



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:19 AM JST

PDB ID : 5XNM / pdb_00005xnm
EMDB ID : EMD-6742
Title : Structure of unstacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2017-05-23
Resolution : 3.20 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

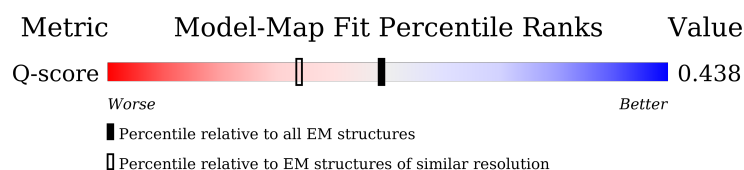
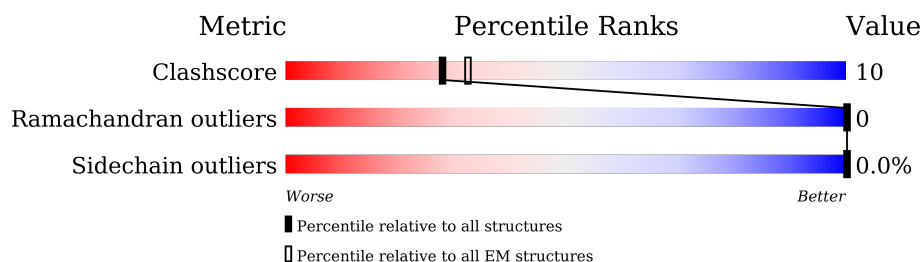
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	1	232	93% 79% 16% 6%
1	2	232	94% 77% 17% 6%
1	5	232	93% 81% 13% 6%
1	6	232	94% 75% 19% 6%

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Mol	Chain	Length	Quality of chain
1	G	232	
1	N	232	
1	Y	232	
1	g	232	
1	n	232	
1	y	232	
2	3	243	
2	7	243	
3	4	210	
3	8	210	
4	A	344	
4	a	344	
5	B	507	
5	b	507	
6	C	473	
6	c	473	
7	D	353	
7	d	353	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	73	
10	h	73	
11	I	36	

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Mol	Chain	Length	Quality of chain
11	i	36	
12	J	40	
12	j	40	
13	K	61	
13	k	61	
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	248	
16	o	248	
17	R	246	
17	r	246	
18	S	244	
18	s	244	
19	T	35	
19	t	35	
20	U	99	
20	u	99	
21	W	54	
21	w	54	
22	X	86	
22	x	86	
23	Z	62	
23	z	62	

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
24	CHL	1	607	X	-	-	-
24	CHL	1	609	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	609	X	-	-	-
24	CHL	3	601	X	-	-	-
24	CHL	3	609	X	-	-	-
24	CHL	5	607	X	-	-	-
24	CHL	5	609	X	-	-	-
24	CHL	6	607	X	-	-	-
24	CHL	6	609	X	-	-	-
24	CHL	7	601	X	-	-	-
24	CHL	7	609	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	Y	601	X	-	-	-
24	CHL	Y	607	X	-	-	-
24	CHL	Y	608	X	-	-	-
24	CHL	Y	609	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	X	-	-	-
24	CHL	s	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	y	601	X	-	-	-
24	CHL	y	607	X	-	-	-
24	CHL	y	608	X	-	-	-
24	CHL	y	609	X	-	-	-

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 92842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
4	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
5	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
6	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	340	Total	C	N	O	S	0	0
			2703	1784	443	464	12		
7	d	340	Total	C	N	O	S	0	0
			2703	1784	443	464	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total	C	N	O	0	0
			612	400	100	112		
8	e	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	34	Total	C	N	O	0	0
			247	168	38	41		
12	j	34	Total	C	N	O	0	0
			247	168	38	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total	C	N	O	0	0
			311	205	49	57		
14	l	37	Total	C	N	O	0	0
			311	205	49	57		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
15	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	214	Total	C	N	O	S	0	0
			1631	1039	260	329	3		
16	o	214	Total	C	N	O	S	0	0
			1631	1039	260	329	3		

- Molecule 17 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		
17	r	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

- Molecule 18 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		
18	s	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		

- Molecule 19 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 20 is a protein called Photosystem II luminal extrinsic protein Tn, PsbTn.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

- Molecule 21 is a protein called Photosystem II reaction center protein W, PSBW.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
21	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

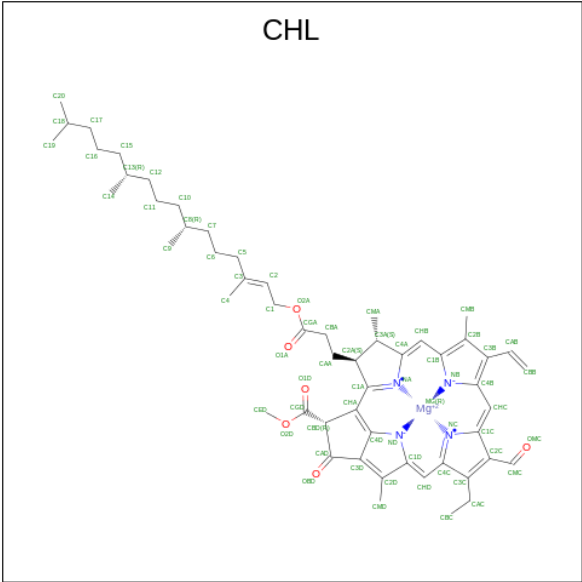
- Molecule 22 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	39	Total	C	N	O		0	0
			276	180	46	50			
22	x	39	Total	C	N	O		0	0
			276	180	46	50			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
23	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 63	C 52	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 62	C 51	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	3	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	3	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	4	1	Total 45	C 34	Mg 1	N 4	O 6	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 63	C 52	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 62	C 51	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0

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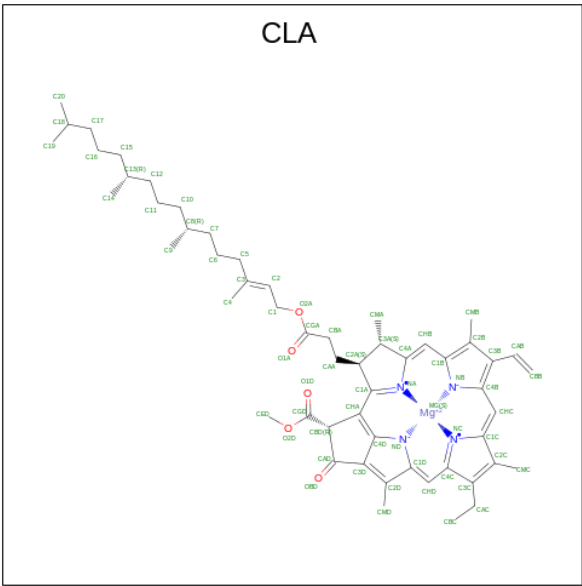
Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	7	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	7	1	Total 53	C 42	Mg 1	N 4	O 6	0
24	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	8	1	Total 45	C 34	Mg 1	N 4	O 6	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	g	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	r	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	r	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	r	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	y	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
			Total	C	Mg	N	O	
			55	45	1	4	5	
			Total	C	Mg	N	O	
25	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
			56	46	1	4	5	
			Total	C	Mg	N	O	
			45	35	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
			Total	C	Mg	N	O	
			55	45	1	4	5	
			Total	C	Mg	N	O	
25	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
			45	35	1	4	5	
			Total	C	Mg	N	O	
			61	51	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
			Total	C	Mg	N	O	
			45	35	1	4	5	
			Total	C	Mg	N	O	
25	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
			45	35	1	4	5	
			Total	C	Mg	N	O	
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0



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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	7	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	7	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 48	C 38	Mg 1	N 4	O 5	0

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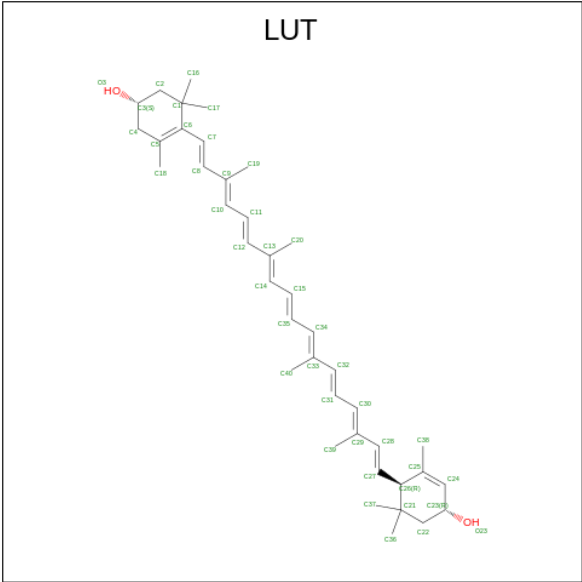
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 48	C 38	Mg 1	N 4	O 5	0

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



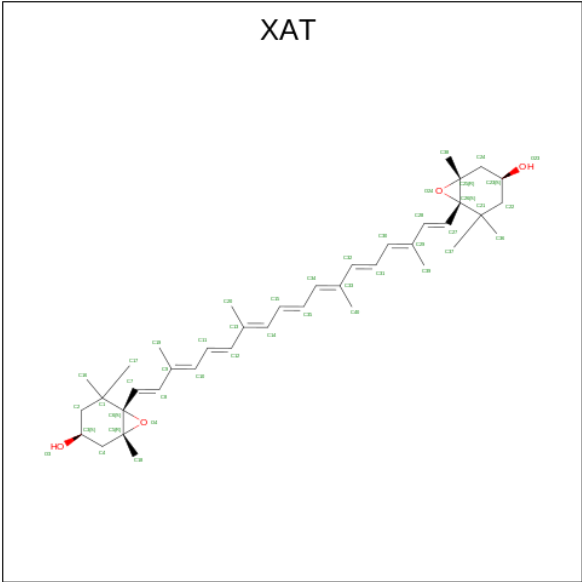
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	N	1	Total	C	O	0
			42	40	2	
26	N	1	Total	C	O	0
			42	40	2	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
26	Y	1	Total	C	O	0
			42	40	2	
26	Y	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	8	1	Total	C	O	0
			42	40	2	
26	g	1	Total	C	O	0
			42	40	2	
26	g	1	Total	C	O	0
			42	40	2	
26	n	1	Total	C	O	0
			42	40	2	
26	n	1	Total	C	O	0
			42	40	2	
26	r	1	Total	C	O	0
			42	40	2	
26	s	1	Total	C	O	0
			42	40	2	
26	s	1	Total	C	O	0
			42	40	2	
26	y	1	Total	C	O	0
			42	40	2	
26	y	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



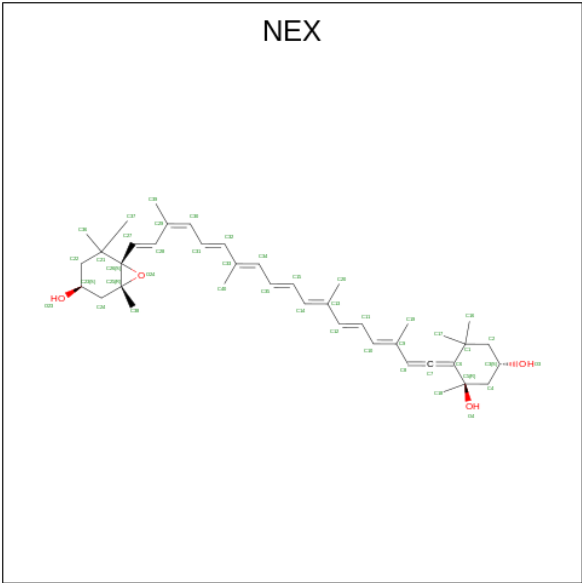
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
27	r	1	Total	C	O	0
			44	40	4	
27	y	1	Total	C	O	0
			44	40	4	

- Molecule 28 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



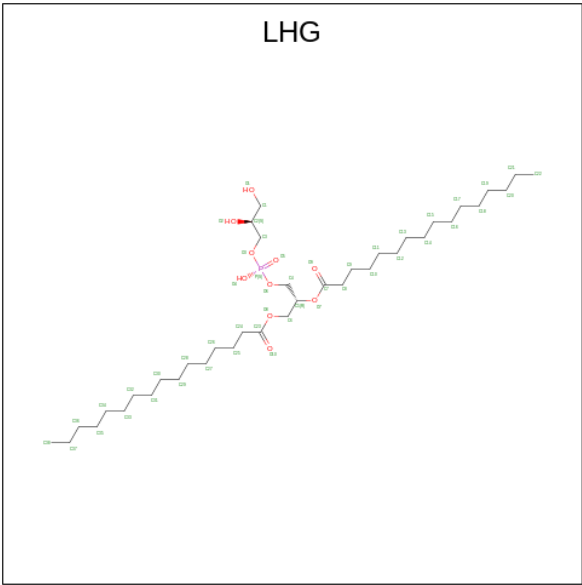
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			44	40	4	
28	S	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	s	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
29	1	1	Total	C	O	P	0
			41	30	10	1	
29	2	1	Total	C	O	P	0
			37	26	10	1	
29	3	1	Total	C	O	P	0
			47	36	10	1	

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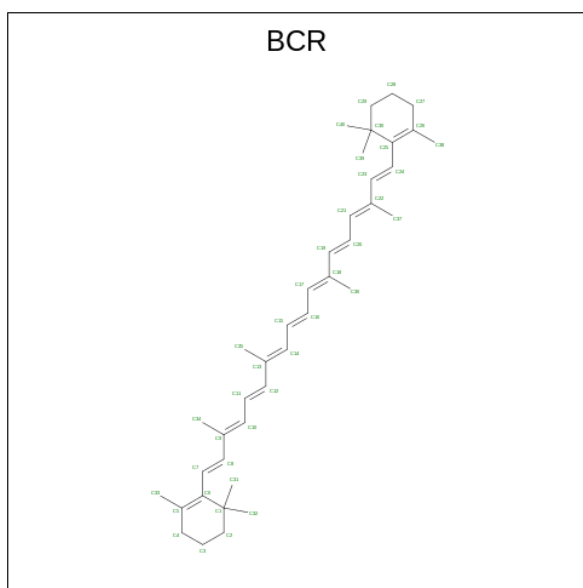
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total 21	C 10	O 10	P 1	0
29	B	1	Total 47	C 36	O 10	P 1	0
29	B	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	D	1	Total 46	C 35	O 10	P 1	0
29	D	1	Total 49	C 38	O 10	P 1	0
29	D	1	Total 43	C 32	O 10	P 1	0
29	G	1	Total 49	C 38	O 10	P 1	0
29	L	1	Total 49	C 38	O 10	P 1	0
29	N	1	Total 49	C 38	O 10	P 1	0
29	R	1	Total 42	C 31	O 10	P 1	0
29	S	1	Total 49	C 38	O 10	P 1	0
29	Y	1	Total 49	C 38	O 10	P 1	0
29	5	1	Total 41	C 30	O 10	P 1	0
29	6	1	Total 37	C 26	O 10	P 1	0
29	7	1	Total 47	C 36	O 10	P 1	0
29	8	1	Total 21	C 10	O 10	P 1	0
29	b	1	Total 47	C 36	O 10	P 1	0
29	b	1	Total 49	C 38	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	c	1	Total	C	O	P	0
			49	38	10	1	
29	c	1	Total	C	O	P	0
			49	38	10	1	
29	c	1	Total	C	O	P	0
			49	38	10	1	
29	d	1	Total	C	O	P	0
			46	35	10	1	
29	d	1	Total	C	O	P	0
			49	38	10	1	
29	d	1	Total	C	O	P	0
			43	32	10	1	
29	g	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	
29	n	1	Total	C	O	P	0
			49	38	10	1	
29	r	1	Total	C	O	P	0
			42	31	10	1	
29	s	1	Total	C	O	P	0
			49	38	10	1	
29	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



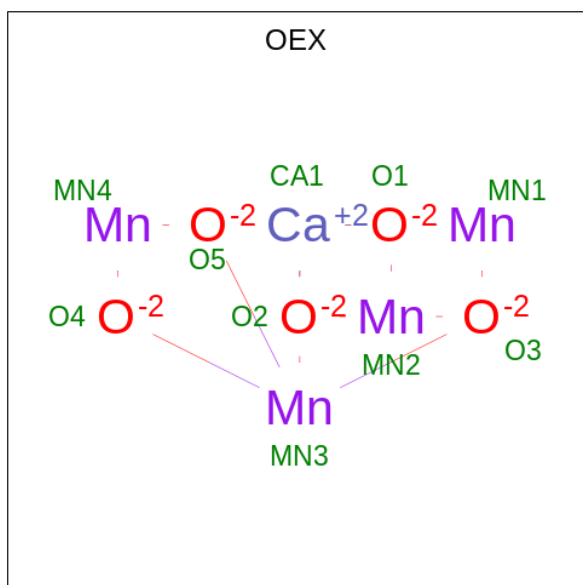
Mol	Chain	Residues	Atoms	AltConf
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	d	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
30	h	1	Total C 40 40	0
30	t	1	Total C 40 40	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

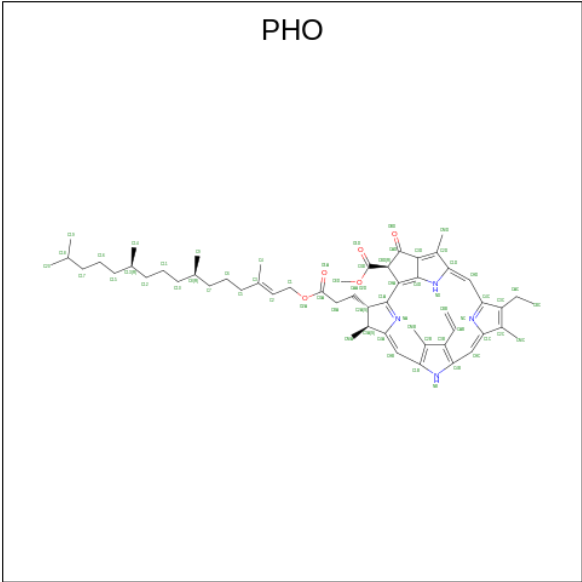


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Ca Mn O 10 1 4 5	0
31	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 32 is FE (II) ION (CCD ID: FE2) (formula: Fe).

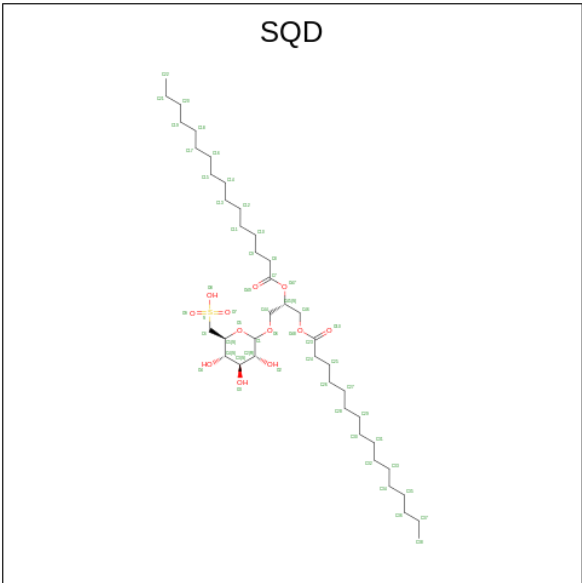
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Fe 1 1	0
32	a	1	Total Fe 1 1	0

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



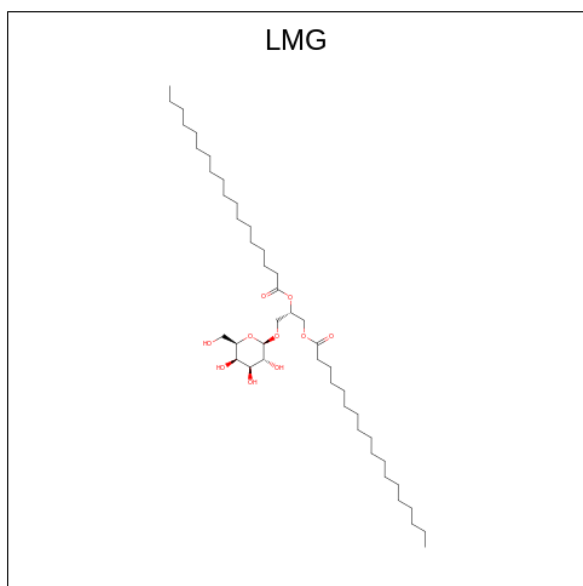
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 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
34	A	1	Total	C	O	S	0
			50	37	12	1	
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			42	29	12	1	
34	a	1	Total	C	O	S	0
			50	37	12	1	
34	a	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



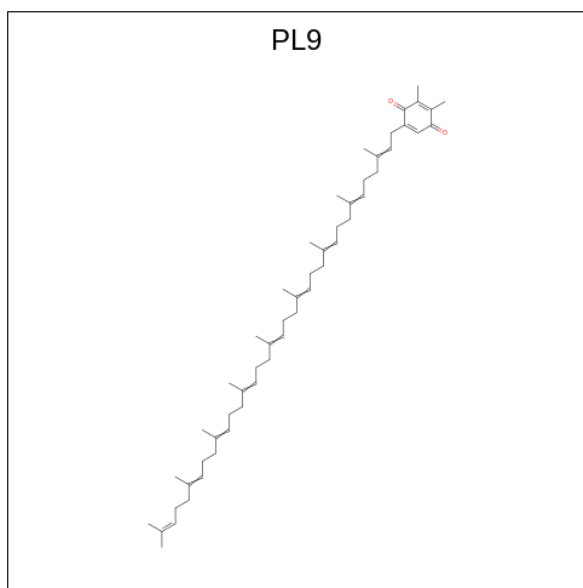
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	
35	A	1	Total	C	O	0
			40	30	10	
35	B	1	Total	C	O	0
			51	41	10	

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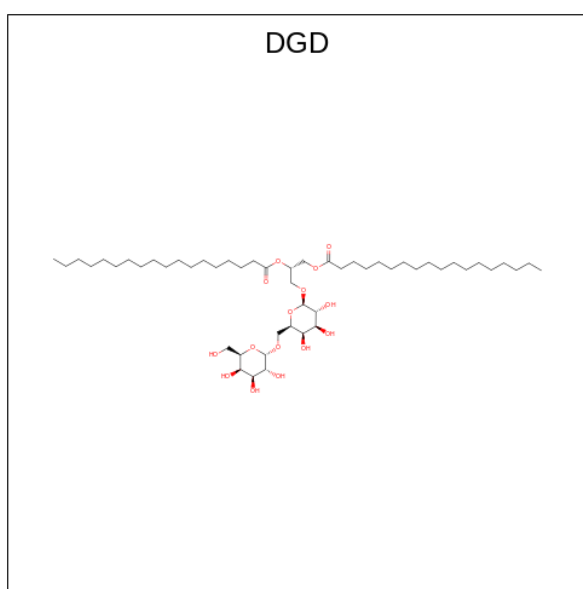
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			55	45	10	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			46	36	10	
35	Z	1	Total	C	O	0
			51	41	10	
35	a	1	Total	C	O	0
			48	38	10	
35	a	1	Total	C	O	0
			40	30	10	
35	b	1	Total	C	O	0
			51	41	10	
35	b	1	Total	C	O	0
			55	45	10	
35	c	1	Total	C	O	0
			51	41	10	
35	d	1	Total	C	O	0
			46	36	10	
35	z	1	Total	C	O	0
			51	41	10	

- Molecule 36 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
36	A	1	Total	C	O	0
			13	11	2	
36	D	1	Total	C	O	0
			55	53	2	
36	a	1	Total	C	O	0
			13	11	2	
36	d	1	Total	C	O	0
			55	53	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



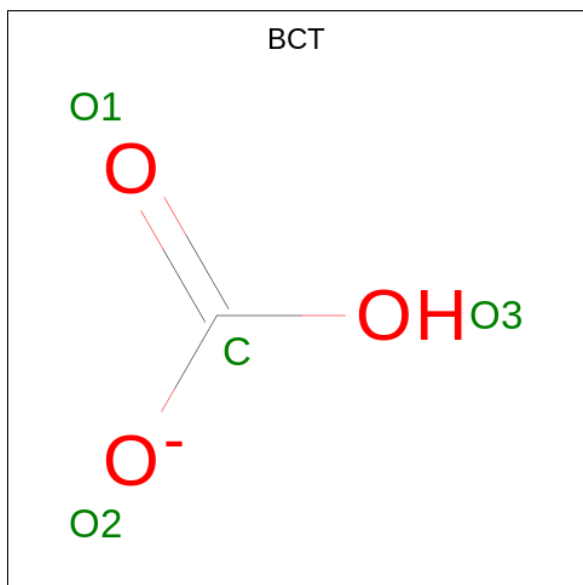
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			55	40	15	
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			60	45	15	
37	H	1	Total	C	O	0
			62	47	15	
37	b	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			55	40	15	

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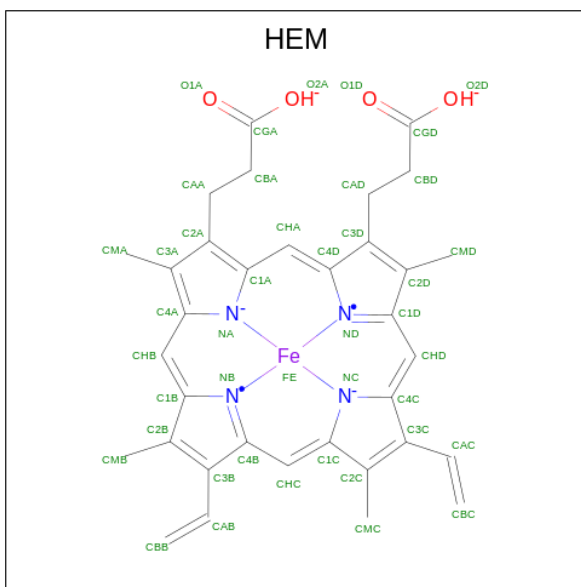
Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			62	47	15	
37	c	1	Total	C	O	0
			60	45	15	
37	h	1	Total	C	O	0
			62	47	15	

- Molecule 38 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

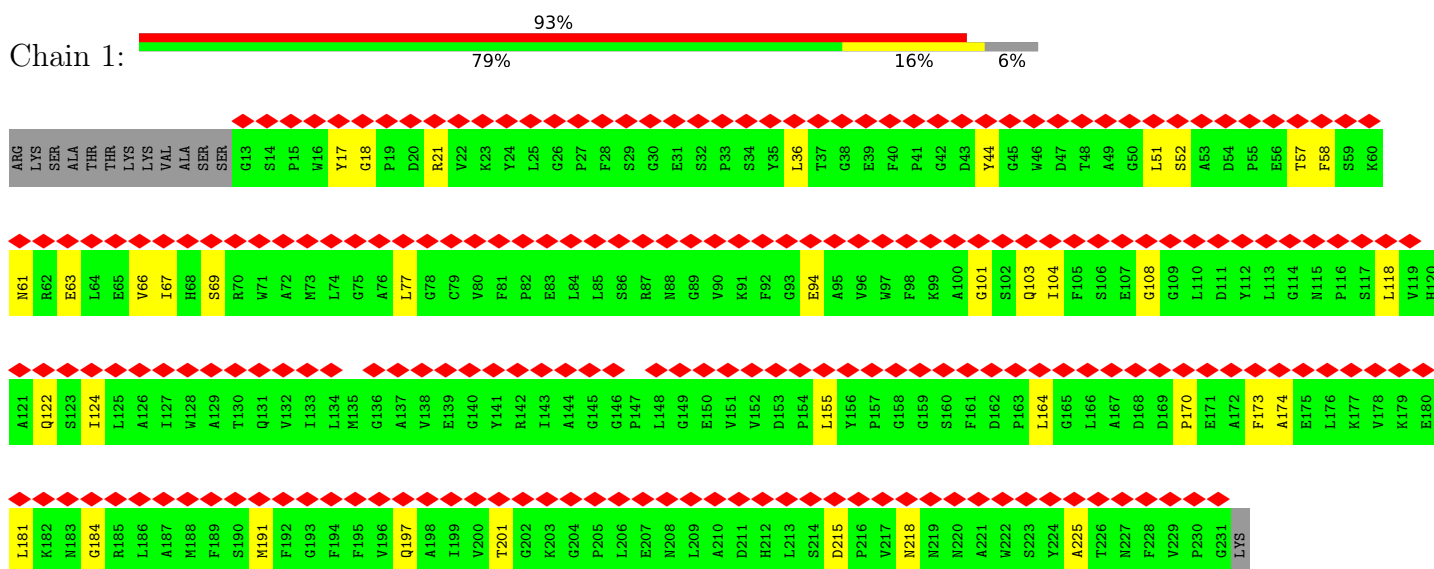


Mol	Chain	Residues	Atoms					AltConf
39	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
39	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

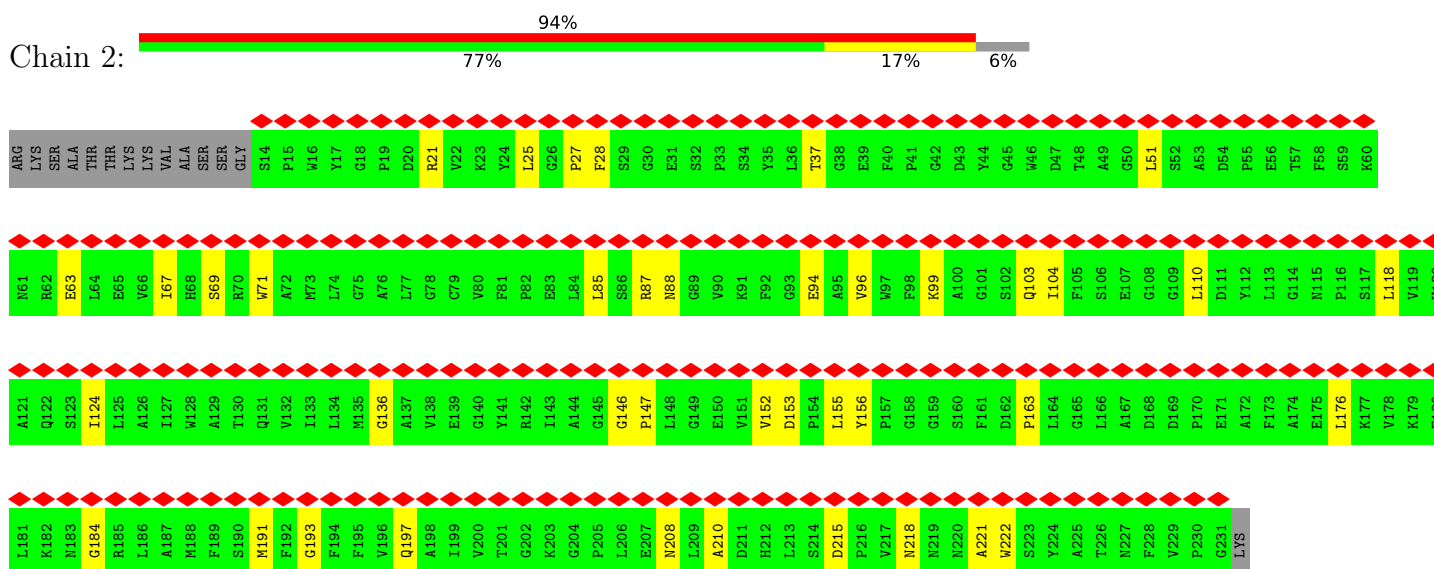
3 Residue-property plots

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

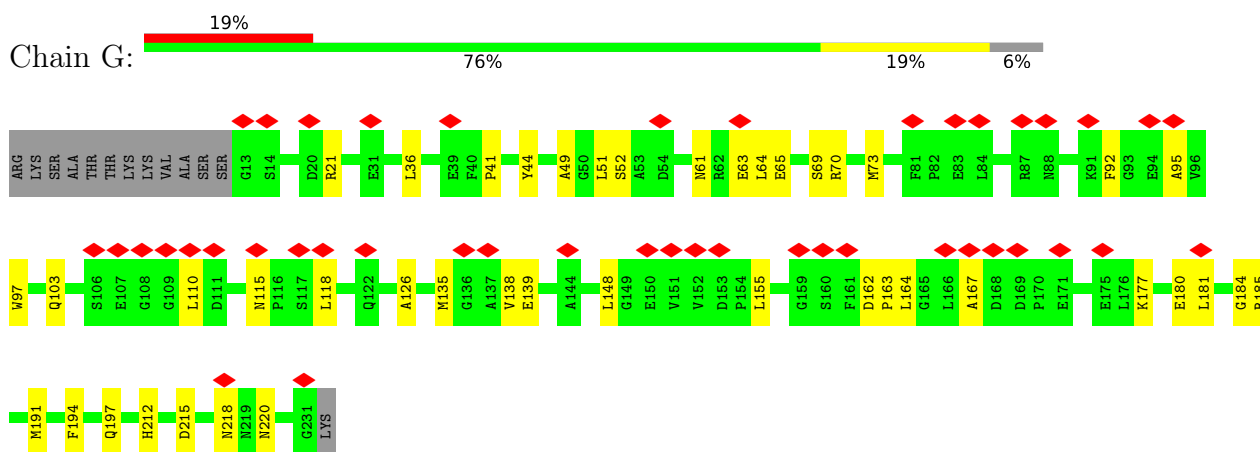
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



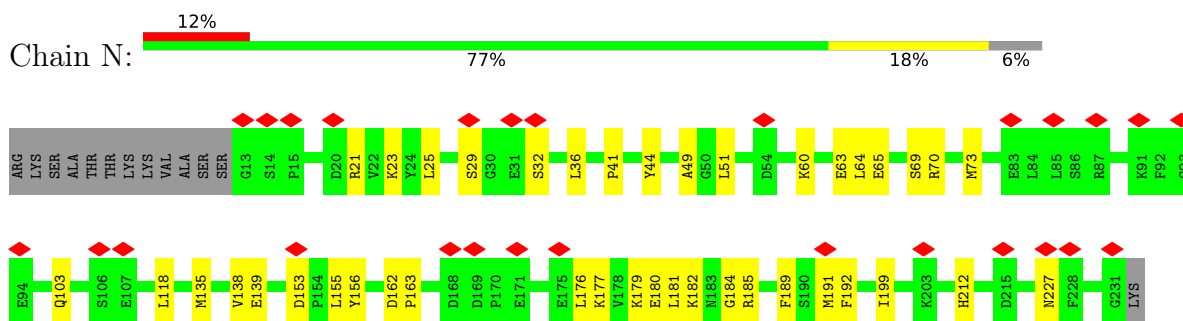
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



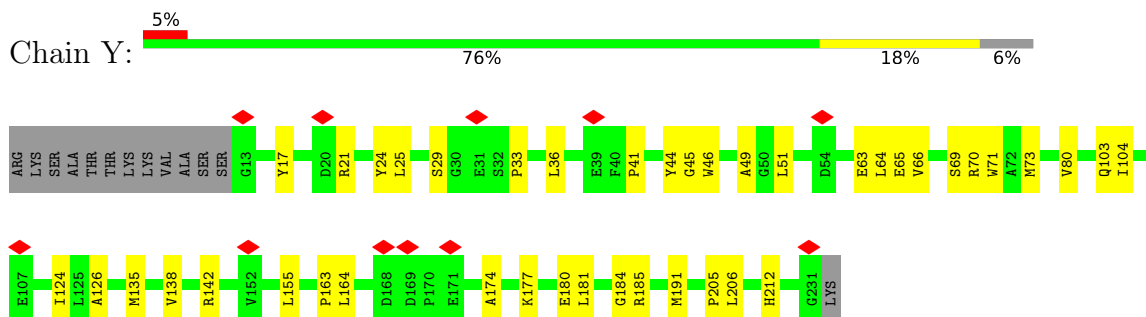
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



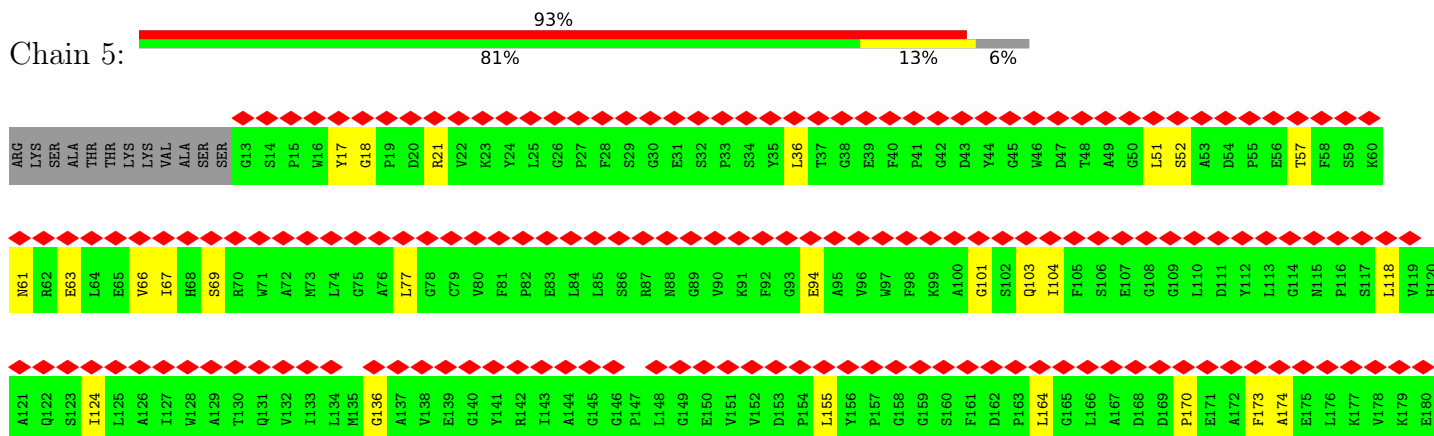
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

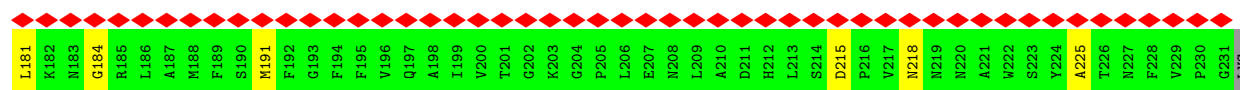


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

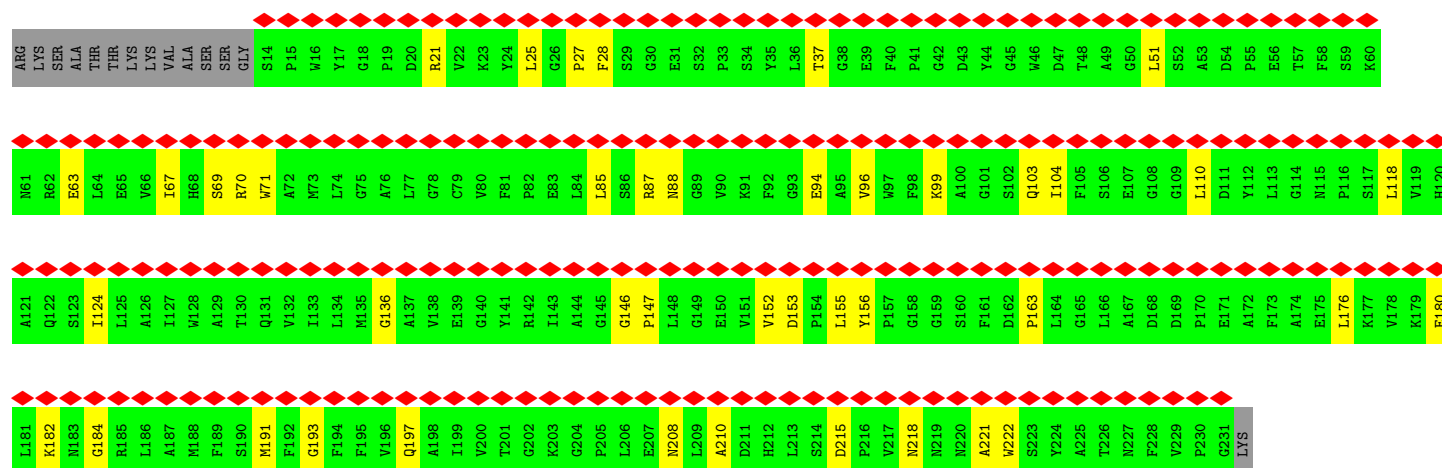
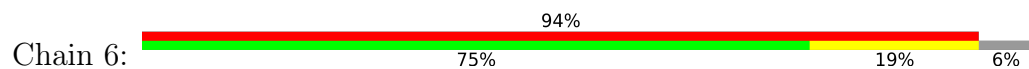


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

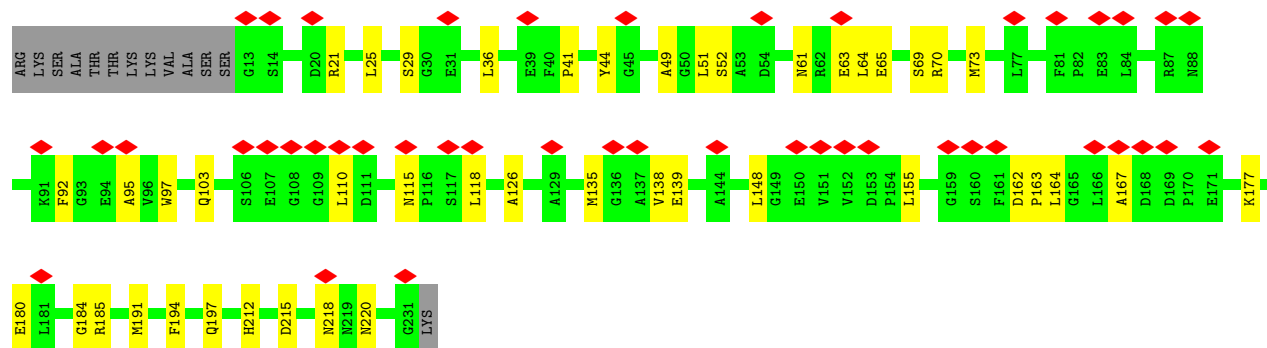
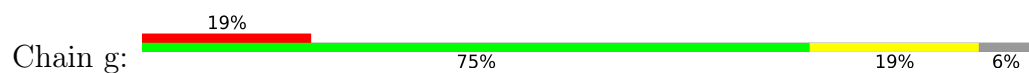




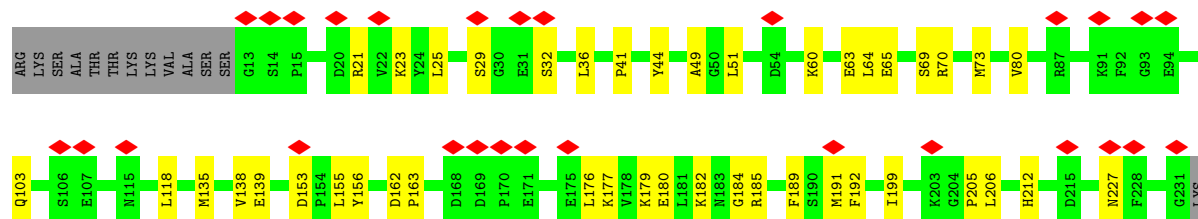
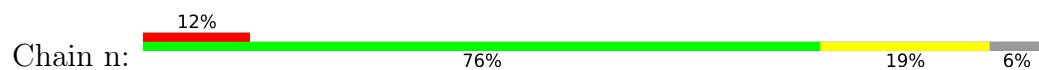
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



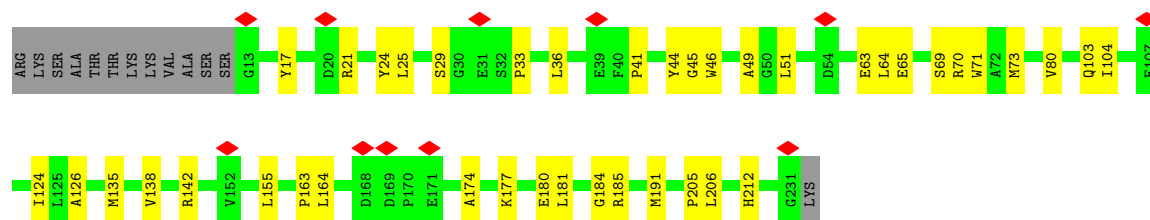
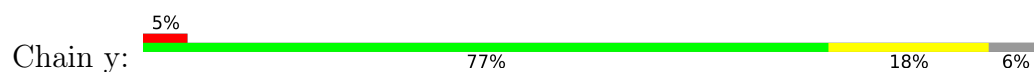
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



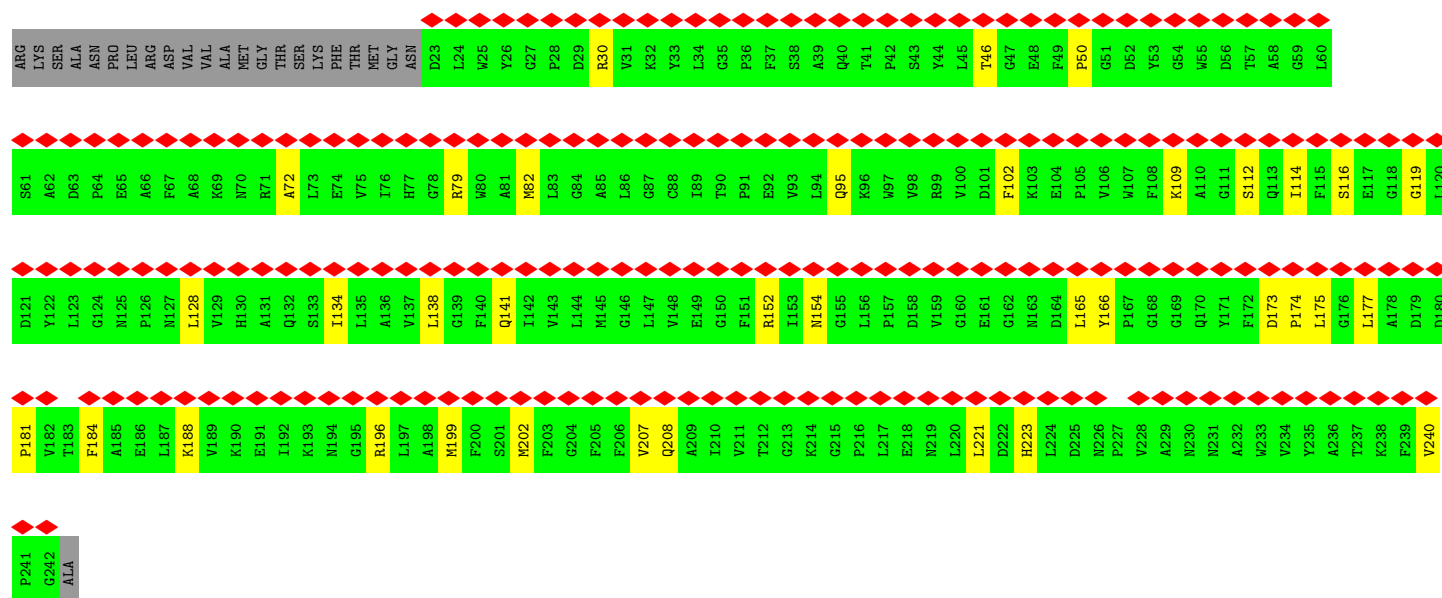
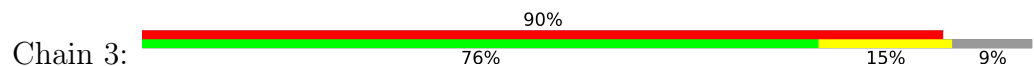
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



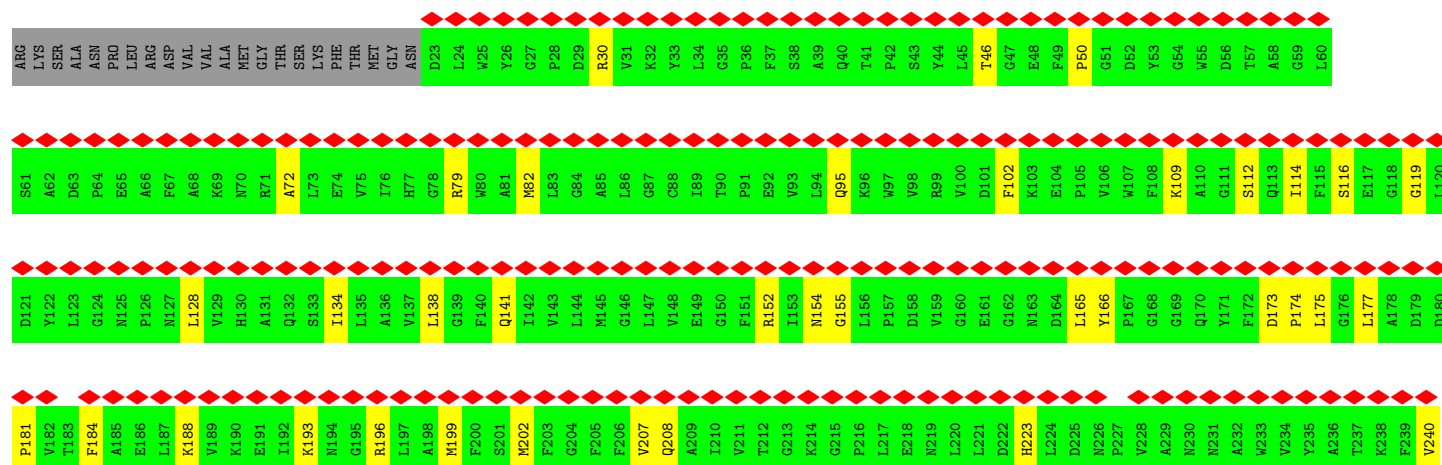
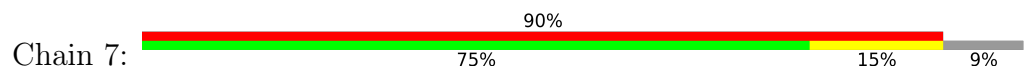
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

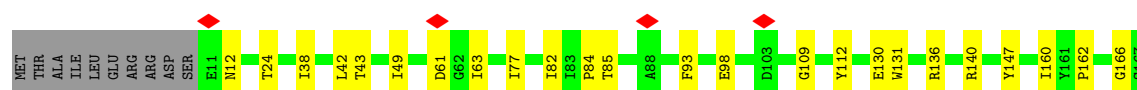


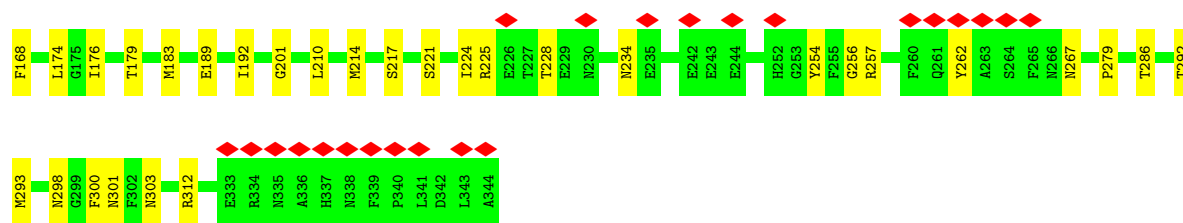
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



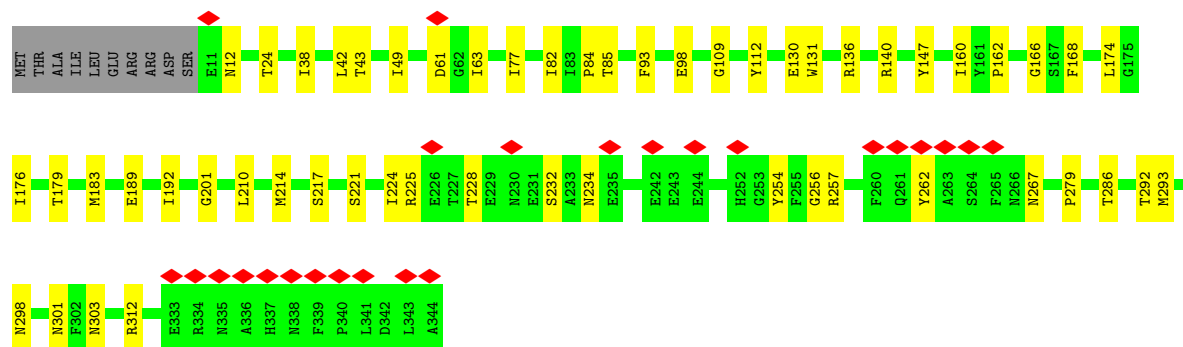
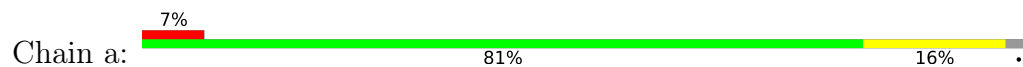
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



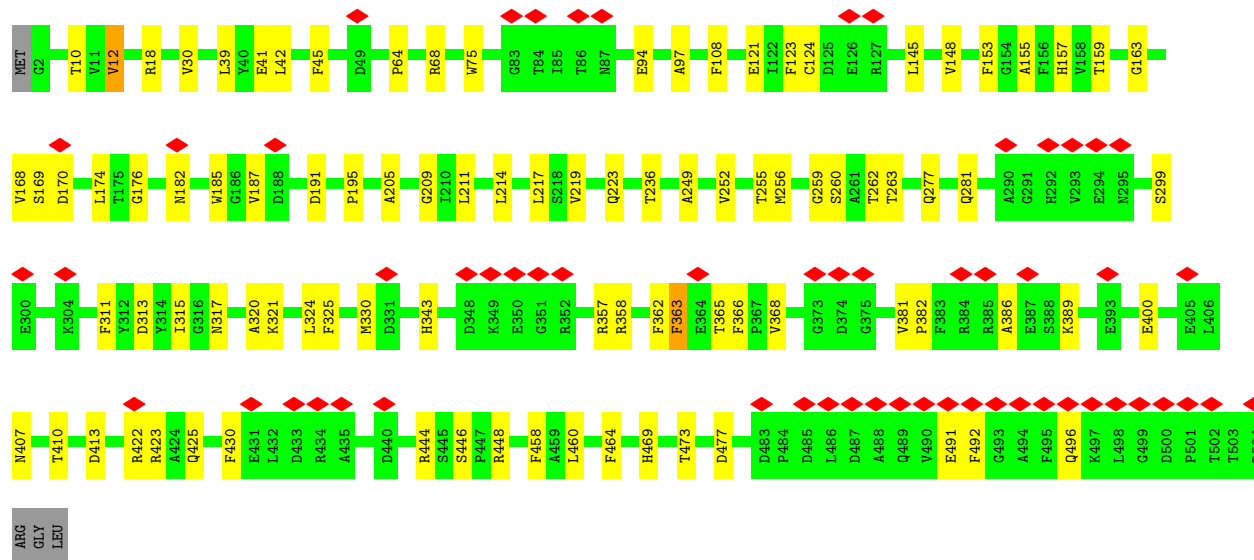
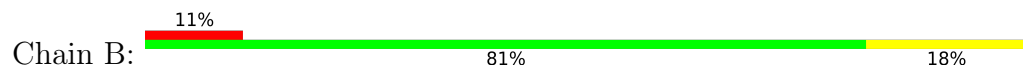




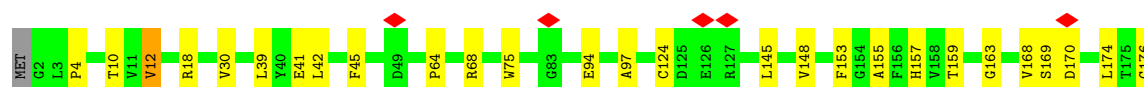
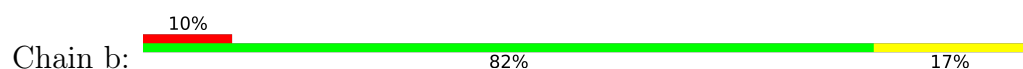
• Molecule 4: Photosystem II protein D1

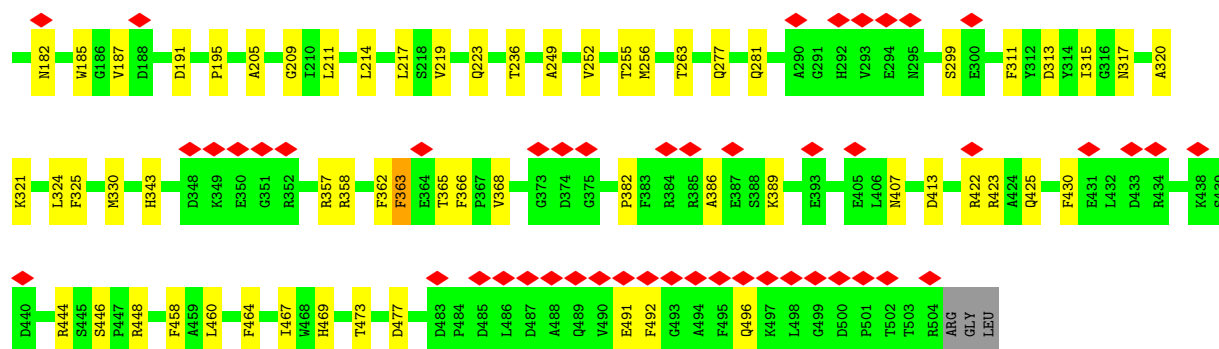


• Molecule 5: Photosystem II CP47 reaction center protein

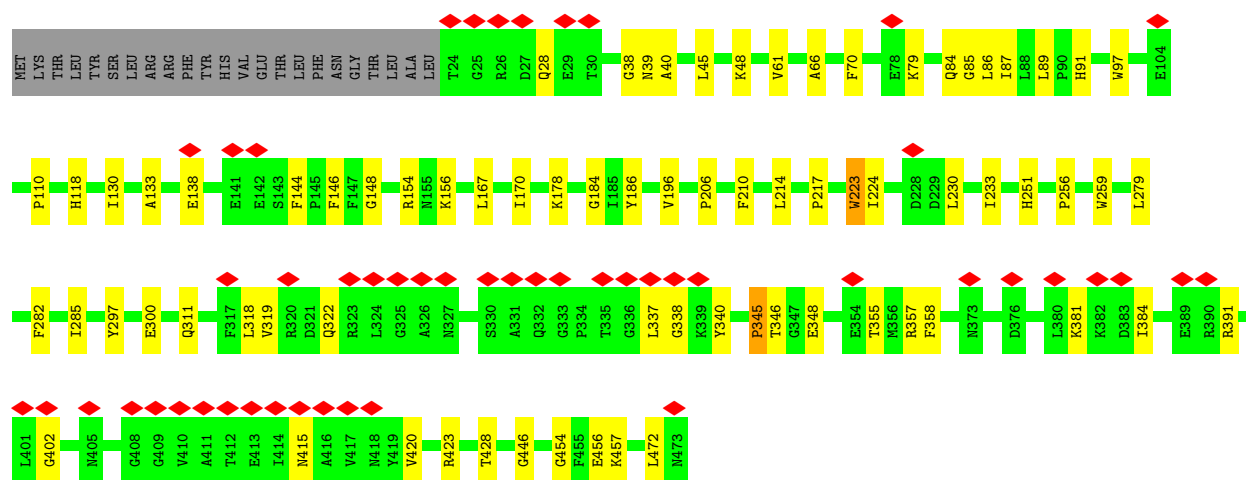
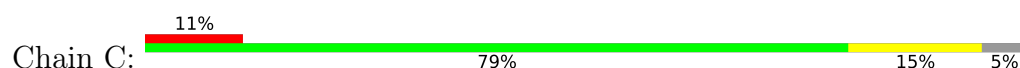


• Molecule 5: Photosystem II CP47 reaction center protein

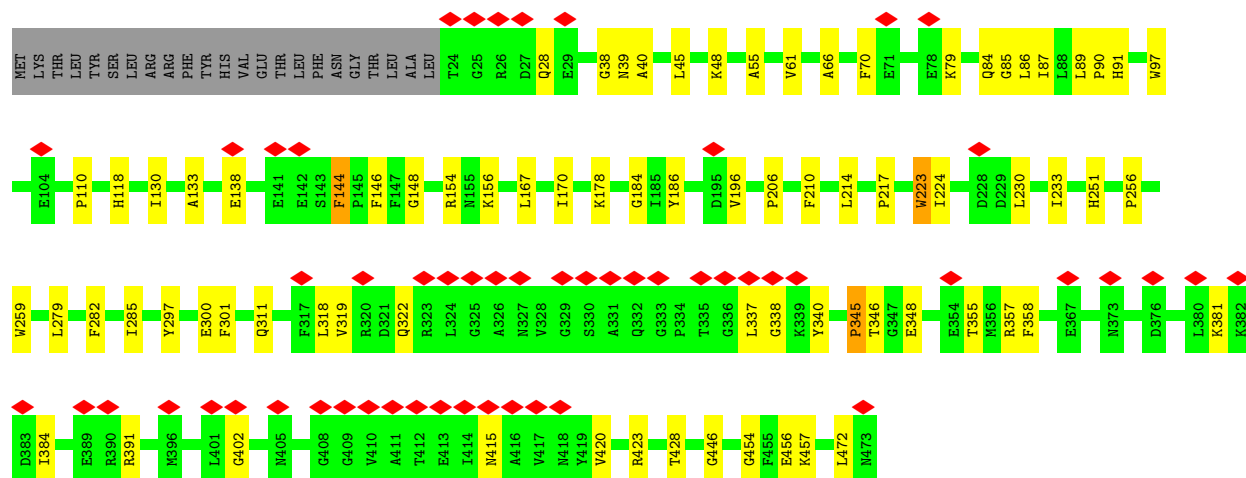
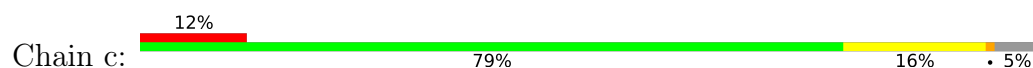




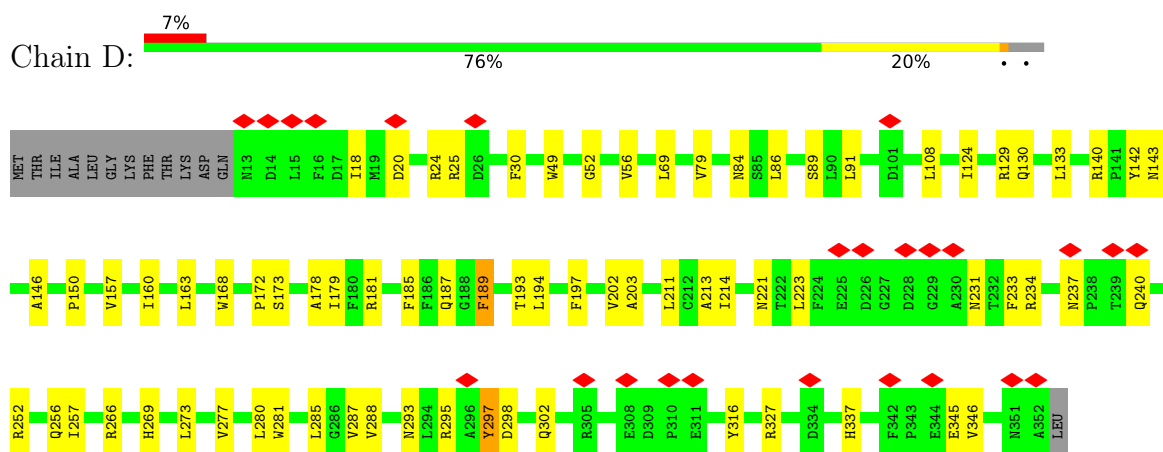
• Molecule 6: Photosystem II CP43 reaction center protein



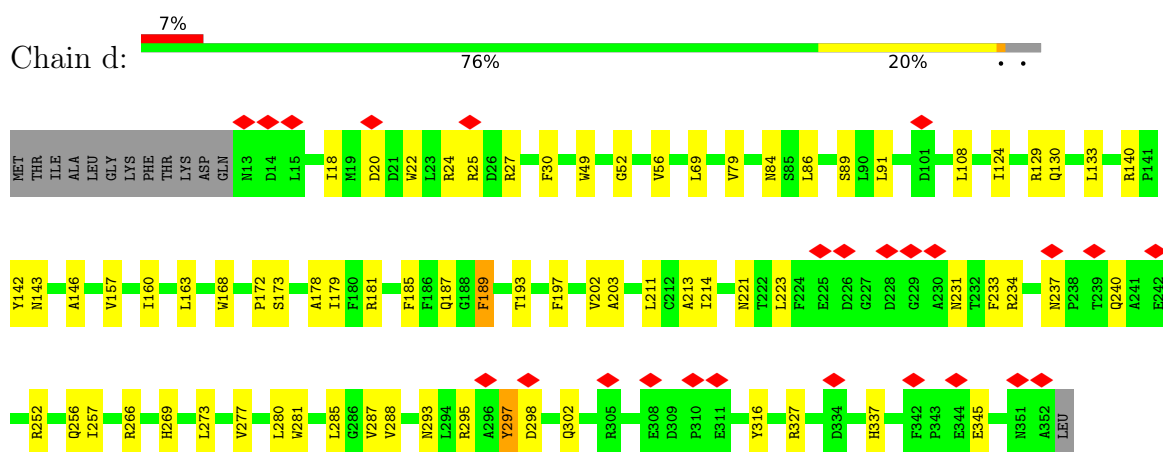
• Molecule 6: Photosystem II CP43 reaction center protein



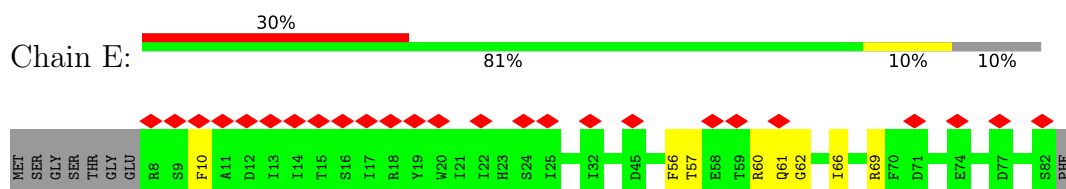
• Molecule 7: Photosystem II D2 protein



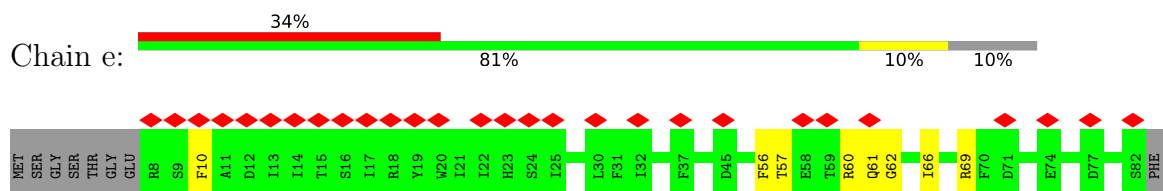
• Molecule 7: Photosystem II D2 protein



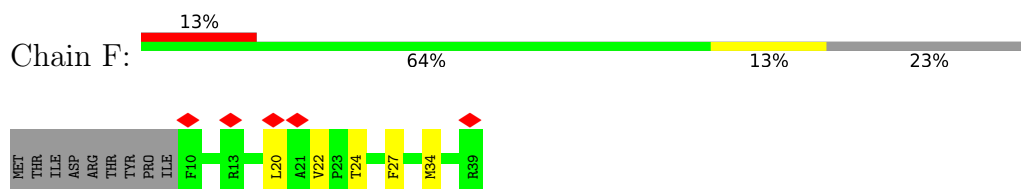
• Molecule 8: Cytochrome b559 subunit alpha



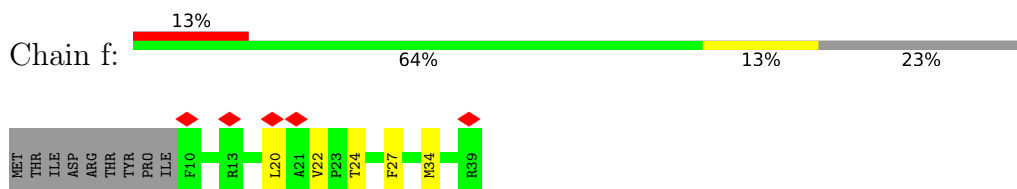
• Molecule 8: Cytochrome b559 subunit alpha



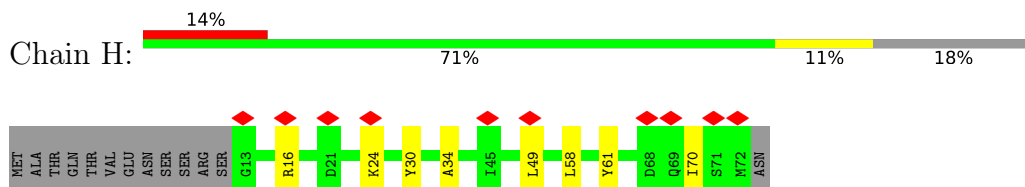
• Molecule 9: Cytochrome b559 subunit beta, PsbF



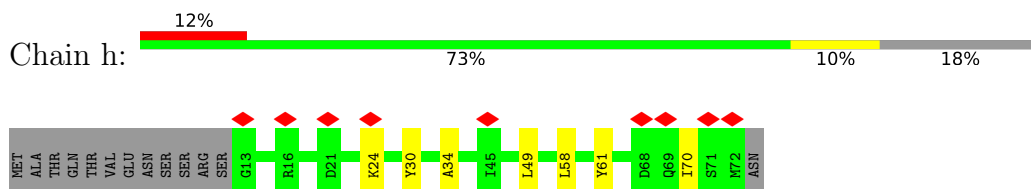
- Molecule 9: Cytochrome b559 subunit beta, PsbF



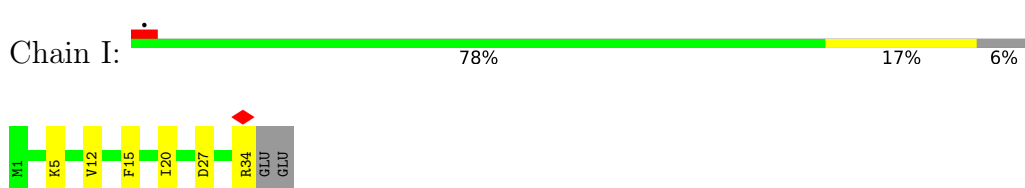
- Molecule 10: Photosystem II reaction center protein H



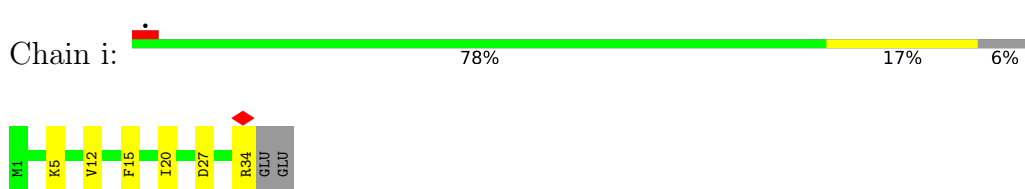
- Molecule 10: Photosystem II reaction center protein H



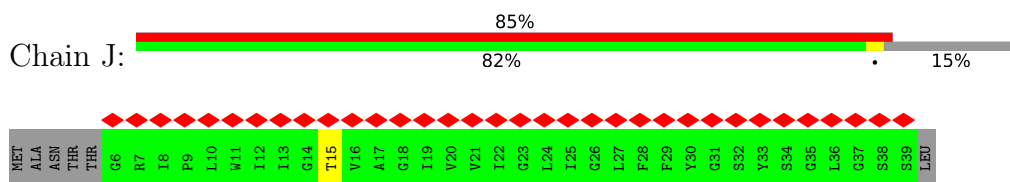
- Molecule 11: Photosystem II reaction center protein I, PsbI



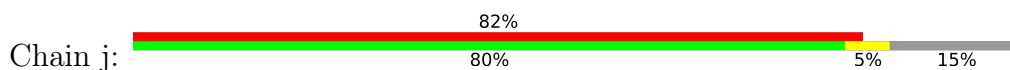
- Molecule 11: Photosystem II reaction center protein I, PsbI



- Molecule 12: Photosystem II reaction center protein J

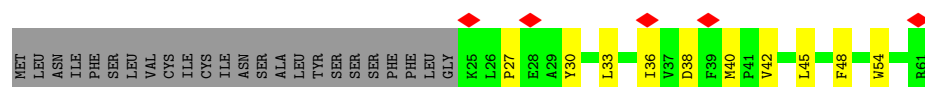
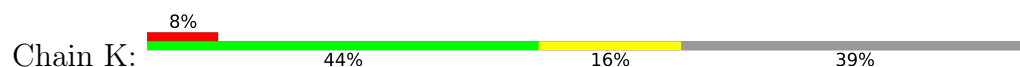


- Molecule 12: Photosystem II reaction center protein J

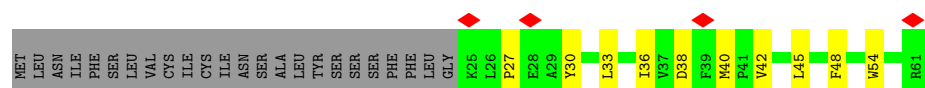
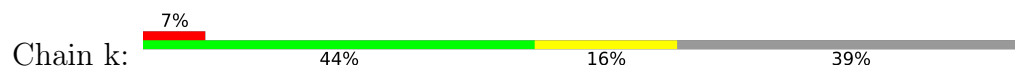




- Molecule 13: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein K



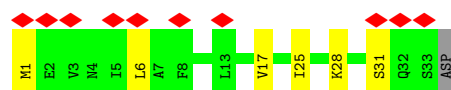
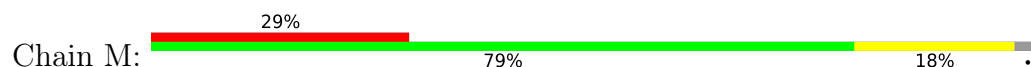
- Molecule 14: Photosystem II reaction center protein L



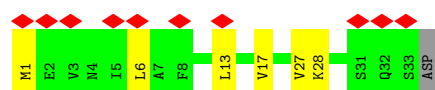
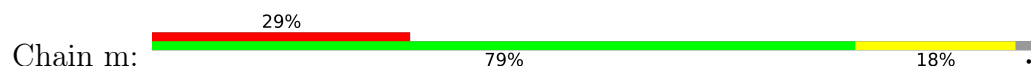
- Molecule 14: Photosystem II reaction center protein L



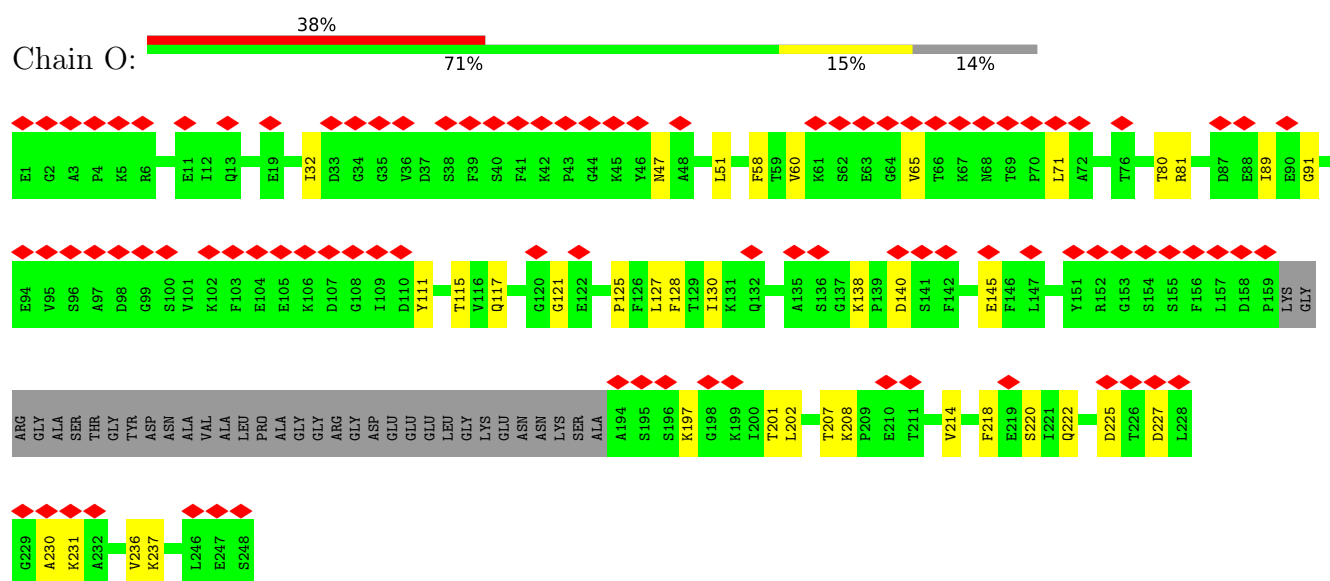
- Molecule 15: Photosystem II reaction center protein M



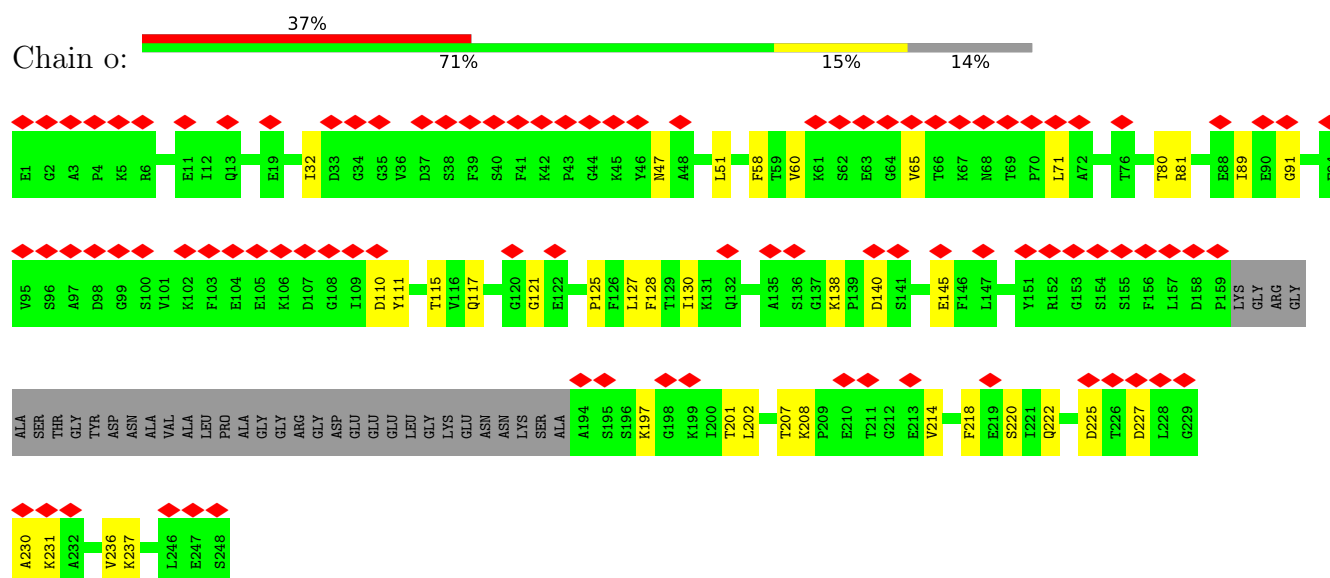
- Molecule 15: Photosystem II reaction center protein M



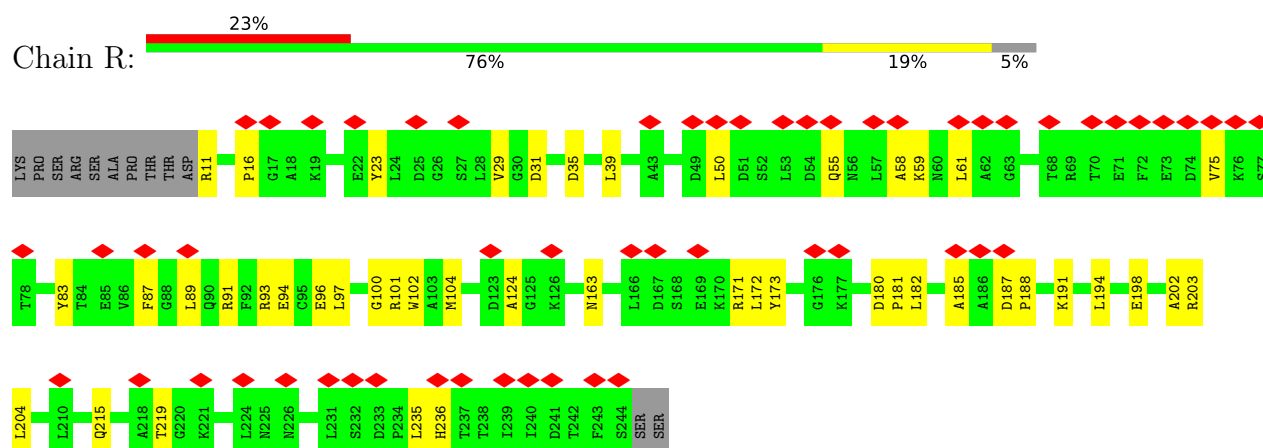
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



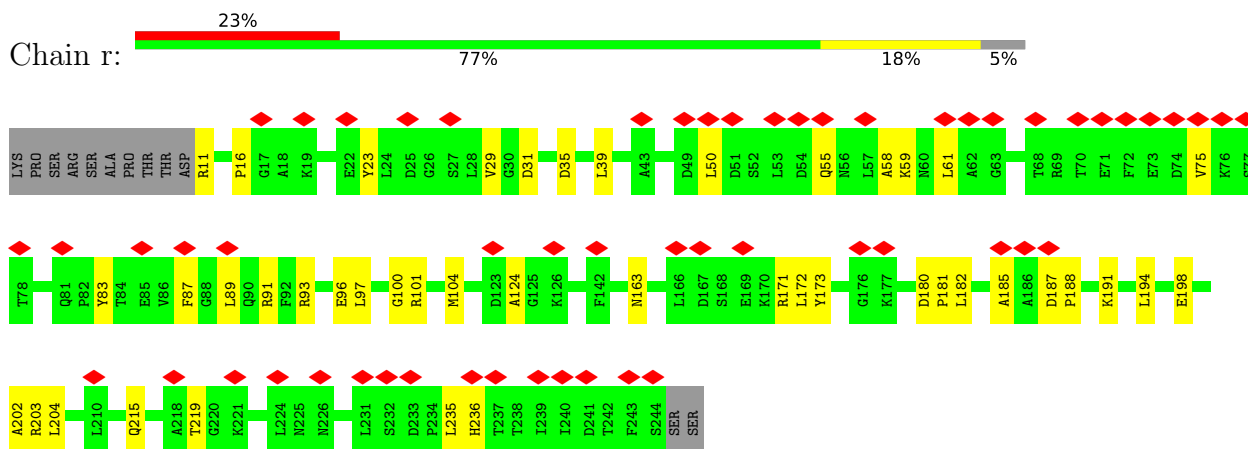
• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



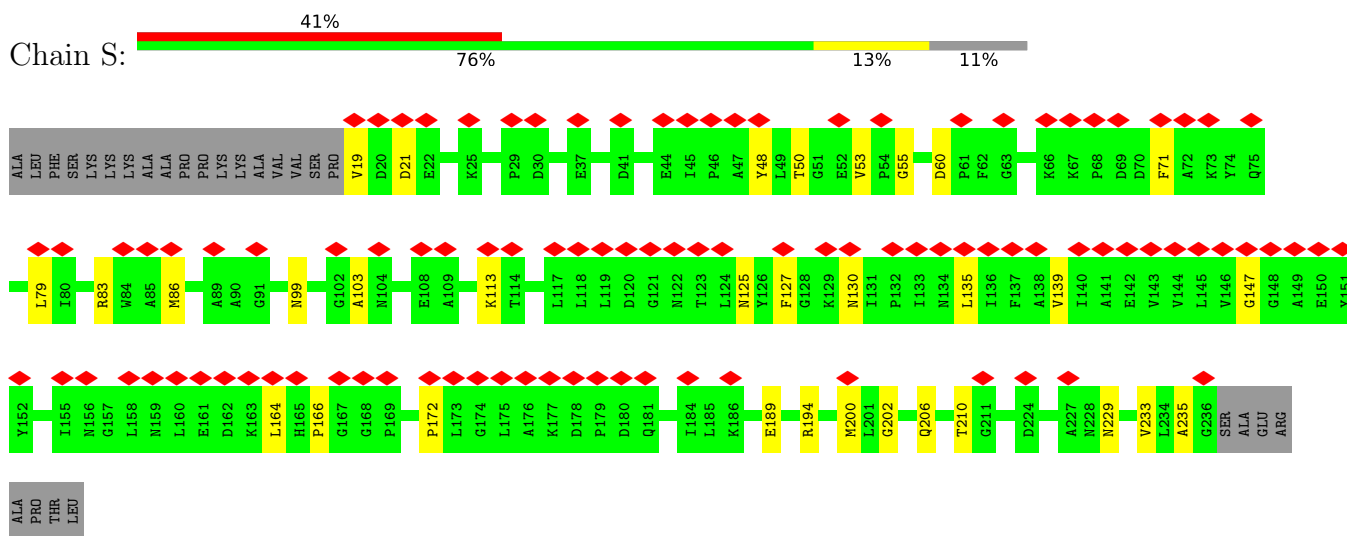
• Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29



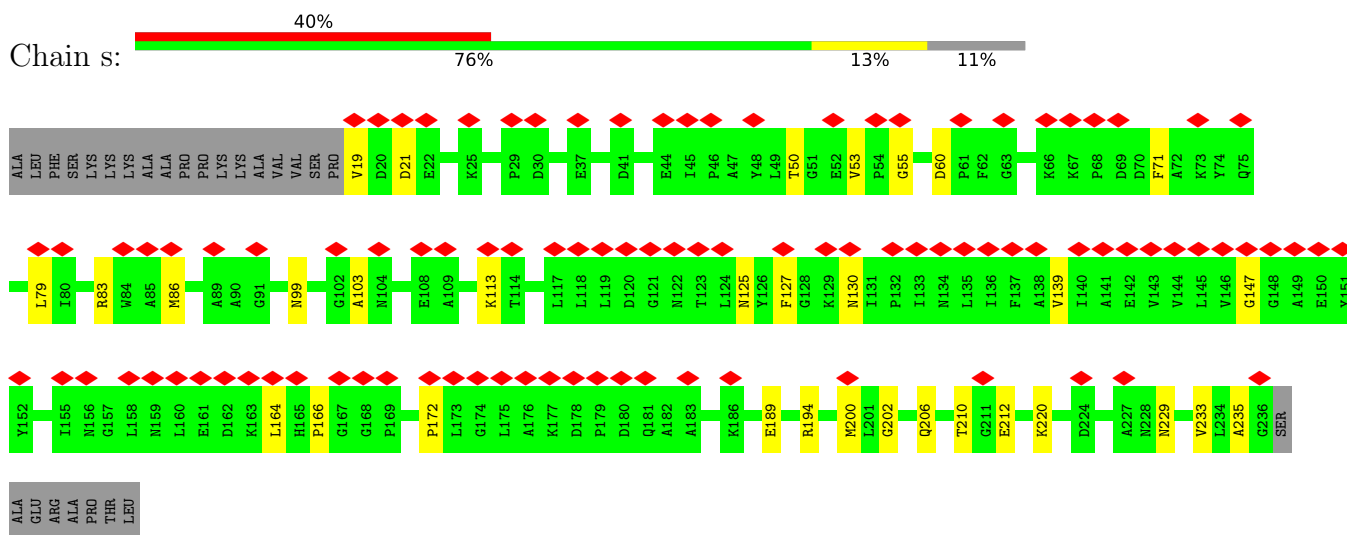
- Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29



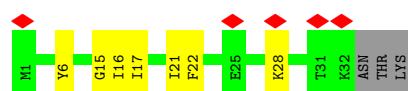
- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



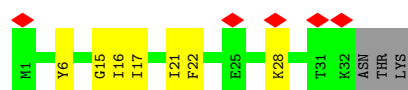
- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



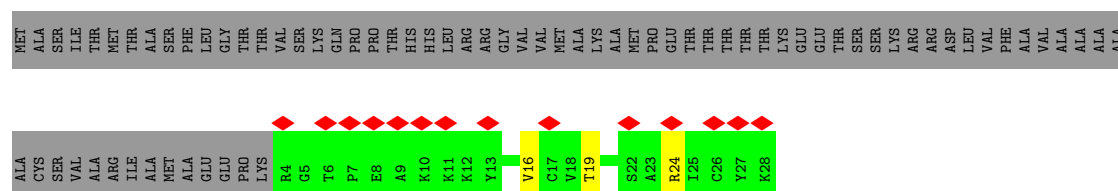
- Molecule 19: Photosystem II reaction center protein T



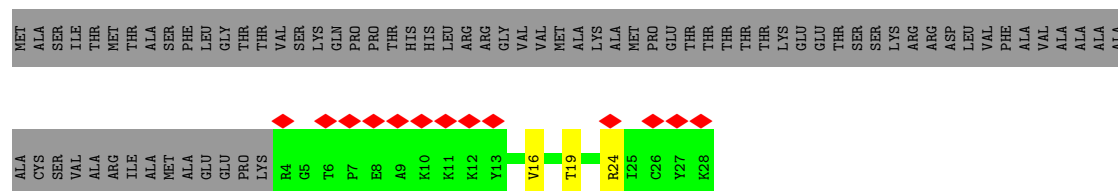
- Molecule 19: Photosystem II reaction center protein T



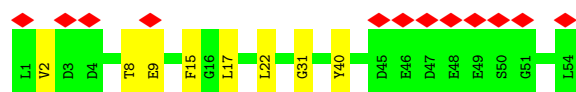
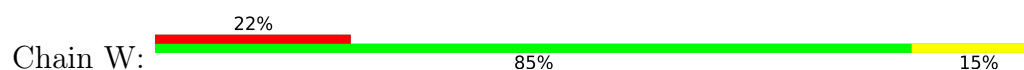
- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



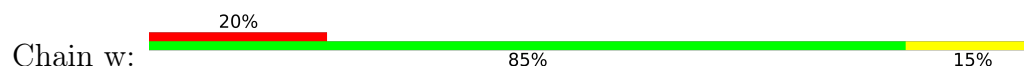
- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



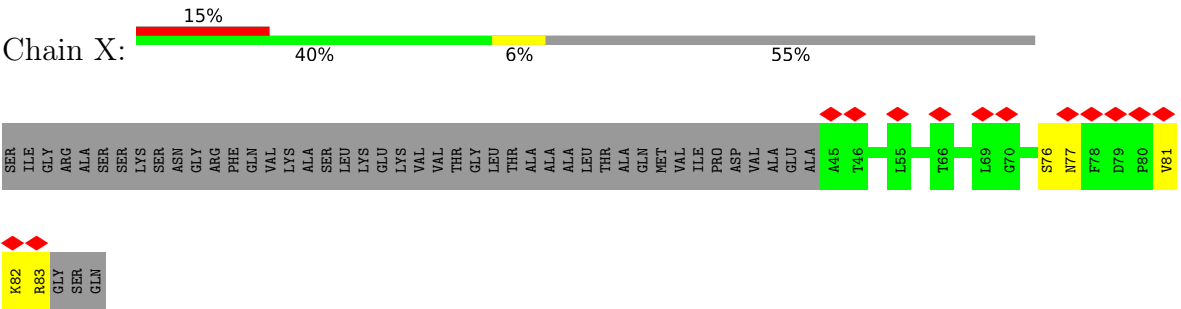
- Molecule 21: Photosystem II reaction center protein W, PSBW



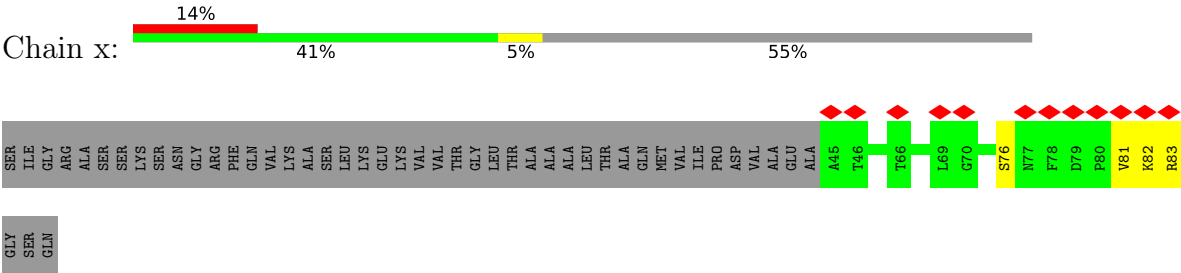
- Molecule 21: Photosystem II reaction center protein W, PSBW



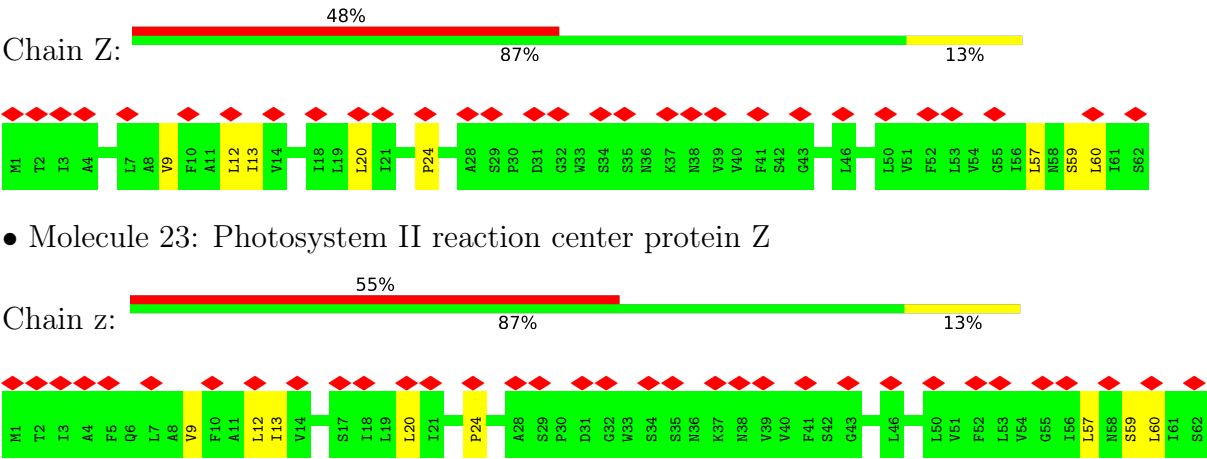
- Molecule 22: Photosystem II reaction center protein X



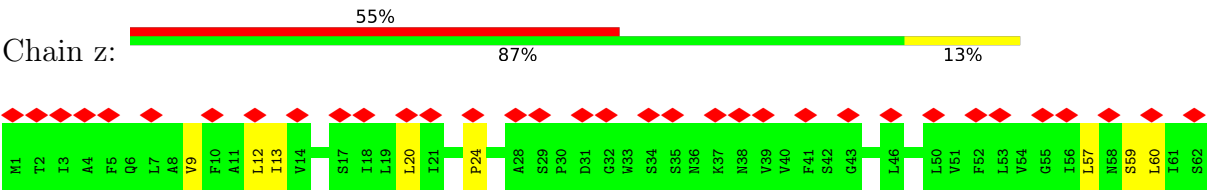
• Molecule 22: Photosystem II reaction center protein X



• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	50237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.42	0/1720	0.55	0/2342
1	2	0.36	0/1716	0.57	1/2337 (0.0%)
1	5	0.42	0/1720	0.55	0/2342
1	6	0.36	0/1716	0.57	1/2337 (0.0%)
1	G	0.41	0/1720	0.54	0/2342
1	N	0.42	0/1720	0.54	1/2342 (0.0%)
1	Y	0.49	0/1720	0.57	0/2342
1	g	0.41	0/1720	0.54	0/2342
1	n	0.42	0/1720	0.54	1/2342 (0.0%)
1	y	0.49	0/1720	0.57	0/2342
2	3	0.42	0/1759	0.58	0/2396
2	7	0.42	0/1759	0.58	0/2396
3	4	0.39	0/1586	0.65	0/2158
3	8	0.39	0/1586	0.66	0/2158
4	A	0.43	0/2697	0.57	0/3677
4	a	0.43	0/2697	0.57	0/3677
5	B	0.51	1/4081 (0.0%)	0.61	1/5556 (0.0%)
5	b	0.51	1/4081 (0.0%)	0.61	1/5556 (0.0%)
6	C	0.34	0/3614	0.57	4/4922 (0.1%)
6	c	0.34	0/3614	0.57	4/4922 (0.1%)
7	D	0.60	0/2795	0.68	3/3812 (0.1%)
7	d	0.60	0/2795	0.68	3/3812 (0.1%)
8	E	0.28	0/630	0.52	0/857
8	e	0.28	0/630	0.52	0/857
9	F	0.45	1/248 (0.4%)	0.51	0/335
9	f	0.44	1/248 (0.4%)	0.51	0/335
10	H	0.45	0/461	0.54	0/626
10	h	0.45	0/461	0.54	0/626
11	I	0.52	0/286	0.67	0/386
11	i	0.53	0/286	0.67	0/386
12	J	0.27	0/253	0.67	0/343
12	j	0.27	0/253	0.67	0/343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	K	0.52	0/318	0.94	2/434 (0.5%)
13	k	0.52	0/318	0.94	2/434 (0.5%)
14	L	0.52	0/319	0.74	1/434 (0.2%)
14	l	0.52	0/319	0.74	1/434 (0.2%)
15	M	0.57	0/260	0.75	0/355
15	m	0.57	0/260	0.75	0/355
16	O	0.39	0/1664	0.55	0/2250
16	o	0.39	0/1664	0.55	0/2250
17	R	0.40	0/1886	0.61	1/2569 (0.0%)
17	r	0.41	0/1886	0.61	1/2569 (0.0%)
18	S	0.27	0/1736	0.55	0/2359
18	s	0.27	0/1736	0.55	0/2359
19	T	0.43	0/269	0.45	0/365
19	t	0.44	0/269	0.46	0/365
20	U	0.33	0/197	0.69	0/264
20	u	0.33	0/197	0.69	0/264
21	W	0.44	0/429	0.54	0/581
21	w	0.44	0/429	0.54	0/581
22	X	0.58	1/279 (0.4%)	0.62	0/380
22	x	0.58	0/279	0.62	0/380
23	Z	0.37	0/474	0.53	0/648
23	z	0.37	0/474	0.53	0/648
All	All	0.44	5/69674 (0.0%)	0.59	28/94824 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	343	HIS	C-N	5.98	1.39	1.33
5	b	343	HIS	C-N	5.98	1.39	1.33
9	F	22	VAL	CA-CB	-5.59	1.51	1.54
9	f	22	VAL	CA-CB	-5.50	1.51	1.54
22	X	77	ASN	CA-C	-5.00	1.46	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	k	42	VAL	CA-C-N	8.86	125.82	120.24
13	k	42	VAL	C-N-CA	8.86	125.82	120.24
13	K	42	VAL	CA-C-N	8.78	125.77	120.24
13	K	42	VAL	C-N-CA	8.78	125.77	120.24
5	B	363	PHE	N-CA-C	6.57	119.31	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	25	0
1	2	1664	0	1593	29	0
1	5	1668	0	1596	24	0
1	6	1664	0	1593	30	0
1	G	1668	0	1596	37	0
1	N	1668	0	1596	36	0
1	Y	1668	0	1596	34	0
1	g	1668	0	1596	39	0
1	n	1668	0	1596	38	0
1	y	1668	0	1596	33	0
2	3	1707	0	1659	29	0
2	7	1707	0	1659	31	0
3	4	1534	0	1486	32	0
3	8	1534	0	1486	36	0
4	A	2616	0	2522	54	0
4	a	2616	0	2522	55	0
5	B	3948	0	3818	83	0
5	b	3948	0	3818	78	0
6	C	3497	0	3422	59	0
6	c	3497	0	3422	62	0
7	D	2703	0	2593	62	0
7	d	2703	0	2593	61	0
8	E	612	0	595	6	0
8	e	612	0	595	7	0
9	F	241	0	246	3	0
9	f	241	0	246	4	0
10	H	452	0	473	12	0
10	h	452	0	473	11	0
11	I	278	0	291	7	0
11	i	278	0	291	7	0
12	J	247	0	258	1	0
12	j	247	0	258	2	0
13	K	306	0	313	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	k	306	0	313	13	0
14	L	311	0	299	20	0
14	l	311	0	299	18	0
15	M	256	0	284	6	0
15	m	256	0	284	6	0
16	O	1631	0	1625	24	0
16	o	1631	0	1625	25	0
17	R	1835	0	1801	43	0
17	r	1835	0	1801	42	0
18	S	1689	0	1670	25	0
18	s	1689	0	1670	24	0
19	T	261	0	280	9	0
19	t	261	0	280	9	0
20	U	193	0	205	4	0
20	u	193	0	205	4	0
21	W	419	0	402	8	0
21	w	419	0	402	8	0
22	X	276	0	301	4	0
22	x	276	0	301	4	0
23	Z	464	0	493	7	0
23	z	464	0	493	7	0
24	1	309	0	244	10	0
24	2	306	0	238	10	0
24	3	316	0	254	15	0
24	4	229	0	152	3	0
24	5	309	0	244	13	0
24	6	306	0	238	11	0
24	7	316	0	254	17	0
24	8	229	0	152	3	0
24	G	355	0	335	15	0
24	N	362	0	350	13	0
24	R	225	0	201	4	0
24	S	196	0	144	5	0
24	Y	362	0	350	16	0
24	g	355	0	335	16	0
24	n	362	0	350	13	0
24	r	225	0	201	3	0
24	s	196	0	144	5	0
24	y	362	0	350	17	0
25	1	412	0	348	12	0
25	2	391	0	314	13	0
25	3	426	0	373	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4	270	0	198	4	0
25	5	412	0	348	11	0
25	6	391	0	314	14	0
25	7	426	0	373	13	0
25	8	270	0	198	5	0
25	A	240	0	242	15	0
25	B	1040	0	1152	55	0
25	C	845	0	936	33	0
25	D	130	0	144	9	0
25	G	477	0	477	21	0
25	N	473	0	468	24	0
25	R	543	0	490	22	0
25	S	465	0	393	7	0
25	Y	473	0	468	23	0
25	a	240	0	242	15	0
25	b	1040	0	1152	56	0
25	c	845	0	936	33	0
25	d	130	0	144	7	0
25	g	477	0	477	23	0
25	n	473	0	468	24	0
25	r	543	0	490	21	0
25	s	465	0	393	7	0
25	y	473	0	468	20	0
26	1	84	0	112	10	0
26	2	84	0	112	7	0
26	3	84	0	112	11	0
26	4	42	0	56	4	0
26	5	84	0	112	11	0
26	6	84	0	112	7	0
26	7	84	0	112	9	0
26	8	42	0	56	3	0
26	G	84	0	112	14	0
26	N	84	0	112	6	0
26	R	42	0	56	4	0
26	S	84	0	112	7	0
26	Y	84	0	112	9	0
26	g	84	0	112	14	0
26	n	84	0	112	9	0
26	r	42	0	56	4	0
26	s	84	0	112	5	0
26	y	84	0	112	6	0
27	1	44	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	2	44	0	56	6	0
27	3	44	0	56	4	0
27	4	44	0	56	5	0
27	5	44	0	56	4	0
27	6	44	0	56	5	0
27	7	44	0	56	7	0
27	8	44	0	56	7	0
27	G	44	0	56	4	0
27	N	44	0	56	6	0
27	R	44	0	56	5	0
27	Y	44	0	56	5	0
27	g	44	0	56	4	0
27	n	44	0	56	7	0
27	r	44	0	56	5	0
27	y	44	0	56	5	0
28	1	44	0	56	3	0
28	2	44	0	56	2	0
28	3	44	0	56	2	0
28	5	44	0	56	3	0
28	6	44	0	56	0	0
28	7	44	0	56	2	0
28	G	44	0	56	3	0
28	N	44	0	56	3	0
28	R	44	0	56	4	0
28	S	44	0	56	1	0
28	Y	44	0	56	1	0
28	g	44	0	56	2	0
28	n	44	0	56	5	0
28	r	44	0	56	2	0
28	s	44	0	56	1	0
28	y	44	0	56	4	0
29	1	41	0	55	0	0
29	2	37	0	44	2	0
29	3	47	0	67	3	0
29	4	21	0	12	1	0
29	5	41	0	55	0	0
29	6	37	0	44	2	0
29	7	47	0	67	4	0
29	8	21	0	12	1	0
29	B	96	0	141	5	0
29	C	147	0	222	7	0
29	D	138	0	195	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	G	49	0	74	2	0
29	L	49	0	74	8	0
29	N	49	0	74	4	0
29	R	42	0	57	3	0
29	S	49	0	74	2	0
29	Y	49	0	74	3	0
29	b	96	0	141	5	0
29	c	147	0	222	9	0
29	d	138	0	195	20	0
29	g	49	0	74	4	0
29	l	49	0	74	8	0
29	n	49	0	74	4	0
29	r	42	0	57	3	0
29	s	49	0	74	2	0
29	y	49	0	74	4	0
30	4	40	0	56	3	0
30	8	40	0	56	3	0
30	A	40	0	56	2	0
30	B	120	0	168	13	0
30	C	160	0	224	15	0
30	D	40	0	56	4	0
30	H	40	0	56	6	0
30	T	40	0	56	3	0
30	a	40	0	56	3	0
30	b	120	0	168	12	0
30	c	160	0	224	16	0
30	d	40	0	56	7	0
30	h	40	0	56	5	0
30	t	40	0	56	7	0
31	A	10	0	0	2	0
31	a	10	0	0	2	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	128	0	148	11	0
33	a	128	0	148	11	0
34	A	104	0	144	8	0
34	B	96	0	126	8	0
34	a	104	0	145	8	0
34	b	96	0	125	7	0
35	A	88	0	116	2	0
35	B	106	0	158	6	0
35	C	51	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	46	0	62	2	0
35	Z	51	0	72	6	0
35	a	88	0	116	2	0
35	b	106	0	158	6	0
35	c	51	0	72	1	0
35	d	46	0	62	3	0
35	z	51	0	72	5	0
36	A	13	0	7	0	0
36	D	55	0	80	6	0
36	a	13	0	7	0	0
36	d	55	0	80	6	0
37	B	59	0	76	1	0
37	C	177	0	228	7	0
37	H	62	0	80	6	0
37	b	59	0	76	1	0
37	c	177	0	228	7	0
37	h	62	0	80	6	0
38	D	4	0	0	1	0
38	d	4	0	0	1	0
39	F	43	0	30	0	0
39	f	43	0	30	0	0
All	All	92842	0	92620	1778	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 10.

The worst 5 of 1778 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7:606:CHL:HBB2	24:7:607:CHL:HBB1	1.57	0.86
24:3:606:CHL:HBB2	24:3:607:CHL:HBB1	1.57	0.85
25:b:603:CLA:H12	10:h:61:TYR:HD2	1.46	0.80
25:B:603:CLA:H12	10:H:61:TYR:HD2	1.46	0.78
25:1:602:CLA:HAB	26:1:1621:LUT:H32	1.66	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	5	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	6	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	G	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	N	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	Y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	g	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	n	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
2	7	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
4	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
5	B	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
5	b	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
7	D	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
7	d	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	57 (98%)	1 (2%)	0	100	100
10	h	58/73 (80%)	57 (98%)	1 (2%)	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	32/40 (80%)	32 (100%)	0	0	100	100
12	j	32/40 (80%)	32 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	31 (100%)	0	0	100	100
15	m	31/34 (91%)	31 (100%)	0	0	100	100
16	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
16	o	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
17	R	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
17	r	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
18	S	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
18	s	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
19	T	30/35 (86%)	30 (100%)	0	0	100	100
19	t	30/35 (86%)	30 (100%)	0	0	100	100
20	U	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
20	u	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
21	W	52/54 (96%)	52 (100%)	0	0	100	100
21	w	52/54 (96%)	52 (100%)	0	0	100	100
22	X	37/86 (43%)	37 (100%)	0	0	100	100
22	x	37/86 (43%)	37 (100%)	0	0	100	100
23	Z	60/62 (97%)	60 (100%)	0	0	100	100
23	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	8596/9536 (90%)	8394 (98%)	202 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	171 (100%)	0	100	100
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100
1	y	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	270 (100%)	0	100	100
4	a	270/279 (97%)	270 (100%)	0	100	100
5	B	400/403 (99%)	399 (100%)	1 (0%)	86	88
5	b	400/403 (99%)	399 (100%)	1 (0%)	86	88
6	C	352/373 (94%)	352 (100%)	0	100	100
6	c	352/373 (94%)	352 (100%)	0	100	100
7	D	274/285 (96%)	274 (100%)	0	100	100
7	d	274/285 (96%)	274 (100%)	0	100	100
8	E	67/73 (92%)	67 (100%)	0	100	100
8	e	67/73 (92%)	67 (100%)	0	100	100
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	49/61 (80%)	49 (100%)	0	100	100
10	h	49/61 (80%)	49 (100%)	0	100	100
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	25/30 (83%)	25 (100%)	0	100	100
12	j	25/30 (83%)	25 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	182/204 (89%)	182 (100%)	0	100	100
16	o	182/204 (89%)	182 (100%)	0	100	100
17	R	191/202 (95%)	191 (100%)	0	100	100
17	r	191/202 (95%)	191 (100%)	0	100	100
18	S	170/190 (90%)	170 (100%)	0	100	100
18	s	170/190 (90%)	170 (100%)	0	100	100
19	T	29/32 (91%)	29 (100%)	0	100	100
19	t	29/32 (91%)	29 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/44 (100%)	44 (100%)	0	100	100
21	w	44/44 (100%)	44 (100%)	0	100	100
22	X	32/67 (48%)	32 (100%)	0	100	100
22	x	32/67 (48%)	32 (100%)	0	100	100
23	Z	54/54 (100%)	54 (100%)	0	100	100
23	z	54/54 (100%)	54 (100%)	0	100	100
All	All	6992/7658 (91%)	6990 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	12	VAL
5	b	12	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
7	d	143	ASN
7	d	351	ASN
16	o	74	GLN
7	D	351	ASN
7	D	323	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 486 ligands modelled in this entry, 2 are monoatomic - leaving 484 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	CLA	2	610	1	54,58,73	1.38	9 (16%)	65,95,113	1.17	6 (9%)
30	BCR	b	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.02	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	509	6	69,73,73	1.24	10 (14%)	83,113,113	1.29	8 (9%)
24	CHL	N	608	-	70,74,74	1.85	17 (24%)	80,114,114	2.92	27 (33%)
25	CLA	G	611	29	64,68,73	1.29	11 (17%)	77,107,113	1.29	5 (6%)
29	LHG	2	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
35	LMG	Z	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.29	5 (8%)
25	CLA	c	513	6	69,73,73	1.22	7 (10%)	83,113,113	1.31	10 (12%)
24	CHL	y	606	-	54,58,74	2.09	18 (33%)	59,94,114	3.13	22 (37%)
28	NEX	Y	1623	-	38,46,46	1.12	2 (5%)	50,70,70	2.70	22 (44%)
25	CLA	R	601	17	53,57,73	1.41	10 (18%)	62,93,113	1.57	9 (14%)
29	LHG	C	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
24	CHL	7	606	-	50,54,74	2.34	18 (36%)	56,90,114	3.37	25 (44%)
25	CLA	8	612	3	49,53,73	1.48	9 (18%)	59,89,113	1.43	8 (13%)
26	LUT	S	1621	-	42,43,43	0.80	0	51,60,60	1.74	15 (29%)
26	LUT	7	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
25	CLA	4	603	3	49,53,73	1.49	11 (22%)	59,89,113	1.38	5 (8%)
28	NEX	5	1623	-	38,46,46	1.13	3 (7%)	50,70,70	2.62	18 (36%)
25	CLA	5	602	1	65,69,73	1.34	11 (16%)	78,108,113	1.21	8 (10%)
25	CLA	c	511	6	69,73,73	1.27	8 (11%)	83,113,113	1.23	6 (7%)
25	CLA	y	610	1	64,68,73	1.31	9 (14%)	77,107,113	1.21	9 (11%)
25	CLA	6	612	1	49,53,73	1.48	9 (18%)	59,89,113	1.39	9 (15%)
35	LMG	A	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
27	XAT	8	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	21 (38%)
30	BCR	4	623	-	41,41,41	0.78	0	56,56,56	2.18	15 (26%)
37	DGD	B	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
25	CLA	y	614	1	52,56,73	1.44	10 (19%)	62,92,113	1.36	7 (11%)
24	CHL	5	607	-	67,71,74	1.94	19 (28%)	76,110,114	3.11	27 (35%)
25	CLA	N	614	1	52,56,73	1.39	10 (19%)	62,92,113	1.37	8 (12%)
29	LHG	4	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
33	PHO	a	408	-	58,69,69	1.97	12 (20%)	56,99,99	1.70	9 (16%)
36	PL9	D	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
25	CLA	A	410	4	64,68,73	1.27	10 (15%)	77,107,113	1.37	9 (11%)
24	CHL	7	608	-	50,54,74	2.23	18 (36%)	56,90,114	3.41	22 (39%)
25	CLA	S	610	18	59,63,73	1.34	8 (13%)	71,101,113	1.29	11 (15%)
25	CLA	s	613	18	59,63,73	1.34	7 (11%)	71,101,113	1.24	4 (5%)
25	CLA	r	603	17	64,68,73	1.30	11 (17%)	77,107,113	1.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	1	605	1	50,54,74	2.28	20 (40%)	56,90,114	3.31	20 (35%)
25	CLA	8	611	29	49,53,73	1.46	8 (16%)	59,89,113	1.30	7 (11%)
26	LUT	G	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)
25	CLA	G	602	1	69,73,73	1.28	11 (15%)	83,113,113	1.38	10 (12%)
25	CLA	R	611	29	53,57,73	1.45	10 (18%)	62,93,113	1.24	7 (11%)
30	BCR	d	404	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
24	CHL	g	601	1	70,74,74	1.87	17 (24%)	80,114,114	2.91	28 (35%)
25	CLA	S	609	18	49,53,73	1.50	5 (10%)	59,89,113	1.32	9 (15%)
25	CLA	g	602	1	69,73,73	1.29	11 (15%)	83,113,113	1.38	10 (12%)
25	CLA	7	604	-	49,53,73	1.47	11 (22%)	59,89,113	1.30	3 (5%)
25	CLA	C	503	6	69,73,73	1.27	8 (11%)	83,113,113	1.24	7 (8%)
29	LHG	b	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
29	LHG	r	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.33	6 (13%)
27	XAT	y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.99	20 (37%)
25	CLA	n	610	1	69,73,73	1.21	9 (13%)	83,113,113	1.25	9 (10%)
25	CLA	3	604	-	49,53,73	1.47	11 (22%)	59,89,113	1.30	4 (6%)
25	CLA	s	602	18	65,69,73	1.30	9 (13%)	78,108,113	1.24	9 (11%)
26	LUT	Y	1620	-	42,43,43	1.08	5 (11%)	51,60,60	1.92	20 (39%)
25	CLA	6	611	29	49,53,73	1.46	10 (20%)	59,89,113	1.45	7 (11%)
26	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
29	LHG	d	409	-	48,48,48	0.80	1 (2%)	51,54,54	1.33	7 (13%)
25	CLA	C	501	6	69,73,73	1.28	7 (10%)	83,113,113	1.14	6 (7%)
24	CHL	n	608	-	70,74,74	1.85	17 (24%)	80,114,114	2.91	27 (33%)
25	CLA	y	603	1	69,73,73	1.29	10 (14%)	83,113,113	1.35	11 (13%)
37	DGD	c	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)
25	CLA	R	613	17	64,68,73	1.29	8 (12%)	77,107,113	1.38	8 (10%)
24	CHL	N	605	1	52,56,74	2.19	18 (34%)	58,92,114	3.31	27 (46%)
29	LHG	C	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
35	LMG	B	2633	-	55,55,55	0.74	2 (3%)	63,63,63	1.36	6 (9%)
33	PHO	A	408	-	58,69,69	1.97	12 (20%)	56,99,99	1.69	8 (14%)
25	CLA	b	612	5	69,73,73	1.40	10 (14%)	83,113,113	1.49	11 (13%)
25	CLA	b	607	5	69,73,73	1.30	11 (15%)	83,113,113	1.31	8 (9%)
24	CHL	S	607	-	62,66,74	2.00	19 (30%)	70,104,114	3.00	26 (37%)
25	CLA	r	602	17	64,68,73	1.29	10 (15%)	77,107,113	1.34	10 (12%)
25	CLA	r	609	17	62,66,73	1.31	11 (17%)	74,104,113	1.25	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	604	5	69,73,73	1.33	11 (15%)	83,113,113	1.30	9 (10%)
24	CHL	S	601	18	50,54,74	2.23	18 (36%)	56,90,114	3.42	26 (46%)
24	CHL	G	606	-	54,58,74	2.15	17 (31%)	59,94,114	3.26	22 (37%)
24	CHL	g	607	-	70,74,74	1.88	18 (25%)	80,114,114	2.92	23 (28%)
25	CLA	n	604	-	54,58,73	1.46	10 (18%)	65,95,113	1.41	9 (13%)
25	CLA	N	611	29	64,68,73	1.28	9 (14%)	77,107,113	1.34	6 (7%)
28	NEX	y	1623	-	38,46,46	1.12	3 (7%)	50,70,70	2.70	22 (44%)
24	CHL	s	607	-	62,66,74	2.00	19 (30%)	70,104,114	3.00	25 (35%)
24	CHL	2	607	-	65,69,74	2.07	20 (30%)	74,108,114	2.85	25 (33%)
25	CLA	3	602	2	64,68,73	1.31	11 (17%)	77,107,113	1.20	7 (9%)
25	CLA	n	614	1	52,56,73	1.39	10 (19%)	62,92,113	1.36	8 (12%)
25	CLA	B	608	-	69,73,73	1.29	11 (15%)	83,113,113	1.31	7 (8%)
25	CLA	3	603	2	59,63,73	1.36	12 (20%)	71,101,113	1.47	8 (11%)
25	CLA	c	505	6	69,73,73	1.23	8 (11%)	83,113,113	1.38	9 (10%)
24	CHL	5	608	-	50,54,74	2.24	17 (34%)	56,90,114	3.36	23 (41%)
24	CHL	2	605	1	50,54,74	2.28	18 (36%)	56,90,114	3.29	22 (39%)
25	CLA	C	507	-	69,73,73	1.23	10 (14%)	83,113,113	1.42	9 (10%)
25	CLA	S	612	18	53,57,73	1.39	7 (13%)	62,93,113	1.32	6 (9%)
34	SQD	a	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.66	13 (20%)
29	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	N	610	1	69,73,73	1.21	9 (13%)	83,113,113	1.25	9 (10%)
26	LUT	N	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
29	LHG	B	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
25	CLA	4	610	3	49,53,73	1.49	9 (18%)	59,89,113	1.27	8 (13%)
26	LUT	6	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
25	CLA	Y	604	-	54,58,73	1.48	10 (18%)	65,95,113	1.43	10 (15%)
25	CLA	6	614	1	49,53,73	1.47	10 (20%)	59,89,113	1.32	8 (13%)
30	BCR	8	623	-	41,41,41	0.79	0	56,56,56	2.18	15 (26%)
25	CLA	c	506	6	69,73,73	1.28	10 (14%)	83,113,113	1.27	7 (8%)
25	CLA	5	604	-	54,58,73	1.44	11 (20%)	65,95,113	1.40	9 (13%)
36	PL9	d	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
25	CLA	b	614	5	69,73,73	1.33	11 (15%)	83,113,113	1.35	9 (10%)
34	SQD	B	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
25	CLA	7	611	29	59,63,73	1.40	11 (18%)	71,101,113	1.38	9 (12%)
28	NEX	R	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.53	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	G	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
35	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
26	LUT	g	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	N	613	1	64,68,73	1.34	9 (14%)	77,107,113	1.52	7 (9%)
24	CHL	s	606	-	50,54,74	2.28	18 (36%)	56,90,114	3.28	21 (37%)
24	CHL	8	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.34	25 (44%)
25	CLA	b	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	8 (9%)
36	PL9	a	414	-	13,13,55	0.74	0	17,17,69	2.09	4 (23%)
25	CLA	b	616	5	69,73,73	1.24	10 (14%)	83,113,113	1.37	10 (12%)
25	CLA	B	612	5	69,73,73	1.40	10 (14%)	83,113,113	1.50	12 (14%)
24	CHL	R	606	-	70,74,74	1.89	17 (24%)	80,114,114	2.91	28 (35%)
30	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
25	CLA	g	604	-	54,58,73	1.46	11 (20%)	65,95,113	1.42	7 (10%)
25	CLA	l	612	1	49,53,73	1.48	11 (22%)	59,89,113	1.54	11 (18%)
24	CHL	N	607	-	70,74,74	1.84	18 (25%)	80,114,114	3.03	22 (27%)
24	CHL	g	608	-	70,74,74	1.88	17 (24%)	80,114,114	2.96	25 (31%)
24	CHL	n	609	1	70,74,74	1.88	20 (28%)	80,114,114	2.76	26 (32%)
38	BCT	d	401	32	2,3,3	1.31	0	2,3,3	4.20	2 (100%)
24	CHL	S	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.27	20 (35%)
37	DGD	b	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
37	DGD	h	102	-	63,63,67	1.21	7 (11%)	77,77,81	1.52	10 (12%)
24	CHL	N	601	1	70,74,74	1.91	18 (25%)	80,114,114	2.87	27 (33%)
25	CLA	s	609	18	49,53,73	1.50	5 (10%)	59,89,113	1.32	9 (15%)
24	CHL	6	606	-	50,54,74	2.24	18 (36%)	56,90,114	3.28	23 (41%)
25	CLA	1	610	1	60,64,73	1.29	8 (13%)	72,102,113	1.23	9 (12%)
25	CLA	B	615	5	69,73,73	1.25	10 (14%)	83,113,113	1.22	10 (12%)
26	LUT	2	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
25	CLA	Y	603	1	69,73,73	1.29	10 (14%)	83,113,113	1.34	11 (13%)
25	CLA	C	511	6	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
25	CLA	1	614	1	49,53,73	1.48	10 (20%)	59,89,113	1.34	9 (15%)
25	CLA	2	612	1	49,53,73	1.48	10 (20%)	59,89,113	1.39	9 (15%)
25	CLA	n	611	29	64,68,73	1.28	9 (14%)	77,107,113	1.34	6 (7%)
26	LUT	n	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
25	CLA	S	613	18	59,63,73	1.34	8 (13%)	71,101,113	1.24	5 (7%)
27	XAT	6	1622	-	39,47,47	1.03	0	54,74,74	2.97	23 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	613	1	49,53,73	1.46	9 (18%)	59,89,113	1.33	8 (13%)
25	CLA	c	507	-	69,73,73	1.23	10 (14%)	83,113,113	1.42	9 (10%)
24	CHL	r	608	-	65,69,74	1.86	15 (23%)	74,108,114	3.01	23 (31%)
35	LMG	C	521	-	51,51,55	0.76	0	59,59,63	1.31	6 (10%)
25	CLA	2	611	29	49,53,73	1.46	10 (20%)	59,89,113	1.45	7 (11%)
25	CLA	b	617	5	69,73,73	1.27	11 (15%)	83,113,113	1.31	8 (9%)
25	CLA	S	603	18	49,53,73	1.49	6 (12%)	59,89,113	1.42	5 (8%)
25	CLA	N	612	1	64,68,73	1.27	10 (15%)	77,107,113	1.33	6 (7%)
24	CHL	2	606	-	50,54,74	2.24	18 (36%)	56,90,114	3.27	23 (41%)
24	CHL	G	605	1	50,54,74	2.24	18 (36%)	56,90,114	3.28	24 (42%)
25	CLA	a	406	-	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
24	CHL	5	609	1	66,70,74	2.05	17 (25%)	75,109,114	2.85	23 (30%)
34	SQD	b	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
25	CLA	C	508	6	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
24	CHL	7	601	2	68,72,74	1.92	17 (25%)	77,111,114	3.03	28 (36%)
25	CLA	g	612	1	64,68,73	1.30	10 (15%)	77,107,113	1.27	9 (11%)
25	CLA	3	612	2	49,53,73	1.49	12 (24%)	59,89,113	1.42	8 (13%)
25	CLA	3	613	2	62,66,73	1.33	11 (17%)	74,104,113	1.33	5 (6%)
26	LUT	R	620	-	42,43,43	0.99	4 (9%)	51,60,60	1.95	18 (35%)
27	XAT	2	1622	-	39,47,47	1.03	0	54,74,74	2.98	22 (40%)
24	CHL	4	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.27	22 (39%)
25	CLA	5	611	29	49,53,73	1.48	12 (24%)	59,89,113	1.46	5 (8%)
25	CLA	C	512	6	69,73,73	1.23	6 (8%)	83,113,113	1.23	6 (7%)
25	CLA	Y	602	1	69,73,73	1.30	11 (15%)	83,113,113	1.26	10 (12%)
24	CHL	3	607	-	57,61,74	2.12	20 (35%)	64,98,114	3.18	23 (35%)
25	CLA	r	610	17	69,73,73	1.21	8 (11%)	83,113,113	1.24	6 (7%)
27	XAT	r	622	-	39,47,47	1.06	2 (5%)	54,74,74	2.72	19 (35%)
25	CLA	2	613	1	49,53,73	1.47	9 (18%)	59,89,113	1.33	8 (13%)
25	CLA	8	604	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	9 (15%)
25	CLA	2	603	1	59,63,73	1.37	10 (16%)	71,101,113	1.41	8 (11%)
25	CLA	B	617	5	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
24	CHL	Y	607	-	70,74,74	1.84	16 (22%)	80,114,114	2.93	21 (26%)
35	LMG	a	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
25	CLA	7	610	2	64,68,73	1.30	10 (15%)	77,107,113	1.19	10 (12%)
27	XAT	1	1622	-	39,47,47	0.95	2 (5%)	54,74,74	2.85	22 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	n	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
24	CHL	2	601	1	50,54,74	2.26	18 (36%)	56,90,114	3.36	25 (44%)
25	CLA	1	613	1	59,63,73	1.35	11 (18%)	71,101,113	1.36	7 (9%)
24	CHL	6	605	1	50,54,74	2.28	18 (36%)	56,90,114	3.29	22 (39%)
24	CHL	y	609	1	70,74,74	1.91	18 (25%)	80,114,114	2.79	29 (36%)
25	CLA	7	614	2	52,56,73	1.46	7 (13%)	62,92,113	1.33	7 (11%)
38	BCT	D	401	32	2,3,3	1.30	0	2,3,3	4.21	2 (100%)
24	CHL	4	609	3	50,54,74	2.20	19 (38%)	56,90,114	3.46	23 (41%)
26	LUT	4	620	-	42,43,43	0.95	2 (4%)	51,60,60	2.09	15 (29%)
29	LHG	y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)
24	CHL	8	601	3	48,53,74	2.42	19 (39%)	53,89,114	3.23	20 (37%)
24	CHL	g	606	-	54,58,74	2.15	16 (29%)	59,94,114	3.25	22 (37%)
24	CHL	Y	606	-	54,58,74	2.09	18 (33%)	59,94,114	3.12	22 (37%)
24	CHL	g	605	1	50,54,74	2.24	17 (34%)	56,90,114	3.28	25 (44%)
30	BCR	A	411	-	41,41,41	0.81	0	56,56,56	1.85	12 (21%)
33	PHO	A	409	-	58,69,69	1.95	9 (15%)	56,99,99	1.75	7 (12%)
31	OEX	A	401	6,4	0,14,14	-	-	-	-	-
25	CLA	g	611	29	64,68,73	1.29	11 (17%)	77,107,113	1.29	5 (6%)
26	LUT	r	620	-	42,43,43	0.98	4 (9%)	51,60,60	1.95	18 (35%)
35	LMG	z	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.29	5 (8%)
25	CLA	R	603	17	64,68,73	1.31	11 (17%)	77,107,113	1.33	9 (11%)
29	LHG	s	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
24	CHL	1	609	1	66,70,74	2.05	17 (25%)	75,109,114	2.85	23 (30%)
25	CLA	8	603	3	49,53,73	1.48	11 (22%)	59,89,113	1.38	5 (8%)
25	CLA	1	603	1	59,63,73	1.38	12 (20%)	71,101,113	1.45	9 (12%)
25	CLA	6	610	1	54,58,73	1.37	9 (16%)	65,95,113	1.17	6 (9%)
25	CLA	5	610	1	60,64,73	1.29	8 (13%)	72,102,113	1.23	8 (11%)
25	CLA	C	506	6	69,73,73	1.28	10 (14%)	83,113,113	1.27	7 (8%)
26	LUT	S	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
25	CLA	N	603	1	69,73,73	1.30	11 (15%)	83,113,113	1.36	11 (13%)
26	LUT	5	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
25	CLA	s	612	18	53,57,73	1.39	7 (13%)	62,93,113	1.32	7 (11%)
25	CLA	4	604	-	49,53,73	1.48	10 (20%)	59,89,113	1.41	7 (11%)
25	CLA	c	508	6	69,73,73	1.25	9 (13%)	83,113,113	1.34	8 (9%)
25	CLA	D	402	7	69,73,73	1.32	12 (17%)	83,113,113	1.39	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	610	5	69,73,73	1.26	12 (17%)	83,113,113	1.32	10 (12%)
25	CLA	y	604	-	54,58,73	1.48	10 (18%)	65,95,113	1.43	10 (15%)
24	CHL	n	606	-	54,58,74	2.13	17 (31%)	59,94,114	3.18	20 (33%)
34	SQD	A	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)
37	DGD	C	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)
30	BCR	B	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	15 (26%)
39	HEM	f	101	8,9	50,50,50	1.34	7 (14%)	66,82,82	1.10	4 (6%)
26	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
25	CLA	B	605	5	69,73,73	1.35	13 (18%)	83,113,113	1.73	17 (20%)
29	LHG	Y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)
30	BCR	c	517	-	41,41,41	0.80	0	56,56,56	2.11	13 (23%)
37	DGD	c	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)
26	LUT	g	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)
25	CLA	G	612	1	64,68,73	1.30	10 (15%)	77,107,113	1.27	9 (11%)
29	LHG	1	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
29	LHG	6	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
29	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
26	LUT	3	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
30	BCR	C	517	-	41,41,41	0.80	0	56,56,56	2.10	13 (23%)
24	CHL	7	609	2	65,69,74	2.05	19 (29%)	74,108,114	2.84	24 (32%)
25	CLA	c	504	-	69,73,73	1.24	8 (11%)	83,113,113	1.24	7 (8%)
29	LHG	b	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
37	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
27	XAT	7	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.07	27 (50%)
25	CLA	7	613	2	62,66,73	1.33	11 (17%)	74,104,113	1.33	5 (6%)
25	CLA	A	407	-	54,58,73	1.41	10 (18%)	65,95,113	1.31	6 (9%)
25	CLA	S	611	29	60,64,73	1.32	7 (11%)	72,102,113	1.24	6 (8%)
29	LHG	d	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
26	LUT	Y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.87	17 (33%)
30	BCR	D	404	-	41,41,41	0.76	0	56,56,56	1.93	14 (25%)
24	CHL	3	608	-	50,54,74	2.23	18 (36%)	56,90,114	3.42	22 (39%)
25	CLA	r	616	17	49,53,73	1.48	12 (24%)	59,89,113	1.44	6 (10%)
26	LUT	1	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.87	14 (27%)
30	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.94	14 (25%)
24	CHL	1	601	1	50,54,74	2.27	17 (34%)	56,90,114	3.34	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	1	1623	-	38,46,46	1.13	4 (10%)	50,70,70	2.62	18 (36%)
25	CLA	5	614	1	49,53,73	1.48	10 (20%)	59,89,113	1.34	9 (15%)
25	CLA	1	602	1	65,69,73	1.34	11 (16%)	78,108,113	1.21	9 (11%)
30	BCR	b	619	-	41,41,41	0.87	2 (4%)	56,56,56	1.86	17 (30%)
30	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
25	CLA	A	405	4	69,73,73	1.30	11 (15%)	83,113,113	1.27	6 (7%)
25	CLA	4	602	3	49,53,73	1.43	10 (20%)	59,89,113	1.49	9 (15%)
24	CHL	5	606	-	50,54,74	2.23	17 (34%)	56,90,114	3.20	21 (37%)
28	NEX	r	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.52	21 (42%)
24	CHL	Y	608	-	70,74,74	1.82	16 (22%)	80,114,114	2.96	22 (27%)
25	CLA	1	604	-	54,58,73	1.44	11 (20%)	65,95,113	1.41	9 (13%)
24	CHL	R	607	-	60,64,74	2.06	18 (30%)	68,102,114	3.14	28 (41%)
28	NEX	S	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	16 (32%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.42	14 (28%)
24	CHL	8	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.27	22 (39%)
25	CLA	s	611	29	60,64,73	1.32	7 (11%)	72,102,113	1.24	6 (8%)
27	XAT	4	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	19 (35%)
26	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
24	CHL	G	609	1	65,69,74	1.96	19 (29%)	74,108,114	2.89	26 (35%)
27	XAT	n	1622	-	39,47,47	0.97	1 (2%)	54,74,74	3.01	23 (42%)
27	XAT	R	622	-	39,47,47	1.05	2 (5%)	54,74,74	2.72	19 (35%)
24	CHL	s	601	18	50,54,74	2.23	18 (36%)	56,90,114	3.43	26 (46%)
36	PL9	A	414	-	13,13,55	0.75	0	17,17,69	2.08	4 (23%)
28	NEX	2	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.41	14 (28%)
25	CLA	a	405	4	69,73,73	1.30	11 (15%)	83,113,113	1.26	7 (8%)
29	LHG	G	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
25	CLA	b	613	5	69,73,73	1.34	8 (11%)	83,113,113	1.52	12 (14%)
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
24	CHL	N	606	-	54,58,74	2.13	17 (31%)	59,94,114	3.17	20 (33%)
29	LHG	D	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	7 (13%)
24	CHL	7	605	2	50,54,74	2.24	18 (36%)	56,90,114	3.34	25 (44%)
26	LUT	N	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
25	CLA	b	603	5	69,73,73	1.27	11 (15%)	83,113,113	1.18	6 (7%)
25	CLA	B	611	-	69,73,73	1.30	10 (14%)	83,113,113	1.42	13 (15%)
37	DGD	C	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	3	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
25	CLA	d	403	7	69,73,73	1.26	11 (15%)	83,113,113	1.27	9 (10%)
25	CLA	c	509	6	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
24	CHL	4	608	-	50,54,74	2.18	18 (36%)	56,90,114	3.33	29 (51%)
25	CLA	c	501	6	69,73,73	1.28	7 (10%)	83,113,113	1.14	6 (7%)
25	CLA	C	513	6	69,73,73	1.22	7 (10%)	83,113,113	1.31	10 (12%)
25	CLA	B	613	5	69,73,73	1.34	8 (11%)	83,113,113	1.52	13 (15%)
25	CLA	R	610	17	69,73,73	1.21	8 (11%)	83,113,113	1.24	6 (7%)
30	BCR	H	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
25	CLA	g	614	1	52,56,73	1.43	10 (19%)	62,92,113	1.22	6 (9%)
30	BCR	c	516	-	41,41,41	0.68	0	56,56,56	1.94	14 (25%)
25	CLA	R	604	-	52,56,73	1.45	11 (21%)	62,92,113	1.45	10 (16%)
24	CHL	n	605	1	52,56,74	2.19	18 (34%)	58,92,114	3.32	27 (46%)
25	CLA	8	602	3	49,53,73	1.43	10 (20%)	59,89,113	1.49	9 (15%)
25	CLA	5	613	1	59,63,73	1.35	11 (18%)	71,101,113	1.35	7 (9%)
26	LUT	s	1621	-	42,43,43	0.80	0	51,60,60	1.73	15 (29%)
24	CHL	1	606	-	50,54,74	2.23	17 (34%)	56,90,114	3.20	21 (37%)
25	CLA	2	604	-	49,53,73	1.46	11 (22%)	59,89,113	1.47	11 (18%)
29	LHG	S	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
24	CHL	3	609	2	65,69,74	2.05	19 (29%)	74,108,114	2.85	24 (32%)
30	BCR	B	619	-	41,41,41	0.87	1 (2%)	56,56,56	1.86	17 (30%)
29	LHG	8	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
25	CLA	r	601	17	53,57,73	1.41	10 (18%)	62,93,113	1.56	9 (14%)
24	CHL	y	607	-	70,74,74	1.85	16 (22%)	80,114,114	2.94	21 (26%)
24	CHL	r	606	-	70,74,74	1.90	17 (24%)	80,114,114	2.90	28 (35%)
27	XAT	N	1622	-	39,47,47	0.96	1 (2%)	54,74,74	3.00	23 (42%)
29	LHG	C	523	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	6 (11%)
29	LHG	R	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.34	6 (13%)
29	LHG	7	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.31	4 (8%)
30	BCR	h	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
28	NEX	N	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	16 (32%)
33	PHO	a	409	-	58,69,69	1.95	9 (15%)	56,99,99	1.75	7 (12%)
24	CHL	Y	609	1	70,74,74	1.91	18 (25%)	80,114,114	2.80	29 (36%)
25	CLA	A	406	-	69,73,73	1.27	10 (14%)	83,113,113	1.37	8 (9%)
25	CLA	C	510	6	69,73,73	1.24	9 (13%)	83,113,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	G	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.85	22 (40%)
25	CLA	7	612	2	49,53,73	1.49	12 (24%)	59,89,113	1.42	8 (13%)
30	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.89	17 (30%)
25	CLA	3	611	29	59,63,73	1.40	11 (18%)	71,101,113	1.38	9 (12%)
25	CLA	d	402	7	69,73,73	1.33	12 (17%)	83,113,113	1.38	14 (16%)
26	LUT	7	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
25	CLA	C	502	6	69,73,73	1.24	7 (10%)	83,113,113	1.41	6 (7%)
24	CHL	1	608	-	50,54,74	2.23	17 (34%)	56,90,114	3.36	23 (41%)
28	NEX	3	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.46	16 (32%)
24	CHL	n	601	1	70,74,74	1.92	18 (25%)	80,114,114	2.87	27 (33%)
25	CLA	G	603	1	69,73,73	1.29	10 (14%)	83,113,113	1.37	10 (12%)
25	CLA	y	602	1	69,73,73	1.30	11 (15%)	83,113,113	1.26	10 (12%)
29	LHG	N	2630	25	48,48,48	0.75	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	4	612	3	49,53,73	1.48	9 (18%)	59,89,113	1.43	8 (13%)
24	CHL	5	605	1	50,54,74	2.28	20 (40%)	56,90,114	3.31	20 (35%)
25	CLA	y	612	1	64,68,73	1.34	10 (15%)	77,107,113	1.32	9 (11%)
25	CLA	Y	611	29	64,68,73	1.36	10 (15%)	77,107,113	1.27	8 (10%)
25	CLA	C	505	6	69,73,73	1.23	8 (11%)	83,113,113	1.38	8 (9%)
25	CLA	2	602	1	65,69,73	1.31	10 (15%)	78,108,113	1.22	9 (11%)
25	CLA	C	504	-	69,73,73	1.24	8 (11%)	83,113,113	1.24	7 (8%)
24	CHL	g	609	1	65,69,74	1.96	19 (29%)	74,108,114	2.89	26 (35%)
30	BCR	t	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.62	23 (41%)
29	LHG	5	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
25	CLA	s	603	18	49,53,73	1.49	6 (12%)	59,89,113	1.42	5 (8%)
28	NEX	7	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.46	16 (32%)
25	CLA	c	502	6	69,73,73	1.24	7 (10%)	83,113,113	1.41	6 (7%)
25	CLA	g	613	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	4 (4%)
26	LUT	G	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	n	612	1	64,68,73	1.27	10 (15%)	77,107,113	1.32	6 (7%)
35	LMG	c	521	-	51,51,55	0.76	1 (1%)	59,59,63	1.31	6 (10%)
25	CLA	R	616	17	49,53,73	1.48	12 (24%)	59,89,113	1.44	6 (10%)
24	CHL	5	601	1	50,54,74	2.26	16 (32%)	56,90,114	3.34	23 (41%)
24	CHL	6	609	1	65,69,74	1.97	17 (26%)	74,108,114	2.89	24 (32%)
25	CLA	B	603	5	69,73,73	1.27	11 (15%)	83,113,113	1.19	6 (7%)
25	CLA	r	604	-	52,56,73	1.45	11 (21%)	62,92,113	1.44	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	603	1	59,63,73	1.37	10 (16%)	71,101,113	1.41	8 (11%)
34	SQD	a	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)
25	CLA	b	609	5	69,73,73	1.22	10 (14%)	83,113,113	1.43	9 (10%)
26	LUT	y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.86	17 (33%)
24	CHL	3	605	2	50,54,74	2.24	18 (36%)	56,90,114	3.34	25 (44%)
24	CHL	3	601	2	68,72,74	1.92	17 (25%)	77,111,114	3.03	28 (36%)
25	CLA	4	611	29	49,53,73	1.46	9 (18%)	59,89,113	1.31	8 (13%)
25	CLA	Y	612	1	64,68,73	1.34	10 (15%)	77,107,113	1.31	8 (10%)
25	CLA	g	610	1	68,72,73	1.23	9 (13%)	81,111,113	1.25	9 (11%)
24	CHL	G	607	-	70,74,74	1.88	18 (25%)	80,114,114	2.93	23 (28%)
30	BCR	c	515	-	41,41,41	0.77	0	56,56,56	1.90	17 (30%)
25	CLA	5	612	1	49,53,73	1.49	11 (22%)	59,89,113	1.55	11 (18%)
29	LHG	3	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.30	4 (8%)
35	LMG	A	415	-	40,40,55	0.88	0	48,48,63	1.32	6 (12%)
24	CHL	2	608	-	50,54,74	2.21	19 (38%)	56,90,114	3.38	20 (35%)
25	CLA	R	609	17	62,66,73	1.31	12 (19%)	74,104,113	1.25	5 (6%)
24	CHL	Y	601	1	70,74,74	1.86	17 (24%)	80,114,114	3.04	28 (35%)
24	CHL	8	609	3	50,54,74	2.21	19 (38%)	56,90,114	3.45	23 (41%)
29	LHG	g	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
25	CLA	B	607	5	69,73,73	1.30	11 (15%)	83,113,113	1.31	8 (9%)
34	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
25	CLA	3	610	2	64,68,73	1.30	10 (15%)	77,107,113	1.19	9 (11%)
25	CLA	6	602	1	65,69,73	1.31	10 (15%)	78,108,113	1.22	9 (11%)
25	CLA	3	614	2	52,56,73	1.46	7 (13%)	62,92,113	1.33	7 (11%)
35	LMG	b	2633	-	55,55,55	0.75	2 (3%)	63,63,63	1.36	6 (9%)
24	CHL	3	606	-	50,54,74	2.34	18 (36%)	56,90,114	3.37	25 (44%)
25	CLA	r	612	17	53,57,73	1.43	10 (18%)	62,93,113	1.43	6 (9%)
25	CLA	G	613	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	4 (4%)
25	CLA	Y	610	1	64,68,73	1.32	9 (14%)	77,107,113	1.21	9 (11%)
25	CLA	2	614	1	49,53,73	1.47	10 (20%)	59,89,113	1.32	7 (11%)
25	CLA	a	407	-	54,58,73	1.41	10 (18%)	65,95,113	1.31	6 (9%)
25	CLA	b	604	5	69,73,73	1.33	11 (15%)	83,113,113	1.29	10 (12%)
28	NEX	g	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
24	CHL	6	607	-	65,69,74	2.07	20 (30%)	74,108,114	2.86	25 (33%)
34	SQD	A	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.67	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	D	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.38	6 (11%)
25	CLA	1	611	29	49,53,73	1.48	12 (24%)	59,89,113	1.45	5 (8%)
25	CLA	c	512	6	69,73,73	1.24	6 (8%)	83,113,113	1.23	6 (7%)
25	CLA	Y	614	1	52,56,73	1.44	10 (19%)	62,92,113	1.35	7 (11%)
24	CHL	y	608	-	70,74,74	1.83	16 (22%)	80,114,114	2.97	22 (27%)
25	CLA	R	602	17	64,68,73	1.29	11 (17%)	77,107,113	1.34	11 (14%)
35	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	B	606	5	69,73,73	1.33	13 (18%)	83,113,113	1.47	10 (12%)
30	BCR	T	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.63	23 (41%)
24	CHL	Y	605	1	52,56,74	2.16	18 (34%)	58,92,114	3.25	22 (37%)
26	LUT	5	1620	-	42,43,43	0.94	2 (4%)	51,60,60	1.87	14 (27%)
24	CHL	6	601	1	50,54,74	2.26	18 (36%)	56,90,114	3.35	25 (44%)
25	CLA	S	602	18	65,69,73	1.29	9 (13%)	78,108,113	1.24	9 (11%)
25	CLA	B	614	5	69,73,73	1.34	11 (15%)	83,113,113	1.35	9 (10%)
24	CHL	N	609	1	70,74,74	1.88	19 (27%)	80,114,114	2.76	26 (32%)
29	LHG	d	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
37	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
24	CHL	r	614	17	46,50,74	2.37	18 (39%)	51,85,114	3.50	20 (39%)
24	CHL	y	601	1	70,74,74	1.86	17 (24%)	80,114,114	3.04	28 (35%)
26	LUT	1	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
25	CLA	S	604	-	54,58,73	1.41	6 (11%)	65,95,113	1.43	7 (10%)
25	CLA	a	410	4	64,68,73	1.27	10 (15%)	77,107,113	1.36	9 (11%)
24	CHL	n	607	-	70,74,74	1.84	18 (25%)	80,114,114	3.03	22 (27%)
25	CLA	b	615	5	69,73,73	1.25	10 (14%)	83,113,113	1.22	10 (12%)
37	DGD	H	102	-	63,63,67	1.21	6 (9%)	77,77,81	1.52	10 (12%)
25	CLA	B	602	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	9 (10%)
25	CLA	B	609	5	69,73,73	1.22	10 (14%)	83,113,113	1.43	9 (10%)
25	CLA	G	610	1	68,72,73	1.23	9 (13%)	81,111,113	1.25	9 (11%)
25	CLA	b	605	5	69,73,73	1.35	14 (20%)	83,113,113	1.72	18 (21%)
29	LHG	c	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
24	CHL	R	614	17	46,50,74	2.37	18 (39%)	51,85,114	3.51	20 (39%)
27	XAT	3	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.06	27 (50%)
24	CHL	G	608	-	70,74,74	1.88	17 (24%)	80,114,114	2.95	25 (31%)
28	NEX	s	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	15 (30%)
24	CHL	1	607	-	67,71,74	1.94	19 (28%)	76,110,114	3.11	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	r	611	29	53,57,73	1.46	10 (18%)	62,93,113	1.24	7 (11%)
29	LHG	D	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
24	CHL	2	609	1	65,69,74	1.97	16 (24%)	74,108,114	2.90	24 (32%)
25	CLA	7	603	2	59,63,73	1.36	12 (20%)	71,101,113	1.46	8 (11%)
35	LMG	d	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.37	6 (11%)
25	CLA	n	613	1	64,68,73	1.34	9 (14%)	77,107,113	1.53	7 (9%)
25	CLA	g	603	1	69,73,73	1.29	10 (14%)	83,113,113	1.37	10 (12%)
26	LUT	8	620	-	42,43,43	0.94	2 (4%)	51,60,60	2.09	15 (29%)
24	CHL	4	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.35	25 (44%)
25	CLA	N	604	-	54,58,73	1.46	10 (18%)	65,95,113	1.41	9 (13%)
25	CLA	R	612	17	53,57,73	1.43	10 (18%)	62,93,113	1.43	6 (9%)
30	BCR	b	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
25	CLA	c	503	6	69,73,73	1.26	8 (11%)	83,113,113	1.23	7 (8%)
29	LHG	D	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
26	LUT	y	1620	-	42,43,43	1.09	5 (11%)	51,60,60	1.91	20 (39%)
25	CLA	c	510	6	69,73,73	1.24	9 (13%)	83,113,113	1.28	8 (9%)
24	CHL	s	608	-	50,54,74	2.27	19 (38%)	56,90,114	3.25	20 (35%)
24	CHL	4	601	3	48,53,74	2.43	19 (39%)	53,89,114	3.23	20 (37%)
25	CLA	G	604	-	54,58,73	1.46	10 (18%)	65,95,113	1.42	7 (10%)
25	CLA	b	606	5	69,73,73	1.33	13 (18%)	83,113,113	1.47	10 (12%)
24	CHL	S	606	-	50,54,74	2.28	18 (36%)	56,90,114	3.28	21 (37%)
25	CLA	Y	613	1	69,73,73	1.34	11 (15%)	83,113,113	1.58	8 (9%)
25	CLA	G	614	1	52,56,73	1.44	10 (19%)	62,92,113	1.23	6 (9%)
25	CLA	s	604	-	54,58,73	1.41	6 (11%)	65,95,113	1.43	7 (10%)
25	CLA	n	603	1	69,73,73	1.29	11 (15%)	83,113,113	1.36	11 (13%)
25	CLA	s	610	18	59,63,73	1.34	8 (13%)	71,101,113	1.29	10 (14%)
25	CLA	8	610	3	49,53,73	1.49	10 (20%)	59,89,113	1.27	8 (13%)
29	LHG	B	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
24	CHL	r	607	-	60,64,74	2.06	18 (30%)	68,102,114	3.15	28 (41%)
25	CLA	7	602	2	64,68,73	1.31	11 (17%)	77,107,113	1.20	7 (9%)
25	CLA	s	614	18	53,57,73	1.37	6 (11%)	62,93,113	1.37	8 (12%)
24	CHL	y	605	1	52,56,74	2.16	18 (34%)	58,92,114	3.25	22 (37%)
25	CLA	N	602	1	69,73,73	1.27	11 (15%)	83,113,113	1.27	9 (10%)
25	CLA	b	608	-	69,73,73	1.29	11 (15%)	83,113,113	1.31	7 (8%)
25	CLA	B	616	5	69,73,73	1.25	10 (14%)	83,113,113	1.37	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	8	608	-	50,54,74	2.18	18 (36%)	56,90,114	3.33	28 (50%)
29	LHG	n	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	7 (13%)
24	CHL	R	608	-	65,69,74	1.86	15 (23%)	74,108,114	3.01	23 (31%)
25	CLA	b	611	-	69,73,73	1.30	10 (14%)	83,113,113	1.42	13 (15%)
25	CLA	y	611	29	64,68,73	1.36	10 (15%)	77,107,113	1.27	8 (10%)
27	XAT	Y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.98	19 (35%)
24	CHL	G	601	1	70,74,74	1.87	17 (24%)	80,114,114	2.91	28 (35%)
25	CLA	S	614	18	53,57,73	1.38	6 (11%)	62,93,113	1.38	8 (12%)
25	CLA	6	604	-	49,53,73	1.46	11 (22%)	59,89,113	1.47	11 (18%)
39	HEM	F	101	8,9	50,50,50	1.34	7 (14%)	66,82,82	1.11	4 (6%)
24	CHL	7	607	-	57,61,74	2.13	20 (35%)	64,98,114	3.19	23 (35%)
30	BCR	a	411	-	41,41,41	0.81	0	56,56,56	1.84	12 (21%)
35	LMG	a	415	-	40,40,55	0.88	0	48,48,63	1.31	6 (12%)
31	OEX	a	401	6,4	0,14,14	-	-	-	-	-
25	CLA	B	610	5	69,73,73	1.26	12 (17%)	83,113,113	1.32	10 (12%)
27	XAT	5	1622	-	39,47,47	0.96	2 (5%)	54,74,74	2.84	22 (40%)
25	CLA	D	403	7	69,73,73	1.26	11 (15%)	83,113,113	1.27	9 (10%)
29	LHG	c	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
34	SQD	b	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
25	CLA	r	613	17	64,68,73	1.29	8 (12%)	77,107,113	1.38	8 (10%)
24	CHL	6	608	-	50,54,74	2.21	19 (38%)	56,90,114	3.38	20 (35%)
25	CLA	5	603	1	59,63,73	1.37	12 (20%)	71,101,113	1.45	9 (12%)
30	BCR	B	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
28	NEX	n	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	17 (34%)
25	CLA	n	602	1	69,73,73	1.27	11 (15%)	83,113,113	1.27	9 (10%)
25	CLA	y	613	1	69,73,73	1.34	11 (15%)	83,113,113	1.58	7 (8%)
27	XAT	g	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.86	22 (40%)

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	CLA	2	610	1	-	5/21/97/115	-
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	509	6	-	8/39/115/115	-
24	CHL	N	608	-	1/1/15/21	14/41/117/117	-
25	CLA	G	611	29	-	13/33/109/115	-
29	LHG	2	2630	25	-	14/41/41/53	-
35	LMG	Z	101	-	-	22/46/66/70	0/1/1/1
25	CLA	c	513	6	-	12/39/115/115	-
24	CHL	y	606	-	-	7/22/98/117	-
28	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	R	601	17	-	11/20/96/115	-
29	LHG	C	2630	-	-	27/53/53/53	-
24	CHL	7	606	-	-	5/17/93/117	-
25	CLA	8	612	3	-	8/15/91/115	-
26	LUT	S	1621	-	-	4/29/67/67	0/2/2/2
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	4	603	3	-	6/15/91/115	-
28	NEX	5	1623	-	-	9/27/83/83	0/3/3/3
25	CLA	5	602	1	-	10/35/111/115	-
25	CLA	c	511	6	-	13/39/115/115	-
25	CLA	y	610	1	-	9/33/109/115	-
25	CLA	6	612	1	-	8/15/91/115	-
35	LMG	A	413	-	-	17/43/63/70	0/1/1/1
27	XAT	8	622	-	-	3/31/93/93	0/4/4/4
30	BCR	4	623	-	-	12/29/63/63	0/2/2/2
37	DGD	B	626	-	-	22/48/88/95	0/2/2/2
25	CLA	y	614	1	-	5/19/95/115	-
24	CHL	5	607	-	1/1/14/21	19/38/114/117	-
25	CLA	N	614	1	-	7/19/95/115	-
29	LHG	4	2630	25	-	8/23/23/53	-
33	PHO	a	408	-	-	6/37/103/103	0/5/6/6
36	PL9	D	405	-	-	8/53/73/73	0/1/1/1
25	CLA	A	410	4	-	8/33/109/115	-
24	CHL	7	608	-	-	8/17/93/117	-
25	CLA	S	610	18	-	6/27/103/115	-
25	CLA	s	613	18	-	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	603	17	-	15/33/109/115	-
24	CHL	1	605	1	-	10/17/93/117	-
25	CLA	8	611	29	-	8/15/91/115	-
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	G	602	1	-	11/39/115/115	-
25	CLA	R	611	29	-	11/20/96/115	-
30	BCR	d	404	-	-	5/29/63/63	0/2/2/2
24	CHL	g	601	1	1/1/15/21	17/41/117/117	-
25	CLA	S	609	18	-	9/15/91/115	-
25	CLA	g	602	1	-	11/39/115/115	-
25	CLA	7	604	-	-	11/15/91/115	-
25	CLA	C	503	6	-	12/39/115/115	-
29	LHG	b	2631	-	-	20/53/53/53	-
29	LHG	r	2630	25	-	16/46/46/53	-
27	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	n	610	1	-	11/39/115/115	-
25	CLA	3	604	-	-	11/15/91/115	-
25	CLA	s	602	18	-	16/35/111/115	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	6	611	29	-	5/15/91/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	d	409	-	-	20/53/53/53	-
25	CLA	C	501	6	-	15/39/115/115	-
24	CHL	n	608	-	1/1/15/21	14/41/117/117	-
25	CLA	y	603	1	-	14/39/115/115	-
37	DGD	c	520	-	-	28/49/89/95	0/2/2/2
25	CLA	R	613	17	-	13/33/109/115	-
24	CHL	N	605	1	-	11/20/96/117	-
29	LHG	C	522	-	-	20/53/53/53	-
35	LMG	B	2633	-	-	21/50/70/70	0/1/1/1
33	PHO	A	408	-	-	6/37/103/103	0/5/6/6
25	CLA	b	612	5	-	12/39/115/115	-
25	CLA	b	607	5	-	13/39/115/115	-
24	CHL	S	607	-	1/1/13/21	13/32/108/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	602	17	-	7/33/109/115	-
25	CLA	r	609	17	-	2/31/107/115	-
25	CLA	B	604	5	-	11/39/115/115	-
24	CHL	S	601	18	-	10/17/93/117	-
24	CHL	G	606	-	-	10/22/98/117	-
24	CHL	g	607	-	1/1/15/21	15/41/117/117	-
25	CLA	n	604	-	-	4/21/97/115	-
25	CLA	N	611	29	-	9/33/109/115	-
28	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	s	607	-	1/1/13/21	13/32/108/117	-
24	CHL	2	607	-	1/1/14/21	20/35/111/117	-
25	CLA	3	602	2	-	15/33/109/115	-
25	CLA	n	614	1	-	7/19/95/115	-
25	CLA	B	608	-	-	13/39/115/115	-
25	CLA	3	603	2	-	11/27/103/115	-
25	CLA	c	505	6	-	13/39/115/115	-
24	CHL	5	608	-	-	3/17/93/117	-
24	CHL	2	605	1	-	10/17/93/117	-
25	CLA	C	507	-	-	21/39/115/115	-
25	CLA	S	612	18	-	3/20/96/115	-
34	SQD	a	418	-	-	22/49/69/69	0/1/1/1
29	LHG	c	523	-	-	21/53/53/53	-
25	CLA	N	610	1	-	11/39/115/115	-
26	LUT	N	1621	-	-	1/29/67/67	0/2/2/2
29	LHG	B	2631	-	-	20/53/53/53	-
25	CLA	4	610	3	-	8/15/91/115	-
26	LUT	6	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	Y	604	-	-	5/21/97/115	-
25	CLA	6	614	1	-	8/15/91/115	-
30	BCR	8	623	-	-	12/29/63/63	0/2/2/2
25	CLA	c	506	6	-	16/39/115/115	-
25	CLA	5	604	-	-	12/21/97/115	-
36	PL9	d	405	-	-	8/53/73/73	0/1/1/1
25	CLA	b	614	5	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
25	CLA	7	611	29	-	12/27/103/115	-
28	NEX	R	623	-	-	4/27/83/83	0/3/3/3
28	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
35	LMG	B	622	-	-	22/46/66/70	0/1/1/1
26	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	N	613	1	-	6/33/109/115	-
24	CHL	s	606	-	-	10/17/93/117	-
24	CHL	8	606	-	-	7/17/93/117	-
25	CLA	b	602	-	-	17/39/115/115	-
36	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CLA	b	616	5	-	14/39/115/115	-
25	CLA	B	612	5	-	12/39/115/115	-
24	CHL	R	606	-	1/1/15/21	23/41/117/117	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2
25	CLA	g	604	-	-	7/21/97/115	-
25	CLA	1	612	1	-	6/15/91/115	-
24	CHL	N	607	-	1/1/15/21	19/41/117/117	-
24	CHL	g	608	-	1/1/15/21	18/41/117/117	-
24	CHL	n	609	1	1/1/15/21	15/41/117/117	-
24	CHL	S	608	-	-	5/17/93/117	-
37	DGD	b	626	-	-	22/48/88/95	0/2/2/2
37	DGD	h	102	-	-	25/51/91/95	0/2/2/2
24	CHL	N	601	1	1/1/15/21	17/41/117/117	-
25	CLA	s	609	18	-	9/15/91/115	-
24	CHL	6	606	-	-	5/17/93/117	-
25	CLA	1	610	1	-	5/29/105/115	-
25	CLA	B	615	5	-	15/39/115/115	-
26	LUT	2	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	Y	603	1	-	14/39/115/115	-
25	CLA	C	511	6	-	13/39/115/115	-
25	CLA	1	614	1	-	6/15/91/115	-
25	CLA	2	612	1	-	8/15/91/115	-
25	CLA	n	611	29	-	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	S	613	18	-	6/27/103/115	-
27	XAT	6	1622	-	-	4/31/93/93	0/4/4/4
25	CLA	6	613	1	-	7/15/91/115	-
25	CLA	c	507	-	-	21/39/115/115	-
24	CHL	r	608	-	1/1/14/21	18/35/111/117	-
35	LMG	C	521	-	-	21/46/66/70	0/1/1/1
25	CLA	2	611	29	-	5/15/91/115	-
25	CLA	b	617	5	-	17/39/115/115	-
25	CLA	S	603	18	-	5/15/91/115	-
25	CLA	N	612	1	-	10/33/109/115	-
24	CHL	2	606	-	-	5/17/93/117	-
24	CHL	G	605	1	-	11/17/93/117	-
25	CLA	a	406	-	-	4/39/115/115	-
24	CHL	5	609	1	1/1/14/21	13/37/113/117	-
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
25	CLA	C	508	6	-	8/39/115/115	-
24	CHL	7	601	2	1/1/14/21	15/39/115/117	-
25	CLA	g	612	1	-	11/33/109/115	-
25	CLA	3	612	2	-	8/15/91/115	-
25	CLA	3	613	2	-	10/31/107/115	-
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
27	XAT	2	1622	-	-	4/31/93/93	0/4/4/4
24	CHL	4	607	-	-	10/17/93/117	-
25	CLA	5	611	29	-	7/15/91/115	-
25	CLA	C	512	6	-	9/39/115/115	-
25	CLA	Y	602	1	-	14/39/115/115	-
24	CHL	3	607	-	-	12/26/102/117	-
25	CLA	r	610	17	-	14/39/115/115	-
27	XAT	r	622	-	-	5/31/93/93	0/4/4/4
25	CLA	2	613	1	-	7/15/91/115	-
25	CLA	8	604	-	-	11/15/91/115	-
25	CLA	2	603	1	-	15/27/103/115	-
25	CLA	B	617	5	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	Y	607	-	1/1/15/21	17/41/117/117	-
35	LMG	a	413	-	-	17/43/63/70	0/1/1/1
25	CLA	7	610	2	-	6/33/109/115	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
26	LUT	n	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	2	601	1	-	8/17/93/117	-
25	CLA	1	613	1	-	9/27/103/115	-
24	CHL	6	605	1	-	10/17/93/117	-
24	CHL	y	609	1	1/1/15/21	14/41/117/117	-
25	CLA	7	614	2	-	5/19/95/115	-
24	CHL	4	609	3	-	9/17/93/117	-
26	LUT	4	620	-	-	5/29/67/67	0/2/2/2
29	LHG	y	2630	25	-	20/53/53/53	-
24	CHL	8	601	3	-	6/15/91/117	-
24	CHL	g	606	-	-	10/22/98/117	-
24	CHL	Y	606	-	-	7/22/98/117	-
24	CHL	g	605	1	-	12/17/93/117	-
30	BCR	A	411	-	-	2/29/63/63	0/2/2/2
33	PHO	A	409	-	-	8/37/103/103	0/5/6/6
25	CLA	g	611	29	-	13/33/109/115	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
35	LMG	z	101	-	-	22/46/66/70	0/1/1/1
25	CLA	R	603	17	-	15/33/109/115	-
29	LHG	s	2630	25	-	24/53/53/53	-
24	CHL	1	609	1	1/1/14/21	13/37/113/117	-
25	CLA	8	603	3	-	6/15/91/115	-
25	CLA	1	603	1	-	12/27/103/115	-
25	CLA	6	610	1	-	5/21/97/115	-
25	CLA	5	610	1	-	5/29/105/115	-
25	CLA	C	506	6	-	16/39/115/115	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	N	603	1	-	14/39/115/115	-
26	LUT	5	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	s	612	18	-	3/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	604	-	-	11/15/91/115	-
25	CLA	c	508	6	-	8/39/115/115	-
25	CLA	D	402	7	-	5/39/115/115	-
25	CLA	b	610	5	-	7/39/115/115	-
25	CLA	y	604	-	-	5/21/97/115	-
24	CHL	n	606	-	-	10/22/98/117	-
34	SQD	A	412	-	-	18/45/65/69	0/1/1/1
37	DGD	C	519	-	-	25/51/91/95	0/2/2/2
30	BCR	B	620	-	-	6/29/63/63	0/2/2/2
39	HEM	f	101	8,9	-	1/14/54/54	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	605	5	-	14/39/115/115	-
29	LHG	Y	2630	25	-	20/53/53/53	-
30	BCR	c	517	-	-	6/29/63/63	0/2/2/2
37	DGD	c	519	-	-	25/51/91/95	0/2/2/2
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	G	612	1	-	11/33/109/115	-
29	LHG	1	2630	25	-	9/45/45/53	-
29	LHG	6	2630	25	-	14/41/41/53	-
29	LHG	l	101	-	-	21/53/53/53	-
26	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
30	BCR	C	517	-	-	6/29/63/63	0/2/2/2
24	CHL	7	609	2	1/1/14/21	14/35/111/117	-
25	CLA	c	504	-	-	12/39/115/115	-
29	LHG	b	2630	-	-	30/51/51/53	-
37	DGD	c	518	-	-	16/44/84/95	0/2/2/2
27	XAT	7	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	7	613	2	-	10/31/107/115	-
25	CLA	A	407	-	-	7/21/97/115	-
25	CLA	S	611	29	-	11/29/105/115	-
29	LHG	d	408	-	-	17/50/50/53	-
26	LUT	Y	1621	-	-	2/29/67/67	0/2/2/2
30	BCR	D	404	-	-	5/29/63/63	0/2/2/2
24	CHL	3	608	-	-	8/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	616	17	-	8/15/91/115	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	CHL	1	601	1	-	7/17/93/117	-
28	NEX	1	1623	-	-	9/27/83/83	0/3/3/3
25	CLA	5	614	1	-	6/15/91/115	-
25	CLA	1	602	1	-	10/35/111/115	-
30	BCR	b	619	-	-	2/29/63/63	0/2/2/2
30	BCR	C	514	-	-	2/29/63/63	0/2/2/2
25	CLA	A	405	4	-	10/39/115/115	-
25	CLA	4	602	3	-	4/15/91/115	-
24	CHL	5	606	-	-	9/17/93/117	-
28	NEX	r	623	-	-	4/27/83/83	0/3/3/3
24	CHL	Y	608	-	1/1/15/21	16/41/117/117	-
25	CLA	1	604	-	-	12/21/97/115	-
24	CHL	R	607	-	1/1/13/21	8/29/105/117	-
28	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
28	NEX	6	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	8	607	-	-	10/17/93/117	-
25	CLA	s	611	29	-	11/29/105/115	-
27	XAT	4	622	-	-	3/31/93/93	0/4/4/4
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	G	609	1	1/1/14/21	11/35/111/117	-
27	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
27	XAT	R	622	-	-	5/31/93/93	0/4/4/4
24	CHL	s	601	18	-	10/17/93/117	-
36	PL9	A	414	-	-	1/5/18/73	0/1/1/1
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	a	405	4	-	10/39/115/115	-
29	LHG	G	2630	25	-	24/53/53/53	-
25	CLA	b	613	5	-	15/39/115/115	-
29	LHG	L	101	-	-	21/53/53/53	-
24	CHL	N	606	-	-	10/22/98/117	-
29	LHG	D	409	-	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	7	605	2	-	12/17/93/117	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	b	603	5	-	12/39/115/115	-
25	CLA	B	611	-	-	11/39/115/115	-
37	DGD	C	520	-	-	28/49/89/95	0/2/2/2
26	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	d	403	7	-	13/39/115/115	-
25	CLA	c	509	6	-	8/39/115/115	-
24	CHL	4	608	-	-	8/17/93/117	-
25	CLA	c	501	6	-	15/39/115/115	-
25	CLA	C	513	6	-	12/39/115/115	-
25	CLA	B	613	5	-	15/39/115/115	-
25	CLA	R	610	17	-	14/39/115/115	-
30	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	g	614	1	-	7/19/95/115	-
30	BCR	c	516	-	-	9/29/63/63	0/2/2/2
25	CLA	R	604	-	-	4/19/95/115	-
24	CHL	n	605	1	-	11/20/96/117	-
25	CLA	8	602	3	-	4/15/91/115	-
25	CLA	5	613	1	-	9/27/103/115	-
26	LUT	s	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	1	606	-	-	9/17/93/117	-
25	CLA	2	604	-	-	9/15/91/115	-
29	LHG	S	2630	25	-	24/53/53/53	-
24	CHL	3	609	2	1/1/14/21	14/35/111/117	-
30	BCR	B	619	-	-	2/29/63/63	0/2/2/2
29	LHG	8	2630	25	-	8/23/23/53	-
25	CLA	r	601	17	-	11/20/96/115	-
24	CHL	y	607	-	1/1/15/21	17/41/117/117	-
24	CHL	r	606	-	1/1/15/21	23/41/117/117	-
27	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
29	LHG	C	523	-	-	21/53/53/53	-
29	LHG	R	2630	25	-	16/46/46/53	-
29	LHG	7	2630	25	-	25/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	h	101	-	-	5/29/63/63	0/2/2/2
28	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
33	PHO	a	409	-	-	8/37/103/103	0/5/6/6
24	CHL	Y	609	1	1/1/15/21	14/41/117/117	-
25	CLA	A	406	-	-	4/39/115/115	-
25	CLA	C	510	6	-	17/39/115/115	-
27	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	7	612	2	-	8/15/91/115	-
30	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	3	611	29	-	12/27/103/115	-
25	CLA	d	402	7	-	5/39/115/115	-
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	C	502	6	-	20/39/115/115	-
24	CHL	1	608	-	-	3/17/93/117	-
28	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	n	601	1	1/1/15/21	17/41/117/117	-
25	CLA	G	603	1	-	11/39/115/115	-
25	CLA	y	602	1	-	14/39/115/115	-
29	LHG	N	2630	25	-	23/53/53/53	-
25	CLA	4	612	3	-	8/15/91/115	-
24	CHL	5	605	1	-	10/17/93/117	-
25	CLA	y	612	1	-	14/33/109/115	-
25	CLA	Y	611	29	-	8/33/109/115	-
25	CLA	C	505	6	-	13/39/115/115	-
25	CLA	2	602	1	-	15/35/111/115	-
25	CLA	C	504	-	-	12/39/115/115	-
24	CHL	g	609	1	1/1/14/21	11/35/111/117	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
29	LHG	5	2630	25	-	9/45/45/53	-
25	CLA	s	603	18	-	5/15/91/115	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	c	502	6	-	20/39/115/115	-
25	CLA	g	613	1	-	13/39/115/115	-
26	LUT	G	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	n	612	1	-	10/33/109/115	-
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
25	CLA	R	616	17	-	8/15/91/115	-
24	CHL	5	601	1	-	7/17/93/117	-
24	CHL	6	609	1	1/1/14/21	17/35/111/117	-
25	CLA	B	603	5	-	12/39/115/115	-
25	CLA	r	604	-	-	4/19/95/115	-
25	CLA	6	603	1	-	15/27/103/115	-
34	SQD	a	412	-	-	18/45/65/69	0/1/1/1
25	CLA	b	609	5	-	5/39/115/115	-
26	LUT	y	1621	-	-	2/29/67/67	0/2/2/2
24	CHL	3	605	2	-	12/17/93/117	-
24	CHL	3	601	2	1/1/14/21	15/39/115/117	-
25	CLA	4	611	29	-	8/15/91/115	-
25	CLA	Y	612	1	-	14/33/109/115	-
25	CLA	g	610	1	-	13/38/114/115	-
24	CHL	G	607	-	1/1/15/21	15/41/117/117	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	CLA	5	612	1	-	6/15/91/115	-
29	LHG	3	2630	25	-	25/51/51/53	-
35	LMG	A	415	-	-	11/35/55/70	0/1/1/1
24	CHL	2	608	-	-	10/17/93/117	-
25	CLA	R	609	17	-	2/31/107/115	-
24	CHL	Y	601	1	1/1/15/21	15/41/117/117	-
24	CHL	8	609	3	-	9/17/93/117	-
29	LHG	g	2630	25	-	24/53/53/53	-
25	CLA	B	607	5	-	13/39/115/115	-
34	SQD	B	623	-	-	17/37/57/69	0/1/1/1
25	CLA	3	610	2	-	6/33/109/115	-
25	CLA	6	602	1	-	15/35/111/115	-
25	CLA	3	614	2	-	5/19/95/115	-
35	LMG	b	2633	-	-	21/50/70/70	0/1/1/1
24	CHL	3	606	-	-	5/17/93/117	-
25	CLA	r	612	17	-	6/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	613	1	-	13/39/115/115	-
25	CLA	Y	610	1	-	9/33/109/115	-
25	CLA	2	614	1	-	8/15/91/115	-
25	CLA	a	407	-	-	7/21/97/115	-
25	CLA	b	604	5	-	11/39/115/115	-
28	NEX	g	1623	-	-	6/27/83/83	0/3/3/3
24	CHL	6	607	-	1/1/14/21	20/35/111/117	-
34	SQD	A	418	-	-	22/49/69/69	0/1/1/1
35	LMG	D	411	-	-	15/41/61/70	0/1/1/1
25	CLA	1	611	29	-	7/15/91/115	-
25	CLA	c	512	6	-	9/39/115/115	-
25	CLA	Y	614	1	-	5/19/95/115	-
24	CHL	y	608	-	1/1/15/21	16/41/117/117	-
25	CLA	R	602	17	-	7/33/109/115	-
35	LMG	b	622	-	-	22/46/66/70	0/1/1/1
25	CLA	B	606	5	-	17/39/115/115	-
30	BCR	T	101	-	-	13/29/63/63	0/2/2/2
24	CHL	Y	605	1	-	8/20/96/117	-
26	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	6	601	1	-	8/17/93/117	-
25	CLA	S	602	18	-	16/35/111/115	-
25	CLA	B	614	5	-	15/39/115/115	-
24	CHL	N	609	1	1/1/15/21	15/41/117/117	-
29	LHG	d	410	-	-	24/47/47/53	-
37	DGD	C	518	-	-	16/44/84/95	0/2/2/2
24	CHL	r	614	17	-	8/12/88/117	-
24	CHL	y	601	1	1/1/15/21	15/41/117/117	-
26	LUT	1	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	S	604	-	-	6/21/97/115	-
25	CLA	a	410	4	-	8/33/109/115	-
24	CHL	n	607	-	1/1/15/21	19/41/117/117	-
25	CLA	b	615	5	-	15/39/115/115	-
37	DGD	H	102	-	-	25/51/91/95	0/2/2/2
25	CLA	B	602	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	609	5	-	5/39/115/115	-
25	CLA	G	610	1	-	13/38/114/115	-
25	CLA	b	605	5	-	14/39/115/115	-
29	LHG	c	522	-	-	20/53/53/53	-
24	CHL	R	614	17	-	8/12/88/117	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
24	CHL	G	608	-	1/1/15/21	18/41/117/117	-
28	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
24	CHL	1	607	-	1/1/14/21	19/38/114/117	-
25	CLA	r	611	29	-	11/20/96/115	-
29	LHG	D	410	-	-	24/47/47/53	-
24	CHL	2	609	1	1/1/14/21	17/35/111/117	-
25	CLA	7	603	2	-	11/27/103/115	-
35	LMG	d	411	-	-	15/41/61/70	0/1/1/1
25	CLA	n	613	1	-	6/33/109/115	-
25	CLA	g	603	1	-	11/39/115/115	-
26	LUT	8	620	-	-	5/29/67/67	0/2/2/2
24	CHL	4	606	-	-	7/17/93/117	-
25	CLA	N	604	-	-	4/21/97/115	-
25	CLA	R	612	17	-	6/20/96/115	-
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	c	503	6	-	12/39/115/115	-
29	LHG	D	408	-	-	17/50/50/53	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	c	510	6	-	17/39/115/115	-
24	CHL	s	608	-	-	5/17/93/117	-
24	CHL	4	601	3	-	6/15/91/117	-
25	CLA	G	604	-	-	7/21/97/115	-
25	CLA	b	606	5	-	17/39/115/115	-
24	CHL	S	606	-	-	10/17/93/117	-
25	CLA	Y	613	1	-	9/39/115/115	-
25	CLA	G	614	1	-	7/19/95/115	-
25	CLA	s	604	-	-	6/21/97/115	-
25	CLA	n	603	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	610	18	-	6/27/103/115	-
25	CLA	8	610	3	-	8/15/91/115	-
29	LHG	B	2630	-	-	30/51/51/53	-
24	CHL	r	607	-	1/1/13/21	8/29/105/117	-
25	CLA	7	602	2	-	14/33/109/115	-
25	CLA	s	614	18	-	5/20/96/115	-
24	CHL	y	605	1	-	8/20/96/117	-
25	CLA	N	602	1	-	14/39/115/115	-
25	CLA	b	608	-	-	13/39/115/115	-
25	CLA	B	616	5	-	14/39/115/115	-
24	CHL	8	608	-	-	8/17/93/117	-
29	LHG	n	2630	25	-	23/53/53/53	-
24	CHL	R	608	-	1/1/14/21	18/35/111/117	-
25	CLA	b	611	-	-	11/39/115/115	-
25	CLA	y	611	29	-	8/33/109/115	-
27	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	G	601	1	1/1/15/21	17/41/117/117	-
25	CLA	S	614	18	-	5/20/96/115	-
25	CLA	6	604	-	-	9/15/91/115	-
39	HEM	F	101	8,9	-	1/14/54/54	-
24	CHL	7	607	-	-	12/26/102/117	-
30	BCR	a	411	-	-	2/29/63/63	0/2/2/2
35	LMG	a	415	-	-	11/35/55/70	0/1/1/1
25	CLA	B	610	5	-	7/39/115/115	-
27	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	D	403	7	-	13/39/115/115	-
29	LHG	c	2630	-	-	27/53/53/53	-
34	SQD	b	623	-	-	17/37/57/69	0/1/1/1
25	CLA	r	613	17	-	13/33/109/115	-
24	CHL	6	608	-	-	10/17/93/117	-
25	CLA	5	603	1	-	12/27/103/115	-
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
28	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	n	602	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	y	613	1	-	9/39/115/115	-
27	XAT	g	1622	-	-	2/31/93/93	0/4/4/4

