



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 02:21 AM JST

PDB ID : 8J5K / pdb_00008j5k
EMDB ID : EMD-35987
Title : Structural insights into photosystem II supercomplex and trimeric FCP antennae of a centric diatom *Cyclotella meneghiniana*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2023-04-23
Resolution : 2.93 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

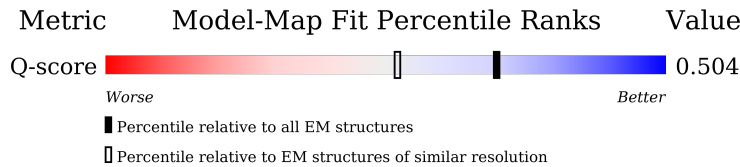
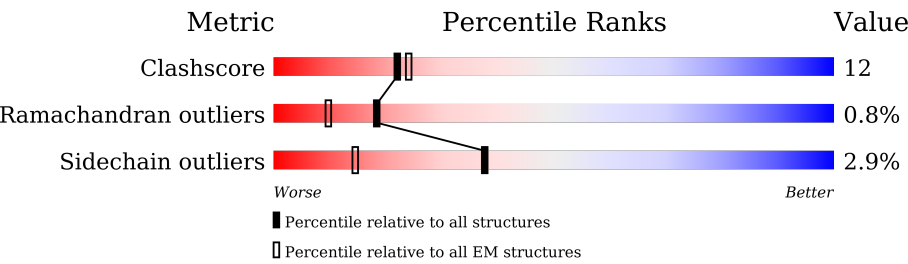
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.93 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.



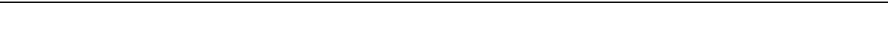
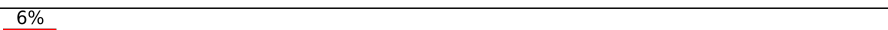
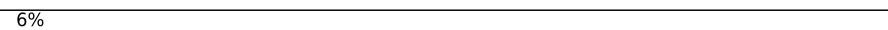
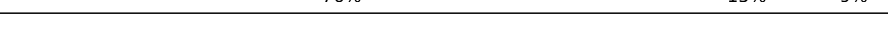
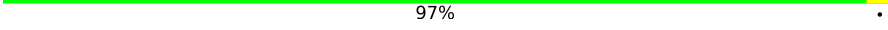
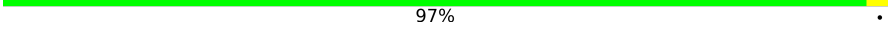
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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

Mol	Chain	Length	Quality of chain
1	A	333	80%20%
1	a	333	81%18%
2	B	481	81%18%
2	b	481	81%18%

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Mol	Chain	Length	Quality of chain
3	C	450	 80% 19%
3	c	450	 80% 20%
4	D	340	 78% 22%
4	d	340	 79% 21%
5	E	75	 80% 20%
5	e	75	 80% 20%
6	F	31	 68% 26% 6%
6	f	31	 68% 26% 6%
7	H	65	 78% 20% .
7	h	65	 78% 20% .
8	I	34	 68% 26% 6%
8	i	34	 68% 26% 6%
9	J	34	 6% 74% 15% 12%
9	j	34	 6% 76% 15% 9%
10	K	37	 68% 30% .
10	k	37	 68% 30% .
11	L	37	 78% 22%
11	l	37	 78% 22%
12	M	41	 73% 24% .
12	m	41	 73% 24% .
13	N	30	 7% 97% .
13	n	30	 10% 97% .
14	O	248	 8% 71% 27% .
14	o	248	 8% 69% 29% .
15	Q	145	 31% 59% 29% 8% .

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Mol	Chain	Length	Quality of chain
15	q	145	
16	T	29	
16	t	29	
17	U	92	
17	u	92	
18	V	136	
18	v	136	
19	W	50	
19	w	50	
20	X	34	
20	x	34	
21	Y	33	
21	y	33	
22	Z	59	
22	z	59	
23	0	169	
23	5	169	
24	2	164	
24	7	164	
25	1	164	
25	6	164	
26	P	214	
26	p	214	
27	4	153	
27	9	153	

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Mol	Chain	Length	Quality of chain
28	3	163	77%
			84%16%
28	8	163	77%
			85%15%

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 71446 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 PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2530	1656	421	439	14		
1	a	333	Total	C	N	O	S	0	0
			2530	1656	421	439	14		

- Molecule 2 is a protein called PsbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	481	Total	C	N	O	S	0	0
			3748	2456	635	646	11		
2	b	481	Total	C	N	O	S	0	0
			3748	2456	635	646	11		

- Molecule 3 is a protein called PsbC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3437	2252	579	595	11		
3	c	450	Total	C	N	O	S	0	0
			3437	2252	579	595	11		

- Molecule 4 is a protein called PsbD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2667	1765	437	455	10		
4	d	340	Total	C	N	O	S	0	0
			2667	1765	437	455	10		

- Molecule 5 is a protein called PsbE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			602	392	101	109		
5	e	75	Total	C	N	O	0	0
			602	392	101	109		

- Molecule 6 is a protein called PsbF.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	31	Total	C	N	O	0	0
			242	166	41	35		
6	f	31	Total	C	N	O	0	0
			242	166	41	35		

- Molecule 7 is a protein called PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			499	331	82	85	1		
7	h	65	Total	C	N	O	S	0	0
			499	331	82	85	1		

- Molecule 8 is a protein called PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			266	179	40	46	1		
8	i	34	Total	C	N	O	S	0	0
			266	179	40	46	1		

- Molecule 9 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	34	Total	C	N	O	0	0
			247	167	38	42		
9	j	34	Total	C	N	O	0	0
			247	167	38	42		

- Molecule 10 is a protein called PsbK.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			294	205	44	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			294	205	44	45		

- Molecule 11 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	37	Total	C	N	O	0	0
			294	197	46	51		
11	l	37	Total	C	N	O	0	0
			294	197	46	51		

- Molecule 12 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	41	Total	C	N	O	0	0
			295	193	49	53		
12	m	41	Total	C	N	O	0	0
			295	193	49	53		

- Molecule 13 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	30	Total	C	N	O	0	0
			150	90	30	30		
13	n	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	248	Total	C	N	O	S	0	0
			1824	1151	304	362	7		
14	o	248	Total	C	N	O	S	0	0
			1824	1151	304	362	7		

- Molecule 15 is a protein called PsbQ'.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Q	145	Total	C	N	O	0	0
			1050	654	182	214		
15	q	145	Total	C	N	O	0	0
			1050	654	182	214		

- Molecule 16 is a protein called PsbT.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			234	164	32	36	2		
16	t	29	Total	C	N	O	S	0	0
			234	164	32	36	2		

- Molecule 17 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	92	Total	C	N	O	S	0	0
			678	436	111	130	1		
17	u	92	Total	C	N	O	S	0	0
			678	436	111	130	1		

- Molecule 18 is a protein called PsbV.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	136	Total	C	N	O	S	0	0
			979	612	169	194	4		
18	v	136	Total	C	N	O	S	0	0
			979	612	169	194	4		

- Molecule 19 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	50	Total	C	N	O	S	0	0
			338	211	56	68	3		
19	w	50	Total	C	N	O	S	0	0
			338	211	56	68	3		

- Molecule 20 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	34	Total	C	N	O	S	0	0
			233	150	39	43	1		
20	x	34	Total	C	N	O	S	0	0
			233	150	39	43	1		

- Molecule 21 is a protein called PsbY.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	33	Total	C	N	O	0	0
			216	137	39	40		
21	y	33	Total	C	N	O	0	0
			216	137	39	40		

- Molecule 22 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	59	Total	C	N	O	S	0	0
			413	270	65	77	1		
22	z	59	Total	C	N	O	S	0	0
			413	270	65	77	1		

- Molecule 23 is a protein called FCPII-G, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	169	Total	C	N	O	S	0	0
			1280	827	211	239	3		
23	0	169	Total	C	N	O	S	0	0
			1280	827	211	239	3		

- Molecule 24 is a protein called FCPII-H2, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7	164	Total	C	N	O	S	0	0
			1222	808	198	212	4		
24	2	164	Total	C	N	O	S	0	0
			1222	808	198	212	4		

- Molecule 25 is a protein called FCPII-H1, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	164	Total	C	N	O	S	0	0
			1209	796	210	201	2		
25	1	164	Total	C	N	O	S	0	0
			1209	796	210	201	2		

- Molecule 26 is a protein called FCPII-I, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	214	Total	C	N	O	S	0	0
			1265	789	230	245	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	214	Total	C	N	O	S	0	0
			1265	789	230	245	1		

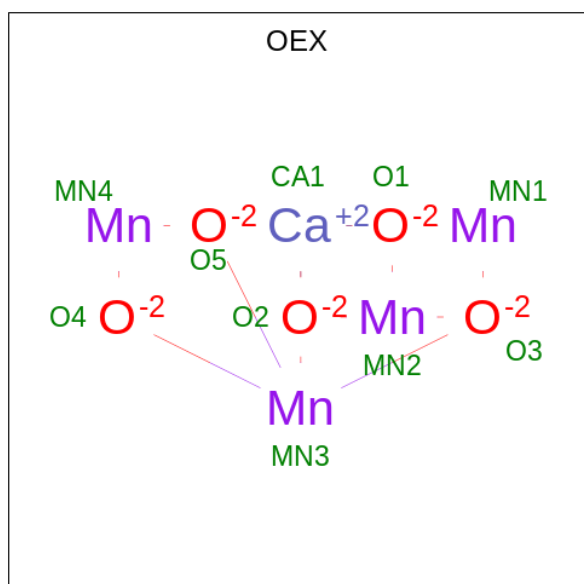
- Molecule 27 is a protein called FCPII-K, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	4	153	Total	C	N	O	0	0
			765	459	153	153		
27	9	153	Total	C	N	O	0	0
			765	459	153	153		

- Molecule 28 is a protein called FCPII-J, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	163	Total	C	N	O	0	0
			992	616	192	184		
28	8	163	Total	C	N	O	0	0
			992	616	192	184		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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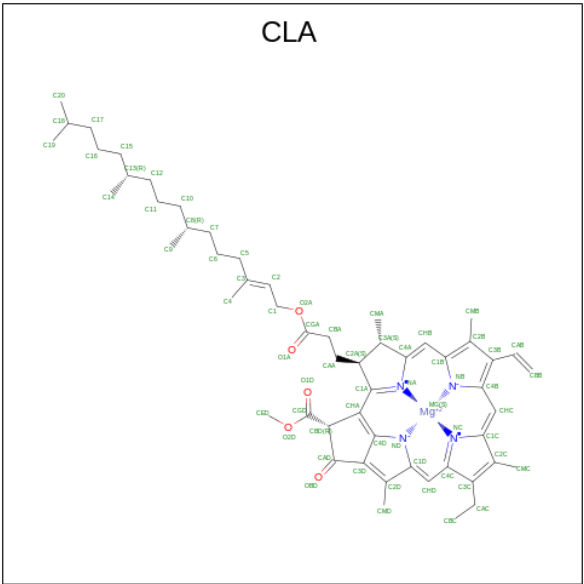
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Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
29	a	1	10	1	4	5	0

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Fe	0
			1	1	
30	a	1	Total	Fe	0
			1	1	

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



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	B	1	Total 61	C 52	Mg 1	N 4	O 4	0
31	B	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	D	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
31	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
31	c	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	d	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	z	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	5	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	5	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	7	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	7	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	7	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	7	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	6	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	6	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	6	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	6	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	6	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	p	1	Total 36	C 30	Mg 1	N 4	O 1	0

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Mol	Chain	Residues	Atoms					AltConf
31	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	p	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	p	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	p	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	p	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	p	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	p	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	p	1	Total 39	C 32	Mg 1	N 4	O 2	0
31	4	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	4	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	4	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	4	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	4	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	4	1	Total 34	C 28	Mg 1	N 4	O 1	0
31	4	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	4	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	3	1	Total 34	C 28	Mg 1	N 4	O 1	0
31	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	3	1	Total 33	C 27	Mg 1	N 4	O 1	0

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	3	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	3	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	3	1	Total 39	C 33	Mg 1	N 4	O 1	0
31	3	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	P	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	P	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	P	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	P	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	P	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	P	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	P	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	P	1	Total 39	C 32	Mg 1	N 4	O 2	0
31	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	9	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	9	1	Total 37	C 31	Mg 1	N 4	O 1	0
31	9	1	Total 38	C 32	Mg 1	N 4	O 1	0

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	9	1	Total 34	C 28	Mg 1	N 4	O 1	0
31	9	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	9	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	8	1	Total 34	C 28	Mg 1	N 4	O 1	0
31	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	8	1	Total 33	C 27	Mg 1	N 4	O 1	0
31	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	8	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	8	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	8	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	8	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	8	1	Total 39	C 33	Mg 1	N 4	O 1	0
31	8	1	Total 35	C 29	Mg 1	N 4	O 1	0
31	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	0	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	0	1	Total 61	C 51	Mg 1	N 4	O 5	0

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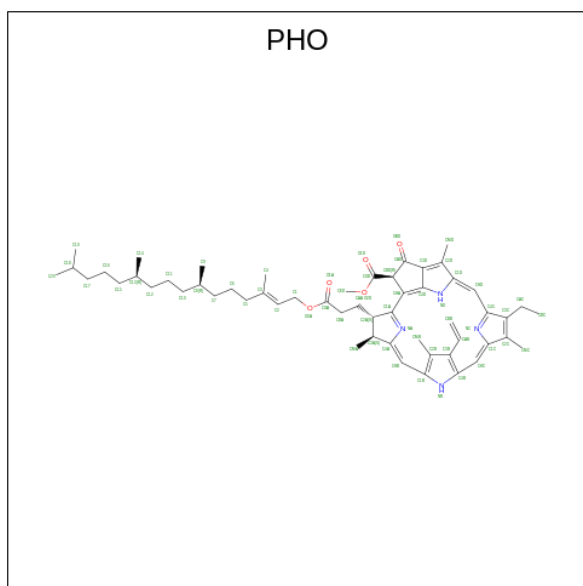
Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	0	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	0	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	0	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	2	1	Total 59	C 49	Mg 1	N 4	O 5	0
31	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	2	1	Total 36	C 30	Mg 1	N 4	O 1	0
31	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	1	1	Total 41	C 33	Mg 1	N 4	O 3	0

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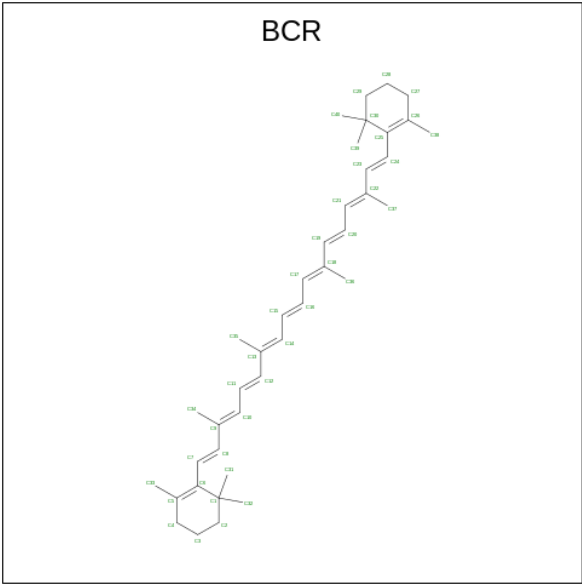
Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	1	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	1	1	Total	C	Mg	N	O	0
			38	32	1	4	1	

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



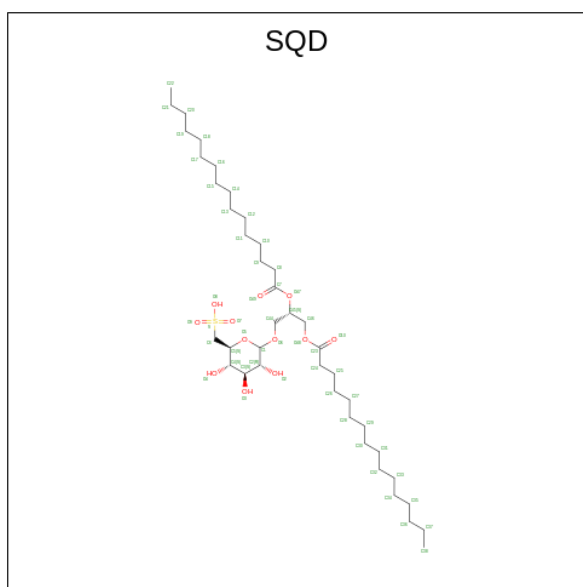
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	
33	C	1	Total	C	0
			40	40	
33	D	1	Total	C	0
			40	40	

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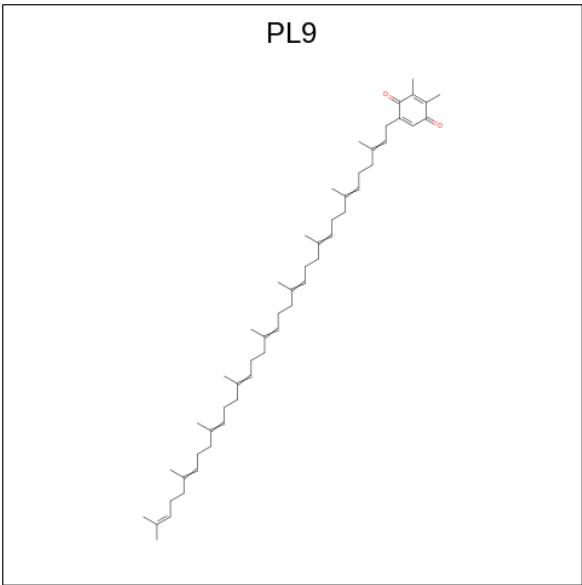
Mol	Chain	Residues	Atoms	AltConf
33	H	1	Total C 40 40	0
33	K	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	h	1	Total C 40 40	0
33	k	1	Total C 40 40	0

- Molecule 34 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).



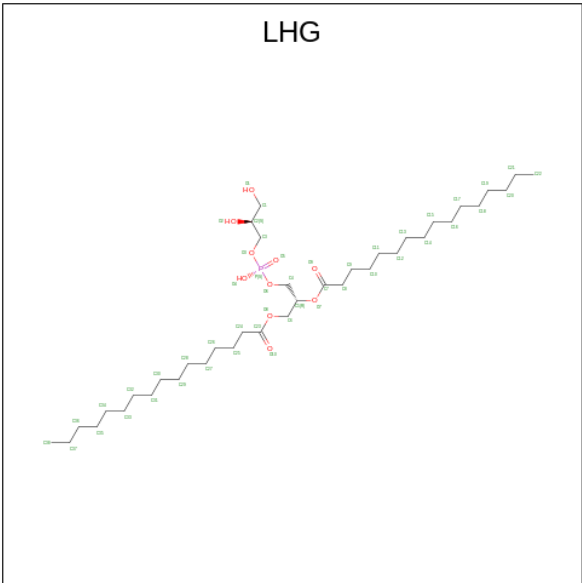
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			40	27	12	1	
34	a	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			40	27	12	1	
34	5	1	Total	C	O	S	0
			48	35	12	1	
34	0	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 35 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).



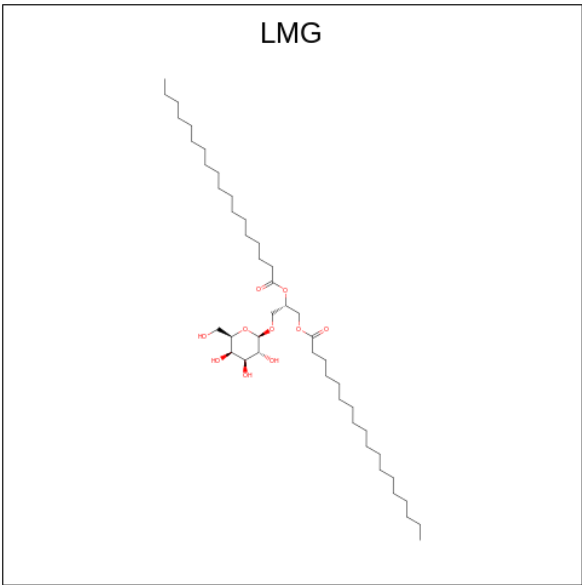
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			32	30	2	
35	D	1	Total	C	O	0
			55	53	2	
35	a	1	Total	C	O	0
			32	30	2	
35	d	1	Total	C	O	0
			55	53	2	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			43	32	10	1	
36	A	1	Total	C	O	P	0
			26	15	10	1	
36	B	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			48	38	9	1	
36	D	1	Total	C	O	P	0
			34	23	10	1	
36	D	1	Total	C	O	P	0
			28	19	8	1	
36	H	1	Total	C	O	P	0
			42	31	10	1	
36	a	1	Total	C	O	P	0
			43	32	10	1	
36	a	1	Total	C	O	P	0
			26	15	10	1	
36	b	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			48	38	9	1	
36	d	1	Total	C	O	P	0
			34	23	10	1	
36	d	1	Total	C	O	P	0
			28	19	8	1	
36	h	1	Total	C	O	P	0
			42	31	10	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	B	1	Total	C	O	0
			28	18	10	
37	C	1	Total	C	O	0
			51	41	10	
37	D	1	Total	C	O	0
			46	36	10	
37	D	1	Total	C	O	0
			37	27	10	
37	D	1	Total	C	O	0
			40	30	10	
37	J	1	Total	C	O	0
			50	40	10	
37	M	1	Total	C	O	0
			51	41	10	
37	M	1	Total	C	O	0
			40	30	10	
37	W	1	Total	C	O	0
			48	38	10	
37	Y	1	Total	C	O	0
			46	36	10	
37	b	1	Total	C	O	0
			28	18	10	
37	c	1	Total	C	O	0
			51	41	10	
37	d	1	Total	C	O	0
			46	36	10	
37	d	1	Total	C	O	0
			37	27	10	

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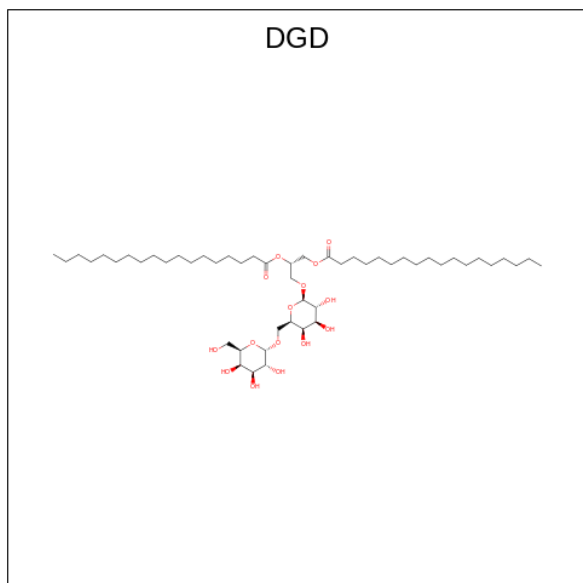
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Mol	Chain	Residues	Atoms			AltConf
37	d	1	Total	C	O	0
			40	30	10	
37	j	1	Total	C	O	0
			50	40	10	
37	m	1	Total	C	O	0
			51	41	10	
37	m	1	Total	C	O	0
			40	30	10	
37	w	1	Total	C	O	0
			48	38	10	
37	y	1	Total	C	O	0
			46	36	10	
37	5	1	Total	C	O	0
			48	38	10	
37	0	1	Total	C	O	0
			48	38	10	

- Molecule 38 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

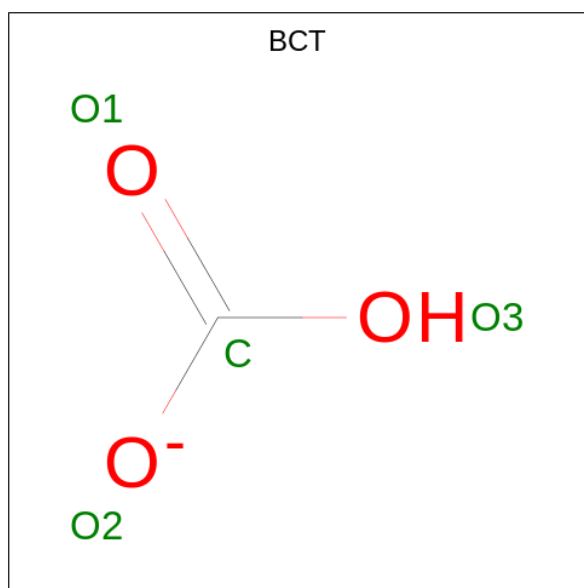
Mol	Chain	Residues	Atoms		AltConf
38	C	1	Total	Cl	0
			1	1	
38	c	1	Total	Cl	0
			1	1	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



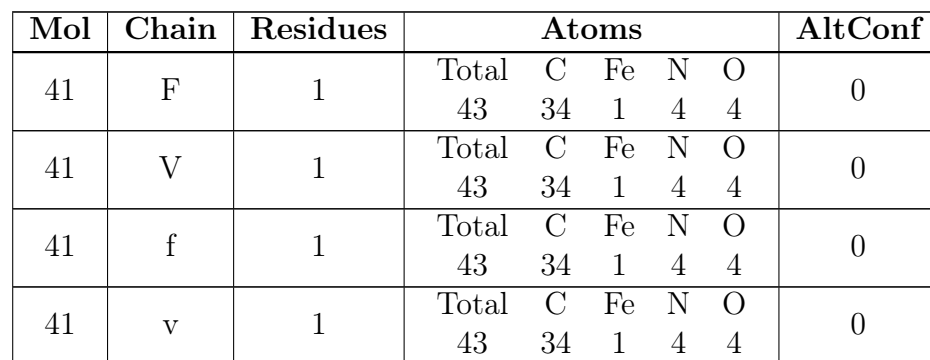
Mol	Chain	Residues	Atoms			AltConf
39	C	1	Total	C	O	0
			55	40	15	
39	C	1	Total	C	O	0
			62	47	15	
39	C	1	Total	C	O	0
			62	47	15	
39	H	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			55	40	15	
39	c	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	h	1	Total	C	O	0
			62	47	15	

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).

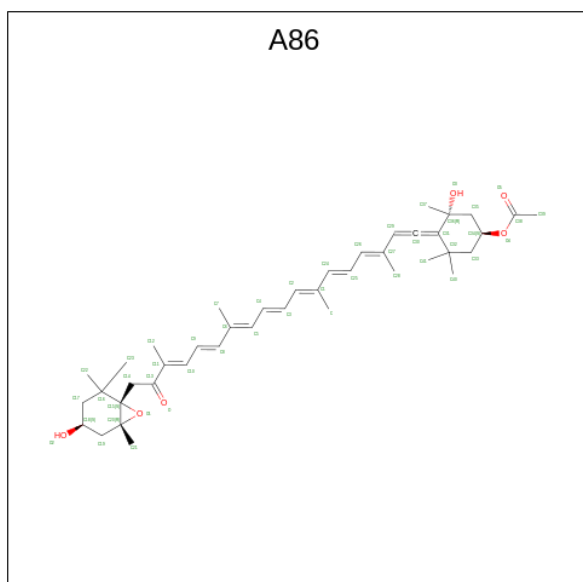


Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



- Molecule 42 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



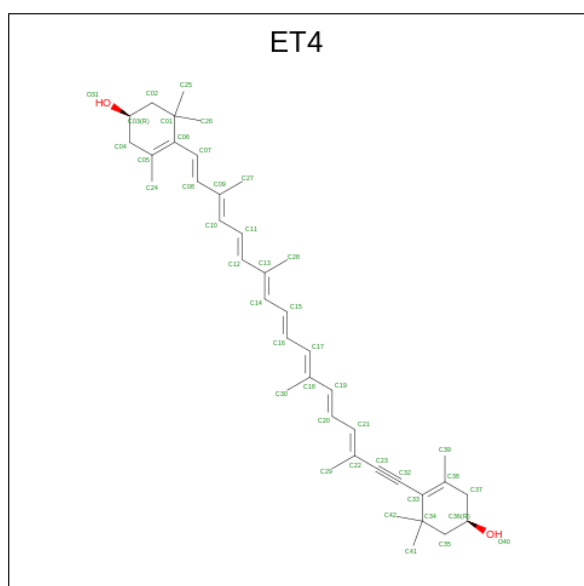
Mol	Chain	Residues	Atoms			AltConf
42	5	1	Total	C	O	0
			48	42	6	
42	5	1	Total	C	O	0
			48	42	6	
42	5	1	Total	C	O	0
			48	42	6	
42	7	1	Total	C	O	0
			48	42	6	
42	7	1	Total	C	O	0
			48	42	6	
42	6	1	Total	C	O	0
			48	42	6	
42	p	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	3	1	Total	C	O	0
			48	42	6	
42	3	1	Total	C	O	0
			48	42	6	
42	P	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	8	1	Total	C	O	0
			48	42	6	
42	8	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	2	1	Total	C	O	0
			48	42	6	

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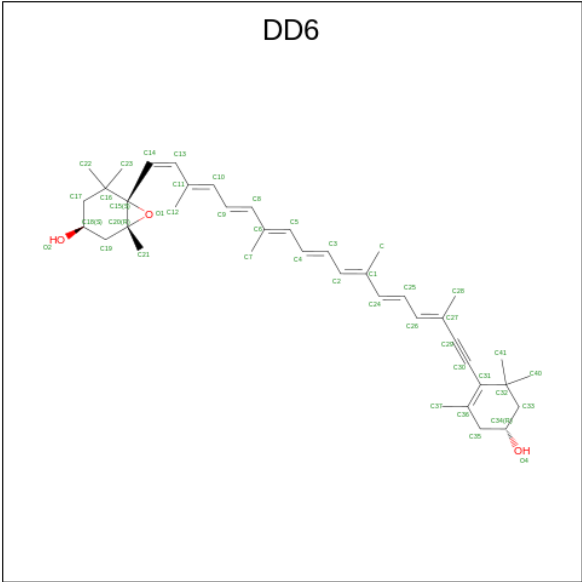
Mol	Chain	Residues	Atoms			AltConf
42	2	1	Total	C	O	0
			48	42	6	
42	1	1	Total	C	O	0
			48	42	6	

- Molecule 43 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},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-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total	C	O	0
			42	40	2	
43	0	1	Total	C	O	0
			42	40	2	

- Molecule 44 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).

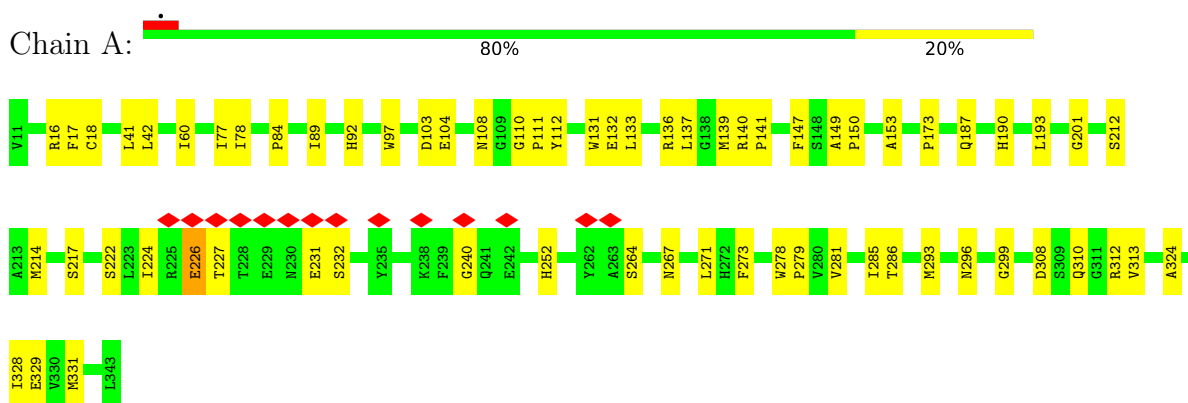


Mol	Chain	Residues	Atoms			AltConf
44	7	1	Total	C	O	0
			43	40	3	
44	7	1	Total	C	O	0
			43	40	3	
44	6	1	Total	C	O	0
			43	40	3	
44	6	1	Total	C	O	0
			43	40	3	
44	p	1	Total	C	O	0
			43	40	3	
44	3	1	Total	C	O	0
			43	40	3	
44	P	1	Total	C	O	0
			43	40	3	
44	8	1	Total	C	O	0
			43	40	3	
44	2	1	Total	C	O	0
			43	40	3	
44	2	1	Total	C	O	0
			43	40	3	
44	1	1	Total	C	O	0
			43	40	3	
44	1	1	Total	C	O	0
			43	40	3	

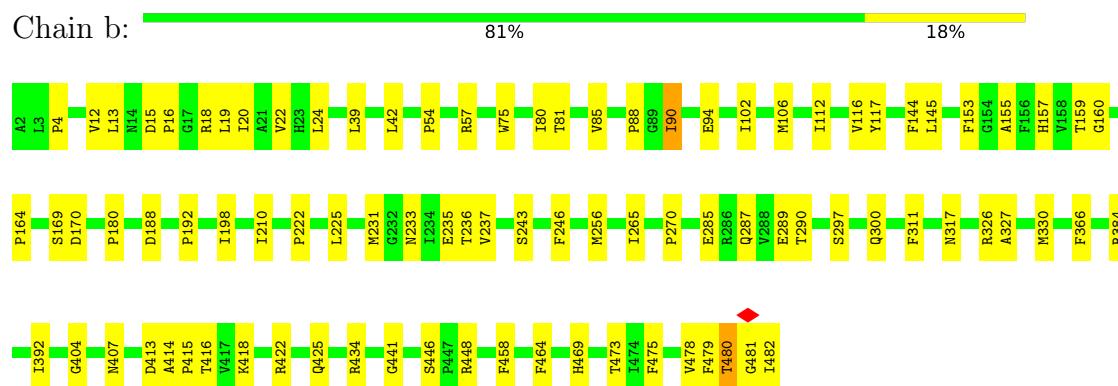
3 Residue-property plots [i](#)

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

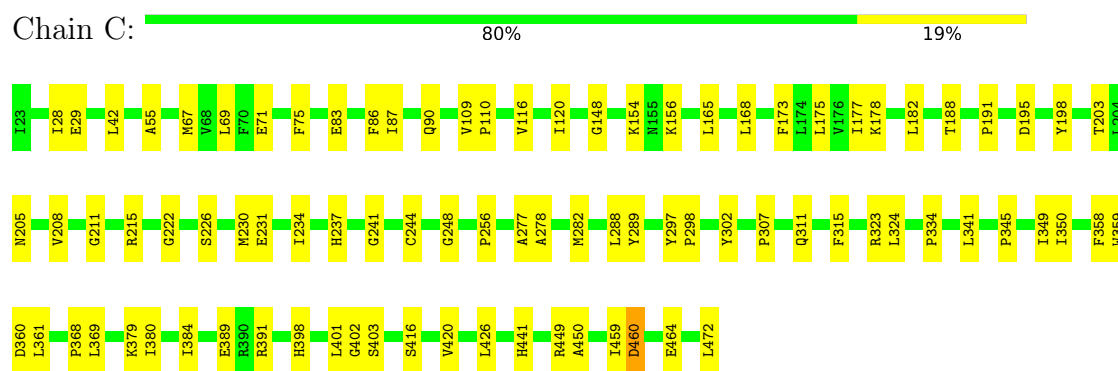
• Molecule 1: PsbA



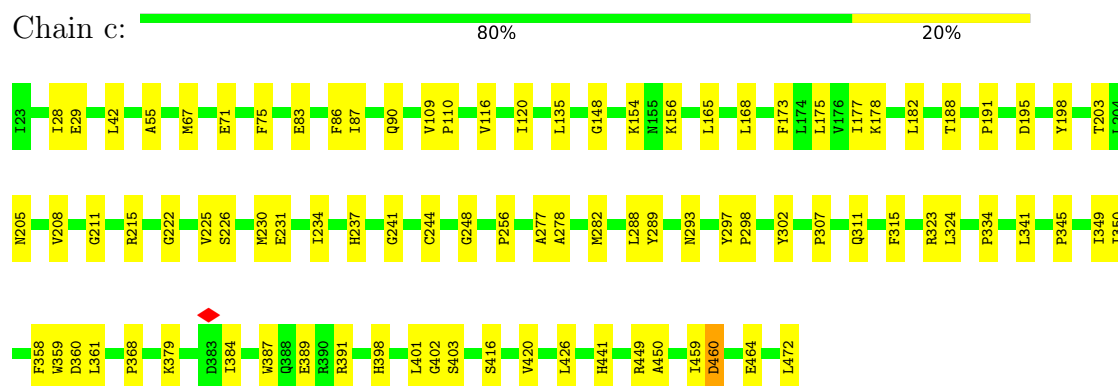
- Molecule 2: PsbB



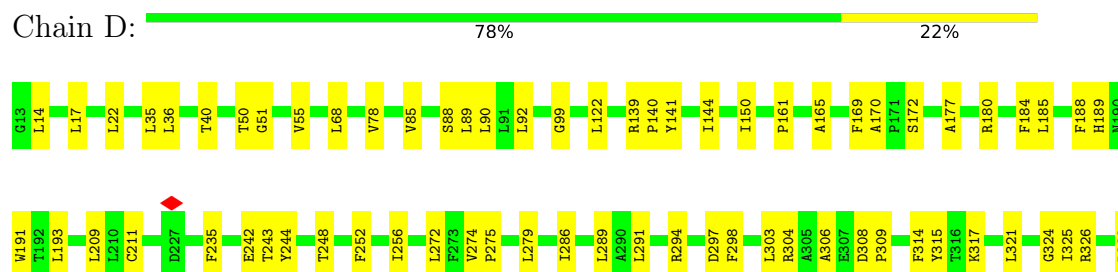
- Molecule 3: PsbC

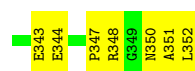


- Molecule 3: PsbC



- Molecule 4: PsbD





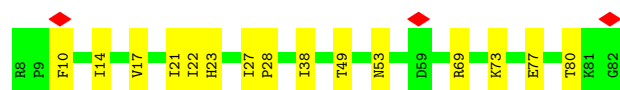
• Molecule 4: PsbD

Chain d: 79% 21%



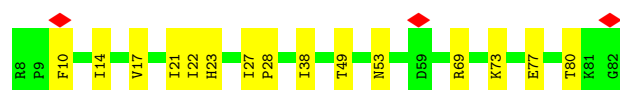
• Molecule 5: PsbE

Chain E: 80% 20%



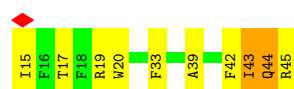
• Molecule 5: PsbE

Chain e: 80% 20%



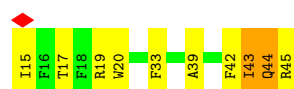
• Molecule 6: PsbF

Chain F: 68% 26% 6%



• Molecule 6: PsbF

Chain f: 68% 26% 6%

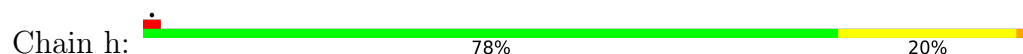


• Molecule 7: PsbH

Chain H: 78% 20%



• Molecule 7: PsbH



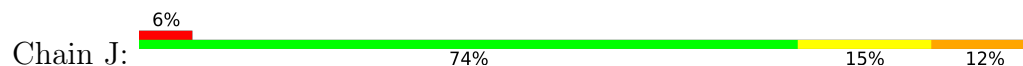
• Molecule 8: PsbI



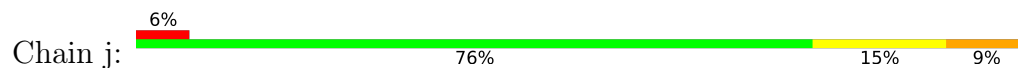
• Molecule 8: PsbI



• Molecule 9: PsbJ



• Molecule 9: PsbJ



• Molecule 10: PsbK



• Molecule 10: PsbK





- Molecule 11: PsbL

Chain L: 78% 22%



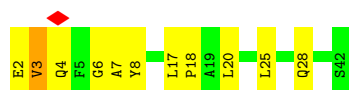
- Molecule 11: PsbL

Chain l: 78% 22%



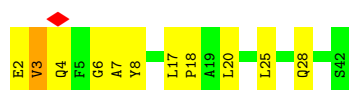
- Molecule 12: PsbM

Chain M: 73% 24% .



- Molecule 12: PsbM

Chain m: 73% 24% .



- Molecule 13: Psb34

Chain N: 7% 97% .



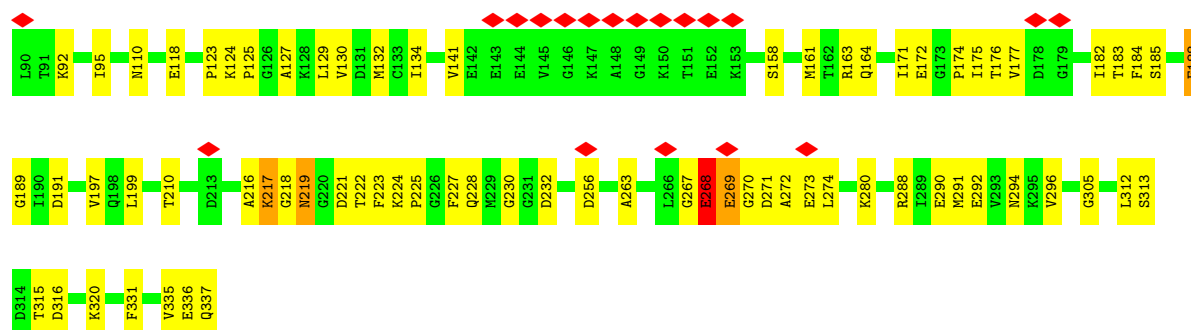
- Molecule 13: Psb34

Chain n: 10% 97% .

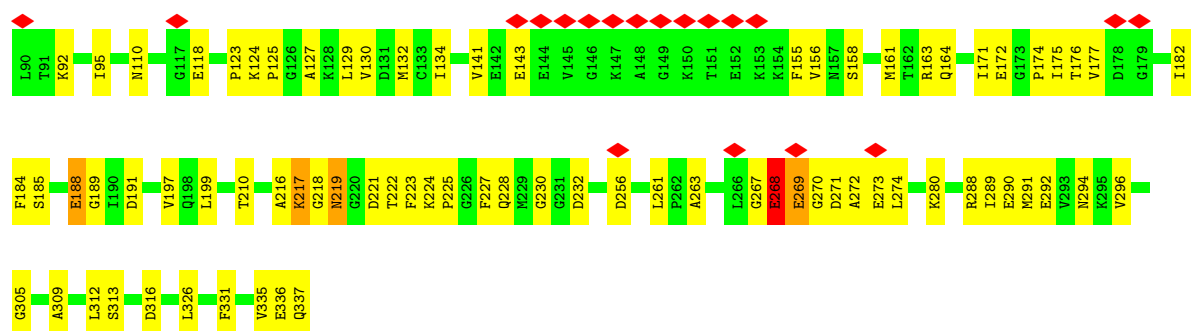


- Molecule 14: PsbO

Chain O: 8% 71% 27% .



• Molecule 14: PsbO



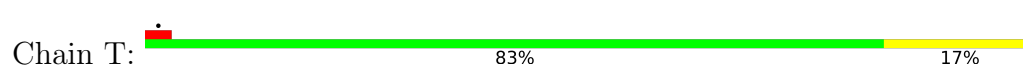
• Molecule 15: PsbQ'



• Molecule 15: PsbQ'

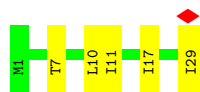
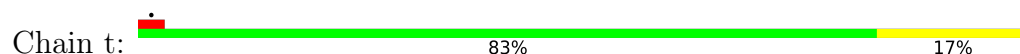


• Molecule 16: PsbT

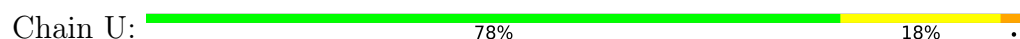




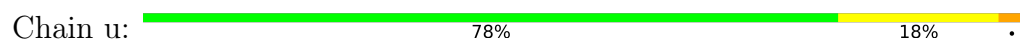
- Molecule 16: PsbT



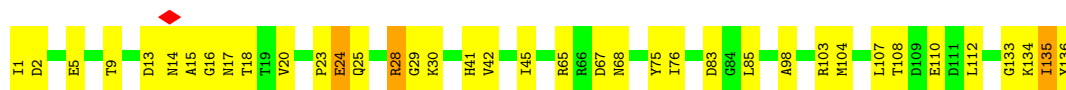
- Molecule 17: PsbU



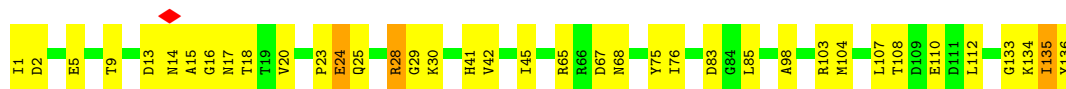
- Molecule 17: PsbU



- Molecule 18: PsbV



- Molecule 18: PsbV



- Molecule 19: PsbW



- Molecule 19: PsbW





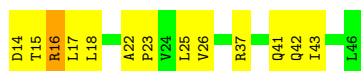
• Molecule 20: PsbX



• Molecule 20: PsbX



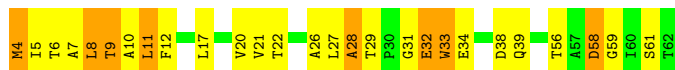
• Molecule 21: PsbY



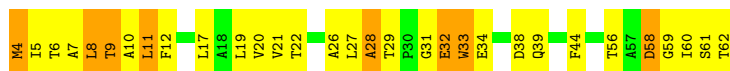
• Molecule 21: PsbY



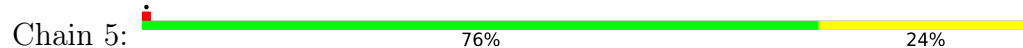
• Molecule 22: PsbZ

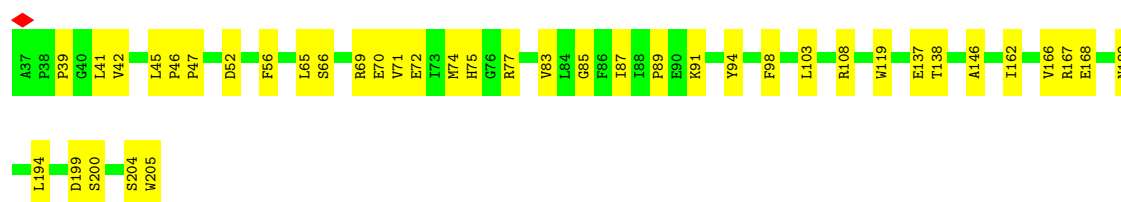


• Molecule 22: PsbZ

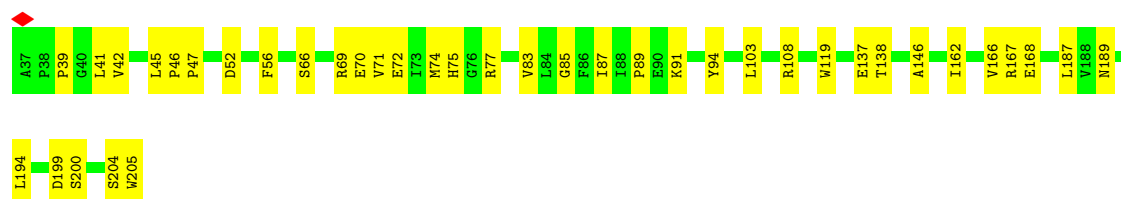
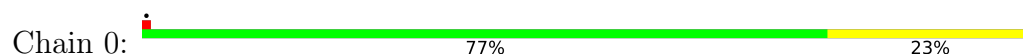


• Molecule 23: FCPH-G, fucoxanthin chlorophyll a/c binding protein

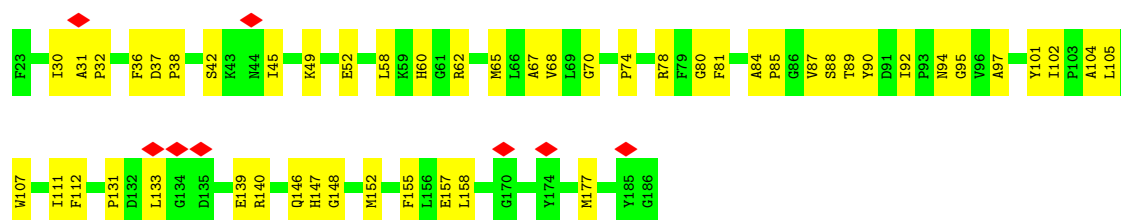




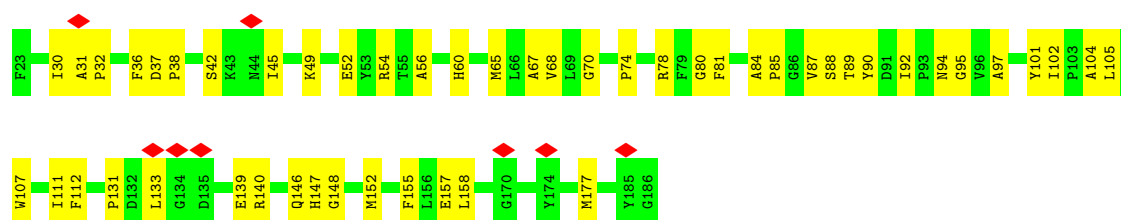
- Molecule 23: FCPH-G, fucoxanthin chlorophyll a/c binding protein



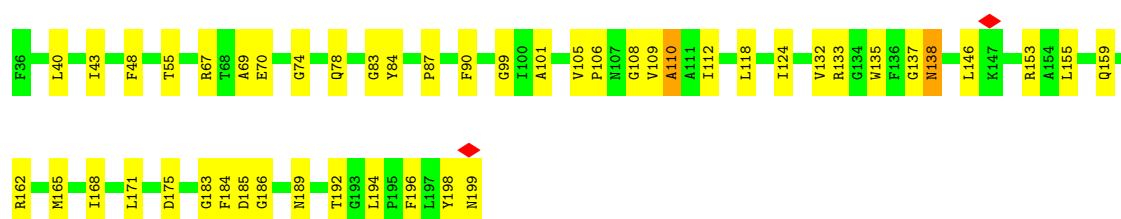
- Molecule 24: FCPH-H2, fucoxanthin chlorophyll a/c binding protein



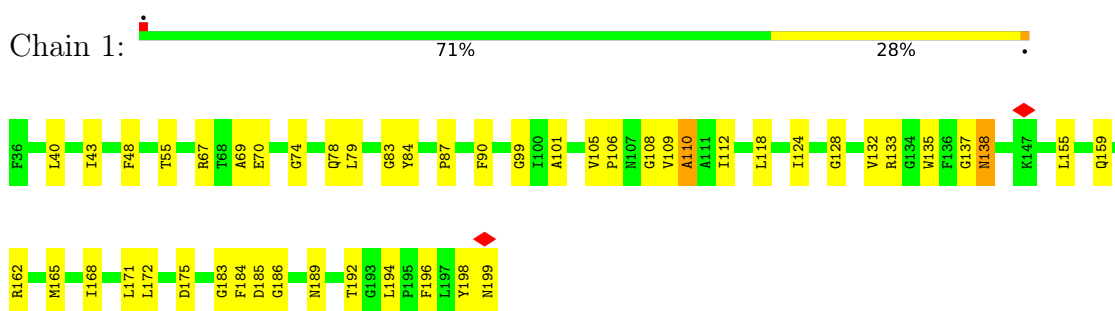
- Molecule 24: FCPH-H2, fucoxanthin chlorophyll a/c binding protein



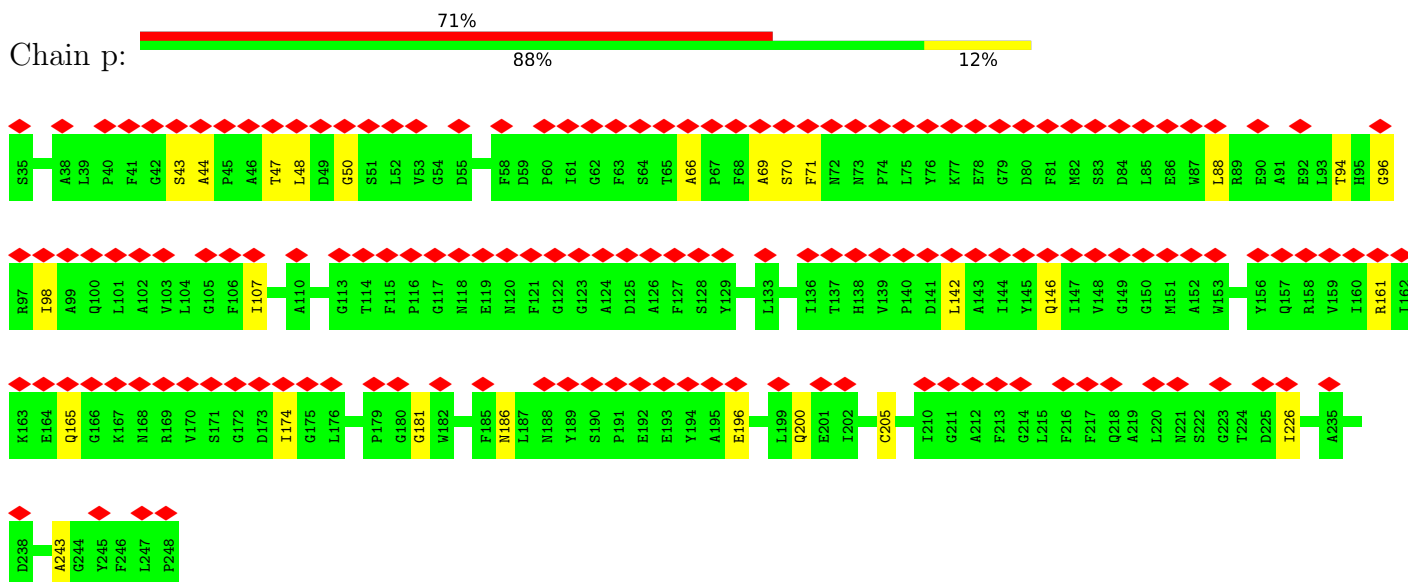
- Molecule 25: FCPH-H1, fucoxanthin chlorophyll a/c binding protein



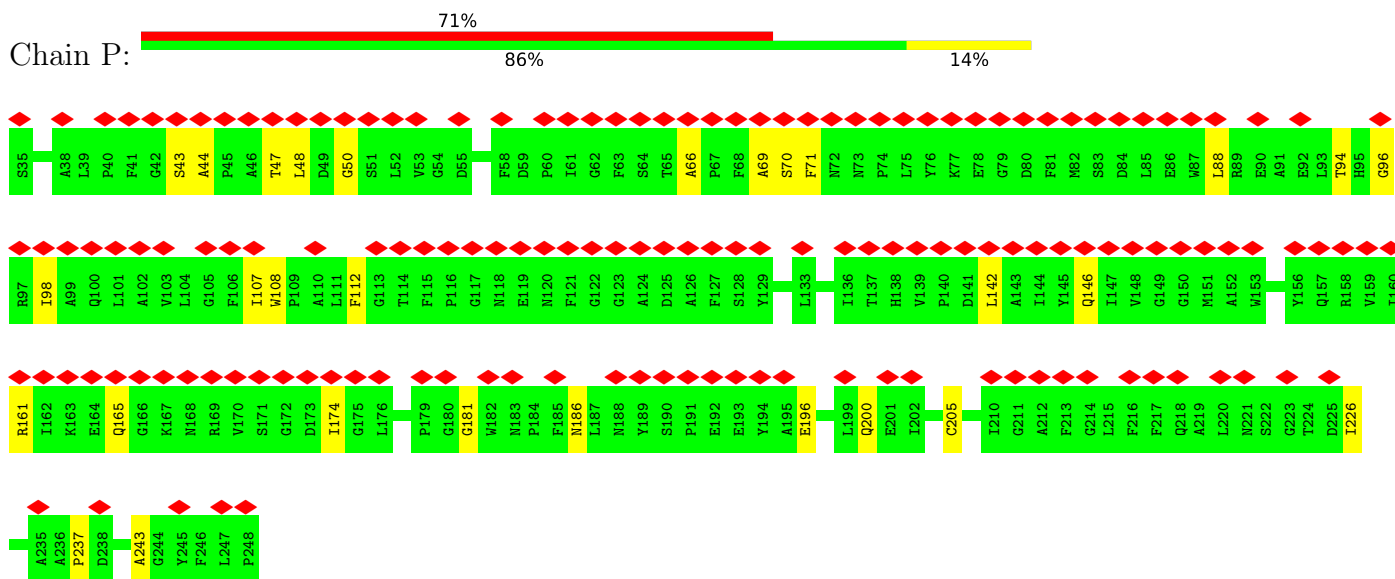
- Molecule 25: FCPH-H1, fucoxanthin chlorophyll a/c binding protein



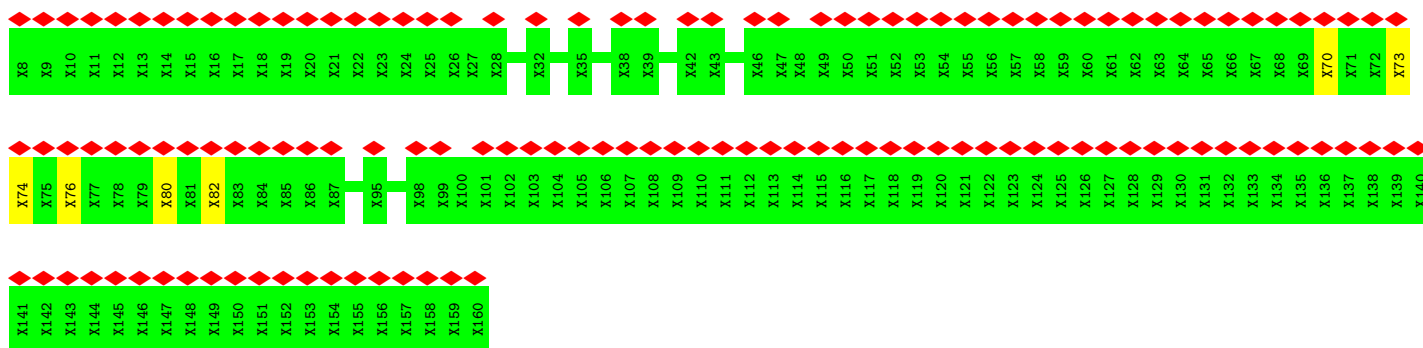
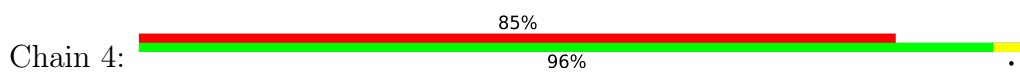
- Molecule 26: FCPH-I, fucoxanthin chlorophyll a/c binding protein



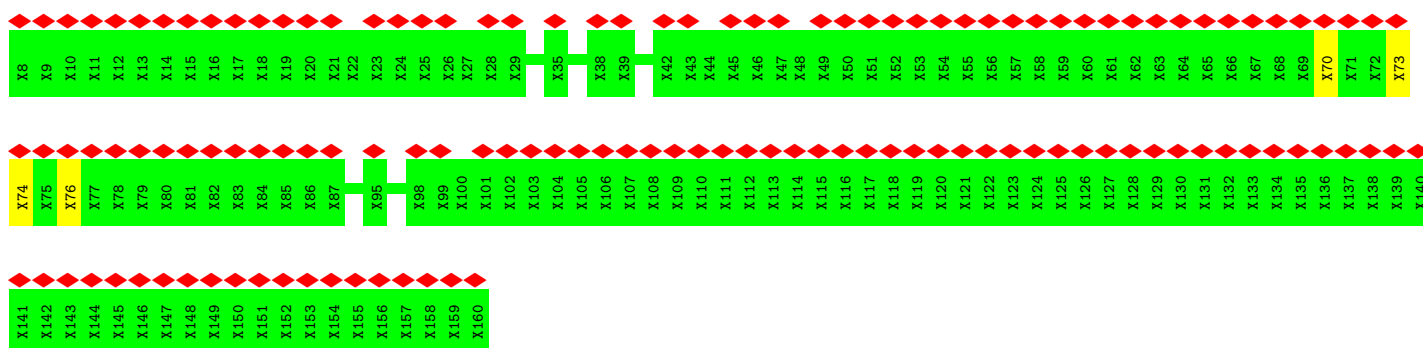
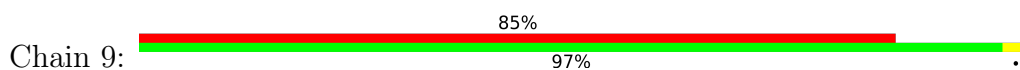
- Molecule 26: FCPH-I, fucoxanthin chlorophyll a/c binding protein



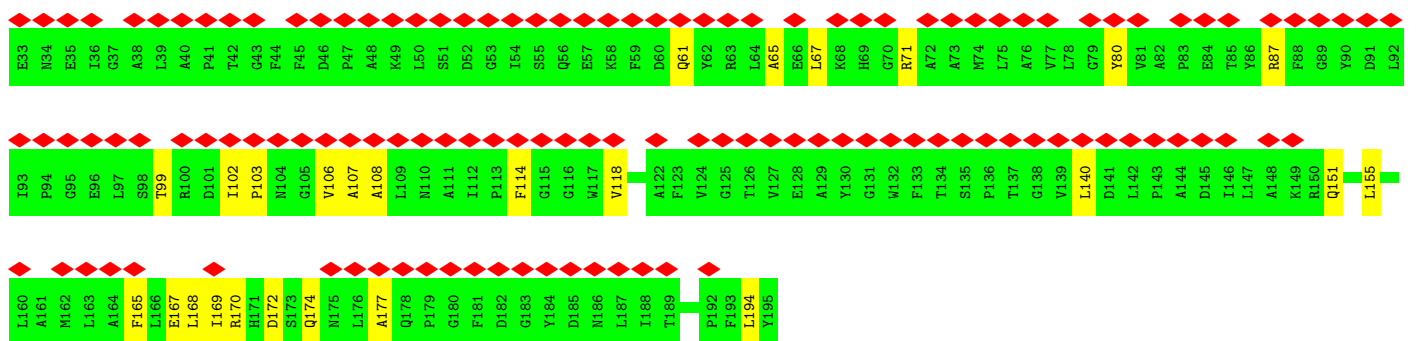
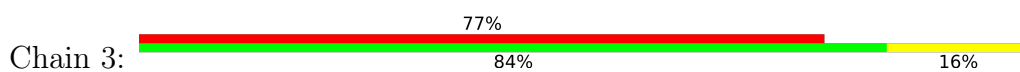
- Molecule 27: FCPH-K, fucoxanthin chlorophyll a/c binding protein



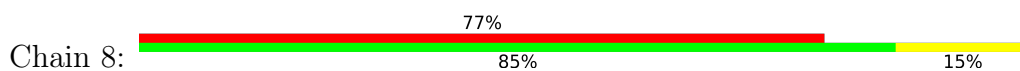
- Molecule 27: FCPH-K, fucoxanthin chlorophyll a/c binding protein



- Molecule 28: FCPH-J, fucoxanthin chlorophyll a/c binding protein



- Molecule 28: FCPH-J, fucoxanthin chlorophyll a/c binding protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.709	Depositor
Minimum map value	-0.314	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.158	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, BCT, OEX, A86, PHO, HEM, FE2, LHG, DGD, CL, PL9, SQD, BCR, LMG, CLA, ET4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.28	0/2609	0.39	0/3563
1	a	0.28	0/2609	0.40	0/3563
2	B	0.24	0/3878	0.36	0/5282
2	b	0.24	0/3878	0.36	0/5282
3	C	0.21	0/3553	0.35	0/4850
3	c	0.22	0/3553	0.35	0/4850
4	D	0.20	0/2759	0.34	0/3766
4	d	0.20	0/2759	0.34	0/3766
5	E	0.20	0/620	0.33	0/847
5	e	0.20	0/620	0.33	0/847
6	F	0.56	0/250	0.64	0/340
6	f	0.56	0/250	0.64	0/340
7	H	0.34	0/509	0.50	0/696
7	h	0.34	0/509	0.50	0/696
8	I	0.40	0/273	0.51	0/371
8	i	0.40	0/273	0.51	0/371
9	J	0.80	2/253 (0.8%)	0.96	4/344 (1.2%)
9	j	0.79	2/253 (0.8%)	0.96	4/344 (1.2%)
10	K	0.51	0/305	0.59	0/420
10	k	0.51	0/305	0.59	0/420
11	L	0.31	0/303	0.43	0/415
11	l	0.31	0/303	0.43	0/415
12	M	0.33	0/299	0.39	0/404
12	m	0.33	0/299	0.39	0/404
14	O	0.24	0/1853	0.40	0/2505
14	o	0.25	0/1853	0.40	0/2505
15	Q	0.35	0/1065	0.63	1/1439 (0.1%)
15	q	0.35	0/1065	0.63	1/1439 (0.1%)
16	T	0.22	0/240	0.34	0/325
16	t	0.23	0/240	0.34	0/325
17	U	0.21	0/693	0.36	0/945
17	u	0.21	0/693	0.36	0/945

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	V	0.33	0/996	0.46	0/1364
18	v	0.33	0/996	0.46	0/1364
19	W	0.46	0/310	0.85	3/421 (0.7%)
19	w	0.42	0/310	0.85	3/421 (0.7%)
20	X	0.35	0/233	0.45	0/315
20	x	0.35	0/233	0.45	0/315
21	Y	0.49	0/216	0.72	0/297
21	y	0.50	0/216	0.72	0/297
22	Z	0.40	0/419	0.45	0/578
22	z	0.40	0/419	0.45	0/578
23	0	0.27	0/1312	0.48	0/1792
23	5	0.27	0/1312	0.49	0/1792
24	2	0.24	0/1258	0.44	0/1714
24	7	0.24	0/1258	0.44	0/1714
25	1	0.31	0/1242	0.47	0/1697
25	6	0.31	0/1242	0.47	0/1697
26	P	0.33	0/1287	0.69	1/1778 (0.1%)
26	p	0.33	0/1287	0.69	1/1778 (0.1%)
28	3	0.39	0/1003	0.65	0/1373
28	8	0.39	0/1003	0.65	0/1373
All	All	0.29	4/55476 (0.0%)	0.46	18/75682 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	j	34	SER	N-CA	5.75	1.54	1.46
9	J	34	SER	N-CA	5.72	1.54	1.46
9	j	33	TYR	CA-C	5.59	1.60	1.52
9	J	33	TYR	CA-C	5.57	1.60	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	33	TYR	N-CA-C	6.89	122.03	112.45
9	j	33	TYR	N-CA-C	6.87	122.00	112.45
9	J	34	SER	N-CA-C	6.75	122.07	107.49
9	j	34	SER	N-CA-C	6.75	122.07	107.49
19	w	97	GLY	N-CA-C	-6.11	102.47	111.03

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	A	2530	0	2400	56	0
1	a	2530	0	2400	53	0
2	B	3748	0	3581	61	0
2	b	3748	0	3581	64	0
3	C	3437	0	3297	74	0
3	c	3437	0	3297	74	0
4	D	2667	0	2551	61	0
4	d	2667	0	2551	57	0
5	E	602	0	576	10	0
5	e	602	0	576	10	0
6	F	242	0	237	12	0
6	f	242	0	237	12	0
7	H	499	0	521	17	0
7	h	499	0	521	16	0
8	I	266	0	264	11	0
8	i	266	0	264	11	0
9	J	247	0	256	7	0
9	j	247	0	256	5	0
10	K	294	0	295	10	0
10	k	294	0	295	10	0
11	L	294	0	281	7	0
11	l	294	0	281	7	0
12	M	295	0	292	6	0
12	m	295	0	292	6	0
13	N	150	0	33	1	0
13	n	150	0	33	1	0
14	O	1824	0	1775	54	0
14	o	1824	0	1775	54	0
15	Q	1050	0	988	67	0
15	q	1050	0	988	65	0
16	T	234	0	241	4	0
16	t	234	0	241	4	0
17	U	678	0	663	16	0
17	u	678	0	663	17	0
18	V	979	0	942	27	0
18	v	979	0	942	28	0
19	W	338	0	254	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	w	338	0	254	18	0
20	X	233	0	254	17	0
20	x	233	0	254	19	0
21	Y	216	0	210	12	0
21	y	216	0	210	11	0
22	Z	413	0	402	22	0
22	z	413	0	402	24	0
23	0	1280	0	1242	42	0
23	5	1280	0	1242	43	0
24	2	1222	0	1142	64	0
24	7	1222	0	1142	63	0
25	1	1209	0	1150	43	0
25	6	1209	0	1150	40	0
26	P	1265	0	946	18	0
26	p	1265	0	946	16	0
27	4	765	0	161	3	0
27	9	765	0	161	2	0
28	3	992	0	778	20	0
28	8	992	0	778	19	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	0	528	0	439	21	0
31	1	580	0	441	14	0
31	2	525	0	395	22	0
31	3	416	0	257	8	0
31	4	372	0	234	0	0
31	5	528	0	439	21	0
31	6	580	0	441	15	0
31	7	525	0	395	22	0
31	8	416	0	257	7	0
31	9	372	0	234	0	0
31	A	174	0	170	4	0
31	B	959	0	994	39	0
31	C	792	0	822	19	0
31	D	186	0	190	4	0
31	P	341	0	213	10	0
31	W	45	0	33	1	0
31	Z	51	0	41	6	0
31	a	174	0	170	3	0
31	b	959	0	994	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	792	0	822	20	0
31	d	186	0	190	4	0
31	p	341	0	213	10	0
31	w	45	0	33	1	0
31	z	51	0	41	6	0
32	A	128	0	148	4	0
32	a	128	0	148	3	0
33	A	40	0	56	3	0
33	B	120	0	168	13	0
33	C	120	0	168	6	0
33	D	40	0	56	2	0
33	H	40	0	56	2	0
33	K	40	0	56	2	0
33	a	40	0	56	3	0
33	b	120	0	168	12	0
33	c	120	0	168	8	0
33	d	40	0	56	1	0
33	h	40	0	56	2	0
33	k	40	0	56	2	0
34	0	48	0	63	5	0
34	5	48	0	63	5	0
34	A	108	0	156	6	0
34	B	94	0	122	3	0
34	a	54	0	78	0	0
34	b	40	0	44	1	0
35	A	32	0	39	3	0
35	D	55	0	80	3	0
35	a	32	0	39	3	0
35	d	55	0	80	4	0
36	A	69	0	81	4	0
36	B	49	0	74	4	0
36	D	110	0	141	9	0
36	H	42	0	54	6	0
36	a	69	0	81	4	0
36	b	49	0	74	4	0
36	d	110	0	141	9	0
36	h	42	0	54	5	0
37	0	48	0	69	1	0
37	5	48	0	69	1	0
37	B	28	0	26	1	0
37	C	51	0	72	4	0
37	D	123	0	156	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	50	0	73	3	0
37	M	91	0	122	2	0
37	W	48	0	66	2	0
37	Y	46	0	62	3	0
37	b	28	0	26	1	0
37	c	51	0	72	4	0
37	d	123	0	156	3	0
37	j	50	0	73	2	0
37	m	91	0	122	2	0
37	w	48	0	66	2	0
37	y	46	0	62	4	0
38	C	1	0	0	0	0
38	c	1	0	0	0	0
39	C	179	0	232	10	0
39	H	62	0	82	4	0
39	c	179	0	232	10	0
39	h	62	0	82	4	0
40	D	4	0	1	0	0
40	d	4	0	1	0	0
41	F	43	0	30	3	0
41	V	43	0	30	6	0
41	f	43	0	30	3	0
41	v	43	0	30	6	0
42	0	144	0	0	1	0
42	1	48	0	0	1	0
42	2	96	0	0	0	0
42	3	96	0	0	0	0
42	4	144	0	0	0	0
42	5	144	0	0	1	0
42	6	48	0	0	1	0
42	7	96	0	0	0	0
42	8	96	0	0	0	0
42	9	144	0	0	0	0
42	P	48	0	0	0	0
42	p	48	0	0	0	0
43	0	42	0	0	0	0
43	5	42	0	0	0	0
44	1	86	0	0	3	0
44	2	86	0	0	24	0
44	3	43	0	0	1	0
44	6	86	0	0	3	0
44	7	86	0	0	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	8	43	0	0	1	0
44	P	43	0	0	7	0
44	p	43	0	0	7	0
All	All	71446	0	64844	1569	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1569 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)
24:7:65:MET:HG2	44:7:304:DD6:C3	1.71	1.19
24:2:65:MET:HG2	44:2:304:DD6:C3	1.71	1.19
31:B:514:CLA:H43	33:B:517:BCR:H383	1.19	1.14
31:b:515:CLA:H43	33:b:518:BCR:H383	1.19	1.13
31:p:604:CLA:C2B	44:p:611:DD6:C37	2.31	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/333 (99%)	316 (96%)	15 (4%)	0	100	100
1	a	331/333 (99%)	316 (96%)	15 (4%)	0	100	100
2	B	479/481 (100%)	456 (95%)	22 (5%)	1 (0%)	43	65
2	b	479/481 (100%)	456 (95%)	22 (5%)	1 (0%)	43	65
3	C	448/450 (100%)	435 (97%)	12 (3%)	1 (0%)	43	65
3	c	448/450 (100%)	435 (97%)	12 (3%)	1 (0%)	43	65
4	D	338/340 (99%)	325 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	338/340 (99%)	325 (96%)	13 (4%)	0	100	100
5	E	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
5	e	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
6	F	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	7
6	f	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	7
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	0	100	100
9	j	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	39/41 (95%)	39 (100%)	0	0	100	100
12	m	39/41 (95%)	39 (100%)	0	0	100	100
14	O	246/248 (99%)	223 (91%)	21 (8%)	2 (1%)	16	36
14	o	246/248 (99%)	223 (91%)	21 (8%)	2 (1%)	16	36
15	Q	143/145 (99%)	113 (79%)	17 (12%)	13 (9%)	0	1
15	q	143/145 (99%)	113 (79%)	17 (12%)	13 (9%)	0	1
16	T	27/29 (93%)	27 (100%)	0	0	100	100
16	t	27/29 (93%)	27 (100%)	0	0	100	100
17	U	90/92 (98%)	82 (91%)	8 (9%)	0	100	100
17	u	90/92 (98%)	82 (91%)	8 (9%)	0	100	100
18	V	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18	40
18	v	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18	40
19	W	42/50 (84%)	36 (86%)	2 (5%)	4 (10%)	0	1
19	w	42/50 (84%)	36 (86%)	2 (5%)	4 (10%)	0	1
20	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	8
20	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Y	31/33 (94%)	26 (84%)	5 (16%)	0	100	100
21	y	31/33 (94%)	26 (84%)	5 (16%)	0	100	100
22	Z	57/59 (97%)	44 (77%)	11 (19%)	2 (4%)	3	7
22	z	57/59 (97%)	44 (77%)	11 (19%)	2 (4%)	3	7
23	0	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
23	5	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
24	2	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
24	7	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
25	1	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21	45
25	6	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21	45
26	P	212/214 (99%)	172 (81%)	38 (18%)	2 (1%)	14	34
26	p	212/214 (99%)	173 (82%)	37 (18%)	2 (1%)	14	34
28	3	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	45
28	8	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	45
All	All	7200/7316 (98%)	6589 (92%)	551 (8%)	60 (1%)	18	36

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	460	ASP
6	F	43	ILE
14	O	268	GLU
15	Q	70	ILE
15	Q	84	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/272 (92%)	242 (97%)	8 (3%)	34	59
1	a	250/272 (92%)	243 (97%)	7 (3%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	370/384 (96%)	360 (97%)	10 (3%)	39	64
2	b	370/384 (96%)	360 (97%)	10 (3%)	39	64
3	C	337/355 (95%)	334 (99%)	3 (1%)	70	82
3	c	337/355 (95%)	334 (99%)	3 (1%)	70	82
4	D	265/272 (97%)	264 (100%)	1 (0%)	84	92
4	d	265/272 (97%)	264 (100%)	1 (0%)	84	92
5	E	65/69 (94%)	64 (98%)	1 (2%)	57	75
5	e	65/69 (94%)	64 (98%)	1 (2%)	57	75
6	F	22/25 (88%)	19 (86%)	3 (14%)	3	10
6	f	22/25 (88%)	19 (86%)	3 (14%)	3	10
7	H	52/54 (96%)	49 (94%)	3 (6%)	18	40
7	h	52/54 (96%)	49 (94%)	3 (6%)	18	40
8	I	30/33 (91%)	27 (90%)	3 (10%)	7	19
8	i	30/33 (91%)	27 (90%)	3 (10%)	7	19
9	J	26/26 (100%)	26 (100%)	0	100	100
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/32 (94%)	29 (97%)	1 (3%)	33	58
10	k	30/32 (94%)	29 (97%)	1 (3%)	33	58
11	L	31/33 (94%)	31 (100%)	0	100	100
11	l	31/33 (94%)	31 (100%)	0	100	100
12	M	26/30 (87%)	24 (92%)	2 (8%)	12	28
12	m	26/30 (87%)	24 (92%)	2 (8%)	12	28
14	O	185/201 (92%)	176 (95%)	9 (5%)	22	47
14	o	185/201 (92%)	176 (95%)	9 (5%)	22	47
15	Q	99/116 (85%)	89 (90%)	10 (10%)	7	19
15	q	99/116 (85%)	89 (90%)	10 (10%)	7	19
16	T	24/26 (92%)	24 (100%)	0	100	100
16	t	24/26 (92%)	24 (100%)	0	100	100
17	U	70/77 (91%)	65 (93%)	5 (7%)	13	31
17	u	70/77 (91%)	65 (93%)	5 (7%)	13	31
18	V	101/114 (89%)	99 (98%)	2 (2%)	48	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	v	101/114 (89%)	99 (98%)	2 (2%)	48	70
19	W	25/34 (74%)	24 (96%)	1 (4%)	28	53
19	w	25/34 (74%)	24 (96%)	1 (4%)	28	53
20	X	25/26 (96%)	24 (96%)	1 (4%)	28	53
20	x	25/26 (96%)	24 (96%)	1 (4%)	28	53
21	Y	18/26 (69%)	16 (89%)	2 (11%)	6	16
21	y	18/26 (69%)	16 (89%)	2 (11%)	6	16
22	Z	39/48 (81%)	32 (82%)	7 (18%)	2	4
22	z	39/48 (81%)	32 (82%)	7 (18%)	2	4
23	0	129/136 (95%)	129 (100%)	0	100	100
23	5	129/136 (95%)	129 (100%)	0	100	100
24	2	110/131 (84%)	109 (99%)	1 (1%)	70	82
24	7	110/131 (84%)	109 (99%)	1 (1%)	70	82
25	1	107/129 (83%)	105 (98%)	2 (2%)	50	71
25	6	107/129 (83%)	105 (98%)	2 (2%)	50	71
26	P	70/166 (42%)	70 (100%)	0	100	100
26	p	70/166 (42%)	70 (100%)	0	100	100
28	3	54/128 (42%)	54 (100%)	0	100	100
28	8	54/128 (42%)	54 (100%)	0	100	100
All	All	5120/5886 (87%)	4971 (97%)	149 (3%)	38	62

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	q	67	PHE
24	7	139	GLU
15	q	78	GLU
18	v	24	GLU
15	Q	78	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
7	h	69	ASN

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Mol	Chain	Res	Type
23	5	185	GLN
10	k	53	GLN
17	u	16	ASN
23	5	196	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 336 ligands modelled in this entry, 4 are monoatomic - leaving 332 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	$\# Z > 2$
33	BCR	c	517	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
31	CLA	2	314	24	41,46,73	1.57	9 (21%)	51,80,113	1.54	8 (15%)
31	CLA	P	603	26	40,45,73	1.58	9 (22%)	50,79,113	1.67	8 (16%)
31	CLA	5	308	-	65,69,73	1.29	8 (12%)	78,108,113	1.35	7 (8%)
43	ET4	5	302	-	41,43,43	1.73	11 (26%)	54,60,60	2.22	17 (31%)
37	LMG	B	520	-	28,28,55	0.95	0	36,36,63	1.34	6 (16%)
42	A86	0	303	-	44,50,50	1.28	4 (9%)	51,76,76	2.43	19 (37%)
31	CLA	6	208	-	51,55,73	1.44	7 (13%)	61,91,113	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	507	-	69,73,73	1.24	8 (11%)	83,113,113	1.35	7 (8%)
39	DGD	C	519	-	63,63,67	0.92	3 (4%)	77,77,81	1.46	12 (15%)
39	DGD	c	520	-	63,63,67	0.85	2 (3%)	77,77,81	0.93	3 (3%)
33	BCR	c	516	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	9 (16%)
33	BCR	H	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
31	CLA	9	208	-	43,48,73	1.58	11 (25%)	51,83,113	1.64	9 (17%)
31	CLA	b	513	2	45,49,73	1.48	8 (17%)	54,84,113	1.60	8 (14%)
34	SQD	B	522	-	53,54,54	0.94	4 (7%)	62,65,65	1.65	12 (19%)
31	CLA	2	312	24	40,44,73	1.70	8 (20%)	49,77,113	1.62	8 (16%)
31	CLA	B	507	-	45,49,73	1.51	9 (20%)	54,84,113	1.54	6 (11%)
31	CLA	A	403	1	69,73,73	1.25	8 (11%)	83,113,113	1.36	8 (9%)
31	CLA	4	213	-	37,43,73	1.77	11 (29%)	49,76,113	1.74	12 (24%)
31	CLA	P	609	-	43,47,73	1.52	9 (20%)	50,81,113	1.58	5 (10%)
44	DD6	1	203	-	39,45,45	2.00	3 (7%)	52,67,67	2.20	17 (32%)
36	LHG	H	103	-	41,41,48	0.65	1 (2%)	44,47,54	1.14	3 (6%)
39	DGD	c	519	-	63,63,67	0.92	3 (4%)	77,77,81	1.46	12 (15%)
33	BCR	h	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	6 (10%)
31	CLA	7	309	24	63,67,73	1.30	9 (14%)	75,105,113	1.34	8 (10%)
37	LMG	b	521	-	28,28,55	0.95	0	36,36,63	1.34	7 (19%)
31	CLA	D	404	4	69,73,73	1.24	10 (14%)	83,113,113	1.33	6 (7%)
37	LMG	0	315	-	48,48,55	0.77	0	56,56,63	1.29	6 (10%)
31	CLA	b	503	2	65,69,73	1.26	8 (12%)	74,106,113	1.29	6 (8%)
44	DD6	7	303	-	39,45,45	2.00	3 (7%)	52,67,67	2.19	17 (32%)
31	CLA	C	504	-	55,59,73	1.39	9 (16%)	66,96,113	1.47	8 (12%)
31	CLA	0	311	-	49,53,73	1.48	7 (14%)	59,89,113	1.49	4 (6%)
31	CLA	p	605	-	40,45,73	1.58	11 (27%)	50,79,113	1.68	7 (14%)
34	SQD	A	409	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
31	CLA	C	509	3	69,73,73	1.24	10 (14%)	83,113,113	1.33	9 (10%)
31	CLA	C	514	3	53,57,73	1.40	8 (15%)	62,93,113	1.46	7 (11%)
31	CLA	b	516	2	69,73,73	1.26	10 (14%)	83,113,113	1.34	5 (6%)
31	CLA	3	314	-	40,43,73	1.67	11 (27%)	51,76,113	1.59	8 (15%)
42	A86	0	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.93	19 (37%)
31	CLA	8	309	-	43,48,73	1.54	9 (20%)	51,83,113	1.74	8 (15%)
31	CLA	c	510	3	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
31	CLA	7	308	24	48,52,73	1.56	8 (16%)	61,88,113	1.50	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	DD6	7	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.51	17 (32%)
31	CLA	0	304	-	45,49,73	1.51	9 (20%)	54,84,113	1.55	6 (11%)
31	CLA	1	209	25	48,52,73	1.56	9 (18%)	61,88,113	1.51	8 (13%)
31	CLA	2	315	24	41,46,73	1.57	7 (17%)	51,80,113	1.54	5 (9%)
42	A86	1	202	-	44,50,50	1.31	4 (9%)	51,76,76	2.90	16 (31%)
31	CLA	c	509	3	69,73,73	1.25	9 (13%)	83,113,113	1.33	8 (9%)
31	CLA	9	209	-	45,49,73	1.50	10 (22%)	54,84,113	1.58	7 (12%)
31	CLA	1	207	25	48,52,73	1.57	9 (18%)	61,88,113	1.47	7 (11%)
42	A86	9	202	-	44,50,50	1.46	5 (11%)	51,76,76	3.56	26 (50%)
31	CLA	5	307	-	65,69,73	1.29	8 (12%)	78,108,113	1.34	6 (7%)
31	CLA	B	513	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	9 (10%)
33	BCR	C	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	7 (12%)
42	A86	7	302	-	44,50,50	1.52	6 (13%)	51,76,76	3.25	18 (35%)
31	CLA	W	202	19	49,53,73	1.46	10 (20%)	59,89,113	1.48	9 (15%)
31	CLA	p	608	26	40,46,73	1.65	11 (27%)	51,80,113	1.59	9 (17%)
32	PHO	a	406	-	58,69,69	1.99	10 (17%)	56,99,99	1.50	6 (10%)
31	CLA	B	504	2	69,73,73	1.24	8 (11%)	83,113,113	1.39	6 (7%)
31	CLA	C	508	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	4 (4%)
31	CLA	B	514	2	64,68,73	1.29	10 (15%)	76,106,113	1.33	7 (9%)
31	CLA	C	505	-	68,72,73	1.24	9 (13%)	81,111,113	1.32	5 (6%)
42	A86	4	202	-	44,50,50	1.47	5 (11%)	51,76,76	3.55	26 (50%)
44	DD6	3	303	-	39,45,45	2.01	3 (7%)	52,67,67	2.77	15 (28%)
31	CLA	2	308	24	48,52,73	1.55	9 (18%)	61,88,113	1.49	7 (11%)
31	CLA	P	604	-	43,48,73	1.52	10 (23%)	51,83,113	1.61	8 (15%)
31	CLA	1	206	25	49,53,73	1.45	8 (16%)	59,89,113	1.51	6 (10%)
31	CLA	p	603	26	40,45,73	1.58	10 (25%)	50,79,113	1.68	8 (16%)
31	CLA	4	211	-	38,42,73	1.71	10 (26%)	48,74,113	1.52	7 (14%)
31	CLA	7	313	24	41,46,73	1.56	7 (17%)	51,80,113	1.52	6 (11%)
31	CLA	C	503	3	68,72,73	1.27	9 (13%)	81,111,113	1.32	7 (8%)
34	SQD	A	411	-	53,54,54	0.94	3 (5%)	62,65,65	1.65	12 (19%)
31	CLA	3	306	28	35,41,73	1.87	11 (31%)	49,72,113	1.71	9 (18%)
33	BCR	B	519	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
31	CLA	3	305	28	44,49,73	1.52	11 (25%)	52,84,113	1.57	5 (9%)
35	PL9	A	410	-	32,32,55	1.11	4 (12%)	39,40,69	1.55	8 (20%)
31	CLA	c	508	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	0	312	-	46,50,73	1.50	7 (15%)	55,85,113	1.47	4 (7%)
31	CLA	6	215	25	41,46,73	1.55	8 (19%)	51,80,113	1.55	6 (11%)
41	HEM	F	101	6,5	50,50,50	1.33	6 (12%)	66,82,82	1.12	5 (7%)
42	A86	5	317	-	44,50,50	1.29	3 (6%)	51,76,76	2.94	18 (35%)
31	CLA	d	403	4	66,70,73	1.34	11 (16%)	82,109,113	1.37	7 (8%)
31	CLA	1	210	25	69,73,73	1.23	8 (11%)	83,113,113	1.34	8 (9%)
31	CLA	6	212	25	45,49,73	1.51	8 (17%)	54,84,113	1.52	6 (11%)
42	A86	3	302	-	44,50,50	1.47	5 (11%)	51,76,76	3.27	23 (45%)
31	CLA	7	305	-	45,49,73	1.52	9 (20%)	54,84,113	1.53	7 (12%)
42	A86	8	302	-	44,50,50	1.47	5 (11%)	51,76,76	3.28	23 (45%)
31	CLA	P	605	-	40,45,73	1.57	11 (27%)	50,79,113	1.67	7 (14%)
31	CLA	C	512	3	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
37	LMG	5	315	-	48,48,55	0.77	0	56,56,63	1.29	6 (10%)
31	CLA	2	307	-	51,55,73	1.44	8 (15%)	61,91,113	1.46	7 (11%)
31	CLA	b	517	2	69,73,73	1.25	10 (14%)	83,113,113	1.32	7 (8%)
31	CLA	a	404	-	53,57,73	1.40	9 (16%)	62,93,113	1.47	8 (12%)
36	LHG	D	411	-	33,33,48	0.72	0	36,39,54	1.35	4 (11%)
31	CLA	B	506	-	69,73,73	1.24	8 (11%)	83,113,113	1.35	8 (9%)
31	CLA	B	503	2	68,72,73	1.25	10 (14%)	81,111,113	1.30	5 (6%)
31	CLA	3	304	-	40,42,73	1.77	13 (32%)	50,74,113	1.70	8 (16%)
31	CLA	9	207	-	41,46,73	1.55	9 (21%)	51,80,113	1.63	5 (9%)
31	CLA	2	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.51	7 (12%)
32	PHO	a	405	-	58,69,69	2.03	10 (17%)	56,99,99	1.59	9 (16%)
31	CLA	5	304	-	45,49,73	1.51	9 (20%)	54,84,113	1.53	6 (11%)
31	CLA	B	510	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
42	A86	8	301	-	44,50,50	1.53	7 (15%)	51,76,76	5.17	24 (47%)
31	CLA	8	307	-	47,50,73	1.48	12 (25%)	56,84,113	1.46	6 (10%)
36	LHG	h	103	-	41,41,48	0.65	1 (2%)	44,47,54	1.13	3 (6%)
39	DGD	C	520	-	63,63,67	0.85	2 (3%)	77,77,81	0.93	3 (3%)
31	CLA	P	601	26	40,44,73	1.66	9 (22%)	49,77,113	1.70	8 (16%)
31	CLA	7	311	24	47,51,73	1.49	8 (17%)	56,86,113	1.40	7 (12%)
31	CLA	4	206	-	39,45,73	1.61	10 (25%)	48,78,113	1.49	5 (10%)
31	CLA	C	511	3	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
36	LHG	A	412	-	42,42,48	0.68	1 (2%)	45,48,54	1.26	5 (11%)
36	LHG	A	413	-	25,25,48	0.81	1 (4%)	28,31,54	1.27	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	C	502	3	69,73,73	1.22	8 (11%)	83,113,113	1.33	6 (7%)
31	CLA	p	609	-	43,47,73	1.52	9 (20%)	50,81,113	1.57	5 (10%)
31	CLA	6	209	25	48,52,73	1.55	9 (18%)	61,88,113	1.50	8 (13%)
31	CLA	3	311	28	43,48,73	1.55	9 (20%)	51,83,113	1.60	7 (13%)
33	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	7 (12%)
41	HEM	v	201	18	50,50,50	1.27	5 (10%)	66,82,82	1.38	8 (12%)
31	CLA	z	101	-	55,59,73	1.42	8 (14%)	66,96,113	1.36	7 (10%)
31	CLA	1	214	25	41,46,73	1.55	8 (19%)	51,80,113	1.56	6 (11%)
31	CLA	A	407	-	64,68,73	1.29	8 (12%)	77,107,113	1.36	10 (12%)
31	CLA	c	502	3	69,73,73	1.22	8 (11%)	83,113,113	1.34	6 (7%)
31	CLA	8	311	28	43,48,73	1.55	9 (20%)	51,83,113	1.60	6 (11%)
31	CLA	6	201	24	48,52,73	1.56	10 (20%)	61,88,113	1.53	8 (13%)
29	OEX	a	401	1,3	0,14,14	-	-	-	-	-
31	CLA	5	306	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	5 (8%)
31	CLA	B	501	-	47,51,73	1.48	9 (19%)	56,86,113	1.47	5 (8%)
33	BCR	B	517	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
33	BCR	C	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	9 (16%)
36	LHG	a	412	-	25,25,48	0.80	1 (4%)	28,31,54	1.27	2 (7%)
40	BCT	D	402	30	2,3,3	1.24	0	2,3,3	4.10	2 (100%)
32	PHO	A	405	-	58,69,69	2.03	10 (17%)	56,99,99	1.59	9 (16%)
31	CLA	6	213	25	43,48,73	1.54	7 (16%)	51,83,113	1.48	5 (9%)
37	LMG	w	201	-	48,48,55	0.76	1 (2%)	56,56,63	1.34	7 (12%)
31	CLA	P	608	26	40,46,73	1.65	11 (27%)	51,80,113	1.57	9 (17%)
39	DGD	C	518	-	56,56,67	0.95	3 (5%)	70,70,81	1.45	11 (15%)
31	CLA	9	213	-	37,43,73	1.78	10 (27%)	49,76,113	1.74	12 (24%)
33	BCR	K	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
31	CLA	7	315	24	41,46,73	1.56	7 (17%)	51,80,113	1.54	6 (11%)
37	LMG	d	408	-	46,46,55	0.77	1 (2%)	54,54,63	1.33	7 (12%)
31	CLA	6	206	25	49,53,73	1.46	7 (14%)	59,89,113	1.52	5 (8%)
31	CLA	6	207	25	48,52,73	1.56	9 (18%)	61,88,113	1.48	7 (11%)
36	LHG	d	411	-	33,33,48	0.72	0	36,39,54	1.34	4 (11%)
31	CLA	2	309	24	63,67,73	1.30	9 (14%)	75,105,113	1.35	8 (10%)
31	CLA	7	312	24	40,44,73	1.70	9 (22%)	49,77,113	1.63	9 (18%)
39	DGD	c	518	-	56,56,67	0.95	3 (5%)	70,70,81	1.45	11 (15%)
42	A86	4	203	-	44,50,50	1.41	3 (6%)	51,76,76	3.55	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	d	410	-	40,40,55	0.94	3 (7%)	48,48,63	1.35	6 (12%)
35	PL9	D	406	-	55,55,55	1.35	5 (9%)	68,69,69	1.56	12 (17%)
42	A86	0	317	-	44,50,50	1.29	3 (6%)	51,76,76	2.94	18 (35%)
31	CLA	B	516	2	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
31	CLA	8	312	28	44,49,73	1.52	8 (18%)	52,84,113	1.48	6 (11%)
42	A86	5	303	-	44,50,50	1.28	4 (9%)	51,76,76	2.43	20 (39%)
31	CLA	2	313	24	41,46,73	1.56	8 (19%)	51,80,113	1.52	6 (11%)
31	CLA	1	201	24	48,52,73	1.56	10 (20%)	61,88,113	1.53	8 (13%)
31	CLA	6	205	-	45,49,73	1.51	7 (15%)	54,84,113	1.50	6 (11%)
34	SQD	B	523	-	39,40,54	1.10	5 (12%)	48,51,65	1.76	12 (25%)
41	HEM	V	201	18	50,50,50	1.27	5 (10%)	66,82,82	1.38	8 (12%)
31	CLA	C	507	3	49,53,73	1.47	9 (18%)	59,89,113	1.45	5 (8%)
31	CLA	p	607	-	38,44,73	1.70	11 (28%)	50,77,113	1.54	6 (12%)
31	CLA	9	210	-	41,46,73	1.56	8 (19%)	51,80,113	1.61	9 (17%)
37	LMG	M	102	-	40,40,55	0.86	1 (2%)	48,48,63	1.30	4 (8%)
42	A86	5	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.93	19 (37%)
31	CLA	c	513	3	68,72,73	1.25	9 (13%)	81,111,113	1.28	6 (7%)
36	LHG	D	407	-	46,47,48	0.63	1 (2%)	45,51,54	1.23	6 (13%)
31	CLA	0	310	23	59,63,73	1.35	9 (15%)	71,101,113	1.35	7 (9%)
34	SQD	b	501	-	39,40,54	1.10	5 (12%)	48,51,65	1.76	12 (25%)
37	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
31	CLA	C	510	3	69,73,73	1.24	9 (13%)	83,113,113	1.35	9 (10%)
31	CLA	9	212	-	41,44,73	1.65	9 (21%)	52,77,113	1.59	7 (13%)
44	DD6	2	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.51	18 (34%)
31	CLA	5	311	-	49,53,73	1.46	8 (16%)	59,89,113	1.49	4 (6%)
31	CLA	p	606	-	39,45,73	1.65	11 (28%)	48,78,113	1.50	6 (12%)
41	HEM	f	101	6,5	50,50,50	1.34	6 (12%)	66,82,82	1.12	5 (7%)
37	LMG	W	201	-	48,48,55	0.76	1 (2%)	56,56,63	1.33	7 (12%)
31	CLA	6	214	25	41,46,73	1.55	8 (19%)	51,80,113	1.55	6 (11%)
31	CLA	8	310	28	41,43,73	1.74	11 (26%)	48,75,113	1.63	7 (14%)
32	PHO	A	406	-	58,69,69	1.99	10 (17%)	56,99,99	1.50	6 (10%)
33	BCR	k	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
31	CLA	P	607	-	38,44,73	1.70	11 (28%)	50,77,113	1.53	7 (14%)
31	CLA	b	506	2	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
36	LHG	B	521	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	404	-	53,57,73	1.40	8 (15%)	62,93,113	1.47	8 (12%)
37	LMG	D	409	-	37,37,55	0.78	0	45,45,63	1.33	7 (15%)
31	CLA	0	314	23	41,46,73	1.56	9 (21%)	51,80,113	1.53	5 (9%)
31	CLA	1	205	-	45,49,73	1.52	8 (17%)	54,84,113	1.49	6 (11%)
31	CLA	0	309	23	45,49,73	1.52	9 (20%)	54,84,113	1.53	7 (12%)
37	LMG	Y	101	-	46,46,55	0.75	1 (2%)	54,54,63	1.38	10 (18%)
31	CLA	c	503	3	68,72,73	1.26	9 (13%)	81,111,113	1.33	7 (8%)
31	CLA	B	515	2	69,73,73	1.26	9 (13%)	83,113,113	1.33	5 (6%)
31	CLA	6	216	25	41,46,73	1.55	7 (17%)	51,80,113	1.49	5 (9%)
37	LMG	d	409	-	37,37,55	0.79	0	45,45,63	1.33	7 (15%)
31	CLA	7	307	-	51,55,73	1.44	8 (15%)	61,91,113	1.46	7 (11%)
31	CLA	0	306	-	49,53,73	1.48	8 (16%)	59,89,113	1.44	5 (8%)
31	CLA	0	307	-	65,69,73	1.30	8 (12%)	78,108,113	1.34	5 (6%)
44	DD6	1	204	-	39,45,45	2.23	4 (10%)	52,67,67	2.34	17 (32%)
31	CLA	c	504	-	55,59,73	1.39	9 (16%)	66,96,113	1.47	8 (12%)
31	CLA	3	307	-	47,50,73	1.48	11 (23%)	56,84,113	1.45	6 (10%)
37	LMG	m	102	-	40,40,55	0.86	1 (2%)	48,48,63	1.30	4 (8%)
42	A86	6	202	-	44,50,50	1.32	4 (9%)	51,76,76	2.90	16 (31%)
43	ET4	0	302	-	41,43,43	1.73	11 (26%)	54,60,60	2.22	17 (31%)
34	SQD	5	316	-	47,48,54	1.03	5 (10%)	56,59,65	1.45	8 (14%)
31	CLA	9	206	-	39,45,73	1.59	10 (25%)	48,78,113	1.49	5 (10%)
36	LHG	d	412	-	27,27,48	0.87	2 (7%)	31,32,54	1.72	4 (12%)
31	CLA	3	310	28	41,43,73	1.73	11 (26%)	48,75,113	1.63	7 (14%)
31	CLA	5	312	-	46,50,73	1.50	8 (17%)	55,85,113	1.46	4 (7%)
31	CLA	4	207	-	41,46,73	1.54	9 (21%)	51,80,113	1.62	5 (9%)
31	CLA	Z	101	-	55,59,73	1.42	8 (14%)	66,96,113	1.36	7 (10%)
37	LMG	J	101	-	50,50,55	0.79	1 (2%)	58,58,63	1.34	6 (10%)
36	LHG	d	407	-	46,47,48	0.63	2 (4%)	45,51,54	1.23	6 (13%)
31	CLA	c	511	3	69,73,73	1.25	10 (14%)	83,113,113	1.26	7 (8%)
31	CLA	P	602	-	45,49,73	1.51	10 (22%)	54,84,113	1.61	10 (18%)
31	CLA	1	211	25	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
31	CLA	P	606	-	39,45,73	1.65	10 (25%)	48,78,113	1.50	6 (12%)
42	A86	9	201	-	44,50,50	1.38	4 (9%)	51,76,76	4.06	22 (43%)
31	CLA	B	505	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
42	A86	4	201	-	44,50,50	1.38	4 (9%)	51,76,76	4.06	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	7	310	24	59,63,73	1.34	9 (15%)	71,101,113	1.38	8 (11%)
39	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.42	10 (12%)
31	CLA	3	312	28	44,49,73	1.51	8 (18%)	52,84,113	1.48	6 (11%)
31	CLA	7	314	24	41,46,73	1.56	9 (21%)	51,80,113	1.55	8 (15%)
31	CLA	c	512	3	69,73,73	1.23	8 (11%)	83,113,113	1.34	6 (7%)
31	CLA	B	512	2	45,49,73	1.48	8 (17%)	54,84,113	1.59	8 (14%)
33	BCR	a	408	-	41,41,41	1.14	2 (4%)	56,56,56	1.16	5 (8%)
31	CLA	0	308	-	65,69,73	1.30	10 (15%)	78,108,113	1.34	8 (10%)
31	CLA	6	211	25	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
31	CLA	b	502	-	47,51,73	1.48	9 (19%)	56,86,113	1.47	5 (8%)
31	CLA	4	208	-	43,48,73	1.58	11 (25%)	51,83,113	1.64	9 (17%)
31	CLA	3	308	-	40,43,73	1.62	11 (27%)	46,73,113	2.44	6 (13%)
33	BCR	A	408	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	6 (10%)
35	PL9	a	410	-	32,32,55	1.10	4 (12%)	39,40,69	1.55	8 (20%)
44	DD6	2	303	-	39,45,45	1.99	3 (7%)	52,67,67	2.20	17 (32%)
31	CLA	D	401	-	63,67,73	1.30	8 (12%)	75,105,113	1.39	9 (12%)
31	CLA	b	508	-	45,49,73	1.50	9 (20%)	54,84,113	1.53	7 (12%)
31	CLA	8	304	-	40,42,73	1.77	13 (32%)	50,74,113	1.69	8 (16%)
44	DD6	6	204	-	39,45,45	2.22	3 (7%)	52,67,67	2.34	17 (32%)
44	DD6	P	611	-	39,45,45	1.99	2 (5%)	52,67,67	1.99	15 (28%)
31	CLA	1	212	25	45,49,73	1.52	8 (17%)	54,84,113	1.50	6 (11%)
33	BCR	C	517	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
44	DD6	8	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.77	15 (28%)
31	CLA	0	305	23	65,69,73	1.31	10 (15%)	78,108,113	1.35	8 (10%)
40	BCT	d	402	30	2,3,3	1.24	0	2,3,3	4.10	2 (100%)
31	CLA	C	513	3	68,72,73	1.25	9 (13%)	81,111,113	1.29	6 (7%)
31	CLA	5	313	23	41,46,73	1.55	8 (19%)	51,80,113	1.55	7 (13%)
31	CLA	2	306	24	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
42	A86	p	610	-	44,50,50	1.44	6 (13%)	51,76,76	3.96	26 (50%)
31	CLA	7	306	24	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
35	PL9	d	406	-	55,55,55	1.35	5 (9%)	68,69,69	1.56	13 (19%)
33	BCR	D	405	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
42	A86	3	301	-	44,50,50	1.53	7 (15%)	51,76,76	5.17	24 (47%)
31	CLA	b	515	2	64,68,73	1.29	10 (15%)	76,106,113	1.33	7 (9%)
31	CLA	D	403	4	66,70,73	1.34	11 (16%)	82,109,113	1.37	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	SQD	a	409	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
36	LHG	b	522	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)
31	CLA	8	313	-	42,47,73	1.54	10 (23%)	52,81,113	1.50	5 (9%)
31	CLA	p	601	26	40,44,73	1.66	9 (22%)	49,77,113	1.72	8 (16%)
31	CLA	4	210	-	41,46,73	1.56	8 (19%)	51,80,113	1.62	9 (17%)
31	CLA	4	209	-	45,49,73	1.51	10 (22%)	54,84,113	1.59	7 (12%)
33	BCR	b	518	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
33	BCR	b	520	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
33	BCR	d	405	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	7 (12%)
31	CLA	8	306	28	35,41,73	1.87	11 (31%)	49,72,113	1.71	9 (18%)
36	LHG	a	411	-	42,42,48	0.68	1 (2%)	45,48,54	1.26	5 (11%)
31	CLA	c	514	3	53,57,73	1.40	8 (15%)	62,93,113	1.46	7 (11%)
31	CLA	b	510	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
29	OEX	A	401	1,3	0,14,14	-	-	-	-	-
31	CLA	c	507	3	49,53,73	1.47	9 (18%)	59,89,113	1.45	5 (8%)
31	CLA	9	211	-	38,42,73	1.71	11 (28%)	48,74,113	1.51	7 (14%)
31	CLA	p	602	-	45,49,73	1.51	10 (22%)	54,84,113	1.61	10 (18%)
31	CLA	3	309	-	43,48,73	1.54	9 (20%)	51,83,113	1.73	8 (15%)
33	BCR	b	519	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	6 (10%)
31	CLA	b	509	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
31	CLA	d	404	4	69,73,73	1.24	9 (13%)	83,113,113	1.33	6 (7%)
31	CLA	1	213	25	43,48,73	1.54	8 (18%)	51,83,113	1.47	5 (9%)
31	CLA	4	212	-	41,44,73	1.66	10 (24%)	52,77,113	1.59	7 (13%)
34	SQD	0	316	-	47,48,54	1.03	5 (10%)	56,59,65	1.45	8 (14%)
42	A86	2	302	-	44,50,50	1.52	6 (13%)	51,76,76	3.25	18 (35%)
36	LHG	D	412	-	27,27,48	0.87	2 (7%)	31,32,54	1.72	4 (12%)
42	A86	9	203	-	44,50,50	1.40	4 (9%)	51,76,76	3.55	21 (41%)
31	CLA	3	313	-	42,47,73	1.54	11 (26%)	52,81,113	1.50	5 (9%)
31	CLA	8	308	-	40,43,73	1.62	11 (27%)	46,73,113	2.44	7 (15%)
31	CLA	d	401	-	63,67,73	1.30	8 (12%)	75,105,113	1.39	9 (12%)
31	CLA	1	215	25	41,46,73	1.54	8 (19%)	51,80,113	1.54	6 (11%)
31	CLA	7	316	-	45,49,73	1.52	8 (17%)	54,84,113	1.51	7 (12%)
31	CLA	1	216	25	41,46,73	1.55	7 (17%)	51,80,113	1.50	5 (9%)
31	CLA	5	310	23	59,63,73	1.35	9 (15%)	71,101,113	1.35	8 (11%)
31	CLA	b	511	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	A86	2	301	-	44,50,50	1.30	3 (6%)	51,76,76	2.97	19 (37%)
42	A86	7	301	-	44,50,50	1.30	3 (6%)	51,76,76	2.97	19 (37%)
31	CLA	b	505	2	69,73,73	1.25	8 (11%)	83,113,113	1.39	7 (8%)
37	LMG	m	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.40	9 (15%)
31	CLA	B	502	2	65,69,73	1.26	9 (13%)	74,106,113	1.28	6 (8%)
31	CLA	w	202	19	49,53,73	1.46	11 (22%)	59,89,113	1.47	9 (15%)
31	CLA	B	508	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
37	LMG	y	101	-	46,46,55	0.75	1 (2%)	54,54,63	1.39	11 (20%)
31	CLA	1	208	-	51,55,73	1.44	7 (13%)	61,91,113	1.44	6 (9%)
31	CLA	c	506	3	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
31	CLA	8	314	-	40,43,73	1.67	11 (27%)	51,76,113	1.58	8 (15%)
31	CLA	9	205	-	39,43,73	1.70	12 (30%)	49,75,113	1.53	6 (12%)
31	CLA	5	305	23	65,69,73	1.31	10 (15%)	78,108,113	1.35	8 (10%)
31	CLA	b	512	2	68,72,73	1.27	10 (14%)	81,111,113	1.35	8 (9%)
44	DD6	p	611	-	39,45,45	1.99	3 (7%)	52,67,67	1.99	15 (28%)
31	CLA	4	205	-	39,43,73	1.69	12 (30%)	49,75,113	1.53	6 (12%)
31	CLA	C	506	3	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
31	CLA	9	204	-	41,46,73	1.58	9 (21%)	51,80,113	1.55	6 (11%)
31	CLA	2	311	24	47,51,73	1.49	8 (17%)	56,86,113	1.40	6 (10%)
44	DD6	6	203	-	39,45,45	2.00	3 (7%)	52,67,67	2.20	17 (32%)
31	CLA	a	403	1	69,73,73	1.26	8 (11%)	83,113,113	1.36	8 (9%)
31	CLA	B	509	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	5 (6%)
31	CLA	2	305	-	45,49,73	1.51	9 (20%)	54,84,113	1.53	7 (12%)
31	CLA	a	407	-	64,68,73	1.28	8 (12%)	77,107,113	1.36	10 (12%)
37	LMG	j	101	-	50,50,55	0.80	1 (2%)	58,58,63	1.34	6 (10%)
31	CLA	5	314	23	41,46,73	1.56	8 (19%)	51,80,113	1.53	5 (9%)
31	CLA	p	604	-	43,48,73	1.52	10 (23%)	51,83,113	1.60	8 (15%)
31	CLA	5	309	23	45,49,73	1.51	9 (20%)	54,84,113	1.53	7 (12%)
31	CLA	0	313	23	41,46,73	1.55	9 (21%)	51,80,113	1.55	7 (13%)
31	CLA	6	210	25	69,73,73	1.23	8 (11%)	83,113,113	1.35	8 (9%)
31	CLA	b	504	2	68,72,73	1.25	9 (13%)	81,111,113	1.30	5 (6%)
37	LMG	M	101	-	51,51,55	0.75	1 (1%)	59,59,63	1.40	9 (15%)
31	CLA	c	505	-	68,72,73	1.25	9 (13%)	81,111,113	1.32	5 (6%)
31	CLA	4	204	-	41,46,73	1.57	9 (21%)	51,80,113	1.55	6 (11%)
37	LMG	D	408	-	46,46,55	0.77	1 (2%)	54,54,63	1.33	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	b	514	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	9 (10%)
33	BCR	B	518	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	6 (10%)
37	LMG	C	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
31	CLA	8	305	28	44,49,73	1.51	11 (25%)	52,84,113	1.58	6 (11%)
31	CLA	2	310	24	59,63,73	1.35	9 (15%)	71,101,113	1.38	8 (11%)
39	DGD	h	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.42	10 (12%)
42	A86	P	610	-	44,50,50	1.44	6 (13%)	51,76,76	3.97	26 (50%)
31	CLA	B	511	2	68,72,73	1.27	10 (14%)	81,111,113	1.35	8 (9%)
37	LMG	D	410	-	40,40,55	0.94	3 (7%)	48,48,63	1.35	6 (12%)

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
33	BCR	c	517	-	-	3/29/63/63	0/2/2/2
31	CLA	2	314	24	-	0/4/80/115	-
31	CLA	P	603	26	-	0/2/78/115	-
31	CLA	5	308	-	-	14/35/111/115	-
43	ET4	5	302	-	-	9/25/67/67	0/2/2/2
37	LMG	B	520	-	-	5/23/43/70	0/1/1/1
42	A86	0	303	-	-	5/34/90/90	0/3/3/3
31	CLA	6	208	-	-	7/18/94/115	-
31	CLA	b	507	-	-	6/39/115/115	-
39	DGD	C	519	-	-	21/51/91/95	0/2/2/2
39	DGD	c	520	-	-	9/51/91/95	0/2/2/2
33	BCR	c	516	-	-	6/29/63/63	0/2/2/2
33	BCR	H	101	-	-	6/29/63/63	0/2/2/2
31	CLA	9	208	-	-	2/8/84/115	-
31	CLA	b	513	2	-	2/10/86/115	-
34	SQD	B	522	-	-	17/49/69/69	0/1/1/1
31	CLA	2	312	24	-	0/2/78/115	-
31	CLA	B	507	-	-	2/10/86/115	-
31	CLA	A	403	1	-	12/39/115/115	-
31	CLA	P	609	-	-	2/6/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DD6	1	203	-	-	2/26/80/80	0/3/3/3
36	LHG	H	103	-	-	10/46/46/53	-
39	DGD	c	519	-	-	21/51/91/95	0/2/2/2
33	BCR	h	101	-	-	6/29/63/63	0/2/2/2
31	CLA	7	309	24	-	10/32/108/115	-
37	LMG	b	521	-	-	5/23/43/70	0/1/1/1
31	CLA	D	404	4	-	9/39/115/115	-
37	LMG	0	315	-	-	25/43/63/70	0/1/1/1
31	CLA	b	503	2	-	14/29/107/115	-
44	DD6	7	303	-	-	2/26/80/80	0/3/3/3
31	CLA	C	504	-	-	5/23/99/115	-
31	CLA	0	311	-	-	9/15/91/115	-
31	CLA	p	605	-	-	2/2/78/115	-
34	SQD	A	409	-	-	16/49/69/69	0/1/1/1
31	CLA	C	509	3	-	14/39/115/115	-
31	CLA	C	514	3	-	4/20/96/115	-
31	CLA	b	516	2	-	8/39/115/115	-
42	A86	0	301	-	-	10/34/90/90	0/3/3/3
31	CLA	8	309	-	-	3/8/84/115	-
31	CLA	c	510	3	-	6/39/115/115	-
31	CLA	7	308	24	-	7/13/89/115	-
44	DD6	7	304	-	-	10/26/80/80	0/3/3/3
31	CLA	0	304	-	-	4/10/86/115	-
31	CLA	1	209	25	-	6/13/89/115	-
31	CLA	2	315	24	-	2/4/80/115	-
42	A86	1	202	-	-	7/34/90/90	0/3/3/3
31	CLA	c	509	3	-	14/39/115/115	-
31	CLA	9	209	-	-	6/10/86/115	-
31	CLA	1	207	25	-	6/13/89/115	-
42	A86	9	202	-	-	7/34/90/90	0/3/3/3
31	CLA	5	307	-	-	21/35/111/115	-
31	CLA	B	513	2	-	7/39/115/115	-
33	BCR	C	515	-	-	3/29/63/63	0/2/2/2
42	A86	7	302	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	W	202	19	-	4/15/91/115	-
31	CLA	p	608	26	-	3/6/78/115	-
32	PHO	a	406	-	-	11/37/103/103	0/5/6/6
31	CLA	B	504	2	-	15/39/115/115	-
31	CLA	C	508	-	-	16/39/115/115	-
31	CLA	B	514	2	-	13/33/109/115	-
31	CLA	C	505	-	-	10/37/113/115	-
42	A86	4	202	-	-	7/34/90/90	0/3/3/3
44	DD6	3	303	-	-	3/26/80/80	0/3/3/3
31	CLA	2	308	24	-	7/13/89/115	-
31	CLA	P	604	-	-	2/8/84/115	-
31	CLA	1	206	25	-	8/15/91/115	-
31	CLA	p	603	26	-	0/2/78/115	-
31	CLA	7	313	24	-	2/4/80/115	-
31	CLA	C	503	3	-	16/37/113/115	-
34	SQD	A	411	-	-	17/49/69/69	0/1/1/1
33	BCR	B	519	-	-	11/29/63/63	0/2/2/2
31	CLA	3	305	28	-	3/10/86/115	-
35	PL9	A	410	-	-	13/25/45/73	0/1/1/1
31	CLA	c	508	-	-	16/39/115/115	-
31	CLA	0	312	-	-	9/12/88/115	-
31	CLA	6	215	25	-	0/4/80/115	-
41	HEM	F	101	6,5	-	4/14/54/54	-
42	A86	5	317	-	-	8/34/90/90	0/3/3/3
31	CLA	d	403	4	-	7/33/109/115	-
31	CLA	1	210	25	-	16/39/115/115	-
31	CLA	6	212	25	-	4/10/86/115	-
42	A86	3	302	-	-	5/34/90/90	0/3/3/3
31	CLA	7	305	-	-	6/10/86/115	-
42	A86	8	302	-	-	5/34/90/90	0/3/3/3
31	CLA	P	605	-	-	2/2/78/115	-
31	CLA	C	512	3	-	10/39/115/115	-
37	LMG	5	315	-	-	25/43/63/70	0/1/1/1
31	CLA	2	307	-	-	5/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	517	2	-	13/39/115/115	-
31	CLA	a	404	-	-	2/20/96/115	-
36	LHG	D	411	-	-	26/38/38/53	-
31	CLA	B	506	-	-	6/39/115/115	-
31	CLA	B	503	2	-	12/37/113/115	-
31	CLA	9	207	-	-	2/4/80/115	-
31	CLA	2	316	-	-	2/10/86/115	-
32	PHO	a	405	-	-	10/37/103/103	0/5/6/6
31	CLA	5	304	-	-	4/10/86/115	-
31	CLA	B	510	-	-	9/39/115/115	-
42	A86	8	301	-	-	11/34/90/90	0/3/3/3
31	CLA	8	307	-	-	2/11/83/115	-
36	LHG	h	103	-	-	10/46/46/53	-
39	DGD	C	520	-	-	9/51/91/95	0/2/2/2
31	CLA	P	601	26	-	2/2/78/115	-
31	CLA	7	311	24	-	7/13/89/115	-
31	CLA	4	206	-	-	2/4/76/115	-
31	CLA	C	511	3	-	13/39/115/115	-
36	LHG	A	412	-	-	13/47/47/53	-
36	LHG	A	413	-	-	13/29/29/53	-
31	CLA	C	502	3	-	14/39/115/115	-
31	CLA	p	609	-	-	2/6/82/115	-
31	CLA	6	209	25	-	6/13/89/115	-
31	CLA	3	311	28	-	2/8/84/115	-
33	BCR	c	515	-	-	3/29/63/63	0/2/2/2
41	HEM	v	201	18	-	6/14/54/54	-
31	CLA	z	101	-	-	8/23/99/115	-
31	CLA	1	214	25	-	0/4/80/115	-
31	CLA	A	407	-	-	4/33/109/115	-
31	CLA	c	502	3	-	14/39/115/115	-
31	CLA	8	311	28	-	2/8/84/115	-
31	CLA	6	201	24	-	4/13/89/115	-
31	CLA	5	306	-	-	4/15/91/115	-
31	CLA	B	501	-	-	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	B	517	-	-	5/29/63/63	0/2/2/2
33	BCR	C	516	-	-	6/29/63/63	0/2/2/2
36	LHG	a	412	-	-	13/29/29/53	-
32	PHO	A	405	-	-	10/37/103/103	0/5/6/6
31	CLA	6	213	25	-	6/8/84/115	-
37	LMG	w	201	-	-	26/43/63/70	0/1/1/1
31	CLA	P	608	26	-	3/6/78/115	-
39	DGD	C	518	-	-	19/44/84/95	0/2/2/2
33	BCR	K	101	-	-	16/29/63/63	0/2/2/2
31	CLA	7	315	24	-	2/4/80/115	-
37	LMG	d	408	-	-	16/41/61/70	0/1/1/1
31	CLA	6	206	25	-	8/15/91/115	-
31	CLA	6	207	25	-	6/13/89/115	-
36	LHG	d	411	-	-	26/38/38/53	-
31	CLA	2	309	24	-	10/32/108/115	-
31	CLA	7	312	24	-	0/2/78/115	-
39	DGD	c	518	-	-	19/44/84/95	0/2/2/2
42	A86	4	203	-	-	5/34/90/90	0/3/3/3
37	LMG	d	410	-	-	16/35/55/70	0/1/1/1
35	PL9	D	406	-	-	8/53/73/73	0/1/1/1
42	A86	0	317	-	-	8/34/90/90	0/3/3/3
31	CLA	B	516	2	-	13/39/115/115	-
31	CLA	8	312	28	-	4/10/86/115	-
42	A86	5	303	-	-	5/34/90/90	0/3/3/3
31	CLA	2	313	24	-	2/4/80/115	-
31	CLA	1	201	24	-	4/13/89/115	-
31	CLA	6	205	-	-	4/10/86/115	-
34	SQD	B	523	-	-	14/35/55/69	0/1/1/1
41	HEM	V	201	18	-	6/14/54/54	-
31	CLA	C	507	3	-	5/15/91/115	-
31	CLA	p	607	-	-	0/2/74/115	-
31	CLA	9	210	-	-	0/4/80/115	-
37	LMG	M	102	-	-	12/35/55/70	0/1/1/1
42	A86	5	301	-	-	10/34/90/90	0/3/3/3
31	CLA	c	513	3	-	17/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	D	407	-	-	23/47/51/53	-
31	CLA	0	310	23	-	5/27/103/115	-
34	SQD	b	501	-	-	14/35/55/69	0/1/1/1
37	LMG	c	521	-	-	27/46/66/70	0/1/1/1
31	CLA	C	510	3	-	6/39/115/115	-
31	CLA	9	212	-	-	0/2/74/115	-
44	DD6	2	304	-	-	10/26/80/80	0/3/3/3
31	CLA	5	311	-	-	9/15/91/115	-
31	CLA	p	606	-	-	2/4/76/115	-
41	HEM	f	101	6,5	-	4/14/54/54	-
37	LMG	W	201	-	-	26/43/63/70	0/1/1/1
31	CLA	6	214	25	-	0/4/80/115	-
31	CLA	8	310	28	-	0/2/74/115	-
32	PHO	A	406	-	-	11/37/103/103	0/5/6/6
33	BCR	k	101	-	-	16/29/63/63	0/2/2/2
31	CLA	P	607	-	-	0/2/74/115	-
31	CLA	b	506	2	-	12/39/115/115	-
36	LHG	B	521	-	-	18/53/53/53	-
31	CLA	A	404	-	-	2/20/96/115	-
37	LMG	D	409	-	-	13/32/52/70	0/1/1/1
31	CLA	0	314	23	-	0/4/80/115	-
31	CLA	1	205	-	-	4/10/86/115	-
31	CLA	0	309	23	-	4/10/86/115	-
37	LMG	Y	101	-	-	18/41/61/70	0/1/1/1
31	CLA	c	503	3	-	16/37/113/115	-
31	CLA	B	515	2	-	8/39/115/115	-
31	CLA	6	216	25	-	2/4/80/115	-
37	LMG	d	409	-	-	13/32/52/70	0/1/1/1
31	CLA	7	307	-	-	5/18/94/115	-
31	CLA	0	306	-	-	4/15/91/115	-
31	CLA	0	307	-	-	21/35/111/115	-
44	DD6	1	204	-	-	5/26/80/80	0/3/3/3
31	CLA	c	504	-	-	5/23/99/115	-
31	CLA	3	307	-	-	2/11/83/115	-
37	LMG	m	102	-	-	12/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A86	6	202	-	-	7/34/90/90	0/3/3/3
43	ET4	0	302	-	-	9/25/67/67	0/2/2/2
34	SQD	5	316	-	-	18/43/63/69	0/1/1/1
31	CLA	9	206	-	-	2/4/76/115	-
36	LHG	d	412	-	-	17/29/29/53	-
31	CLA	3	310	28	-	0/2/74/115	-
31	CLA	5	312	-	-	9/12/88/115	-
31	CLA	4	207	-	-	2/4/80/115	-
31	CLA	Z	101	-	-	8/23/99/115	-
37	LMG	J	101	-	-	29/45/65/70	0/1/1/1
36	LHG	d	407	-	-	23/47/51/53	-
31	CLA	c	511	3	-	13/39/115/115	-
31	CLA	P	602	-	-	2/10/86/115	-
31	CLA	1	211	25	-	5/27/103/115	-
31	CLA	P	606	-	-	2/4/76/115	-
42	A86	9	201	-	-	7/34/90/90	1/3/3/3
31	CLA	B	505	2	-	12/39/115/115	-
42	A86	4	201	-	-	7/34/90/90	1/3/3/3
31	CLA	7	310	24	-	10/27/103/115	-
39	DGD	H	102	-	-	16/51/91/95	0/2/2/2
31	CLA	3	312	28	-	4/10/86/115	-
31	CLA	7	314	24	-	0/4/80/115	-
31	CLA	c	512	3	-	10/39/115/115	-
31	CLA	B	512	2	-	2/10/86/115	-
33	BCR	a	408	-	-	4/29/63/63	0/2/2/2
31	CLA	0	308	-	-	14/35/111/115	-
31	CLA	6	211	25	-	5/27/103/115	-
31	CLA	b	502	-	-	5/13/89/115	-
31	CLA	4	208	-	-	2/8/84/115	-
31	CLA	3	308	-	-	4/6/66/115	-
33	BCR	A	408	-	-	4/29/63/63	0/2/2/2
35	PL9	a	410	-	-	13/25/45/73	0/1/1/1
44	DD6	2	303	-	-	2/26/80/80	0/3/3/3
31	CLA	D	401	-	-	4/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	508	-	-	2/10/86/115	-
44	DD6	6	204	-	-	5/26/80/80	0/3/3/3
44	DD6	P	611	-	-	5/26/80/80	0/3/3/3
31	CLA	1	212	25	-	4/10/86/115	-
33	BCR	C	517	-	-	3/29/63/63	0/2/2/2
44	DD6	8	303	-	-	2/26/80/80	0/3/3/3
31	CLA	0	305	23	-	17/35/111/115	-
31	CLA	C	513	3	-	17/37/113/115	-
31	CLA	5	313	23	-	2/4/80/115	-
31	CLA	2	306	24	-	3/15/91/115	-
42	A86	p	610	-	-	9/34/90/90	0/3/3/3
31	CLA	7	306	24	-	3/15/91/115	-
35	PL9	d	406	-	-	8/53/73/73	0/1/1/1
33	BCR	D	405	-	-	5/29/63/63	0/2/2/2
42	A86	3	301	-	-	11/34/90/90	0/3/3/3
31	CLA	b	515	2	-	13/33/109/115	-
31	CLA	D	403	4	-	7/33/109/115	-
34	SQD	a	409	-	-	16/49/69/69	0/1/1/1
36	LHG	b	522	-	-	18/53/53/53	-
31	CLA	8	313	-	-	3/6/82/115	-
31	CLA	p	601	26	-	2/2/78/115	-
31	CLA	4	210	-	-	0/4/80/115	-
31	CLA	4	209	-	-	6/10/86/115	-
33	BCR	b	518	-	-	5/29/63/63	0/2/2/2
33	BCR	b	520	-	-	11/29/63/63	0/2/2/2
33	BCR	d	405	-	-	5/29/63/63	0/2/2/2
36	LHG	a	411	-	-	13/47/47/53	-
31	CLA	c	514	3	-	4/20/96/115	-
31	CLA	b	510	-	-	12/39/115/115	-
31	CLA	c	507	3	-	5/15/91/115	-
31	CLA	p	602	-	-	2/10/86/115	-
31	CLA	3	309	-	-	3/8/84/115	-
33	BCR	b	519	-	-	5/29/63/63	0/2/2/2
31	CLA	b	509	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	d	404	4	-	9/39/115/115	-
31	CLA	1	213	25	-	6/8/84/115	-
31	CLA	4	212	-	-	0/2/74/115	-
34	SQD	0	316	-	-	18/43/63/69	0/1/1/1
42	A86	2	302	-	-	8/34/90/90	0/3/3/3
36	LHG	D	412	-	-	17/29/29/53	-
42	A86	9	203	-	-	5/34/90/90	0/3/3/3
31	CLA	3	313	-	-	3/6/82/115	-
31	CLA	8	308	-	-	4/6/66/115	-
31	CLA	d	401	-	-	4/32/108/115	-
31	CLA	1	215	25	-	0/4/80/115	-
31	CLA	7	316	-	-	2/10/86/115	-
31	CLA	1	216	25	-	2/4/80/115	-
31	CLA	5	310	23	-	5/27/103/115	-
31	CLA	b	511	-	-	9/39/115/115	-
42	A86	2	301	-	-	8/34/90/90	0/3/3/3
42	A86	7	301	-	-	8/34/90/90	0/3/3/3
31	CLA	b	505	2	-	15/39/115/115	-
37	LMG	m	101	-	-	18/46/66/70	0/1/1/1
31	CLA	B	502	2	-	14/29/107/115	-
31	CLA	w	202	19	-	4/15/91/115	-
31	CLA	B	508	2	-	8/39/115/115	-
37	LMG	y	101	-	-	18/41/61/70	0/1/1/1
31	CLA	1	208	-	-	7/18/94/115	-
31	CLA	c	506	3	-	18/39/115/115	-
31	CLA	9	205	-	-	0/2/70/115	-
31	CLA	5	305	23	-	17/35/111/115	-
31	CLA	b	512	2	-	11/37/113/115	-
44	DD6	p	611	-	-	5/26/80/80	0/3/3/3
31	CLA	4	205	-	-	0/2/70/115	-
31	CLA	C	506	3	-	18/39/115/115	-
31	CLA	9	204	-	-	2/4/80/115	-
31	CLA	2	311	24	-	7/13/89/115	-
44	DD6	6	203	-	-	2/26/80/80	0/3/3/3
31	CLA	a	403	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	509	-	-	12/39/115/115	-
31	CLA	2	305	-	-	6/10/86/115	-
31	CLA	a	407	-	-	4/33/109/115	-
37	LMG	j	101	-	-	29/45/65/70	0/1/1/1
31	CLA	5	314	23	-	0/4/80/115	-
31	CLA	p	604	-	-	2/8/84/115	-
31	CLA	5	309	23	-	4/10/86/115	-
31	CLA	0	313	23	-	2/4/80/115	-
31	CLA	6	210	25	-	16/39/115/115	-
31	CLA	b	504	2	-	12/37/113/115	-
37	LMG	M	101	-	-	18/46/66/70	0/1/1/1
31	CLA	c	505	-	-	10/37/113/115	-
31	CLA	4	204	-	-	2/4/80/115	-
37	LMG	D	408	-	-	16/41/61/70	0/1/1/1
31	CLA	b	514	2	-	7/39/115/115	-
33	BCR	B	518	-	-	5/29/63/63	0/2/2/2
37	LMG	C	521	-	-	27/46/66/70	0/1/1/1
31	CLA	8	305	28	-	3/10/86/115	-
31	CLA	2	310	24	-	10/27/103/115	-
39	DGD	h	102	-	-	16/51/91/95	0/2/2/2
42	A86	P	610	-	-	9/34/90/90	0/3/3/3
31	CLA	B	511	2	-	11/37/113/115	-
37	LMG	D	410	-	-	16/35/55/70	0/1/1/1

The worst 5 of 2255 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	204	DD6	C29-C27	-9.33	1.24	1.42
44	6	204	DD6	C29-C27	-9.29	1.24	1.42
32	A	406	PHO	C1B-C2B	9.10	1.49	1.39
32	a	406	PHO	C1B-C2B	9.10	1.49	1.39
32	A	405	PHO	C1B-C2B	9.08	1.49	1.39

The worst 5 of 2727 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	8	301	A86	O1-C20-C19	-20.74	97.80	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	3	301	A86	O1-C20-C19	-20.71	97.83	113.38
42	3	301	A86	C40-C32-C31	-17.41	94.89	110.47
42	8	301	A86	C40-C32-C31	-17.36	94.94	110.47
42	p	610	A86	O1-C15-C14	-15.87	81.36	113.21

There are no chirality outliers.

