



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 01:01 AM JST

PDB ID : 9LK5 / pdb_00009lk5
EMDB ID : EMD-63168
Title : The structure of Lhcb8-C2S2 PSII-LHCII supercomplex from *Arabidopsis thaliana*
Authors : Zhou, Q.; Caferri, R.; Shan, J.Y.; Amelii, A.; Bassi, R.; Liu, Z.F.
Deposited on : 2025-01-16
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

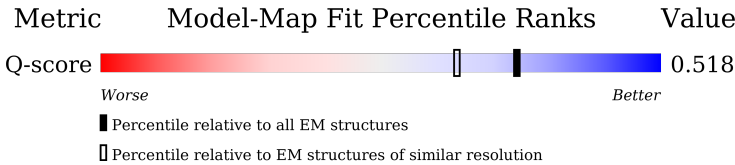
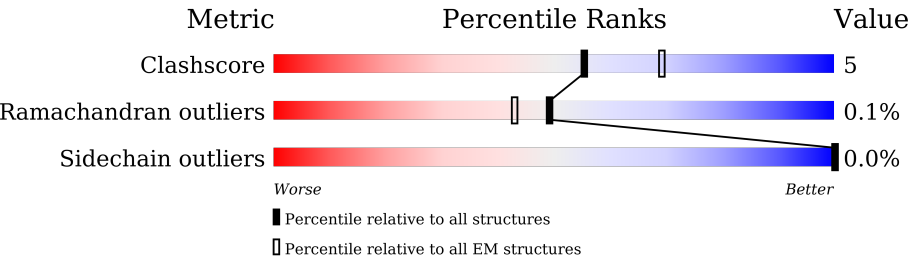
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



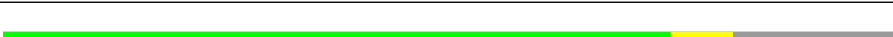
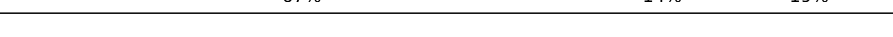
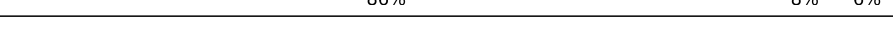
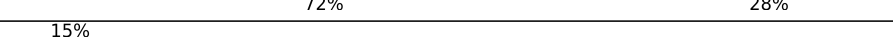
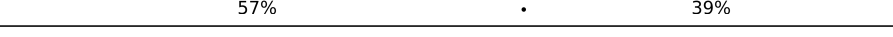
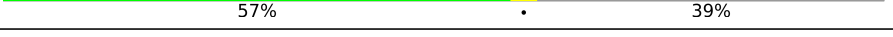
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	353	
1	a	353	
2	B	508	
2	b	508	

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Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	g	267	
7	n	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	61	
11	k	61	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	

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Mol	Chain	Length	Quality of chain
14	o	332	
15	S	280	
15	s	280	
16	T	33	
16	t	33	
17	U	103	
17	u	103	
18	W	133	
18	w	133	
19	X	116	
19	x	116	
20	Y	265	
20	y	265	
21	Z	62	
21	z	62	
22	R	286	
22	r	286	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	BCT	A	407	-	-	X	-
27	BCT	a	408	-	-	X	-
33	PL9	D	406	-	X	-	-
33	PL9	d	406	-	X	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 71232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		
1	a	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		
2	b	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		
3	c	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		
4	d	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	71	Total	C	N	O	0	0
			576	377	93	106		
5	e	71	Total	C	N	O	0	0
			576	377	93	106		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			235	156	41	37	1		
6	f	30	Total	C	N	O	S	0	0
			235	156	41	37	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
8	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			277	190	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	29	Total	C	N	O	0	0
			219	152	33	34		
10	j	29	Total	C	N	O	0	0
			219	152	33	34		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			301	211	44	45	1		
11	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			309	204	48	57		
12	l	37	Total	C	N	O	0	0
			309	204	48	57		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			250	172	36	42		
13	m	32	Total	C	N	O	0	0
			250	172	36	42		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		
14	o	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	23	Total	C	N	O	S	0	0
			179	114	31	31	3		
17	u	23	Total	C	N	O	S	0	0
			179	114	31	31	3		

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
18	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 19 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	38	Total	C	N	O	0	0
			267	176	42	49		
19	x	38	Total	C	N	O	0	0
			267	176	42	49		

- Molecule 20 is a protein called Chlorophyll a-b binding protein 2.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		
20	y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
21	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		
22	R	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	277	GLY	-	expression tag	UNP Q9S7W1
r	278	GLY	-	expression tag	UNP Q9S7W1
r	279	GLY	-	expression tag	UNP Q9S7W1
r	280	GLY	-	expression tag	UNP Q9S7W1
r	281	HIS	-	expression tag	UNP Q9S7W1
r	282	HIS	-	expression tag	UNP Q9S7W1
r	283	HIS	-	expression tag	UNP Q9S7W1
r	284	HIS	-	expression tag	UNP Q9S7W1
r	285	HIS	-	expression tag	UNP Q9S7W1
r	286	HIS	-	expression tag	UNP Q9S7W1
R	277	GLY	-	expression tag	UNP Q9S7W1
R	278	GLY	-	expression tag	UNP Q9S7W1
R	279	GLY	-	expression tag	UNP Q9S7W1
R	280	GLY	-	expression tag	UNP Q9S7W1
R	281	HIS	-	expression tag	UNP Q9S7W1
R	282	HIS	-	expression tag	UNP Q9S7W1
R	283	HIS	-	expression tag	UNP Q9S7W1
R	284	HIS	-	expression tag	UNP Q9S7W1
R	285	HIS	-	expression tag	UNP Q9S7W1
R	286	HIS	-	expression tag	UNP Q9S7W1

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	C	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	N	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	Y	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	c	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	g	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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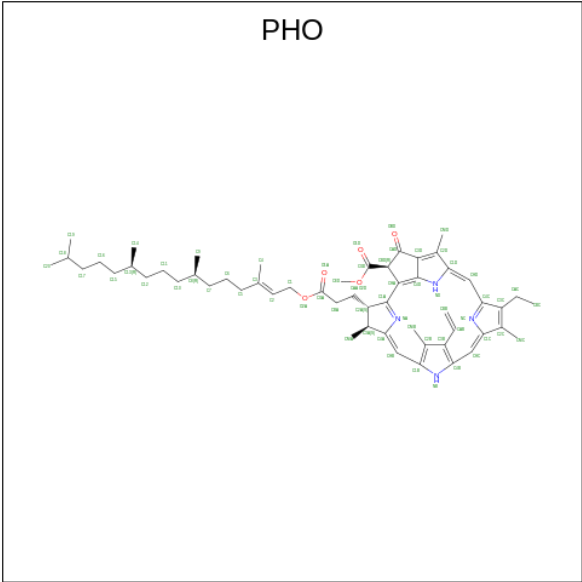
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	s	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	s	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	s	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	n	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	y	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 50	C 40	Mg 1	N 4	O 5	0

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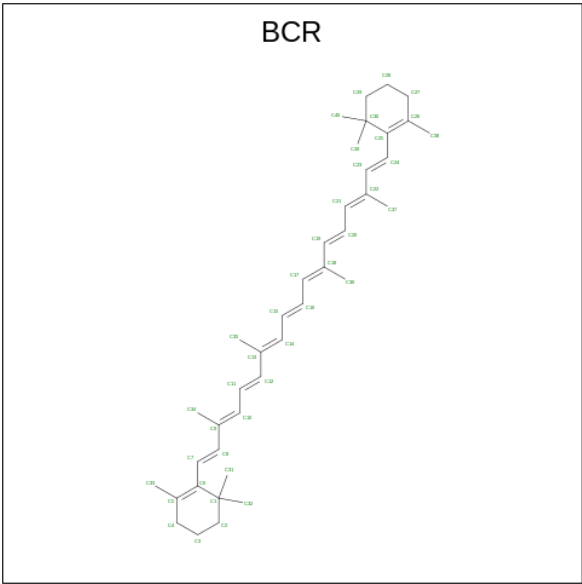
Mol	Chain	Residues	Atoms					AltConf
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



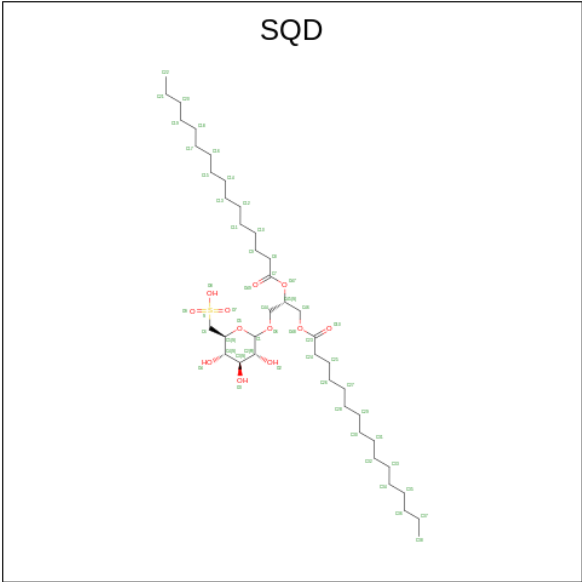
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



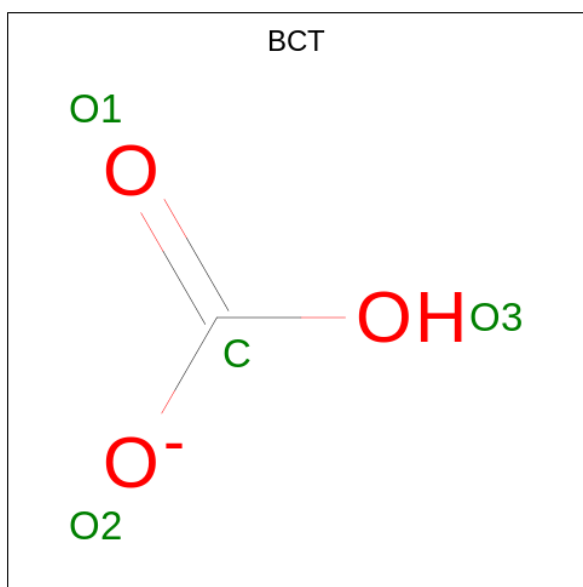
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



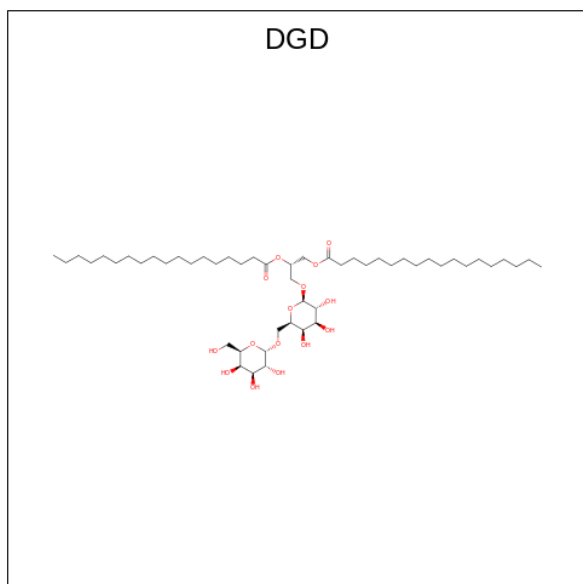
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	C	1	Total	C	O	S	0
			45	32	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			50	37	12	1	
26	b	1	Total	C	O	S	0
			54	41	12	1	
26	c	1	Total	C	O	S	0
			45	32	12	1	
26	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			59	44	15	

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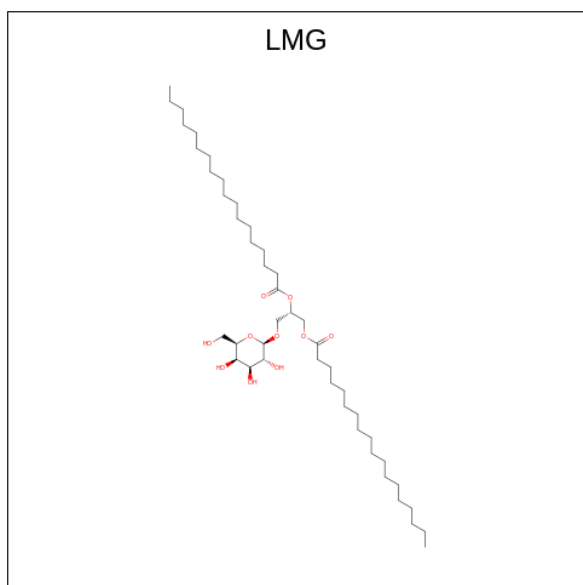
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Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			59	44	15	
28	B	1	Total	C	O	0
			56	41	15	
28	C	1	Total	C	O	0
			55	40	15	
28	D	1	Total	C	O	0
			62	47	15	
28	b	1	Total	C	O	0
			56	41	15	
28	c	1	Total	C	O	0
			55	40	15	
28	d	1	Total	C	O	0
			62	47	15	

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	B	1	Total	C	O	0
			40	30	10	
30	C	1	Total	C	O	0
			48	38	10	
30	C	1	Total	C	O	0
			50	40	10	
30	D	1	Total	C	O	0
			46	36	10	
30	S	1	Total	C	O	0
			55	45	10	
30	W	1	Total	C	O	0
			51	41	10	
30	a	1	Total	C	O	0
			48	38	10	
30	b	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			50	40	10	
30	d	1	Total	C	O	0
			46	36	10	
30	s	1	Total	C	O	0
			55	45	10	
30	w	1	Total	C	O	0
			51	41	10	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

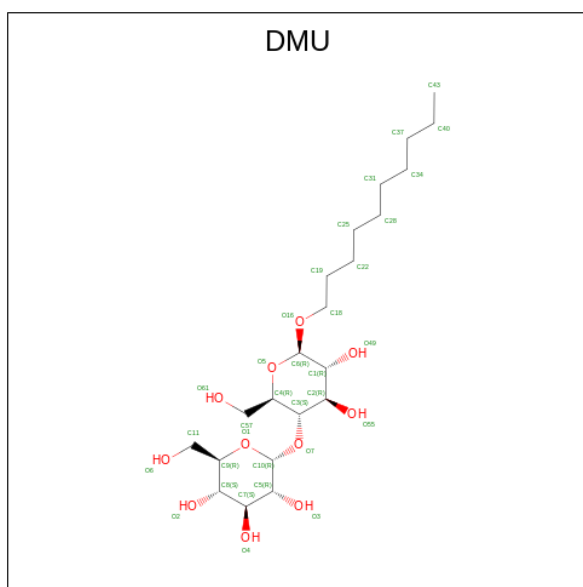


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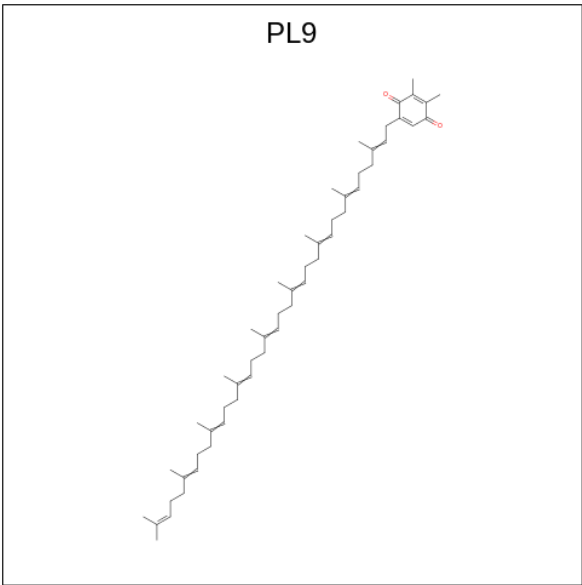
Mol	Chain	Residues	Atoms				AltConf
31	b	1	Total	C	O	P	0
			46	35	10	1	
31	b	1	Total	C	O	P	0
			40	29	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	g	1	Total	C	O	P	0
			46	35	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	r	1	Total	C	O	P	0
			42	31	10	1	
31	s	1	Total	C	O	P	0
			49	38	10	1	
31	n	1	Total	C	O	P	0
			49	38	10	1	
31	y	1	Total	C	O	P	0
			49	38	10	1	
31	R	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 32 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



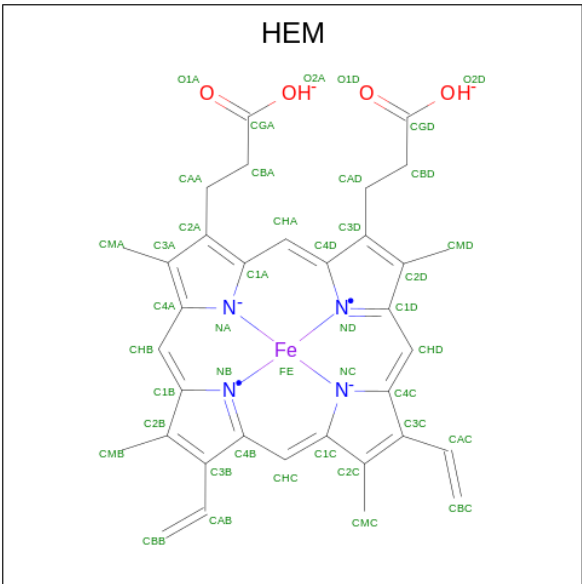
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			33	22	11	
32	C	1	Total	C	O	0
			33	22	11	
32	S	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	s	1	Total	C	O	0
			33	22	11	

- Molecule 33 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).



Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			55	53	2	
33	d	1	Total	C	O	0
			55	53	2	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



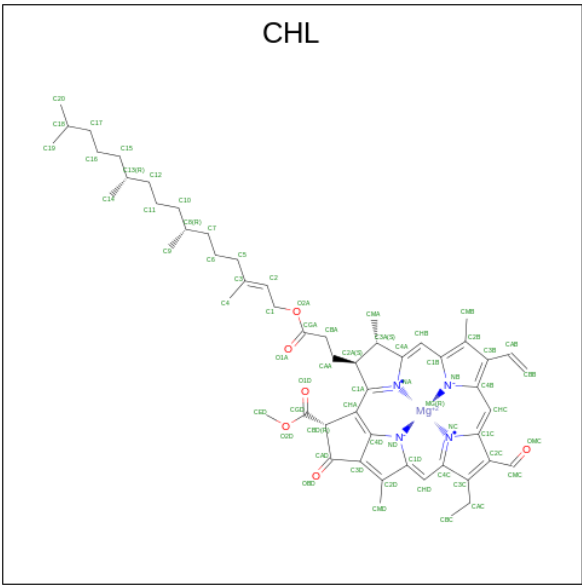
Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 35 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
35	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
35	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	N	1	Total 46	C 35	Mg 1	N 4	O 6	0

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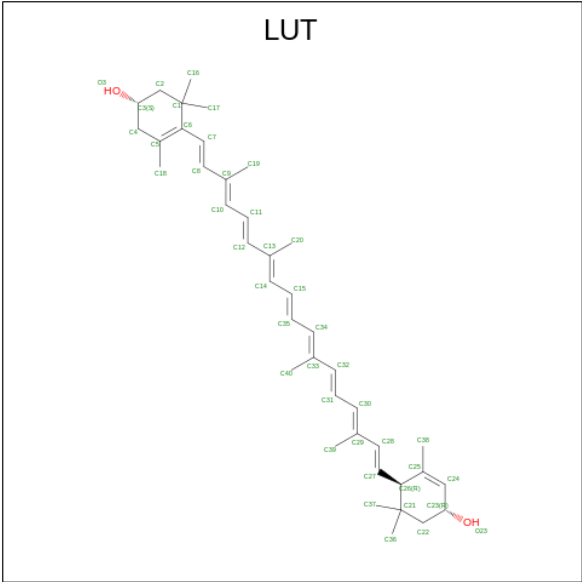
Mol	Chain	Residues	Atoms					AltConf
35	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
35	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
35	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	r	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
35	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
35	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
35	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
35	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	y	1	Total 51	C 40	Mg 1	N 4	O 6	0
35	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
35	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
35	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
35	R	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



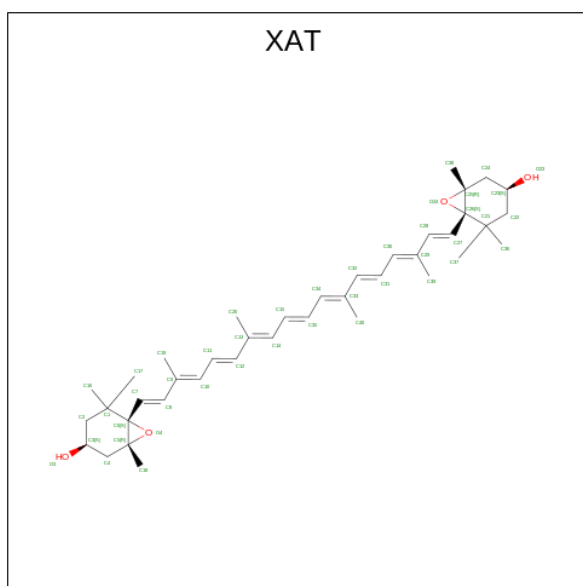
Mol	Chain	Residues	Atoms			AltConf
36	G	1	Total	C	O	0
			42	40	2	
36	G	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	r	1	Total	C	O	0
			42	40	2	
36	s	1	Total	C	O	0
			42	40	2	
36	s	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
36	n	1	Total	C	O	0
			42	40	2	
36	y	1	Total	C	O	0
			42	40	2	
36	y	1	Total	C	O	0
			42	40	2	
36	R	1	Total	C	O	0
			42	40	2	

- Molecule 37 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



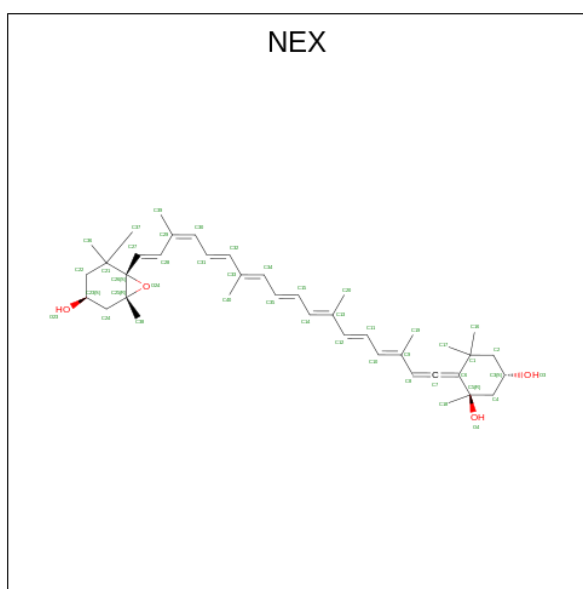
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	40	4	
37	G	1	Total	C	O	0
			44	40	4	
37	Y	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
37	y	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	

- Molecule 38 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



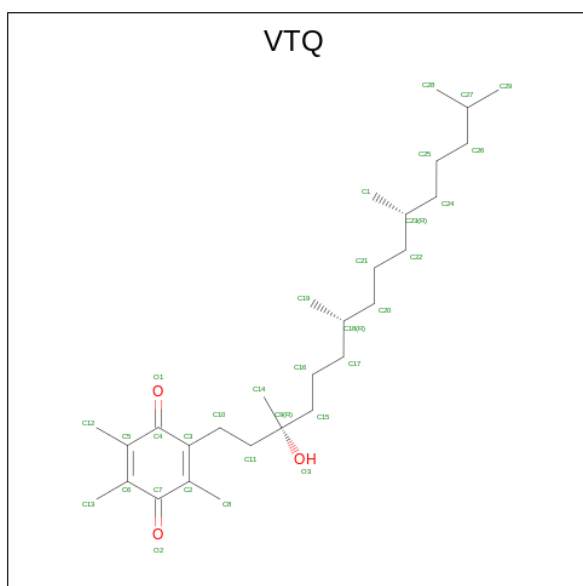
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			44	40	4	
38	N	1	Total	C	O	0
			44	40	4	
38	S	1	Total	C	O	0
			44	40	4	
38	Y	1	Total	C	O	0
			44	40	4	
38	g	1	Total	C	O	0
			44	40	4	
38	r	1	Total	C	O	0
			44	40	4	
38	s	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
38	n	1	Total	C	O	0
			44	40	4	
38	R	1	Total	C	O	0
			44	40	4	
38	R	1	Total	C	O	0
			44	40	4	

- Molecule 39 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula: $C_{29}H_{50}O_3$).

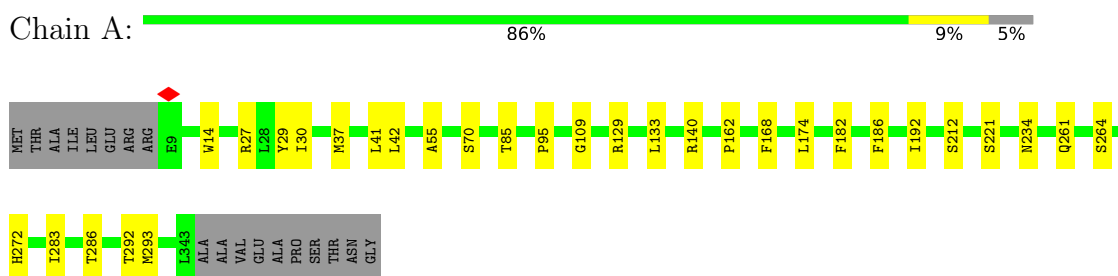


Mol	Chain	Residues	Atoms			AltConf
39	W	1	Total	C	O	0
			32	29	3	
39	w	1	Total	C	O	0
			32	29	3	

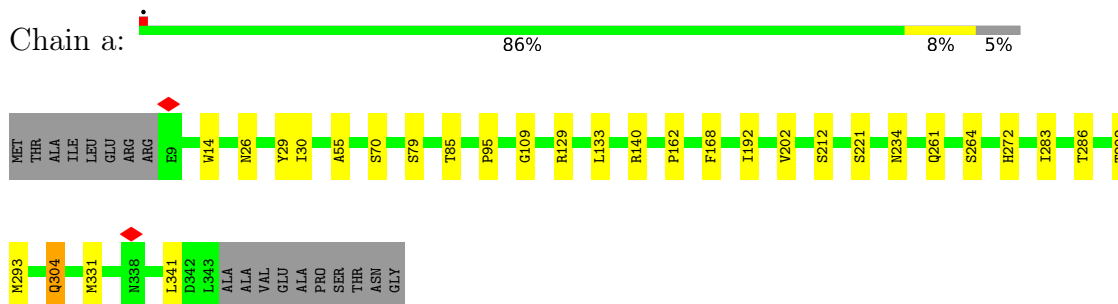
3 Residue-property plots [i](#)

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.

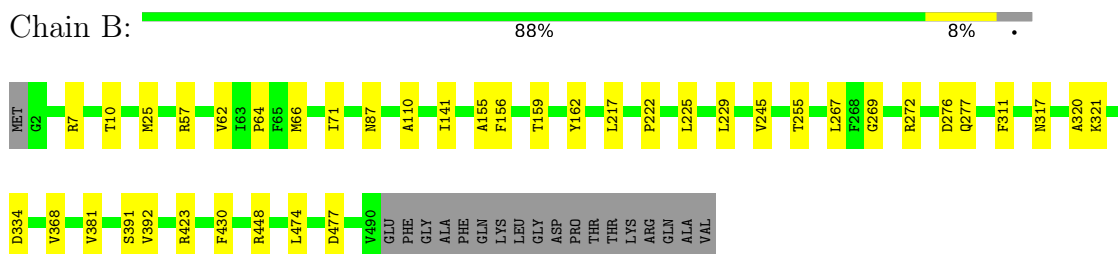
- Molecule 1: Photosystem II protein D1



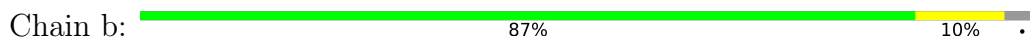
- Molecule 1: Photosystem II protein D1

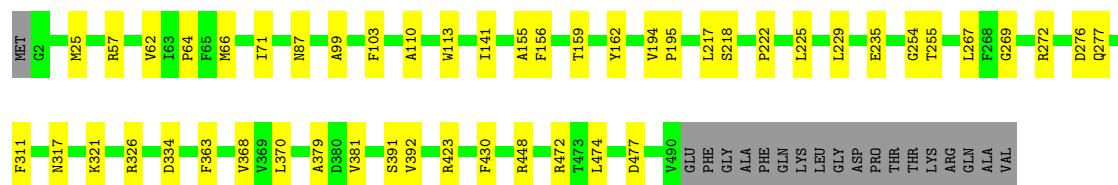


- Molecule 2: Photosystem II CP47 reaction center protein



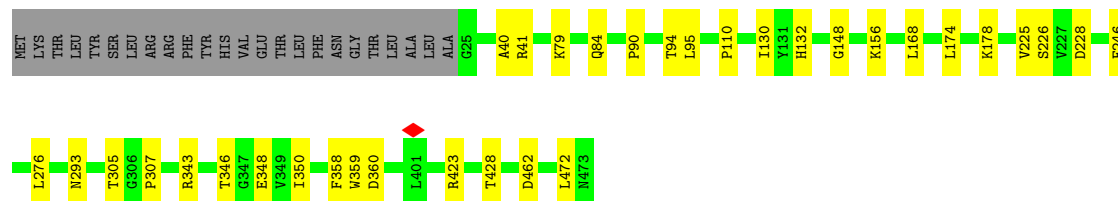
- Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 7% 5%



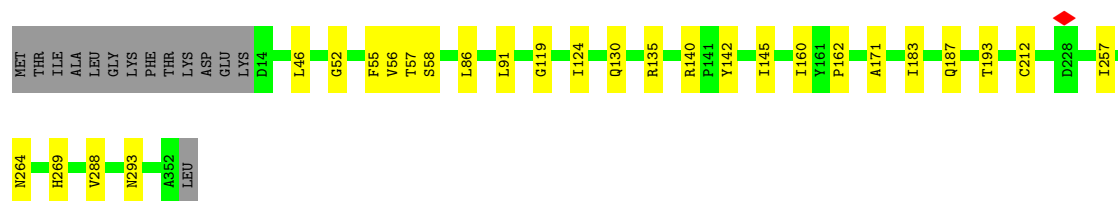
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 88% 7% 5%



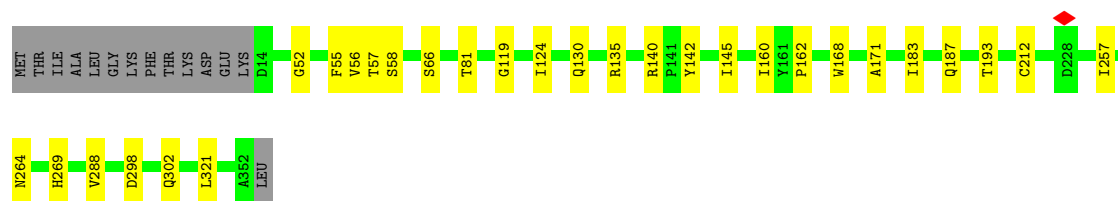
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .

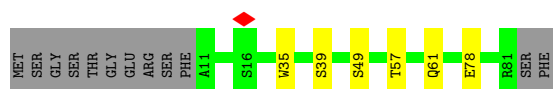
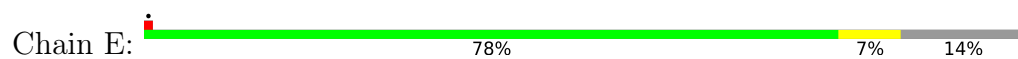


• Molecule 4: Photosystem II D2 protein

Chain d: 88% 8% .



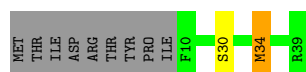
• Molecule 5: Cytochrome b559 subunit alpha



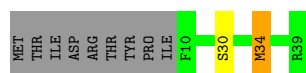
- Molecule 5: Cytochrome b559 subunit alpha



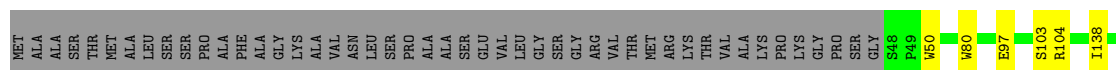
- Molecule 6: Cytochrome b559 subunit beta



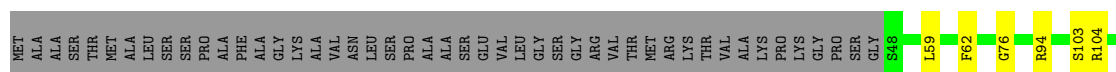
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

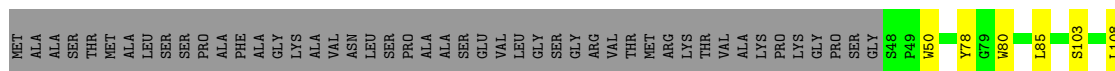


- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

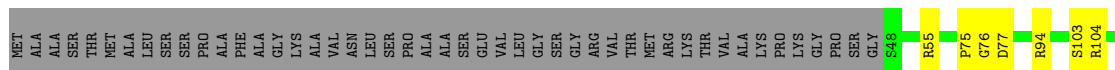


- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

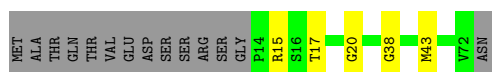




- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic



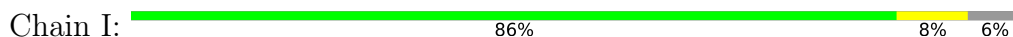
- Molecule 8: Photosystem II reaction center protein H



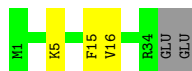
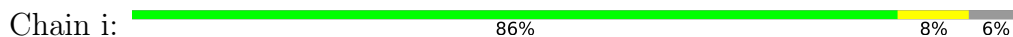
- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I

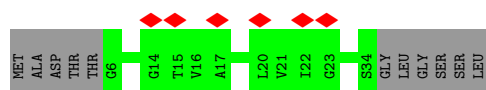


- Molecule 9: Photosystem II reaction center protein I

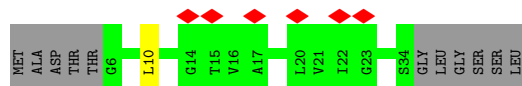


- Molecule 10: Photosystem II reaction center protein J

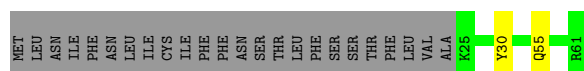




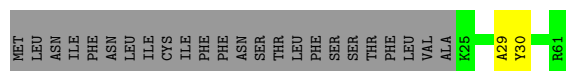
- Molecule 10: Photosystem II reaction center protein J



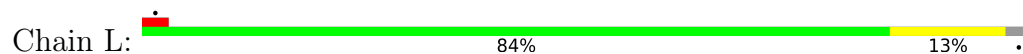
- Molecule 11: Photosystem II reaction center protein K



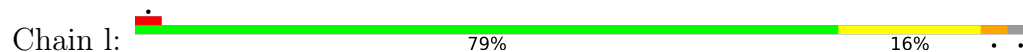
- Molecule 11: Photosystem II reaction center protein K



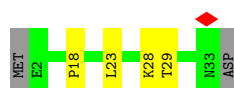
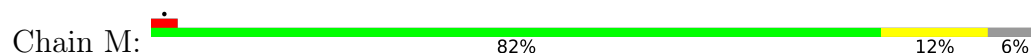
- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein M



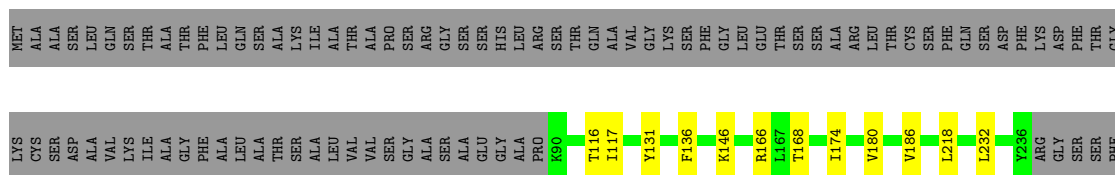
- Molecule 13: Photosystem II reaction center protein M

Chain m:  82% 12% 6%



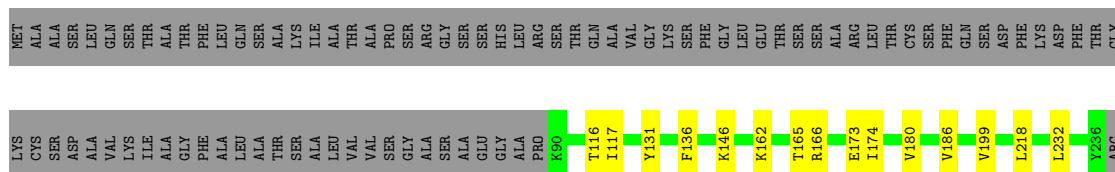
- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:  53% 6% 40%



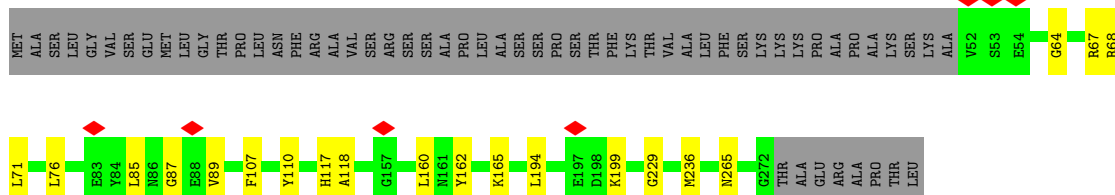
- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain o:  52% 7% 40%



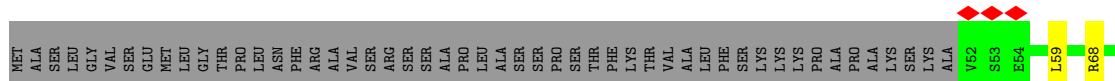
- Molecule 15: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:  72% 7% 21%



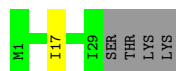
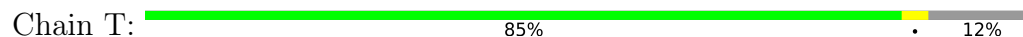
- Molecule 15: Chlorophyll a-b binding protein CP26, chloroplastic

Chain s:  71% 8% 21%

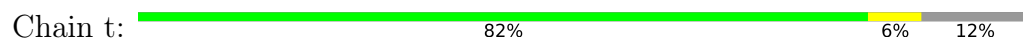




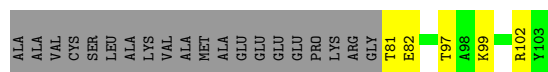
- Molecule 16: Photosystem II reaction center protein T



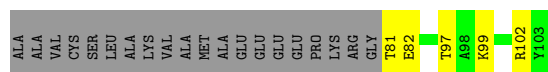
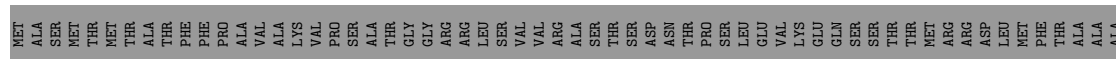
- Molecule 16: Photosystem II reaction center protein T



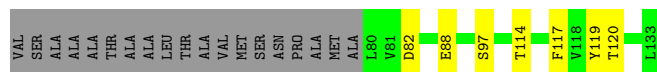
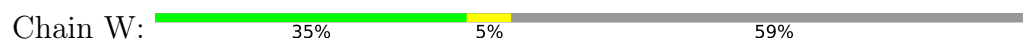
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic



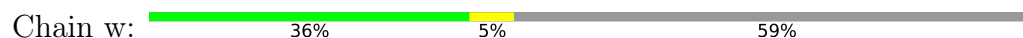
- Molecule 17: Photosystem II 5 kDa protein, chloroplastic

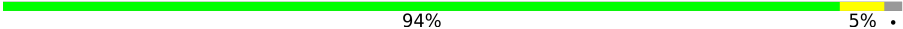


- Molecule 18: Photosystem II reaction center W protein, chloroplastic



- Molecule 18: Photosystem II reaction center W protein, chloroplastic



Chain Z:  94% 5% .



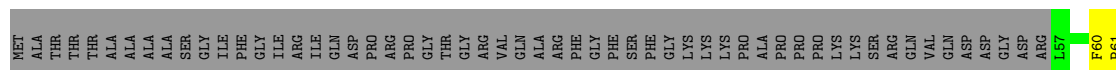
- Molecule 21: Photosystem II reaction center protein Z

Chain z:  92% 6% .



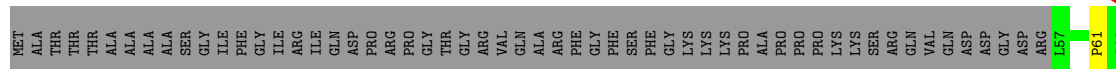
- Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain r:  72% 5% 23%



- Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain R:  71% 6% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.356	Depositor
Minimum map value	-16.319	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, PHO, PL9, LUT, LMG, SQD, CLA, LHG, DMU, BCT, BCR, HEM, FE2, NEX, VTQ, CHL, XAT

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	0.25	0/2704	0.54	0/3687
1	a	0.27	0/2704	0.56	1/3687 (0.0%)
2	B	0.22	0/3959	0.44	0/5394
2	b	0.22	0/3959	0.46	0/5394
3	C	0.23	0/3595	0.49	0/4899
3	c	0.23	0/3595	0.49	0/4899
4	D	0.24	0/2789	0.51	0/3803
4	d	0.24	0/2789	0.49	0/3803
5	E	0.30	0/593	0.79	1/808 (0.1%)
5	e	0.30	0/593	0.84	4/808 (0.5%)
6	F	0.31	0/241	0.78	2/327 (0.6%)
6	f	0.32	0/241	0.81	1/327 (0.3%)
7	G	0.23	0/1716	0.47	1/2336 (0.0%)
7	N	0.23	0/1716	0.47	0/2336
7	g	0.25	0/1716	0.55	1/2336 (0.0%)
7	n	0.22	0/1716	0.44	0/2336
8	H	0.29	0/447	0.52	0/608
8	h	0.30	0/447	0.58	0/608
9	I	0.28	0/285	0.58	0/385
9	i	0.28	0/285	0.56	0/385
10	J	0.23	0/225	0.43	0/306
10	j	0.23	0/225	0.42	0/306
11	K	0.47	0/312	0.86	0/428
11	k	0.44	0/312	0.89	0/428
12	L	0.23	0/317	0.52	0/431
12	l	0.29	0/317	0.62	0/431
13	M	0.41	0/254	0.69	0/348
13	m	0.35	0/254	0.71	0/348
14	O	0.23	0/1556	0.62	4/2104 (0.2%)
14	o	0.26	0/1556	0.66	4/2104 (0.2%)
15	S	0.26	0/1750	0.57	0/2376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	s	0.25	0/1750	0.54	0/2376
16	T	0.23	0/246	0.53	0/333
16	t	0.29	0/246	0.65	0/333
17	U	0.13	0/181	0.39	0/242
17	u	0.12	0/181	0.40	0/242
18	W	0.24	0/438	0.54	0/594
18	w	0.22	0/438	0.47	0/594
19	X	0.25	0/270	0.48	0/367
19	x	0.25	0/270	0.49	0/367
20	Y	0.23	0/1753	0.51	0/2385
20	y	0.23	0/1753	0.51	0/2385
21	Z	0.30	0/468	0.64	0/641
21	z	0.33	0/468	0.71	0/641
22	R	0.25	0/1766	0.58	0/2403
22	r	0.23	0/1766	0.52	0/2403
All	All	0.25	0/55162	0.54	19/75082 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	34	MET	CB-CG-SD	-6.43	93.41	112.70
14	O	311	THR	CA-C-N	6.36	133.69	121.54
14	O	311	THR	C-N-CA	6.36	133.69	121.54
14	o	311	THR	CA-C-N	6.21	133.40	121.54
14	o	311	THR	C-N-CA	6.21	133.40	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	413	GLU	Peptide

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	2623	0	2527	22	0
1	a	2623	0	2527	24	0
2	B	3829	0	3707	30	0
2	b	3829	0	3707	36	0
3	C	3480	0	3409	27	0
3	c	3480	0	3409	28	0
4	D	2696	0	2585	22	0
4	d	2696	0	2585	25	0
5	E	576	0	559	3	0
5	e	576	0	559	4	0
6	F	235	0	242	1	0
6	f	235	0	242	1	0
7	G	1666	0	1593	12	0
7	N	1666	0	1593	19	0
7	g	1666	0	1593	12	0
7	n	1666	0	1593	18	0
8	H	438	0	465	4	0
8	h	438	0	465	8	0
9	I	277	0	289	3	0
9	i	277	0	289	3	0
10	J	219	0	231	0	0
10	j	219	0	231	1	0
11	K	301	0	313	2	0
11	k	301	0	313	2	0
12	L	309	0	298	5	0
12	l	309	0	298	6	0
13	M	250	0	273	5	0
13	m	250	0	273	4	0
14	O	1523	0	1504	11	0
14	o	1523	0	1504	12	0
15	S	1705	0	1681	14	0
15	s	1705	0	1681	15	0
16	T	239	0	255	1	0
16	t	239	0	255	2	0
17	U	179	0	190	3	0
17	u	179	0	190	3	0
18	W	427	0	405	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	w	427	0	405	5	0
19	X	267	0	292	0	0
19	x	267	0	292	1	0
20	Y	1699	0	1630	17	0
20	y	1699	0	1630	17	0
21	Z	458	0	490	2	0
21	z	458	0	490	4	0
22	R	1718	0	1691	13	0
22	r	1718	0	1691	11	0
23	A	175	0	170	6	0
23	B	1040	0	1152	23	0
23	C	810	0	854	21	0
23	D	195	0	216	9	0
23	G	448	0	429	9	0
23	N	435	0	396	7	0
23	R	511	0	493	11	0
23	S	415	0	313	8	0
23	Y	466	0	454	15	0
23	a	125	0	131	5	0
23	b	1040	0	1152	22	0
23	c	810	0	854	16	0
23	d	245	0	255	8	0
23	g	448	0	429	9	0
23	n	435	0	396	8	0
23	r	511	0	493	8	0
23	s	415	0	313	6	0
23	y	466	0	454	12	0
24	A	64	0	74	3	0
24	D	64	0	74	5	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	120	0	168	10	0
25	D	40	0	56	1	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	a	40	0	56	4	0
25	b	120	0	168	11	0
25	c	80	0	112	6	0
25	d	40	0	56	1	0
25	h	40	0	56	2	0
25	k	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	z	40	0	56	2	0
26	A	50	0	67	0	0
26	B	54	0	78	3	0
26	C	45	0	54	2	0
26	L	54	0	78	1	0
26	a	50	0	67	2	0
26	b	54	0	78	3	0
26	c	45	0	54	1	0
26	l	54	0	78	4	0
27	A	4	0	0	2	0
27	a	4	0	0	2	0
28	A	59	0	76	1	0
28	B	115	0	146	4	0
28	C	55	0	68	2	0
28	D	62	0	82	3	0
28	b	56	0	70	0	0
28	c	55	0	68	2	0
28	d	62	0	82	5	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	91	0	122	6	0
30	C	98	0	139	2	0
30	D	46	0	62	1	0
30	S	55	0	86	0	0
30	W	51	0	75	0	0
30	a	48	0	66	0	0
30	b	91	0	122	6	0
30	c	50	0	73	0	0
30	d	46	0	62	0	0
30	s	55	0	86	0	0
30	w	51	0	75	0	0
31	B	135	0	192	3	0
31	C	49	0	74	2	0
31	D	98	0	148	4	0
31	G	46	0	65	2	0
31	L	98	0	148	4	0
31	N	49	0	74	2	0
31	R	42	0	57	1	0
31	S	49	0	74	3	0
31	W	49	0	74	1	0
31	Y	49	0	74	3	0
31	b	135	0	192	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	98	0	148	2	0
31	d	98	0	148	7	0
31	g	46	0	65	4	0
31	l	98	0	148	3	0
31	n	49	0	74	1	0
31	r	42	0	57	1	0
31	s	49	0	74	2	0
31	y	49	0	74	3	0
32	C	66	0	84	2	0
32	S	33	0	42	1	0
32	c	66	0	84	2	0
32	s	33	0	42	1	0
33	D	55	0	80	2	0
33	d	55	0	80	0	0
34	F	43	0	30	1	0
34	f	43	0	30	1	0
35	G	325	0	286	7	0
35	N	338	0	305	9	0
35	R	153	0	119	2	0
35	S	184	0	125	5	0
35	Y	365	0	354	13	0
35	g	325	0	286	8	0
35	n	338	0	305	11	0
35	r	153	0	119	2	0
35	s	184	0	125	3	0
35	y	365	0	354	15	0
36	G	84	0	112	6	0
36	N	84	0	112	9	0
36	R	42	0	56	4	0
36	S	84	0	112	6	0
36	Y	84	0	112	7	0
36	g	84	0	112	5	0
36	n	84	0	112	7	0
36	r	42	0	56	3	0
36	s	84	0	112	4	0
36	y	84	0	112	7	0
37	G	88	0	112	4	0
37	R	44	0	56	1	0
37	Y	44	0	56	5	0
37	g	88	0	112	6	0
37	r	44	0	56	2	0
37	y	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	44	0	56	1	0
38	N	44	0	56	3	0
38	R	88	0	112	6	0
38	S	44	0	56	1	0
38	Y	44	0	56	1	0
38	g	44	0	56	1	0
38	n	44	0	56	1	0
38	r	44	0	56	1	0
38	s	44	0	56	1	0
39	W	32	0	50	0	0
39	w	32	0	50	0	0
All	All	71232	0	71854	714	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 5.

The worst 5 of 714 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)
23:Y:311:CLA:HAB	36:Y:316:LUT:H32	1.62	0.80
3:c:276:LEU:HD21	23:c:508:CLA:HAB	1.69	0.75
23:s:609:CLA:HAB	36:s:614:LUT:H32	1.70	0.74
3:C:276:LEU:HD21	23:C:509:CLA:HAB	1.69	0.74
23:n:602:CLA:HAB	36:n:616:LUT:H32	1.68	0.74

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	333/353 (94%)	314 (94%)	19 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	333/353 (94%)	315 (95%)	18 (5%)	0	100	100
2	B	487/508 (96%)	467 (96%)	20 (4%)	0	100	100
2	b	487/508 (96%)	469 (96%)	18 (4%)	0	100	100
3	C	447/473 (94%)	432 (97%)	15 (3%)	0	100	100
3	c	447/473 (94%)	434 (97%)	13 (3%)	0	100	100
4	D	337/353 (96%)	327 (97%)	10 (3%)	0	100	100
4	d	337/353 (96%)	329 (98%)	8 (2%)	0	100	100
5	E	69/83 (83%)	65 (94%)	4 (6%)	0	100	100
5	e	69/83 (83%)	63 (91%)	6 (9%)	0	100	100
6	F	28/39 (72%)	26 (93%)	2 (7%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	0	100	100
7	G	217/267 (81%)	206 (95%)	10 (5%)	1 (0%)	24	60
7	N	217/267 (81%)	207 (95%)	10 (5%)	0	100	100
7	g	217/267 (81%)	208 (96%)	8 (4%)	1 (0%)	24	60
7	n	217/267 (81%)	204 (94%)	13 (6%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	32/36 (89%)	32 (100%)	0	0	100	100
9	i	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
10	J	27/40 (68%)	27 (100%)	0	0	100	100
10	j	27/40 (68%)	27 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
13	m	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
14	O	194/332 (58%)	180 (93%)	14 (7%)	0	100	100
14	o	194/332 (58%)	176 (91%)	17 (9%)	1 (0%)	24	60
15	S	219/280 (78%)	200 (91%)	19 (9%)	0	100	100
15	s	219/280 (78%)	206 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	T	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
16	t	27/33 (82%)	27 (100%)	0	0	100	100
17	U	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
17	u	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
18	W	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
18	w	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
19	X	36/116 (31%)	36 (100%)	0	0	100	100
19	x	36/116 (31%)	36 (100%)	0	0	100	100
20	Y	218/265 (82%)	211 (97%)	6 (3%)	1 (0%)	24	60
20	y	218/265 (82%)	209 (96%)	8 (4%)	1 (0%)	24	60
21	Z	59/62 (95%)	59 (100%)	0	0	100	100
21	z	59/62 (95%)	59 (100%)	0	0	100	100
22	R	218/286 (76%)	210 (96%)	8 (4%)	0	100	100
22	r	218/286 (76%)	209 (96%)	9 (4%)	0	100	100
All	All	6790/8470 (80%)	6501 (96%)	284 (4%)	5 (0%)	49	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	o	312	ASP
20	y	152	ILE
20	Y	152	ILE
7	g	153	VAL
7	G	153	VAL

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	272/285 (95%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	272/285 (95%)	272 (100%)	0	100	100
2	B	387/402 (96%)	387 (100%)	0	100	100
2	b	387/402 (96%)	387 (100%)	0	100	100
3	C	352/373 (94%)	352 (100%)	0	100	100
3	c	352/373 (94%)	352 (100%)	0	100	100
4	D	271/283 (96%)	271 (100%)	0	100	100
4	d	271/283 (96%)	271 (100%)	0	100	100
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	167/201 (83%)	167 (100%)	0	100	100
7	N	167/201 (83%)	167 (100%)	0	100	100
7	g	167/201 (83%)	167 (100%)	0	100	100
7	n	167/201 (83%)	167 (100%)	0	100	100
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	31/33 (94%)	31 (100%)	0	100	100
9	i	31/33 (94%)	31 (100%)	0	100	100
10	J	22/30 (73%)	22 (100%)	0	100	100
10	j	22/30 (73%)	22 (100%)	0	100	100
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	34 (97%)	1 (3%)	37	70
13	M	28/30 (93%)	28 (100%)	0	100	100
13	m	28/30 (93%)	28 (100%)	0	100	100
14	O	170/268 (63%)	170 (100%)	0	100	100
14	o	170/268 (63%)	170 (100%)	0	100	100
15	S	172/219 (78%)	172 (100%)	0	100	100
15	s	172/219 (78%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	U	19/82 (23%)	19 (100%)	0	100	100
17	u	19/82 (23%)	19 (100%)	0	100	100
18	W	47/102 (46%)	47 (100%)	0	100	100
18	w	47/102 (46%)	47 (100%)	0	100	100
19	X	32/92 (35%)	32 (100%)	0	100	100
19	x	32/92 (35%)	32 (100%)	0	100	100
20	Y	173/209 (83%)	173 (100%)	0	100	100
20	y	173/209 (83%)	173 (100%)	0	100	100
21	Z	53/54 (98%)	53 (100%)	0	100	100
21	z	53/54 (98%)	53 (100%)	0	100	100
22	R	178/226 (79%)	178 (100%)	0	100	100
22	r	178/226 (79%)	178 (100%)	0	100	100
All	All	5542/6758 (82%)	5541 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	34	ASN

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

Mol	Chain	Res	Type
7	g	243	ASN
20	y	164	GLN
14	o	307	GLN
7	n	165	GLN
22	R	126	GLN

5.3.3 RNA ⓘ

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 338 ligands modelled in this entry, 2 are monoatomic - leaving 336 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	$\# Z > 2$
25	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.71	13 (23%)
32	DMU	c	522	-	34,34,34	0.58	0	45,45,45	0.81	1 (2%)
23	CLA	B	609	2	69,73,73	1.26	7 (10%)	83,113,113	1.20	5 (6%)
23	CLA	B	612	2	69,73,73	1.22	8 (11%)	83,113,113	1.37	6 (7%)
35	CHL	g	607	-	47,51,74	1.46	7 (14%)	52,86,114	1.50	7 (13%)
31	LHG	l	103	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	3 (5%)
39	VTQ	W	202	-	30,32,32	0.42	0	39,44,44	0.50	0
35	CHL	n	607	-	50,54,74	1.43	7 (14%)	56,90,114	1.58	9 (16%)
31	LHG	R	317	23	41,41,48	1.01	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	C	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.34	6 (7%)
23	CLA	c	509	3	69,73,73	1.26	7 (10%)	83,113,113	1.20	5 (6%)
35	CHL	y	308	-	70,74,74	1.20	8 (11%)	80,114,114	1.36	9 (11%)
23	CLA	g	603	7	69,73,73	1.26	7 (10%)	83,113,113	1.25	8 (9%)
23	CLA	y	303	20	65,69,73	1.28	7 (10%)	78,108,113	1.20	5 (6%)
35	CHL	y	302	20	70,74,74	1.20	8 (11%)	80,114,114	1.24	7 (8%)
31	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
25	BCR	B	619	-	41,41,41	0.68	0	56,56,56	1.73	11 (19%)
30	LMG	a	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	L	102	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	2 (3%)
35	CHL	y	307	-	54,58,74	1.38	7 (12%)	59,94,114	1.45	8 (13%)
23	CLA	b	611	2	69,73,73	1.26	7 (10%)	83,113,113	1.19	5 (6%)
35	CHL	G	606	-	47,51,74	1.47	7 (14%)	52,86,114	1.45	10 (19%)
23	CLA	S	314	15	45,49,73	1.51	8 (17%)	54,84,113	1.47	8 (14%)
31	LHG	n	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
23	CLA	y	313	20	64,68,73	1.30	7 (10%)	77,107,113	1.29	10 (12%)
23	CLA	A	402	-	54,58,73	1.43	7 (12%)	65,95,113	1.42	7 (10%)
23	CLA	g	613	7	62,66,73	1.32	6 (9%)	74,104,113	1.27	4 (5%)
35	CHL	N	608	-	70,74,74	1.21	8 (11%)	80,114,114	1.22	7 (8%)
35	CHL	R	308	-	65,69,74	1.27	8 (12%)	74,108,114	1.31	9 (12%)
28	DGD	B	624	-	60,60,67	0.89	2 (3%)	74,74,81	0.91	2 (2%)
35	CHL	G	601	7	70,74,74	1.24	7 (10%)	80,114,114	1.28	7 (8%)
31	LHG	B	622	-	45,45,48	0.96	2 (4%)	48,51,54	0.99	3 (6%)
35	CHL	g	608	-	70,74,74	1.20	8 (11%)	80,114,114	1.16	5 (6%)
28	DGD	d	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.94	2 (2%)
26	SQD	b	602	-	53,54,54	1.20	4 (7%)	62,65,65	3.65	8 (12%)
37	XAT	G	617	-	39,47,47	0.87	0	54,74,74	2.51	16 (29%)
23	CLA	y	314	20	69,73,73	1.25	7 (10%)	83,113,113	1.23	4 (4%)
23	CLA	R	303	22	64,68,73	1.31	10 (15%)	77,107,113	1.18	5 (6%)
38	NEX	n	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	16 (32%)
31	LHG	s	617	23	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
23	CLA	b	609	-	69,73,73	1.25	8 (11%)	83,113,113	1.20	5 (6%)
35	CHL	y	310	20	70,74,74	1.27	10 (14%)	80,114,114	1.36	9 (11%)
23	CLA	G	602	7	69,73,73	1.26	9 (13%)	83,113,113	1.11	4 (4%)
24	PHO	D	402	-	58,69,69	1.19	3 (5%)	56,99,99	1.74	8 (14%)
35	CHL	Y	307	-	54,58,74	1.39	7 (12%)	59,94,114	1.47	8 (13%)
23	CLA	B	601	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	7 (8%)
37	XAT	g	620	-	39,47,47	0.92	0	54,74,74	2.47	18 (33%)
33	PL9	d	406	-	55,55,55	4.32	23 (41%)	68,69,69	3.64	33 (48%)
35	CHL	S	308	-	53,57,74	1.38	6 (11%)	59,93,114	1.41	10 (16%)
28	DGD	A	408	-	60,60,67	0.91	2 (3%)	74,74,81	0.96	3 (4%)
39	VTQ	w	201	-	30,32,32	0.42	0	39,44,44	0.50	0
23	CLA	n	613	7	64,68,73	1.30	6 (9%)	77,107,113	1.31	7 (9%)
36	LUT	g	615	-	42,43,43	0.73	0	51,60,60	1.53	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	g	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.04	3 (6%)
25	BCR	C	519	-	41,41,41	0.67	0	56,56,56	1.96	15 (26%)
23	CLA	b	618	2	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
36	LUT	S	315	-	42,43,43	0.74	0	51,60,60	1.60	11 (21%)
26	SQD	L	103	-	53,54,54	1.18	4 (7%)	62,65,65	1.10	6 (9%)
23	CLA	S	313	15	59,63,73	1.35	7 (11%)	71,101,113	1.30	3 (4%)
23	CLA	G	611	31	64,68,73	1.29	8 (12%)	77,107,113	1.23	5 (6%)
28	DGD	B	626	-	57,57,67	0.96	2 (3%)	71,71,81	1.04	4 (5%)
23	CLA	c	513	3	69,73,73	1.25	8 (11%)	83,113,113	1.23	8 (9%)
23	CLA	C	506	3	62,66,73	1.29	7 (11%)	74,104,113	1.29	8 (10%)
35	CHL	y	306	20	55,59,74	1.36	7 (12%)	62,96,114	1.34	9 (14%)
23	CLA	Y	304	20	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	r	602	22	64,68,73	1.31	9 (14%)	77,107,113	1.18	6 (7%)
23	CLA	C	512	3	69,73,73	1.27	6 (8%)	83,113,113	1.29	5 (6%)
27	BCT	A	407	29	2,3,3	0.87	0	2,3,3	3.25	2 (100%)
36	LUT	y	316	-	42,43,43	0.72	0	51,60,60	1.52	10 (19%)
31	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)
31	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
26	SQD	l	101	-	53,54,54	1.19	4 (7%)	62,65,65	1.09	4 (6%)
36	LUT	G	615	-	42,43,43	0.73	0	51,60,60	1.54	10 (19%)
23	CLA	n	612	7	49,53,73	1.50	7 (14%)	59,89,113	1.44	6 (10%)
25	BCR	H	101	-	41,41,41	0.71	0	56,56,56	1.56	7 (12%)
38	NEX	S	317	-	38,46,46	0.86	1 (2%)	50,70,70	2.26	17 (34%)
23	CLA	G	610	7	68,72,73	1.23	7 (10%)	81,111,113	1.20	7 (8%)
25	BCR	A	405	-	41,41,41	0.68	0	56,56,56	1.69	12 (21%)
23	CLA	B	615	2	69,73,73	1.23	7 (10%)	83,113,113	1.34	9 (10%)
23	CLA	b	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.33	6 (7%)
37	XAT	R	315	-	39,47,47	0.88	0	54,74,74	2.51	19 (35%)
23	CLA	b	613	2	69,73,73	1.23	8 (11%)	83,113,113	1.19	6 (7%)
23	CLA	d	404	4	69,73,73	1.23	6 (8%)	83,113,113	1.23	5 (6%)
28	DGD	b	625	-	57,57,67	0.95	2 (3%)	71,71,81	1.06	4 (5%)
32	DMU	c	519	-	34,34,34	0.54	0	45,45,45	1.50	5 (11%)
23	CLA	R	312	22	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
23	CLA	b	612	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
35	CHL	n	606	-	50,54,74	1.44	7 (14%)	56,90,114	1.39	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	502	3	69,73,73	1.27	8 (11%)	83,113,113	1.14	6 (7%)
38	NEX	s	616	-	38,46,46	0.89	1 (2%)	50,70,70	2.35	20 (40%)
23	CLA	r	601	22	53,57,73	1.45	7 (13%)	62,93,113	1.32	5 (8%)
23	CLA	n	614	7	45,49,73	1.51	7 (15%)	54,84,113	1.34	5 (9%)
23	CLA	n	603	7	63,67,73	1.31	7 (11%)	75,105,113	1.31	6 (8%)
38	NEX	G	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.34	16 (32%)
23	CLA	N	603	7	63,67,73	1.33	7 (11%)	75,105,113	1.35	6 (8%)
24	PHO	a	403	-	58,69,69	1.19	4 (6%)	56,99,99	1.73	8 (14%)
25	BCR	z	101	-	41,41,41	0.71	0	56,56,56	1.63	9 (16%)
35	CHL	Y	306	20	55,59,74	1.37	7 (12%)	62,96,114	1.32	9 (14%)
25	BCR	K	101	-	41,41,41	0.65	0	56,56,56	1.80	16 (28%)
30	LMG	b	601	-	40,40,55	1.06	2 (5%)	48,48,63	1.00	2 (4%)
23	CLA	s	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.41	9 (15%)
23	CLA	N	613	7	64,68,73	1.30	6 (9%)	77,107,113	1.30	7 (9%)
23	CLA	R	310	22	69,73,73	1.26	8 (11%)	83,113,113	1.22	5 (6%)
31	LHG	C	518	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
23	CLA	y	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.35	6 (9%)
23	CLA	C	509	3	69,73,73	1.25	9 (13%)	83,113,113	1.24	7 (8%)
23	CLA	N	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.37	7 (10%)
23	CLA	c	507	-	69,73,73	1.23	7 (10%)	83,113,113	1.31	7 (8%)
34	HEM	F	101	6,5	50,50,50	1.48	7 (14%)	66,82,82	1.33	7 (10%)
30	LMG	b	622	-	51,51,55	0.94	2 (3%)	59,59,63	0.99	3 (5%)
33	PL9	D	406	-	55,55,55	4.31	22 (40%)	68,69,69	3.66	33 (48%)
35	CHL	G	609	7	65,69,74	1.29	7 (10%)	74,108,114	1.47	8 (10%)
23	CLA	S	310	15	49,53,73	1.48	7 (14%)	59,89,113	1.31	8 (13%)
23	CLA	B	610	-	69,73,73	1.23	8 (11%)	83,113,113	1.27	6 (7%)
23	CLA	C	510	3	69,73,73	1.27	9 (13%)	83,113,113	1.21	5 (6%)
37	XAT	G	620	-	39,47,47	0.91	0	54,74,74	2.47	17 (31%)
35	CHL	N	607	-	50,54,74	1.44	7 (14%)	56,90,114	1.55	8 (14%)
35	CHL	g	606	-	47,51,74	1.44	6 (12%)	52,86,114	1.41	7 (13%)
23	CLA	s	603	15	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
23	CLA	s	610	31	46,50,73	1.50	8 (17%)	55,85,113	1.37	4 (7%)
23	CLA	C	507	3	55,59,73	1.38	9 (16%)	66,96,113	1.56	8 (12%)
37	XAT	Y	301	-	39,47,47	0.91	0	54,74,74	2.56	18 (33%)
35	CHL	R	306	-	50,54,74	1.44	6 (12%)	56,90,114	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	CHL	N	605	7	52,56,74	1.37	7 (13%)	58,92,114	1.59	10 (17%)
23	CLA	r	612	22	69,73,73	1.26	9 (13%)	83,113,113	1.25	8 (9%)
23	CLA	b	616	2	69,73,73	1.25	8 (11%)	83,113,113	1.21	9 (10%)
25	BCR	a	405	-	41,41,41	0.69	0	56,56,56	1.70	11 (19%)
26	SQD	a	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
30	LMG	s	619	-	55,55,55	0.90	2 (3%)	63,63,63	0.98	4 (6%)
35	CHL	N	609	7	70,74,74	1.23	7 (10%)	80,114,114	1.41	9 (11%)
37	XAT	g	617	-	39,47,47	0.89	0	54,74,74	2.51	16 (29%)
23	CLA	A	401	1	69,73,73	1.26	8 (11%)	83,113,113	1.20	4 (4%)
23	CLA	d	401	-	69,73,73	1.23	7 (10%)	83,113,113	1.29	7 (8%)
35	CHL	y	309	-	70,74,74	1.22	8 (11%)	80,114,114	1.24	8 (10%)
23	CLA	g	611	31	64,68,73	1.30	7 (10%)	77,107,113	1.23	4 (5%)
25	BCR	B	618	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
31	LHG	N	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.05	4 (7%)
23	CLA	y	311	20	64,68,73	1.29	9 (14%)	77,107,113	1.24	8 (10%)
23	CLA	R	309	22	62,66,73	1.32	7 (11%)	74,104,113	1.22	6 (8%)
31	LHG	b	626	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)
35	CHL	n	605	7	52,56,74	1.37	6 (11%)	58,92,114	1.56	9 (15%)
38	NEX	N	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	15 (30%)
31	LHG	G	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.05	3 (6%)
23	CLA	s	602	15	50,54,73	1.46	8 (16%)	60,90,113	1.28	5 (8%)
36	LUT	n	616	-	42,43,43	0.76	0	51,60,60	1.54	13 (25%)
23	CLA	S	304	15	49,53,73	1.48	6 (12%)	59,89,113	1.41	4 (6%)
23	CLA	Y	314	20	69,73,73	1.25	7 (10%)	83,113,113	1.23	4 (4%)
36	LUT	n	615	-	42,43,43	0.72	0	51,60,60	1.53	11 (21%)
35	CHL	s	605	-	50,54,74	1.46	8 (16%)	56,90,114	1.44	5 (8%)
31	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	Y	313	20	64,68,73	1.30	7 (10%)	77,107,113	1.30	8 (10%)
35	CHL	r	606	-	50,54,74	1.43	7 (14%)	56,90,114	1.34	6 (10%)
23	CLA	y	312	31	64,68,73	1.30	7 (10%)	77,107,113	1.26	5 (6%)
23	CLA	s	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
36	LUT	s	614	-	42,43,43	0.74	0	51,60,60	1.59	11 (21%)
23	CLA	B	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.16	7 (8%)
35	CHL	r	607	-	65,69,74	1.26	7 (10%)	74,108,114	1.27	8 (10%)
23	CLA	g	610	7	68,72,73	1.24	6 (8%)	81,111,113	1.13	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	402	-	54,58,73	1.44	8 (14%)	65,95,113	1.36	6 (9%)
32	DMU	s	618	-	34,34,34	0.54	0	45,45,45	0.98	1 (2%)
23	CLA	S	311	31	46,50,73	1.50	7 (15%)	55,85,113	1.32	5 (9%)
25	BCR	b	620	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
35	CHL	Y	309	-	70,74,74	1.22	8 (11%)	80,114,114	1.24	8 (10%)
23	CLA	R	311	31	45,49,73	1.52	7 (15%)	54,84,113	1.41	4 (7%)
25	BCR	b	619	-	41,41,41	0.70	0	56,56,56	1.68	12 (21%)
23	CLA	G	603	7	69,73,73	1.25	6 (8%)	83,113,113	1.25	7 (8%)
35	CHL	N	601	7	70,74,74	1.21	7 (10%)	80,114,114	1.30	9 (11%)
35	CHL	Y	308	-	70,74,74	1.20	8 (11%)	80,114,114	1.36	9 (11%)
30	LMG	B	623	-	40,40,55	1.06	2 (5%)	48,48,63	0.99	2 (4%)
23	CLA	a	404	1	64,68,73	1.28	7 (10%)	77,107,113	1.27	7 (9%)
23	CLA	s	608	15	49,53,73	1.49	7 (14%)	59,89,113	1.36	7 (11%)
23	CLA	r	603	22	64,68,73	1.29	8 (12%)	77,107,113	1.27	5 (6%)
23	CLA	C	511	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	5 (6%)
32	DMU	C	520	-	34,34,34	0.54	0	45,45,45	1.48	5 (11%)
23	CLA	B	611	2	69,73,73	1.24	9 (13%)	83,113,113	1.19	5 (6%)
23	CLA	c	504	-	64,68,73	1.30	7 (10%)	77,107,113	1.23	3 (3%)
23	CLA	B	616	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
36	LUT	Y	317	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
35	CHL	n	601	7	70,74,74	1.20	7 (10%)	80,114,114	1.31	7 (8%)
23	CLA	b	603	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	8 (9%)
23	CLA	G	612	7	49,53,73	1.48	6 (12%)	59,89,113	1.39	7 (11%)
26	SQD	c	520	-	44,45,54	1.31	4 (9%)	53,56,65	3.95	8 (15%)
23	CLA	b	615	2	69,73,73	1.25	8 (11%)	83,113,113	1.24	5 (6%)
32	DMU	S	319	-	34,34,34	0.53	0	45,45,45	0.97	2 (4%)
31	LHG	B	627	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)
23	CLA	b	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.17	7 (8%)
30	LMG	W	203	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	3 (5%)
23	CLA	r	610	31	45,49,73	1.52	7 (15%)	54,84,113	1.42	4 (7%)
23	CLA	r	609	22	69,73,73	1.24	8 (11%)	83,113,113	1.16	7 (8%)
35	CHL	G	608	-	70,74,74	1.21	7 (10%)	80,114,114	1.17	5 (6%)
35	CHL	G	605	7	50,54,74	1.45	8 (16%)	56,90,114	1.34	8 (14%)
31	LHG	W	201	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	c	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.25	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	n	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.33	6 (9%)
23	CLA	C	508	-	69,73,73	1.24	6 (8%)	83,113,113	1.32	7 (8%)
23	CLA	C	504	3	69,73,73	1.25	6 (8%)	83,113,113	1.20	4 (4%)
30	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
38	NEX	Y	318	-	38,46,46	0.92	1 (2%)	50,70,70	3.98	18 (36%)
23	CLA	S	312	15	49,53,73	1.47	7 (14%)	59,89,113	1.50	7 (11%)
23	CLA	b	605	2	69,73,73	1.24	8 (11%)	83,113,113	1.20	6 (7%)
23	CLA	B	606	2	69,73,73	1.25	8 (11%)	83,113,113	1.21	6 (7%)
36	LUT	R	314	-	42,43,43	0.73	0	51,60,60	1.60	10 (19%)
23	CLA	B	613	2	69,73,73	1.24	7 (10%)	83,113,113	1.24	5 (6%)
23	CLA	G	614	7	46,50,73	1.50	7 (15%)	55,85,113	1.30	7 (12%)
23	CLA	S	303	15	50,54,73	1.46	8 (16%)	60,90,113	1.30	4 (6%)
30	LMG	w	202	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
30	LMG	d	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.98	2 (3%)
36	LUT	Y	316	-	42,43,43	0.71	0	51,60,60	1.48	9 (17%)
23	CLA	s	613	15	45,49,73	1.50	8 (17%)	54,84,113	1.45	7 (12%)
23	CLA	s	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.29	3 (4%)
23	CLA	R	305	-	52,56,73	1.43	8 (15%)	62,92,113	1.36	7 (11%)
23	CLA	s	611	15	49,53,73	1.51	7 (14%)	59,89,113	1.41	8 (13%)
36	LUT	G	616	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
25	BCR	c	518	-	41,41,41	0.67	0	56,56,56	1.82	13 (23%)
38	NEX	R	301	-	38,46,46	0.91	1 (2%)	50,70,70	4.00	18 (36%)
23	CLA	c	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.19	5 (6%)
35	CHL	R	307	-	50,54,74	1.44	7 (14%)	56,90,114	1.35	7 (12%)
23	CLA	G	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.34	6 (9%)
35	CHL	n	609	7	70,74,74	1.23	7 (10%)	80,114,114	1.40	8 (10%)
23	CLA	c	512	3	60,64,73	1.33	6 (10%)	72,102,113	1.35	6 (8%)
31	LHG	b	624	-	45,45,48	0.96	2 (4%)	48,51,54	0.98	2 (4%)
28	DGD	c	515	-	56,56,67	0.92	2 (3%)	70,70,81	1.01	3 (4%)
35	CHL	r	605	-	50,54,74	1.44	6 (12%)	56,90,114	1.38	7 (12%)
25	BCR	b	621	-	41,41,41	0.68	0	56,56,56	1.72	10 (17%)
23	CLA	b	617	2	69,73,73	1.23	7 (10%)	83,113,113	1.34	8 (9%)
31	LHG	y	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	D	403	4	69,73,73	1.28	9 (13%)	83,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	CHL	g	609	7	65,69,74	1.27	8 (12%)	74,108,114	1.22	7 (9%)
23	CLA	C	513	3	60,64,73	1.33	5 (8%)	72,102,113	1.33	7 (9%)
23	CLA	c	505	3	62,66,73	1.29	7 (11%)	74,104,113	1.28	7 (9%)
23	CLA	c	508	3	69,73,73	1.25	8 (11%)	83,113,113	1.23	7 (8%)
28	DGD	C	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.02	3 (4%)
23	CLA	a	401	1	69,73,73	1.25	8 (11%)	83,113,113	1.21	4 (4%)
23	CLA	y	315	20	49,53,73	1.48	8 (16%)	59,89,113	1.31	5 (8%)
35	CHL	s	607	-	53,57,74	1.38	6 (11%)	59,93,114	1.34	10 (16%)
31	LHG	Y	319	23	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
23	CLA	S	305	-	54,58,73	1.43	9 (16%)	65,95,113	1.36	7 (10%)
35	CHL	N	606	-	50,54,74	1.44	8 (16%)	56,90,114	1.41	12 (21%)
23	CLA	Y	303	20	65,69,73	1.29	6 (9%)	78,108,113	1.21	5 (6%)
24	PHO	a	402	-	58,69,69	1.21	5 (8%)	56,99,99	1.83	7 (12%)
23	CLA	B	603	2	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
23	CLA	b	608	2	69,73,73	1.24	8 (11%)	83,113,113	1.21	6 (7%)
34	HEM	f	101	6,5	50,50,50	1.48	7 (14%)	66,82,82	1.32	7 (10%)
23	CLA	y	304	20	69,73,73	1.28	7 (10%)	83,113,113	1.31	7 (8%)
36	LUT	s	615	-	42,43,43	0.73	0	51,60,60	1.47	8 (15%)
23	CLA	Y	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.38	7 (10%)
23	CLA	Y	315	20	49,53,73	1.47	6 (12%)	59,89,113	1.32	5 (8%)
35	CHL	S	307	-	47,51,74	1.45	6 (12%)	52,86,114	1.53	7 (13%)
31	LHG	S	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
25	BCR	D	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
23	CLA	B	604	2	69,73,73	1.27	7 (10%)	83,113,113	1.32	5 (6%)
35	CHL	G	607	-	47,51,74	1.46	7 (14%)	52,86,114	1.46	6 (11%)
23	CLA	c	506	3	55,59,73	1.40	8 (14%)	66,96,113	1.36	7 (10%)
27	BCT	a	408	29	2,3,3	0.87	0	2,3,3	3.26	2 (100%)
36	LUT	y	317	-	42,43,43	0.74	0	51,60,60	1.50	10 (19%)
23	CLA	R	304	22	64,68,73	1.29	8 (12%)	77,107,113	1.31	5 (6%)
25	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.72	14 (25%)
23	CLA	n	611	31	64,68,73	1.30	6 (9%)	77,107,113	1.33	7 (9%)
23	CLA	b	607	2	69,73,73	1.25	7 (10%)	83,113,113	1.39	7 (8%)
23	CLA	r	611	22	69,73,73	1.26	7 (10%)	83,113,113	1.24	4 (4%)
36	LUT	N	616	-	42,43,43	0.75	0	51,60,60	1.49	11 (21%)
35	CHL	S	302	15	50,54,74	1.43	7 (14%)	56,90,114	1.46	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	k	101	-	41,41,41	0.65	0	56,56,56	1.84	15 (26%)
23	CLA	N	611	31	64,68,73	1.30	6 (9%)	77,107,113	1.33	7 (9%)
23	CLA	B	608	2	69,73,73	1.24	8 (11%)	83,113,113	1.24	7 (8%)
30	LMG	c	521	-	50,50,55	0.97	2 (4%)	58,58,63	1.07	4 (6%)
23	CLA	R	302	22	53,57,73	1.45	7 (13%)	62,93,113	1.31	5 (8%)
31	LHG	c	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
35	CHL	Y	310	20	70,74,74	1.27	9 (12%)	80,114,114	1.37	8 (10%)
23	CLA	C	505	-	64,68,73	1.29	6 (9%)	77,107,113	1.24	4 (5%)
32	DMU	C	523	-	34,34,34	0.59	0	45,45,45	0.81	1 (2%)
26	SQD	A	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
25	BCR	h	101	-	41,41,41	0.70	0	56,56,56	1.59	9 (16%)
38	NEX	g	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.45	16 (32%)
23	CLA	g	612	7	49,53,73	1.48	8 (16%)	59,89,113	1.37	4 (6%)
23	CLA	N	610	7	63,67,73	1.28	7 (11%)	75,105,113	1.23	7 (9%)
23	CLA	C	514	3	69,73,73	1.26	8 (11%)	83,113,113	1.24	8 (9%)
35	CHL	g	605	7	50,54,74	1.44	8 (16%)	56,90,114	1.34	8 (14%)
38	NEX	R	316	-	38,46,46	0.86	1 (2%)	50,70,70	2.30	16 (32%)
23	CLA	A	404	1	64,68,73	1.27	7 (10%)	77,107,113	1.27	8 (10%)
38	NEX	r	615	-	38,46,46	0.90	1 (2%)	50,70,70	2.31	18 (36%)
23	CLA	c	501	3	69,73,73	1.27	9 (13%)	83,113,113	1.17	6 (7%)
23	CLA	g	602	7	69,73,73	1.25	7 (10%)	83,113,113	1.12	4 (4%)
26	SQD	B	625	-	53,54,54	1.20	4 (7%)	62,65,65	3.67	8 (12%)
23	CLA	Y	311	20	64,68,73	1.28	8 (12%)	77,107,113	1.18	6 (7%)
23	CLA	N	614	7	45,49,73	1.52	6 (13%)	54,84,113	1.33	5 (9%)
23	CLA	r	604	-	52,56,73	1.44	7 (13%)	62,92,113	1.37	6 (9%)
23	CLA	g	614	7	46,50,73	1.49	7 (15%)	55,85,113	1.31	7 (12%)
23	CLA	b	614	2	69,73,73	1.23	8 (11%)	83,113,113	1.36	6 (7%)
37	XAT	y	301	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
31	LHG	b	623	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	G	613	7	62,66,73	1.32	7 (11%)	74,104,113	1.25	4 (5%)
23	CLA	n	610	7	63,67,73	1.28	7 (11%)	75,105,113	1.20	7 (9%)
25	BCR	d	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
35	CHL	g	601	7	70,74,74	1.23	7 (10%)	80,114,114	1.28	8 (10%)
25	BCR	B	617	-	41,41,41	0.70	0	56,56,56	1.66	12 (21%)
30	LMG	C	501	-	48,48,55	0.95	2 (4%)	56,56,63	1.06	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	N	612	7	49,53,73	1.51	7 (14%)	59,89,113	1.46	6 (10%)
23	CLA	S	309	15	49,53,73	1.51	7 (14%)	59,89,113	1.33	4 (6%)
23	CLA	n	602	7	65,69,73	1.27	8 (12%)	78,108,113	1.35	8 (10%)
36	LUT	g	616	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
24	PHO	A	403	-	58,69,69	1.22	5 (8%)	56,99,99	1.85	7 (12%)
37	XAT	r	614	-	39,47,47	0.89	0	54,74,74	2.49	17 (31%)
23	CLA	D	404	4	69,73,73	1.24	6 (8%)	83,113,113	1.23	4 (4%)
23	CLA	N	602	7	65,69,73	1.28	8 (12%)	78,108,113	1.34	9 (11%)
23	CLA	g	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.33	6 (9%)
23	CLA	b	610	2	69,73,73	1.23	7 (10%)	83,113,113	1.23	7 (8%)
23	CLA	D	401	-	69,73,73	1.24	8 (11%)	83,113,113	1.27	7 (8%)
30	LMG	C	522	-	50,50,55	0.96	2 (4%)	58,58,63	1.08	4 (6%)
31	LHG	l	102	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	B	605	2	69,73,73	1.25	7 (10%)	83,113,113	1.37	7 (8%)
35	CHL	S	306	-	50,54,74	1.47	6 (12%)	56,90,114	1.50	9 (16%)
31	LHG	r	616	23	41,41,48	1.00	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	c	510	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)
30	LMG	D	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.97	2 (3%)
26	SQD	C	521	-	44,45,54	1.31	4 (9%)	53,56,65	3.96	8 (15%)
35	CHL	n	608	-	70,74,74	1.22	8 (11%)	80,114,114	1.19	6 (7%)
36	LUT	S	316	-	42,43,43	0.77	0	51,60,60	1.48	8 (15%)
31	LHG	D	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.94	2 (3%)
35	CHL	Y	302	20	70,74,74	1.21	8 (11%)	80,114,114	1.25	7 (8%)
31	LHG	c	517	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
23	CLA	d	403	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
36	LUT	r	613	-	42,43,43	0.73	0	51,60,60	1.67	11 (21%)
25	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.61	9 (16%)
30	LMG	S	301	-	55,55,55	0.90	2 (3%)	63,63,63	0.97	4 (6%)
23	CLA	Y	312	31	64,68,73	1.30	7 (10%)	77,107,113	1.27	5 (6%)
23	CLA	B	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.20	9 (10%)
35	CHL	s	601	15	50,54,74	1.44	7 (14%)	56,90,114	1.47	5 (8%)
23	CLA	c	502	3	69,73,73	1.25	7 (10%)	83,113,113	1.34	6 (7%)
23	CLA	B	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.20	5 (6%)
36	LUT	N	615	-	42,43,43	0.72	0	51,60,60	1.48	9 (17%)
23	CLA	R	313	22	69,73,73	1.25	7 (10%)	83,113,113	1.22	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	D	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.92	2 (2%)
35	CHL	s	606	-	47,51,74	1.46	6 (12%)	52,86,114	1.56	8 (15%)
23	CLA	r	608	22	62,66,73	1.31	7 (11%)	74,104,113	1.22	5 (6%)

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
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
32	DMU	c	522	-	-	5/19/59/59	0/2/2/2
23	CLA	B	609	2	-	14/39/115/115	-
23	CLA	B	612	2	-	18/39/115/115	-
35	CHL	g	607	-	-	7/14/90/117	-
31	LHG	l	103	-	-	18/53/53/53	-
39	VTQ	W	202	-	-	3/25/49/49	0/1/1/1
35	CHL	n	607	-	-	11/17/93/117	-
31	LHG	R	317	23	-	8/46/46/53	-
23	CLA	C	503	3	-	13/39/115/115	-
23	CLA	c	509	3	-	11/39/115/115	-
35	CHL	y	308	-	-	22/41/117/117	-
23	CLA	g	603	7	-	8/39/115/115	-
23	CLA	y	303	20	-	18/35/111/115	-
35	CHL	y	302	20	-	16/41/117/117	-
31	LHG	D	408	-	-	7/53/53/53	-
25	BCR	B	619	-	-	6/29/63/63	0/2/2/2
30	LMG	a	407	-	-	2/43/63/70	0/1/1/1
31	LHG	L	102	-	-	18/53/53/53	-
35	CHL	y	307	-	-	10/22/98/117	-
23	CLA	b	611	2	-	13/39/115/115	-
35	CHL	G	606	-	-	8/14/90/117	-
23	CLA	S	314	15	-	8/10/86/115	-
31	LHG	n	618	23	-	10/53/53/53	-
23	CLA	y	313	20	-	9/33/109/115	-
23	CLA	A	402	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	613	7	-	13/31/107/115	-
35	CHL	N	608	-	-	10/41/117/117	-
35	CHL	R	308	-	-	13/35/111/117	-
28	DGD	B	624	-	-	7/48/88/95	0/2/2/2
35	CHL	G	601	7	-	20/41/117/117	-
31	LHG	B	622	-	-	11/50/50/53	-
35	CHL	g	608	-	-	18/41/117/117	-
28	DGD	d	410	-	-	9/51/91/95	0/2/2/2
26	SQD	b	602	-	-	20/49/69/69	0/1/1/1
37	XAT	G	617	-	-	1/31/93/93	0/4/4/4
23	CLA	y	314	20	-	15/39/115/115	-
23	CLA	R	303	22	-	15/33/109/115	-
38	NEX	n	617	-	-	5/27/83/83	0/3/3/3
31	LHG	s	617	23	-	9/53/53/53	-
23	CLA	b	609	-	-	16/39/115/115	-
35	CHL	y	310	20	-	21/41/117/117	-
23	CLA	G	602	7	-	20/39/115/115	-
24	PHO	D	402	-	-	6/37/103/103	0/5/6/6
35	CHL	Y	307	-	-	10/22/98/117	-
23	CLA	B	601	-	-	15/39/115/115	-
37	XAT	g	620	-	-	0/31/93/93	0/4/4/4
33	PL9	d	406	-	-	25/53/73/73	0/1/1/1
35	CHL	S	308	-	-	12/21/97/117	-
28	DGD	A	408	-	-	8/48/88/95	0/2/2/2
39	VTQ	w	201	-	-	3/25/49/49	0/1/1/1
23	CLA	n	613	7	-	14/33/109/115	-
36	LUT	g	615	-	-	3/29/67/67	0/2/2/2
31	LHG	g	619	23	-	10/50/50/53	-
25	BCR	C	519	-	-	0/29/63/63	0/2/2/2
23	CLA	b	618	2	-	14/39/115/115	-
36	LUT	S	315	-	-	2/29/67/67	0/2/2/2
26	SQD	L	103	-	-	15/49/69/69	0/1/1/1
23	CLA	S	313	15	-	11/27/103/115	-
23	CLA	G	611	31	-	5/33/109/115	-
28	DGD	B	626	-	-	13/45/85/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	3	-	9/39/115/115	-
23	CLA	C	506	3	-	13/31/107/115	-
35	CHL	y	306	20	-	13/23/99/117	-
23	CLA	Y	304	20	-	13/39/115/115	-
23	CLA	r	602	22	-	18/33/109/115	-
23	CLA	C	512	3	-	16/39/115/115	-
36	LUT	y	316	-	-	2/29/67/67	0/2/2/2
31	LHG	d	407	-	-	12/53/53/53	-
31	LHG	d	408	-	-	9/53/53/53	-
26	SQD	l	101	-	-	17/49/69/69	0/1/1/1
36	LUT	G	615	-	-	2/29/67/67	0/2/2/2
23	CLA	n	612	7	-	10/15/91/115	-
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
38	NEX	S	317	-	-	4/27/83/83	0/3/3/3
23	CLA	G	610	7	-	13/38/114/115	-
25	BCR	A	405	-	-	2/29/63/63	0/2/2/2
23	CLA	B	615	2	-	16/39/115/115	-
23	CLA	b	606	2	-	11/39/115/115	-
37	XAT	R	315	-	-	1/31/93/93	0/4/4/4
23	CLA	b	613	2	-	12/39/115/115	-
23	CLA	d	404	4	-	17/39/115/115	-
28	DGD	b	625	-	-	12/45/85/95	0/2/2/2
32	DMU	c	519	-	-	6/19/59/59	0/2/2/2
23	CLA	R	312	22	-	14/39/115/115	-
23	CLA	b	612	-	-	11/39/115/115	-
35	CHL	n	606	-	-	7/17/93/117	-
23	CLA	C	502	3	-	14/39/115/115	-
38	NEX	s	616	-	-	2/27/83/83	0/3/3/3
23	CLA	r	601	22	-	13/20/96/115	-
23	CLA	n	614	7	-	5/10/86/115	-
23	CLA	n	603	7	-	12/32/108/115	-
38	NEX	G	618	-	-	3/27/83/83	0/3/3/3
23	CLA	N	603	7	-	13/32/108/115	-
24	PHO	a	403	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
35	CHL	Y	306	20	-	13/23/99/117	-
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LMG	b	601	-	-	3/35/55/70	0/1/1/1
23	CLA	s	609	15	-	6/15/91/115	-
23	CLA	N	613	7	-	14/33/109/115	-
23	CLA	R	310	22	-	11/39/115/115	-
31	LHG	C	518	-	-	11/53/53/53	-
23	CLA	y	305	-	-	9/21/97/115	-
23	CLA	C	509	3	-	11/39/115/115	-
23	CLA	N	604	-	-	7/21/97/115	-
23	CLA	c	507	-	-	10/39/115/115	-
34	HEM	F	101	6,5	-	5/14/54/54	-
30	LMG	b	622	-	-	7/46/66/70	0/1/1/1
33	PL9	D	406	-	-	26/53/73/73	0/1/1/1
35	CHL	G	609	7	-	12/35/111/117	-
23	CLA	S	310	15	-	9/15/91/115	-
23	CLA	B	610	-	-	11/39/115/115	-
23	CLA	C	510	3	-	11/39/115/115	-
37	XAT	G	620	-	-	0/31/93/93	0/4/4/4
35	CHL	N	607	-	-	11/17/93/117	-
35	CHL	g	606	-	-	4/14/90/117	-
23	CLA	s	603	15	-	7/15/91/115	-
23	CLA	s	610	31	-	6/12/88/115	-
23	CLA	C	507	3	-	5/23/99/115	-
37	XAT	Y	301	-	-	0/31/93/93	0/4/4/4
35	CHL	R	306	-	-	7/17/93/117	-
35	CHL	N	605	7	-	12/20/96/117	-
23	CLA	r	612	22	-	11/39/115/115	-
23	CLA	b	616	2	-	18/39/115/115	-
25	BCR	a	405	-	-	2/29/63/63	0/2/2/2
26	SQD	a	406	-	-	8/45/65/69	0/1/1/1
30	LMG	s	619	-	-	5/50/70/70	0/1/1/1
35	CHL	N	609	7	-	16/41/117/117	-
37	XAT	g	617	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	401	1	-	10/39/115/115	-
23	CLA	d	401	-	-	14/39/115/115	-
35	CHL	y	309	-	-	13/41/117/117	-
23	CLA	g	611	31	-	6/33/109/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	LHG	N	618	23	-	9/53/53/53	-
23	CLA	y	311	20	-	8/33/109/115	-
23	CLA	R	309	22	-	7/31/107/115	-
31	LHG	b	626	-	-	13/44/44/53	-
35	CHL	n	605	7	-	12/20/96/117	-
38	NEX	N	617	-	-	4/27/83/83	0/3/3/3
31	LHG	G	619	23	-	11/50/50/53	-
23	CLA	s	602	15	-	10/17/93/115	-
36	LUT	n	616	-	-	1/29/67/67	0/2/2/2
23	CLA	S	304	15	-	7/15/91/115	-
23	CLA	Y	314	20	-	13/39/115/115	-
36	LUT	n	615	-	-	3/29/67/67	0/2/2/2
35	CHL	s	605	-	-	8/17/93/117	-
31	LHG	B	621	-	-	11/53/53/53	-
23	CLA	Y	313	20	-	9/33/109/115	-
35	CHL	r	606	-	-	7/17/93/117	-
23	CLA	y	312	31	-	10/33/109/115	-
23	CLA	s	604	-	-	5/21/97/115	-
36	LUT	s	614	-	-	2/29/67/67	0/2/2/2
23	CLA	B	602	2	-	15/39/115/115	-
35	CHL	r	607	-	-	13/35/111/117	-
23	CLA	g	610	7	-	15/38/114/115	-
23	CLA	d	402	-	-	12/21/97/115	-
32	DMU	s	618	-	-	5/19/59/59	0/2/2/2
23	CLA	S	311	31	-	6/12/88/115	-
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
35	CHL	Y	309	-	-	14/41/117/117	-
23	CLA	R	311	31	-	7/10/86/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	G	603	7	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CHL	N	601	7	-	11/41/117/117	-
35	CHL	Y	308	-	-	24/41/117/117	-
30	LMG	B	623	-	-	3/35/55/70	0/1/1/1
23	CLA	a	404	1	-	14/33/109/115	-
23	CLA	s	608	15	-	6/15/91/115	-
23	CLA	r	603	22	-	8/33/109/115	-
23	CLA	C	511	3	-	15/39/115/115	-
32	DMU	C	520	-	-	7/19/59/59	0/2/2/2
23	CLA	B	611	2	-	11/39/115/115	-
23	CLA	c	504	-	-	5/33/109/115	-
23	CLA	B	616	2	-	12/39/115/115	-
36	LUT	Y	317	-	-	1/29/67/67	0/2/2/2
35	CHL	n	601	7	-	16/41/117/117	-
23	CLA	b	603	-	-	15/39/115/115	-
23	CLA	G	612	7	-	9/15/91/115	-
26	SQD	c	520	-	-	2/40/60/69	0/1/1/1
23	CLA	b	615	2	-	15/39/115/115	-
32	DMU	S	319	-	-	4/19/59/59	0/2/2/2
31	LHG	B	627	-	-	13/44/44/53	-
23	CLA	b	604	2	-	12/39/115/115	-
30	LMG	W	203	-	-	7/46/66/70	0/1/1/1
23	CLA	r	610	31	-	6/10/86/115	-
23	CLA	r	609	22	-	12/39/115/115	-
35	CHL	G	608	-	-	17/41/117/117	-
35	CHL	G	605	7	-	12/17/93/117	-
31	LHG	W	201	-	-	9/53/53/53	-
23	CLA	c	511	3	-	13/39/115/115	-
23	CLA	n	604	-	-	6/21/97/115	-
23	CLA	C	508	-	-	12/39/115/115	-
23	CLA	C	504	3	-	19/39/115/115	-
30	LMG	B	620	-	-	9/46/66/70	0/1/1/1
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
23	CLA	S	312	15	-	6/15/91/115	-
23	CLA	b	605	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	606	2	-	9/39/115/115	-
36	LUT	R	314	-	-	2/29/67/67	0/2/2/2
23	CLA	B	613	2	-	15/39/115/115	-
23	CLA	G	614	7	-	7/12/88/115	-
23	CLA	S	303	15	-	8/17/93/115	-
30	LMG	w	202	-	-	7/46/66/70	0/1/1/1
30	LMG	d	409	-	-	3/41/61/70	0/1/1/1
36	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	s	613	15	-	8/10/86/115	-
23	CLA	s	612	15	-	11/27/103/115	-
23	CLA	R	305	-	-	10/19/95/115	-
23	CLA	s	611	15	-	4/15/91/115	-
36	LUT	G	616	-	-	1/29/67/67	0/2/2/2
25	BCR	c	518	-	-	2/29/63/63	0/2/2/2
38	NEX	R	301	-	-	4/27/83/83	0/3/3/3
23	CLA	c	503	3	-	18/39/115/115	-
35	CHL	R	307	-	-	7/17/93/117	-
23	CLA	G	604	-	-	11/20/96/115	-
35	CHL	n	609	7	-	15/41/117/117	-
23	CLA	c	512	3	-	8/29/105/115	-
31	LHG	b	624	-	-	9/50/50/53	-
28	DGD	c	515	-	-	4/44/84/95	0/2/2/2
35	CHL	r	605	-	-	7/17/93/117	-
25	BCR	b	621	-	-	4/29/63/63	0/2/2/2
23	CLA	b	617	2	-	20/39/115/115	-
31	LHG	y	318	23	-	12/53/53/53	-
31	LHG	L	101	-	-	8/53/53/53	-
23	CLA	D	403	4	-	7/39/115/115	-
35	CHL	g	609	7	-	14/35/111/117	-
23	CLA	C	513	3	-	8/29/105/115	-
23	CLA	c	505	3	-	15/31/107/115	-
23	CLA	c	508	3	-	13/39/115/115	-
28	DGD	C	517	-	-	4/44/84/95	0/2/2/2
23	CLA	a	401	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	y	315	20	-	6/15/91/115	-
35	CHL	s	607	-	-	14/21/97/117	-
31	LHG	Y	319	23	-	12/53/53/53	-
23	CLA	S	305	-	-	7/21/97/115	-
35	CHL	N	606	-	-	9/17/93/117	-
23	CLA	Y	303	20	-	18/35/111/115	-
24	PHO	a	402	-	-	14/37/103/103	0/5/6/6
23	CLA	B	603	2	-	19/39/115/115	-
23	CLA	b	608	2	-	12/39/115/115	-
34	HEM	f	101	6,5	-	5/14/54/54	-
23	CLA	y	304	20	-	13/39/115/115	-
36	LUT	s	615	-	-	3/29/67/67	0/2/2/2
23	CLA	Y	305	-	-	9/21/97/115	-
23	CLA	Y	315	20	-	6/15/91/115	-
35	CHL	S	307	-	-	7/14/90/117	-
31	LHG	S	318	23	-	10/53/53/53	-
25	BCR	D	405	-	-	7/29/63/63	0/2/2/2
23	CLA	B	604	2	-	11/39/115/115	-
35	CHL	G	607	-	-	6/14/90/117	-
23	CLA	c	506	3	-	8/23/99/115	-
36	LUT	y	317	-	-	1/29/67/67	0/2/2/2
23	CLA	R	304	22	-	9/33/109/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
23	CLA	n	611	31	-	11/33/109/115	-
23	CLA	b	607	2	-	13/39/115/115	-
23	CLA	r	611	22	-	12/39/115/115	-
36	LUT	N	616	-	-	1/29/67/67	0/2/2/2
35	CHL	S	302	15	-	9/17/93/117	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	N	611	31	-	11/33/109/115	-
23	CLA	B	608	2	-	14/39/115/115	-
30	LMG	c	521	-	-	9/45/65/70	0/1/1/1
23	CLA	R	302	22	-	12/20/96/115	-
31	LHG	c	516	-	-	9/53/53/53	-
35	CHL	Y	310	20	-	20/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	-	-	7/33/109/115	-
32	DMU	C	523	-	-	6/19/59/59	0/2/2/2
26	SQD	A	406	-	-	5/45/65/69	0/1/1/1
25	BCR	h	101	-	-	7/29/63/63	0/2/2/2
38	NEX	g	618	-	-	2/27/83/83	0/3/3/3
23	CLA	g	612	7	-	9/15/91/115	-
23	CLA	N	610	7	-	9/32/108/115	-
23	CLA	C	514	3	-	7/39/115/115	-
35	CHL	g	605	7	-	12/17/93/117	-
38	NEX	R	316	-	-	5/27/83/83	0/3/3/3
23	CLA	A	404	1	-	14/33/109/115	-
38	NEX	r	615	-	-	5/27/83/83	0/3/3/3
23	CLA	c	501	3	-	14/39/115/115	-
23	CLA	g	602	7	-	16/39/115/115	-
26	SQD	B	625	-	-	19/49/69/69	0/1/1/1
23	CLA	Y	311	20	-	8/33/109/115	-
23	CLA	N	614	7	-	5/10/86/115	-
23	CLA	r	604	-	-	10/19/95/115	-
23	CLA	g	614	7	-	7/12/88/115	-
23	CLA	b	614	2	-	18/39/115/115	-
37	XAT	y	301	-	-	0/31/93/93	0/4/4/4
31	LHG	b	623	-	-	11/53/53/53	-
23	CLA	G	613	7	-	14/31/107/115	-
23	CLA	n	610	7	-	10/32/108/115	-
25	BCR	d	405	-	-	7/29/63/63	0/2/2/2
35	CHL	g	601	7	-	19/41/117/117	-
25	BCR	B	617	-	-	6/29/63/63	0/2/2/2
30	LMG	C	501	-	-	5/43/63/70	0/1/1/1
23	CLA	N	612	7	-	9/15/91/115	-
23	CLA	S	309	15	-	10/15/91/115	-
23	CLA	n	602	7	-	10/35/111/115	-
36	LUT	g	616	-	-	0/29/67/67	0/2/2/2
24	PHO	A	403	-	-	13/37/103/103	0/5/6/6
37	XAT	r	614	-	-	1/31/93/93	0/4/4/4
23	CLA	D	404	4	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	N	602	7	-	13/35/111/115	-
23	CLA	g	604	-	-	9/20/96/115	-
23	CLA	b	610	2	-	18/39/115/115	-
23	CLA	D	401	-	-	16/39/115/115	-
30	LMG	C	522	-	-	9/45/65/70	0/1/1/1
31	LHG	l	102	-	-	9/53/53/53	-
23	CLA	B	605	2	-	13/39/115/115	-
35	CHL	S	306	-	-	10/17/93/117	-
31	LHG	r	616	23	-	6/46/46/53	-
23	CLA	c	510	3	-	15/39/115/115	-
30	LMG	D	409	-	-	3/41/61/70	0/1/1/1
26	SQD	C	521	-	-	2/40/60/69	0/1/1/1
35	CHL	n	608	-	-	10/41/117/117	-
36	LUT	S	316	-	-	2/29/67/67	0/2/2/2
31	LHG	D	407	-	-	11/53/53/53	-
35	CHL	Y	302	20	-	17/41/117/117	-
31	LHG	c	517	-	-	12/53/53/53	-
23	CLA	d	403	4	-	11/39/115/115	-
36	LUT	r	613	-	-	2/29/67/67	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
30	LMG	S	301	-	-	5/50/70/70	0/1/1/1
23	CLA	Y	312	31	-	11/33/109/115	-
23	CLA	B	614	2	-	23/39/115/115	-
35	CHL	s	601	15	-	8/17/93/117	-
23	CLA	c	502	3	-	13/39/115/115	-
23	CLA	B	607	-	-	15/39/115/115	-
36	LUT	N	615	-	-	2/29/67/67	0/2/2/2
23	CLA	R	313	22	-	11/39/115/115	-
28	DGD	D	410	-	-	4/51/91/95	0/2/2/2
35	CHL	s	606	-	-	6/14/90/117	-
23	CLA	r	608	22	-	9/31/107/115	-

The worst 5 of 1723 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	406	PL9	C23-C24	10.33	1.57	1.33
33	D	406	PL9	C23-C24	10.29	1.57	1.33
33	d	406	PL9	C38-C39	10.14	1.57	1.33
33	D	406	PL9	C38-C39	10.02	1.57	1.33
33	d	406	PL9	C18-C19	9.68	1.56	1.33

The worst 5 of 2385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	625	SQD	O9-S-C6	-20.17	82.96	106.94
26	C	521	SQD	O9-S-C6	-20.02	83.14	106.94
26	c	520	SQD	O9-S-C6	-19.99	83.18	106.94
26	b	602	SQD	O9-S-C6	-19.91	83.27	106.94
38	R	301	NEX	C17-C1-C6	-17.45	94.86	110.47

There are no chirality outliers.