The worst 5 of 4240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	409	PHO	C1B-C2B	8.72	1.49	1.39
33	A	409	PHO	C1B-C2B	8.72	1.49	1.39
33	A	408	PHO	C1B-C2B	8.68	1.49	1.39
33	a	408	PHO	C1B-C2B	8.63	1.49	1.39
33	a	409	PHO	C3B-C4B	7.22	1.49	1.41

The worst 5 of 6137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	1622	XAT	O24-C25-C24	10.52	121.28	113.38
27	1	1622	XAT	O24-C25-C24	10.51	121.28	113.38
24	N	607	CHL	C2B-C1B-NB	10.44	117.23	110.23
24	5	607	CHL	C2B-C1B-NB	10.41	117.21	110.23
24	n	607	CHL	C2B-C1B-NB	10.39	117.20	110.23

5 of 44 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	607	CHL	C8
24	1	609	CHL	C8
24	2	607	CHL	C8
24	2	609	CHL	C8
24	3	601	CHL	C8

5 of 5095 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	C2B-C3B-CAB-CBB
24	1	606	CHL	C4B-C3B-CAB-CBB
24	1	606	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

429 monomers are involved in 1087 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	2	610	CLA	3	0
30	b	620	BCR	2	0
24	N	608	CHL	2	0
25	G	611	CLA	1	0
29	2	2630	LHG	2	0
35	Z	101	LMG	6	0
25	c	513	CLA	3	0
24	y	606	CHL	1	0
28	Y	1623	NEX	1	0
29	C	2630	LHG	4	0
24	7	606	CHL	4	0
25	8	612	CLA	2	0
26	S	1621	LUT	4	0
26	7	1621	LUT	3	0
25	4	603	CLA	1	0
28	5	1623	NEX	3	0
25	5	602	CLA	4	0
25	c	511	CLA	9	0
25	y	610	CLA	1	0
25	6	612	CLA	2	0
35	A	413	LMG	2	0
27	8	622	XAT	7	0
30	4	623	BCR	3	0
37	B	626	DGD	1	0
24	5	607	CHL	4	0
29	4	2630	LHG	1	0
33	a	408	PHO	7	0
36	D	405	PL9	6	0
25	A	410	CLA	6	0
24	7	608	CHL	3	0
25	S	610	CLA	1	0
25	s	613	CLA	1	0
25	r	603	CLA	2	0
25	8	611	CLA	1	0
26	G	1621	LUT	6	0
25	G	602	CLA	3	0
25	R	611	CLA	3	0
30	d	404	BCR	7	0
24	g	601	CHL	4	0
25	S	609	CLA	1	0
25	g	602	CLA	3	0
25	C	503	CLA	2	0
29	b	2631	LHG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	r	2630	LHG	3	0
27	y	1622	XAT	5	0
25	n	610	CLA	4	0
26	Y	1620	LUT	4	0
25	6	611	CLA	1	0
26	6	1620	LUT	4	0
29	d	409	LHG	11	0
25	C	501	CLA	4	0
24	n	608	CHL	3	0
25	y	603	CLA	6	0
37	c	520	DGD	2	0
25	R	613	CLA	2	0
29	C	522	LHG	2	0
35	B	2633	LMG	2	0
33	A	408	PHO	7	0
25	b	612	CLA	5	0
25	b	607	CLA	3	0
24	S	607	CHL	3	0
25	r	602	CLA	5	0
25	r	609	CLA	3	0
25	B	604	CLA	4	0
24	G	606	CHL	1	0
24	g	607	CHL	4	0
25	n	604	CLA	1	0
25	N	611	CLA	2	0
28	y	1623	NEX	4	0
24	s	607	CHL	3	0
24	2	607	CHL	2	0
25	3	602	CLA	3	0
25	B	608	CLA	3	0
25	3	603	CLA	1	0
25	c	505	CLA	1	0
24	5	608	CHL	1	0
24	2	605	CHL	1	0
25	C	507	CLA	5	0
34	a	418	SQD	6	0
29	c	523	LHG	1	0
25	N	610	CLA	4	0
26	N	1621	LUT	4	0
29	B	2631	LHG	5	0
25	4	610	CLA	1	0
26	6	1621	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	604	CLA	2	0
25	6	614	CLA	1	0
30	8	623	BCR	3	0
25	c	506	CLA	3	0
25	5	604	CLA	1	0
36	d	405	PL9	6	0
25	b	614	CLA	4	0
34	B	621	SQD	5	0
25	7	611	CLA	2	0
28	R	623	NEX	4	0
28	G	1623	NEX	3	0
35	B	622	LMG	4	0
26	g	1620	LUT	8	0
25	N	613	CLA	4	0
24	s	606	CHL	2	0
24	8	606	CHL	1	0
25	b	602	CLA	4	0
25	b	616	CLA	4	0
25	B	612	CLA	3	0
24	R	606	CHL	1	0
30	c	514	BCR	2	0
25	g	604	CLA	2	0
25	1	612	CLA	2	0
24	N	607	CHL	4	0
24	g	608	CHL	4	0
24	n	609	CHL	5	0
38	d	401	BCT	1	0
24	S	608	CHL	1	0
37	b	626	DGD	1	0
37	h	102	DGD	6	0
24	N	601	CHL	1	0
25	s	609	CLA	1	0
24	6	606	CHL	3	0
25	1	610	CLA	2	0
25	B	615	CLA	5	0
26	2	1621	LUT	3	0
25	Y	603	CLA	7	0
25	C	511	CLA	9	0
25	2	612	CLA	2	0
25	n	611	CLA	2	0
26	n	1620	LUT	5	0
25	S	613	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	1622	XAT	5	0
25	6	613	CLA	2	0
25	c	507	CLA	5	0
24	r	608	CHL	1	0
35	C	521	LMG	1	0
25	S	603	CLA	2	0
25	N	612	CLA	4	0
24	2	606	CHL	3	0
24	G	605	CHL	1	0
25	a	406	CLA	2	0
24	5	609	CHL	6	0
34	b	621	SQD	4	0
25	C	508	CLA	2	0
24	7	601	CHL	2	0
25	g	612	CLA	2	0
25	3	613	CLA	3	0
26	R	620	LUT	4	0
27	2	1622	XAT	6	0
25	C	512	CLA	1	0
25	Y	602	CLA	5	0
24	3	607	CHL	6	0
25	r	610	CLA	1	0
27	r	622	XAT	5	0
25	2	613	CLA	2	0
25	8	604	CLA	1	0
25	2	603	CLA	2	0
25	B	617	CLA	1	0
24	Y	607	CHL	3	0
35	a	413	LMG	2	0
25	7	610	CLA	3	0
27	1	1622	XAT	4	0
26	n	1621	LUT	4	0
25	1	613	CLA	1	0
24	6	605	CHL	1	0
24	y	609	CHL	2	0
38	D	401	BCT	1	0
26	4	620	LUT	4	0
29	y	2630	LHG	4	0
24	g	606	CHL	2	0
24	g	605	CHL	1	0
30	A	411	BCR	2	0
33	A	409	PHO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	401	OEX	2	0
25	g	611	CLA	1	0
26	r	620	LUT	4	0
35	z	101	LMG	5	0
25	R	603	CLA	2	0
29	s	2630	LHG	2	0
24	l	609	CHL	4	0
25	8	603	CLA	1	0
25	1	603	CLA	2	0
25	6	610	CLA	3	0
25	5	610	CLA	2	0
25	C	506	CLA	2	0
26	S	1620	LUT	3	0
25	N	603	CLA	4	0
26	5	1621	LUT	4	0
25	c	508	CLA	2	0
25	D	402	CLA	7	0
25	b	610	CLA	2	0
25	y	604	CLA	2	0
24	n	606	CHL	2	0
34	A	412	SQD	2	0
37	C	519	DGD	3	0
30	B	620	BCR	3	0
26	s	1620	LUT	2	0
25	B	605	CLA	7	0
29	Y	2630	LHG	3	0
30	c	517	BCR	10	0
37	c	519	DGD	3	0
26	g	1621	LUT	6	0
25	G	612	CLA	1	0
29	6	2630	LHG	2	0
29	l	101	LHG	8	0
26	3	1621	LUT	4	0
30	C	517	BCR	9	0
24	7	609	CHL	4	0
25	c	504	CLA	1	0
29	b	2630	LHG	2	0
37	c	518	DGD	3	0
27	7	1622	XAT	7	0
25	7	613	CLA	2	0
25	A	407	CLA	1	0
25	S	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	408	LHG	5	0
26	Y	1621	LUT	5	0
30	D	404	BCR	4	0
24	3	608	CHL	2	0
25	r	616	CLA	2	0
26	1	1620	LUT	6	0
30	C	516	BCR	2	0
28	1	1623	NEX	3	0
25	1	602	CLA	4	0
30	b	619	BCR	5	0
30	C	514	BCR	2	0
25	A	405	CLA	5	0
24	5	606	CHL	2	0
28	r	623	NEX	2	0
24	Y	608	CHL	3	0
25	1	604	CLA	1	0
24	R	607	CHL	1	0
28	S	1623	NEX	1	0
24	8	607	CHL	1	0
25	s	611	CLA	1	0
27	4	622	XAT	5	0
26	2	1620	LUT	4	0
24	G	609	CHL	2	0
27	n	1622	XAT	7	0
27	R	622	XAT	5	0
28	2	1623	NEX	2	0
25	a	405	CLA	5	0
29	G	2630	LHG	2	0
25	b	613	CLA	6	0
29	L	101	LHG	8	0
24	N	606	CHL	3	0
29	D	409	LHG	11	0
24	7	605	CHL	1	0
26	N	1620	LUT	2	0
25	b	603	CLA	9	0
25	B	611	CLA	5	0
37	C	520	DGD	2	0
26	3	1620	LUT	7	0
25	d	403	CLA	2	0
24	4	608	CHL	1	0
25	c	501	CLA	4	0
25	C	513	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	613	CLA	7	0
25	R	610	CLA	1	0
30	H	101	BCR	6	0
25	g	614	CLA	2	0
30	c	516	BCR	2	0
25	R	604	CLA	1	0
25	5	613	CLA	1	0
26	s	1621	LUT	3	0
24	1	606	CHL	2	0
25	2	604	CLA	1	0
29	S	2630	LHG	2	0
24	3	609	CHL	3	0
30	B	619	BCR	4	0
29	8	2630	LHG	1	0
24	y	607	CHL	2	0
24	r	606	CHL	1	0
27	N	1622	XAT	6	0
29	C	523	LHG	1	0
29	R	2630	LHG	3	0
29	7	2630	LHG	4	0
30	h	101	BCR	5	0
28	N	1623	NEX	3	0
33	a	409	PHO	4	0
24	Y	609	CHL	2	0
25	A	406	CLA	3	0
25	C	510	CLA	5	0
27	G	1622	XAT	4	0
30	C	515	BCR	2	0
25	3	611	CLA	2	0
25	d	402	CLA	5	0
26	7	1620	LUT	6	0
25	C	502	CLA	1	0
24	1	608	CHL	1	0
28	3	1623	NEX	2	0
24	n	601	CHL	1	0
25	G	603	CLA	3	0
25	y	602	CLA	3	0
29	N	2630	LHG	4	0
25	4	612	CLA	2	0
24	5	605	CHL	1	0
25	y	612	CLA	2	0
25	Y	611	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	505	CLA	1	0
25	2	602	CLA	3	0
25	C	504	CLA	1	0
24	g	609	CHL	3	0
30	t	101	BCR	7	0
25	s	603	CLA	1	0
28	7	1623	NEX	2	0
25	c	502	CLA	1	0
25	g	613	CLA	5	0
26	G	1620	LUT	8	0
25	n	612	CLA	4	0
35	c	521	LMG	1	0
25	R	616	CLA	4	0
24	6	609	CHL	5	0
25	B	603	CLA	8	0
25	r	604	CLA	1	0
25	6	603	CLA	1	0
34	a	412	SQD	2	0
26	y	1621	LUT	3	0
24	3	605	CHL	1	0
24	3	601	CHL	2	0
25	4	611	CLA	1	0
25	Y	612	CLA	3	0
25	g	610	CLA	6	0
24	G	607	CHL	4	0
30	c	515	BCR	2	0
25	5	612	CLA	2	0
29	3	2630	LHG	3	0
24	2	608	CHL	2	0
25	R	609	CLA	4	0
24	Y	601	CHL	7	0
29	g	2630	LHG	4	0
25	B	607	CLA	4	0
34	B	623	SQD	5	0
25	3	610	CLA	2	0
25	6	602	CLA	3	0
35	b	2633	LMG	2	0
24	3	606	CHL	4	0
25	r	612	CLA	2	0
25	G	613	CLA	5	0
25	Y	610	CLA	2	0
25	2	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	407	CLA	1	0
25	b	604	CLA	3	0
28	g	1623	NEX	2	0
24	6	607	CHL	2	0
34	A	418	SQD	6	0
35	D	411	LMG	2	0
25	c	512	CLA	1	0
24	y	608	CHL	3	0
25	R	602	CLA	4	0
35	b	622	LMG	4	0
25	B	606	CLA	4	0
30	T	101	BCR	3	0
24	Y	605	CHL	1	0
26	5	1620	LUT	7	0
25	B	614	CLA	4	0
24	N	609	CHL	5	0
29	d	410	LHG	4	0
37	C	518	DGD	3	0
24	y	601	CHL	8	0
26	1	1621	LUT	4	0
25	S	604	CLA	1	0
25	a	410	CLA	7	0
24	n	607	CHL	3	0
25	b	615	CLA	5	0
37	H	102	DGD	6	0
25	B	602	CLA	4	0
25	G	610	CLA	6	0
25	b	605	CLA	8	0
29	c	522	LHG	3	0
27	3	1622	XAT	4	0
24	G	608	CHL	4	0
28	s	1623	NEX	1	0
24	1	607	CHL	4	0
25	r	611	CLA	3	0
29	D	410	LHG	4	0
24	2	609	CHL	4	0
25	7	603	CLA	2	0
35	d	411	LMG	3	0
25	n	613	CLA	4	0
25	g	603	CLA	4	0
26	8	620	LUT	3	0
24	4	606	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	604	CLA	1	0
25	R	612	CLA	2	0
30	b	618	BCR	5	0
25	c	503	CLA	2	0
29	D	408	LHG	4	0
26	y	1620	LUT	3	0
25	c	510	CLA	4	0
24	s	608	CHL	1	0
24	4	601	CHL	1	0
25	G	604	CLA	2	0
25	b	606	CLA	5	0
24	S	606	CHL	2	0
25	Y	613	CLA	2	0
25	G	614	CLA	2	0
25	s	604	CLA	1	0
25	n	603	CLA	4	0
25	s	610	CLA	1	0
25	8	610	CLA	1	0
29	B	2630	LHG	2	0
24	r	607	CHL	1	0
25	7	602	CLA	4	0
25	s	614	CLA	1	0
24	y	605	CHL	1	0
25	N	602	CLA	8	0
25	b	608	CLA	2	0
25	B	616	CLA	4	0
24	8	608	CHL	1	0
29	n	2630	LHG	4	0
24	R	608	CHL	2	0
25	b	611	CLA	4	0
25	y	611	CLA	4	0
27	Y	1622	XAT	5	0
24	G	601	CHL	4	0
25	6	604	CLA	2	0
24	7	607	CHL	6	0
30	a	411	BCR	3	0
31	a	401	OEX	2	0
25	B	610	CLA	1	0
27	5	1622	XAT	4	0
25	D	403	CLA	2	0
29	c	2630	LHG	5	0
34	b	623	SQD	5	0

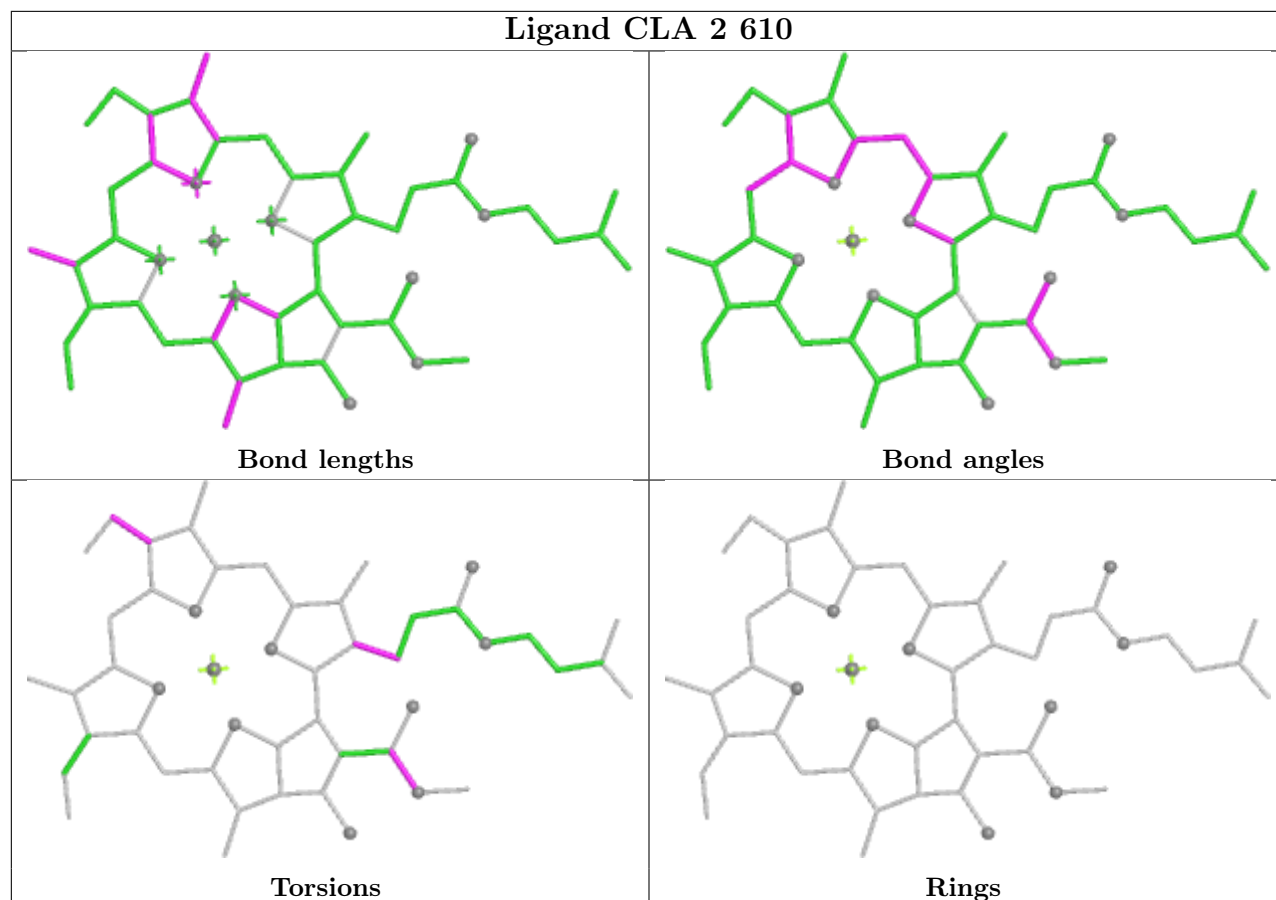
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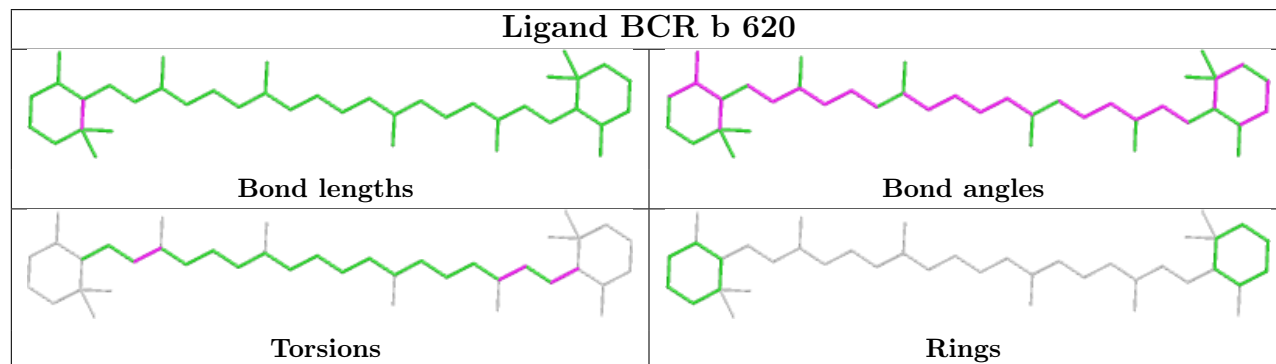
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	r	613	CLA	2	0
24	6	608	CHL	2	0
25	5	603	CLA	1	0
30	B	618	BCR	6	0
28	n	1623	NEX	5	0
25	n	602	CLA	8	0
25	y	613	CLA	2	0
27	g	1622	XAT	4	0

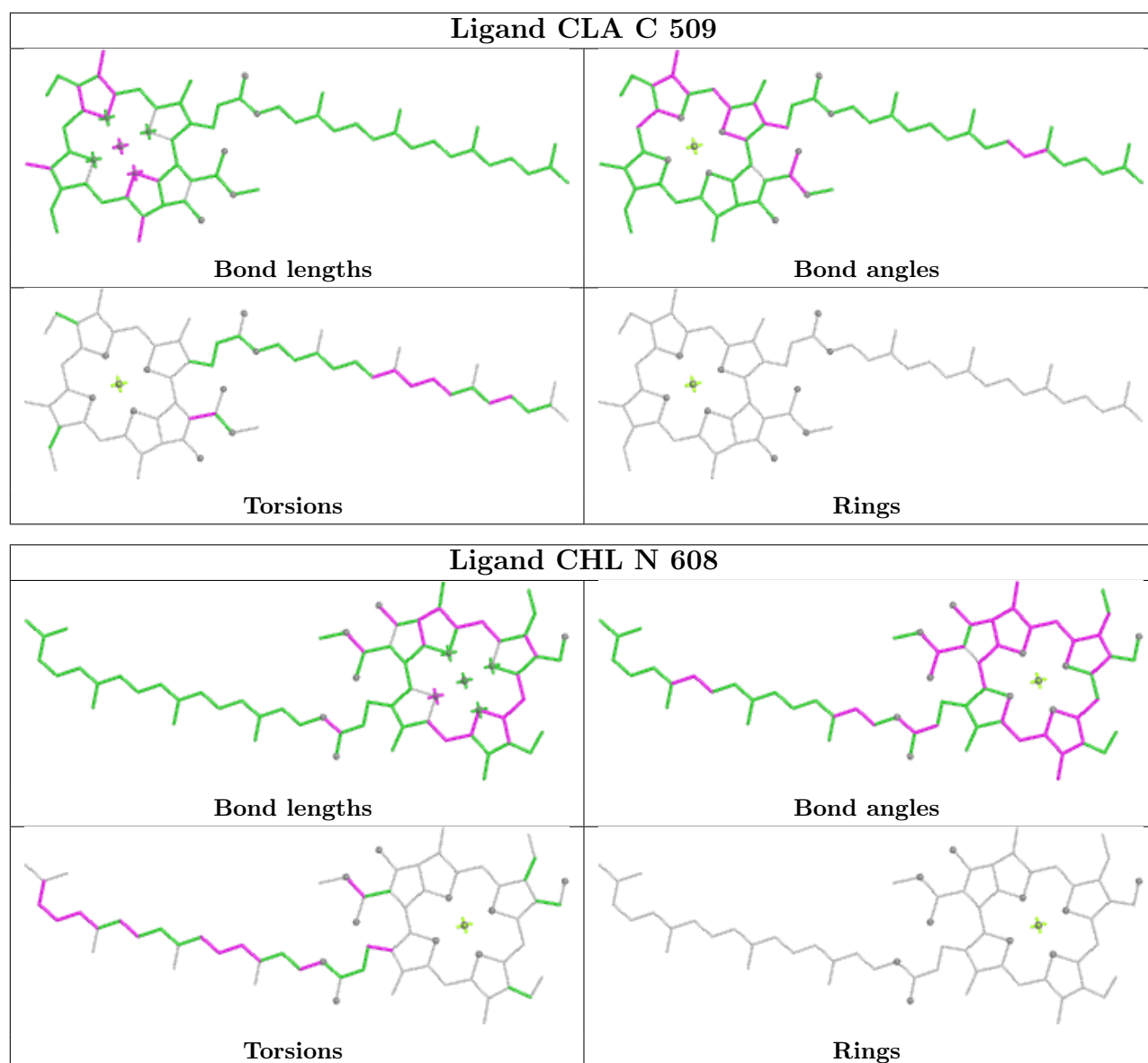
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

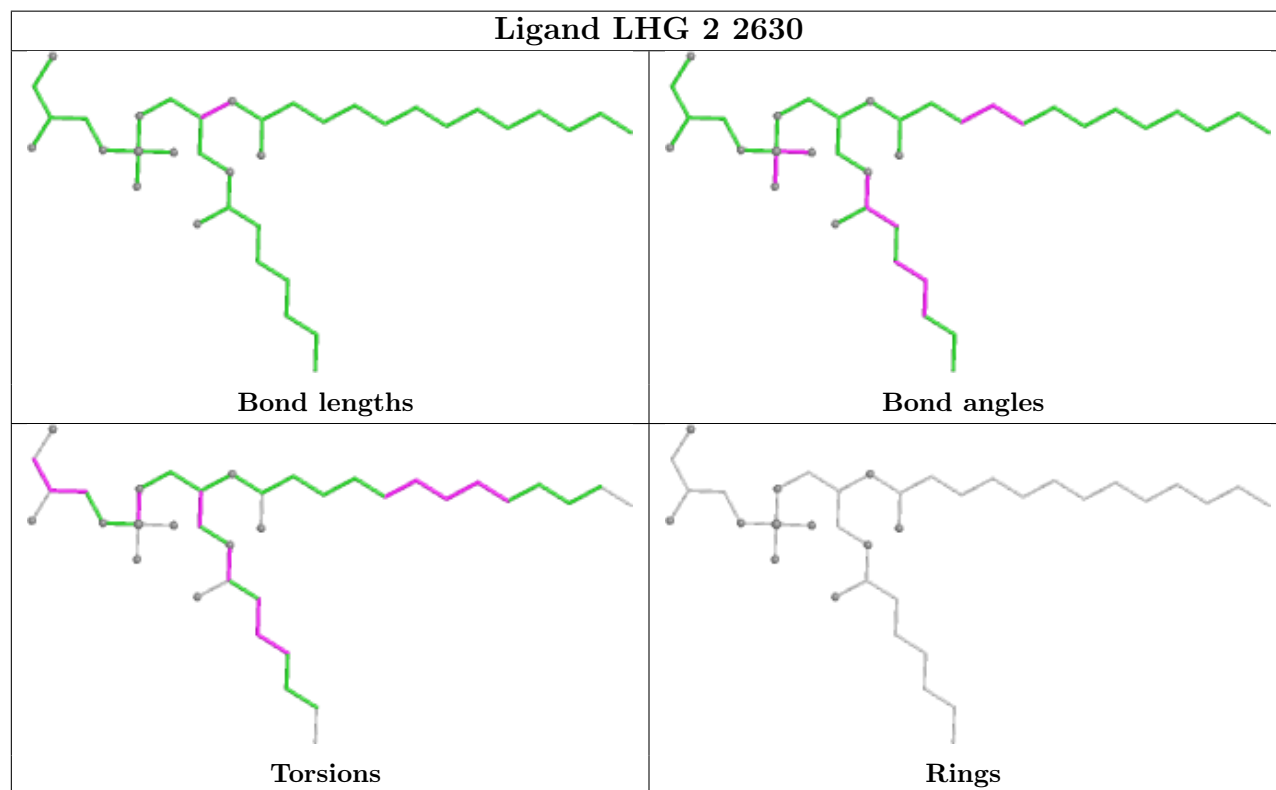
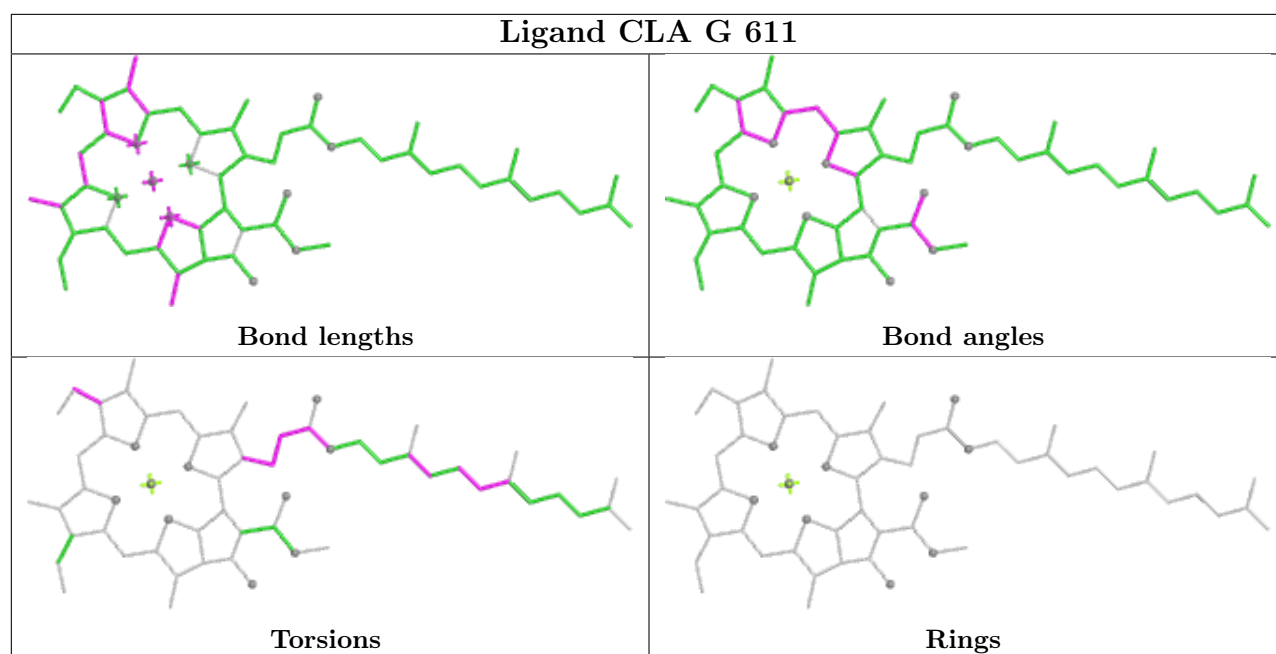
Ligand CLA 2 610

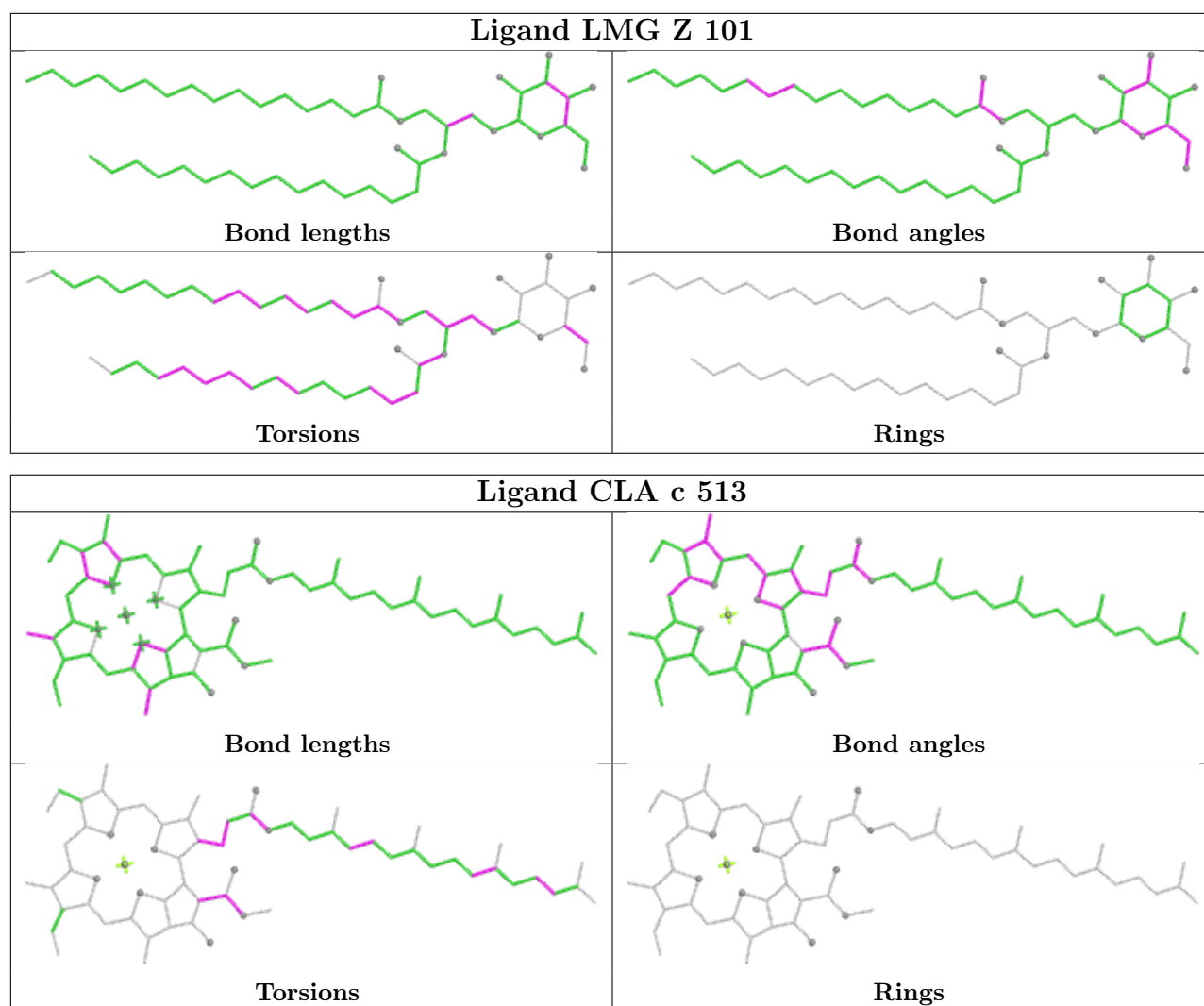


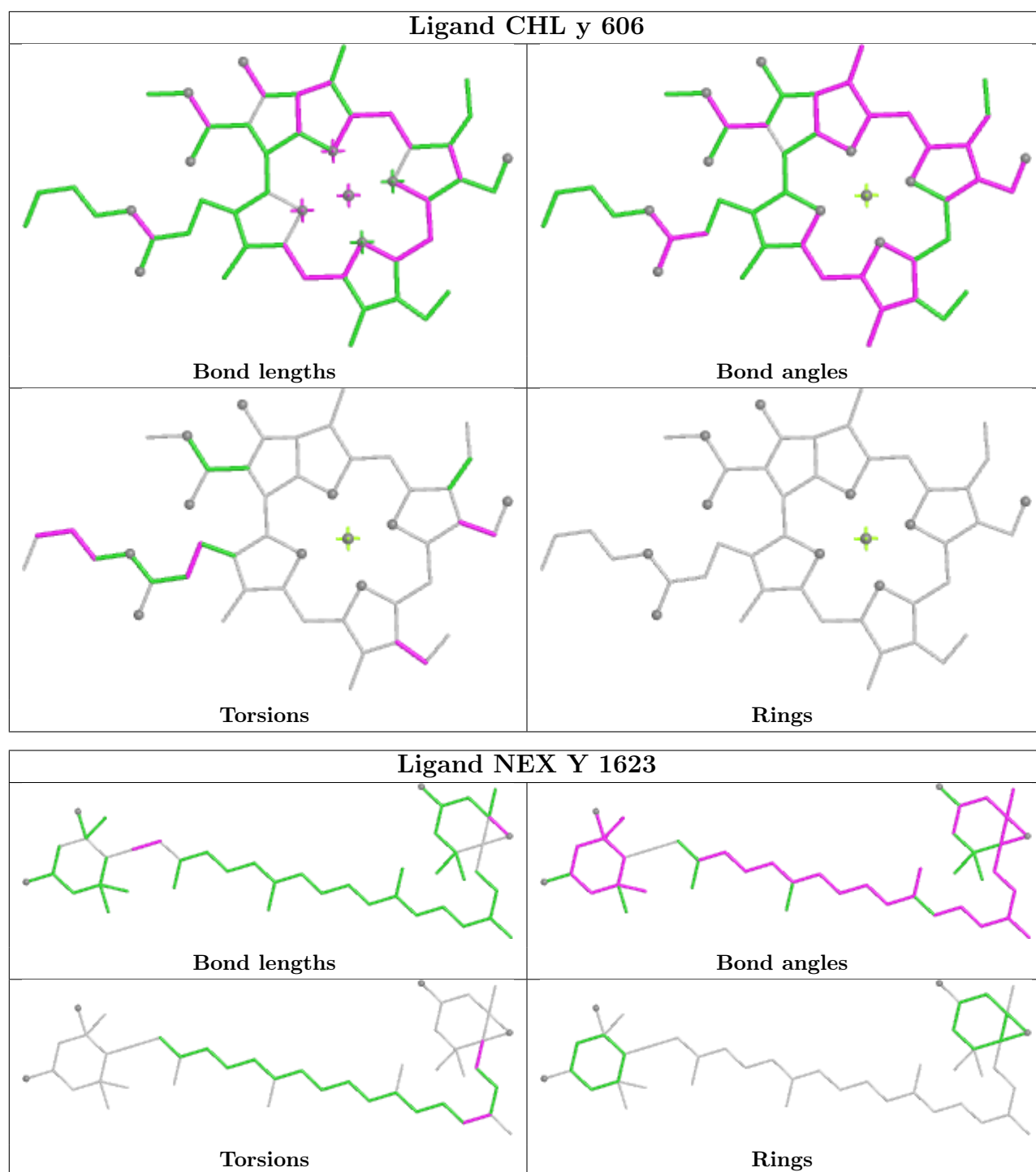
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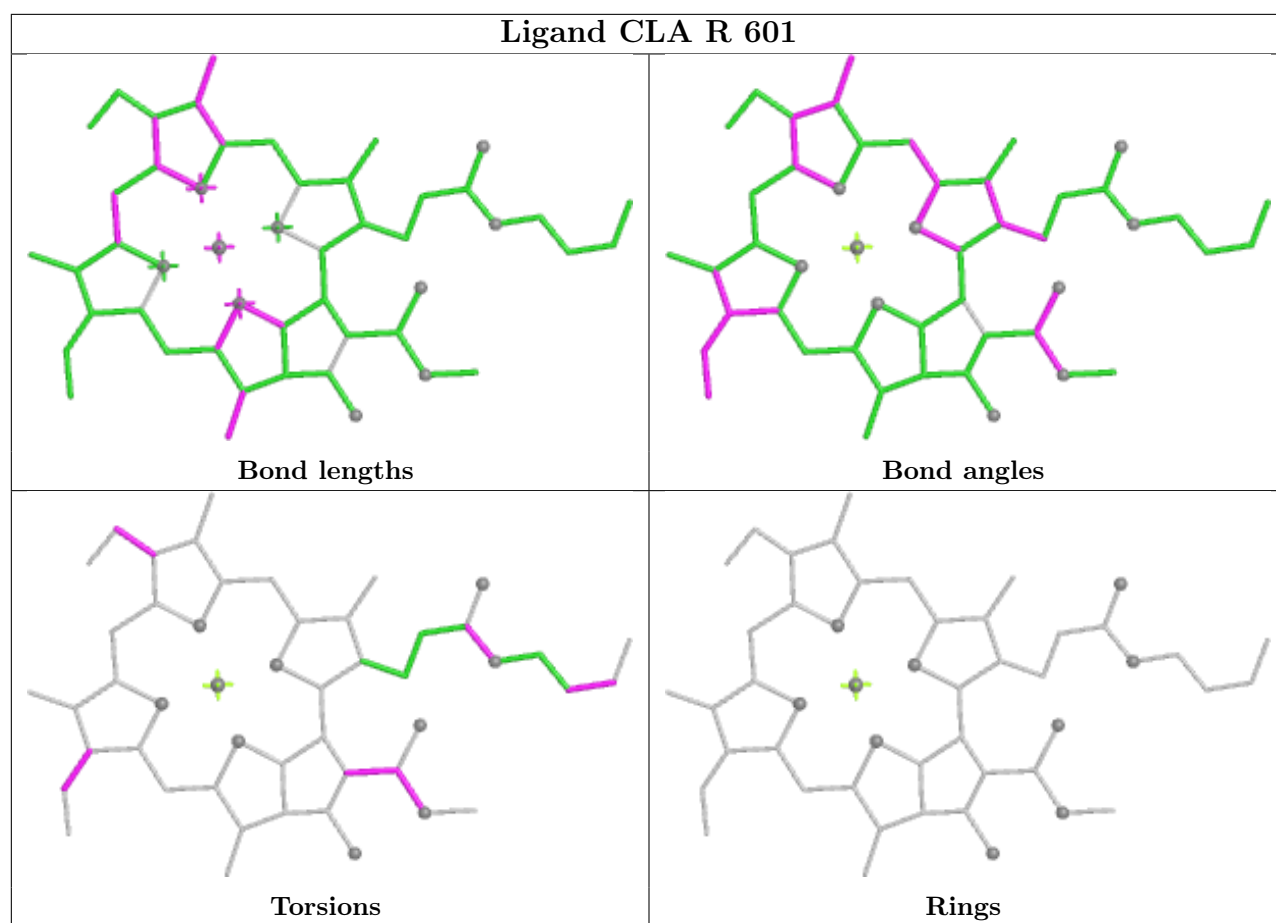


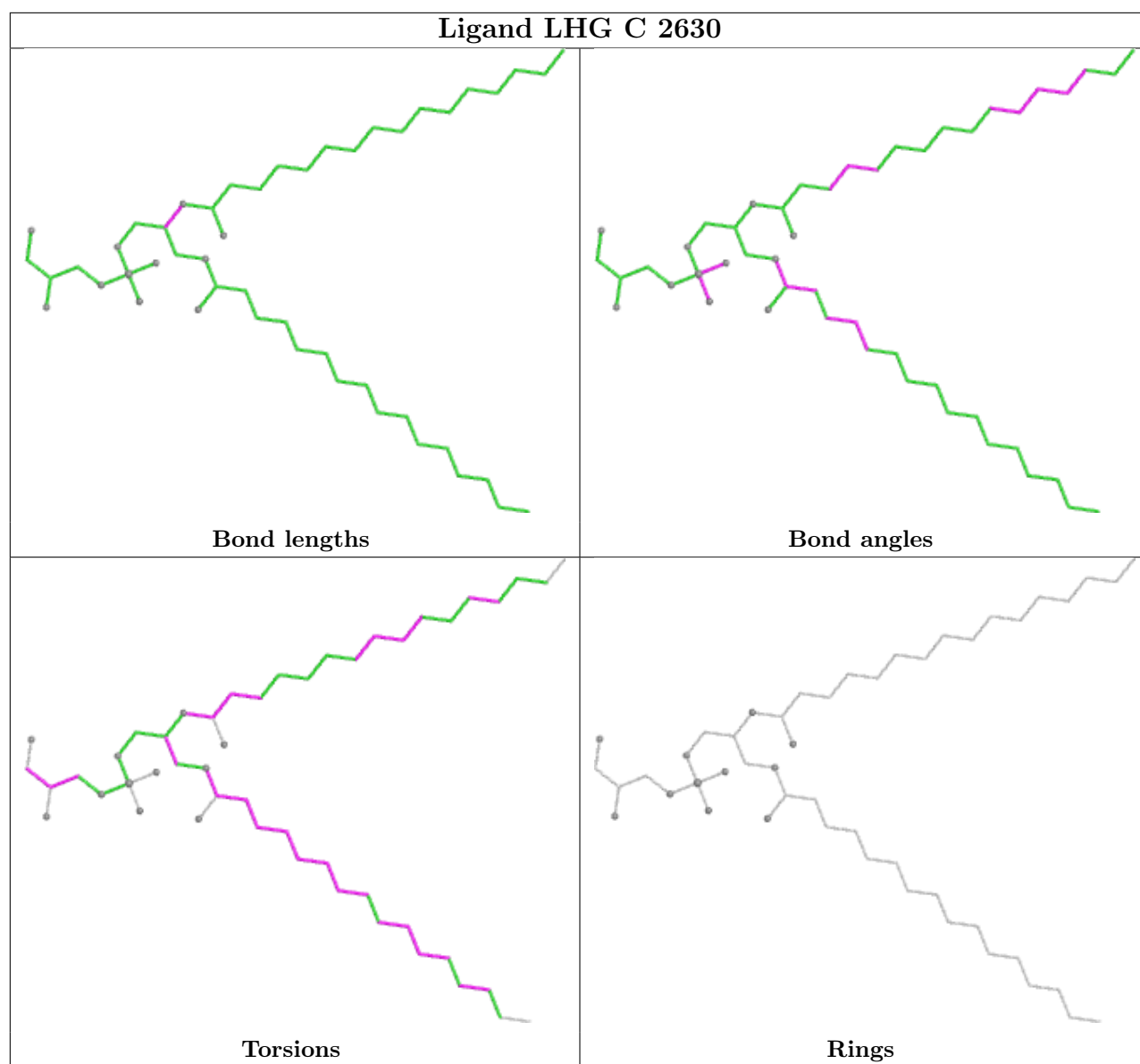




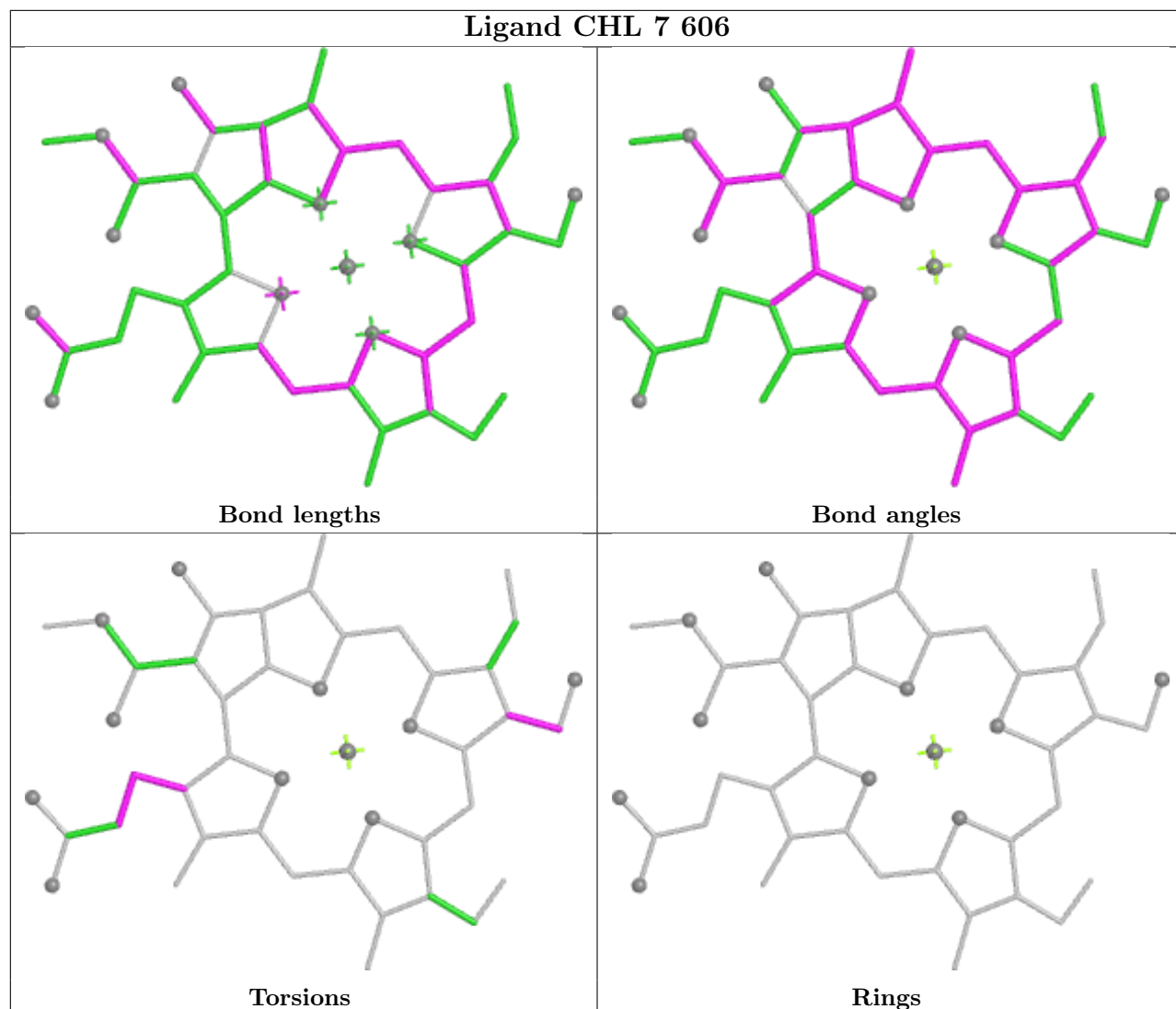




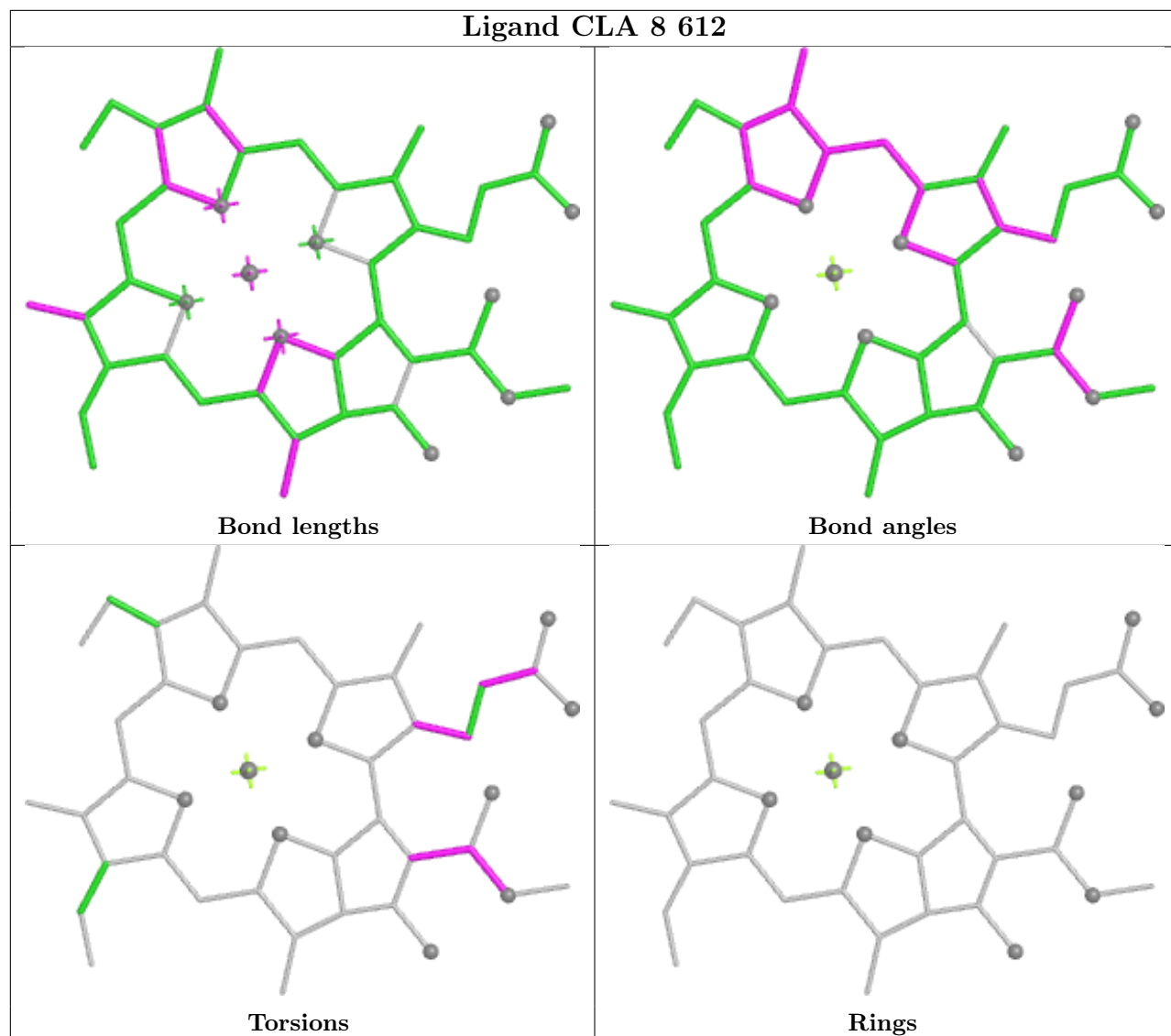




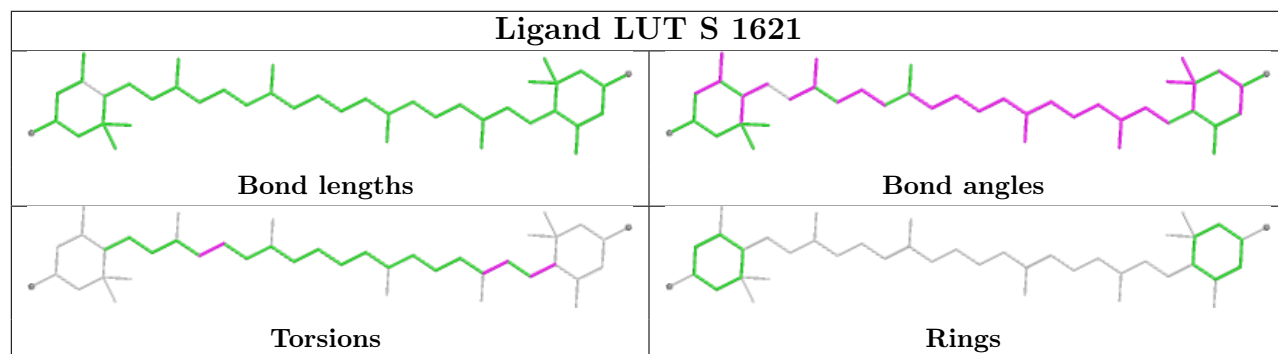
Ligand CHL 7 606

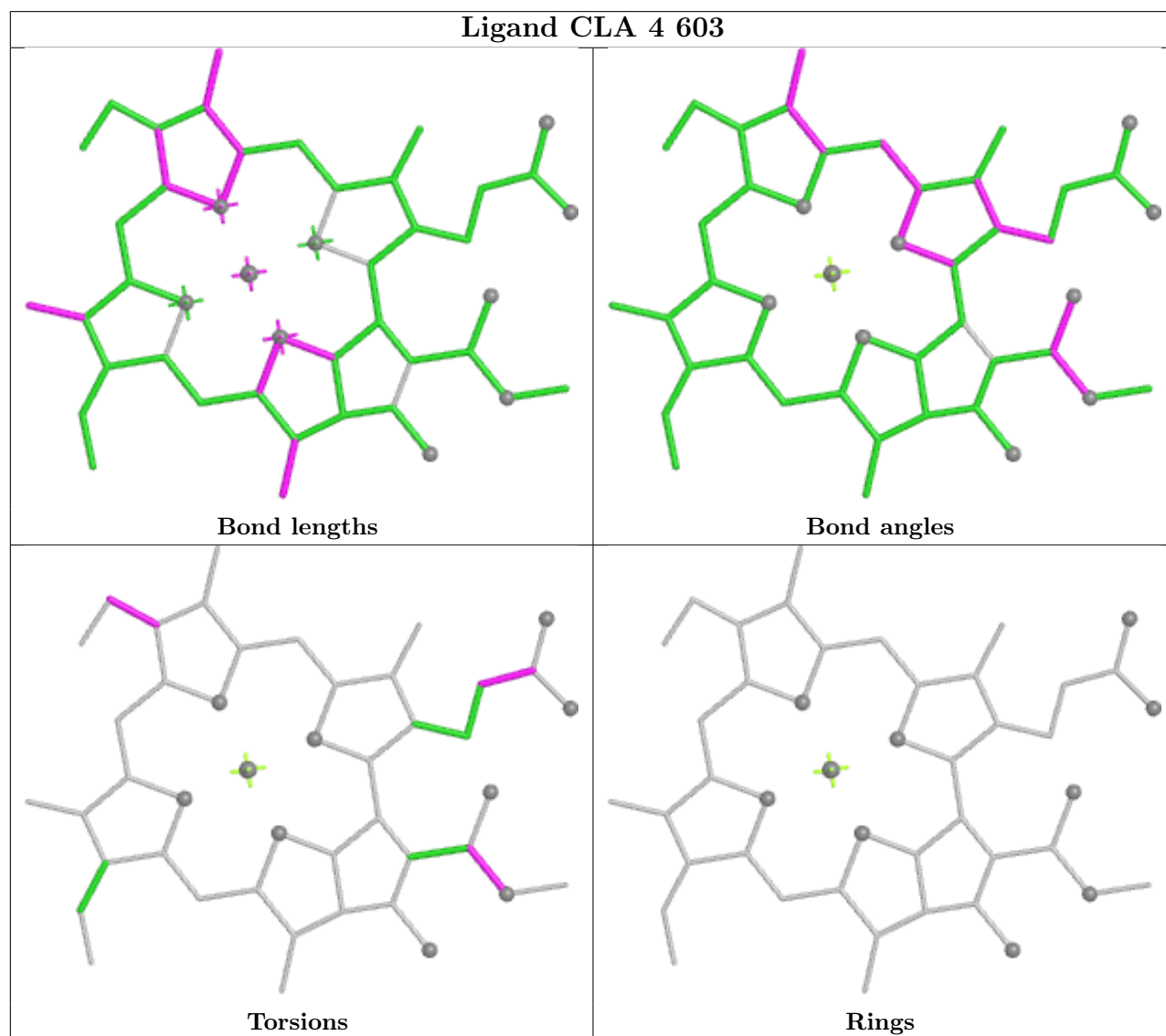
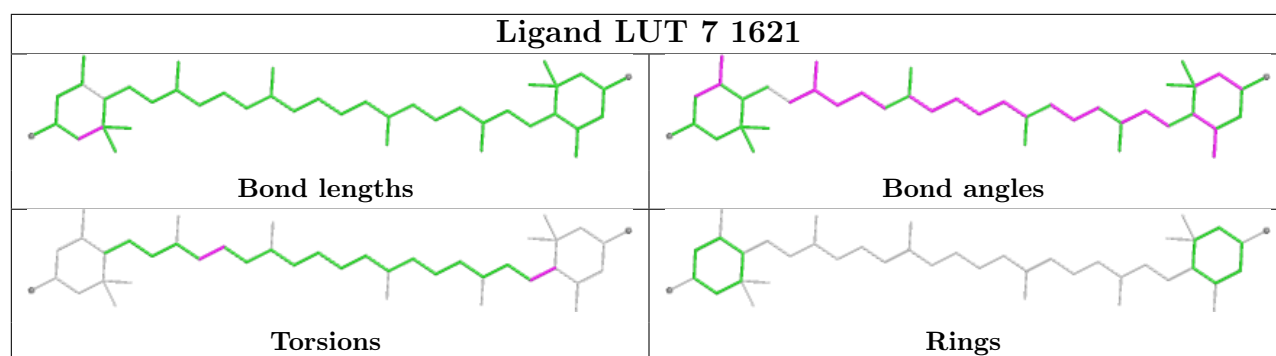


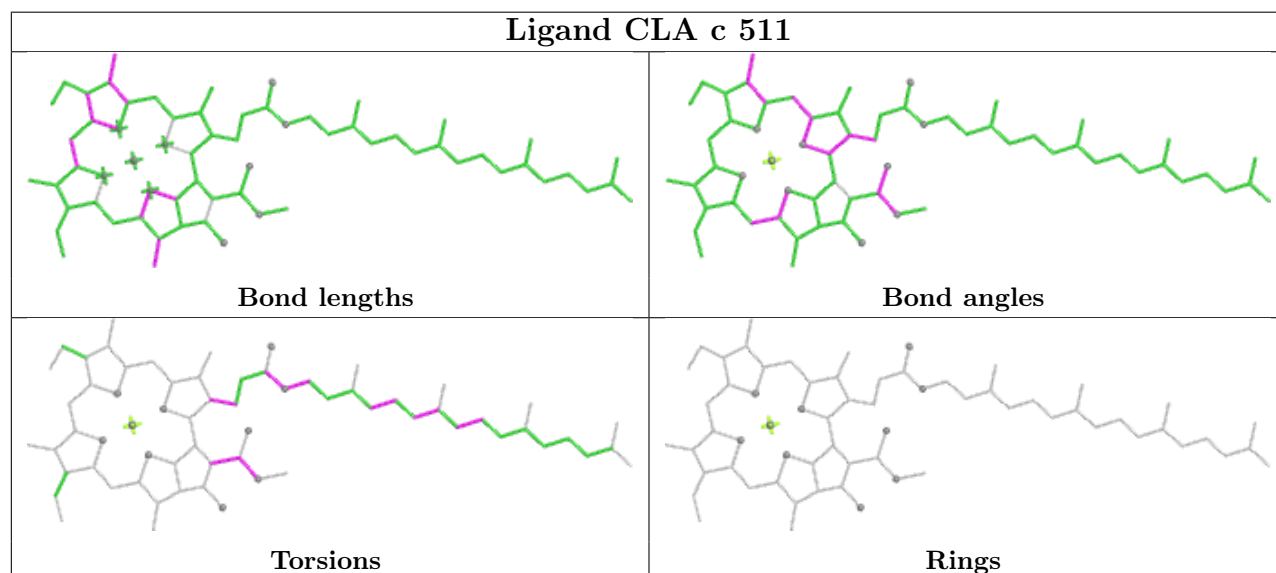
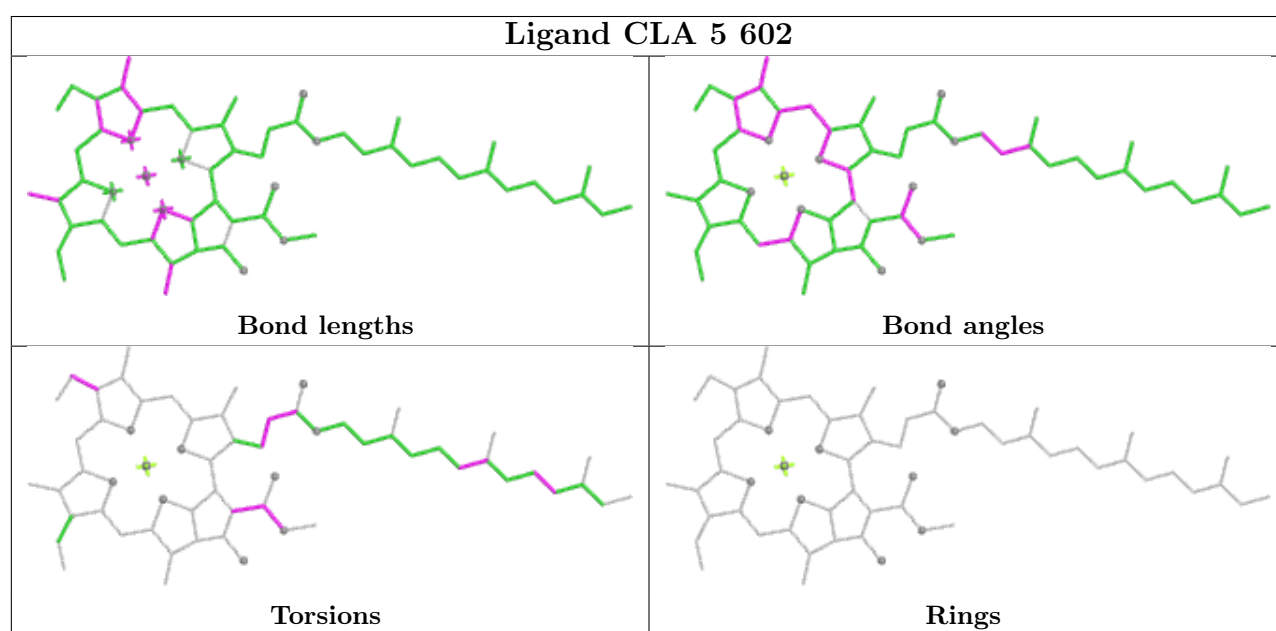
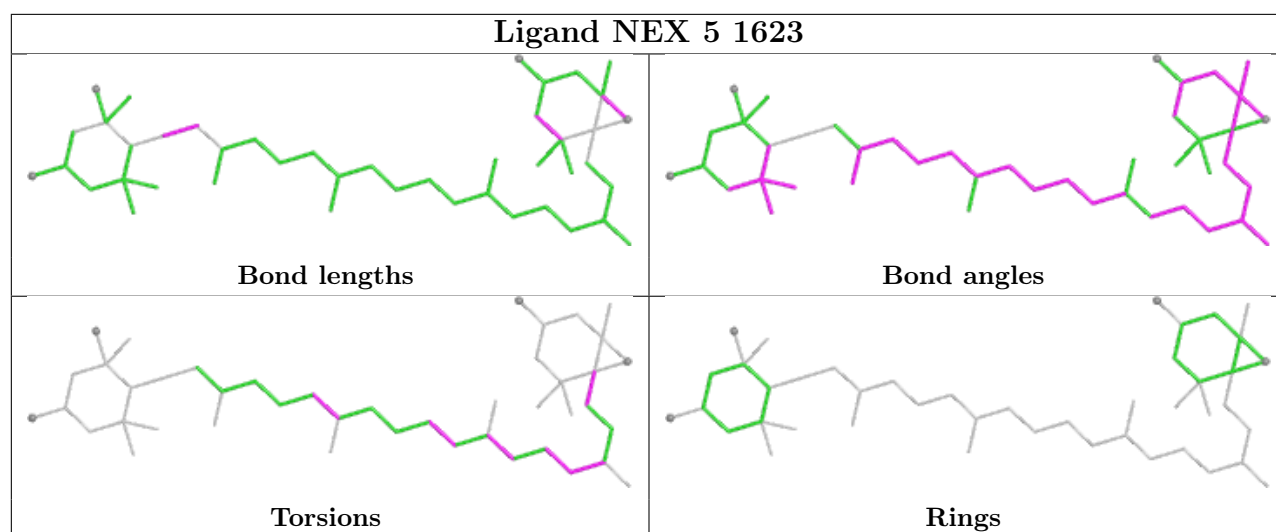
Ligand CLA 8 612



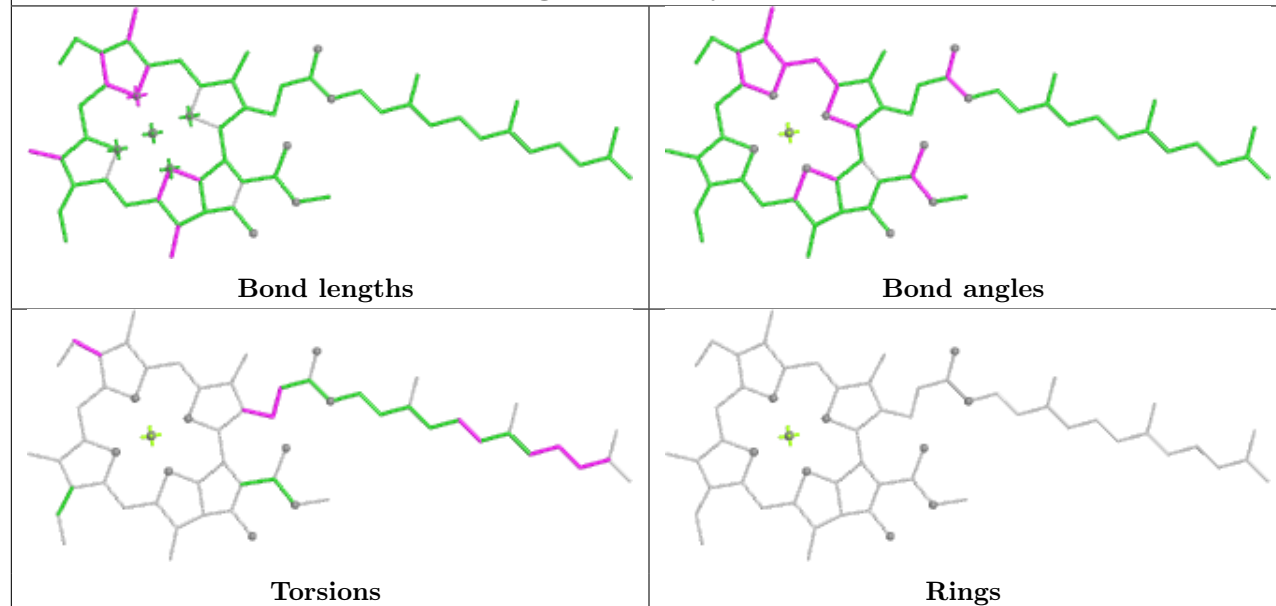
Ligand LUT S 1621



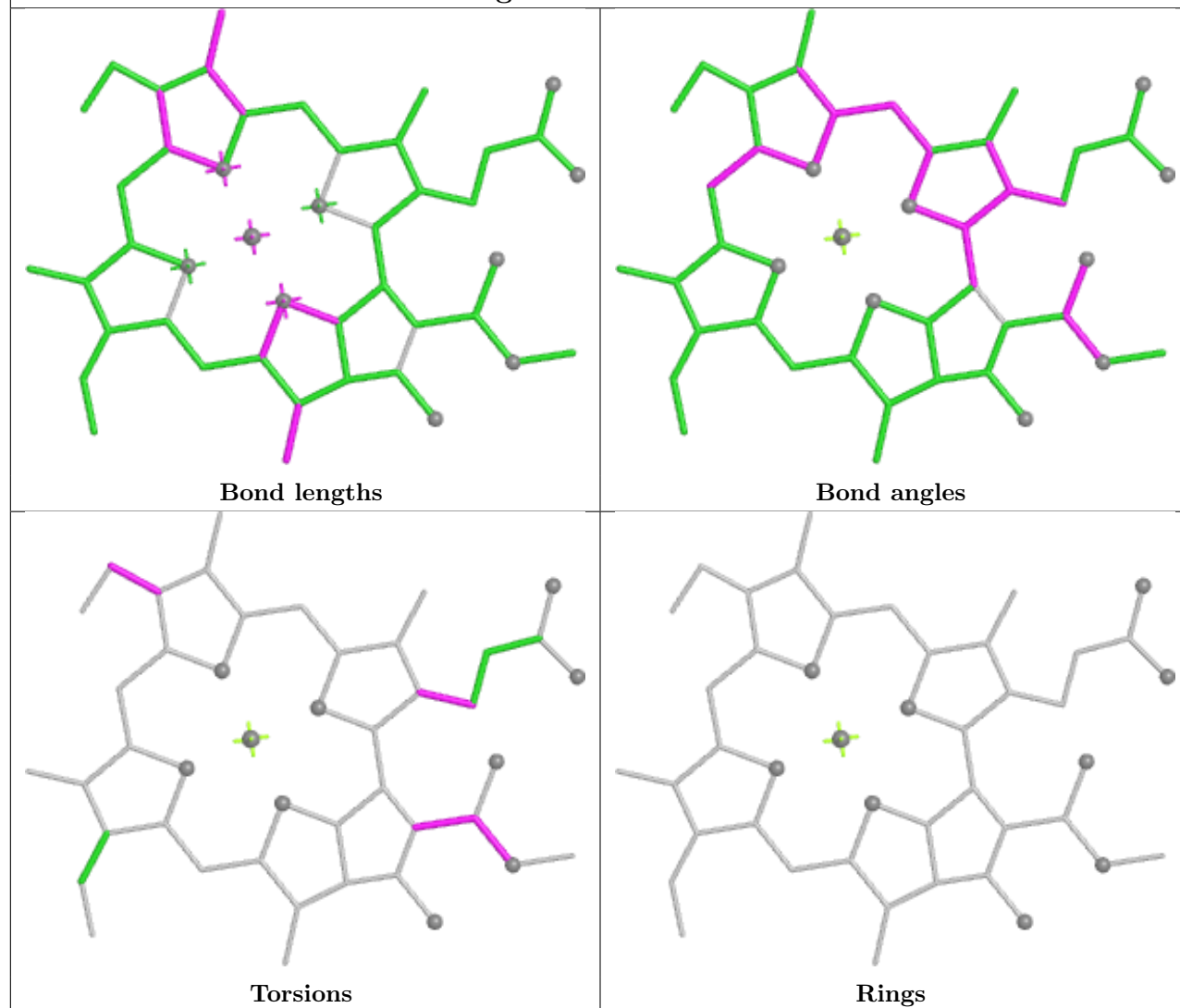


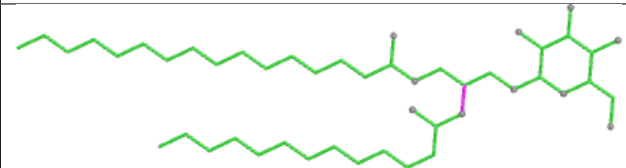
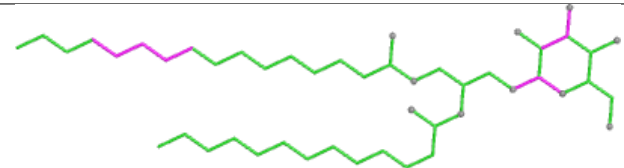
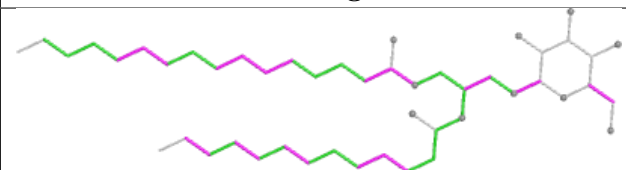
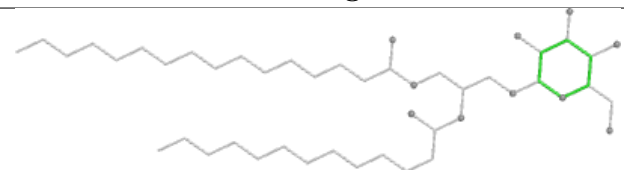


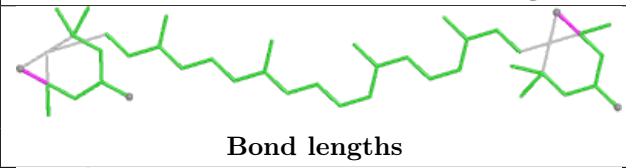
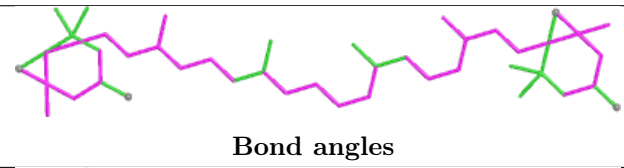
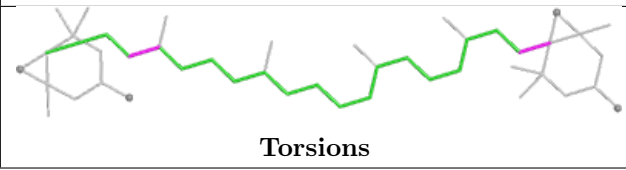
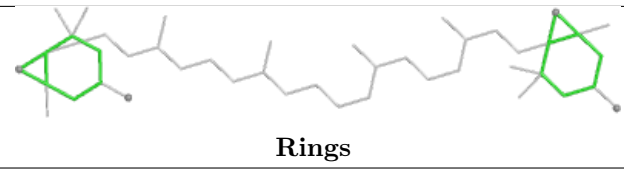
Ligand CLA y 610

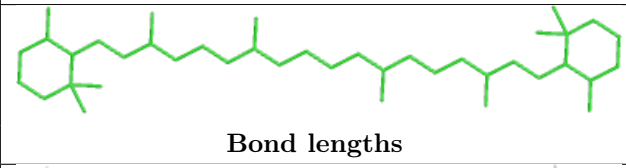
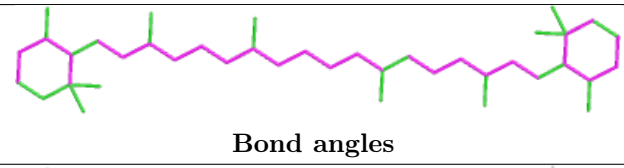
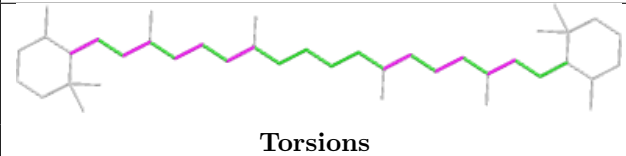
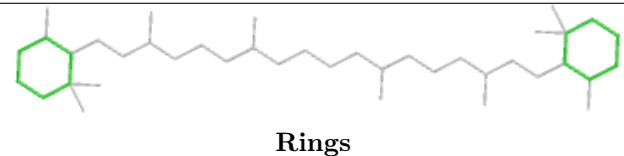


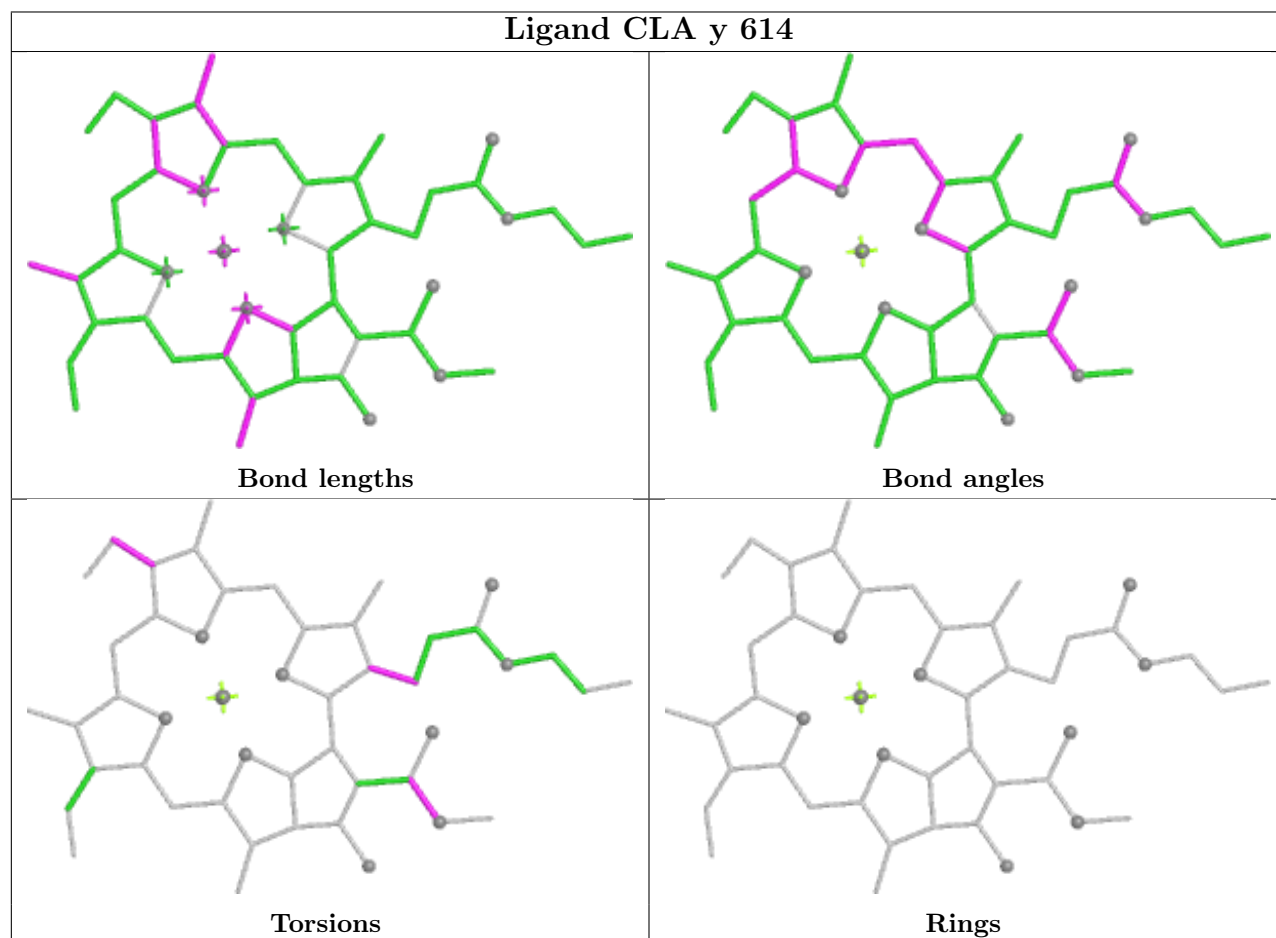
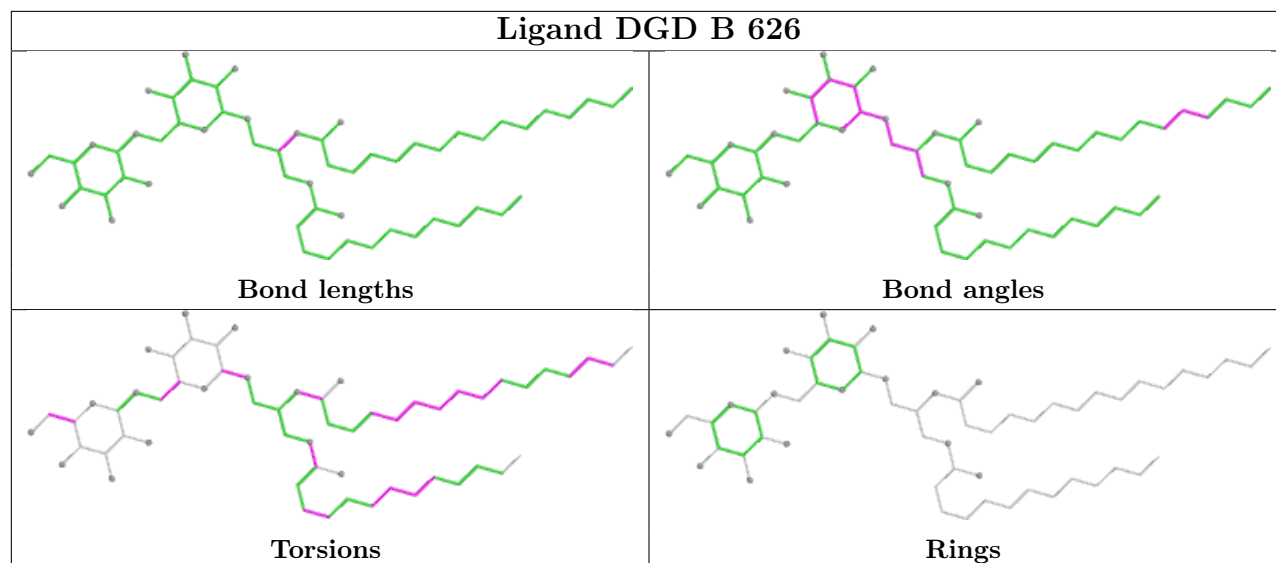
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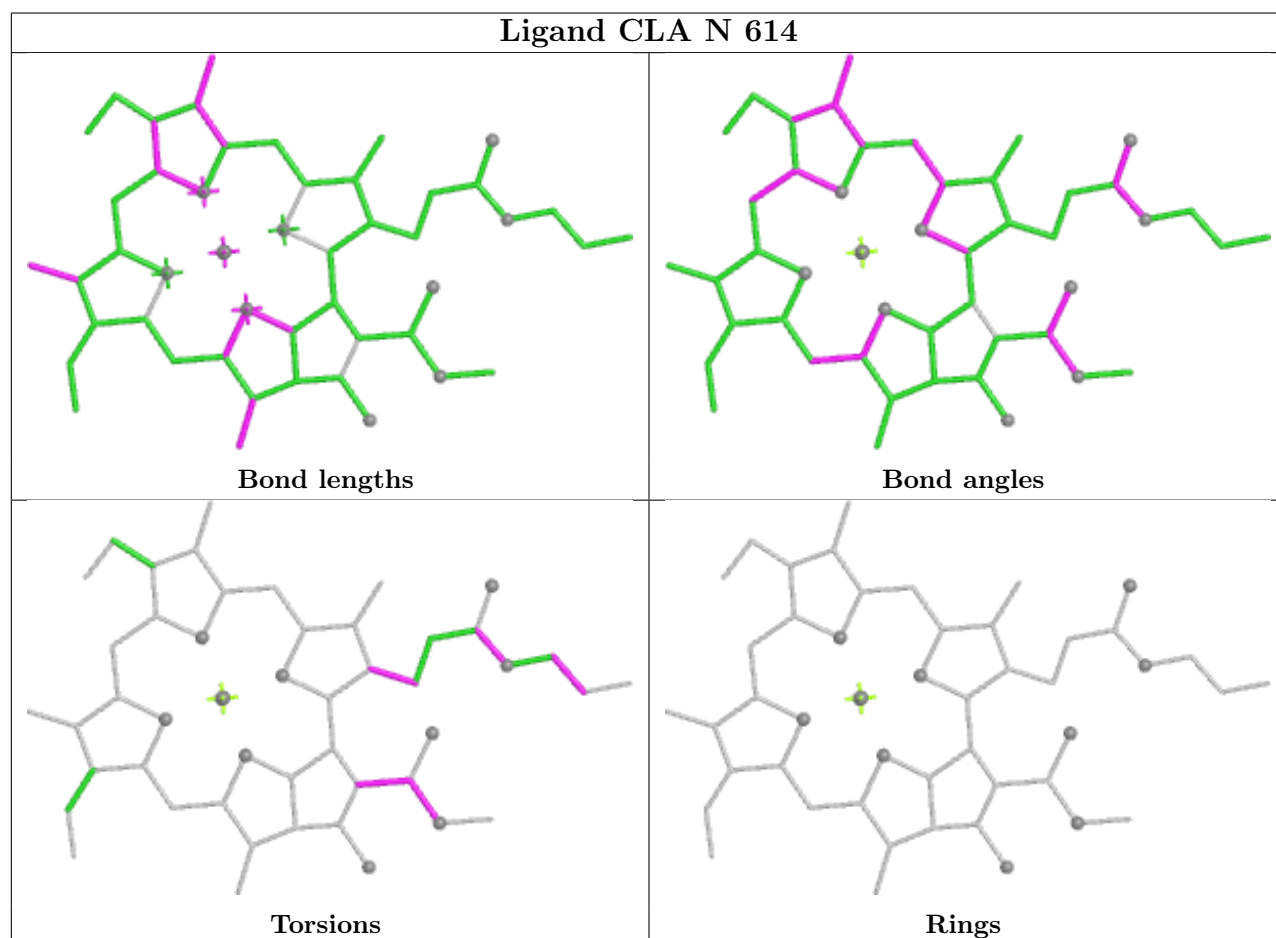
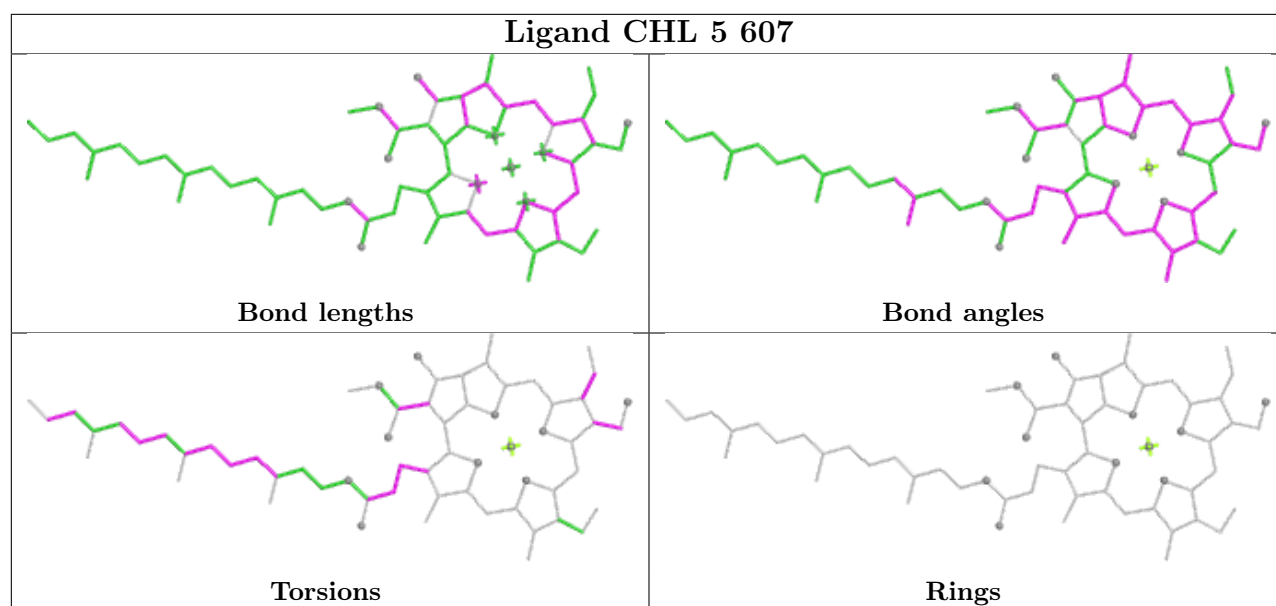


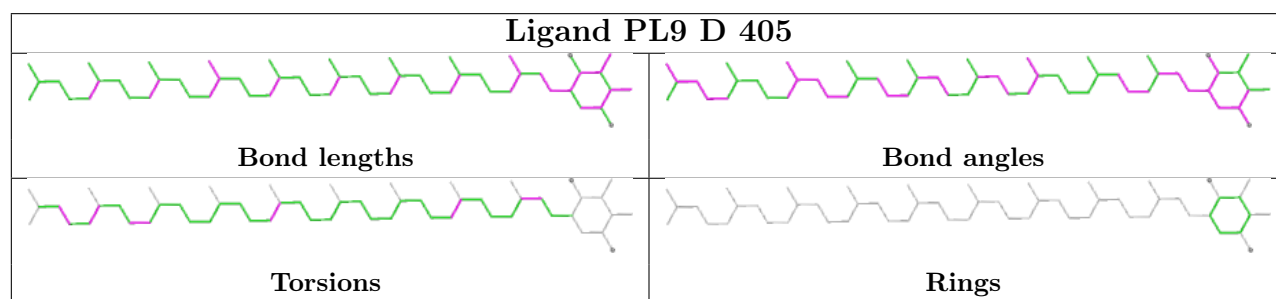
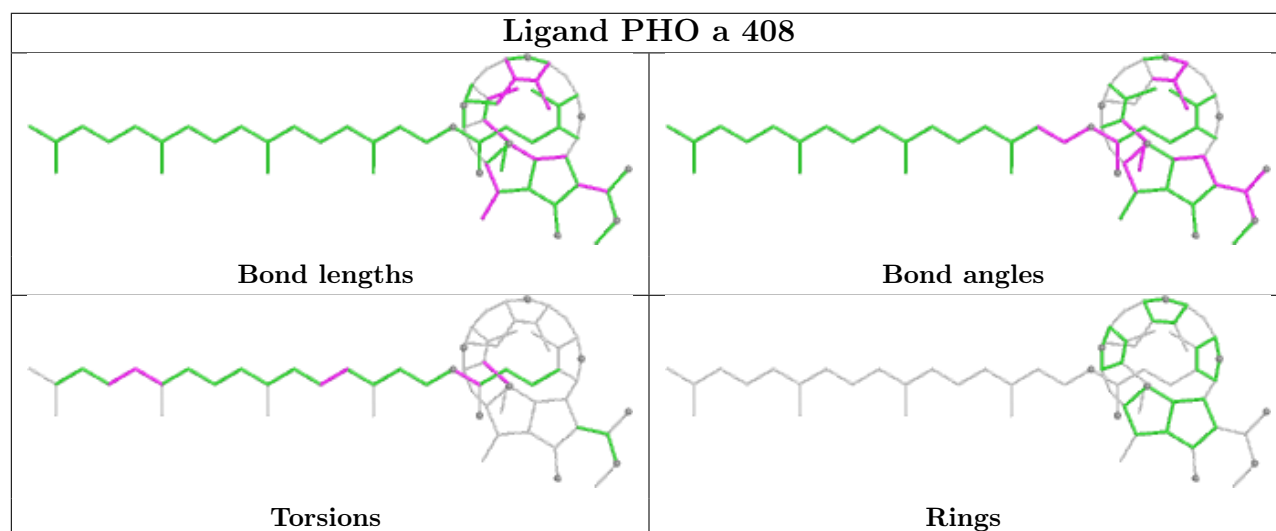
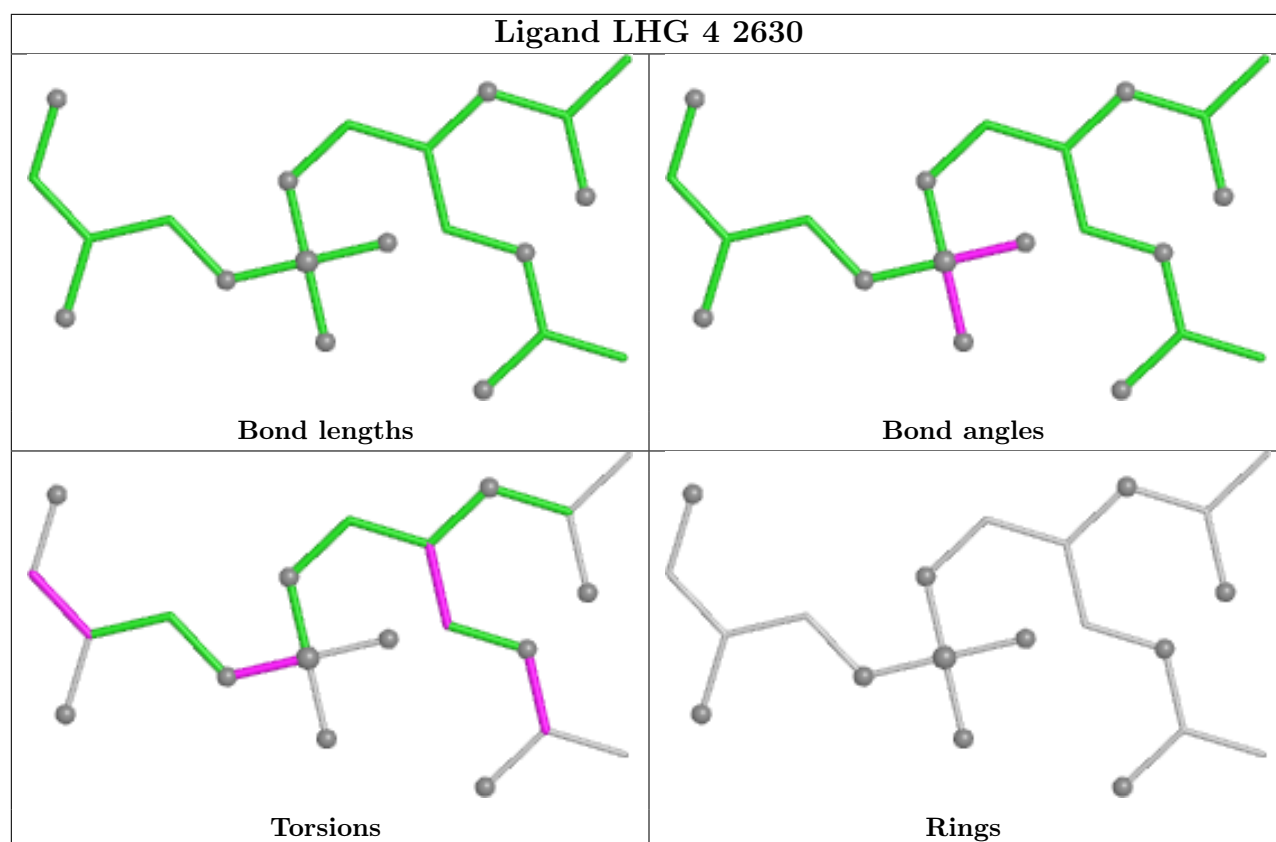
Ligand LMG A 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 8 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

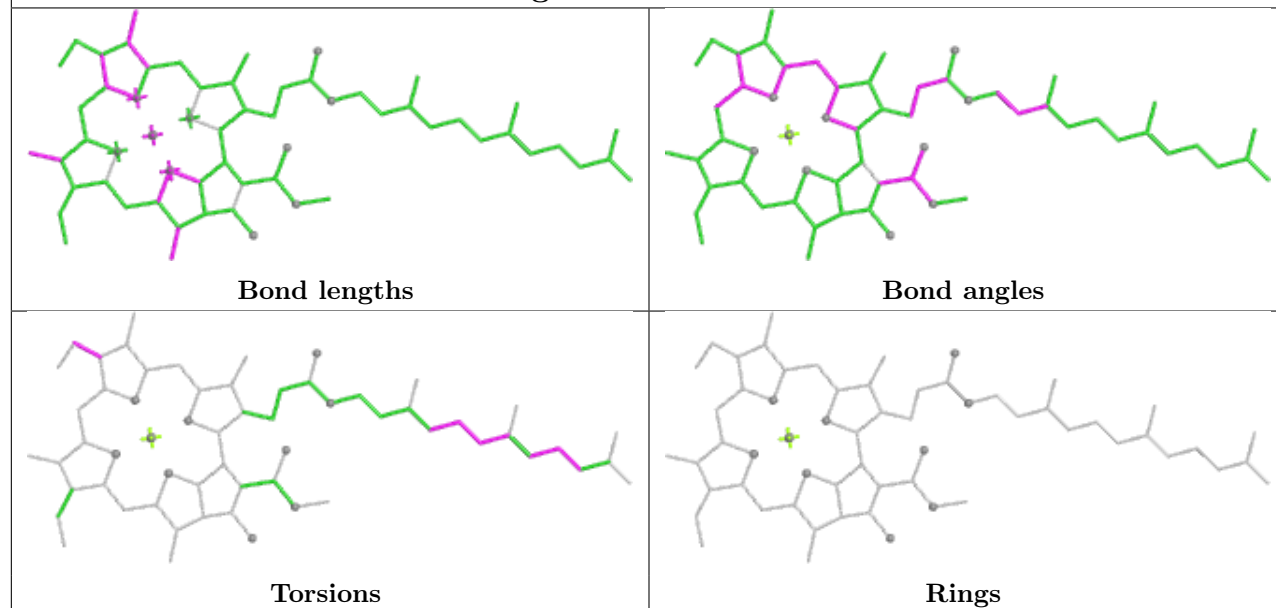
Ligand BCR 4 623	
	
Bond lengths	Bond angles
	
Torsions	Rings



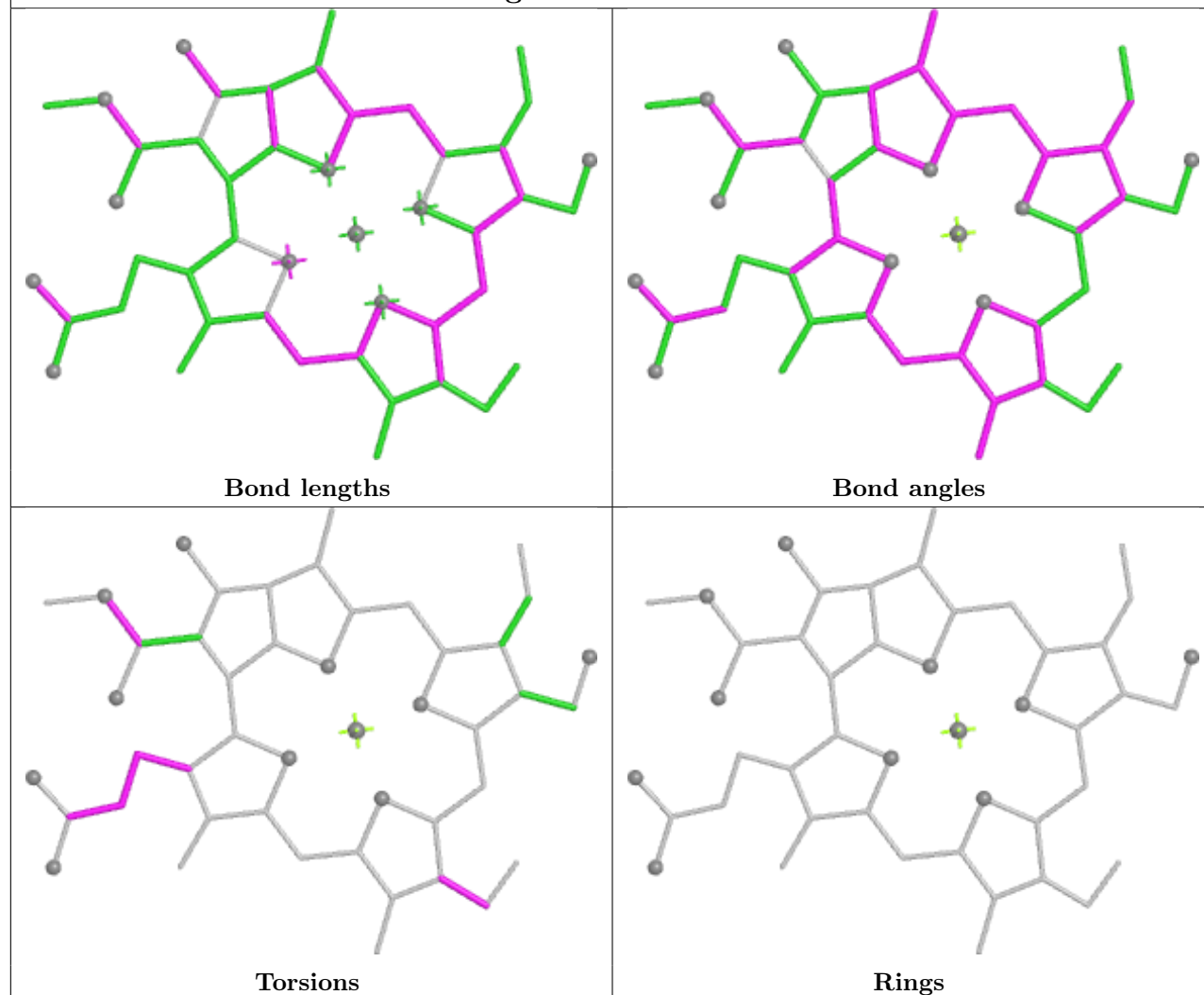




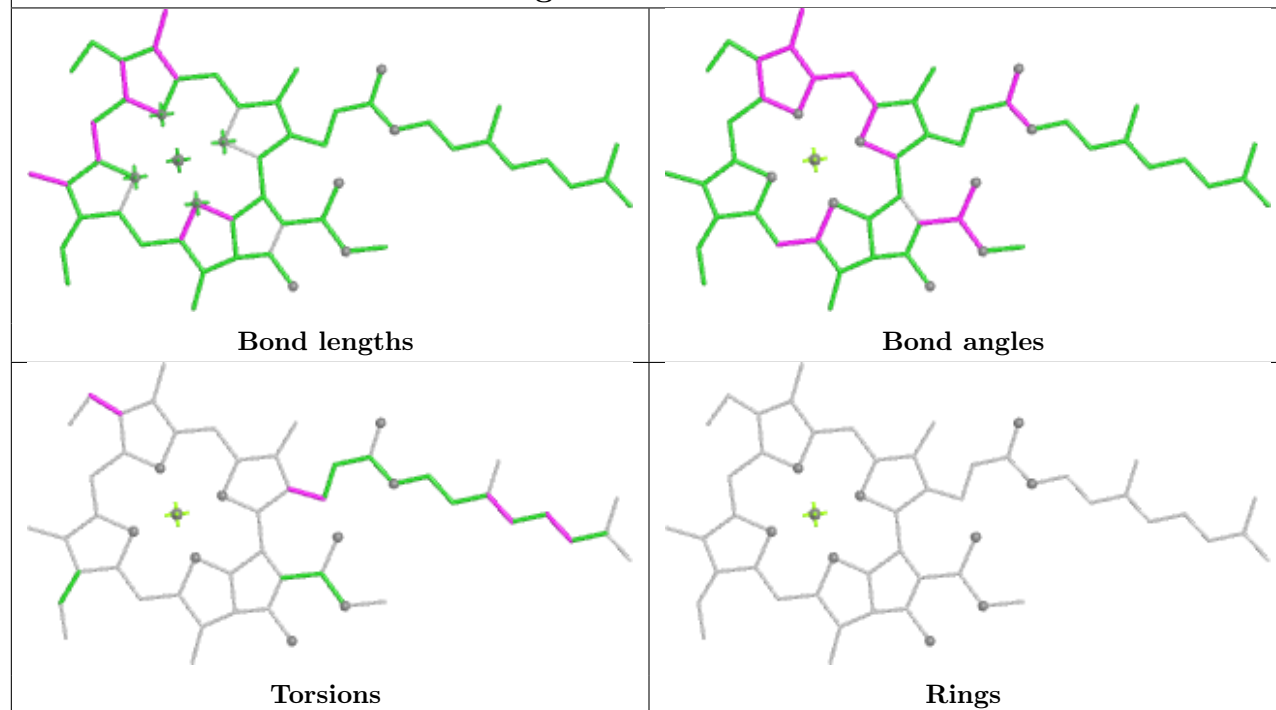
Ligand CLA A 410



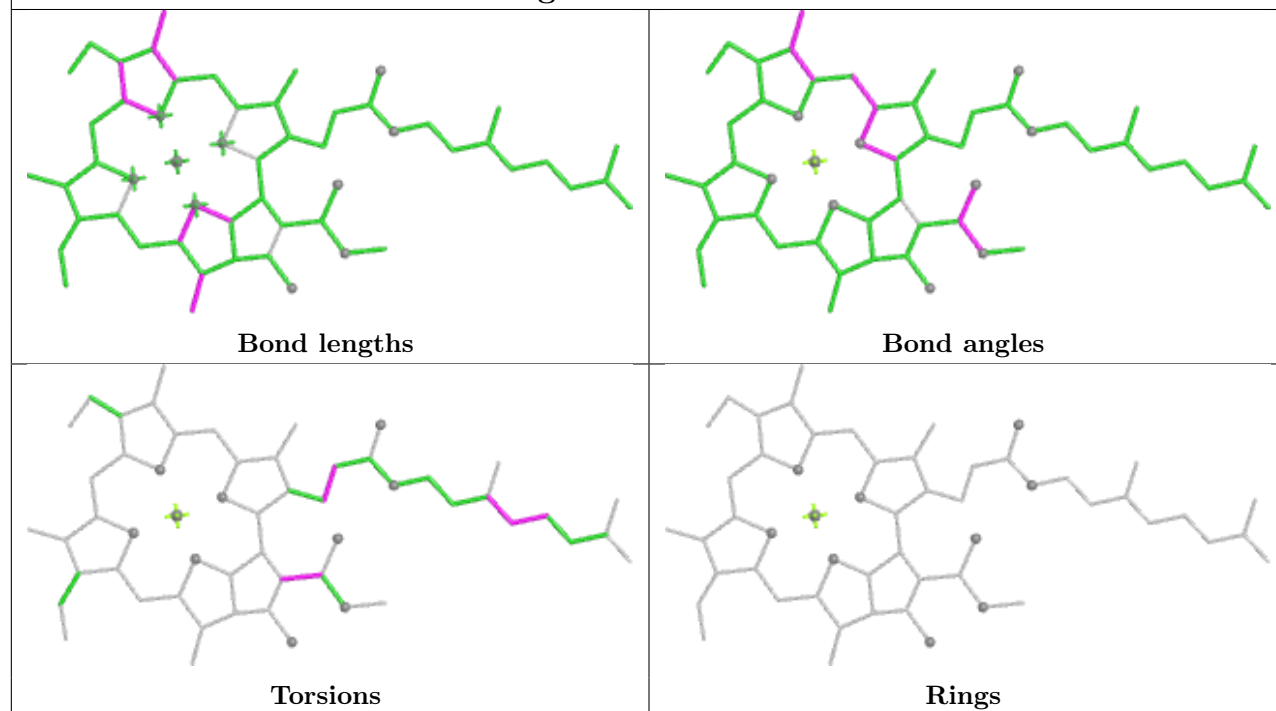
Ligand CHL 7 608



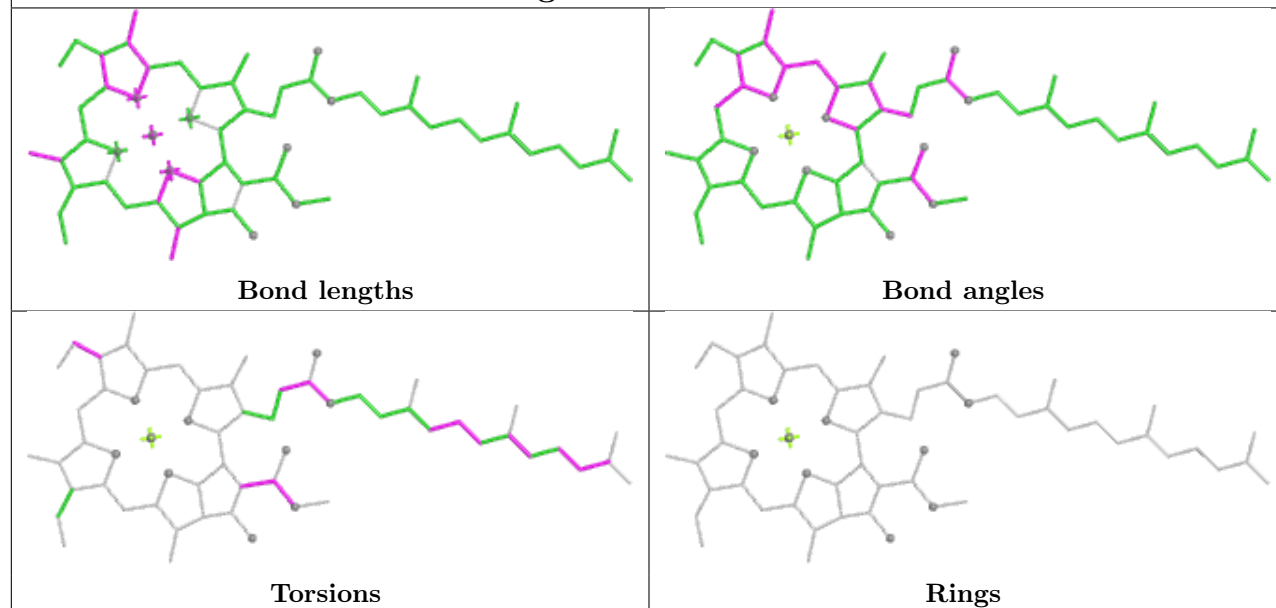
Ligand CLA S 610



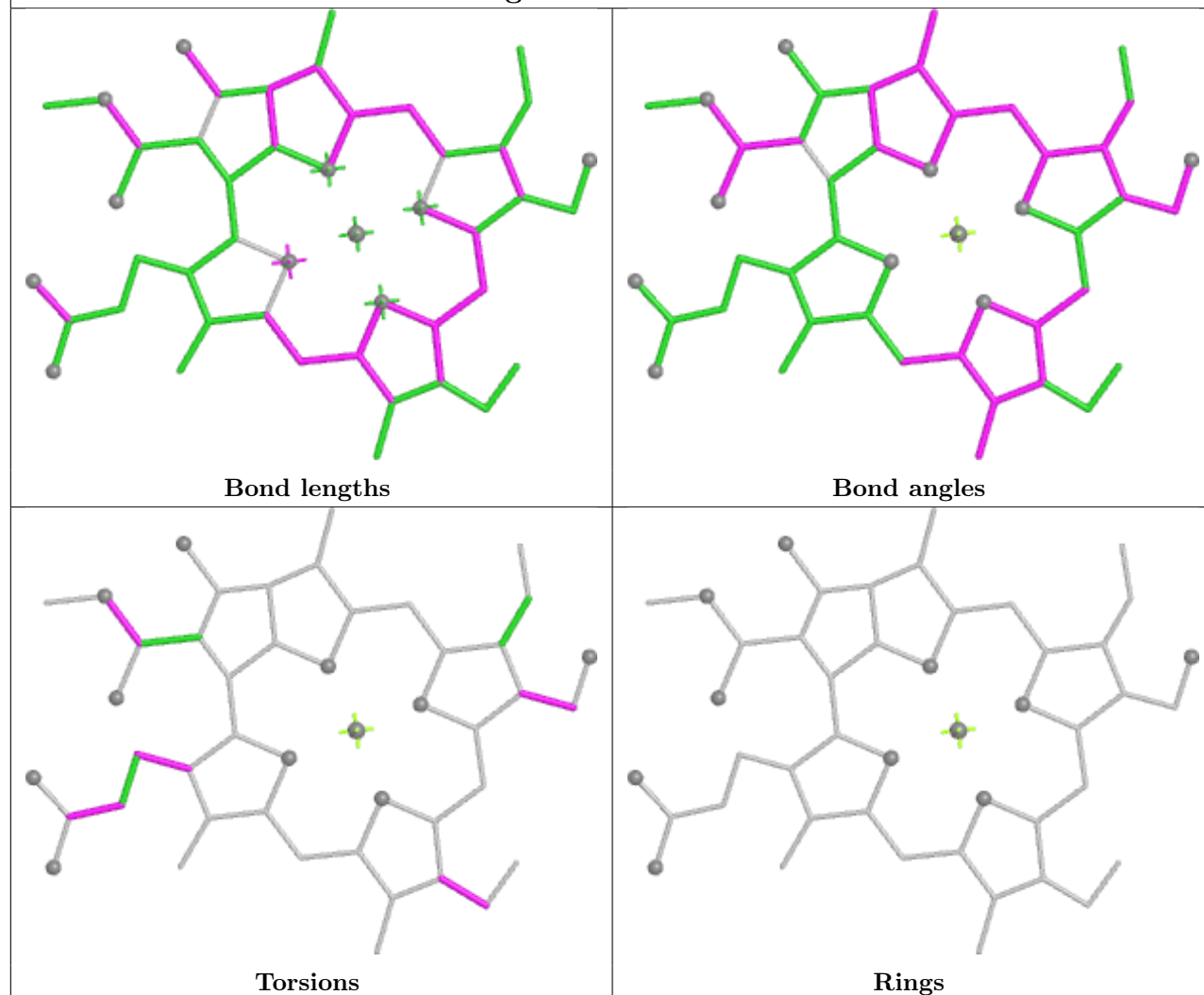
Ligand CLA s 613



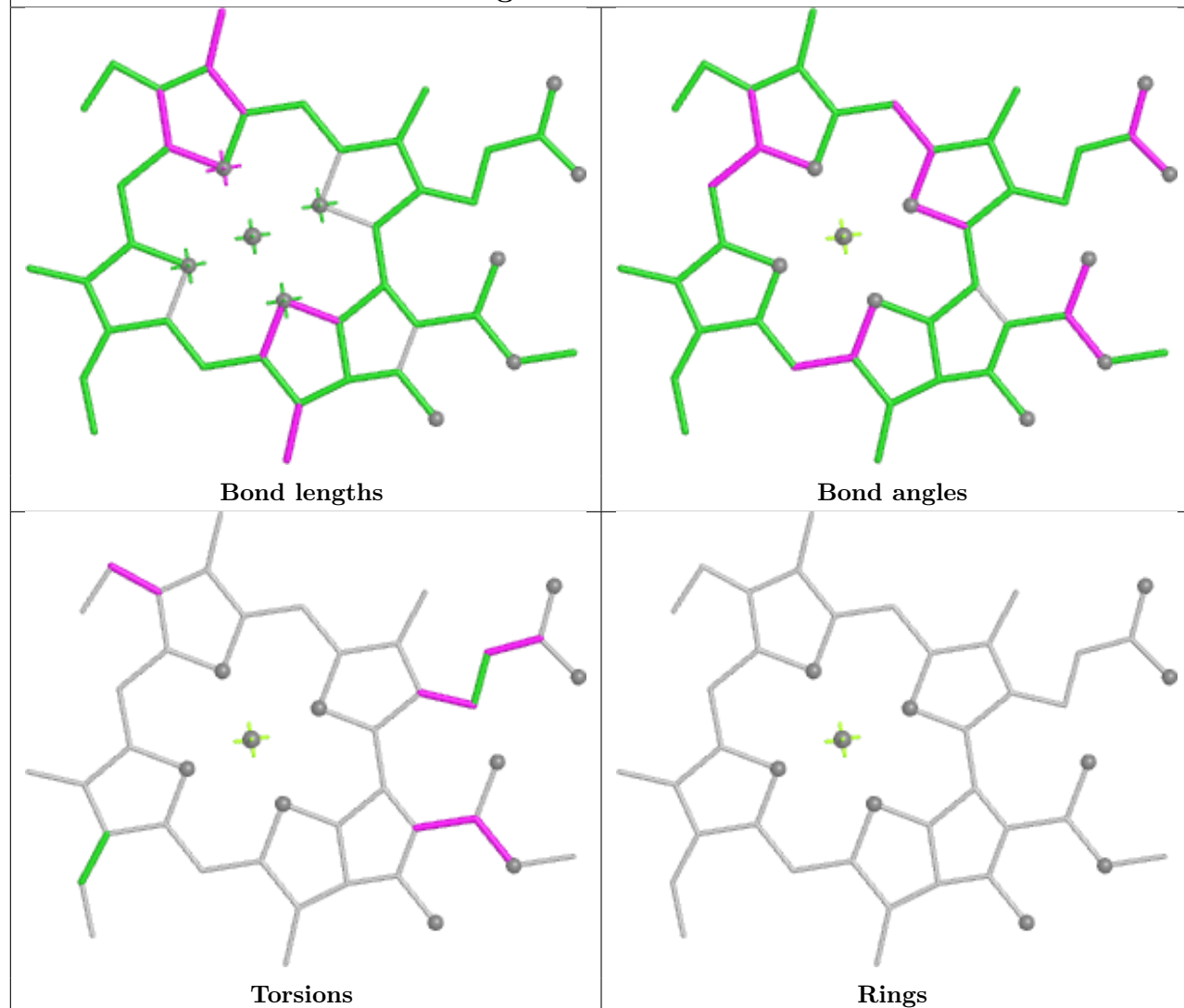
Ligand CLA r 603



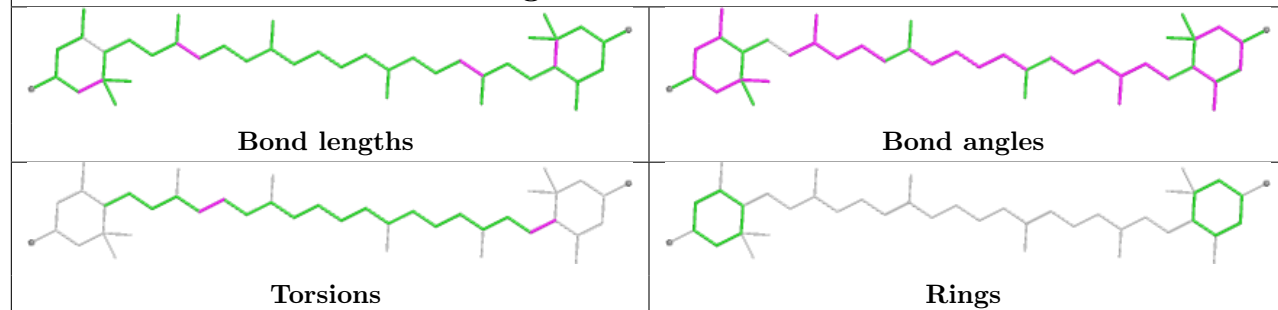
Ligand CHL 1 605

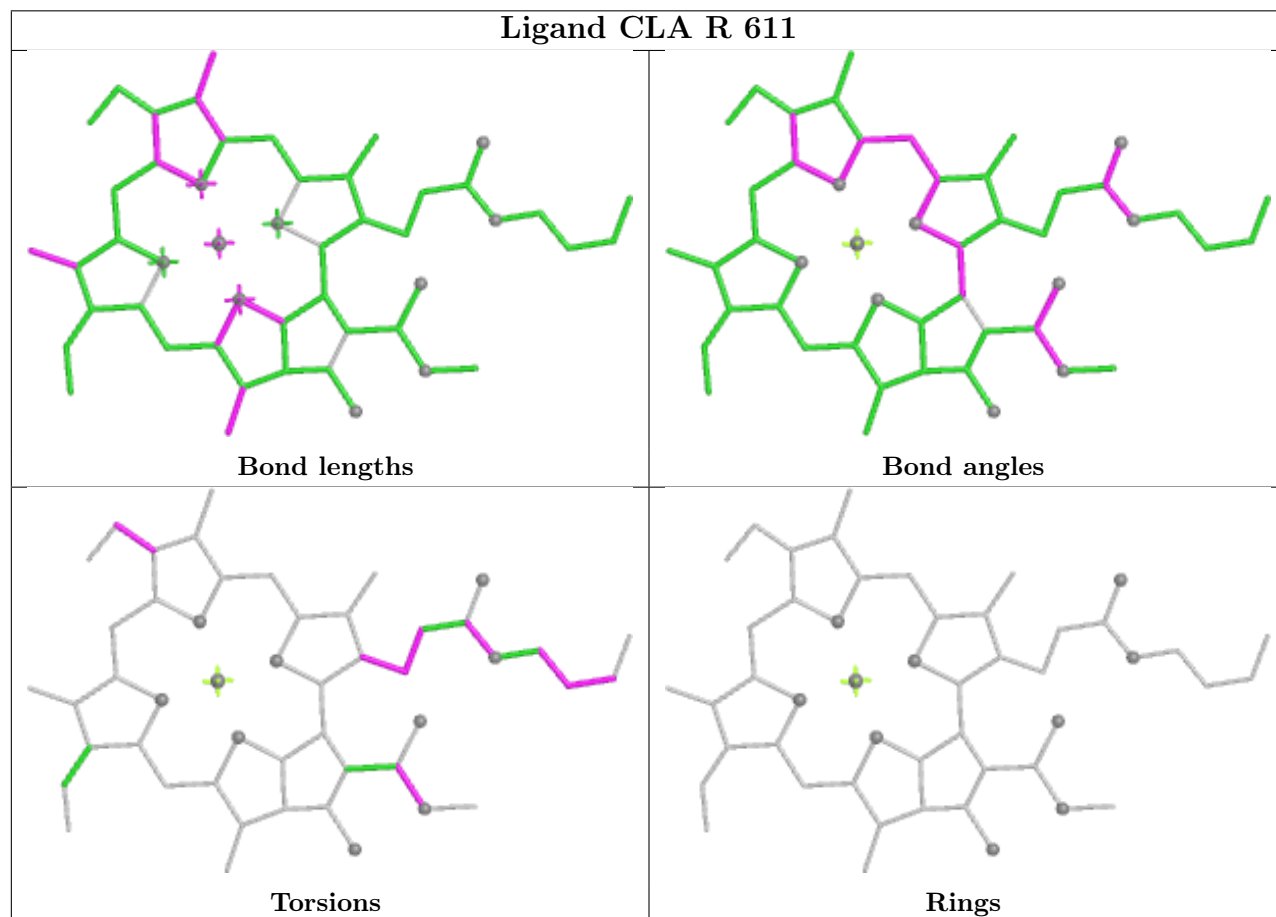
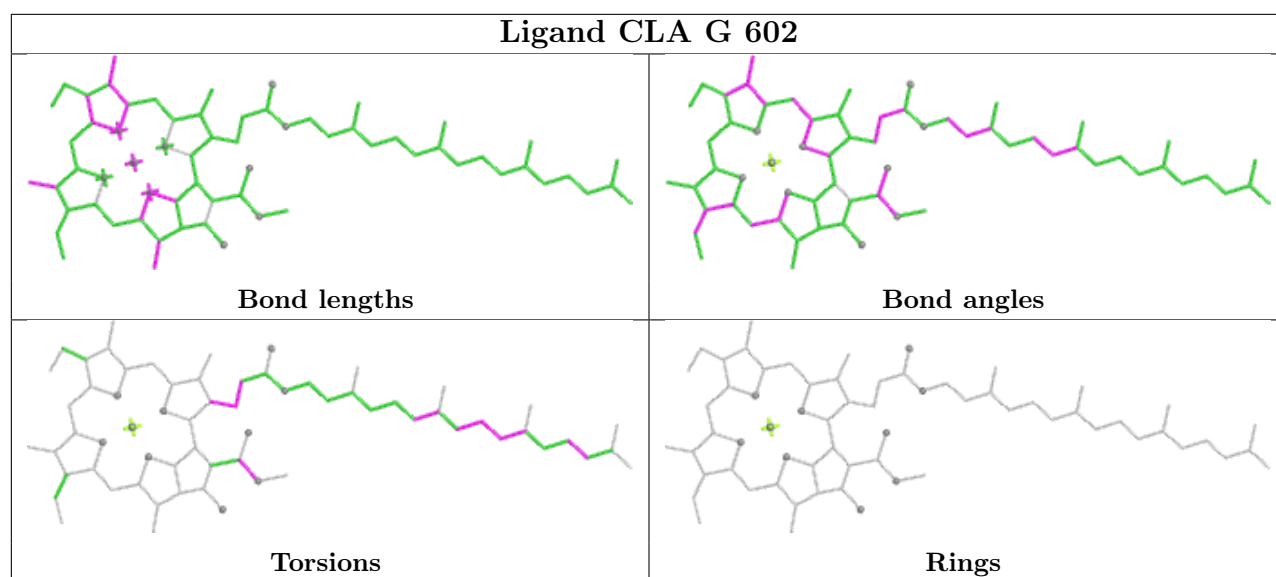


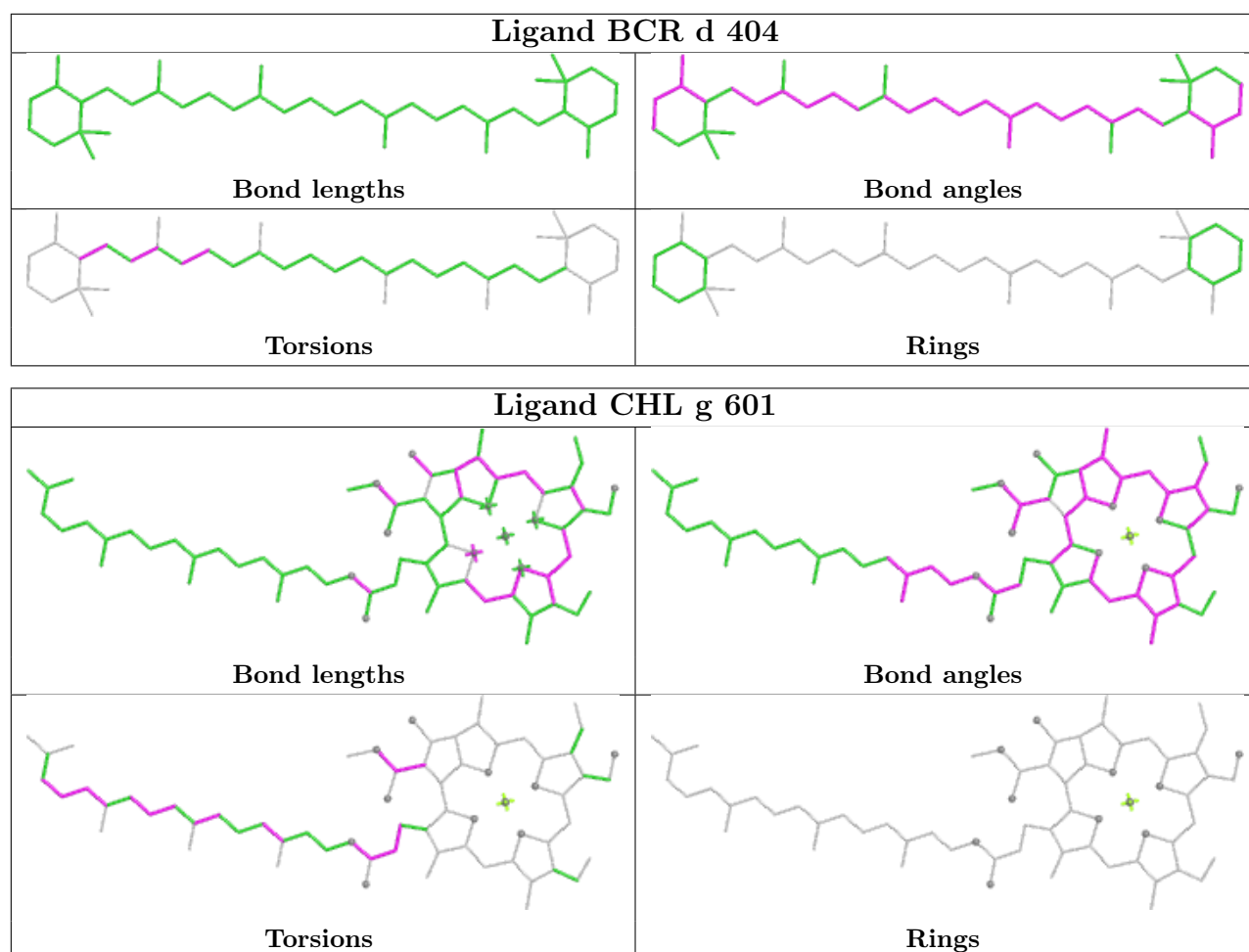
Ligand CLA 8 611

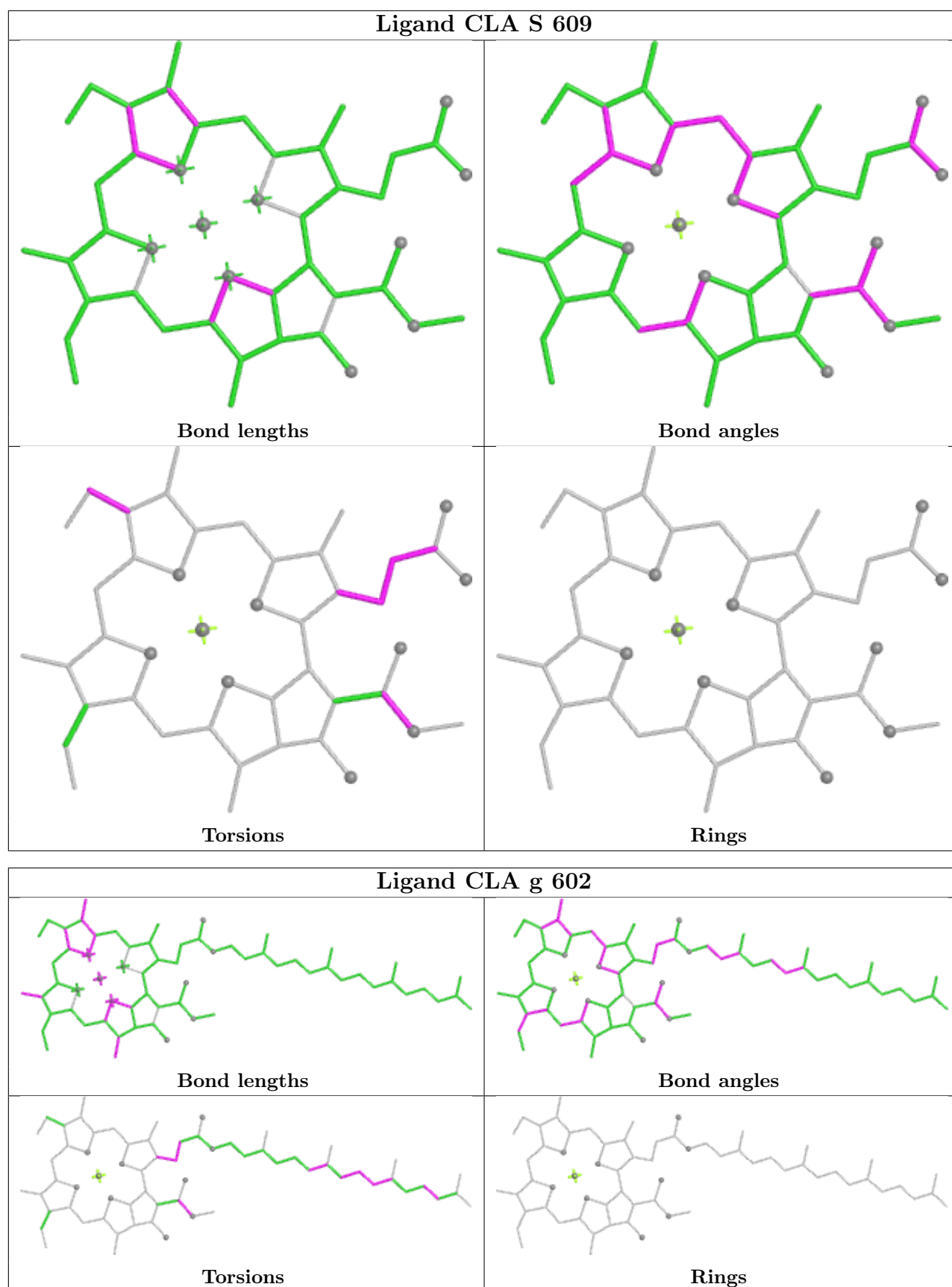


Ligand LUT G 1621

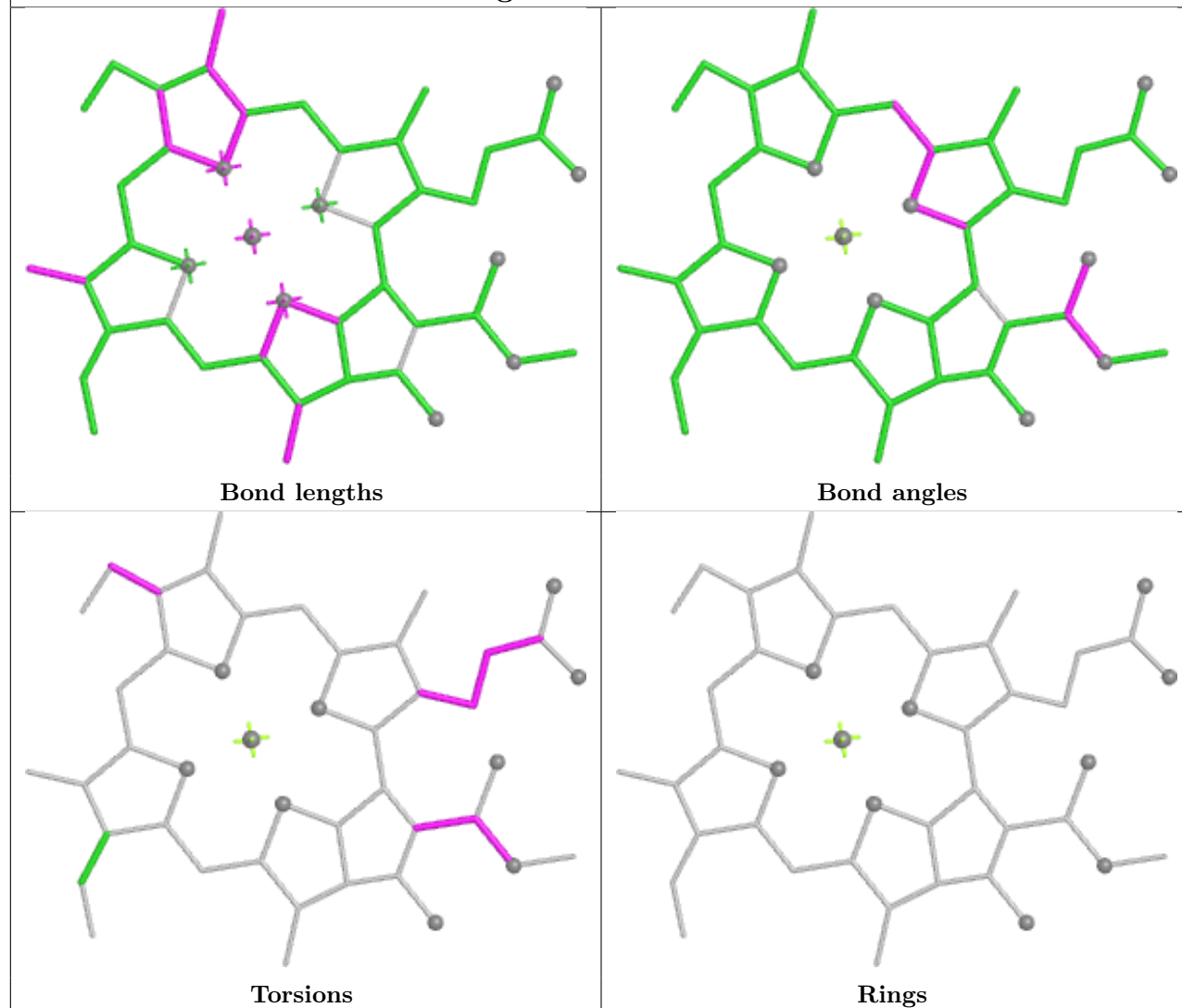




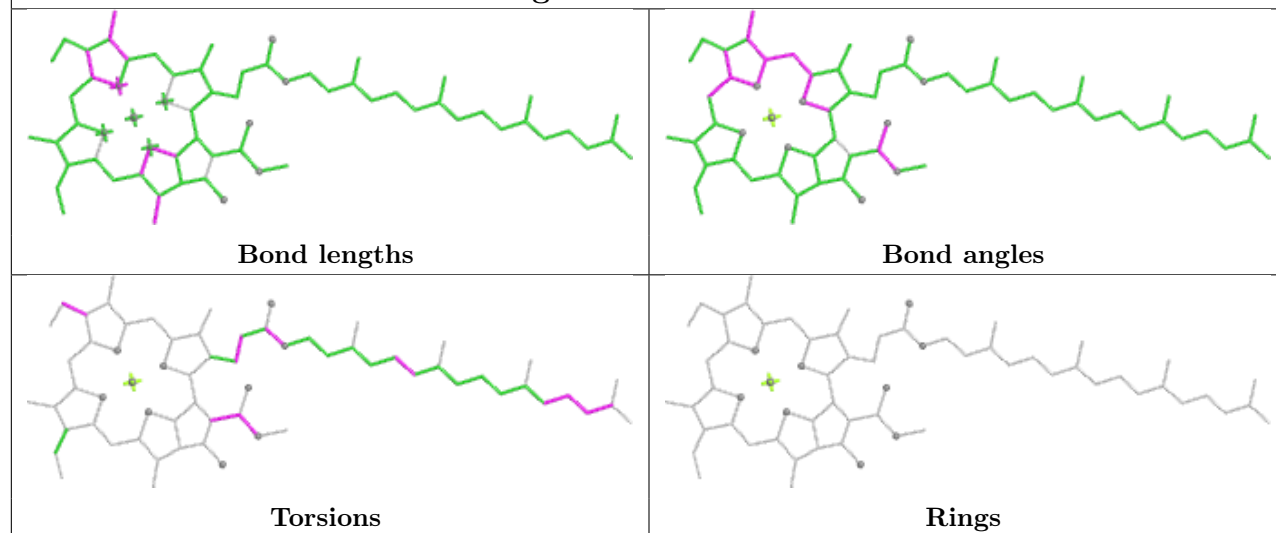


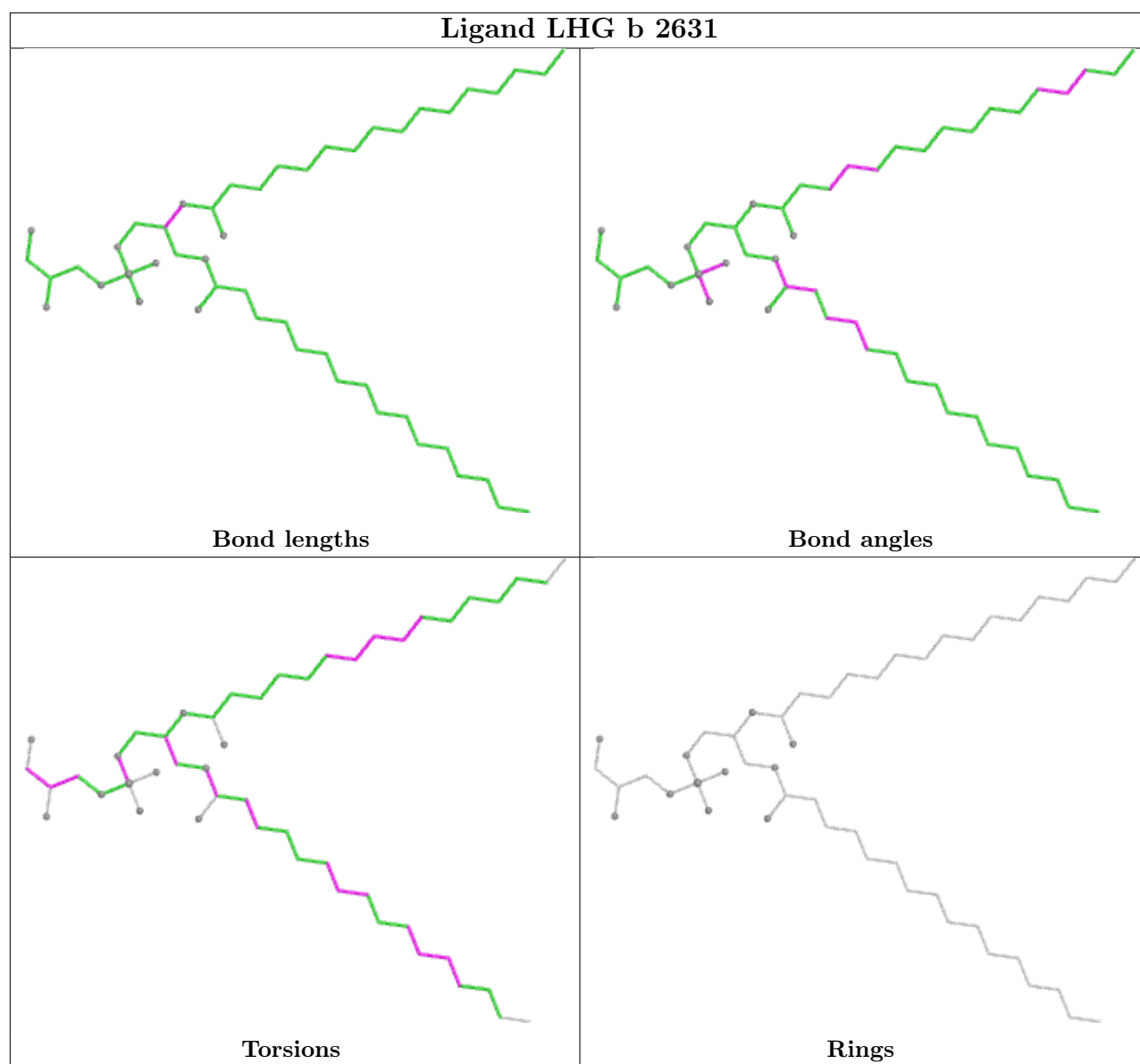


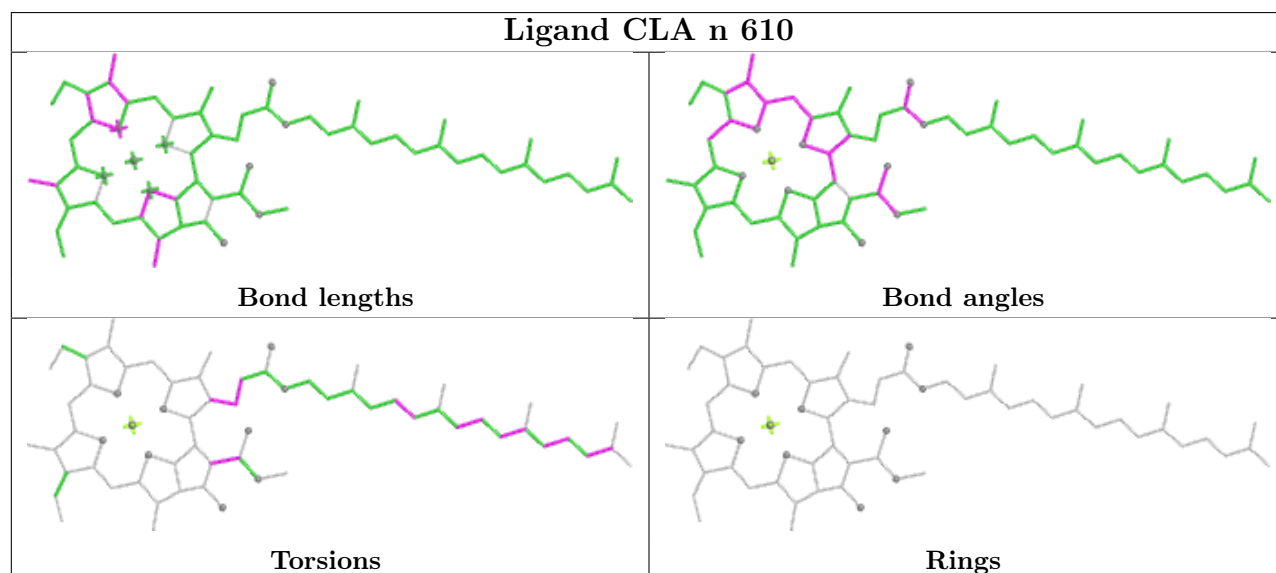
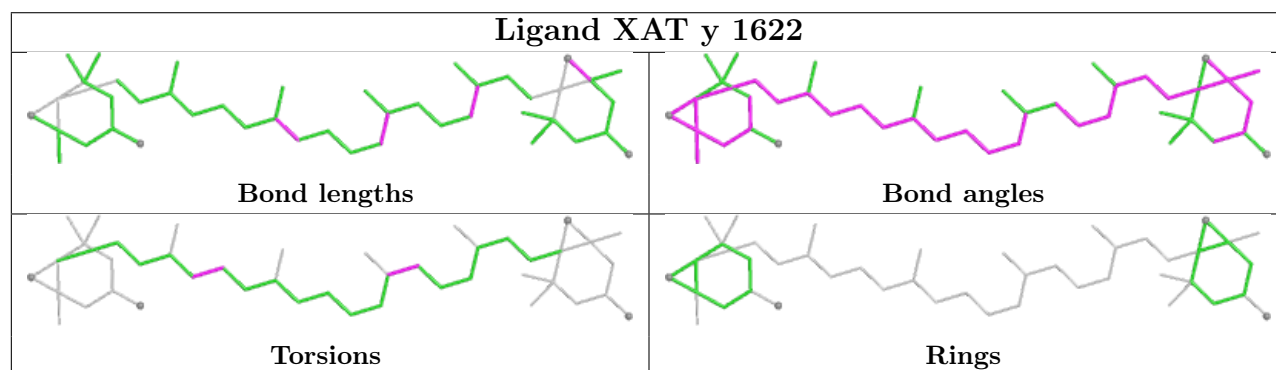
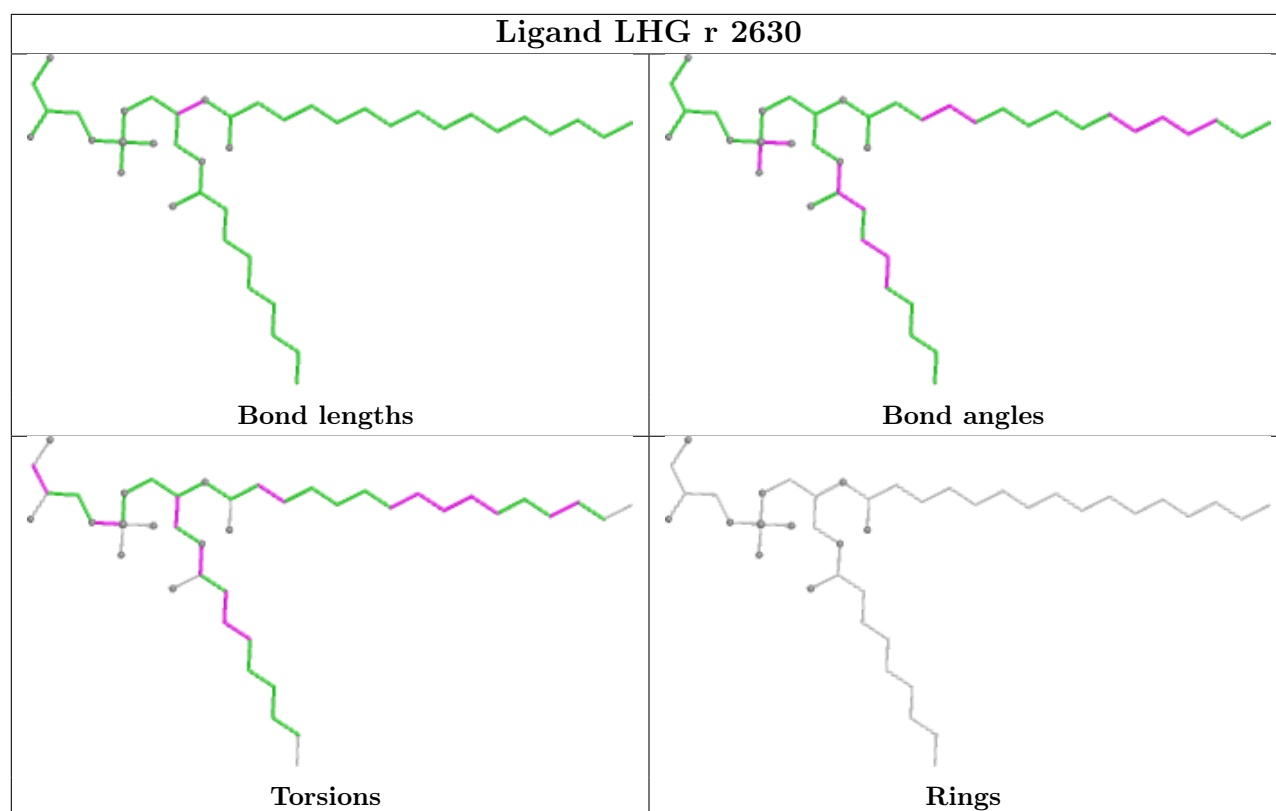
Ligand CLA 7 604



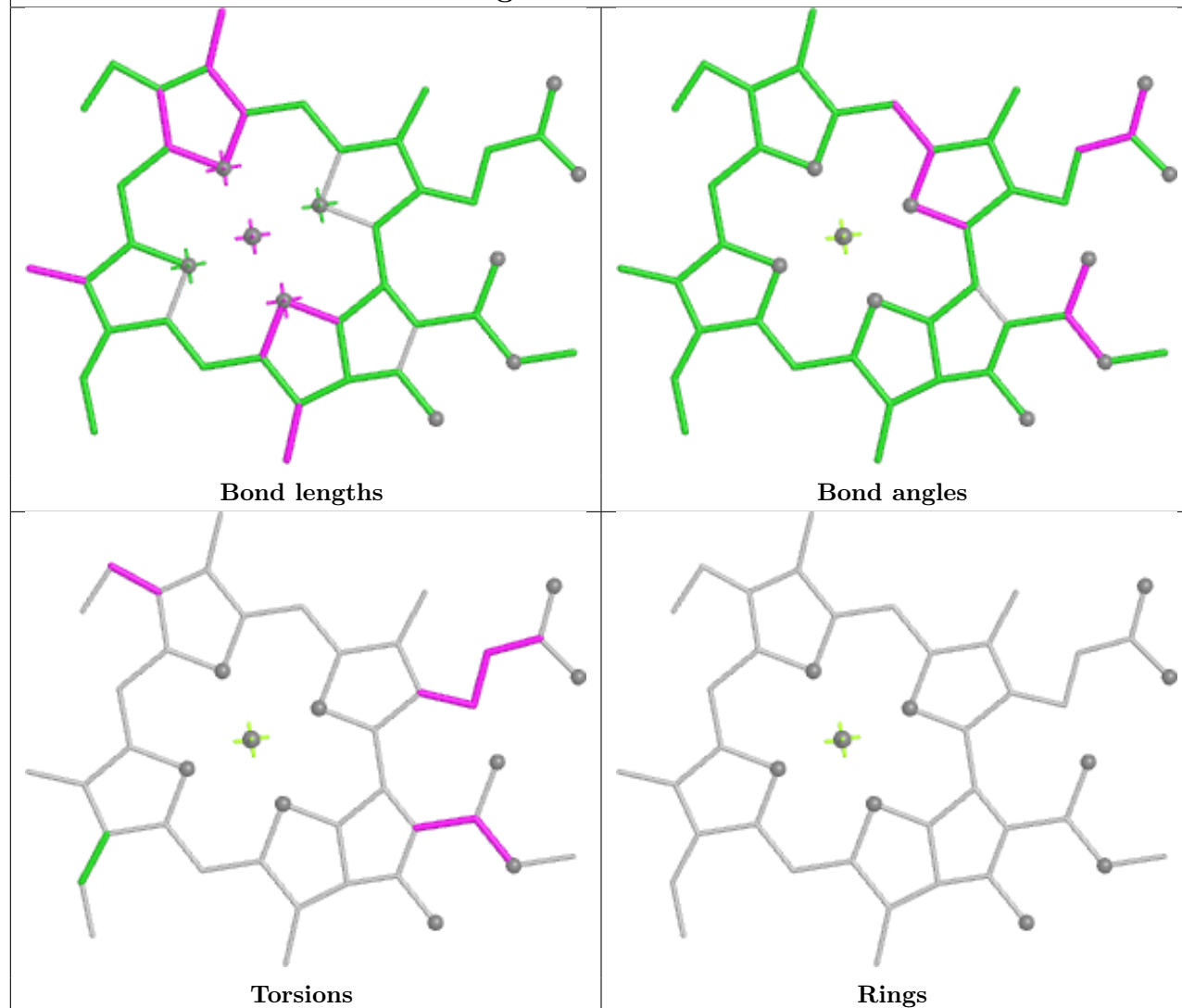
Ligand CLA C 503



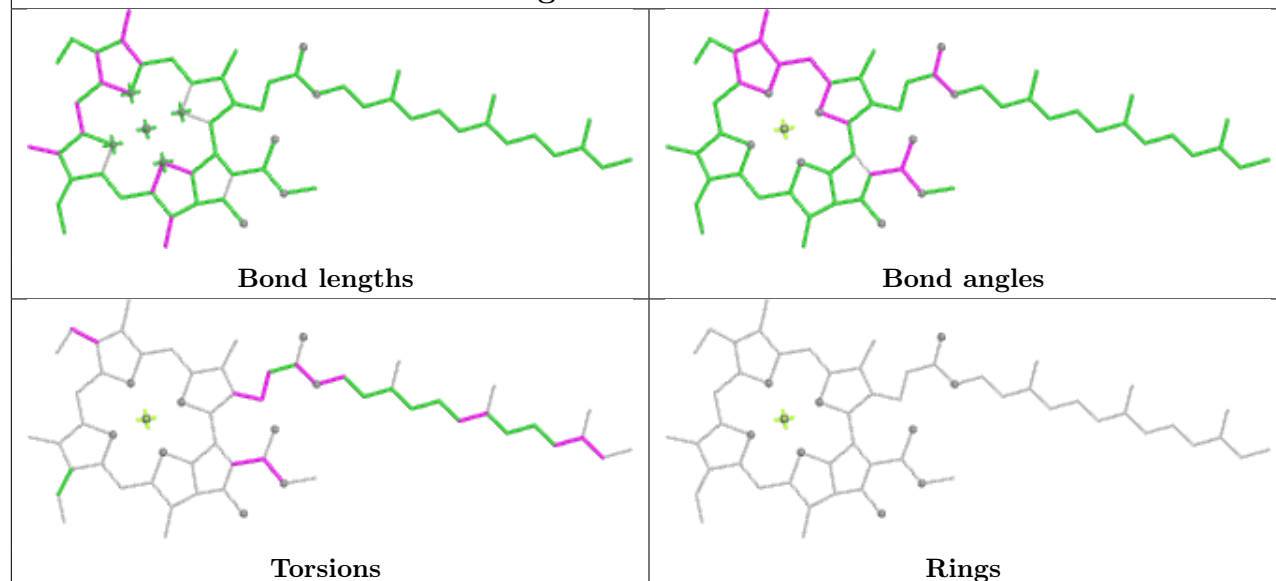


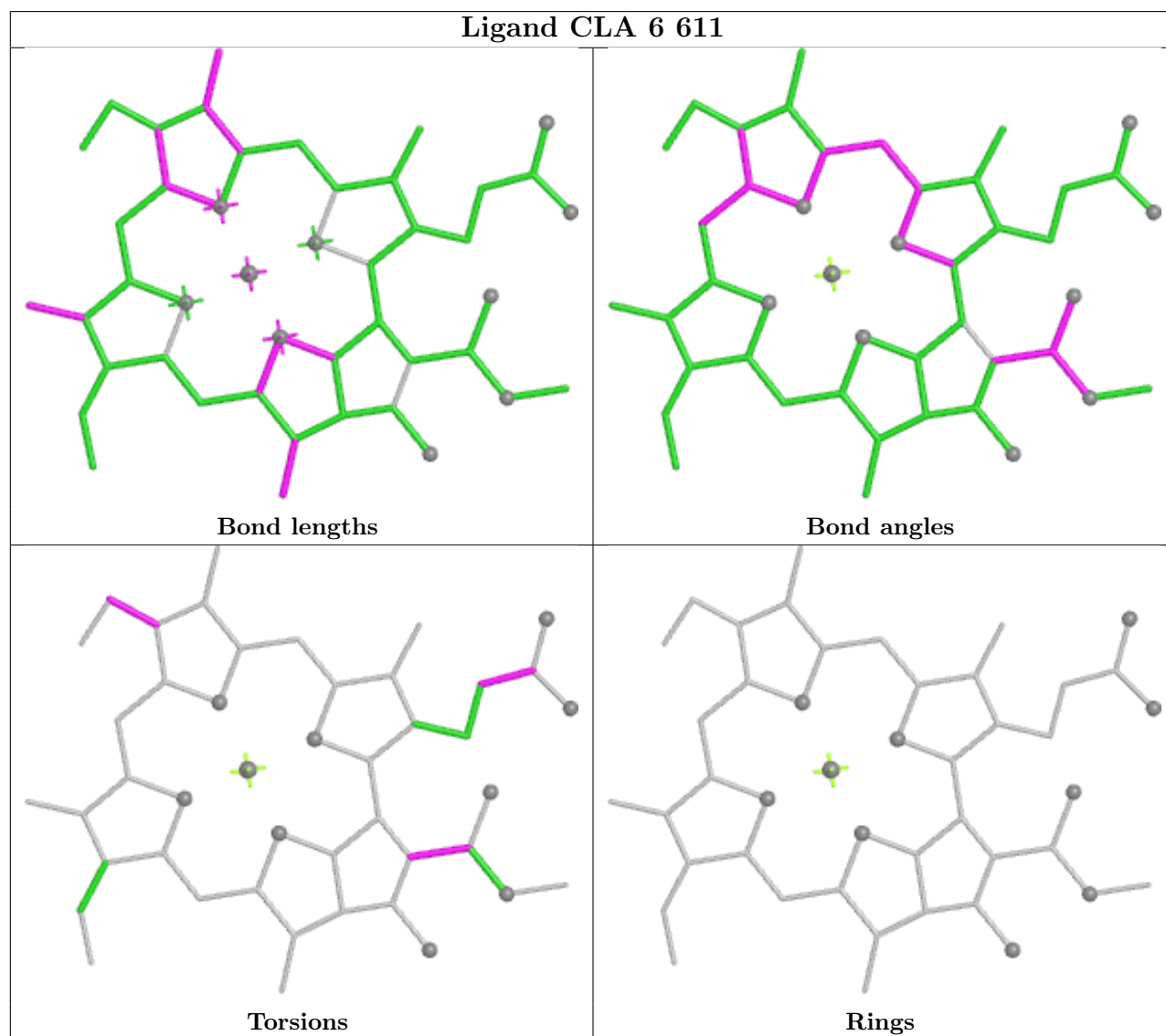
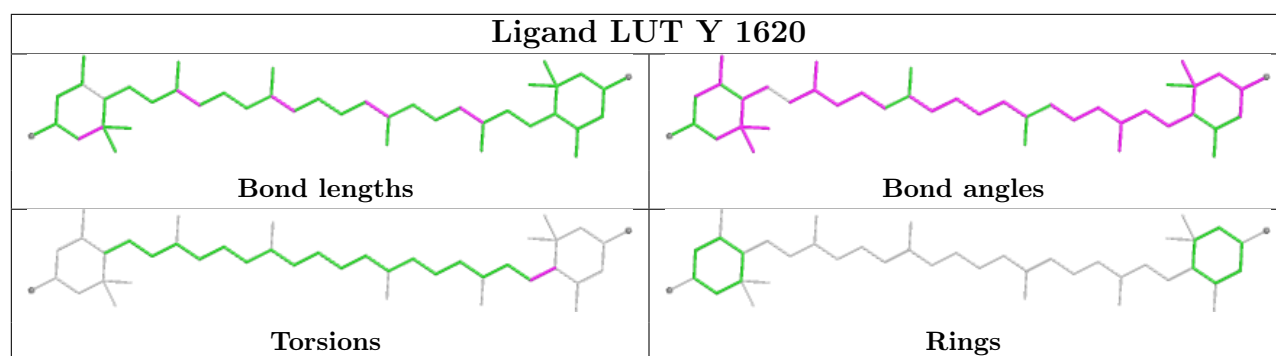


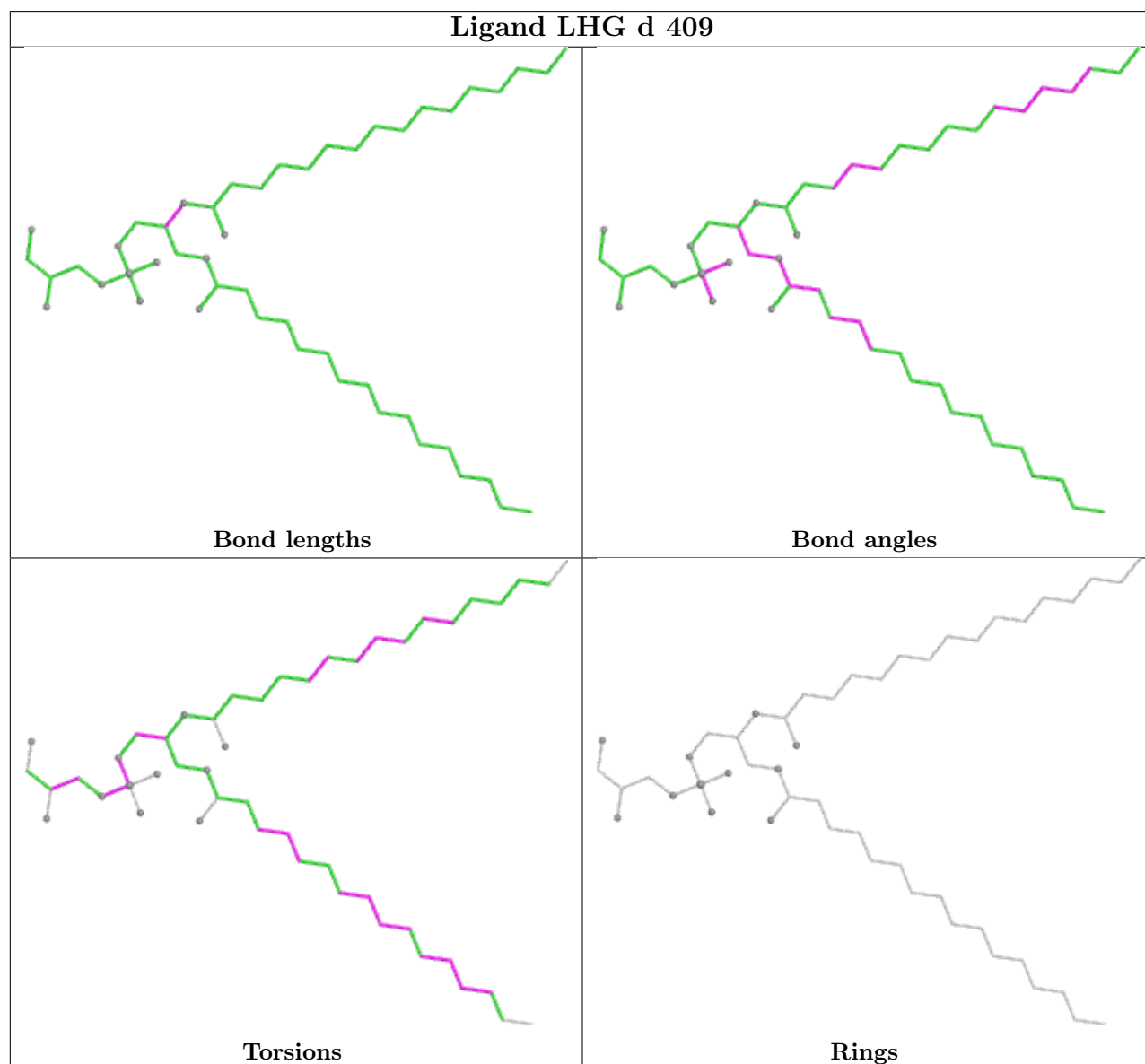
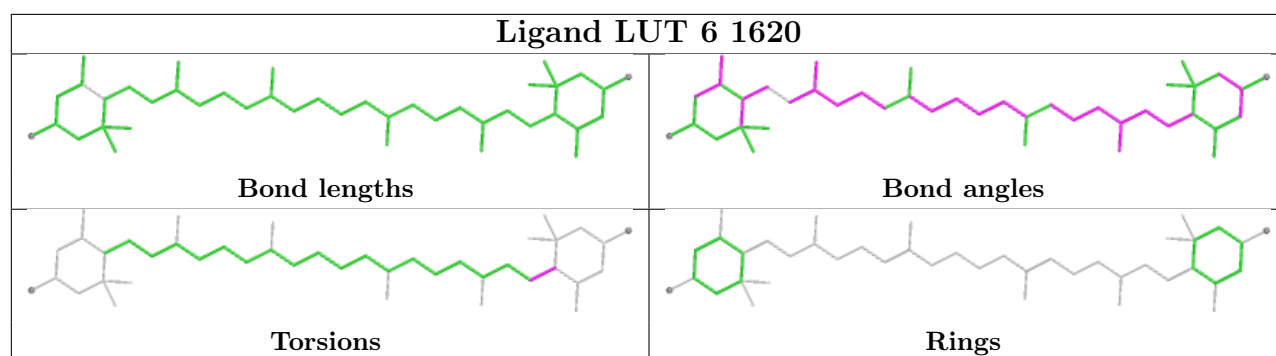
Ligand CLA 3 604

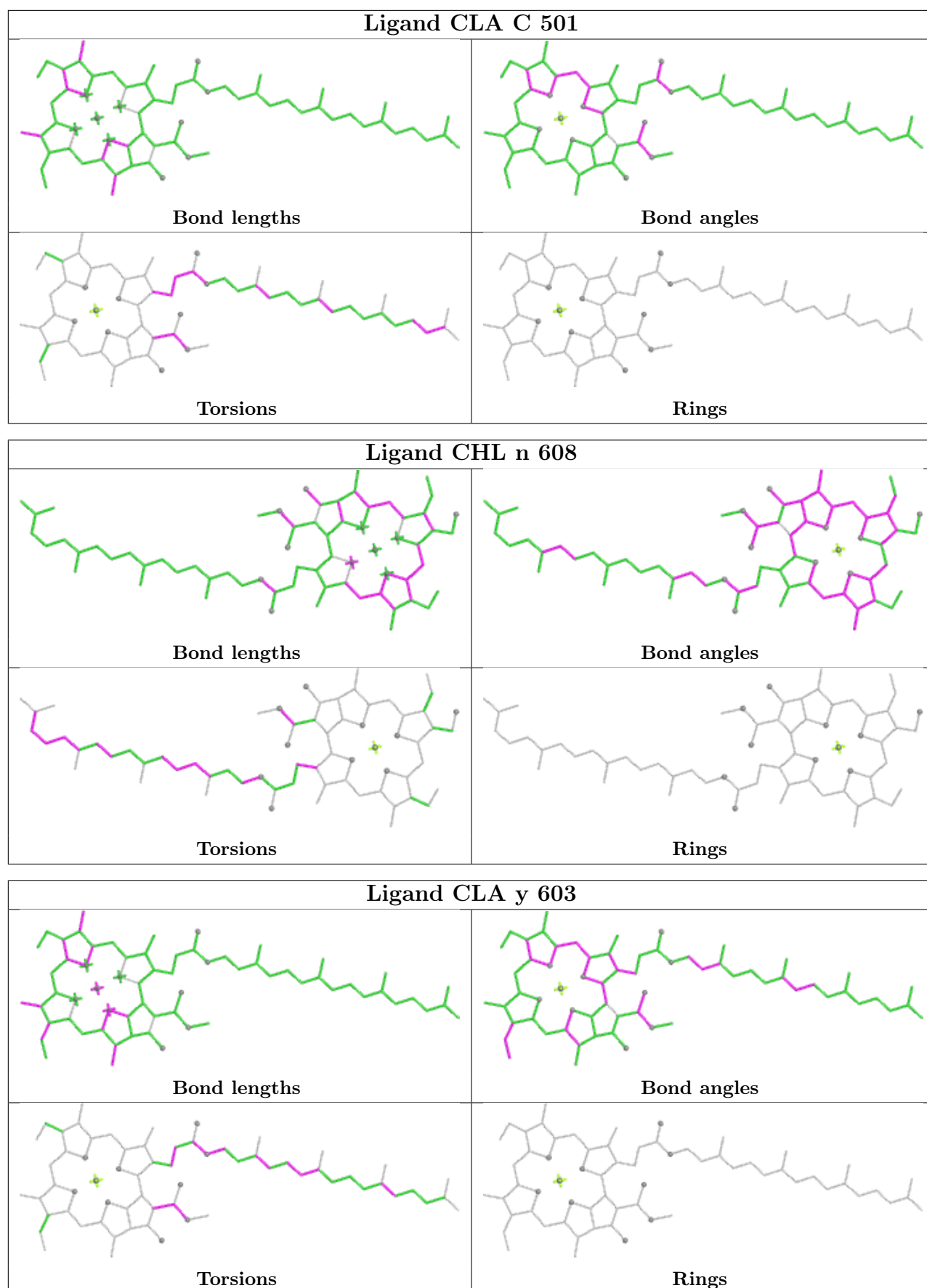


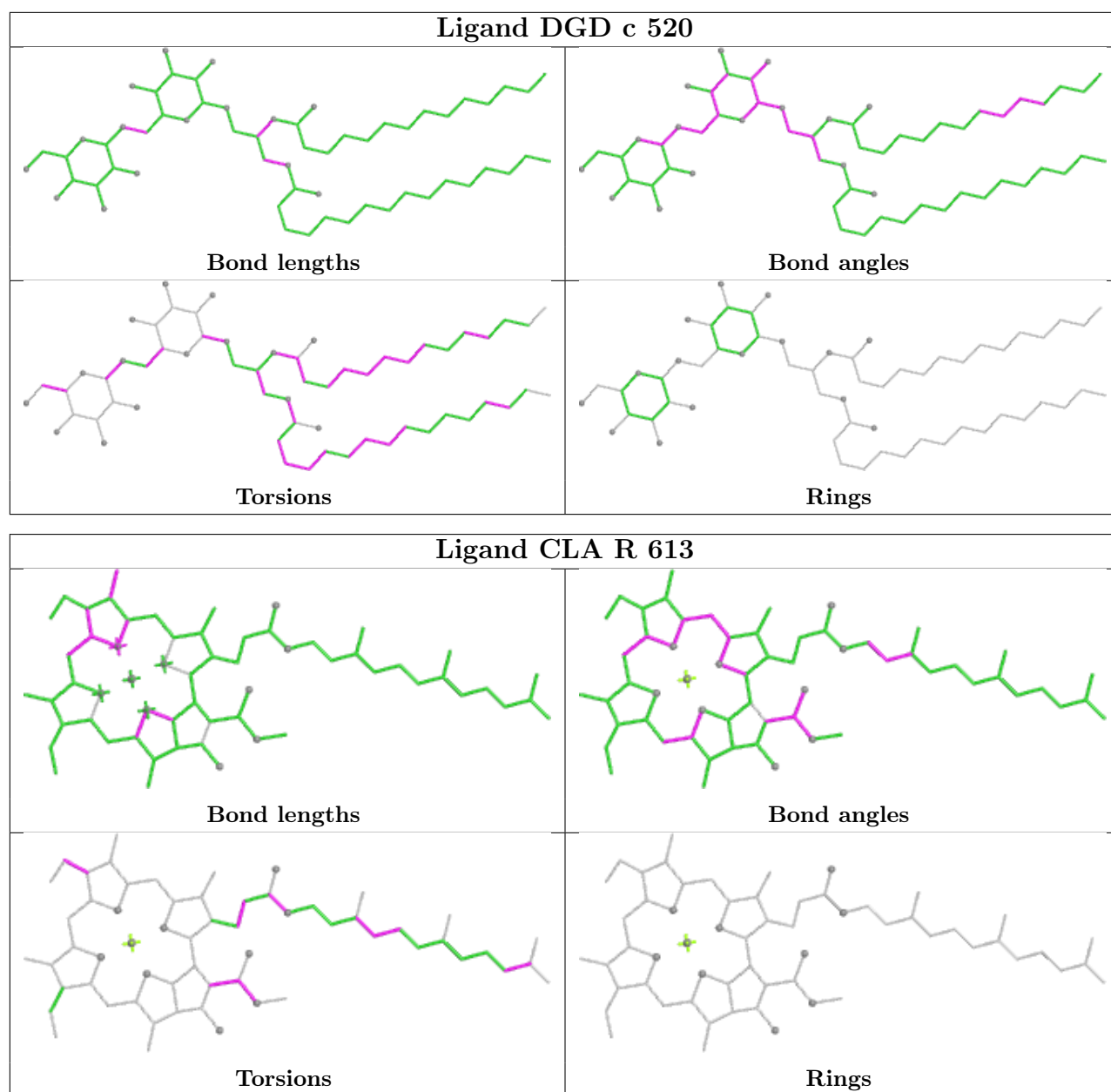
Ligand CLA s 602

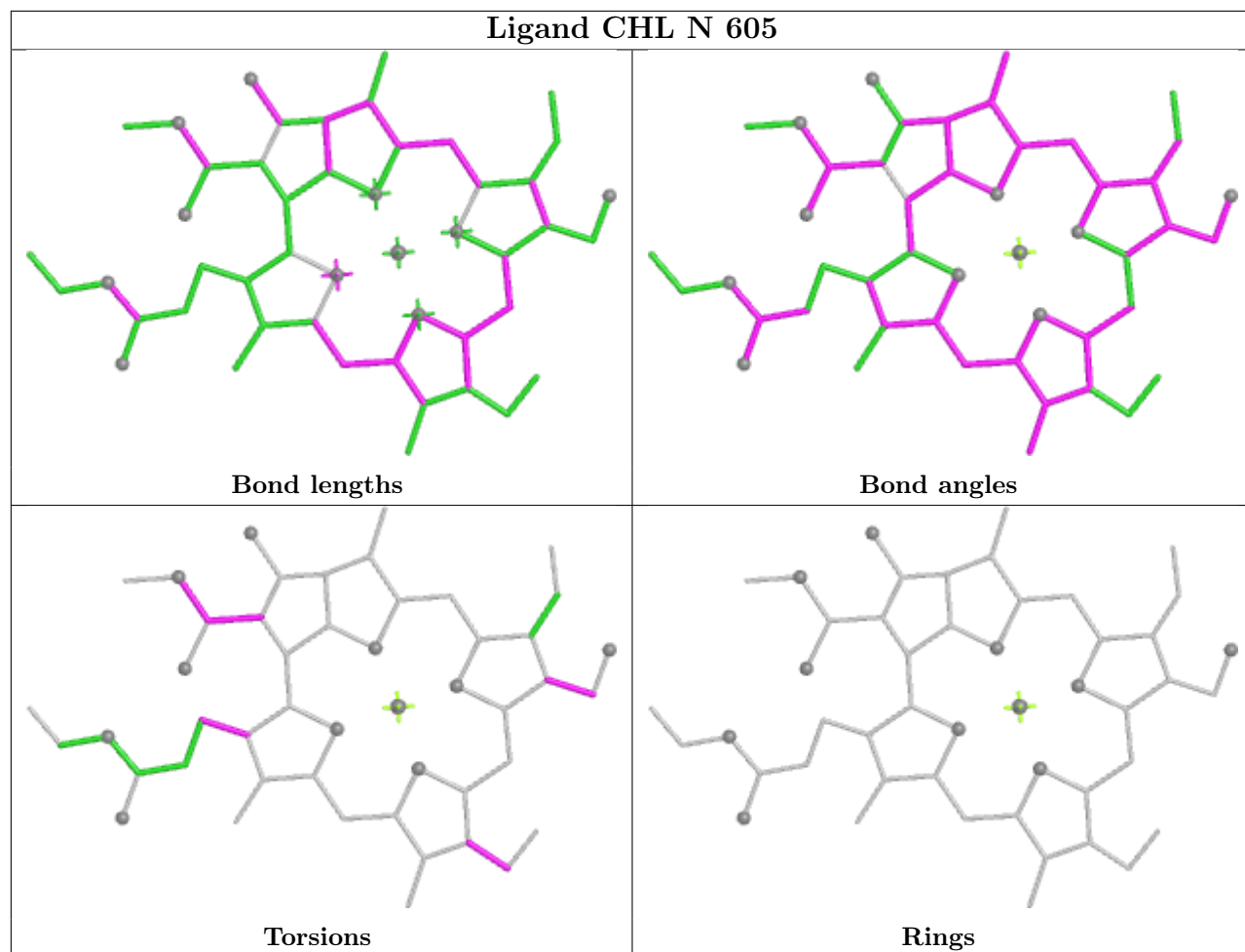


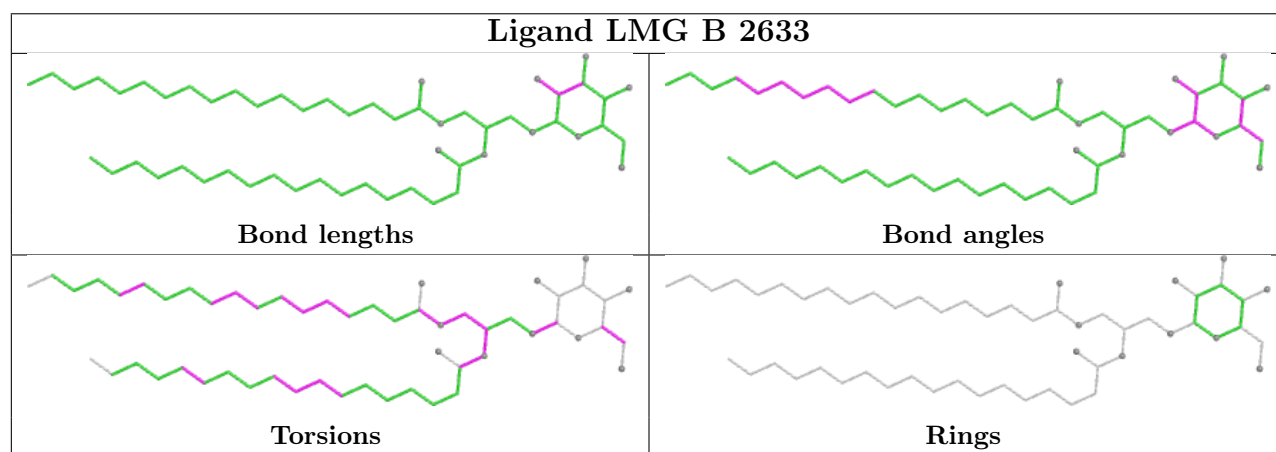
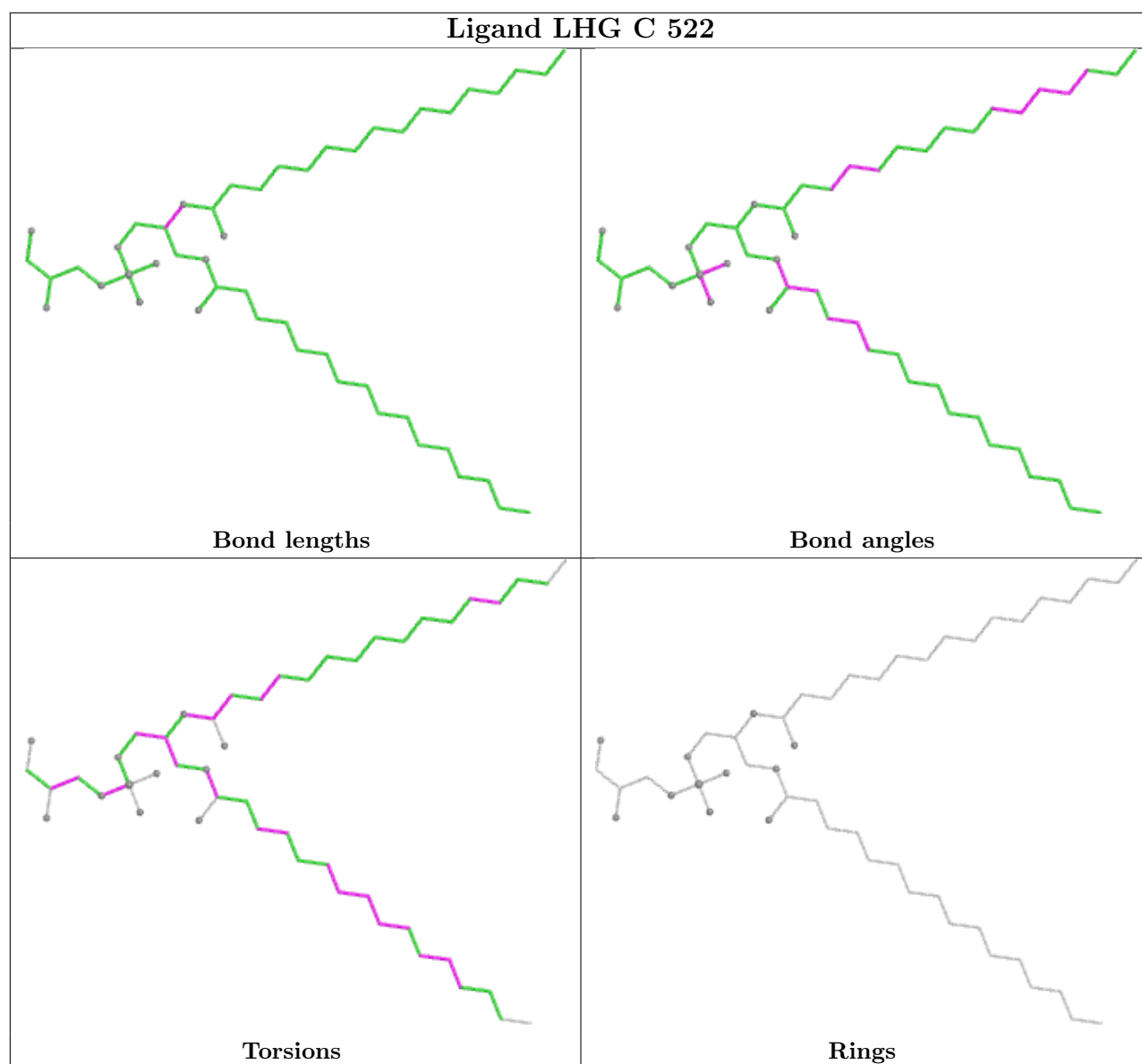


