



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 06:25 PM JST

PDB ID : 6KAC / pdb_00006kac
EMDB ID : EMD-9955
Title : Cryo-EM structure of the C2S2-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Sheng, X.; Li, A.J.; Song, D.F.; Liu, Z.F.
Deposited on : 2019-06-21
Resolution : 2.70 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

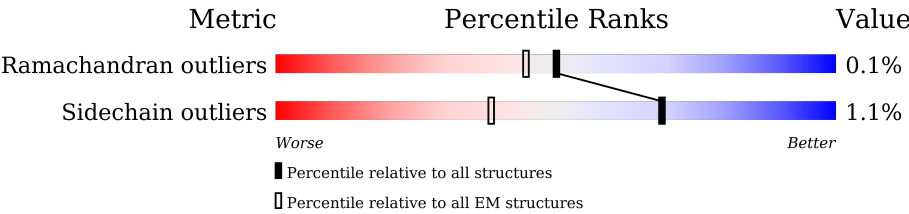
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.










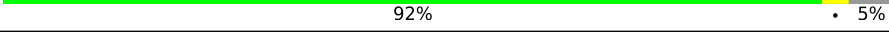



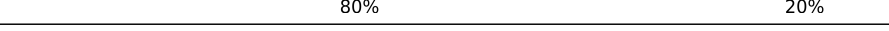







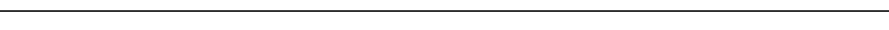

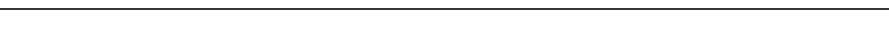
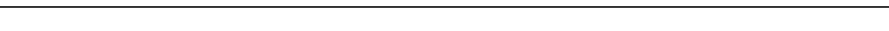


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	352	
1	a	352	
2	B	508	
2	b	508	
3	V	33	
3	v	33	
4	C	461	
4	c	461	
5	D	352	
5	d	352	




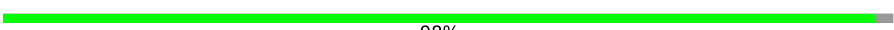
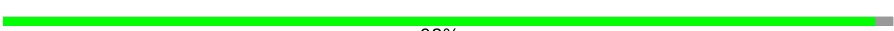





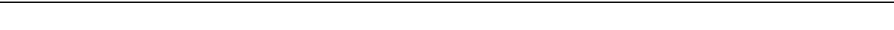

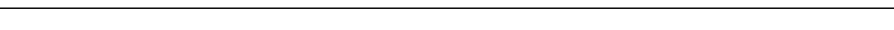
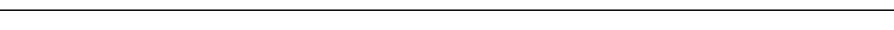
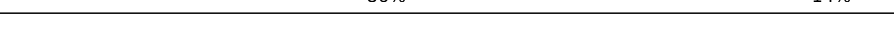



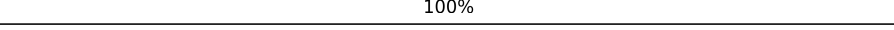
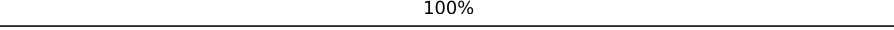
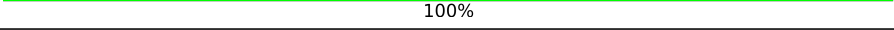
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Mol	Chain	Length	Quality of chain
6	E	82	 91% • 7%
6	e	82	 91% • 7%
7	F	44	 70% 30%
7	f	44	 70% 30%
8	H	88	 75% • 23%
8	h	88	 75% • 23%
9	I	37	 92% • 5%
9	i	37	 92% • 5%
10	J	42	 86% 14%
10	j	42	 86% 14%
11	K	46	 80% 20%
11	k	46	 80% 20%
12	L	38	 84% 8% 8%
12	l	38	 84% 8% 8%
13	M	34	 88% 12%
13	m	34	 88% 12%
14	O	291	 80% • 18%
14	o	291	 80% • 18%
15	P	245	 77% 23%
15	p	245	 76% 23%
16	Q	199	 73% • 26%
16	q	199	 73% • 26%
17	T	31	 94% • •
17	t	31	 94% • •
18	W	115	 48% • 51%

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Mol	Chain	Length	Quality of chain
18	w	115	
19	X	101	
19	x	101	
20	Z	62	
20	z	62	
21	N	257	
21	n	257	
22	G	249	
22	g	249	
23	R	280	
23	r	280	
24	S	289	
24	s	289	
25	Y	256	
25	y	256	
26	U	178	
26	u	178	
27	0	25	
27	1	25	
28	3	25	
28	4	25	

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
32	CLA	A	405	X	-	-	-
32	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	B	602	X	-	-	-
32	CLA	B	603	X	-	-	-
32	CLA	B	605	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-
32	CLA	B	609	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	612	X	-	-	-
32	CLA	B	613	X	-	-	-
32	CLA	B	614	X	-	-	-
32	CLA	B	615	X	-	-	-
32	CLA	B	616	X	-	-	-
32	CLA	B	617	X	-	-	-
32	CLA	C	501	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	504	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	D	402	X	-	-	-
32	CLA	G	602	X	-	-	-
32	CLA	G	603	X	-	-	-
32	CLA	G	604	X	-	-	-
32	CLA	G	610	X	-	-	-
32	CLA	G	611	X	-	-	-
32	CLA	G	612	X	-	-	-
32	CLA	G	614	X	-	-	-
32	CLA	N	602	X	-	-	-
32	CLA	N	603	X	-	-	-
32	CLA	N	604	X	-	-	-
32	CLA	N	610	X	-	-	-
32	CLA	N	611	X	-	-	-
32	CLA	N	612	X	-	-	-
32	CLA	N	614	X	-	-	-
32	CLA	R	602	X	-	-	-
32	CLA	R	603	X	-	-	-
32	CLA	R	604	X	-	-	-
32	CLA	R	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	R	610	X	-	-	-
32	CLA	S	602	X	-	-	-
32	CLA	S	603	X	-	-	-
32	CLA	S	604	X	-	-	-
32	CLA	S	605	X	-	-	-
32	CLA	S	609	X	-	-	-
32	CLA	S	610	X	-	-	-
32	CLA	S	611	X	-	-	-
32	CLA	S	612	X	-	-	-
32	CLA	S	614	X	-	-	-
32	CLA	Y	602	X	-	-	-
32	CLA	Y	603	X	-	-	-
32	CLA	Y	604	X	-	-	-
32	CLA	Y	610	X	-	-	-
32	CLA	Y	611	X	-	-	-
32	CLA	Y	612	X	-	-	-
32	CLA	Y	614	X	-	-	-
32	CLA	a	405	X	-	-	-
32	CLA	a	407	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-
32	CLA	b	616	X	-	-	-
32	CLA	b	617	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	d	402	X	-	-	-
32	CLA	g	602	X	-	-	-
32	CLA	g	603	X	-	-	-
32	CLA	g	604	X	-	-	-
32	CLA	g	610	X	-	-	-
32	CLA	g	611	X	-	-	-
32	CLA	g	612	X	-	-	-
32	CLA	g	614	X	-	-	-
32	CLA	n	602	X	-	-	-
32	CLA	n	603	X	-	-	-
32	CLA	n	604	X	-	-	-
32	CLA	n	610	X	-	-	-
32	CLA	n	611	X	-	-	-
32	CLA	n	612	X	-	-	-
32	CLA	n	614	X	-	-	-
32	CLA	r	602	X	-	-	-
32	CLA	r	603	X	-	-	-
32	CLA	r	604	X	-	-	-
32	CLA	r	609	X	-	-	-
32	CLA	r	610	X	-	-	-
32	CLA	s	602	X	-	-	-
32	CLA	s	603	X	-	-	-
32	CLA	s	604	X	-	-	-
32	CLA	s	605	X	-	-	-
32	CLA	s	609	X	-	-	-
32	CLA	s	610	X	-	-	-
32	CLA	s	611	X	-	-	-
32	CLA	s	612	X	-	-	-
32	CLA	s	614	X	-	-	-
32	CLA	y	602	X	-	-	-
32	CLA	y	603	X	-	-	-
32	CLA	y	604	X	-	-	-
32	CLA	y	610	X	-	-	-
32	CLA	y	611	X	-	-	-
32	CLA	y	612	X	-	-	-
32	CLA	y	614	X	-	-	-
43	CHL	G	601	X	-	-	-
43	CHL	G	605	X	-	-	-
43	CHL	G	606	X	-	-	-
43	CHL	G	607	X	-	-	-
43	CHL	G	608	X	-	-	-
43	CHL	G	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	CHL	N	601	X	-	-	-
43	CHL	N	605	X	-	-	-
43	CHL	N	606	X	-	-	-
43	CHL	N	607	X	-	-	-
43	CHL	N	608	X	-	-	-
43	CHL	N	609	X	-	-	-
43	CHL	R	606	X	-	-	-
43	CHL	R	607	X	-	-	-
43	CHL	R	608	X	-	-	-
43	CHL	S	601	X	-	-	-
43	CHL	S	606	X	-	-	-
43	CHL	S	607	X	-	-	-
43	CHL	S	608	X	-	-	-
43	CHL	Y	601	X	-	-	-
43	CHL	Y	605	X	-	-	-
43	CHL	Y	606	X	-	-	-
43	CHL	Y	607	X	-	-	-
43	CHL	Y	608	X	-	-	-
43	CHL	Y	609	X	-	-	-
43	CHL	g	601	X	-	-	-
43	CHL	g	605	X	-	-	-
43	CHL	g	606	X	-	-	-
43	CHL	g	607	X	-	-	-
43	CHL	g	608	X	-	-	-
43	CHL	g	609	X	-	-	-
43	CHL	n	601	X	-	-	-
43	CHL	n	605	X	-	-	-
43	CHL	n	606	X	-	-	-
43	CHL	n	607	X	-	-	-
43	CHL	n	608	X	-	-	-
43	CHL	n	609	X	-	-	-
43	CHL	r	606	X	-	-	-
43	CHL	r	607	X	-	-	-
43	CHL	r	608	X	-	-	-
43	CHL	s	601	X	-	-	-
43	CHL	s	606	X	-	-	-
43	CHL	s	607	X	-	-	-
43	CHL	s	608	X	-	-	-
43	CHL	y	601	X	-	-	-
43	CHL	y	605	X	-	-	-
43	CHL	y	606	X	-	-	-
43	CHL	y	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	CHL	y	608	X	-	-	-
43	CHL	y	609	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 77947 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		
1	a	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		
2	b	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			224	147	37	40		
3	v	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		
4	c	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		
5	d	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			619	404	102	113			
6	e	76	Total	C	N	O	S	0	0
			619	404	102	113			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	68	Total	C	N	O	S	0	0
			519	347	77	93	2		
8	h	68	Total	C	N	O	S	0	0
			519	347	77	93	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		
9	i	35	Total	C	N	O	S	0	0
			283	193	43	45	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			262	178	40	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			262	178	40	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		
11	k	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		
12	l	35	Total	C	N	O	0	0
			290	196	45	49		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	30	Total	C	N	O	0	0
			230	158	32	40		
13	m	30	Total	C	N	O	0	0
			230	158	32	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		
14	o	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		
15	p	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total	C	N	O	0	0
			1192	746	214	232		
16	q	148	Total	C	N	O	0	0
			1192	746	214	232		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
17	t	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		
18	w	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

- Molecule 19 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	35	Total	C	N	O	0	0
			242	159	39	44		
19	x	35	Total	C	N	O	0	0
			242	159	39	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
20	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
21	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
22	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		
23	r	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		
24	s	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
25	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

- Molecule 26 is a protein called Predicted protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	24	Total	C	N	O	0	0
			184	113	32	39		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	u	24	Total	C	N	O	0	0
			184	113	32	39		

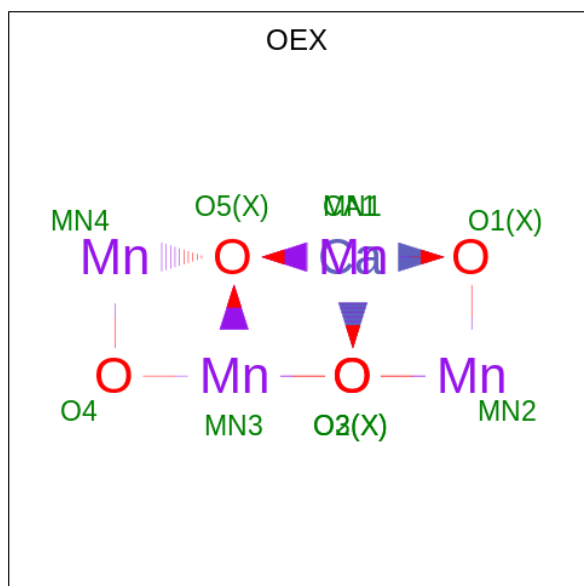
- Molecule 27 is a protein called 10 kDa photosystem II polypeptide PsbR (potential).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	25	Total	C	N	O	0	0
			121	71	25	25		
27	0	25	Total	C	N	O	0	0
			121	71	25	25		

- Molecule 28 is a protein called Unidentified Stromal Protein (USP).

Mol	Chain	Residues	Atoms				AltConf	Trace
28	4	25	Total	C	N	O	0	0
			169	109	29	31		
28	3	25	Total	C	N	O	0	0
			169	109	29	31		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

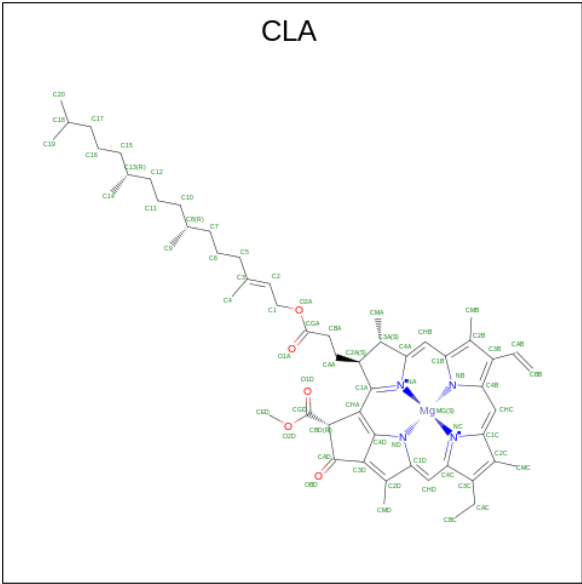
- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Cl	0
			2	2	
31	a	2	Total	Cl	0
			2	2	

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



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

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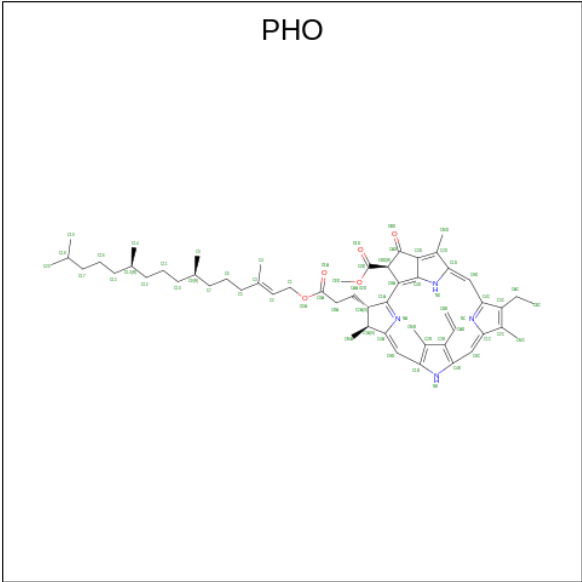
Mol	Chain	Residues	Atoms					AltConf
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	r	1	Total 41	C 33	Mg 1	N 4	O 3	0

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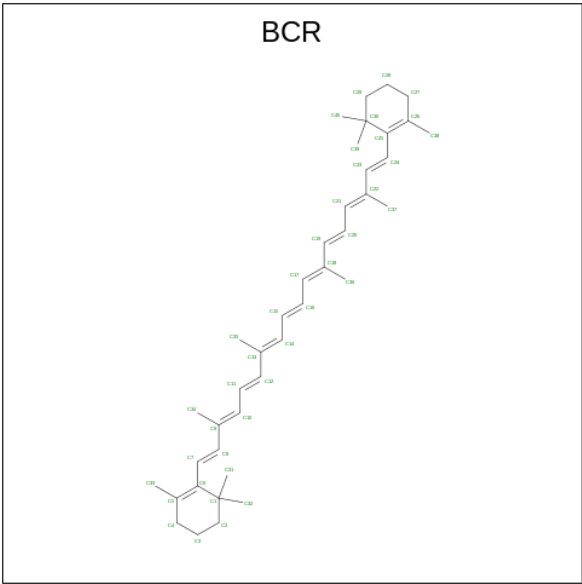
Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



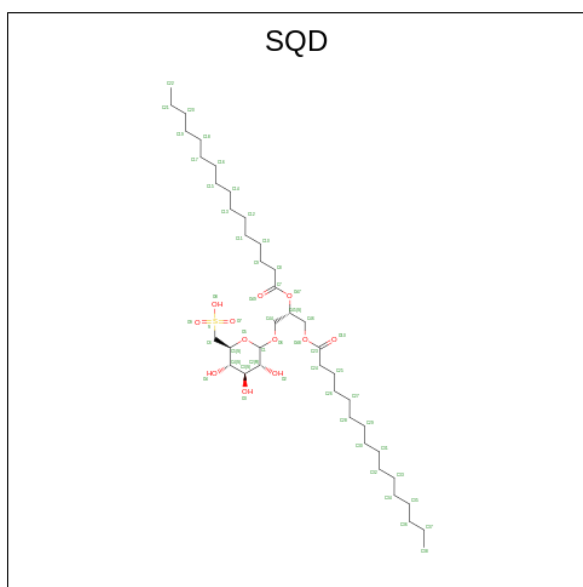
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



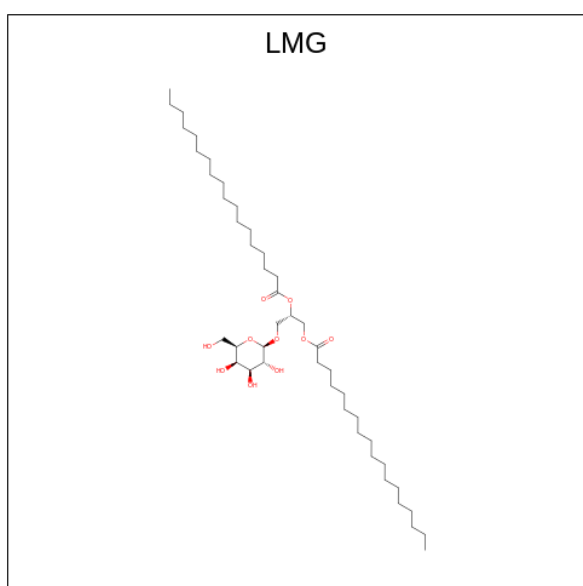
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	D	1	Total C 40 40	0
34	H	1	Total C 40 40	0
34	a	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	b	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	c	1	Total C 40 40	0
34	d	1	Total C 40 40	0
34	h	1	Total C 40 40	0

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



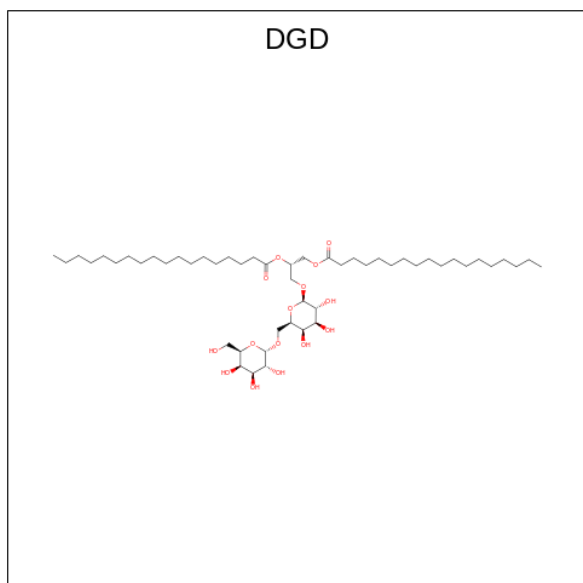
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			54	41	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	
35	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			48	38	10	
36	B	1	Total	C	O	0
			51	41	10	
36	C	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			46	36	10	
36	H	1	Total	C	O	0
			48	38	10	
36	a	1	Total	C	O	0
			48	38	10	
36	b	1	Total	C	O	0
			51	41	10	
36	c	1	Total	C	O	0
			51	41	10	
36	d	1	Total	C	O	0
			46	36	10	
36	h	1	Total	C	O	0
			48	38	10	