5 of 3166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	401	CLA	CBD-CGD-O2D-CED
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	402	CLA	C2B-C3B-CAB-CBB
23	A	402	CLA	C4B-C3B-CAB-CBB
23	A	402	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

260 monomers are involved in 465 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	516	BCR	1	0
32	c	522	DMU	1	0
23	B	612	CLA	4	0
31	l	103	LHG	1	0
35	n	607	CHL	2	0
31	R	317	LHG	1	0
23	C	503	CLA	3	0
23	c	509	CLA	3	0
35	y	308	CHL	5	0
23	g	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	y	302	CHL	3	0
31	D	408	LHG	3	0
25	B	619	BCR	4	0
31	L	102	LHG	1	0
35	y	307	CHL	1	0
23	b	611	CLA	1	0
23	S	314	CLA	1	0
31	n	618	LHG	1	0
23	y	313	CLA	2	0
23	A	402	CLA	1	0
23	g	613	CLA	1	0
35	N	608	CHL	3	0
35	R	308	CHL	1	0
28	B	624	DGD	4	0
35	G	601	CHL	5	0
31	B	622	LHG	1	0
35	g	608	CHL	1	0
28	d	410	DGD	5	0
26	b	602	SQD	3	0
37	G	617	XAT	2	0
23	R	303	CLA	2	0
38	n	617	NEX	1	0
31	s	617	LHG	2	0
23	b	609	CLA	3	0
35	y	310	CHL	4	0
23	G	602	CLA	4	0
24	D	402	PHO	5	0
23	B	601	CLA	1	0
37	g	620	XAT	5	0
35	S	308	CHL	2	0
28	A	408	DGD	1	0
36	g	615	LUT	3	0
31	g	619	LHG	4	0
25	C	519	BCR	3	0
23	b	618	CLA	2	0
36	S	315	LUT	2	0
26	L	103	SQD	1	0
23	c	513	CLA	3	0
35	y	306	CHL	1	0
23	Y	304	CLA	4	0
23	r	602	CLA	1	0
23	C	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	407	BCT	2	0
36	y	316	LUT	4	0
31	d	407	LHG	2	0
31	d	408	LHG	5	0
26	l	101	SQD	4	0
36	G	615	LUT	4	0
23	n	612	CLA	2	0
25	H	101	BCR	3	0
38	S	317	NEX	1	0
23	G	610	CLA	2	0
25	A	405	BCR	1	0
23	b	606	CLA	1	0
37	R	315	XAT	1	0
32	c	519	DMU	1	0
23	b	612	CLA	1	0
35	n	606	CHL	1	0
23	C	502	CLA	1	0
38	s	616	NEX	1	0
23	r	601	CLA	1	0
23	n	603	CLA	1	0
38	G	618	NEX	1	0
24	a	403	PHO	4	0
25	z	101	BCR	2	0
25	K	101	BCR	1	0
30	b	601	LMG	2	0
23	s	609	CLA	2	0
23	R	310	CLA	3	0
31	C	518	LHG	2	0
23	y	305	CLA	2	0
23	C	509	CLA	3	0
23	N	604	CLA	1	0
23	c	507	CLA	2	0
34	F	101	HEM	1	0
30	b	622	LMG	4	0
33	D	406	PL9	2	0
23	S	310	CLA	2	0
23	B	610	CLA	1	0
23	C	510	CLA	1	0
37	G	620	XAT	2	0
35	N	607	CHL	1	0
23	s	603	CLA	1	0
23	C	507	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	Y	301	XAT	5	0
35	N	605	CHL	1	0
23	r	612	CLA	1	0
23	b	616	CLA	3	0
25	a	405	BCR	4	0
26	a	406	SQD	2	0
35	N	609	CHL	1	0
37	g	617	XAT	1	0
23	A	401	CLA	2	0
23	d	401	CLA	3	0
35	y	309	CHL	1	0
31	N	618	LHG	2	0
23	y	311	CLA	3	0
23	R	309	CLA	1	0
38	N	617	NEX	3	0
31	G	619	LHG	2	0
23	s	602	CLA	2	0
36	n	616	LUT	3	0
23	S	304	CLA	1	0
36	n	615	LUT	4	0
31	B	621	LHG	1	0
23	Y	313	CLA	2	0
23	y	312	CLA	1	0
36	s	614	LUT	2	0
23	B	602	CLA	2	0
35	r	607	CHL	2	0
23	g	610	CLA	1	0
23	d	402	CLA	1	0
32	s	618	DMU	1	0
23	S	311	CLA	1	0
25	b	620	BCR	2	0
35	Y	309	CHL	2	0
23	R	311	CLA	2	0
25	b	619	BCR	5	0
23	G	603	CLA	1	0
35	N	601	CHL	3	0
35	Y	308	CHL	4	0
30	B	623	LMG	1	0
23	a	404	CLA	2	0
23	r	603	CLA	1	0
23	C	511	CLA	3	0
32	C	520	DMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	611	CLA	2	0
23	B	616	CLA	1	0
36	Y	317	LUT	2	0
35	n	601	CHL	4	0
26	c	520	SQD	1	0
23	b	615	CLA	4	0
32	S	319	DMU	1	0
31	B	627	LHG	1	0
23	b	604	CLA	1	0
23	r	610	CLA	1	0
23	r	609	CLA	1	0
35	G	608	CHL	2	0
31	W	201	LHG	1	0
23	c	511	CLA	1	0
23	n	604	CLA	1	0
23	C	508	CLA	3	0
23	C	504	CLA	2	0
30	B	620	LMG	5	0
38	Y	318	NEX	1	0
23	b	605	CLA	1	0
23	B	606	CLA	2	0
36	R	314	LUT	4	0
23	B	613	CLA	5	0
23	G	614	CLA	1	0
23	S	303	CLA	2	0
36	Y	316	LUT	5	0
23	R	305	CLA	1	0
23	s	611	CLA	1	0
36	G	616	LUT	2	0
25	c	518	BCR	4	0
38	R	301	NEX	3	0
23	c	503	CLA	2	0
35	R	307	CHL	1	0
35	n	609	CHL	2	0
31	b	624	LHG	2	0
28	c	515	DGD	2	0
25	b	621	BCR	4	0
23	b	617	CLA	1	0
31	y	318	LHG	3	0
31	L	101	LHG	3	0
23	D	403	CLA	6	0
35	g	609	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	508	CLA	2	0
28	C	517	DGD	2	0
23	a	401	CLA	3	0
35	s	607	CHL	3	0
31	Y	319	LHG	3	0
23	S	305	CLA	1	0
23	Y	303	CLA	2	0
23	B	603	CLA	1	0
23	b	608	CLA	4	0
34	f	101	HEM	1	0
23	y	304	CLA	4	0
36	s	615	LUT	2	0
23	Y	305	CLA	2	0
35	S	307	CHL	2	0
31	S	318	LHG	3	0
25	D	405	BCR	1	0
23	B	604	CLA	2	0
23	c	506	CLA	1	0
27	a	408	BCT	2	0
36	y	317	LUT	3	0
25	c	514	BCR	2	0
23	n	611	CLA	1	0
36	N	616	LUT	4	0
25	k	101	BCR	3	0
23	N	611	CLA	1	0
23	B	608	CLA	1	0
23	R	302	CLA	1	0
31	c	516	LHG	2	0
35	Y	310	CHL	5	0
32	C	523	DMU	1	0
25	h	101	BCR	2	0
38	g	618	NEX	1	0
23	N	610	CLA	2	0
23	C	514	CLA	4	0
35	g	605	CHL	1	0
38	R	316	NEX	3	0
23	A	404	CLA	3	0
38	r	615	NEX	1	0
23	g	602	CLA	5	0
26	B	625	SQD	3	0
23	Y	311	CLA	4	0
23	r	604	CLA	1	0

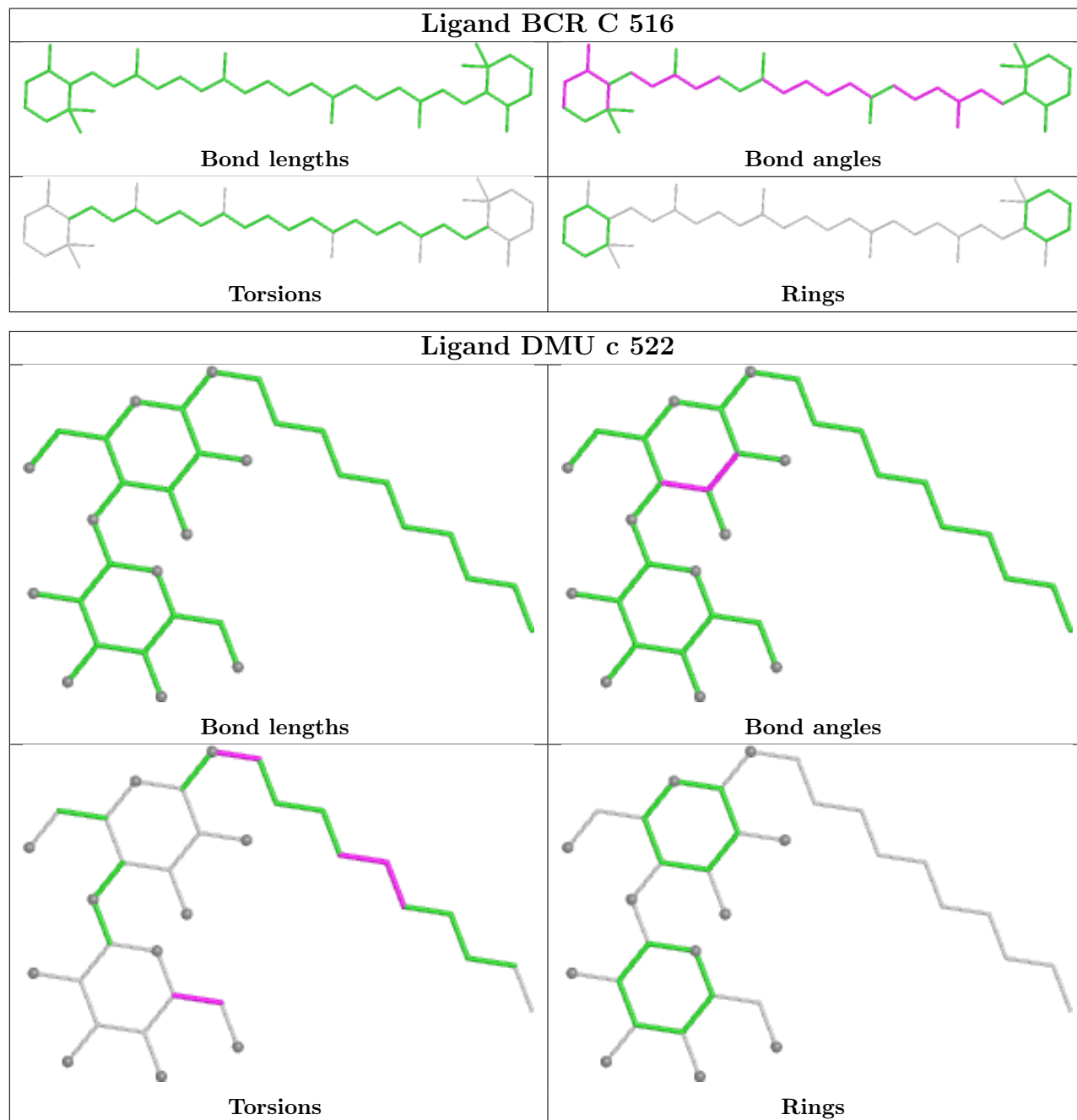
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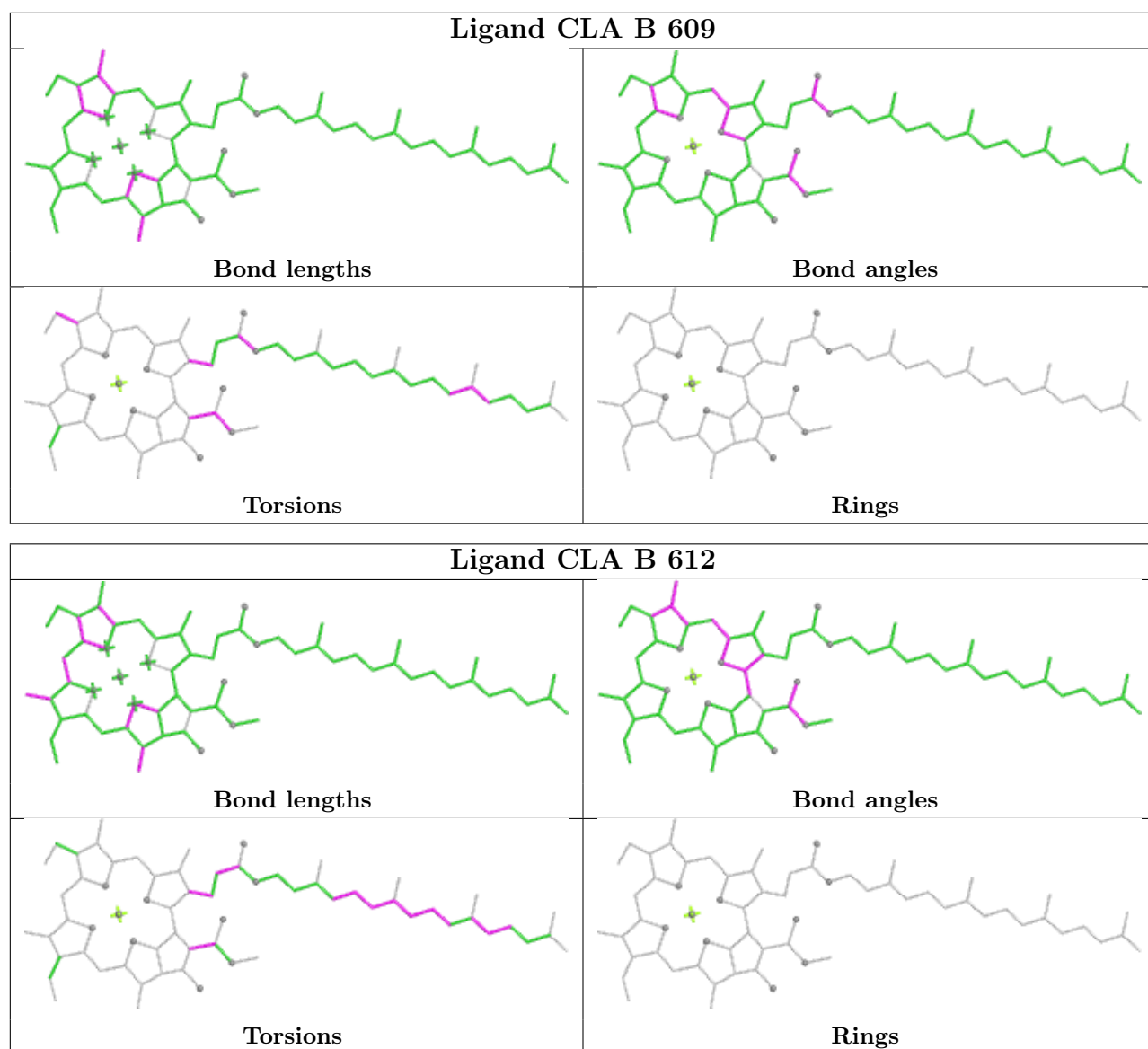
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	g	614	CLA	1	0
23	b	614	CLA	2	0
37	y	301	XAT	6	0
31	b	623	LHG	1	0
23	G	613	CLA	2	0
23	n	610	CLA	2	0
25	d	405	BCR	1	0
35	g	601	CHL	5	0
25	B	617	BCR	4	0
30	C	501	LMG	2	0
23	N	612	CLA	2	0
23	n	602	CLA	1	0
36	g	616	LUT	2	0
24	A	403	PHO	3	0
37	r	614	XAT	2	0
23	N	602	CLA	1	0
23	g	604	CLA	1	0
23	b	610	CLA	3	0
23	D	401	CLA	3	0
31	l	102	LHG	2	0
35	S	306	CHL	3	0
31	r	616	LHG	1	0
23	c	510	CLA	1	0
30	D	409	LMG	1	0
26	C	521	SQD	2	0
35	n	608	CHL	3	0
36	S	316	LUT	4	0
31	D	407	LHG	1	0
35	Y	302	CHL	2	0
23	d	403	CLA	4	0
36	r	613	LUT	3	0
25	C	515	BCR	7	0
23	Y	312	CLA	1	0
23	B	614	CLA	3	0
23	c	502	CLA	3	0
23	B	607	CLA	3	0
36	N	615	LUT	5	0
23	R	313	CLA	2	0
28	D	410	DGD	3	0
23	r	608	CLA	2	0

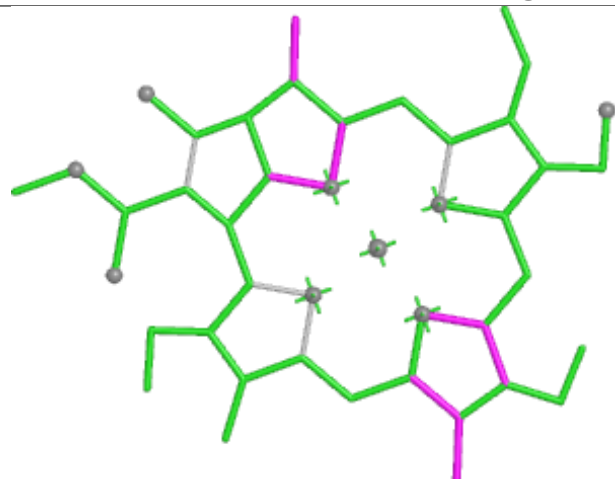
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

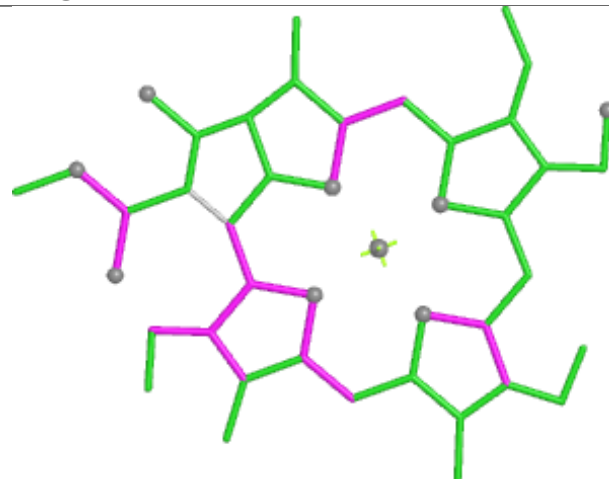




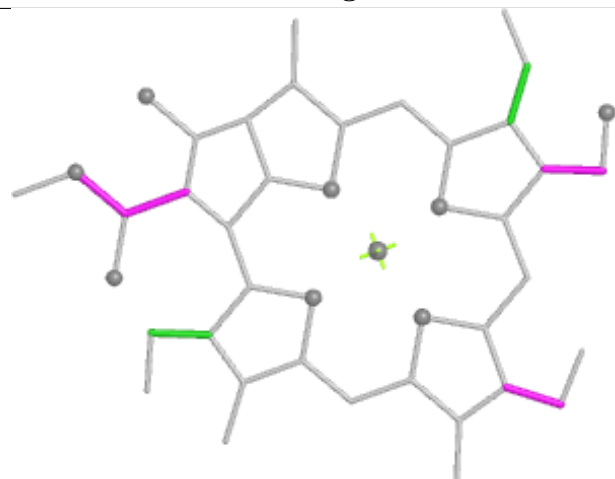
Ligand CHL g 607



Bond lengths



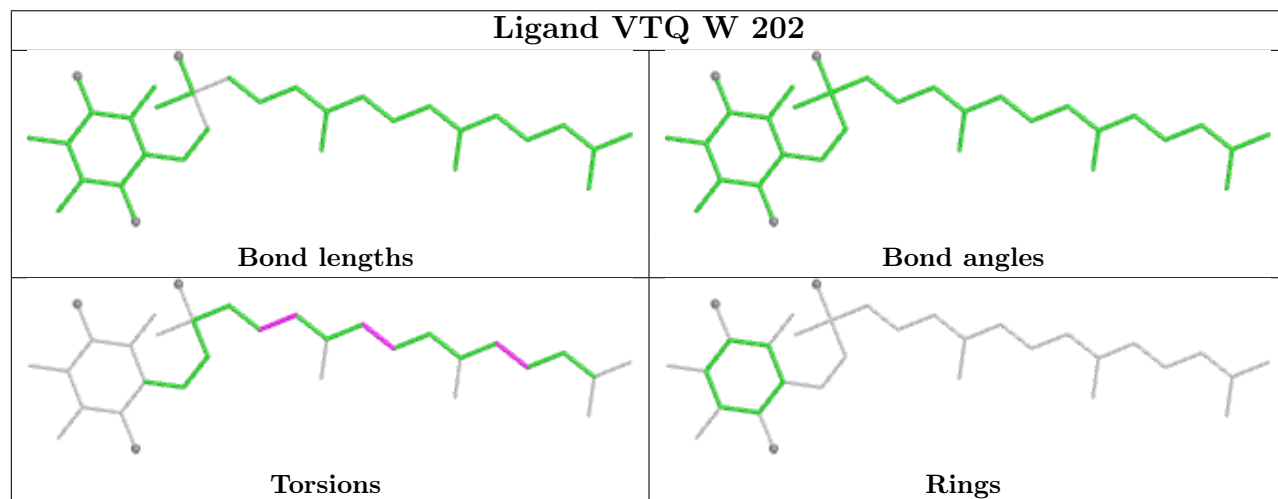
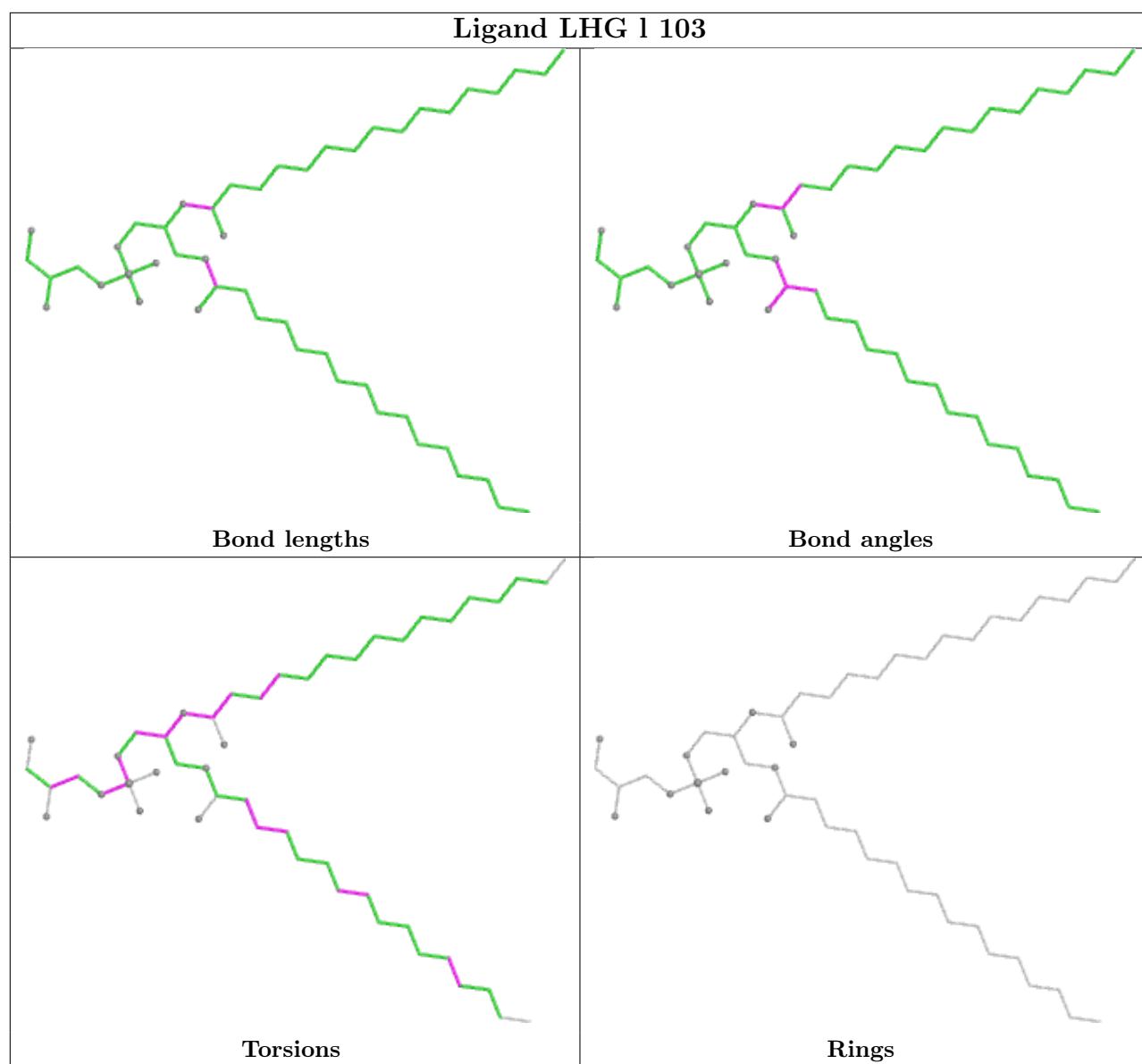
Bond angles



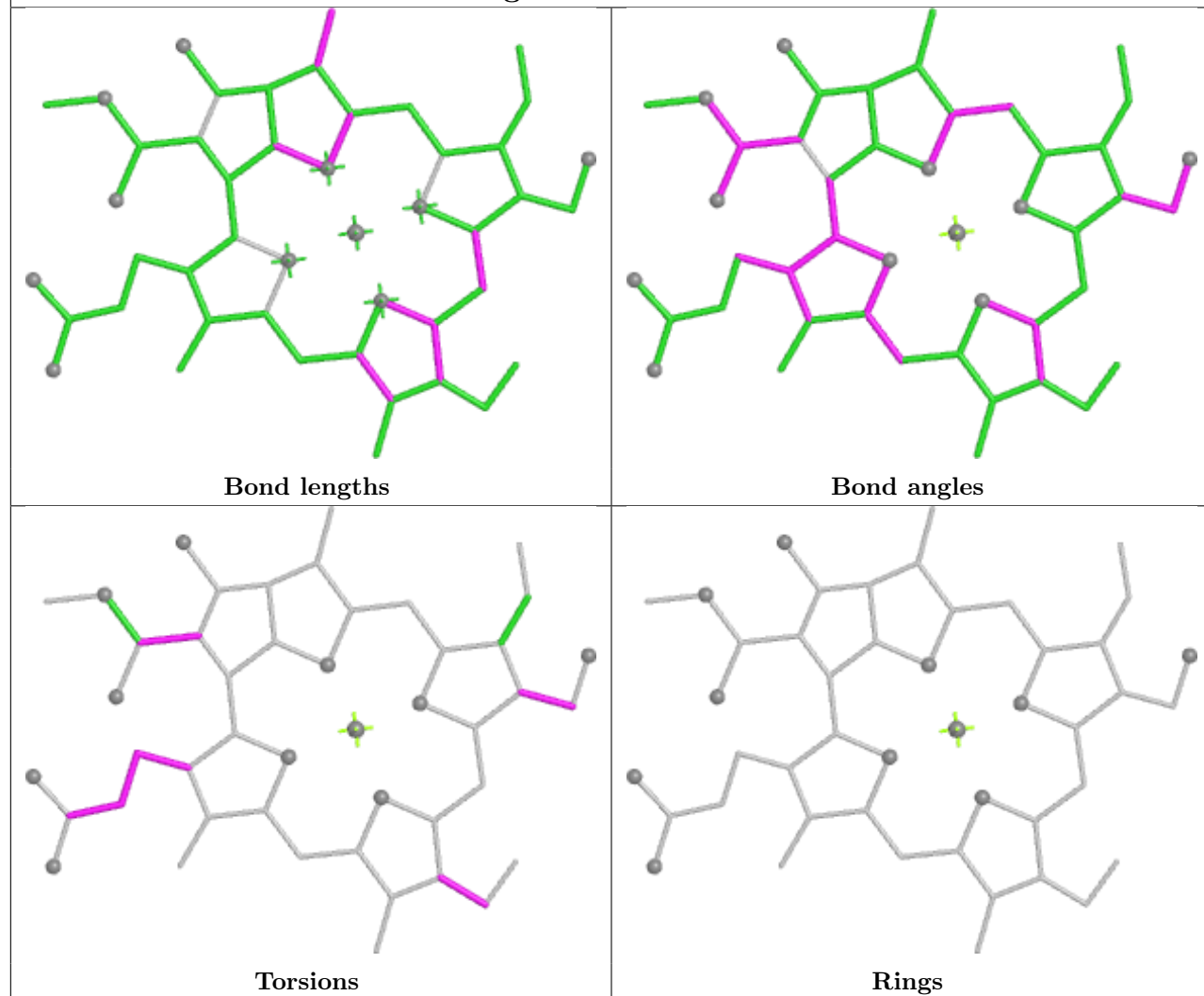
Torsions

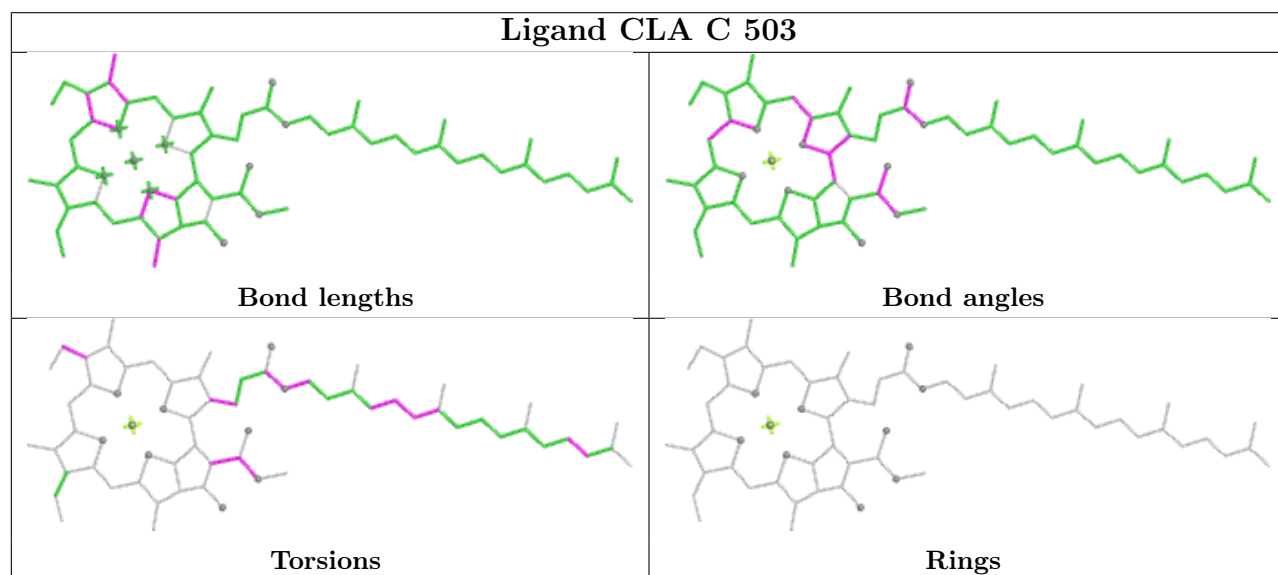
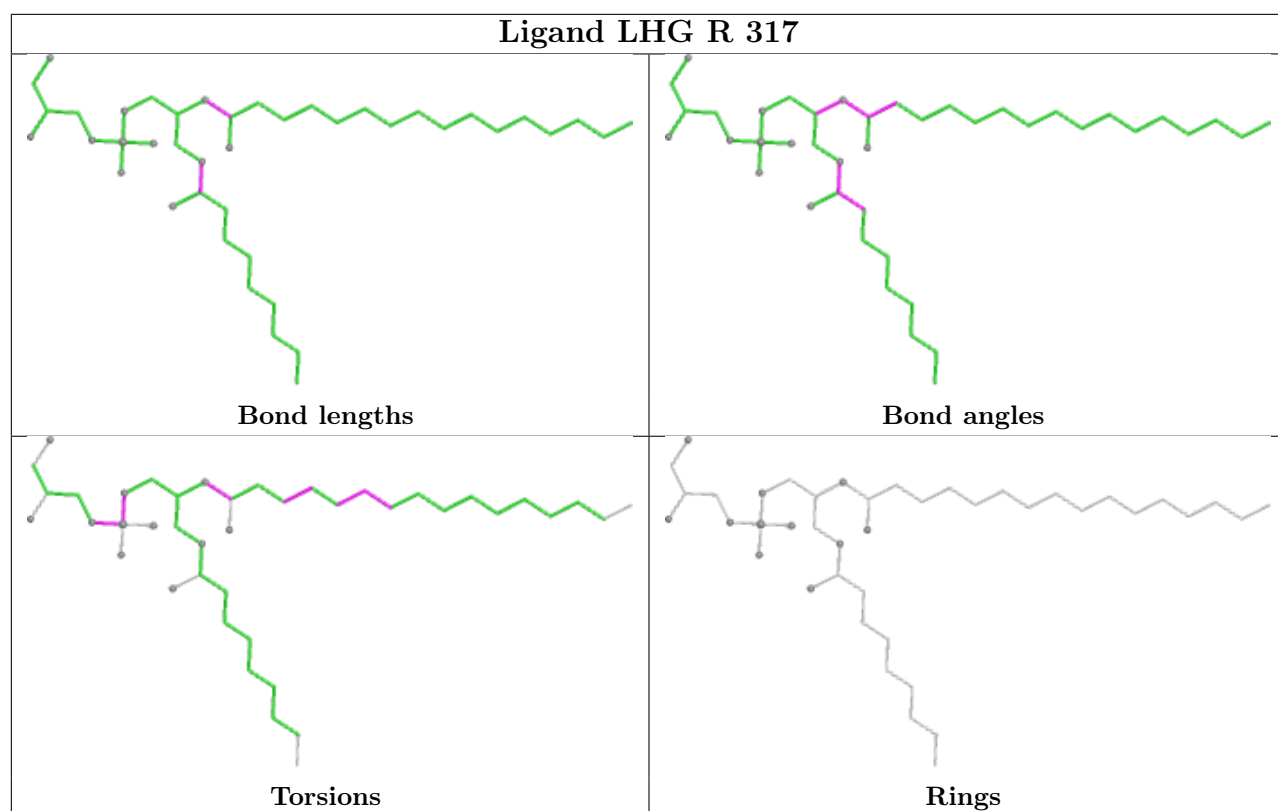


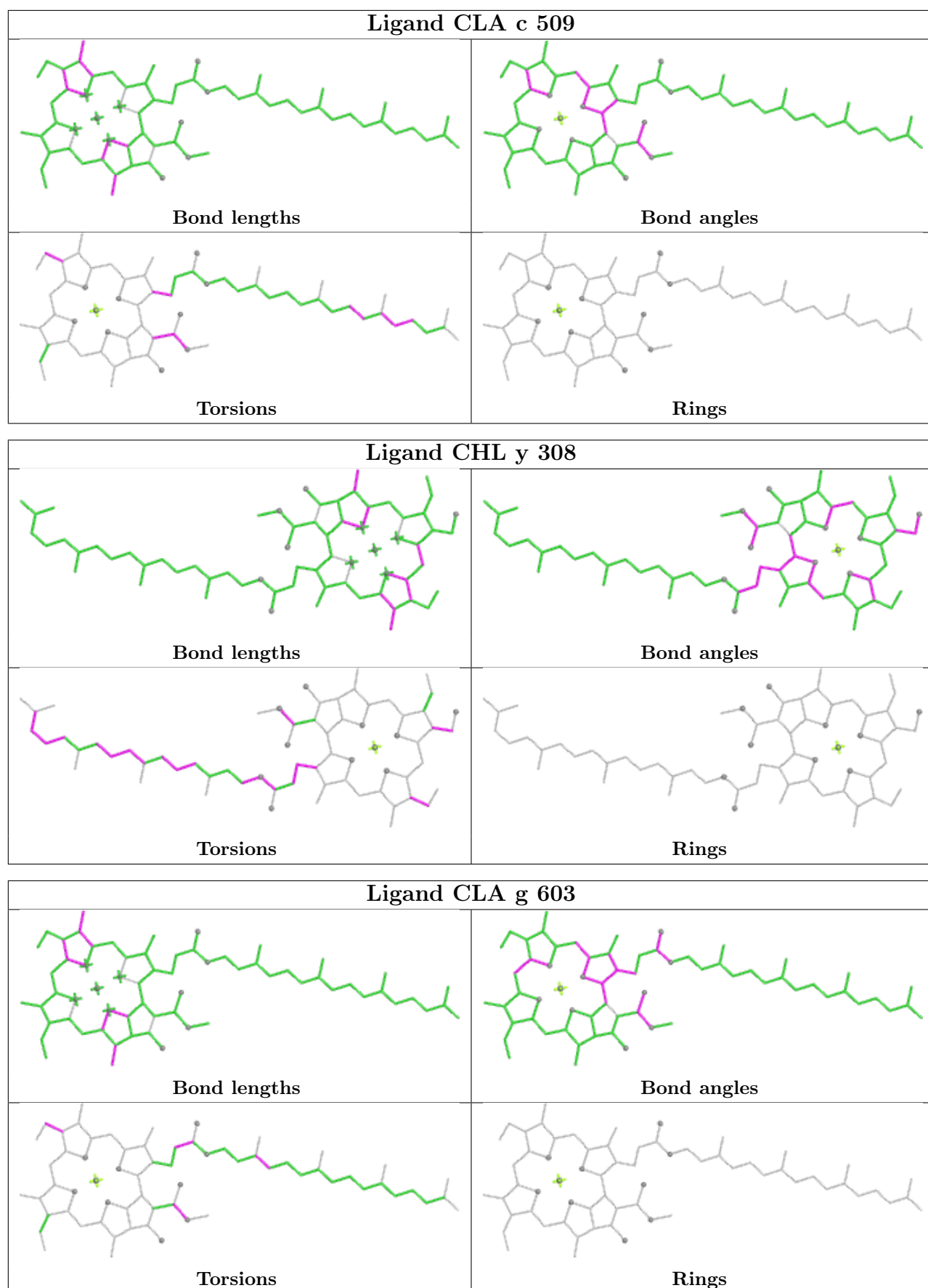
Rings

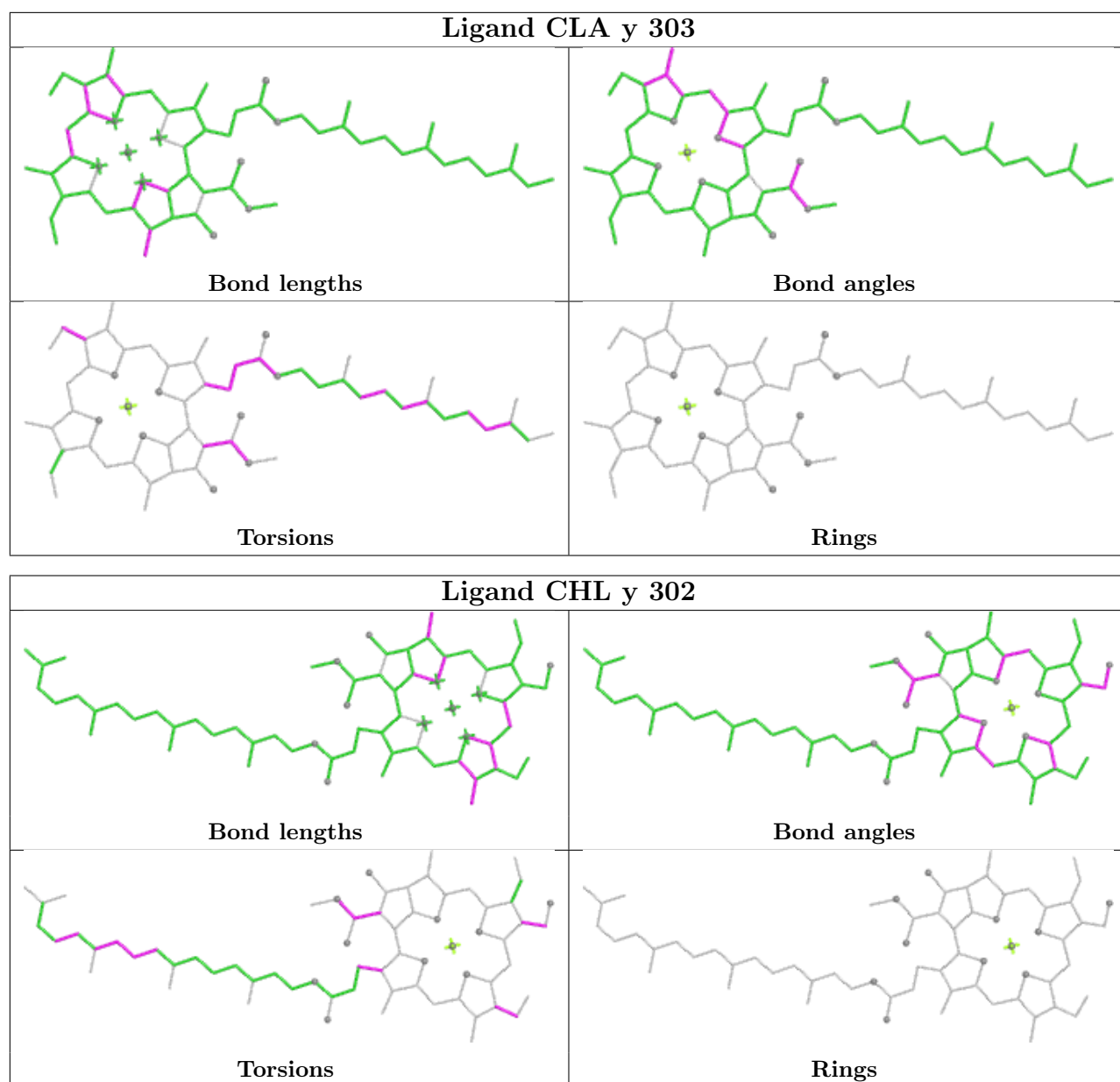


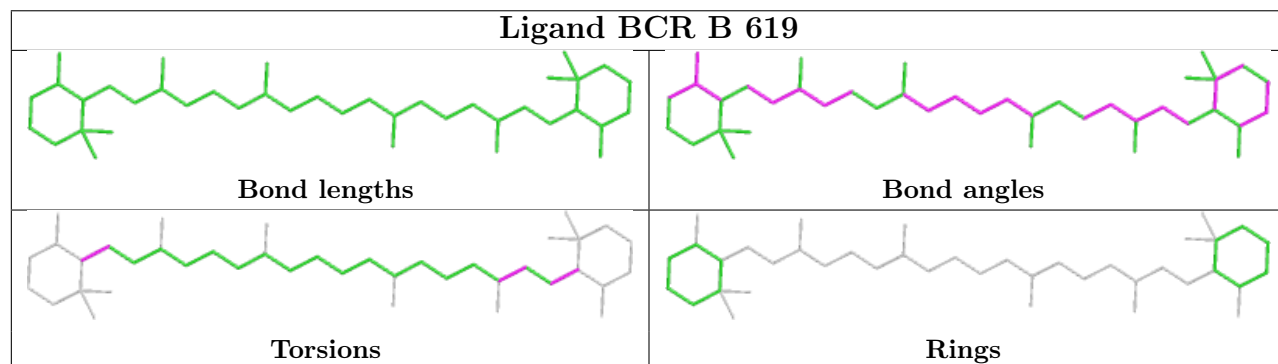
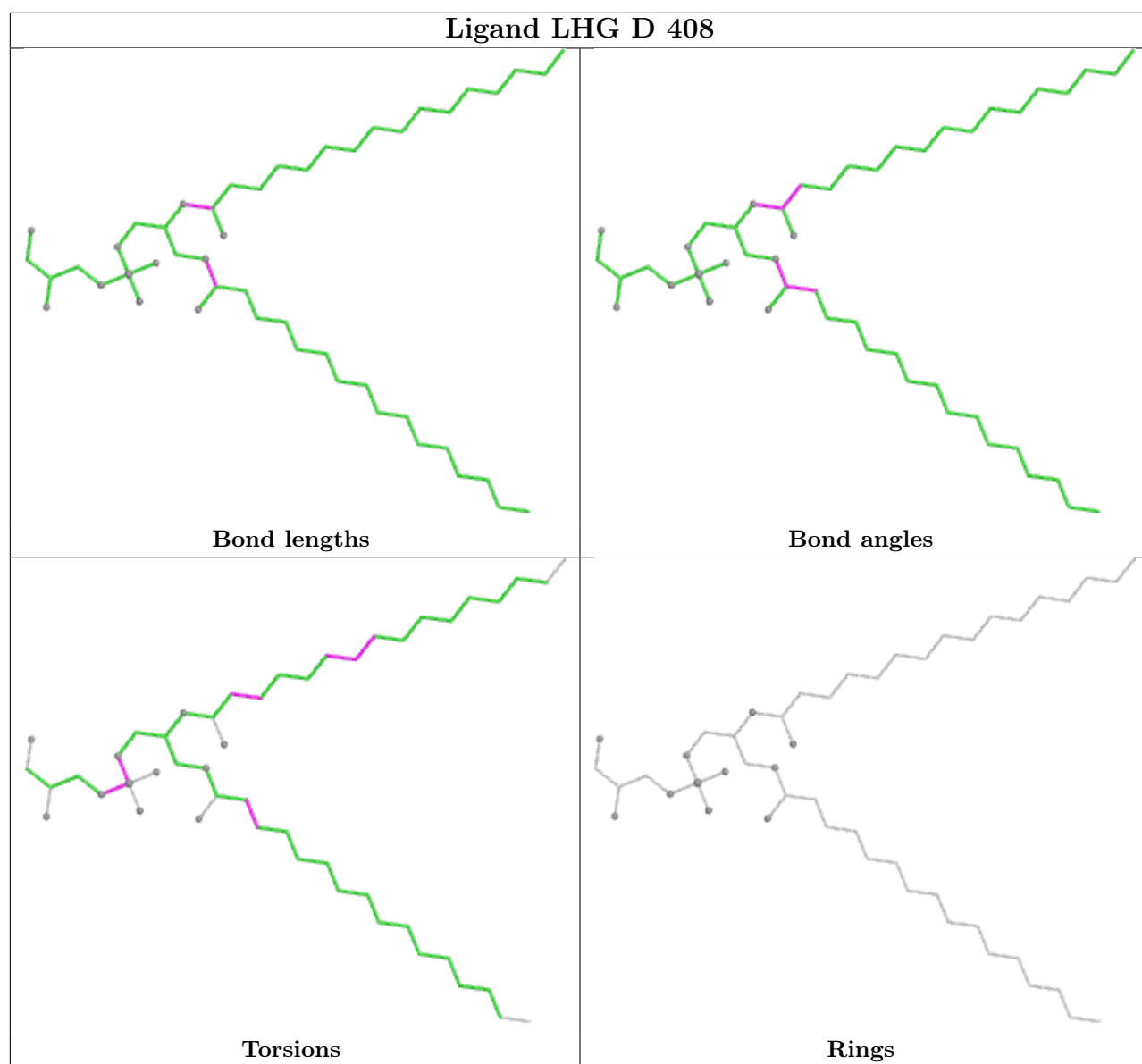
Ligand CHL n 607

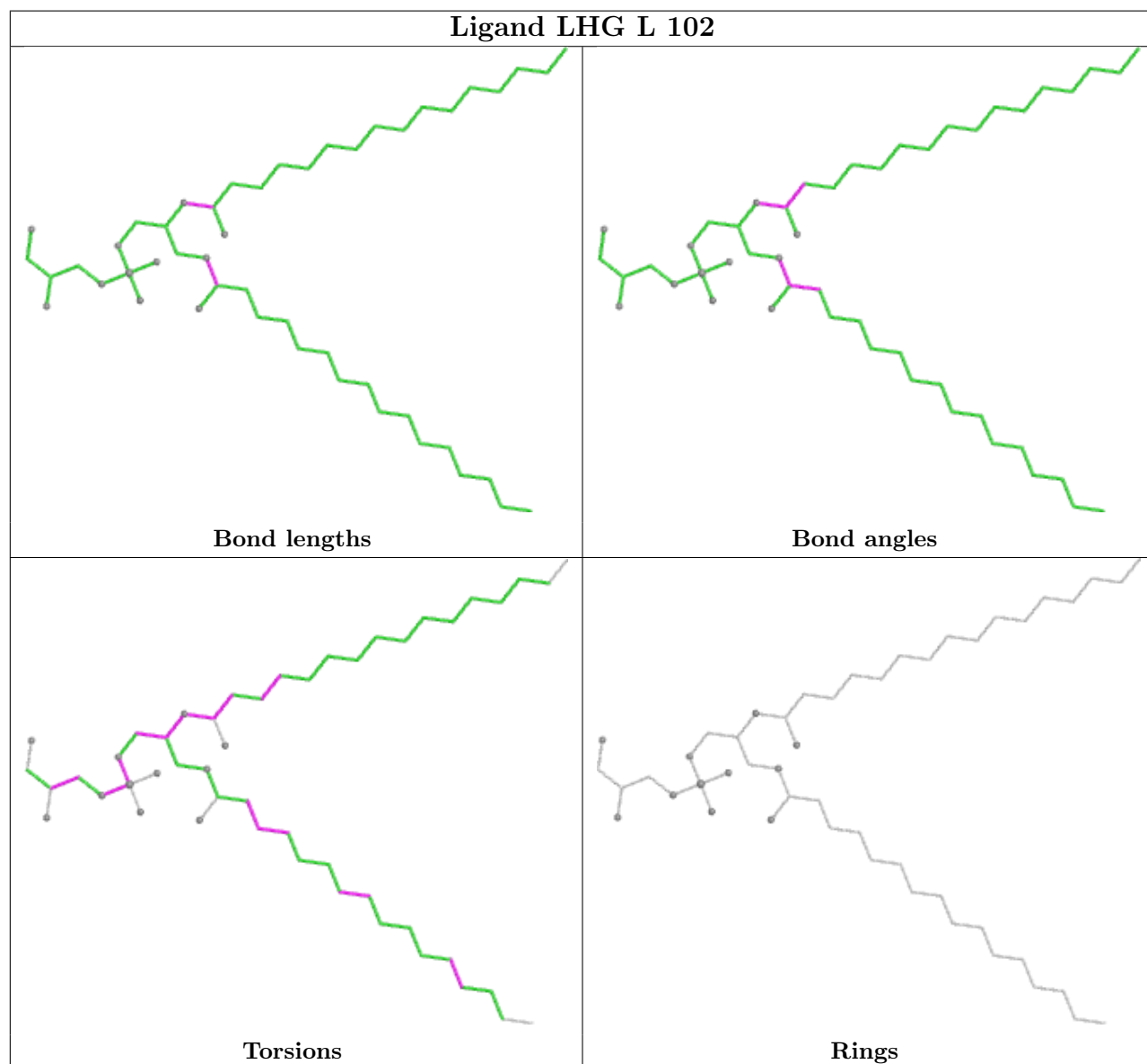
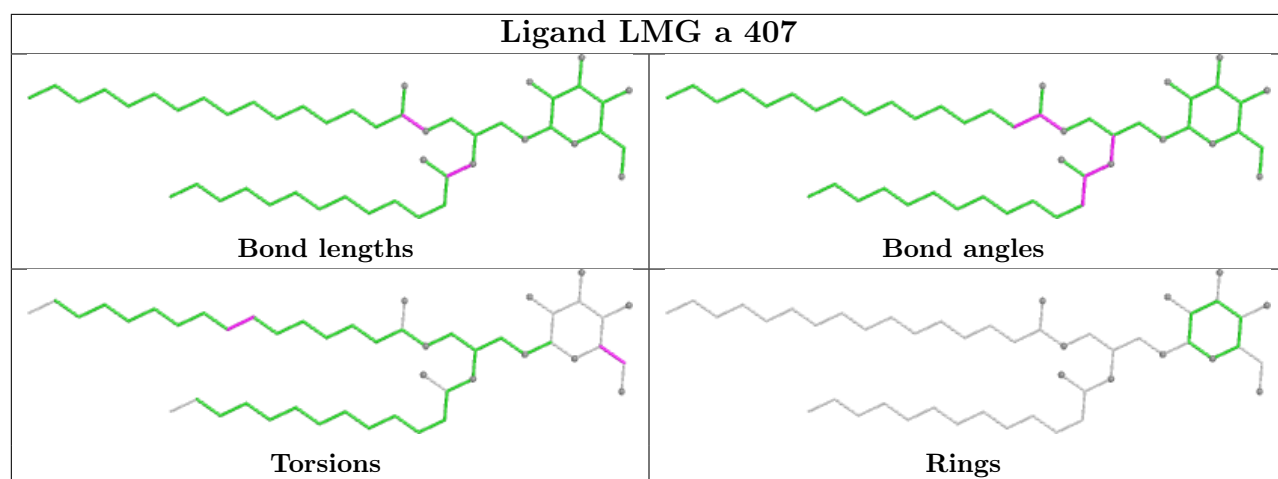


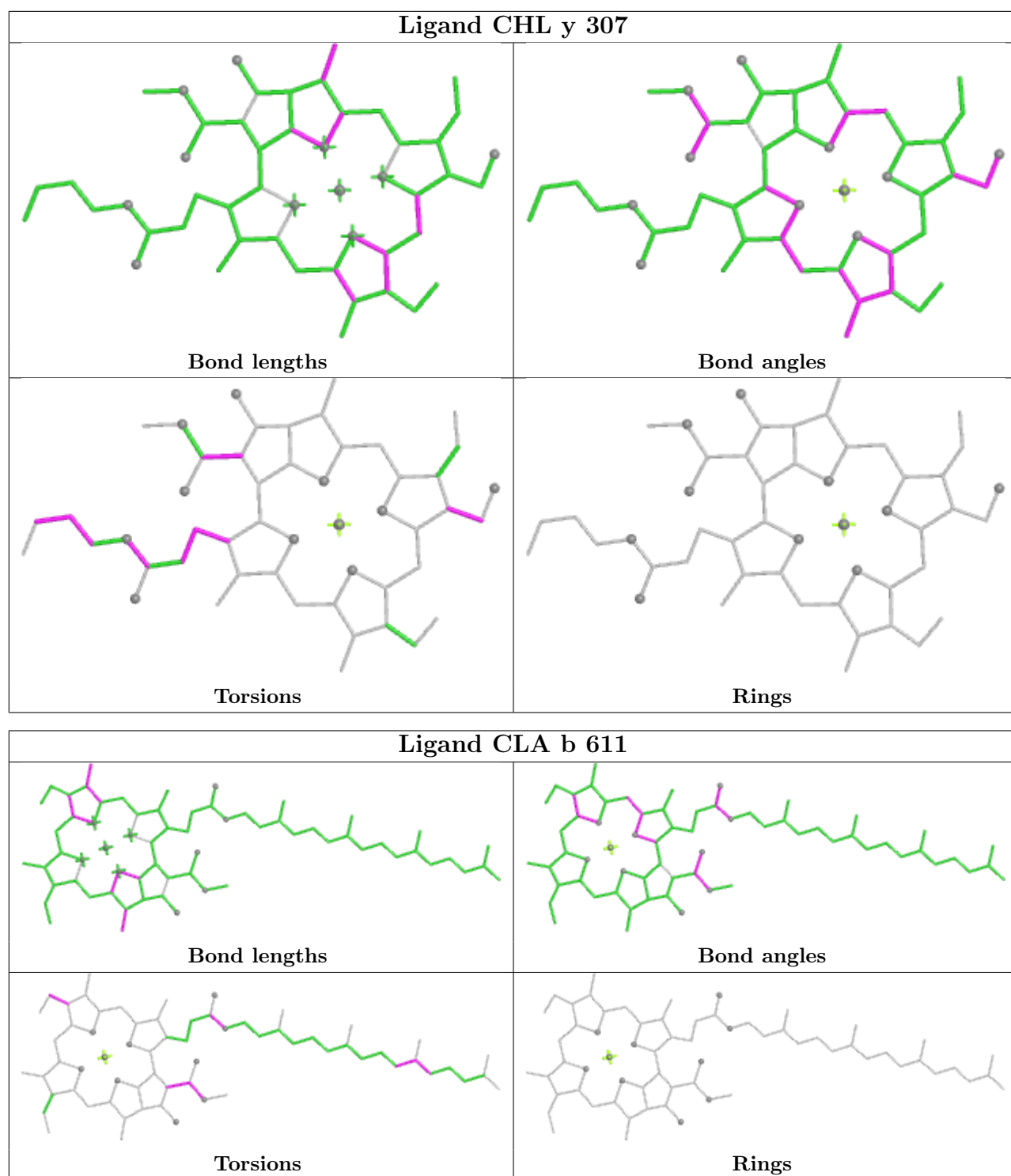


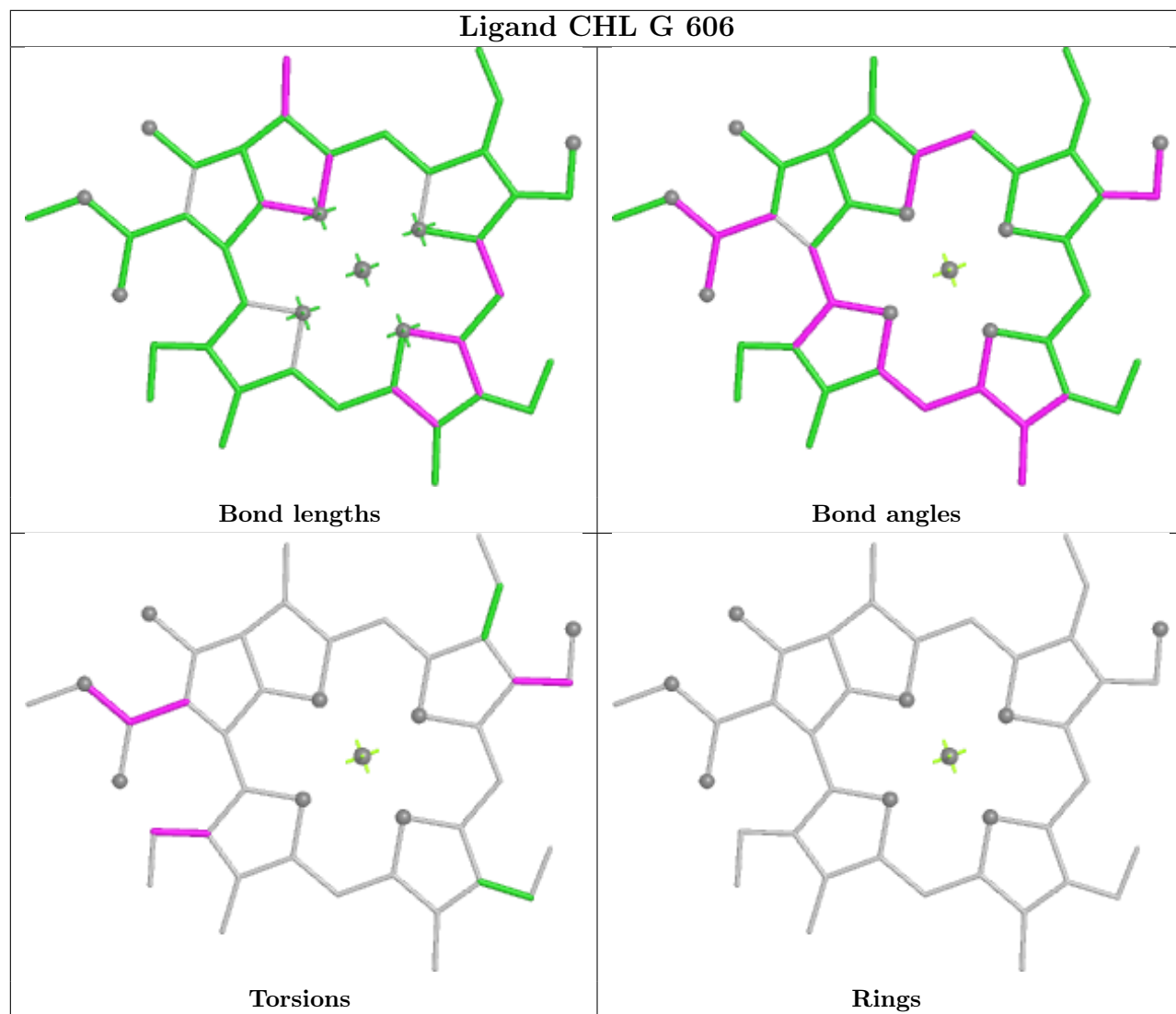




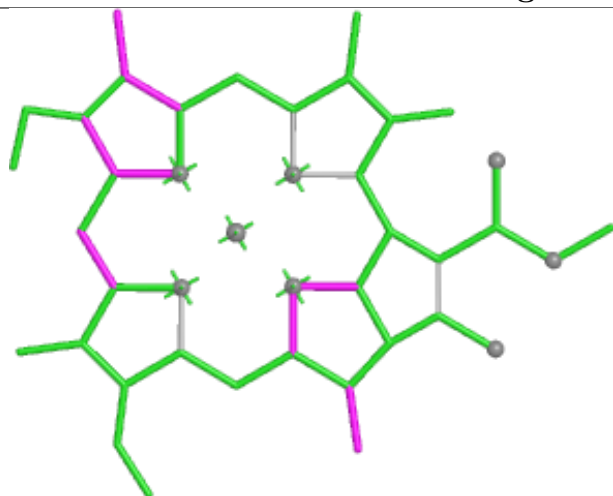








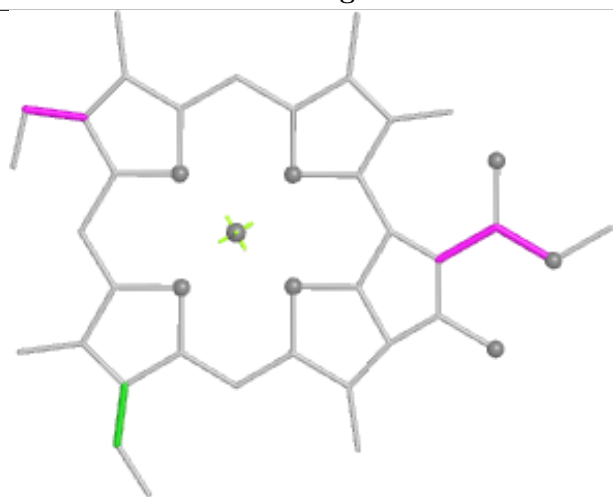
Ligand CLA S 314



Bond lengths



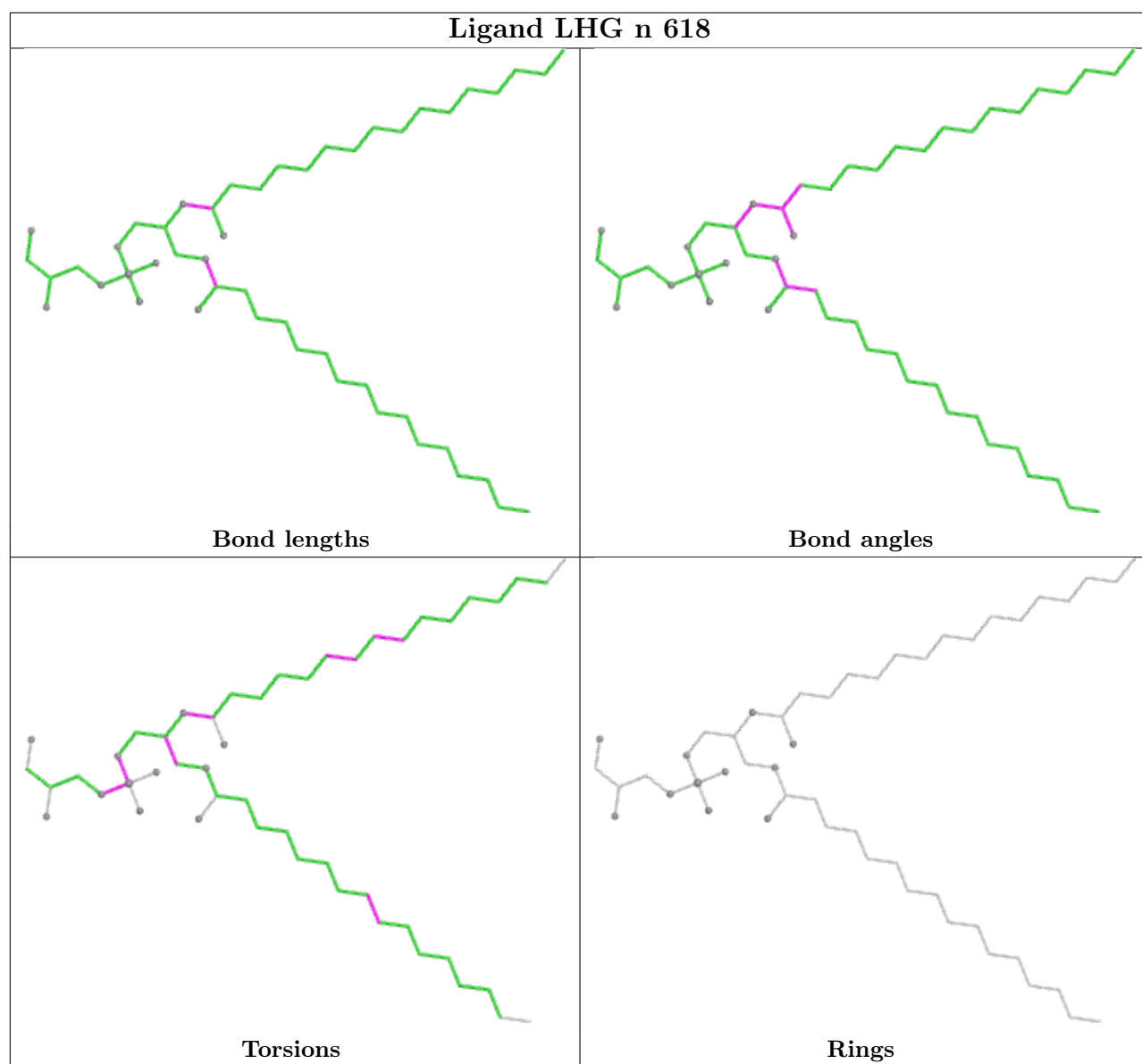
Bond angles

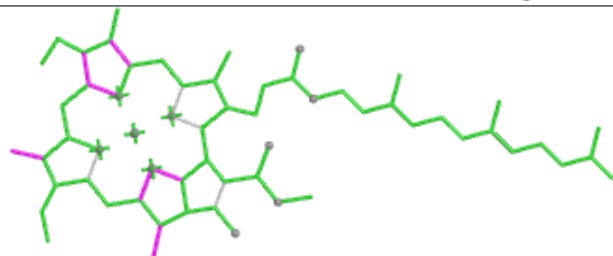
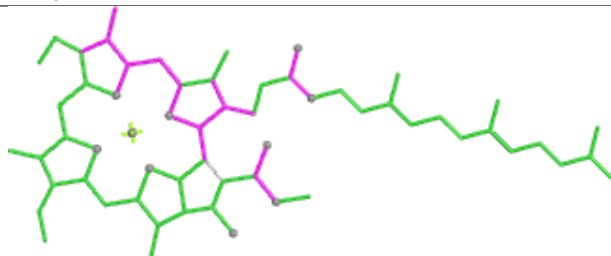
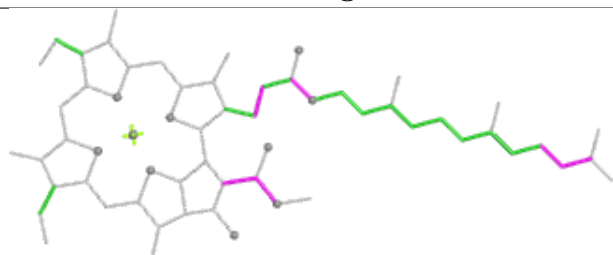
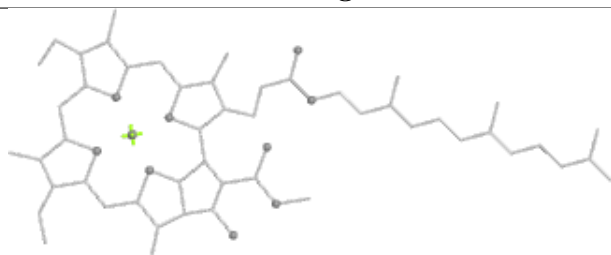
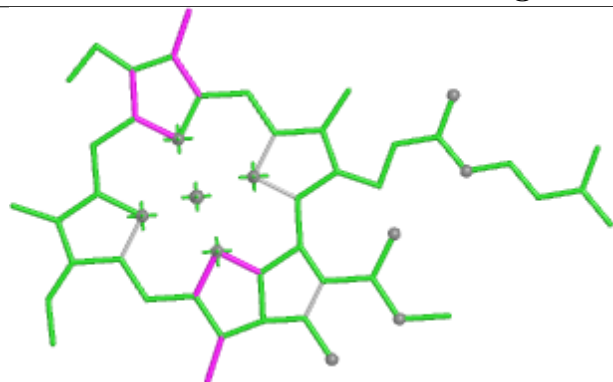
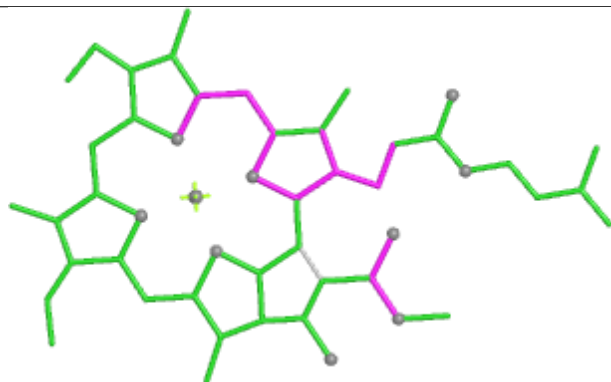
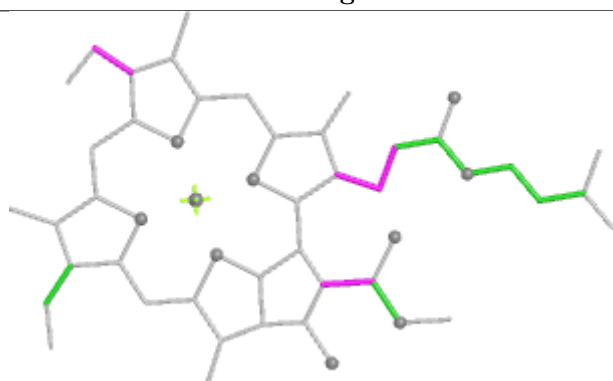
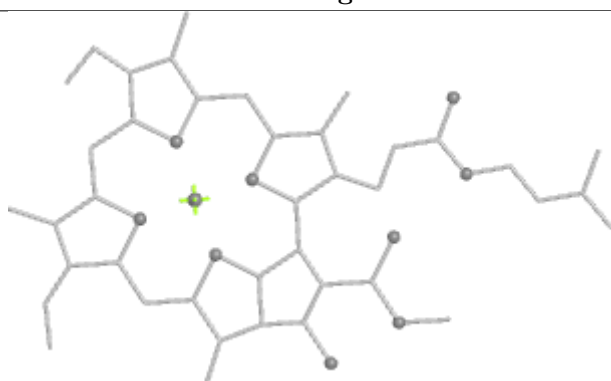


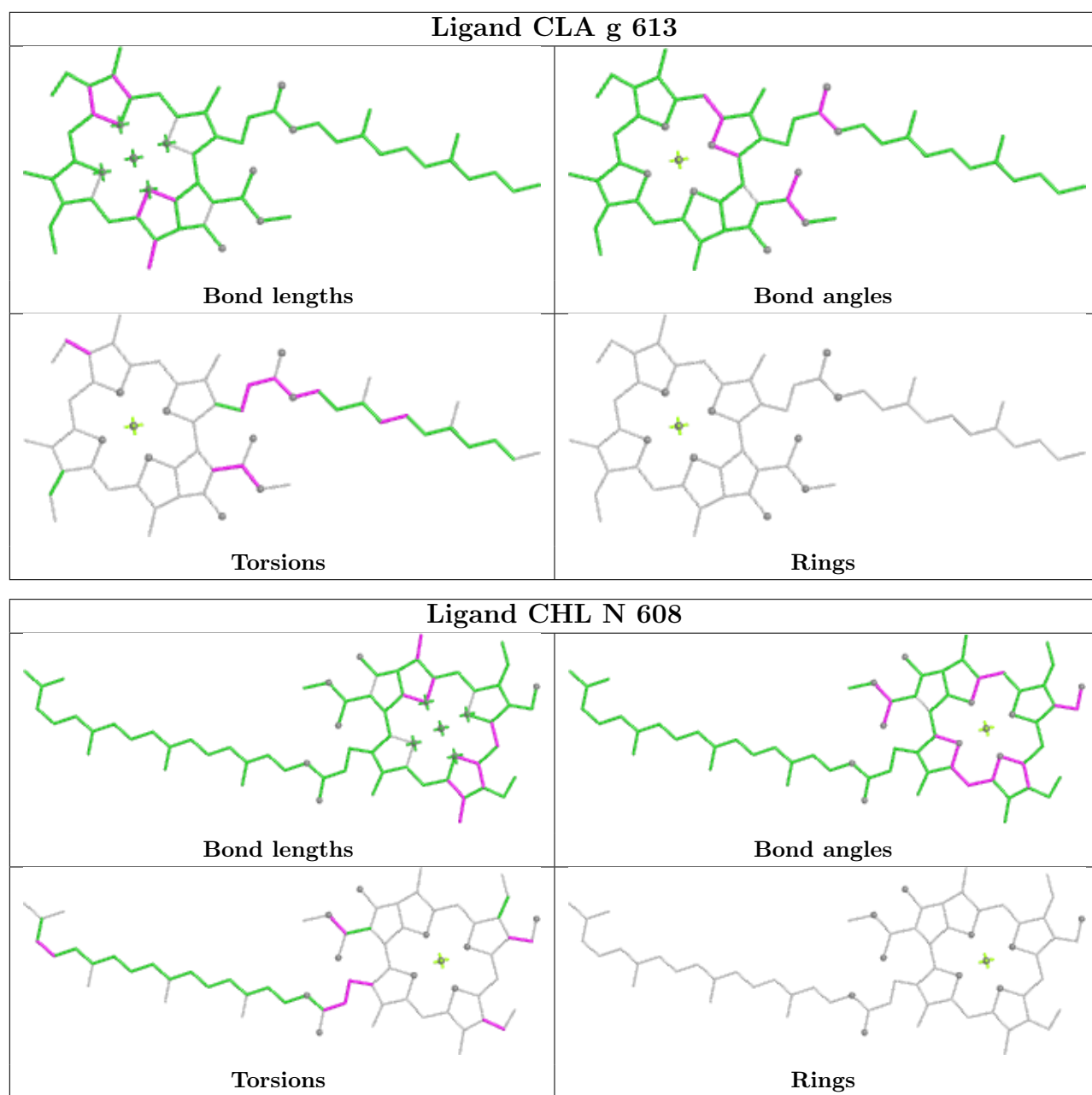
Torsions

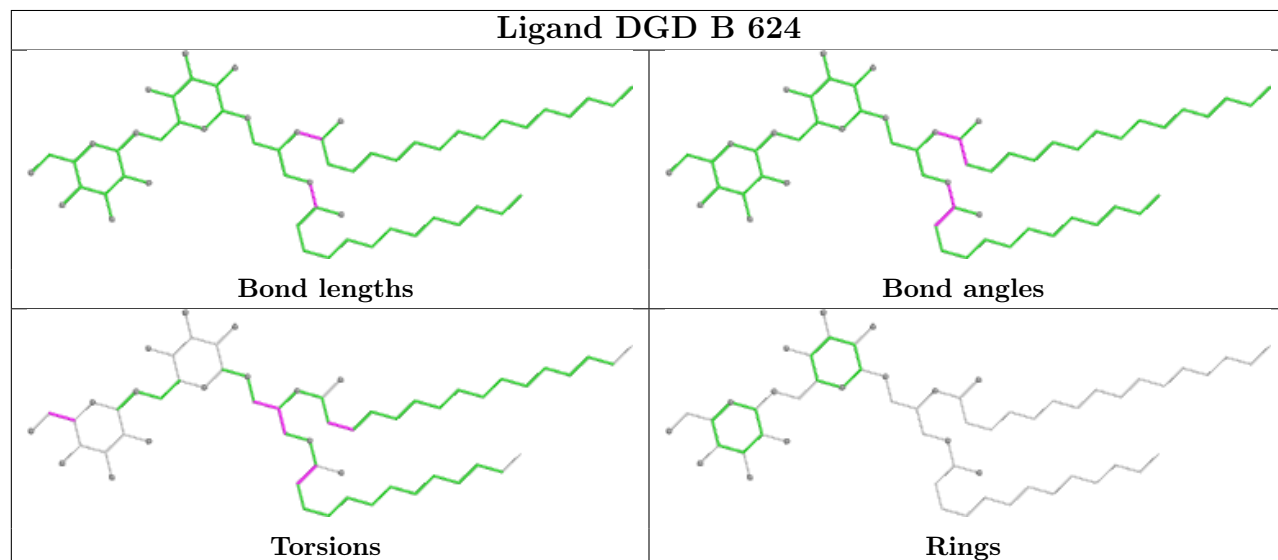
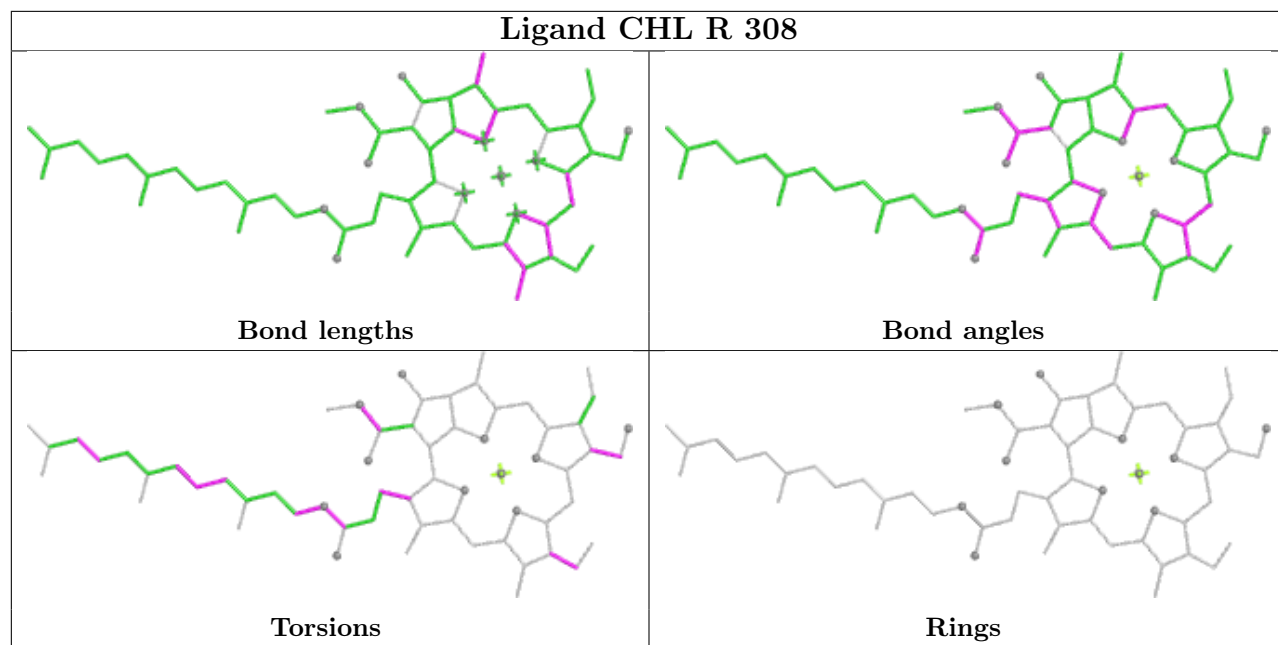


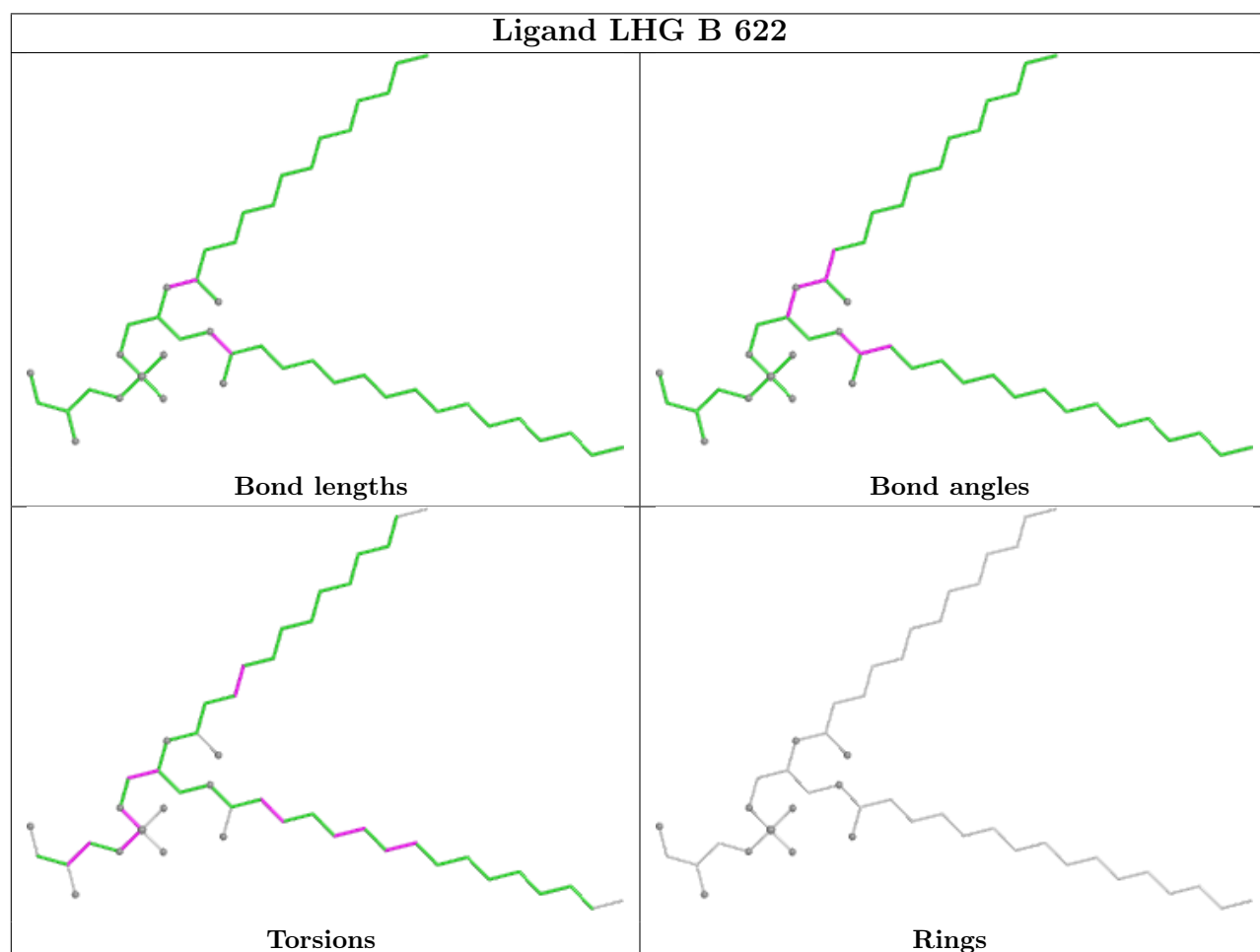
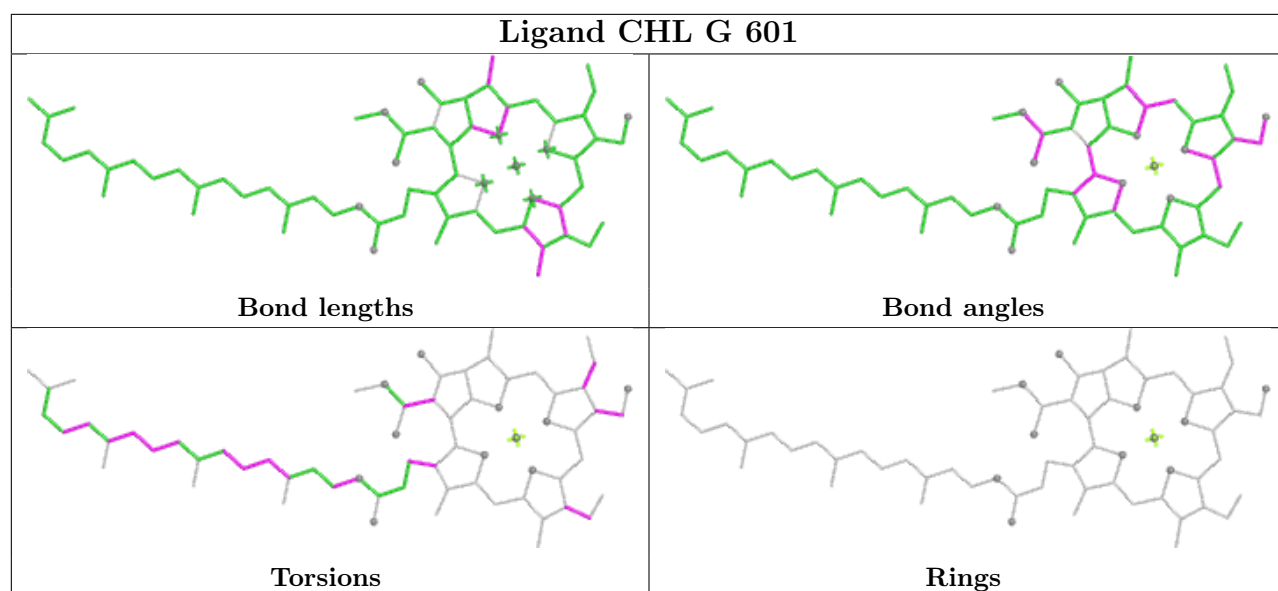
Rings

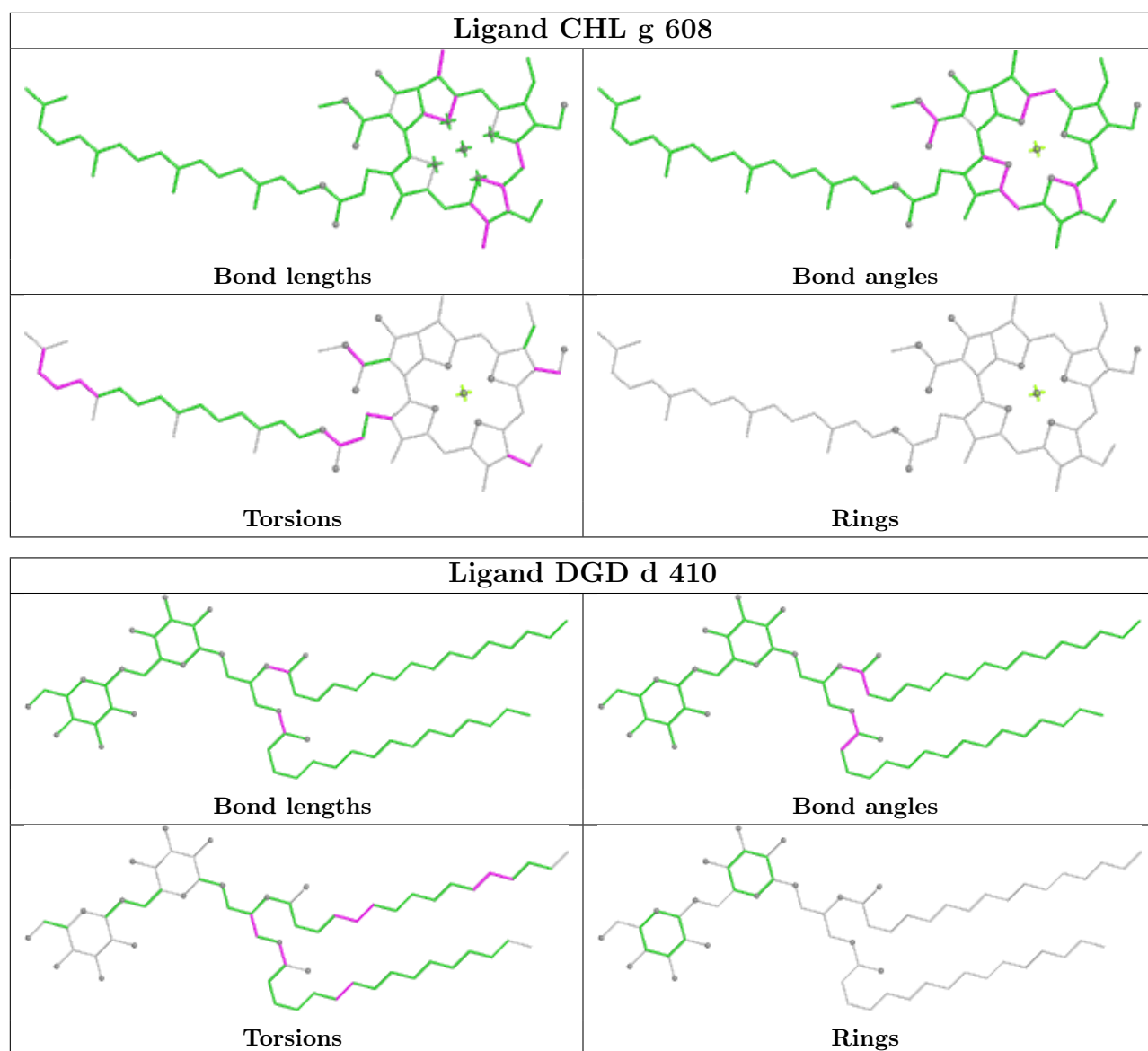


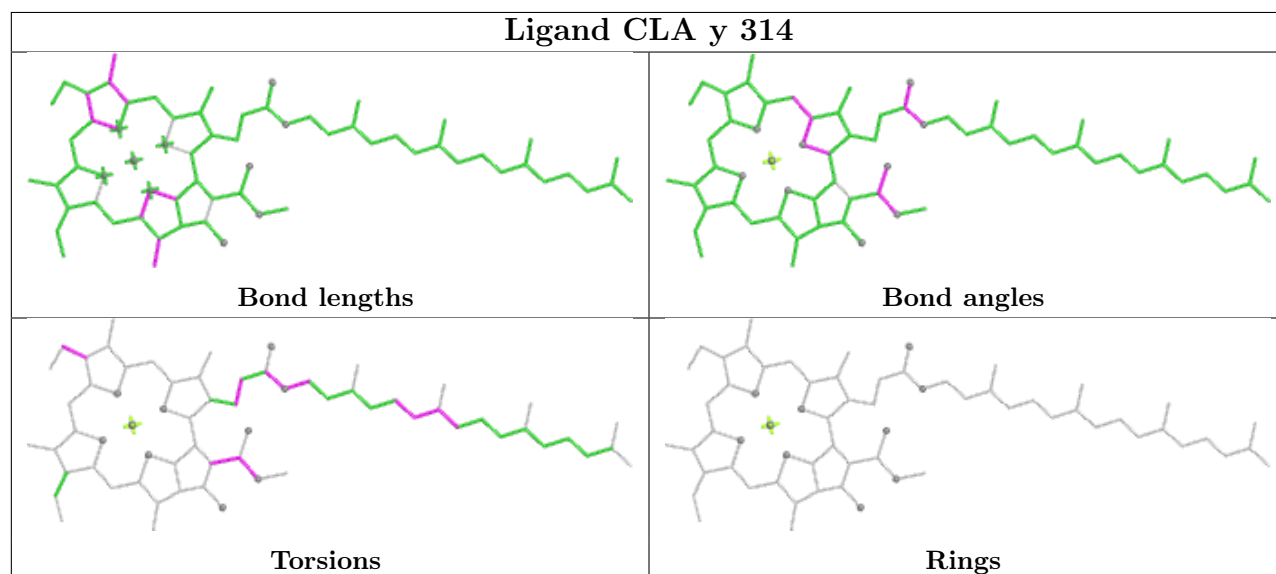
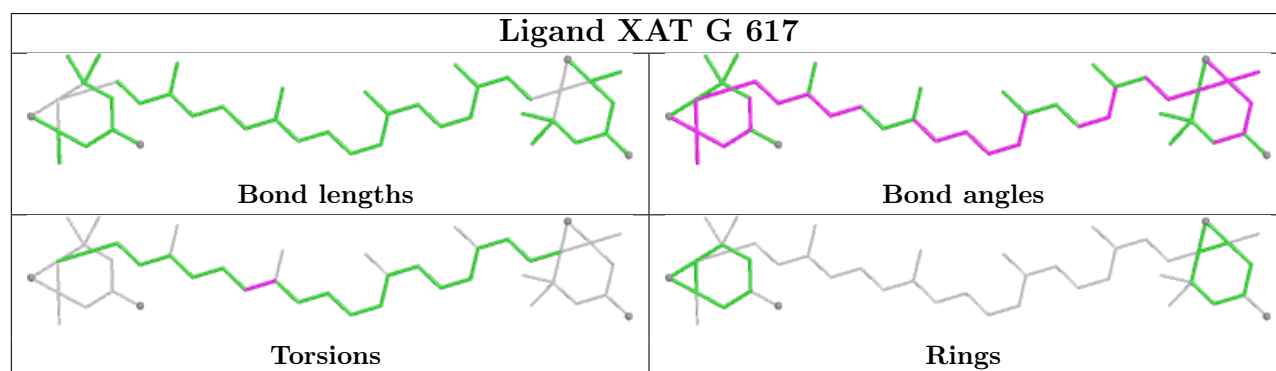
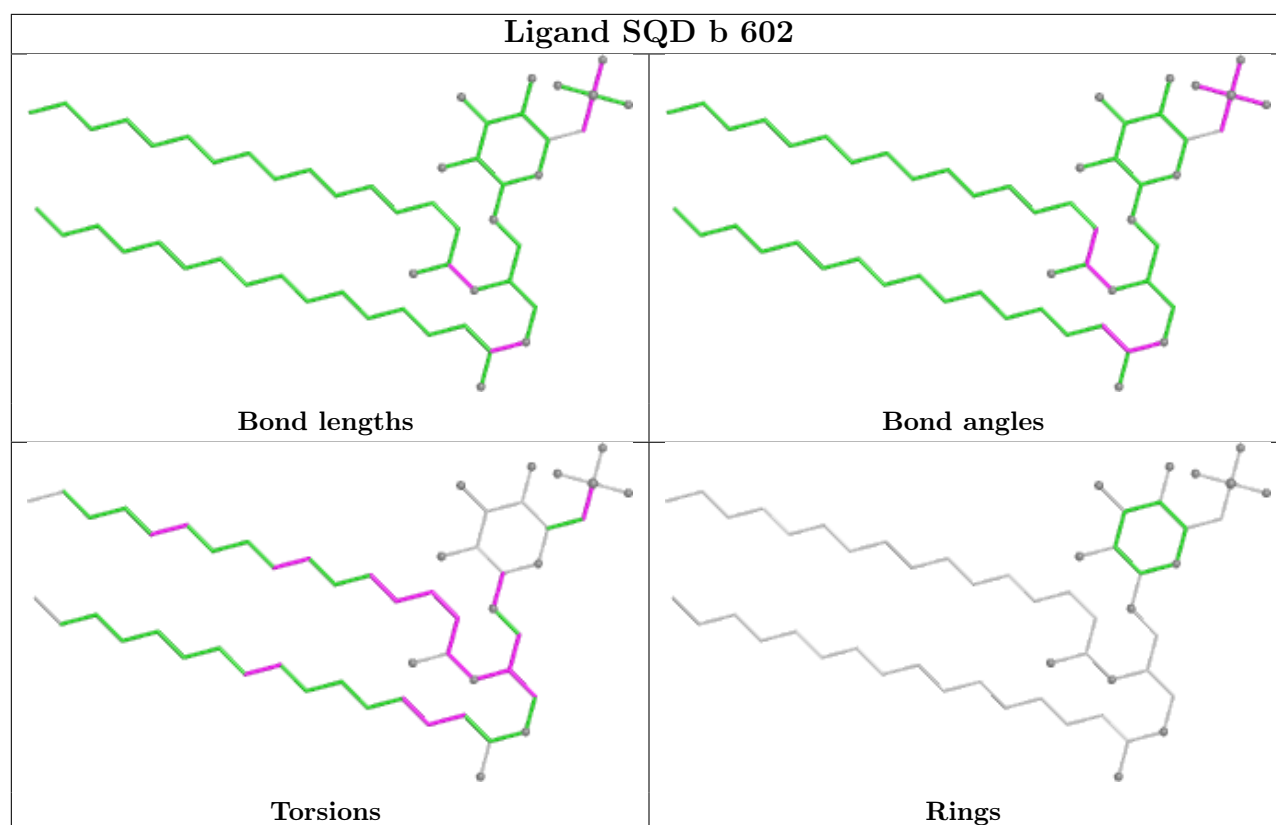
Ligand CLA y 313**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 402****Bond lengths****Bond angles****Torsions****Rings**

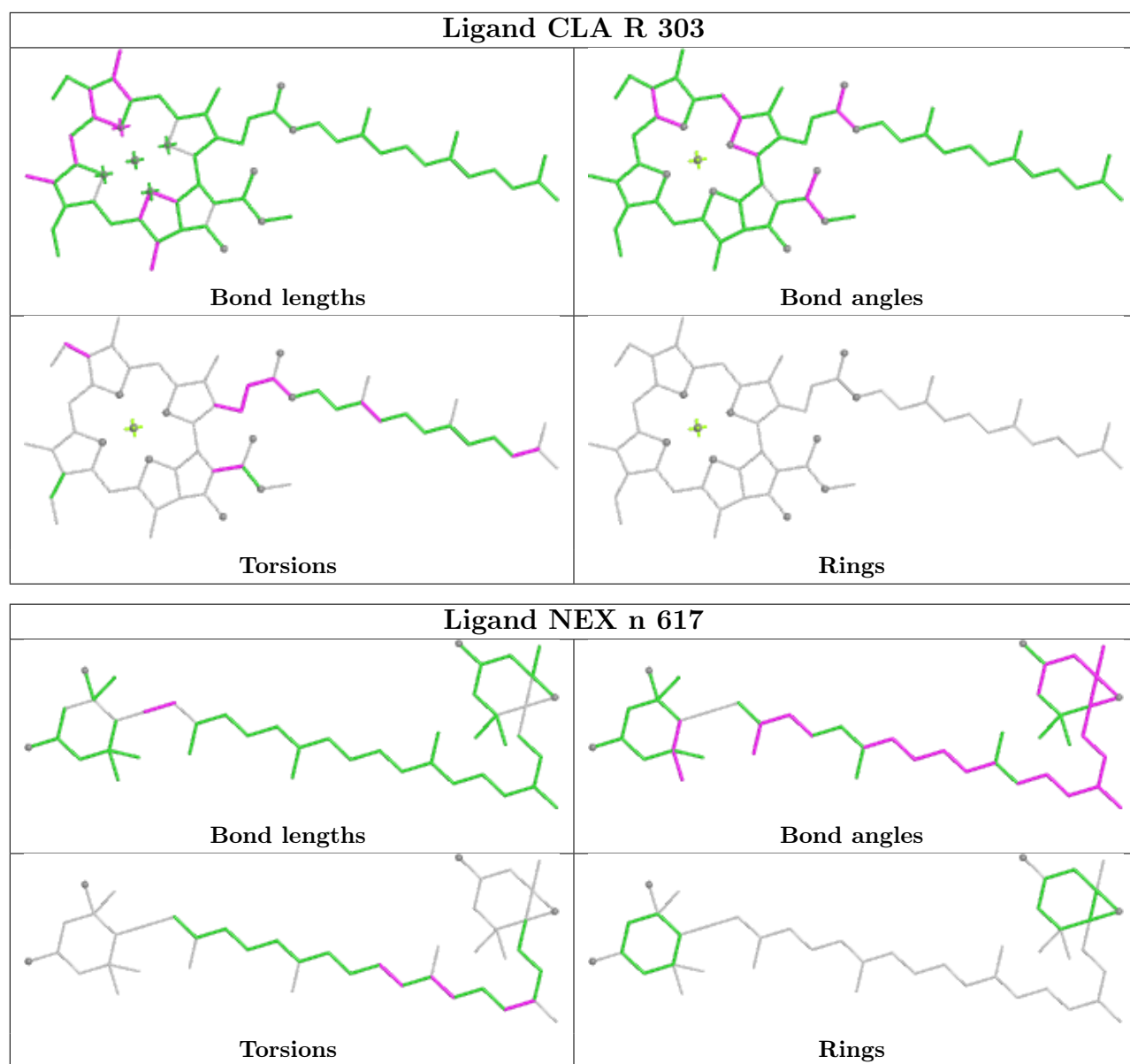


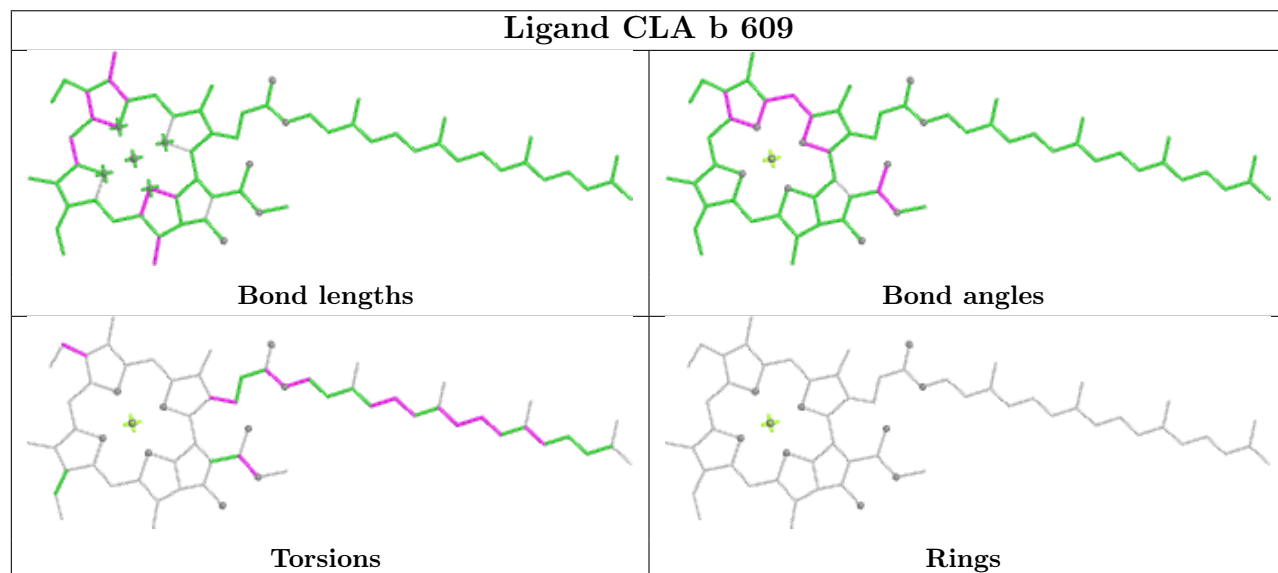
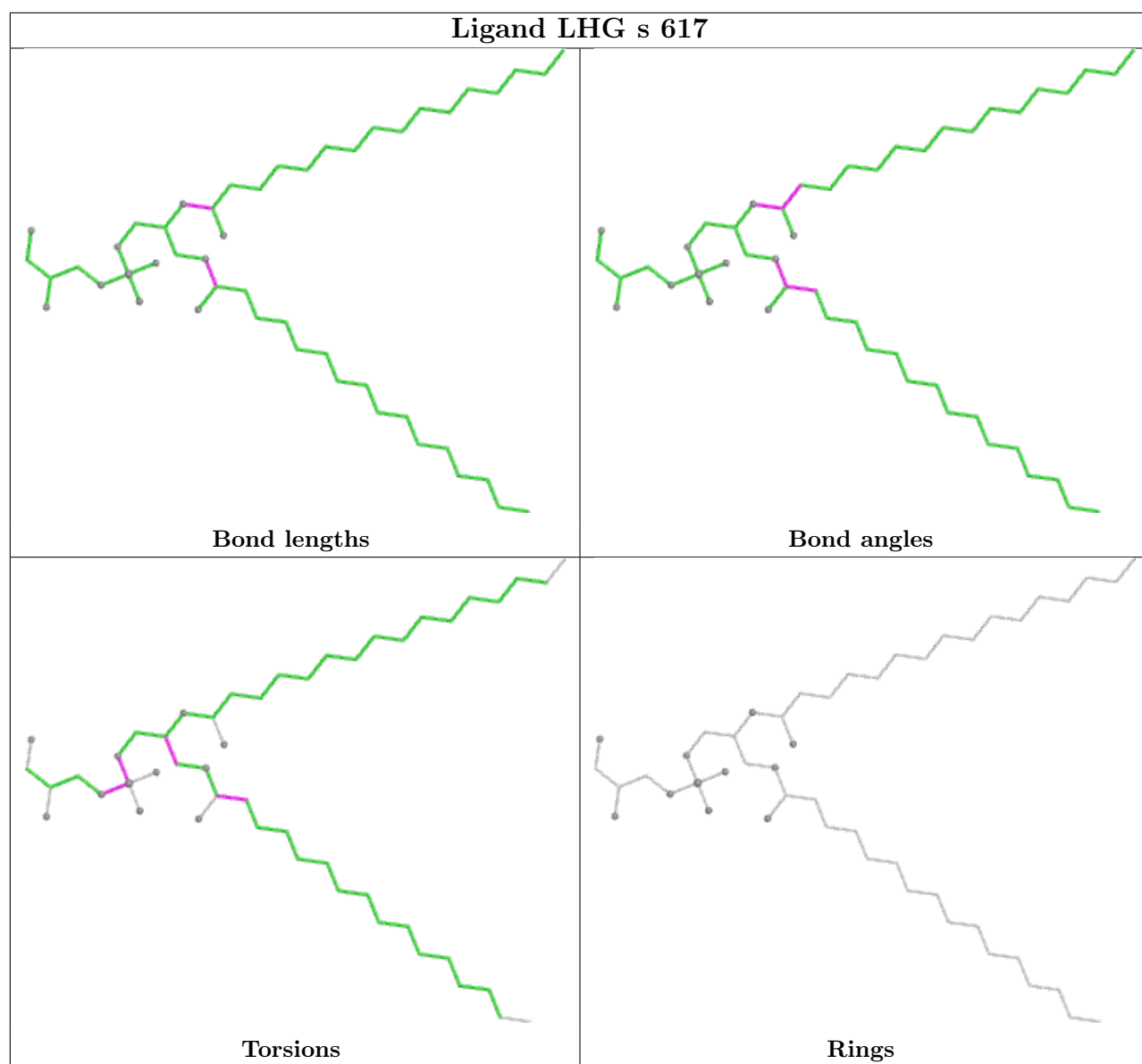


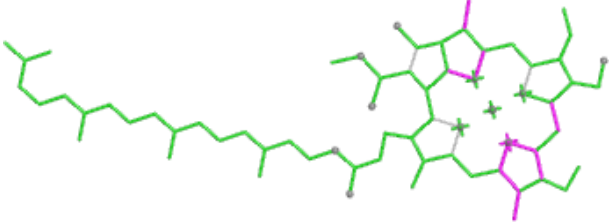
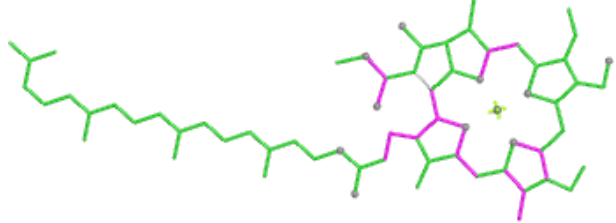
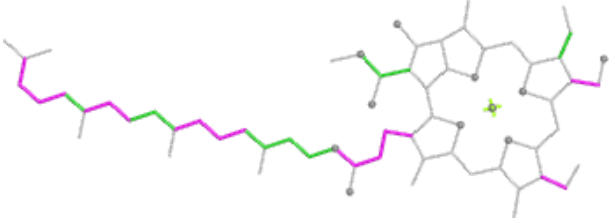
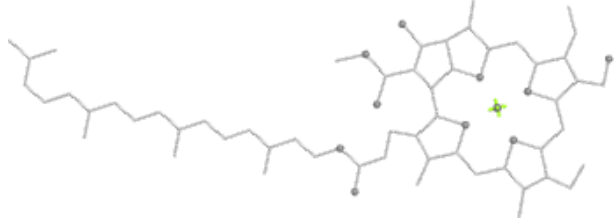
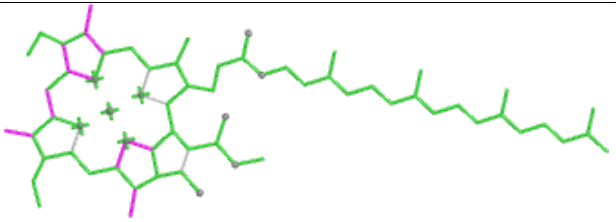
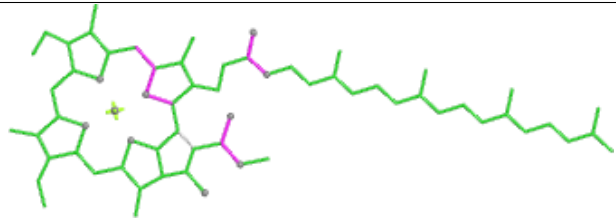
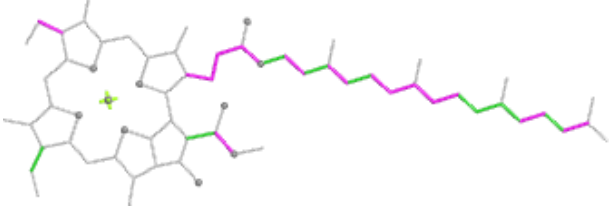
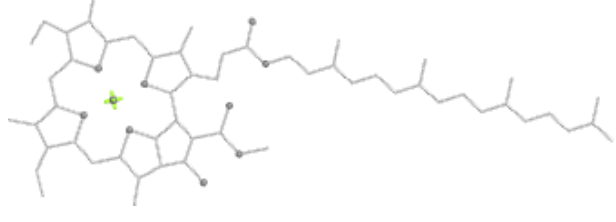
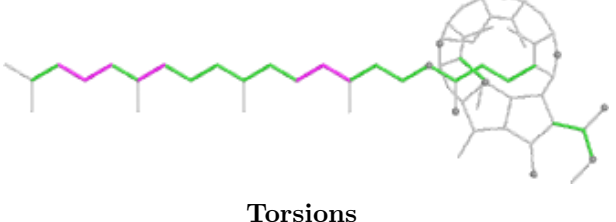
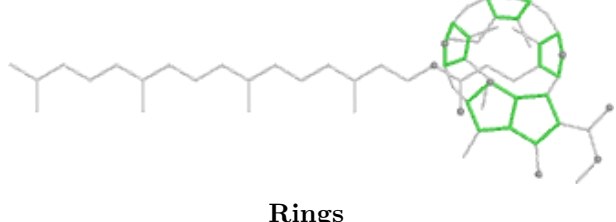


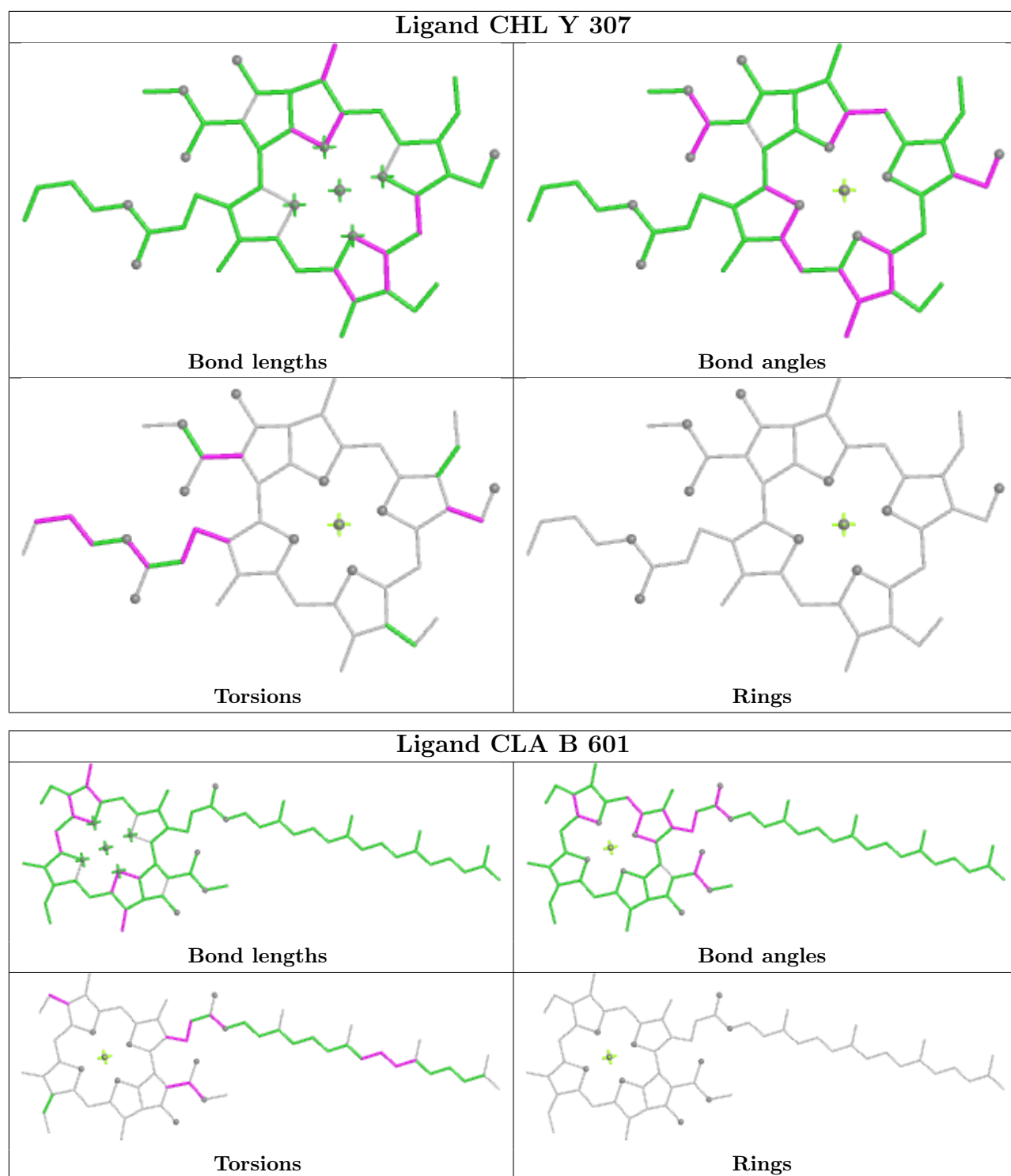


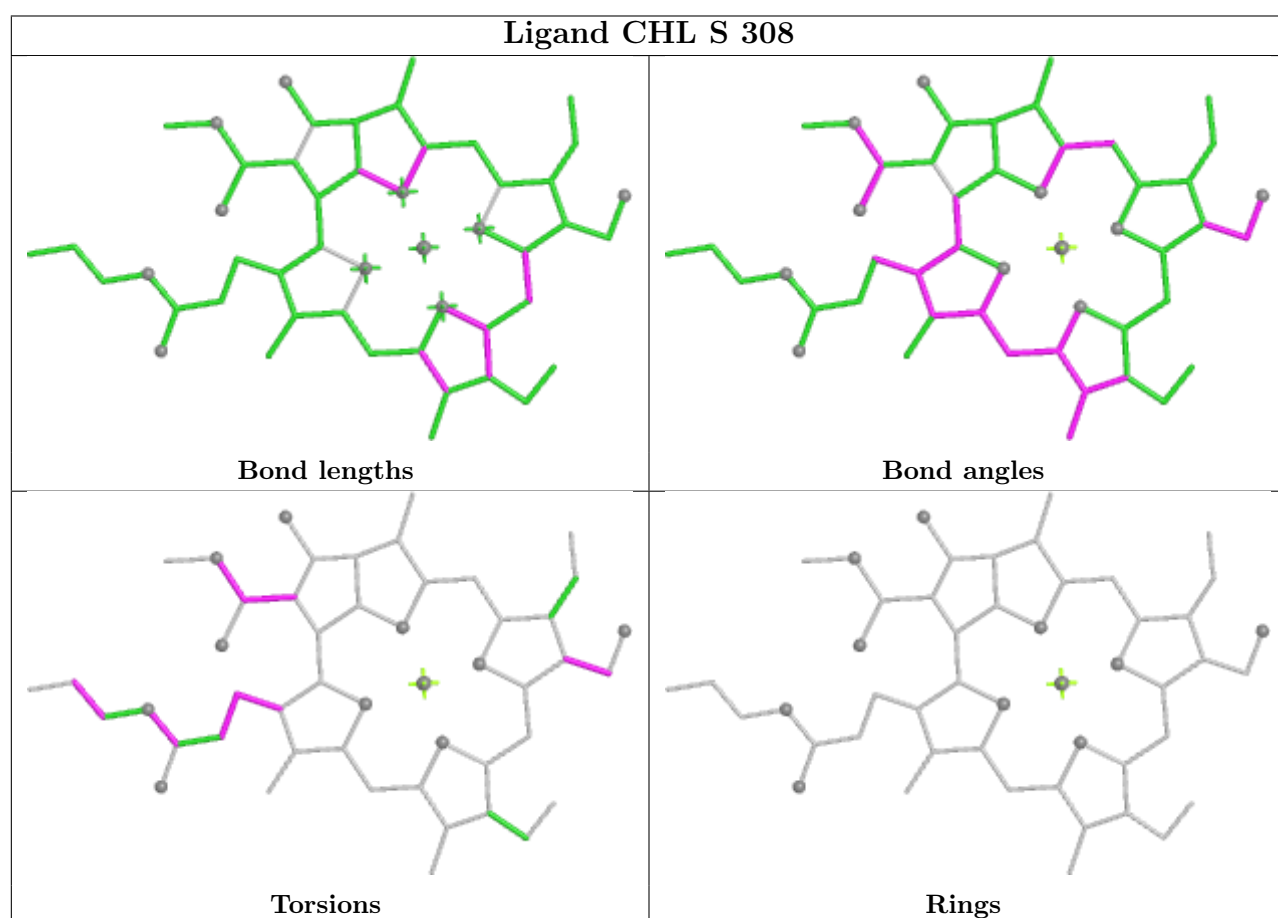
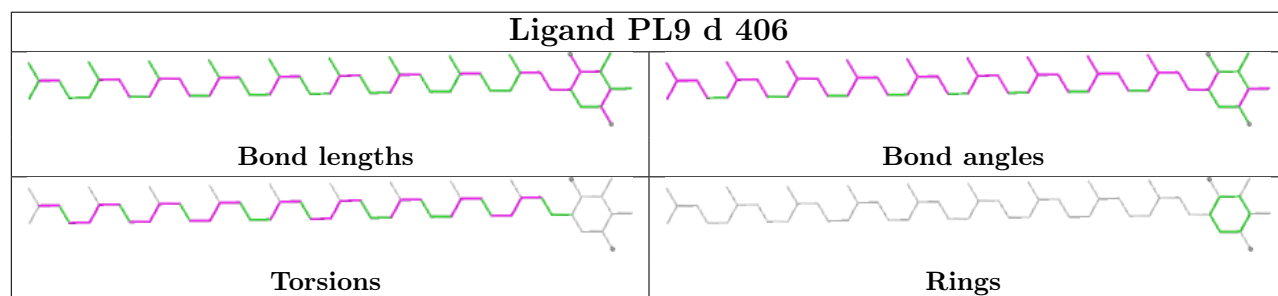
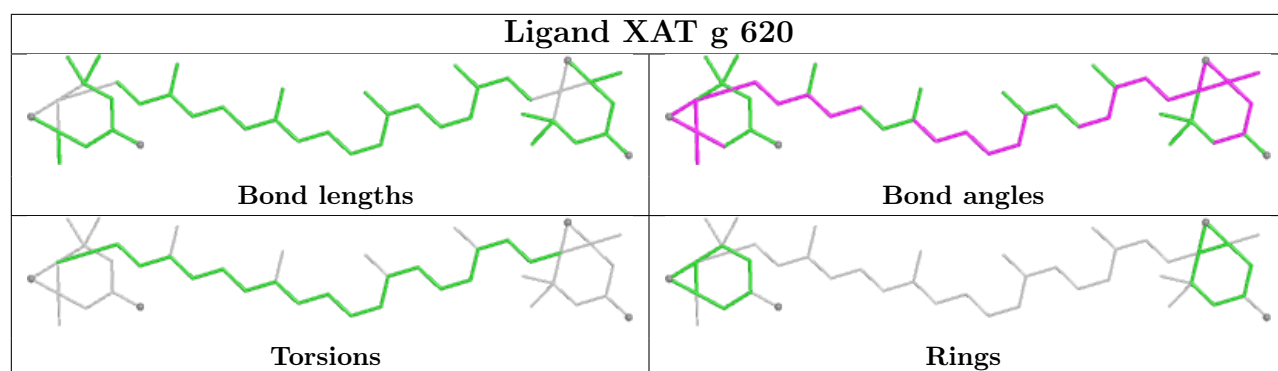


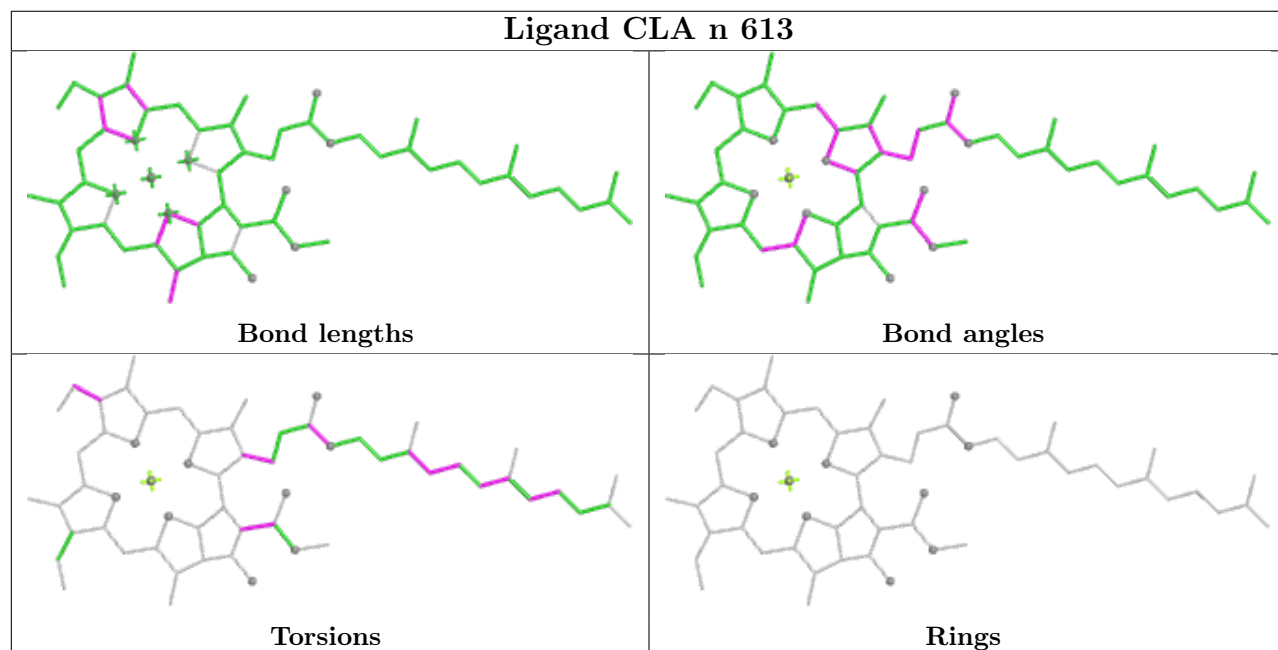
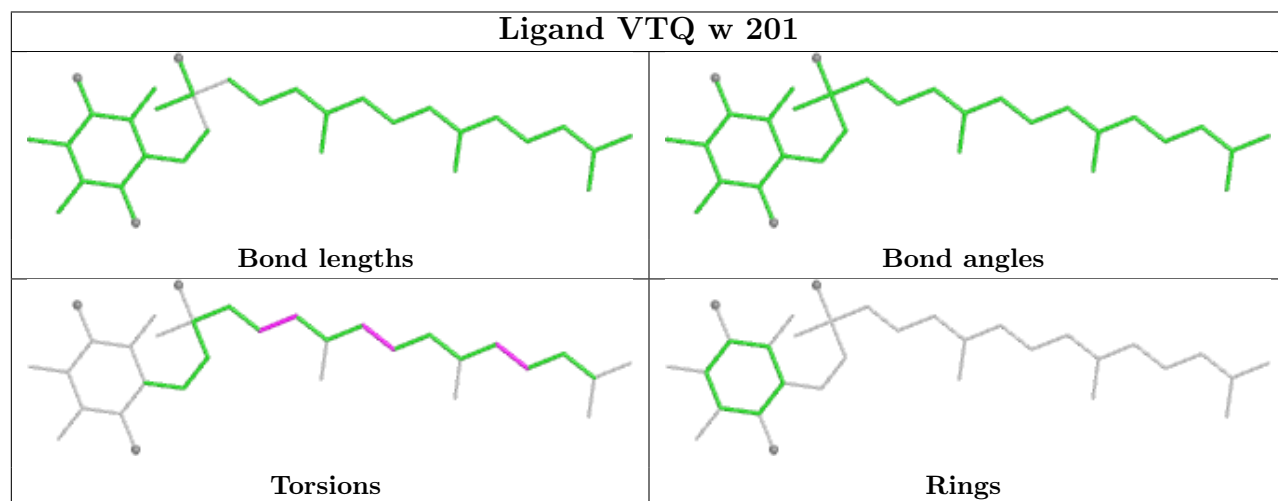
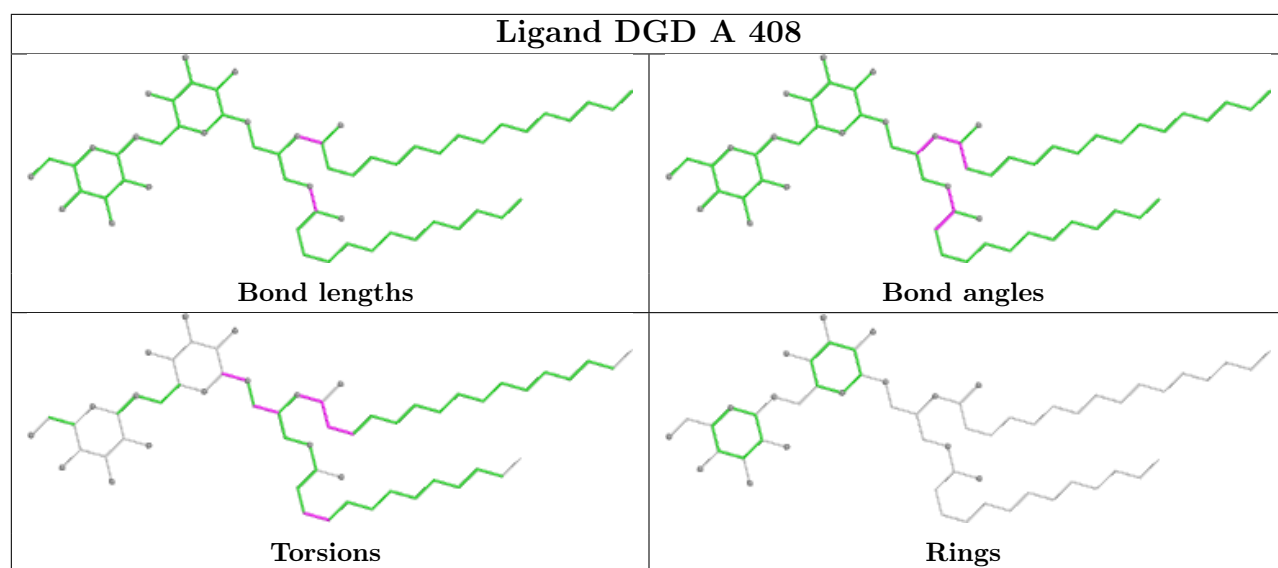


