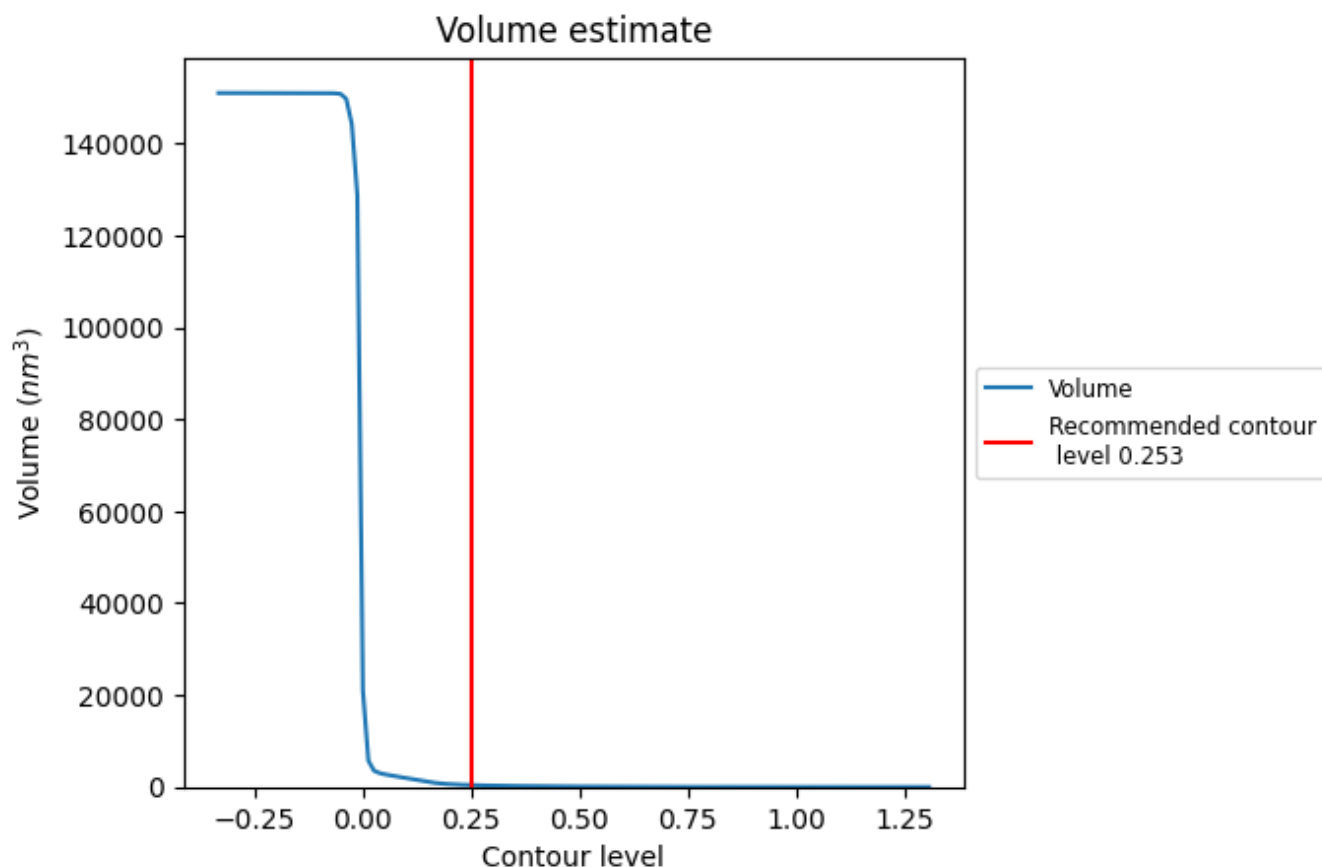
This section contains the results of statistical analysis of the map.

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.