5 of 2609 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	B	501	CLA	CAD-CBD-CGD-O1D
31	B	501	CLA	CAD-CBD-CGD-O2D
31	B	516	CLA	C2B-C3B-CAB-CBB
31	B	516	CLA	C4B-C3B-CAB-CBB
31	C	502	CLA	CHA-CBD-CGD-O1D

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	4	201	A86	C31-C32-C33-C34-C35-C36
42	9	201	A86	C31-C32-C33-C34-C35-C36

217 monomers are involved in 516 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	517	BCR	4	0
31	P	603	CLA	2	0
31	5	308	CLA	6	0
37	B	520	LMG	1	0
42	0	303	A86	1	0
31	b	507	CLA	3	0
39	C	519	DGD	5	0
39	c	520	DGD	6	0
33	c	516	BCR	2	0
33	H	101	BCR	2	0
31	b	513	CLA	1	0
34	B	522	SQD	2	0
31	2	312	CLA	1	0
31	A	403	CLA	4	0
44	1	203	DD6	1	0
36	H	103	LHG	6	0
39	c	519	DGD	5	0
33	h	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	309	CLA	6	0
37	b	521	LMG	1	0
31	D	404	CLA	3	0
37	0	315	LMG	1	0
31	b	503	CLA	1	0
44	7	303	DD6	18	0
31	0	311	CLA	2	0
34	A	409	SQD	3	0
31	C	509	CLA	5	0
31	b	516	CLA	2	0
31	3	314	CLA	1	0
31	c	510	CLA	2	0
44	7	304	DD6	7	0
31	0	304	CLA	3	0
31	1	209	CLA	1	0
42	1	202	A86	1	0
31	c	509	CLA	5	0
31	5	307	CLA	3	0
31	B	513	CLA	2	0
33	C	515	BCR	1	0
31	W	202	CLA	1	0
32	a	406	PHO	1	0
31	B	504	CLA	7	0
31	B	514	CLA	7	0
31	C	505	CLA	2	0
44	3	303	DD6	1	0
31	P	604	CLA	5	0
31	1	206	CLA	4	0
31	p	603	CLA	2	0
34	A	411	SQD	3	0
33	B	519	BCR	4	0
31	3	305	CLA	1	0
35	A	410	PL9	3	0
31	c	508	CLA	1	0
41	F	101	HEM	3	0
31	1	210	CLA	5	0
31	7	305	CLA	1	0
31	C	512	CLA	3	0
37	5	315	LMG	1	0
31	2	307	CLA	3	0
31	b	517	CLA	4	0
36	D	411	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	506	CLA	4	0
31	B	503	CLA	2	0
32	a	405	PHO	2	0
31	5	304	CLA	3	0
31	B	510	CLA	3	0
36	h	103	LHG	5	0
39	C	520	DGD	7	0
31	C	511	CLA	2	0
36	A	412	LHG	2	0
36	A	413	LHG	2	0
31	C	502	CLA	3	0
31	6	209	CLA	1	0
31	3	311	CLA	1	0
33	c	515	BCR	2	0
41	v	201	HEM	6	0
31	z	101	CLA	6	0
31	1	214	CLA	1	0
31	c	502	CLA	3	0
31	8	311	CLA	1	0
31	6	201	CLA	2	0
31	B	501	CLA	1	0
33	B	517	BCR	7	0
33	C	516	BCR	1	0
36	a	412	LHG	2	0
32	A	405	PHO	3	0
37	w	201	LMG	2	0
39	C	518	DGD	1	0
33	K	101	BCR	2	0
31	6	206	CLA	4	0
36	d	411	LHG	2	0
31	2	309	CLA	6	0
31	7	312	CLA	1	0
39	c	518	DGD	2	0
37	d	410	LMG	2	0
35	D	406	PL9	3	0
31	B	516	CLA	5	0
31	8	312	CLA	1	0
42	5	303	A86	1	0
31	1	201	CLA	2	0
34	B	523	SQD	1	0
41	V	201	HEM	6	0
31	C	507	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	p	607	CLA	1	0
37	M	102	LMG	1	0
36	D	407	LHG	5	0
31	0	310	CLA	1	0
34	b	501	SQD	1	0
37	c	521	LMG	4	0
31	C	510	CLA	2	0
44	2	304	DD6	6	0
31	5	311	CLA	2	0
41	f	101	HEM	3	0
37	W	201	LMG	2	0
31	6	214	CLA	1	0
31	8	310	CLA	1	0
32	A	406	PHO	1	0
33	k	101	BCR	2	0
31	P	607	CLA	1	0
31	b	506	CLA	3	0
36	B	521	LHG	4	0
37	D	409	LMG	2	0
31	0	314	CLA	3	0
37	Y	101	LMG	3	0
31	B	515	CLA	2	0
37	d	409	LMG	3	0
31	7	307	CLA	3	0
31	0	307	CLA	3	0
44	1	204	DD6	2	0
31	3	307	CLA	1	0
37	m	102	LMG	1	0
42	6	202	A86	1	0
34	5	316	SQD	5	0
36	d	412	LHG	2	0
31	3	310	CLA	1	0
31	Z	101	CLA	6	0
37	J	101	LMG	3	0
36	d	407	LHG	5	0
31	c	511	CLA	2	0
31	P	602	CLA	2	0
31	1	211	CLA	1	0
31	B	505	CLA	4	0
31	7	310	CLA	7	0
39	H	102	DGD	4	0
31	3	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	512	CLA	3	0
31	B	512	CLA	2	0
33	a	408	BCR	3	0
31	0	308	CLA	6	0
31	6	211	CLA	2	0
31	b	502	CLA	1	0
31	3	308	CLA	1	0
33	A	408	BCR	3	0
35	a	410	PL9	3	0
44	2	303	DD6	18	0
31	D	401	CLA	1	0
44	6	204	DD6	2	0
44	P	611	DD6	7	0
33	C	517	BCR	4	0
44	8	303	DD6	1	0
31	0	305	CLA	3	0
31	5	313	CLA	1	0
31	2	306	CLA	5	0
31	7	306	CLA	4	0
35	d	406	PL9	4	0
33	D	405	BCR	2	0
31	b	515	CLA	8	0
36	b	522	LHG	4	0
31	8	313	CLA	1	0
33	b	518	BCR	5	0
33	b	520	BCR	5	0
33	d	405	BCR	1	0
36	a	411	LHG	2	0
31	b	510	CLA	2	0
31	c	507	CLA	1	0
31	p	602	CLA	2	0
33	b	519	BCR	2	0
31	b	509	CLA	2	0
31	d	404	CLA	3	0
34	0	316	SQD	5	0
36	D	412	LHG	2	0
31	3	313	CLA	1	0
31	8	308	CLA	1	0
31	d	401	CLA	1	0
31	5	310	CLA	1	0
31	b	511	CLA	3	0
31	b	505	CLA	7	0

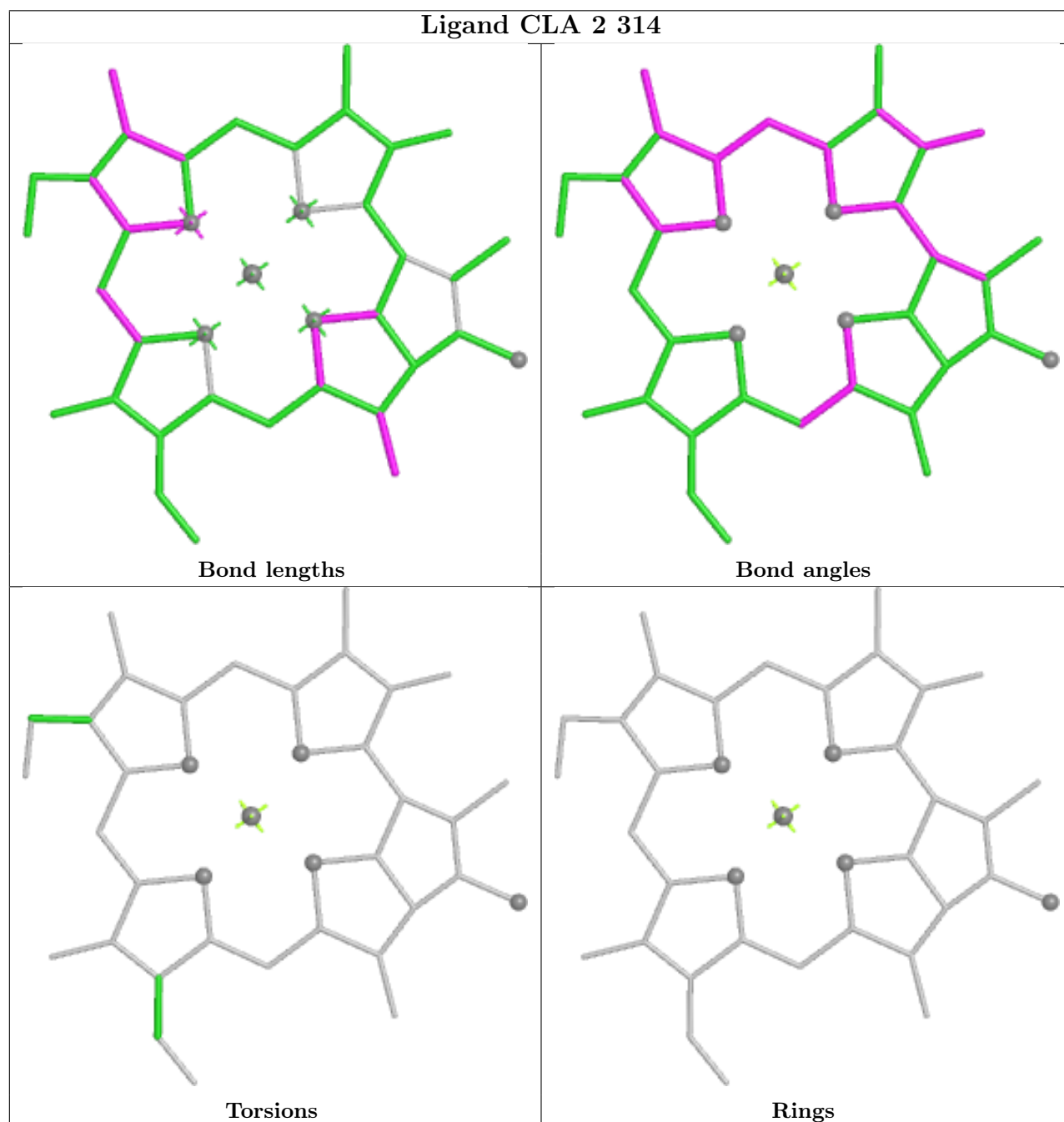
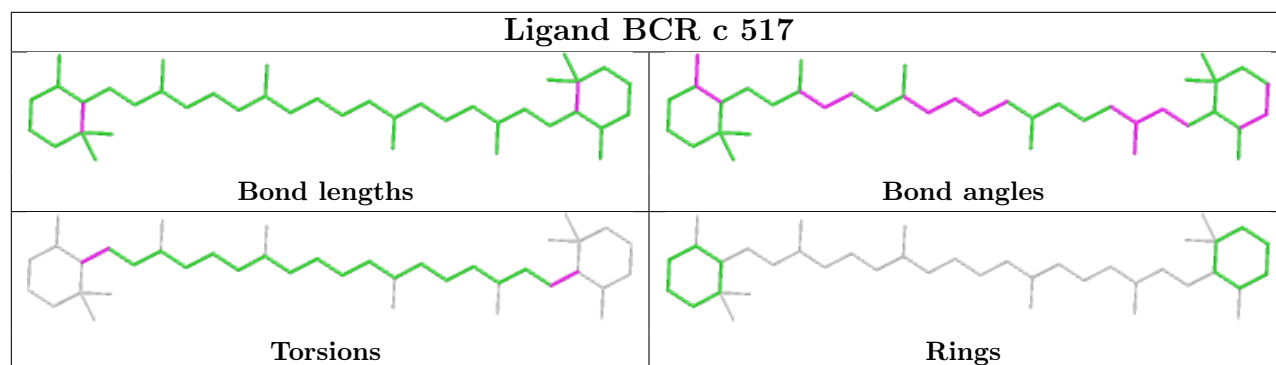
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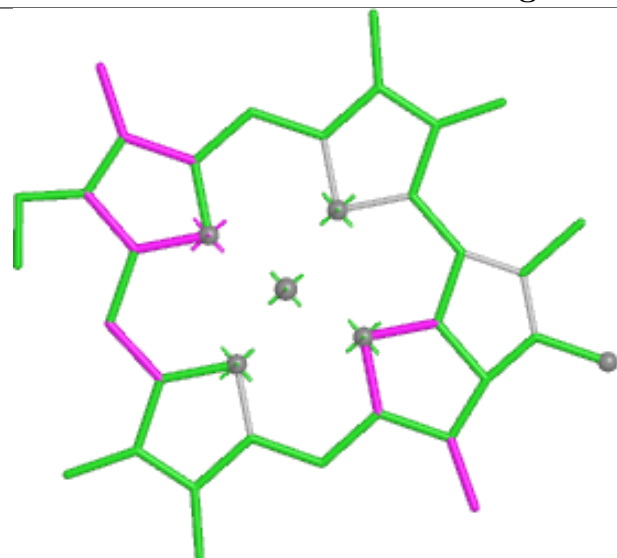
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	m	101	LMG	1	0
31	B	502	CLA	1	0
31	w	202	CLA	1	0
31	B	508	CLA	3	0
37	y	101	LMG	4	0
31	c	506	CLA	2	0
31	8	314	CLA	1	0
31	5	305	CLA	3	0
31	b	512	CLA	1	0
44	p	611	DD6	7	0
31	C	506	CLA	2	0
44	6	203	DD6	1	0
31	a	403	CLA	3	0
31	B	509	CLA	2	0
31	2	305	CLA	1	0
37	j	101	LMG	2	0
31	5	314	CLA	3	0
31	p	604	CLA	5	0
31	0	313	CLA	1	0
31	6	210	CLA	5	0
31	b	504	CLA	2	0
37	M	101	LMG	1	0
31	c	505	CLA	2	0
31	b	514	CLA	1	0
33	B	518	BCR	2	0
37	C	521	LMG	4	0
31	8	305	CLA	1	0
31	2	310	CLA	6	0
39	h	102	DGD	4	0
31	B	511	CLA	1	0
37	D	410	LMG	2	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.



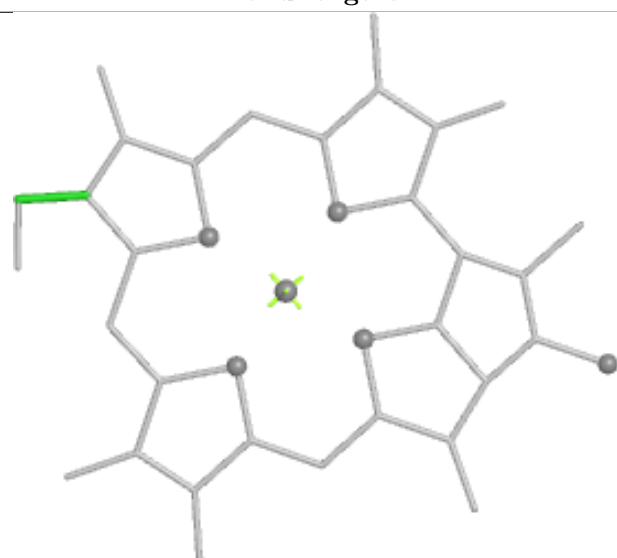
Ligand CLA P 603



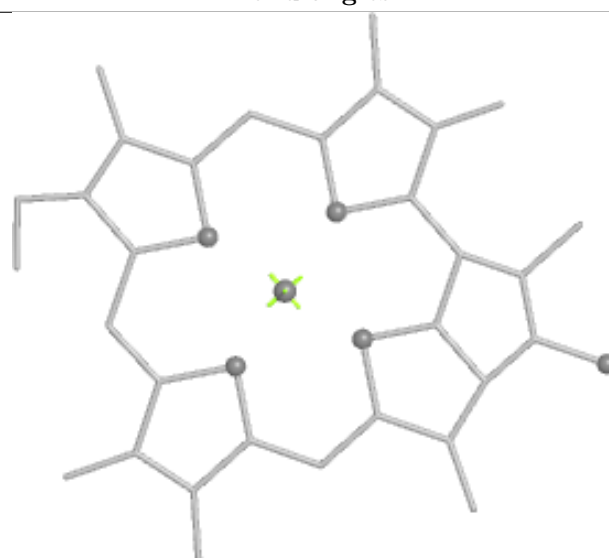
Bond lengths



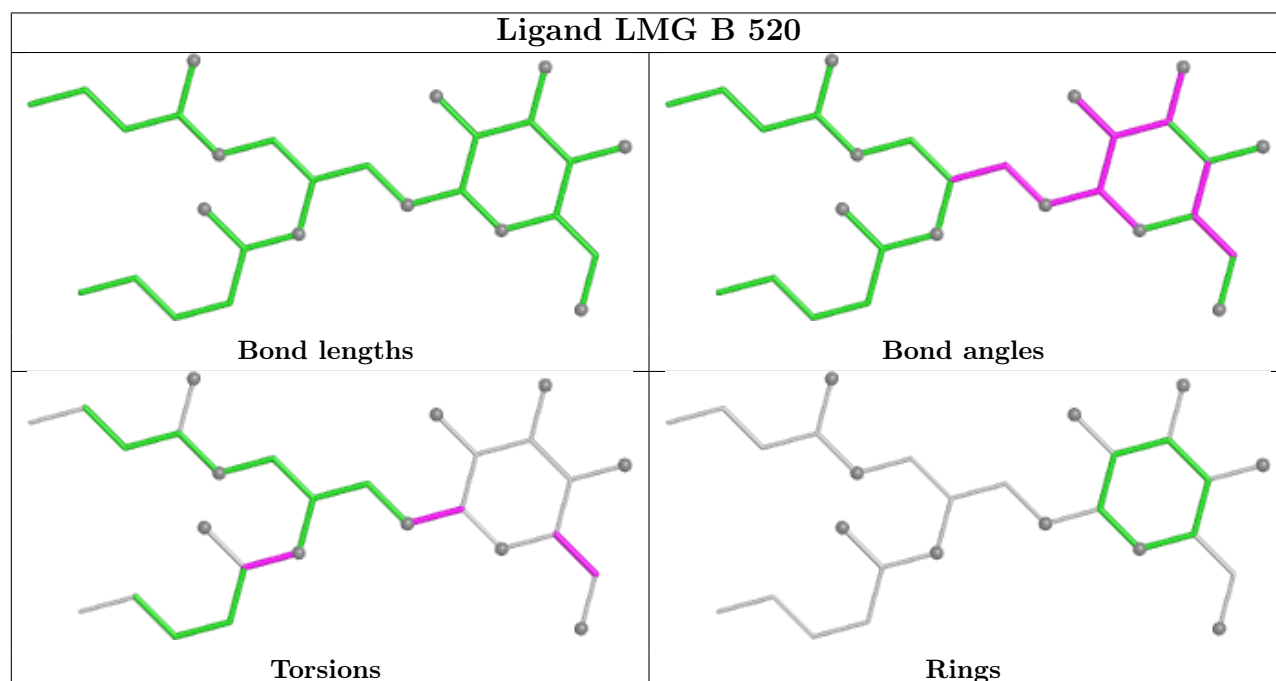
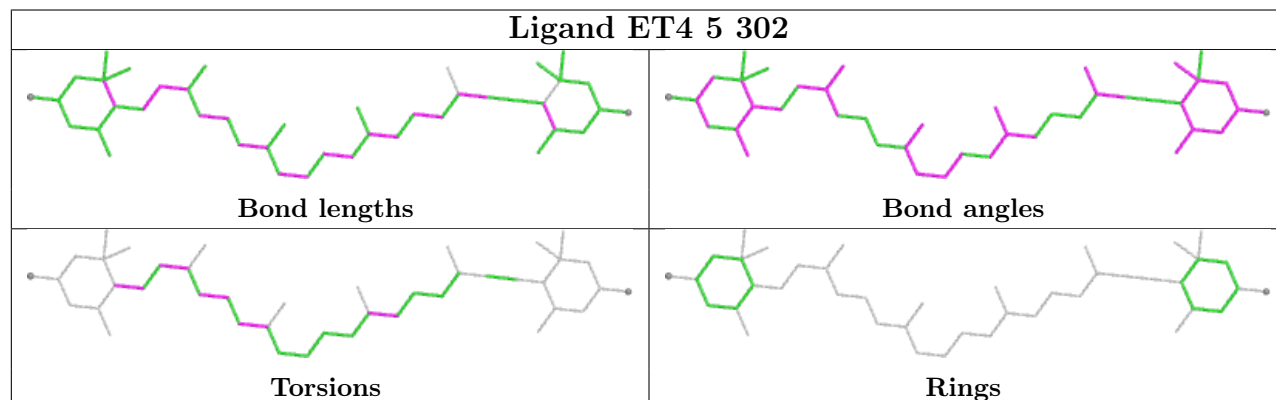
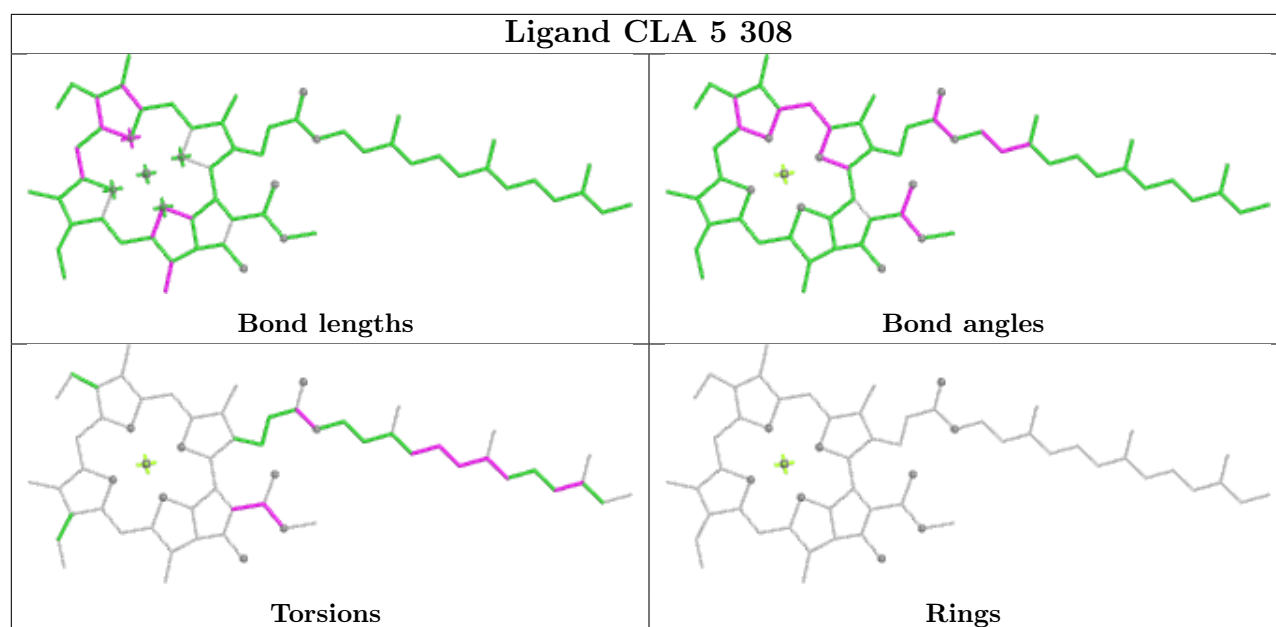
Bond angles

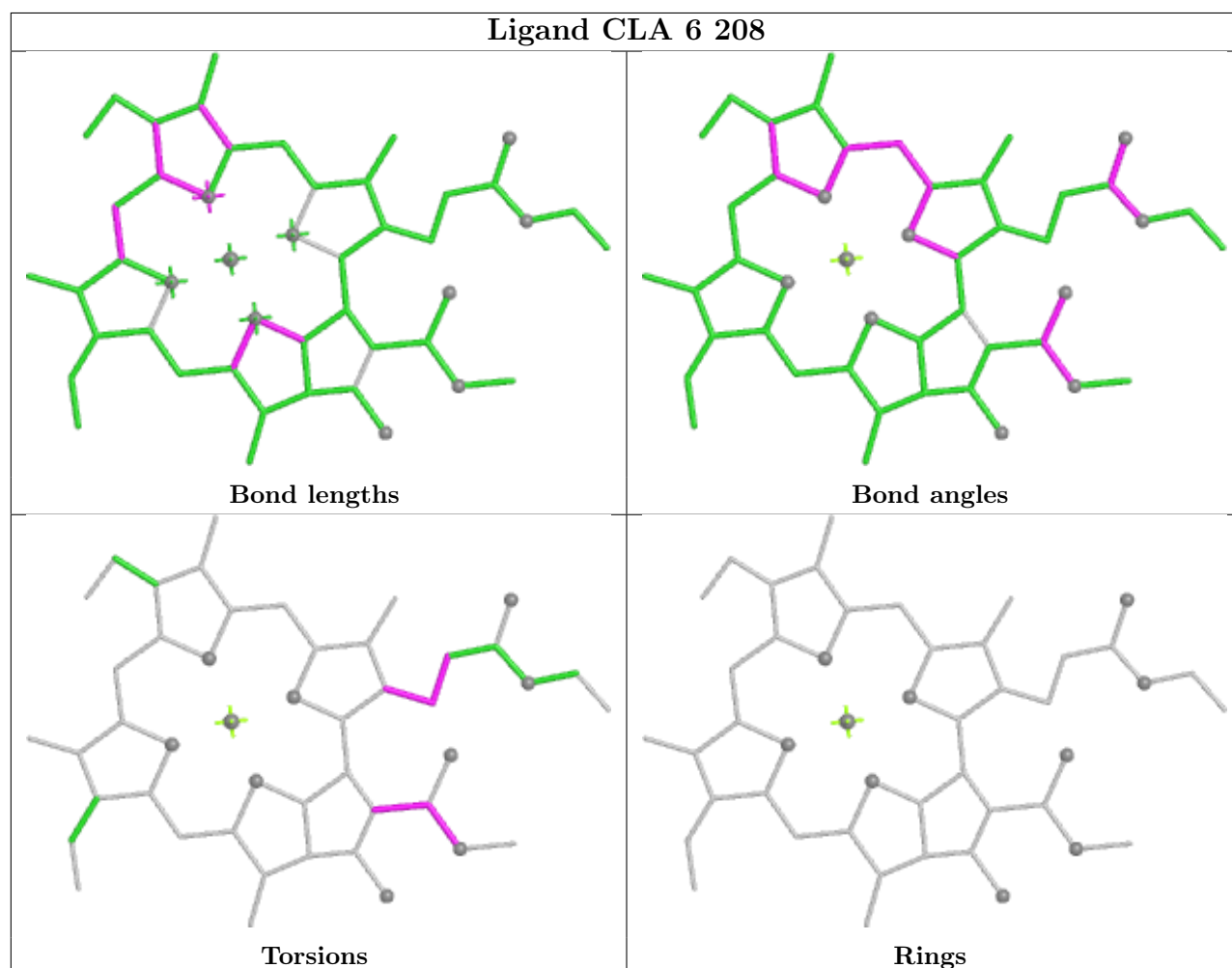
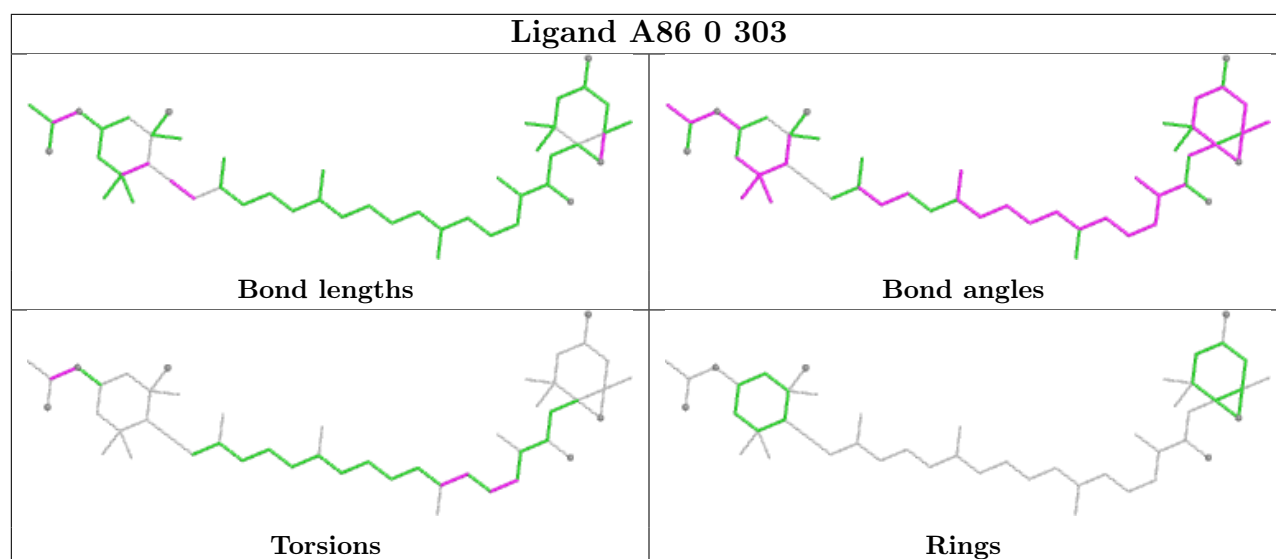


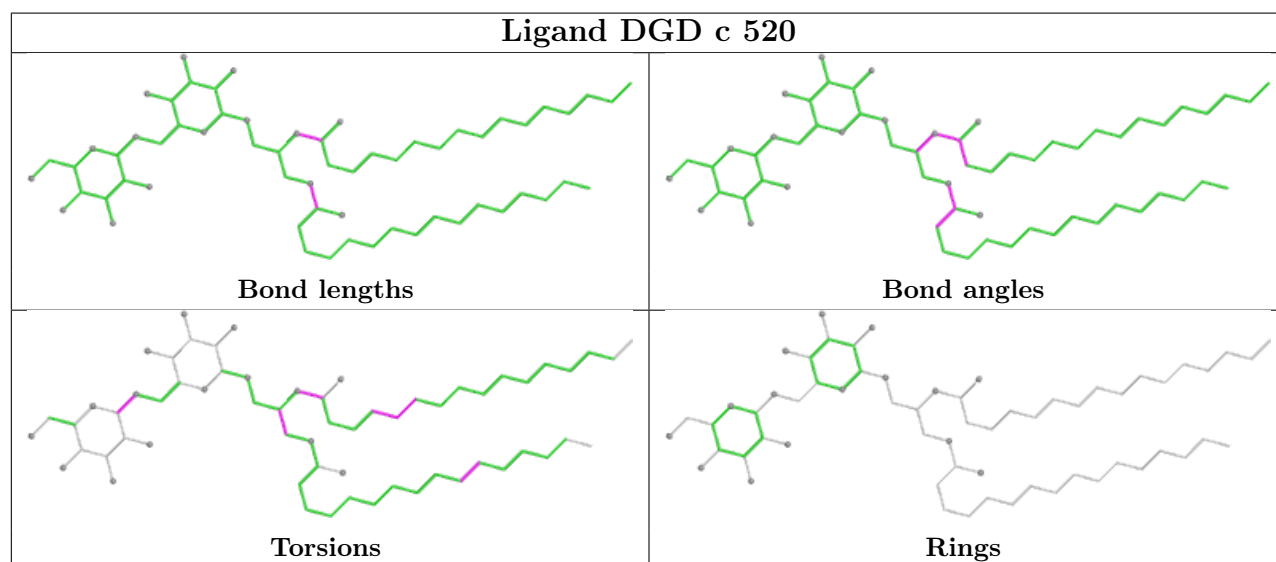
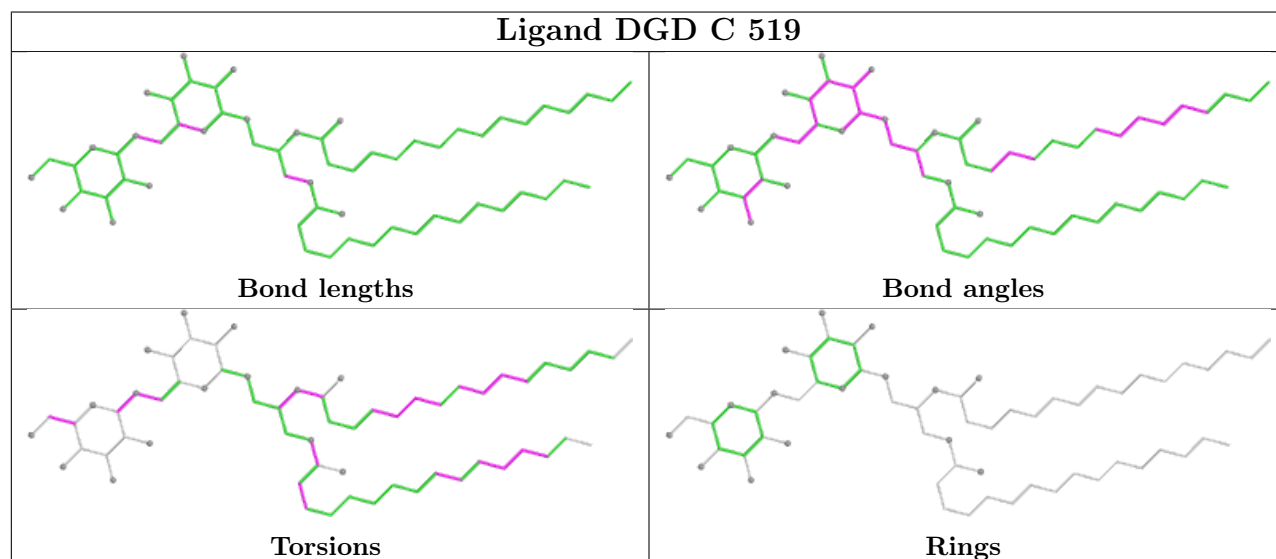
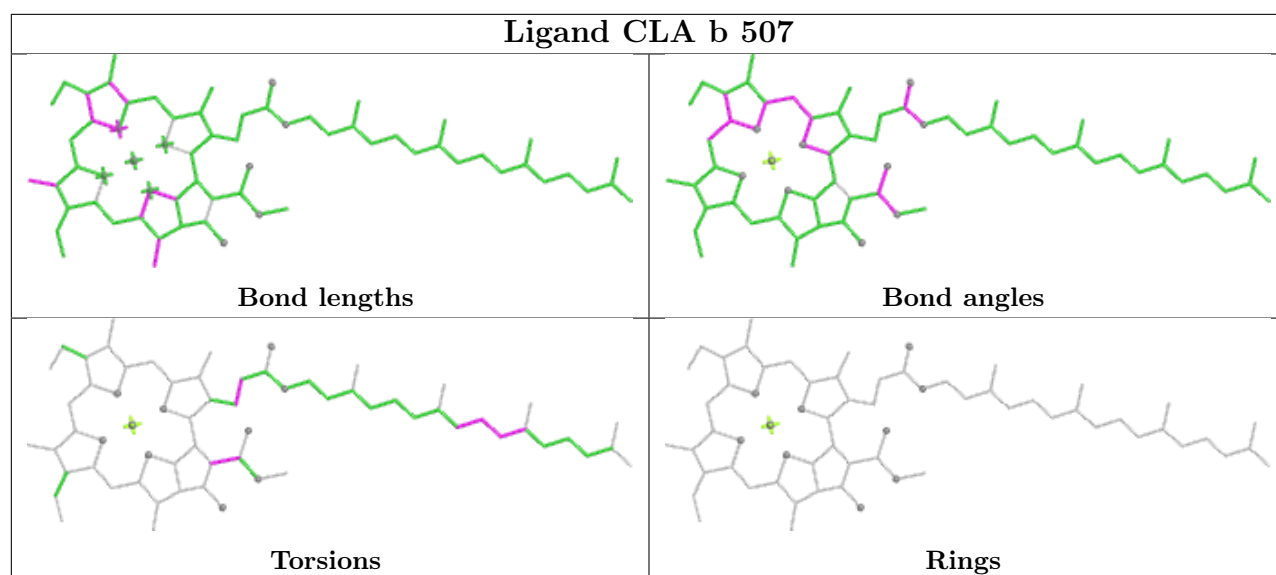
Torsions

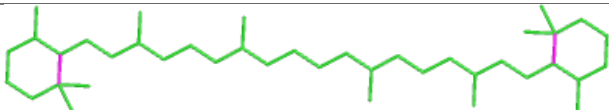
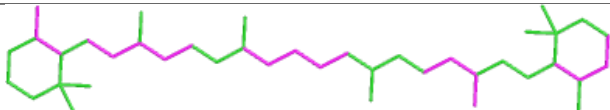
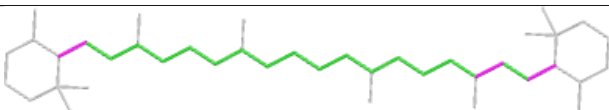
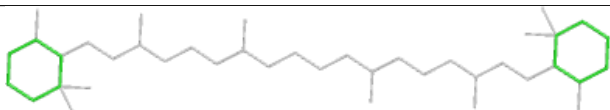


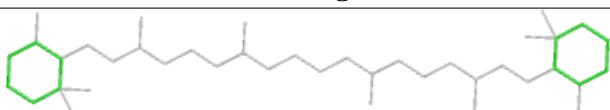
Rings



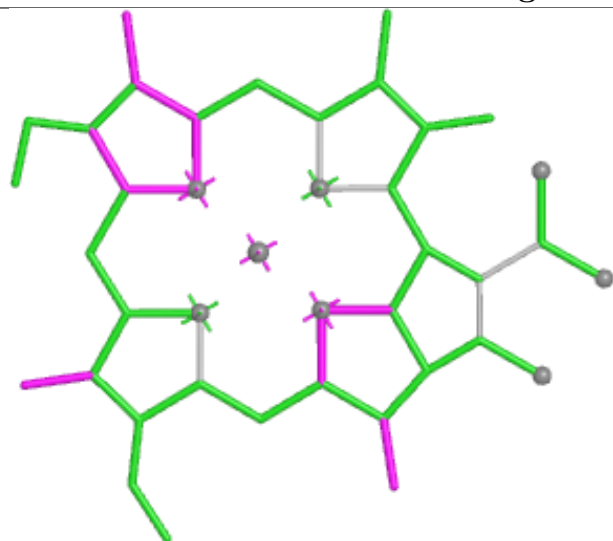




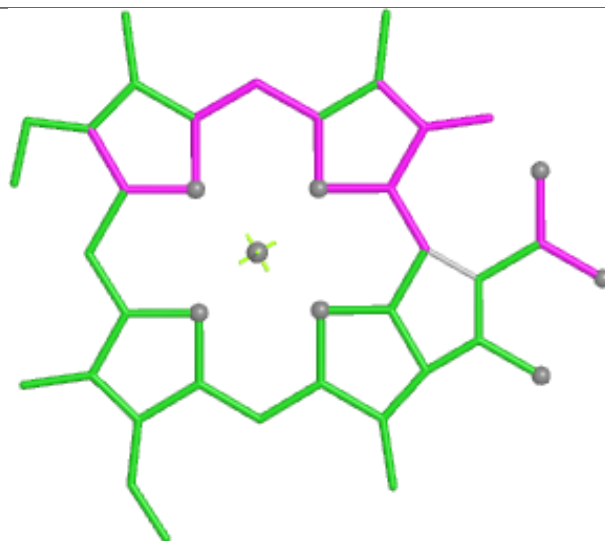
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

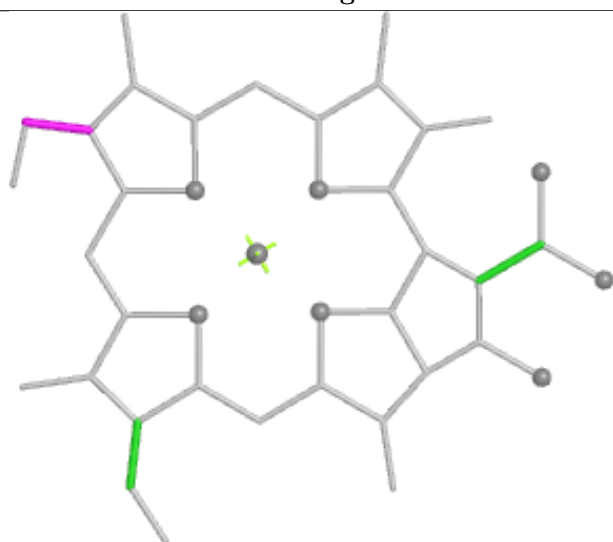
Ligand CLA 9 208



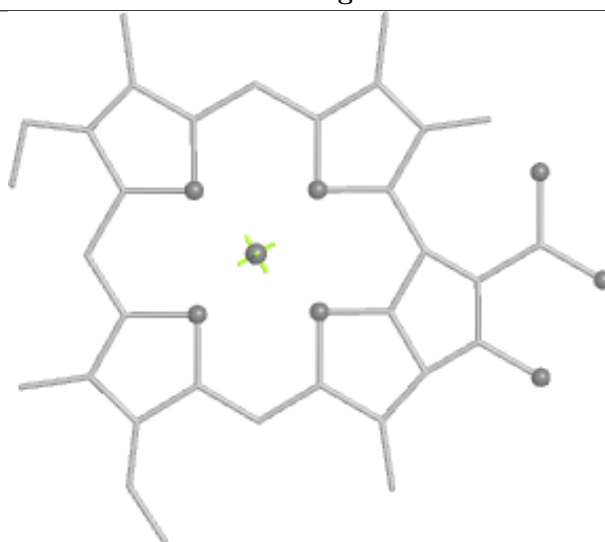
Bond lengths



Bond angles

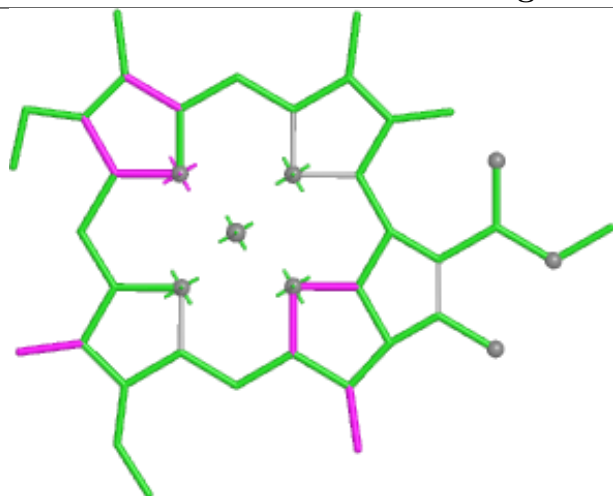


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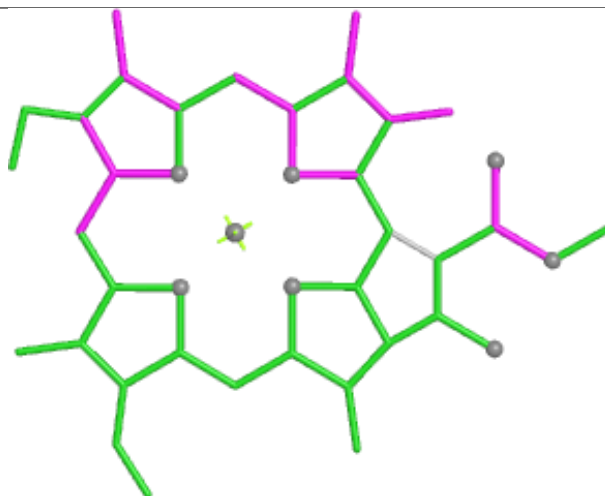


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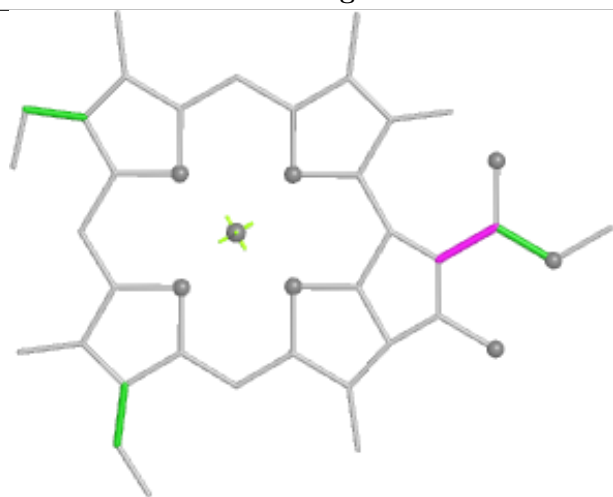
Ligand CLA b 513



Bond lengths



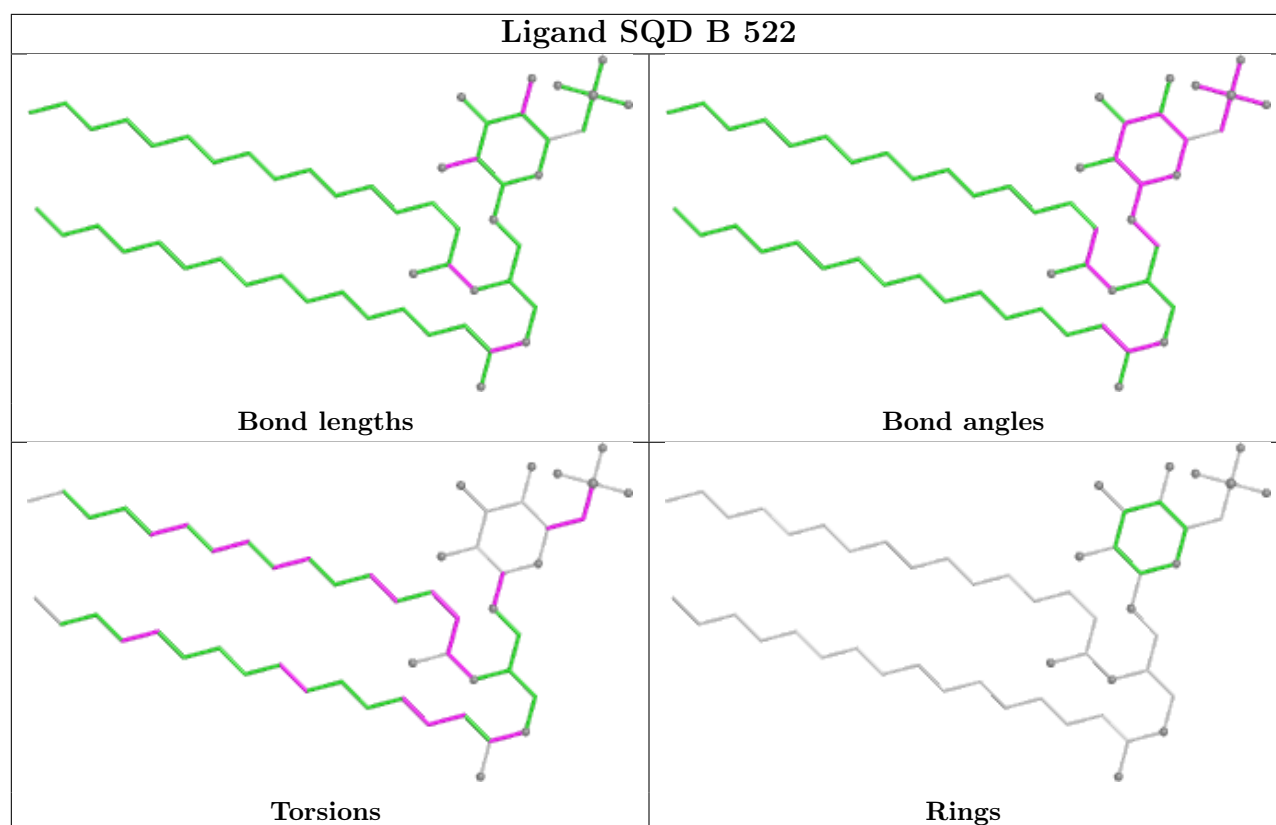
Bond angles



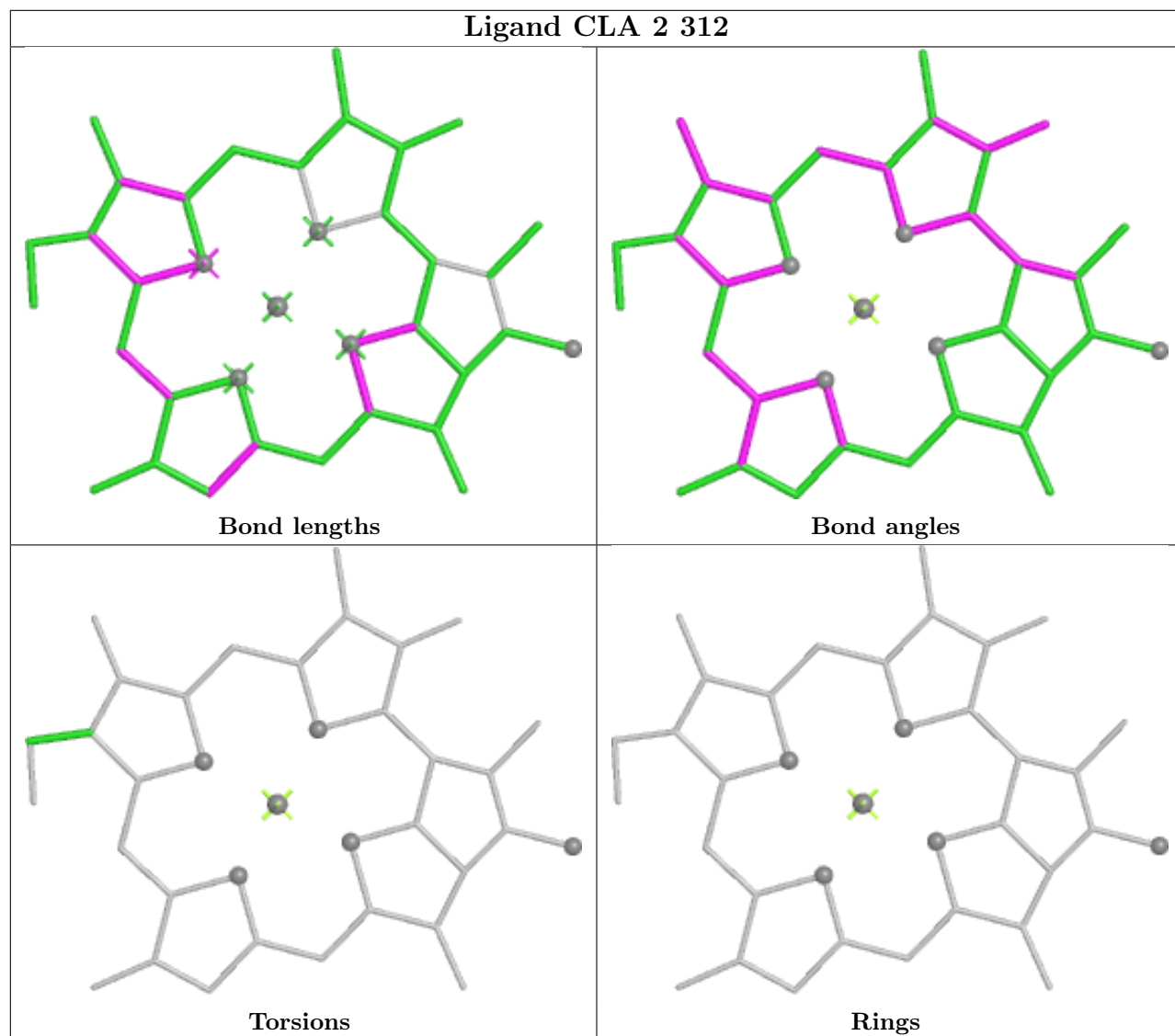
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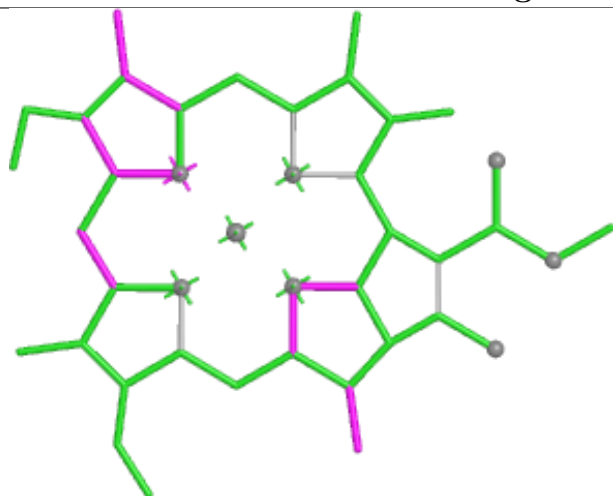
Rings



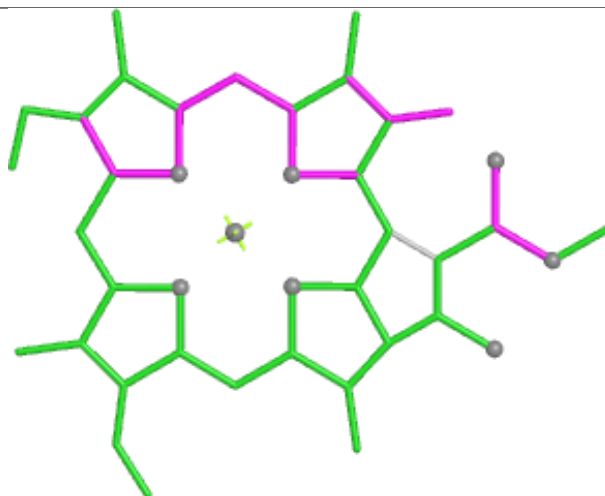
Ligand CLA 2 312



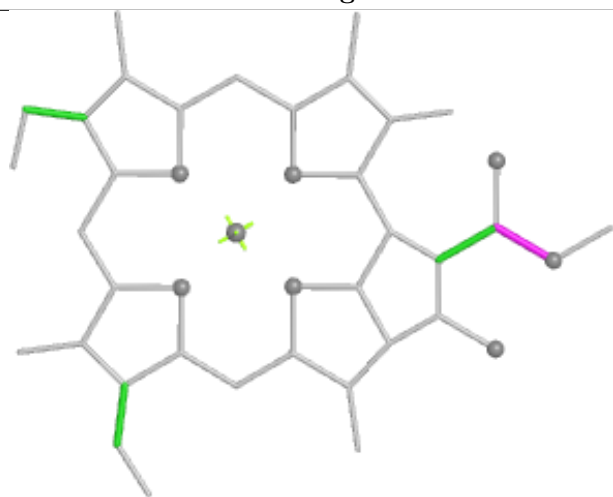
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Bond lengths



Bond angles

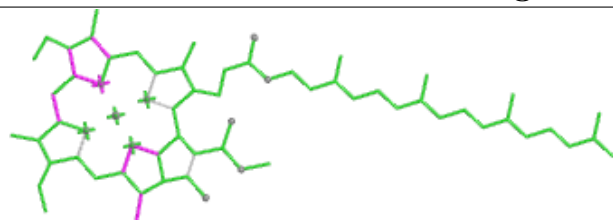


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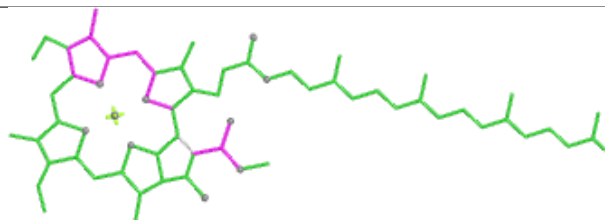


Rings

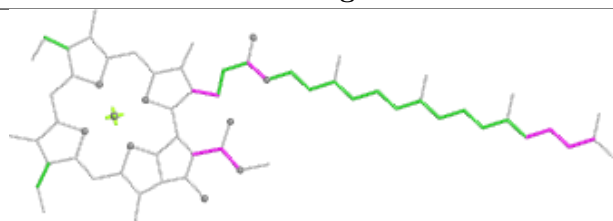
Ligand CLA A 403



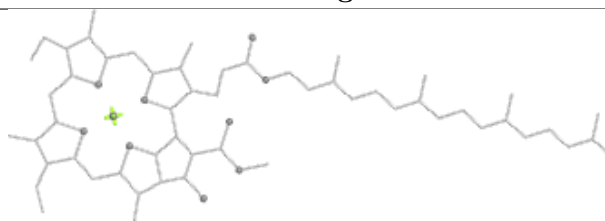
Bond lengths



Bond angles

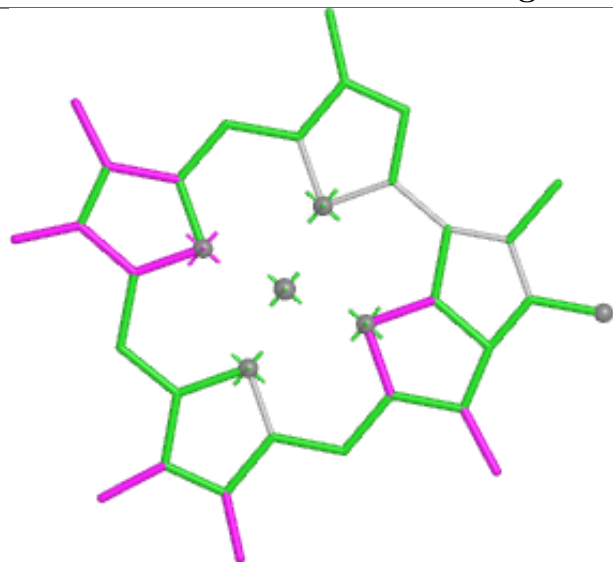


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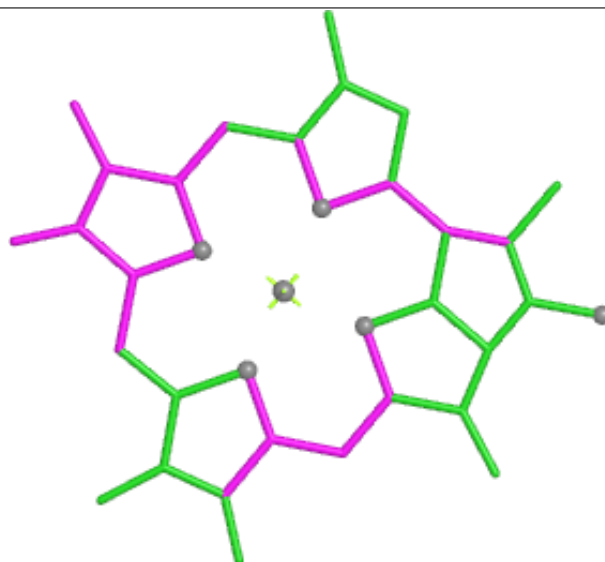


Rings

Ligand CLA 4 213



Bond lengths



Bond angles

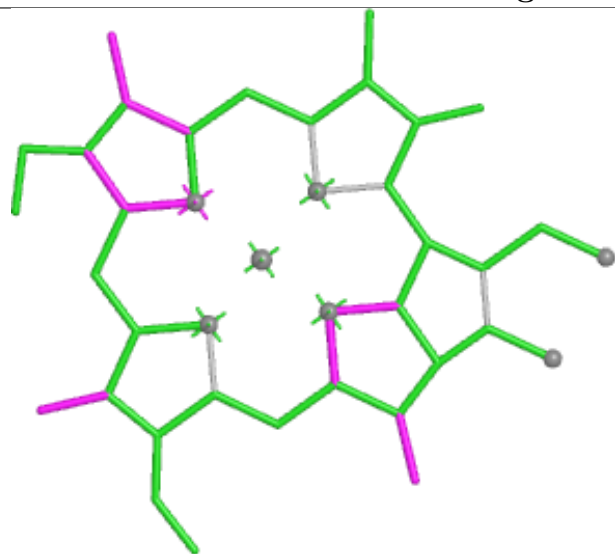


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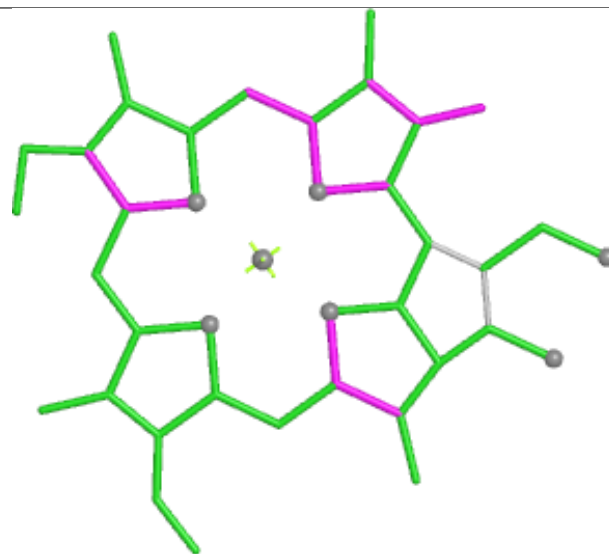


Rings

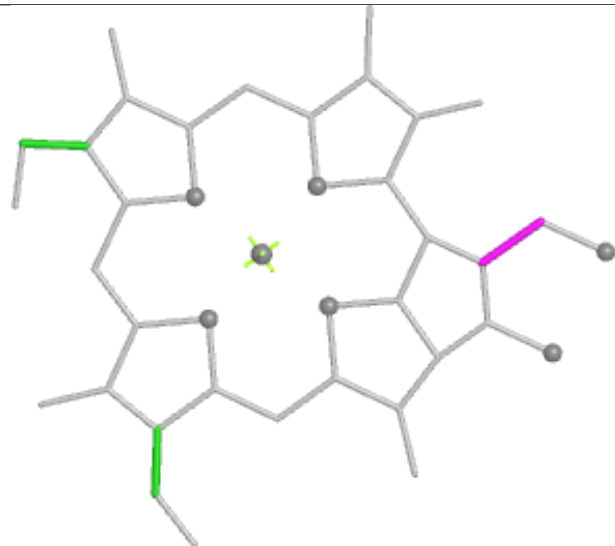
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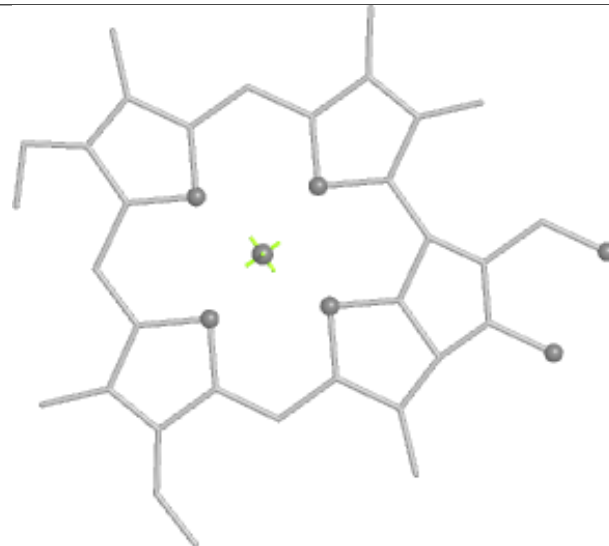
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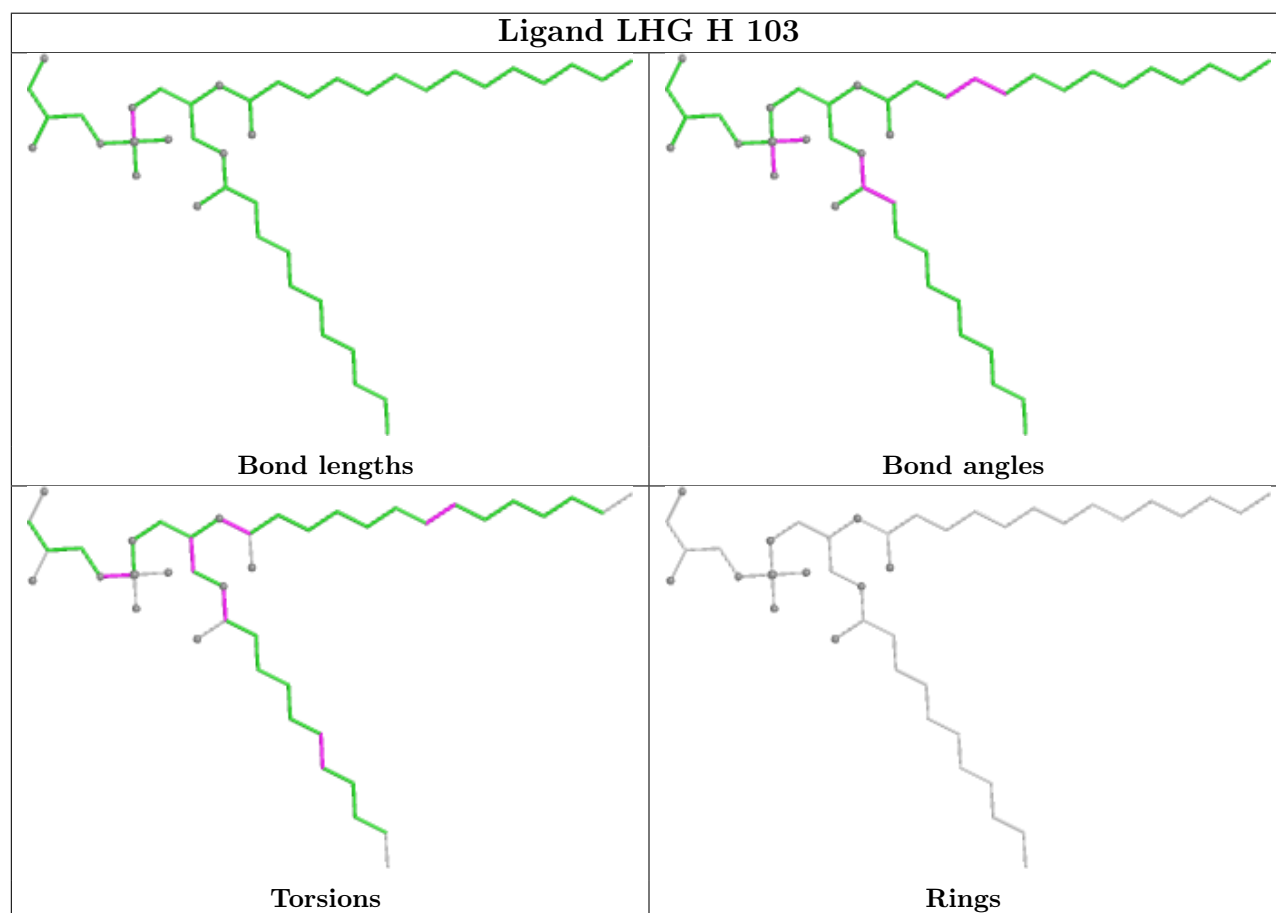
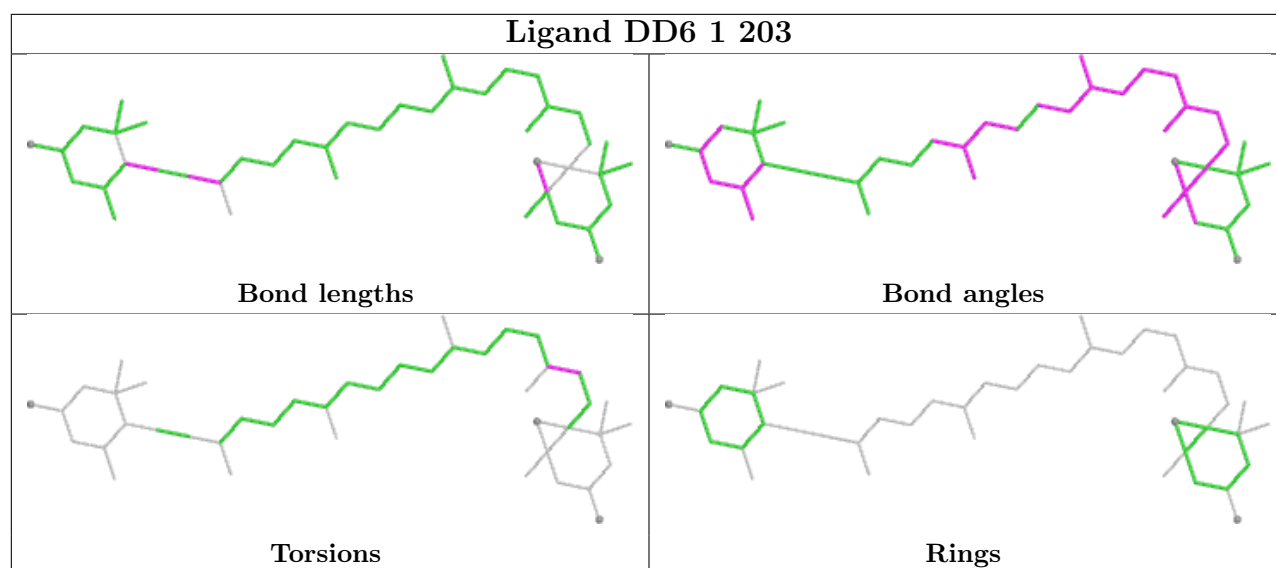
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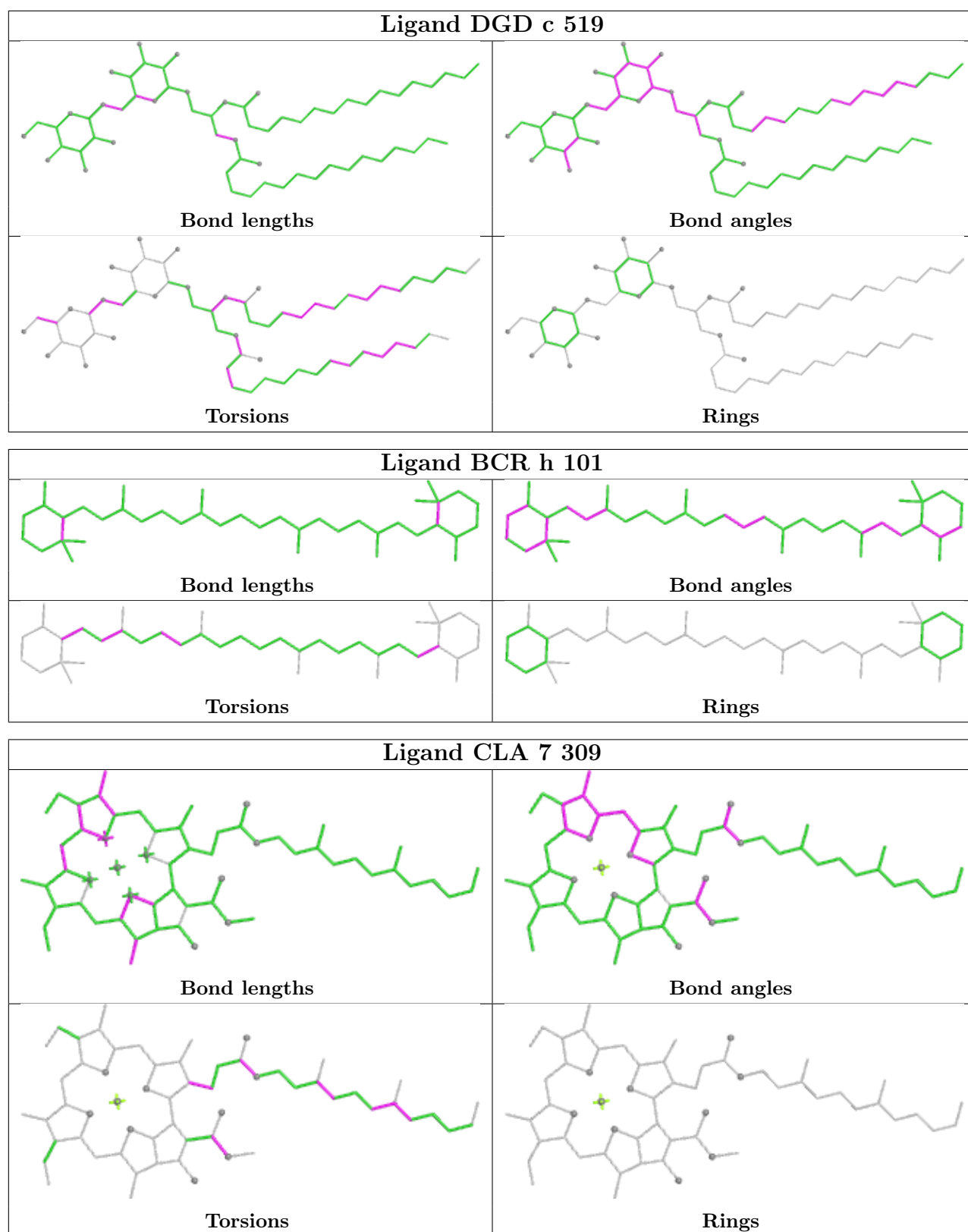


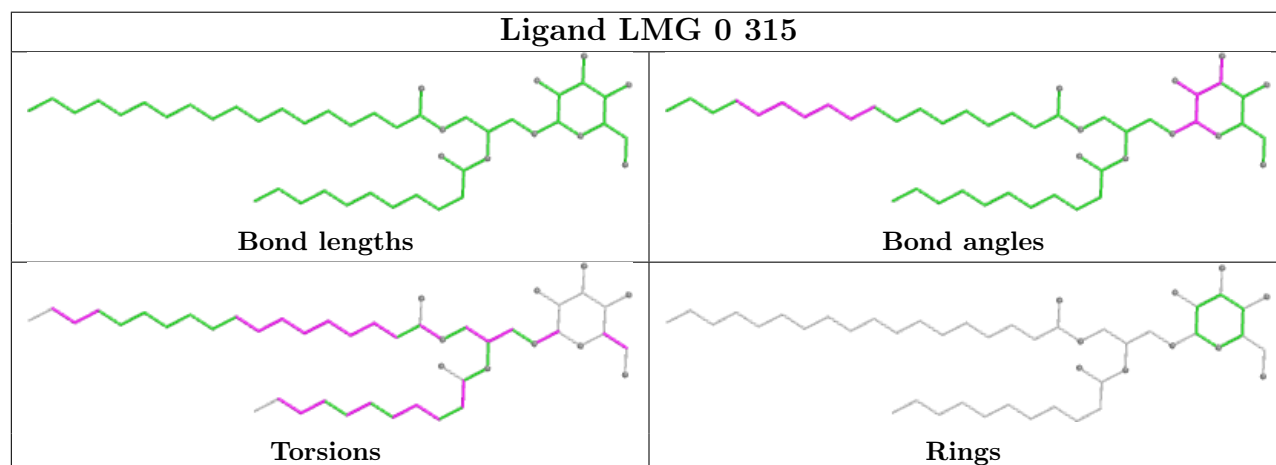
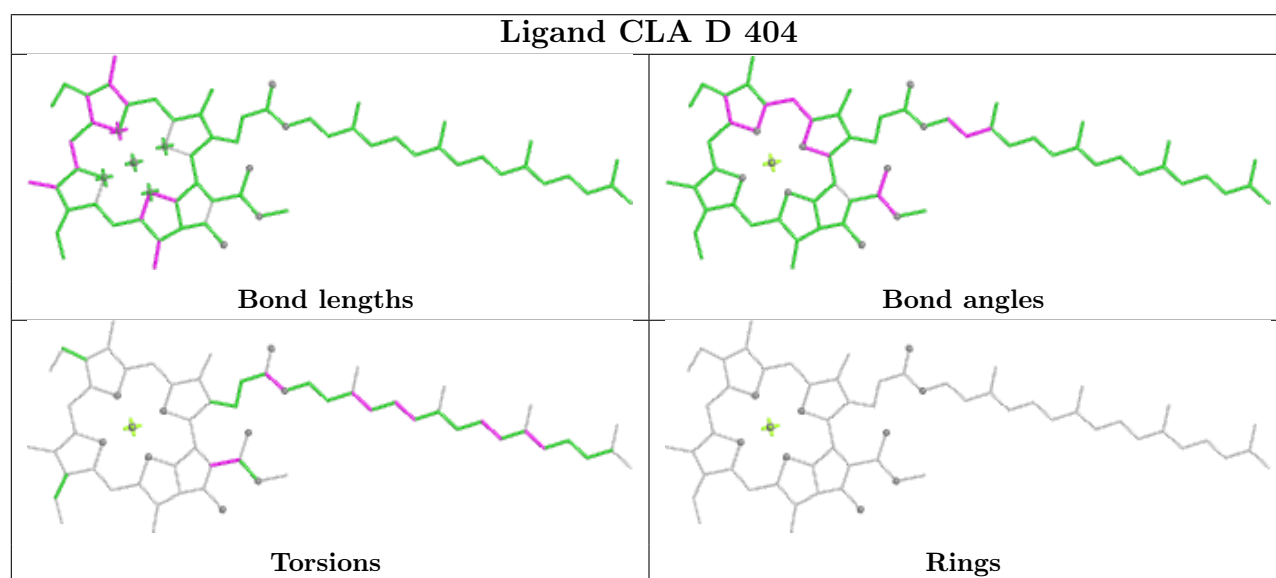
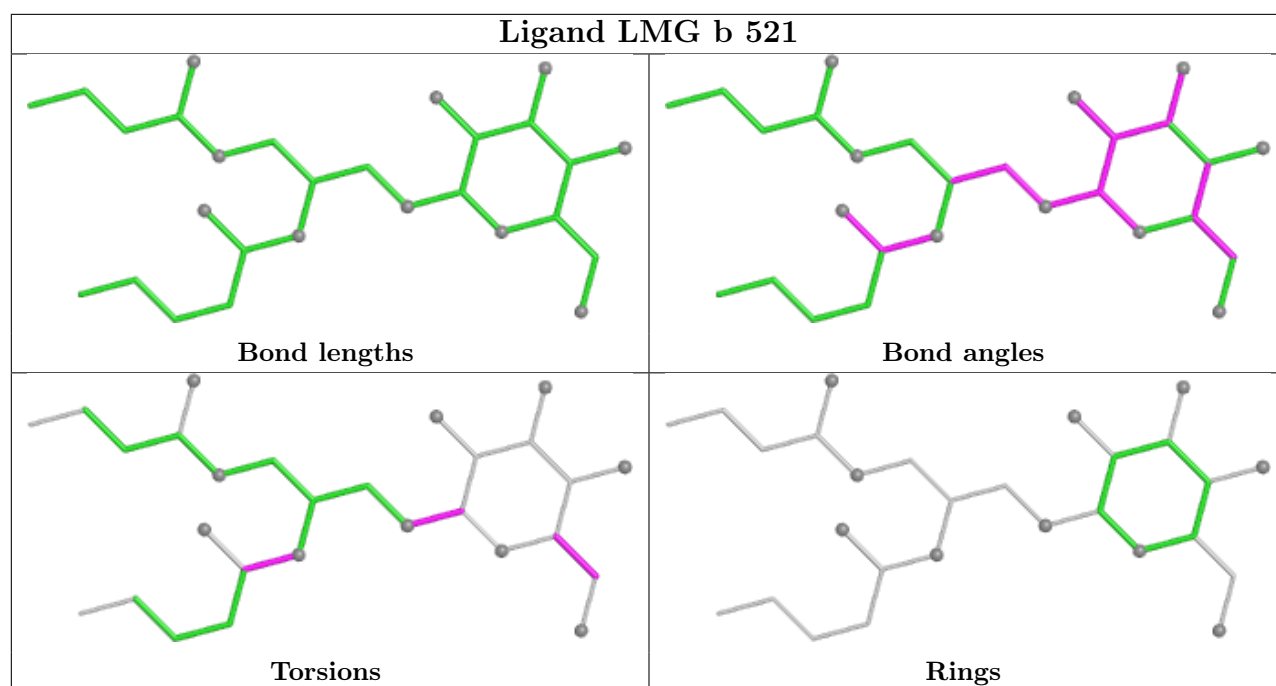
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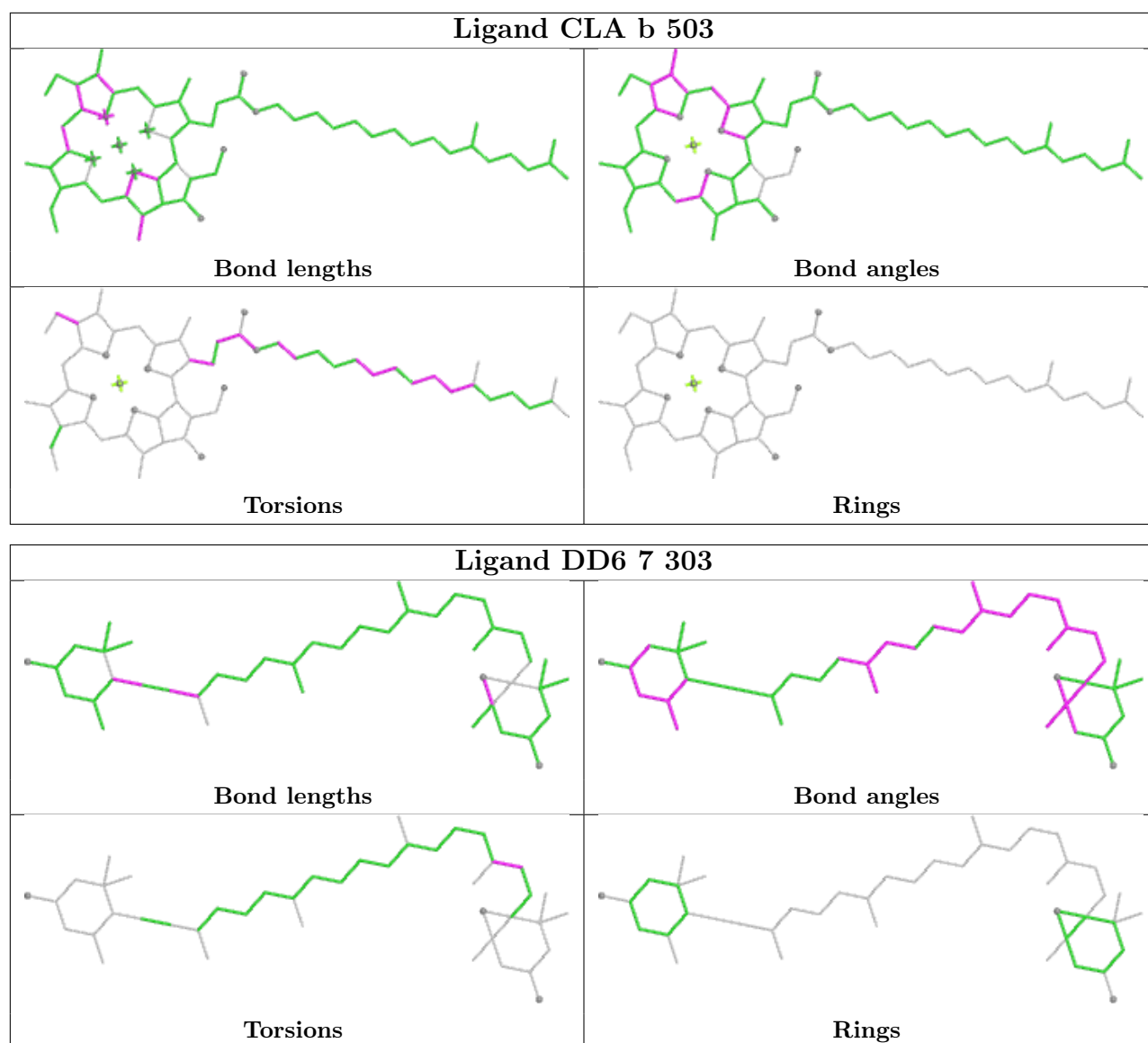


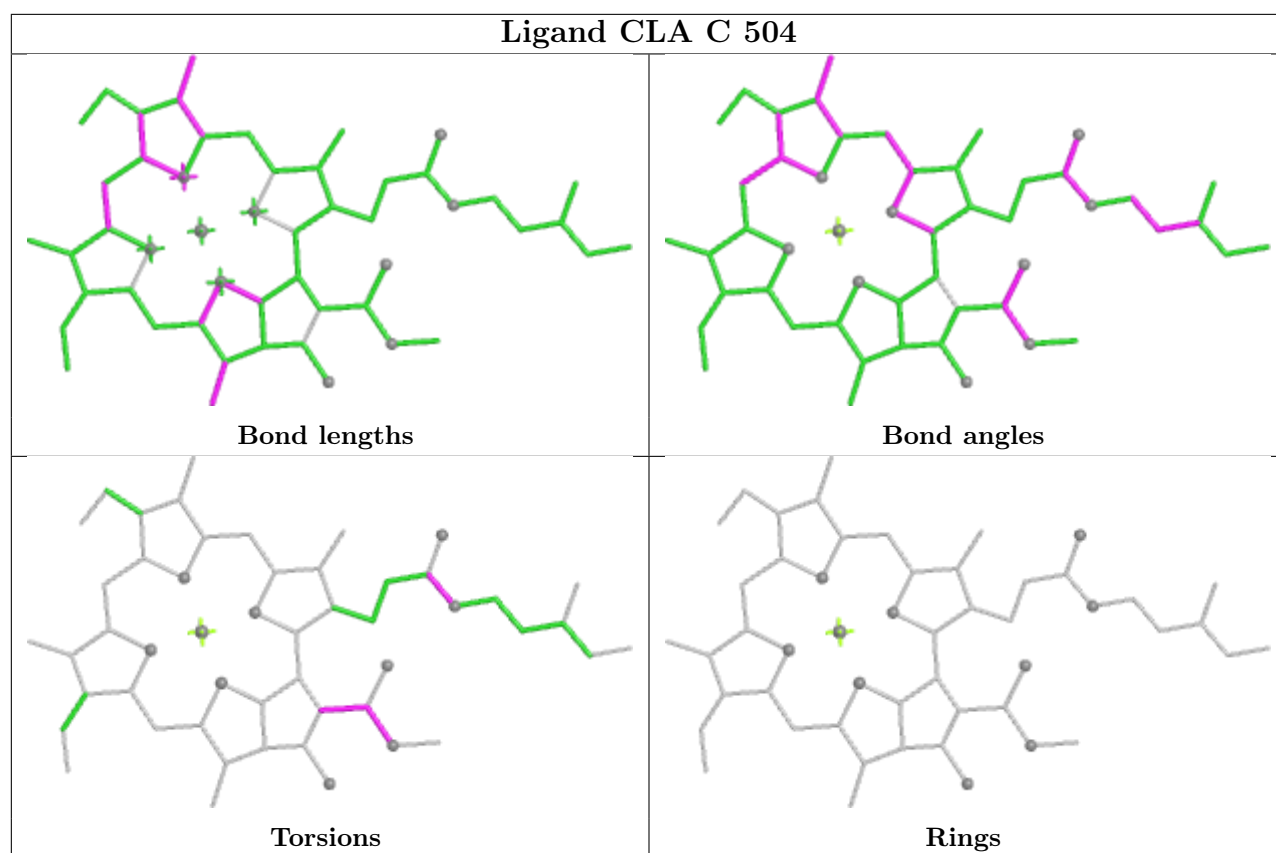
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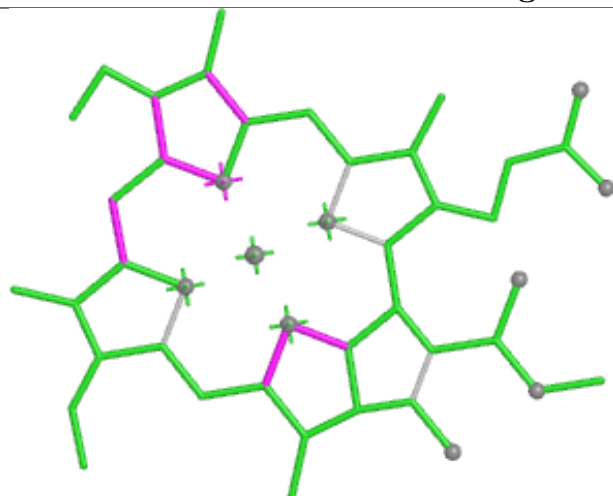




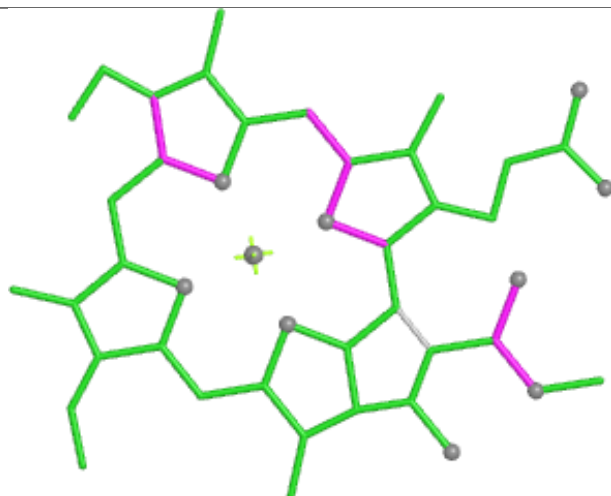




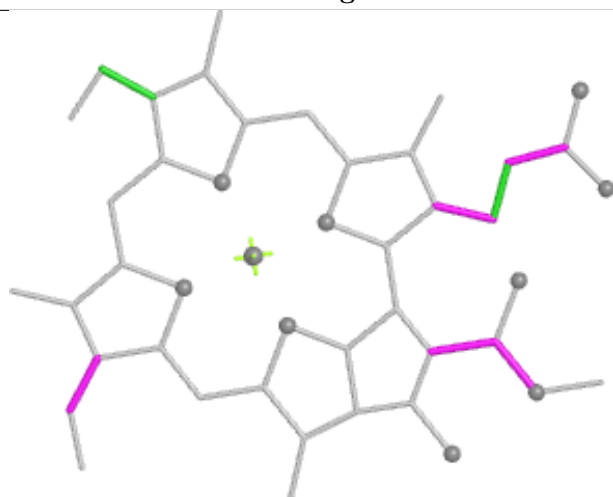
Ligand CLA 0 311



Bond lengths



Bond angles

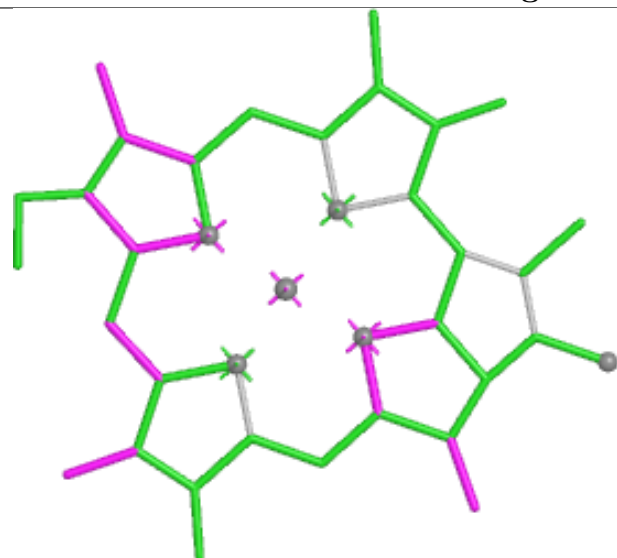


Torsions

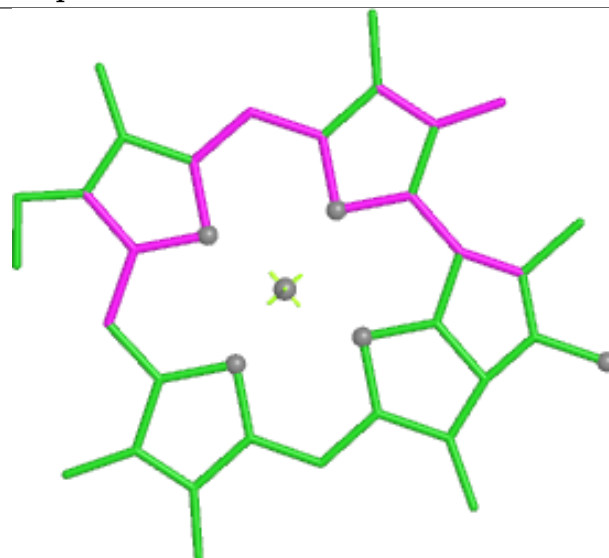


Rings

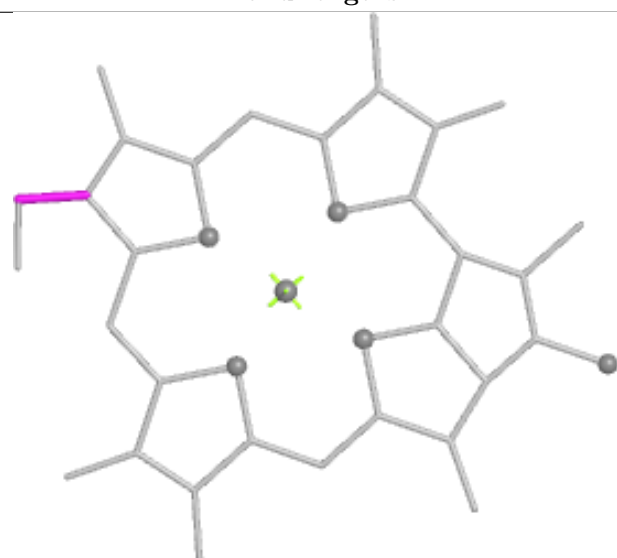
Ligand CLA p 605



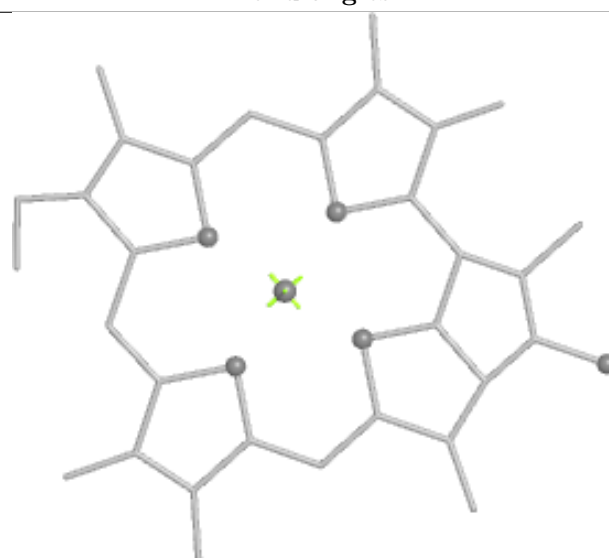
Bond lengths



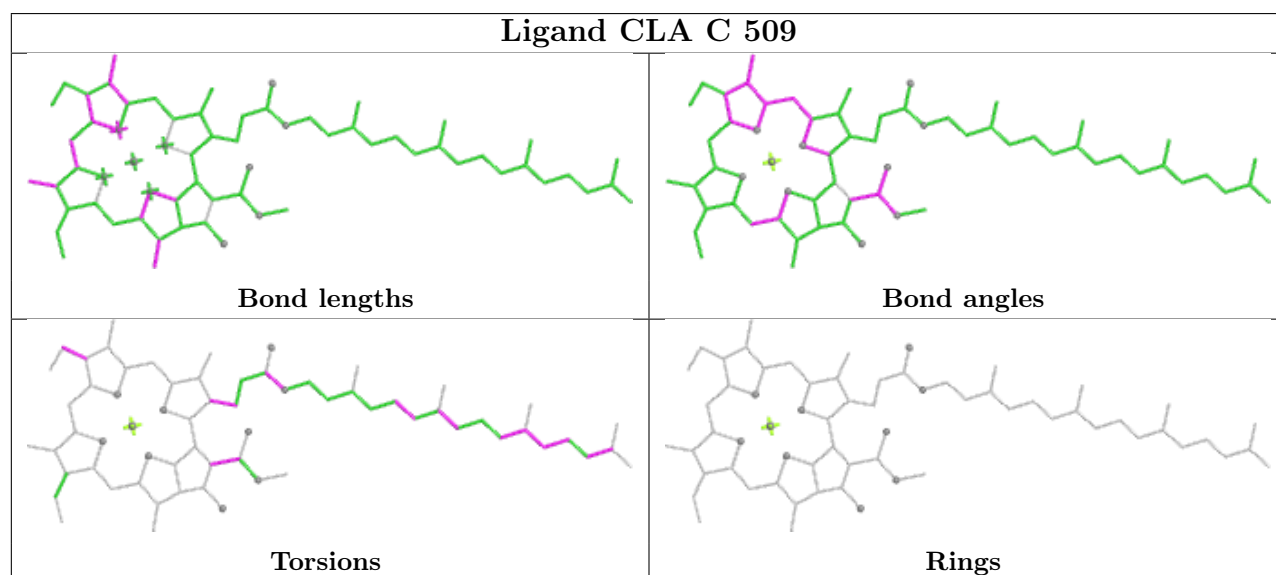
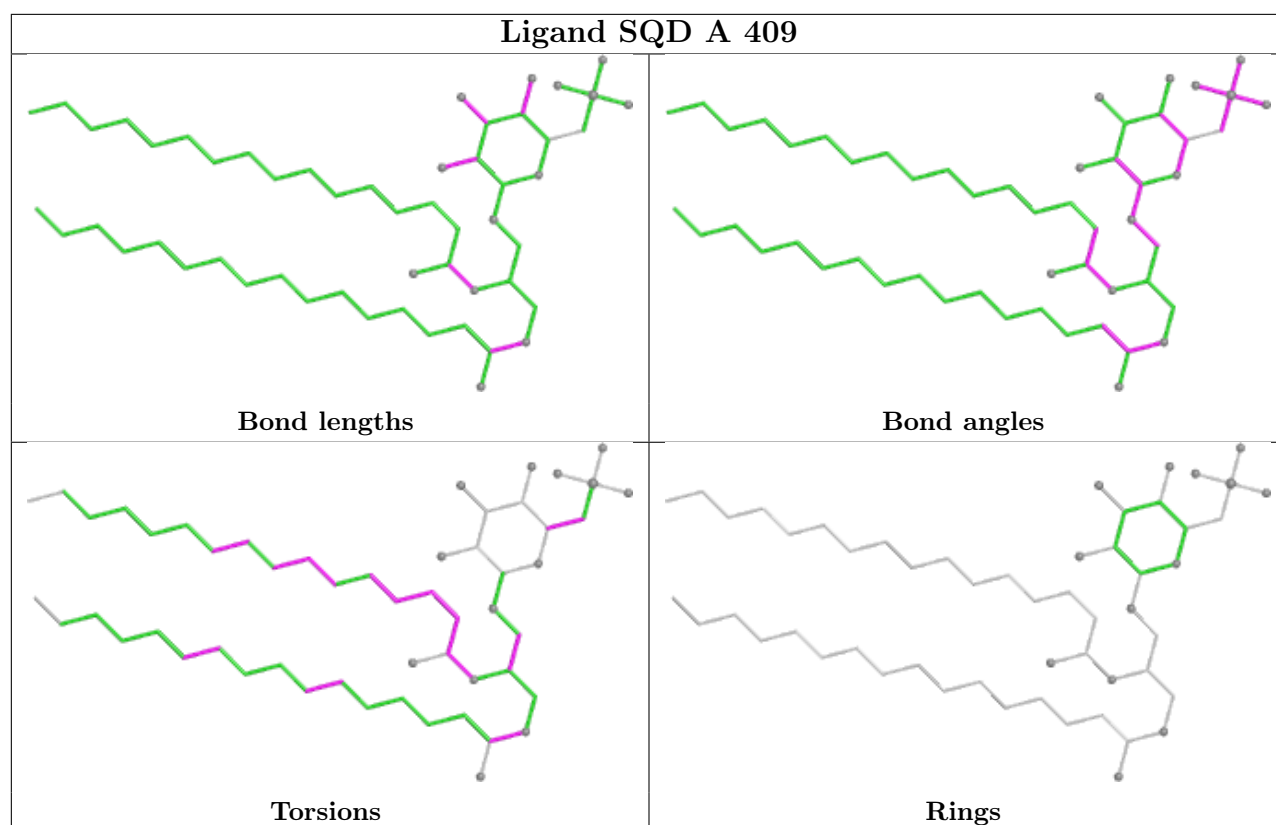
Bond angles



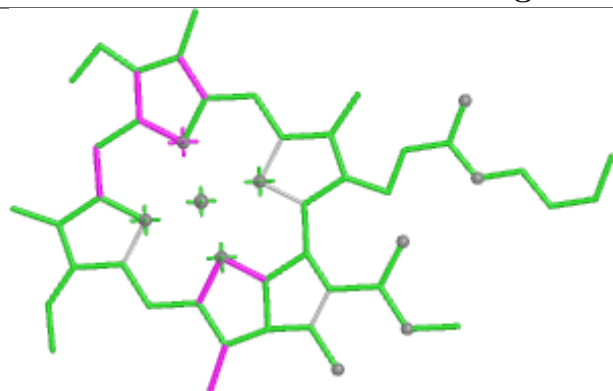
Torsions



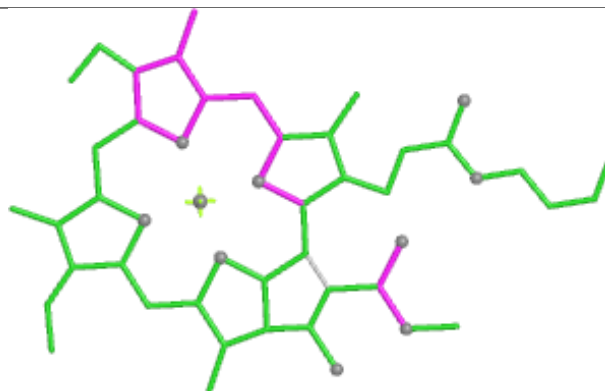
Rings



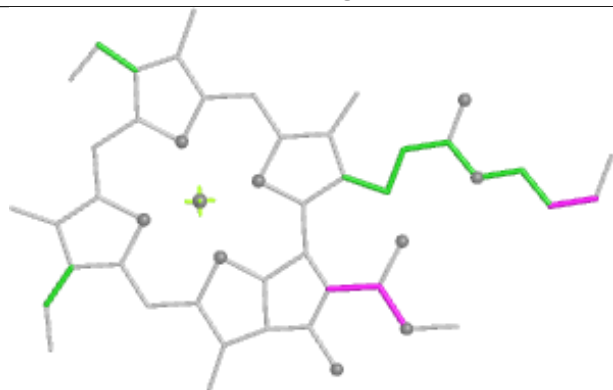
Ligand CLA C 514



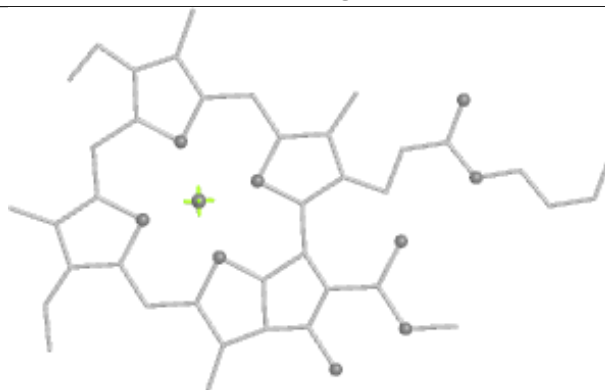
Bond lengths



Bond angles

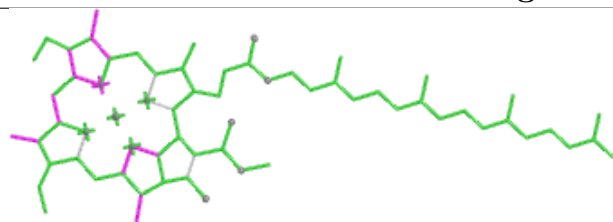


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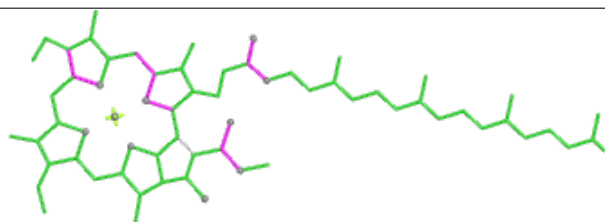


Rings

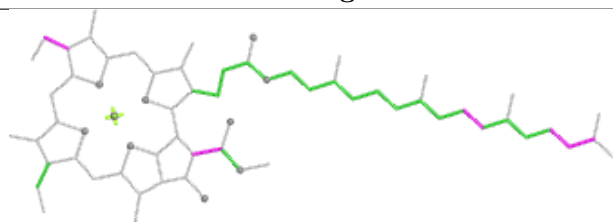
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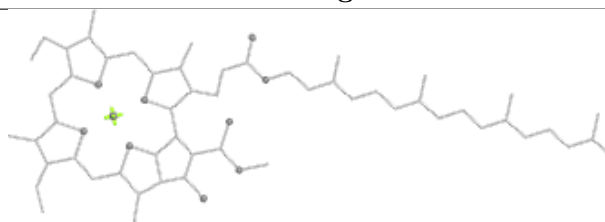
Bond lengths



Bond angles



Torsions

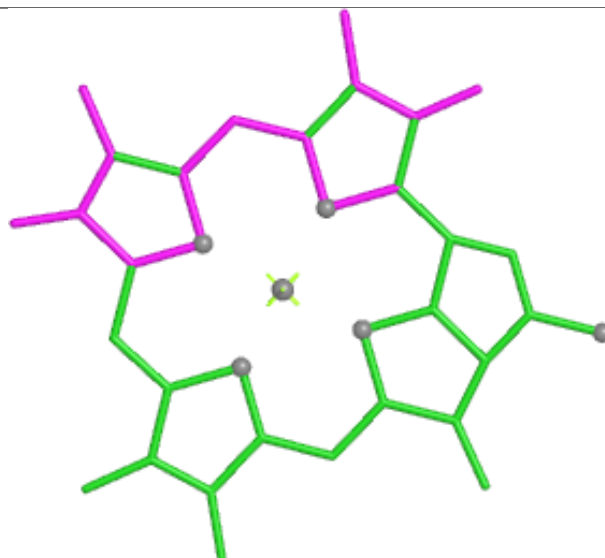


Rings

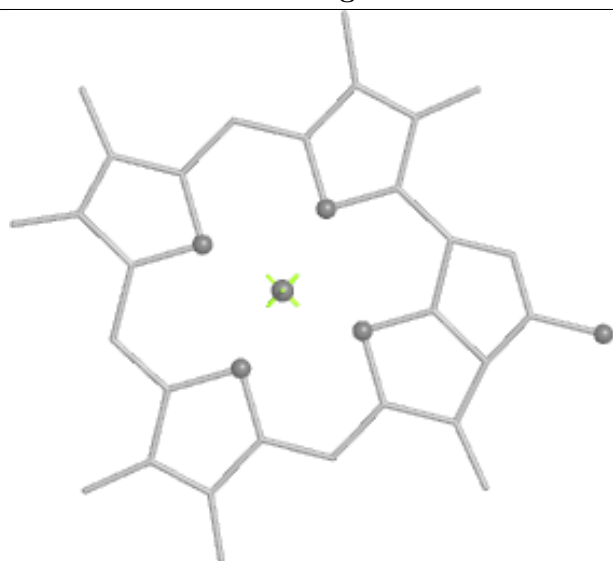
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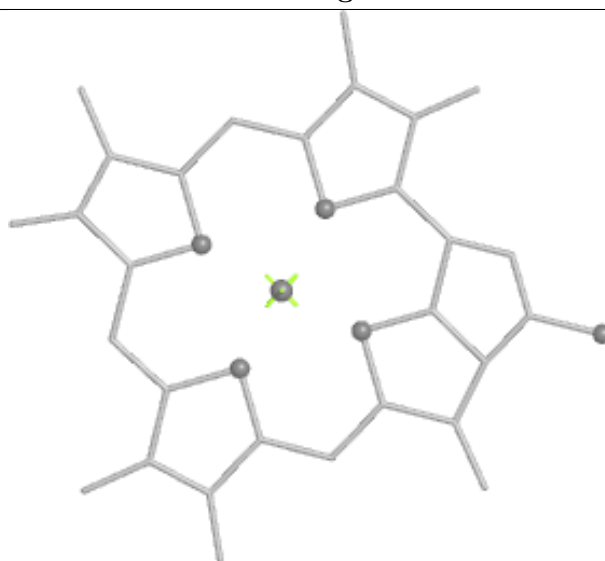
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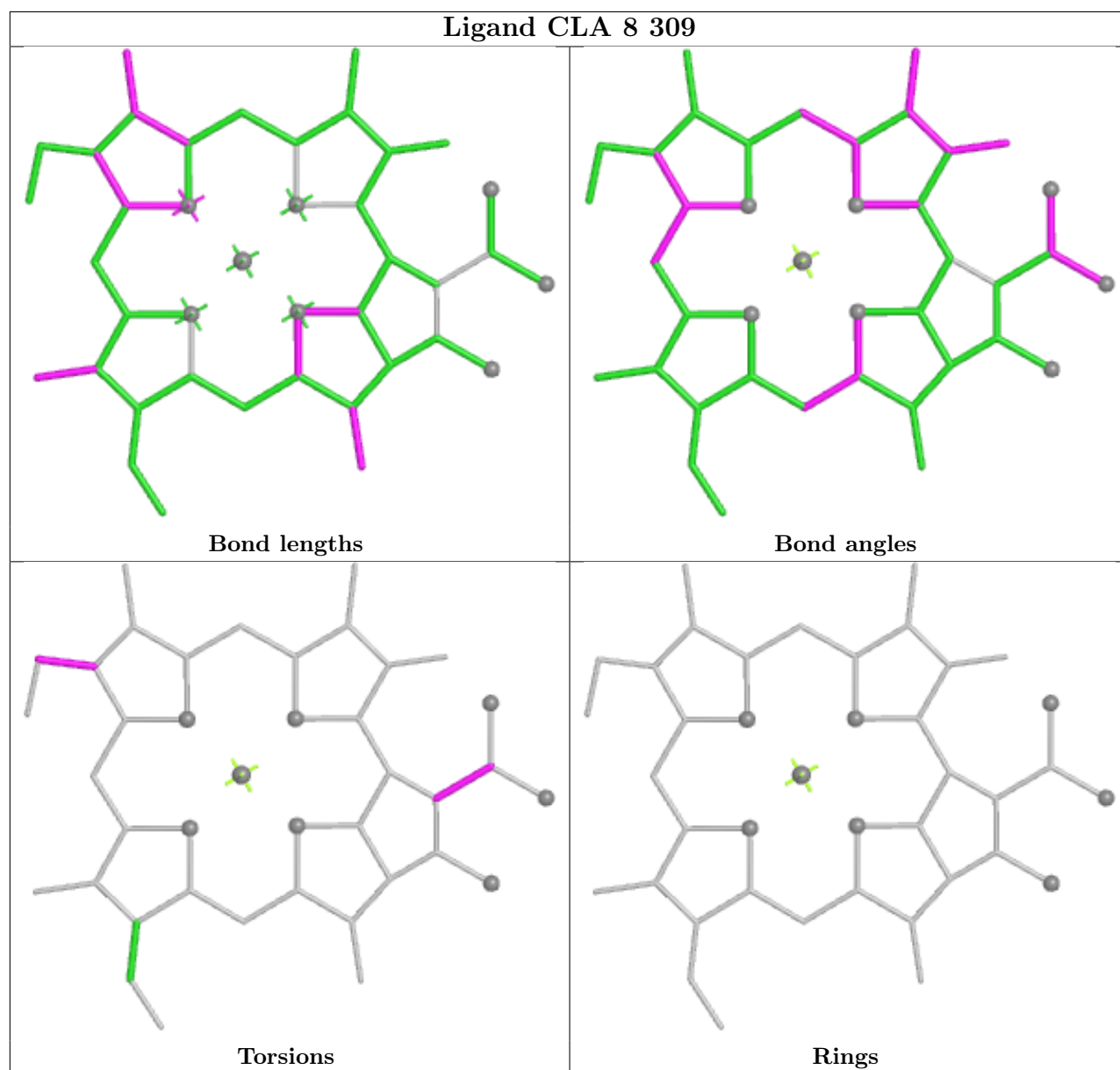
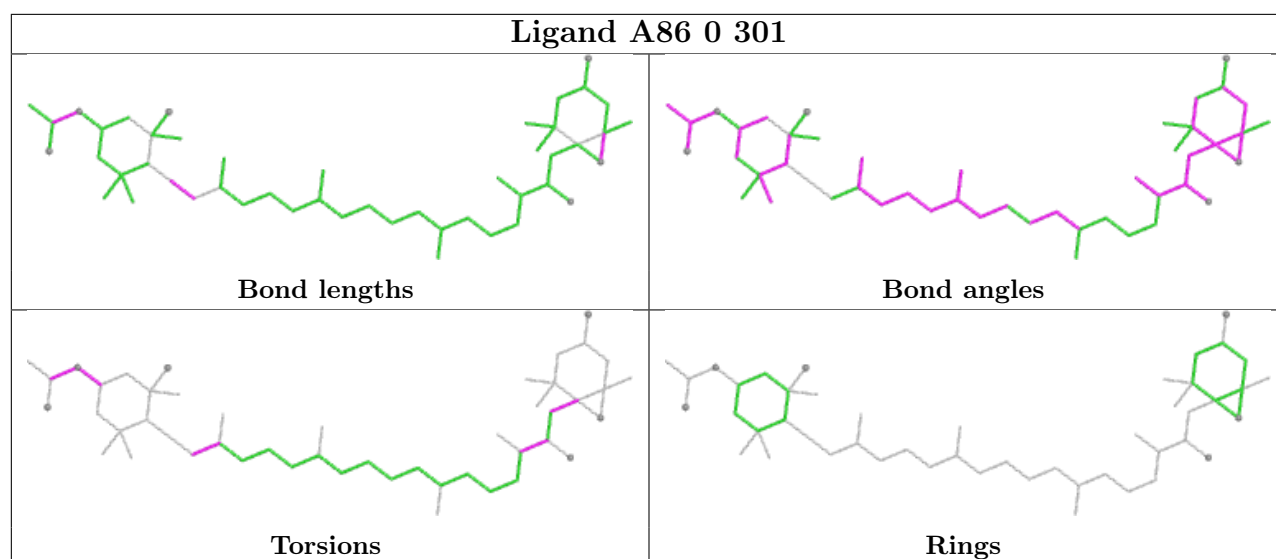
Bond angles



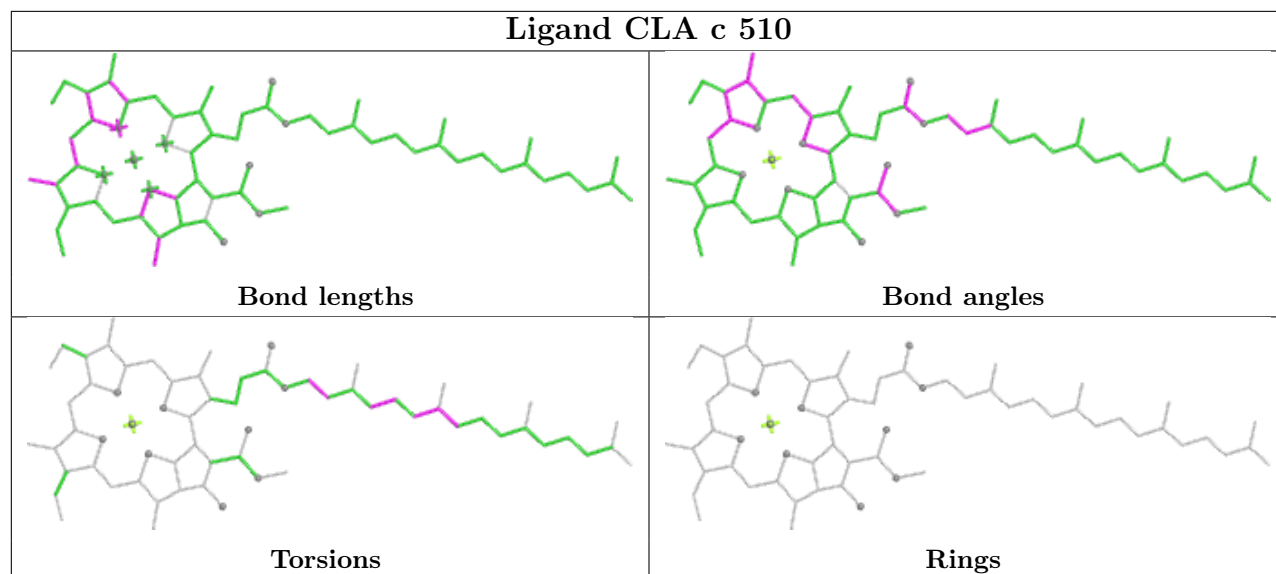
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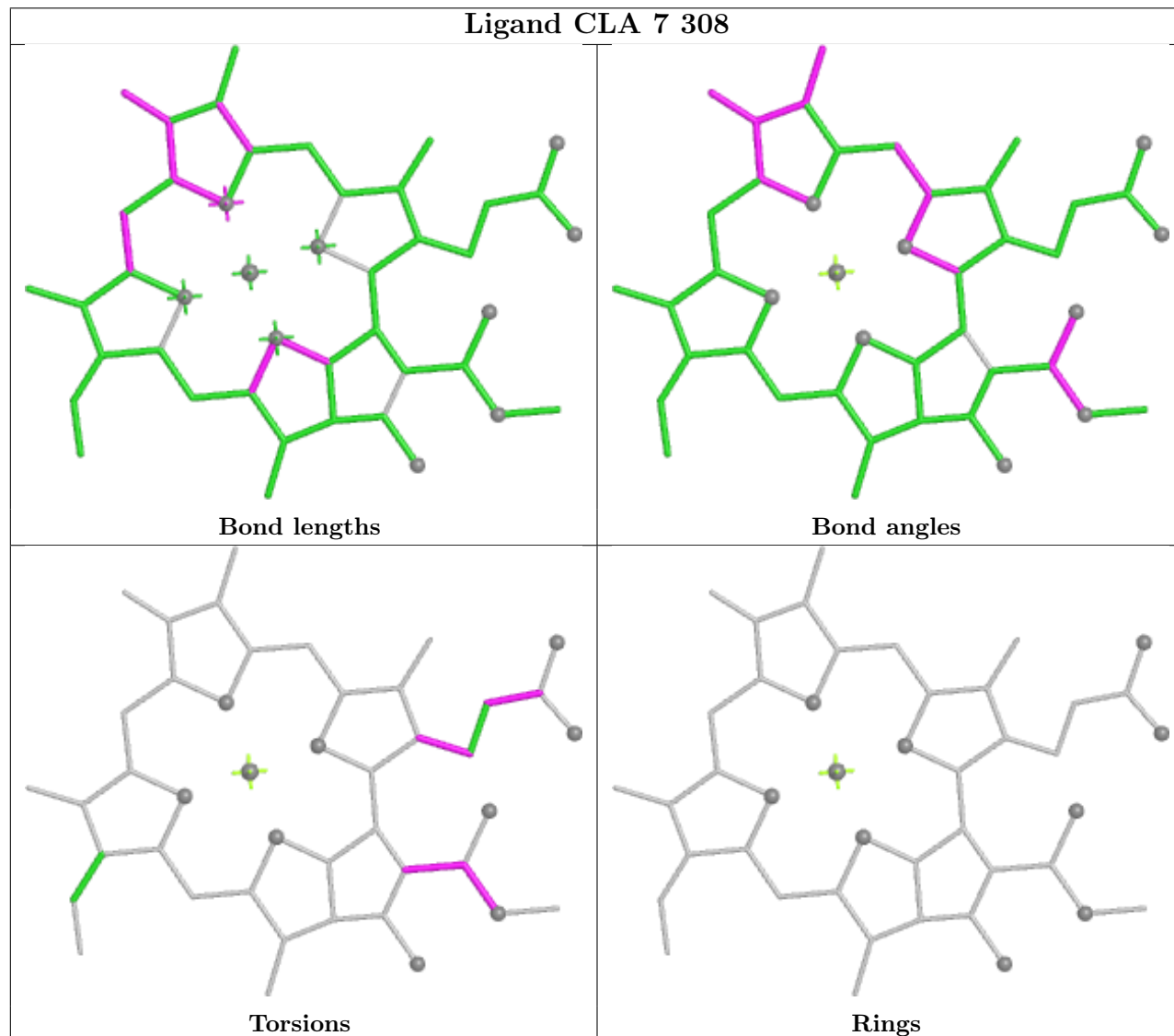
Rings

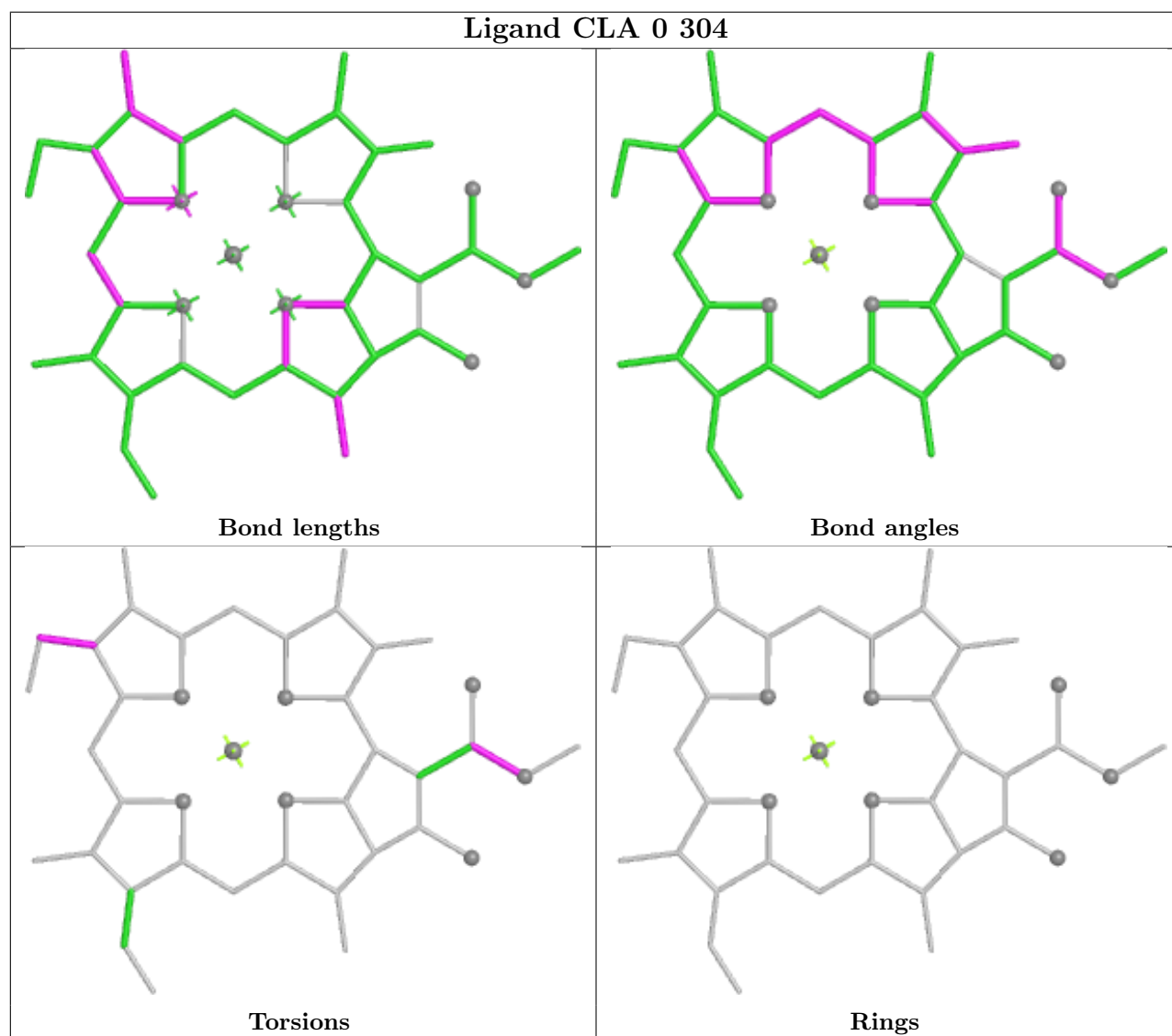
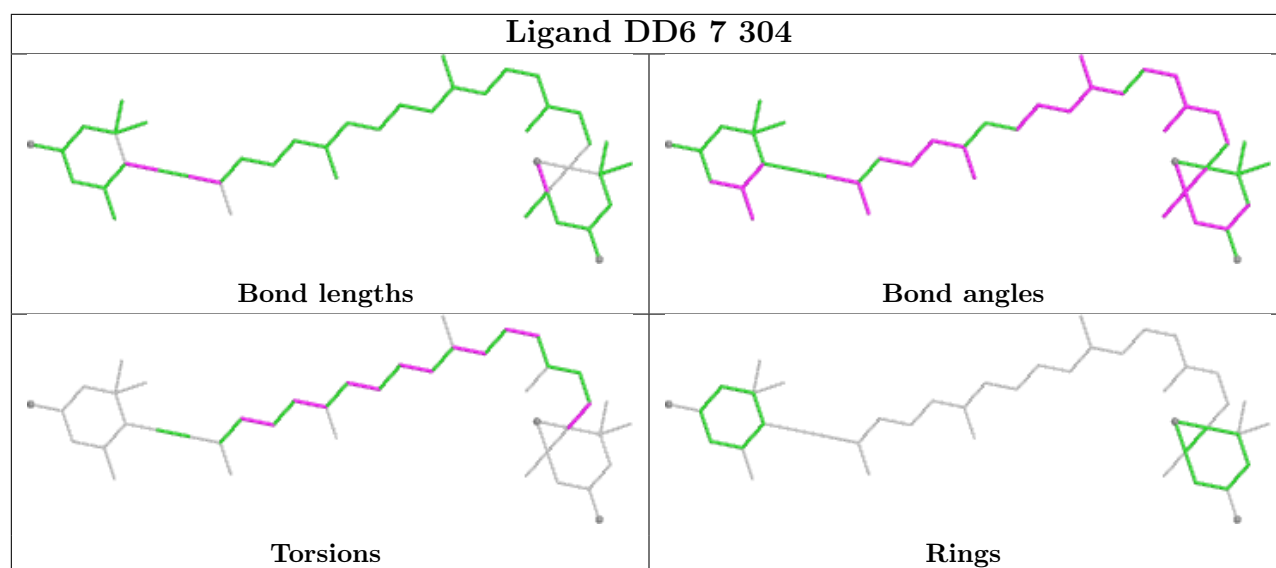


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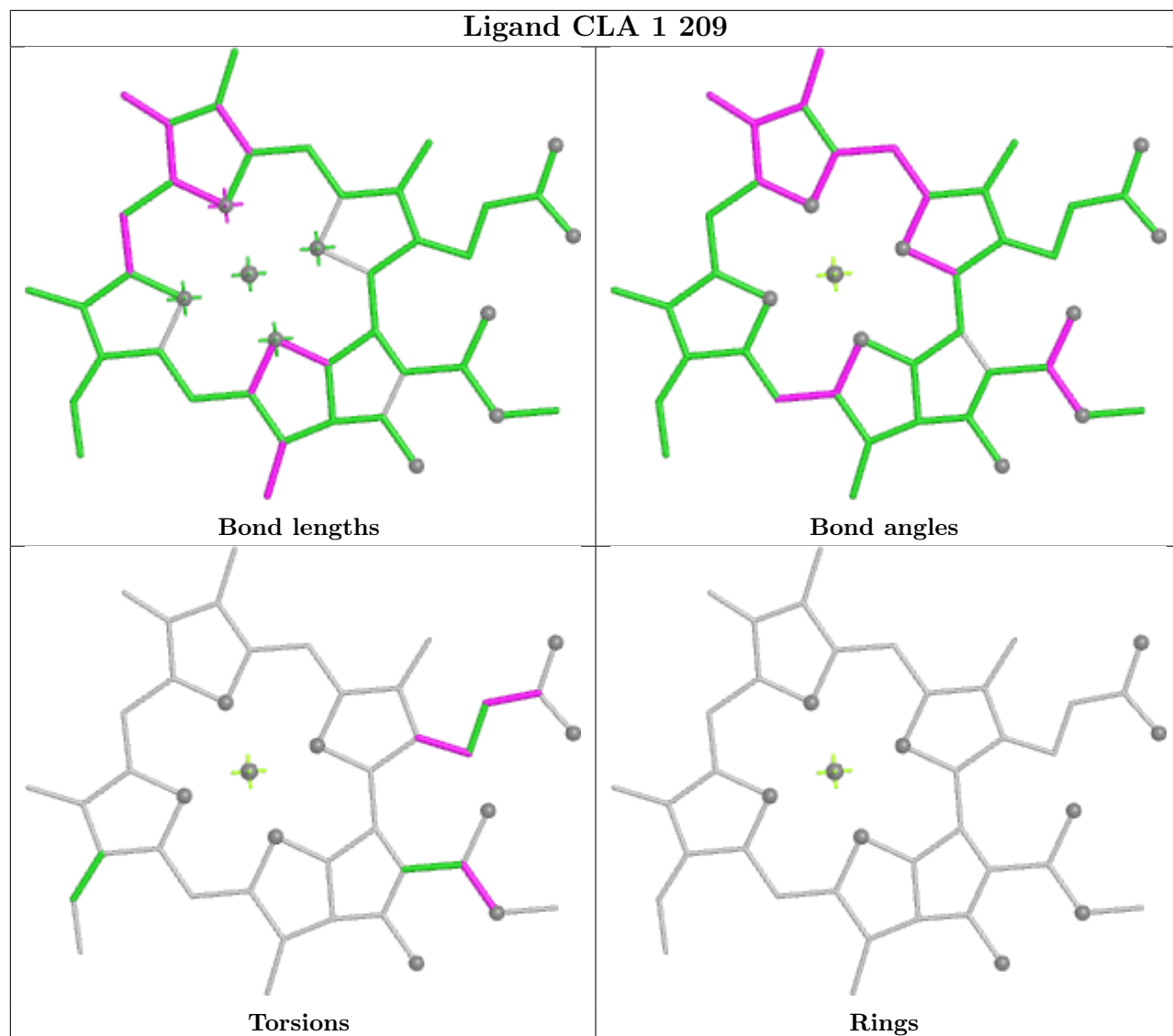


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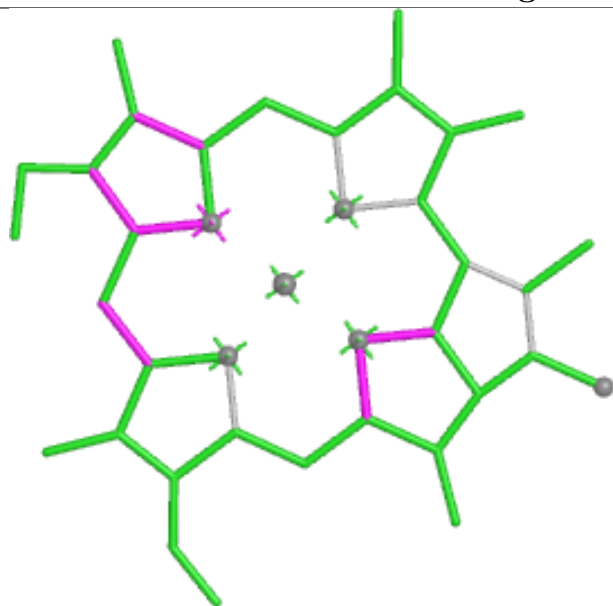




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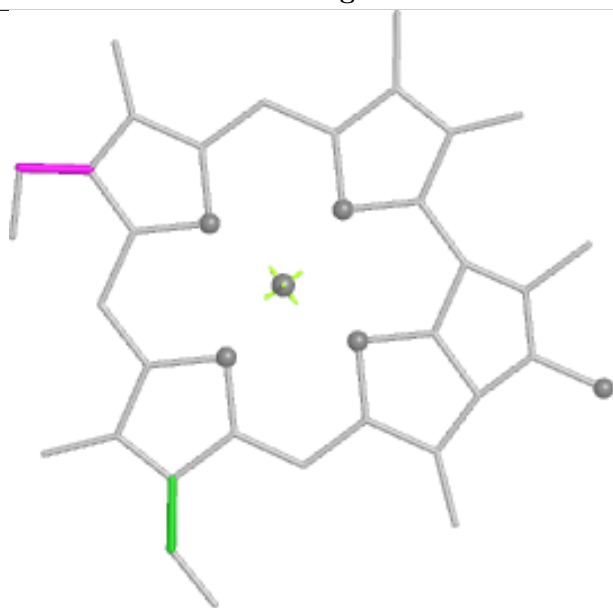
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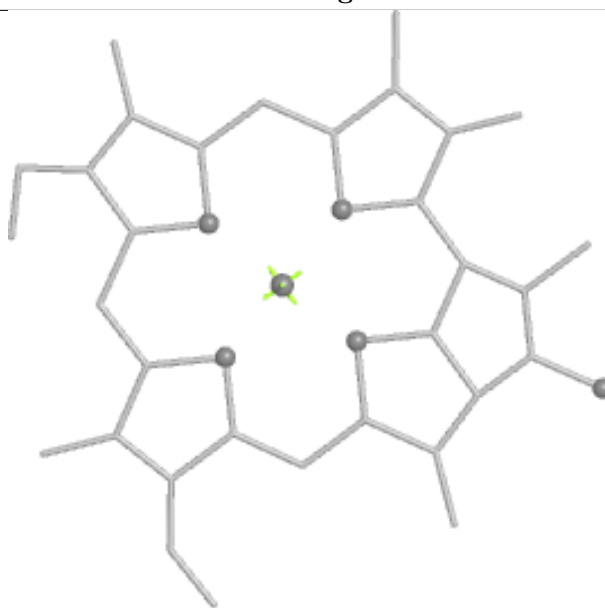
Bond lengths