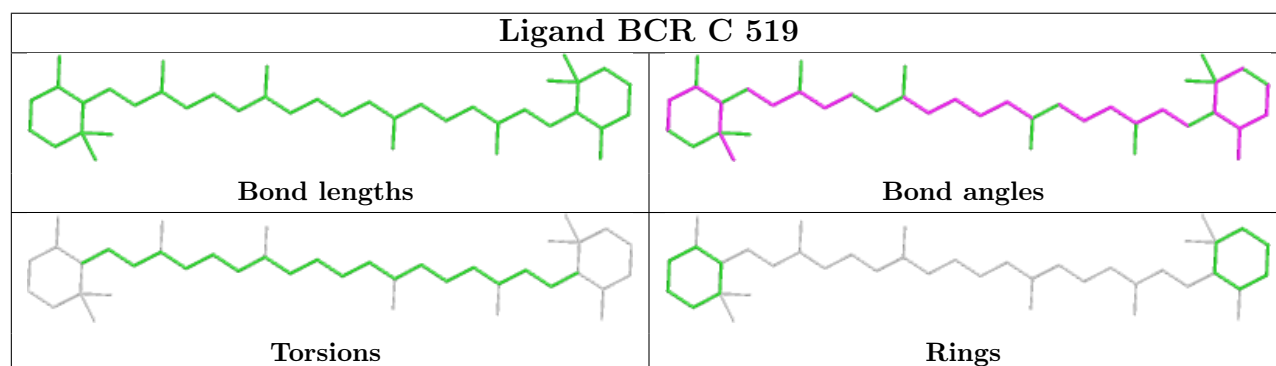
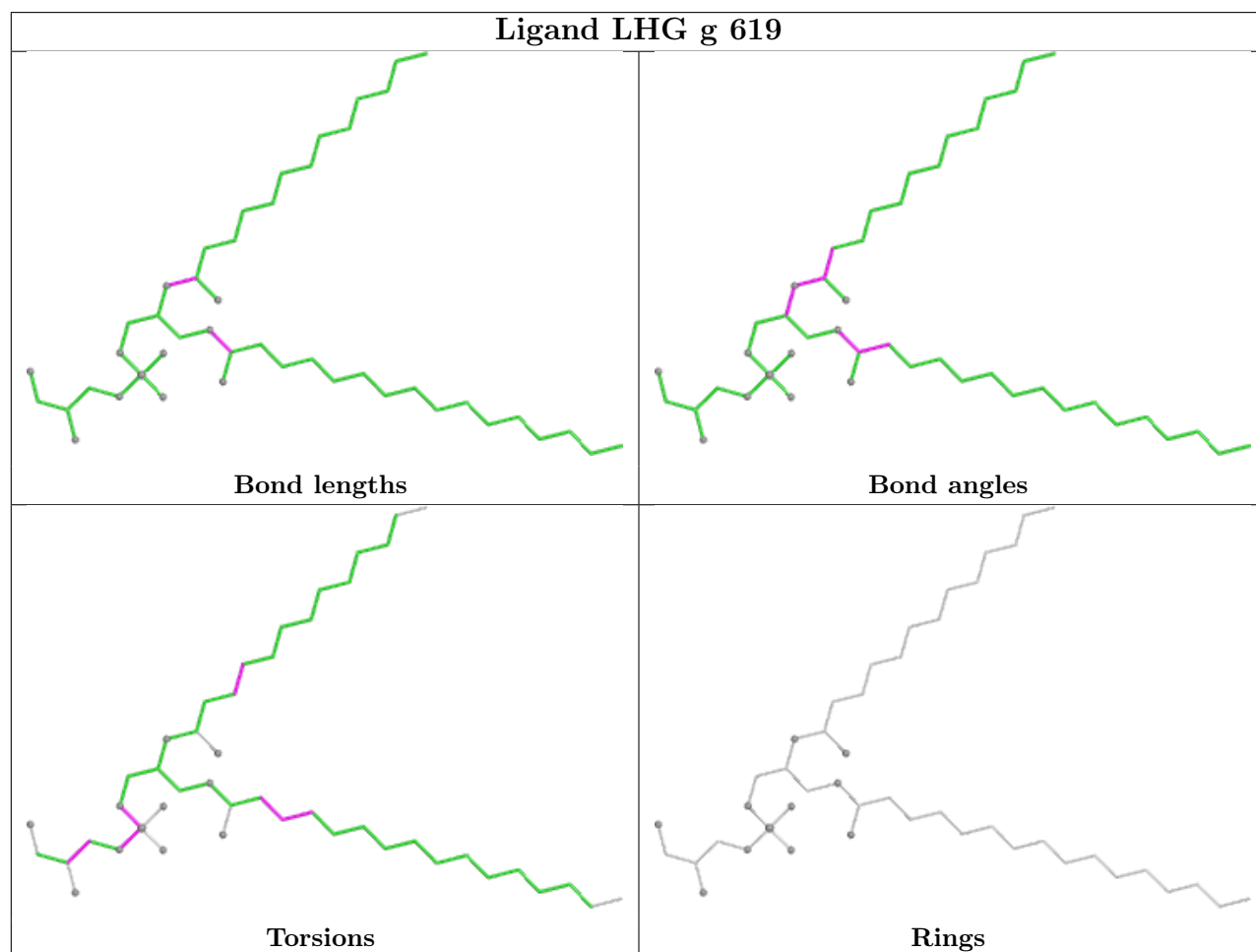
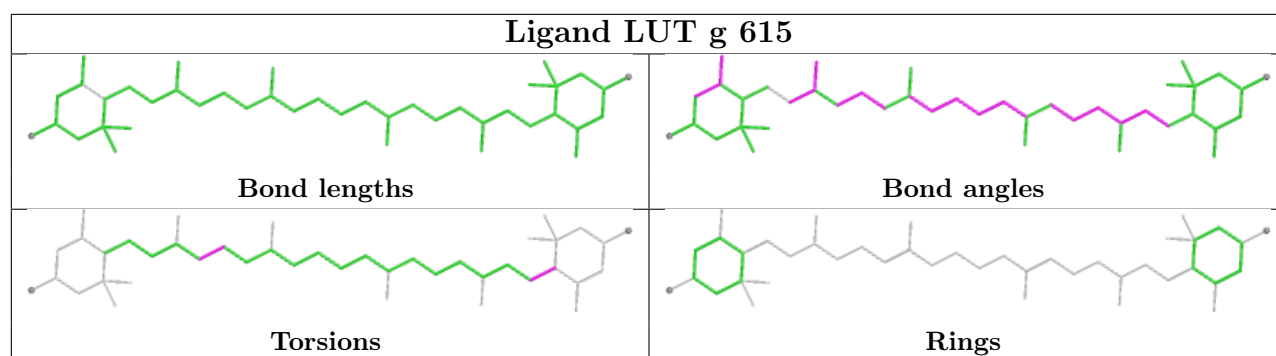


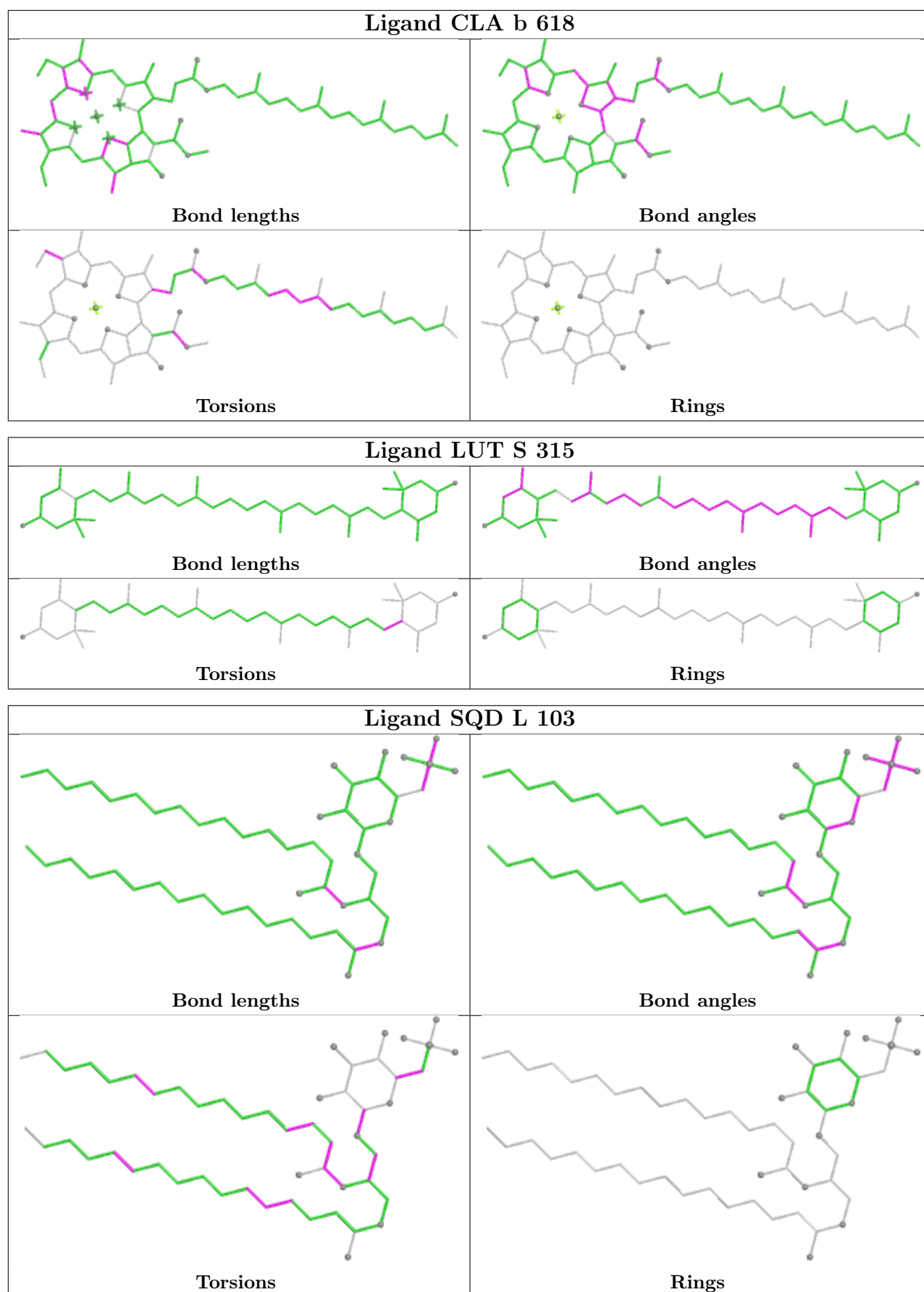
Ligand CHL y 310	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA G 602	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings



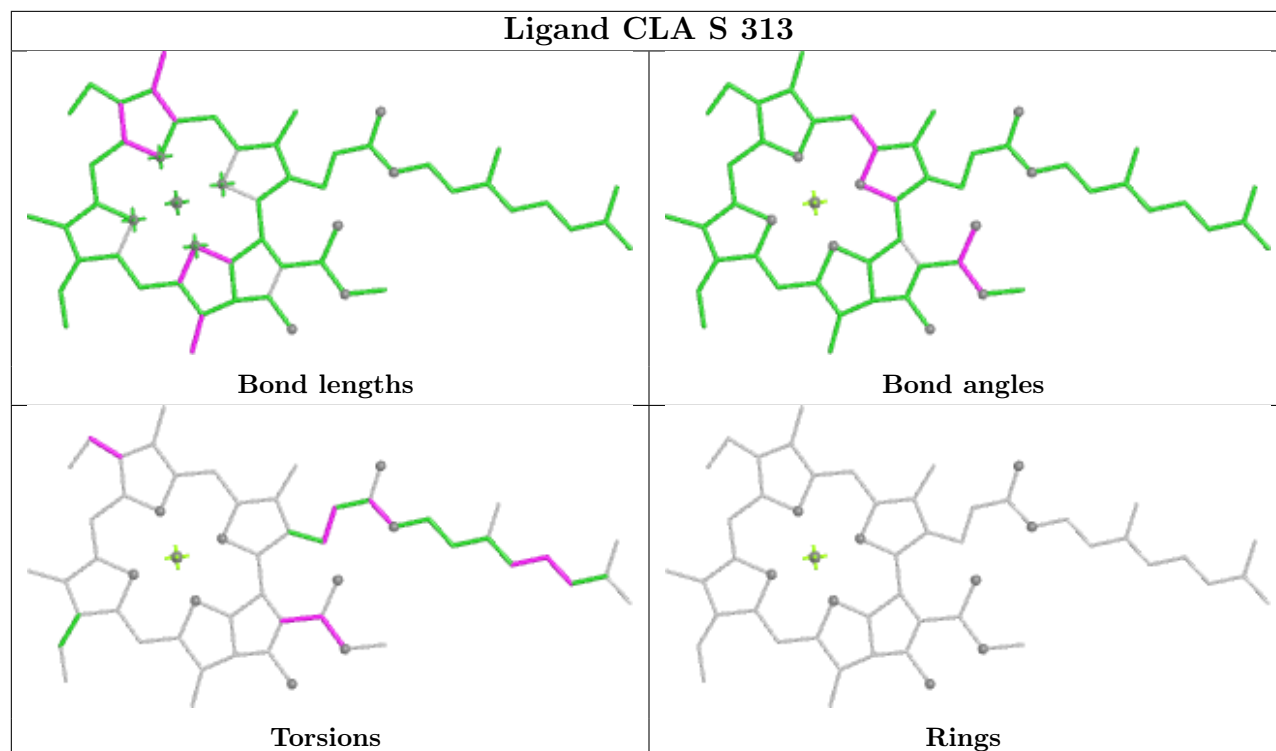




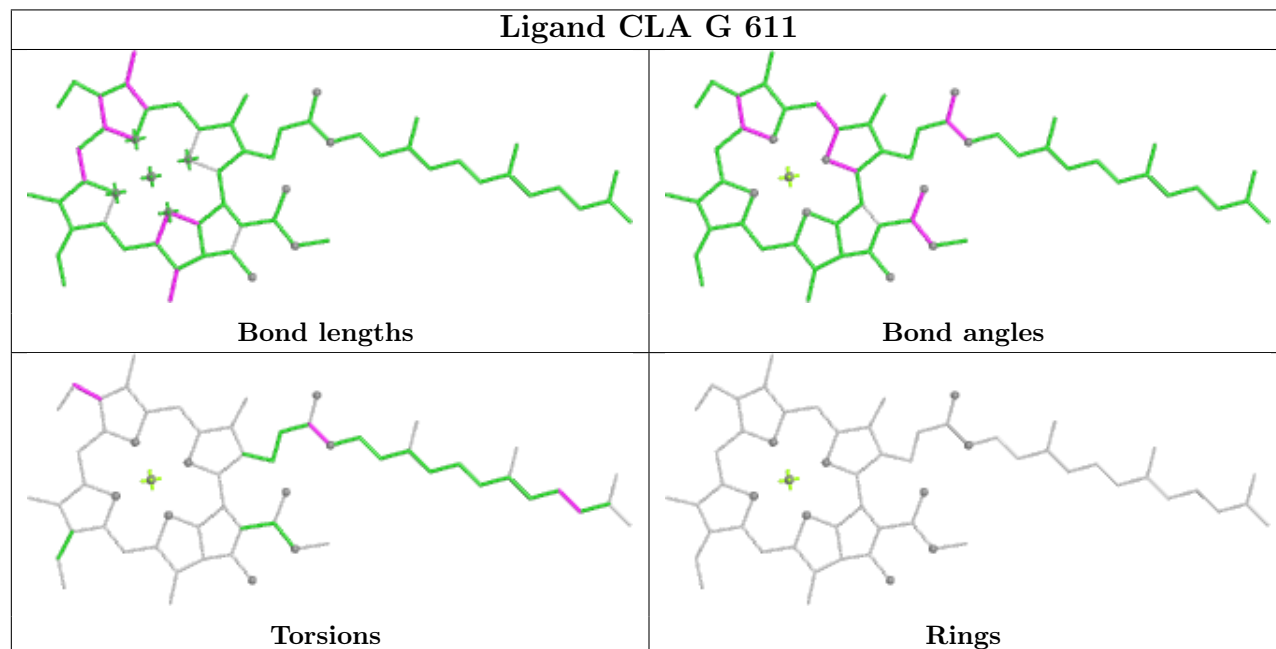


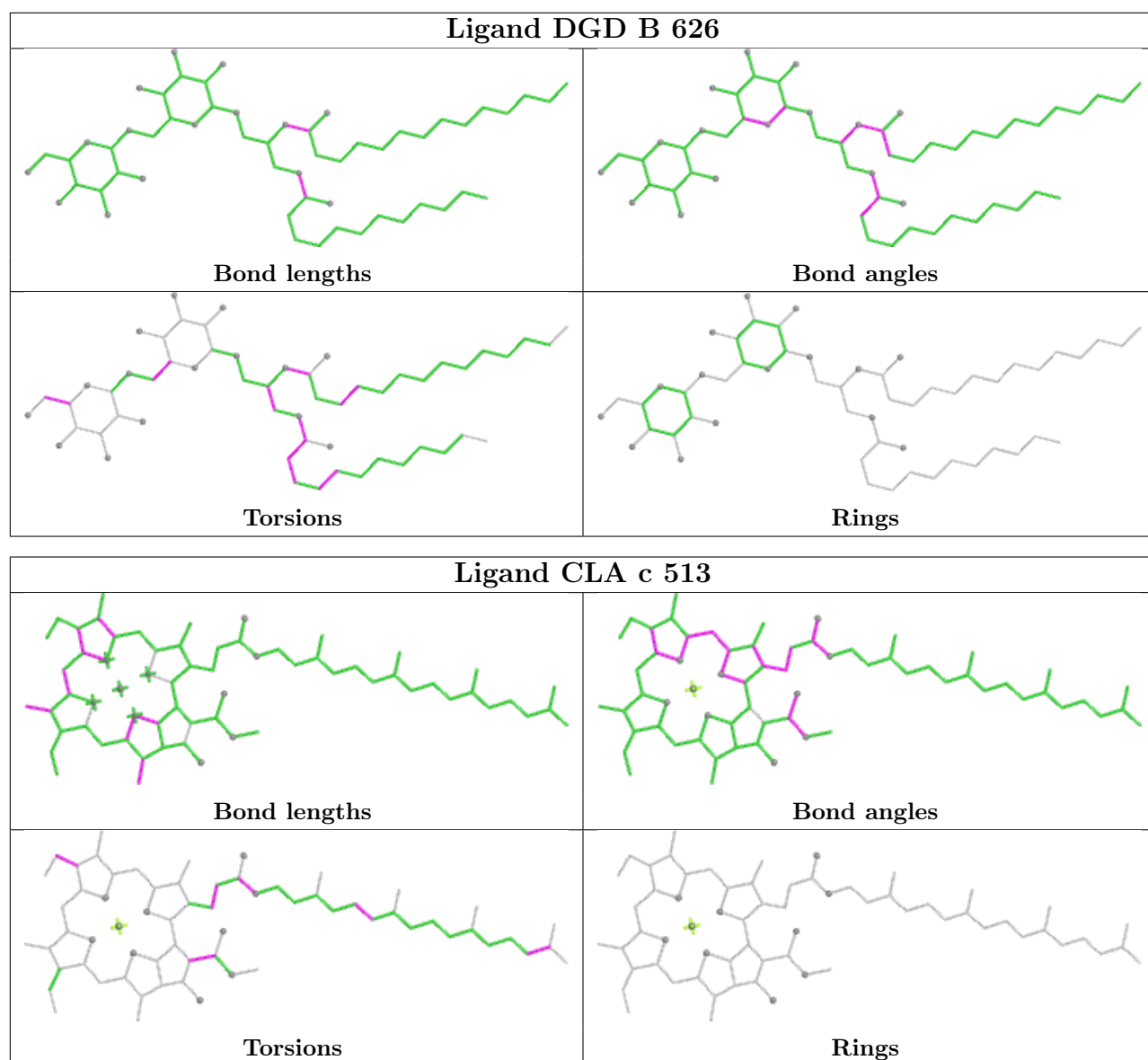


Ligand CLA S 313

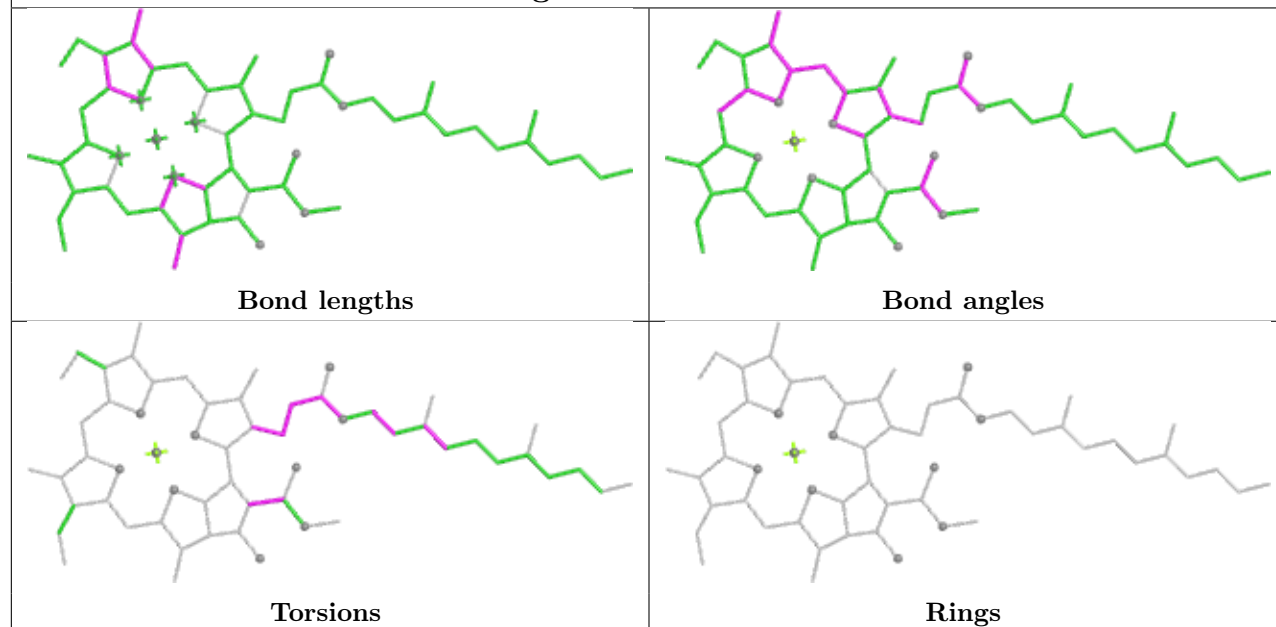


Ligand CLA G 611

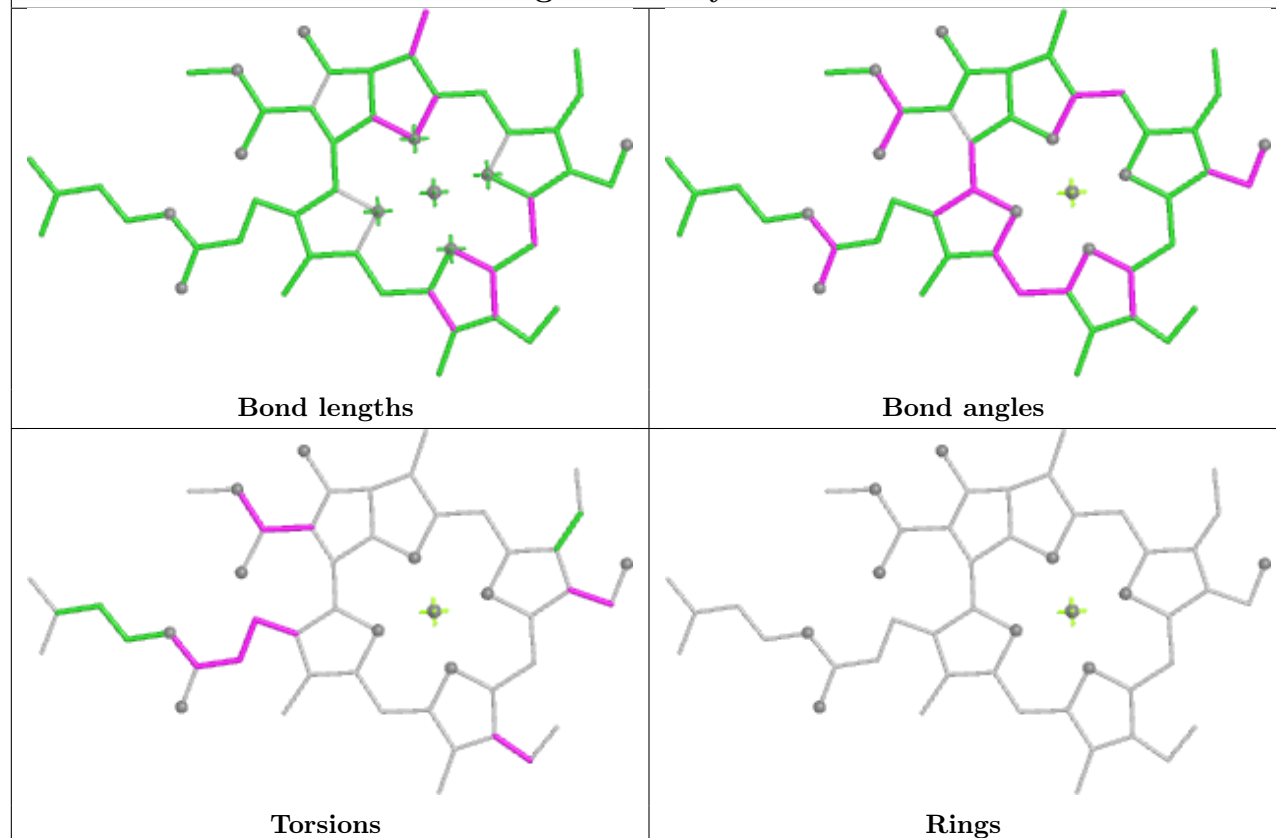


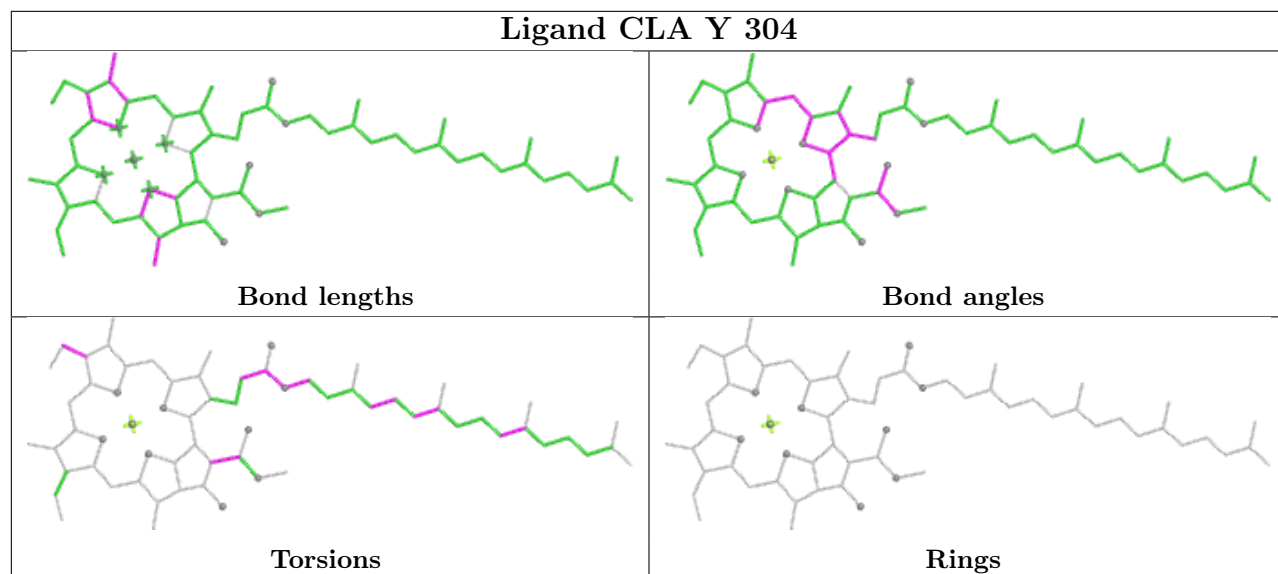
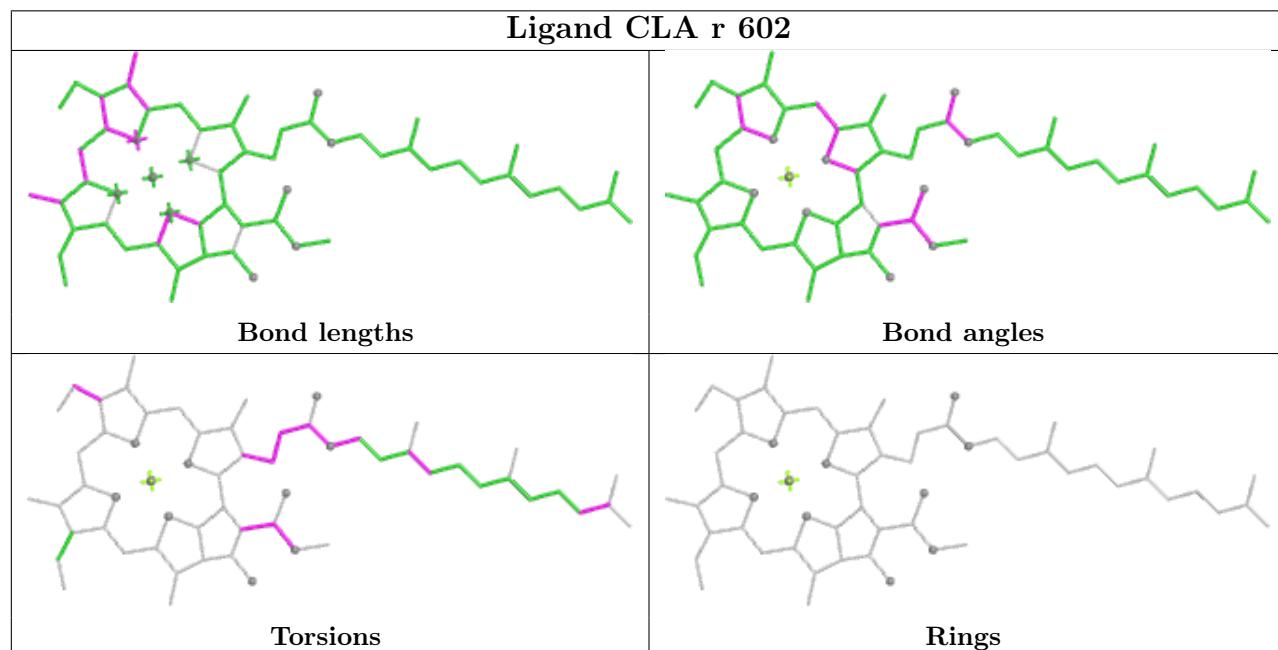


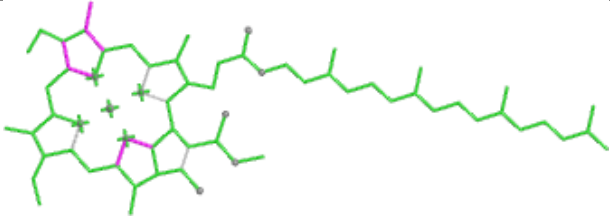
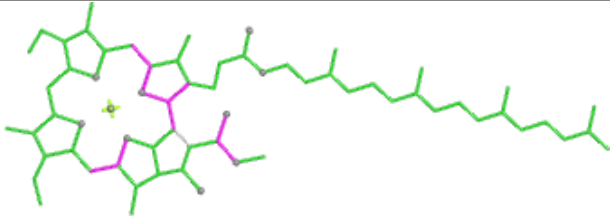
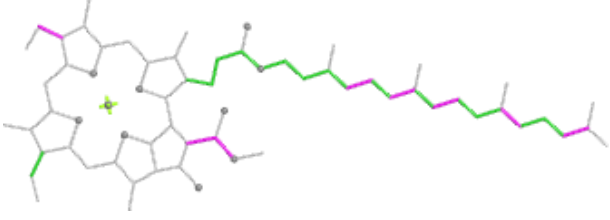
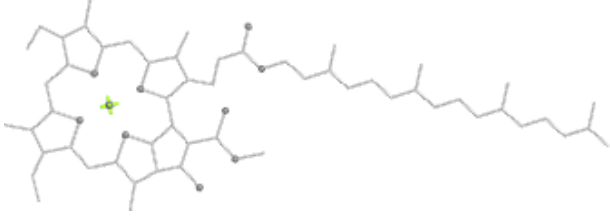
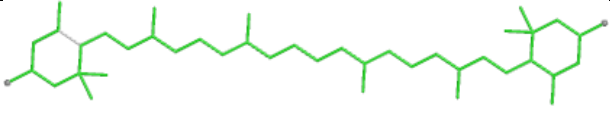
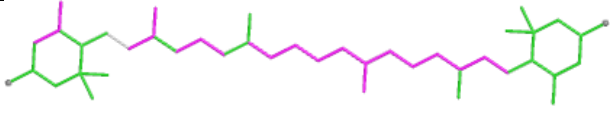
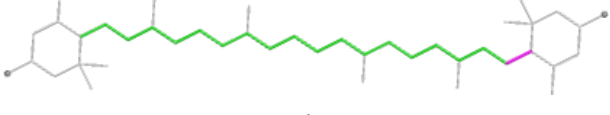
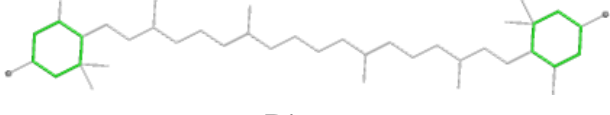
Ligand CLA C 506

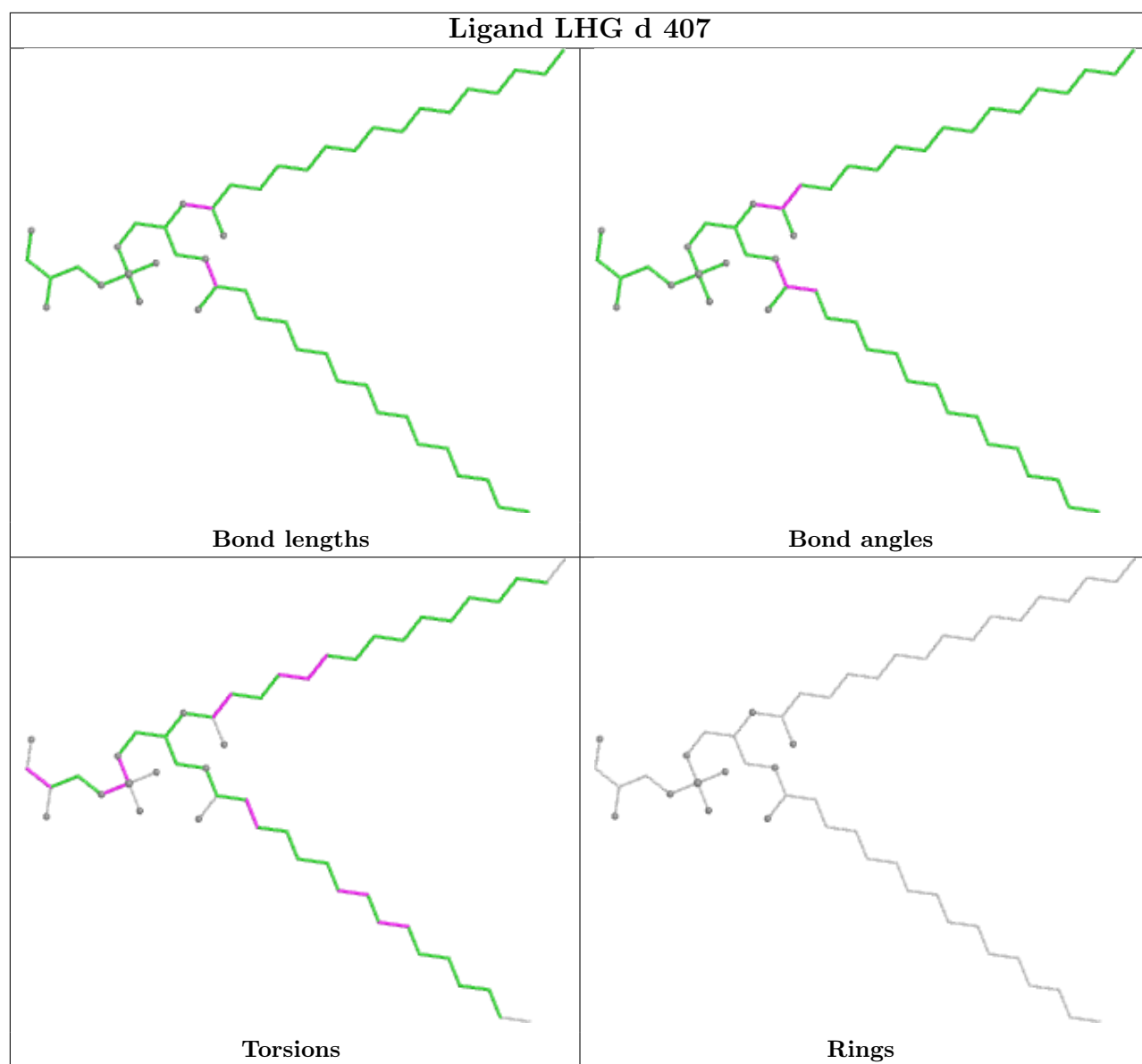


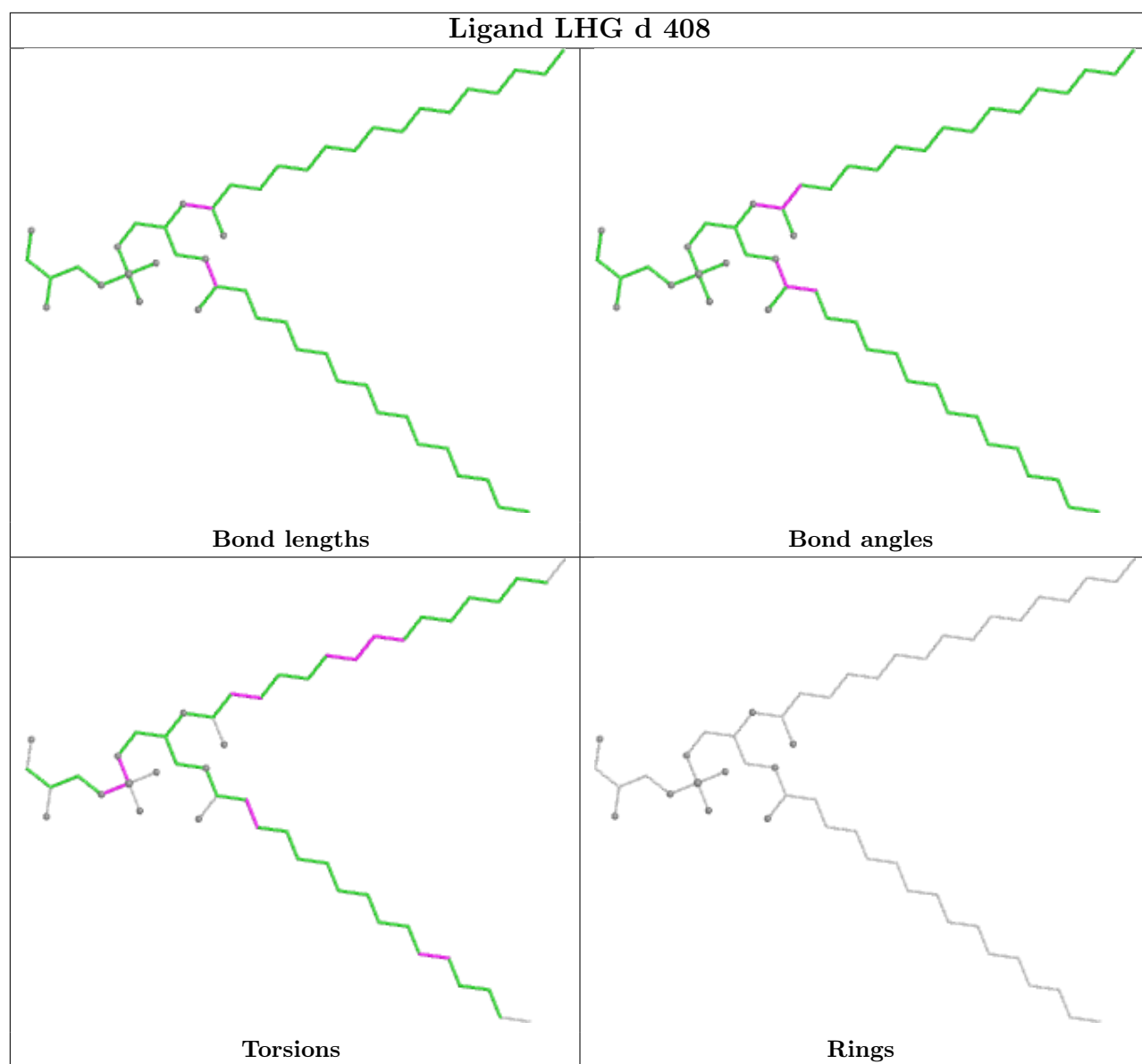
Ligand CHL y 306

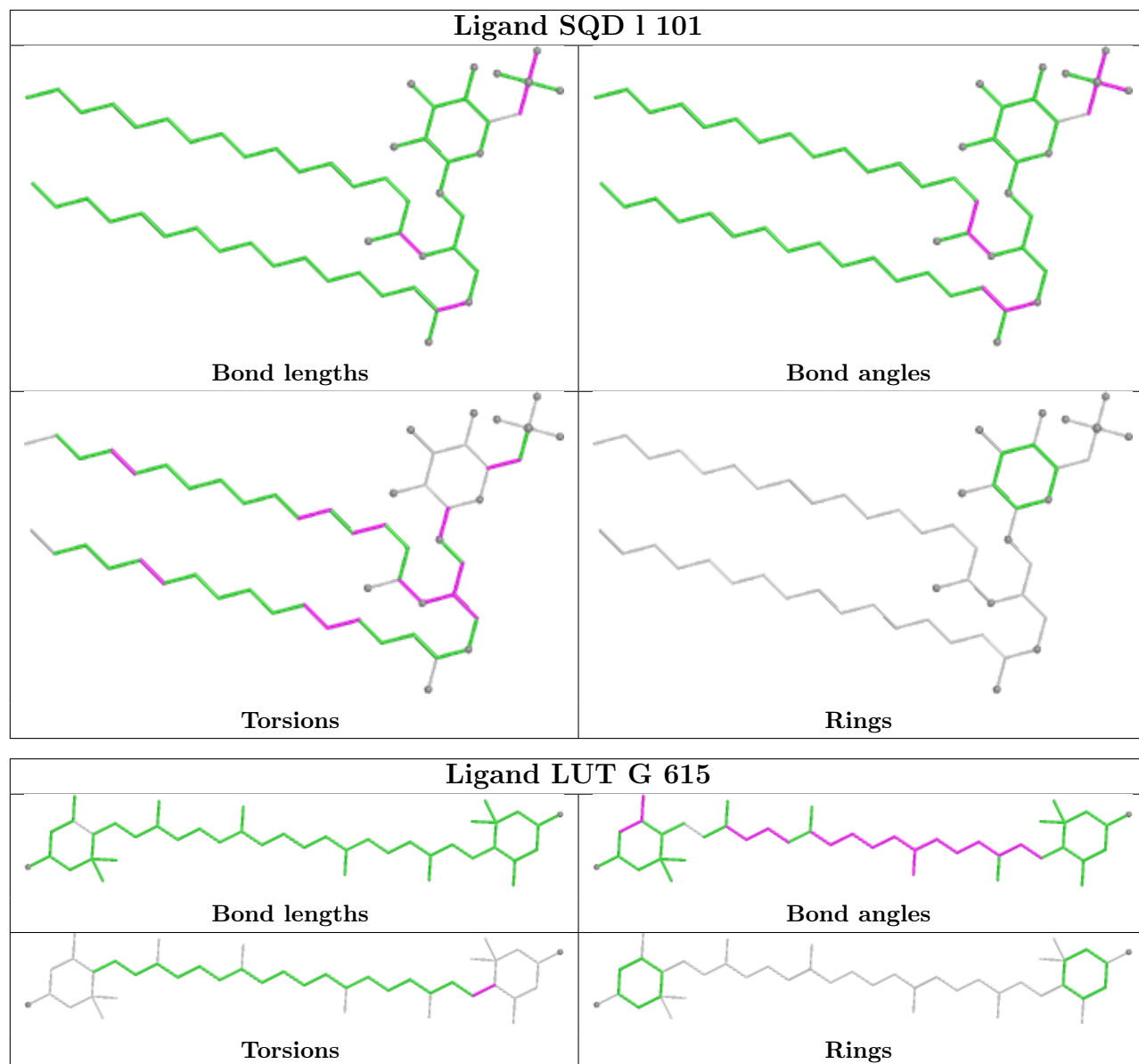


Ligand CLA Y 304**Ligand CLA r 602**

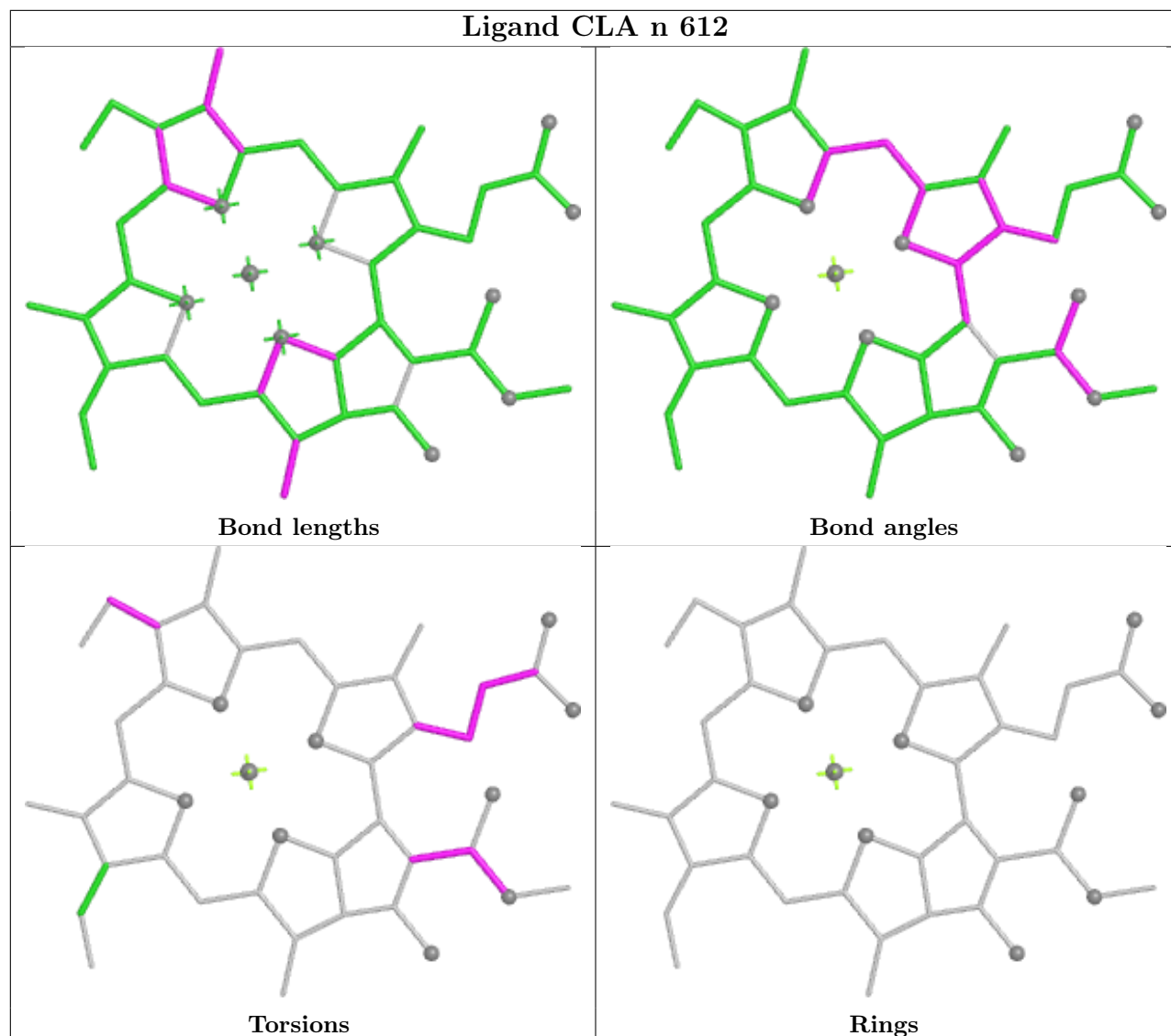
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT y 316	
 Bond lengths	 Bond angles
 Torsions	 Rings



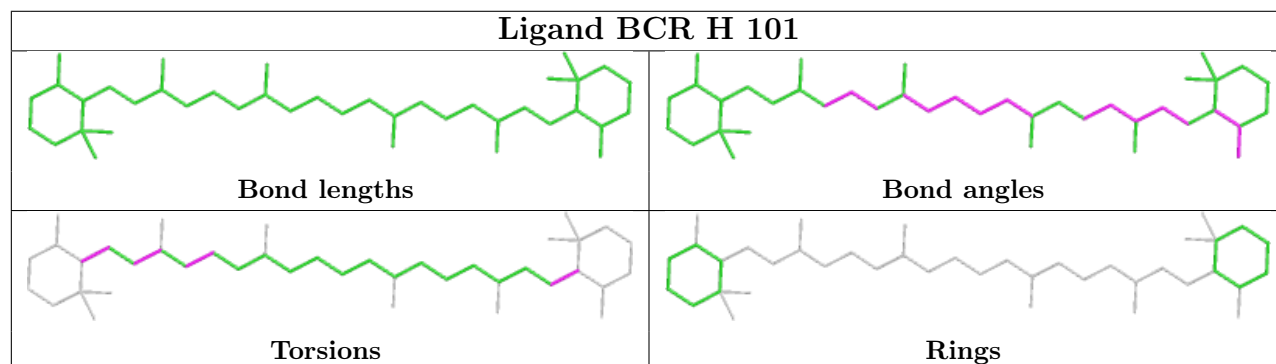


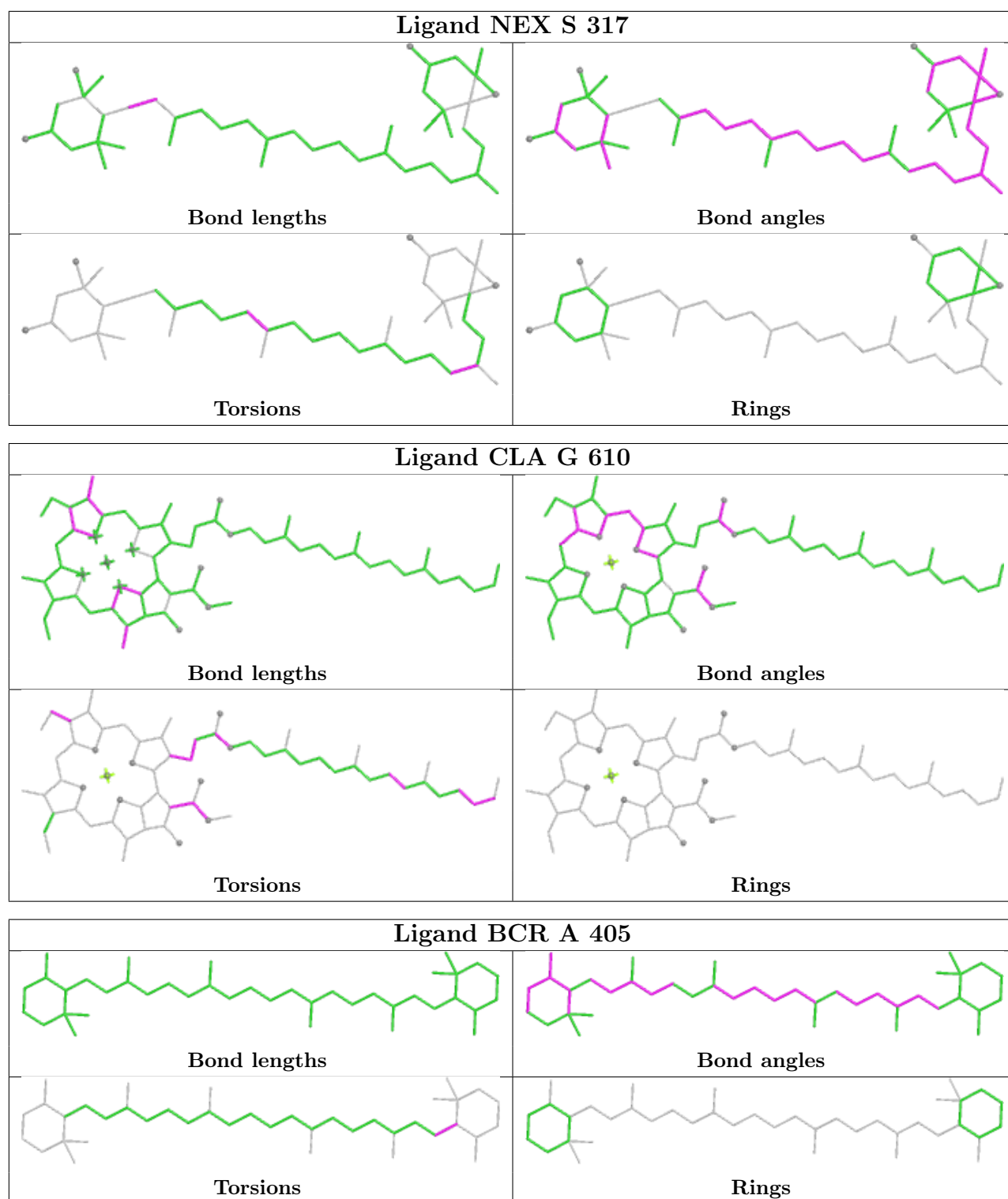


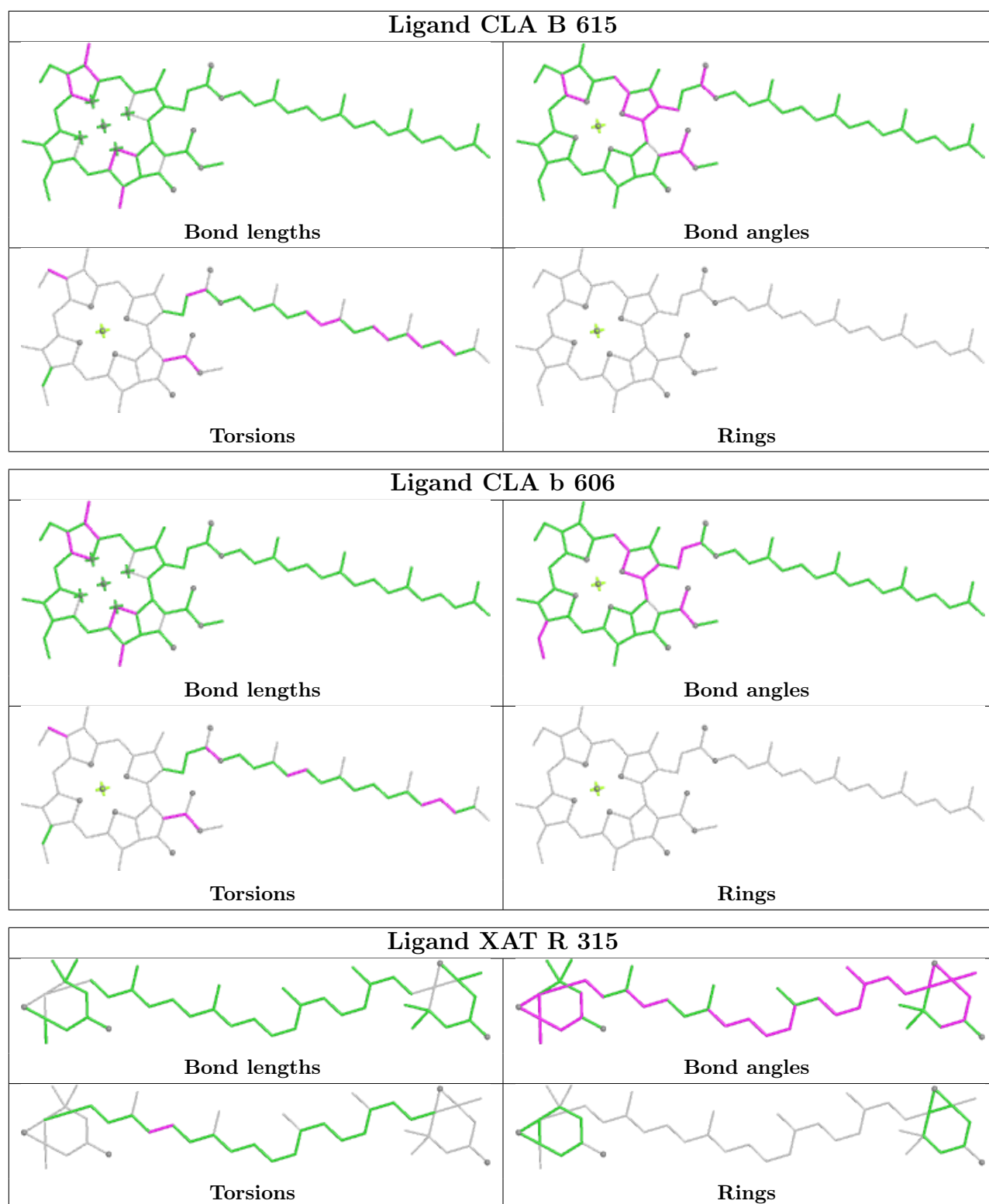
Ligand CLA n 612

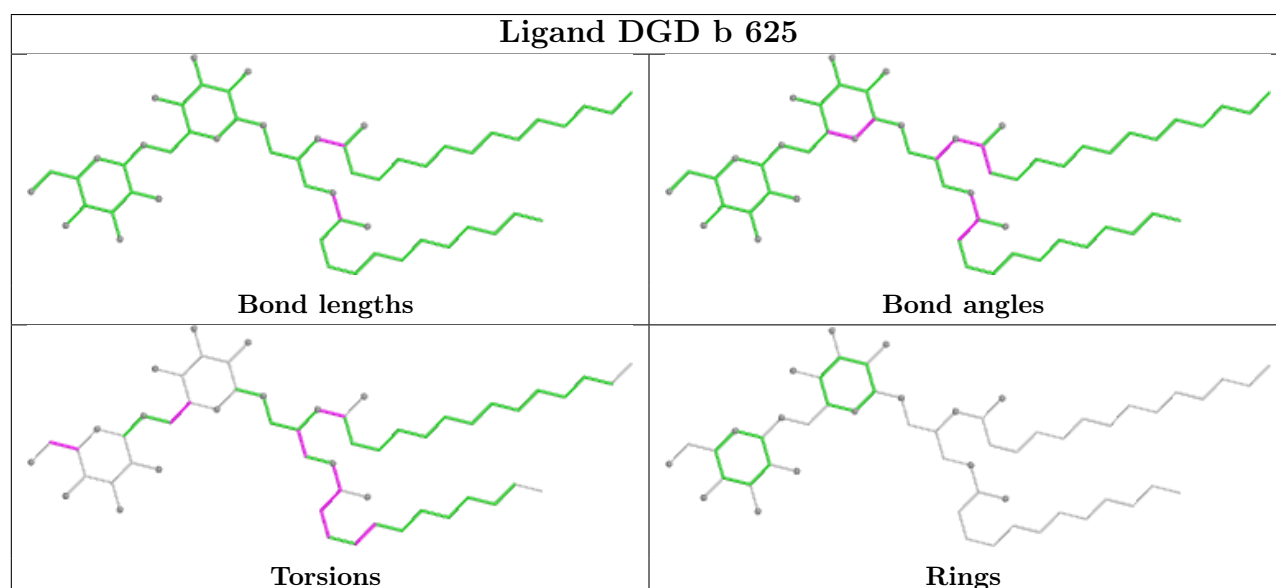
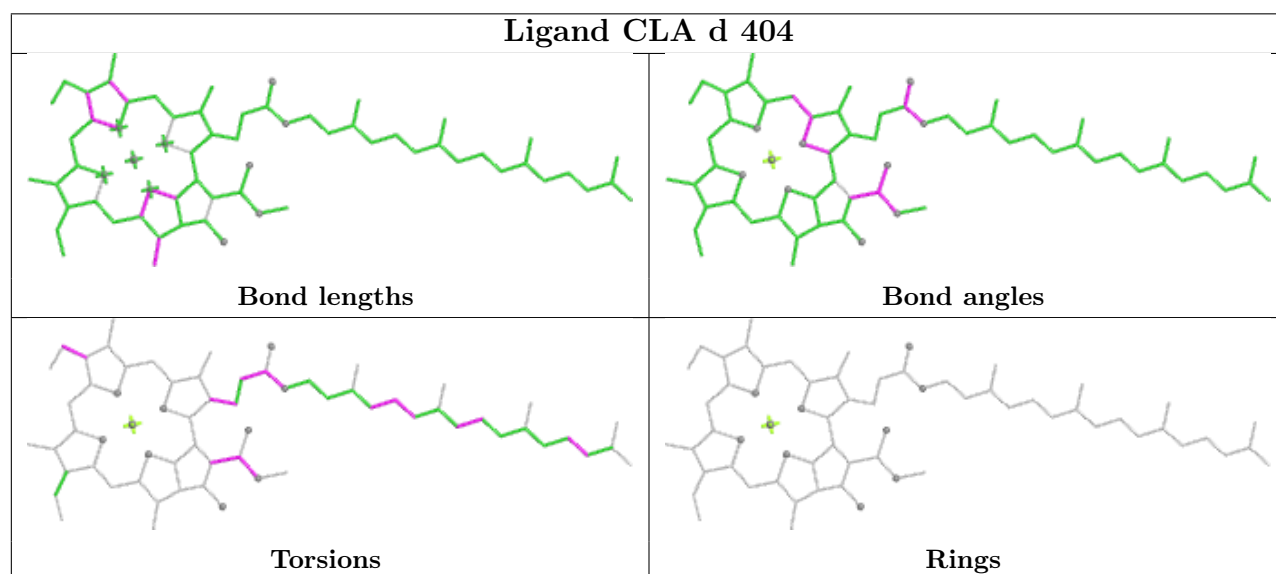
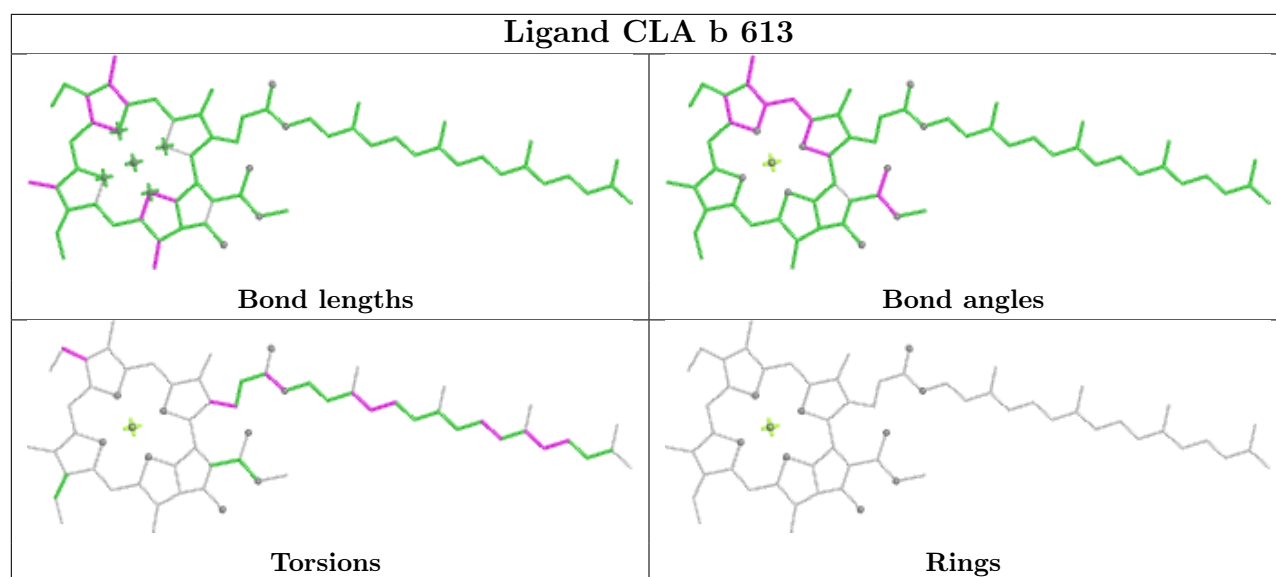


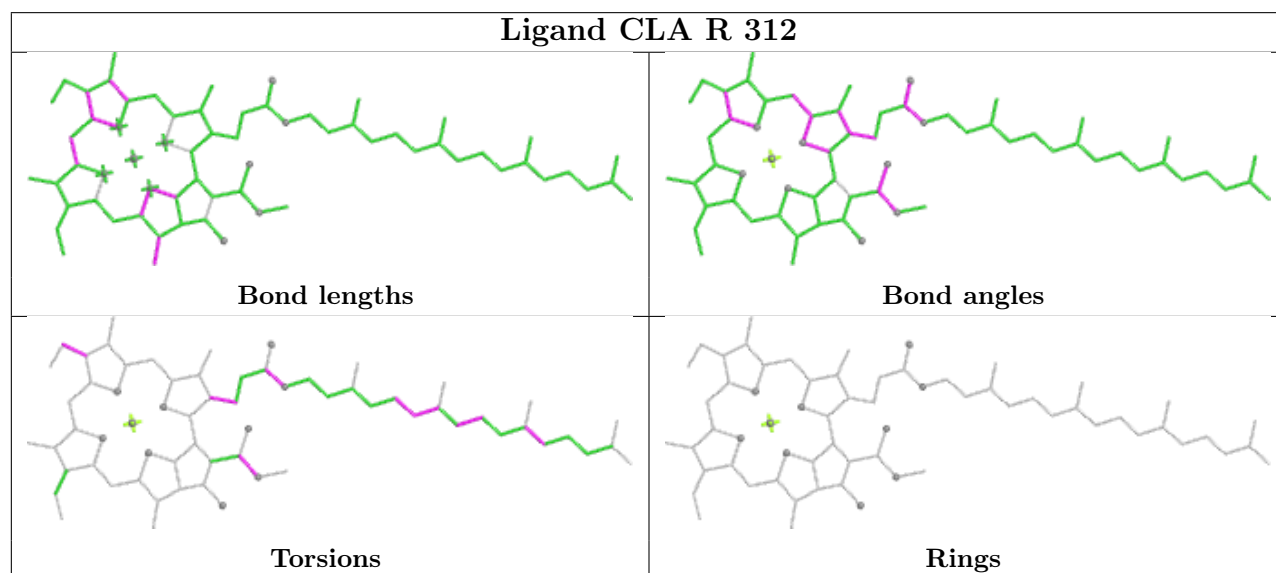
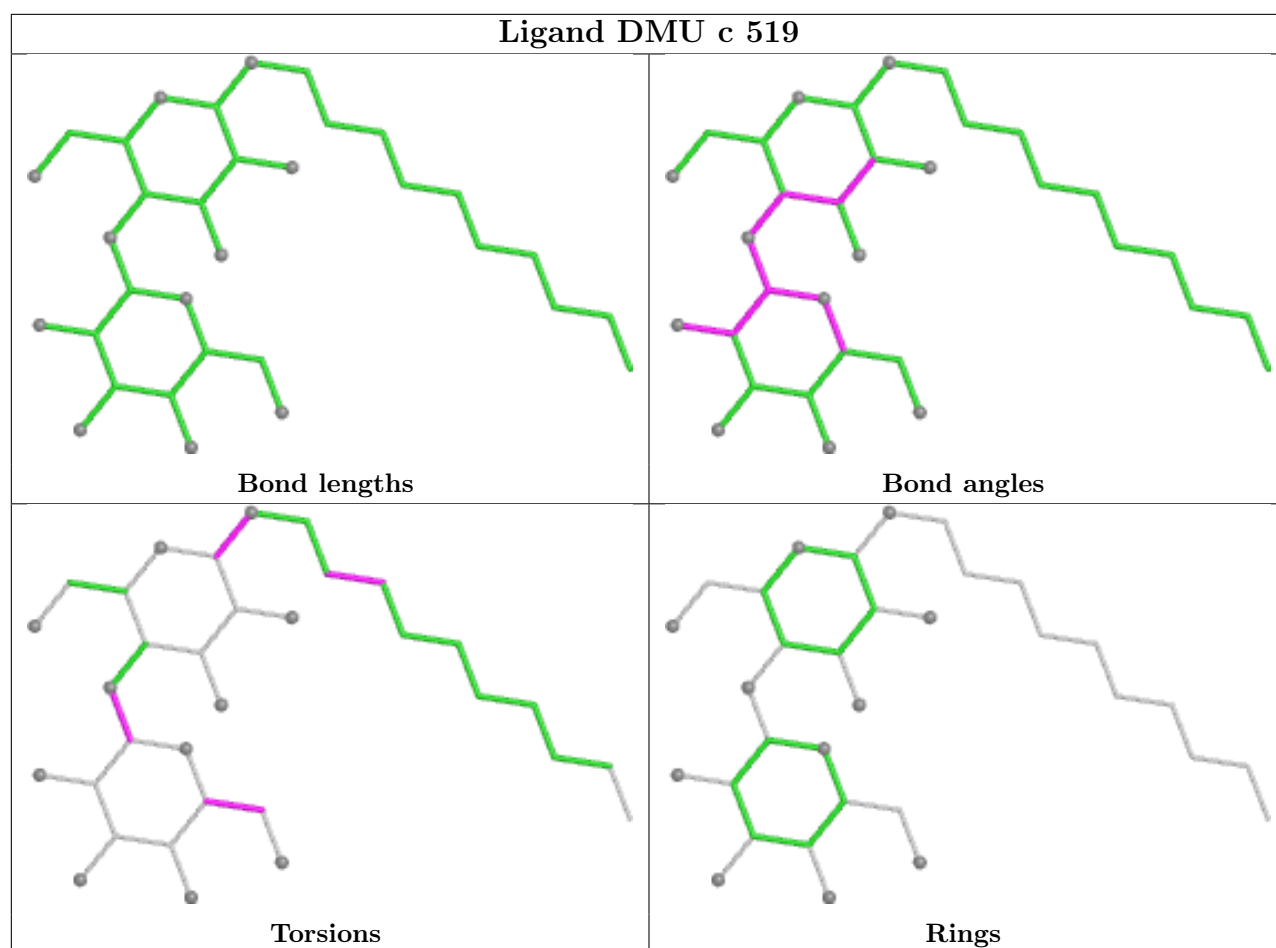
Ligand BCR H 101



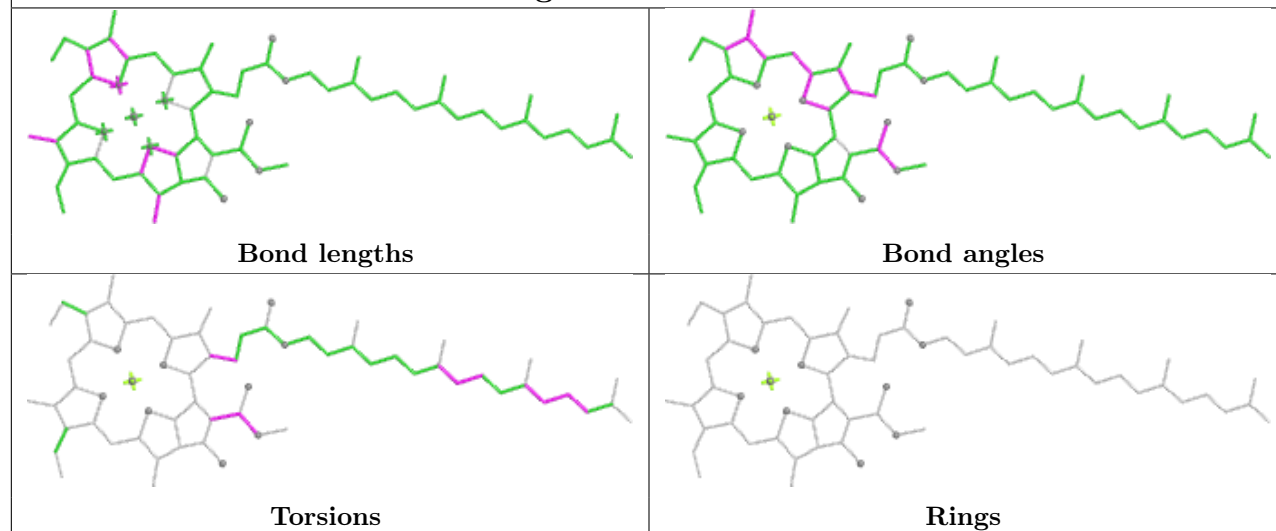




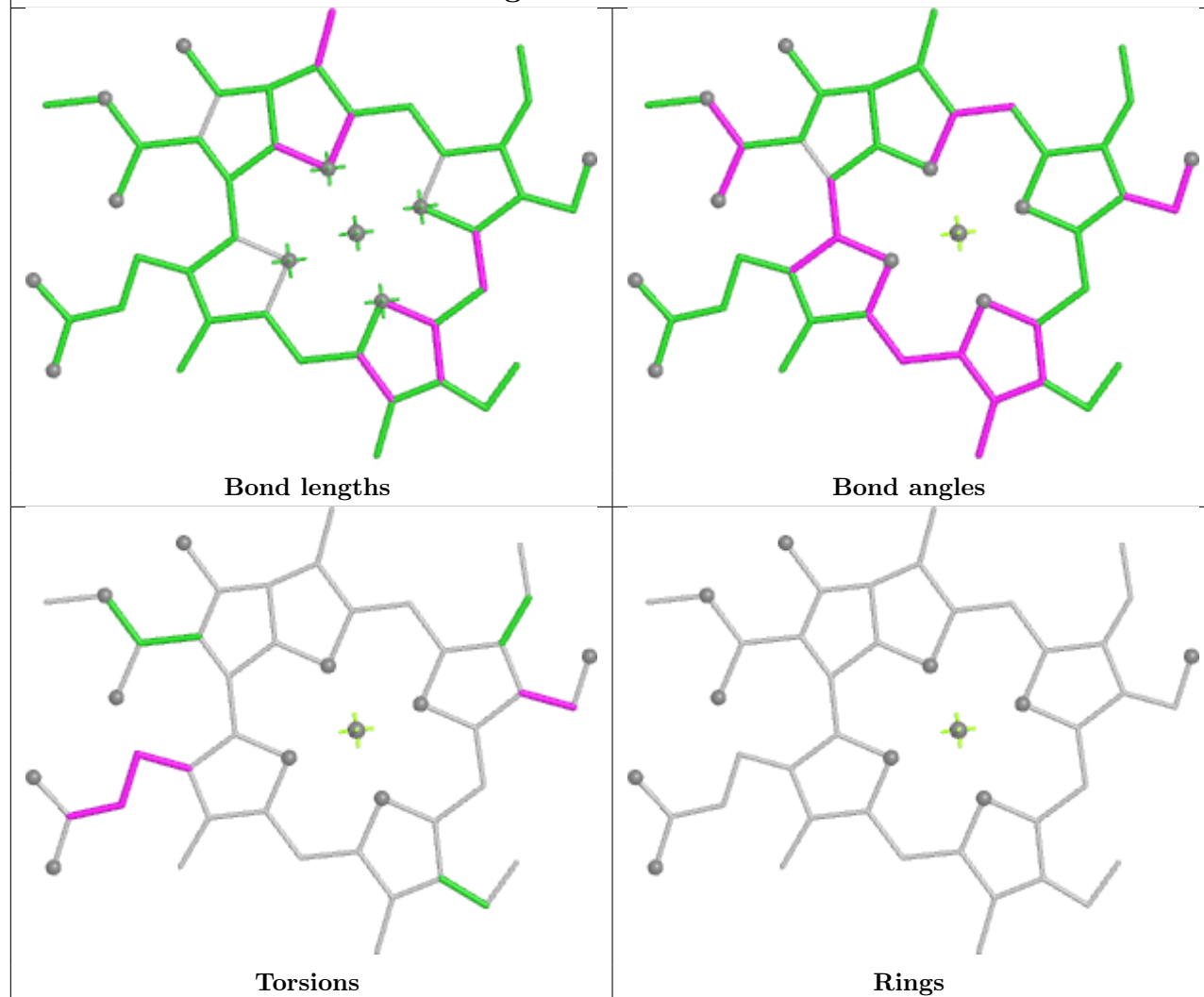


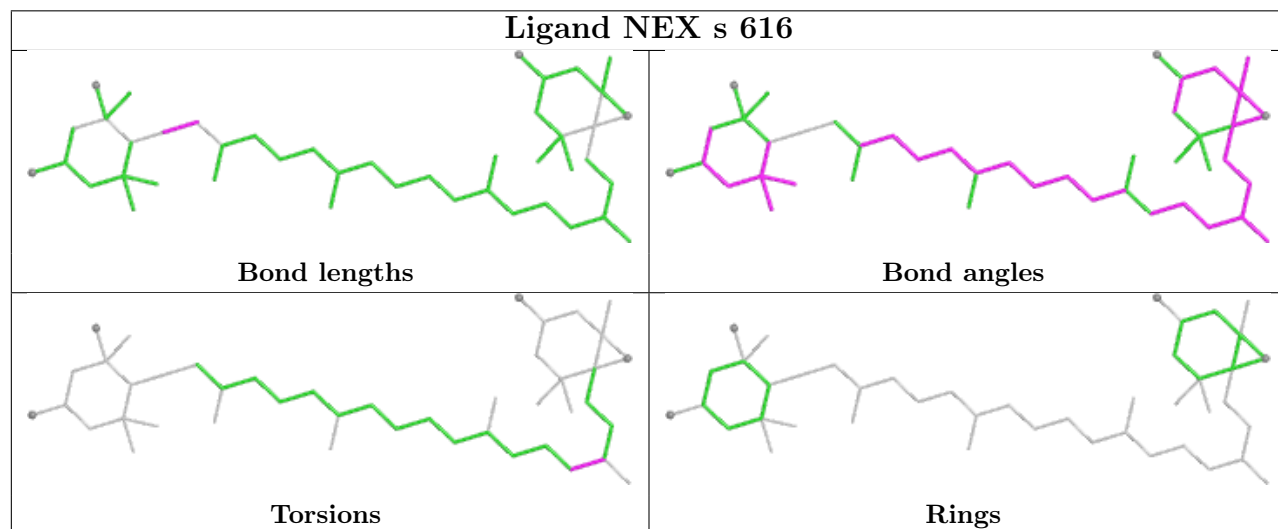
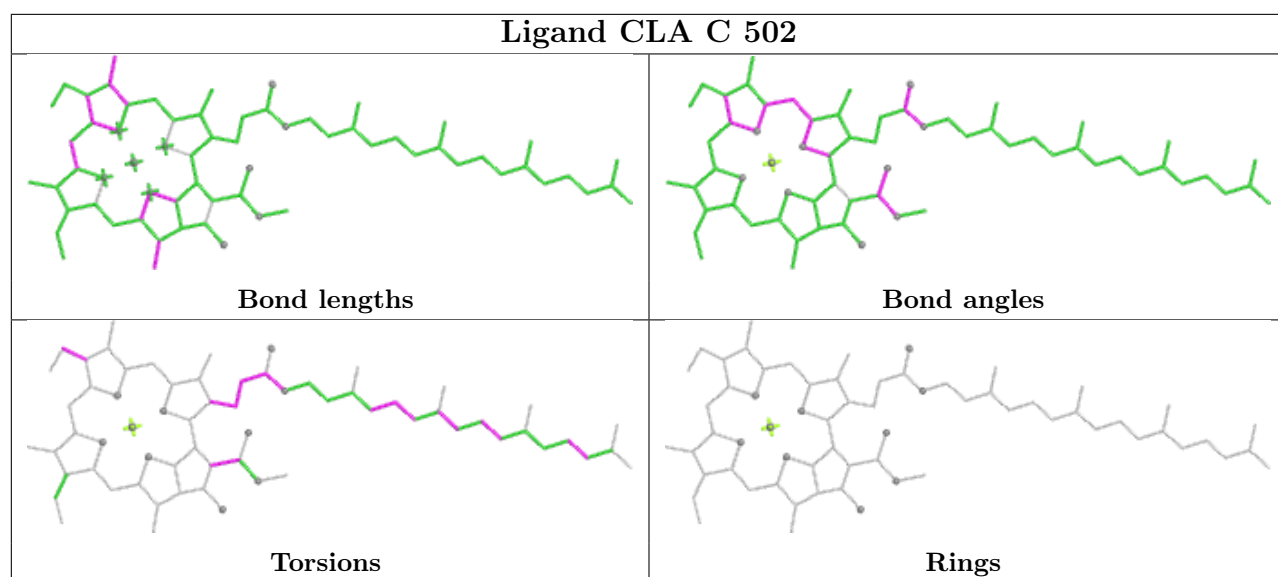


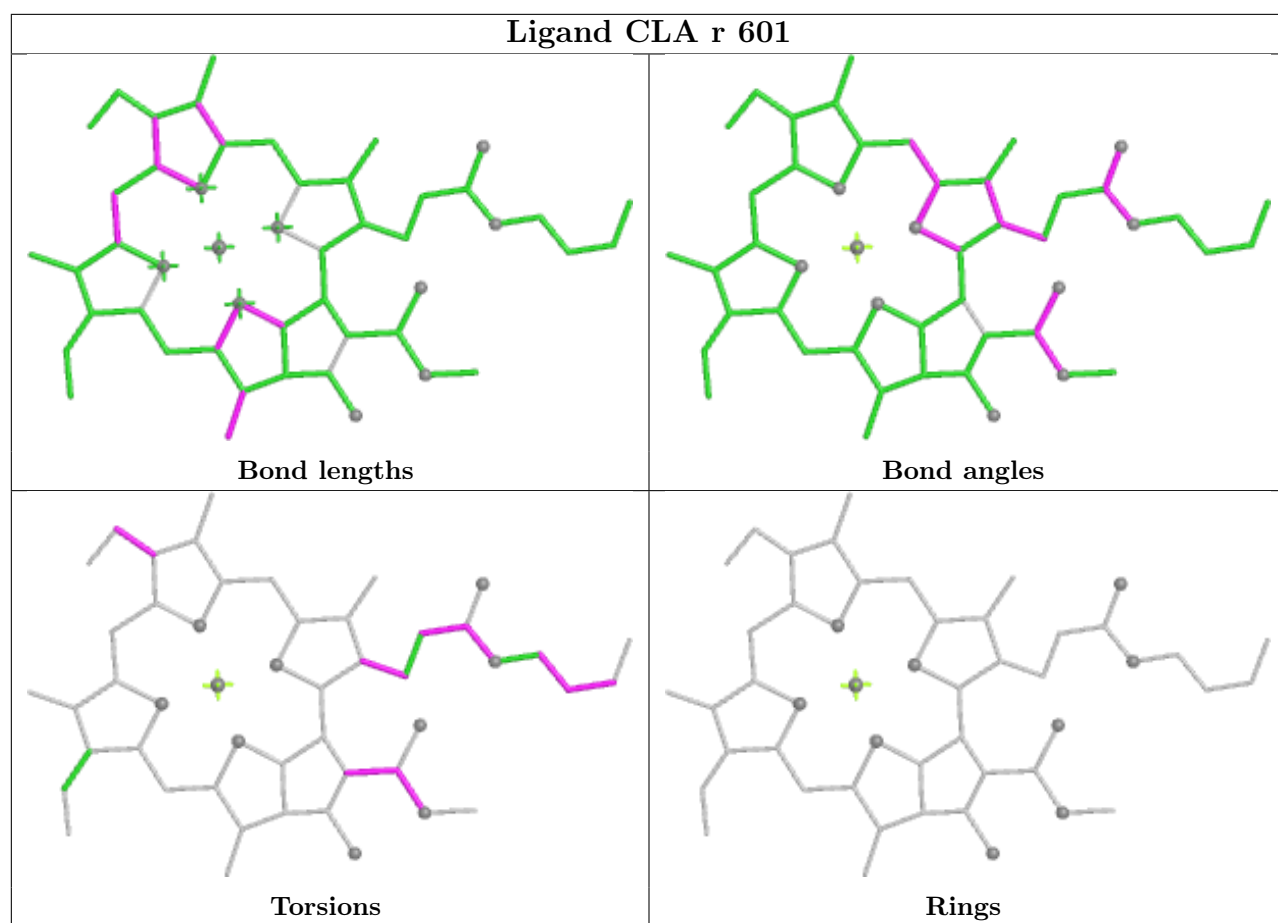
Ligand CLA b 612



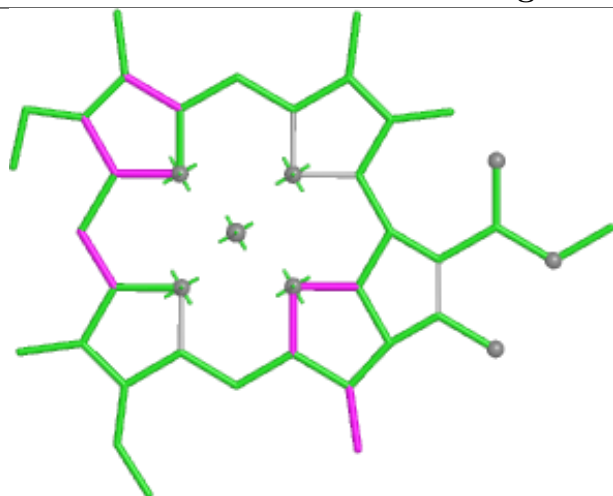
Ligand CHL n 606



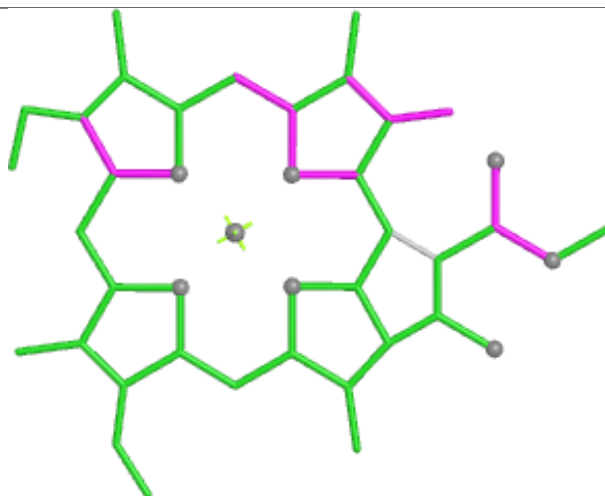




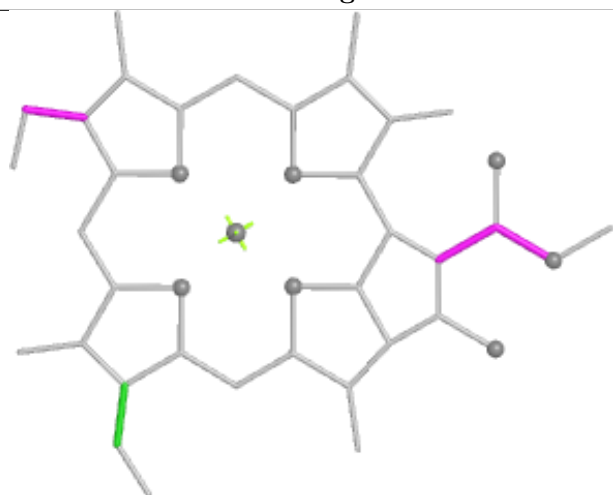
Ligand CLA n 614



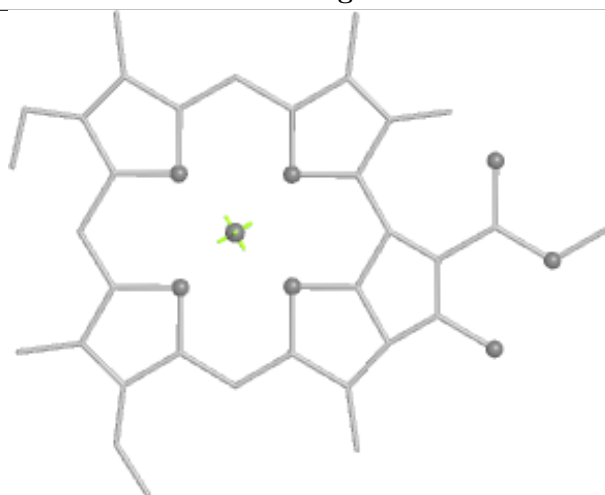
Bond lengths



Bond angles

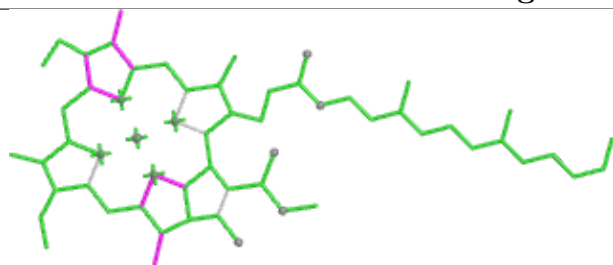


Torsions

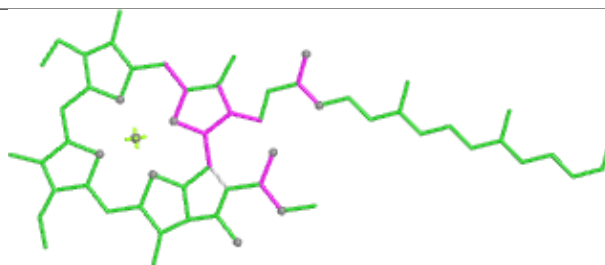


Rings

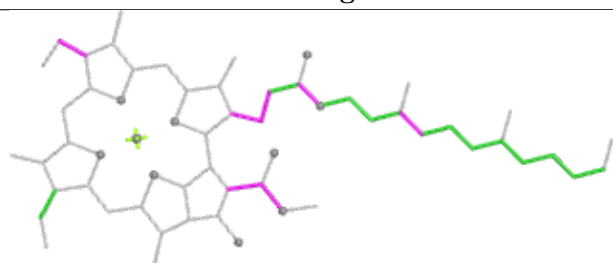
Ligand CLA n 603



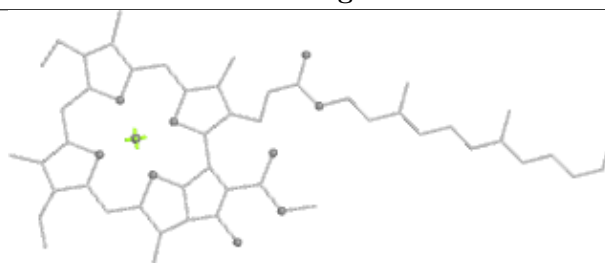
Bond lengths



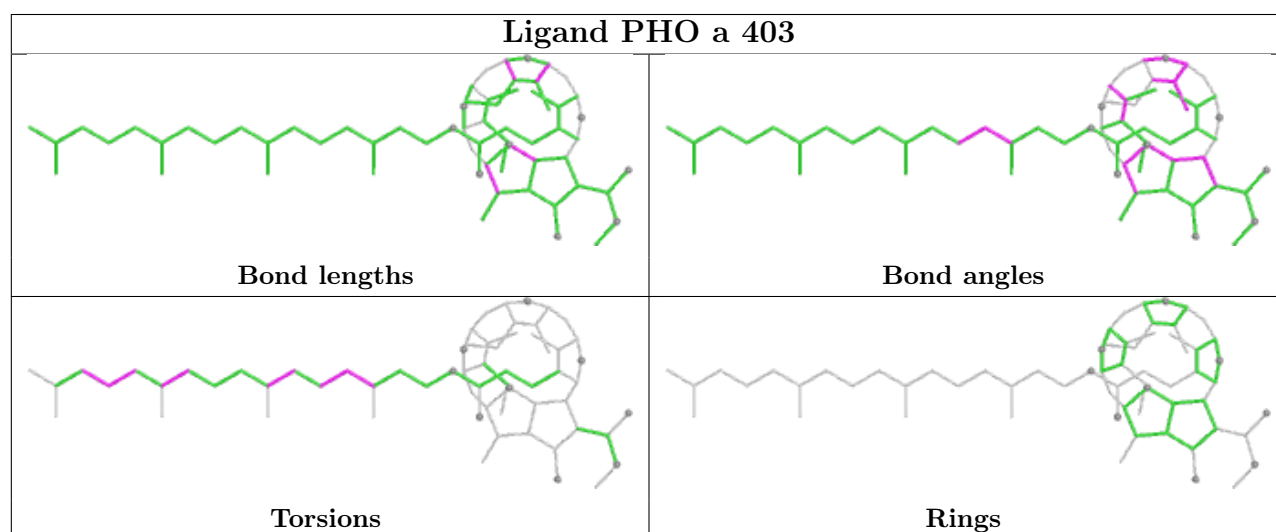
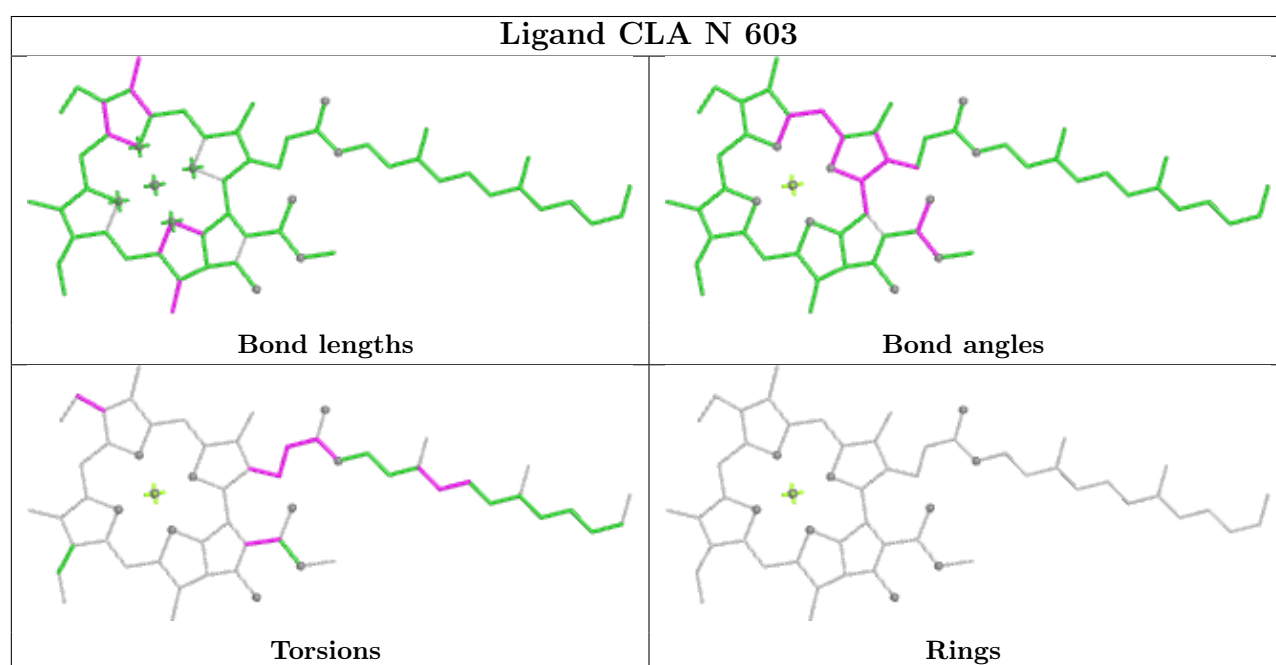
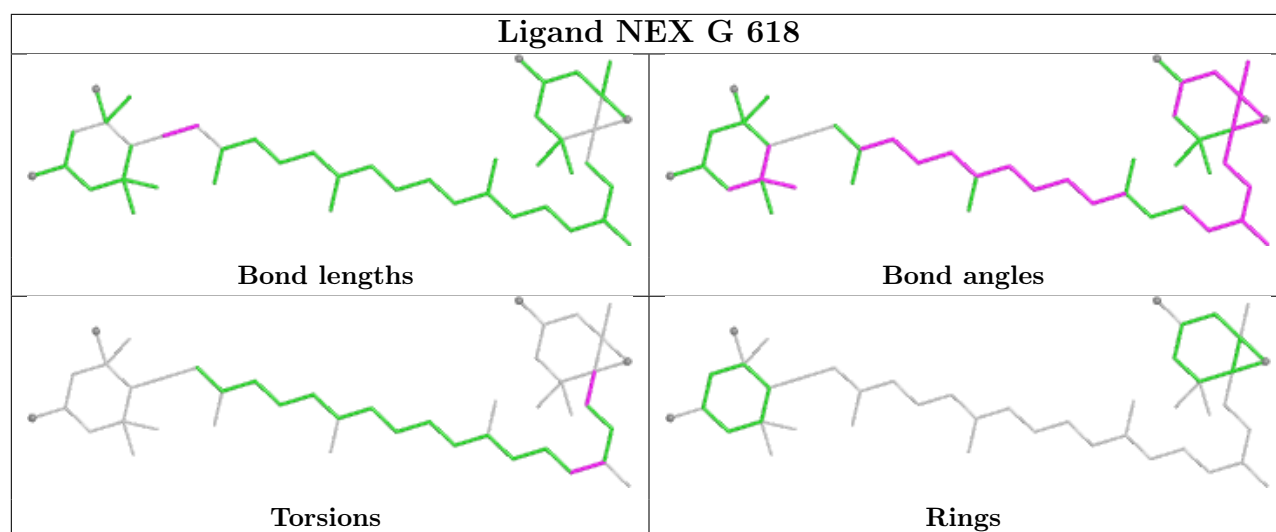
Bond angles

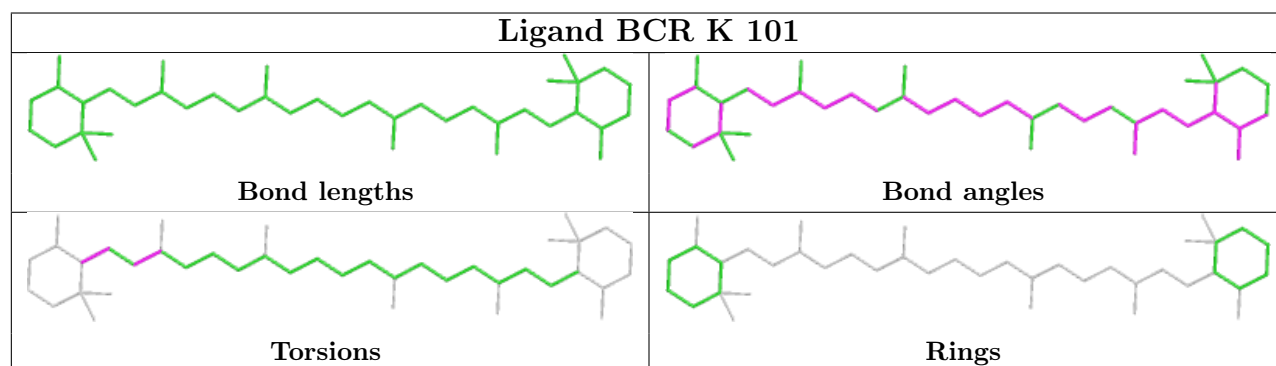
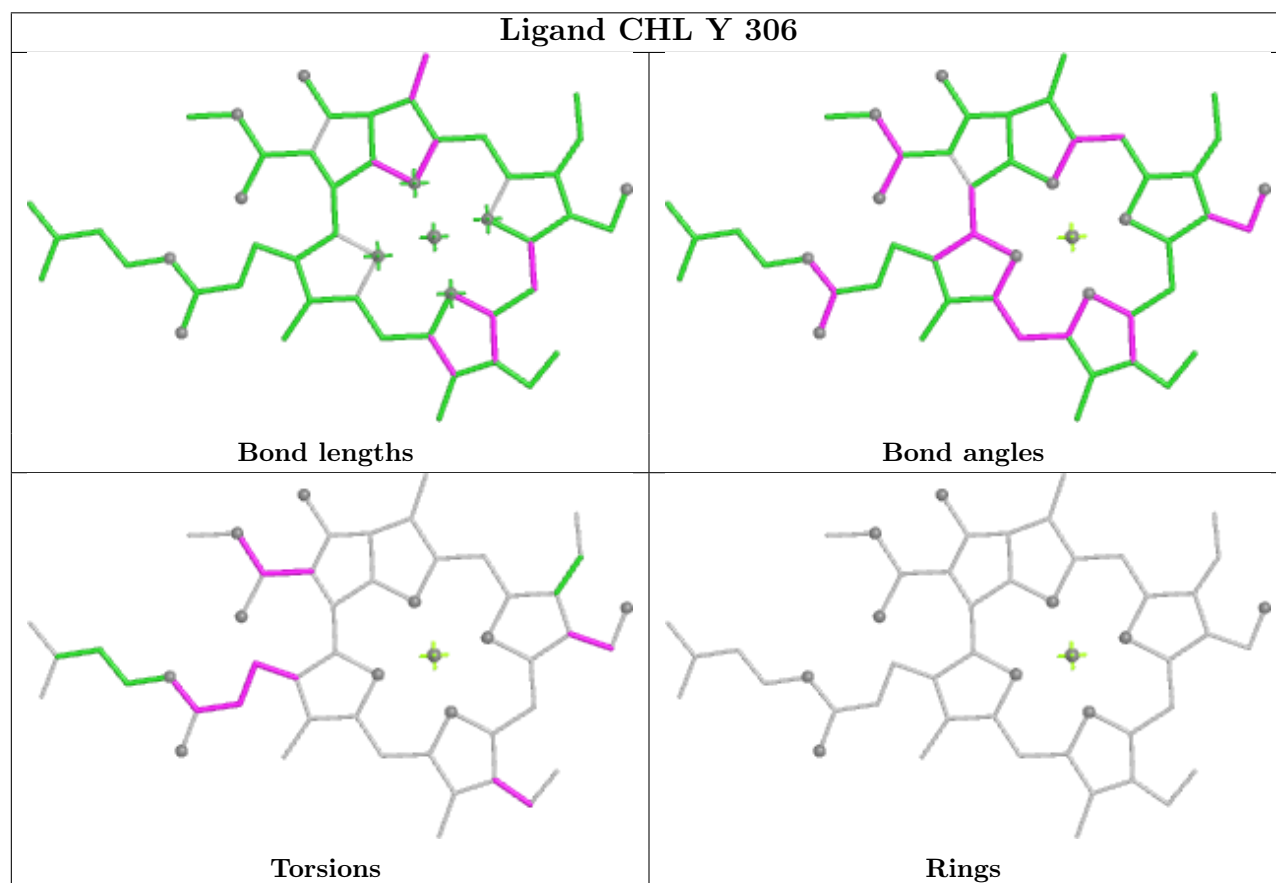
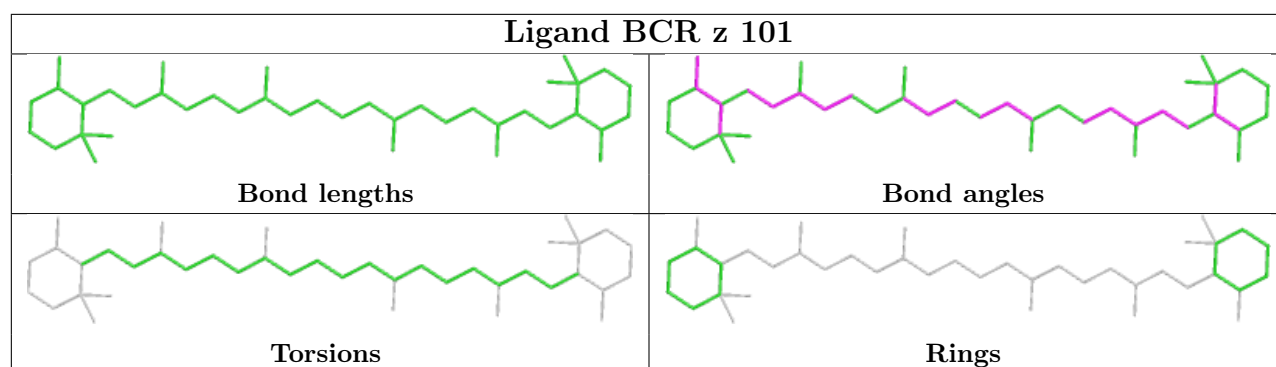