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



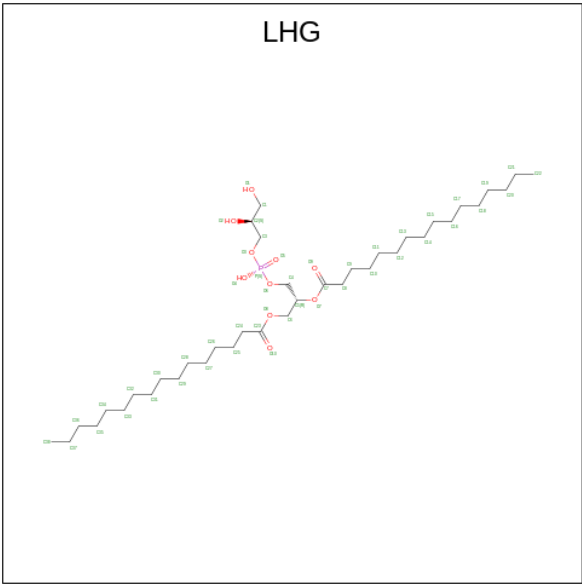
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			55	40	15	

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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
			59	44	15	
37	C	1	Total	C	O	0
			66	51	15	
37	C	1	Total	C	O	0
			66	51	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
			59	44	15	
37	c	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			66	51	15	

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



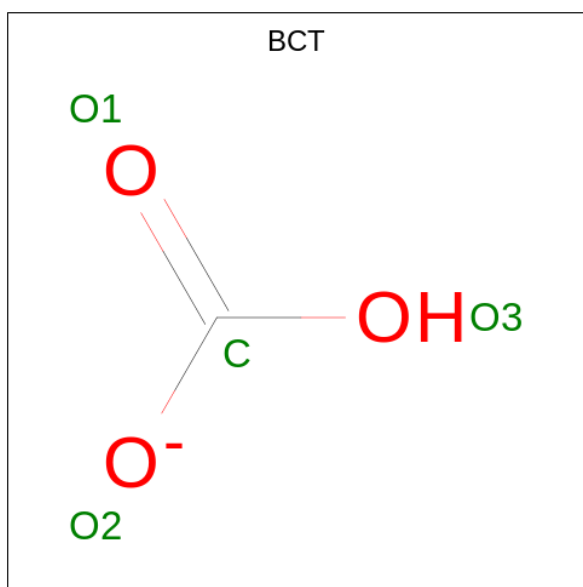
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	

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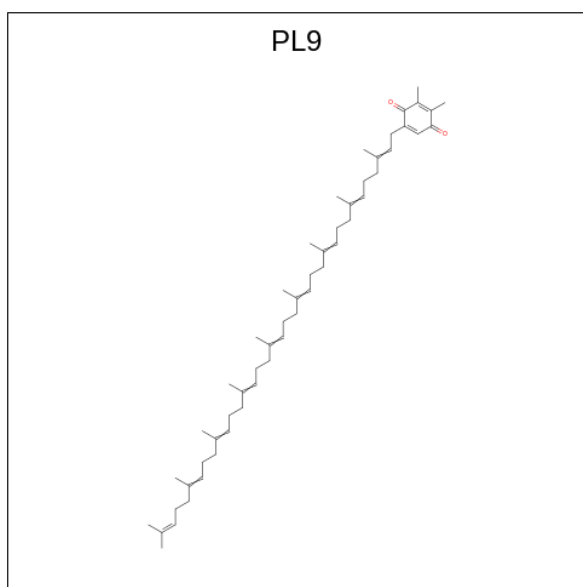
Mol	Chain	Residues	Atoms				AltConf
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			44	33	10	1	
38	d	1	Total	C	O	P	0
			49	38	10	1	
38	d	1	Total	C	O	P	0
			39	28	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	n	1	Total	C	O	P	0
			49	38	10	1	
38	g	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			45	34	10	1	
38	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 40 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).



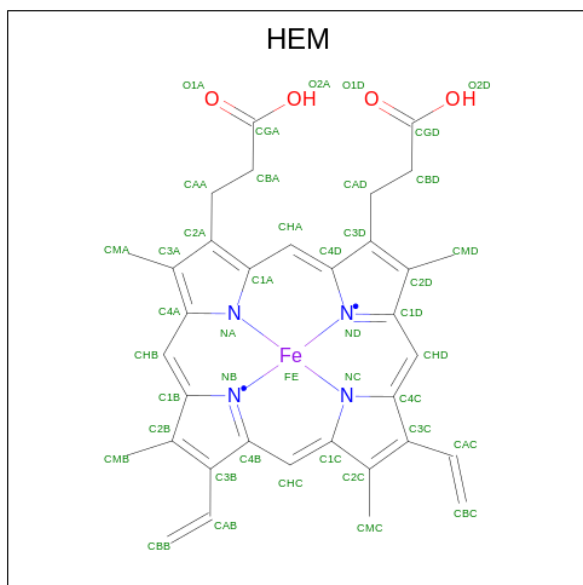
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			55	53	2	

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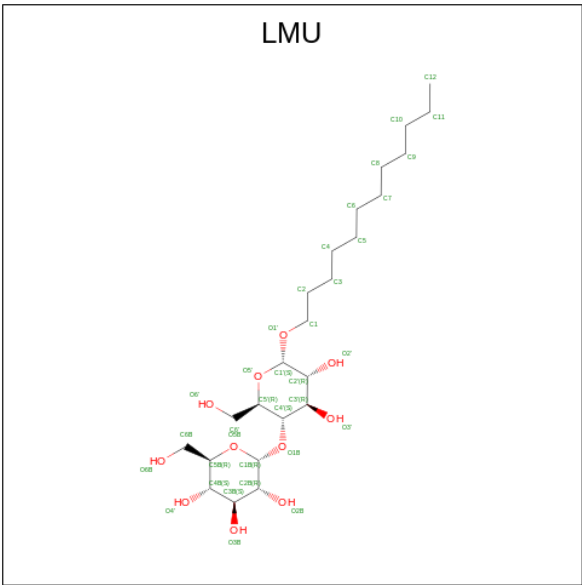
Mol	Chain	Residues	Atoms			AltConf
40	d	1	Total	C	O	0
			55	53	2	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



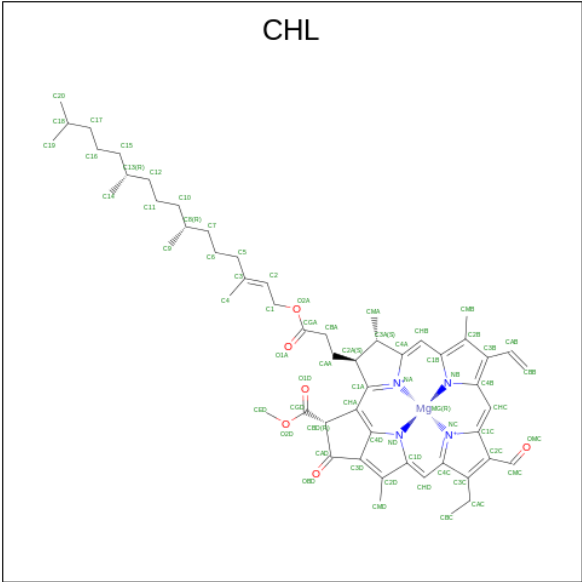
Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
42	Z	1	Total	C	O	0
			35	24	11	
42	Z	1	Total	C	O	0
			35	24	11	
42	Y	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	y	1	Total	C	O	0
			35	24	11	

- Molecule 43 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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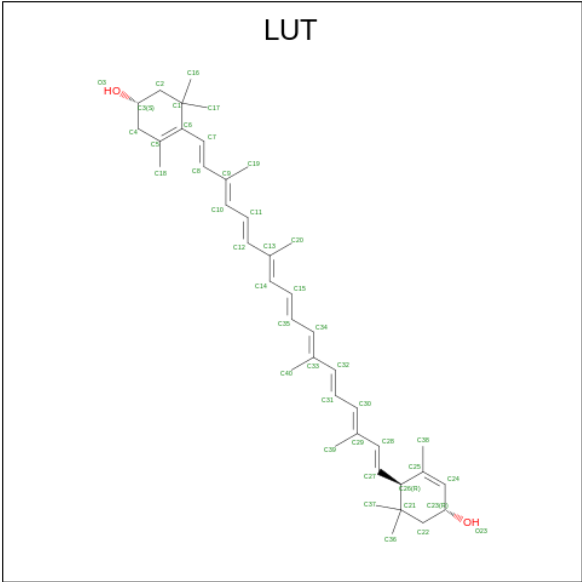
Mol	Chain	Residues	Atoms					AltConf
43	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
43	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
43	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
43	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 44 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



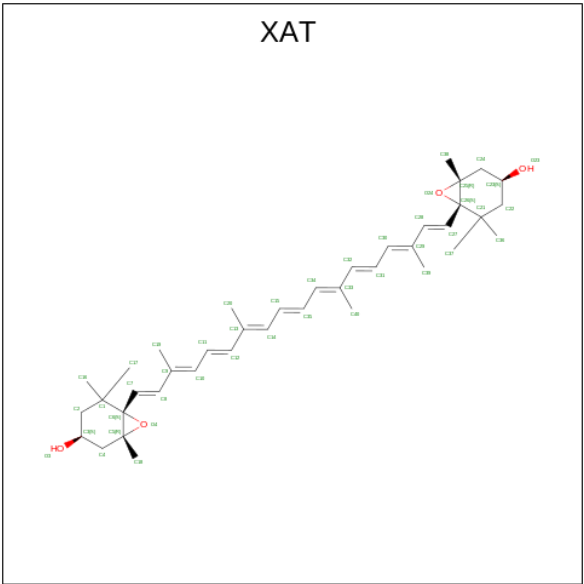
Mol	Chain	Residues	Atoms			AltConf
44	N	1	Total	C	O	0
			42	40	2	
44	N	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	n	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
44	y	1	Total	C	O	0
			42	40	2	
44	y	1	Total	C	O	0
			42	40	2	

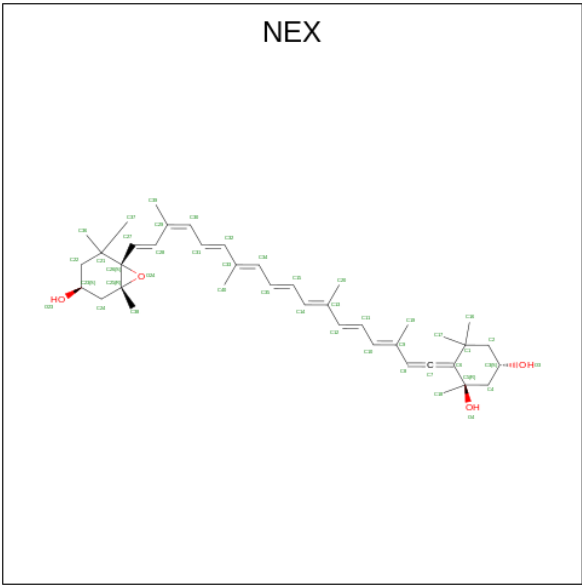
- Molecule 45 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
45	N	1	Total	C	O	0
			44	40	4	
45	G	1	Total	C	O	0
			44	40	4	
45	R	1	Total	C	O	0
			44	40	4	
45	Y	1	Total	C	O	0
			44	40	4	
45	n	1	Total	C	O	0
			44	40	4	
45	g	1	Total	C	O	0
			44	40	4	
45	r	1	Total	C	O	0
			44	40	4	
45	y	1	Total	C	O	0
			44	40	4	

- Molecule 46 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
46	N	1	Total	C	O	0
			44	40	4	
46	G	1	Total	C	O	0
			44	40	4	
46	R	1	Total	C	O	0
			44	40	4	
46	S	1	Total	C	O	0
			44	40	4	
46	Y	1	Total	C	O	0
			44	40	4	
46	n	1	Total	C	O	0
			44	40	4	
46	g	1	Total	C	O	0
			44	40	4	
46	r	1	Total	C	O	0
			44	40	4	
46	s	1	Total	C	O	0
			44	40	4	
46	y	1	Total	C	O	0
			44	40	4	

- Molecule 47 is water.

Mol	Chain	Residues	Atoms		AltConf
47	A	40	Total 40	O 40	0
47	B	57	Total 57	O 57	0
47	V	6	Total 6	O 6	0
47	C	28	Total 28	O 28	0
47	D	28	Total 28	O 28	0
47	E	6	Total 6	O 6	0
47	F	3	Total 3	O 3	0
47	H	7	Total 7	O 7	0
47	I	5	Total 5	O 5	0
47	J	1	Total 1	O 1	0
47	L	1	Total 1	O 1	0
47	M	3	Total 3	O 3	0
47	O	43	Total 43	O 43	0
47	P	23	Total 23	O 23	0
47	Q	20	Total 20	O 20	0
47	T	3	Total 3	O 3	0
47	W	3	Total 3	O 3	0
47	X	1	Total 1	O 1	0
47	Z	3	Total 3	O 3	0
47	N	3	Total 3	O 3	0
47	G	6	Total 6	O 6	0
47	Y	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
47	a	40	Total 40	O 40	0
47	b	57	Total 57	O 57	0
47	v	6	Total 6	O 6	0
47	c	28	Total 28	O 28	0
47	d	28	Total 28	O 28	0
47	e	6	Total 6	O 6	0
47	f	3	Total 3	O 3	0
47	h	7	Total 7	O 7	0
47	i	5	Total 5	O 5	0
47	j	1	Total 1	O 1	0
47	l	1	Total 1	O 1	0
47	m	2	Total 2	O 2	0
47	o	43	Total 43	O 43	0
47	p	23	Total 23	O 23	0
47	q	20	Total 20	O 20	0
47	t	3	Total 3	O 3	0
47	w	3	Total 3	O 3	0
47	x	1	Total 1	O 1	0
47	z	3	Total 3	O 3	0
47	n	3	Total 3	O 3	0
47	g	6	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
47	y	8	Total	O	0
			8	8	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1

Chain A:  94% 5%



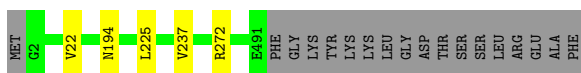
- Molecule 1: Photosystem II protein D1

Chain a:  94% 5%



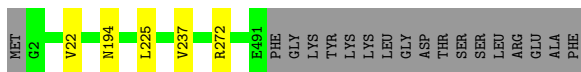
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  95%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  95%



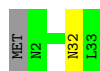
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  94%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  94%



- Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 95%



- Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 96%



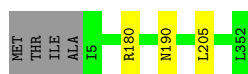
- Molecule 5: Photosystem II D2 protein

Chain D: 98%



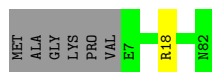
- Molecule 5: Photosystem II D2 protein

Chain d: 98%



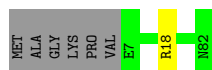
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 91% 7%



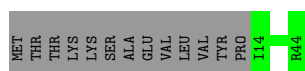
- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 91% 7%

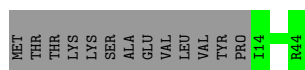


- Molecule 7: Cytochrome b559 subunit beta

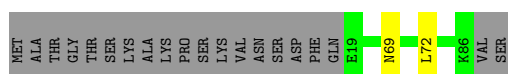
Chain F: 70% 30%



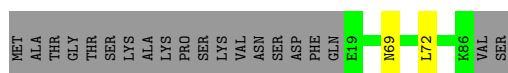
- Molecule 7: Cytochrome b559 subunit beta



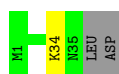
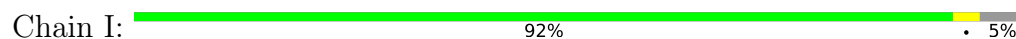
- Molecule 8: Photosystem II reaction center protein H



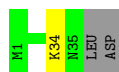
- Molecule 8: Photosystem II reaction center protein H



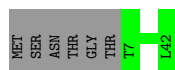
- Molecule 9: Photosystem II reaction center protein I



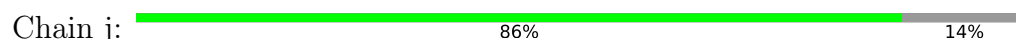
- Molecule 9: Photosystem II reaction center protein I

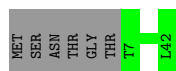


- Molecule 10: Photosystem II reaction center protein J

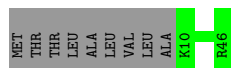
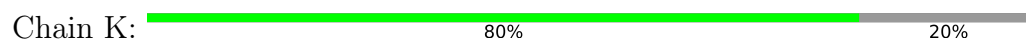


- Molecule 10: Photosystem II reaction center protein J

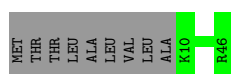
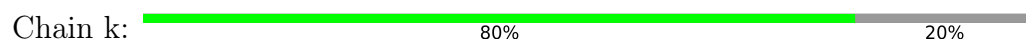




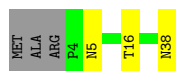
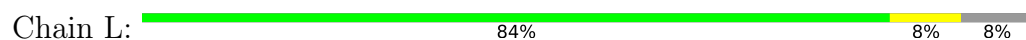
- Molecule 11: Photosystem II reaction center protein K



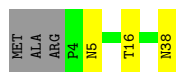
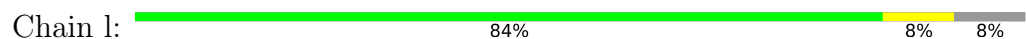
- Molecule 11: Photosystem II reaction center protein K



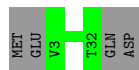
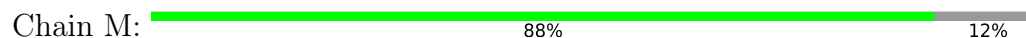
- Molecule 12: Photosystem II reaction center protein L



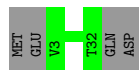
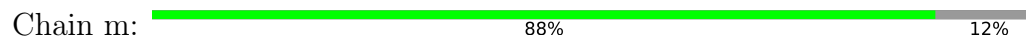
- Molecule 12: Photosystem II reaction center protein L



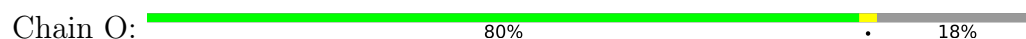
- Molecule 13: Photosystem II reaction center protein M

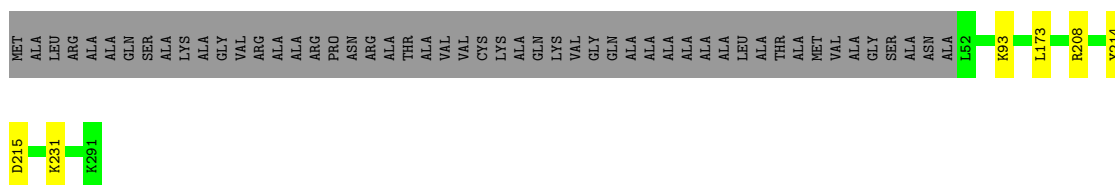


- Molecule 13: Photosystem II reaction center protein M



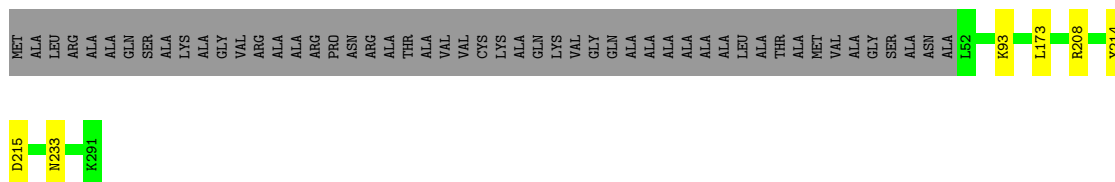
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic





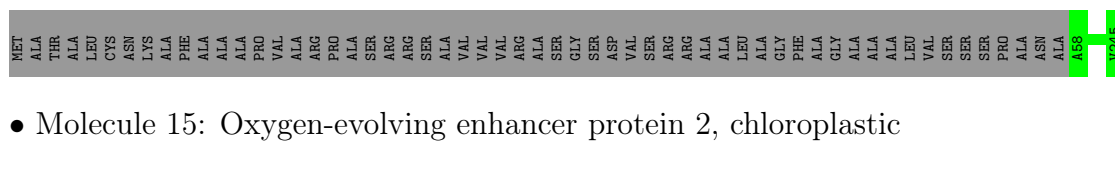
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 80% 18%