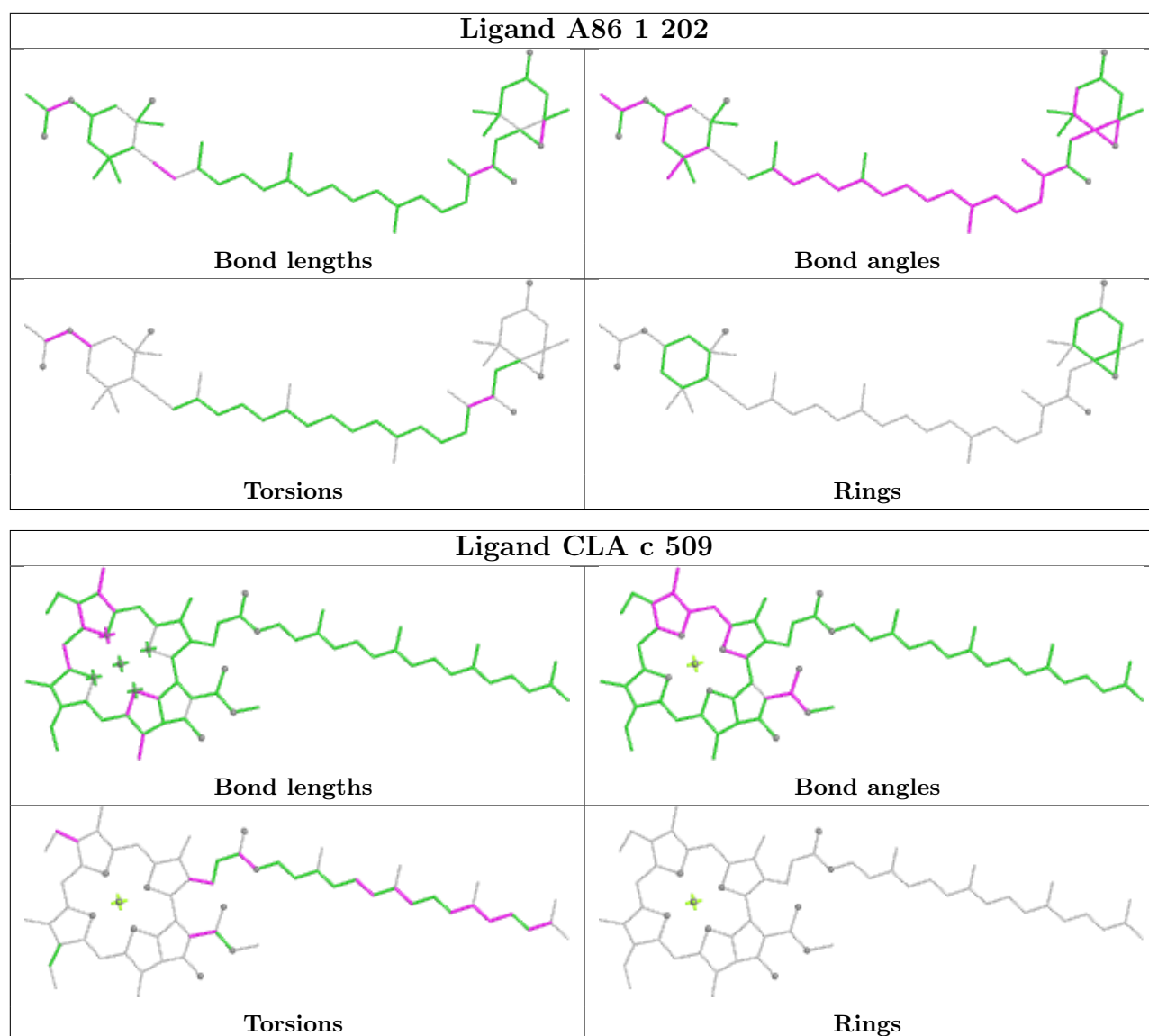
Bond angles



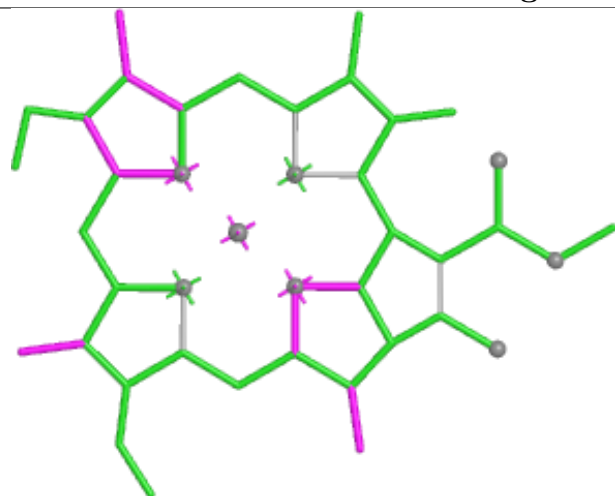
Torsions



Rings



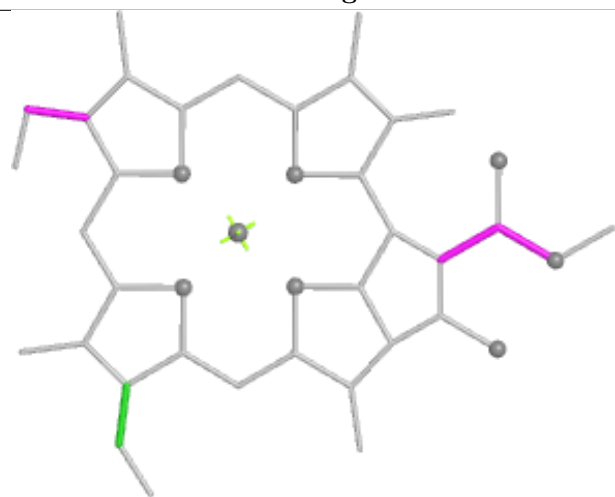
Ligand CLA 9 209



Bond lengths



Bond angles

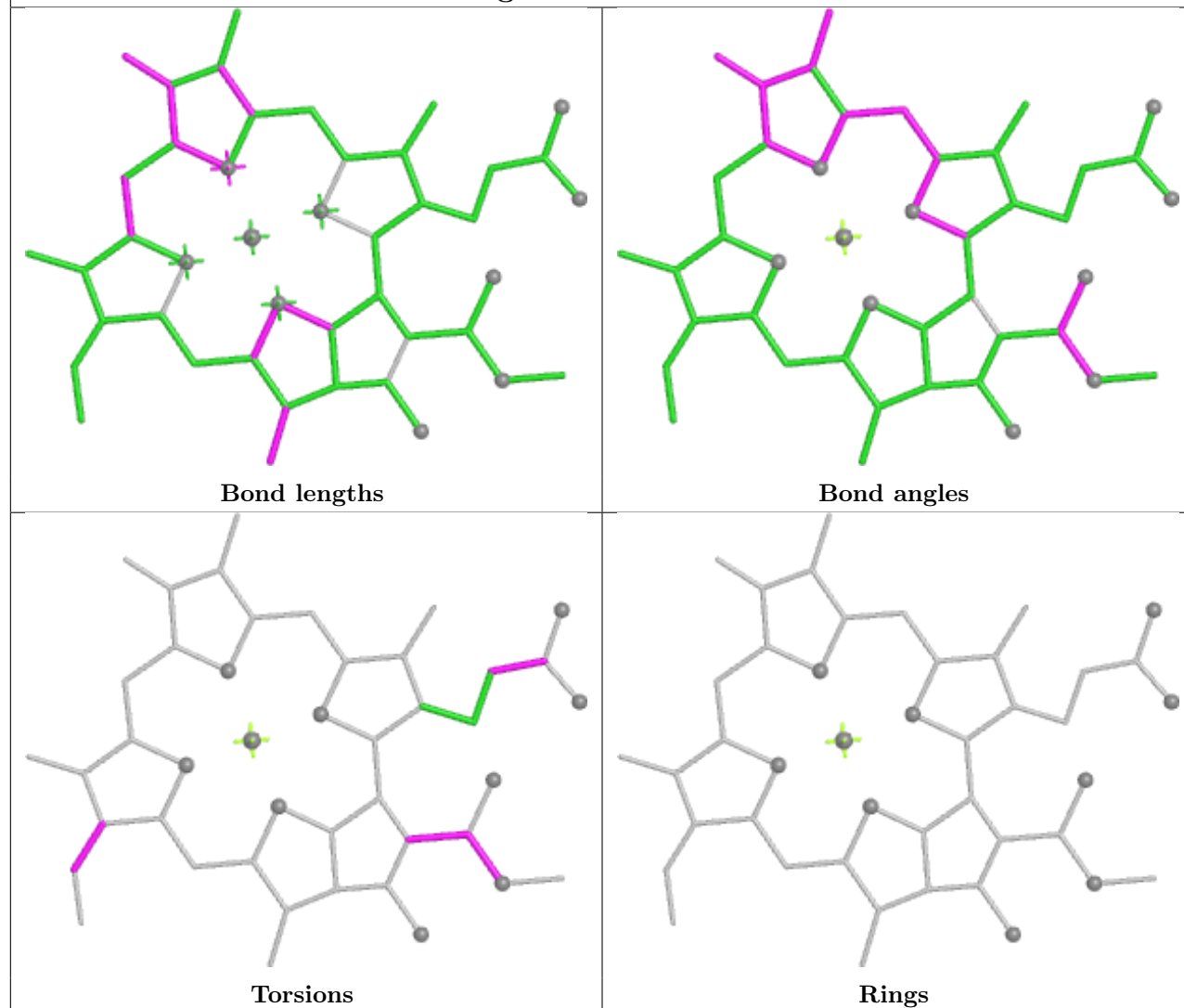


Torsions

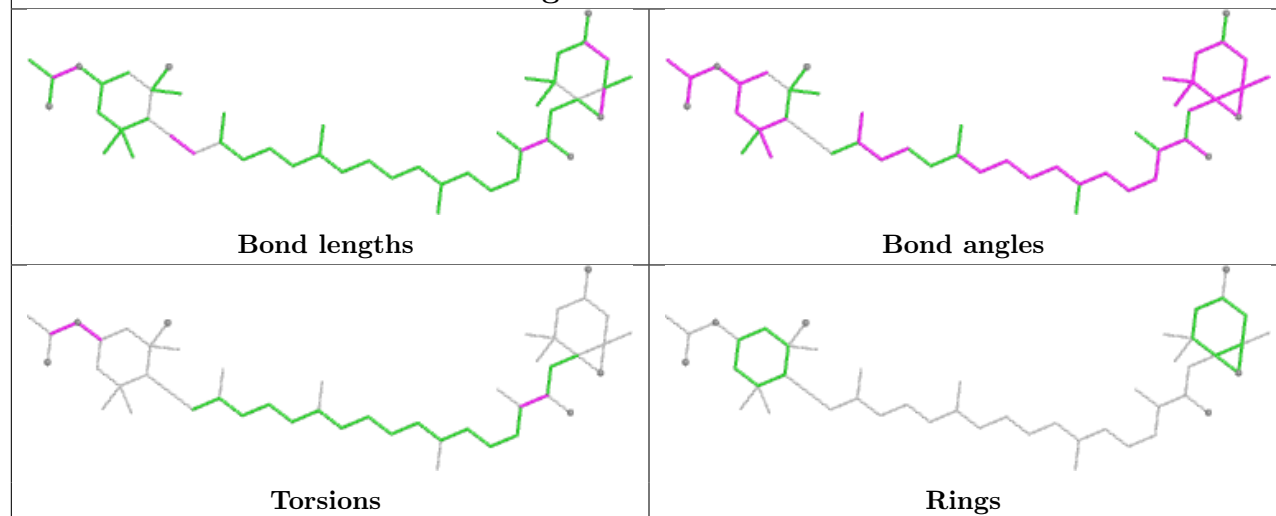


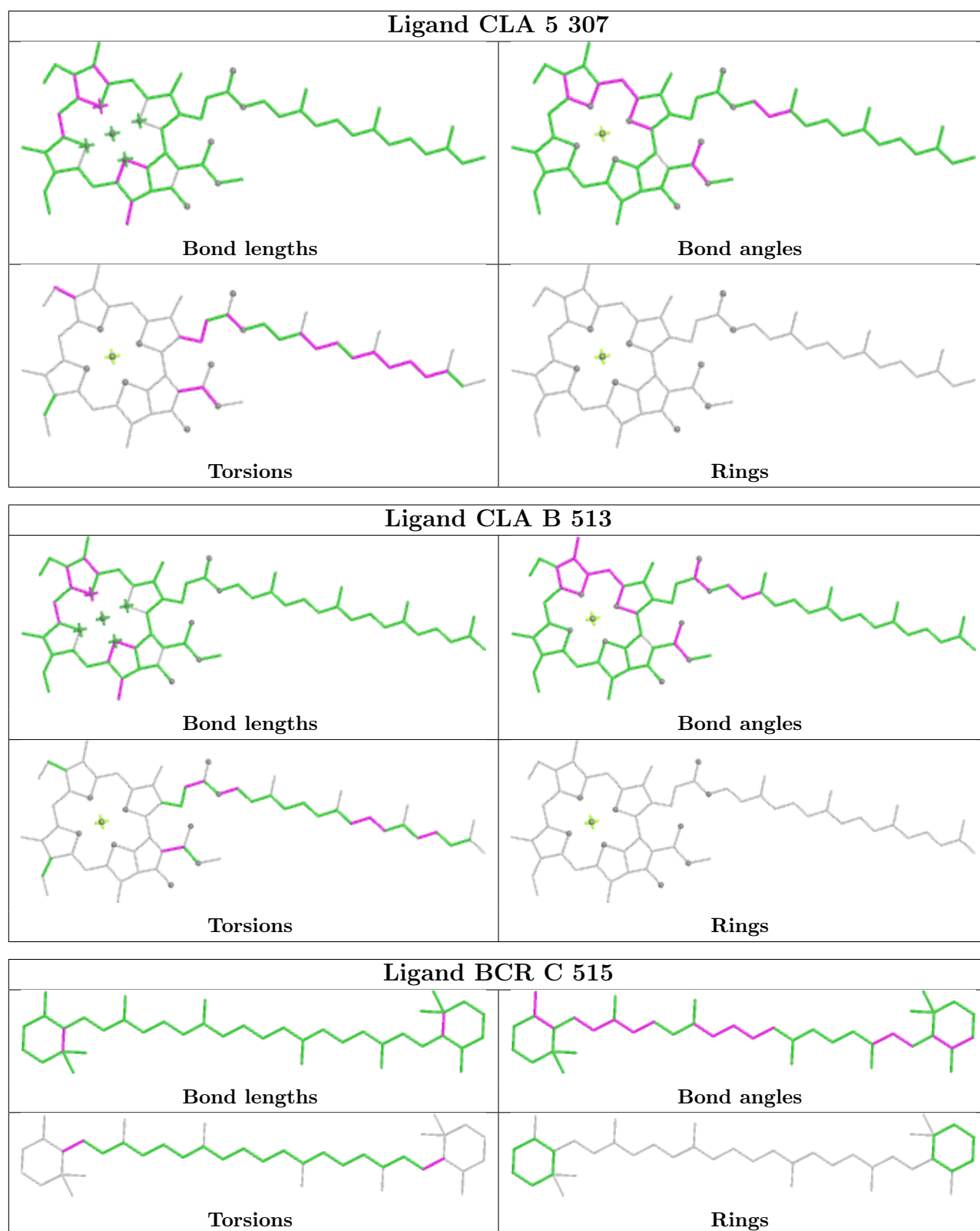
Rings

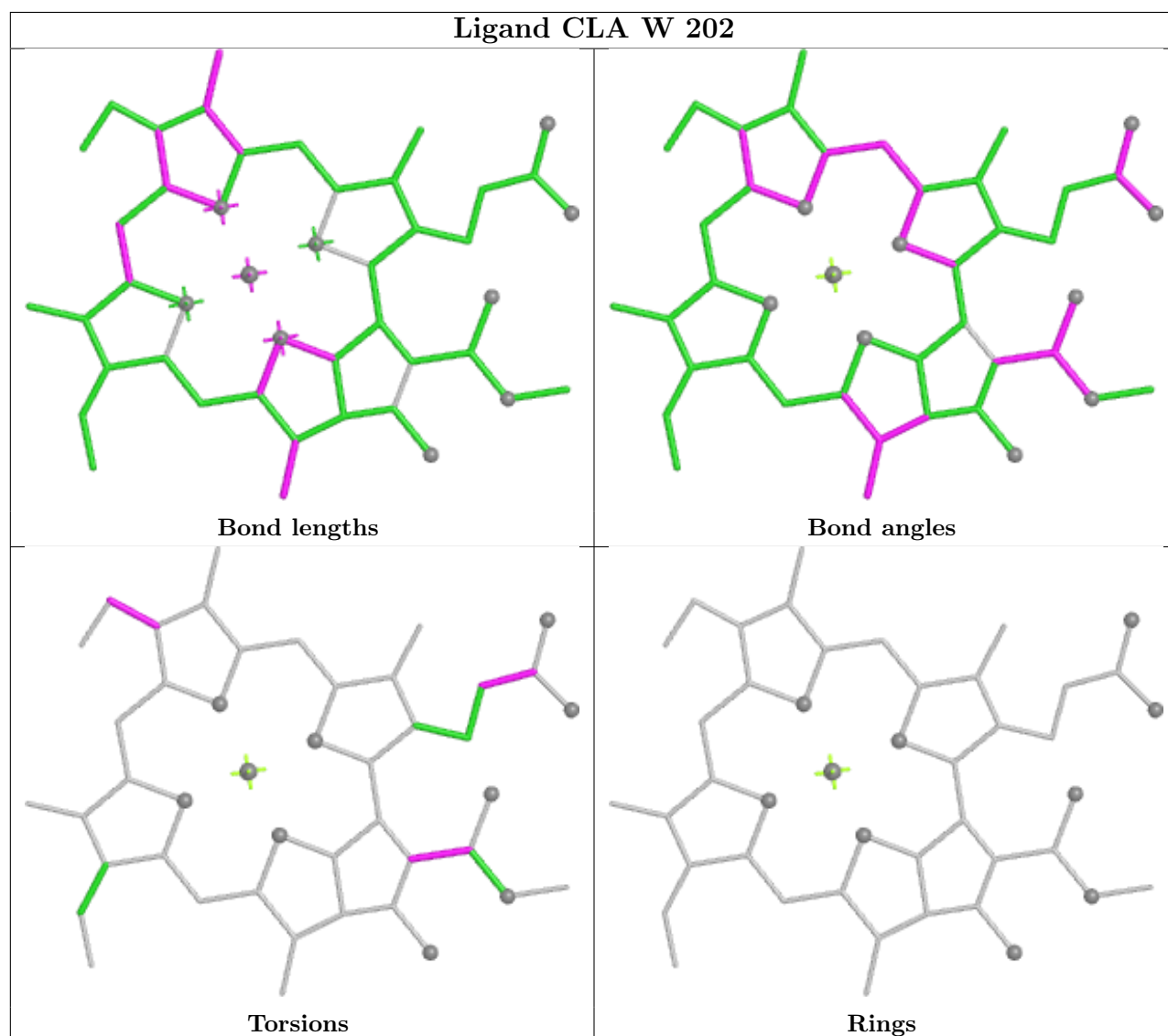
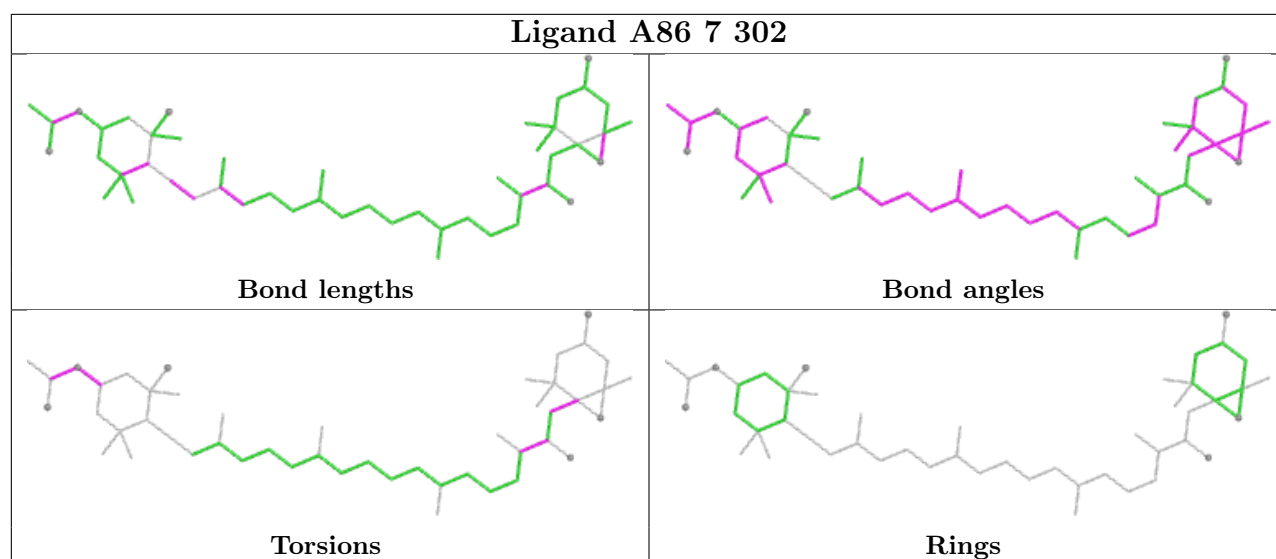
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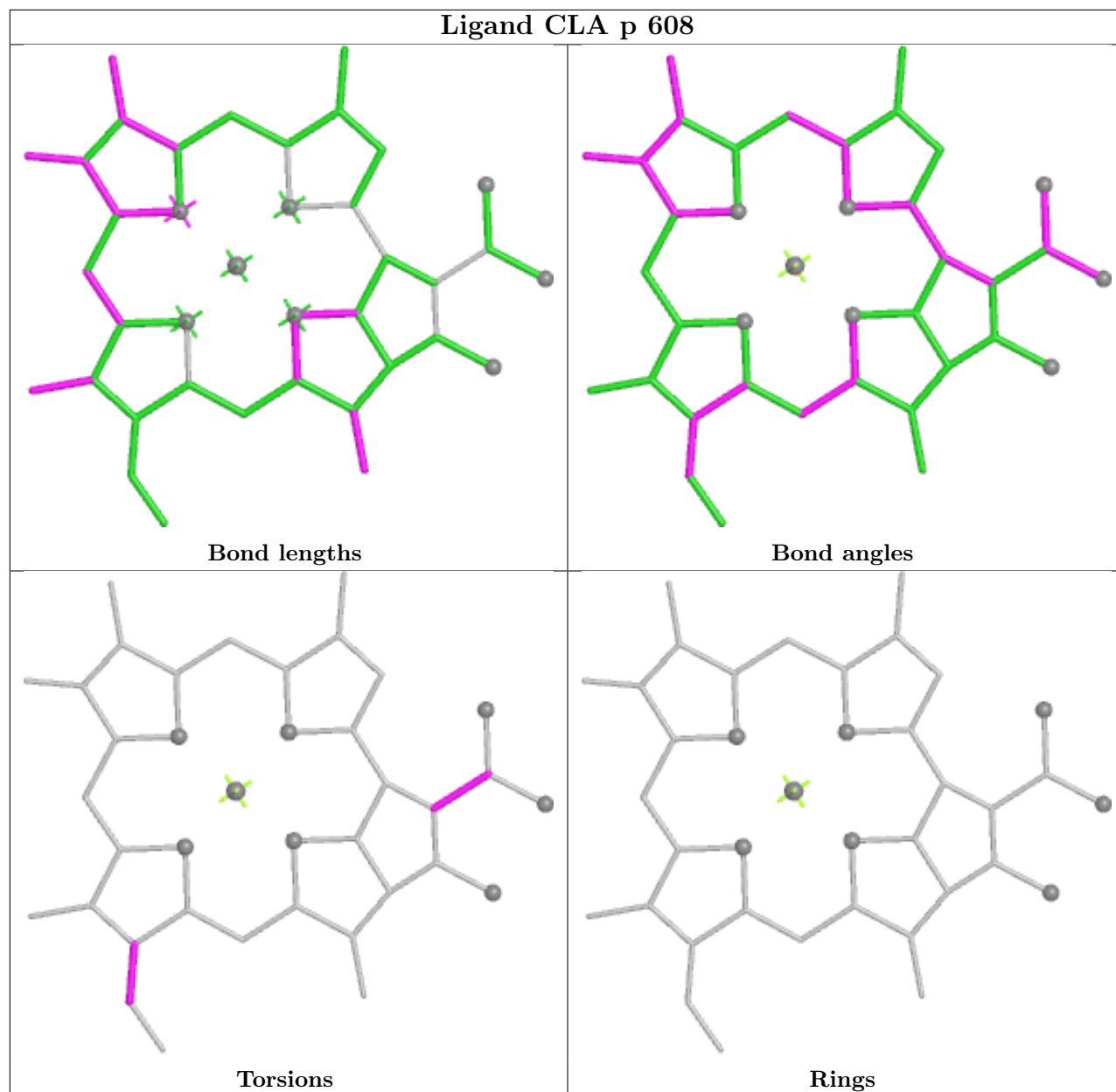
Ligand A86 9 202



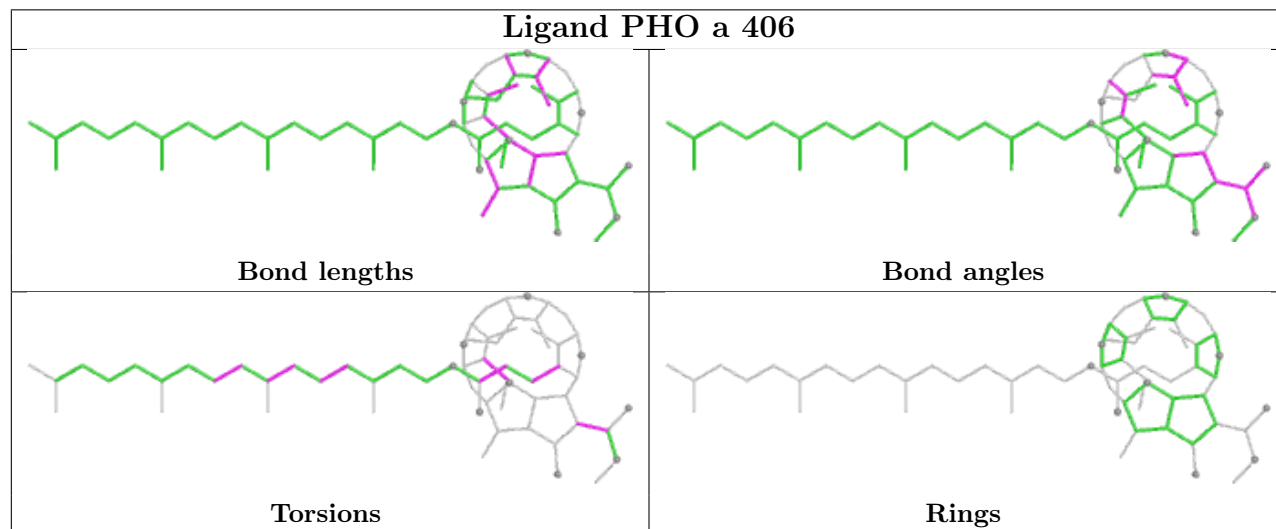


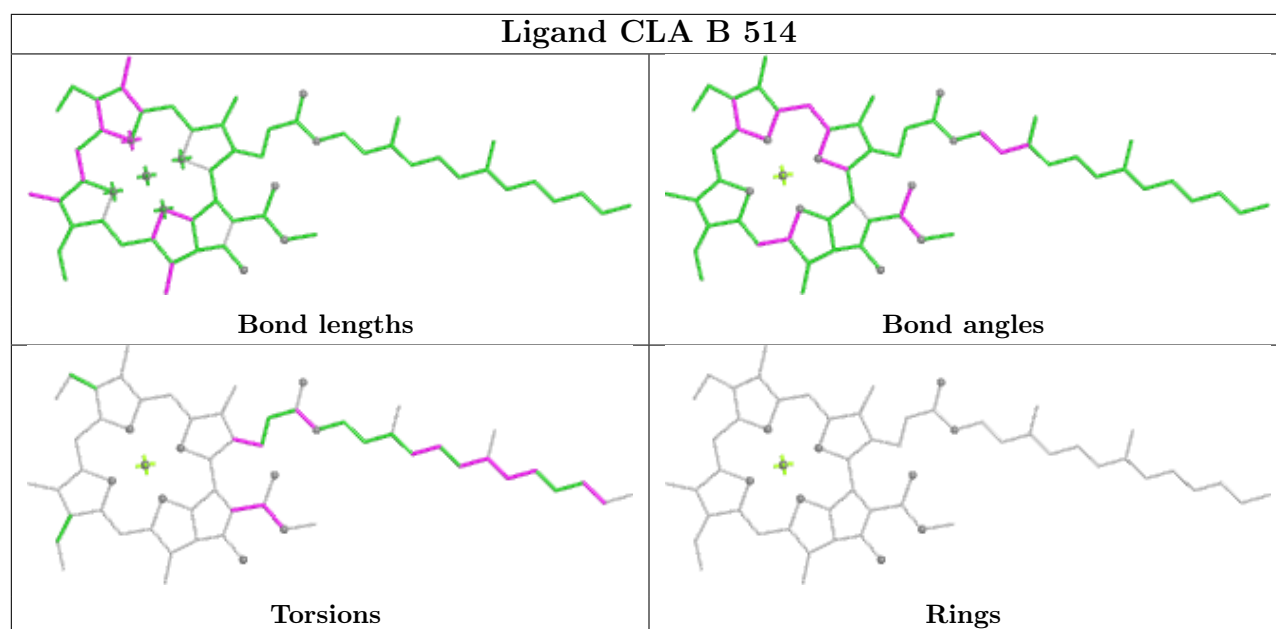
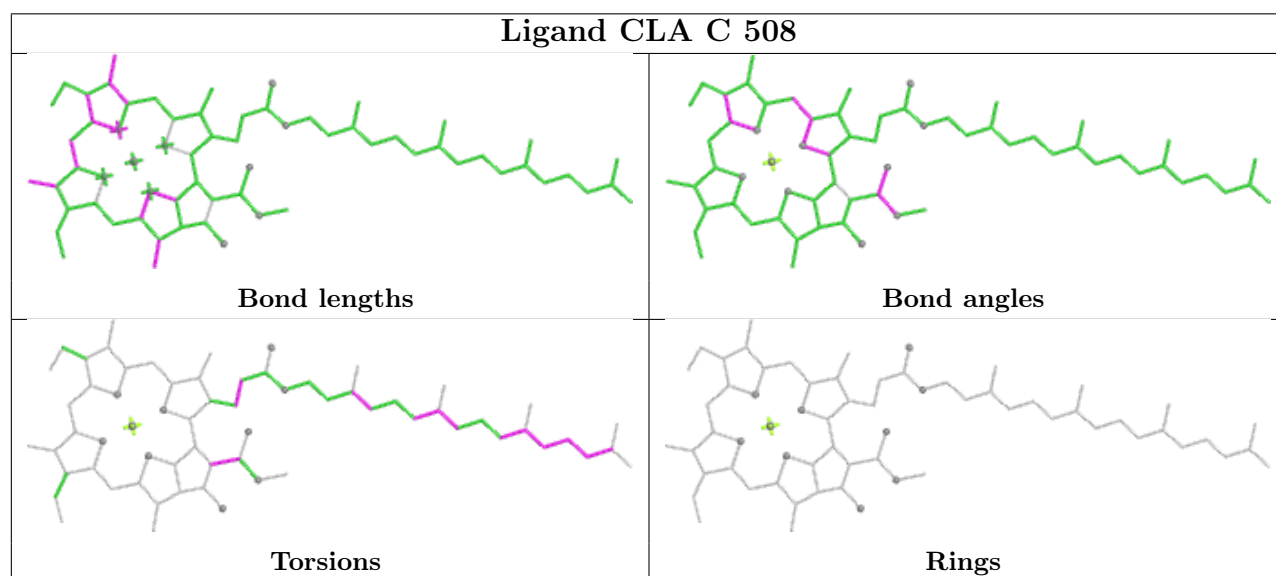
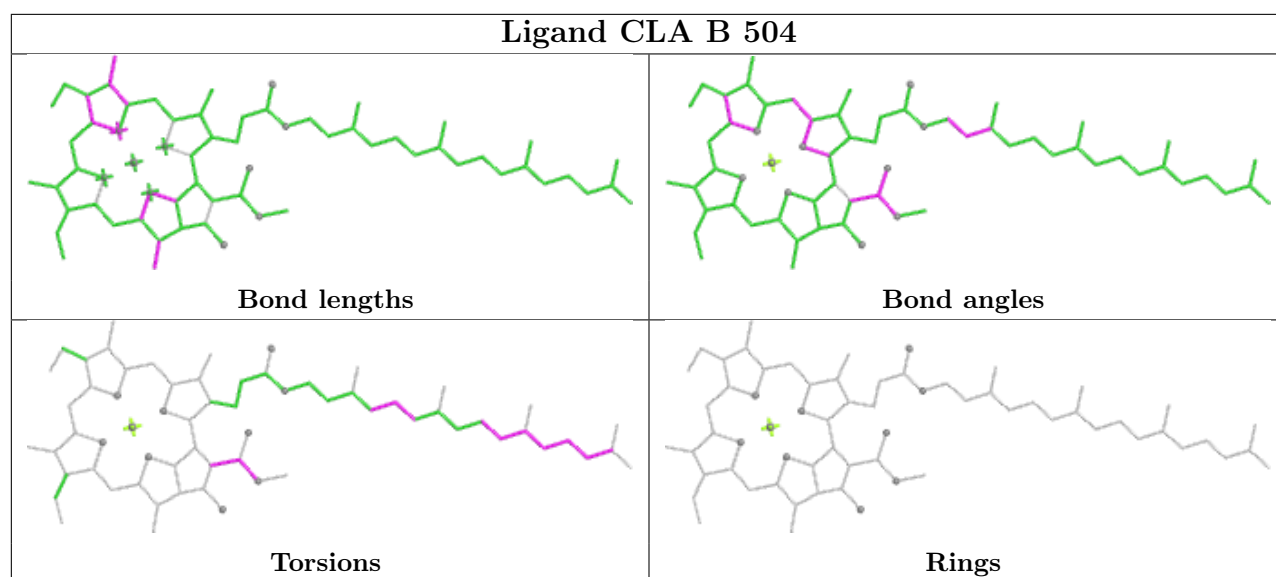


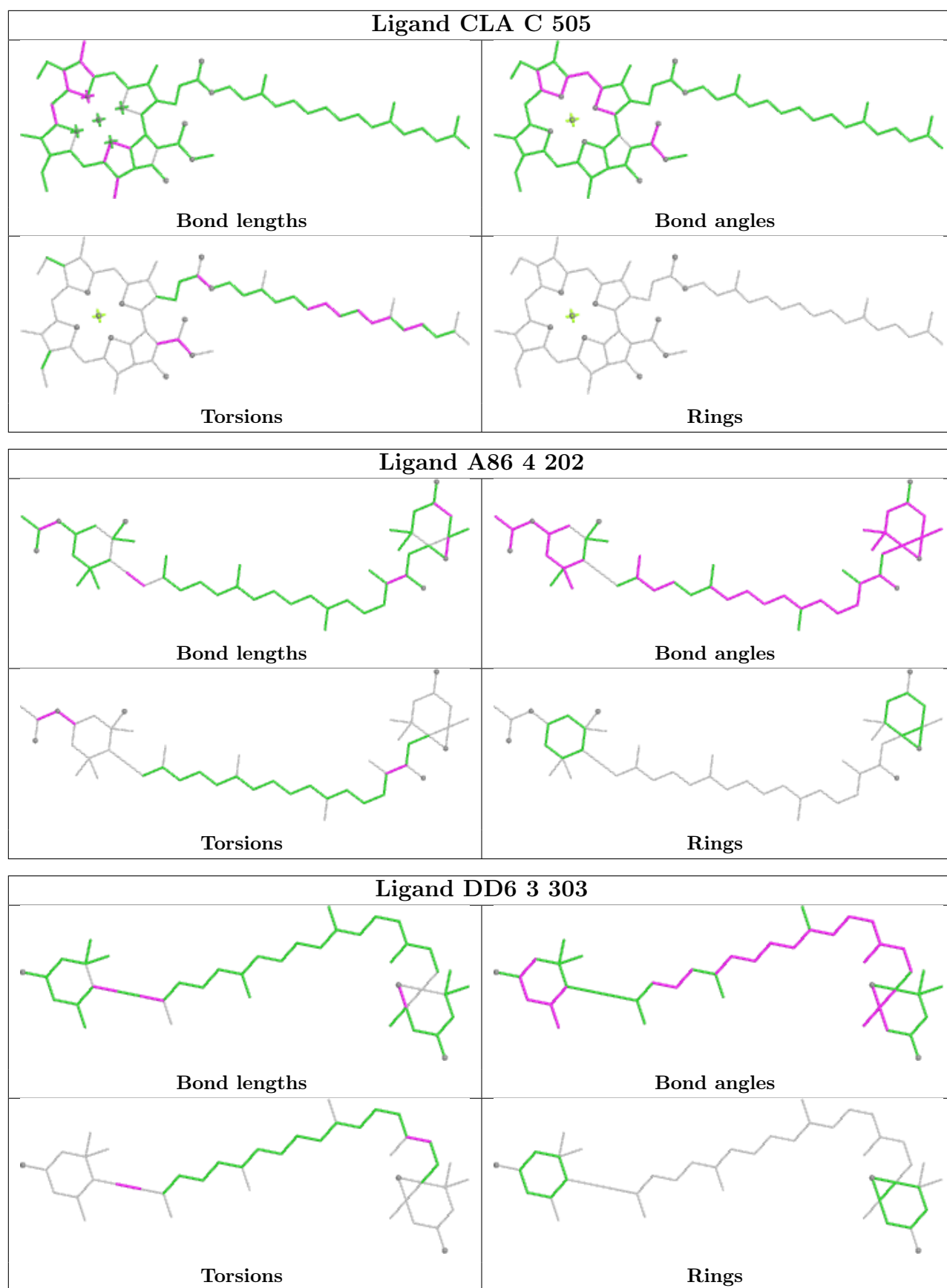
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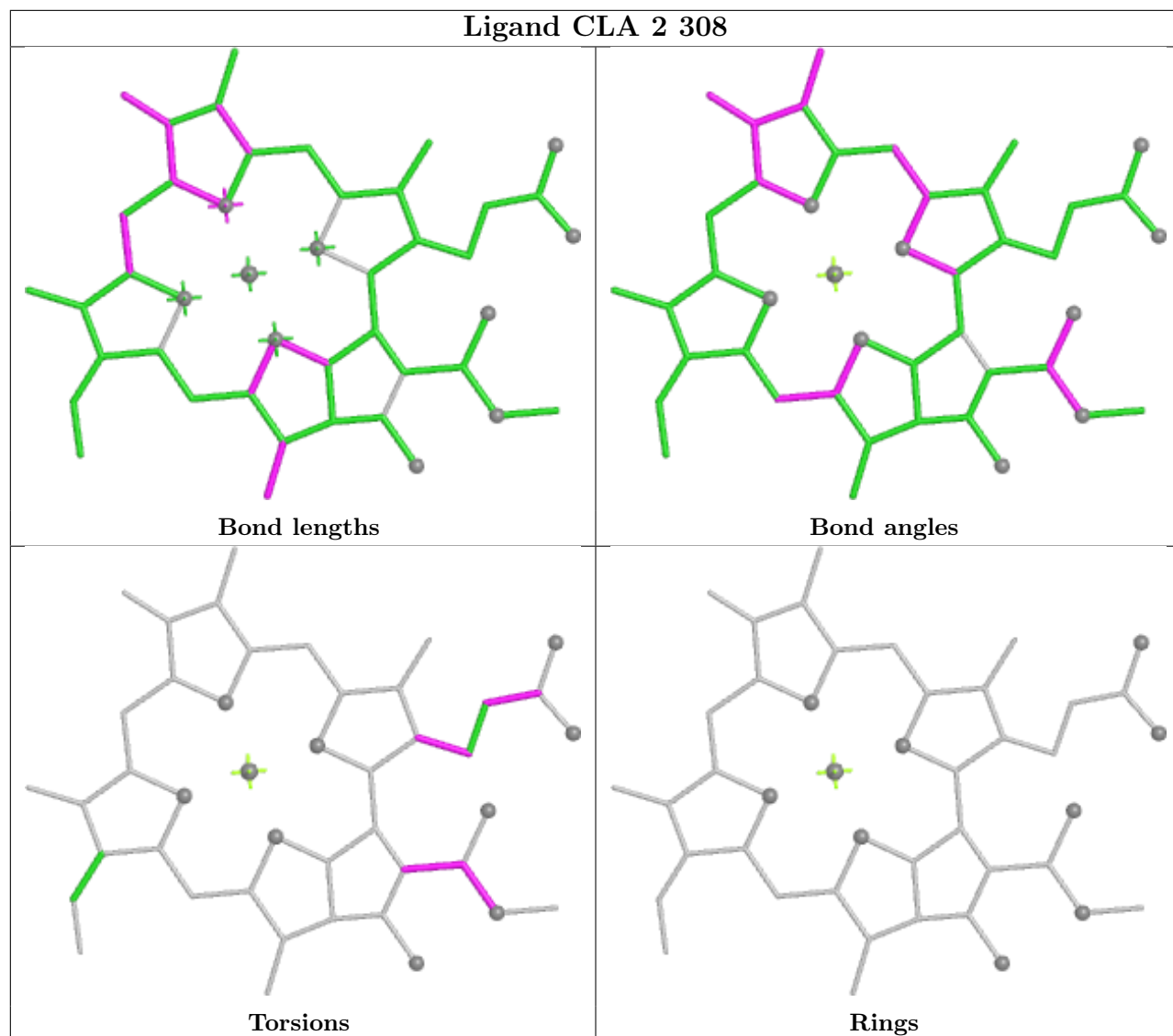
Ligand PHO a 406



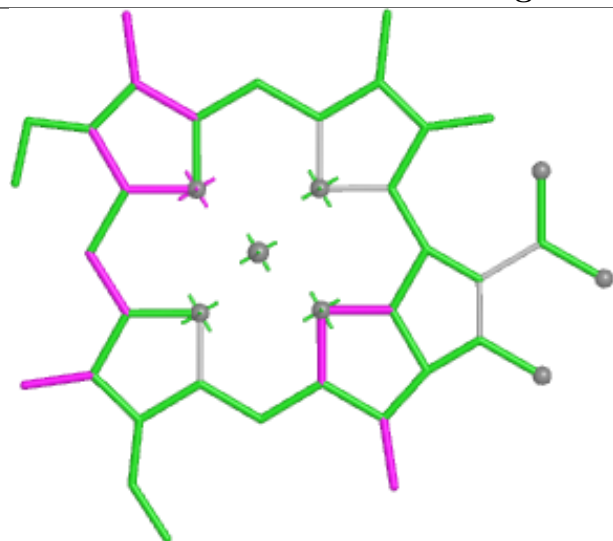




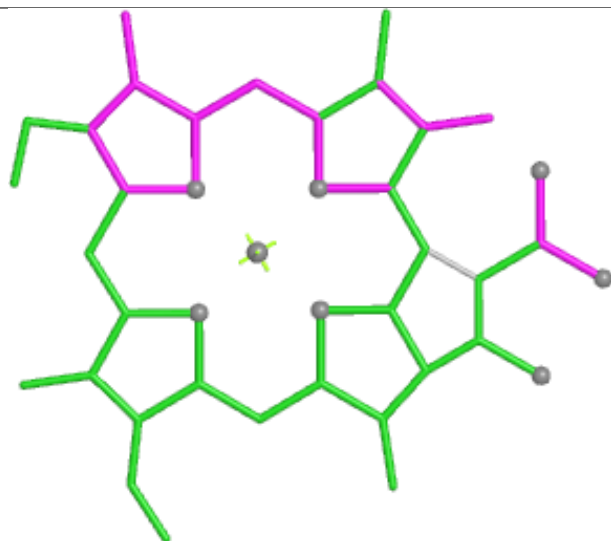
Ligand CLA 2 308



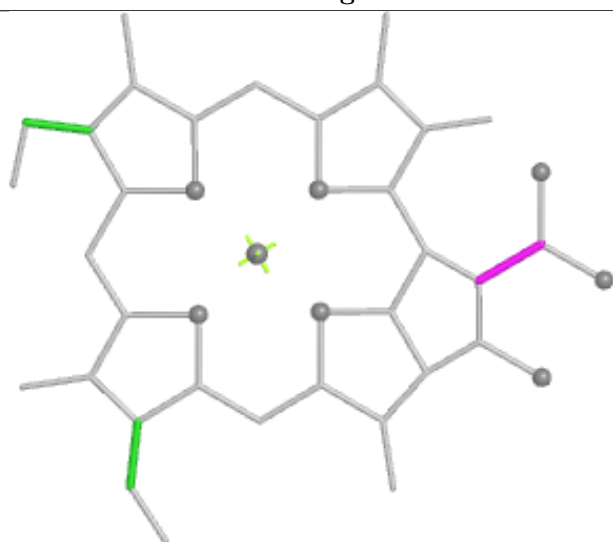
Ligand CLA P 604



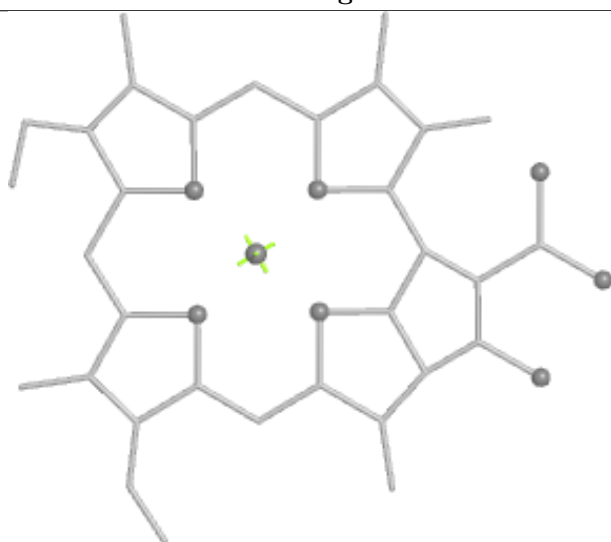
Bond lengths



Bond angles

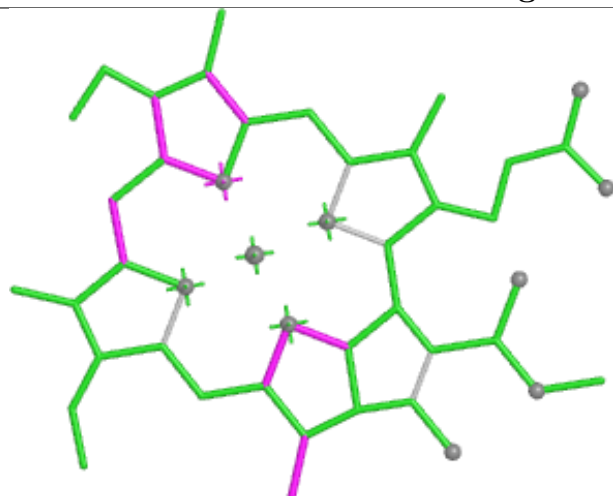


Torsions

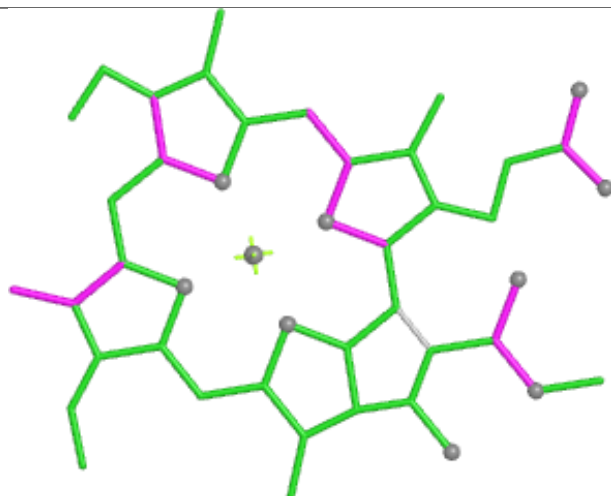


Rings

Ligand CLA 1 206



Bond lengths



Bond angles

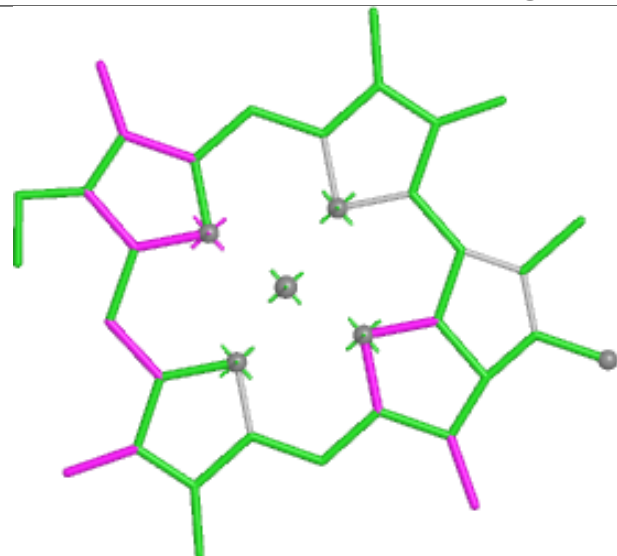


Torsions



Rings

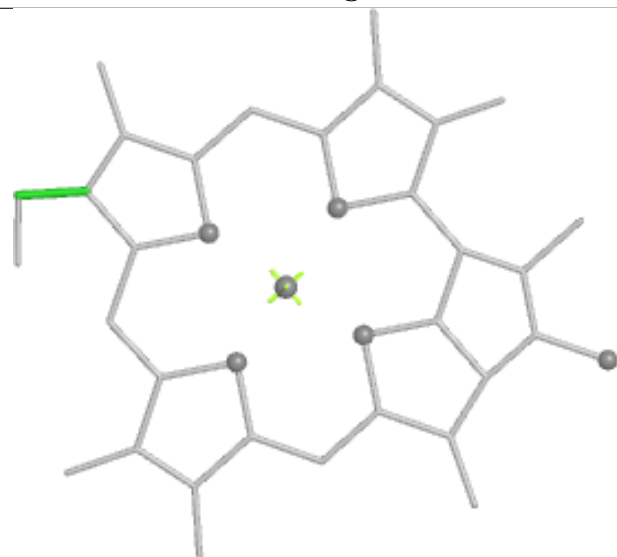
Ligand CLA p 603



Bond lengths



Bond angles

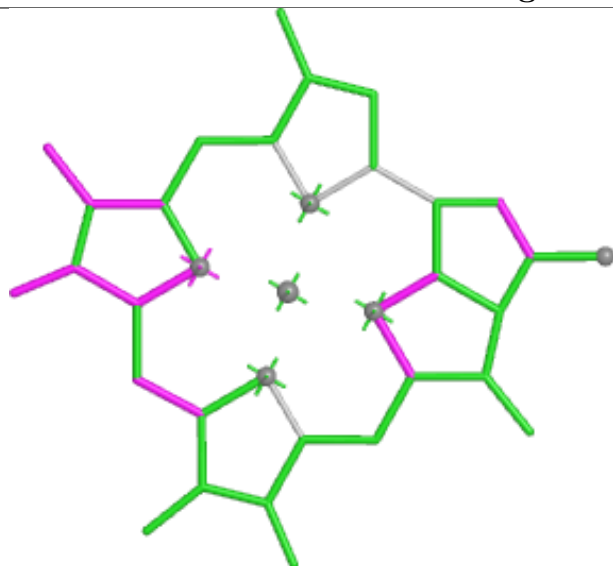


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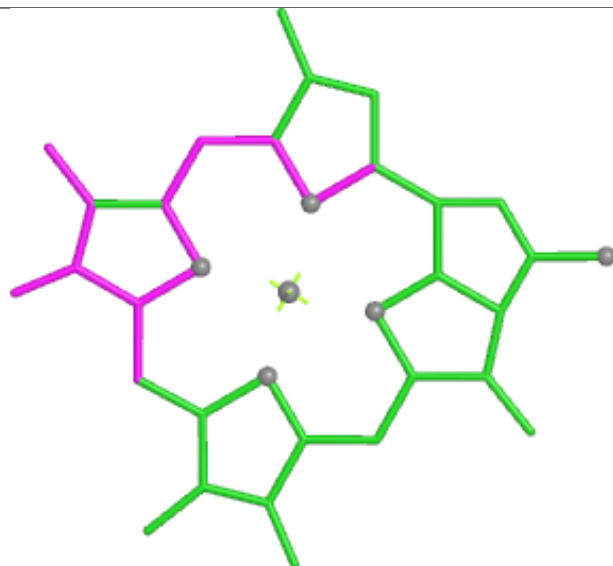


Rings

Ligand CLA 4 211



Bond lengths



Bond angles

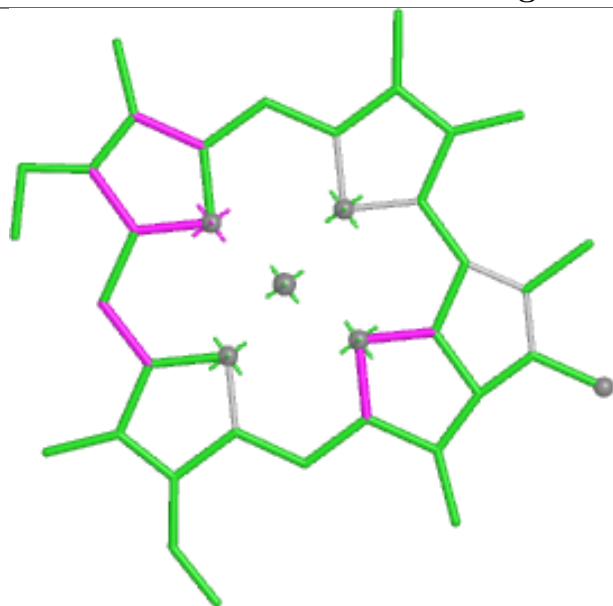


Torsions

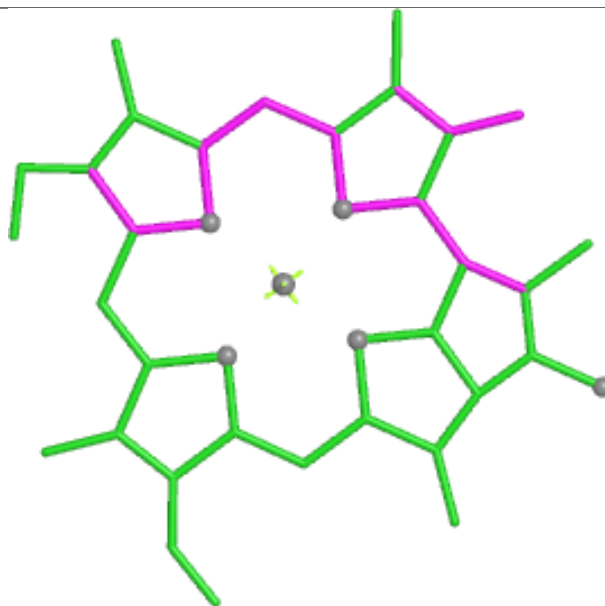


Rings

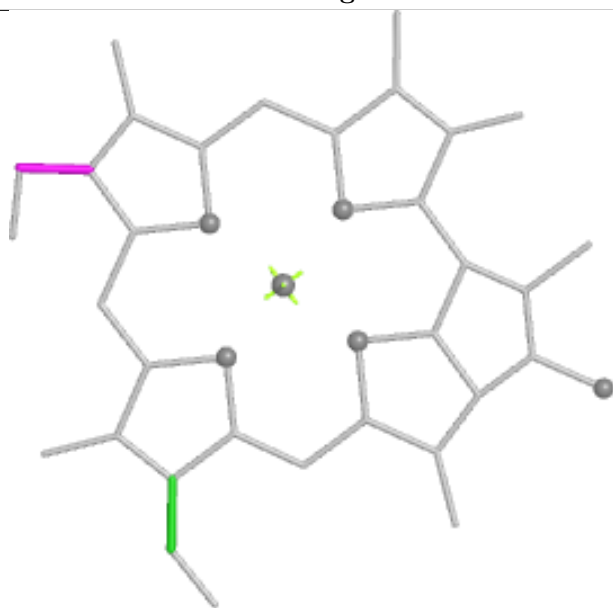
Ligand CLA 7 313



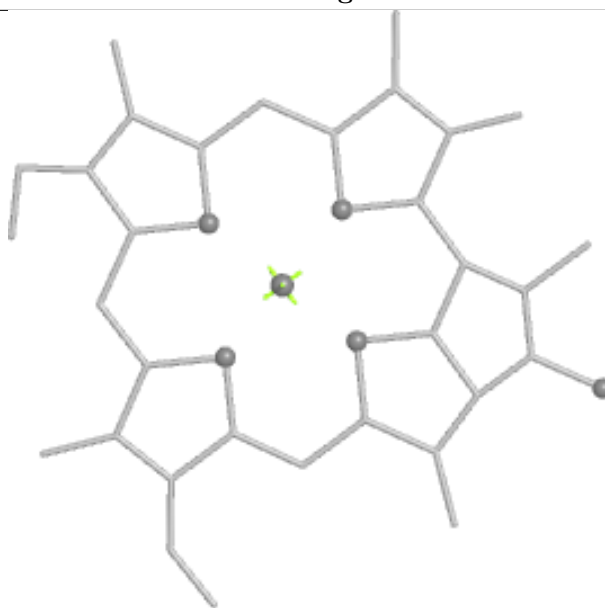
Bond lengths



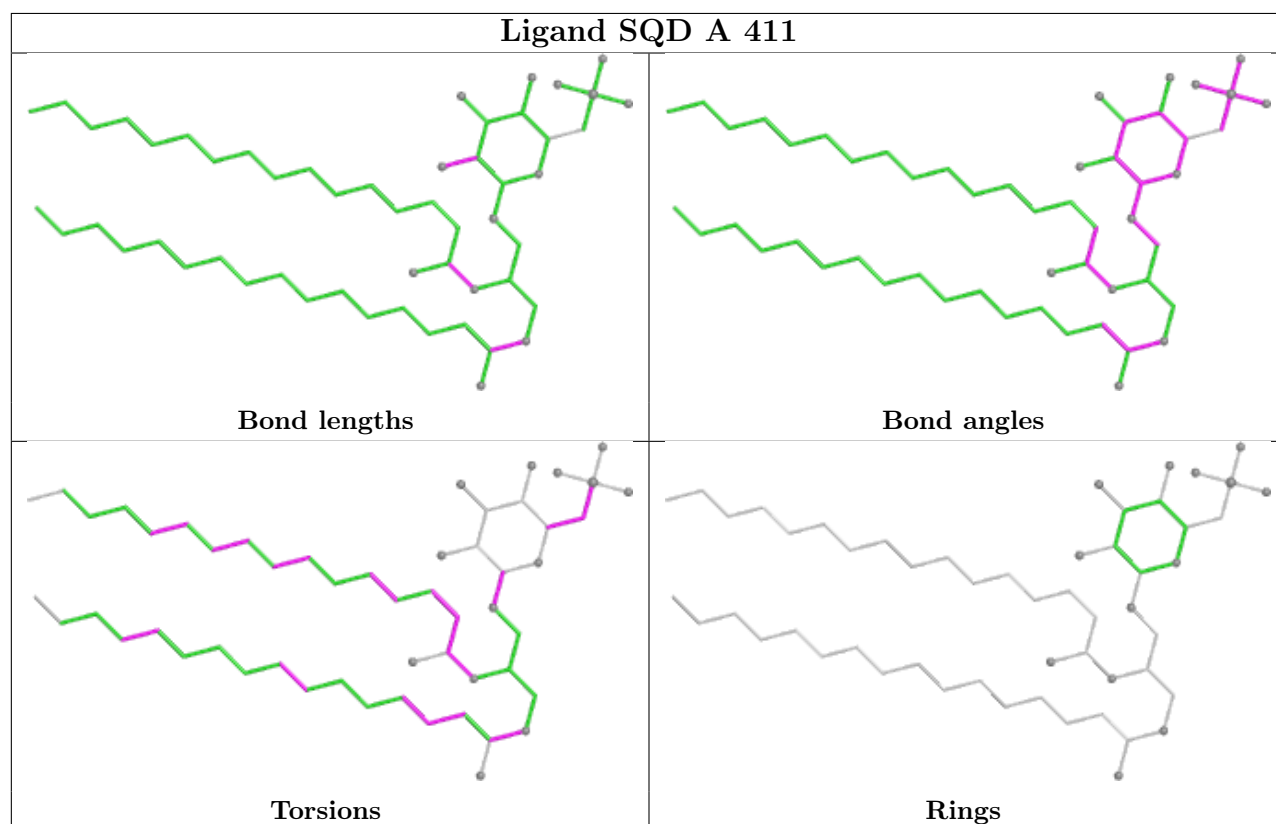
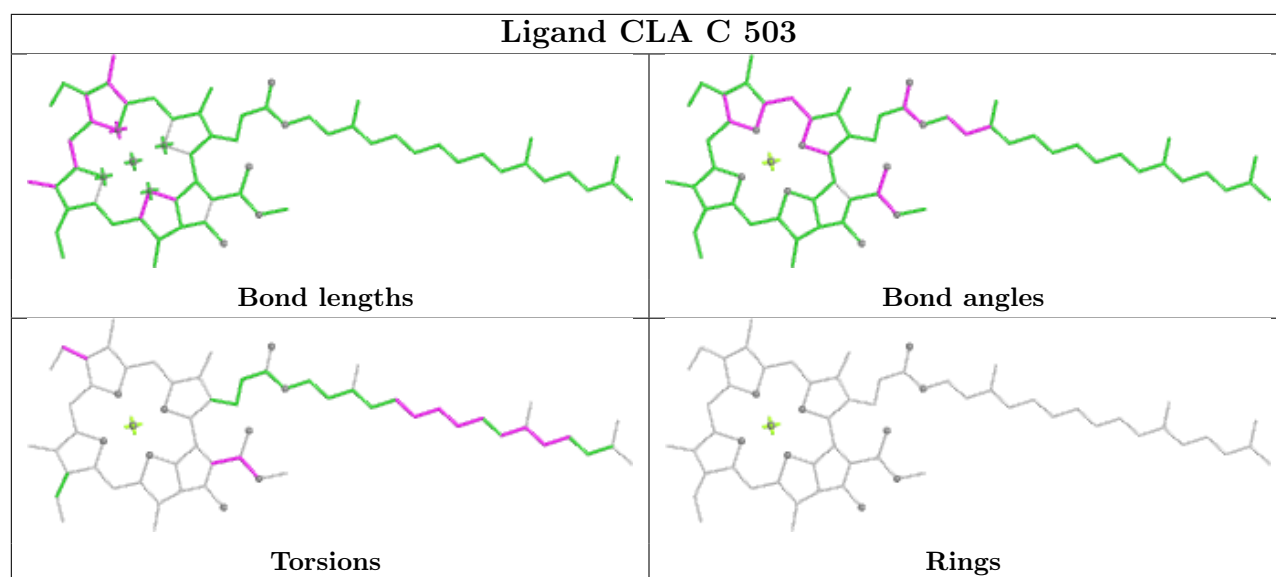
Bond angles



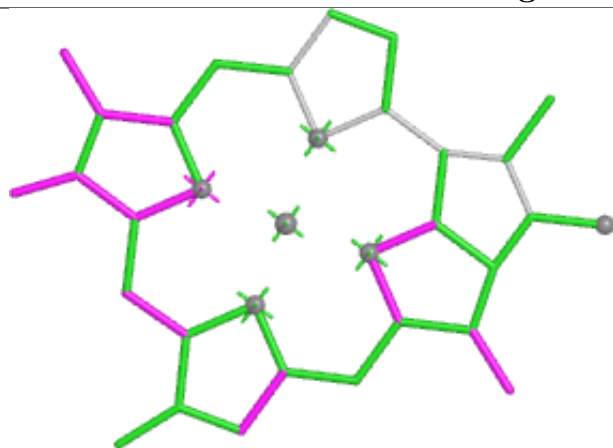
Torsions



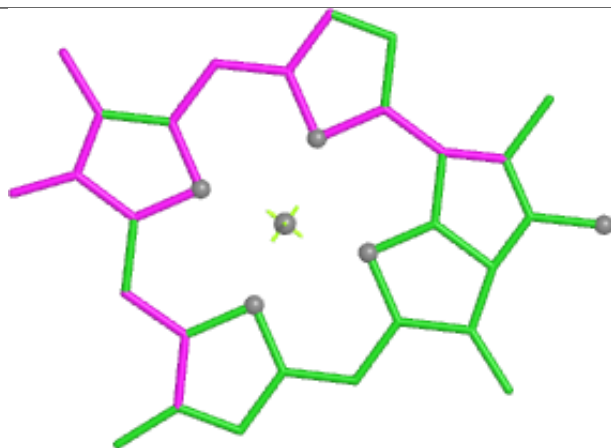
Rings



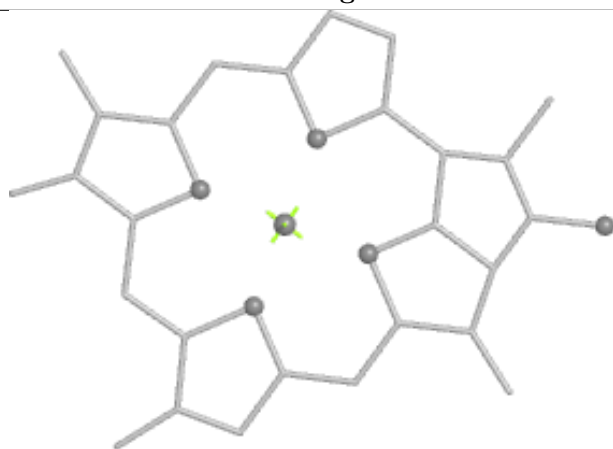
Ligand CLA 3 306



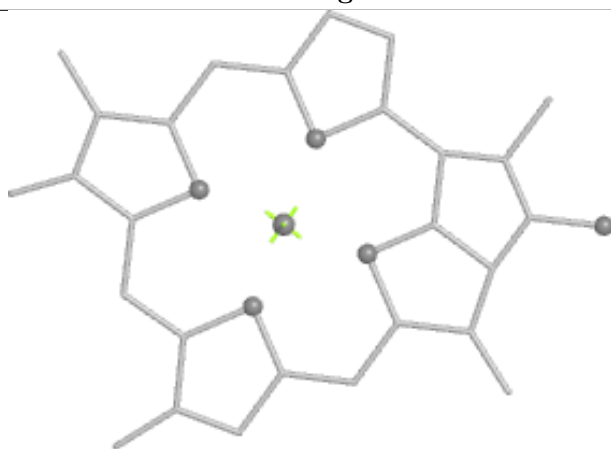
Bond lengths



Bond angles

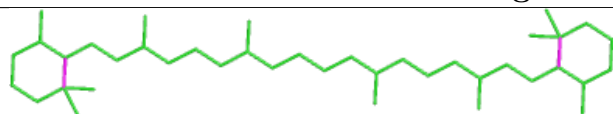


Torsions

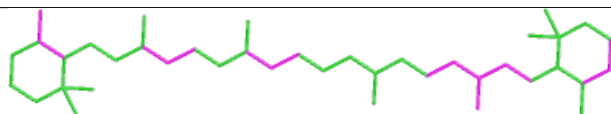


Rings

Ligand BCR B 519



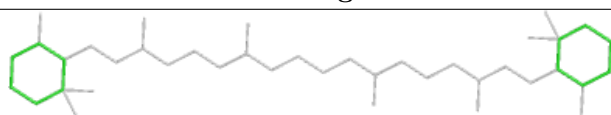
Bond lengths



Bond angles

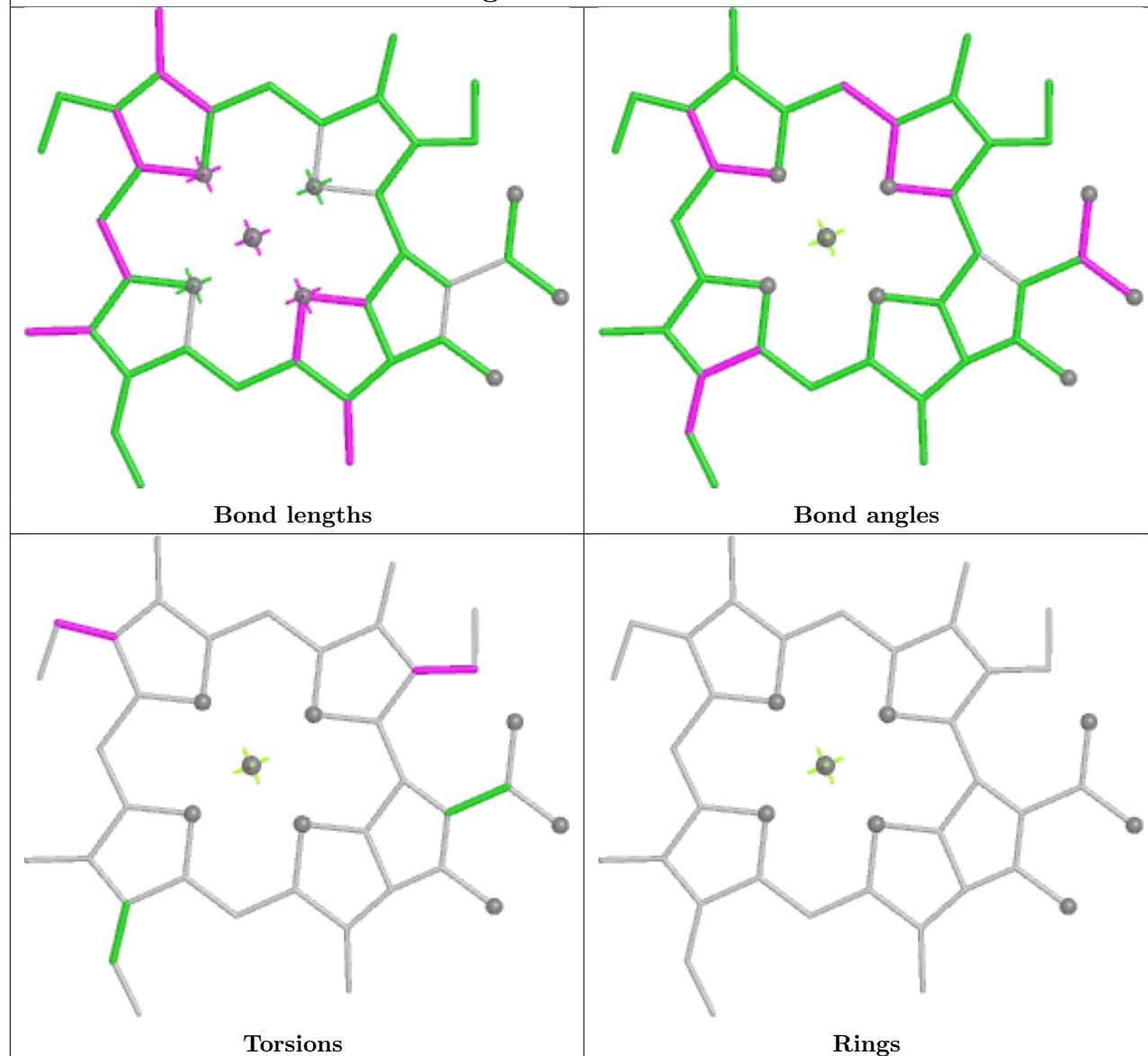


Torsions

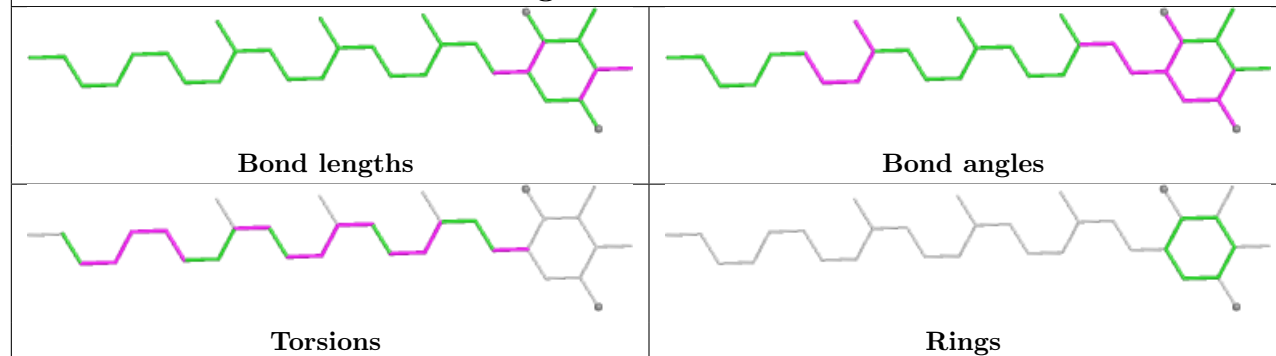


Rings

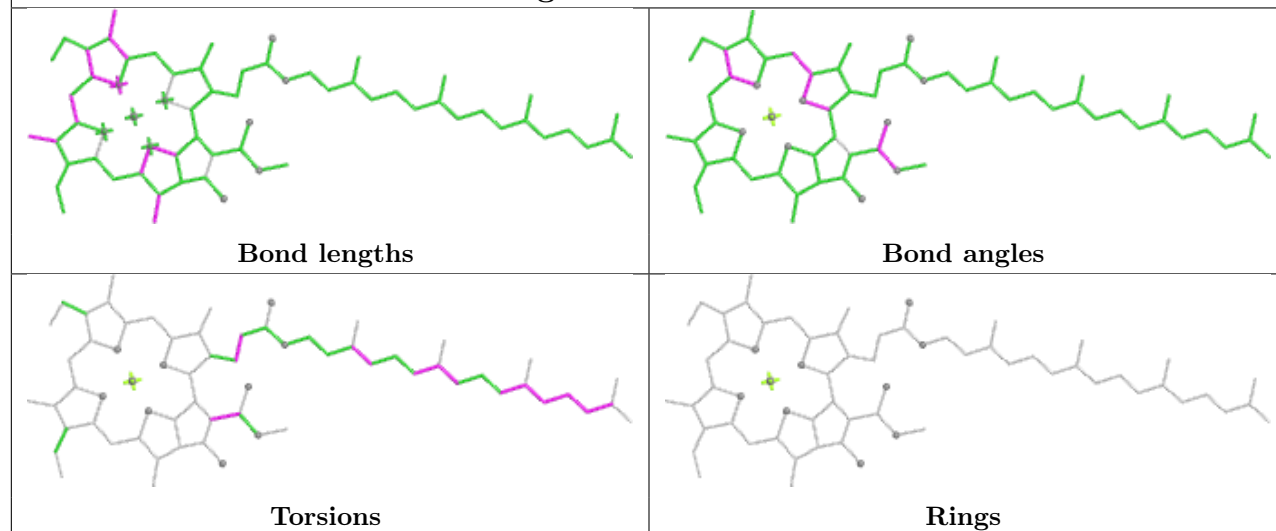
Ligand CLA 3 305



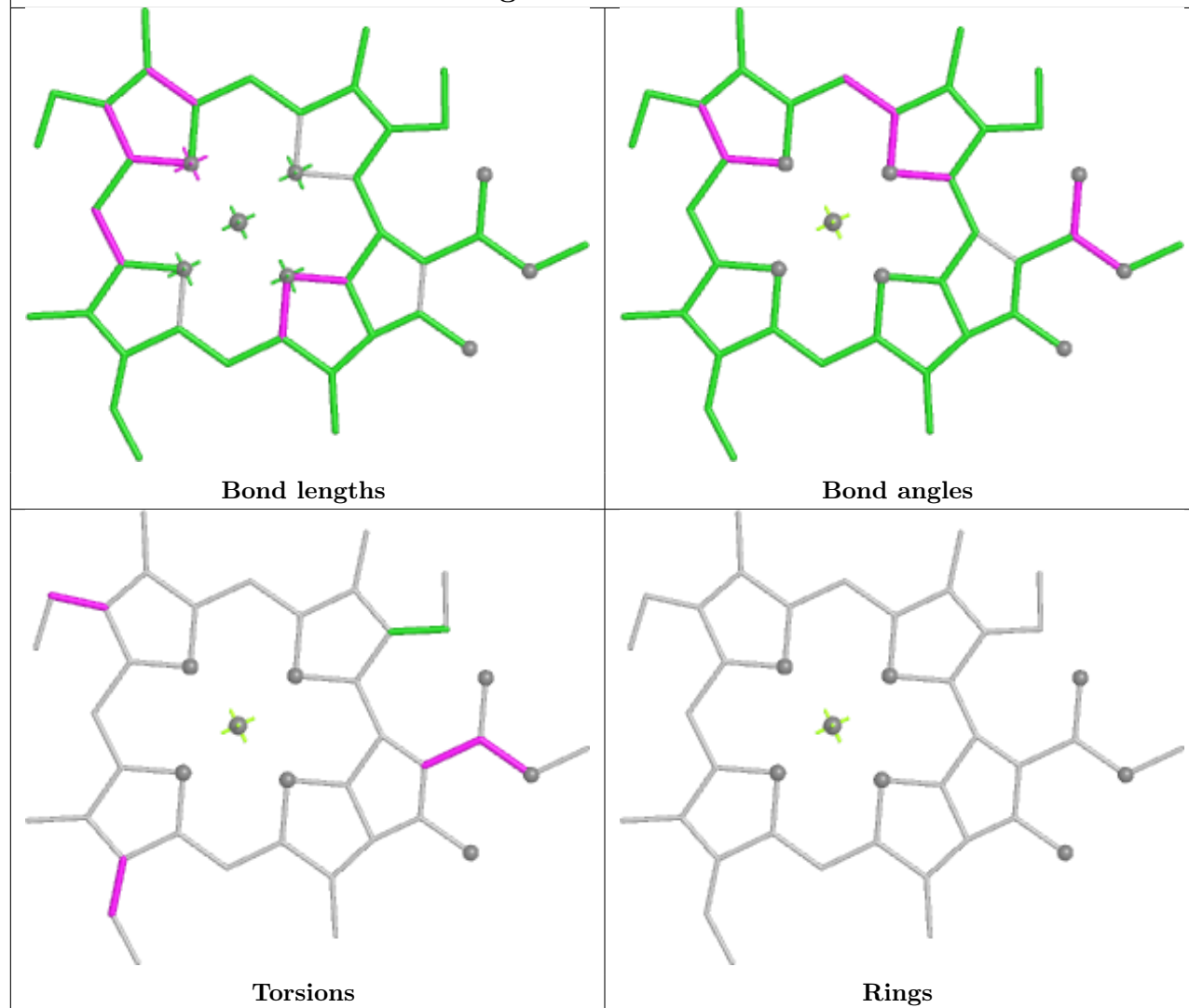
Ligand PL9 A 410



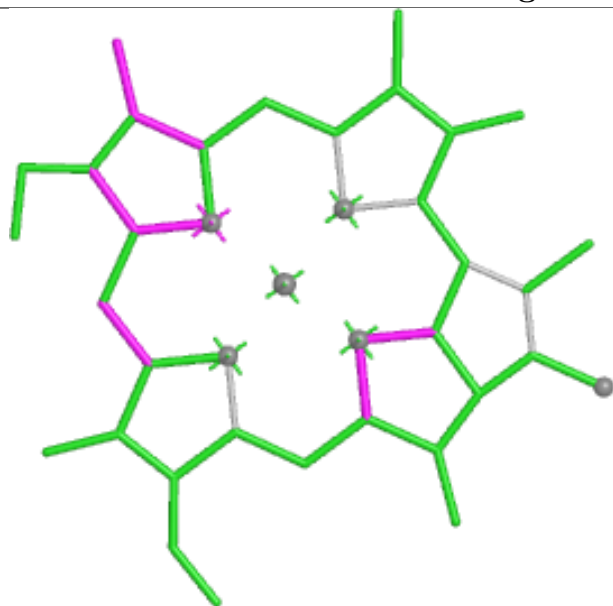
Ligand CLA c 508



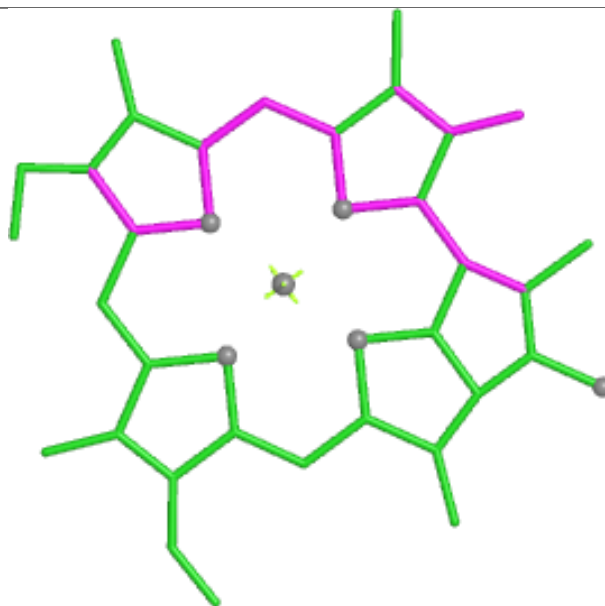
Ligand CLA 0 312



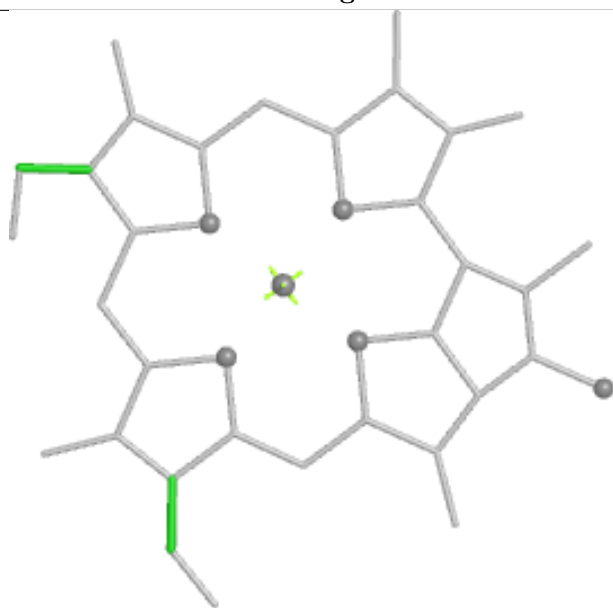
Ligand CLA 6 215



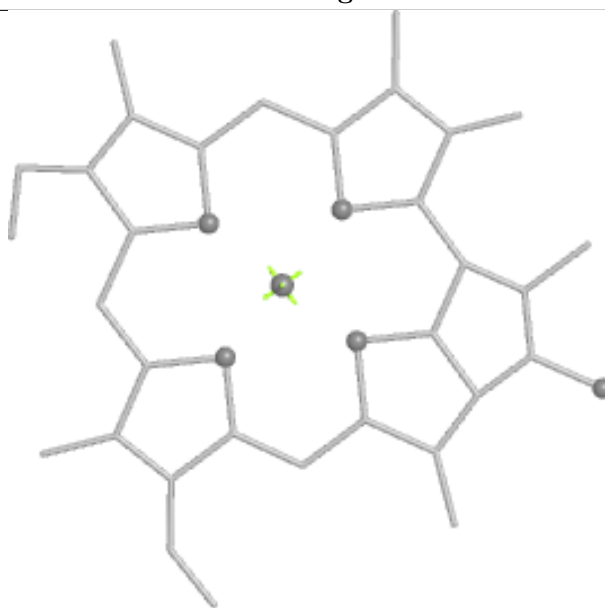
Bond lengths



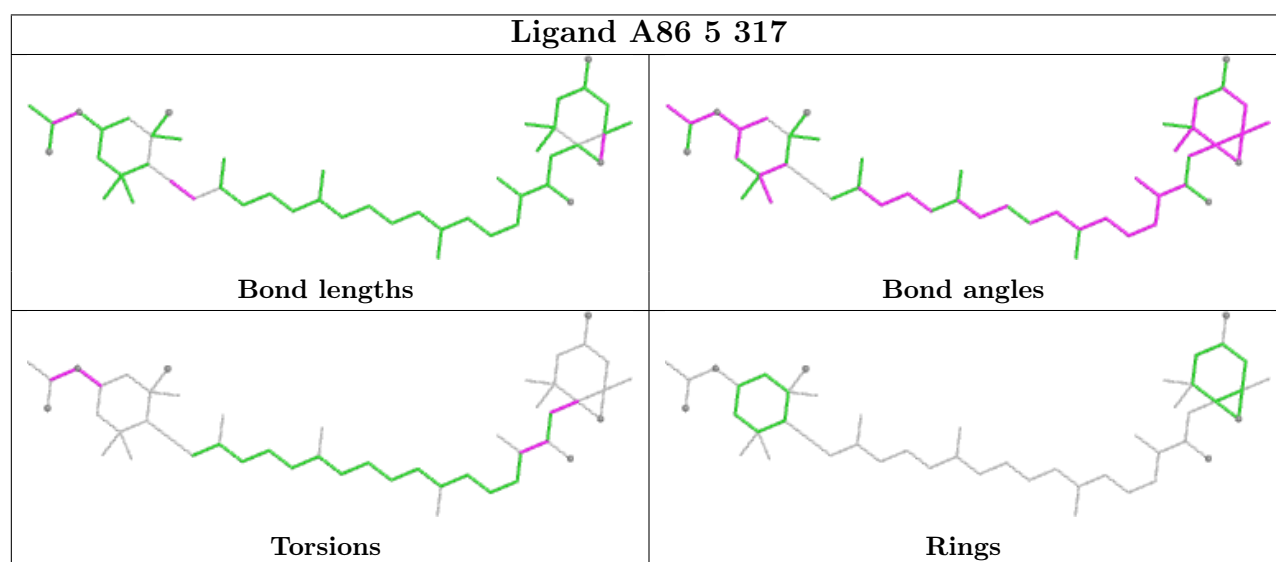
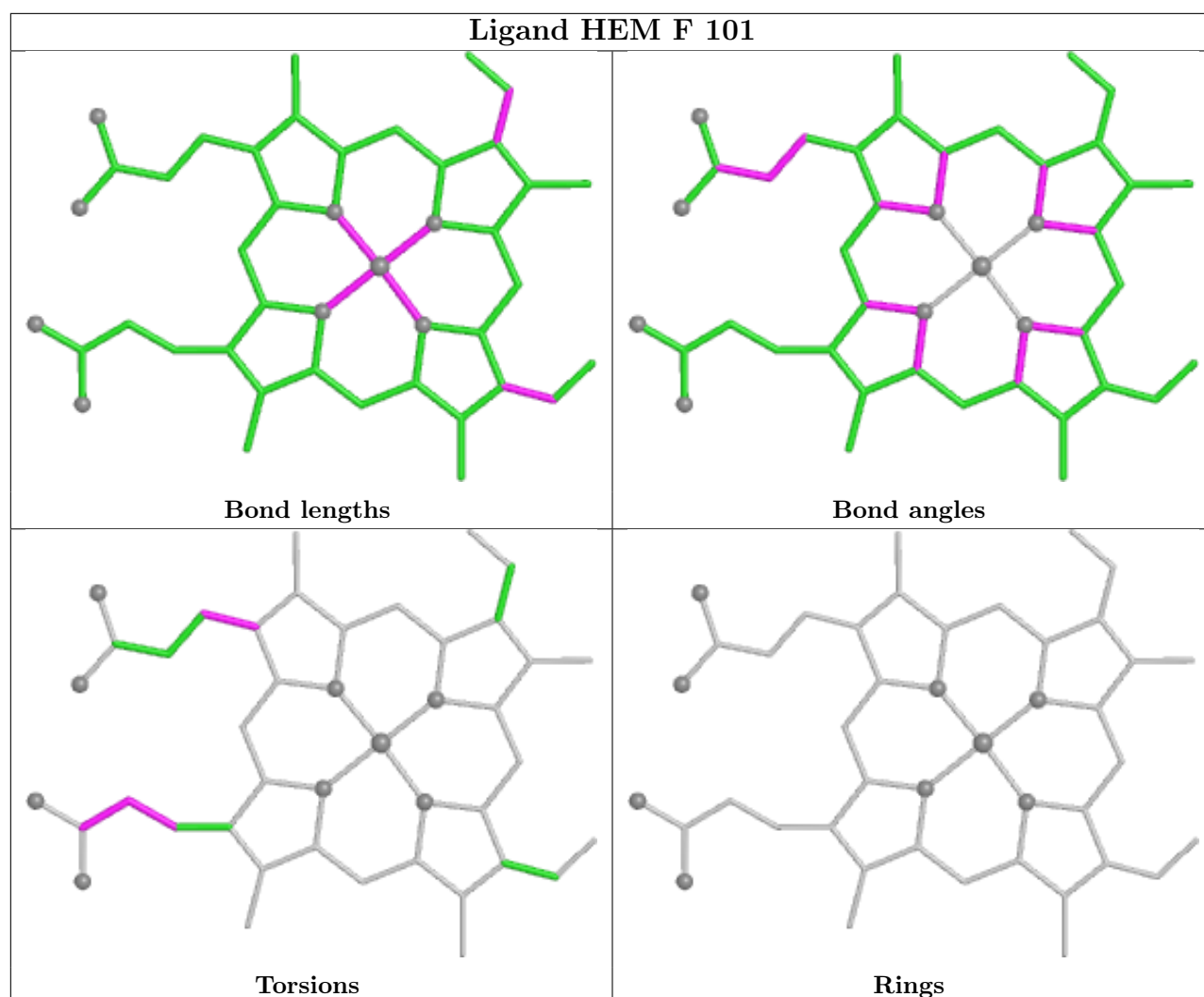
Bond angles

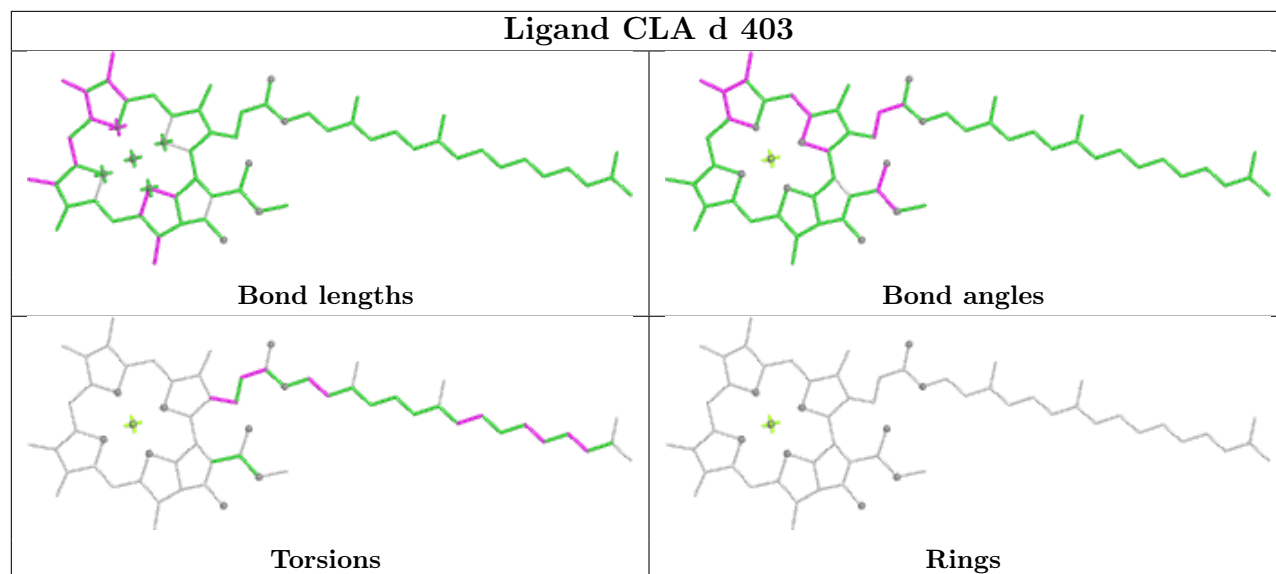
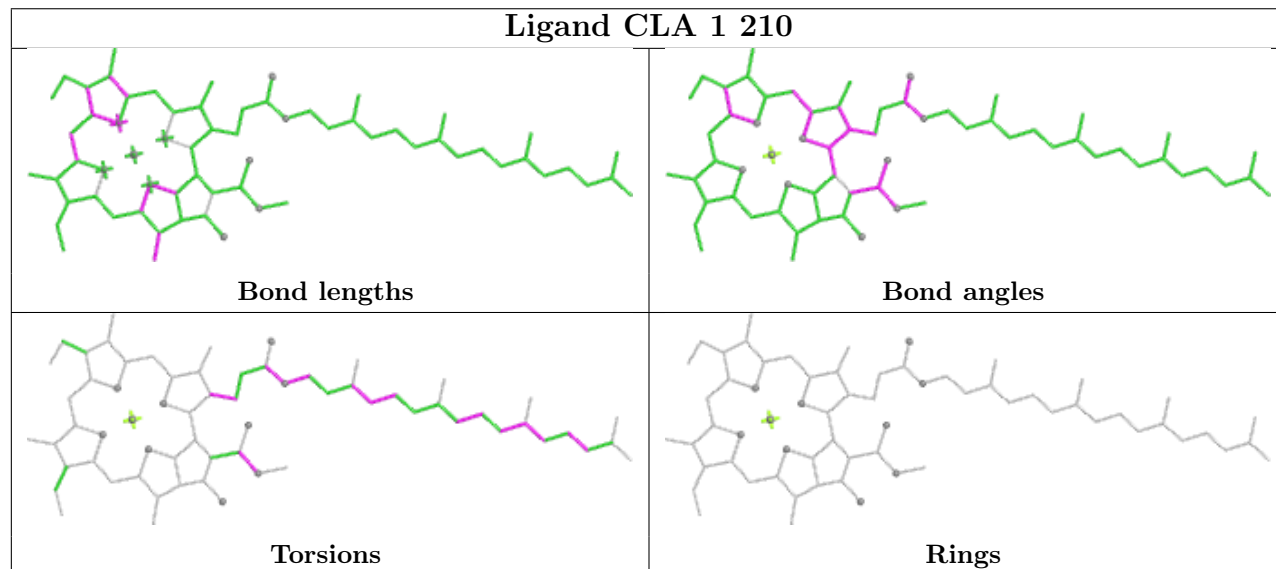


Torsions

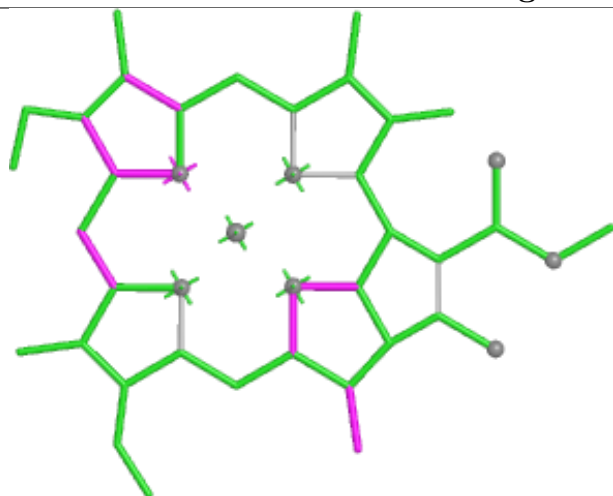


Rings

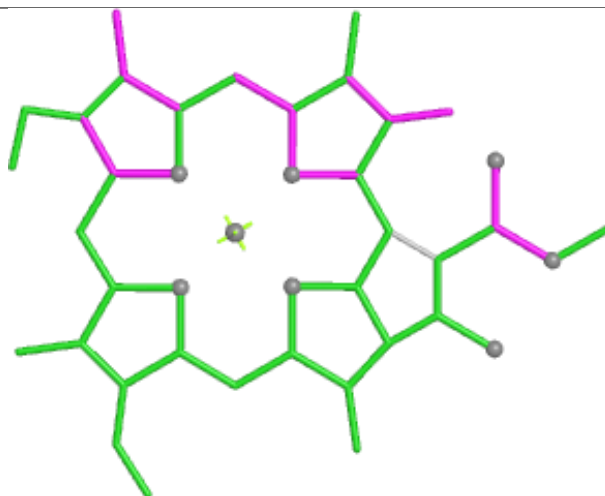


Ligand CLA d 403**Ligand CLA 1 210**

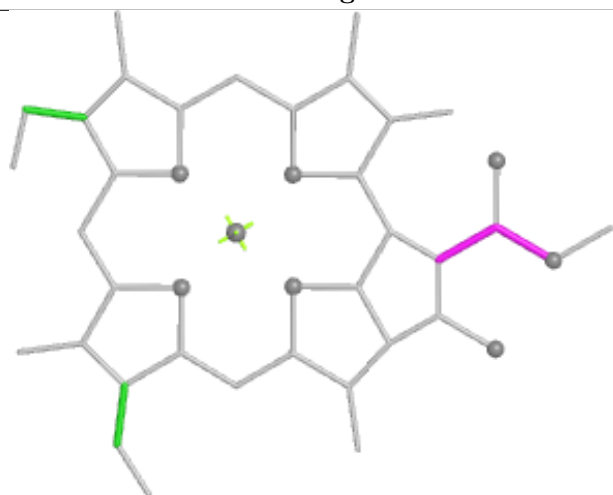
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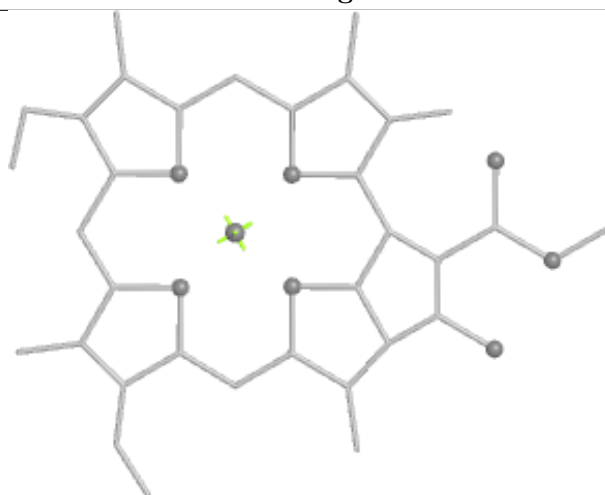
Bond lengths



Bond angles

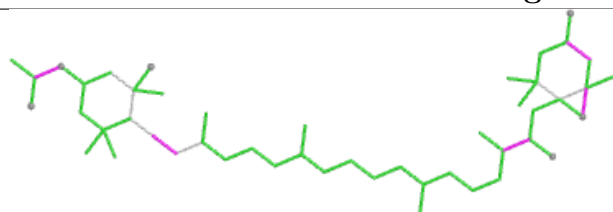


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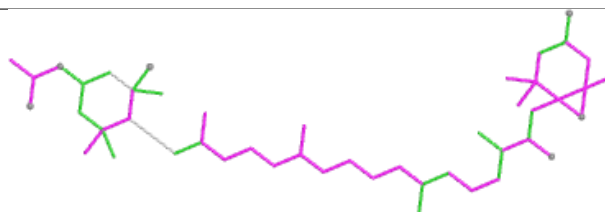


Rings

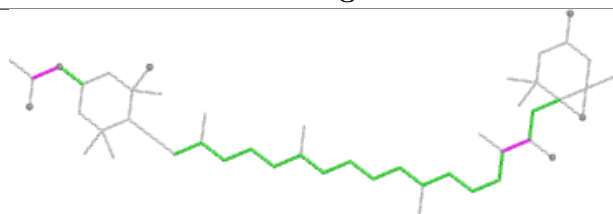
Ligand A86 3 302



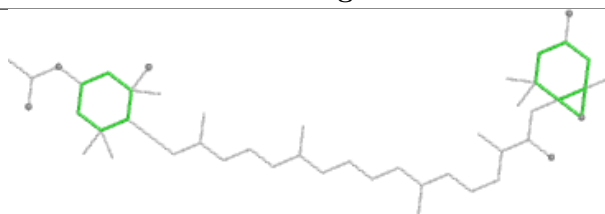
Bond lengths



Bond angles

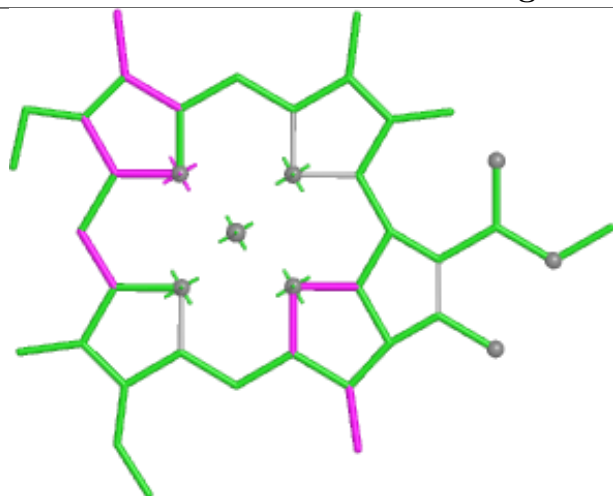


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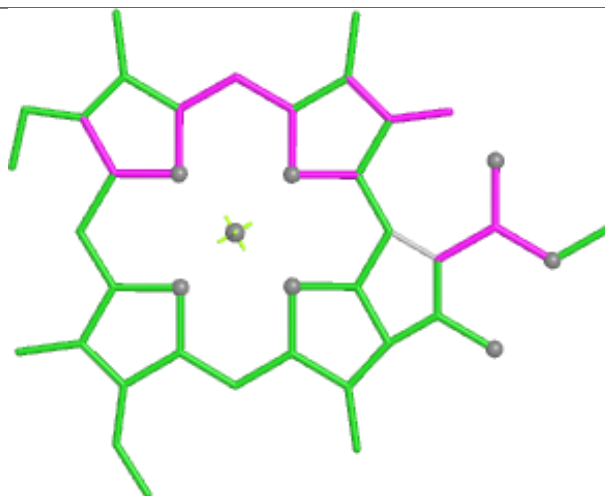


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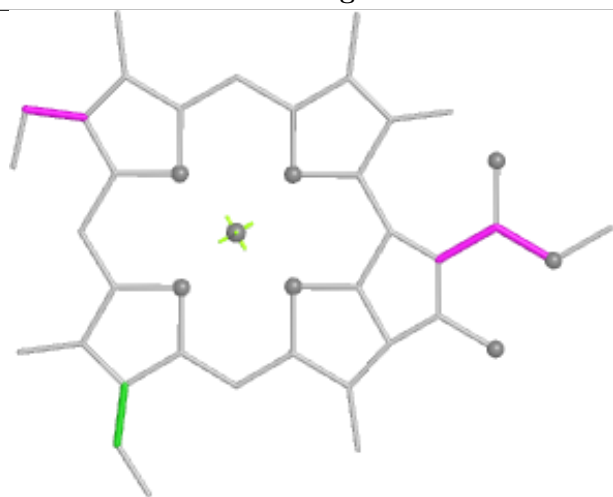
Ligand CLA 7 305



Bond lengths



Bond angles

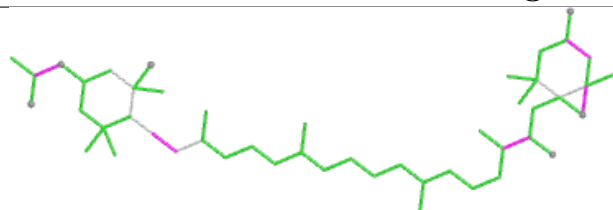


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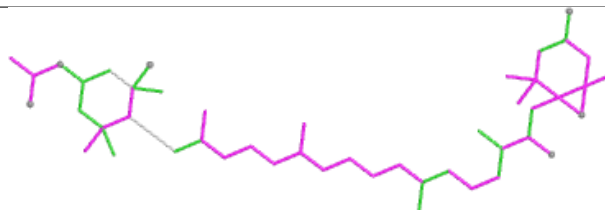


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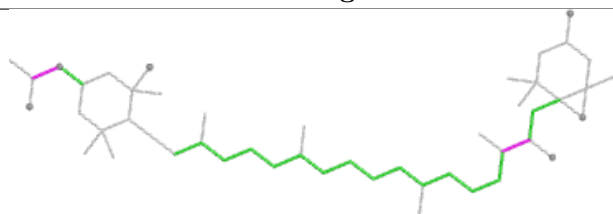
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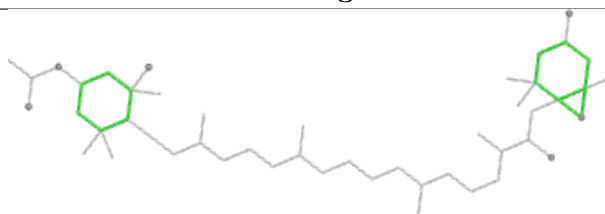
Bond lengths



Bond angles

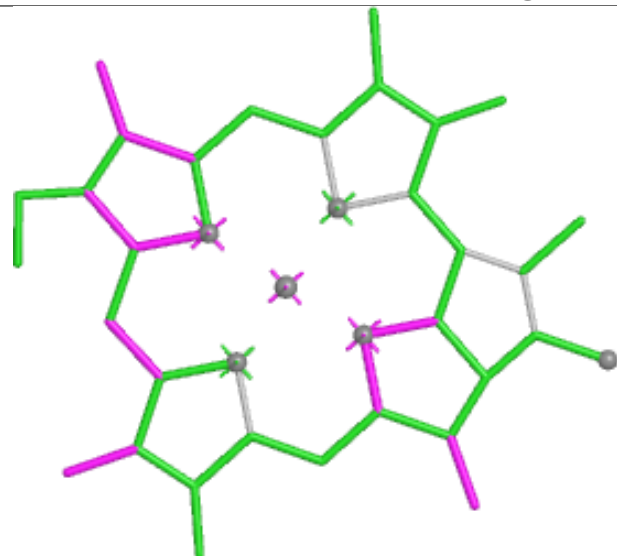


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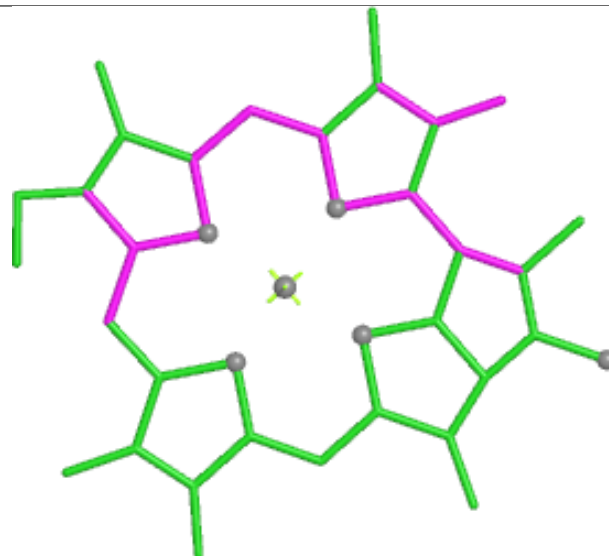


Rings

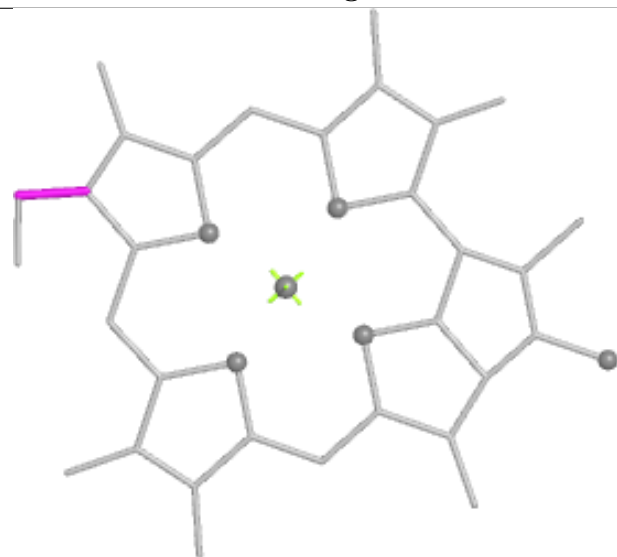
Ligand CLA P 605



Bond lengths



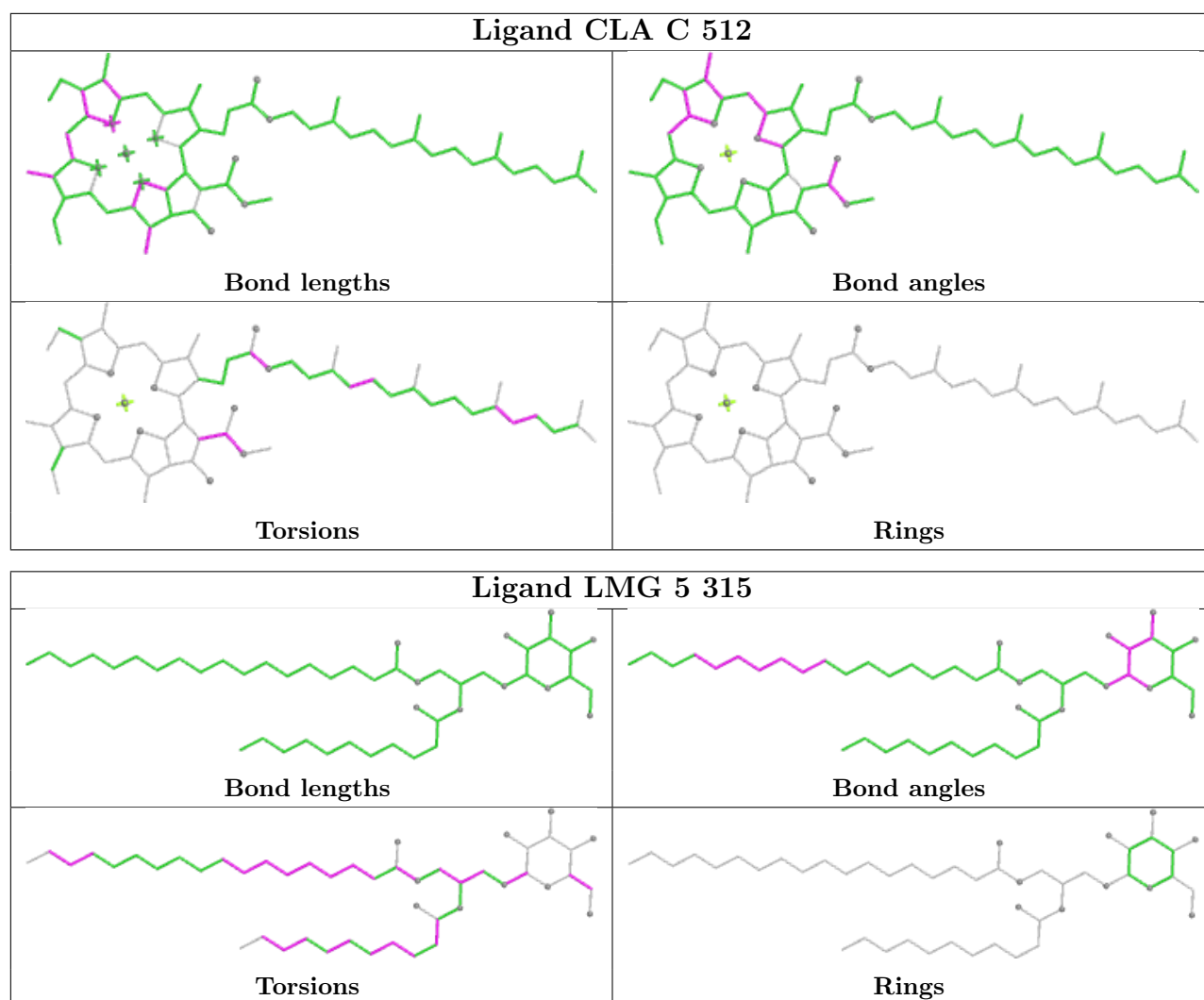
Bond angles



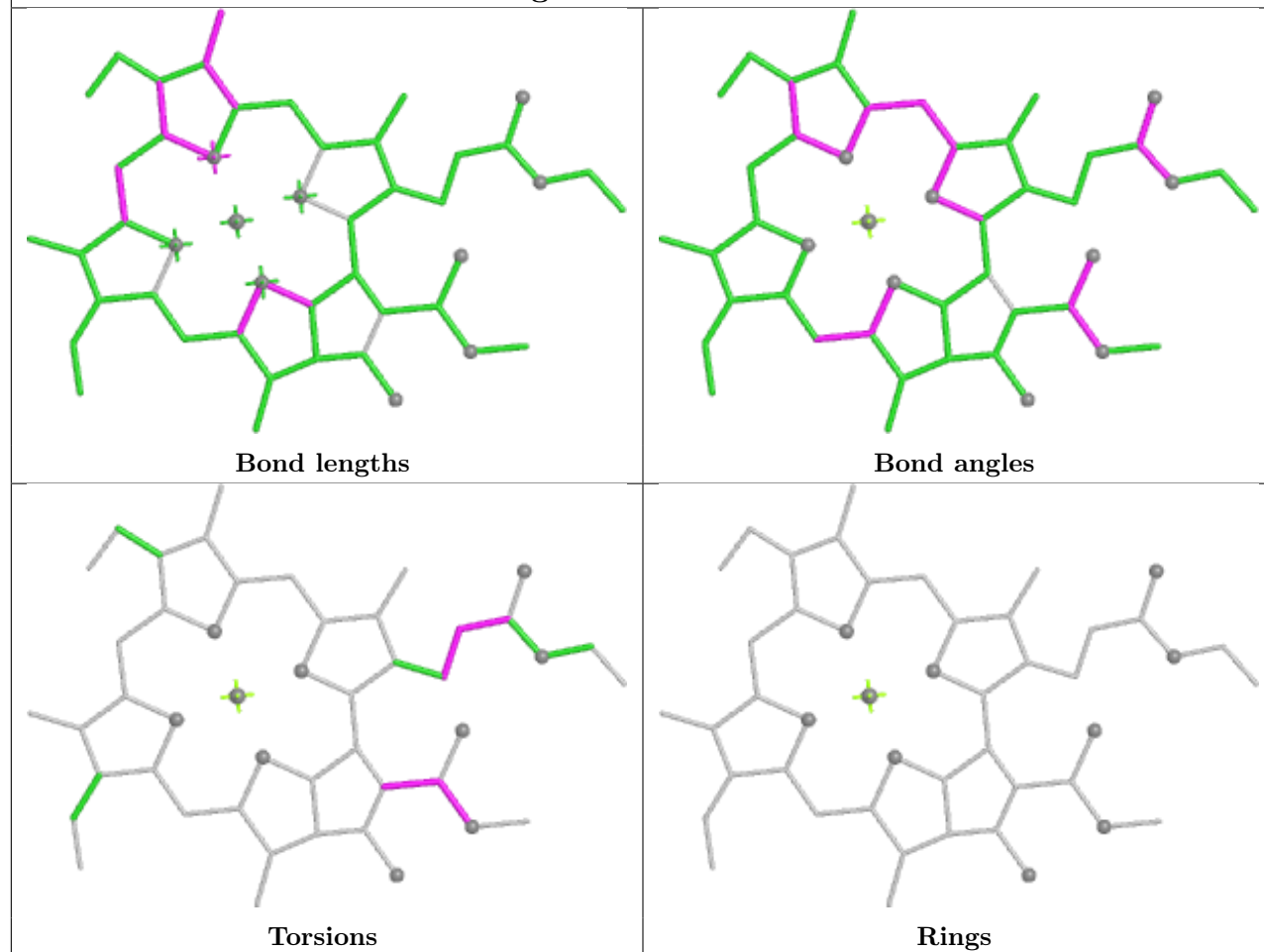
Torsions



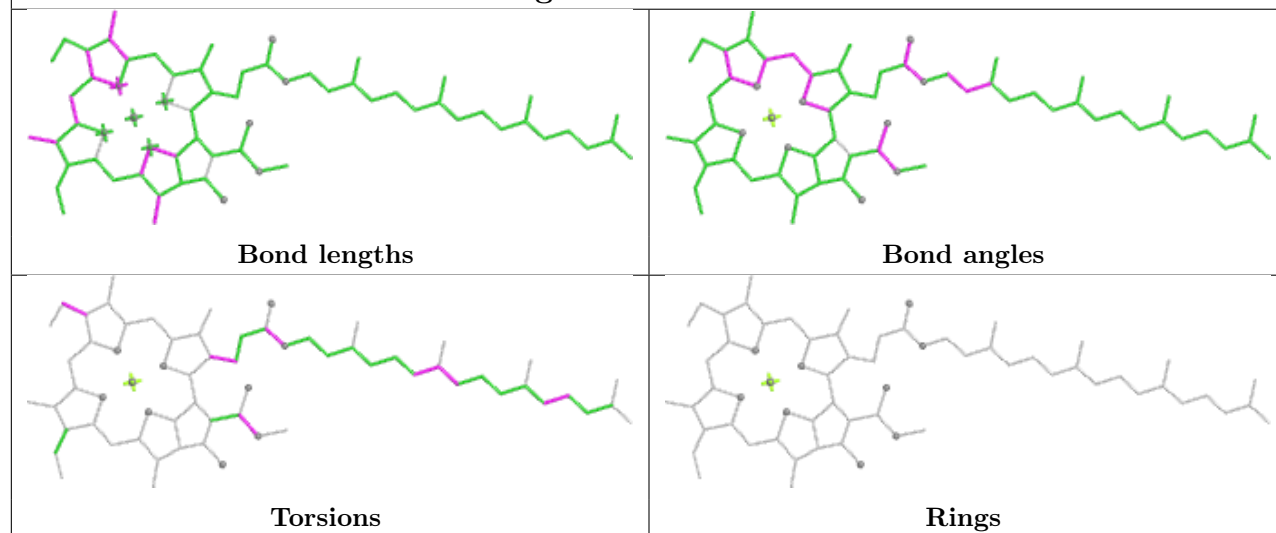
Rings



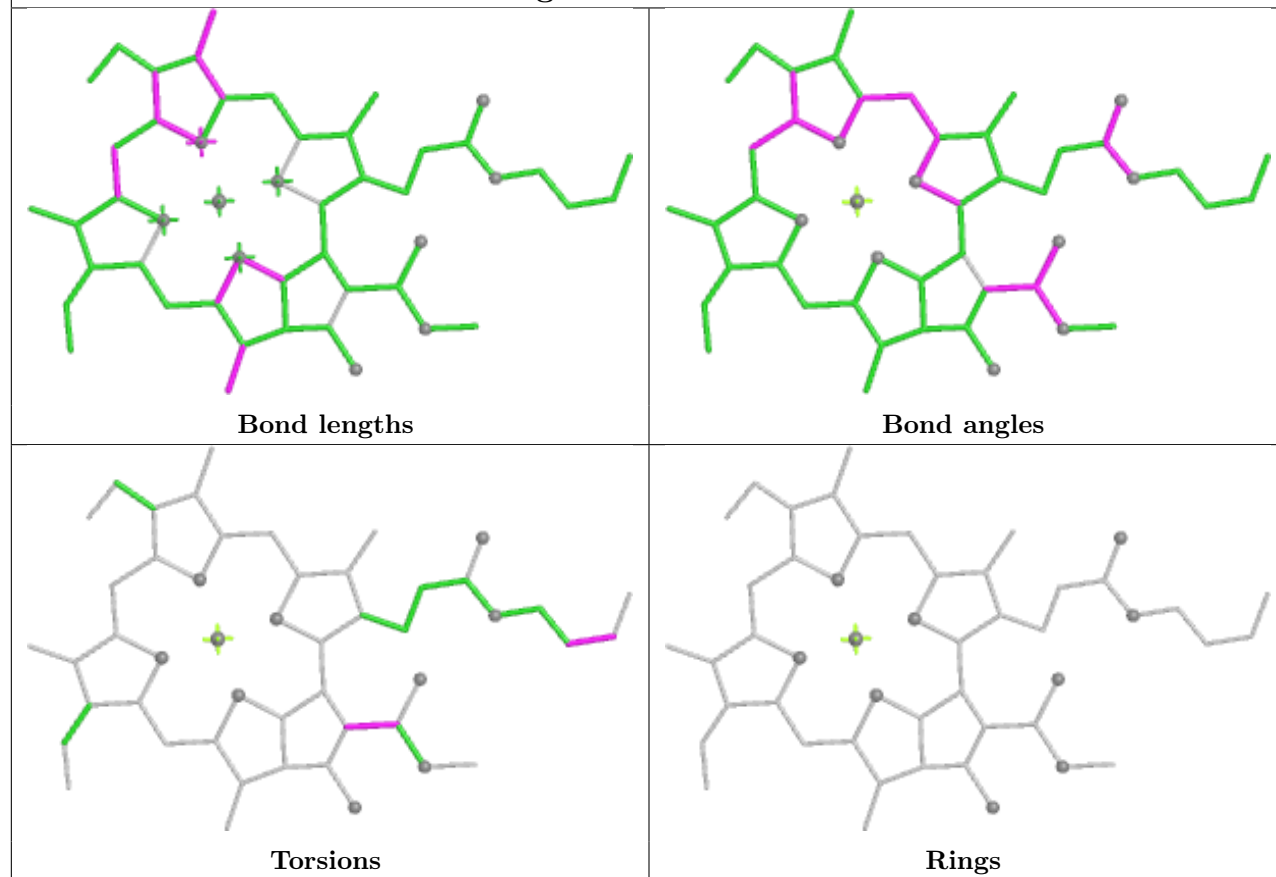
Ligand CLA 2 307



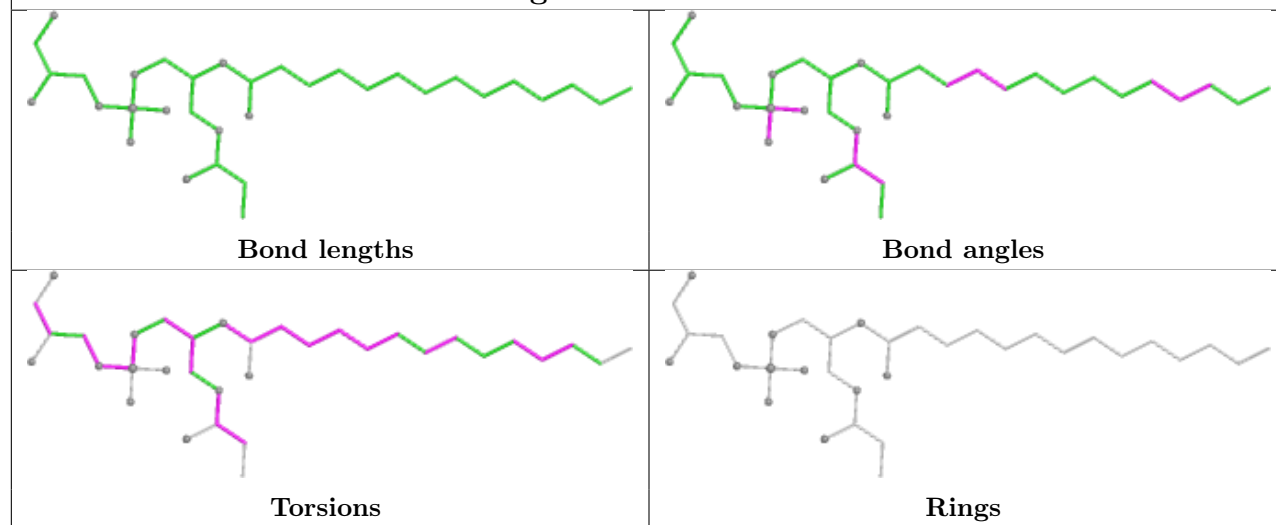
Ligand CLA b 517

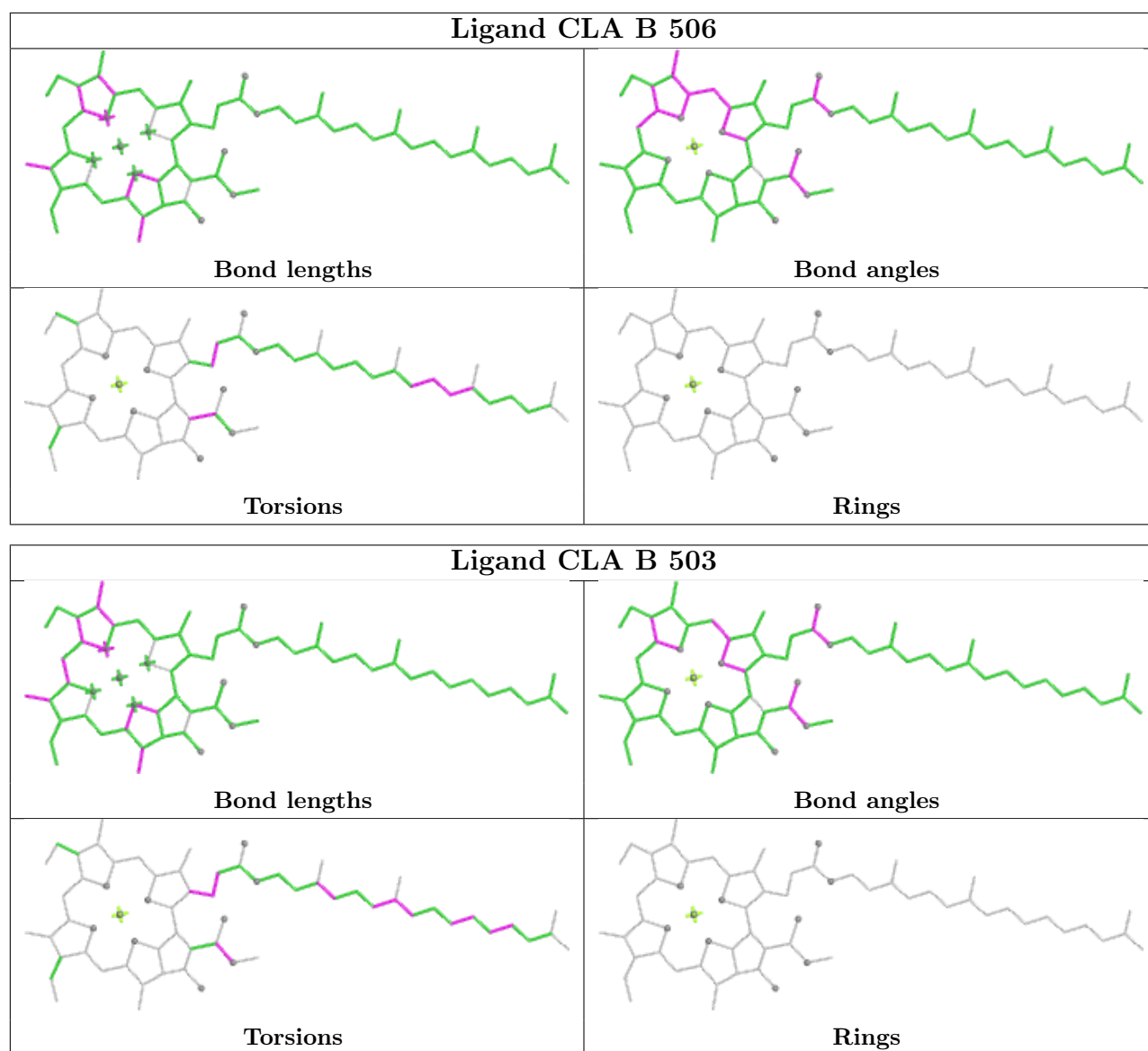


Ligand CLA a 404

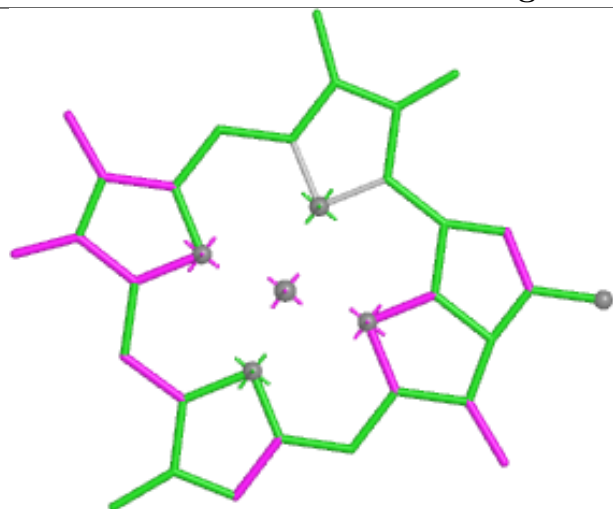


Ligand LHG D 411





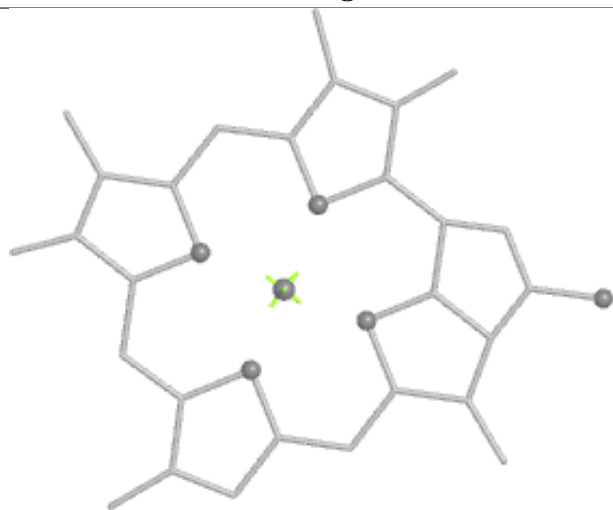
Ligand CLA 3 304



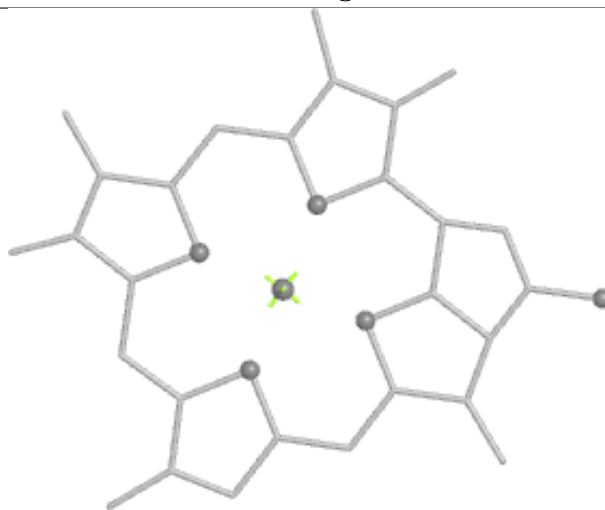
Bond lengths



Bond angles

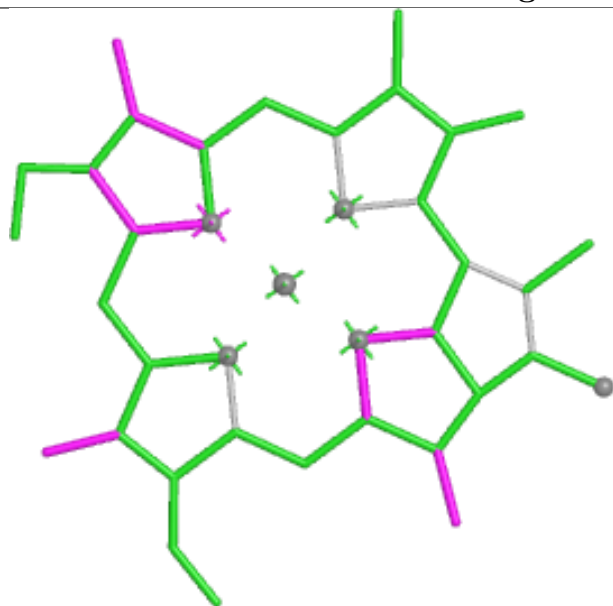


Torsions



Rings

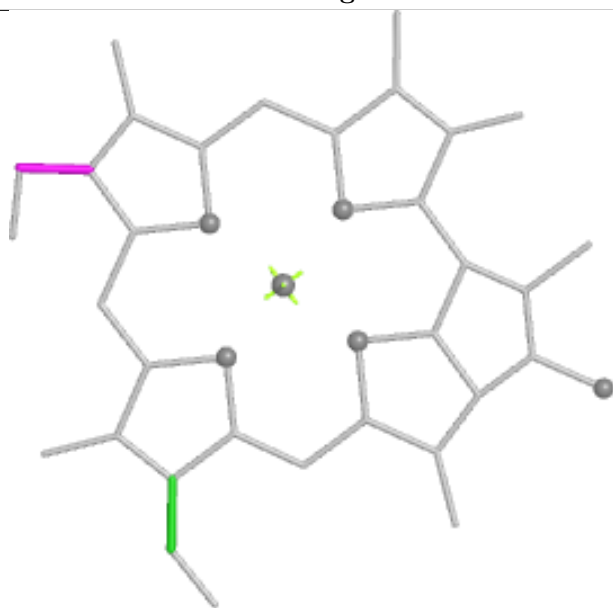
Ligand CLA 9 207



Bond lengths



Bond angles

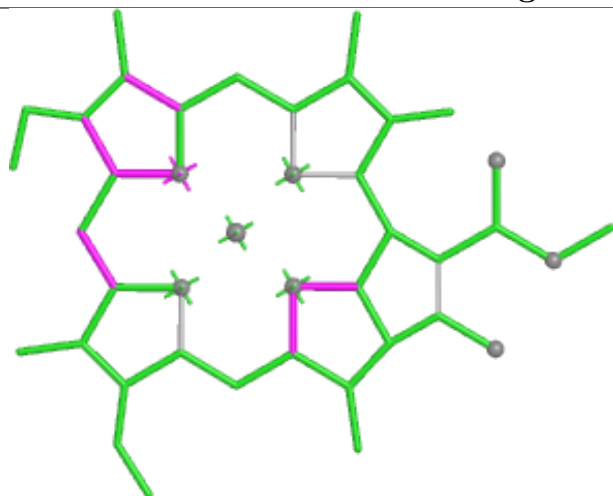


Torsions

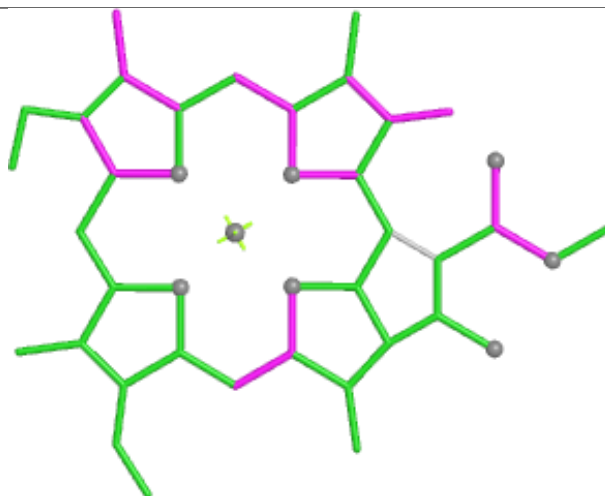


Rings

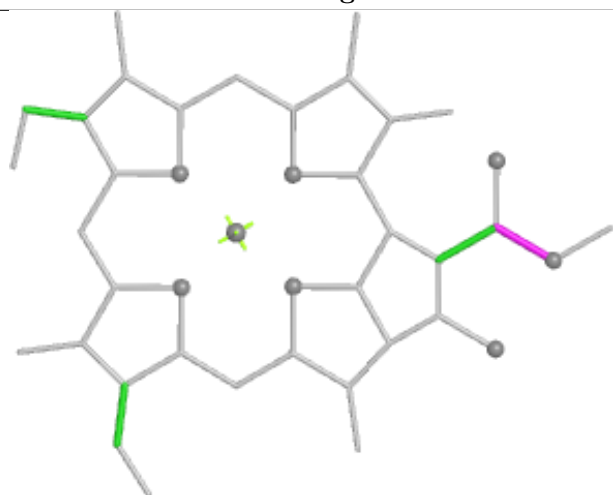
Ligand CLA 2 316



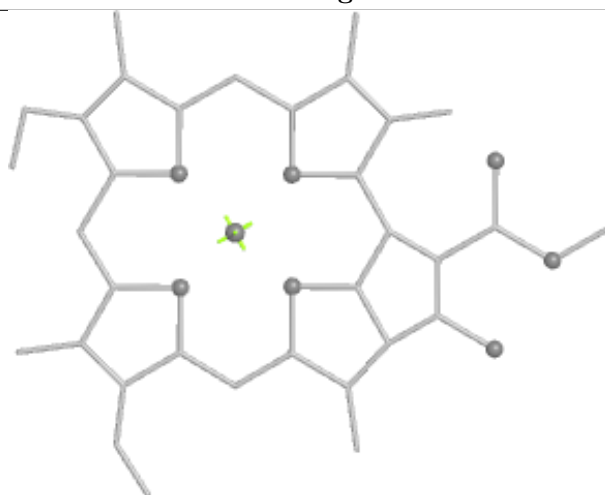
Bond lengths



Bond angles

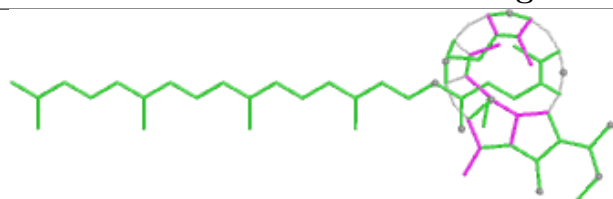


Torsions

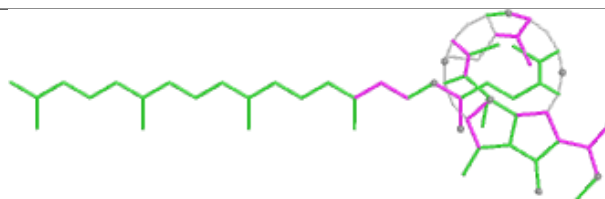


Rings

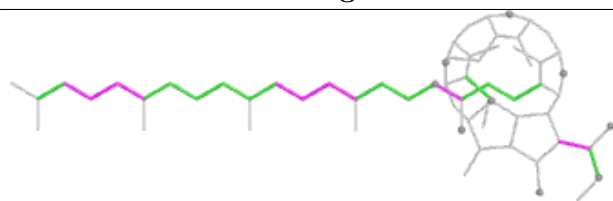
Ligand PHO a 405



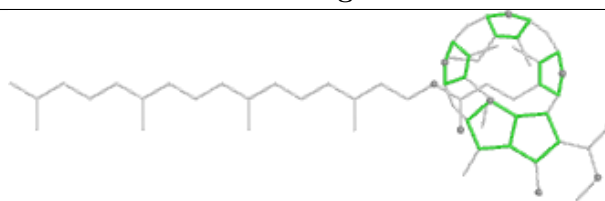
Bond lengths



Bond angles

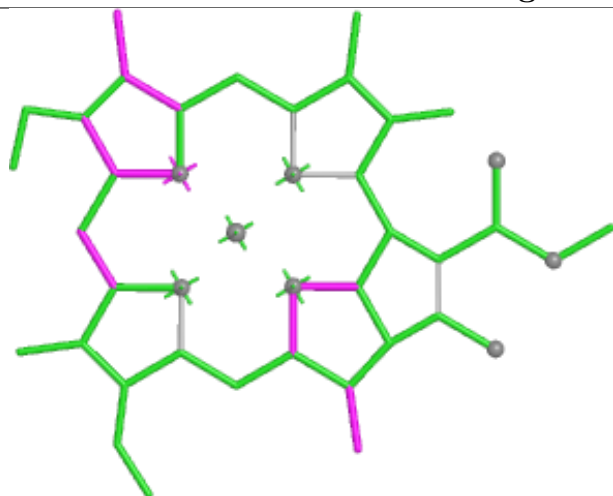


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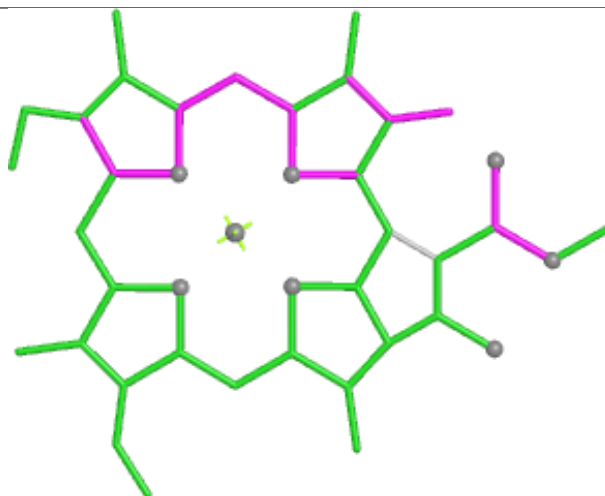