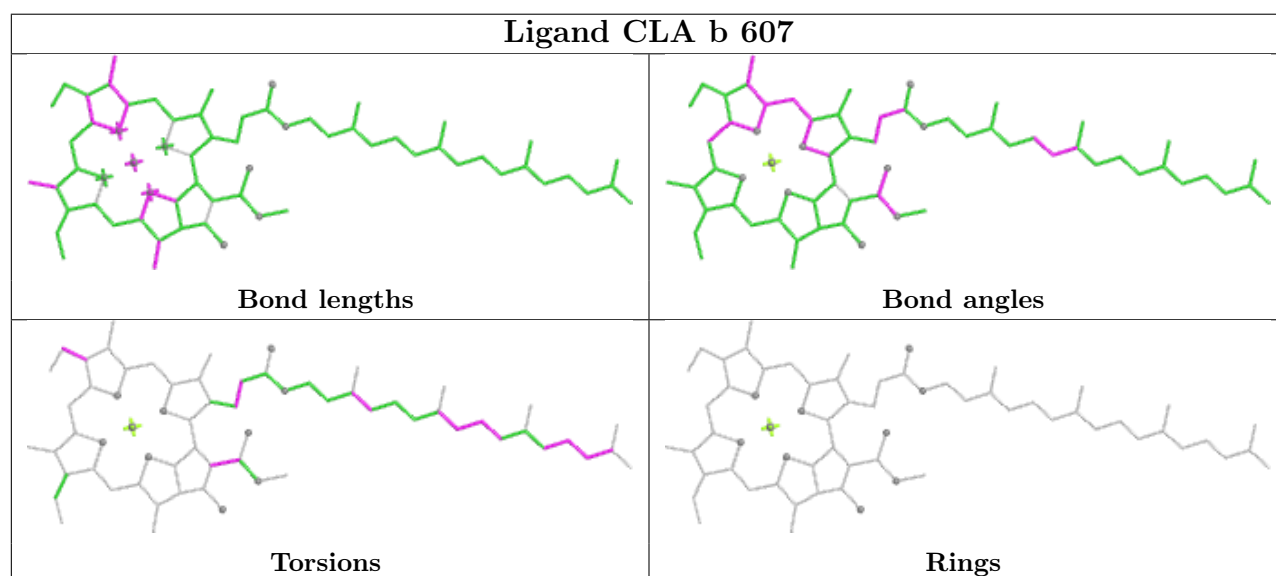
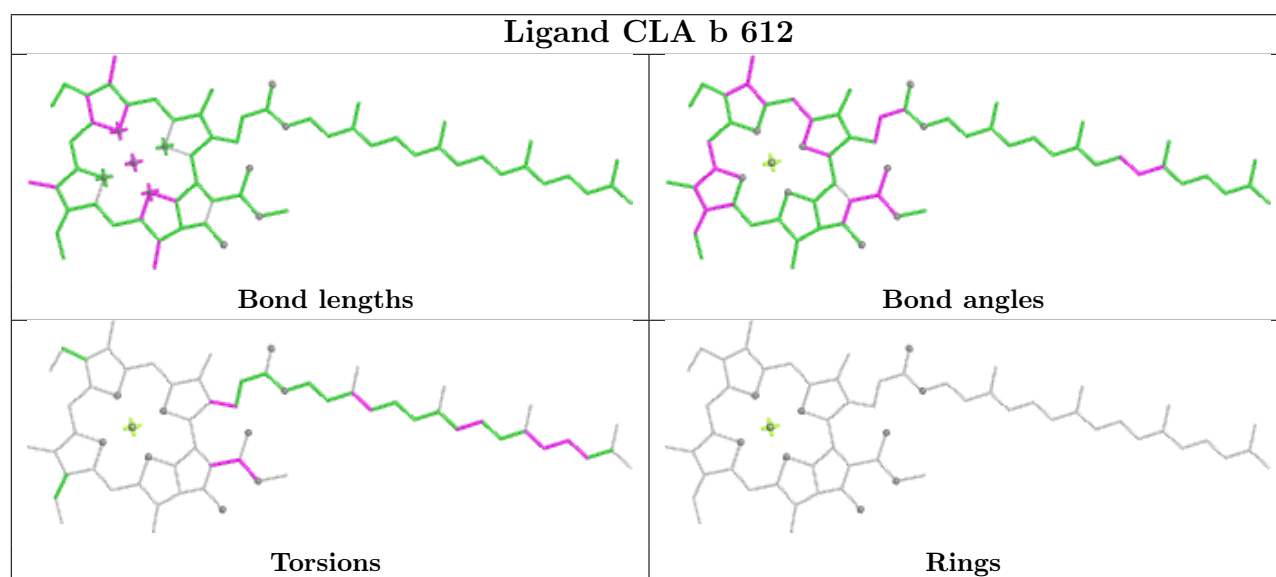
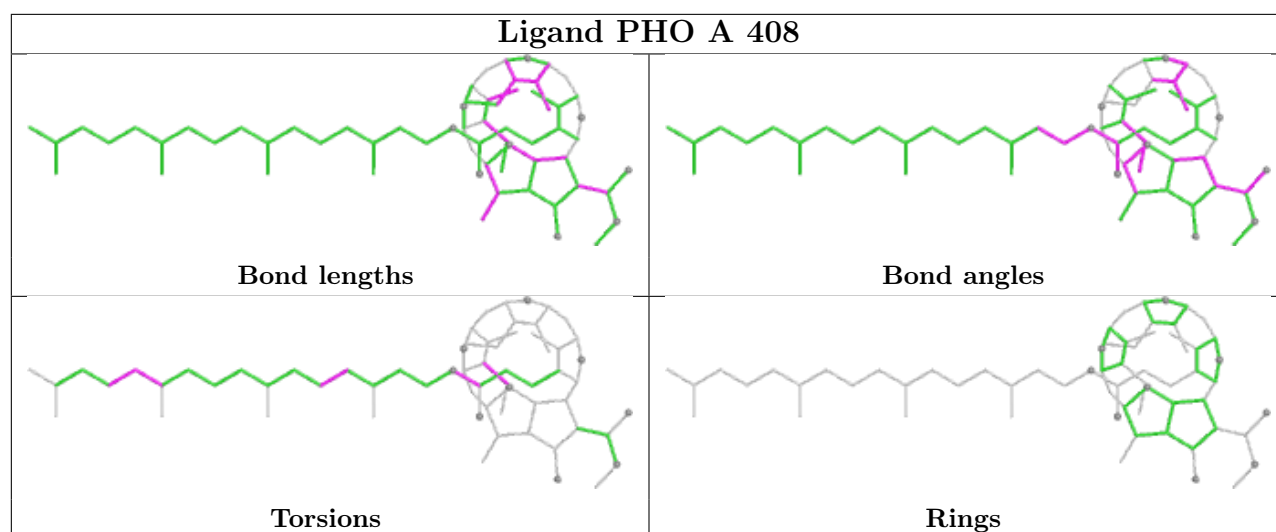


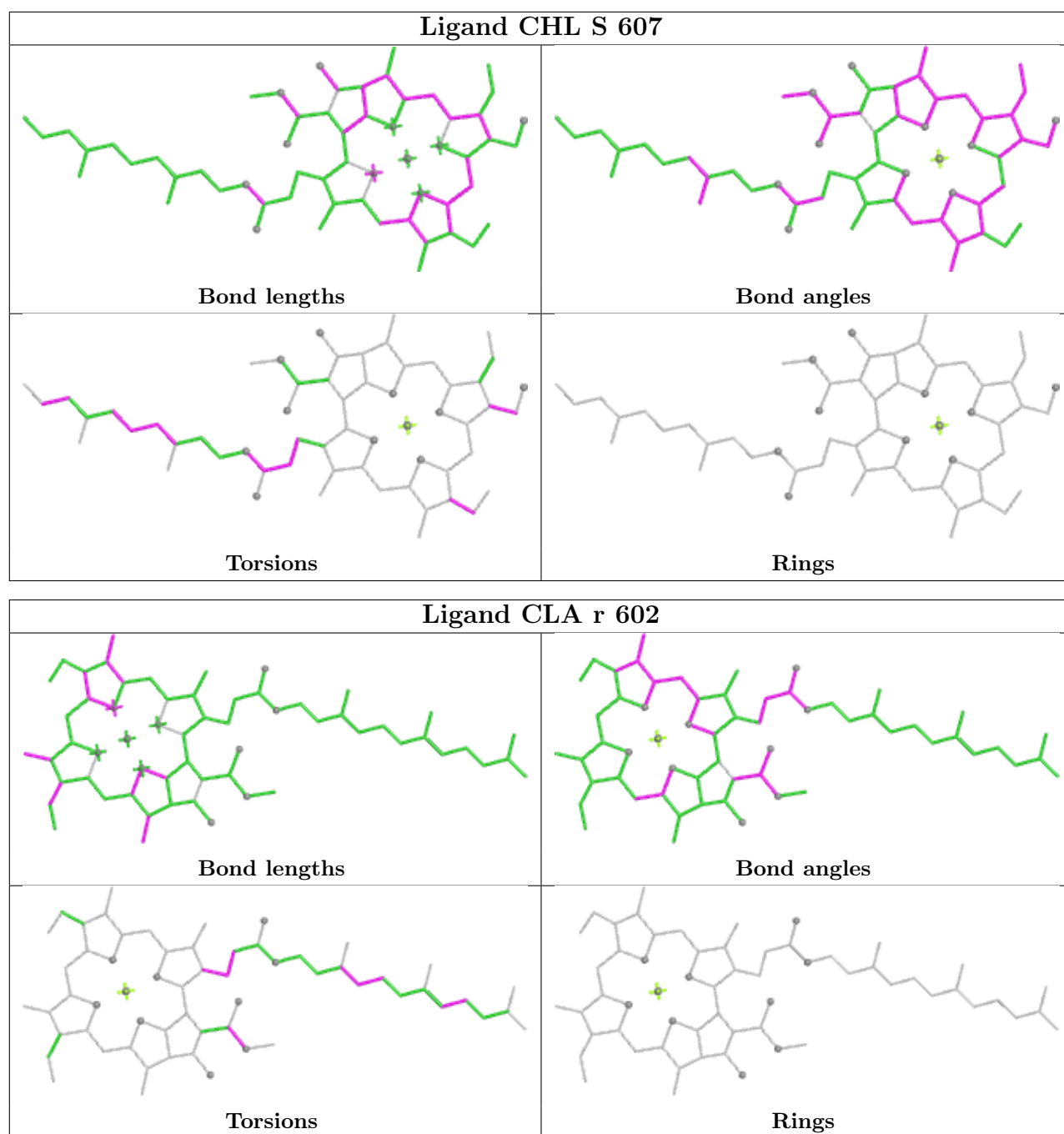


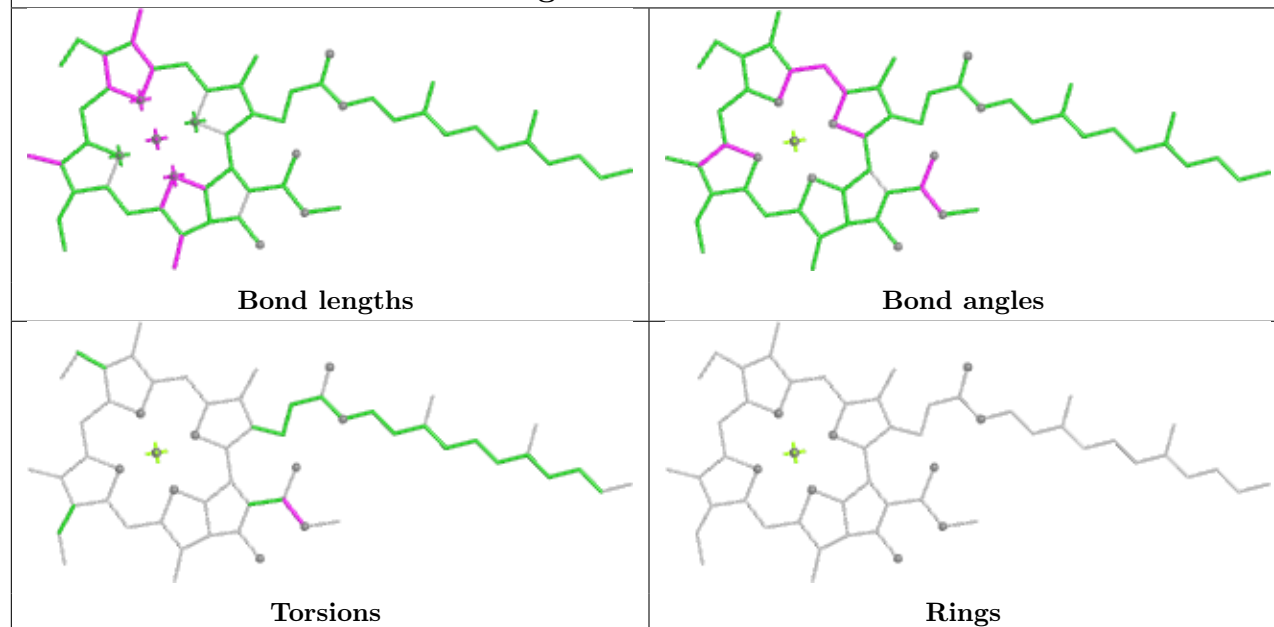
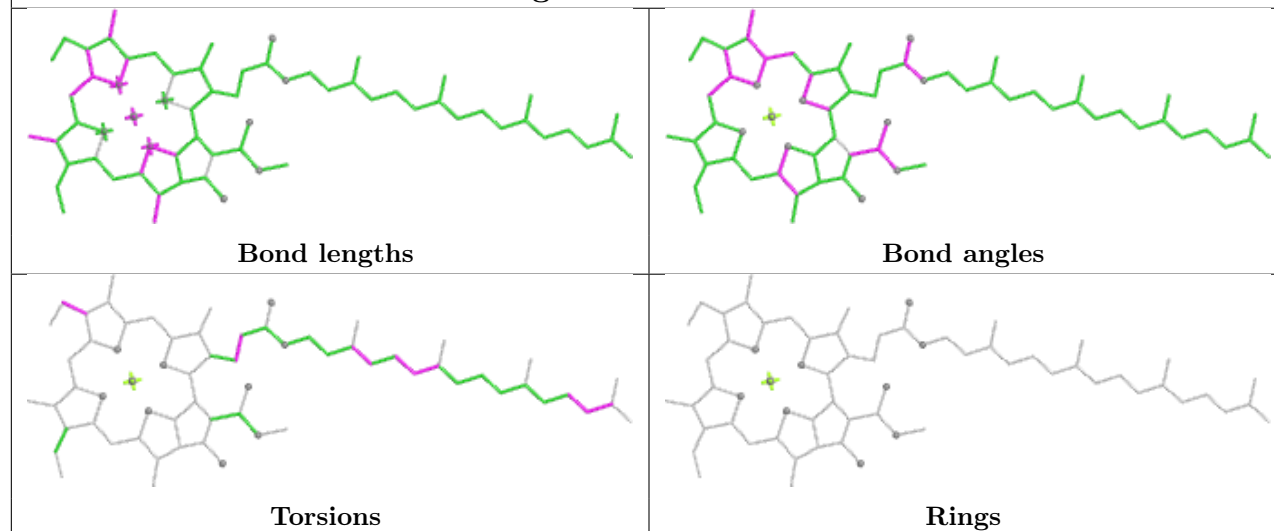




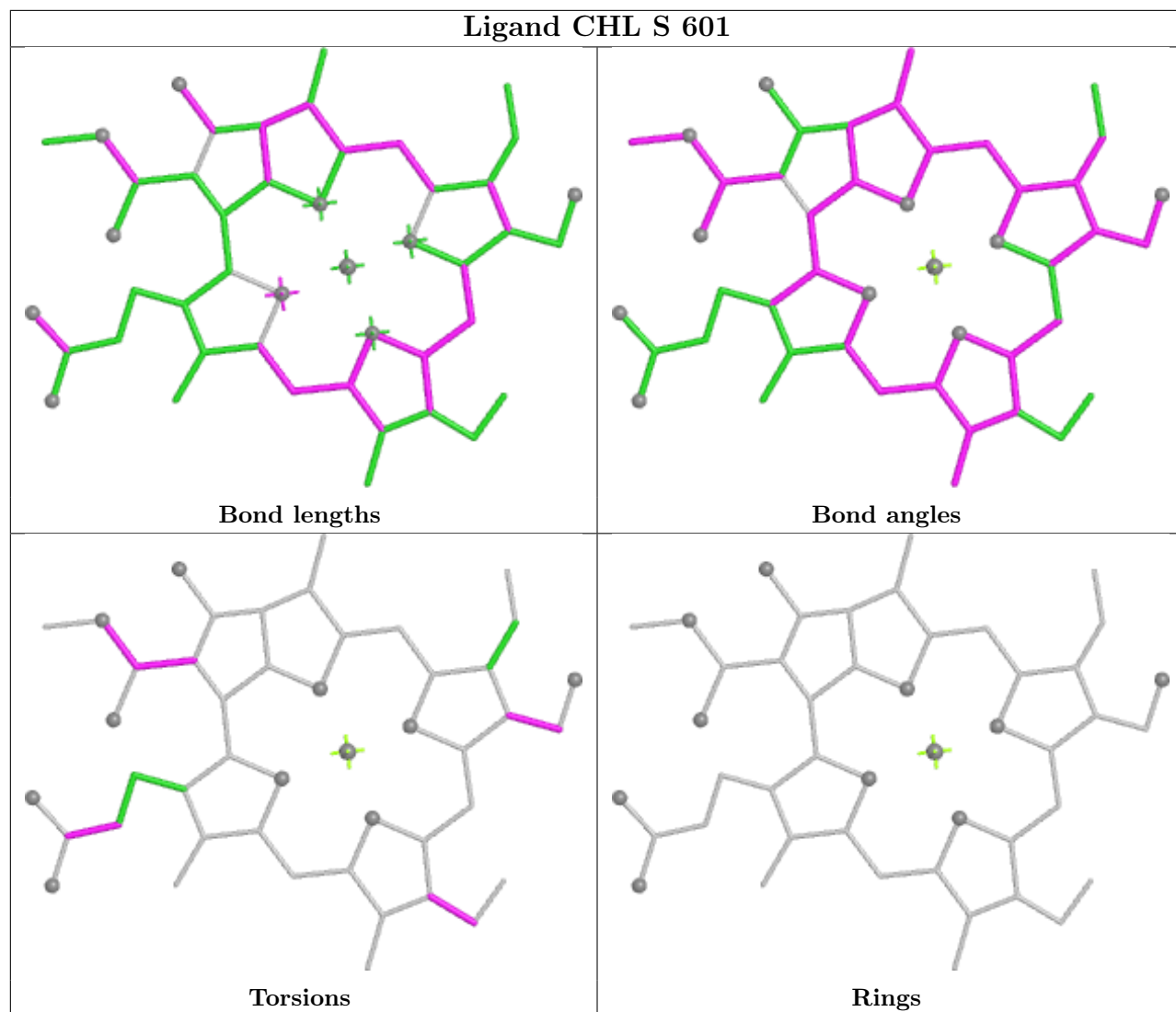


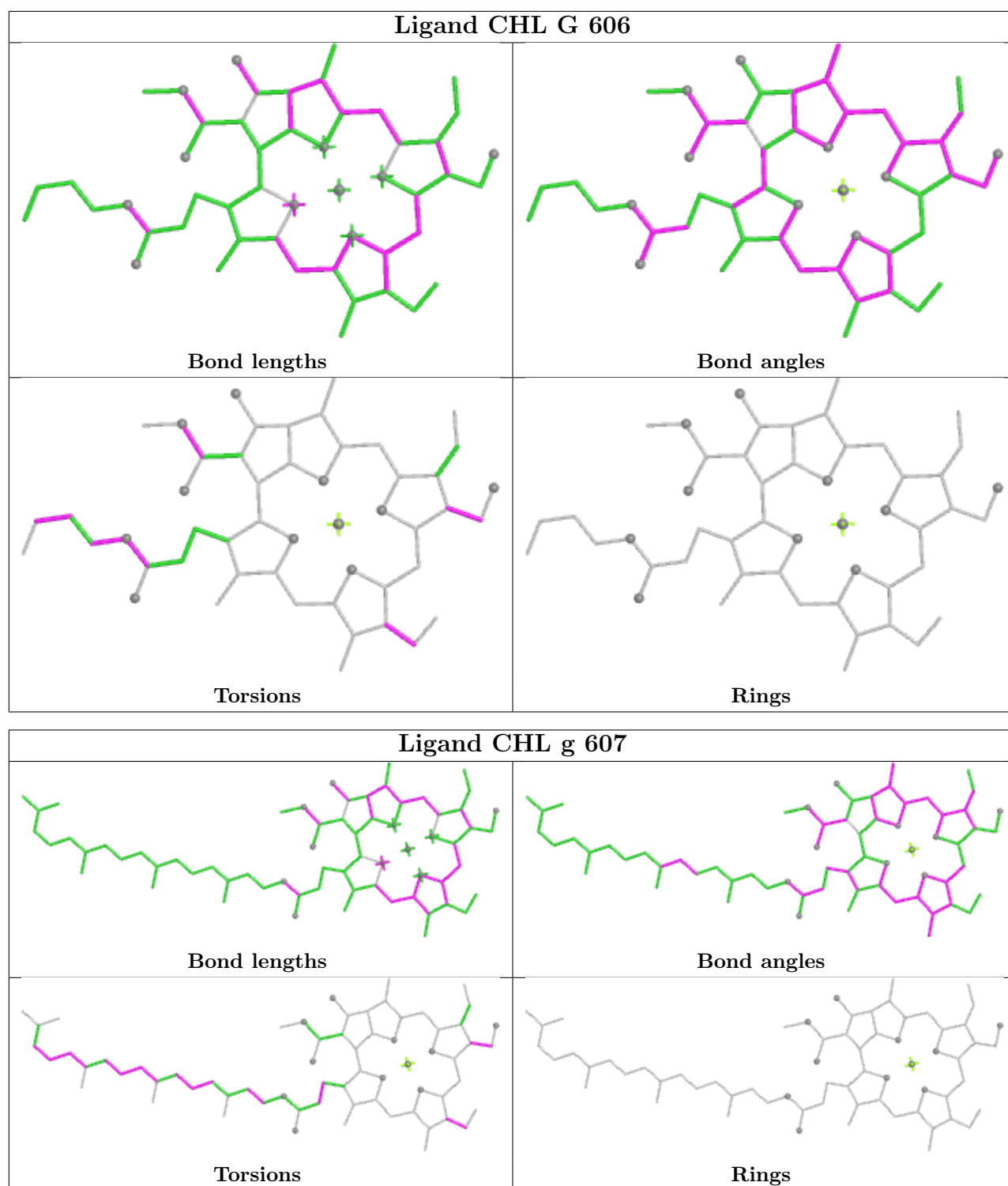




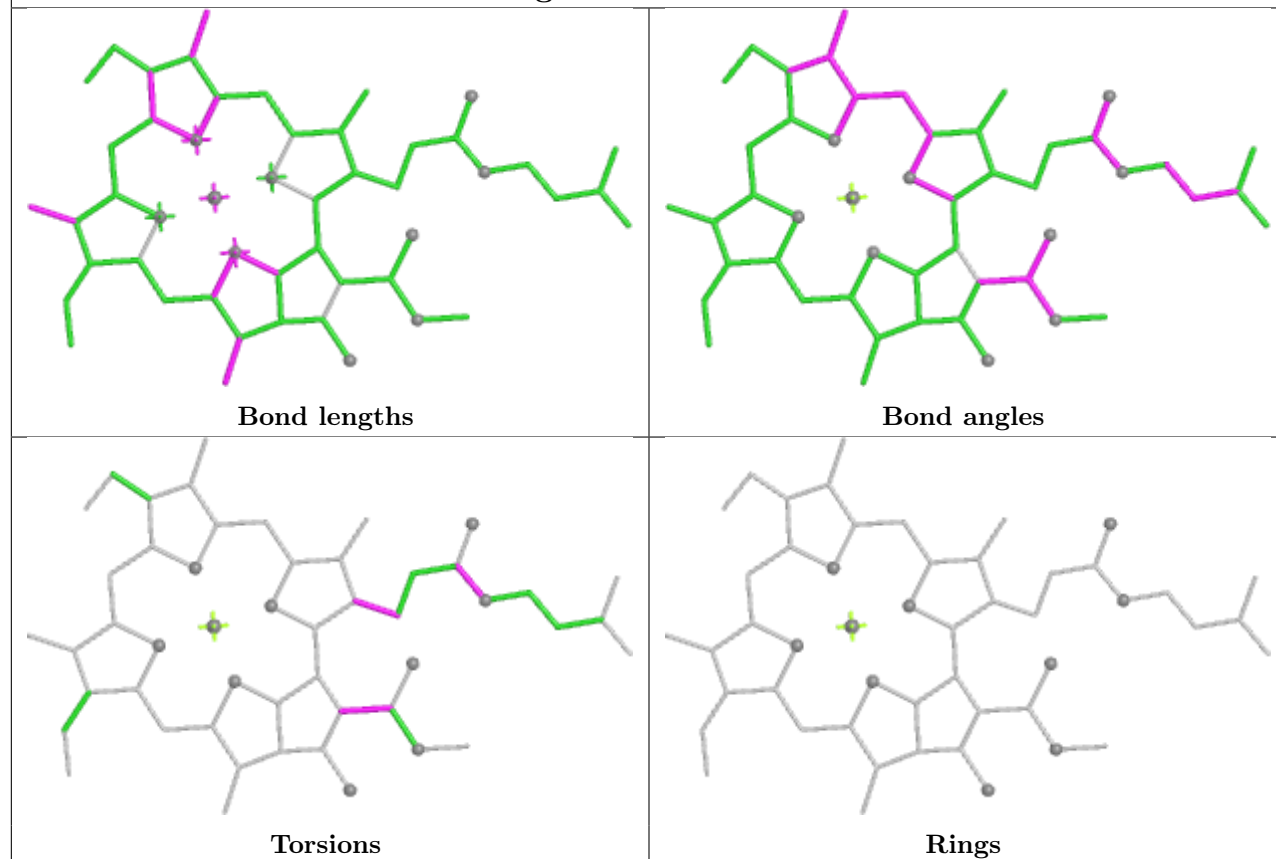
Ligand CLA r 609**Ligand CLA B 604**

Ligand CHL S 601

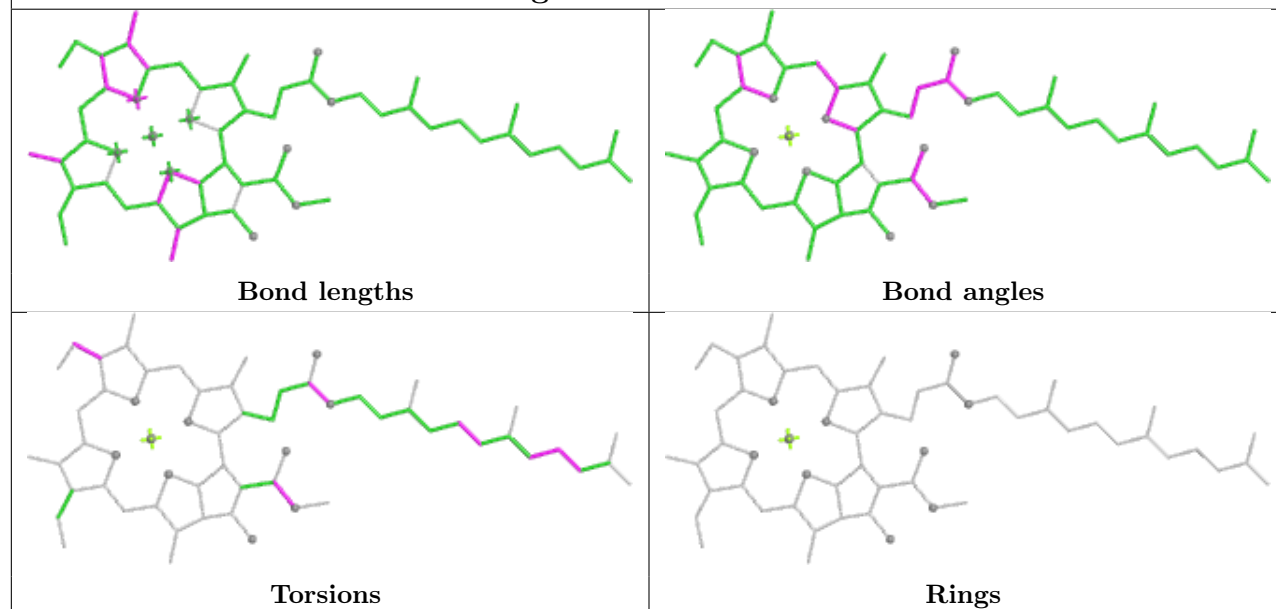


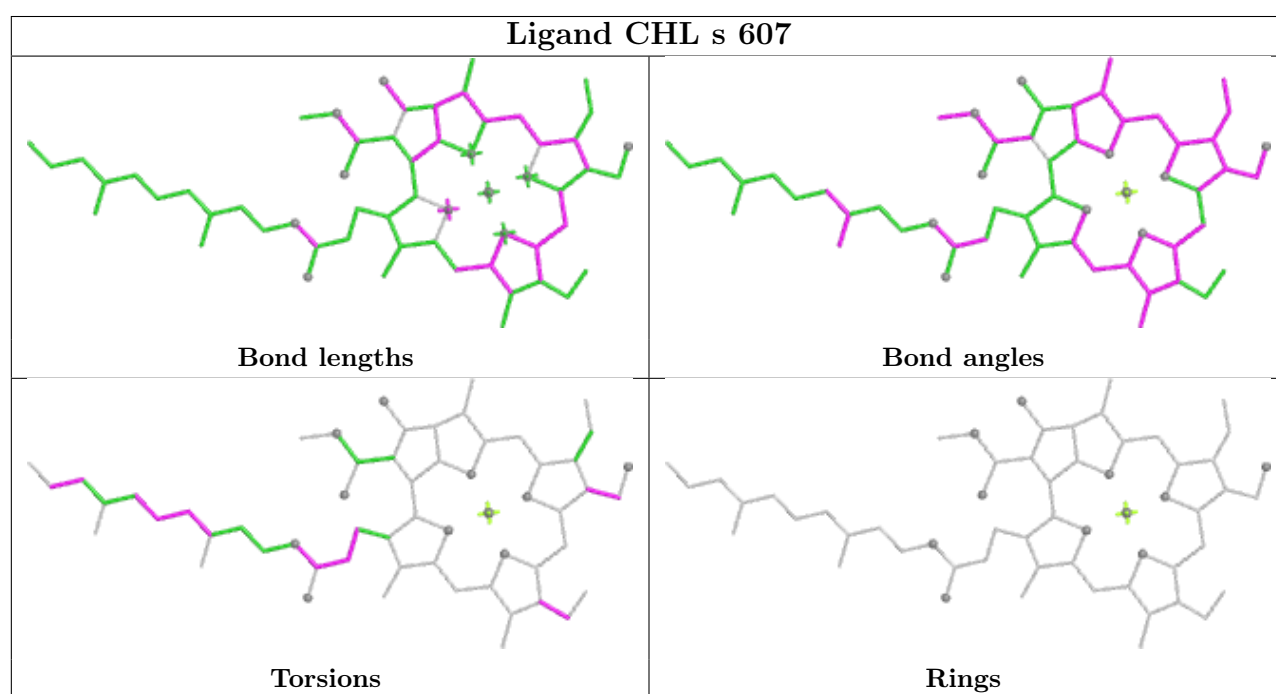
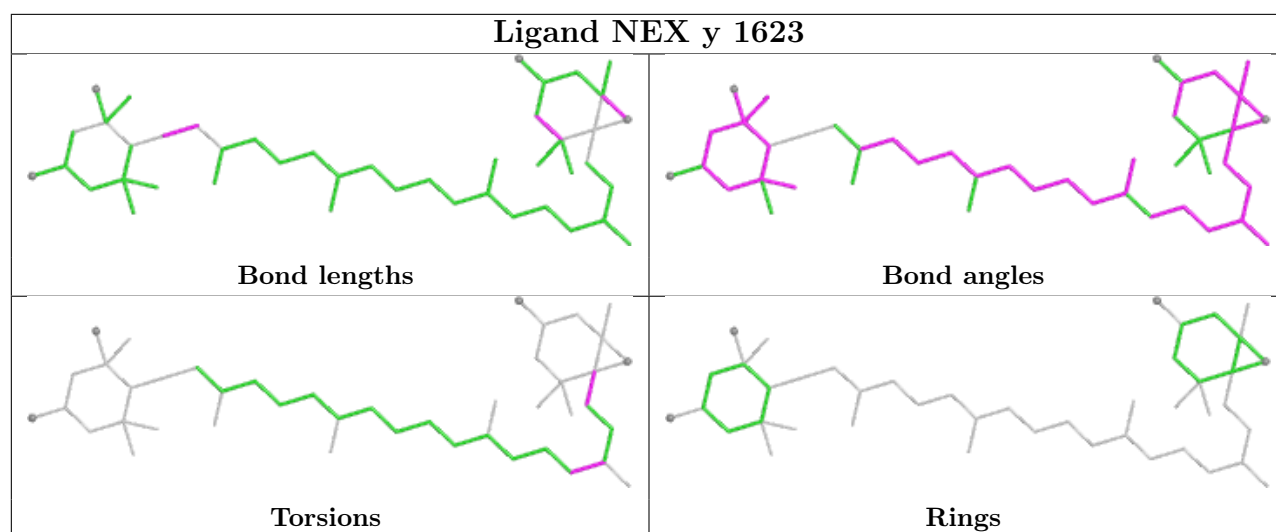


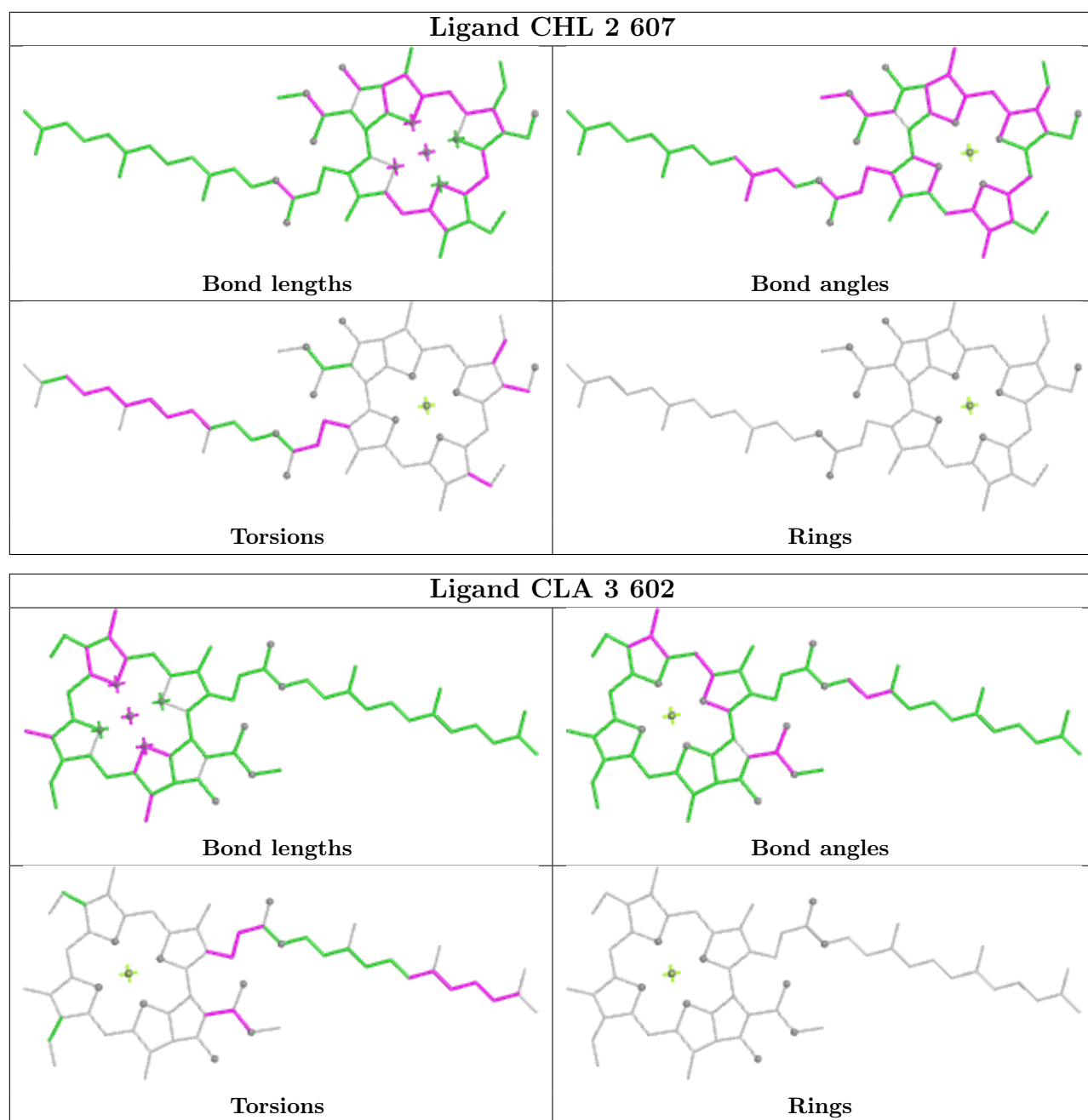
Ligand CLA n 604



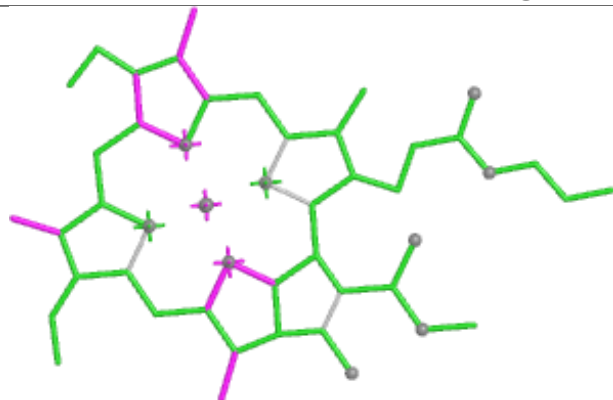
Ligand CLA N 611



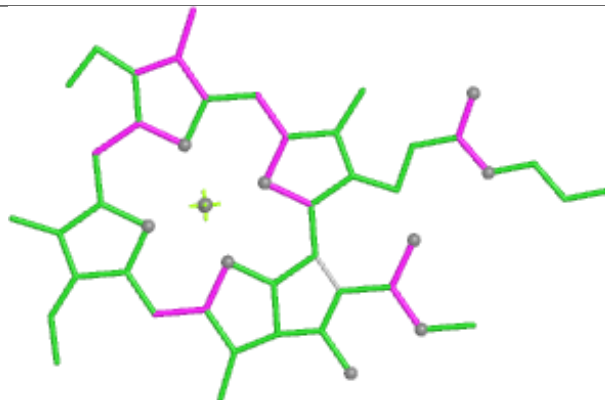




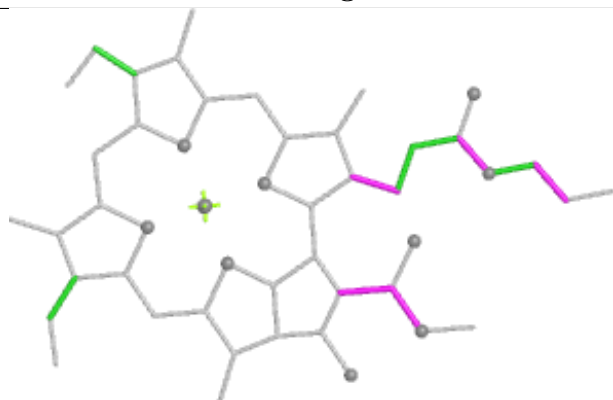
Ligand CLA n 614



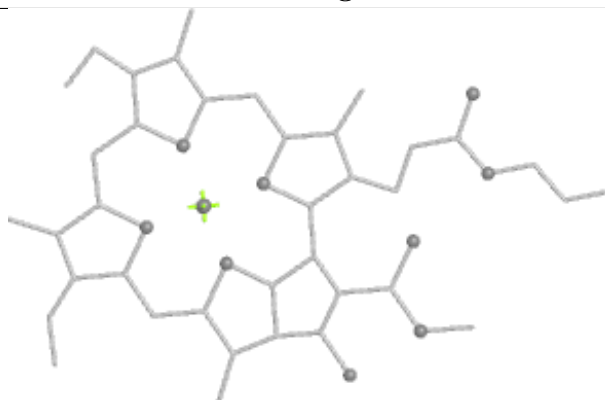
Bond lengths



Bond angles

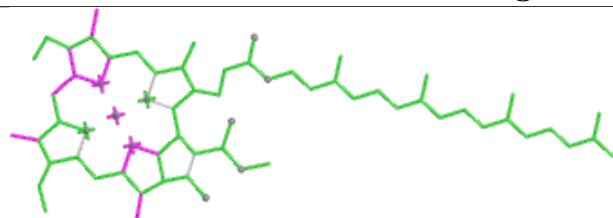


Torsions

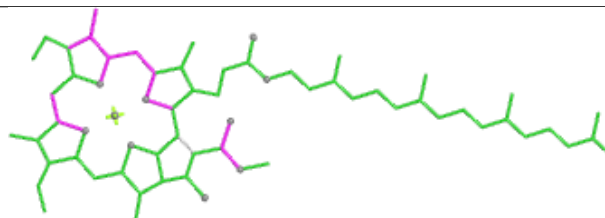


Rings

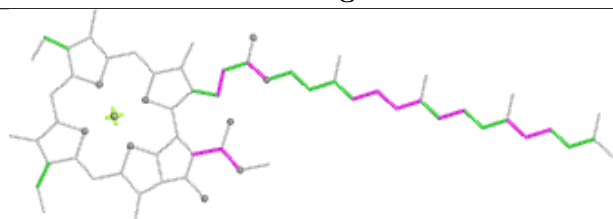
Ligand CLA B 608



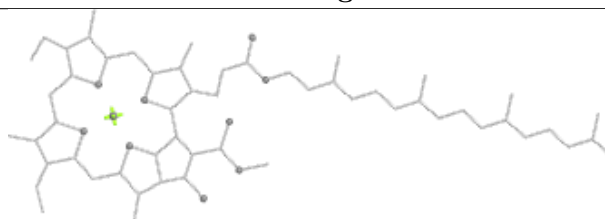
Bond lengths



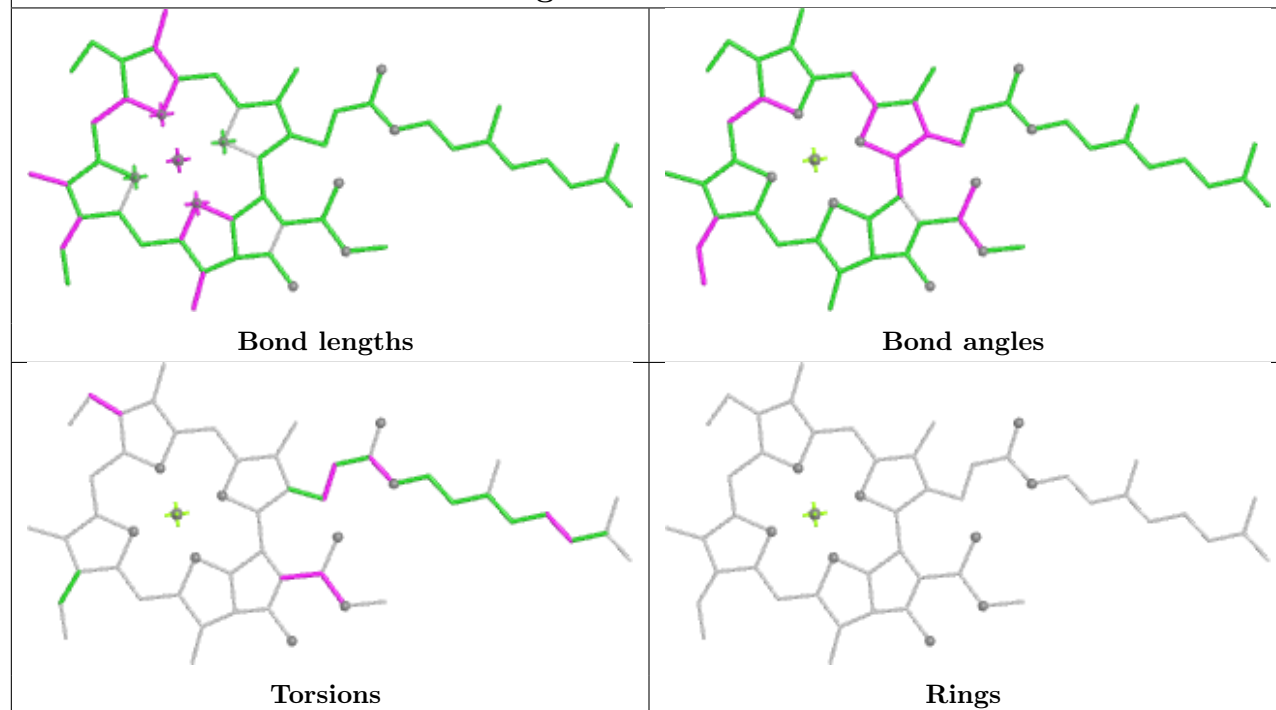
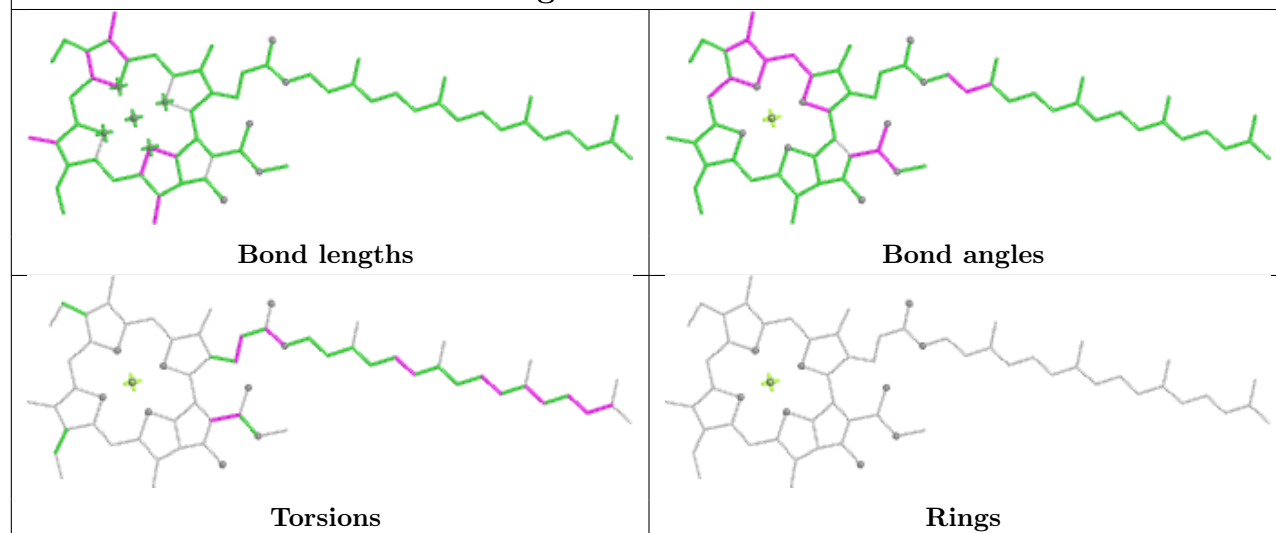
Bond angles



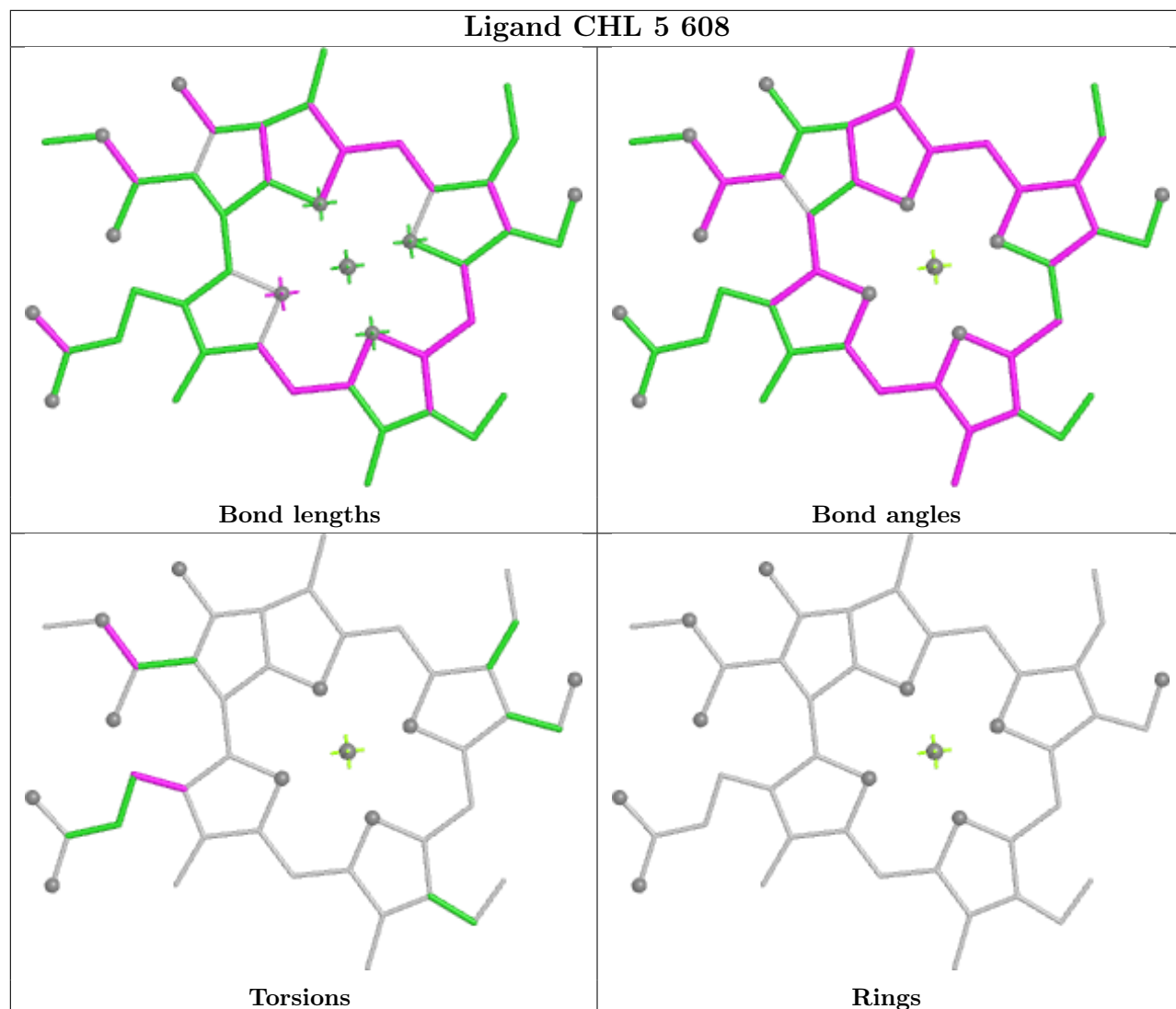
Torsions



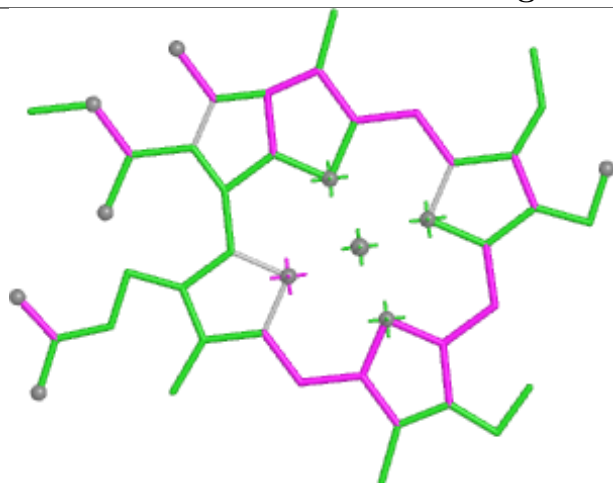
Rings

Ligand CLA 3 603**Ligand CLA c 505**

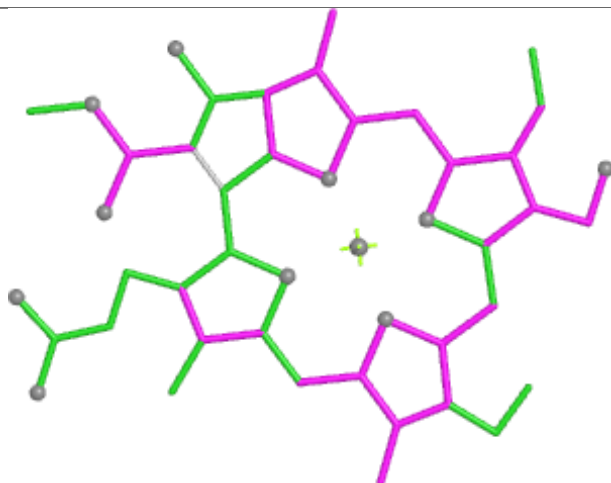
Ligand CHL 5 608



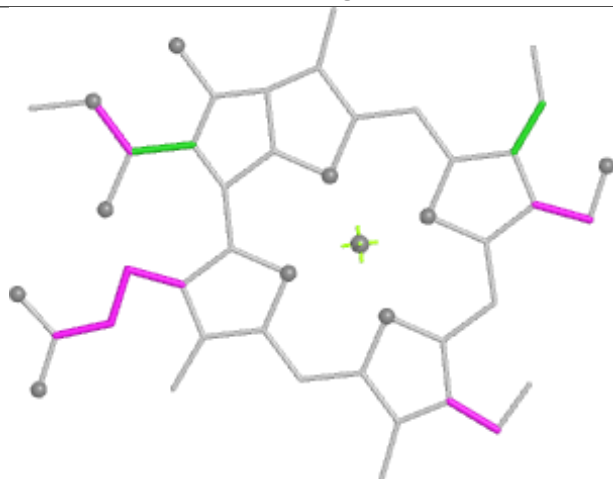
Ligand CHL 2 605



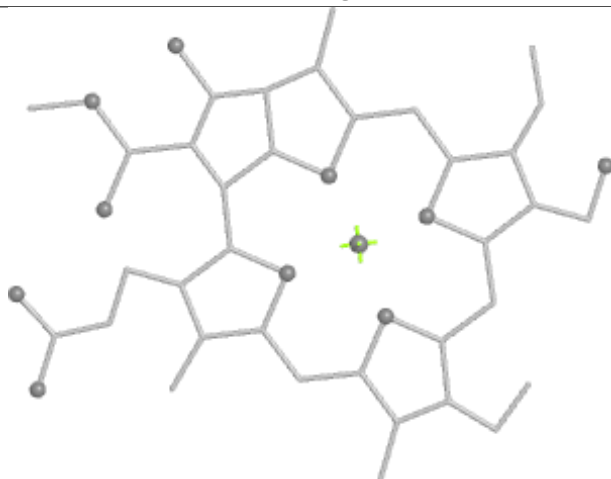
Bond lengths



Bond angles

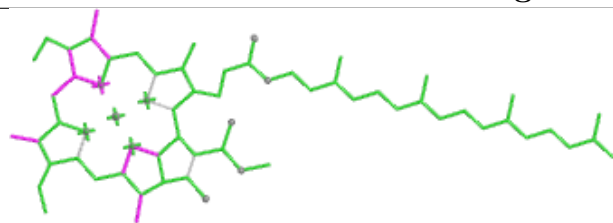


Torsions

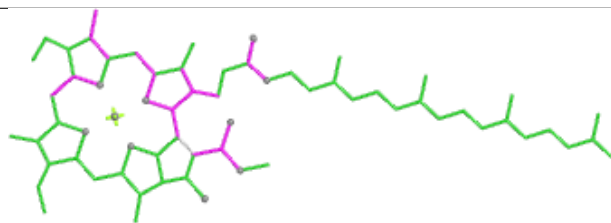


Rings

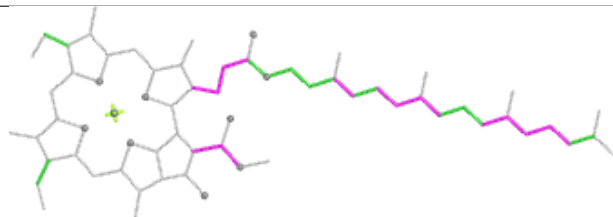
Ligand CLA C 507



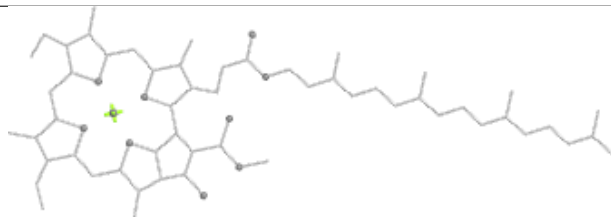
Bond lengths



Bond angles

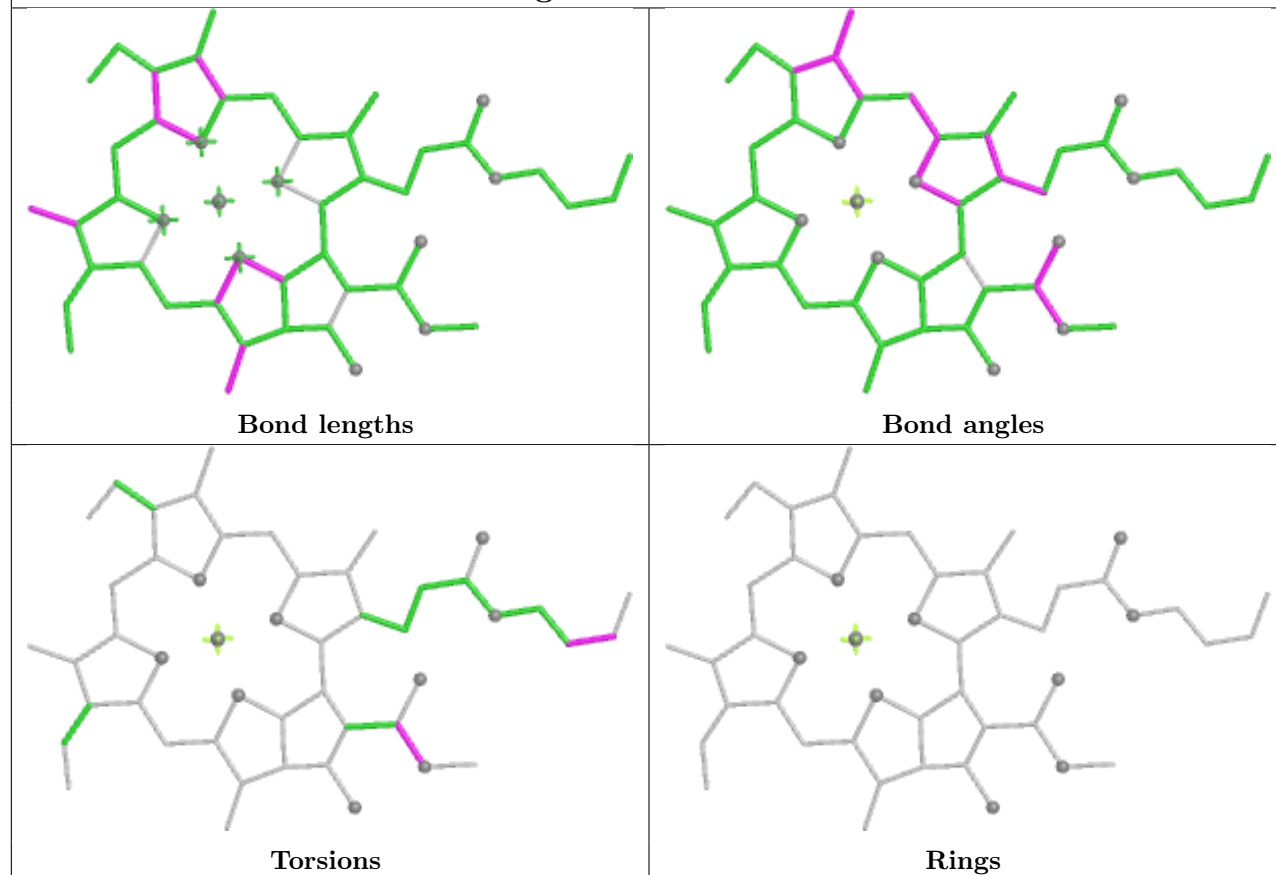


Torsions

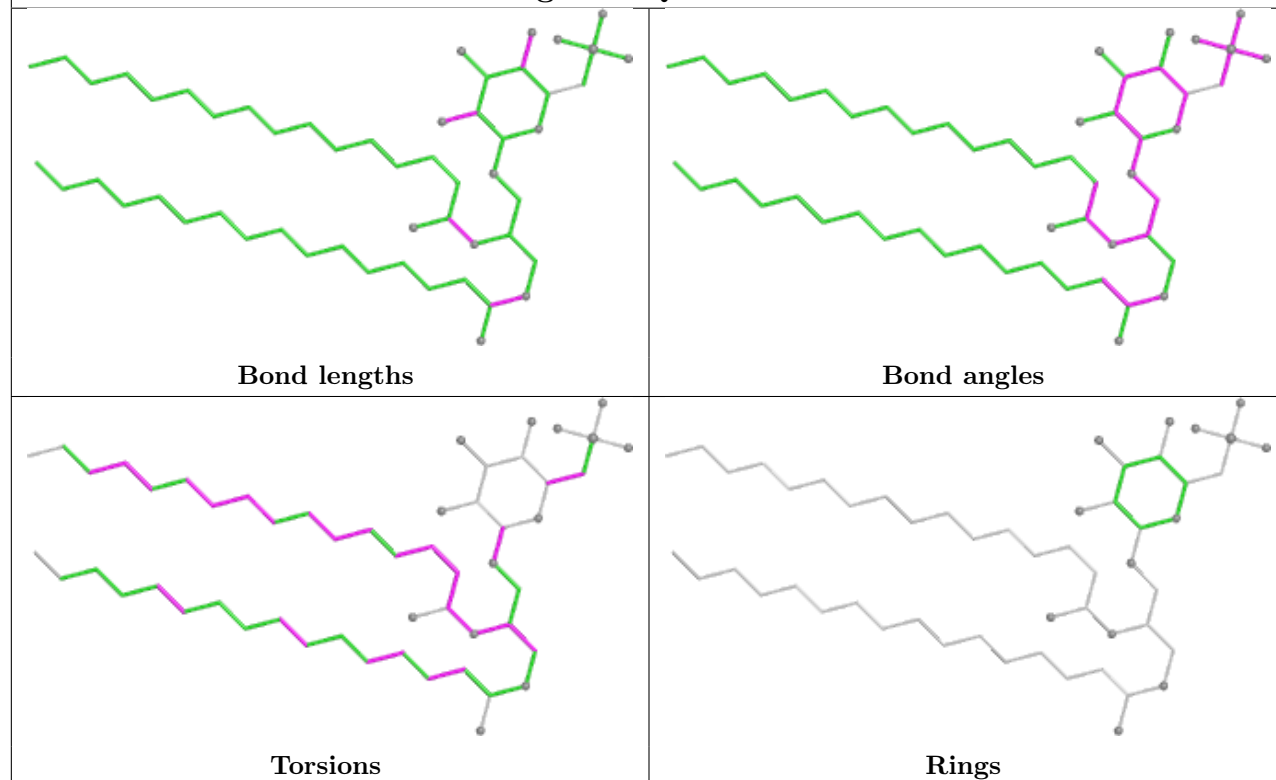


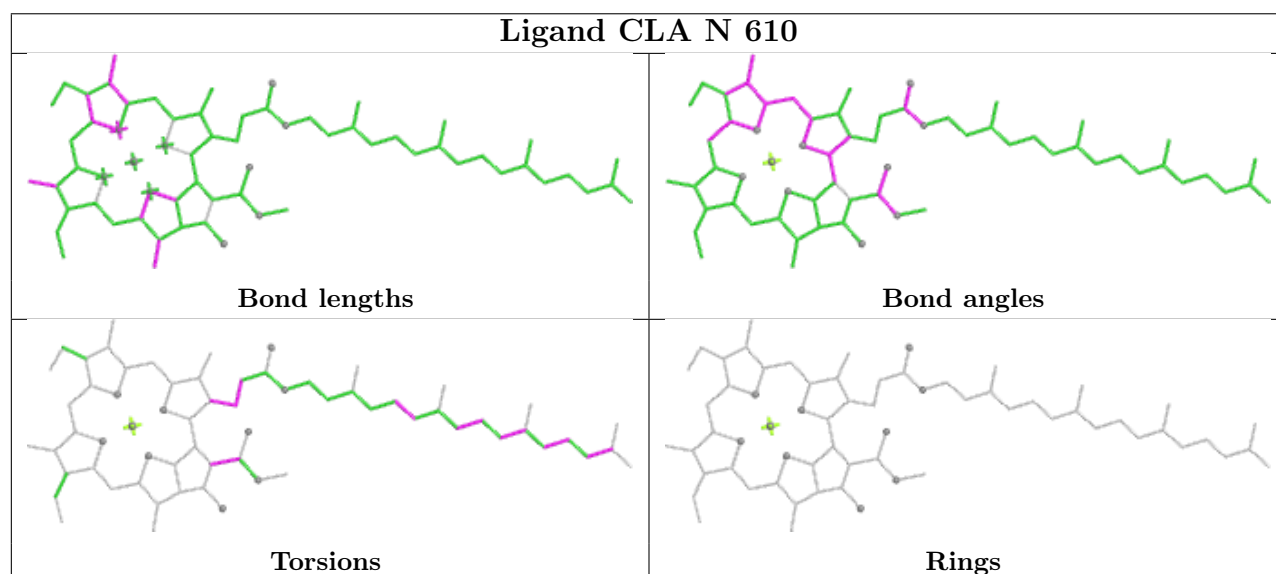
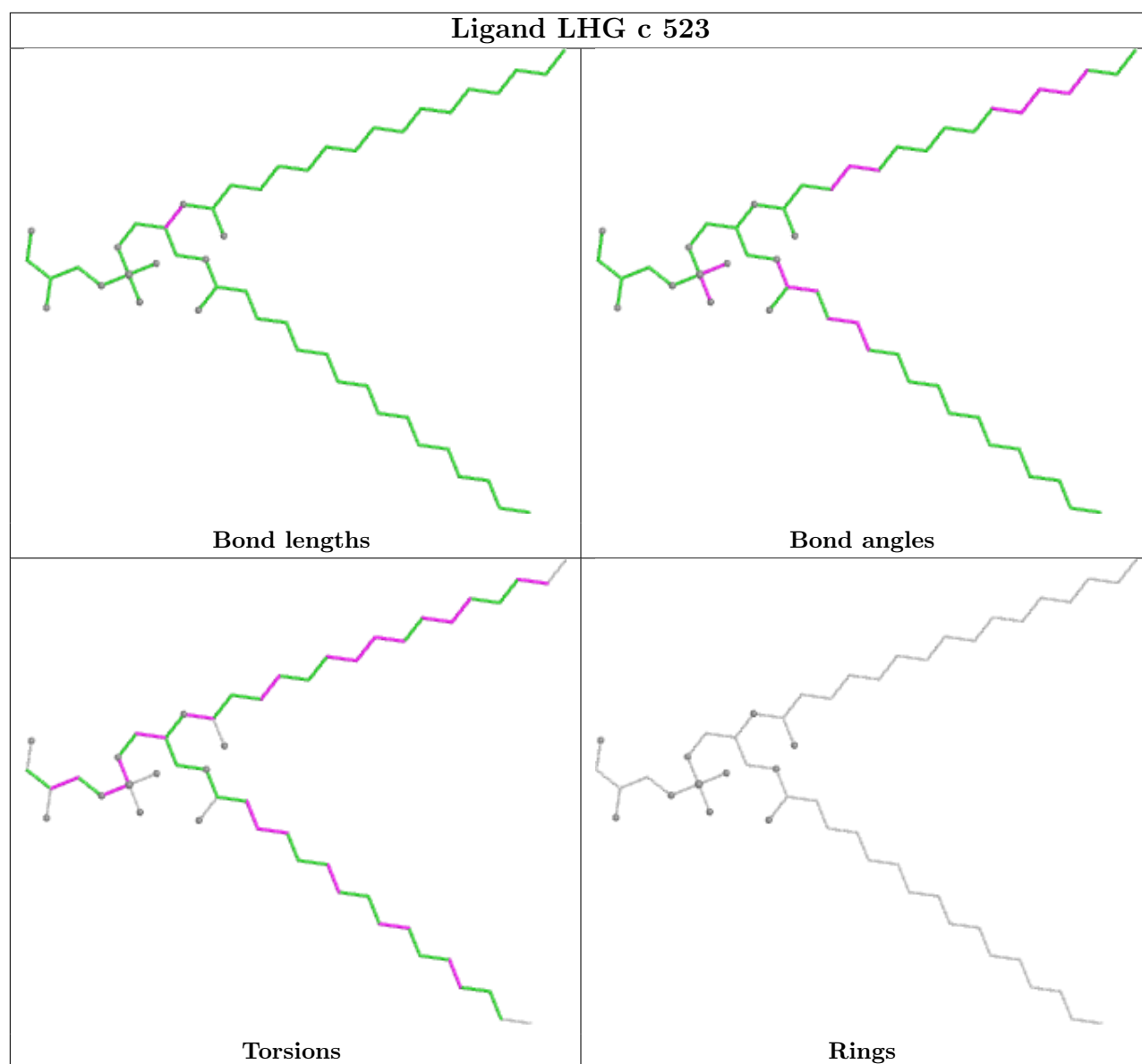
Rings

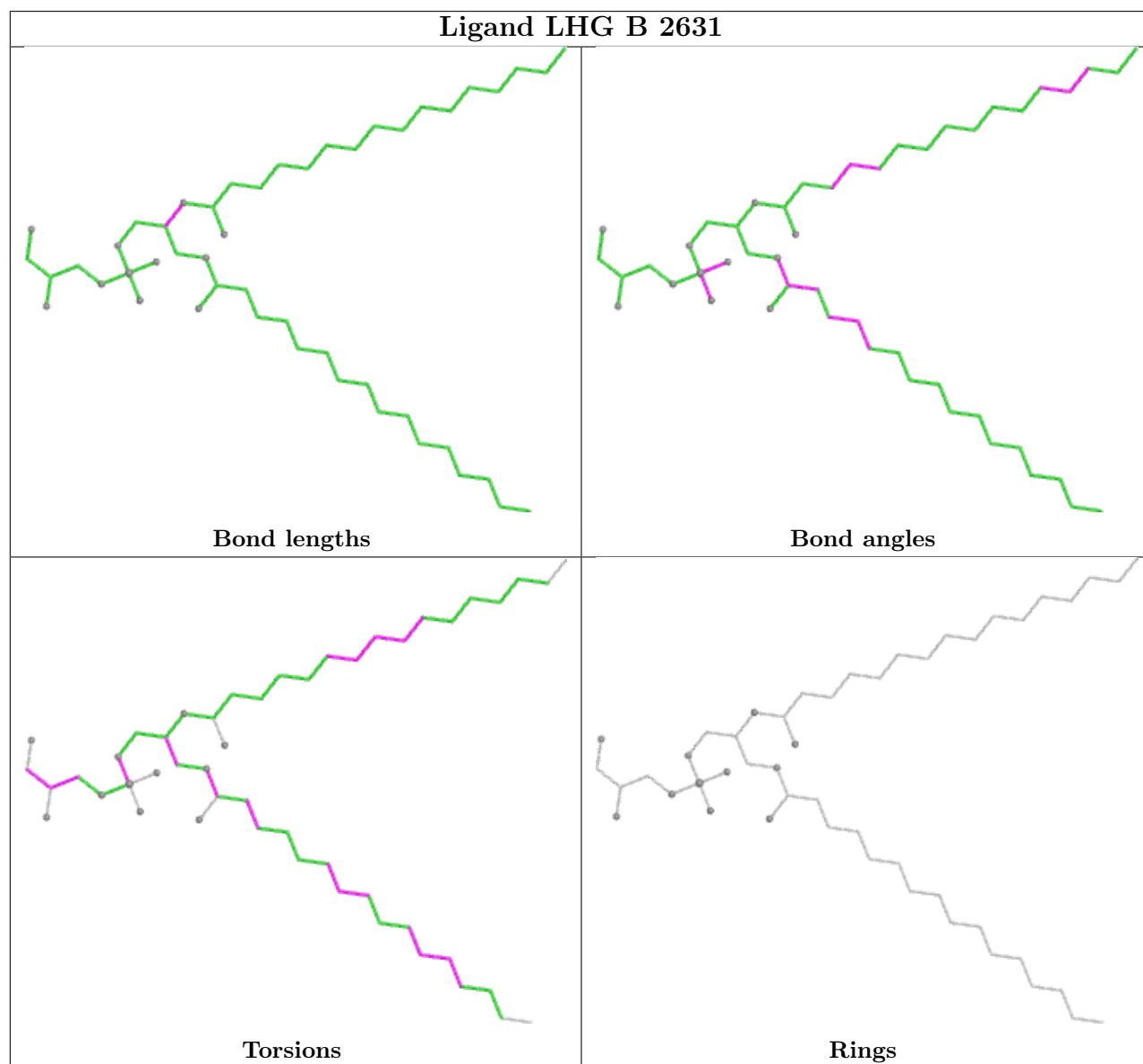
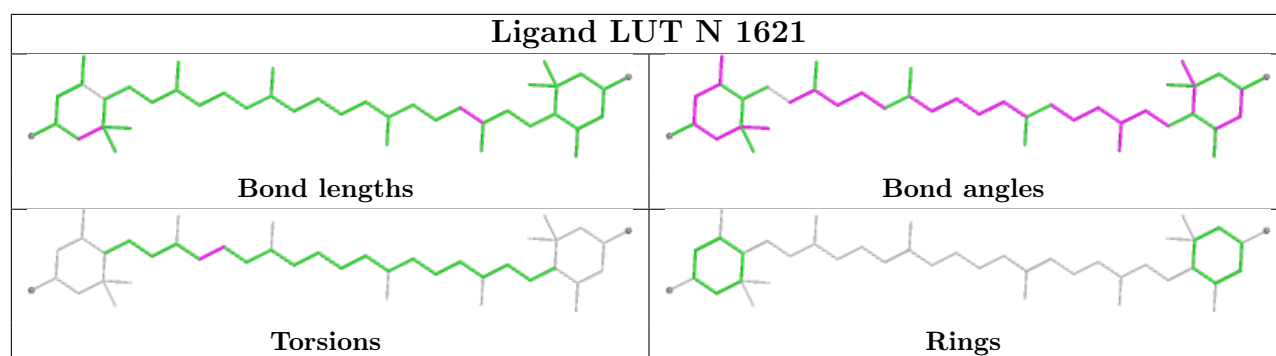
Ligand CLA S 612



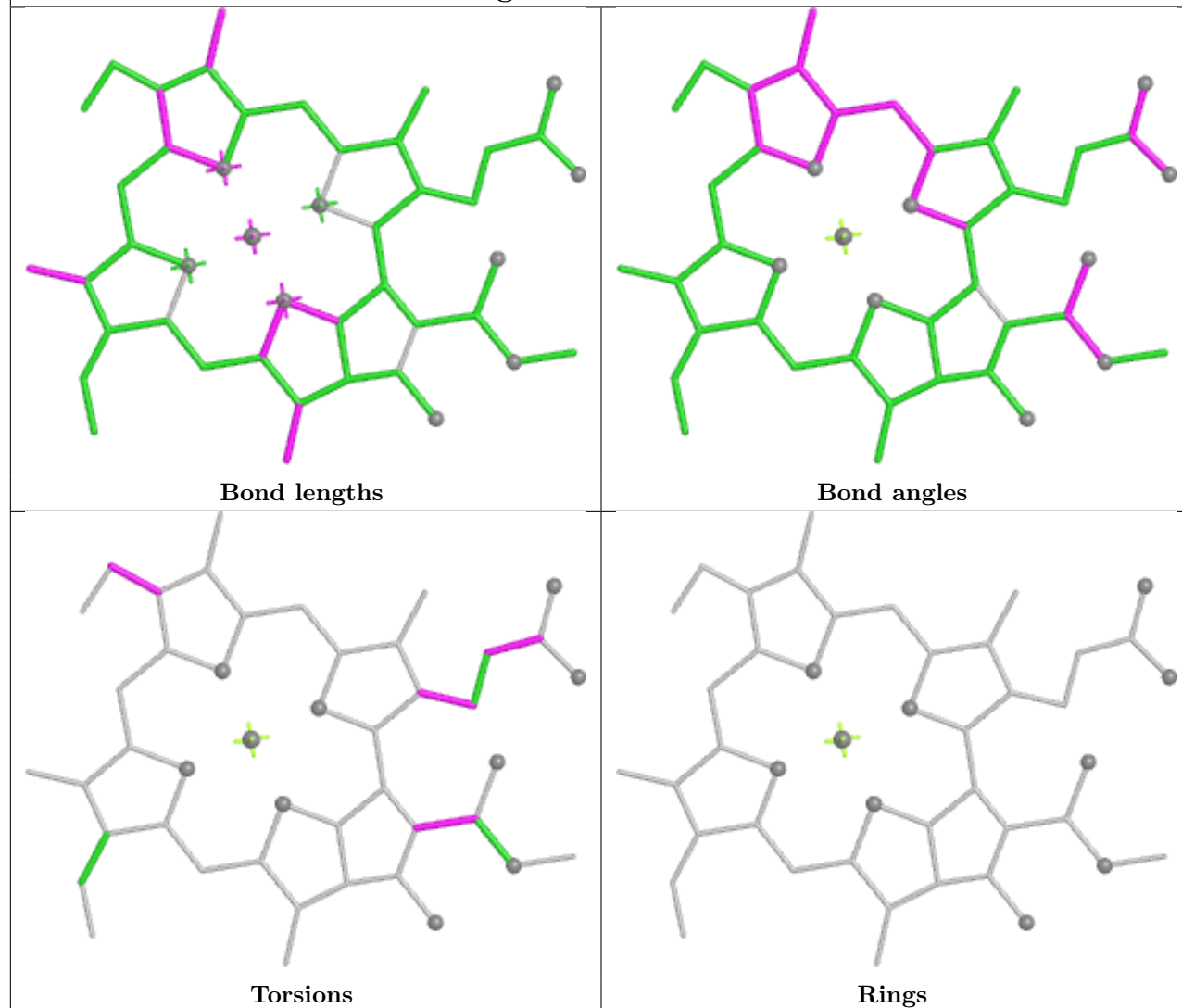
Ligand SQD a 418



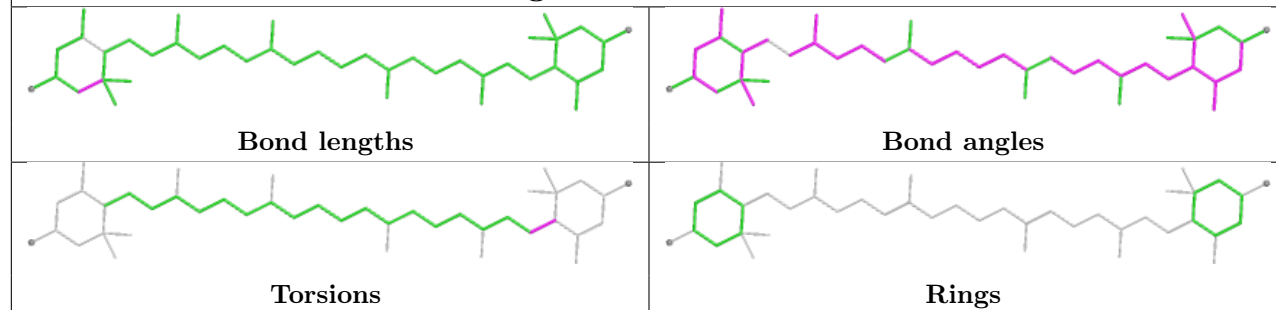


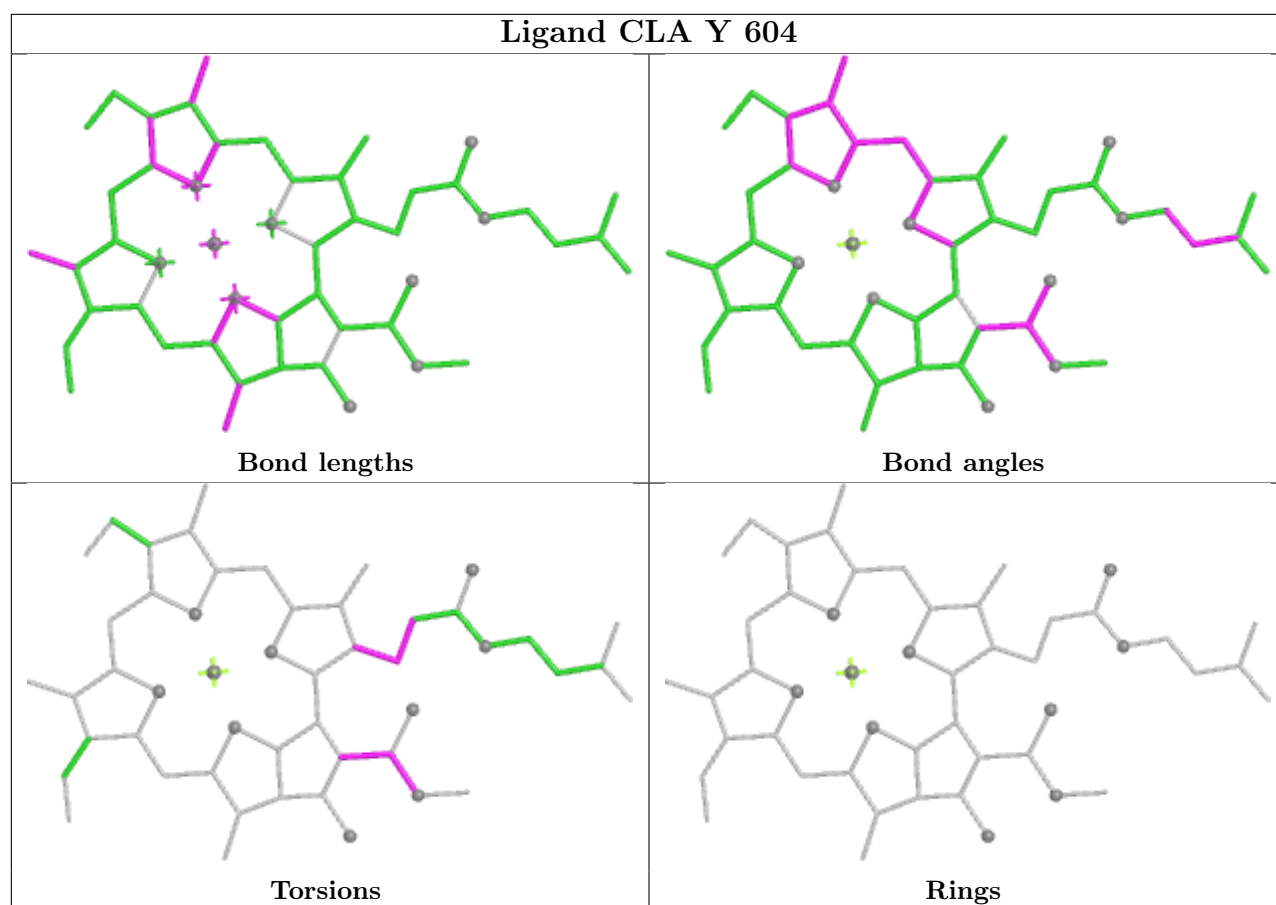


Ligand CLA 4 610

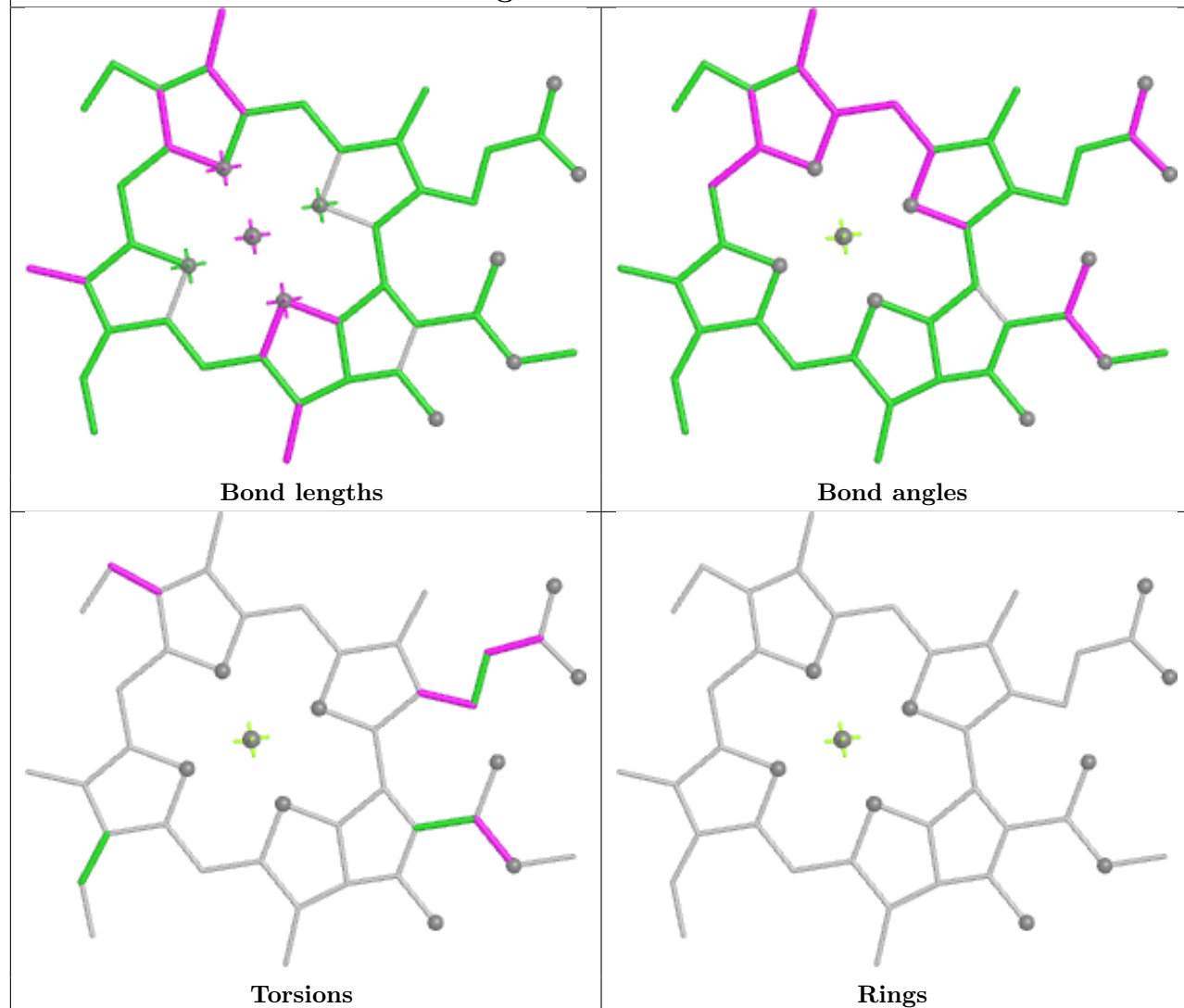


Ligand LUT 6 1621

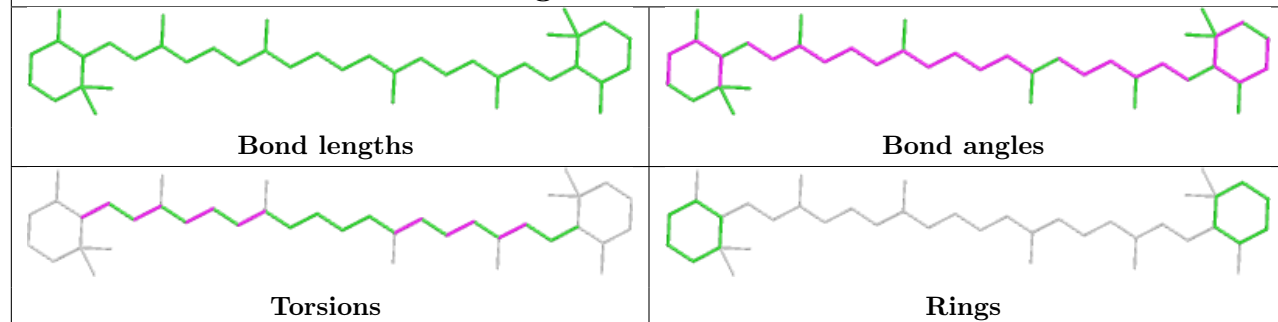


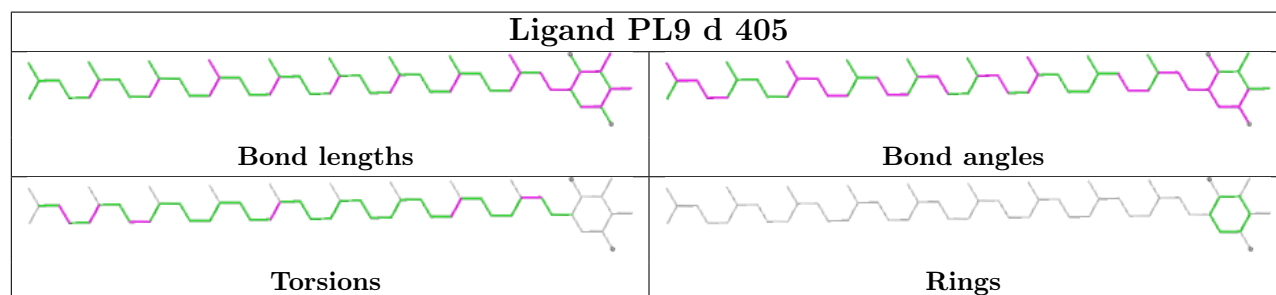
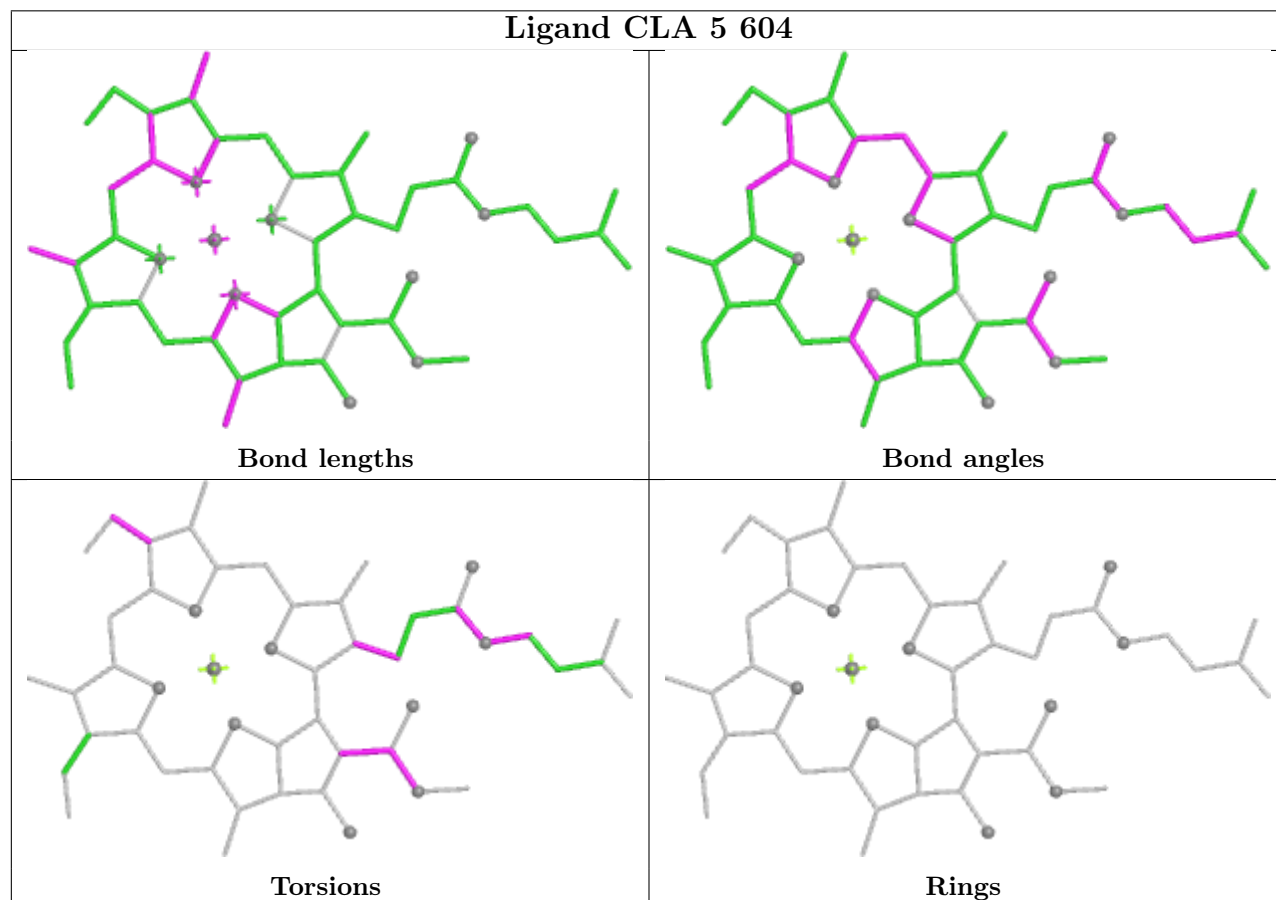
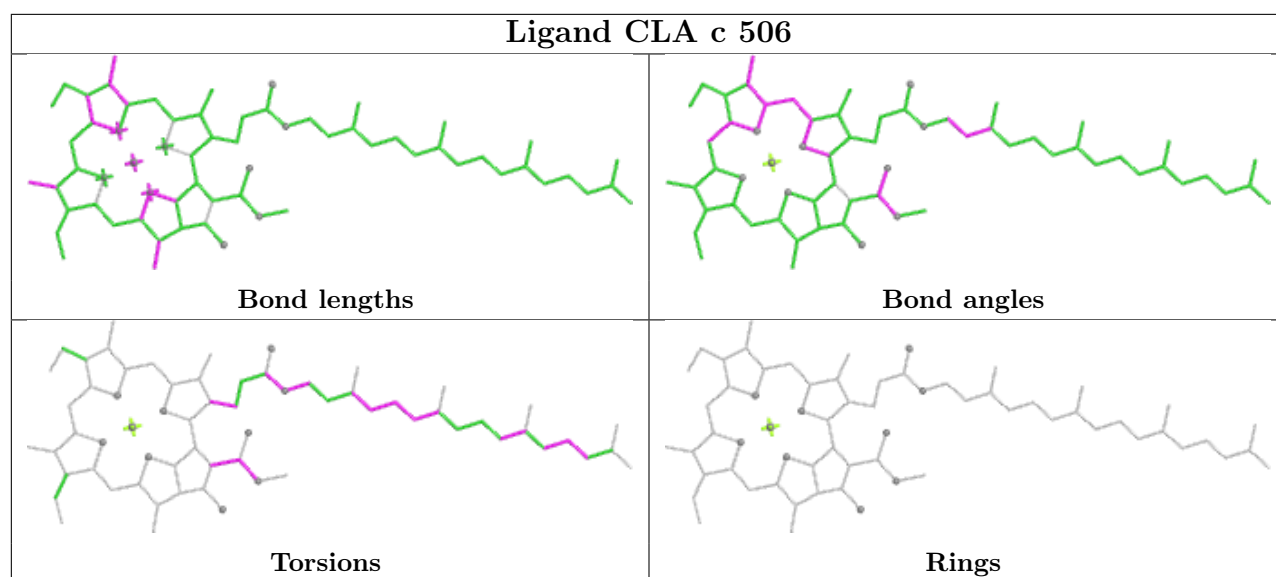


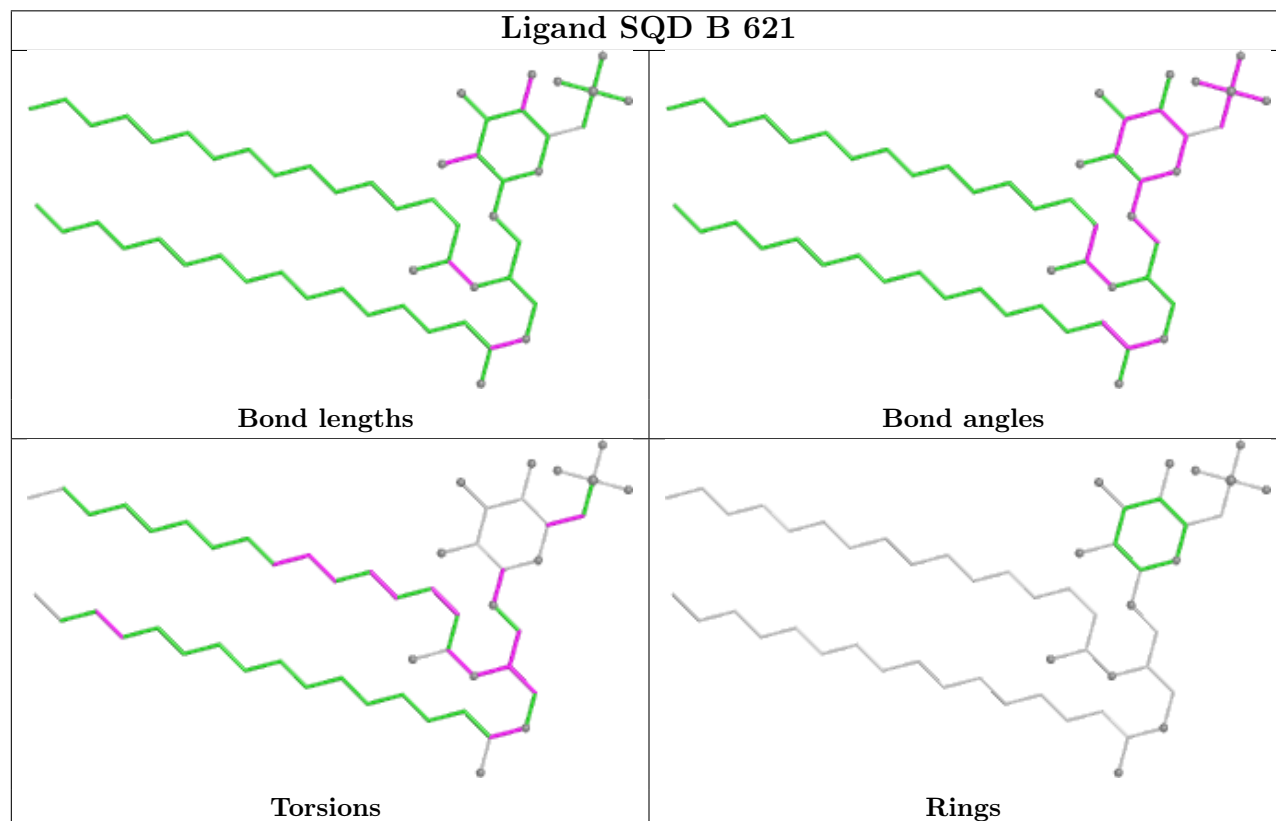
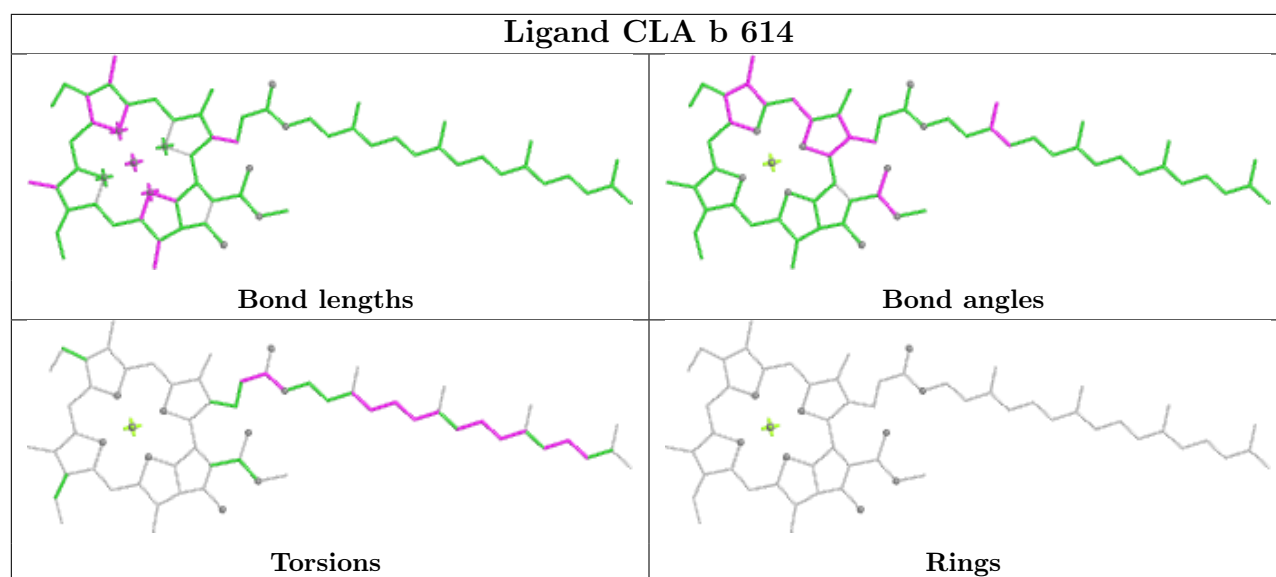
Ligand CLA 6 614

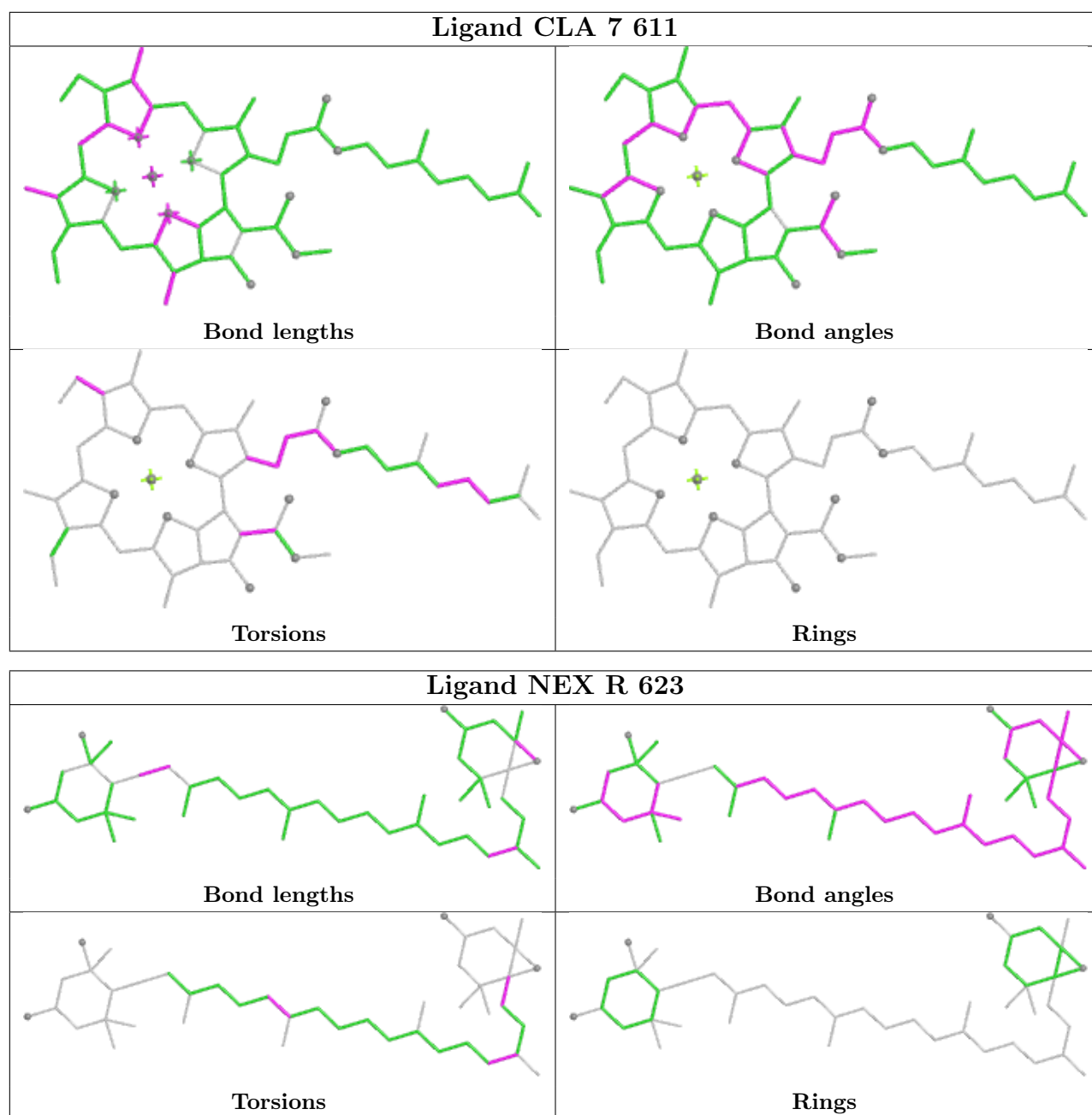


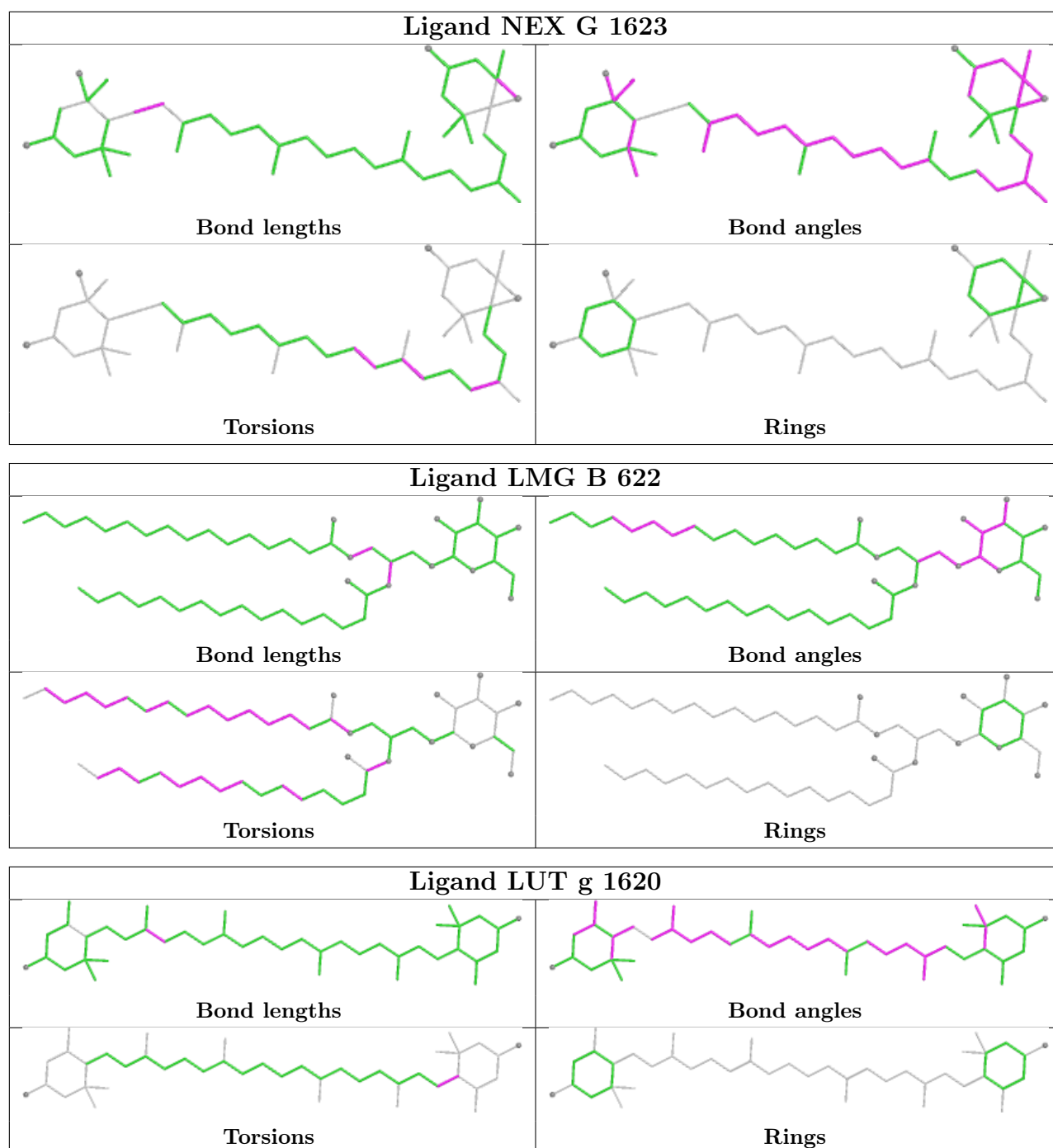
Ligand BCR 8 623



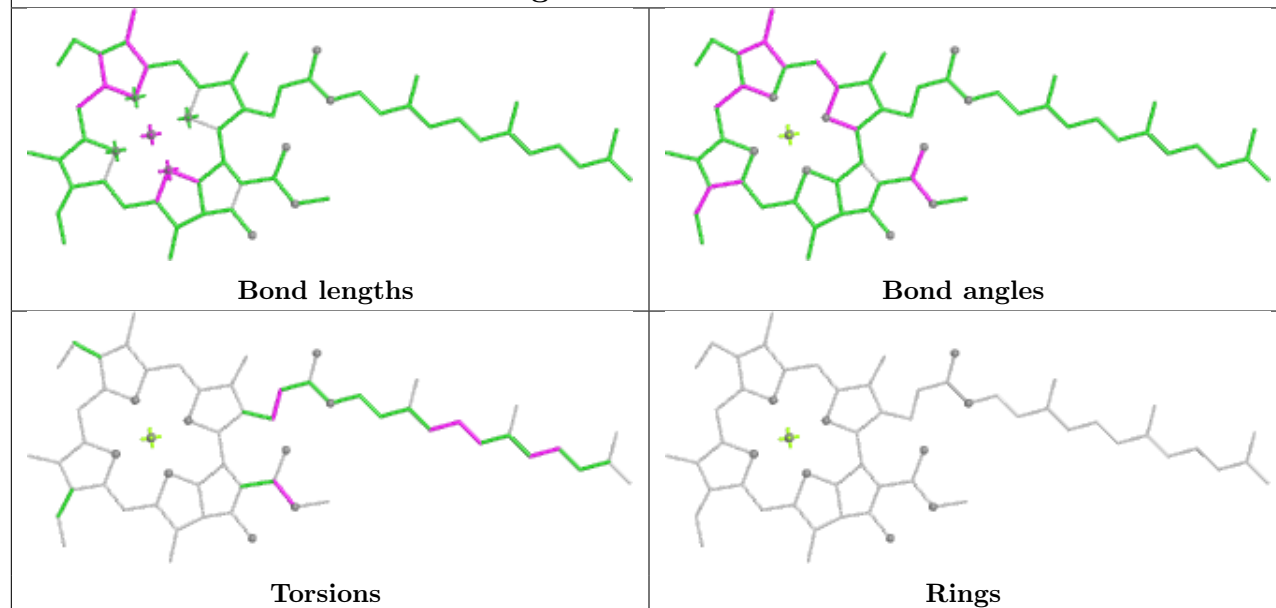




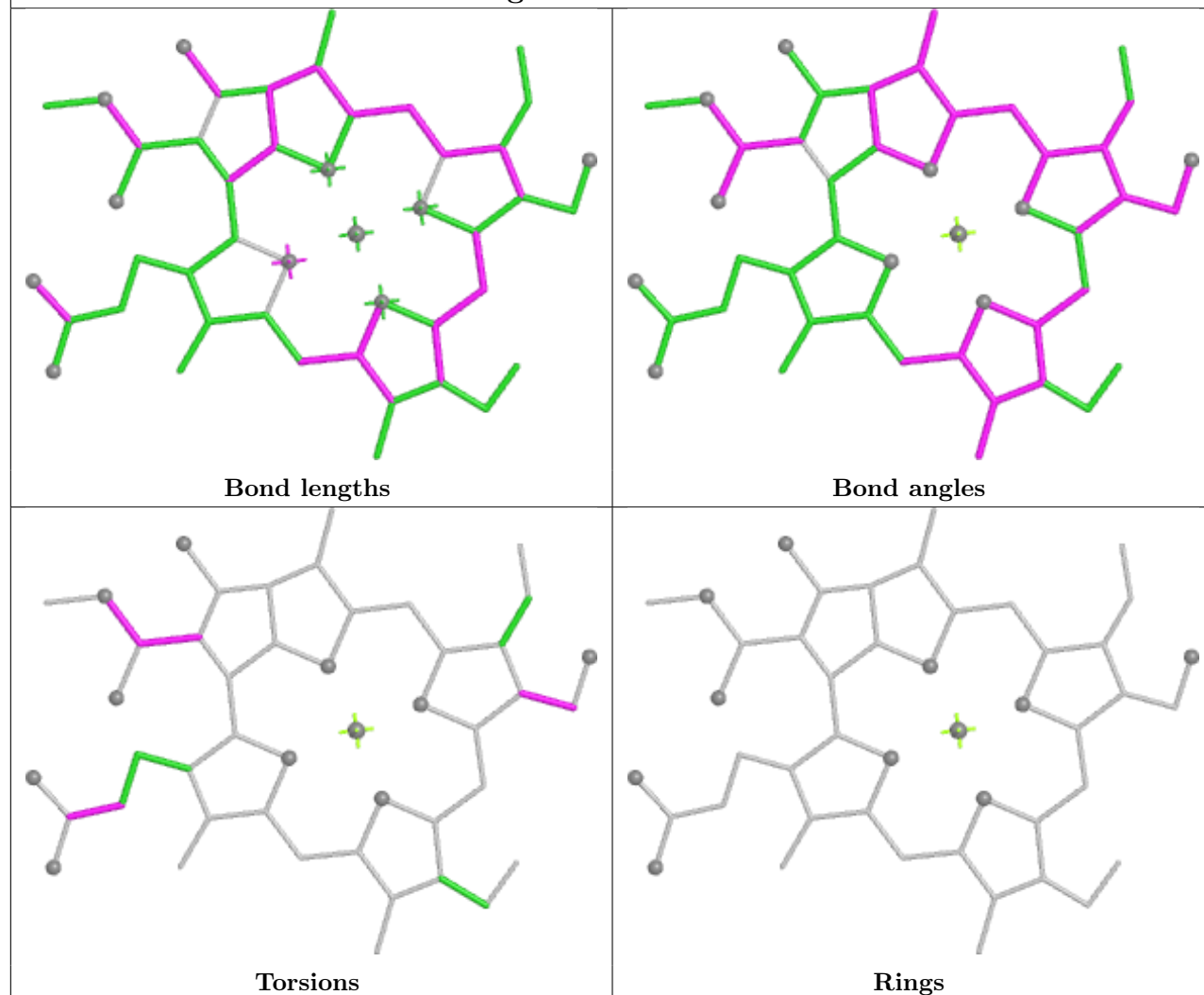




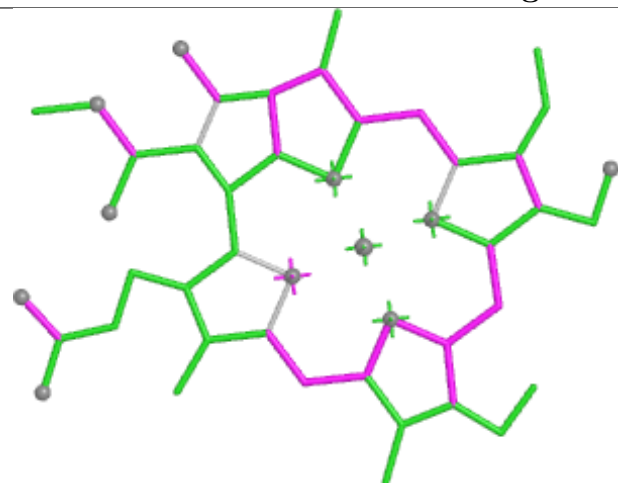
Ligand CLA N 613



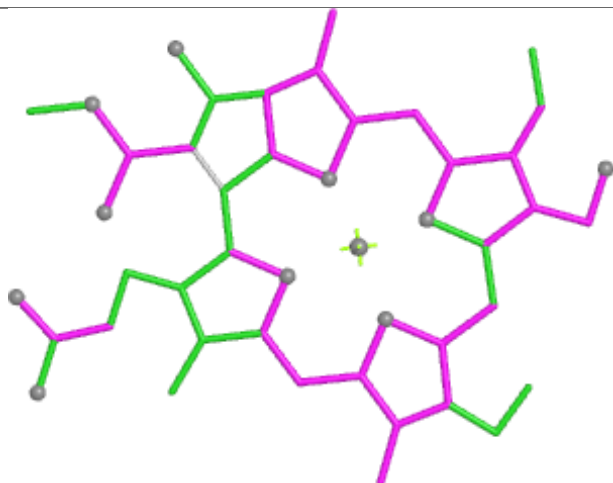
Ligand CHL s 606



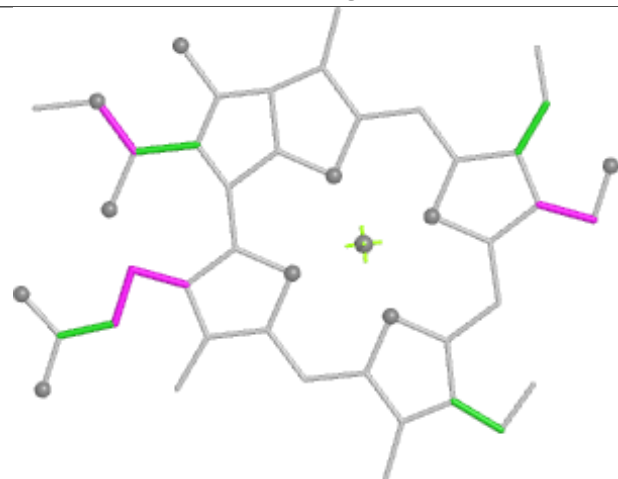
Ligand CHL 8 606



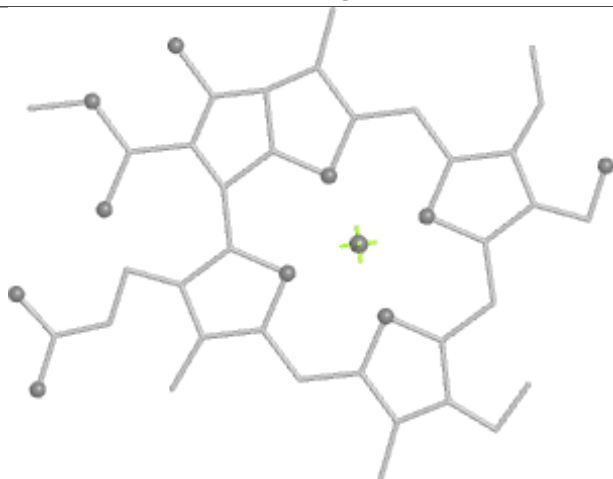
Bond lengths



Bond angles

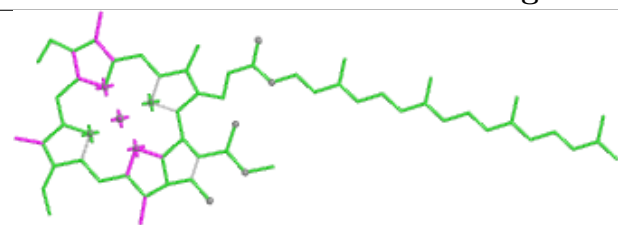


Torsions

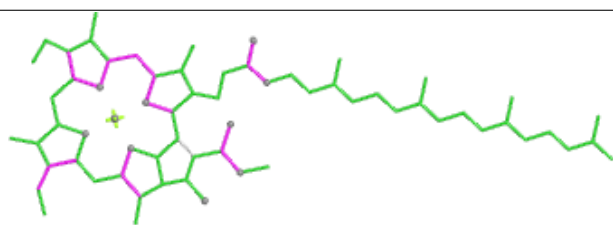


Rings

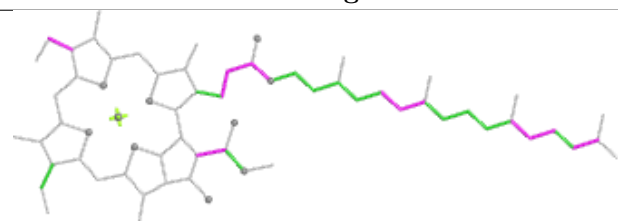
Ligand CLA b 602



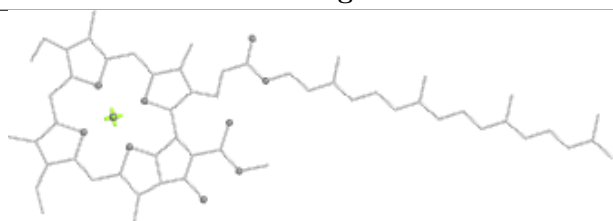
Bond lengths



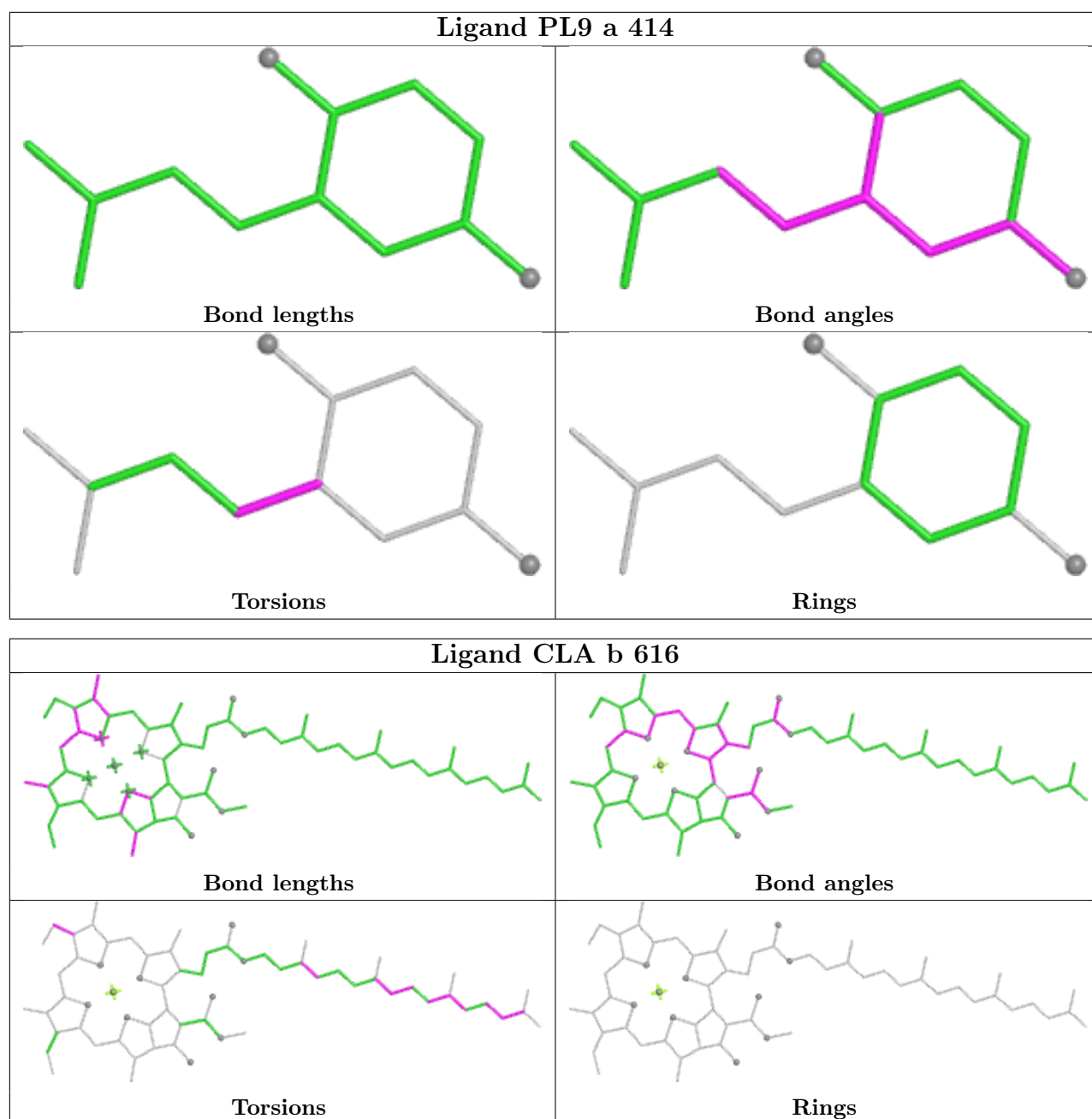
Bond angles

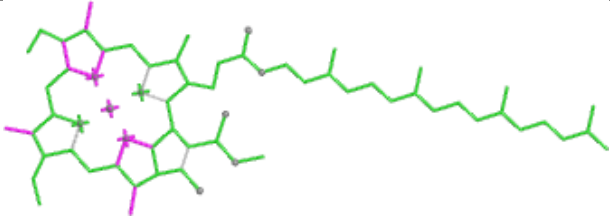
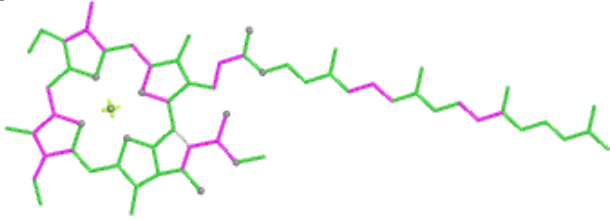
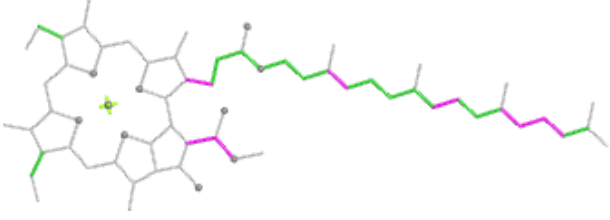
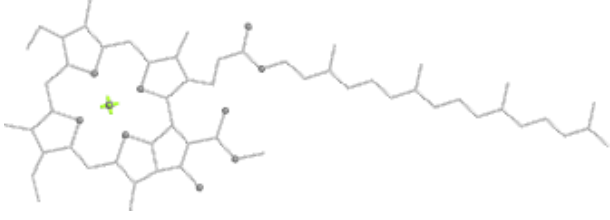
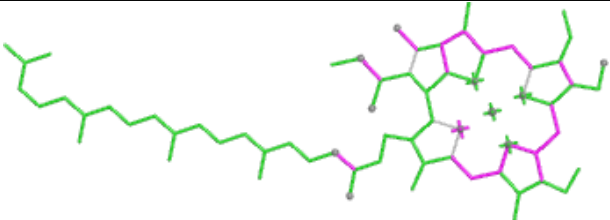
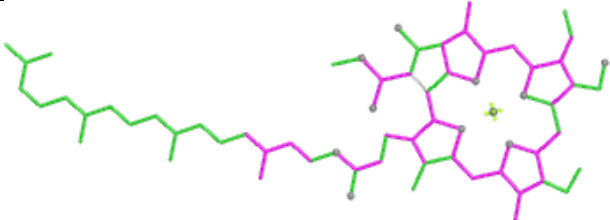
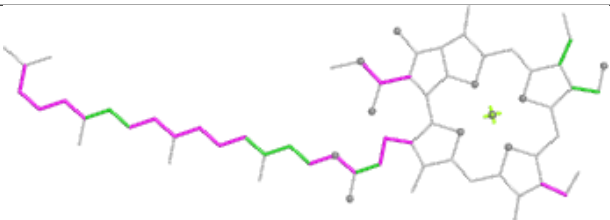
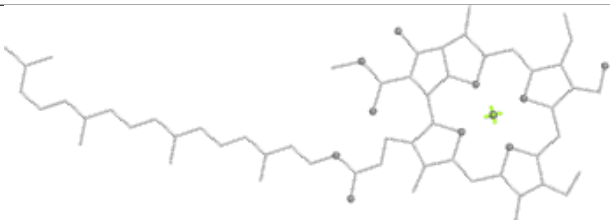
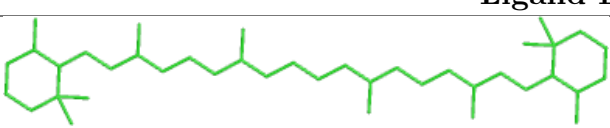
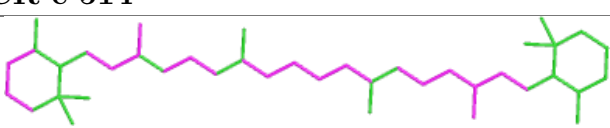
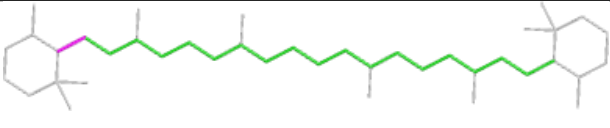
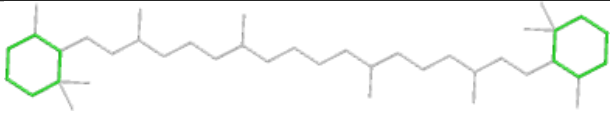


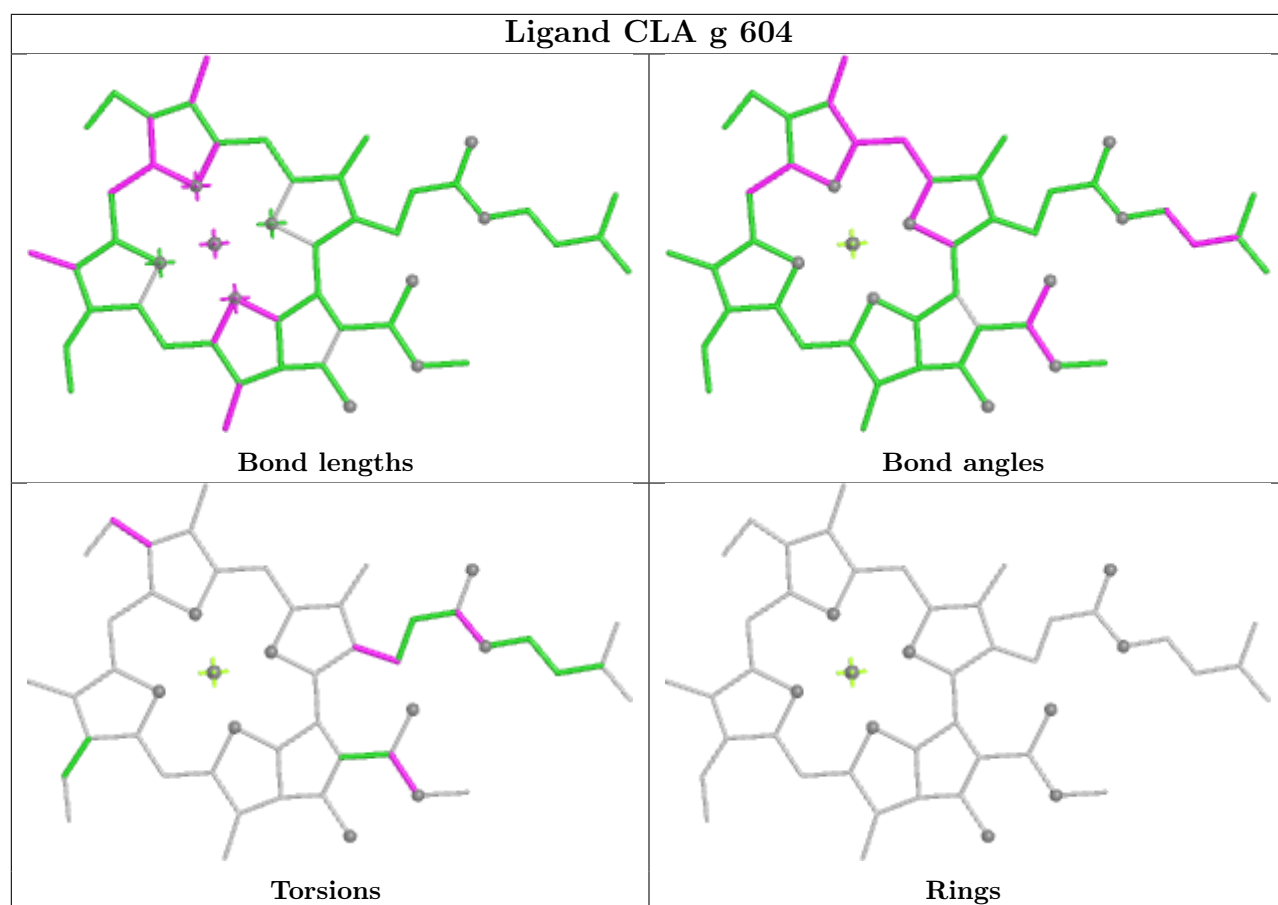
Torsions



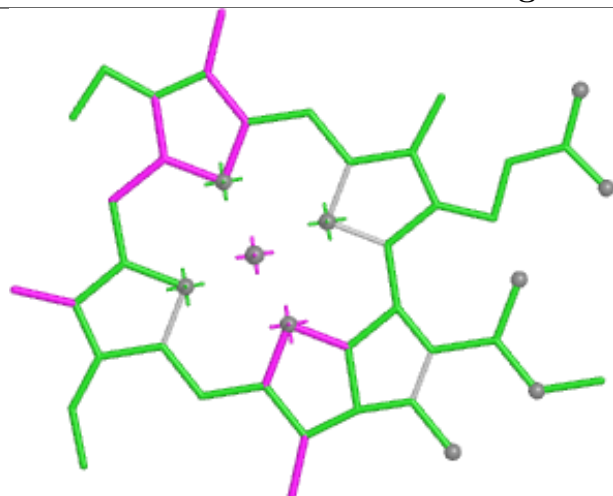
Rings



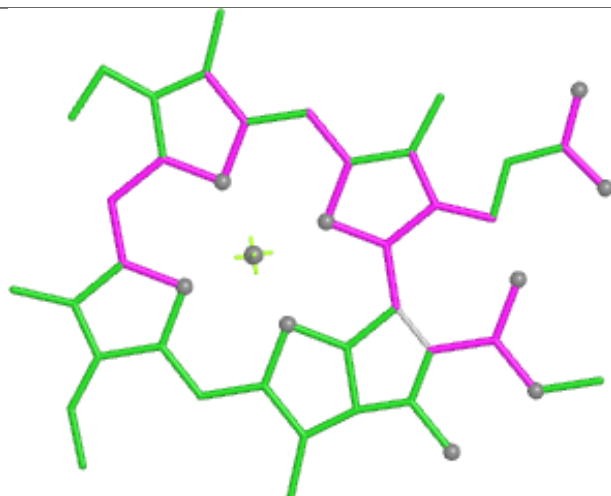
Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL R 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings



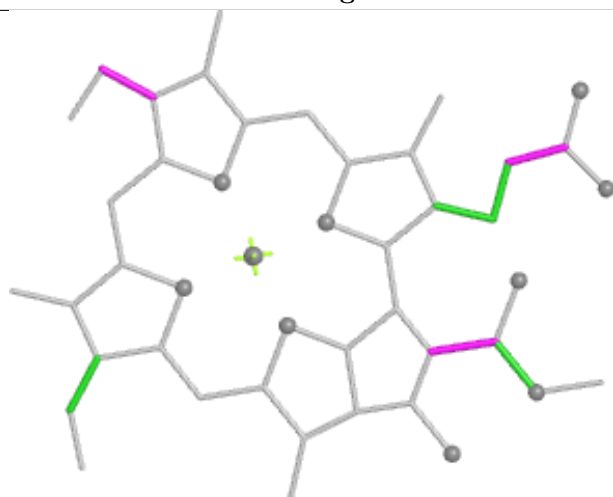
Ligand CLA 1 612



Bond lengths



Bond angles

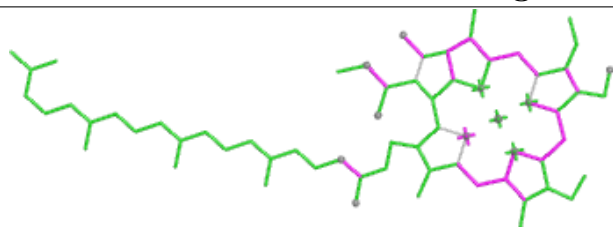


Torsions

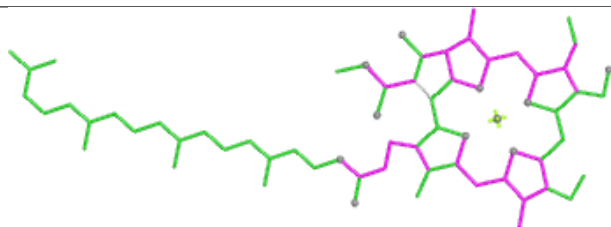


Rings

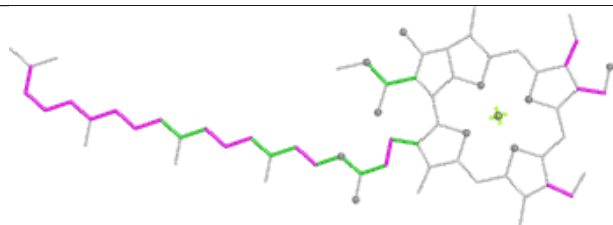
Ligand CHL N 607



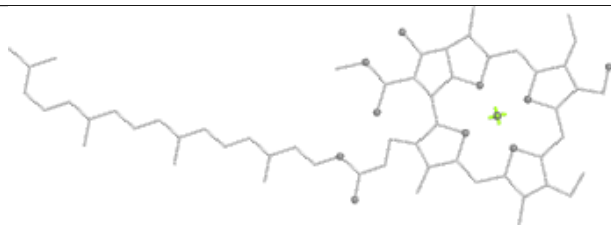
Bond lengths



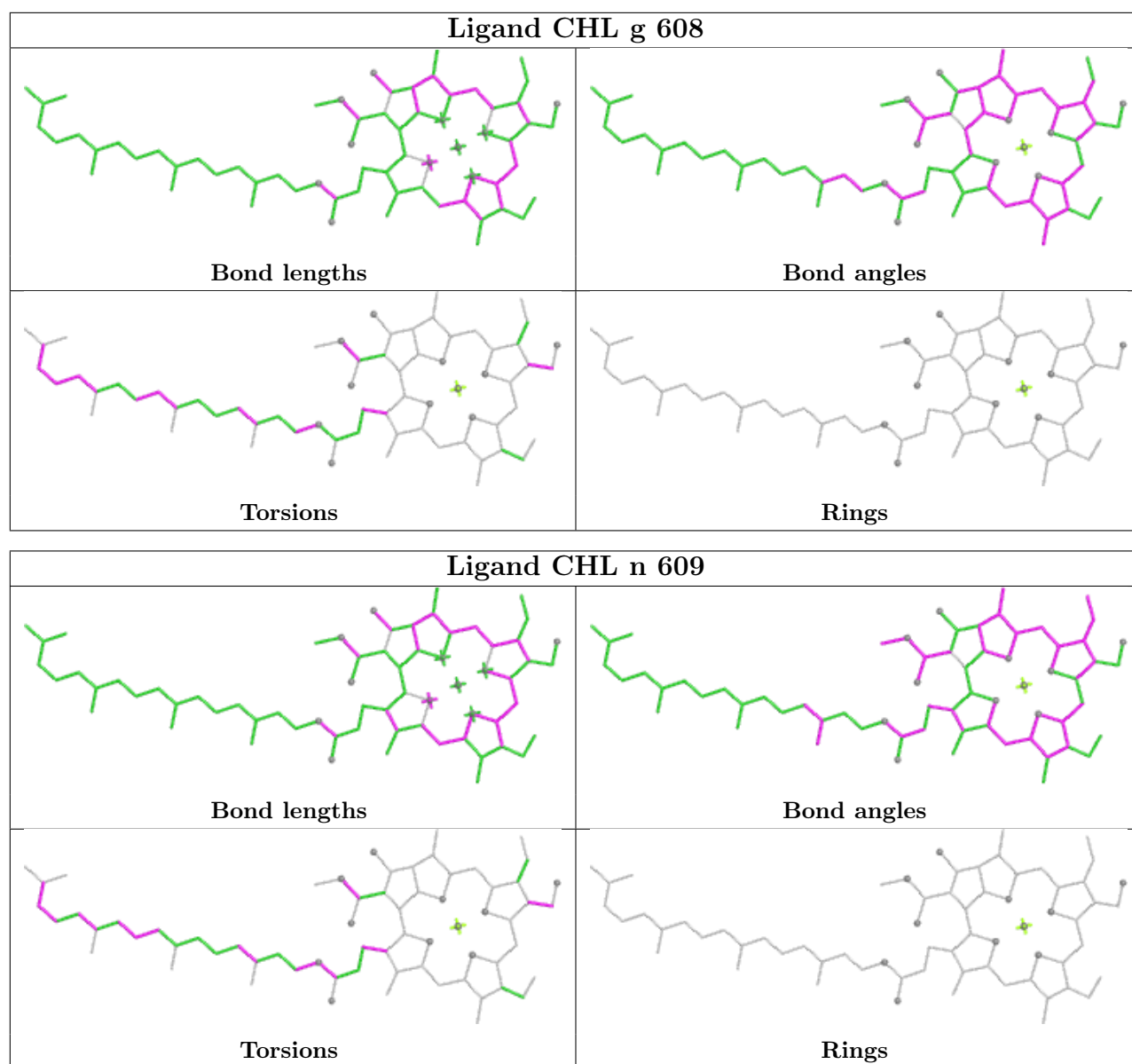
Bond angles



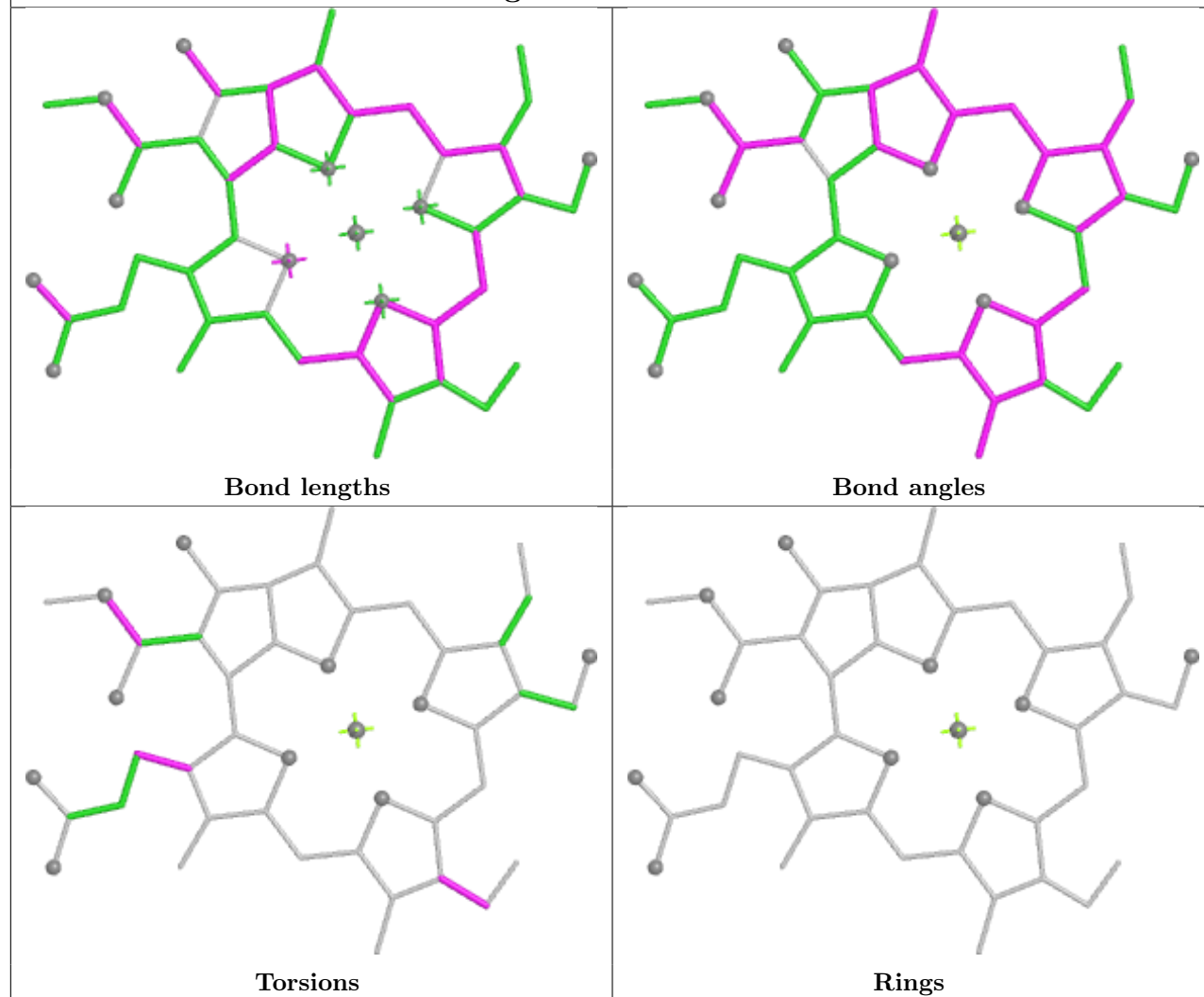
Torsions



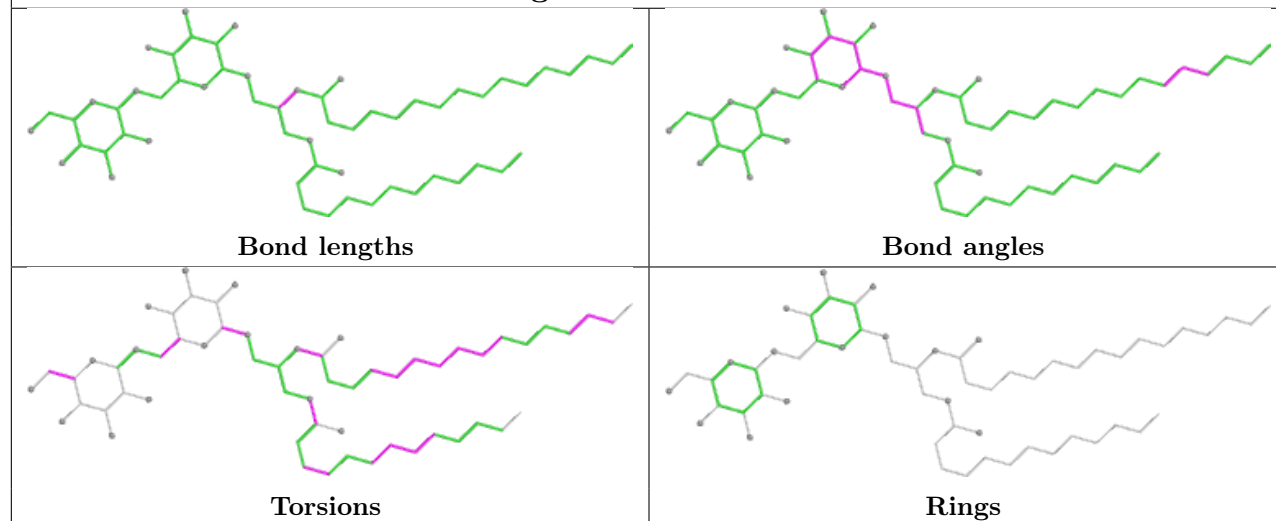
Rings

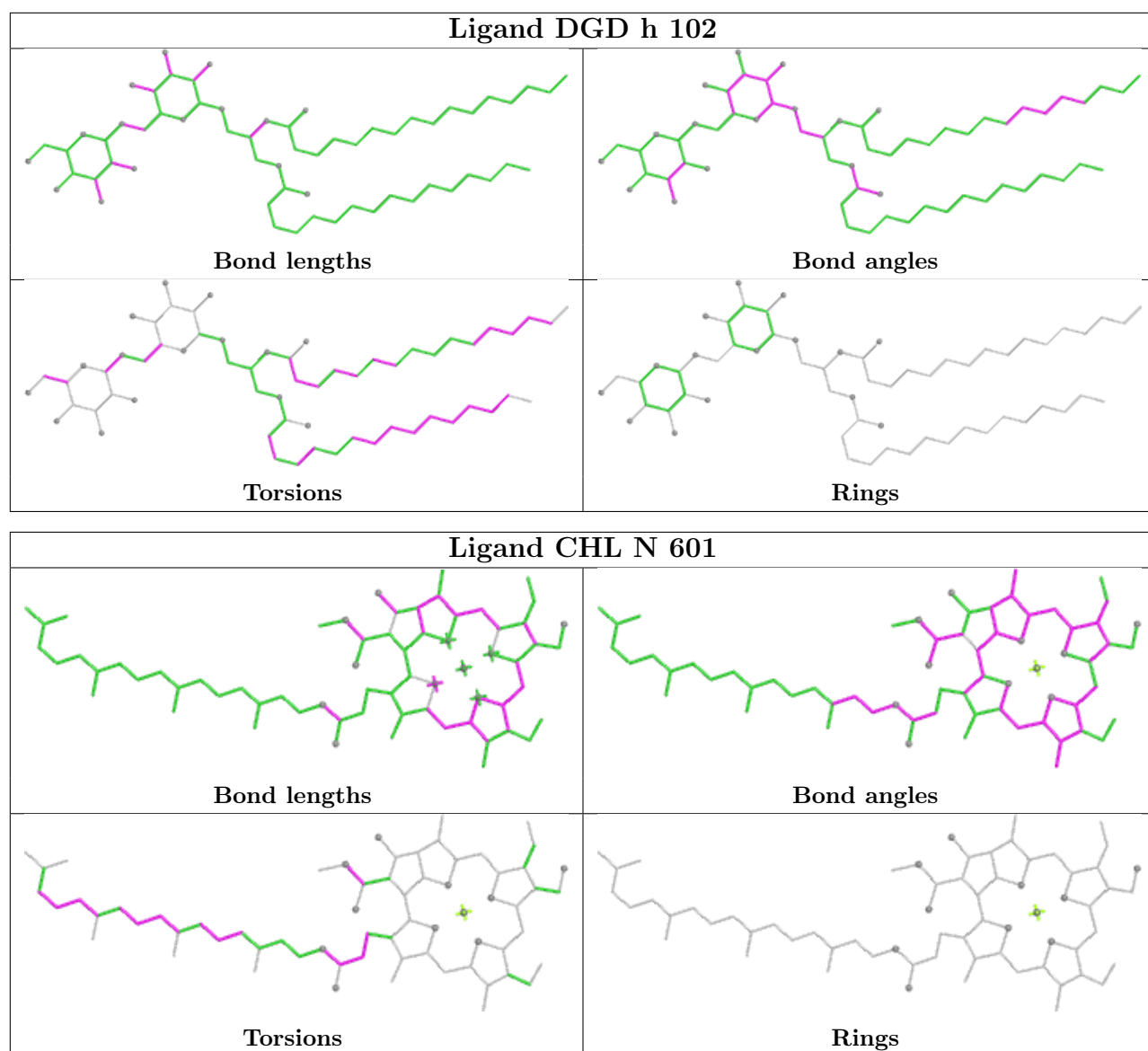


Ligand CHL S 608

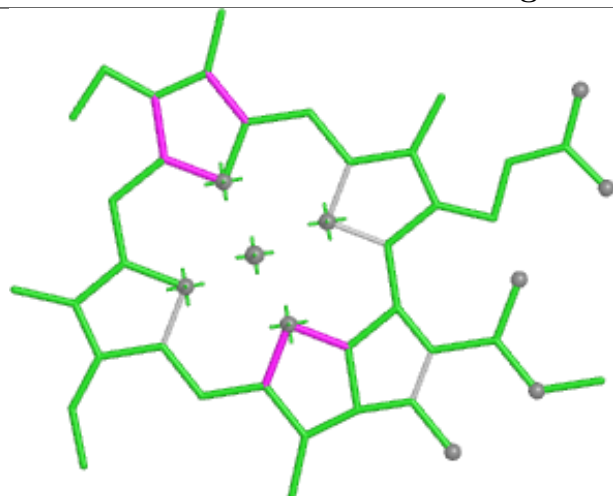


Ligand DGD b 626

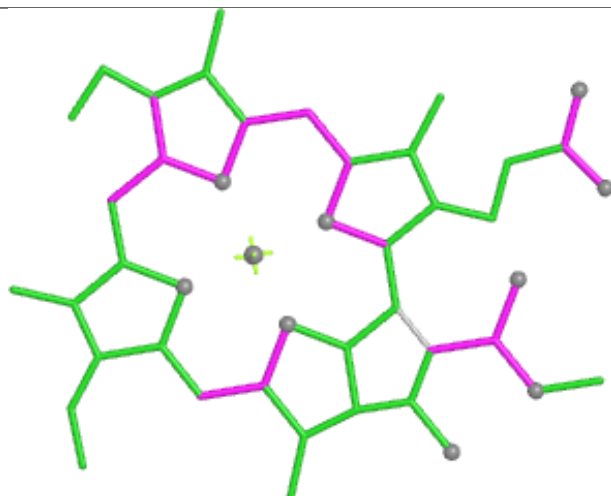




Ligand CLA s 609



Bond lengths



Bond angles

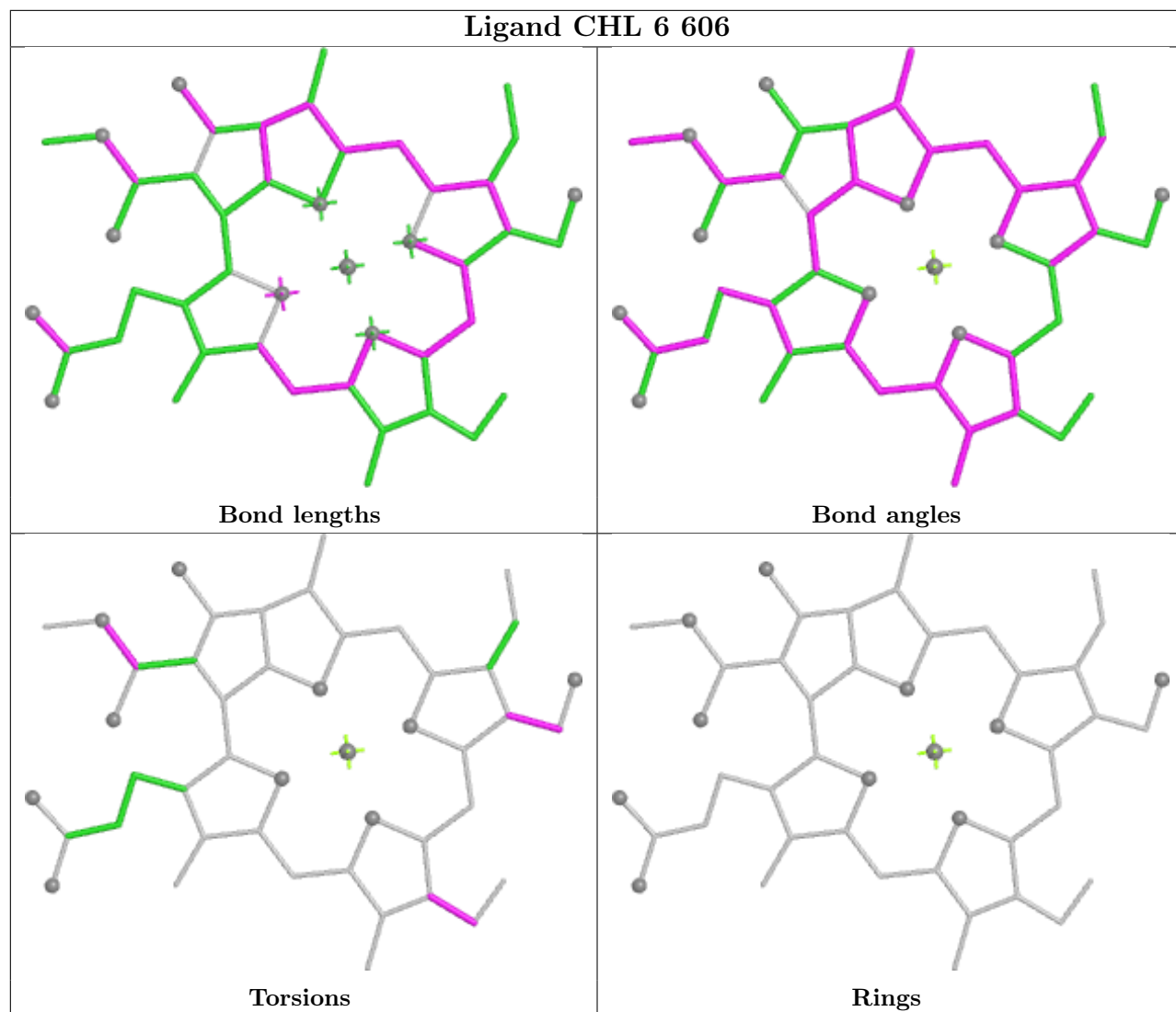


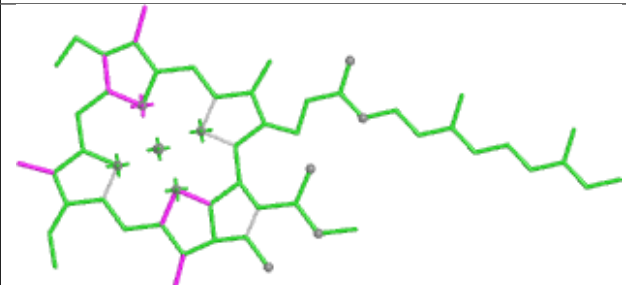
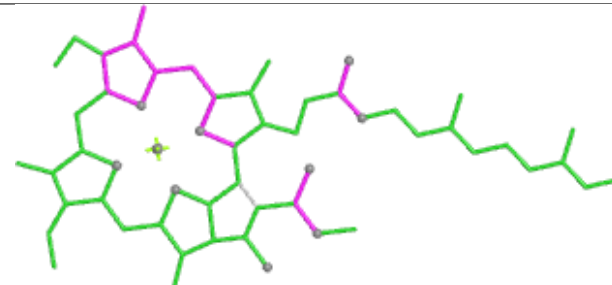
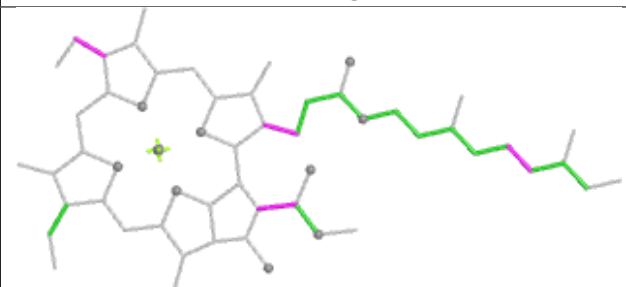
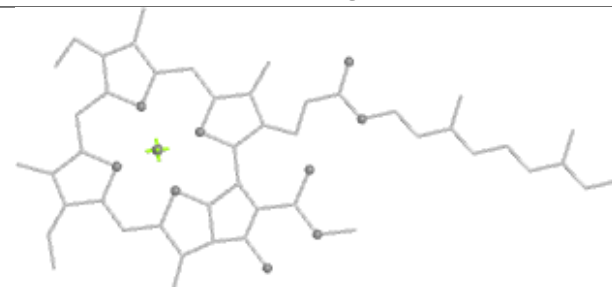
Torsions

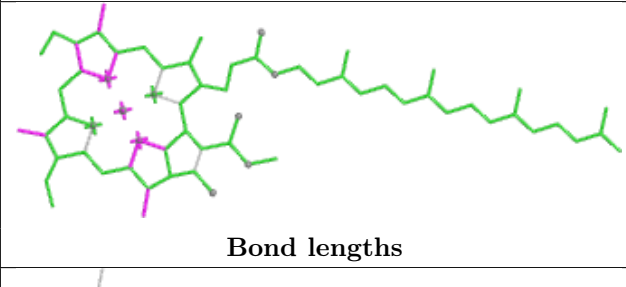
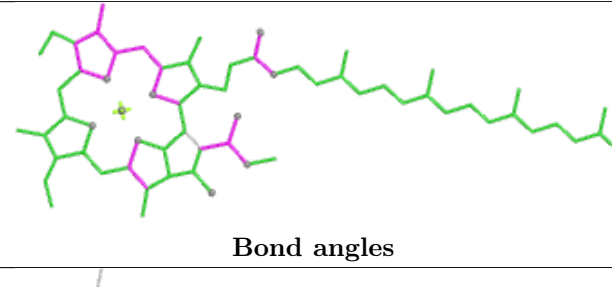
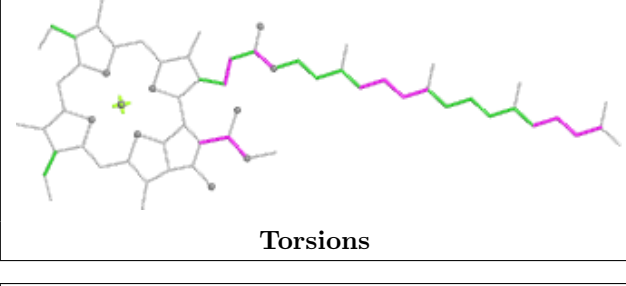
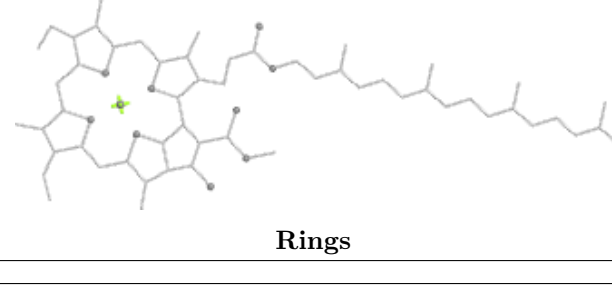


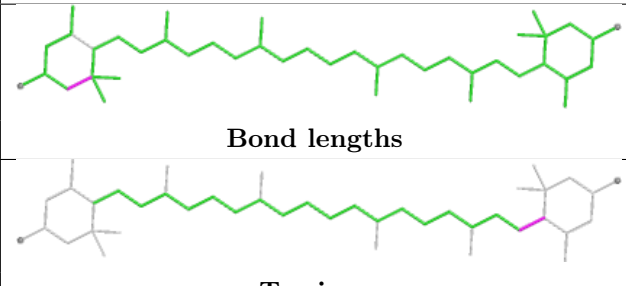
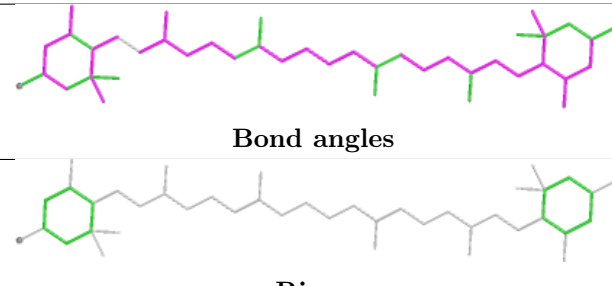
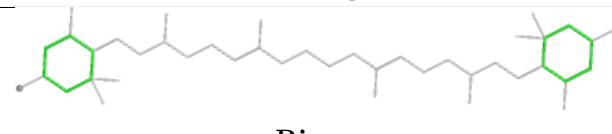
Rings

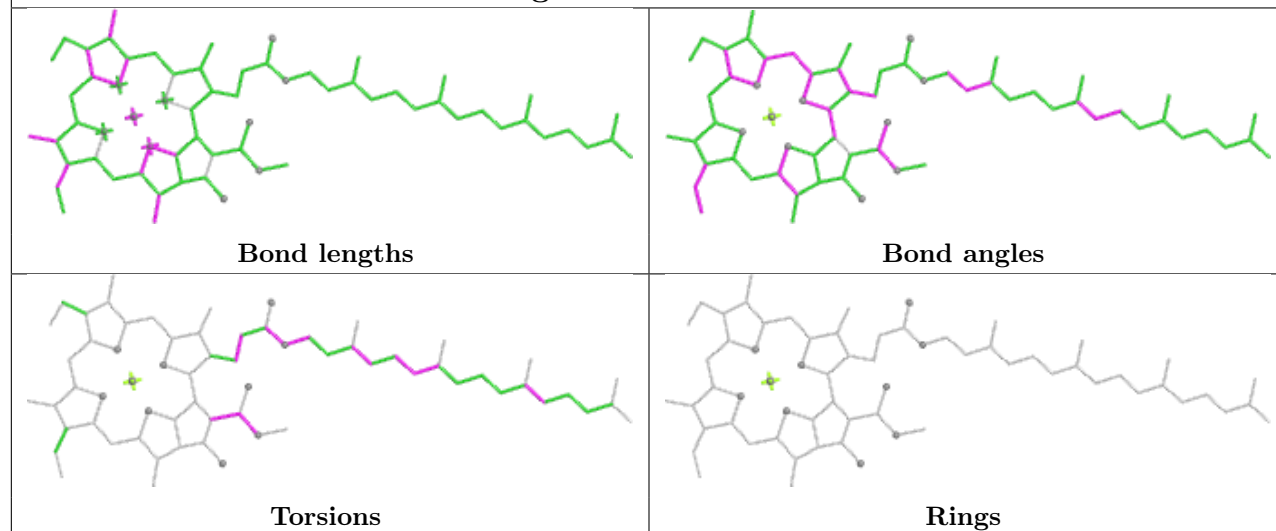
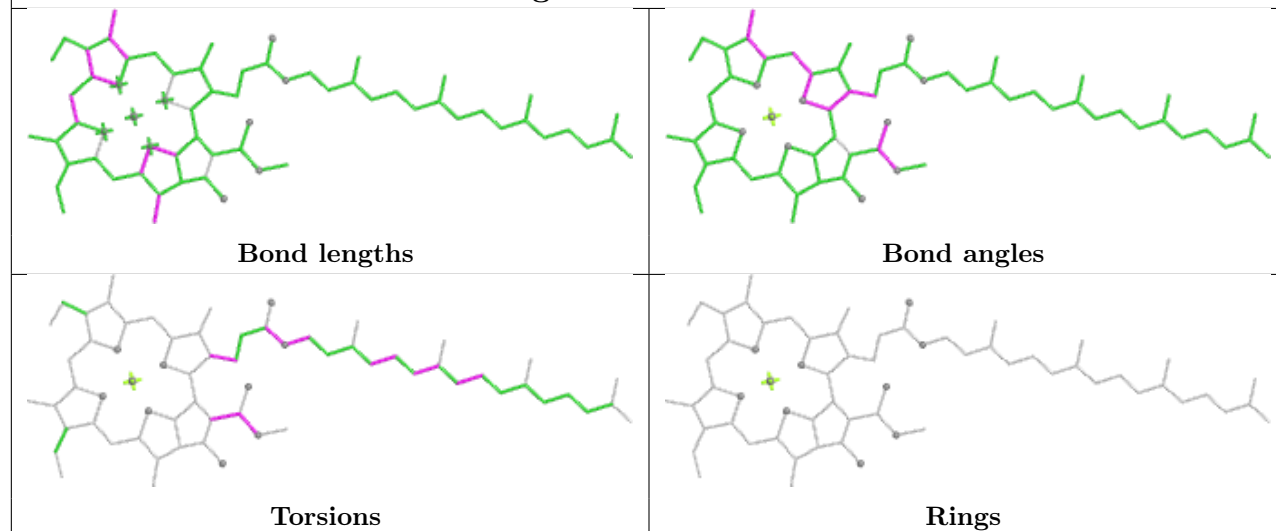
Ligand CHL 6 606



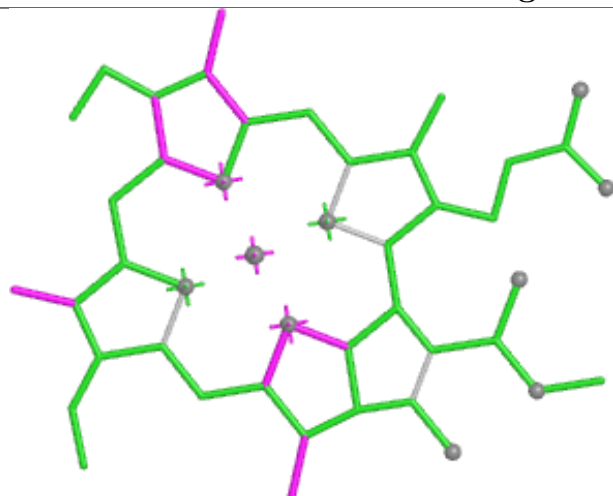
Ligand CLA 1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