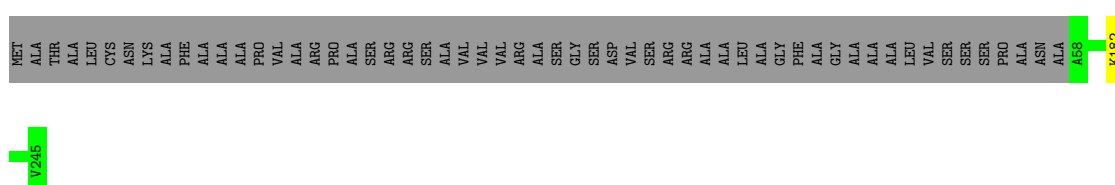
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P: 77% 23%



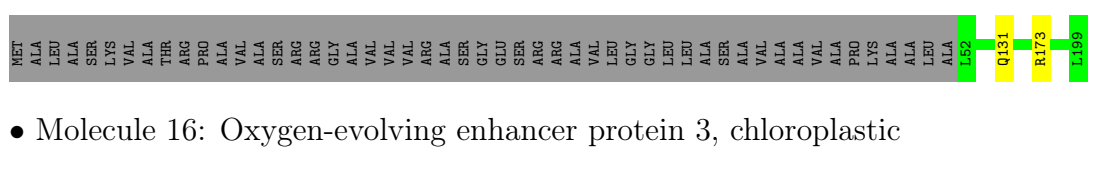
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p: 76% 23%



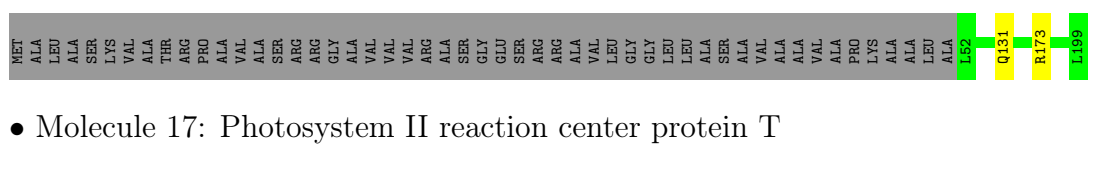
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain Q: 73% 26%



- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain q: 73% 26%



- Molecule 17: Photosystem II reaction center protein T

Chain T:

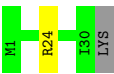
94%



• Molecule 17: Photosystem II reaction center protein T

Chain t:

94%

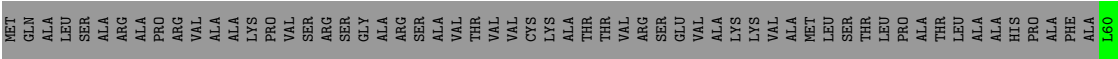


• Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain W:

48%

51%

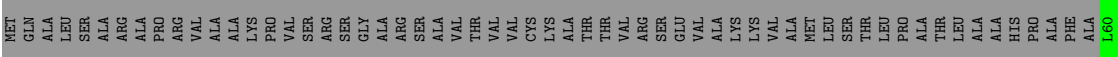


• Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain w:

48%

51%

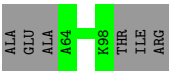
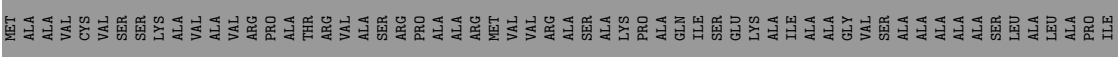


• Molecule 19: 4.1 kDa photosystem II subunit

Chain X:

35%

65%

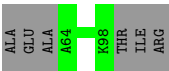


• Molecule 19: 4.1 kDa photosystem II subunit

Chain x:

35%

65%



- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  98% .




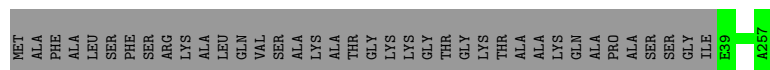
- Molecule 20: Photosystem II reaction center protein Z

Chain z:  98% .




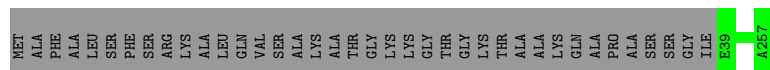
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain N:  85% 15%




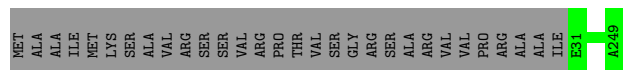
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain n:  85% 15%




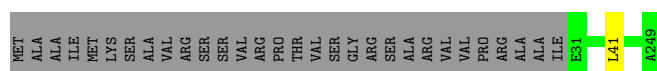
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain G:  88% 12%



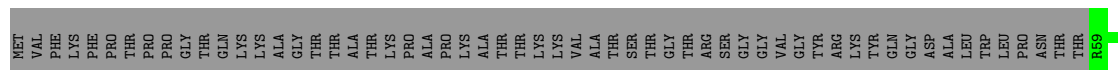
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain g:  88% 12%



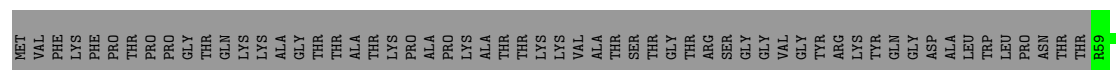
- Molecule 23: Chlorophyll a-b binding protein CP29

Chain R:  65% 35%



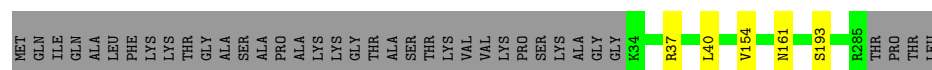
- Molecule 23: Chlorophyll a-b binding protein CP29

Chain r: 65% 35%

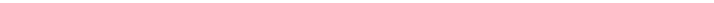


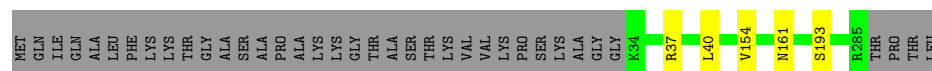
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain S: 85% • 13%



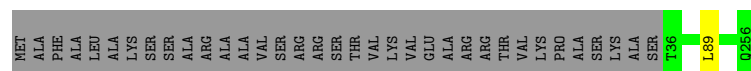
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain s:  85% • 13%



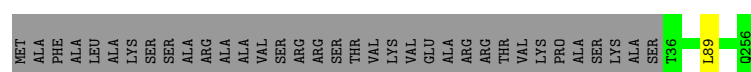
- Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain Y: 86% 14%



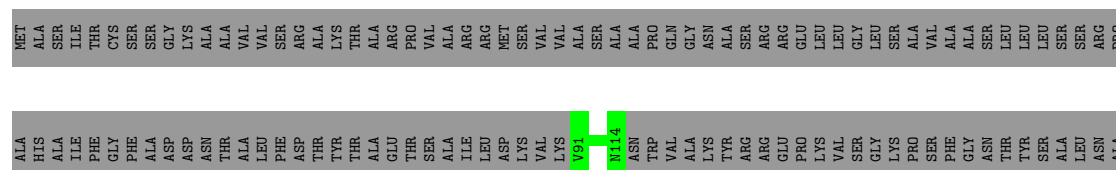
- Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain y: 86% 14%



- Molecule 26: Predicted protein

Chain U: 13% 87%



LEU ALA GLY HIS PHE ASN SER PHE GLY THR ALA PRO ILE PRO LYS LYS ARG LEU GLU ARG LEU GLN LYS LEU ASP ASP ALA THR LEU THR ASN ARG

- Molecule 26: Predicted protein

Chain u:  13% 87%

MET ALA SER ILE THR CYS SER SER GLY LYS ALA VAL VAL SER ARG LYS THR LYS THR ALA ARG PRO VAL ARG ARG MET SER VAL VAL ALA SER ALA PRO GLN GLY ASN ALA SER ARG ARG GLU LEU LEU GLY SER VAL VAL ALA SER LEU LEU SER ARG PRO

ALA HIS ALA ILE PHE GLY PHE ALA ASP ASN THR ALA THR ALA LEU PHE ASP THR TVR THR ALA GLU THR SER VAL ILE LEU ASP LYS VAL LYS V91 V114 ASN TRP VAL ALA LYS TYR ARG ARG GLU PRO LYS VAL SER GLY LYS PRO SER PHE GLY ASN THR TYR SER ALA LEU SER ARG PRO

LEU ALA GLY HIS PHE ASN SER PHE GLY THR ALA PRO ILE PRO LYS LYS ARG LEU GLU ARG LEU GLN LYS LEU ASP ASP ALA THR LEU THR ASN ARG

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 3:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	258242	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 ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2718	0.60	0/3706
1	a	0.50	0/2718	0.60	0/3706
2	B	0.44	0/3964	0.57	1/5397 (0.0%)
2	b	0.44	0/3964	0.57	1/5397 (0.0%)
3	V	0.31	0/224	0.65	0/307
3	v	0.30	0/224	0.69	0/307
4	C	0.48	0/3619	0.57	1/4931 (0.0%)
4	c	0.48	0/3619	0.57	1/4931 (0.0%)
5	D	0.50	0/2866	0.62	1/3909 (0.0%)
5	d	0.49	0/2866	0.62	1/3909 (0.0%)
6	E	0.37	0/637	0.53	0/869
6	e	0.37	0/637	0.53	0/869
7	F	0.32	0/258	0.54	0/349
7	f	0.31	0/258	0.55	0/349
8	H	0.36	0/530	0.61	1/725 (0.1%)
8	h	0.36	0/530	0.61	1/725 (0.1%)
9	I	0.47	0/291	0.59	0/394
9	i	0.47	0/291	0.59	0/394
10	J	0.32	0/268	0.60	0/366
10	j	0.33	0/268	0.60	0/366
11	K	0.47	0/309	0.65	0/425
11	k	0.47	0/309	0.65	0/425
12	L	0.42	0/298	0.55	0/405
12	l	0.42	0/298	0.55	0/405
13	M	0.38	0/234	0.54	0/321
13	m	0.38	0/234	0.54	0/321
14	O	0.38	0/1839	0.64	3/2482 (0.1%)
14	o	0.38	0/1839	0.64	3/2482 (0.1%)
15	P	0.33	0/1473	0.57	0/1987
15	p	0.33	0/1473	0.56	0/1987
16	Q	0.30	0/1204	0.52	0/1616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	q	0.30	0/1204	0.52	0/1616
17	T	0.38	0/254	0.54	0/343
17	t	0.38	0/254	0.54	0/343
18	W	0.40	0/445	0.59	0/603
18	w	0.40	0/445	0.59	0/603
19	X	0.27	0/244	0.52	0/330
19	x	0.28	0/244	0.52	0/330
20	Z	0.31	0/469	0.55	0/644
20	z	0.32	0/469	0.55	0/644
21	N	0.35	0/1720	0.53	0/2341
21	n	0.35	0/1720	0.53	0/2341
22	G	0.33	0/1717	0.52	0/2337
22	g	0.33	0/1717	0.52	0/2337
23	R	0.32	0/1429	0.55	0/1934
23	r	0.32	0/1429	0.55	0/1934
24	S	0.36	0/1968	0.57	1/2679 (0.0%)
24	s	0.36	0/1968	0.57	1/2679 (0.0%)
25	Y	0.40	0/1746	0.56	1/2375 (0.0%)
25	y	0.40	0/1746	0.55	1/2375 (0.0%)
26	U	0.30	0/184	0.66	0/246
26	u	0.30	0/184	0.66	0/246
27	0	0.26	0/120	0.35	0/164
27	1	0.26	0/120	0.35	0/164
28	3	0.35	0/174	0.63	0/237
28	4	0.33	0/174	0.63	0/237
All	All	0.41	0/62404	0.57	18/84844 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	215	ASP	CB-CG-OD1	8.52	125.97	118.30
14	o	215	ASP	CB-CG-OD1	8.40	125.86	118.30
25	Y	89	LEU	CA-CB-CG	6.97	131.33	115.30
25	y	89	LEU	CA-CB-CG	6.96	131.30	115.30
4	C	368	LEU	CA-CB-CG	6.46	130.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
1	a	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
2	B	488/508 (96%)	477 (98%)	11 (2%)	0	100	100
2	b	488/508 (96%)	478 (98%)	10 (2%)	0	100	100
3	V	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
3	v	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
4	C	447/461 (97%)	421 (94%)	25 (6%)	1 (0%)	44	68
4	c	447/461 (97%)	422 (94%)	24 (5%)	1 (0%)	44	68
5	D	346/352 (98%)	334 (96%)	12 (4%)	0	100	100
5	d	346/352 (98%)	332 (96%)	14 (4%)	0	100	100
6	E	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
6	e	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
7	F	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
7	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
8	H	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
8	h	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
9	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
9	i	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
10	J	34/42 (81%)	34 (100%)	0	0	100	100
10	j	34/42 (81%)	34 (100%)	0	0	100	100
11	K	35/46 (76%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	k	35/46 (76%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
12	l	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
13	M	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
13	m	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
14	O	238/291 (82%)	224 (94%)	14 (6%)	0	100	100
14	o	238/291 (82%)	221 (93%)	17 (7%)	0	100	100
15	P	186/245 (76%)	180 (97%)	6 (3%)	0	100	100
15	p	186/245 (76%)	179 (96%)	7 (4%)	0	100	100
16	Q	146/199 (73%)	139 (95%)	7 (5%)	0	100	100
16	q	146/199 (73%)	138 (94%)	8 (6%)	0	100	100
17	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
17	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
18	W	54/115 (47%)	50 (93%)	4 (7%)	0	100	100
18	w	54/115 (47%)	50 (93%)	4 (7%)	0	100	100
19	X	33/101 (33%)	31 (94%)	2 (6%)	0	100	100
19	x	33/101 (33%)	32 (97%)	1 (3%)	0	100	100
20	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
21	N	217/257 (84%)	202 (93%)	15 (7%)	0	100	100
21	n	217/257 (84%)	201 (93%)	16 (7%)	0	100	100
22	G	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
22	g	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
23	R	179/280 (64%)	169 (94%)	10 (6%)	0	100	100
23	r	179/280 (64%)	167 (93%)	12 (7%)	0	100	100
24	S	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	55
24	s	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	55
25	Y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
25	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
26	U	22/178 (12%)	19 (86%)	3 (14%)	0	100	100
26	u	22/178 (12%)	19 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	23/25 (92%)	23 (100%)	0	0	100	100
27	1	23/25 (92%)	23 (100%)	0	0	100	100
28	3	23/25 (92%)	17 (74%)	6 (26%)	0	100	100
28	4	23/25 (92%)	18 (78%)	5 (22%)	0	100	100
All	All	7742/9440 (82%)	7357 (95%)	381 (5%)	4 (0%)	50	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	211	TRP
4	c	211	TRP
24	S	193	SER
24	s	193	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/289 (95%)	270 (98%)	4 (2%)	60	83
1	a	274/289 (95%)	270 (98%)	4 (2%)	60	83
2	B	392/407 (96%)	388 (99%)	4 (1%)	73	89
2	b	392/407 (96%)	388 (99%)	4 (1%)	73	89
3	V	26/27 (96%)	25 (96%)	1 (4%)	28	56
3	v	26/27 (96%)	25 (96%)	1 (4%)	28	56
4	C	352/362 (97%)	345 (98%)	7 (2%)	50	78
4	c	352/362 (97%)	346 (98%)	6 (2%)	56	81
5	D	278/281 (99%)	276 (99%)	2 (1%)	81	93
5	d	278/281 (99%)	276 (99%)	2 (1%)	81	93
6	E	67/71 (94%)	66 (98%)	1 (2%)	60	83
6	e	67/71 (94%)	66 (98%)	1 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	25/37 (68%)	25 (100%)	0	100	100
7	f	25/37 (68%)	25 (100%)	0	100	100
8	H	58/75 (77%)	57 (98%)	1 (2%)	56	81
8	h	58/75 (77%)	57 (98%)	1 (2%)	56	81
9	I	32/34 (94%)	31 (97%)	1 (3%)	35	64
9	i	32/34 (94%)	31 (97%)	1 (3%)	35	64
10	J	27/32 (84%)	27 (100%)	0	100	100
10	j	27/32 (84%)	27 (100%)	0	100	100
11	K	31/38 (82%)	31 (100%)	0	100	100
11	k	31/38 (82%)	31 (100%)	0	100	100
12	L	33/35 (94%)	30 (91%)	3 (9%)	7	19
12	l	33/35 (94%)	30 (91%)	3 (9%)	7	19
13	M	26/30 (87%)	26 (100%)	0	100	100
13	m	26/30 (87%)	26 (100%)	0	100	100
14	O	195/222 (88%)	192 (98%)	3 (2%)	60	83
14	o	195/222 (88%)	192 (98%)	3 (2%)	60	83
15	P	150/185 (81%)	150 (100%)	0	100	100
15	p	150/185 (81%)	149 (99%)	1 (1%)	81	93
16	Q	126/157 (80%)	124 (98%)	2 (2%)	58	82
16	q	126/157 (80%)	124 (98%)	2 (2%)	58	82
17	T	27/28 (96%)	26 (96%)	1 (4%)	29	58
17	t	27/28 (96%)	26 (96%)	1 (4%)	29	58
18	W	44/87 (51%)	43 (98%)	1 (2%)	45	74
18	w	44/87 (51%)	43 (98%)	1 (2%)	45	74
19	X	25/67 (37%)	25 (100%)	0	100	100
19	x	25/67 (37%)	25 (100%)	0	100	100
20	Z	51/52 (98%)	51 (100%)	0	100	100
20	z	51/52 (98%)	51 (100%)	0	100	100
21	N	169/194 (87%)	169 (100%)	0	100	100
21	n	169/194 (87%)	169 (100%)	0	100	100
22	G	164/187 (88%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	g	164/187 (88%)	163 (99%)	1 (1%)	84	94
23	R	144/218 (66%)	143 (99%)	1 (1%)	81	93
23	r	144/218 (66%)	143 (99%)	1 (1%)	81	93
24	S	190/217 (88%)	187 (98%)	3 (2%)	58	82
24	s	190/217 (88%)	187 (98%)	3 (2%)	58	82
25	Y	170/196 (87%)	170 (100%)	0	100	100
25	y	170/196 (87%)	170 (100%)	0	100	100
26	U	21/141 (15%)	21 (100%)	0	100	100
26	u	21/141 (15%)	21 (100%)	0	100	100
28	3	8/8 (100%)	8 (100%)	0	100	100
28	4	8/8 (100%)	8 (100%)	0	100	100
All	All	6210/7354 (84%)	6139 (99%)	71 (1%)	69	87