Rings

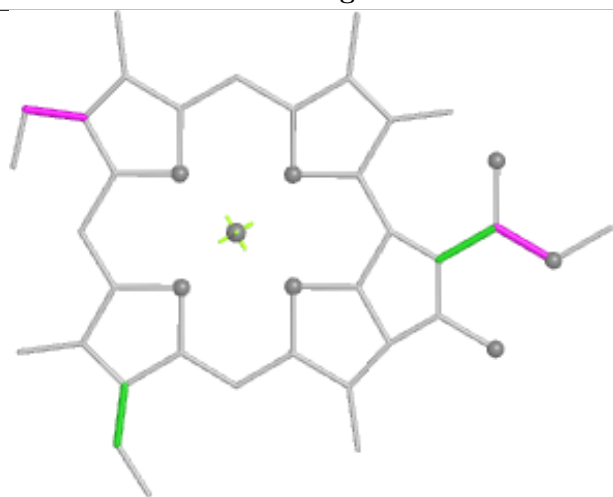
Ligand CLA 5 304



Bond lengths



Bond angles

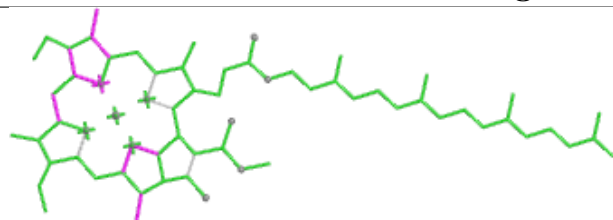


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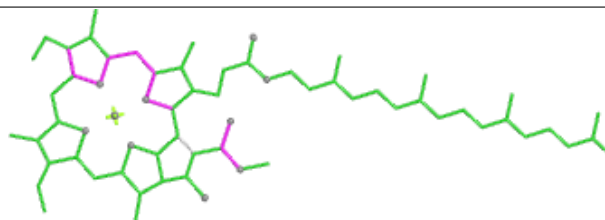


Rings

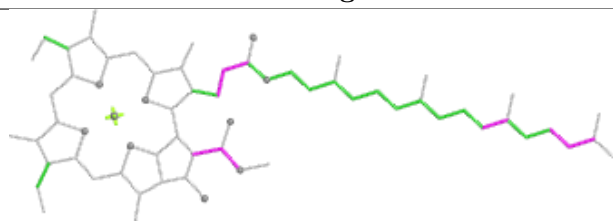
Ligand CLA B 510



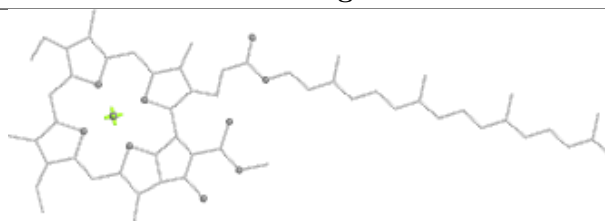
Bond lengths



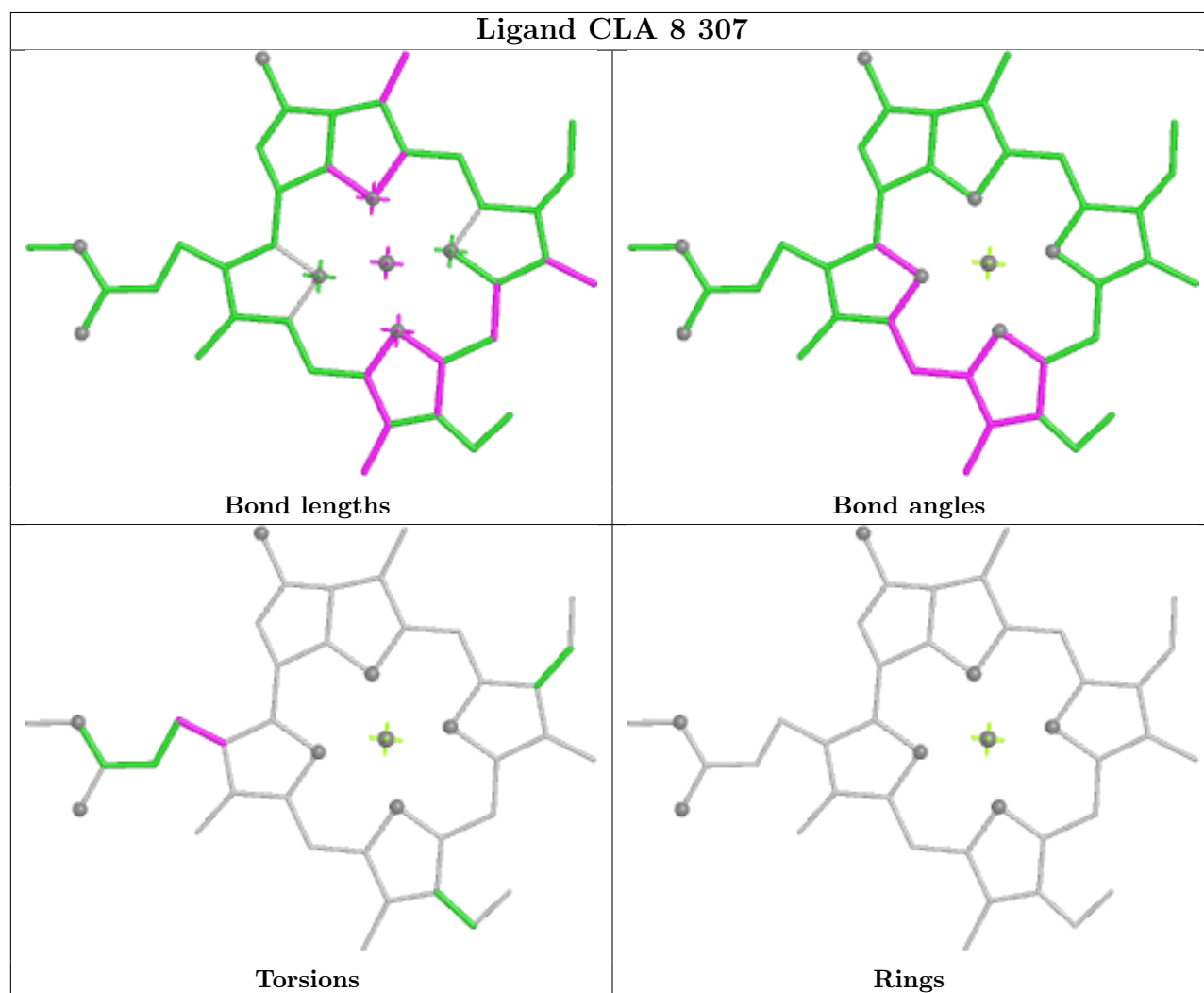
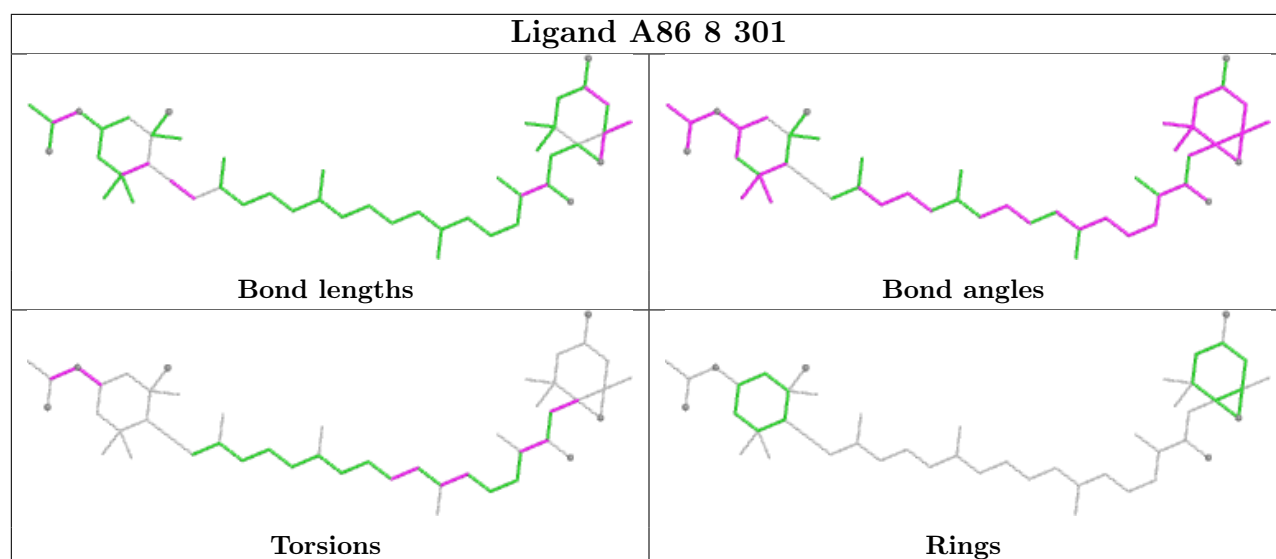
Bond angles

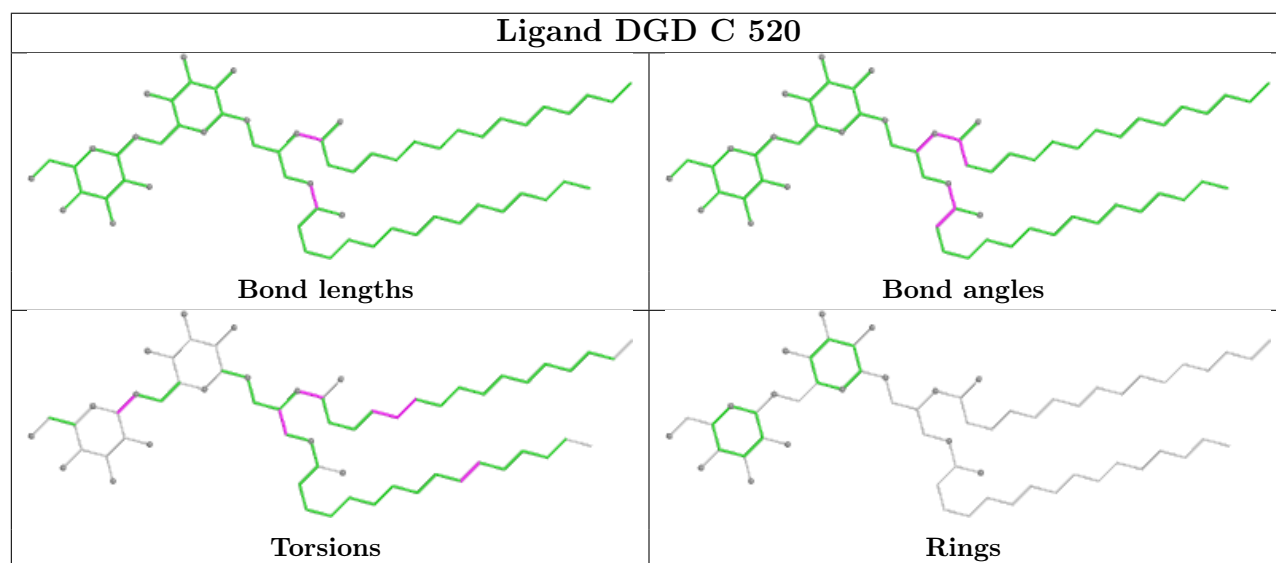
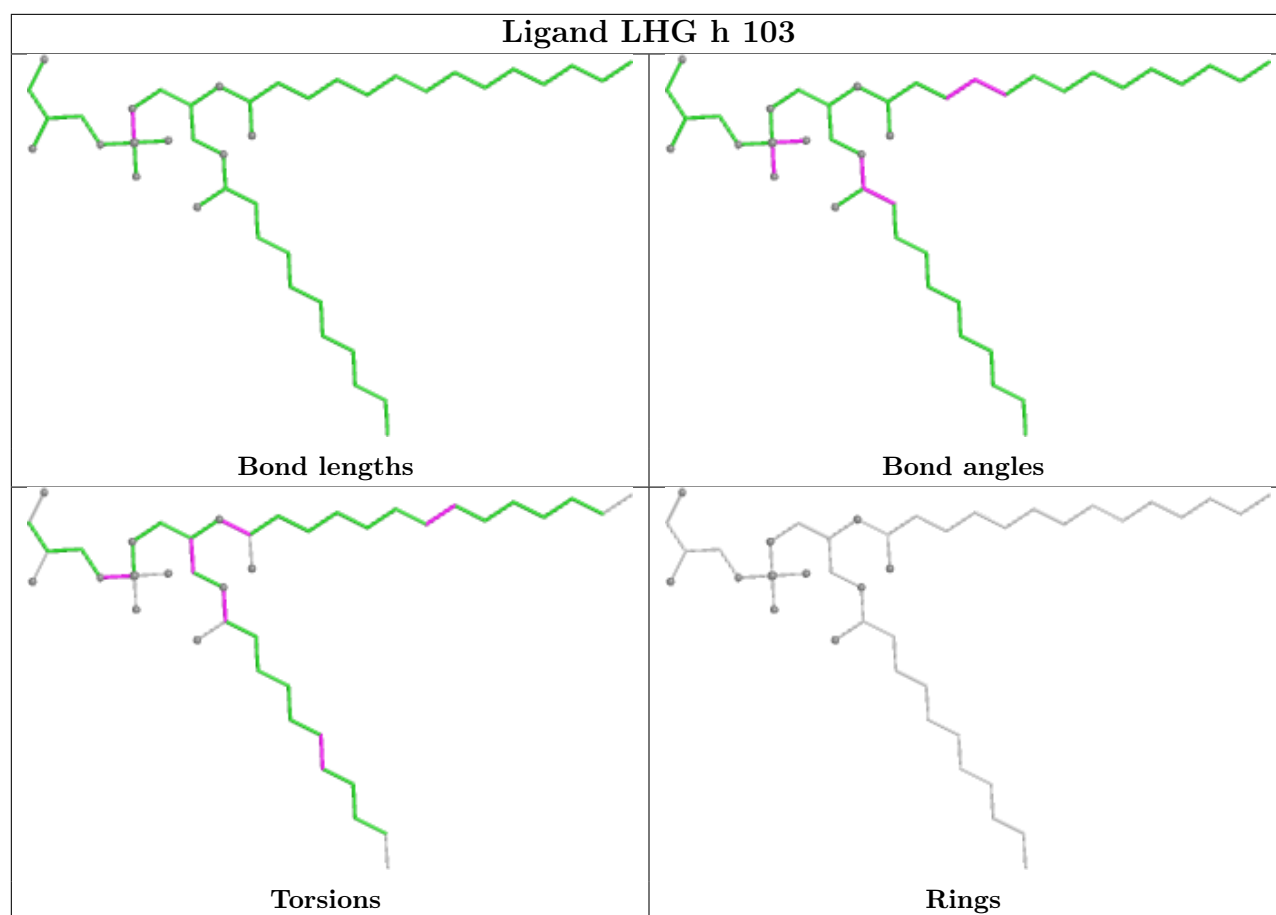


Torsions

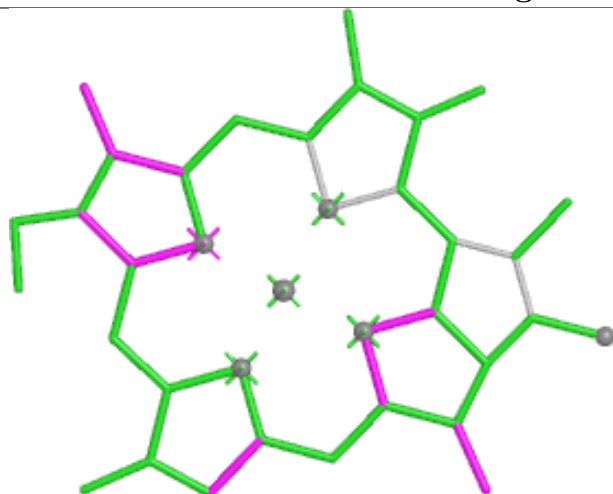


Rings

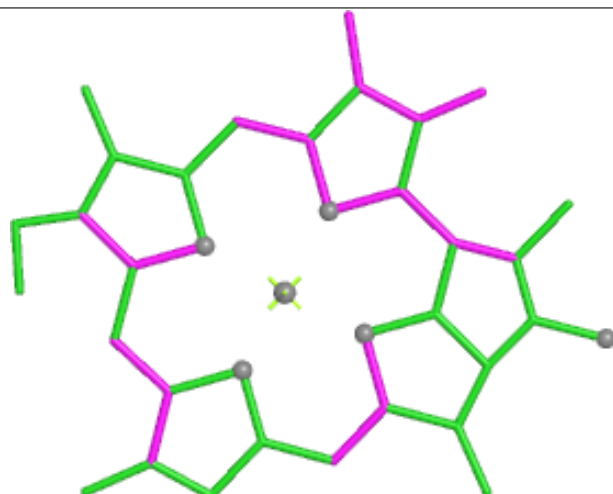




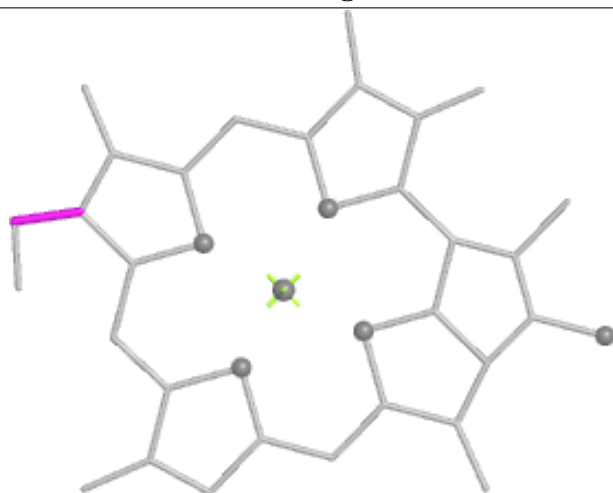
Ligand CLA P 601



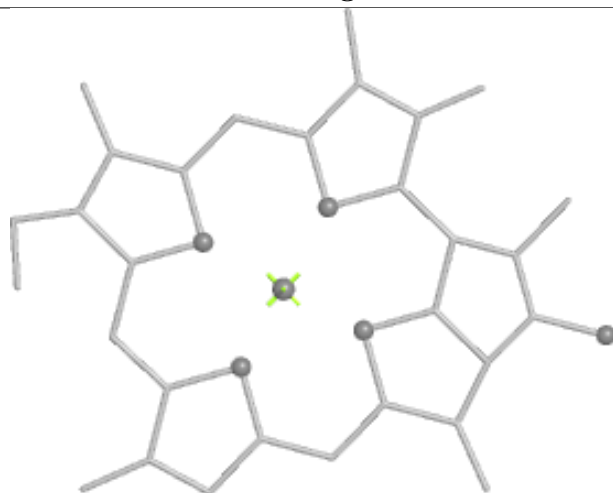
Bond lengths



Bond angles

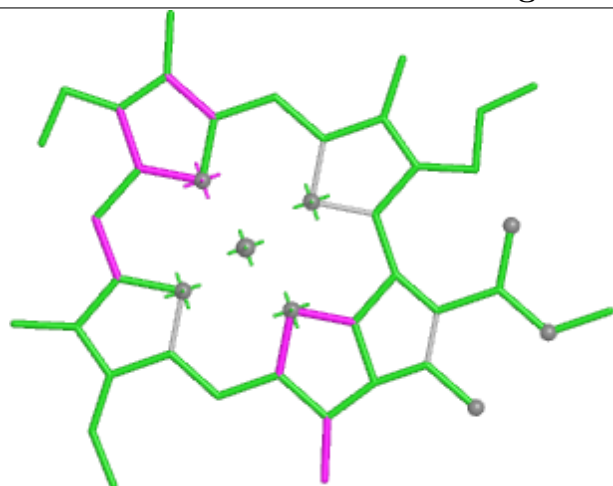


Torsions

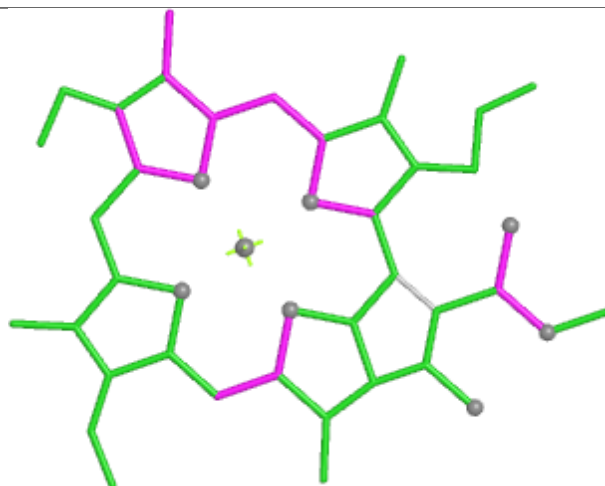


Rings

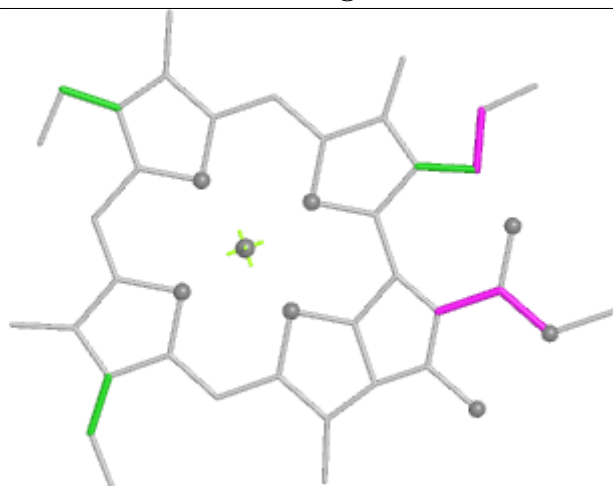
Ligand CLA 7 311



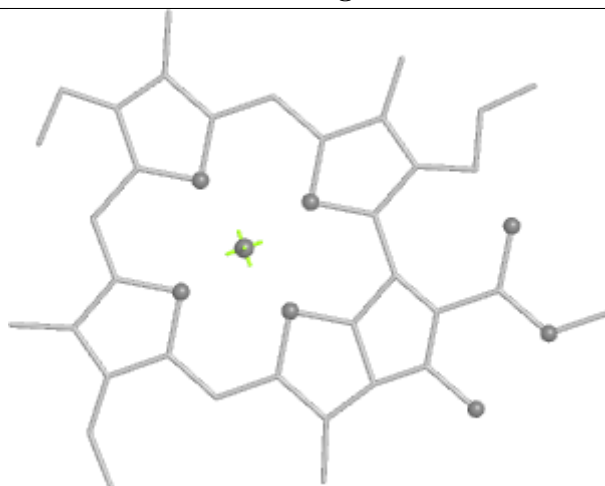
Bond lengths



Bond angles

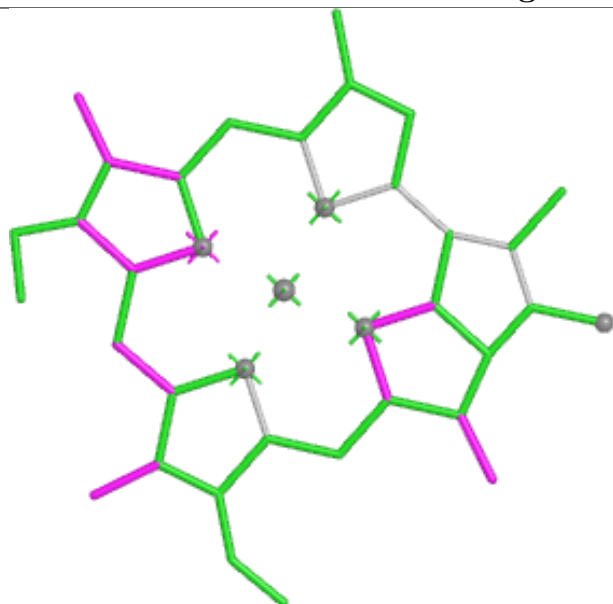


Torsions

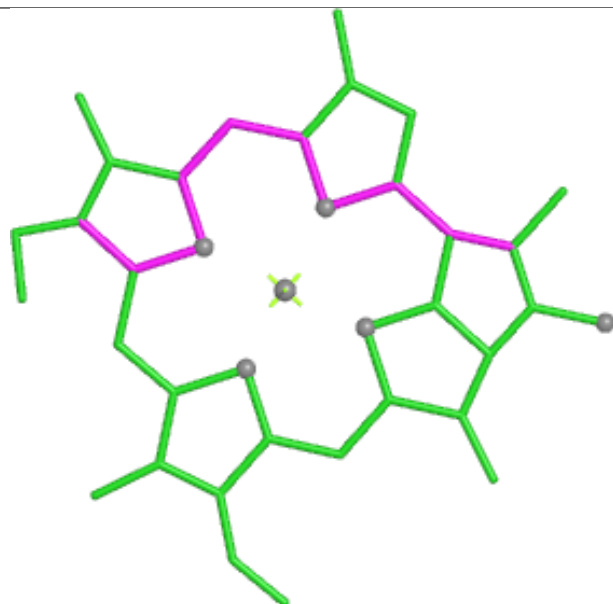


Rings

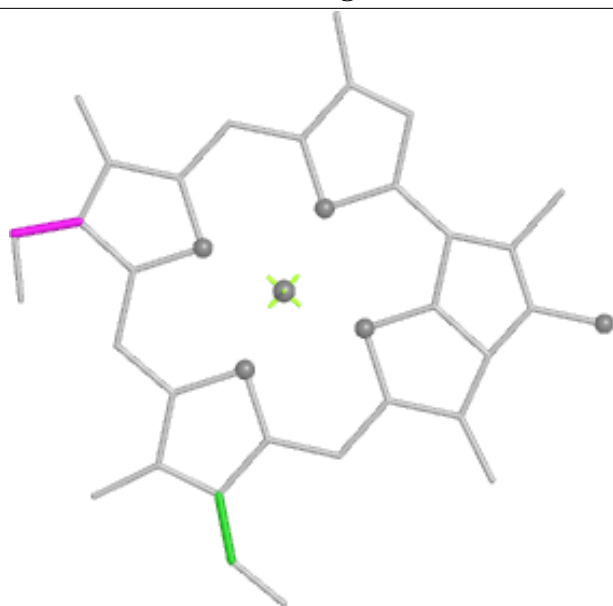
Ligand CLA 4 206



Bond lengths



Bond angles

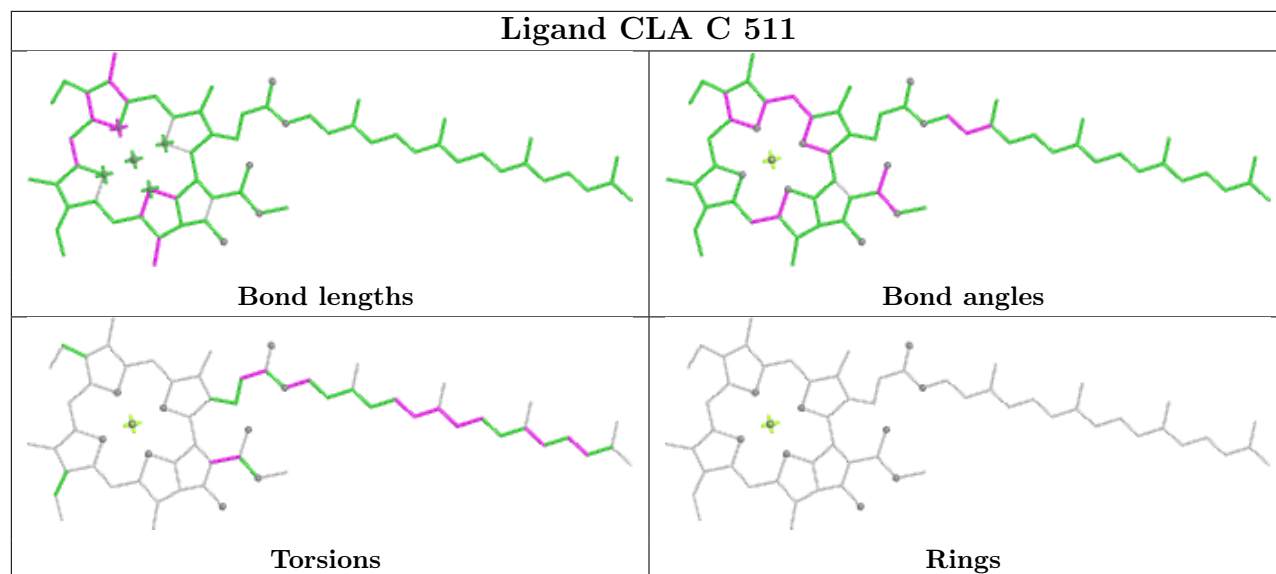


Torsions

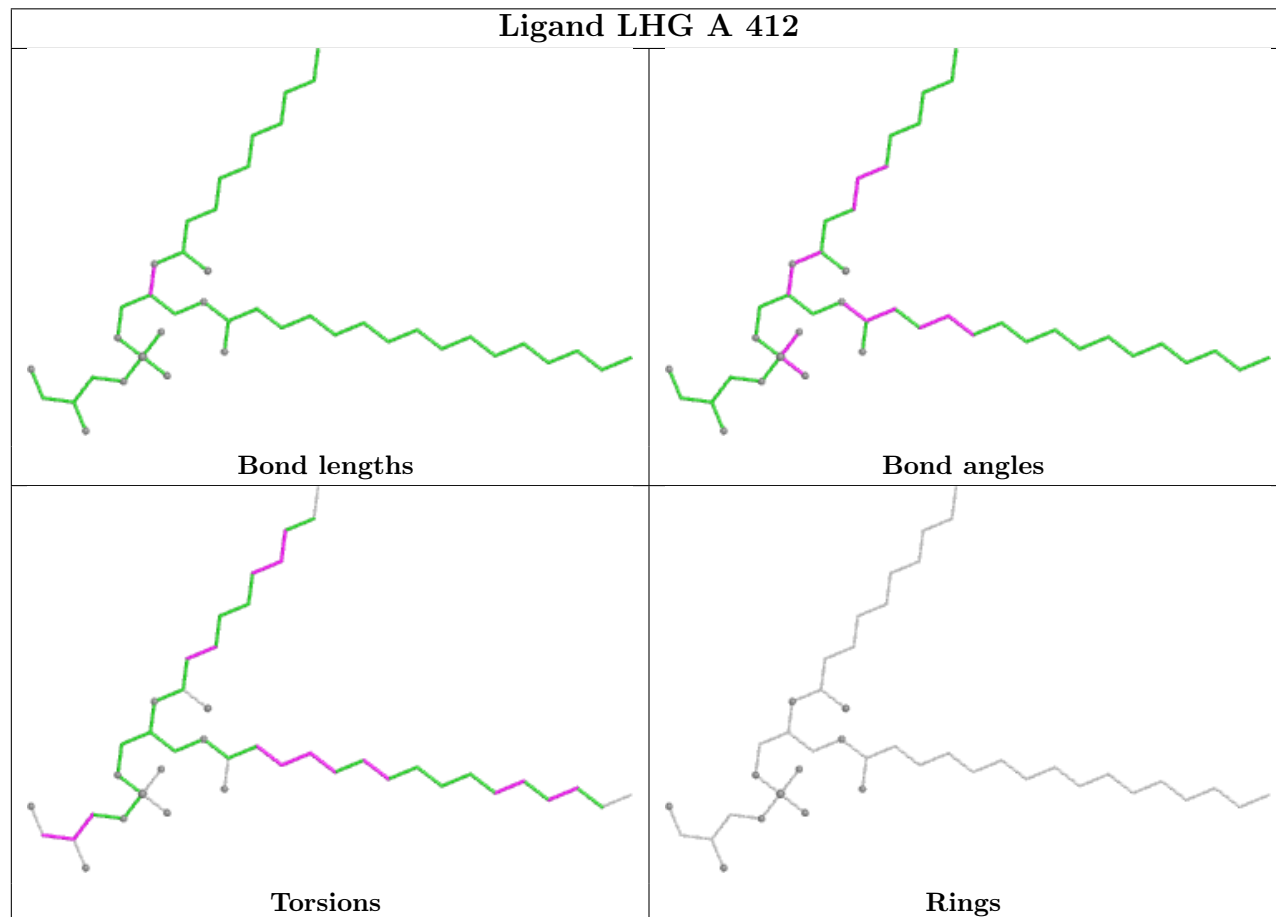


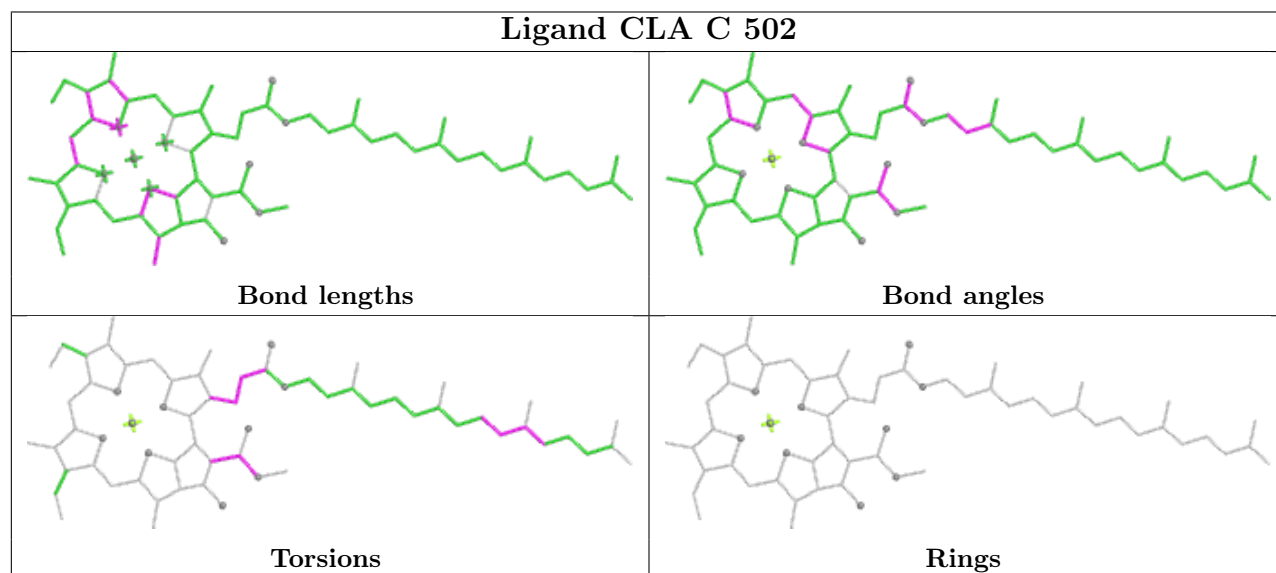
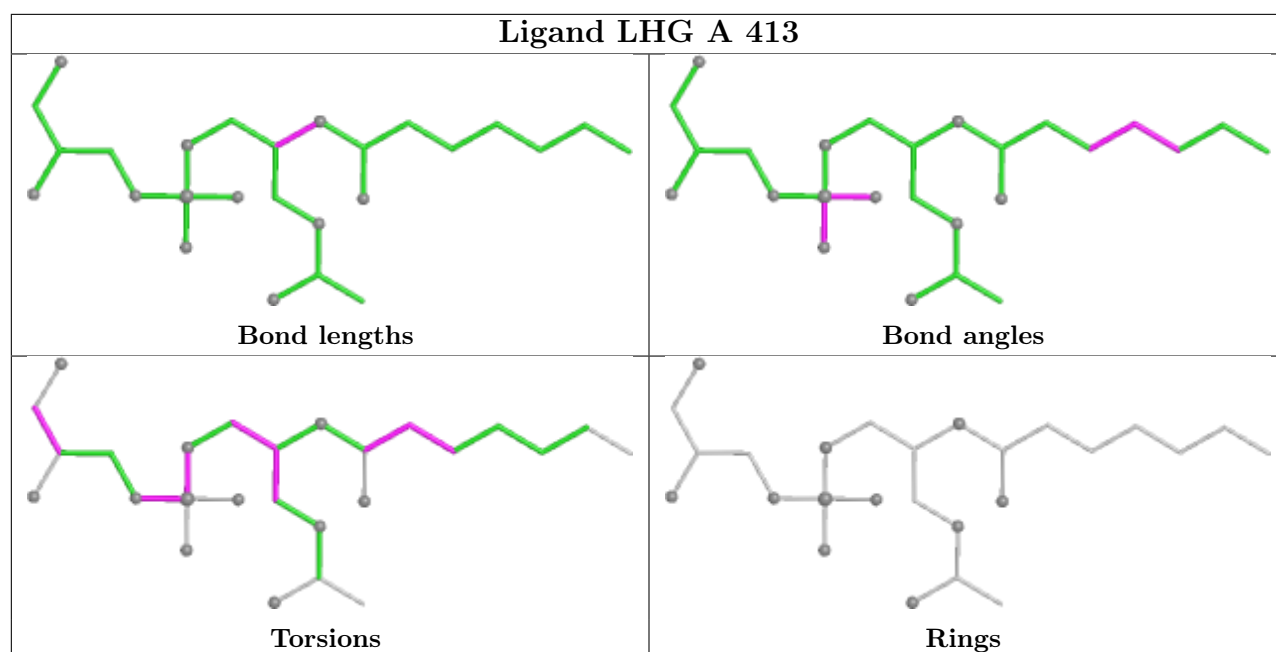
Rings

Ligand CLA C 511

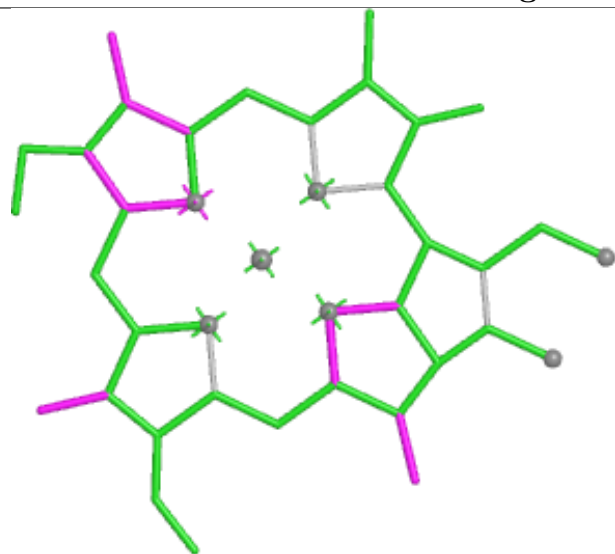


Ligand LHG A 412

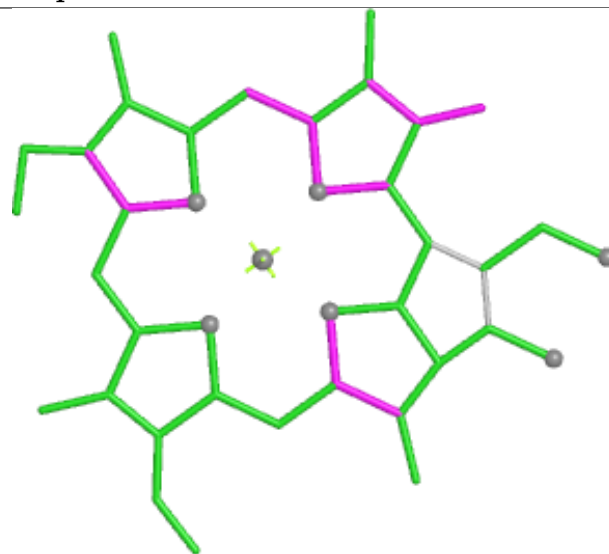




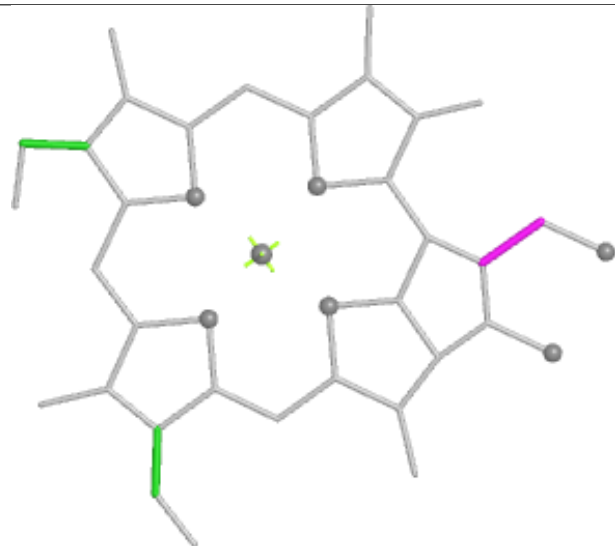
Ligand CLA p 609



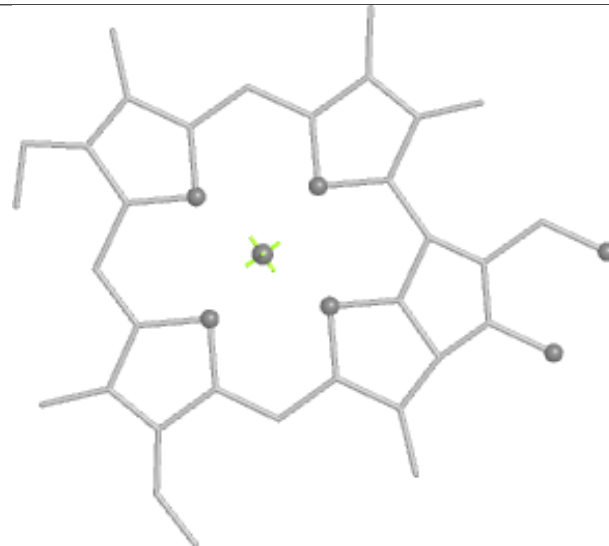
Bond lengths



Bond angles

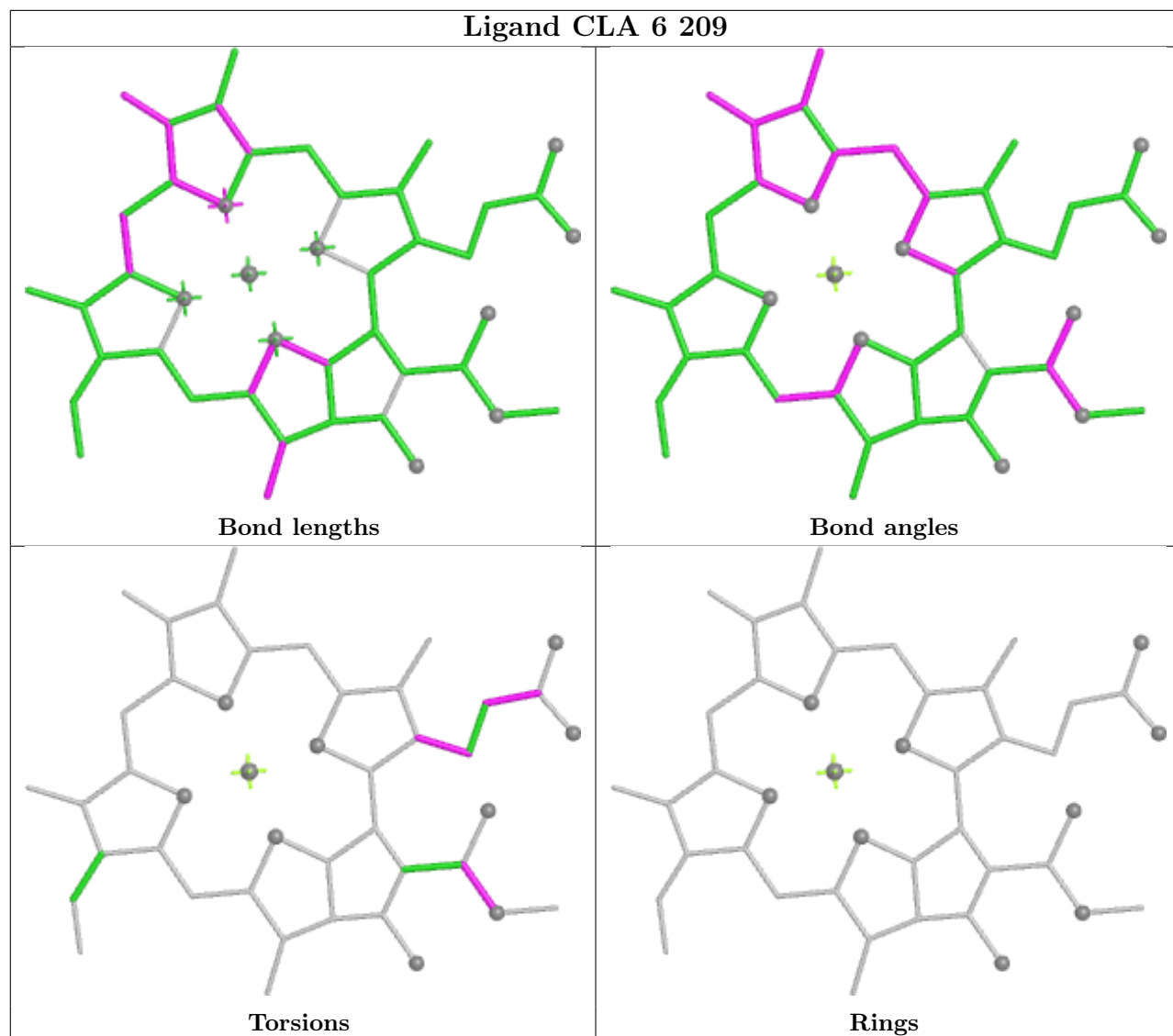


Torsions

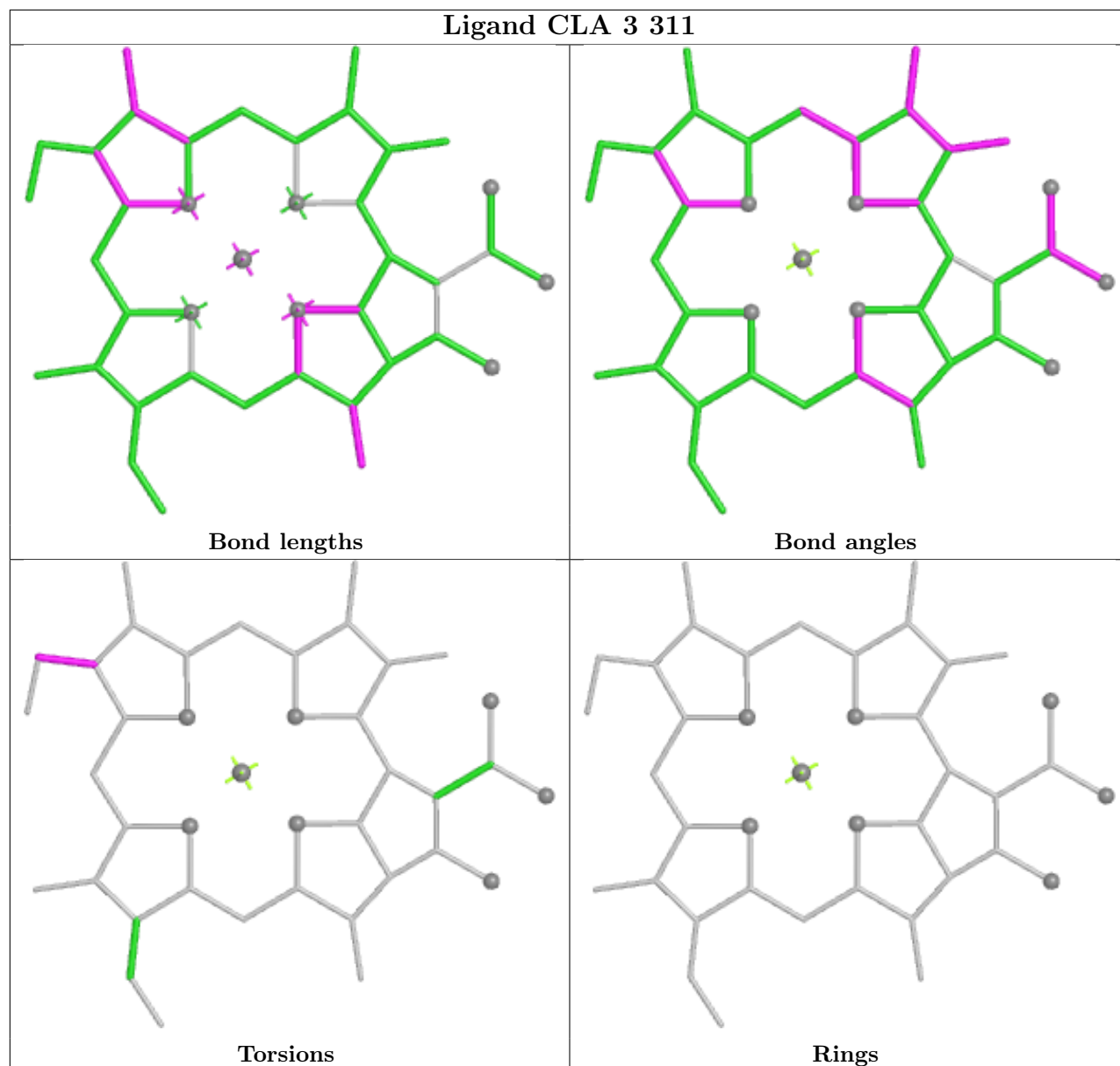


Rings

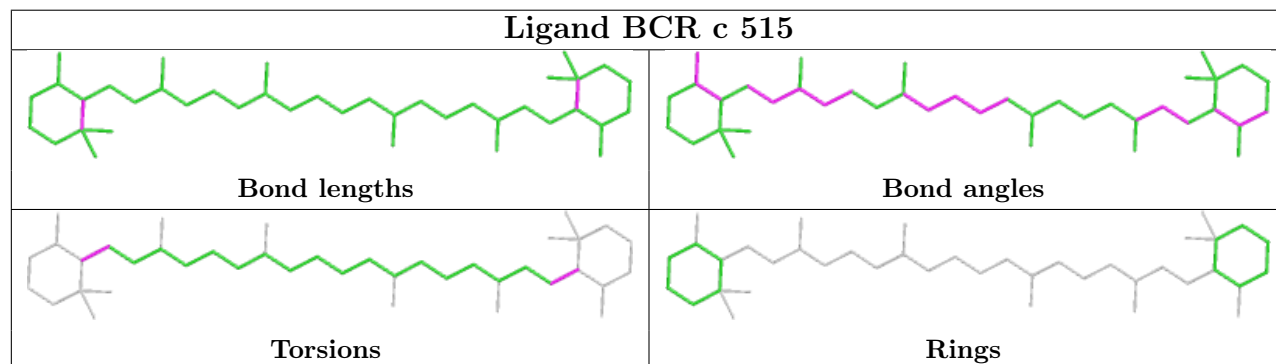
Ligand CLA 6 209

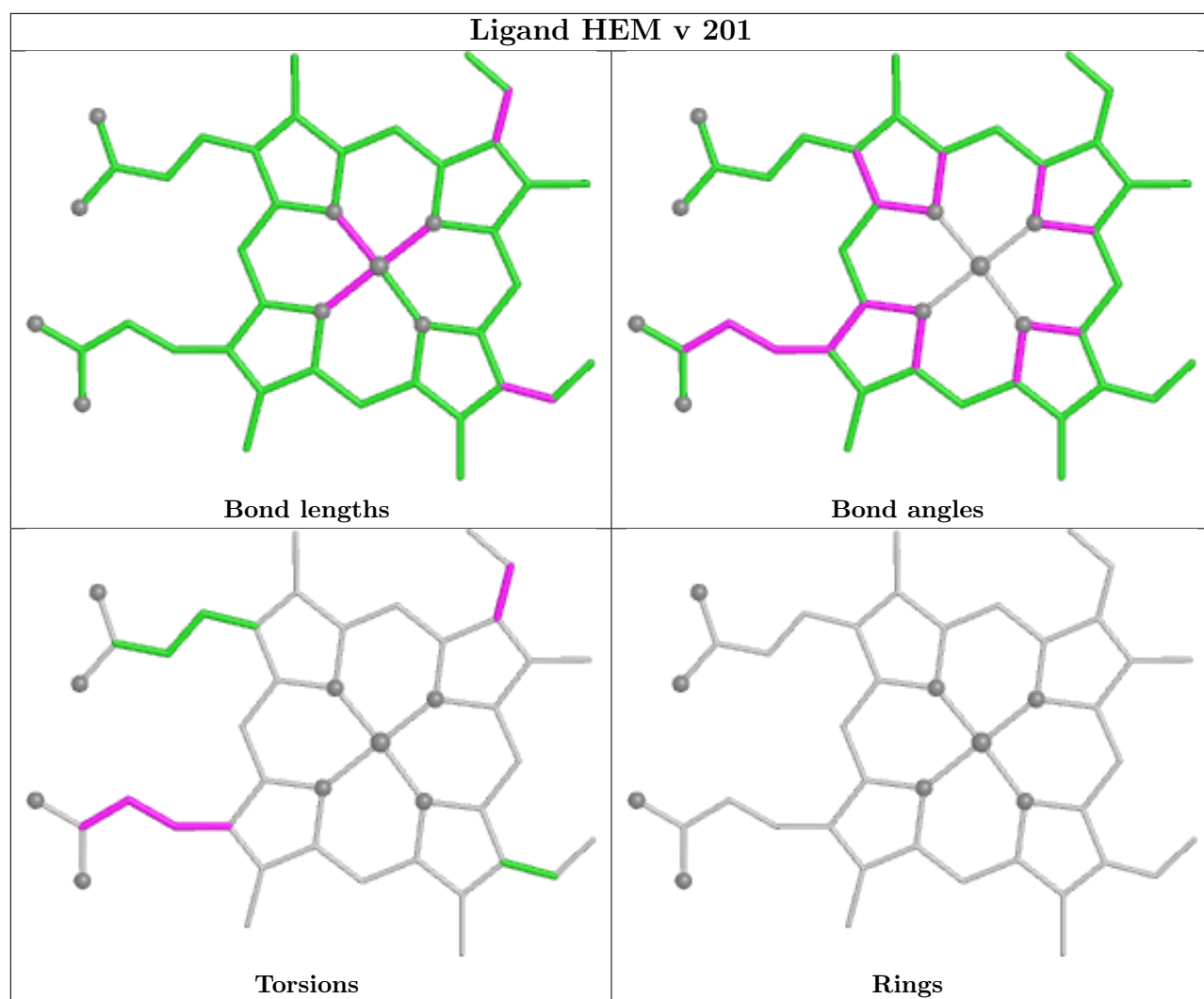


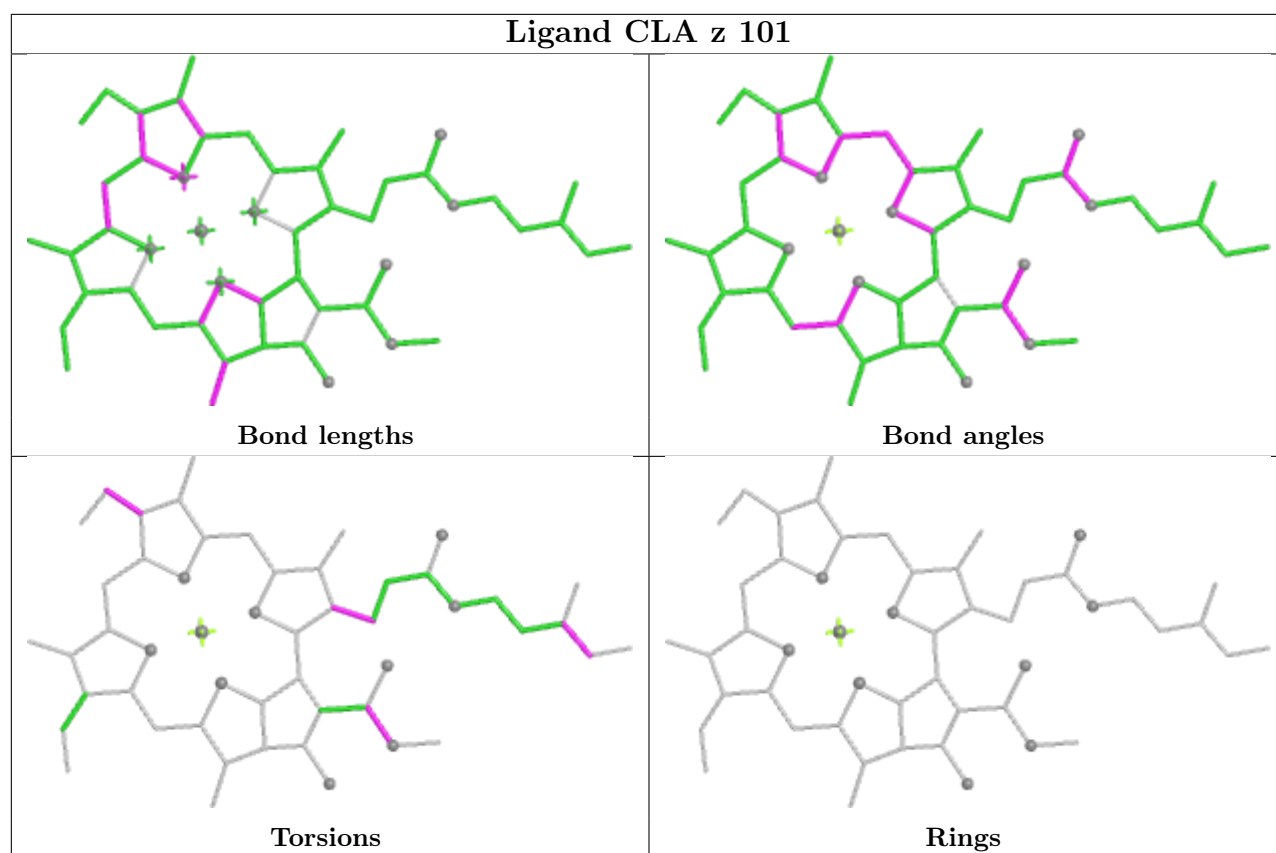
Ligand CLA 3 311



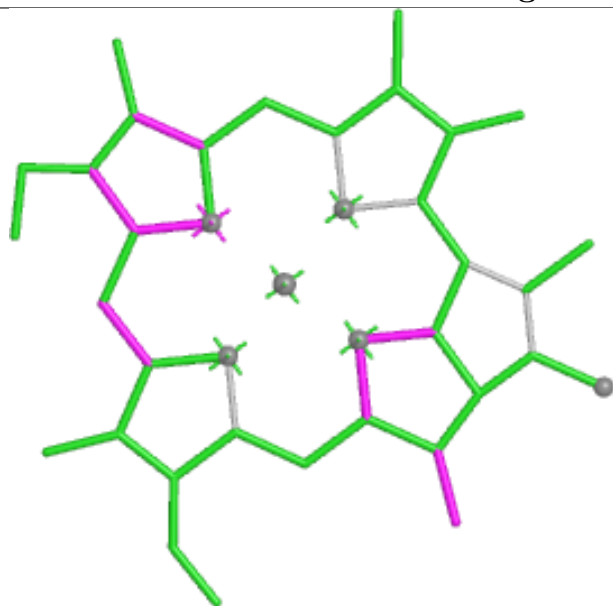
Ligand BCR c 515







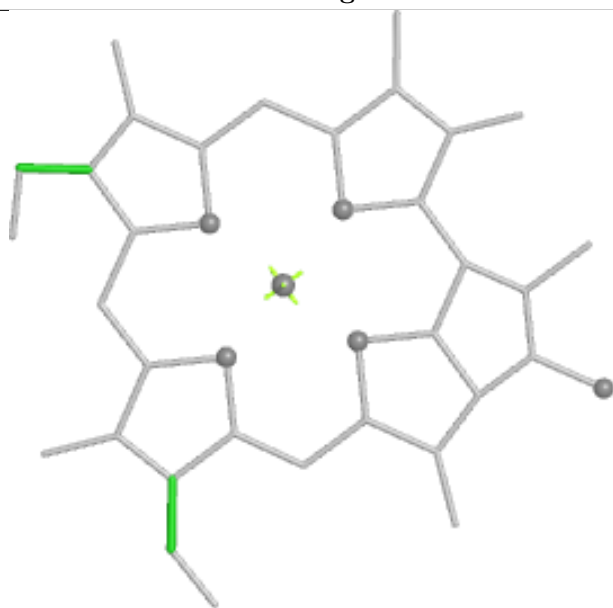
Ligand CLA 1 214



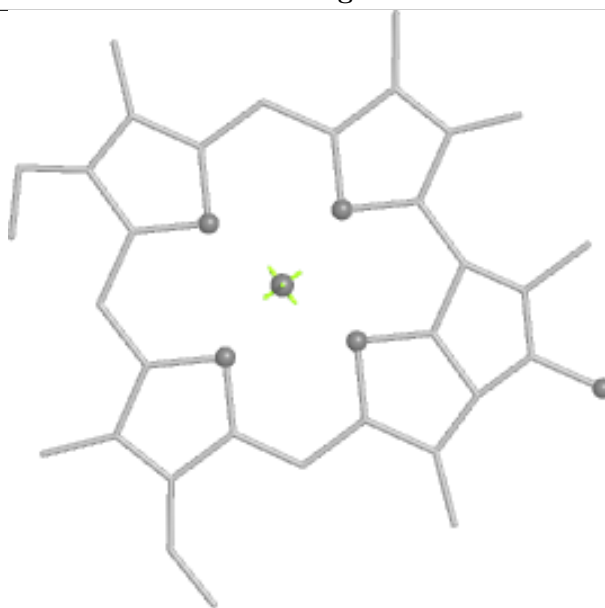
Bond lengths



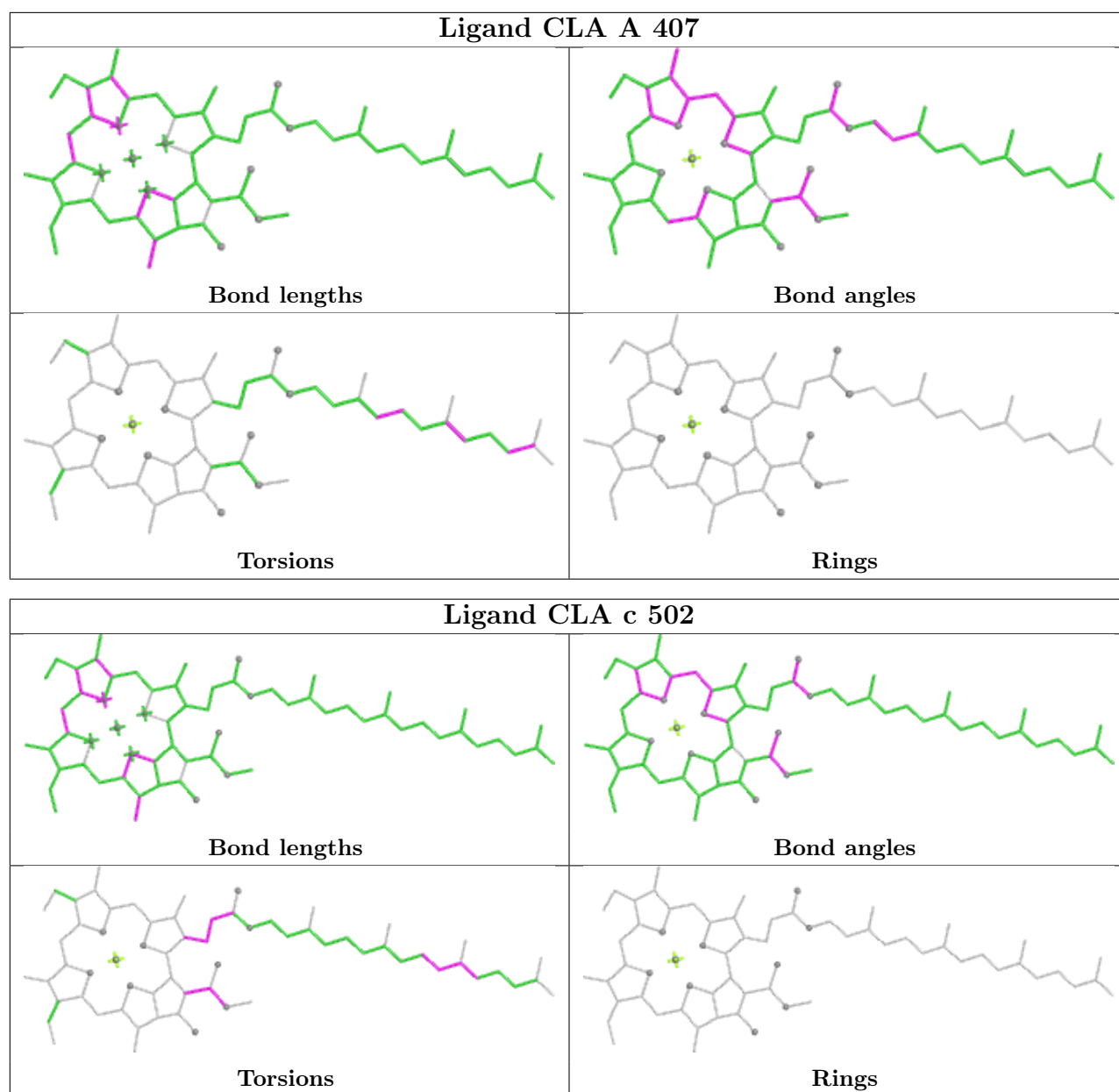
Bond angles



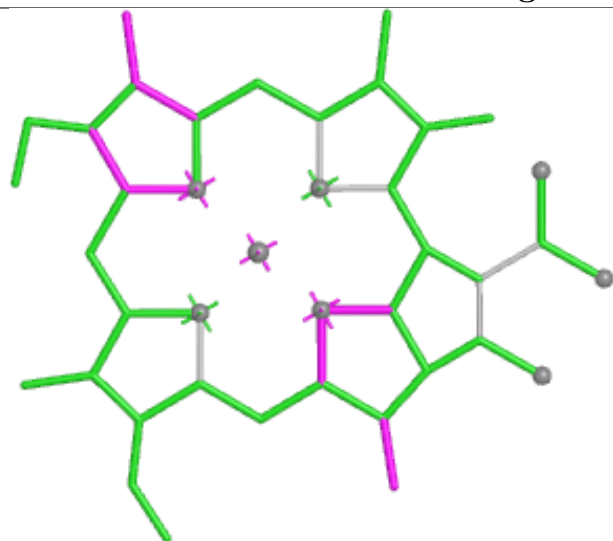
Torsions



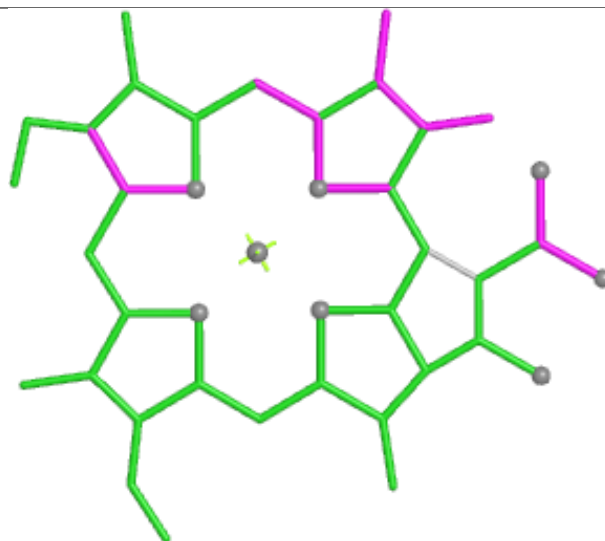
Rings



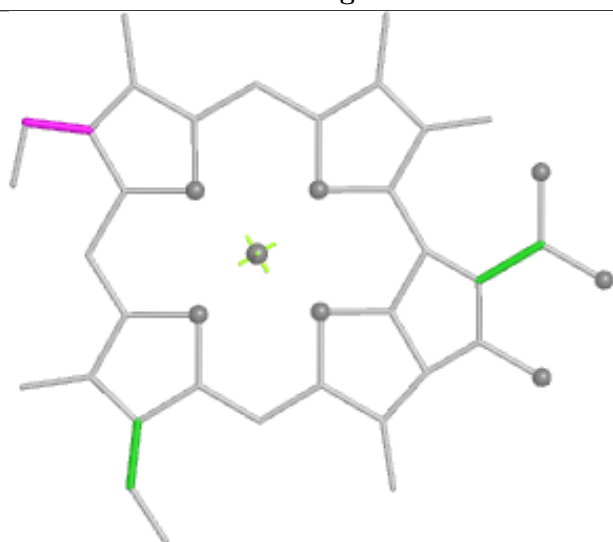
Ligand CLA 8 311



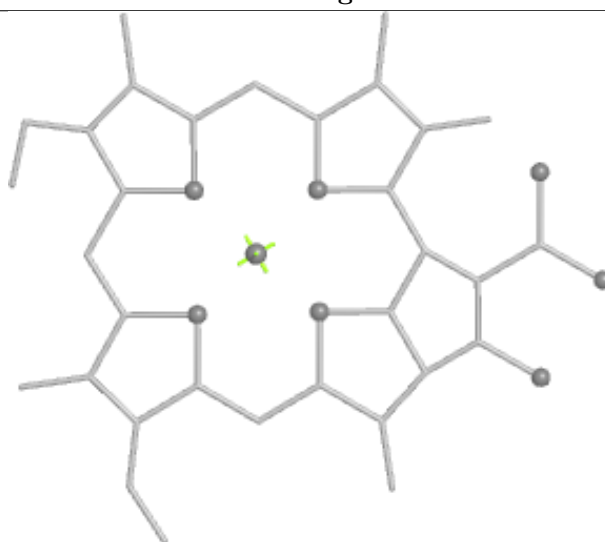
Bond lengths



Bond angles

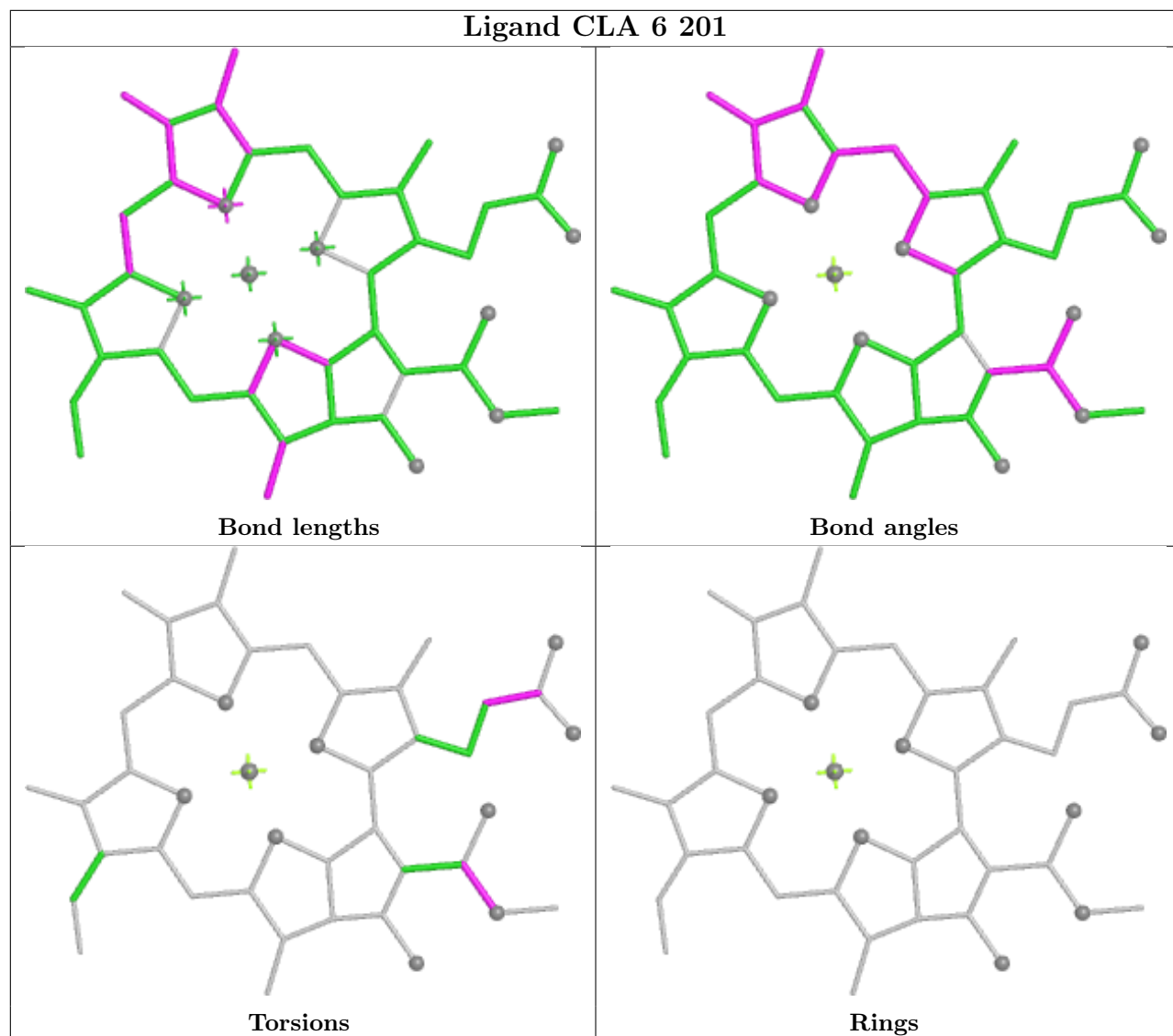


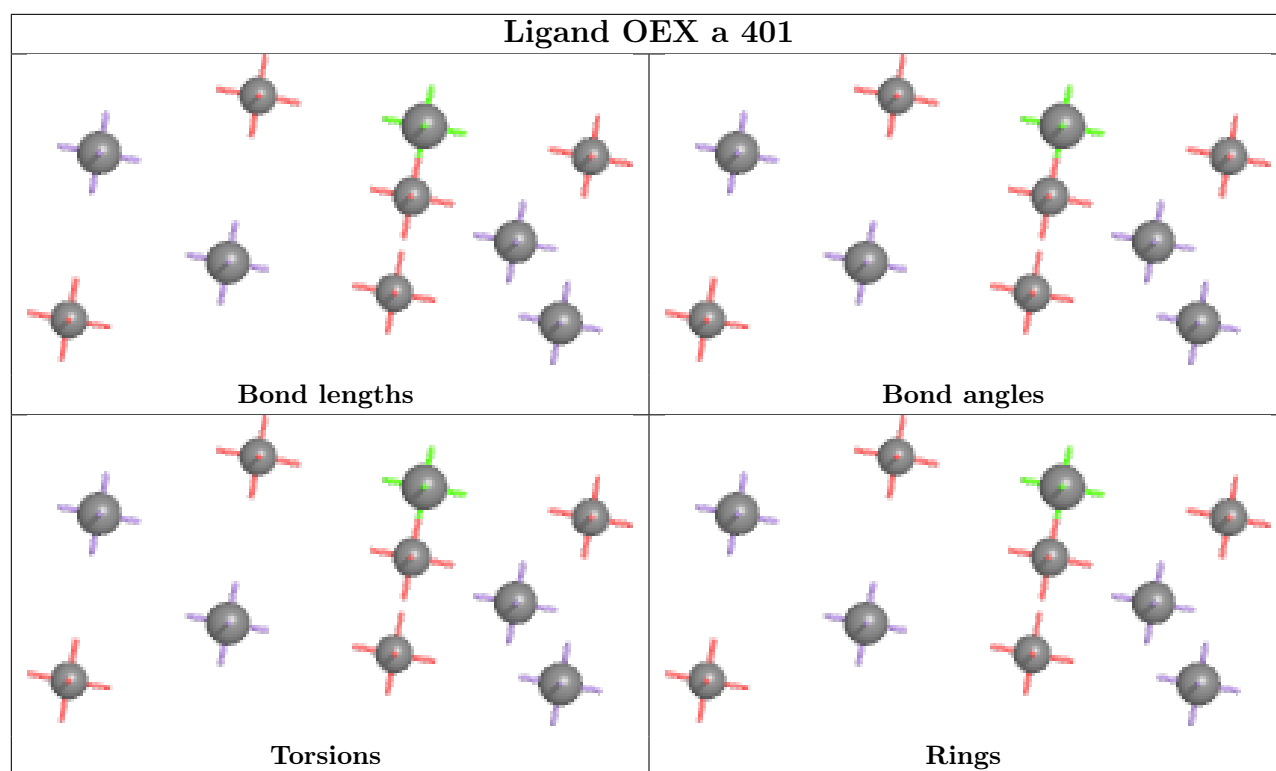
Torsions



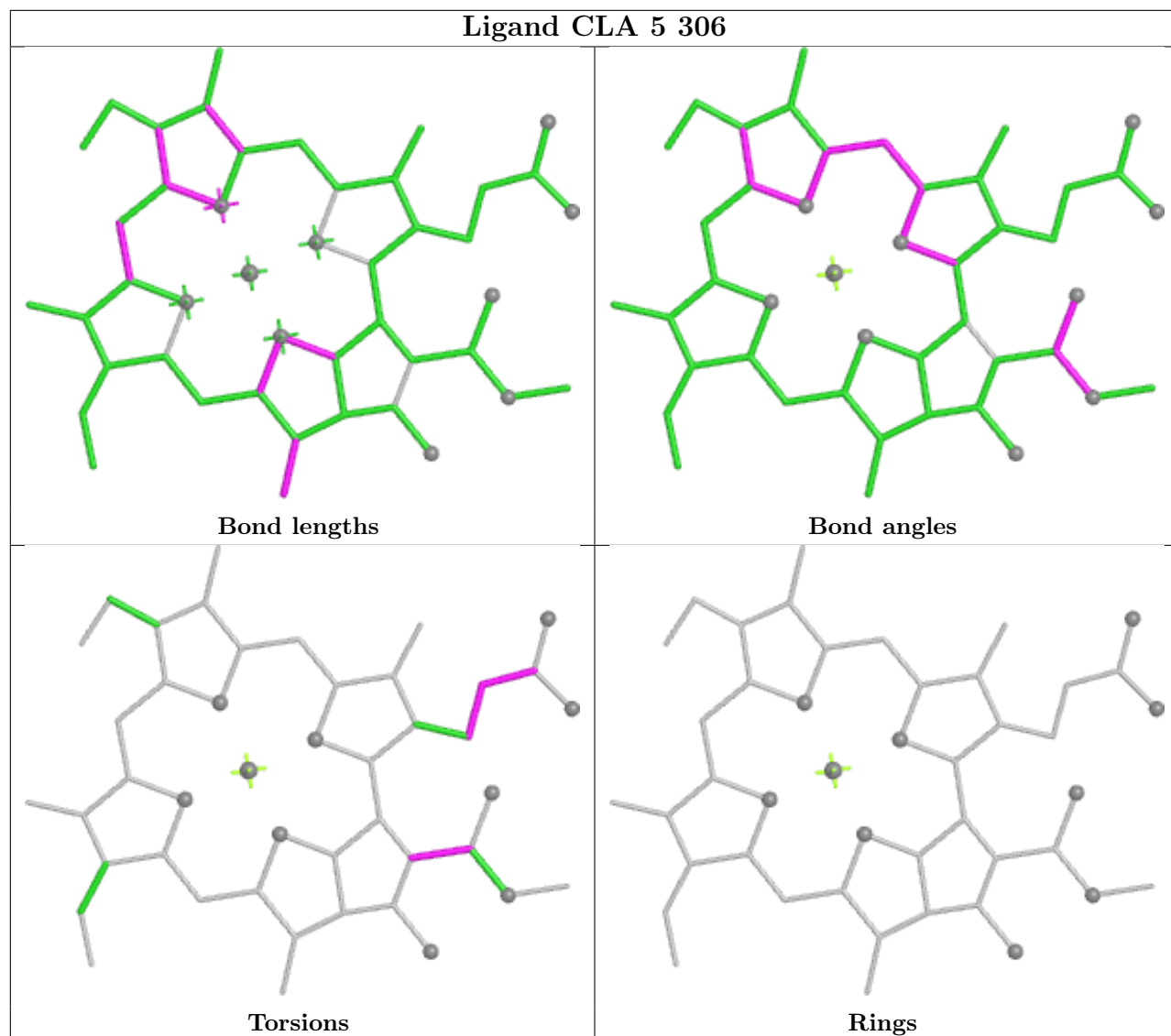
Rings

Ligand CLA 6 201

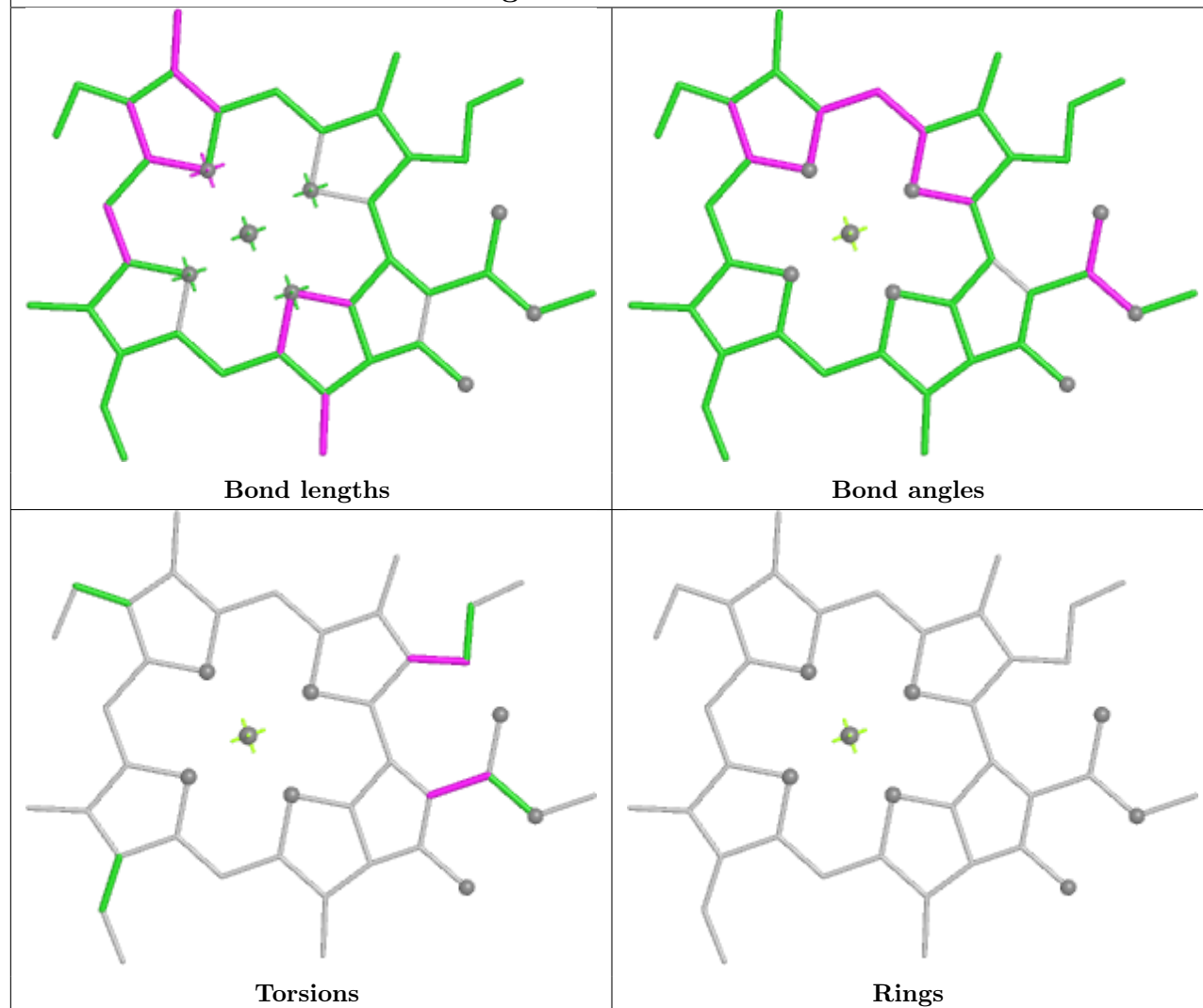




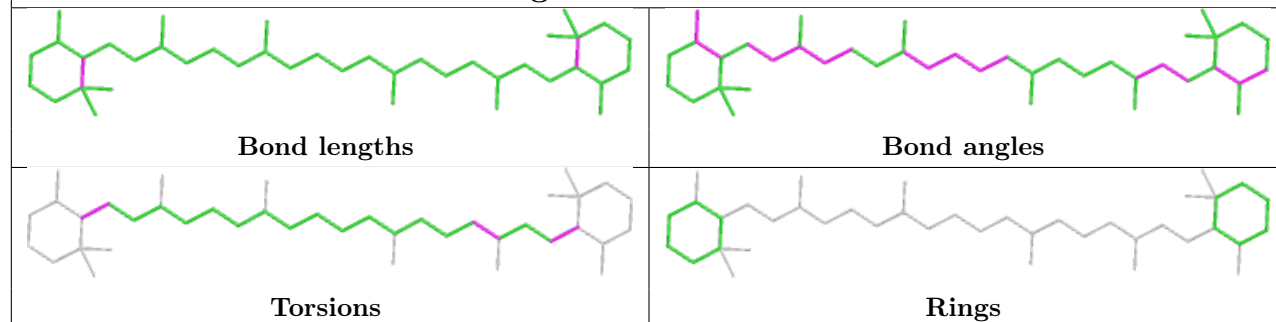
Ligand CLA 5 306

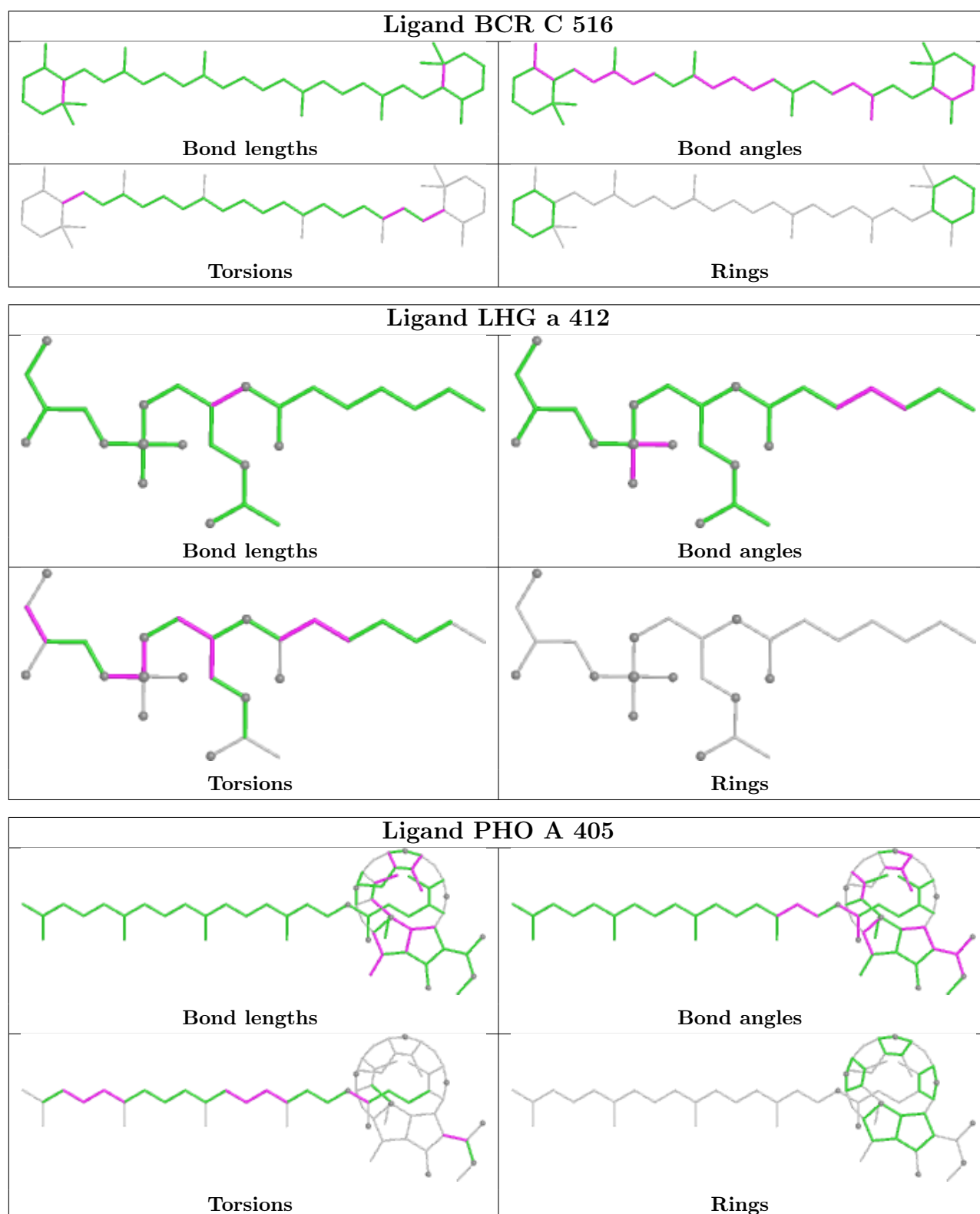


Ligand CLA B 501

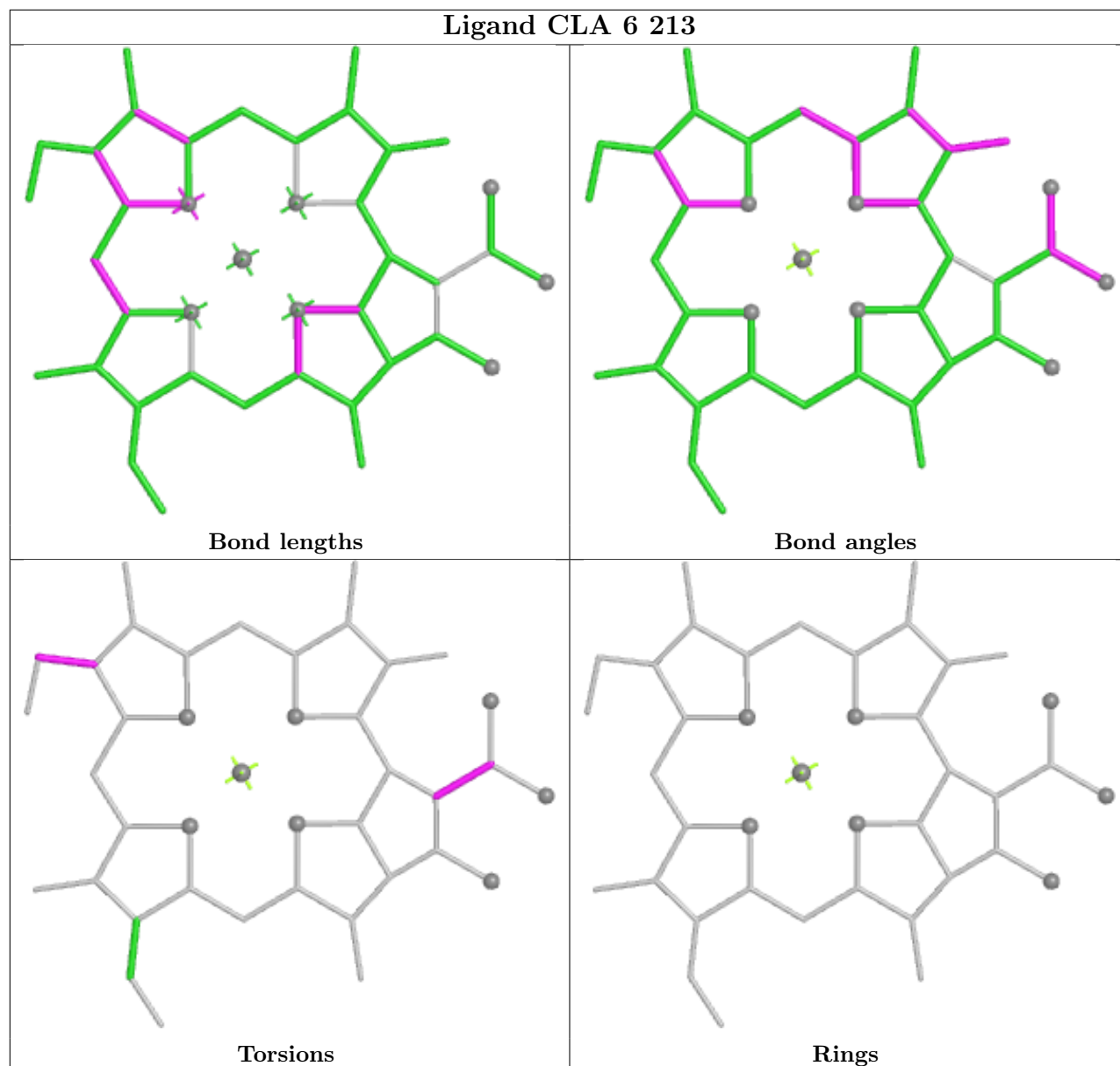


Ligand BCR B 517

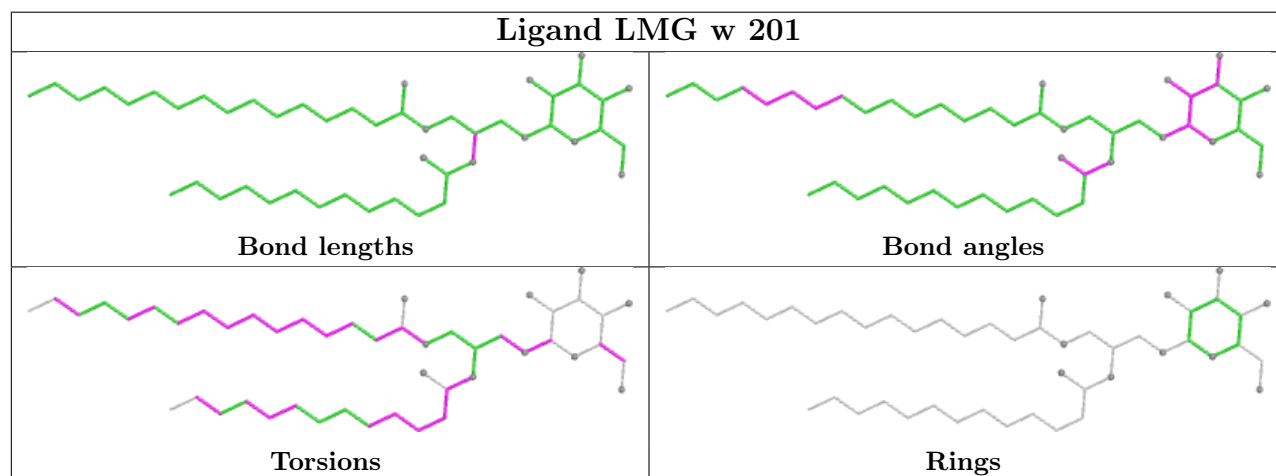




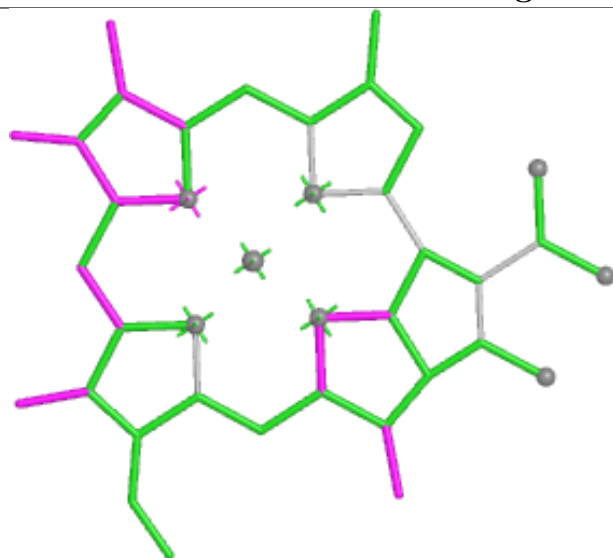
Ligand CLA 6 213



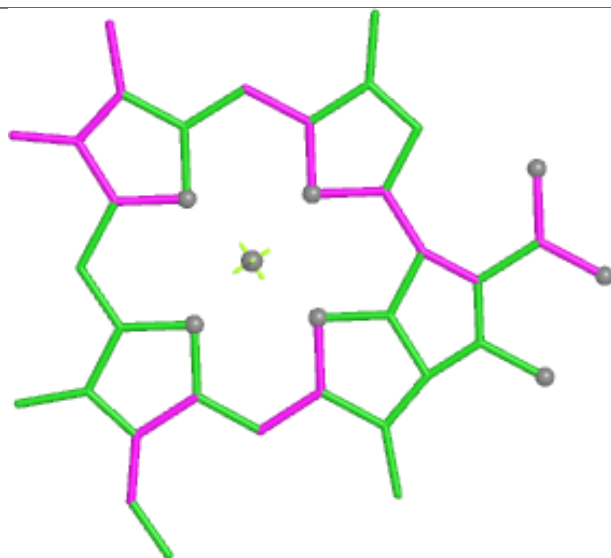
Ligand LMG w 201



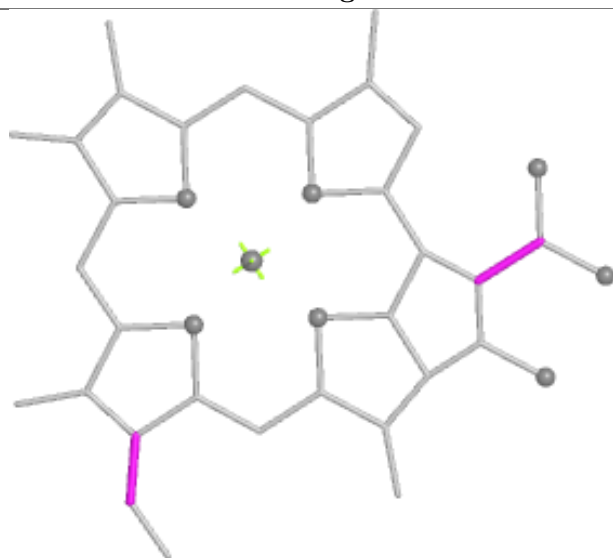
Ligand CLA P 608



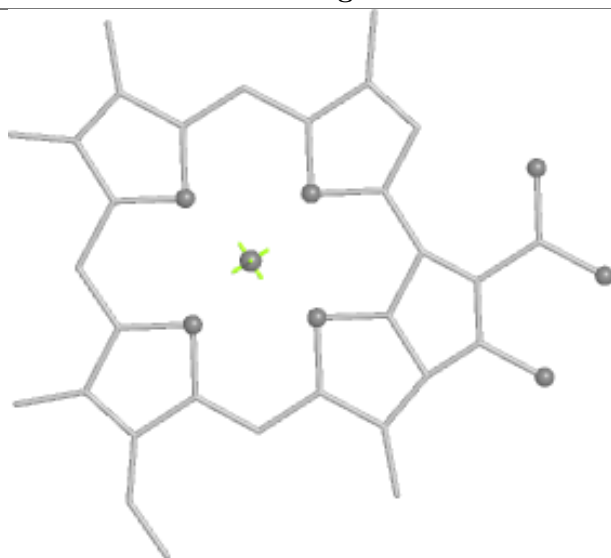
Bond lengths



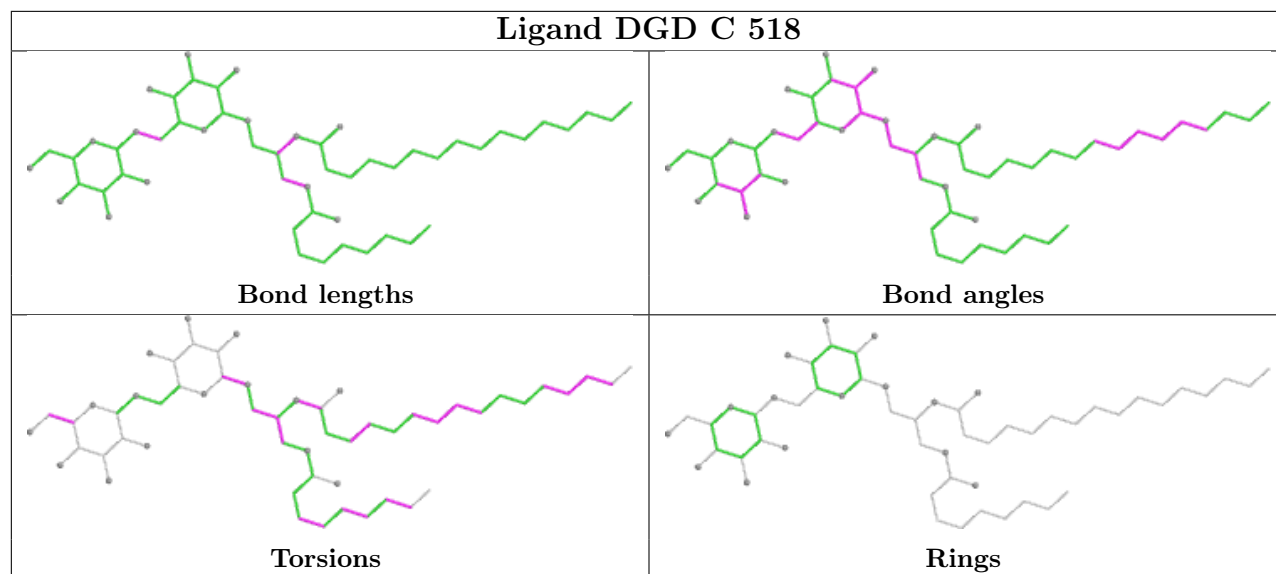
Bond angles



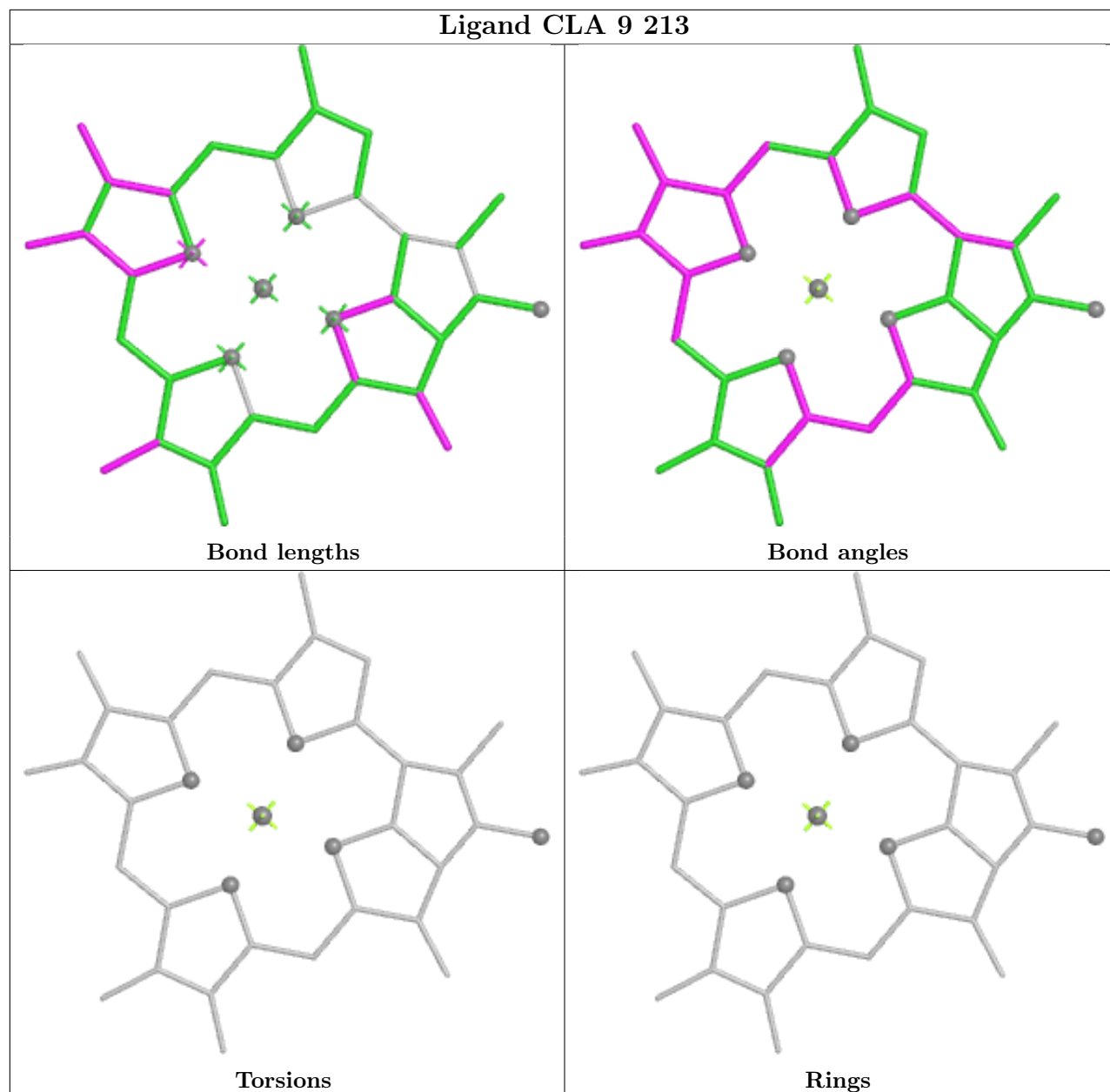
Torsions



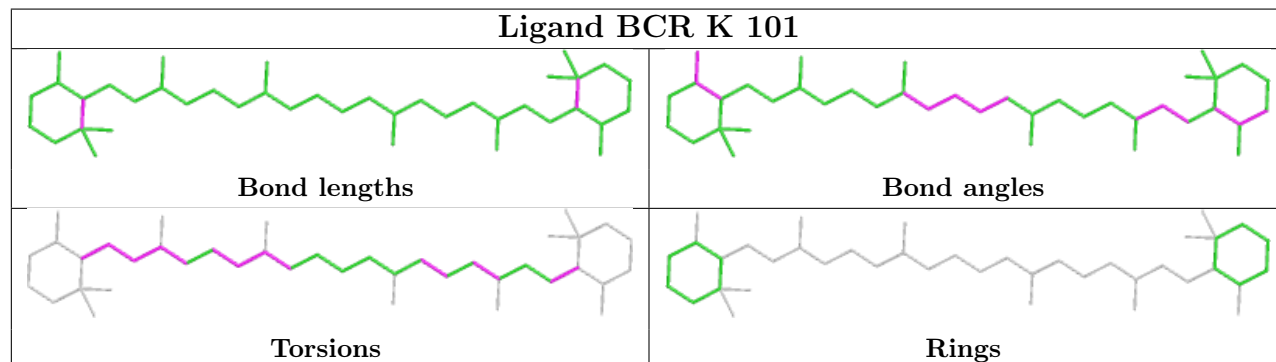
Rings



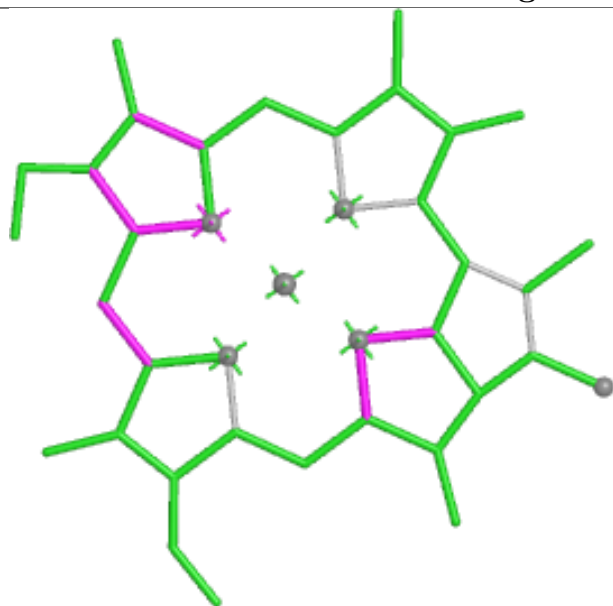
Ligand CLA 9 213



Ligand BCR K 101



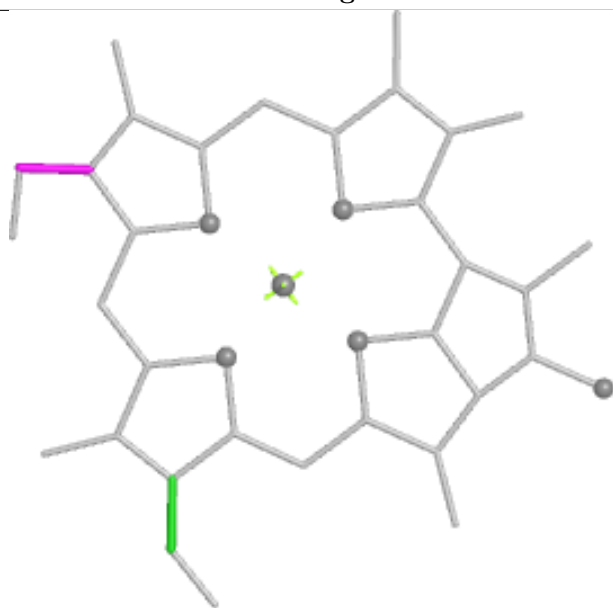
Ligand CLA 7 315



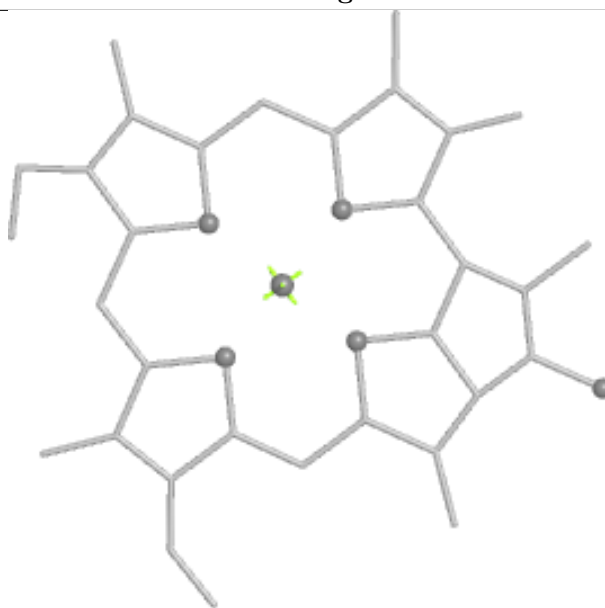
Bond lengths



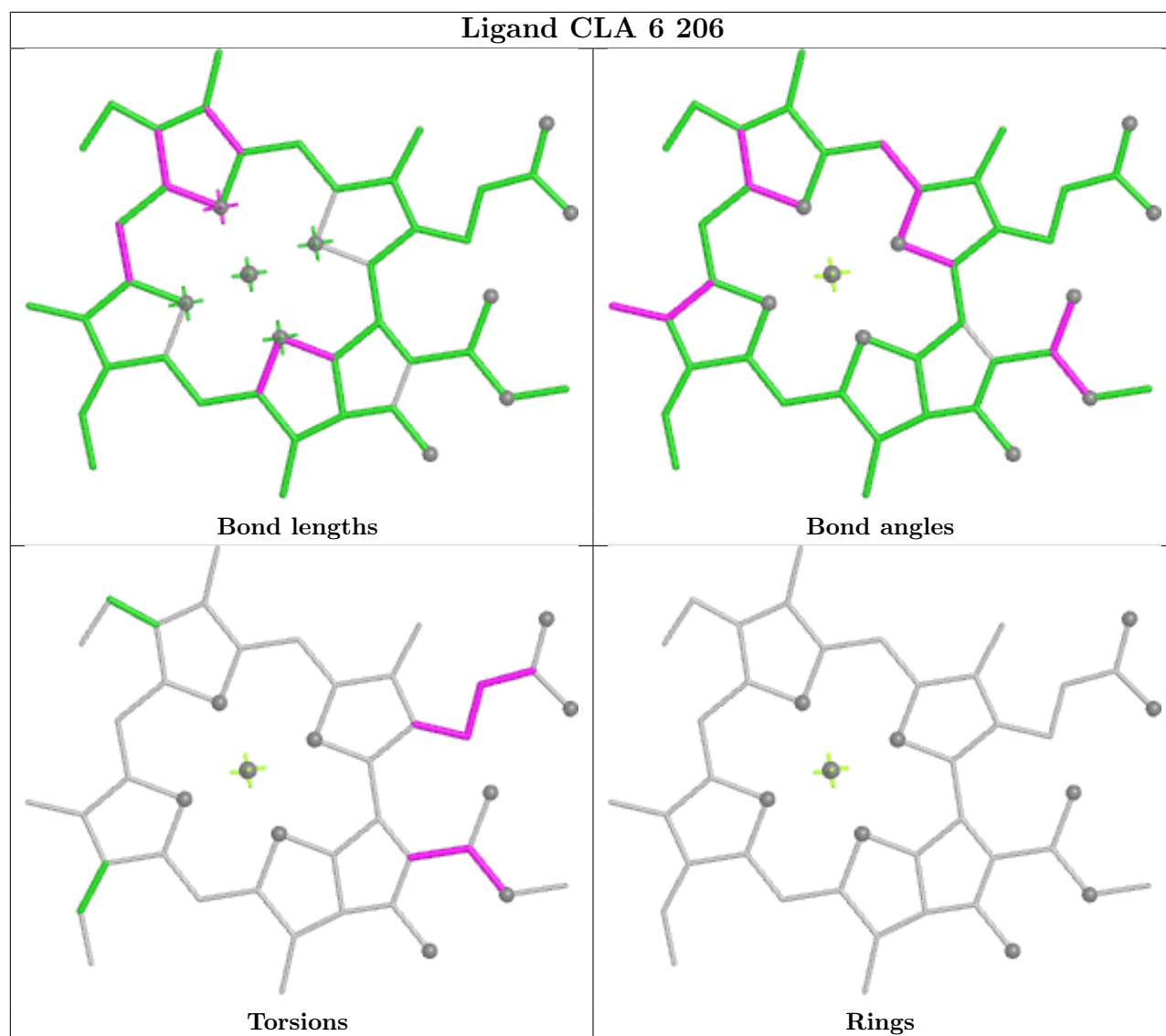
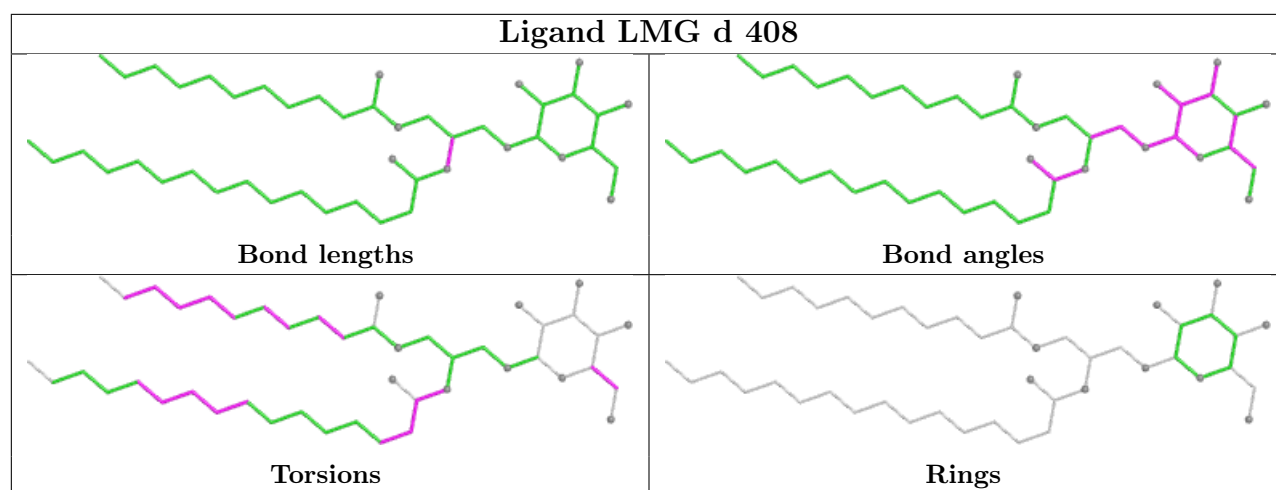
Bond angles