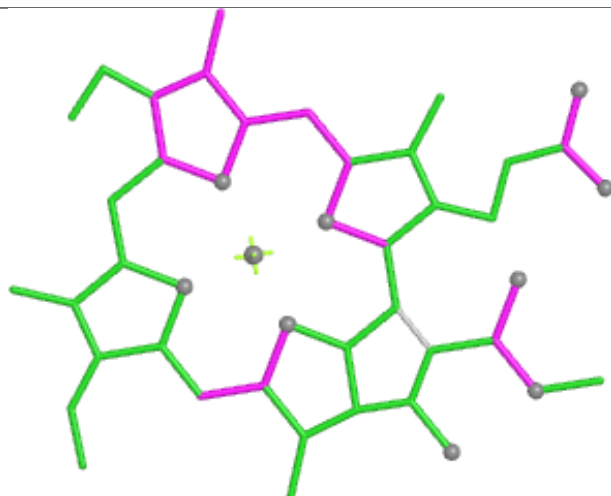
Ligand LUT 2 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 603**Ligand CLA C 511**

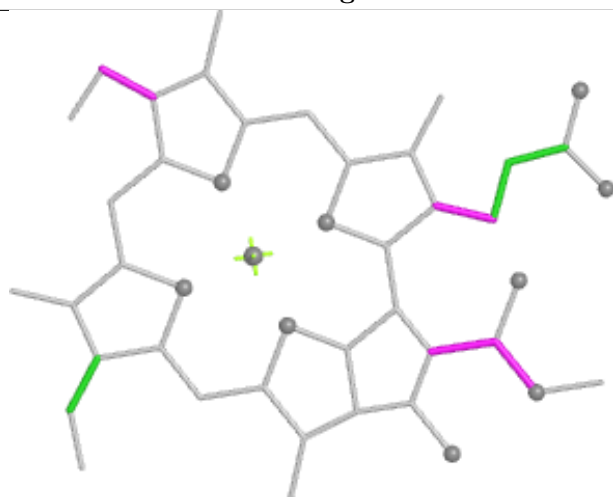
Ligand CLA 1 614



Bond lengths



Bond angles

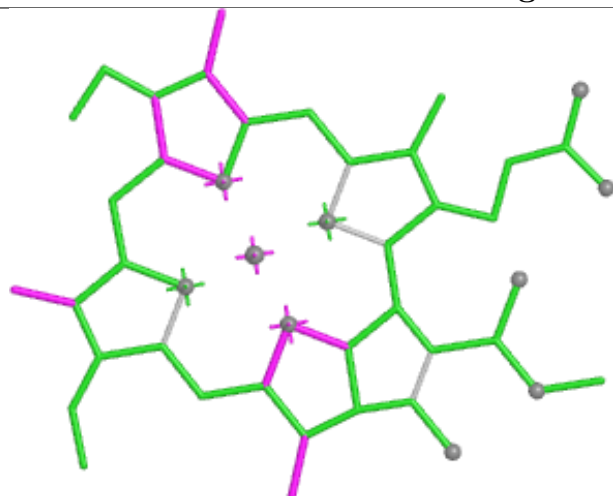


Torsions

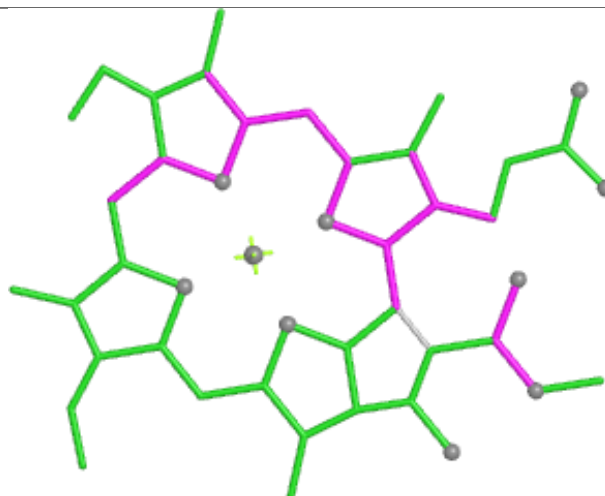


Rings

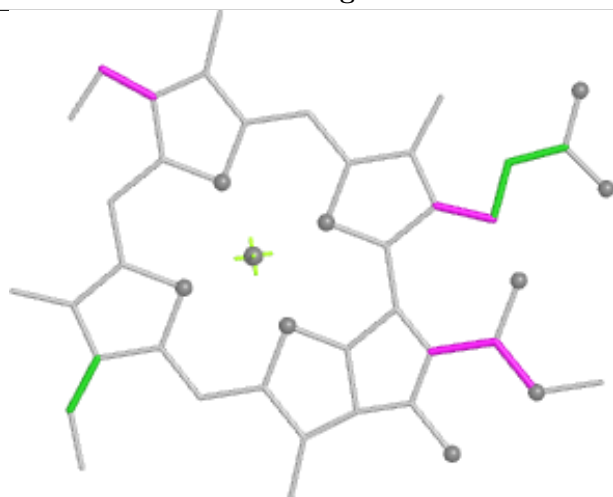
Ligand CLA 2 612



Bond lengths



Bond angles

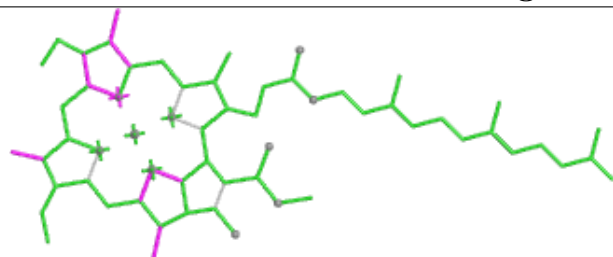


Torsions

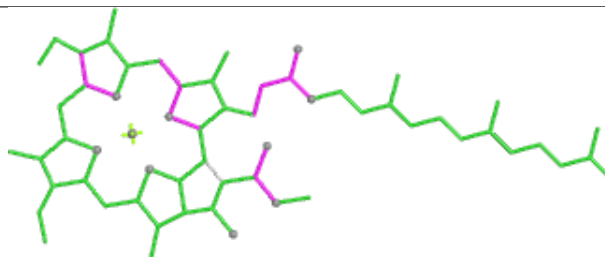


Rings

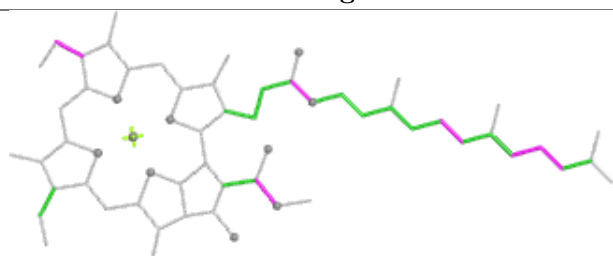
Ligand CLA n 611



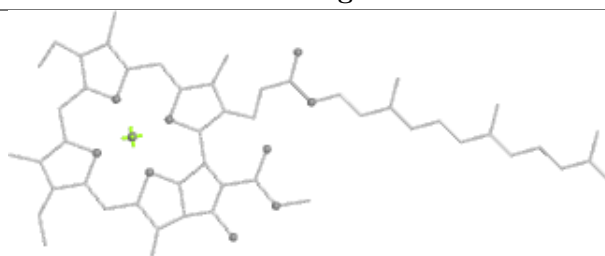
Bond lengths



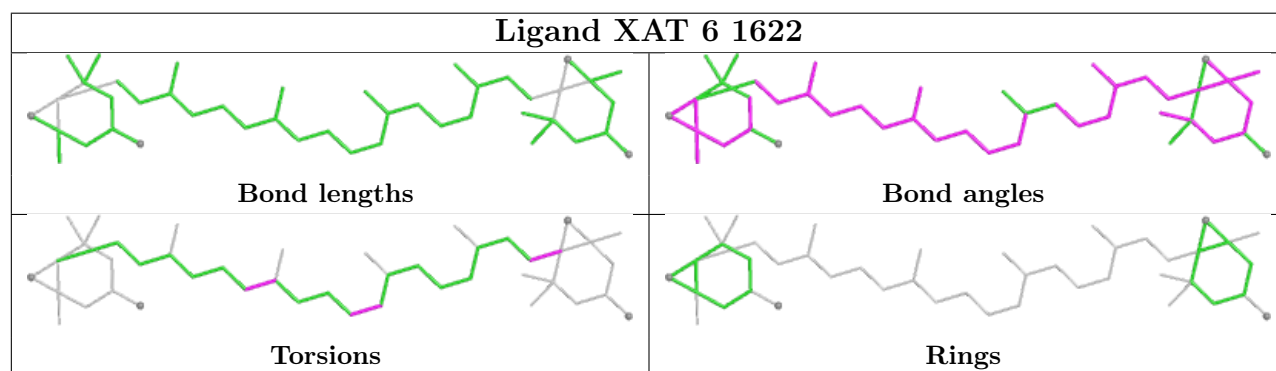
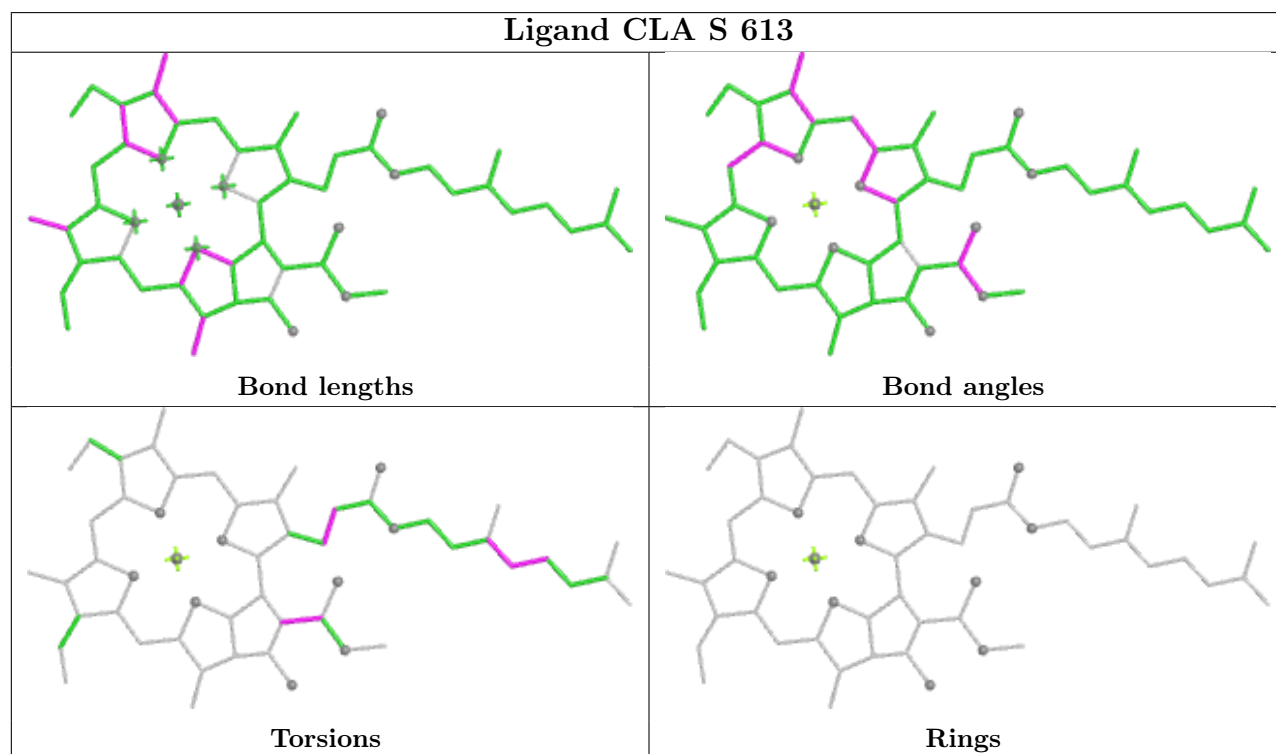
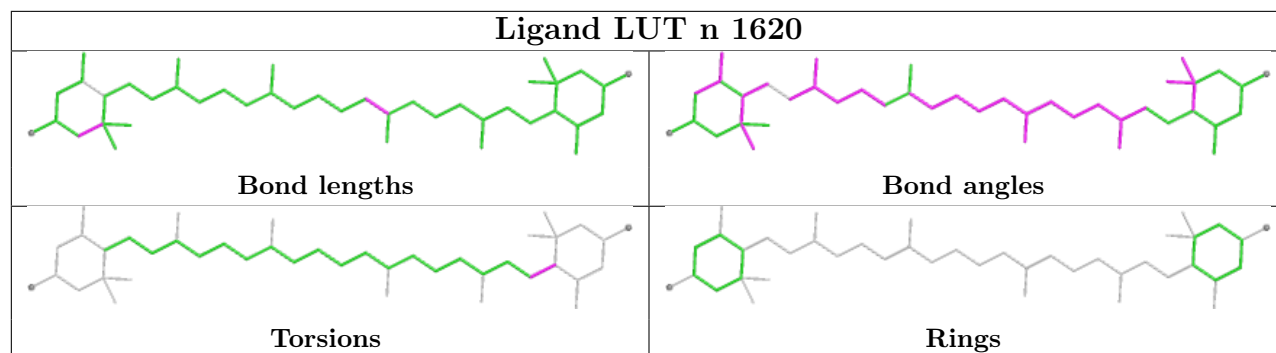
Bond angles



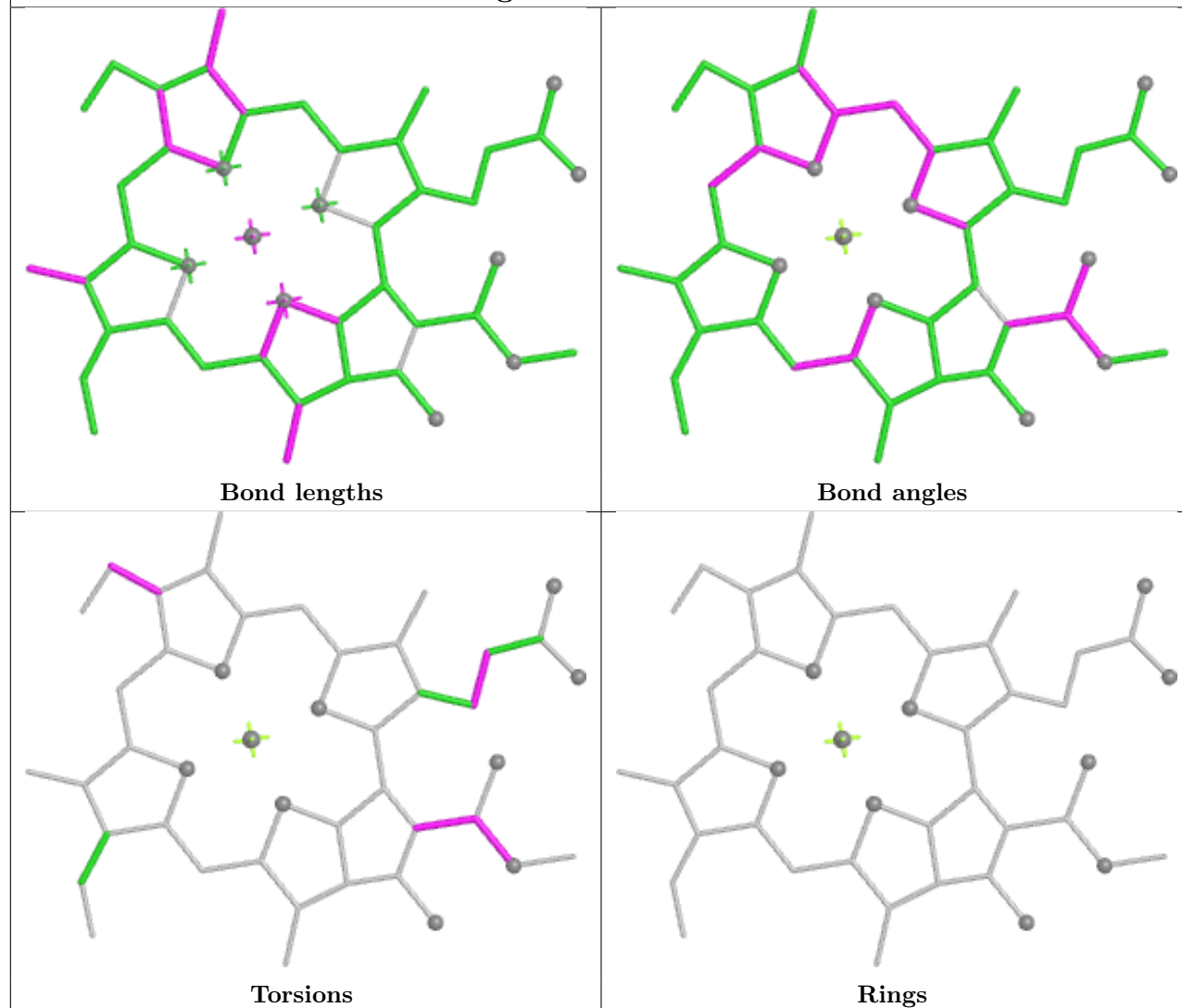
Torsions



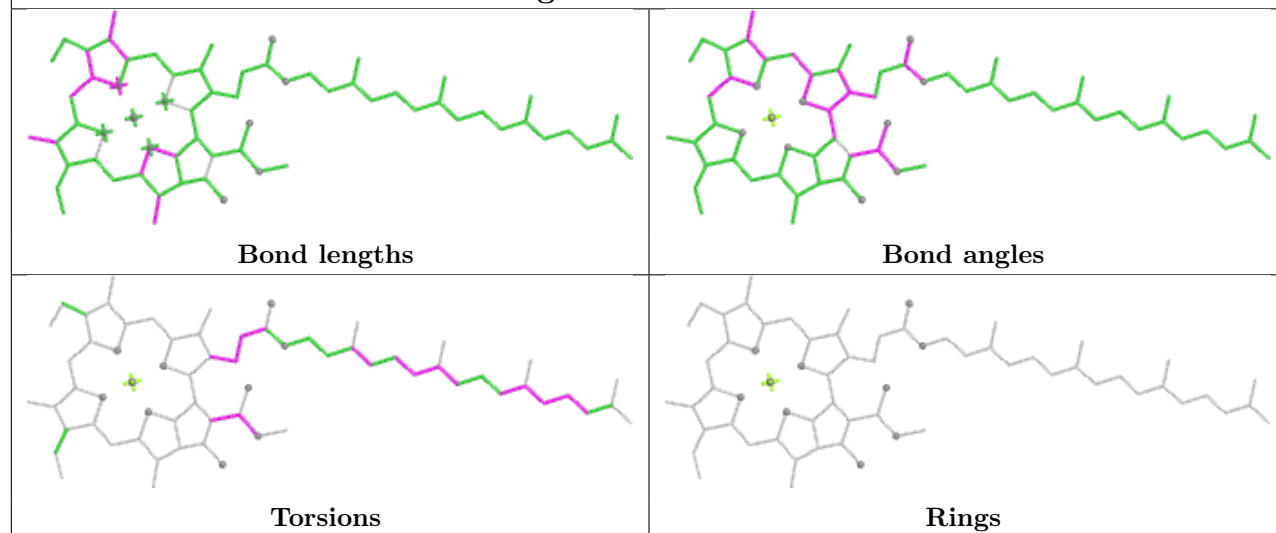
Rings

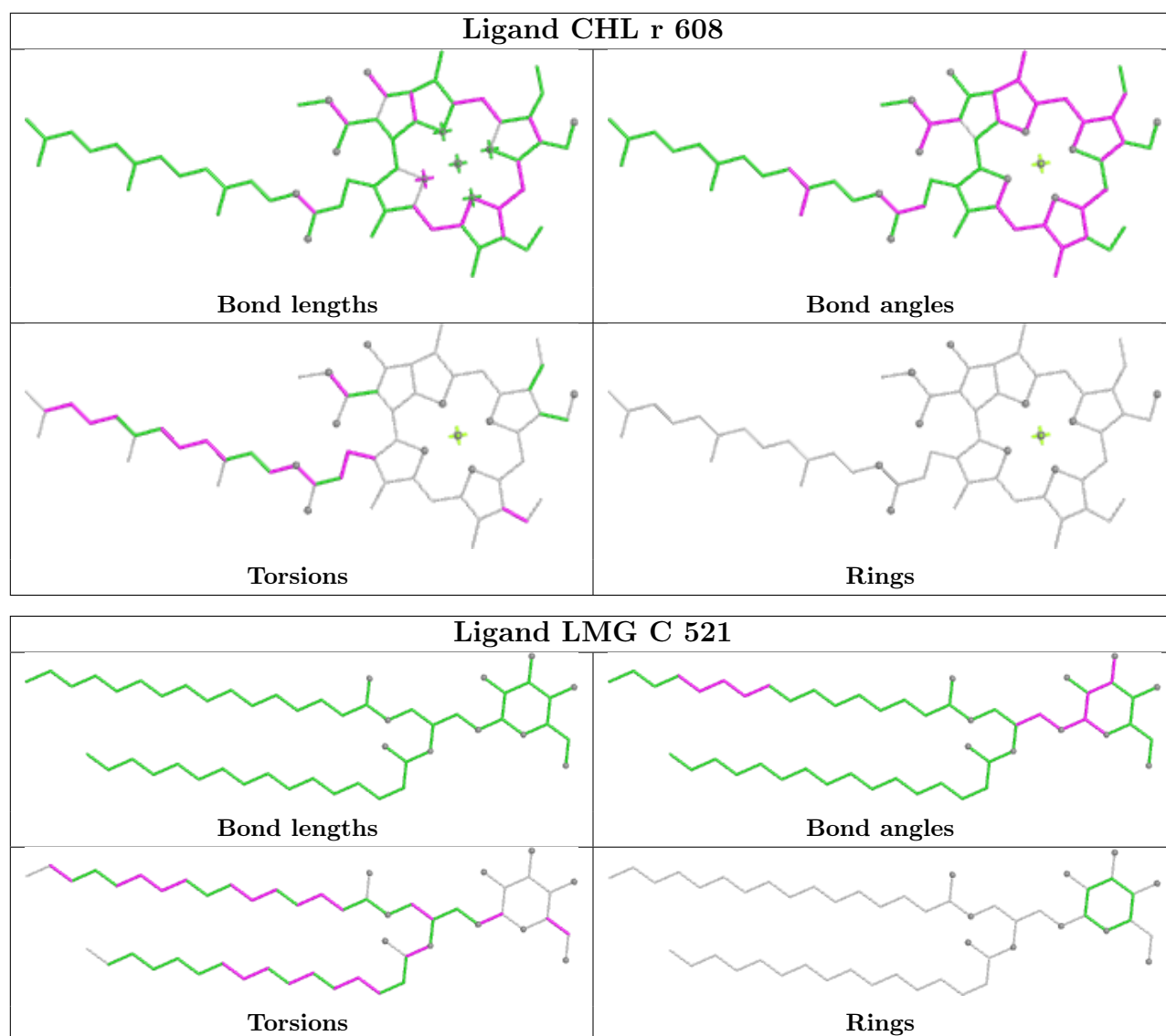


Ligand CLA 6 613

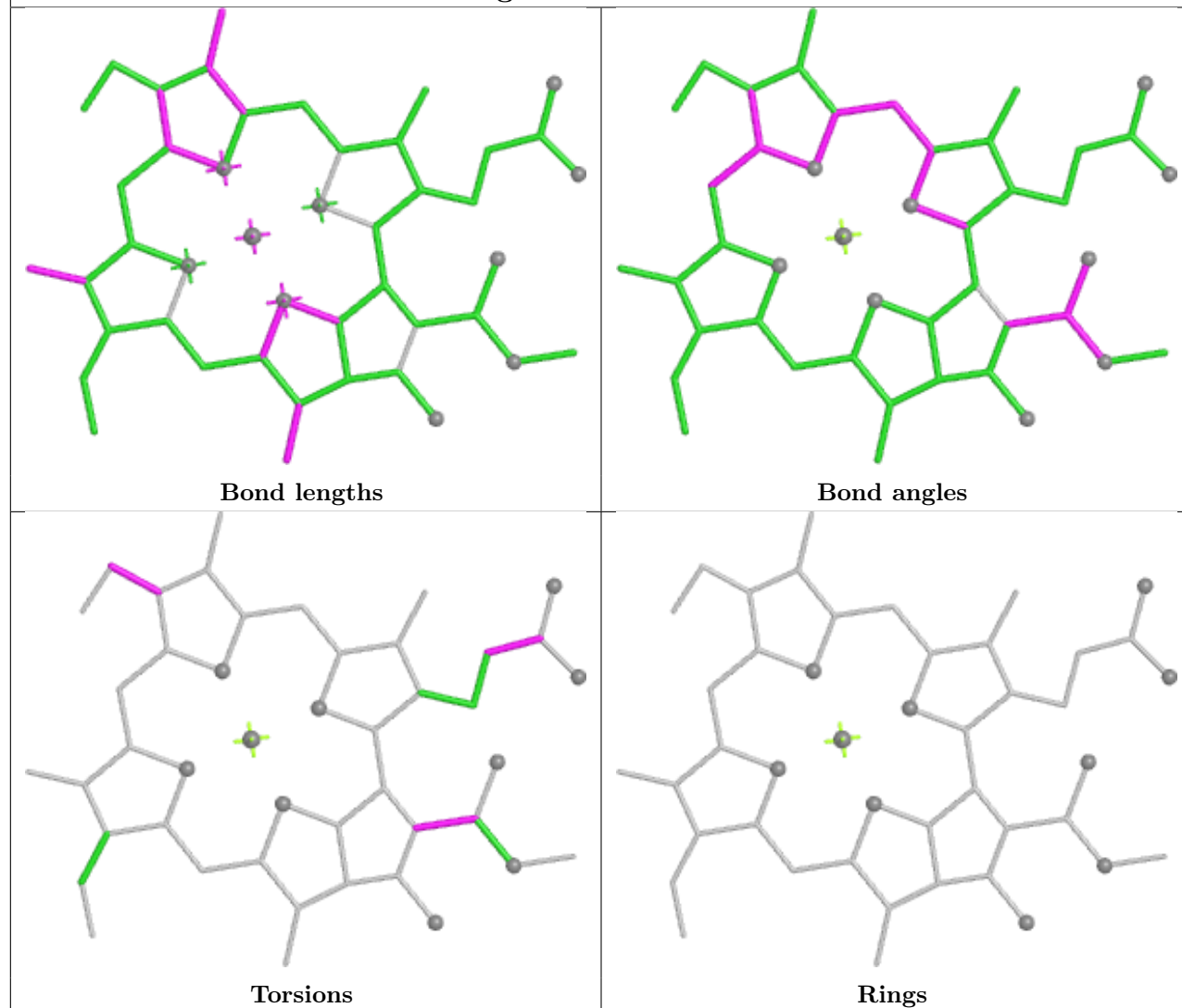


Ligand CLA c 507

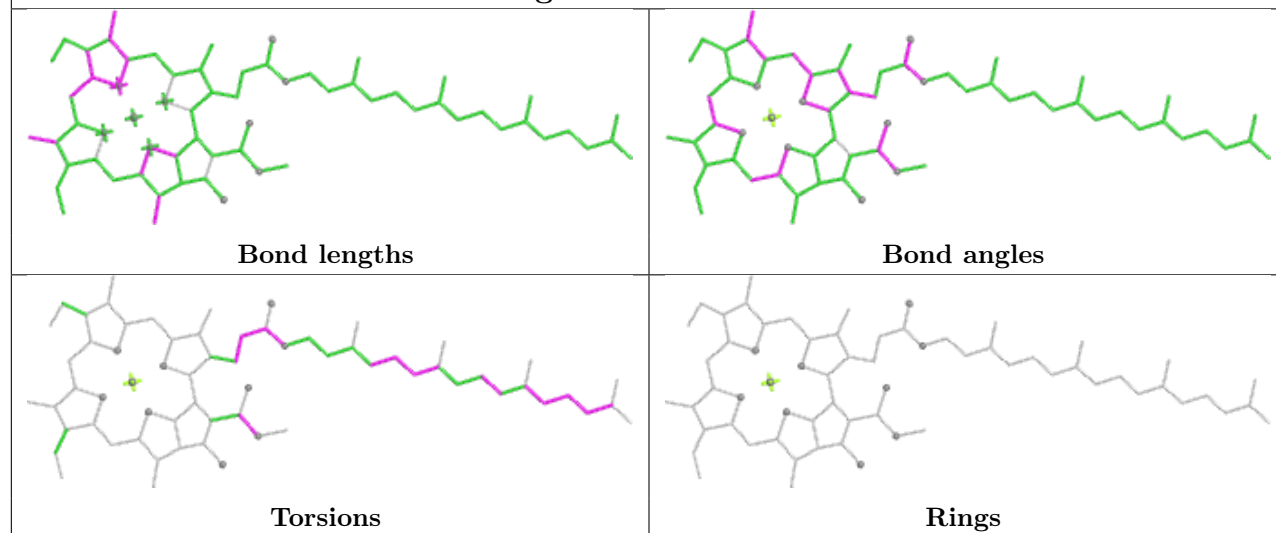




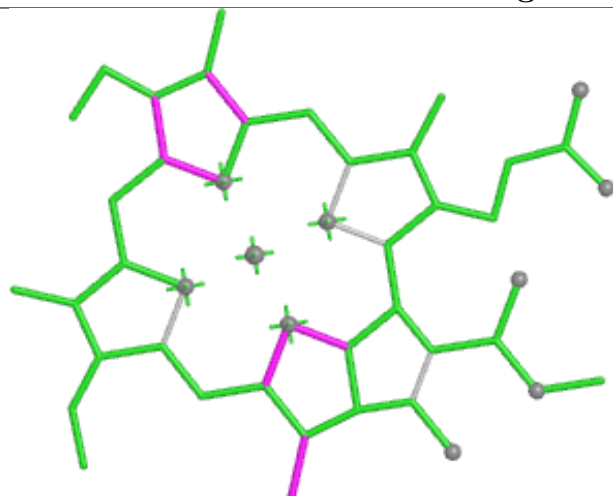
Ligand CLA 2 611



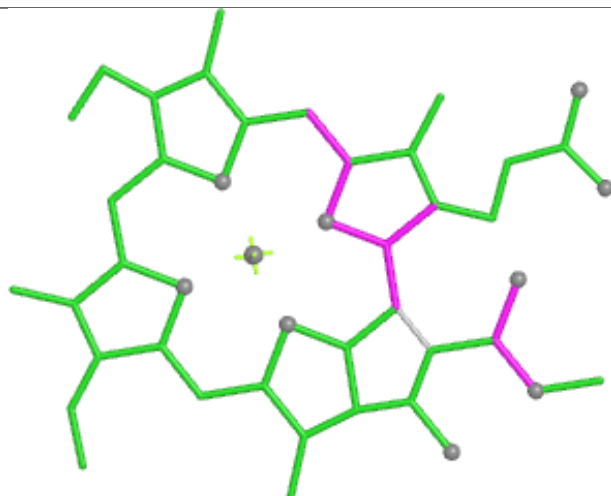
Ligand CLA b 617



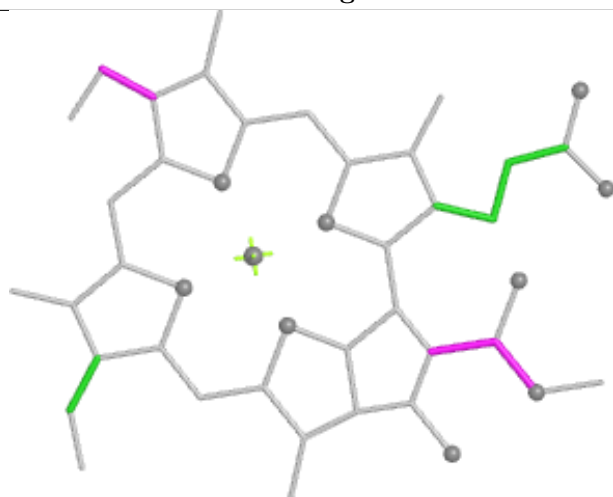
Ligand CLA S 603



Bond lengths



Bond angles

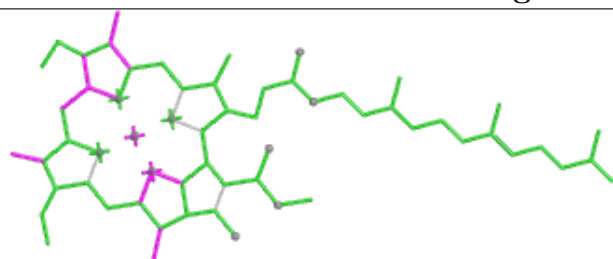


Torsions

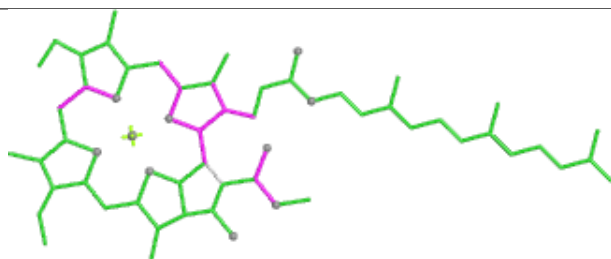


Rings

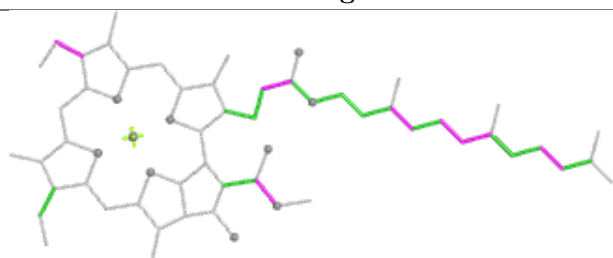
Ligand CLA N 612



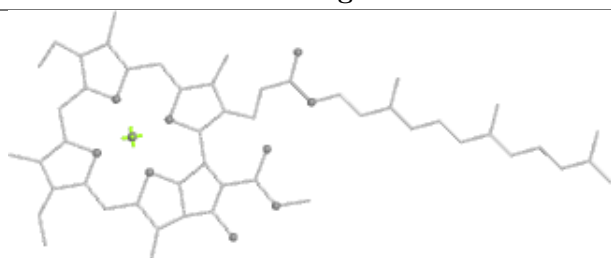
Bond lengths



Bond angles

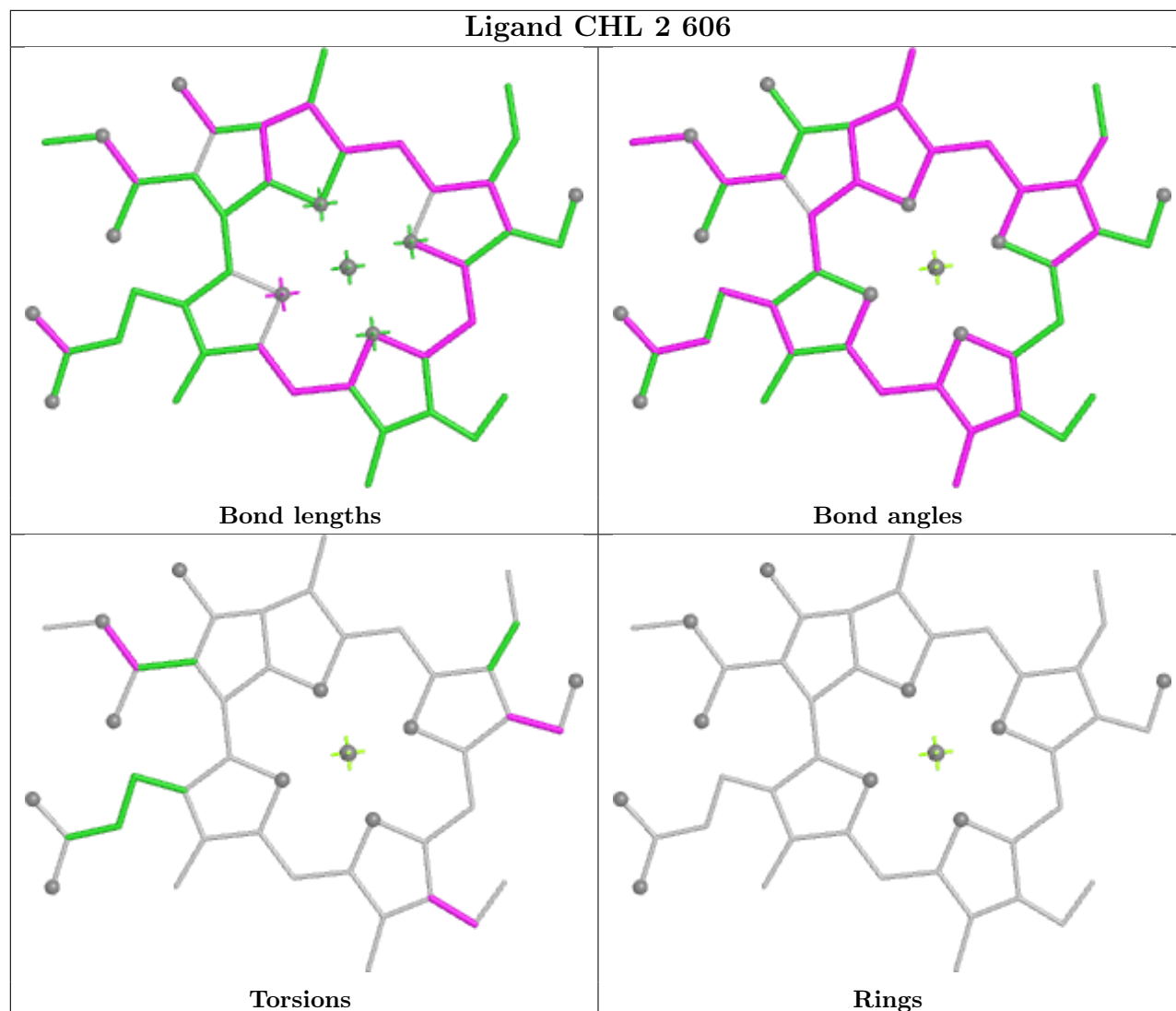


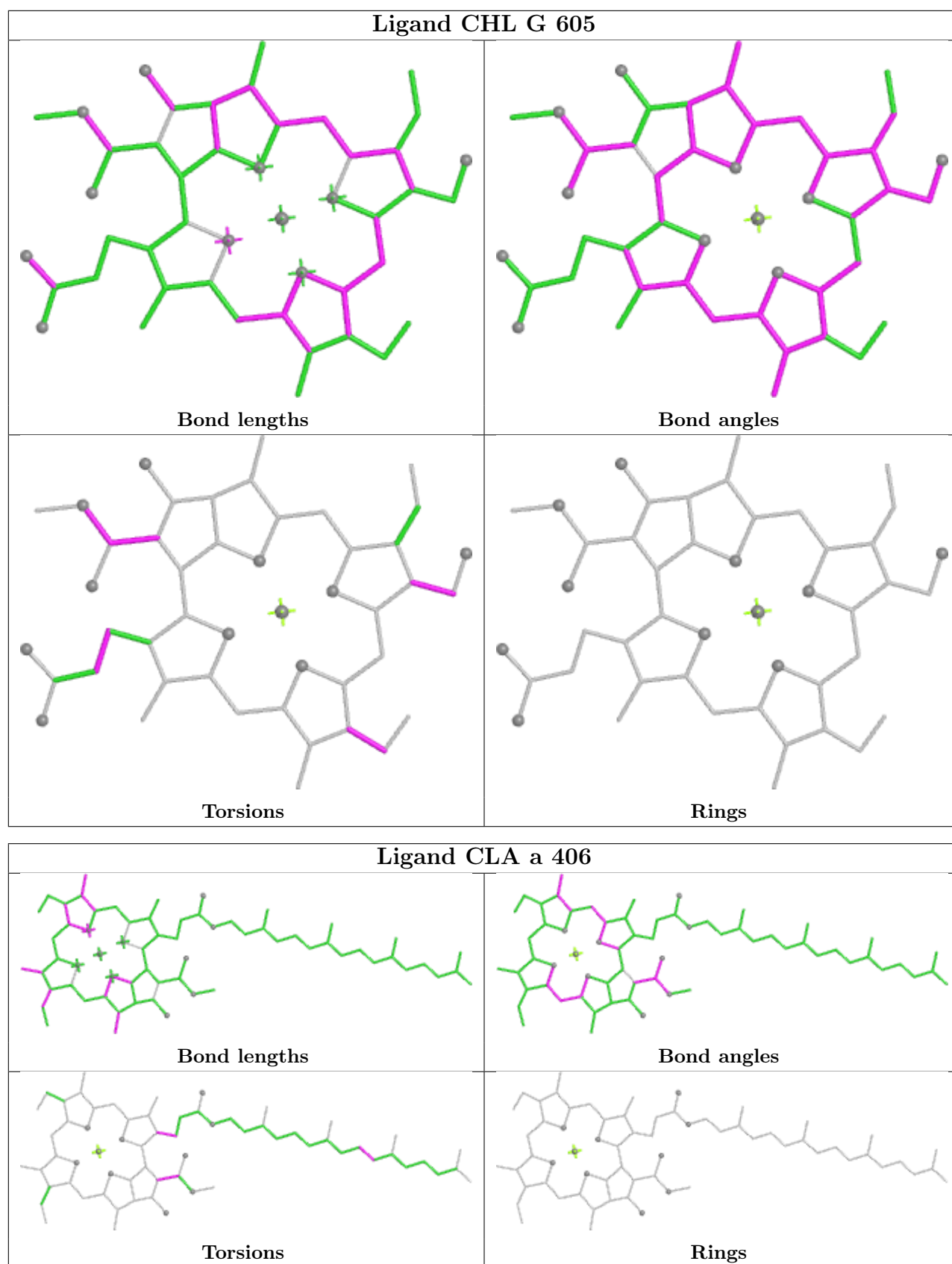
Torsions

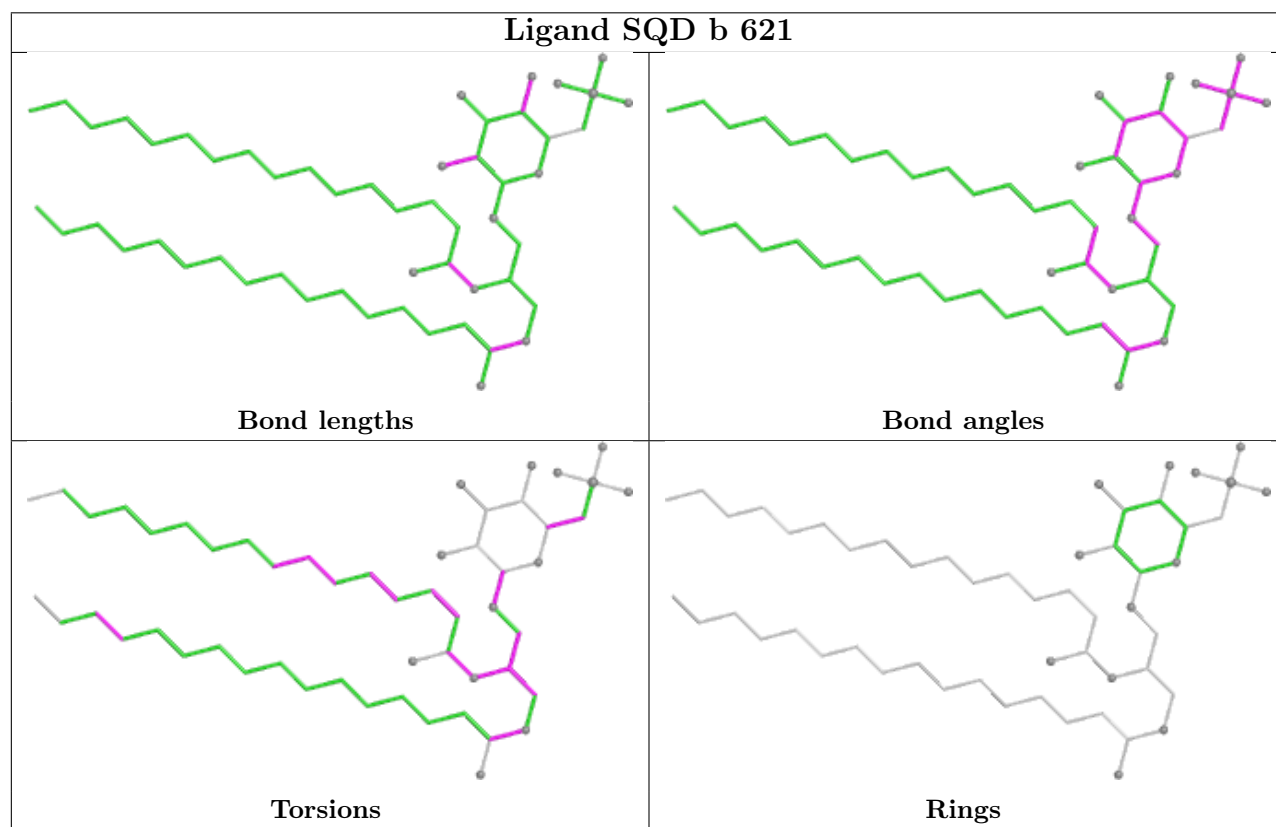
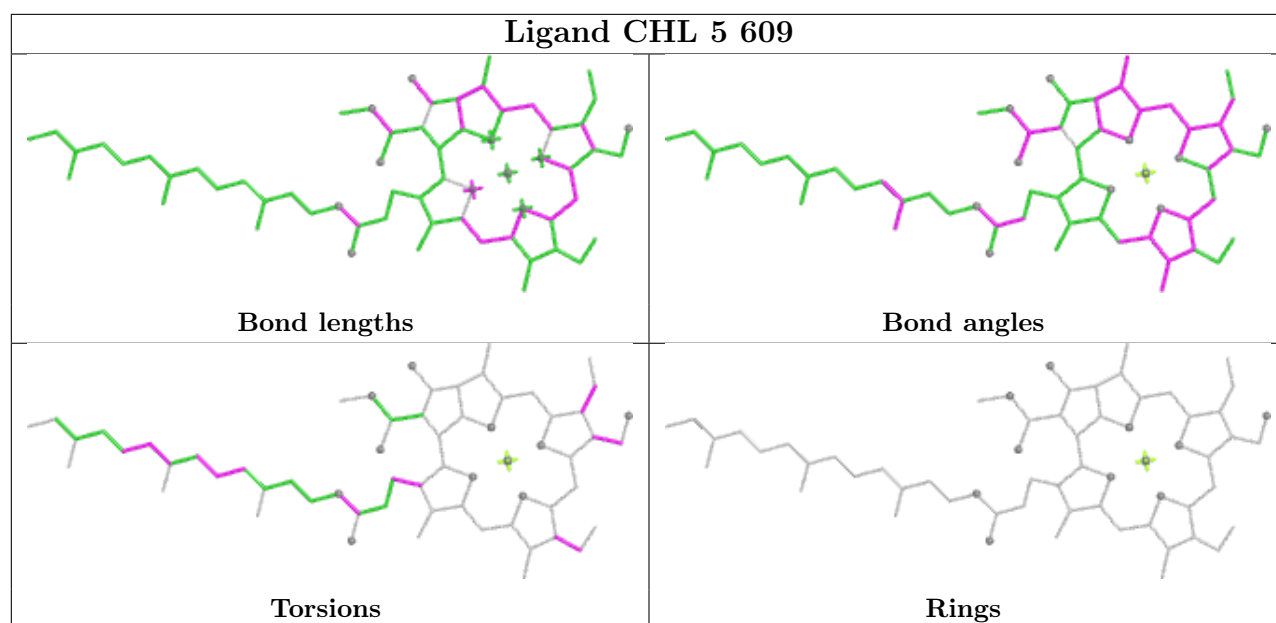


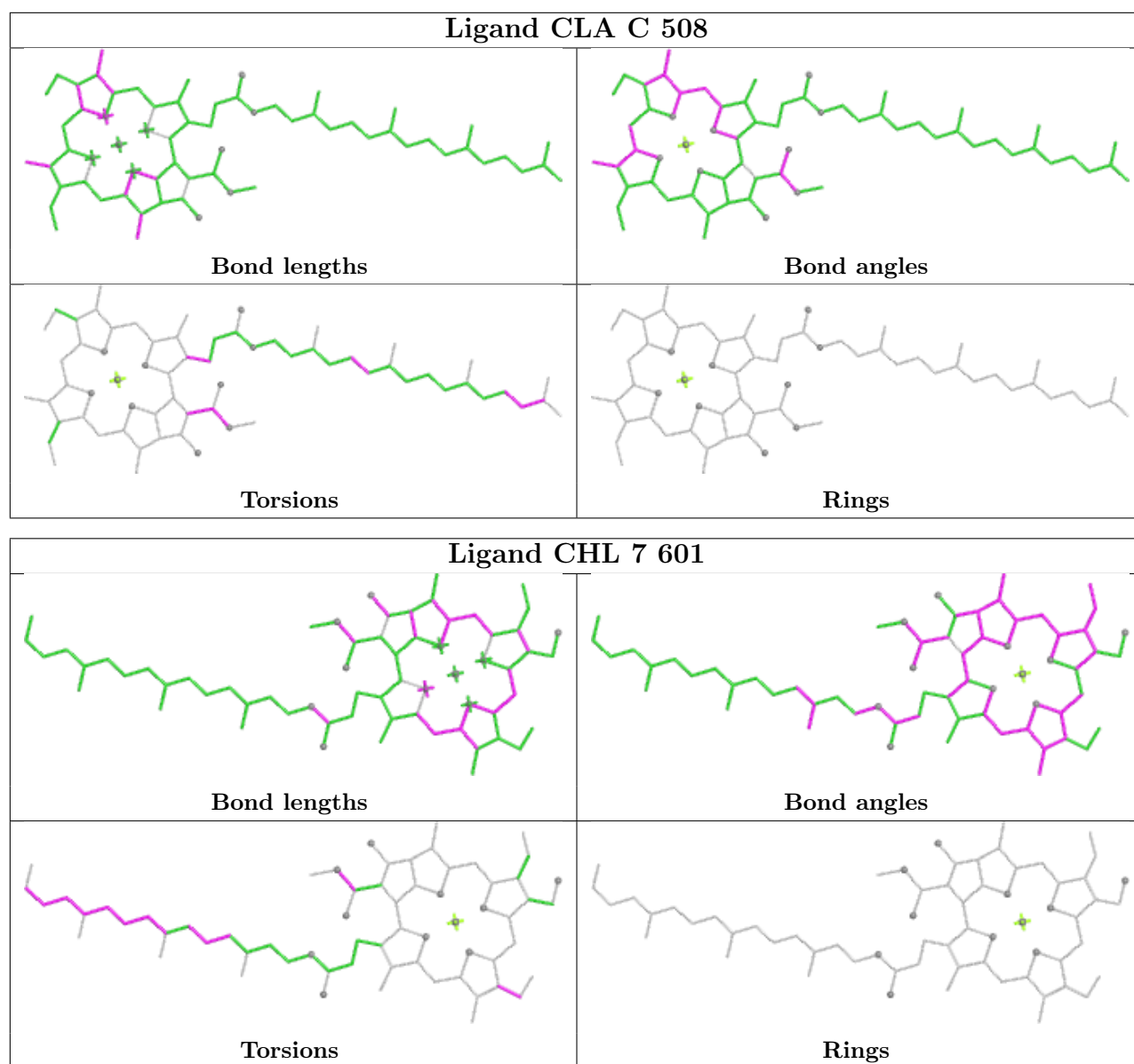
Rings

Ligand CHL 2 606

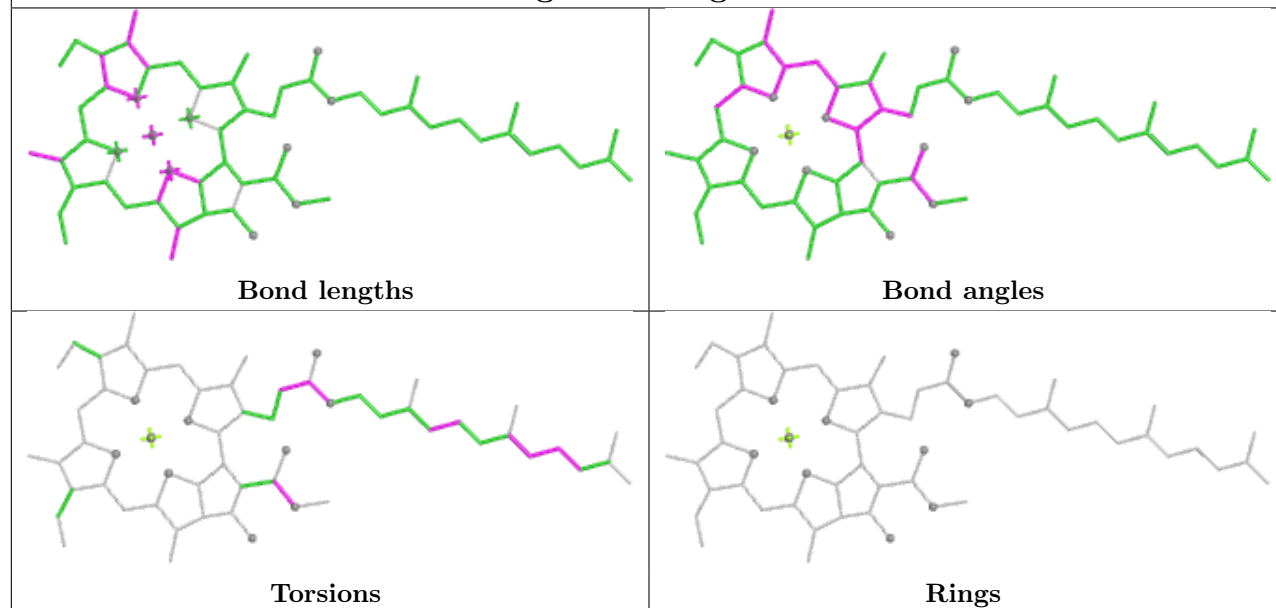




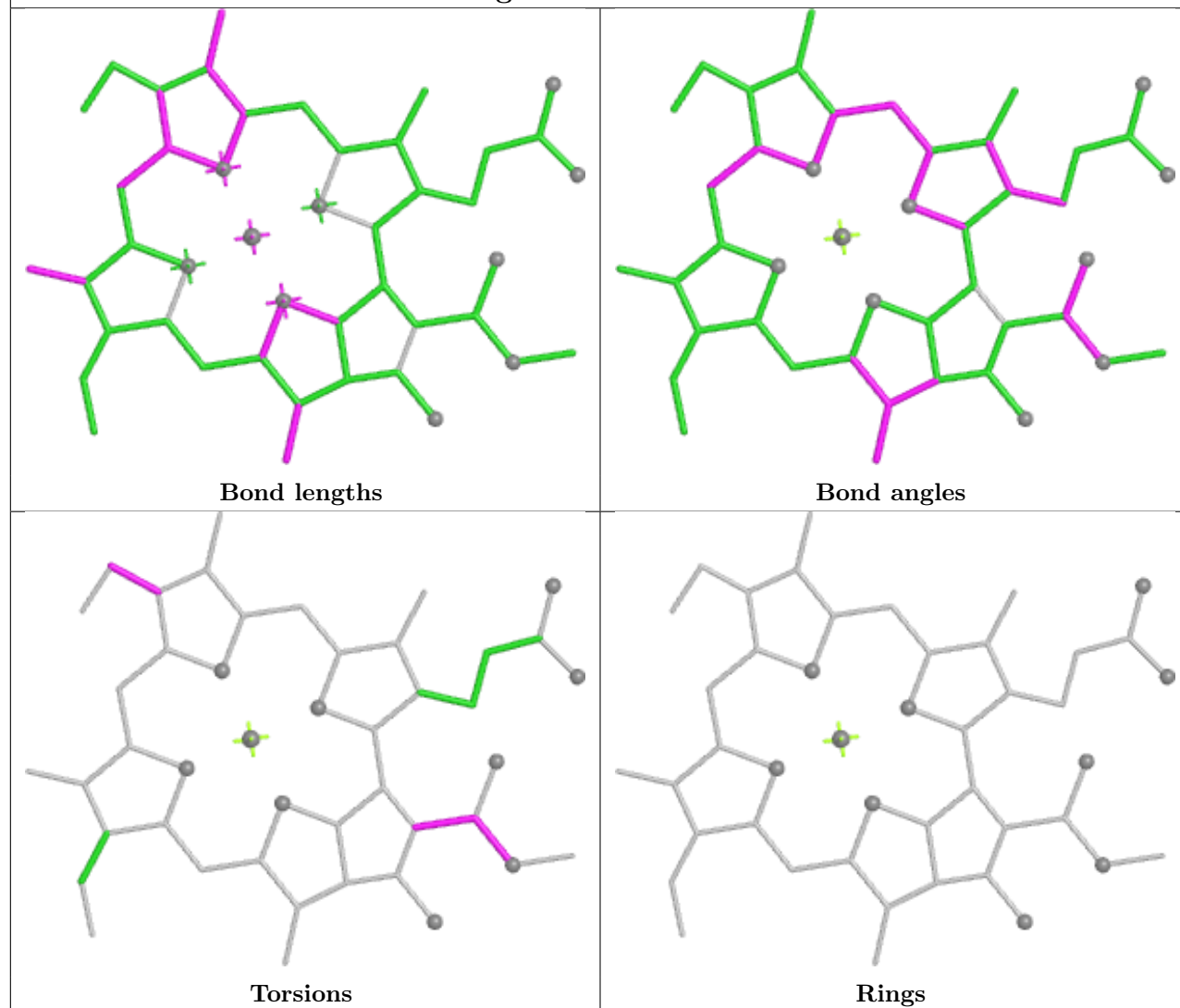


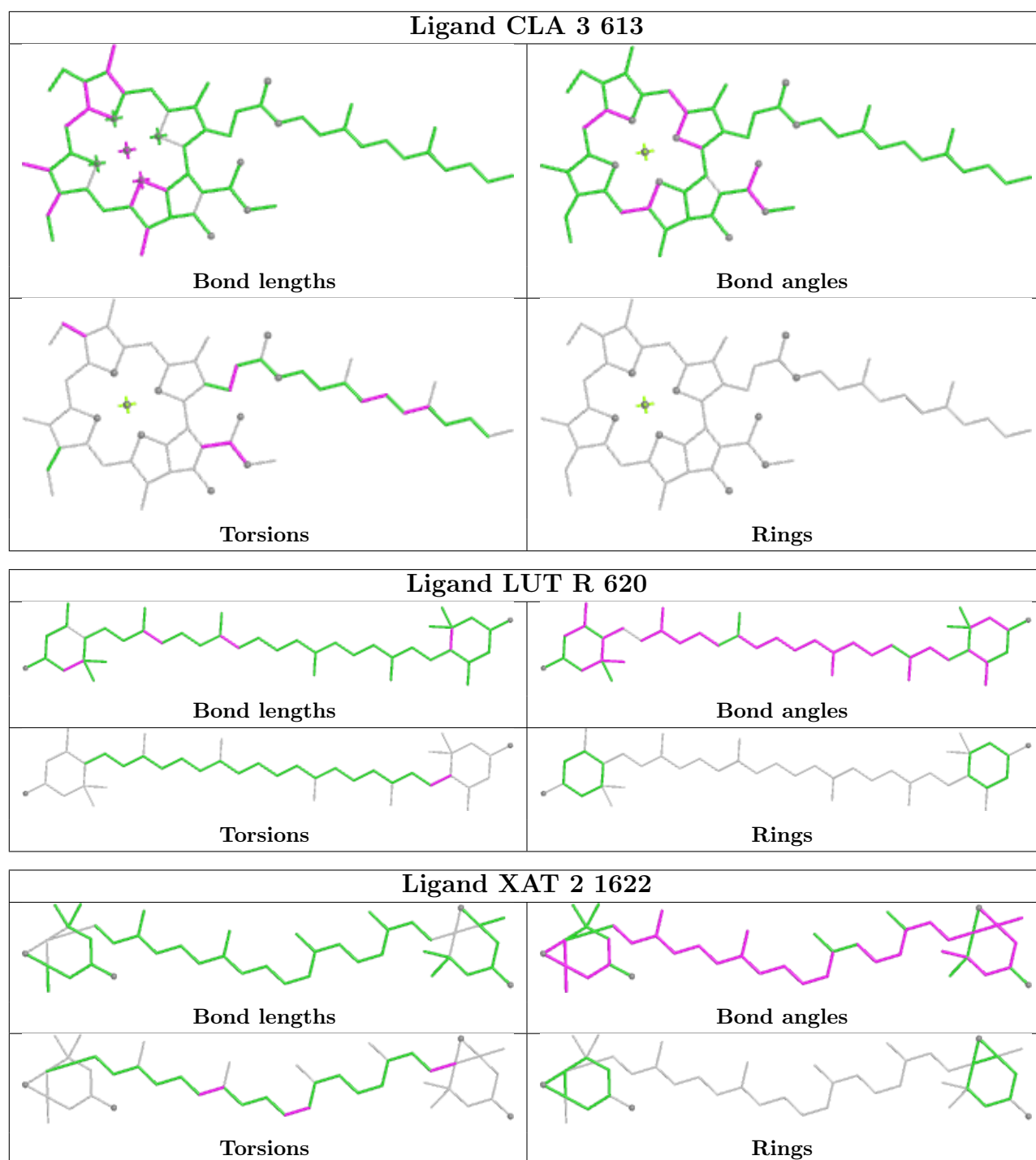


Ligand CLA g 612

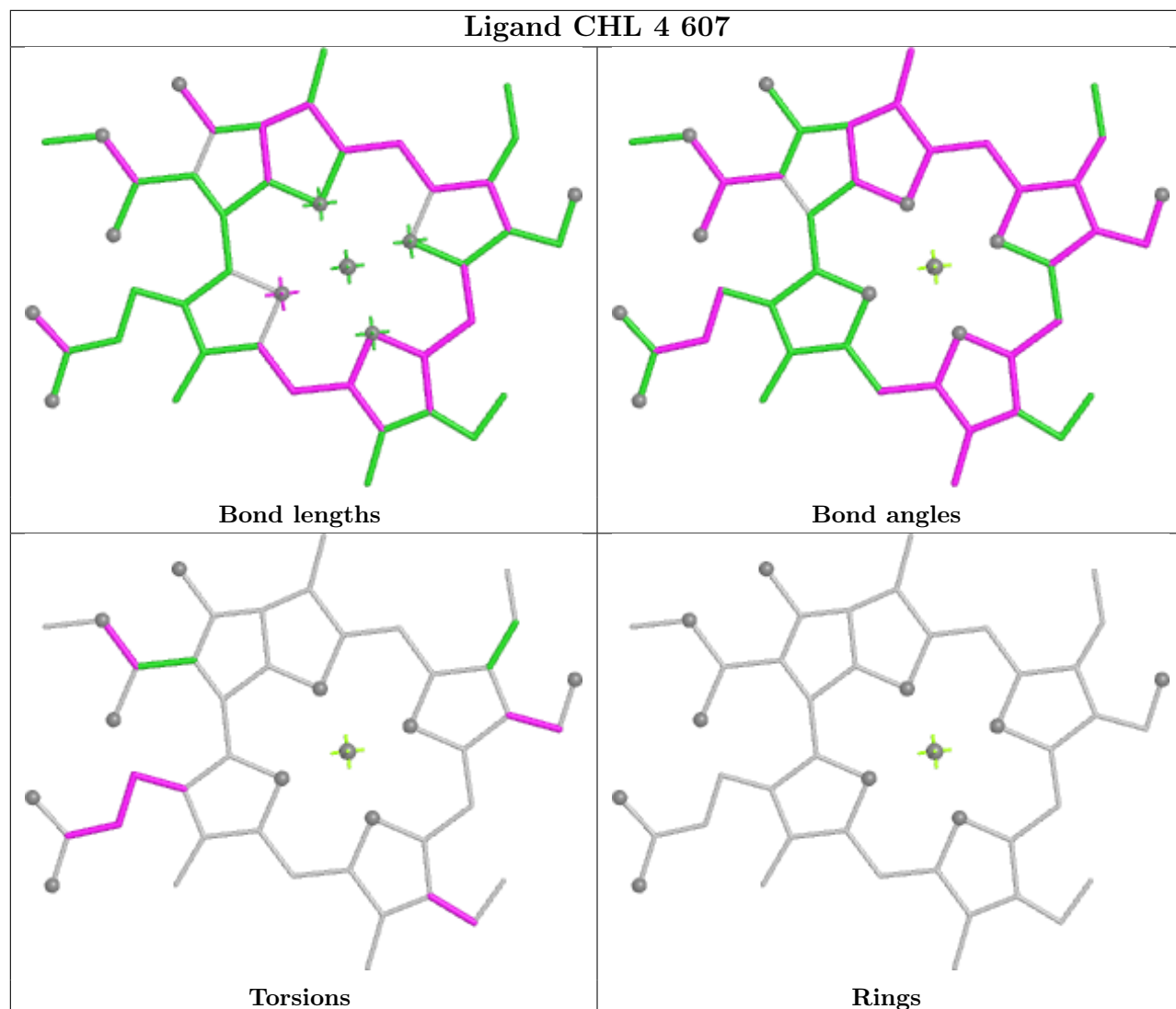


Ligand CLA 3 612

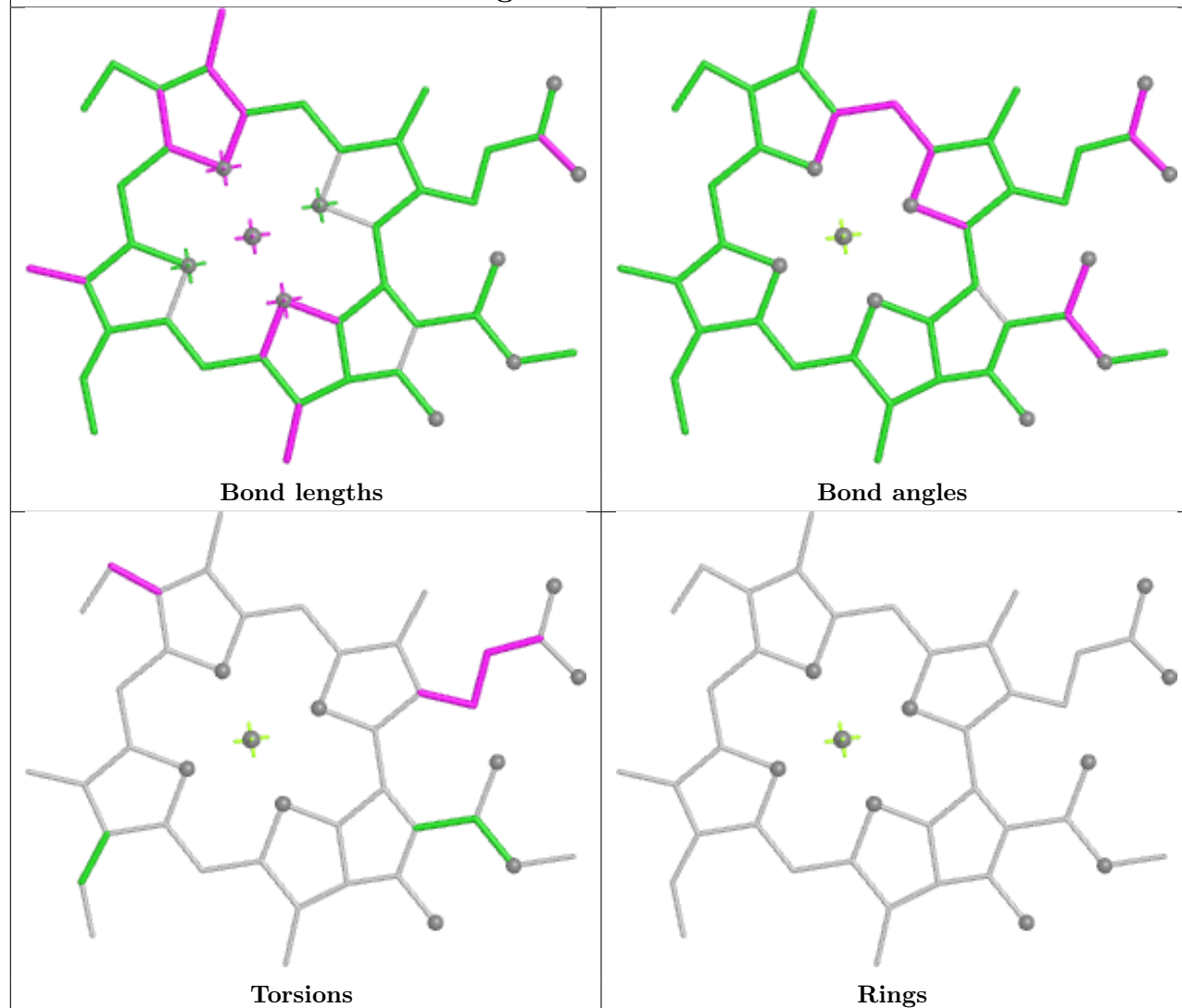




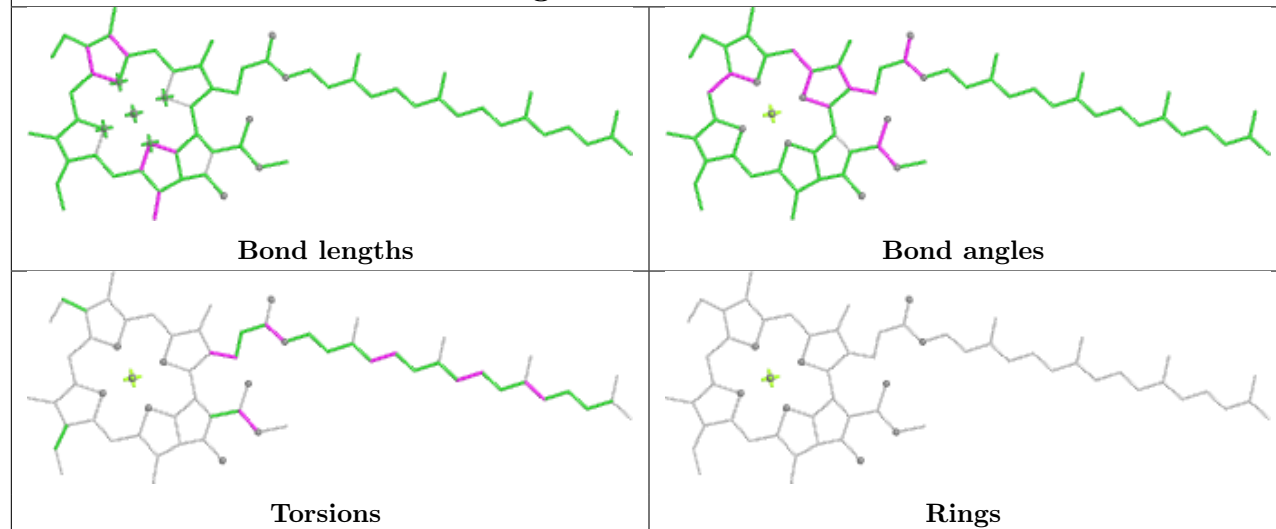
Ligand CHL 4 607

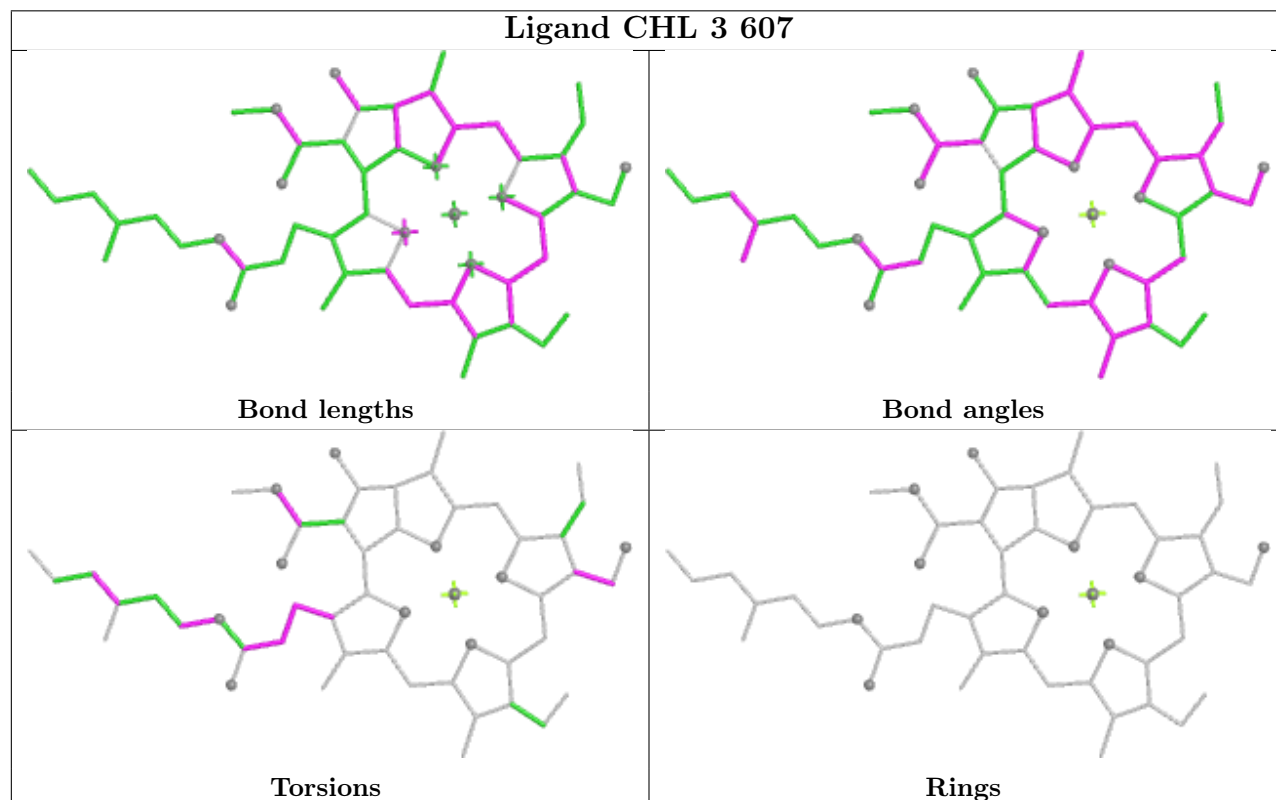
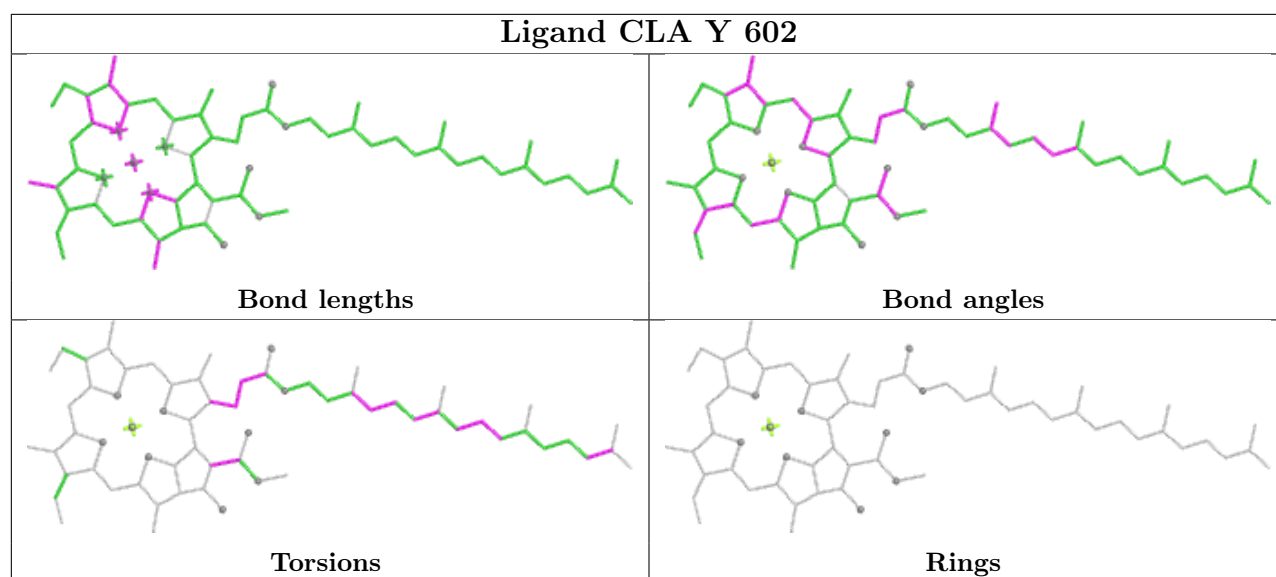


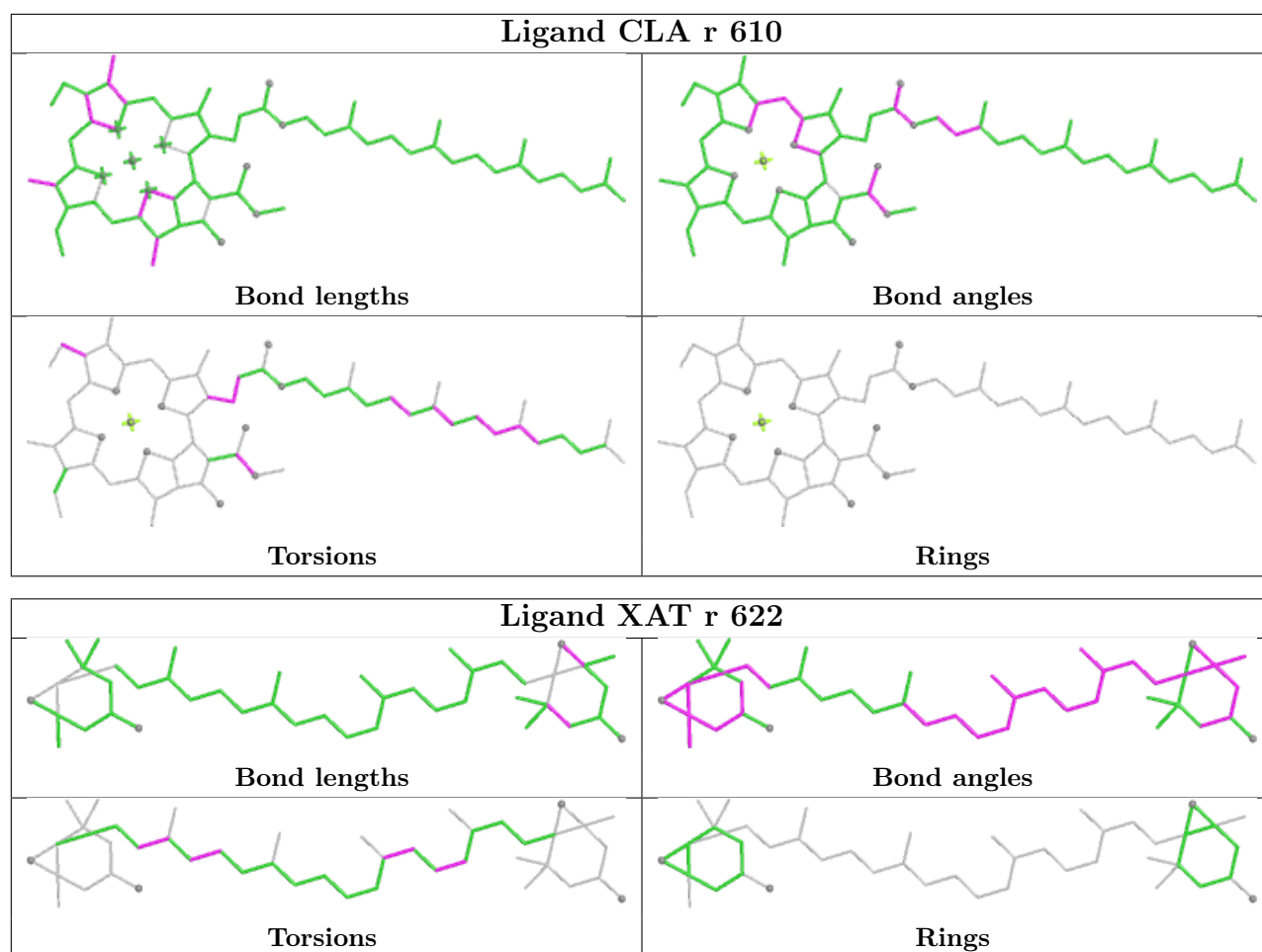
Ligand CLA 5 611



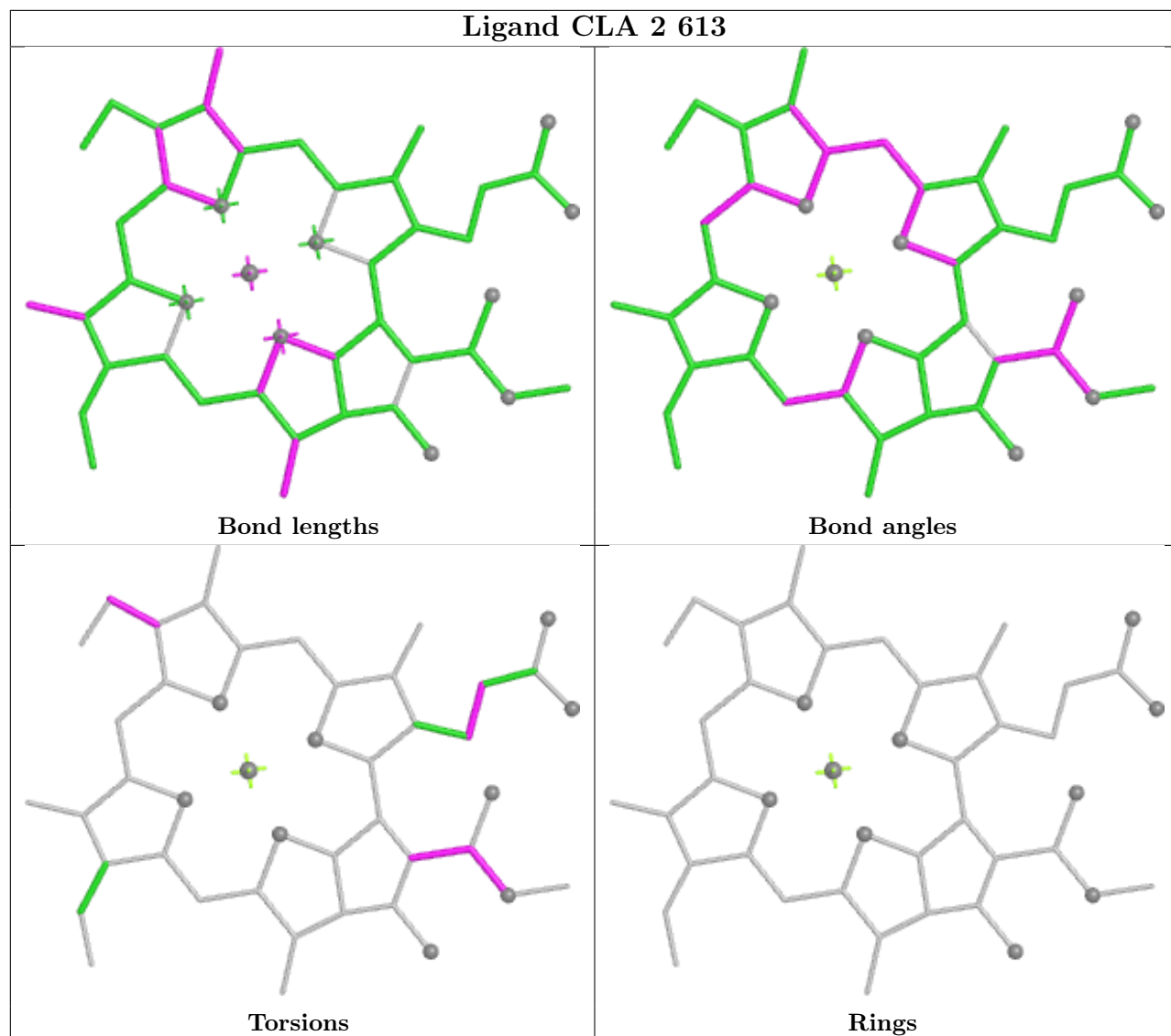
Ligand CLA C 512



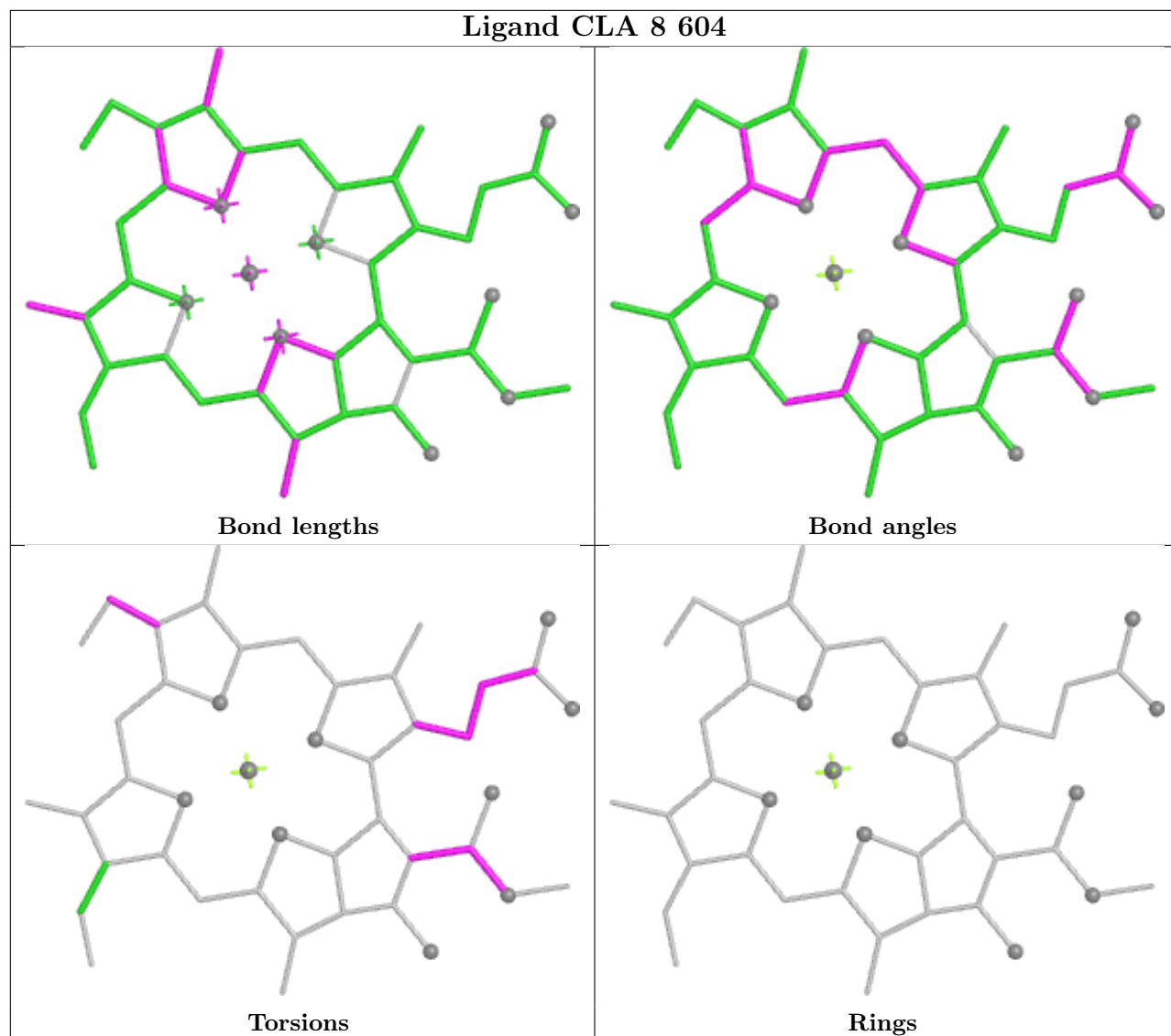


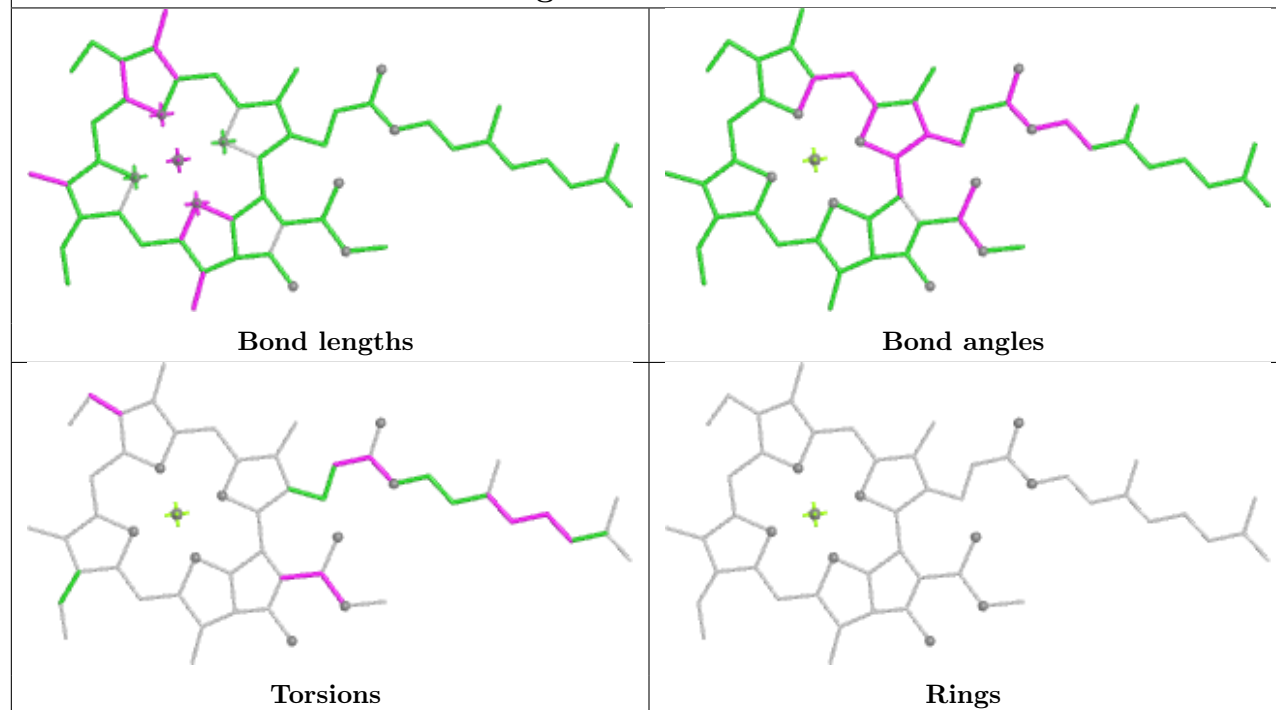
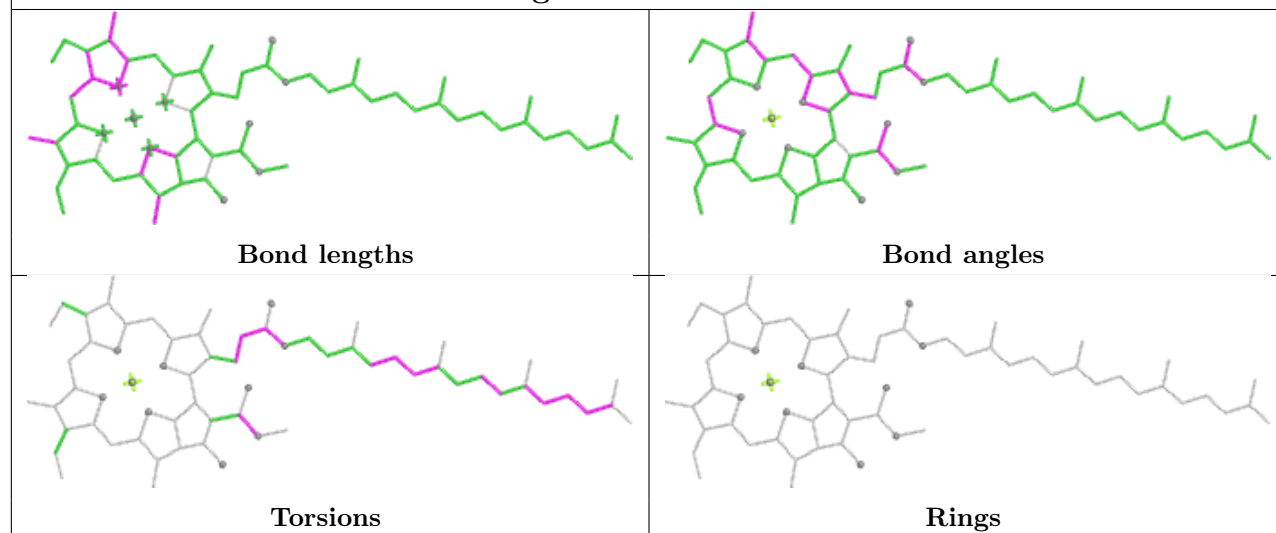


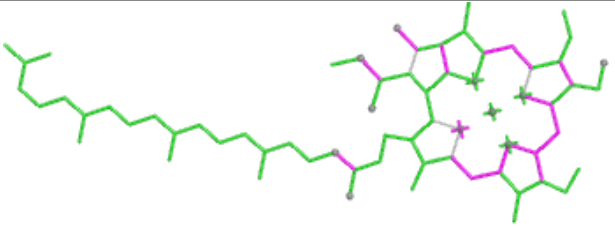
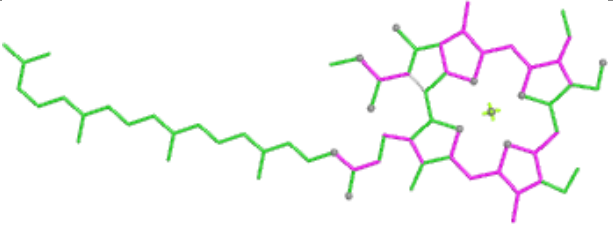
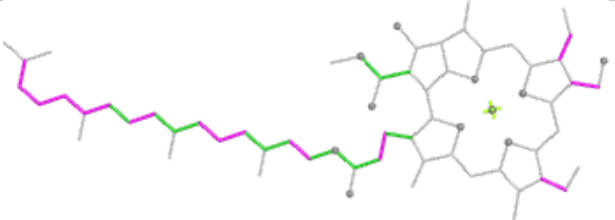
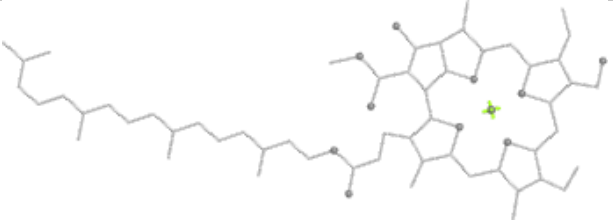
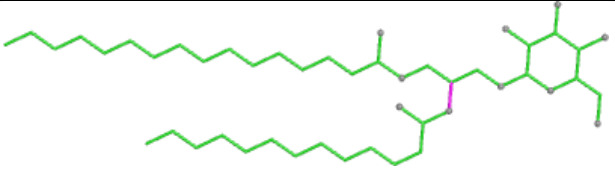
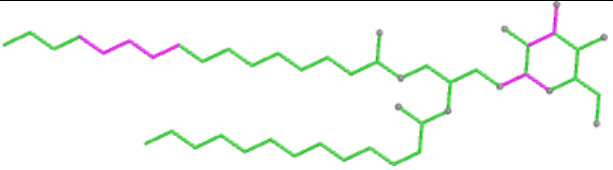
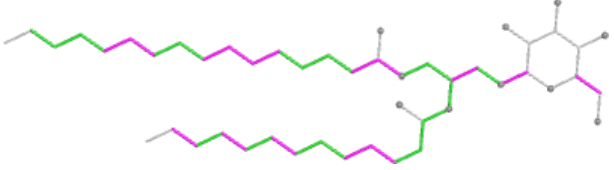
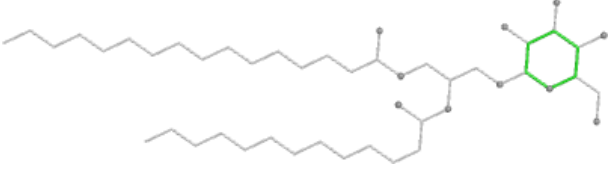
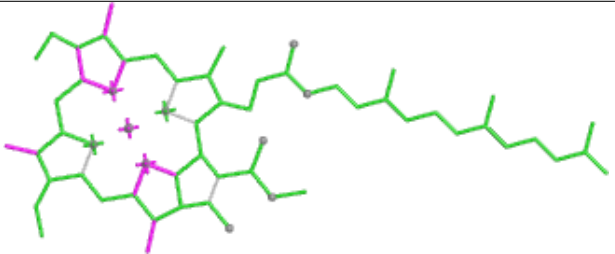
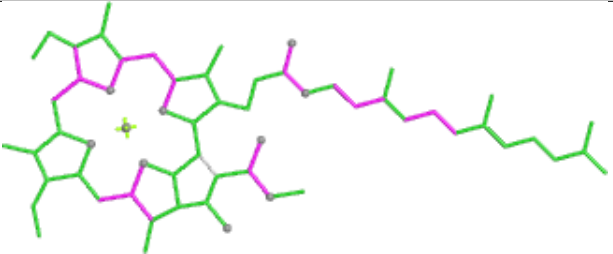
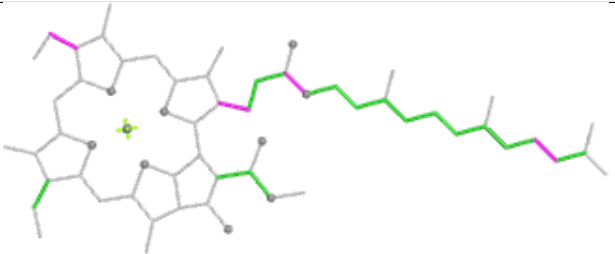
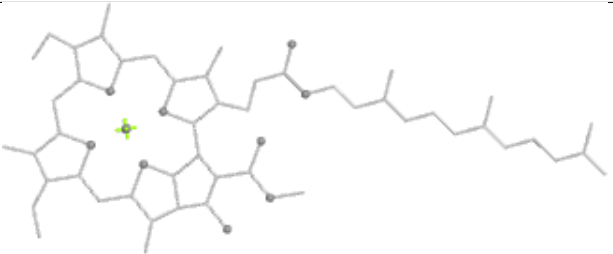
Ligand CLA 2 613

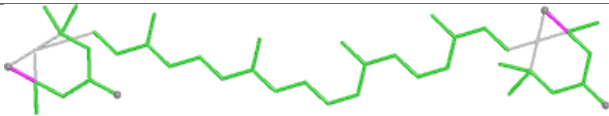
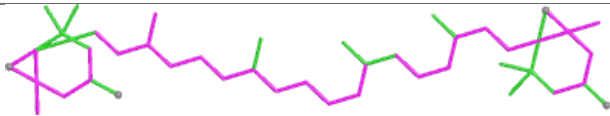
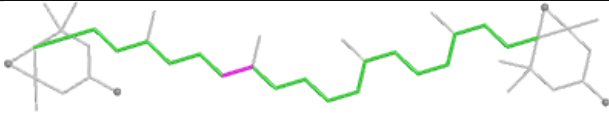
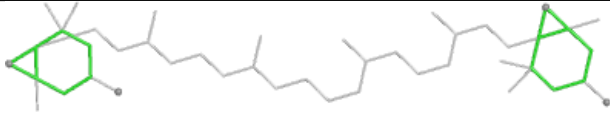


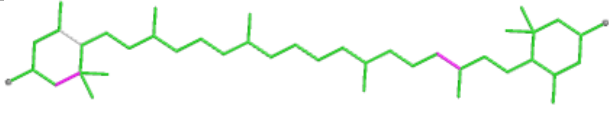
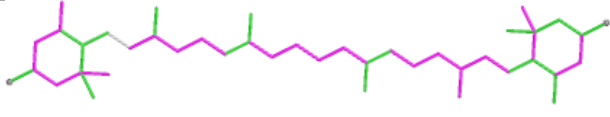
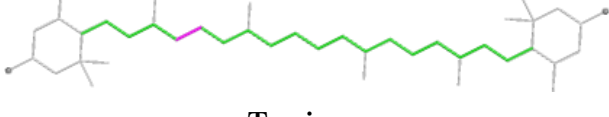
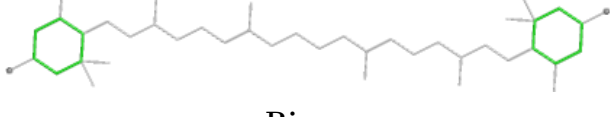
Ligand CLA 8 604



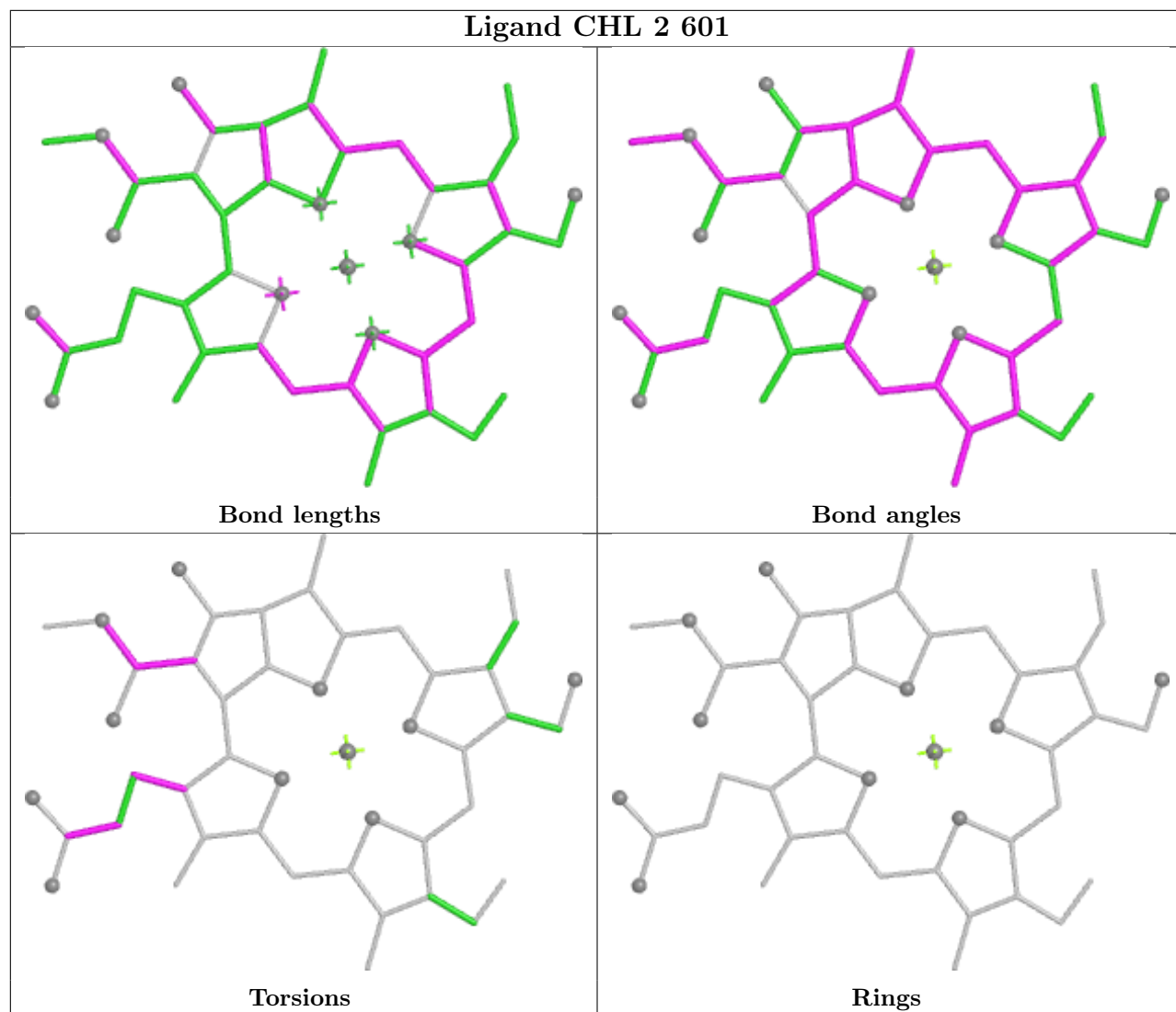
Ligand CLA 2 603**Ligand CLA B 617**

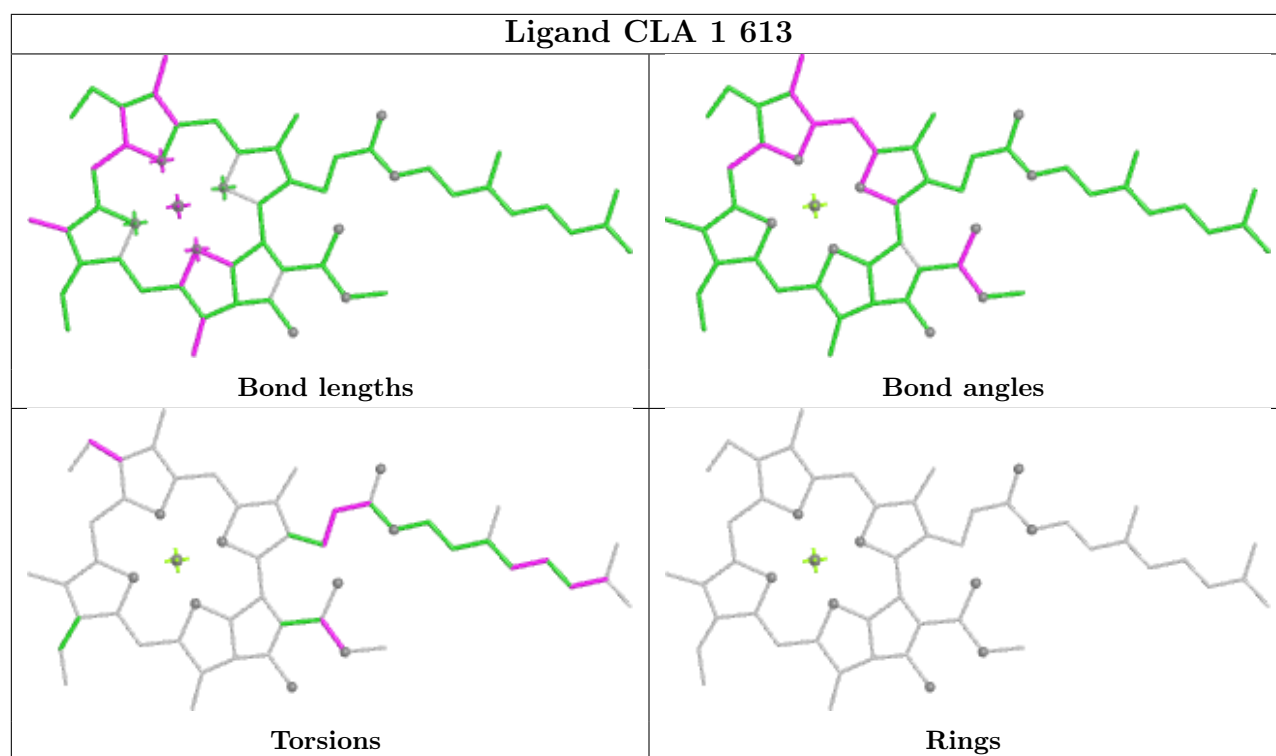
Ligand CHL Y 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 7 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 1 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

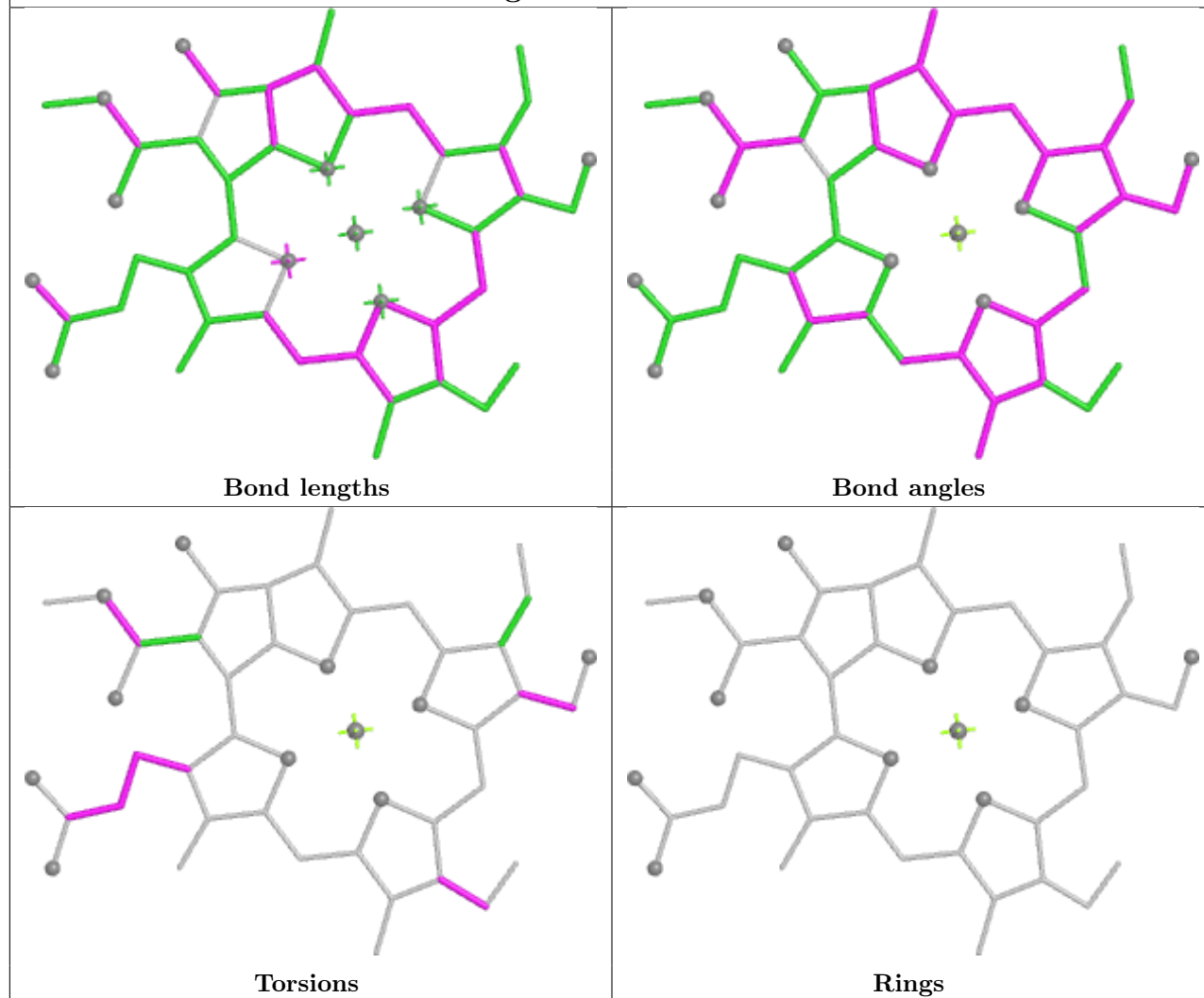
Ligand LUT n 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 2 601

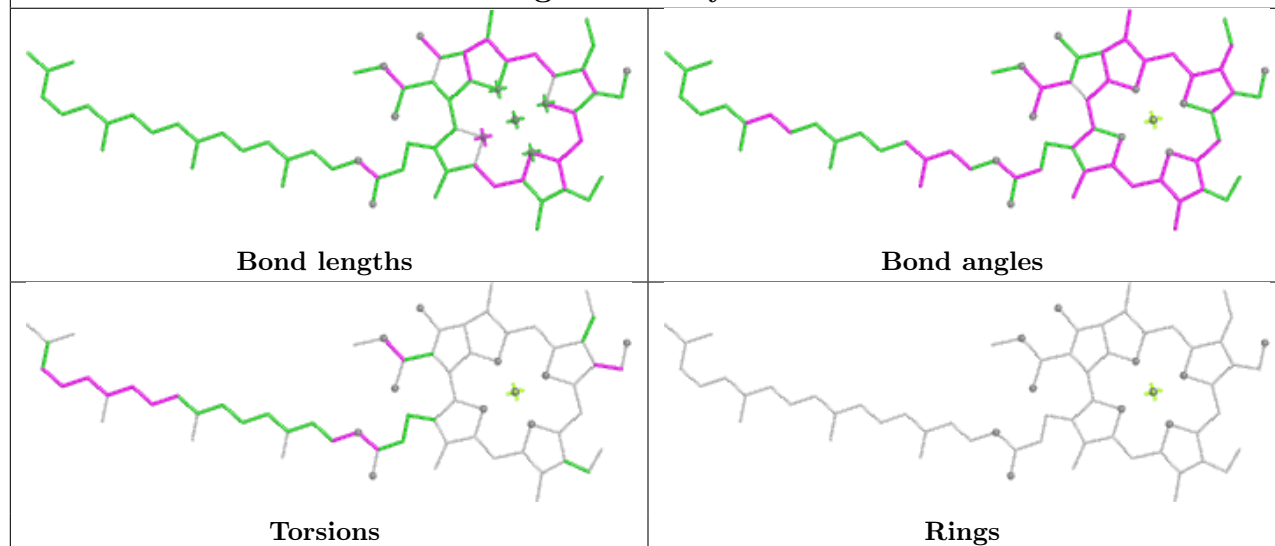


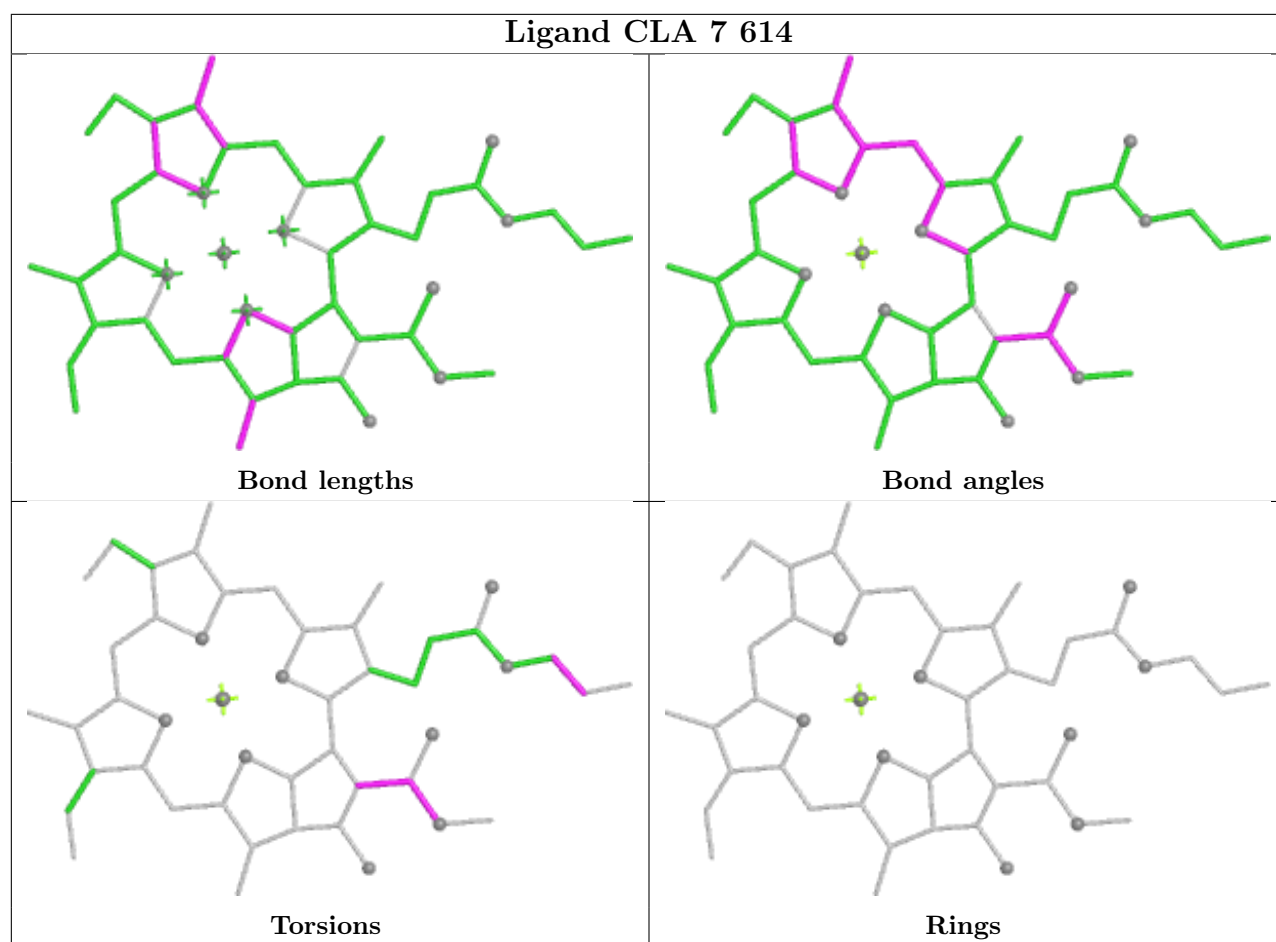


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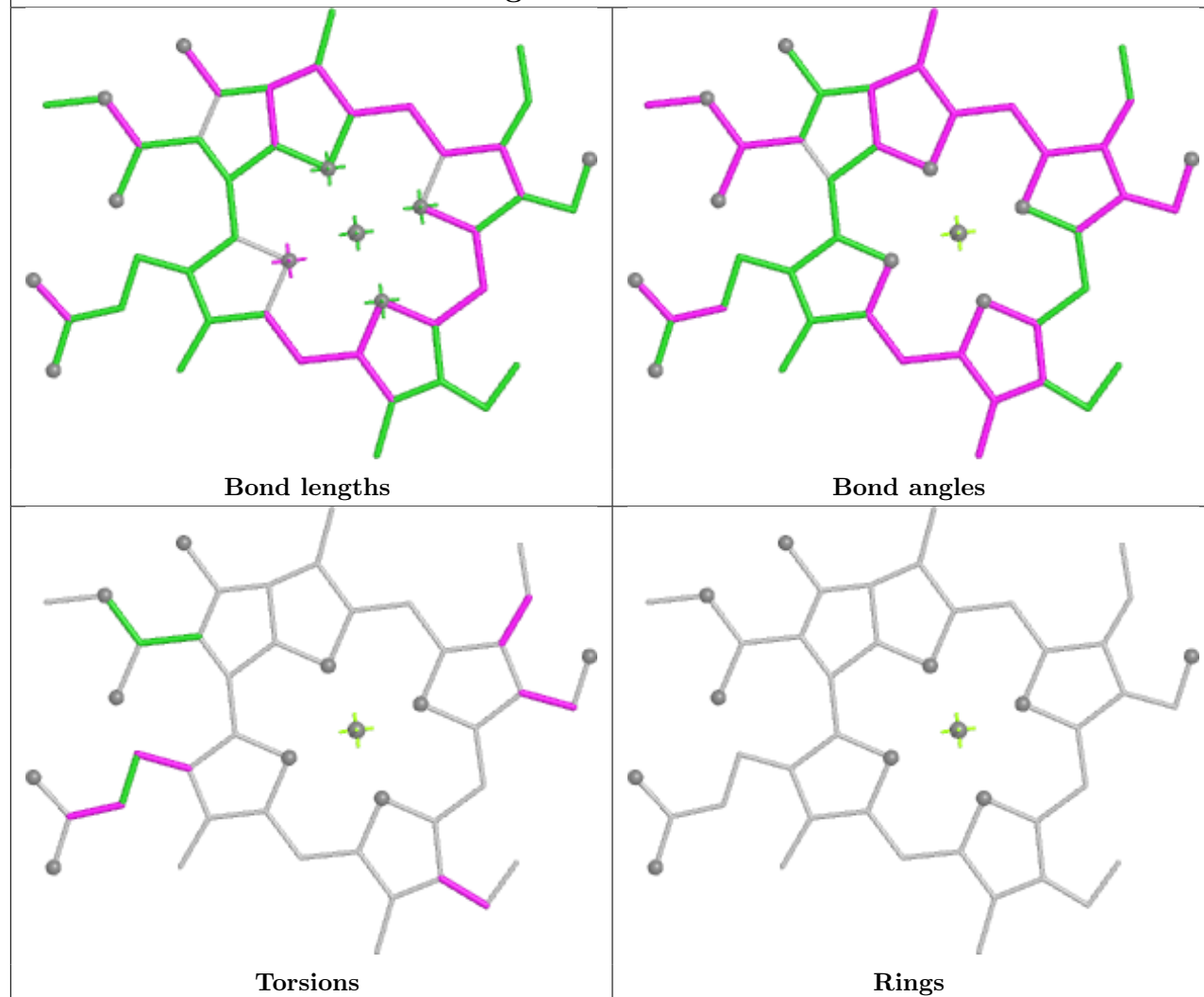


Ligand CHL y 609

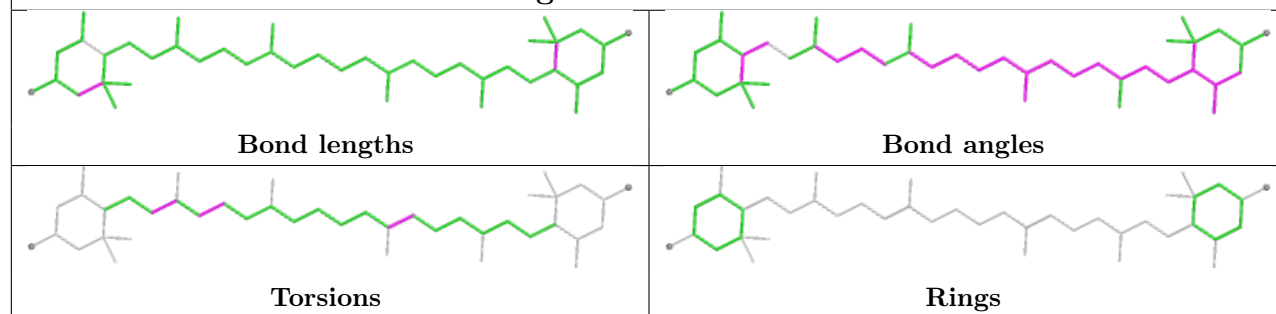


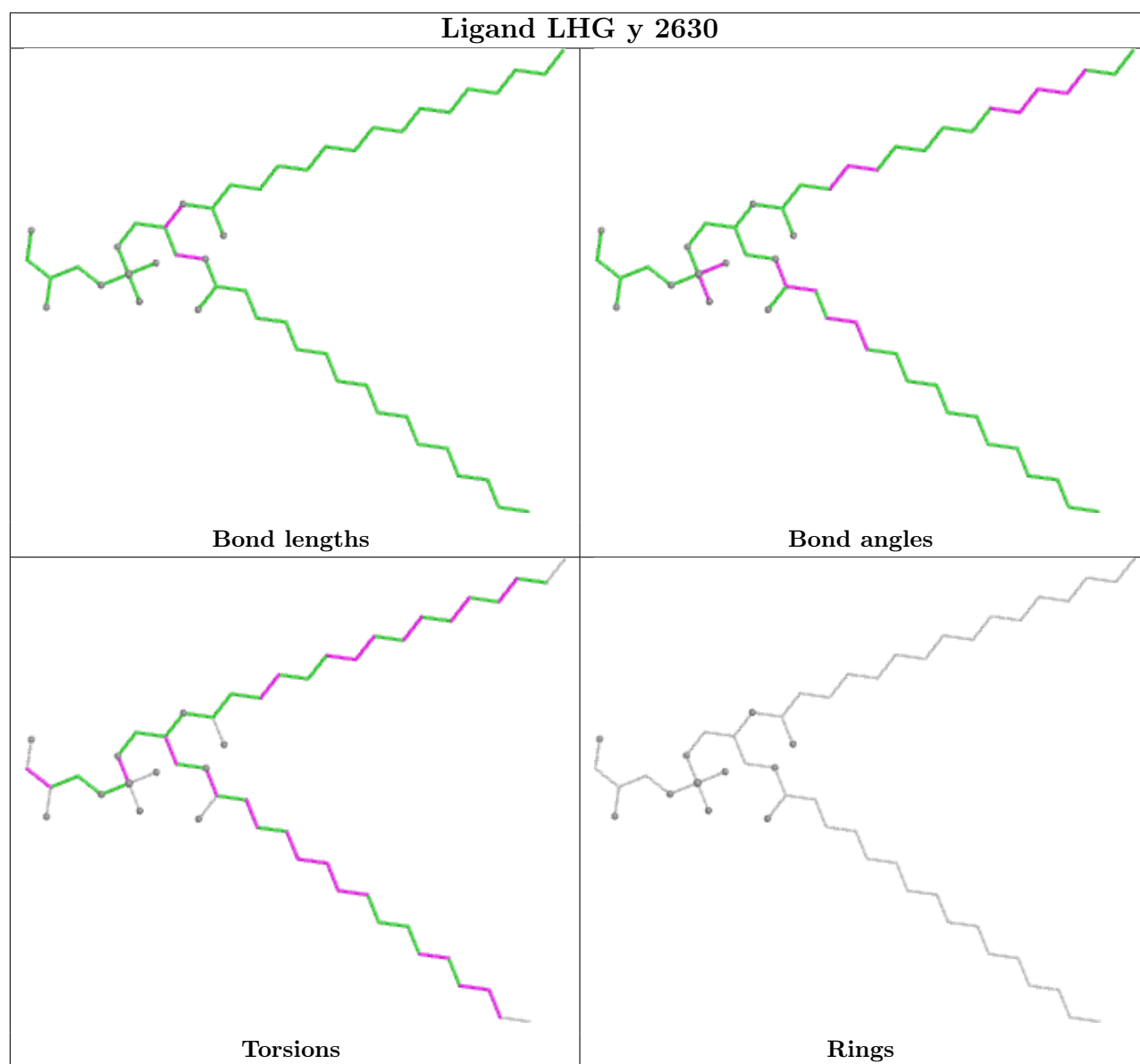


Ligand CHL 4 609

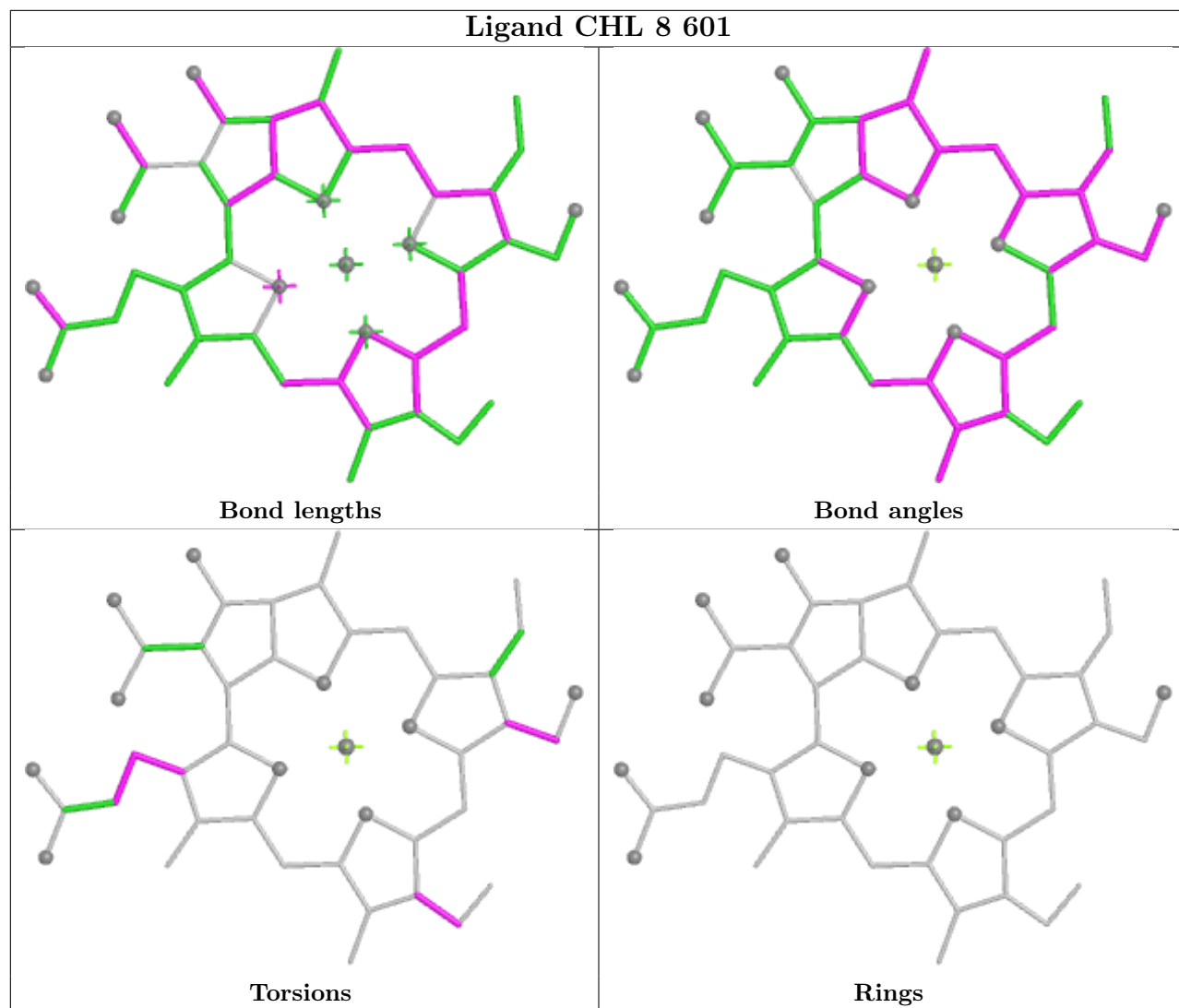


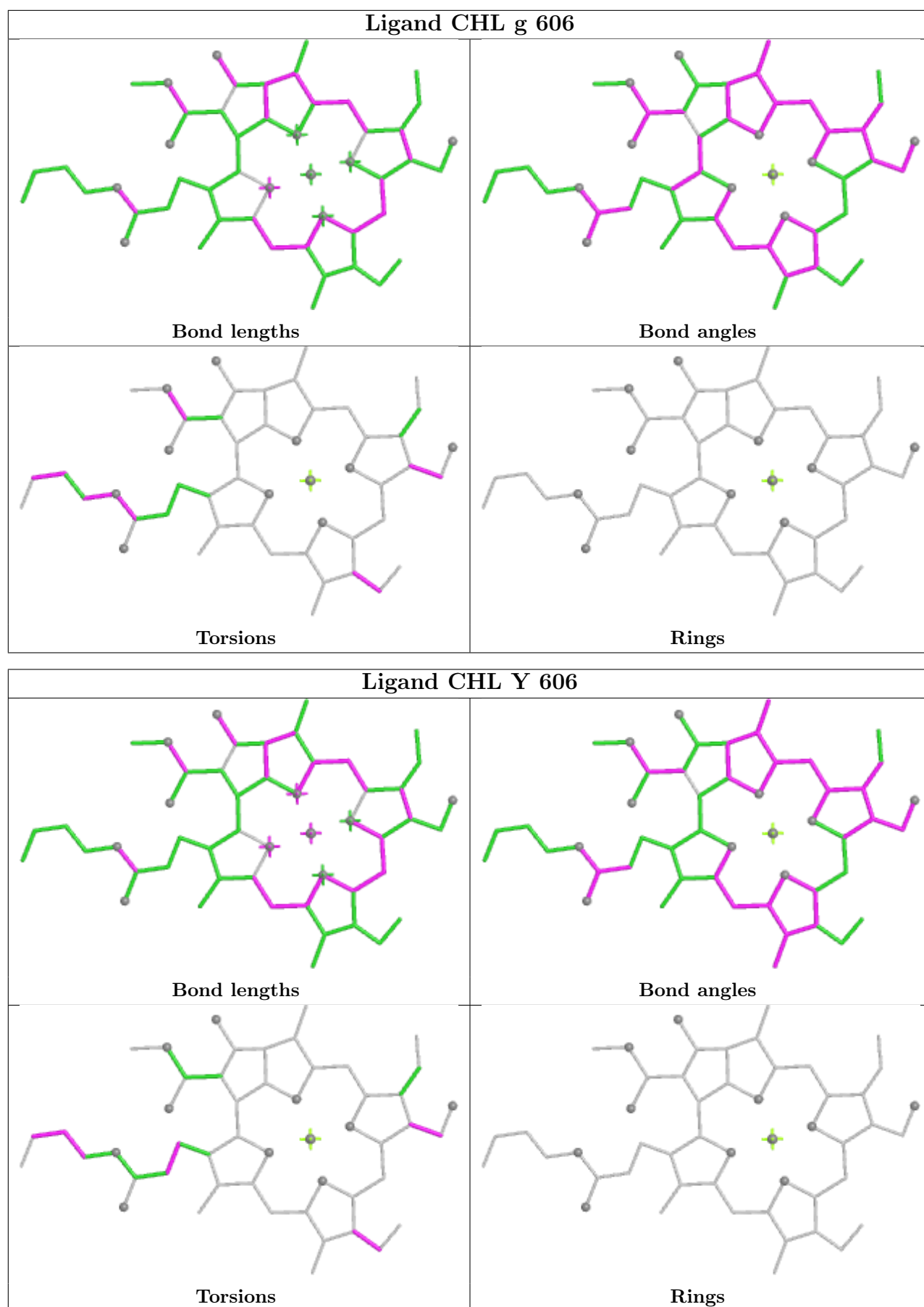
Ligand LUT 4 620



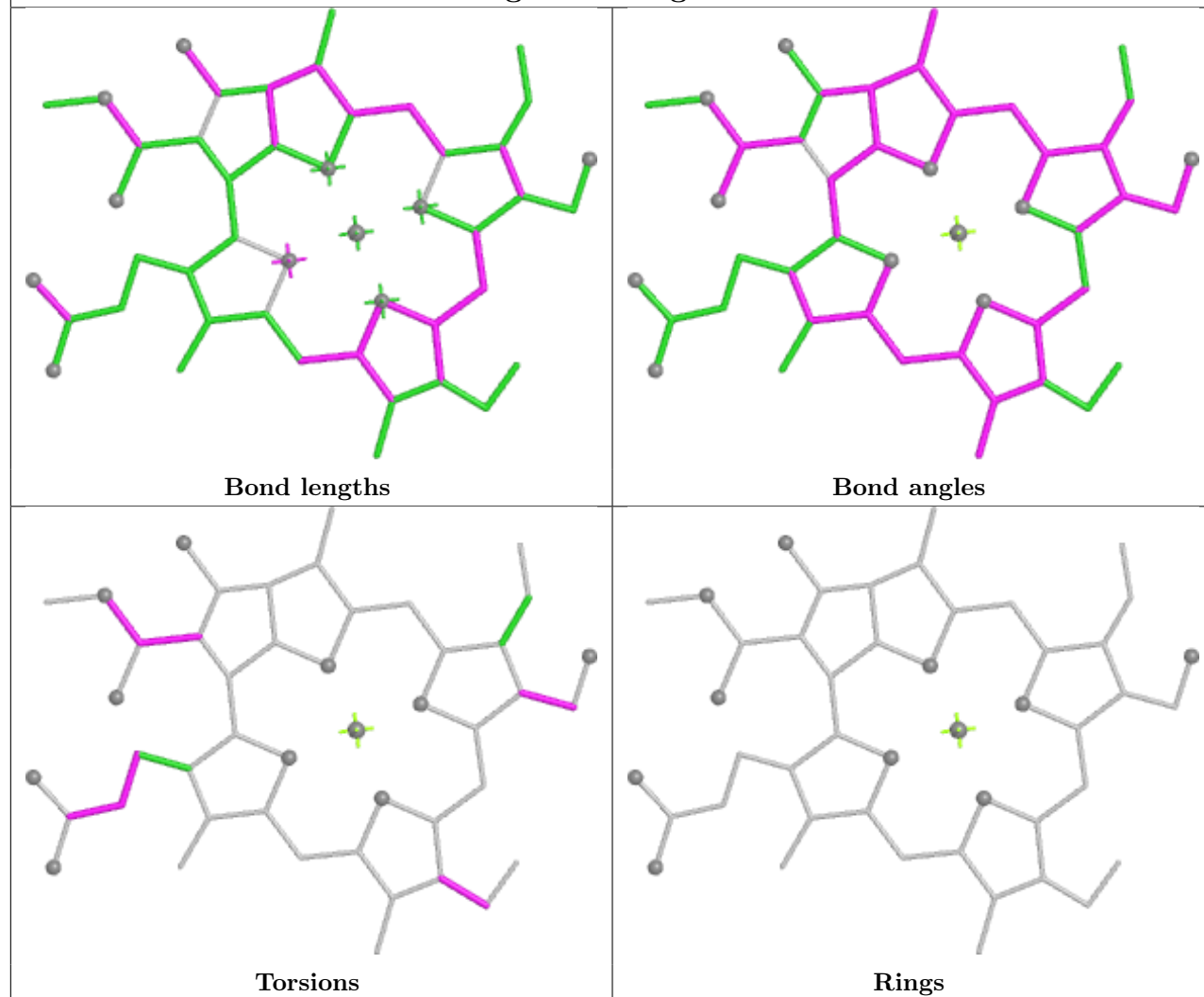


Ligand CHL 8 601

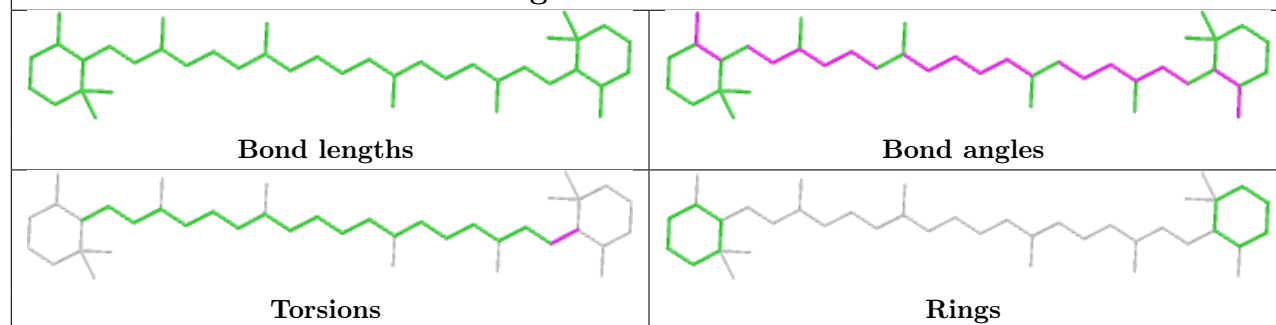


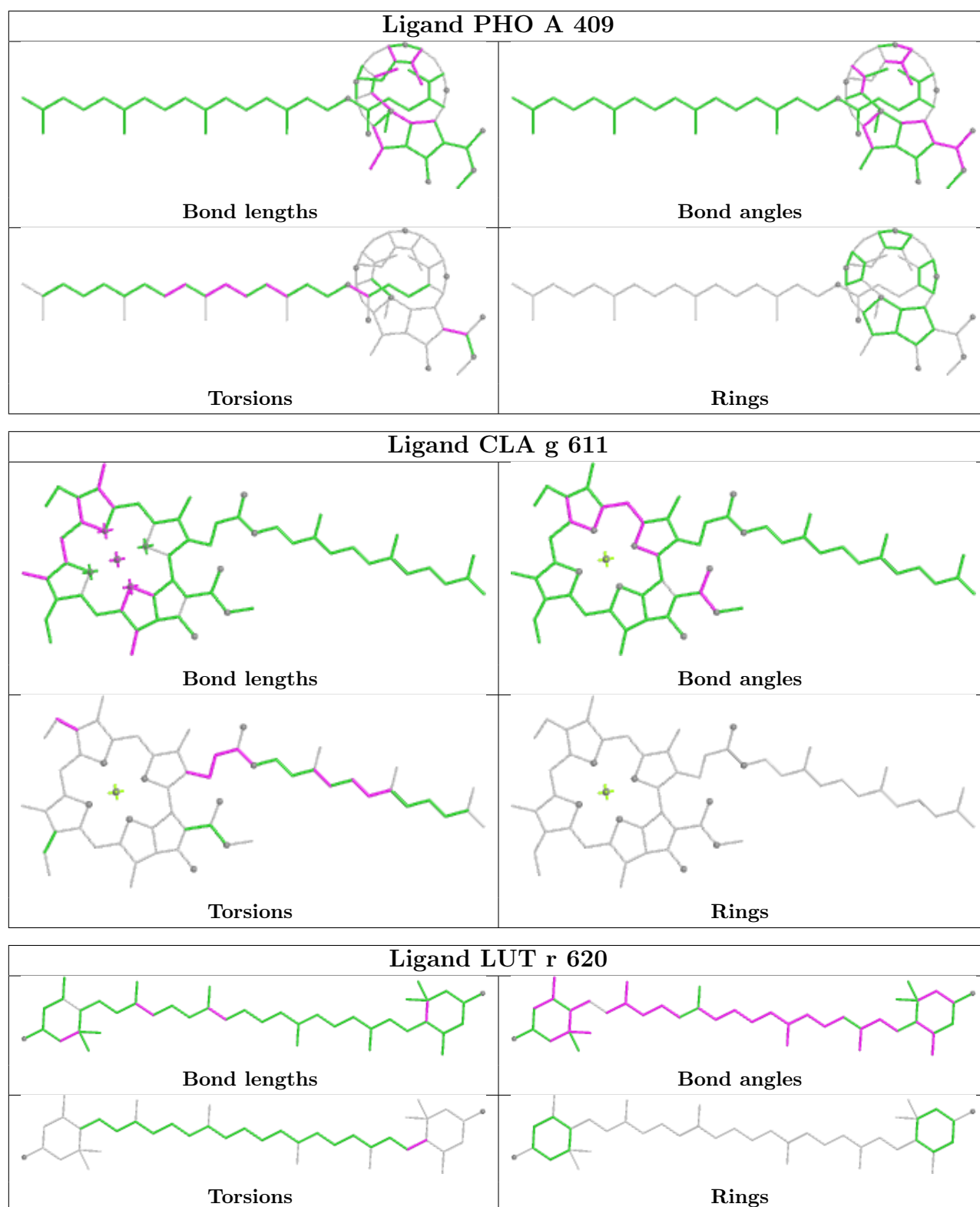


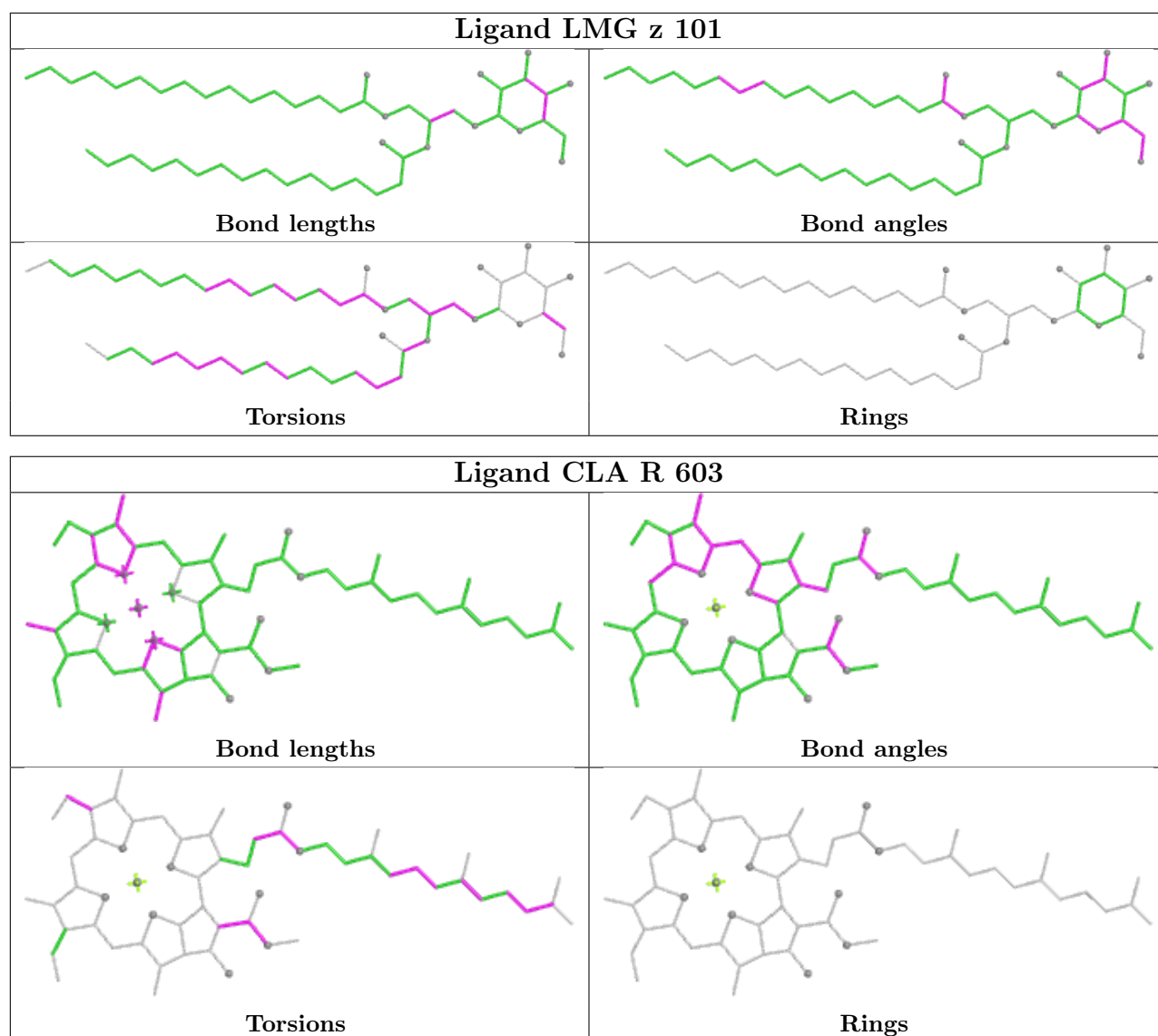
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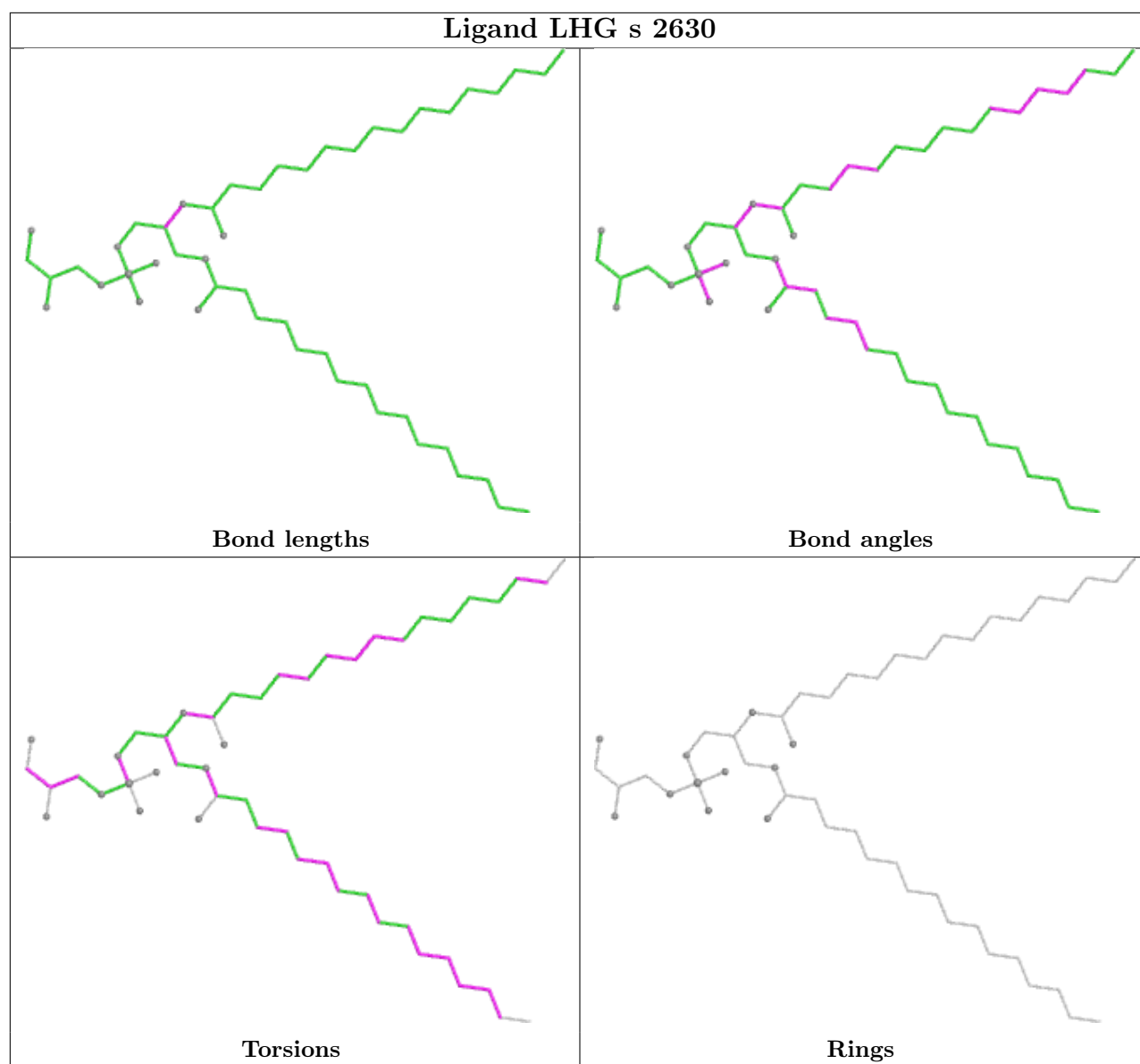


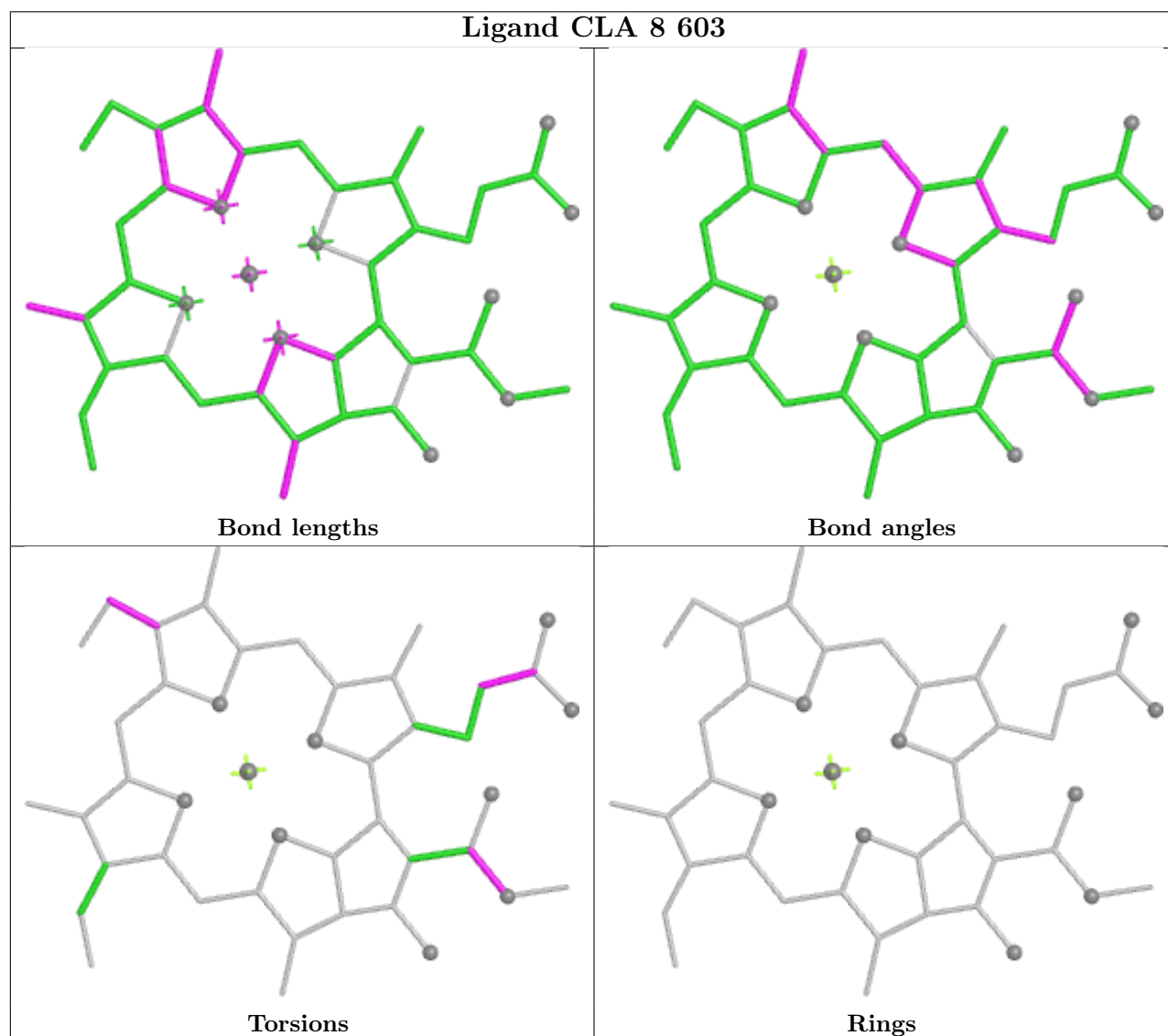
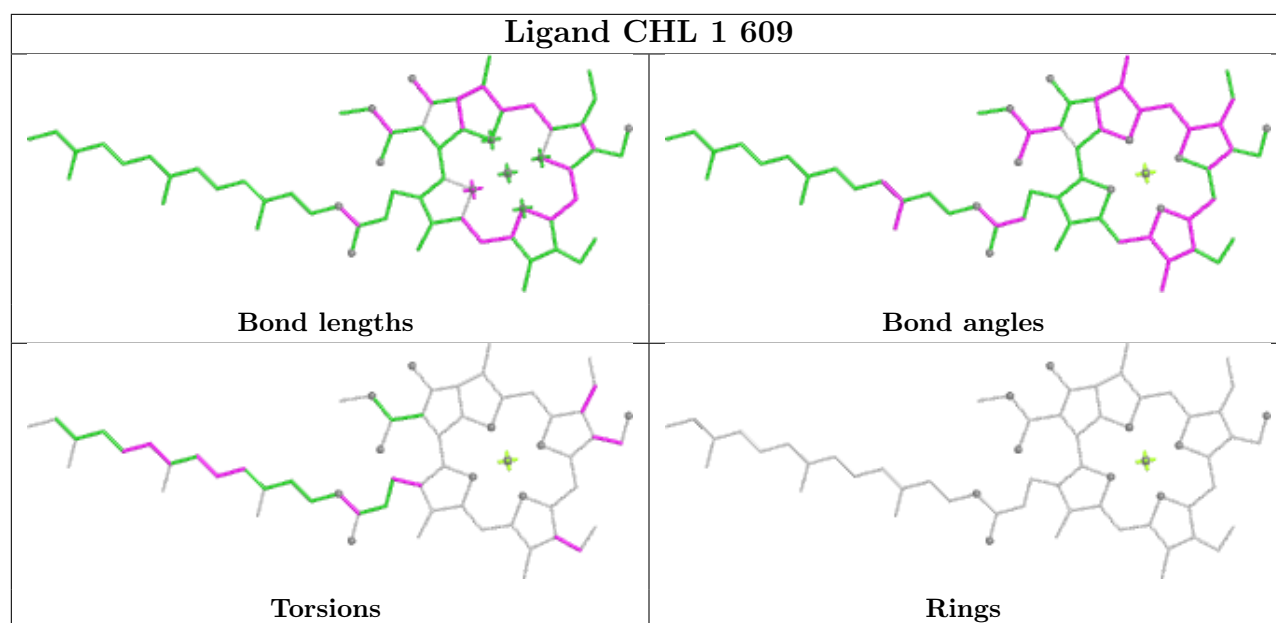
Ligand BCR A 411



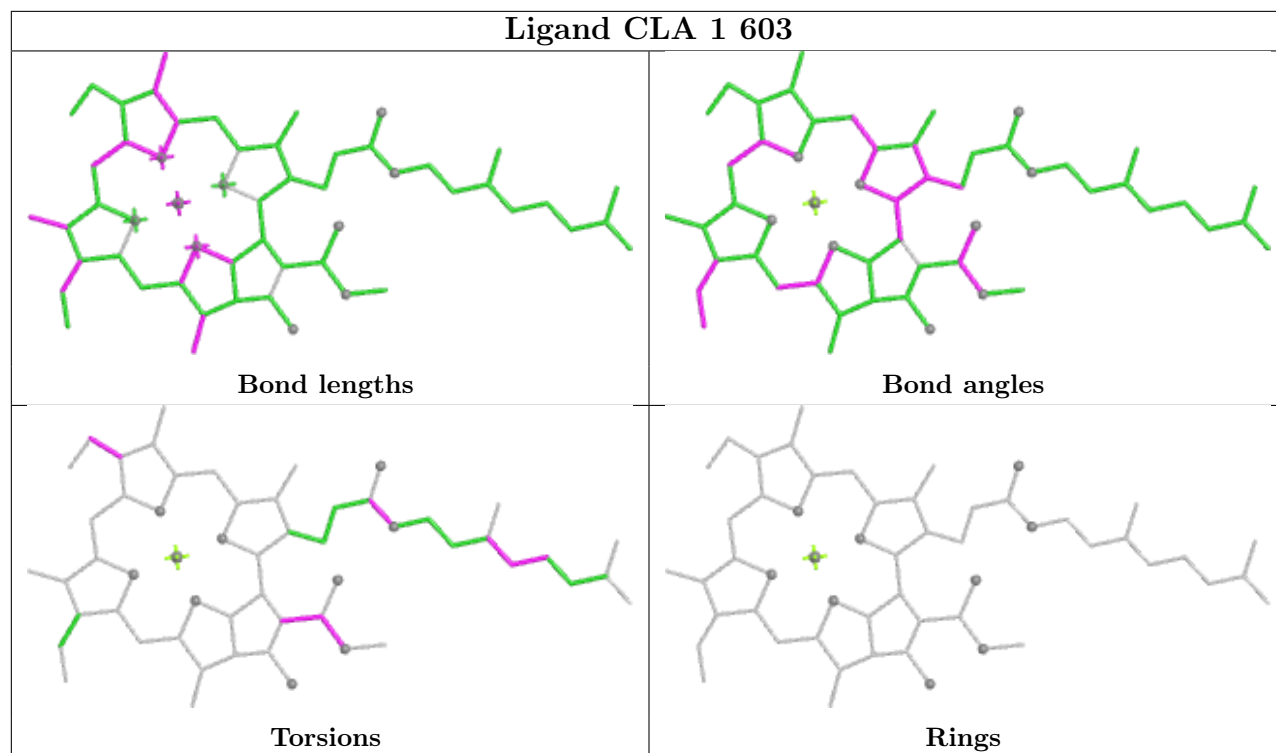




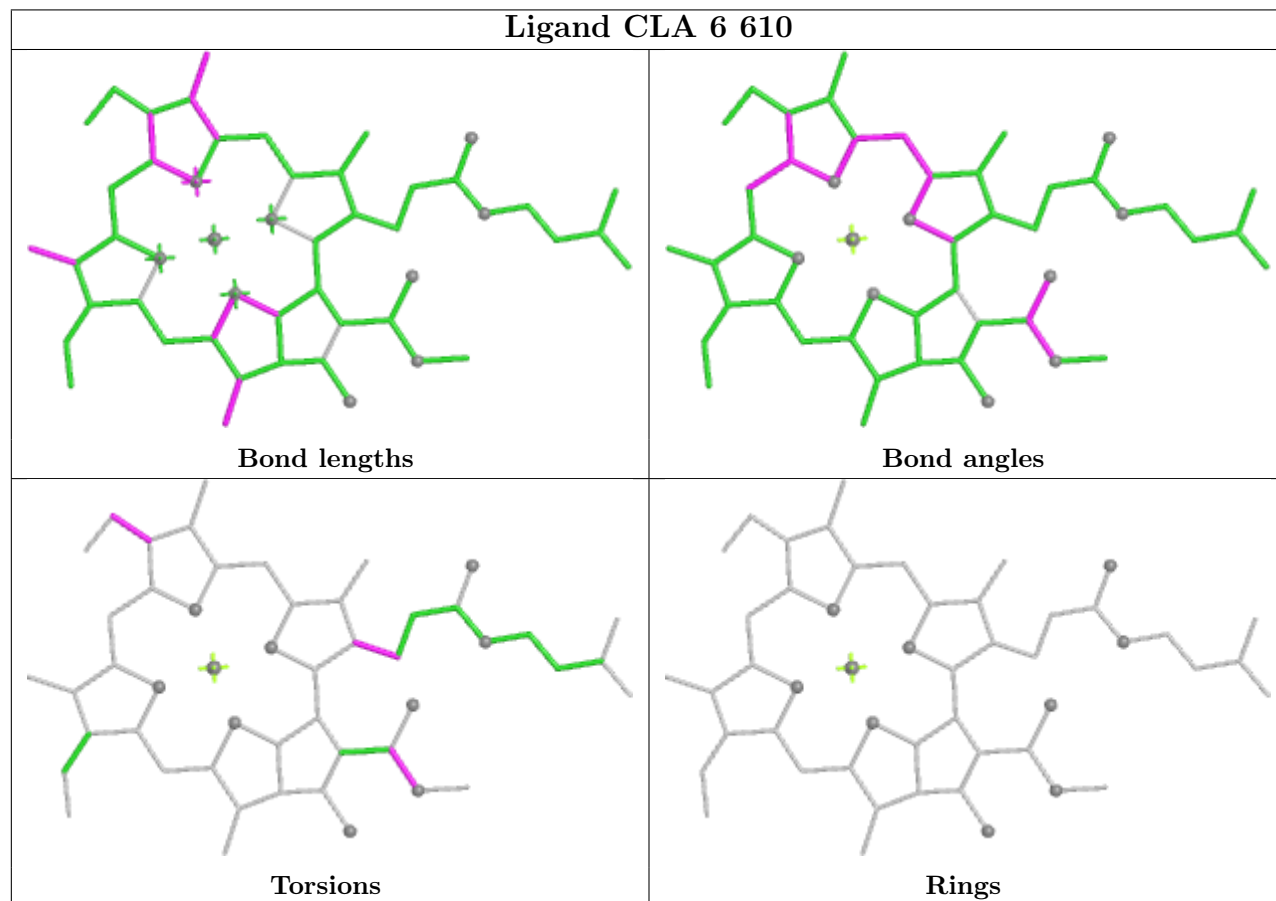


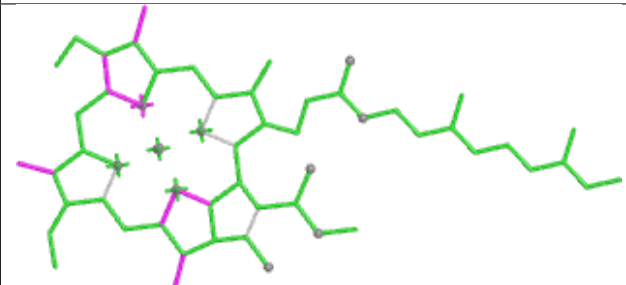
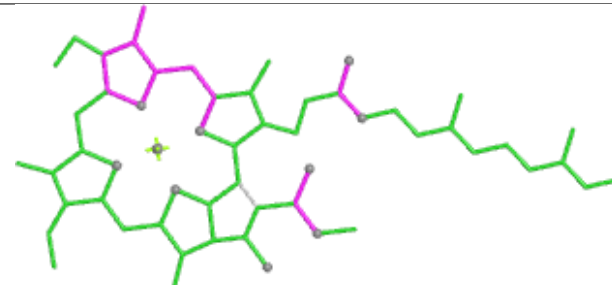
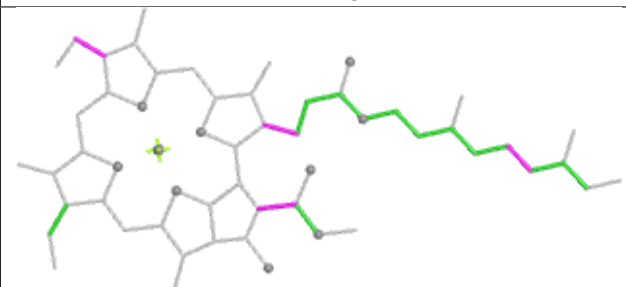
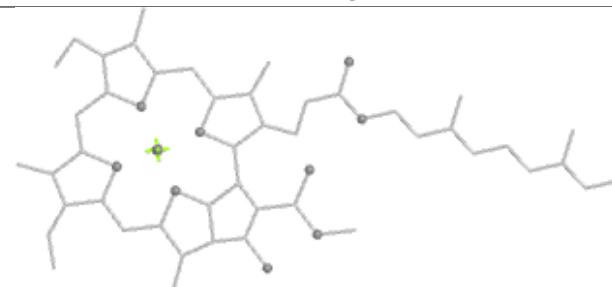


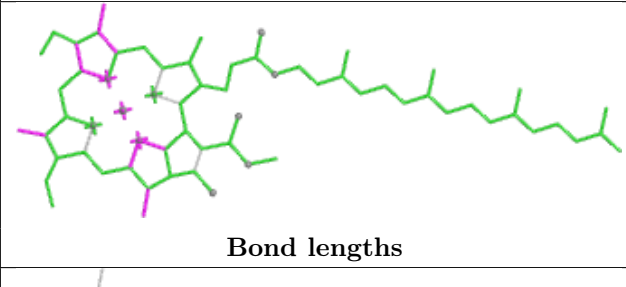
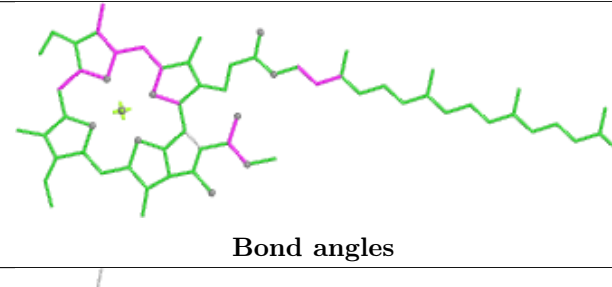
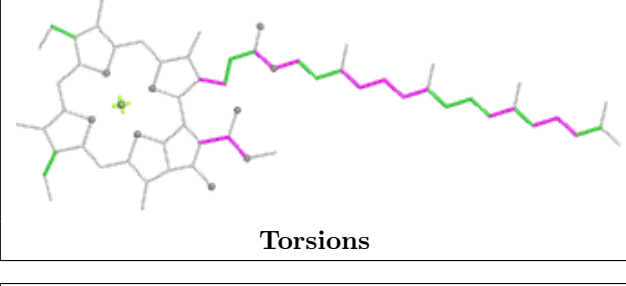
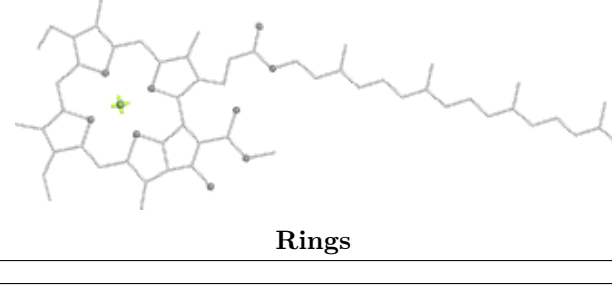
Ligand CLA 1 603

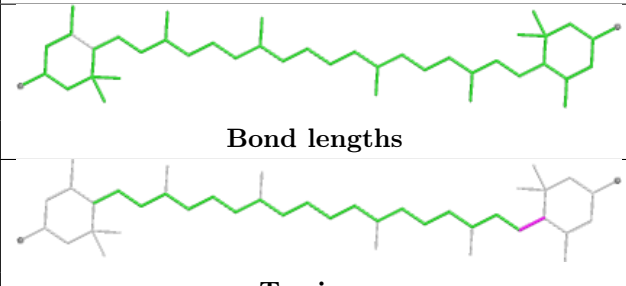
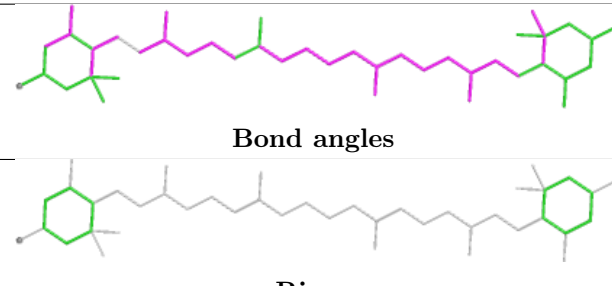
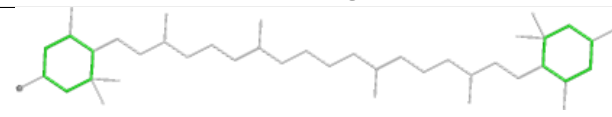


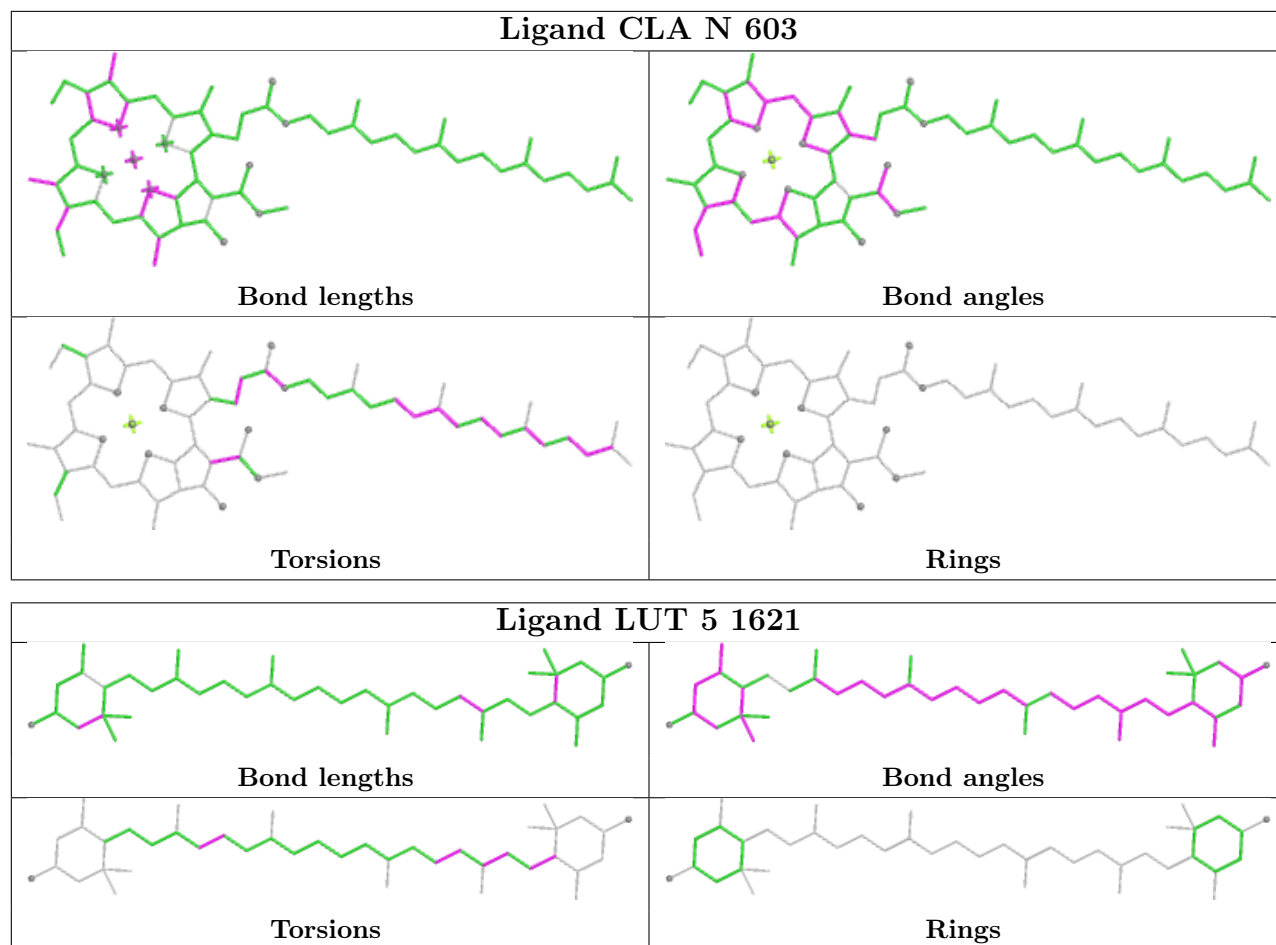
Ligand CLA 6 610

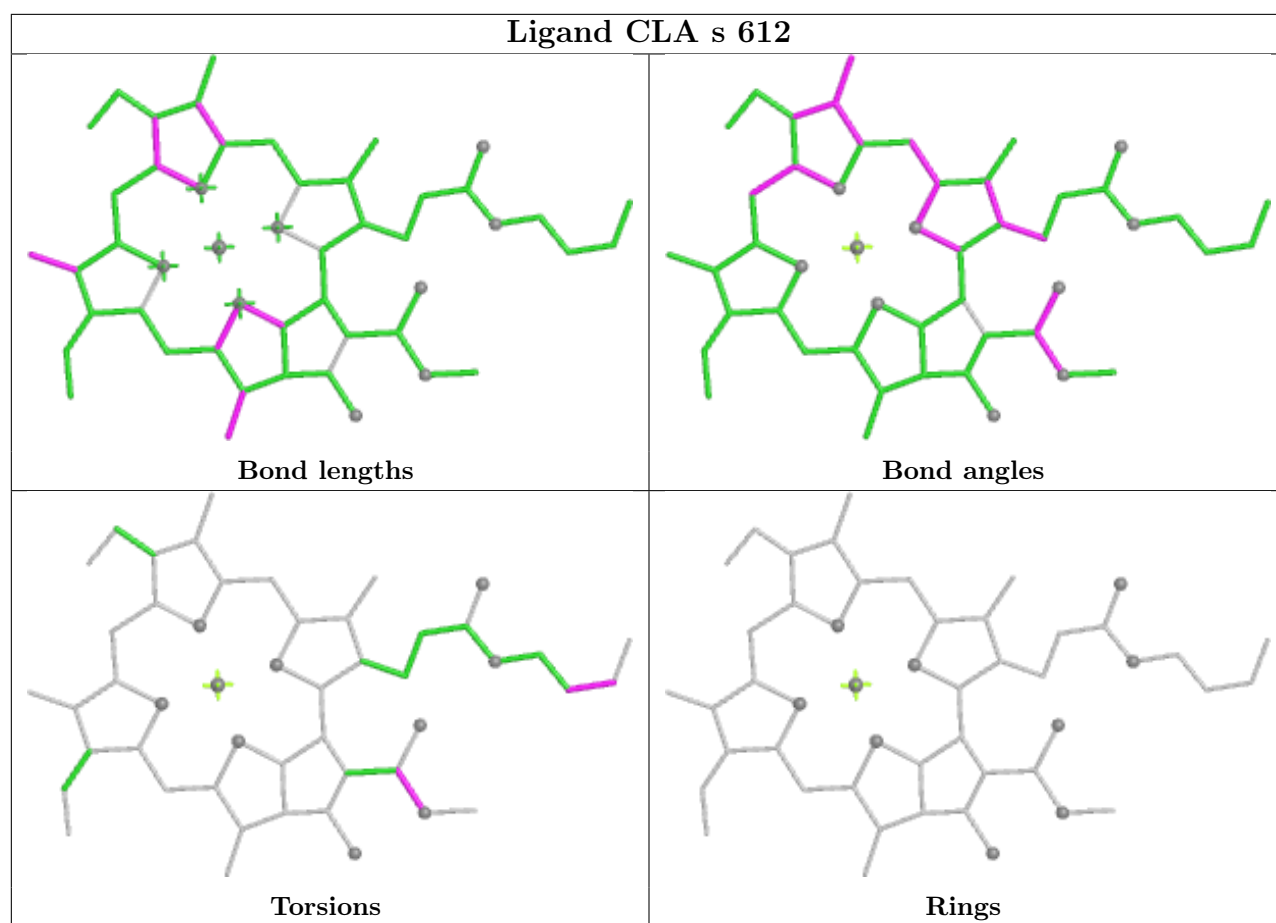


Ligand CLA 5 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

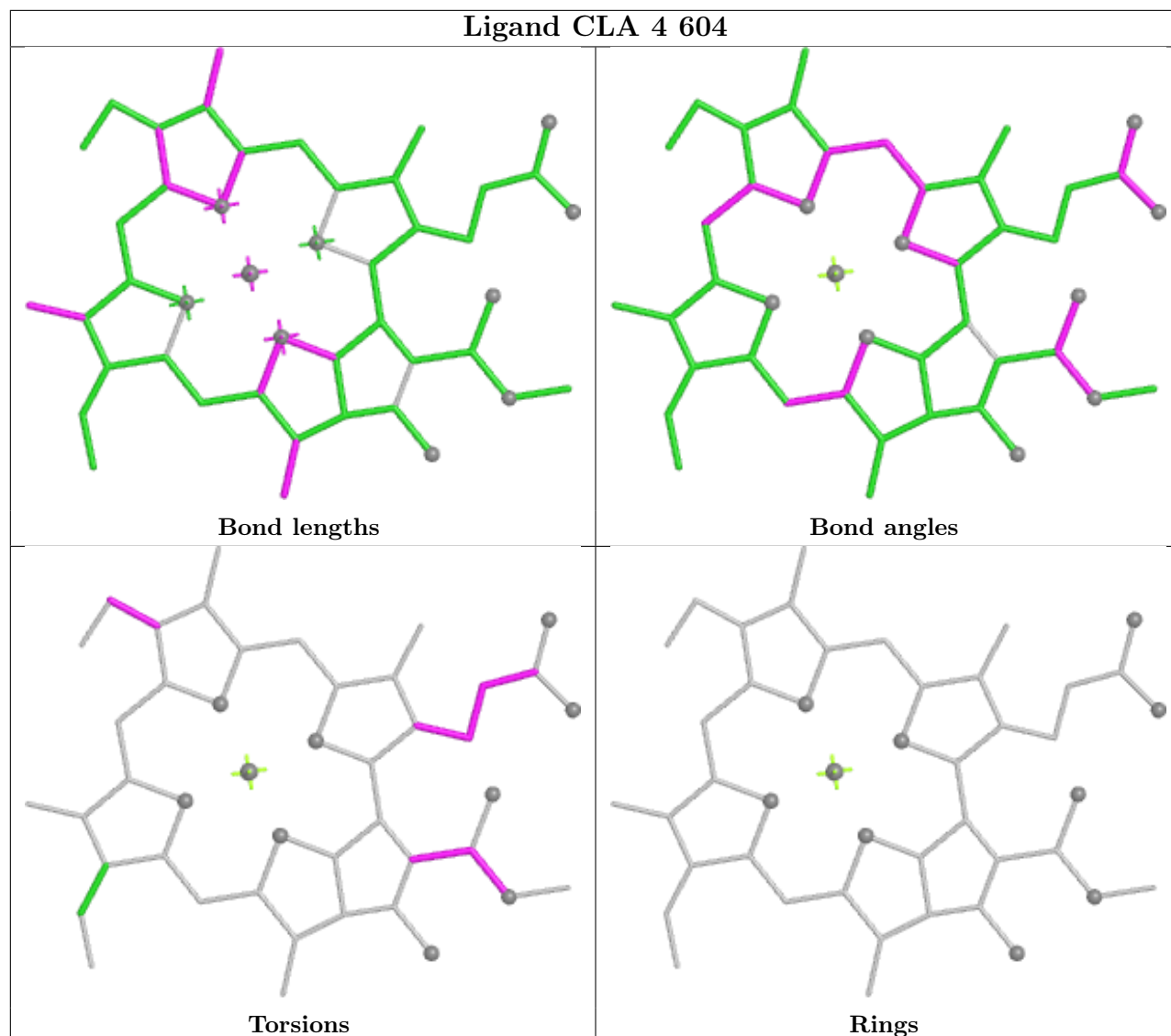
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT S 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