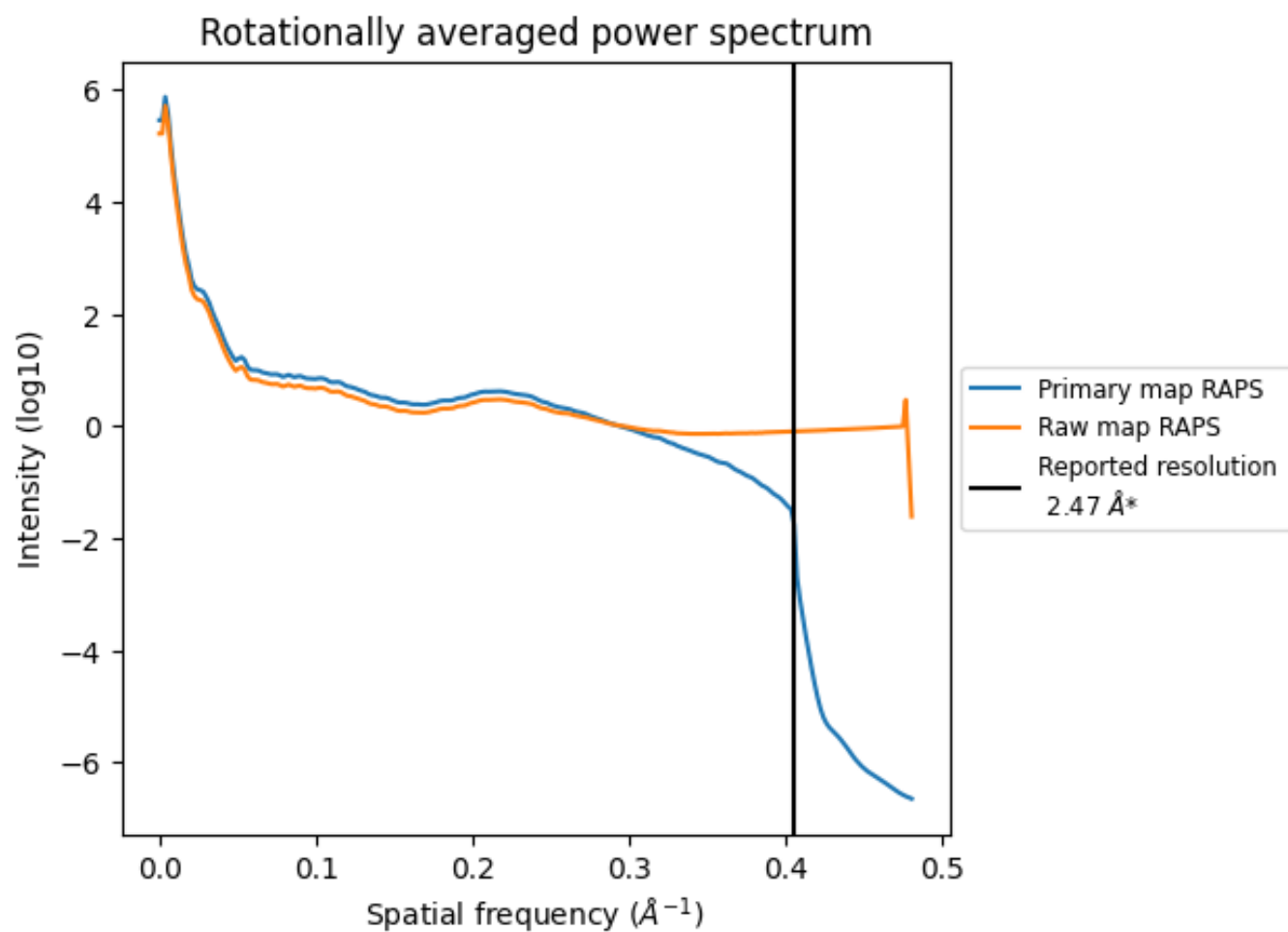
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 394 nm^3 ; this corresponds to an approximate mass of 356 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 ⓘ