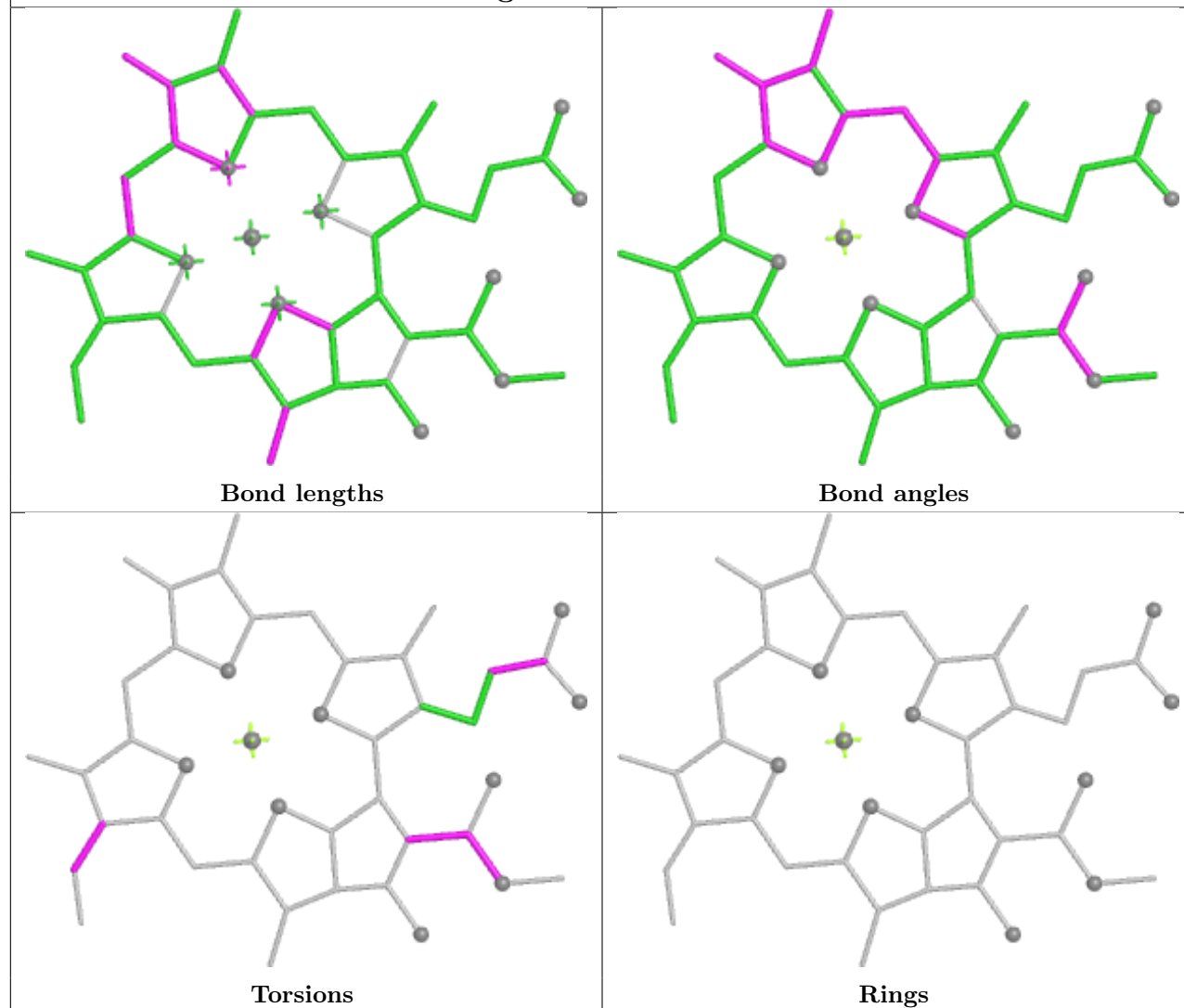
Torsions



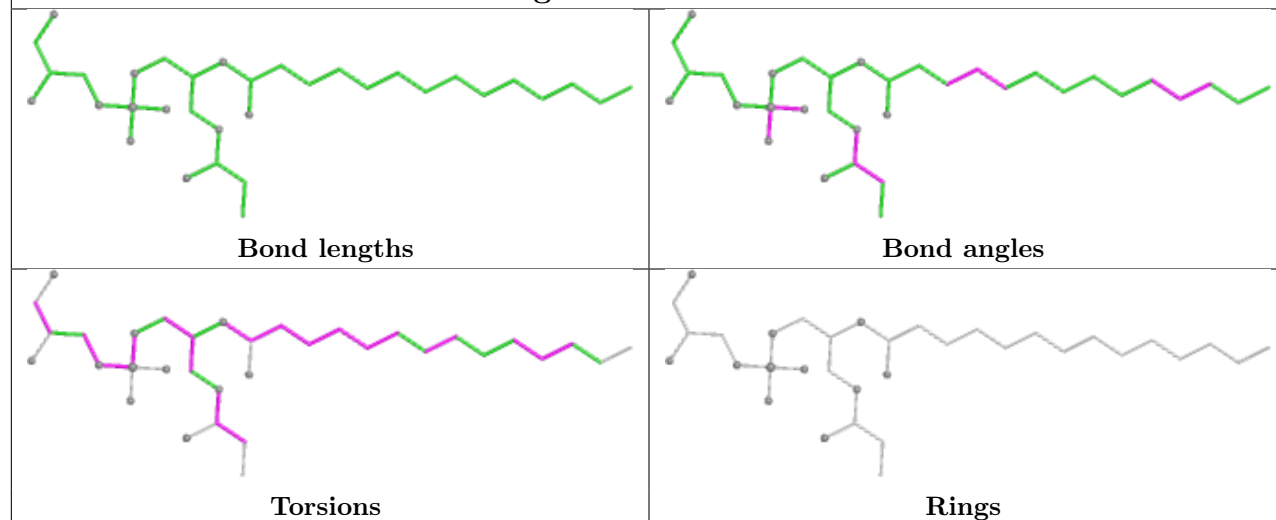
Rings



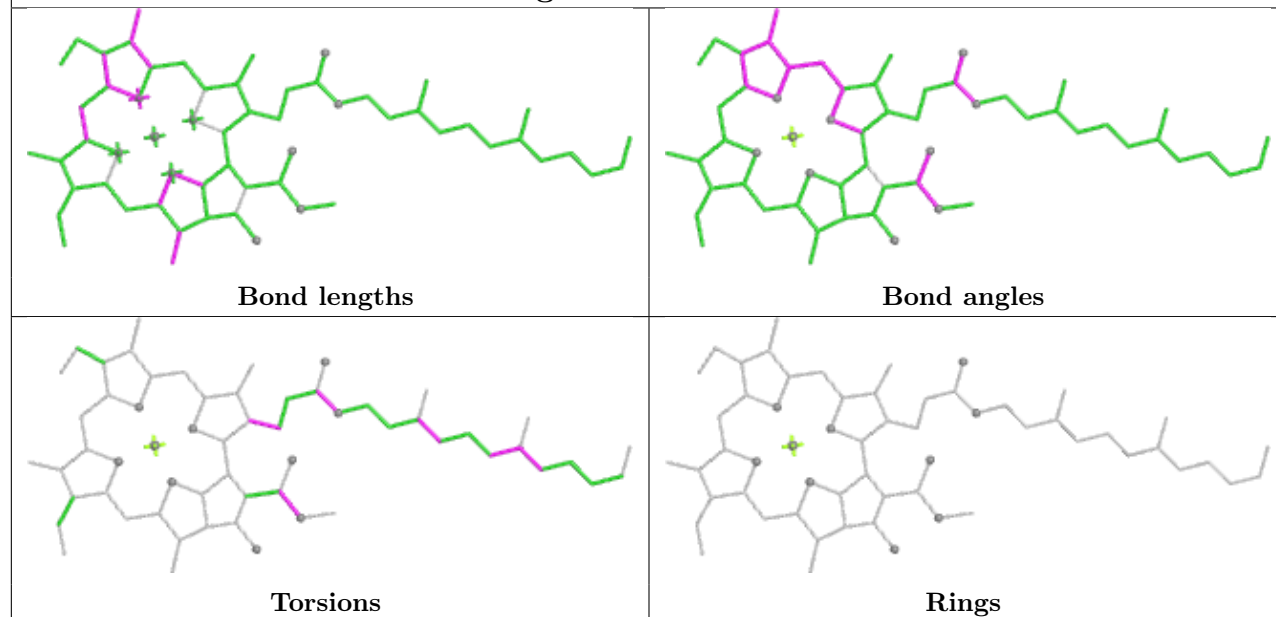
Ligand CLA 6 207



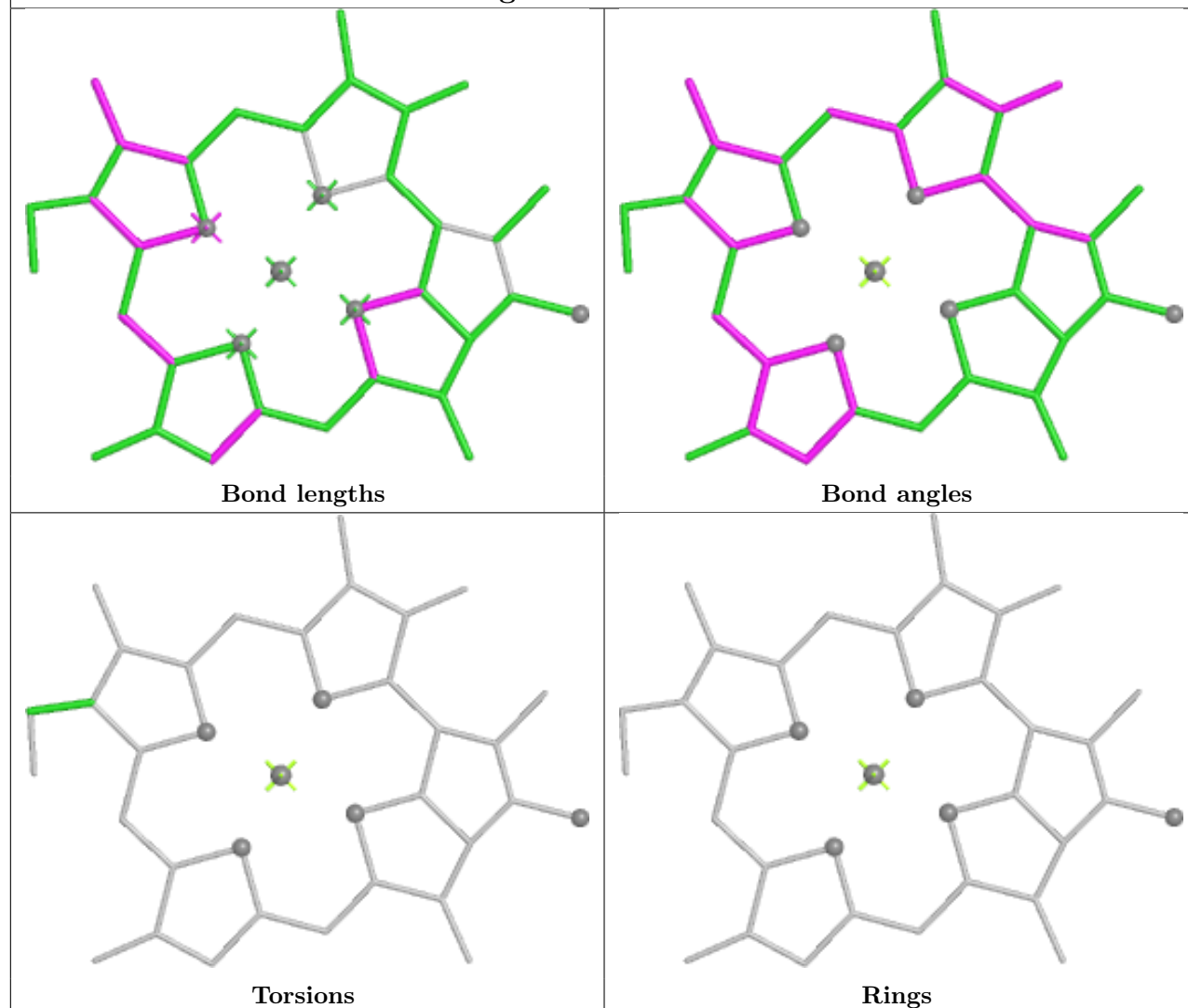
Ligand LHG d 411

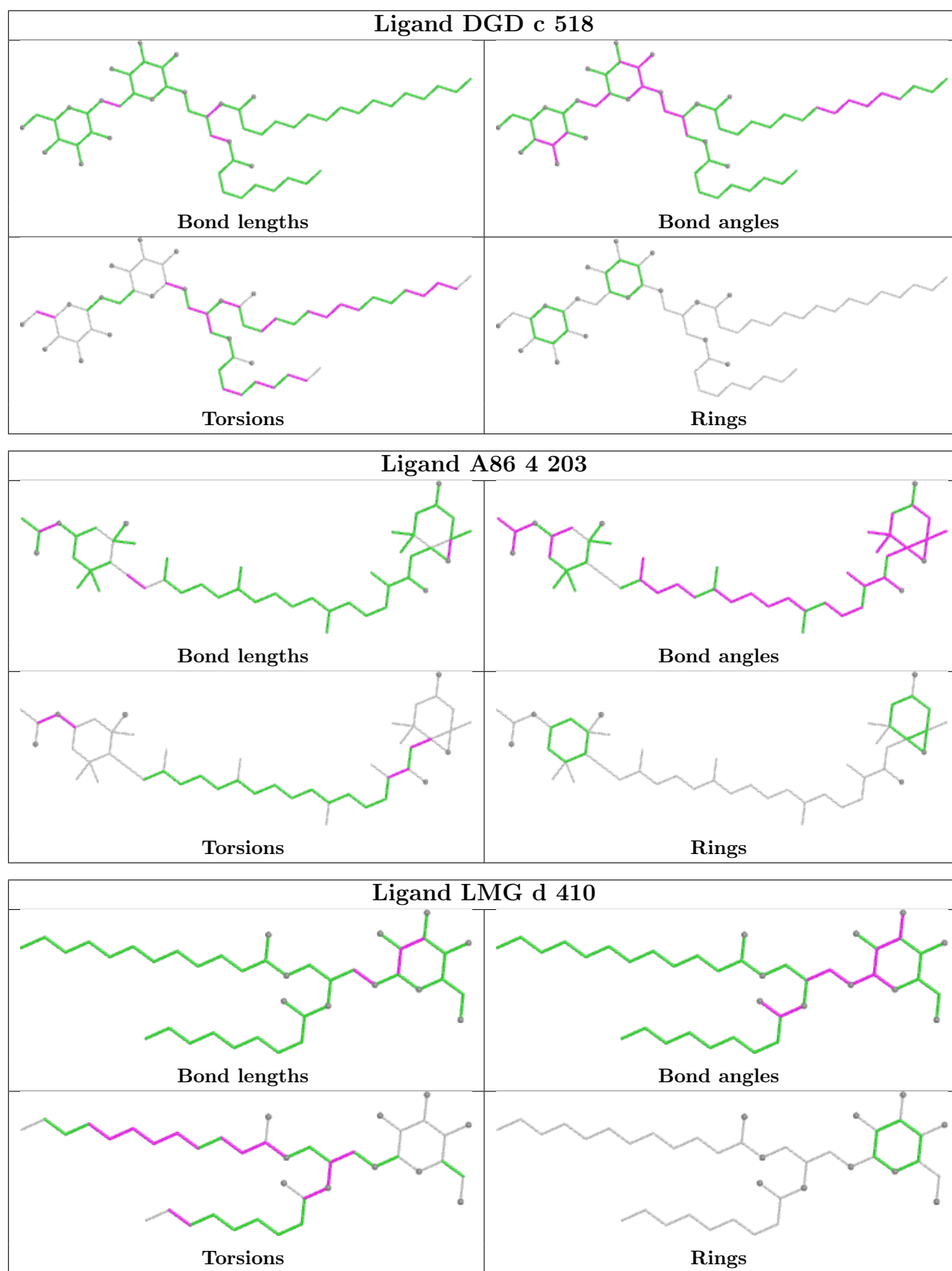


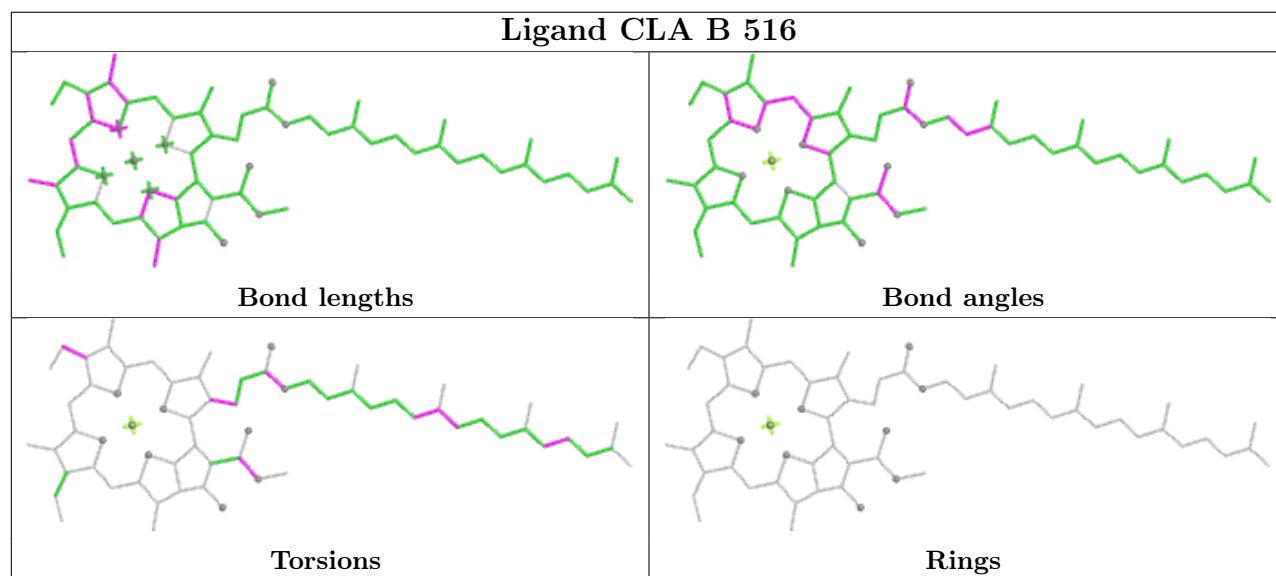
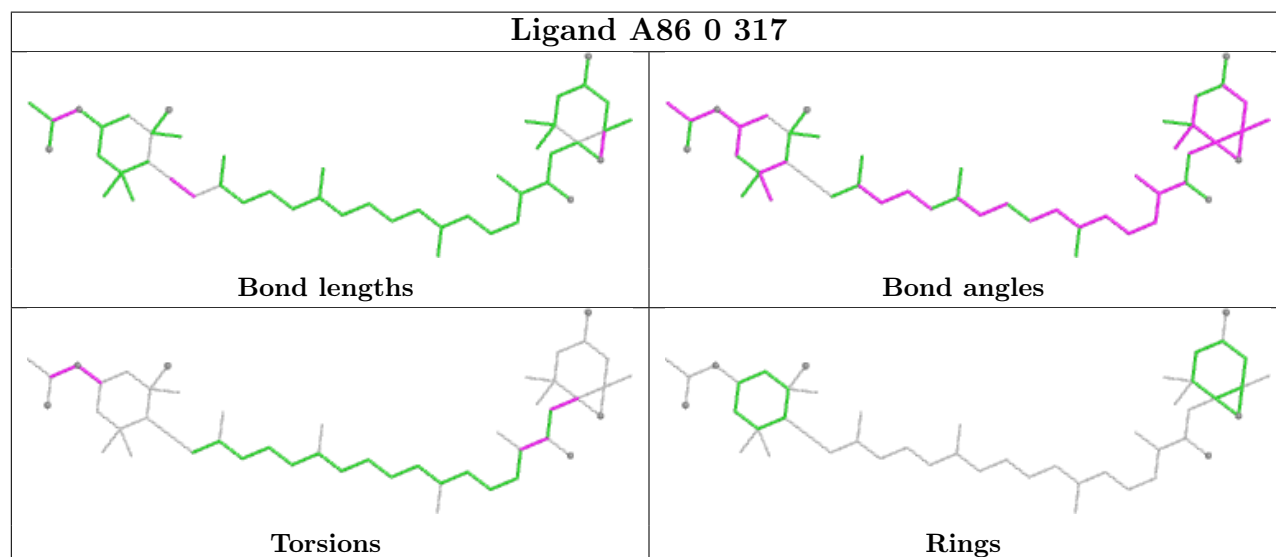
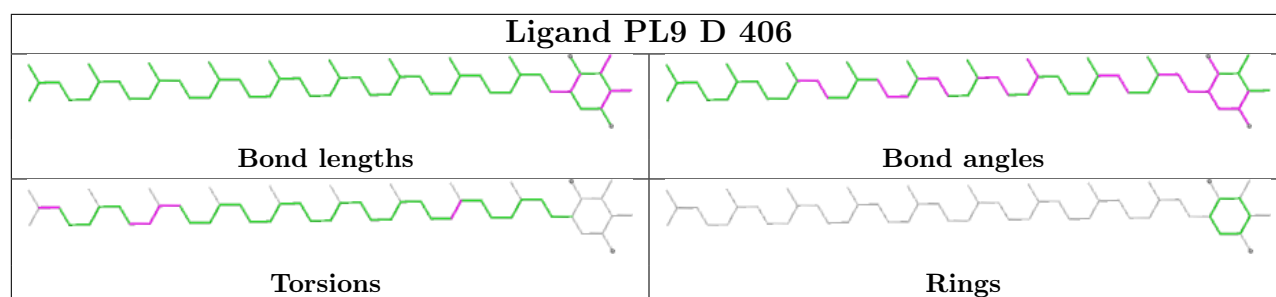
Ligand CLA 2 309



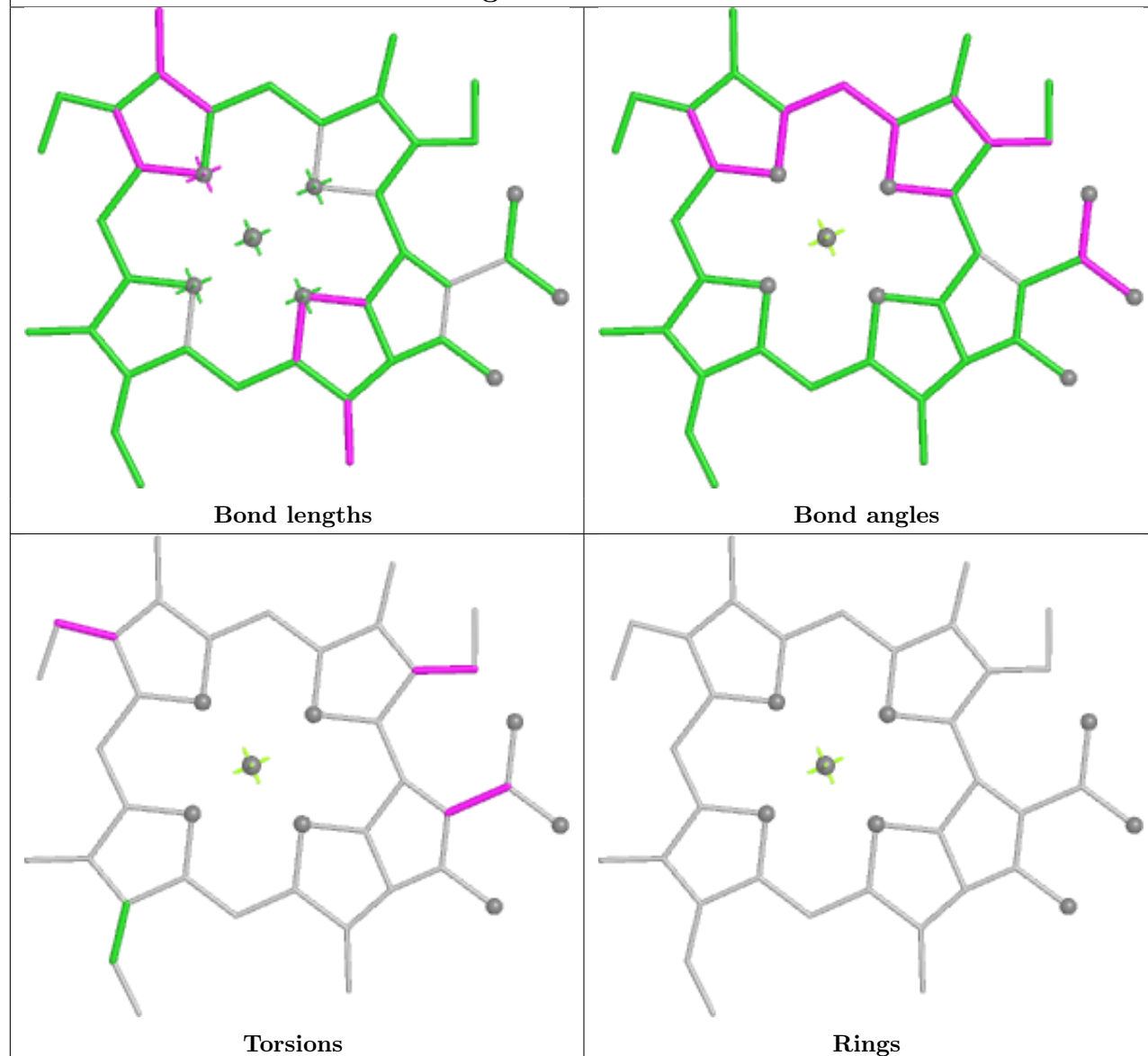
Ligand CLA 7 312



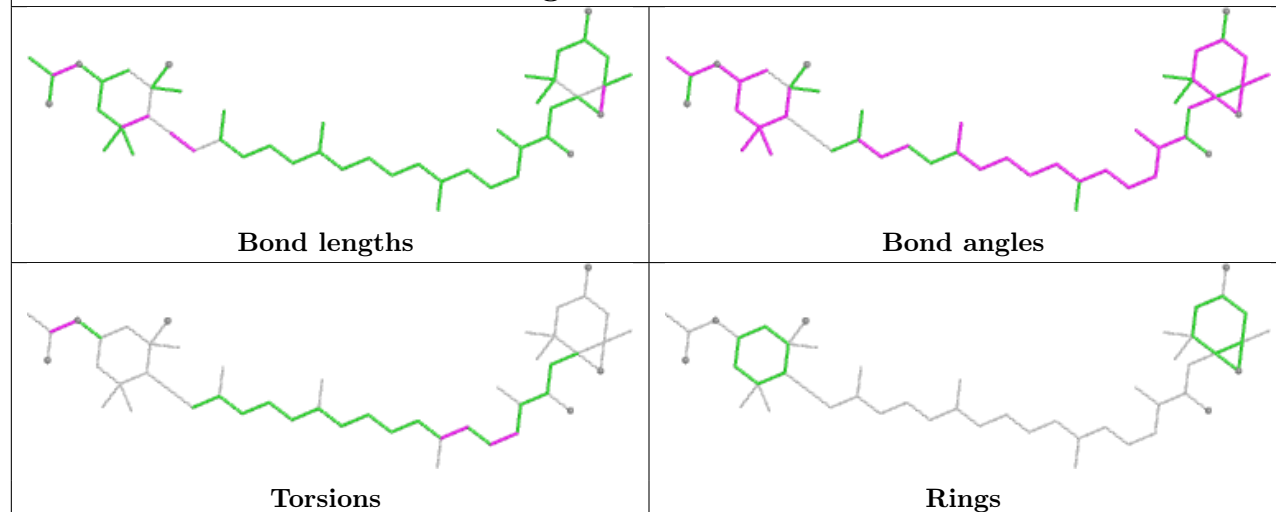




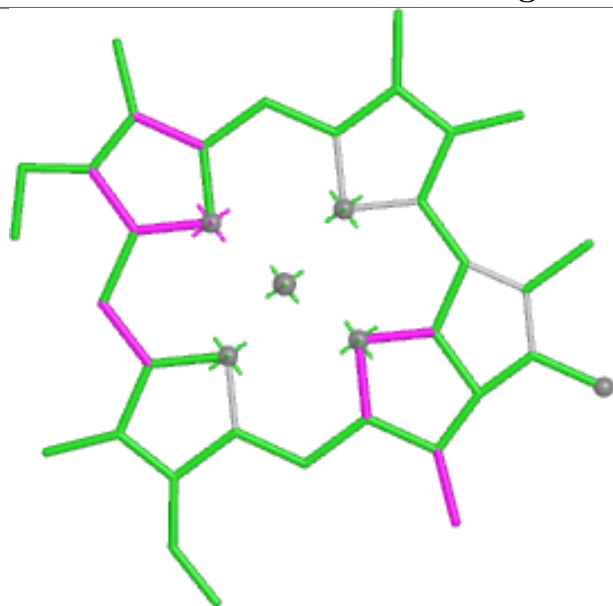
Ligand CLA 8 312



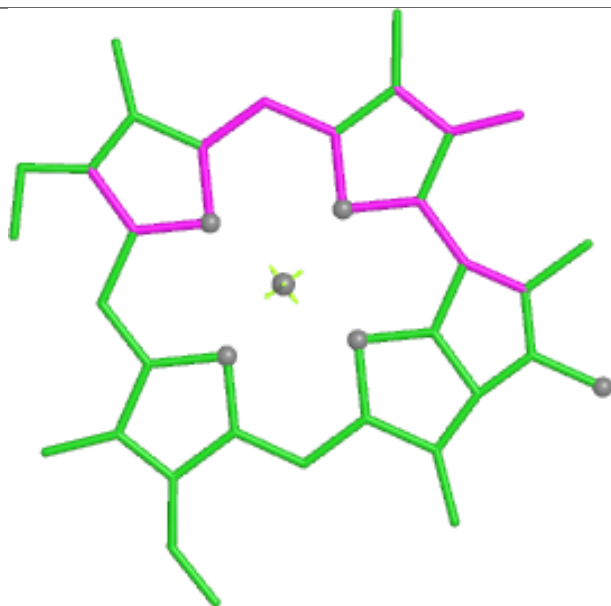
Ligand A86 5 303



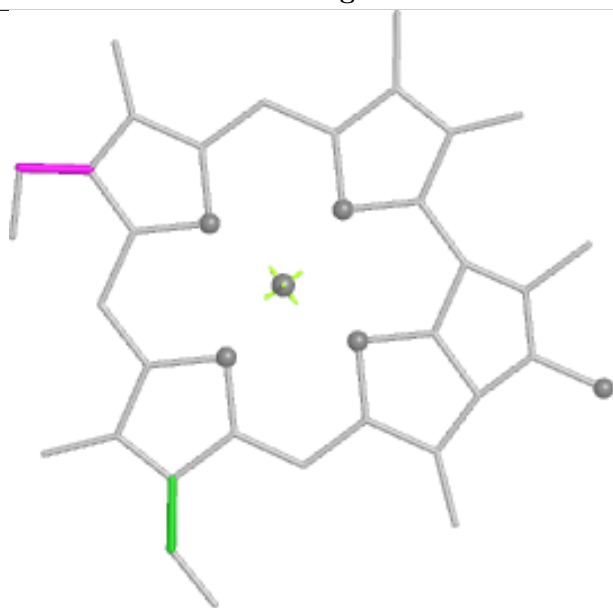
Ligand CLA 2 313



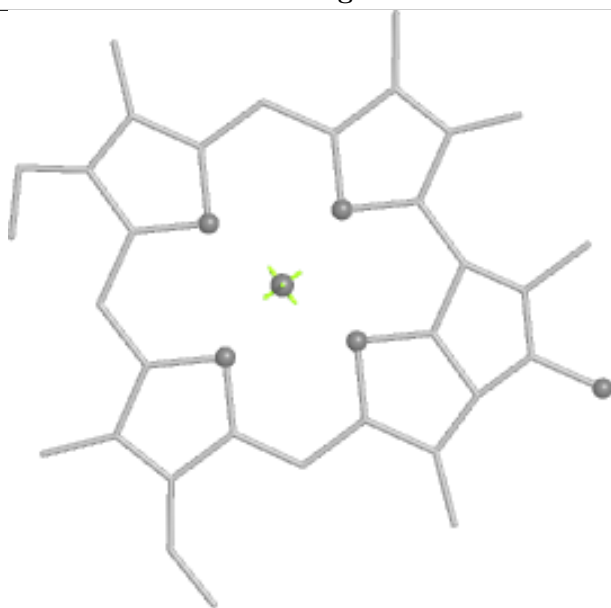
Bond lengths



Bond angles

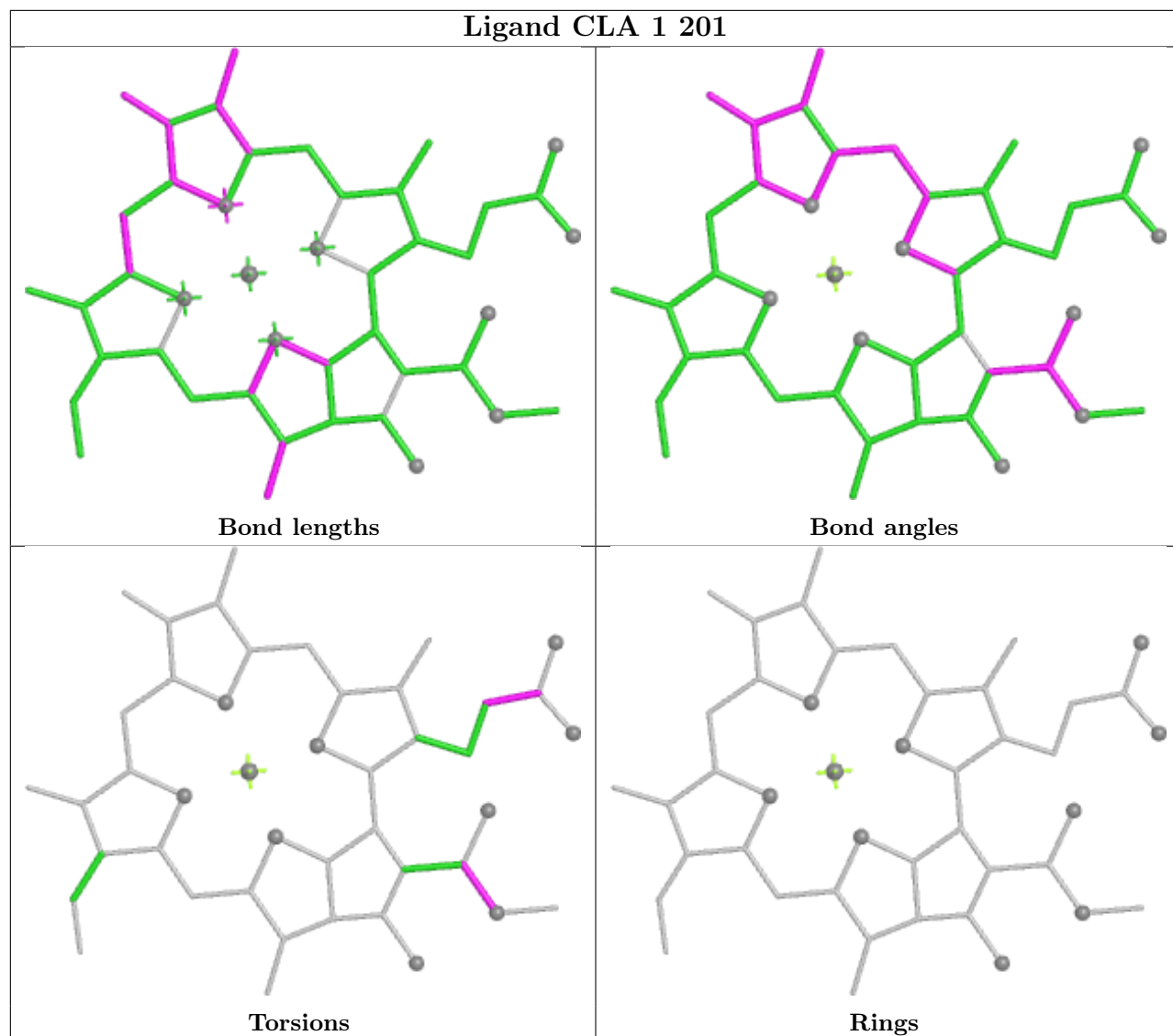


Torsions

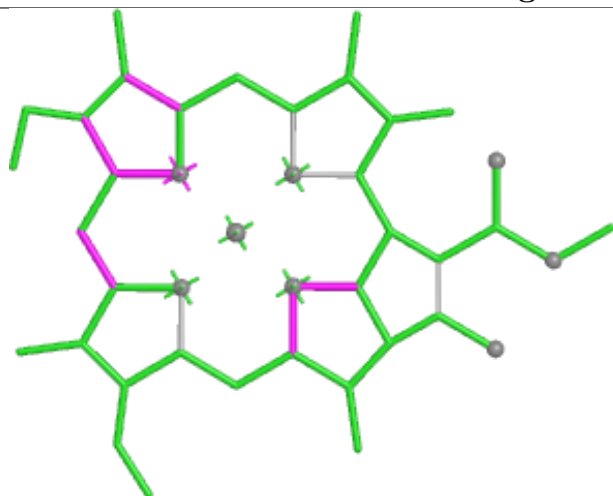


Rings

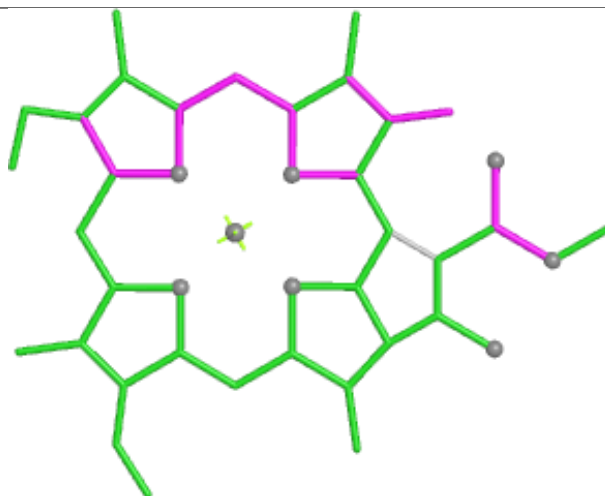
Ligand CLA 1 201



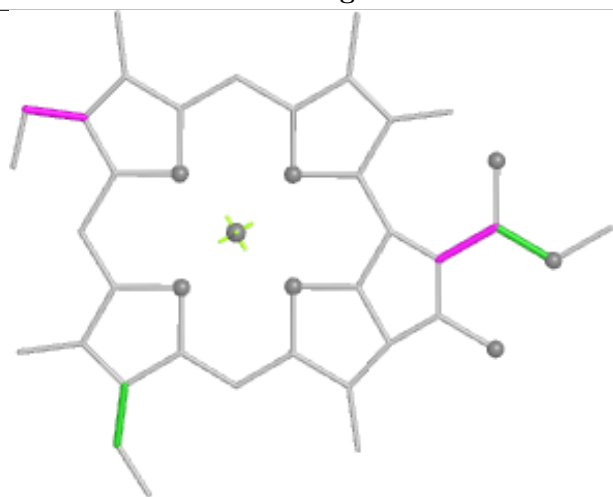
Ligand CLA 6 205



Bond lengths



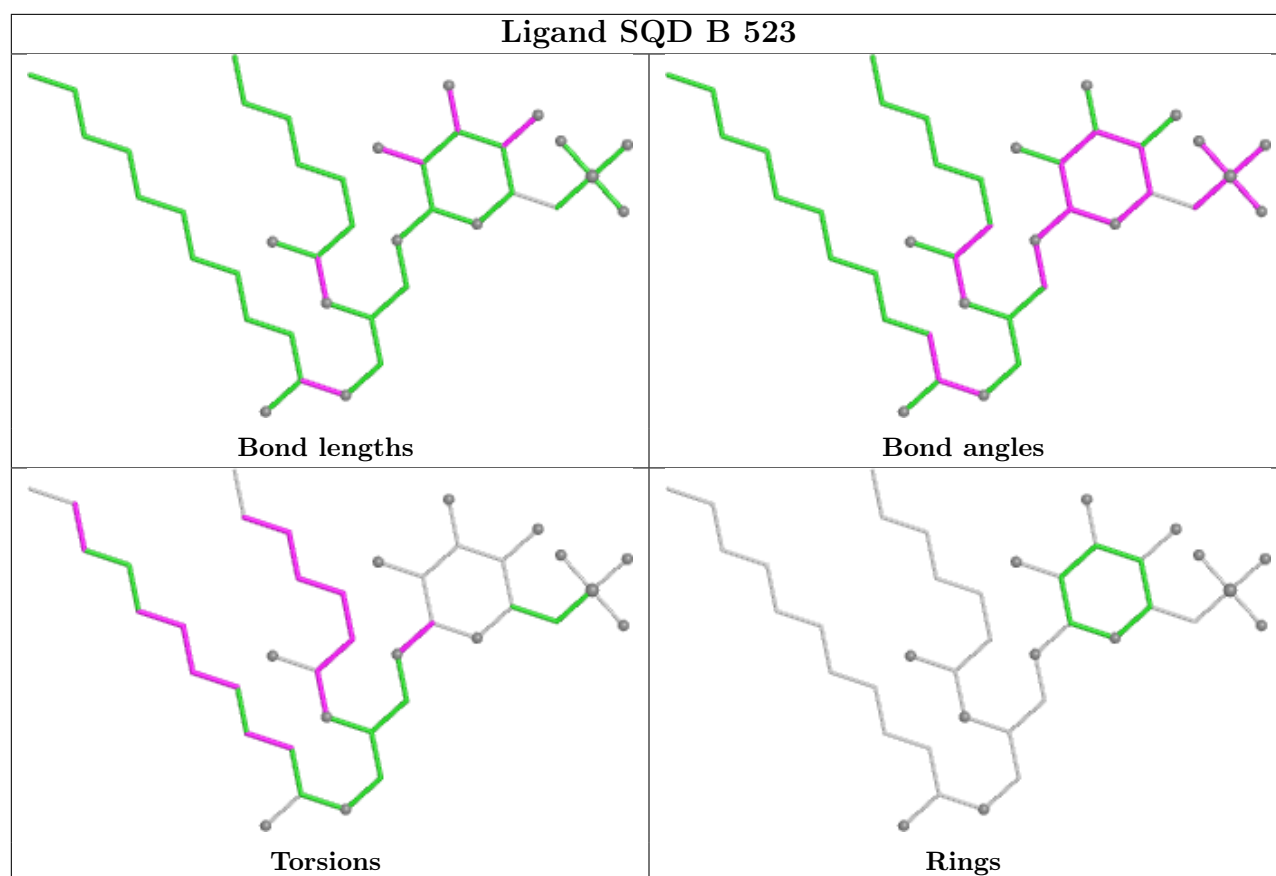
Bond angles

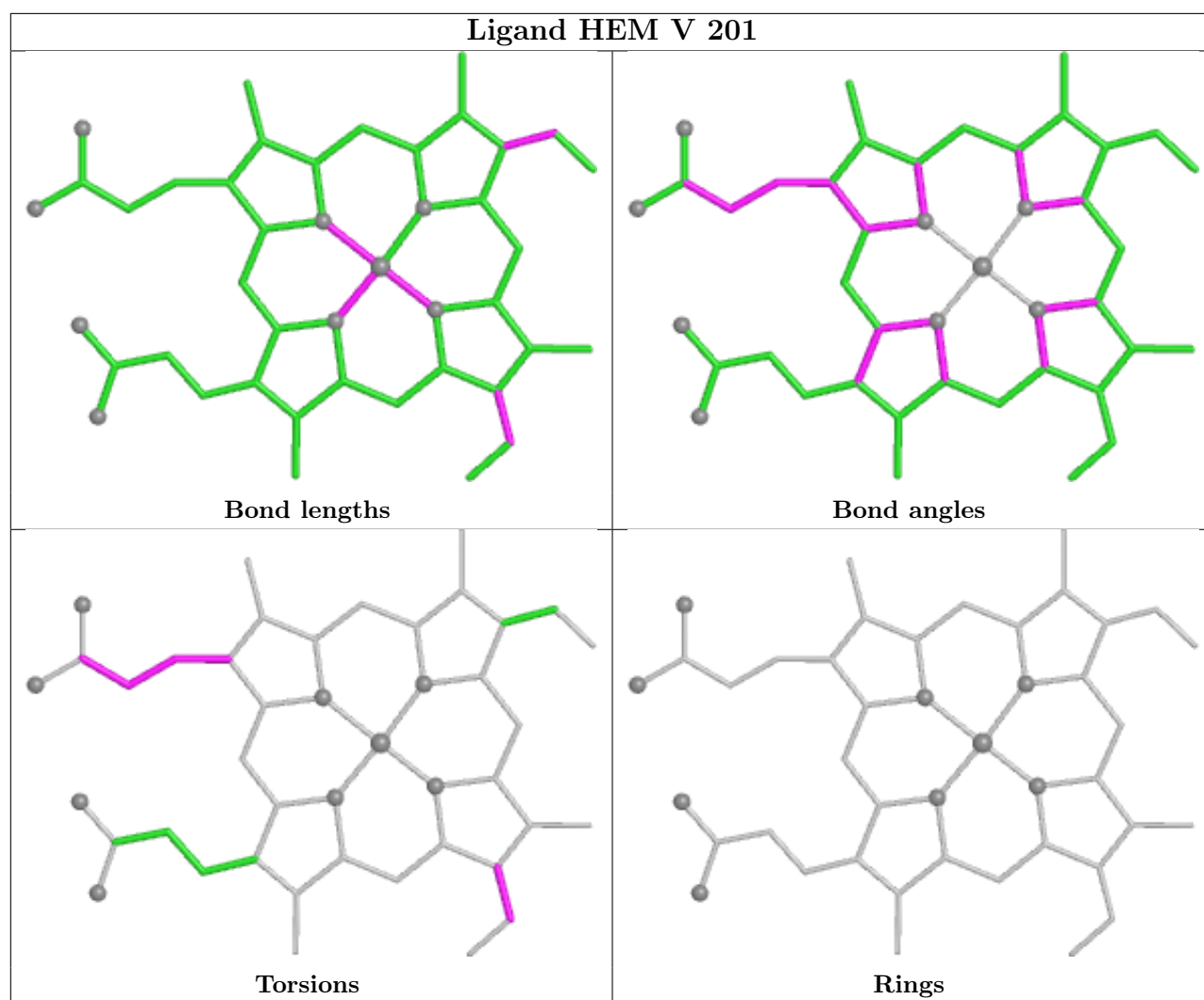


Torsions

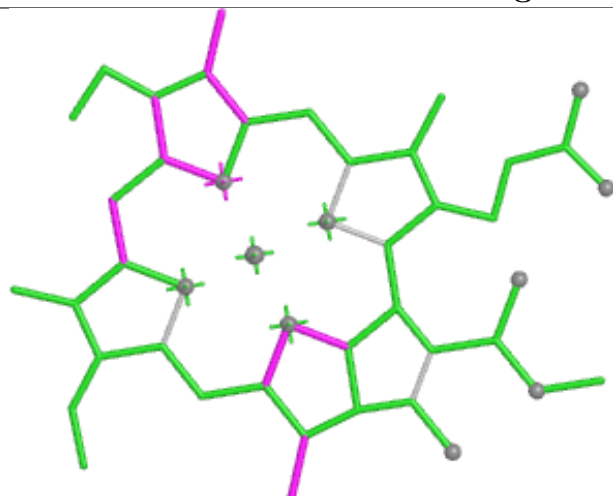


Rings

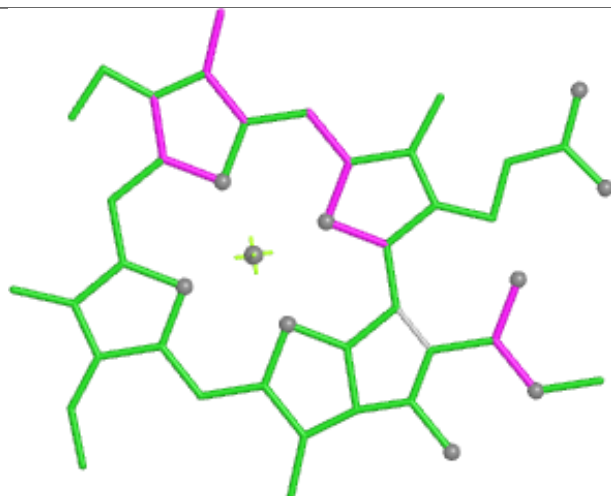




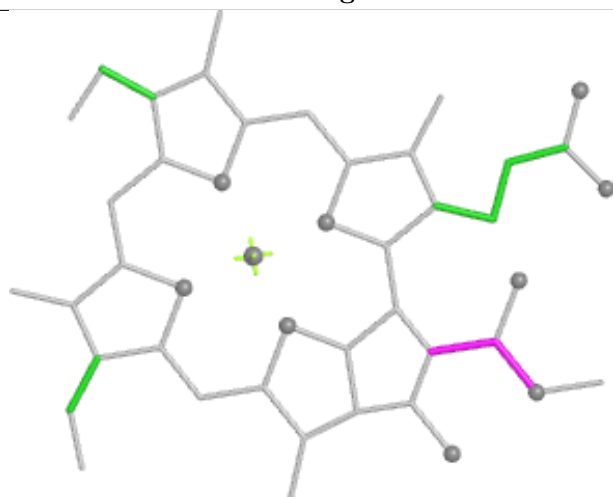
Ligand CLA C 507



Bond lengths



Bond angles

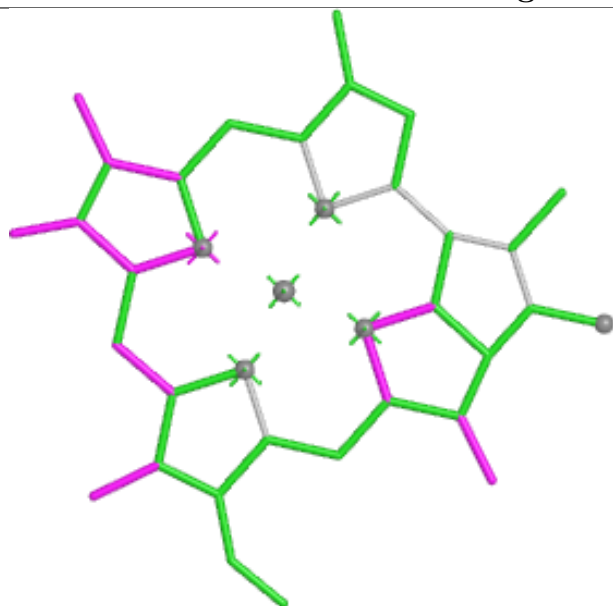


Torsions

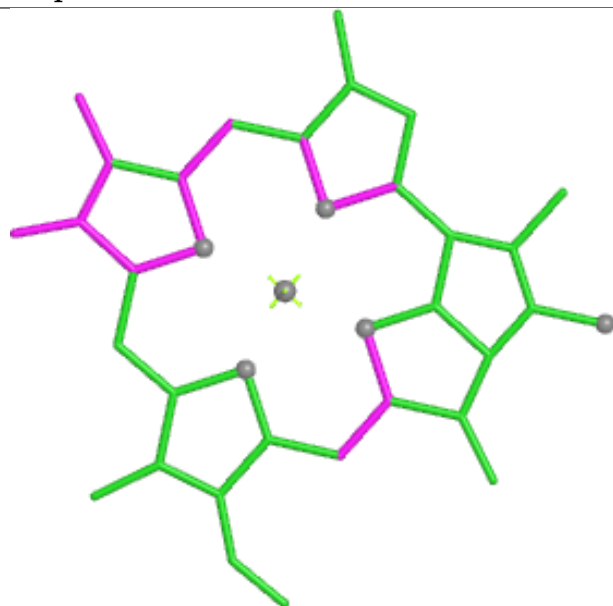


Rings

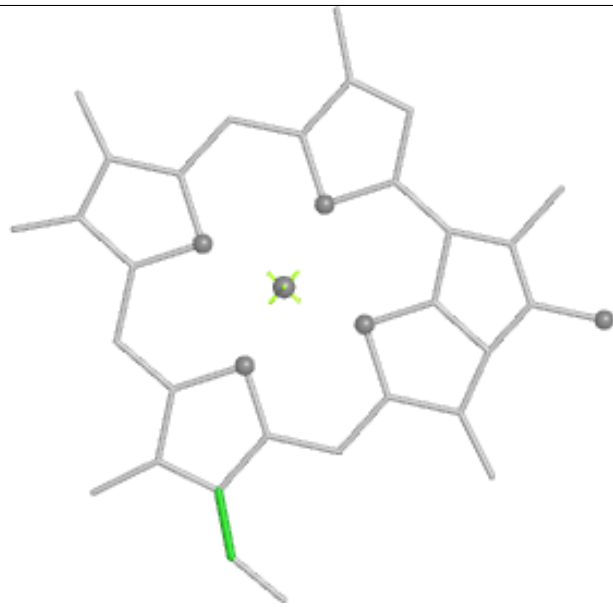
Ligand CLA p 607



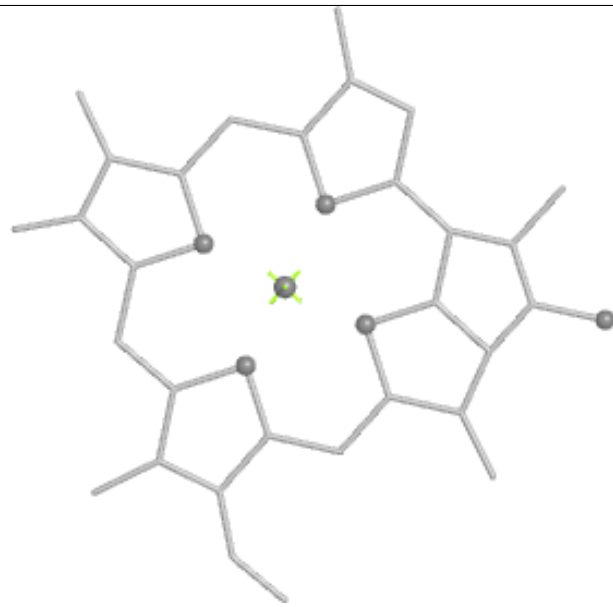
Bond lengths



Bond angles

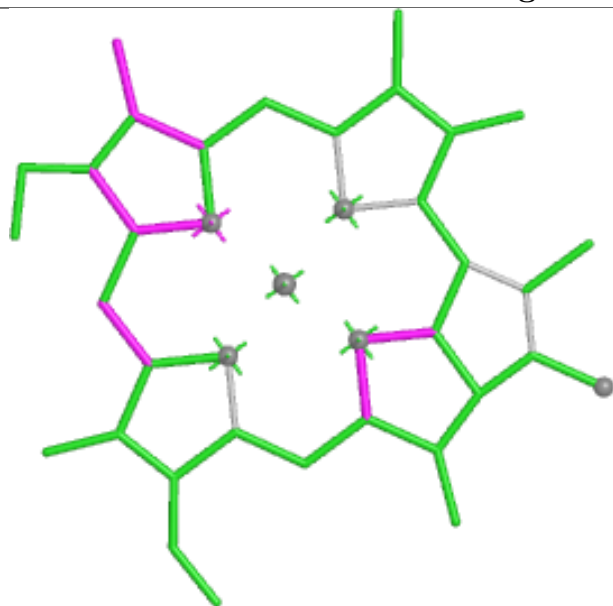


Torsions



Rings

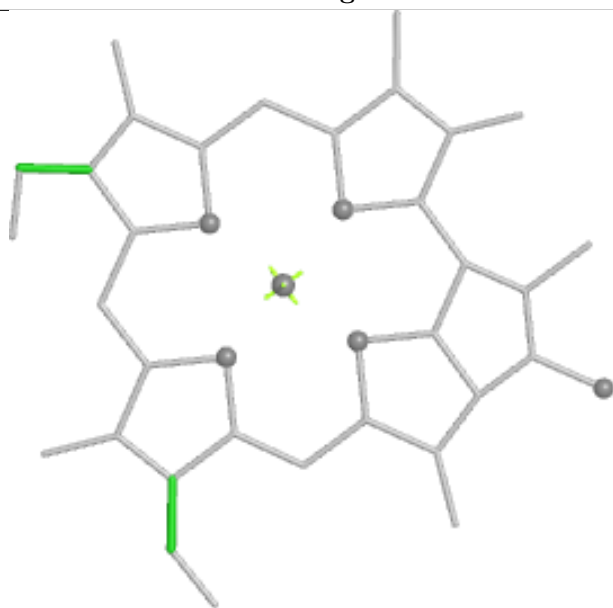
Ligand CLA 9 210



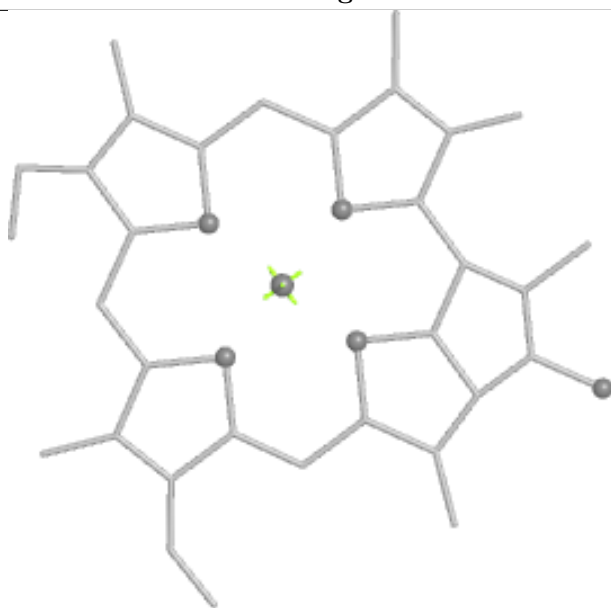
Bond lengths



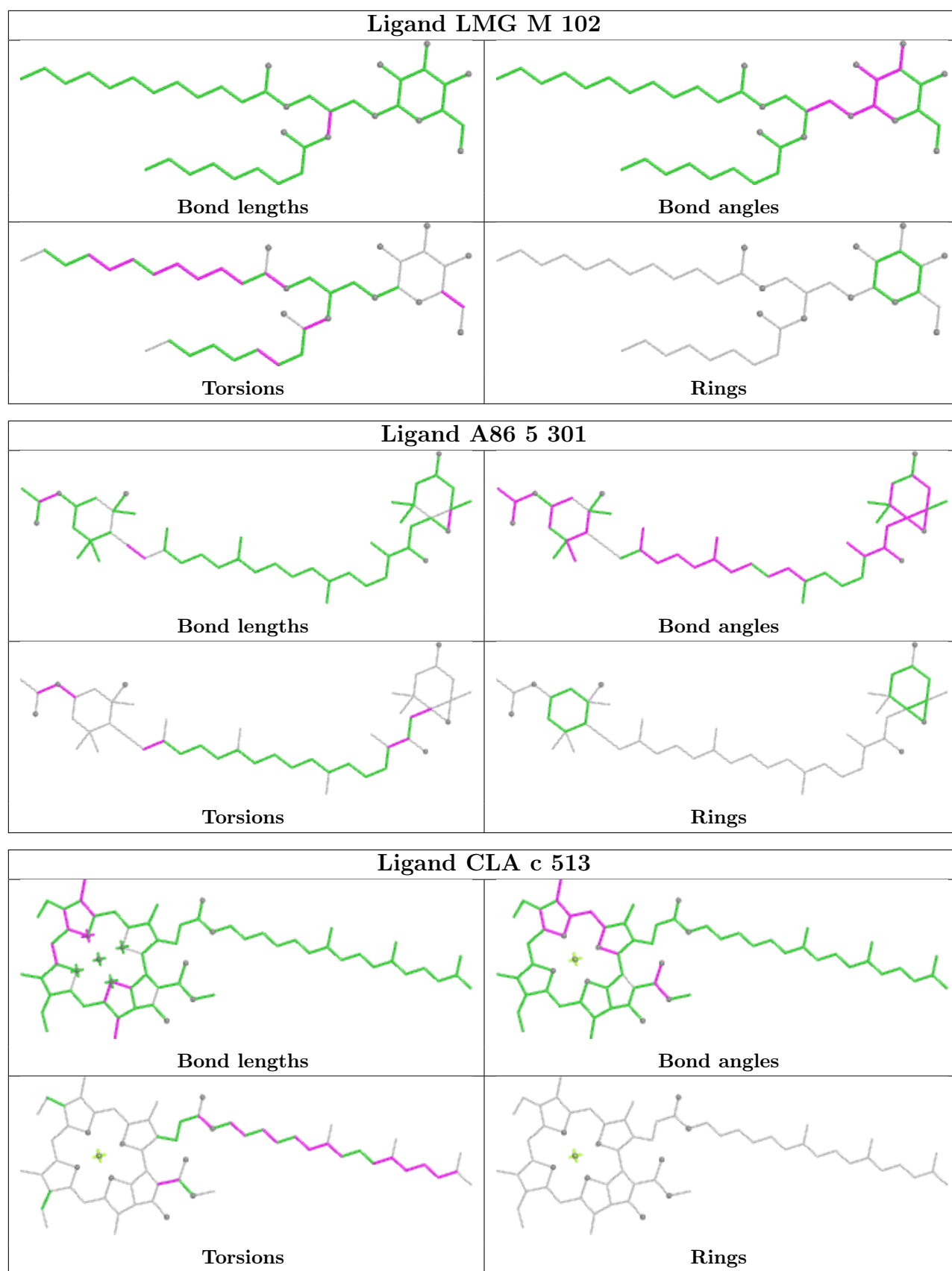
Bond angles

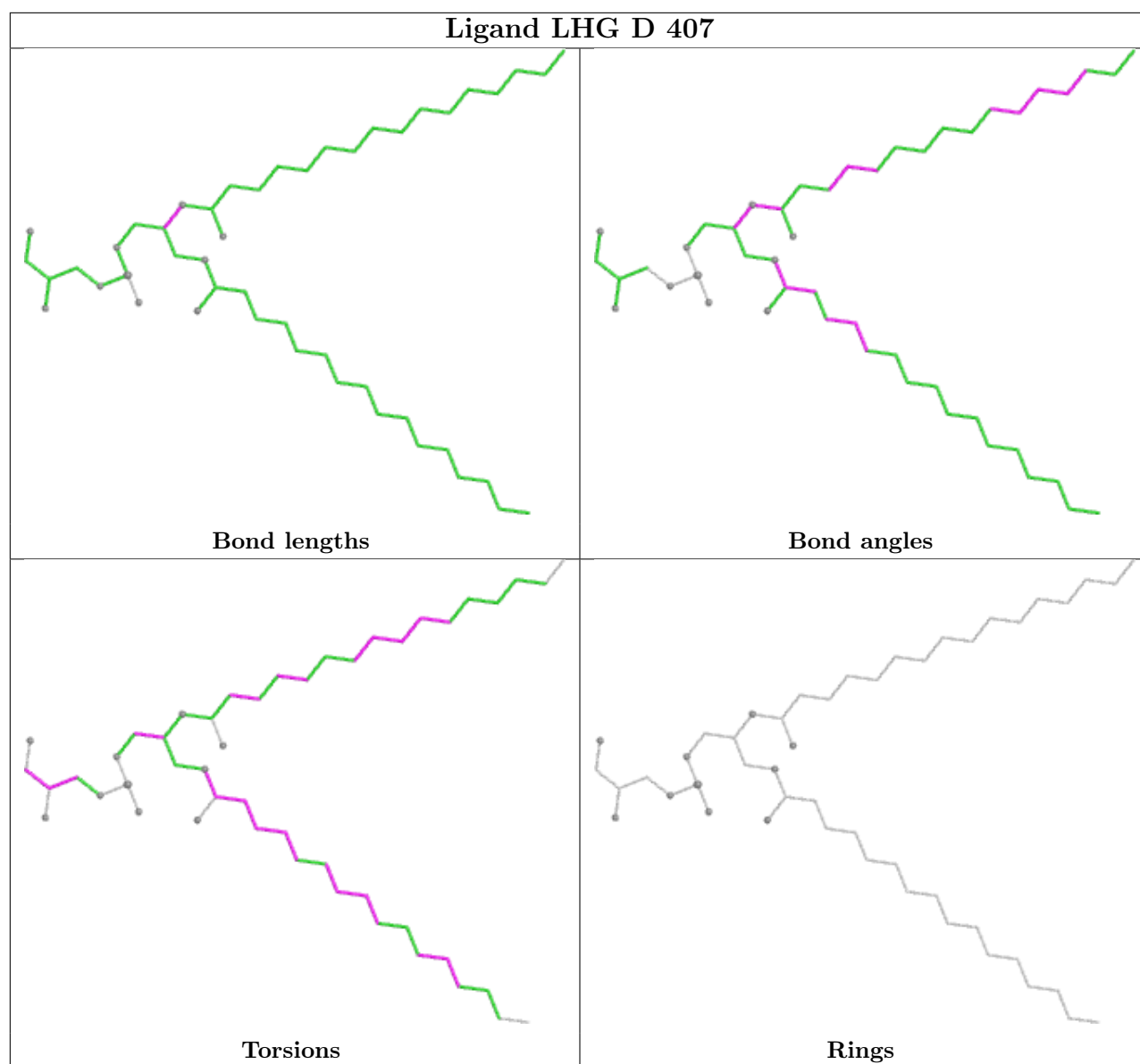


Torsions

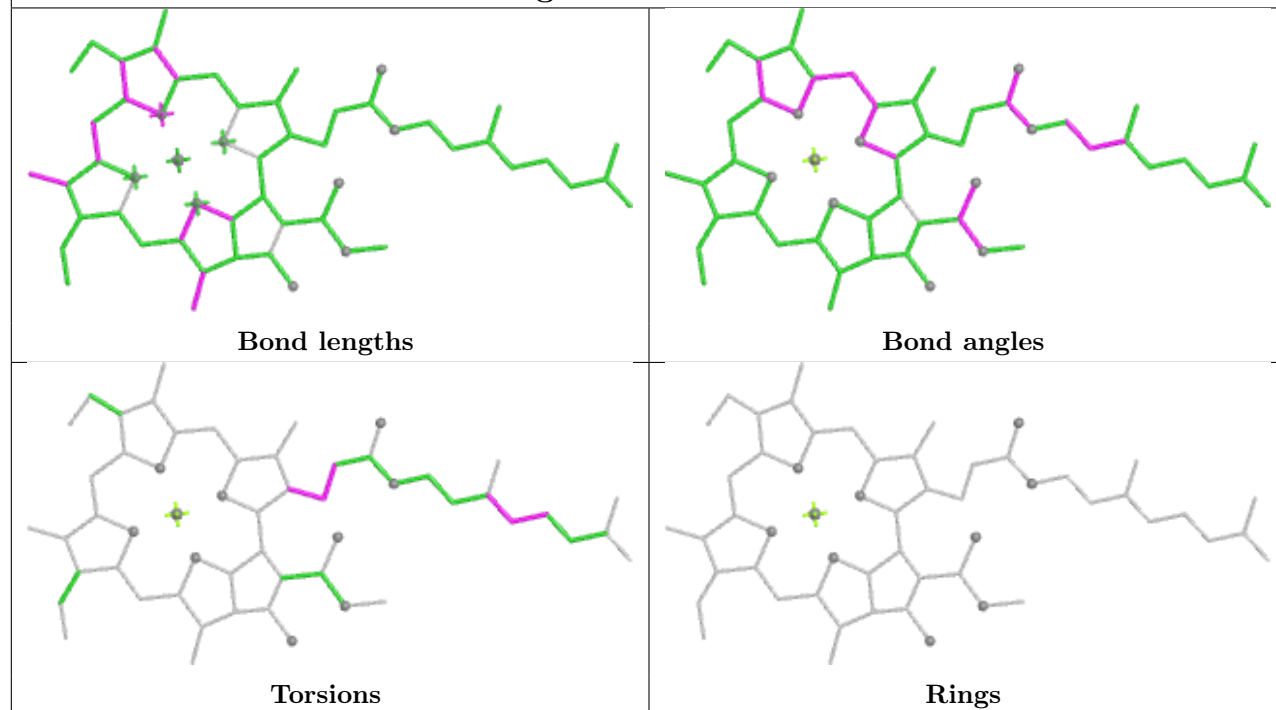


Rings

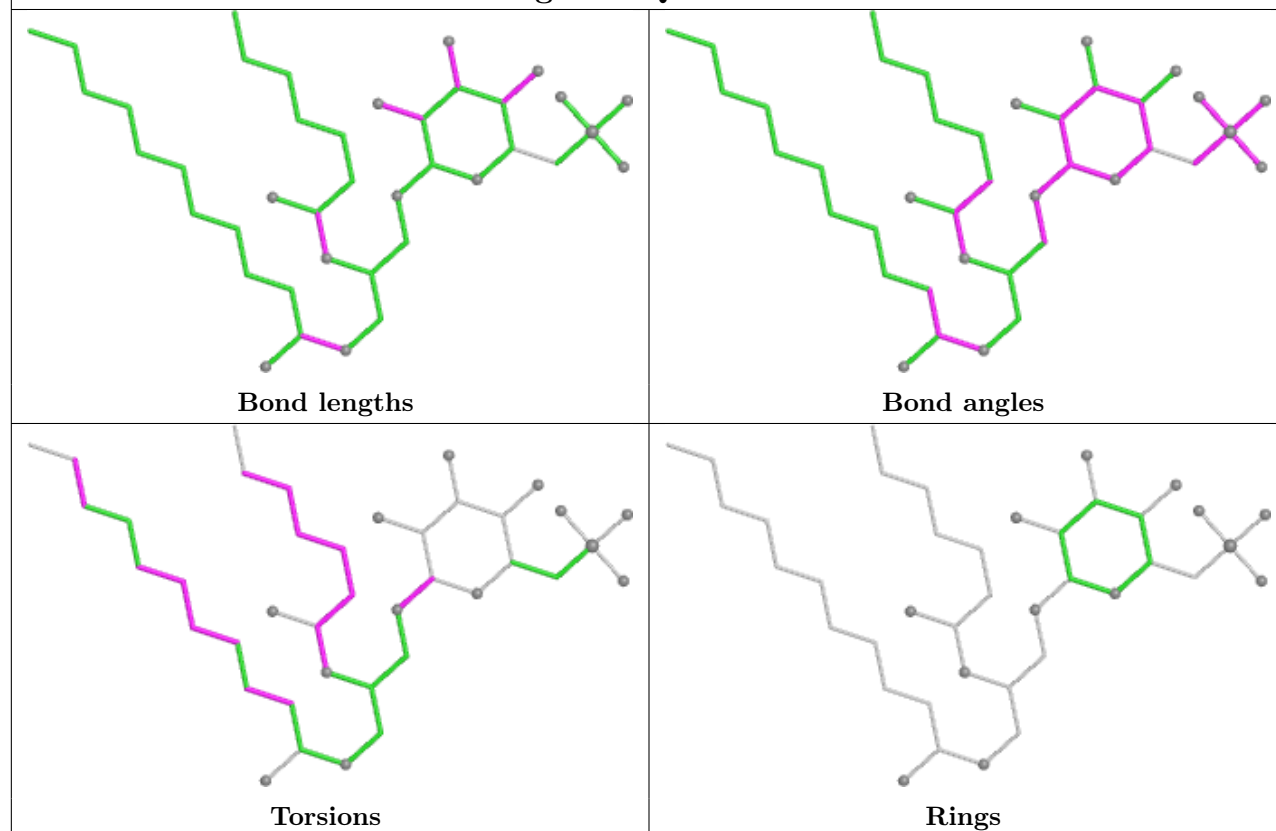


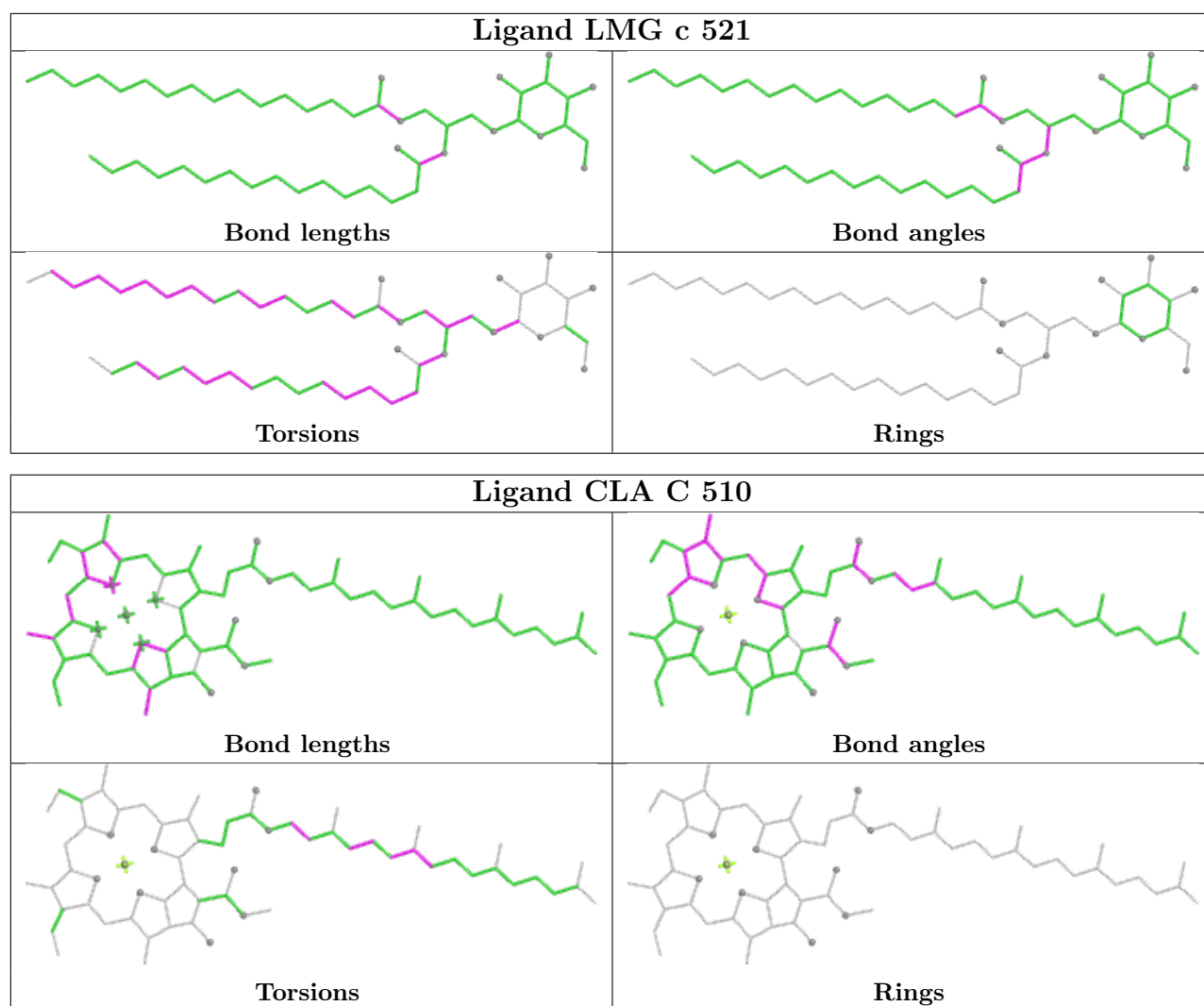


Ligand CLA 0 310

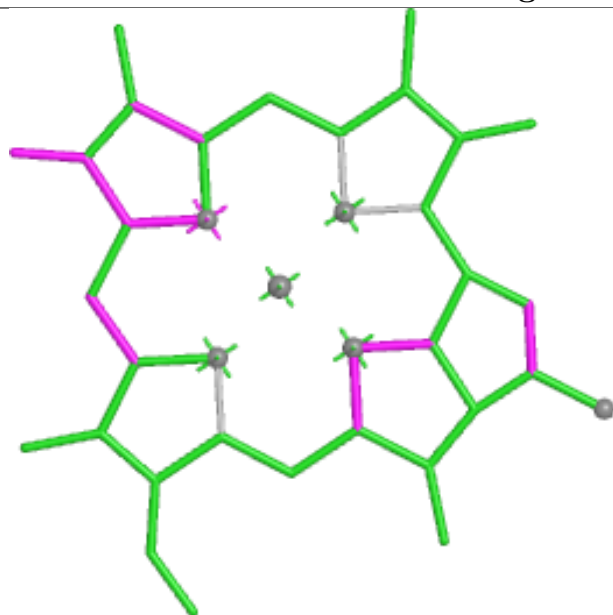


Ligand SQD b 501

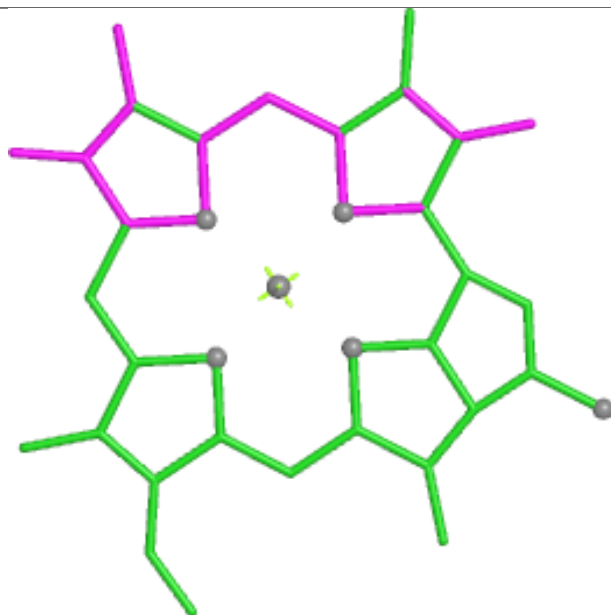




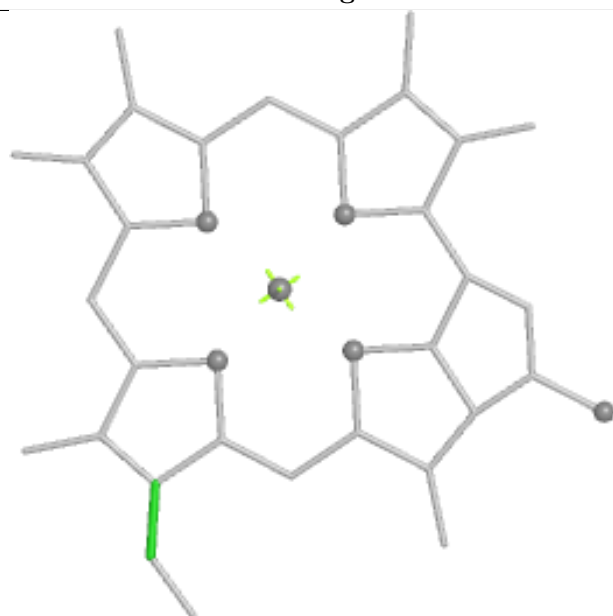
Ligand CLA 9 212



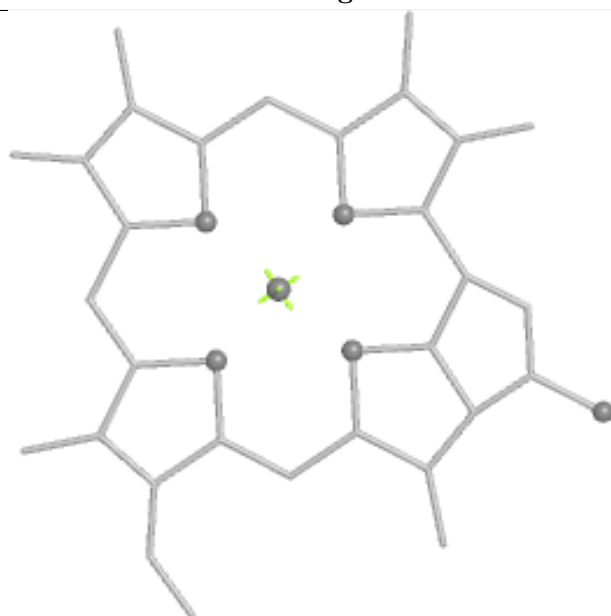
Bond lengths



Bond angles

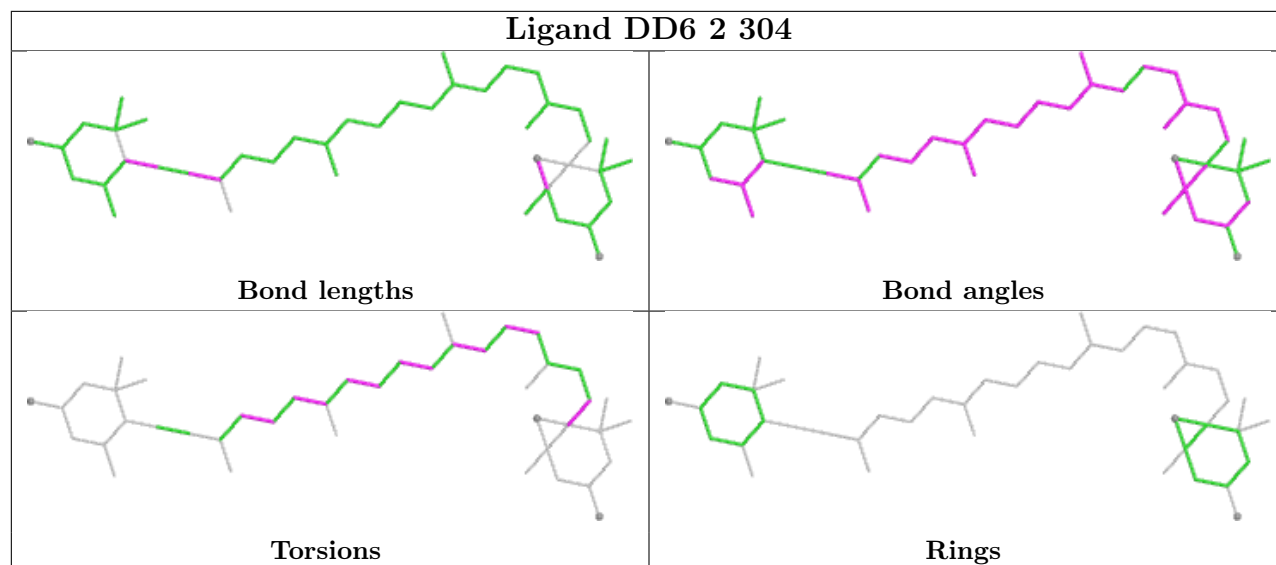


Torsions

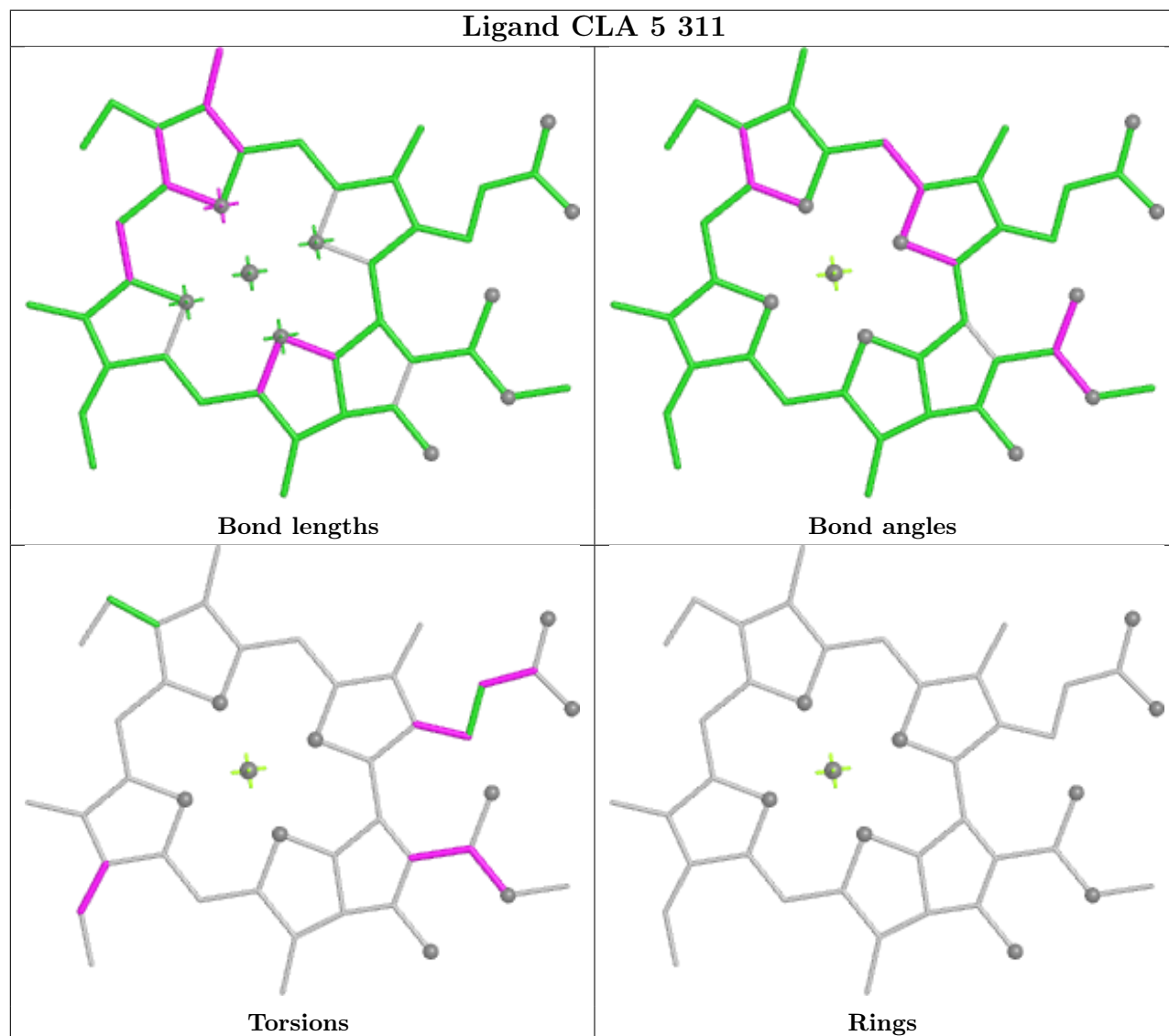


Rings

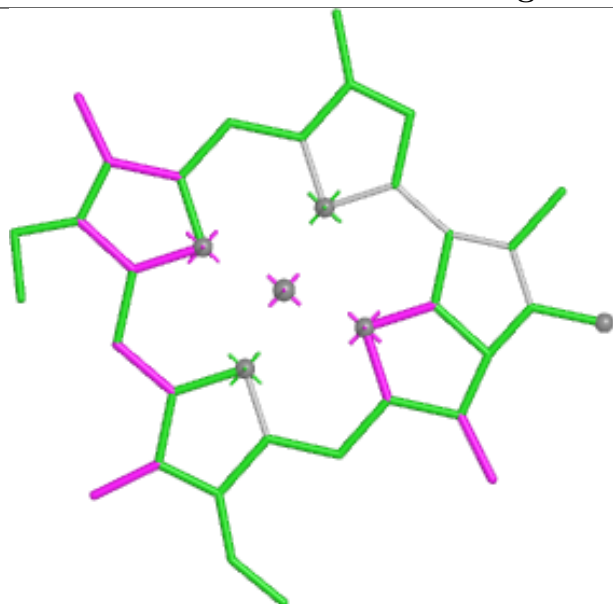
Ligand DD6 2 304



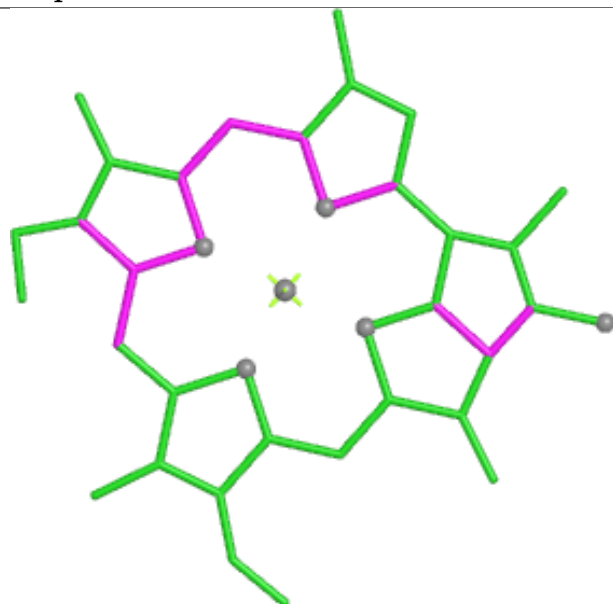
Ligand CLA 5 311



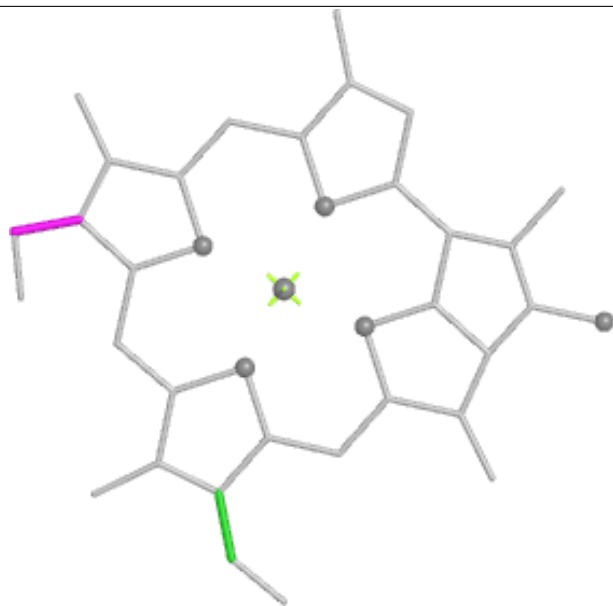
Ligand CLA p 606



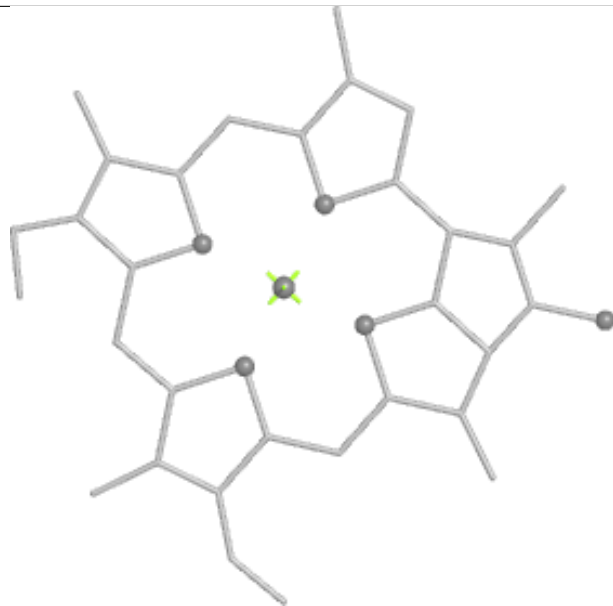
Bond lengths



Bond angles

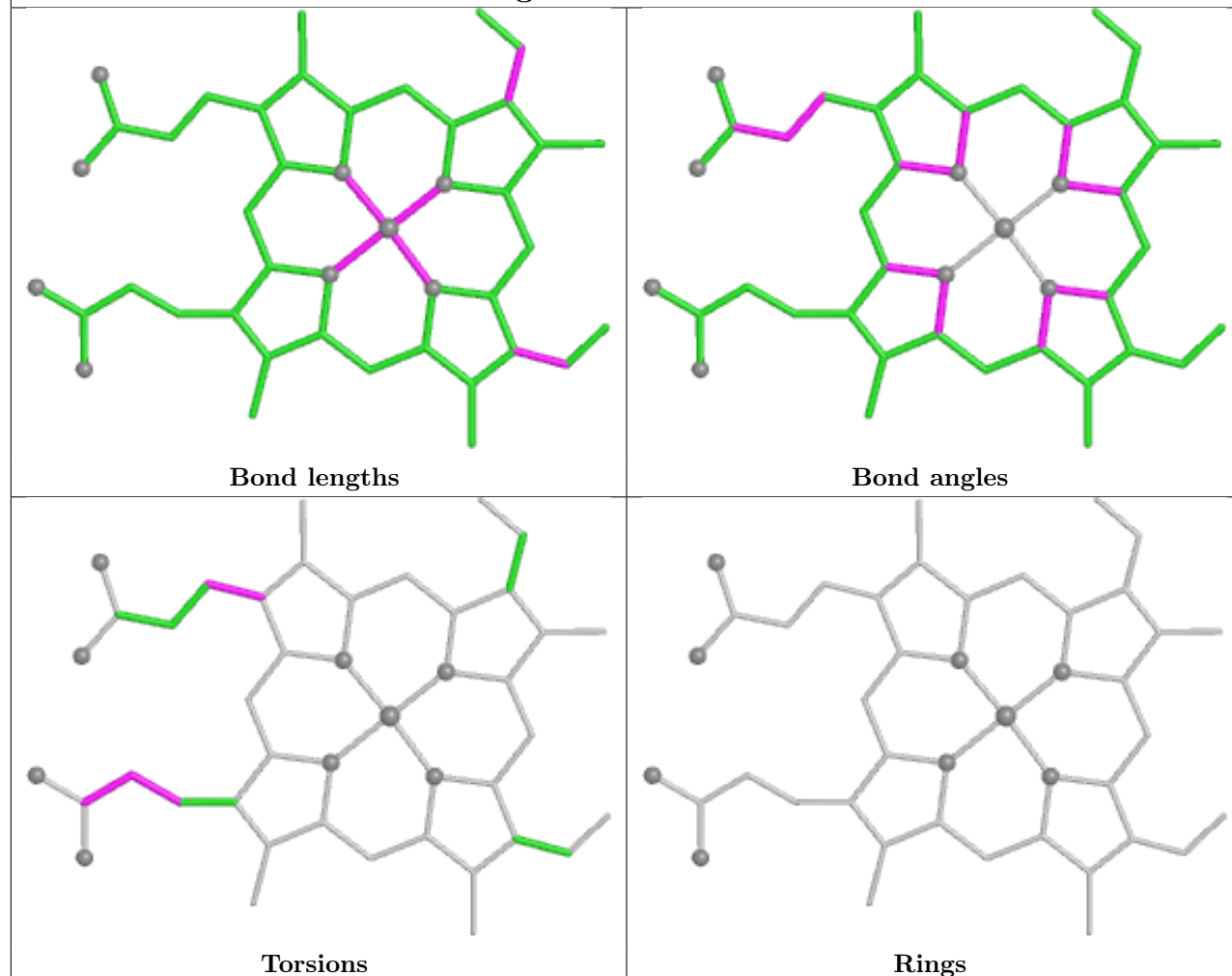


Torsions

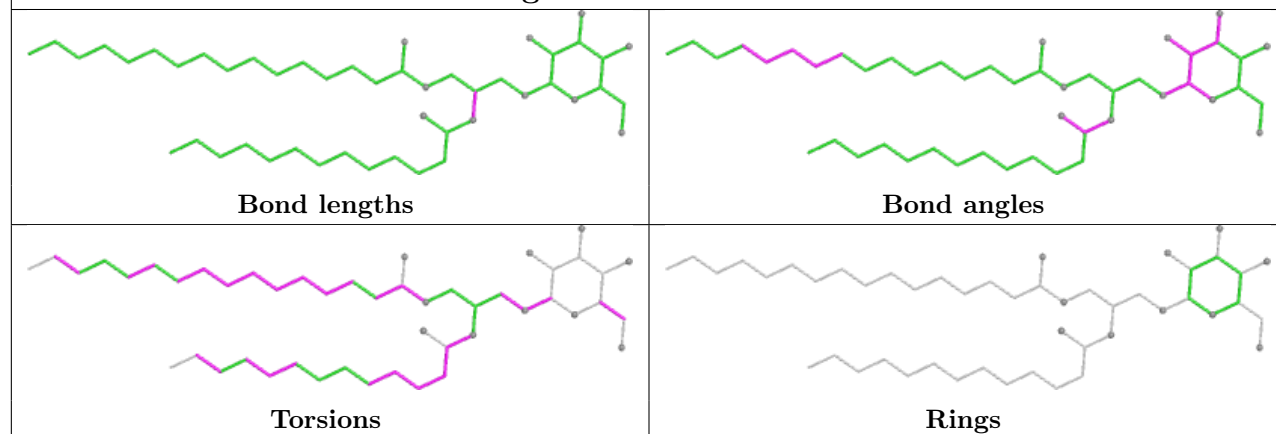


Rings

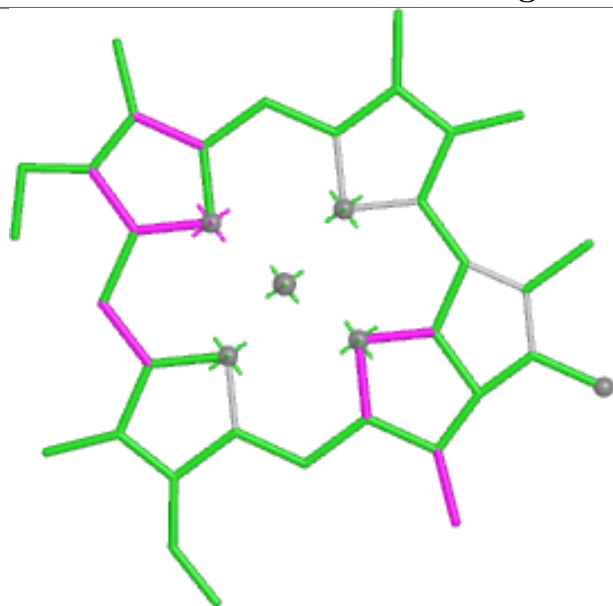
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Ligand LMG W 201



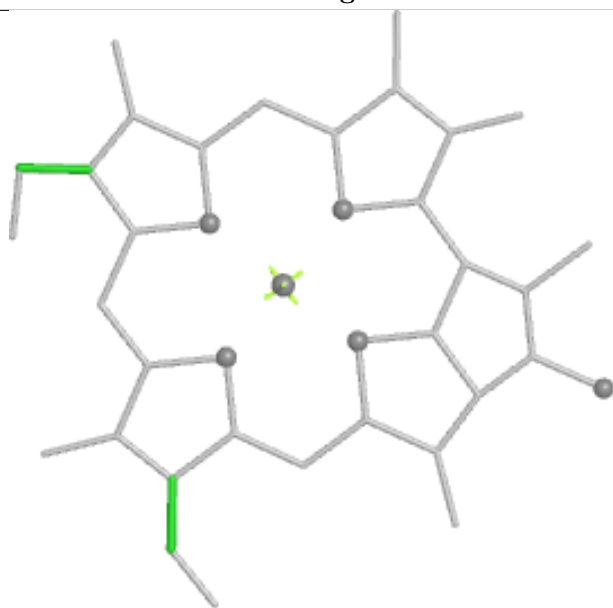
Ligand CLA 6 214



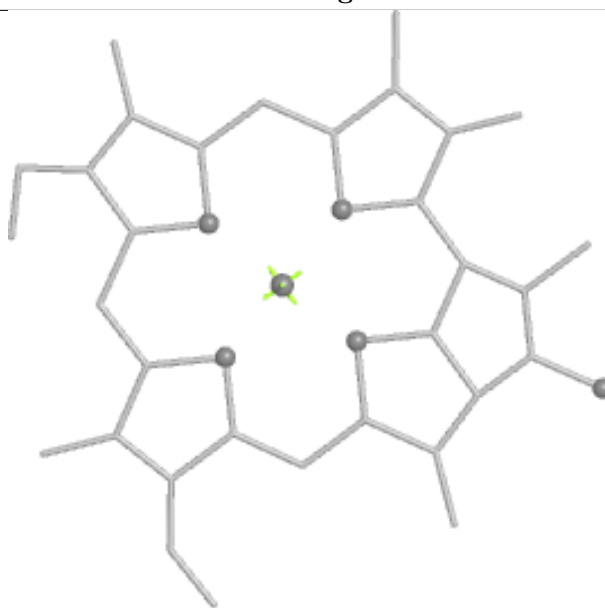
Bond lengths



Bond angles

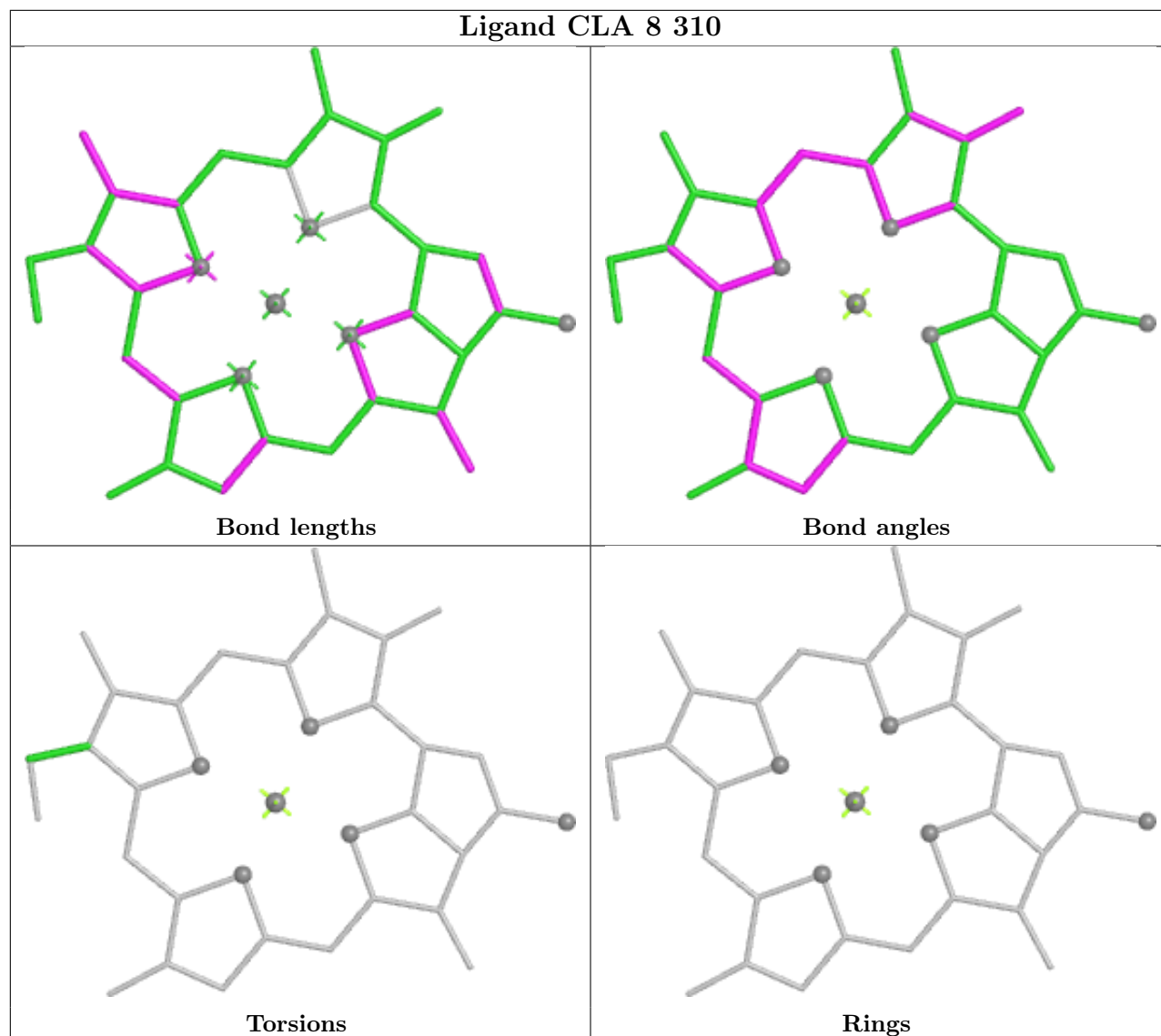


Torsions

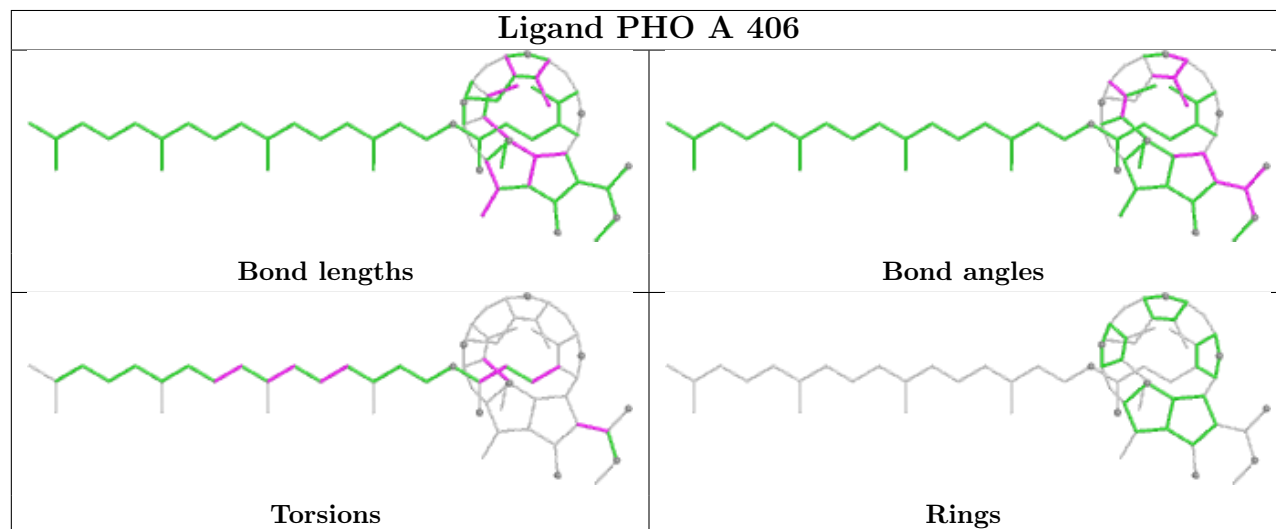


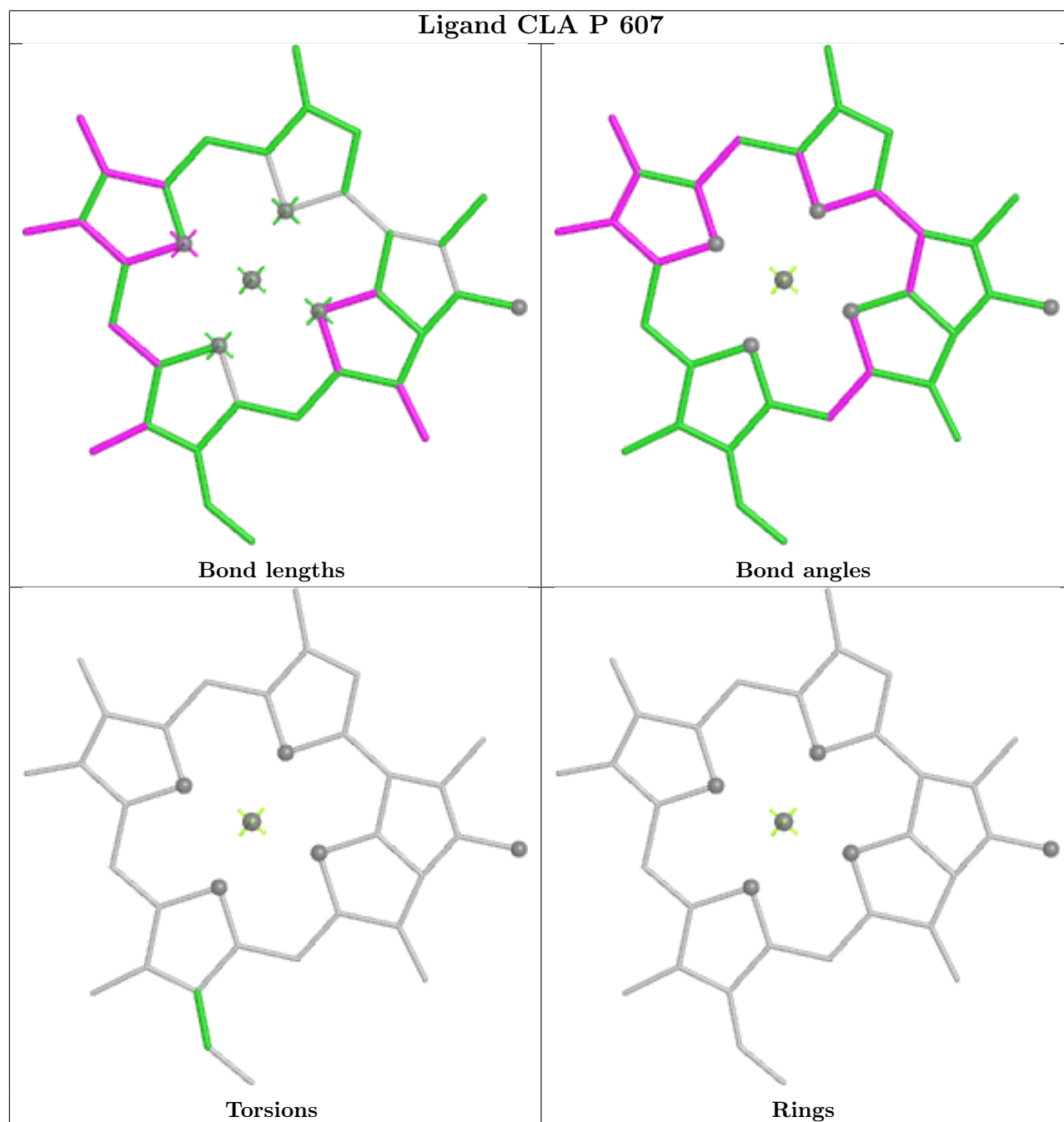
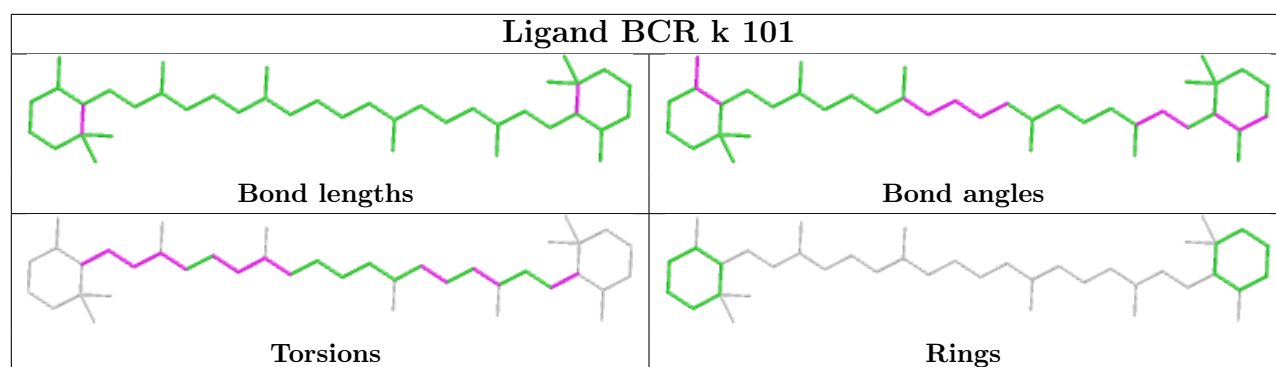
Rings

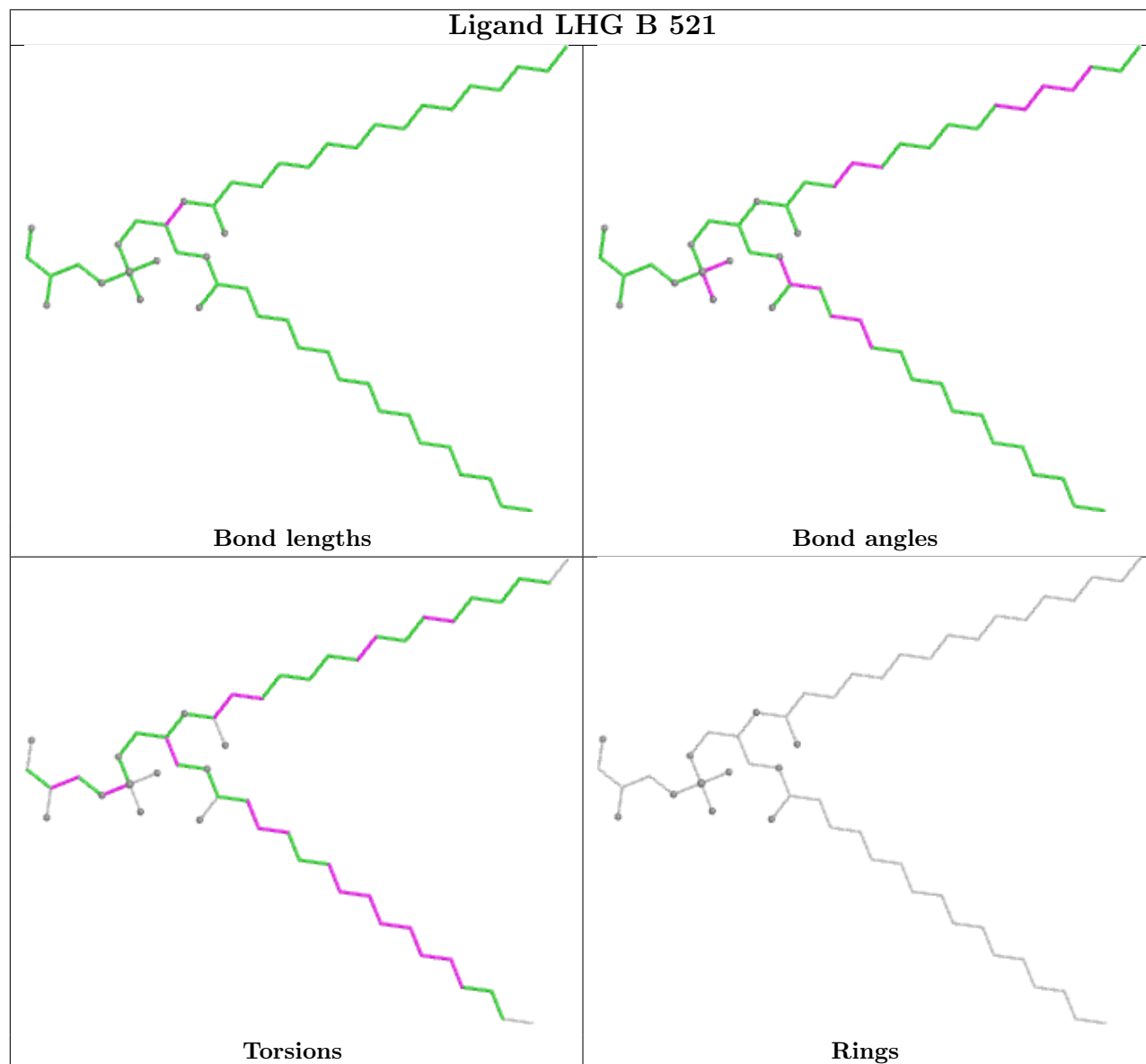
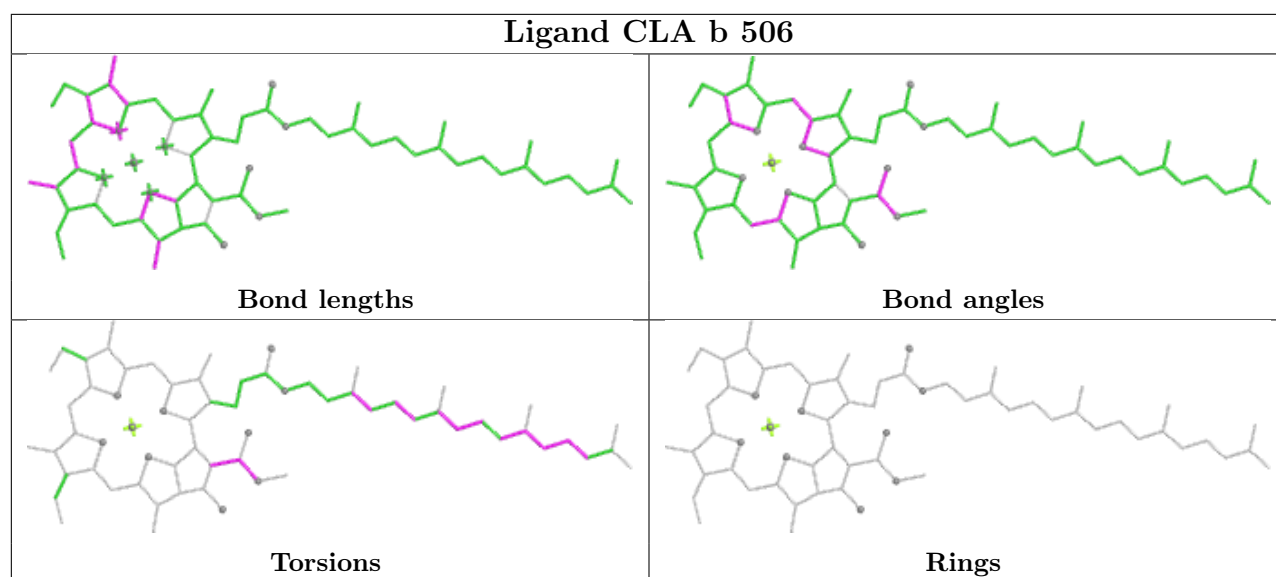
Ligand CLA 8 310



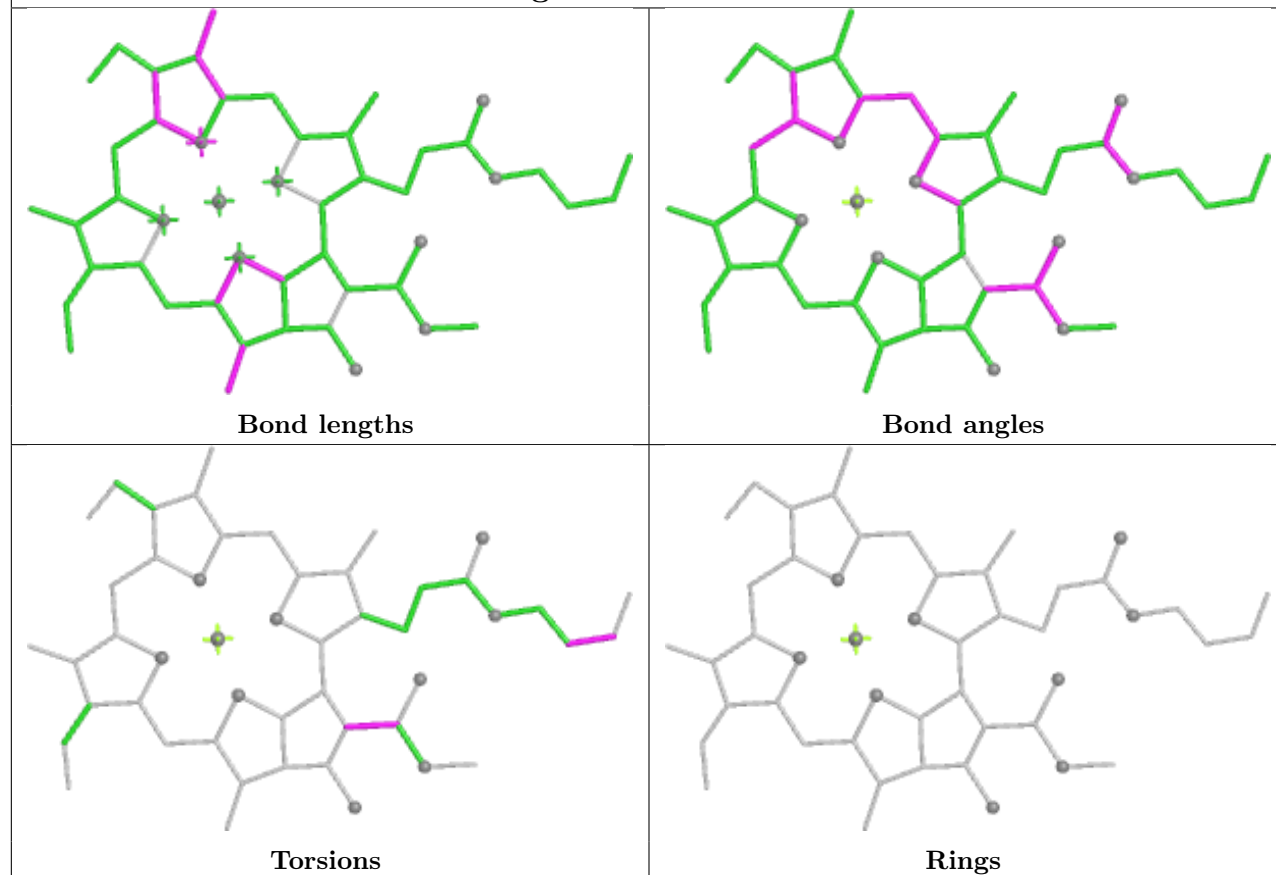
Ligand PHO A 406



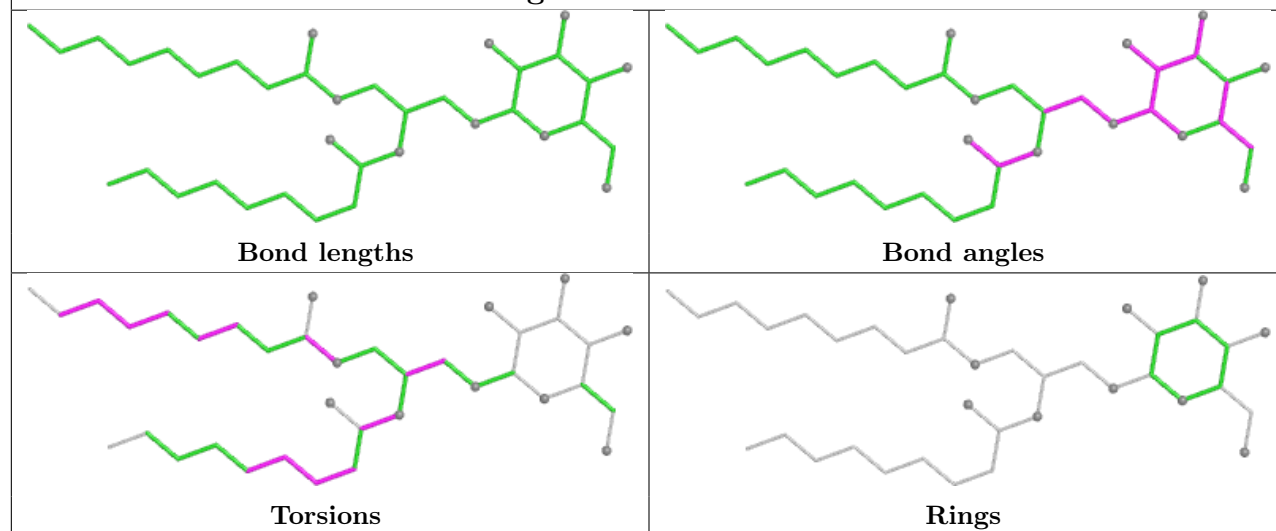




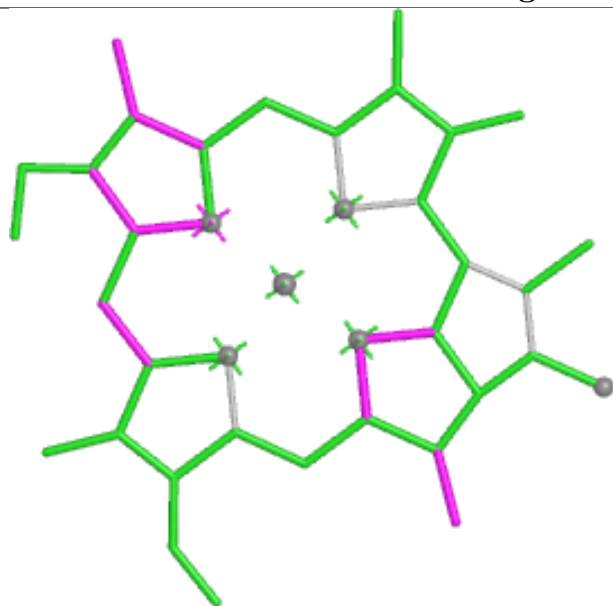
Ligand CLA A 404



Ligand LMG D 409



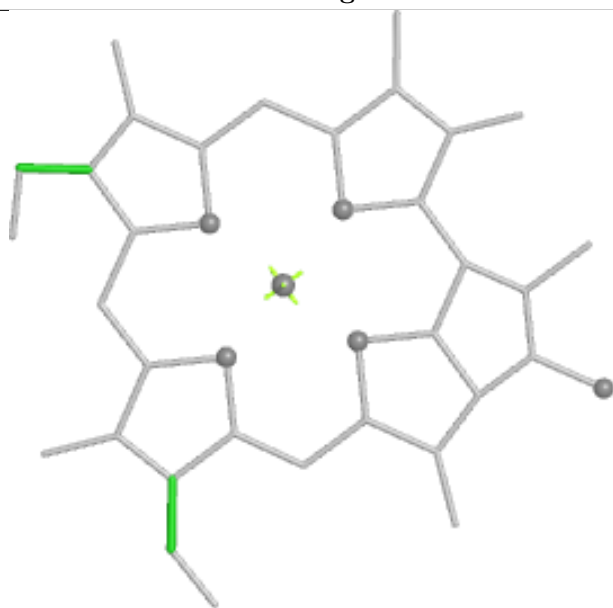
Ligand CLA 0 314



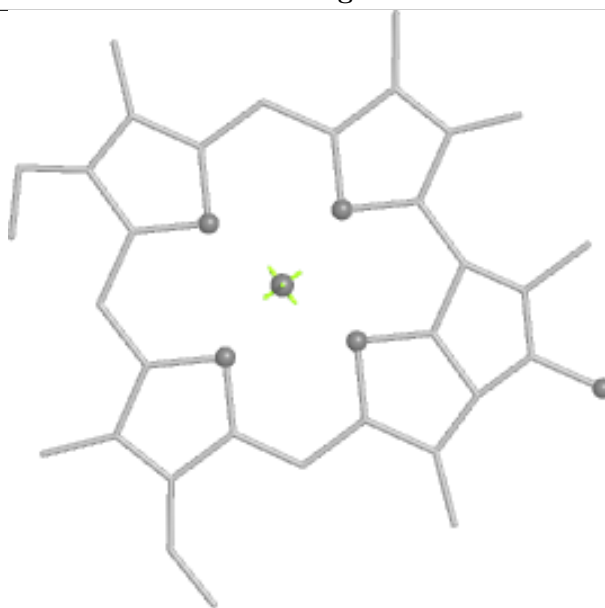
Bond lengths



Bond angles

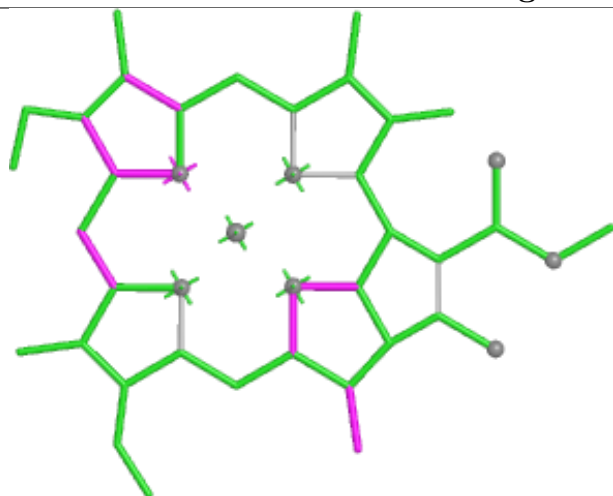


Torsions



Rings

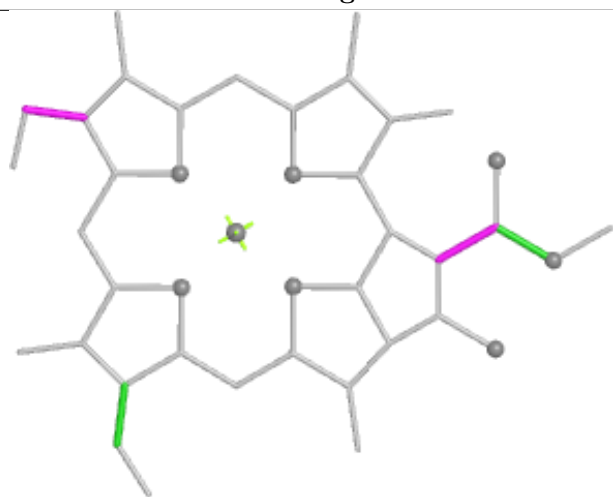
Ligand CLA 1 205



Bond lengths



Bond angles

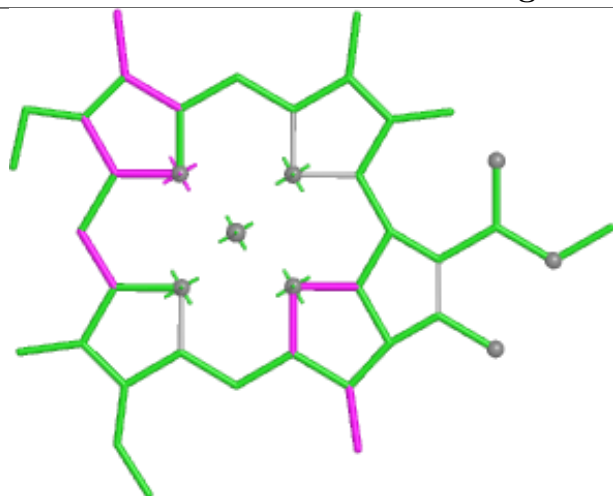


Torsions

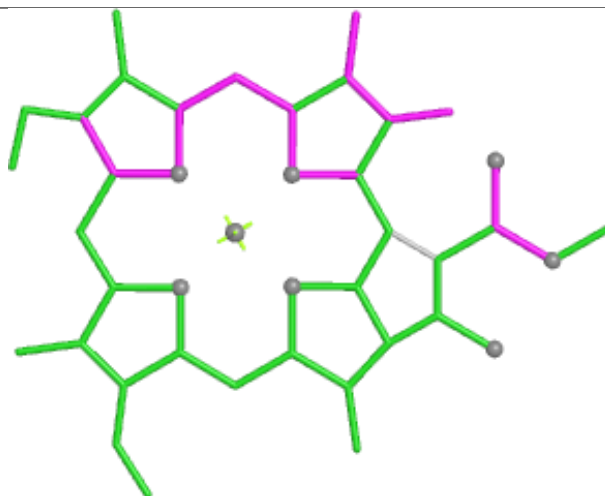


Rings

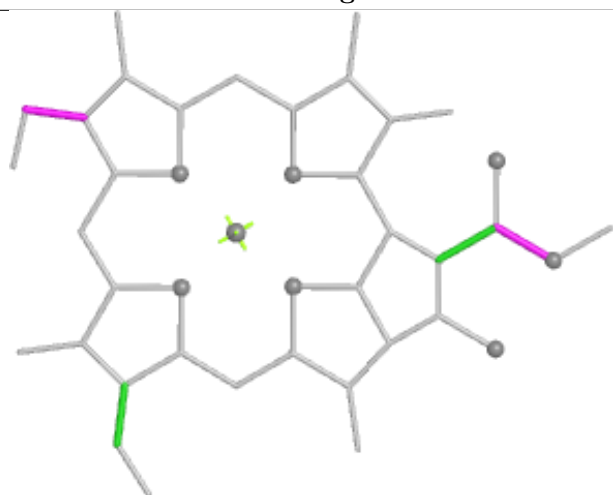
Ligand CLA 0 309



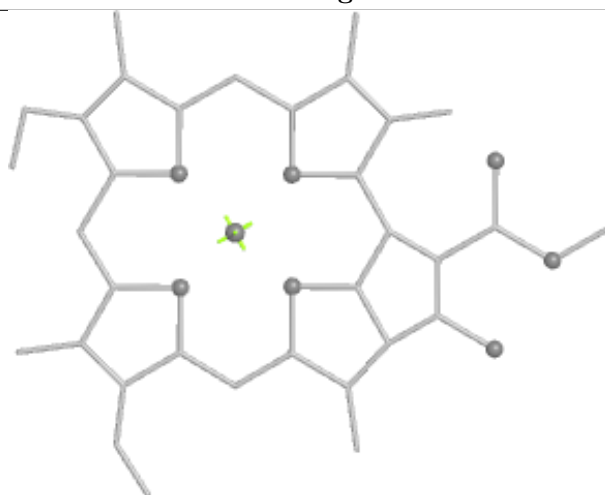
Bond lengths



Bond angles

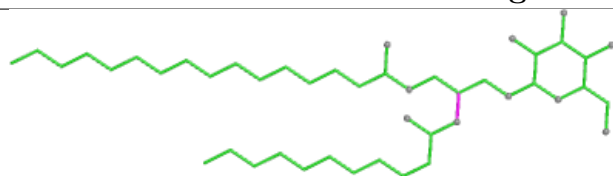


Torsions

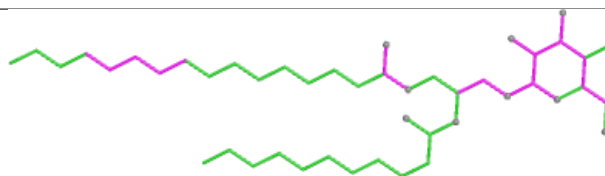


Rings

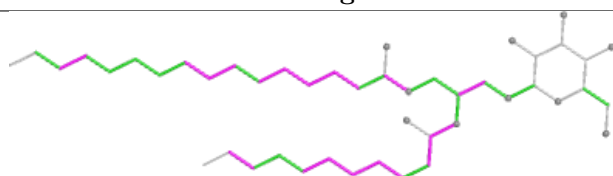
Ligand LMG Y 101



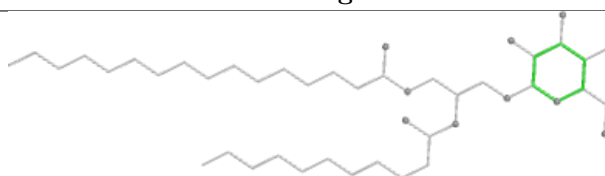
Bond lengths



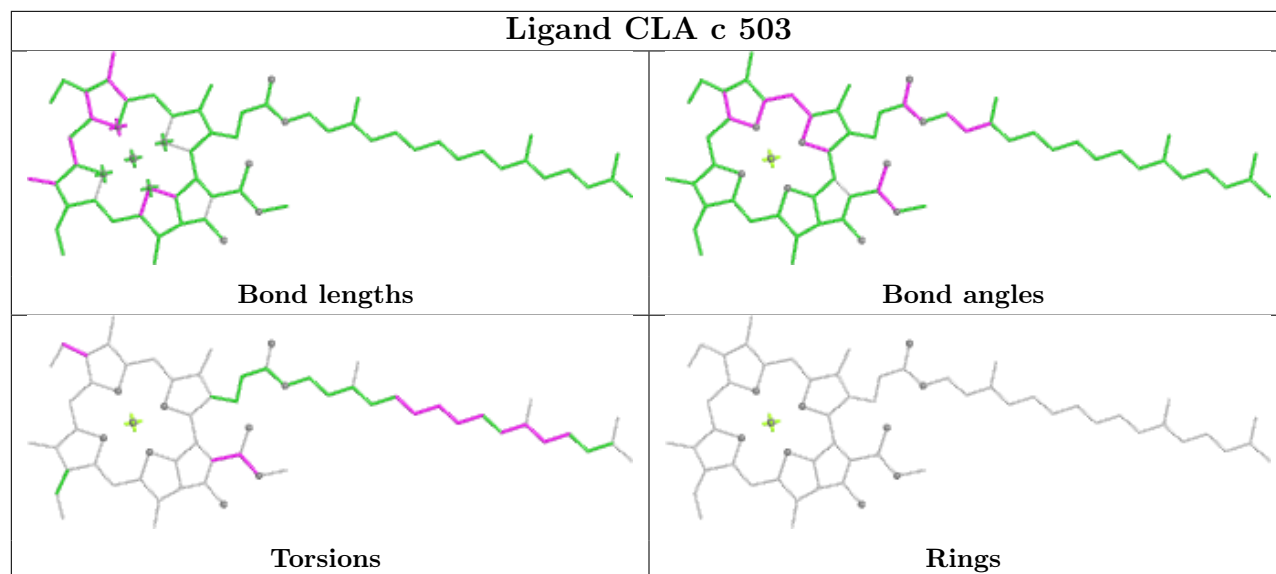
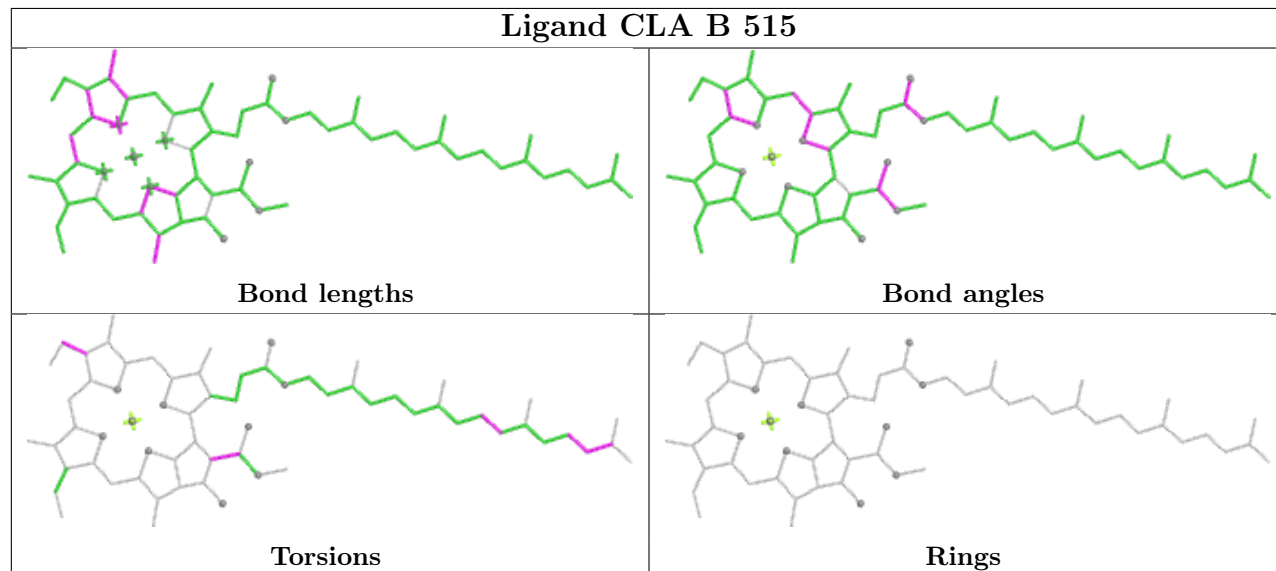
Bond angles