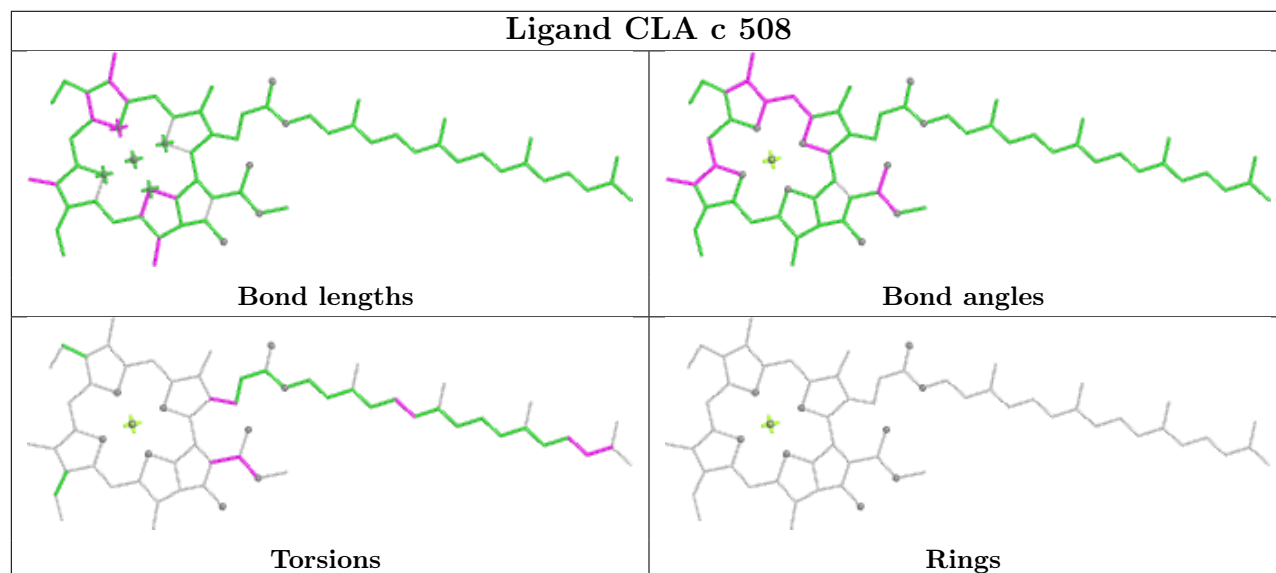


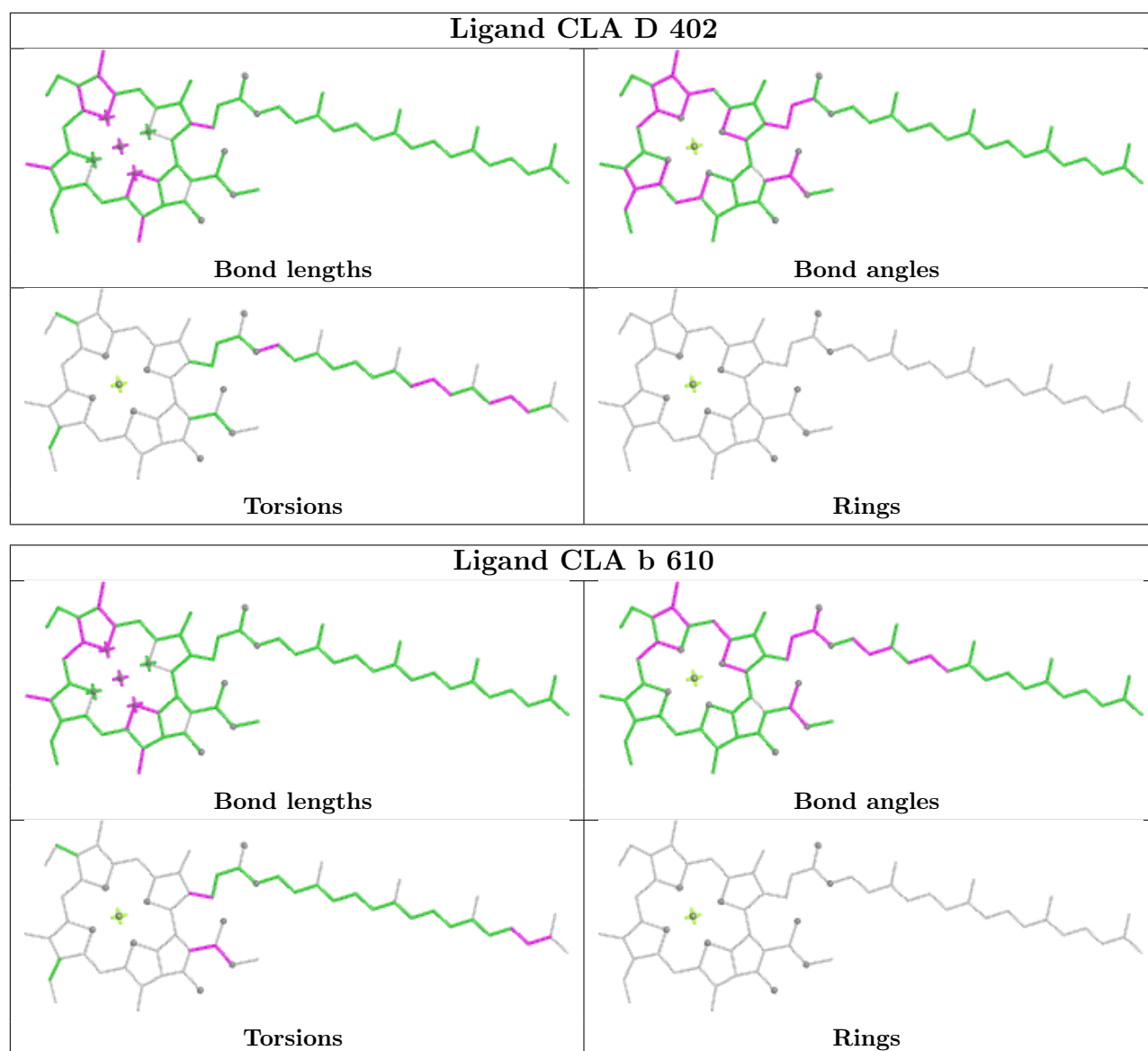


Ligand CLA 4 604

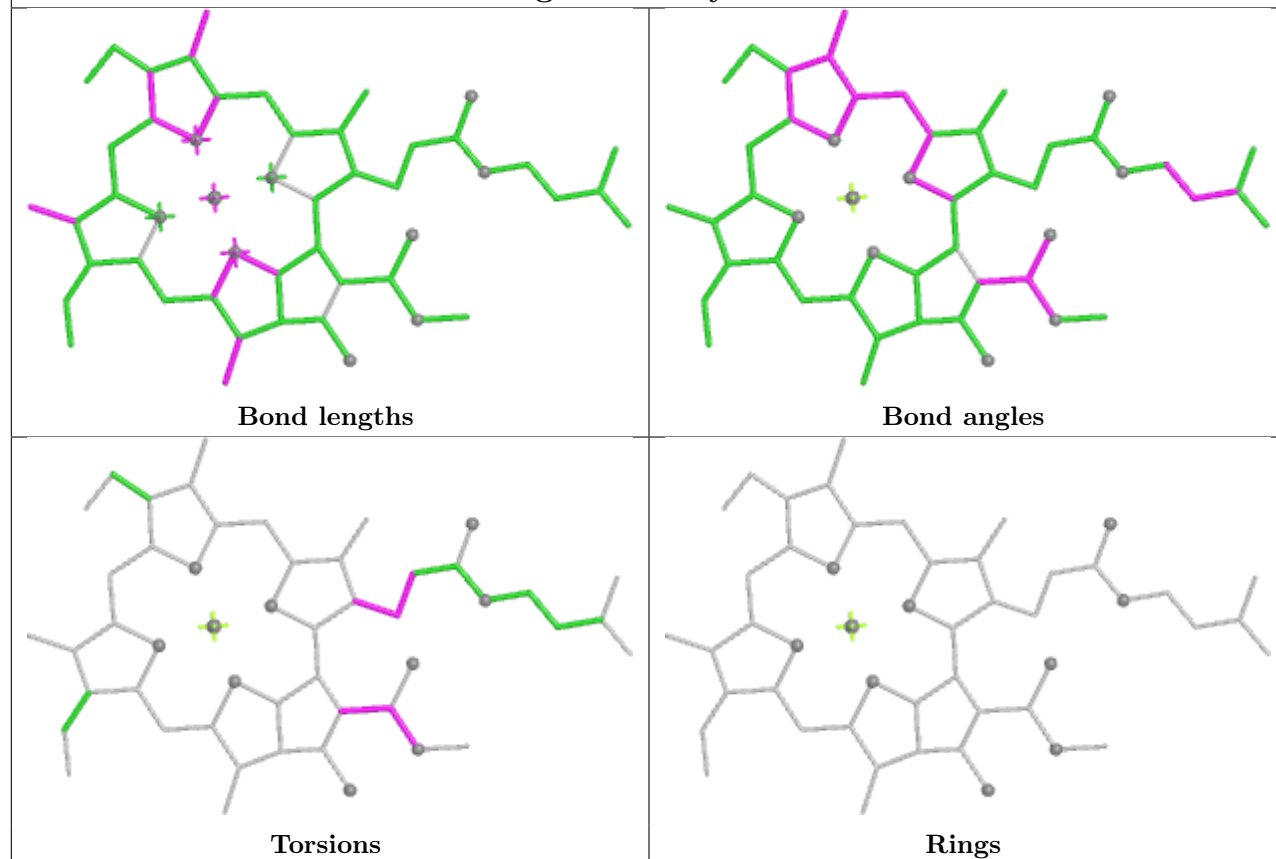


Ligand CLA c 508

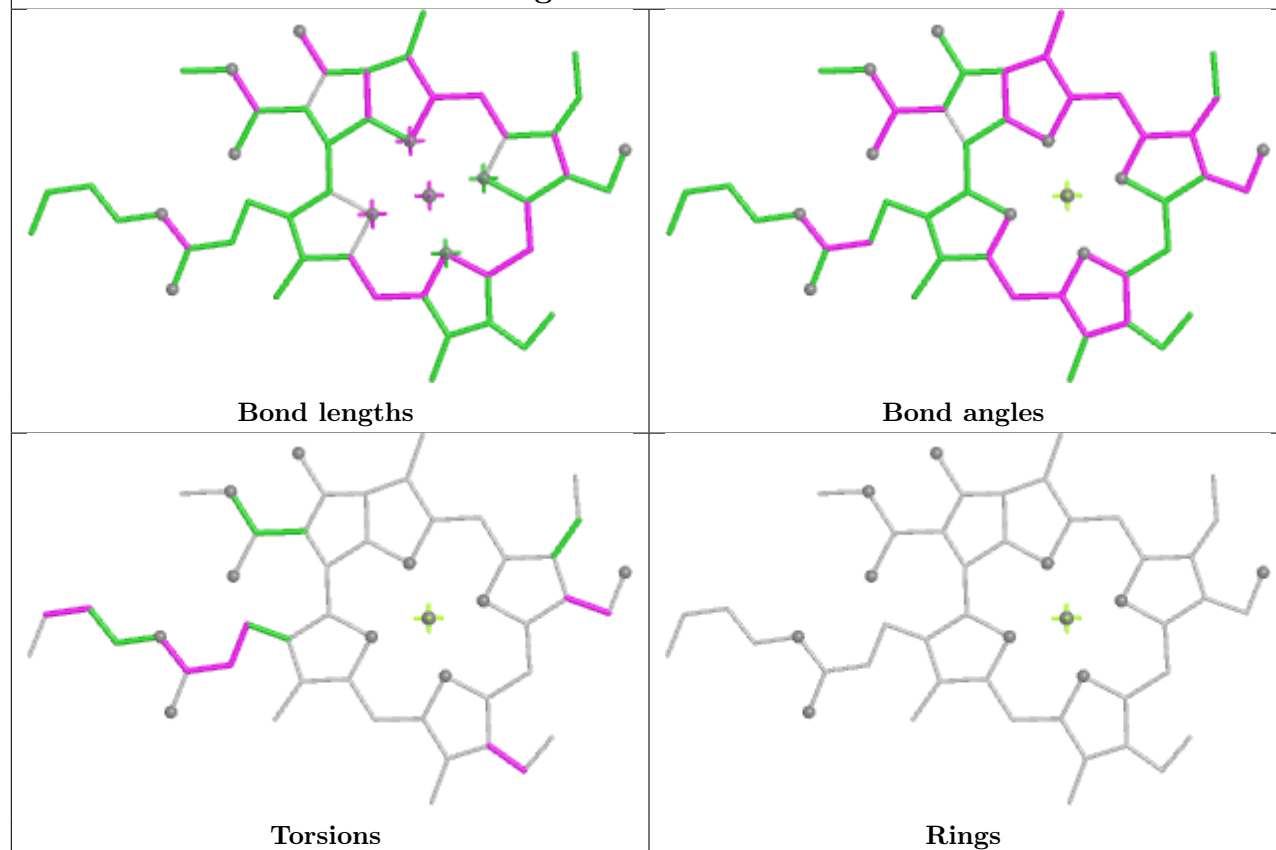


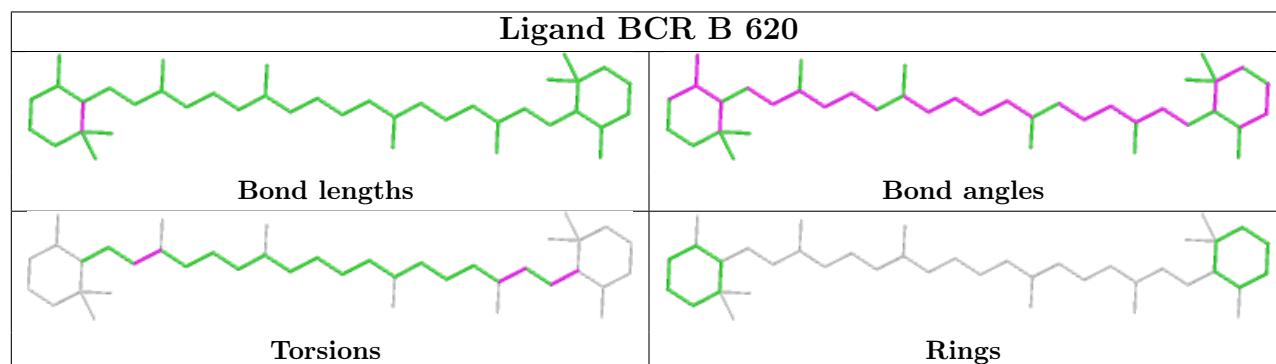
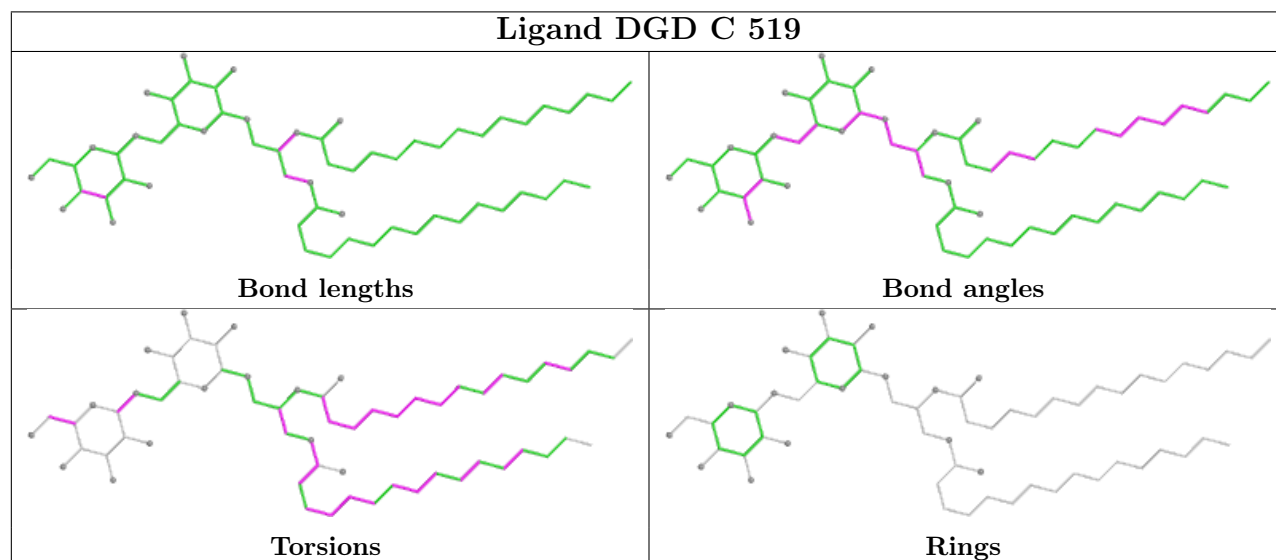
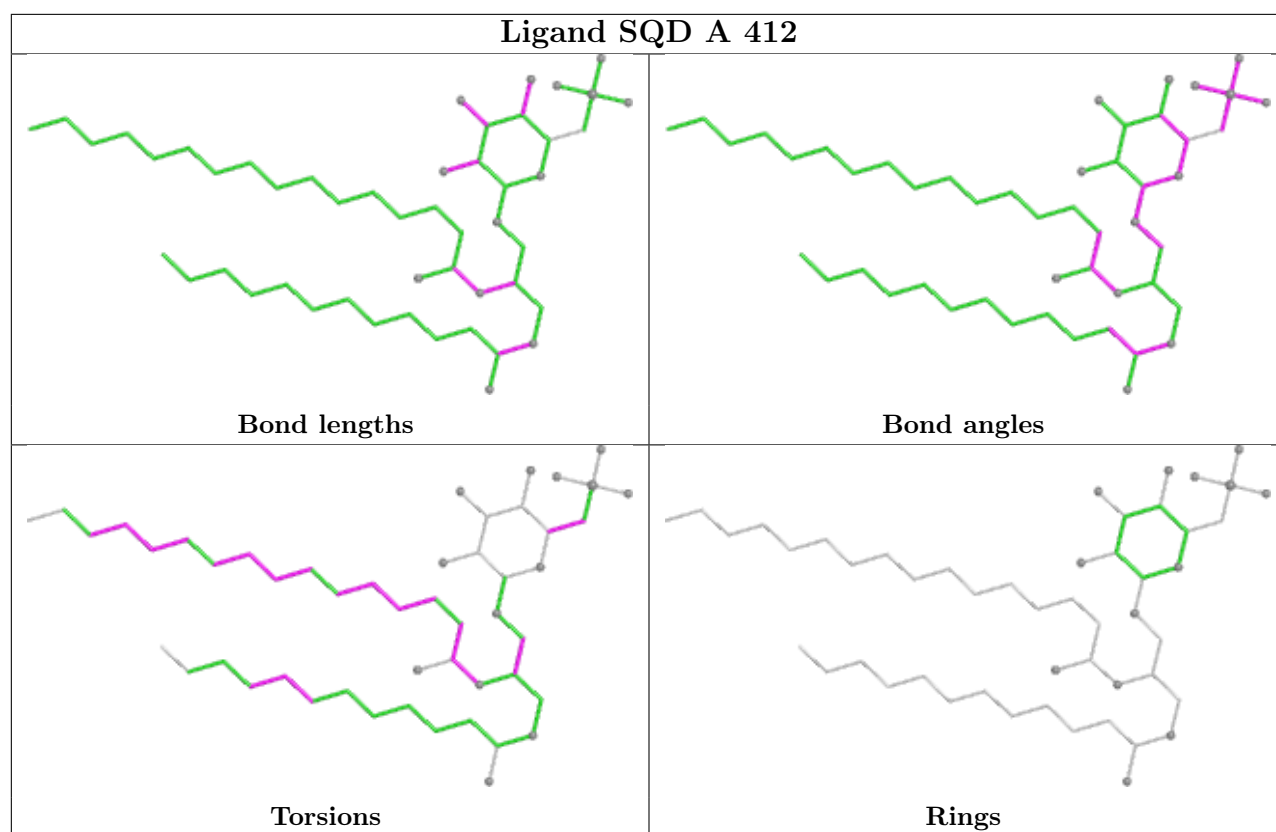


Ligand CLA y 604

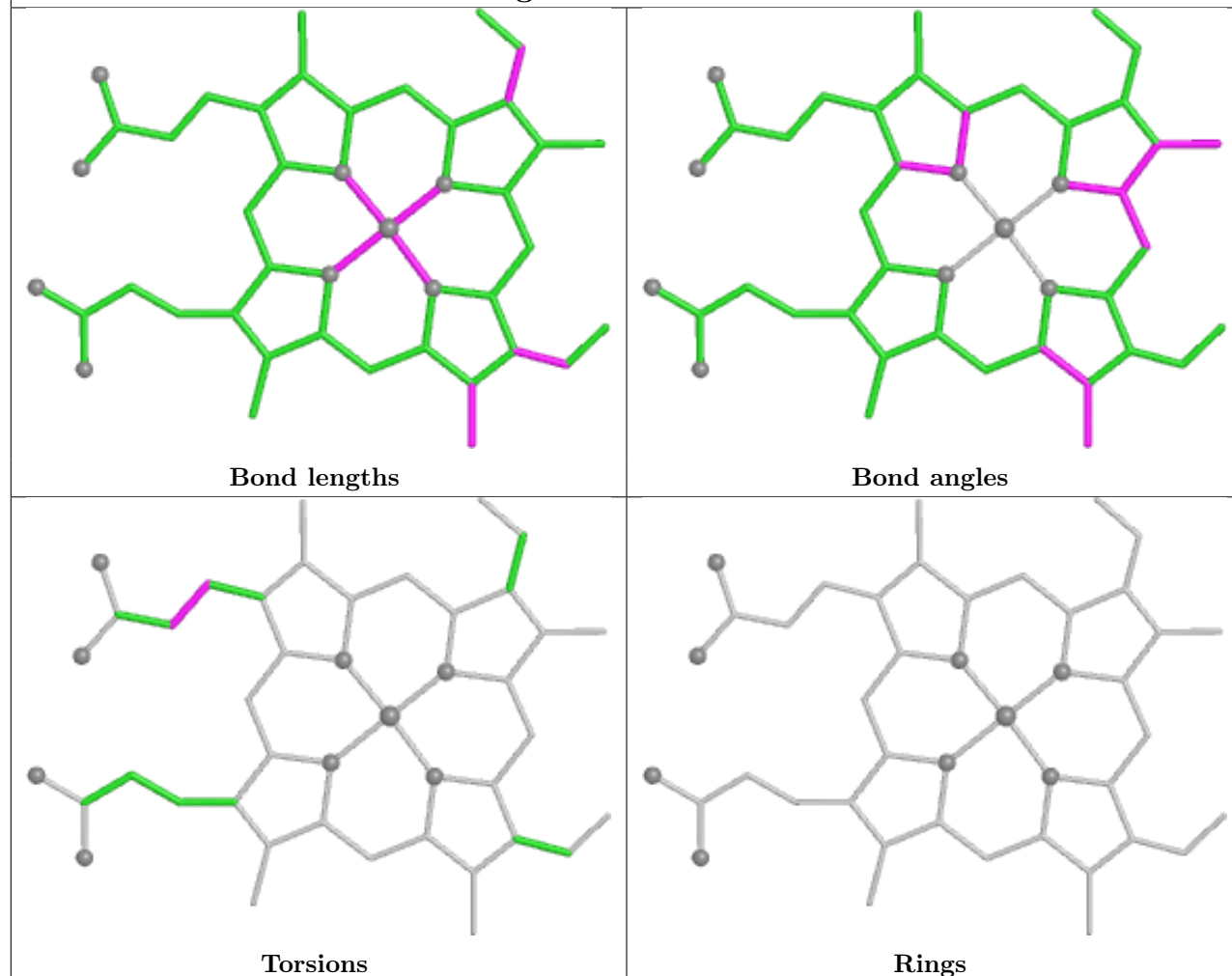


Ligand CHL n 606

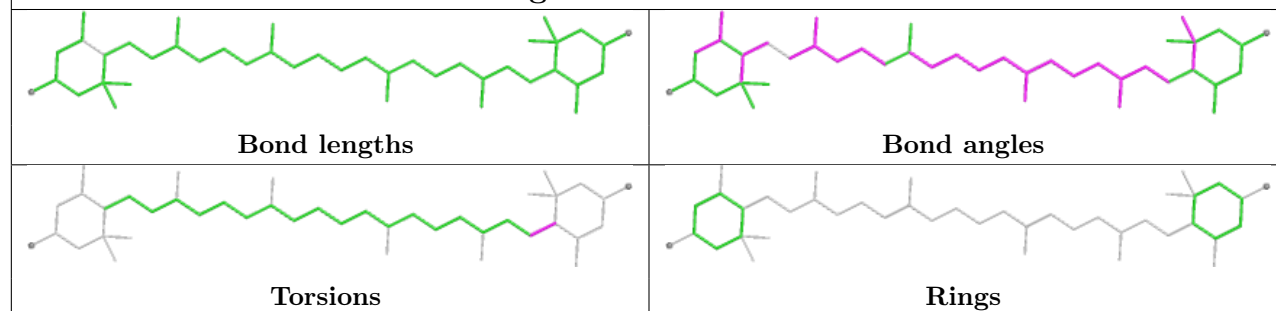


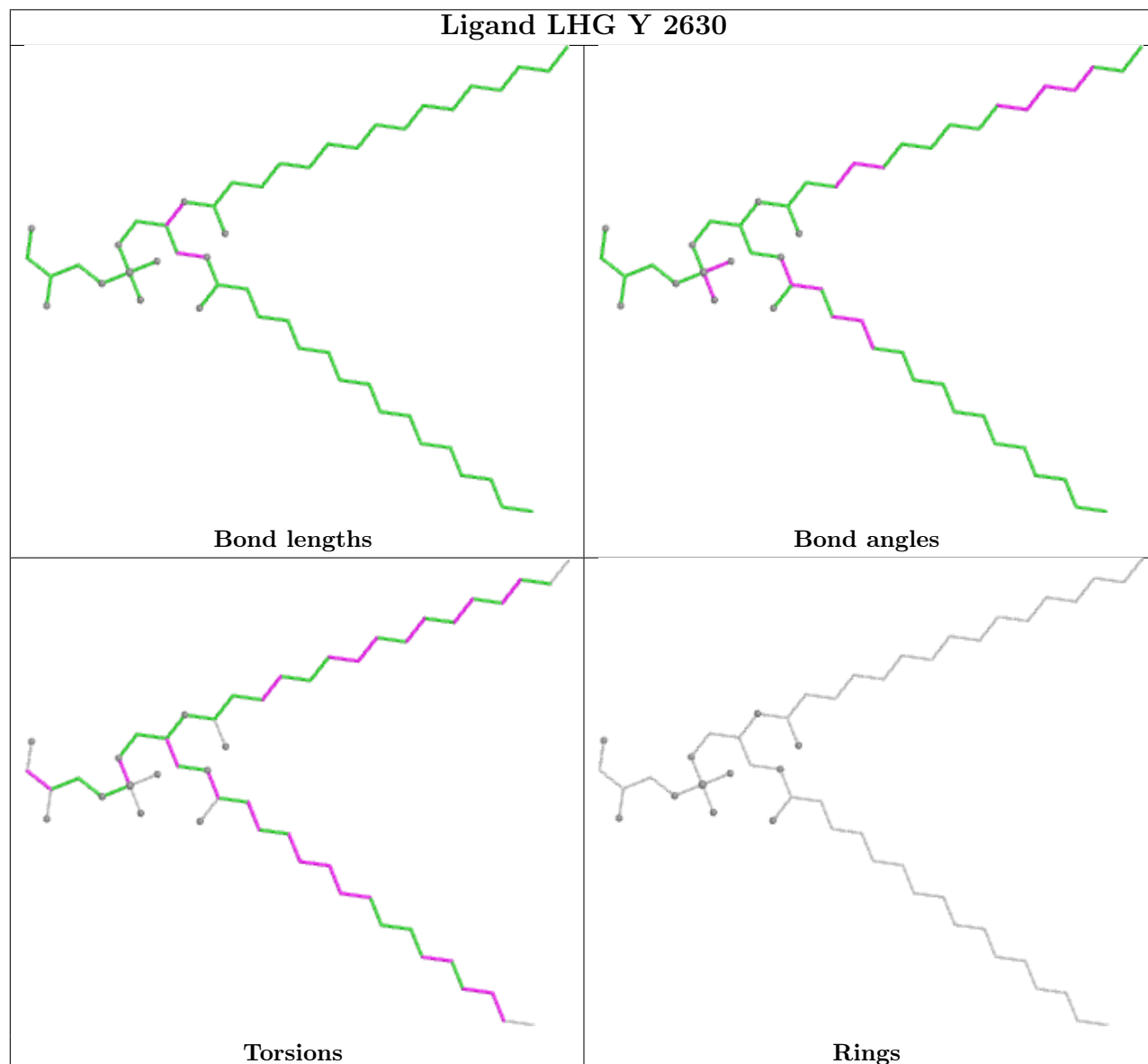
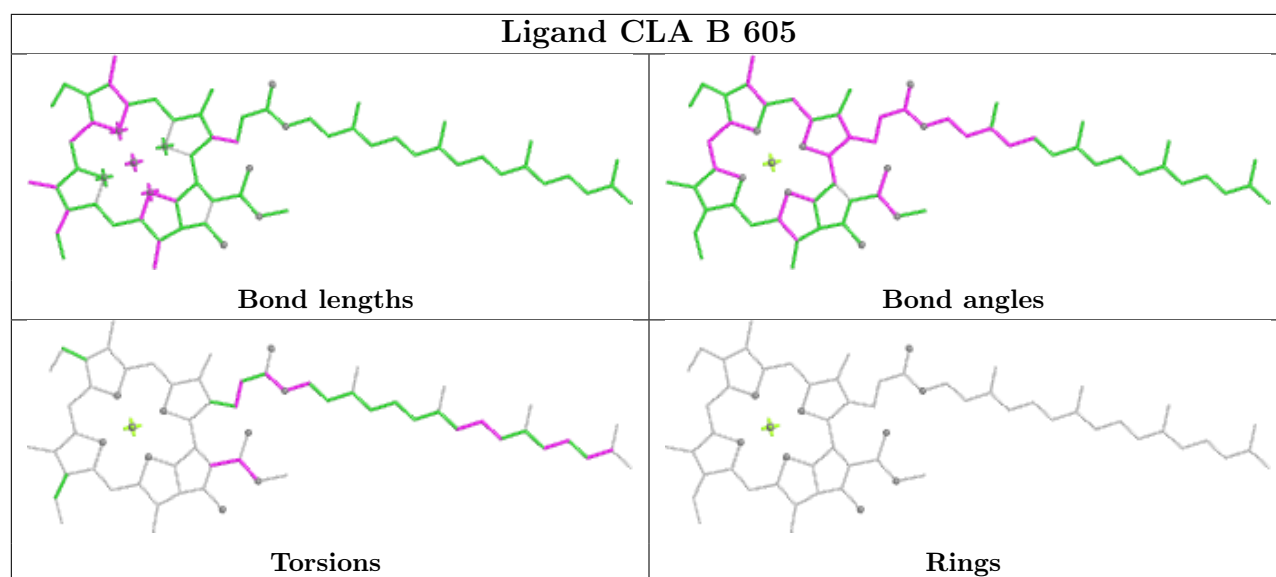


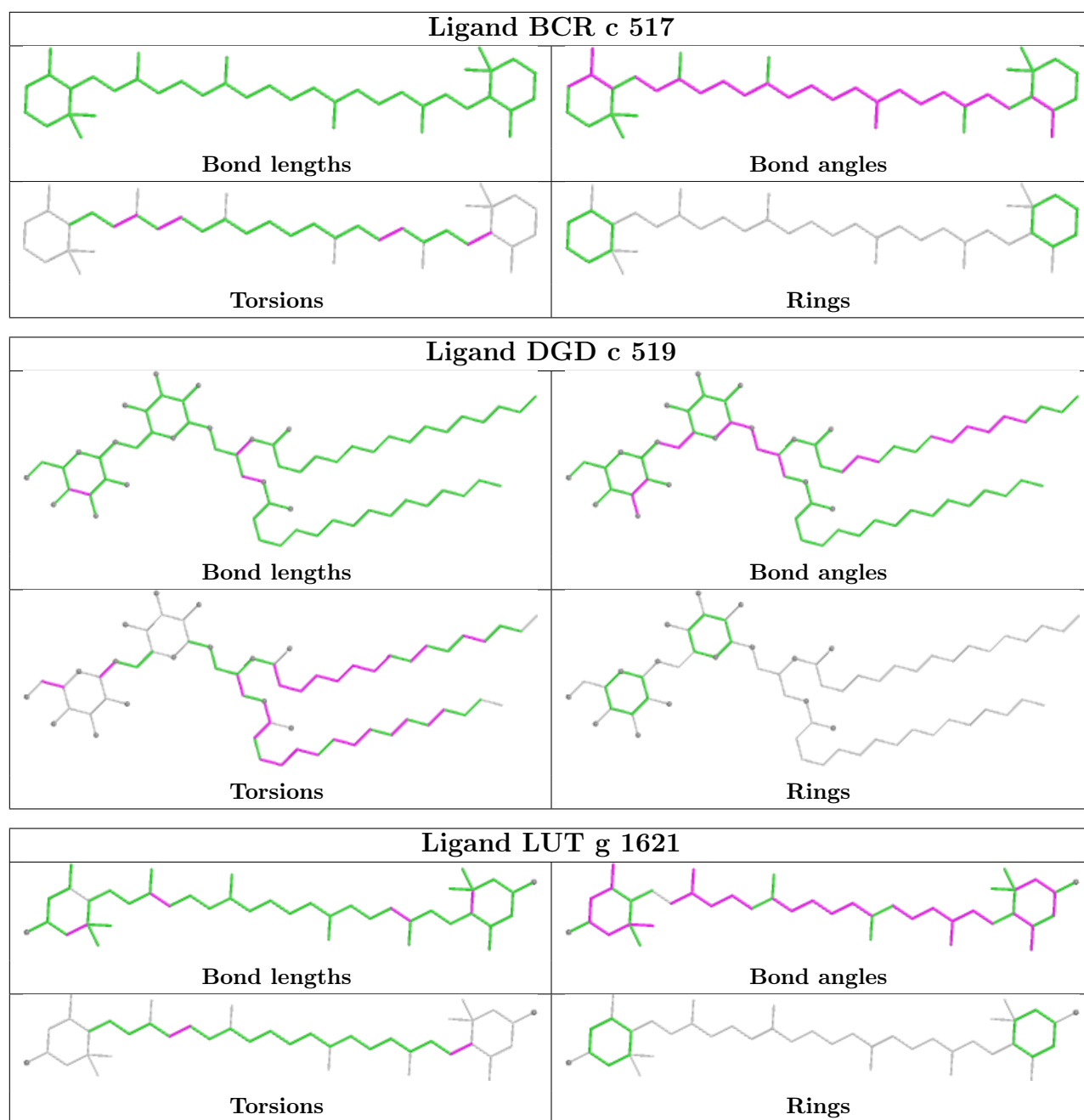
Ligand HEM f 101

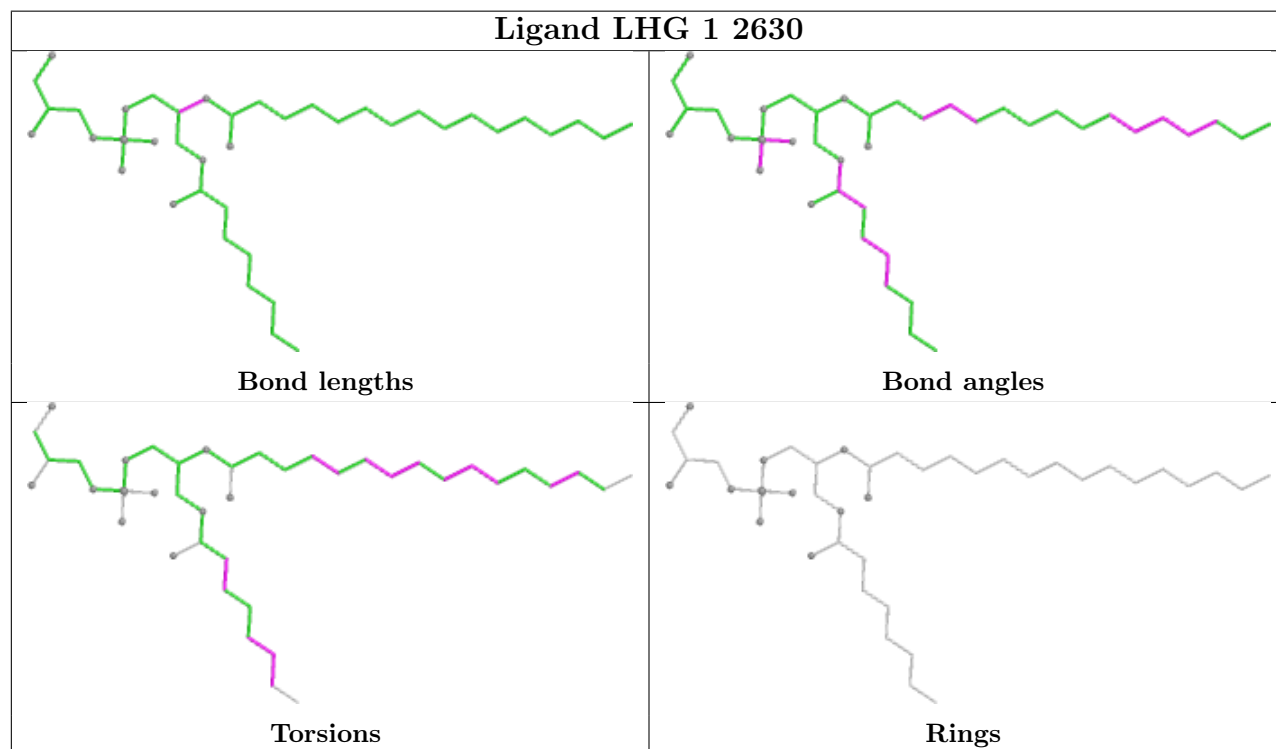
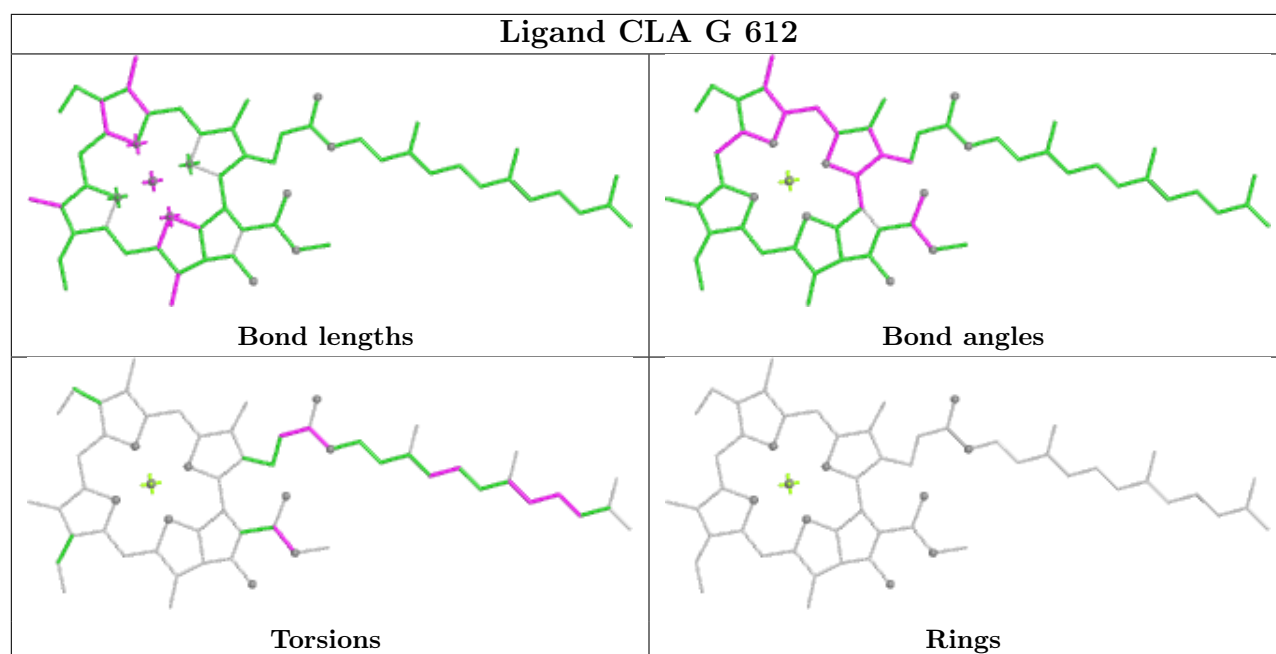


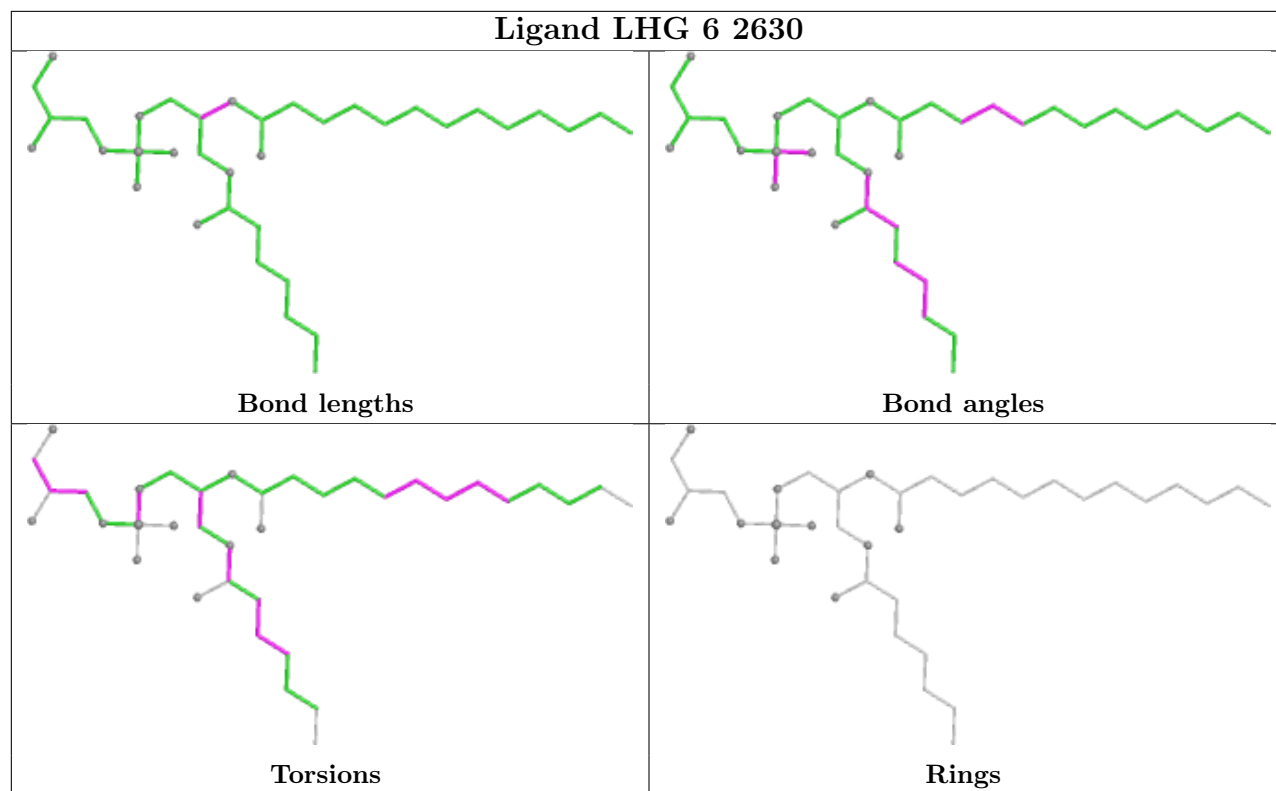
Ligand LUT s 1620

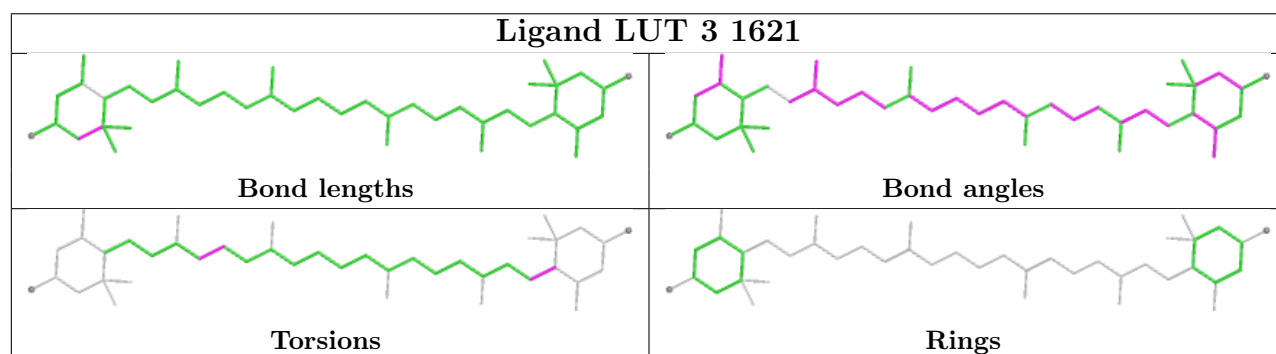
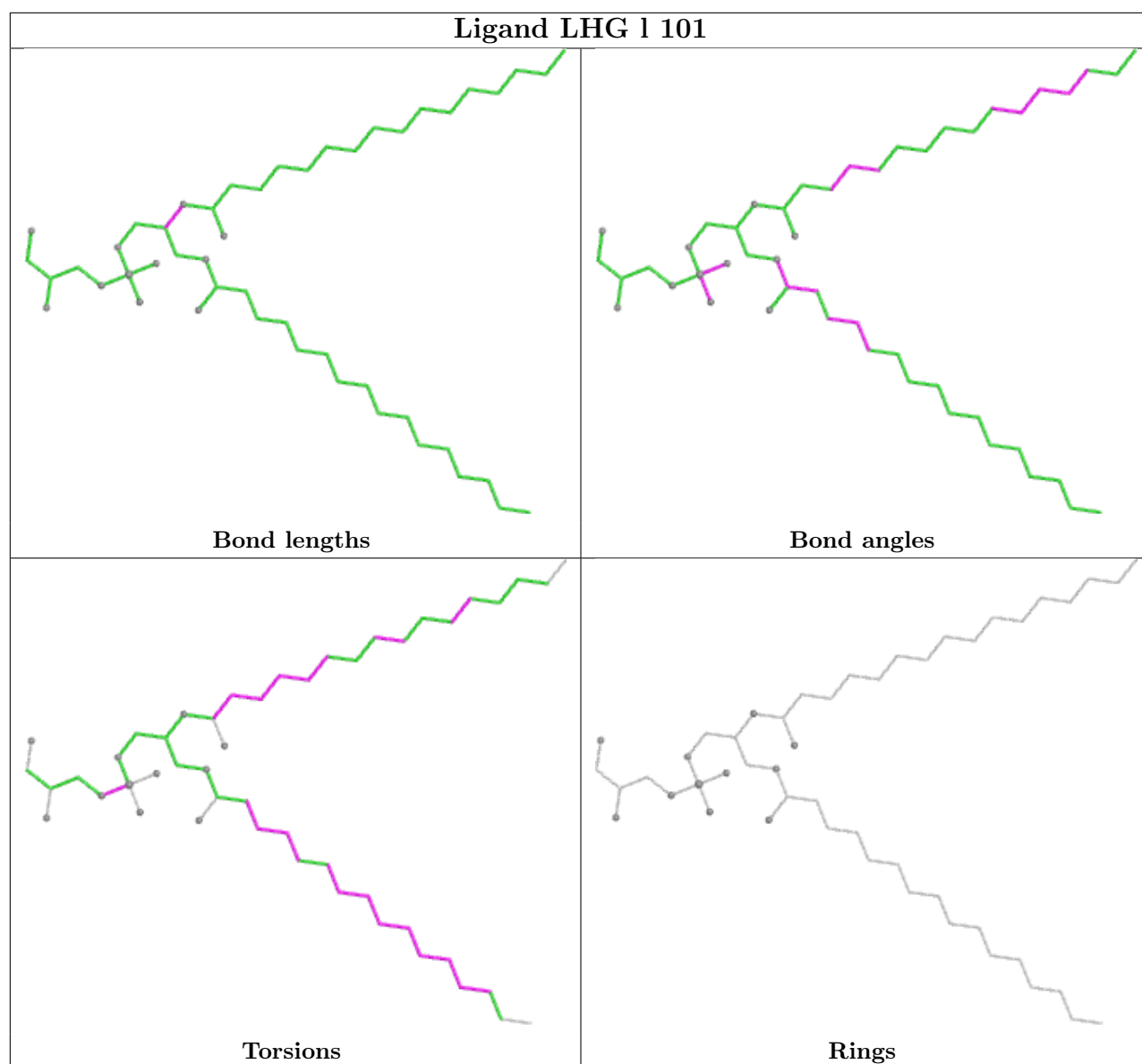


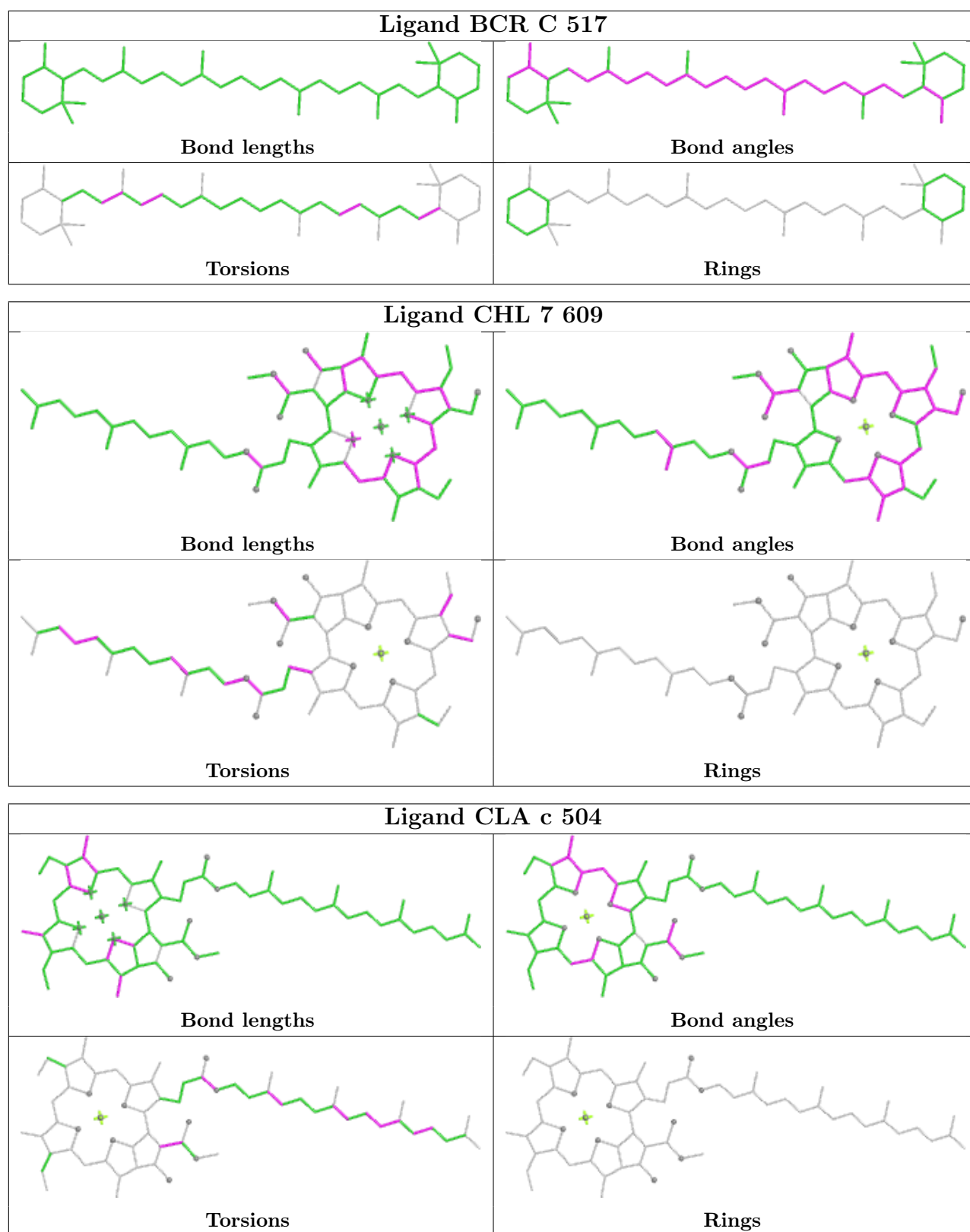


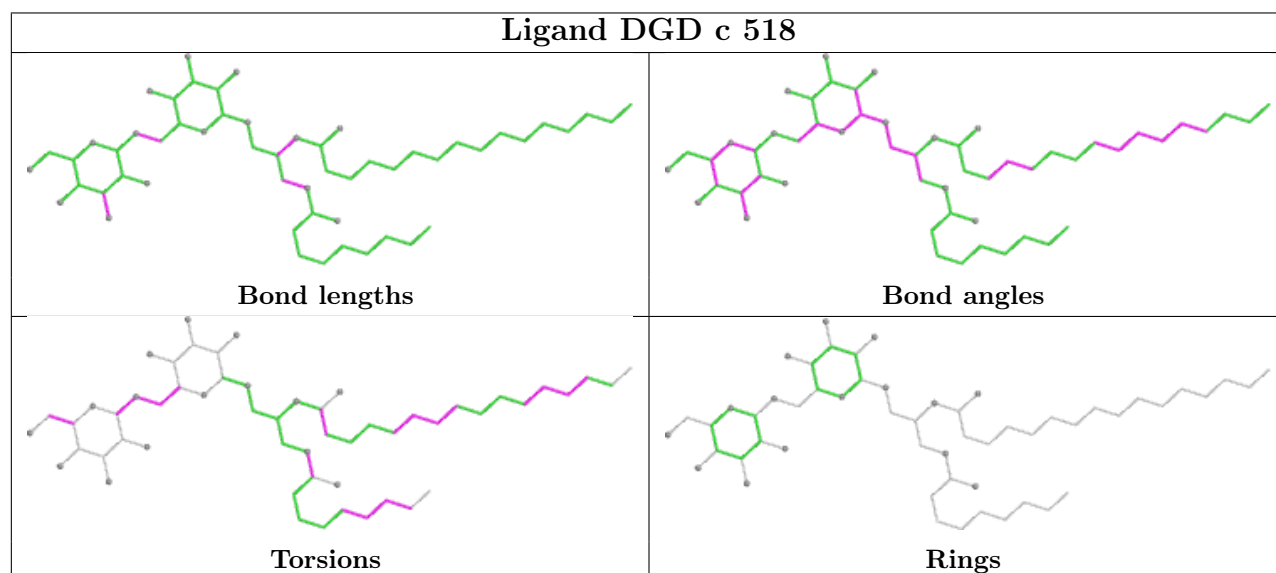
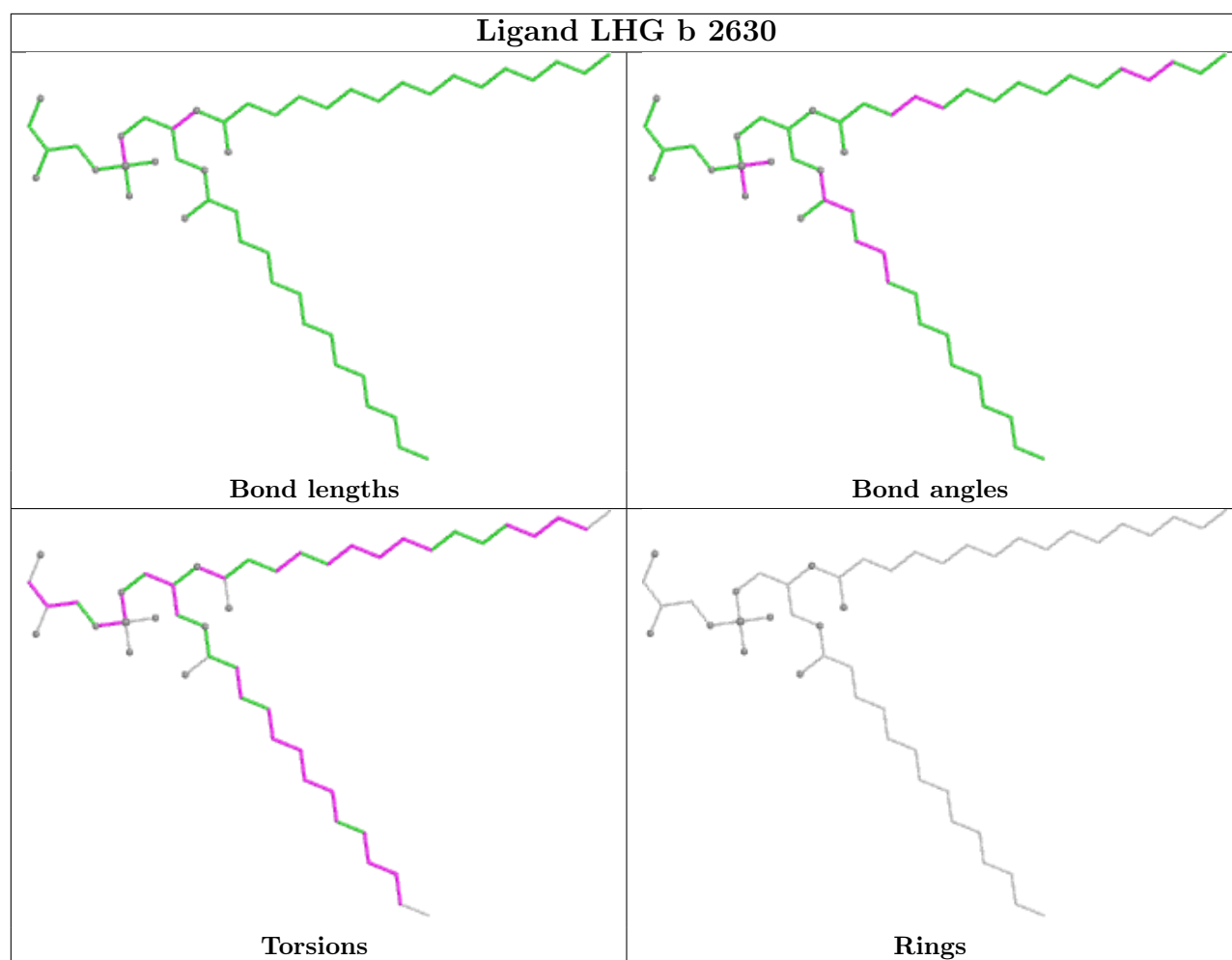


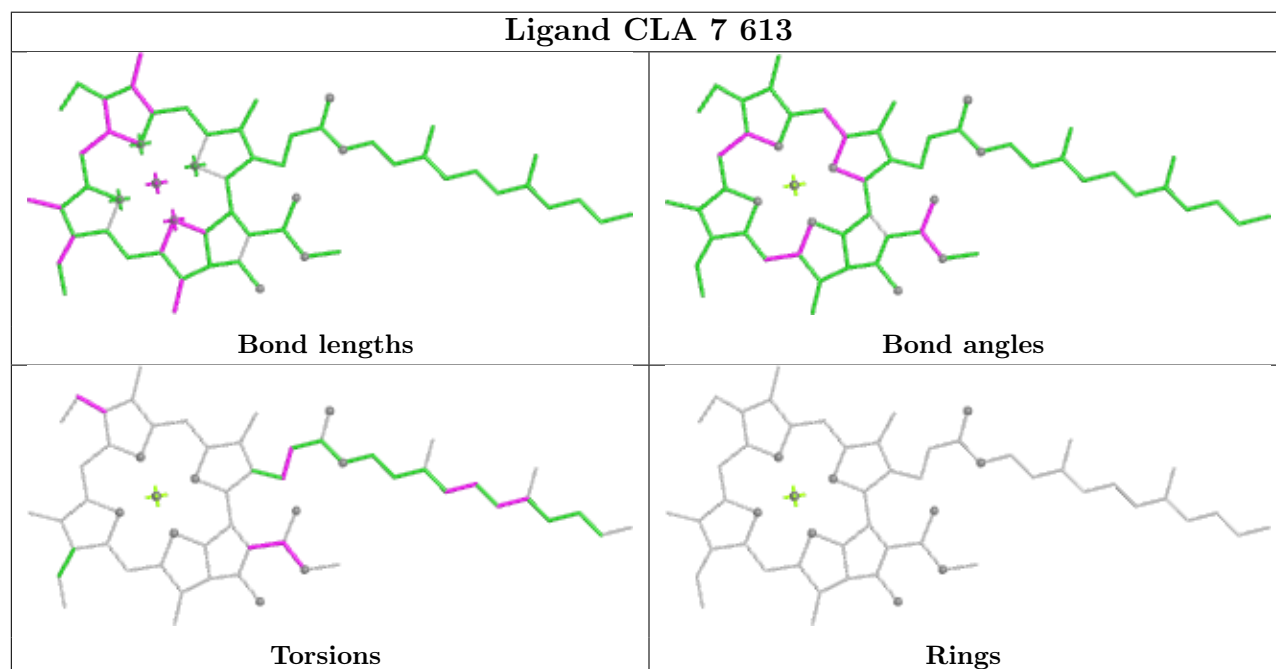
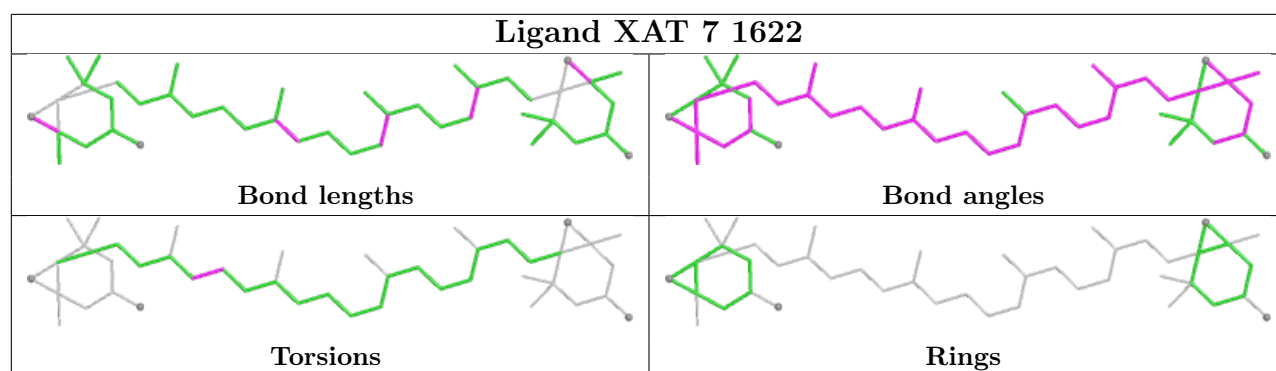




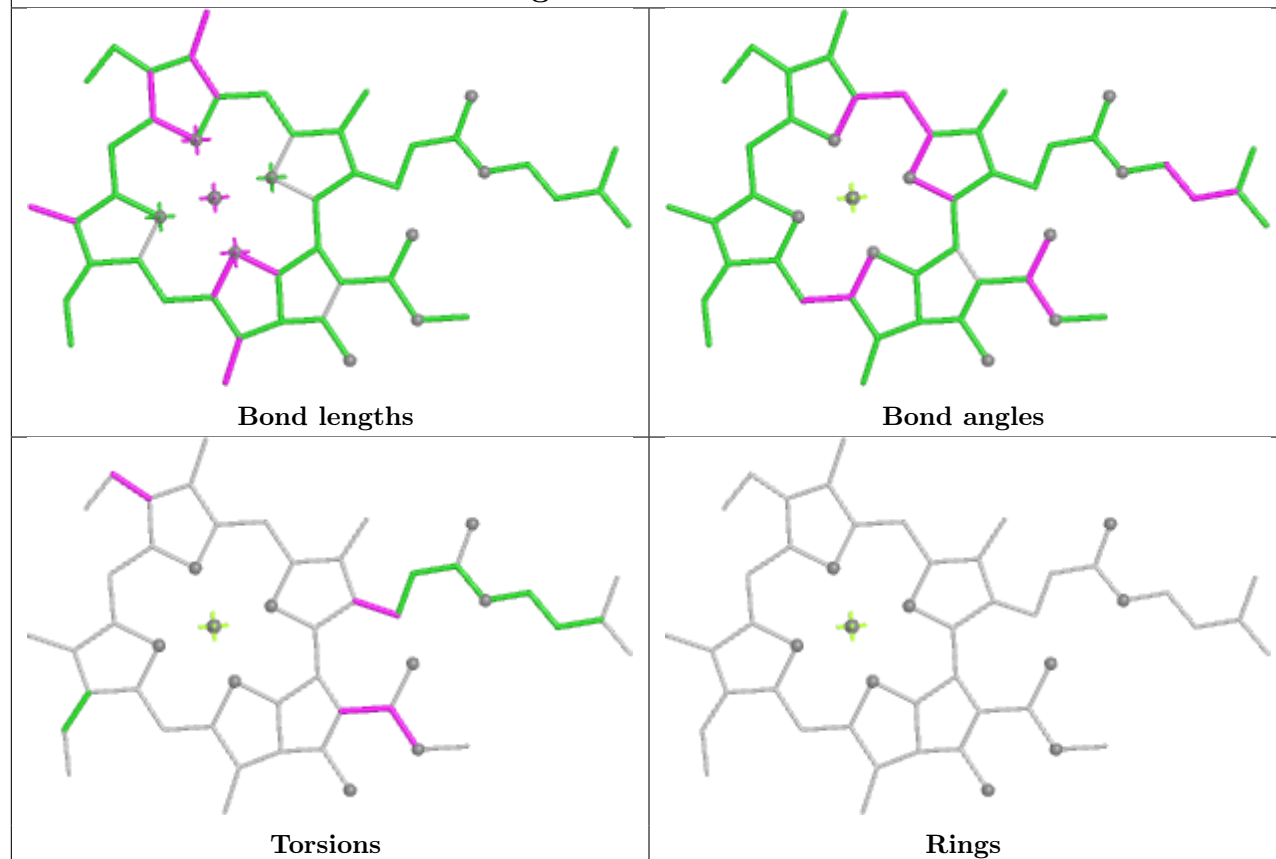




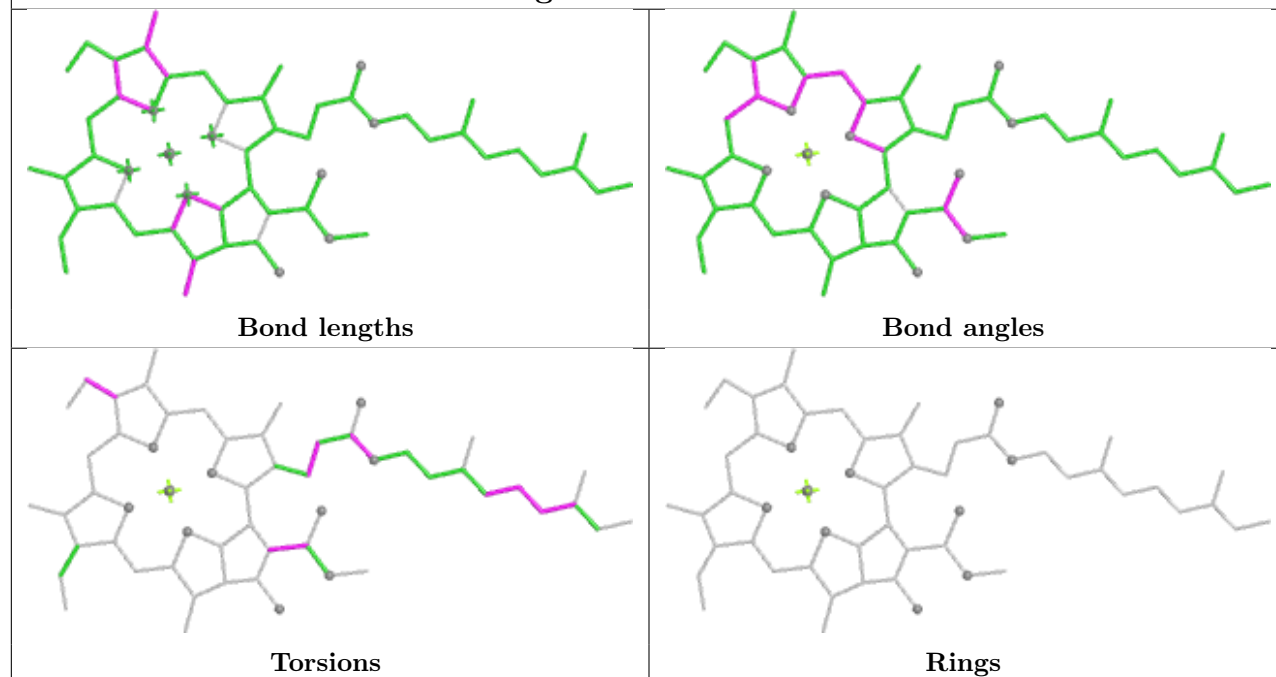


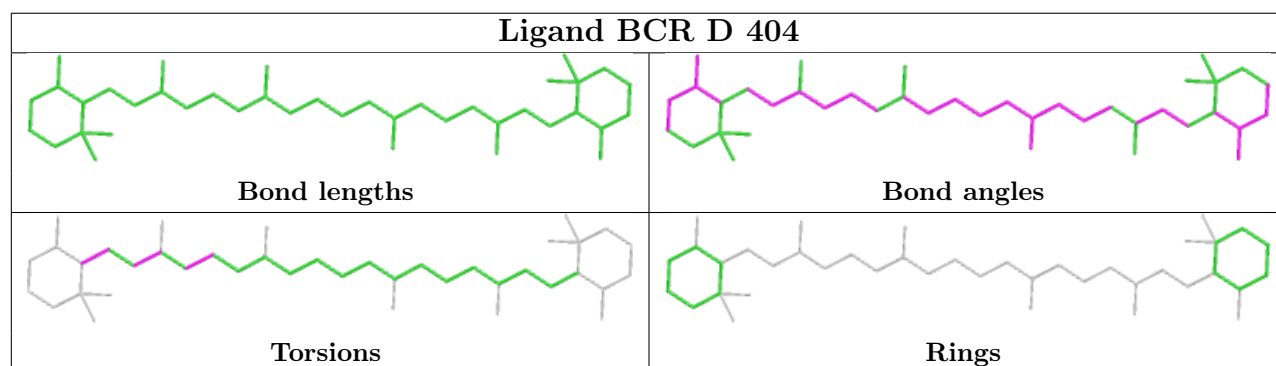
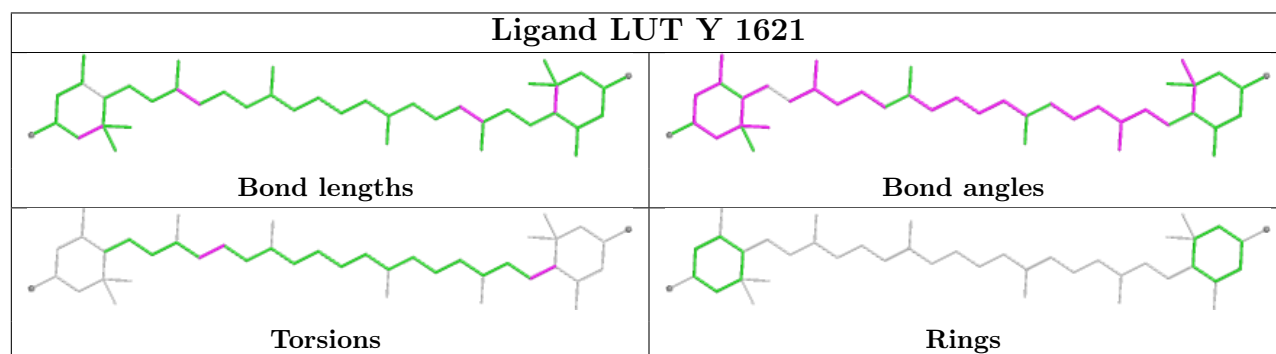
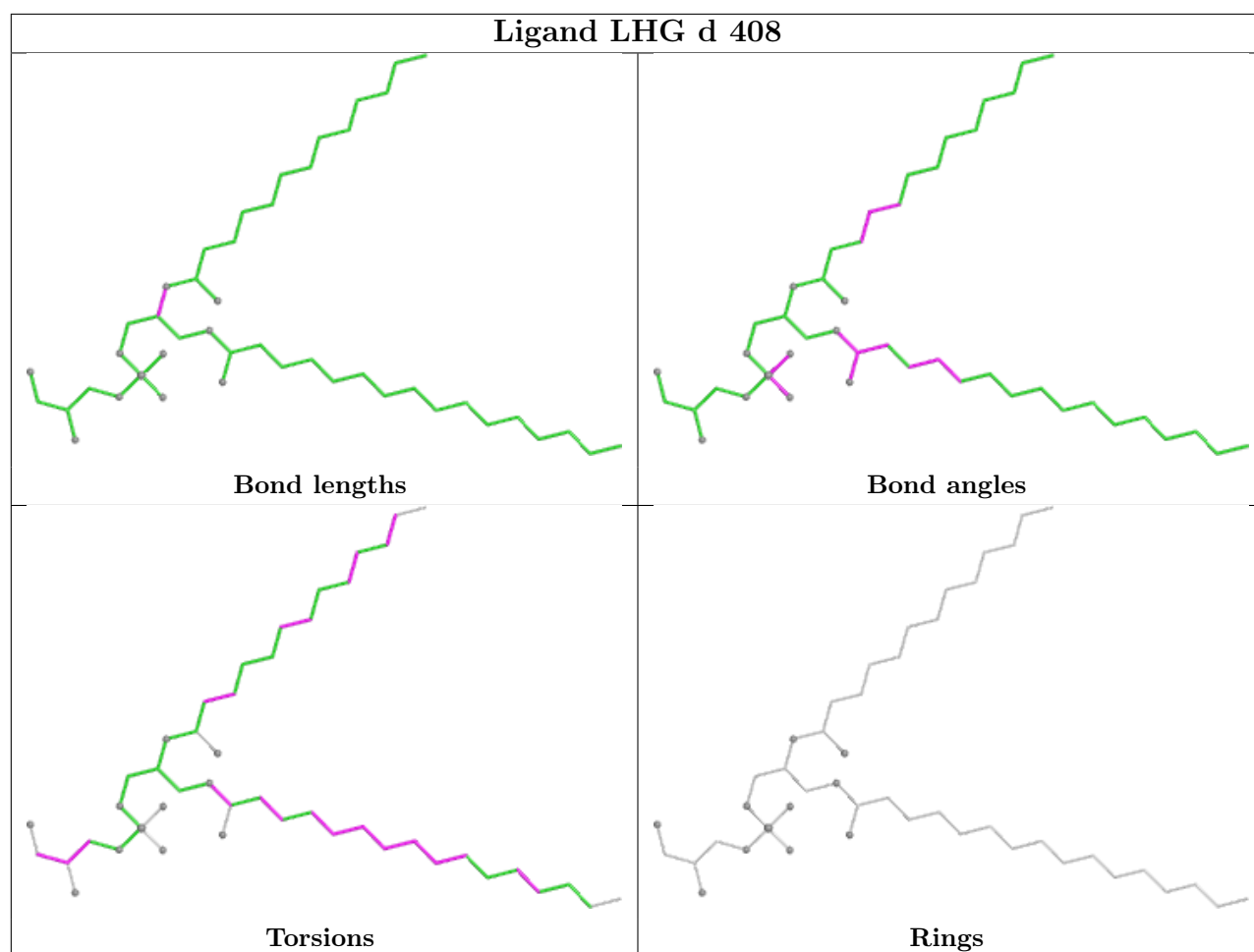


Ligand CLA A 407

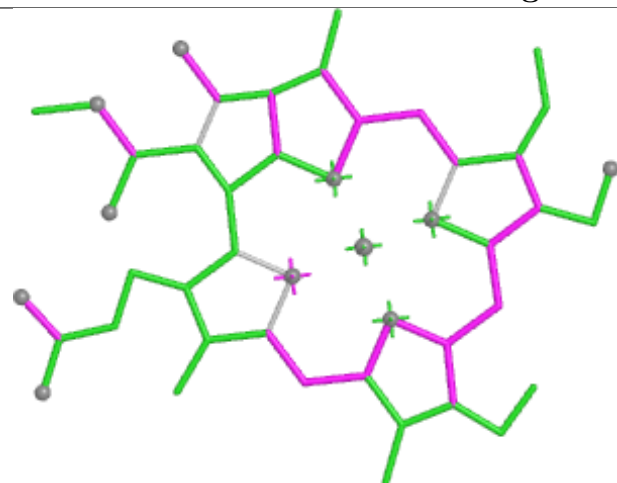


Ligand CLA S 611

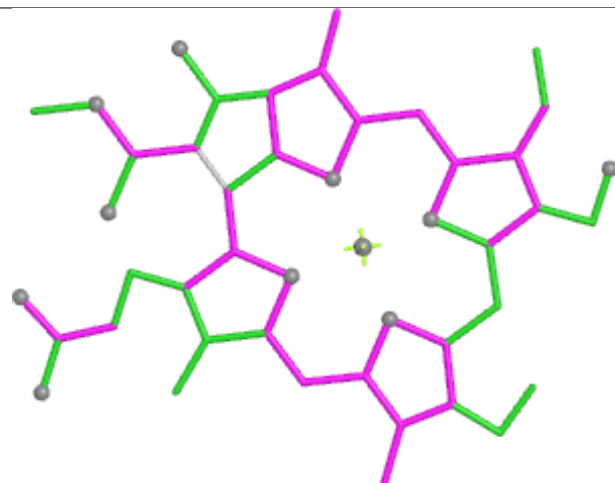




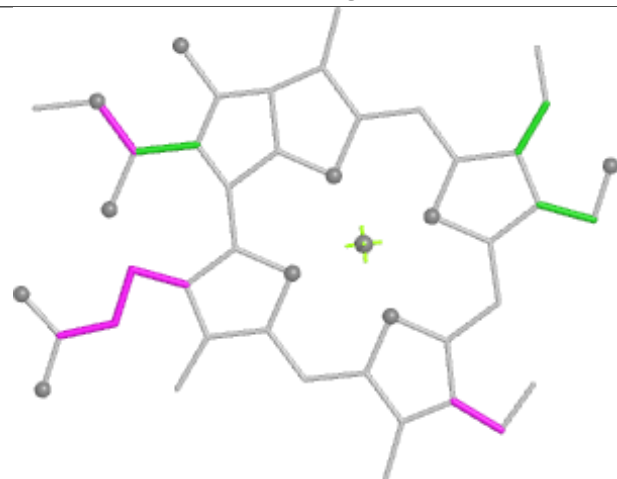
Ligand CHL 3 608



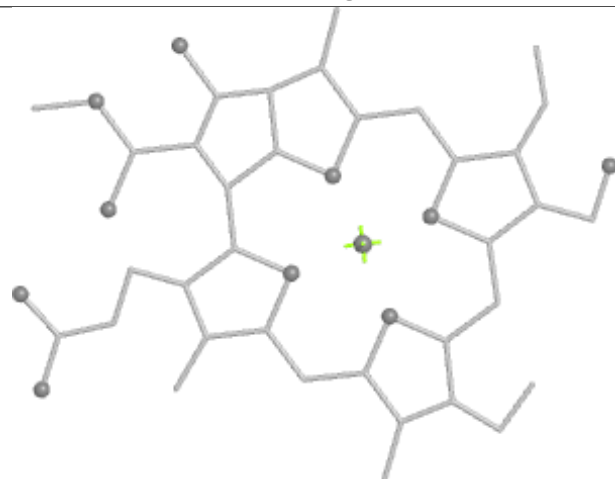
Bond lengths



Bond angles

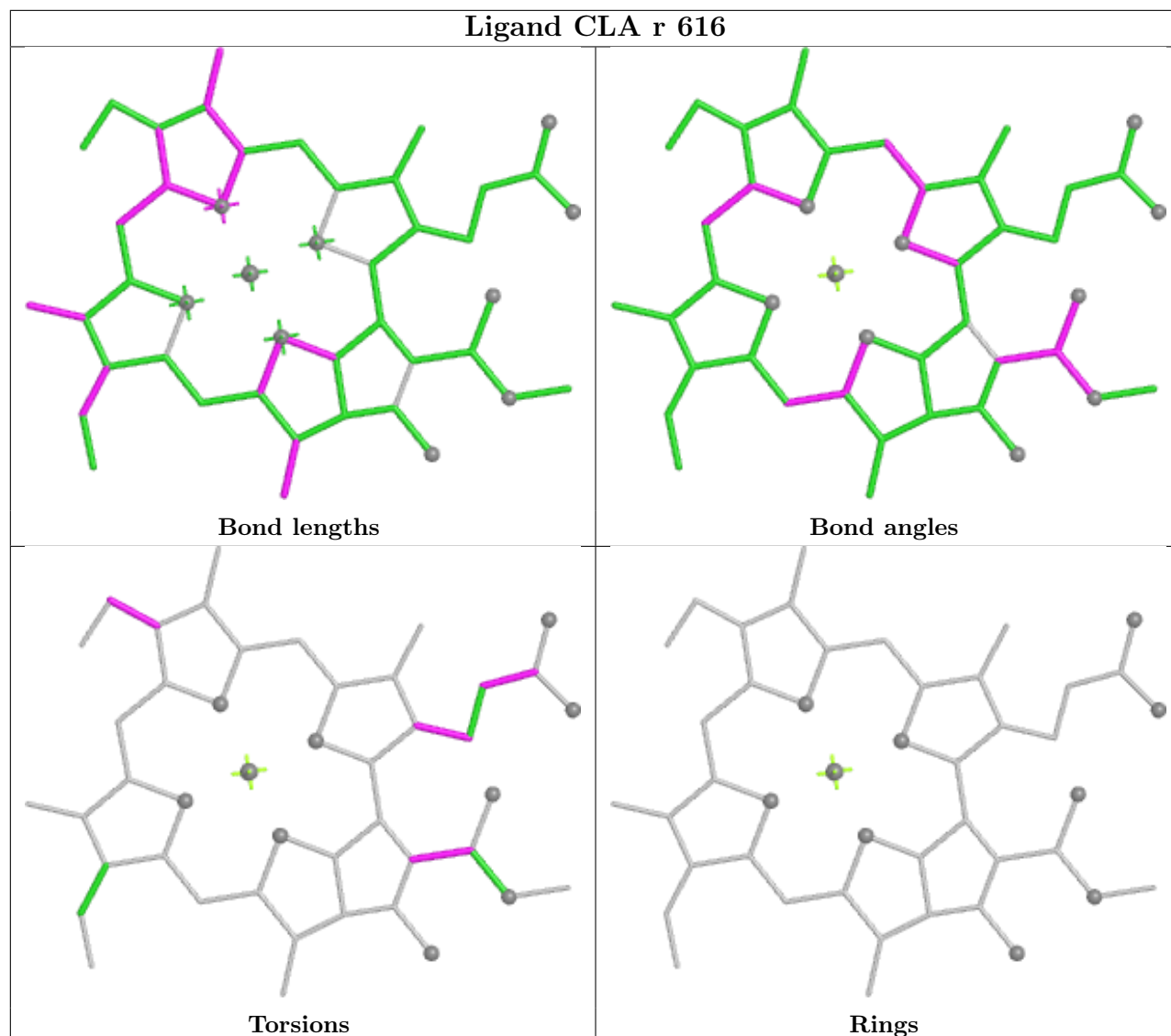


Torsions

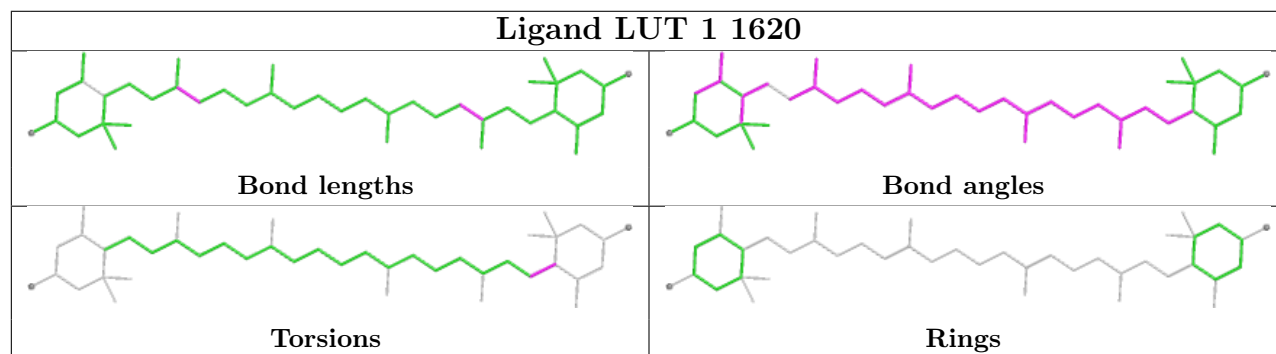


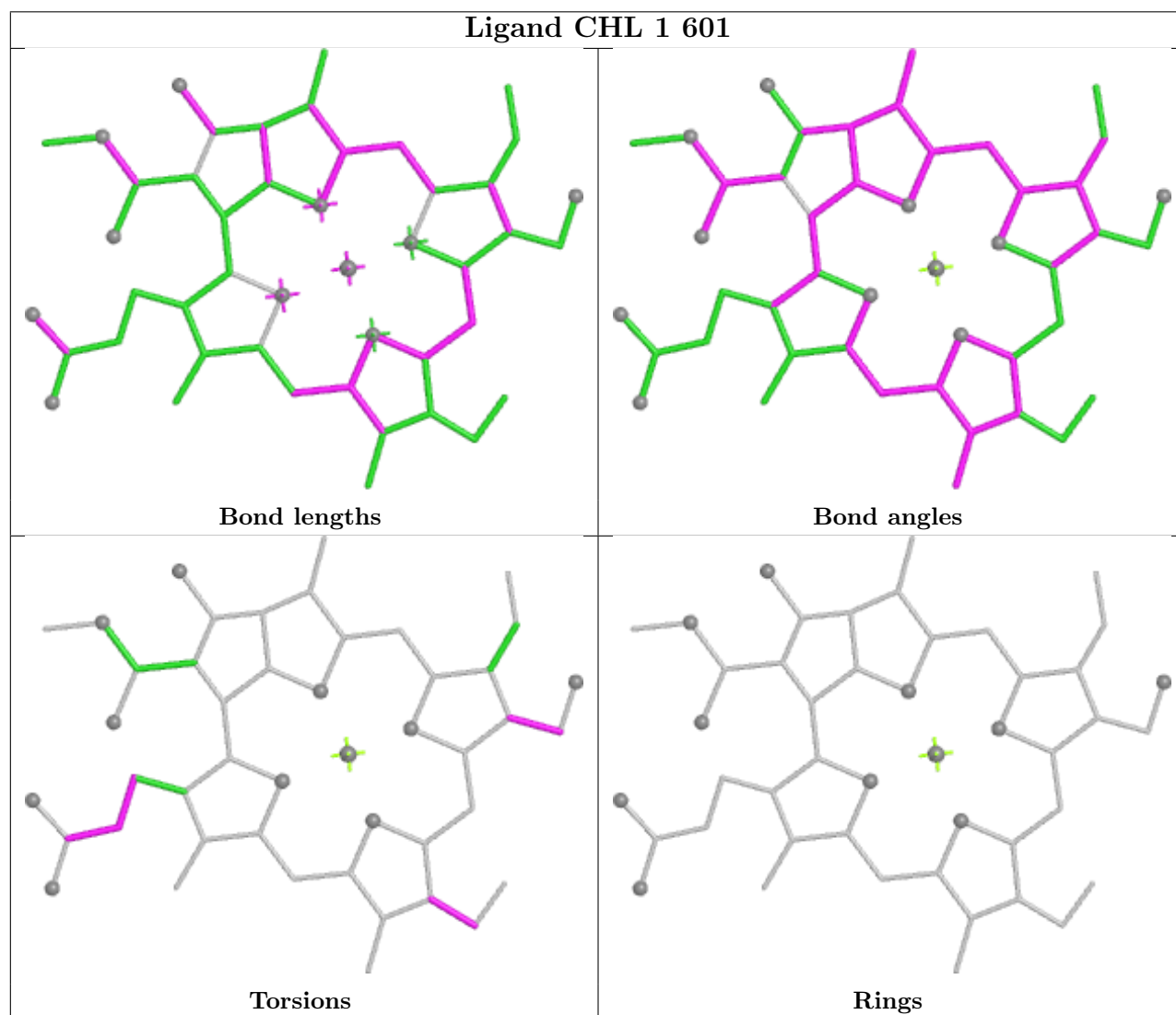
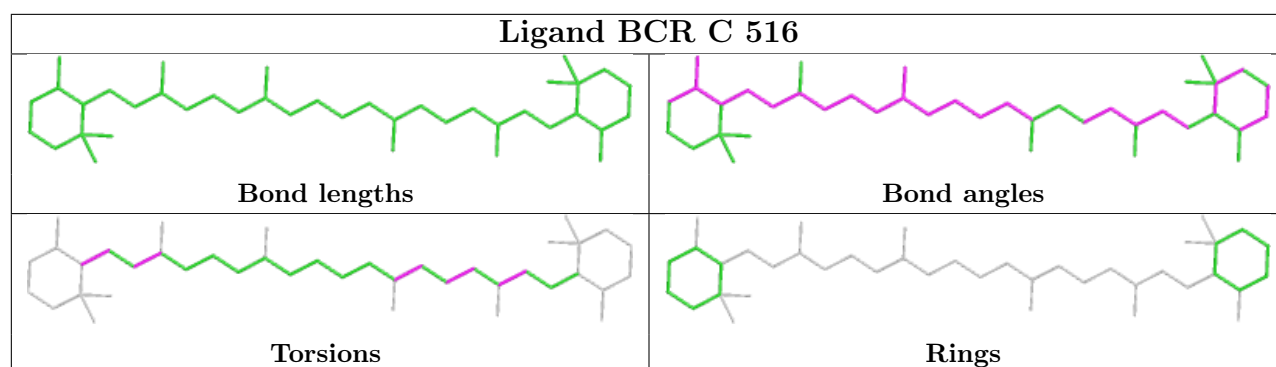
Rings

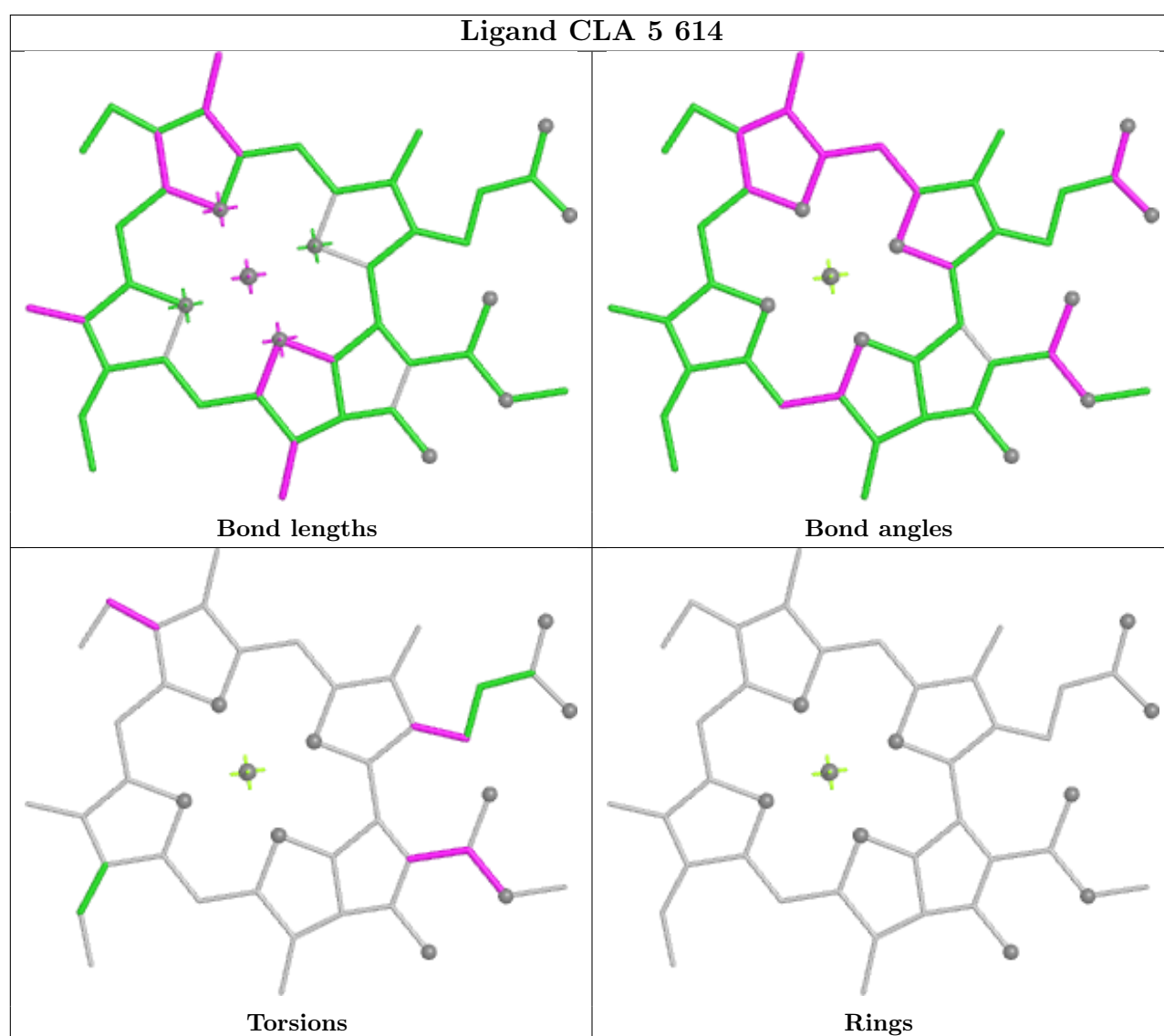
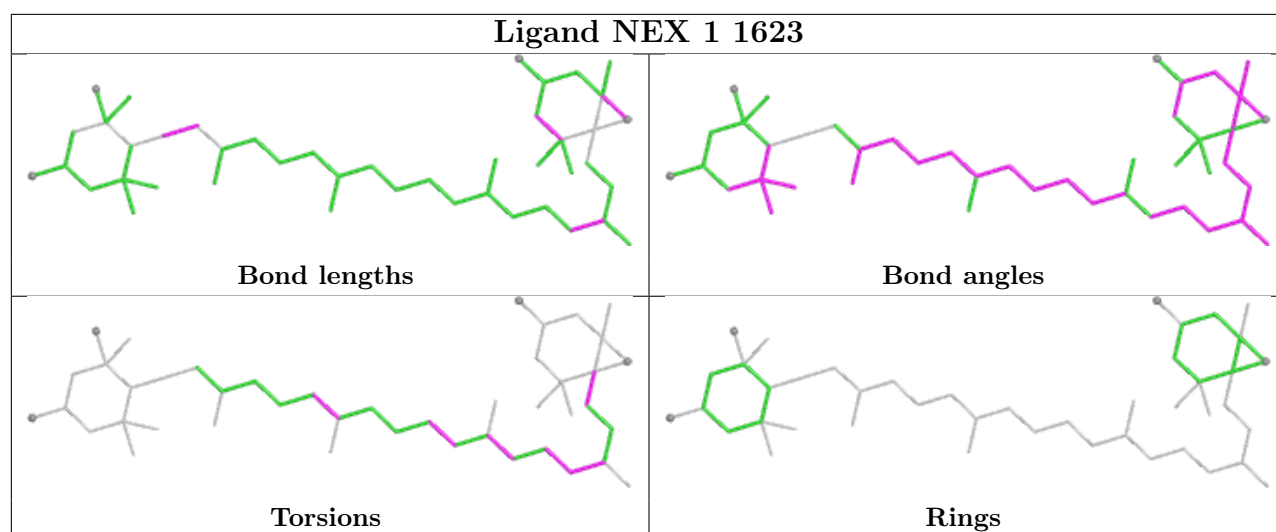
Ligand CLA r 616

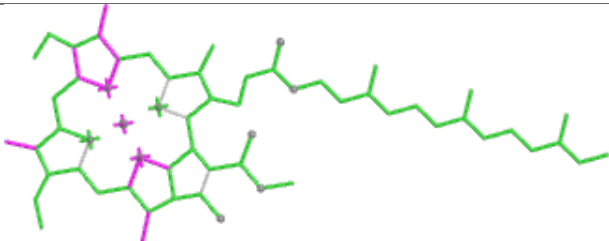
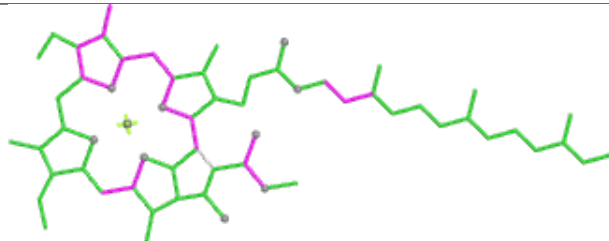
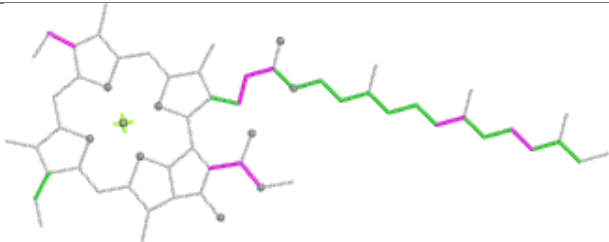
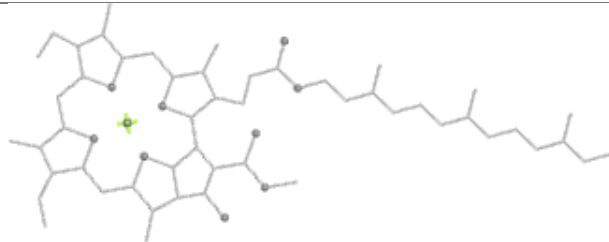


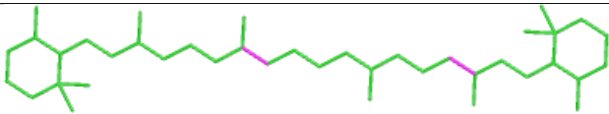
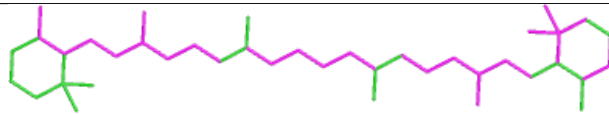
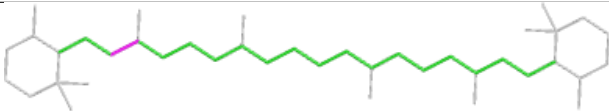
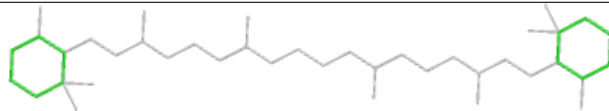
Ligand LUT 1 1620

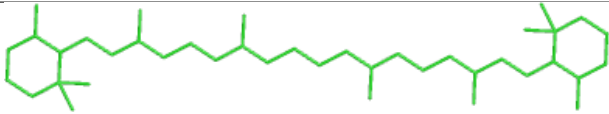
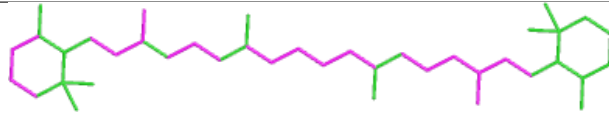
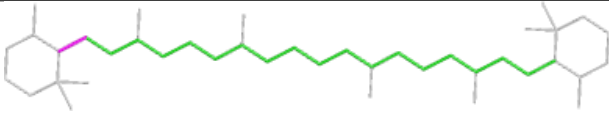
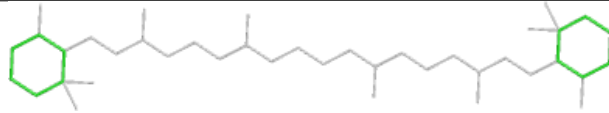




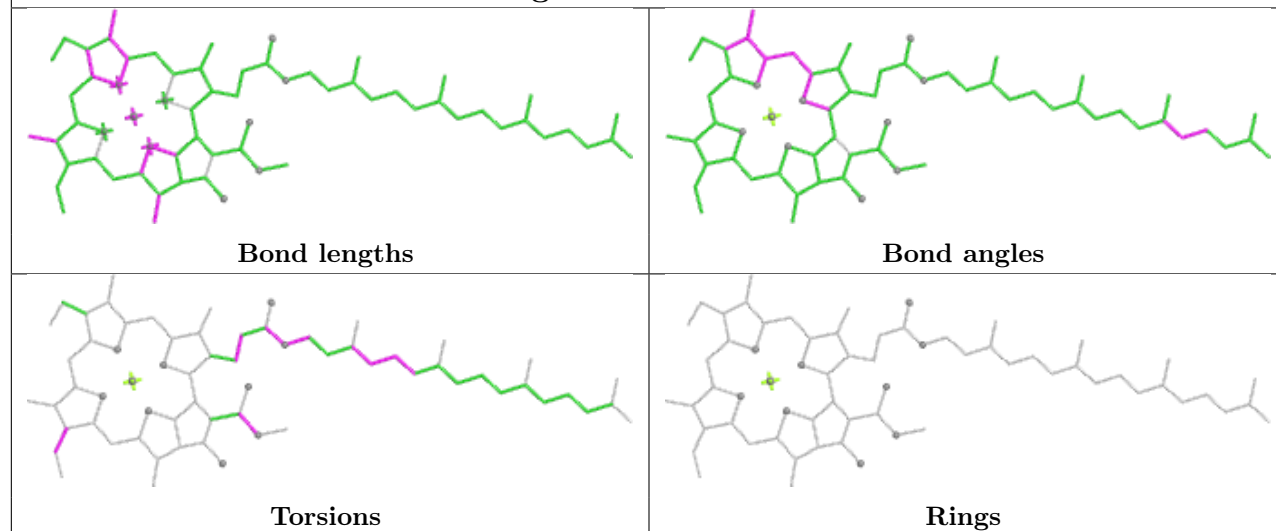


Ligand CLA 1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

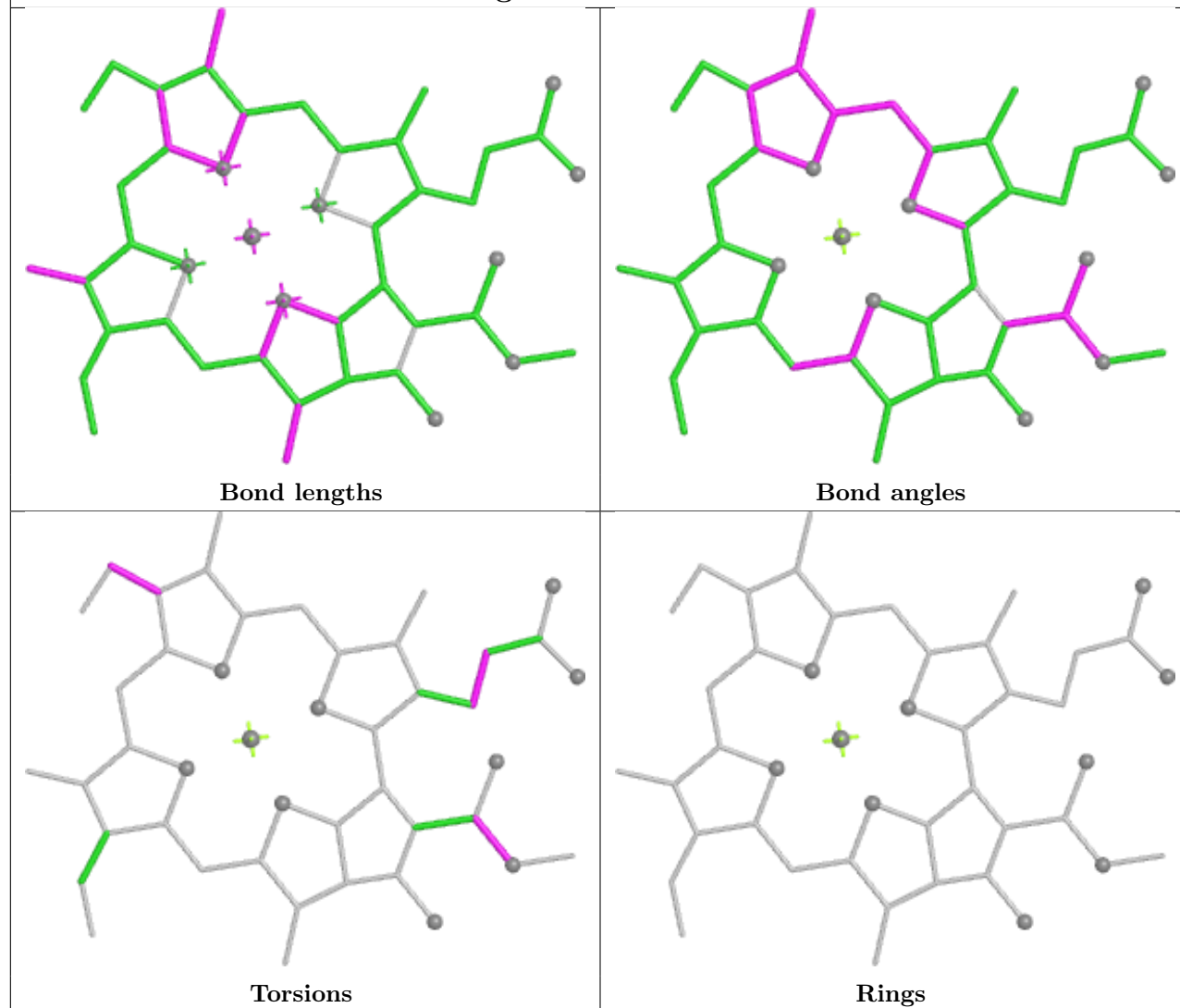
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

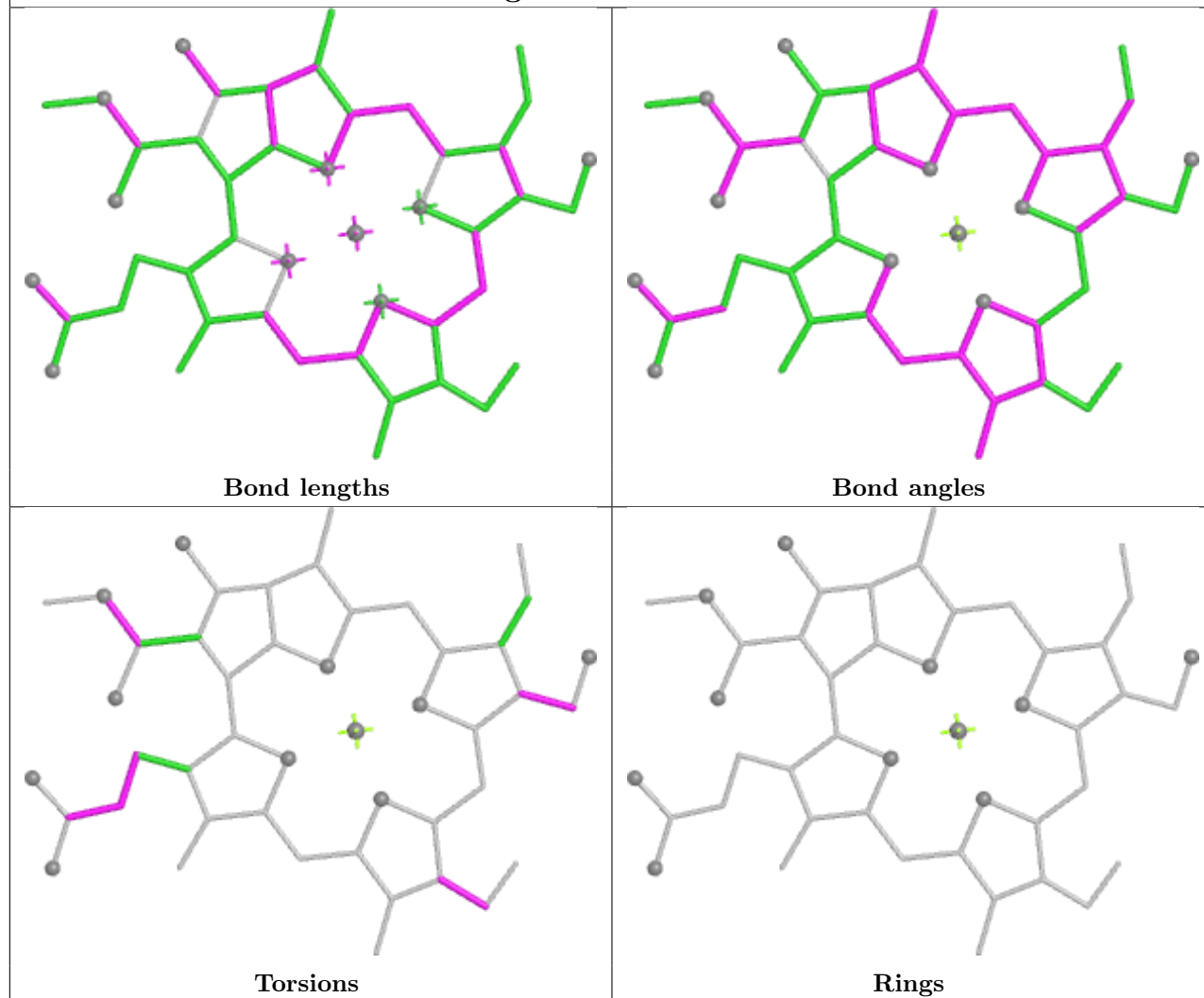
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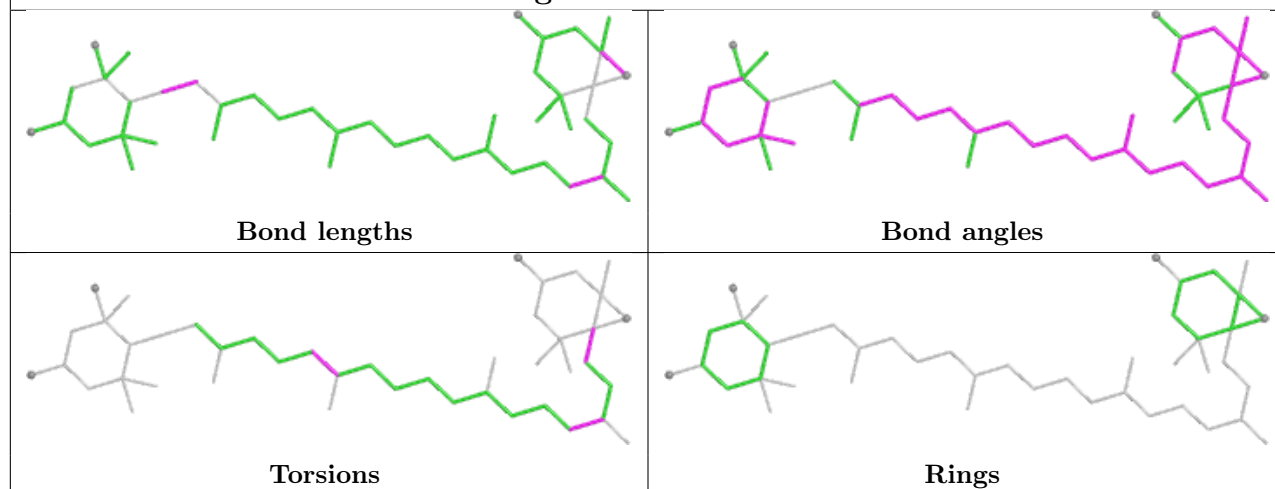
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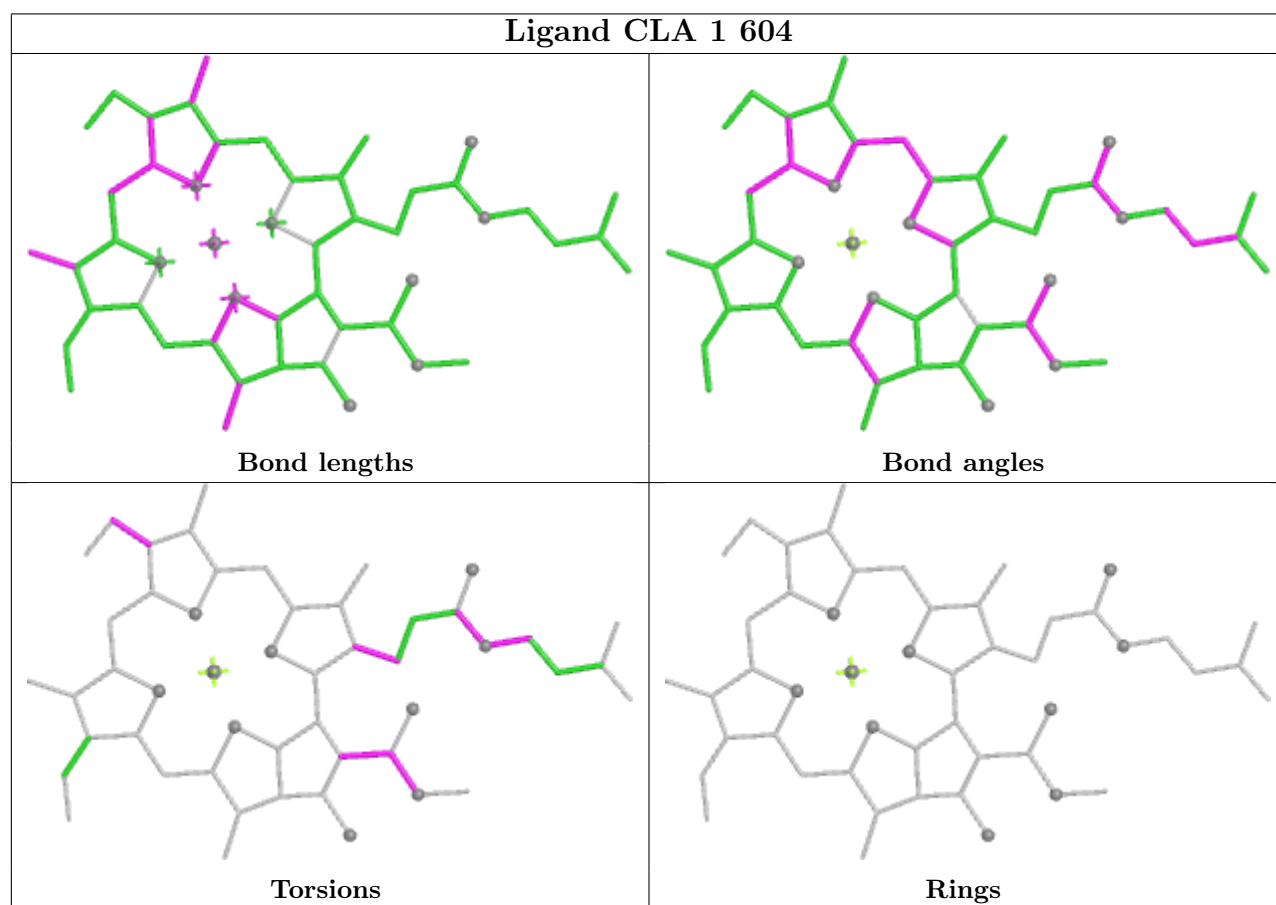
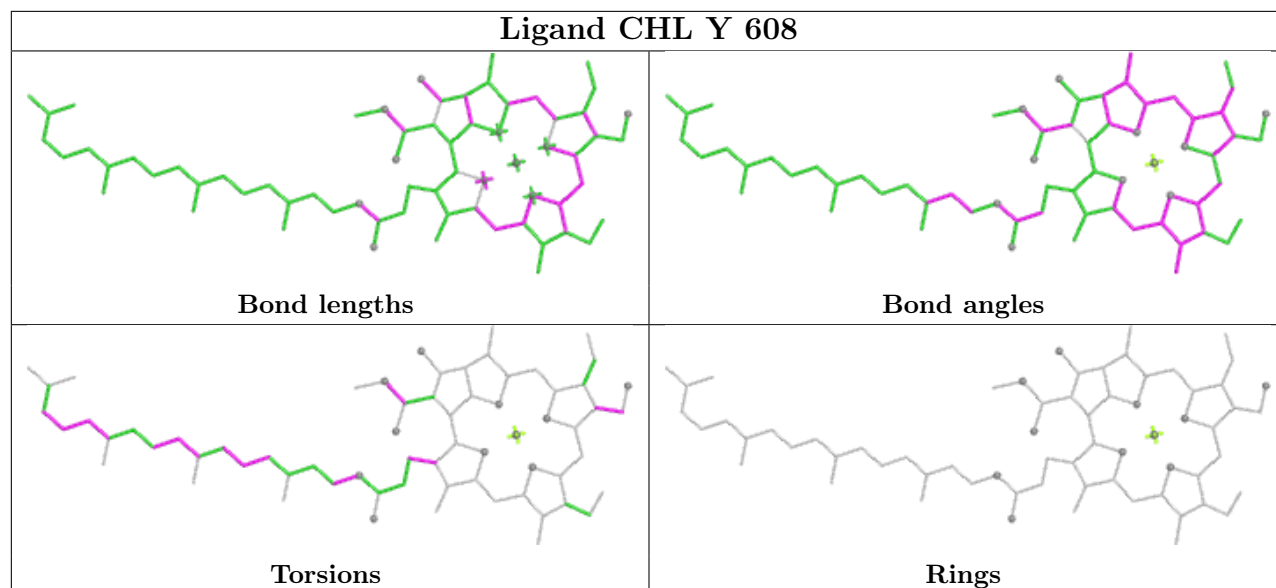


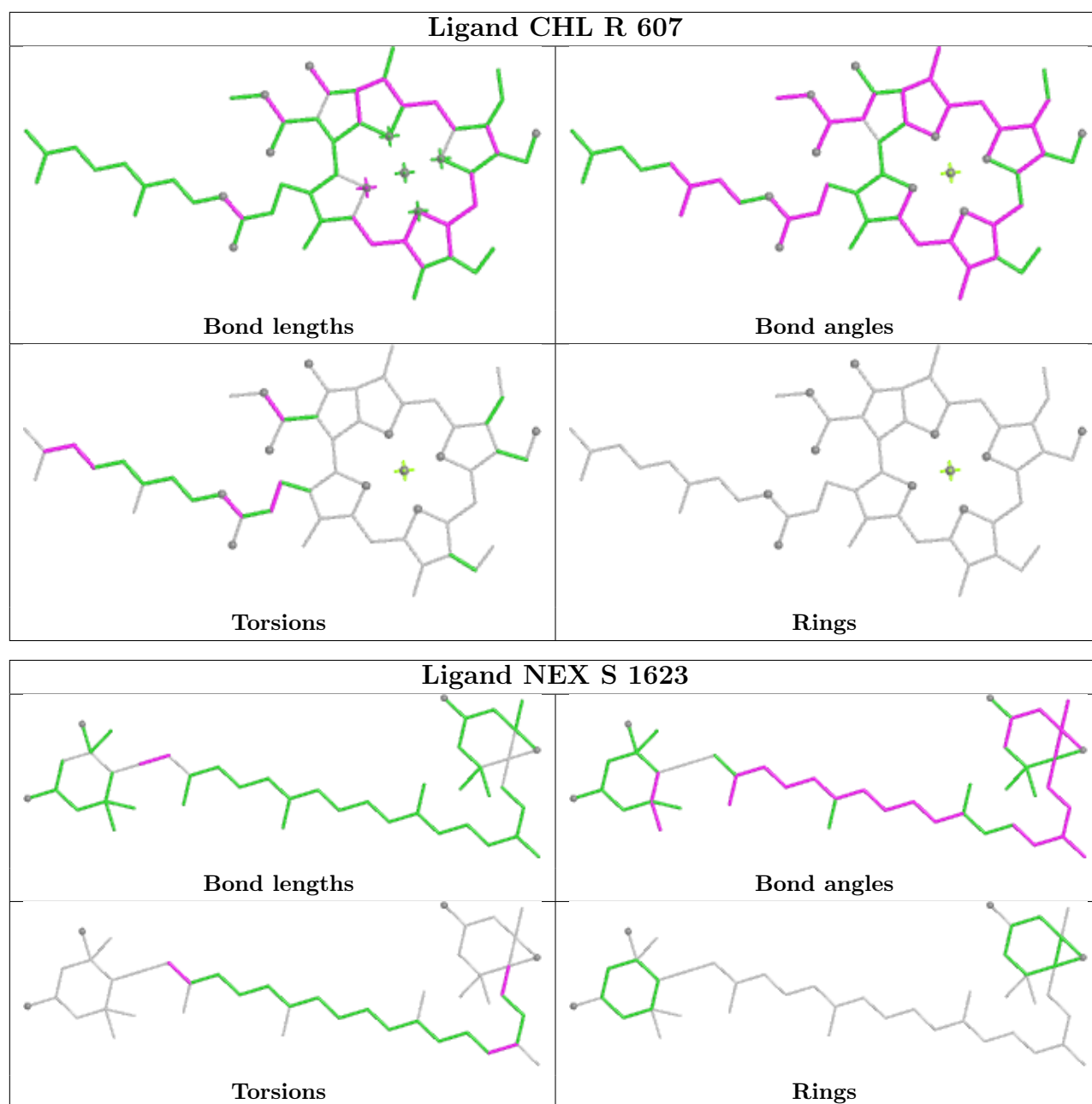
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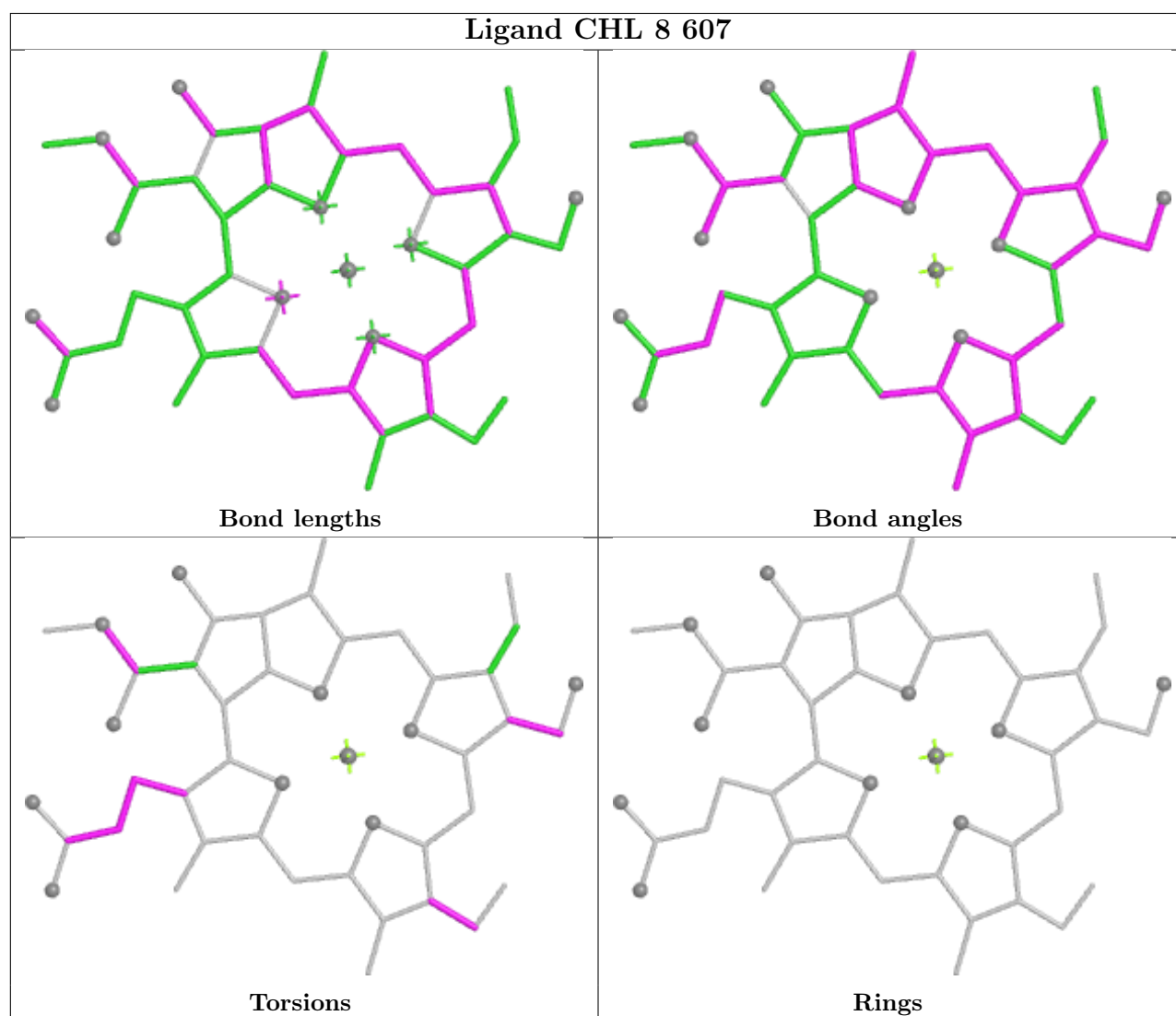
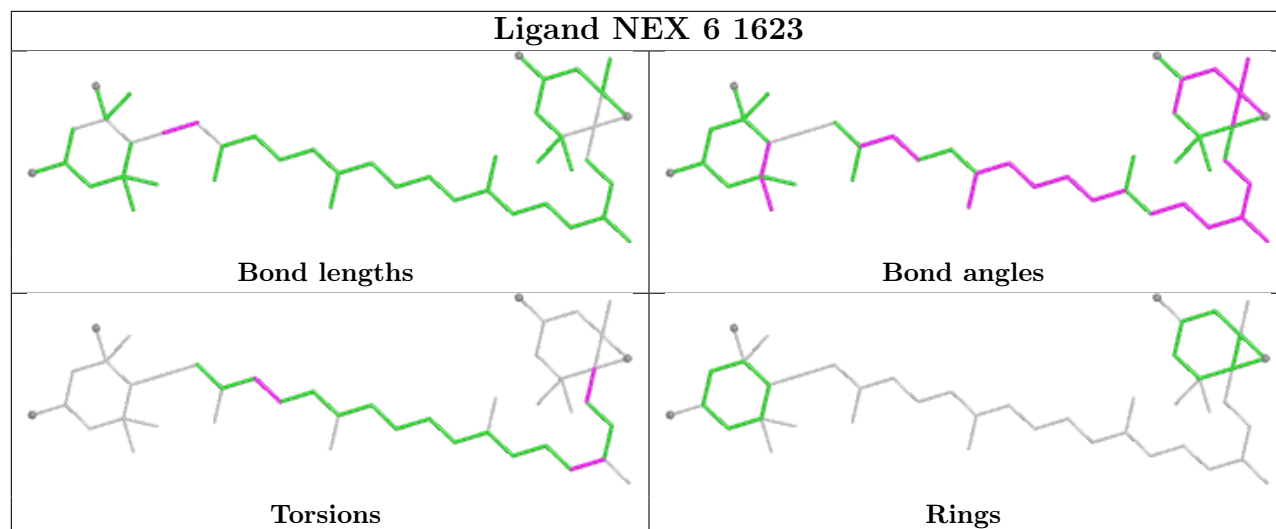


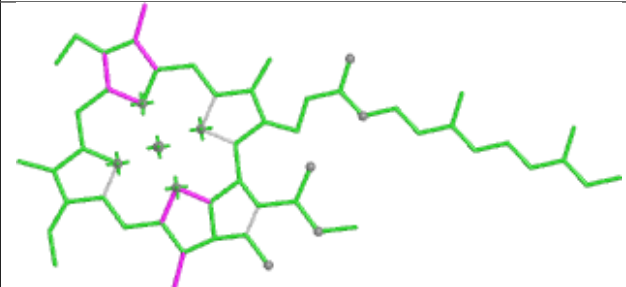
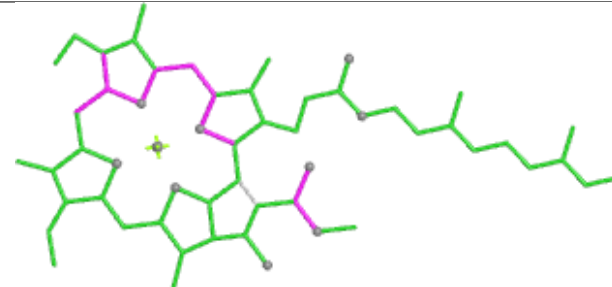
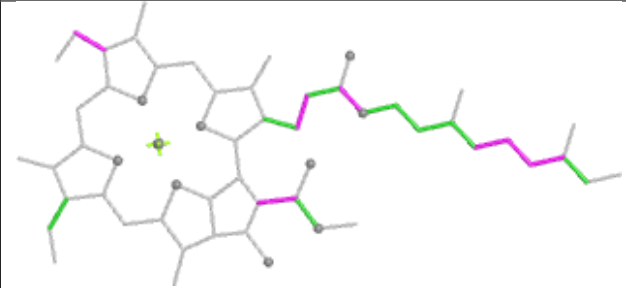
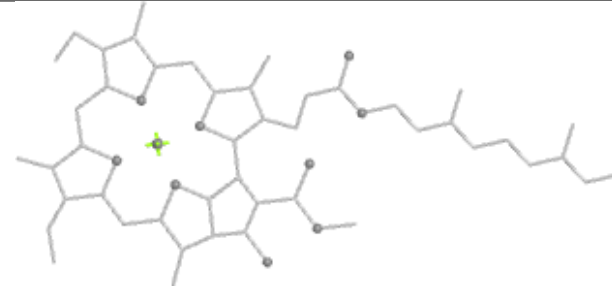
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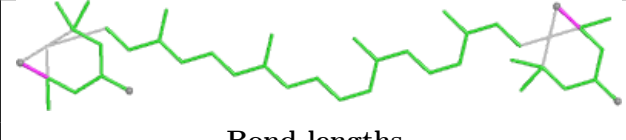
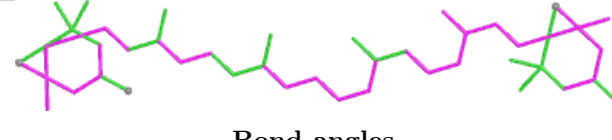
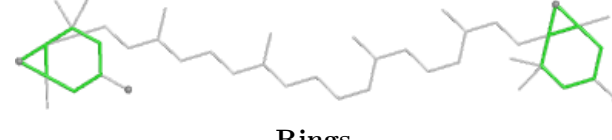


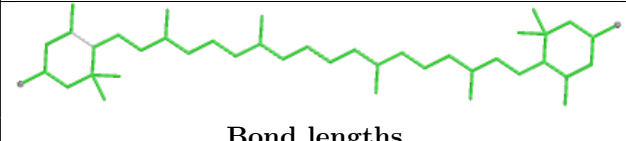
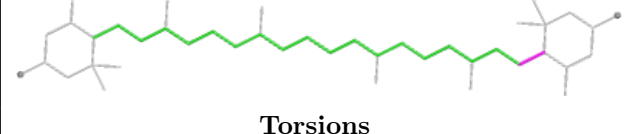
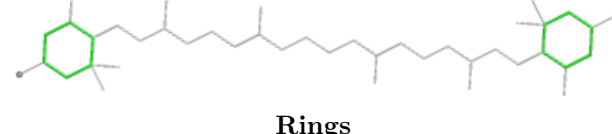


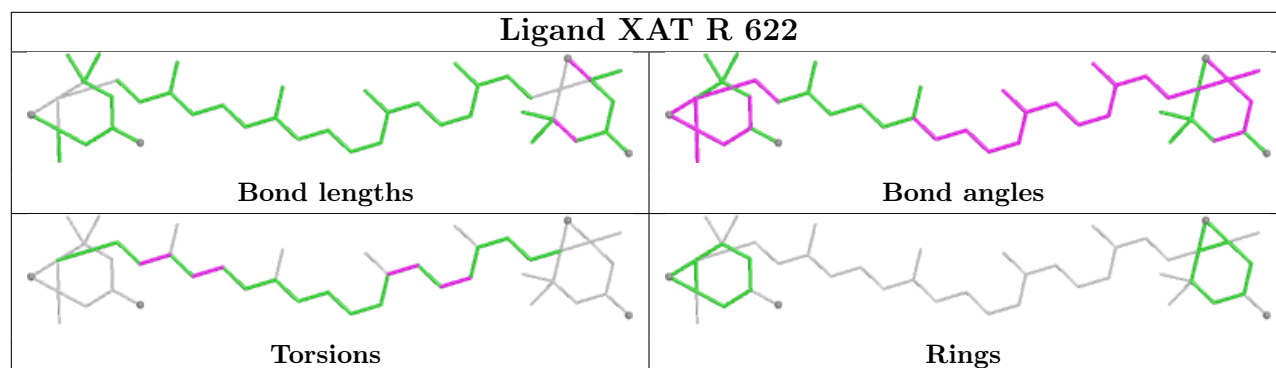
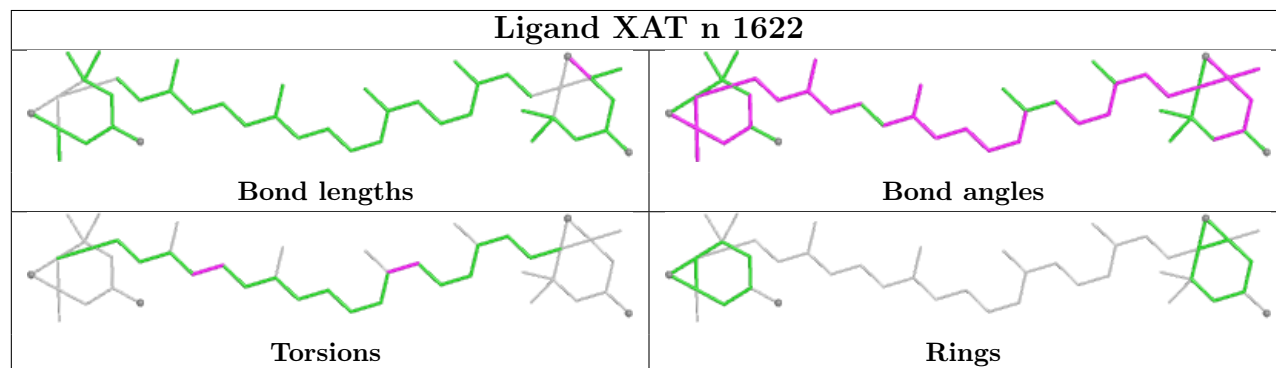
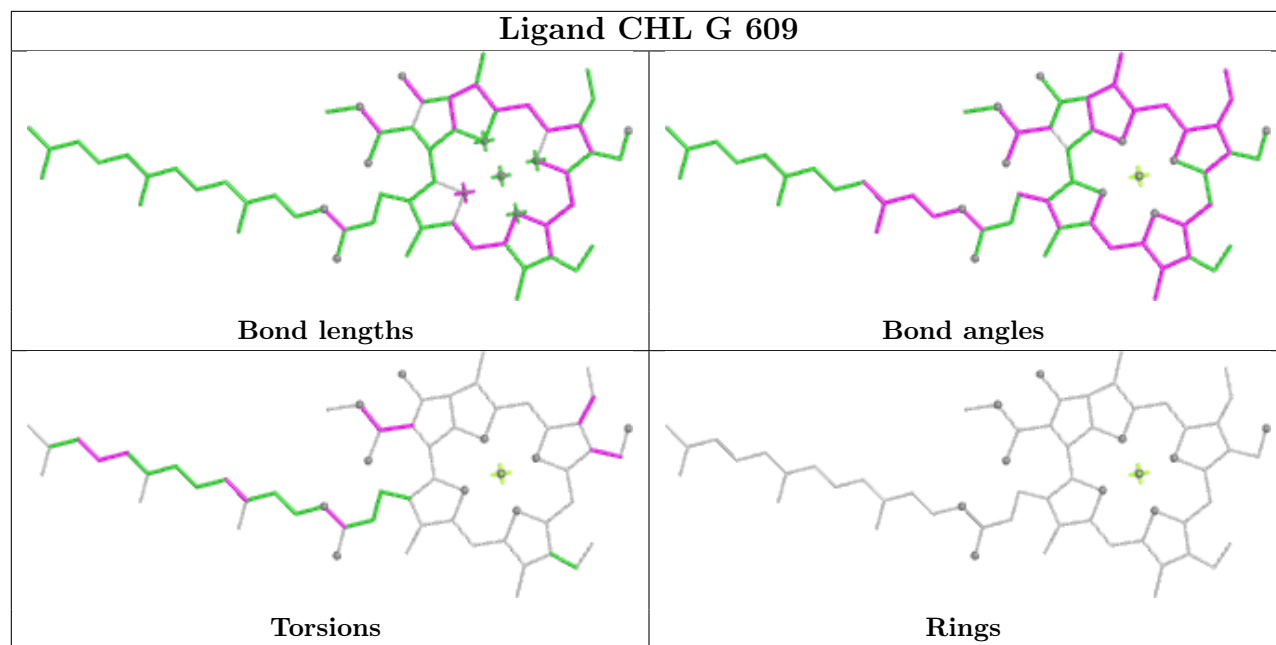




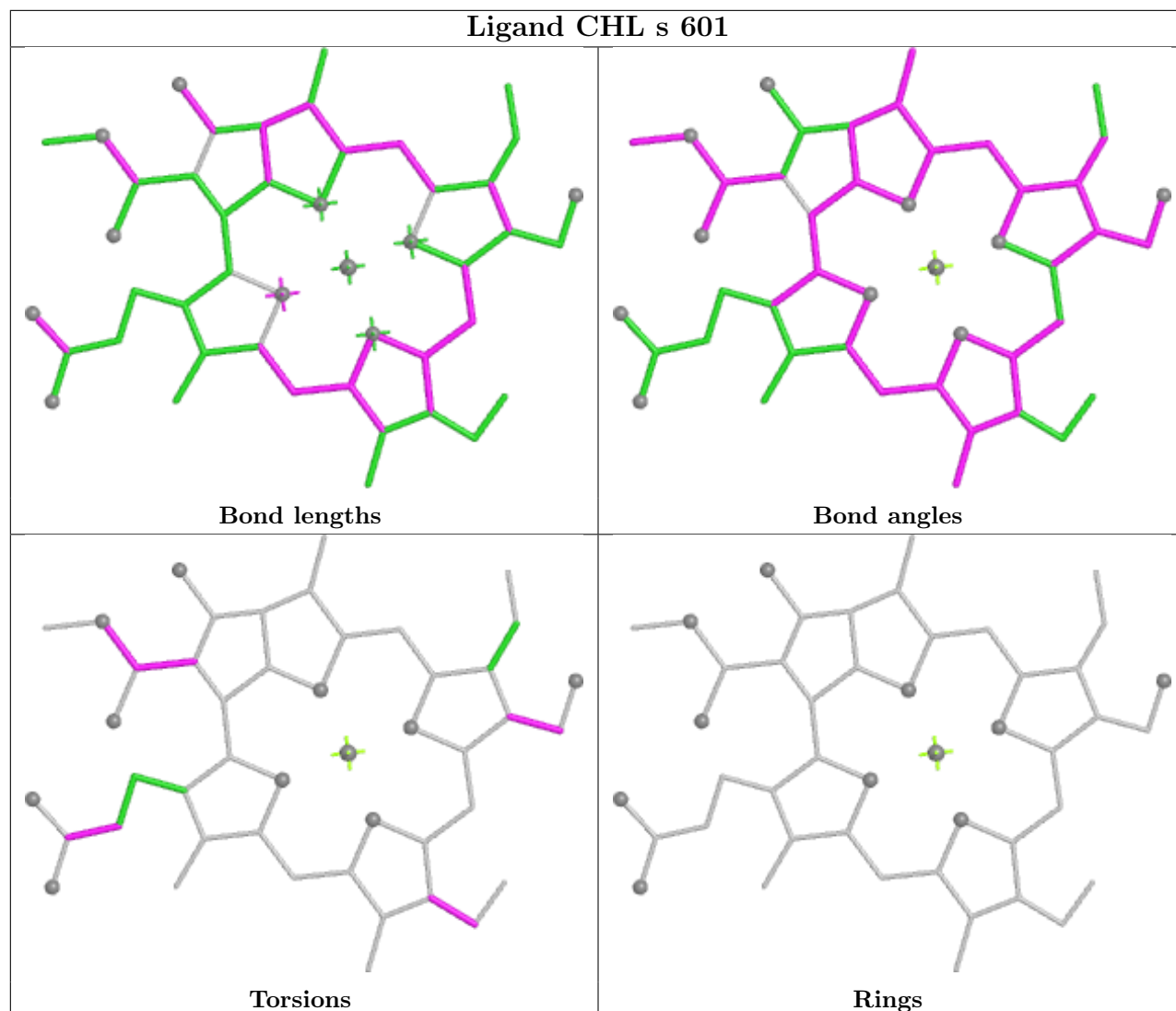
Ligand CLA s 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

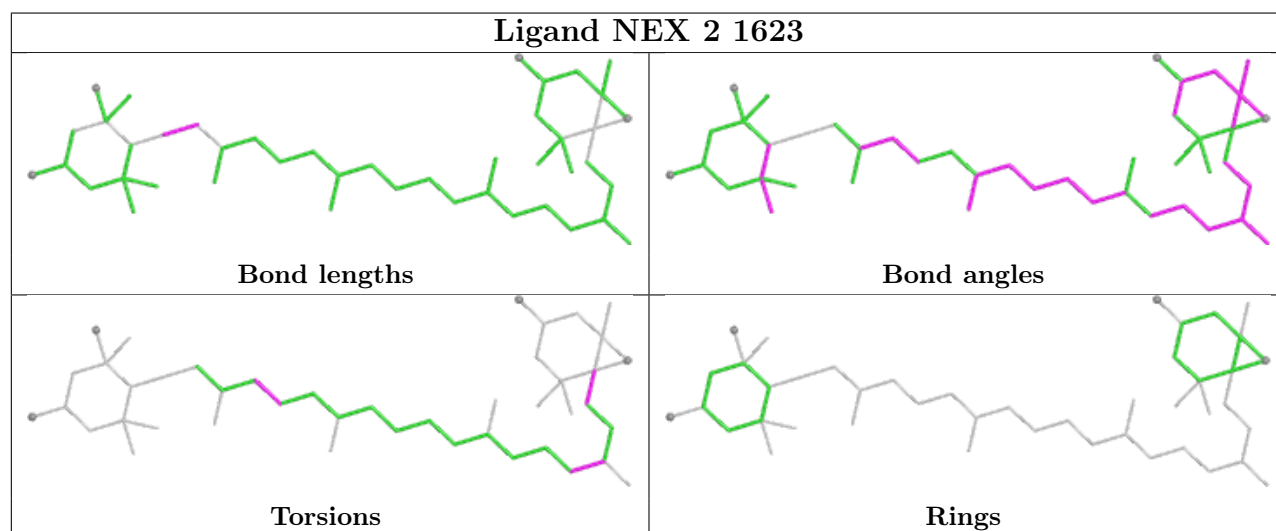
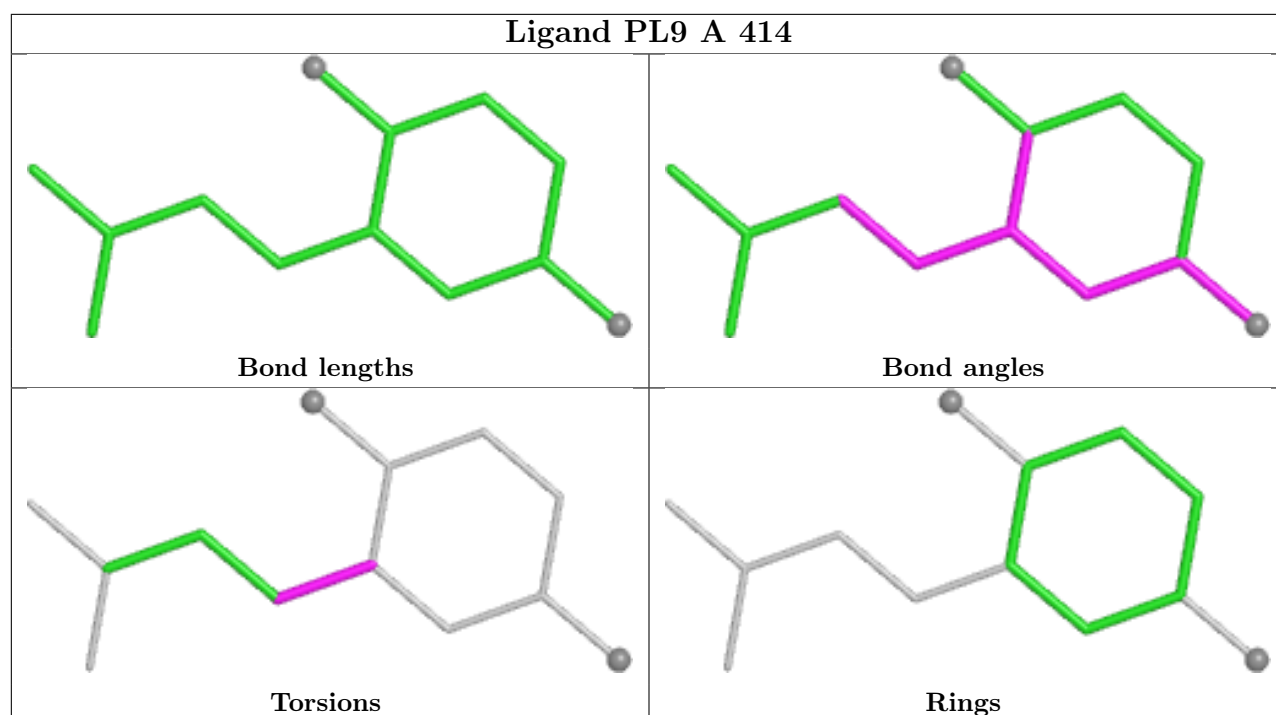
Ligand XAT 4 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

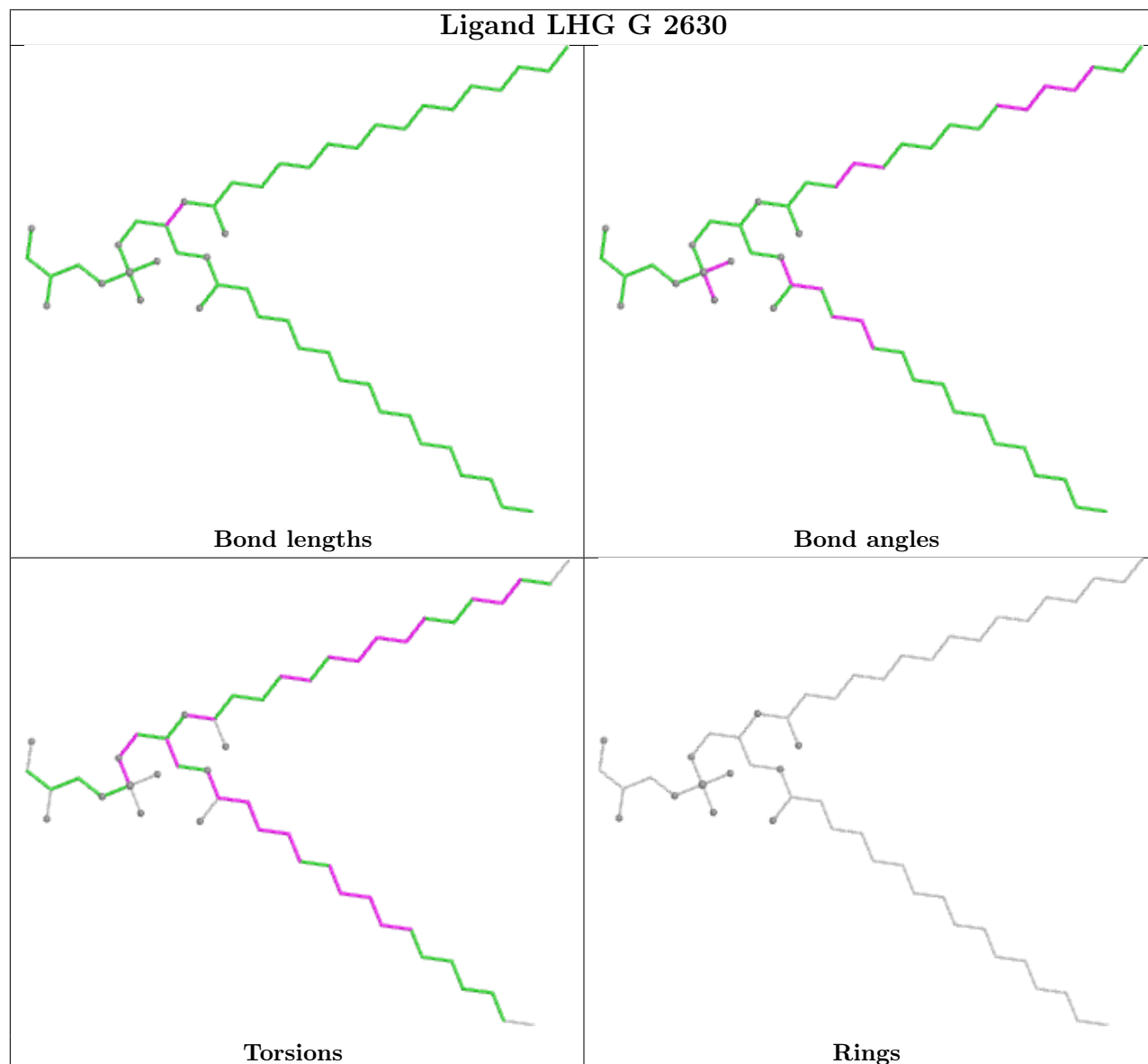
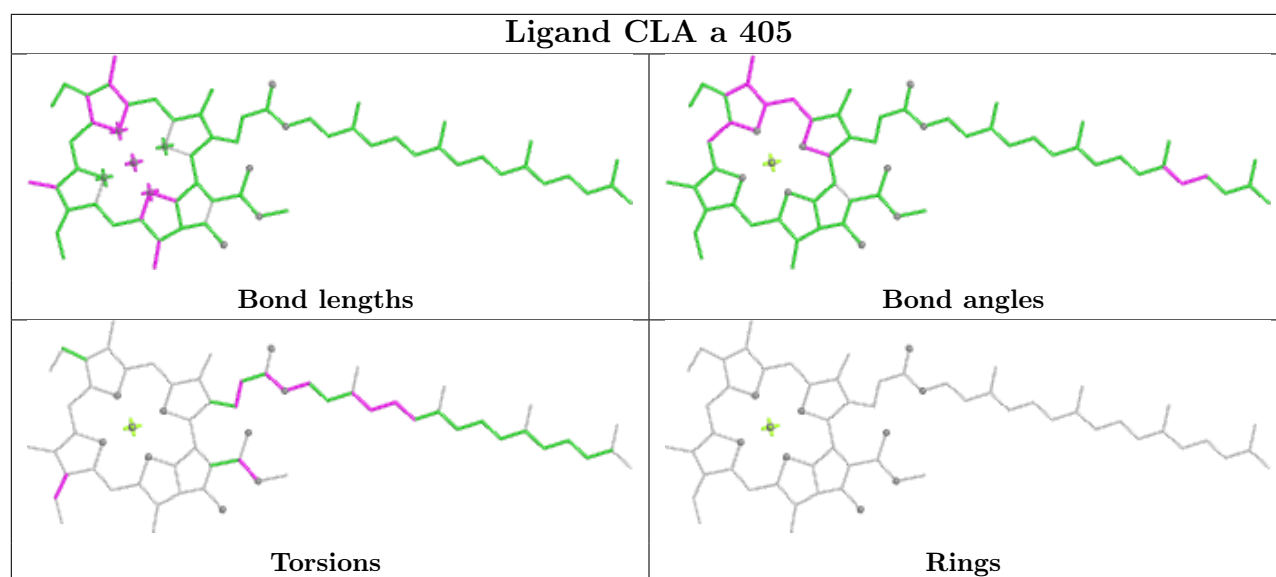
Ligand LUT 2 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

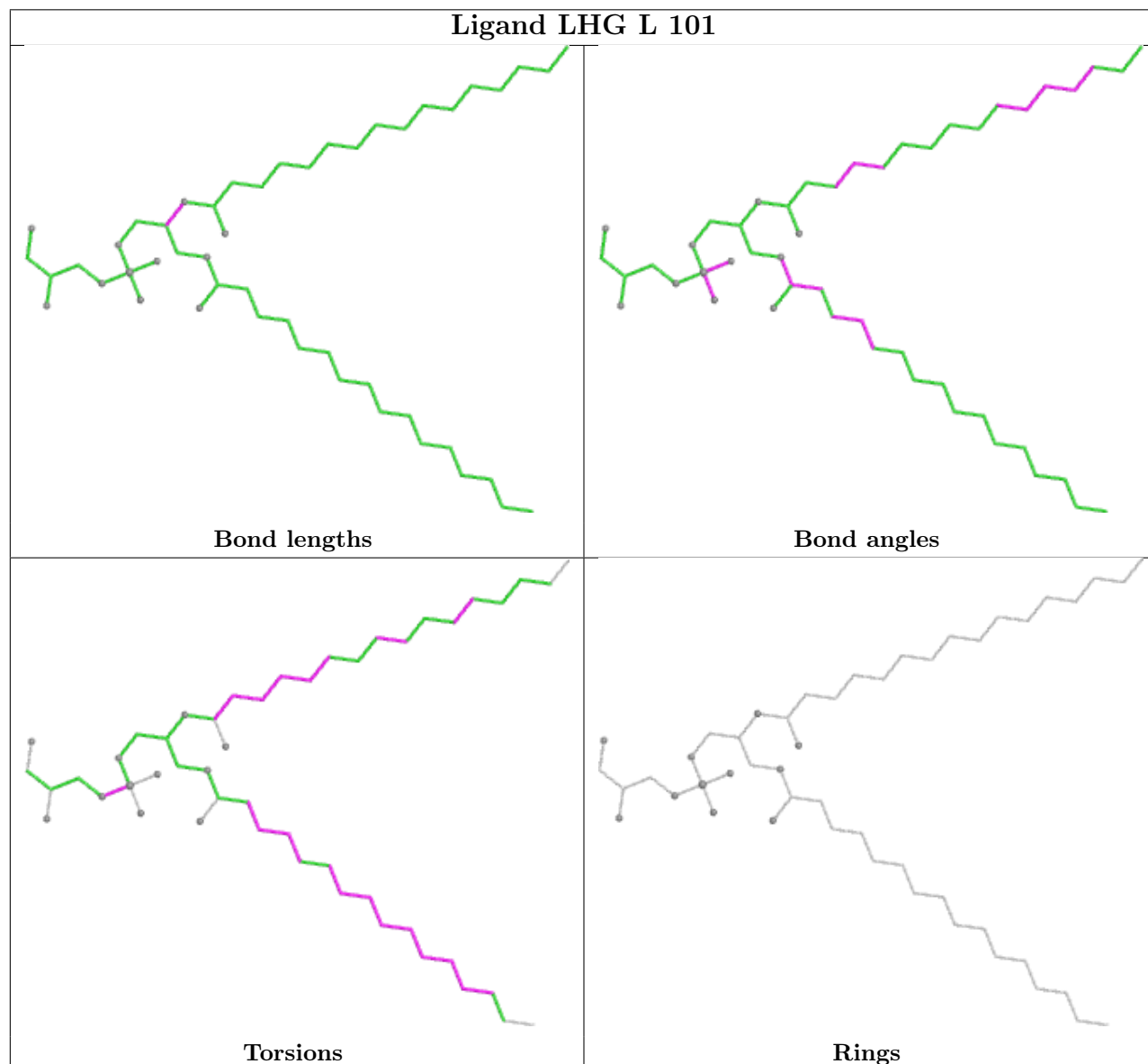
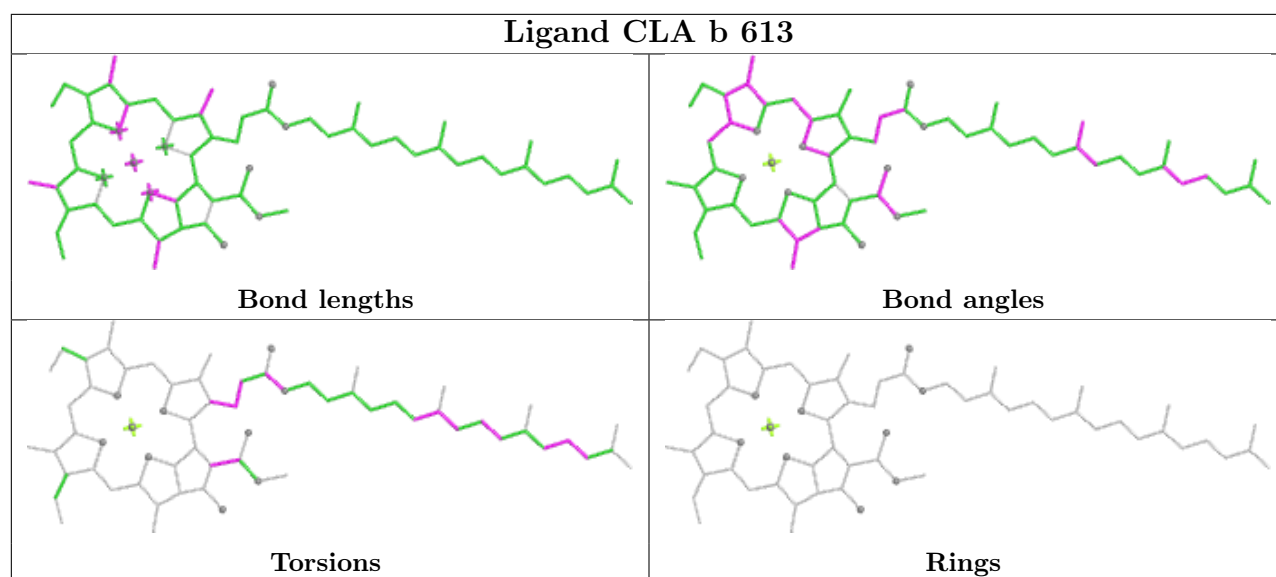


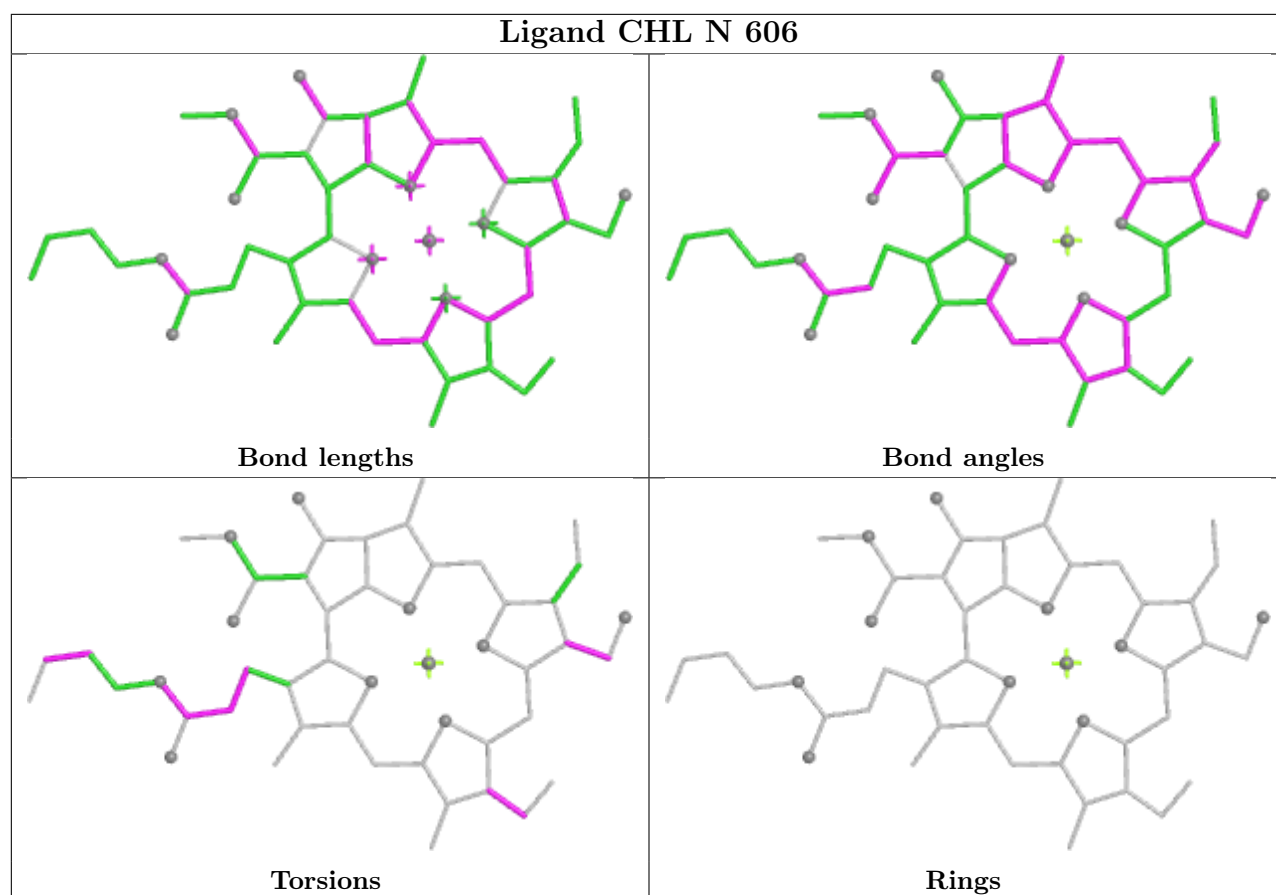
Ligand CHL s 601

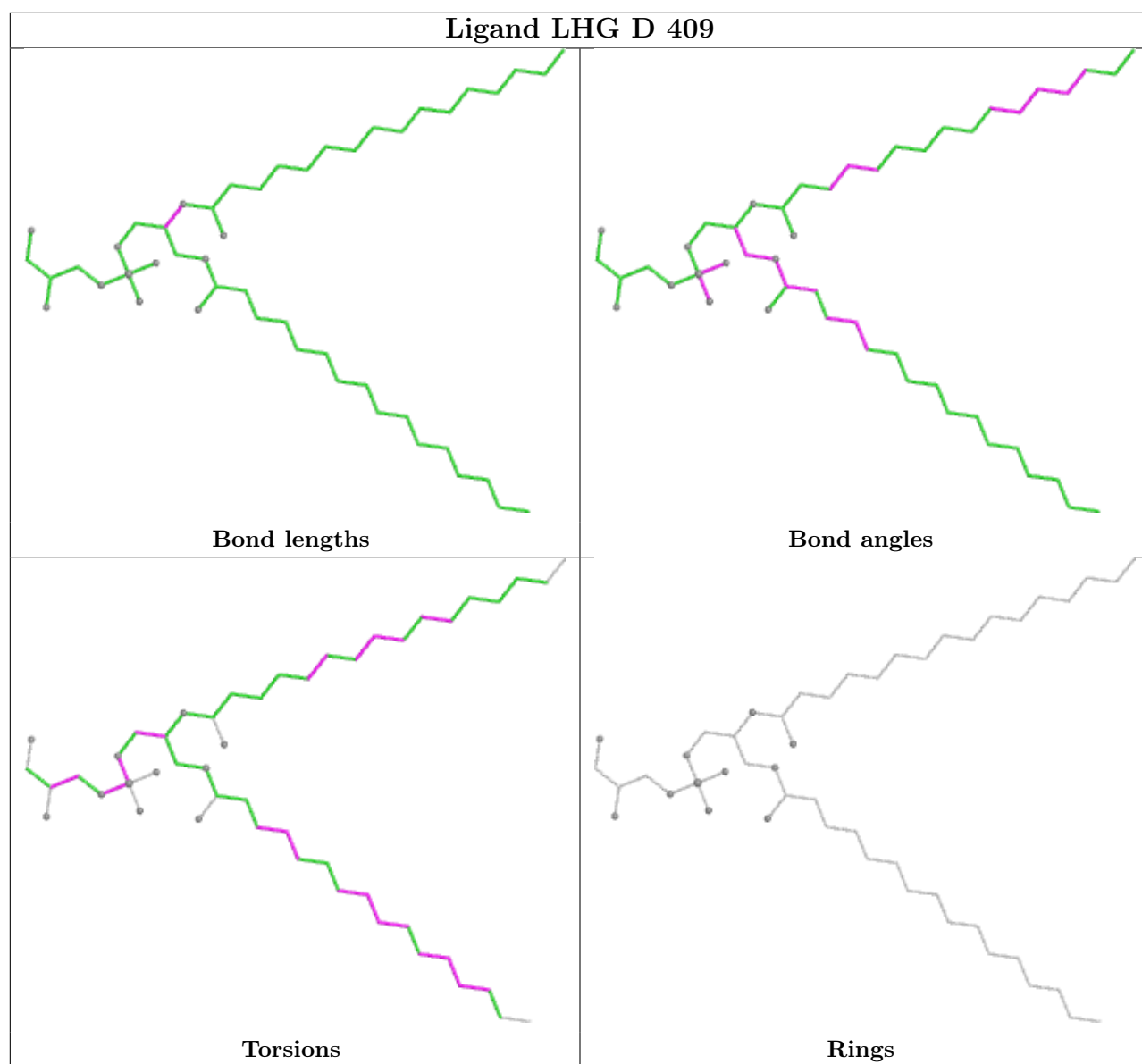




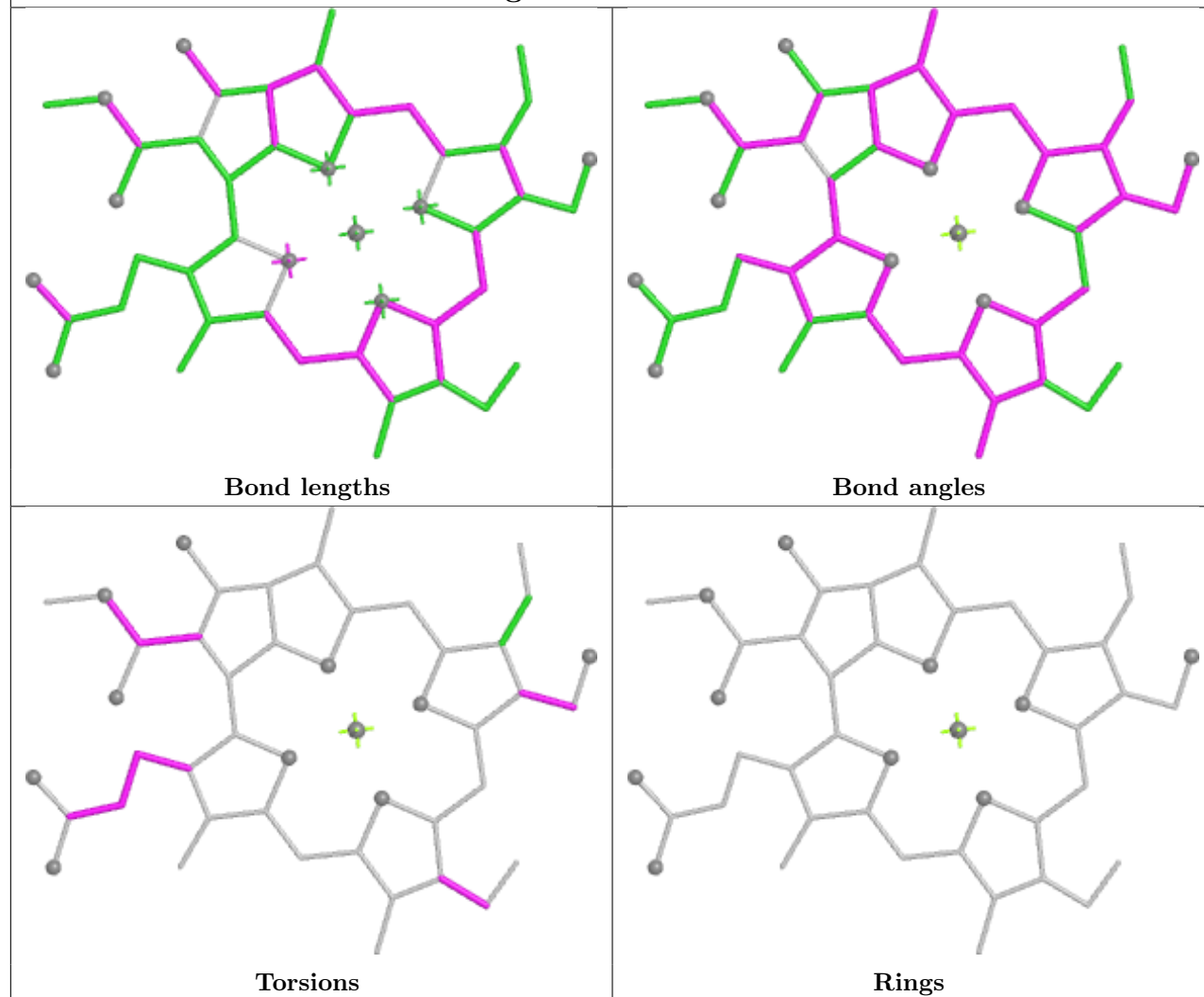




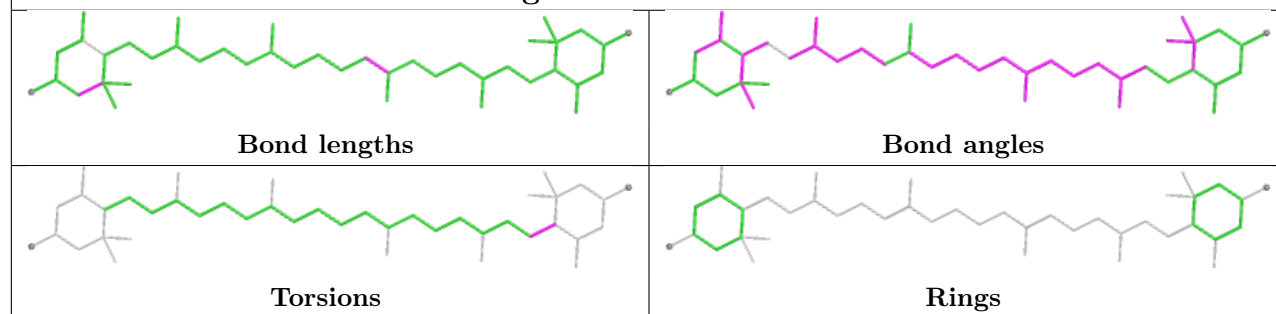


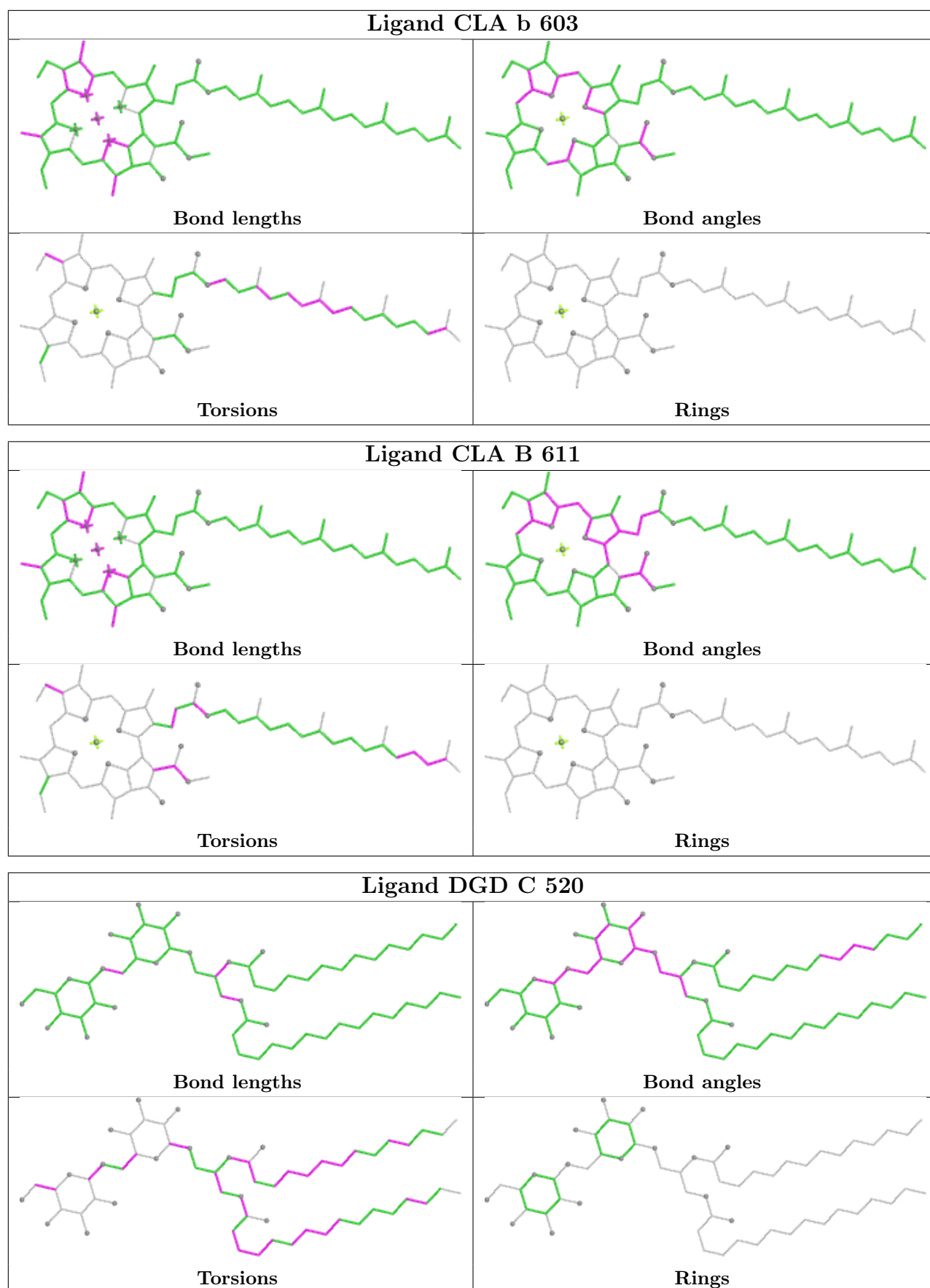


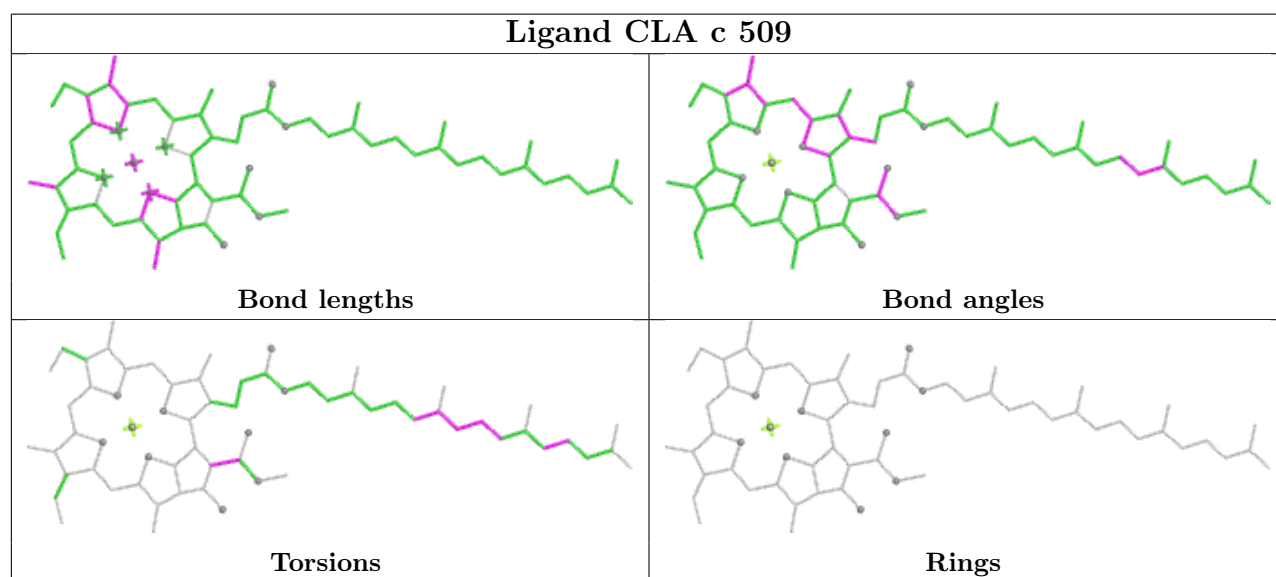
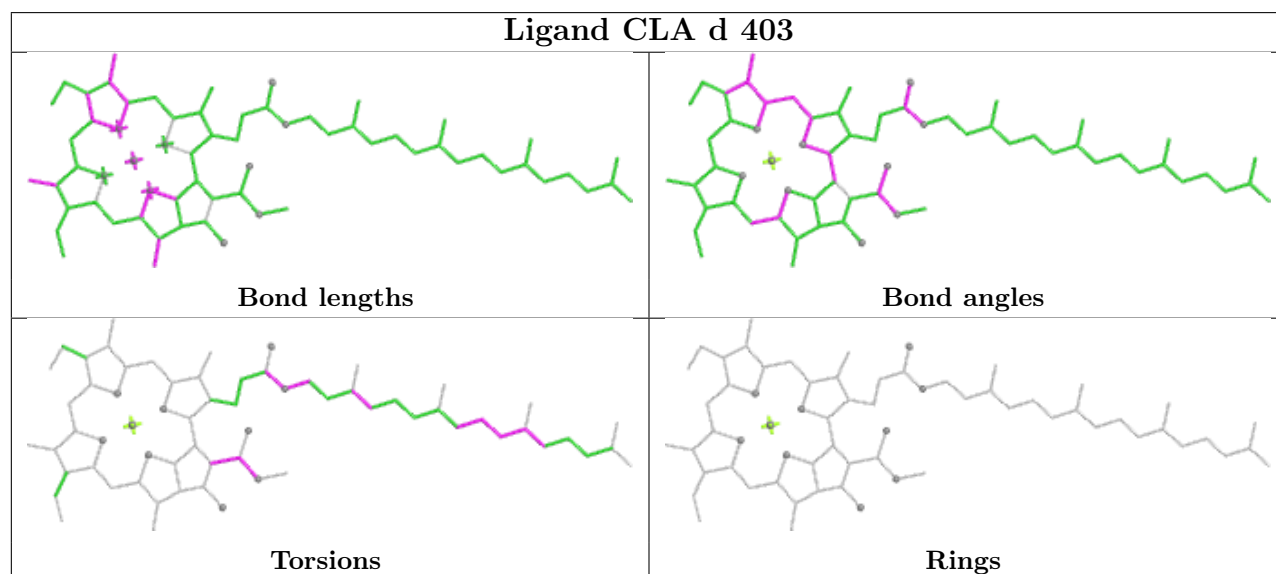
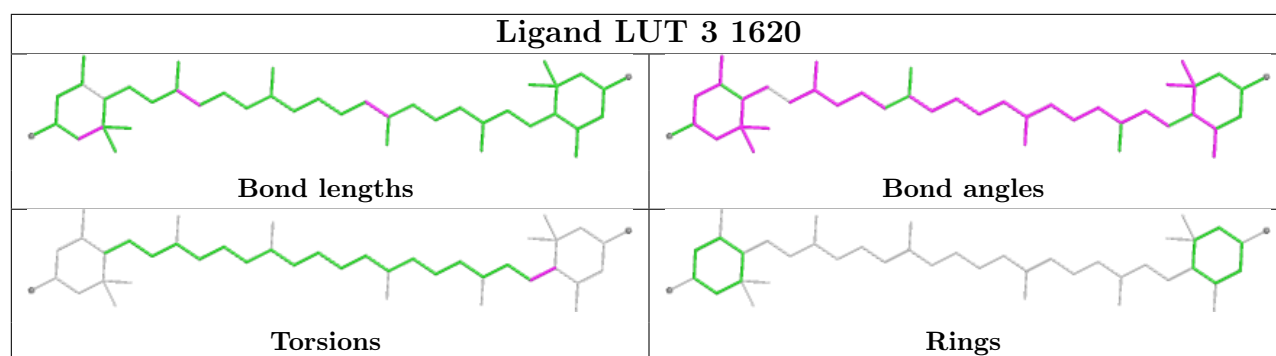
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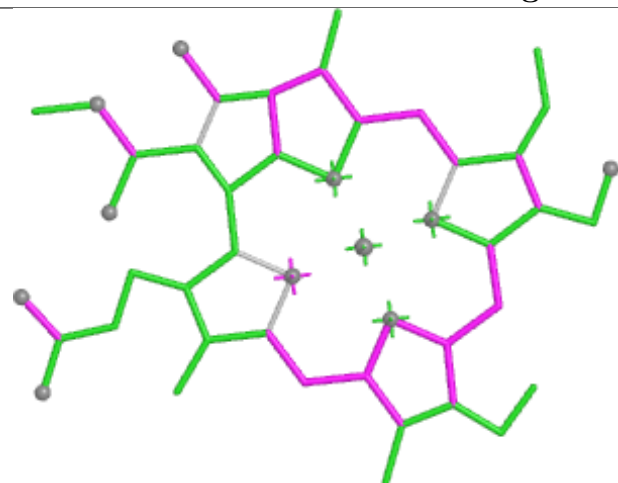
Ligand LUT N 1620