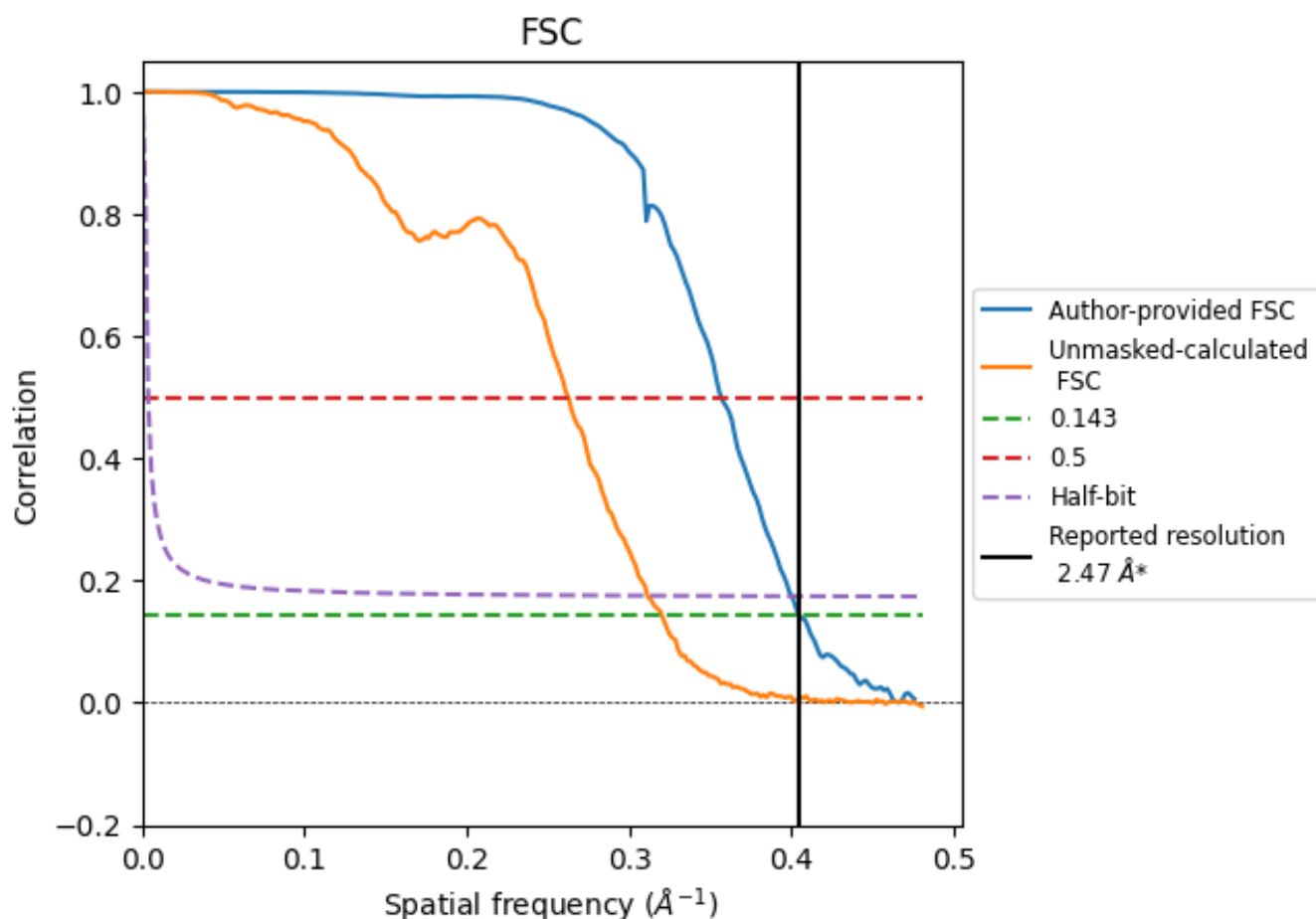


*Reported resolution corresponds to spatial frequency of 0.405 $\text{\AA}^{-1}$

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 0.405 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