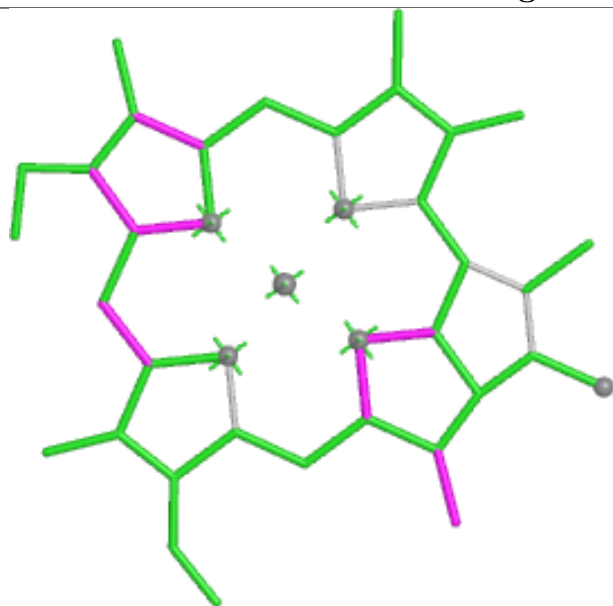
Torsions



Rings

Ligand CLA c 503**Ligand CLA B 515**

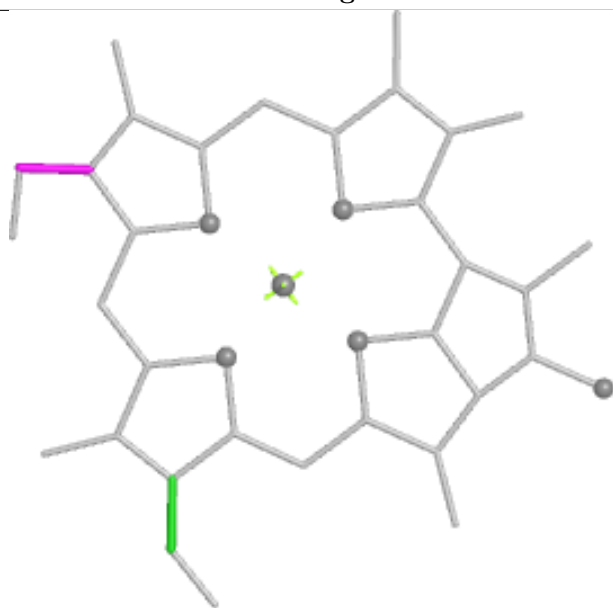
Ligand CLA 6 216



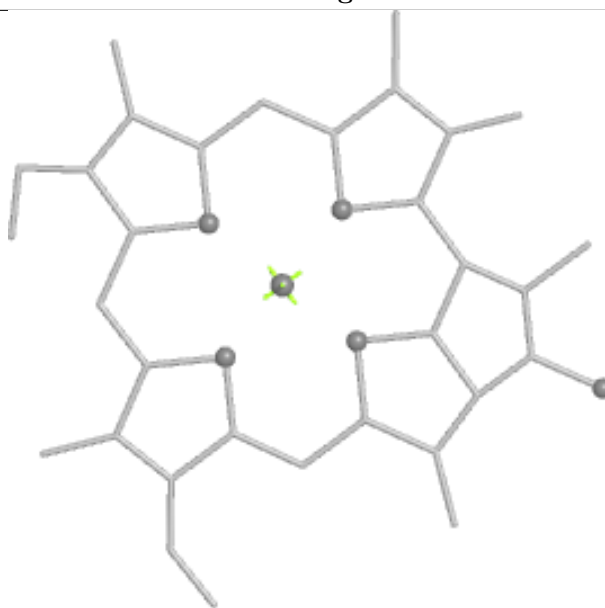
Bond lengths



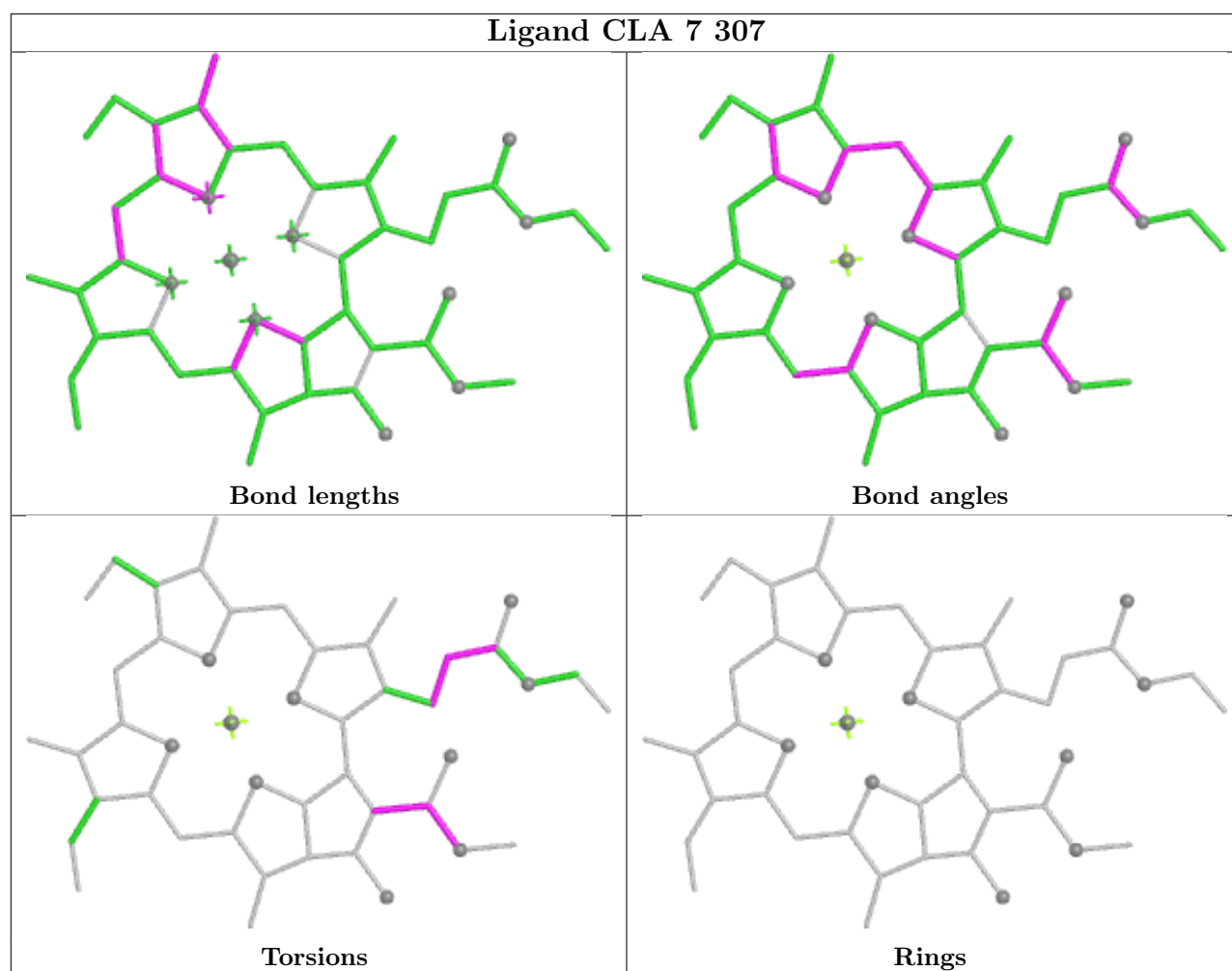
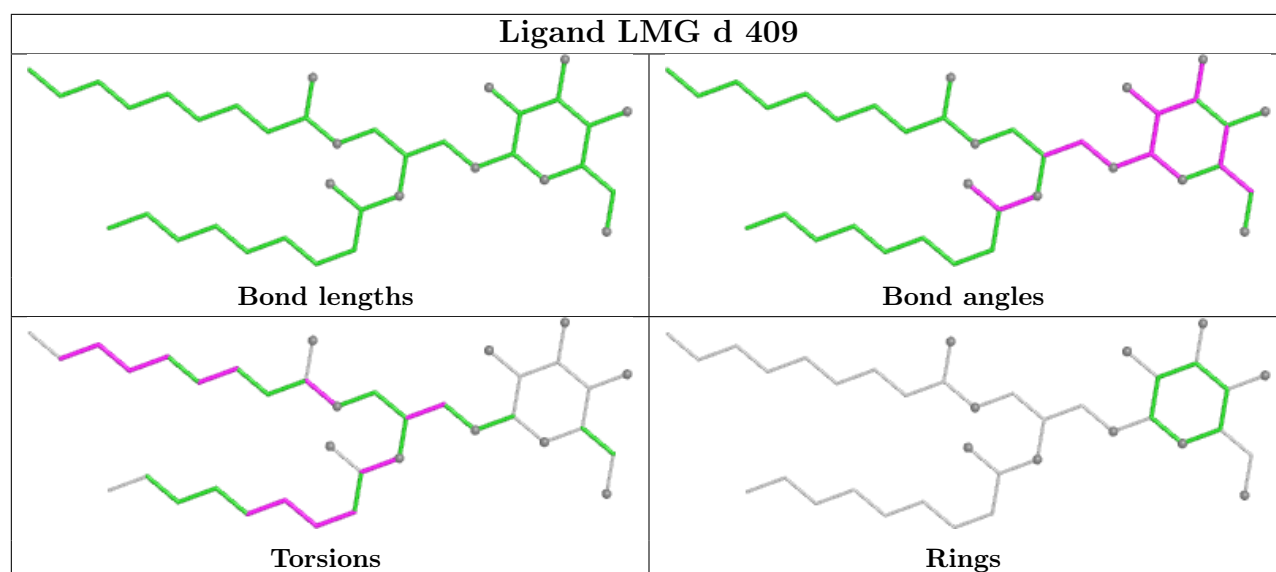
Bond angles



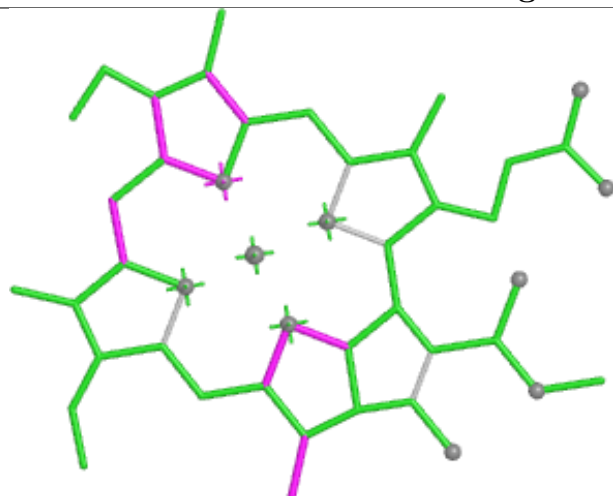
Torsions



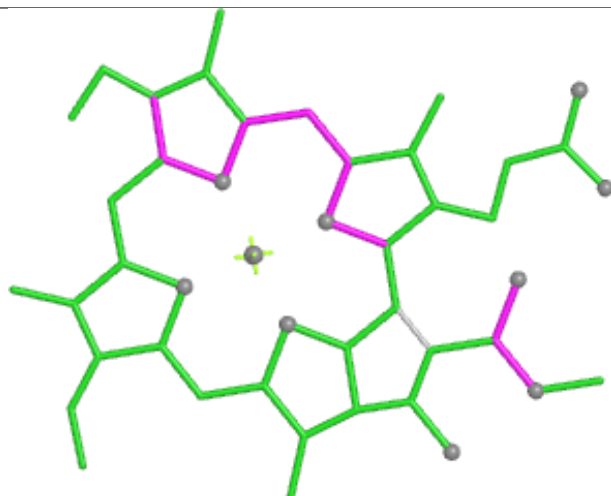
Rings



Ligand CLA 0 306



Bond lengths



Bond angles

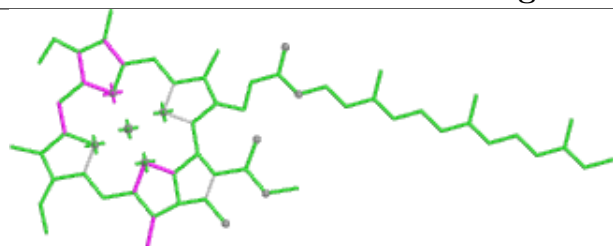


Torsions

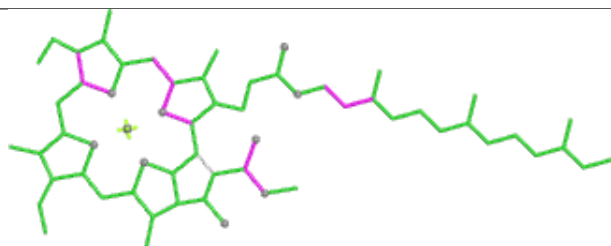


Rings

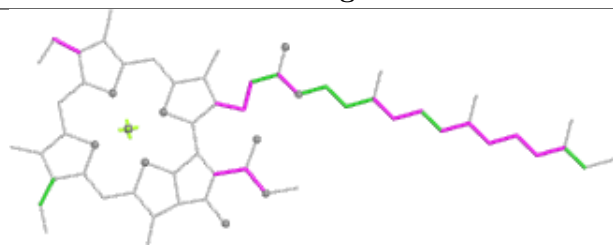
Ligand CLA 0 307



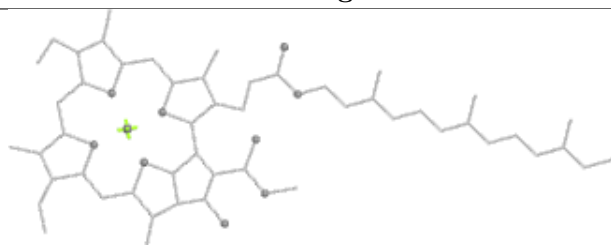
Bond lengths



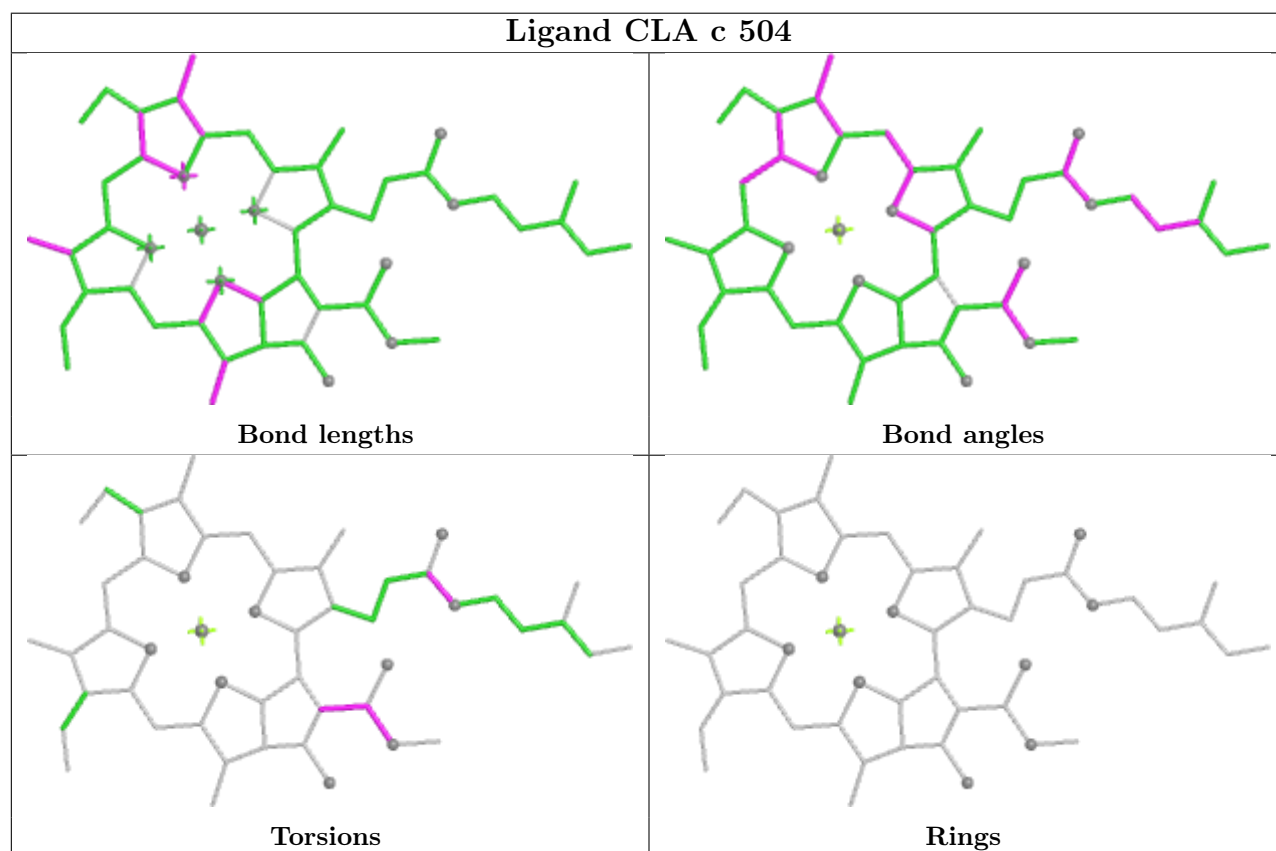
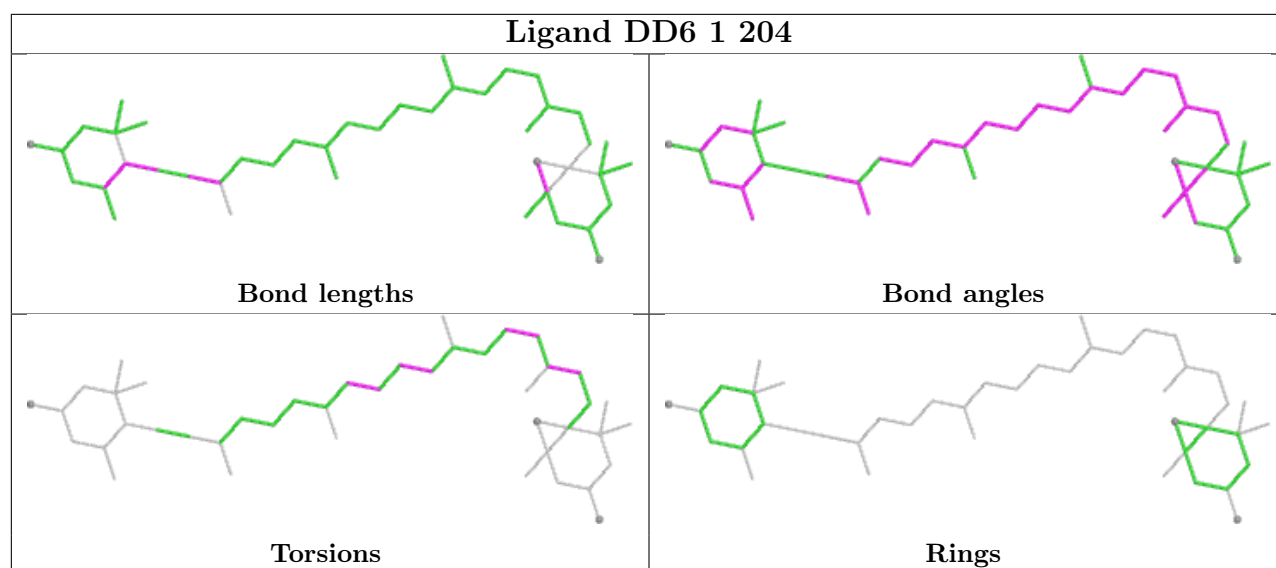
Bond angles

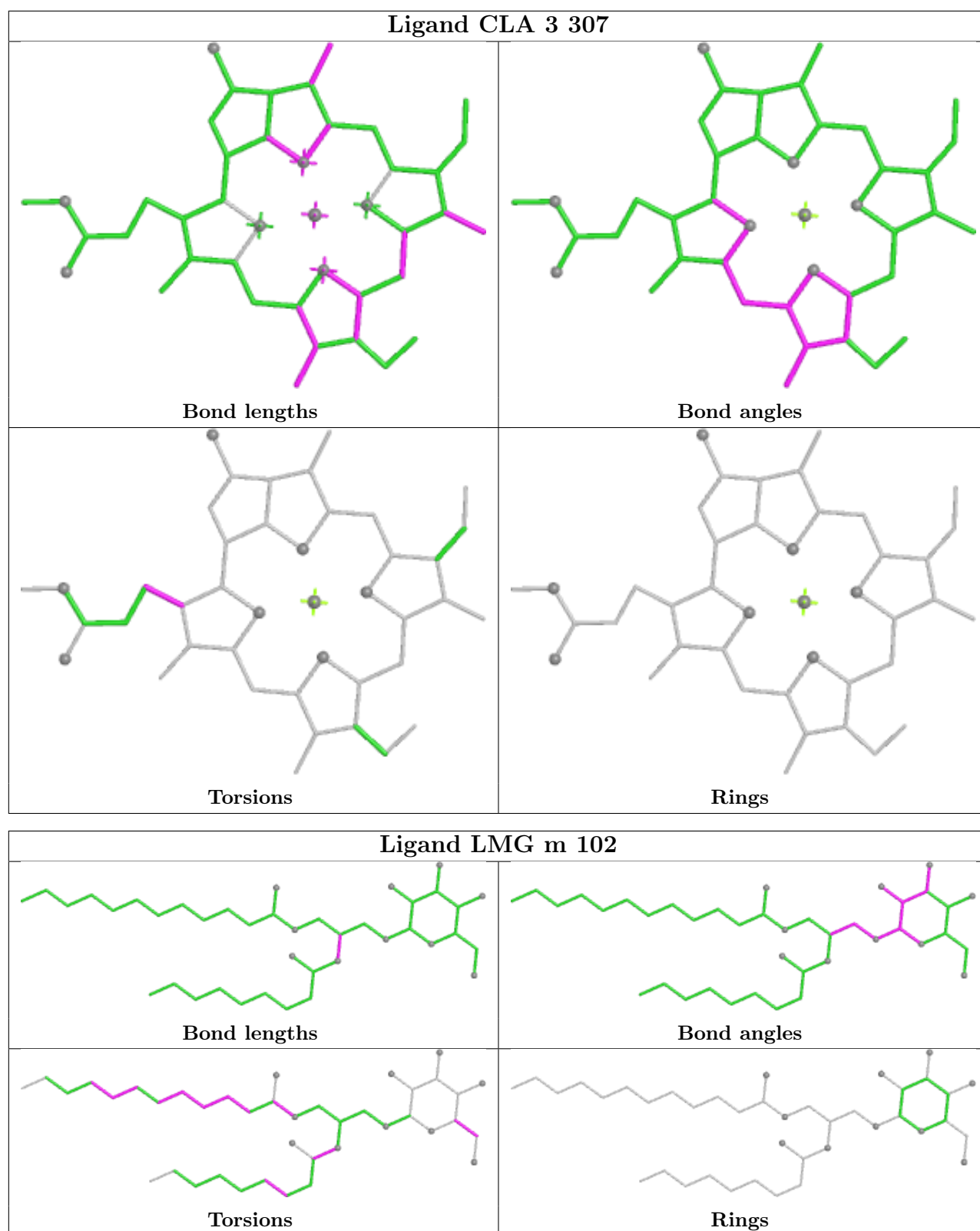


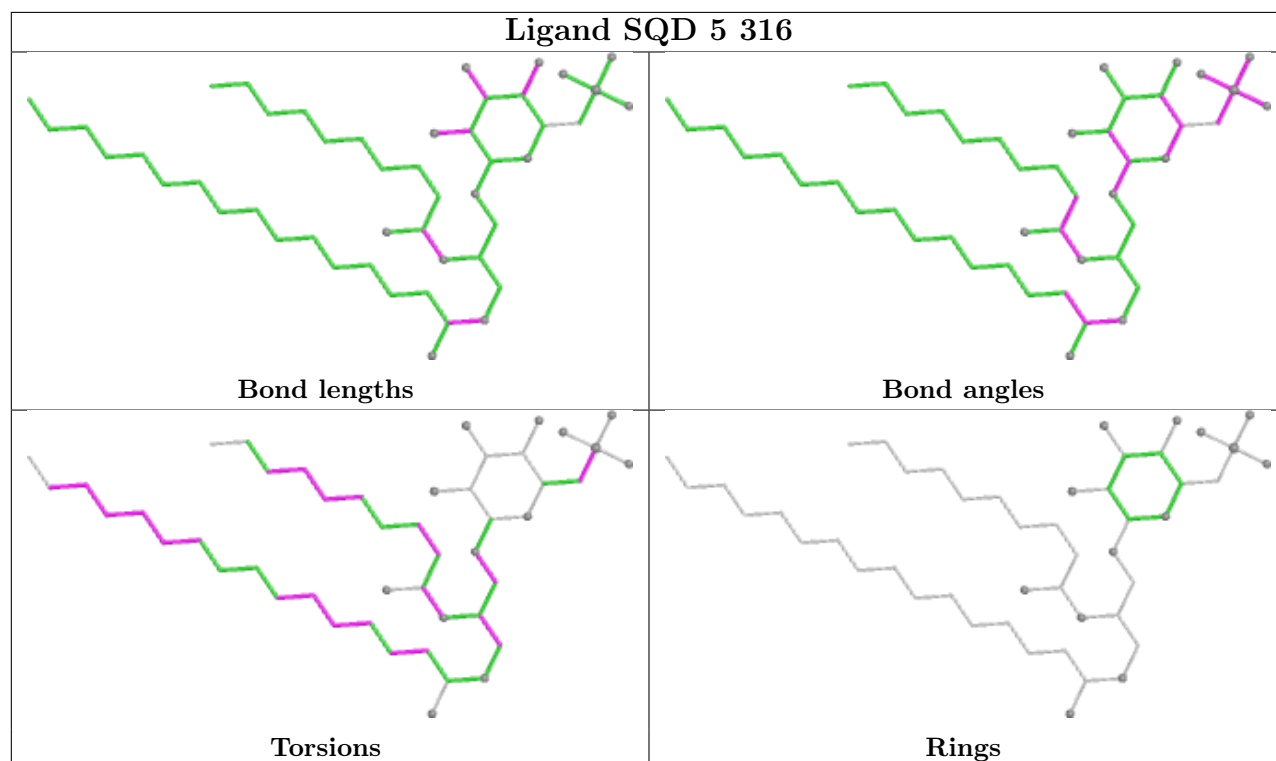
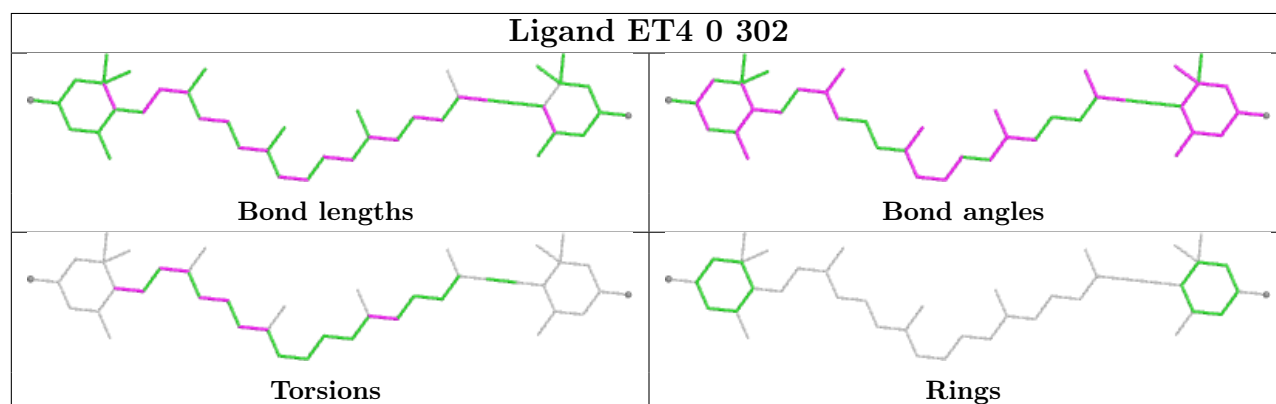
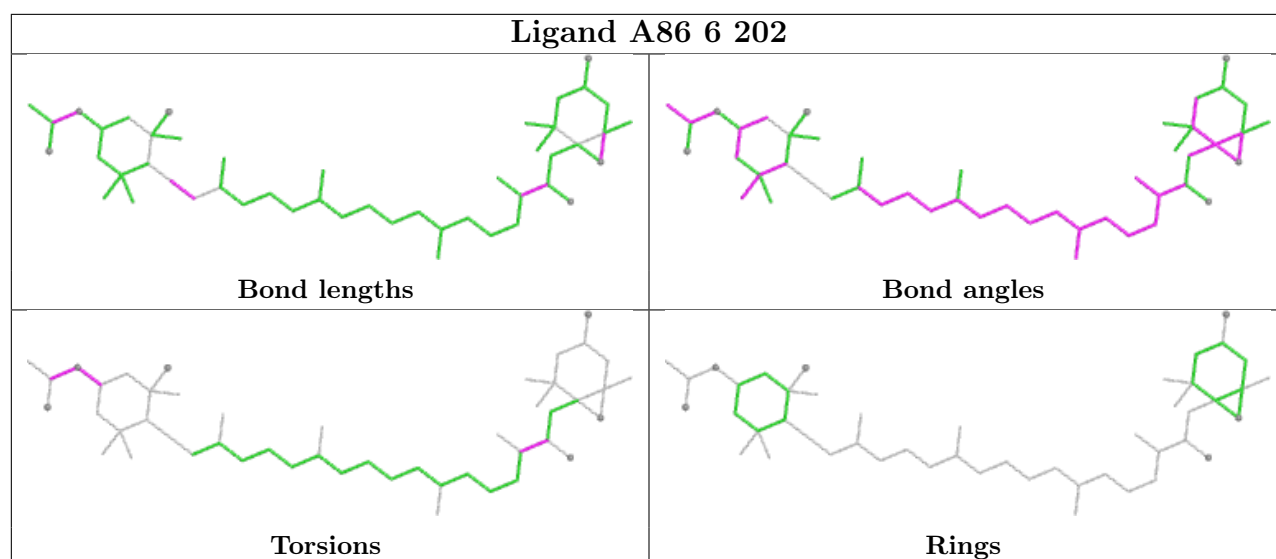
Torsions



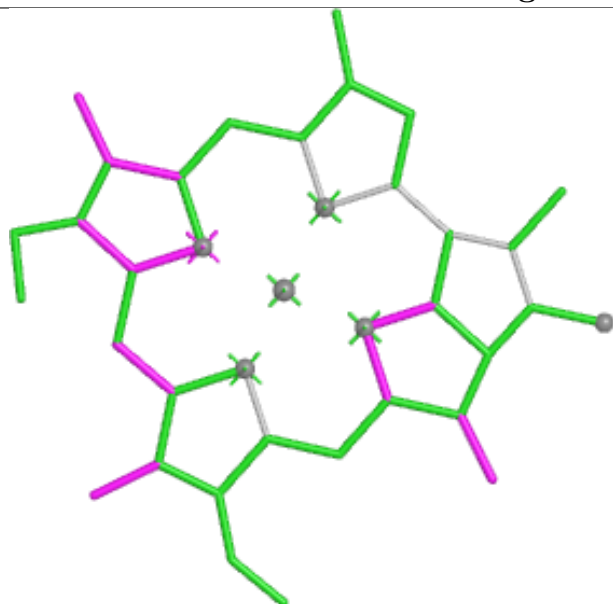
Rings



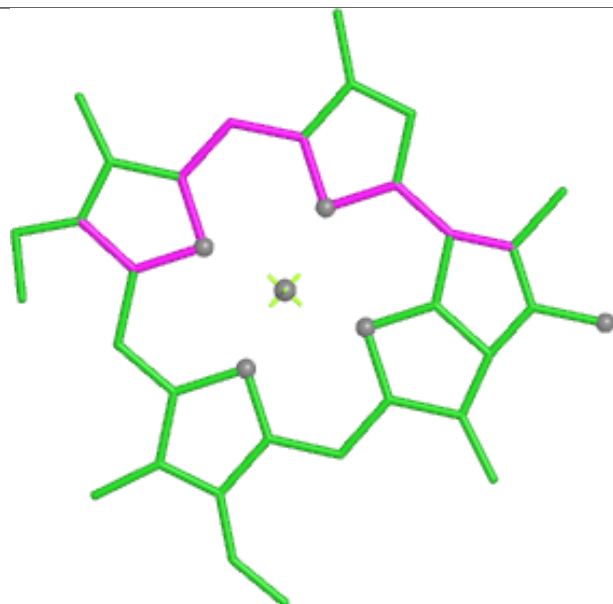




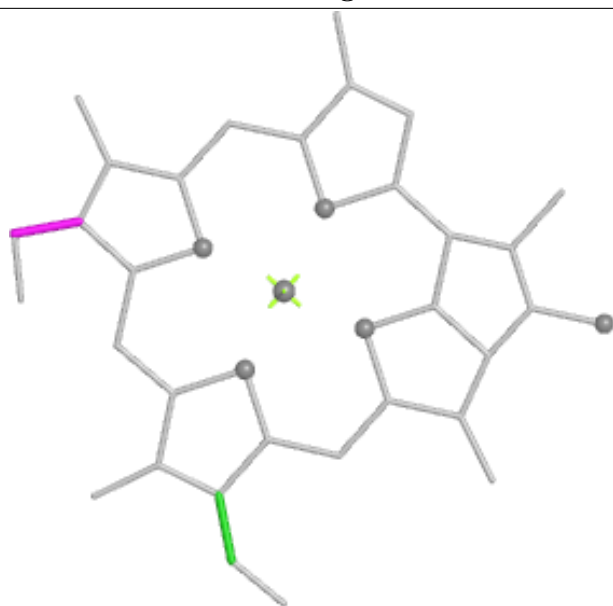
Ligand CLA 9 206



Bond lengths



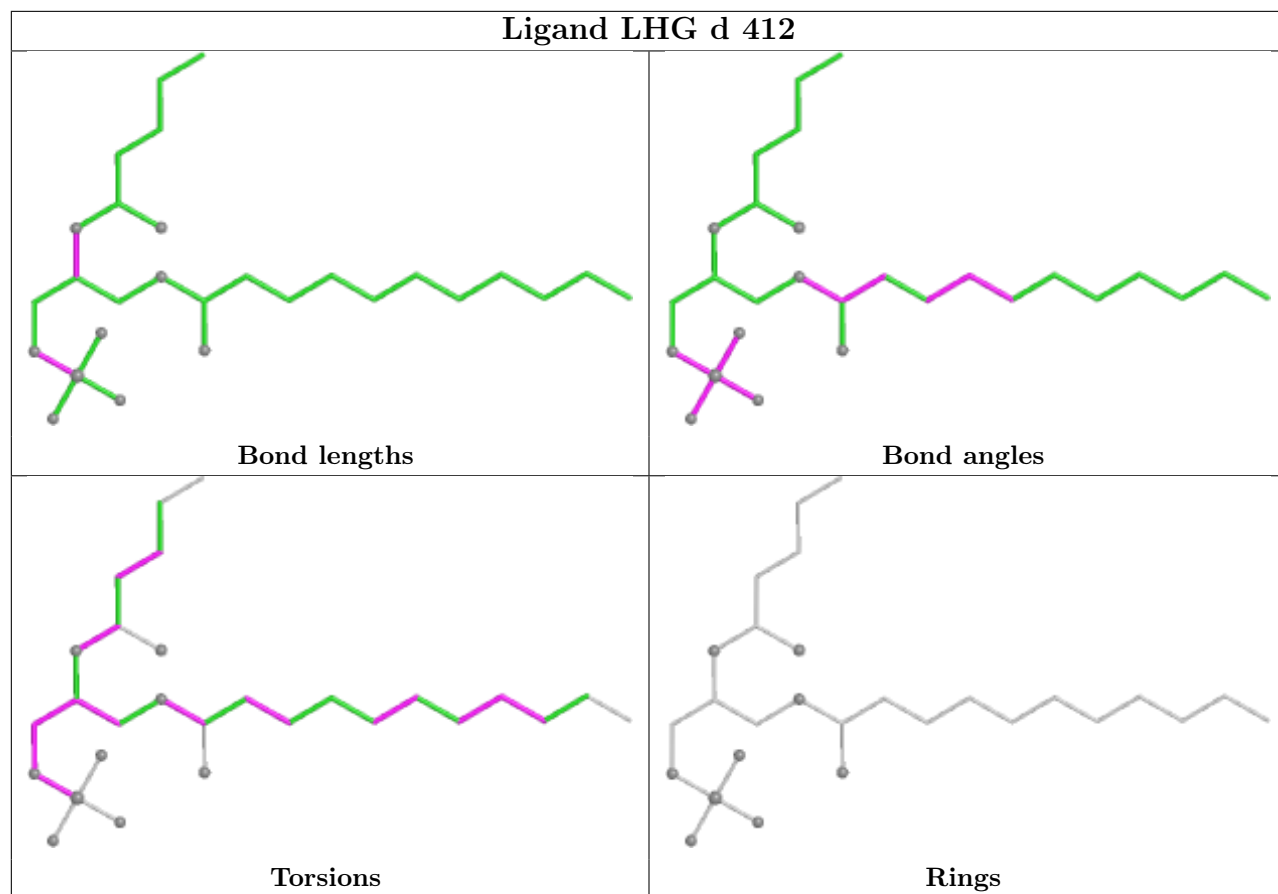
Bond angles



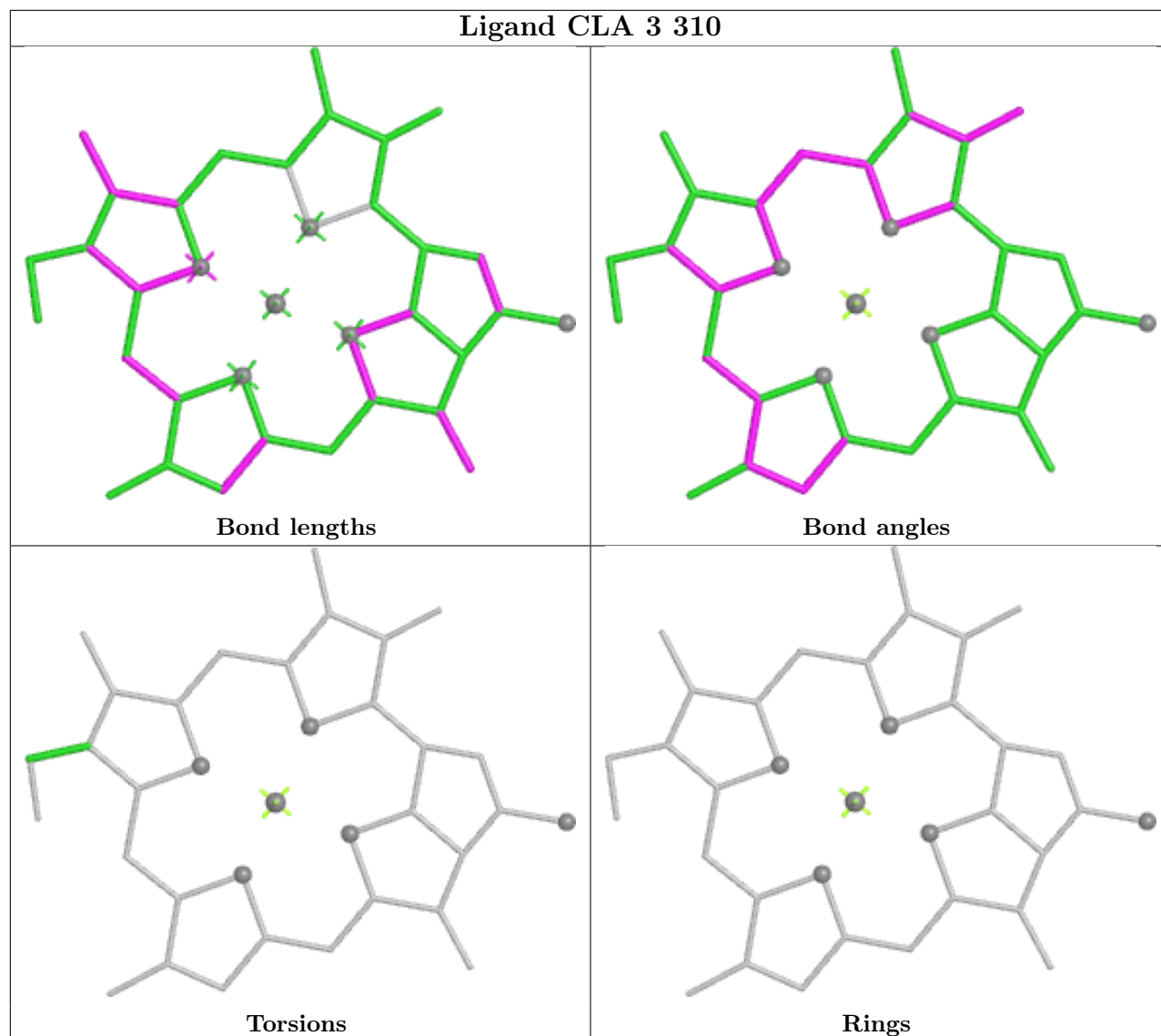
Torsions



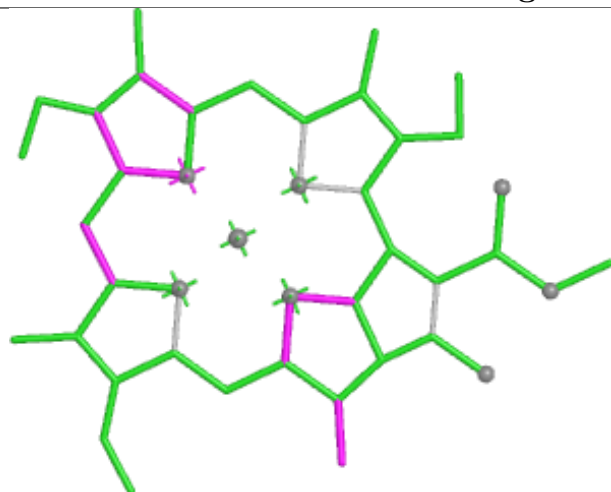
Rings



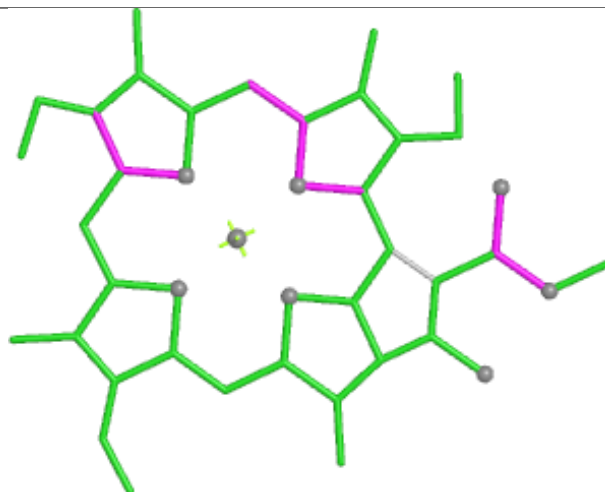
Ligand CLA 3 310



Ligand CLA 5 312



Bond lengths



Bond angles

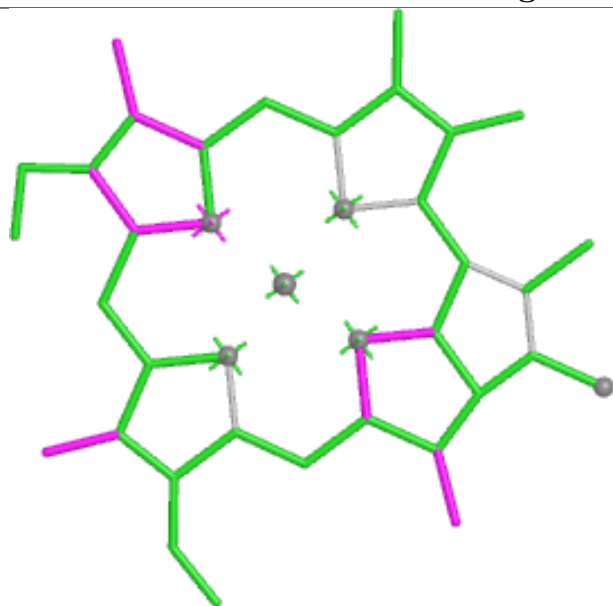


Torsions



Rings

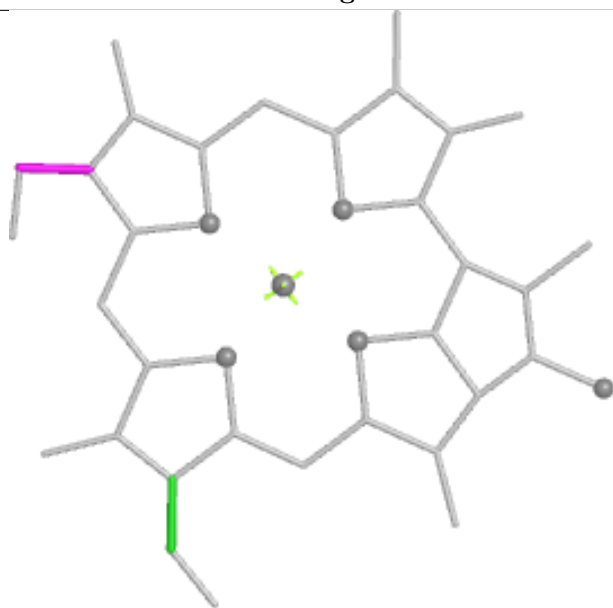
Ligand CLA 4 207



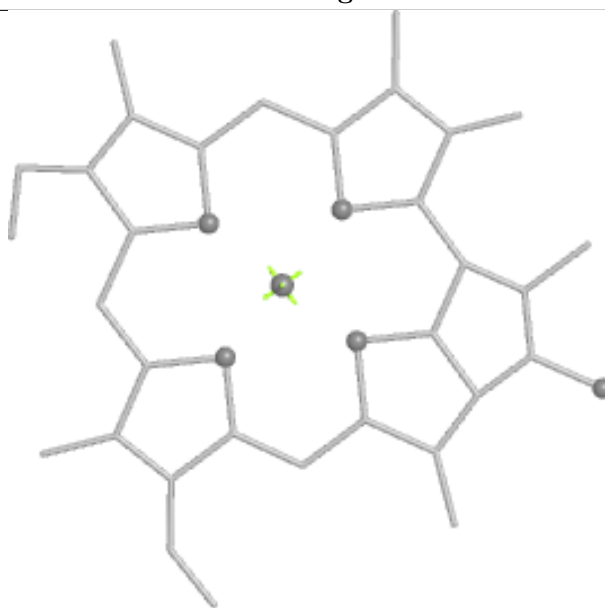
Bond lengths



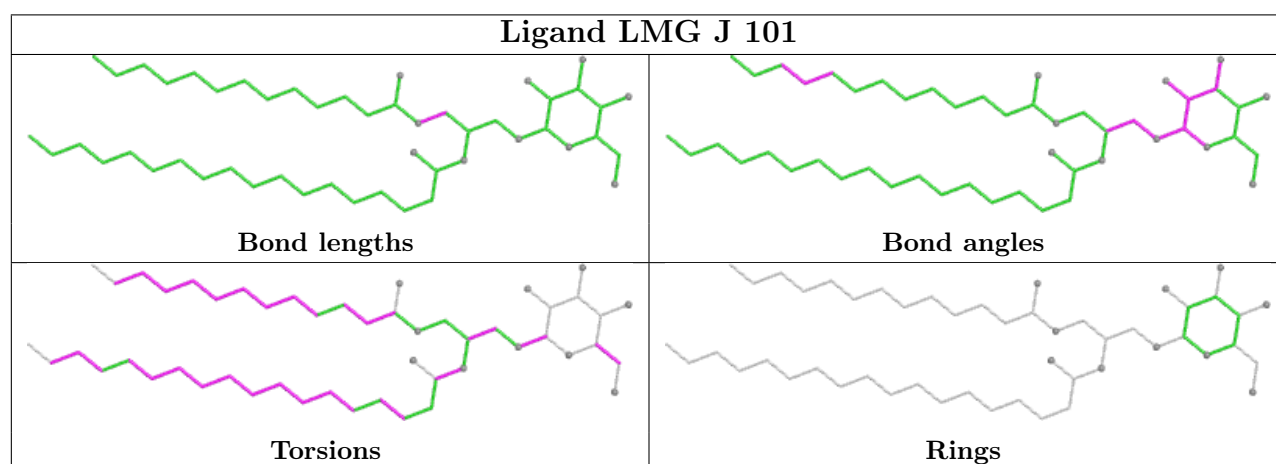
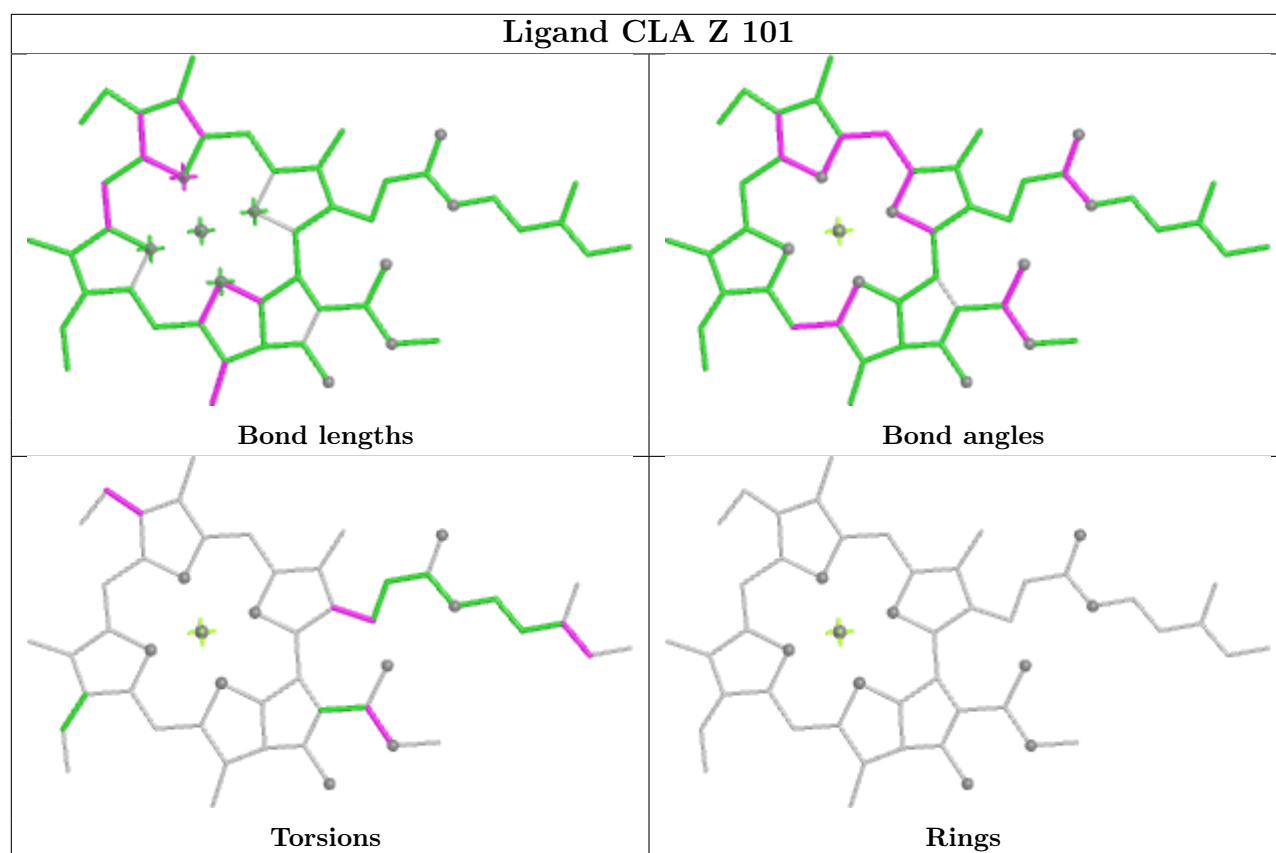
Bond angles

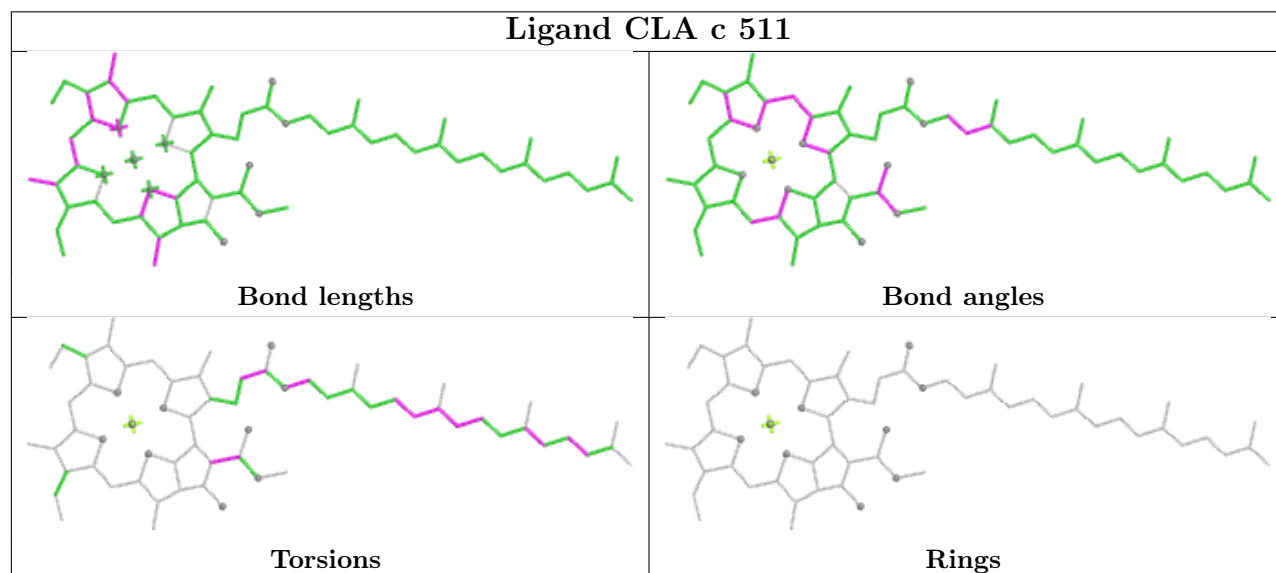
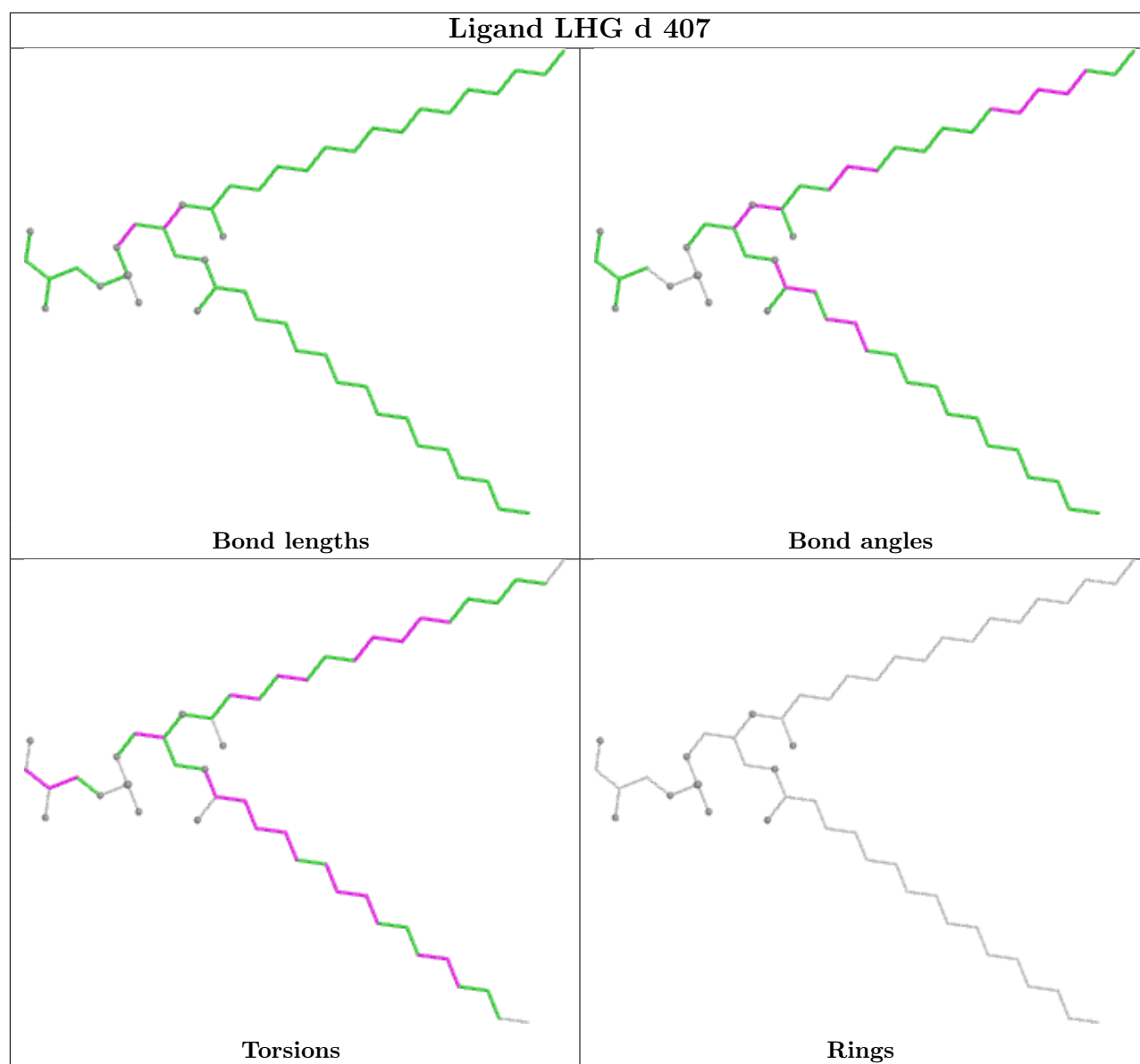


Torsions

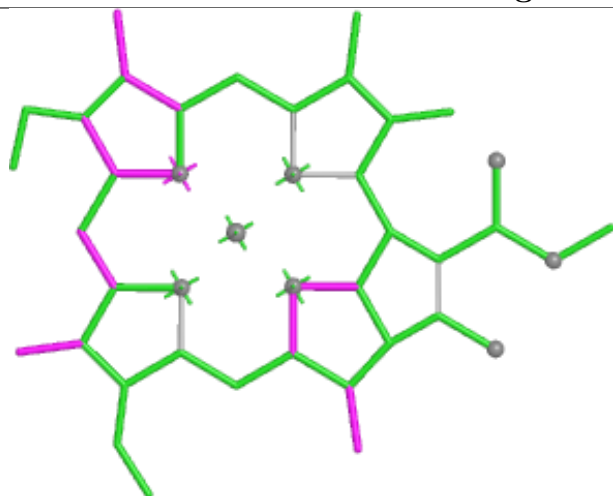


Rings

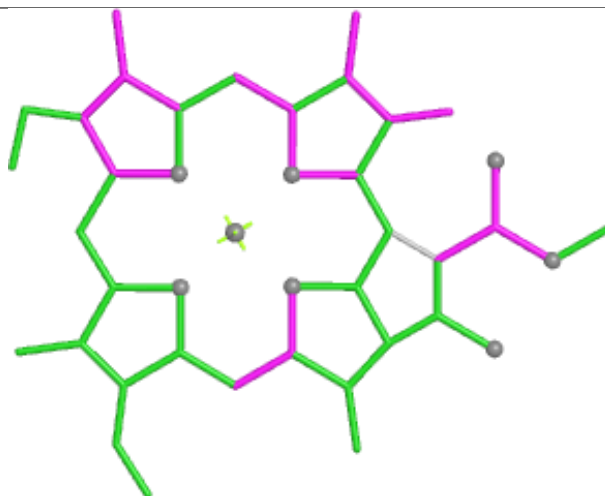




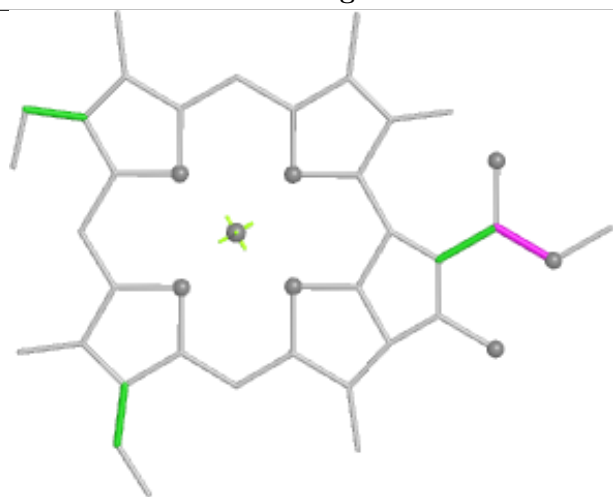
Ligand CLA P 602



Bond lengths



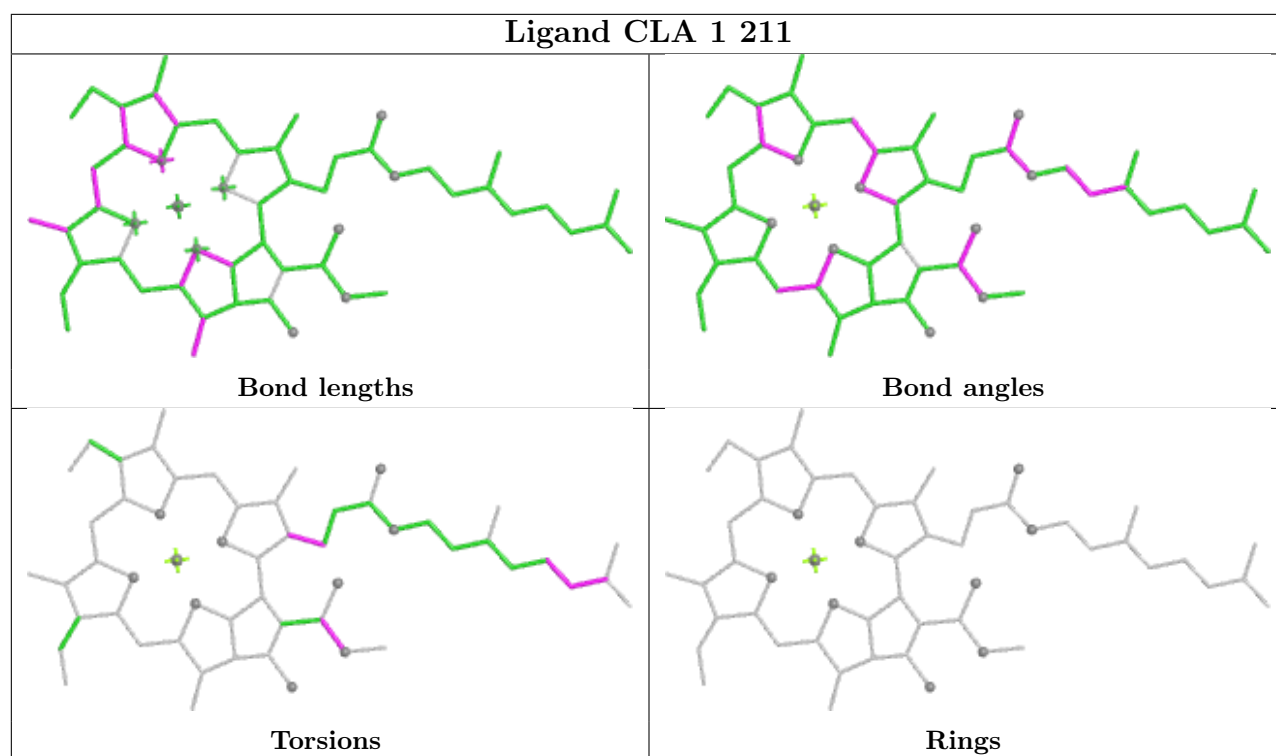
Bond angles

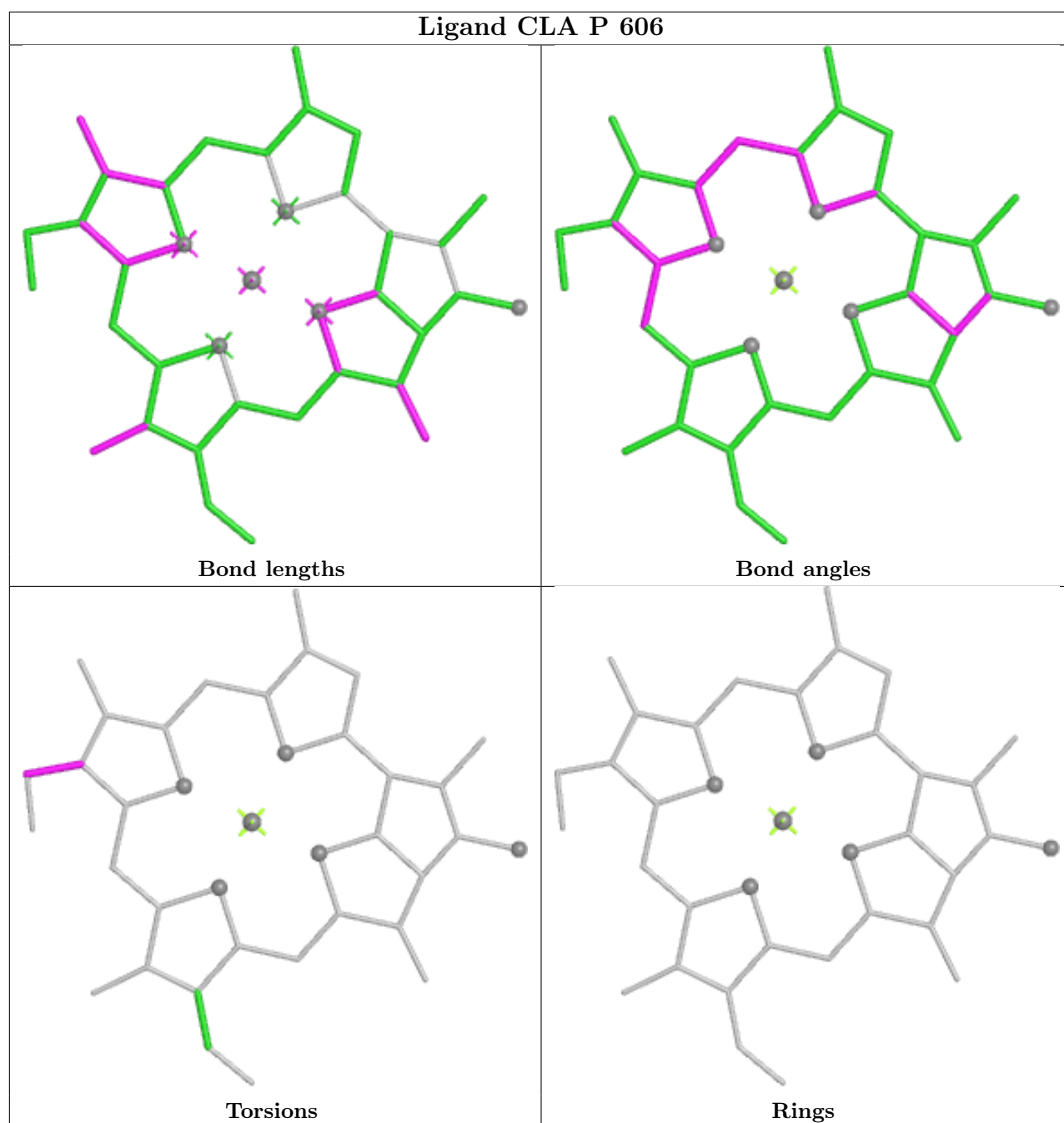


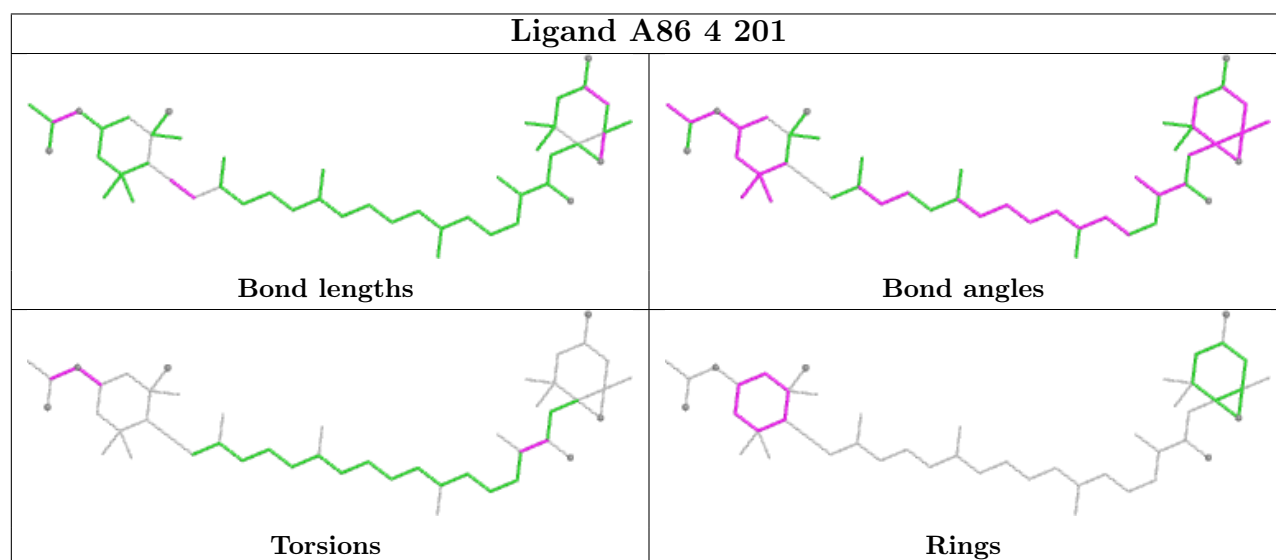
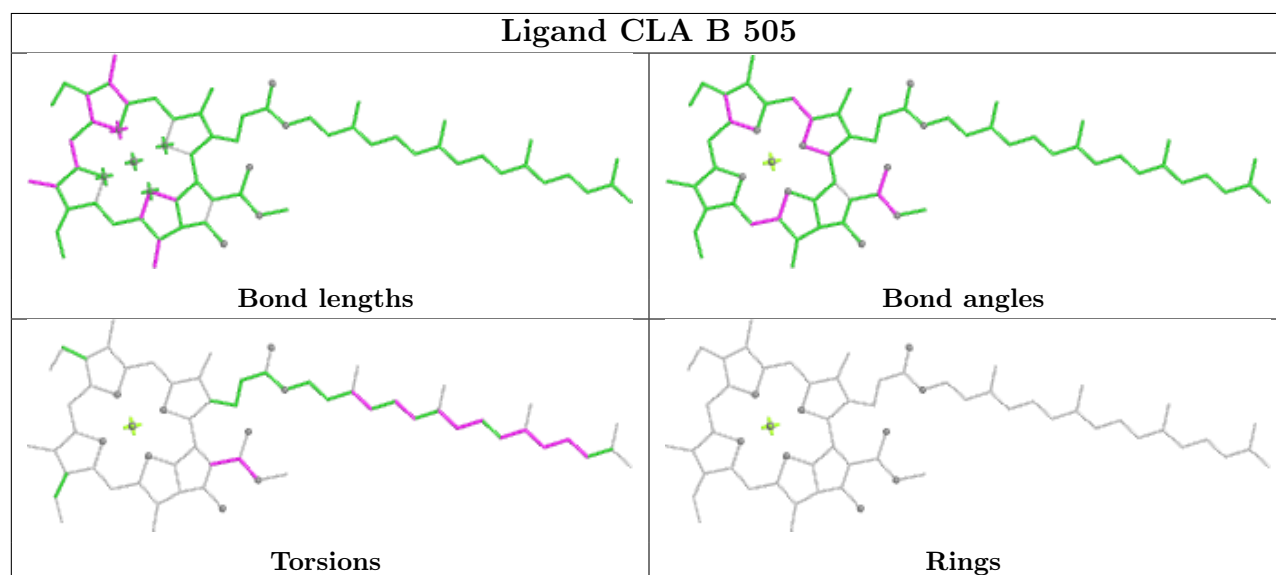
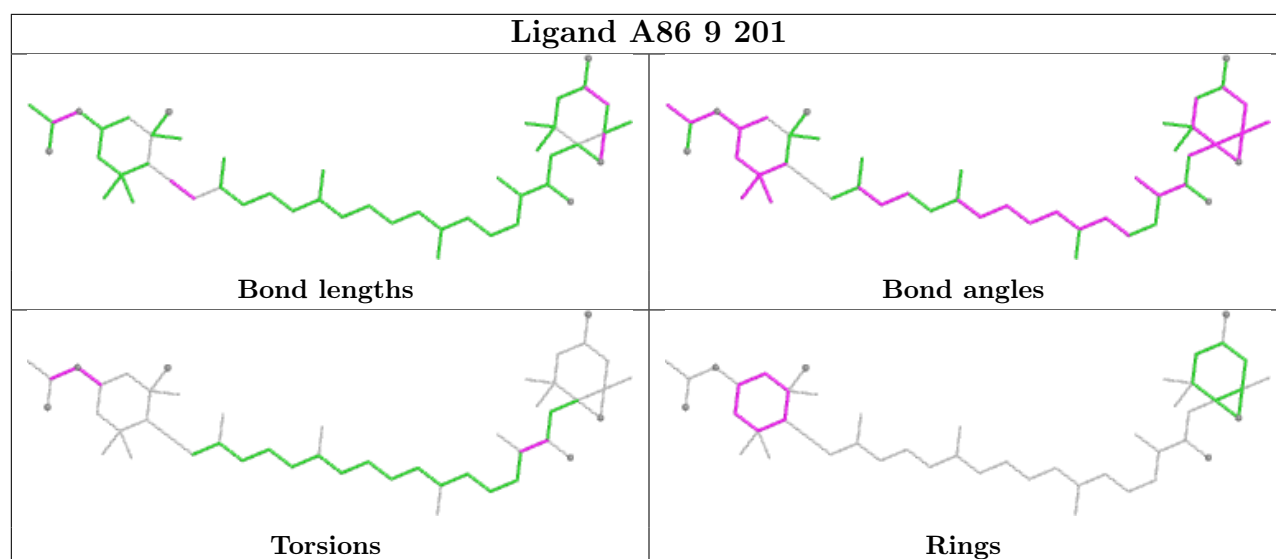
Torsions

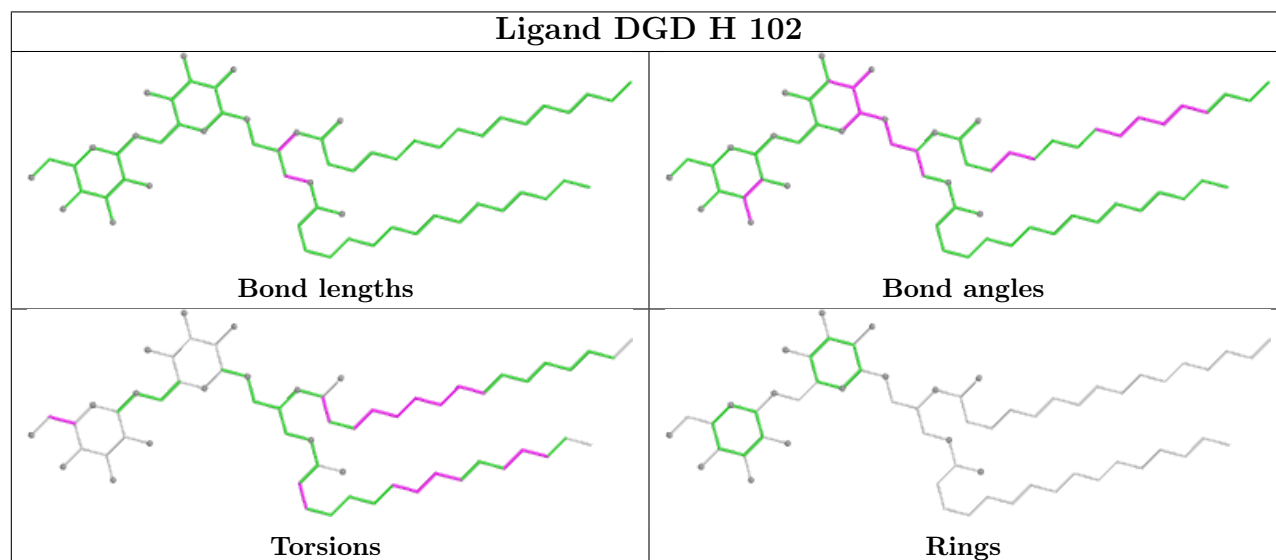
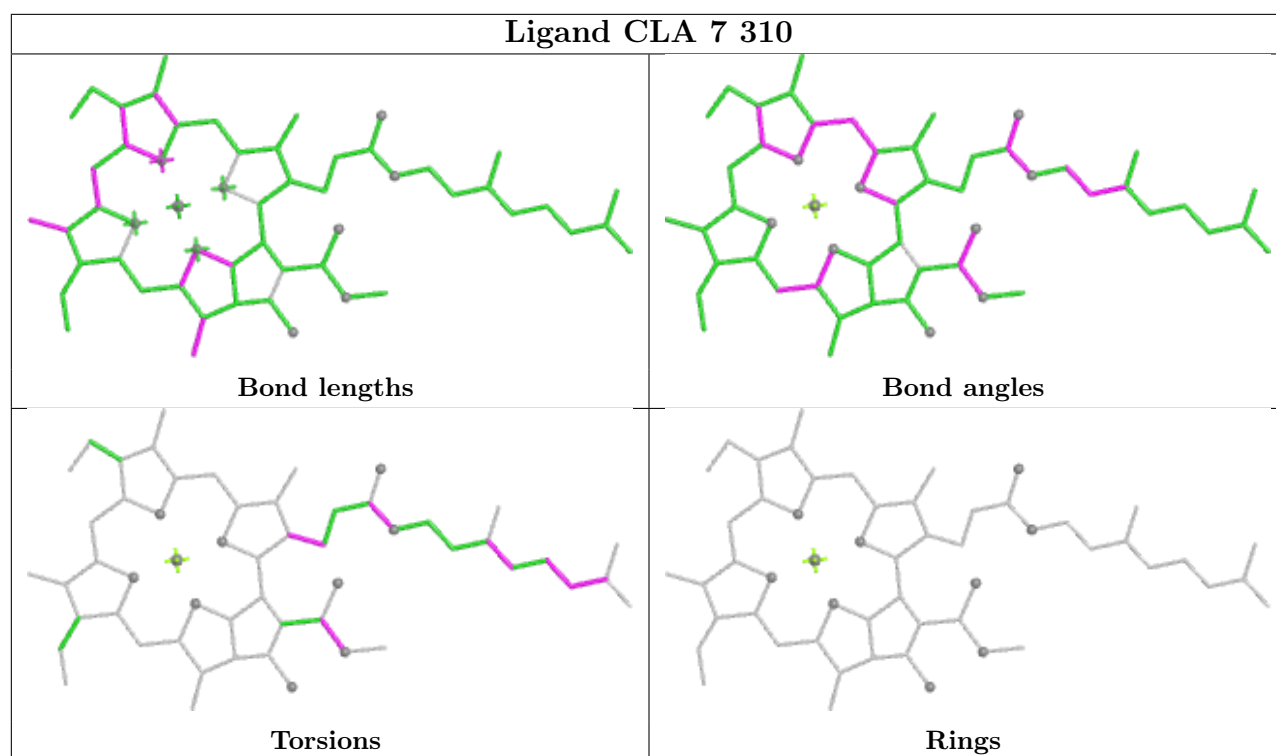


Rings

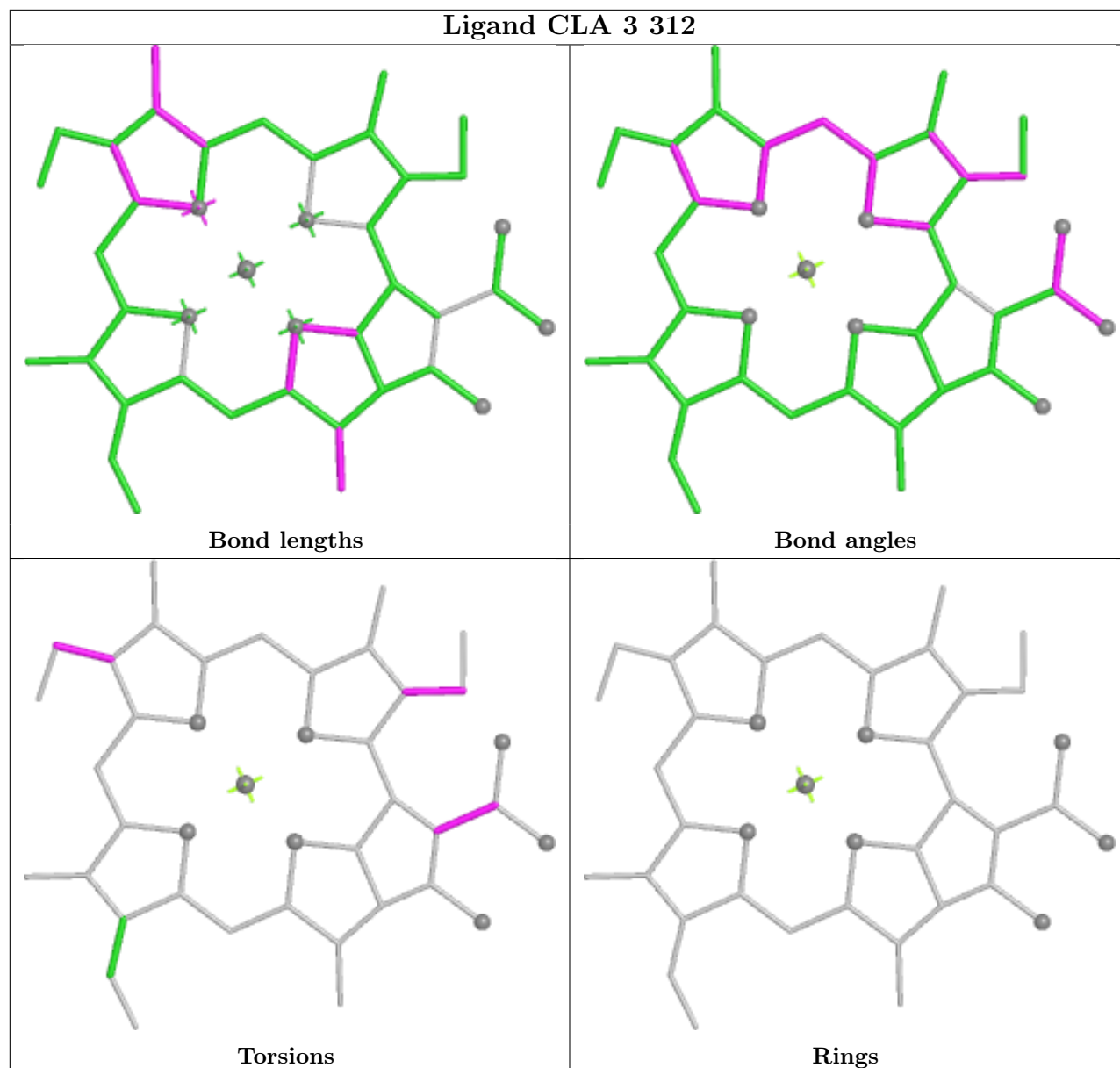




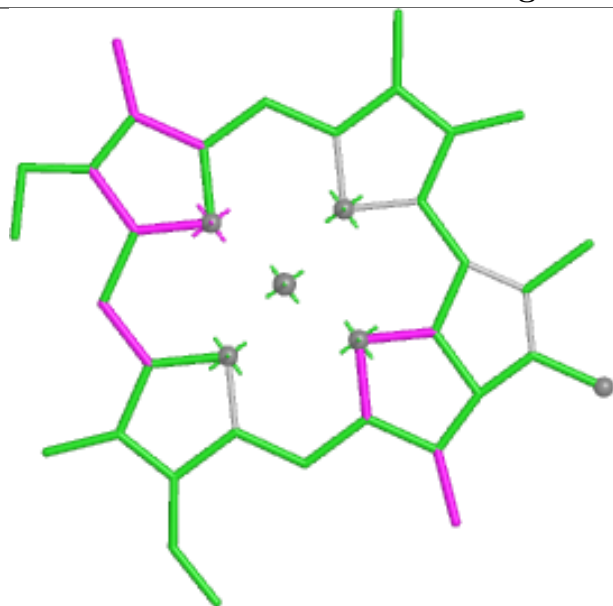




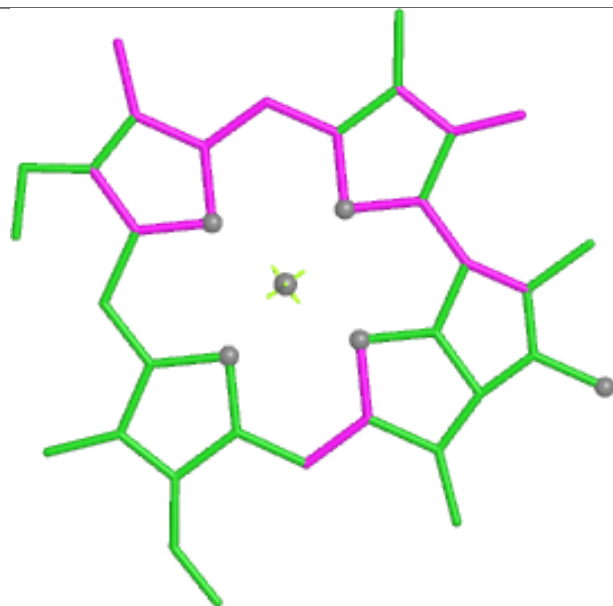
Ligand CLA 3 312



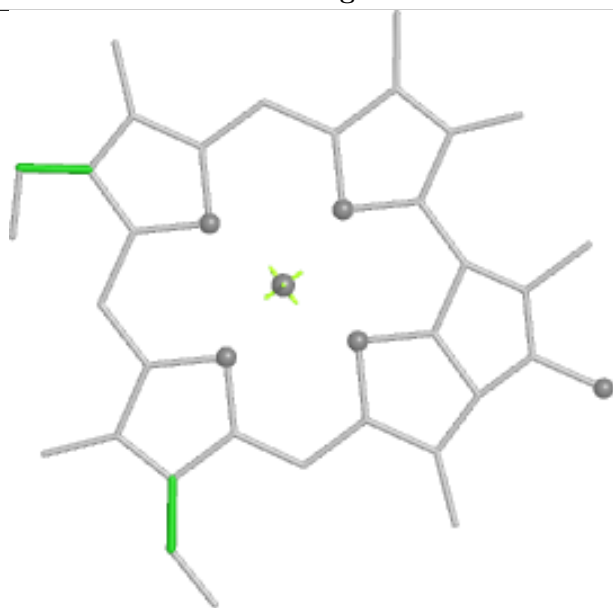
Ligand CLA 7 314



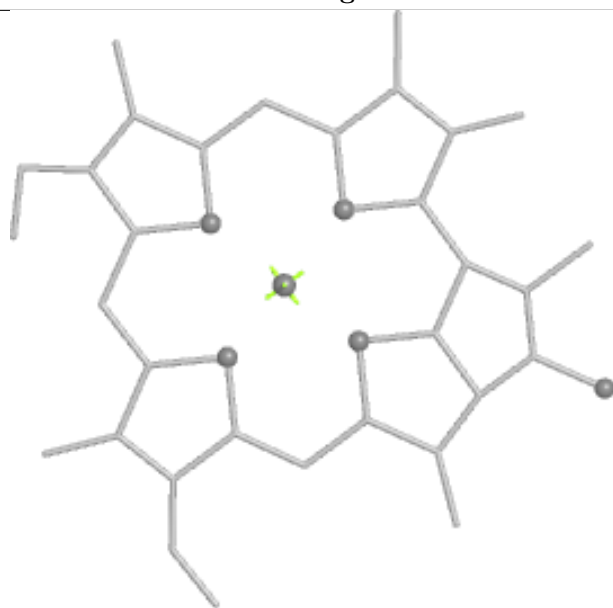
Bond lengths



Bond angles

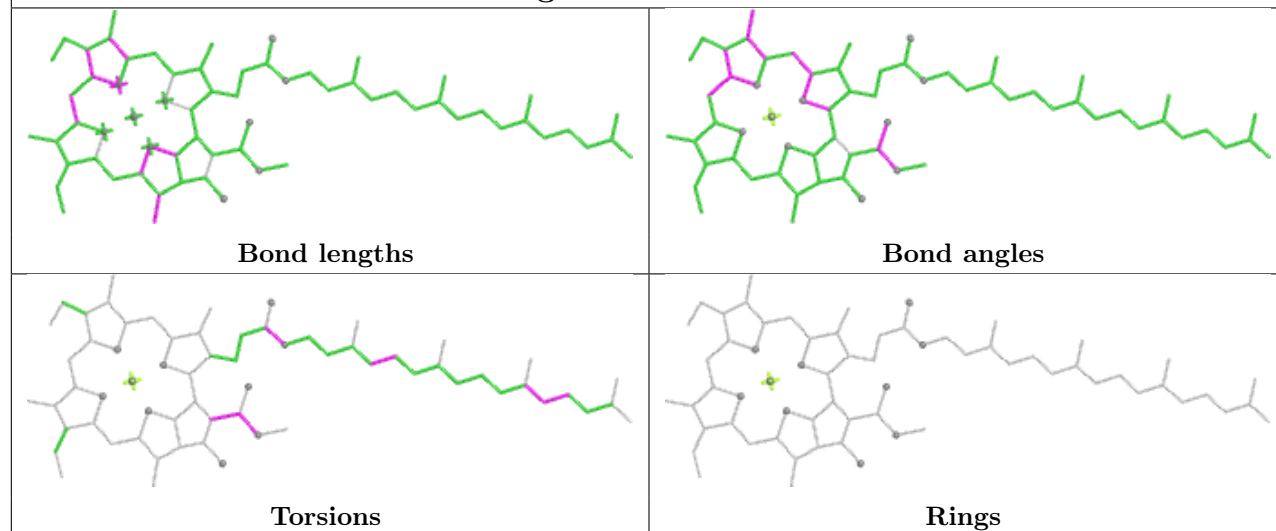


Torsions

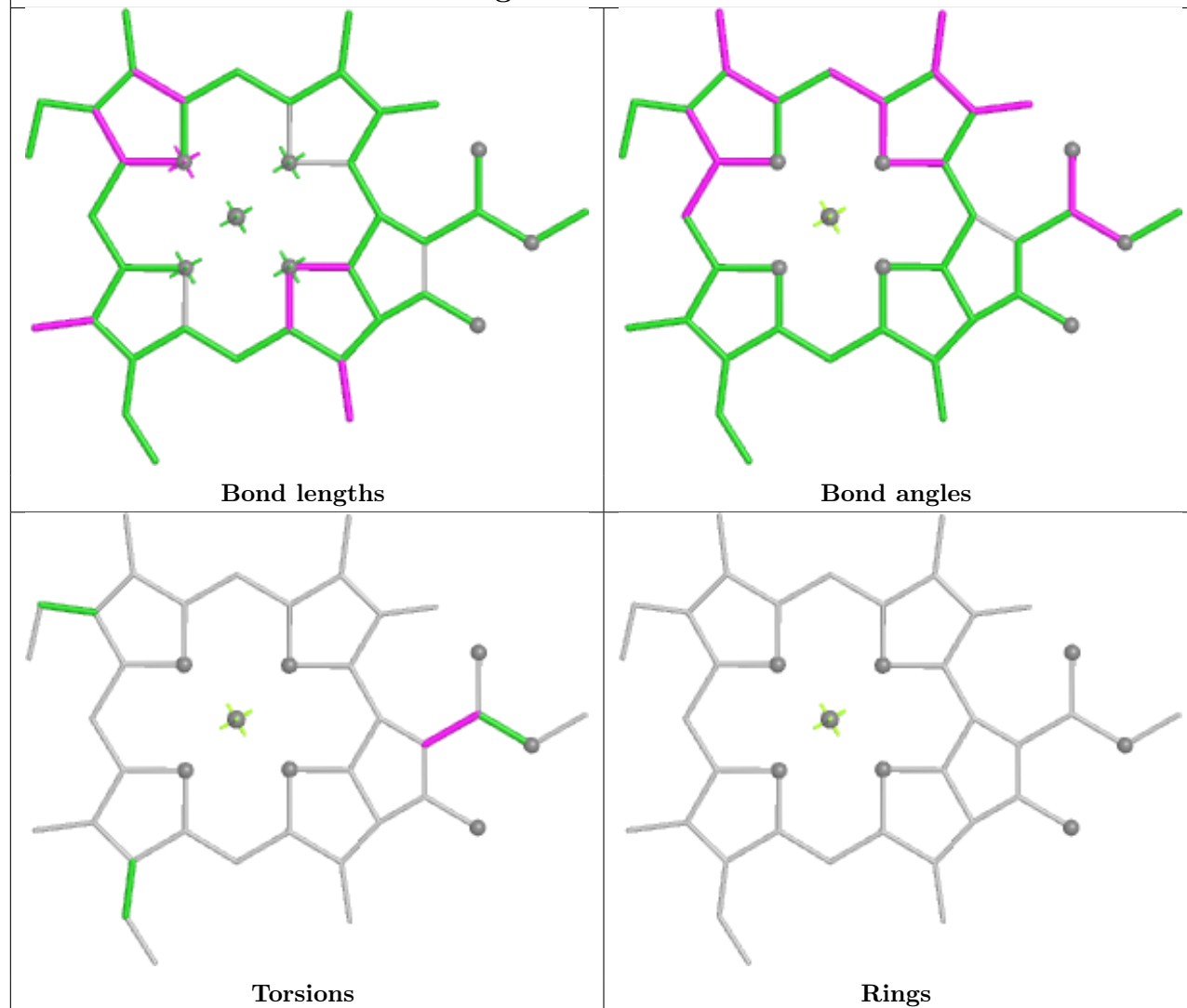


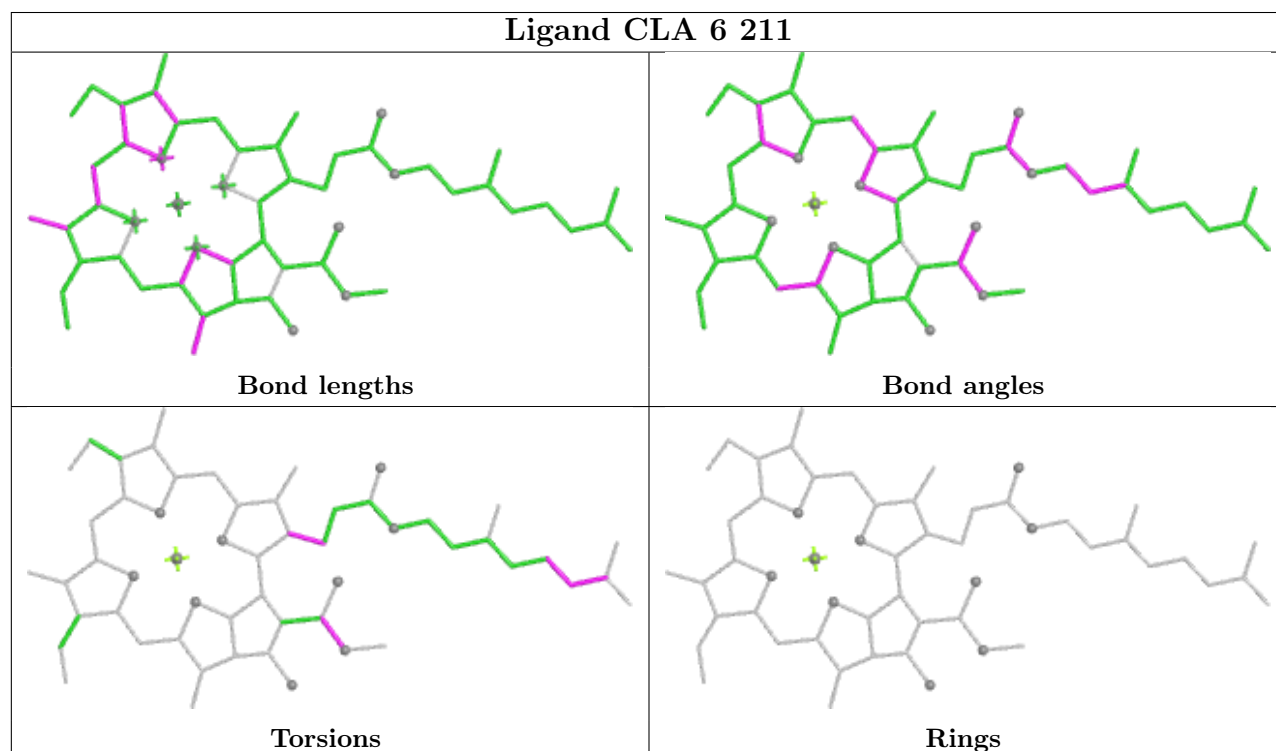
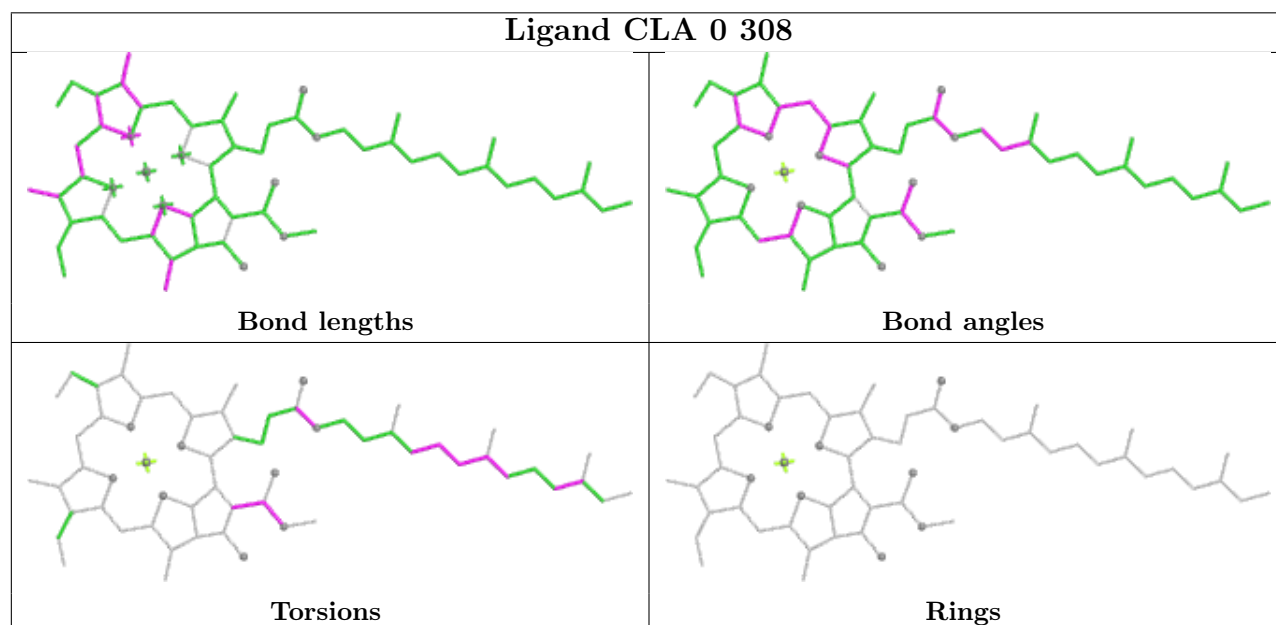
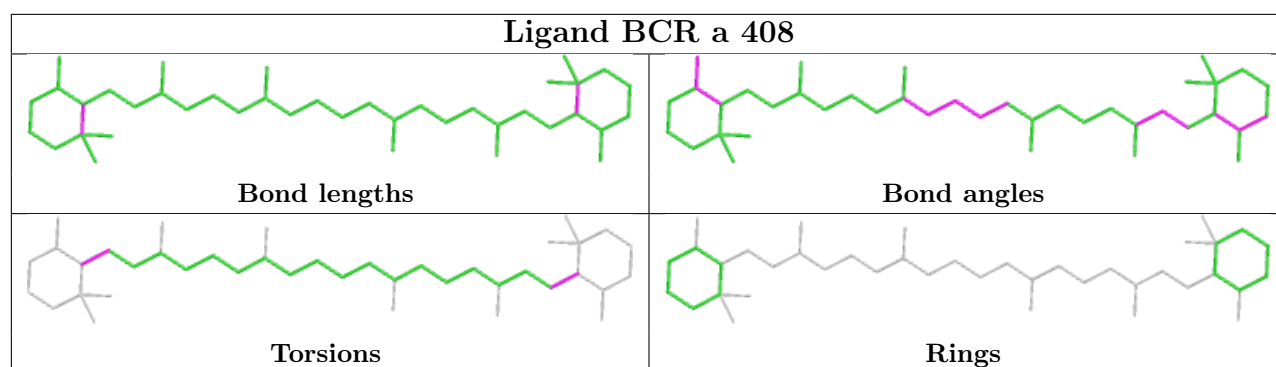
Rings

Ligand CLA c 512

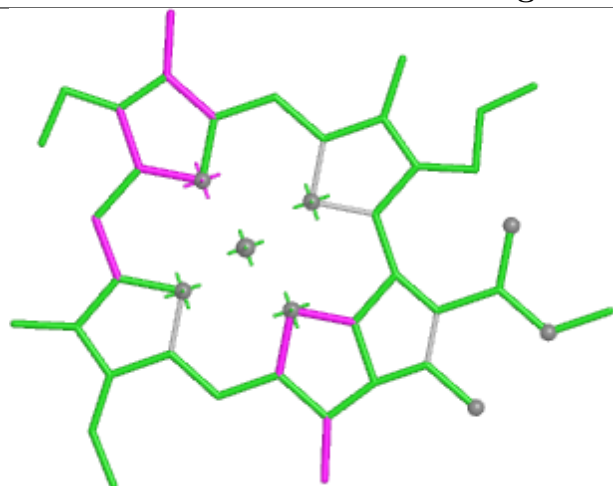


Ligand CLA B 512

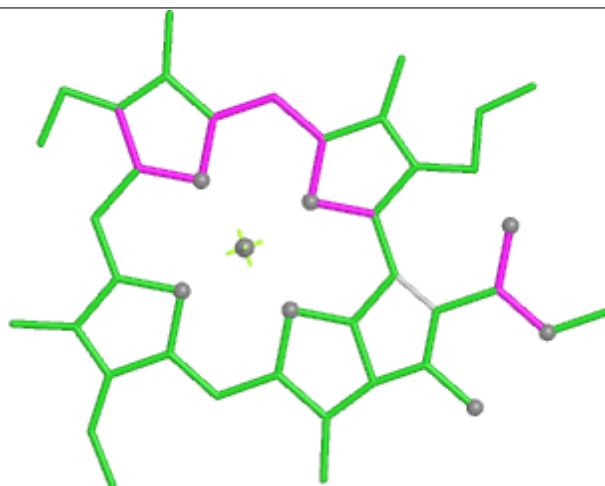




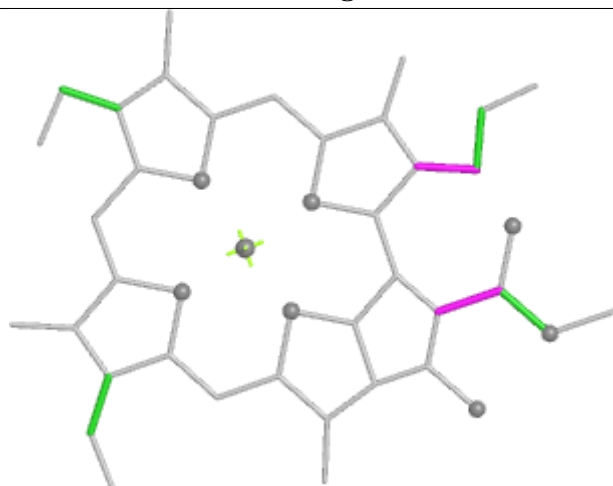
Ligand CLA b 502



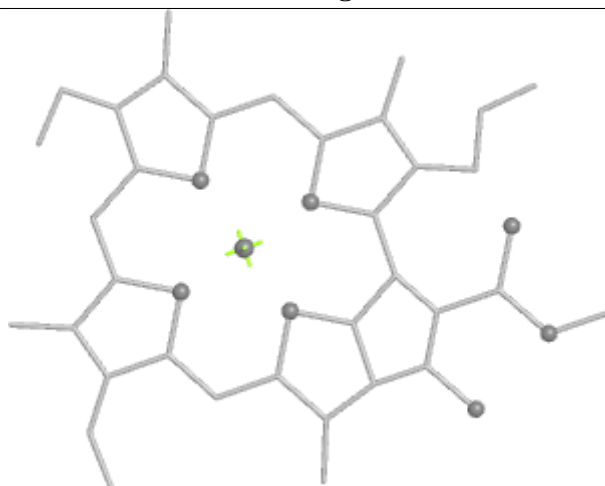
Bond lengths



Bond angles

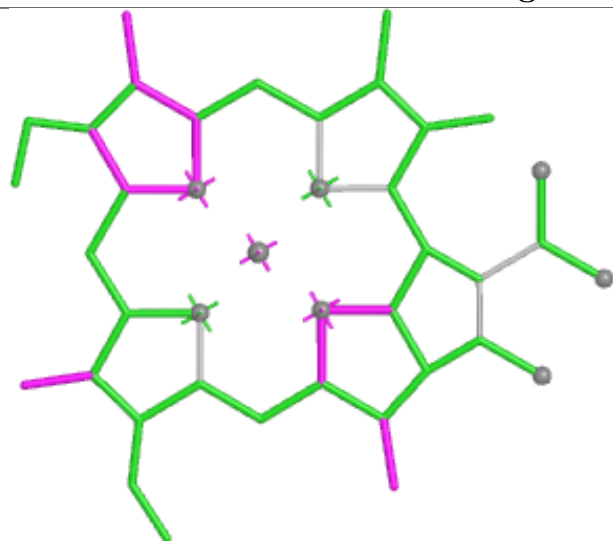


Torsions

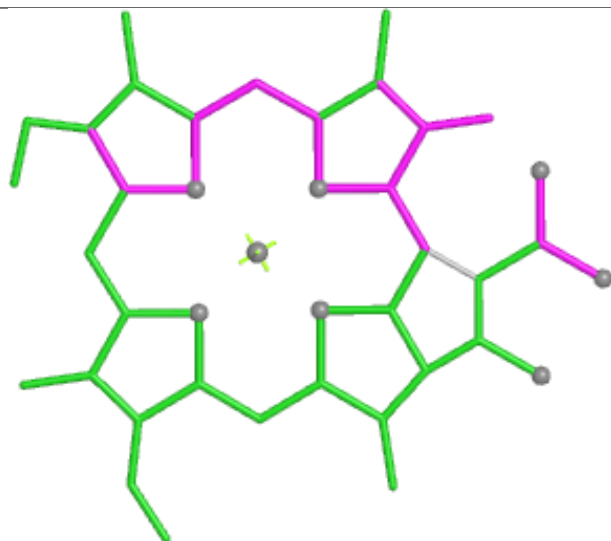


Rings

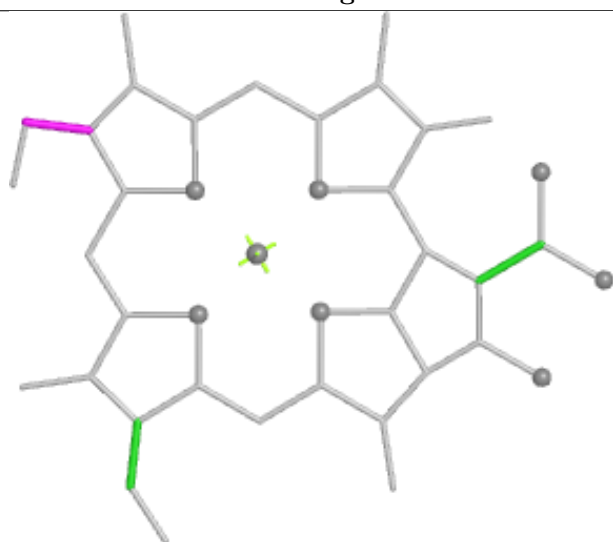
Ligand CLA 4 208



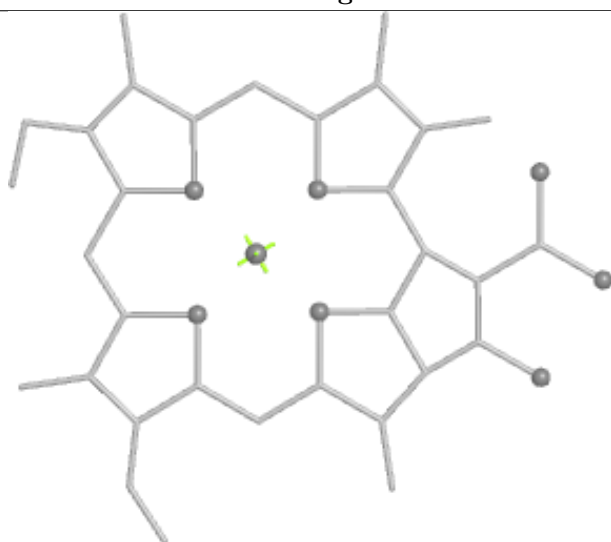
Bond lengths



Bond angles

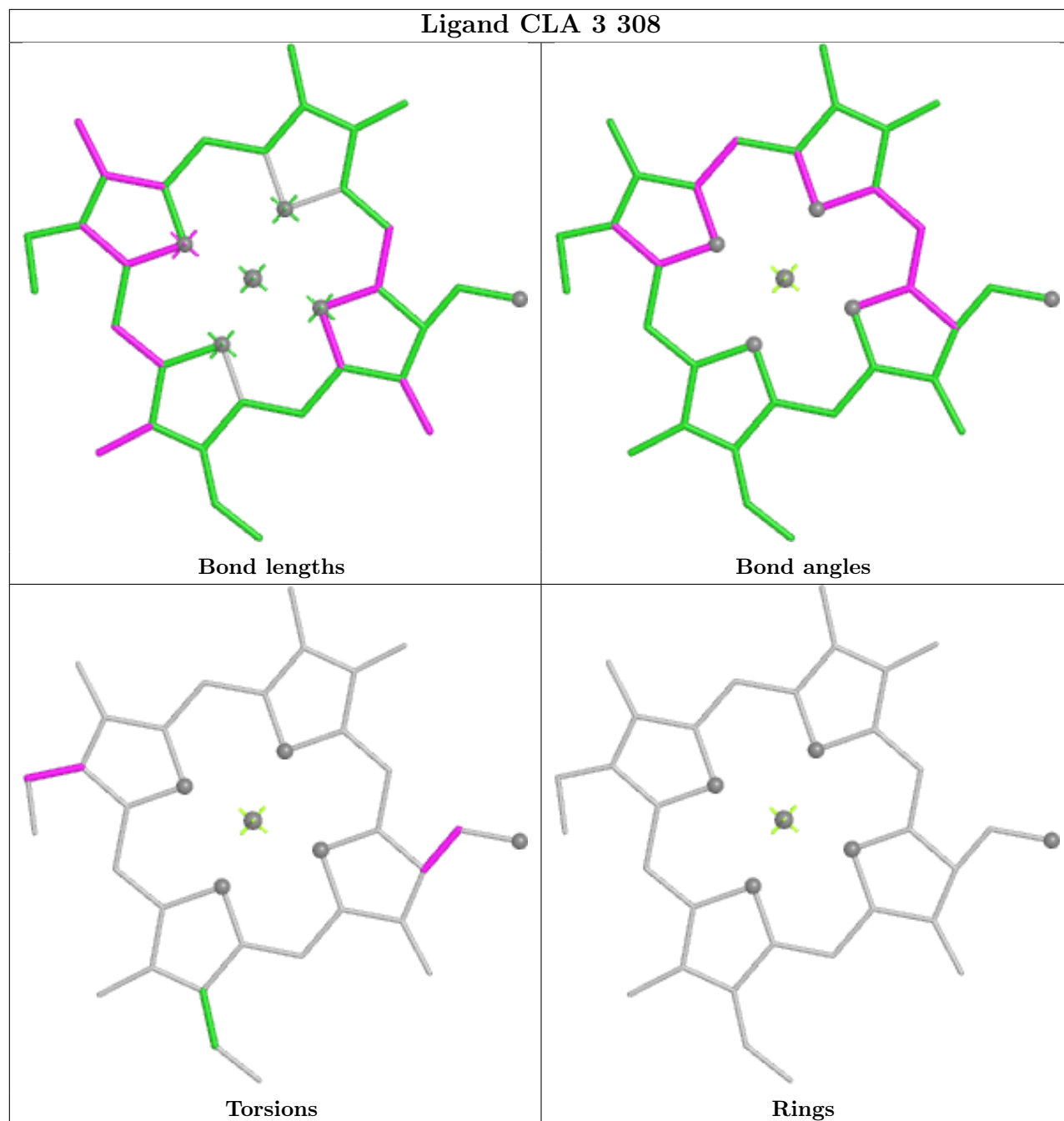


Torsions

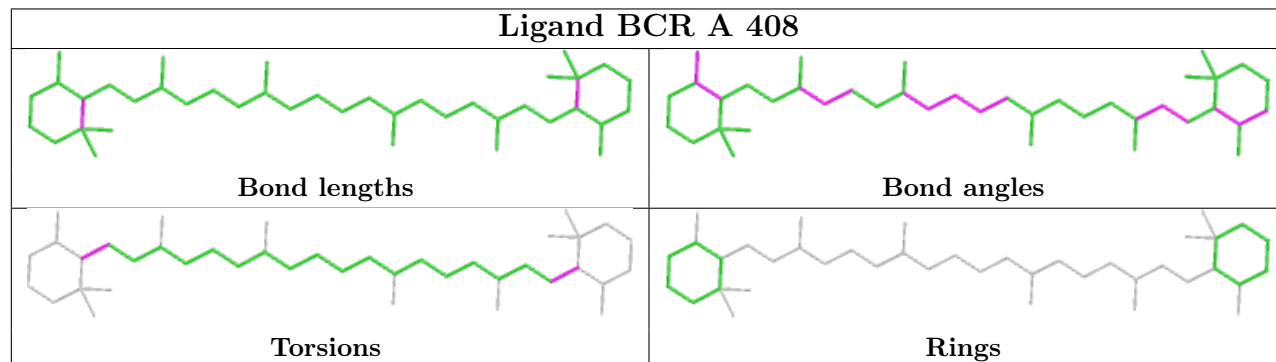


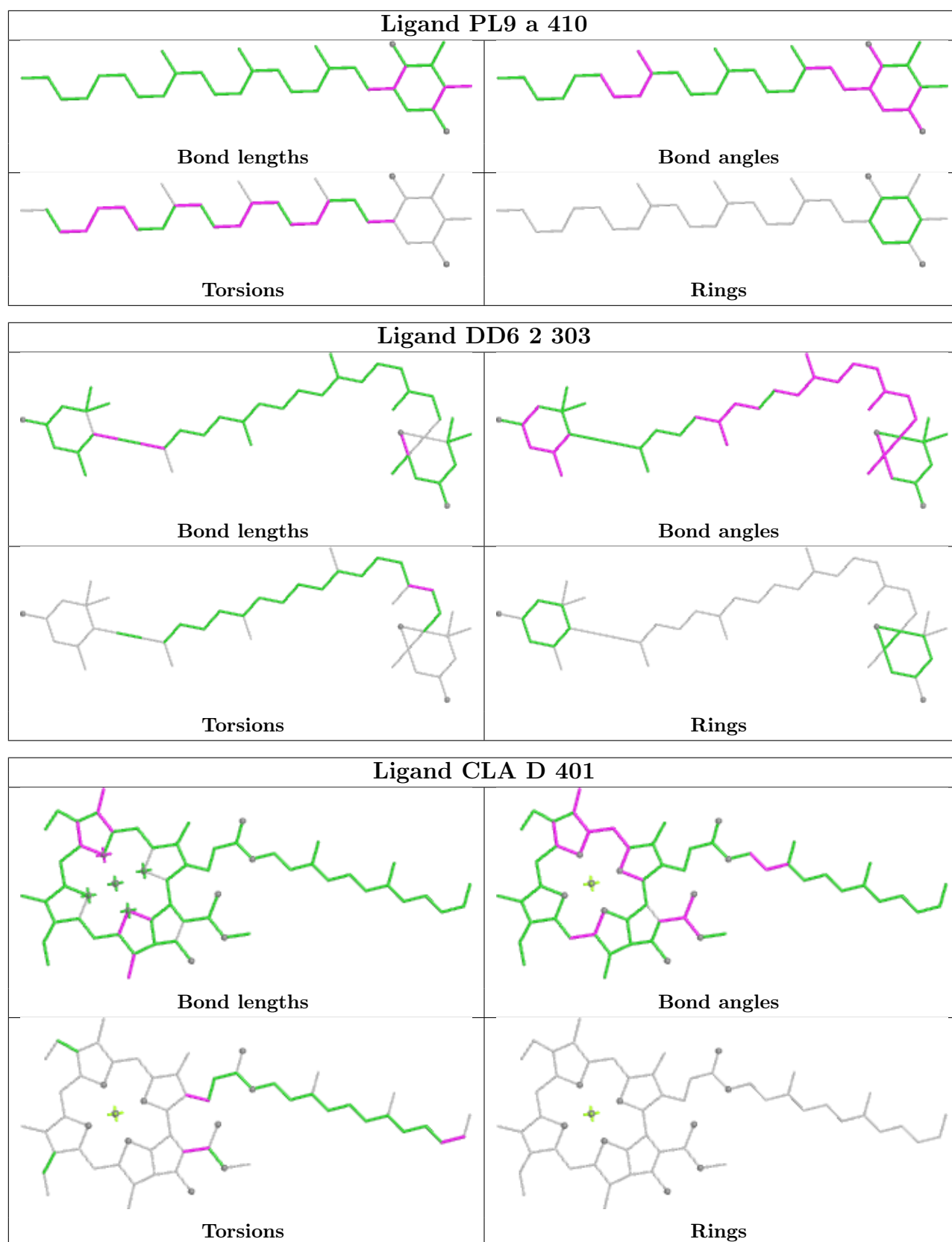
Rings

Ligand CLA 3 308

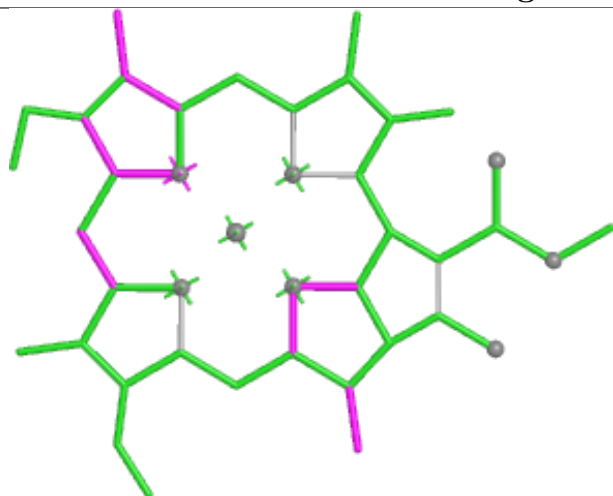


Ligand BCR A 408

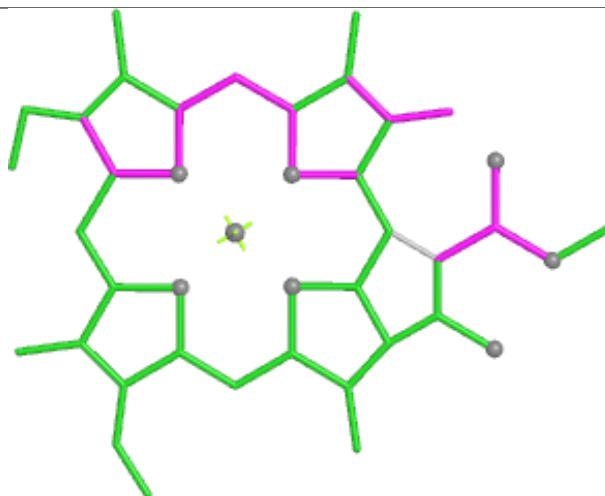




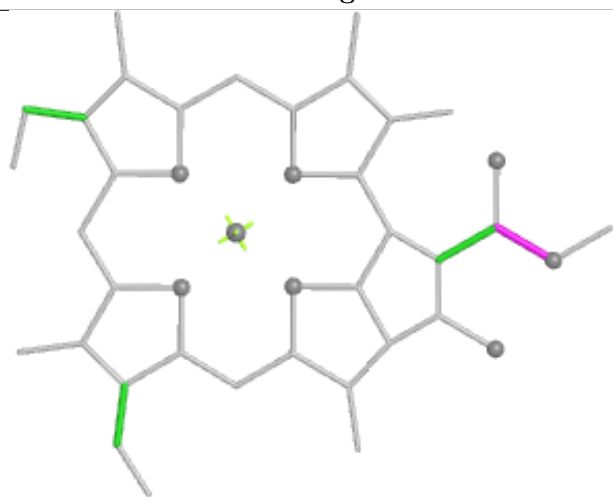
Ligand CLA b 508



Bond lengths



Bond angles

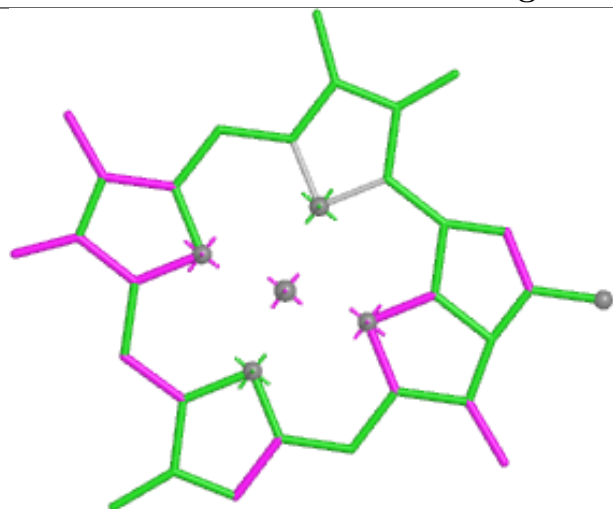


Torsions



Rings

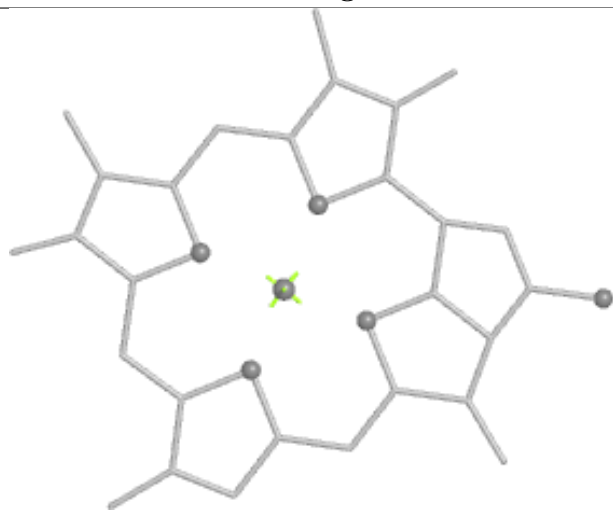
Ligand CLA 8 304



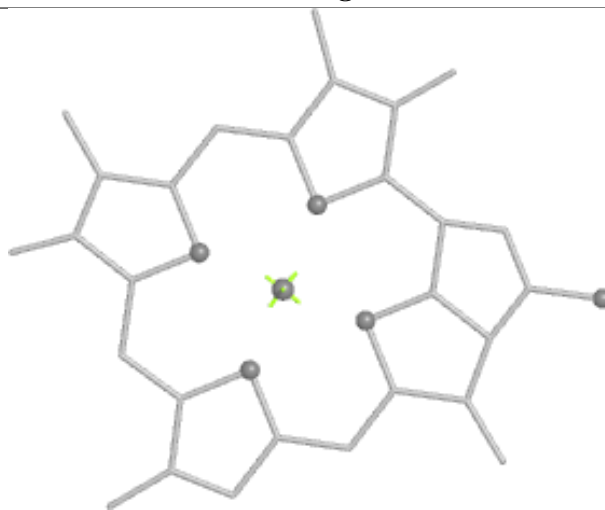
Bond lengths



Bond angles

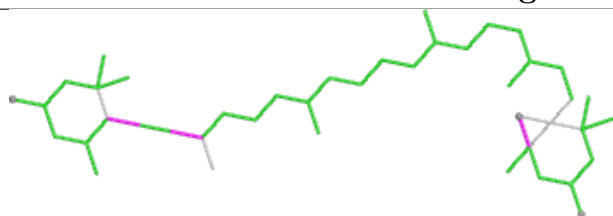


Torsions

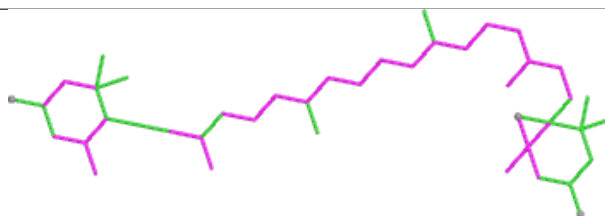


Rings

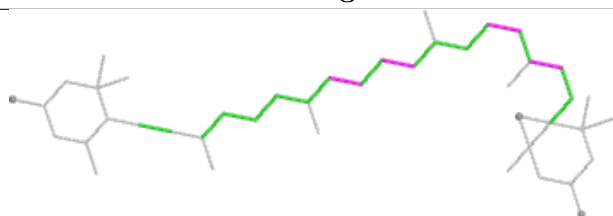
Ligand DD6 6 204



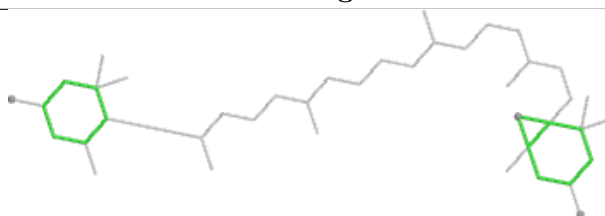
Bond lengths



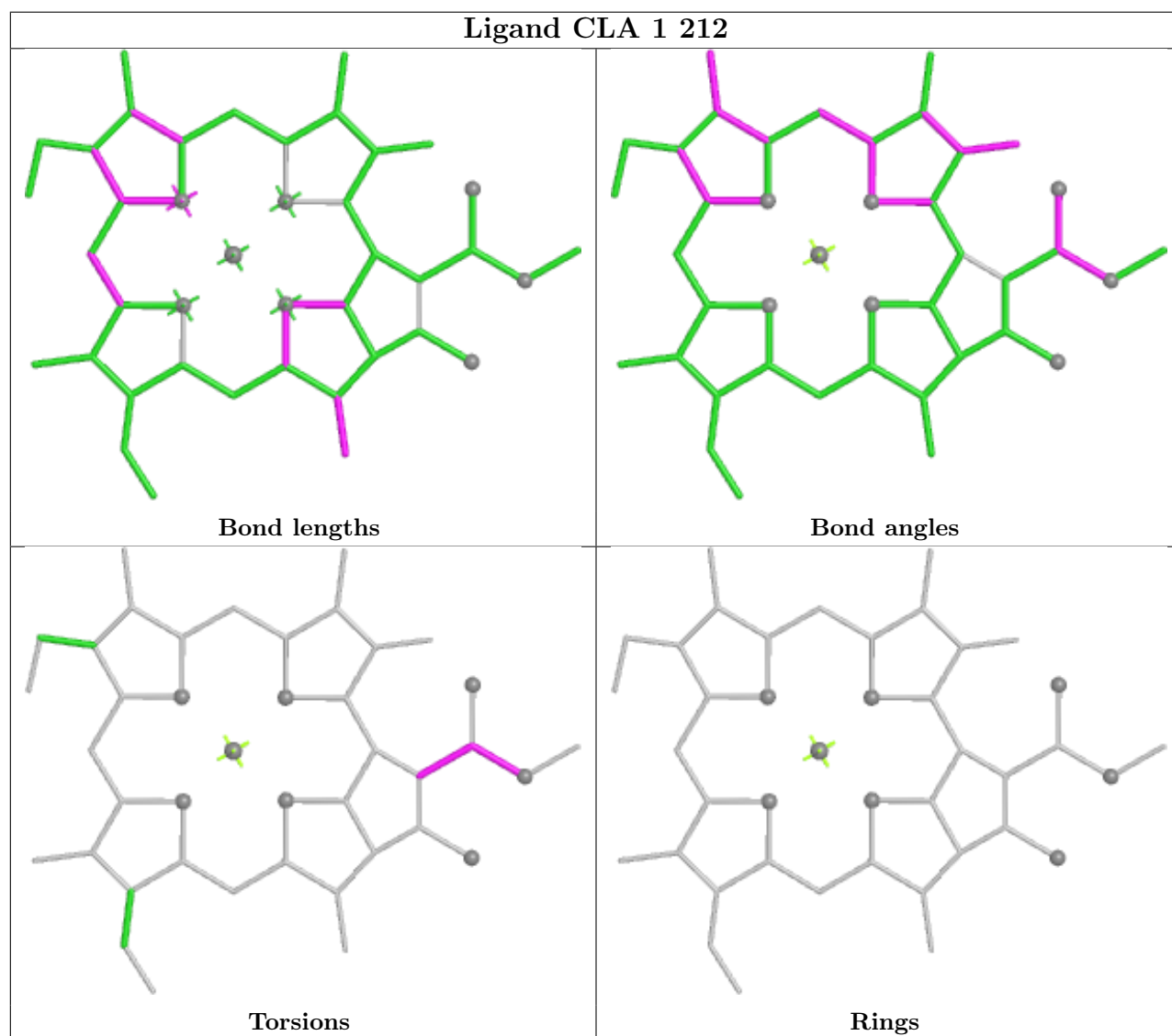
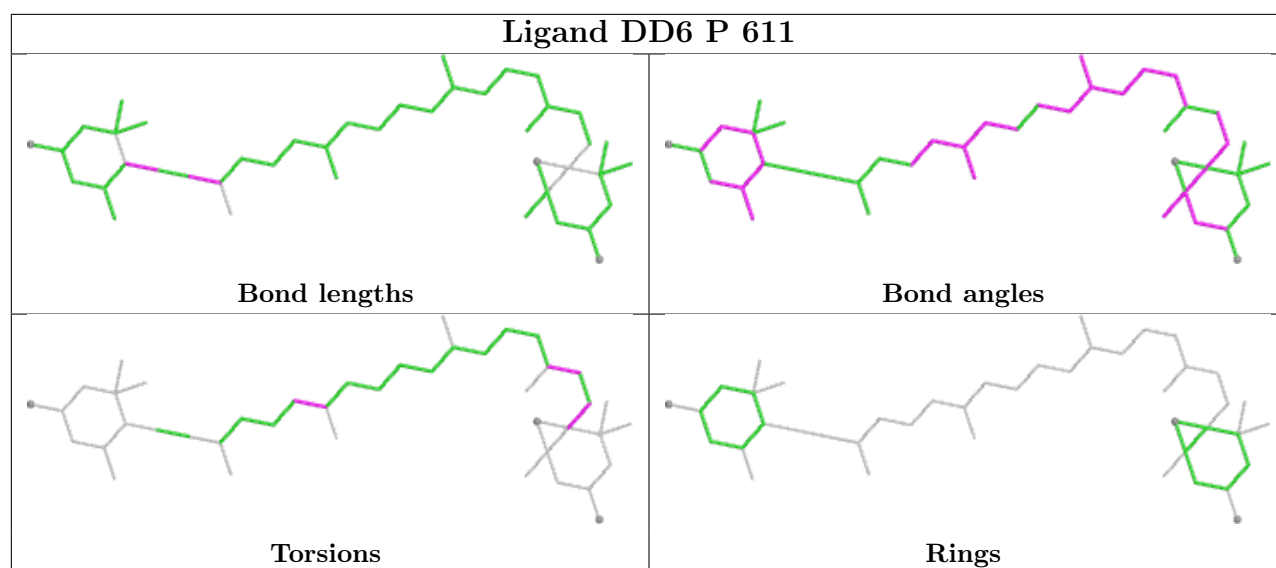
Bond angles