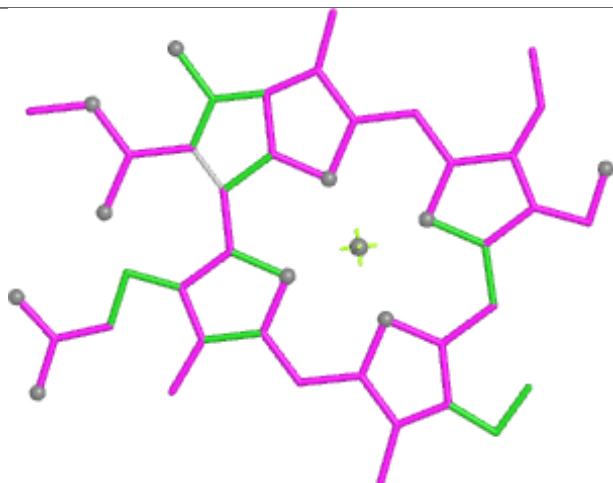




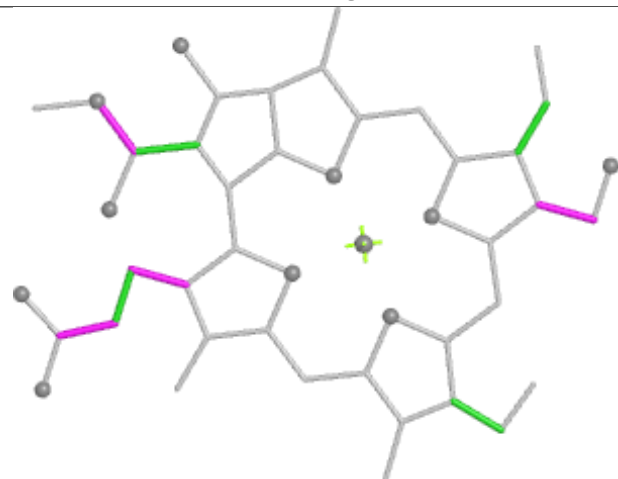
Ligand CHL 4 608



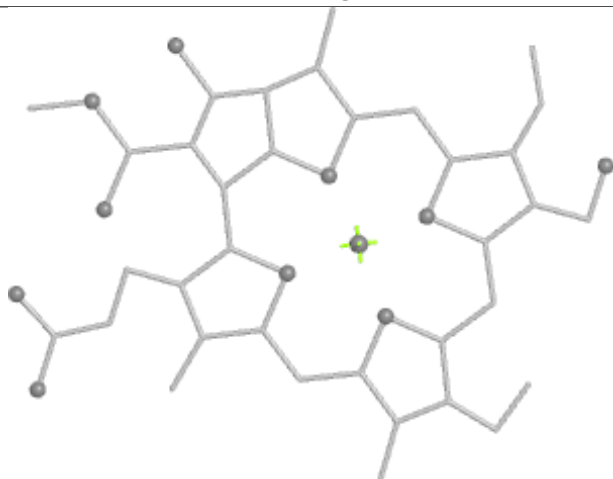
Bond lengths



Bond angles

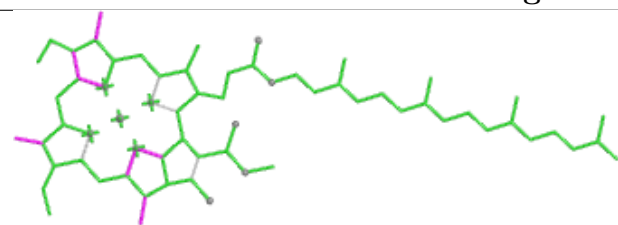


Torsions

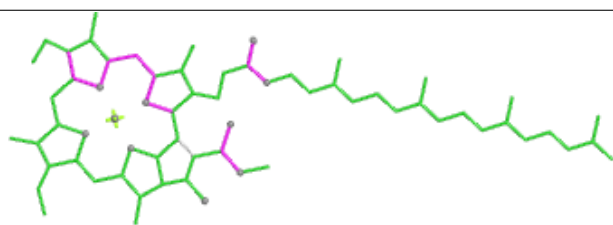


Rings

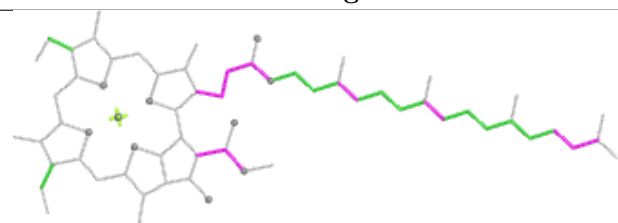
Ligand CLA c 501



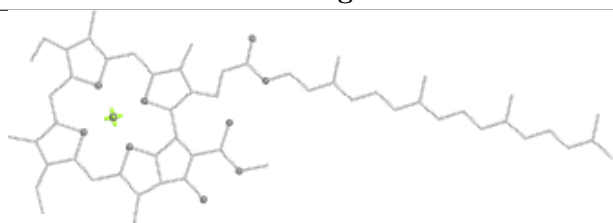
Bond lengths



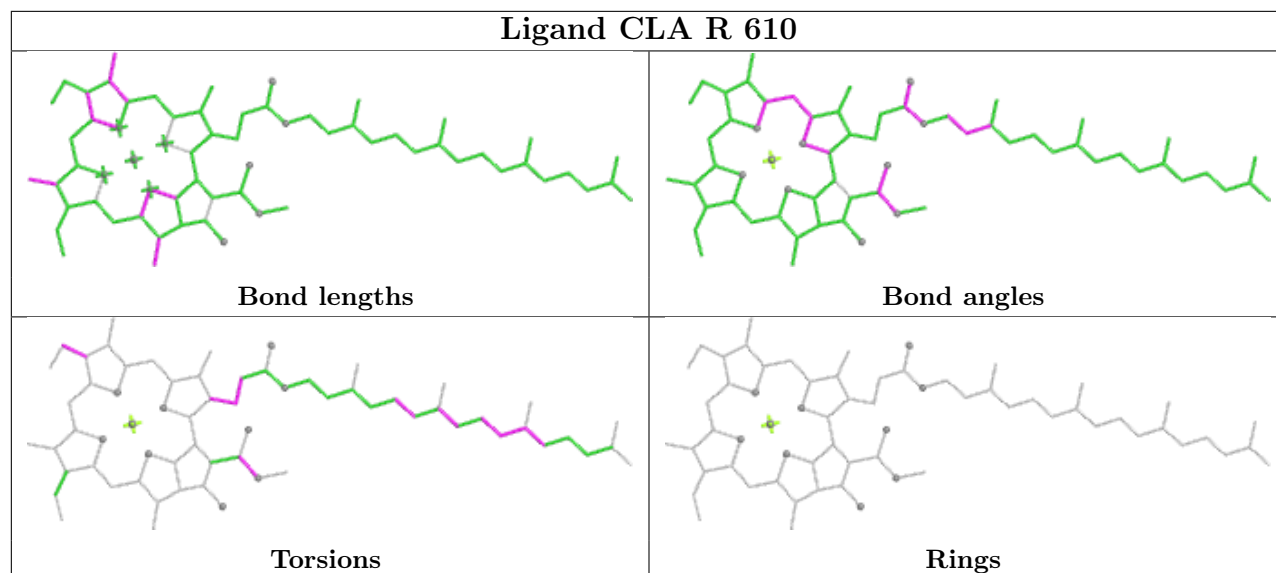
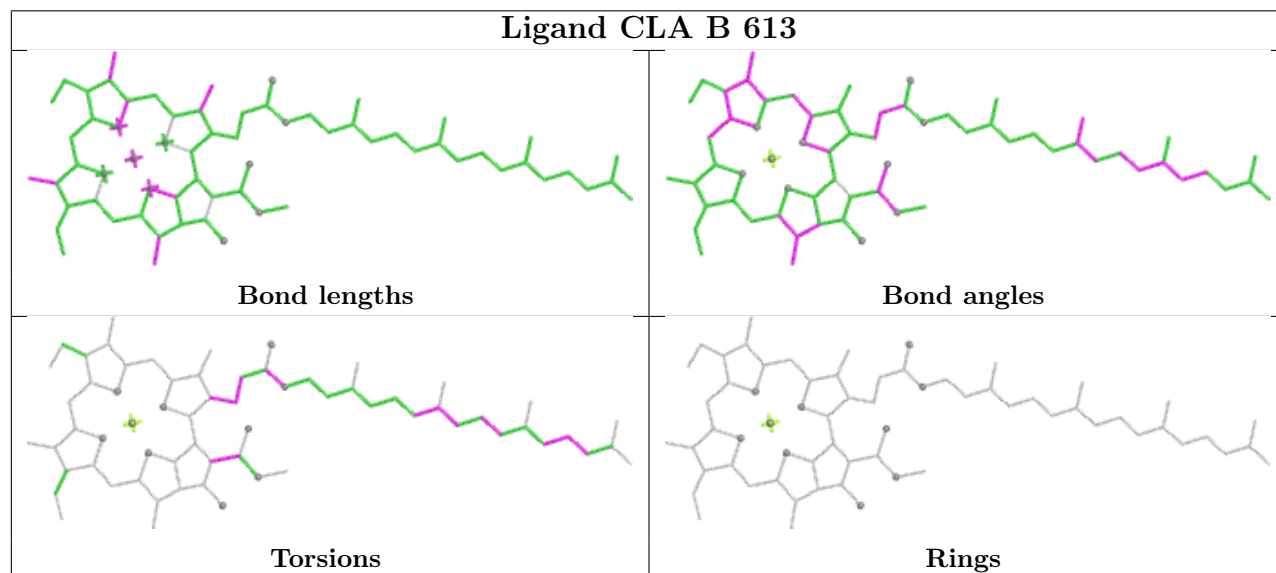
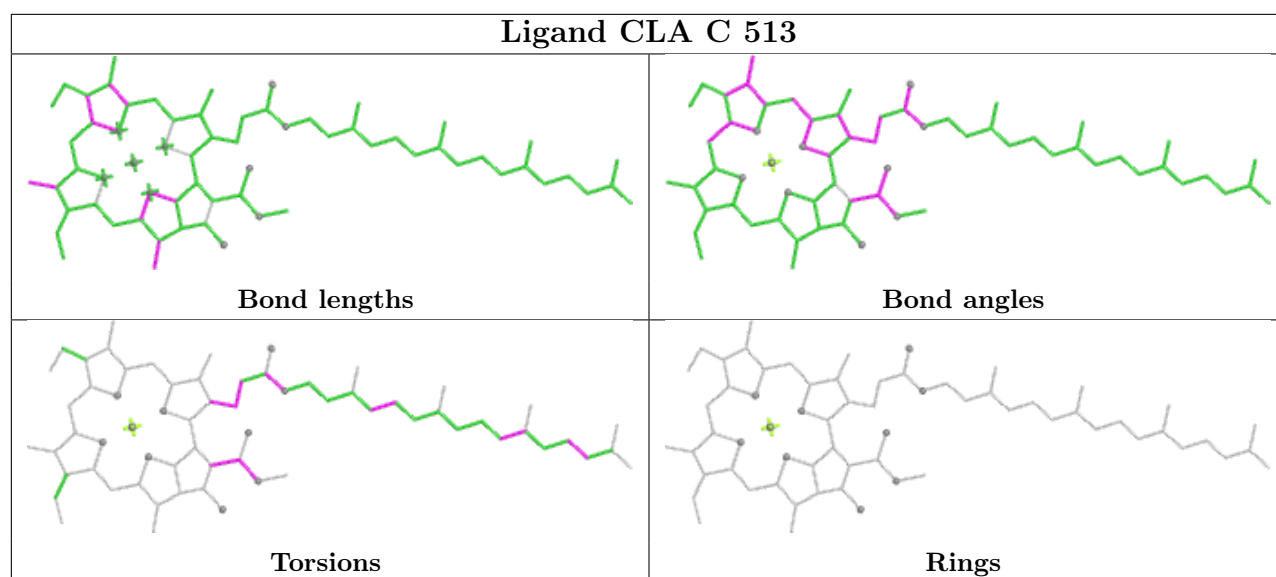
Bond angles

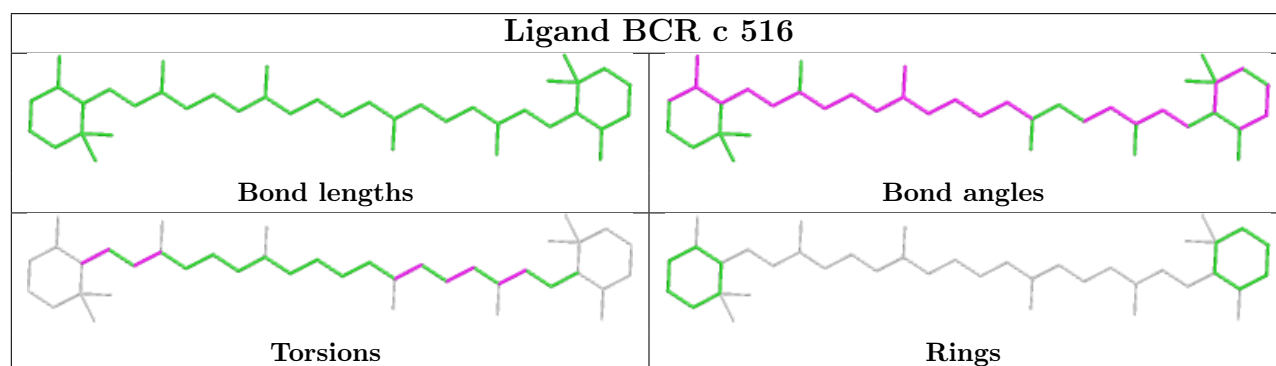
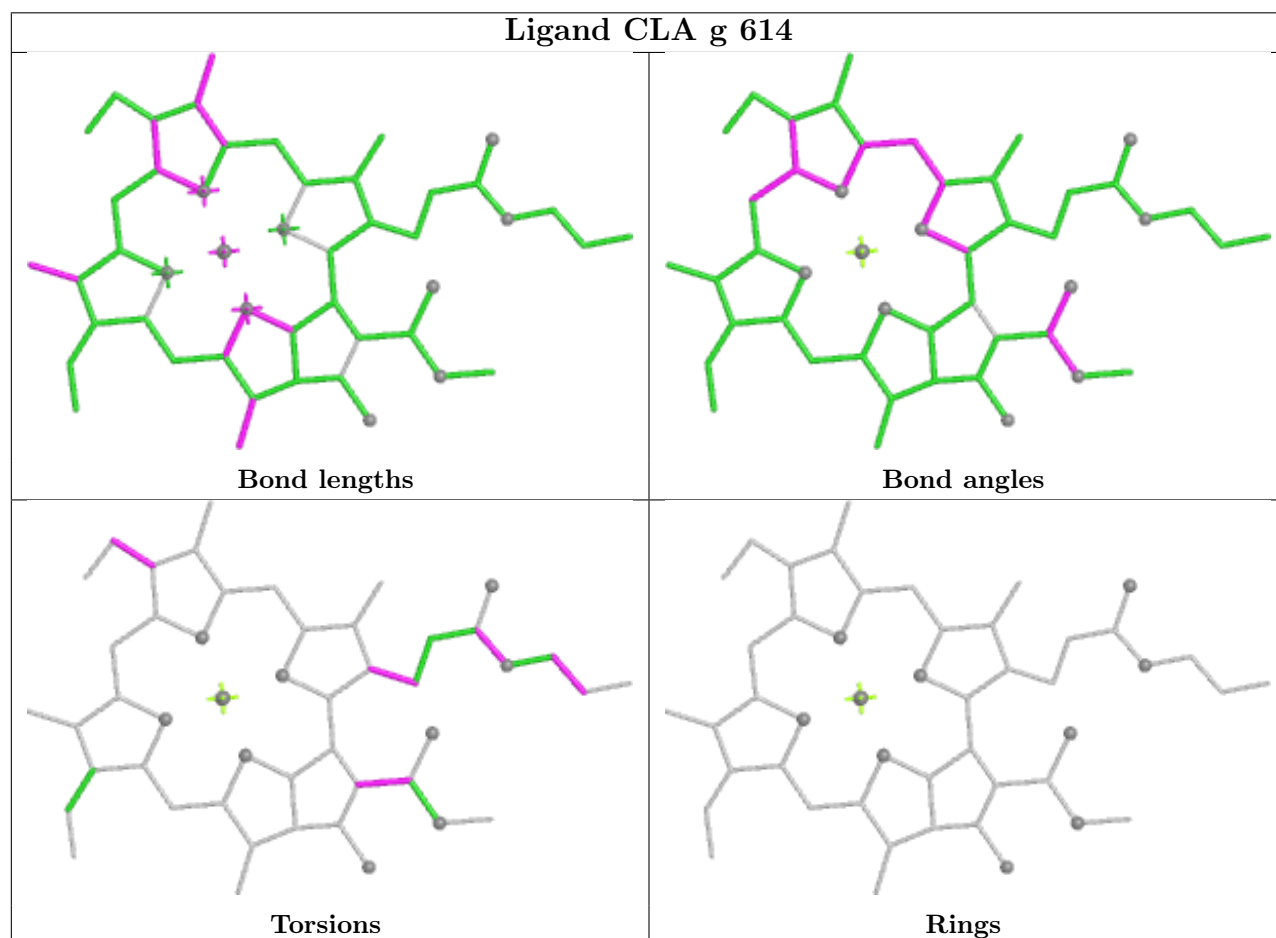
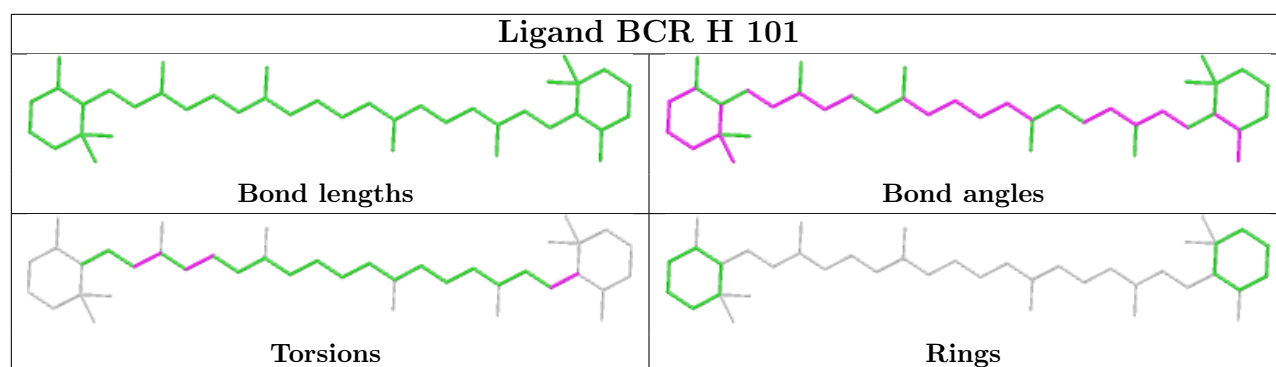


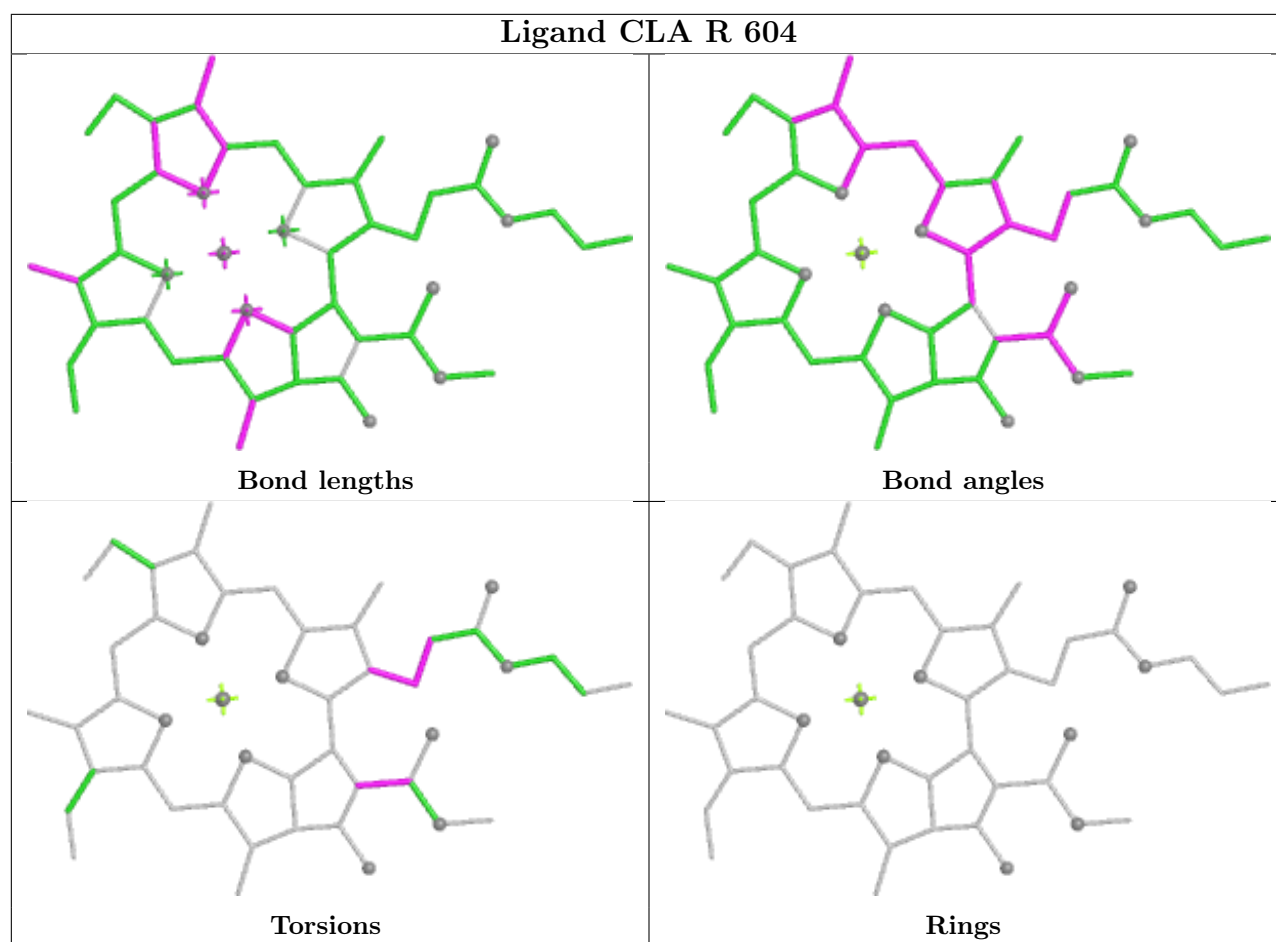
Torsions



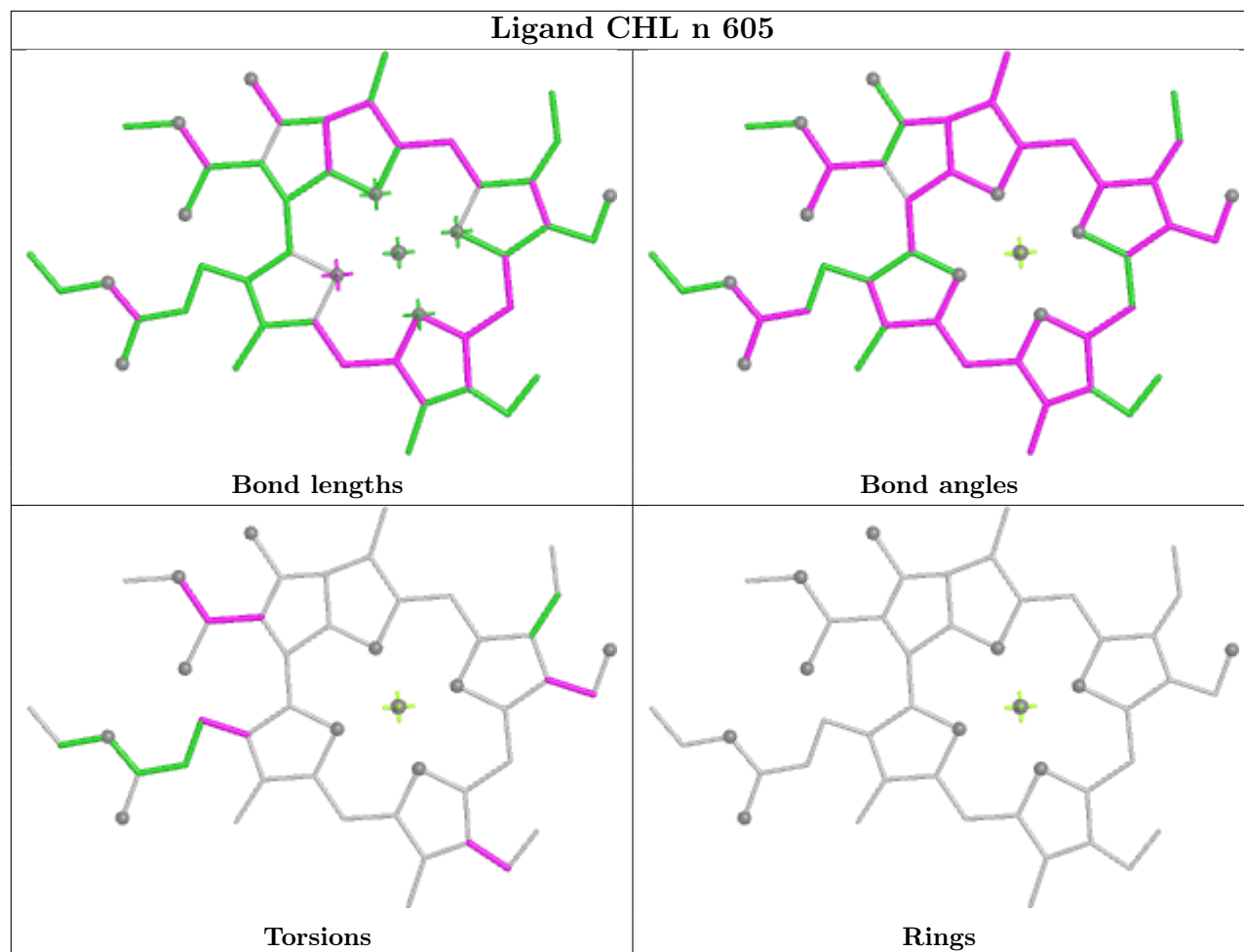
Rings



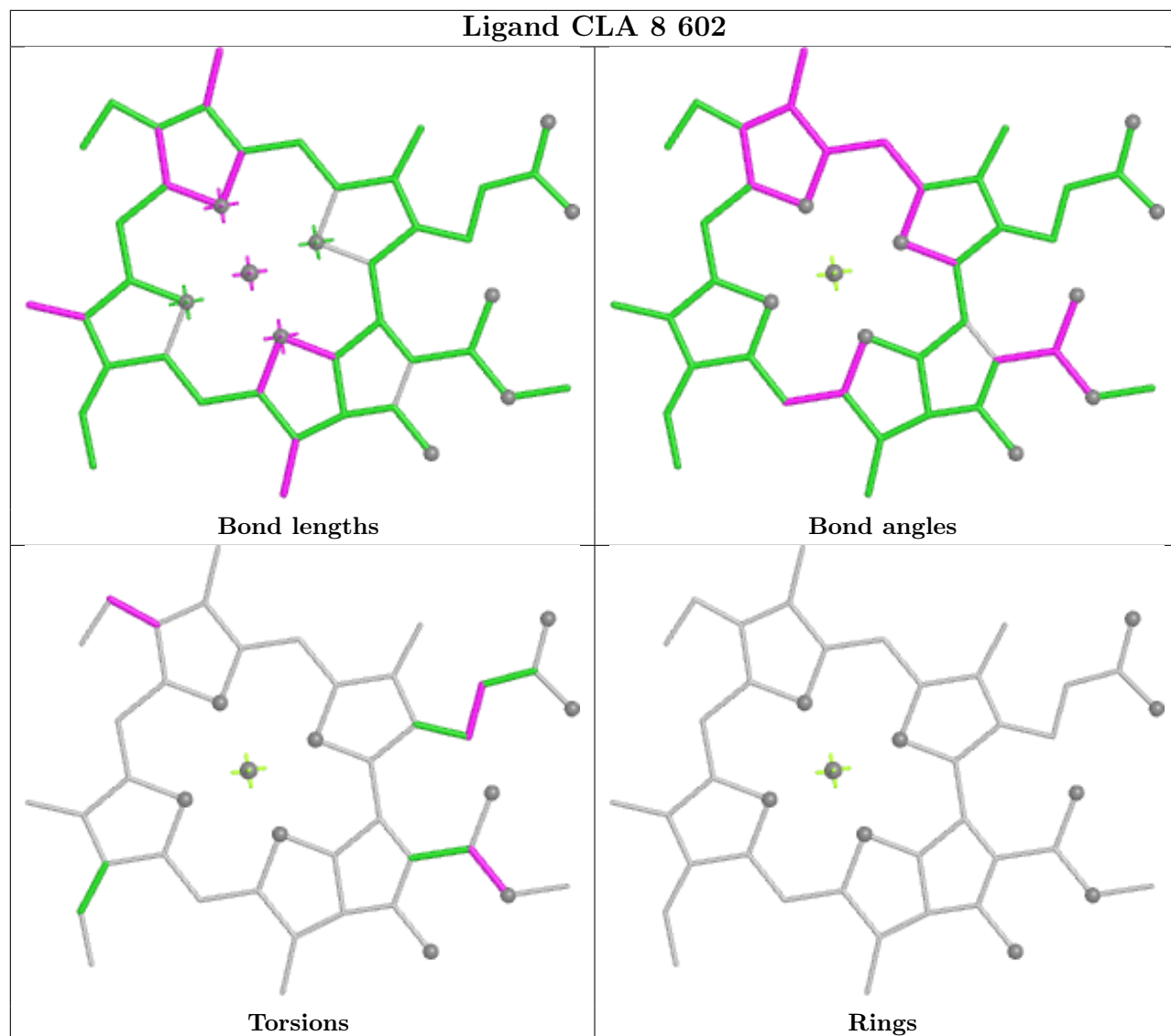


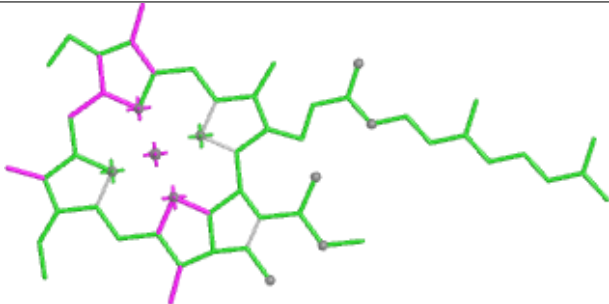
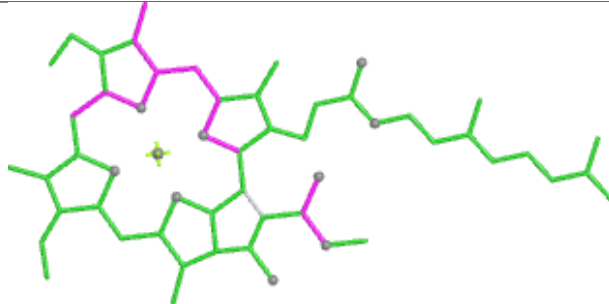
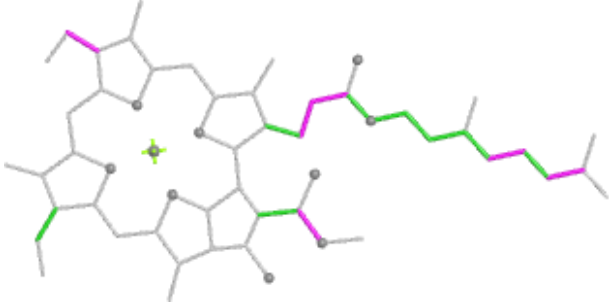
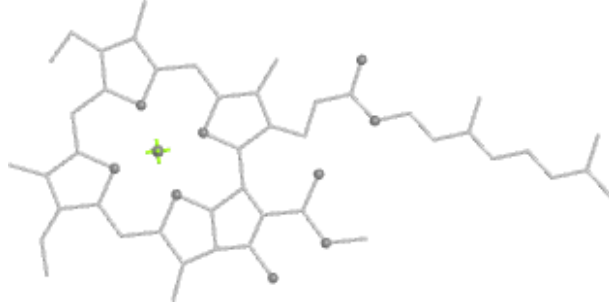


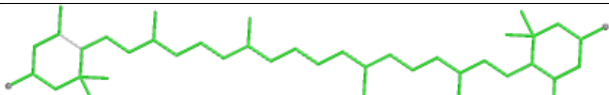
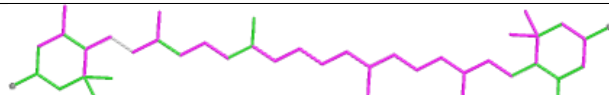
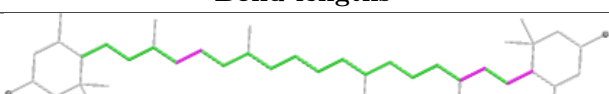
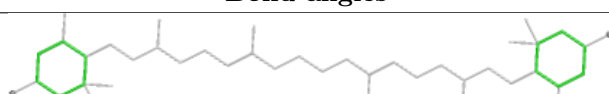
Ligand CHL n 605



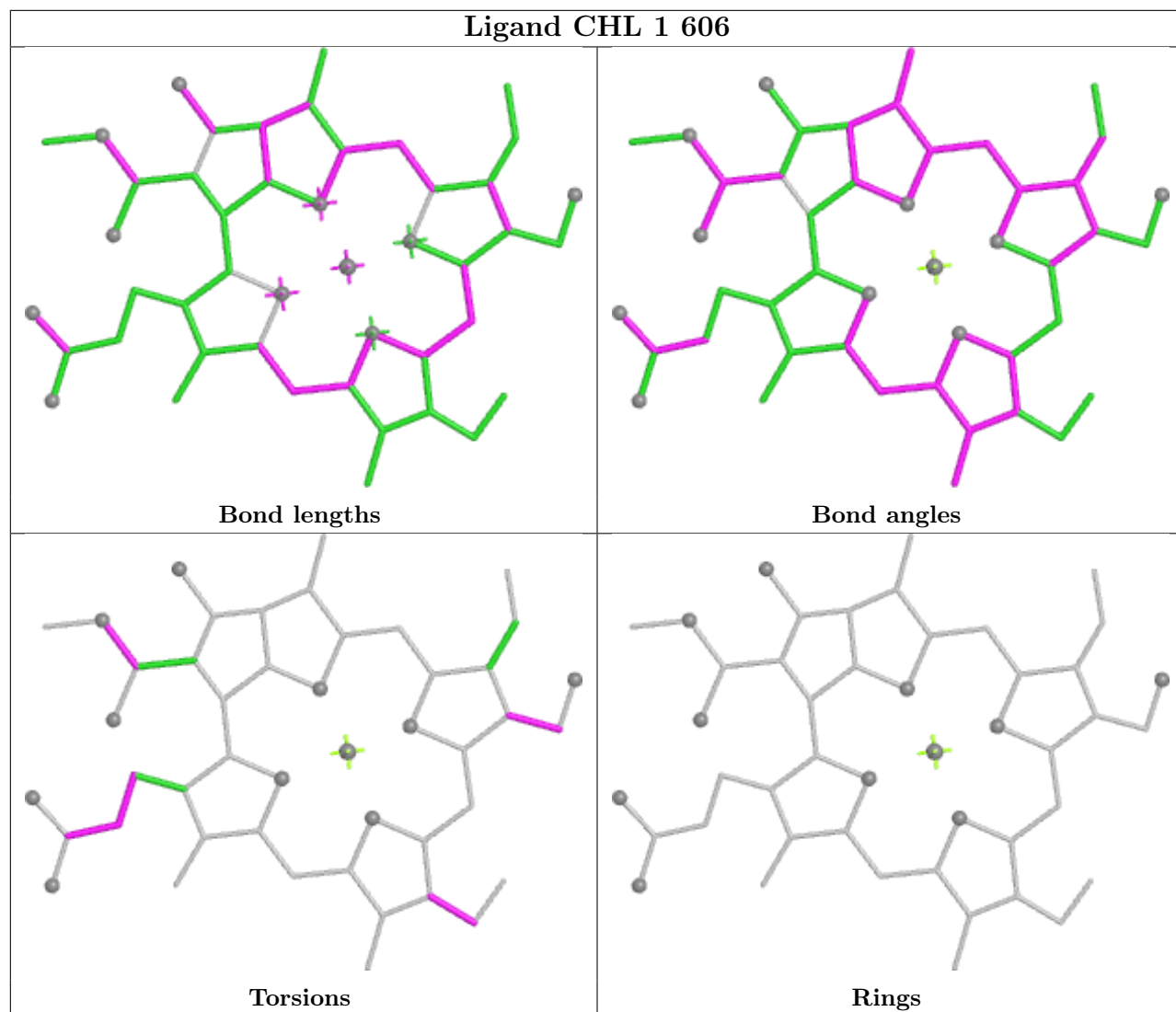
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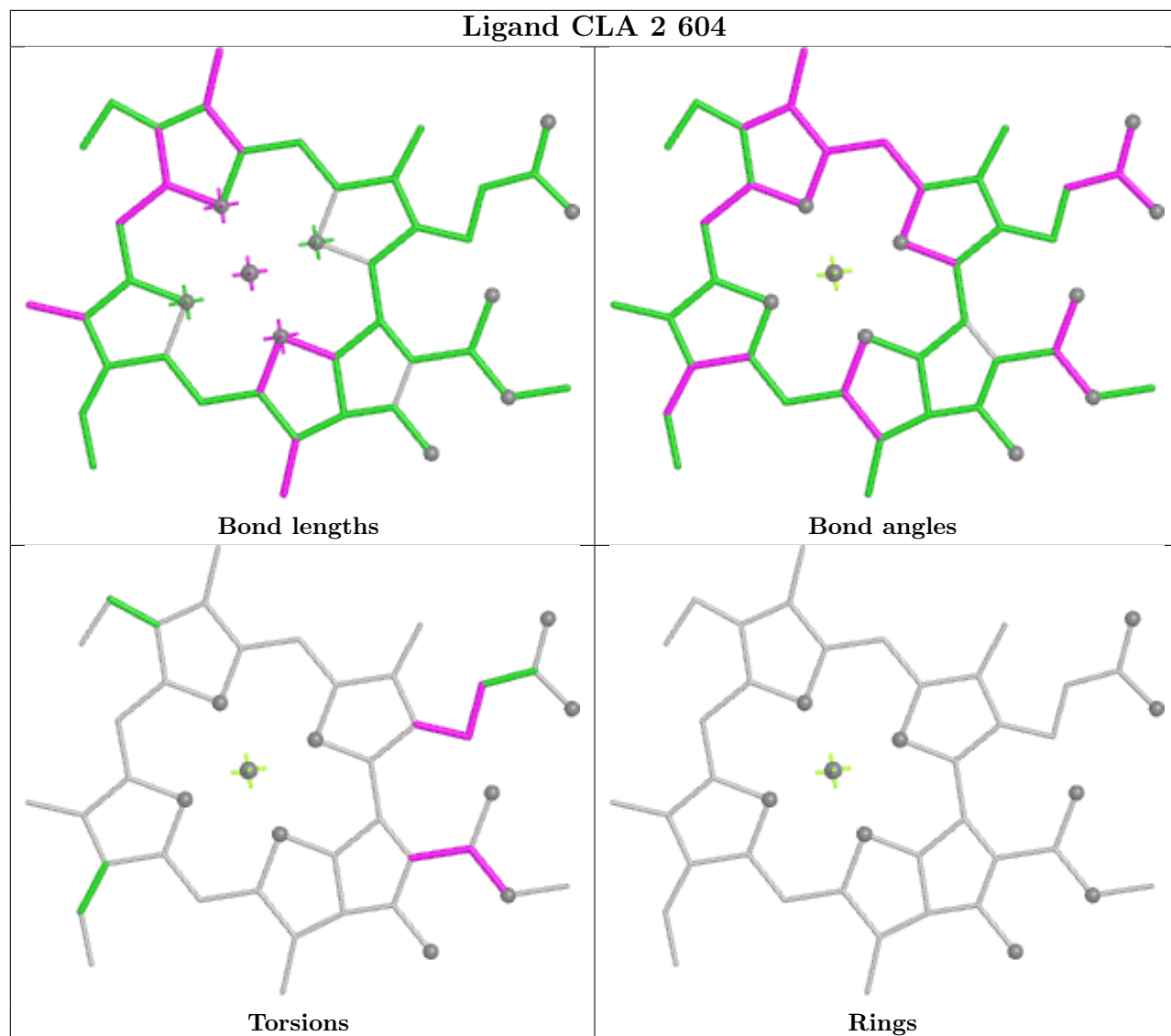
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Bond lengths	Bond angles
	
Torsions	Rings

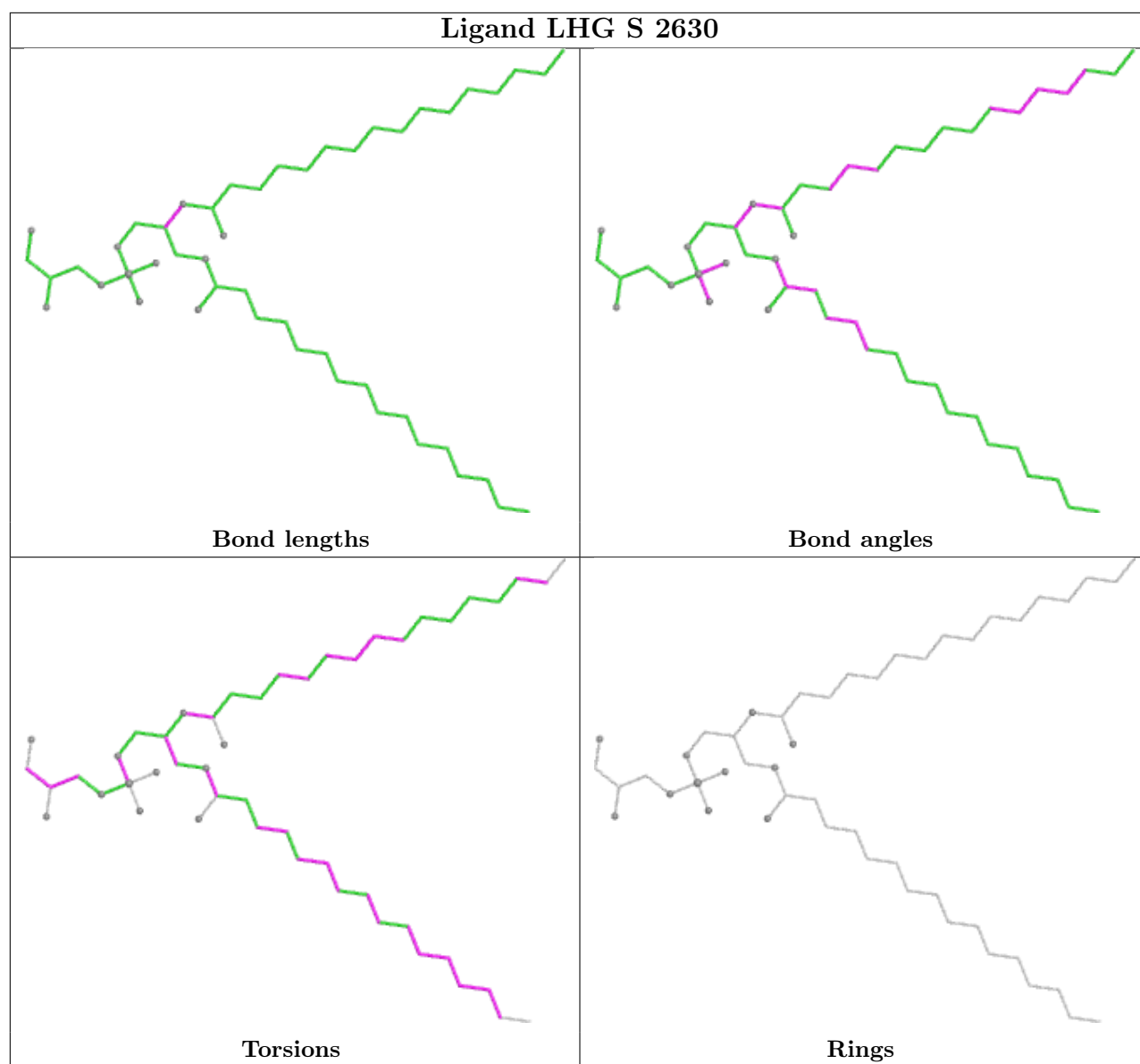
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Bond lengths	Bond angles
	
Torsions	Rings

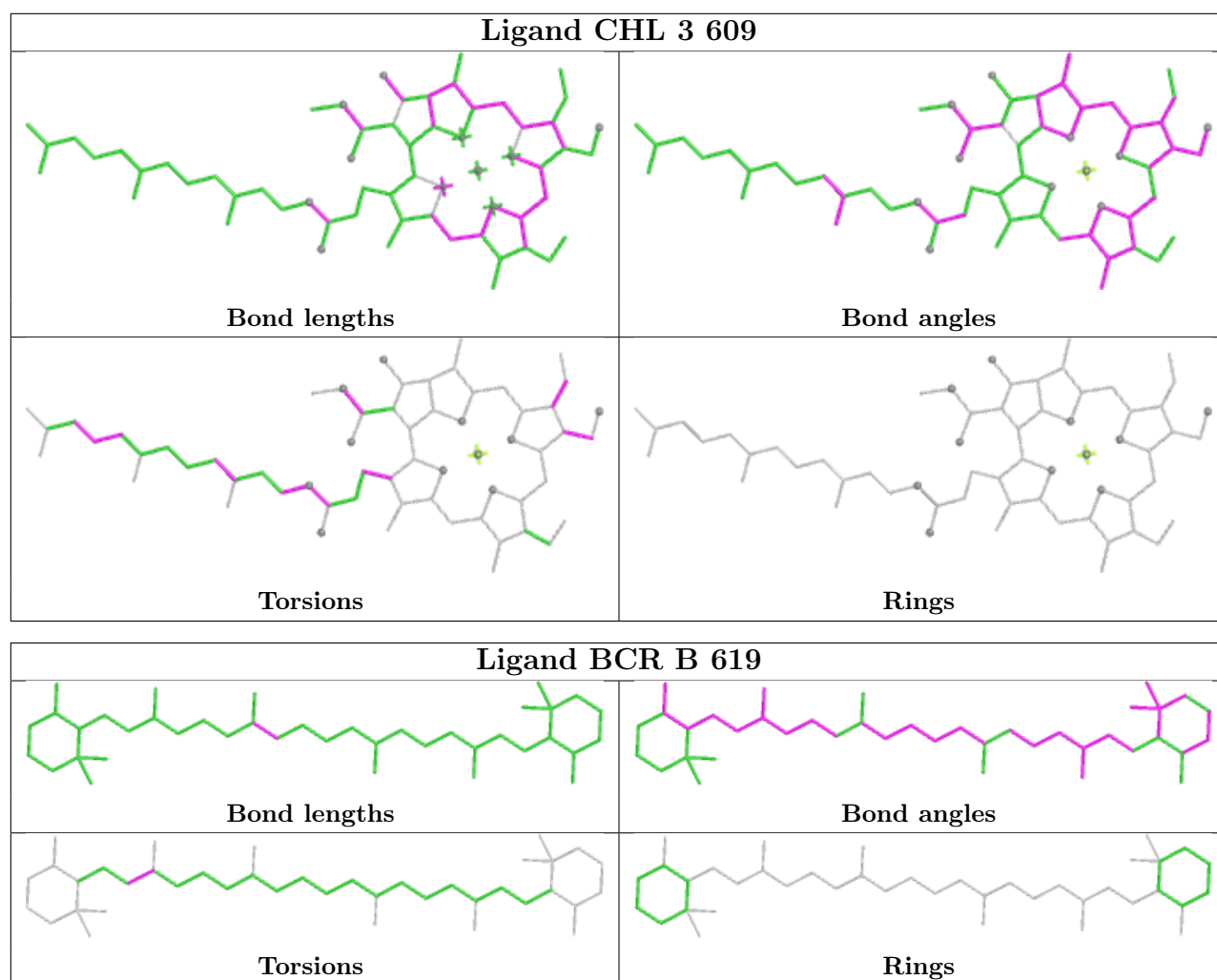
Ligand CHL 1 606

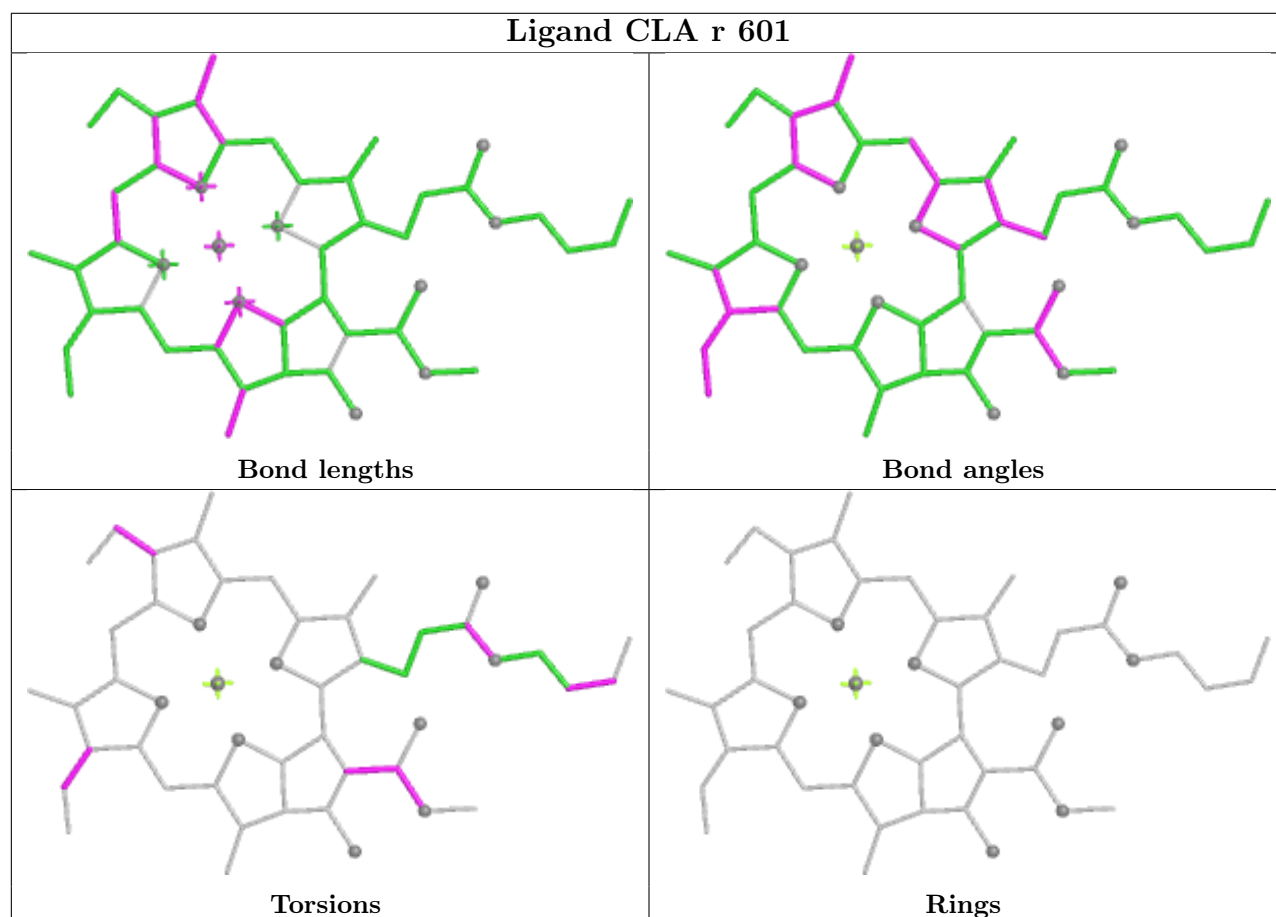
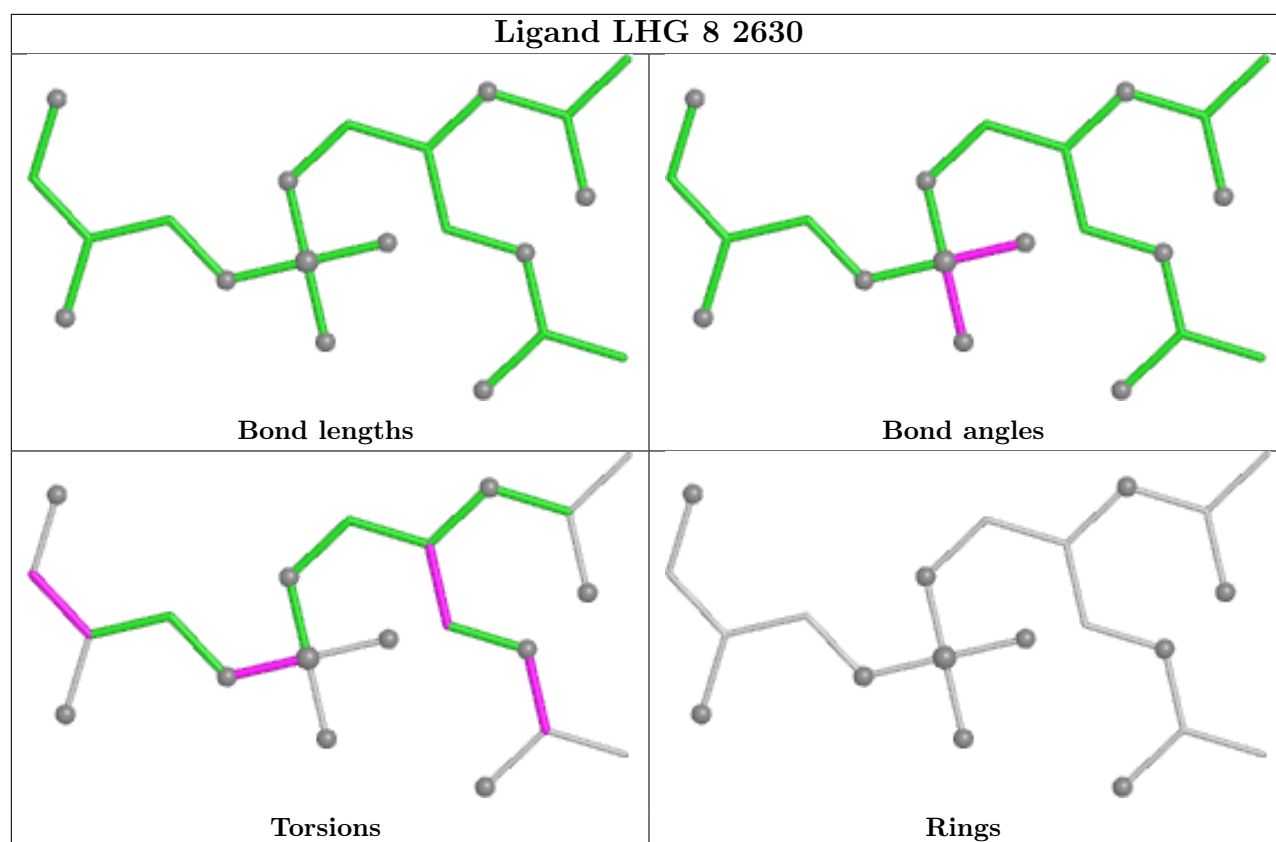


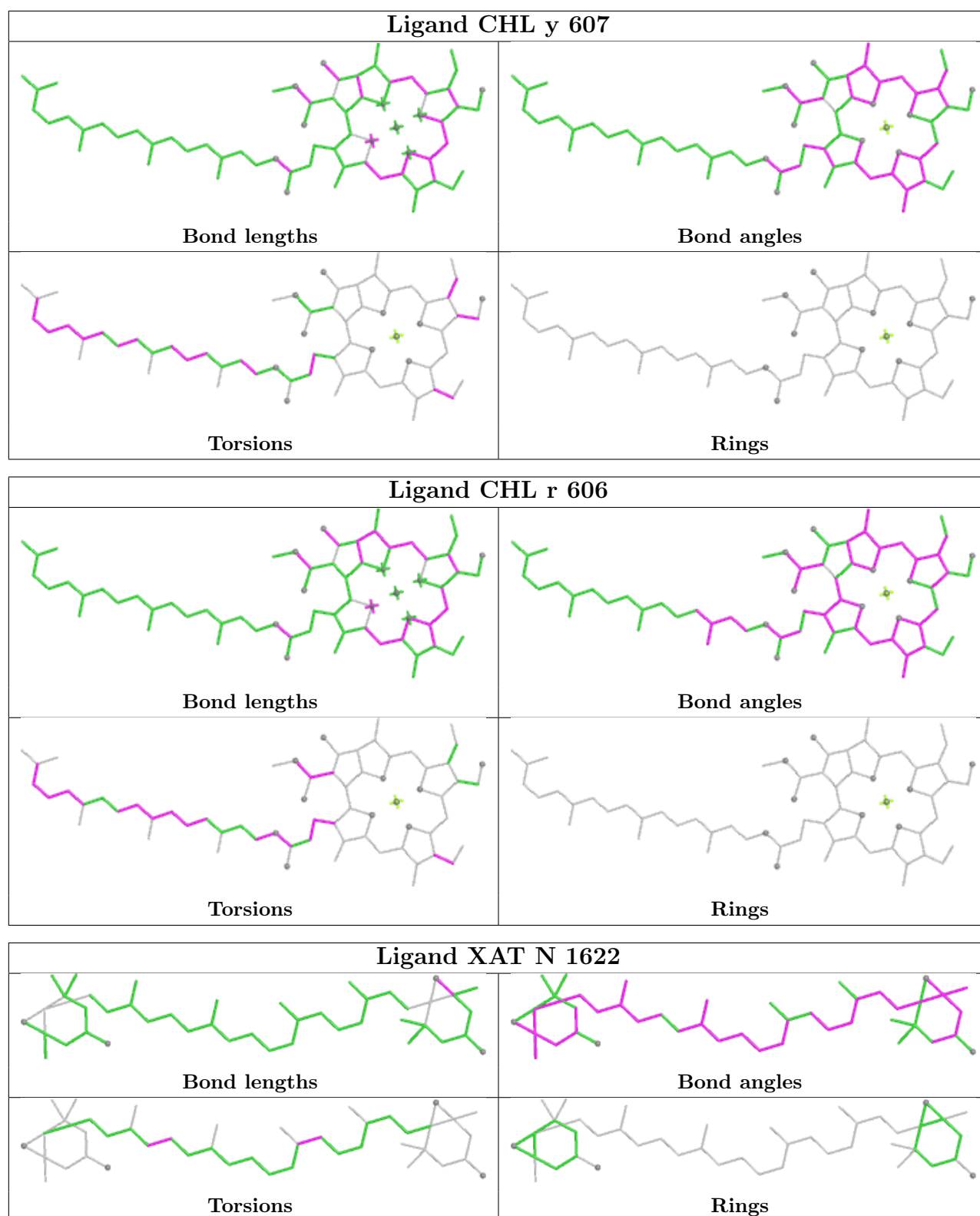
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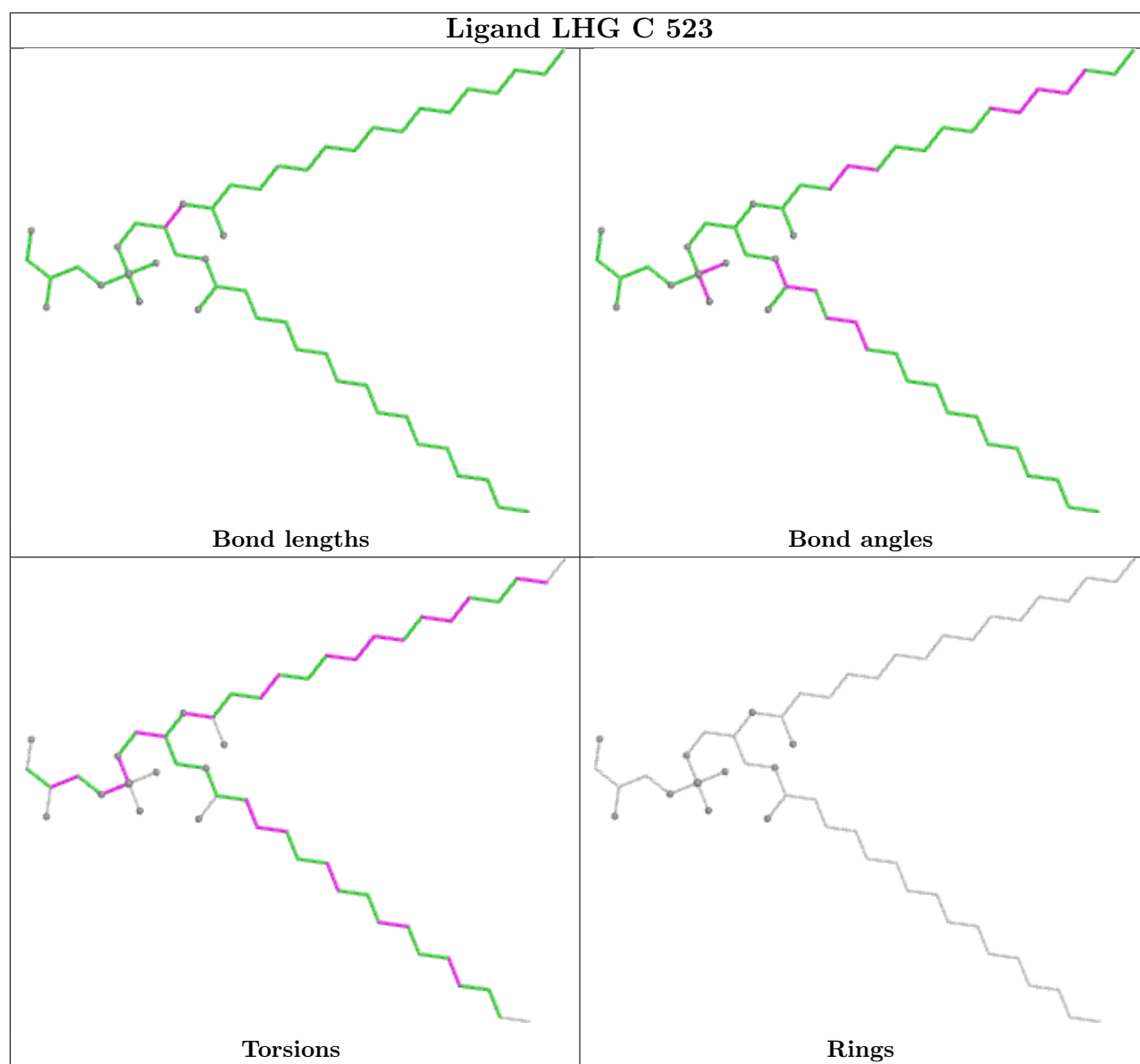


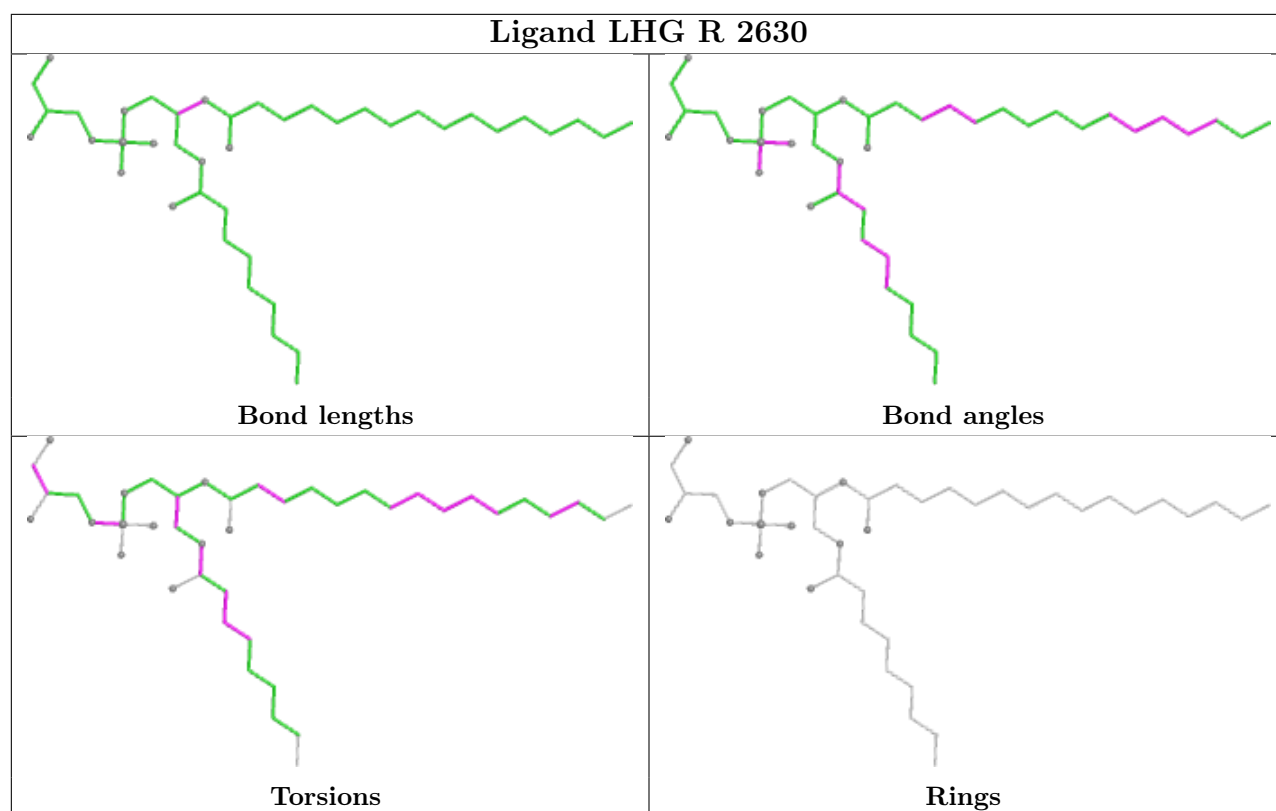


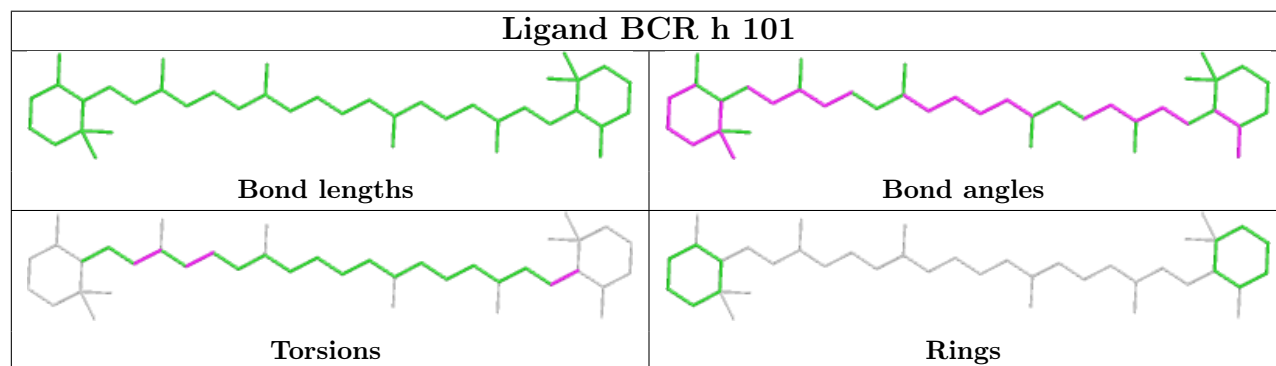
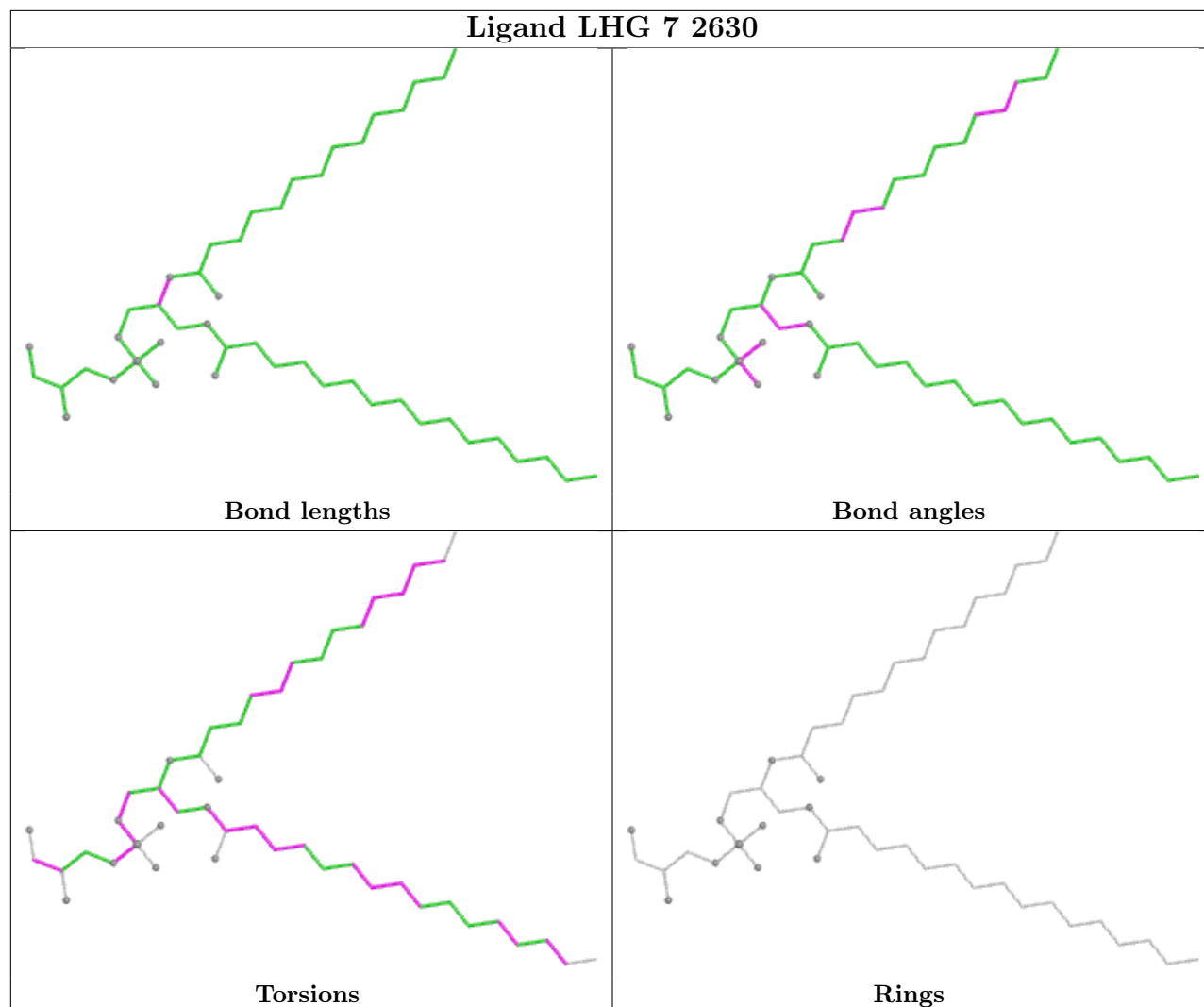


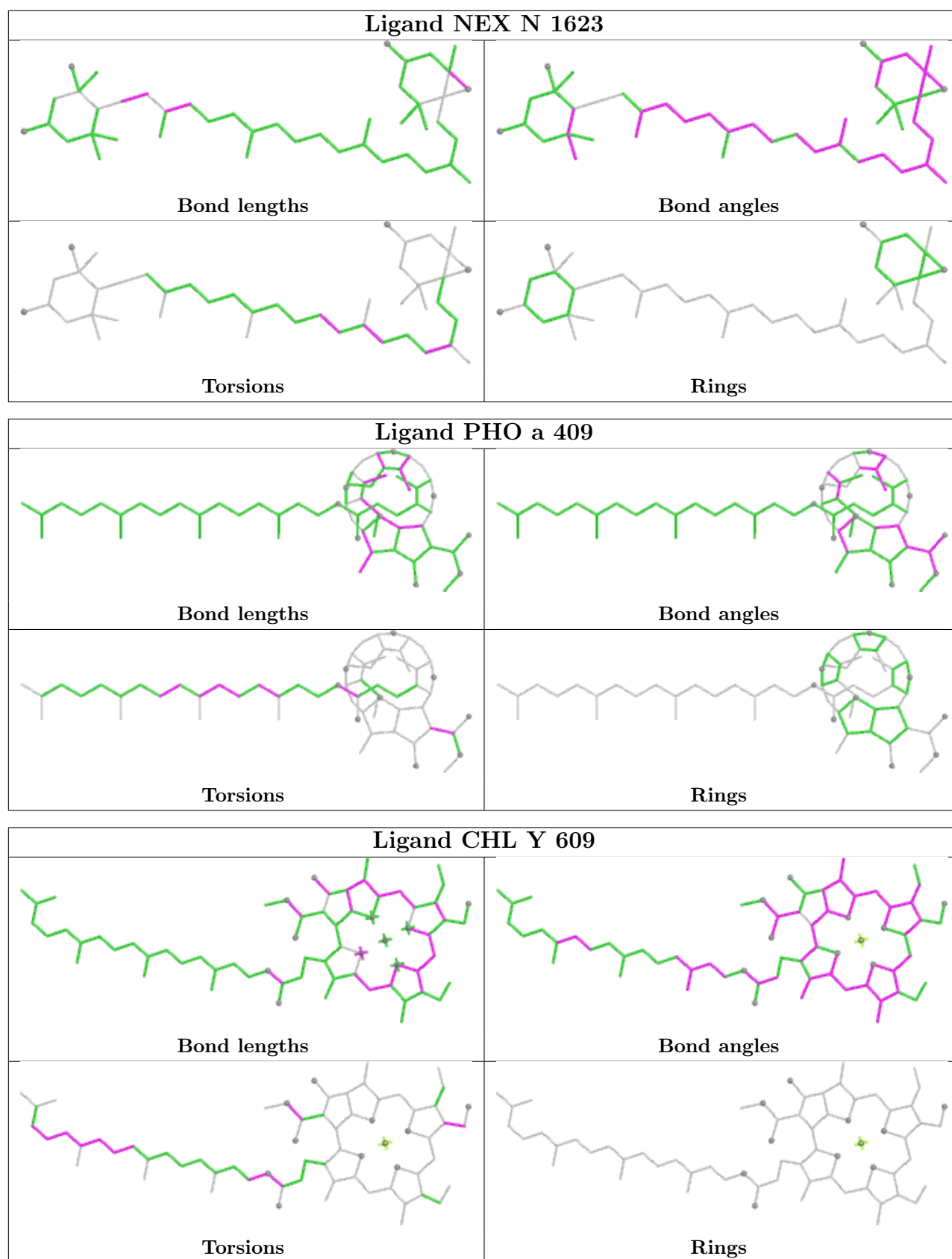


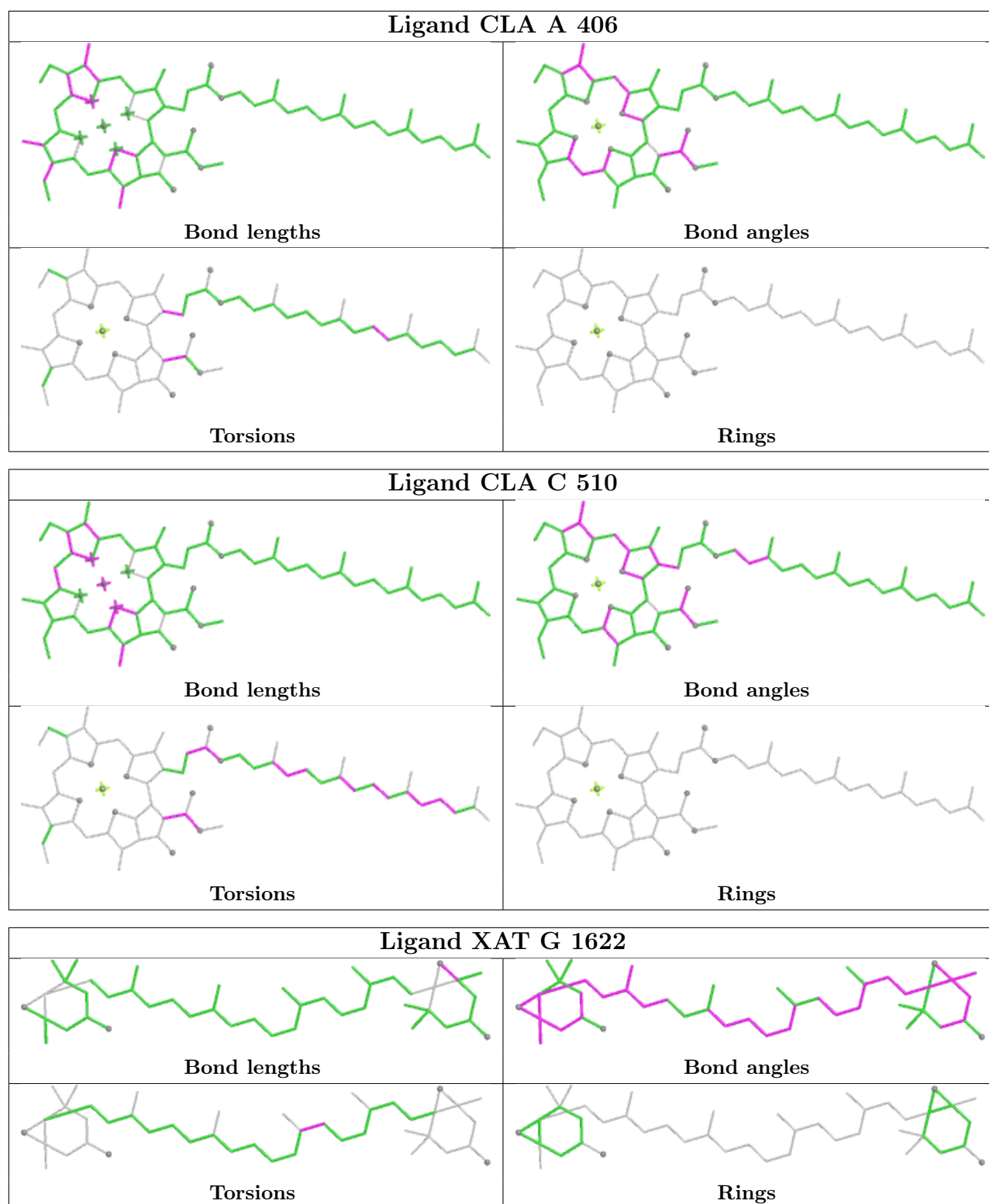




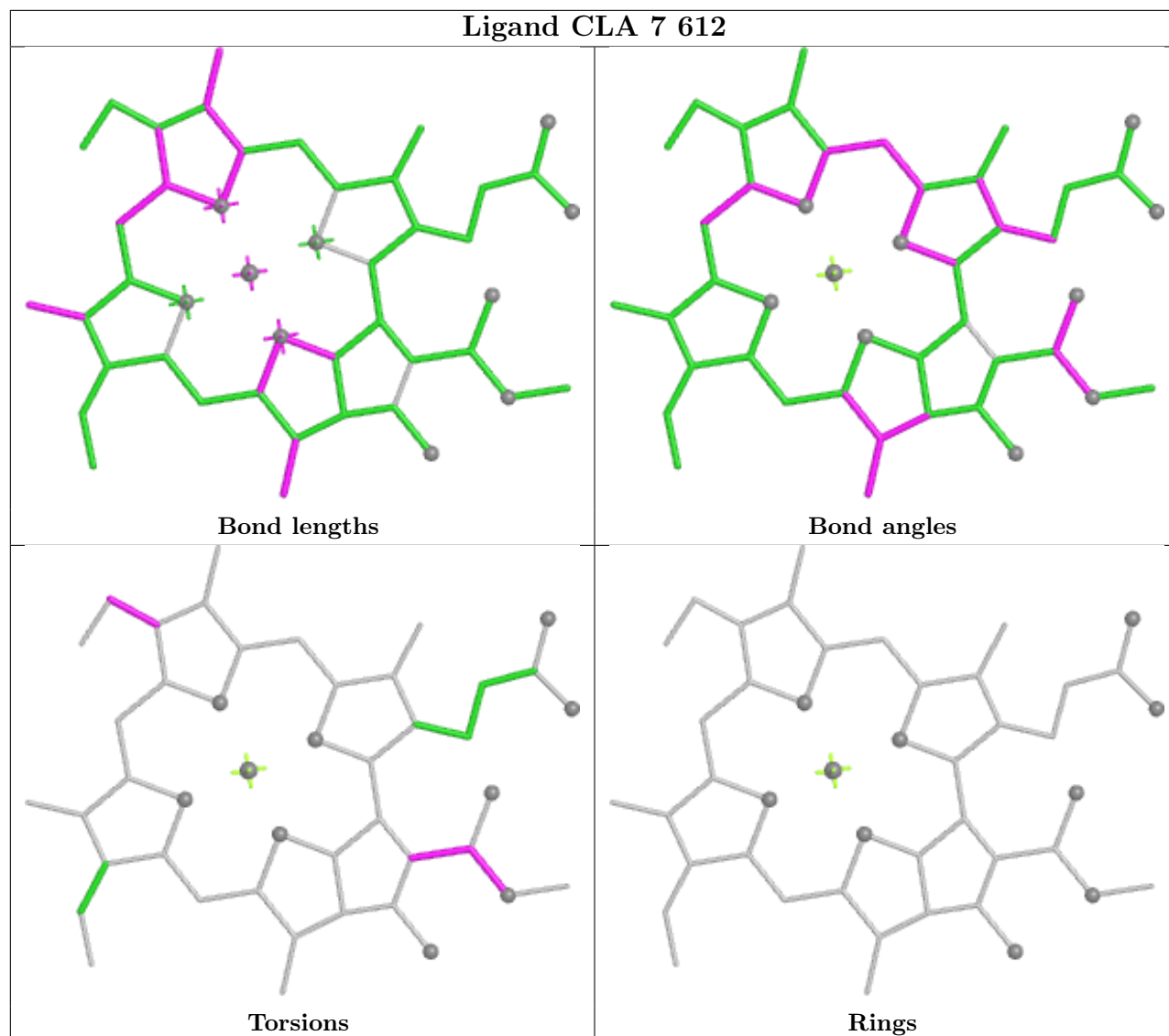




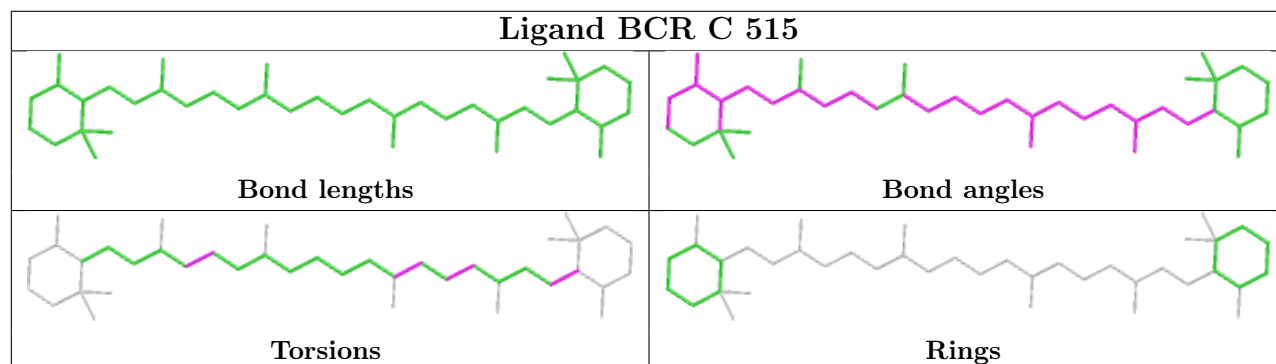


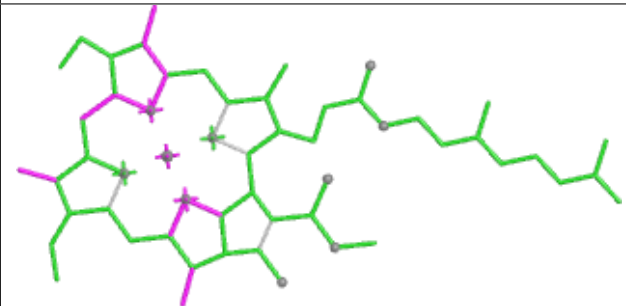
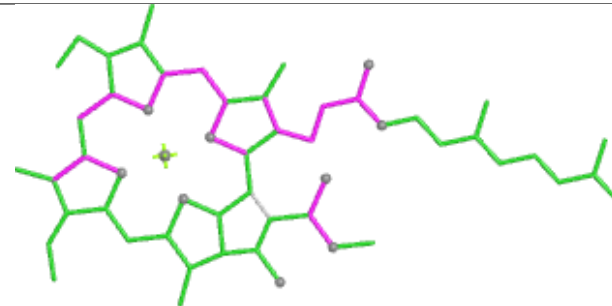
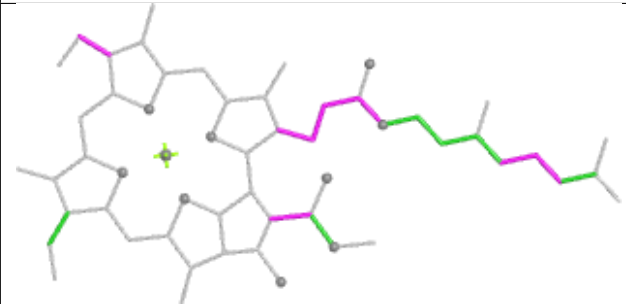
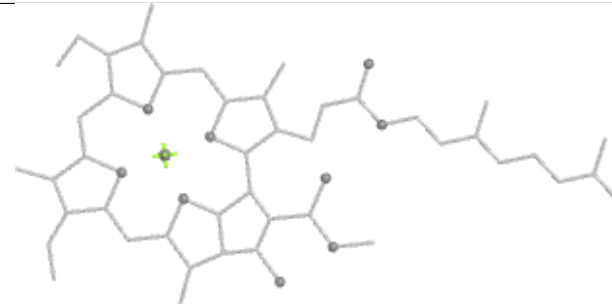


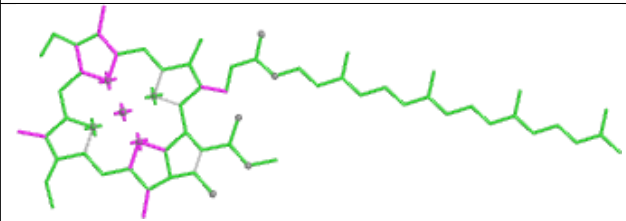
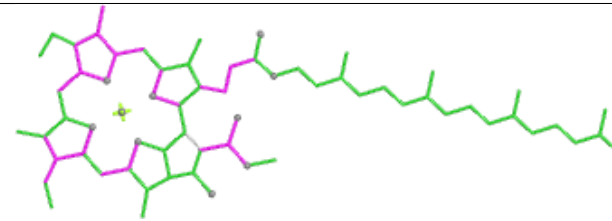
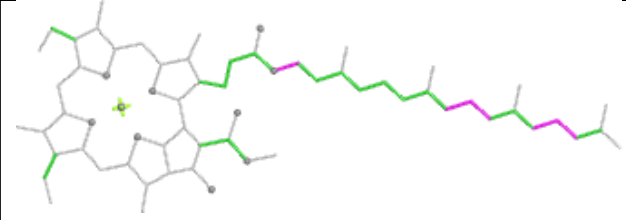
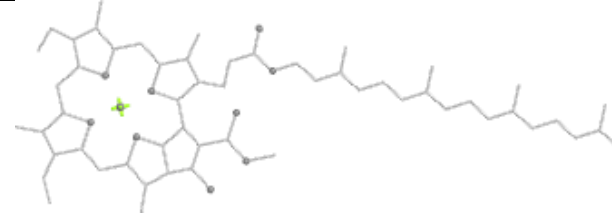
Ligand CLA 7 612

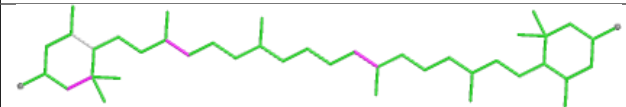
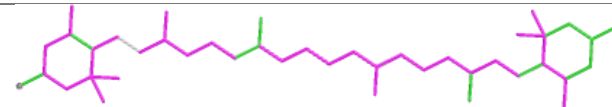
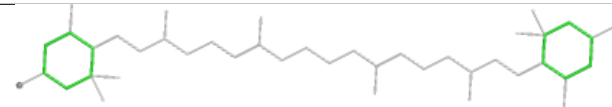


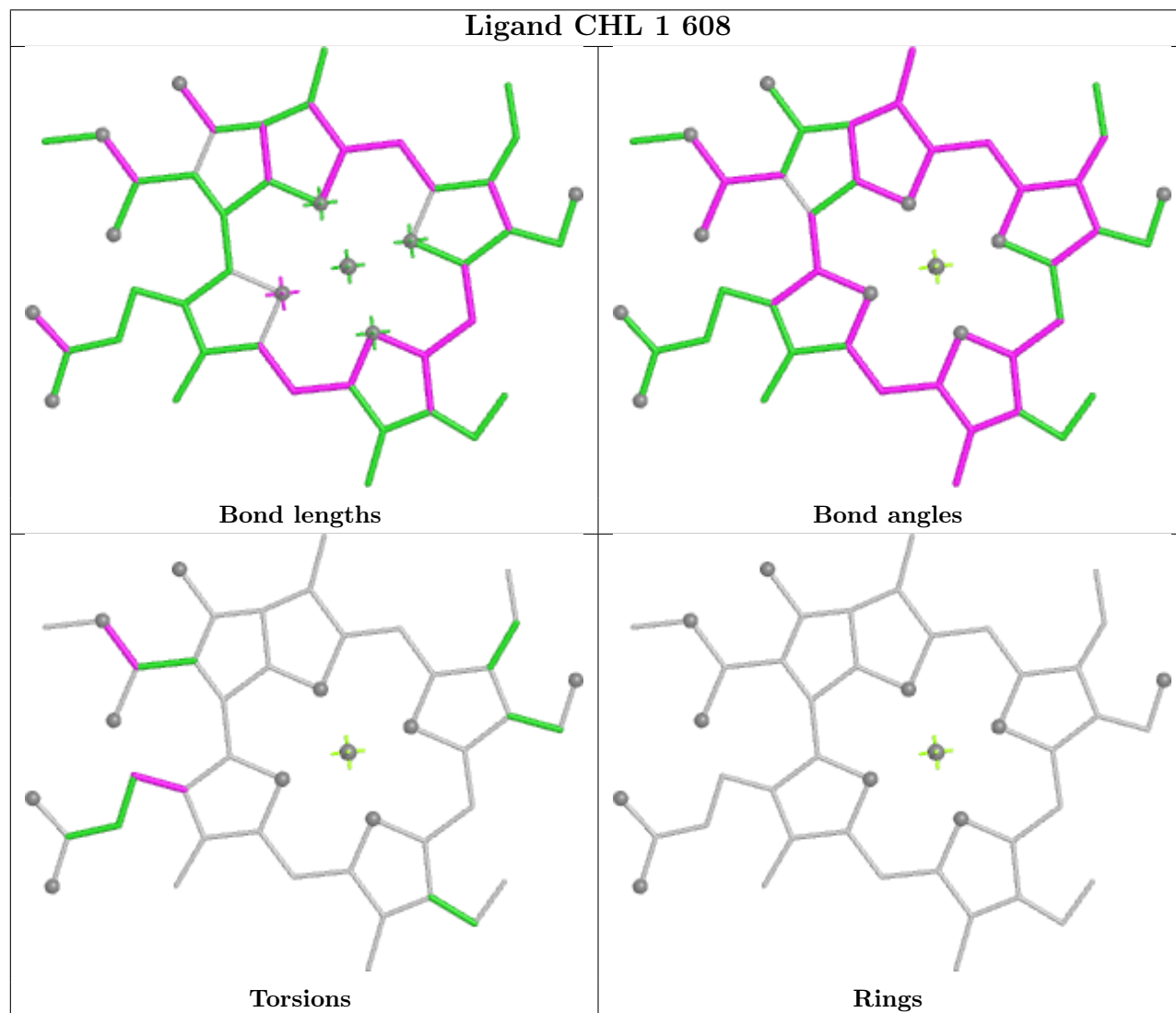
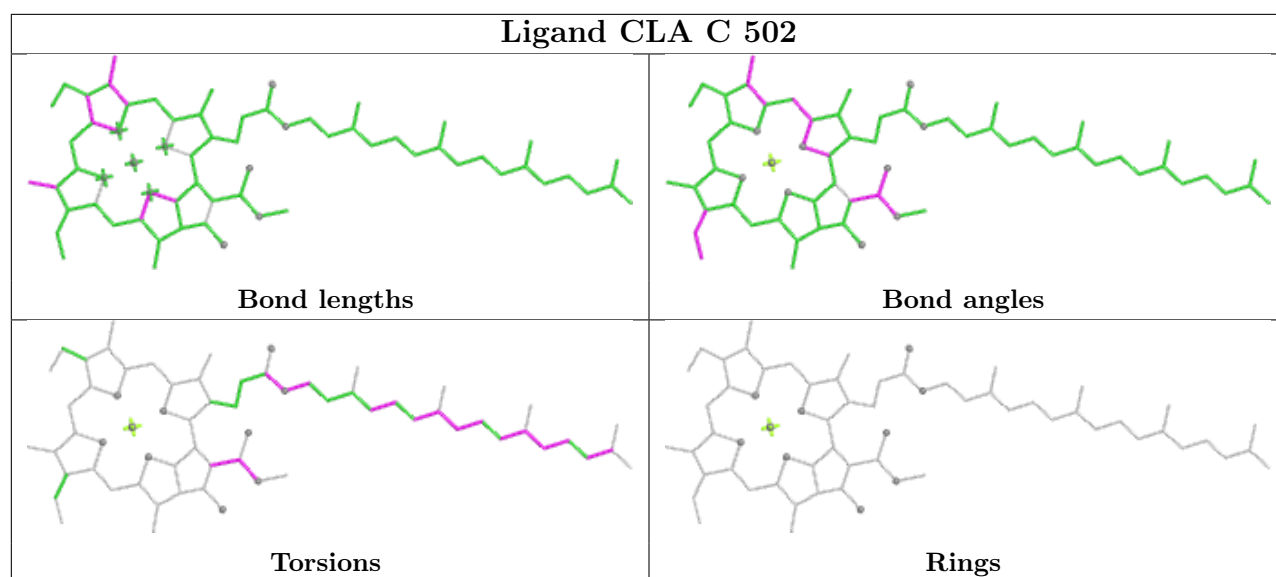
Ligand BCR C 515

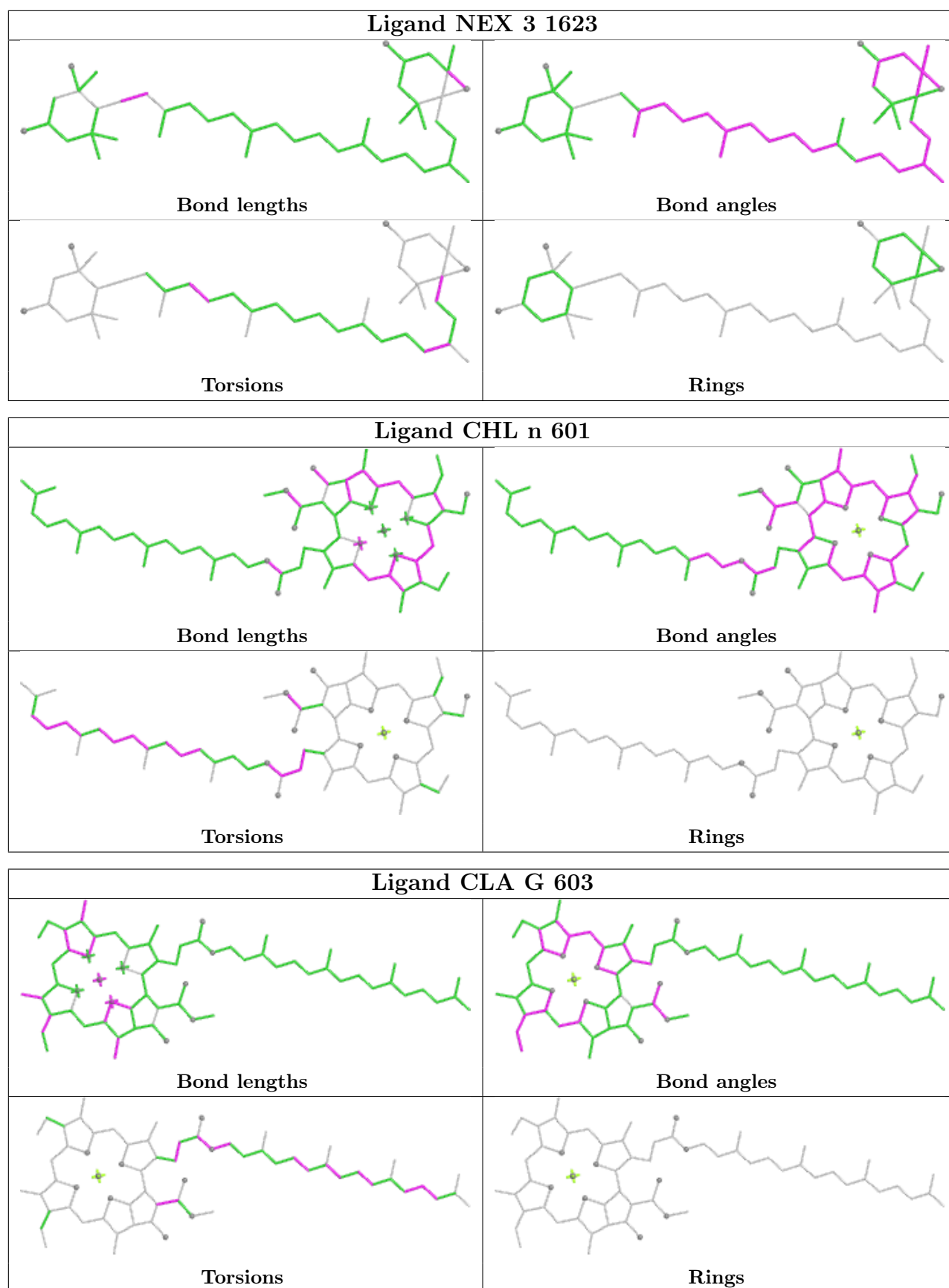


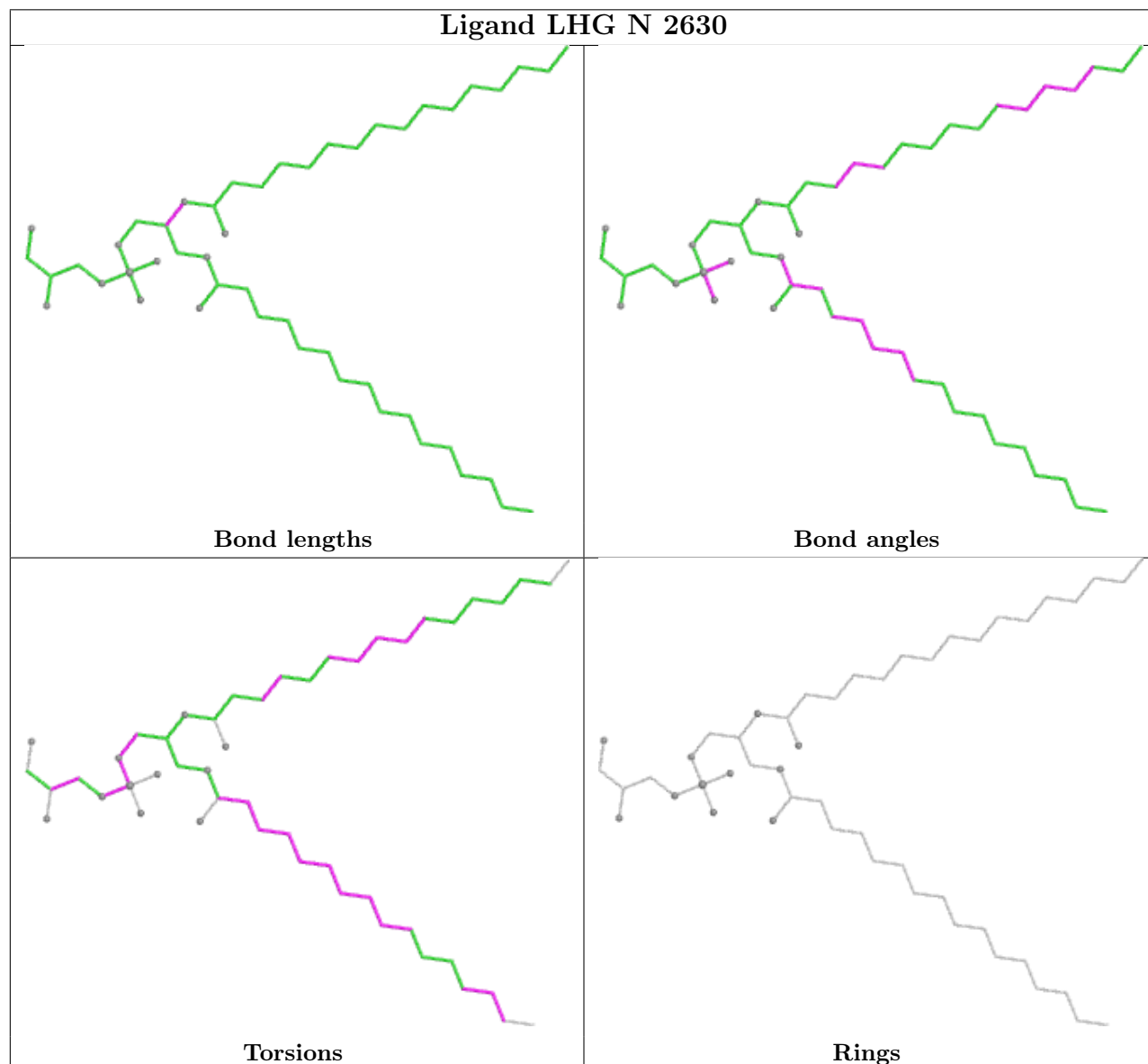
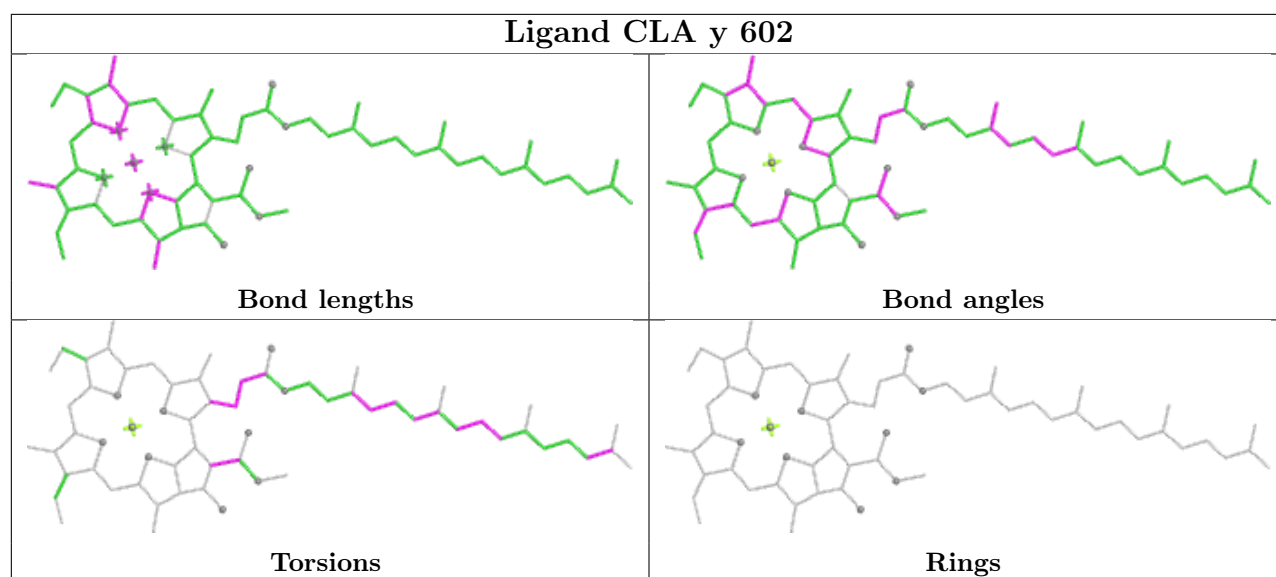
Ligand CLA 3 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

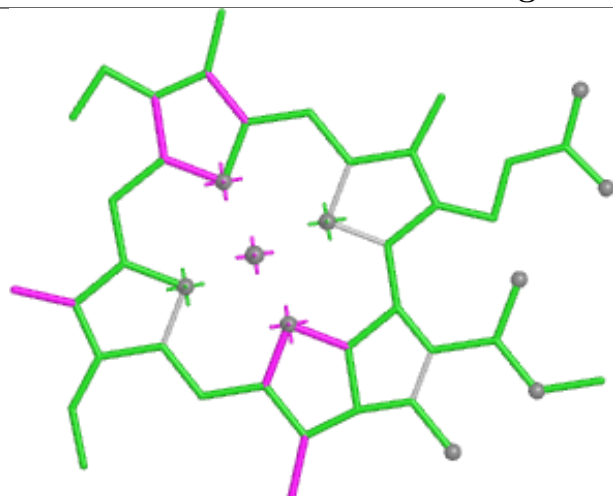
Ligand LUT 7 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings



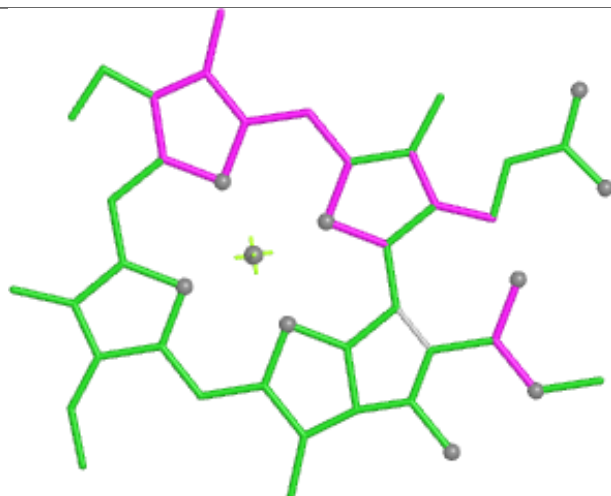




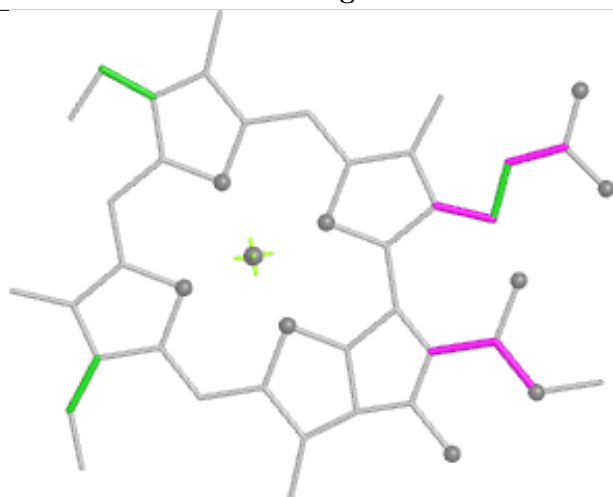
Ligand CLA 4 612



Bond lengths



Bond angles

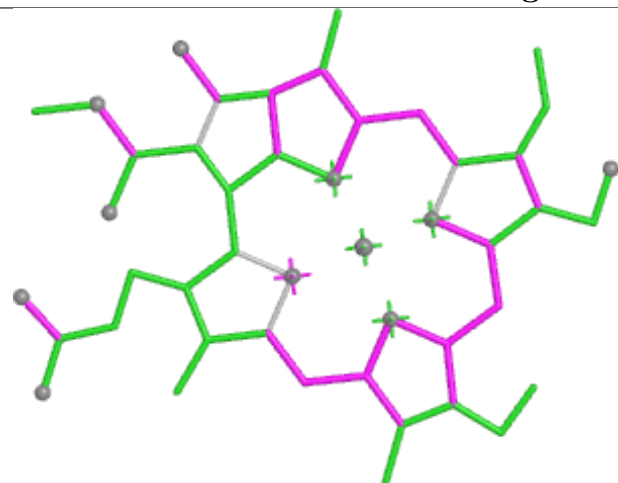


Torsions

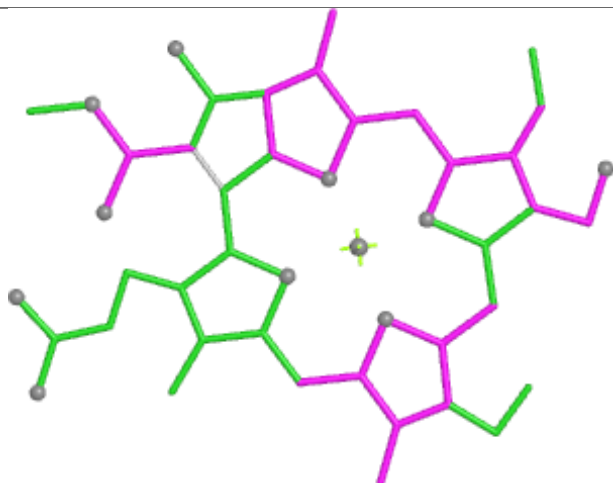


Rings

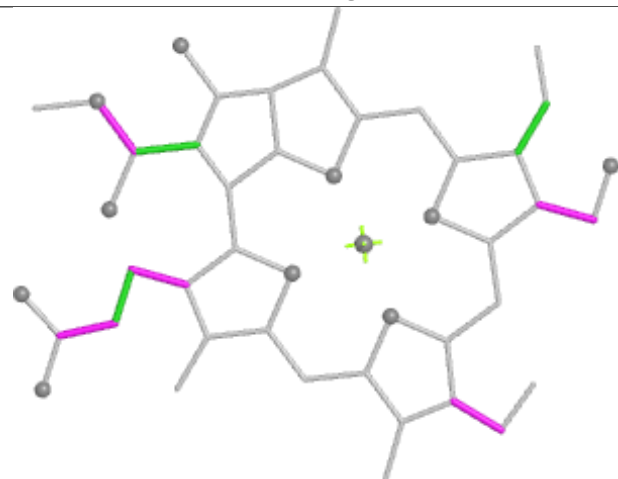
Ligand CHL 5 605



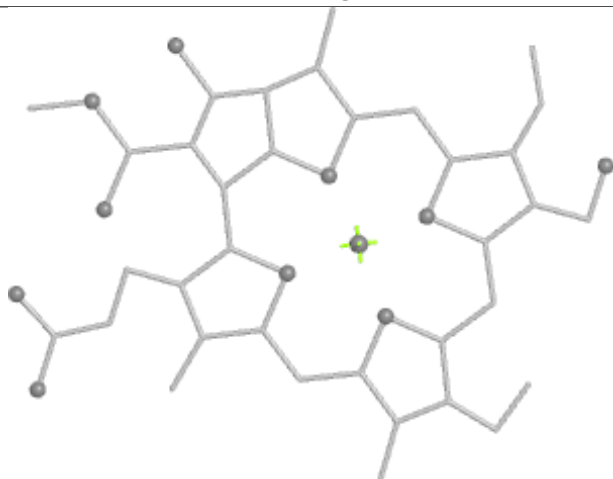
Bond lengths



Bond angles

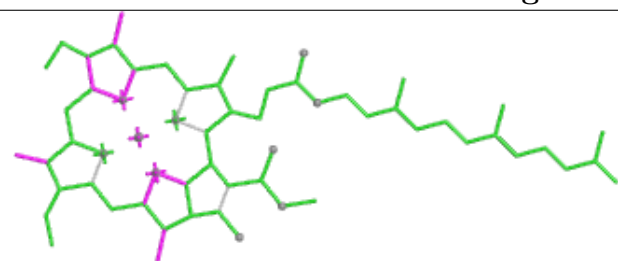


Torsions

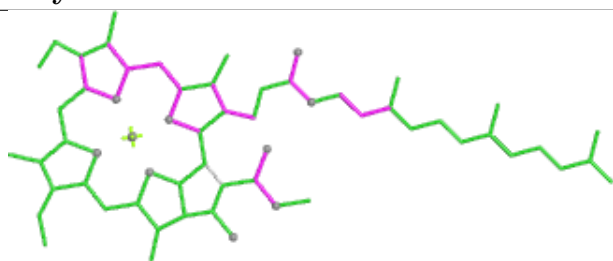


Rings

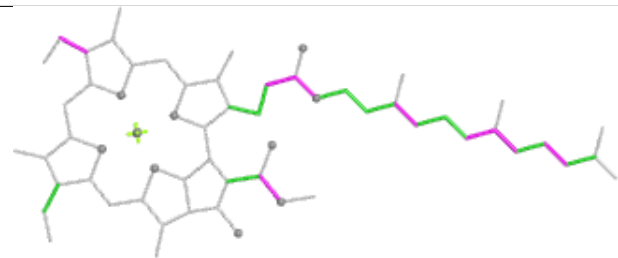
Ligand CLA y 612



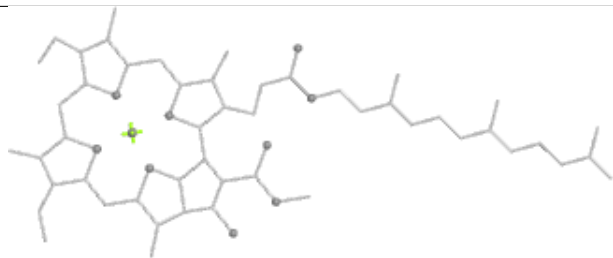
Bond lengths



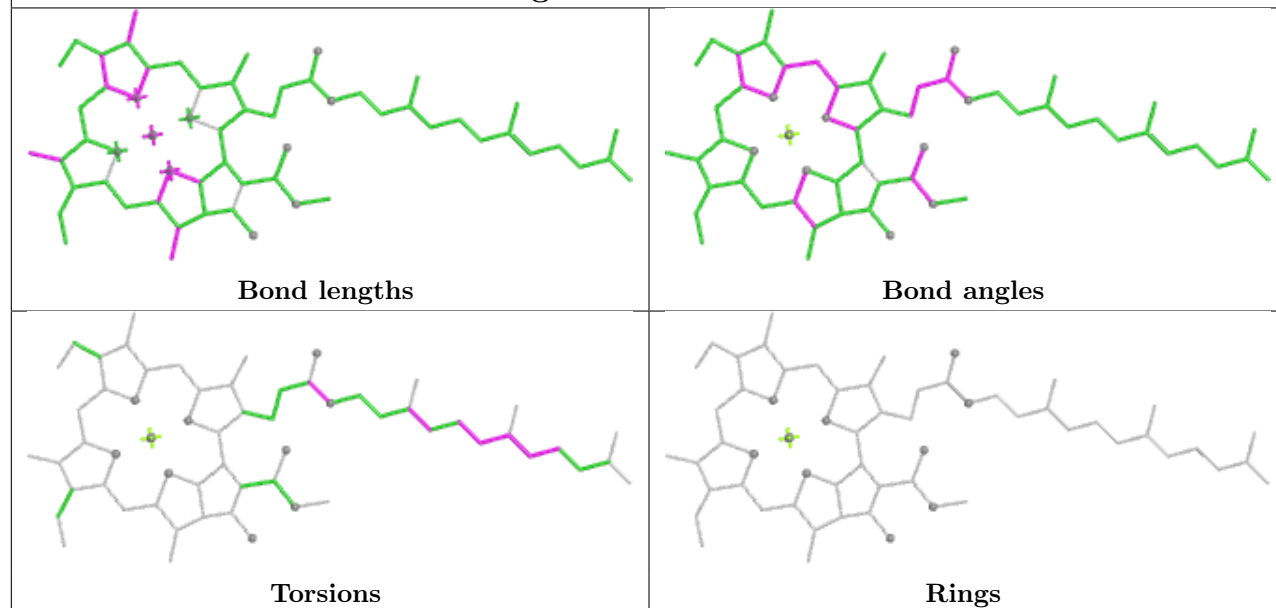
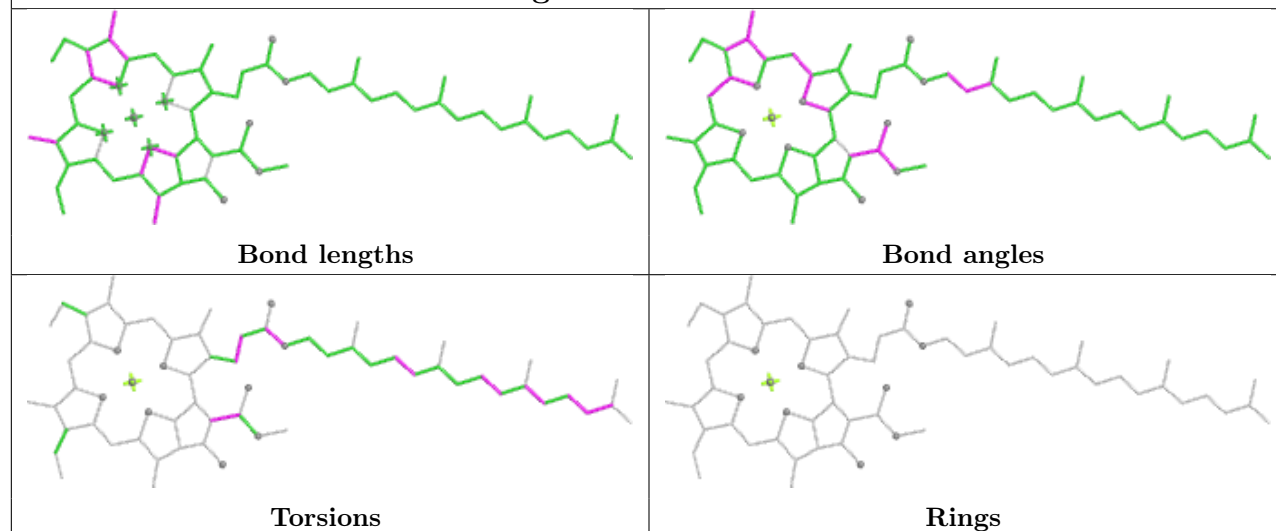
Bond angles

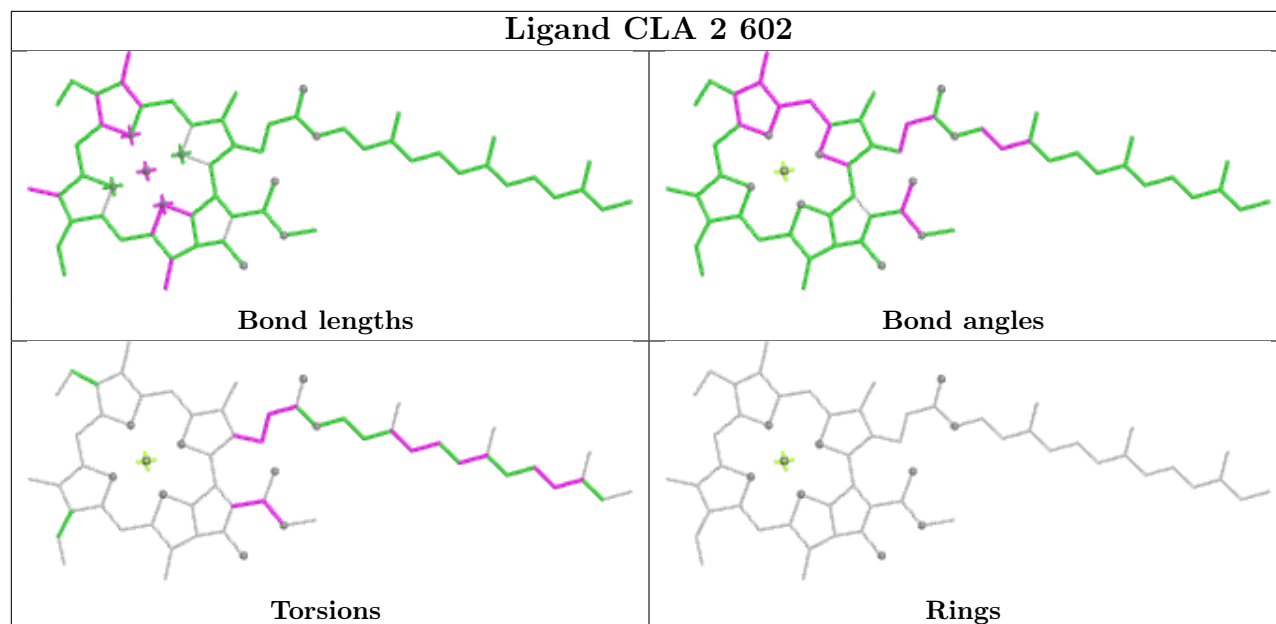
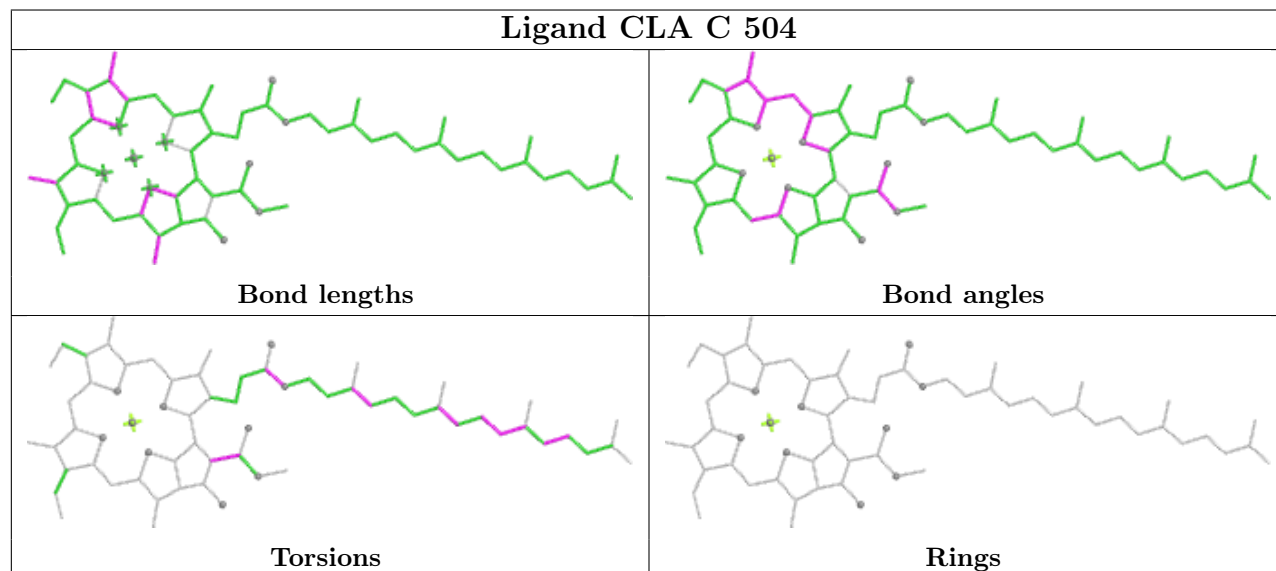


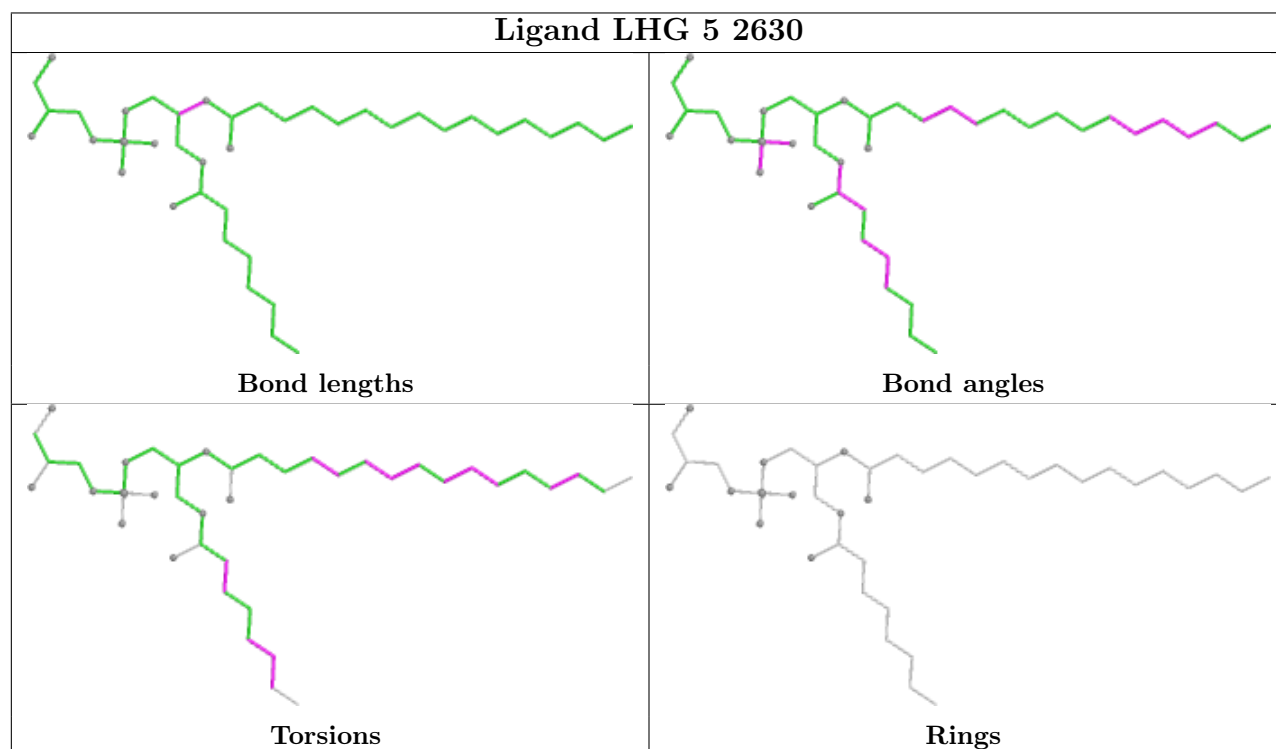
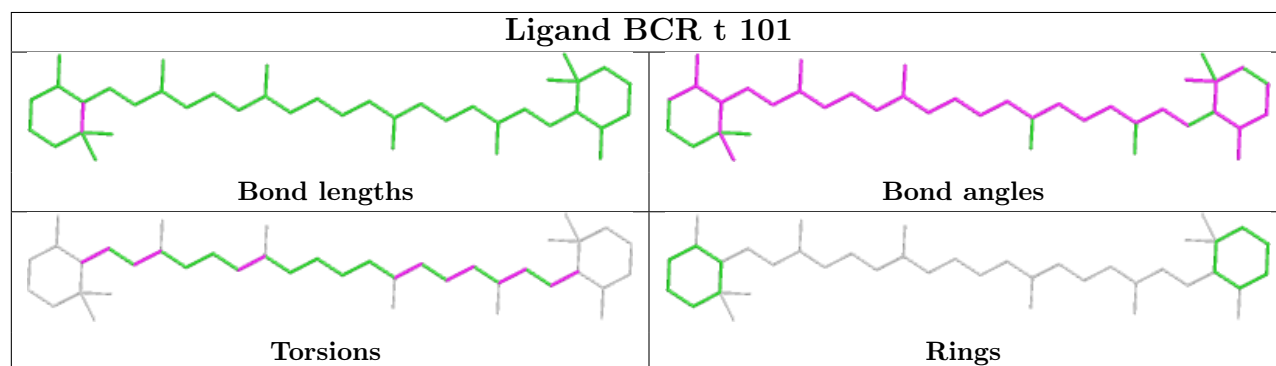
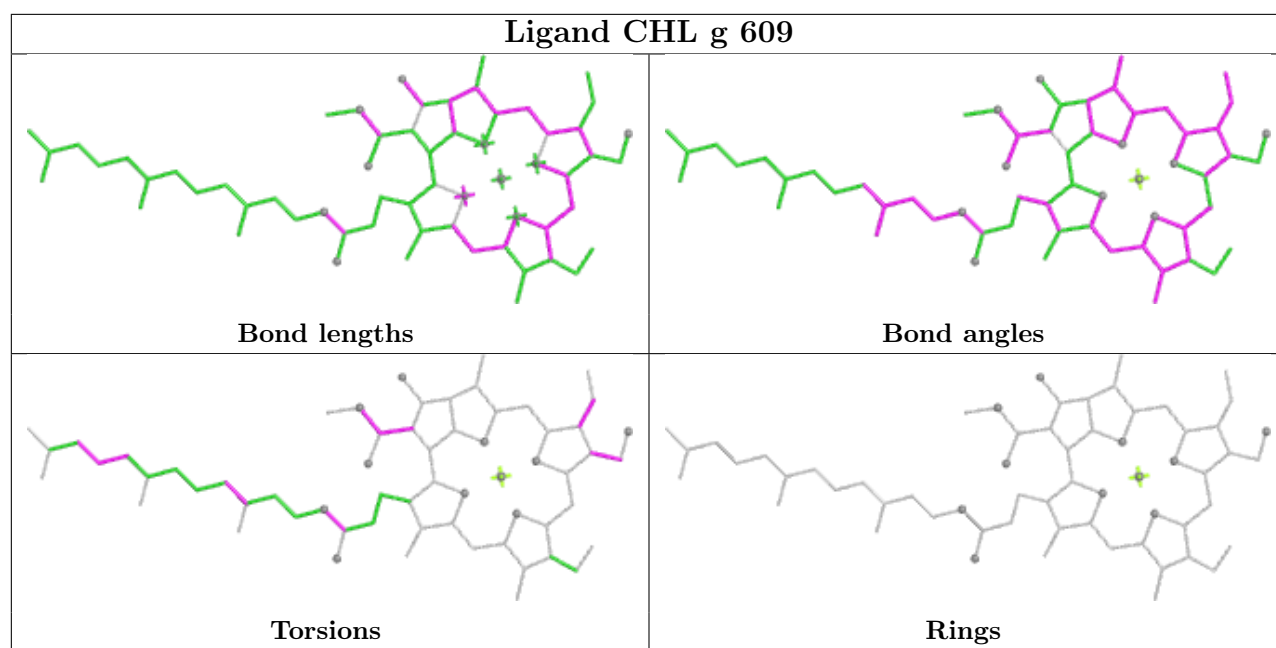
Torsions



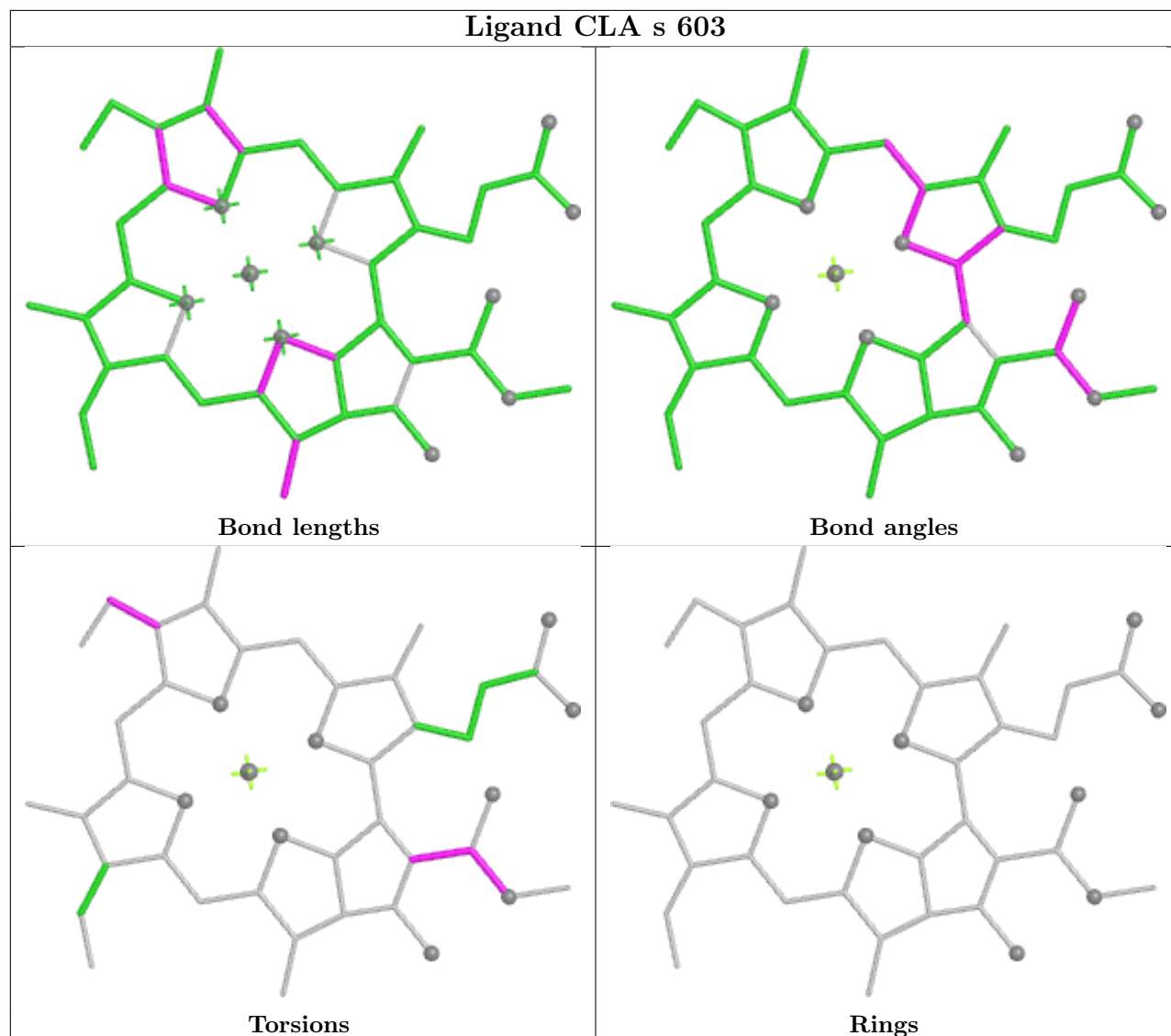
Rings

Ligand CLA Y 611**Ligand CLA C 505**

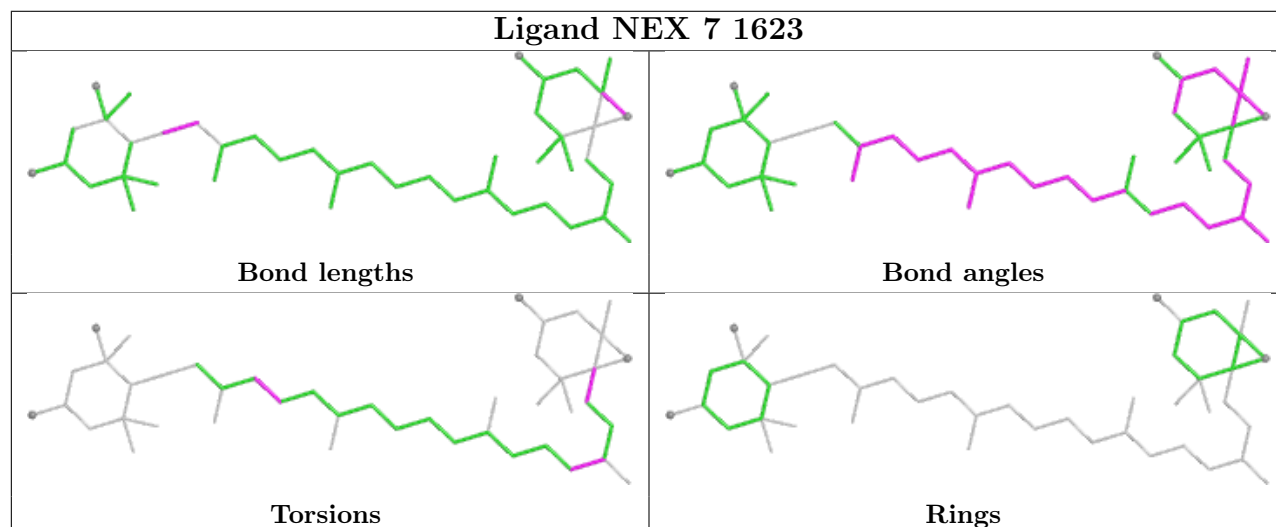
Ligand CLA 2 602**Ligand CLA C 504**

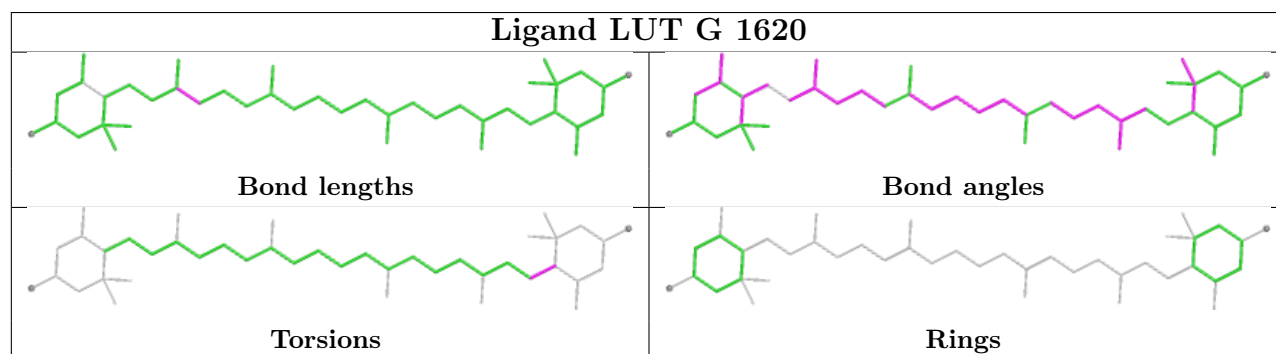
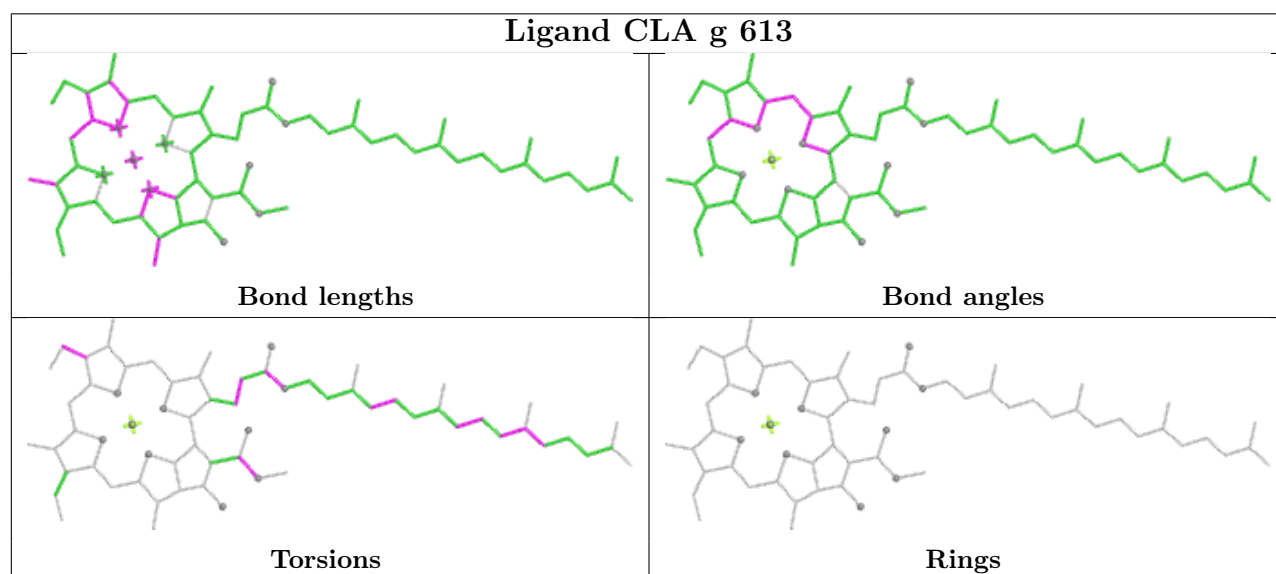
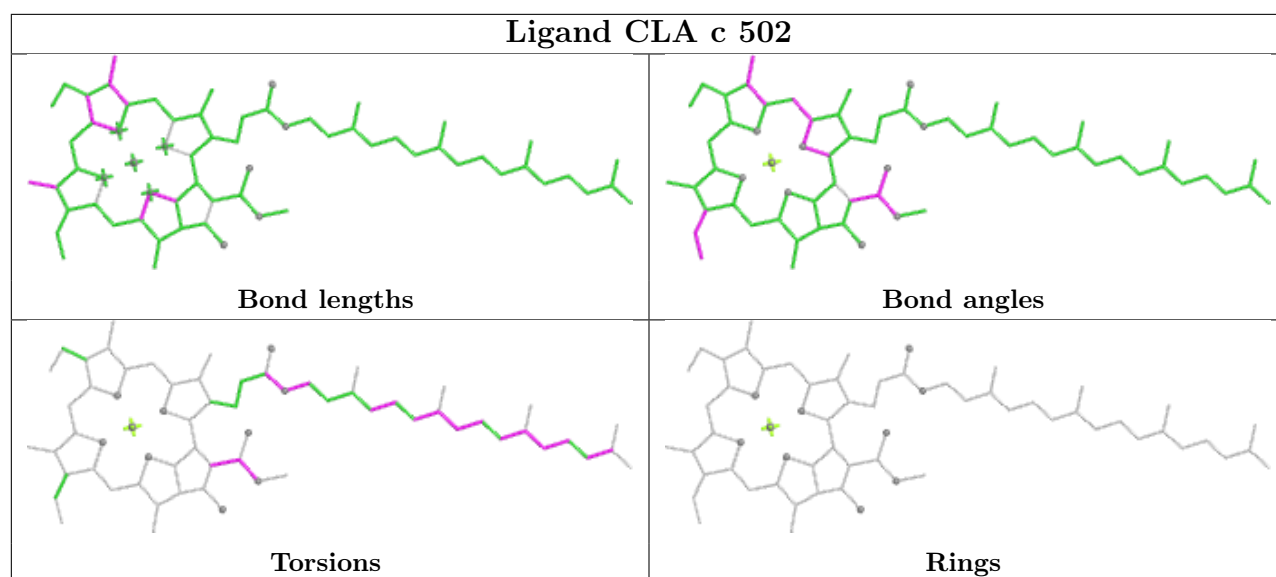


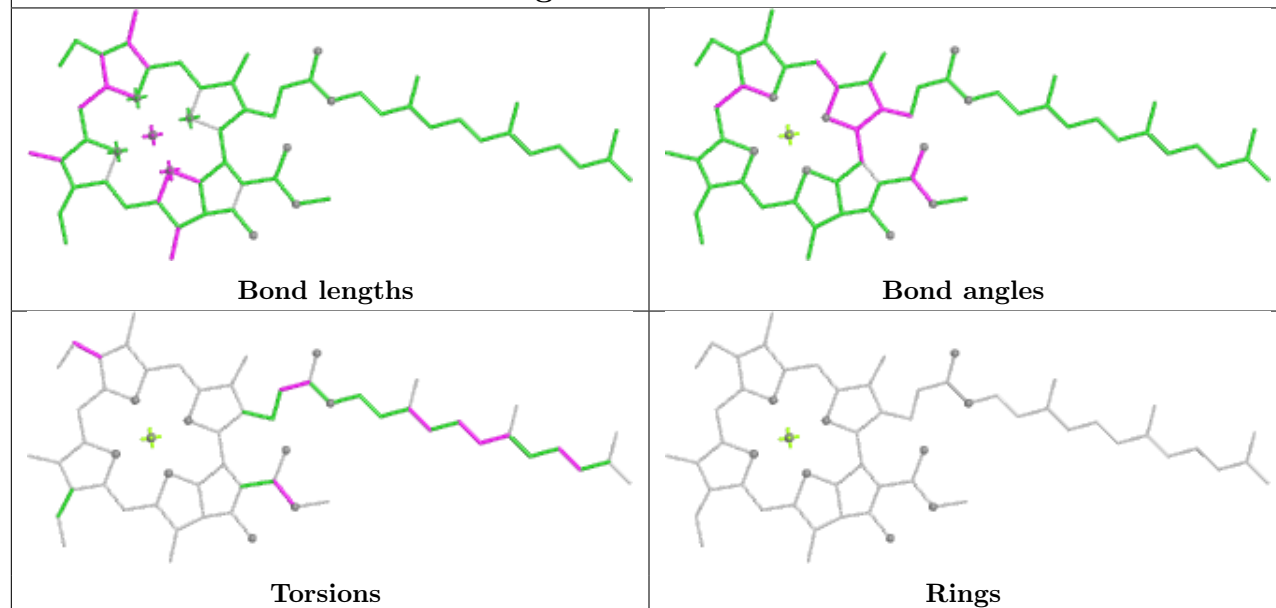
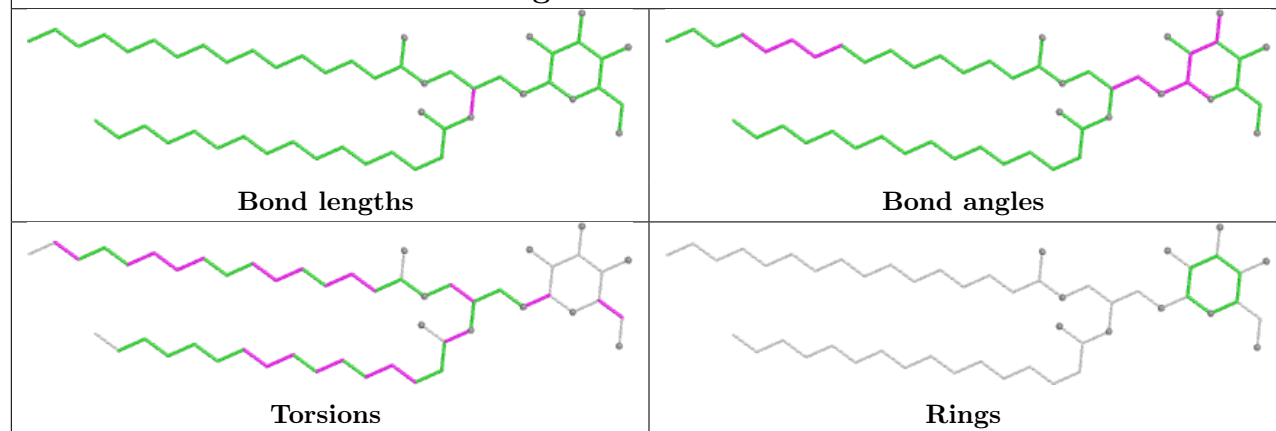
Ligand CLA s 603



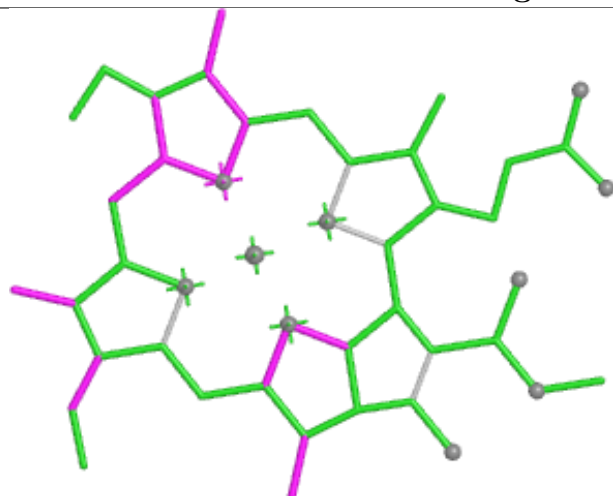
Ligand NEX 7 1623



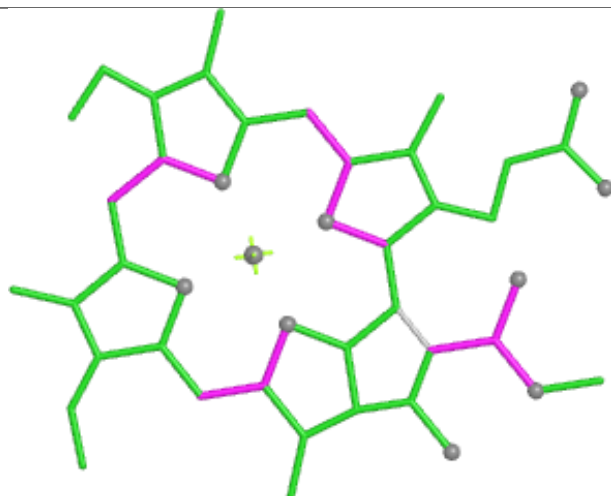


Ligand CLA n 612**Ligand LMG c 521**

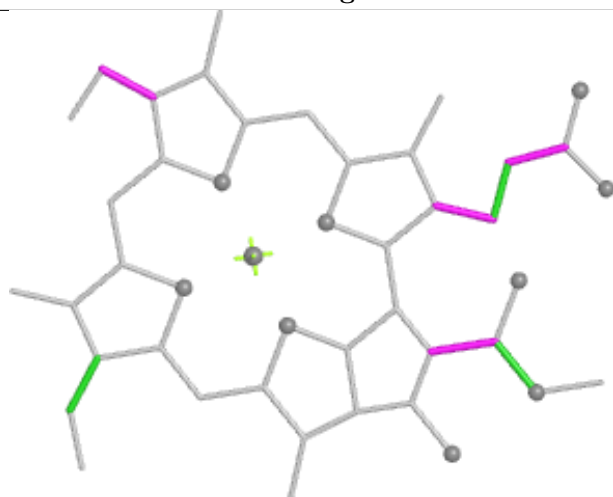
Ligand CLA R 616



Bond lengths



Bond angles

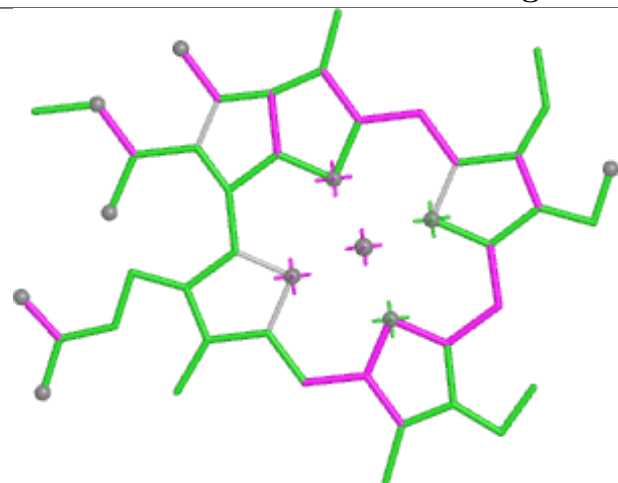


Torsions

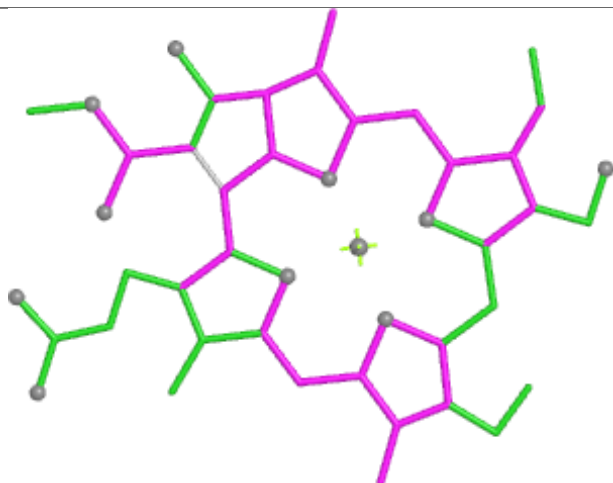


Rings

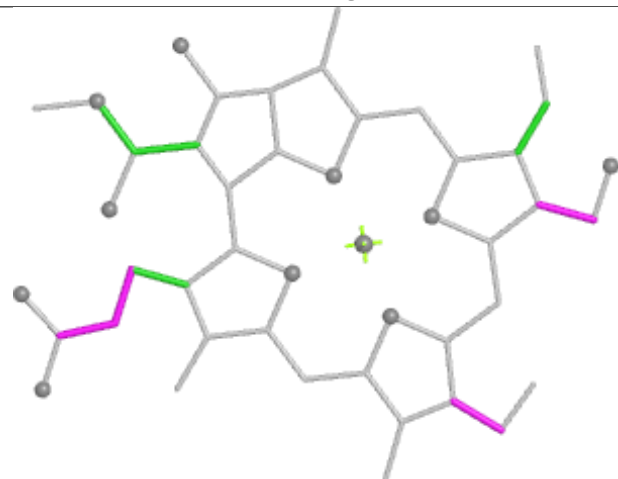
Ligand CHL 5 601



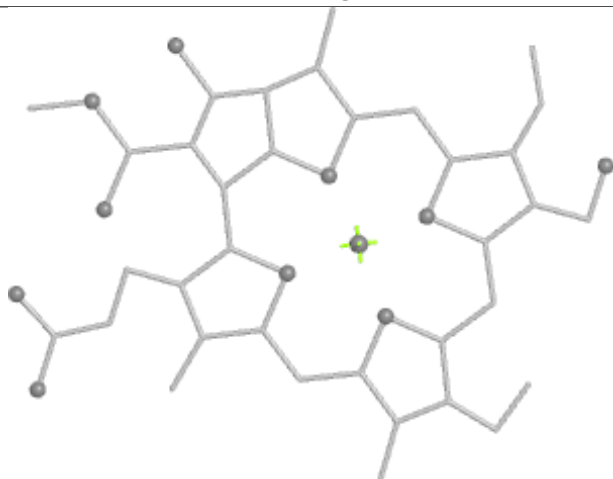
Bond lengths



Bond angles

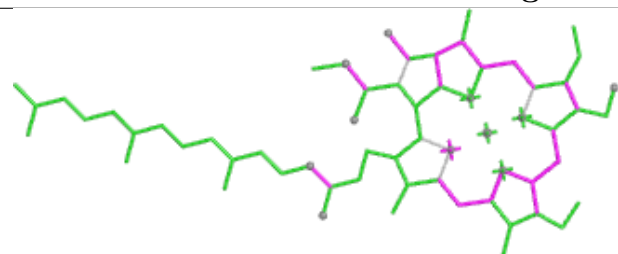


Torsions

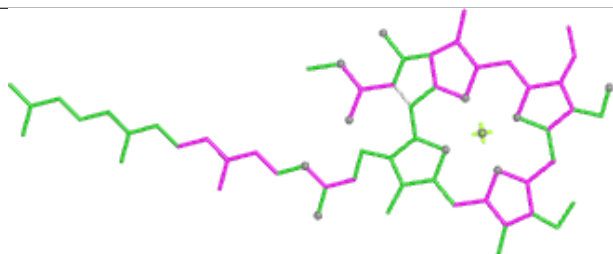


Rings

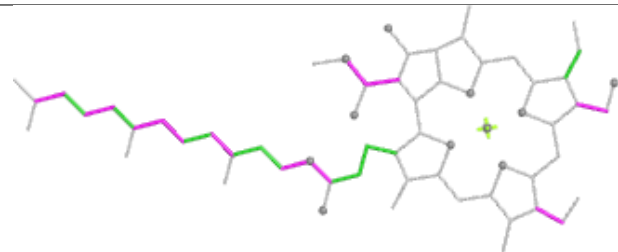
Ligand CHL 6 609



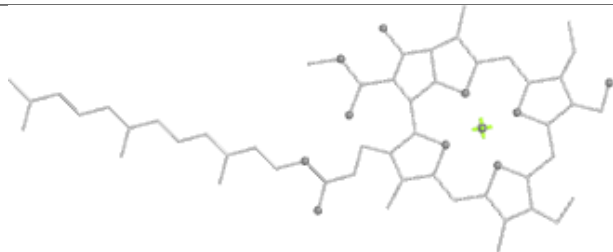
Bond lengths



Bond angles

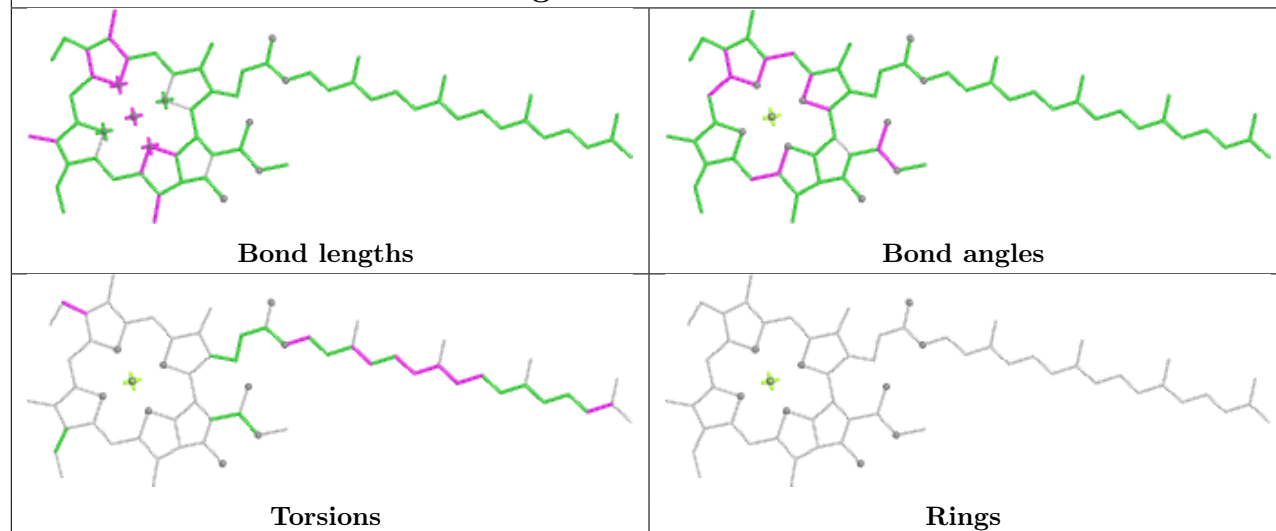


Torsions

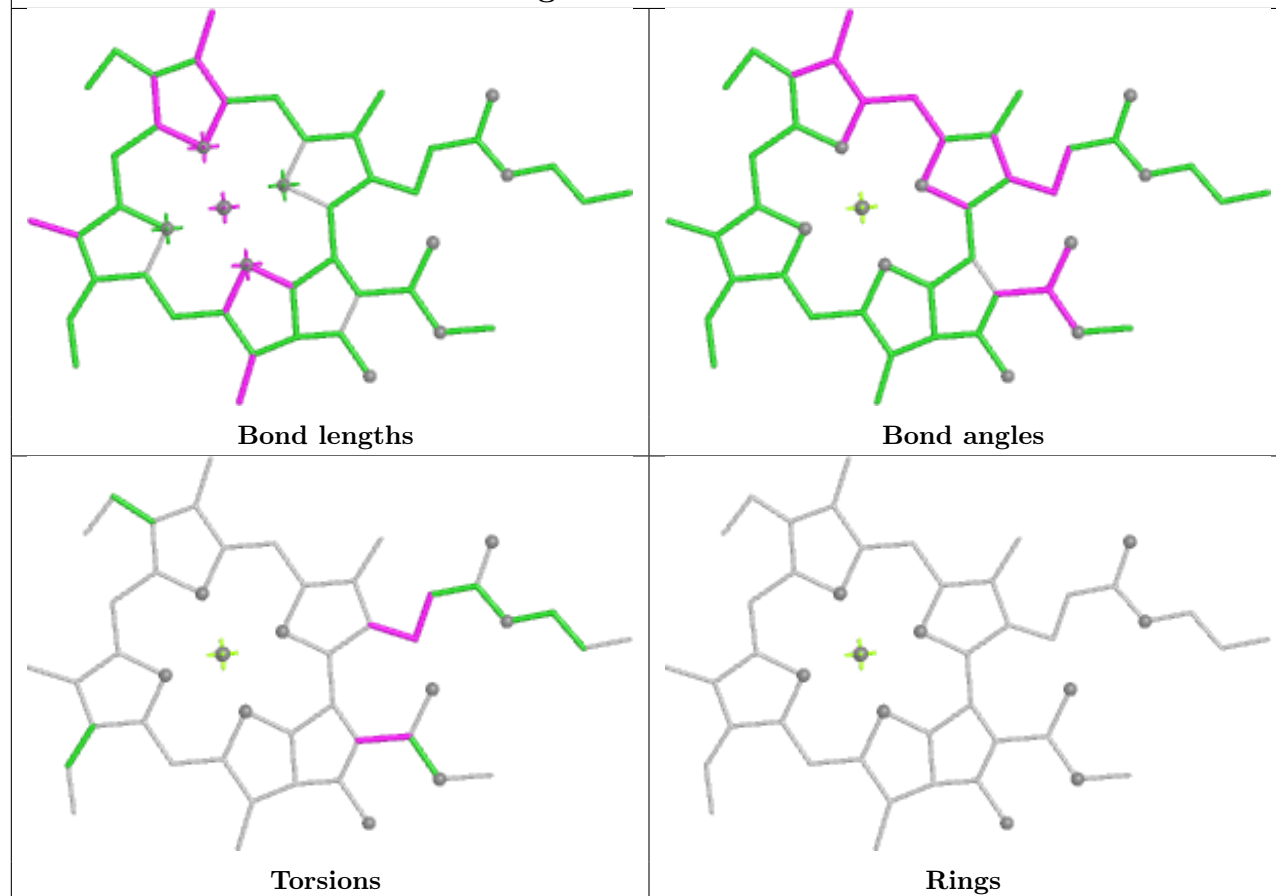


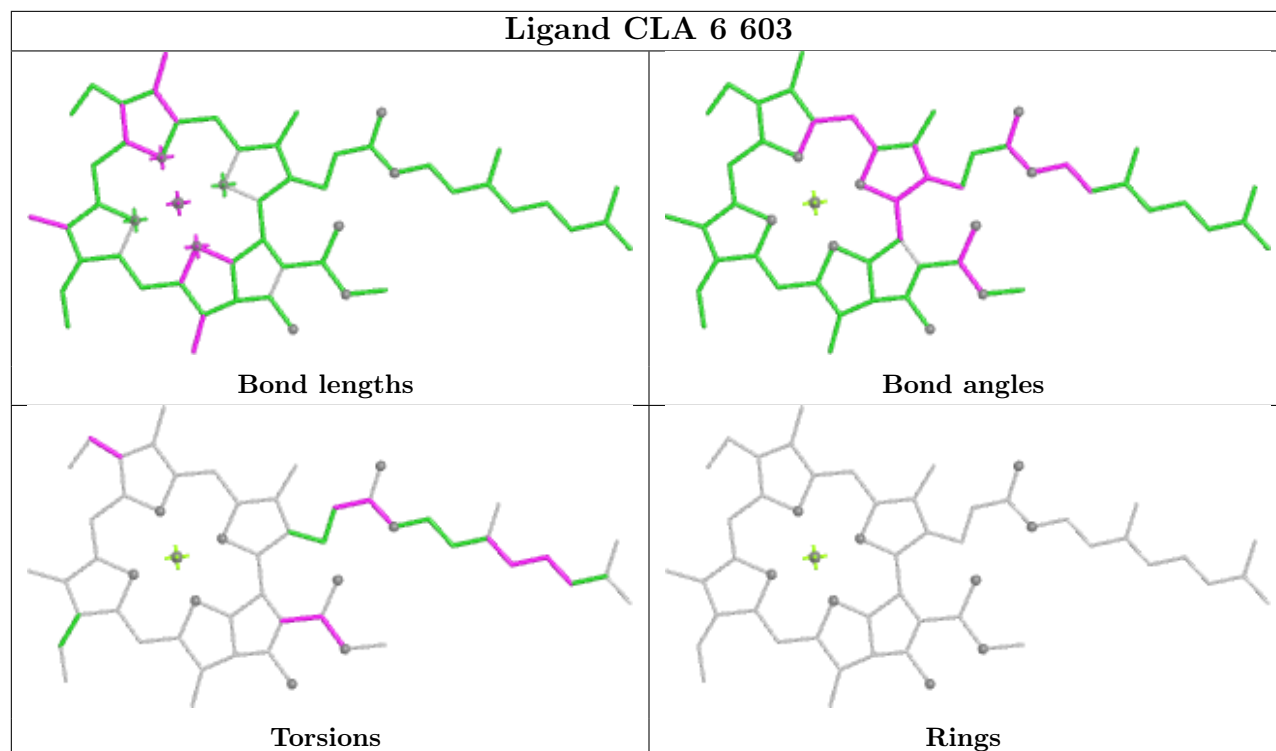
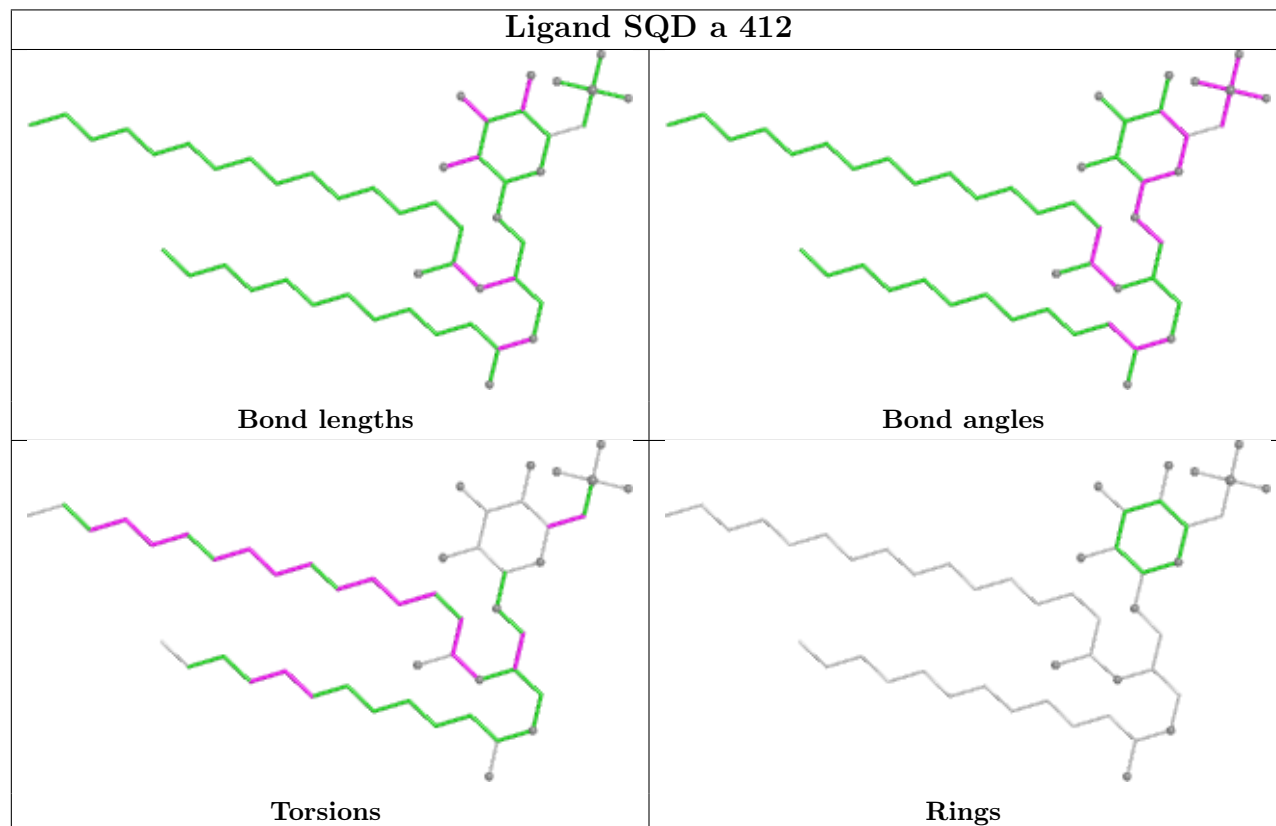
Rings