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	38	ASN
14	o	208	ARG
18	w	114	LYS
14	O	93	LYS
12	L	38	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
5	d	190	ASN
22	g	214	GLN
12	l	5	ASN
15	p	221	GLN
25	y	233	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 318 ligands modelled in this entry, 6 are monoatomic - leaving 312 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	CLA	b	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.66	9 (11%)
32	CLA	N	602	21	65,73,73	1.48	7 (10%)	76,113,113	1.31	8 (10%)
36	LMG	H	102	-	48,48,55	0.92	2 (4%)	56,56,63	1.08	3 (5%)
43	CHL	G	608	-	44,52,74	2.17	13 (29%)	46,87,114	3.26	17 (36%)
32	CLA	B	604	-	65,73,73	1.51	9 (13%)	76,113,113	1.40	11 (14%)
34	BCR	D	404	-	41,41,41	0.72	0	56,56,56	1.92	21 (37%)
32	CLA	A	407	47	49,57,73	1.63	7 (14%)	55,93,113	1.71	8 (14%)
32	CLA	b	616	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
32	CLA	B	614	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	8 (10%)
32	CLA	B	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	7 (9%)
34	BCR	h	101	-	41,41,41	0.71	0	56,56,56	2.00	13 (23%)
32	CLA	G	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.39	8 (14%)
34	BCR	c	517	-	41,41,41	0.74	0	56,56,56	1.92	16 (28%)
43	CHL	g	609	22	66,74,74	1.85	14 (21%)	73,114,114	2.74	23 (31%)
42	LMU	Z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.14	4 (8%)
32	CLA	c	507	47	65,73,73	1.44	9 (13%)	76,113,113	1.54	10 (13%)
32	CLA	a	405	-	65,73,73	1.53	8 (12%)	76,113,113	1.57	10 (13%)
46	NEX	n	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.33	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	y	611	38	65,73,73	1.46	9 (13%)	76,113,113	1.41	8 (10%)
44	LUT	N	1621	-	42,43,43	0.79	0	51,60,60	1.52	7 (13%)
32	CLA	Y	602	25	65,73,73	1.50	8 (12%)	76,113,113	1.34	9 (11%)
32	CLA	B	609	-	65,73,73	1.41	7 (10%)	76,113,113	1.47	7 (9%)
34	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.84	15 (26%)
43	CHL	y	605	25	46,54,74	2.23	15 (32%)	49,90,114	3.18	19 (38%)
32	CLA	n	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.34	7 (9%)
46	NEX	G	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.40	15 (30%)
42	LMU	y	2632	-	36,36,36	1.14	2 (5%)	47,47,47	1.13	5 (10%)
45	XAT	Y	1622	-	39,47,47	0.95	2 (5%)	54,74,74	4.34	24 (44%)
32	CLA	n	614	-	49,57,73	1.75	7 (14%)	55,93,113	1.41	8 (14%)
32	CLA	c	510	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	7 (9%)
32	CLA	b	617	-	65,73,73	1.43	8 (12%)	76,113,113	1.42	9 (11%)
32	CLA	g	602	22	65,73,73	1.51	8 (12%)	76,113,113	1.31	8 (10%)
32	CLA	C	508	-	65,73,73	1.41	7 (10%)	76,113,113	1.56	8 (10%)
43	CHL	Y	609	25	66,74,74	1.82	13 (19%)	73,114,114	2.76	22 (30%)
32	CLA	G	610	22	65,73,73	1.44	8 (12%)	76,113,113	1.37	8 (10%)
43	CHL	n	606	-	46,54,74	2.22	14 (30%)	49,90,114	3.14	17 (34%)
35	SQD	b	621	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	5 (8%)
32	CLA	b	608	47	65,73,73	1.45	8 (12%)	76,113,113	1.42	7 (9%)
35	SQD	A	412	-	50,51,54	1.21	4 (8%)	59,62,65	3.80	9 (15%)
34	BCR	H	101	-	41,41,41	0.70	0	56,56,56	2.00	12 (21%)
43	CHL	N	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.79	22 (30%)
35	SQD	a	412	-	50,51,54	1.21	4 (8%)	59,62,65	3.79	9 (15%)
36	LMG	h	102	-	48,48,55	0.92	2 (4%)	56,56,63	1.10	3 (5%)
32	CLA	s	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.59	8 (14%)
32	CLA	a	406	47	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
43	CHL	S	601	24	46,54,74	2.26	14 (30%)	49,90,114	3.16	22 (44%)
46	NEX	r	625	-	38,46,46	0.99	2 (5%)	50,70,70	2.48	16 (32%)
32	CLA	B	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	11 (14%)
43	CHL	N	606	-	46,54,74	2.22	15 (32%)	49,90,114	3.14	17 (34%)
46	NEX	S	1623	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	17 (34%)
32	CLA	n	612	21	45,53,73	1.79	7 (15%)	52,89,113	1.51	10 (19%)
36	LMG	a	413	-	48,48,55	0.96	2 (4%)	56,56,63	1.06	4 (7%)
32	CLA	c	501	-	65,73,73	1.49	9 (13%)	76,113,113	1.29	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	S	614	-	48,56,73	1.70	8 (16%)	55,92,113	1.38	8 (14%)
32	CLA	S	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.58	8 (14%)
32	CLA	C	505	-	65,73,73	1.43	10 (15%)	76,113,113	1.47	10 (13%)
44	LUT	g	1621	-	42,43,43	0.81	0	51,60,60	1.56	11 (21%)
34	BCR	c	514	-	41,41,41	0.84	0	56,56,56	1.69	10 (17%)
32	CLA	b	606	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	7 (9%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.97	2 (2%)
34	BCR	C	516	-	41,41,41	0.83	0	56,56,56	1.89	18 (32%)
32	CLA	c	511	4	65,73,73	1.40	8 (12%)	76,113,113	1.48	8 (10%)
36	LMG	b	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	4 (6%)
32	CLA	Y	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	10 (13%)
32	CLA	n	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.37	6 (7%)
43	CHL	G	601	22	66,74,74	1.79	12 (18%)	73,114,114	2.70	23 (31%)
32	CLA	Y	613	25	65,73,73	1.48	10 (15%)	76,113,113	1.44	9 (11%)
43	CHL	Y	606	-	66,74,74	1.84	15 (22%)	73,114,114	2.65	20 (27%)
45	XAT	g	1622	-	39,47,47	0.94	0	54,74,74	2.82	20 (37%)
32	CLA	s	609	24	41,49,73	1.89	7 (17%)	47,84,113	1.52	8 (17%)
38	LHG	D	410	-	38,38,48	1.00	2 (5%)	41,44,54	1.00	2 (4%)
32	CLA	G	602	22	65,73,73	1.51	7 (10%)	76,113,113	1.31	7 (9%)
38	LHG	y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.19	5 (9%)
34	BCR	B	619	-	41,41,41	0.72	0	56,56,56	1.94	13 (23%)
37	DGD	C	524	-	67,67,67	0.82	2 (2%)	81,81,81	1.00	4 (4%)
33	PHO	A	408	-	51,69,69	1.06	5 (9%)	47,99,99	1.33	8 (17%)
45	XAT	G	1622	-	39,47,47	0.93	0	54,74,74	2.83	20 (37%)
32	CLA	g	613	22	65,73,73	1.50	11 (16%)	76,113,113	1.51	6 (7%)
32	CLA	r	609	23	45,53,73	1.78	6 (13%)	52,89,113	1.62	9 (17%)
32	CLA	B	616	-	65,73,73	1.48	9 (13%)	76,113,113	1.36	10 (13%)
32	CLA	R	603	-	49,57,73	1.72	7 (14%)	55,93,113	1.55	10 (18%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	6 (8%)
38	LHG	D	409	-	48,48,48	0.88	3 (6%)	51,54,54	0.97	3 (5%)
32	CLA	C	506	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
34	BCR	B	620	-	41,41,41	0.73	0	56,56,56	1.75	13 (23%)
37	DGD	c	524	-	67,67,67	0.82	2 (2%)	81,81,81	1.00	4 (4%)
32	CLA	s	603	-	42,50,73	1.82	7 (16%)	48,85,113	1.68	10 (20%)
43	CHL	n	605	21	66,74,74	1.80	15 (22%)	73,114,114	2.85	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
42	LMU	Z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.21	5 (10%)
35	SQD	B	621	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	5 (8%)
38	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	3 (5%)
38	LHG	C	2630	-	46,46,48	0.91	2 (4%)	49,52,54	1.03	3 (6%)
41	HEM	f	101	6,7	41,50,50	1.46	4 (9%)	45,82,82	1.35	5 (11%)
32	CLA	c	505	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	10 (13%)
29	OEX	A	401	4,1	0,15,15	-	-	-		
46	NEX	s	1623	-	38,46,46	1.03	3 (7%)	50,70,70	2.38	17 (34%)
32	CLA	S	603	-	42,50,73	1.83	9 (21%)	48,85,113	1.70	10 (20%)
46	NEX	R	625	-	38,46,46	0.90	1 (2%)	50,70,70	2.45	17 (34%)
42	LMU	Y	2632	-	36,36,36	1.13	2 (5%)	47,47,47	1.12	5 (10%)
34	BCR	d	404	-	41,41,41	0.71	0	56,56,56	1.92	21 (37%)
32	CLA	d	403	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	9 (11%)
44	LUT	s	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.72	16 (31%)
43	CHL	S	607	-	43,51,74	2.25	13 (30%)	45,86,114	3.22	16 (35%)
32	CLA	b	612	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	10 (13%)
32	CLA	B	603	-	65,73,73	1.42	7 (10%)	76,113,113	1.31	9 (11%)
32	CLA	s	611	38	49,57,73	1.63	7 (14%)	55,93,113	1.48	6 (10%)
43	CHL	s	607	-	43,51,74	2.25	13 (30%)	45,86,114	3.23	16 (35%)
32	CLA	n	603	-	65,73,73	1.52	9 (13%)	76,113,113	1.40	8 (10%)
32	CLA	N	614	-	49,57,73	1.74	7 (14%)	55,93,113	1.41	8 (14%)
32	CLA	n	610	21	65,73,73	1.44	7 (10%)	76,113,113	1.34	8 (10%)
39	BCT	d	401	30	2,3,3	1.29	0	2,3,3	4.18	2 (100%)
43	CHL	r	607	-	50,58,74	2.17	16 (32%)	52,94,114	3.09	21 (40%)
32	CLA	Y	604	-	65,73,73	1.50	9 (13%)	76,113,113	1.36	7 (9%)
32	CLA	b	615	-	65,73,73	1.45	8 (12%)	76,113,113	1.33	7 (9%)
43	CHL	R	607	-	50,58,74	2.17	16 (32%)	52,94,114	3.09	21 (40%)
32	CLA	S	611	38	49,57,73	1.64	7 (14%)	55,93,113	1.49	7 (12%)
45	XAT	y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.35	24 (44%)
32	CLA	n	602	21	65,73,73	1.48	7 (10%)	76,113,113	1.31	8 (10%)
45	XAT	r	624	-	39,47,47	0.88	2 (5%)	54,74,74	2.62	18 (33%)
32	CLA	G	613	22	65,73,73	1.50	10 (15%)	76,113,113	1.51	6 (7%)
46	NEX	N	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.37	15 (30%)
44	LUT	G	1621	-	42,43,43	0.82	0	51,60,60	1.56	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	s	610	24	49,57,73	1.81	9 (18%)	55,93,113	1.33	9 (16%)
44	LUT	G	1620	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)
43	CHL	n	608	-	50,58,74	2.08	13 (26%)	52,94,114	3.22	18 (34%)
32	CLA	B	615	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	7 (9%)
32	CLA	C	501	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	11 (14%)
32	CLA	r	610	23	41,49,73	1.86	8 (19%)	47,84,113	1.48	7 (14%)
38	LHG	N	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
43	CHL	N	605	21	66,74,74	1.80	15 (22%)	73,114,114	2.85	24 (32%)
45	XAT	n	1622	-	39,47,47	0.98	1 (2%)	54,74,74	2.66	22 (40%)
32	CLA	g	603	-	65,73,73	1.50	8 (12%)	76,113,113	1.39	12 (15%)
40	PL9	D	405	-	55,55,55	2.01	14 (25%)	68,69,69	1.46	15 (22%)
32	CLA	R	610	23	41,49,73	1.86	8 (19%)	47,84,113	1.48	7 (14%)
43	CHL	G	606	-	50,58,74	2.14	14 (28%)	52,94,114	3.08	19 (36%)
32	CLA	s	602	24	49,57,73	1.66	7 (14%)	55,93,113	1.47	8 (14%)
46	NEX	Y	1623	-	38,46,46	0.97	2 (5%)	50,70,70	2.46	17 (34%)
38	LHG	n	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
32	CLA	g	604	-	49,57,73	1.72	7 (14%)	55,93,113	1.53	6 (10%)
43	CHL	G	607	-	50,58,74	2.14	14 (28%)	52,94,114	3.09	22 (42%)
34	BCR	b	620	-	41,41,41	0.73	0	56,56,56	1.74	13 (23%)
44	LUT	Y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.71	10 (19%)
32	CLA	b	607	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	8 (10%)
44	LUT	Y	1620	-	42,43,43	0.93	3 (7%)	51,60,60	1.90	15 (29%)
32	CLA	S	602	24	49,57,73	1.67	7 (14%)	55,93,113	1.47	9 (16%)
32	CLA	N	603	-	65,73,73	1.52	10 (15%)	76,113,113	1.40	8 (10%)
32	CLA	y	603	-	65,73,73	1.49	10 (15%)	76,113,113	1.41	10 (13%)
32	CLA	G	611	38	45,53,73	1.76	7 (15%)	52,89,113	1.59	8 (15%)
32	CLA	C	503	-	65,73,73	1.51	8 (12%)	76,113,113	1.40	10 (13%)
34	BCR	C	515	-	41,41,41	0.85	1 (2%)	56,56,56	1.98	19 (33%)
43	CHL	Y	605	25	46,54,74	2.22	15 (32%)	49,90,114	3.18	19 (38%)
32	CLA	g	612	22	43,51,73	1.83	7 (16%)	49,86,113	1.59	9 (18%)
32	CLA	C	509	-	65,73,73	1.44	11 (16%)	76,113,113	1.58	10 (13%)
43	CHL	Y	607	-	66,74,74	1.81	14 (21%)	73,114,114	2.67	21 (28%)
32	CLA	A	406	47	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
33	PHO	a	409	-	51,69,69	1.04	4 (7%)	47,99,99	1.33	5 (10%)
32	CLA	c	504	47	65,73,73	1.50	10 (15%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	B	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.67	9 (11%)
39	BCT	D	401	30	2,3,3	1.29	0	2,3,3	4.17	2 (100%)
42	LMU	z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.14	4 (8%)
32	CLA	b	603	-	65,73,73	1.43	7 (10%)	76,113,113	1.32	9 (11%)
32	CLA	r	603	-	49,57,73	1.73	7 (14%)	55,93,113	1.55	10 (18%)
32	CLA	s	614	-	48,56,73	1.69	8 (16%)	55,92,113	1.39	8 (14%)
38	LHG	Y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.19	5 (9%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
34	BCR	c	516	-	41,41,41	0.83	0	56,56,56	1.89	18 (32%)
38	LHG	S	2630	32	44,44,48	0.94	2 (4%)	47,50,54	1.00	2 (4%)
32	CLA	d	402	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	7 (9%)
45	XAT	N	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.66	23 (42%)
32	CLA	c	513	-	65,73,73	1.40	9 (13%)	76,113,113	1.44	9 (11%)
46	NEX	g	1623	-	38,46,46	0.92	1 (2%)	50,70,70	2.38	16 (32%)
32	CLA	R	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.50	7 (12%)
43	CHL	G	609	22	66,74,74	1.85	13 (19%)	73,114,114	2.73	22 (30%)
32	CLA	b	614	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	8 (10%)
32	CLA	c	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	9 (11%)
32	CLA	b	604	-	65,73,73	1.51	9 (13%)	76,113,113	1.41	11 (14%)
32	CLA	A	405	-	65,73,73	1.53	8 (12%)	76,113,113	1.56	10 (13%)
32	CLA	c	508	-	65,73,73	1.42	7 (10%)	76,113,113	1.58	8 (10%)
34	BCR	a	411	-	41,41,41	0.76	0	56,56,56	1.70	14 (25%)
44	LUT	N	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.57	10 (19%)
38	LHG	D	408	-	43,43,48	0.95	2 (4%)	46,49,54	1.02	2 (4%)
32	CLA	G	604	-	49,57,73	1.72	8 (16%)	55,93,113	1.52	6 (10%)
32	CLA	g	611	38	45,53,73	1.77	7 (15%)	52,89,113	1.58	8 (15%)
43	CHL	s	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.22	19 (41%)
32	CLA	y	602	25	65,73,73	1.51	8 (12%)	76,113,113	1.34	9 (11%)
43	CHL	g	605	22	48,56,74	2.36	16 (33%)	51,92,114	3.05	19 (37%)
43	CHL	N	601	21	66,74,74	1.81	13 (19%)	73,114,114	2.68	20 (27%)
32	CLA	S	609	24	41,49,73	1.90	7 (17%)	47,84,113	1.52	8 (17%)
43	CHL	G	605	22	48,56,74	2.36	16 (33%)	51,92,114	3.05	19 (37%)
43	CHL	g	607	-	50,58,74	2.14	14 (28%)	52,94,114	3.09	22 (42%)
45	XAT	R	624	-	39,47,47	0.88	1 (2%)	54,74,74	2.61	17 (31%)
36	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	y	609	25	66,74,74	1.82	13 (19%)	73,114,114	2.76	22 (30%)
41	HEM	F	101	6,7	41,50,50	1.45	4 (9%)	45,82,82	1.35	6 (13%)
43	CHL	n	601	21	66,74,74	1.81	13 (19%)	73,114,114	2.67	20 (27%)
44	LUT	g	1620	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
32	CLA	G	612	22	43,51,73	1.83	8 (18%)	49,86,113	1.59	9 (18%)
32	CLA	S	605	24	50,58,73	1.70	7 (14%)	58,95,113	1.51	11 (18%)
32	CLA	B	608	47	65,73,73	1.45	8 (12%)	76,113,113	1.41	7 (9%)
43	CHL	s	608	-	49,57,74	2.18	15 (30%)	52,93,114	3.13	19 (36%)
32	CLA	b	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.50	11 (14%)
32	CLA	N	612	21	45,53,73	1.80	8 (17%)	52,89,113	1.50	10 (19%)
43	CHL	y	601	25	66,74,74	1.80	14 (21%)	73,114,114	2.67	26 (35%)
32	CLA	B	611	47	65,73,73	1.48	8 (12%)	76,113,113	1.55	11 (14%)
32	CLA	g	610	22	65,73,73	1.44	8 (12%)	76,113,113	1.37	8 (10%)
33	PHO	a	408	-	51,69,69	1.06	5 (9%)	47,99,99	1.32	8 (17%)
34	BCR	C	514	-	41,41,41	0.84	0	56,56,56	1.69	10 (17%)
38	LHG	c	2630	-	46,46,48	0.92	2 (4%)	49,52,54	1.03	3 (6%)
32	CLA	B	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	8 (10%)
32	CLA	D	402	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
33	PHO	A	409	-	51,69,69	1.04	4 (7%)	47,99,99	1.34	6 (12%)
34	BCR	C	517	-	41,41,41	0.74	0	56,56,56	1.93	15 (26%)
36	LMG	D	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.15	4 (7%)
43	CHL	R	608	-	46,54,74	2.26	15 (32%)	49,90,114	3.10	20 (40%)
32	CLA	B	617	-	65,73,73	1.42	8 (12%)	76,113,113	1.41	9 (11%)
32	CLA	B	607	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	8 (10%)
37	DGD	C	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
32	CLA	c	509	-	65,73,73	1.44	11 (16%)	76,113,113	1.57	10 (13%)
36	LMG	d	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.16	4 (7%)
44	LUT	S	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.71	16 (31%)
32	CLA	Y	611	38	65,73,73	1.45	8 (12%)	76,113,113	1.42	8 (10%)
36	LMG	A	413	-	48,48,55	0.95	2 (4%)	56,56,63	1.07	4 (7%)
29	OEX	a	401	4,1	0,15,15	-	-	-	-	-
32	CLA	Y	610	25	65,73,73	1.46	9 (13%)	76,113,113	1.29	7 (9%)
43	CHL	N	608	-	50,58,74	2.08	13 (26%)	52,94,114	3.21	18 (34%)
37	DGD	C	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	5 (7%)
32	CLA	c	512	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	C	502	-	65,73,73	1.46	11 (16%)	76,113,113	1.50	6 (7%)
32	CLA	R	609	23	45,53,73	1.78	6 (13%)	52,89,113	1.60	9 (17%)
32	CLA	Y	614	-	54,62,73	1.59	8 (14%)	62,99,113	1.36	8 (12%)
32	CLA	y	613	25	65,73,73	1.49	10 (15%)	76,113,113	1.44	9 (11%)
32	CLA	B	602	47	65,73,73	1.47	8 (12%)	76,113,113	1.38	8 (10%)
44	LUT	y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.71	10 (19%)
38	LHG	G	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.96	3 (5%)
32	CLA	S	610	24	49,57,73	1.80	9 (18%)	55,93,113	1.32	7 (12%)
32	CLA	b	611	47	65,73,73	1.48	8 (12%)	76,113,113	1.55	10 (13%)
32	CLA	s	605	24	50,58,73	1.69	7 (14%)	58,95,113	1.51	11 (18%)
42	LMU	z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.21	5 (10%)
32	CLA	c	502	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	6 (7%)
43	CHL	Y	608	-	50,58,74	2.10	14 (28%)	52,94,114	3.23	19 (36%)
46	NEX	y	1623	-	38,46,46	0.92	2 (5%)	50,70,70	2.45	17 (34%)
32	CLA	c	503	-	65,73,73	1.51	8 (12%)	76,113,113	1.39	9 (11%)
38	LHG	d	409	-	48,48,48	0.89	3 (6%)	51,54,54	0.97	3 (5%)
43	CHL	g	608	-	44,52,74	2.18	14 (31%)	46,87,114	3.26	18 (39%)
43	CHL	y	608	-	50,58,74	2.10	14 (28%)	52,94,114	3.22	19 (36%)
32	CLA	a	407	47	49,57,73	1.64	7 (14%)	55,93,113	1.70	7 (12%)
32	CLA	C	510	-	65,73,73	1.42	9 (13%)	76,113,113	1.50	7 (9%)
32	CLA	C	513	-	65,73,73	1.40	9 (13%)	76,113,113	1.45	9 (11%)
32	CLA	D	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	9 (11%)
32	CLA	C	507	47	65,73,73	1.44	9 (13%)	76,113,113	1.54	10 (13%)