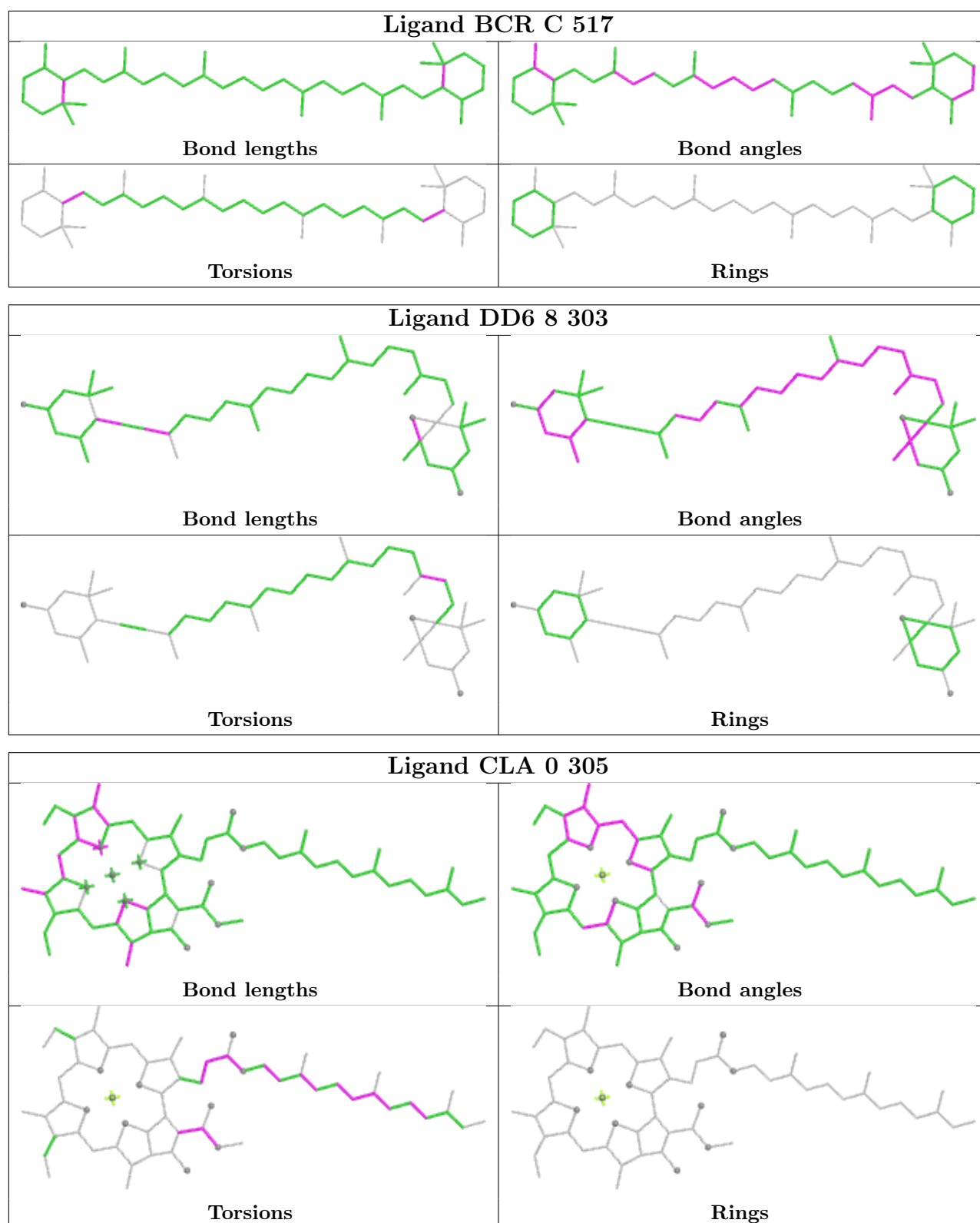


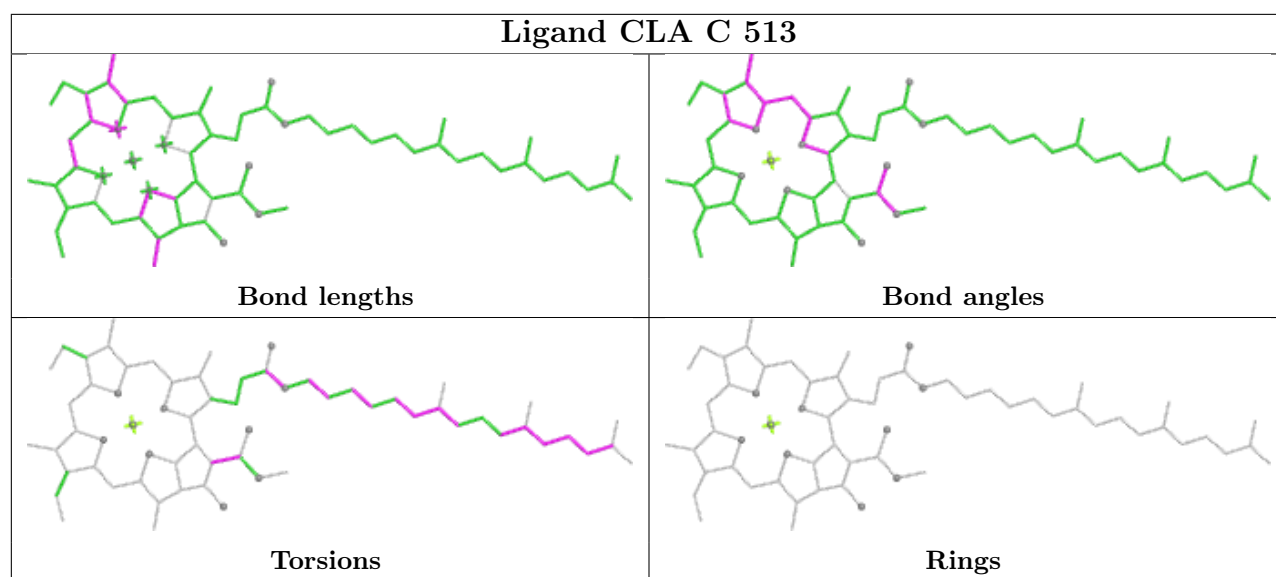
Torsions



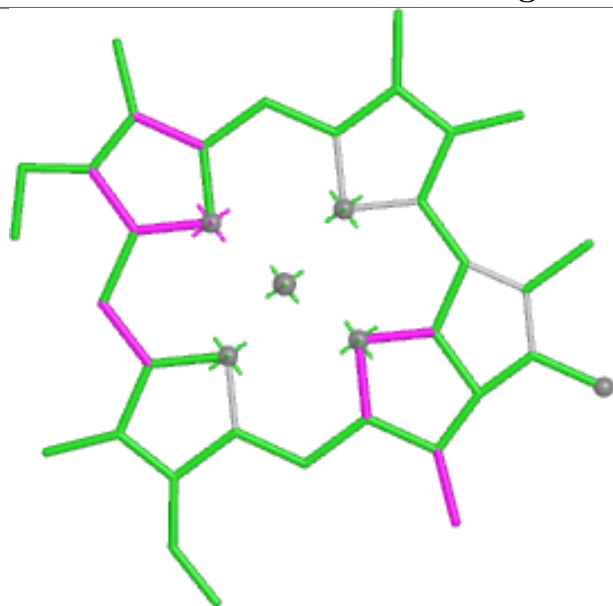
Rings







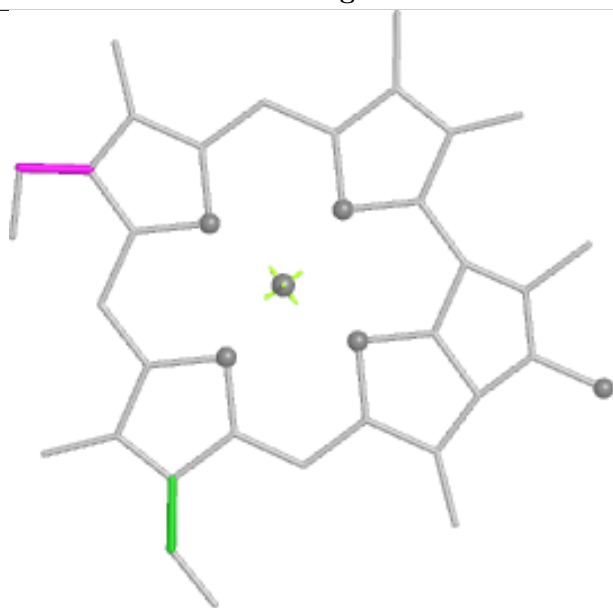
Ligand CLA 5 313



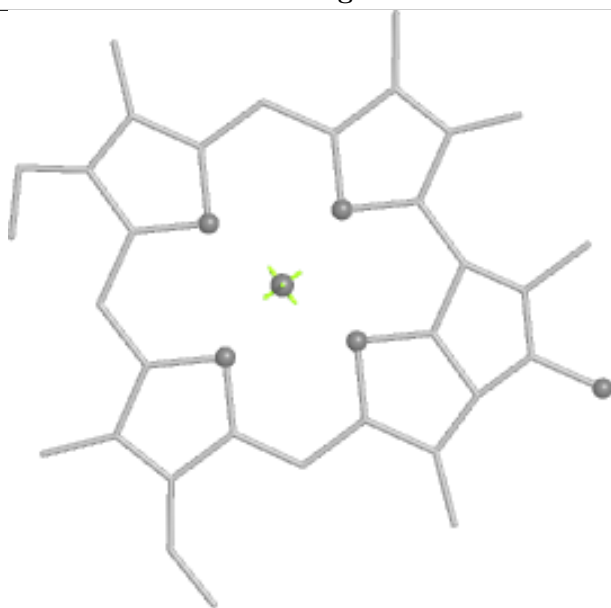
Bond lengths



Bond angles

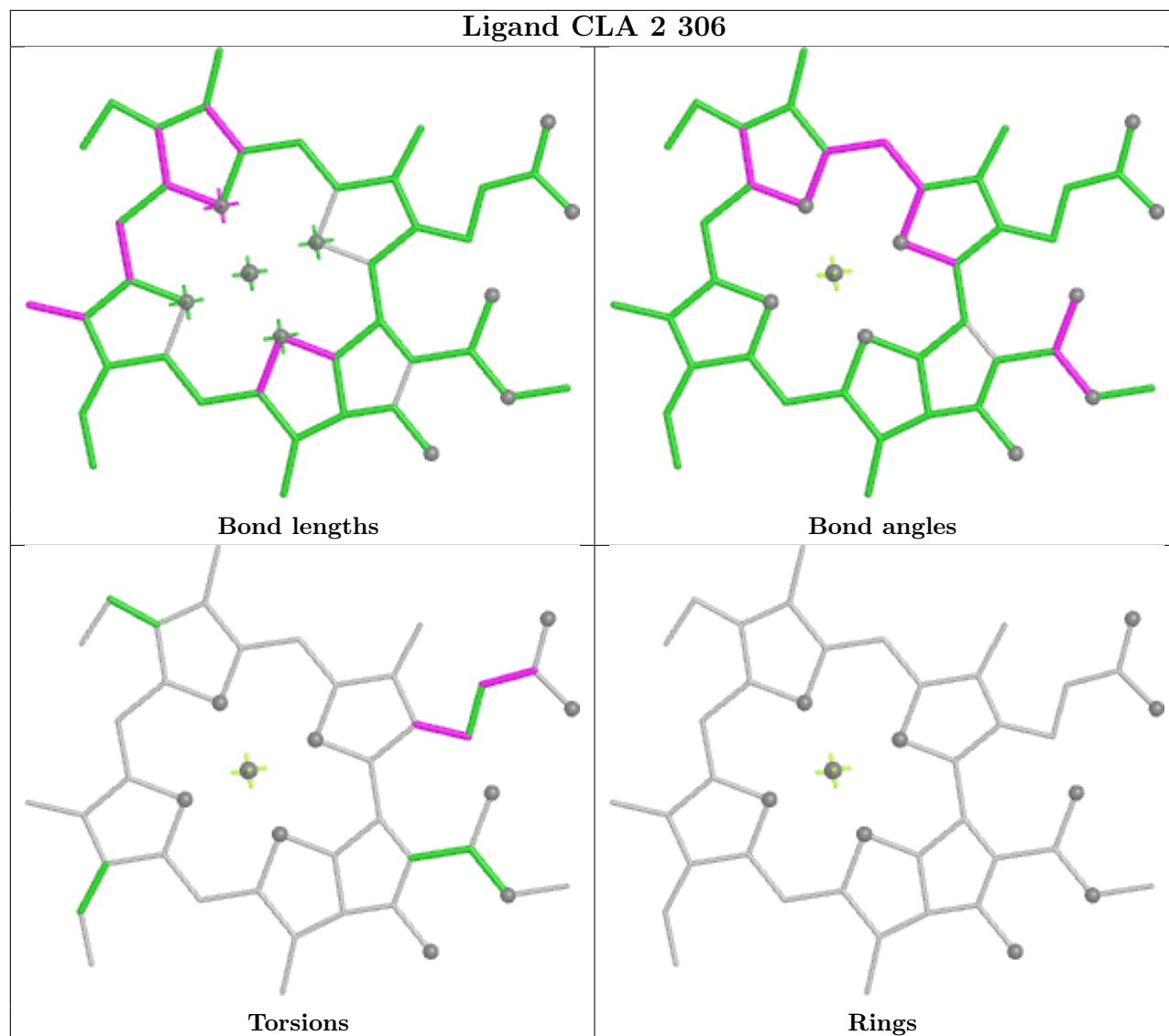


Torsions

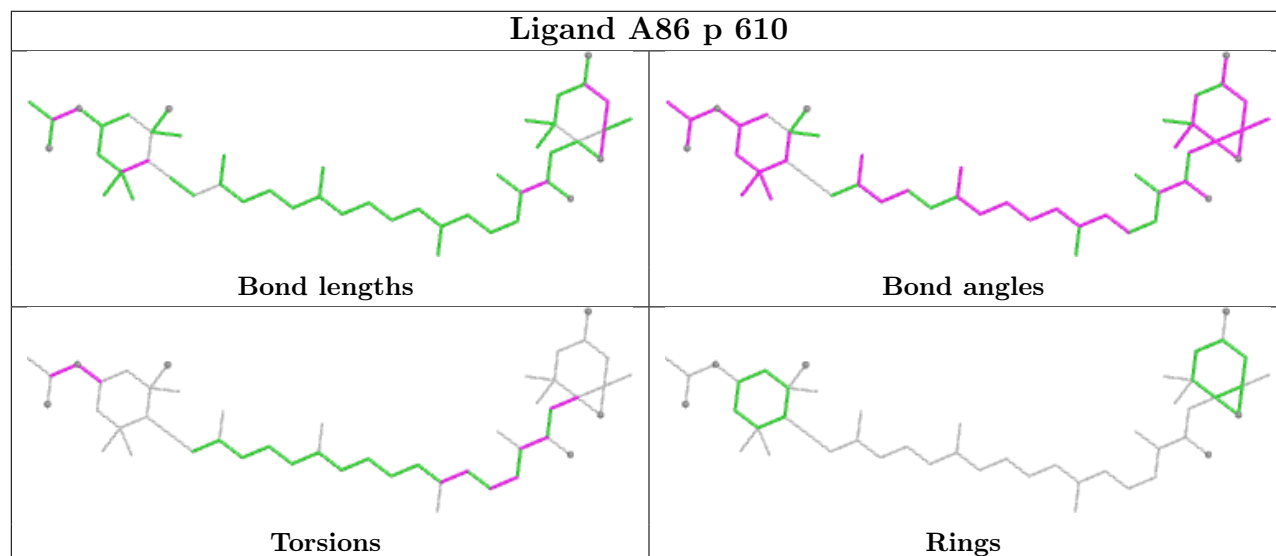


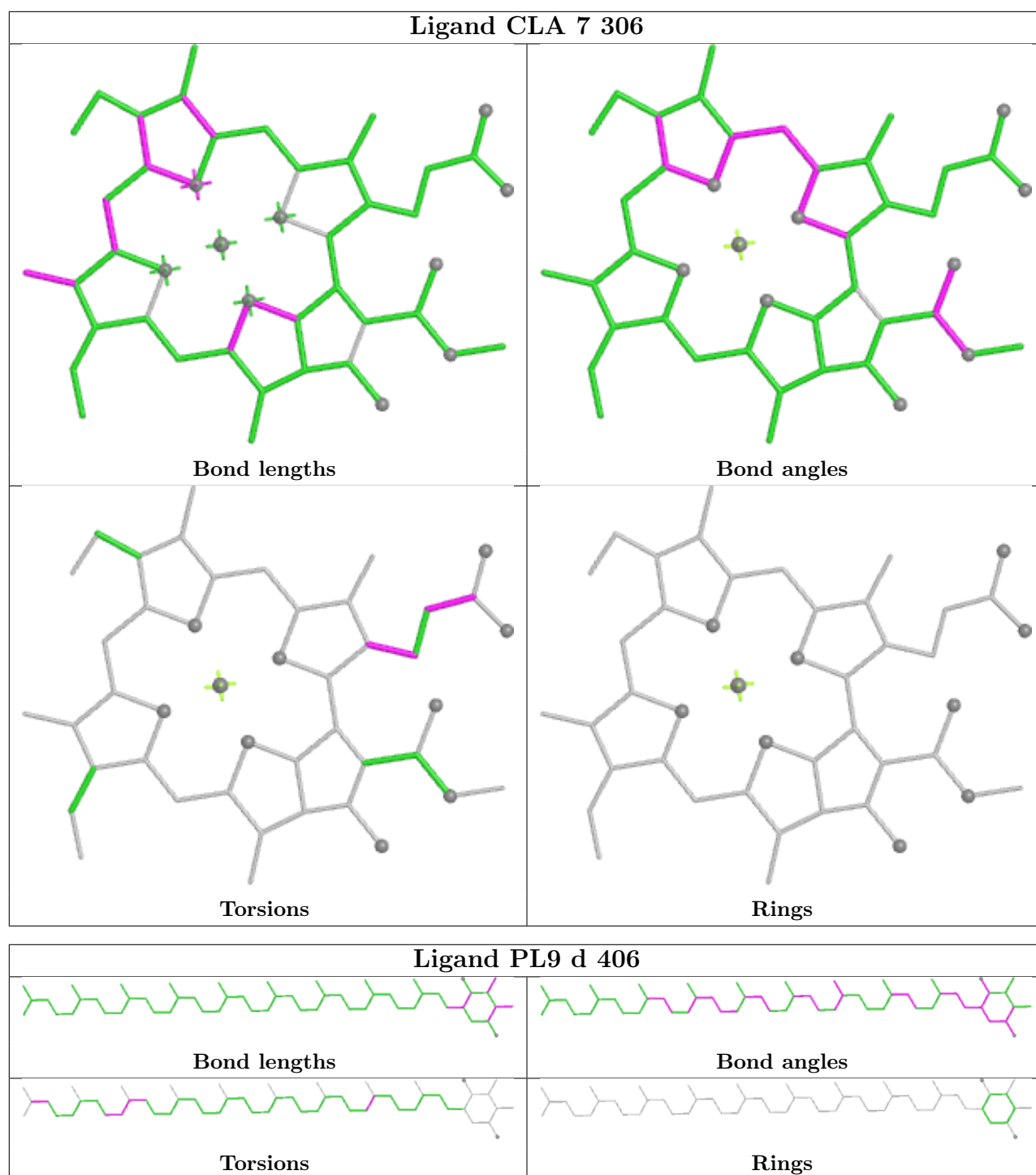
Rings

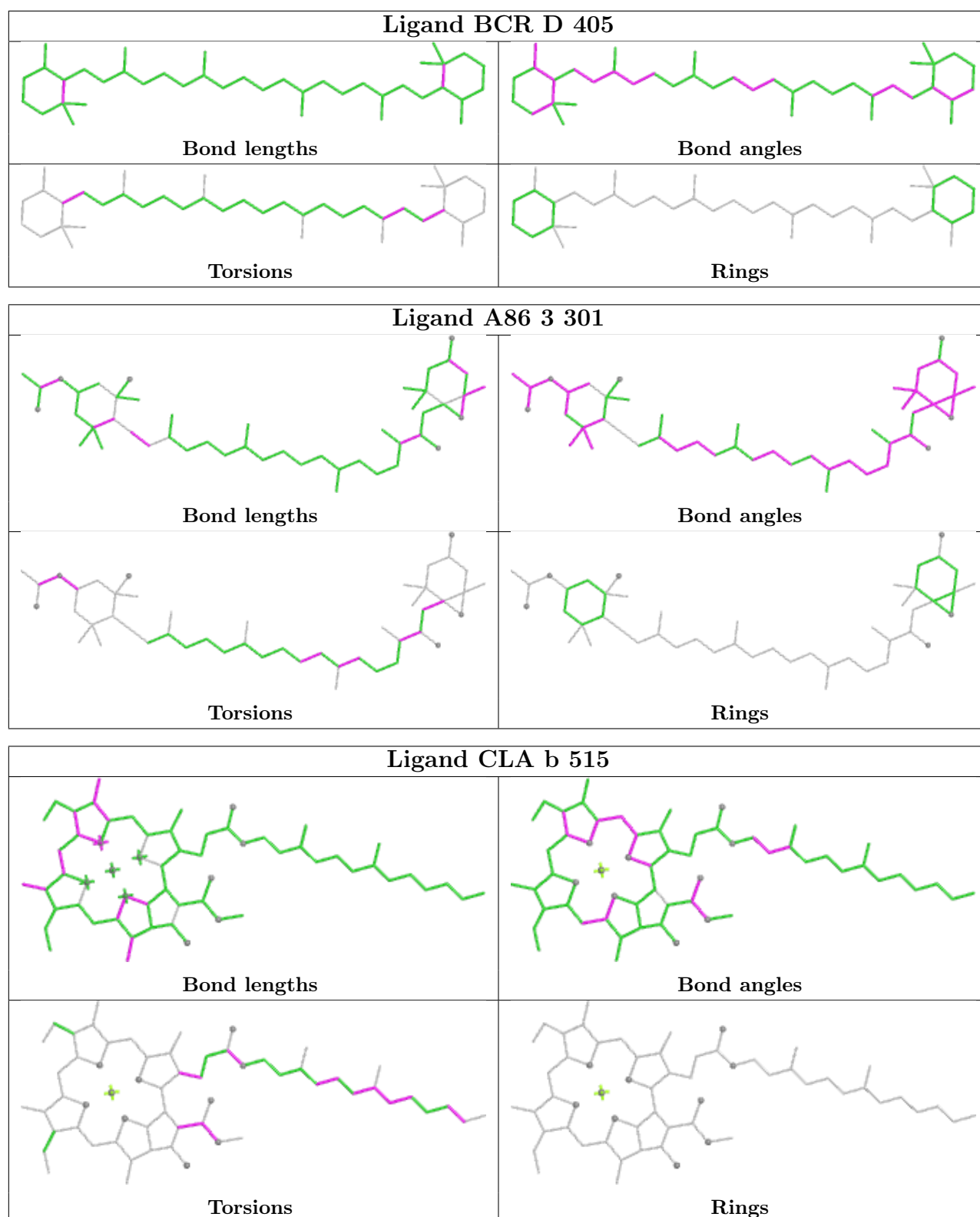
Ligand CLA 2 306

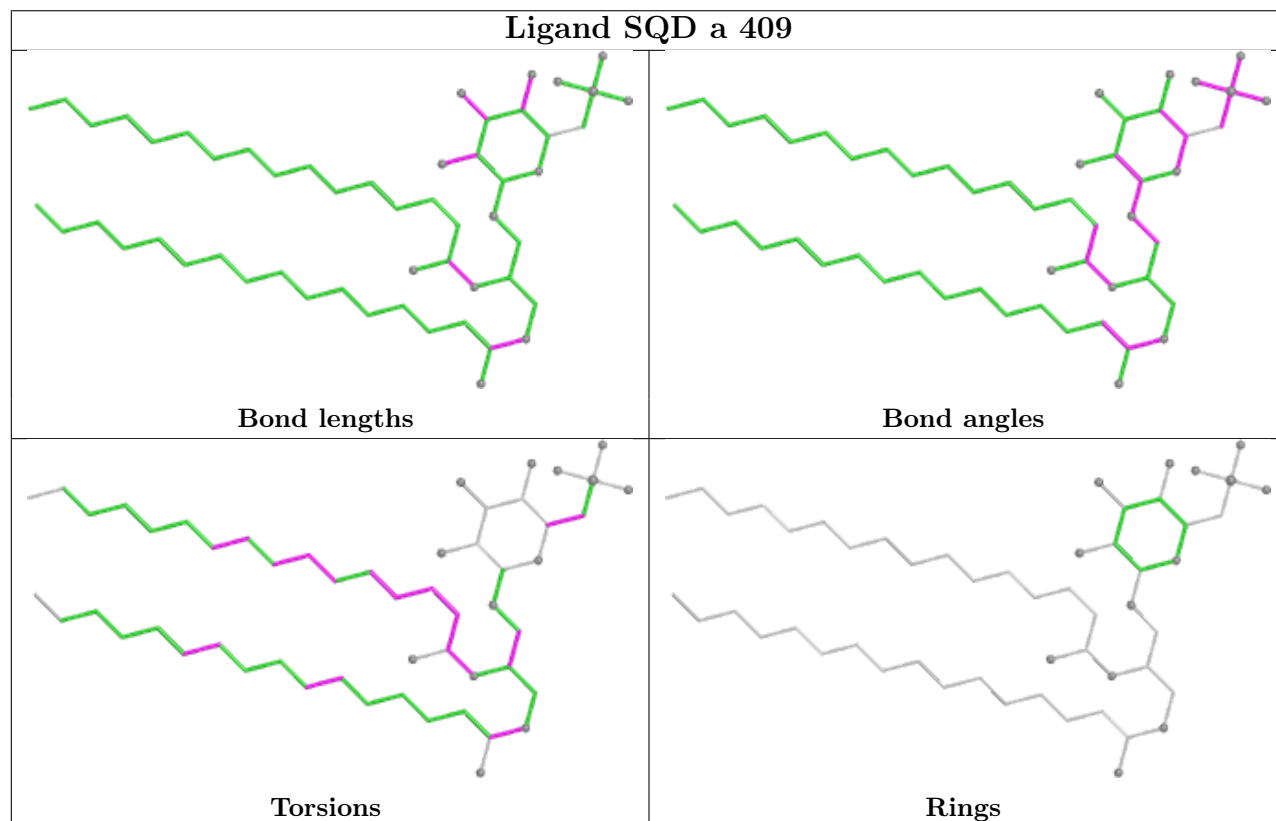
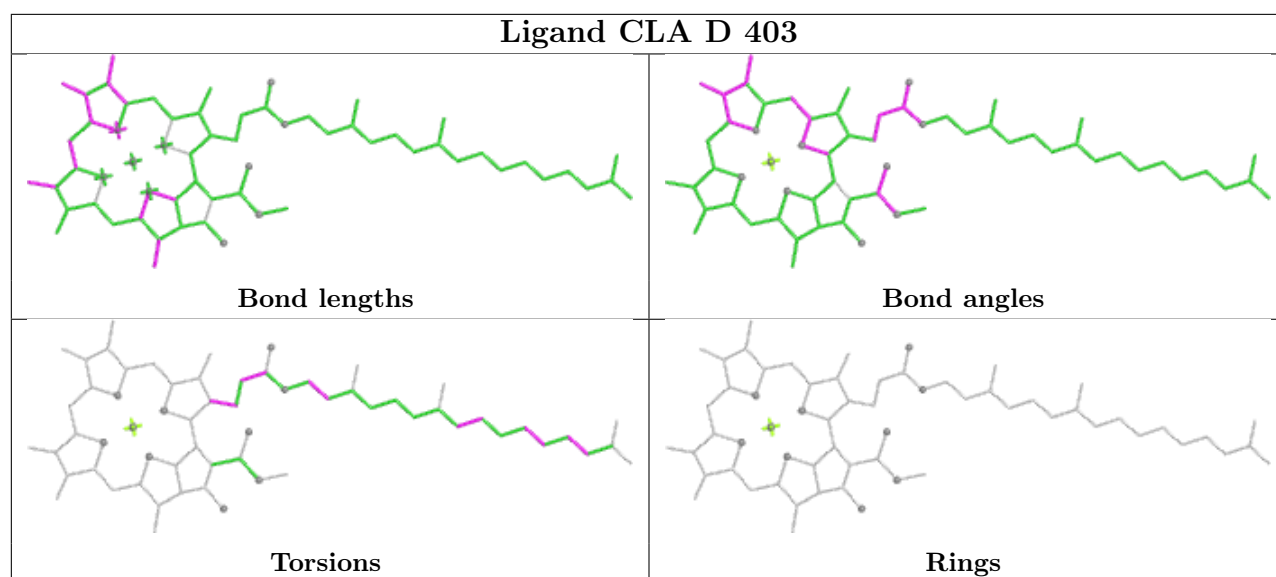


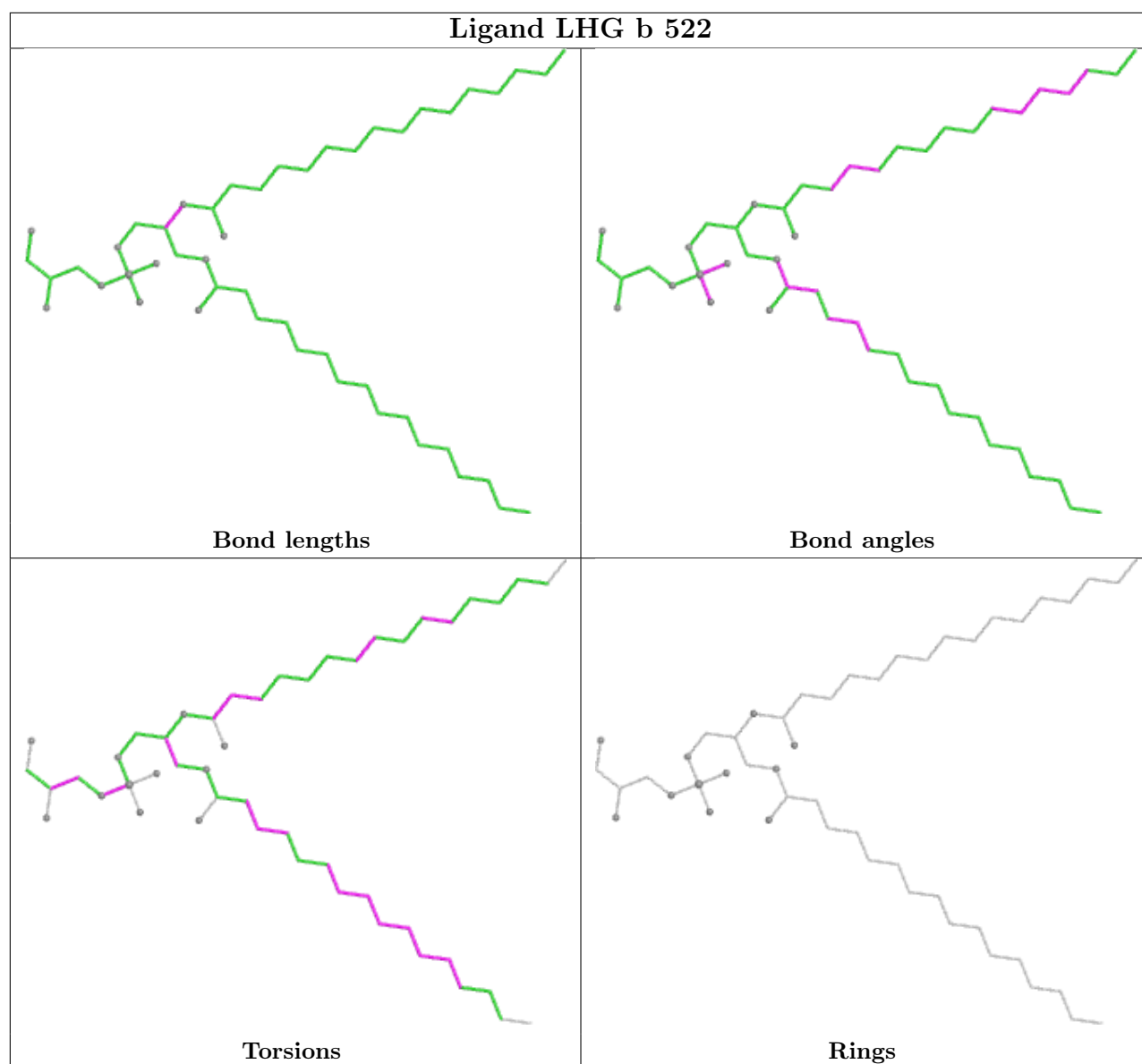
Ligand A86 p 610



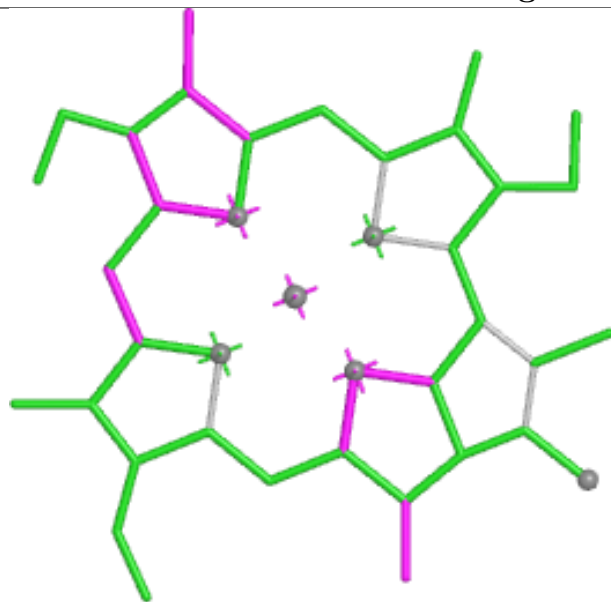








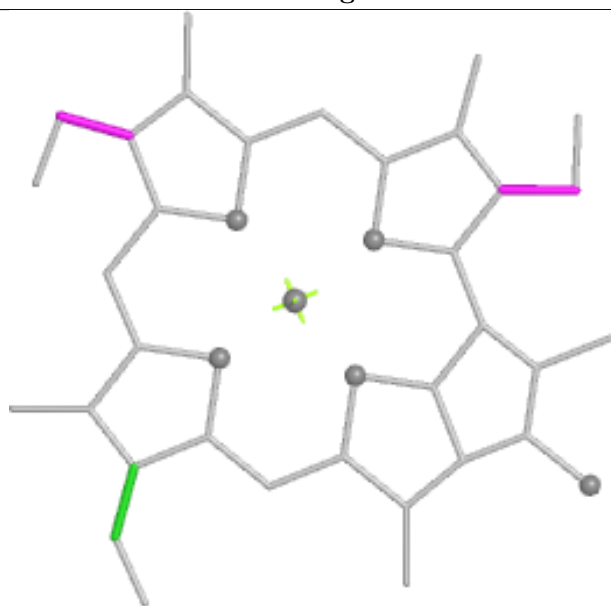
Ligand CLA 8 313



Bond lengths



Bond angles

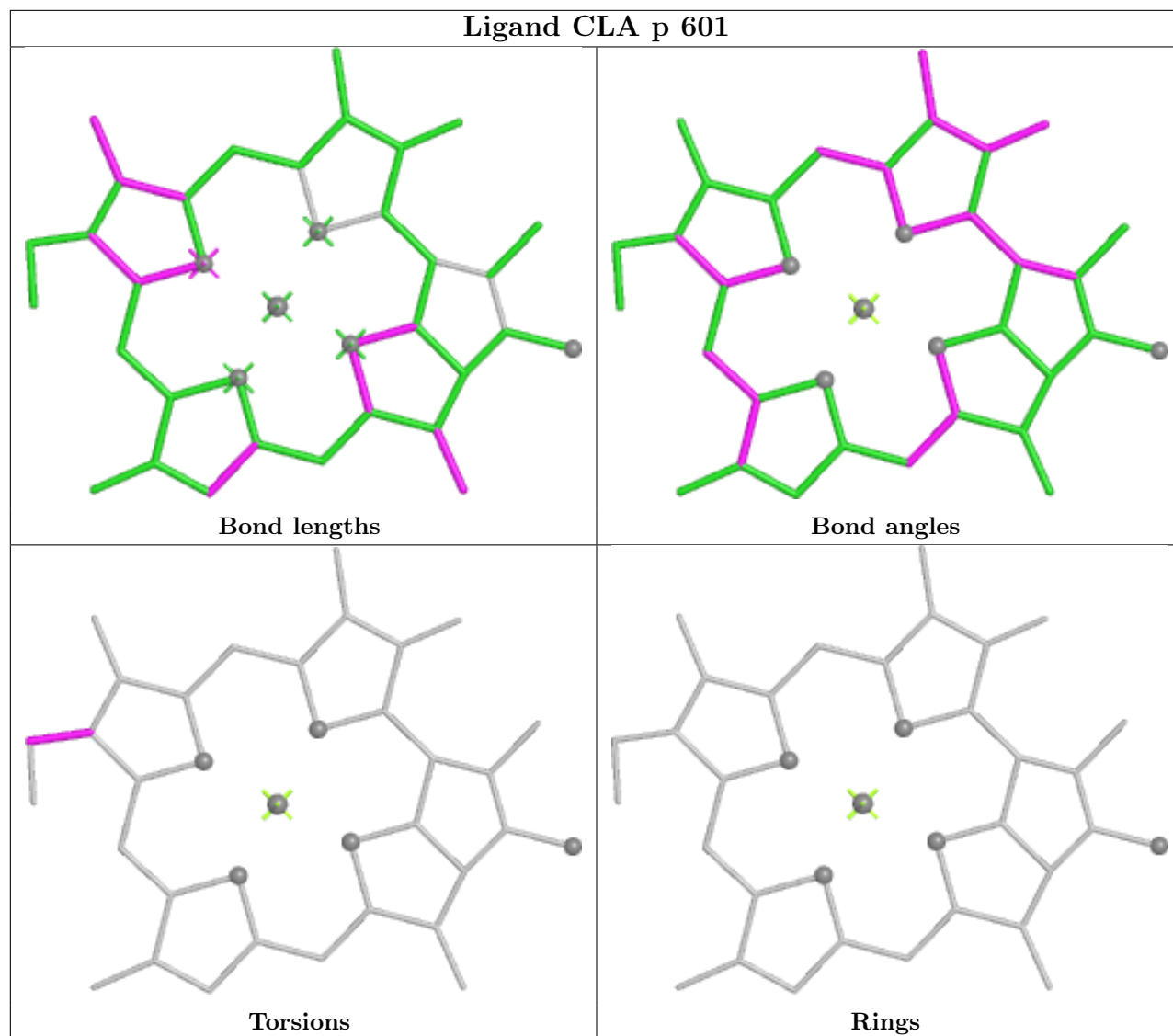


Torsions

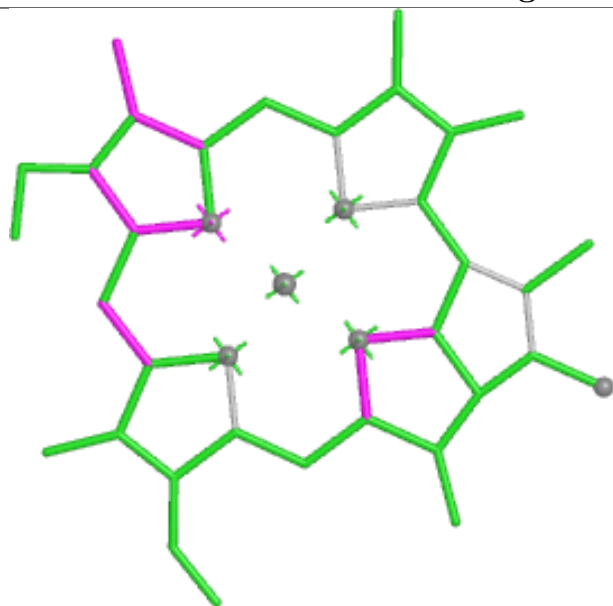


Rings

Ligand CLA p 601



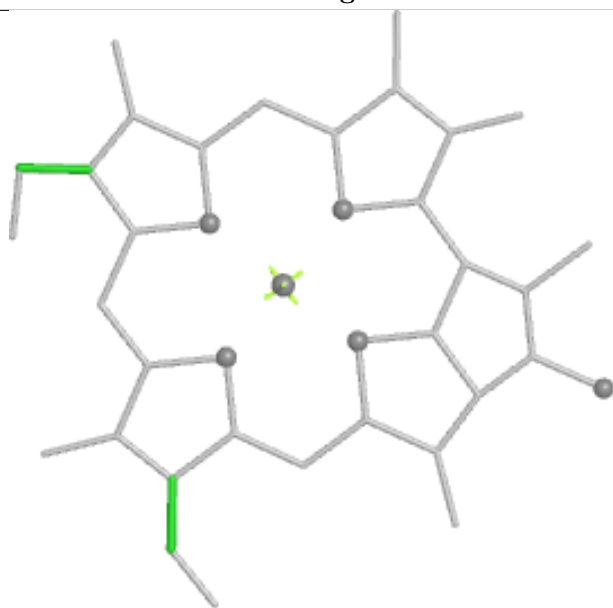
Ligand CLA 4 210



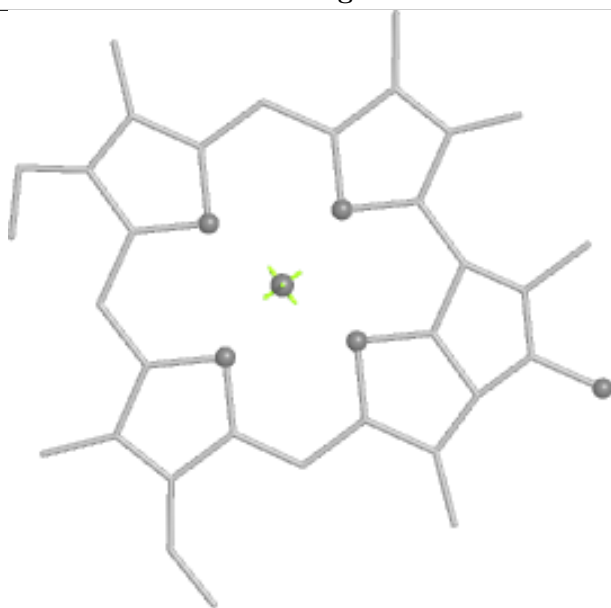
Bond lengths



Bond angles

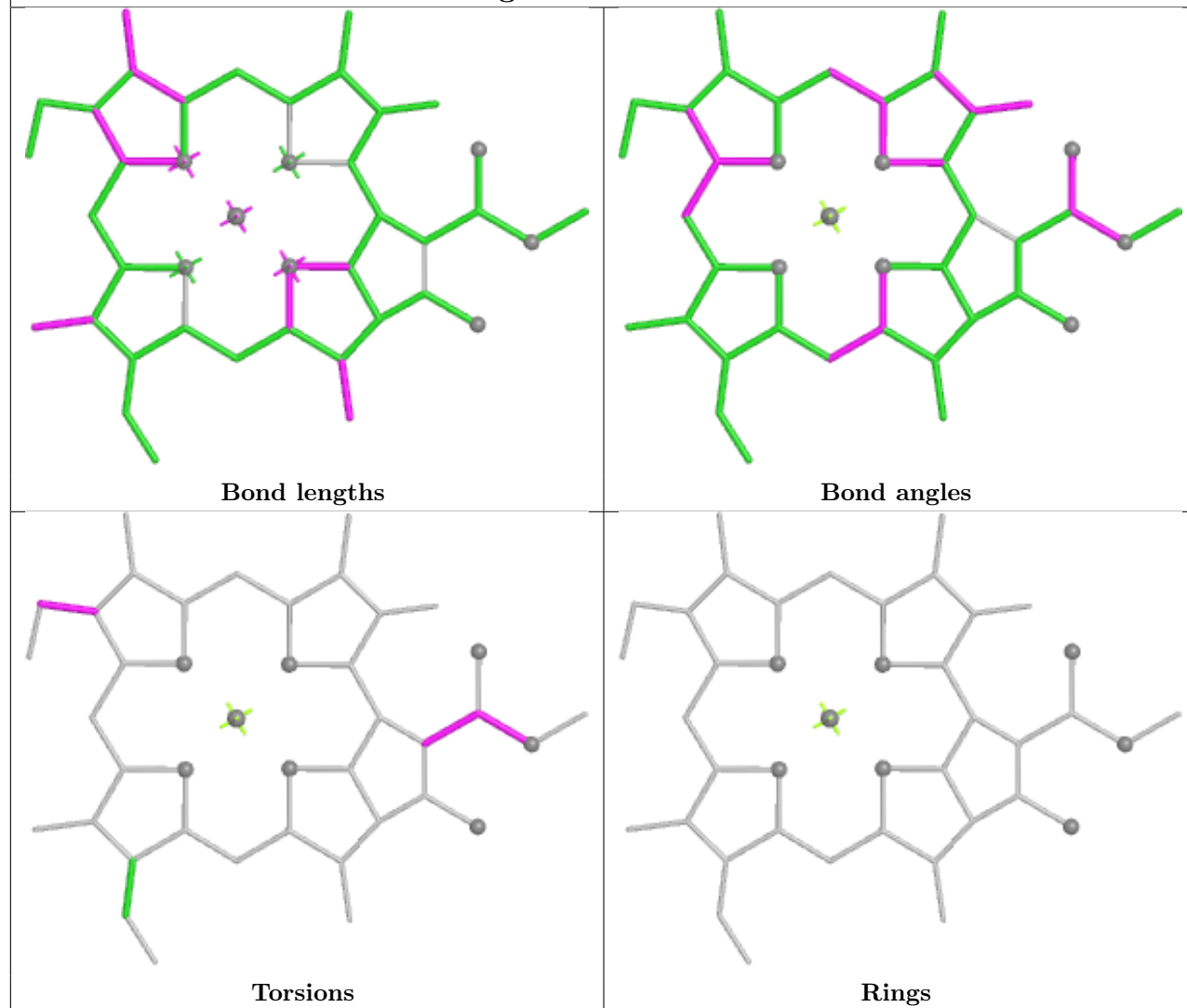


Torsions

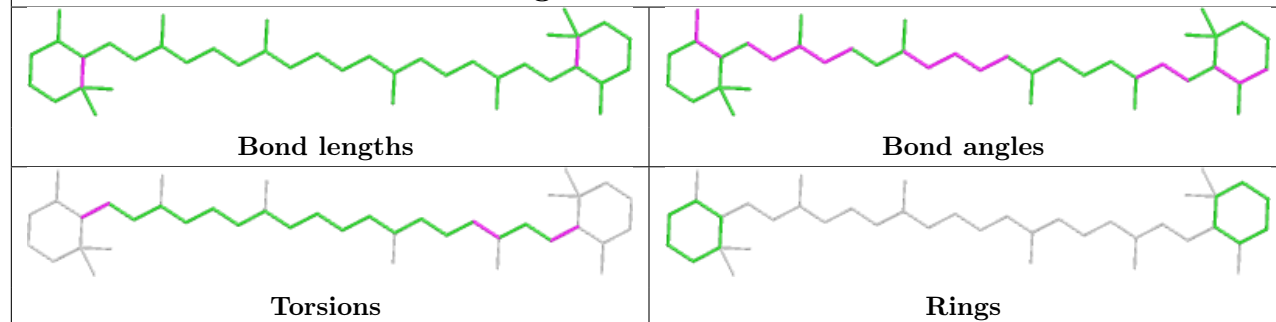


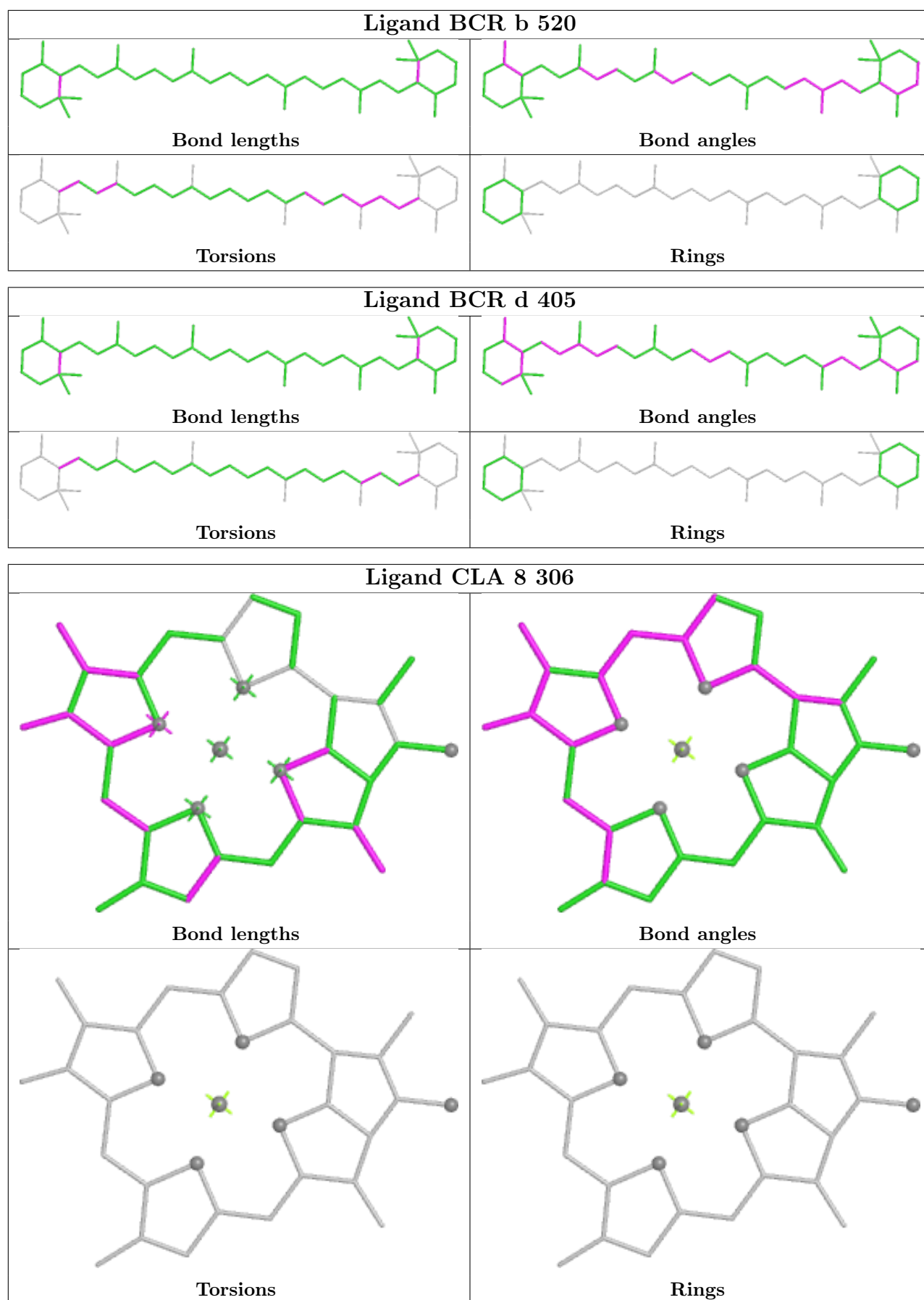
Rings

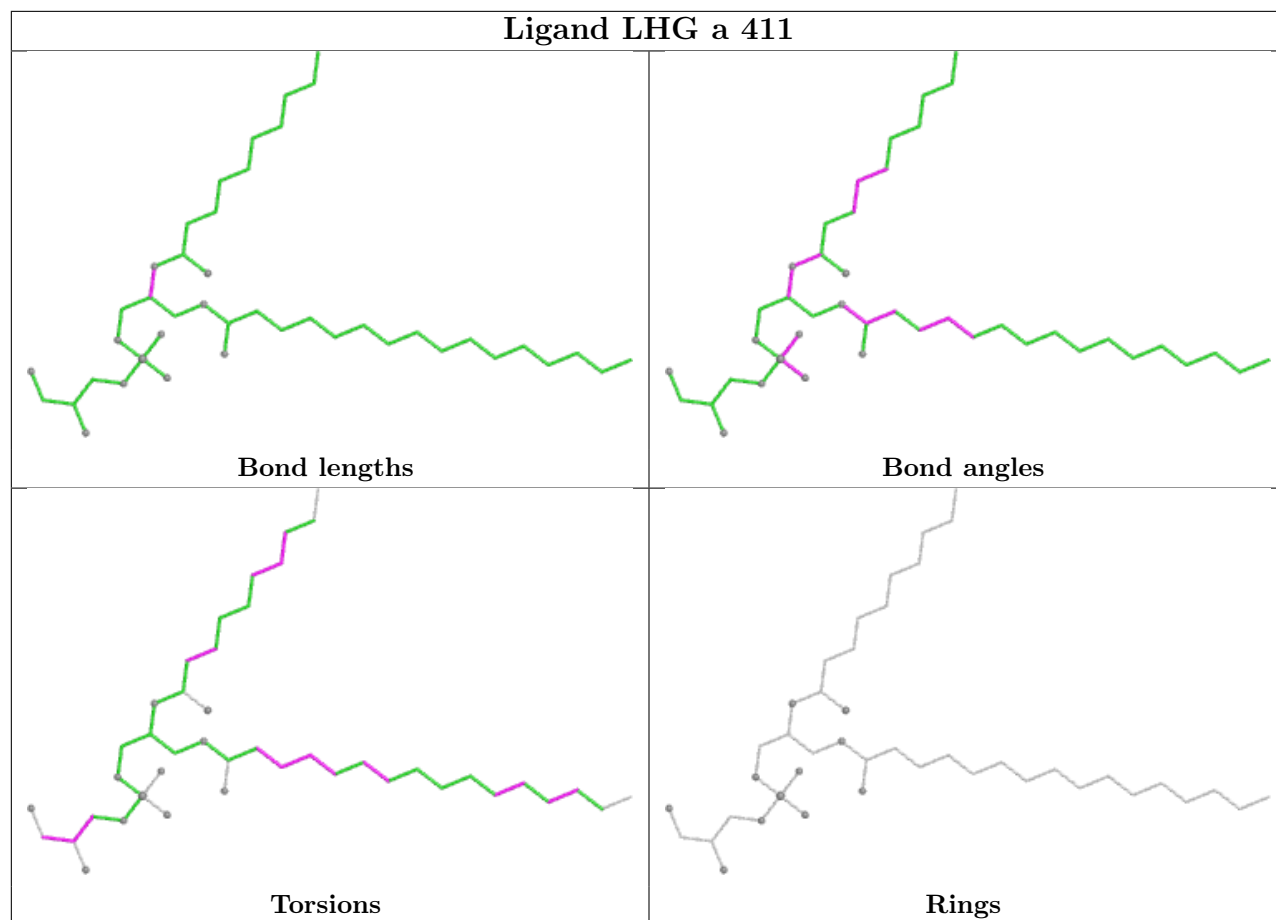
Ligand CLA 4 209



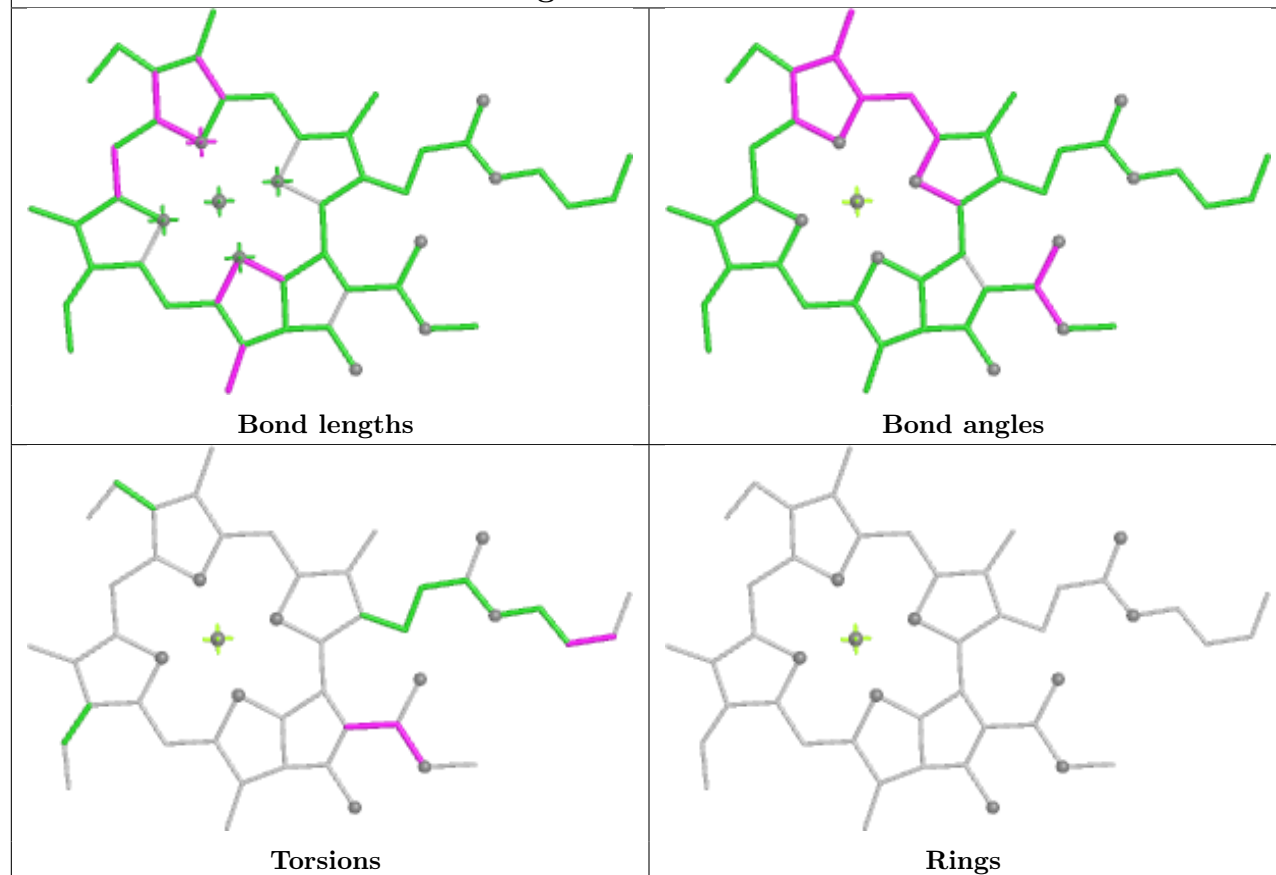
Ligand BCR b 518



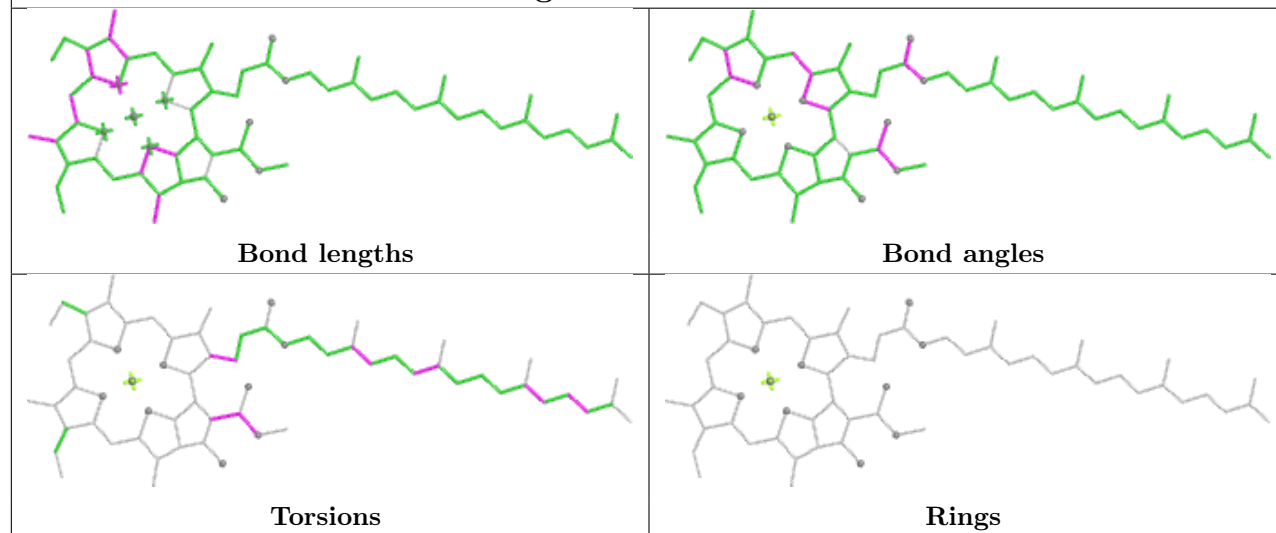


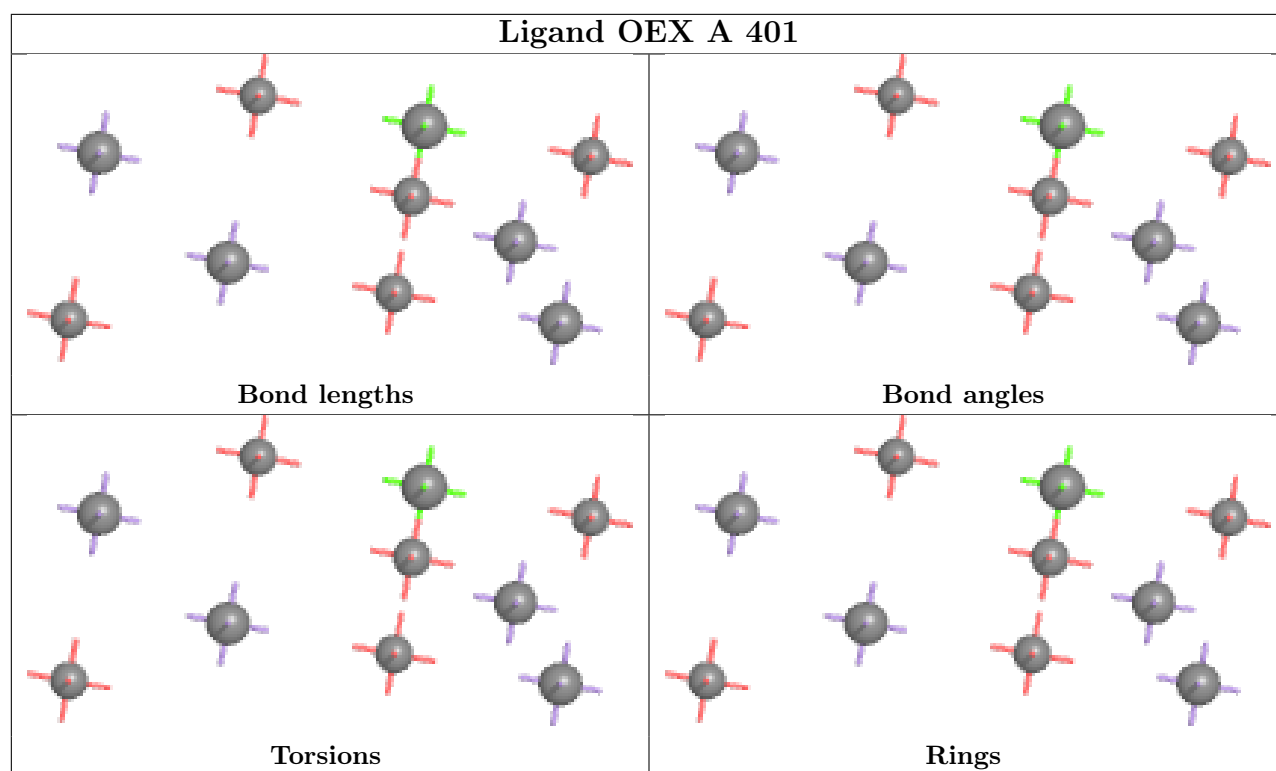


Ligand CLA c 514

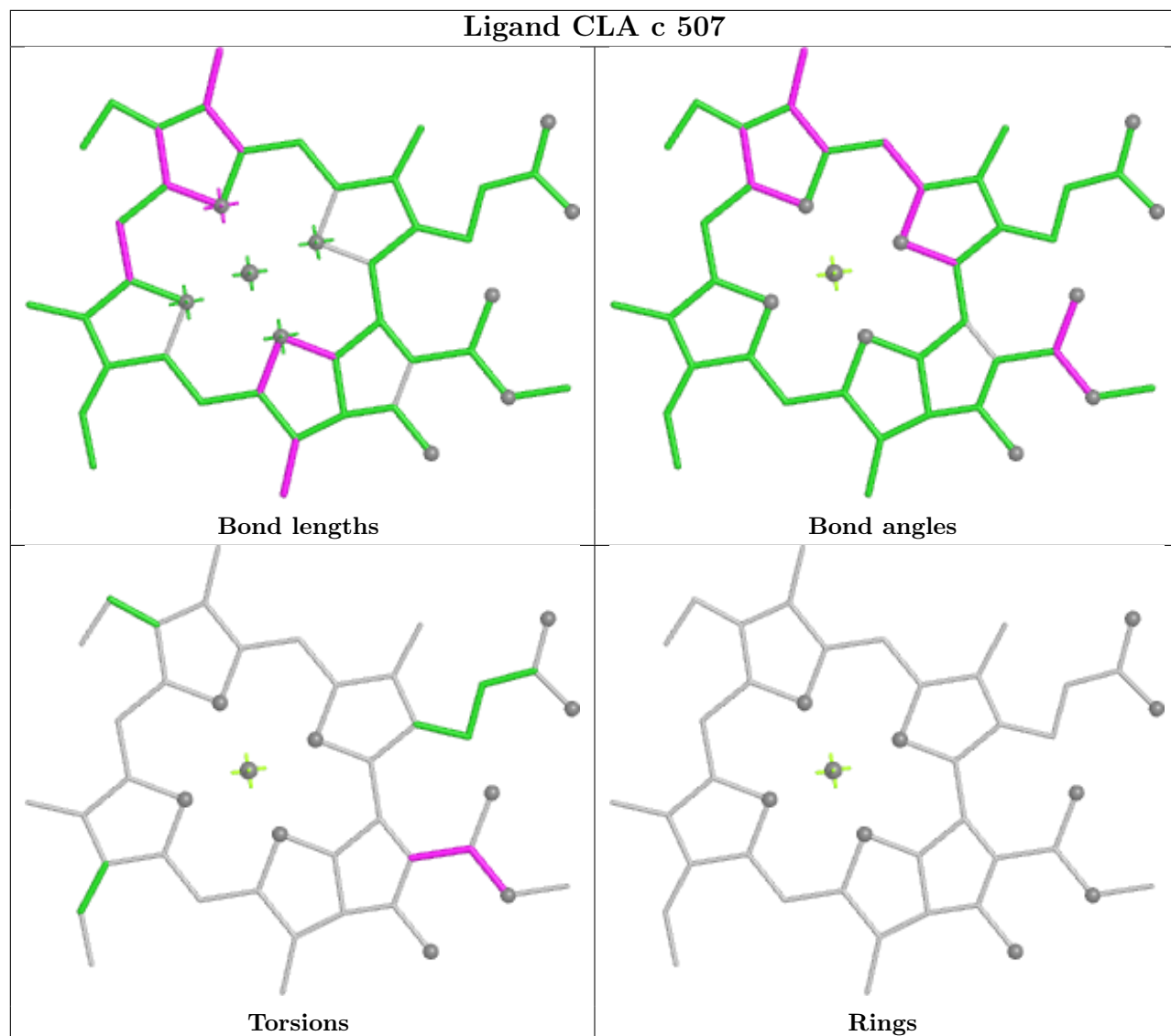


Ligand CLA b 510

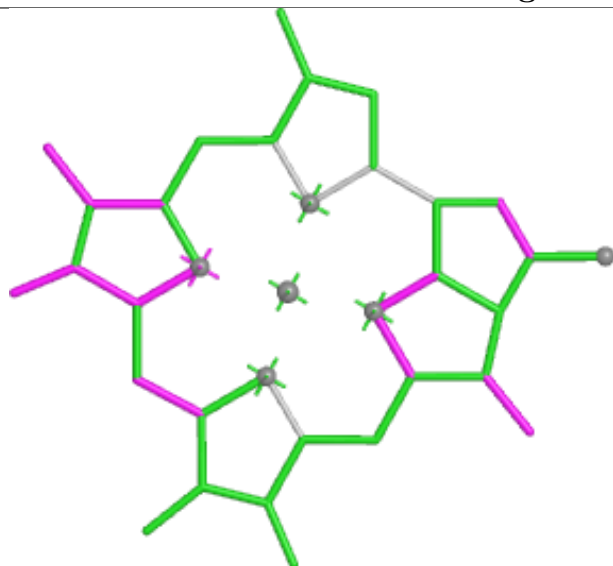




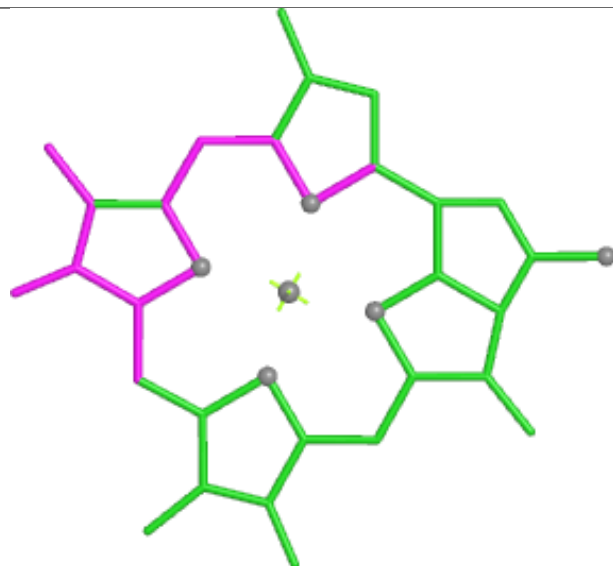
Ligand CLA c 507



Ligand CLA 9 211



Bond lengths



Bond angles

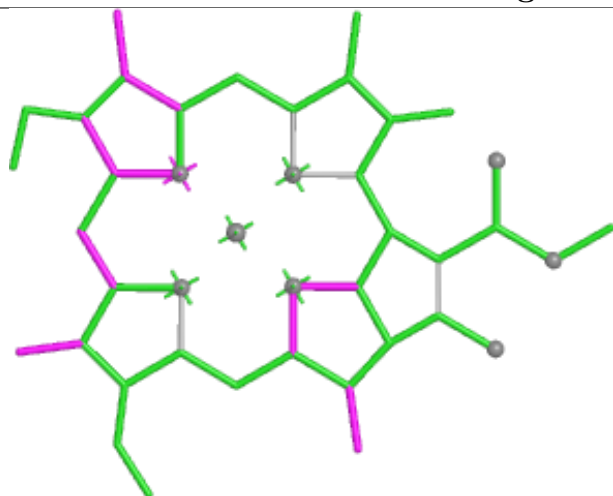


Torsions

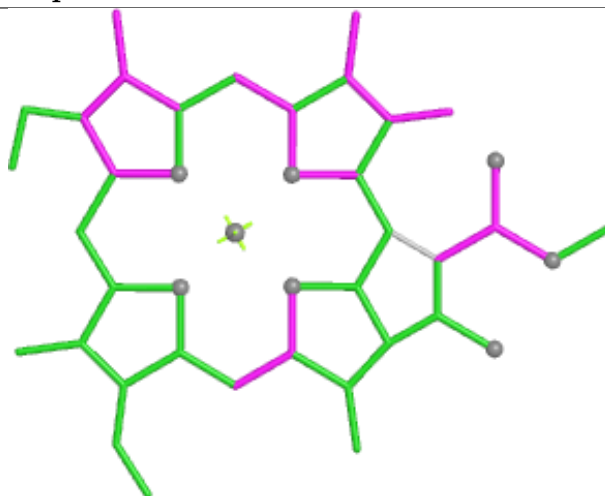


Rings

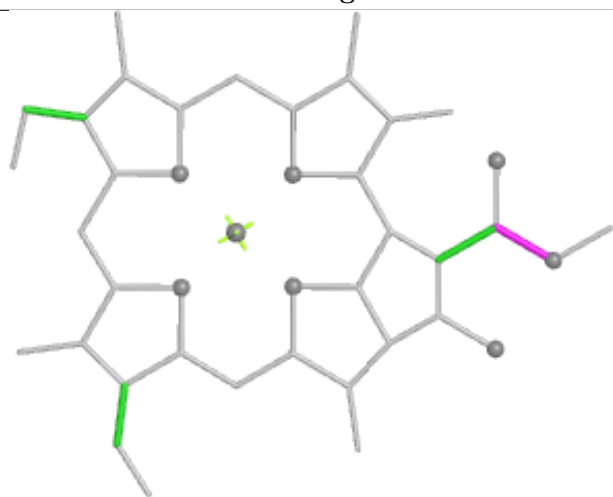
Ligand CLA p 602



Bond lengths



Bond angles

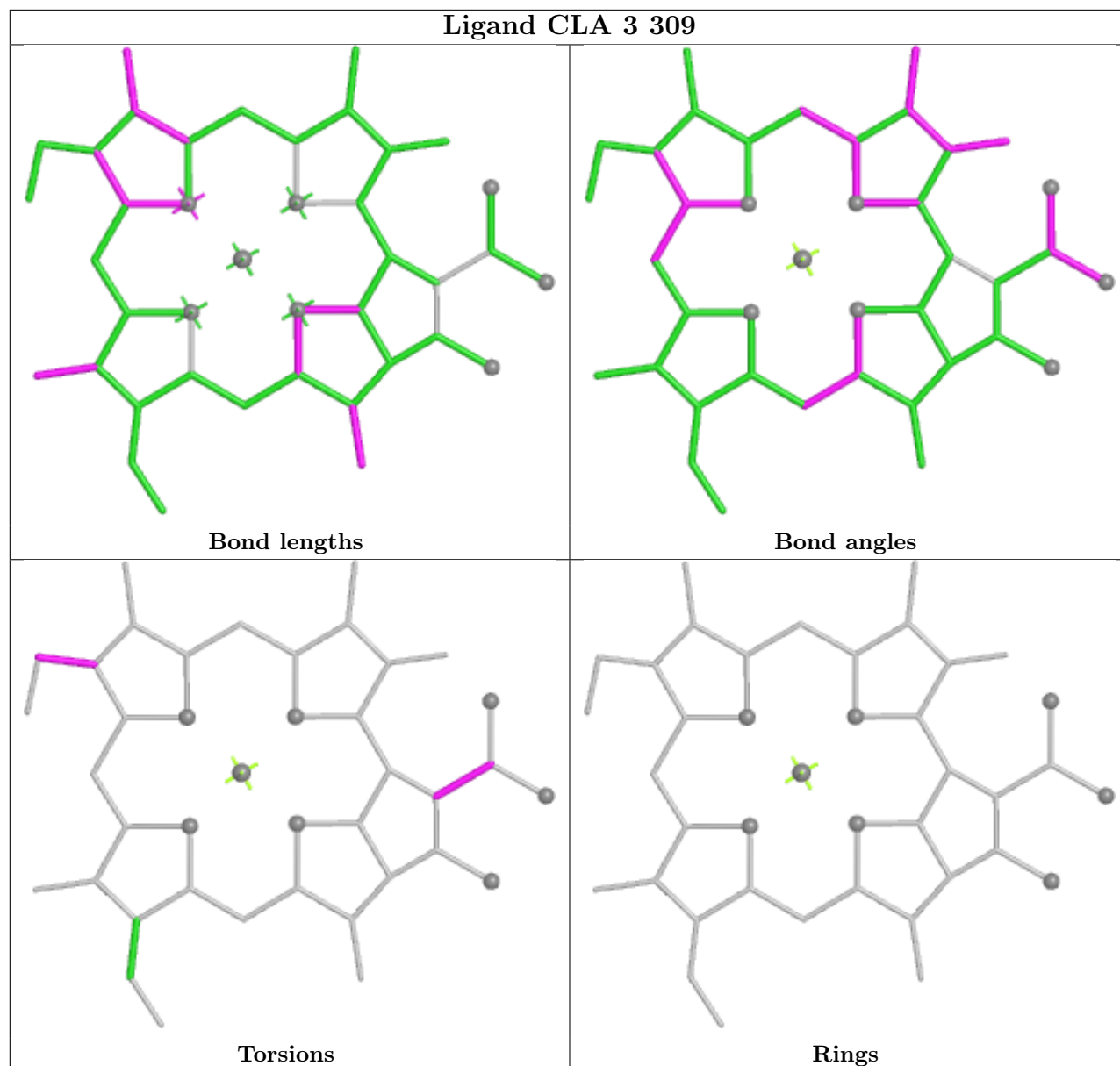


Torsions

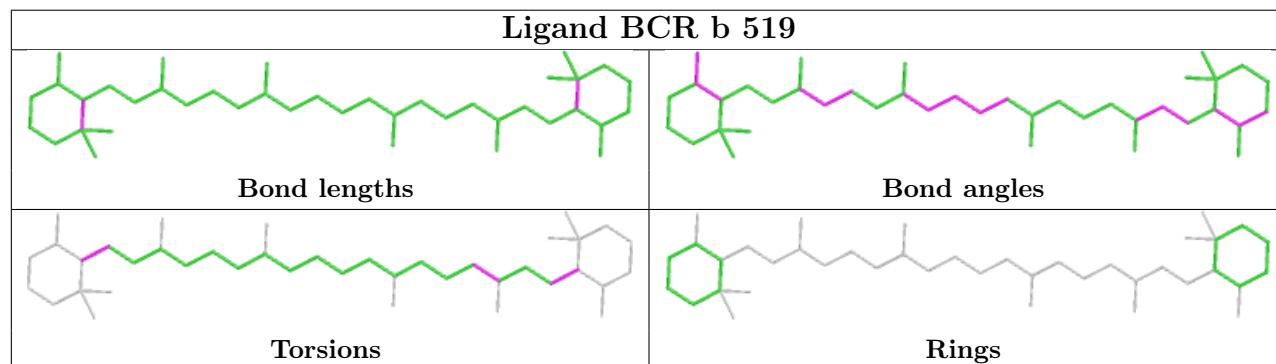


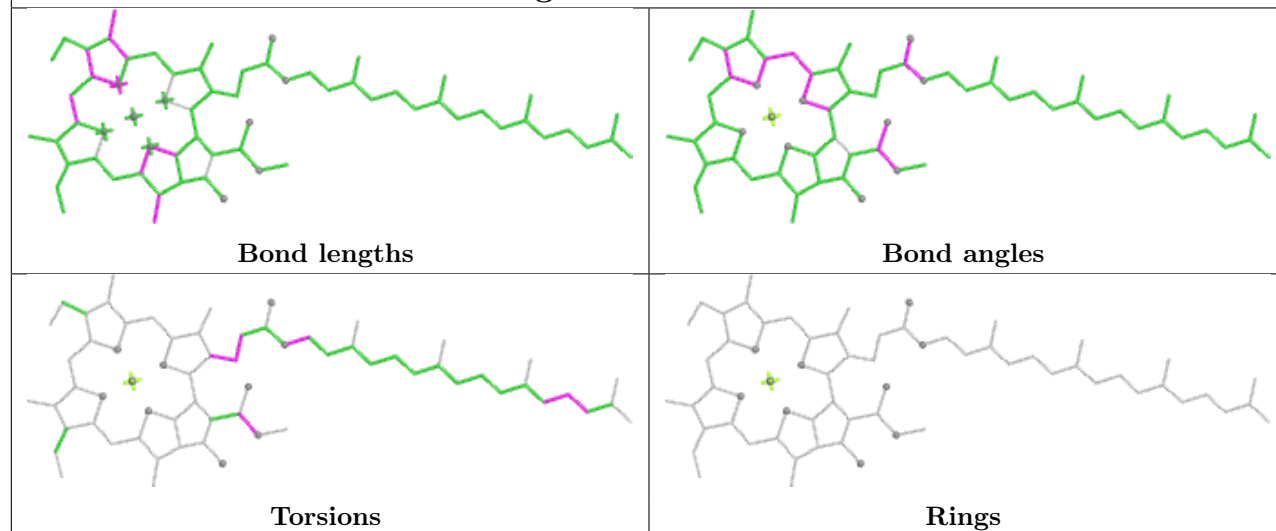
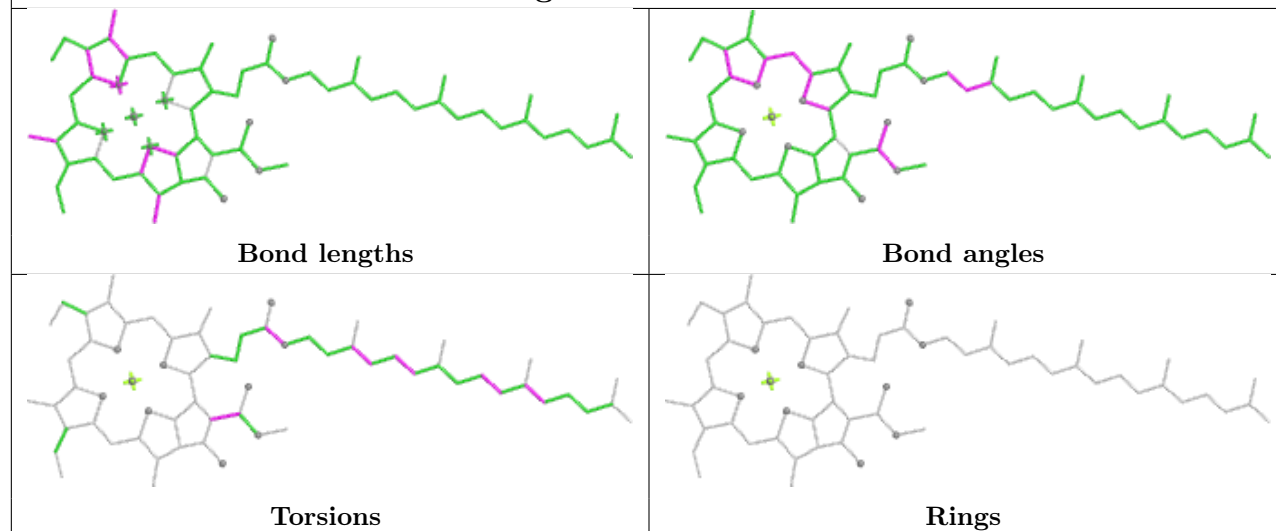
Rings

Ligand CLA 3 309

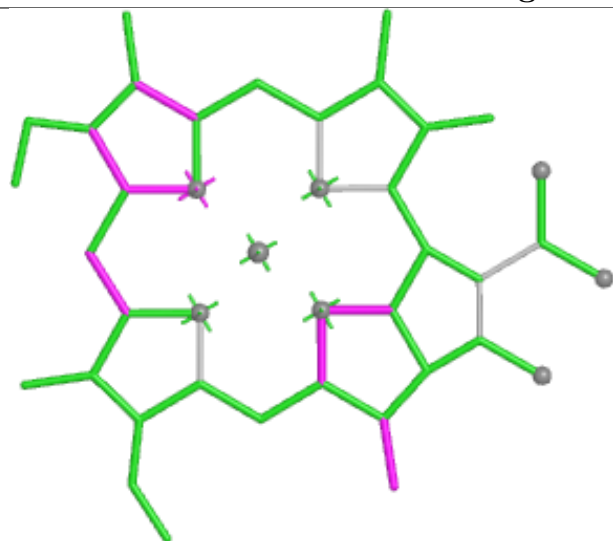


Ligand BCR b 519

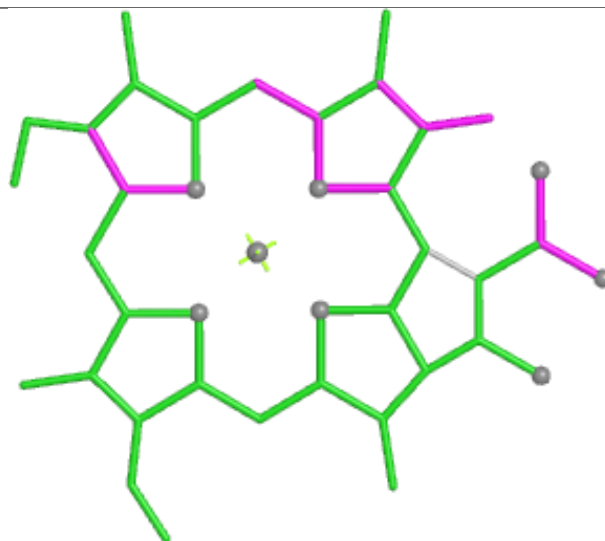


Ligand CLA b 509**Ligand CLA d 404**

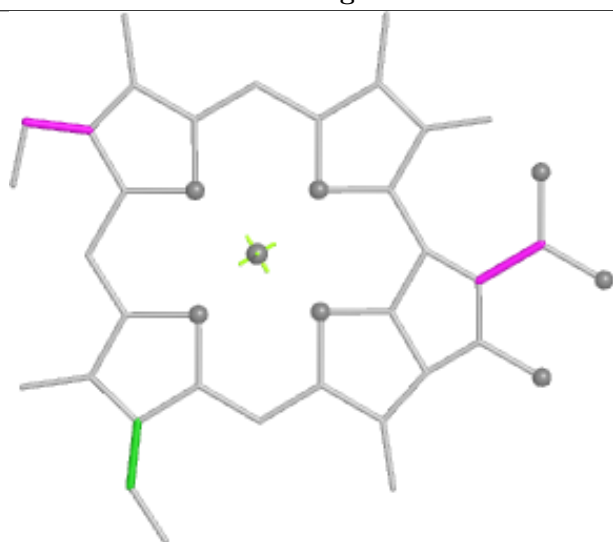
Ligand CLA 1 213



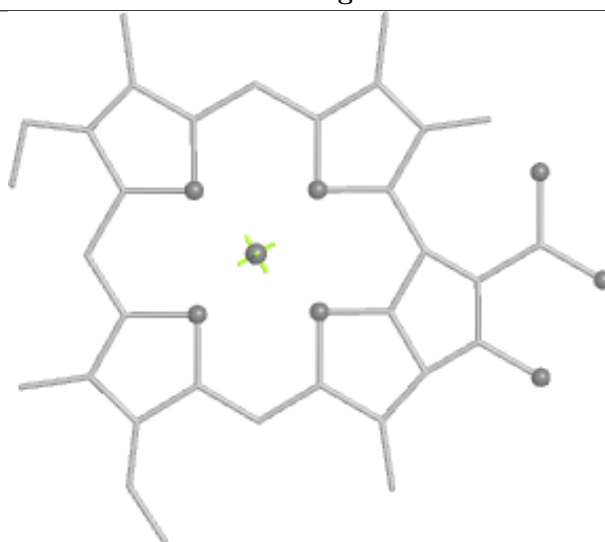
Bond lengths



Bond angles

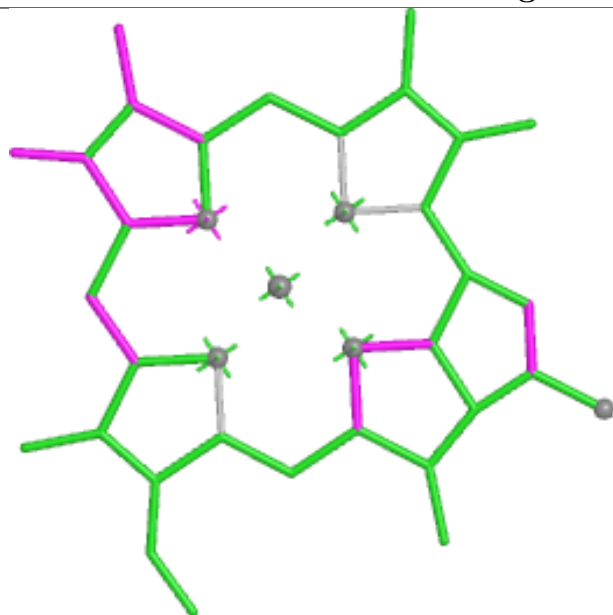


Torsions

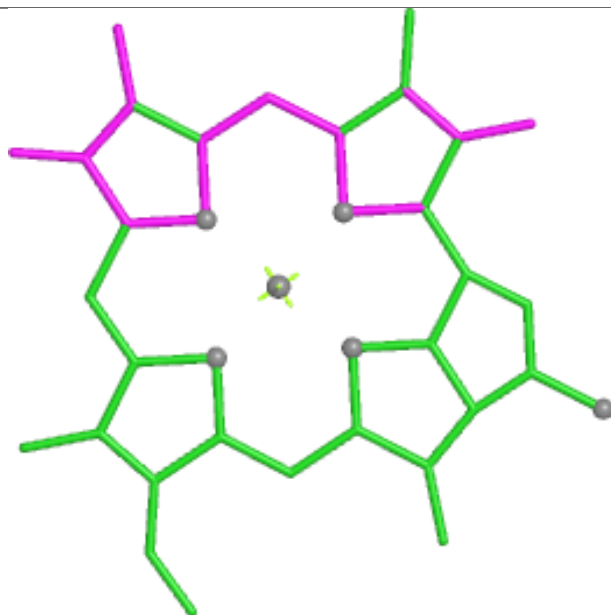


Rings

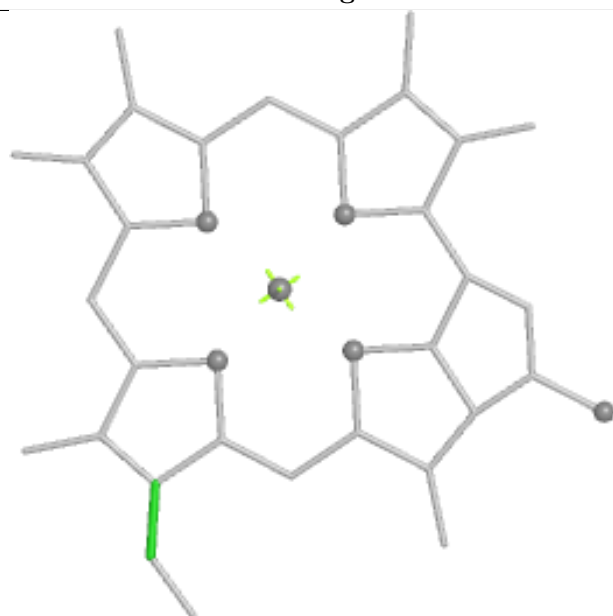
Ligand CLA 4 212



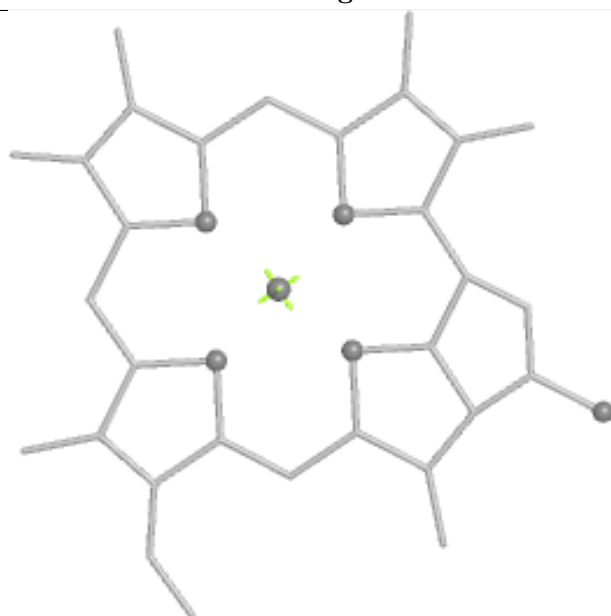
Bond lengths



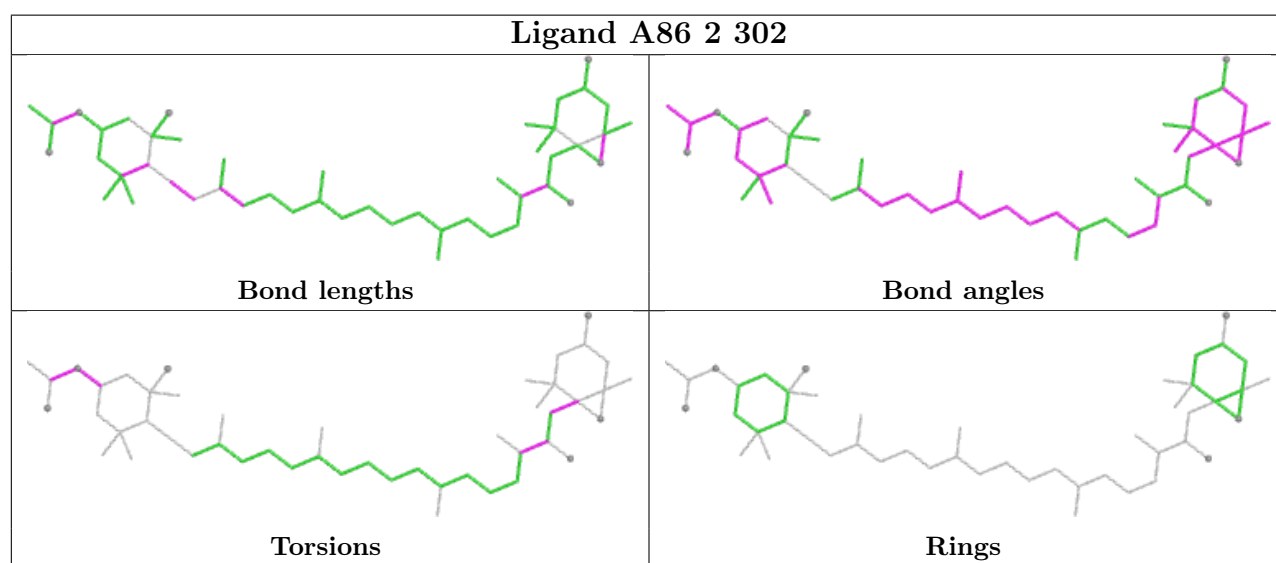
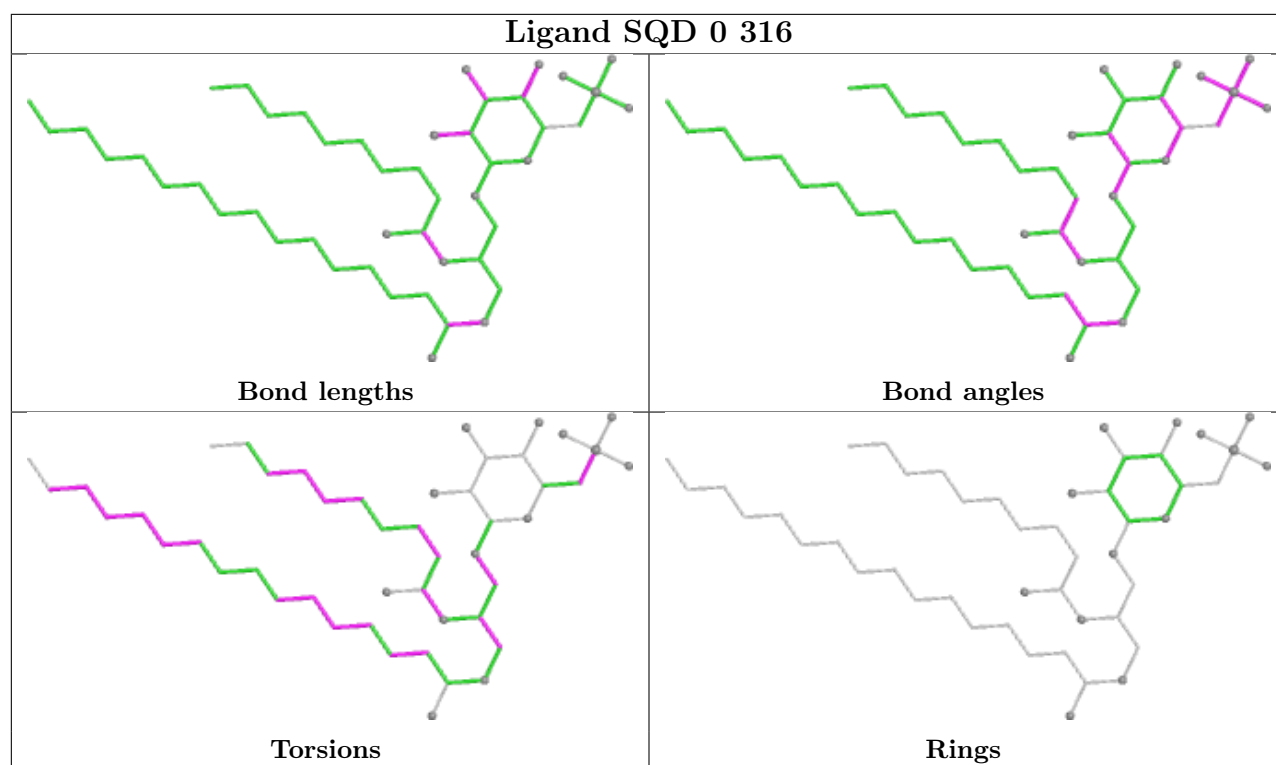
Bond angles

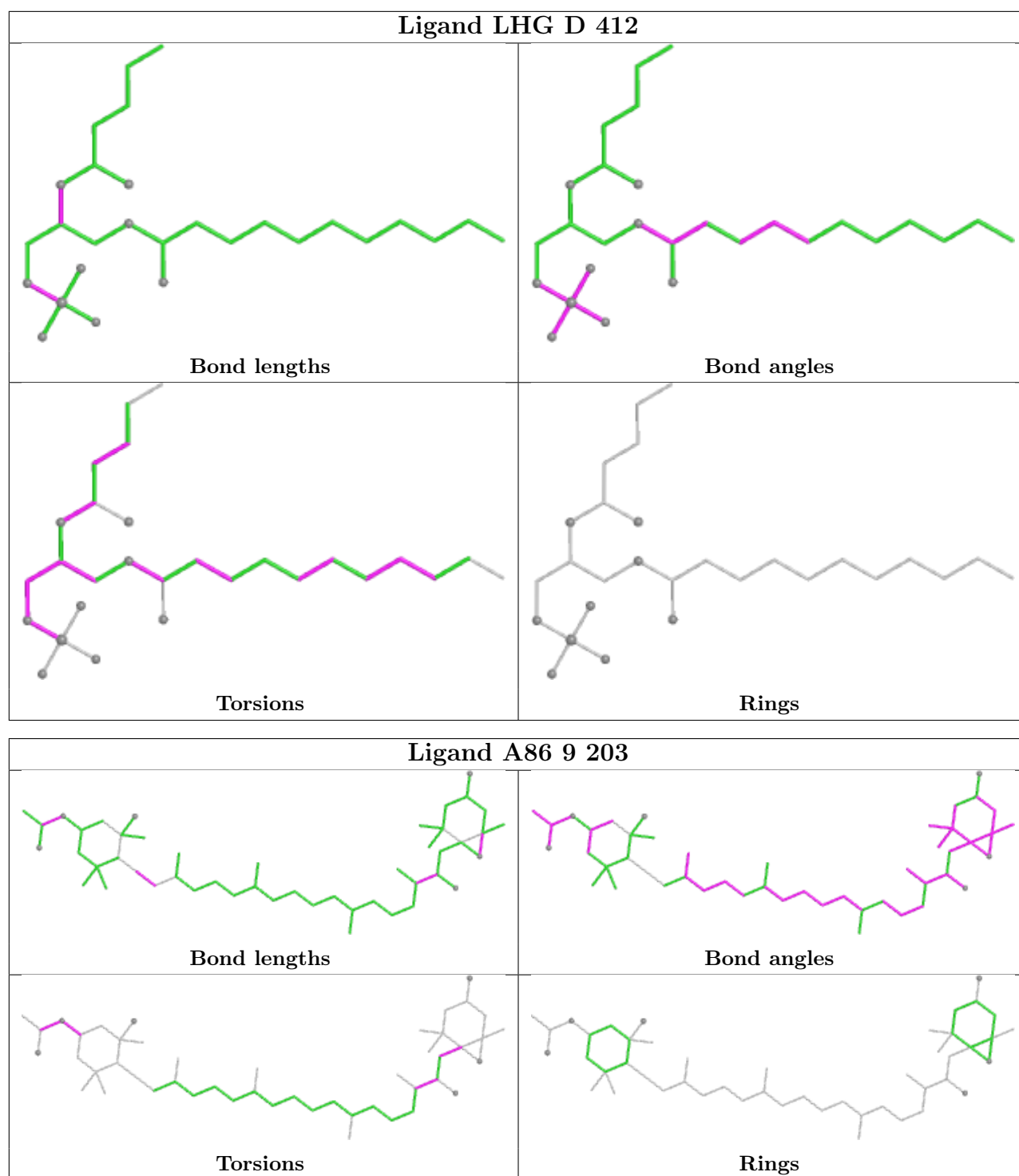


Torsions

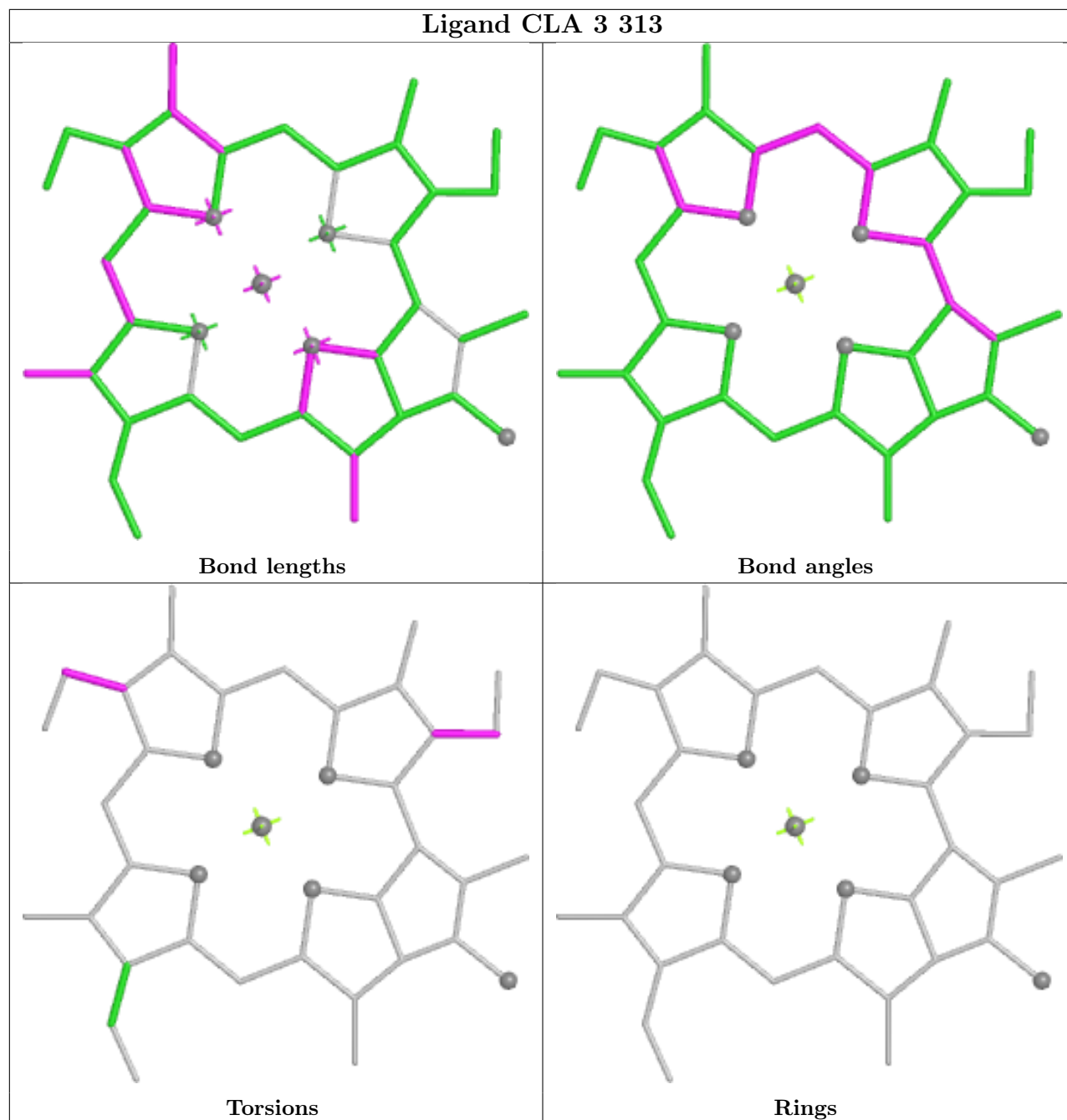


Rings

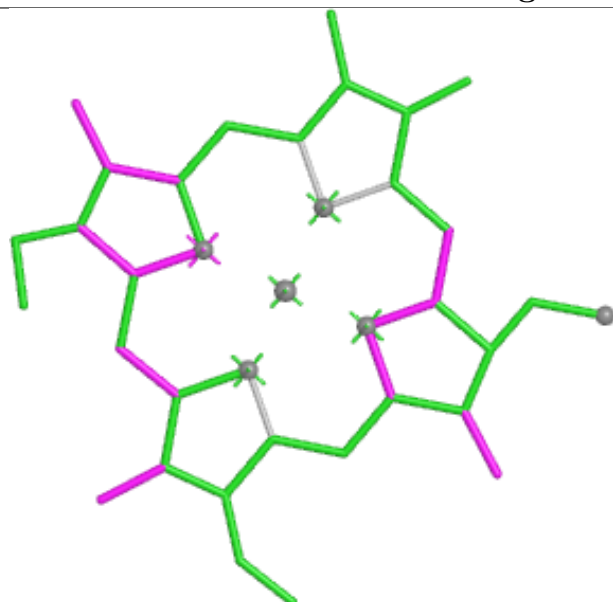




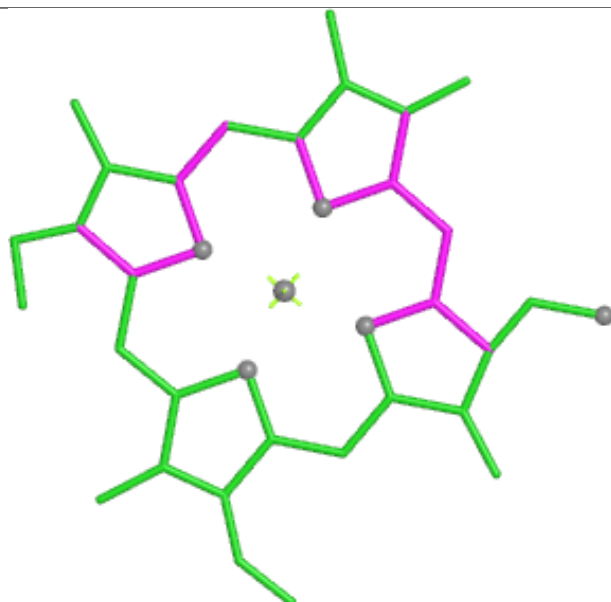
Ligand CLA 3 313



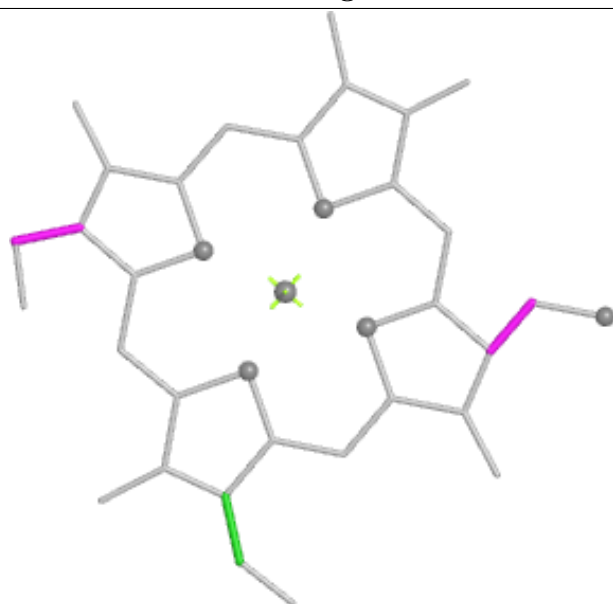
Ligand CLA 8 308



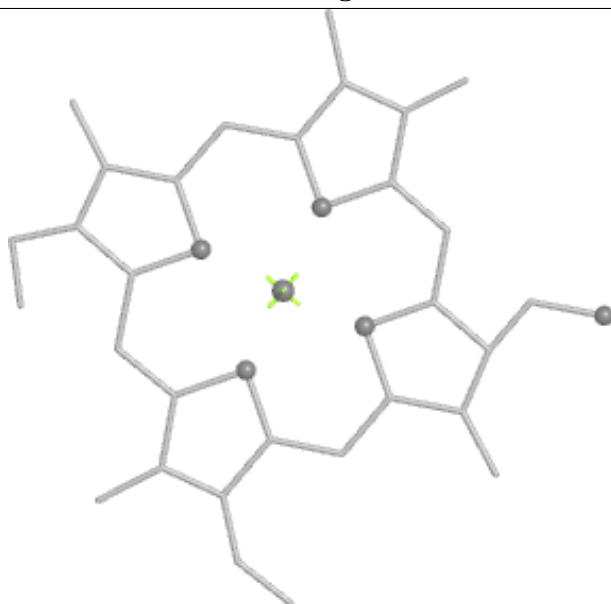
Bond lengths



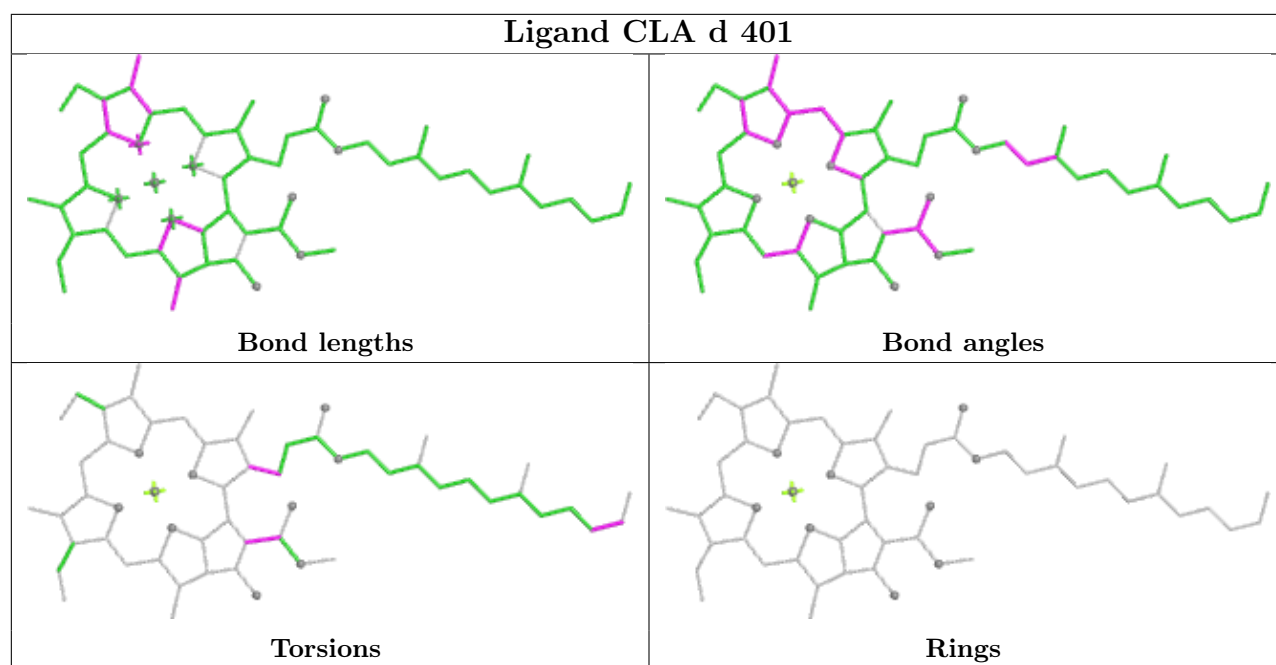
Bond angles



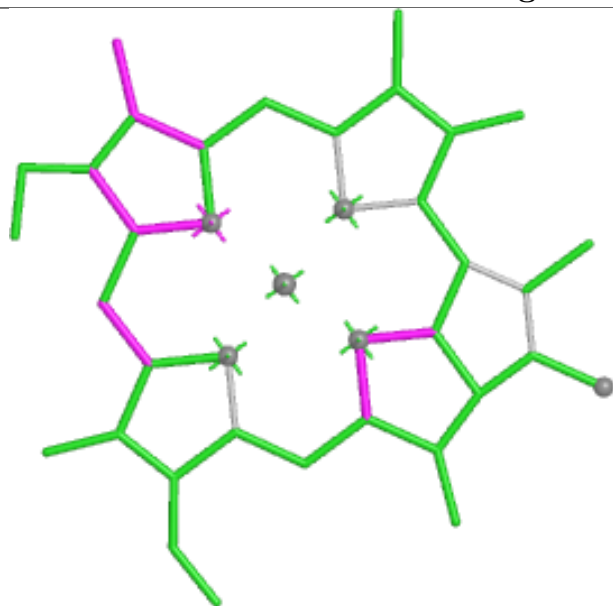
Torsions



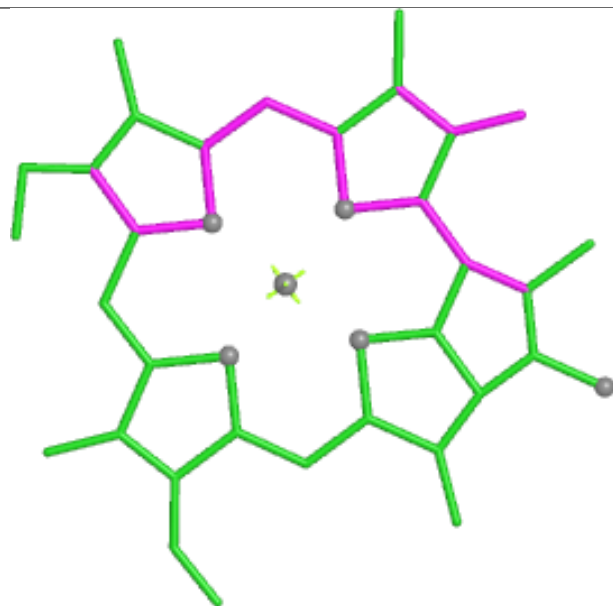
Rings



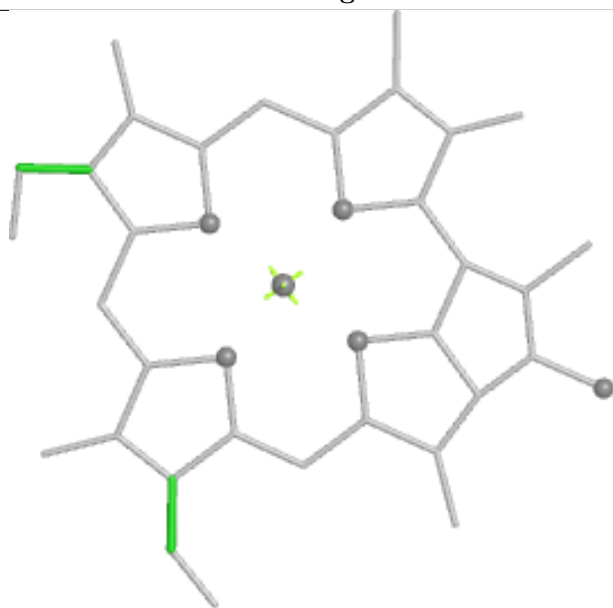
Ligand CLA 1 215



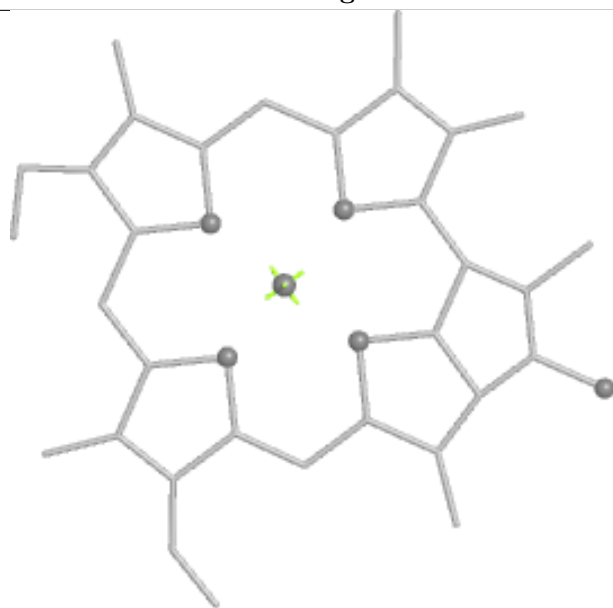
Bond lengths



Bond angles

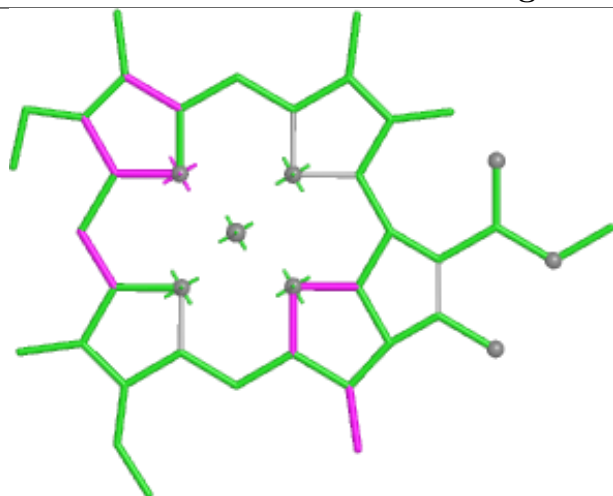


Torsions

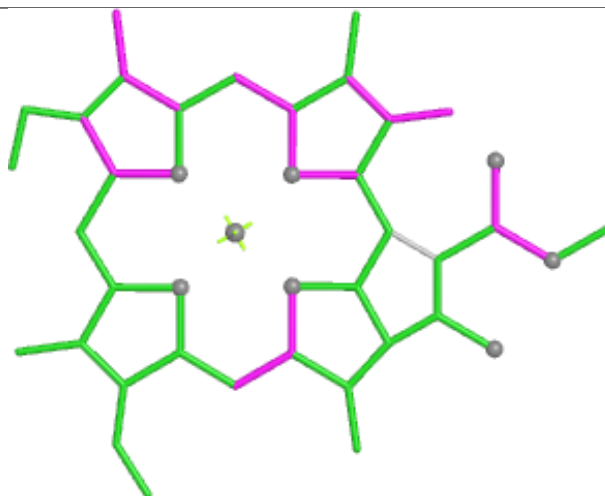


Rings

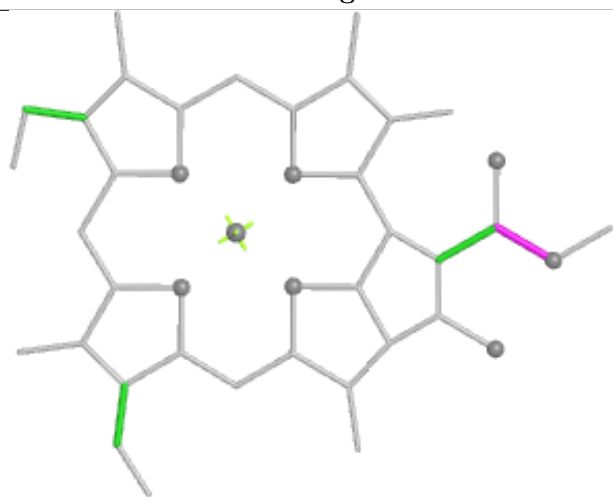
Ligand CLA 7 316



Bond lengths



Bond angles

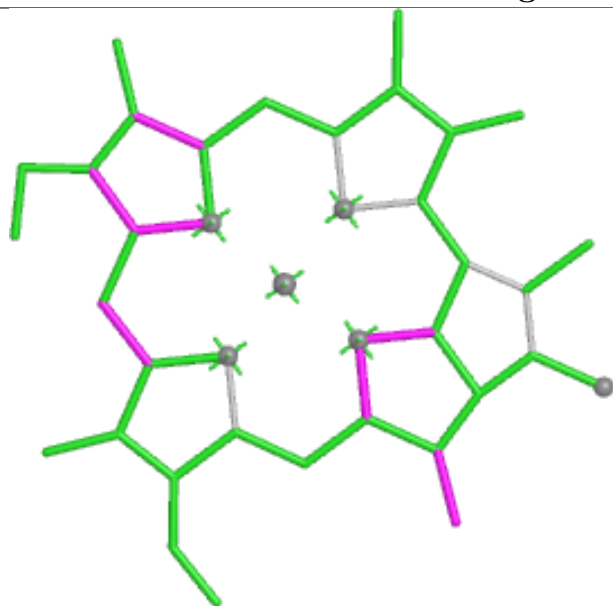


Torsions



Rings

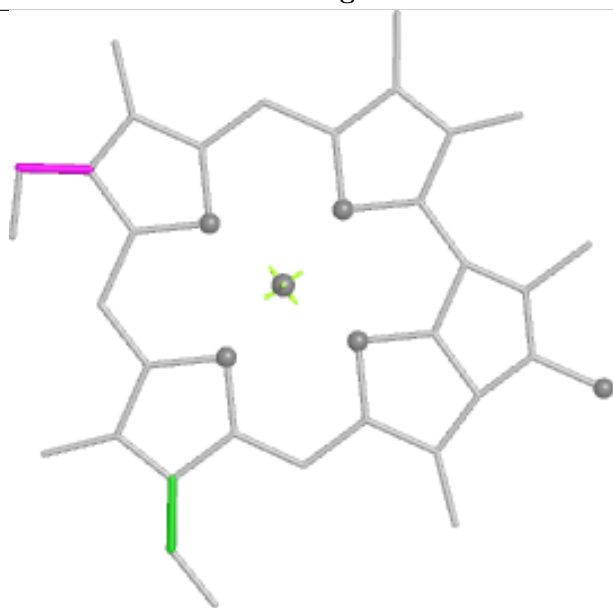
Ligand CLA 1 216



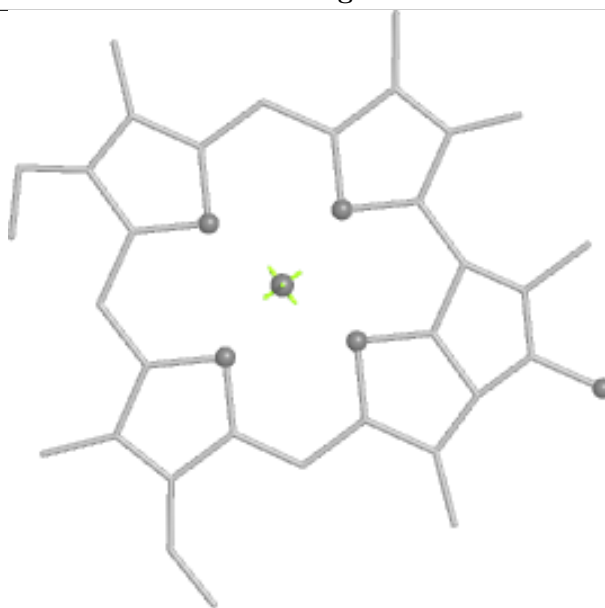
Bond lengths



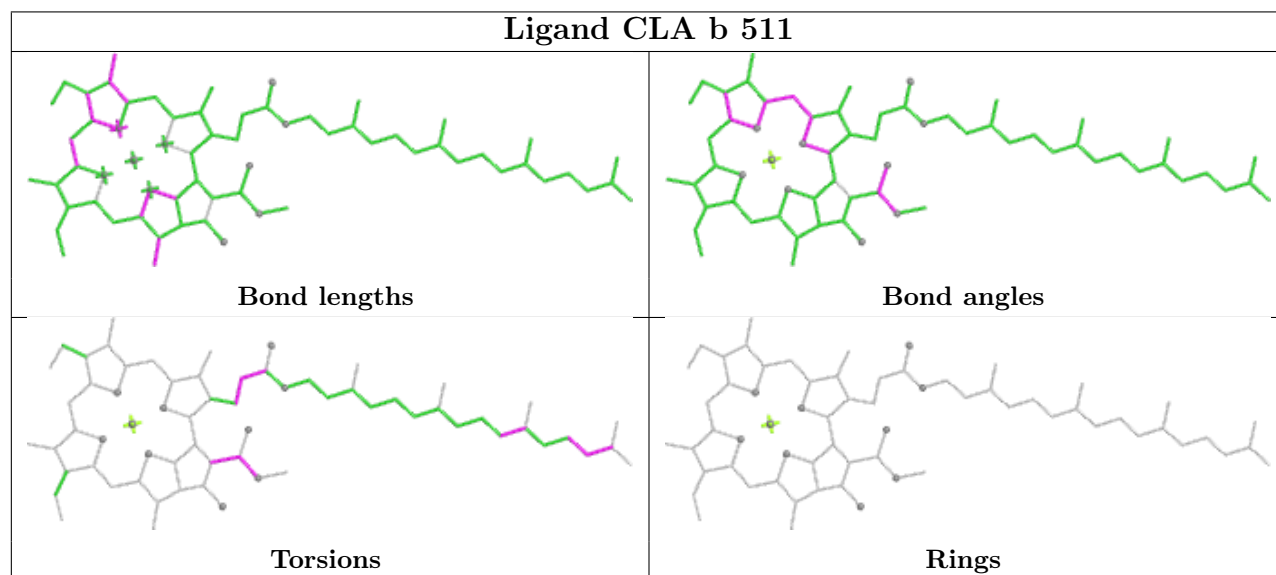
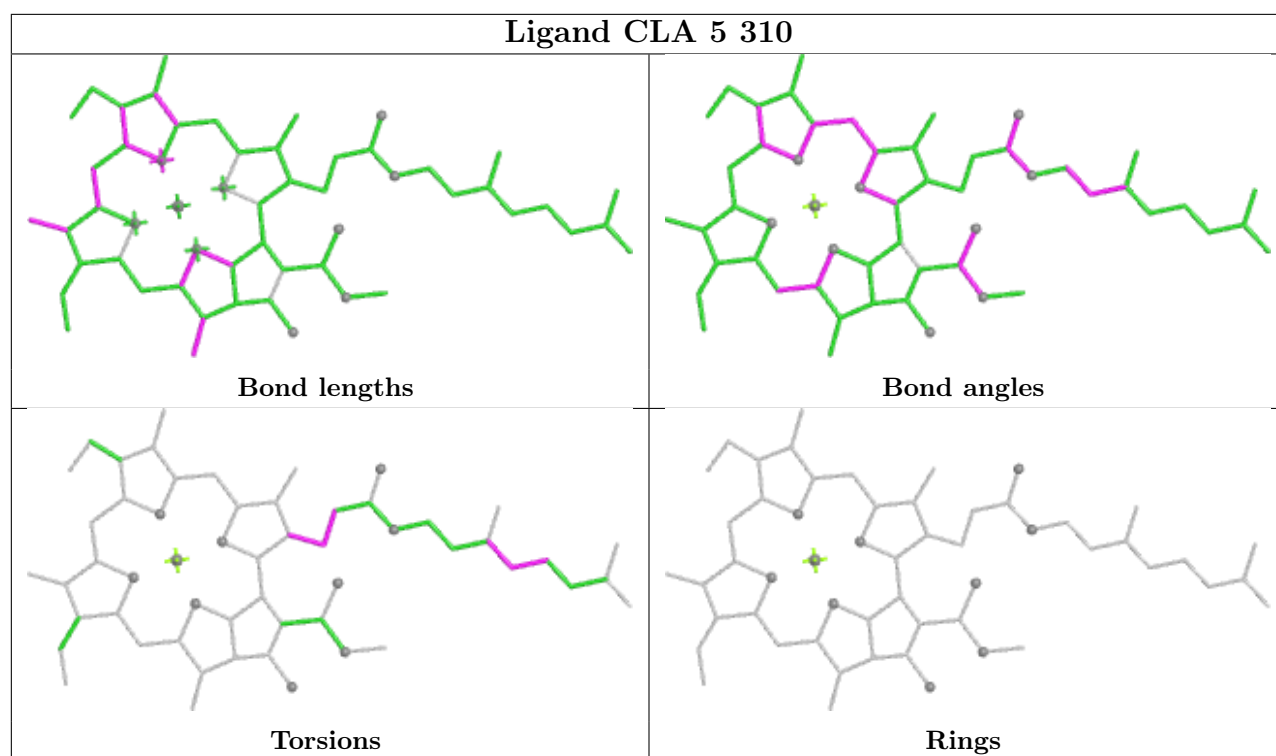
Bond angles