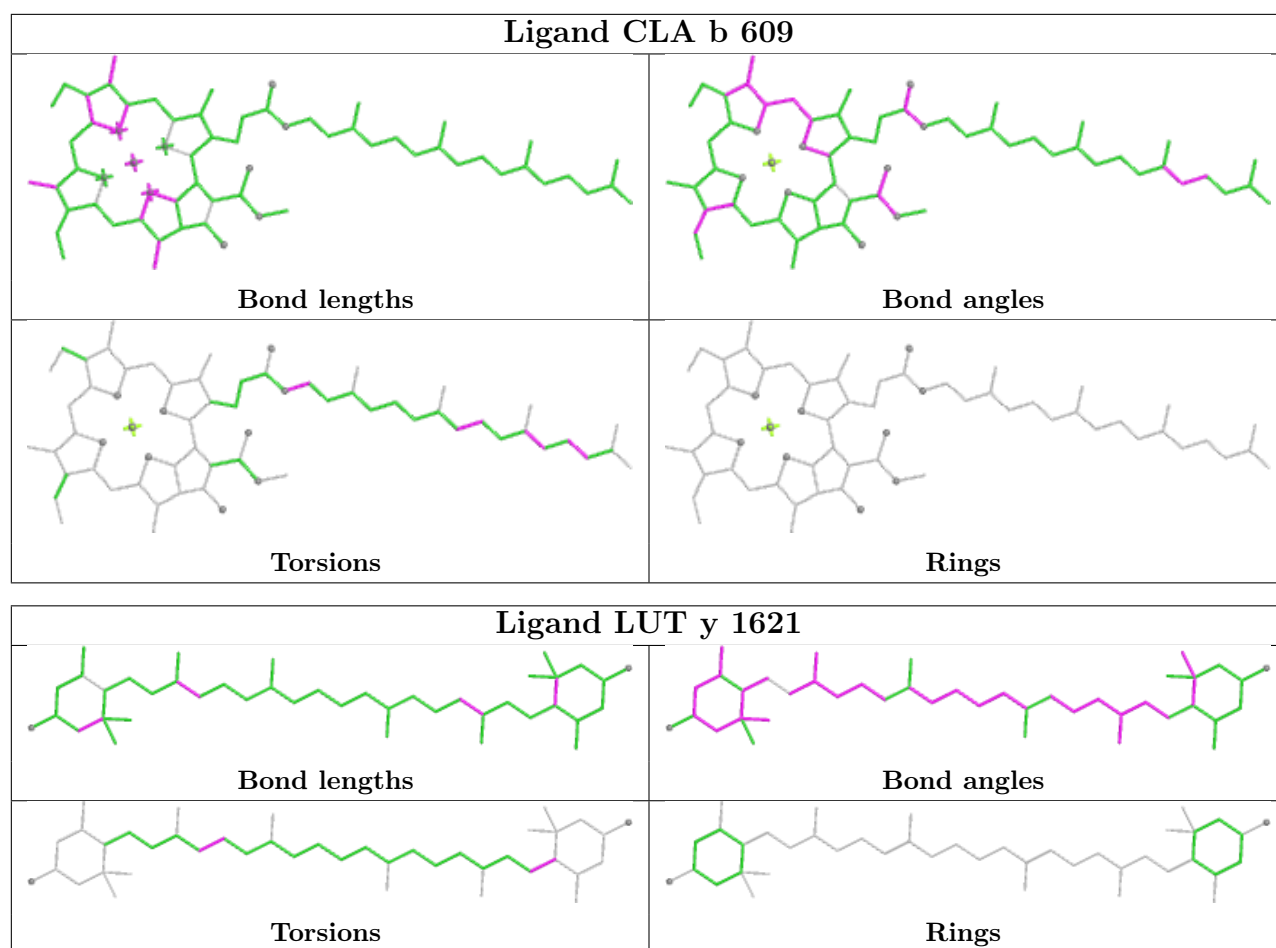
Ligand CLA B 603



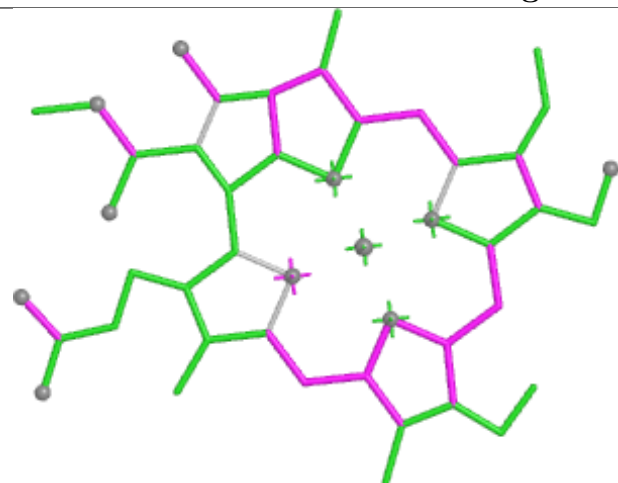
Ligand CLA r 604



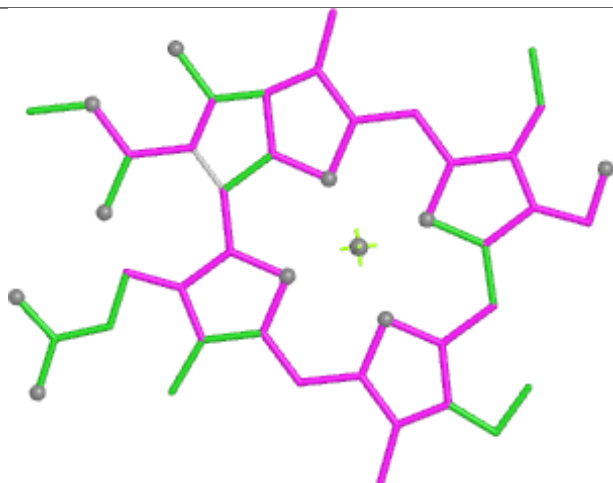
Ligand CLA 6 603**Ligand SQD a 412**



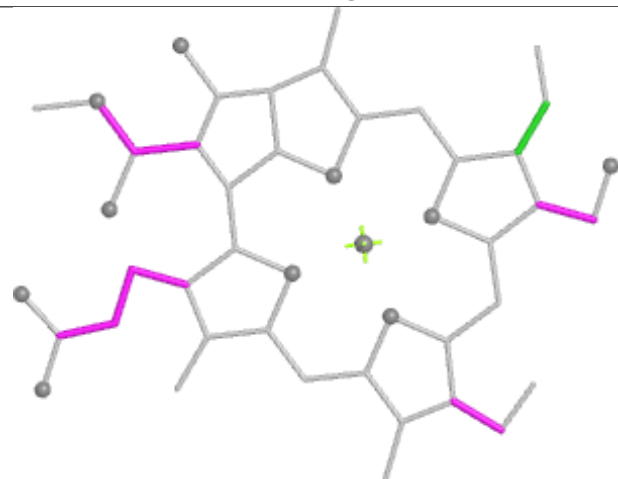
Ligand CHL 3 605



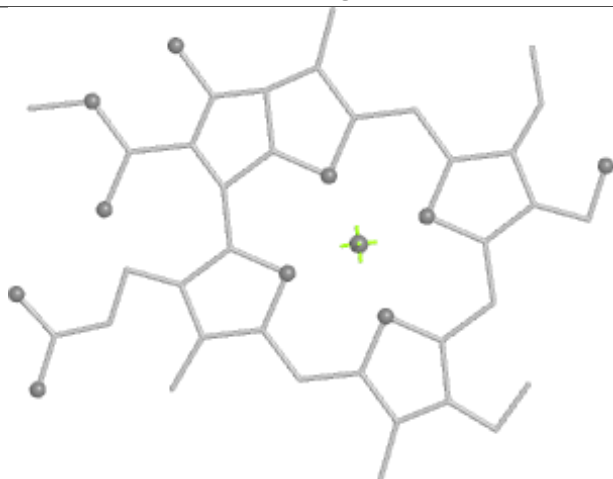
Bond lengths



Bond angles

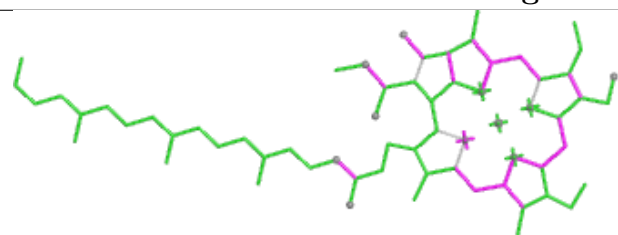


Torsions

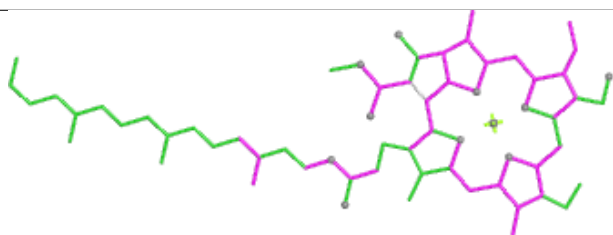


Rings

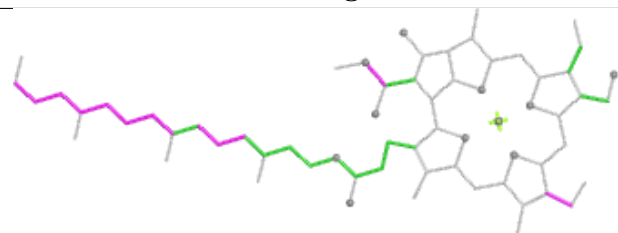
Ligand CHL 3 601



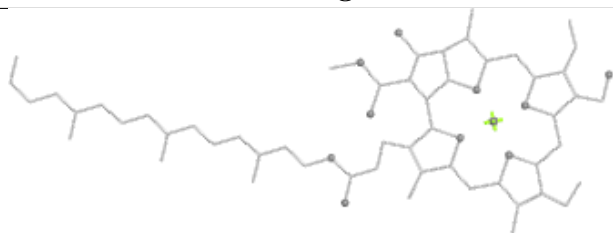
Bond lengths



Bond angles

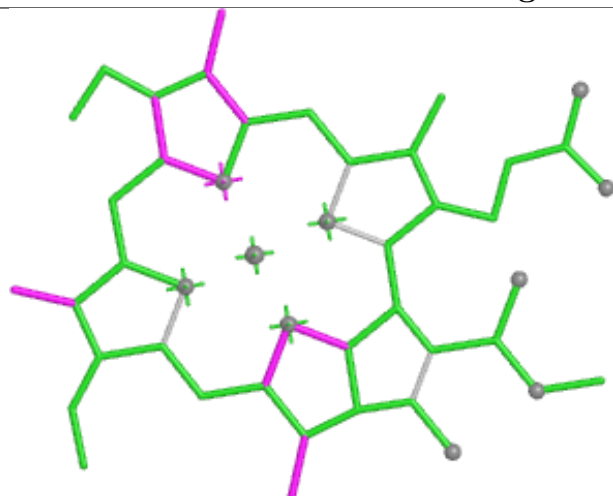


Torsions

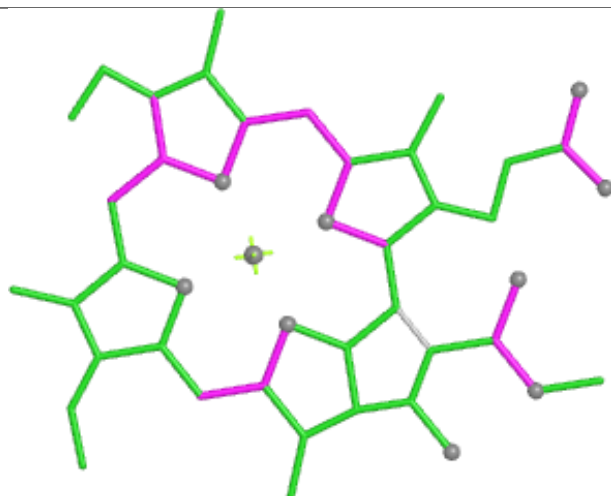


Rings

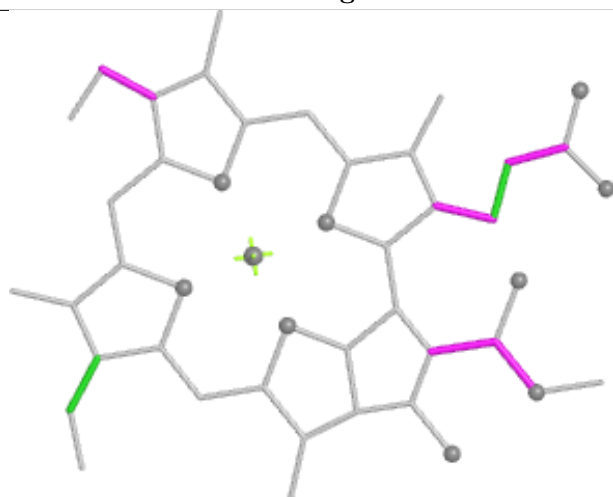
Ligand CLA 4 611



Bond lengths



Bond angles

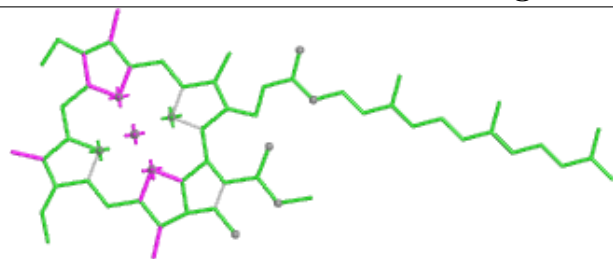


Torsions

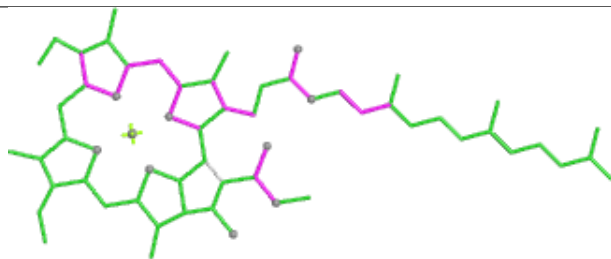


Rings

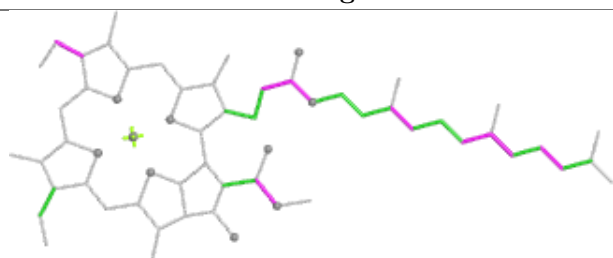
Ligand CLA Y 612



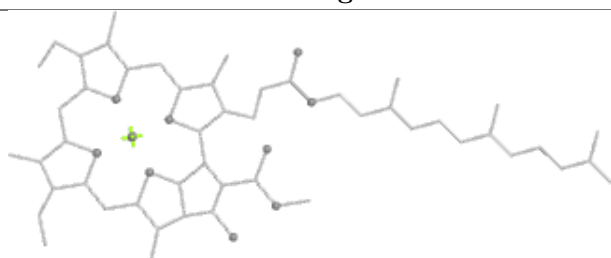
Bond lengths



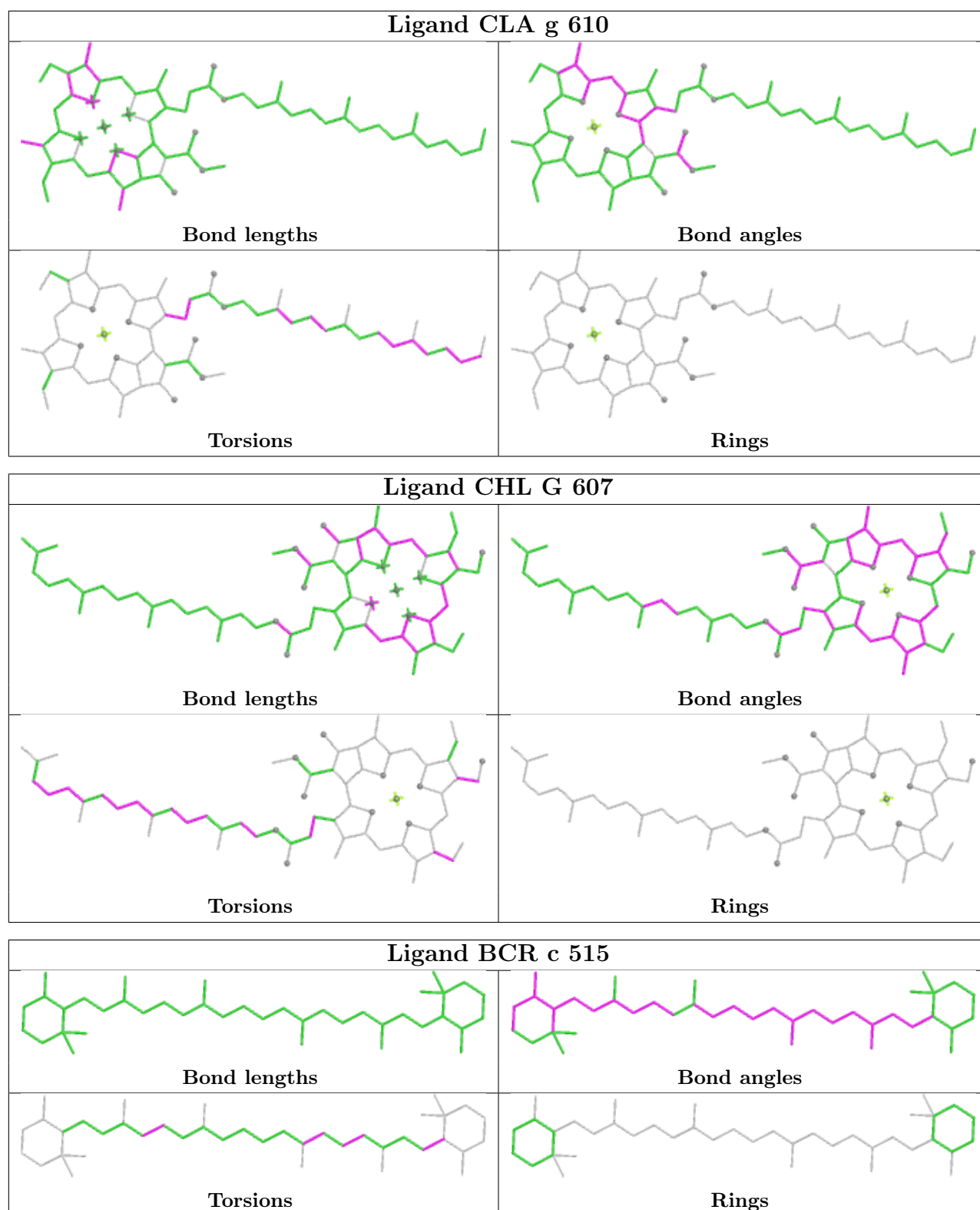
Bond angles



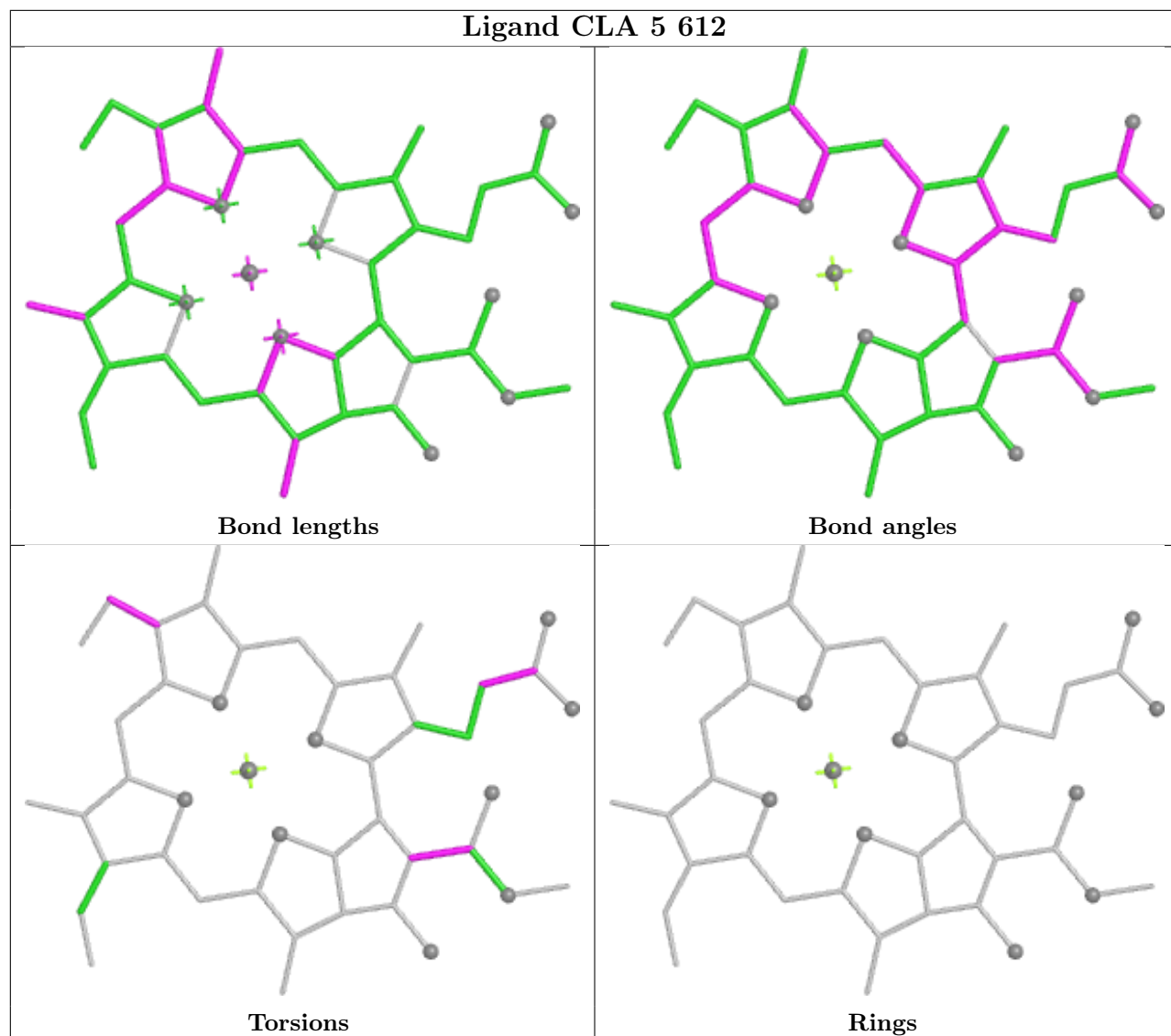
Torsions

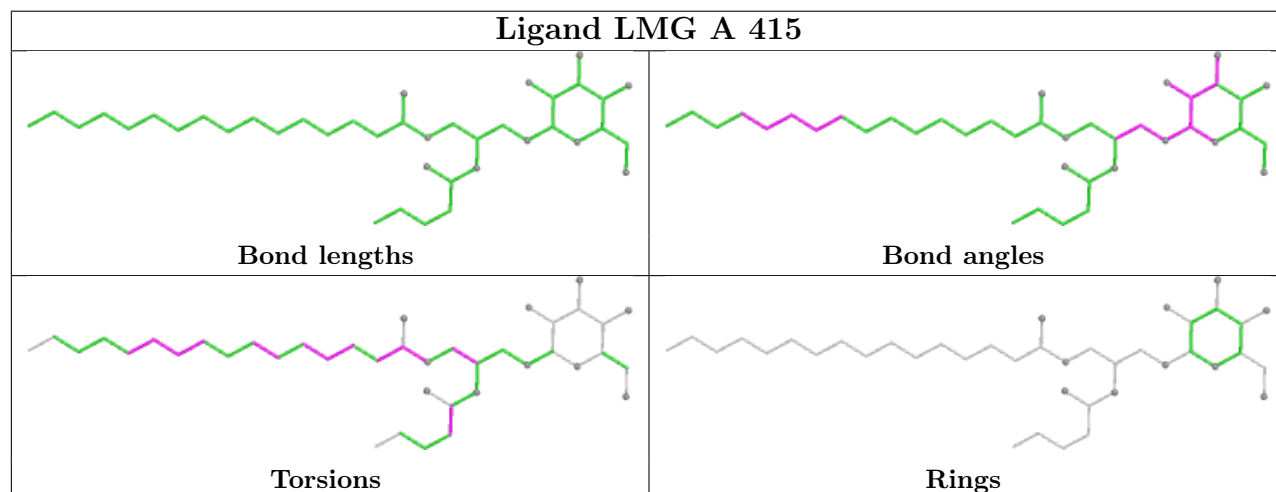
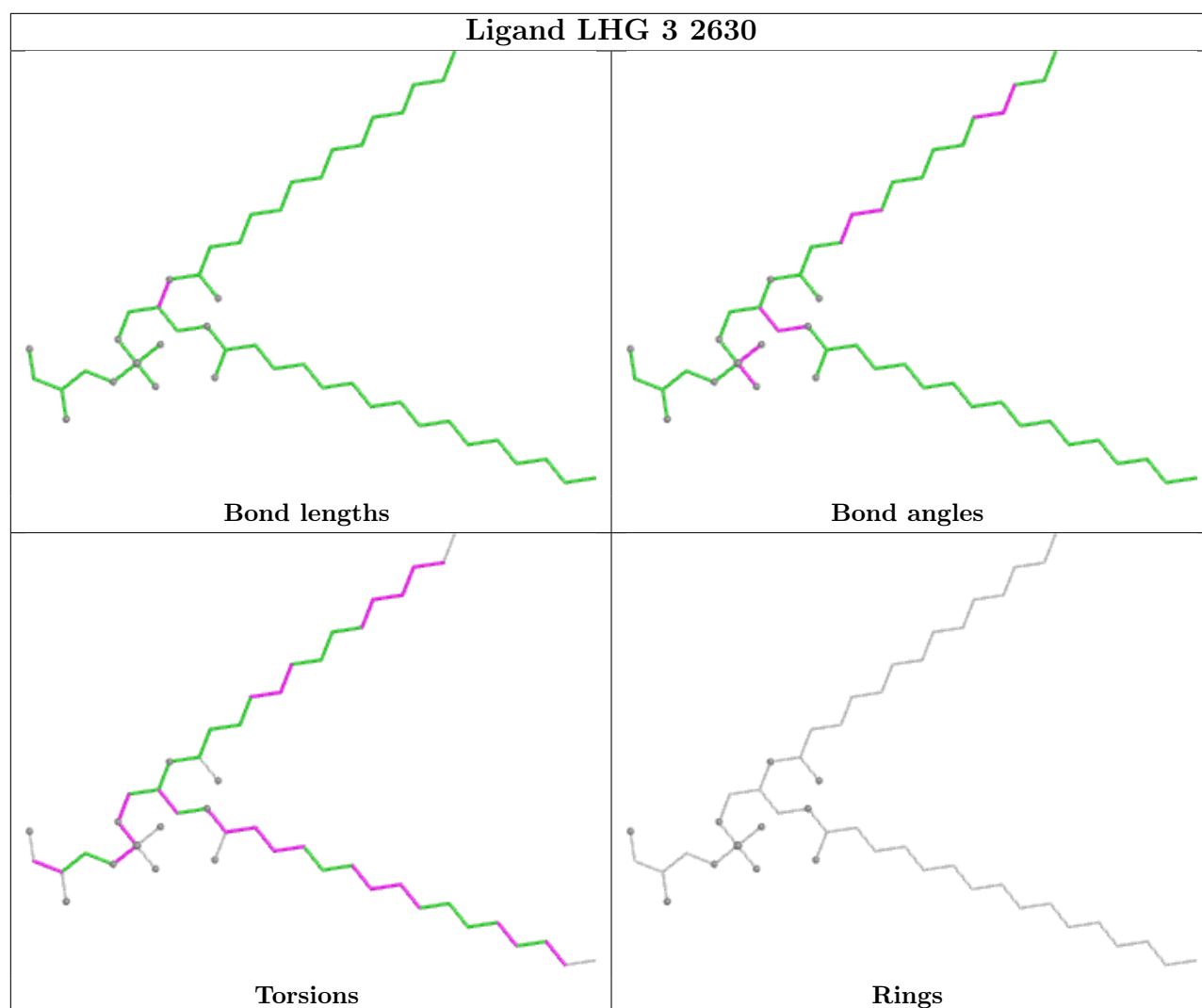


Rings

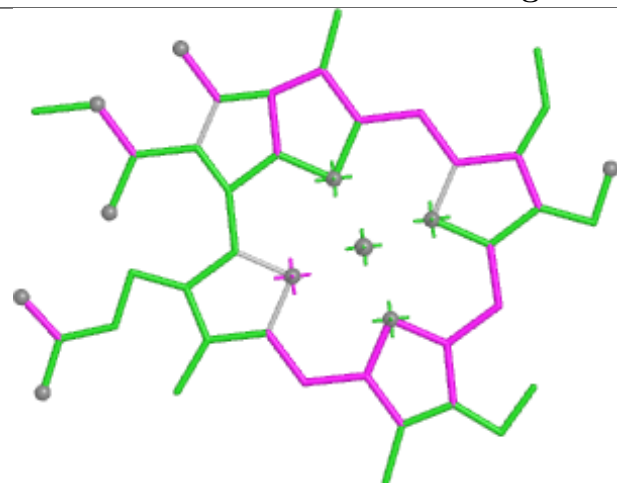


Ligand CLA 5 612

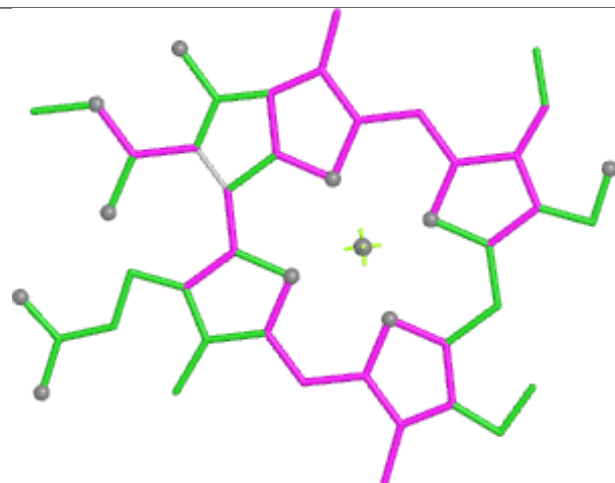




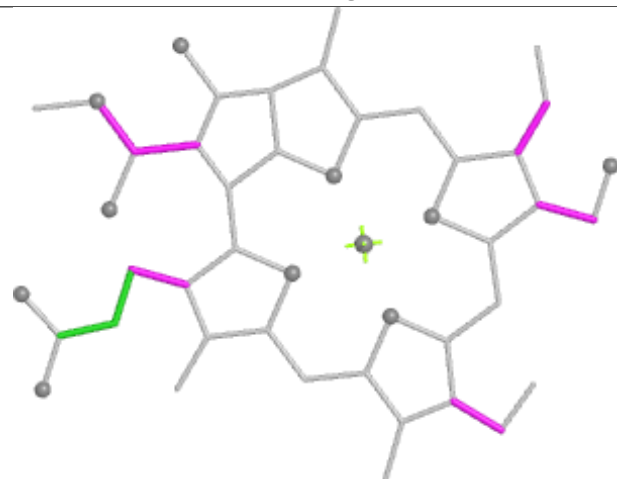
Ligand CHL 2 608



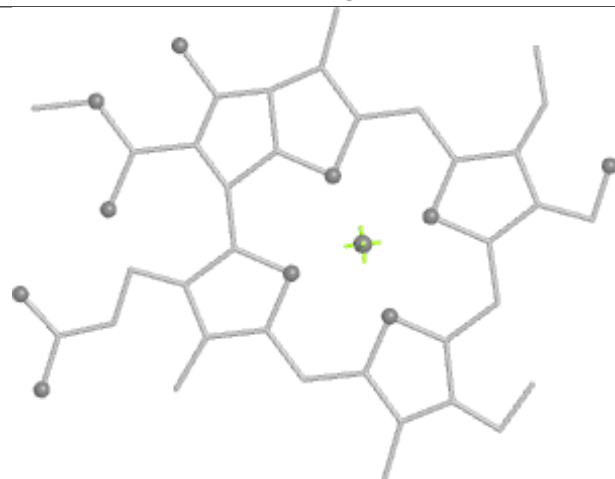
Bond lengths



Bond angles

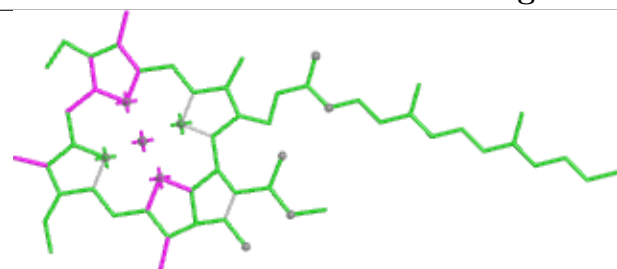


Torsions

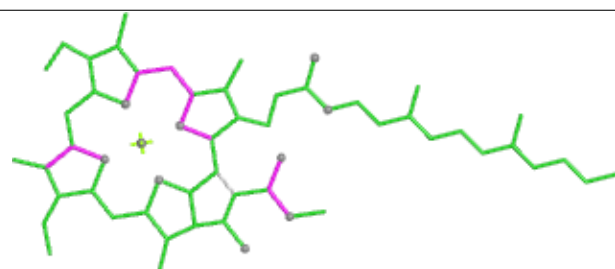


Rings

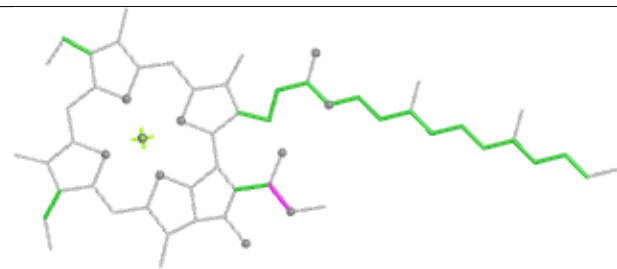
Ligand CLA R 609



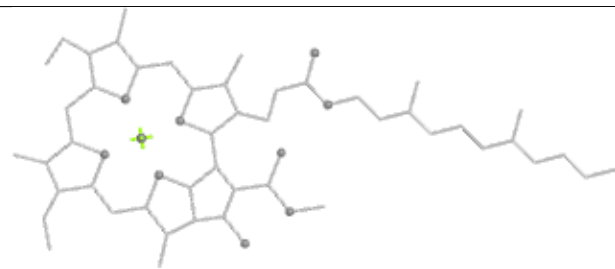
Bond lengths



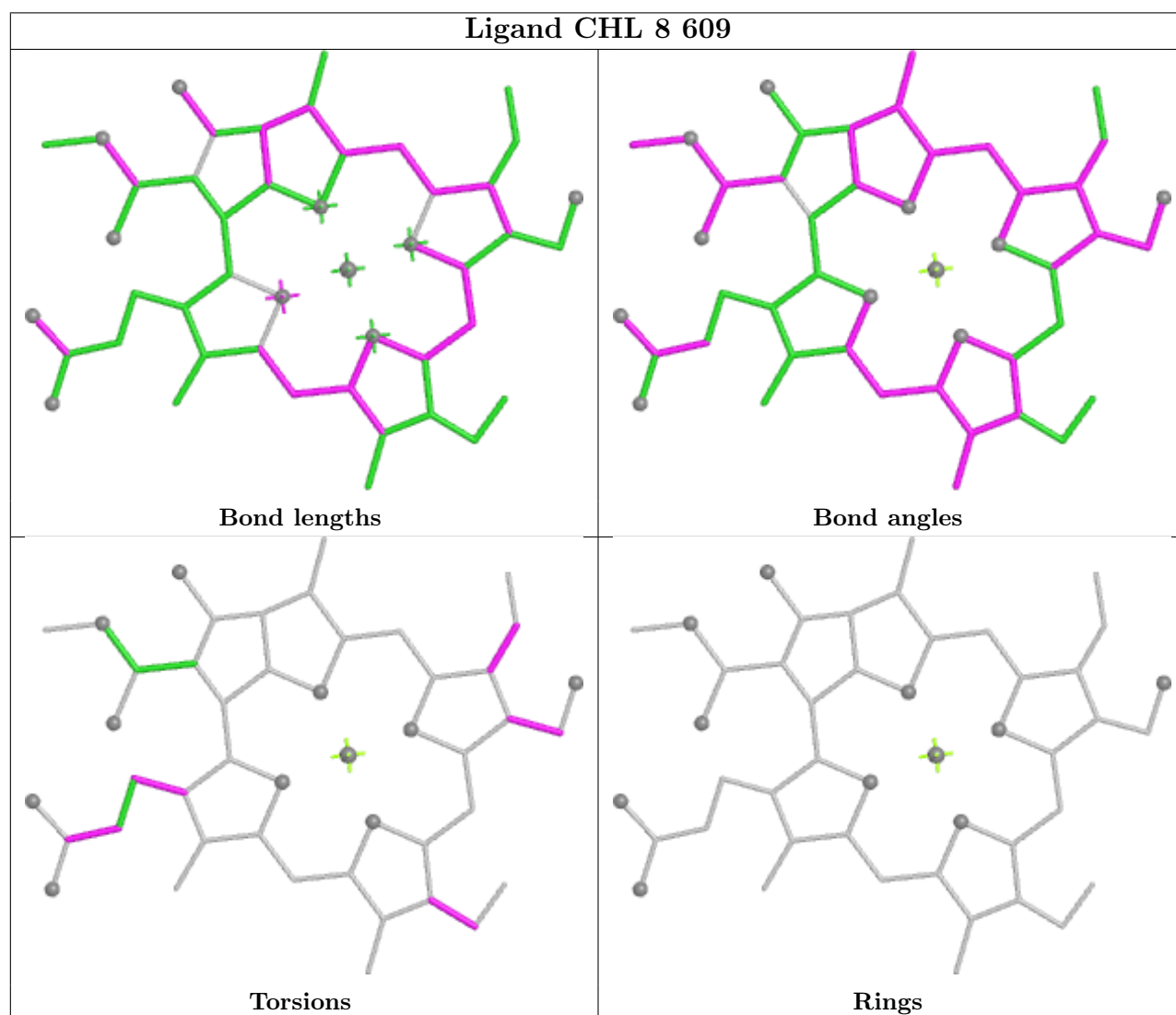
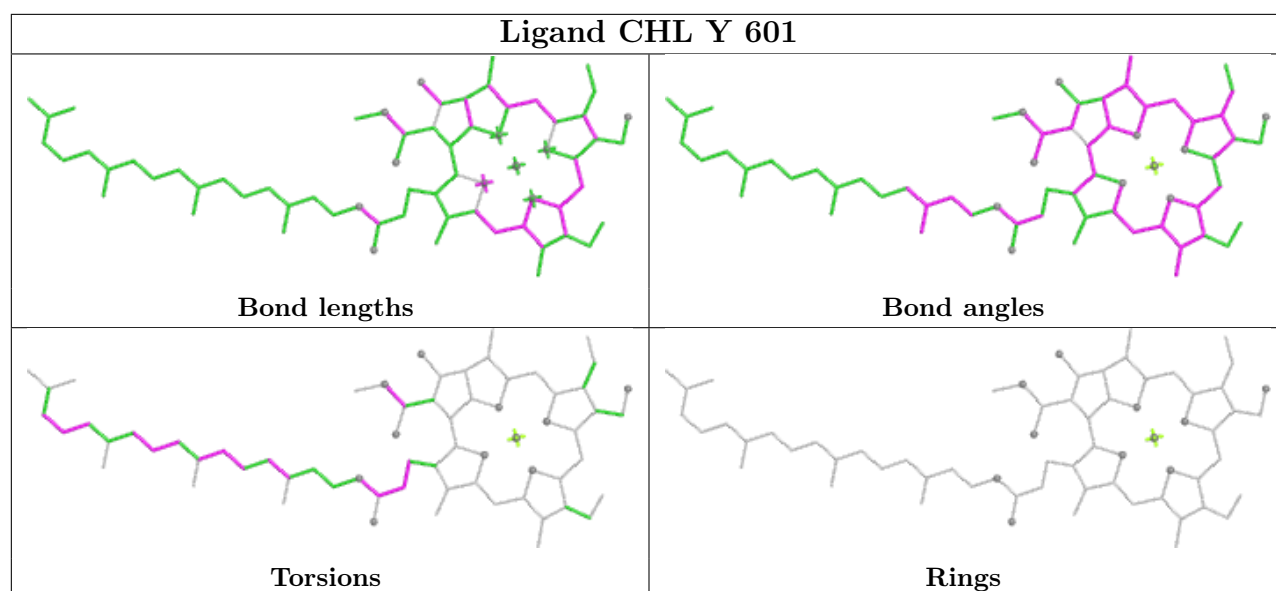
Bond angles

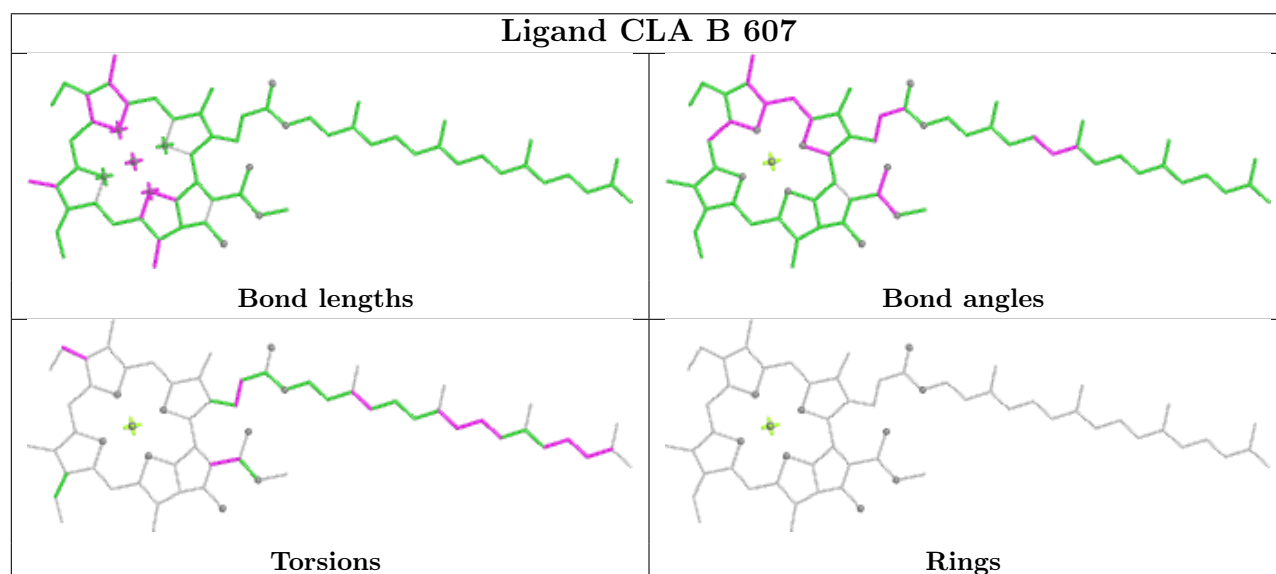
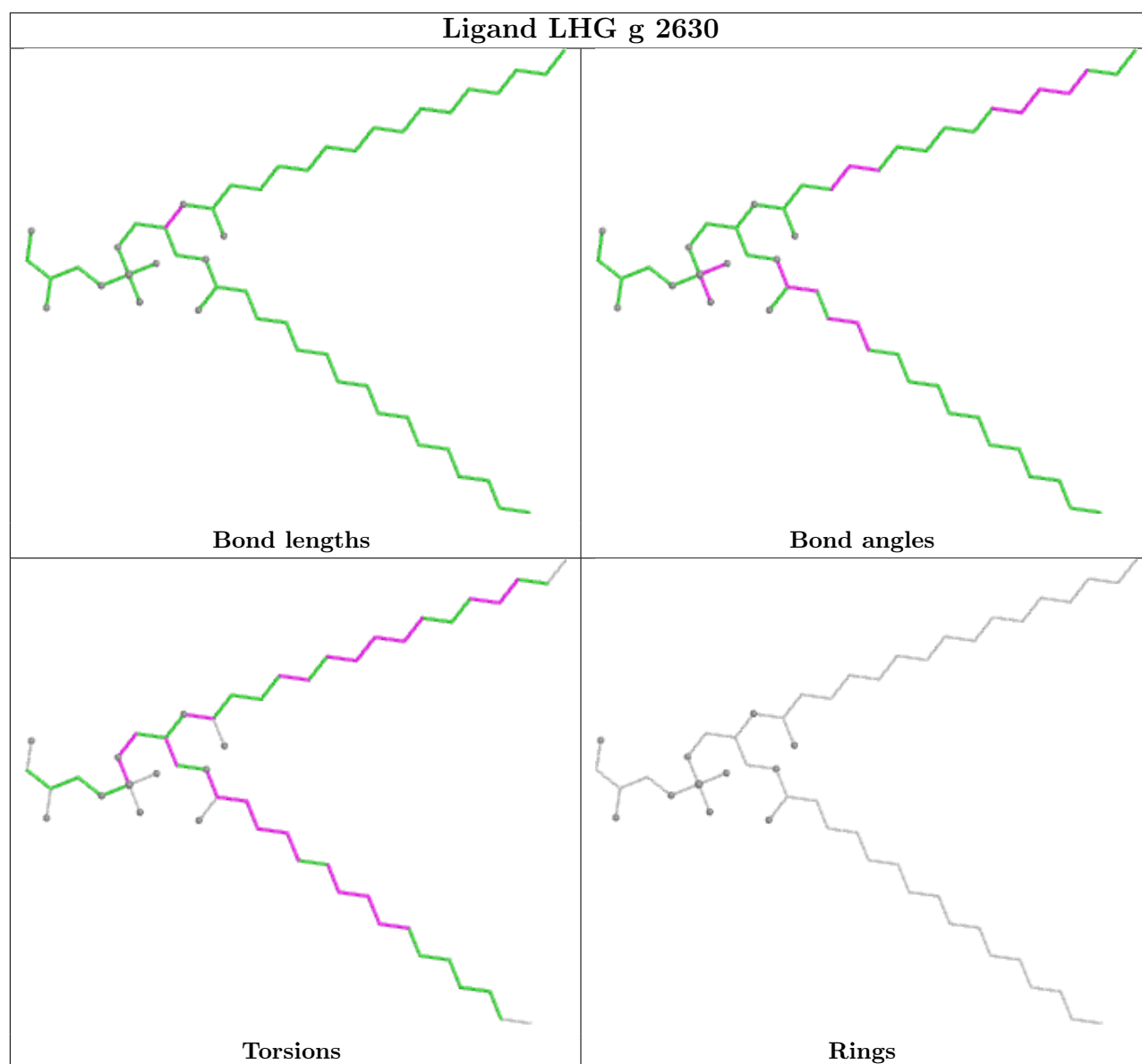


Torsions

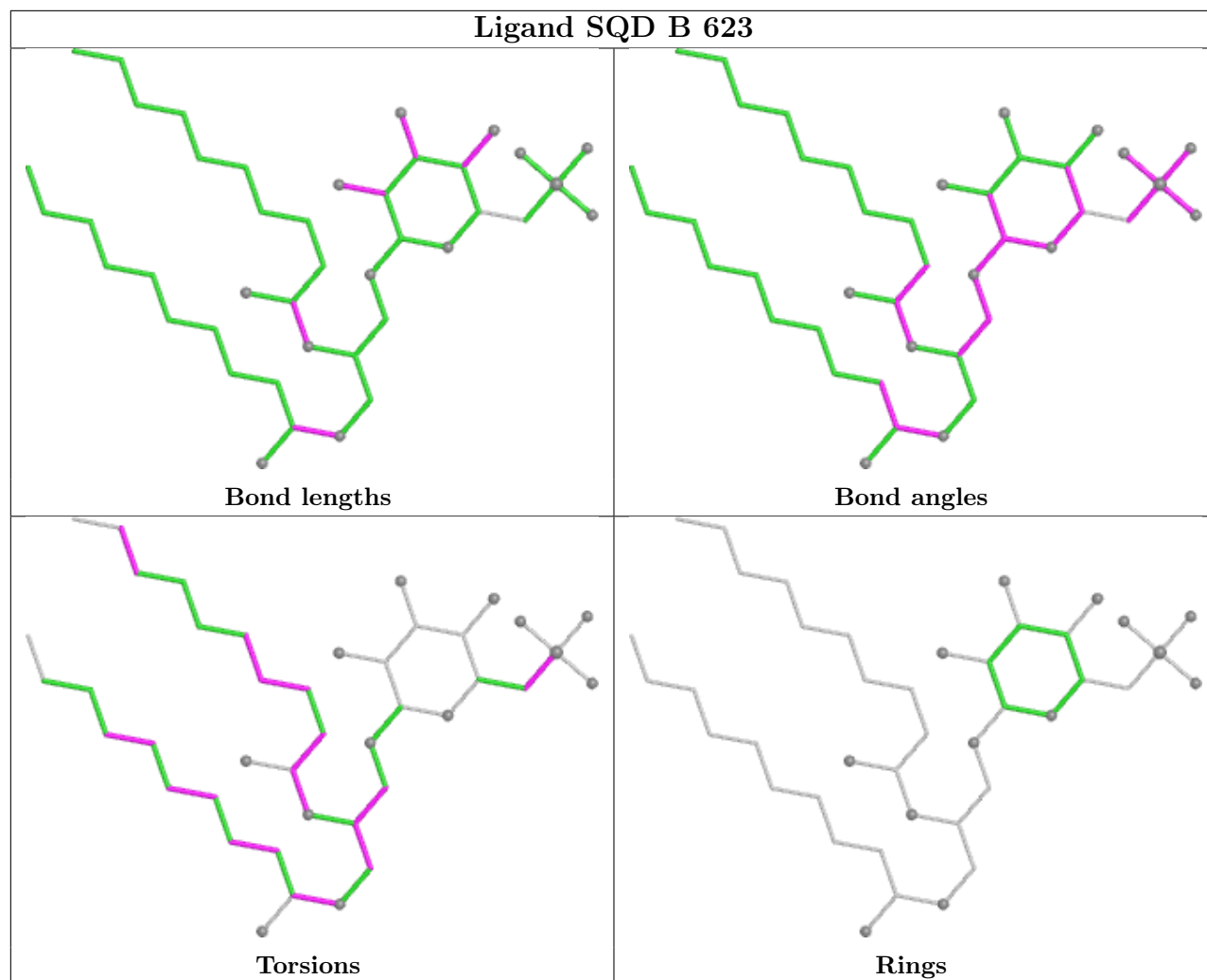


Rings

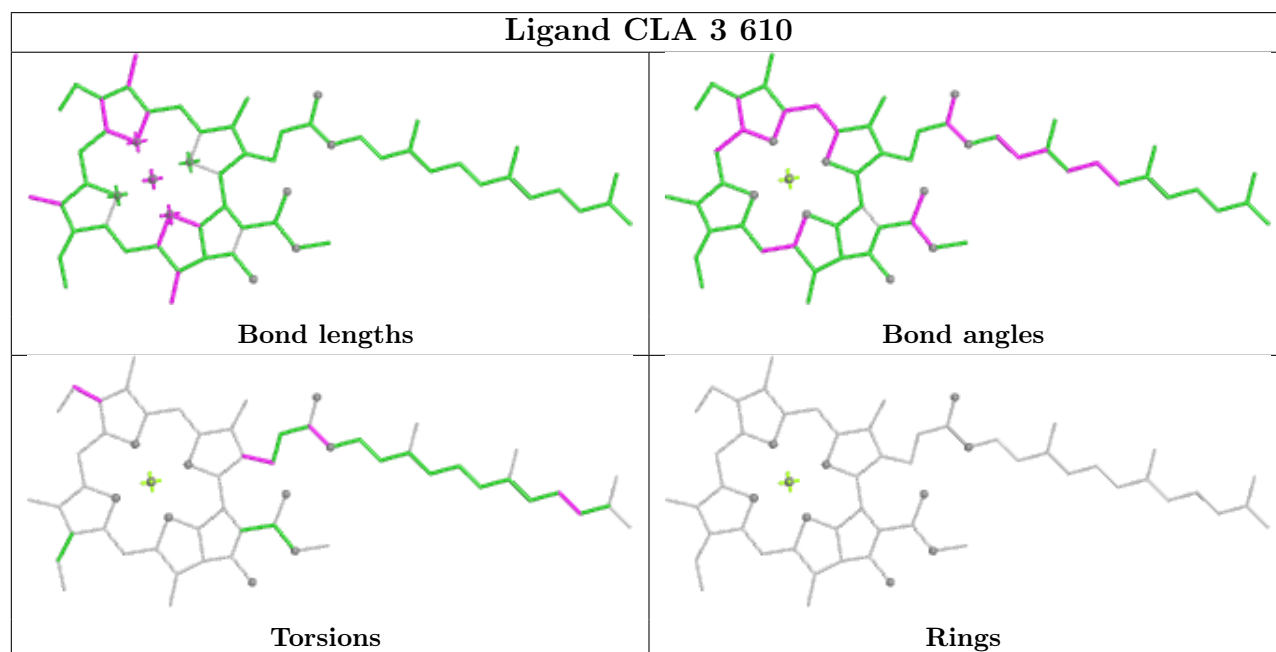




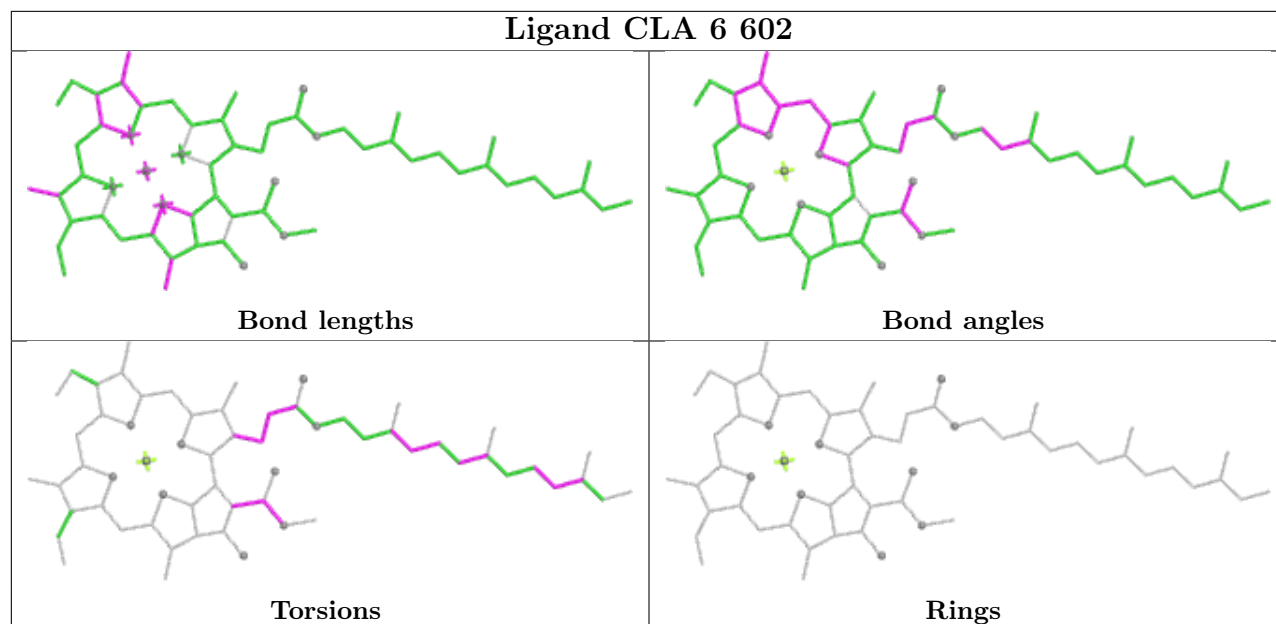
Ligand SQD B 623



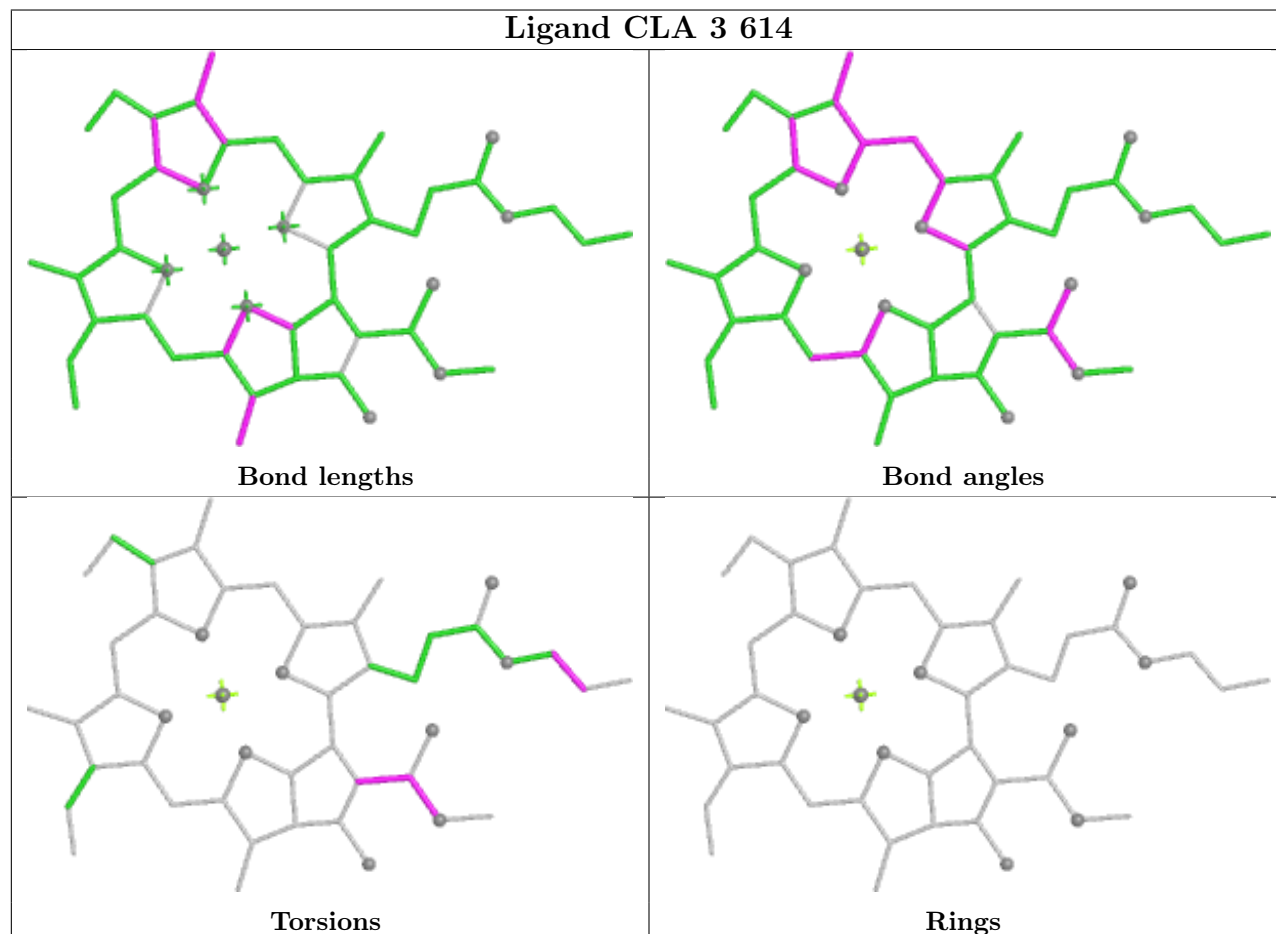
Ligand CLA 3 610

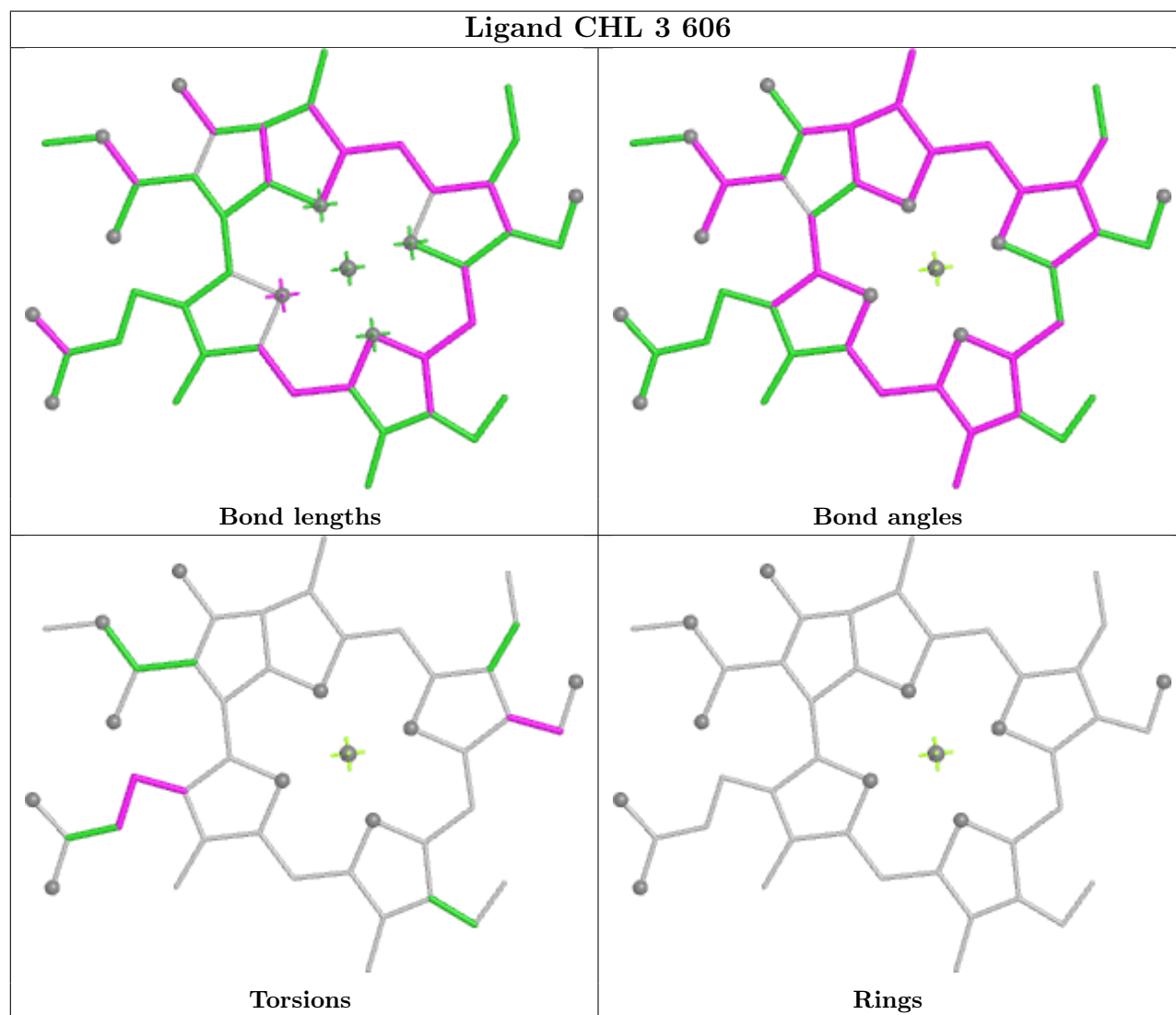
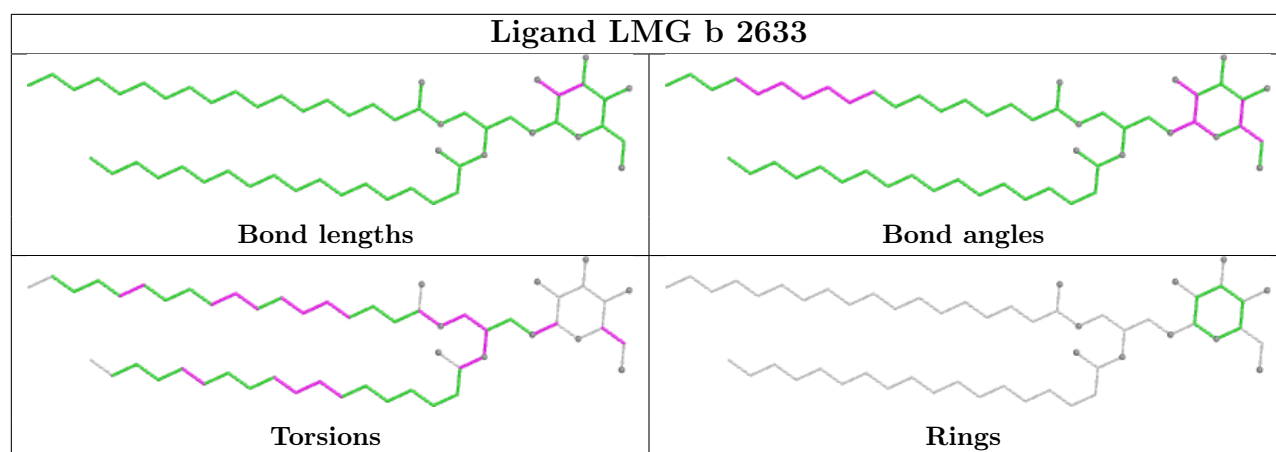


Ligand CLA 6 602

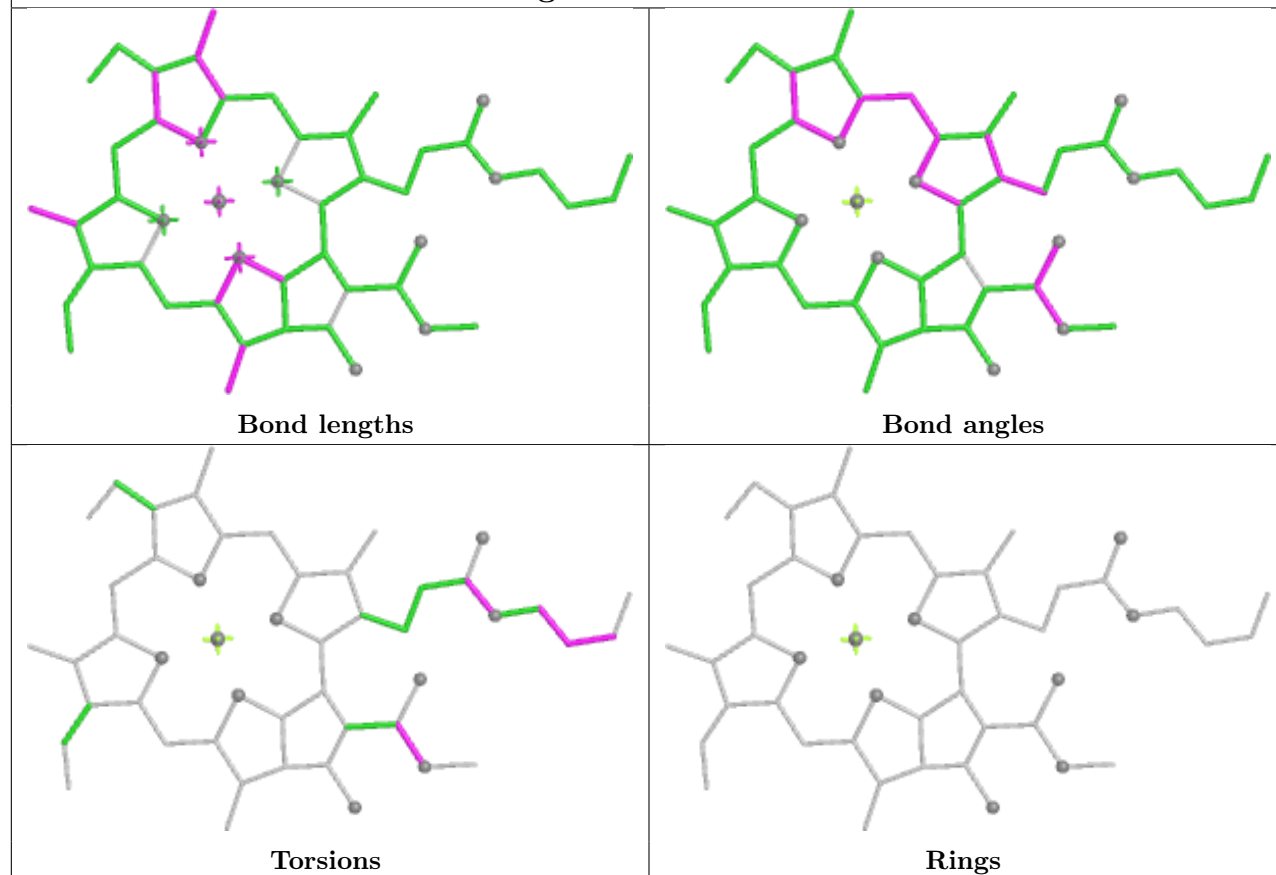


Ligand CLA 3 614

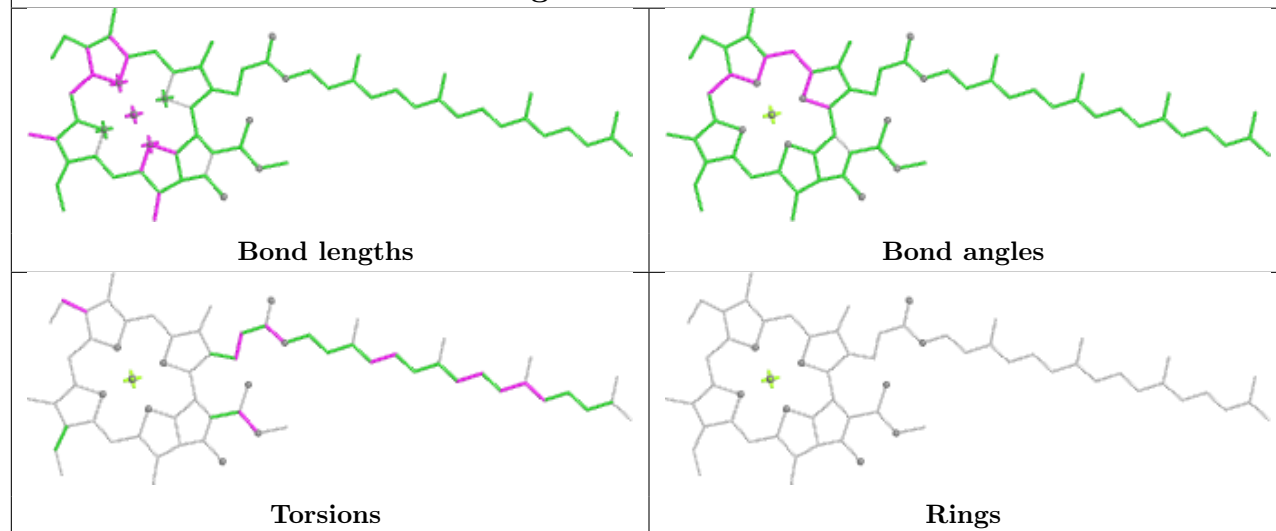




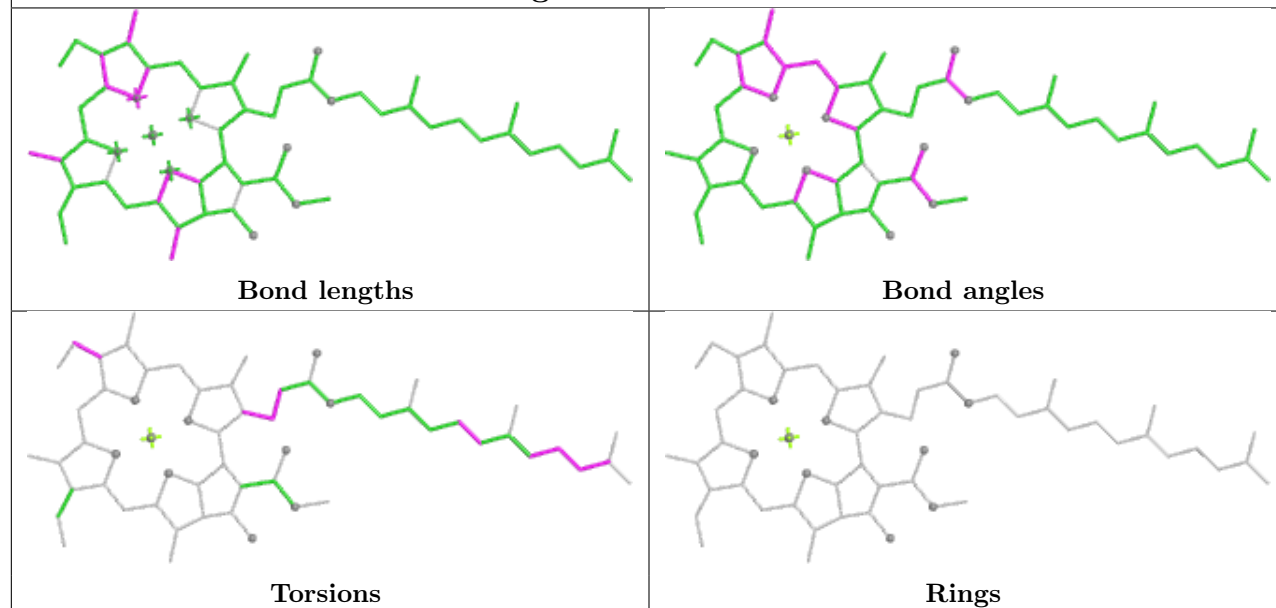
Ligand CLA r 612



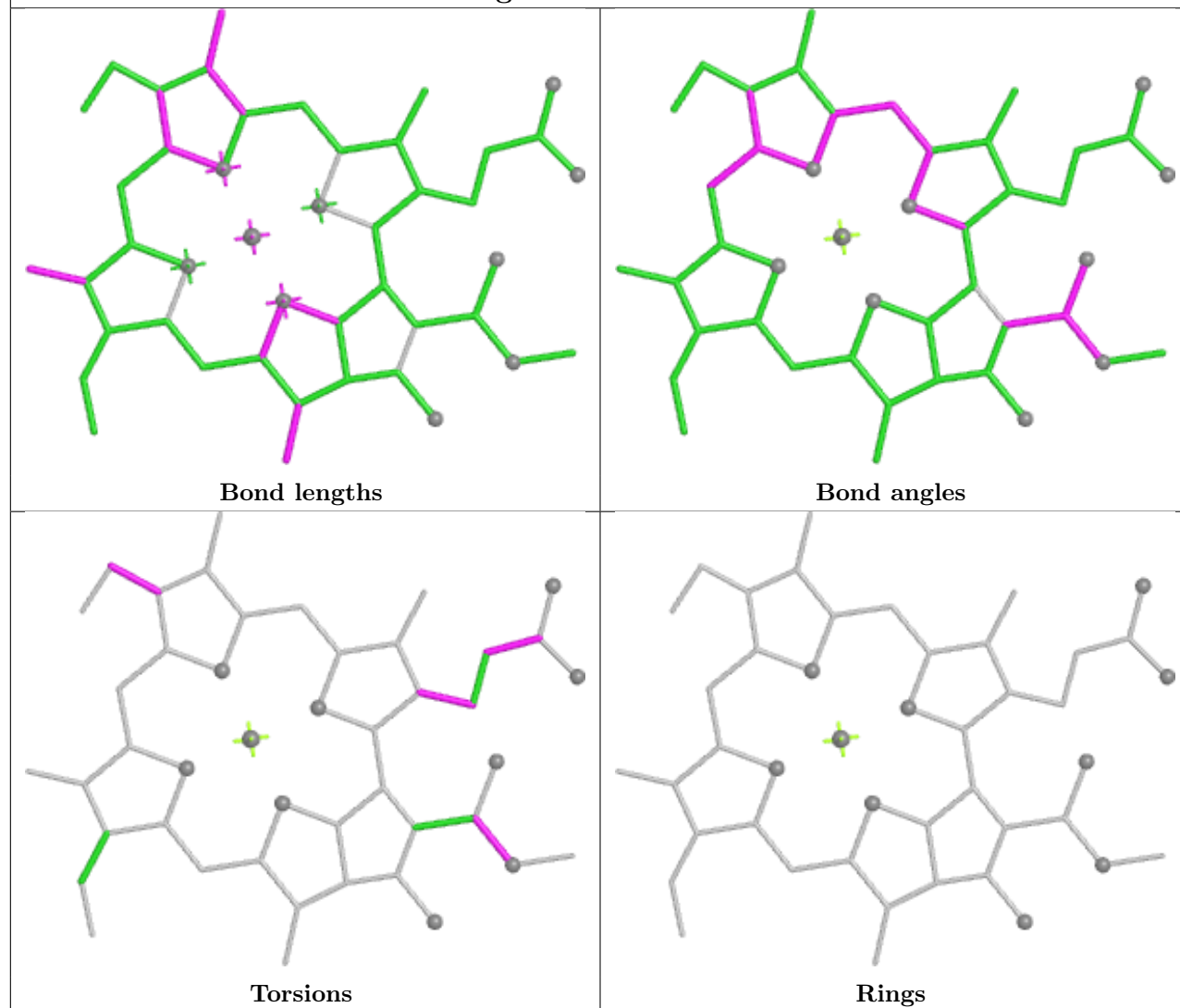
Ligand CLA G 613



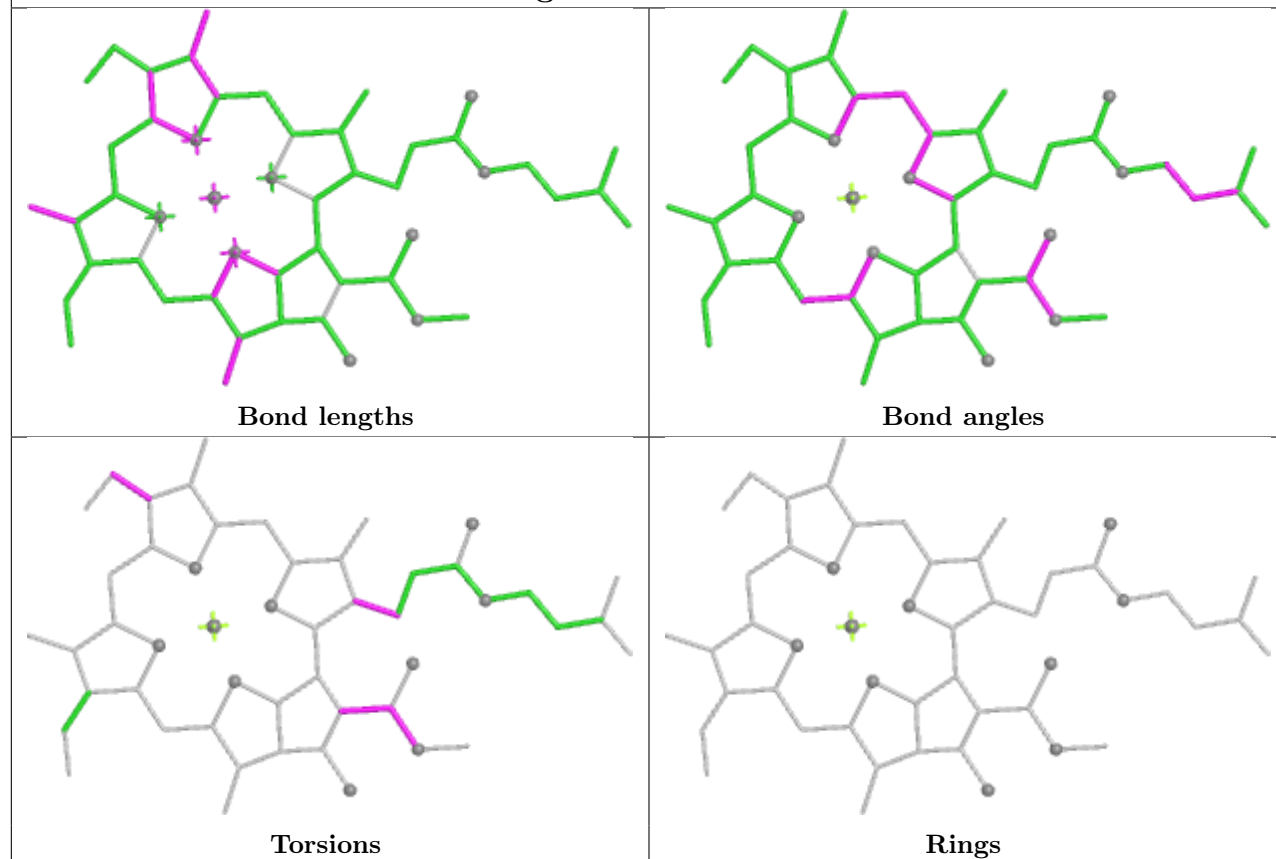
Ligand CLA Y 610



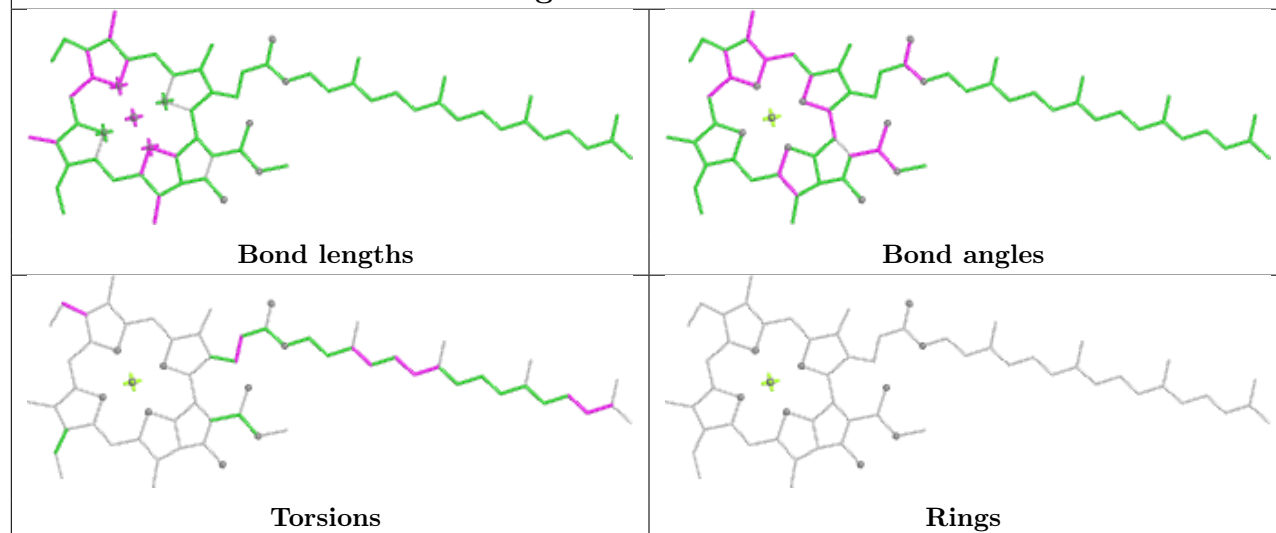
Ligand CLA 2 614

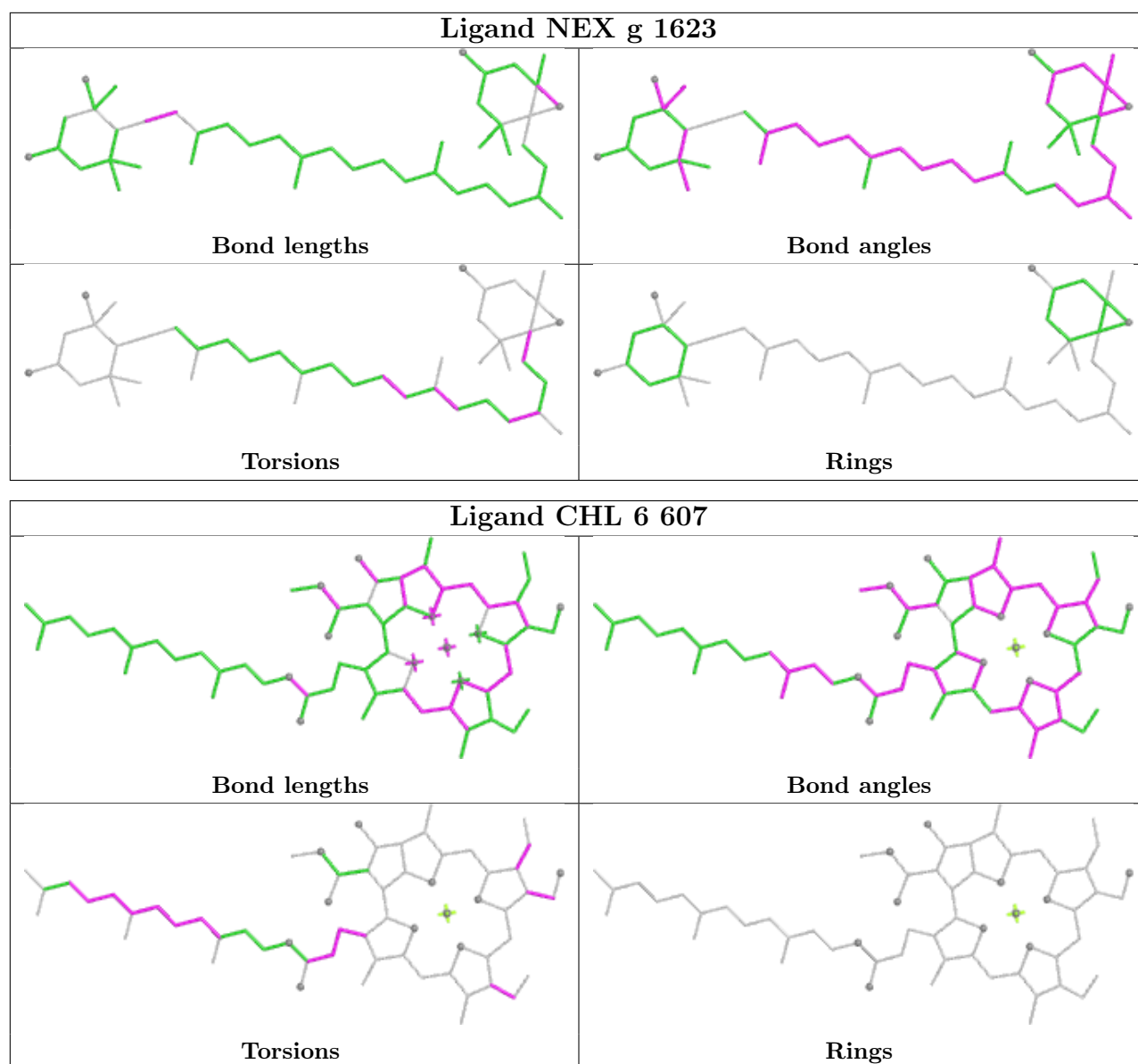


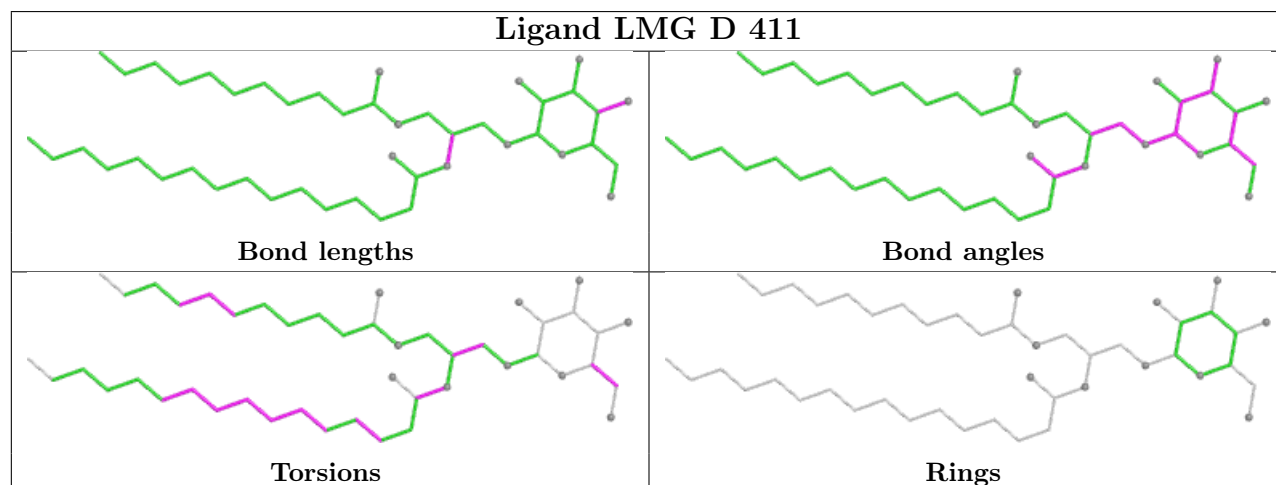
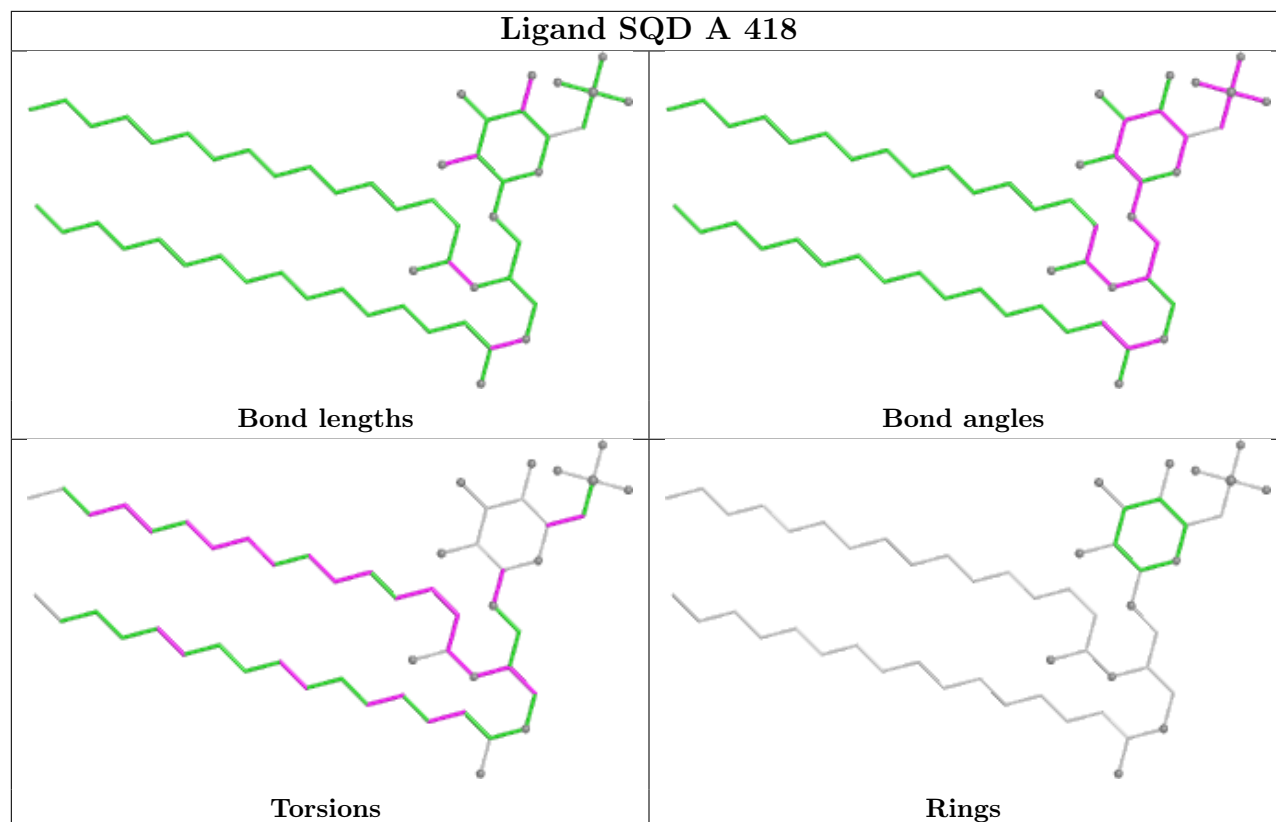
Ligand CLA a 407



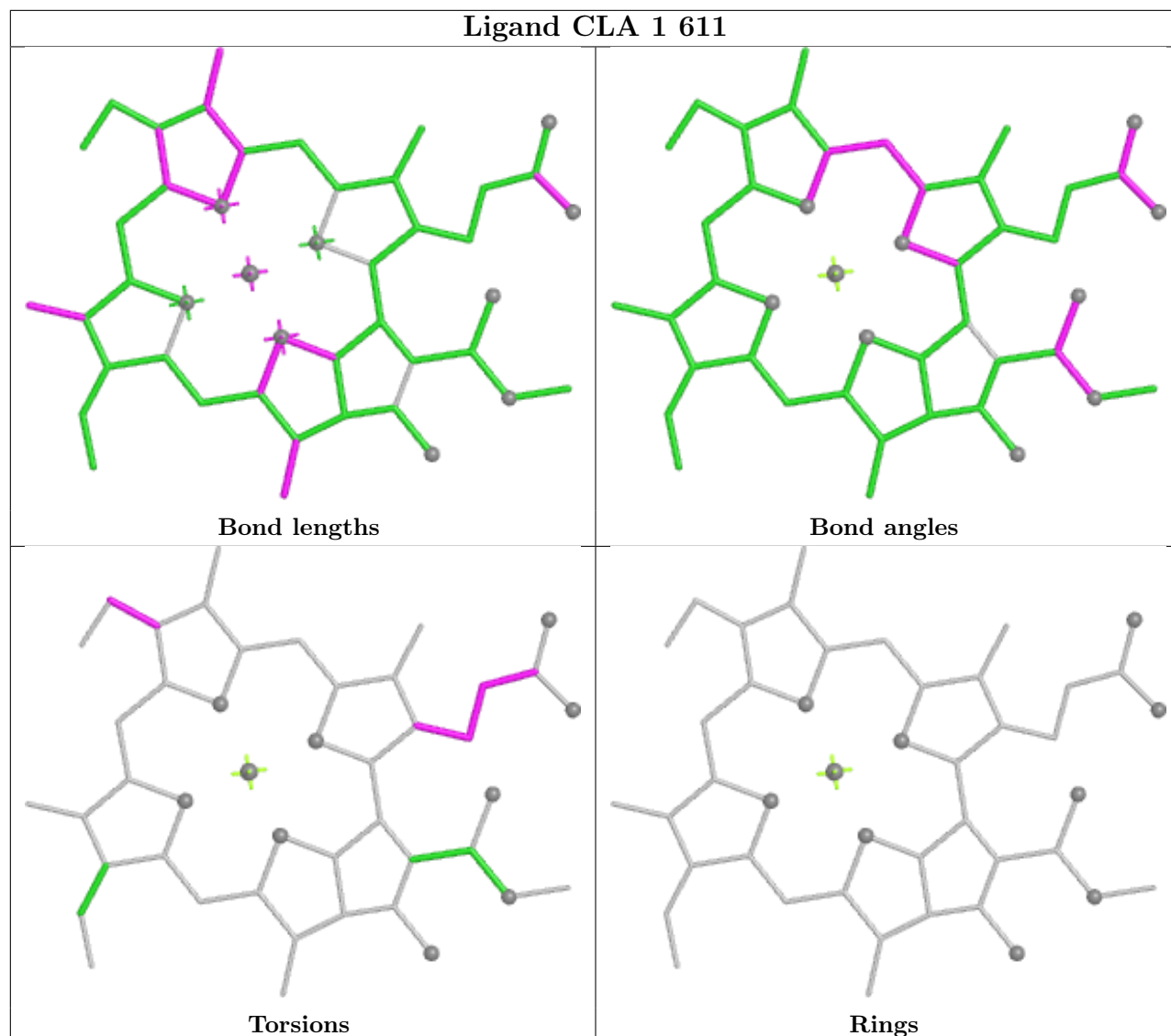
Ligand CLA b 604



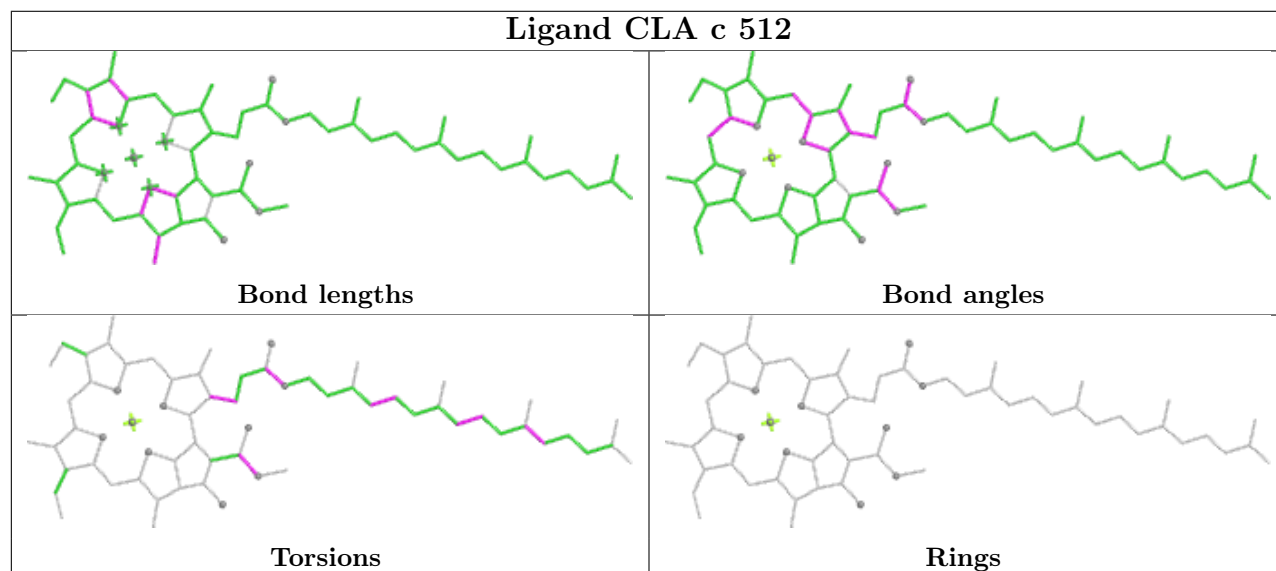




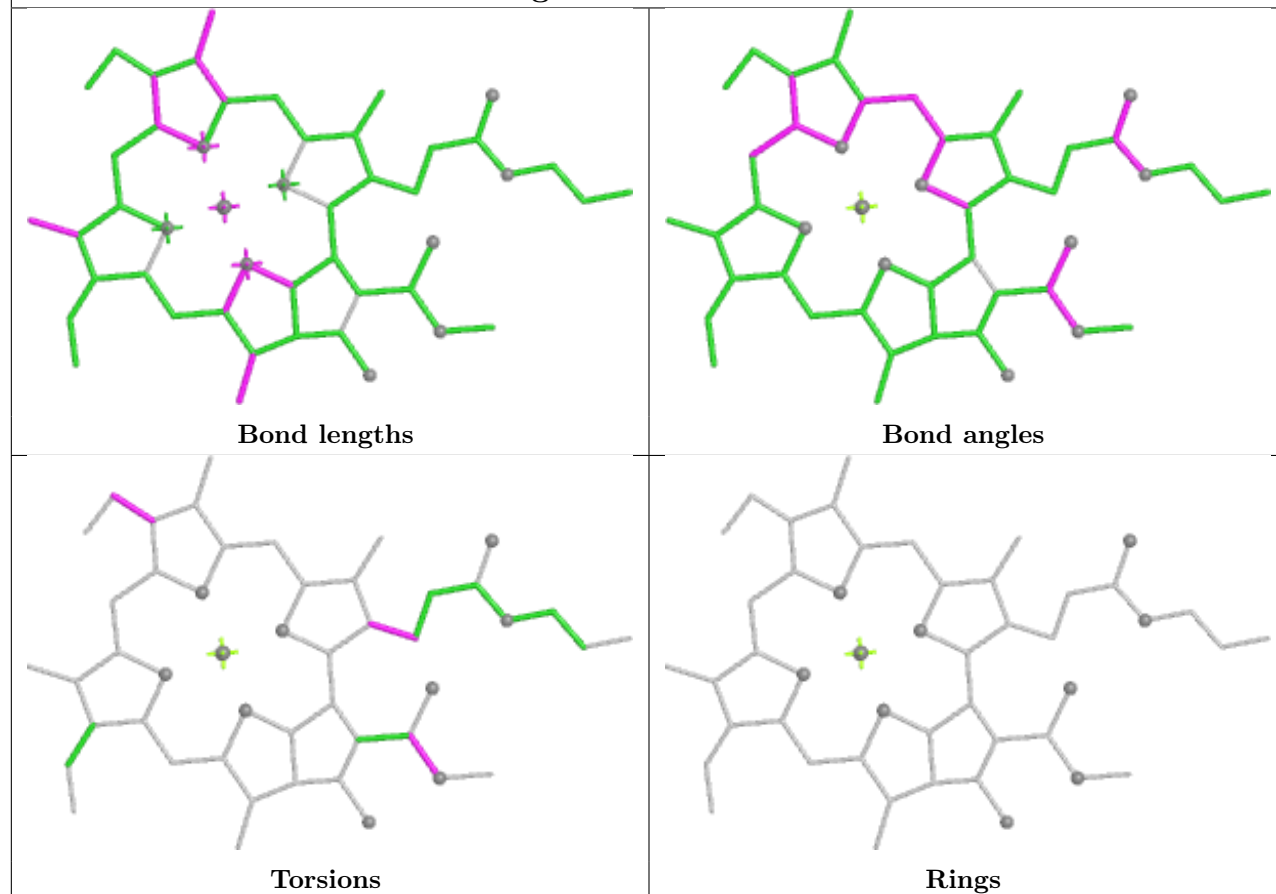
Ligand CLA 1 611



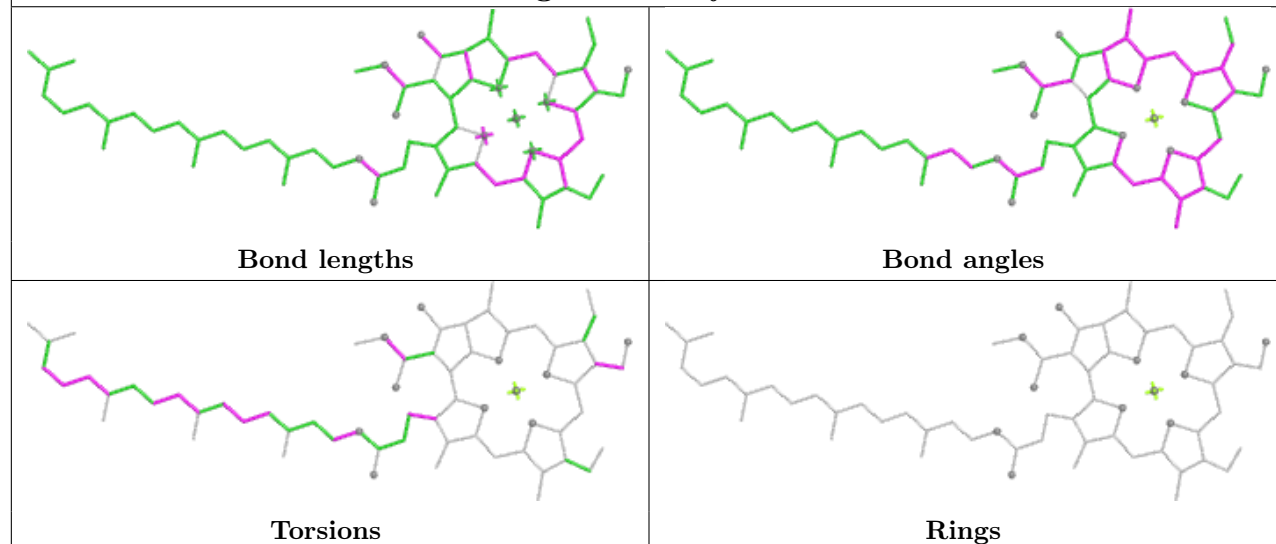
Ligand CLA c 512

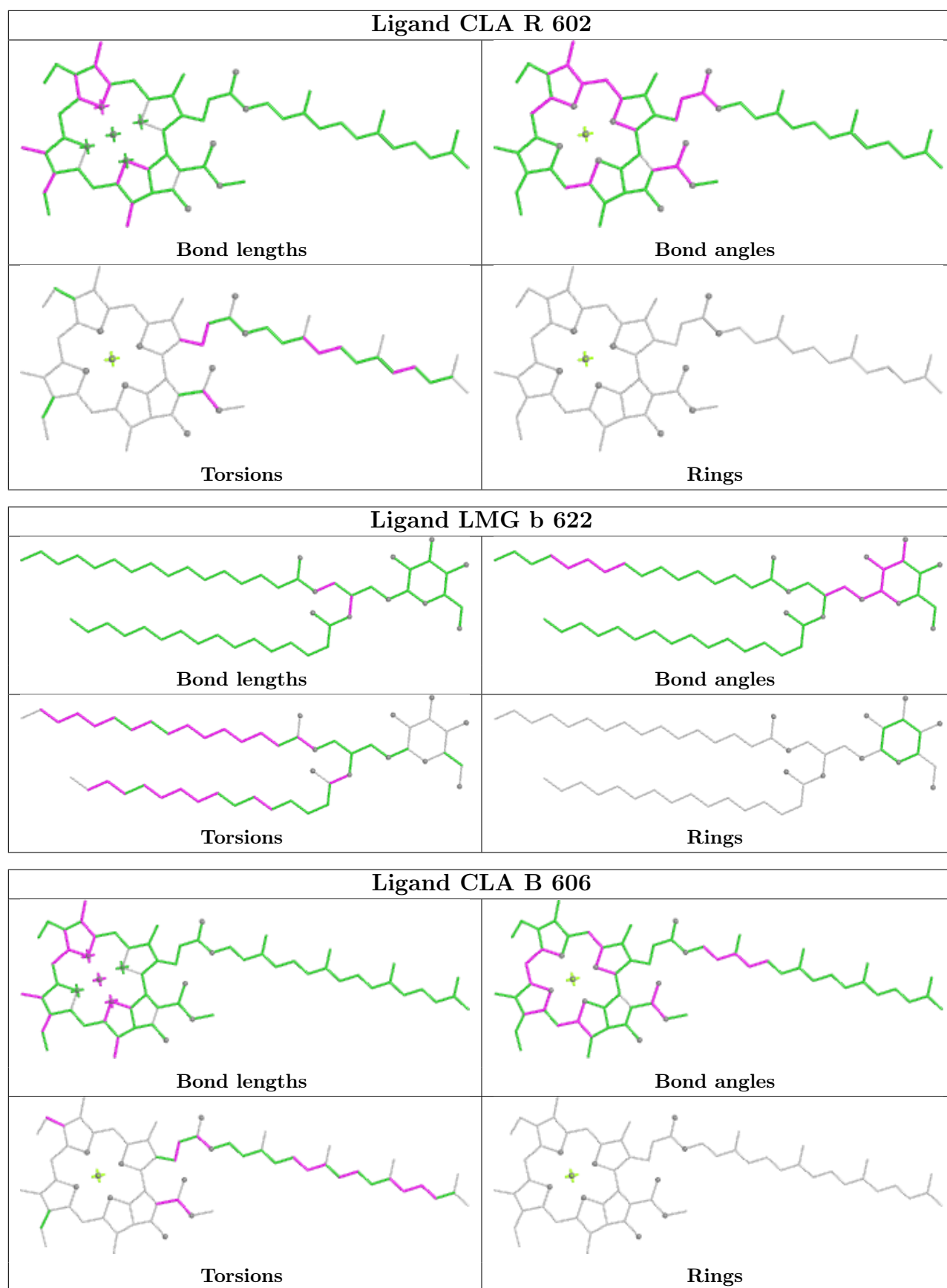


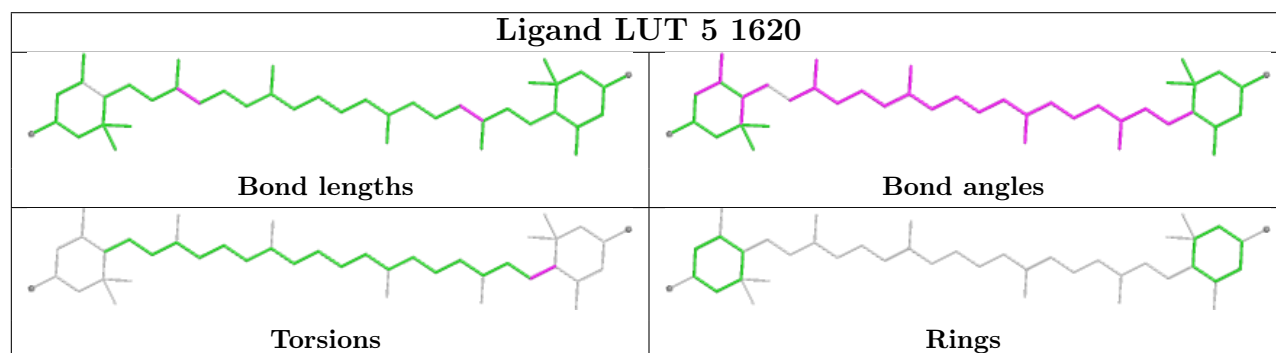
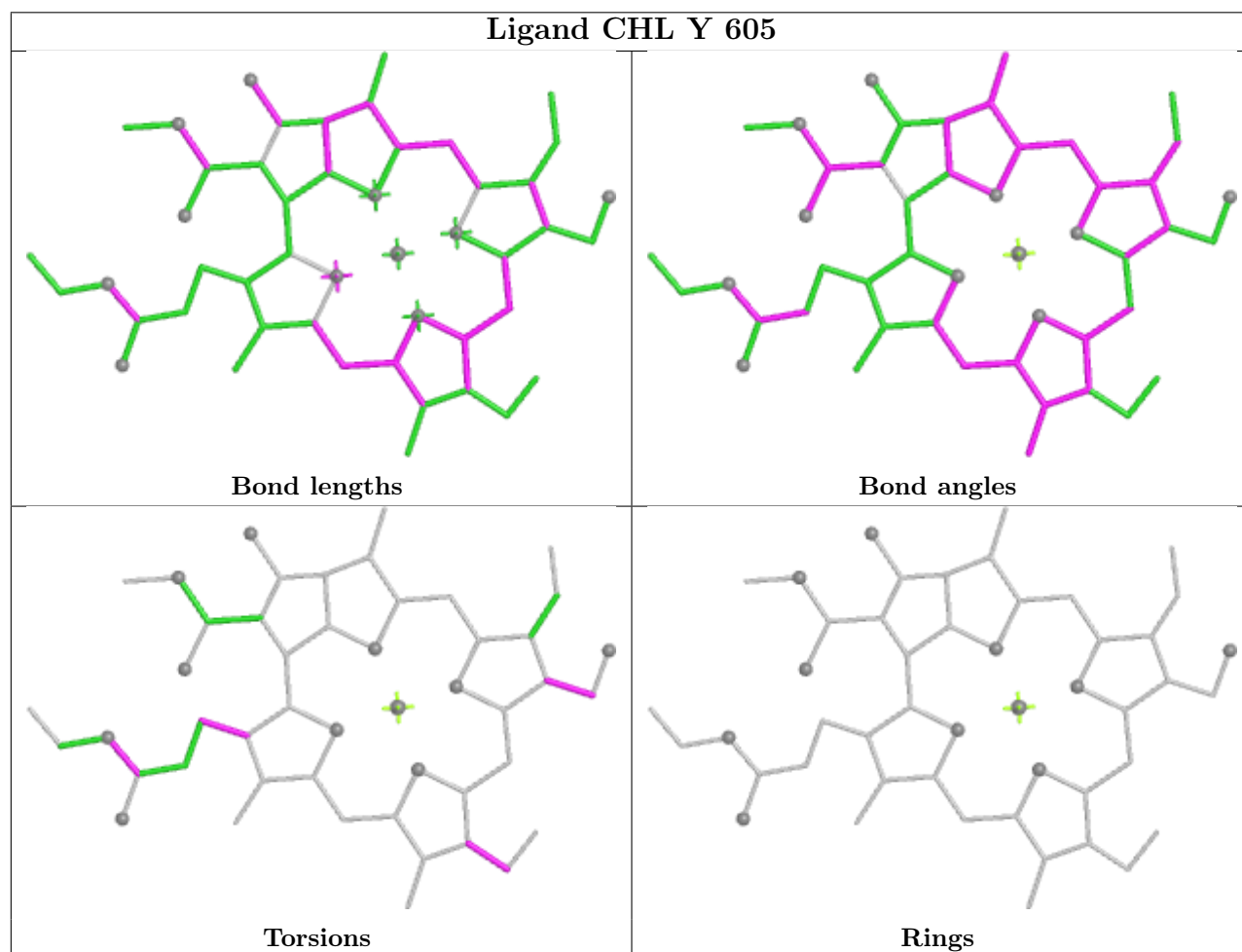
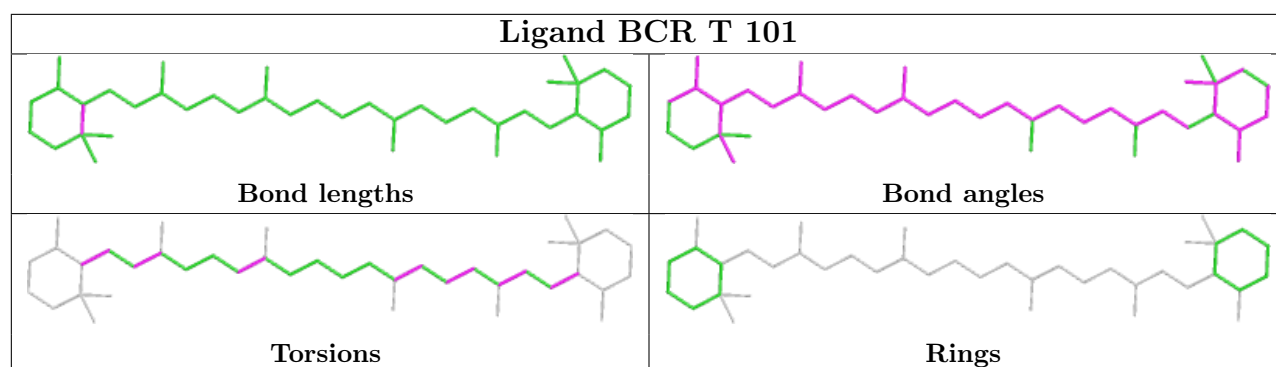
Ligand CLA Y 614



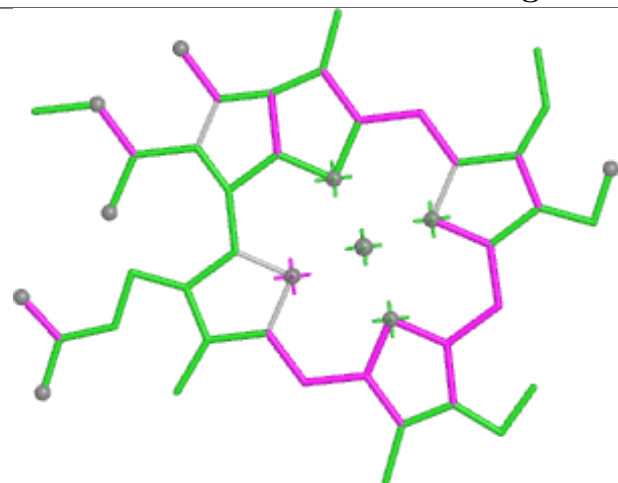
Ligand CHL y 608



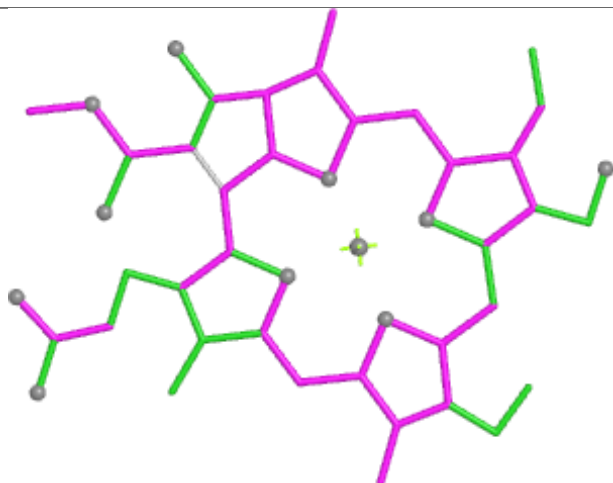




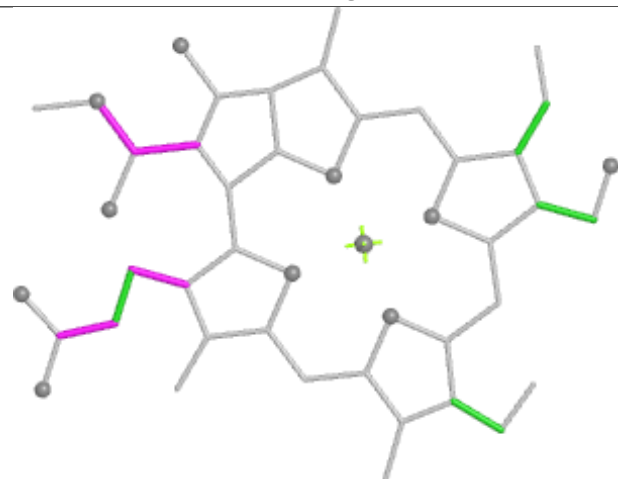
Ligand CHL 6 601



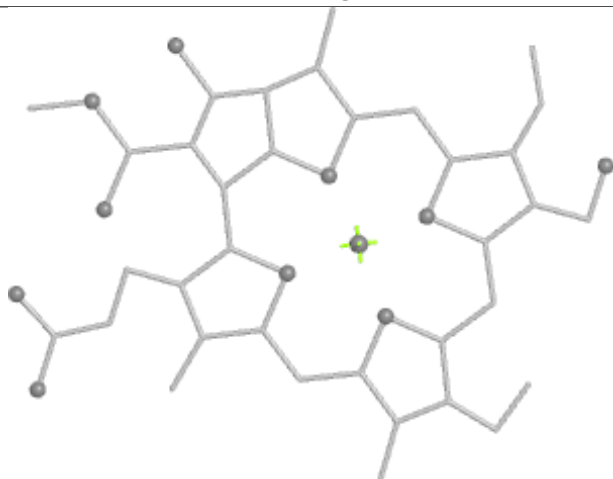
Bond lengths



Bond angles

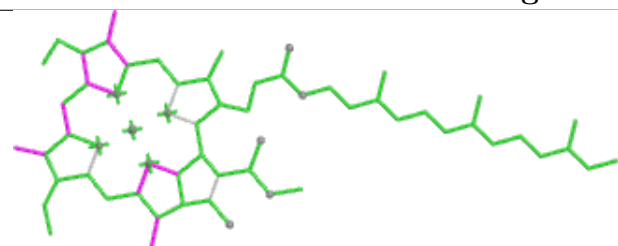


Torsions

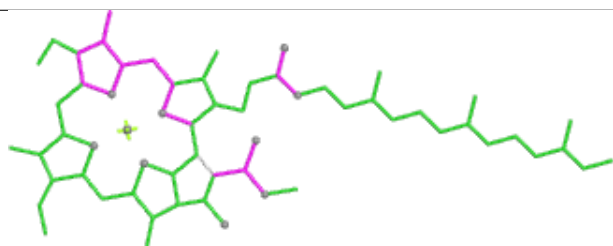


Rings

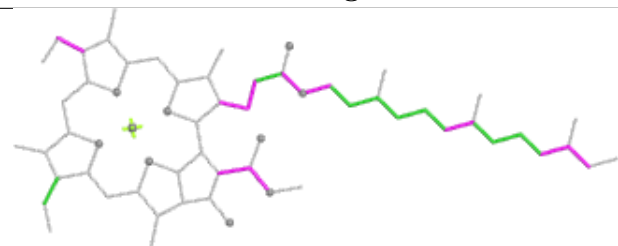
Ligand CLA S 602



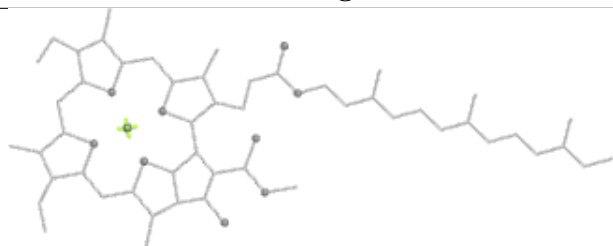
Bond lengths



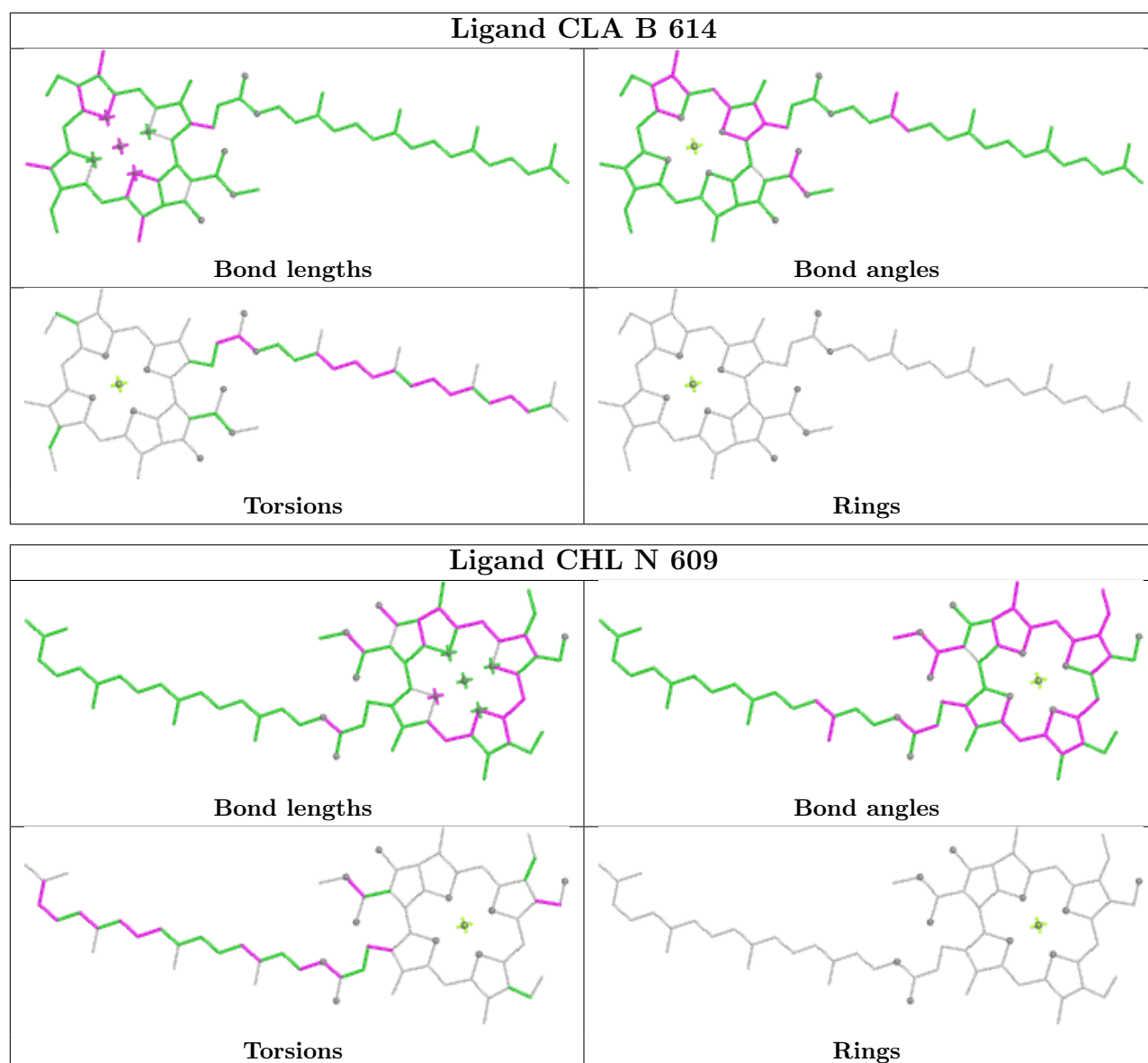
Bond angles

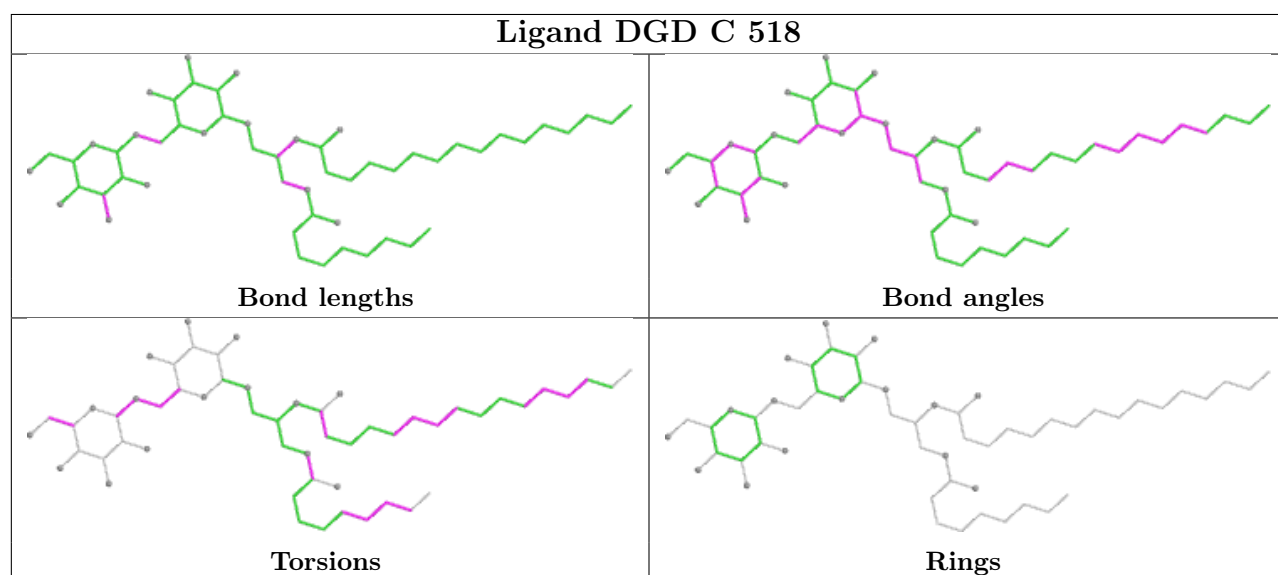
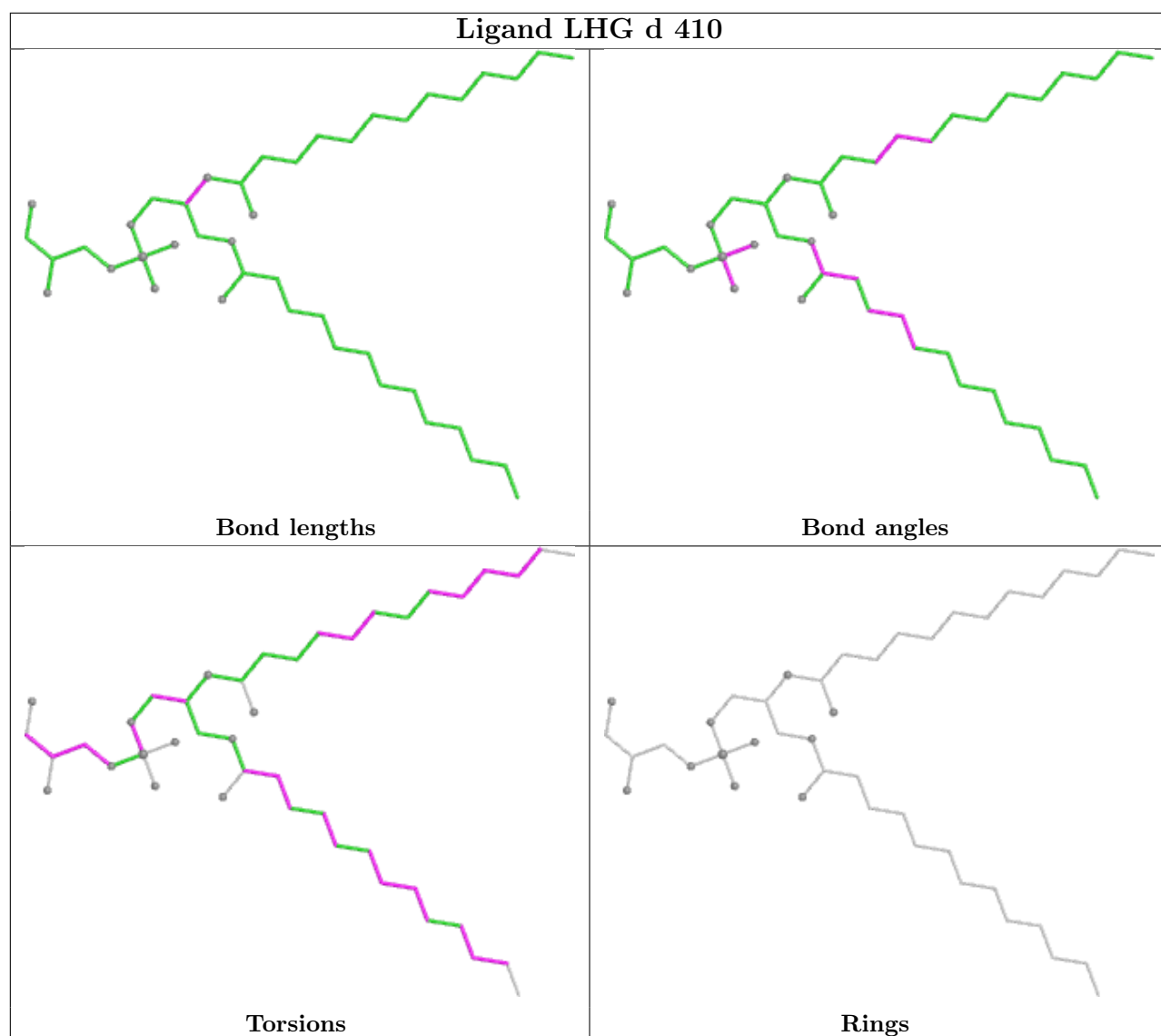


Torsions

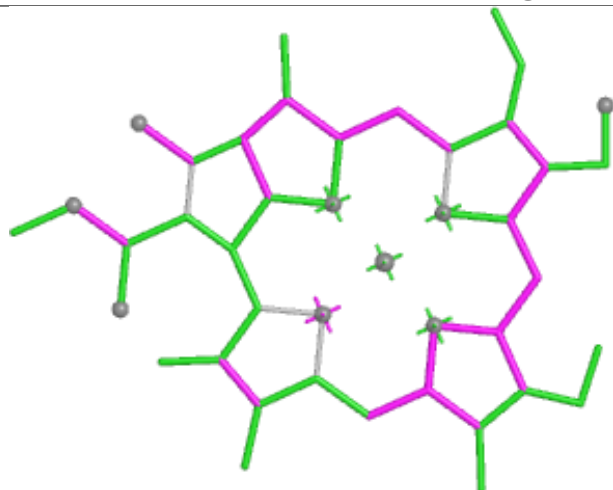


Rings

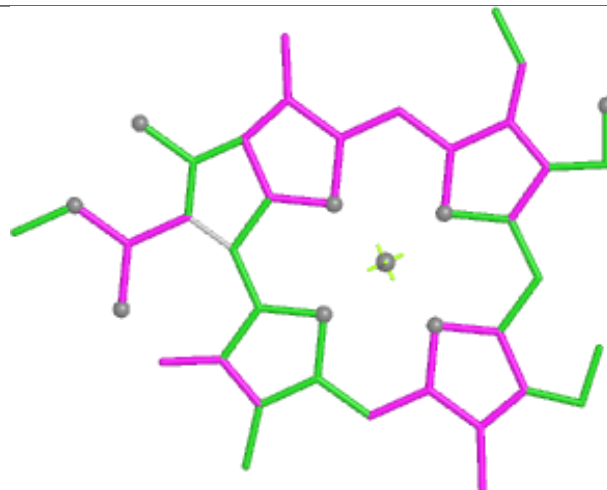




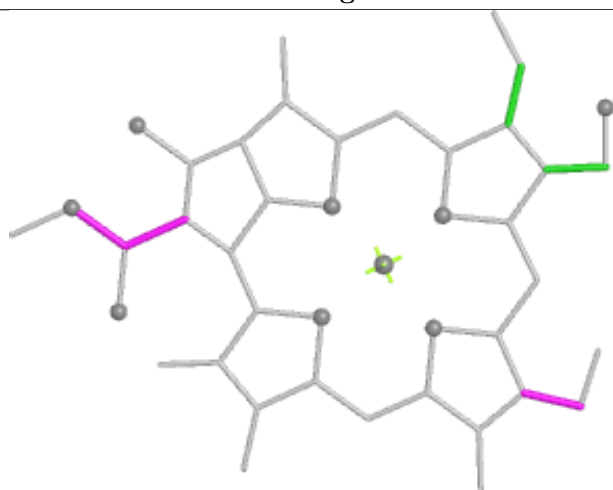
Ligand CHL r 614



Bond lengths



Bond angles

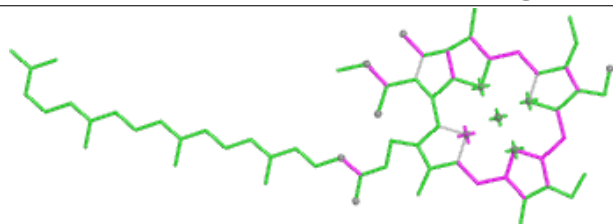


Torsions

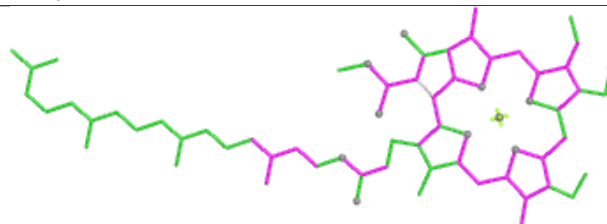


Rings

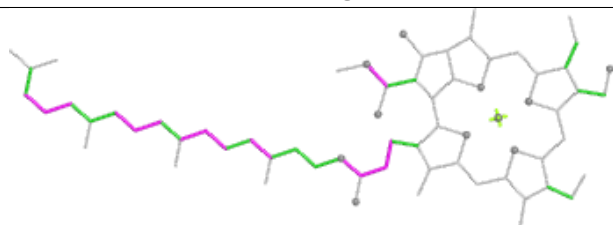
Ligand CHL y 601



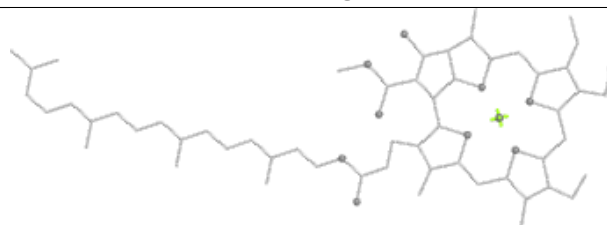
Bond lengths



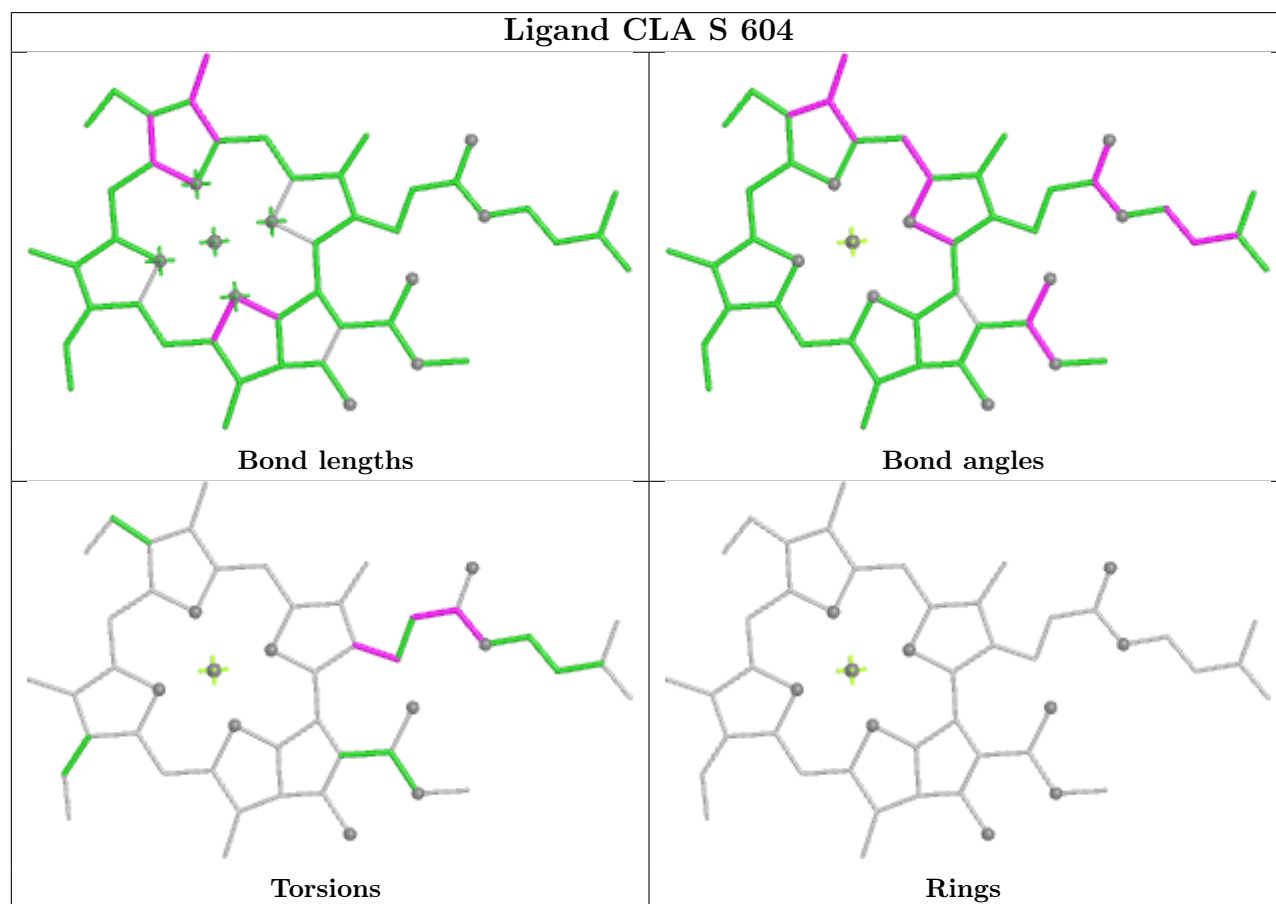
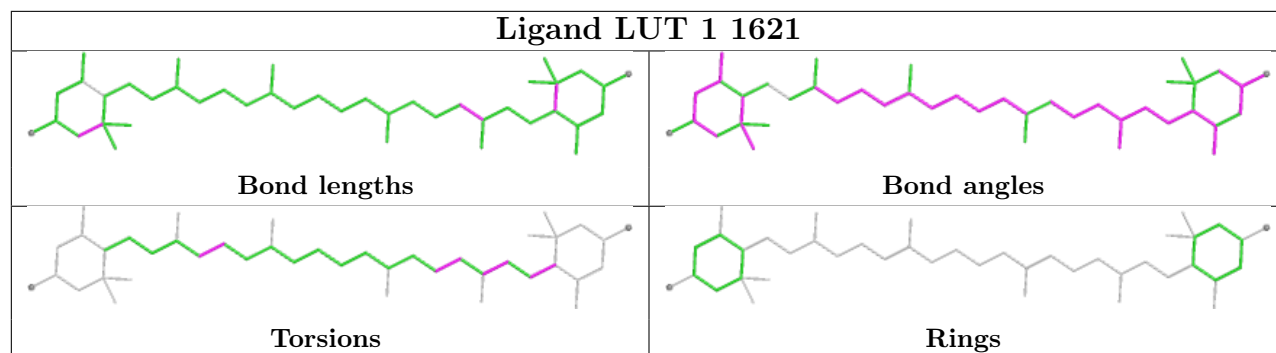
Bond angles

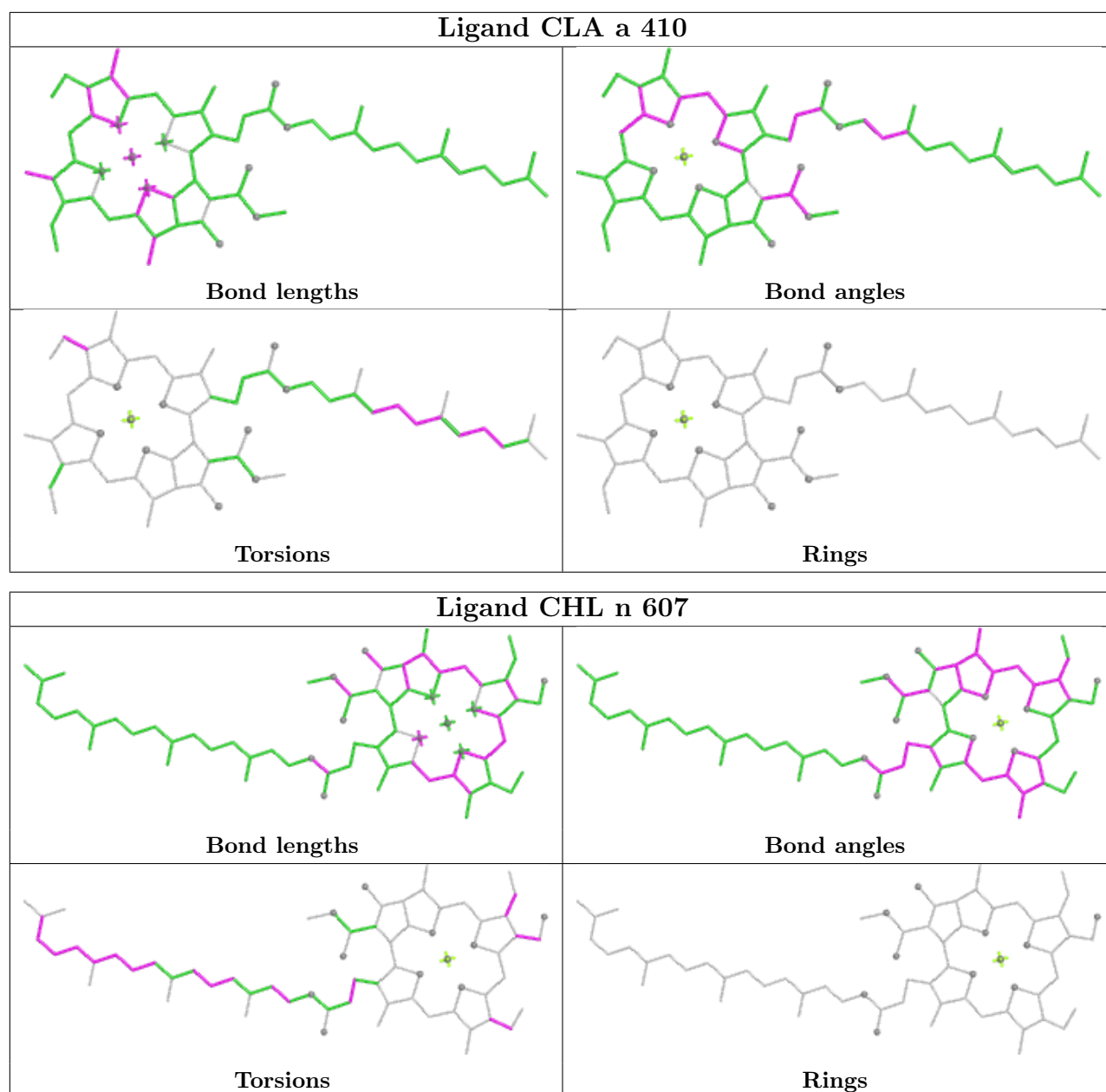


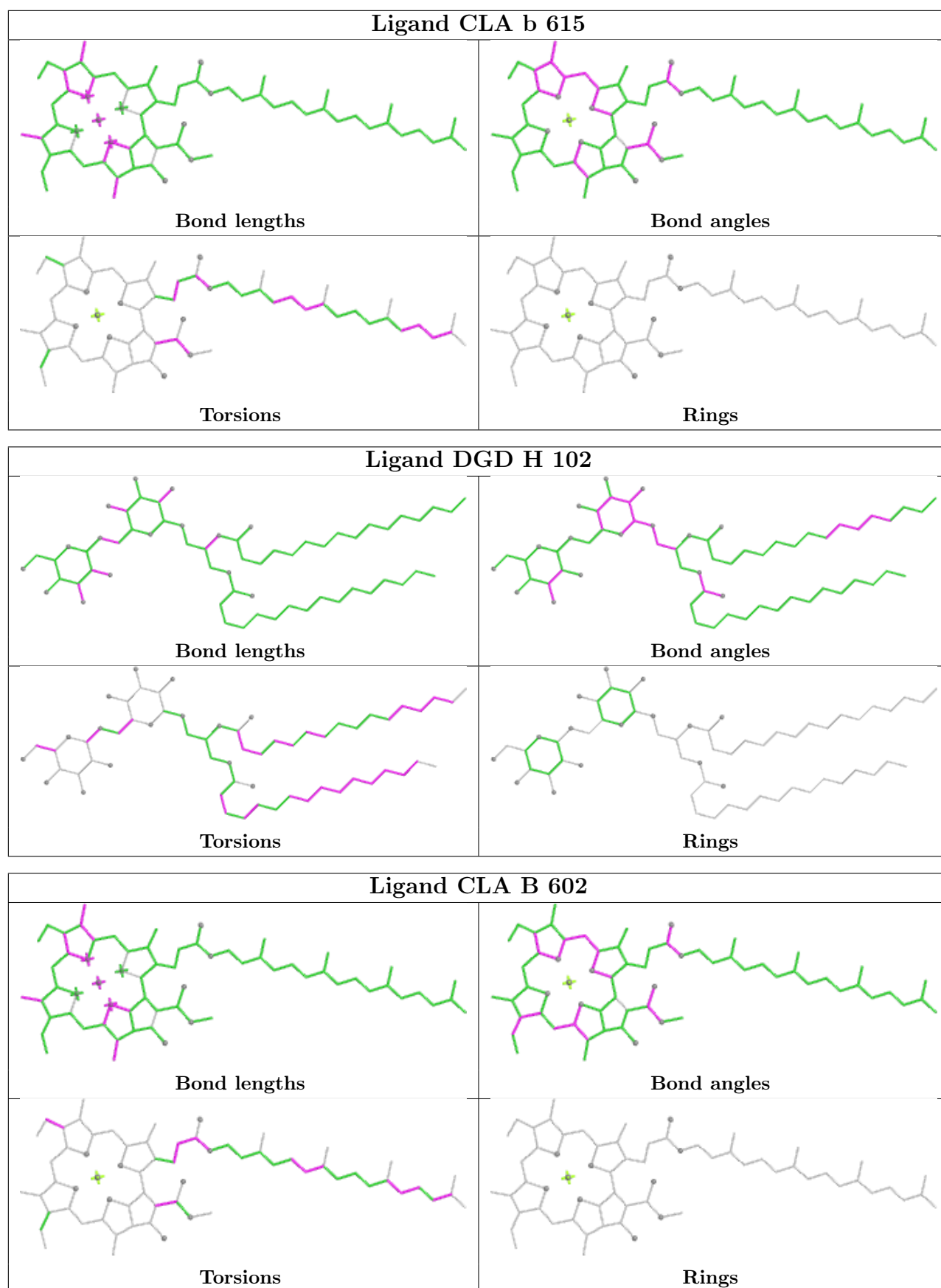
Torsions

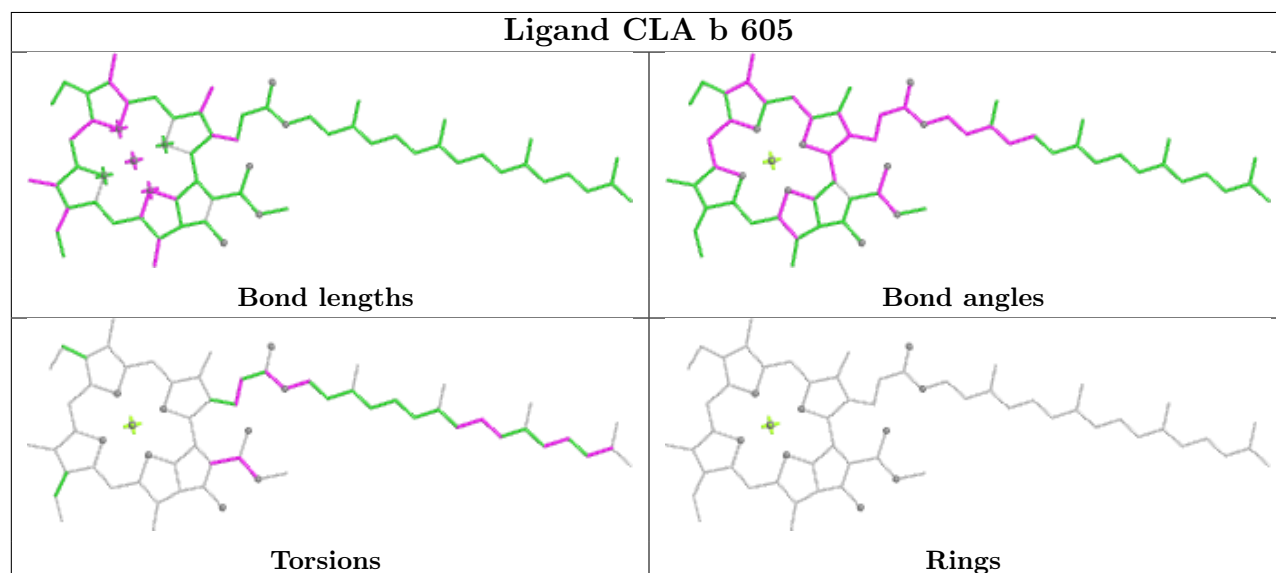
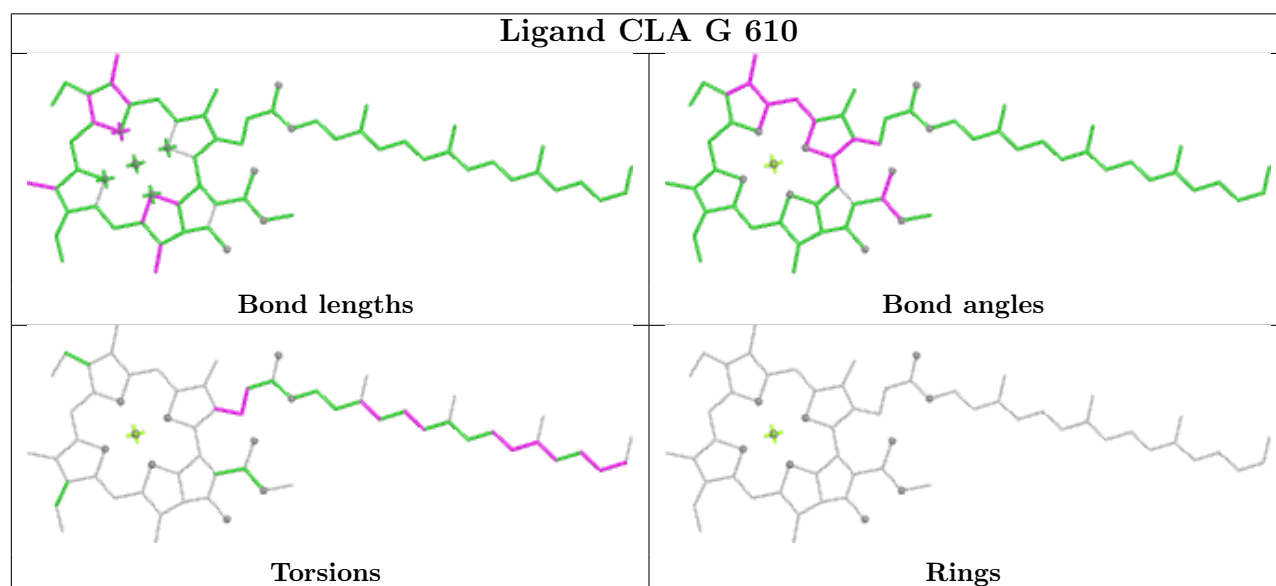
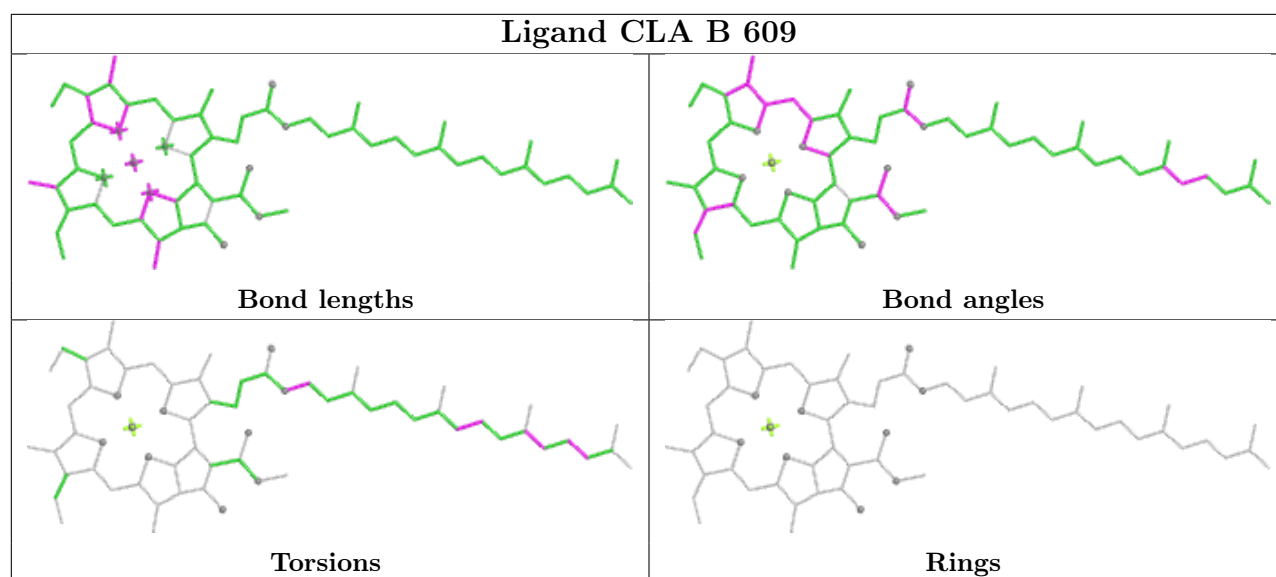


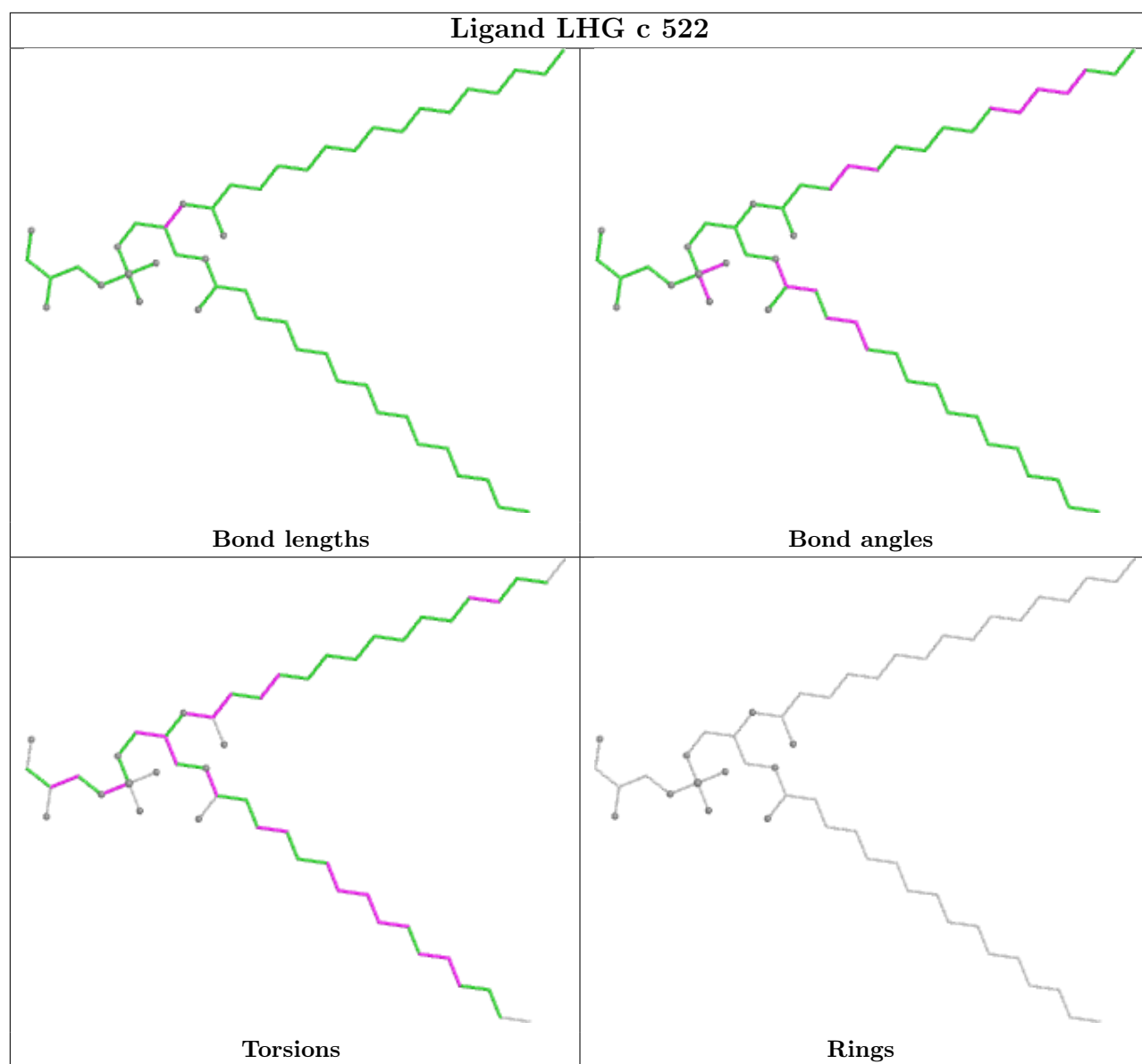
Rings



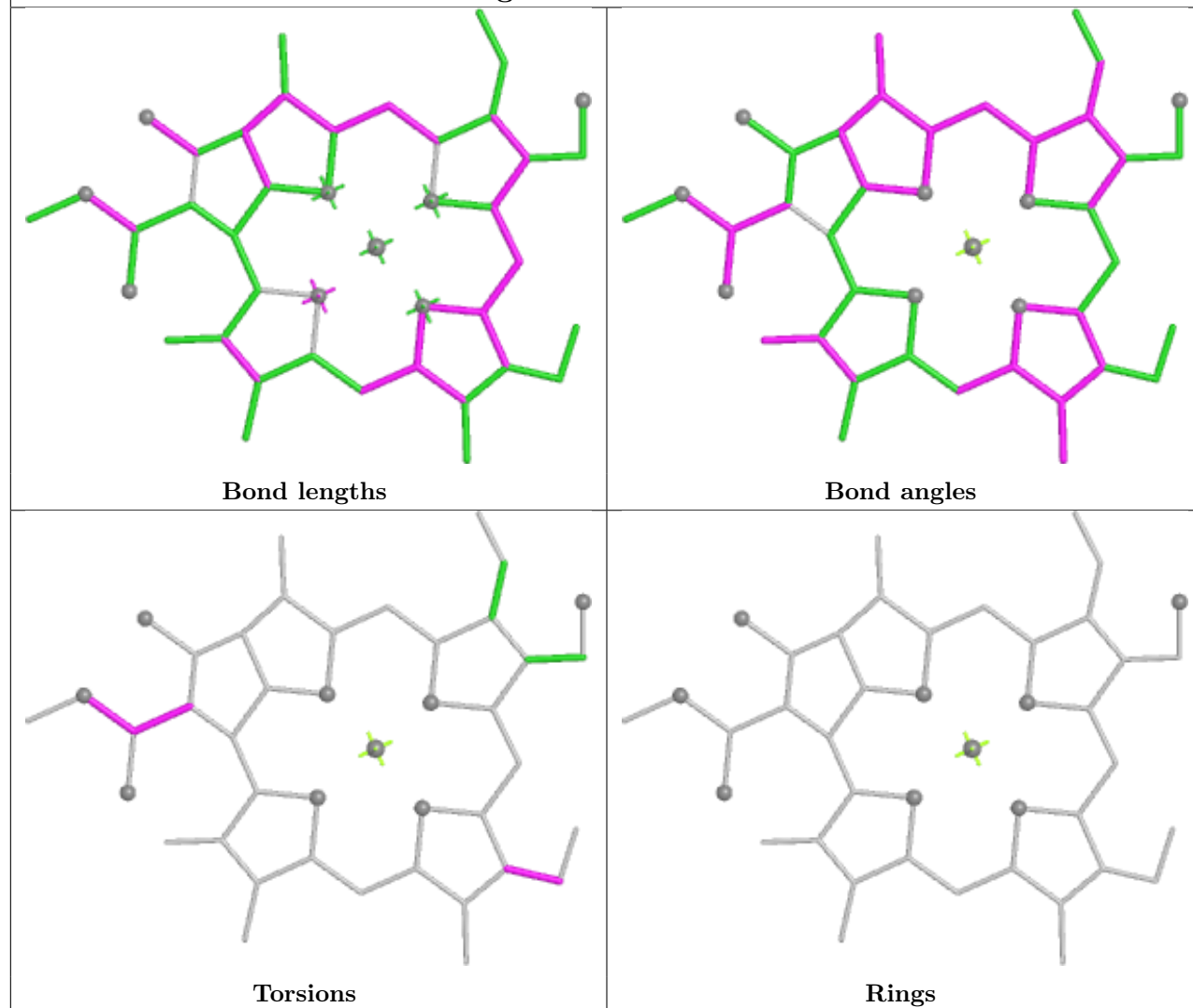




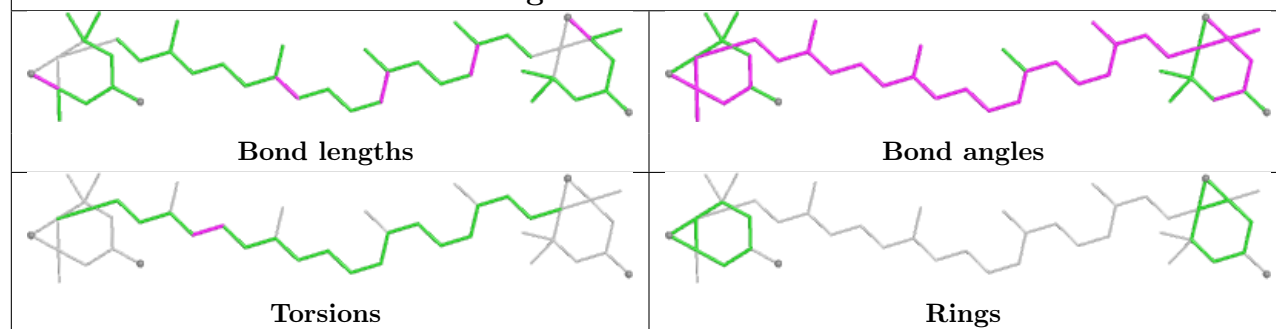


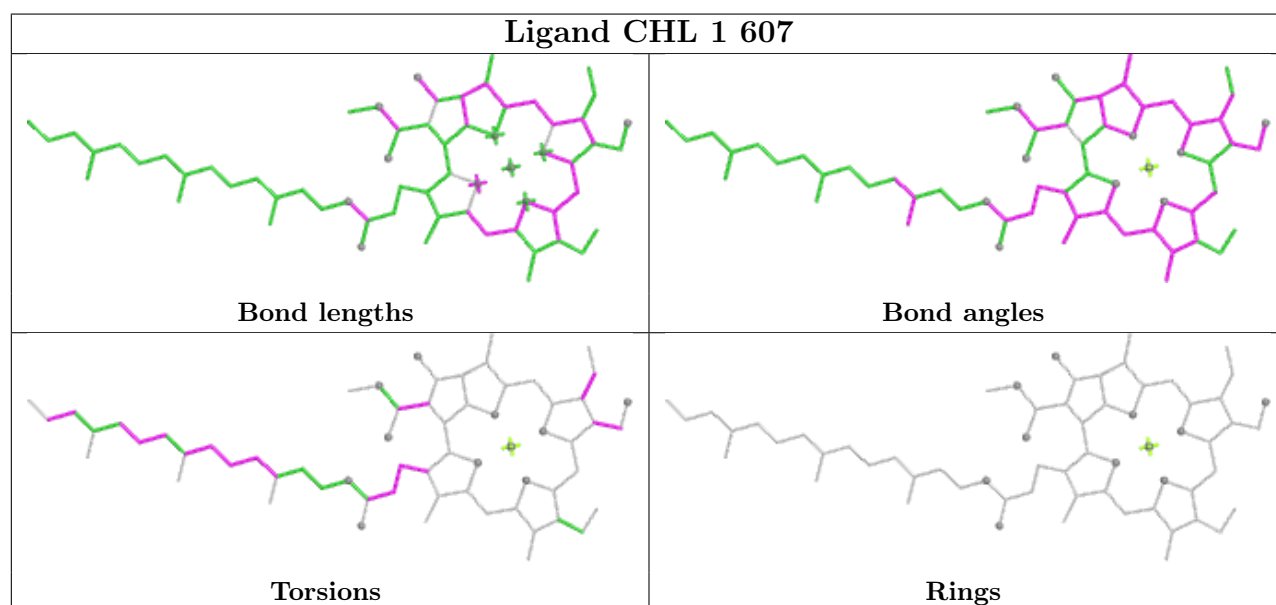
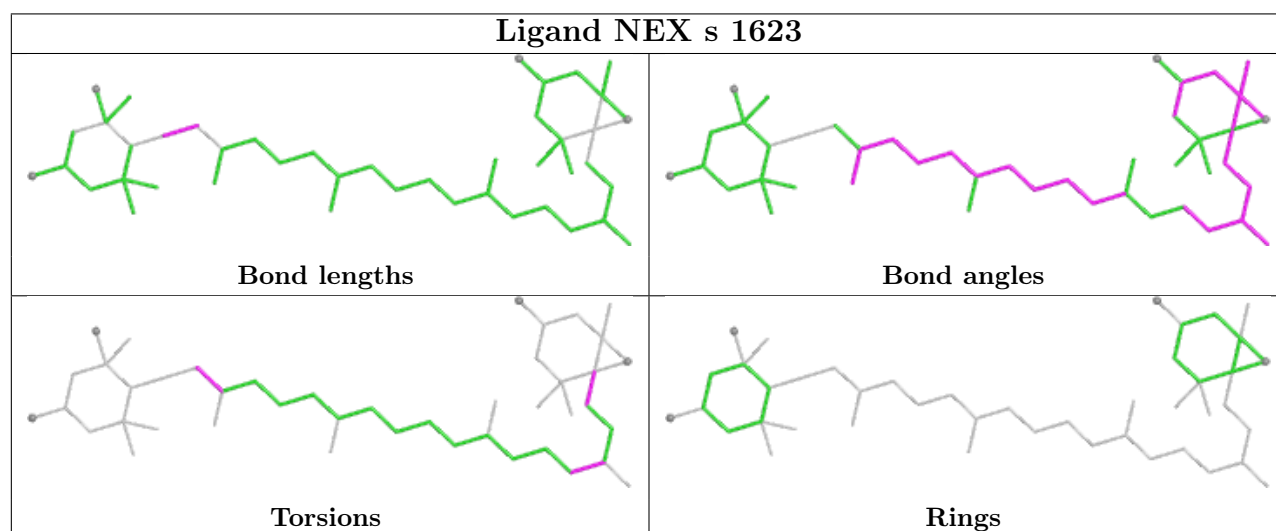
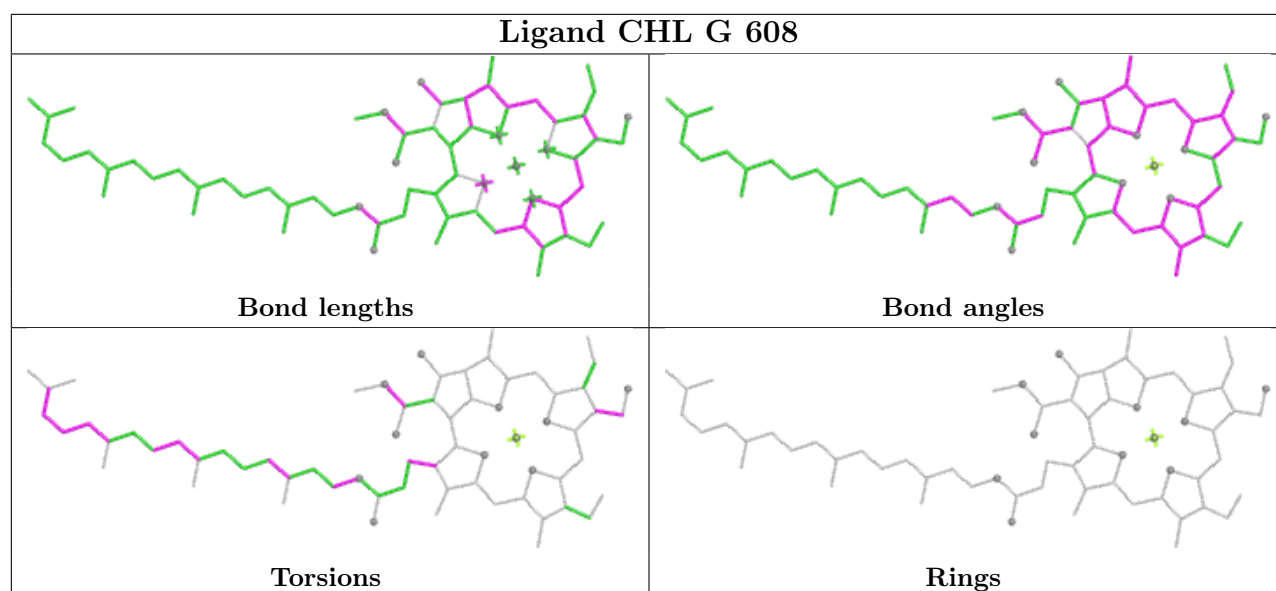


Ligand CHL R 614

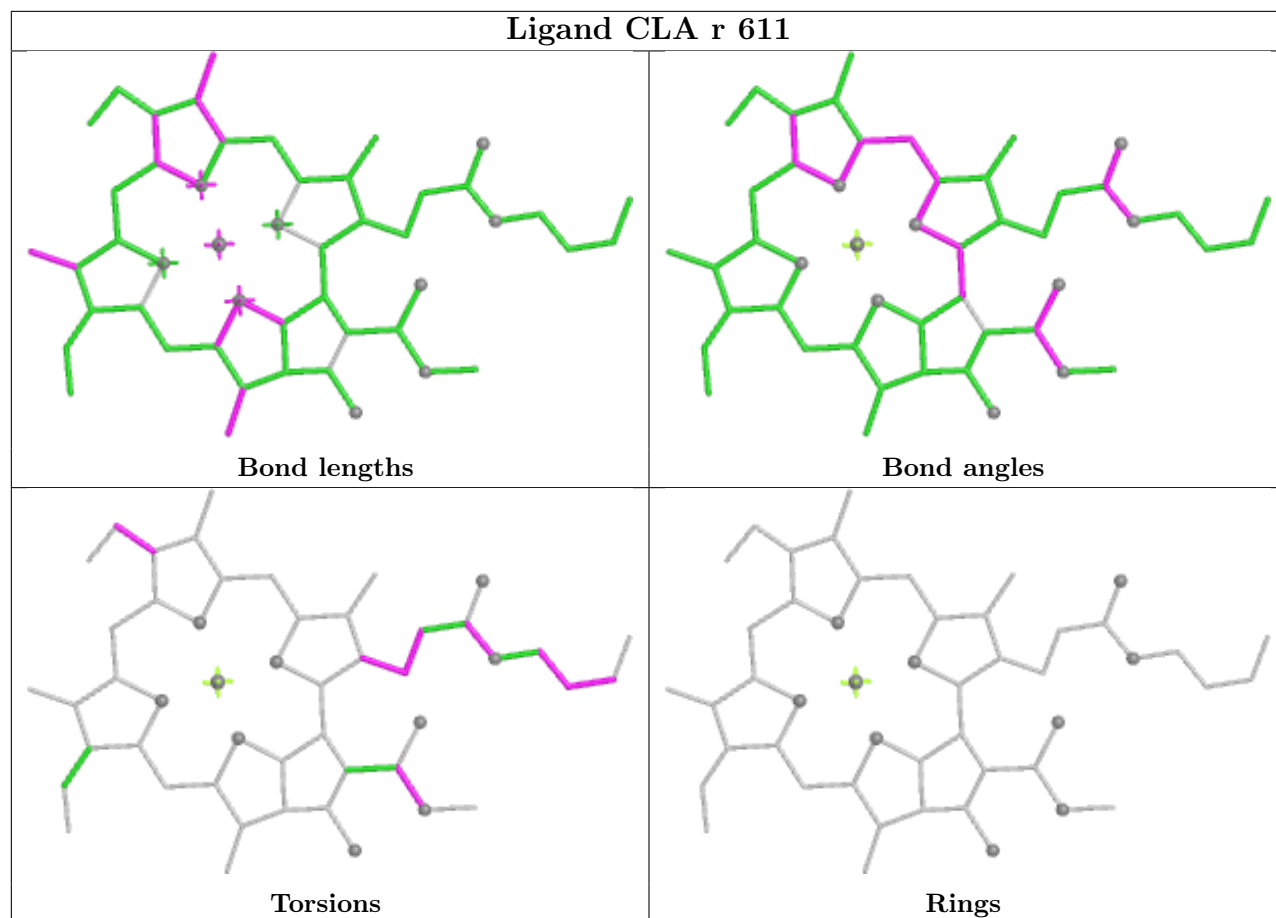


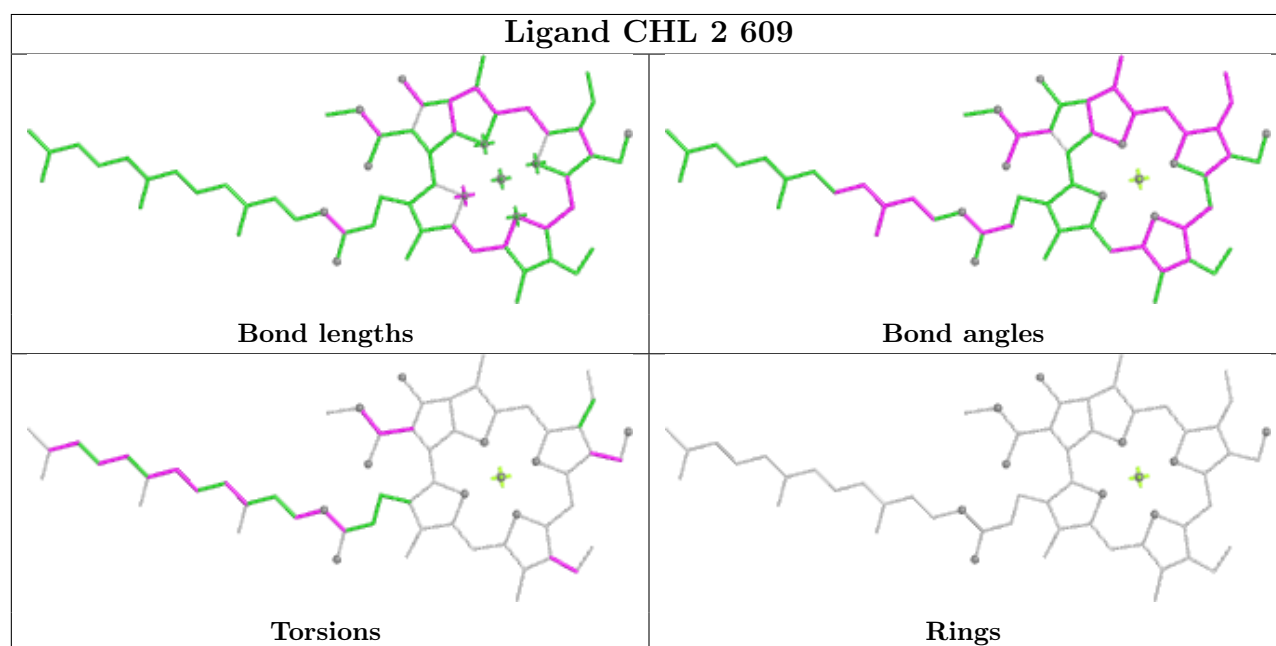
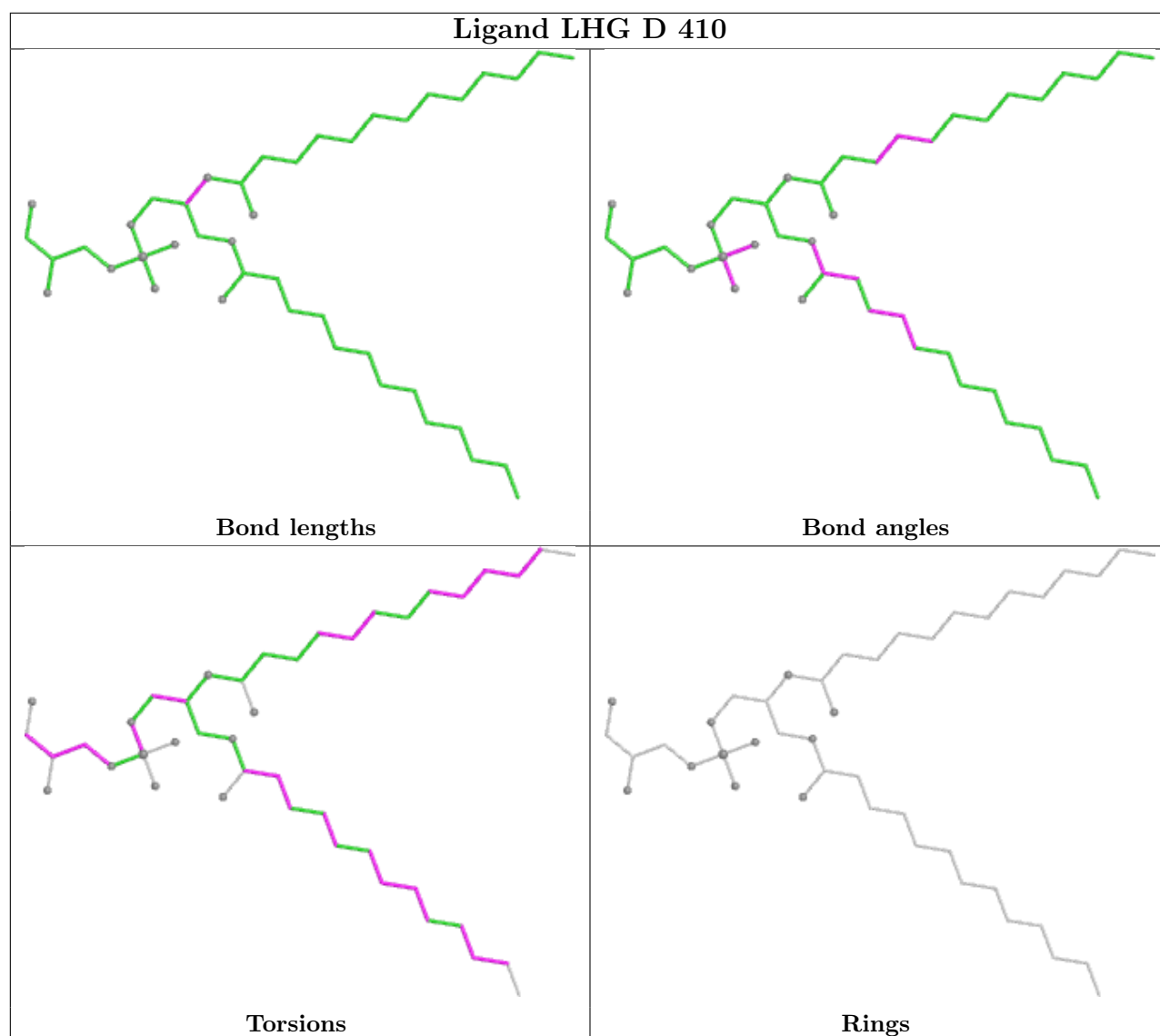
Ligand XAT 3 1622