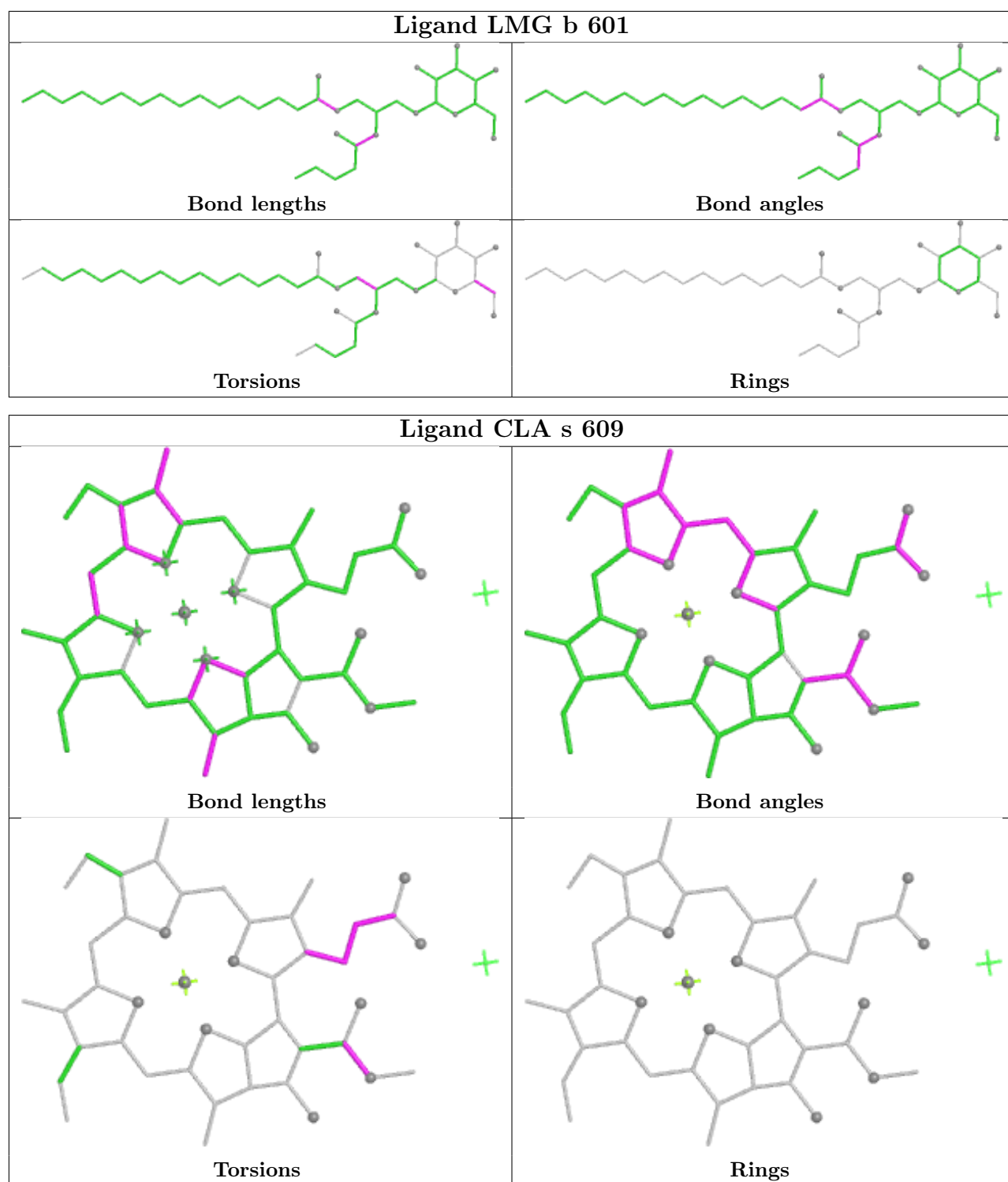
Torsions

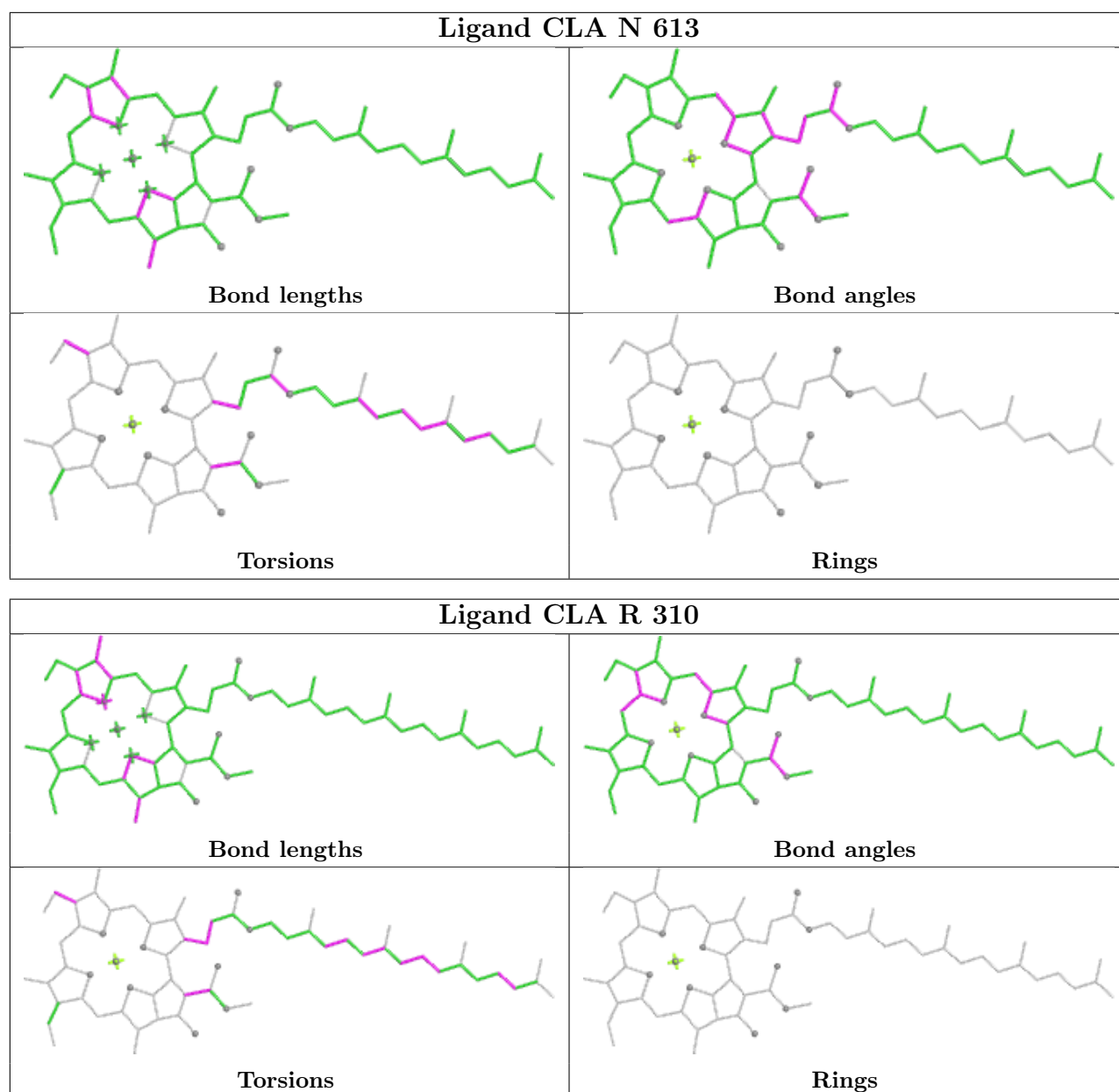


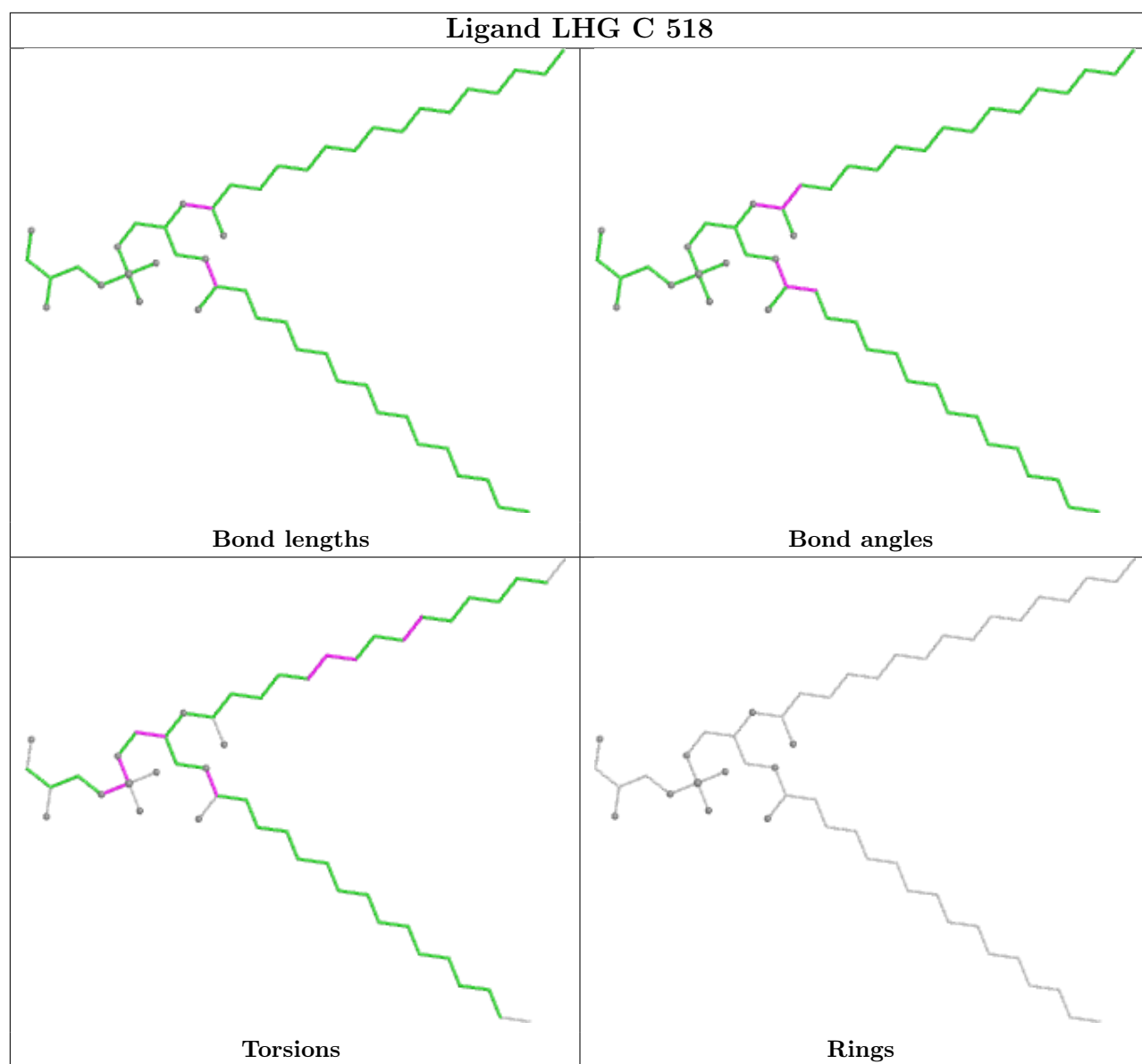
Rings



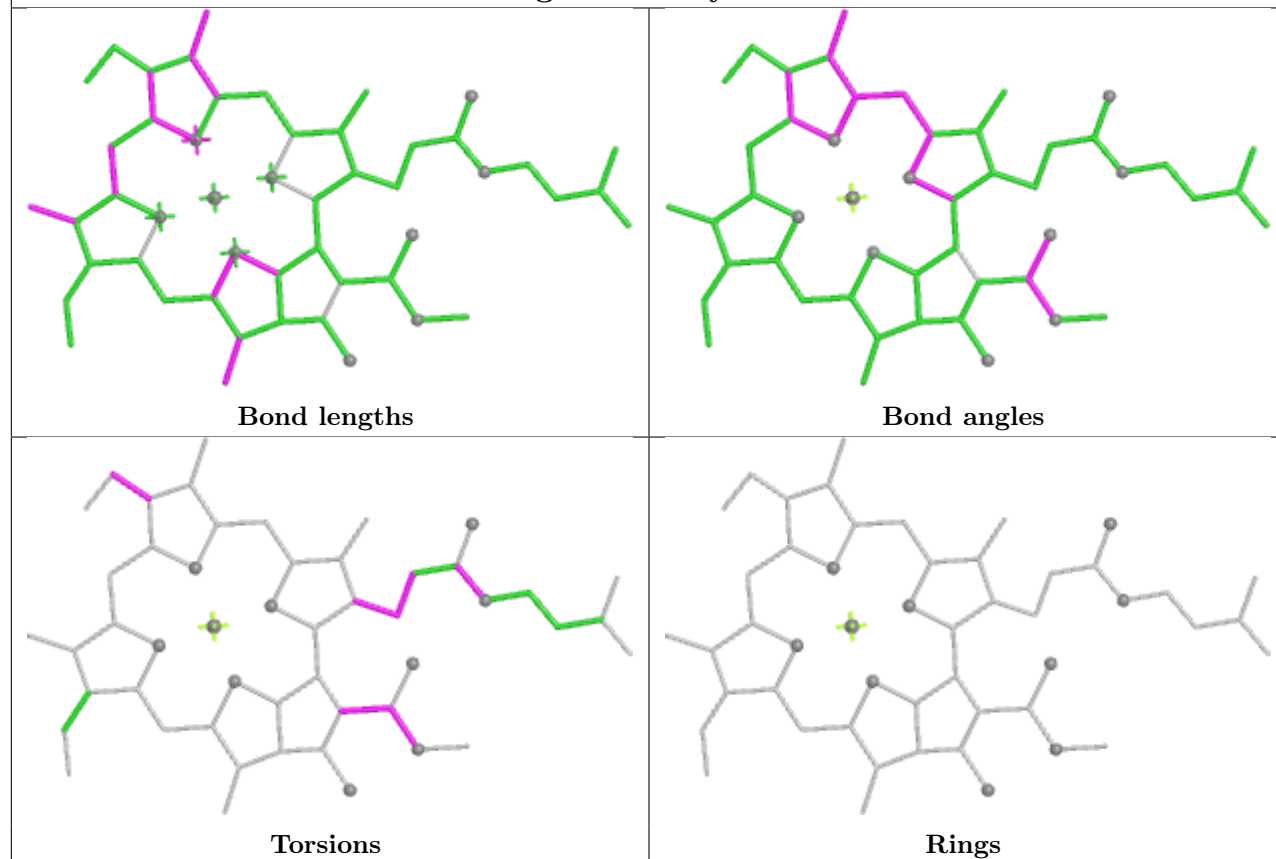




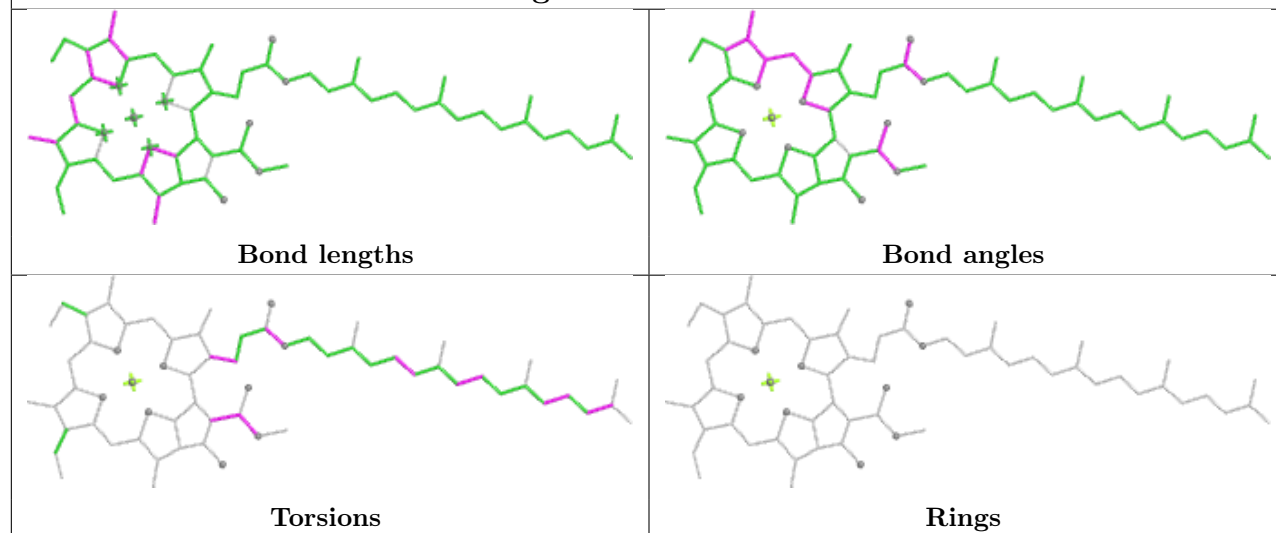




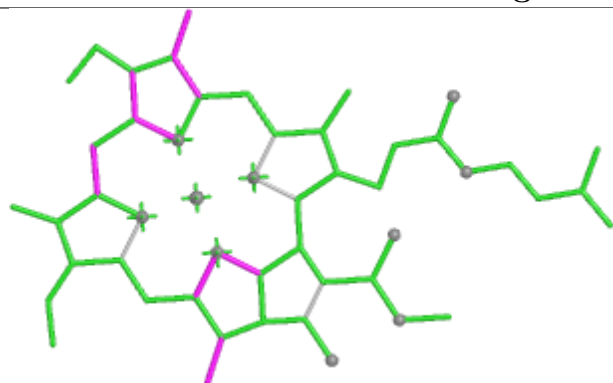
Ligand CLA y 305



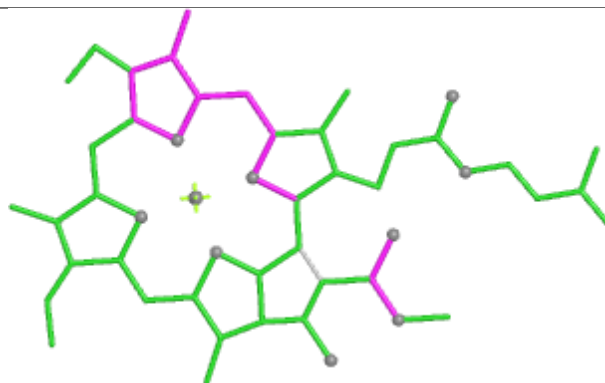
Ligand CLA C 509



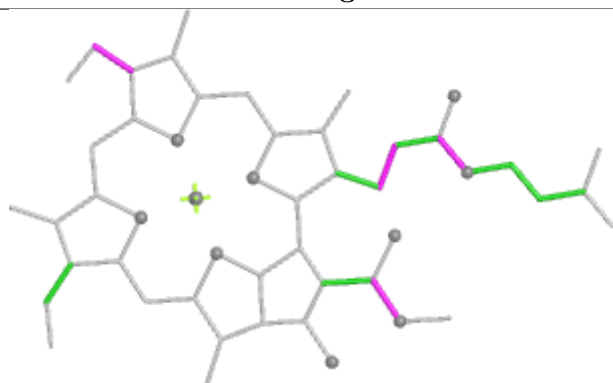
Ligand CLA N 604



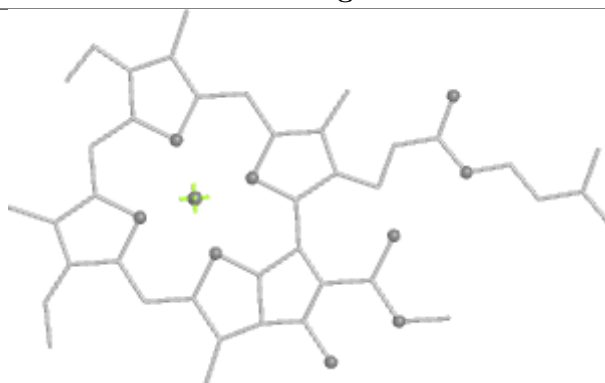
Bond lengths



Bond angles

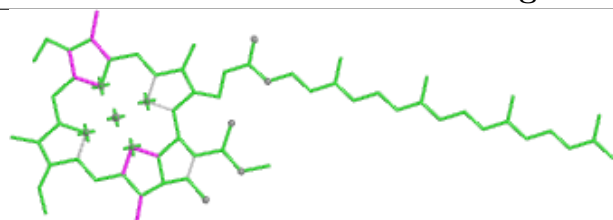


Torsions

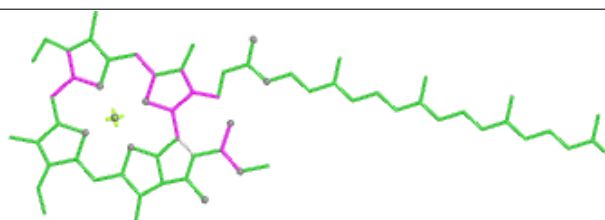


Rings

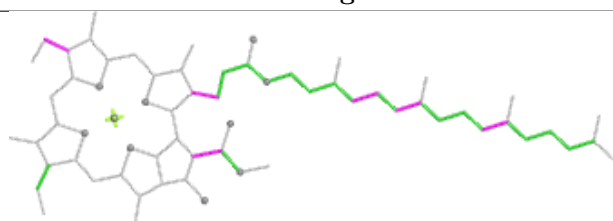
Ligand CLA c 507



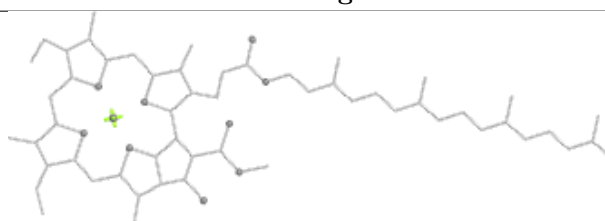
Bond lengths



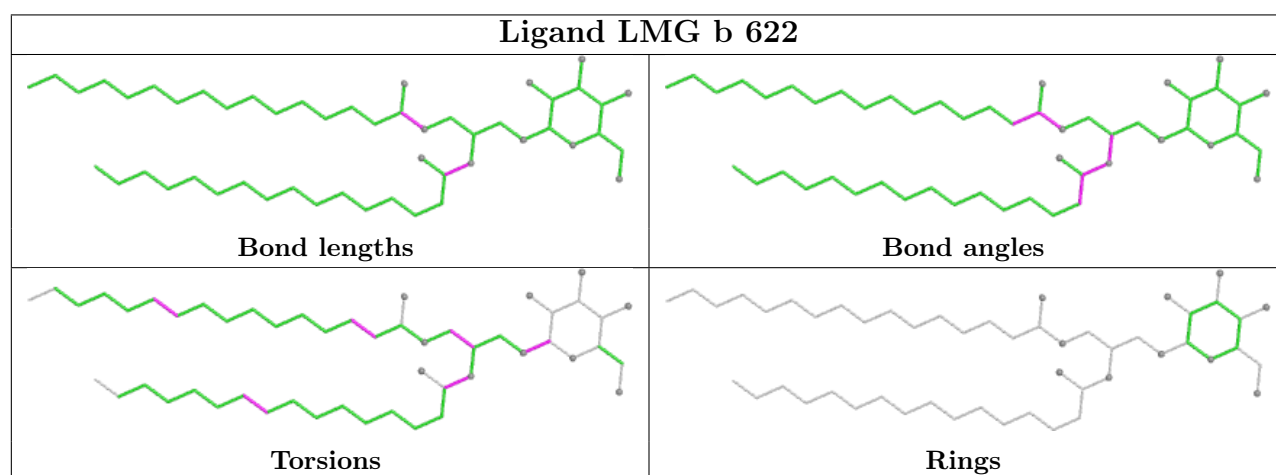
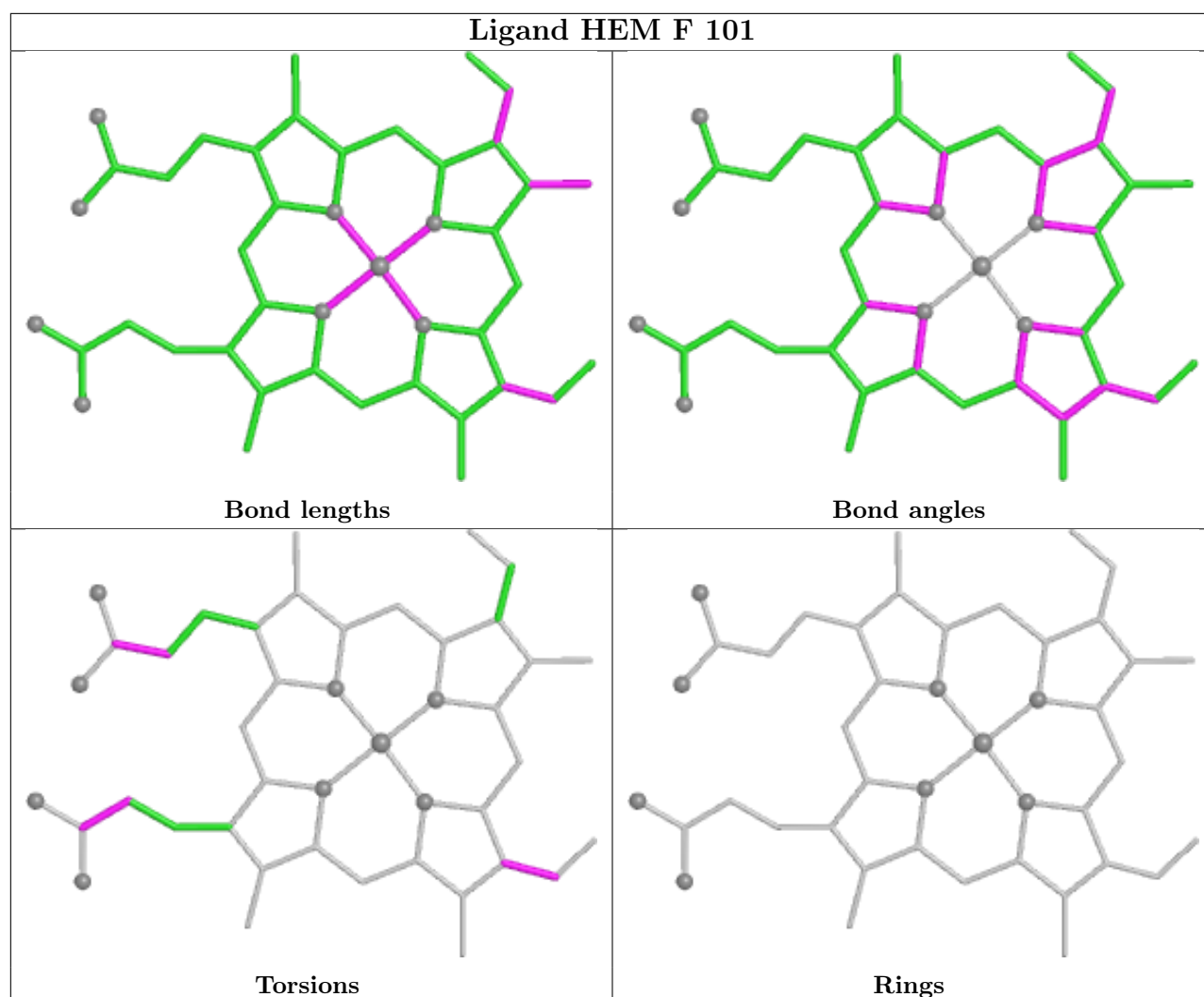
Bond angles

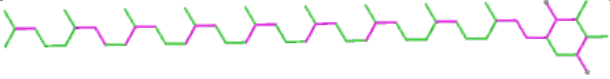
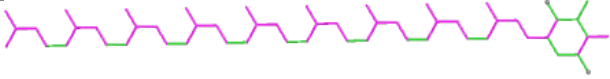
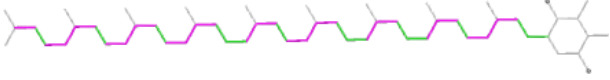
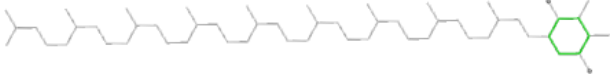
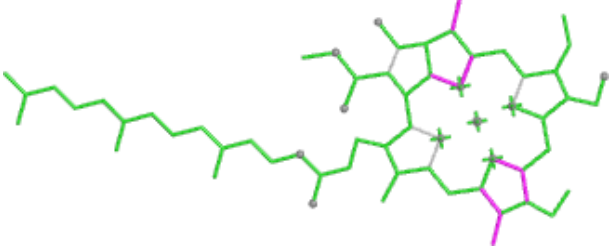
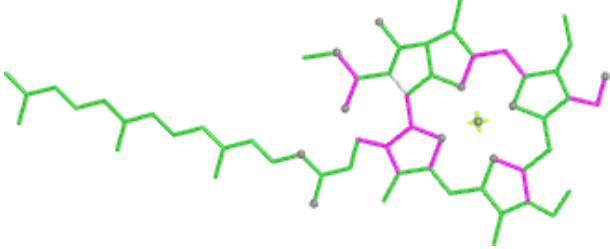
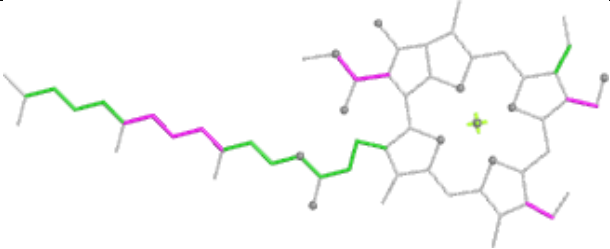
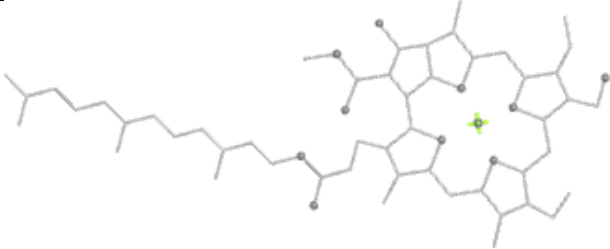


Torsions

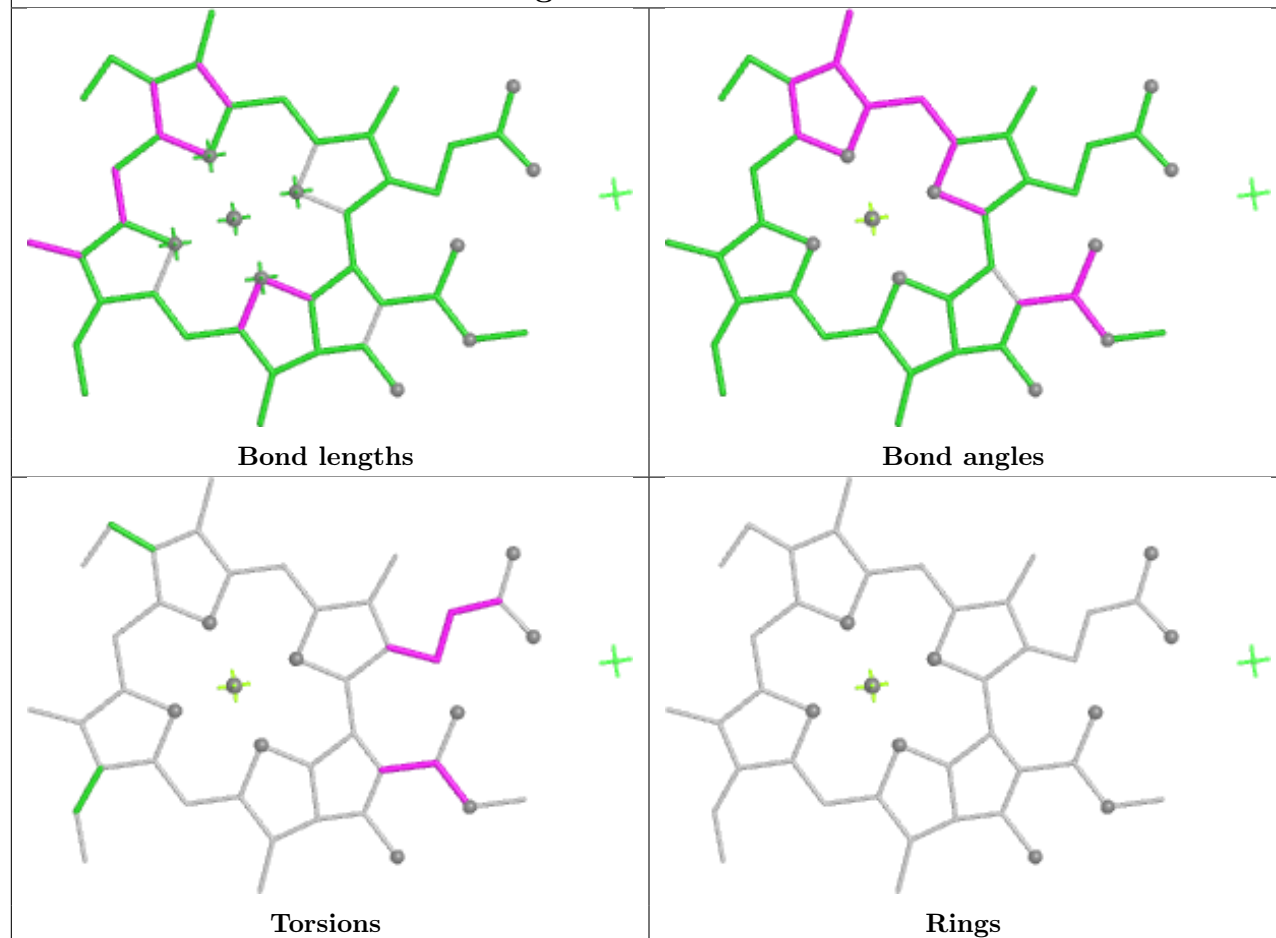


Rings

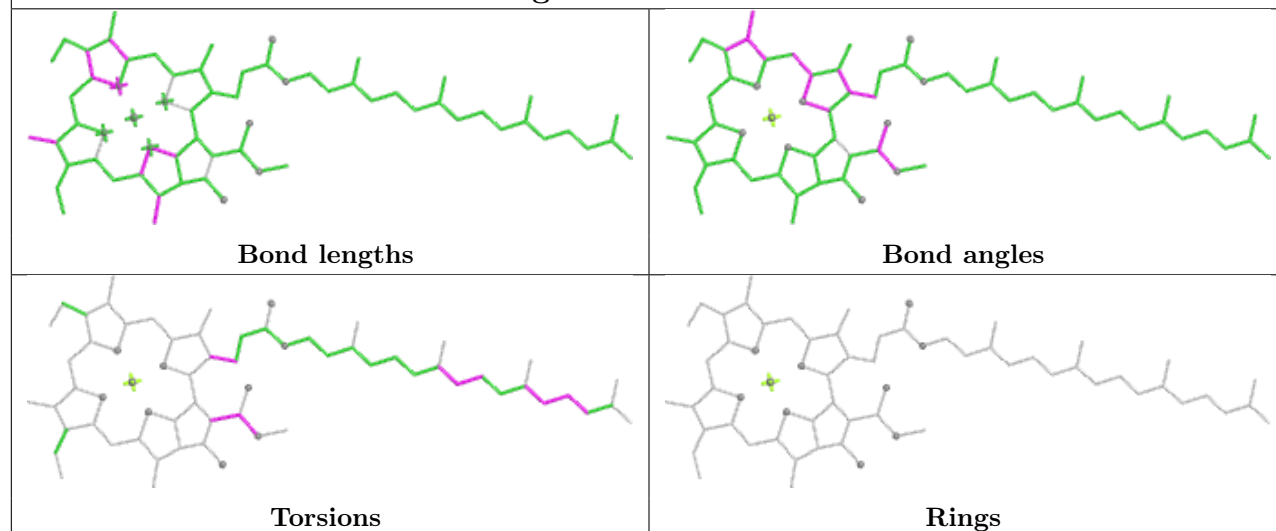


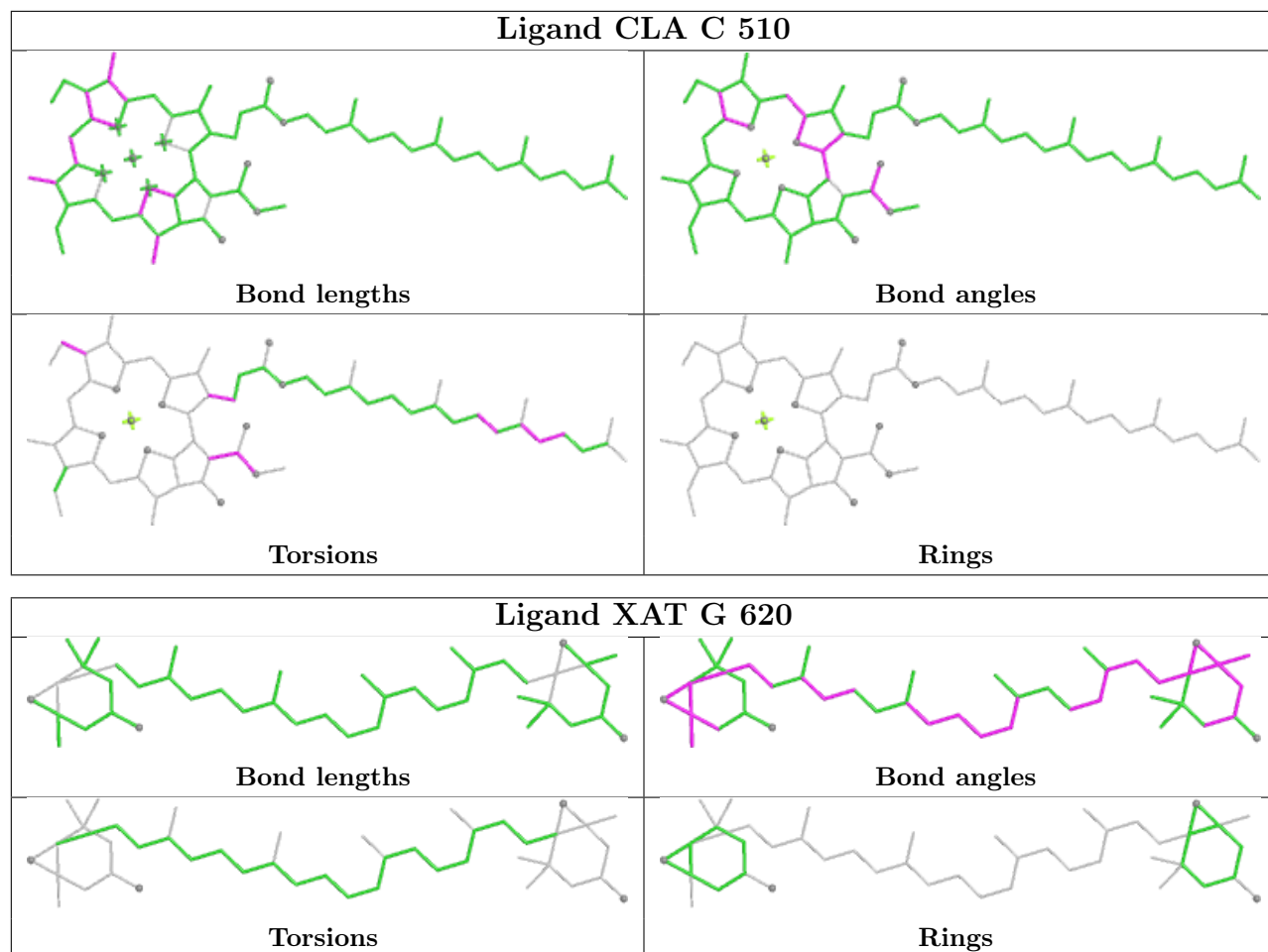
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL G 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

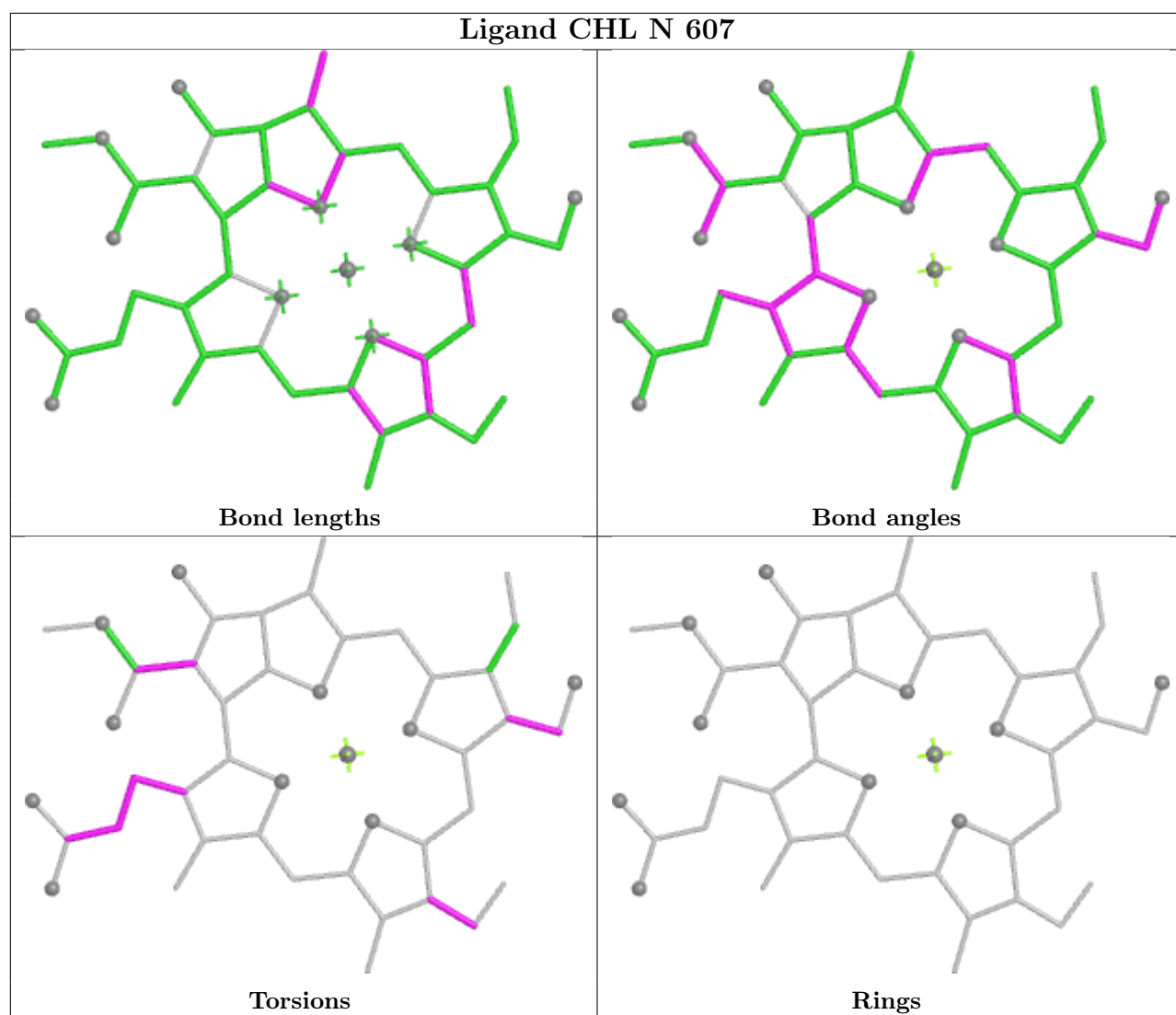
Ligand CLA S 310



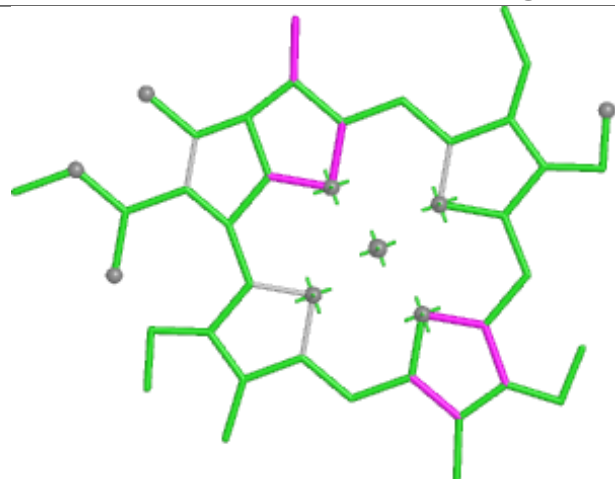
Ligand CLA B 610



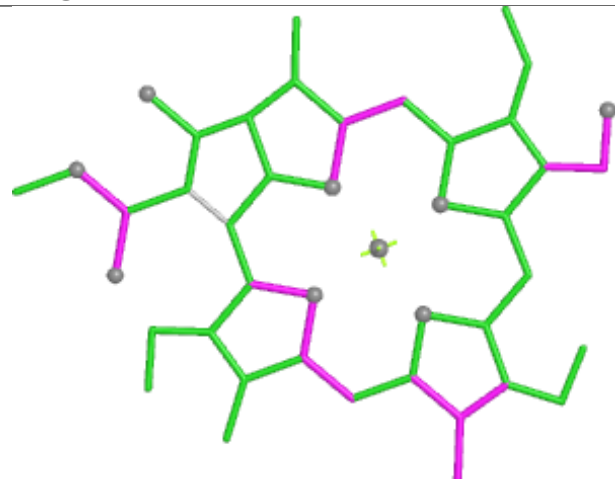




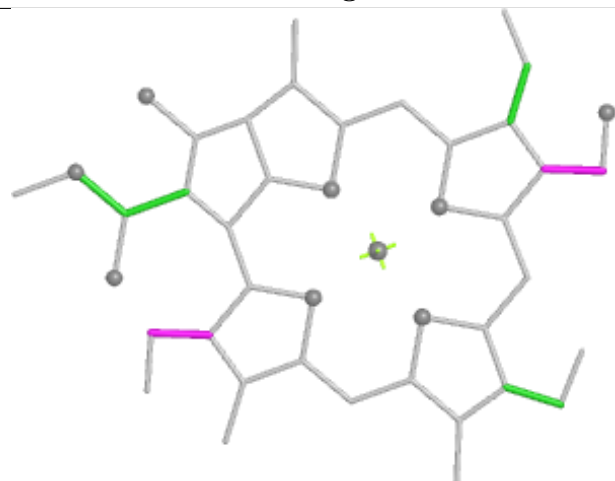
Ligand CHL g 606



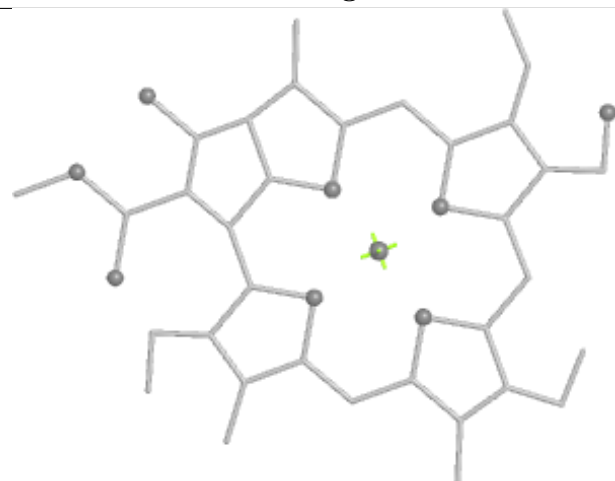
Bond lengths



Bond angles

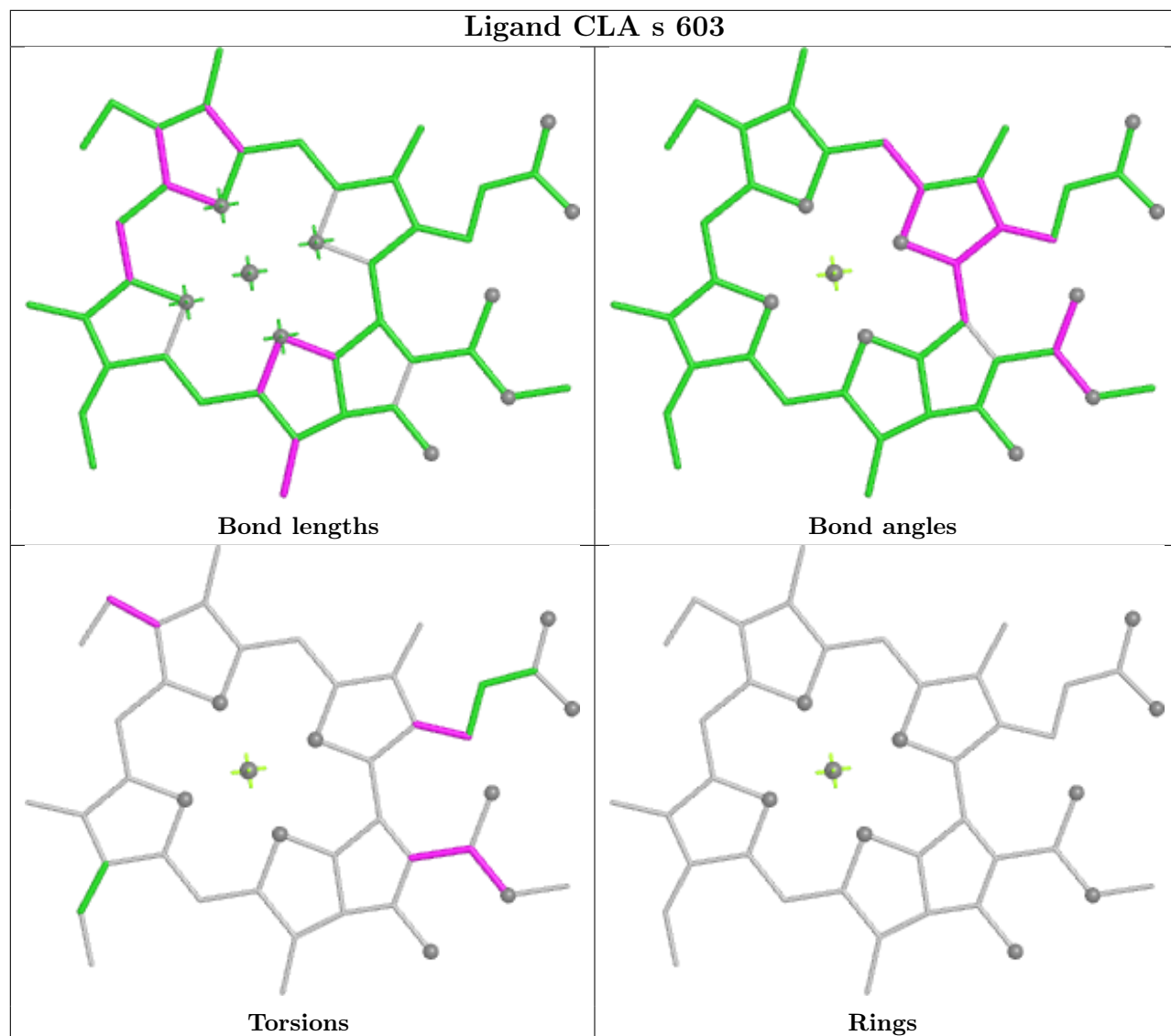


Torsions

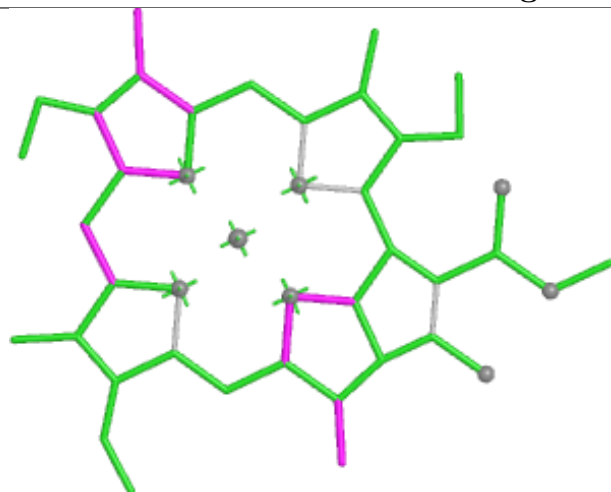


Rings

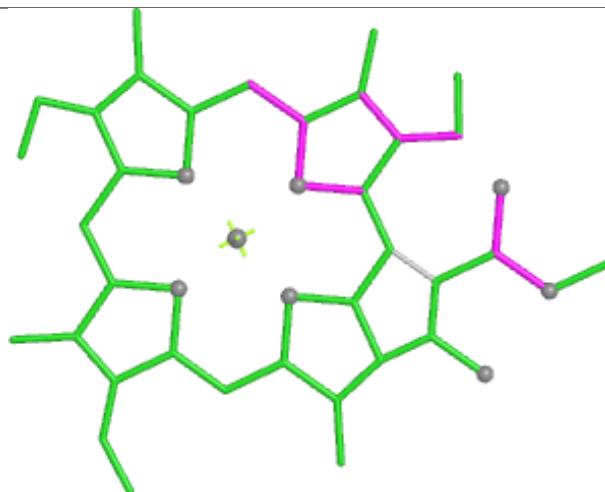
Ligand CLA s 603



Ligand CLA s 610



Bond lengths



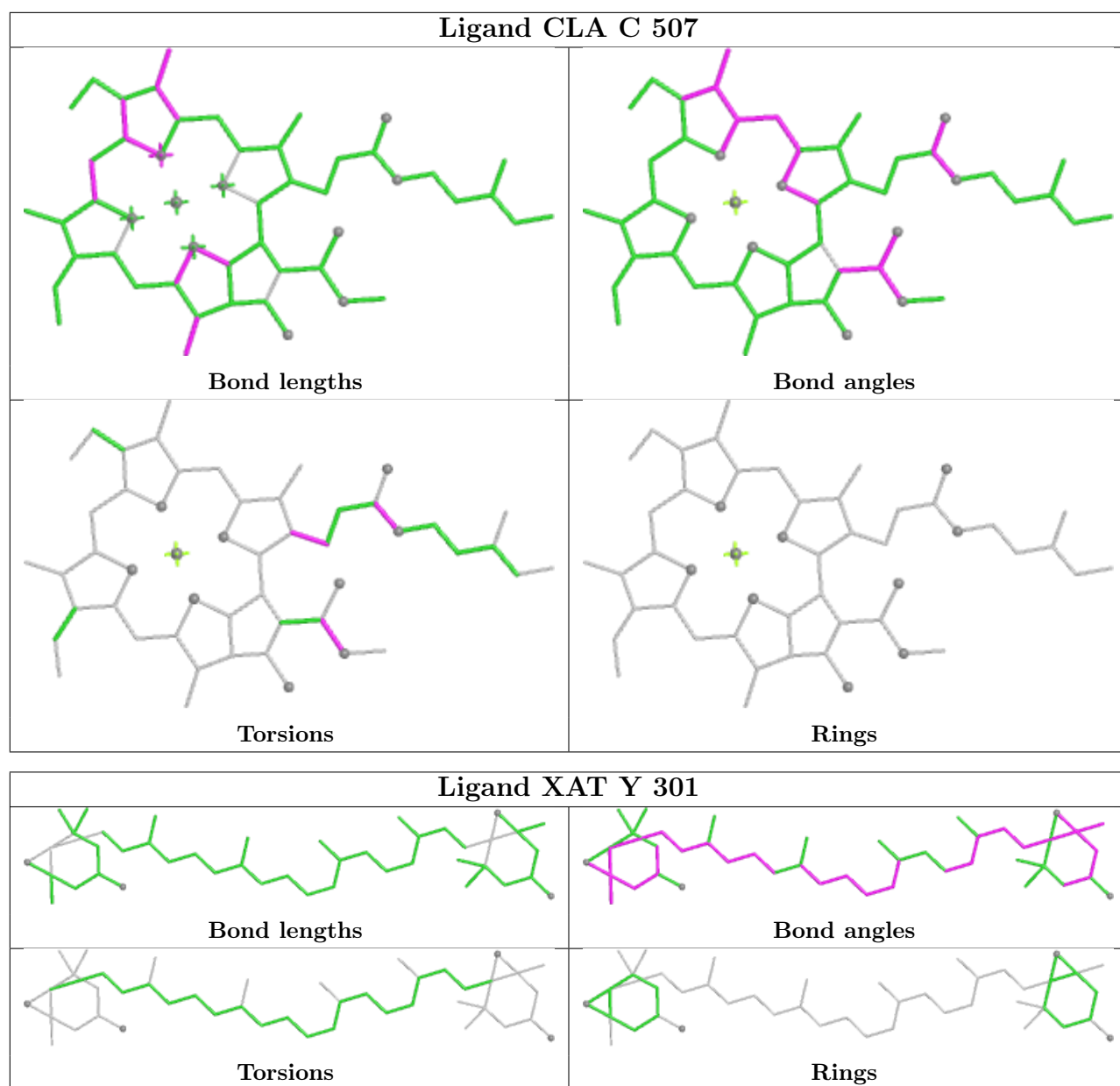
Bond angles



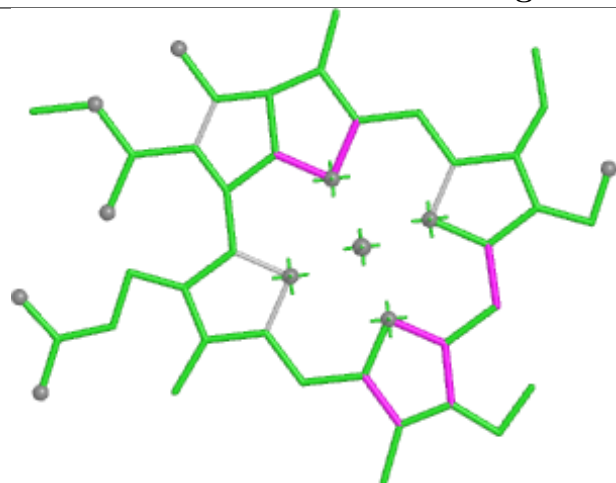
Torsions



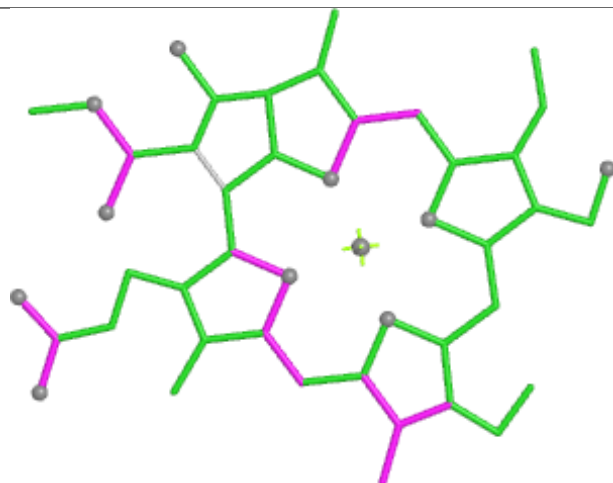
Rings



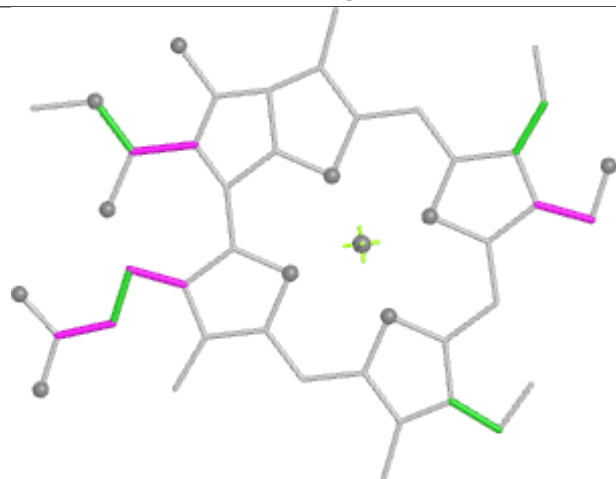
Ligand CHL R 306



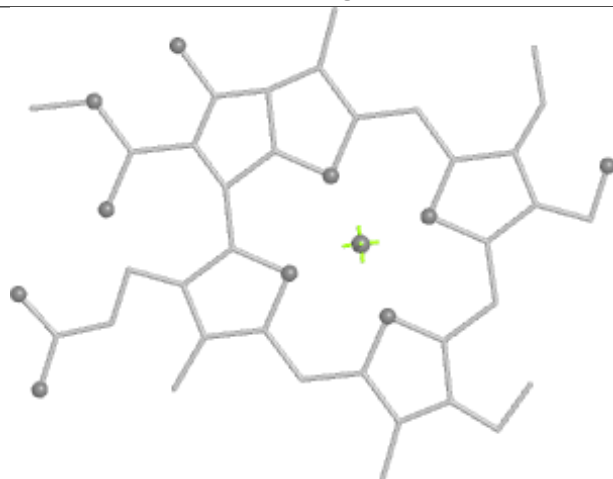
Bond lengths



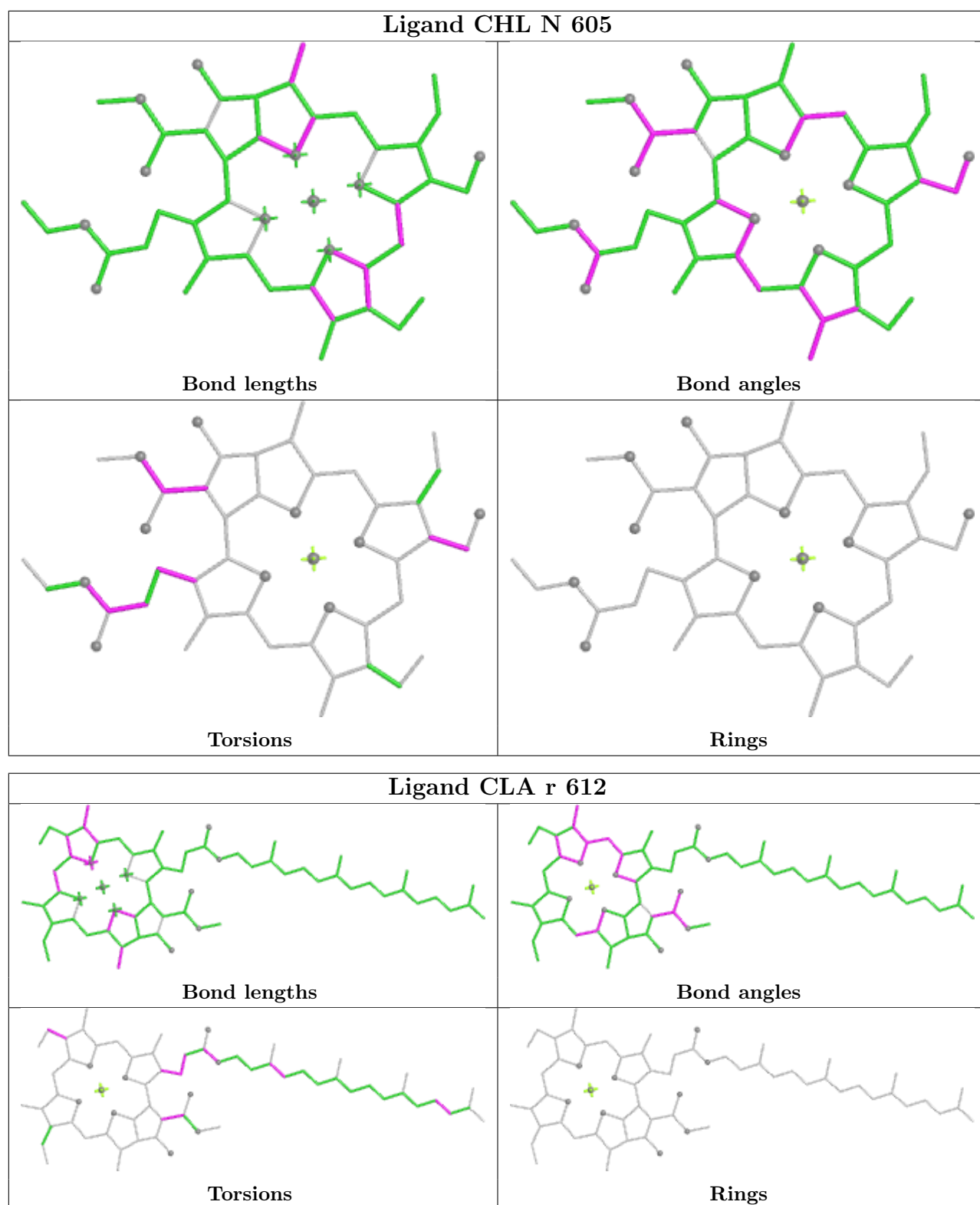
Bond angles

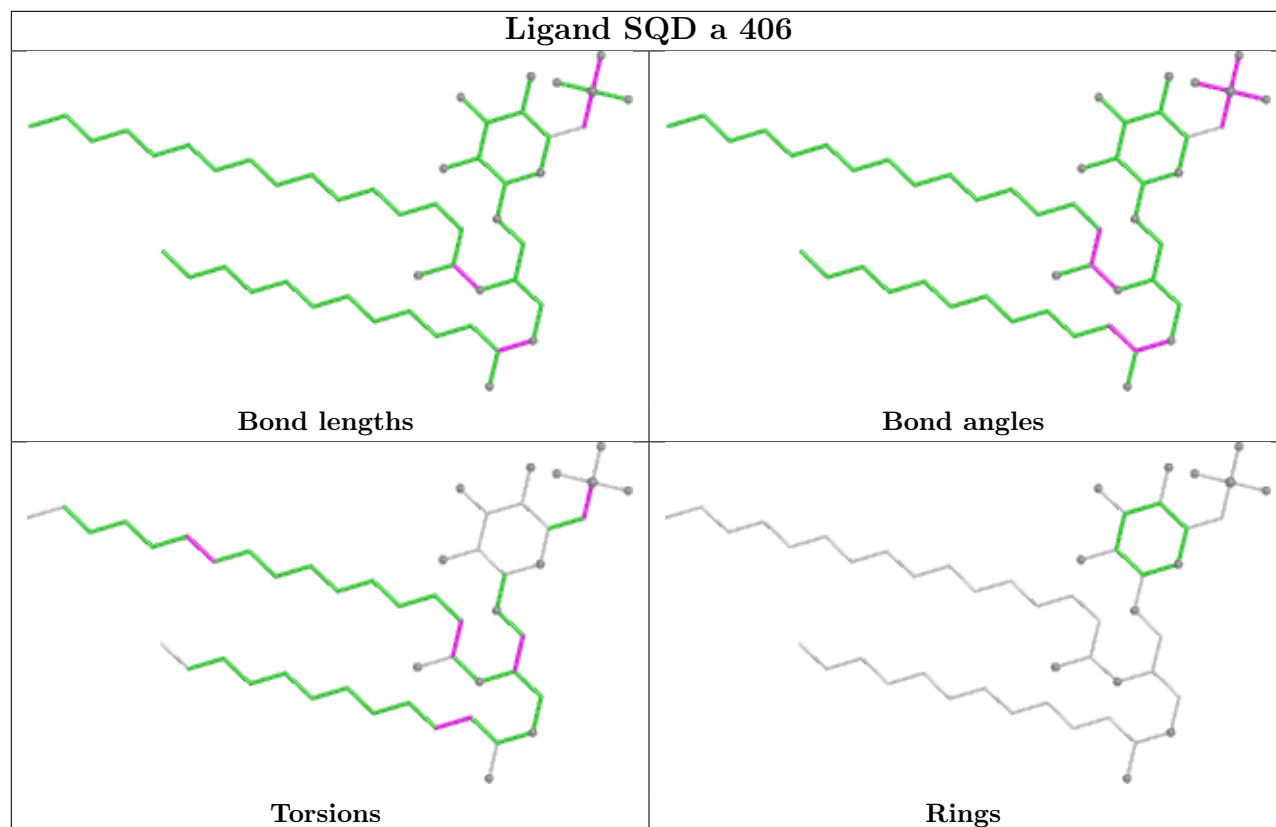
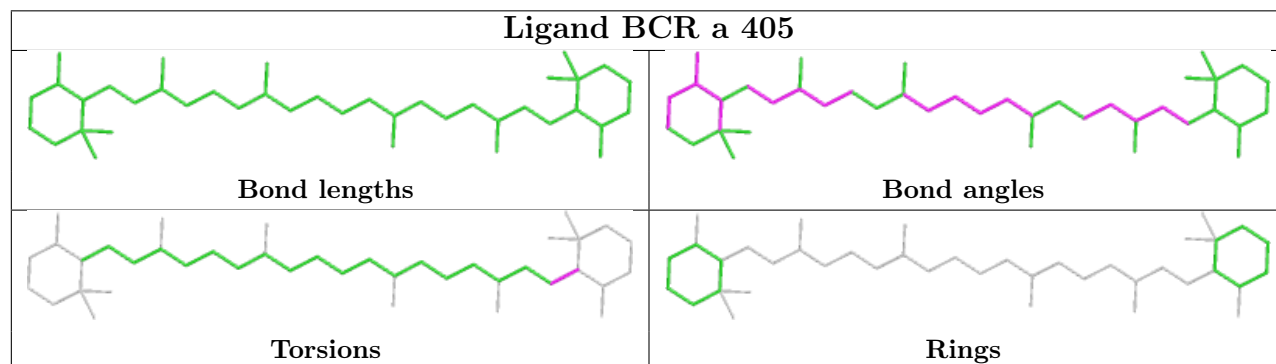
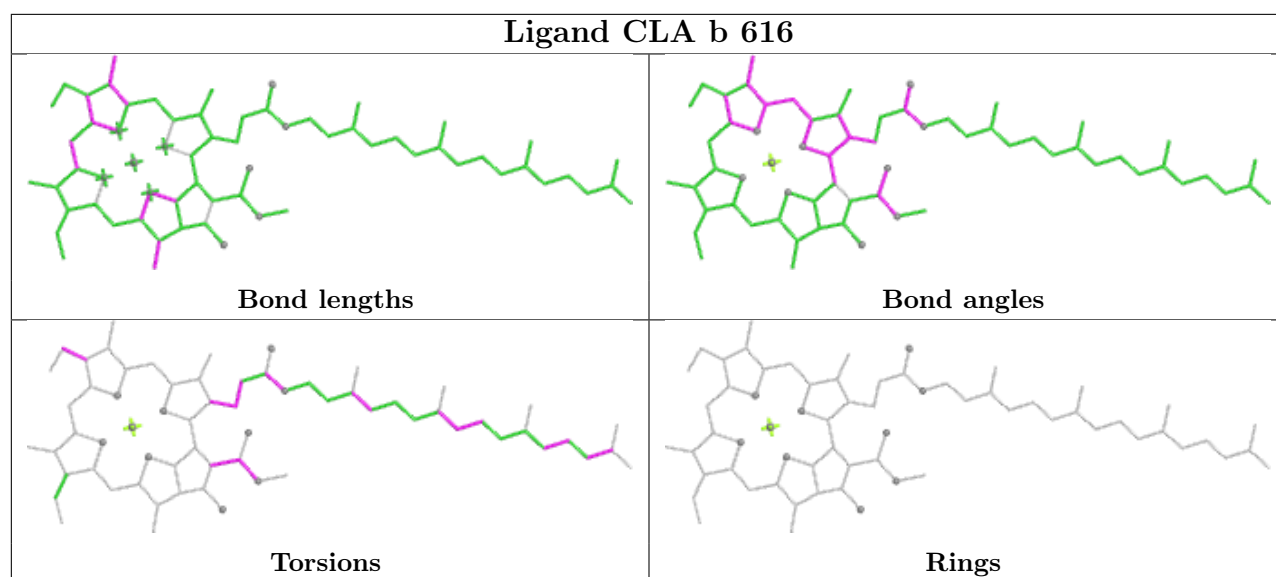


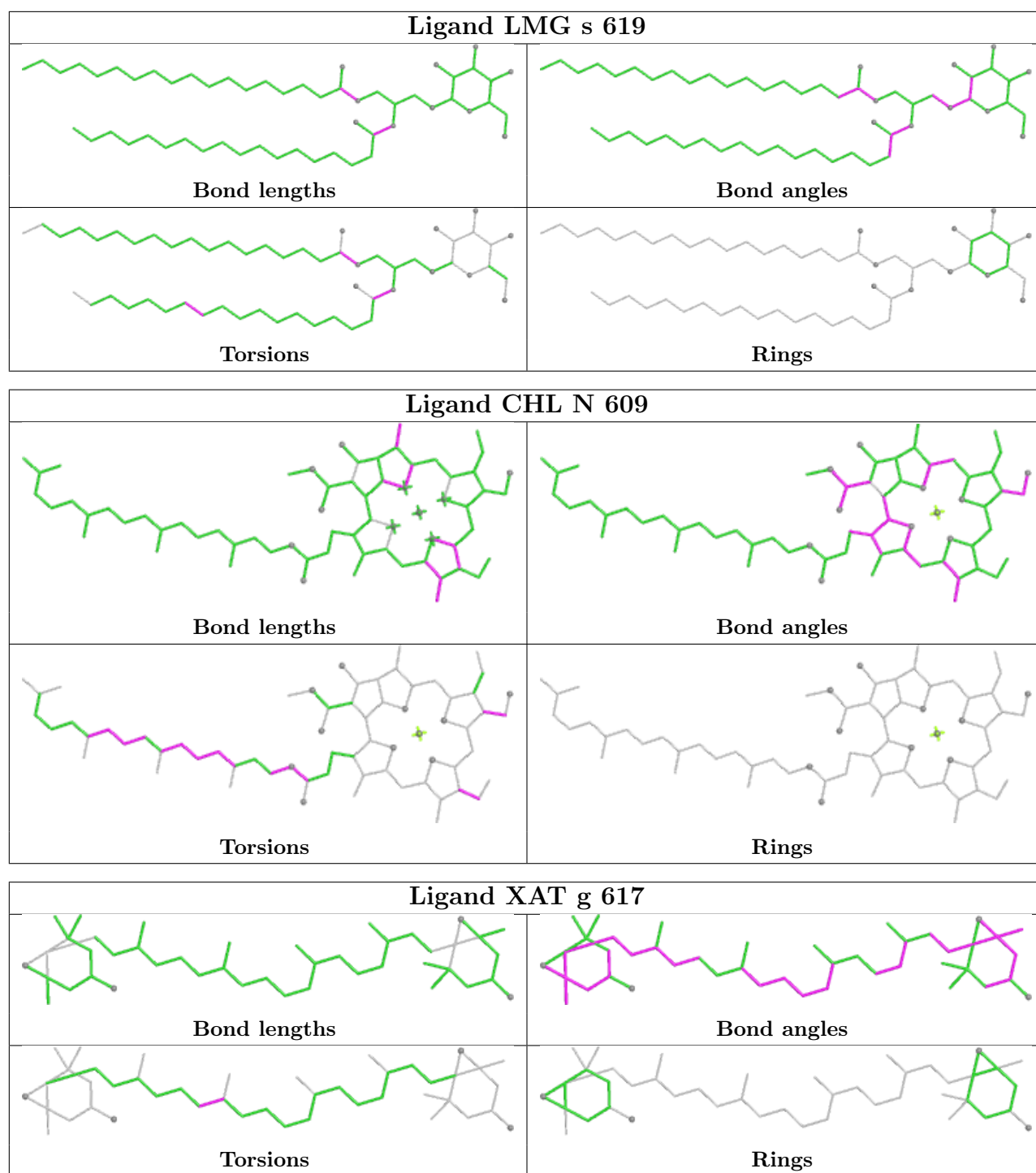
Torsions

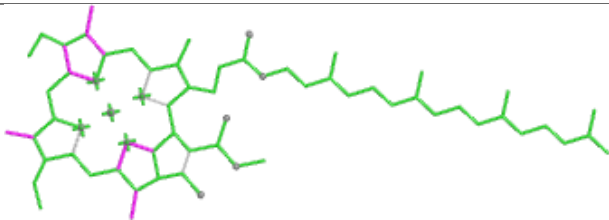
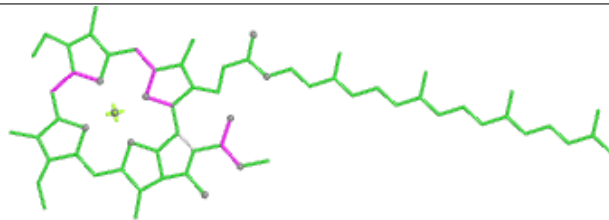
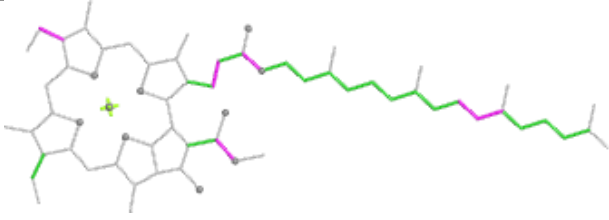
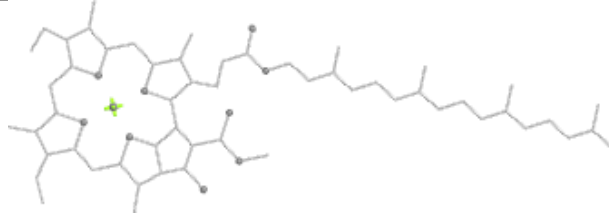


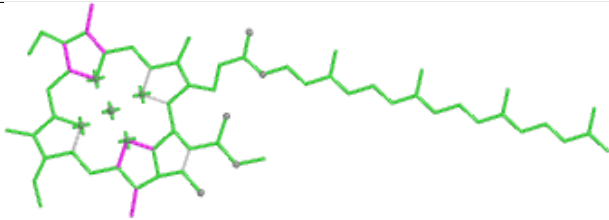
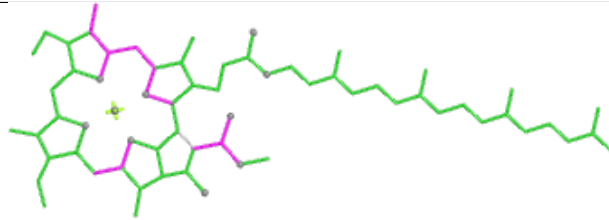
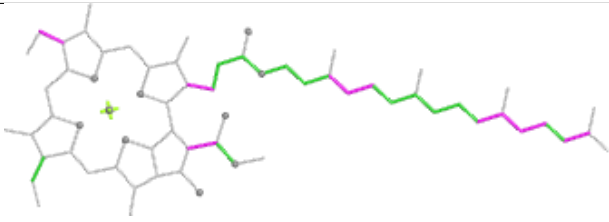
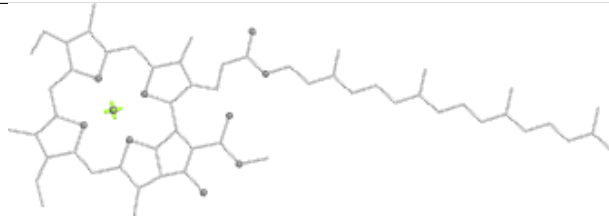
Rings

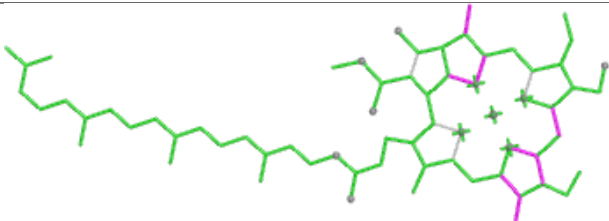
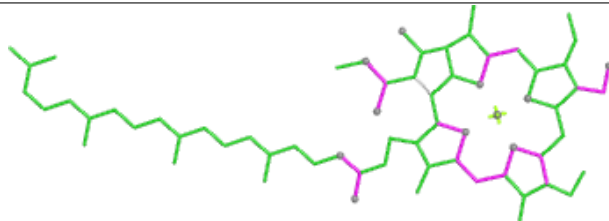
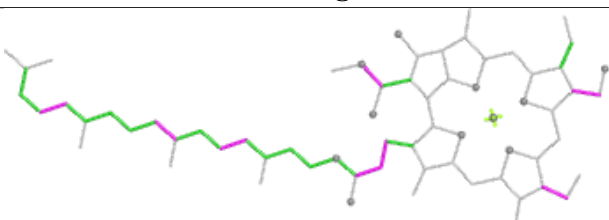
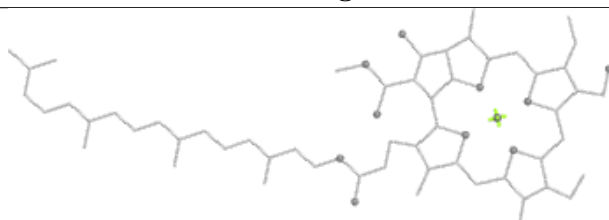


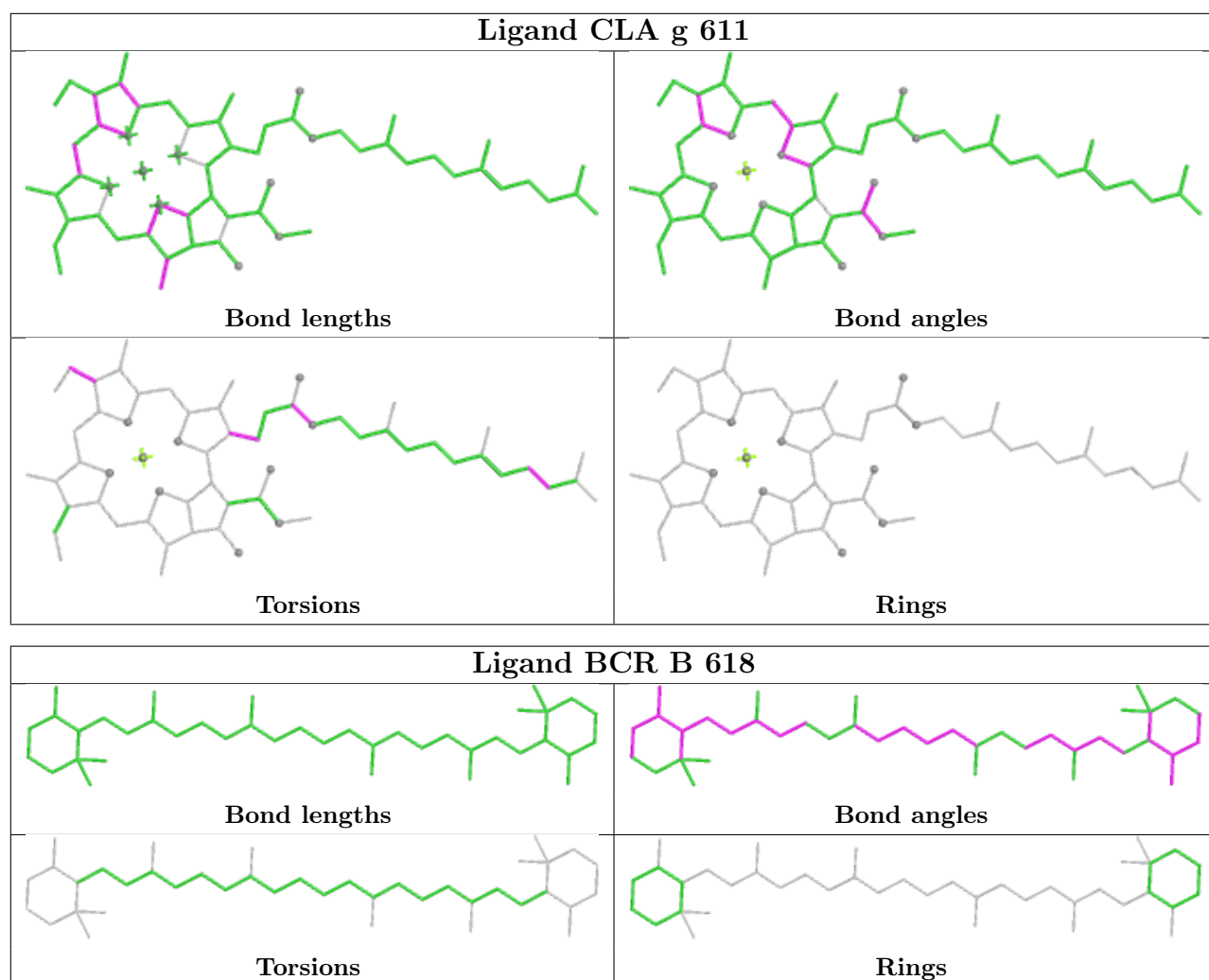


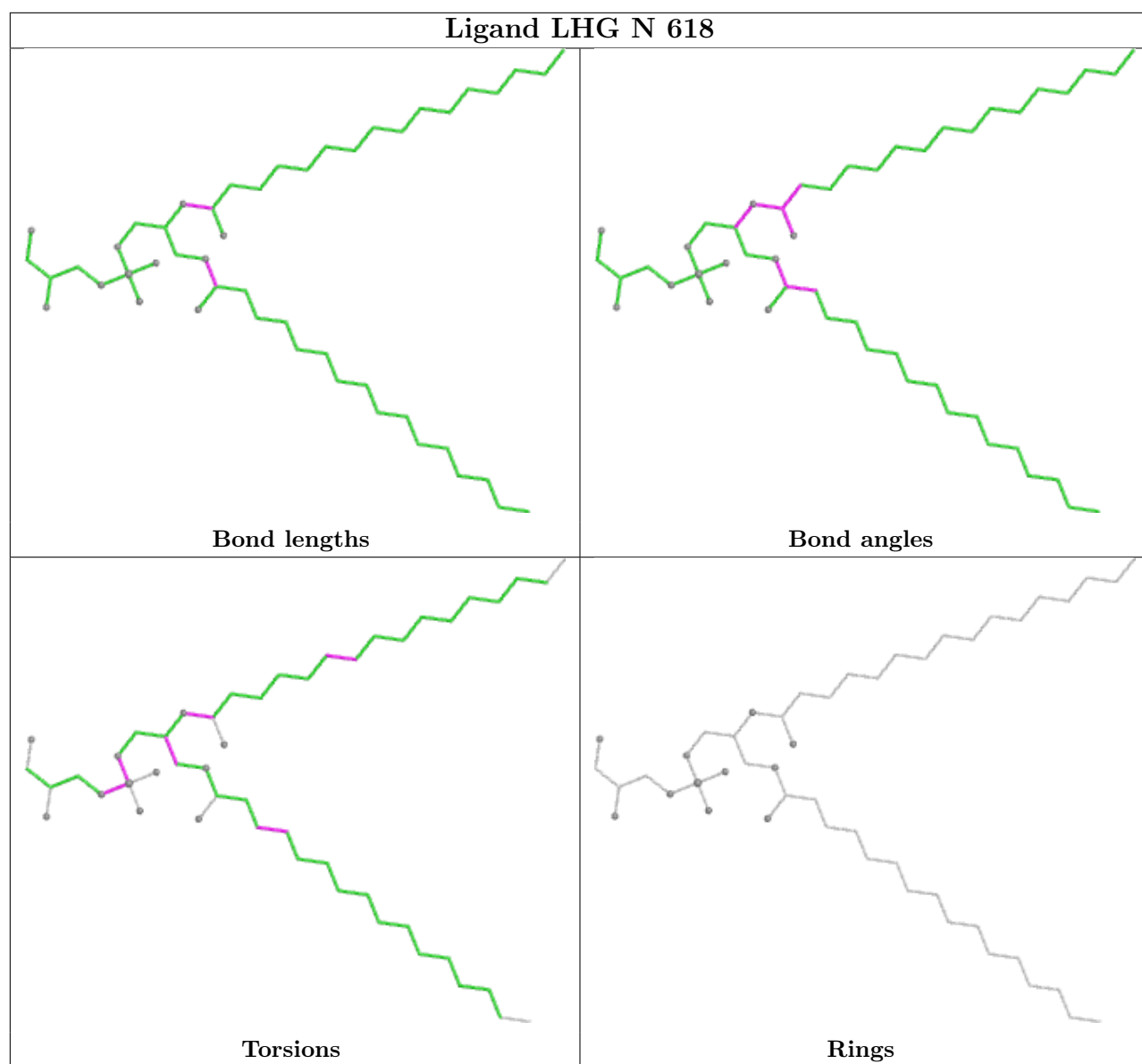


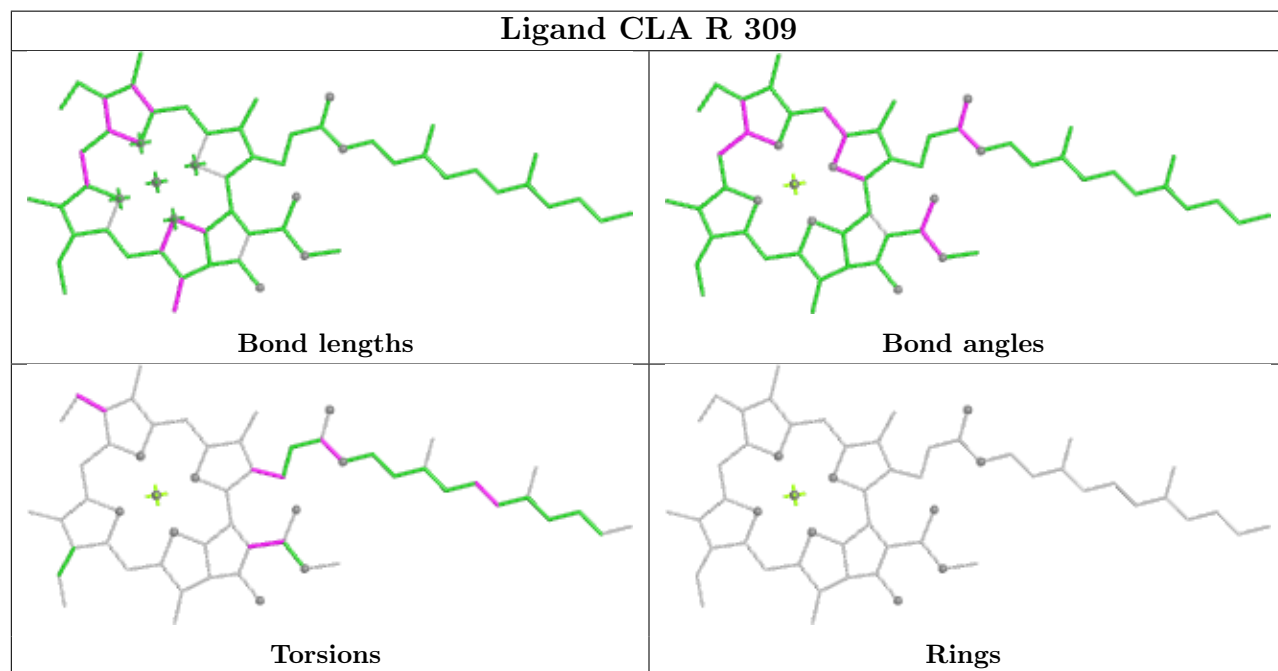
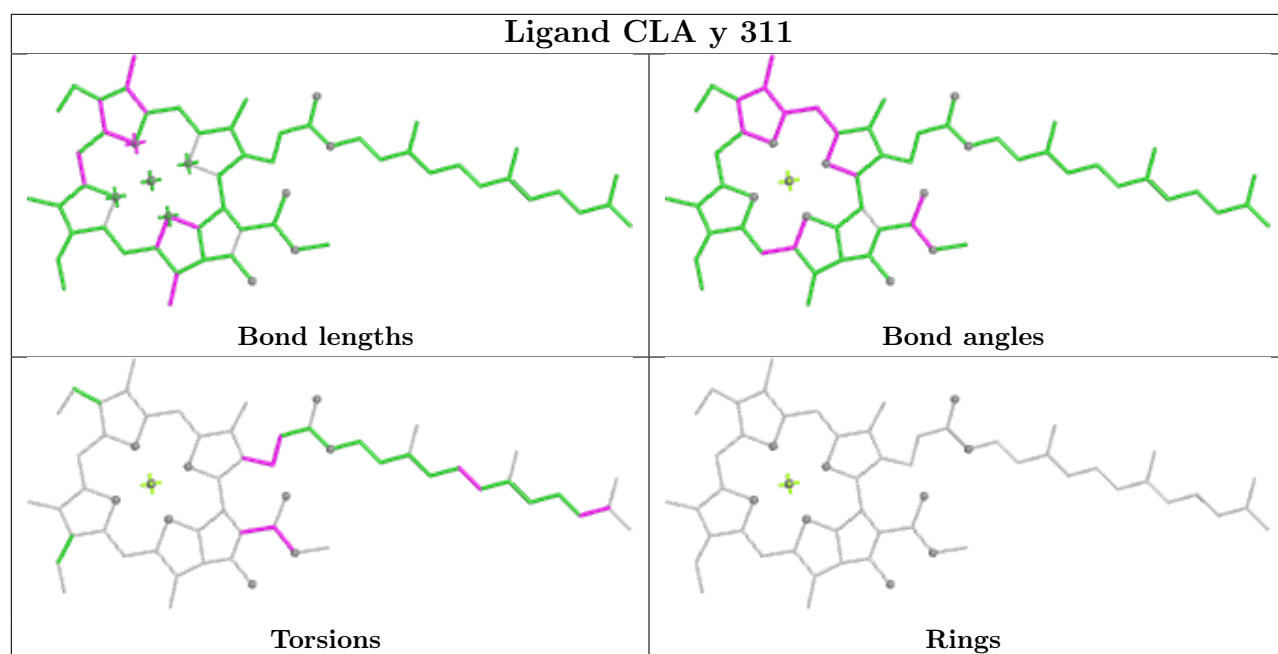
Ligand CLA A 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

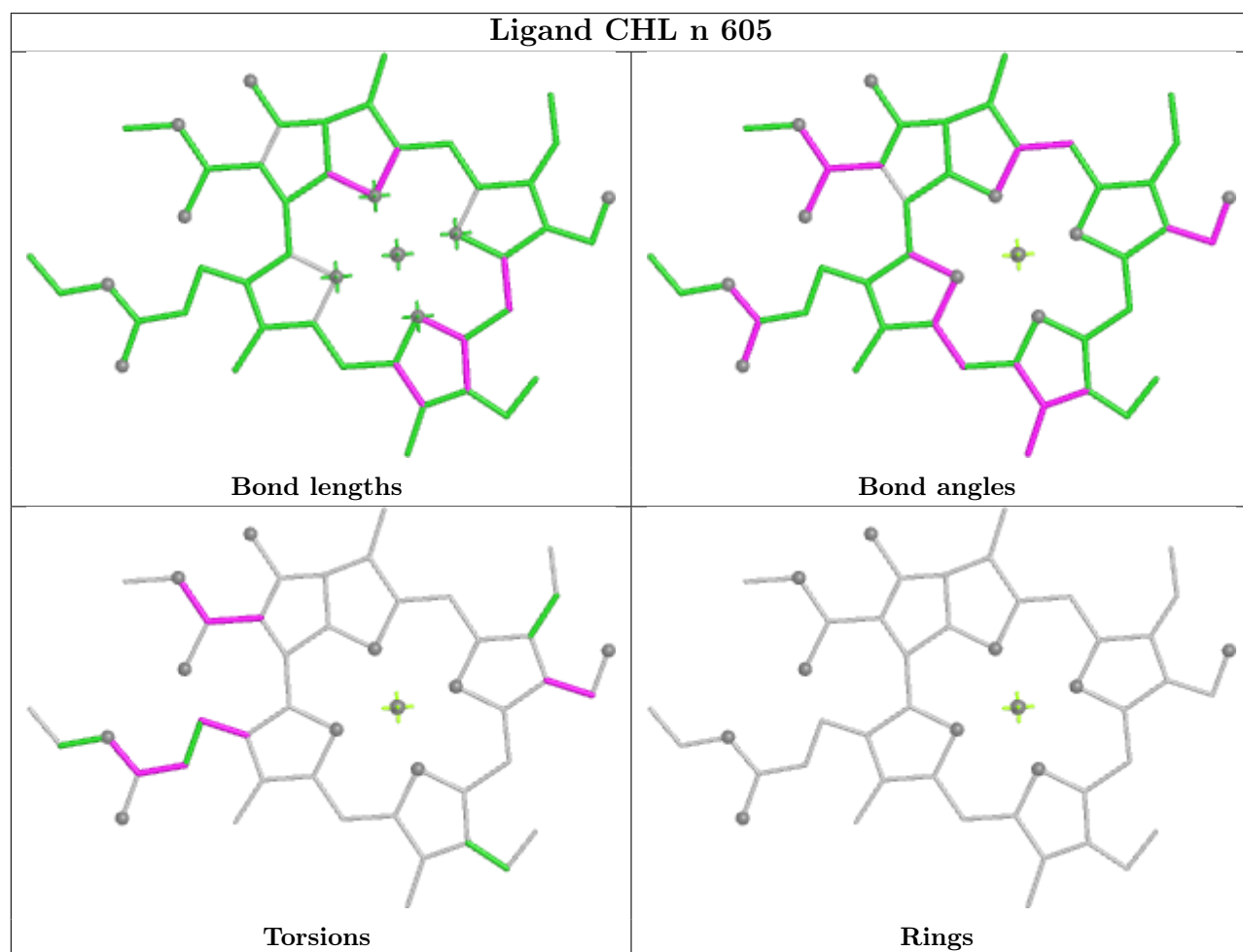
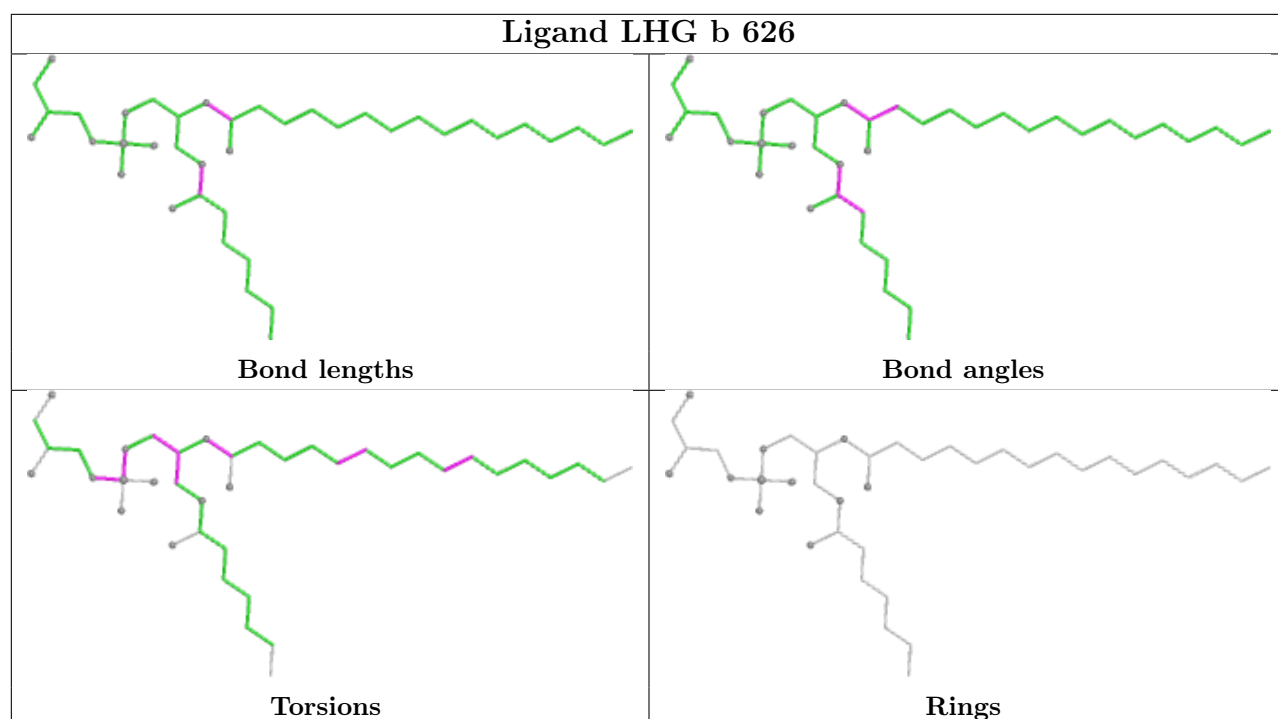
Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

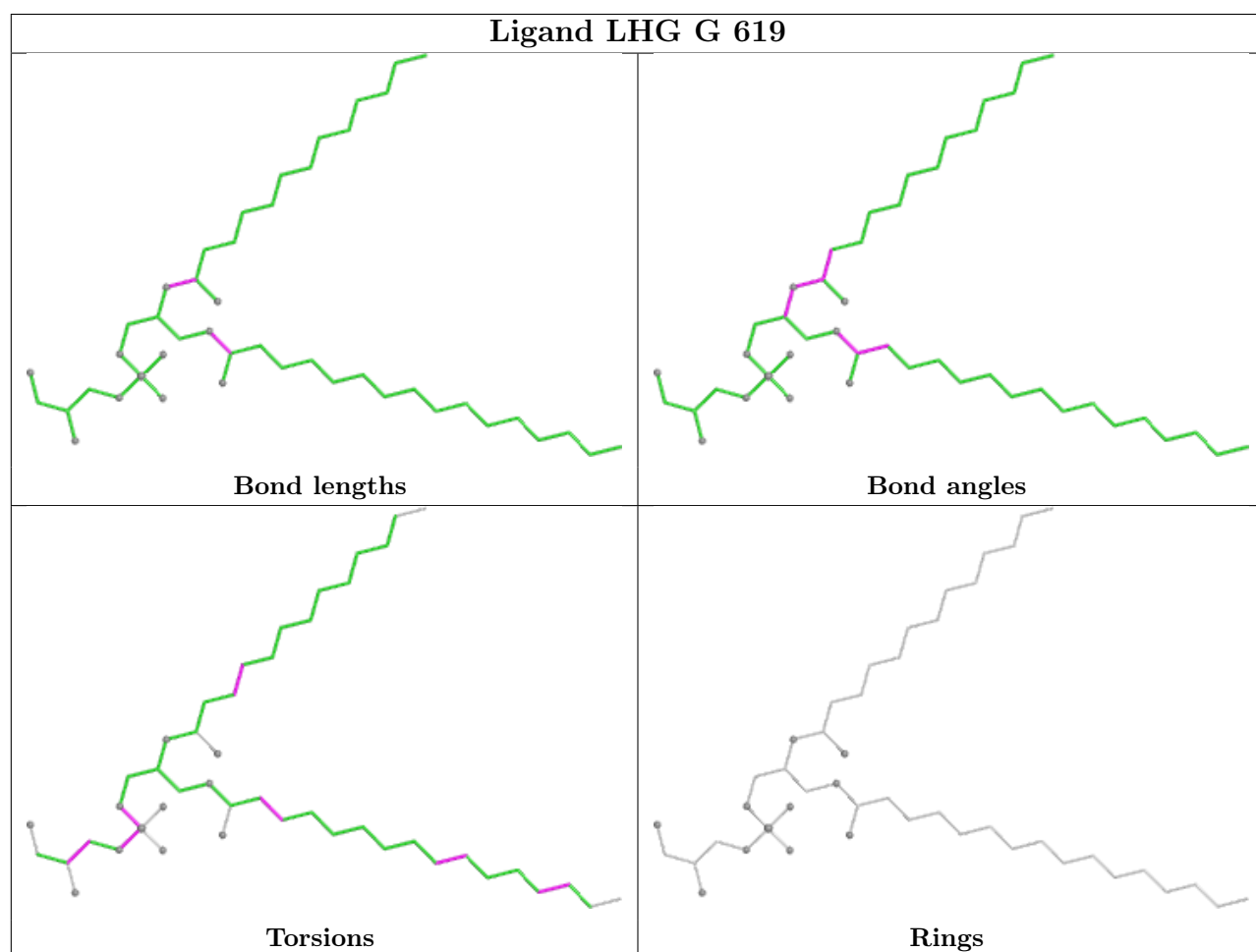
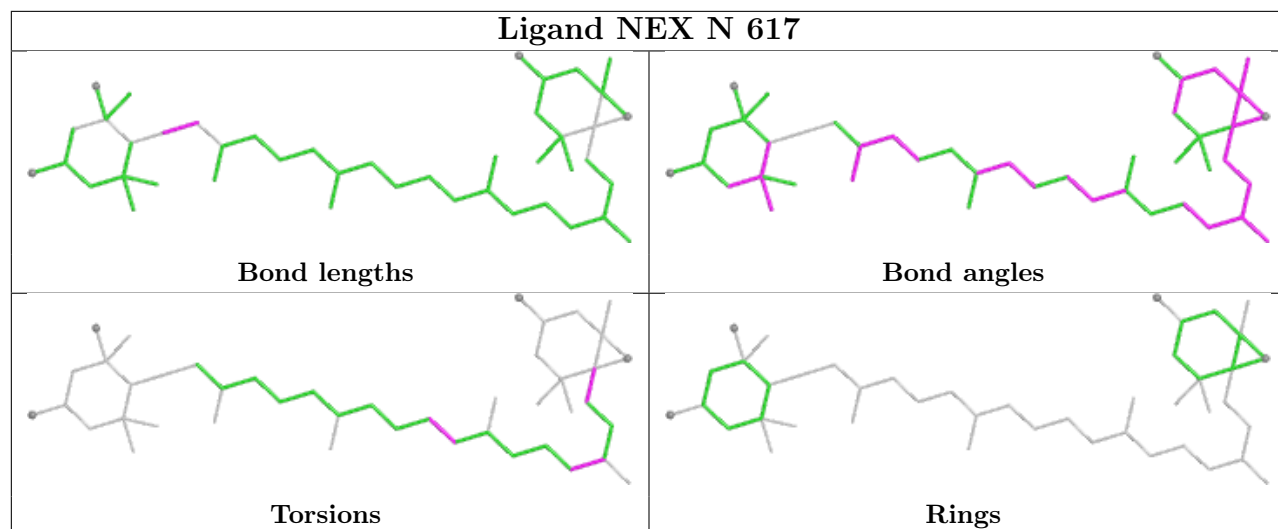
Ligand CHL y 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

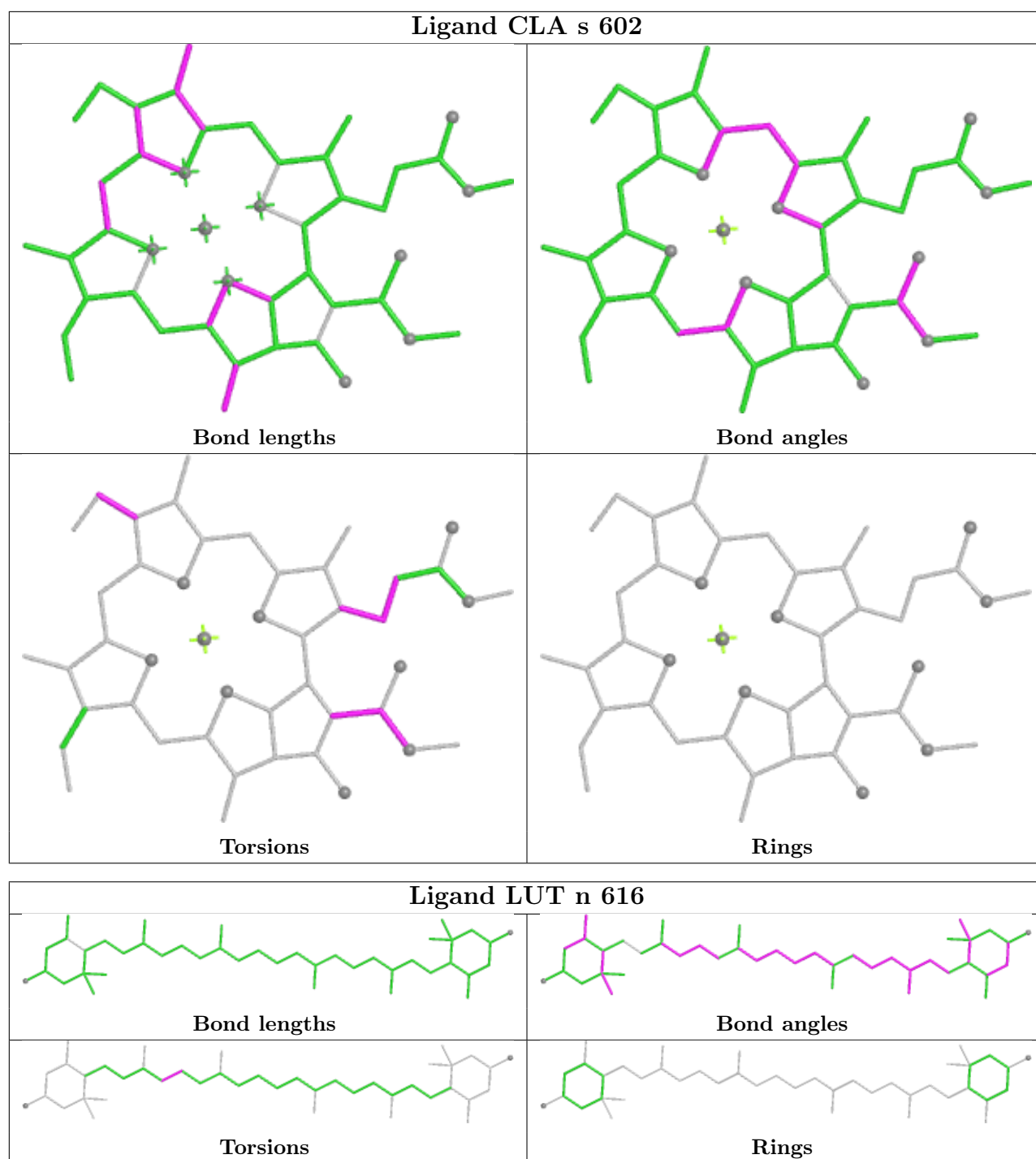




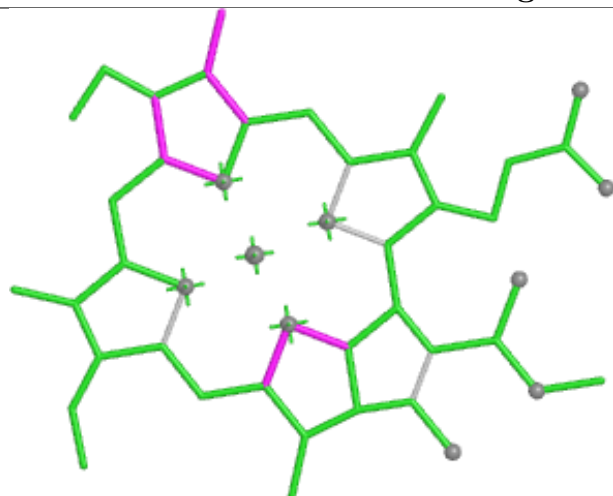




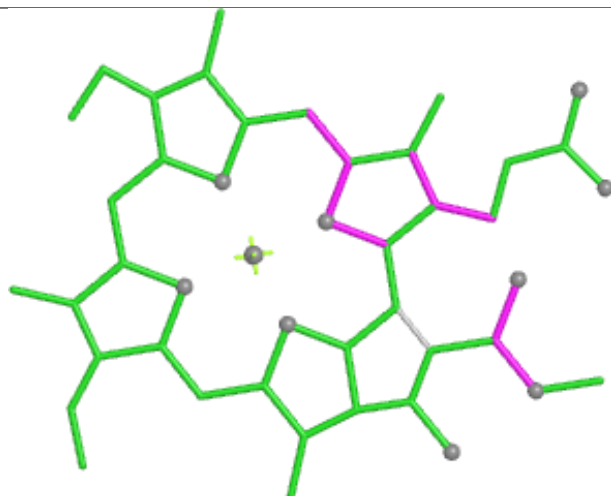




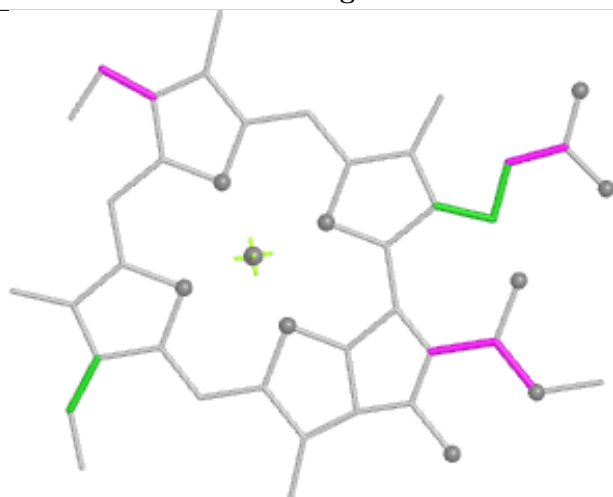
Ligand CLA S 304



Bond lengths



Bond angles

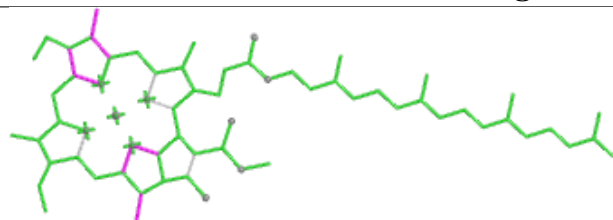


Torsions

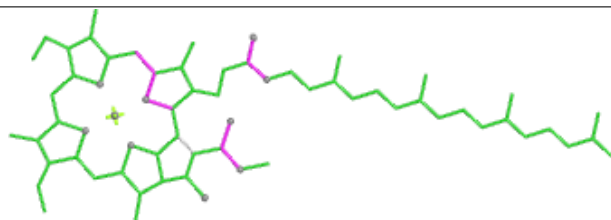


Rings

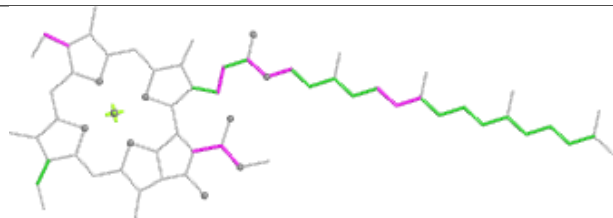
Ligand CLA Y 314



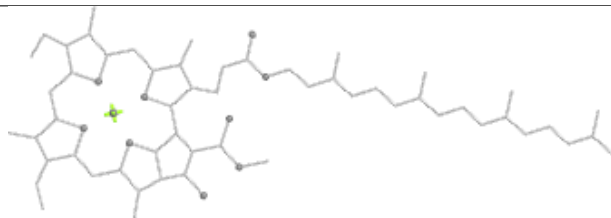
Bond lengths



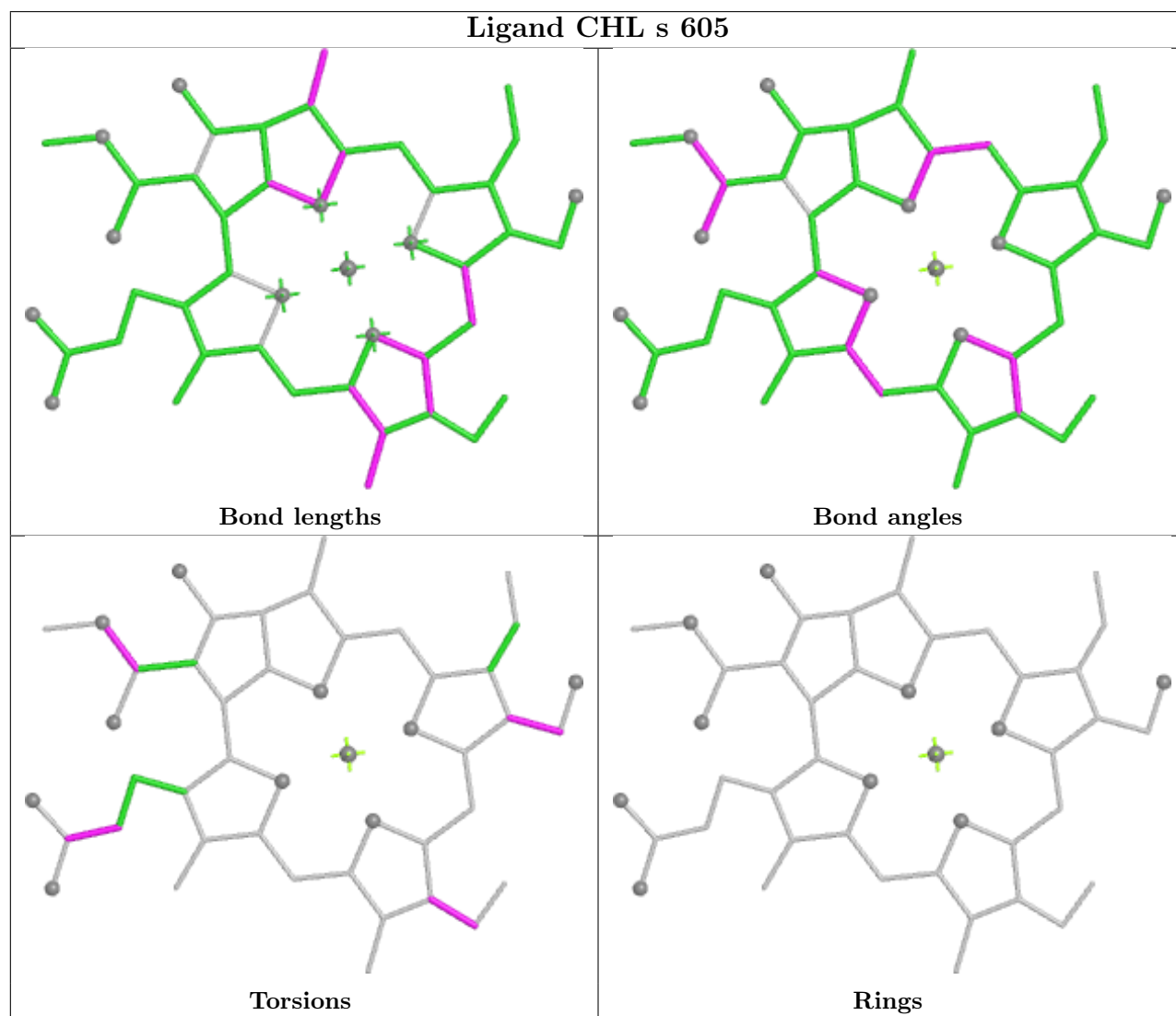
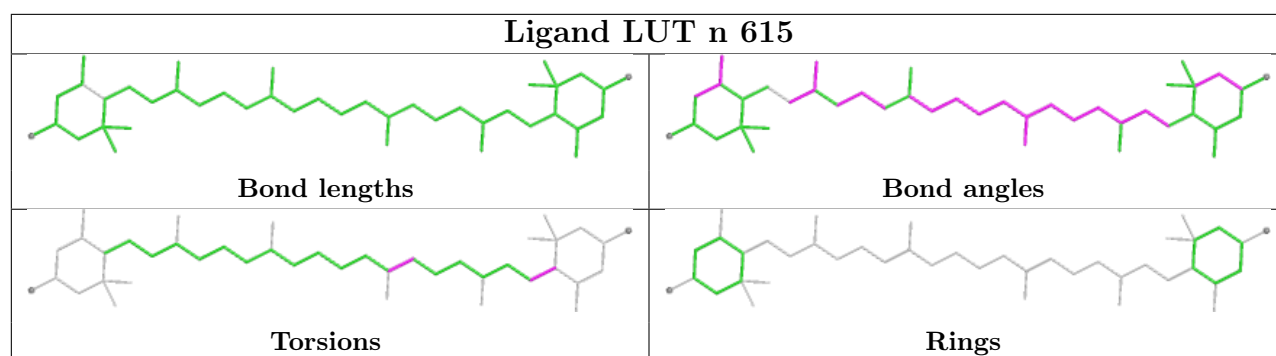
Bond angles