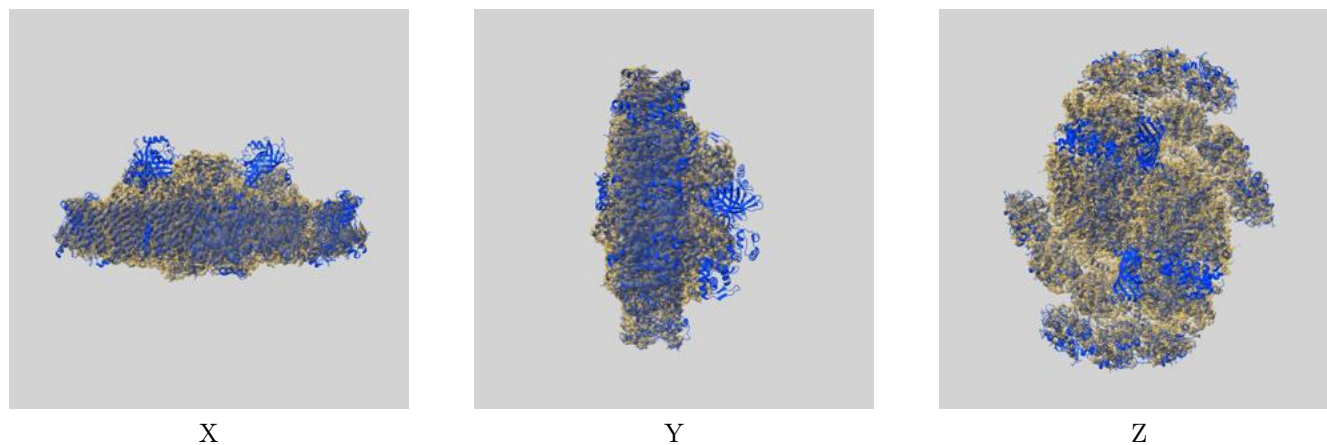
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.47	2.80	2.50
Unmasked-calculated*	3.12	3.81	3.21

*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 3.12 differs from the reported value 2.47 by more than 10 %

9 Map-model fit [i](#)

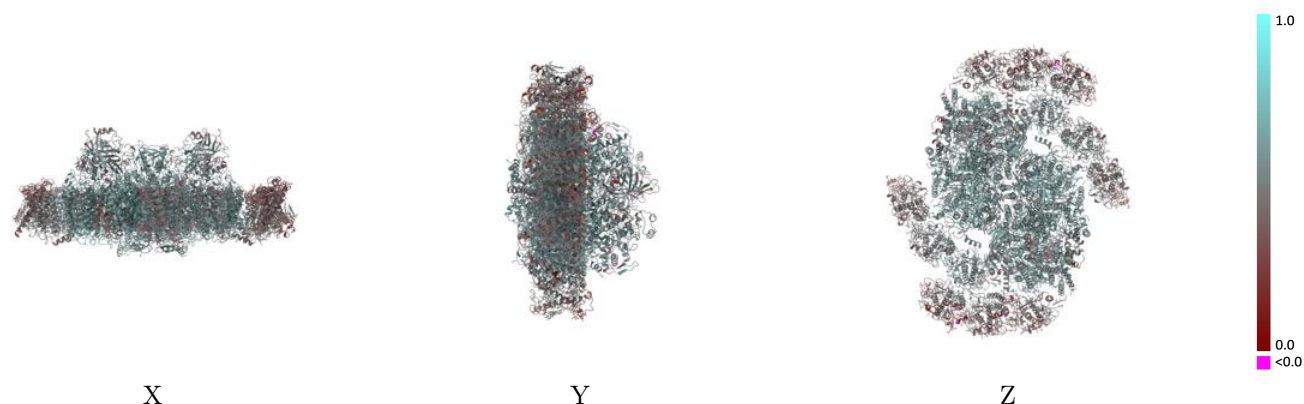
This section contains information regarding the fit between EMDB map EMD-37414 and PDB model 8WB4. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