43	CHL	n	609	21	66,74,74	1.87	14 (21%)	73,114,114	2.66	20 (27%)
38	LHG	g	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.95	3 (5%)
32	CLA	y	610	25	65,73,73	1.46	9 (13%)	76,113,113	1.29	7 (9%)
43	CHL	y	607	-	66,74,74	1.81	14 (21%)	73,114,114	2.68	21 (28%)
32	CLA	g	614	-	49,57,73	1.72	7 (14%)	55,93,113	1.40	8 (14%)
32	CLA	r	604	-	49,57,73	1.70	7 (14%)	55,93,113	1.50	7 (12%)
44	LUT	y	1620	-	42,43,43	0.92	3 (7%)	51,60,60	1.90	14 (27%)
43	CHL	R	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.27	20 (43%)
32	CLA	n	611	38	49,57,73	1.69	8 (16%)	55,93,113	1.45	8 (14%)
37	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.12	6 (7%)
32	CLA	R	602	23	60,68,73	1.61	8 (13%)	70,107,113	1.35	9 (12%)
32	CLA	G	603	-	65,73,73	1.50	9 (13%)	76,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	b	619	-	41,41,41	0.72	0	56,56,56	1.95	13 (23%)
32	CLA	B	612	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	9 (11%)
32	CLA	N	613	21	65,73,73	1.53	10 (15%)	76,113,113	1.37	6 (7%)
43	CHL	s	601	24	46,54,74	2.25	14 (30%)	49,90,114	3.17	21 (42%)
32	CLA	b	602	47	65,73,73	1.47	8 (12%)	76,113,113	1.39	8 (10%)
32	CLA	r	602	23	60,68,73	1.61	8 (13%)	70,107,113	1.35	9 (12%)
32	CLA	A	410	-	60,68,73	1.47	9 (15%)	70,107,113	1.48	9 (12%)
32	CLA	b	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.39	8 (10%)
34	BCR	c	515	-	41,41,41	0.84	1 (2%)	56,56,56	1.98	18 (32%)
32	CLA	Y	612	25	65,73,73	1.47	10 (15%)	76,113,113	1.31	8 (10%)
38	LHG	l	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	3 (5%)
32	CLA	a	410	-	60,68,73	1.47	8 (13%)	70,107,113	1.46	9 (12%)
43	CHL	r	608	-	46,54,74	2.27	15 (32%)	49,90,114	3.09	19 (38%)
43	CHL	g	606	-	50,58,74	2.14	14 (28%)	52,94,114	3.08	18 (34%)
32	CLA	C	512	-	65,73,73	1.42	10 (15%)	76,113,113	1.47	8 (10%)
38	LHG	d	410	-	38,38,48	1.00	2 (5%)	41,44,54	1.00	2 (4%)
34	BCR	b	618	-	41,41,41	0.76	0	56,56,56	1.84	15 (26%)
32	CLA	C	504	47	65,73,73	1.50	10 (15%)	76,113,113	1.41	8 (10%)
32	CLA	N	611	38	49,57,73	1.70	8 (16%)	55,93,113	1.44	8 (14%)
43	CHL	g	601	22	66,74,74	1.81	12 (18%)	73,114,114	2.71	23 (31%)
43	CHL	n	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.80	22 (30%)
32	CLA	y	604	-	65,73,73	1.50	8 (12%)	76,113,113	1.36	7 (9%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.13	6 (7%)
32	CLA	s	613	24	49,57,73	1.81	10 (20%)	55,93,113	1.45	6 (10%)
43	CHL	N	609	21	66,74,74	1.86	13 (19%)	73,114,114	2.67	20 (27%)
34	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.70	13 (23%)
44	LUT	n	1621	-	42,43,43	0.79	0	51,60,60	1.52	7 (13%)
38	LHG	d	408	-	43,43,48	0.95	2 (4%)	46,49,54	1.02	2 (4%)
44	LUT	n	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.56	10 (19%)
43	CHL	S	606	-	44,52,74	2.16	13 (29%)	46,87,114	3.24	19 (41%)
32	CLA	C	511	4	65,73,73	1.41	8 (12%)	76,113,113	1.49	8 (10%)
32	CLA	b	609	-	65,73,73	1.41	7 (10%)	76,113,113	1.48	7 (9%)
32	CLA	S	613	24	49,57,73	1.80	10 (20%)	55,93,113	1.44	6 (10%)
43	CHL	r	606	-	44,52,74	2.15	13 (29%)	46,87,114	3.28	19 (41%)
32	CLA	s	612	24	45,53,73	1.75	10 (22%)	52,89,113	1.57	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	Y	601	25	66,74,74	1.80	14 (21%)	73,114,114	2.67	26 (35%)
32	CLA	N	610	21	65,73,73	1.44	7 (10%)	76,113,113	1.35	8 (10%)
36	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	4 (6%)
40	PL9	d	405	-	55,55,55	2.02	13 (23%)	68,69,69	1.46	14 (20%)
37	DGD	C	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.97	2 (2%)
38	LHG	s	2630	32	44,44,48	0.94	2 (4%)	47,50,54	1.00	2 (4%)
43	CHL	S	608	-	49,57,74	2.19	15 (30%)	52,93,114	3.15	20 (38%)
32	CLA	S	612	24	45,53,73	1.75	10 (22%)	52,89,113	1.57	8 (15%)
44	LUT	s	1621	-	42,43,43	0.80	0	51,60,60	1.71	13 (25%)
32	CLA	y	614	-	54,62,73	1.59	8 (14%)	62,99,113	1.36	8 (12%)
32	CLA	y	612	25	65,73,73	1.46	9 (13%)	76,113,113	1.31	8 (10%)
32	CLA	N	604	-	65,73,73	1.48	8 (12%)	76,113,113	1.33	7 (9%)
44	LUT	S	1621	-	42,43,43	0.79	0	51,60,60	1.71	14 (27%)
43	CHL	y	606	-	66,74,74	1.84	15 (22%)	73,114,114	2.64	20 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	613	-	1/1/15/20	9/37/115/115	-
32	CLA	N	602	21	1/1/15/20	12/37/115/115	-
36	LMG	H	102	-	-	14/43/63/70	0/1/1/1
43	CHL	G	608	-	3/3/15/26	7/13/111/137	-
32	CLA	B	604	-	-	12/37/115/115	-
34	BCR	D	404	-	-	2/29/63/63	0/2/2/2
32	CLA	A	407	47	1/1/11/20	2/18/96/115	-
32	CLA	b	616	-	1/1/15/20	13/37/115/115	-
32	CLA	B	614	-	1/1/15/20	10/37/115/115	-
32	CLA	B	606	-	1/1/15/20	9/37/115/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
32	CLA	G	614	-	1/1/11/20	11/18/96/115	-
34	BCR	c	517	-	-	1/29/63/63	0/2/2/2
43	CHL	g	609	22	3/3/20/26	21/39/137/137	-
42	LMU	Z	2635	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	507	47	1/1/15/20	11/37/115/115	-
32	CLA	a	405	-	1/1/15/20	15/37/115/115	-
46	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
32	CLA	y	611	38	1/1/15/20	11/37/115/115	-
44	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	Y	602	25	1/1/15/20	10/37/115/115	-
32	CLA	B	609	-	1/1/15/20	14/37/115/115	-
34	BCR	B	618	-	-	2/29/63/63	0/2/2/2
43	CHL	y	605	25	3/3/16/26	9/15/113/137	-
32	CLA	n	604	-	1/1/15/20	11/37/115/115	-
46	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
42	LMU	y	2632	-	-	9/21/61/61	0/2/2/2
45	XAT	Y	1622	-	-	4/31/93/93	0/4/4/4
32	CLA	n	614	-	1/1/11/20	8/18/96/115	-
32	CLA	c	510	-	1/1/15/20	17/37/115/115	-
32	CLA	b	617	-	1/1/15/20	16/37/115/115	-
32	CLA	g	602	22	1/1/15/20	16/37/115/115	-
32	CLA	C	508	-	1/1/15/20	13/37/115/115	-
43	CHL	Y	609	25	3/3/20/26	16/39/137/137	-
32	CLA	G	610	22	1/1/15/20	13/37/115/115	-
43	CHL	n	606	-	3/3/16/26	7/15/113/137	-
35	SQD	b	621	-	-	15/49/69/69	0/1/1/1
32	CLA	b	608	47	1/1/15/20	12/37/115/115	-
35	SQD	A	412	-	-	15/46/66/69	0/1/1/1
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
43	CHL	N	607	-	3/3/20/26	20/39/137/137	-
35	SQD	a	412	-	-	15/46/66/69	0/1/1/1
36	LMG	h	102	-	-	15/43/63/70	0/1/1/1
32	CLA	s	604	-	1/1/11/20	7/18/96/115	-
32	CLA	a	406	47	-	9/37/115/115	-
43	CHL	S	601	24	3/3/16/26	8/15/113/137	-
46	NEX	r	625	-	-	5/27/83/83	0/3/3/3
32	CLA	B	605	-	1/1/15/20	13/37/115/115	-
43	CHL	N	606	-	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
32	CLA	n	612	21	1/1/11/20	4/13/91/115	-
36	LMG	a	413	-	-	17/43/63/70	0/1/1/1
32	CLA	c	501	-	1/1/15/20	16/37/115/115	-
32	CLA	S	614	-	1/1/11/20	4/17/95/115	-
32	CLA	S	604	-	1/1/11/20	7/18/96/115	-
32	CLA	C	505	-	-	14/37/115/115	-
44	LUT	g	1621	-	-	5/29/67/67	0/2/2/2
34	BCR	c	514	-	-	2/29/63/63	0/2/2/2
32	CLA	b	606	-	1/1/15/20	9/37/115/115	-
37	DGD	c	520	-	-	14/48/88/95	0/2/2/2
34	BCR	C	516	-	-	8/29/63/63	0/2/2/2
32	CLA	c	511	4	-	12/37/115/115	-
36	LMG	b	622	-	-	4/46/66/70	0/1/1/1
32	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
32	CLA	n	613	21	-	12/37/115/115	-
43	CHL	G	601	22	3/3/20/26	14/39/137/137	-
32	CLA	Y	613	25	-	13/37/115/115	-
43	CHL	Y	606	-	3/3/20/26	15/39/137/137	-
45	XAT	g	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	s	609	24	1/1/10/20	2/8/86/115	-
38	LHG	D	410	-	-	13/43/43/53	-
32	CLA	G	602	22	1/1/15/20	16/37/115/115	-
38	LHG	y	2630	32	-	18/53/53/53	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
37	DGD	C	524	-	-	10/55/95/95	0/2/2/2
33	PHO	A	408	-	-	12/37/103/103	0/5/6/6
45	XAT	G	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	g	613	22	-	16/37/115/115	-
32	CLA	r	609	23	1/1/11/20	8/13/91/115	-
32	CLA	B	616	-	1/1/15/20	14/37/115/115	-
32	CLA	C	506	-	-	4/37/115/115	-
37	DGD	c	518	-	-	10/44/84/95	0/2/2/2
38	LHG	D	409	-	-	20/53/53/53	-
32	CLA	R	603	-	1/1/11/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
37	DGD	c	524	-	-	10/55/95/95	0/2/2/2
32	CLA	s	603	-	1/1/10/20	5/10/88/115	-
43	CHL	n	605	21	3/3/20/26	17/39/137/137	-
36	LMG	c	521	-	-	5/46/66/70	0/1/1/1
42	LMU	Z	2634	-	-	9/21/61/61	0/2/2/2
35	SQD	B	621	-	-	16/49/69/69	0/1/1/1
38	LHG	L	101	-	-	20/53/53/53	-
38	LHG	C	2630	-	-	15/51/51/53	-
41	HEM	f	101	6,7	-	2/12/54/54	-
32	CLA	c	505	-	-	14/37/115/115	-
46	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
32	CLA	S	603	-	1/1/10/20	5/10/88/115	-
46	NEX	R	625	-	-	5/27/83/83	0/3/3/3
42	LMU	Y	2632	-	-	9/21/61/61	0/2/2/2
34	BCR	d	404	-	-	2/29/63/63	0/2/2/2
32	CLA	d	403	-	-	12/37/115/115	-
44	LUT	s	1620	-	-	4/29/67/67	0/2/2/2
43	CHL	S	607	-	3/3/15/26	4/12/110/137	-
32	CLA	b	612	-	1/1/15/20	11/37/115/115	-
32	CLA	B	603	-	1/1/15/20	14/37/115/115	-
32	CLA	s	611	38	1/1/11/20	7/18/96/115	-
43	CHL	s	607	-	3/3/15/26	3/12/110/137	-
32	CLA	n	603	-	1/1/15/20	14/37/115/115	-
32	CLA	N	614	-	1/1/11/20	7/18/96/115	-
32	CLA	n	610	21	1/1/15/20	3/37/115/115	-
43	CHL	r	607	-	3/3/16/26	7/20/118/137	-
32	CLA	Y	604	-	1/1/15/20	14/37/115/115	-
32	CLA	b	615	-	1/1/15/20	21/37/115/115	-
43	CHL	R	607	-	3/3/16/26	7/20/118/137	-
32	CLA	S	611	38	1/1/11/20	7/18/96/115	-
45	XAT	y	1622	-	-	4/31/93/93	0/4/4/4
32	CLA	n	602	21	1/1/15/20	13/37/115/115	-
45	XAT	r	624	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	G	613	22	-	16/37/115/115	-
46	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
44	LUT	G	1621	-	-	5/29/67/67	0/2/2/2
32	CLA	s	610	24	1/1/11/20	6/18/96/115	-
44	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	n	608	-	3/3/16/26	5/20/118/137	-
32	CLA	B	615	-	1/1/15/20	21/37/115/115	-
32	CLA	C	501	-	1/1/15/20	16/37/115/115	-
32	CLA	r	610	23	1/1/10/20	3/8/86/115	-
43	CHL	N	605	21	3/3/20/26	17/39/137/137	-
38	LHG	N	2630	32	-	12/53/53/53	-
45	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	g	603	-	1/1/15/20	14/37/115/115	-
40	PL9	D	405	-	-	14/53/73/73	0/1/1/1
32	CLA	R	610	23	1/1/10/20	3/8/86/115	-
43	CHL	G	606	-	3/3/16/26	8/20/118/137	-
32	CLA	s	602	24	1/1/11/20	8/18/96/115	-
46	NEX	Y	1623	-	-	8/27/83/83	0/3/3/3
38	LHG	n	2630	32	-	12/53/53/53	-
32	CLA	g	604	-	1/1/11/20	10/18/96/115	-
43	CHL	G	607	-	3/3/16/26	8/20/118/137	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
44	LUT	Y	1621	-	-	5/29/67/67	0/2/2/2
32	CLA	b	607	-	1/1/15/20	11/37/115/115	-
44	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	S	602	24	1/1/11/20	8/18/96/115	-
32	CLA	N	603	-	1/1/15/20	14/37/115/115	-
32	CLA	y	603	-	1/1/15/20	14/37/115/115	-
32	CLA	G	611	38	1/1/11/20	3/13/91/115	-
32	CLA	C	503	-	1/1/15/20	9/37/115/115	-
34	BCR	C	515	-	-	7/29/63/63	0/2/2/2
43	CHL	Y	605	25	3/3/16/26	9/15/113/137	-
32	CLA	g	612	22	1/1/10/20	4/11/89/115	-
32	CLA	C	509	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CHL	Y	607	-	3/3/20/26	22/39/137/137	-
32	CLA	A	406	47	-	9/37/115/115	-
33	PHO	a	409	-	-	3/37/103/103	0/5/6/6
32	CLA	c	504	47	1/1/15/20	13/37/115/115	-
32	CLA	B	613	-	1/1/15/20	9/37/115/115	-
42	LMU	z	2635	-	-	10/21/61/61	0/2/2/2
32	CLA	b	603	-	1/1/15/20	14/37/115/115	-
32	CLA	r	603	-	1/1/11/20	11/18/96/115	-
32	CLA	s	614	-	1/1/11/20	4/17/95/115	-
38	LHG	Y	2630	32	-	18/53/53/53	-
37	DGD	c	523	-	-	15/55/95/95	0/2/2/2
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
38	LHG	S	2630	32	-	9/49/49/53	-
32	CLA	d	402	-	1/1/15/20	9/37/115/115	-
45	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	c	513	-	1/1/15/20	19/37/115/115	-
46	NEX	g	1623	-	-	2/27/83/83	0/3/3/3
32	CLA	R	604	-	1/1/11/20	7/18/96/115	-
43	CHL	G	609	22	3/3/20/26	21/39/137/137	-
32	CLA	b	614	-	1/1/15/20	10/37/115/115	-
32	CLA	c	506	-	-	4/37/115/115	-
32	CLA	b	604	-	-	12/37/115/115	-
32	CLA	A	405	-	1/1/15/20	15/37/115/115	-
32	CLA	c	508	-	1/1/15/20	13/37/115/115	-
34	BCR	a	411	-	-	5/29/63/63	0/2/2/2
44	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
38	LHG	D	408	-	-	17/48/48/53	-
32	CLA	G	604	-	1/1/11/20	10/18/96/115	-
32	CLA	g	611	38	1/1/11/20	3/13/91/115	-
43	CHL	s	606	-	3/3/15/26	5/13/111/137	-
32	CLA	y	602	25	1/1/15/20	10/37/115/115	-
43	CHL	g	605	22	3/3/16/26	4/18/116/137	-
43	CHL	N	601	21	3/3/20/26	17/39/137/137	-
32	CLA	S	609	24	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CHL	G	605	22	3/3/16/26	4/18/116/137	-
43	CHL	g	607	-	3/3/16/26	8/20/118/137	-
45	XAT	R	624	-	-	1/31/93/93	0/4/4/4
43	CHL	y	609	25	3/3/20/26	17/39/137/137	-
36	LMG	C	521	-	-	5/46/66/70	0/1/1/1
41	HEM	F	101	6,7	-	2/12/54/54	-
43	CHL	n	601	21	3/3/20/26	17/39/137/137	-
44	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	G	612	22	1/1/10/20	4/11/89/115	-
32	CLA	S	605	24	1/1/12/20	6/19/97/115	-
32	CLA	B	608	47	1/1/15/20	12/37/115/115	-
43	CHL	s	608	-	3/3/16/26	10/19/117/137	-
32	CLA	b	605	-	1/1/15/20	13/37/115/115	-
32	CLA	N	612	21	1/1/11/20	4/13/91/115	-
43	CHL	y	601	25	3/3/20/26	19/39/137/137	-
32	CLA	B	611	47	1/1/15/20	7/37/115/115	-
32	CLA	g	610	22	1/1/15/20	13/37/115/115	-
33	PHO	a	408	-	-	11/37/103/103	0/5/6/6
34	BCR	C	514	-	-	2/29/63/63	0/2/2/2
38	LHG	c	2630	-	-	15/51/51/53	-
32	CLA	D	402	-	1/1/15/20	9/37/115/115	-
32	CLA	B	610	-	-	15/37/115/115	-
33	PHO	A	409	-	-	1/37/103/103	0/5/6/6
34	BCR	C	517	-	-	1/29/63/63	0/2/2/2
36	LMG	D	411	-	-	10/41/61/70	0/1/1/1
43	CHL	R	608	-	3/3/16/26	5/15/113/137	-
32	CLA	B	617	-	1/1/15/20	16/37/115/115	-
32	CLA	B	607	-	1/1/15/20	11/37/115/115	-
37	DGD	C	523	-	-	15/55/95/95	0/2/2/2
32	CLA	c	509	-	1/1/15/20	10/37/115/115	-
36	LMG	d	411	-	-	10/41/61/70	0/1/1/1
44	LUT	S	1620	-	-	4/29/67/67	0/2/2/2
32	CLA	Y	611	38	1/1/15/20	11/37/115/115	-
36	LMG	A	413	-	-	17/43/63/70	0/1/1/1
32	CLA	Y	610	25	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CHL	N	608	-	3/3/16/26	5/20/118/137	-
37	DGD	C	518	-	-	11/44/84/95	0/2/2/2
32	CLA	c	512	-	1/1/15/20	15/37/115/115	-
32	CLA	C	502	-	-	8/37/115/115	-
32	CLA	R	609	23	1/1/11/20	8/13/91/115	-
32	CLA	Y	614	-	1/1/12/20	6/24/102/115	-
32	CLA	y	613	25	-	13/37/115/115	-
32	CLA	B	602	47	1/1/15/20	12/37/115/115	-
44	LUT	y	1621	-	-	5/29/67/67	0/2/2/2
38	LHG	G	2630	32	-	17/53/53/53	-
32	CLA	S	610	24	1/1/11/20	6/18/96/115	-
32	CLA	b	611	47	1/1/15/20	7/37/115/115	-
32	CLA	s	605	24	1/1/12/20	6/19/97/115	-
42	LMU	z	2634	-	-	9/21/61/61	0/2/2/2
32	CLA	c	502	-	-	8/37/115/115	-
43	CHL	Y	608	-	3/3/16/26	4/20/118/137	-
46	NEX	y	1623	-	-	9/27/83/83	0/3/3/3
32	CLA	c	503	-	1/1/15/20	10/37/115/115	-
43	CHL	g	608	-	3/3/15/26	7/13/111/137	-
38	LHG	d	409	-	-	19/53/53/53	-
43	CHL	y	608	-	3/3/16/26	4/20/118/137	-
32	CLA	a	407	47	1/1/11/20	2/18/96/115	-
32	CLA	C	510	-	1/1/15/20	17/37/115/115	-
32	CLA	C	513	-	1/1/15/20	19/37/115/115	-
32	CLA	D	403	-	-	12/37/115/115	-
32	CLA	C	507	47	1/1/15/20	11/37/115/115	-
43	CHL	n	609	21	3/3/20/26	21/39/137/137	-
38	LHG	g	2630	32	-	17/53/53/53	-
32	CLA	y	610	25	1/1/15/20	5/37/115/115	-
43	CHL	y	607	-	3/3/20/26	22/39/137/137	-
32	CLA	g	614	-	1/1/11/20	11/18/96/115	-
32	CLA	r	604	-	1/1/11/20	7/18/96/115	-
44	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	R	606	-	3/3/15/26	5/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	n	611	38	1/1/11/20	12/18/96/115	-
37	DGD	C	519	-	-	11/51/91/95	0/2/2/2
32	CLA	R	602	23	1/1/14/20	5/31/109/115	-
32	CLA	G	603	-	1/1/15/20	14/37/115/115	-
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
32	CLA	B	612	-	1/1/15/20	11/37/115/115	-
32	CLA	N	613	21	-	12/37/115/115	-
43	CHL	s	601	24	3/3/16/26	8/15/113/137	-
32	CLA	b	602	47	1/1/15/20	12/37/115/115	-
32	CLA	r	602	23	1/1/14/20	5/31/109/115	-
32	CLA	A	410	-	-	4/31/109/115	-
32	CLA	b	610	-	-	15/37/115/115	-
34	BCR	c	515	-	-	7/29/63/63	0/2/2/2
32	CLA	Y	612	25	1/1/15/20	16/37/115/115	-
38	LHG	l	101	-	-	20/53/53/53	-
32	CLA	a	410	-	-	4/31/109/115	-
43	CHL	r	608	-	3/3/16/26	5/15/113/137	-
43	CHL	g	606	-	3/3/16/26	8/20/118/137	-
32	CLA	C	512	-	1/1/15/20	15/37/115/115	-
38	LHG	d	410	-	-	13/43/43/53	-
34	BCR	b	618	-	-	2/29/63/63	0/2/2/2
32	CLA	C	504	47	1/1/15/20	13/37/115/115	-
32	CLA	N	611	38	1/1/11/20	12/18/96/115	-
43	CHL	g	601	22	3/3/20/26	14/39/137/137	-
43	CHL	n	607	-	3/3/20/26	20/39/137/137	-
32	CLA	y	604	-	1/1/15/20	13/37/115/115	-
37	DGD	c	519	-	-	13/51/91/95	0/2/2/2
32	CLA	s	613	24	-	8/18/96/115	-
43	CHL	N	609	21	3/3/20/26	21/39/137/137	-
34	BCR	A	411	-	-	5/29/63/63	0/2/2/2
44	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
38	LHG	d	408	-	-	18/48/48/53	-
44	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
43	CHL	S	606	-	3/3/15/26	5/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	C	511	4	-	12/37/115/115	-
32	CLA	b	609	-	1/1/15/20	14/37/115/115	-
32	CLA	S	613	24	-	8/18/96/115	-
43	CHL	r	606	-	3/3/15/26	5/13/111/137	-
32	CLA	s	612	24	1/1/11/20	4/13/91/115	-
43	CHL	Y	601	25	3/3/20/26	19/39/137/137	-
32	CLA	N	610	21	1/1/15/20	3/37/115/115	-
36	LMG	B	622	-	-	4/46/66/70	0/1/1/1
40	PL9	d	405	-	-	14/53/73/73	0/1/1/1
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
38	LHG	s	2630	32	-	9/49/49/53	-
43	CHL	S	608	-	3/3/16/26	10/19/117/137	-
32	CLA	S	612	24	1/1/11/20	4/13/91/115	-
44	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	y	614	-	1/1/12/20	6/24/102/115	-
32	CLA	y	612	25	1/1/15/20	16/37/115/115	-
32	CLA	N	604	-	1/1/15/20	12/37/115/115	-
44	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
43	CHL	y	606	-	3/3/20/26	15/39/137/137	-