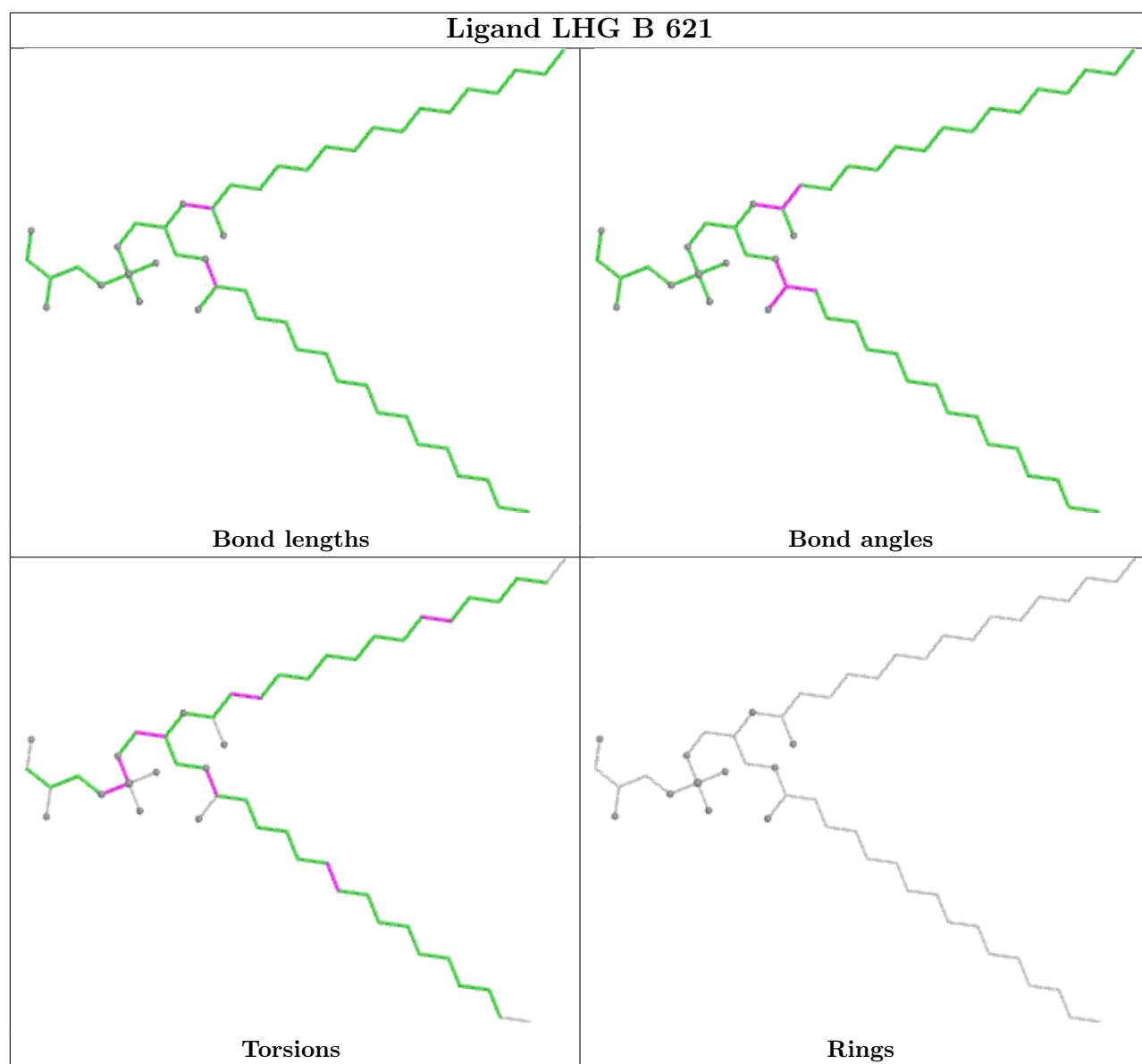


Torsions

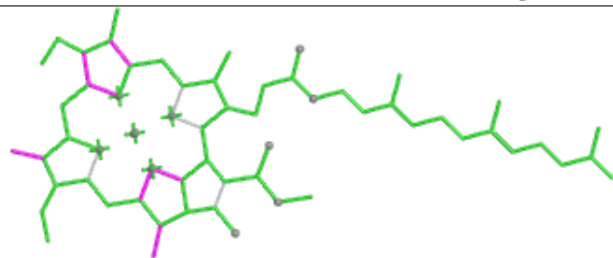


Rings

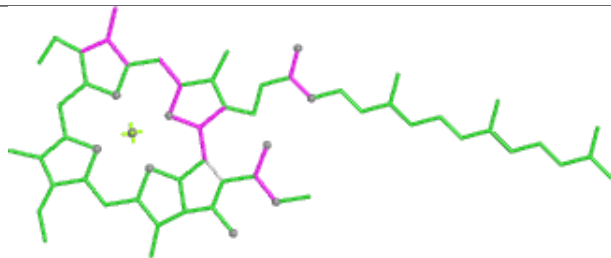




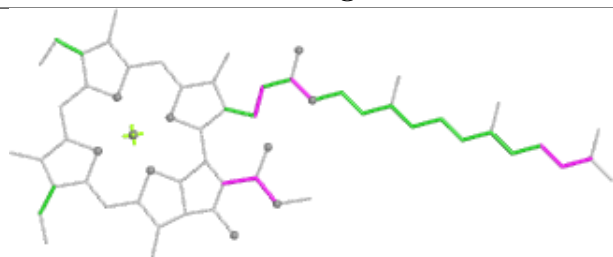
Ligand CLA Y 313



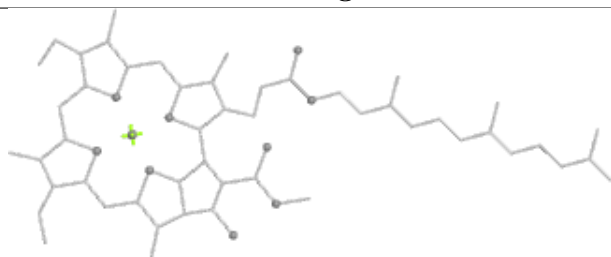
Bond lengths



Bond angles

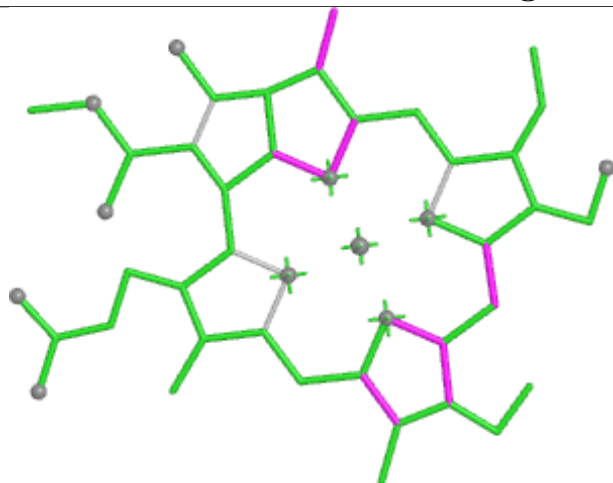


Torsions

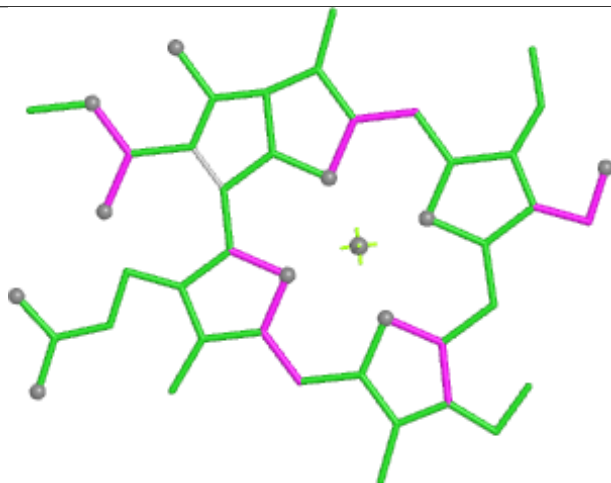


Rings

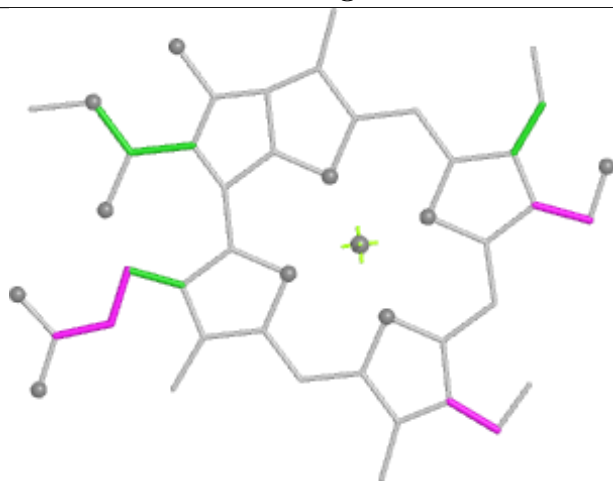
Ligand CHL r 606



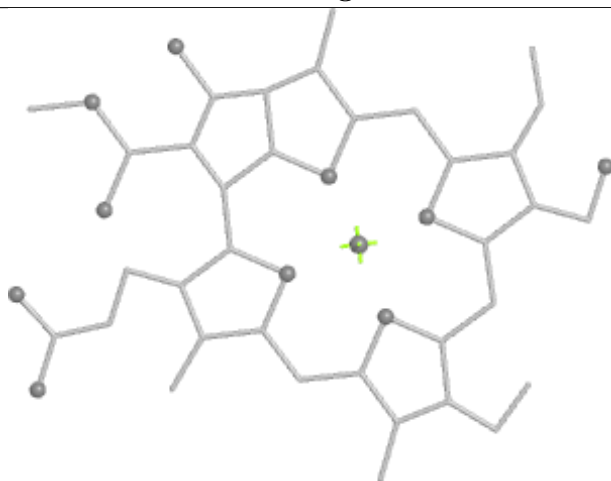
Bond lengths



Bond angles

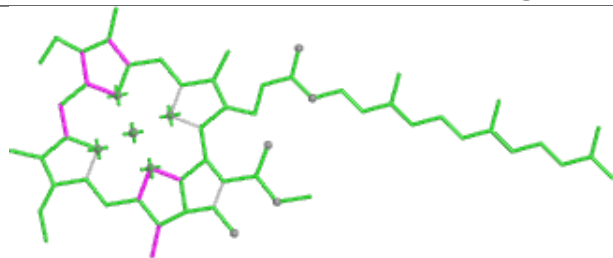


Torsions

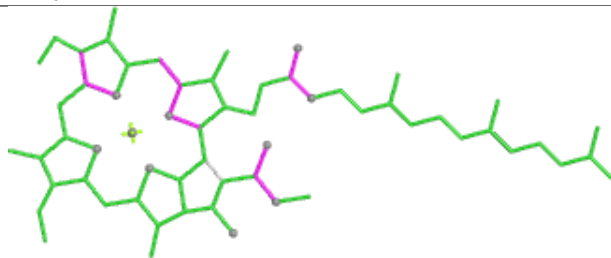


Rings

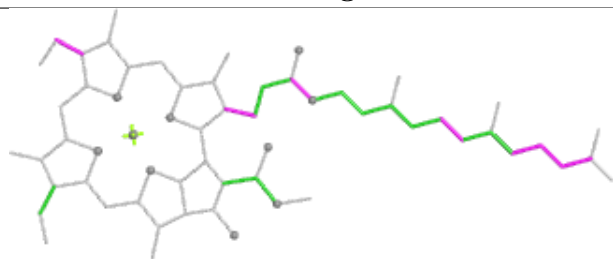
Ligand CLA y 312



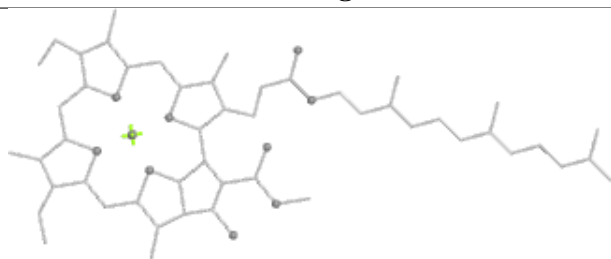
Bond lengths



Bond angles

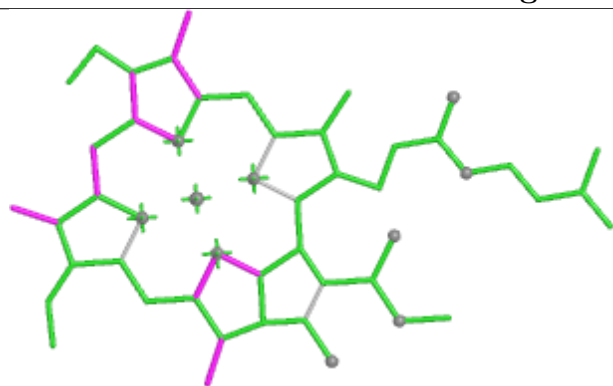


Torsions

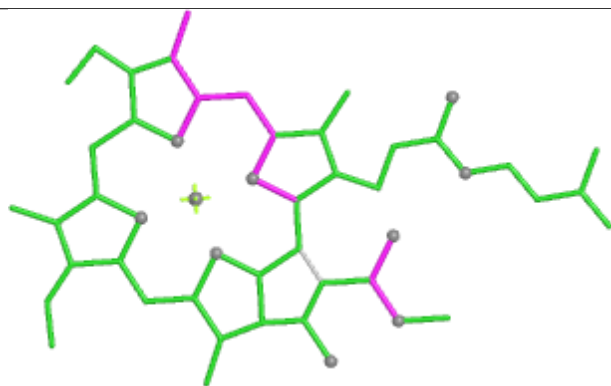


Rings

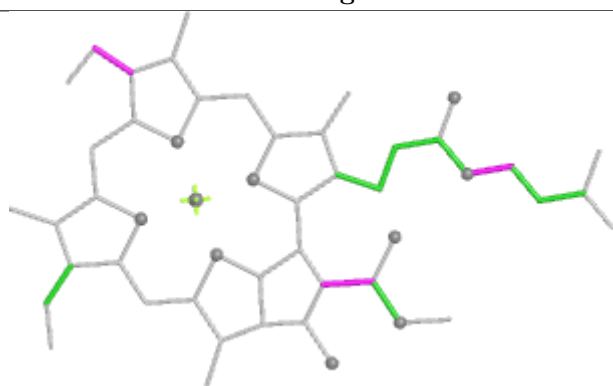
Ligand CLA s 604



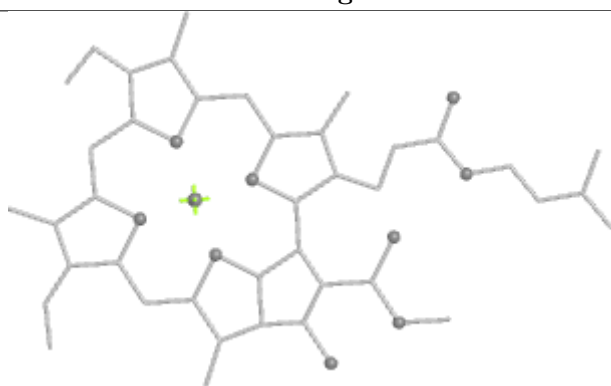
Bond lengths



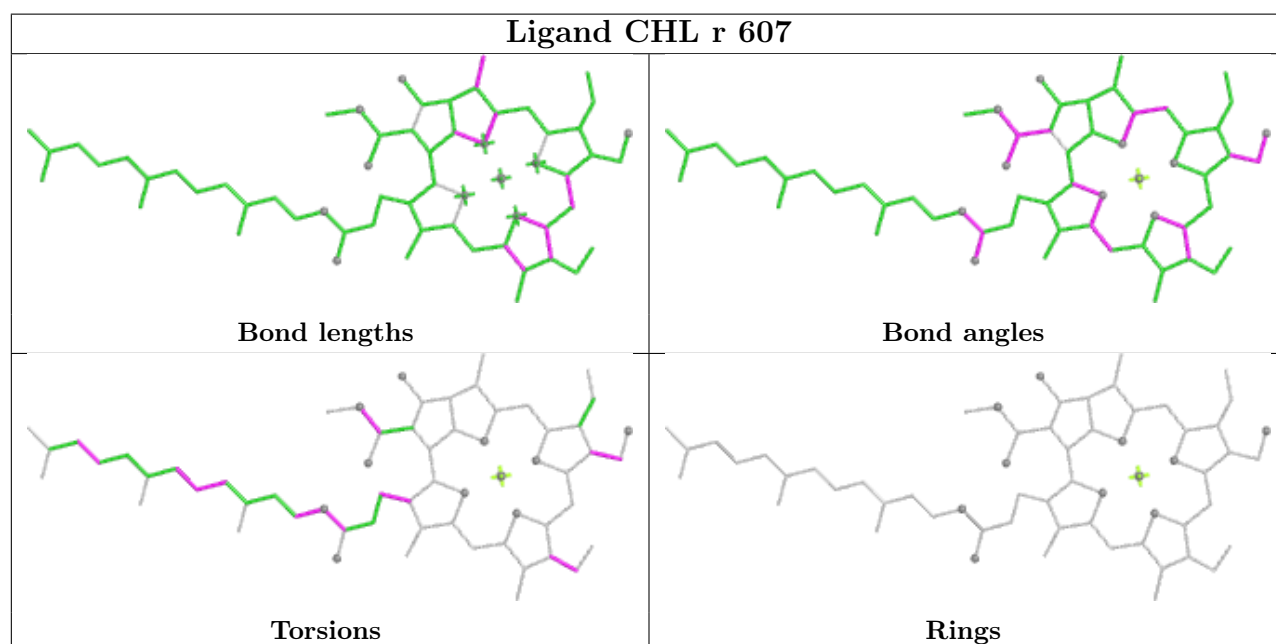
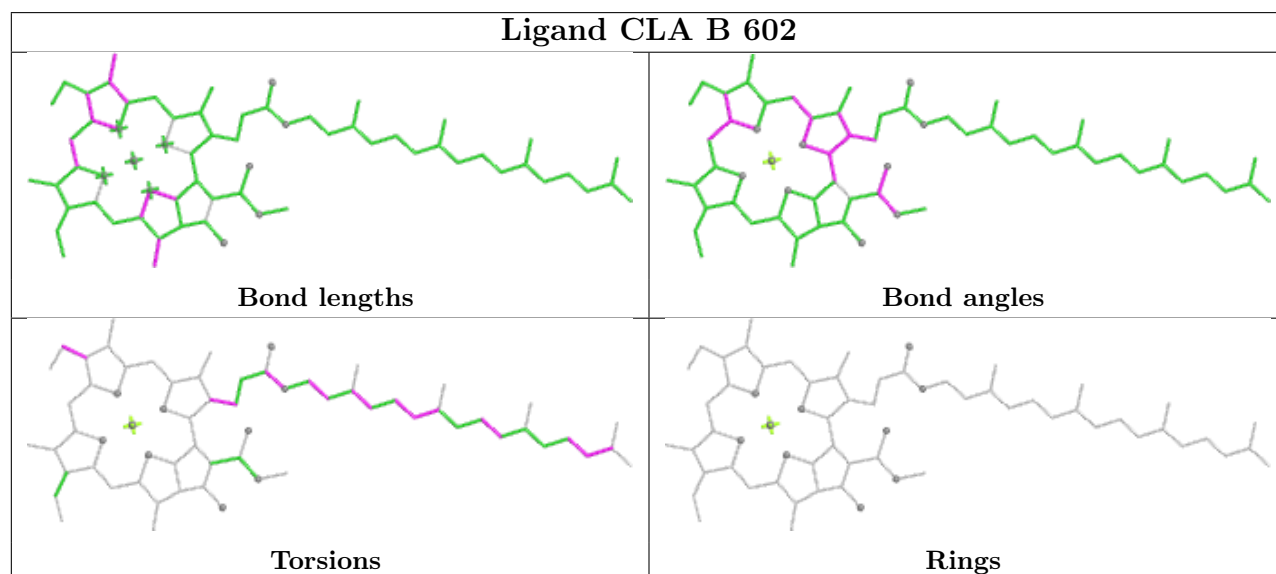
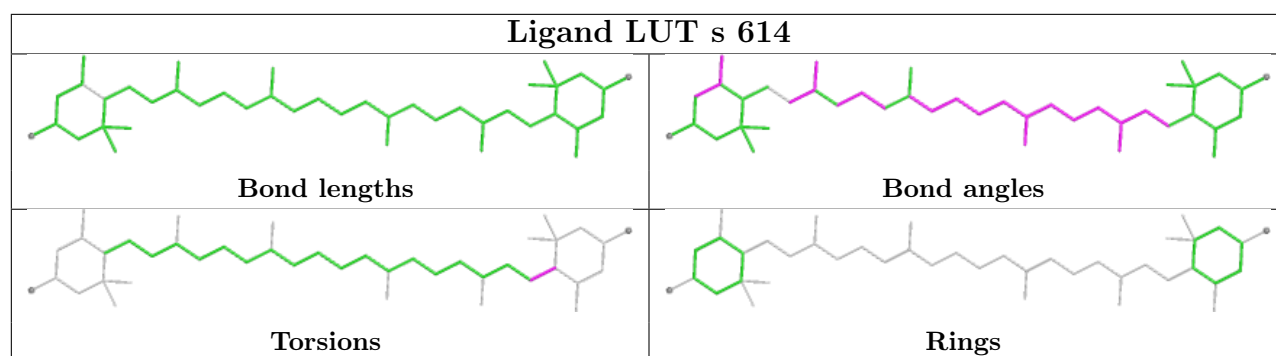
Bond angles

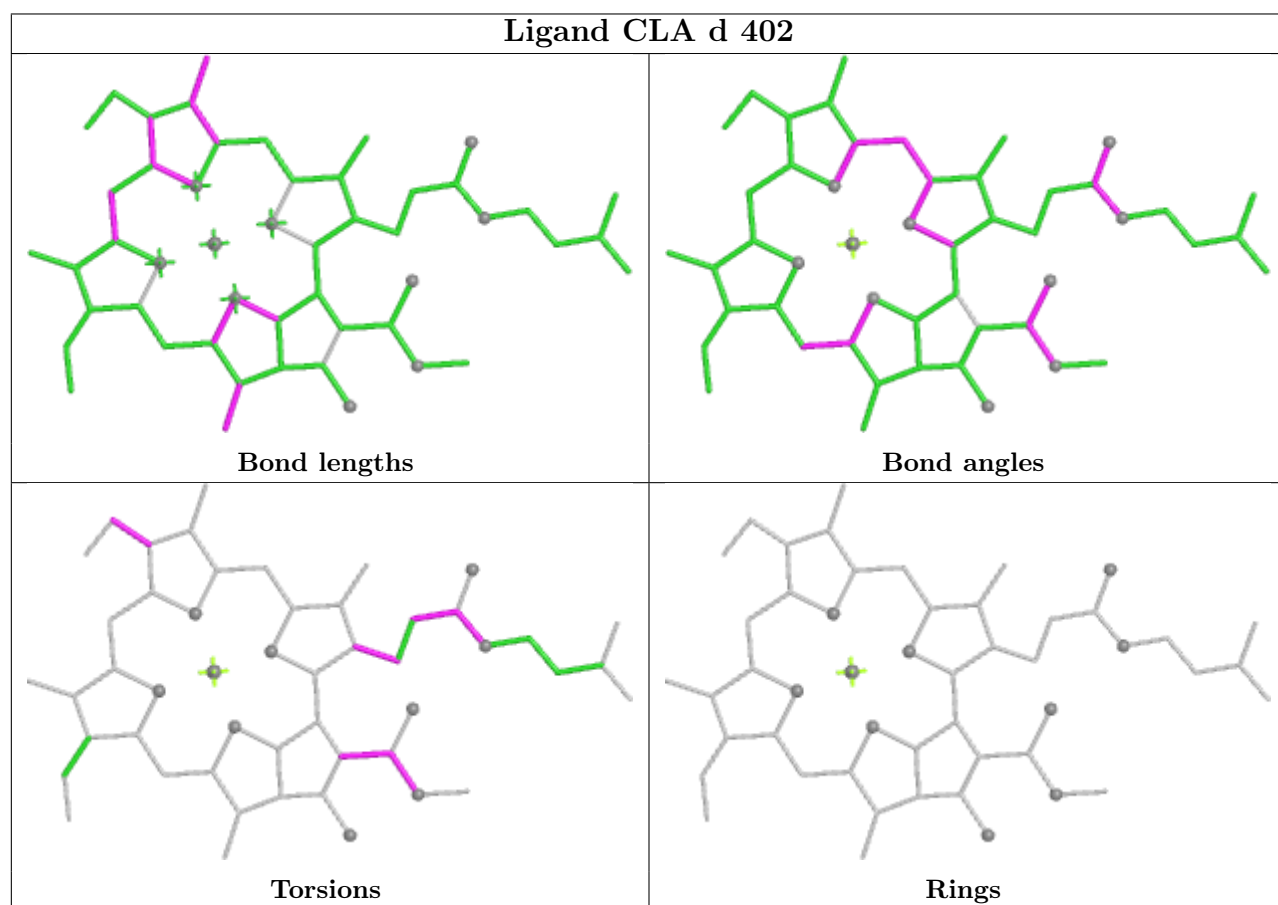
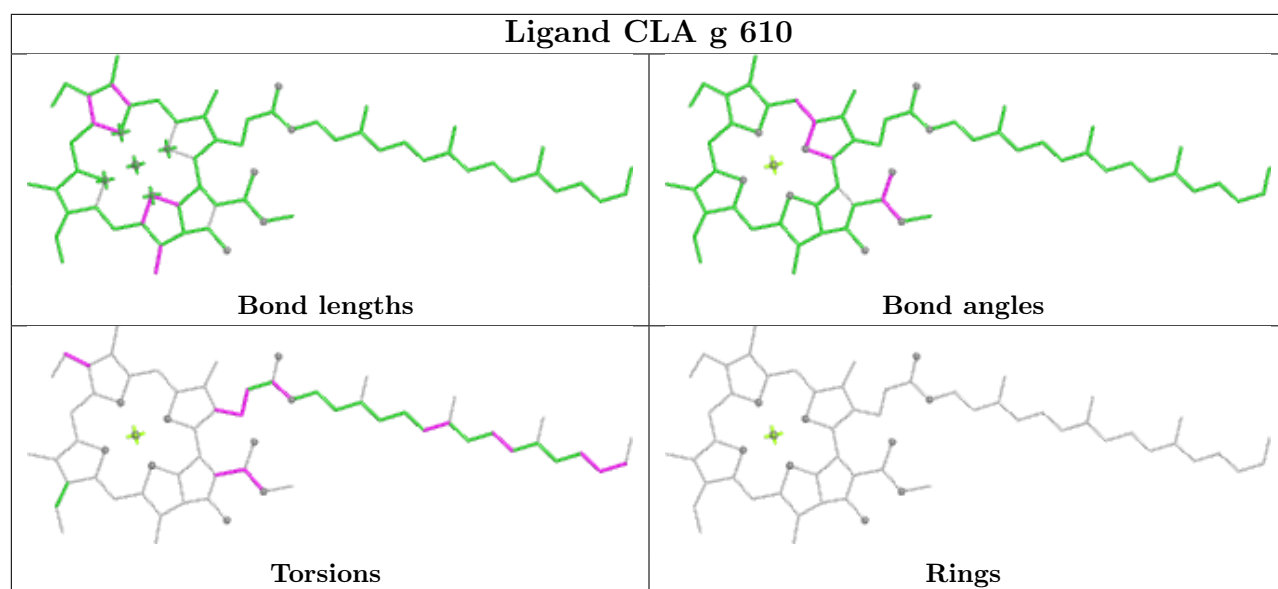


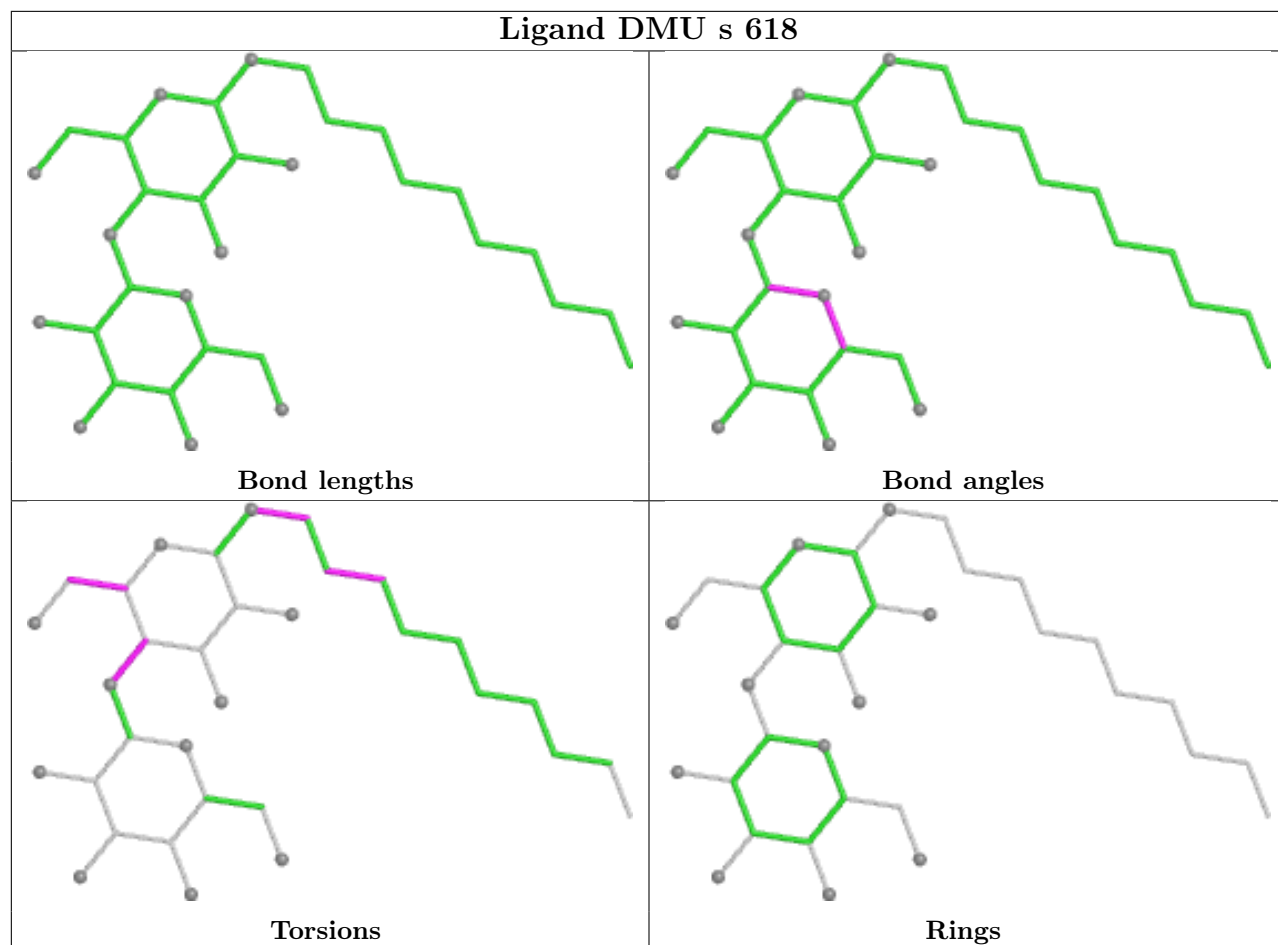
Torsions



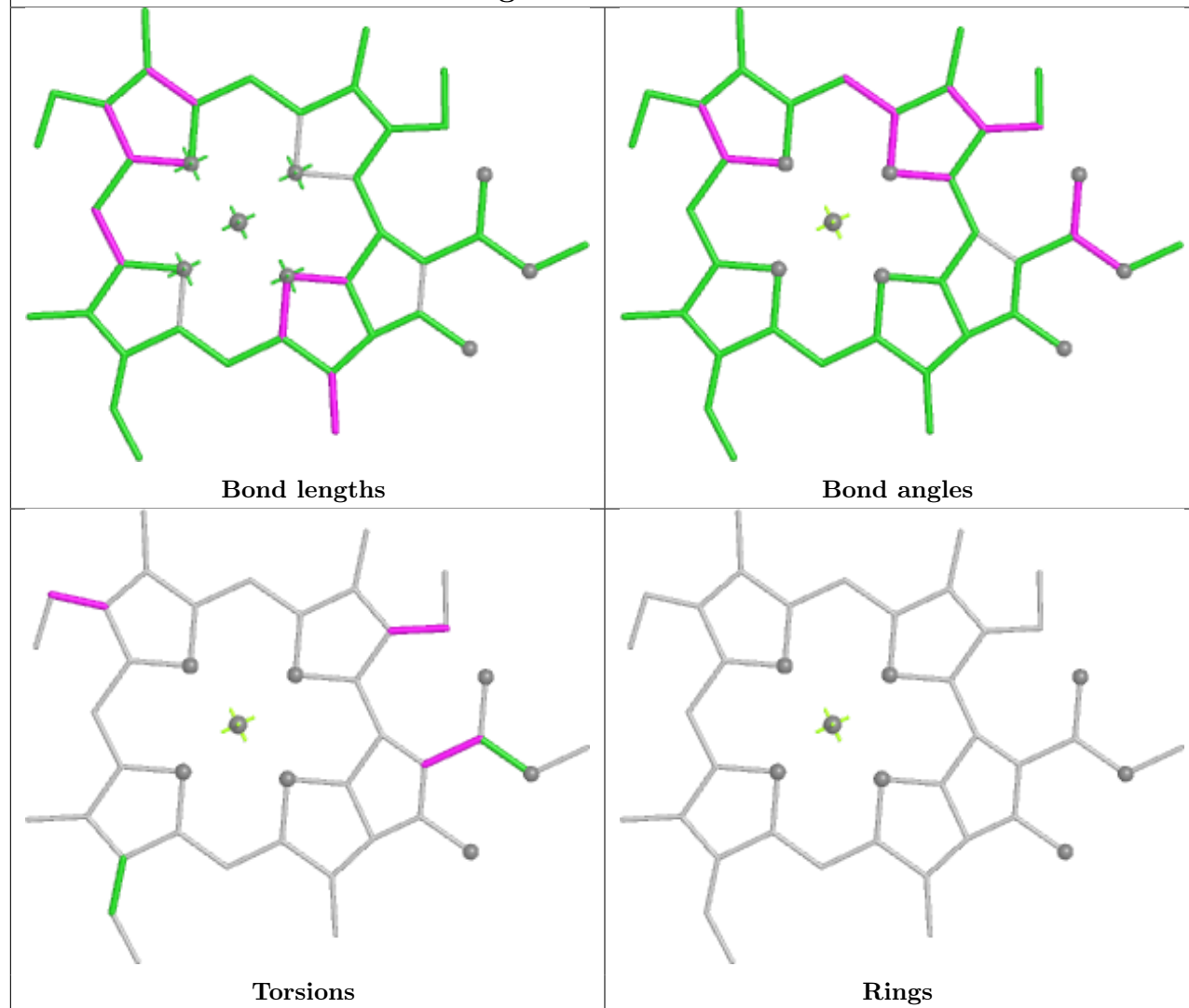
Rings



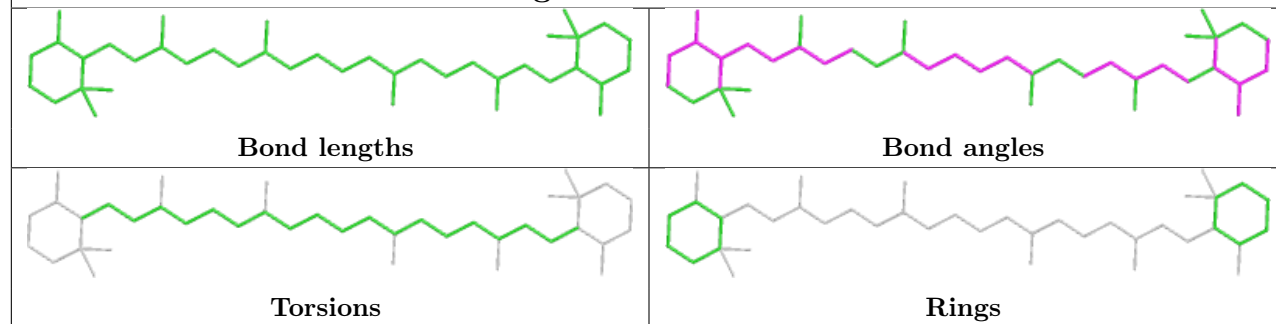


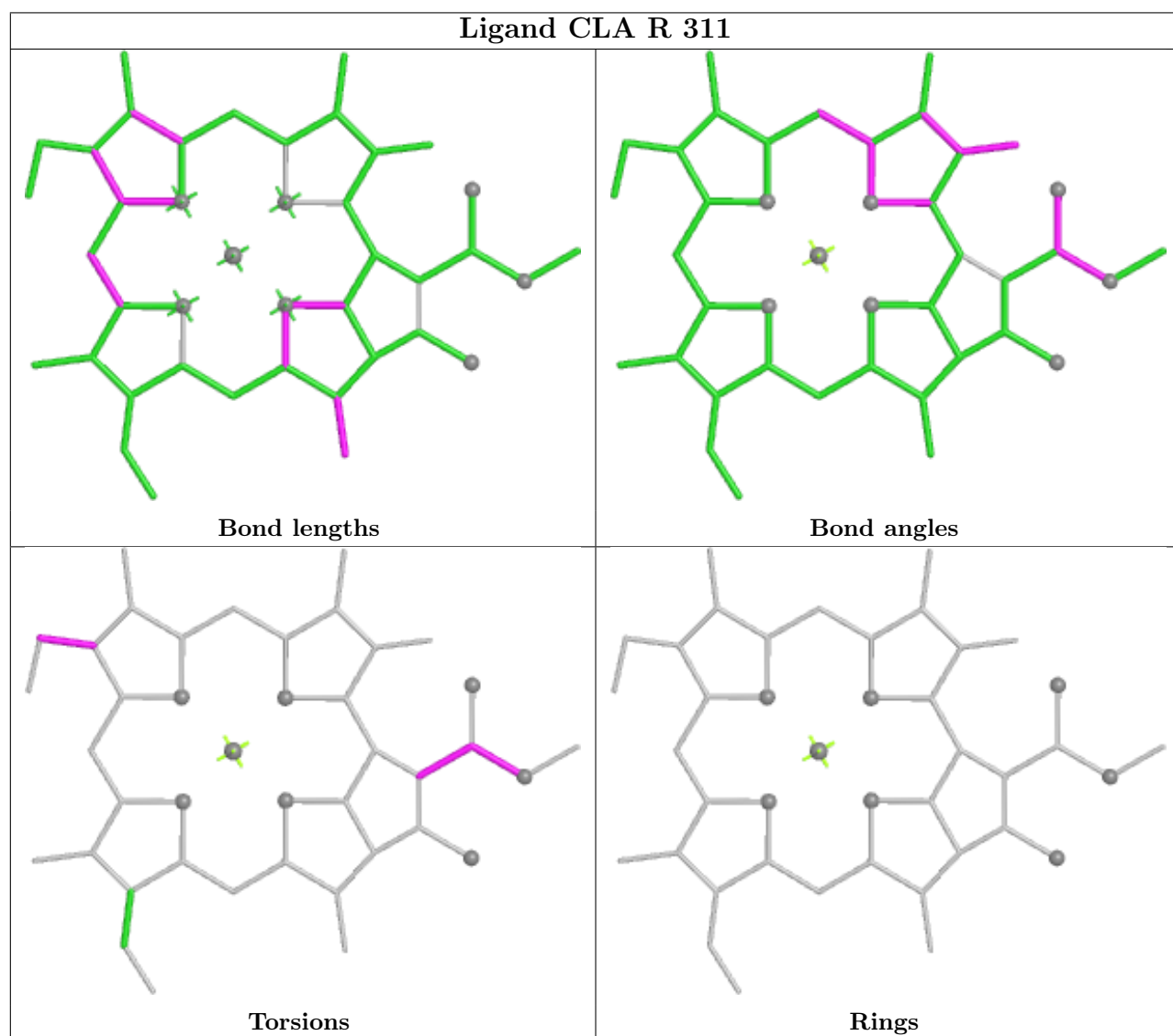
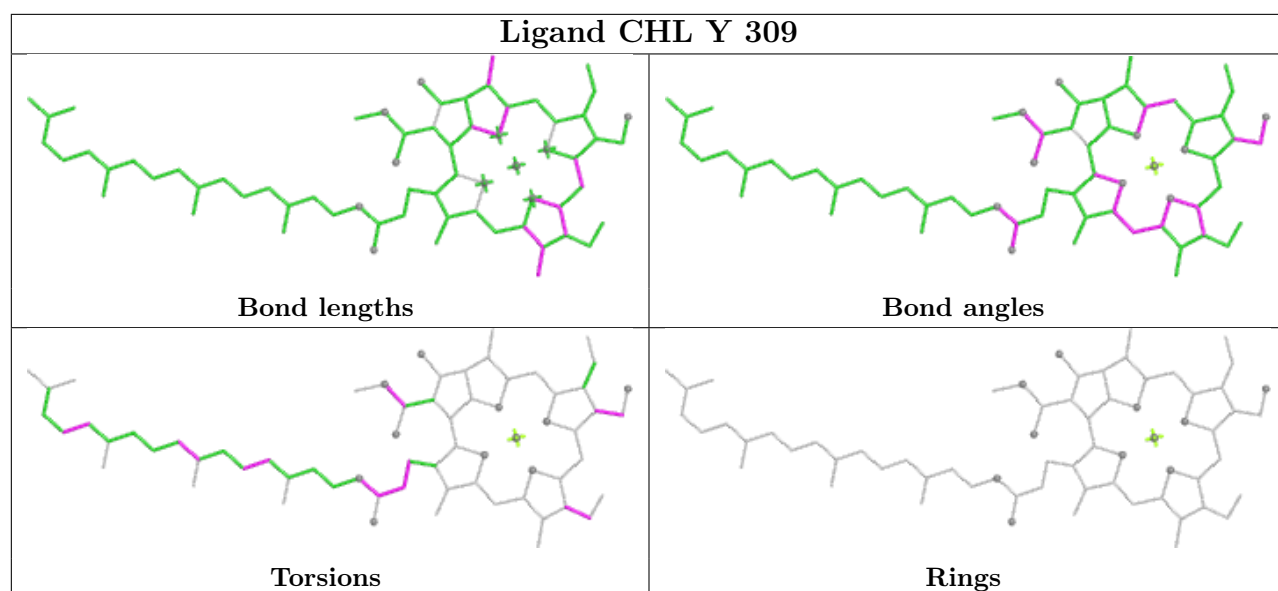


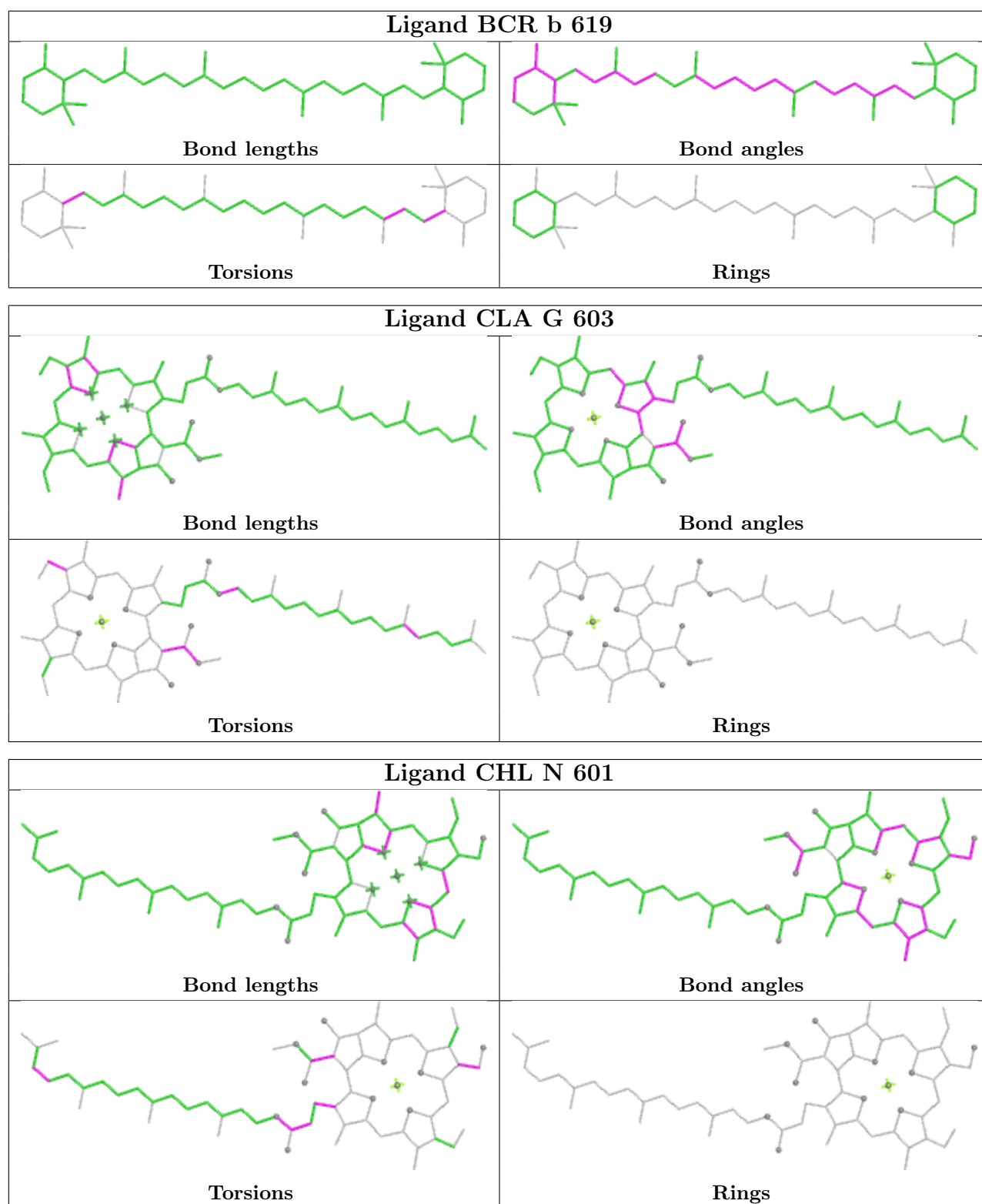
Ligand CLA S 311

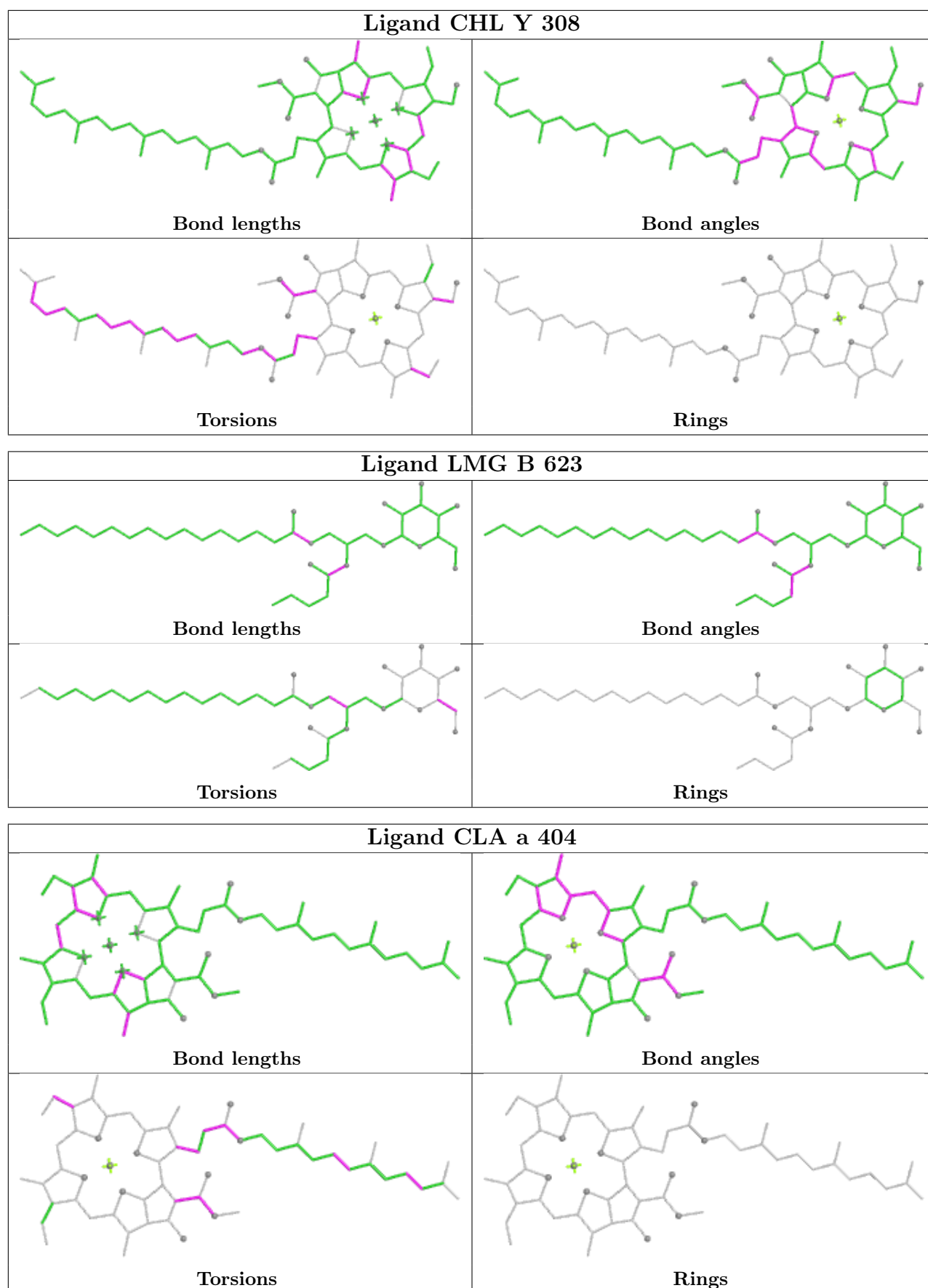


Ligand BCR b 620

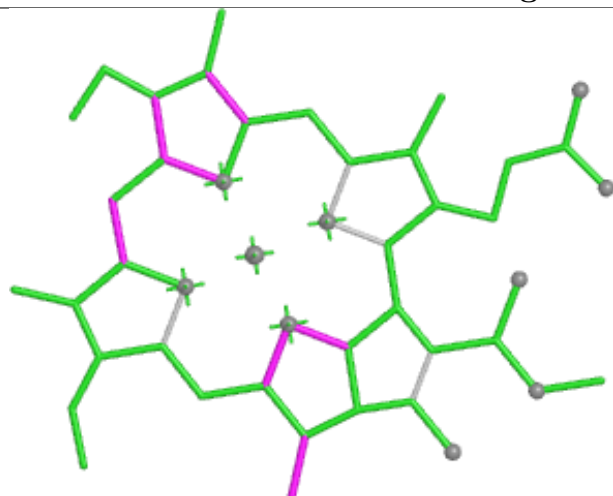




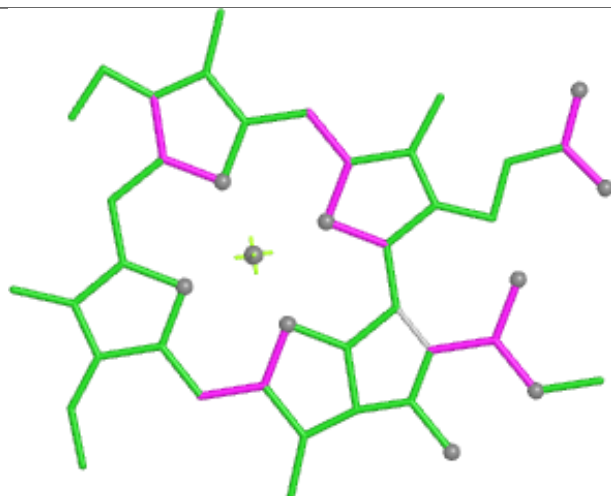




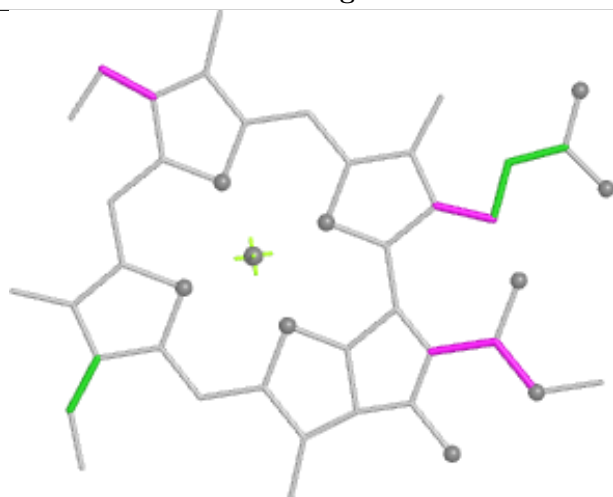
Ligand CLA s 608



Bond lengths



Bond angles

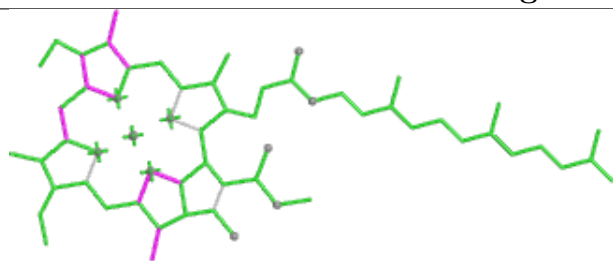


Torsions

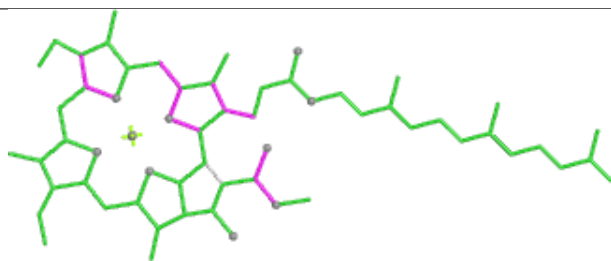


Rings

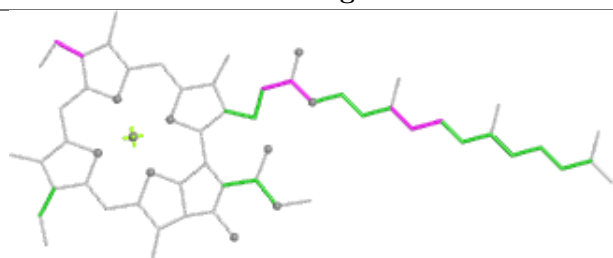
Ligand CLA r 603



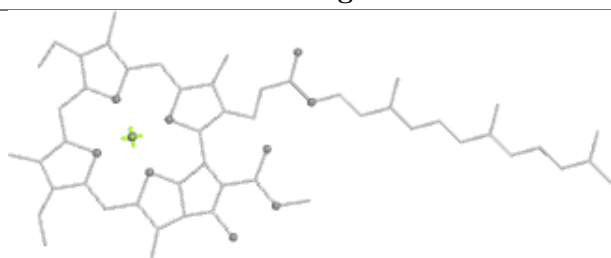
Bond lengths



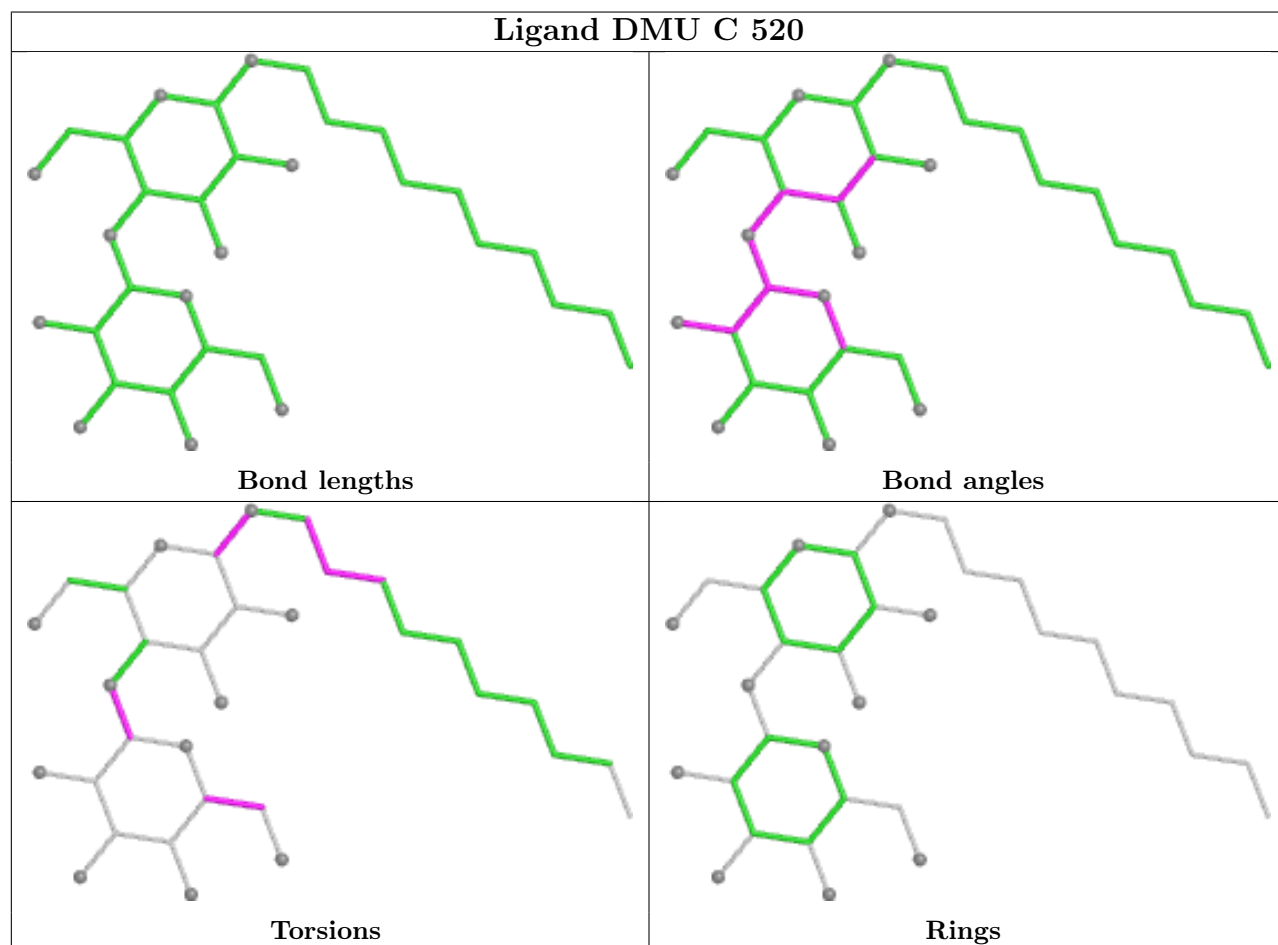
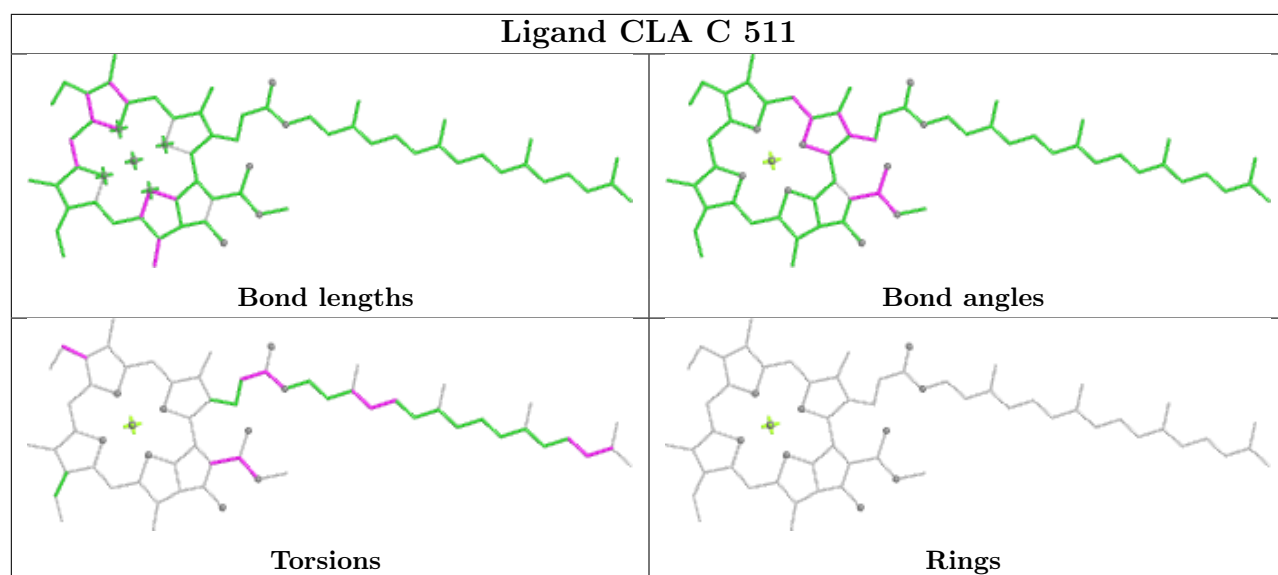
Bond angles

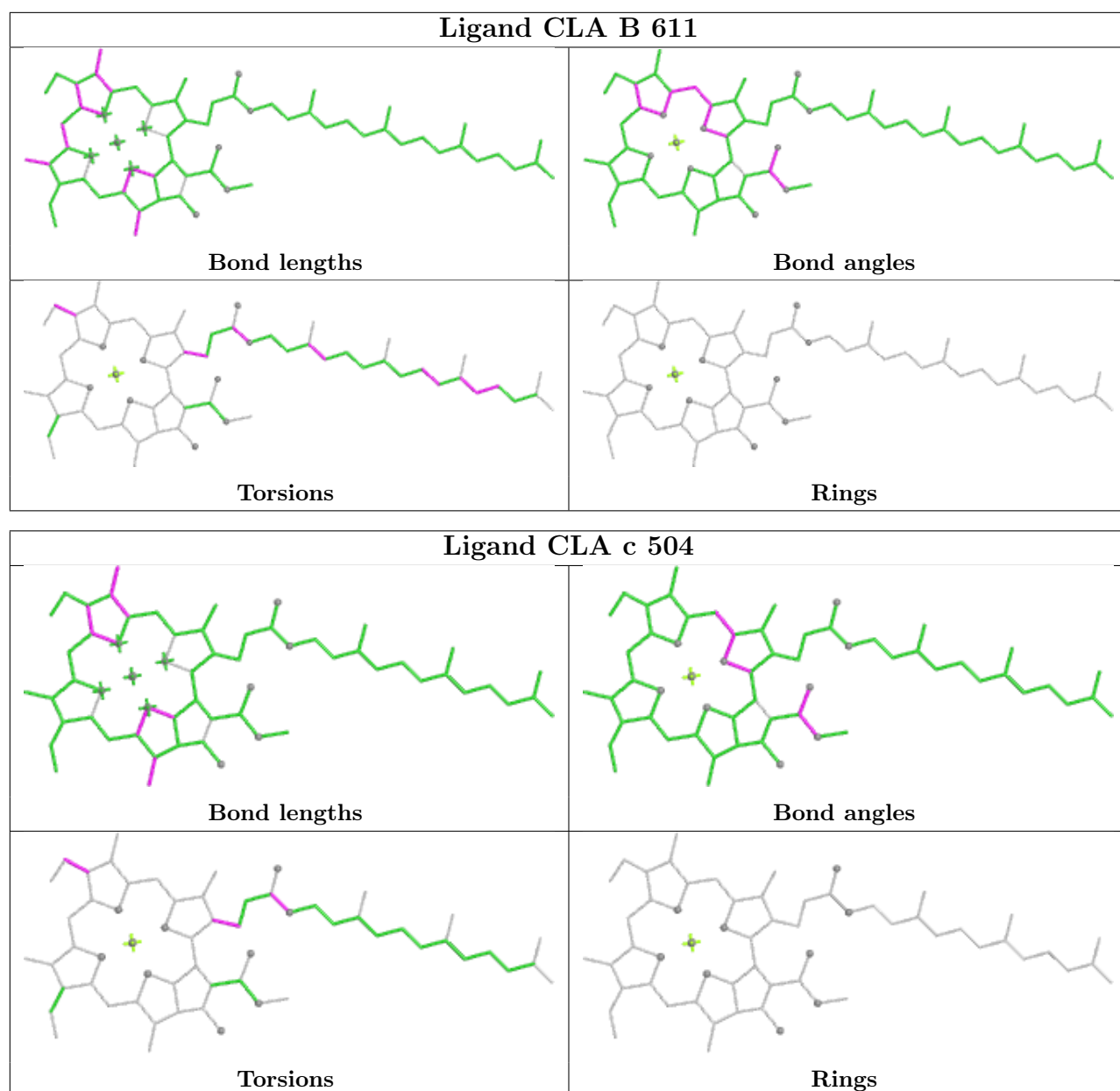


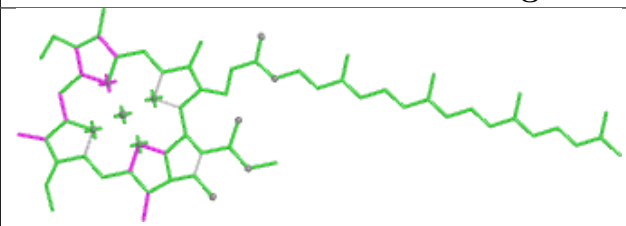
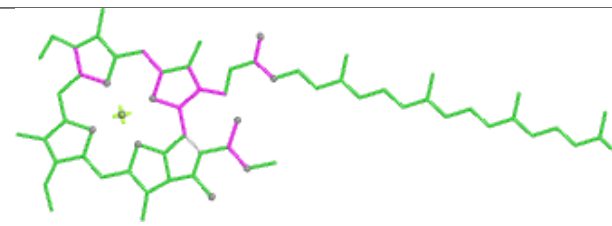
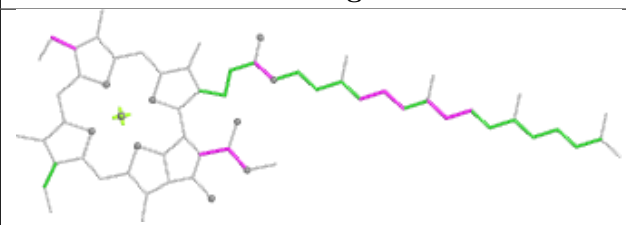
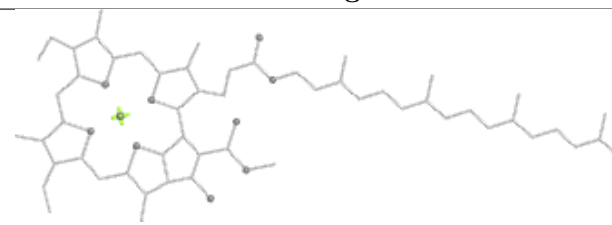
Torsions

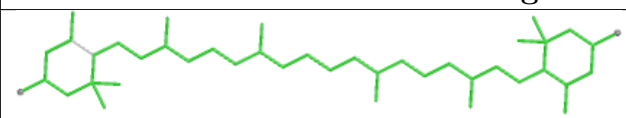
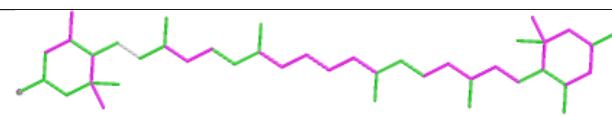
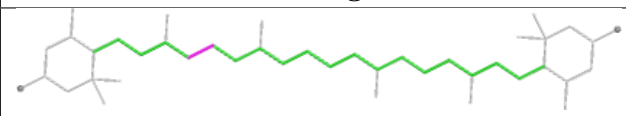
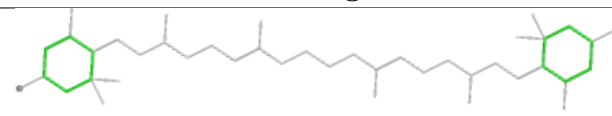


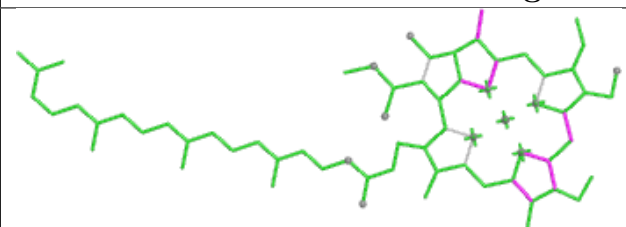
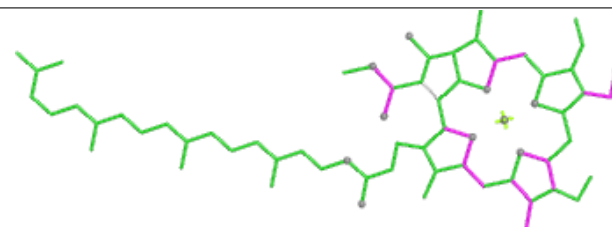
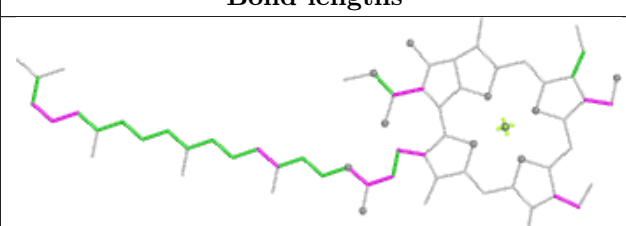
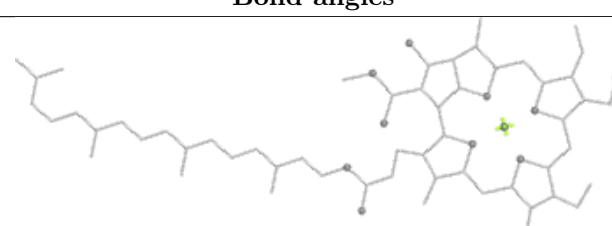
Rings



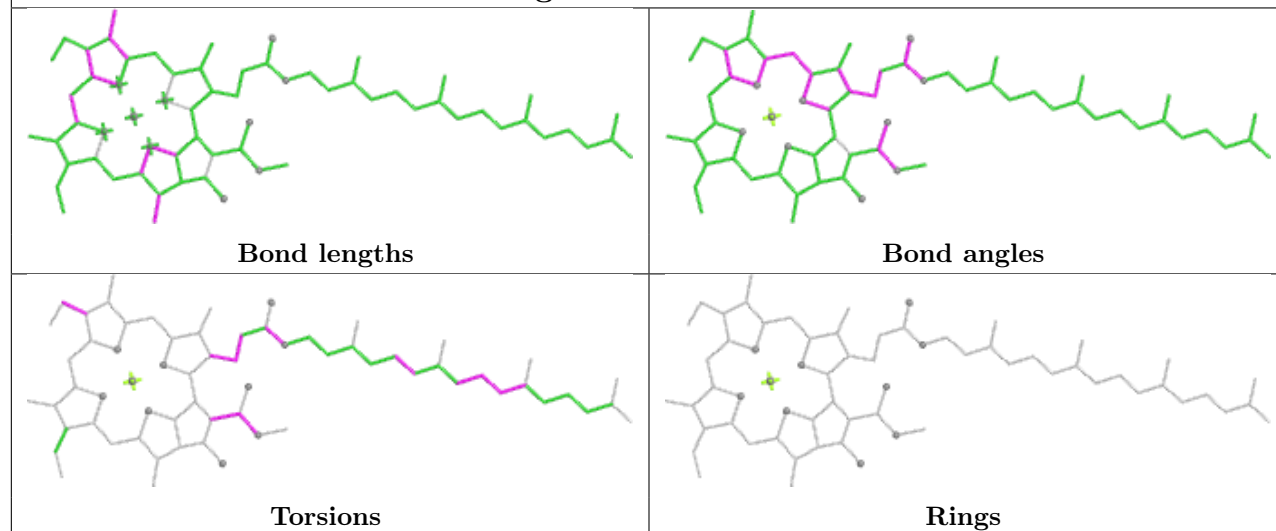


Ligand CLA B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

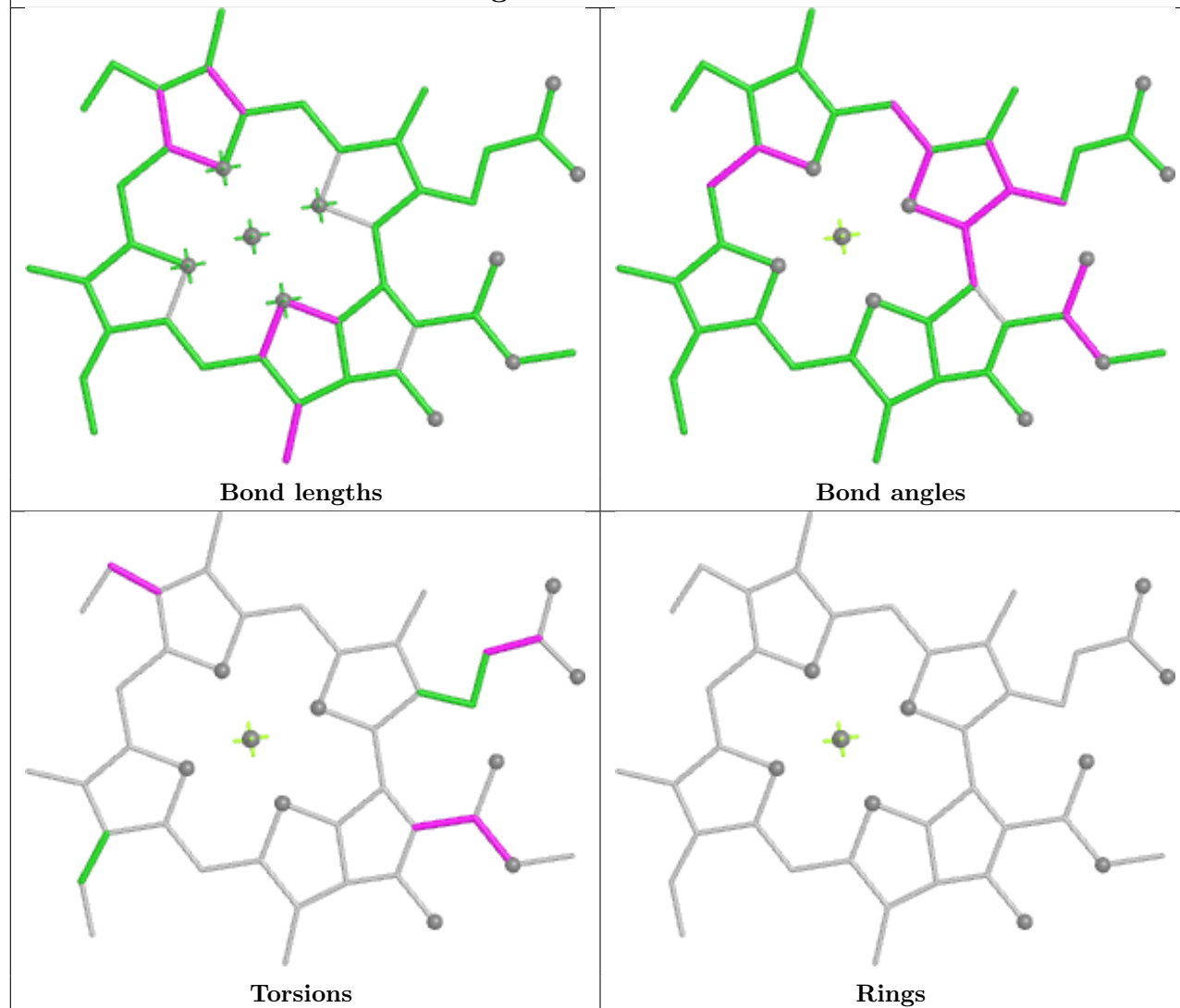
Ligand LUT Y 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

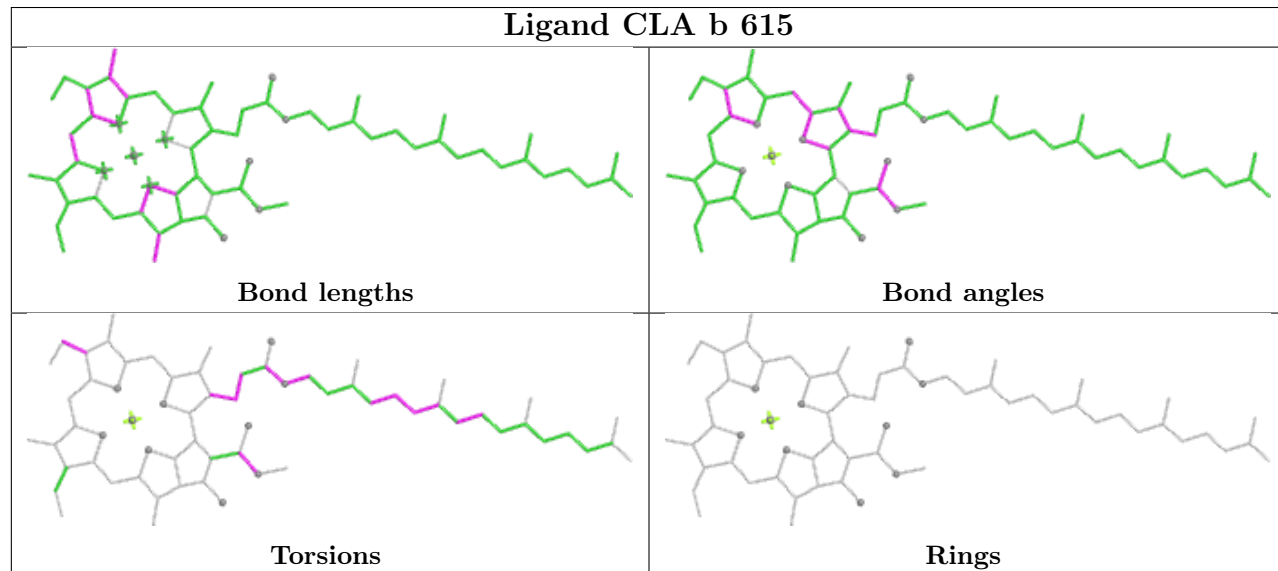
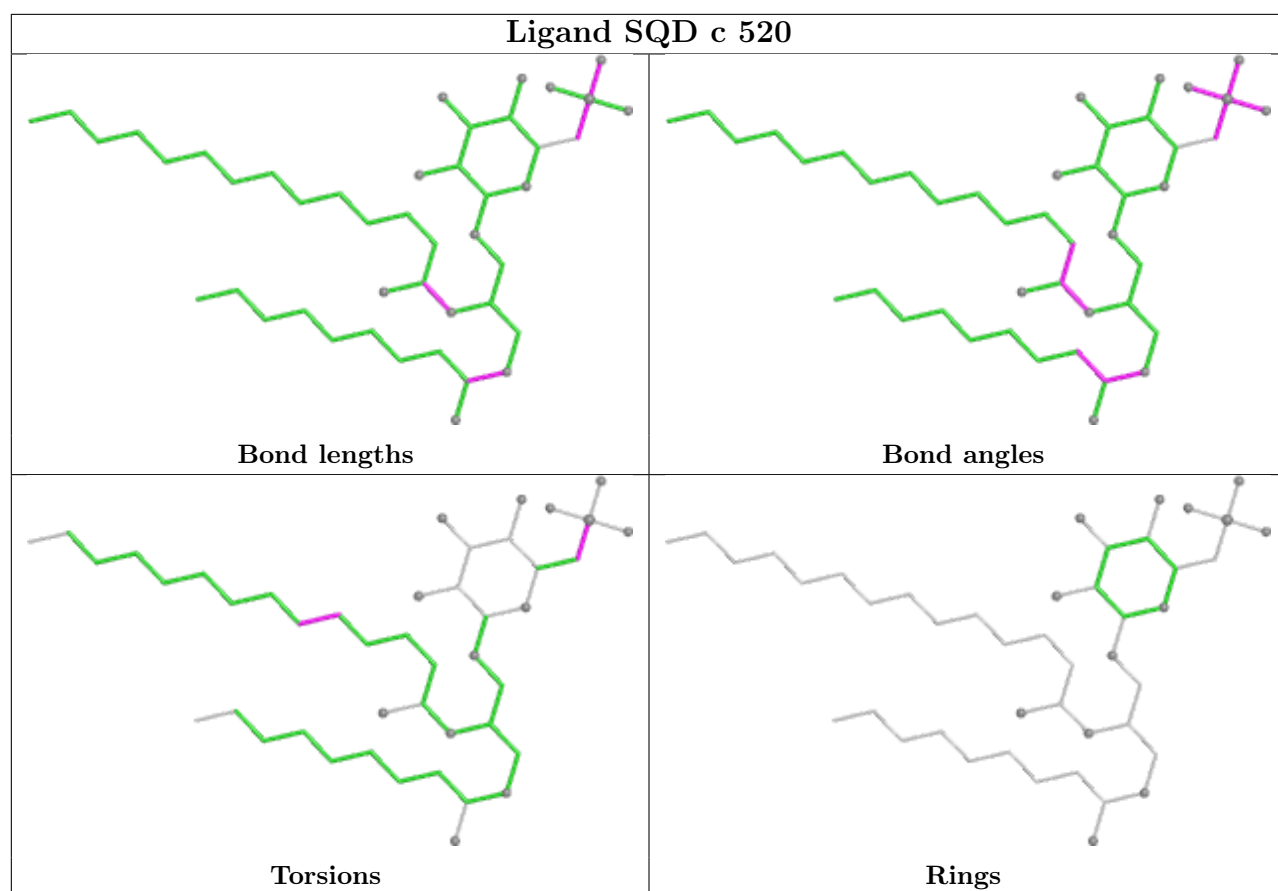
Ligand CHL n 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

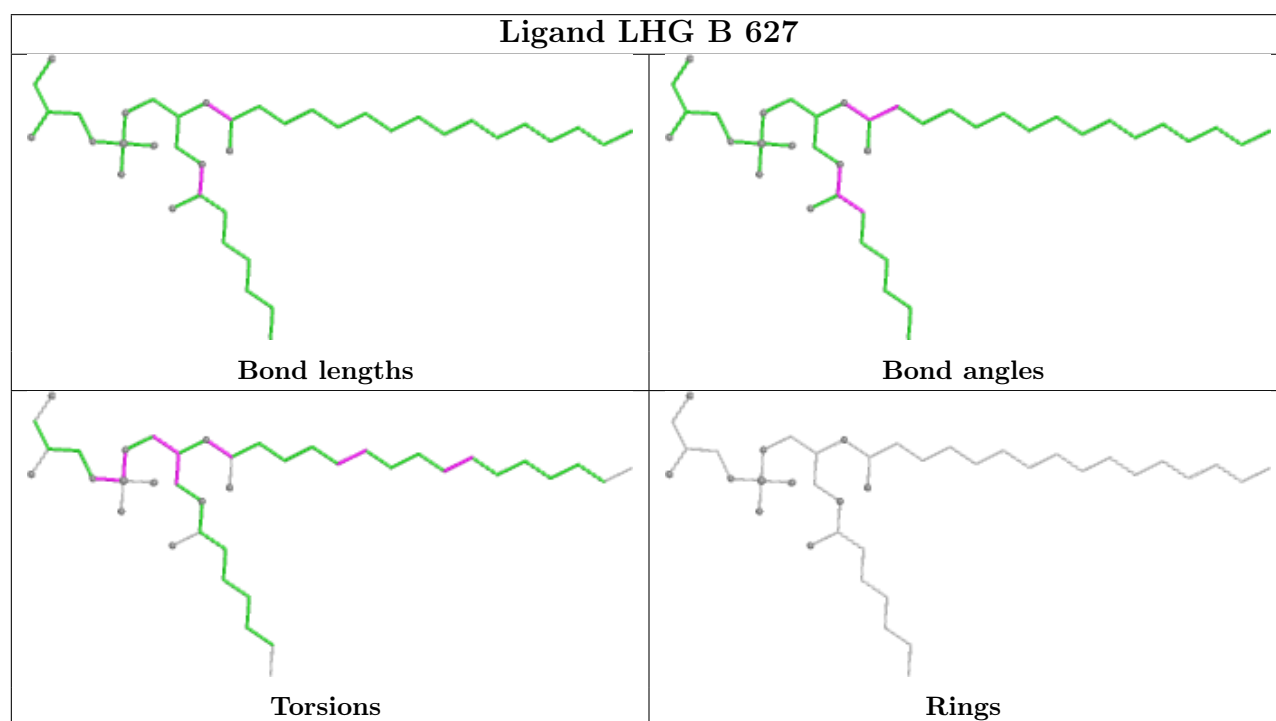
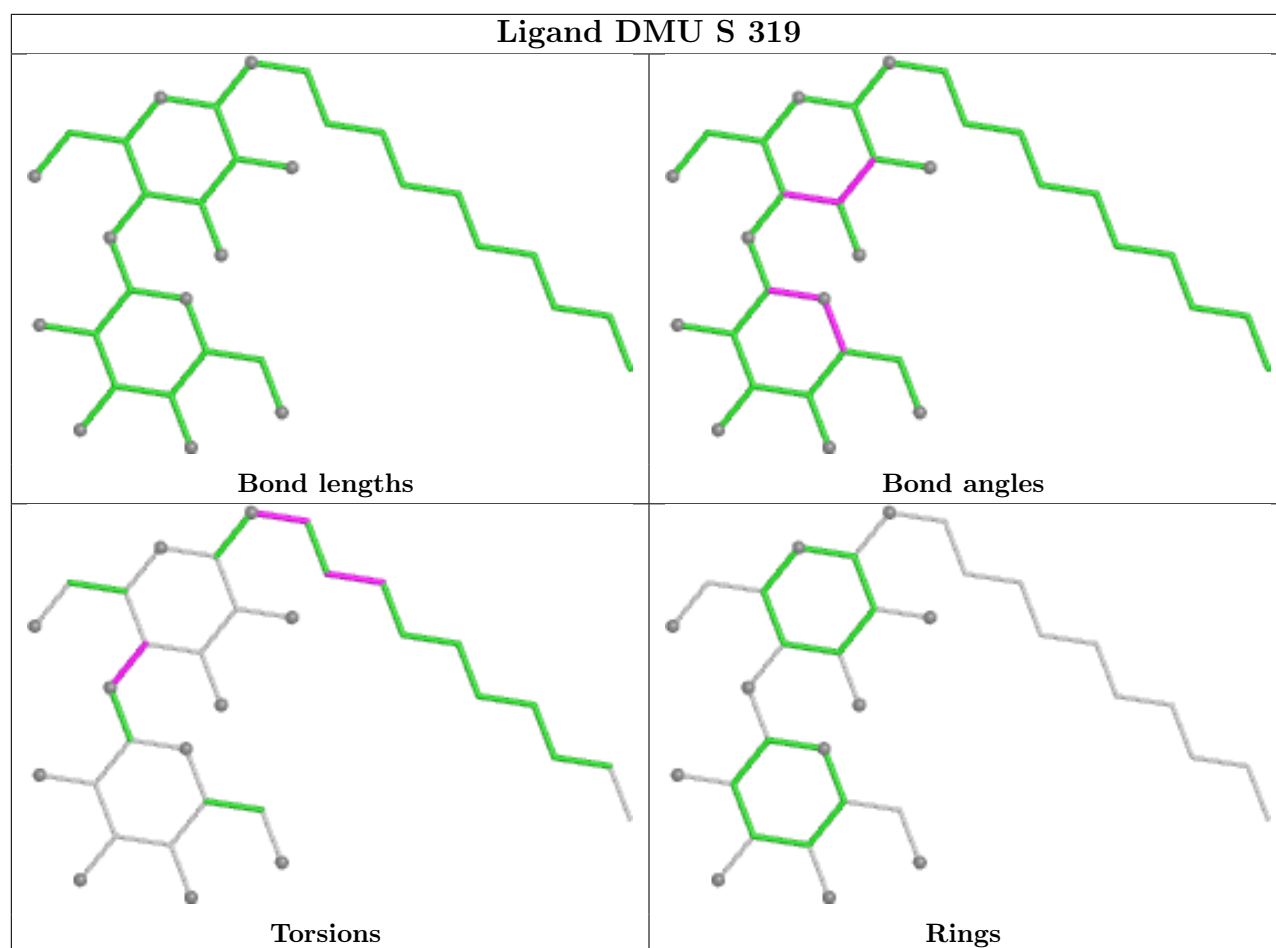
Ligand CLA b 603

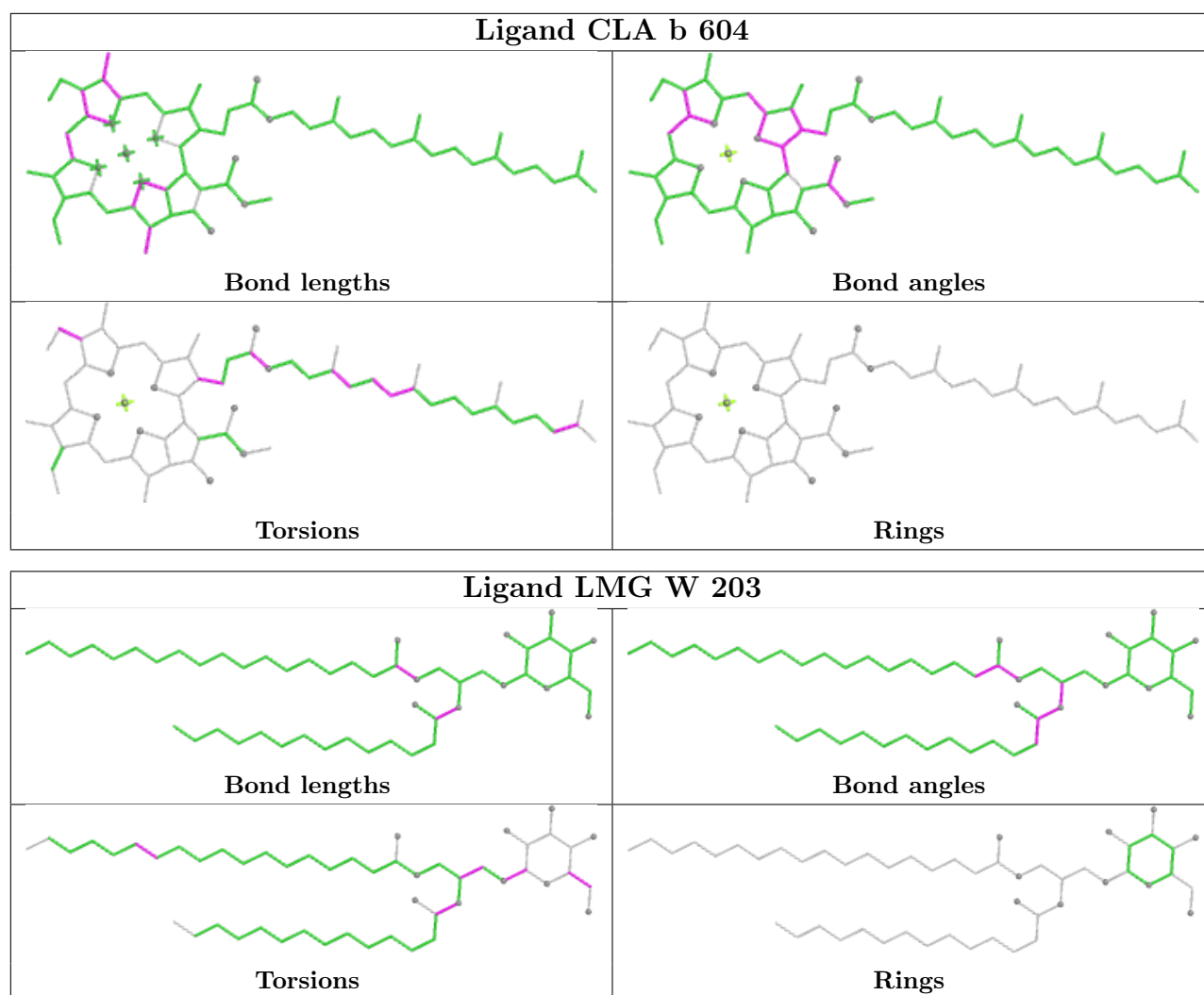


Ligand CLA G 612

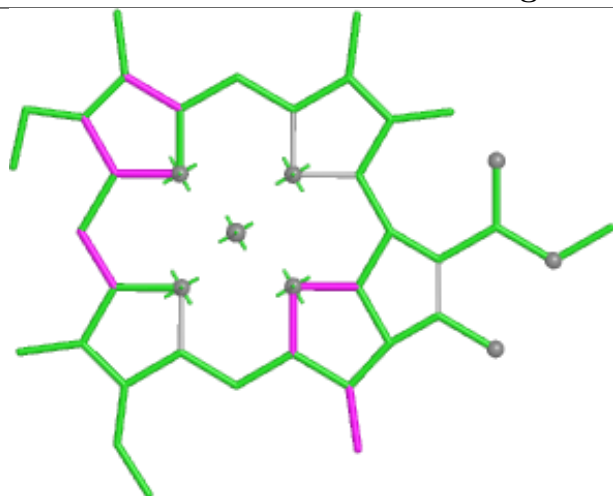








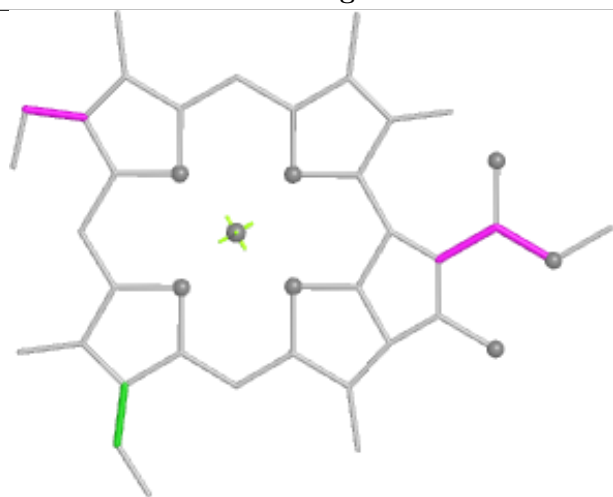
Ligand CLA r 610



Bond lengths



Bond angles

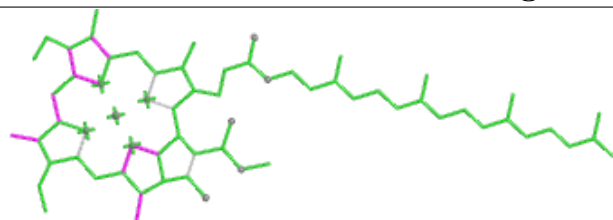


Torsions

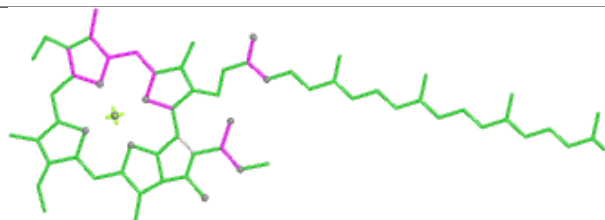


Rings

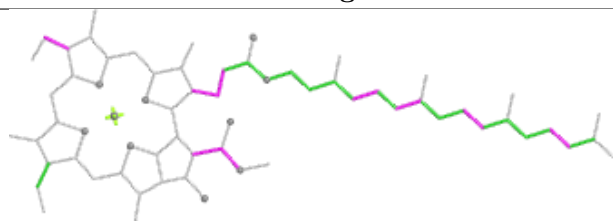
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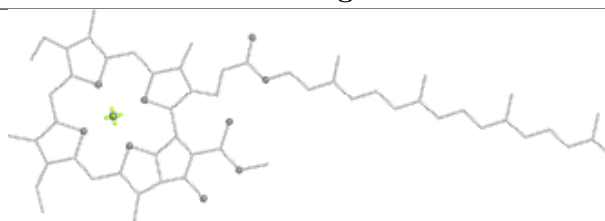
Bond lengths



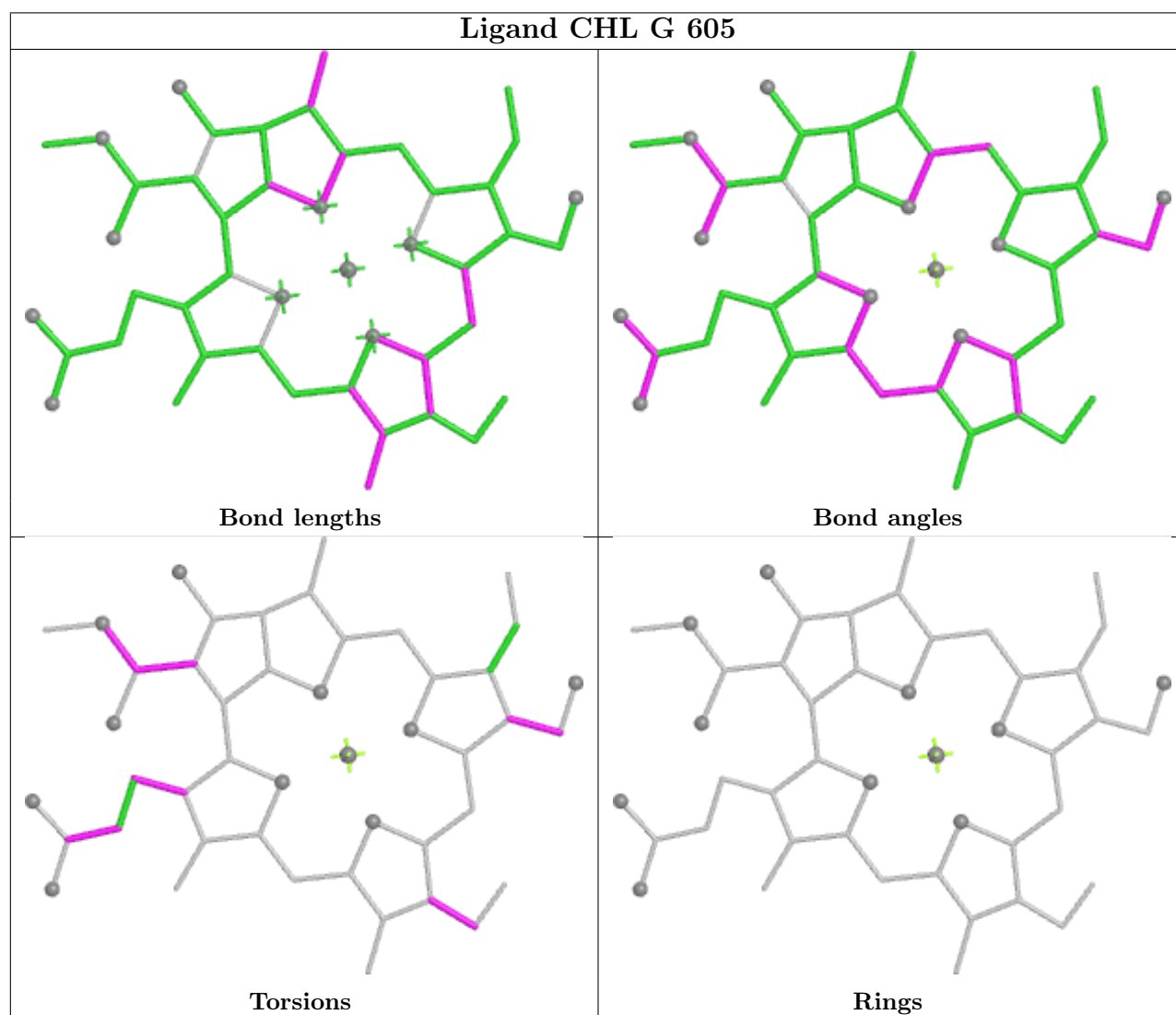
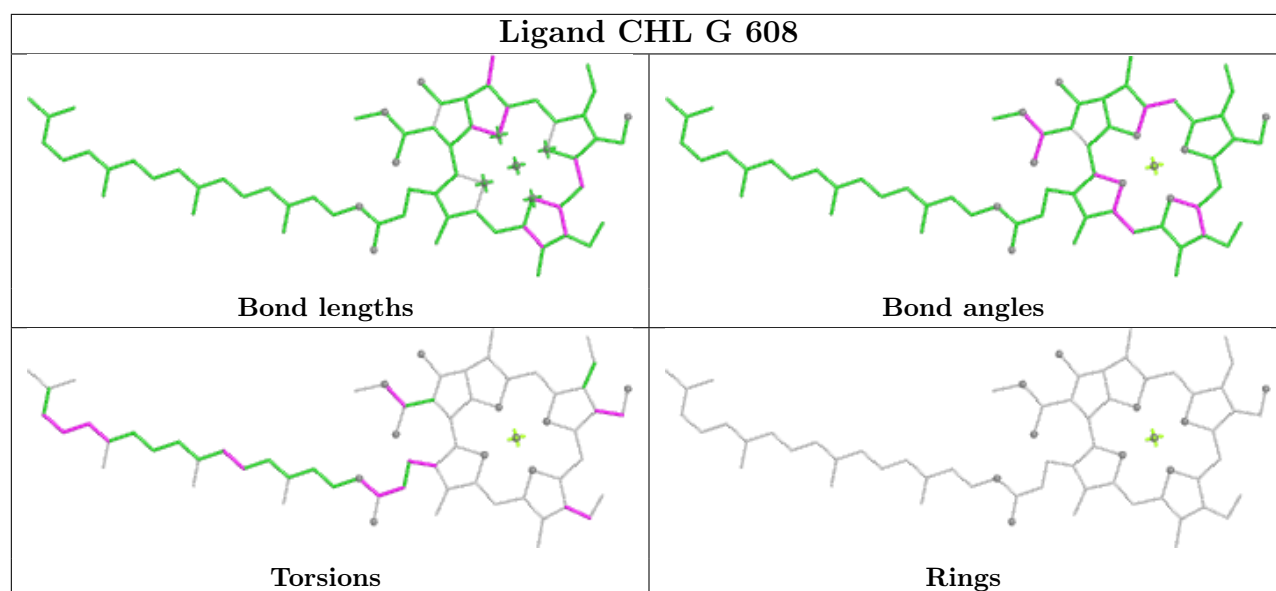
Bond angles

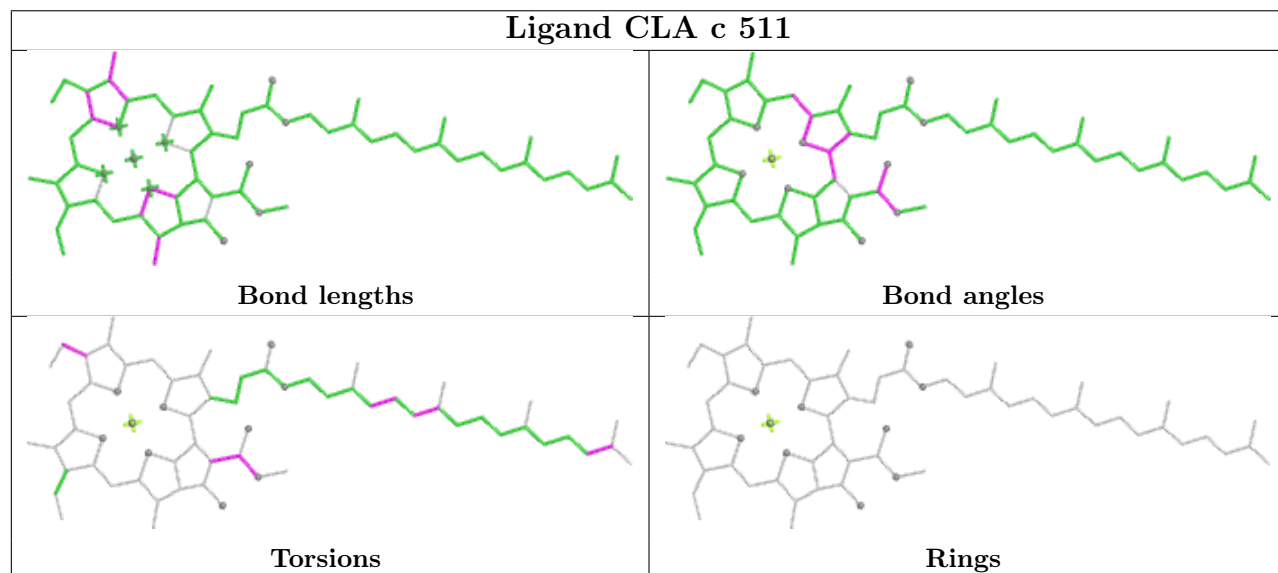
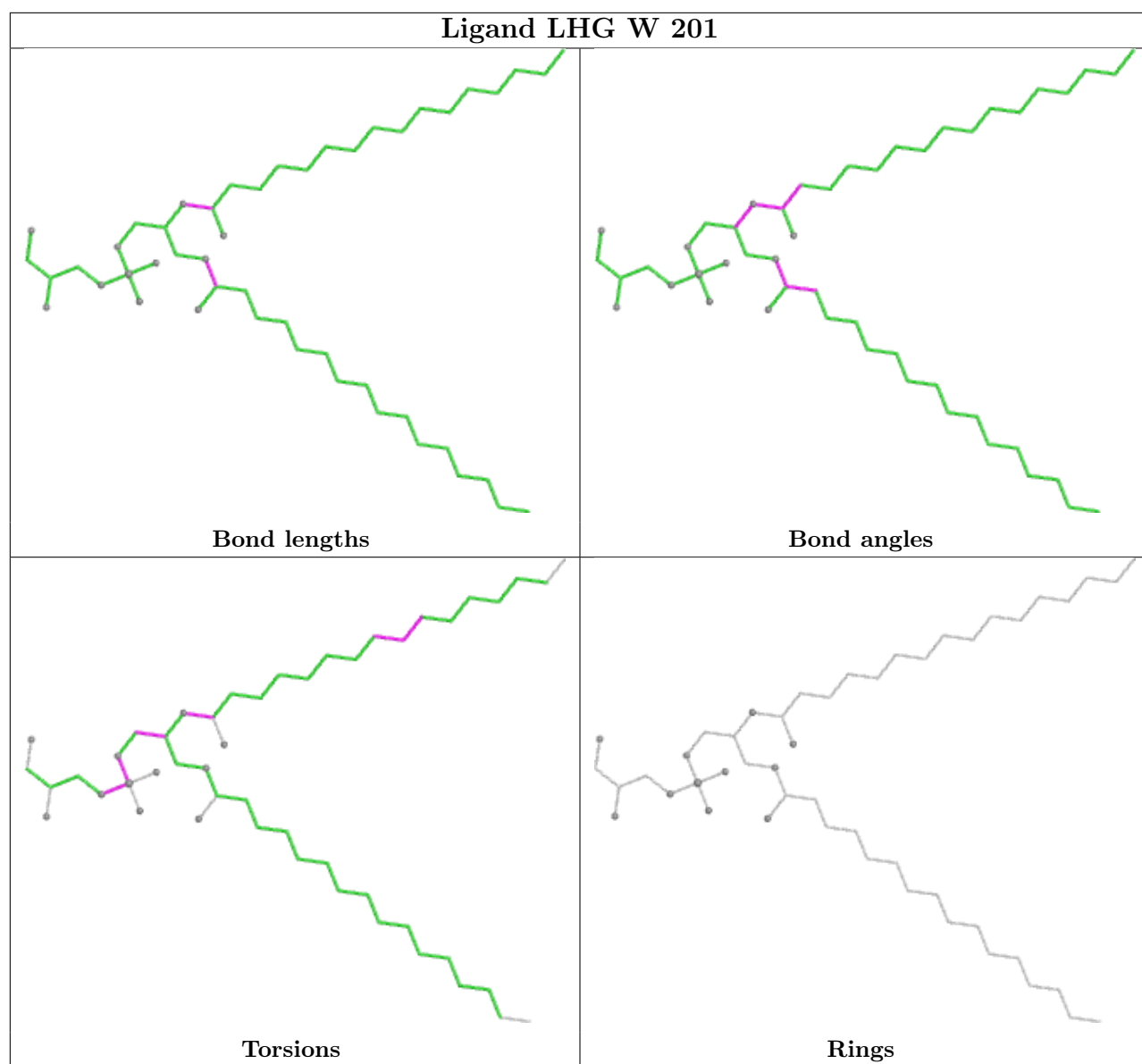


Torsions

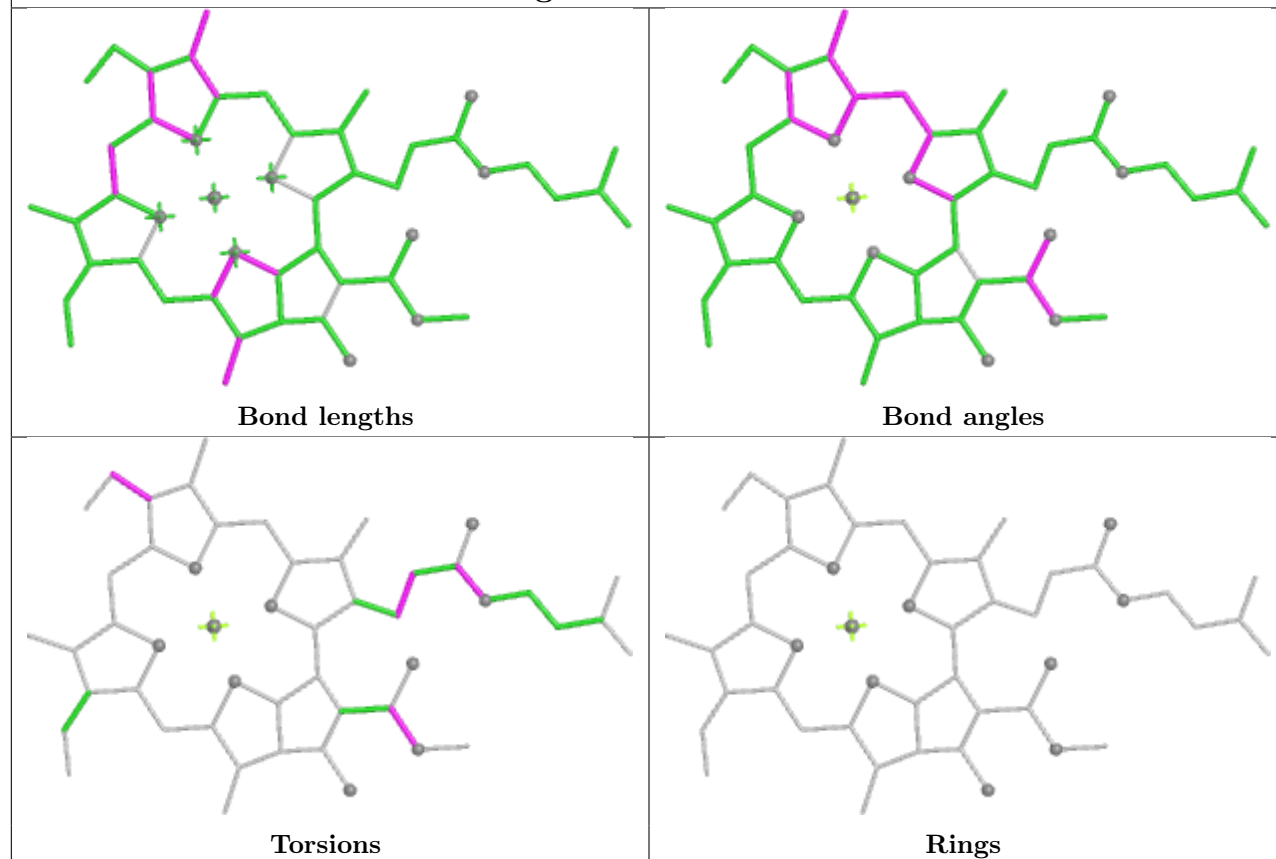


Rings

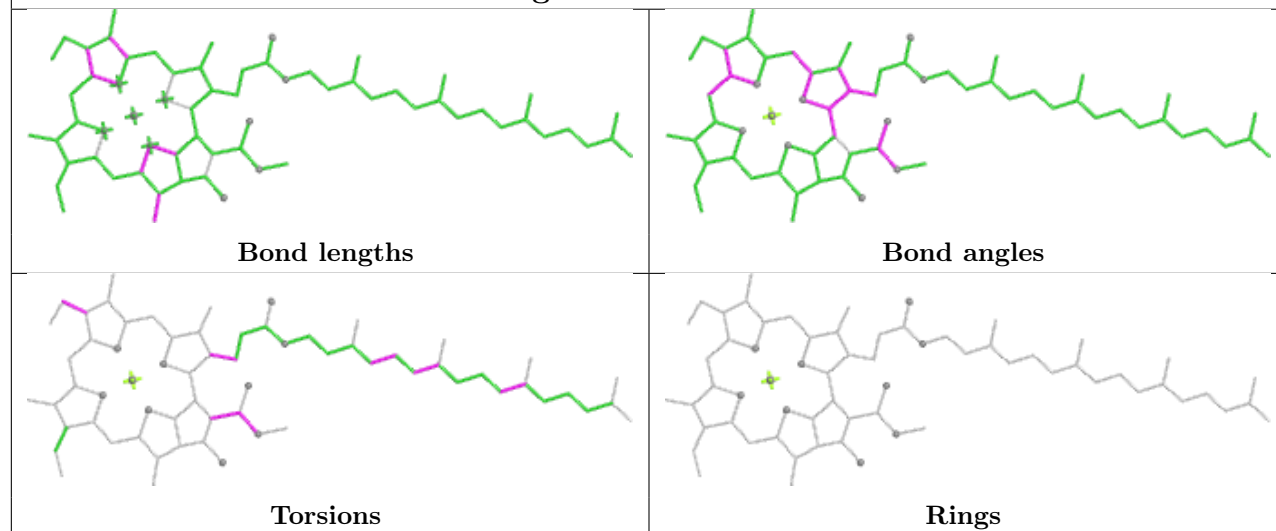


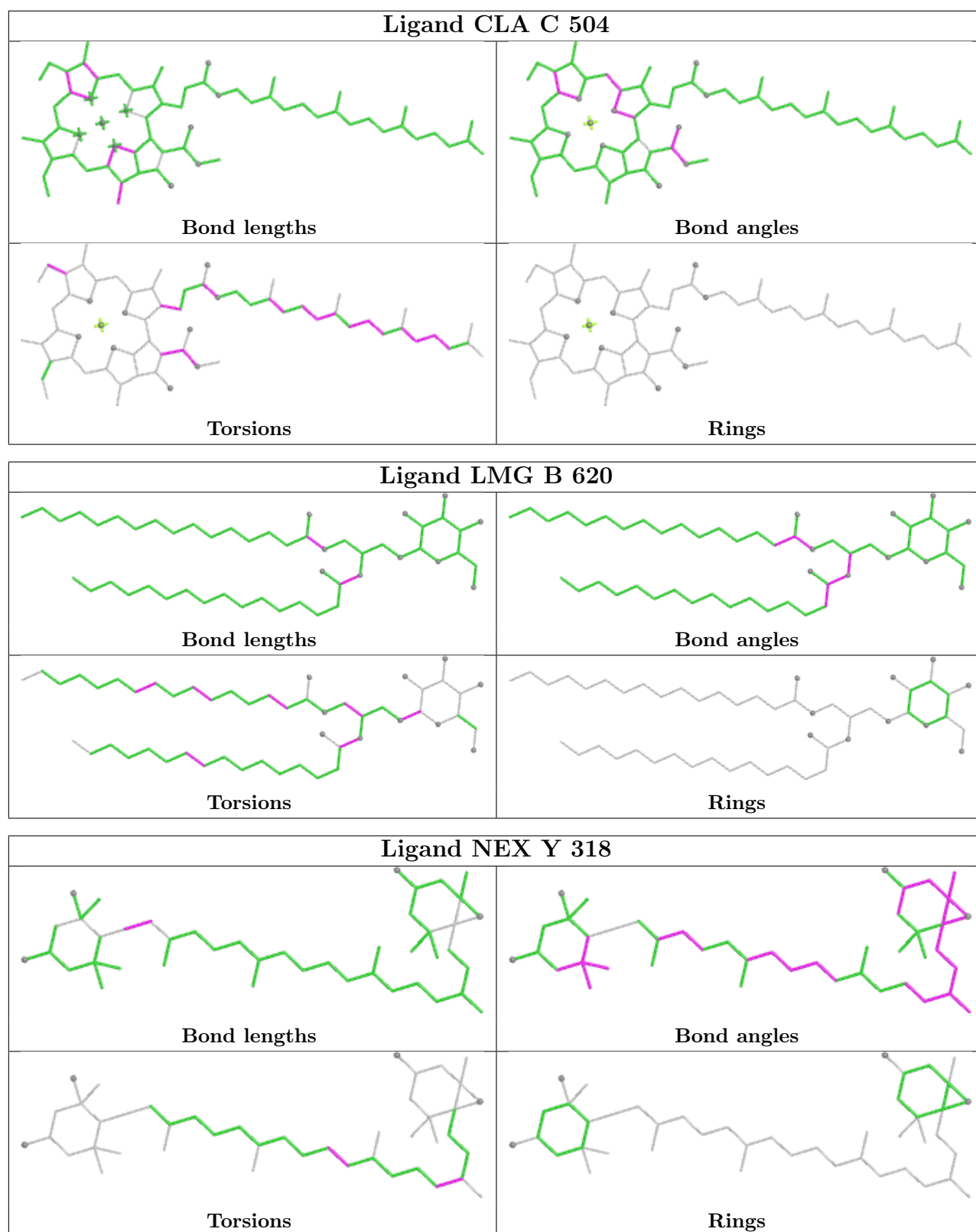


Ligand CLA n 604

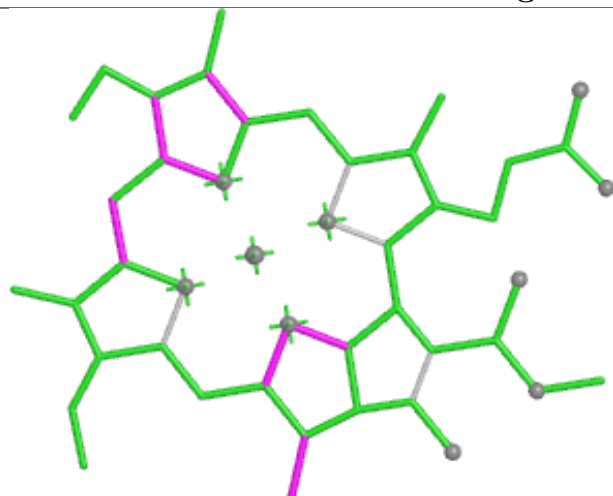


Ligand CLA C 508

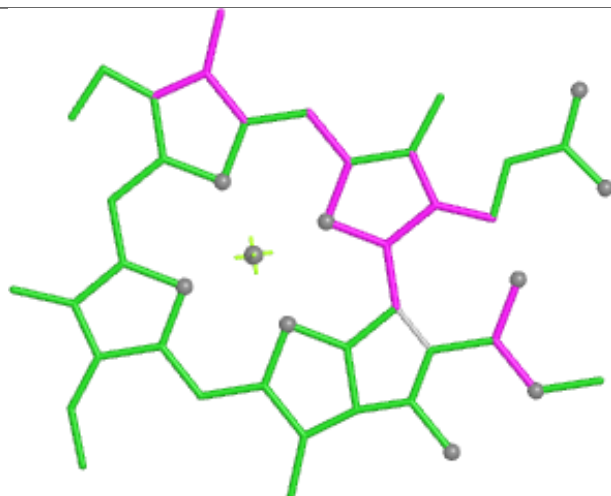




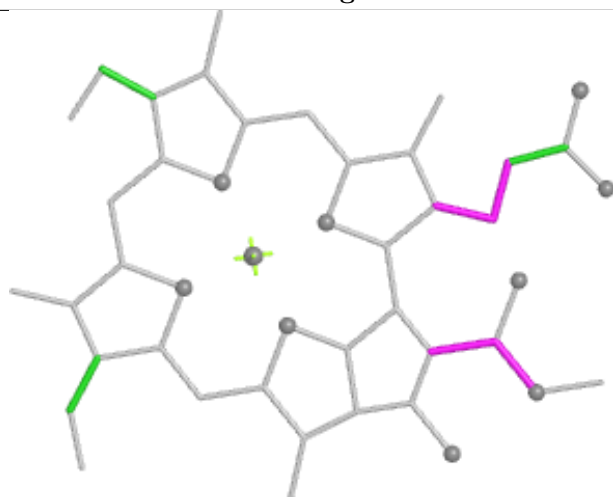
Ligand CLA S 312



Bond lengths



Bond angles

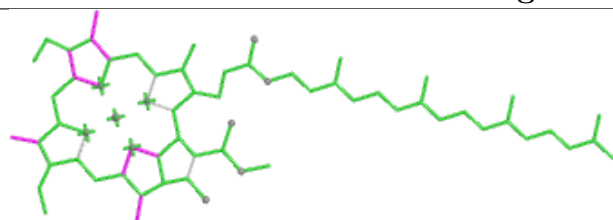


Torsions

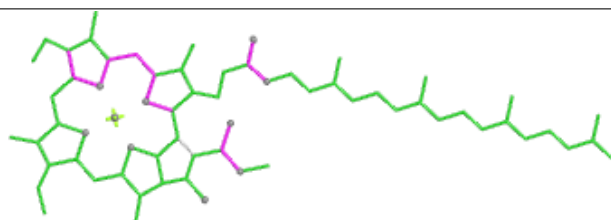


Rings

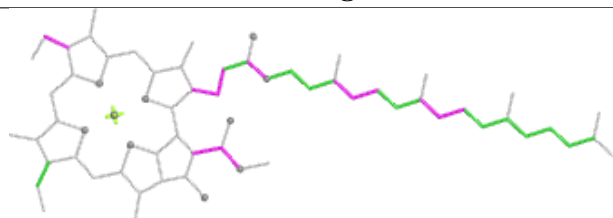
Ligand CLA b 605



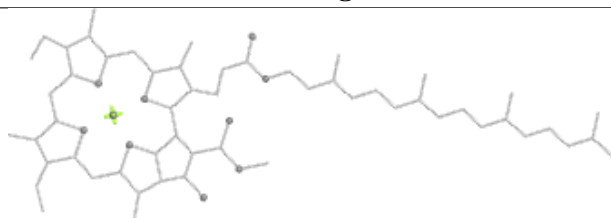
Bond lengths



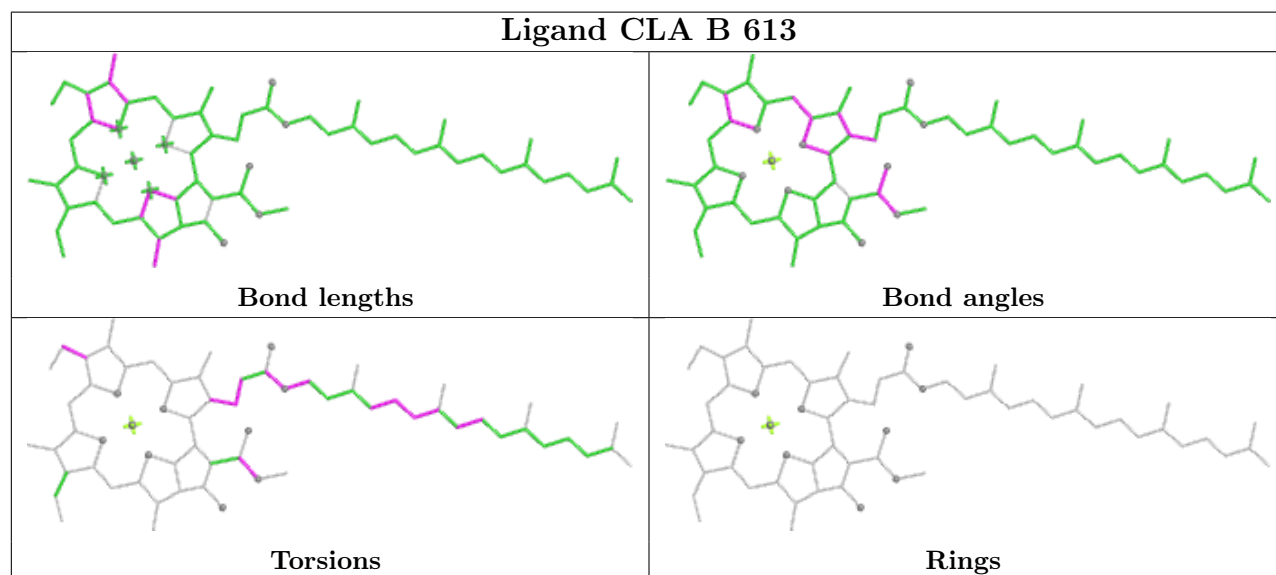
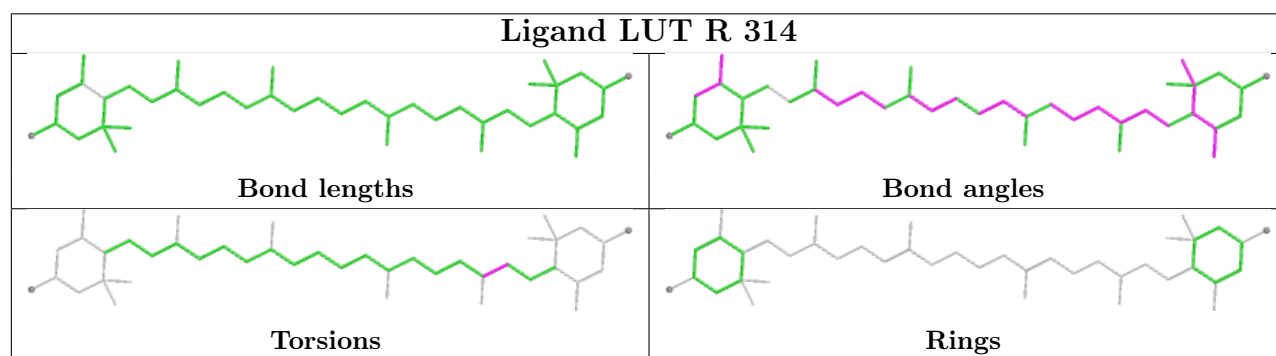
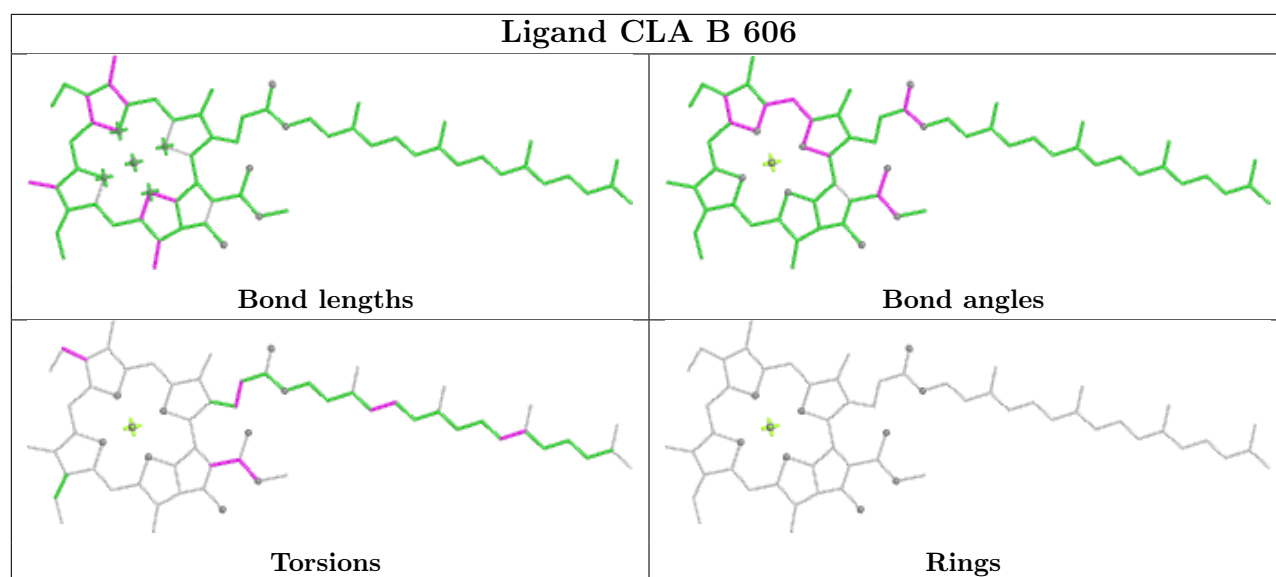
Bond angles