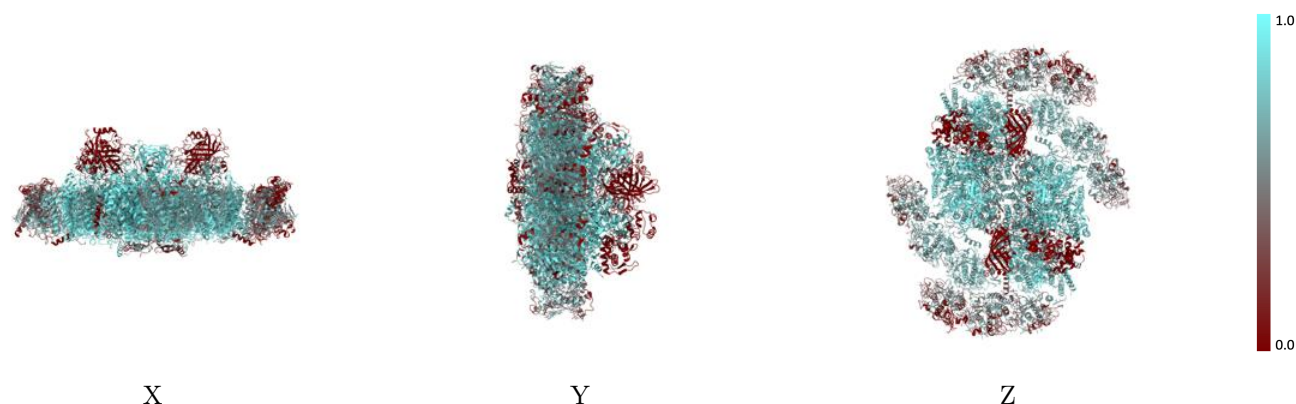
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