The worst 5 of 2131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	613	CLA	C4B-NB	7.90	1.42	1.35
32	s	613	CLA	C4B-NB	7.89	1.42	1.35
32	r	602	CLA	C4B-NB	7.82	1.42	1.35
32	s	610	CLA	C4B-NB	7.81	1.42	1.35
32	R	602	CLA	C4B-NB	7.80	1.42	1.35

The worst 5 of 3324 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	412	SQD	O9-S-C6	-20.28	82.84	106.94
35	a	412	SQD	O9-S-C6	-20.18	82.95	106.94
45	y	1622	XAT	C37-C21-C36	-17.09	82.16	107.37
45	Y	1622	XAT	C37-C21-C36	-17.08	82.17	107.37
45	y	1622	XAT	C37-C21-C22	-15.00	82.91	108.98

5 of 272 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	407	CLA	ND
32	B	602	CLA	ND
32	B	603	CLA	ND
32	B	605	CLA	ND

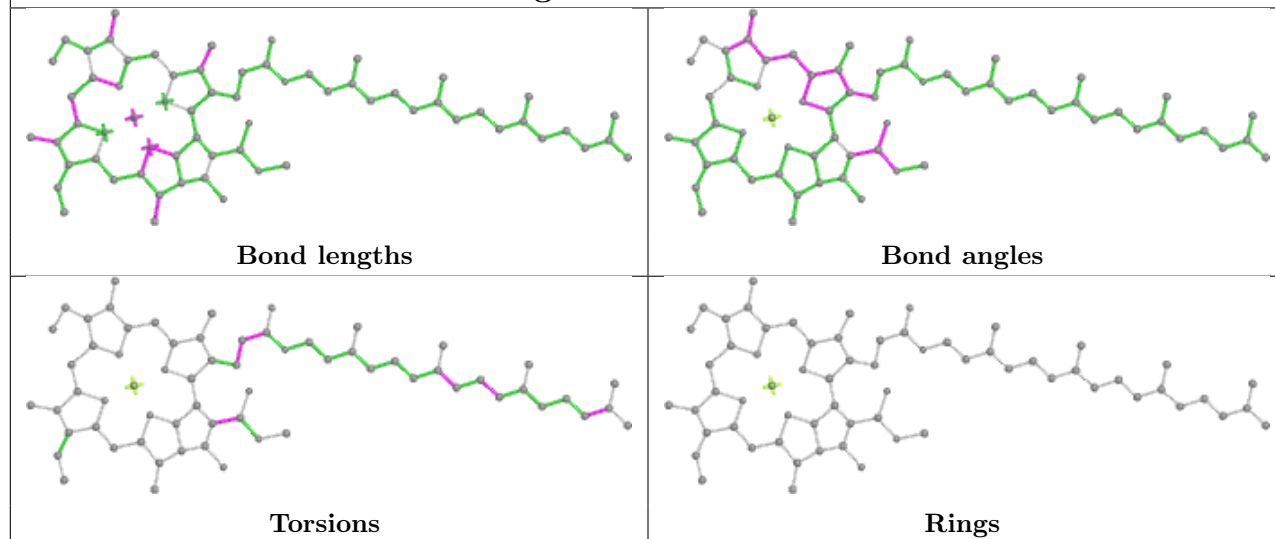
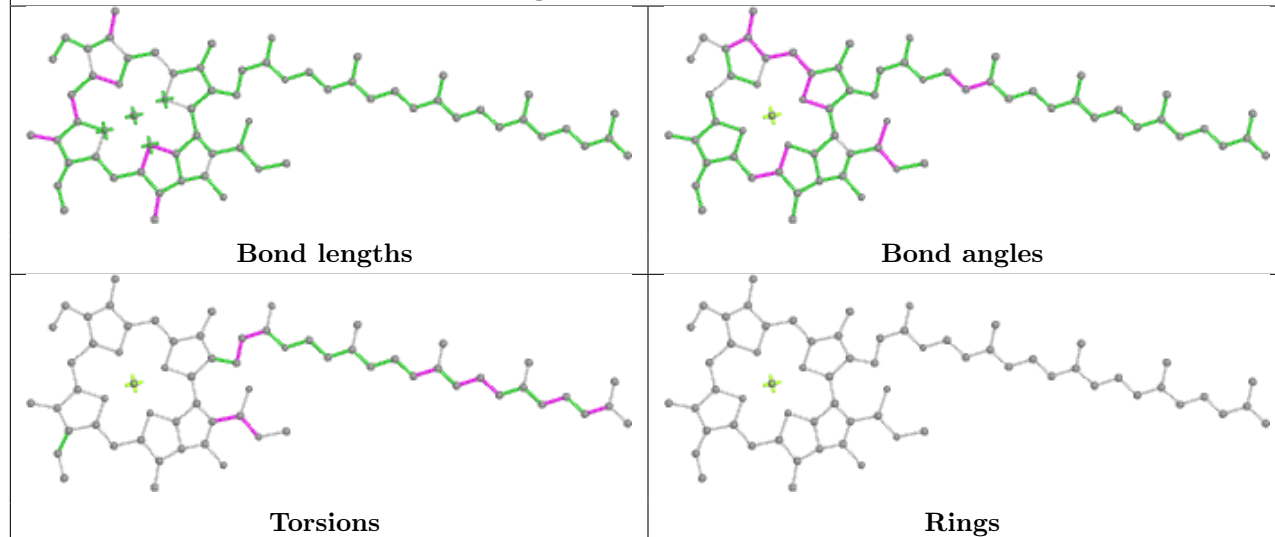
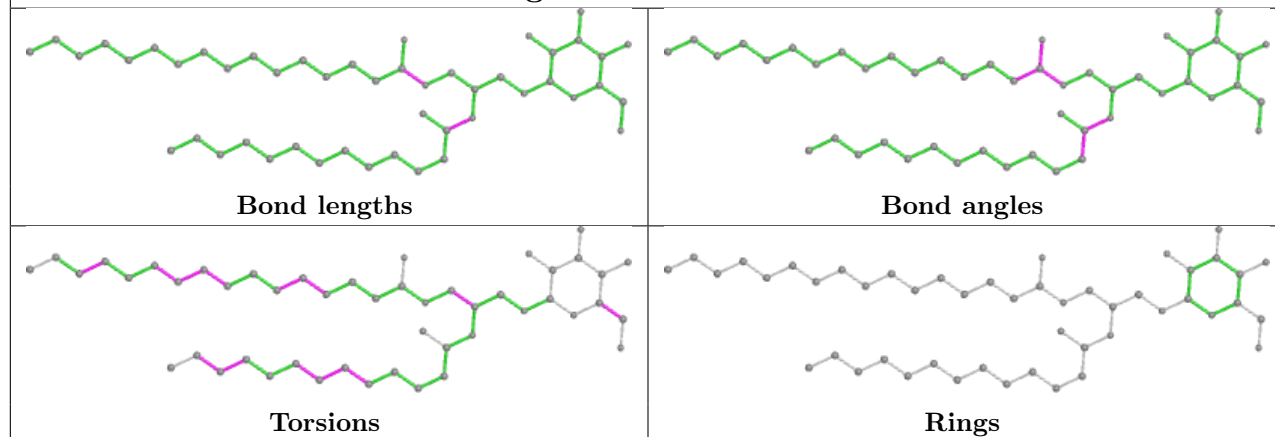
5 of 2937 torsion outliers are listed below:

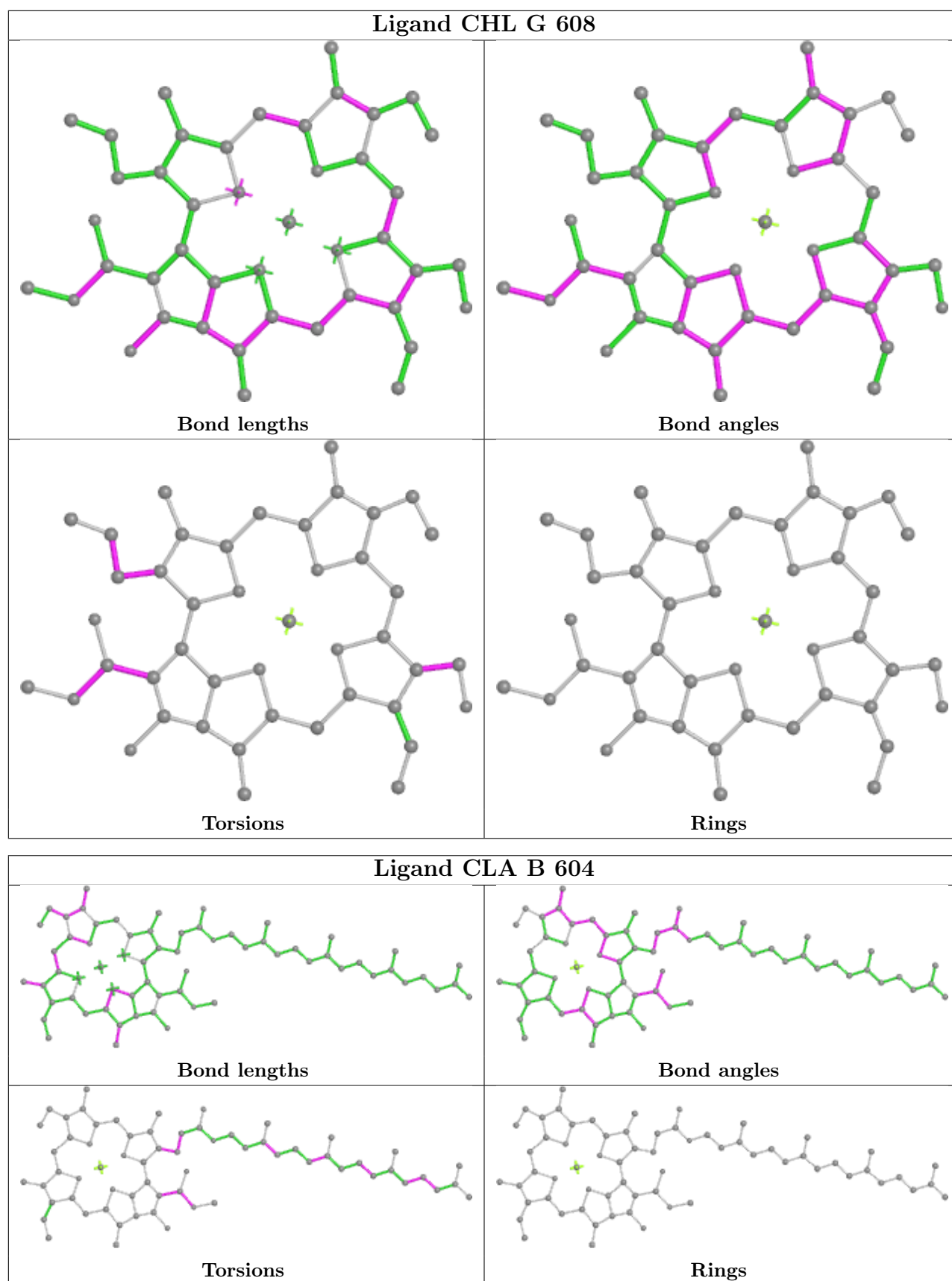
Mol	Chain	Res	Type	Atoms
32	A	406	CLA	CHA-CBD-CGD-O1D
32	A	406	CLA	CHA-CBD-CGD-O2D
32	B	603	CLA	C2-C3-C5-C6
32	B	603	CLA	C4-C3-C5-C6
32	B	604	CLA	C2-C3-C5-C6

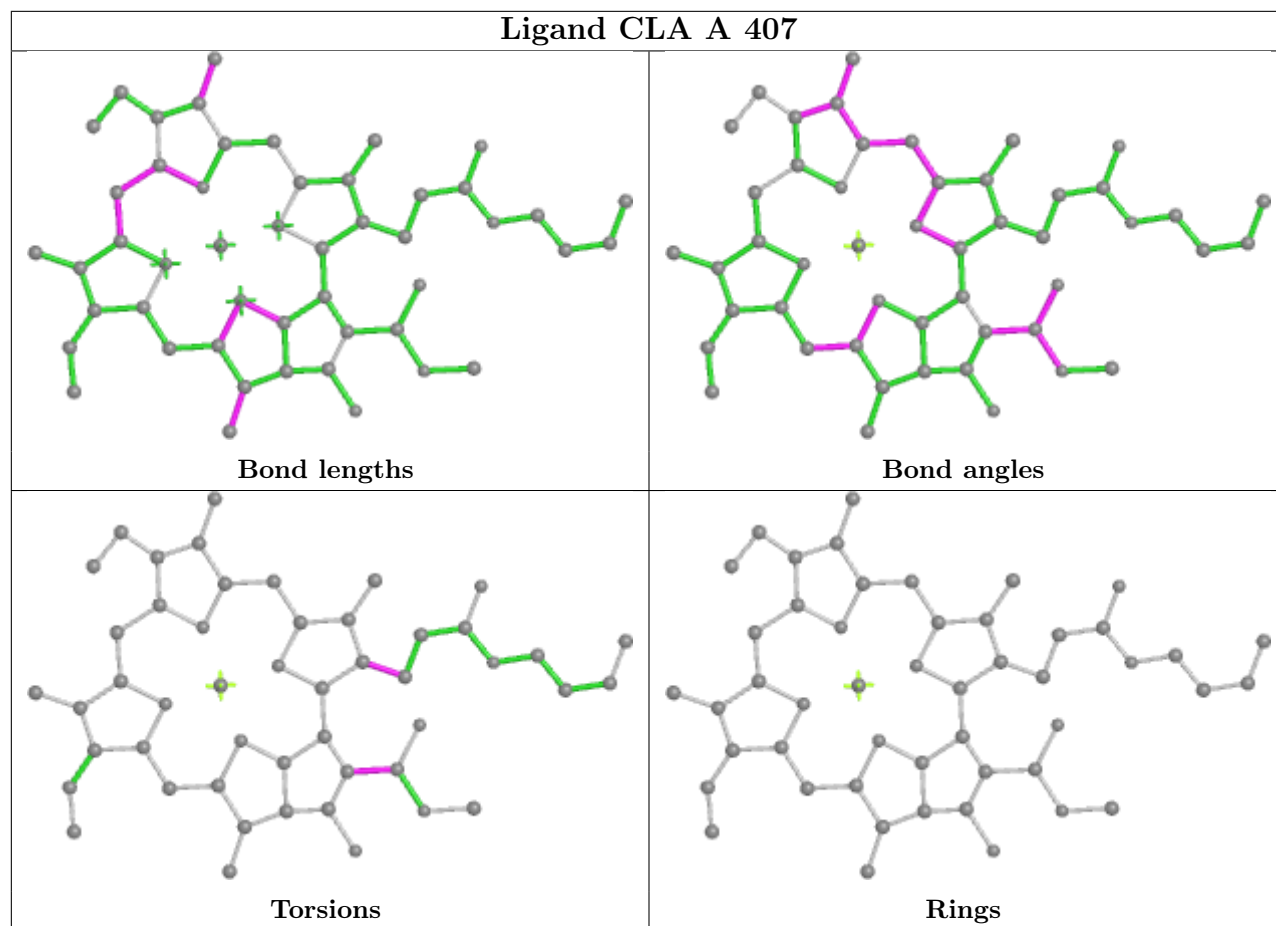
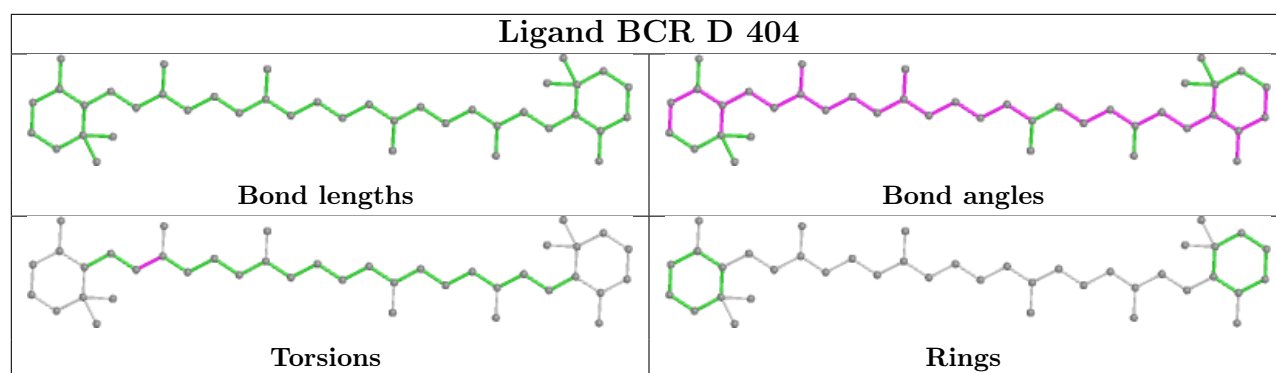
There are no ring outliers.