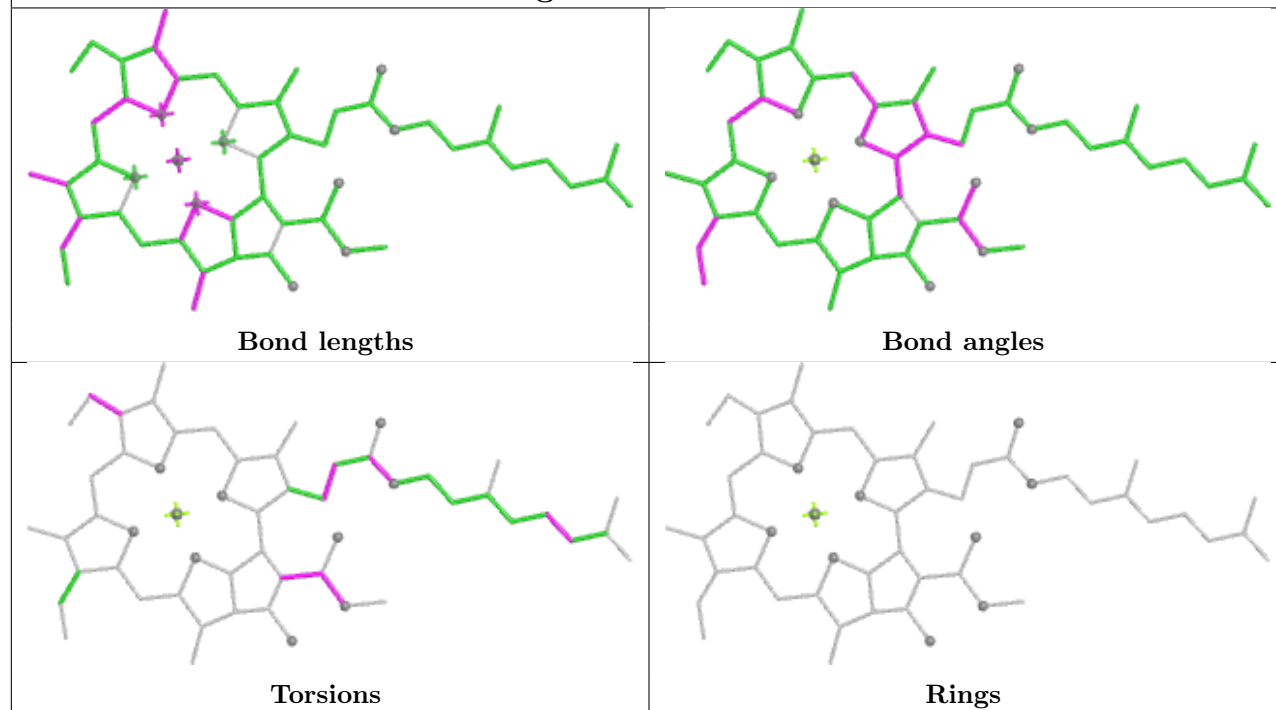
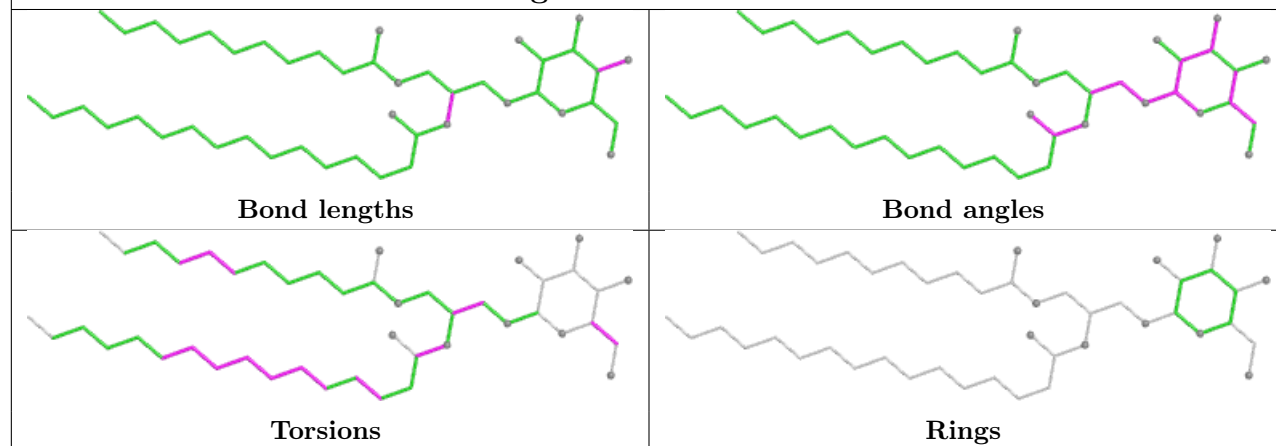


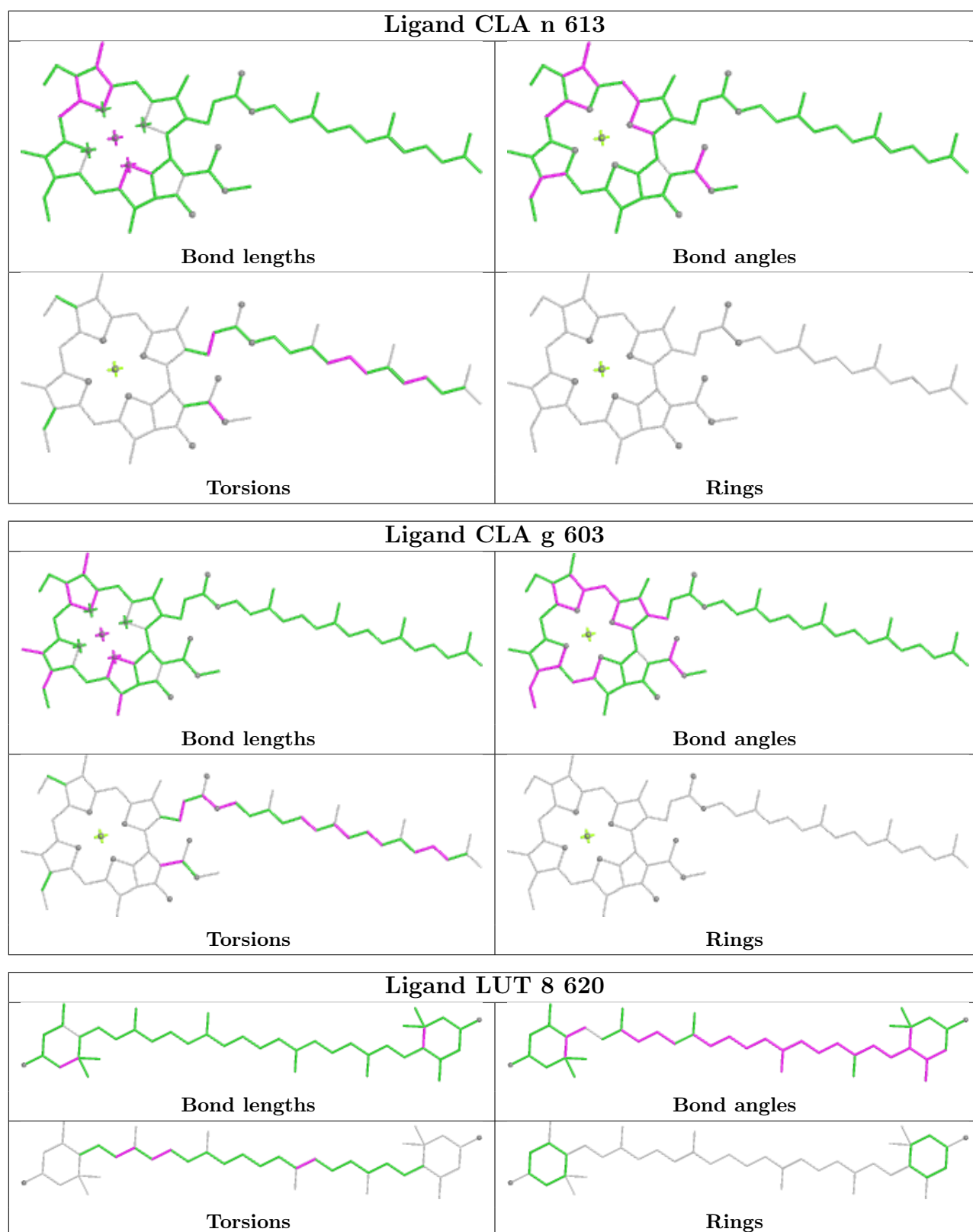


Ligand CLA r 611

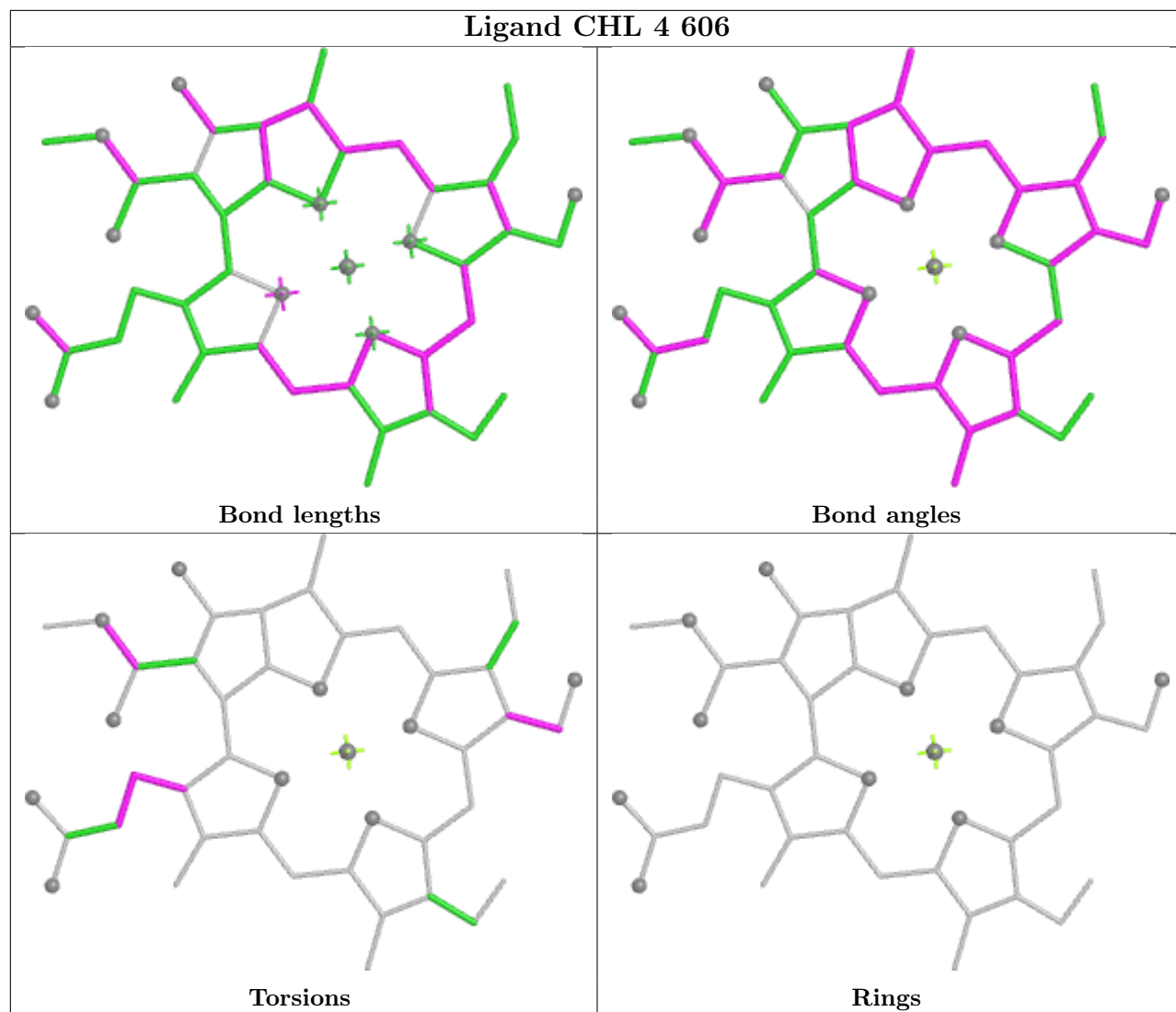


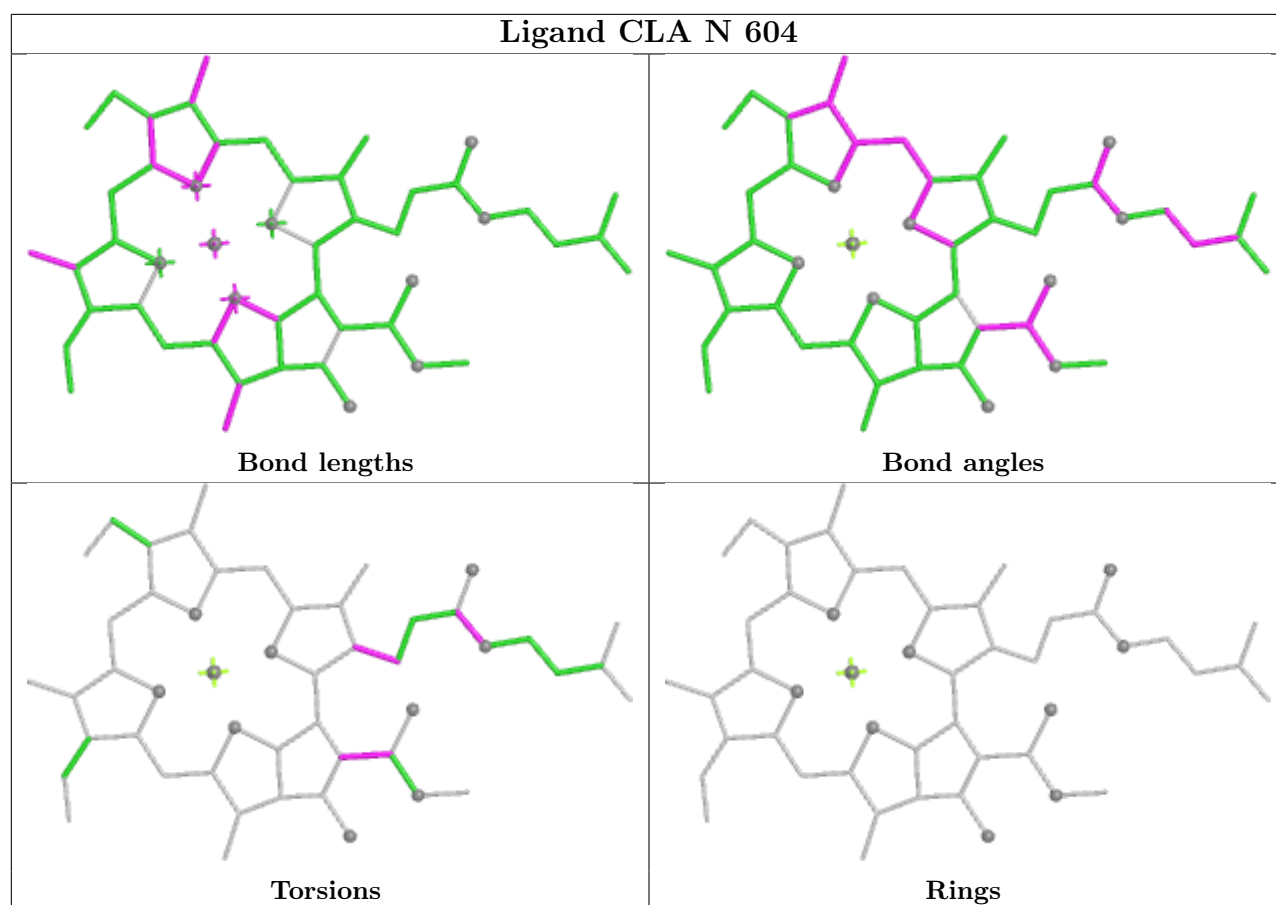


Ligand CLA 7 603**Ligand LMG d 411**

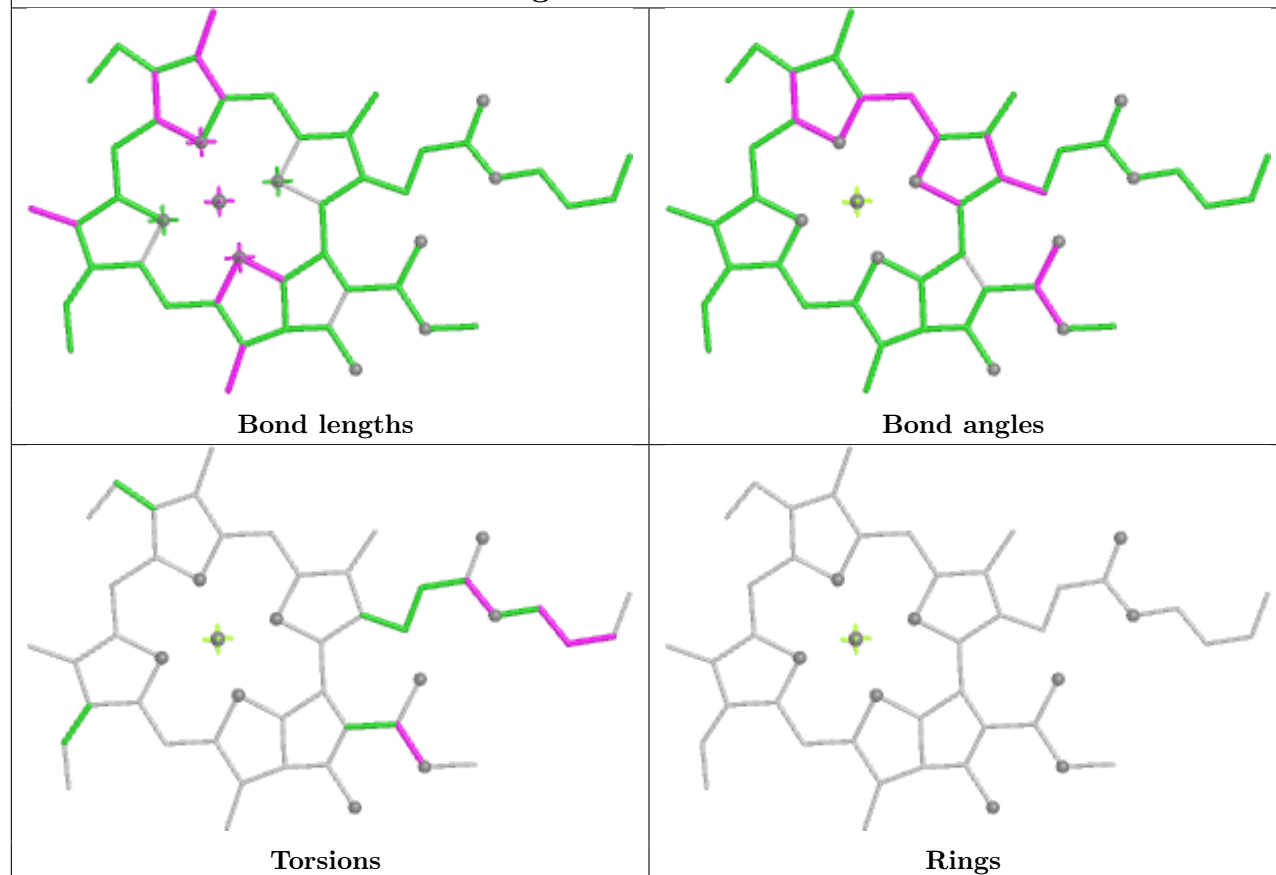


Ligand CHL 4 606

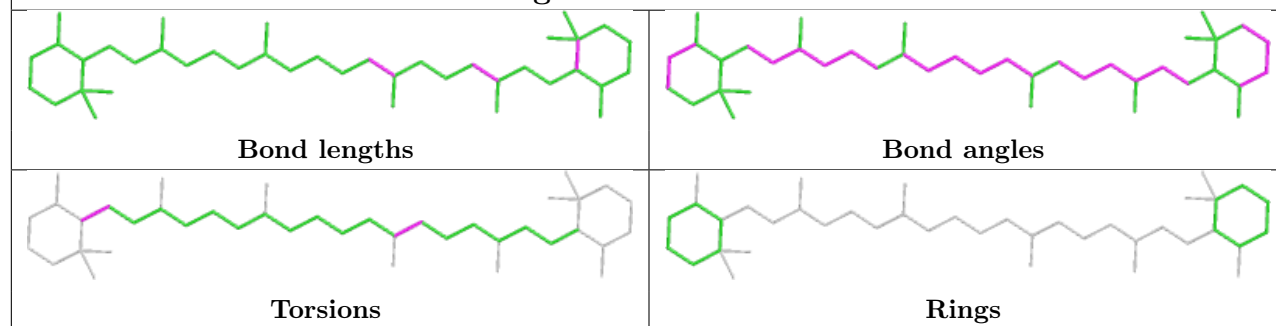


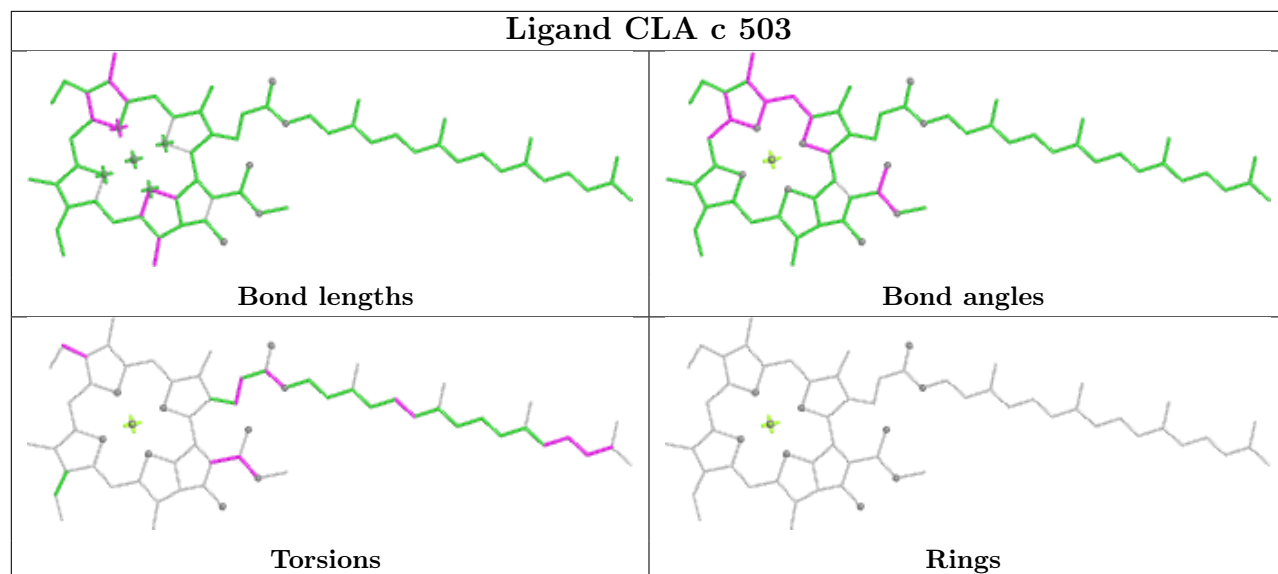
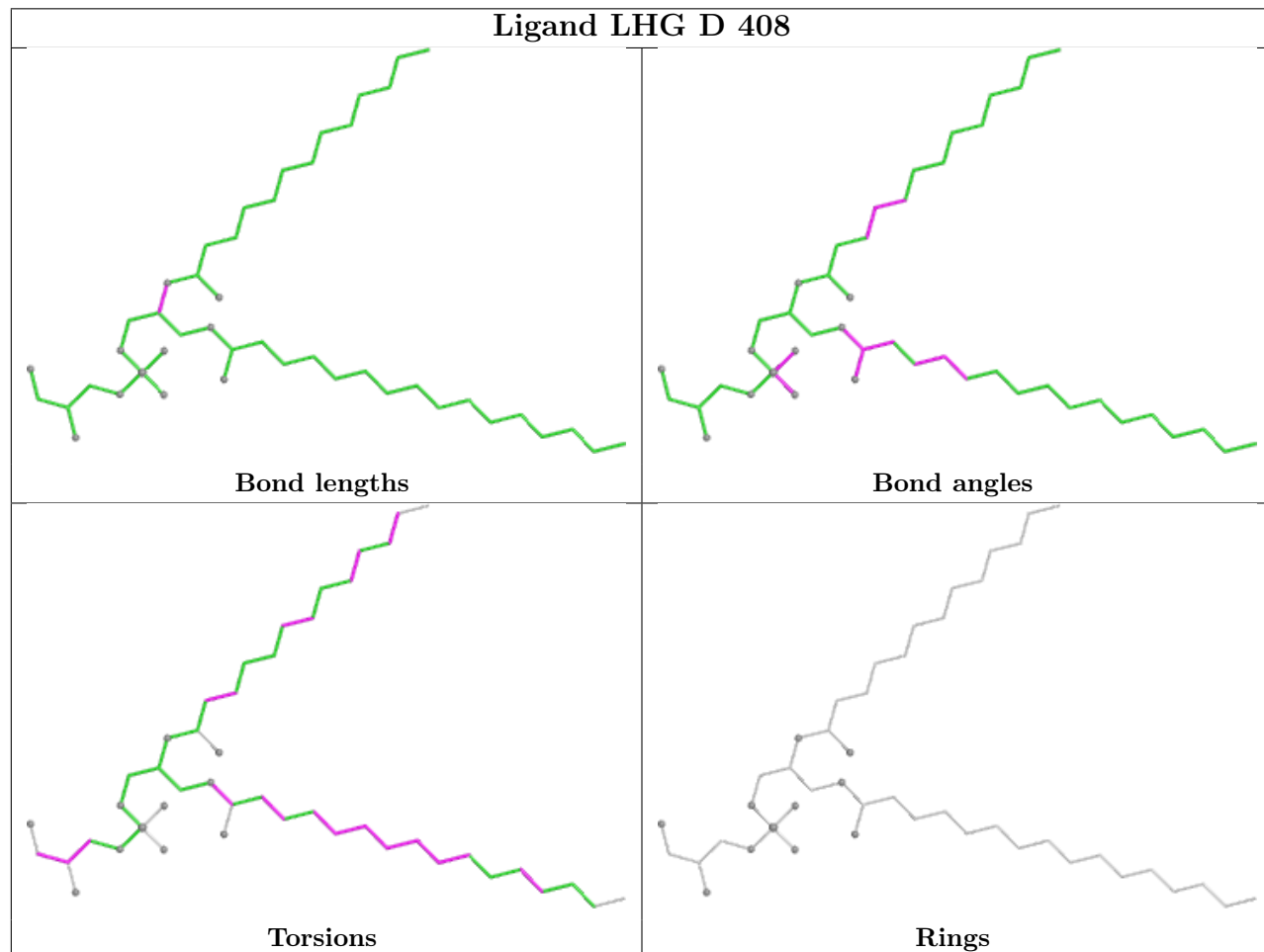


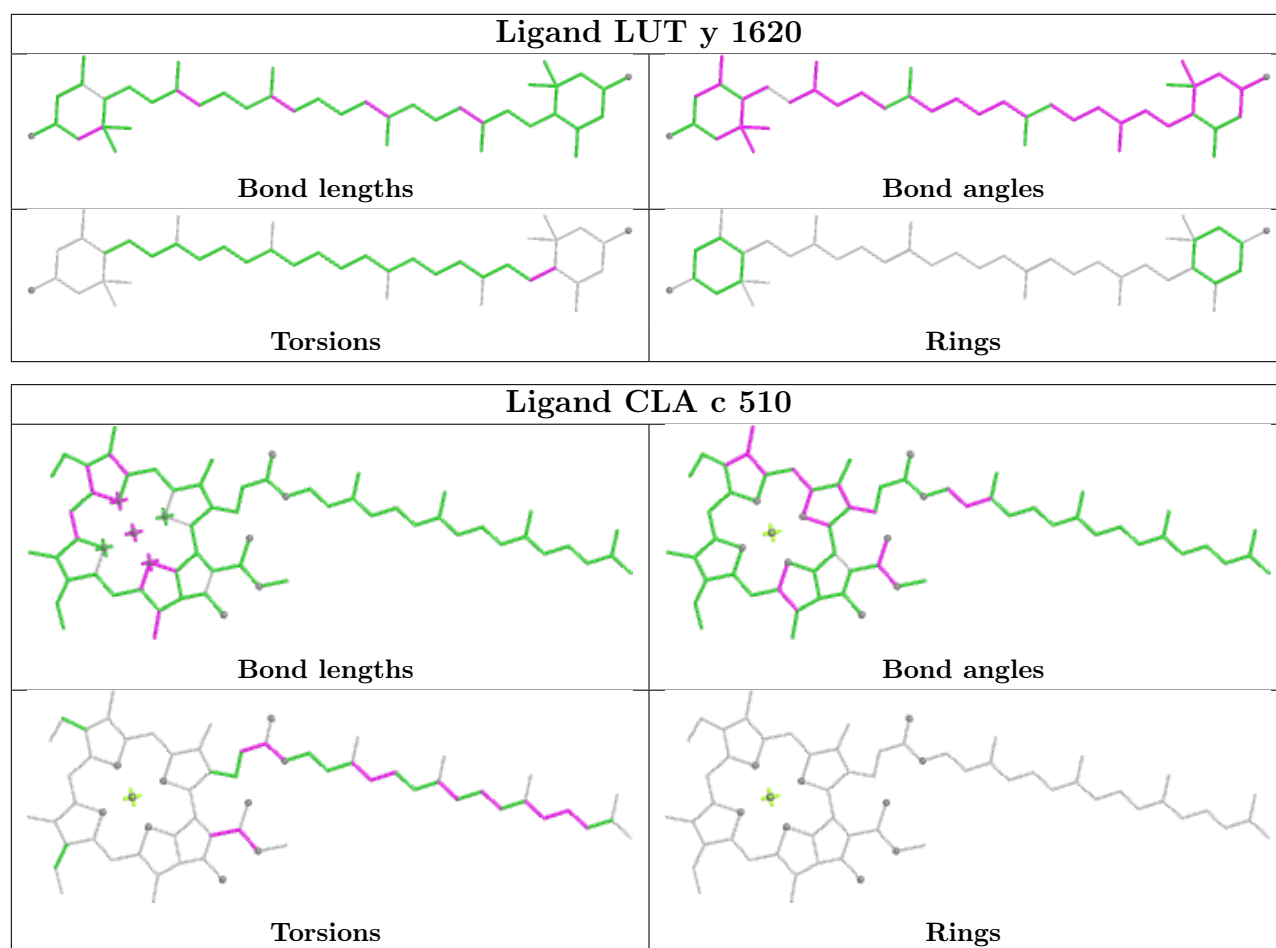
Ligand CLA R 612



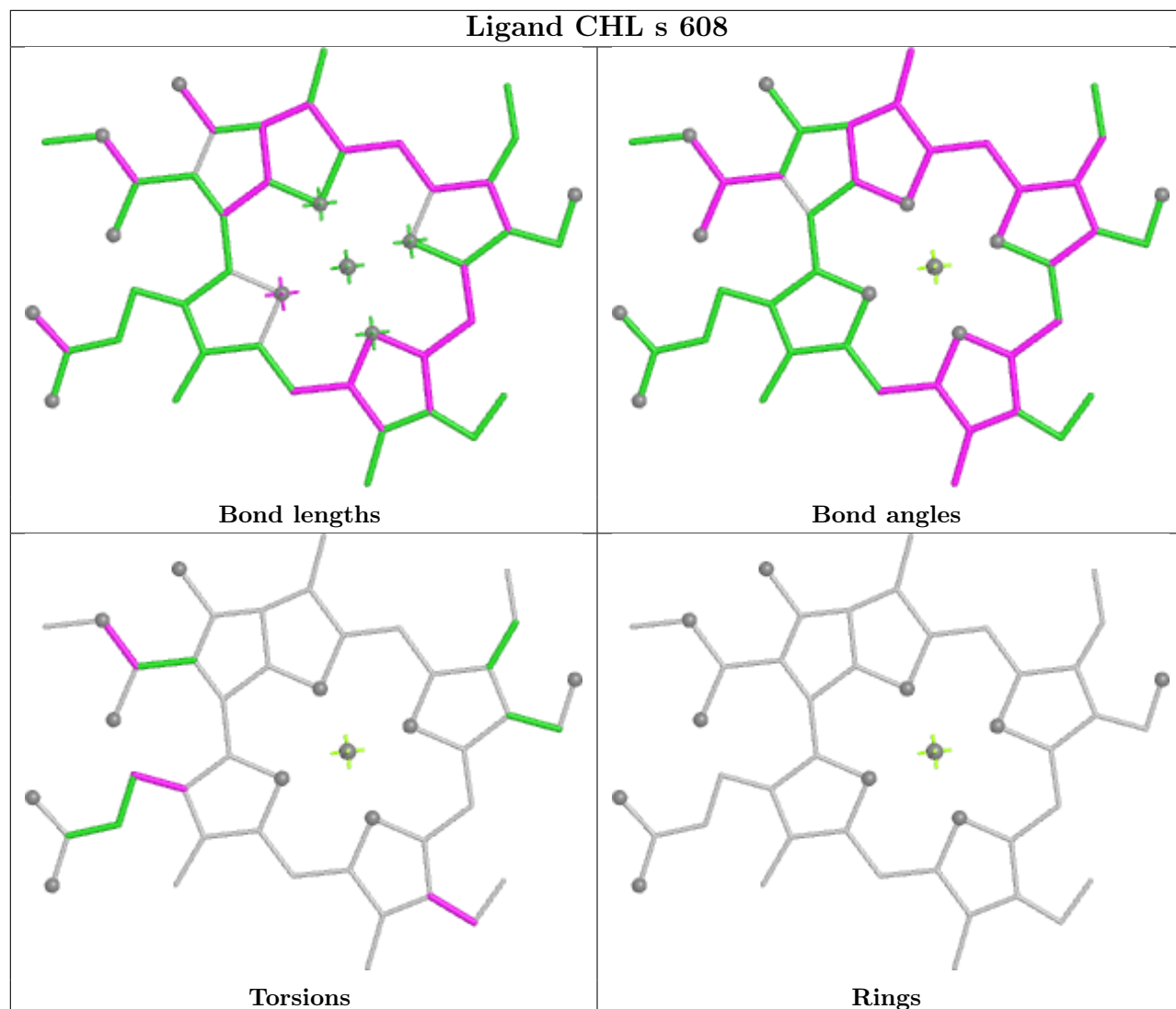
Ligand BCR b 618



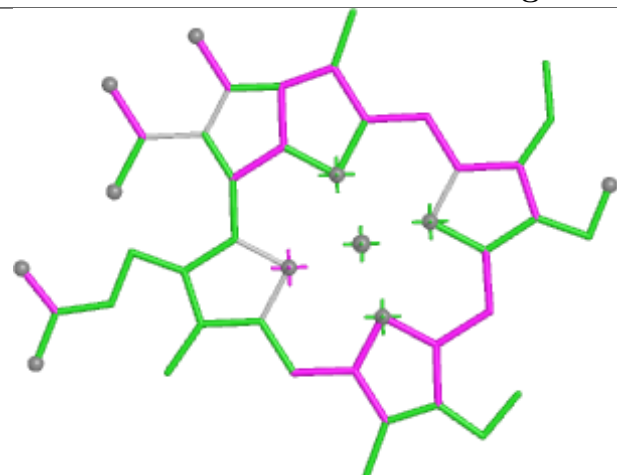
Ligand CLA c 503**Ligand LHG D 408**



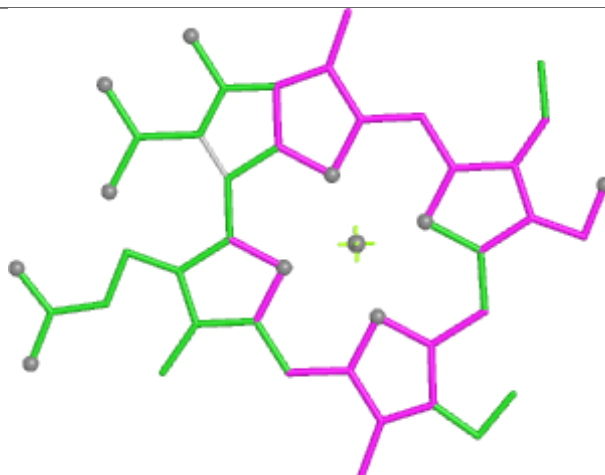
Ligand CHL s 608



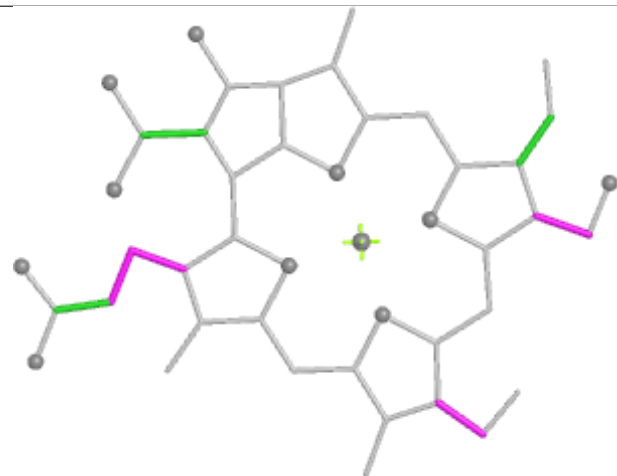
Ligand CHL 4 601



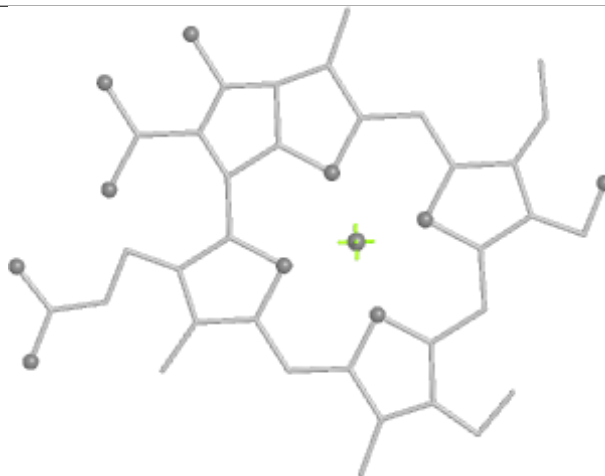
Bond lengths



Bond angles

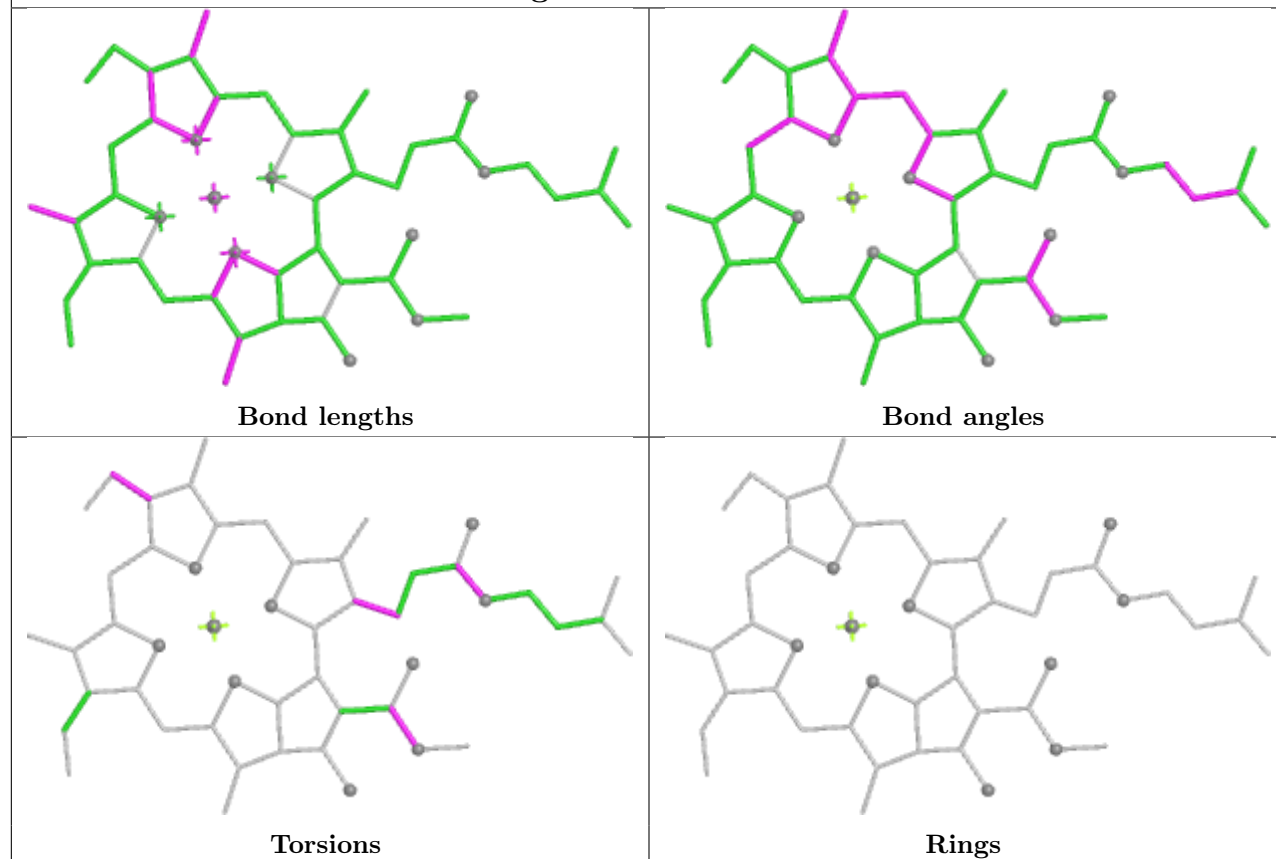


Torsions

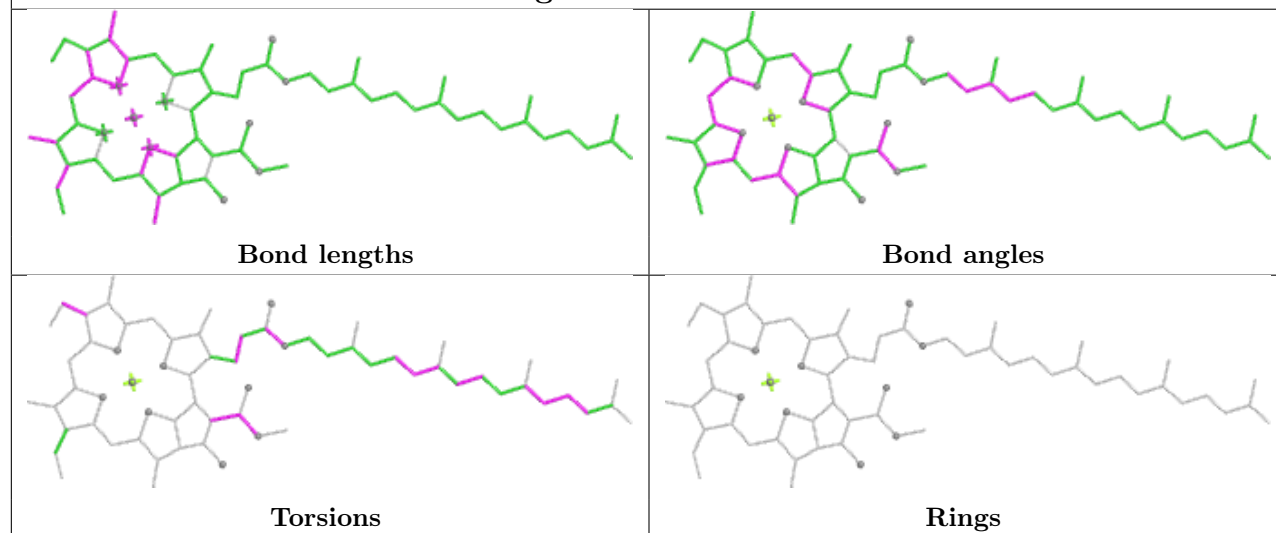


Rings

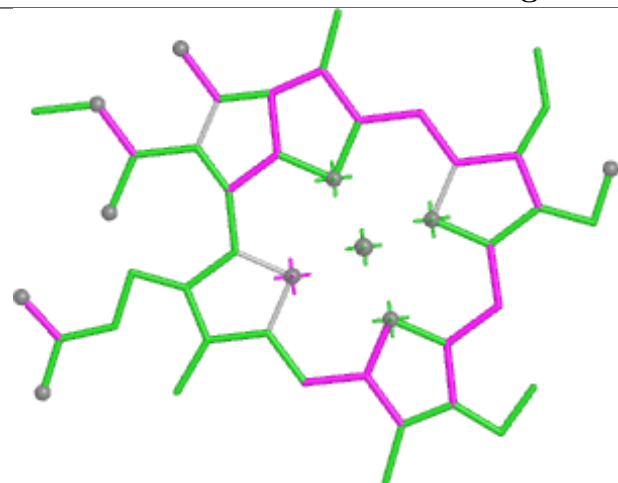
Ligand CLA G 604



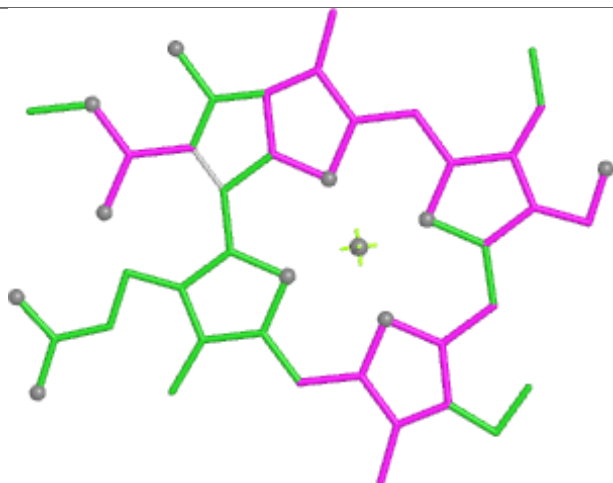
Ligand CLA b 606



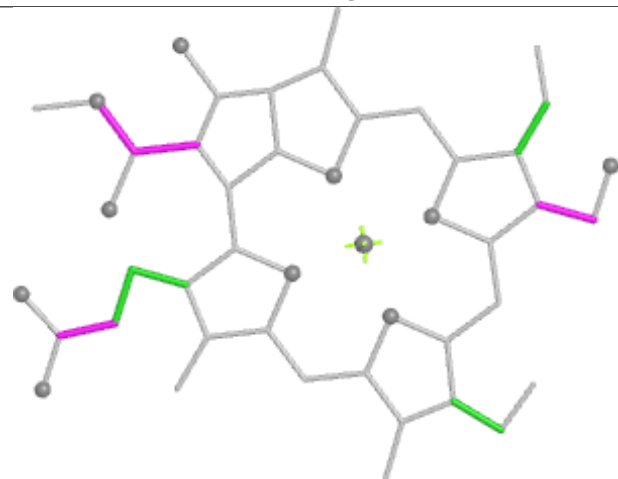
Ligand CHL S 606



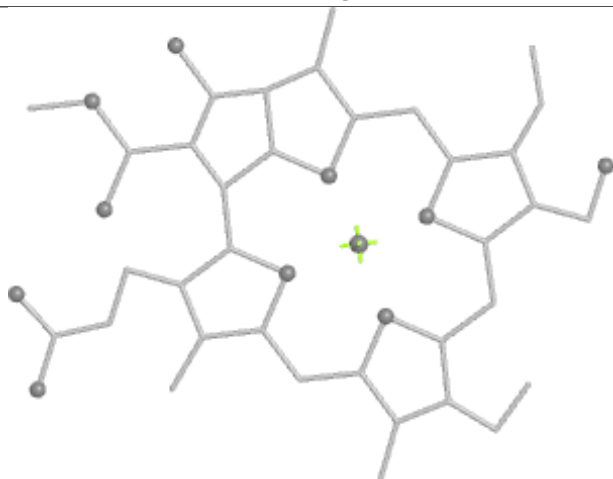
Bond lengths



Bond angles

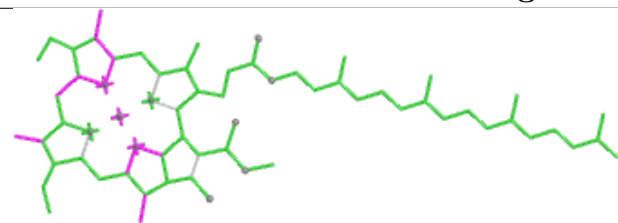


Torsions

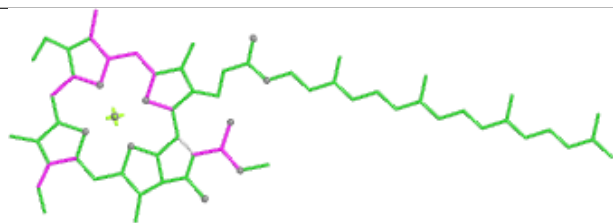


Rings

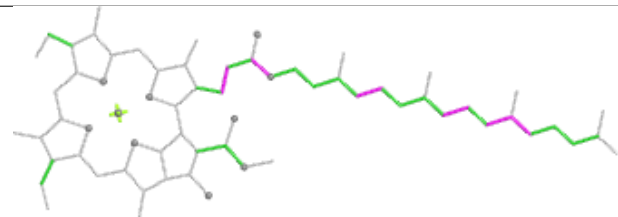
Ligand CLA Y 613



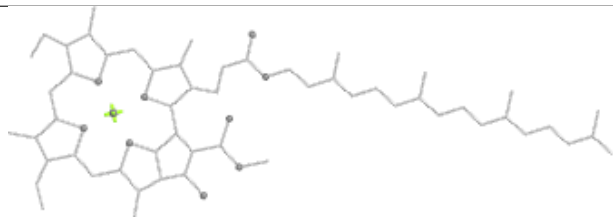
Bond lengths



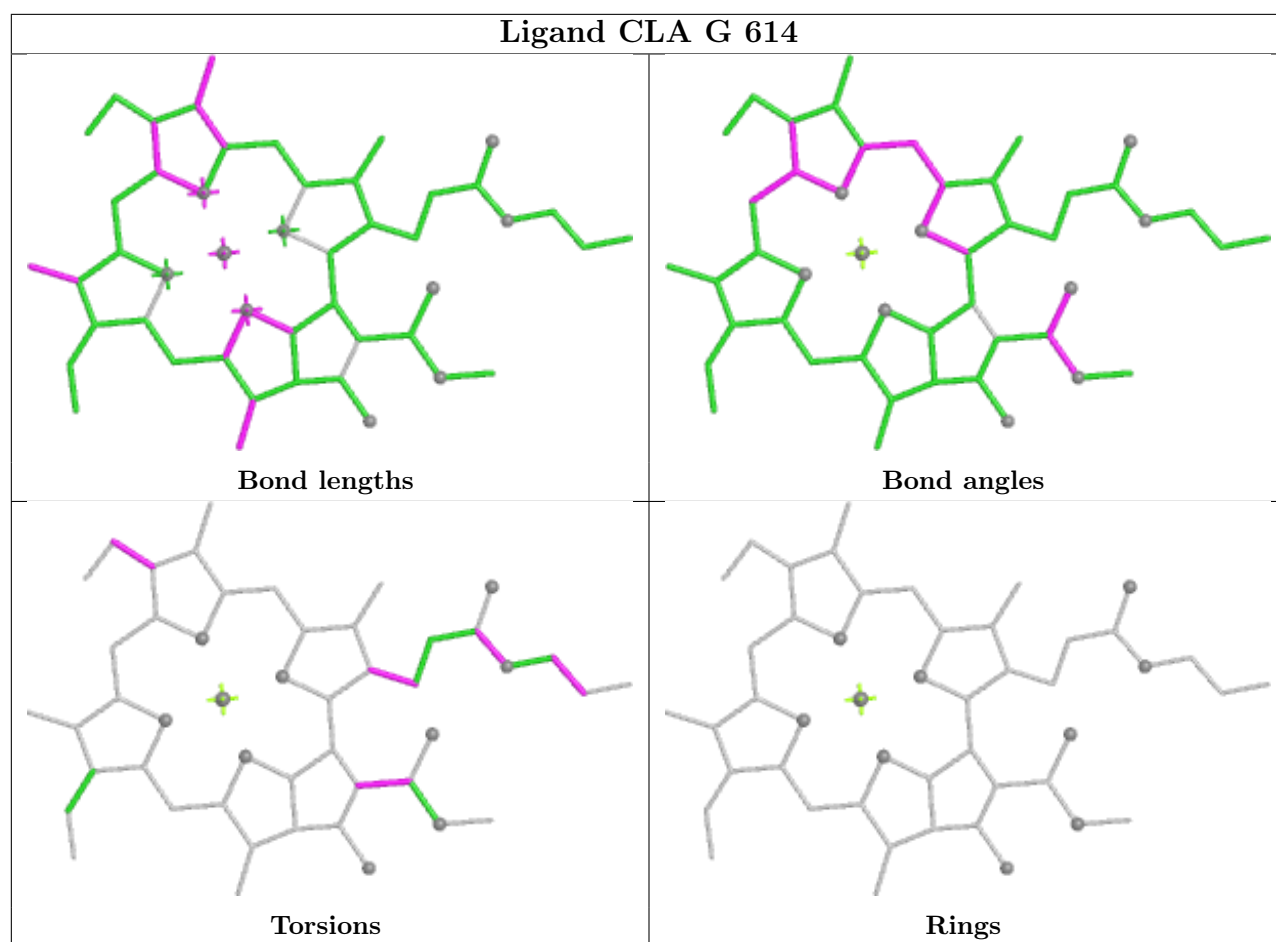
Bond angles



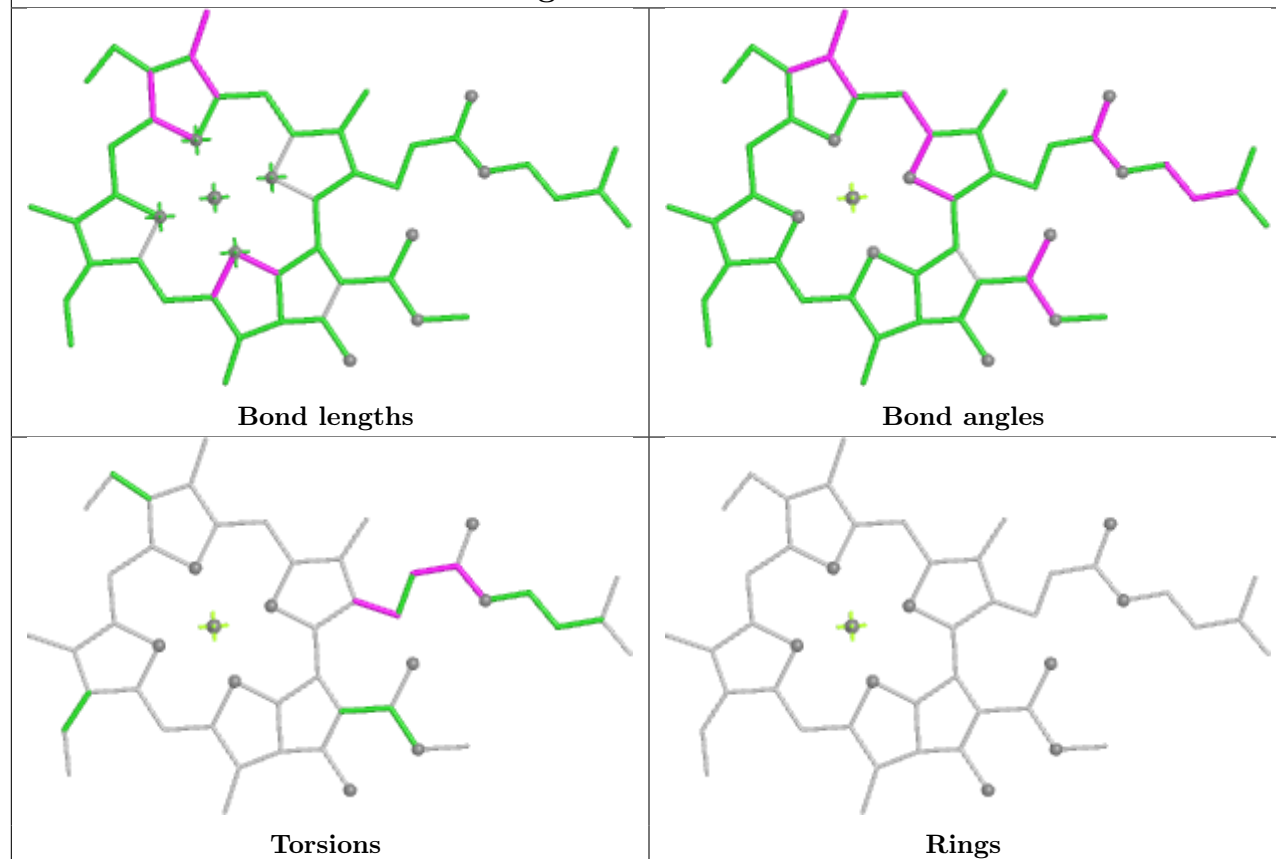
Torsions



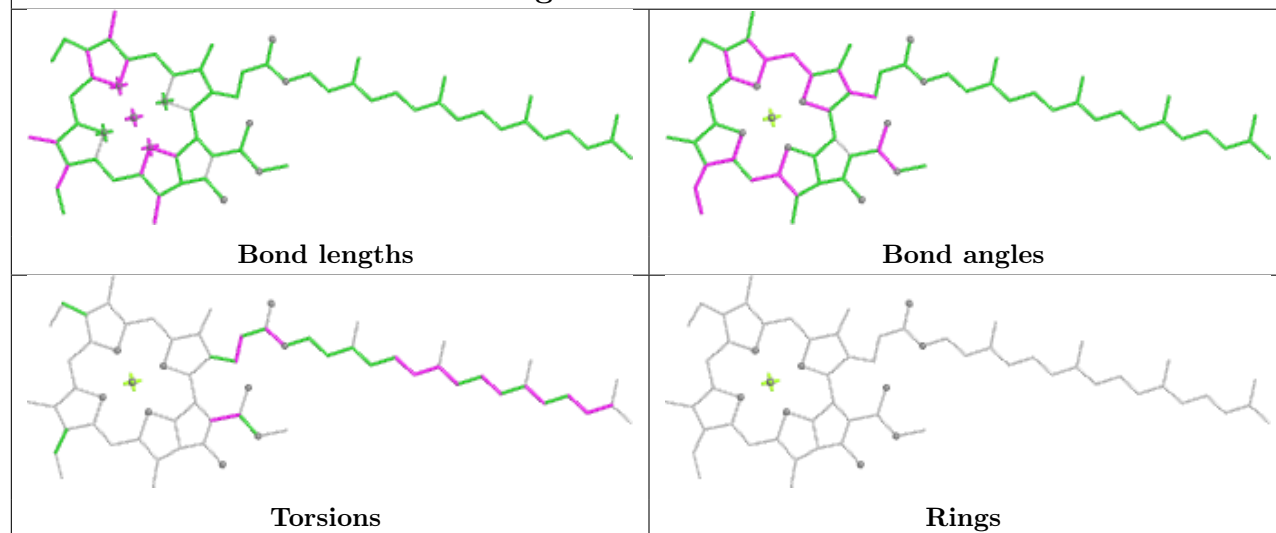
Rings

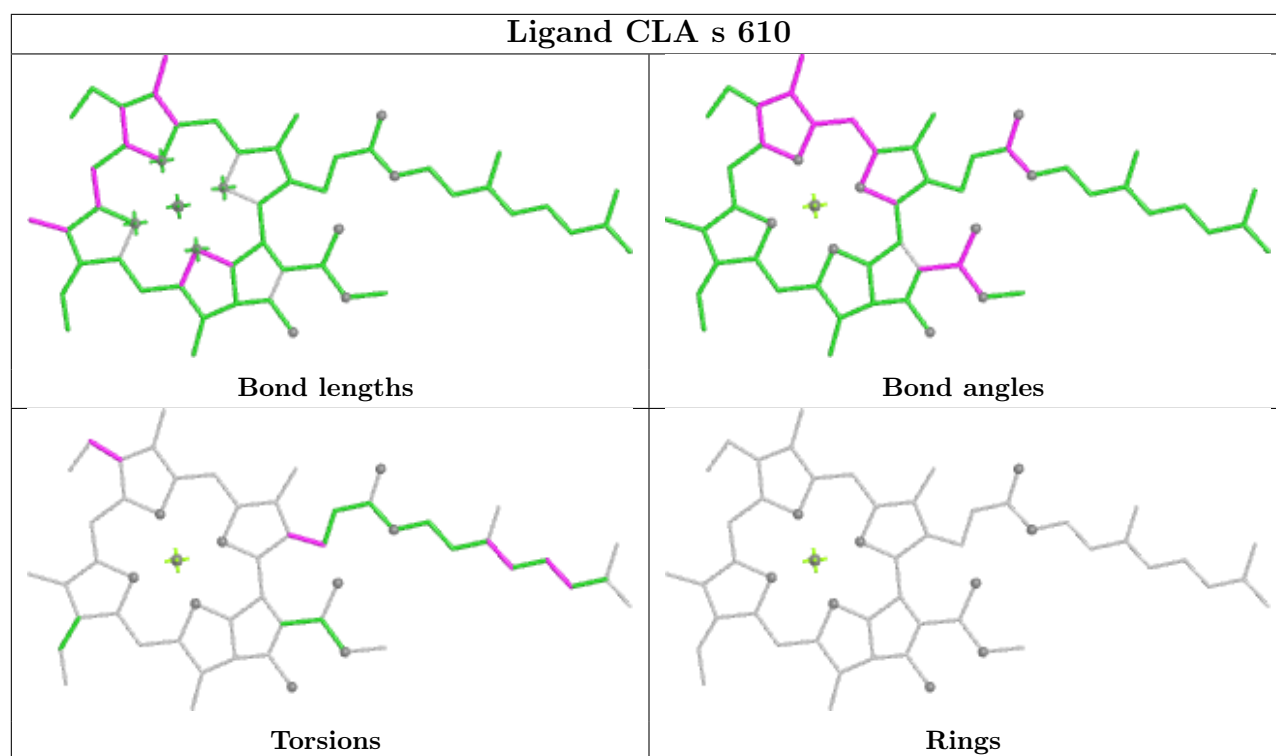


Ligand CLA s 604

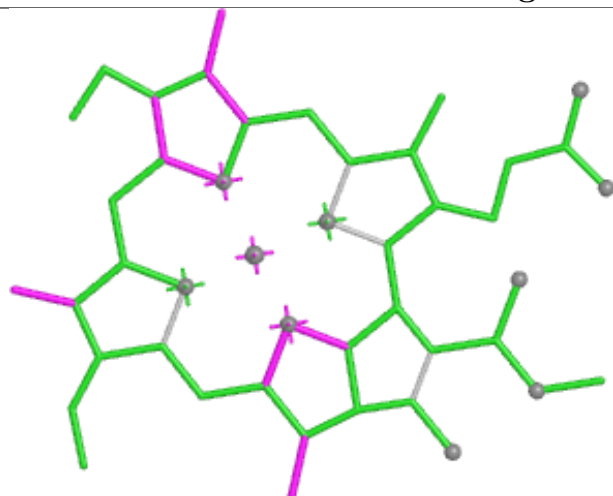


Ligand CLA n 603

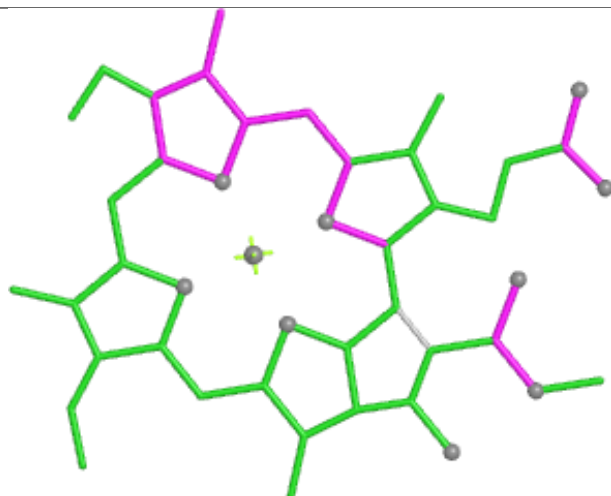




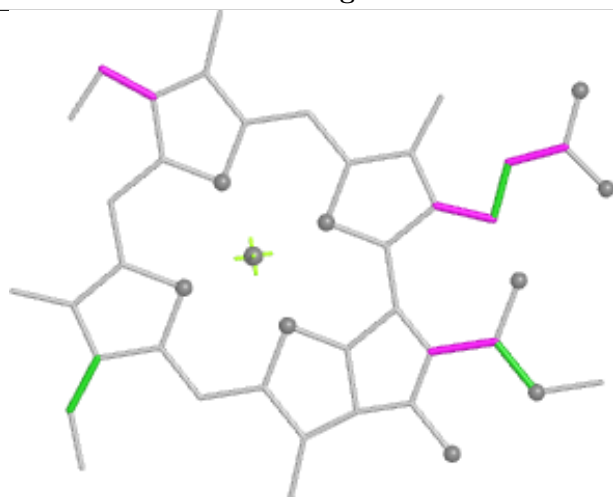
Ligand CLA 8 610



Bond lengths



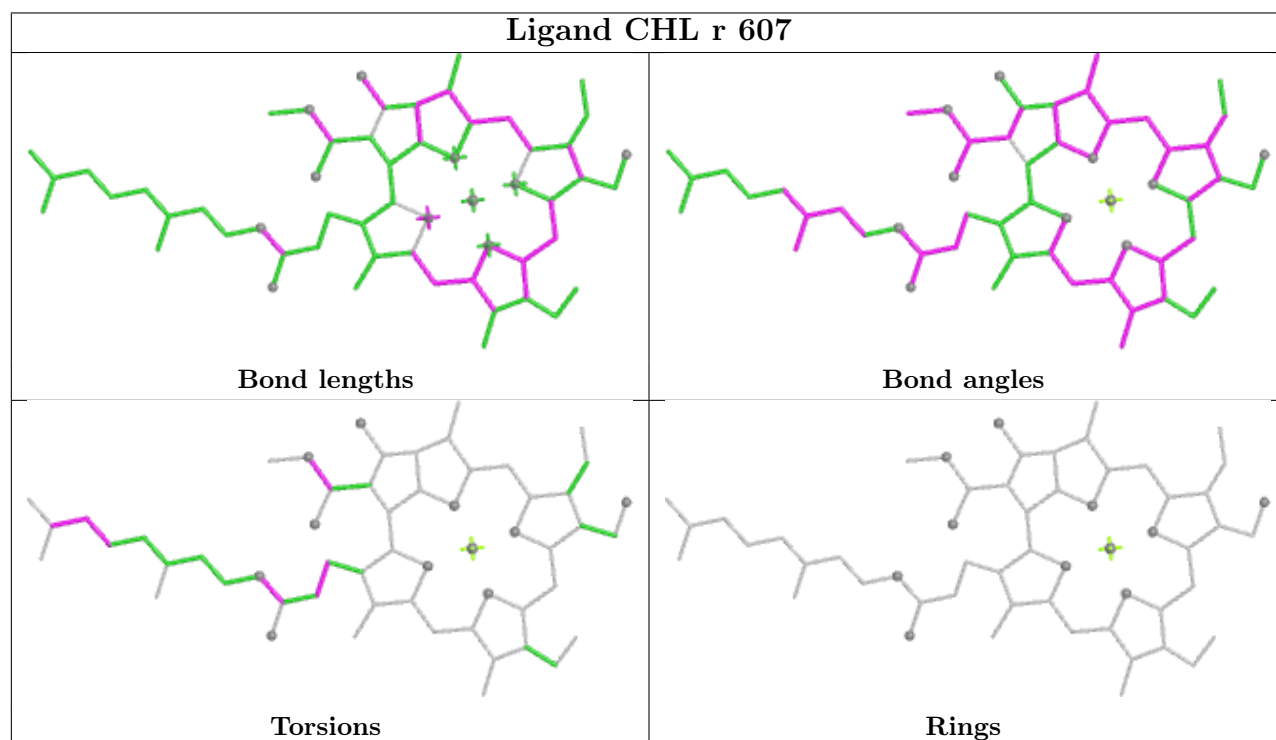
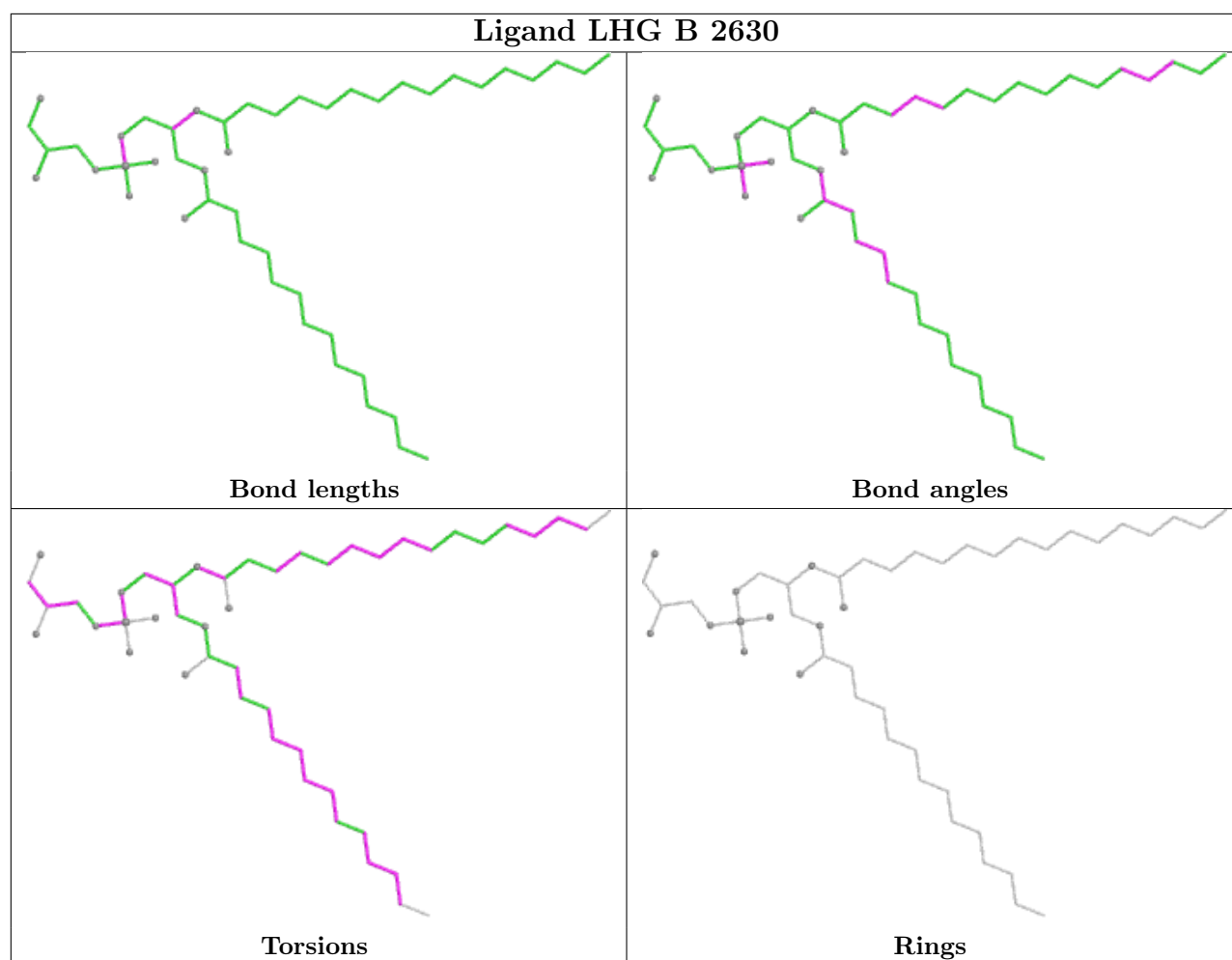
Bond angles



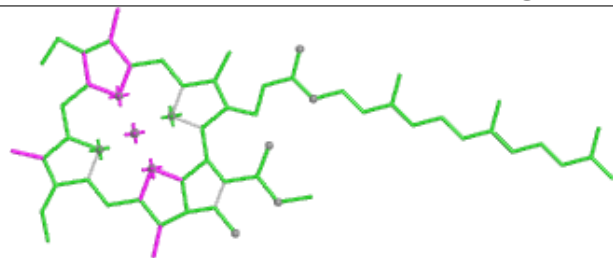
Torsions



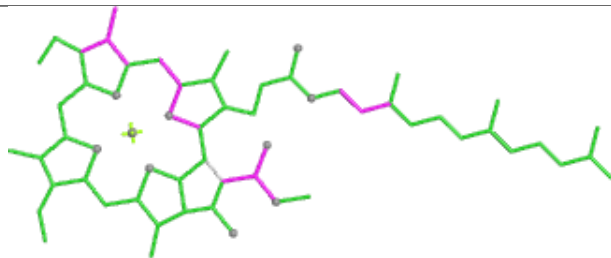
Rings



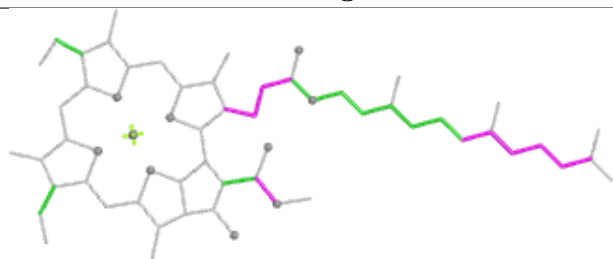
Ligand CLA 7 602



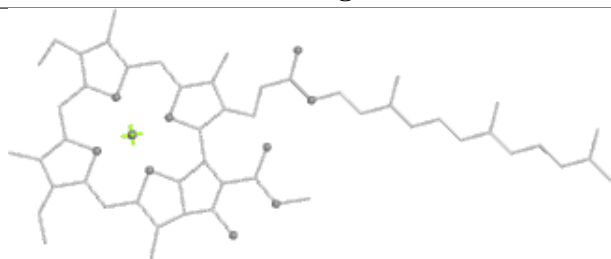
Bond lengths



Bond angles

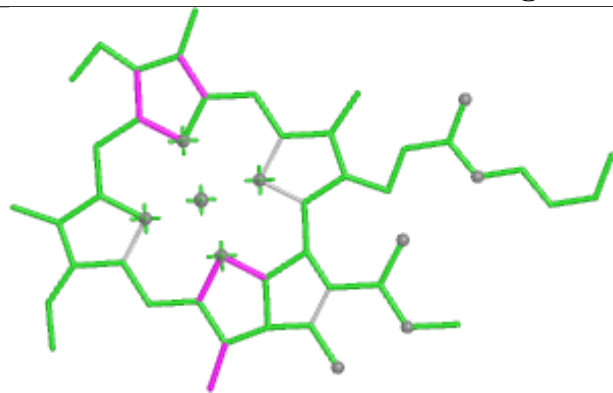


Torsions

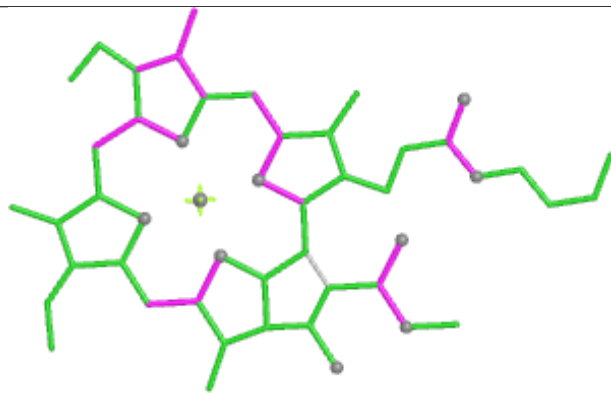


Rings

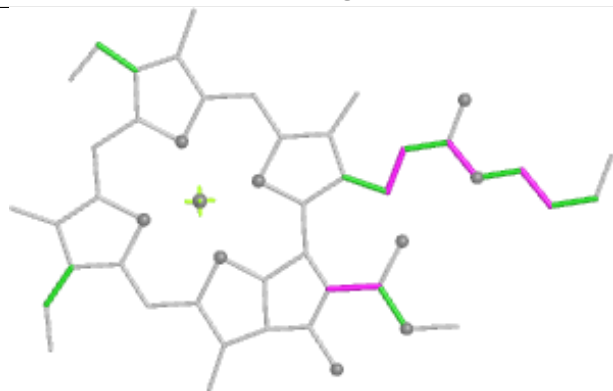
Ligand CLA s 614



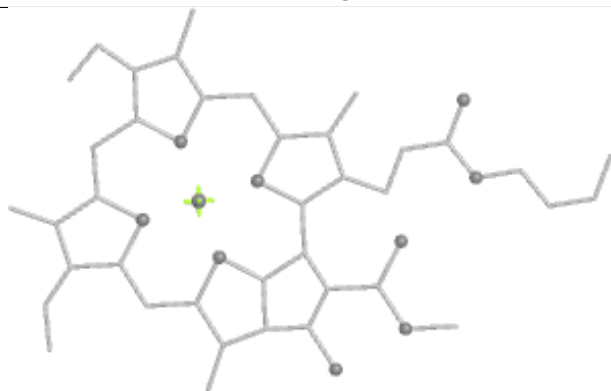
Bond lengths



Bond angles

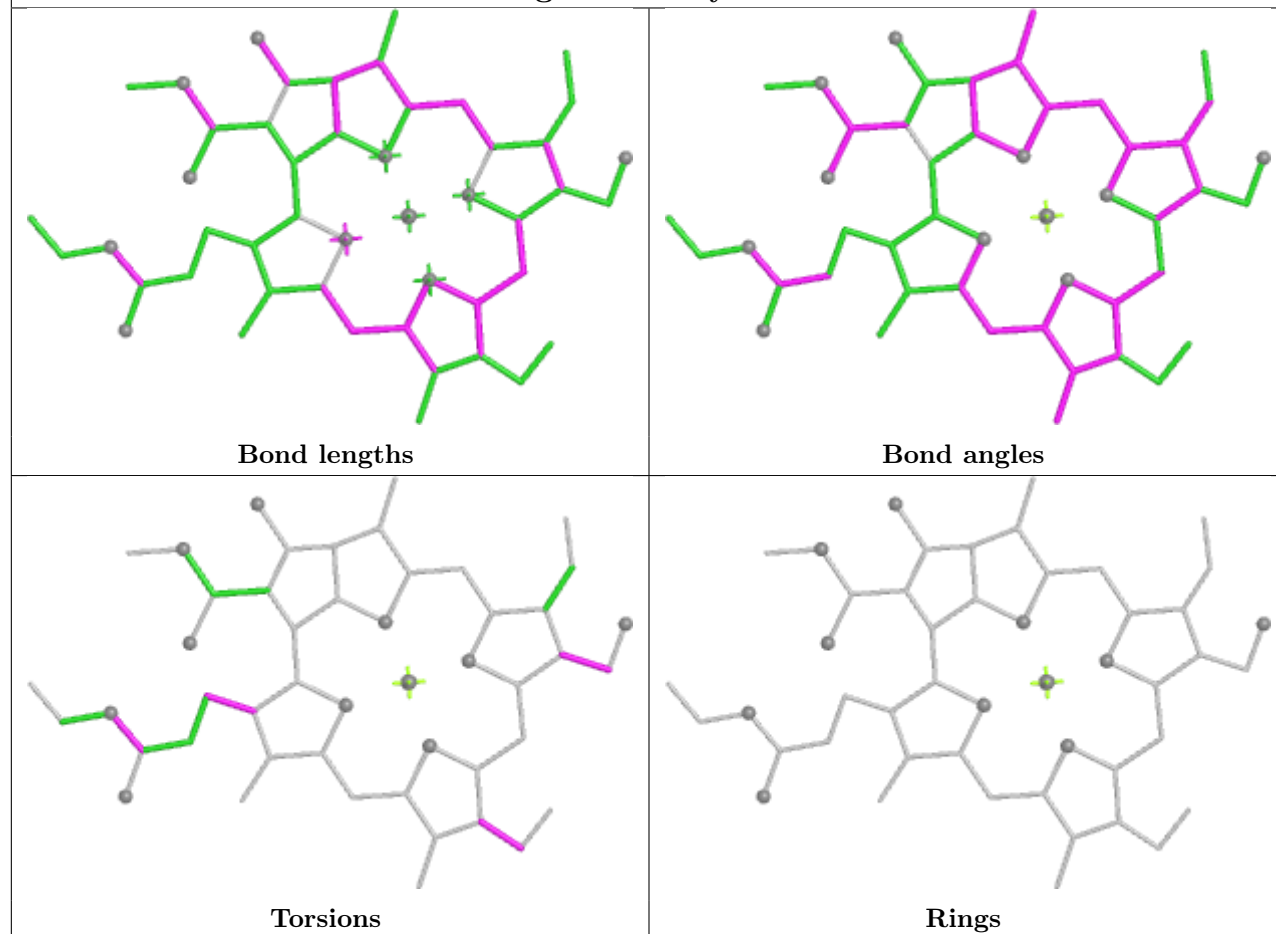


Torsions

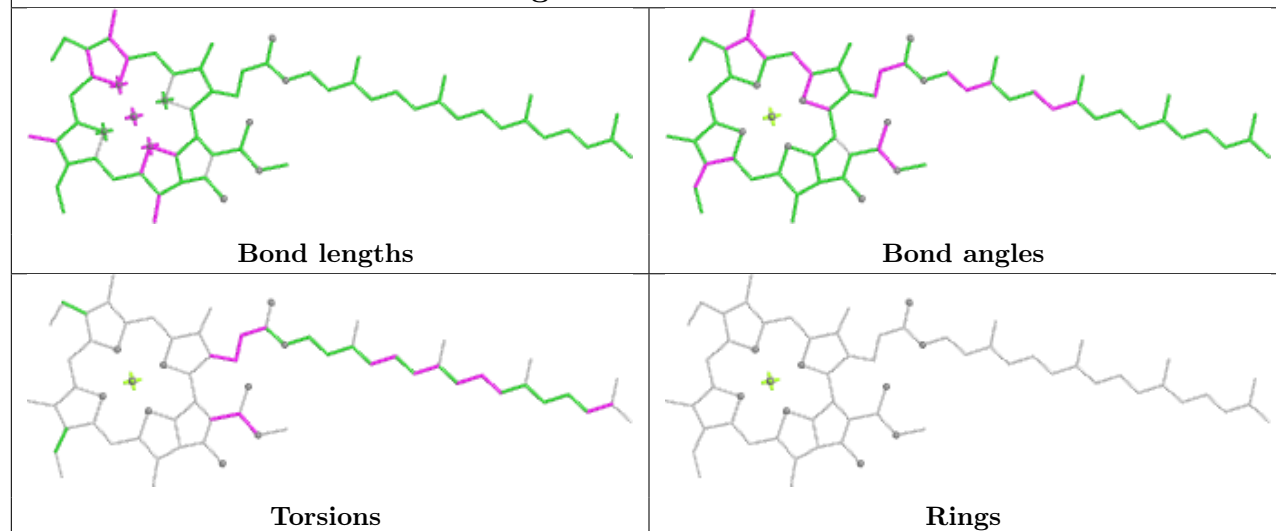


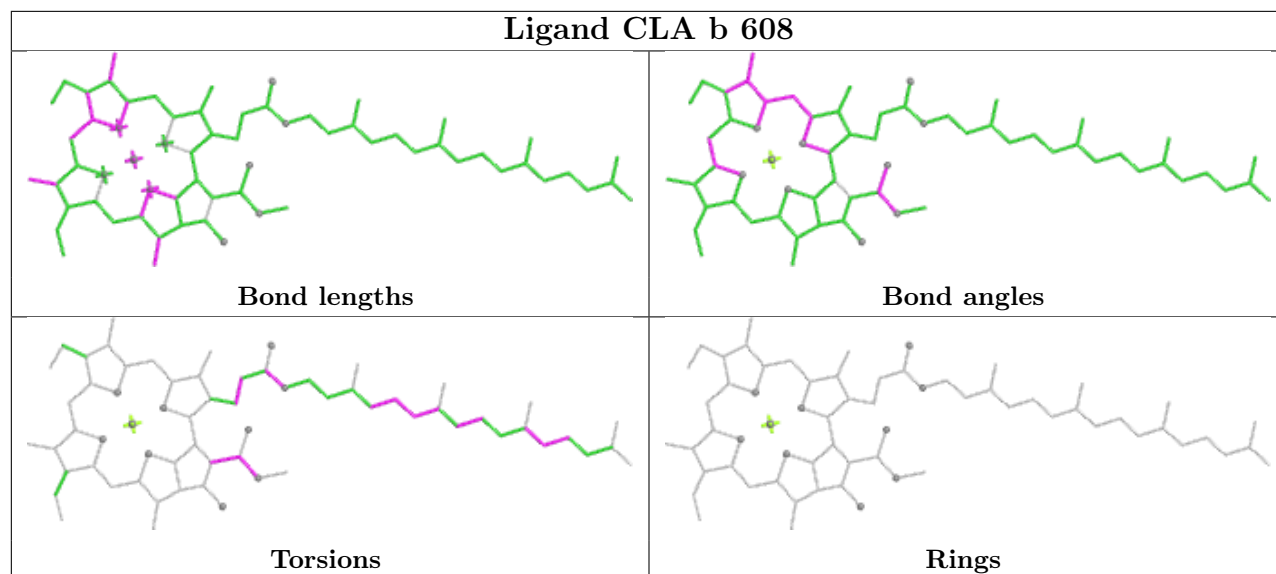
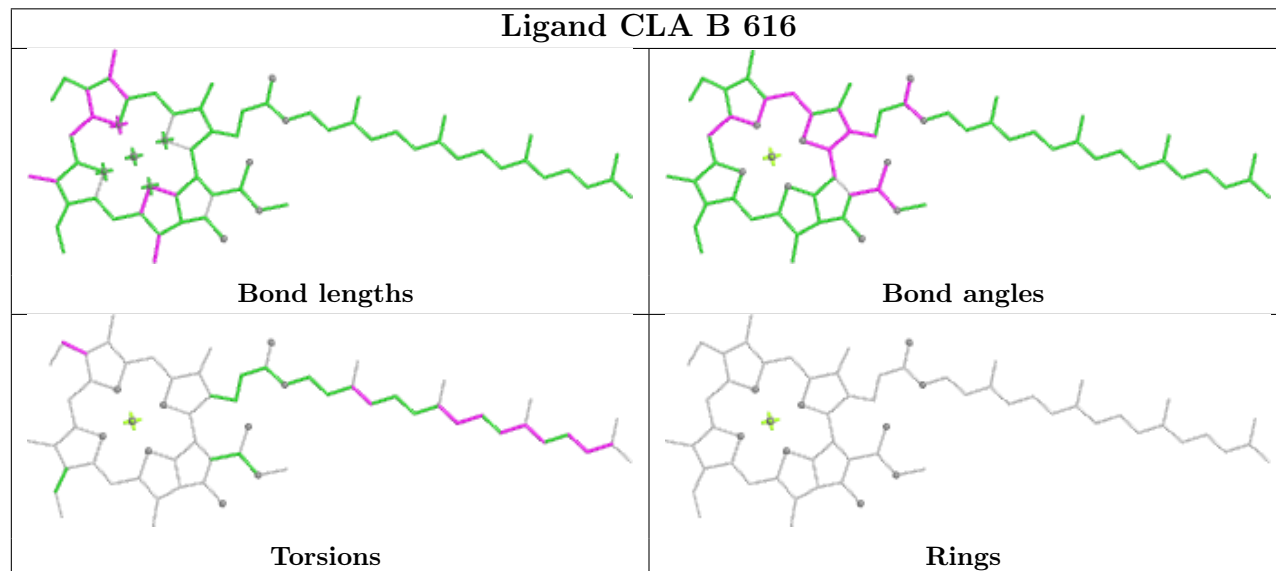
Rings

Ligand CHL y 605

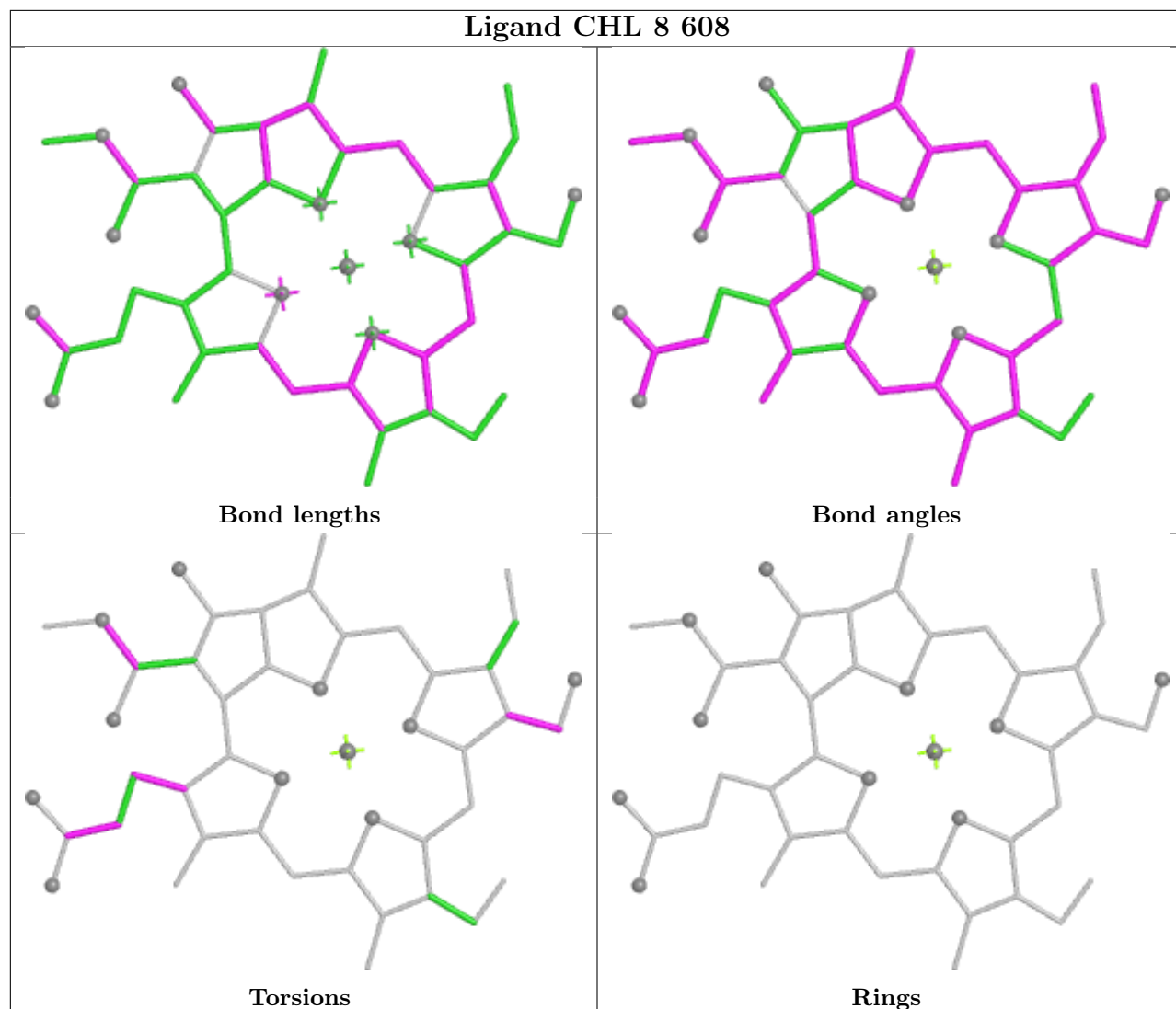


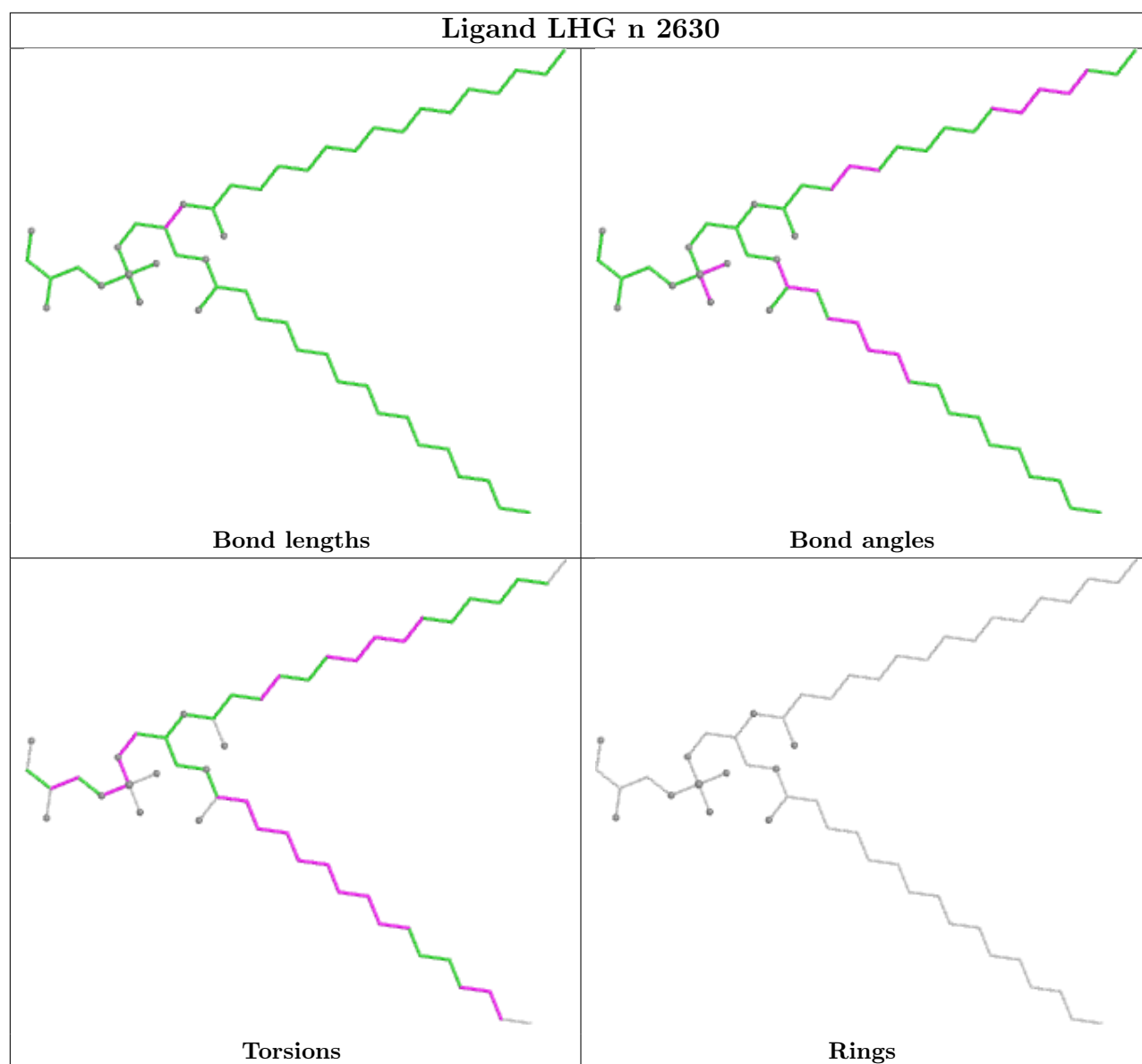
Ligand CLA N 602

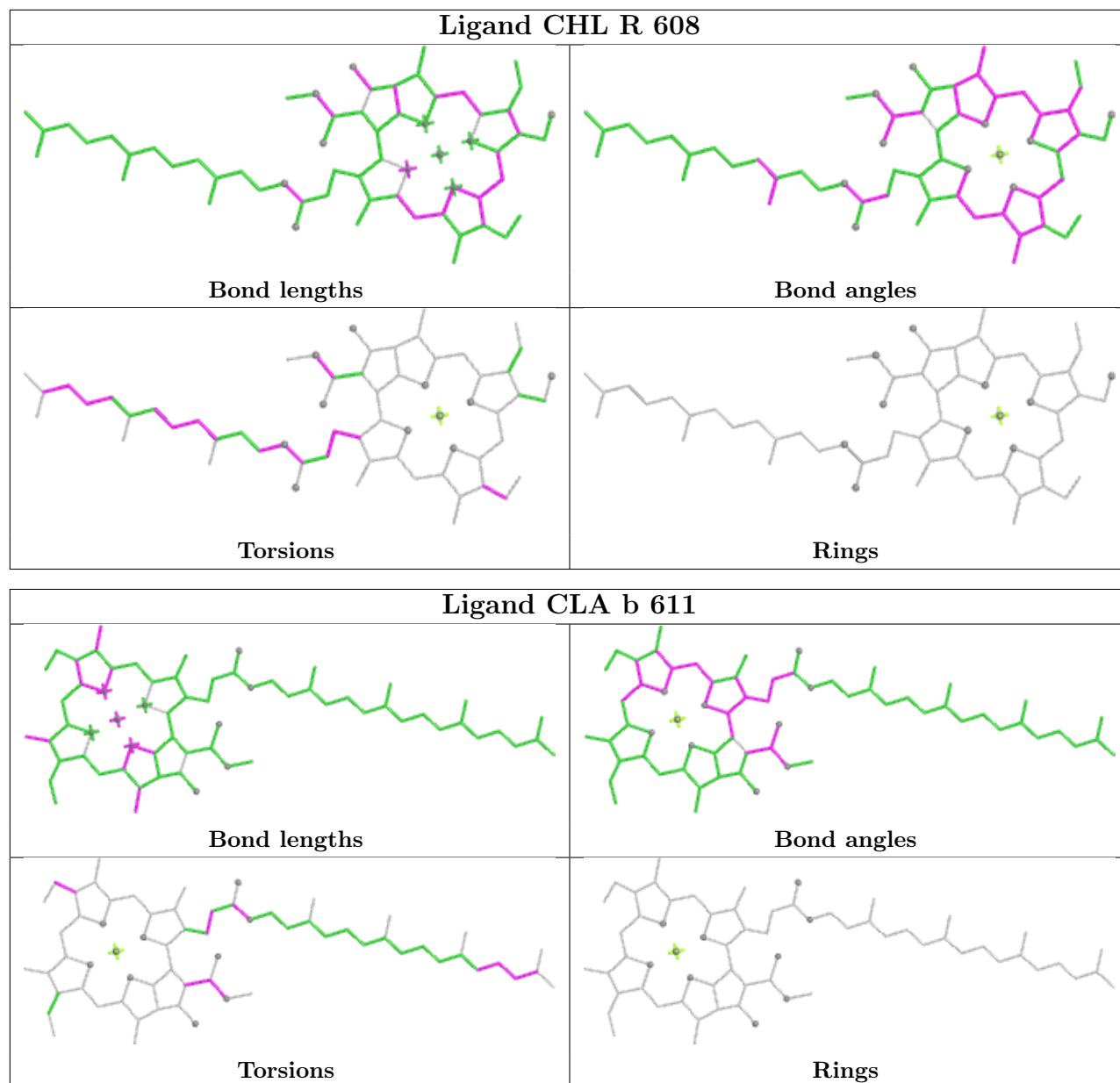


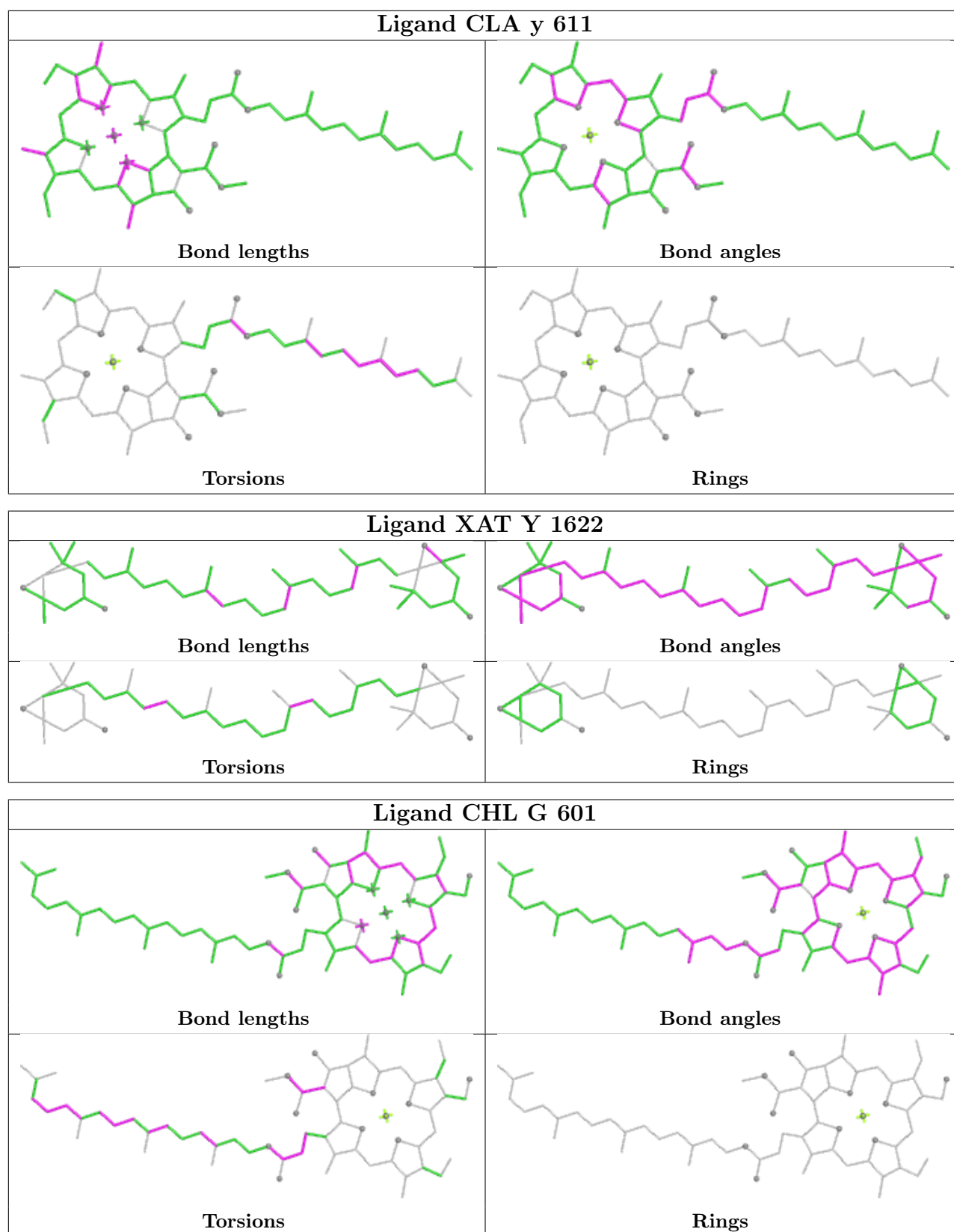
Ligand CLA b 608**Ligand CLA B 616**

Ligand CHL 8 608

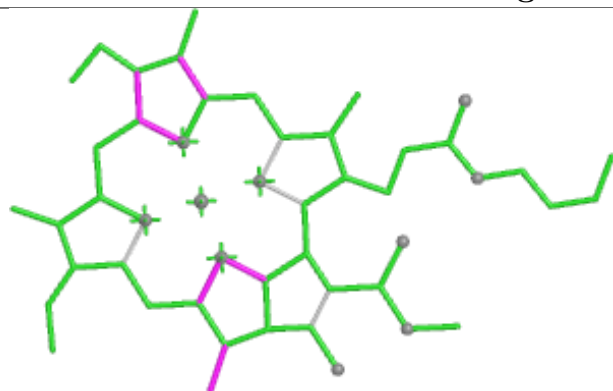




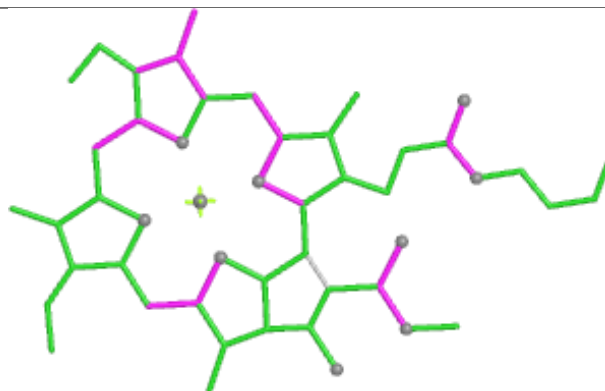




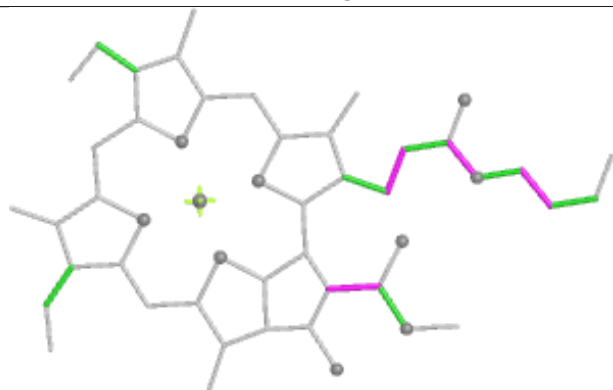
Ligand CLA S 614



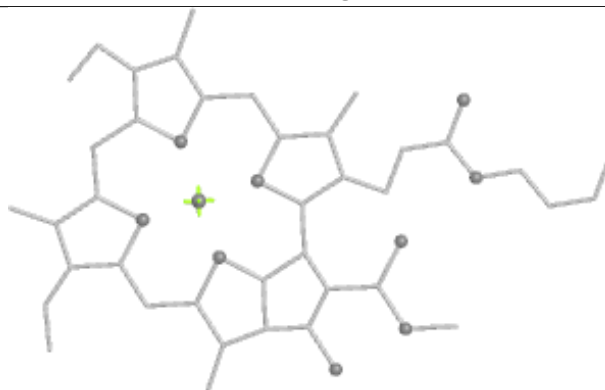
Bond lengths



Bond angles

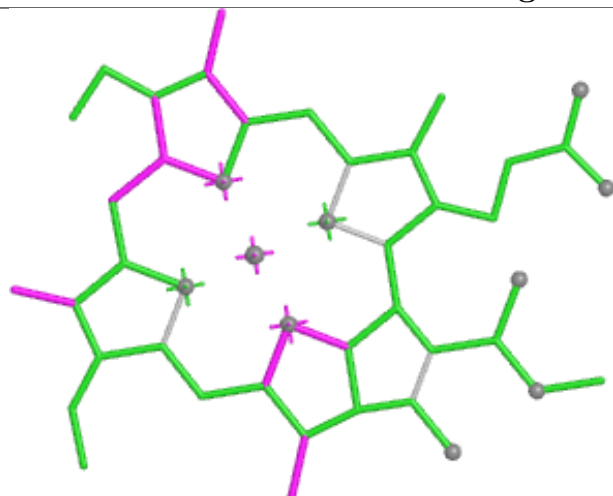


Torsions

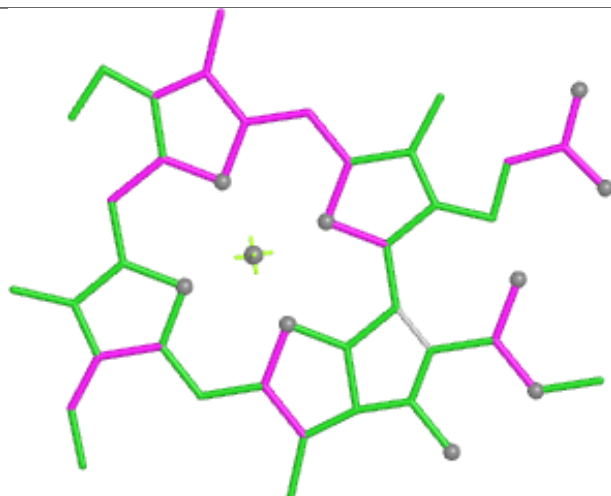


Rings

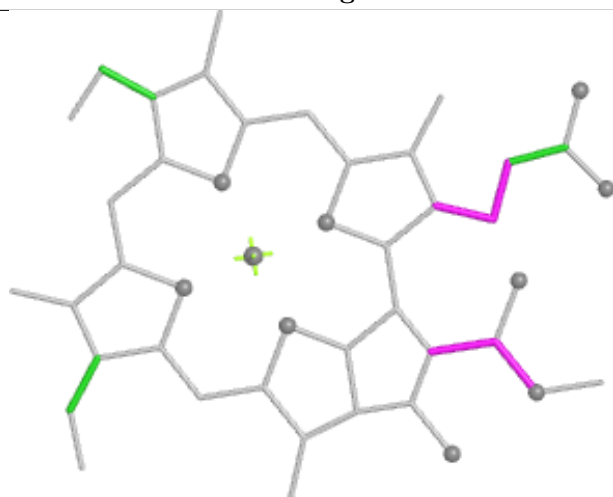
Ligand CLA 6 604



Bond lengths



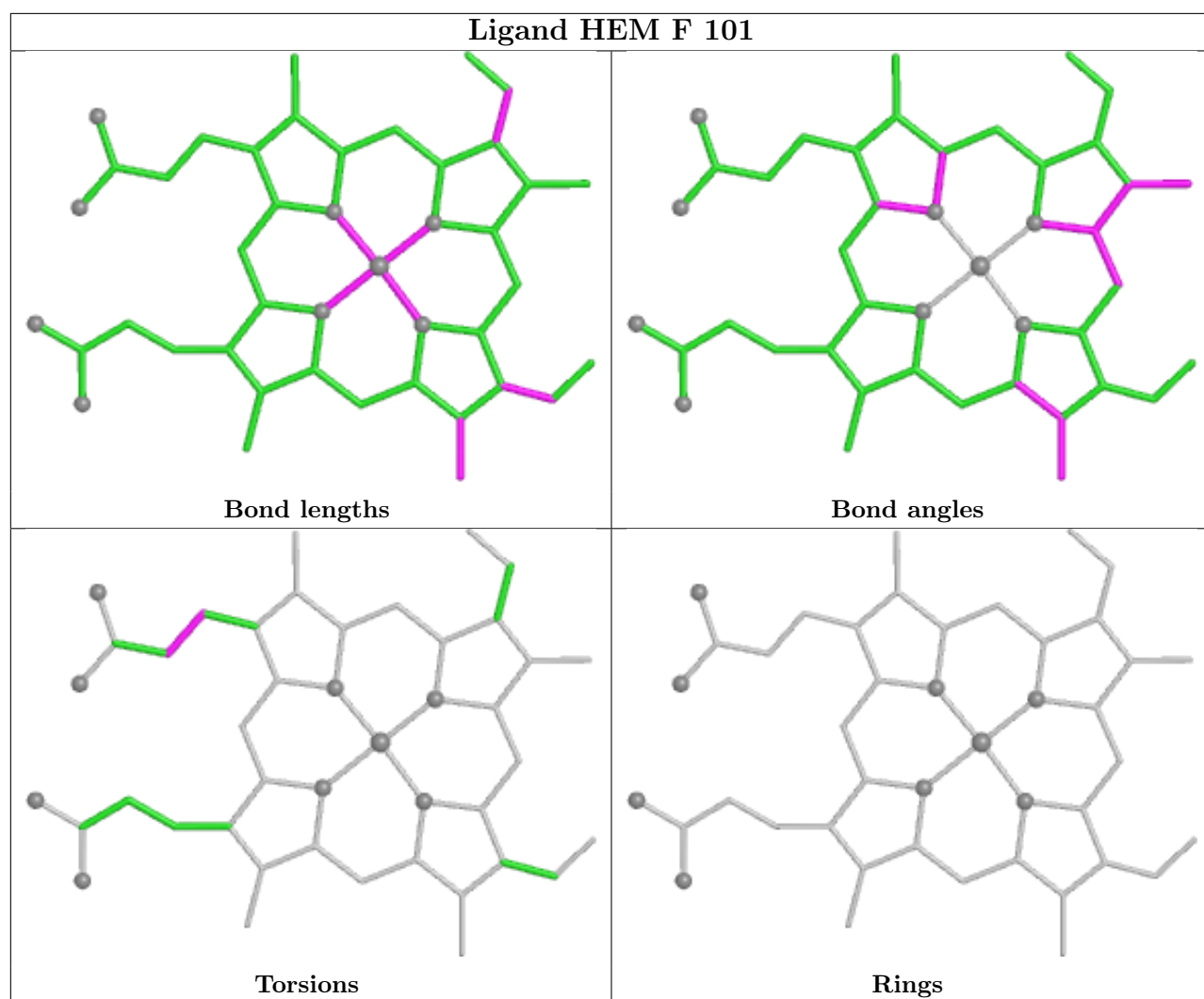
Bond angles

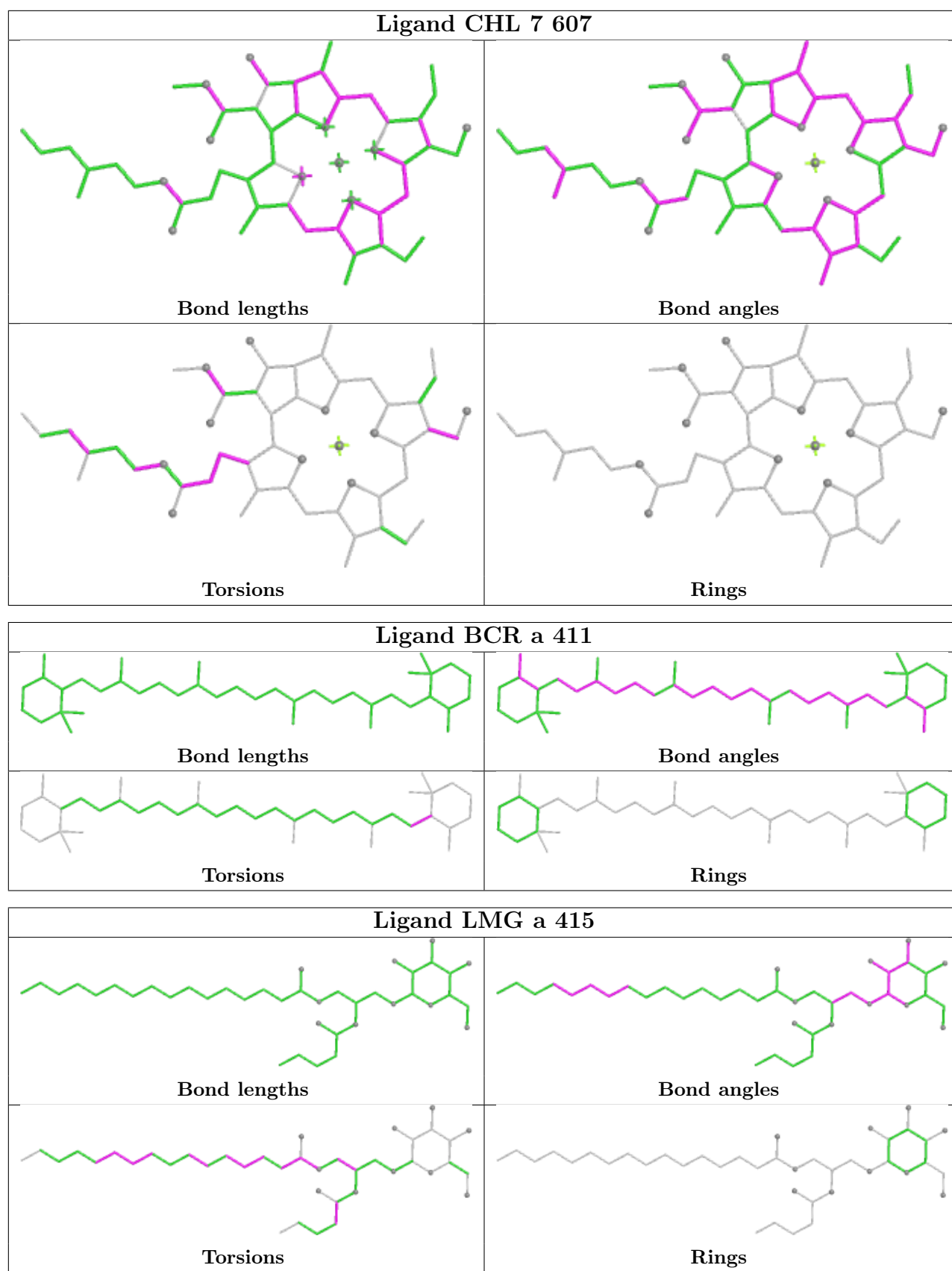


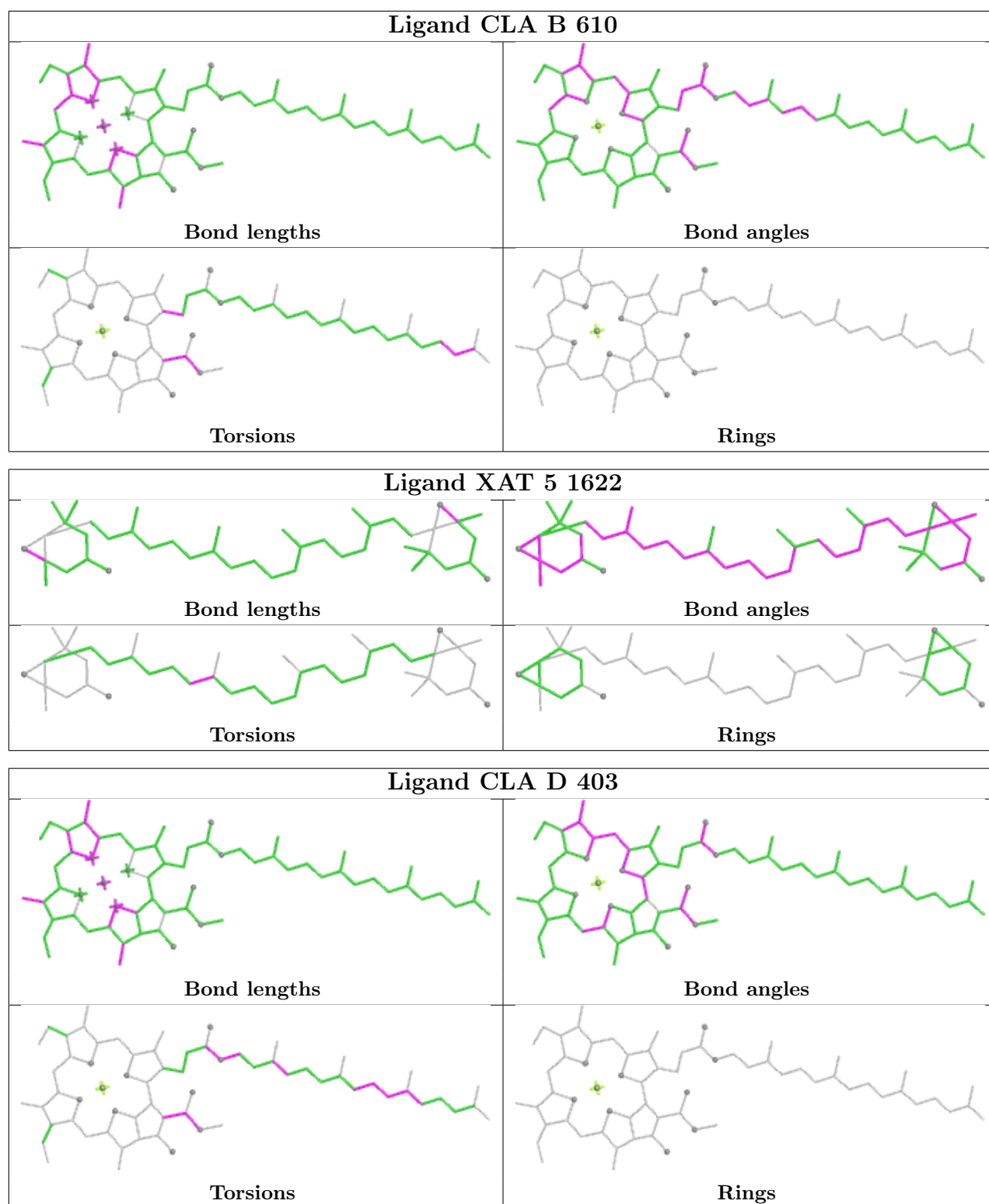
Torsions

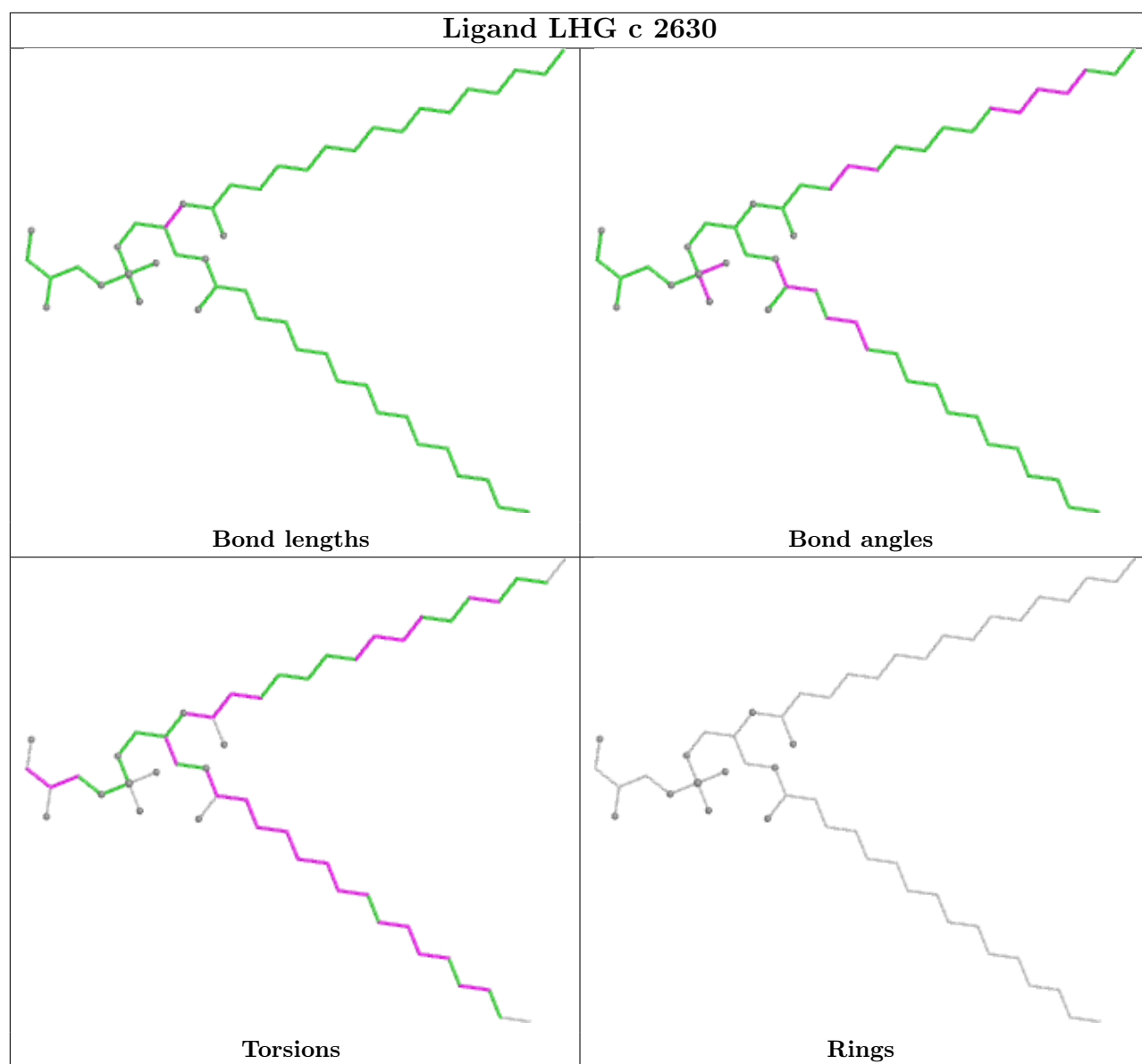


Rings

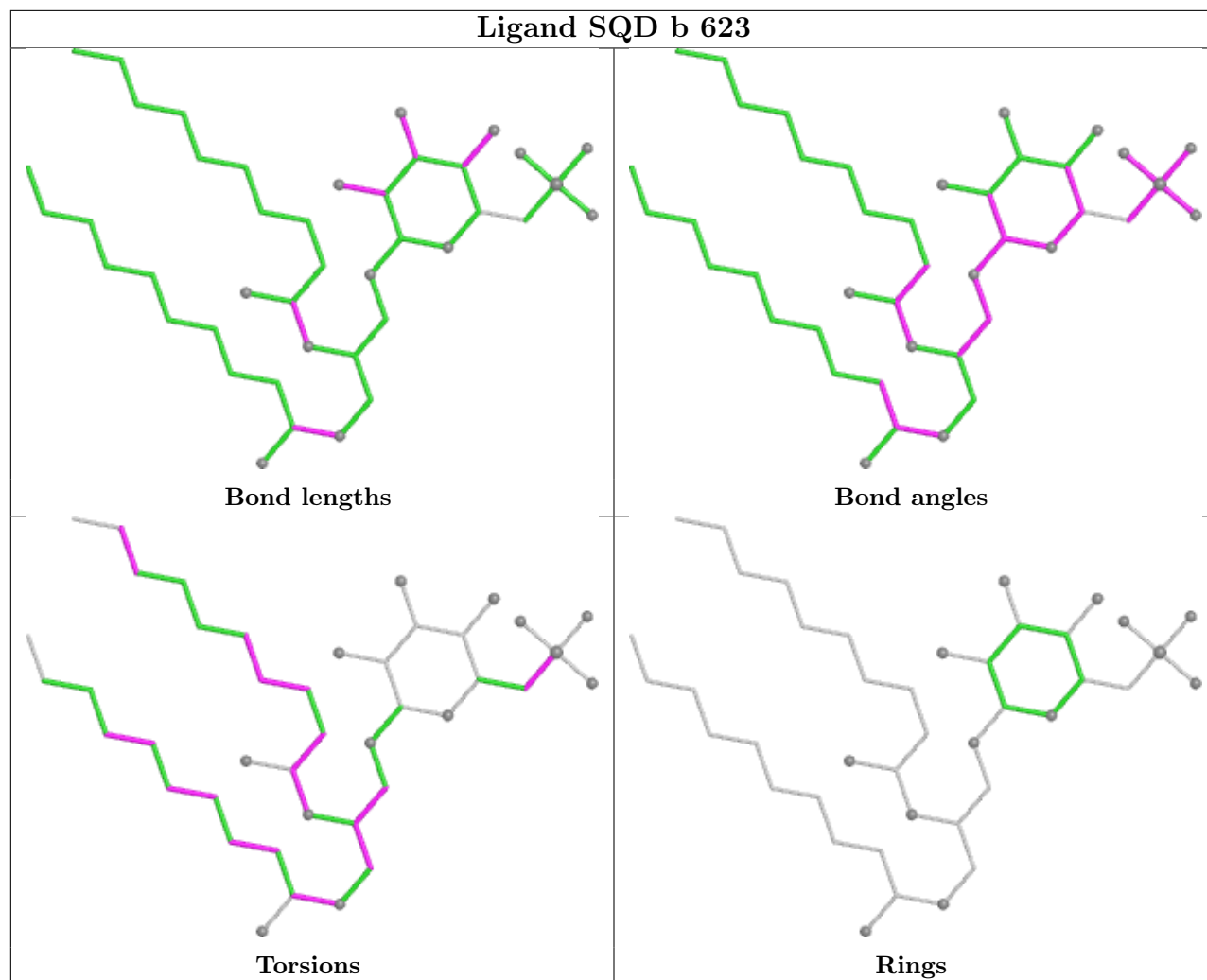




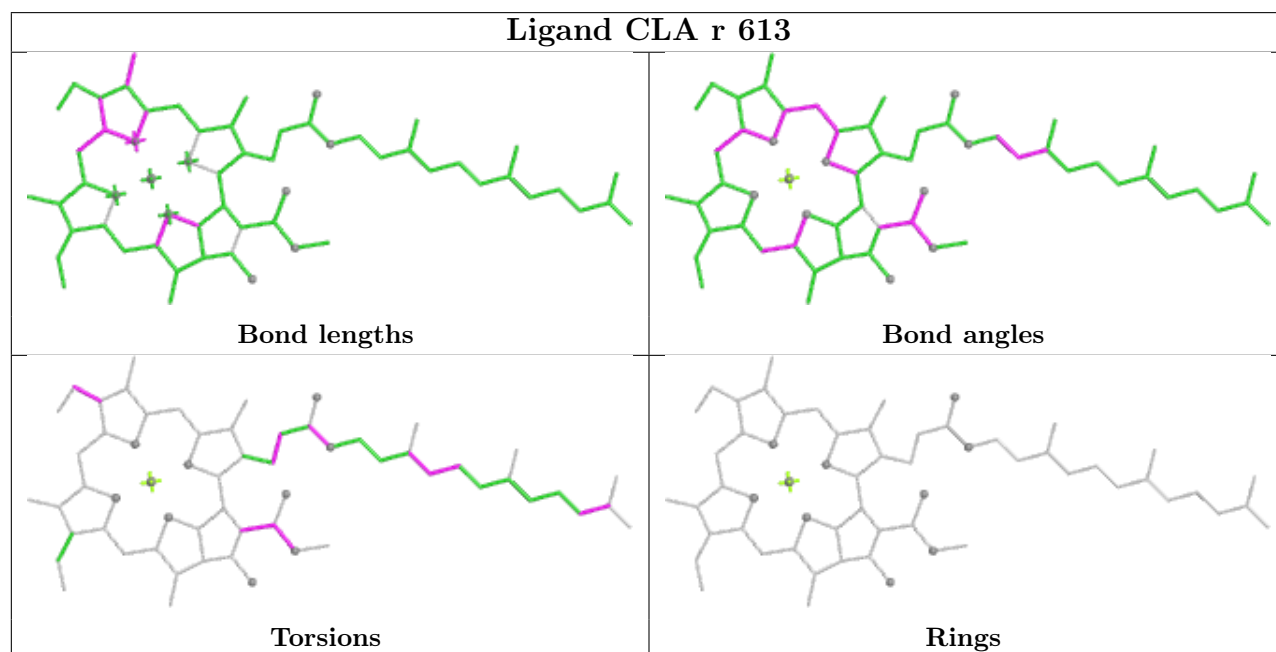




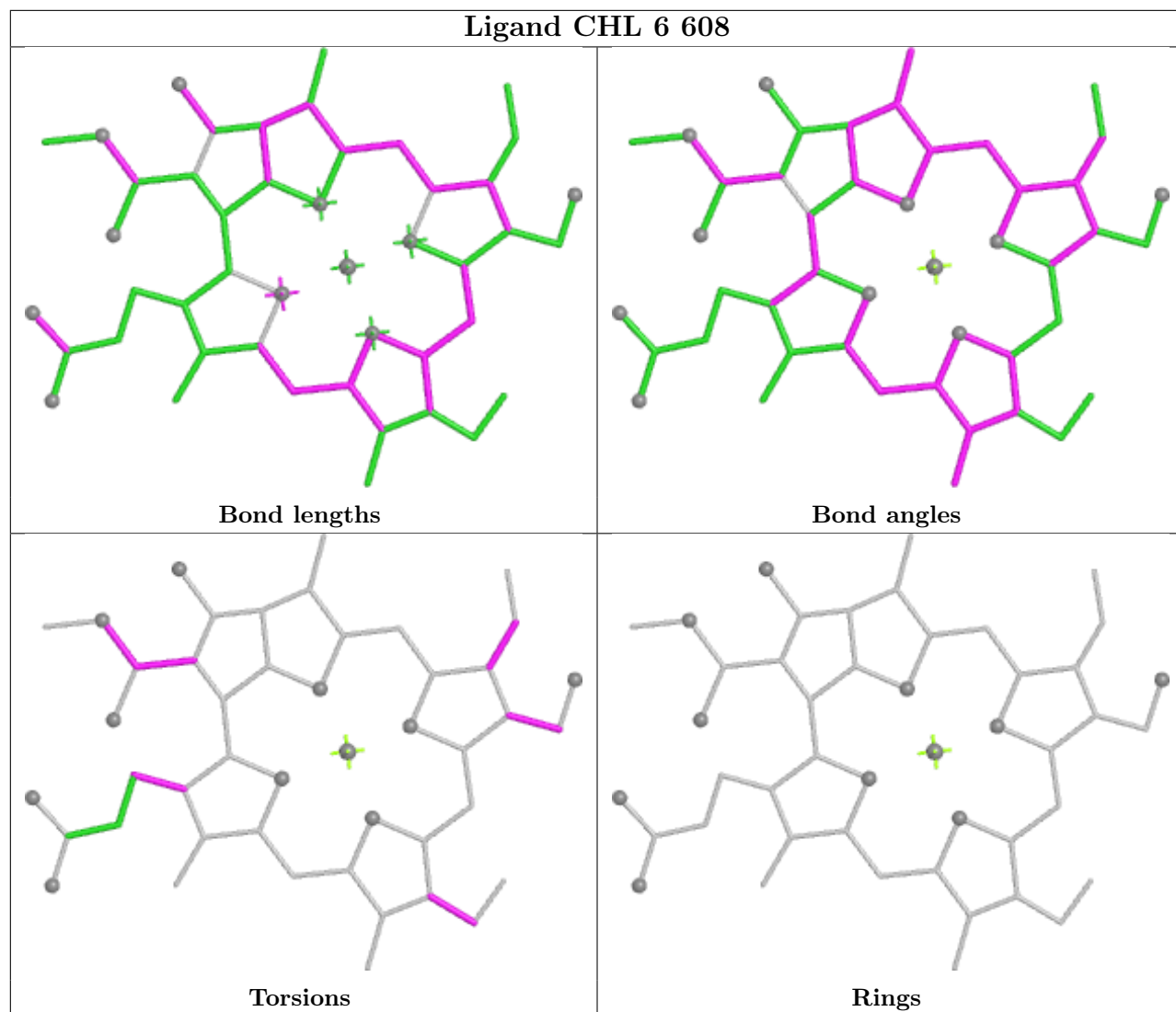
Ligand SQD b 623

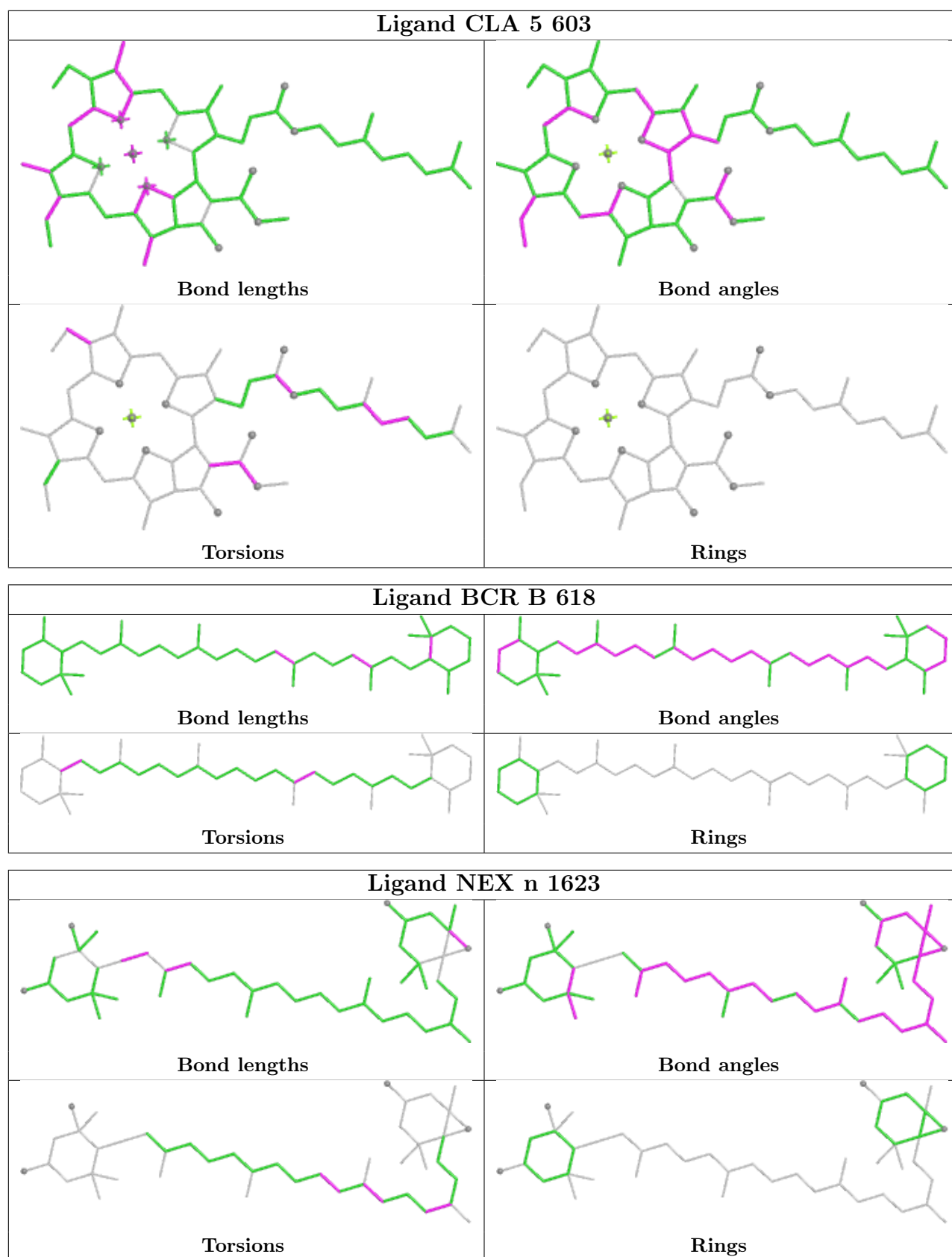


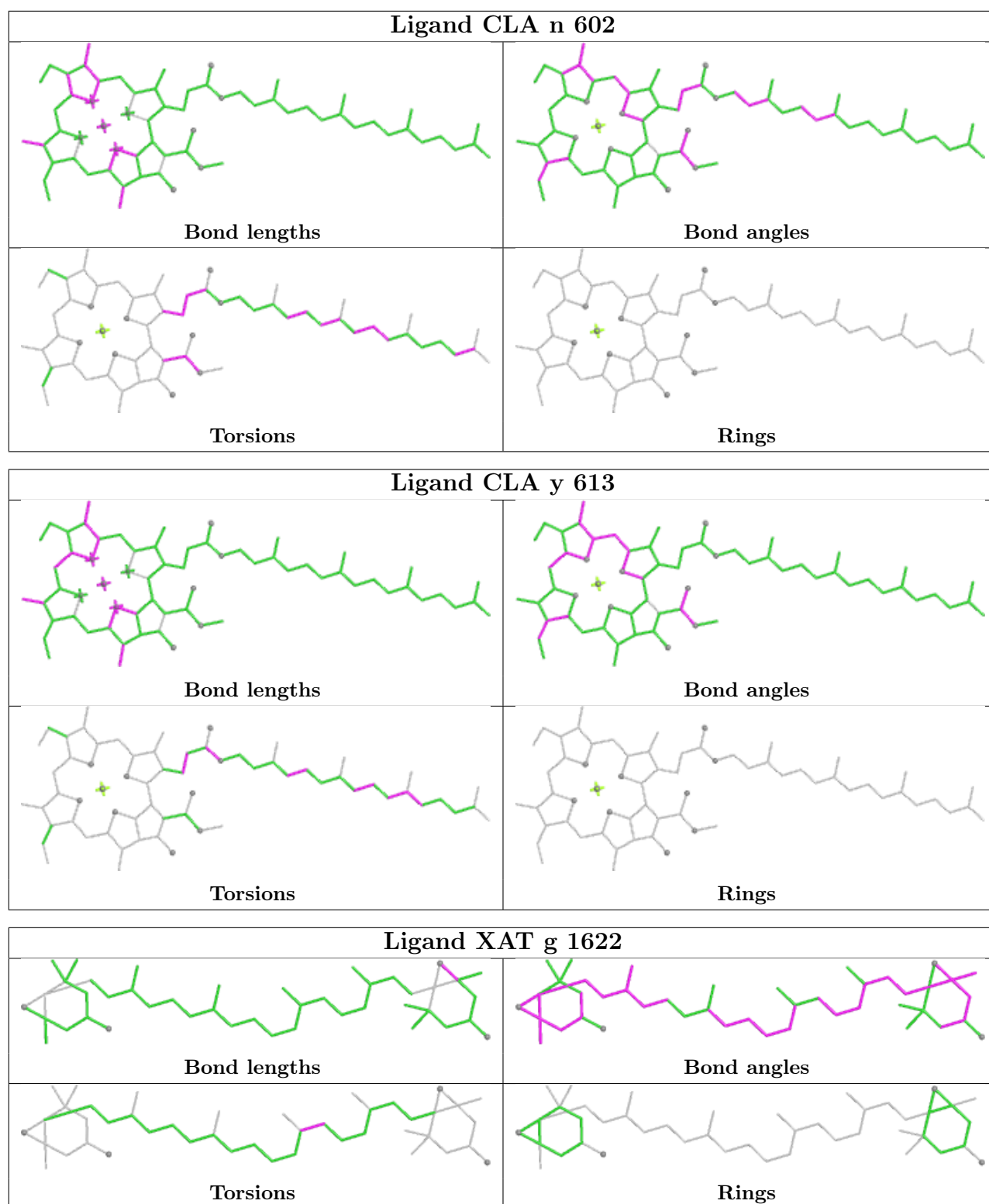
Ligand CLA r 613



Ligand CHL 6 608







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

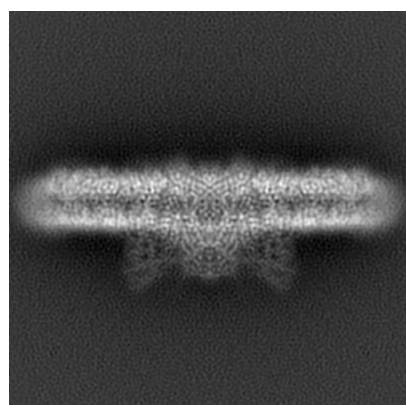
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6742. These allow visual inspection of the internal detail of the map and identification of artifacts.

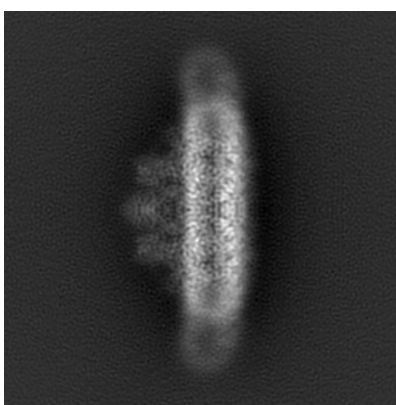
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

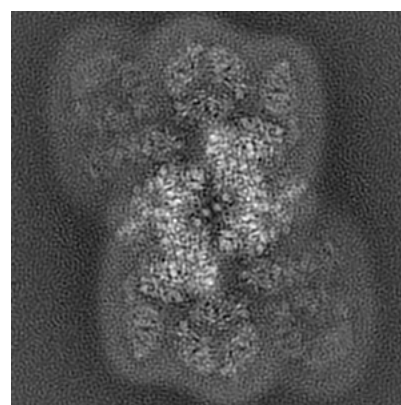
6.1.1 Primary map



X



Y

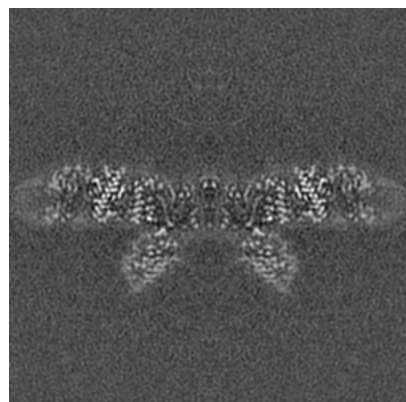


Z

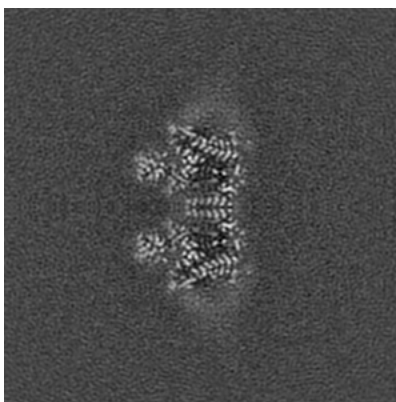
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

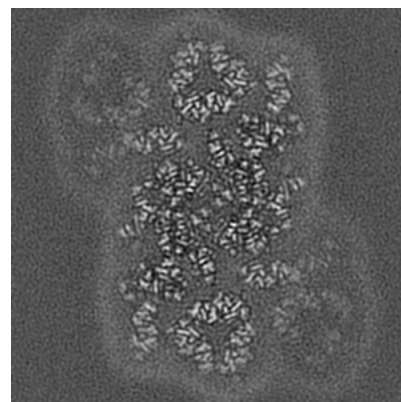
6.2.1 Primary map



X Index: 150



Y Index: 150

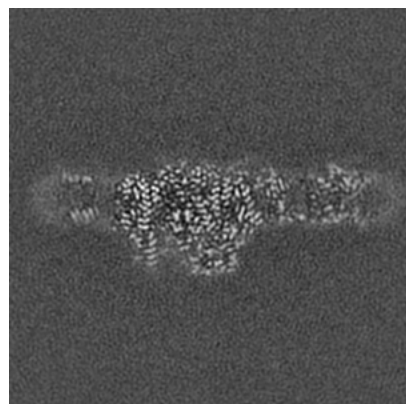


Z Index: 150

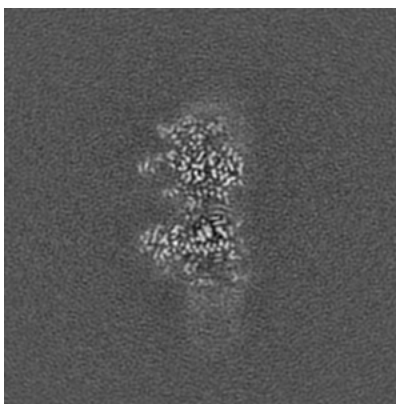
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

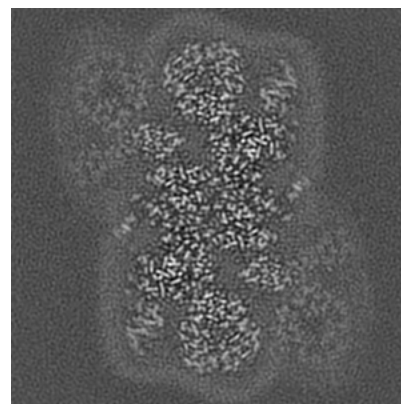
6.3.1 Primary map



X Index: 122



Y Index: 162

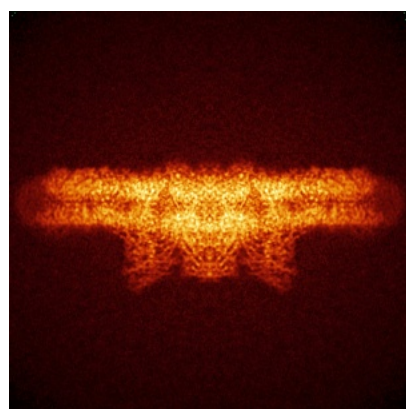


Z Index: 164

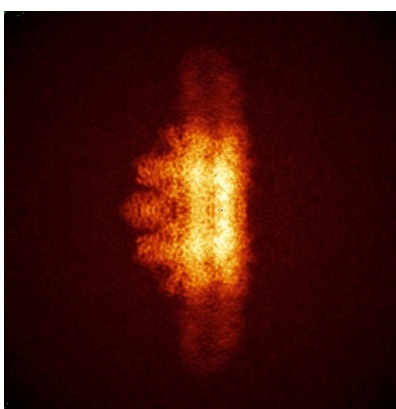
The images above show the largest variance slices of the map in three orthogonal directions.

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

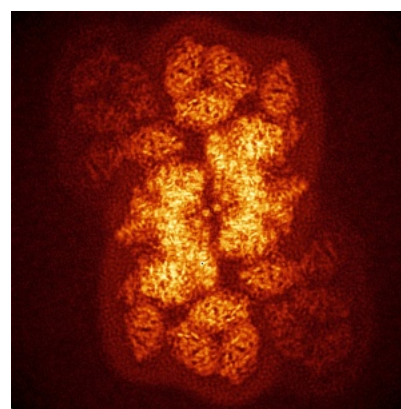
6.4.1 Primary map



X



Y

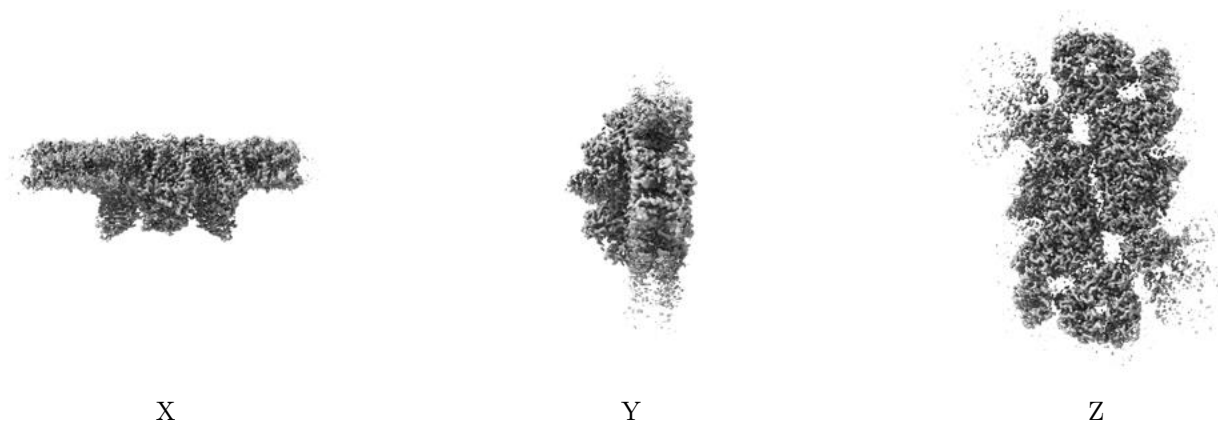


Z

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

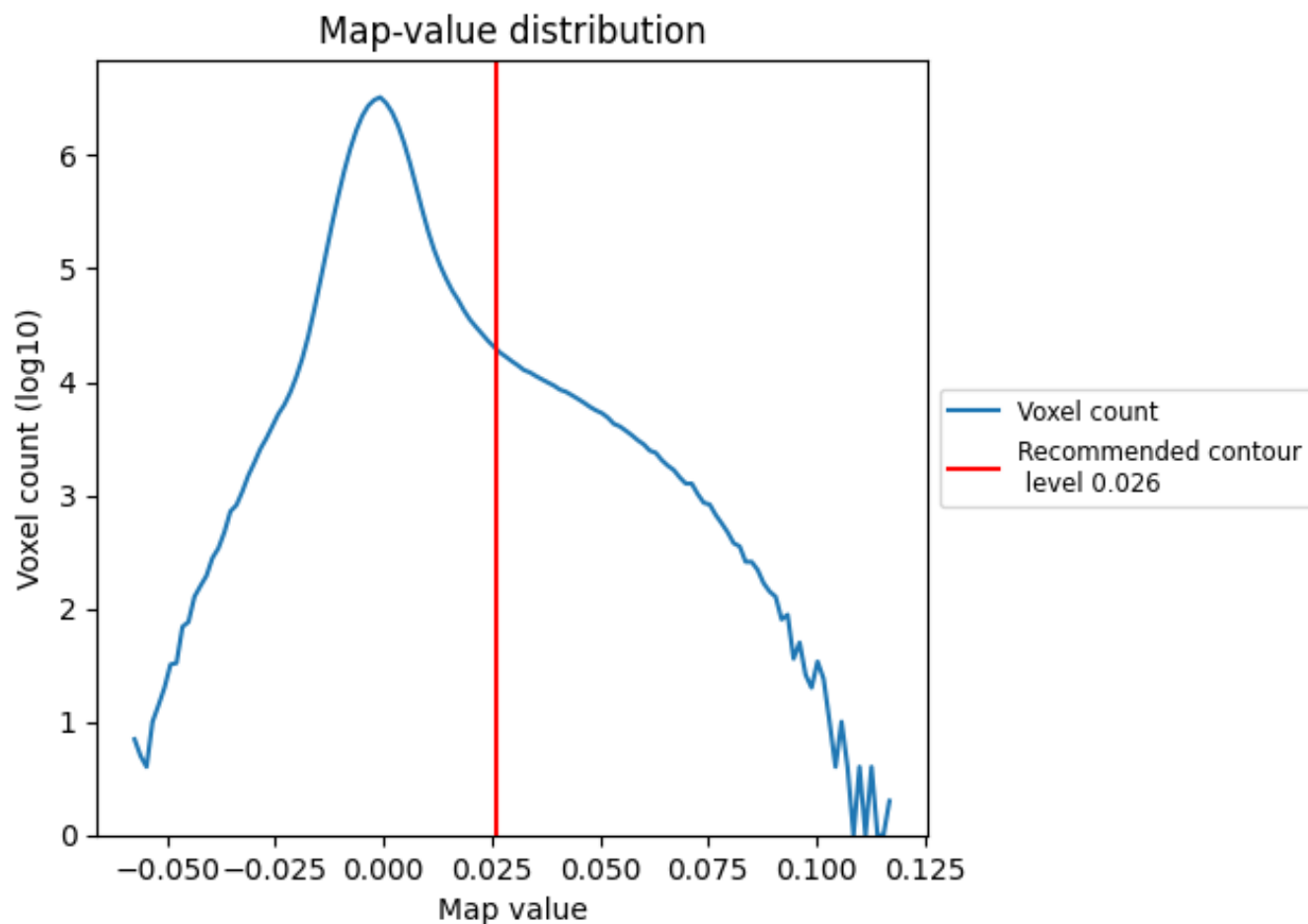
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

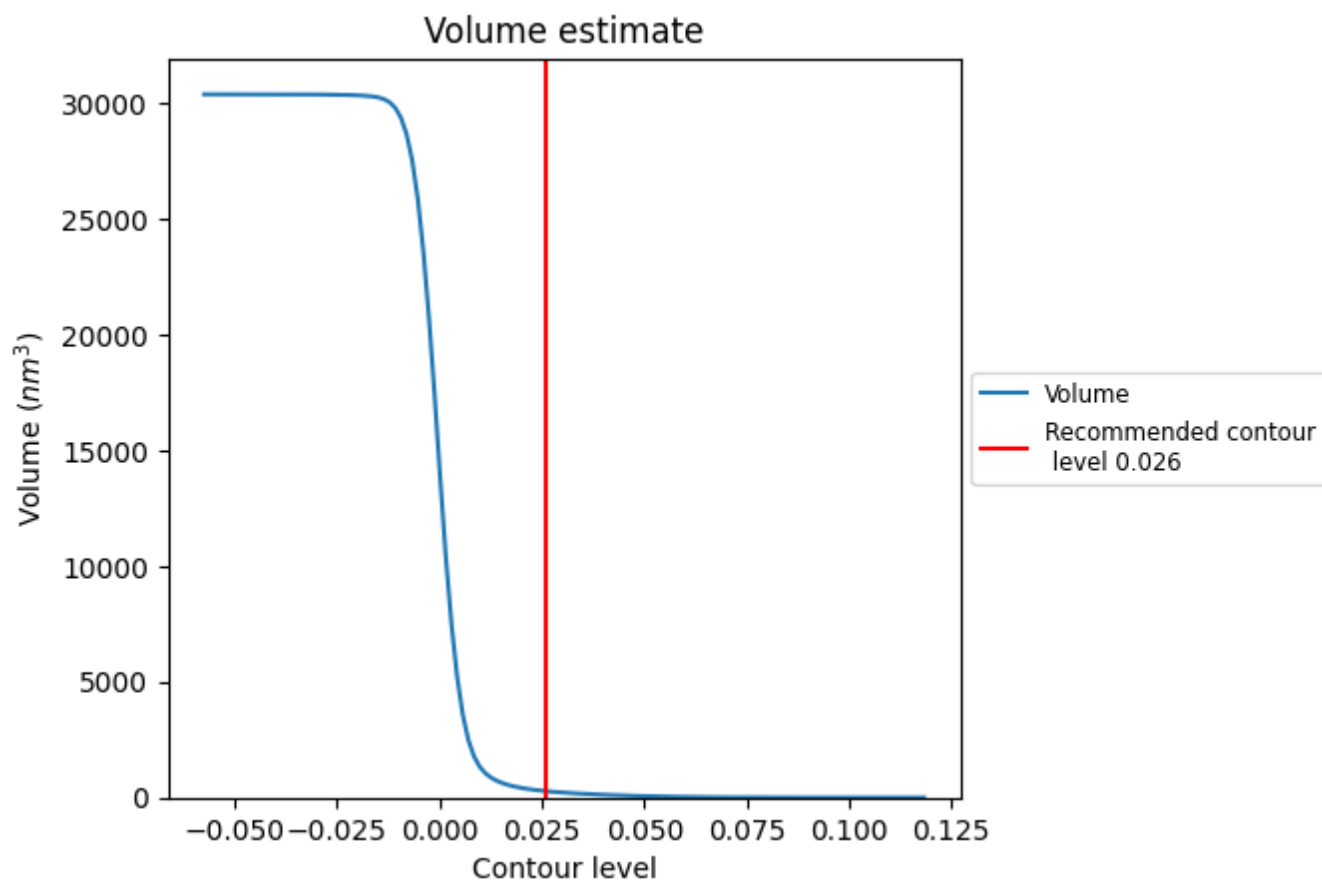
This section contains the results of statistical analysis of the map.

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.

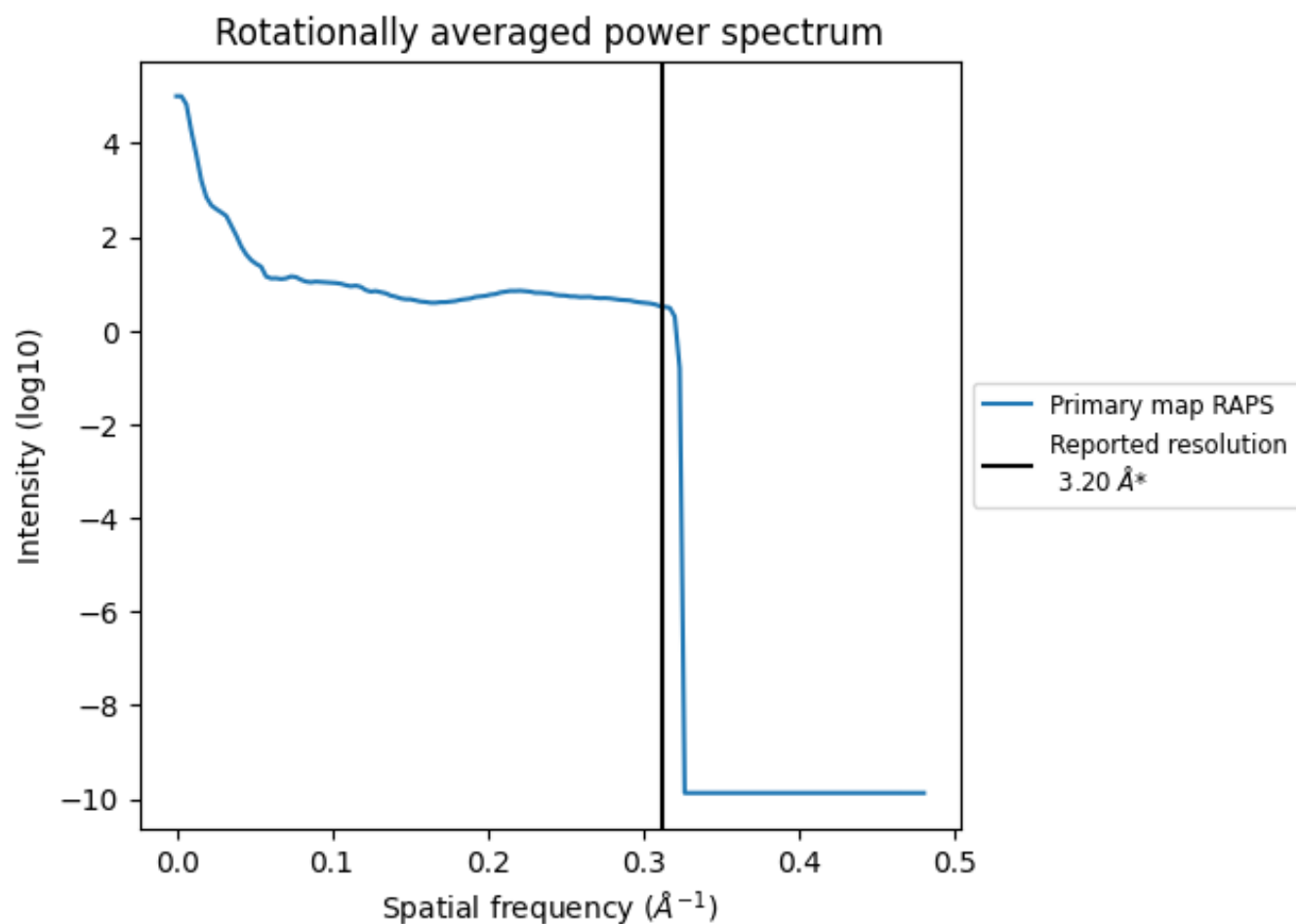
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 249 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 0.312 Å⁻¹

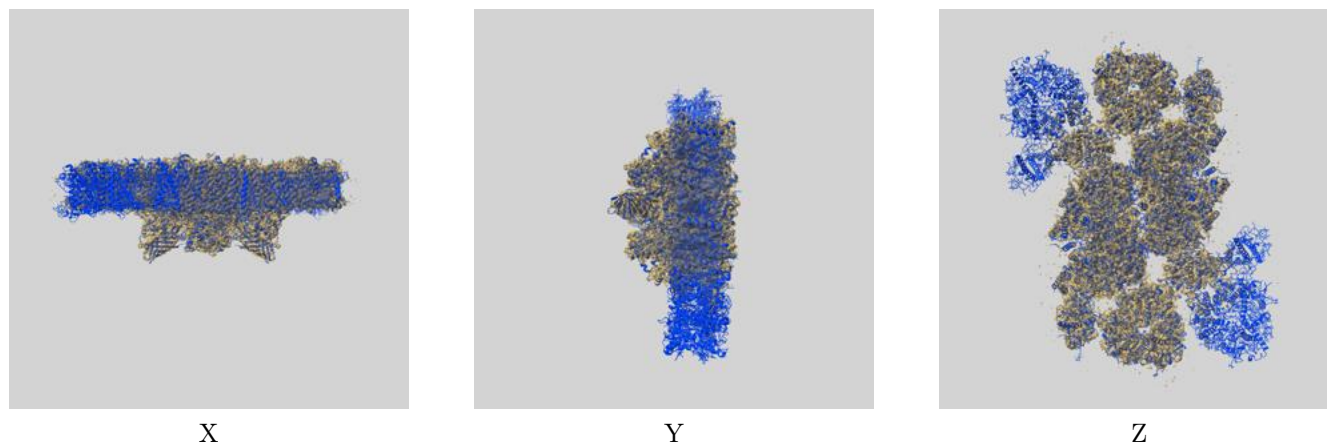
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

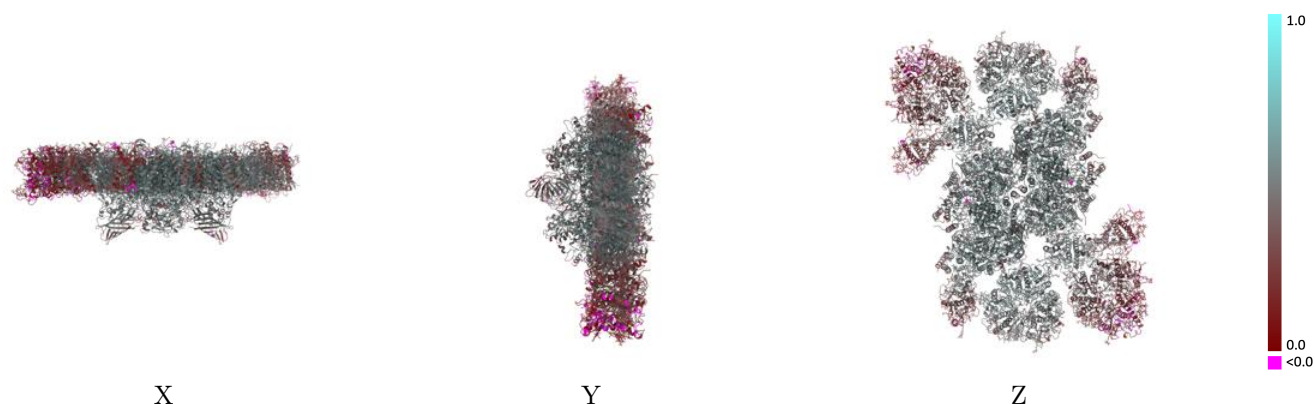
This section contains information regarding the fit between EMDB map EMD-6742 and PDB model 5XNM. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



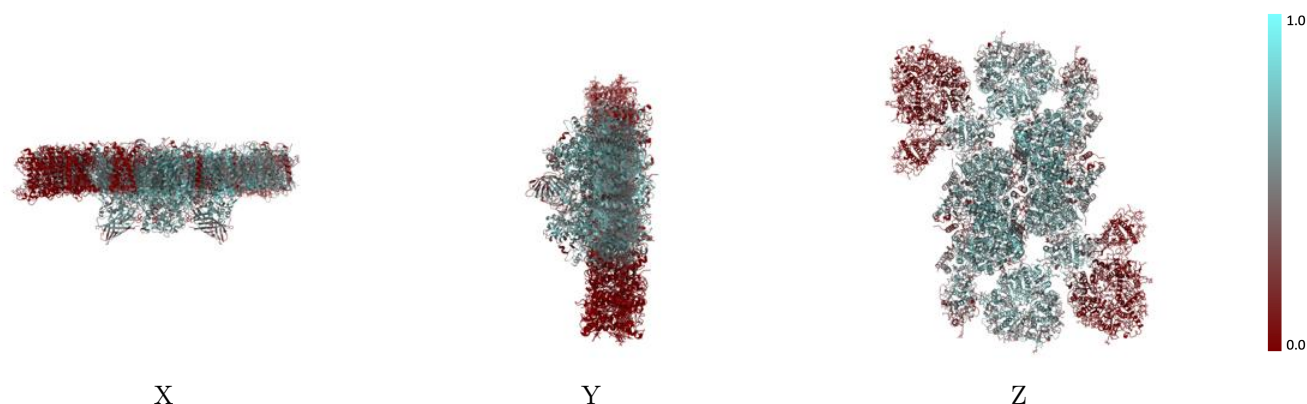
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



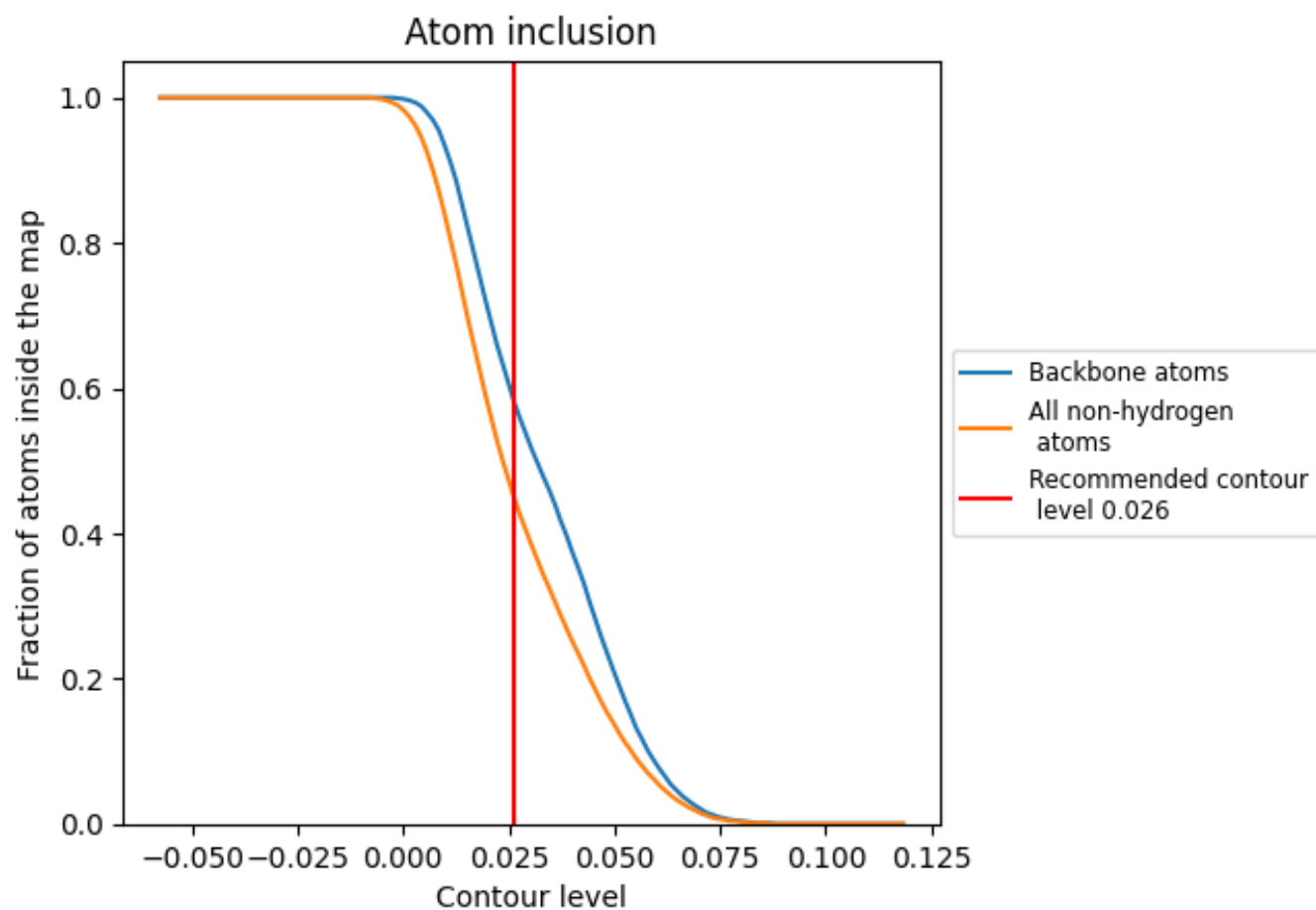
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4540	 0.4380
1	 0.0860	 0.2990
2	 0.0030	 0.1580
3	 0.0400	 0.2970
4	 0.0390	 0.2450
5	 0.0870	 0.2990
6	 0.0030	 0.1560
7	 0.0390	 0.2950
8	 0.0390	 0.2440
A	 0.6450	 0.5320
B	 0.6120	 0.5170
C	 0.5920	 0.5110
D	 0.6600	 0.5410
E	 0.4810	 0.4190
F	 0.5240	 0.4390
G	 0.5320	 0.4690
H	 0.5590	 0.5160
I	 0.6670	 0.5430
J	 0.0910	 0.3730
K	 0.5830	 0.4850
L	 0.5940	 0.5140
M	 0.4780	 0.4670
N	 0.5510	 0.4770
O	 0.4200	 0.4010
R	 0.5310	 0.4820
S	 0.4280	 0.3750
T	 0.5100	 0.5200
U	 0.3420	 0.4140
W	 0.5760	 0.4860
X	 0.4200	 0.4390
Y	 0.6590	 0.5350
Z	 0.3880	 0.4010
a	 0.6480	 0.5320
b	 0.6150	 0.5180
c	 0.5940	 0.5110



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Chain	Atom inclusion	Q-score
d	 0.6580	 0.5400
e	 0.4760	 0.4190
f	 0.5200	 0.4380
g	 0.5310	 0.4630
h	 0.5540	 0.5110
i	 0.6850	 0.5440
j	 0.0950	 0.3710
k	 0.5890	 0.4840
l	 0.5940	 0.5190
m	 0.4670	 0.4620
n	 0.5490	 0.4720
o	 0.4200	 0.4030
r	 0.5260	 0.4830
s	 0.4280	 0.3740
t	 0.5070	 0.5170
u	 0.3480	 0.4170
w	 0.5790	 0.4920
x	 0.4270	 0.4410
y	 0.6610	 0.5320
z	 0.3880	 0.3920