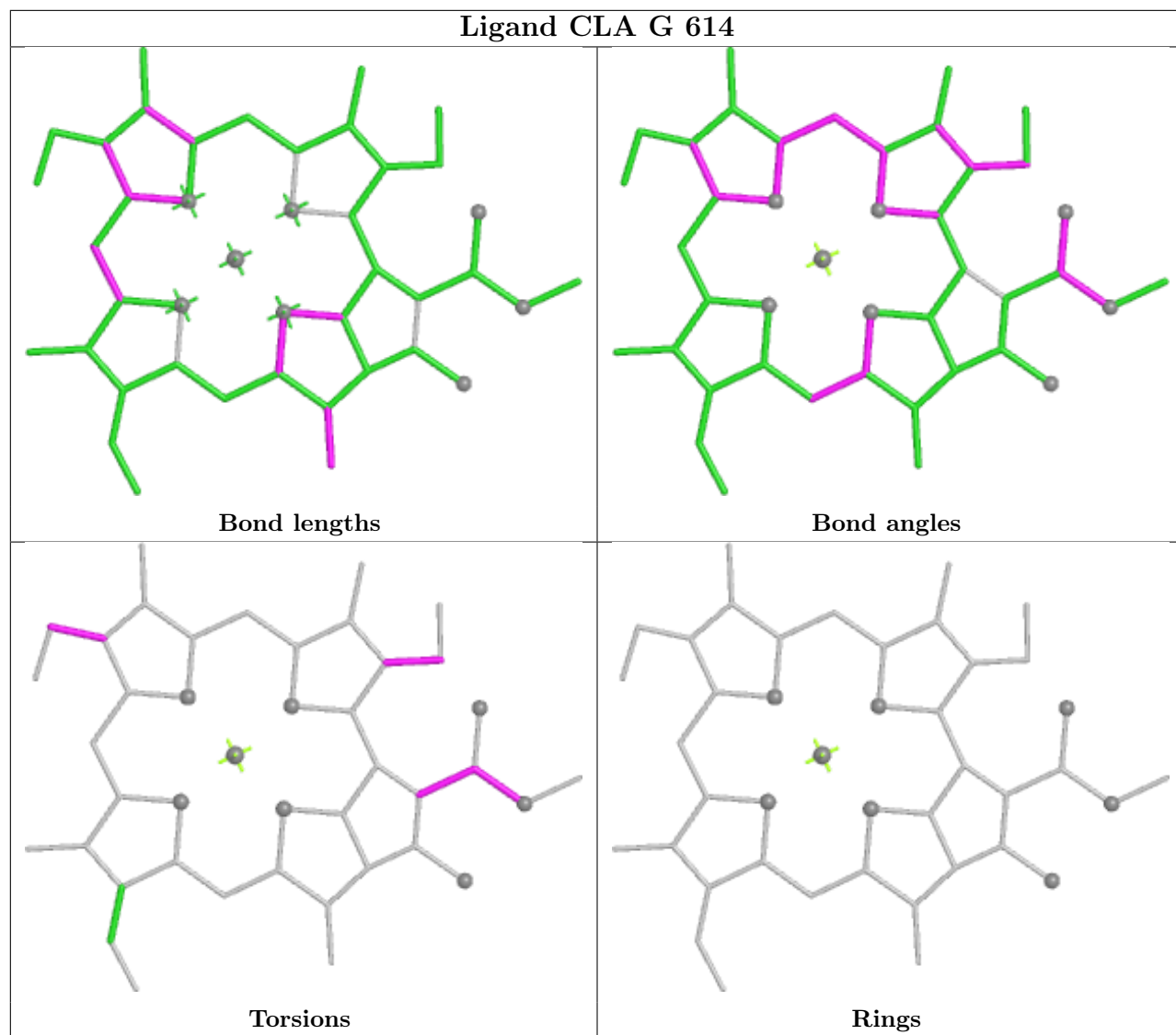


Torsions

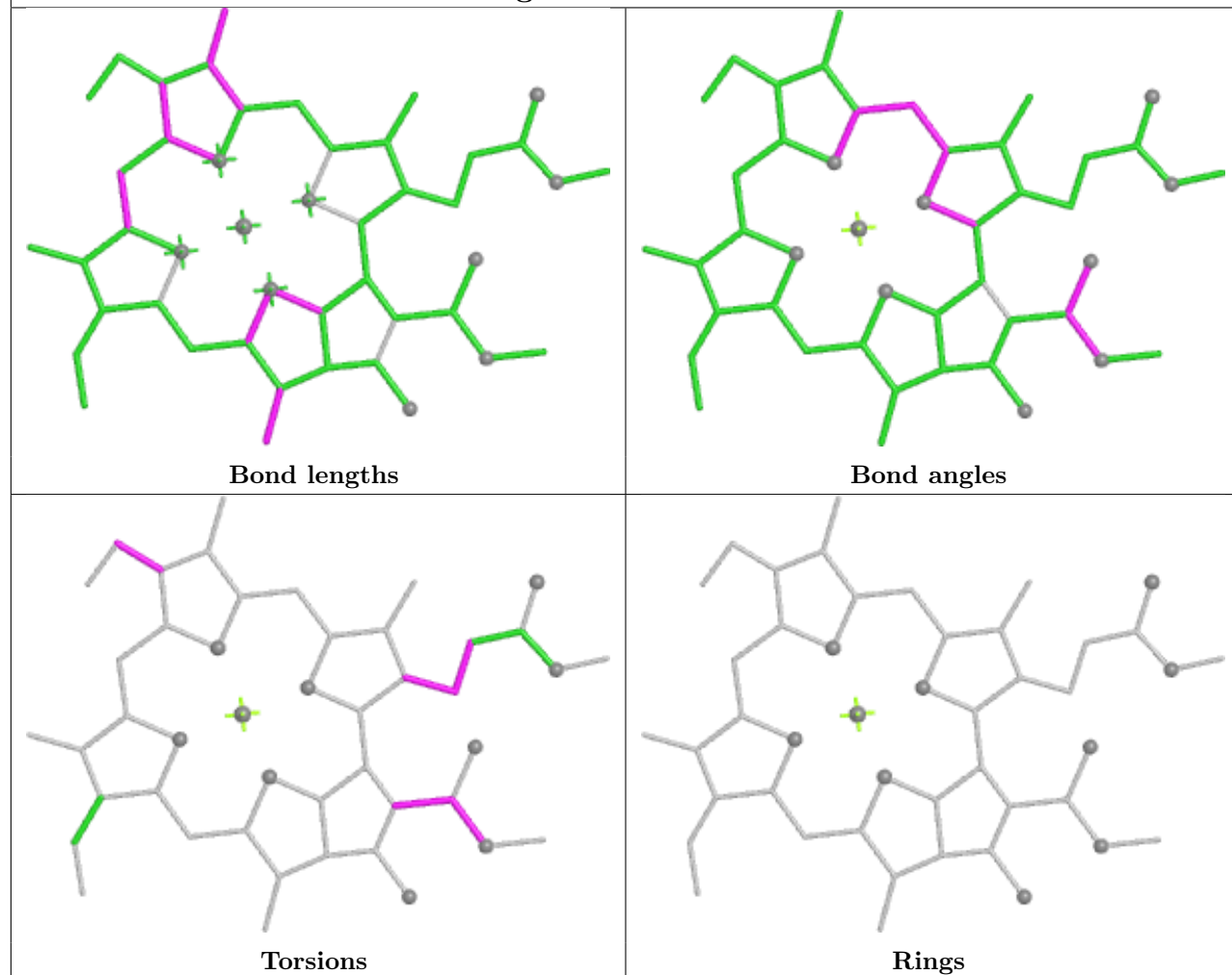


Rings

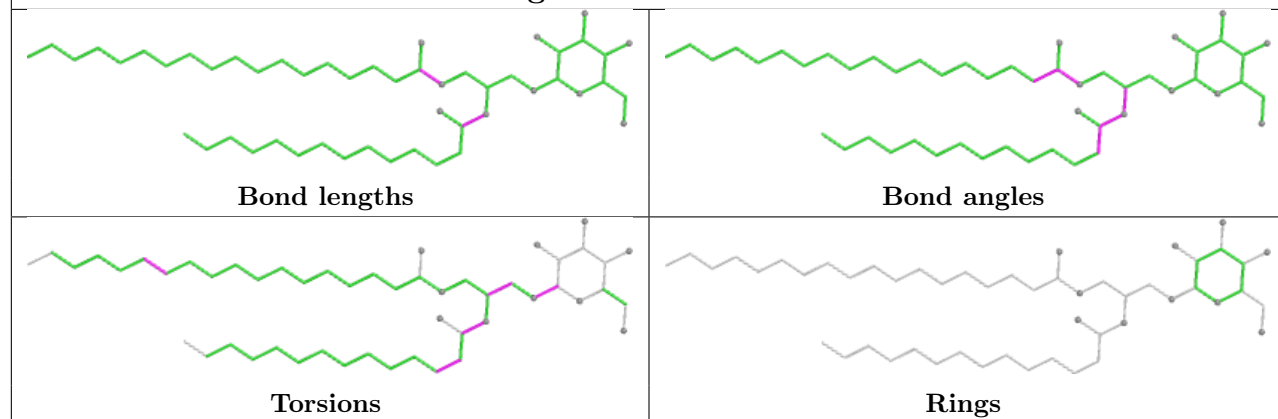


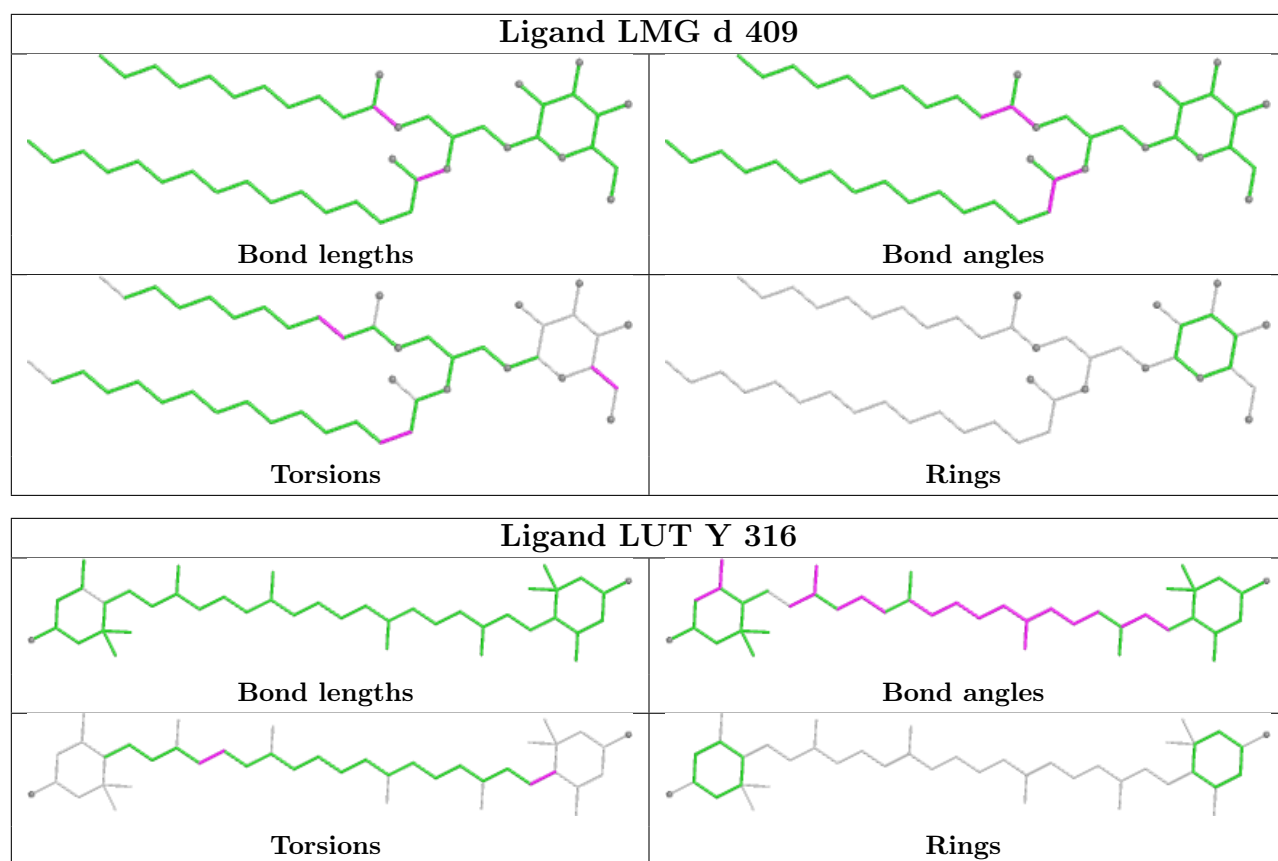


Ligand CLA S 303

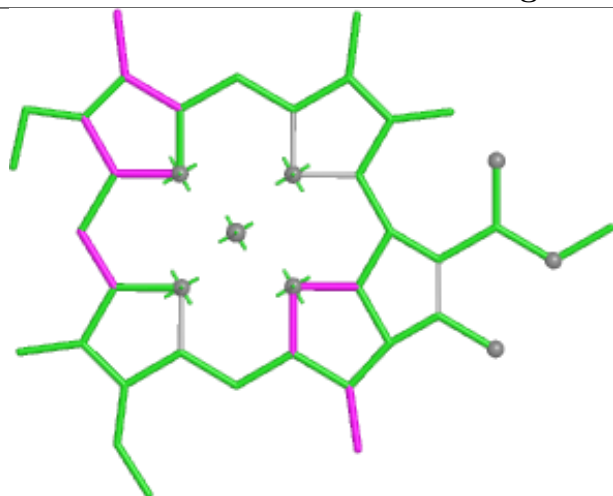


Ligand LMG w 202

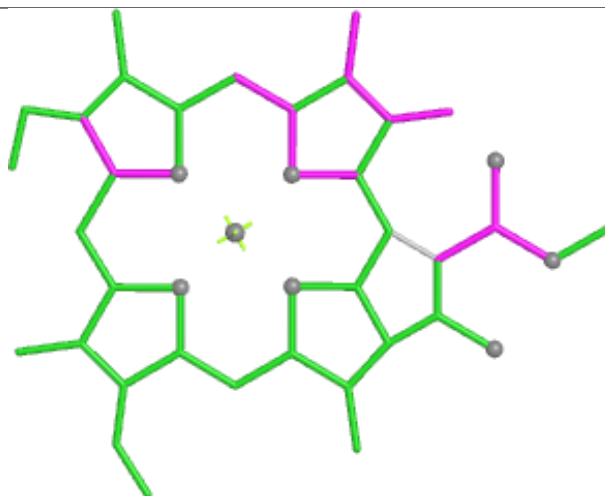




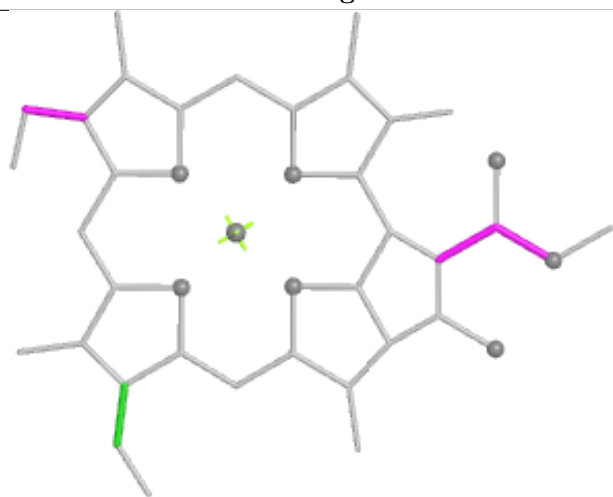
Ligand CLA s 613



Bond lengths



Bond angles

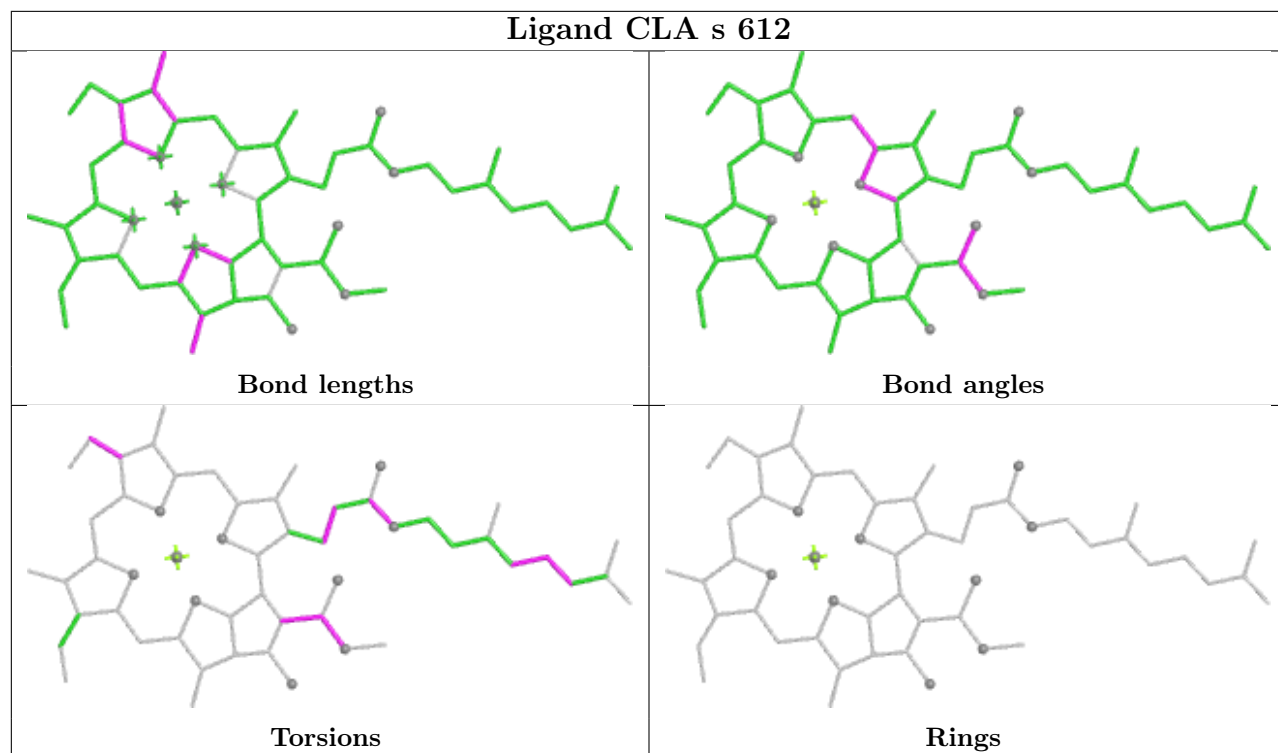


Torsions

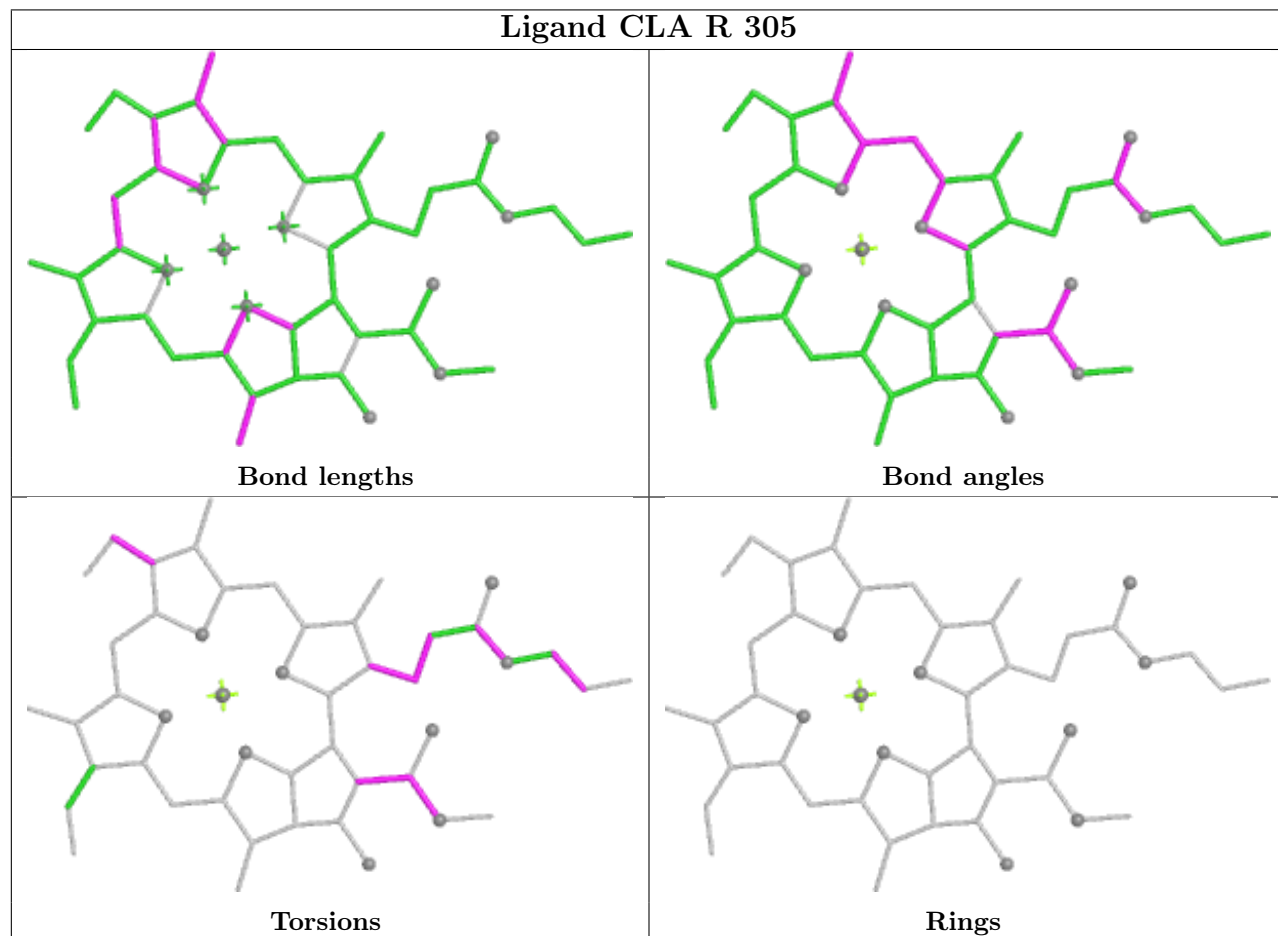


Rings

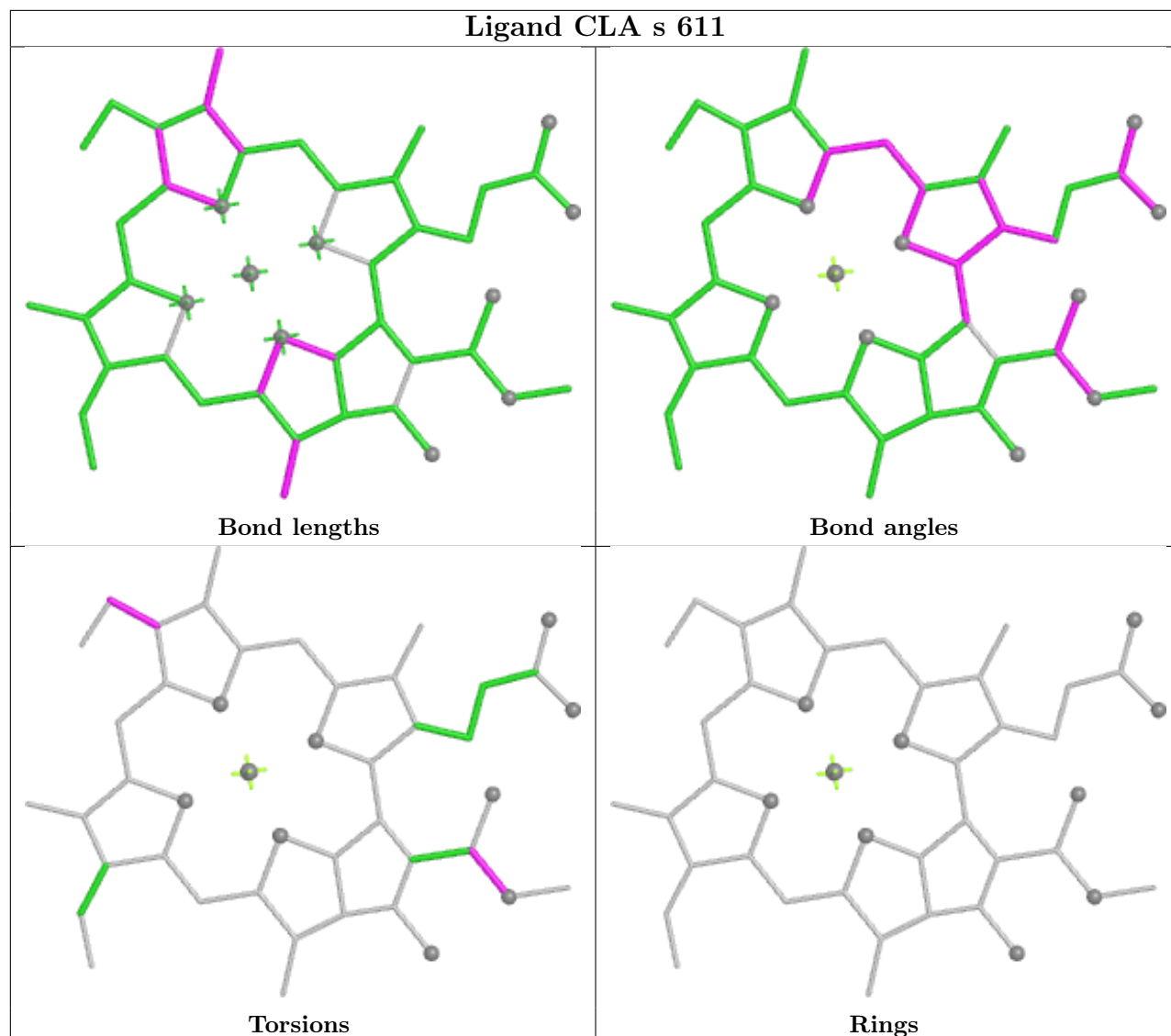
Ligand CLA s 612



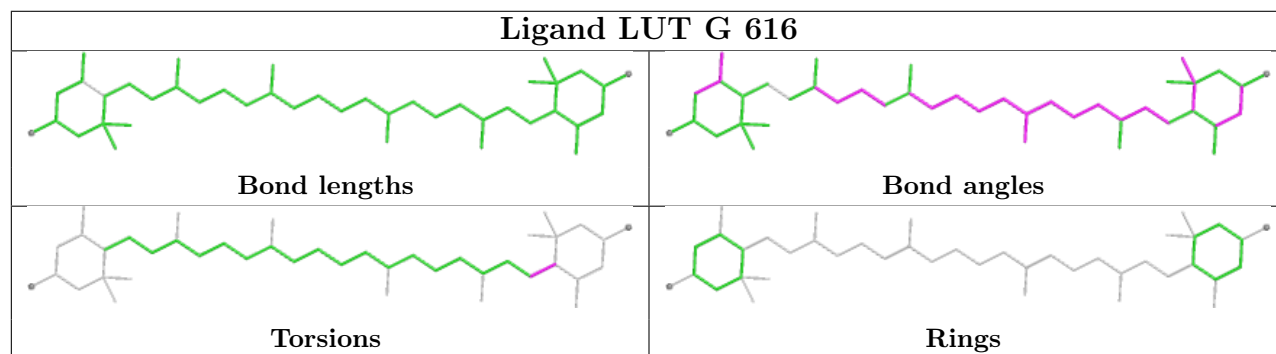
Ligand CLA R 305

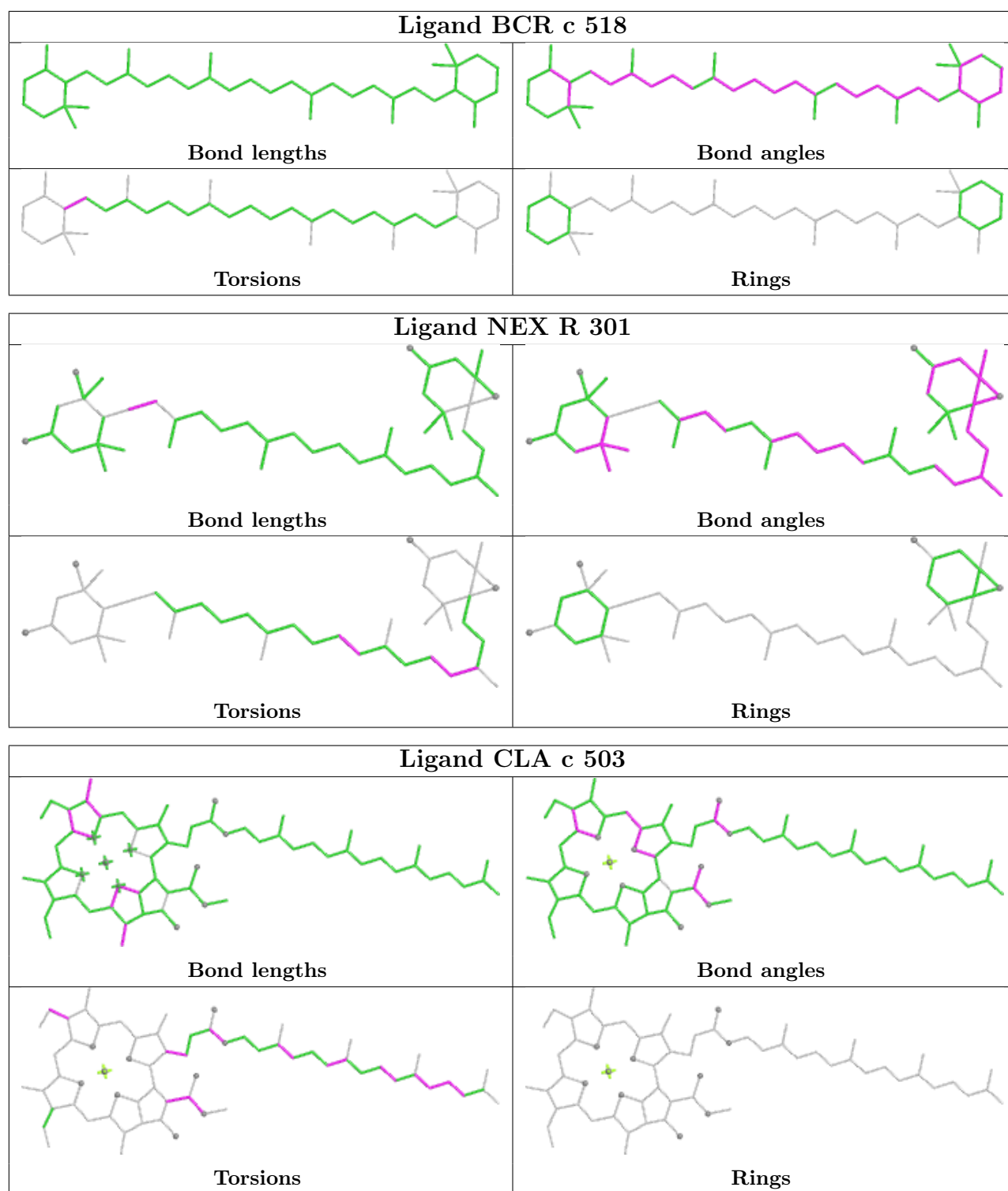


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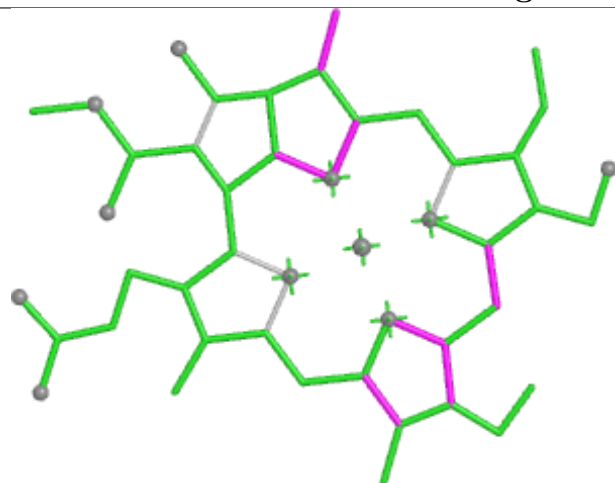


Ligand LUT G 616

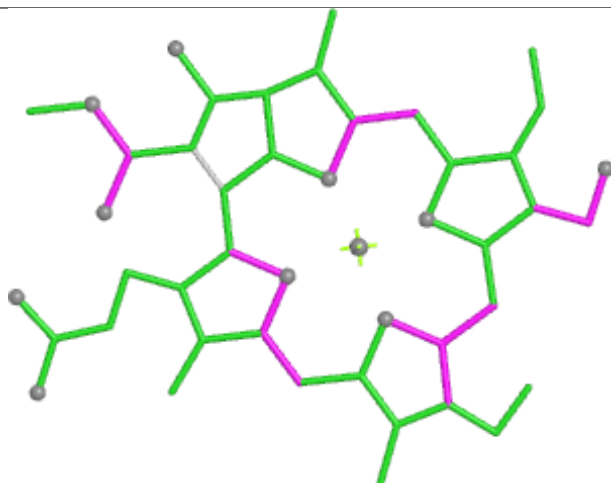




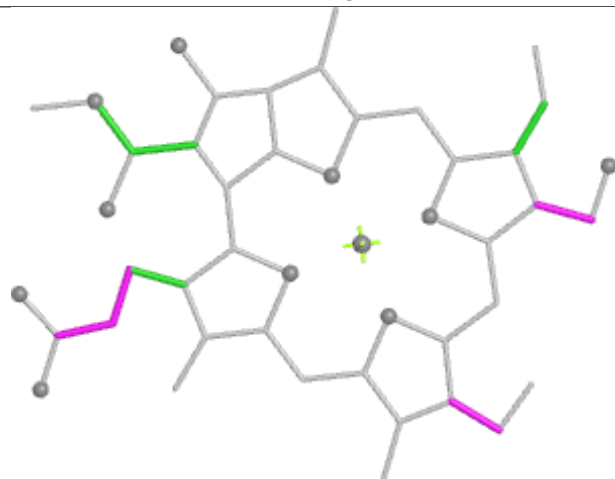
Ligand CHL R 307



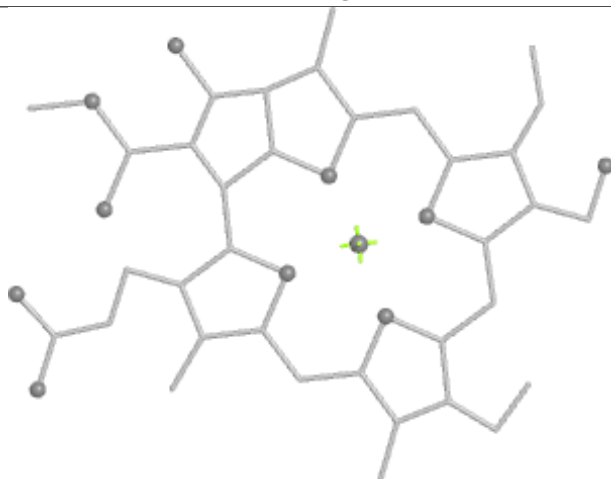
Bond lengths



Bond angles

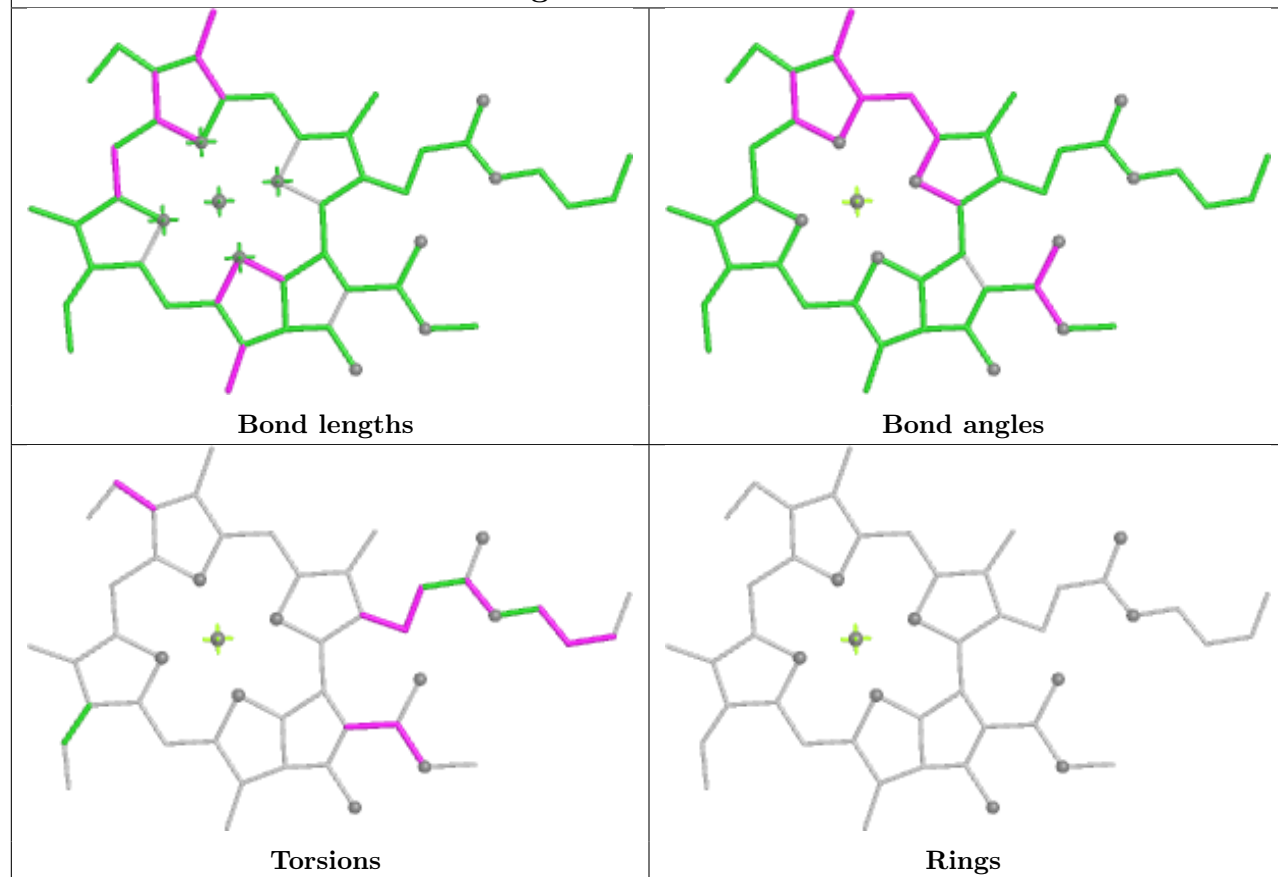


Torsions

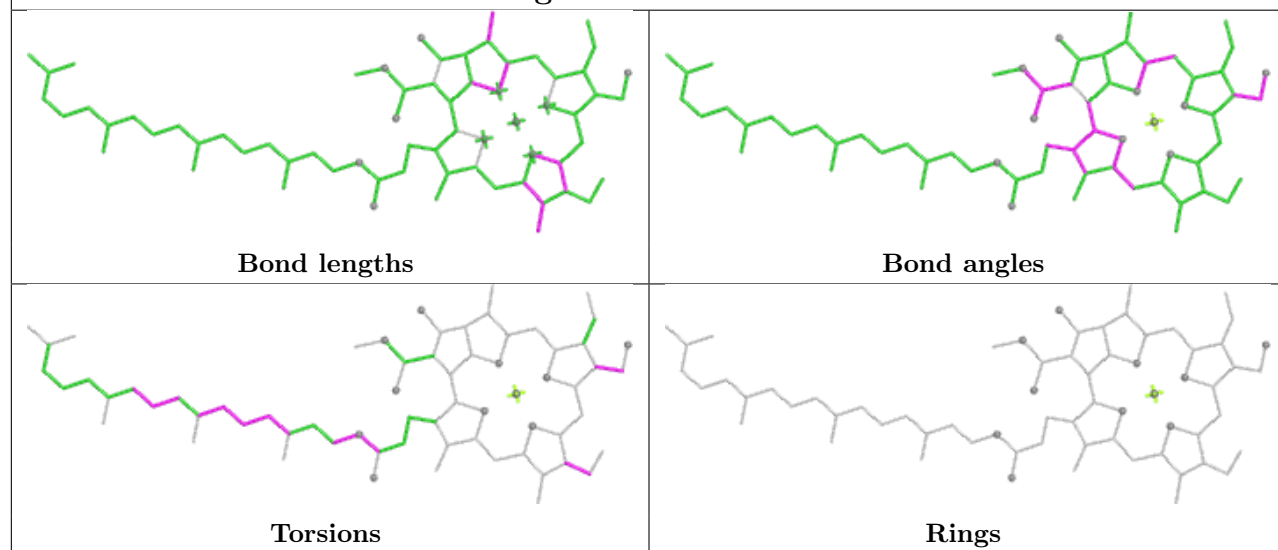


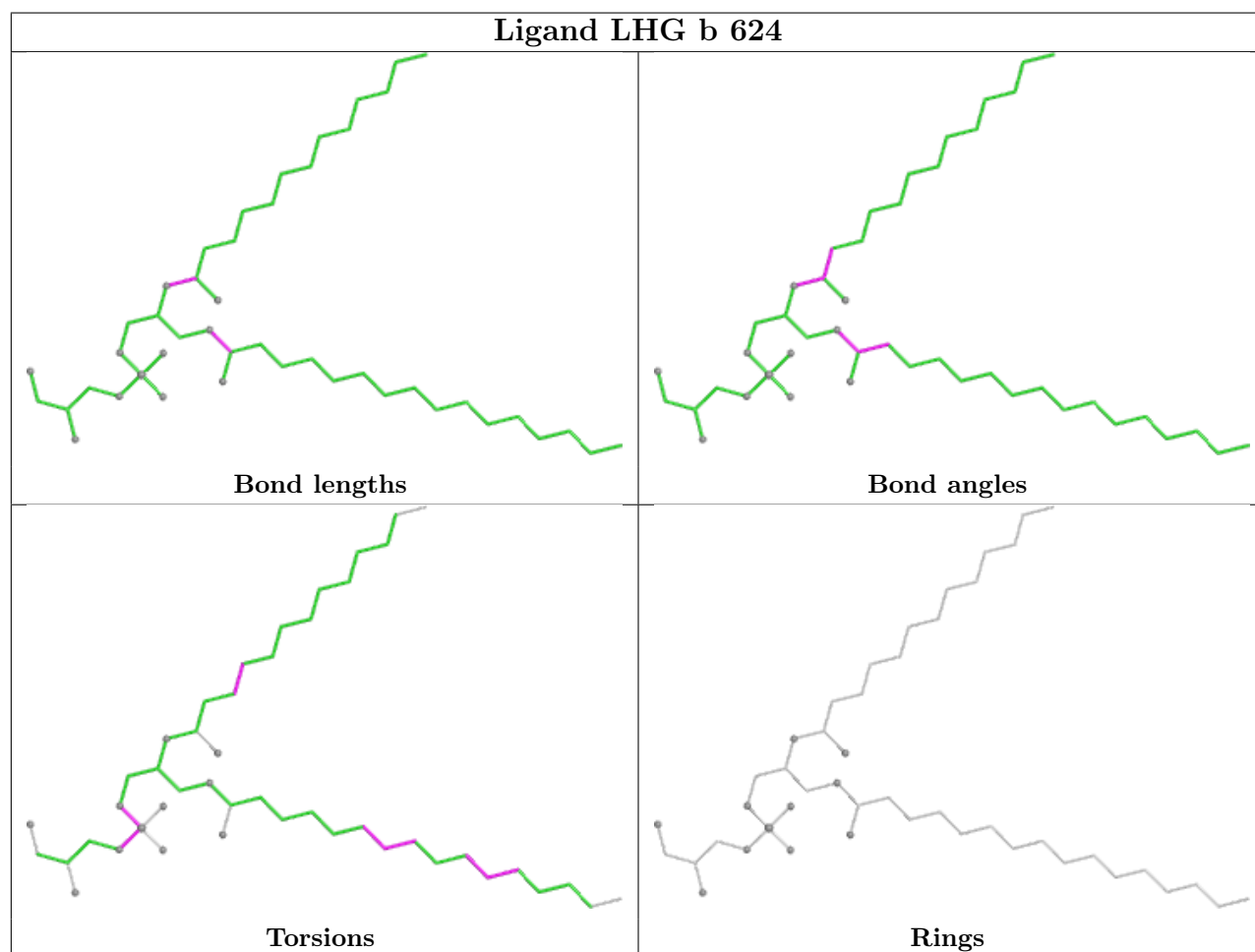
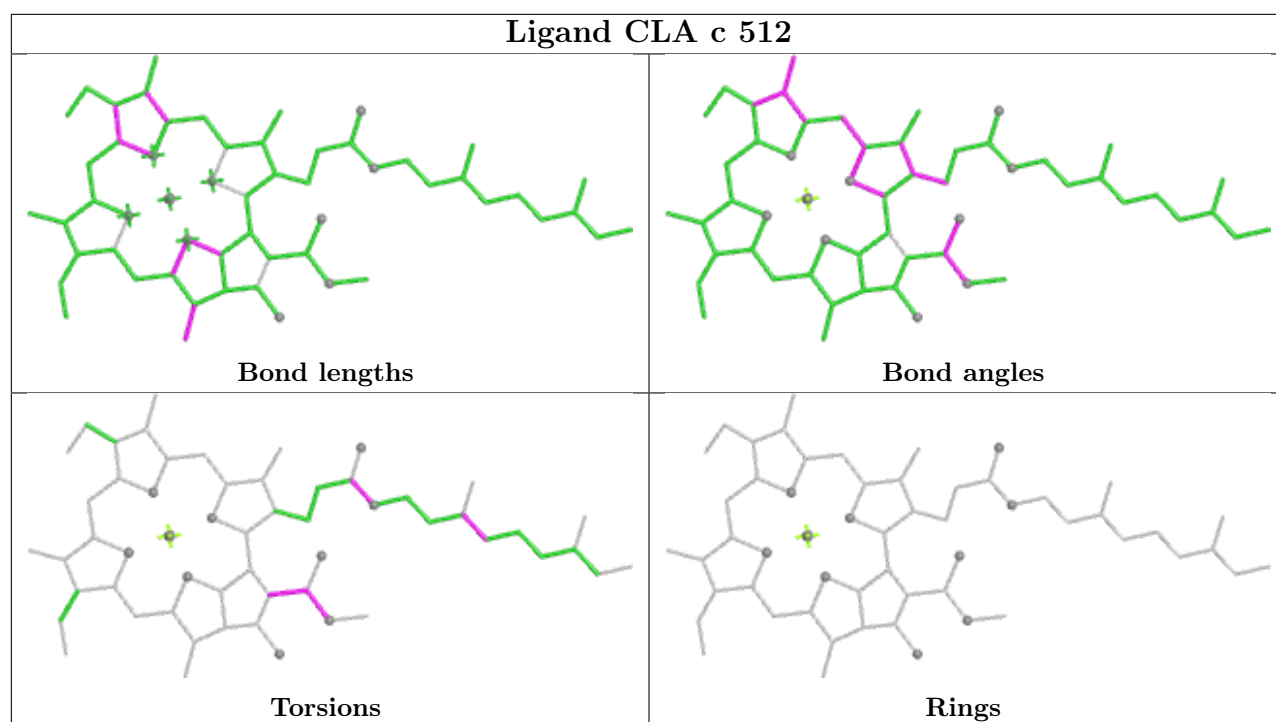
Rings

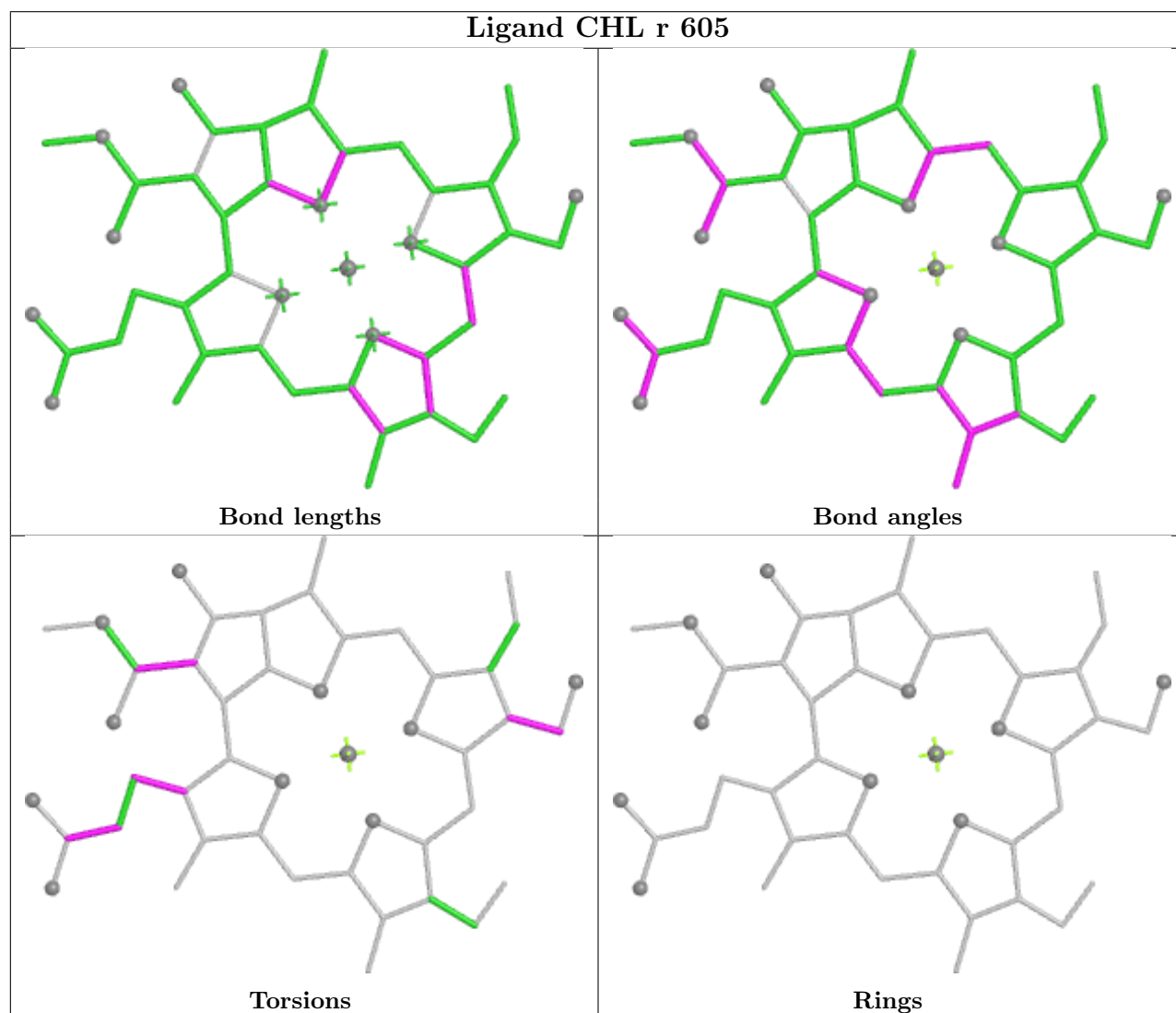
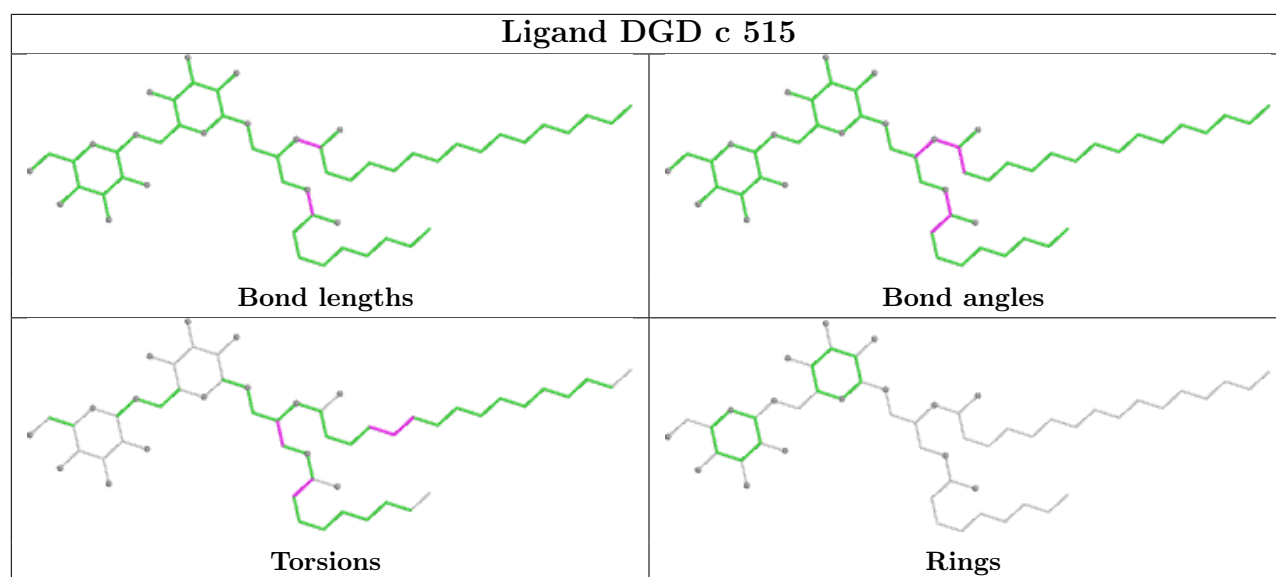
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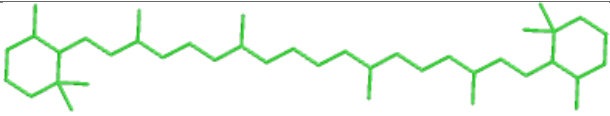
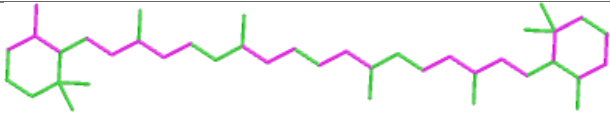
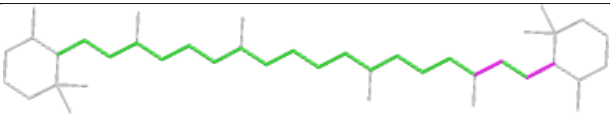
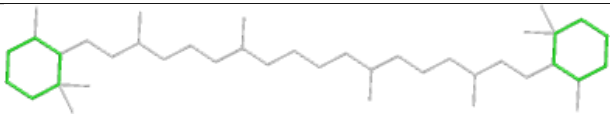


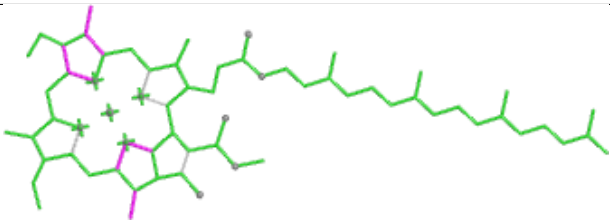
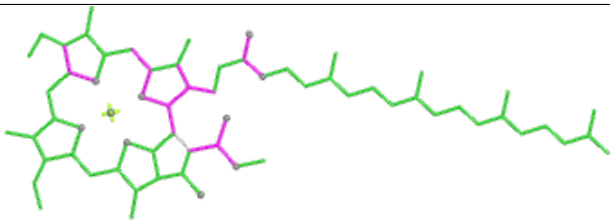
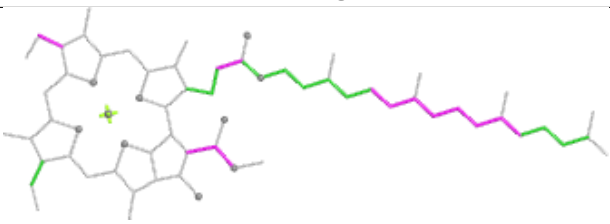
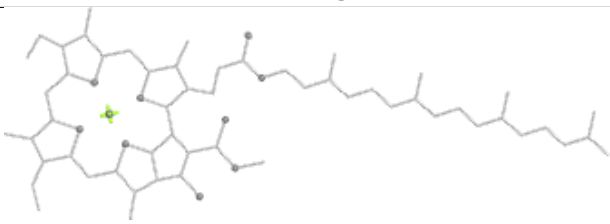
Ligand CHL n 609

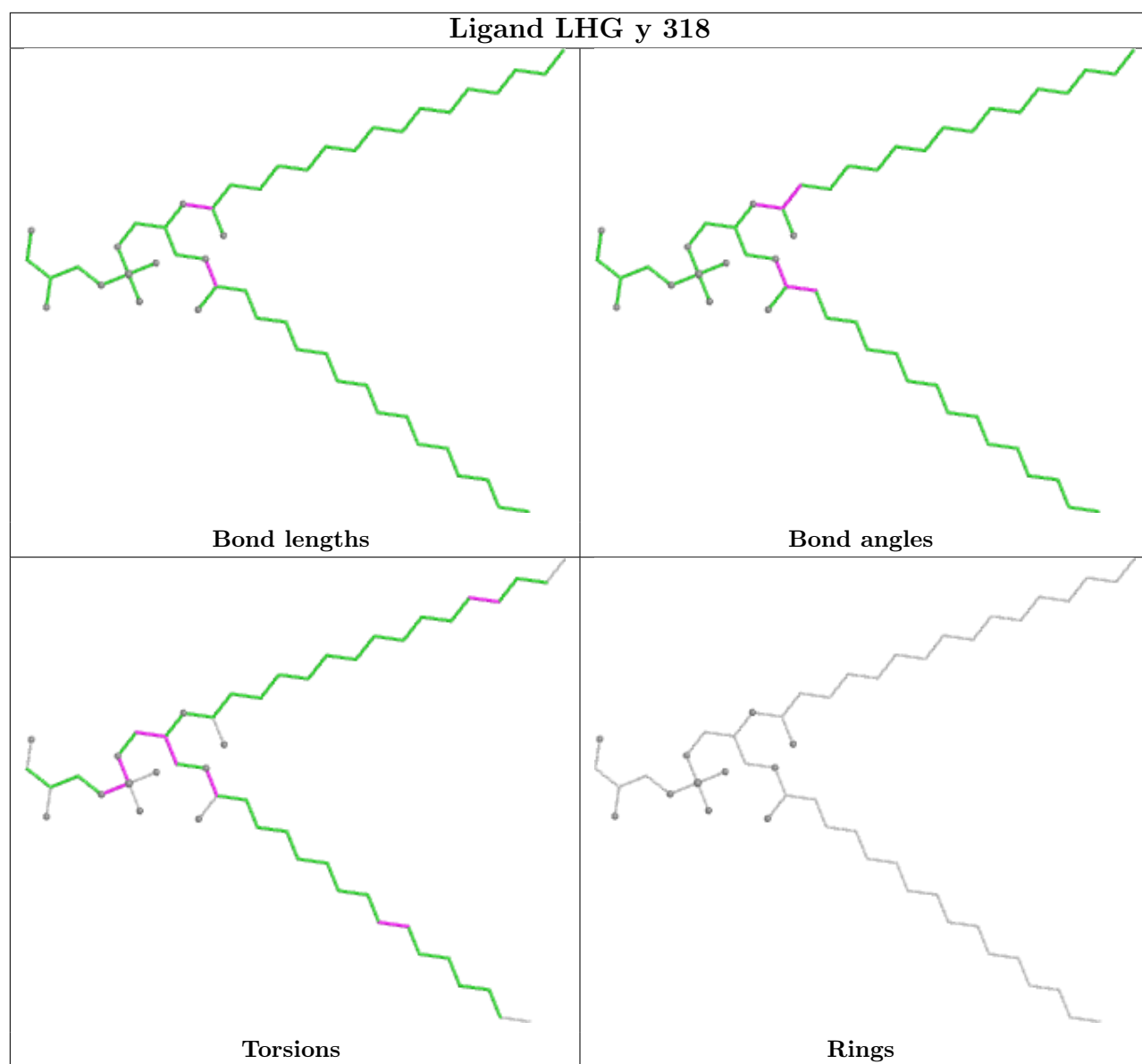


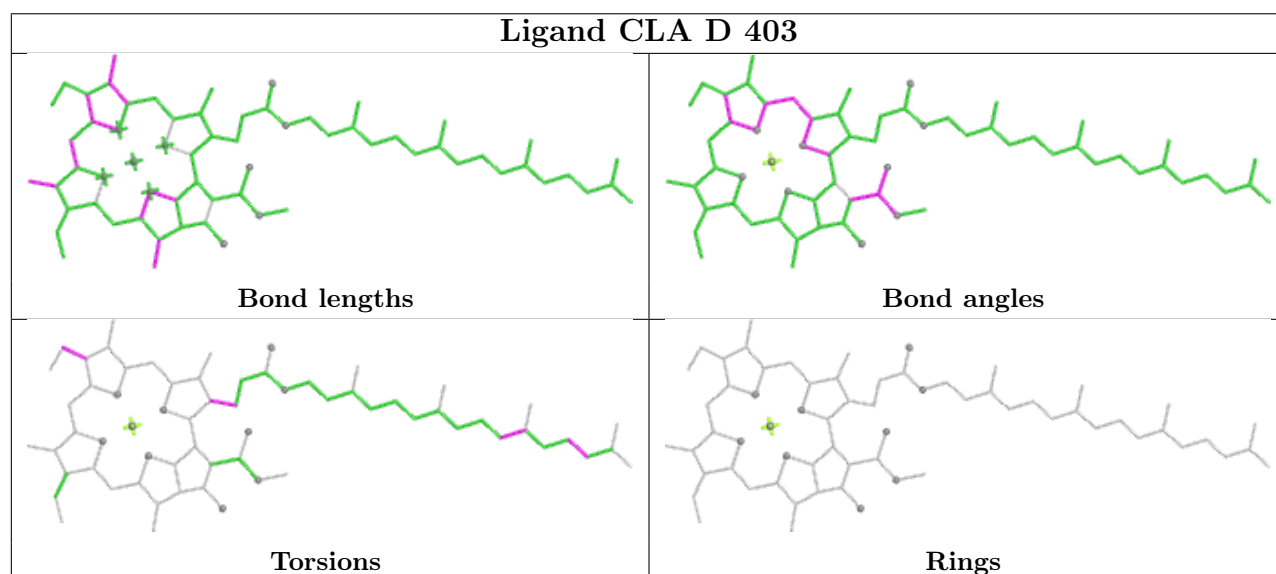
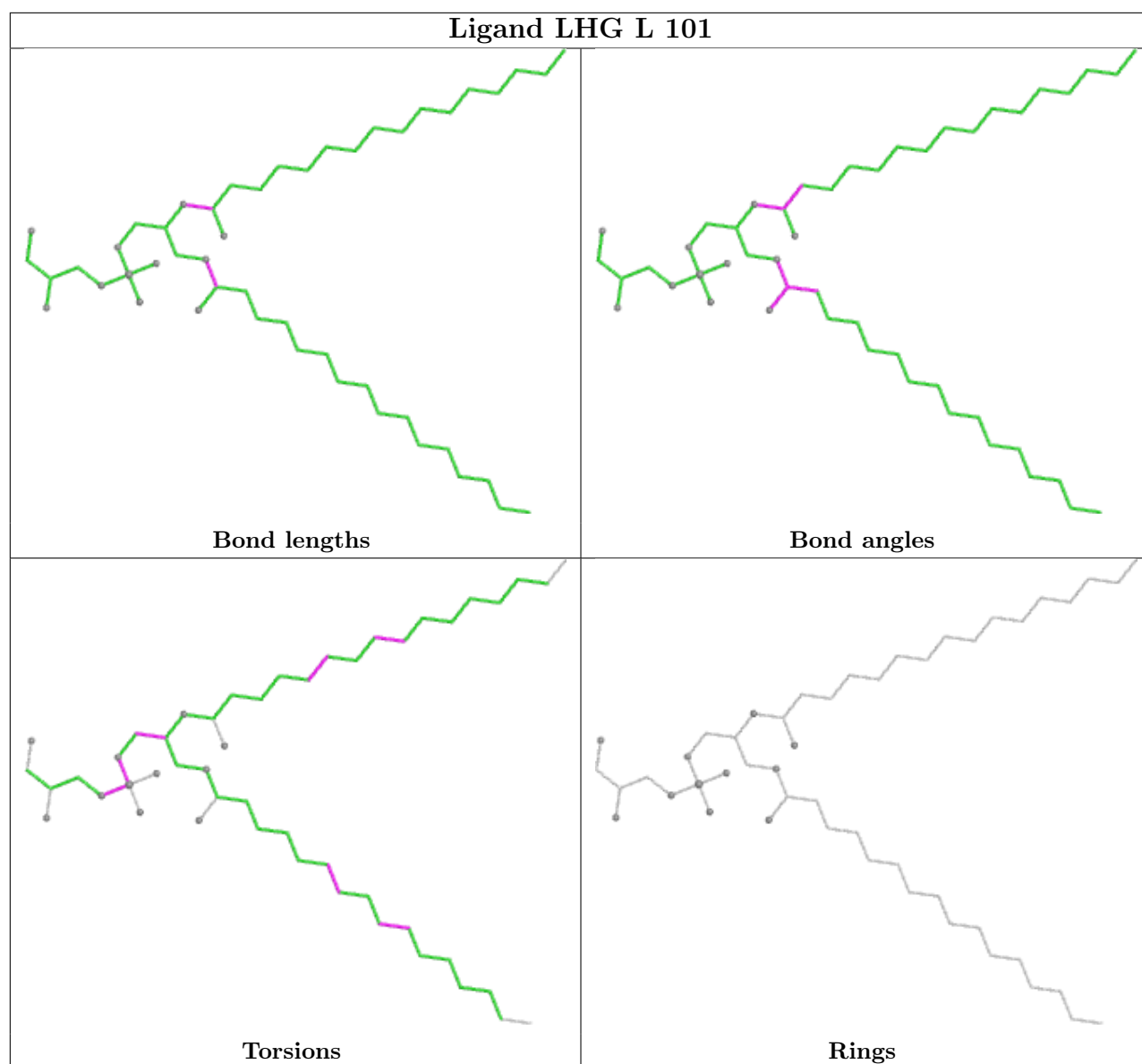


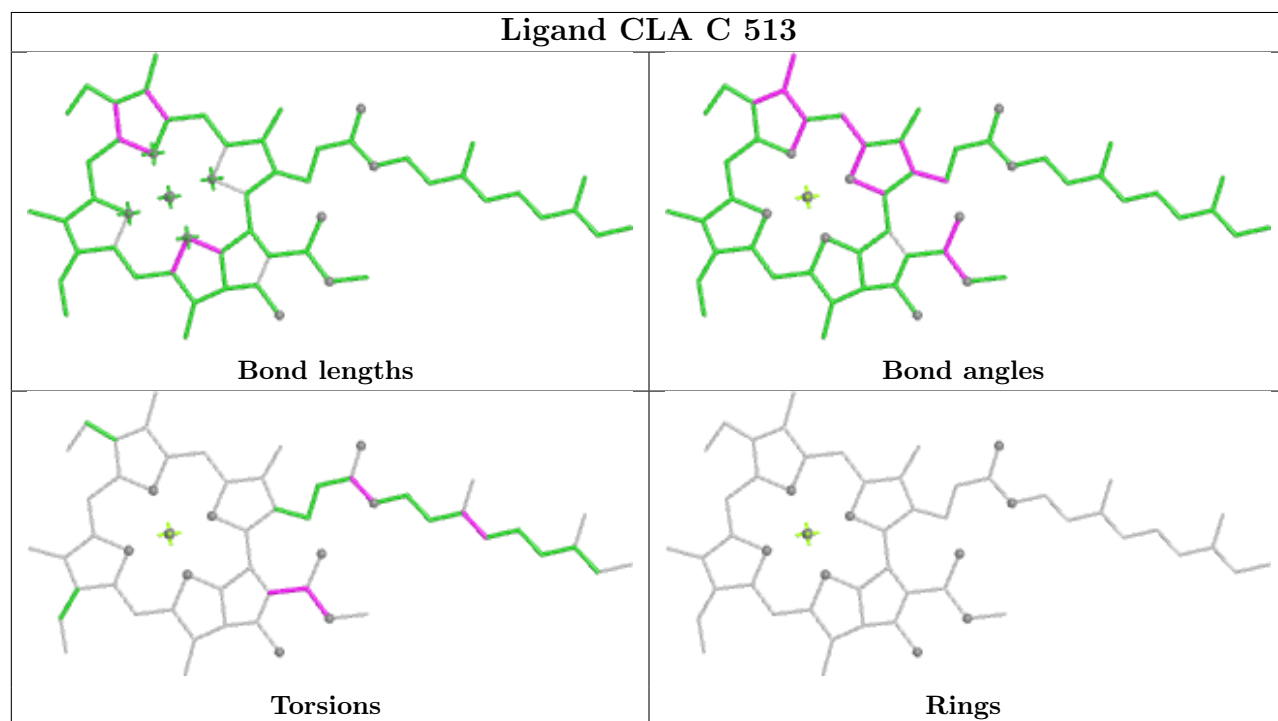
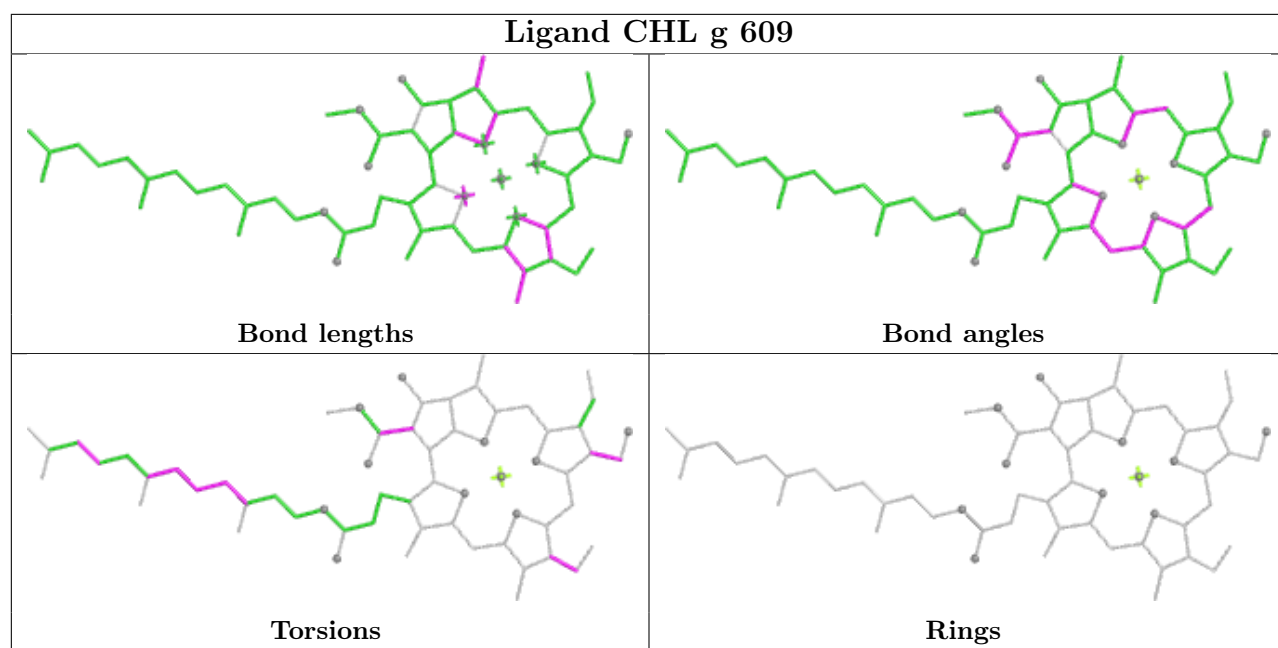


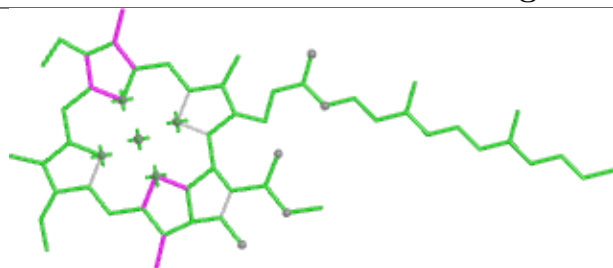
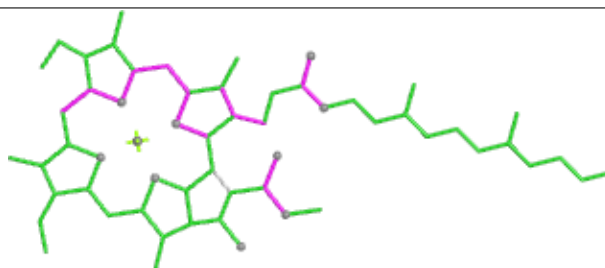
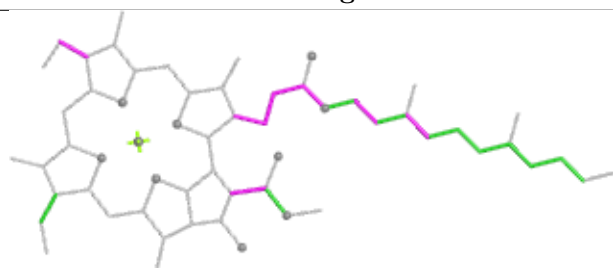
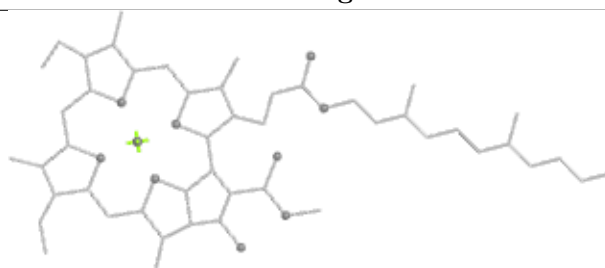
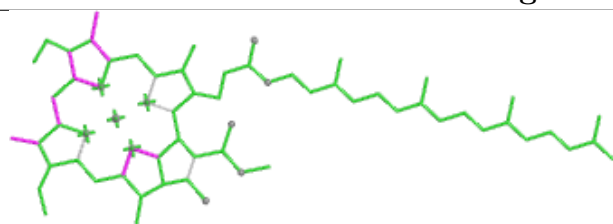
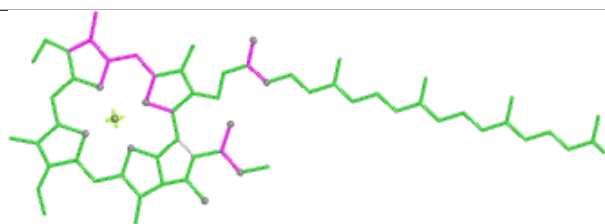
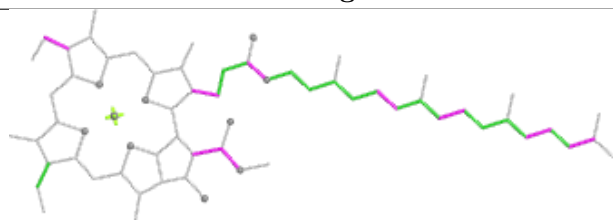
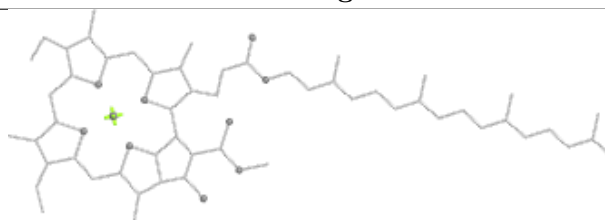
Ligand BCR b 621			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

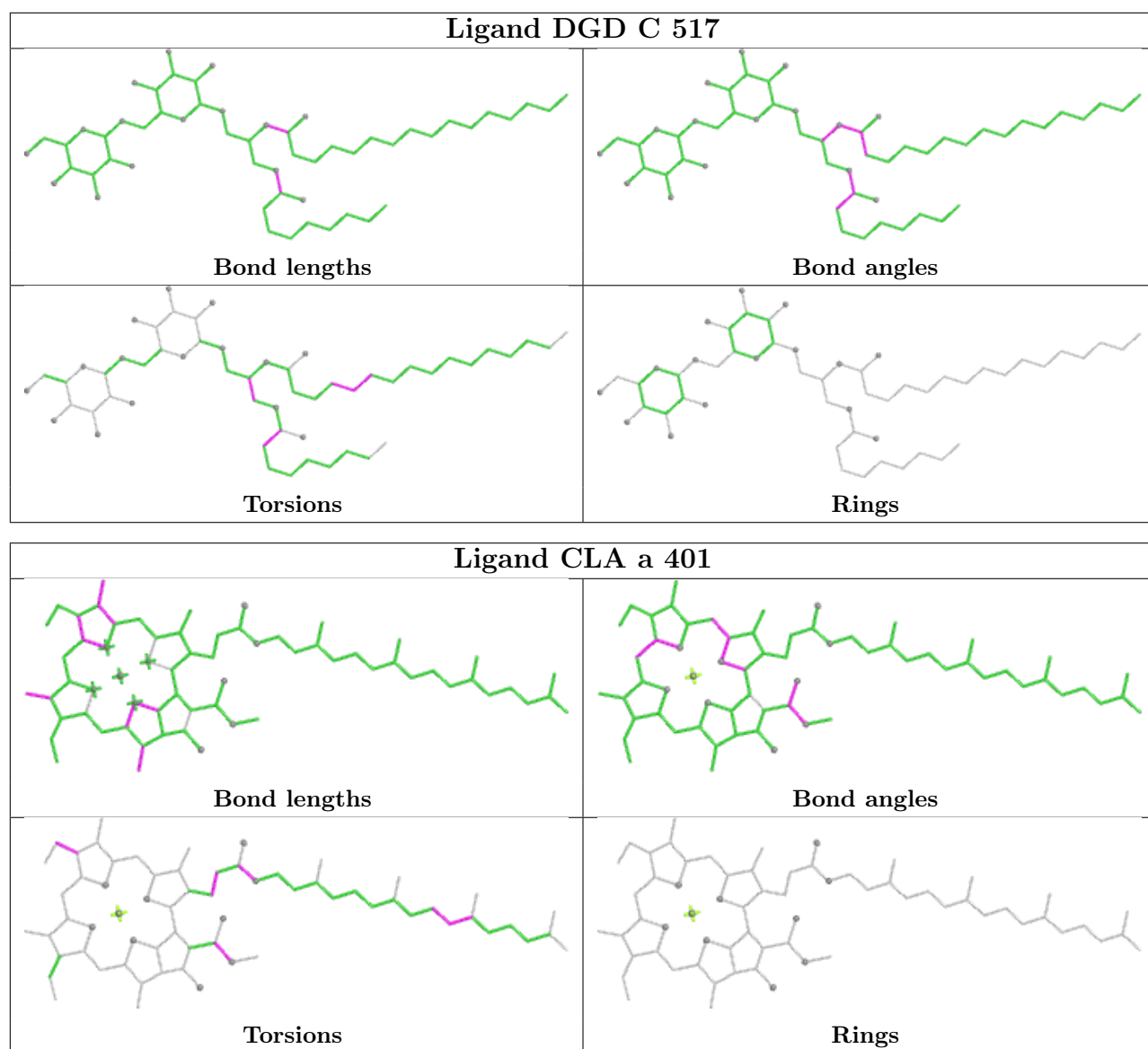
Ligand CLA b 617			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



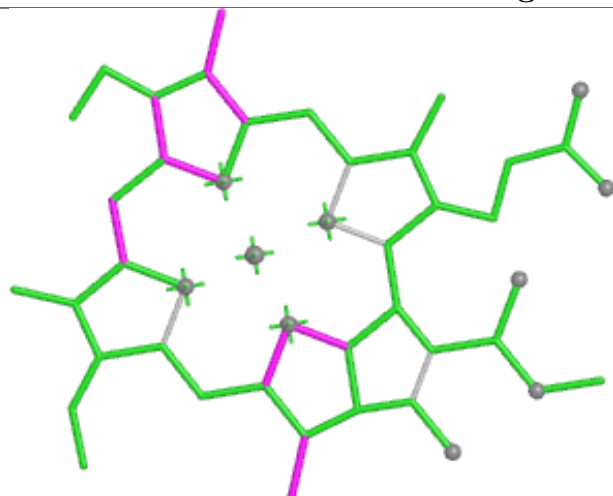




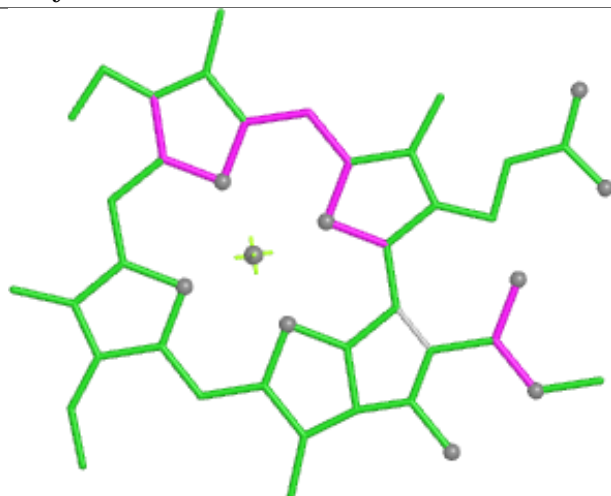
Ligand CLA c 505**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA c 508****Bond lengths****Bond angles****Torsions****Rings**



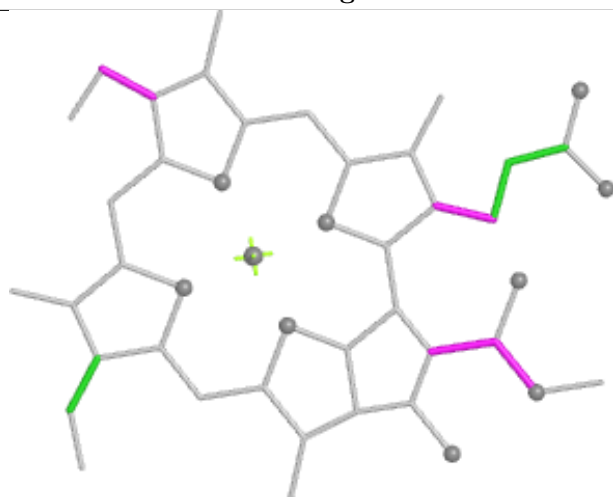
Ligand CLA y 315



Bond lengths



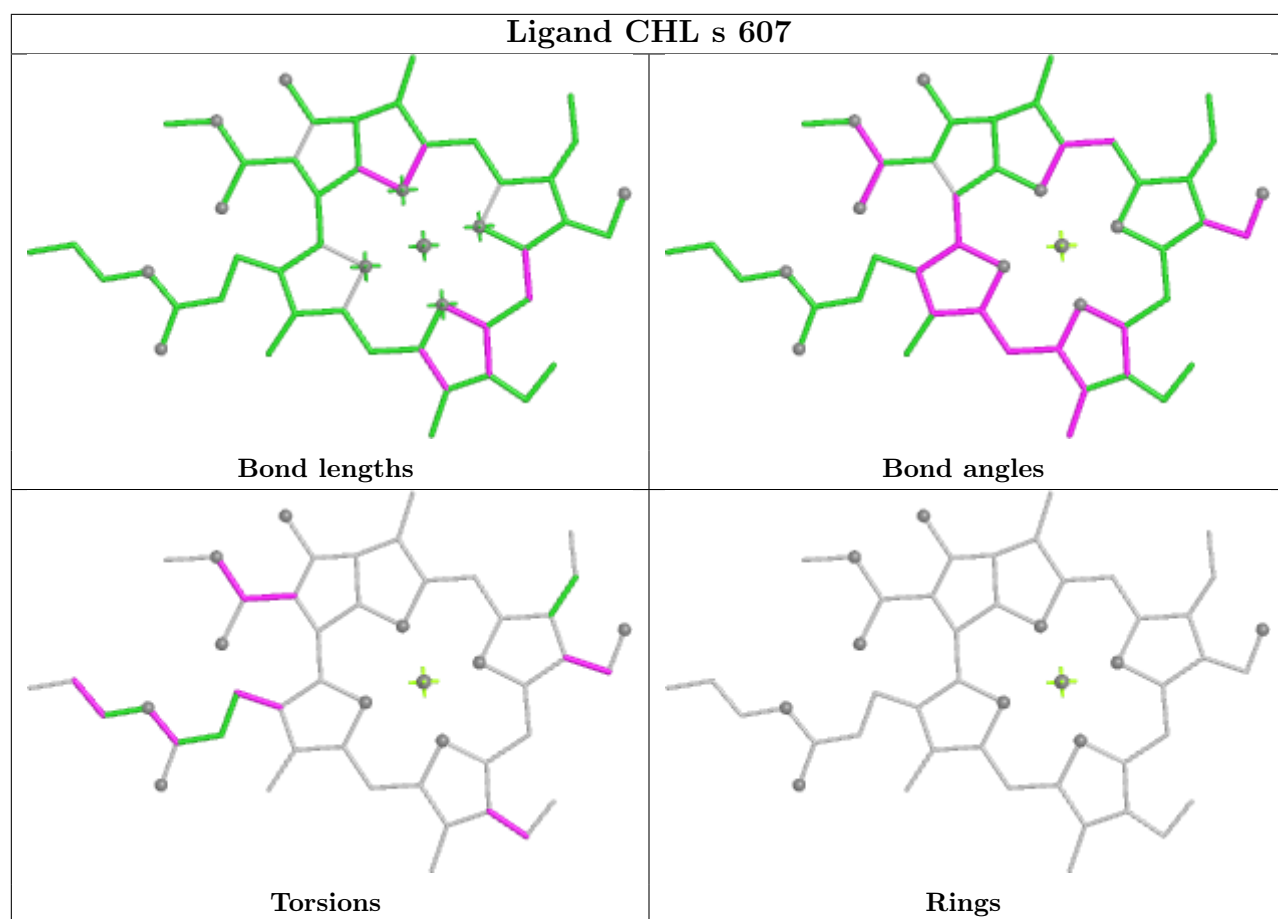
Bond angles

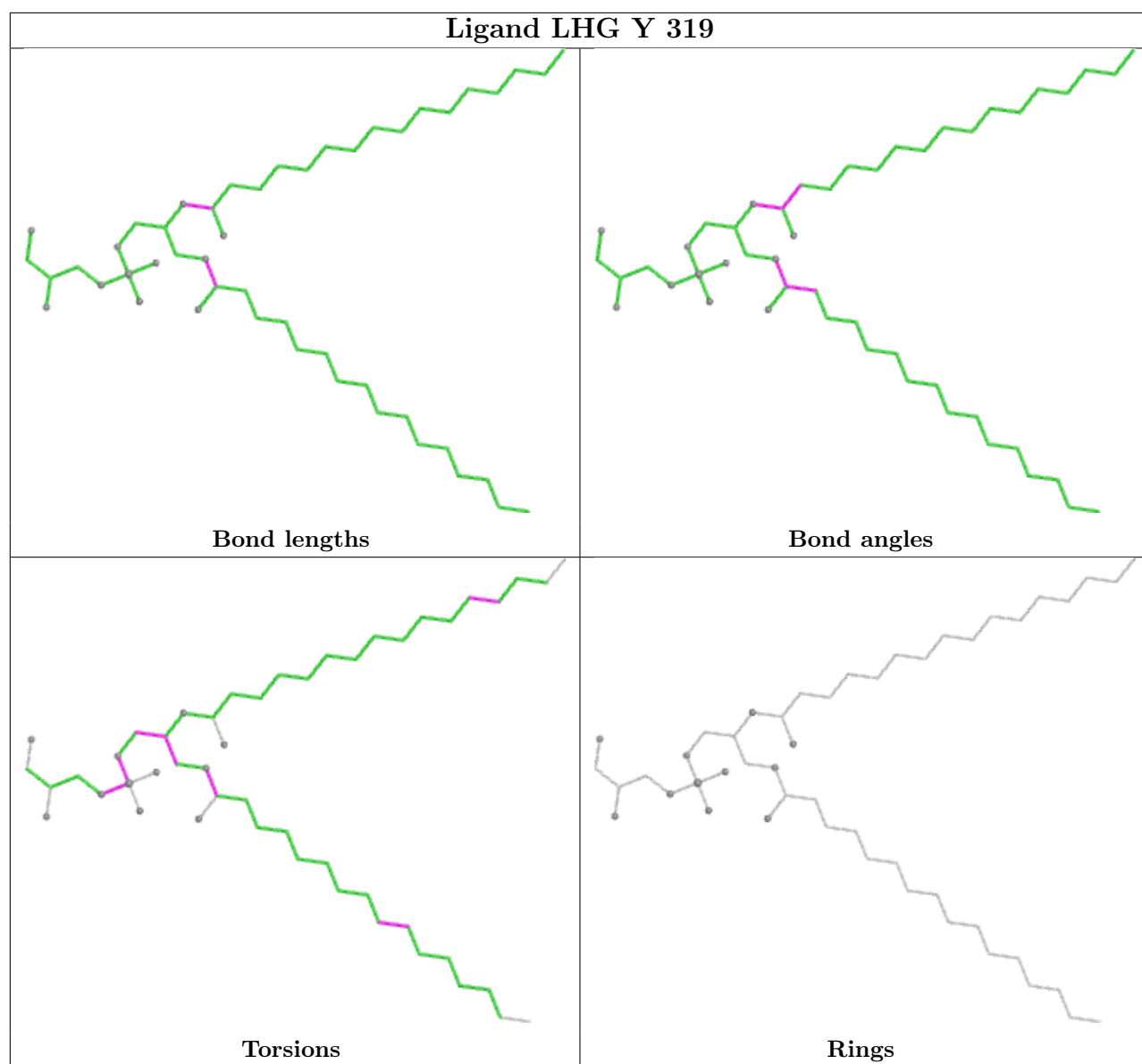


Torsions

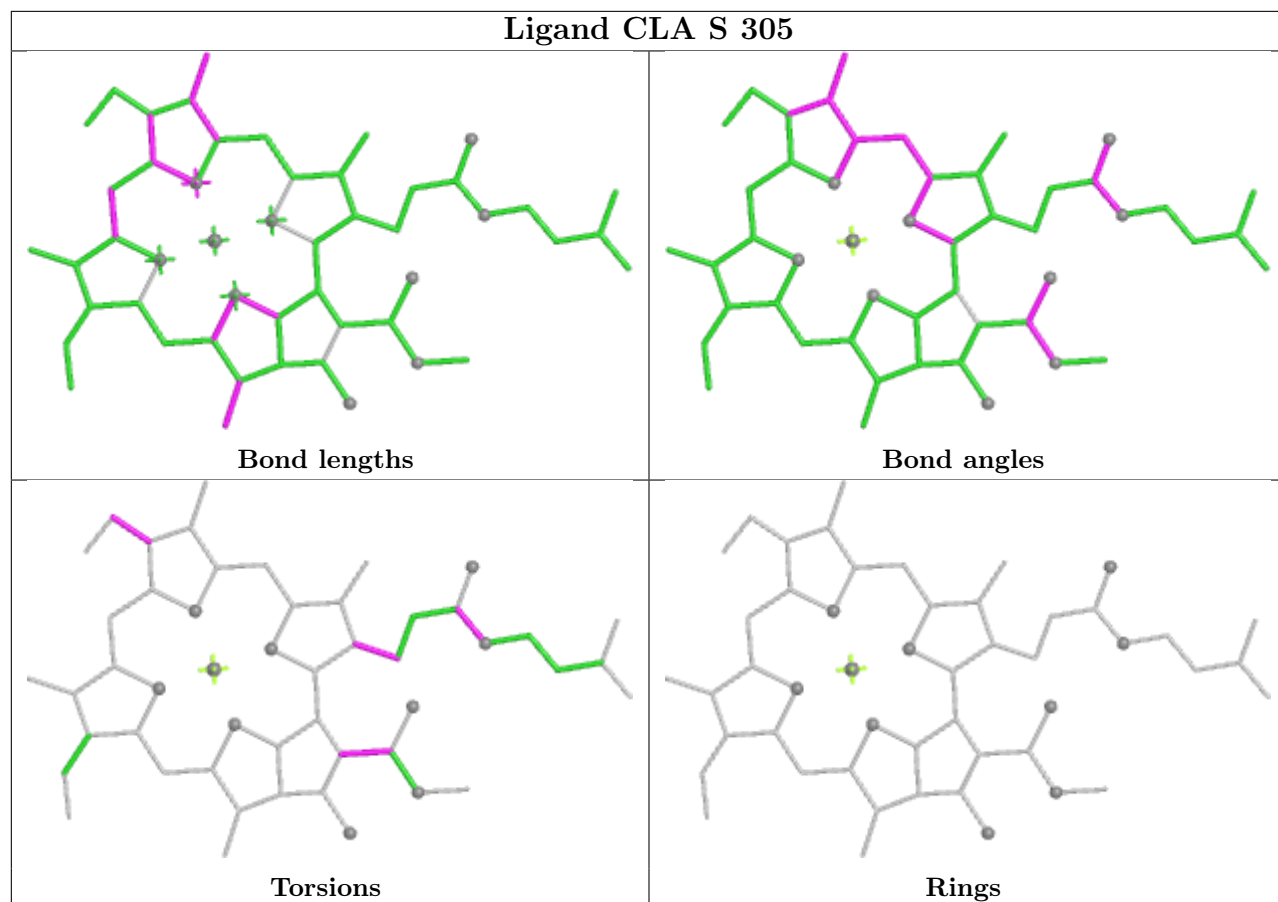


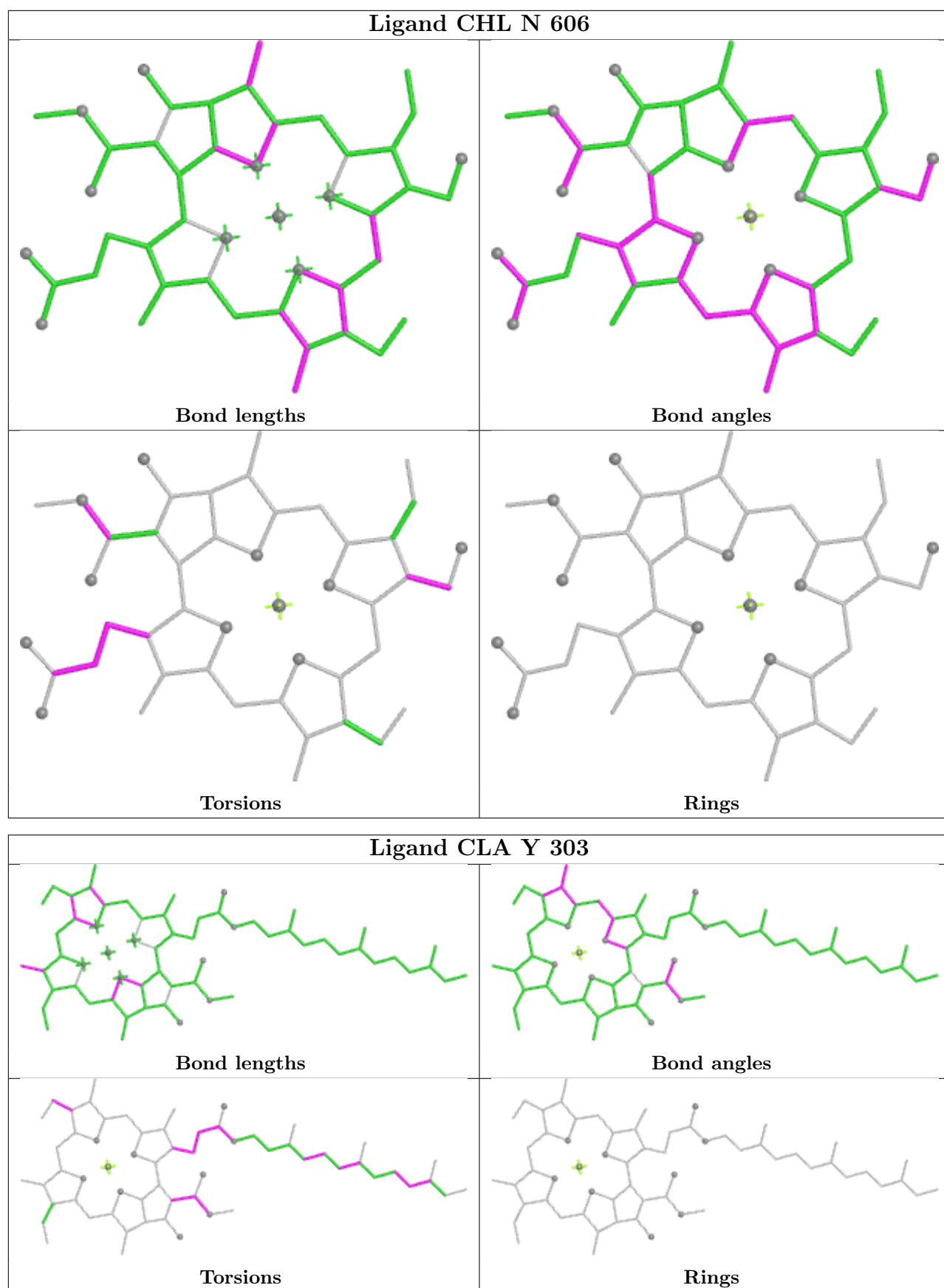
Rings

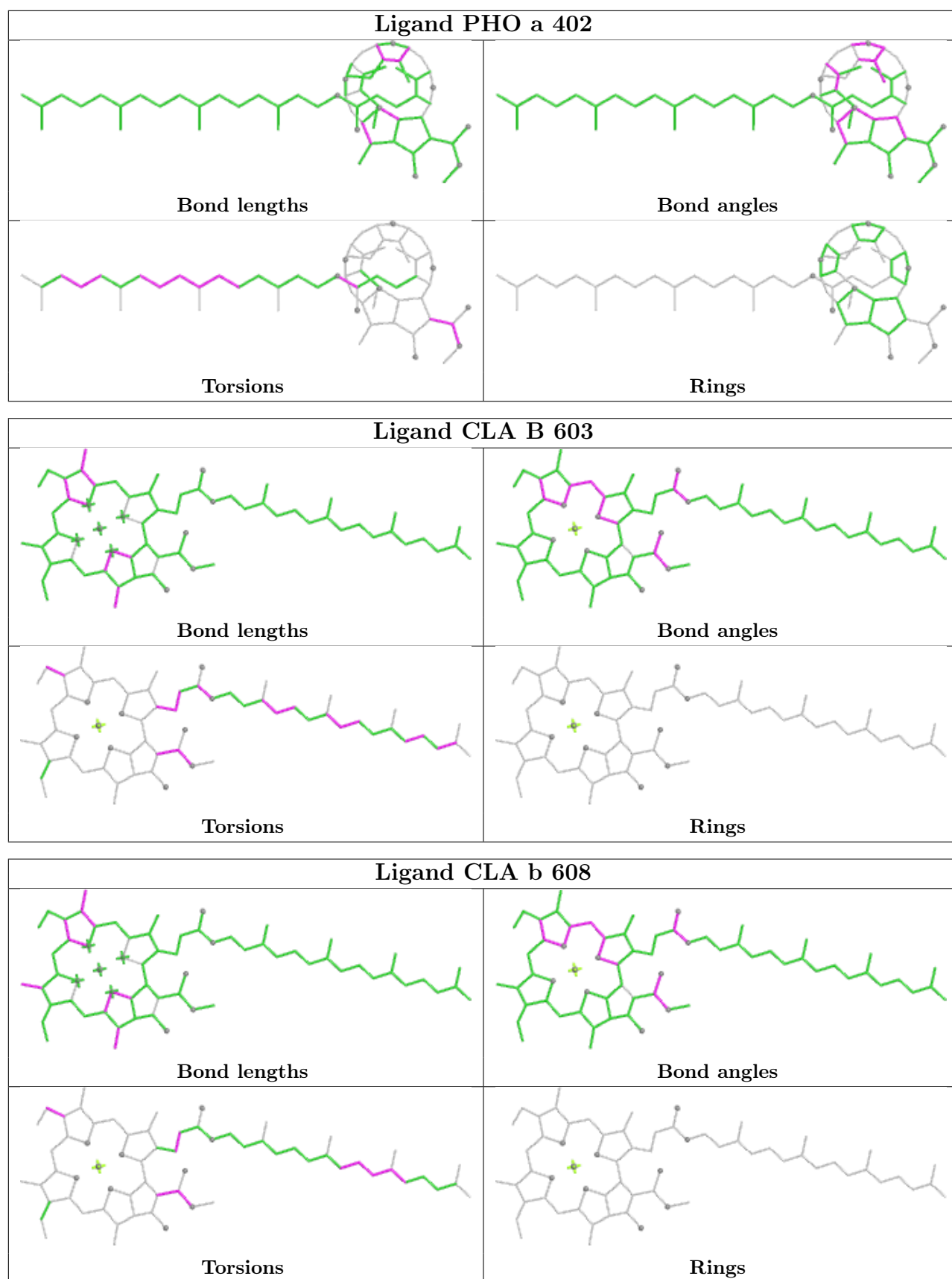




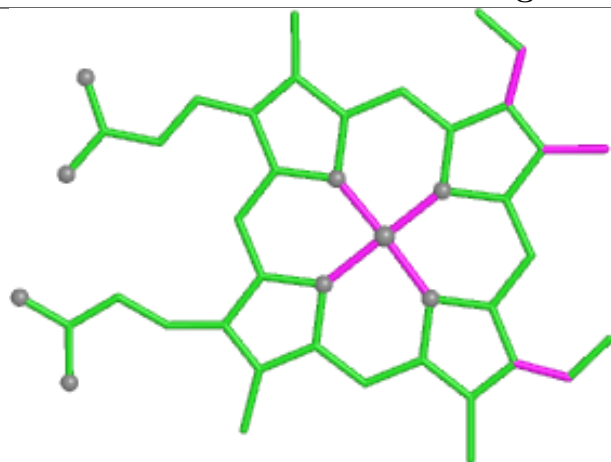
Ligand CLA S 305



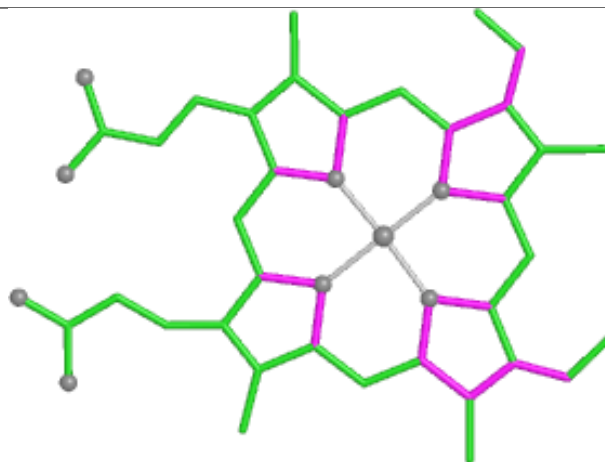




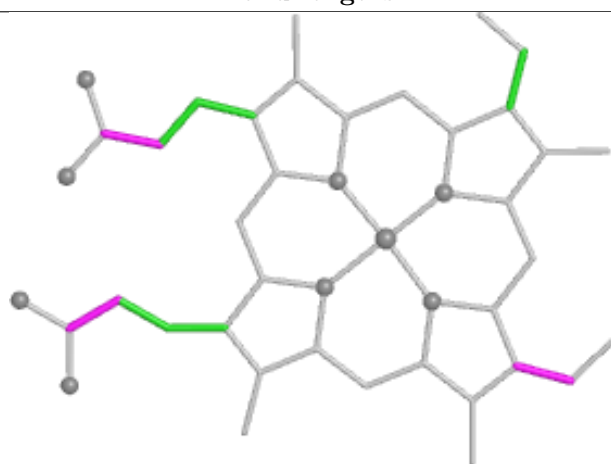
Ligand HEM f 101



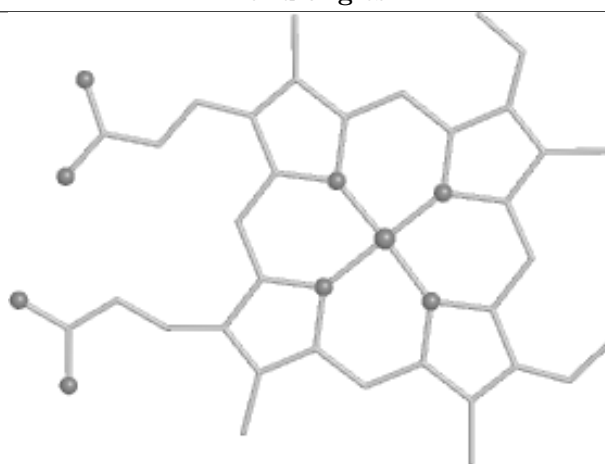
Bond lengths



Bond angles

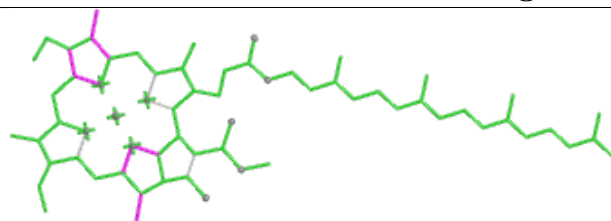


Torsions

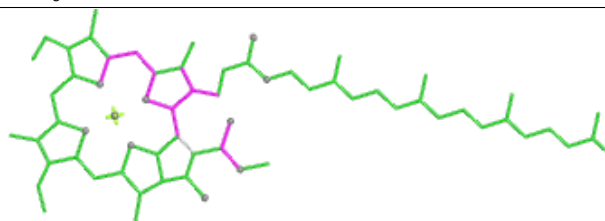


Rings

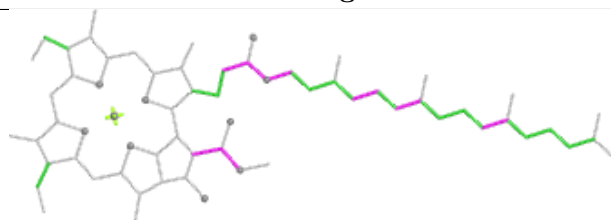
Ligand CLA y 304



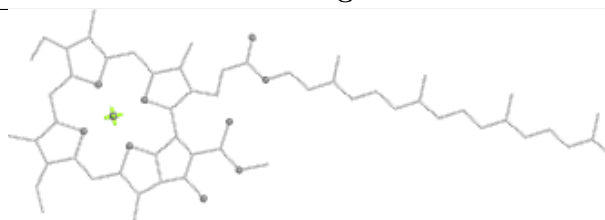
Bond lengths



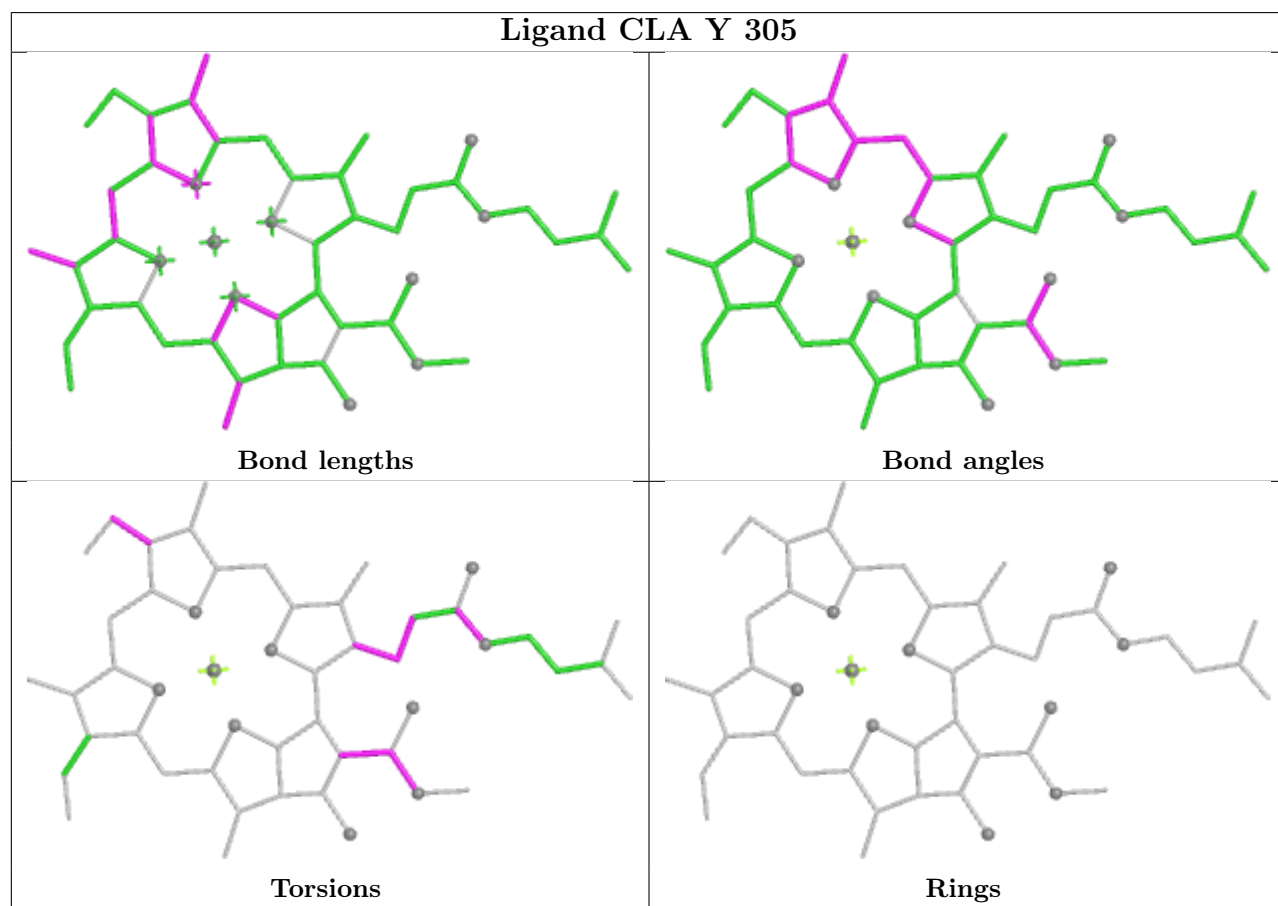
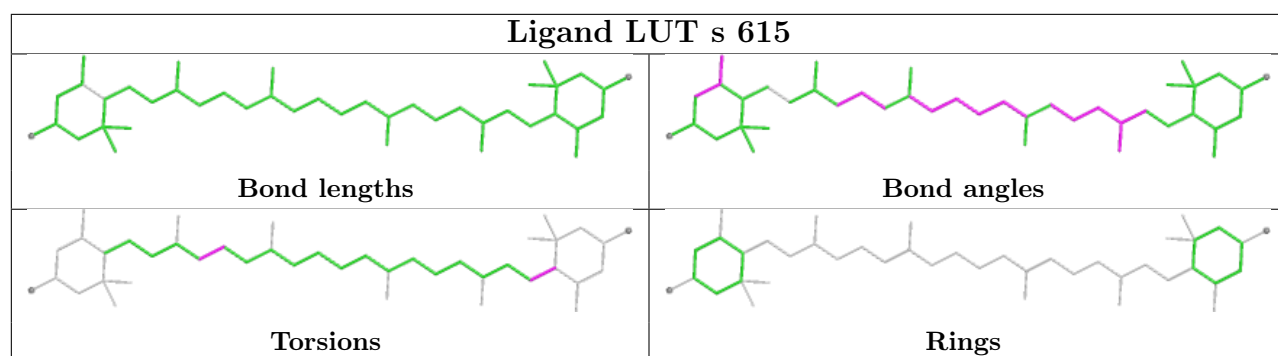
Bond angles