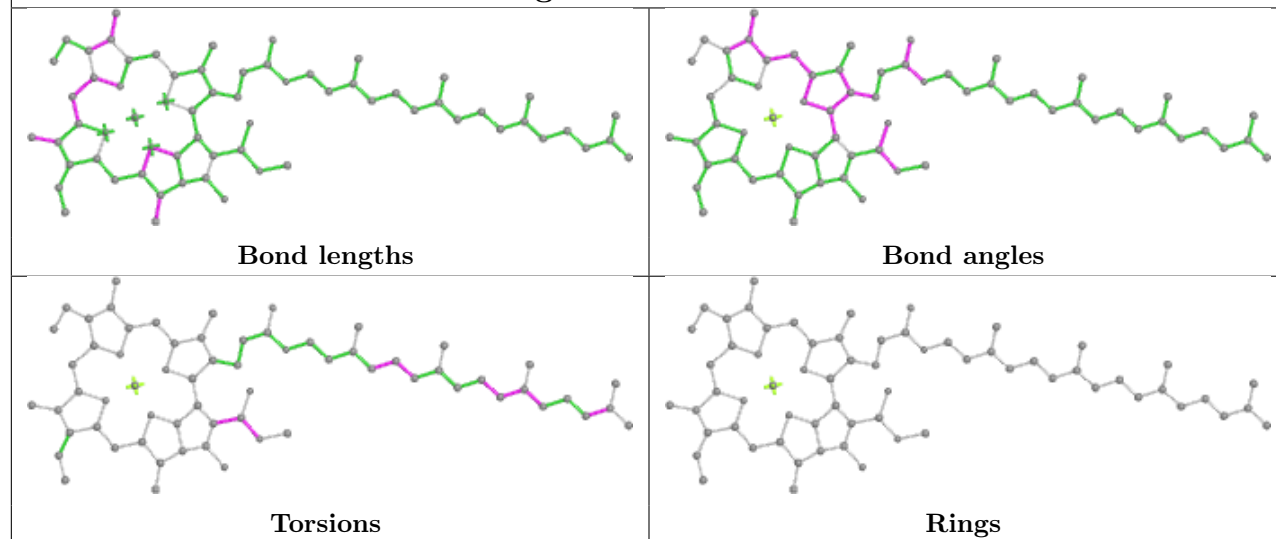
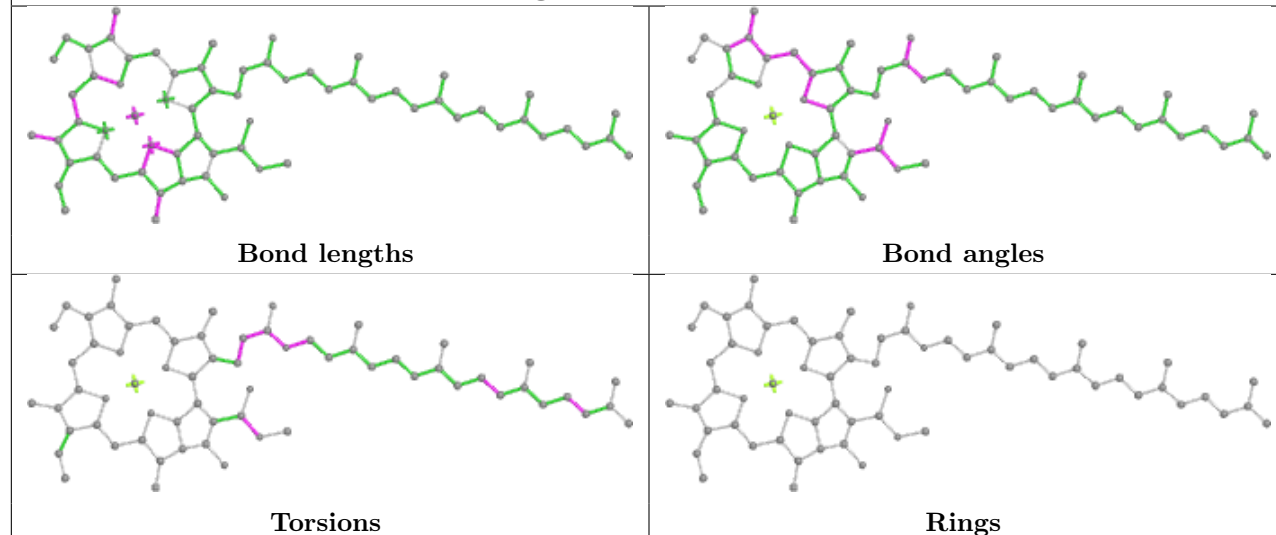
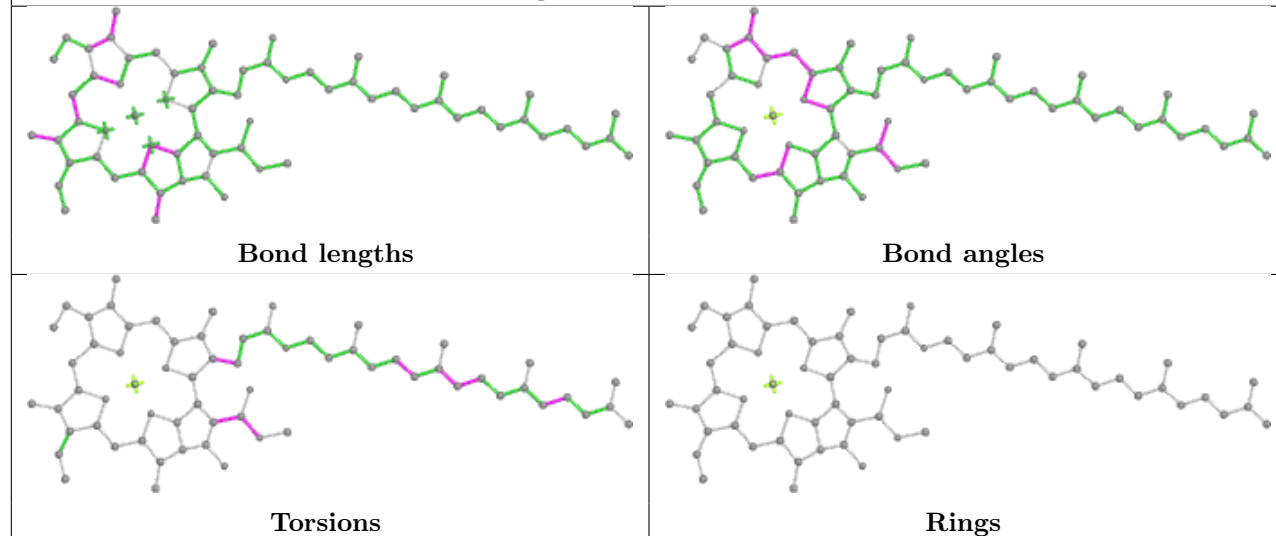
No monomer is involved in short contacts.

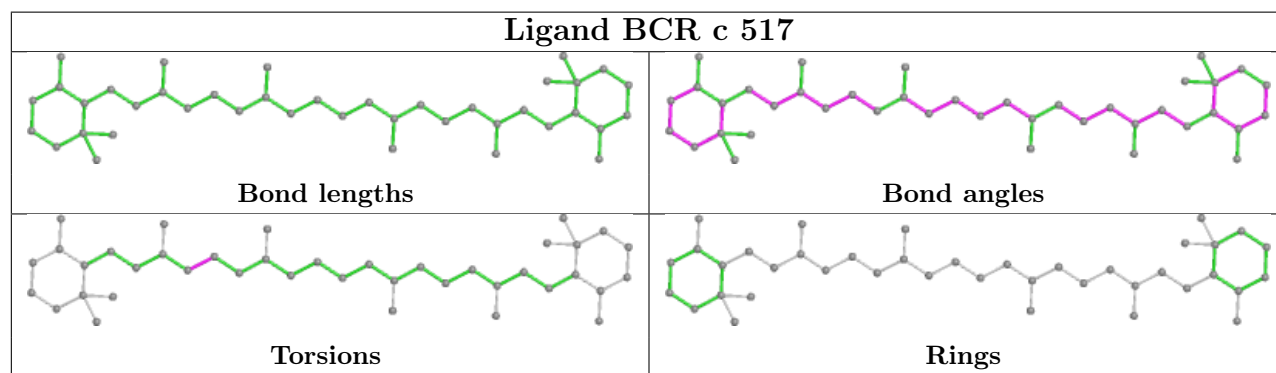
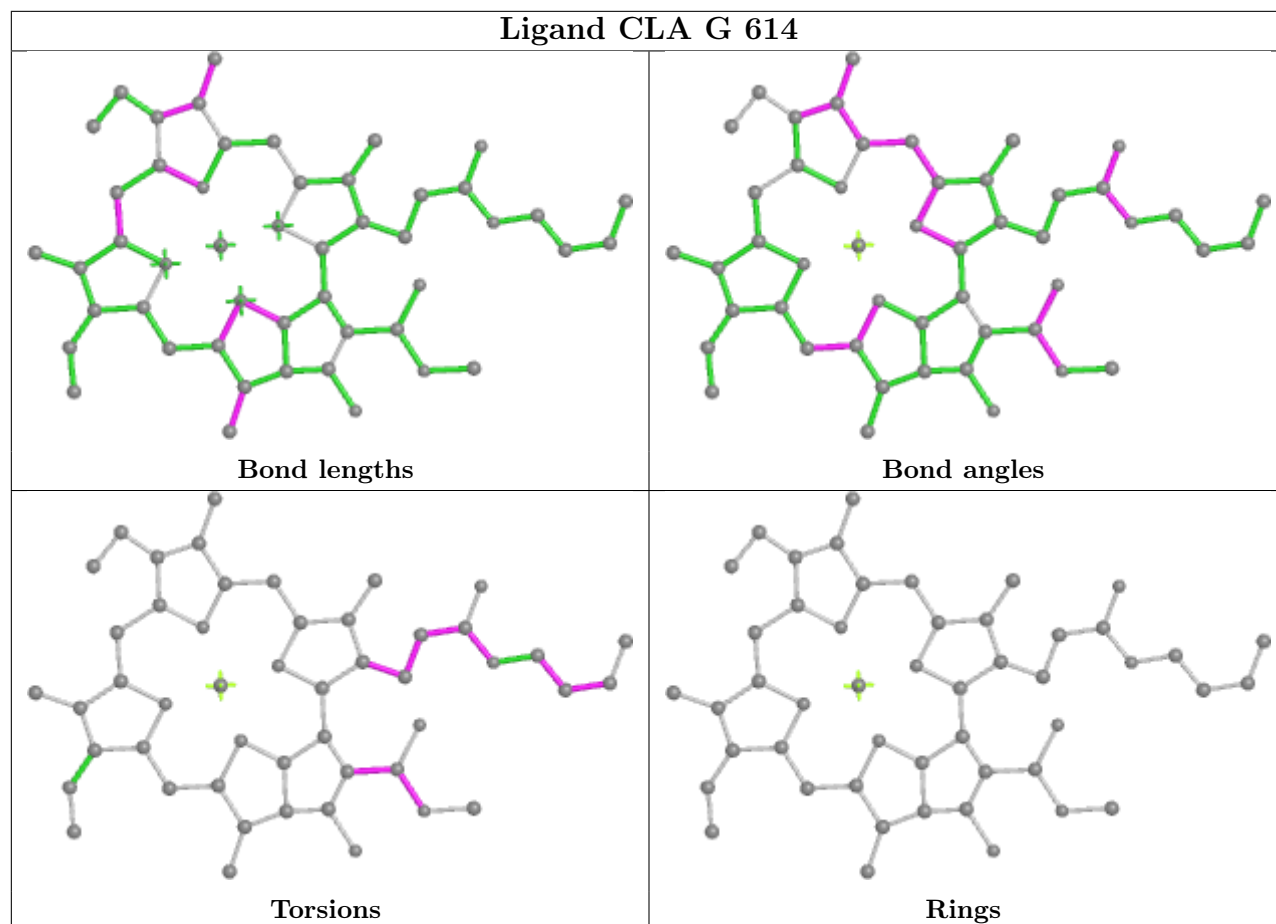
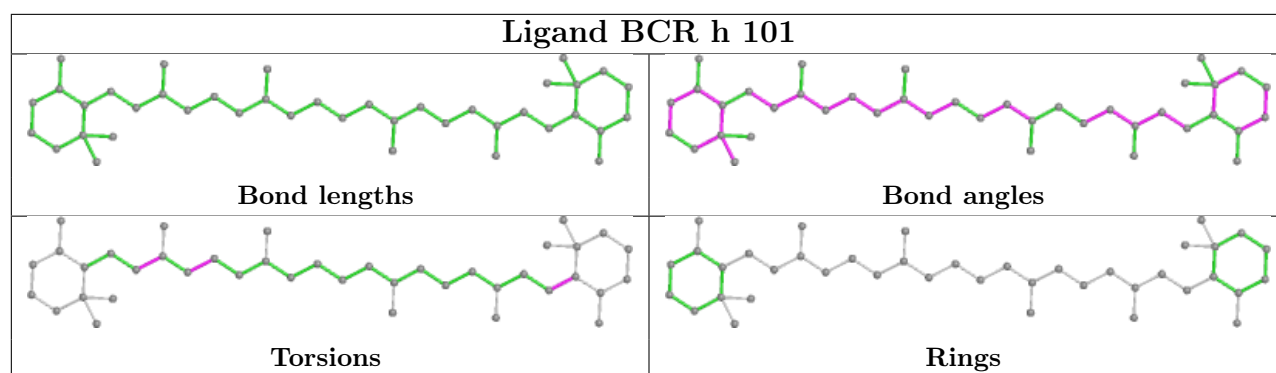
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

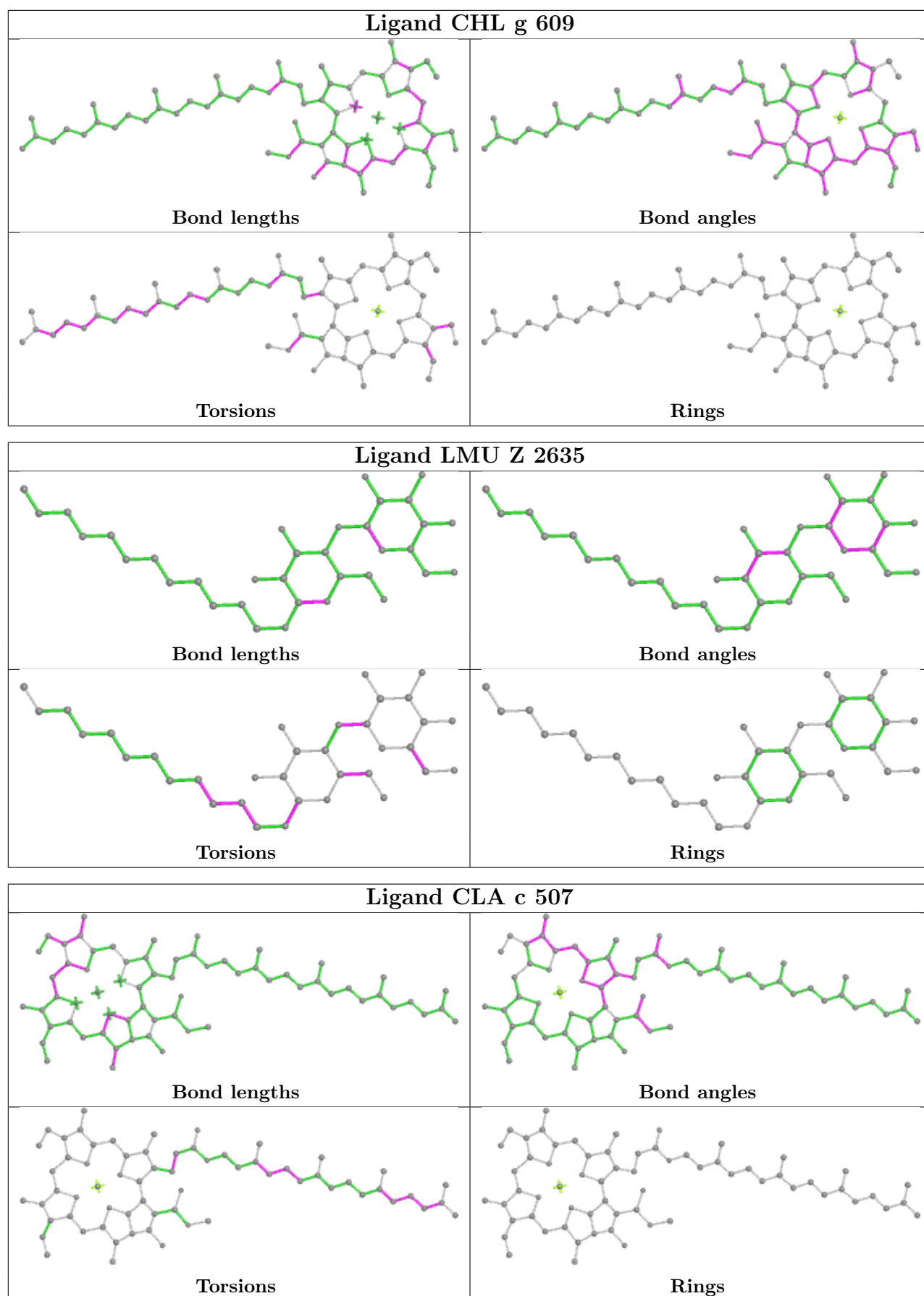
Ligand CLA b 613**Ligand CLA N 602****Ligand LMG H 102**