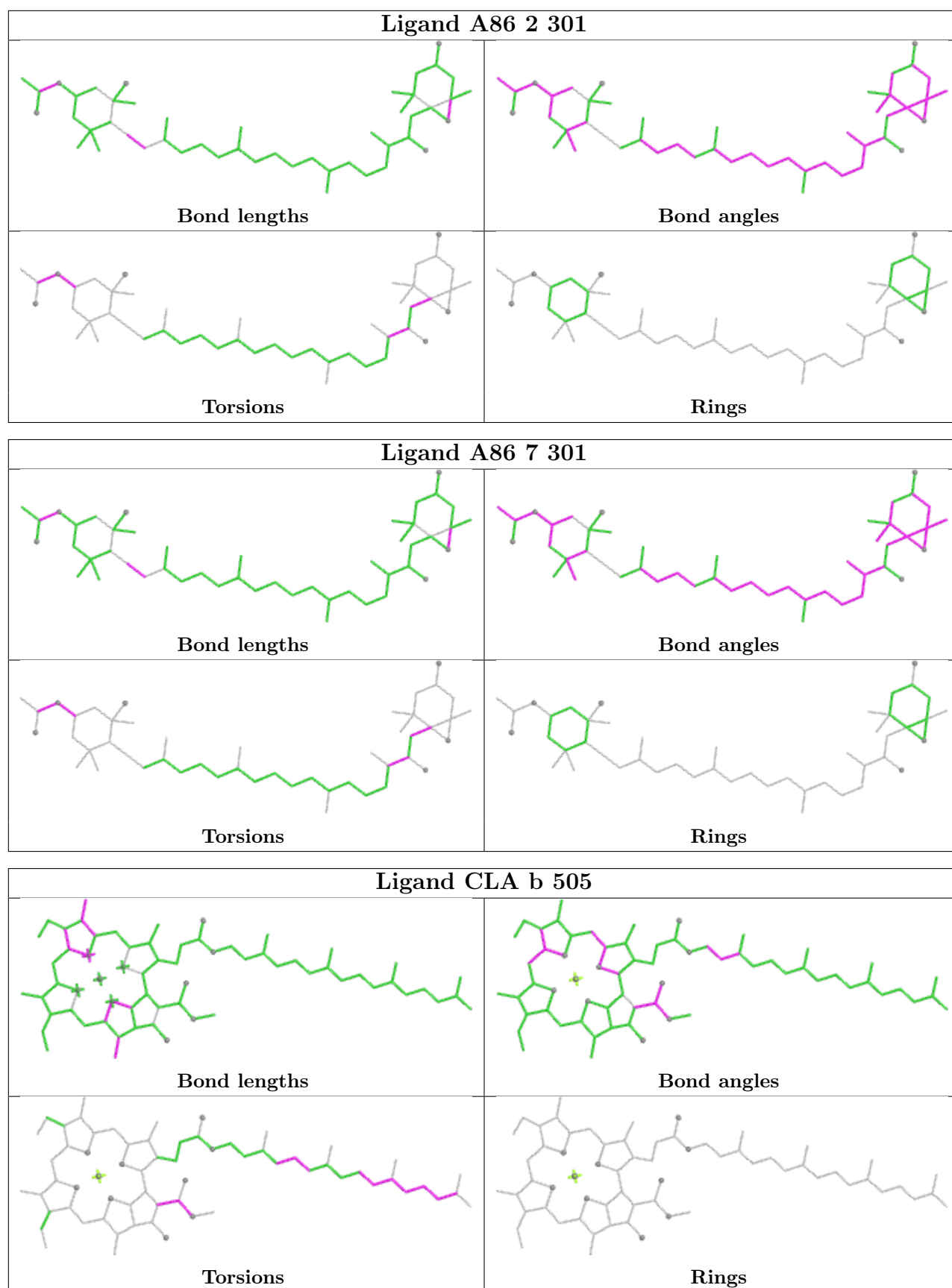


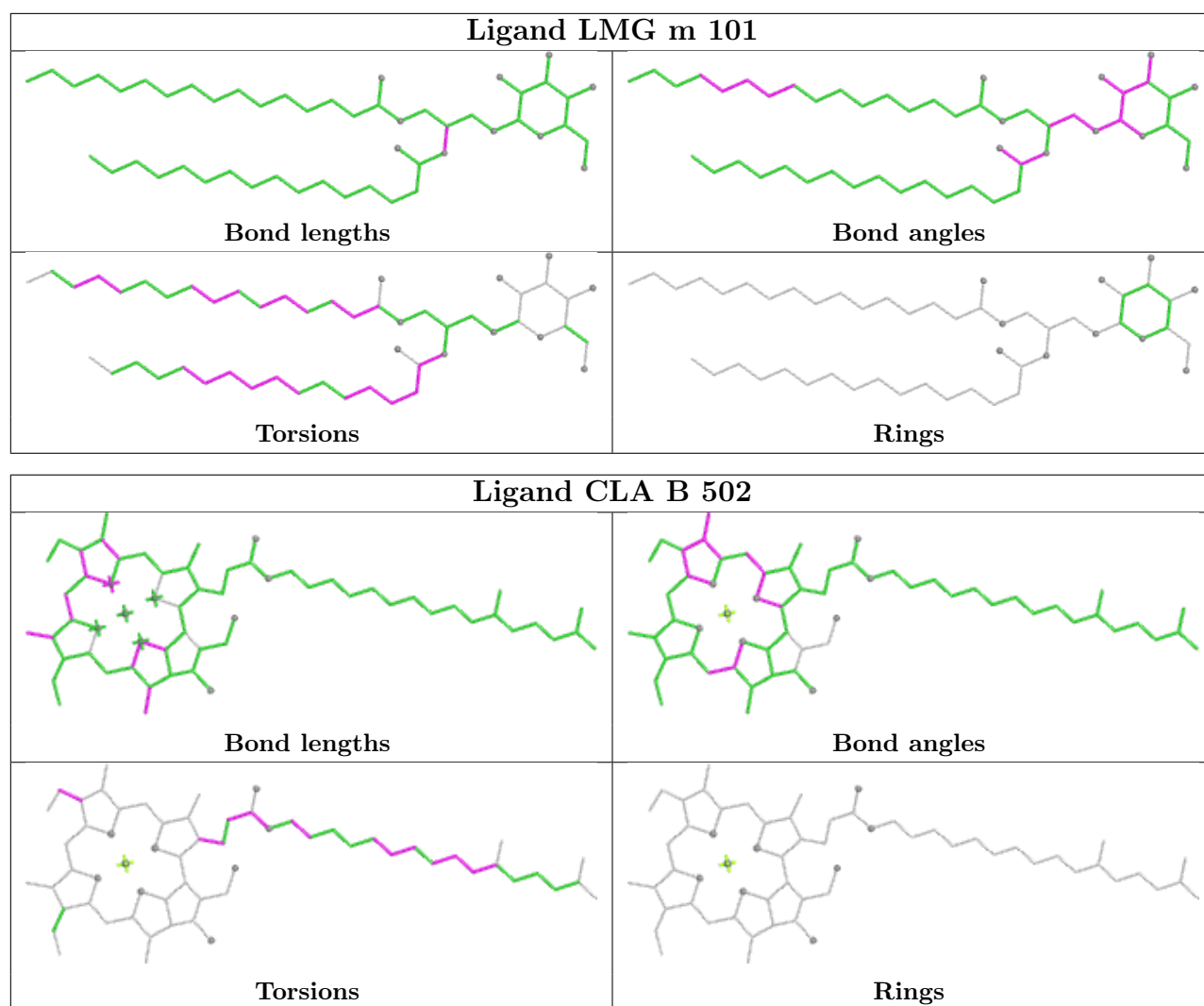
Torsions

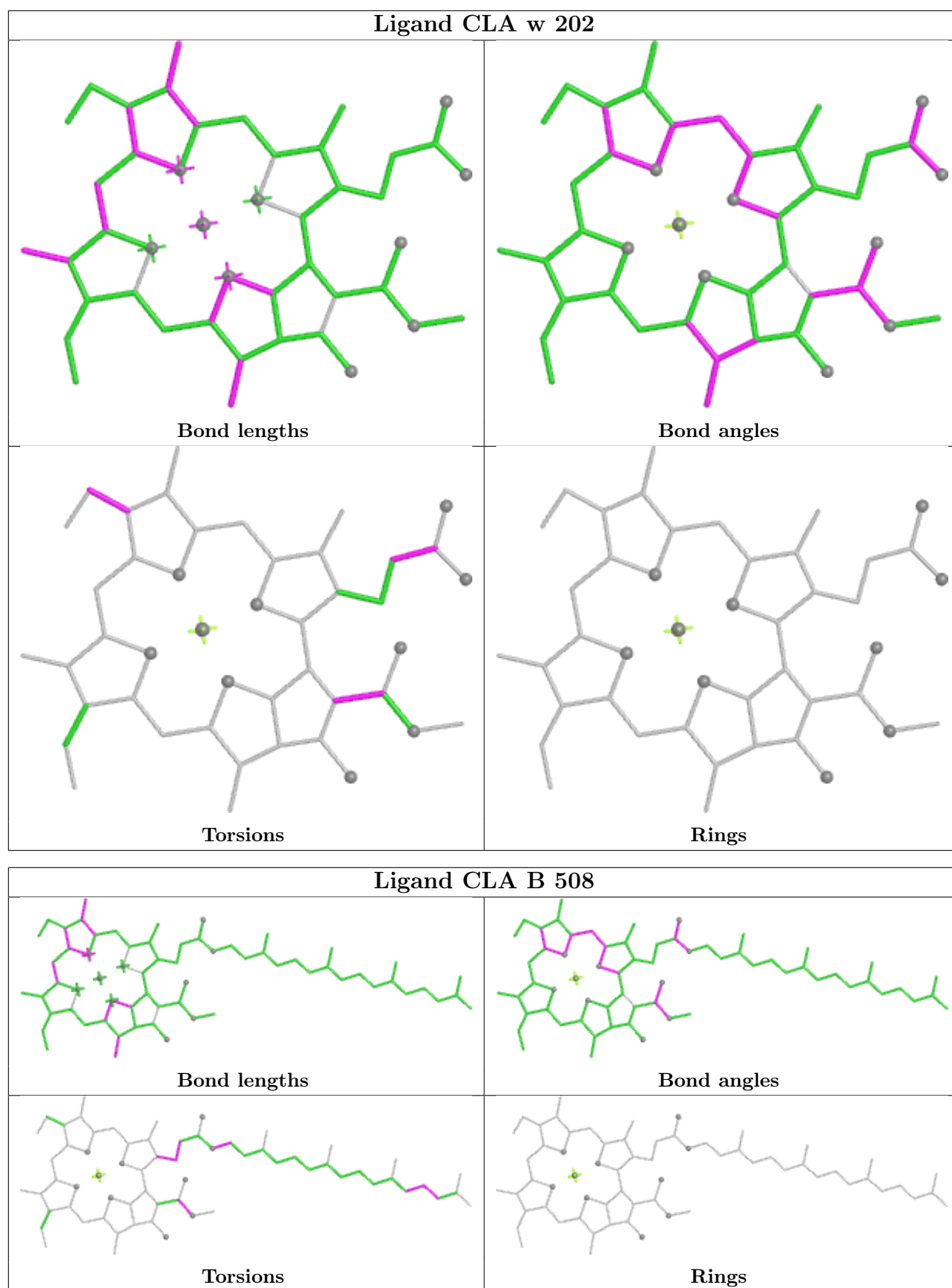


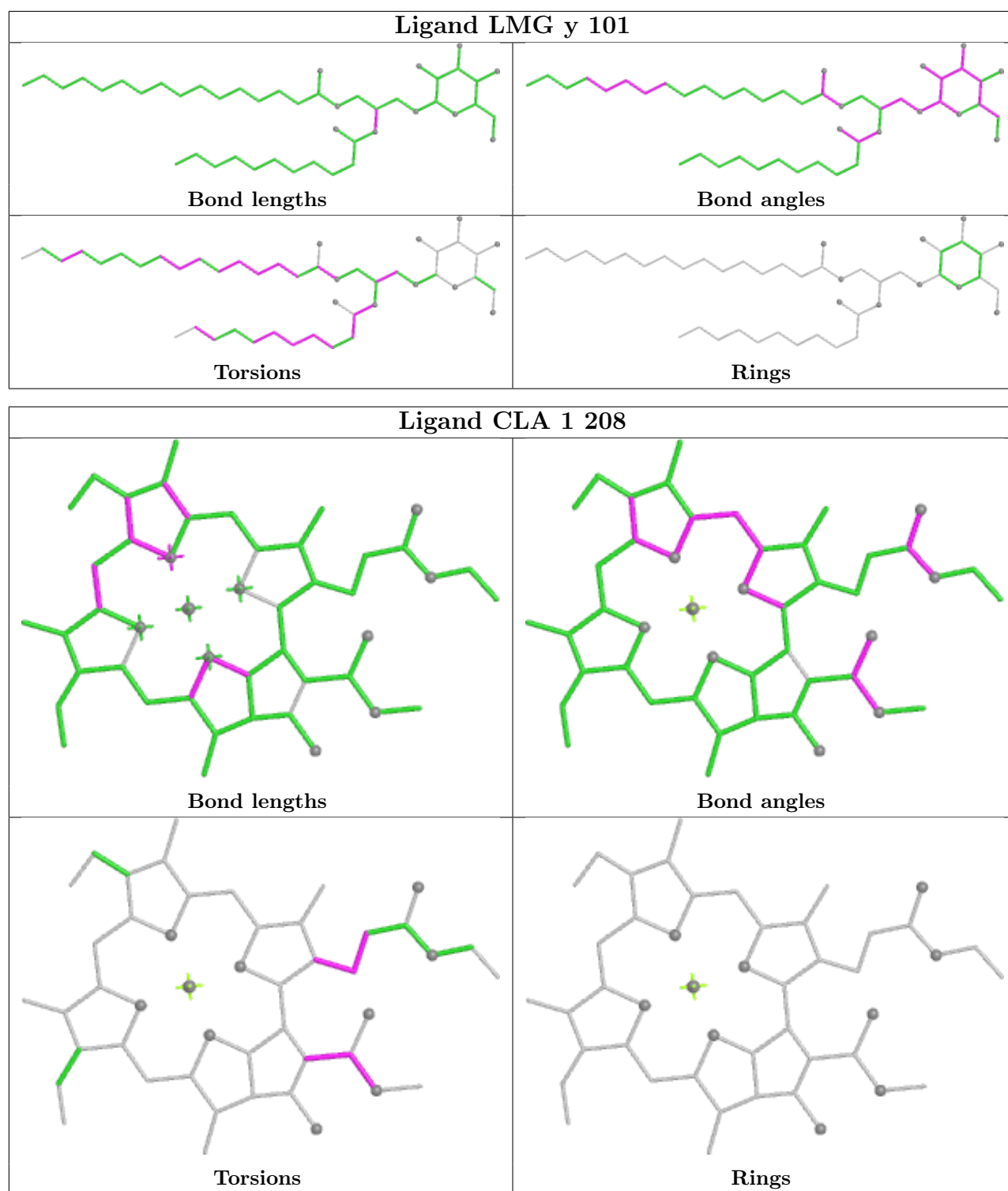
Rings

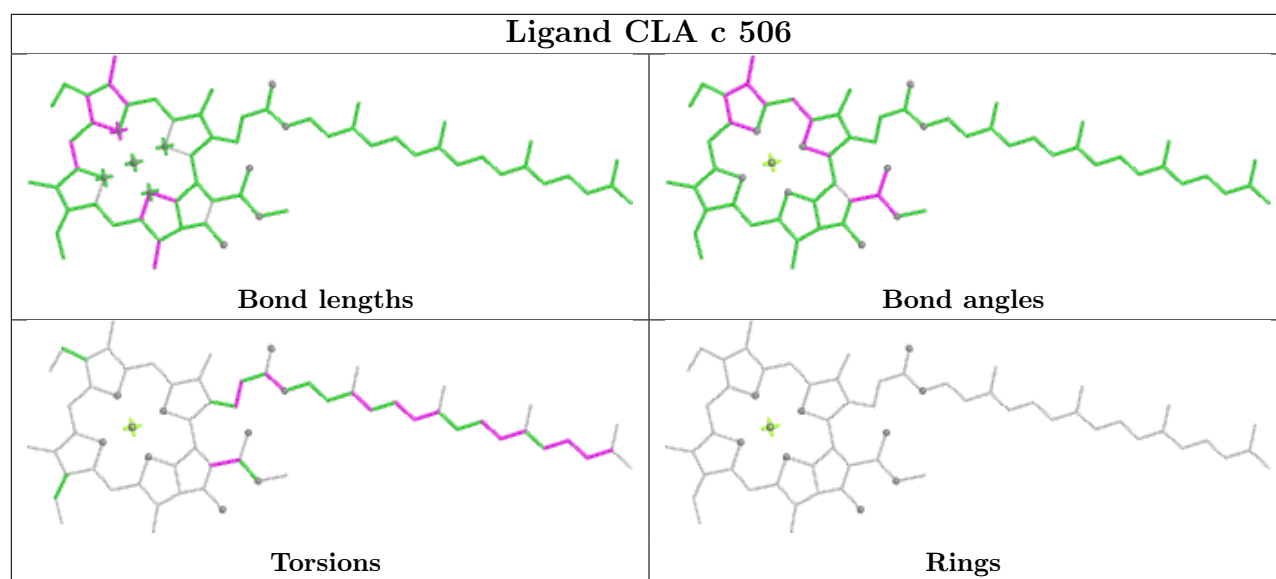








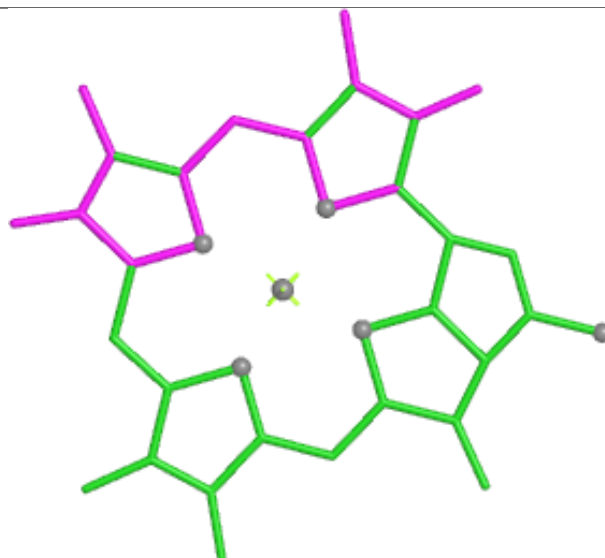




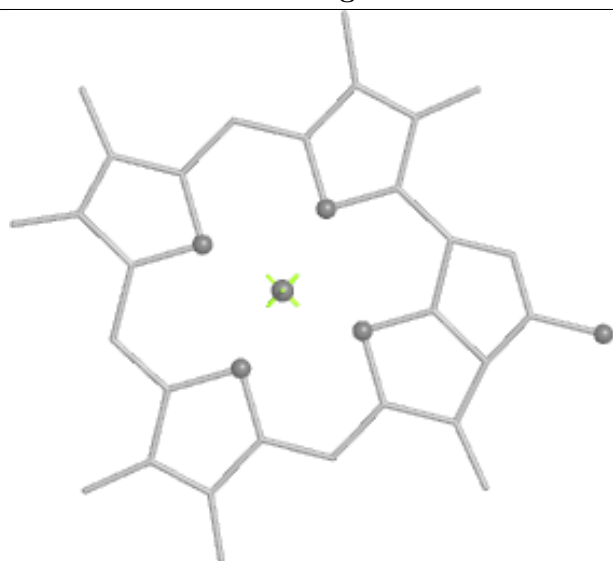
Ligand CLA 8 314



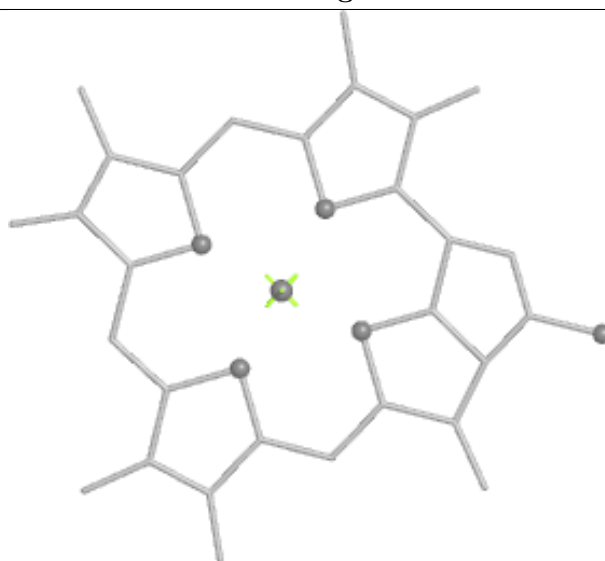
Bond lengths



Bond angles

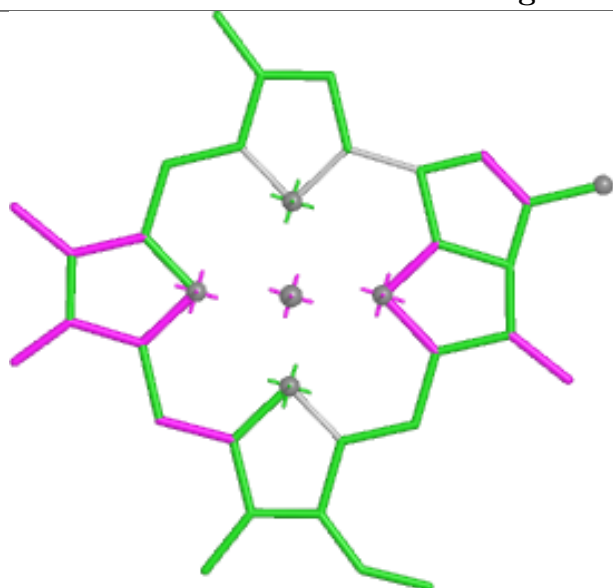


Torsions

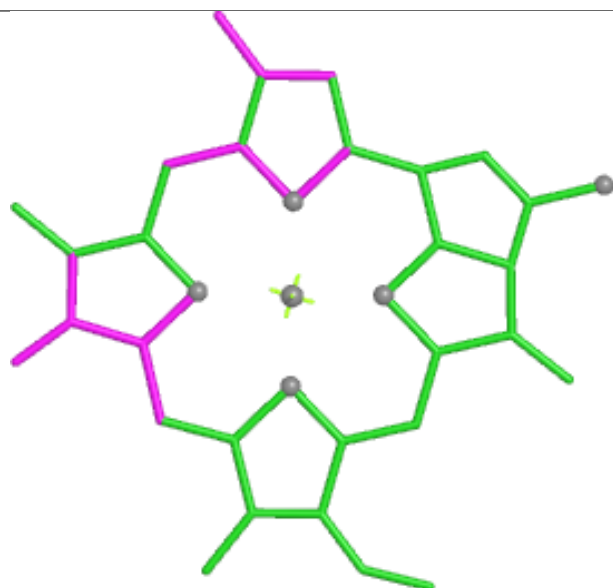


Rings

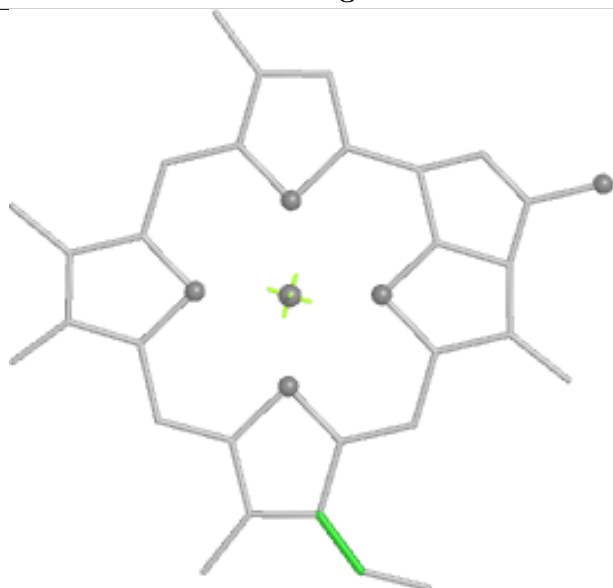
Ligand CLA 9 205



Bond lengths



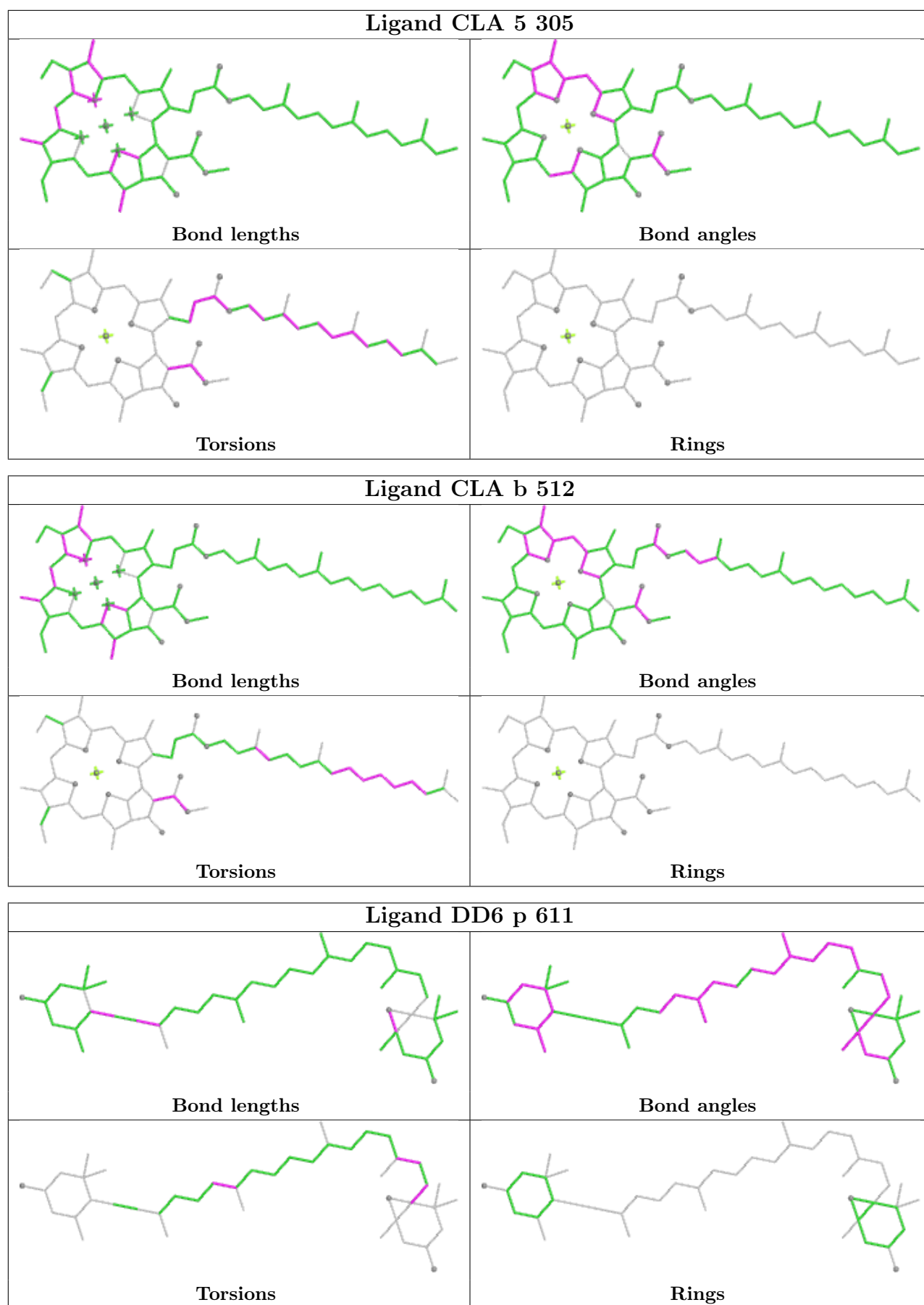
Bond angles



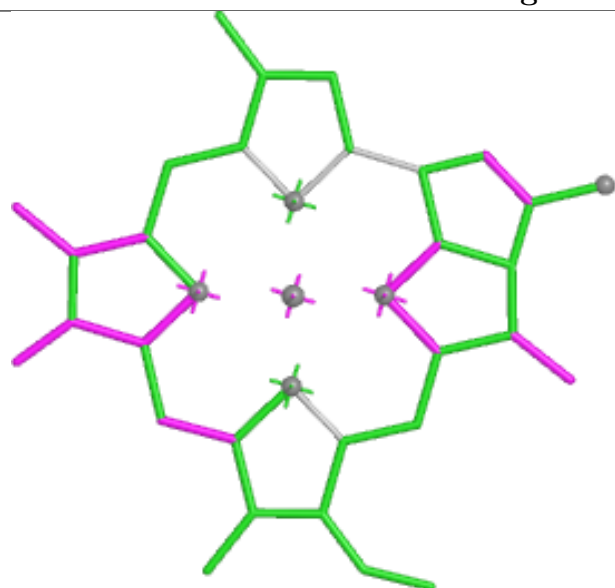
Torsions



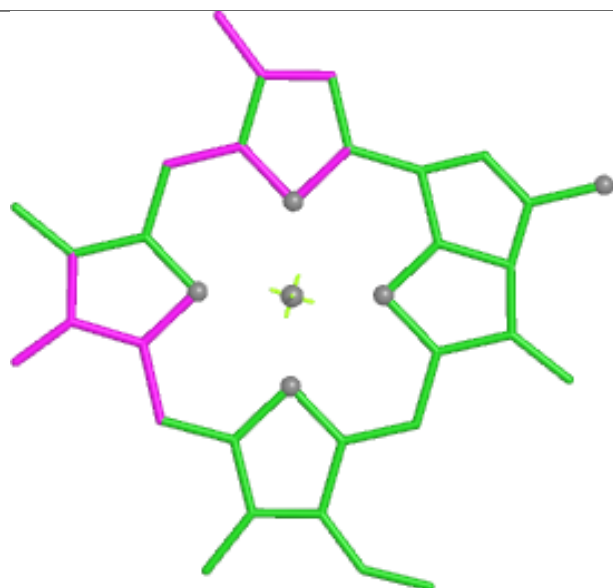
Rings



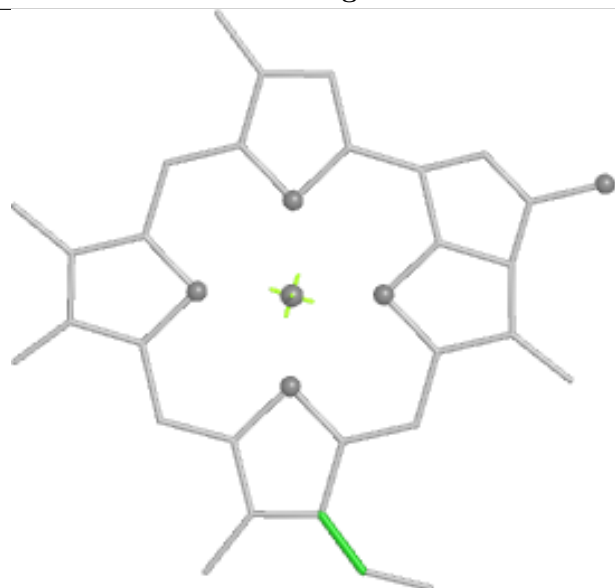
Ligand CLA 4 205



Bond lengths



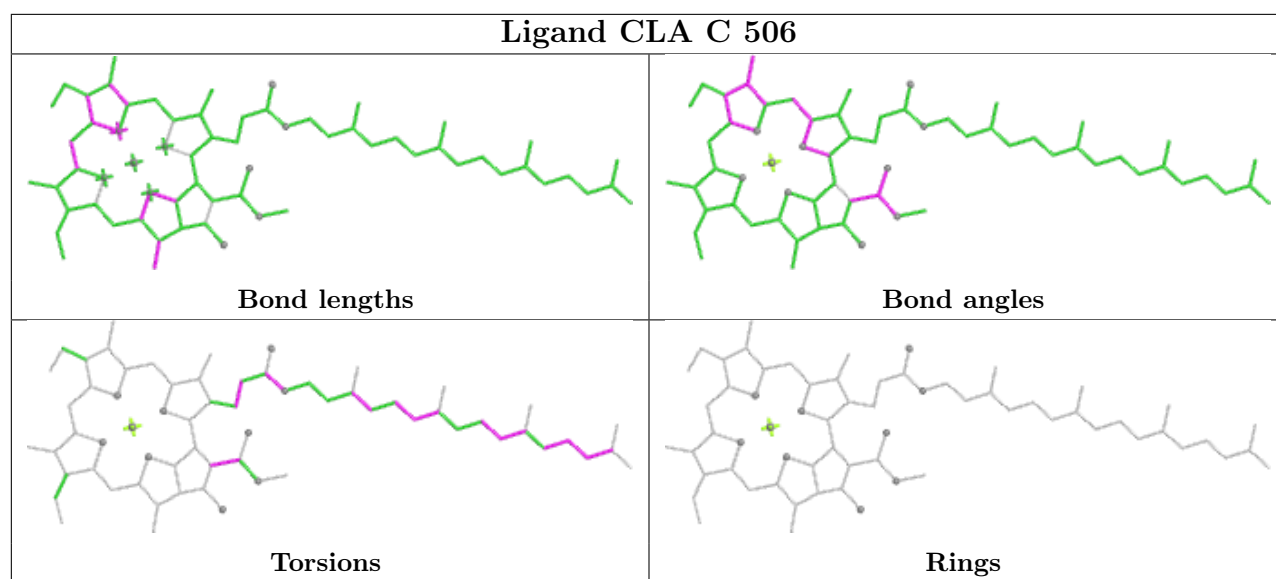
Bond angles



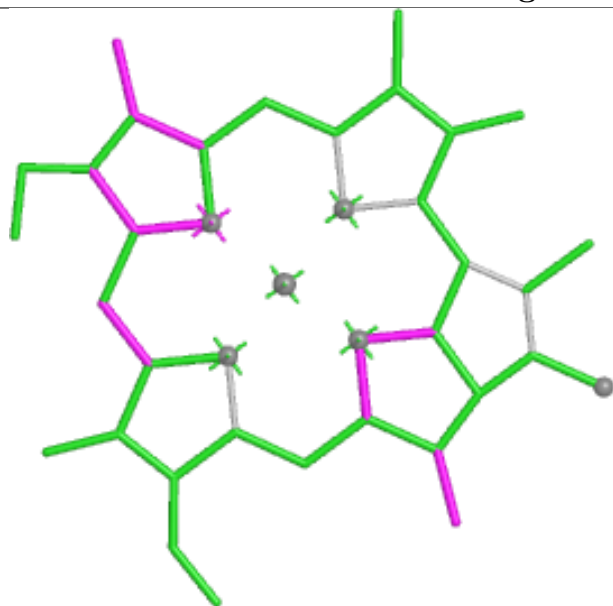
Torsions



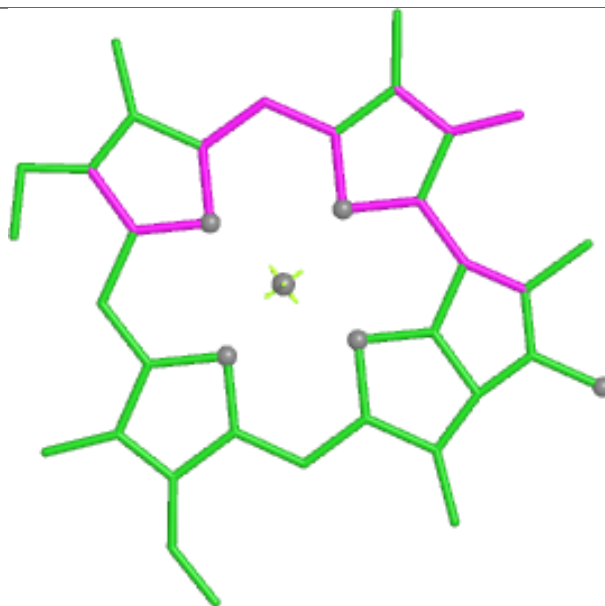
Rings



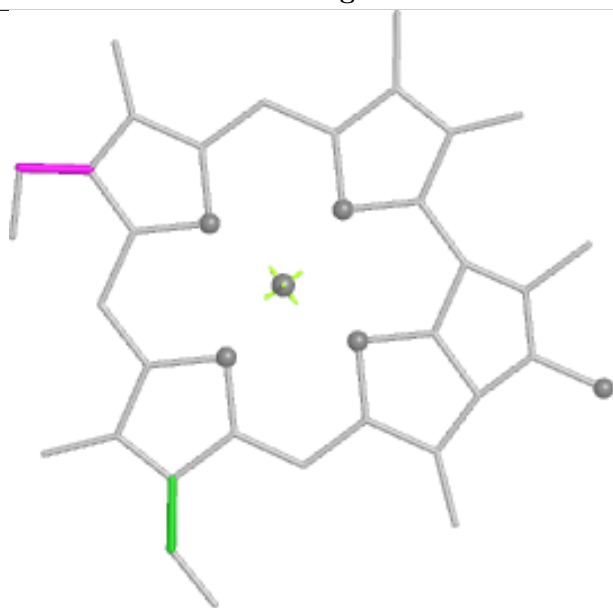
Ligand CLA 9 204



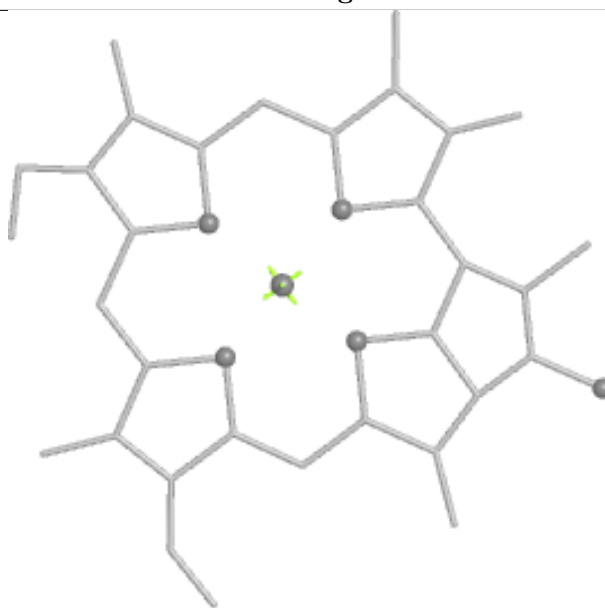
Bond lengths



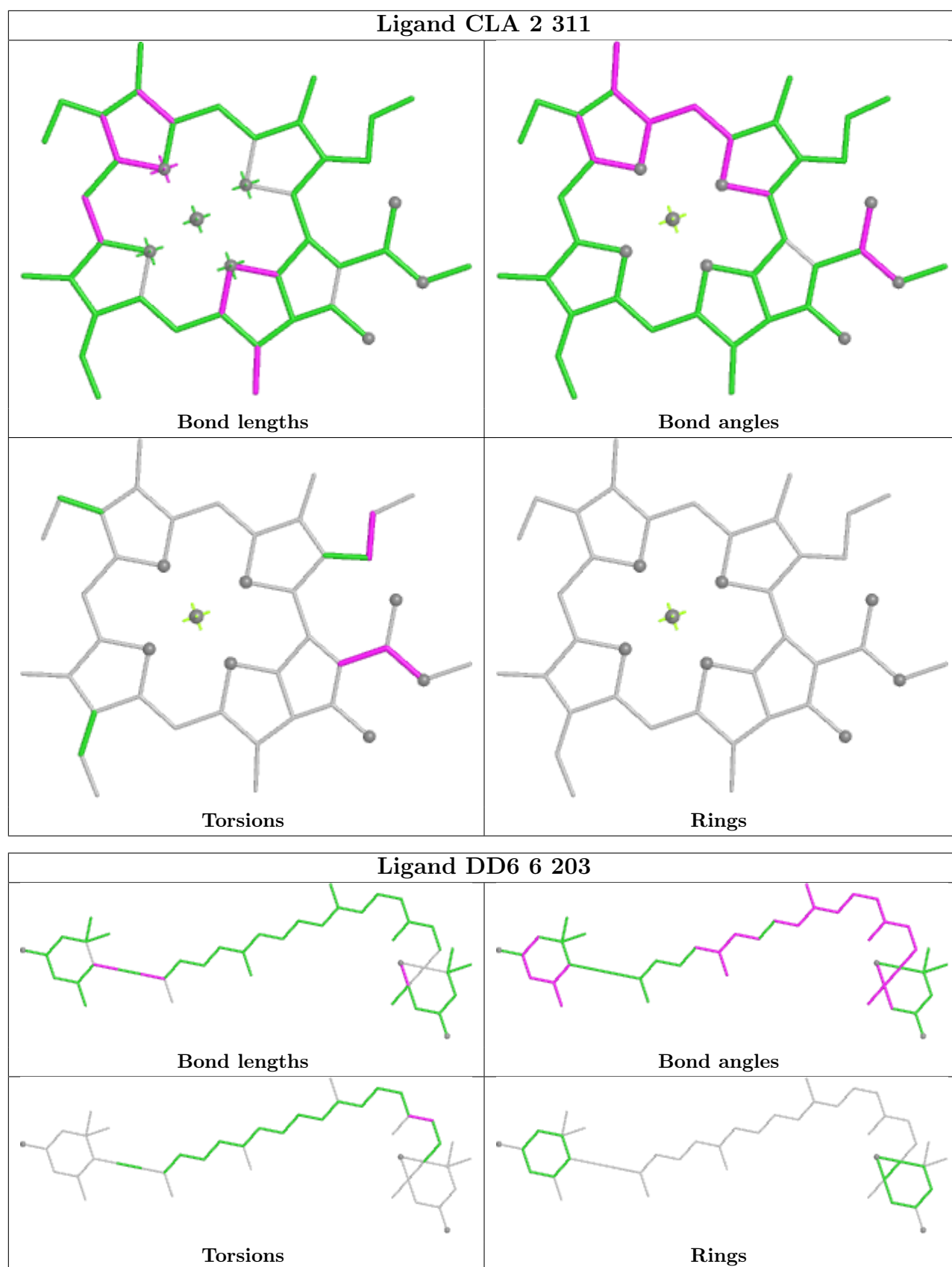
Bond angles

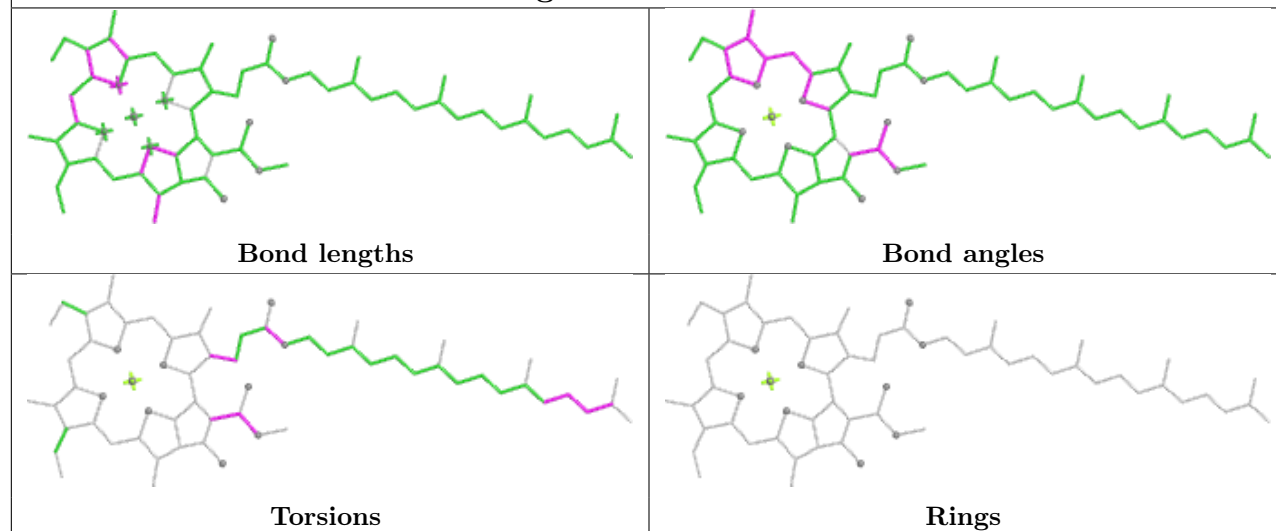
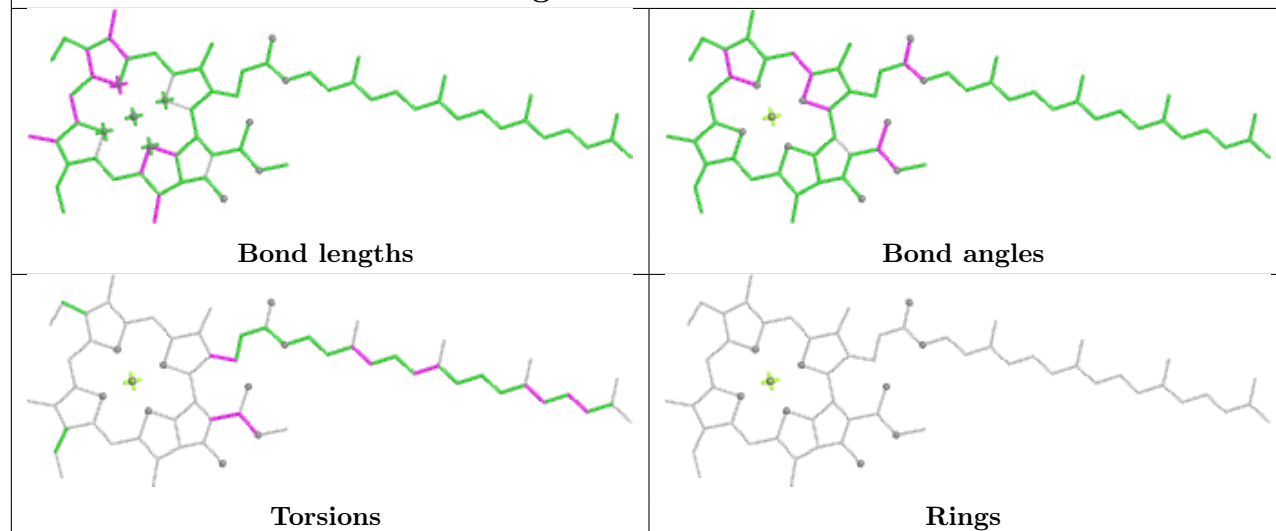


Torsions

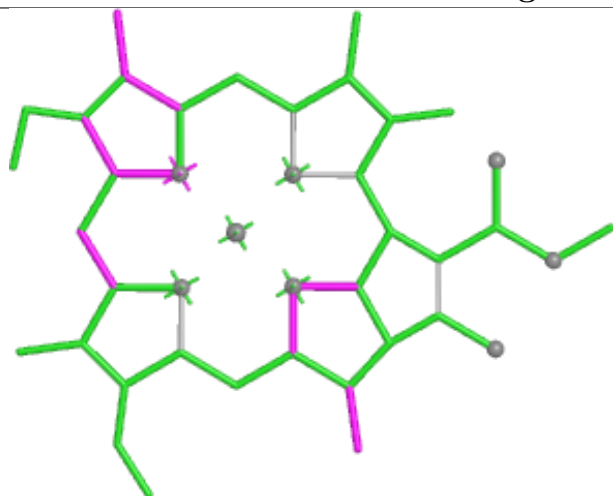


Rings

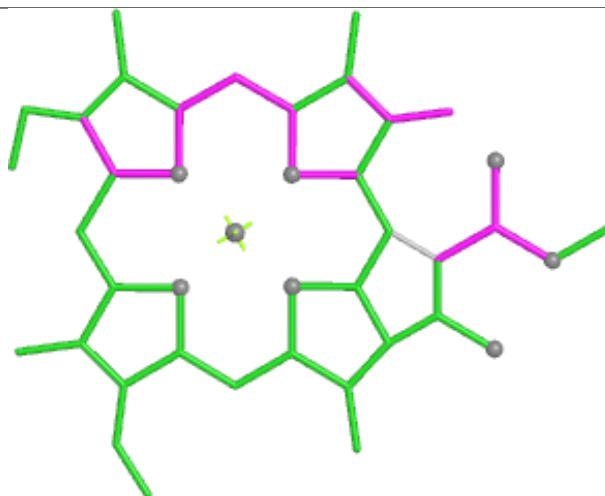


Ligand CLA a 403**Ligand CLA B 509**

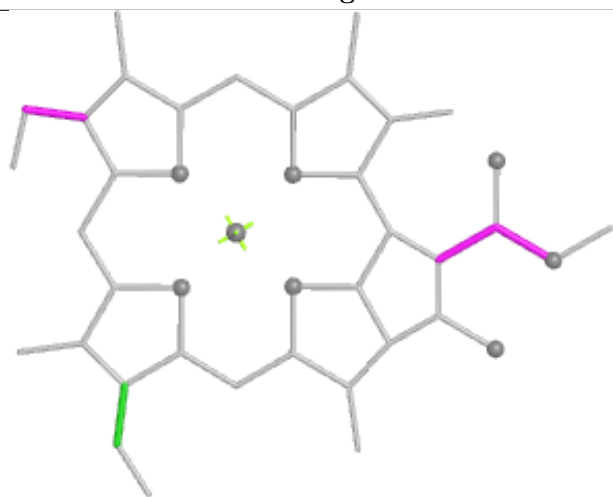
Ligand CLA 2 305



Bond lengths



Bond angles

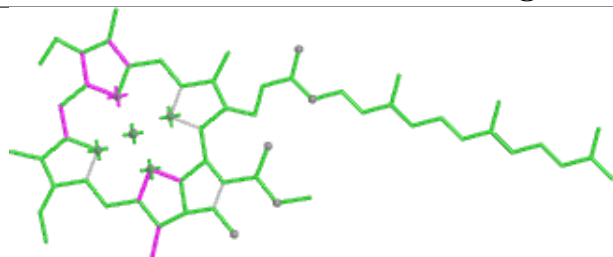


Torsions

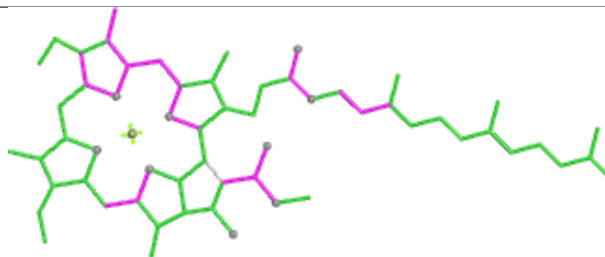


Rings

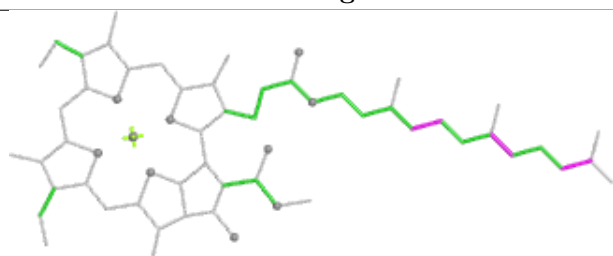
Ligand CLA a 407



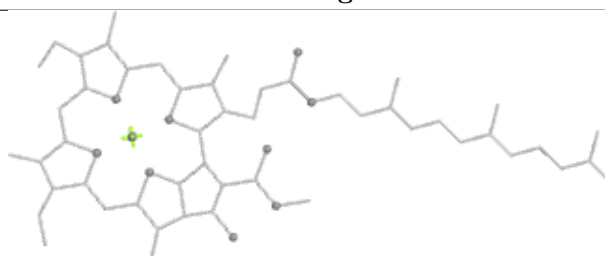
Bond lengths



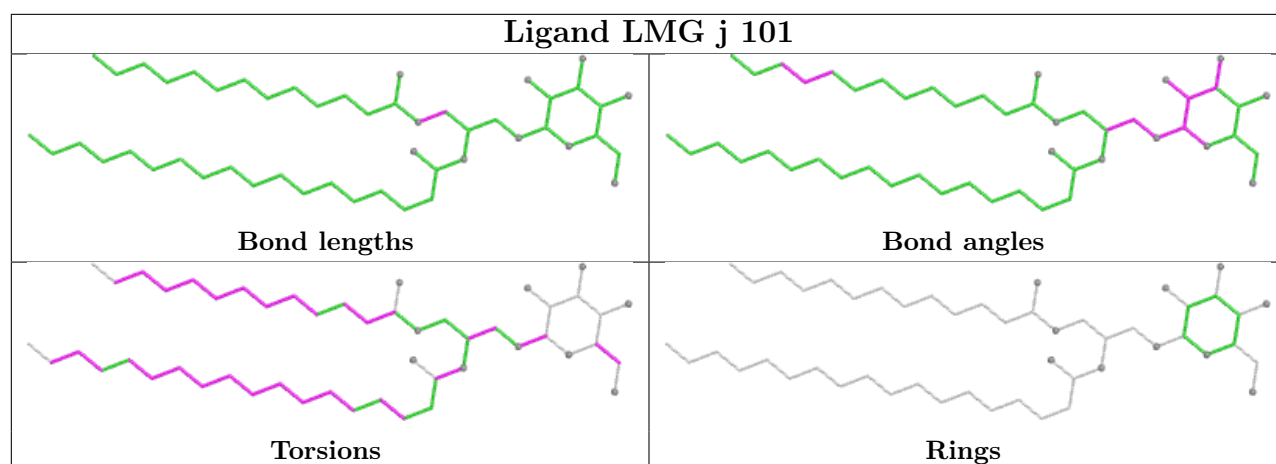
Bond angles



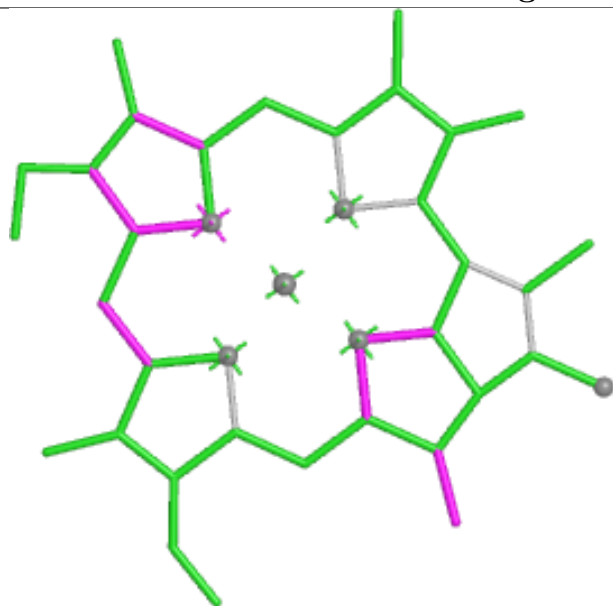
Torsions



Rings



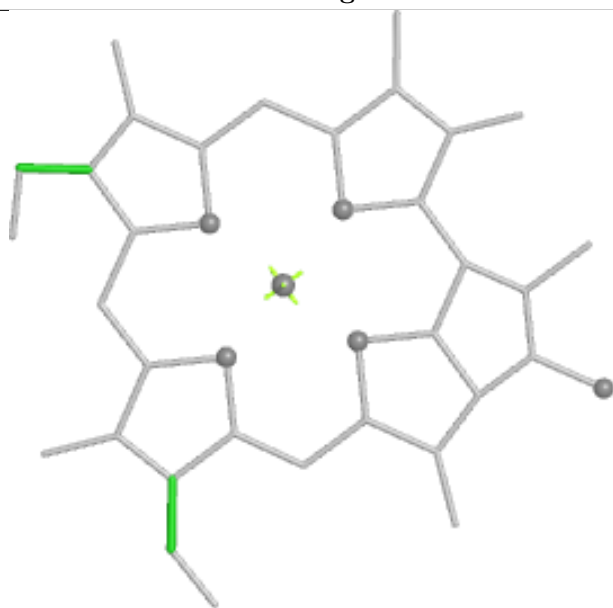
Ligand CLA 5 314



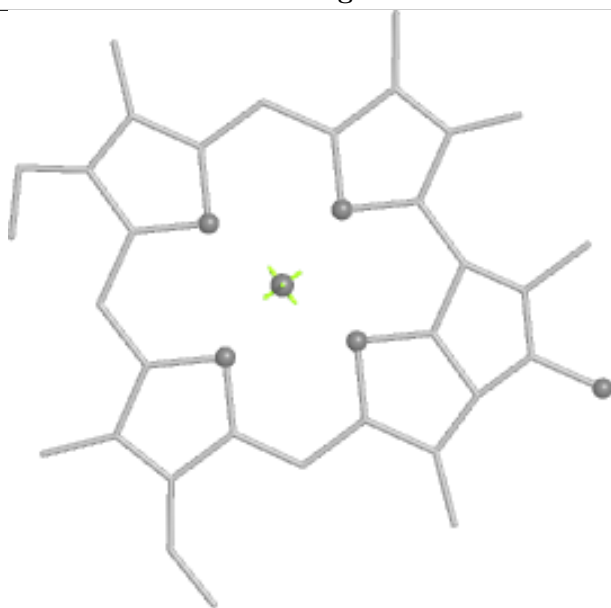
Bond lengths



Bond angles

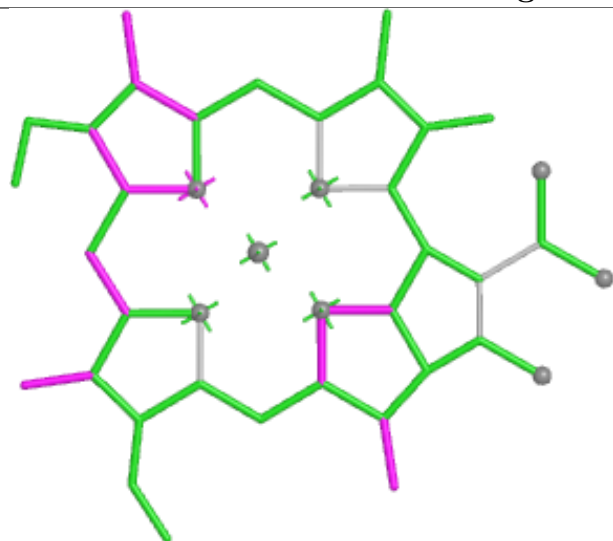


Torsions

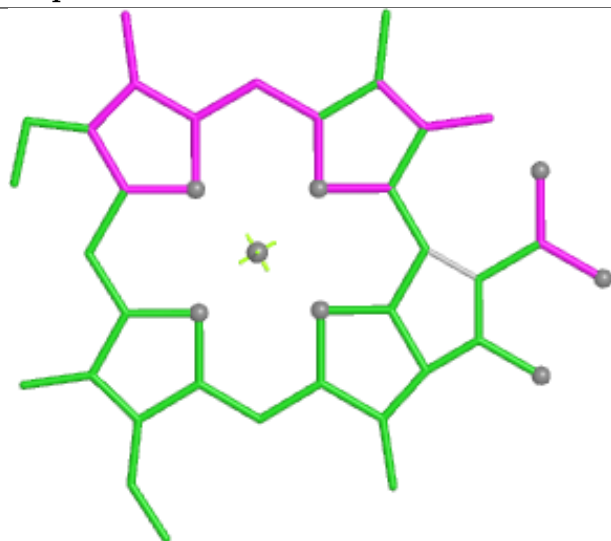


Rings

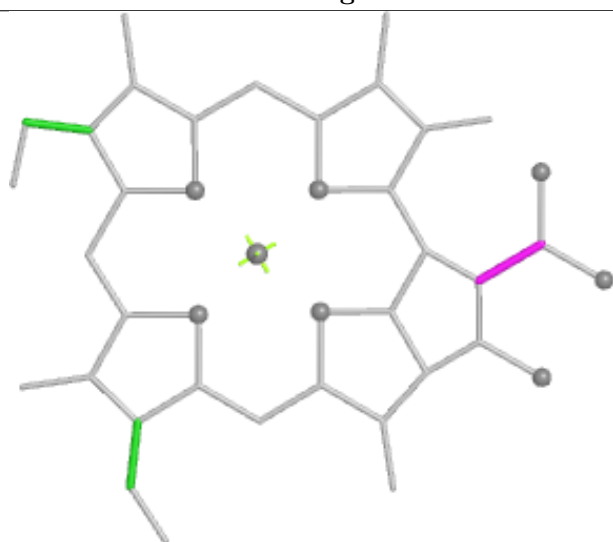
Ligand CLA p 604



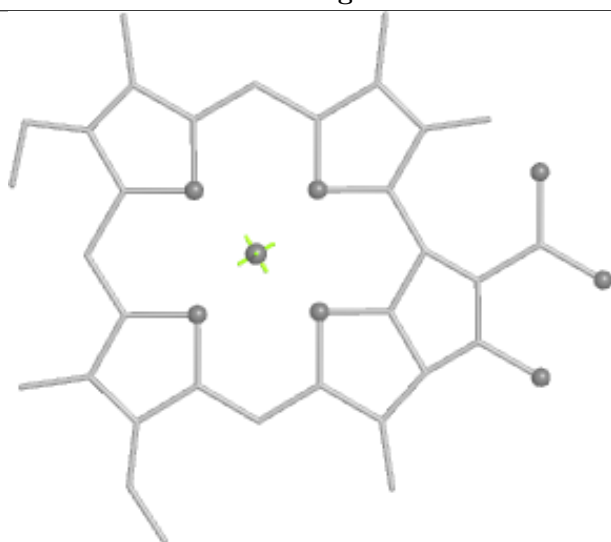
Bond lengths



Bond angles

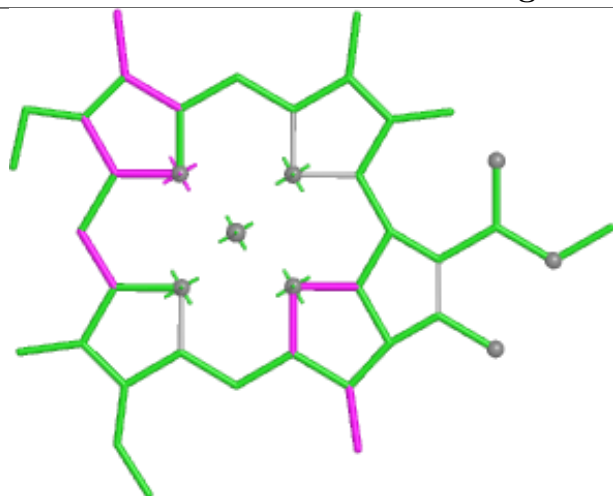


Torsions

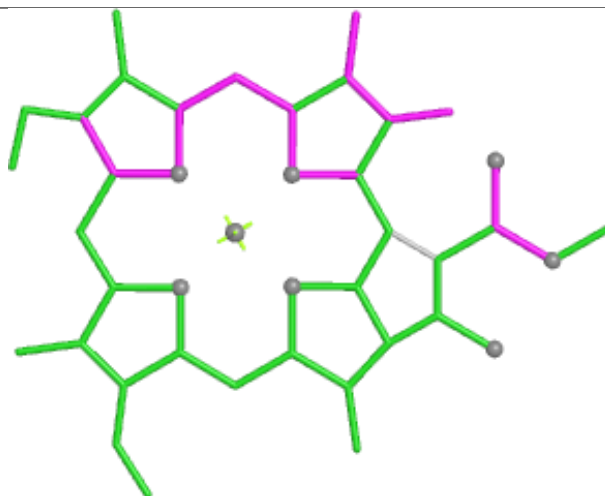


Rings

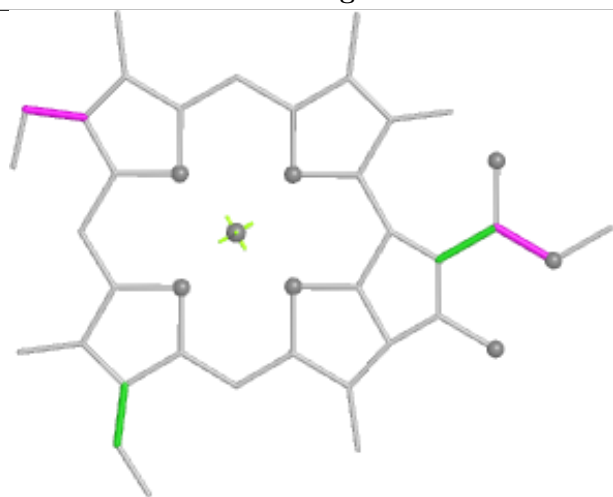
Ligand CLA 5 309



Bond lengths



Bond angles

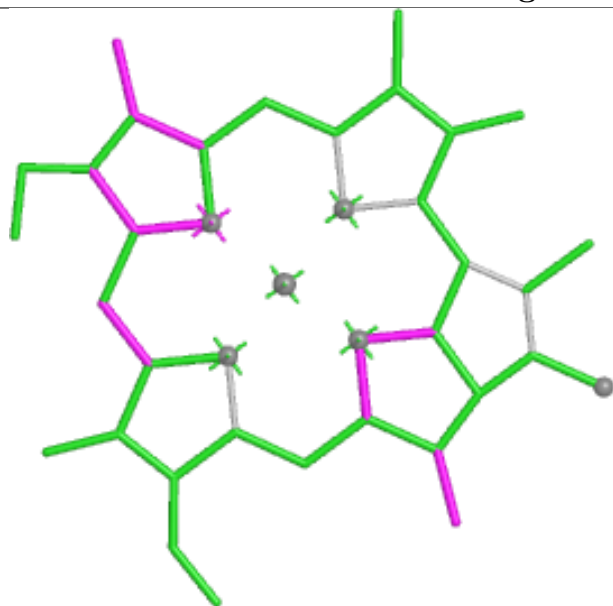


Torsions



Rings

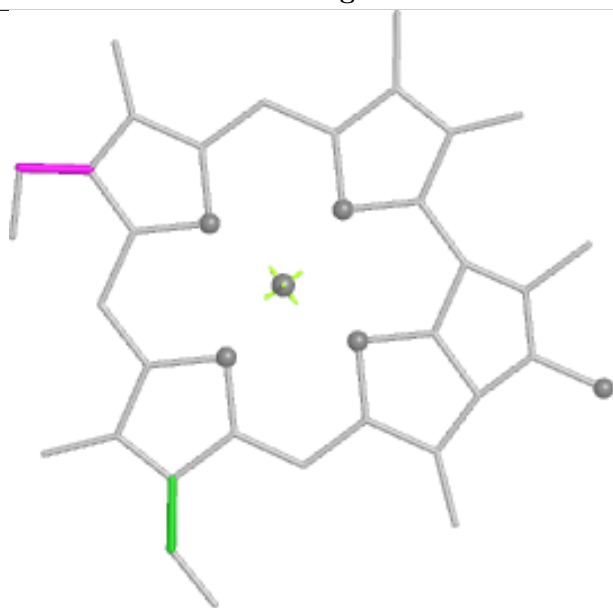
Ligand CLA 0 313



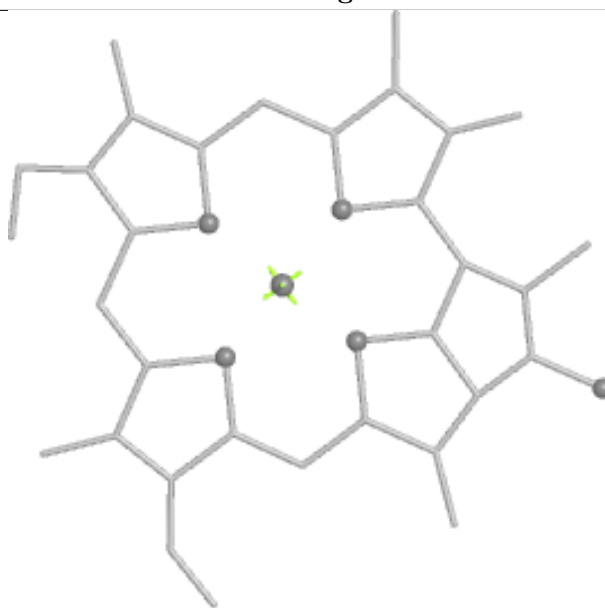
Bond lengths



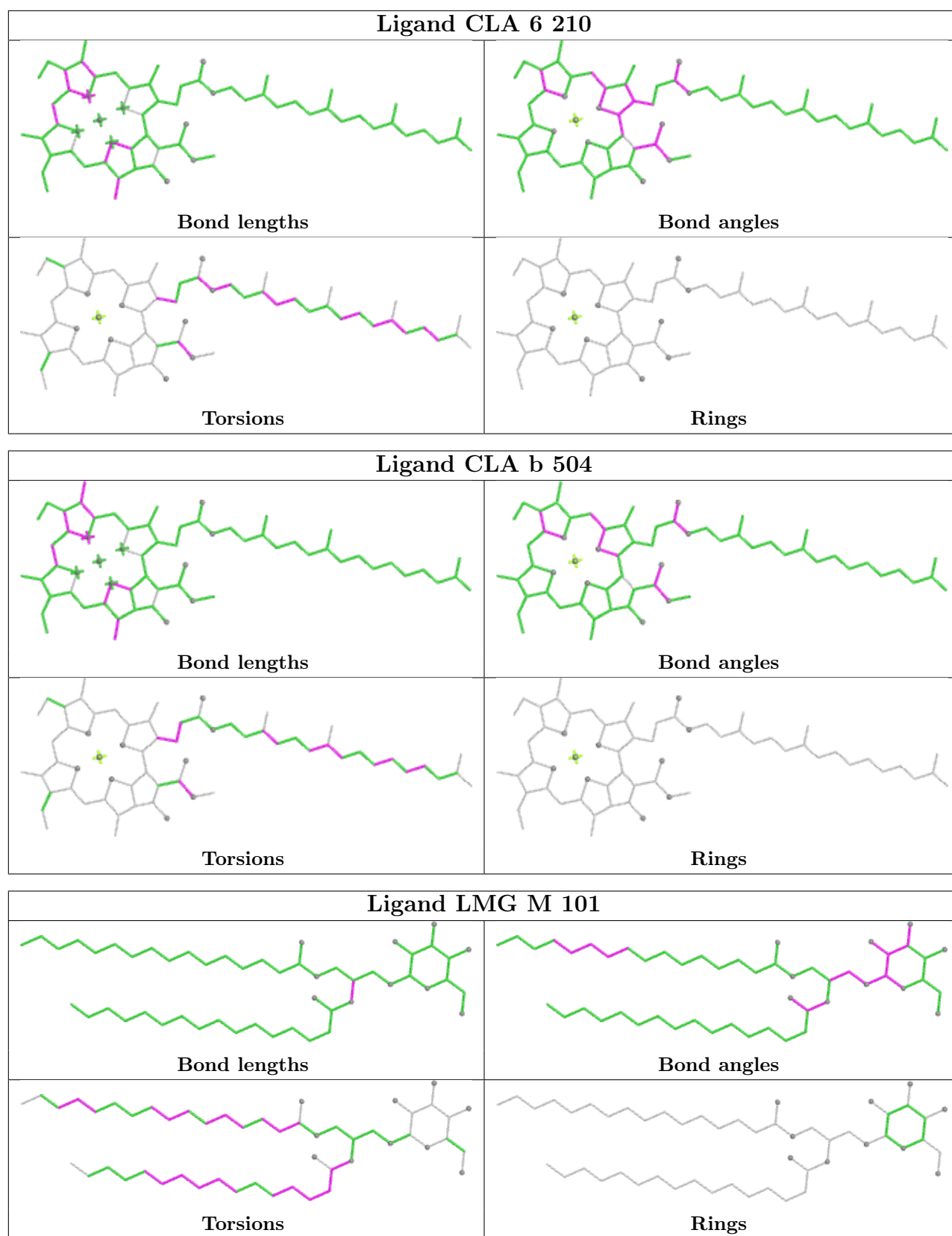
Bond angles

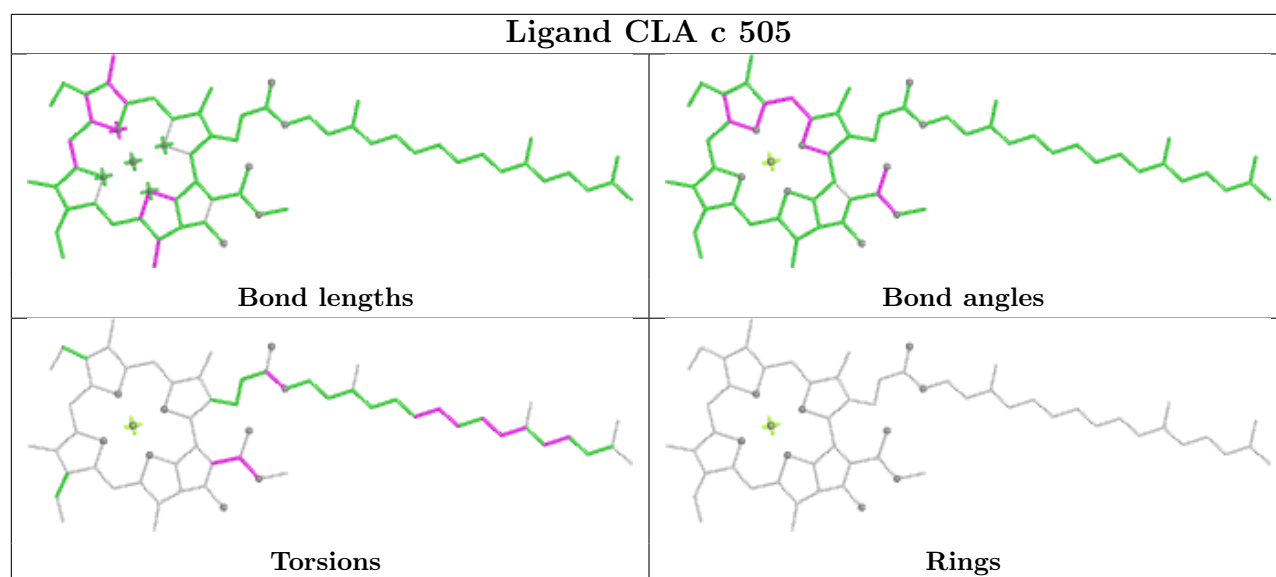


Torsions

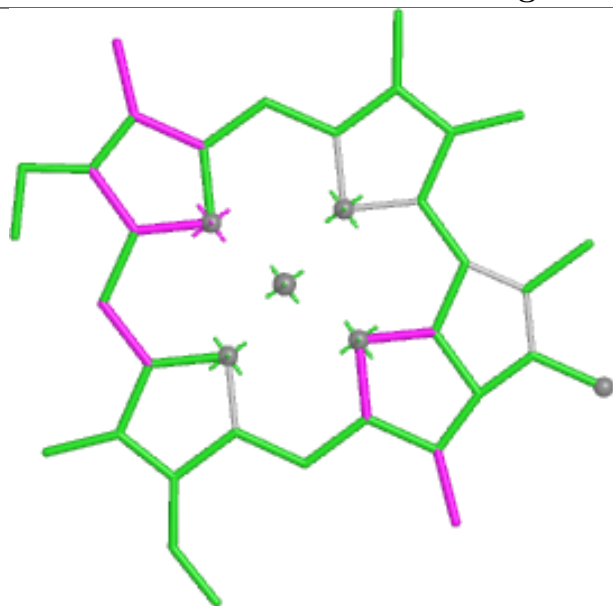


Rings

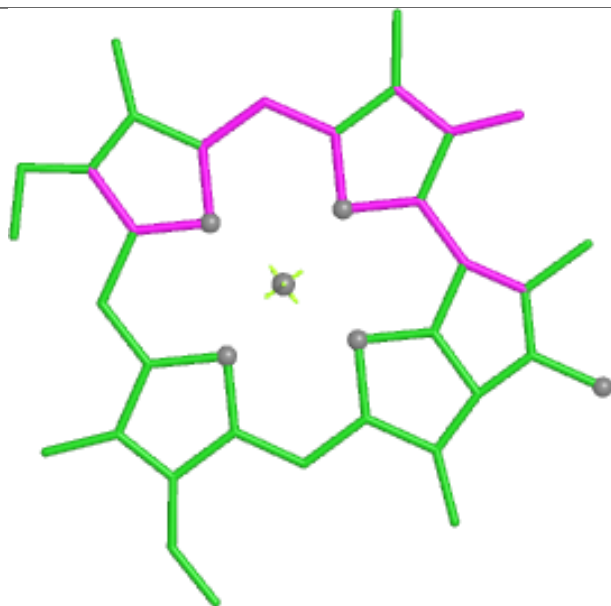




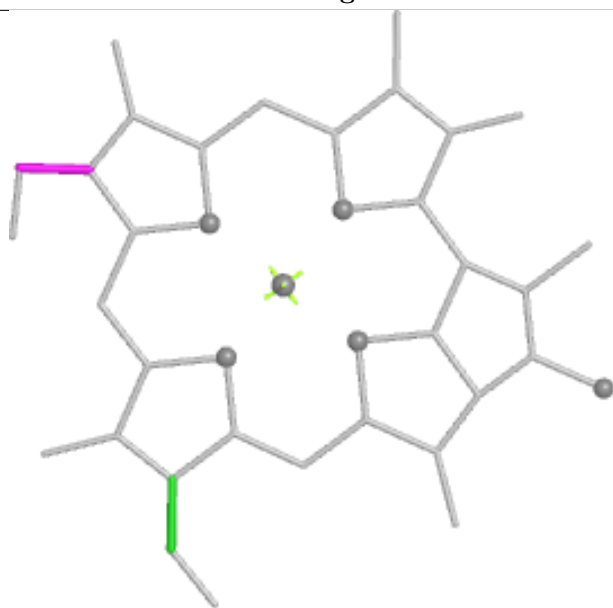
Ligand CLA 4 204



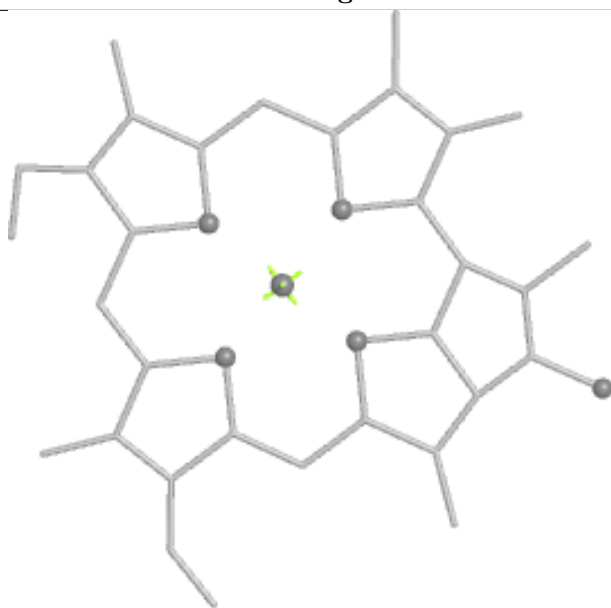
Bond lengths



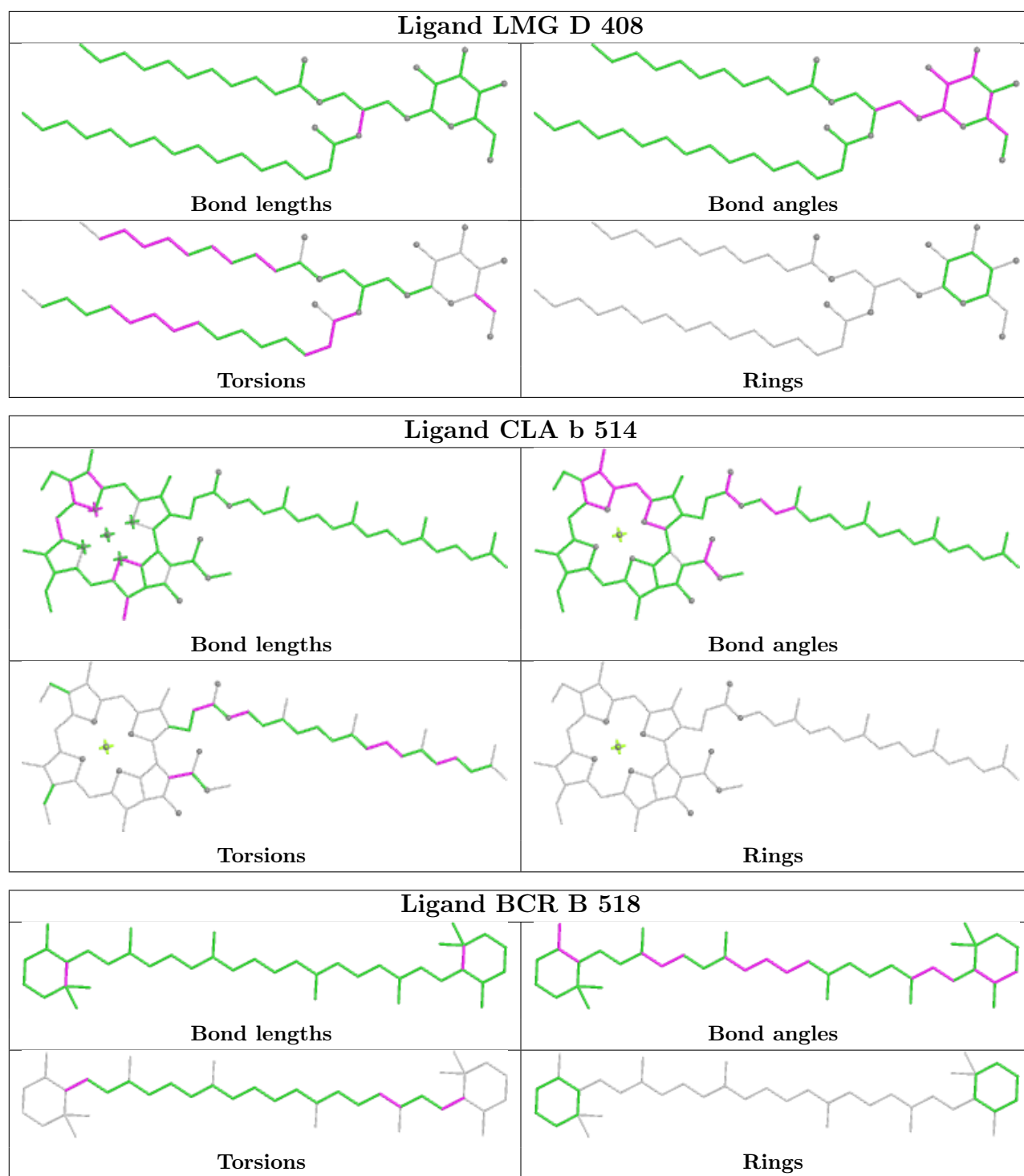
Bond angles

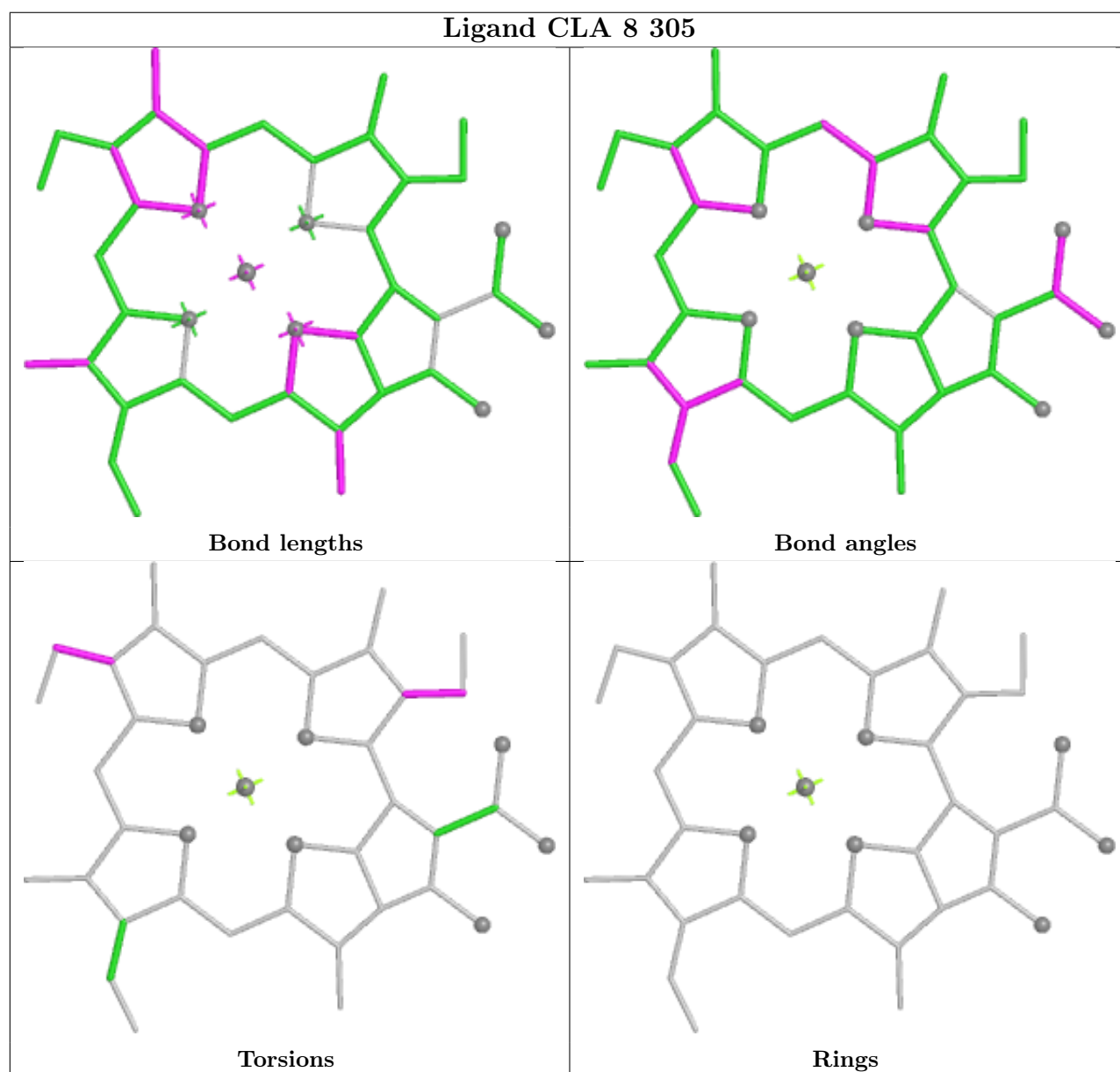
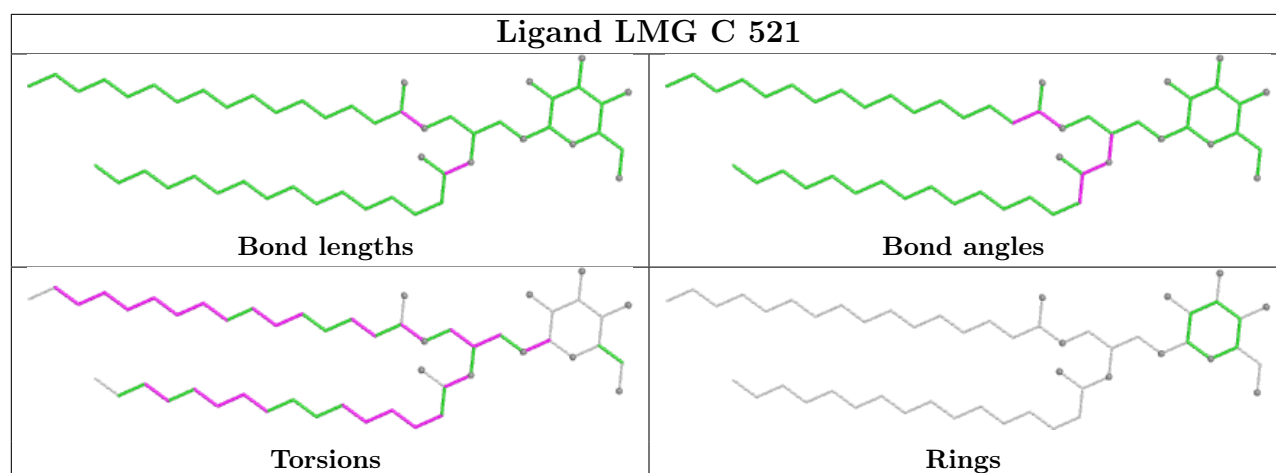


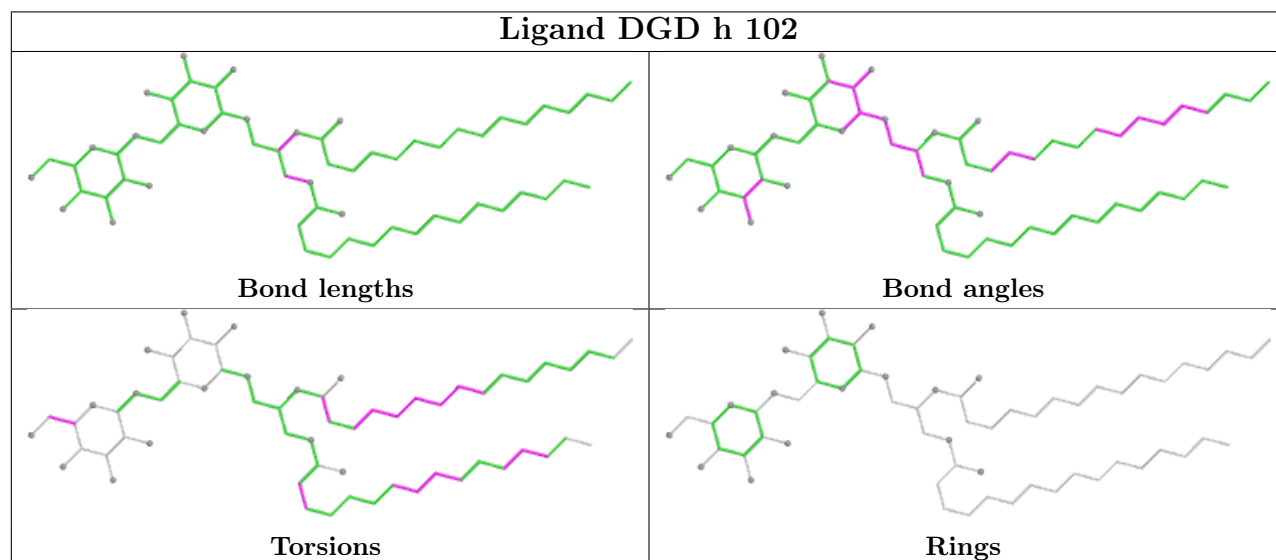
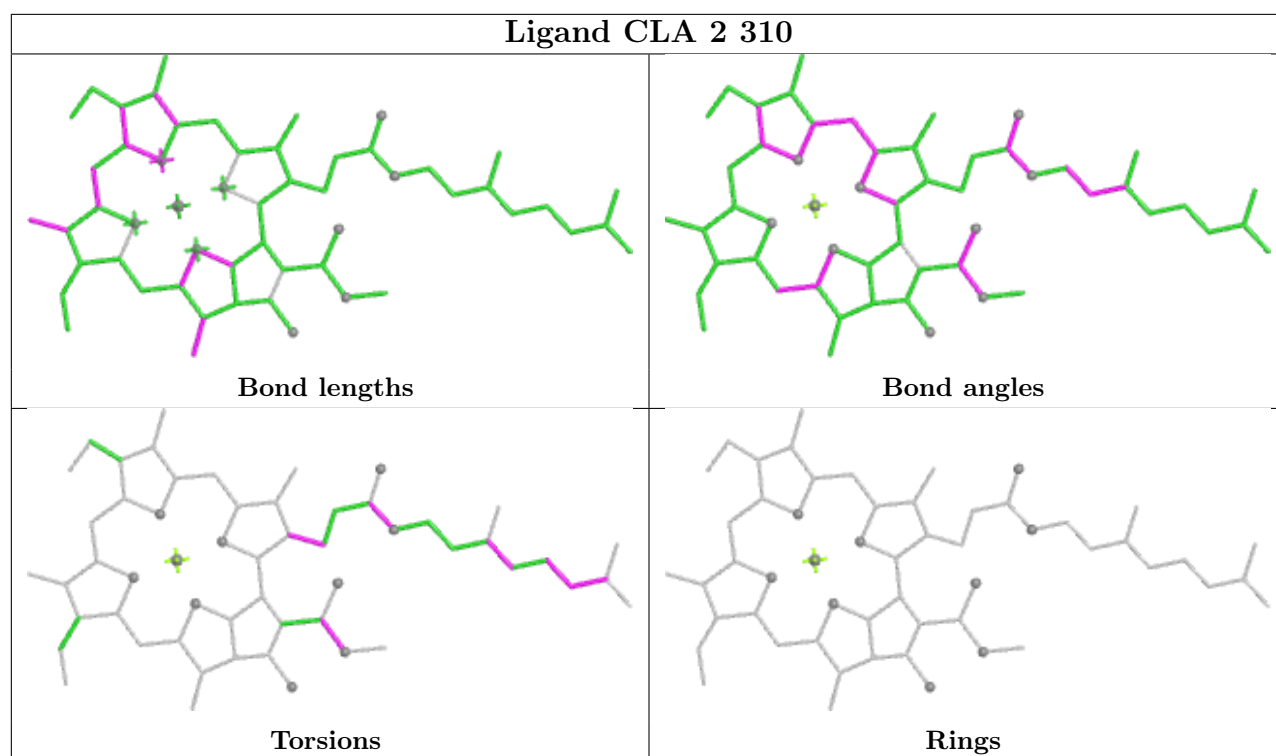
Torsions

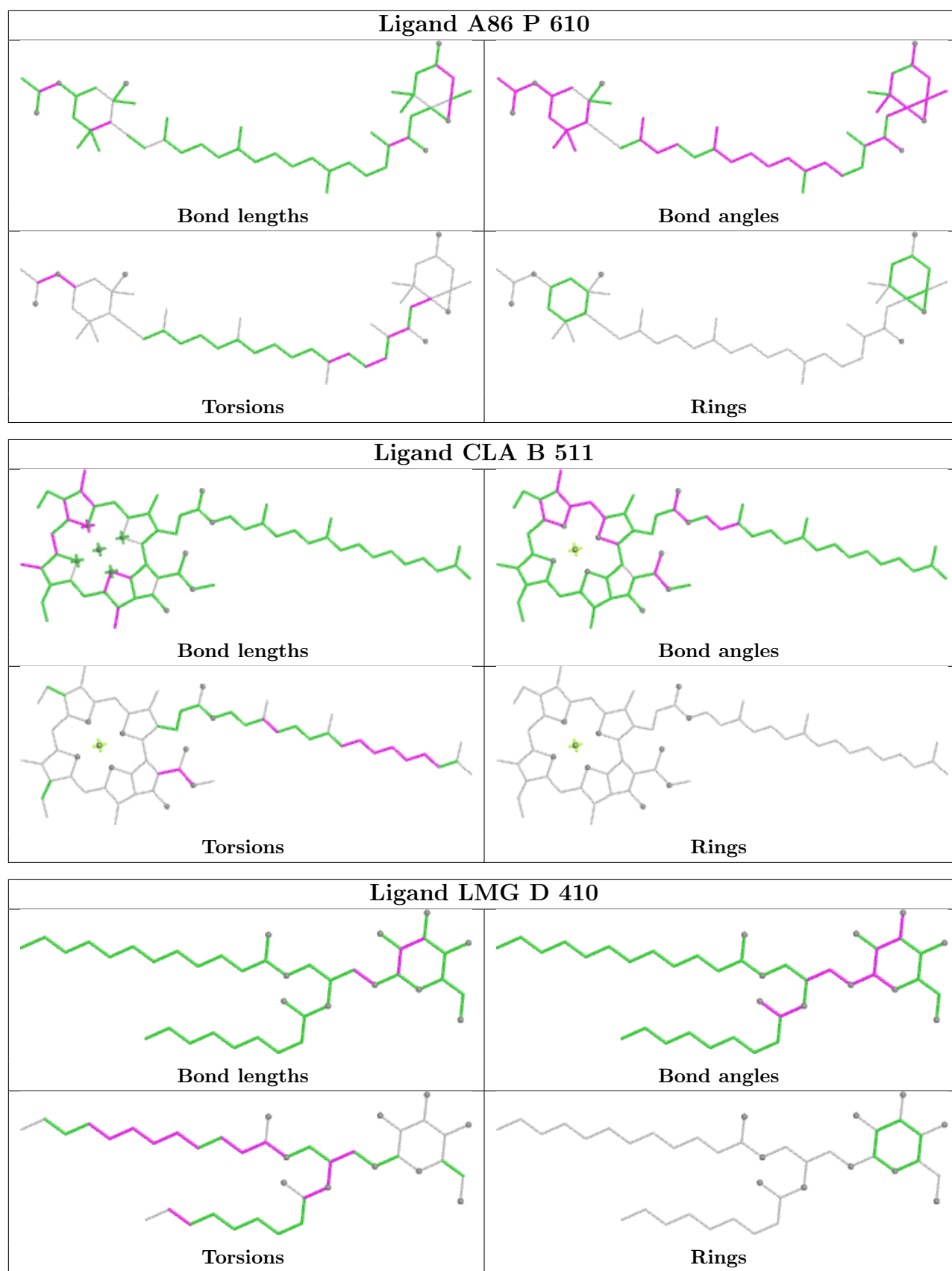


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

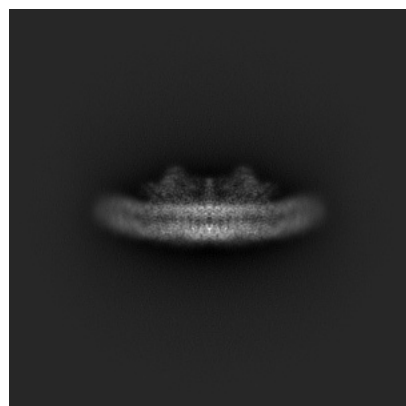
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35987. These allow visual inspection of the internal detail of the map and identification of artifacts.

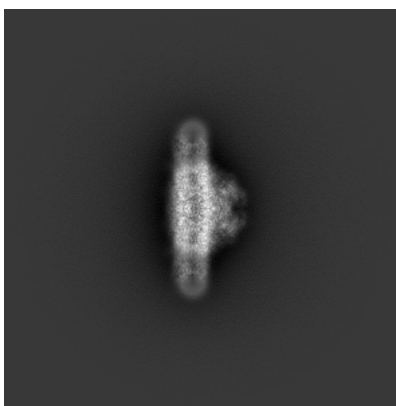
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

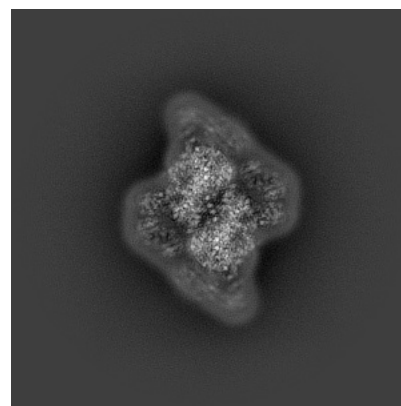
6.1.1 Primary map



X

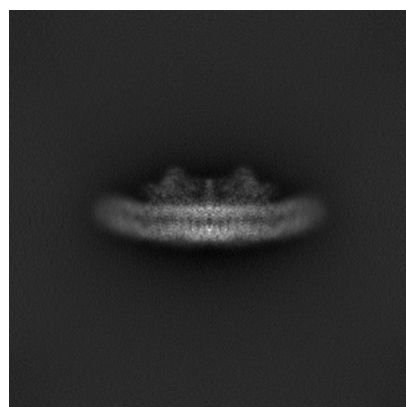


Y

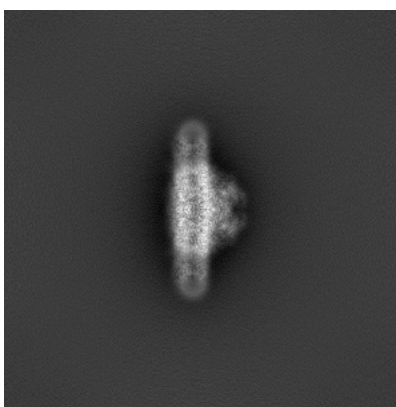


Z

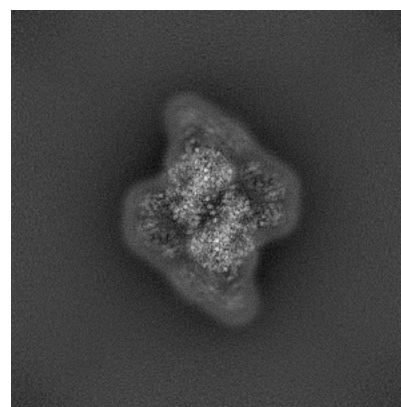
6.1.2 Raw map



X



Y

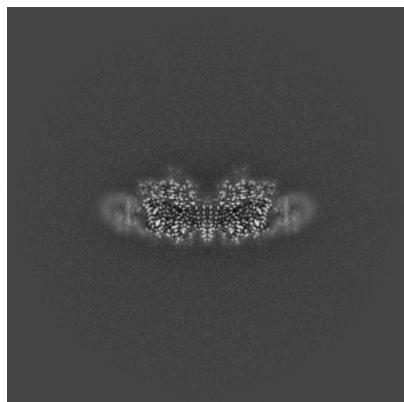


Z

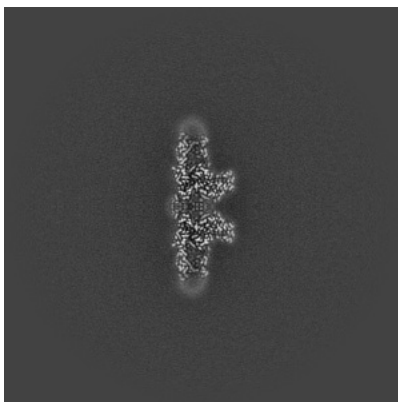
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

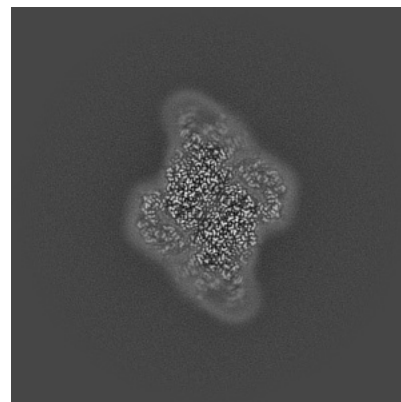
6.2.1 Primary map



X Index: 256

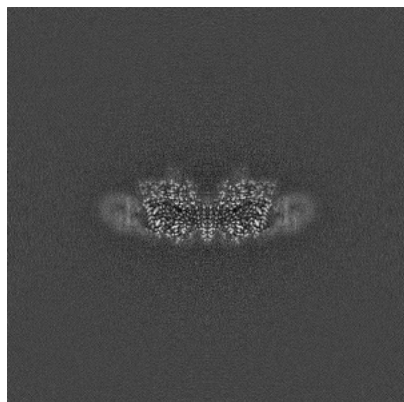


Y Index: 256

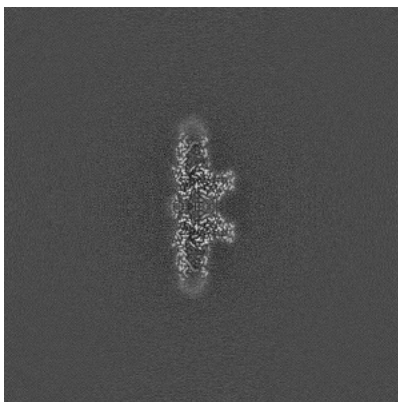


Z Index: 256

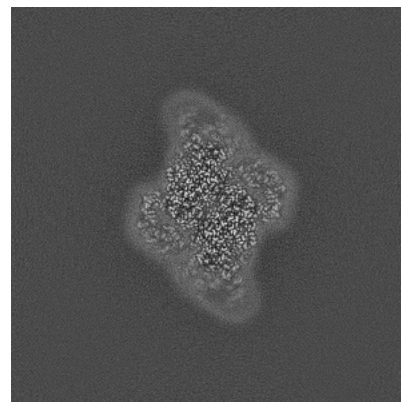
6.2.2 Raw map



X Index: 256



Y Index: 256

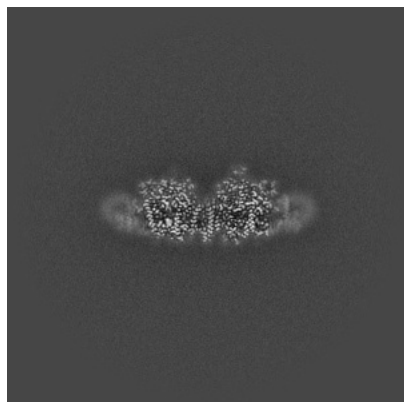


Z Index: 256

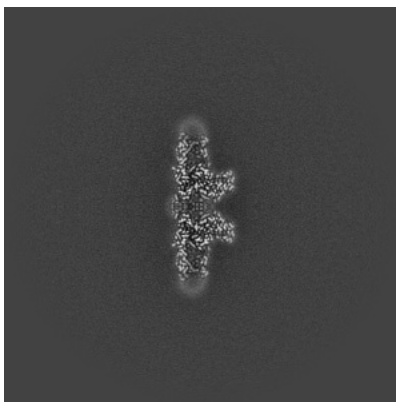
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

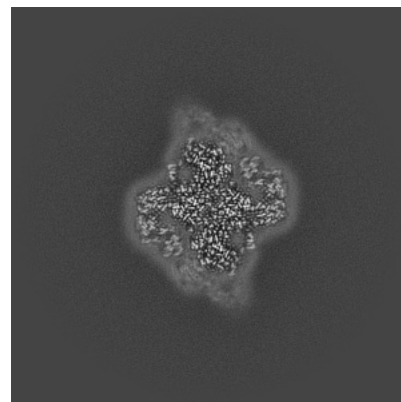
6.3.1 Primary map



X Index: 254

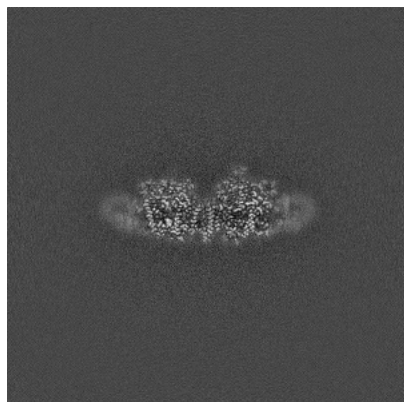


Y Index: 256

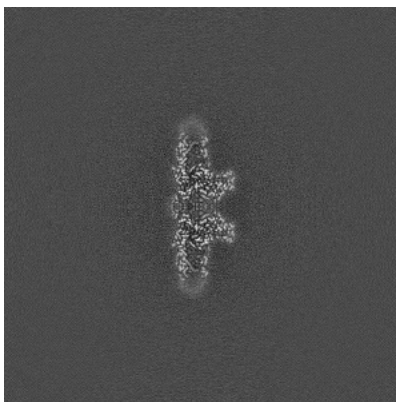


Z Index: 230

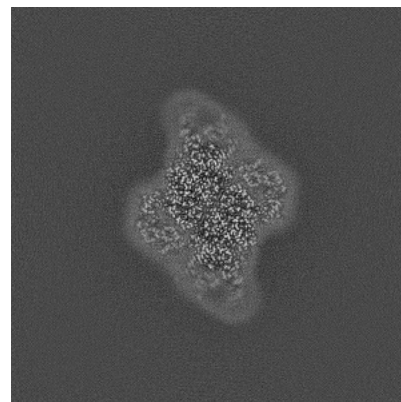
6.3.2 Raw map



X Index: 254



Y Index: 256

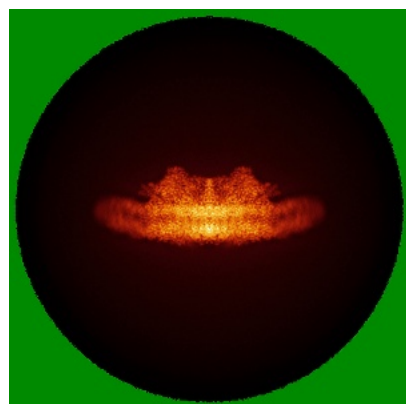


Z Index: 255

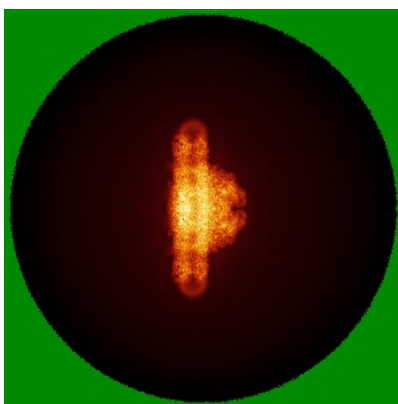
The images above show the largest variance slices of the map in three orthogonal directions.

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

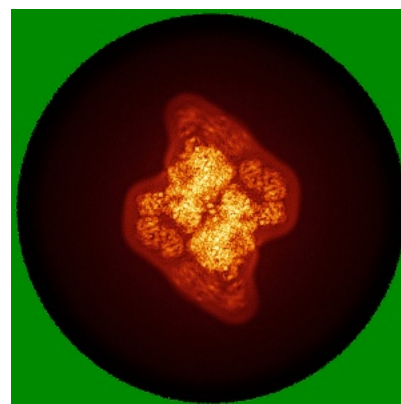
6.4.1 Primary map



X

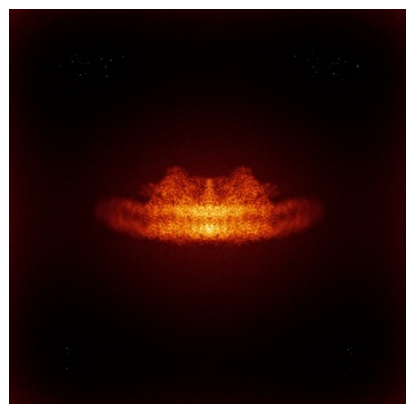


Y

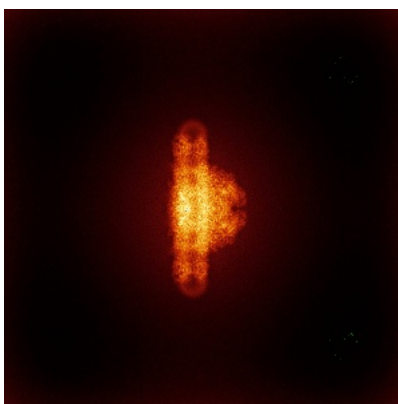


Z

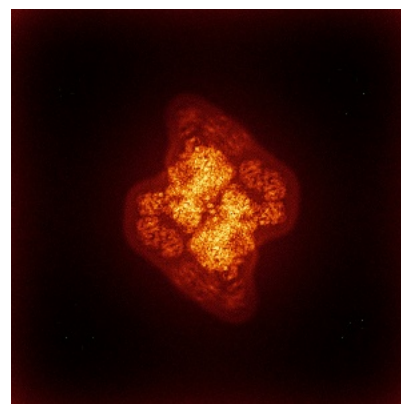
6.4.2 Raw map



X



Y

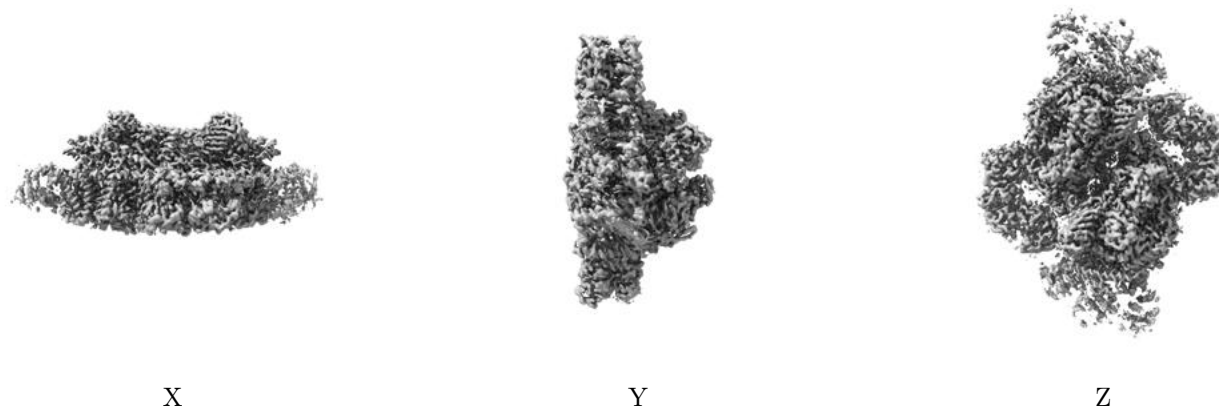


Z

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.

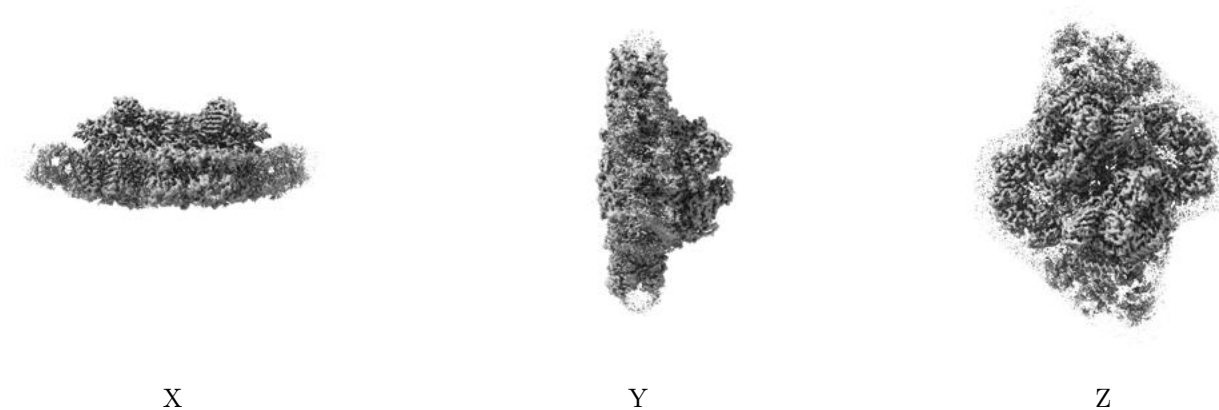
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.158. 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.

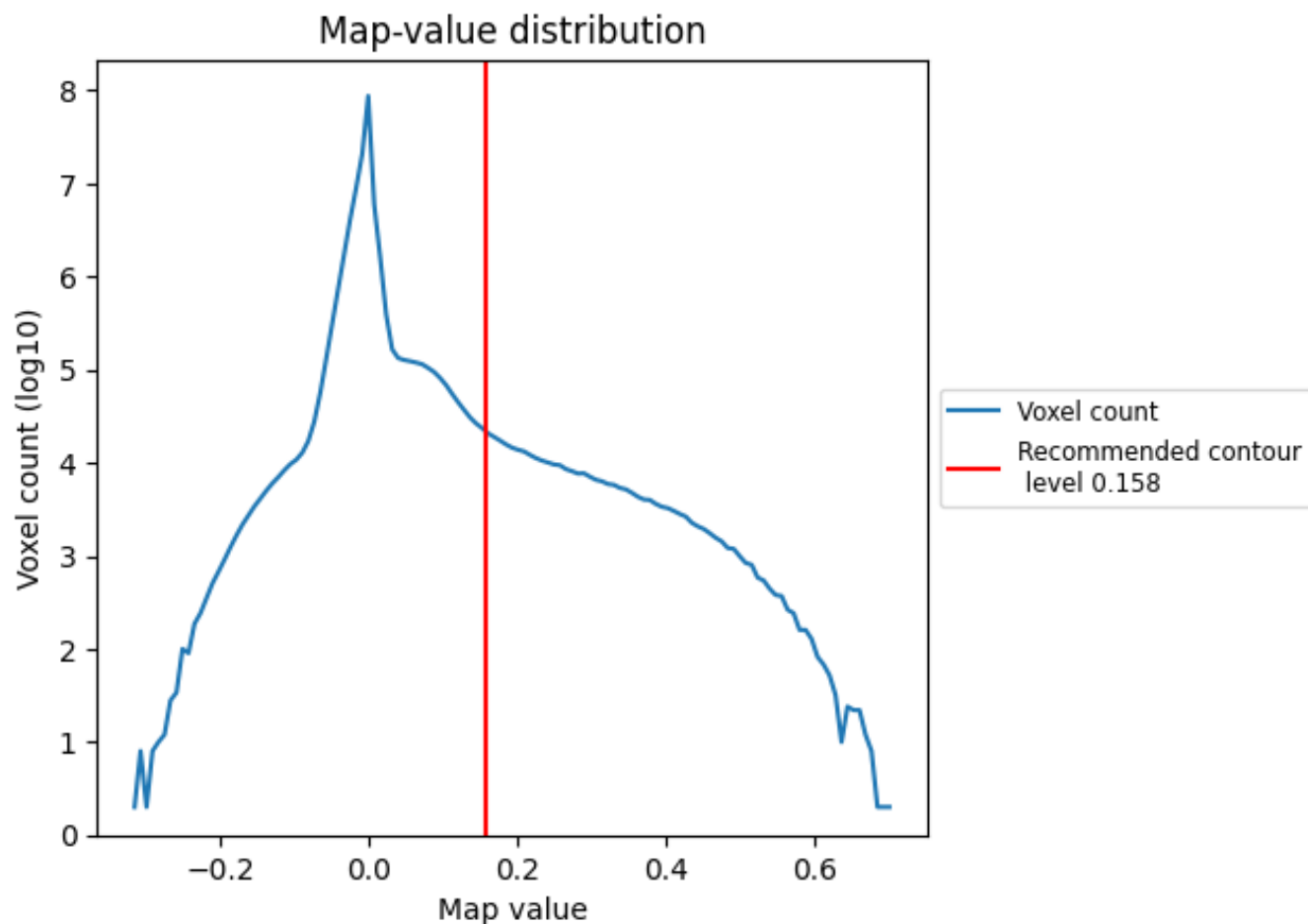
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

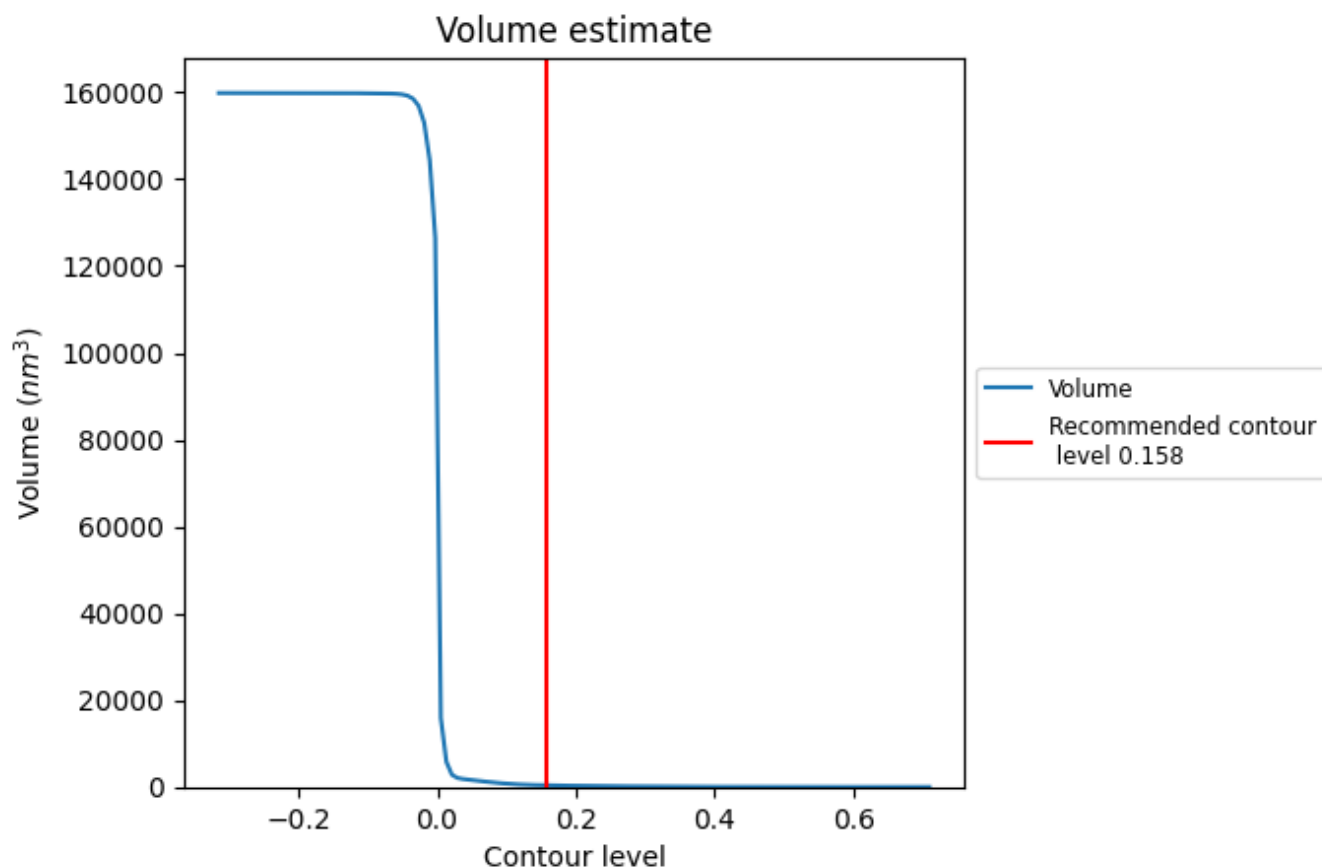
This section contains the results of statistical analysis of the map.

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.

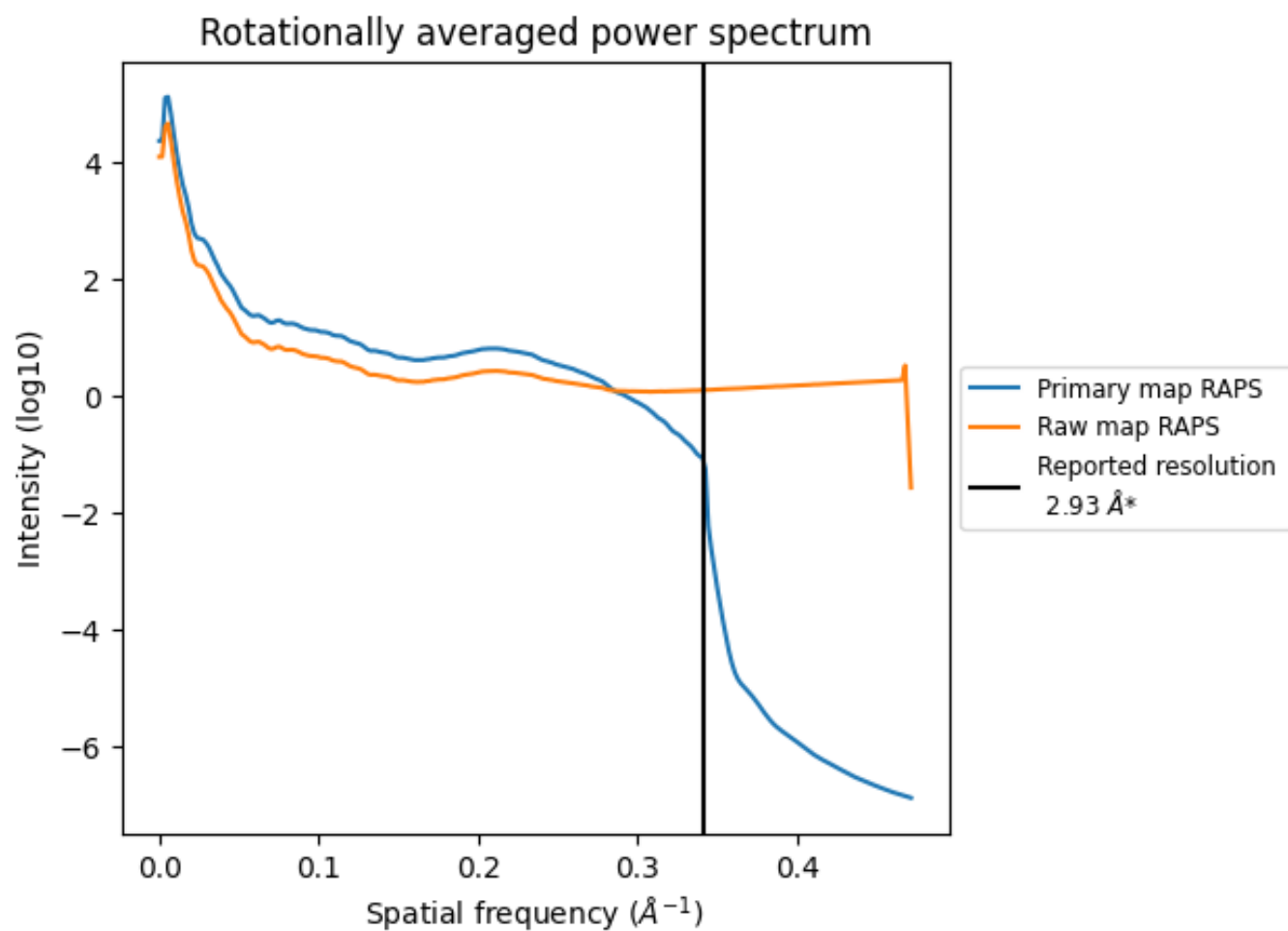
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 339 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 ⓘ

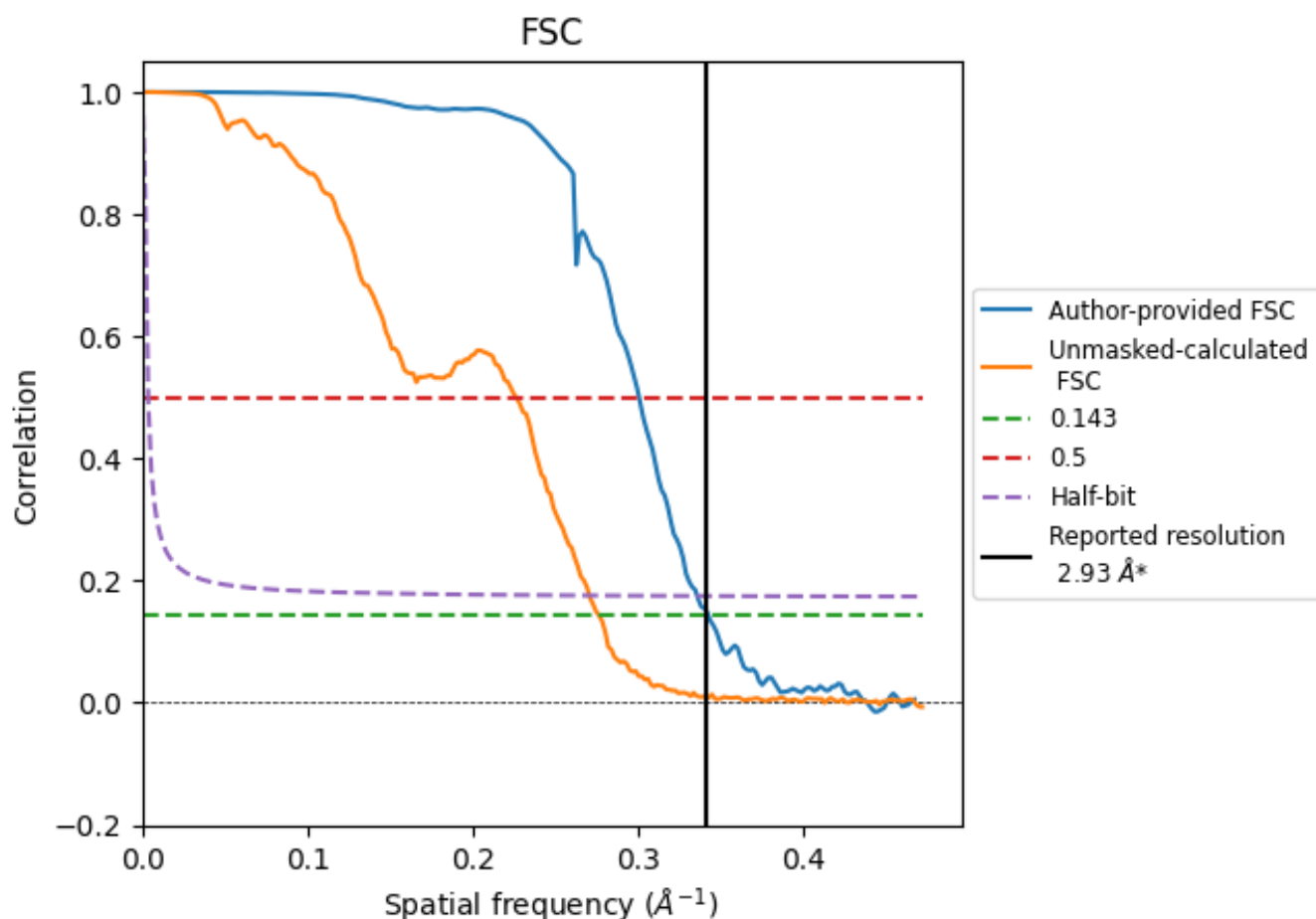


*Reported resolution corresponds to spatial frequency of $0.341 \text{ \AA}^{-1}$

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 $0.341 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

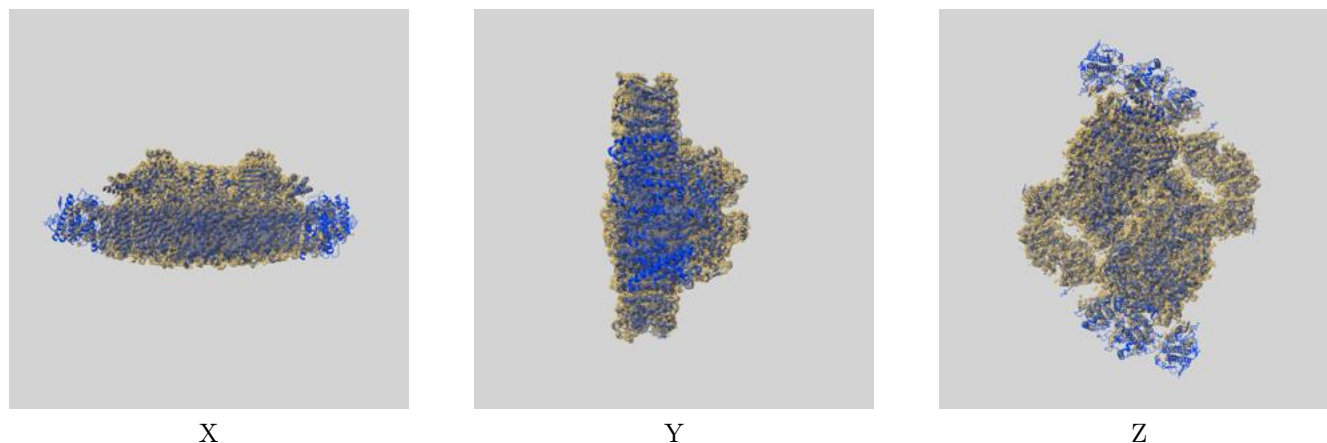
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.33	2.98
Unmasked-calculated*	3.62	4.42	3.70

*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 3.62 differs from the reported value 2.93 by more than 10 %

9 Map-model fit [i](#)

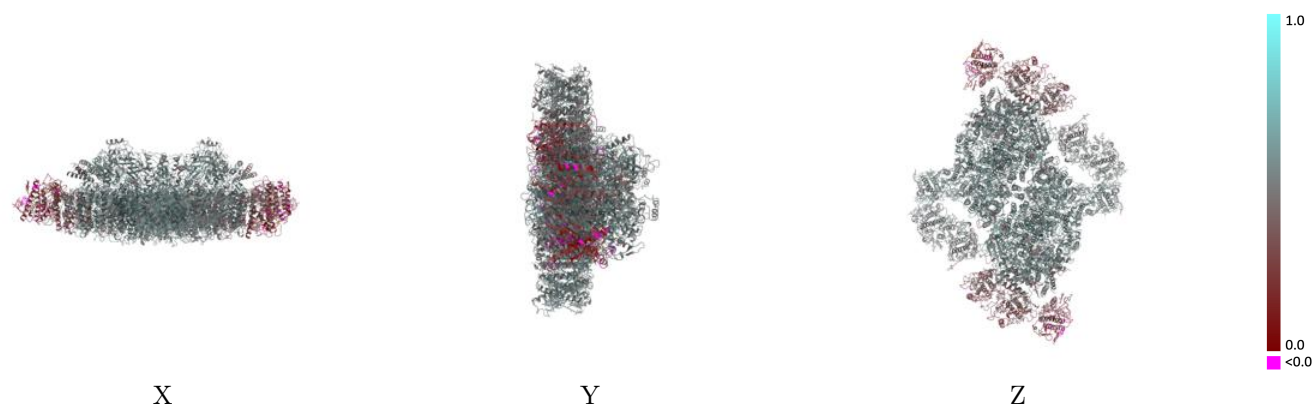
This section contains information regarding the fit between EMDB map EMD-35987 and PDB model 8J5K. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



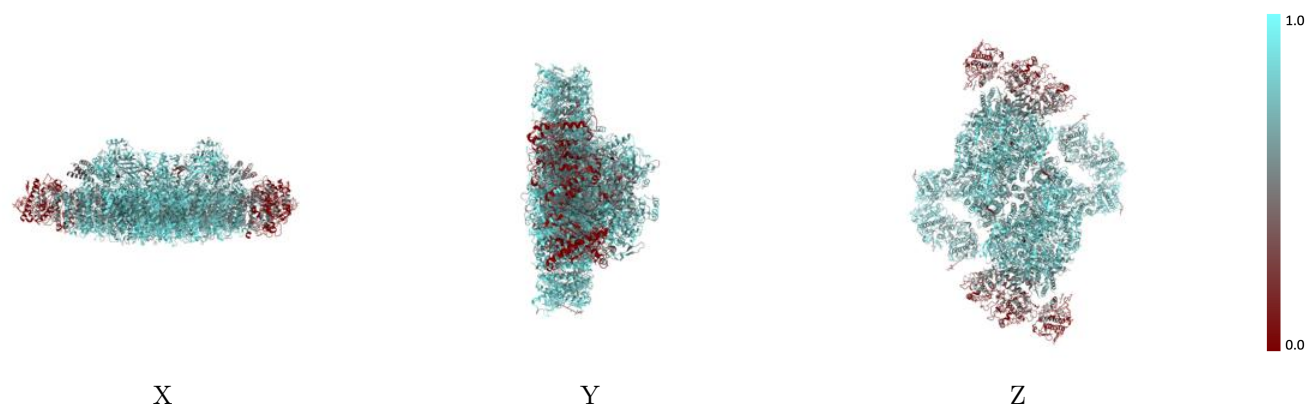
The images above show the 3D surface view of the map at the recommended contour level 0.158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



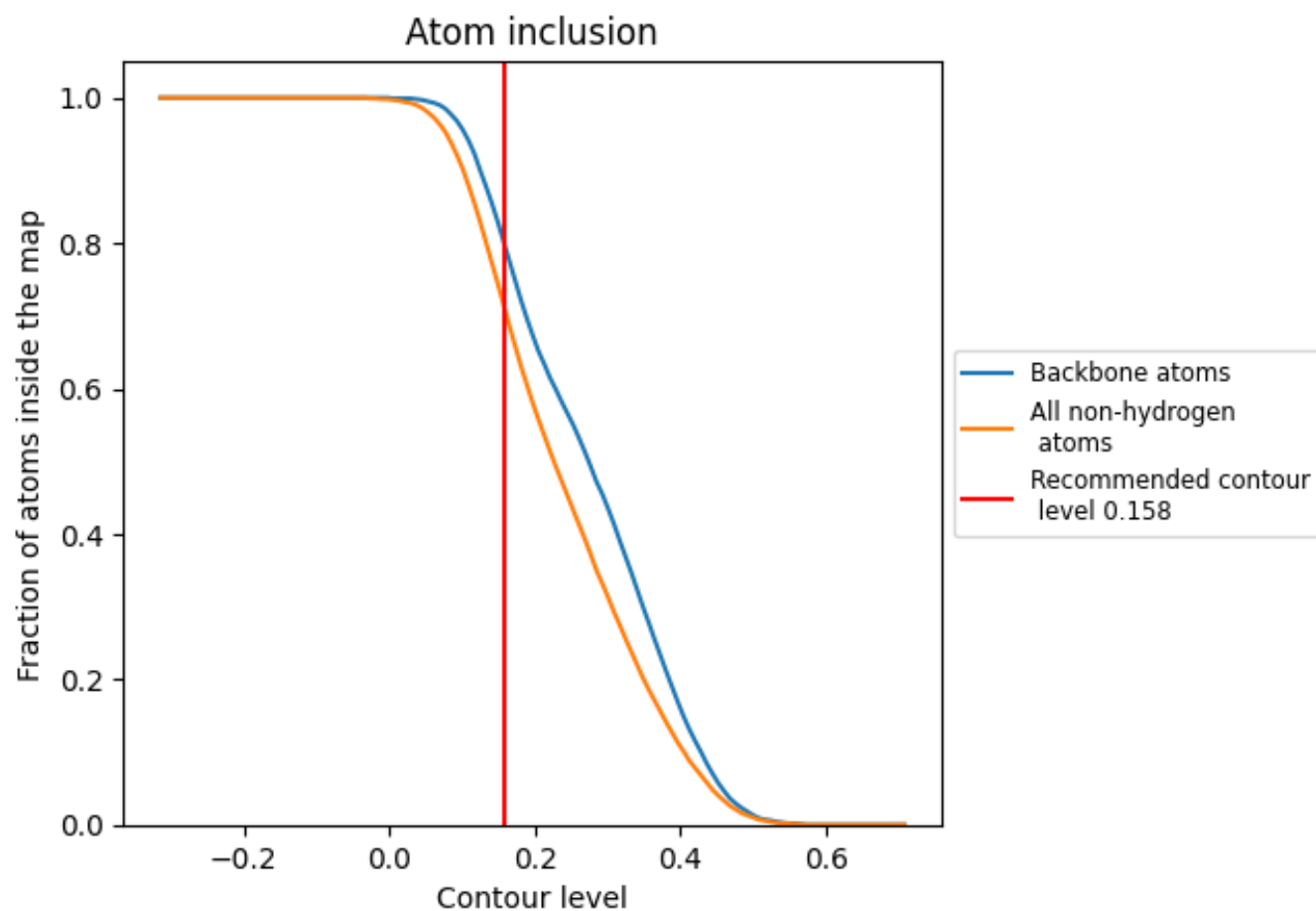
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.158).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.5040
0	 0.7910	 0.5330
1	 0.7530	 0.5000
2	 0.6890	 0.4730
3	 0.2070	 0.2790
4	 0.1270	 0.1640
5	 0.7910	 0.5340
6	 0.7530	 0.5000
7	 0.6880	 0.4740
8	 0.2140	 0.2820
9	 0.1320	 0.1850
A	 0.8080	 0.5670
B	 0.8430	 0.5670
C	 0.8320	 0.5600
D	 0.8480	 0.5720
E	 0.7890	 0.5110
F	 0.8080	 0.5150
H	 0.8140	 0.5580
I	 0.8520	 0.5500
J	 0.6470	 0.5260
K	 0.7820	 0.5170
L	 0.8580	 0.5820
M	 0.7210	 0.5590
N	 0.7000	 0.4400
O	 0.7150	 0.5260
P	 0.2690	 0.2840
Q	 0.5210	 0.4800
T	 0.7490	 0.5580
U	 0.7670	 0.5160
V	 0.7710	 0.5320
W	 0.7160	 0.4810
X	 0.7790	 0.5410
Y	 0.6610	 0.4860
Z	 0.7290	 0.4790
a	 0.8200	 0.5700



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.8480	 0.5690
c	 0.8310	 0.5600
d	 0.8460	 0.5730
e	 0.7840	 0.5110
f	 0.8080	 0.5160
h	 0.8090	 0.5590
i	 0.8440	 0.5450
j	 0.6400	 0.5240
k	 0.7820	 0.5120
l	 0.8510	 0.5740
m	 0.7260	 0.5600
n	 0.7130	 0.4310
o	 0.7190	 0.5250
p	 0.2710	 0.2870
q	 0.5150	 0.4750
t	 0.7530	 0.5600
u	 0.7590	 0.5170
v	 0.7800	 0.5300
w	 0.7180	 0.4830
x	 0.7880	 0.5390
y	 0.6580	 0.4930
z	 0.7310	 0.4820