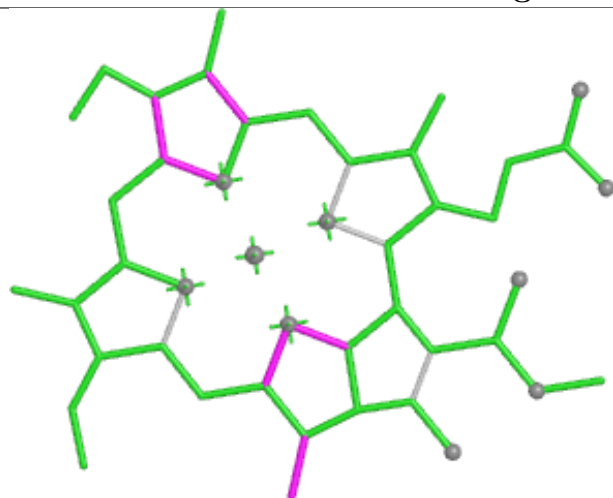
Torsions



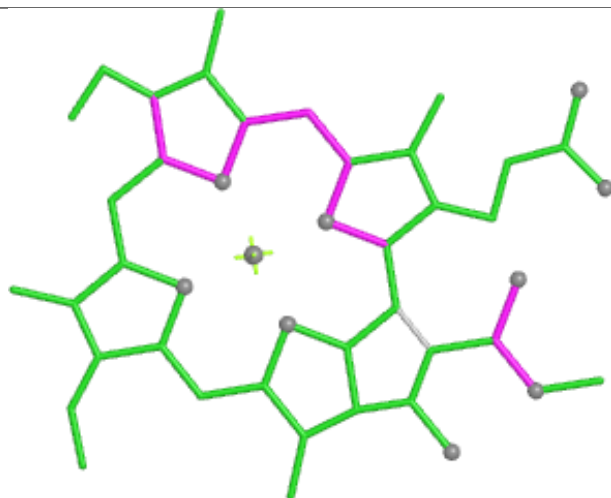
Rings



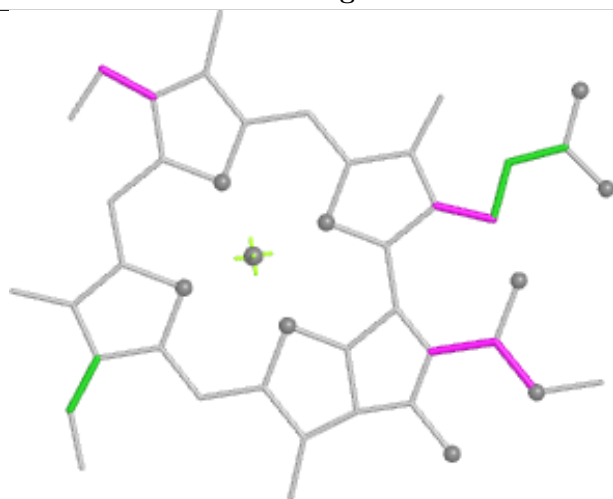
Ligand CLA Y 315



Bond lengths



Bond angles

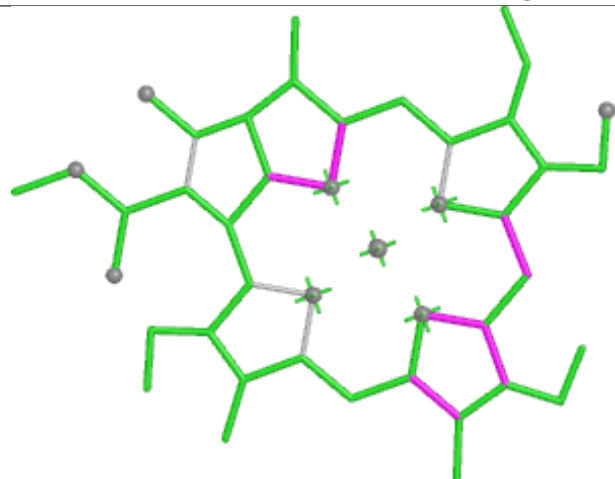


Torsions

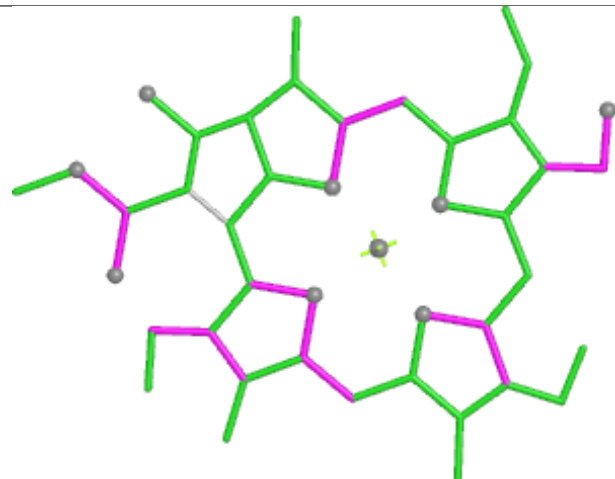


Rings

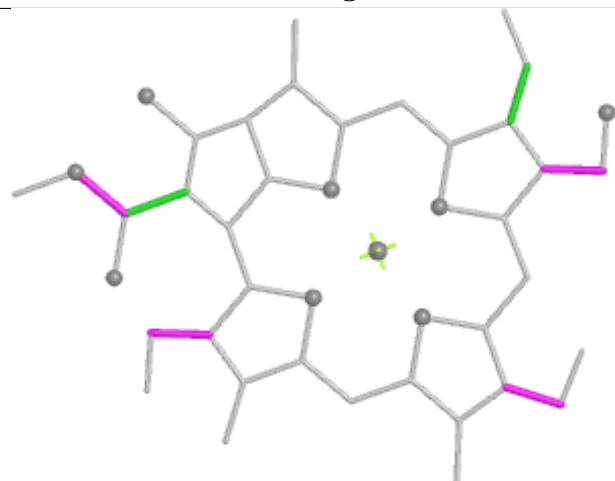
Ligand CHL S 307



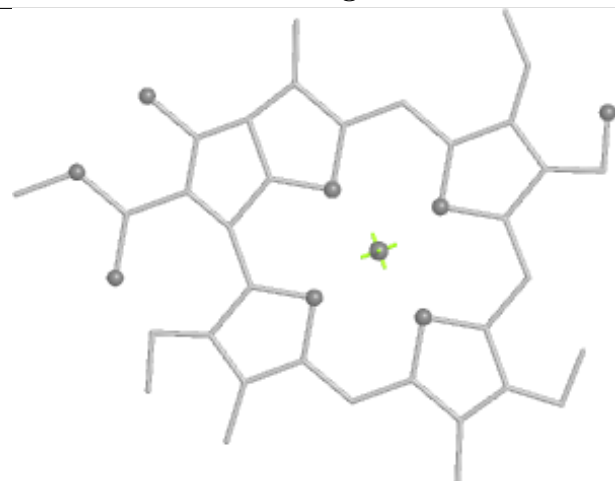
Bond lengths



Bond angles

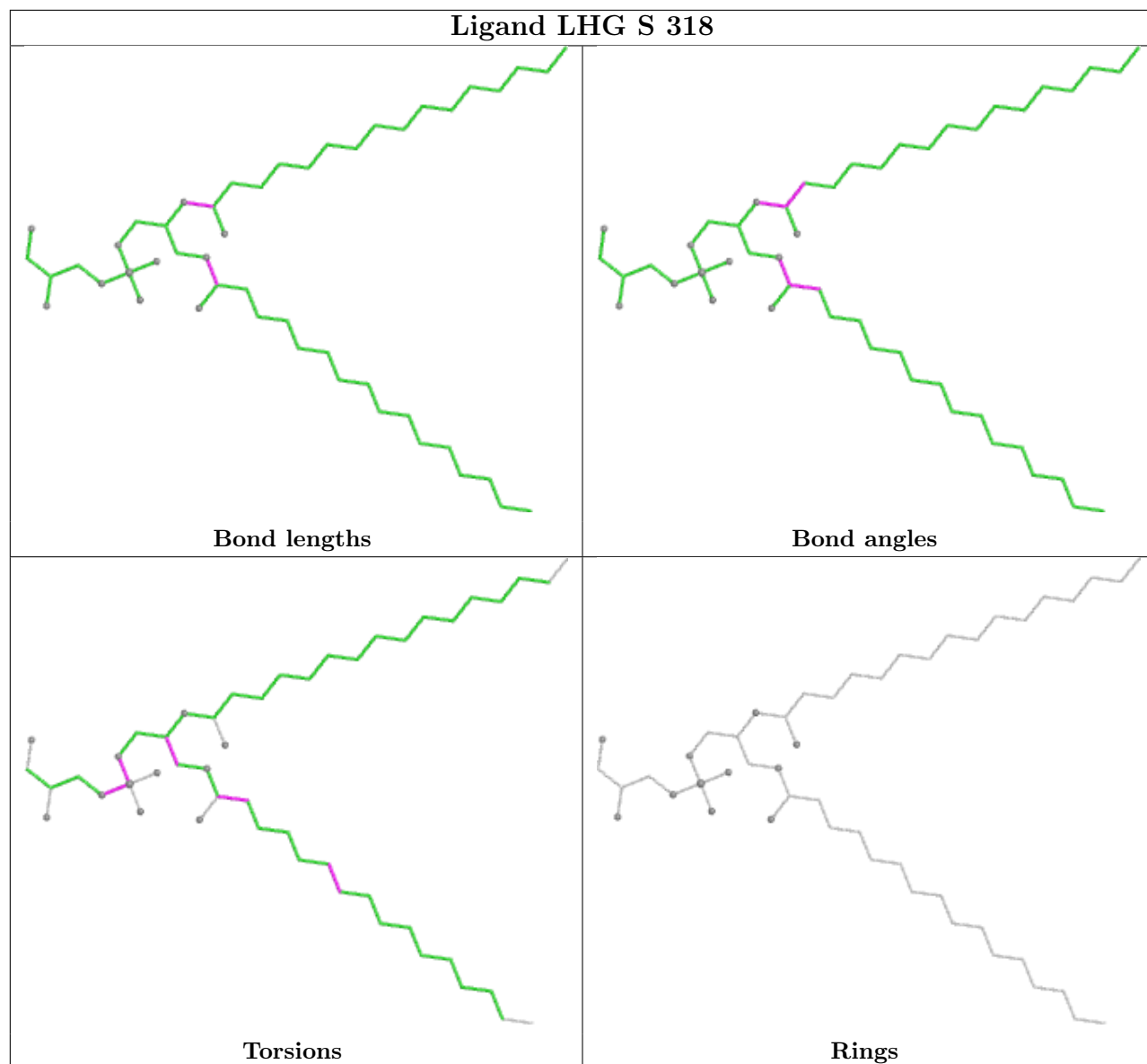


Torsions

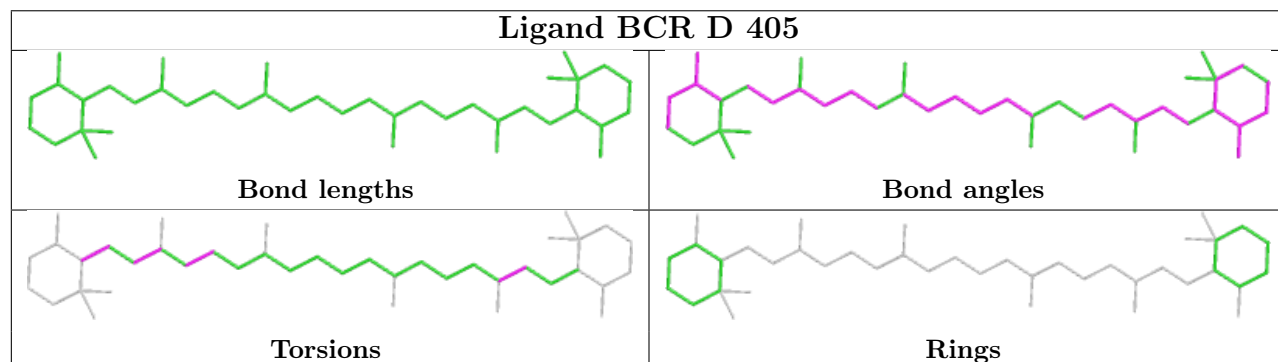


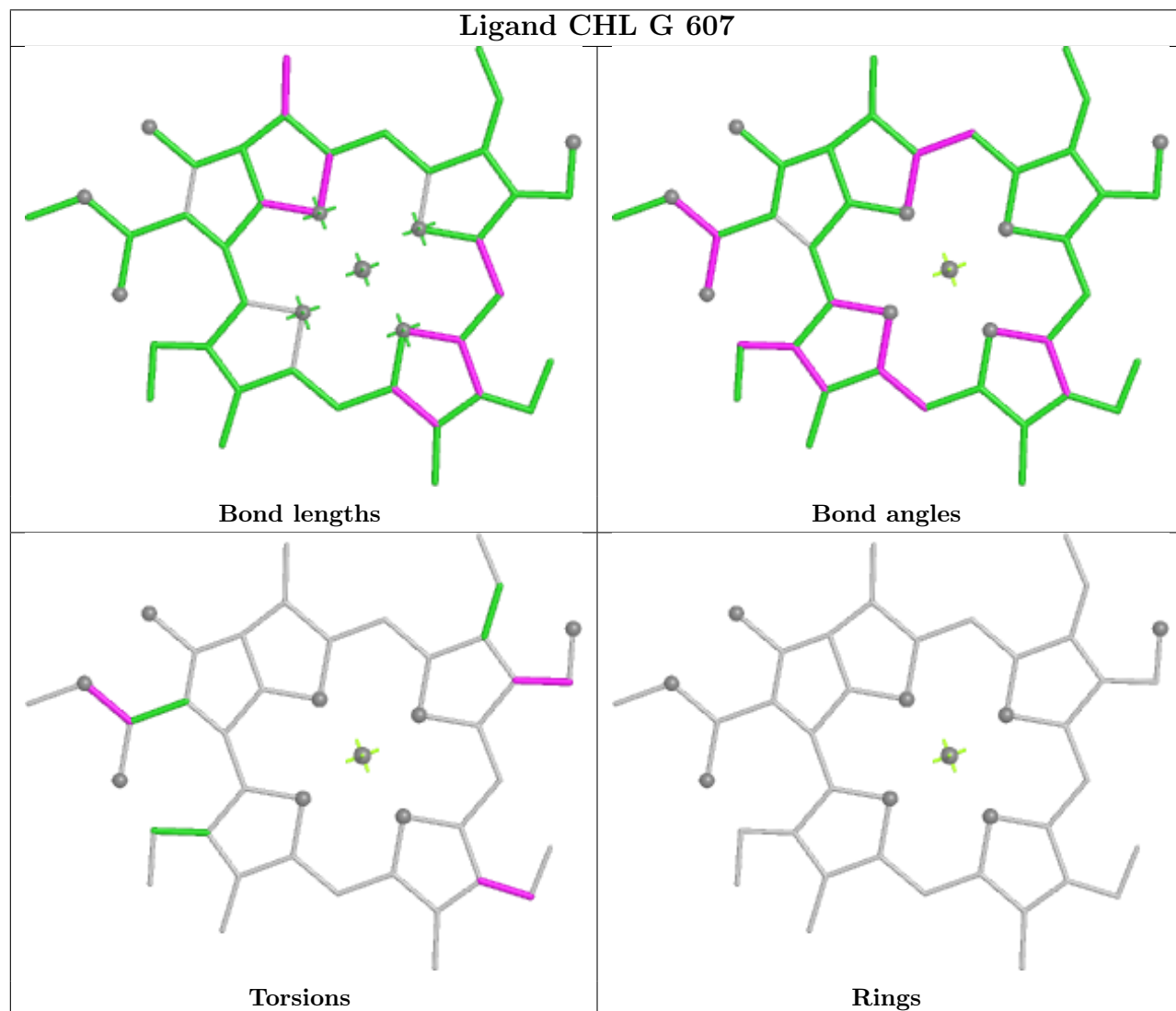
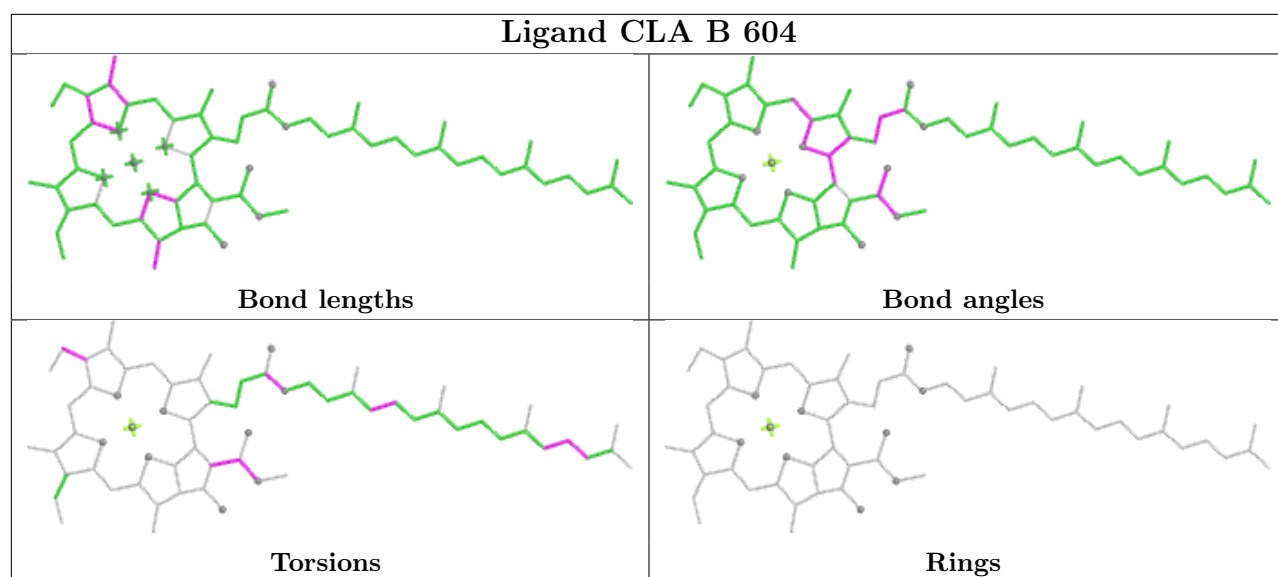
Rings

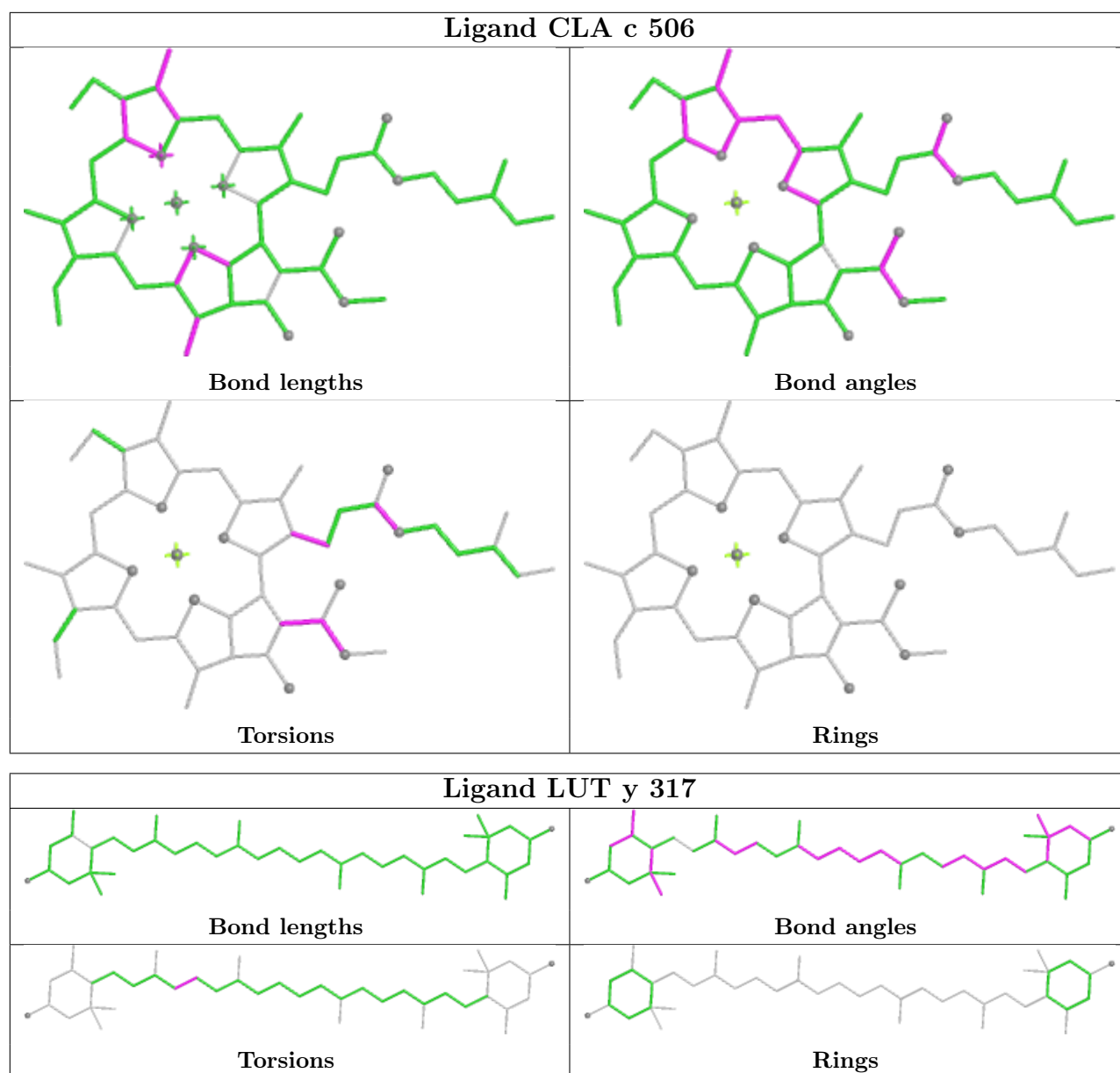
Ligand LHG S 318



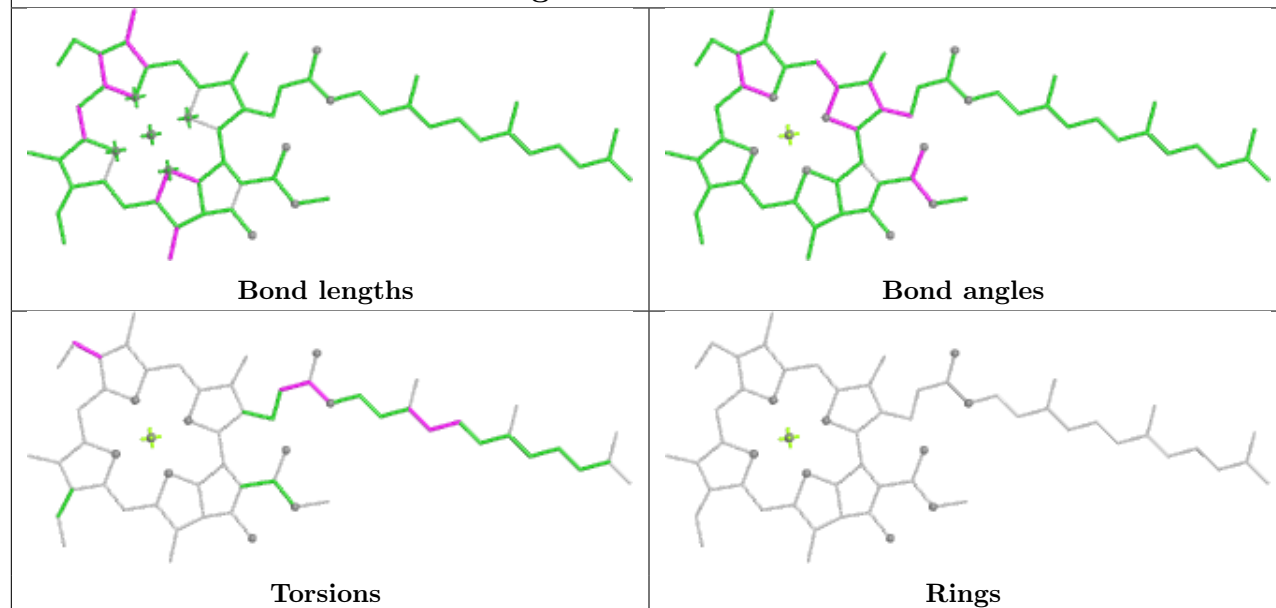
Ligand BCR D 405



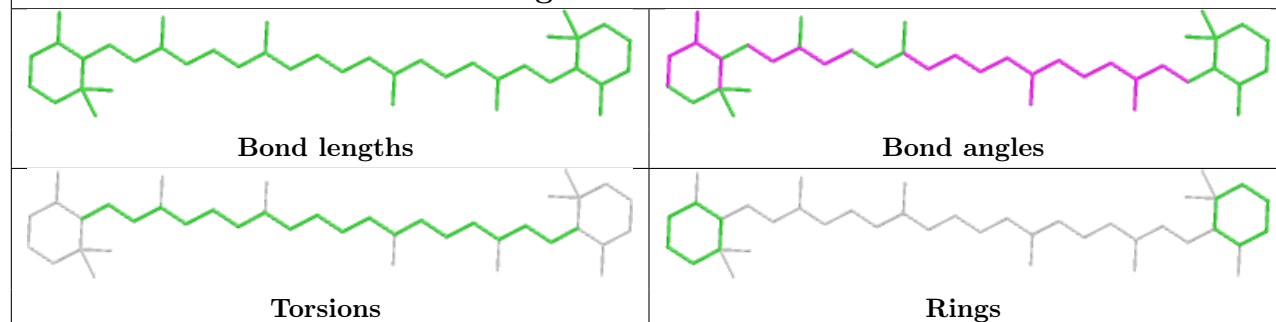




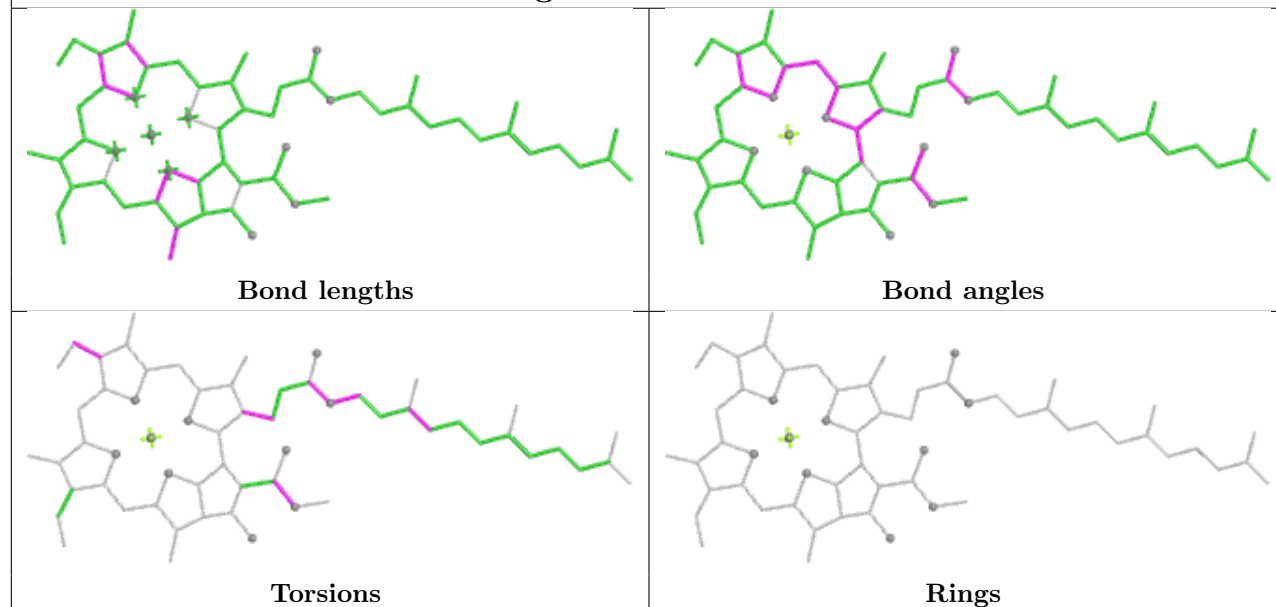
Ligand CLA R 304

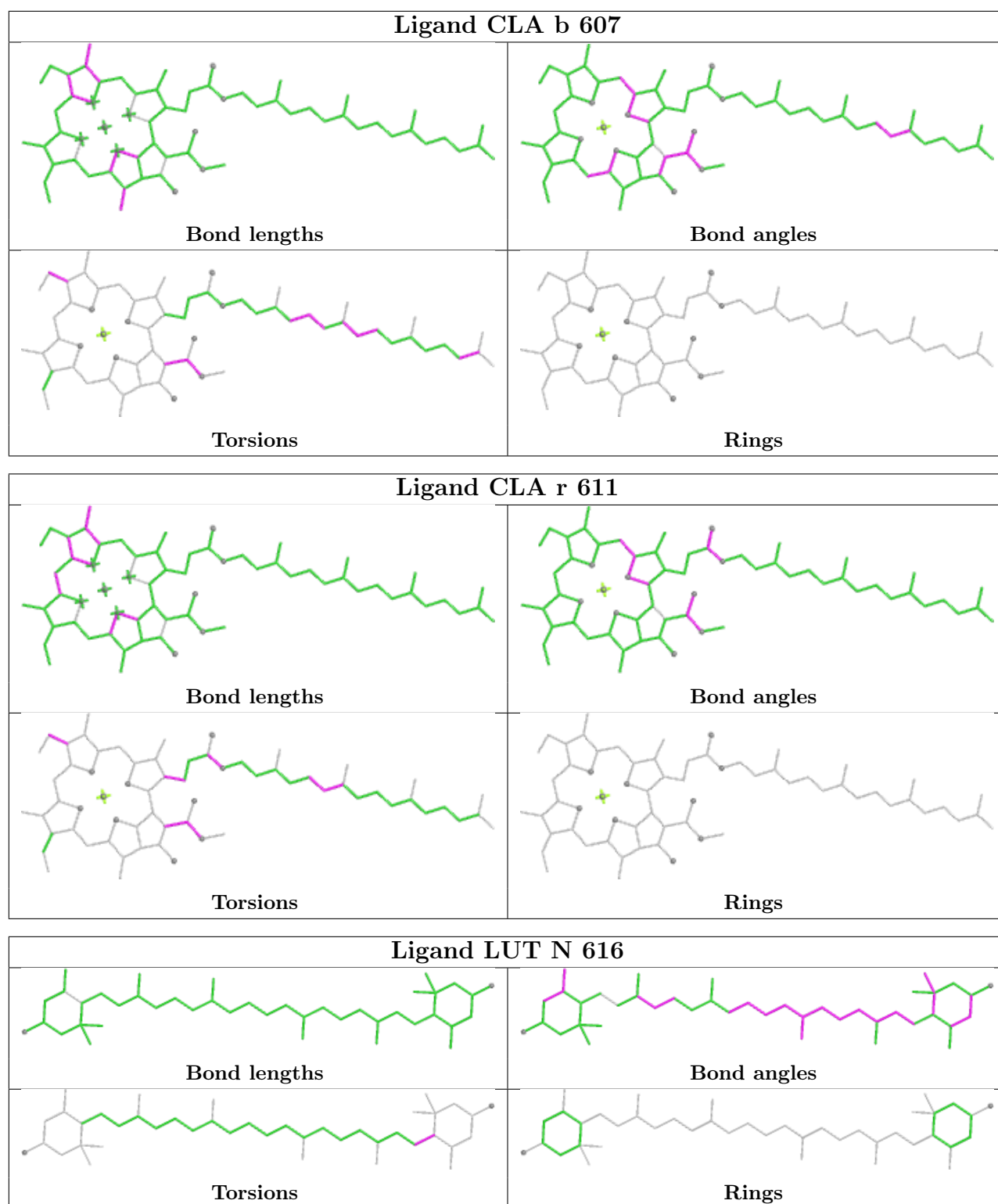


Ligand BCR c 514

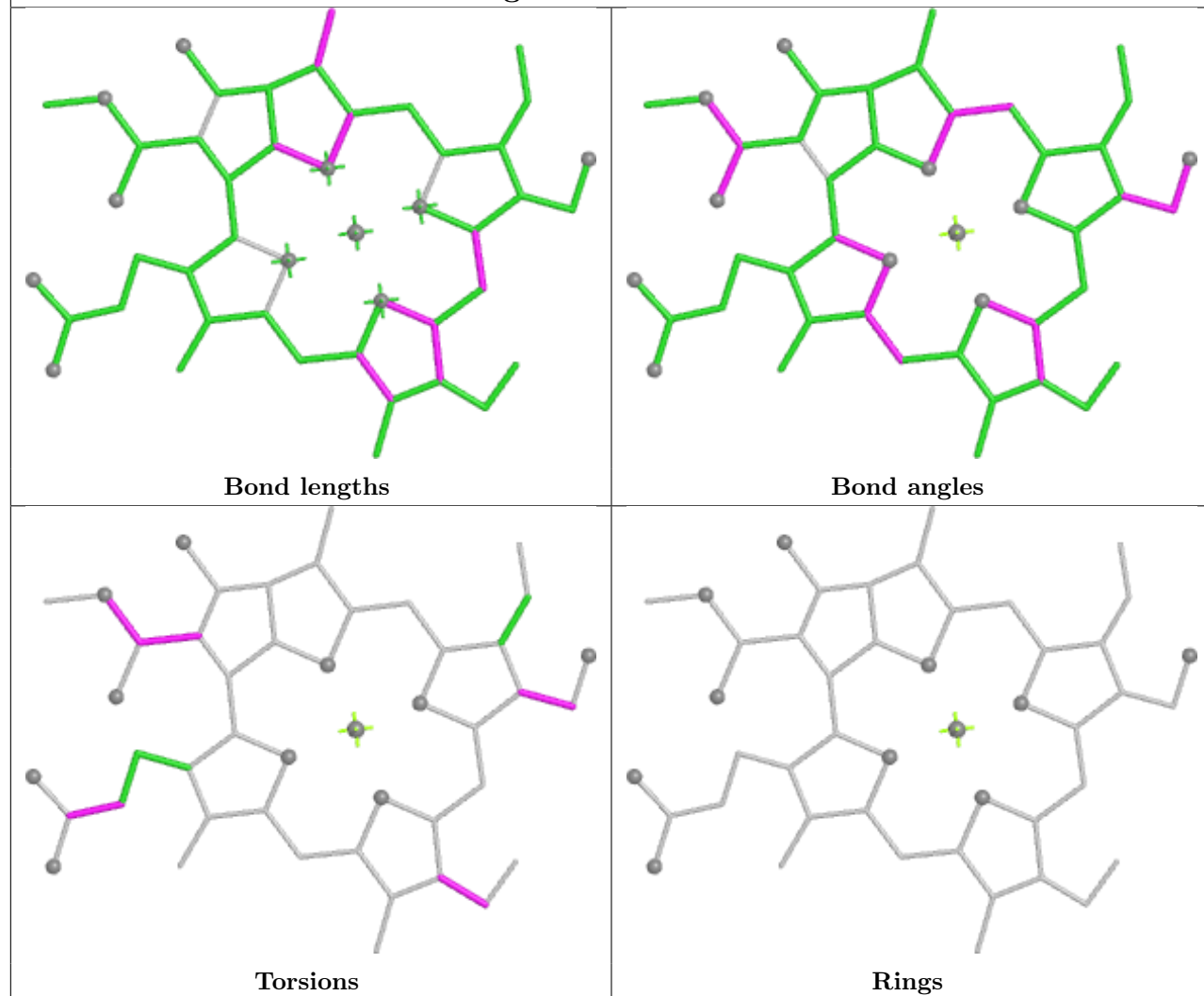


Ligand CLA n 611

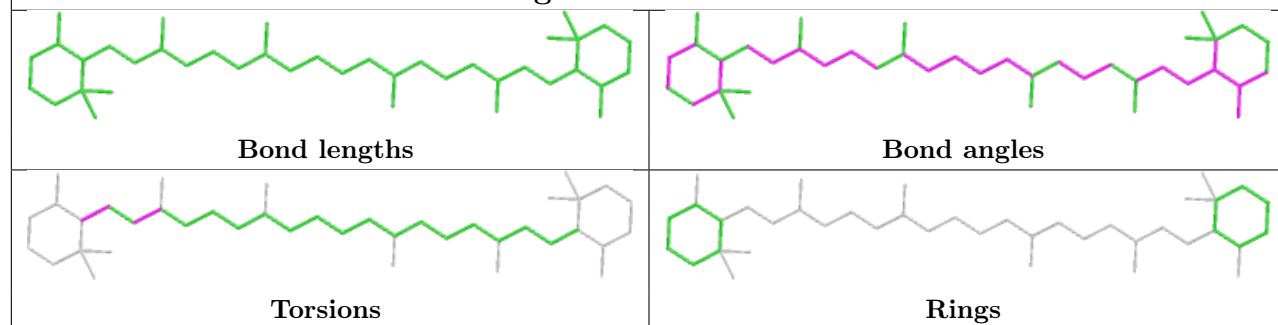


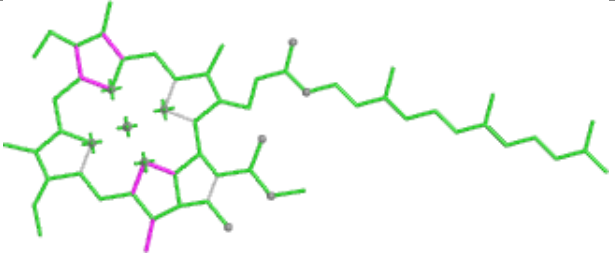
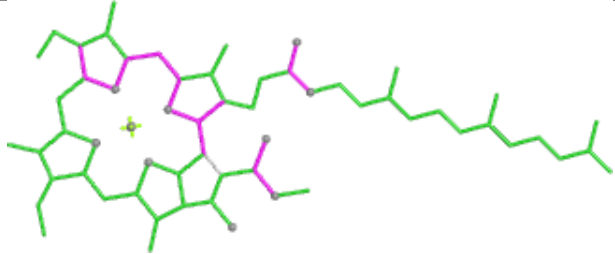
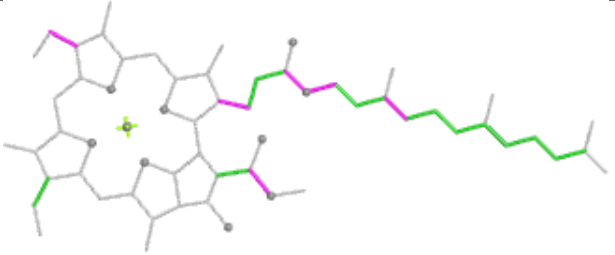
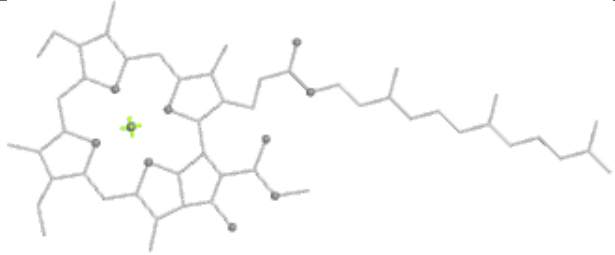
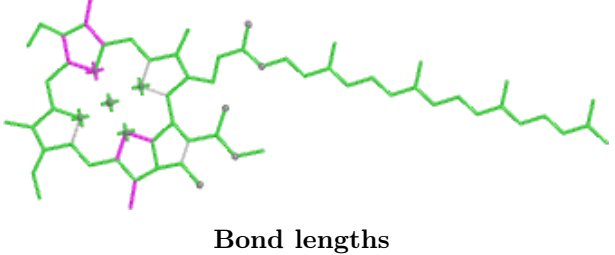
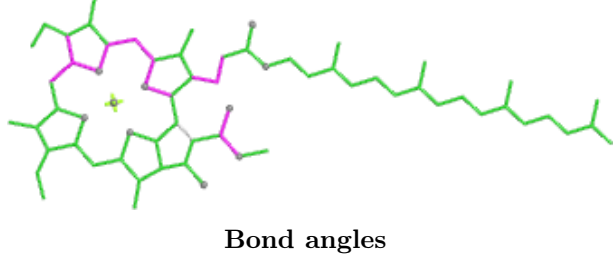
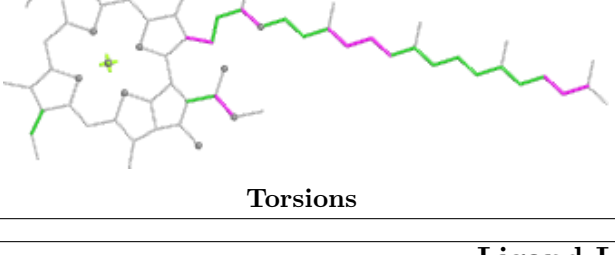
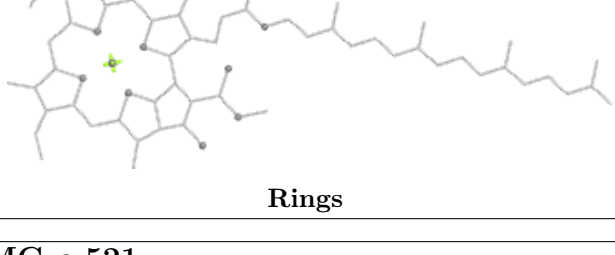
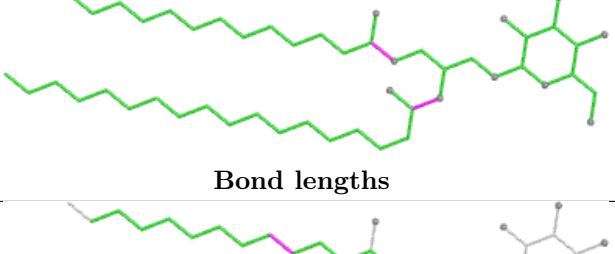
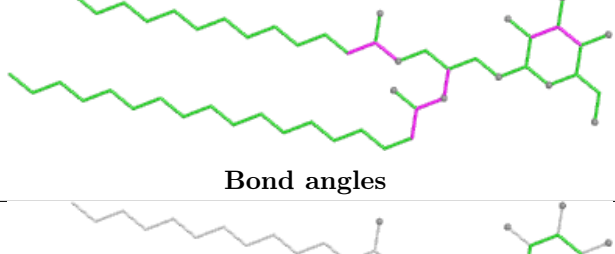
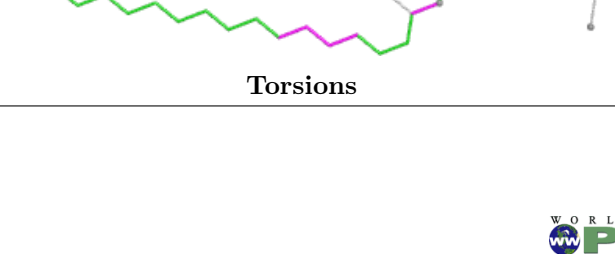


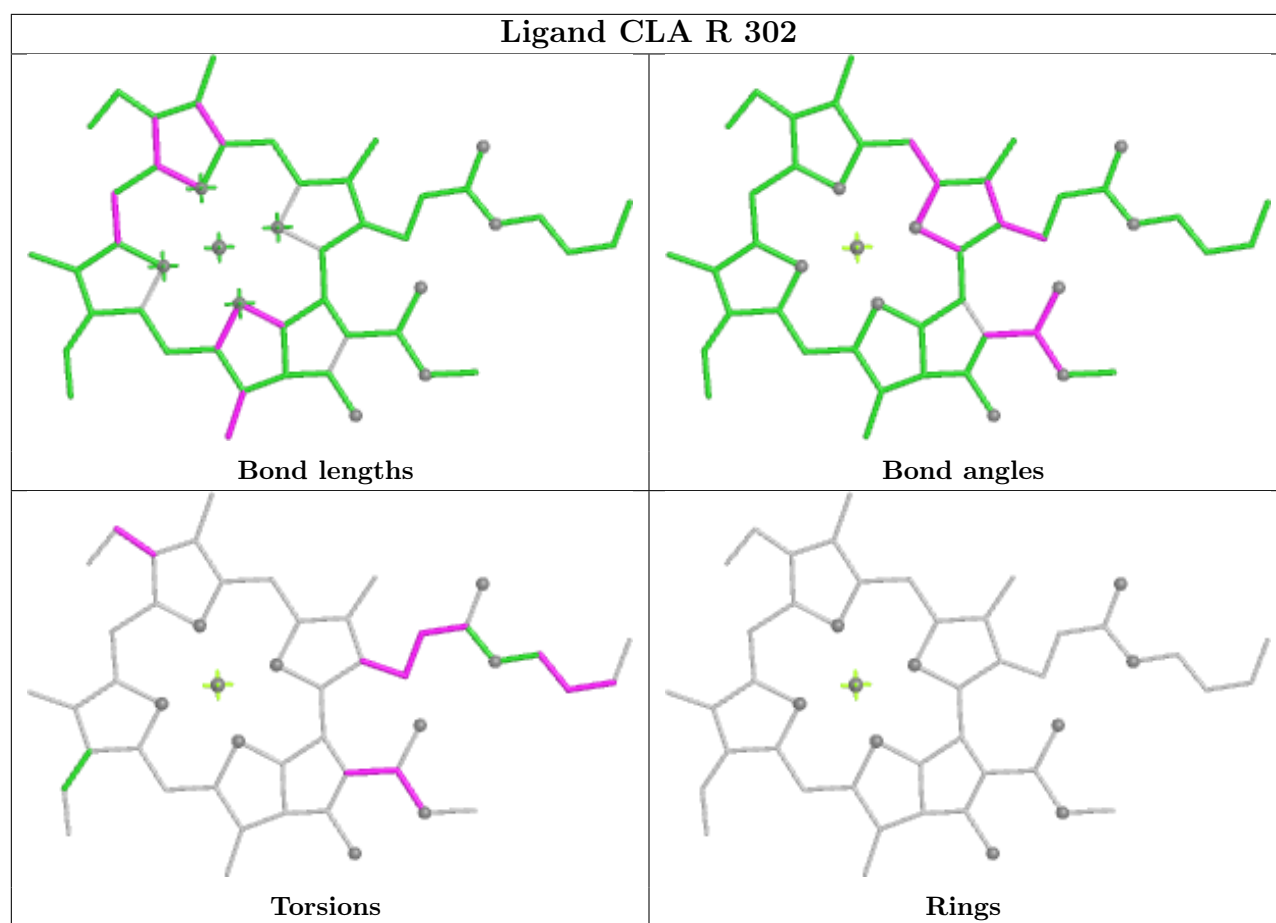
Ligand CHL S 302

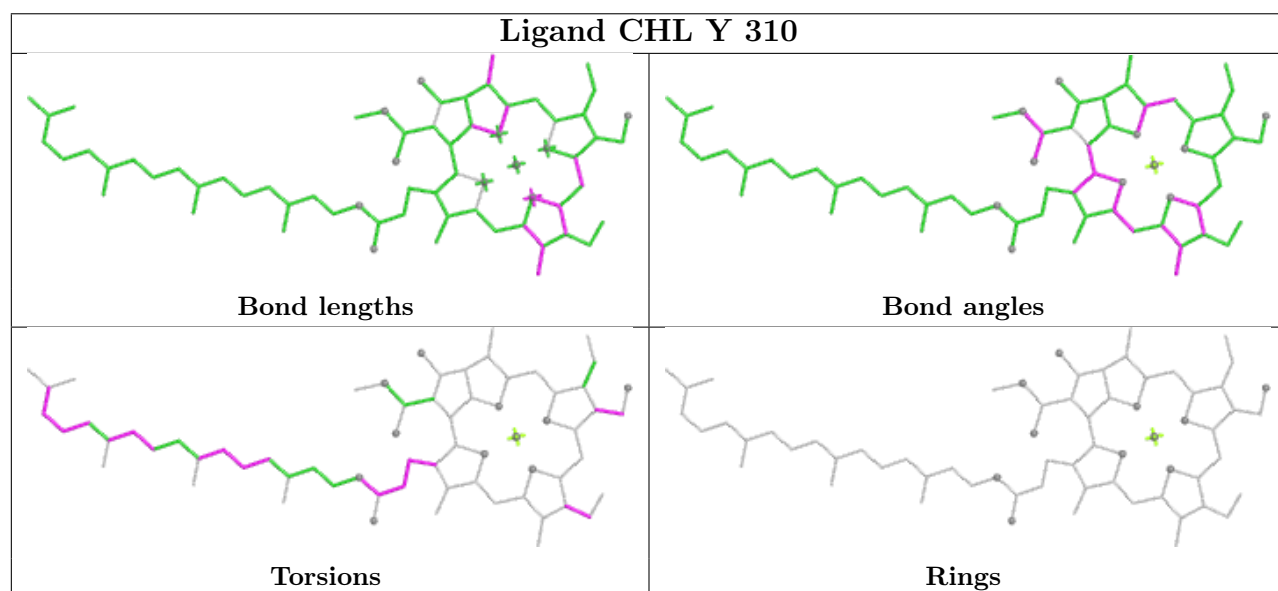
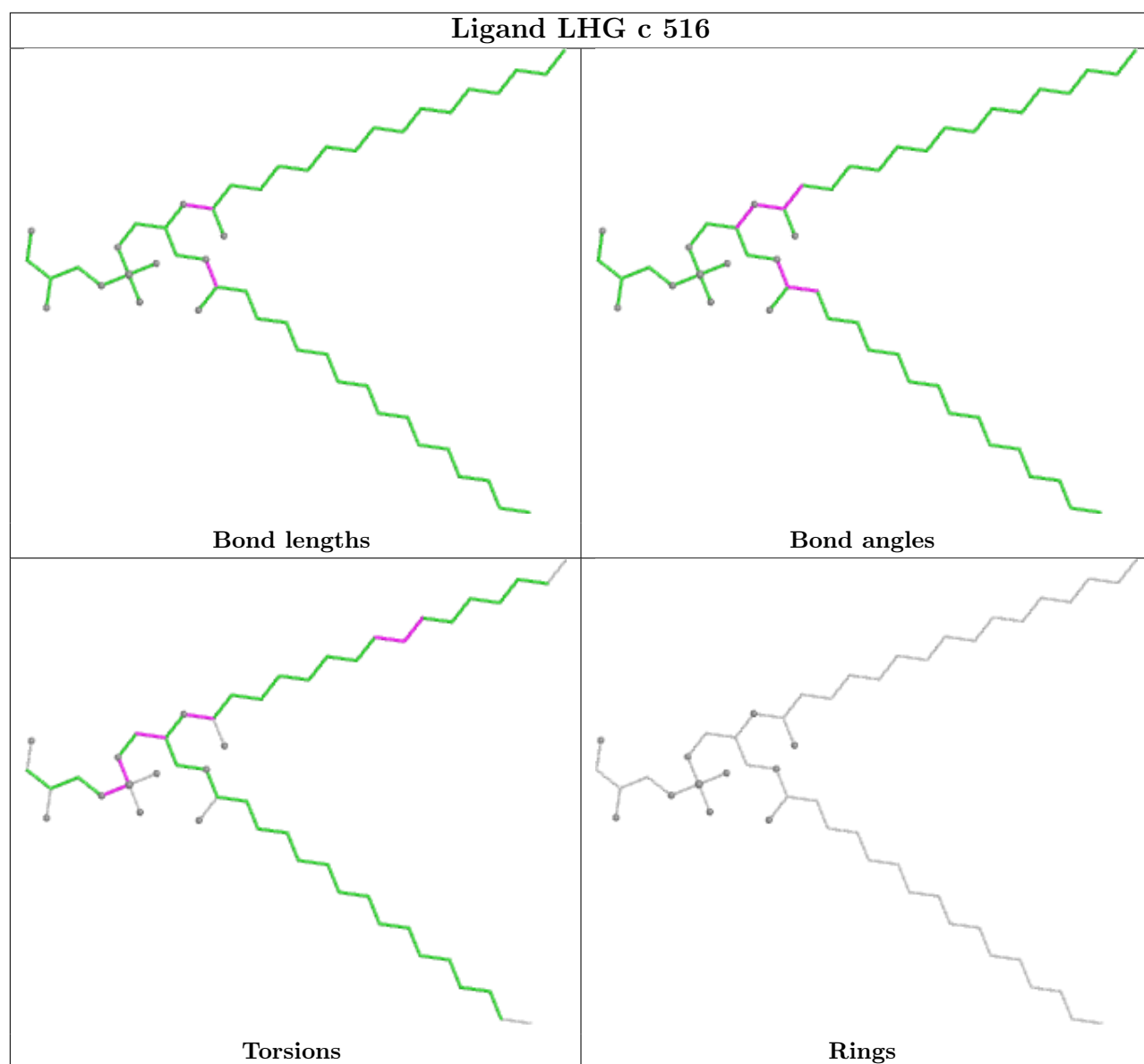


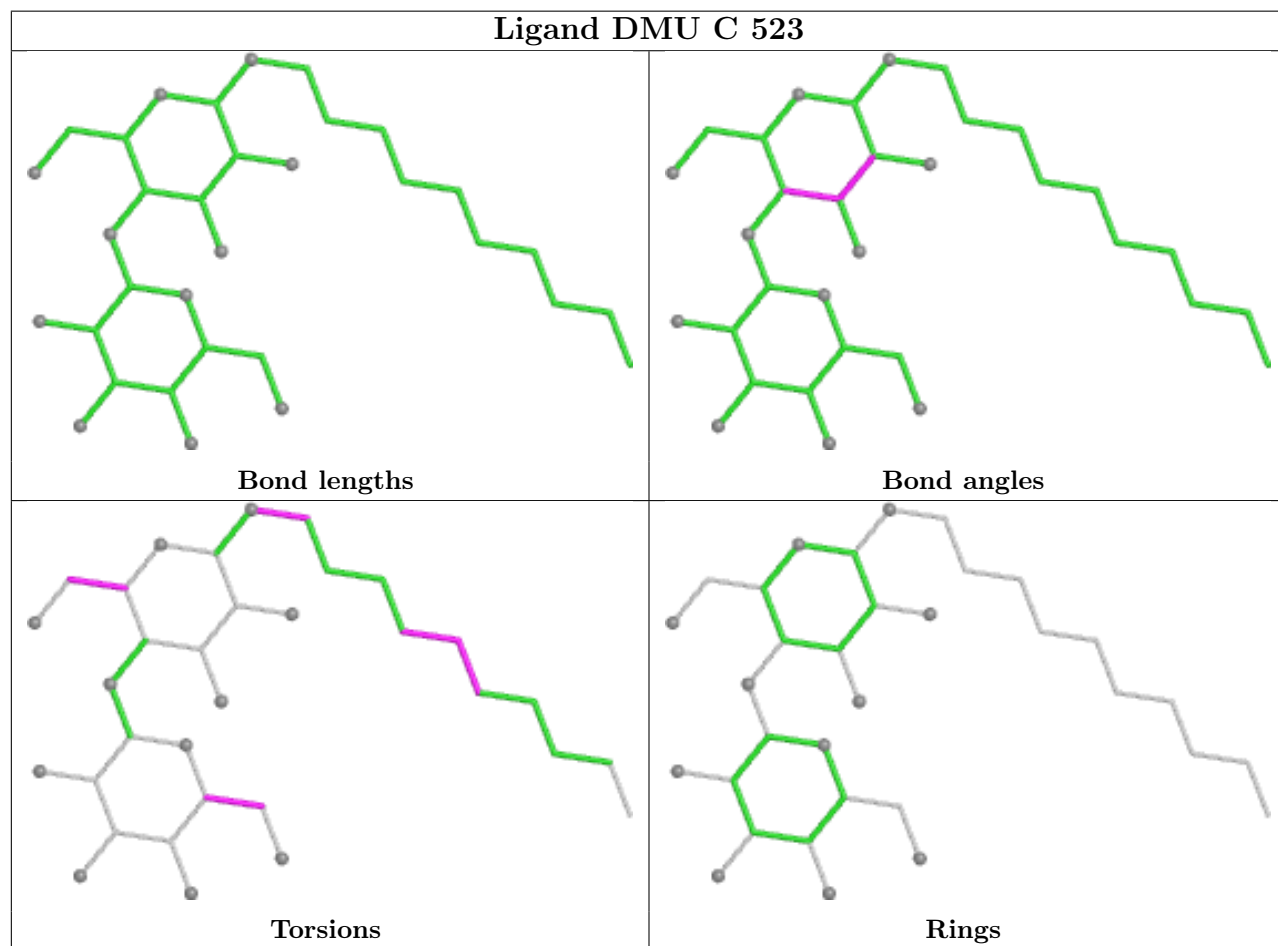
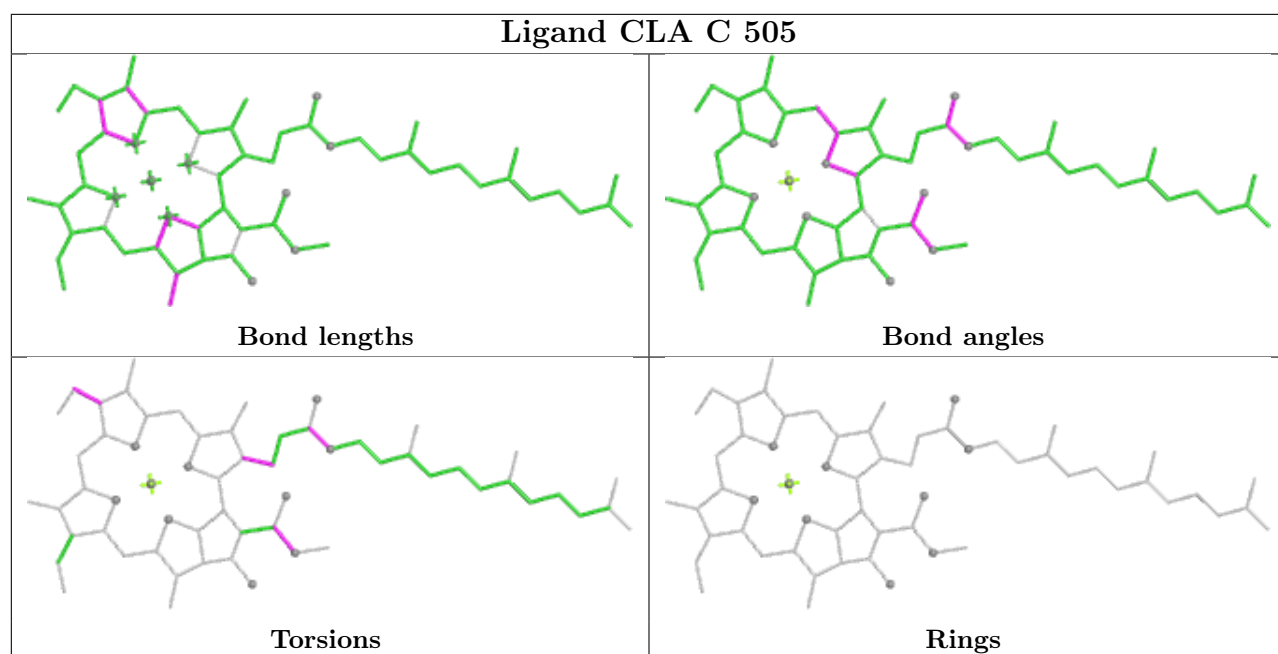
Ligand BCR k 101

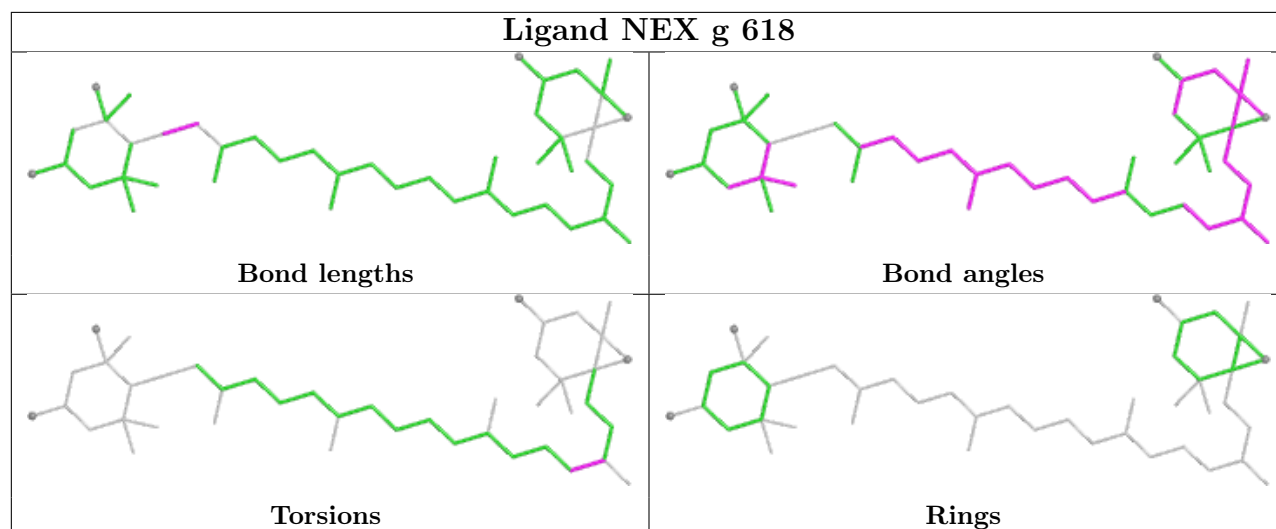
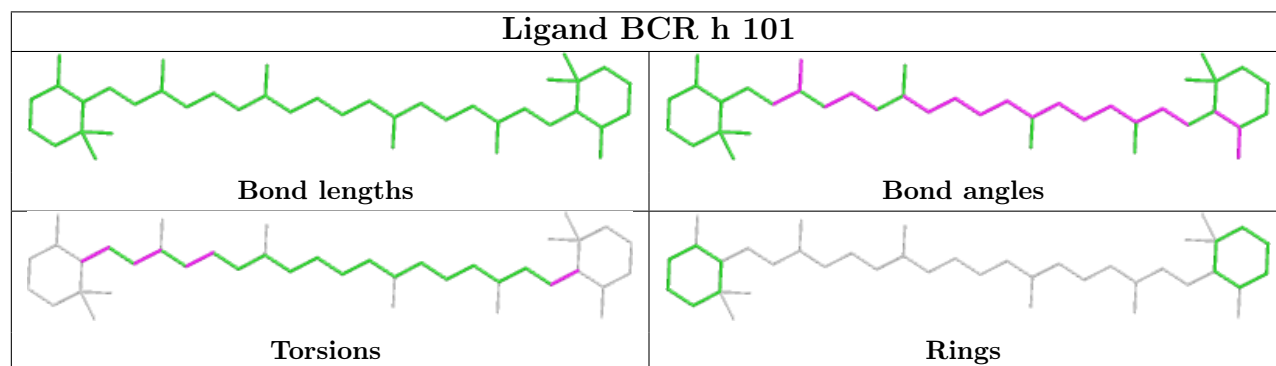
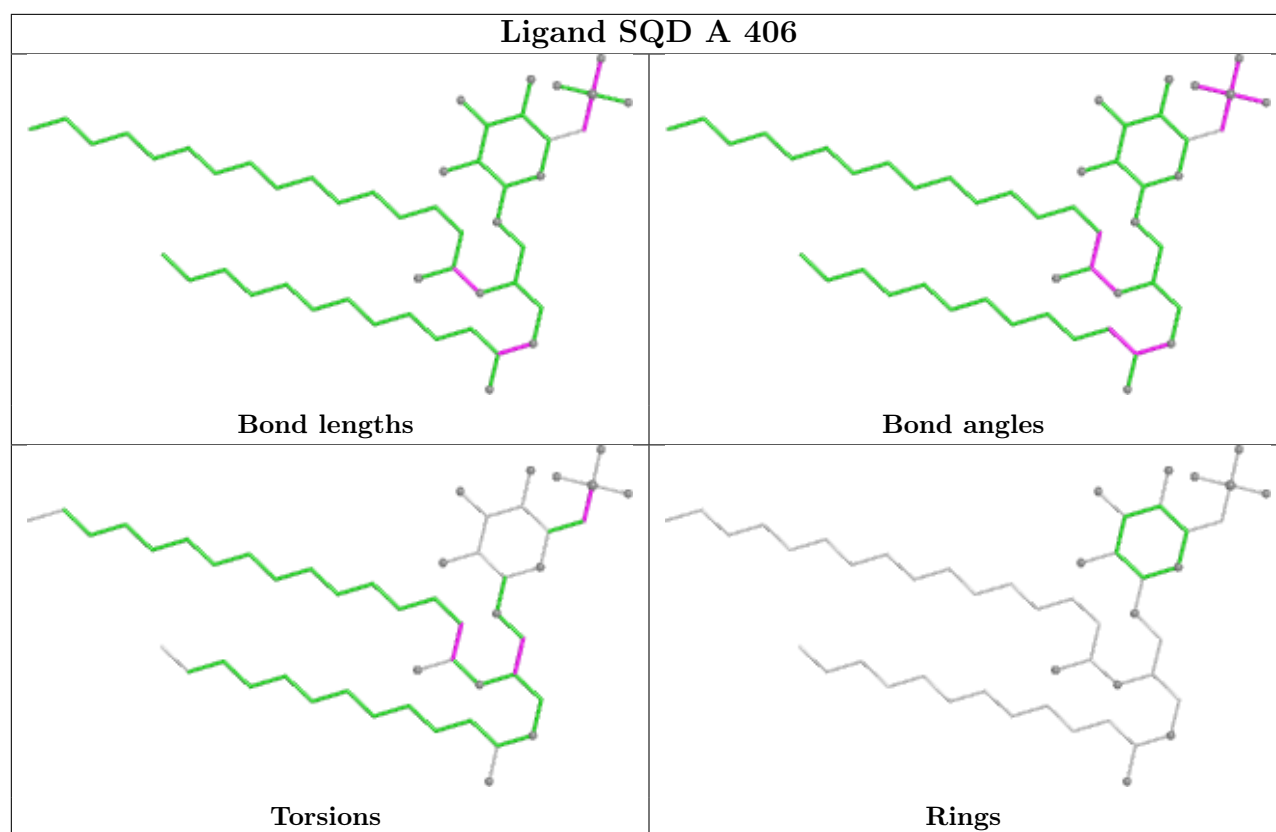


Ligand CLA N 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

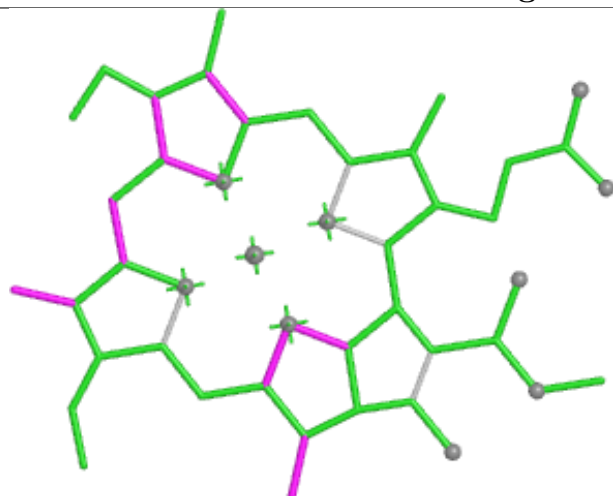




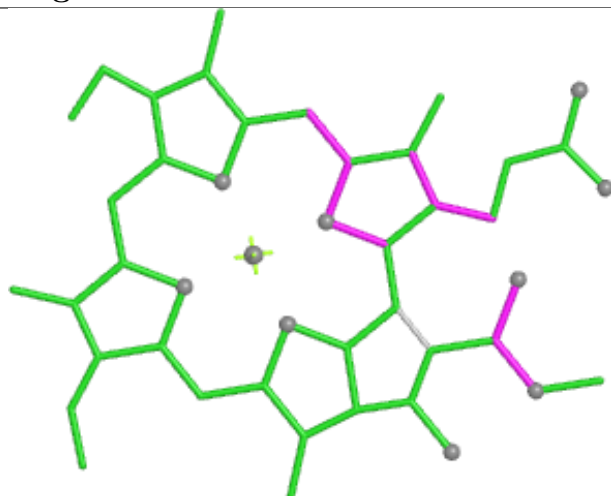




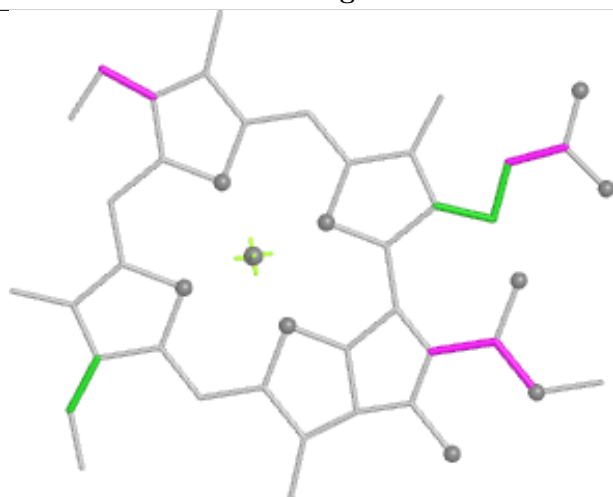
Ligand CLA g 612



Bond lengths



Bond angles

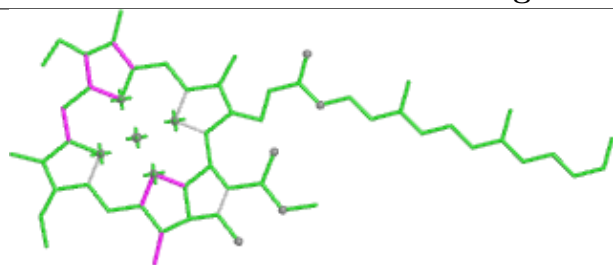


Torsions

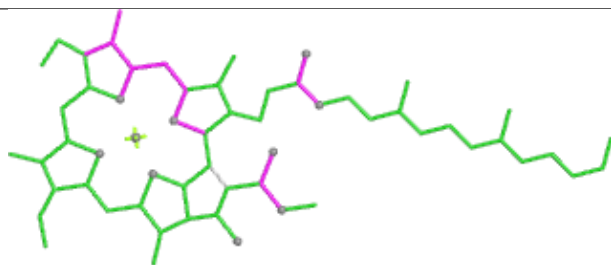


Rings

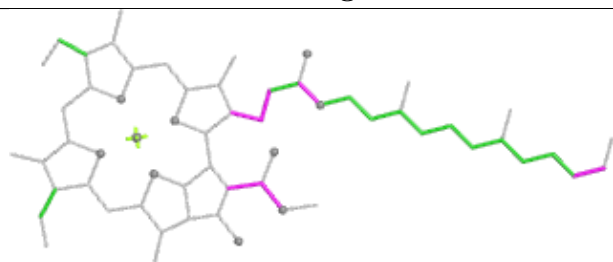
Ligand CLA N 610



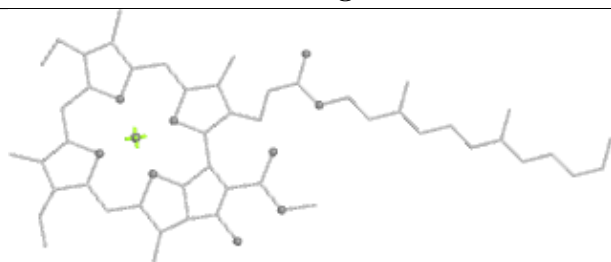
Bond lengths



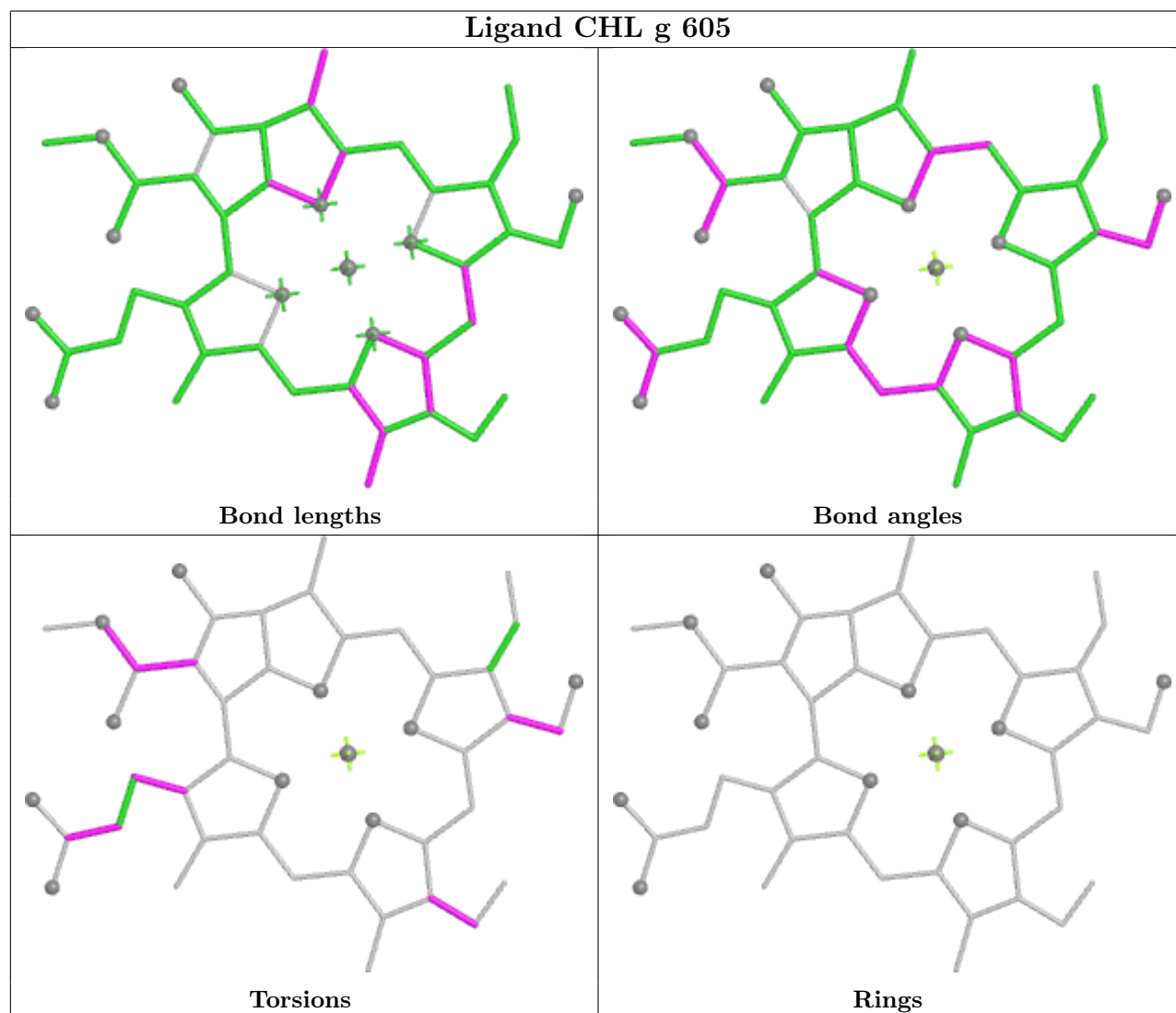
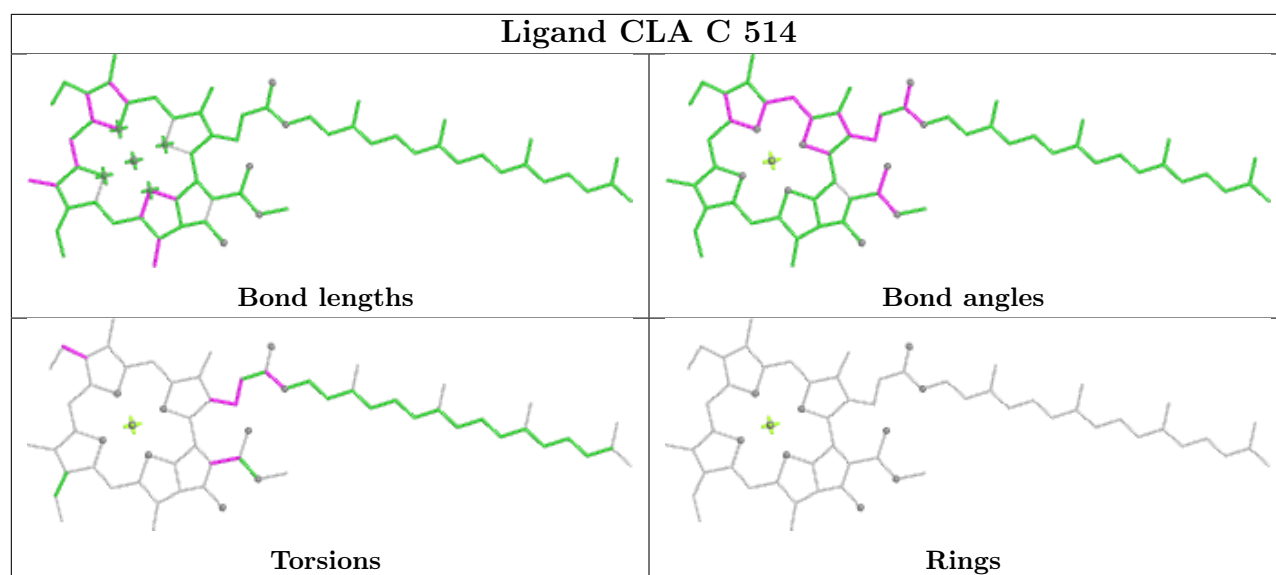
Bond angles

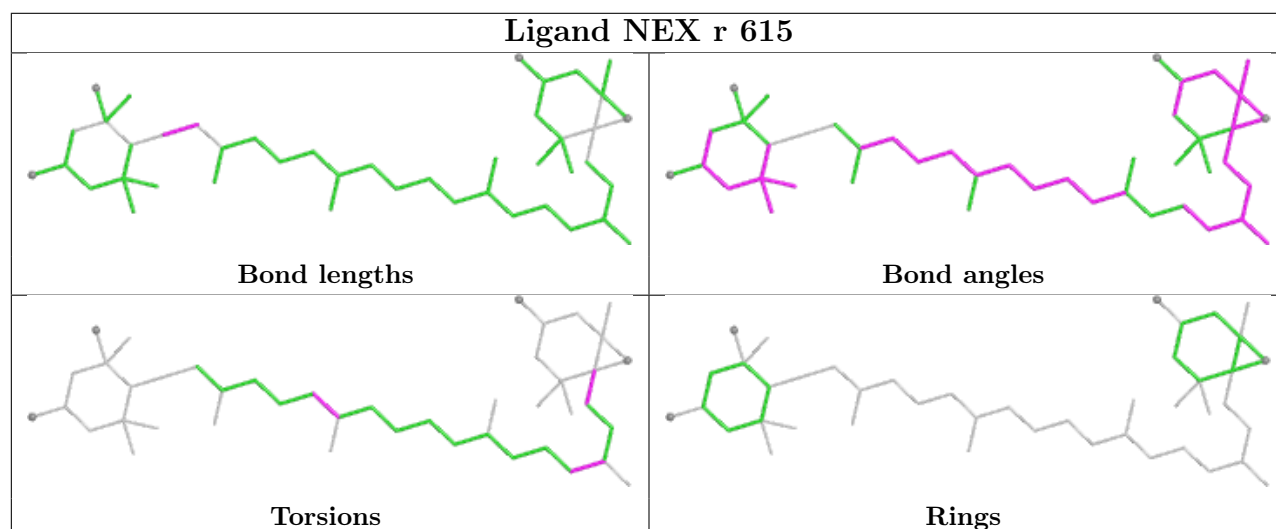
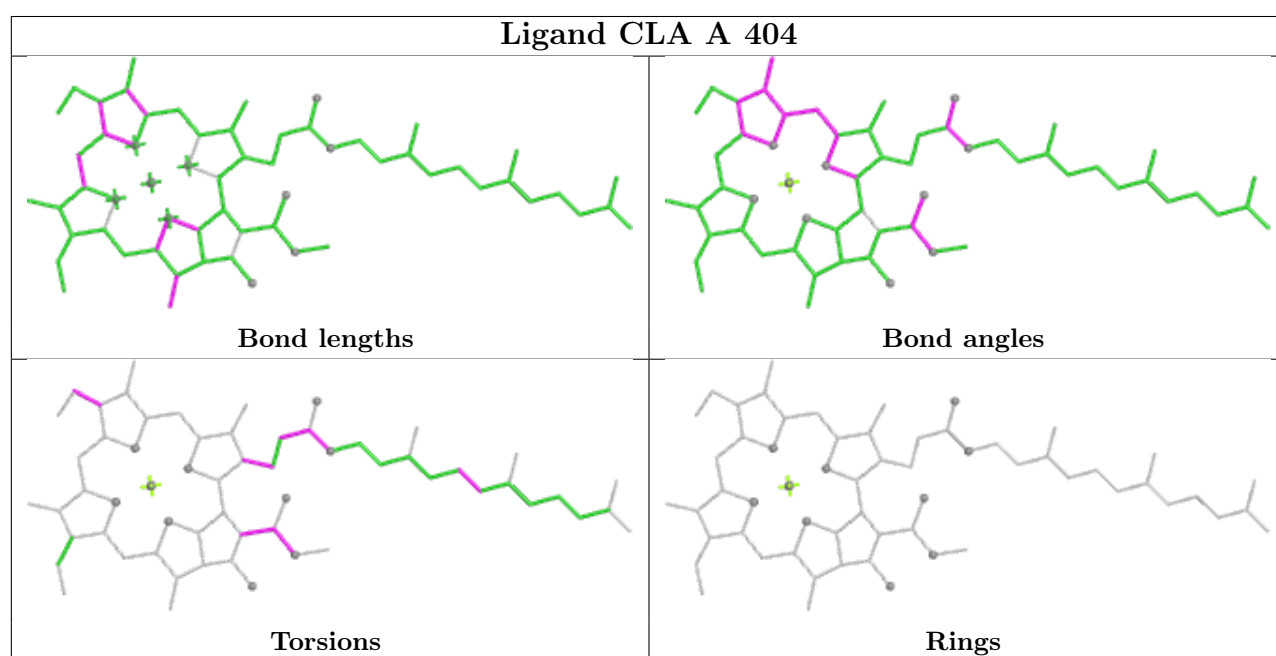
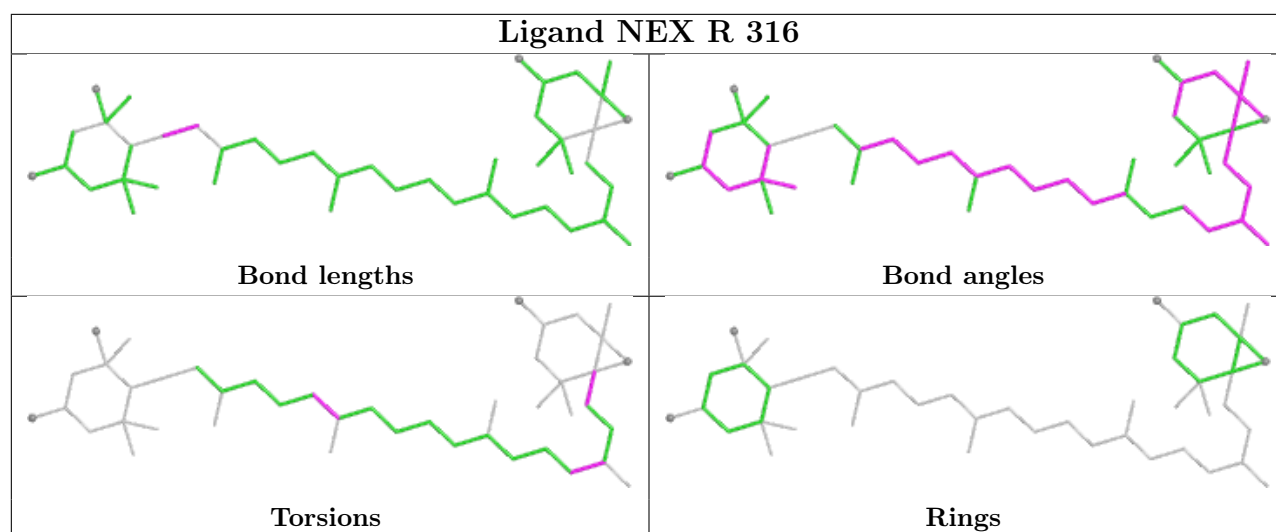


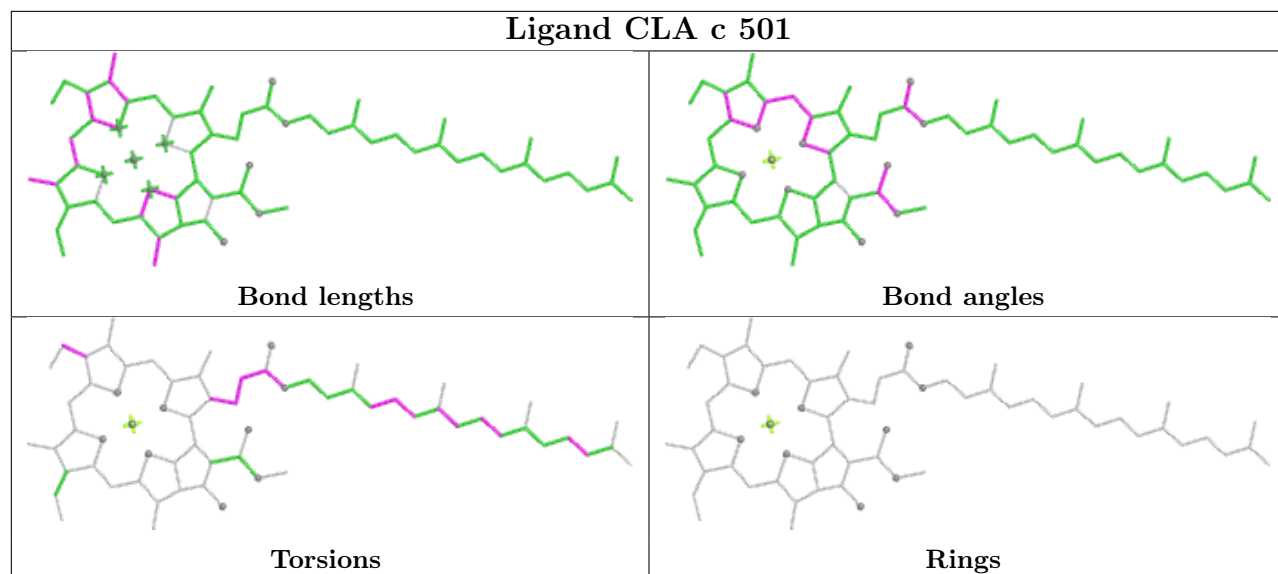
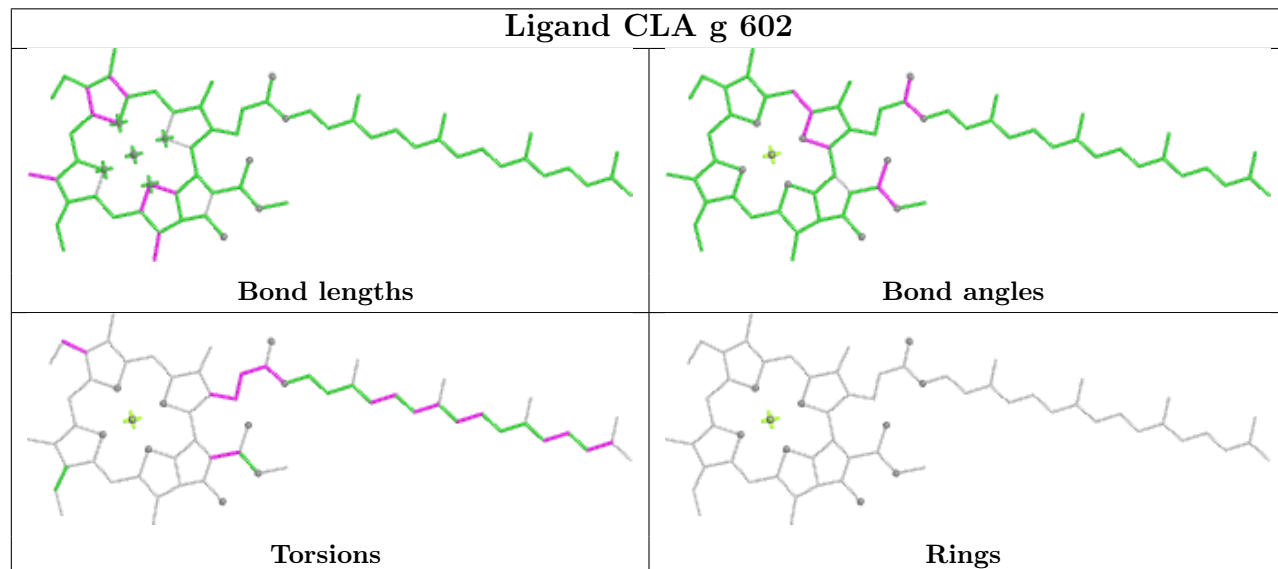
Torsions

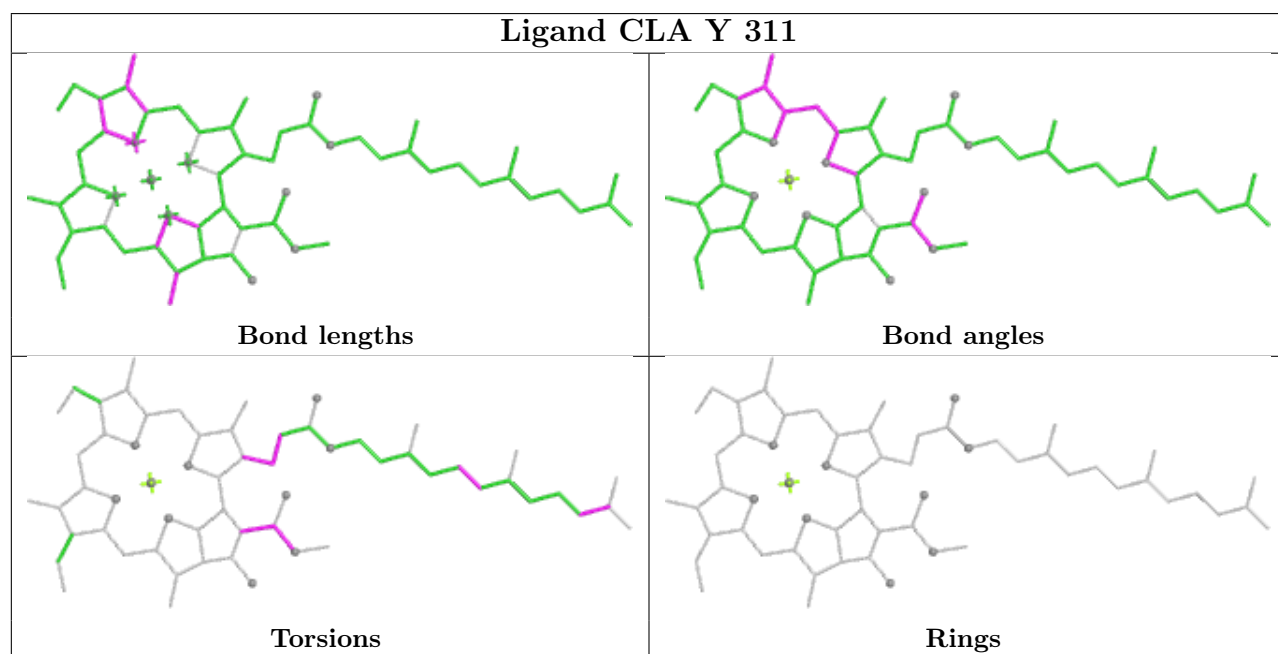
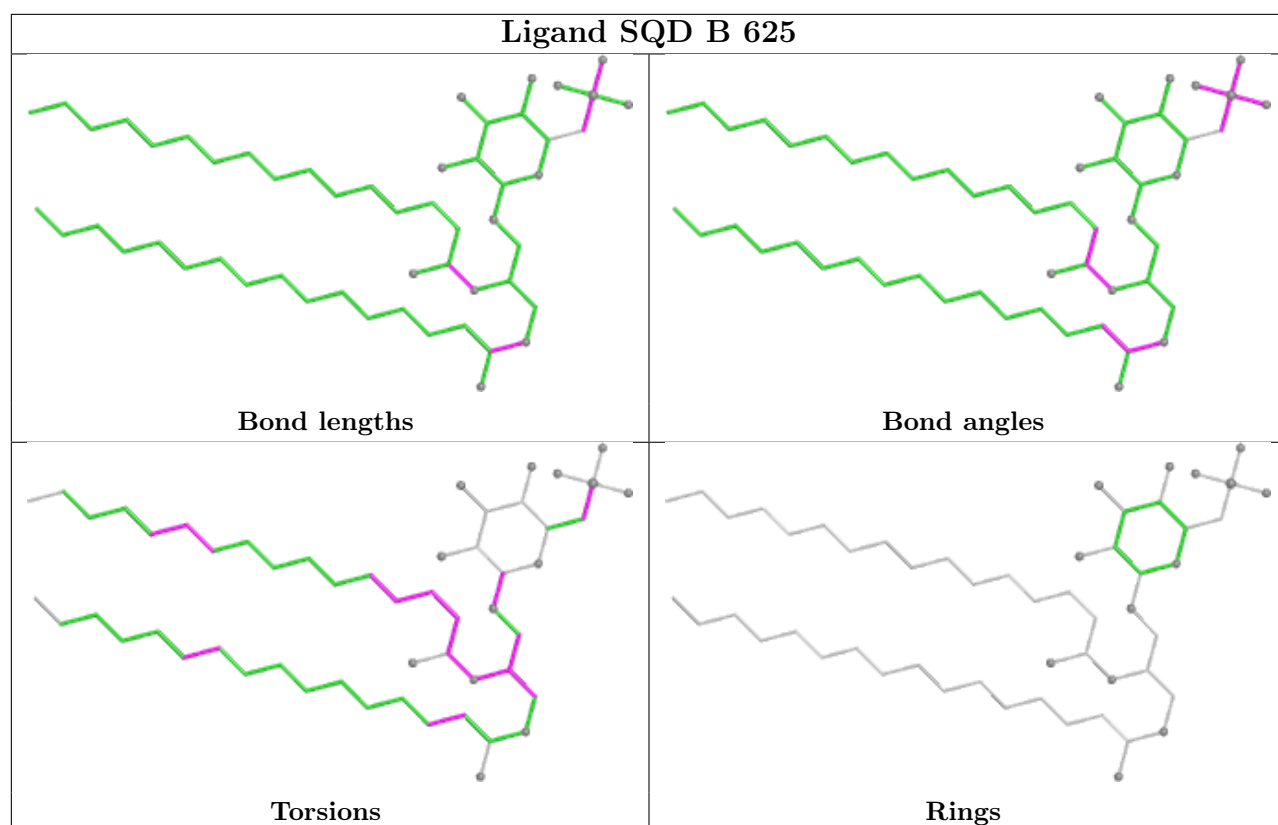


Rings

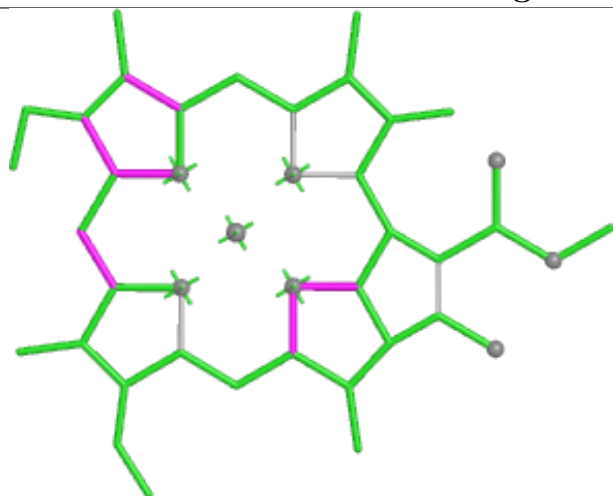




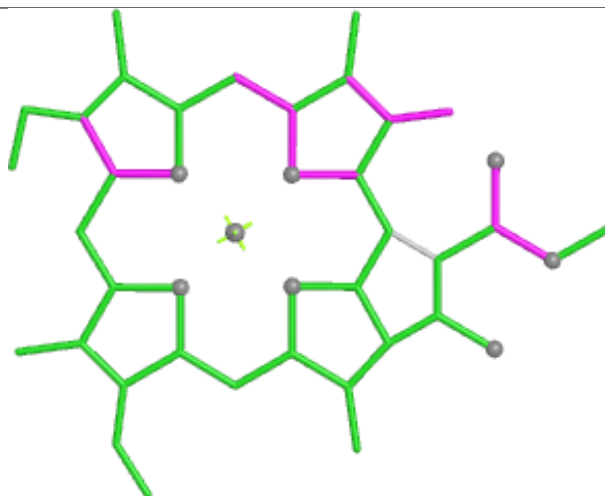
Ligand CLA c 501**Ligand CLA g 602**



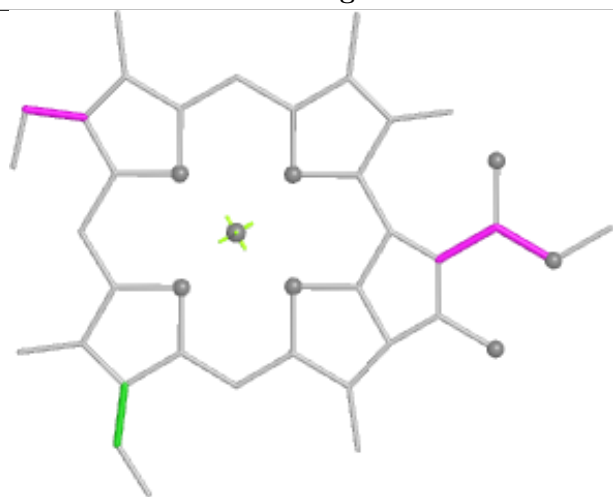
Ligand CLA N 614



Bond lengths



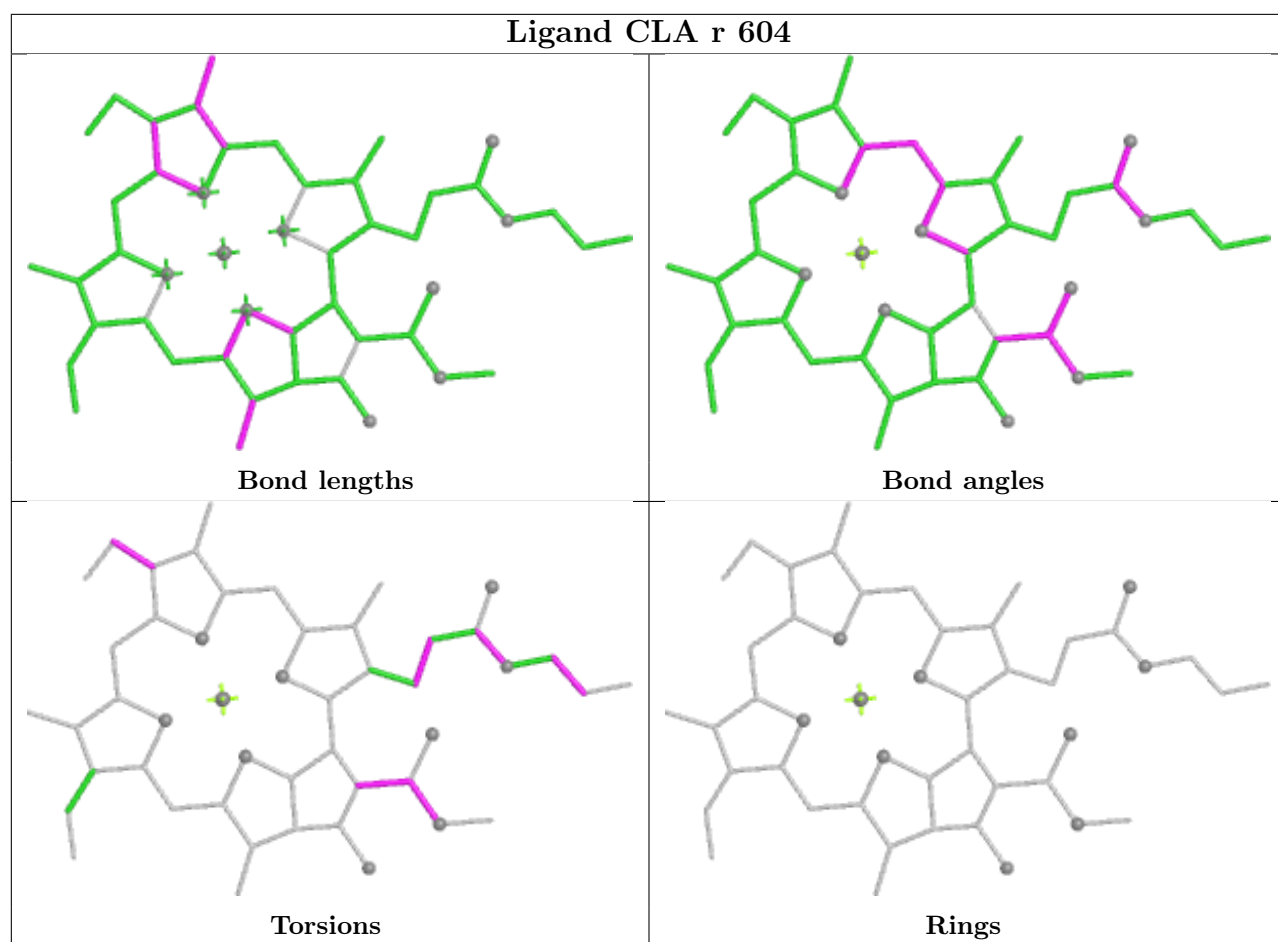
Bond angles

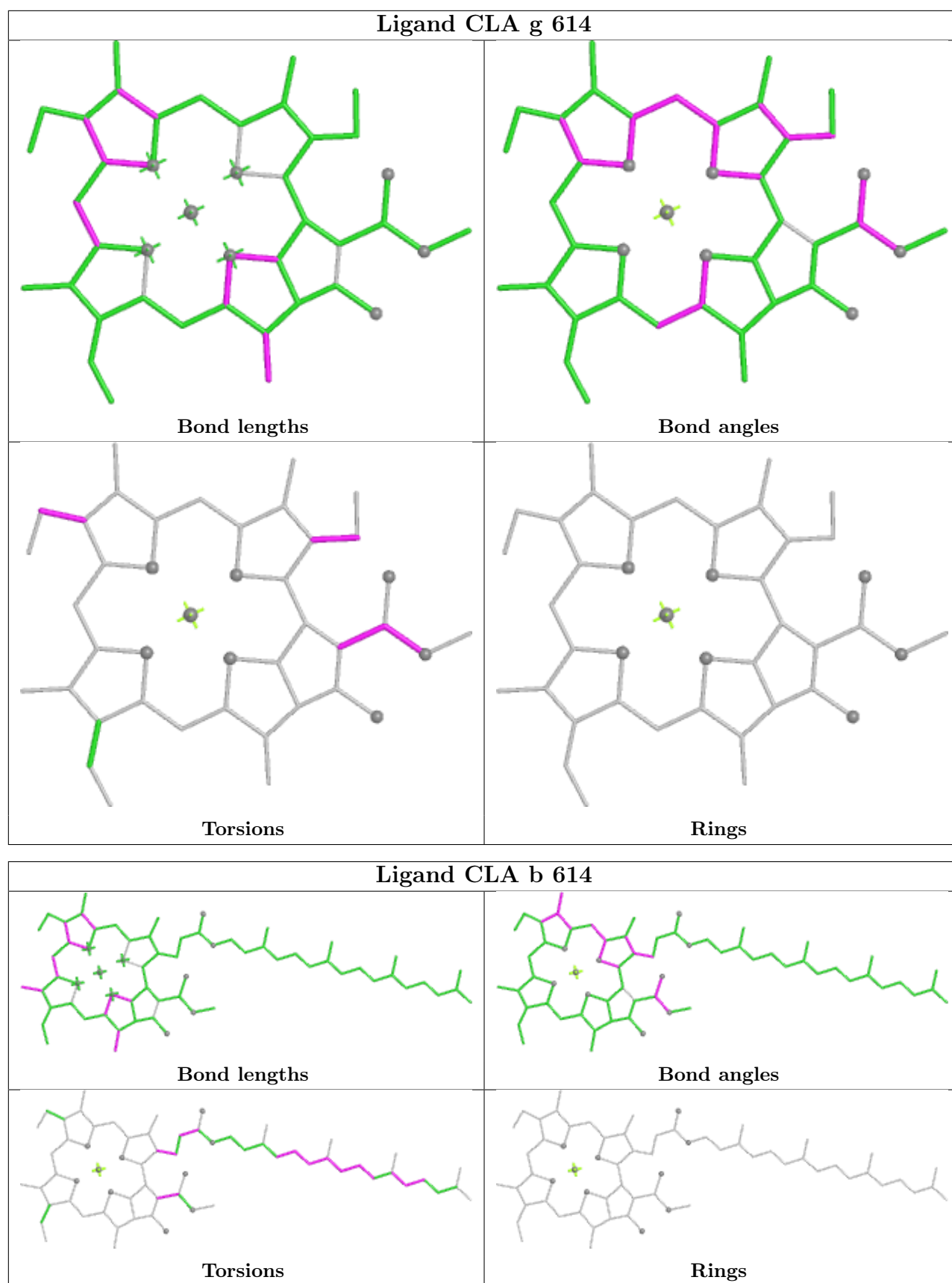


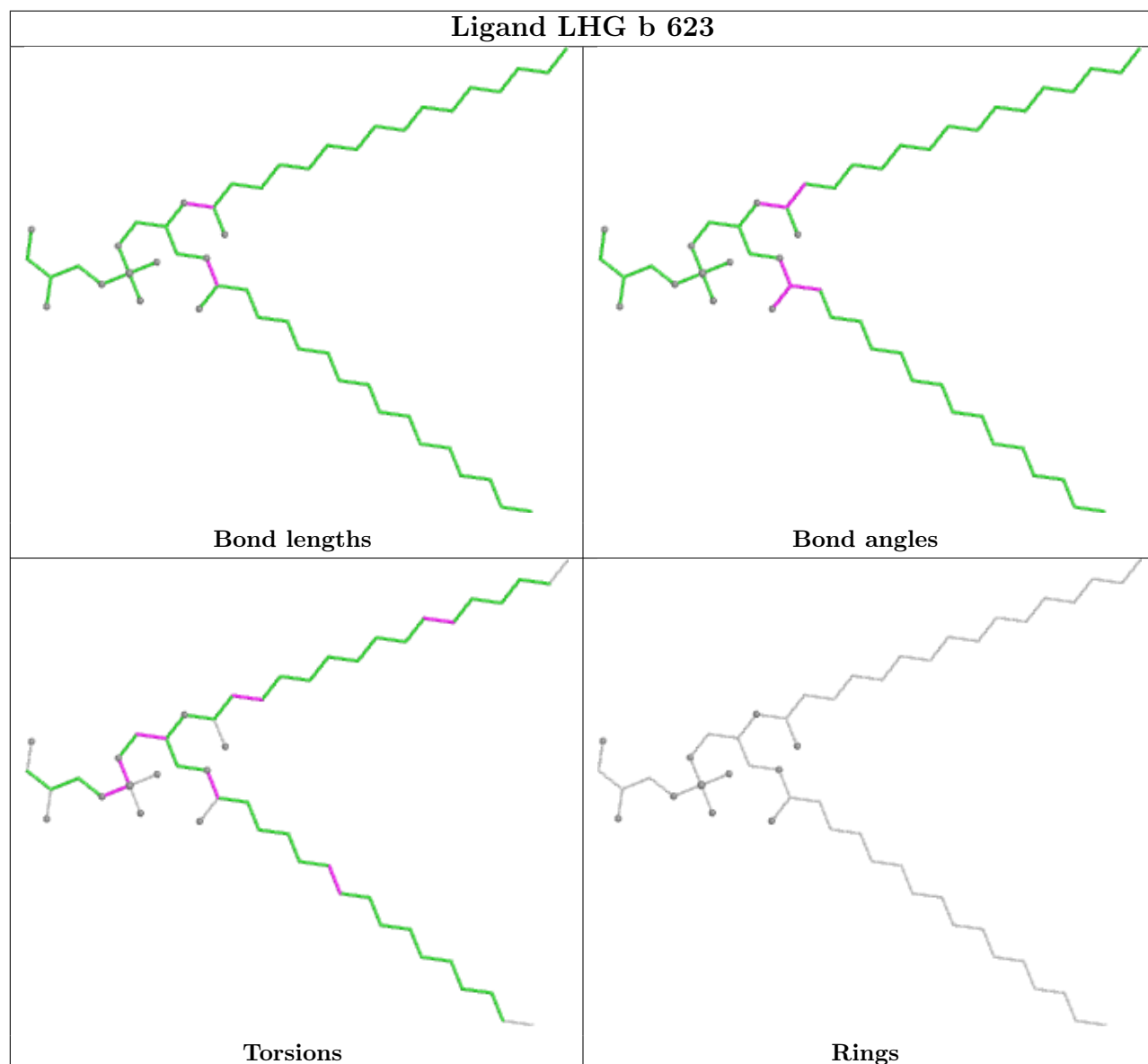
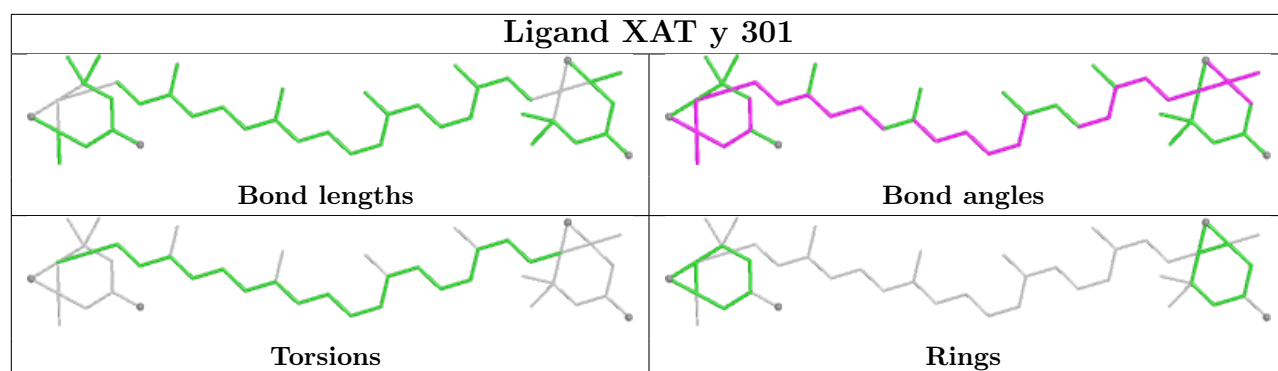
Torsions

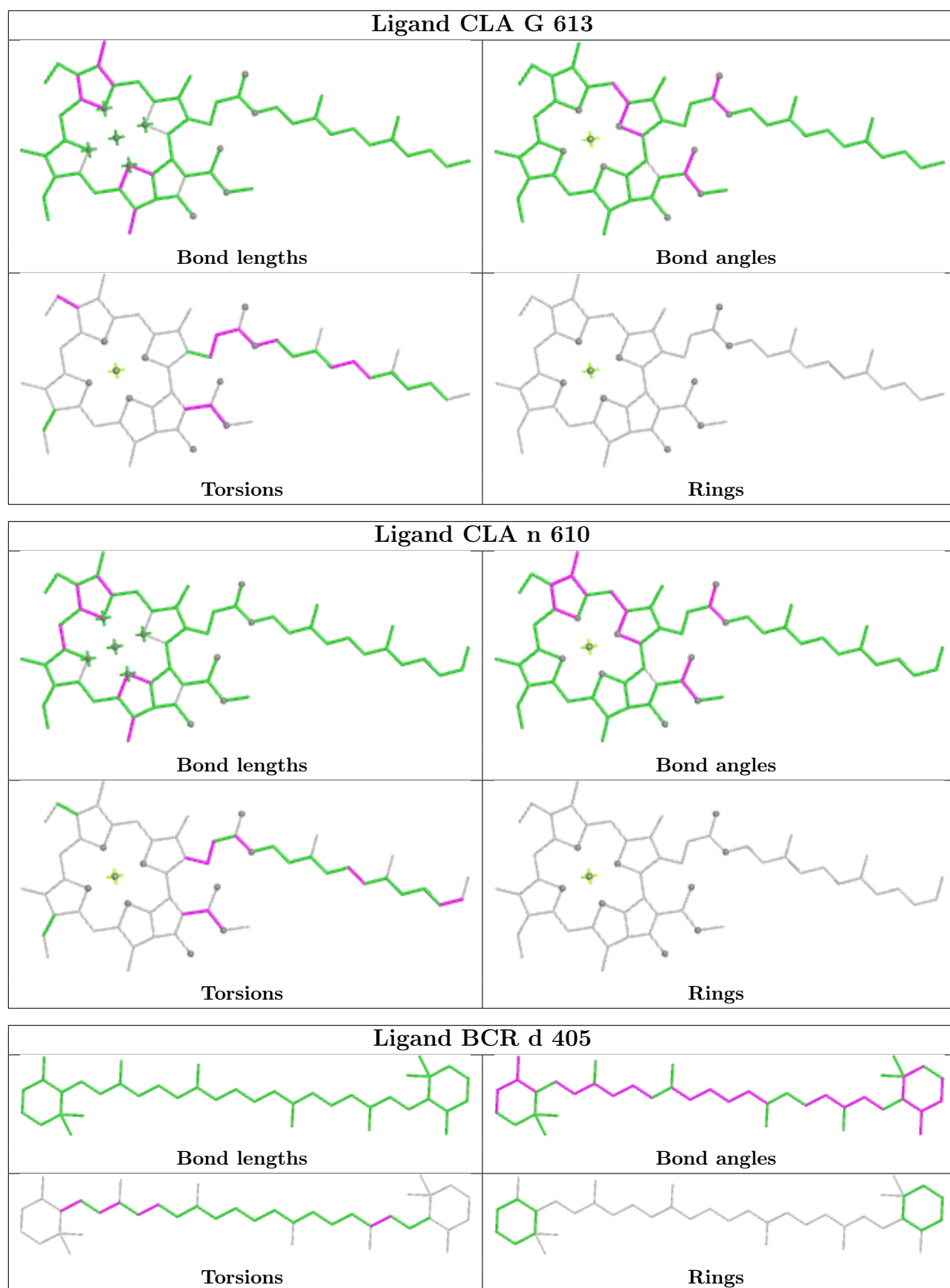


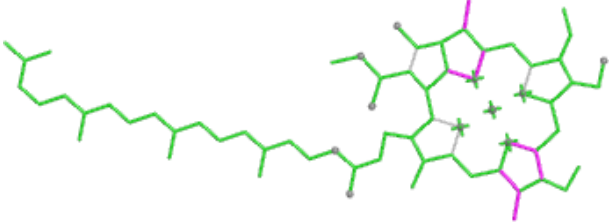
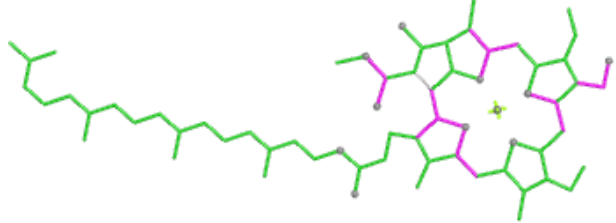
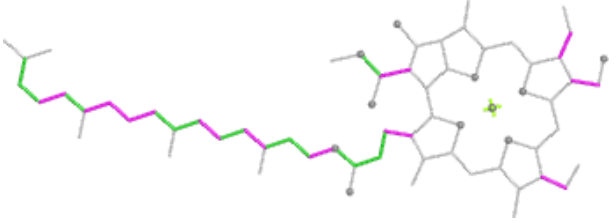
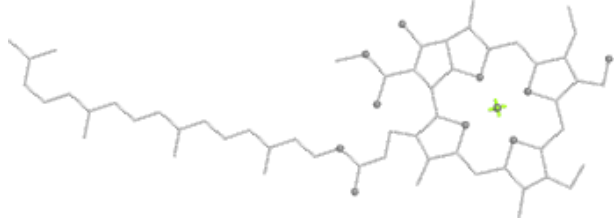
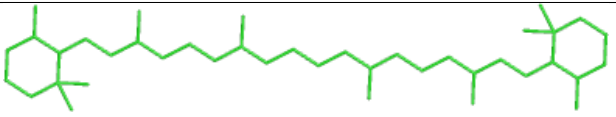
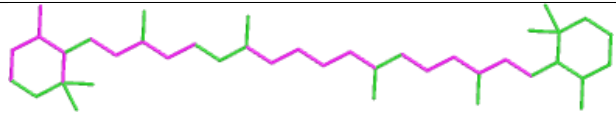
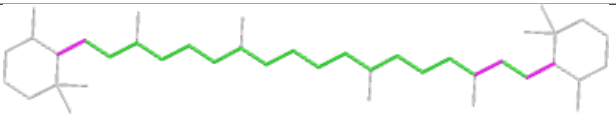
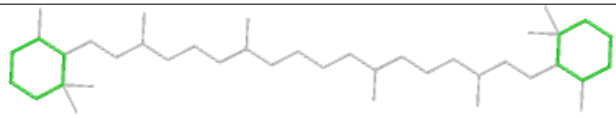
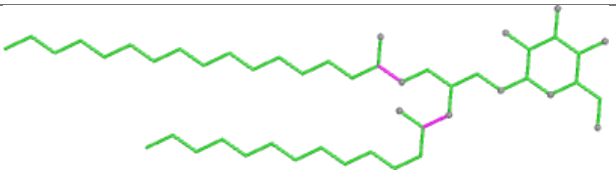
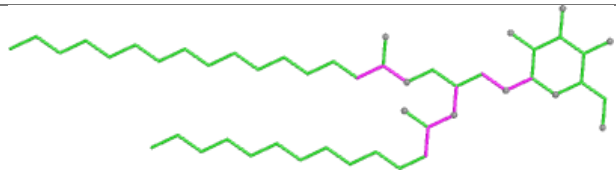
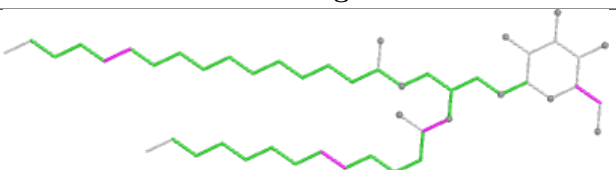
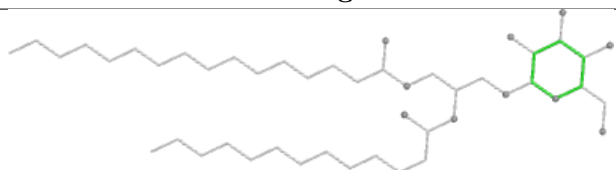
Rings