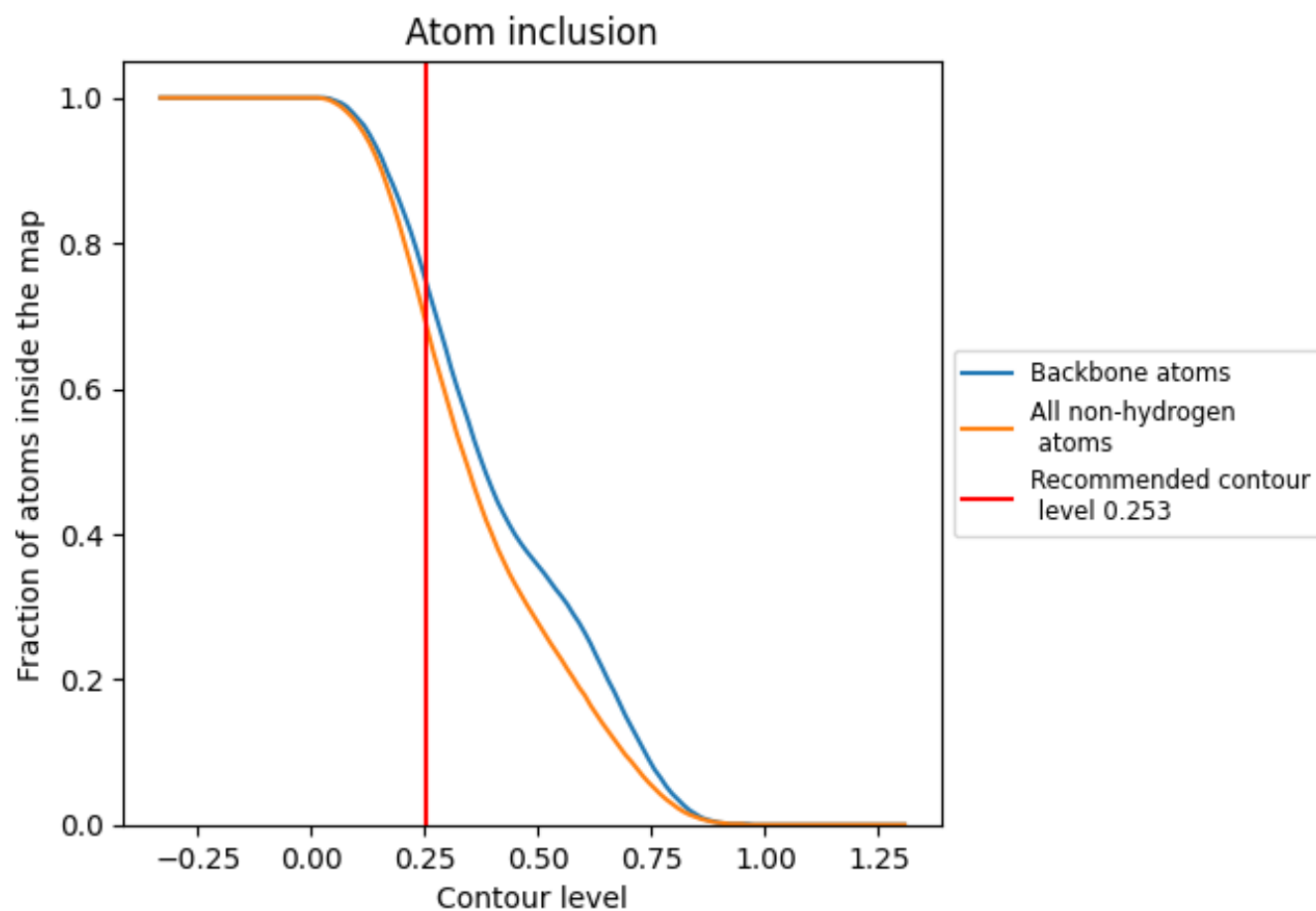
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.253).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.5390
0	 0.3220	 0.3940
1	 0.5160	 0.4300
2	 0.7030	 0.5030
3	 0.8210	 0.5590
4	 0.3280	 0.3940
5	 0.3860	 0.4010
6	 0.4790	 0.4320
7	 0.5140	 0.4320
8	 0.7060	 0.5030
9	 0.8200	 0.5590
A	 0.9490	 0.6200
B	 0.9280	 0.6140
C	 0.9050	 0.6000
D	 0.9620	 0.6290
E	 0.7590	 0.5330
F	 0.8680	 0.5520
G	 0.4320	 0.5120
H	 0.9650	 0.6130
I	 0.9890	 0.6320
J	 0.2870	 0.4670
K	 0.9140	 0.5930
L	 0.9340	 0.6010
M	 0.9440	 0.6050
O	 0.0060	 0.4920
P	 0.4830	 0.4330
Q	 0.0570	 0.5560
R	 0.4620	 0.4100
S	 0.6270	 0.5060
T	 0.9250	 0.6230
U	 0.0110	 0.4830
V	 0.0170	 0.5160
W	 0.8750	 0.5900
X	 0.8780	 0.5930
Y	 0.6150	 0.4860



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.7650	 0.5140
a	 0.9470	 0.6180
b	 0.9290	 0.6150
c	 0.9040	 0.6010
d	 0.9620	 0.6310
e	 0.7600	 0.5390
f	 0.8430	 0.5560
g	 0.4160	 0.4930
h	 0.9650	 0.6160
i	 0.9890	 0.6260
j	 0.2870	 0.4630
k	 0.9110	 0.5940
l	 0.9340	 0.5980
m	 0.9350	 0.6030
o	 0.0070	 0.4880
p	 0.3940	 0.4020
q	 0.0570	 0.5540
r	 0.4620	 0.4120
s	 0.6270	 0.5080
t	 0.9250	 0.6230
u	 0.0110	 0.4850
v	 0.0160	 0.5190
w	 0.8750	 0.5860
x	 0.8780	 0.5880
y	 0.6110	 0.4880
z	 0.7570	 0.5180