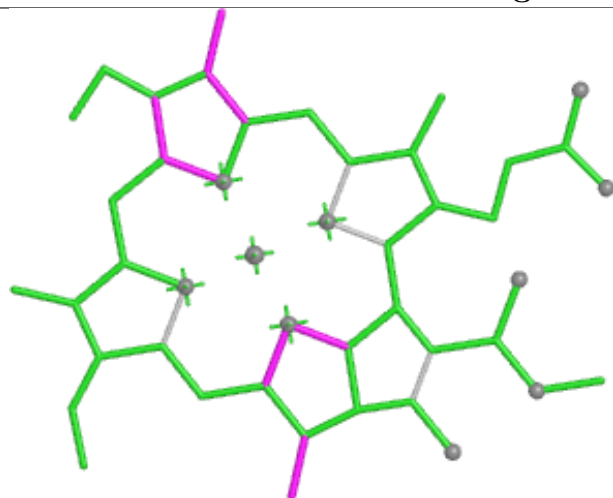




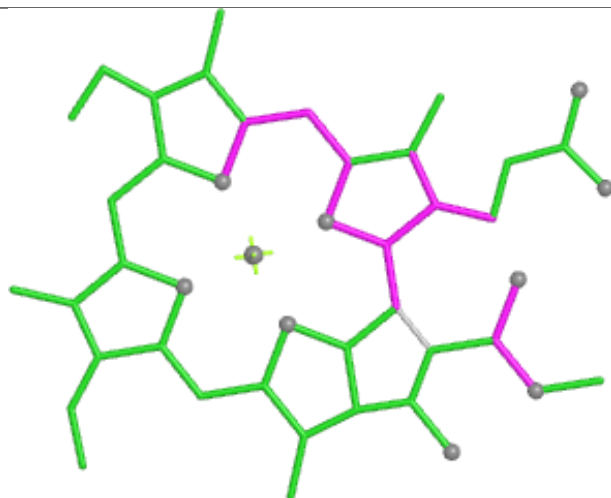


Ligand CHL g 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

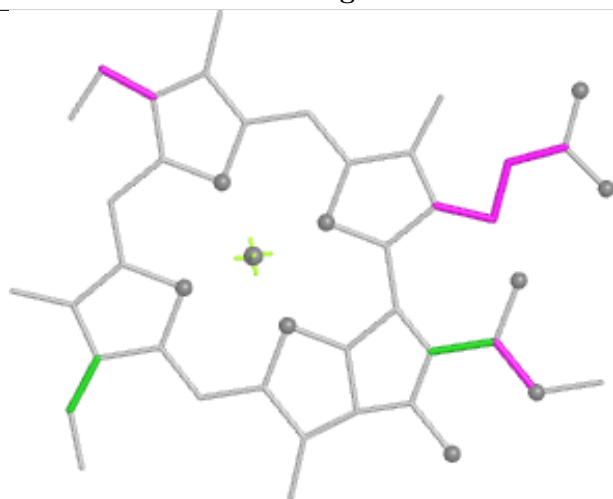
Ligand CLA N 612



Bond lengths



Bond angles

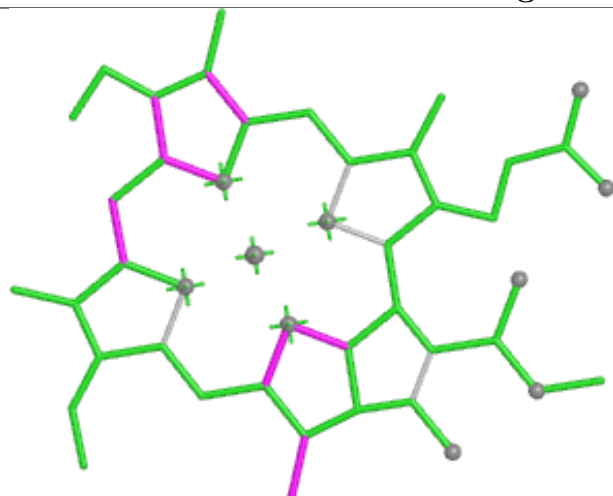


Torsions

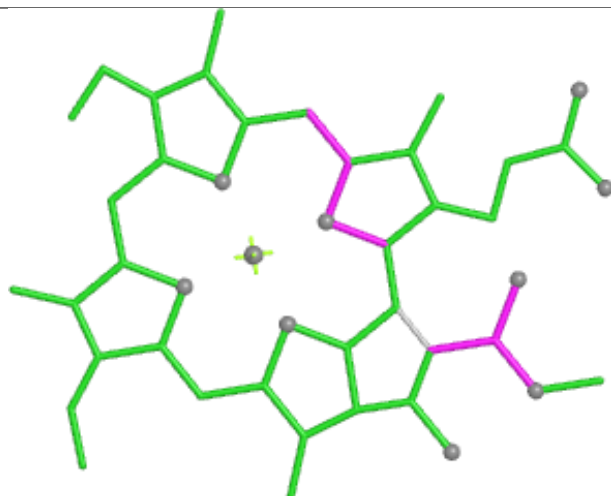


Rings

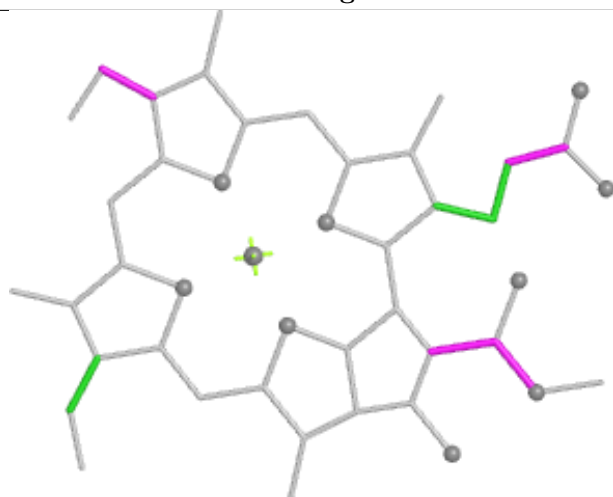
Ligand CLA S 309



Bond lengths



Bond angles

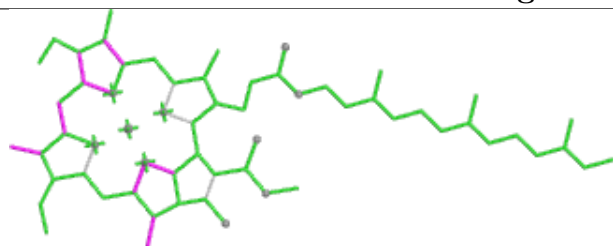


Torsions

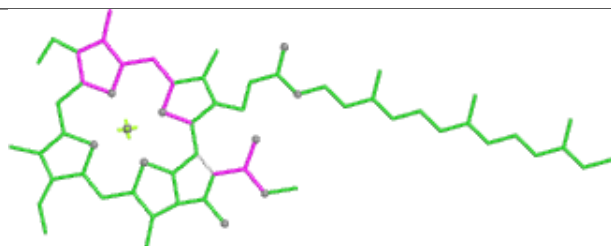


Rings

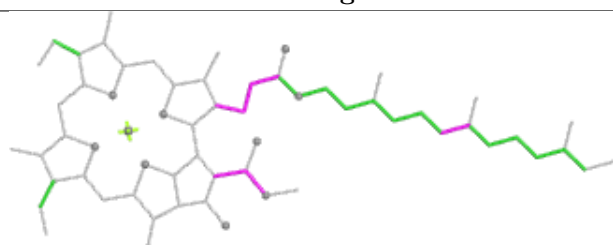
Ligand CLA n 602



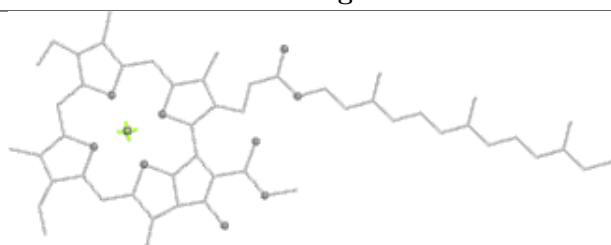
Bond lengths



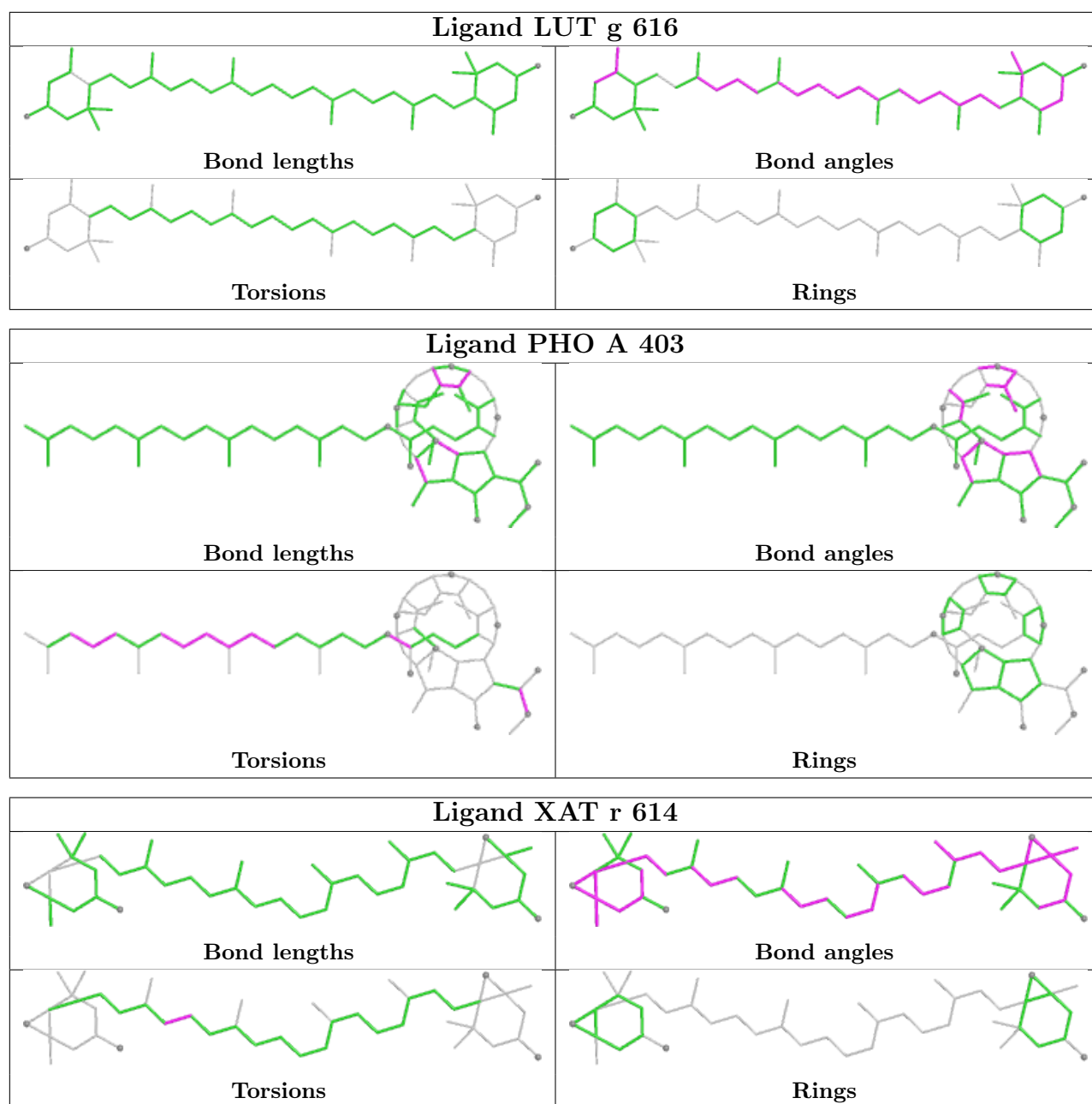
Bond angles

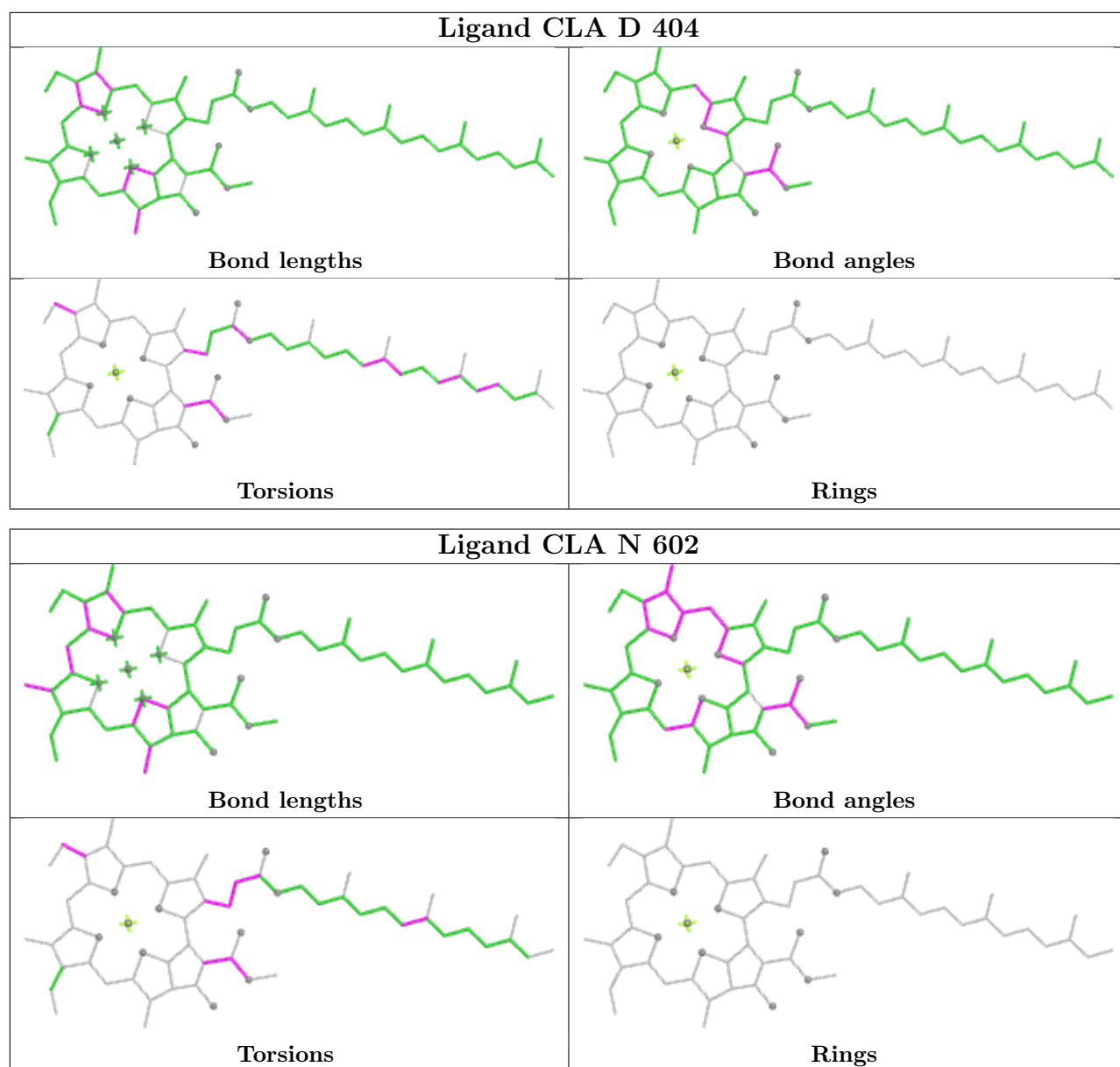


Torsions

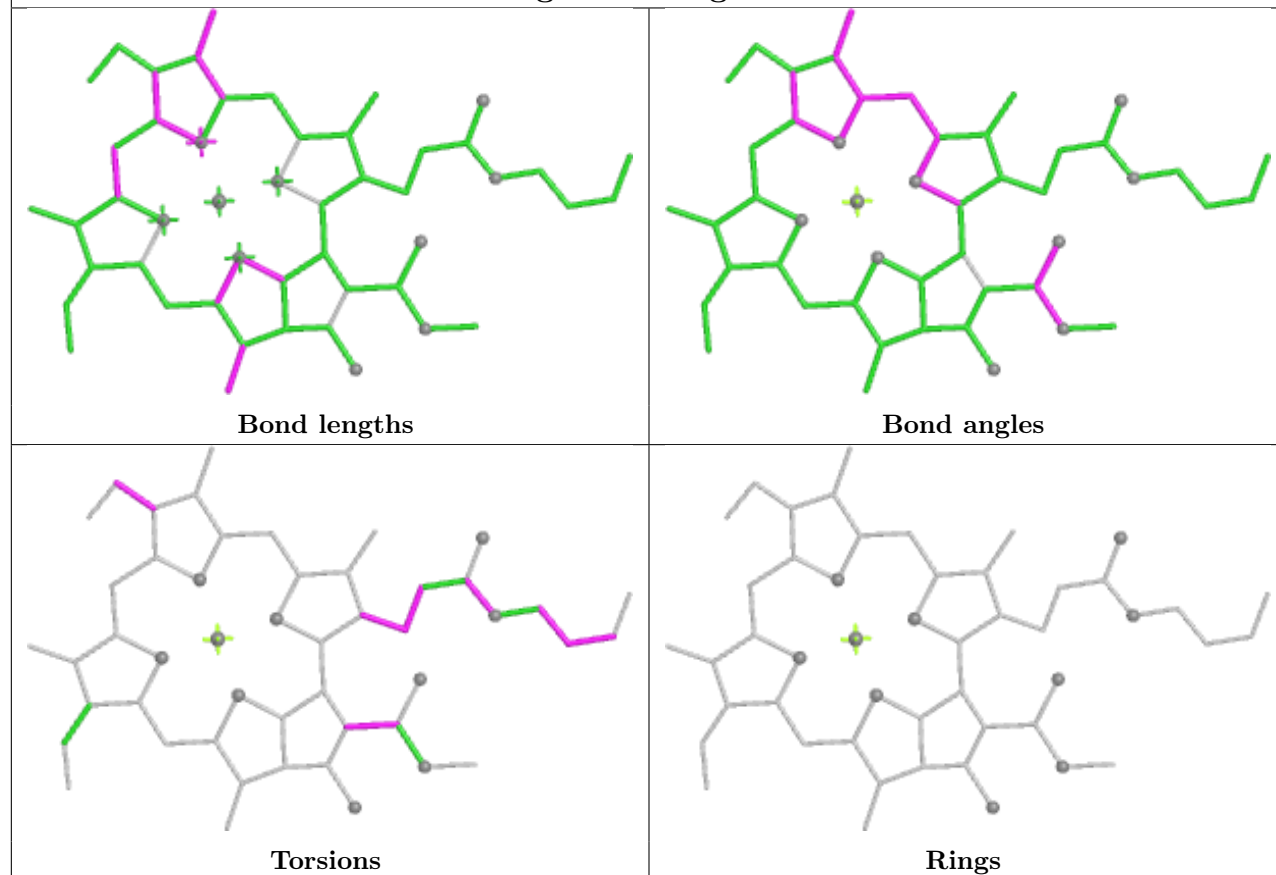


Rings

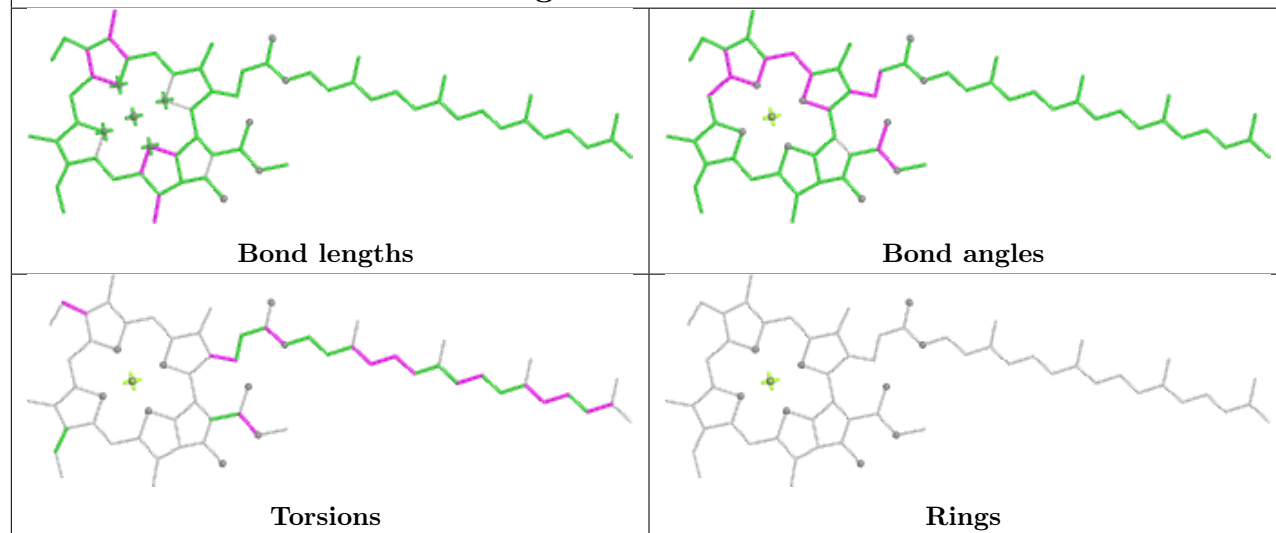


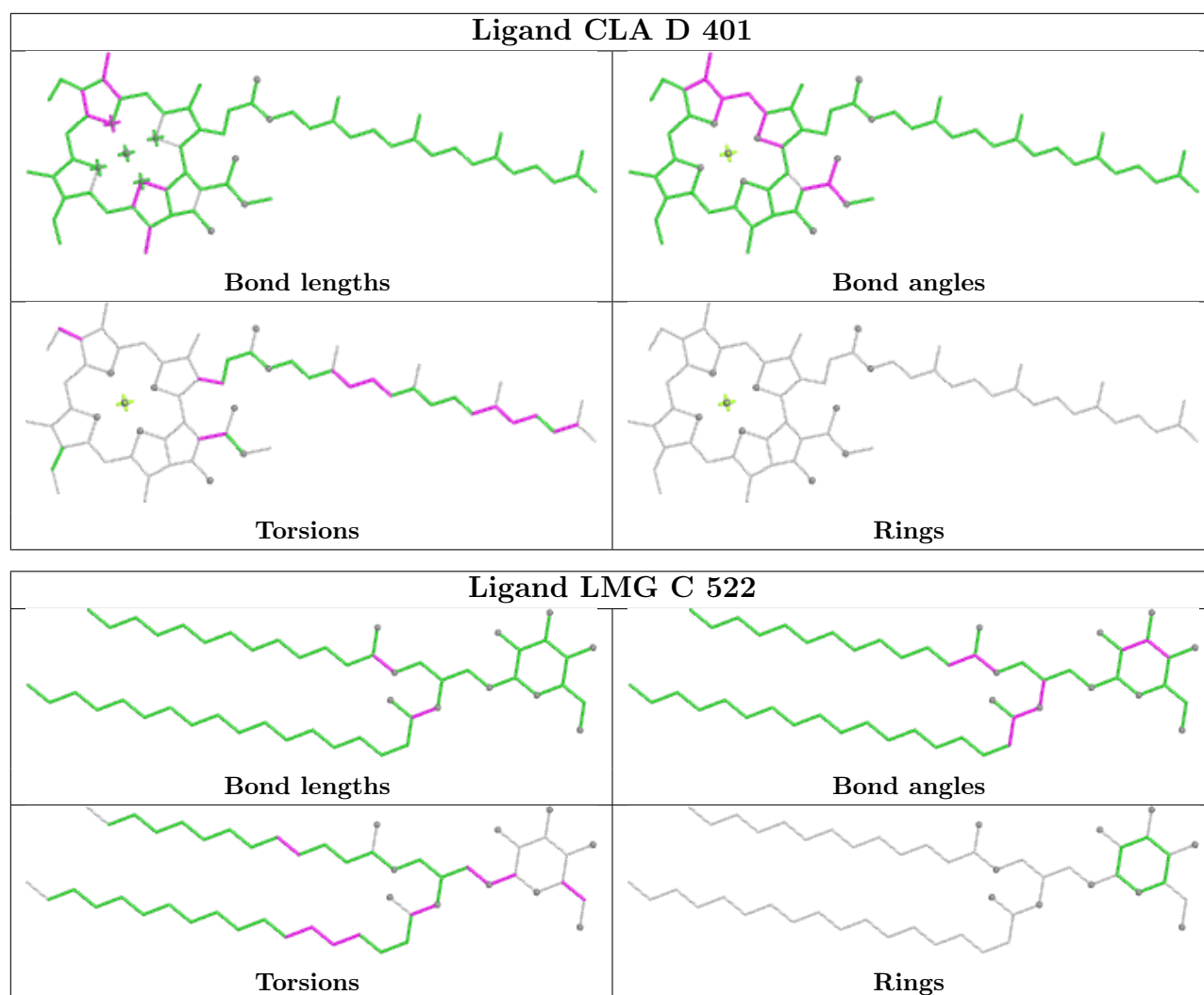


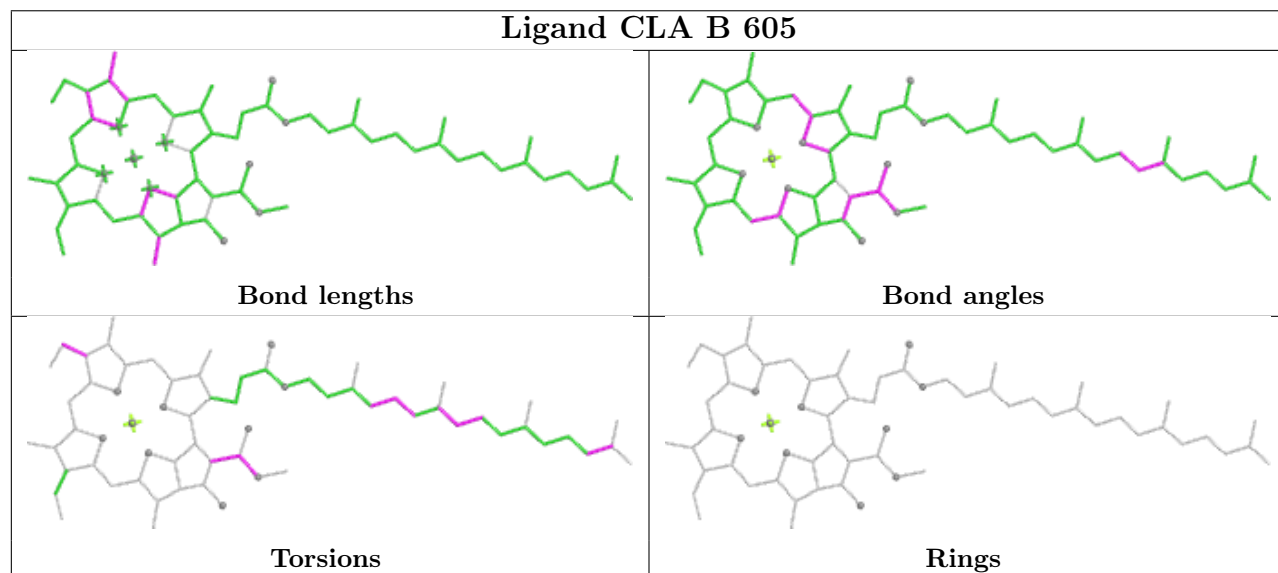
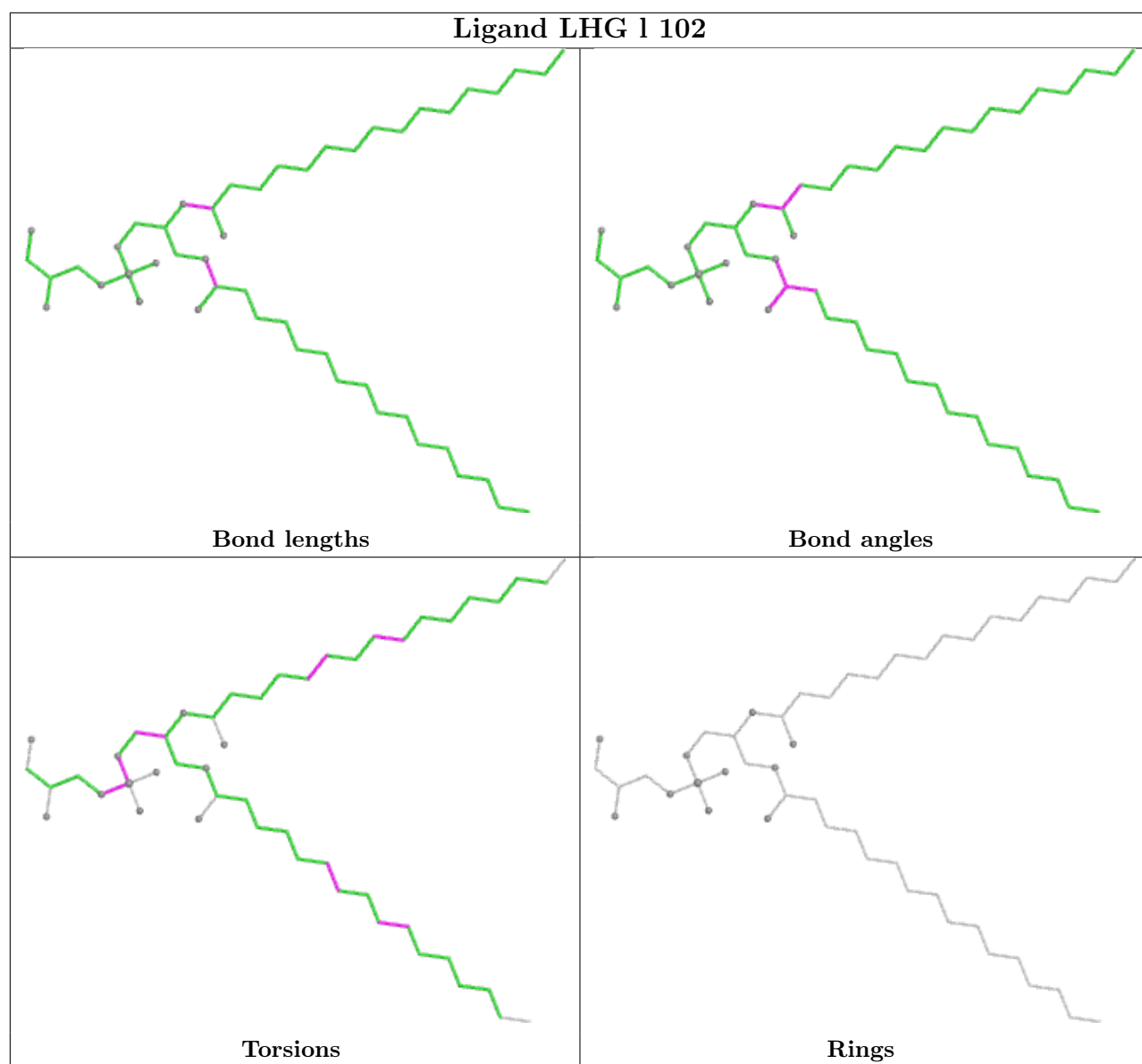
Ligand CLA g 604



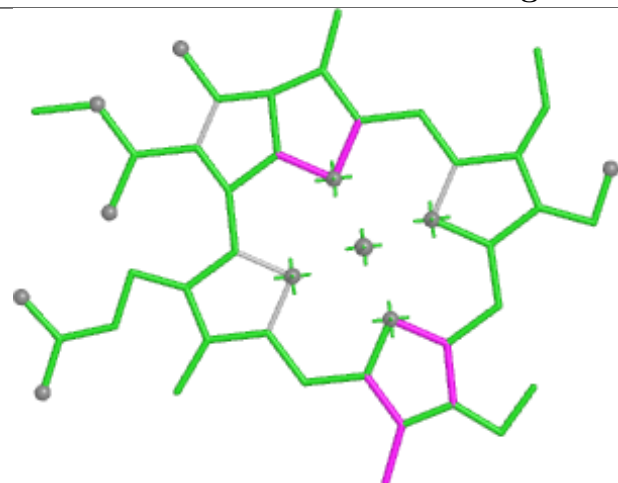
Ligand CLA b 610



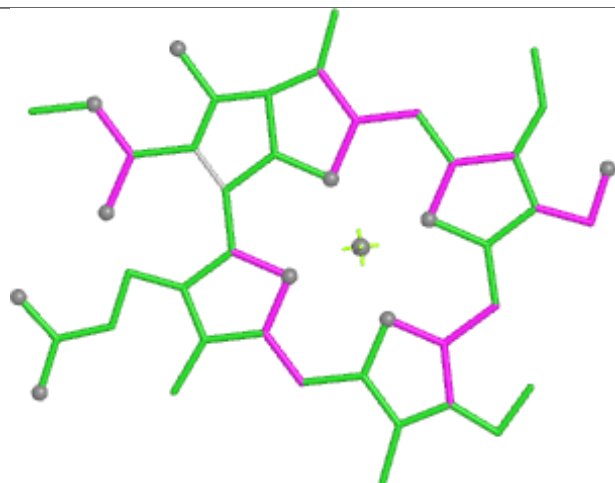




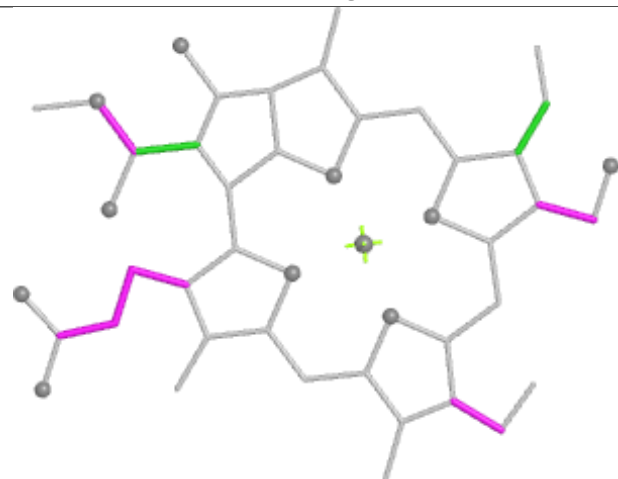
Ligand CHL S 306



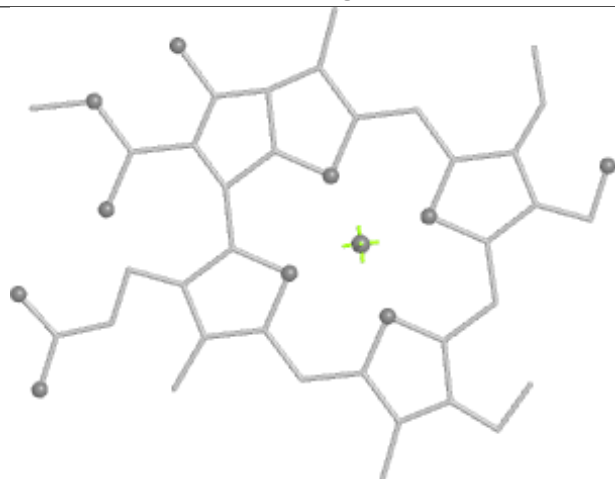
Bond lengths



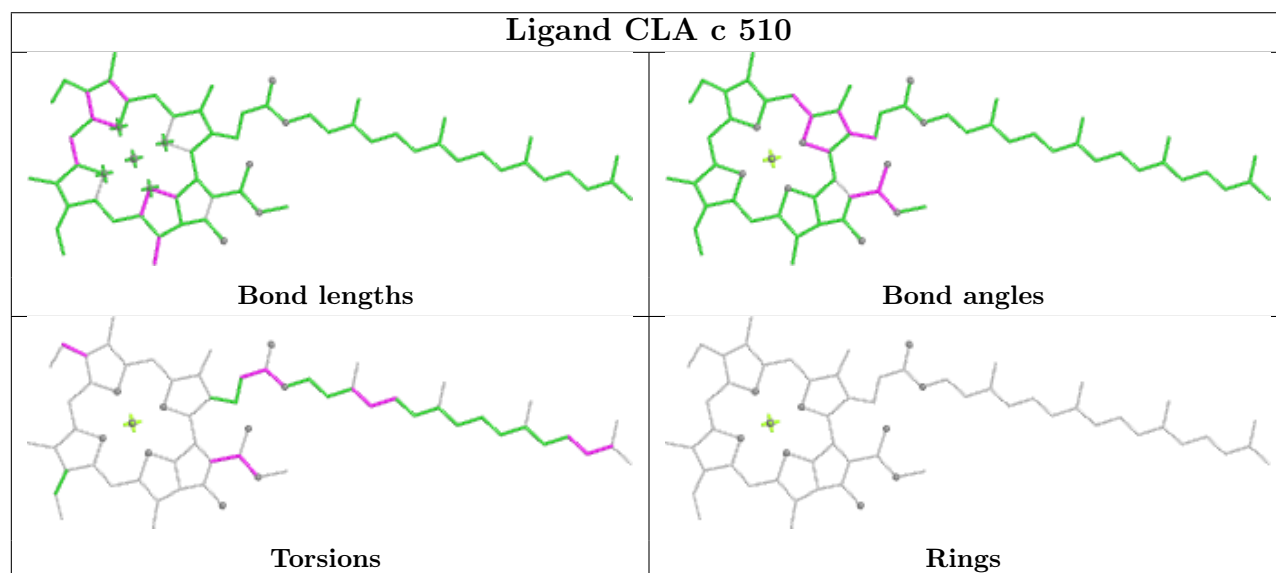
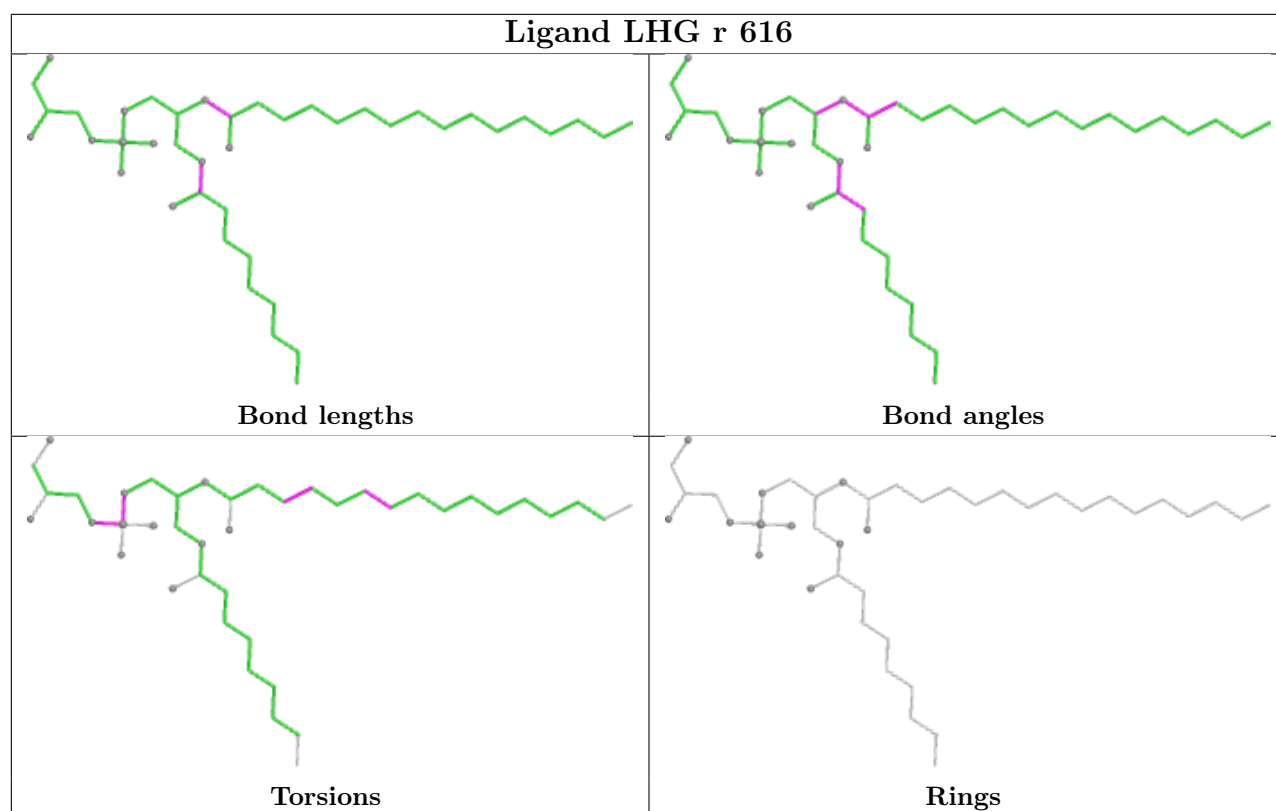
Bond angles

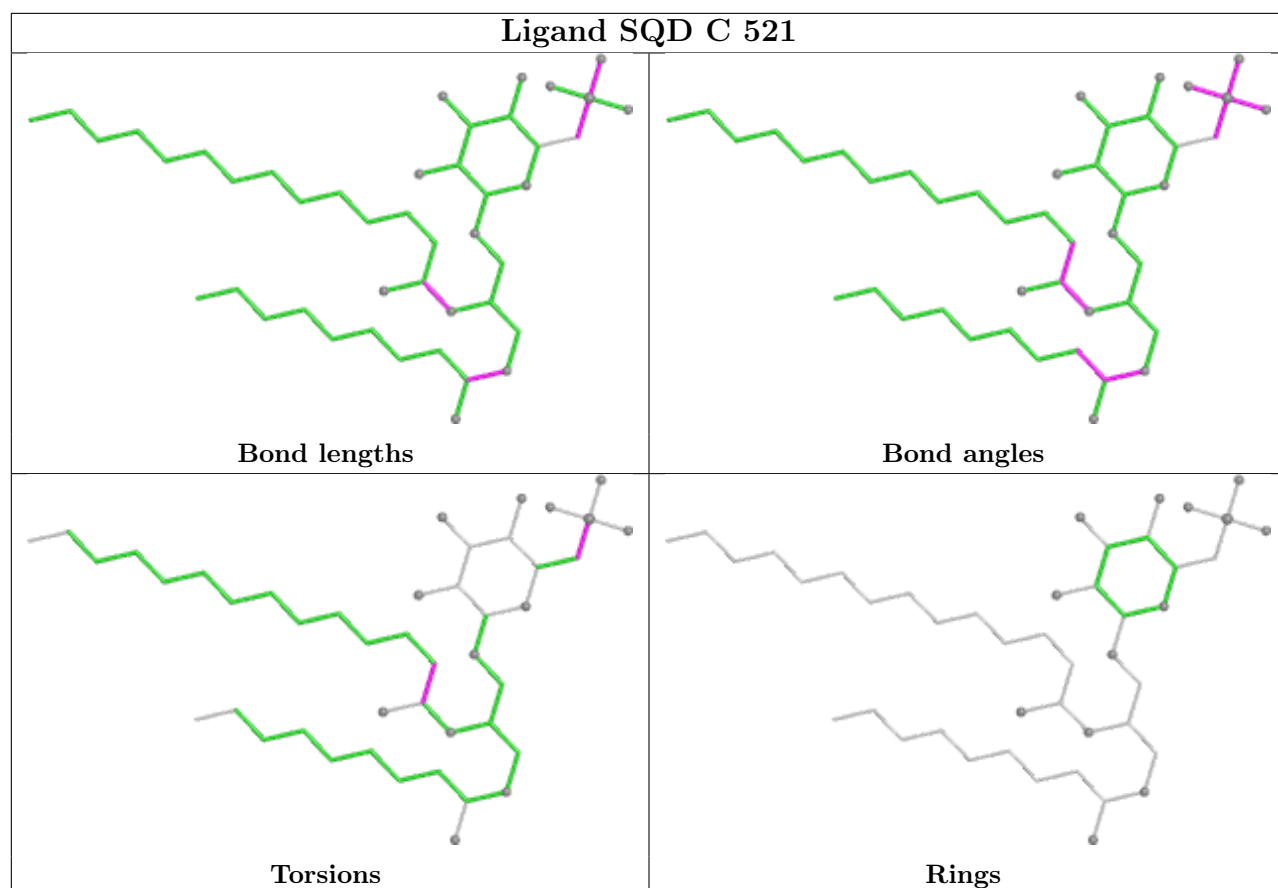
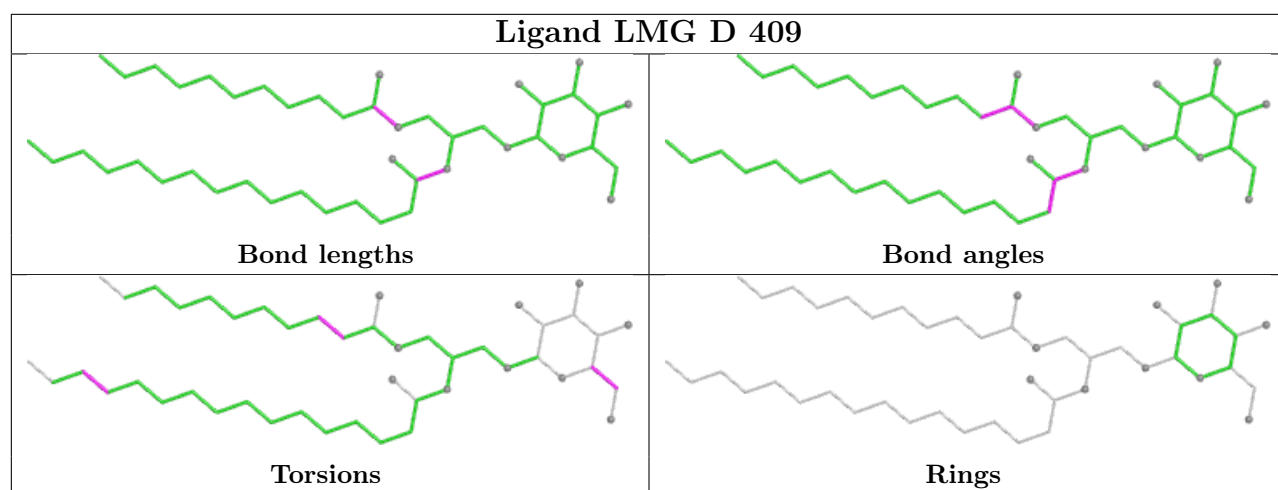


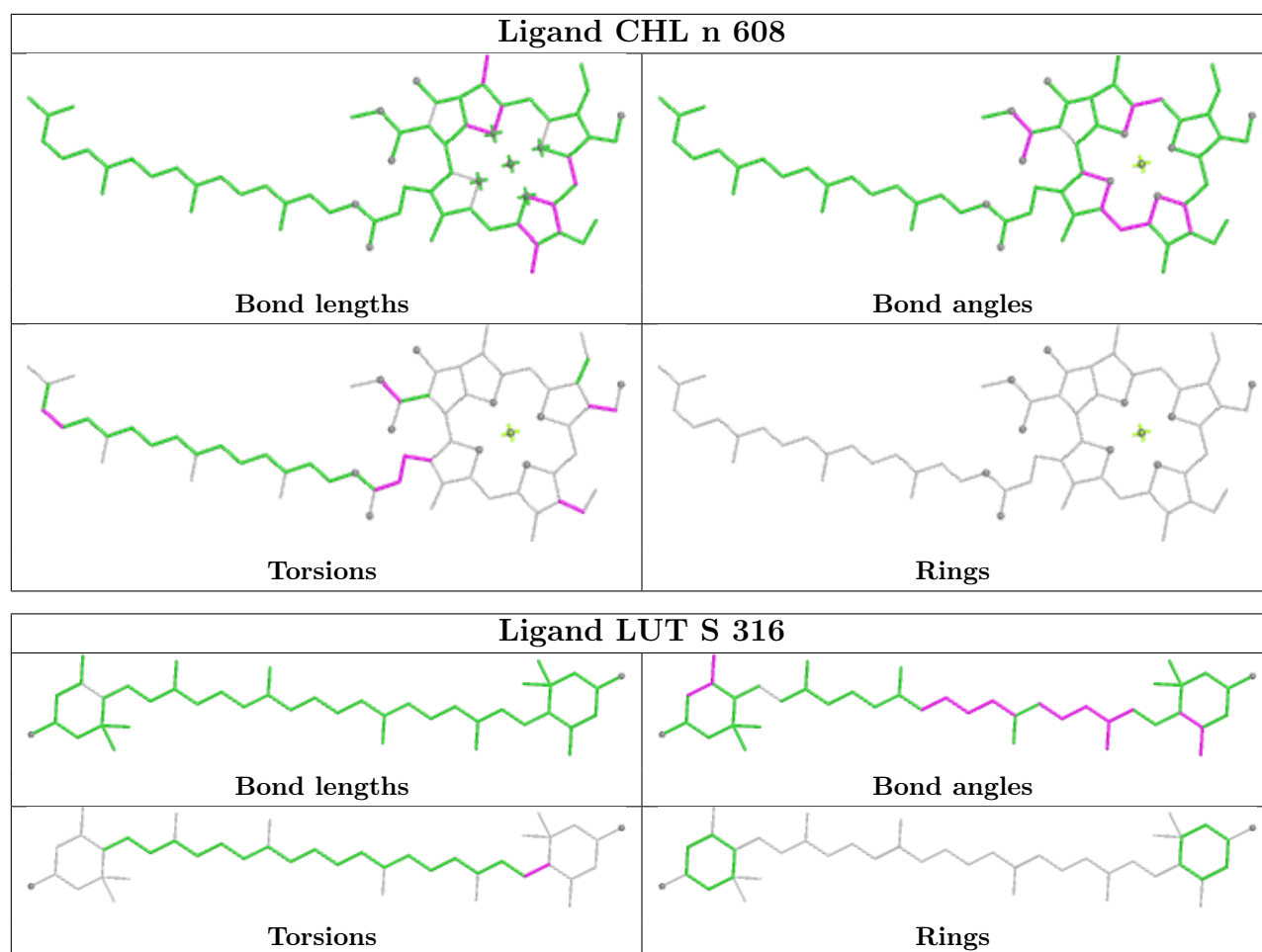
Torsions

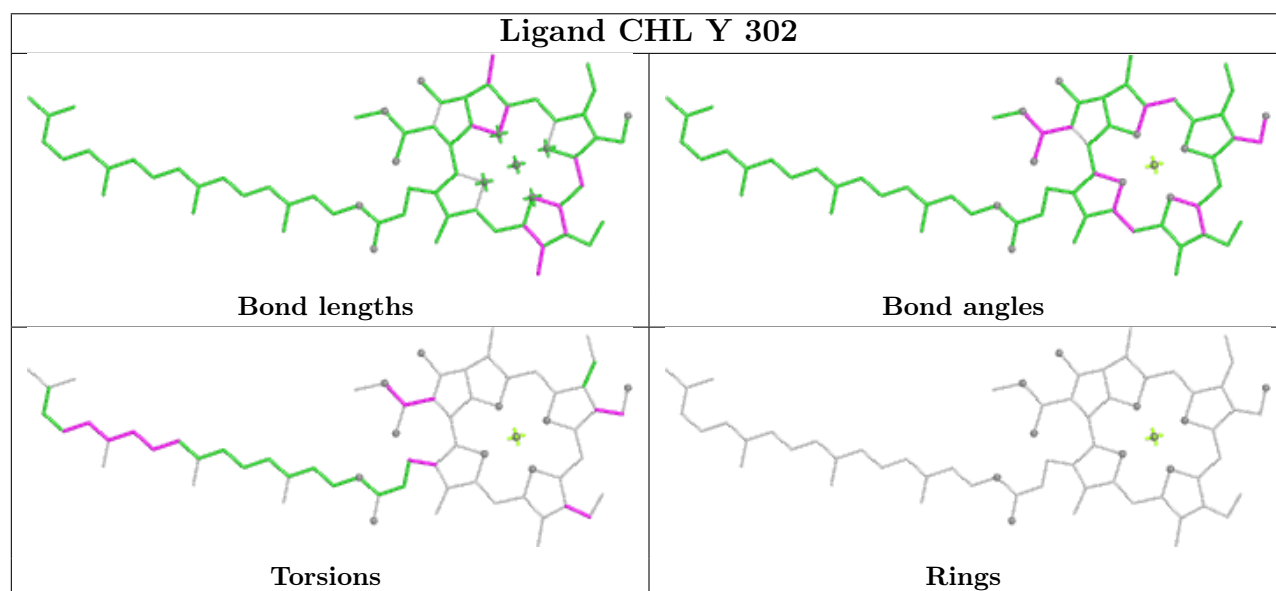
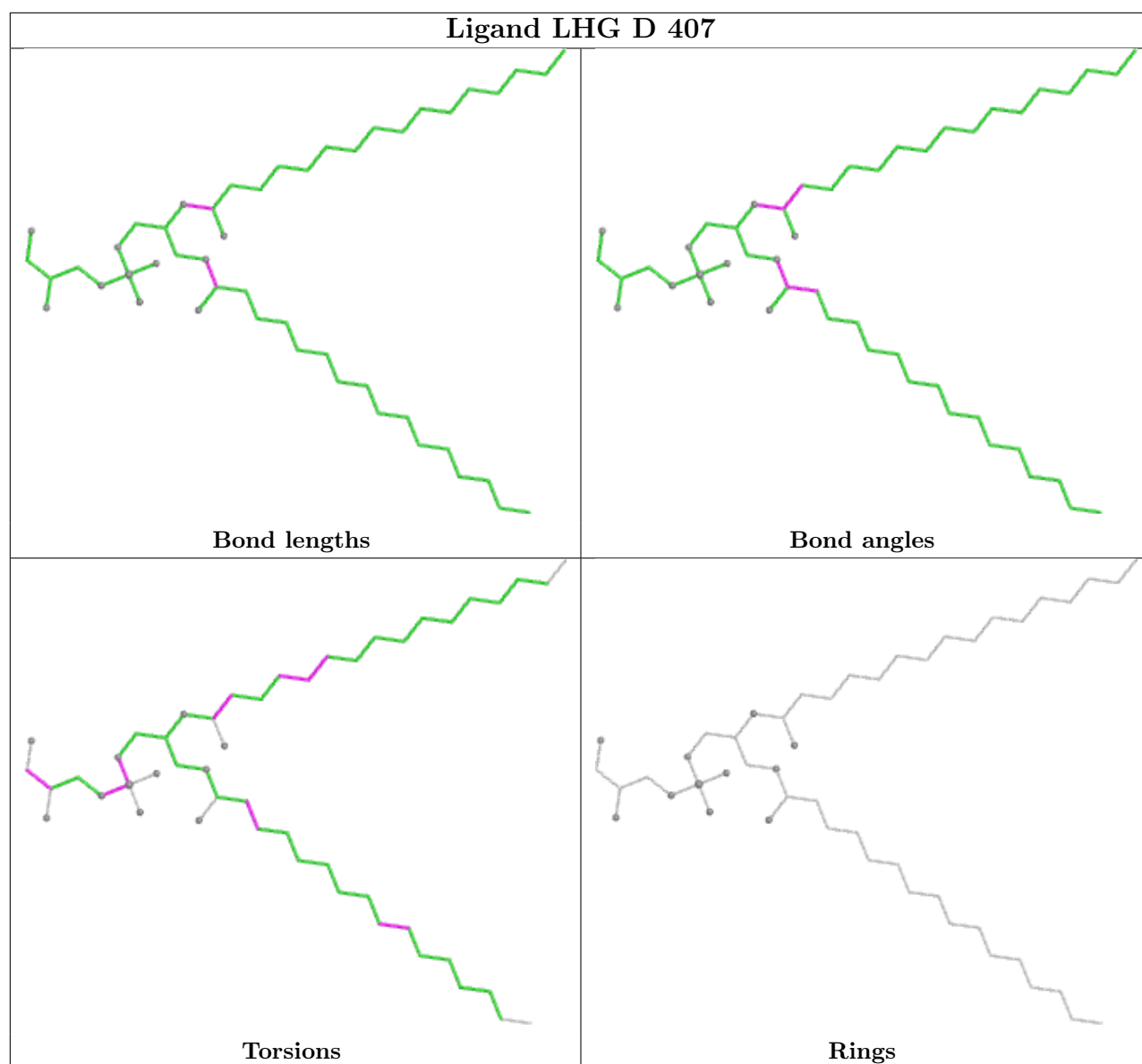


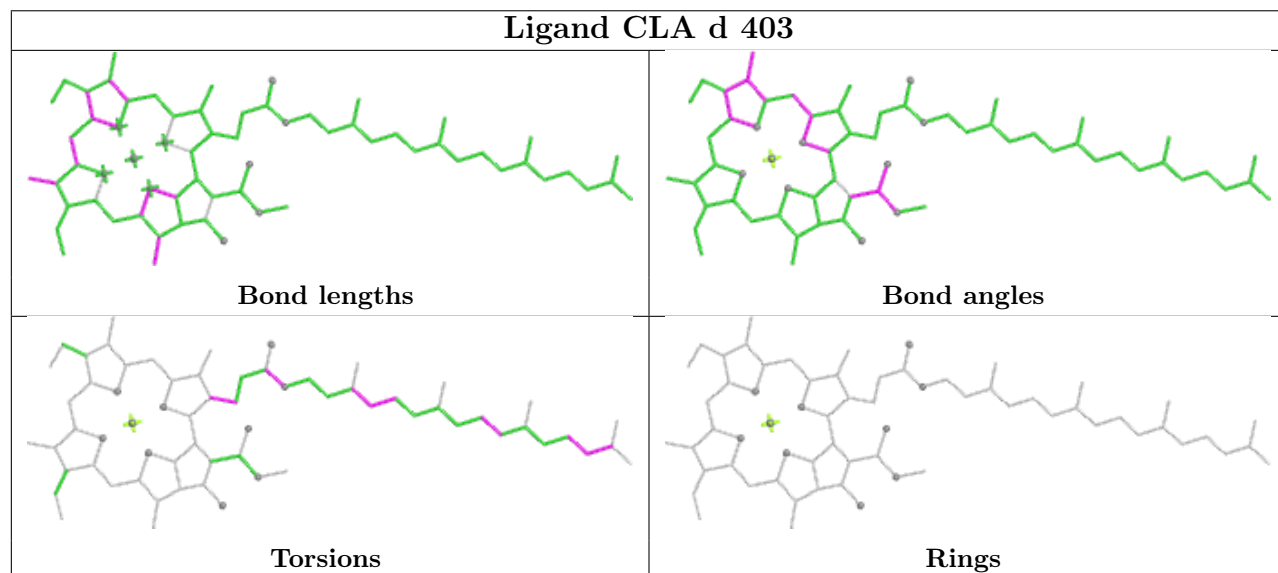
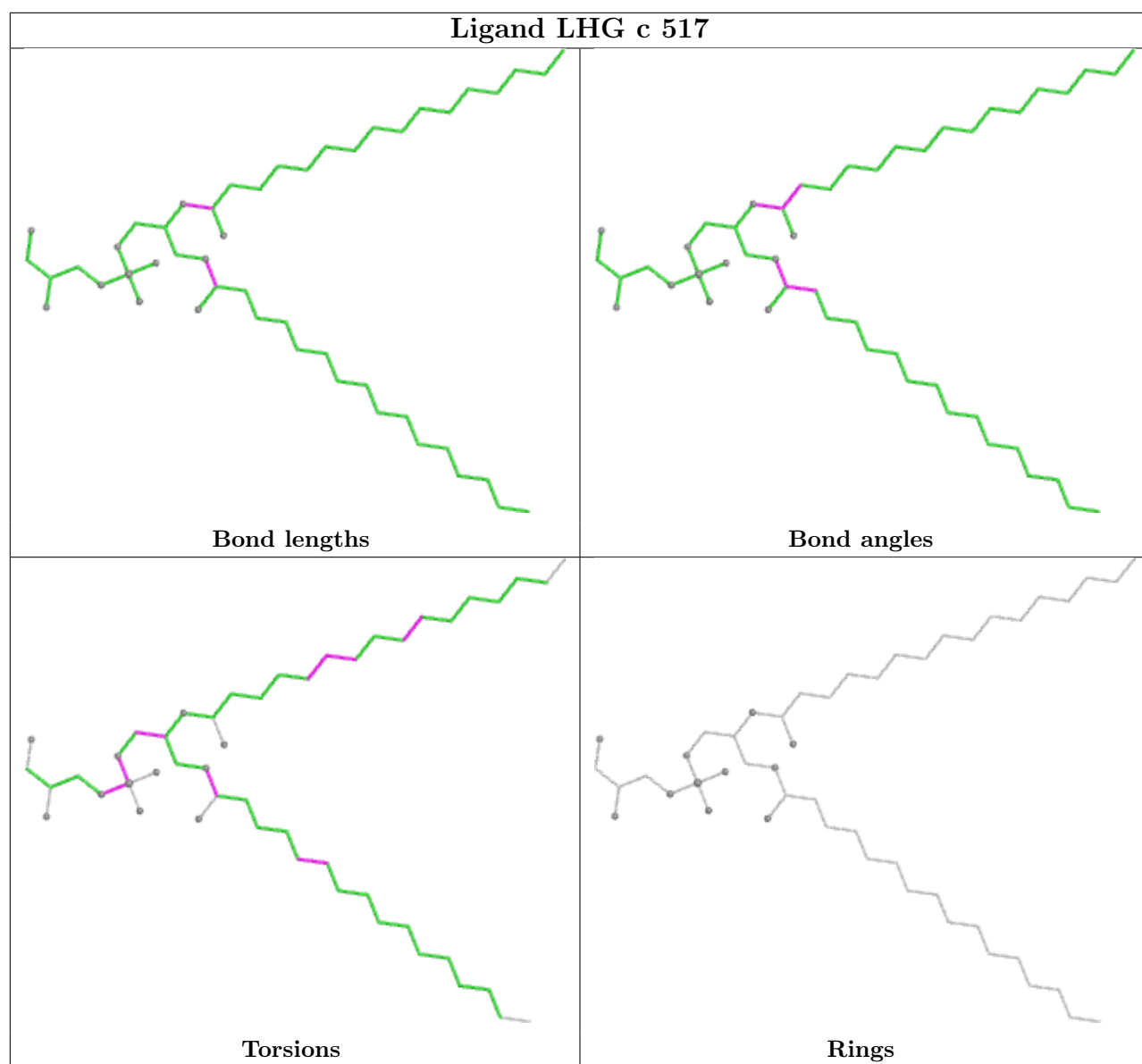
Rings

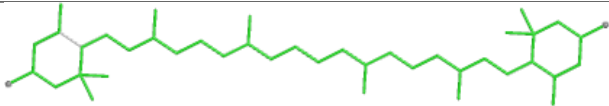
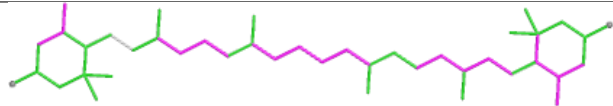
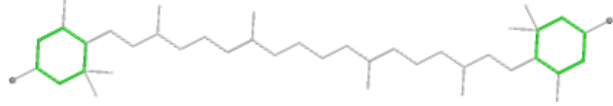


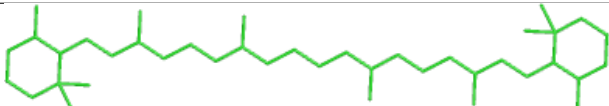
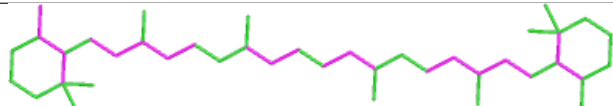
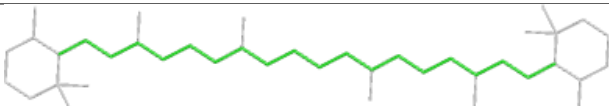
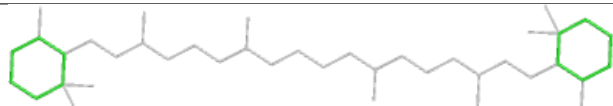


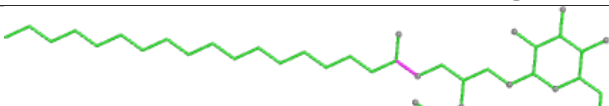
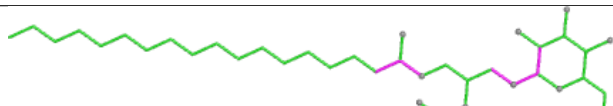
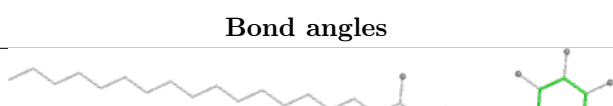


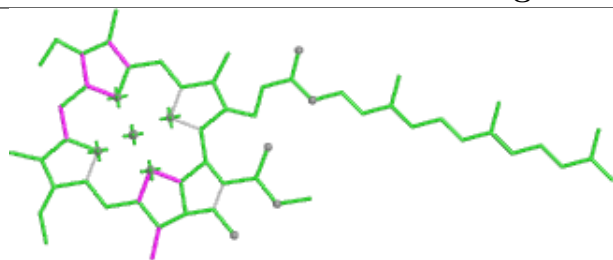
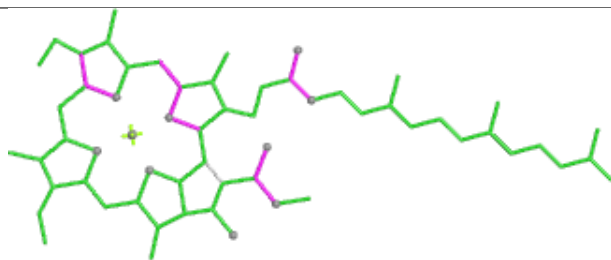
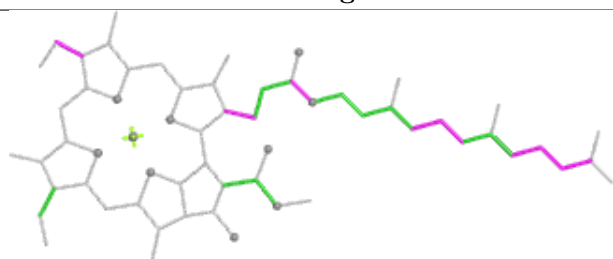
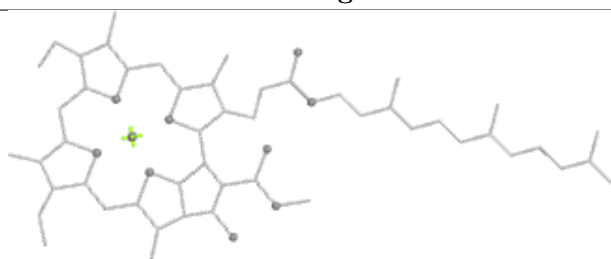
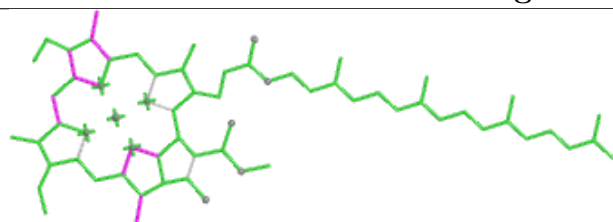
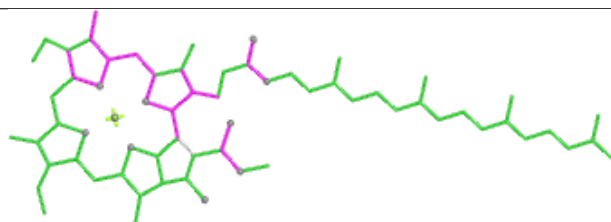
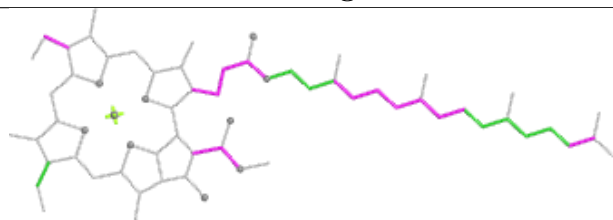
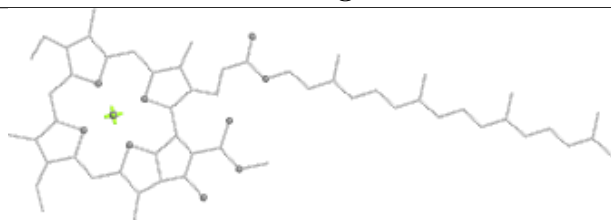




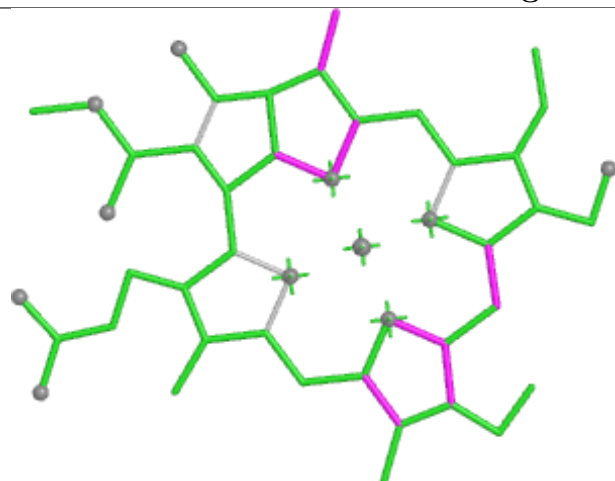
Ligand LUT r 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

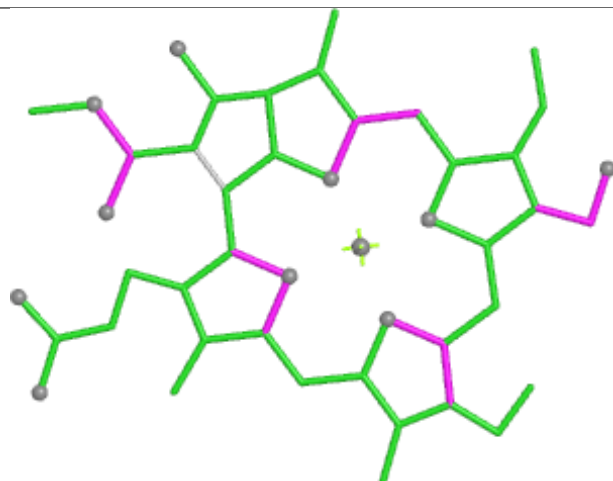
Ligand LMG S 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 312**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 614****Bond lengths****Bond angles****Torsions****Rings**

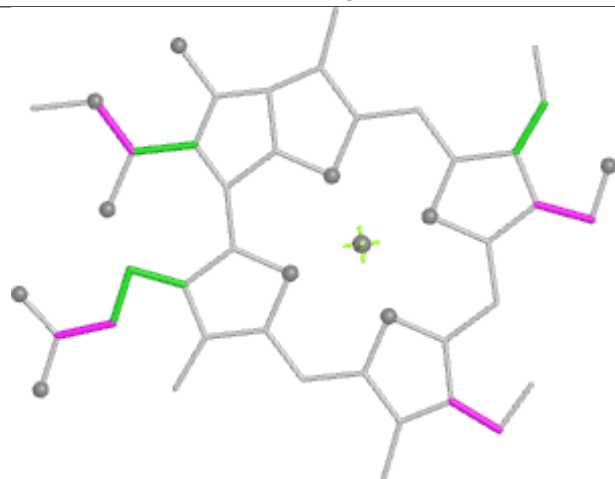
Ligand CHL s 601



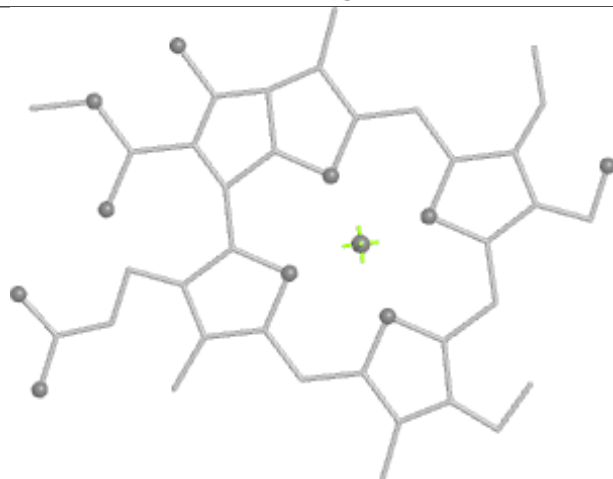
Bond lengths



Bond angles

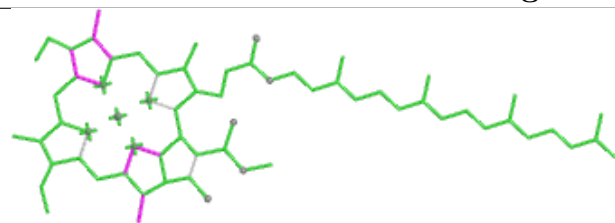


Torsions

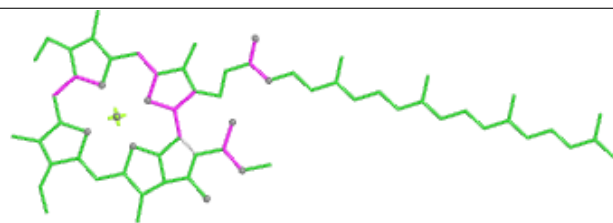


Rings

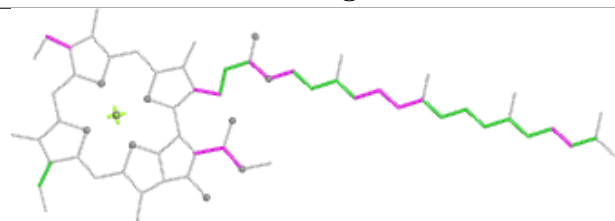
Ligand CLA c 502



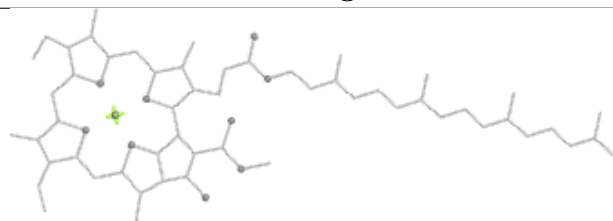
Bond lengths



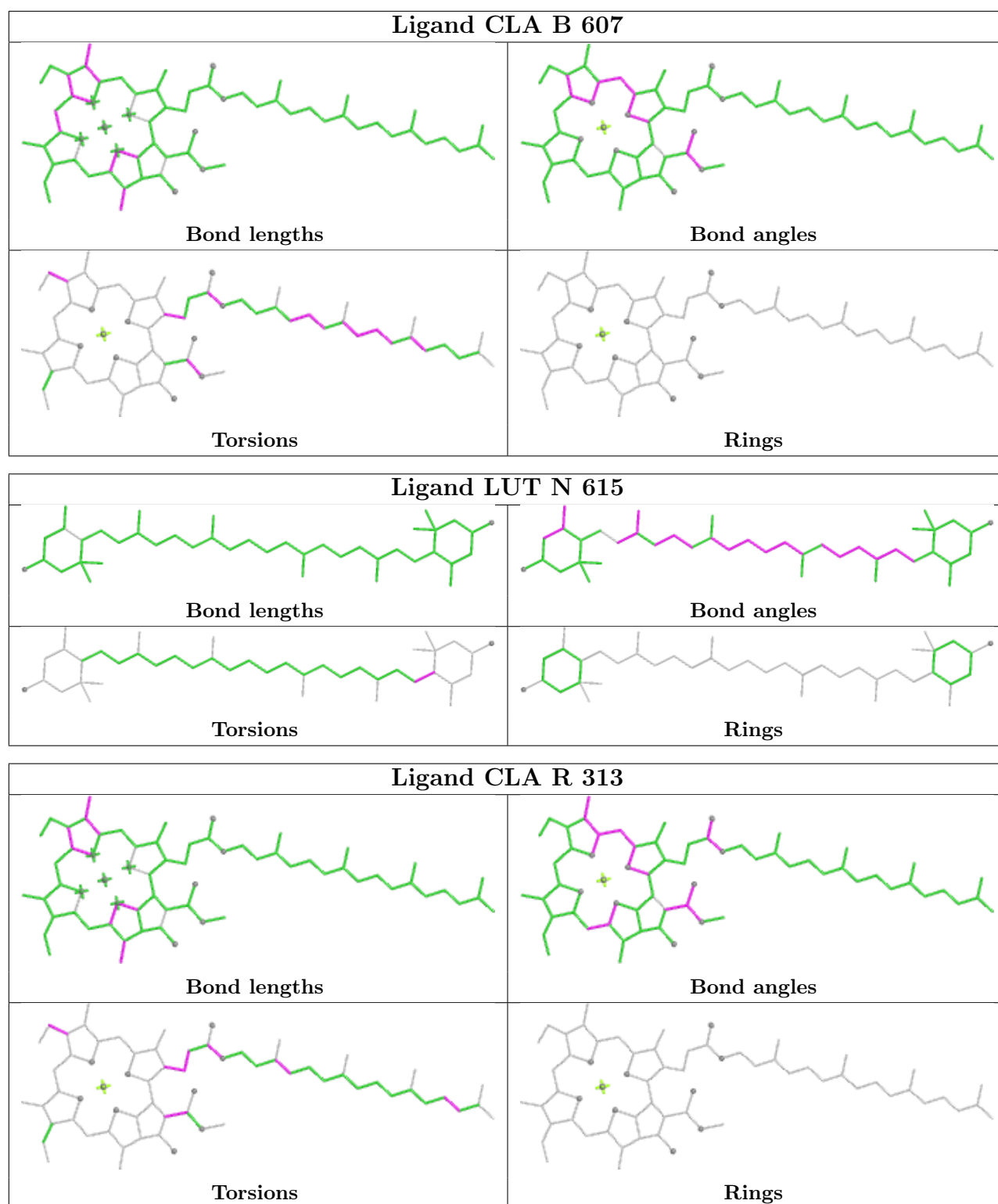
Bond angles

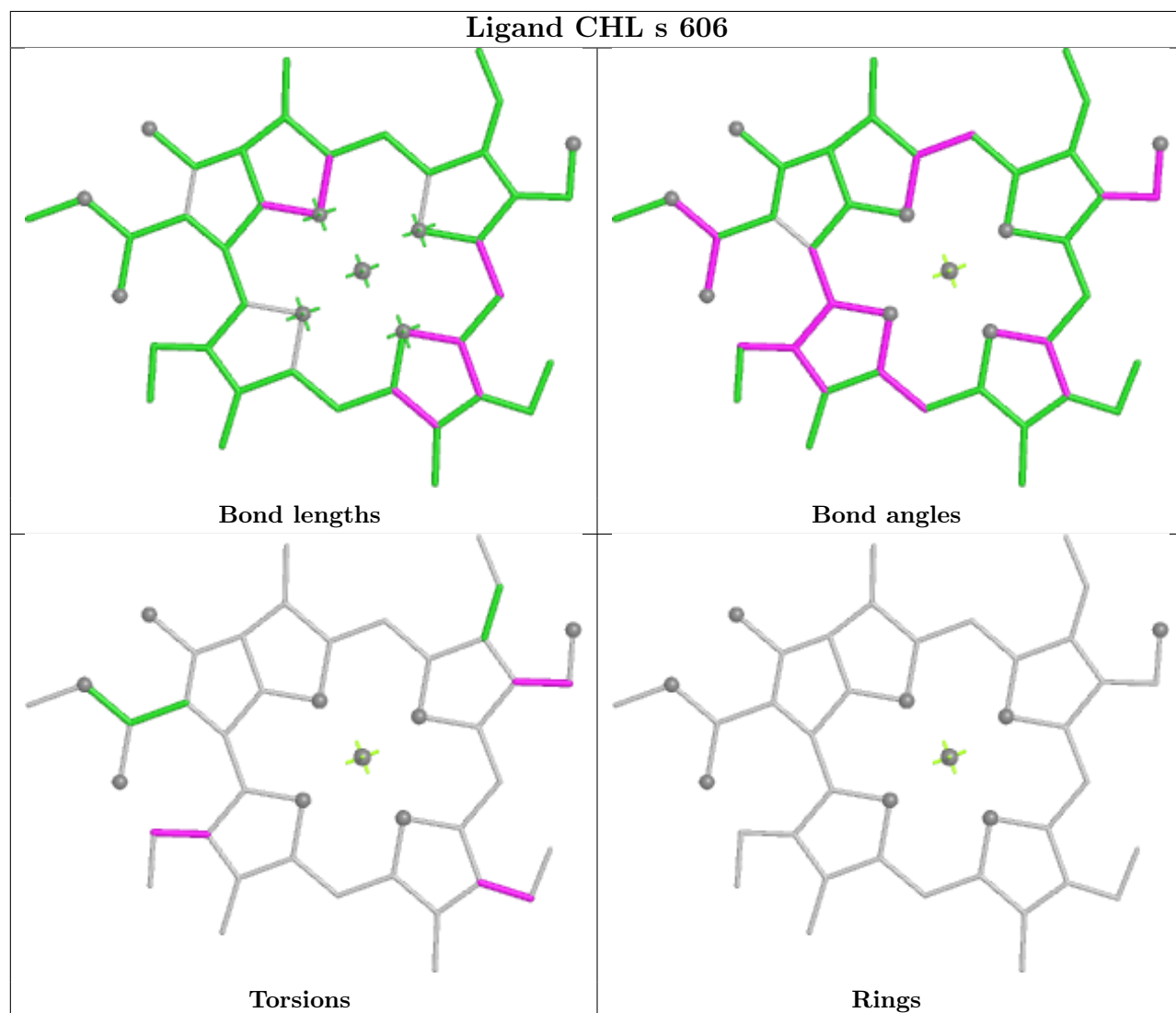
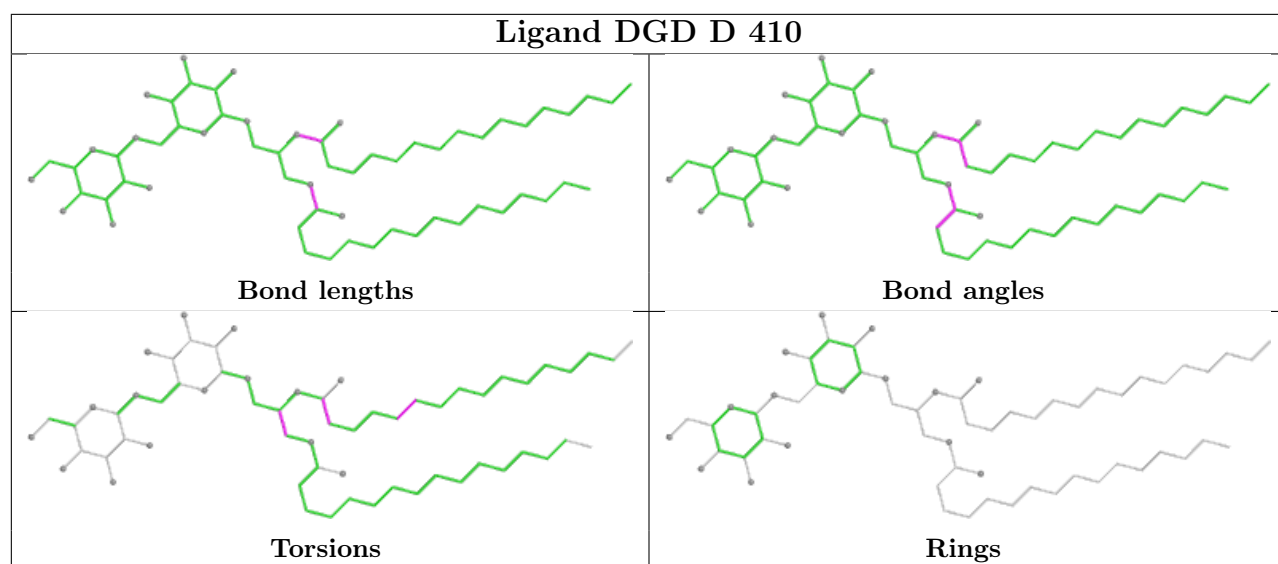


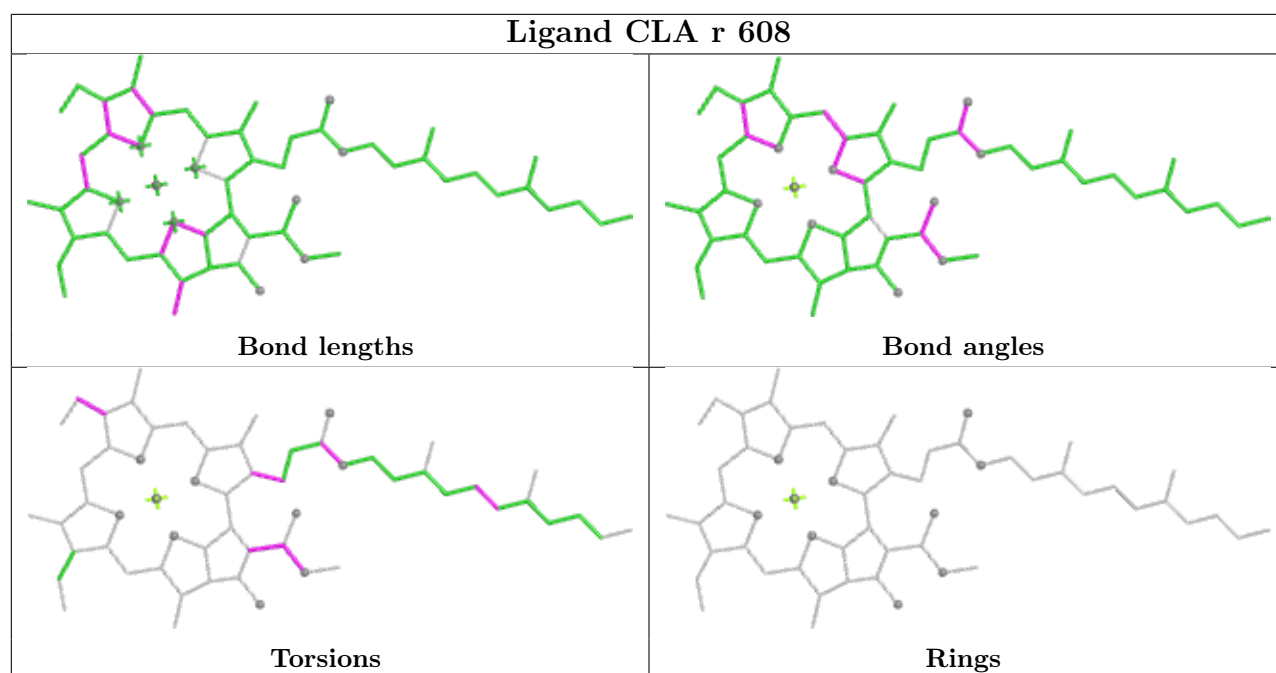
Torsions



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.

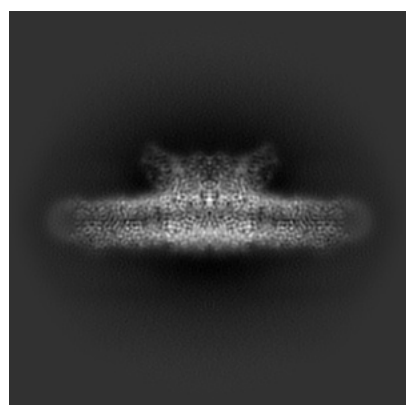
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63168. These allow visual inspection of the internal detail of the map and identification of artifacts.

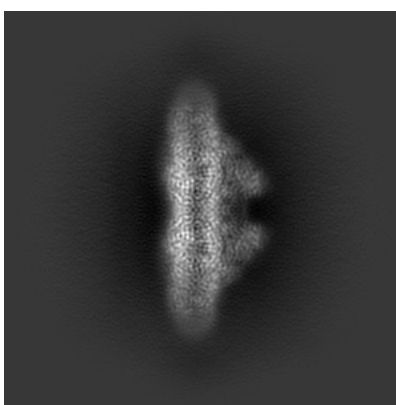
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

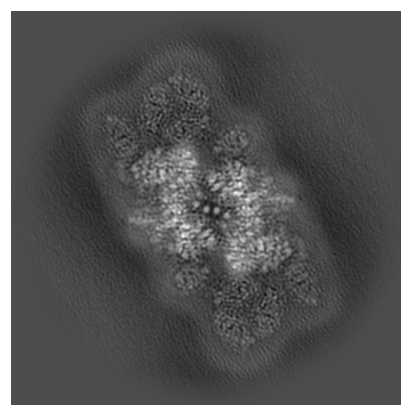
6.1.1 Primary map



X



Y

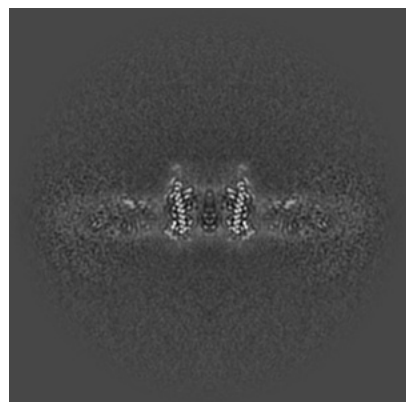


Z

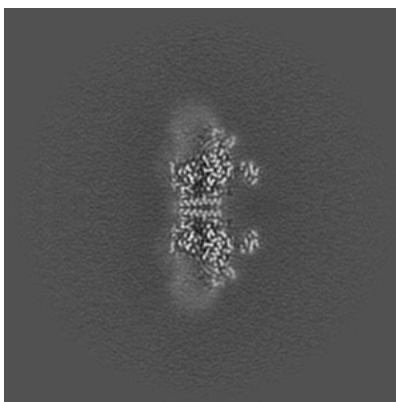
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

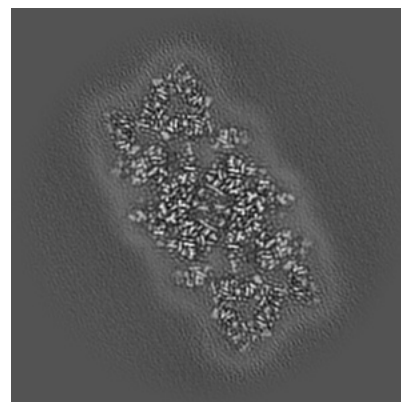
6.2.1 Primary map



X Index: 180



Y Index: 180

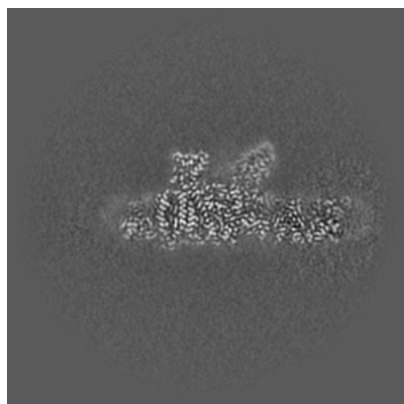


Z Index: 180

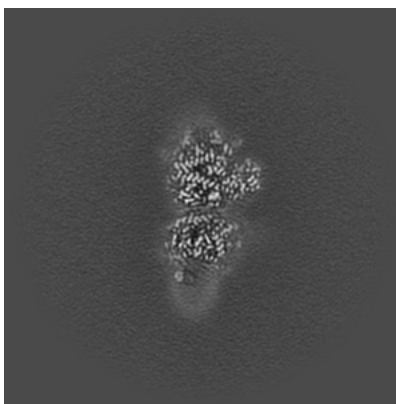
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

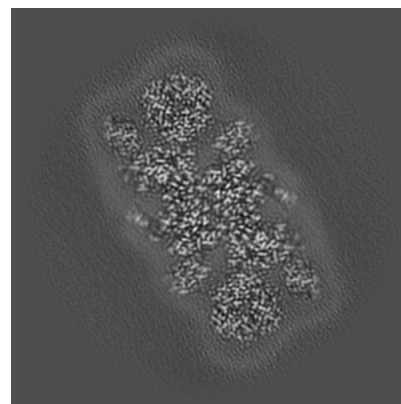
6.3.1 Primary map



X Index: 155



Y Index: 194

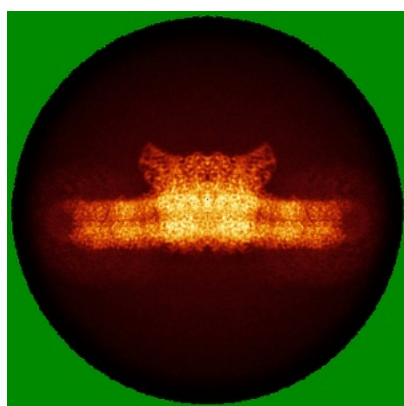


Z Index: 164

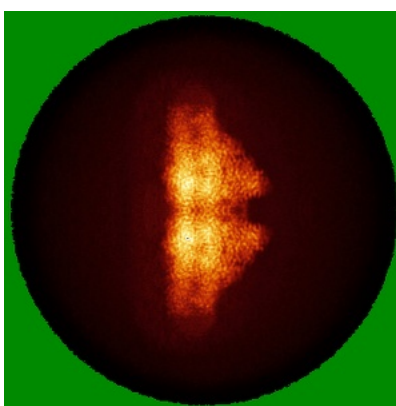
The images above show the largest variance slices of the map in three orthogonal directions.

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

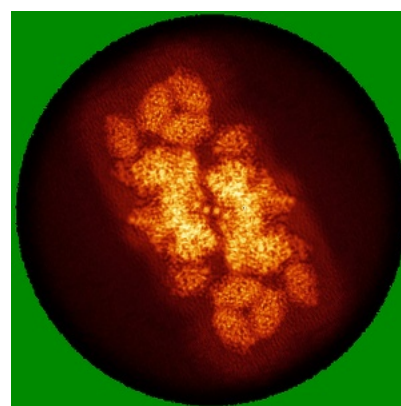
6.4.1 Primary map



X



Y



Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

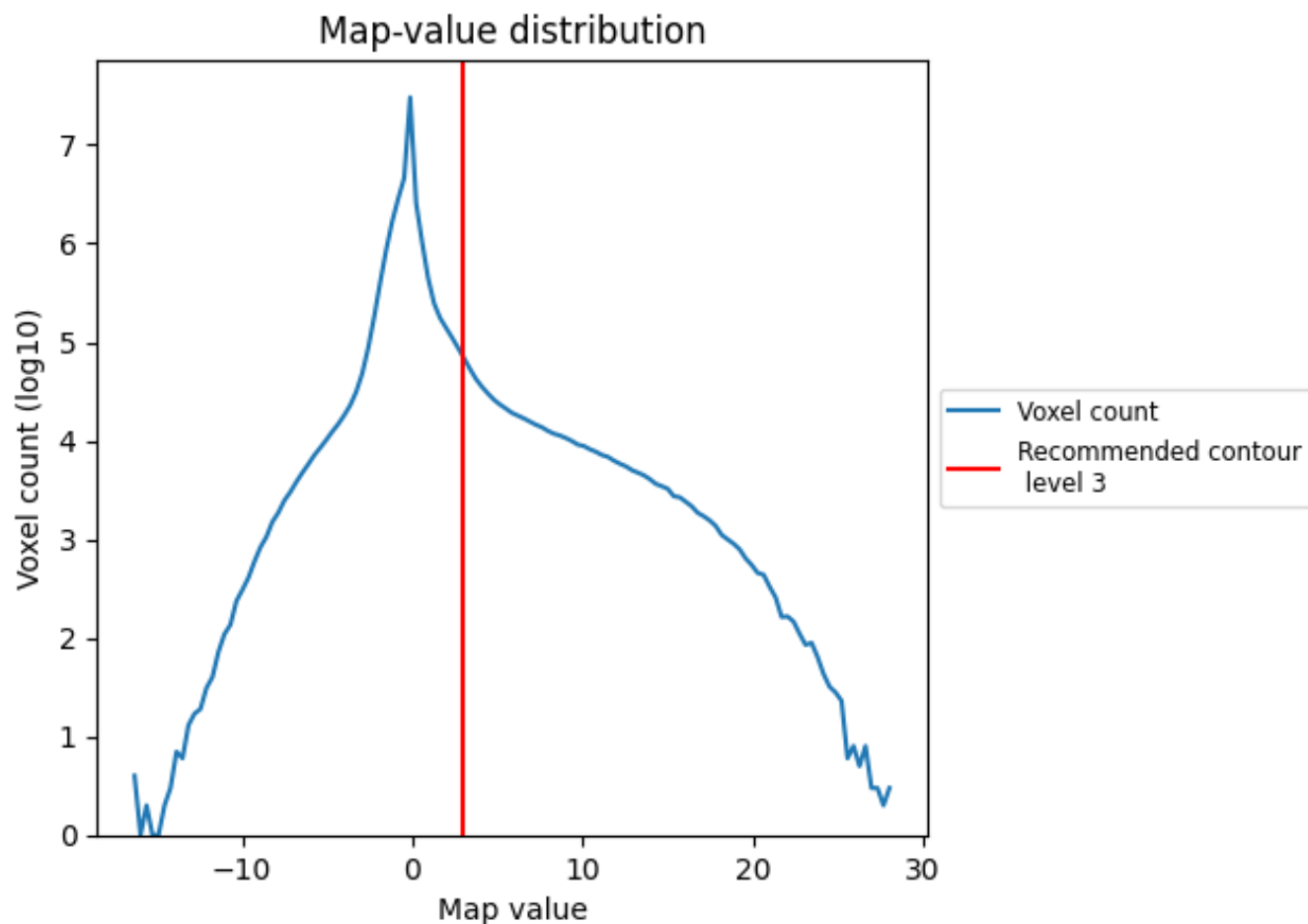
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

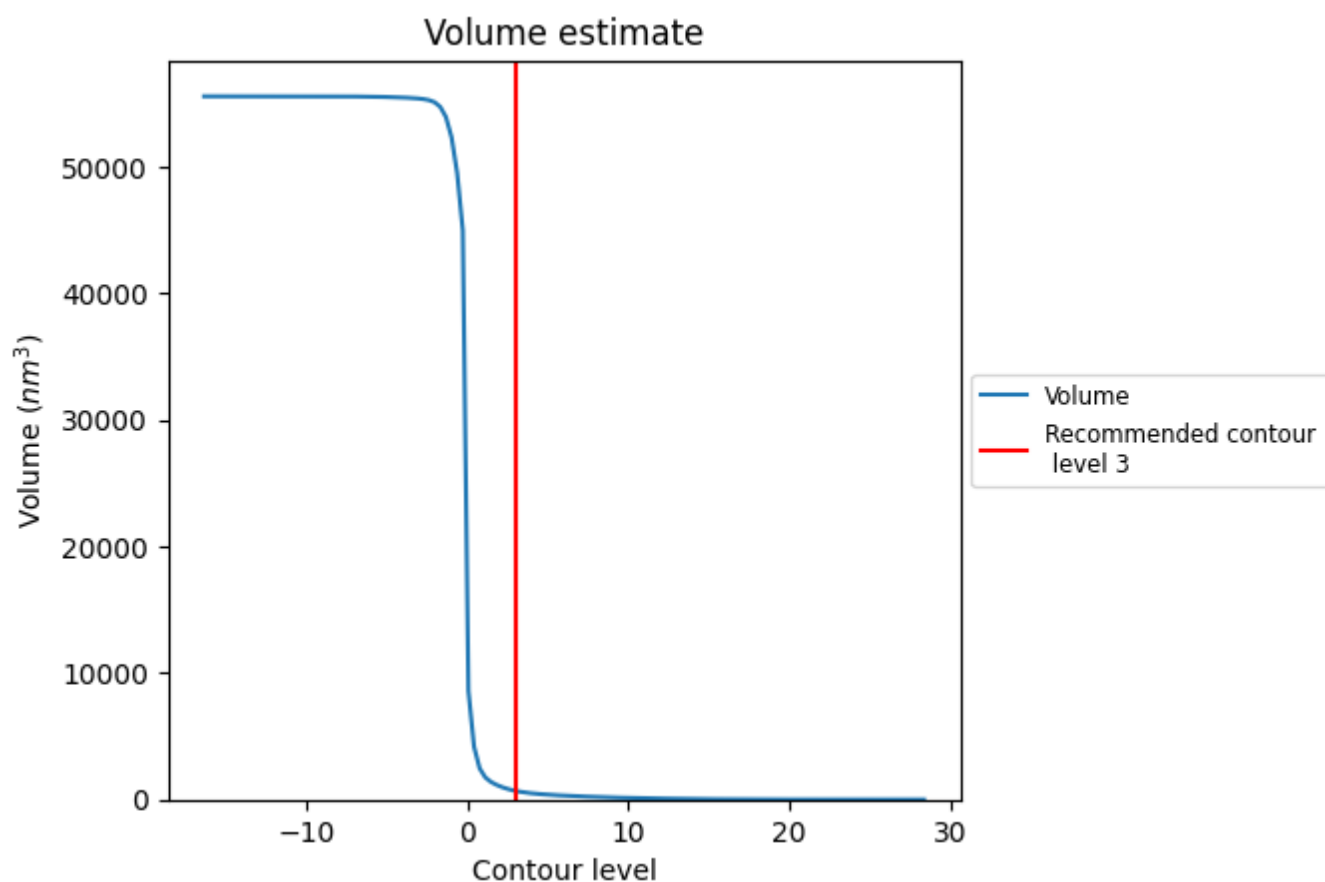
This section contains the results of statistical analysis of the map.

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.

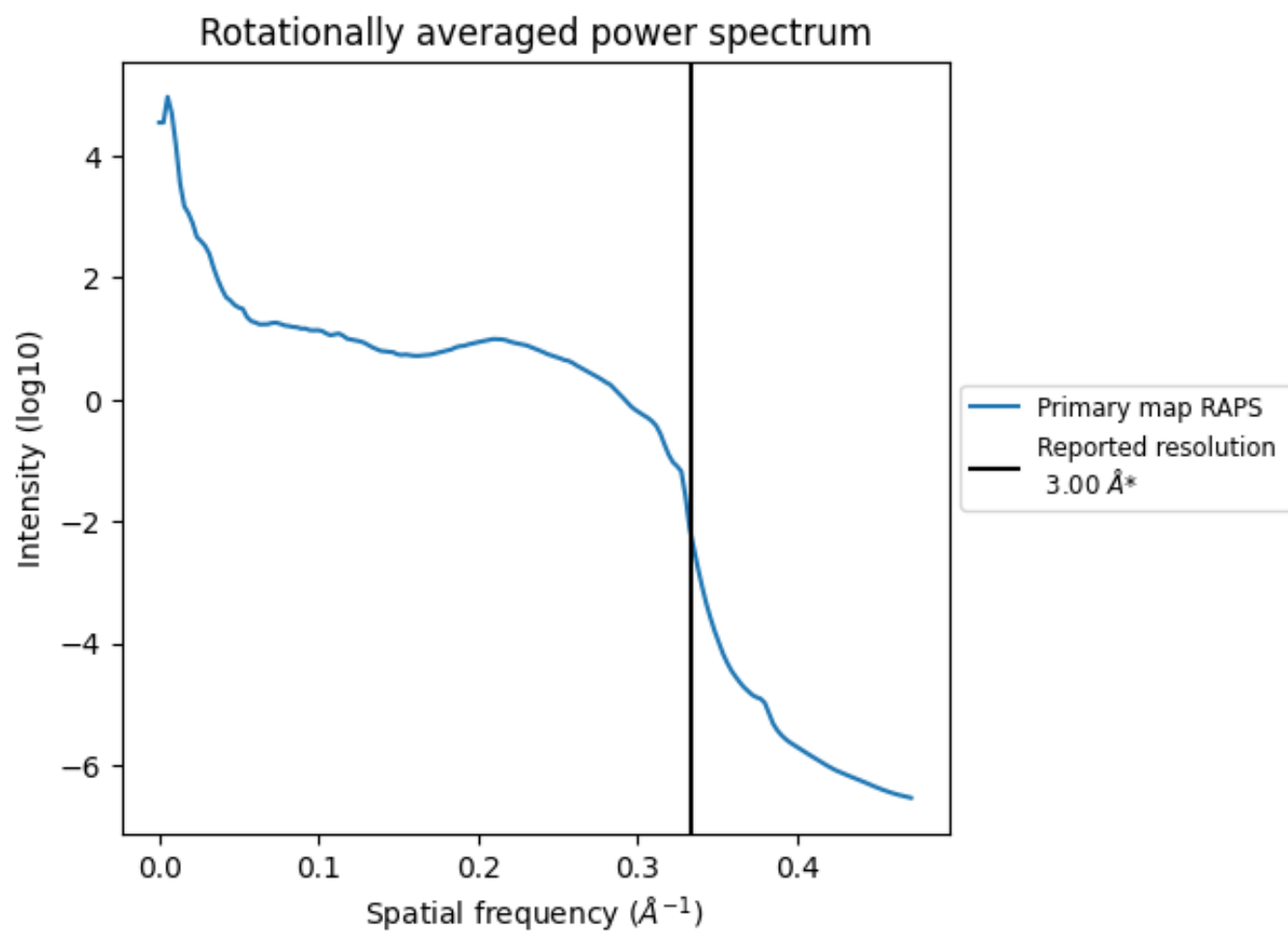
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 690 nm³; this corresponds to an approximate mass of 624 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 0.333 $\text{\AA}^{-1}$

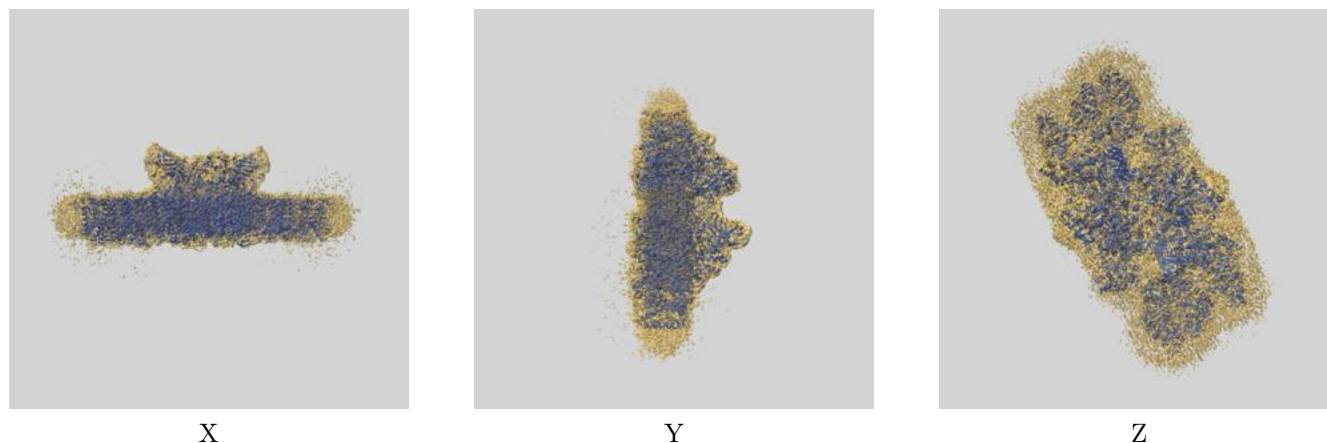
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

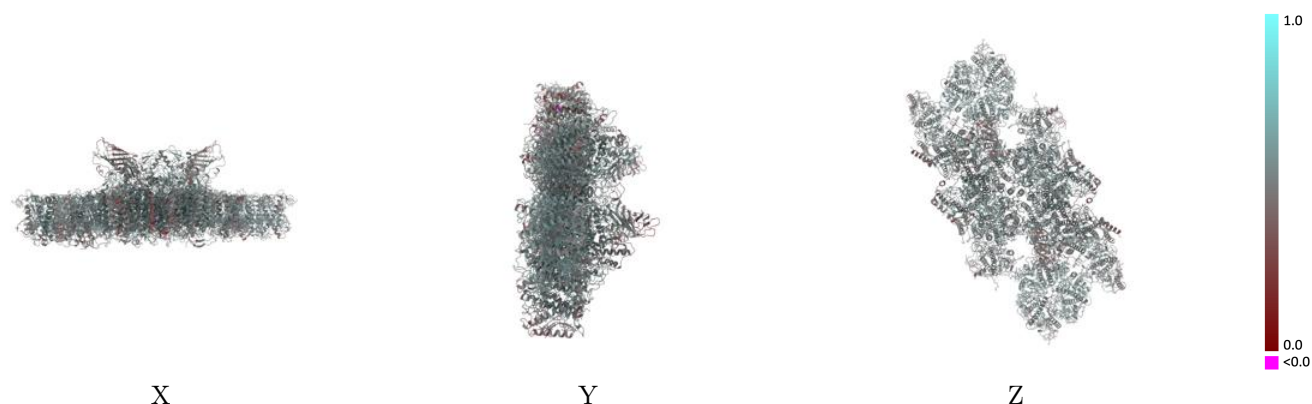
This section contains information regarding the fit between EMDB map EMD-63168 and PDB model 9LK5. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



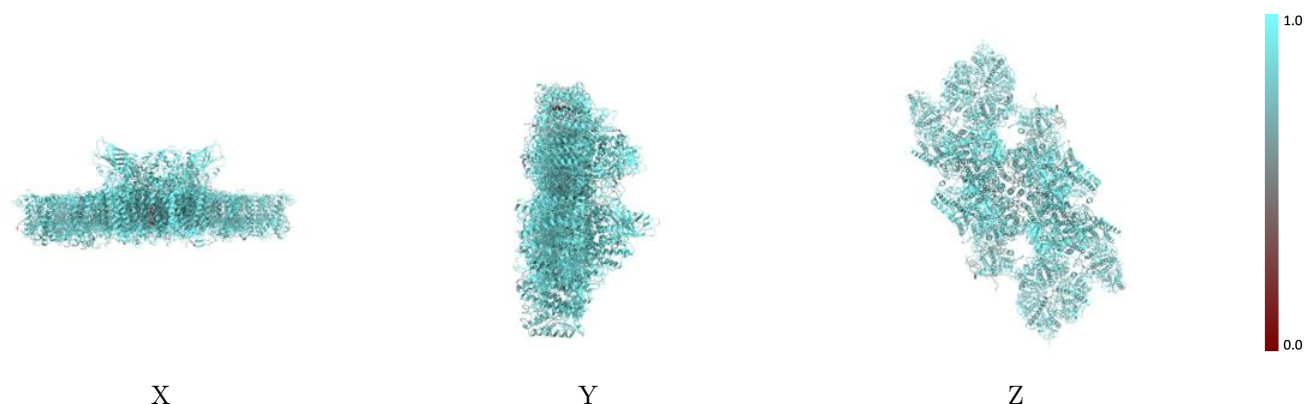
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



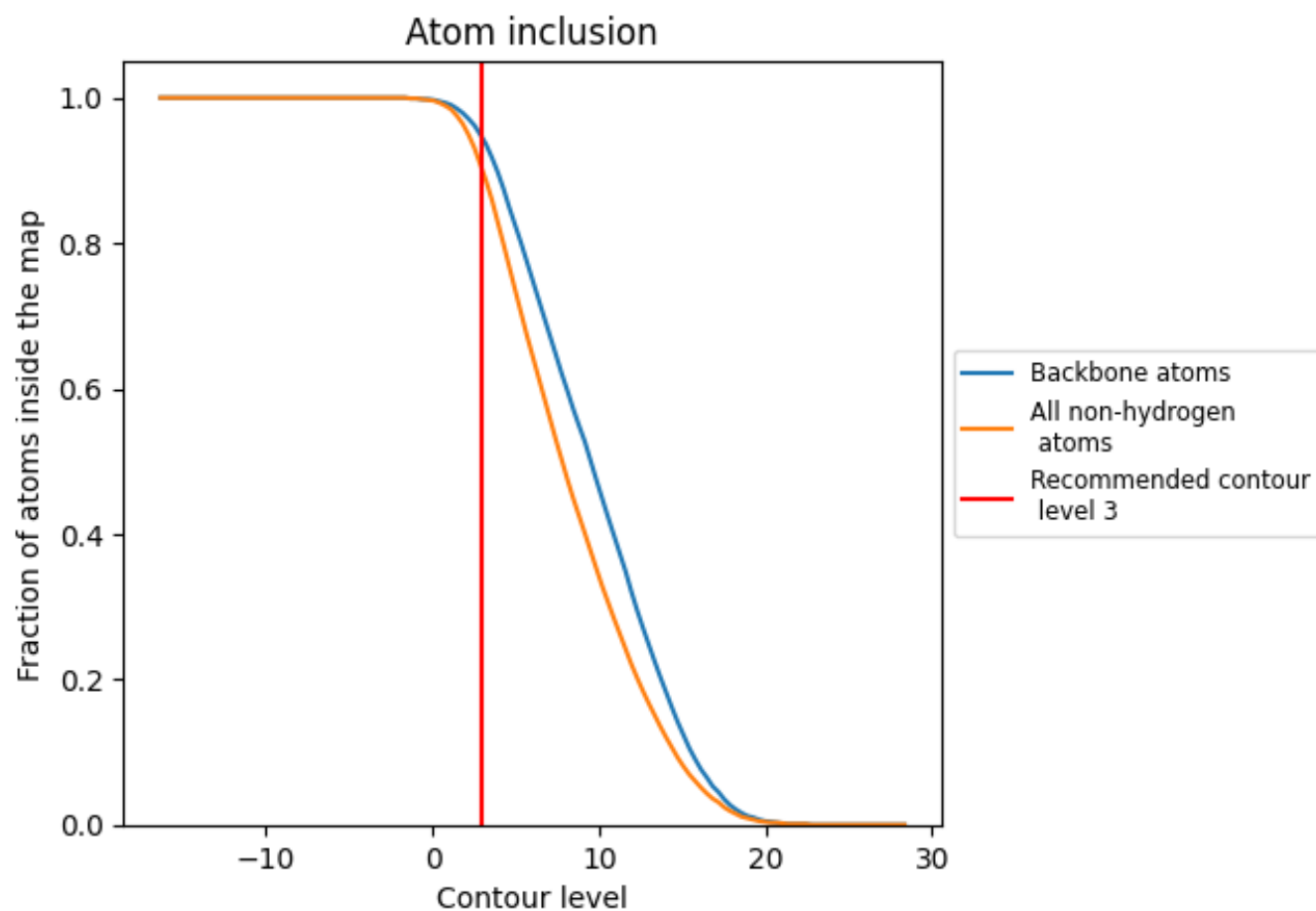
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5180
A	 0.9390	 0.5340
B	 0.9400	 0.5440
C	 0.9310	 0.5240
D	 0.9470	 0.5450
E	 0.9160	 0.4170
F	 0.9070	 0.4570
G	 0.8560	 0.5250
H	 0.9390	 0.5300
I	 0.9670	 0.5430
J	 0.6820	 0.3290
K	 0.8690	 0.4710
L	 0.8900	 0.5250
M	 0.8830	 0.4970
N	 0.8900	 0.5430
O	 0.8950	 0.4240
R	 0.8310	 0.4860
S	 0.8270	 0.4920
T	 0.9240	 0.5250
U	 0.7090	 0.4720
W	 0.8520	 0.5190
X	 0.8500	 0.4700
Y	 0.9070	 0.5580
Z	 0.8640	 0.4290
a	 0.9420	 0.5360
b	 0.9430	 0.5440
c	 0.9300	 0.5240
d	 0.9470	 0.5440
e	 0.9220	 0.4190
f	 0.9140	 0.4560
g	 0.8530	 0.5240
h	 0.9390	 0.5280
i	 0.9670	 0.5490
j	 0.6820	 0.3310
k	 0.8750	 0.4720



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Chain	Atom inclusion	Q-score
l	 0.8920	 0.5270
m	 0.8680	 0.4860
n	 0.8810	 0.5410
o	 0.8980	 0.4230
r	 0.8400	 0.4830
s	 0.8210	 0.4920
t	 0.9150	 0.5270
u	 0.7200	 0.4620
w	 0.8730	 0.5140
x	 0.8350	 0.4650
y	 0.9060	 0.5560
z	 0.8690	 0.4320