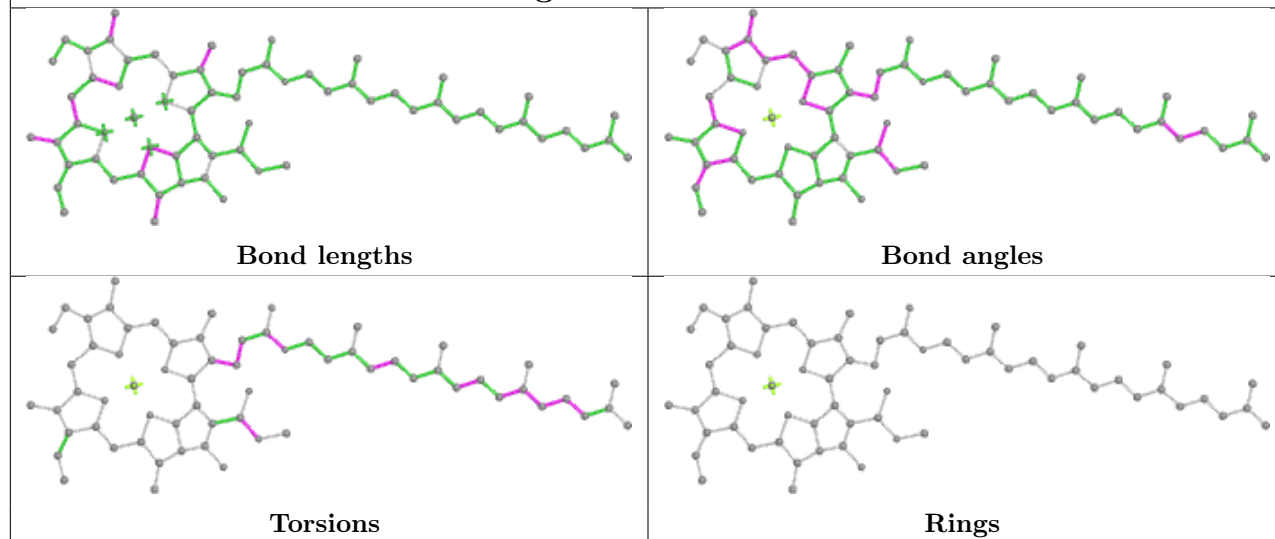


Ligand CLA b 616**Ligand CLA B 614****Ligand CLA B 606**

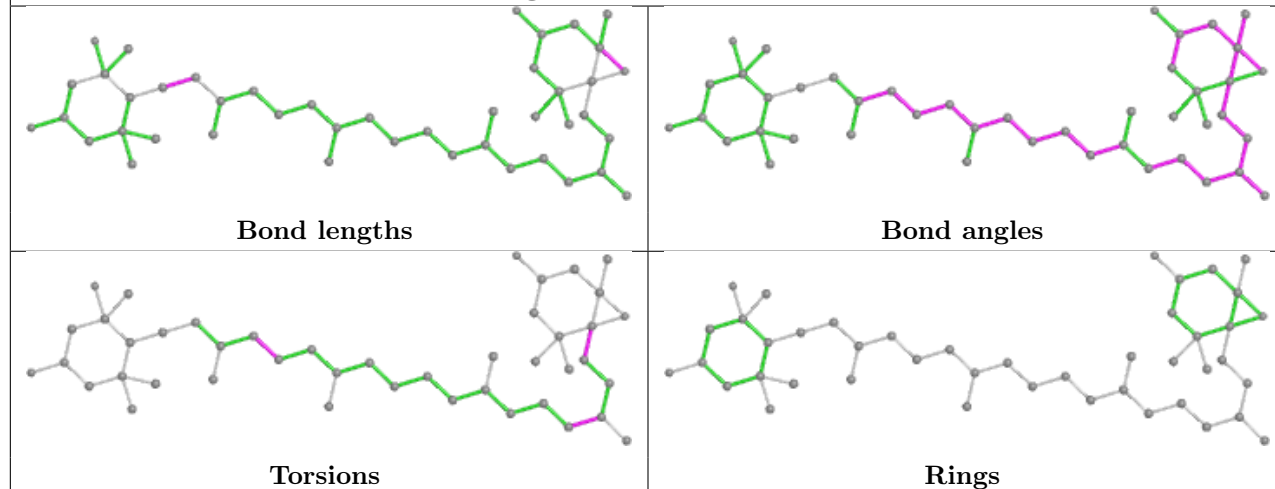




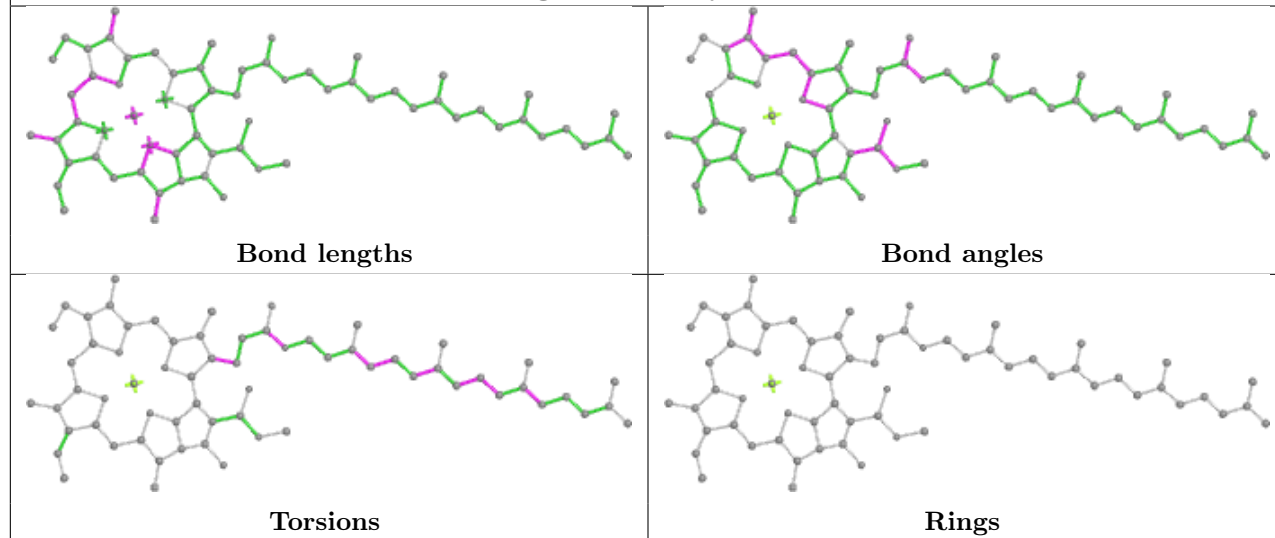
Ligand CLA a 405

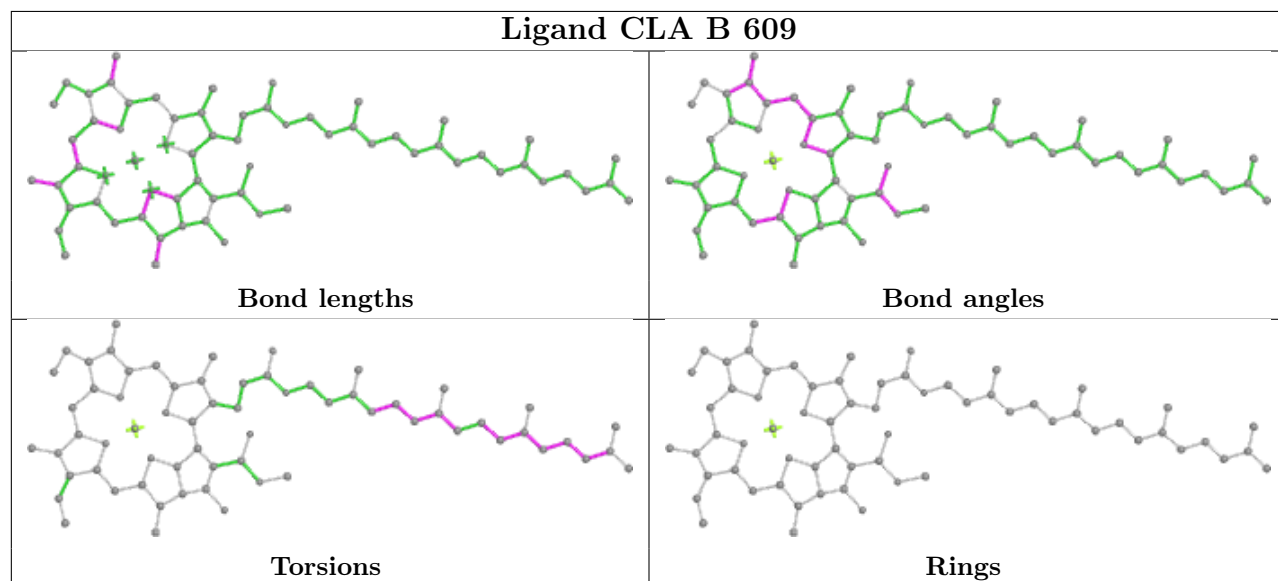
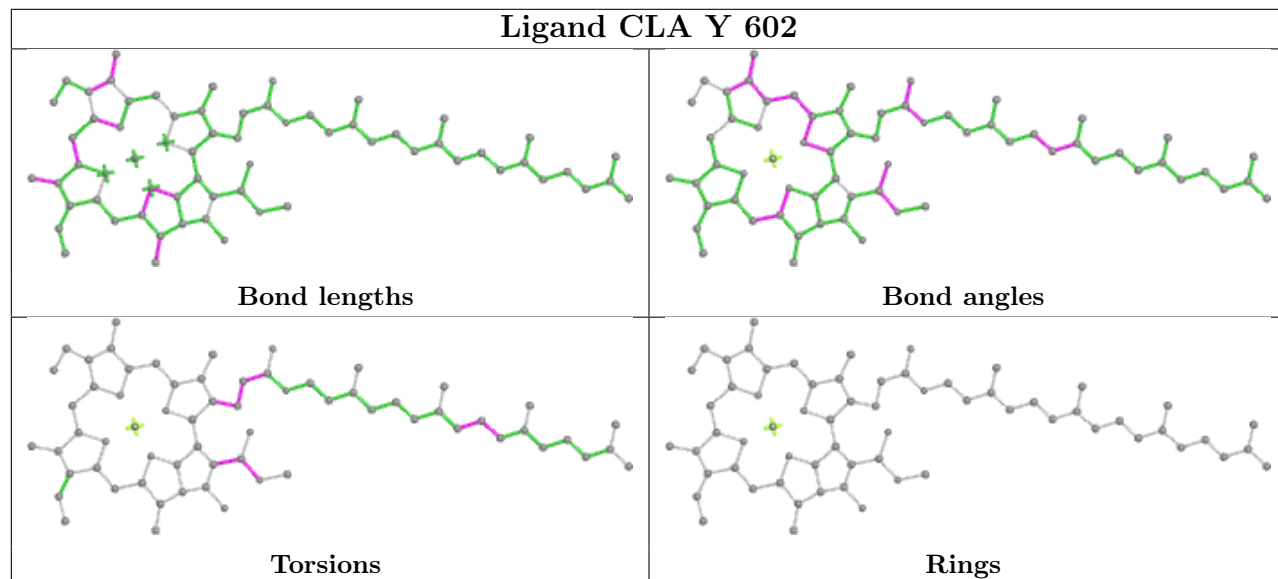
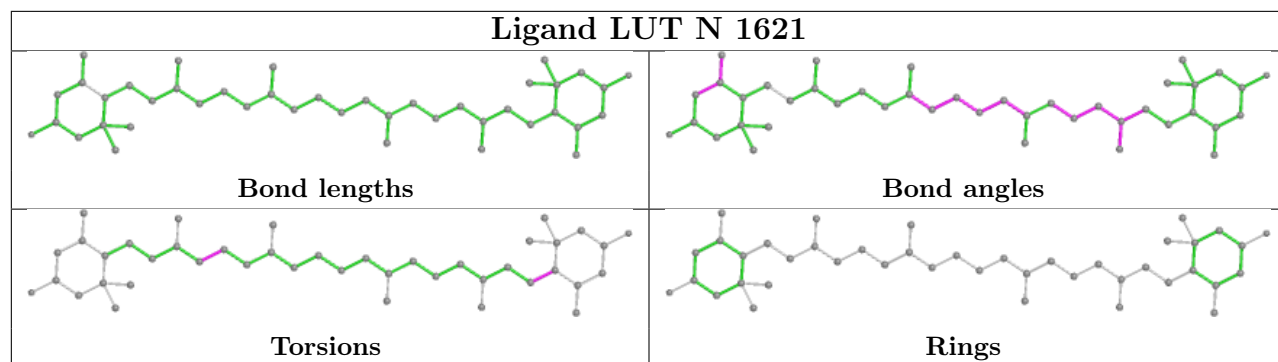


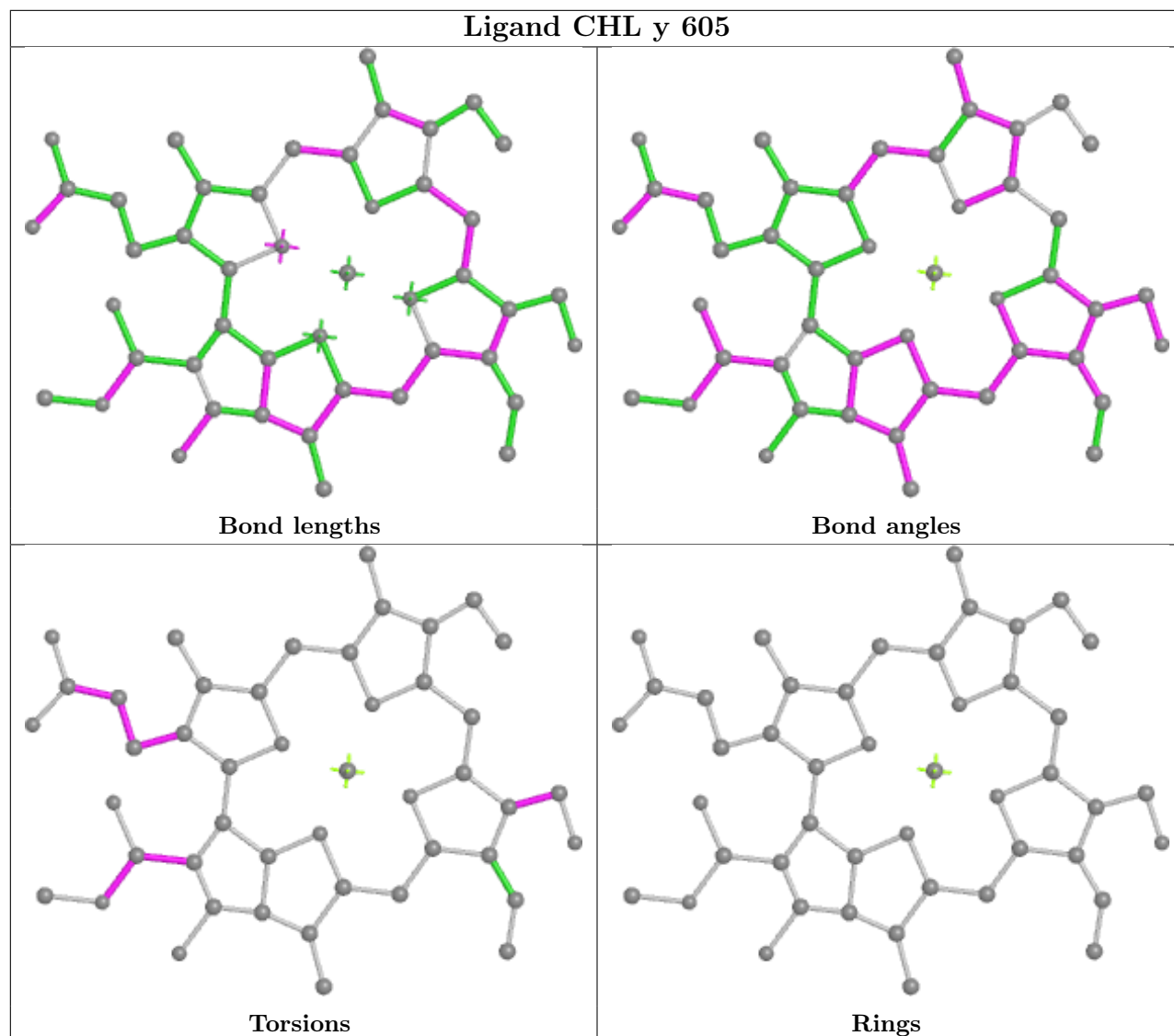
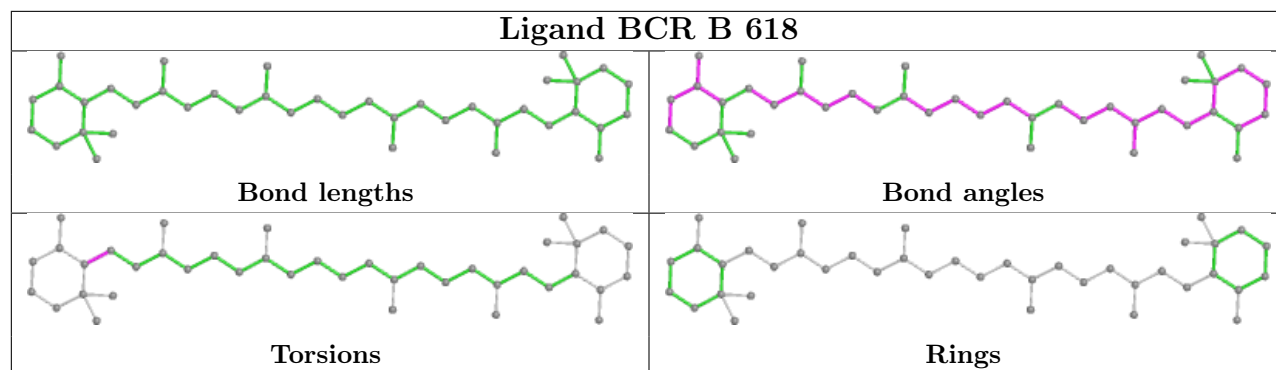
Ligand NEX n 1623

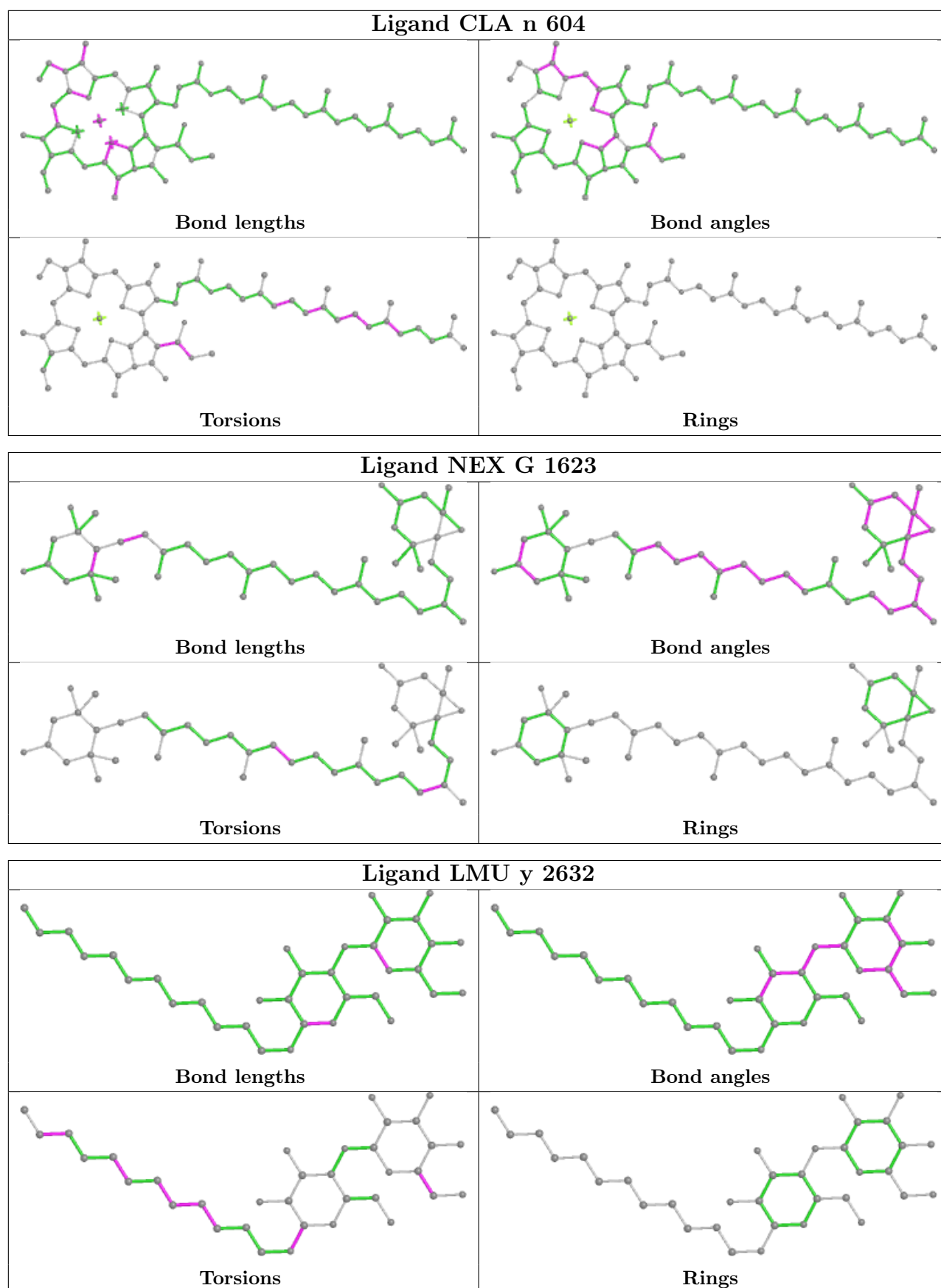


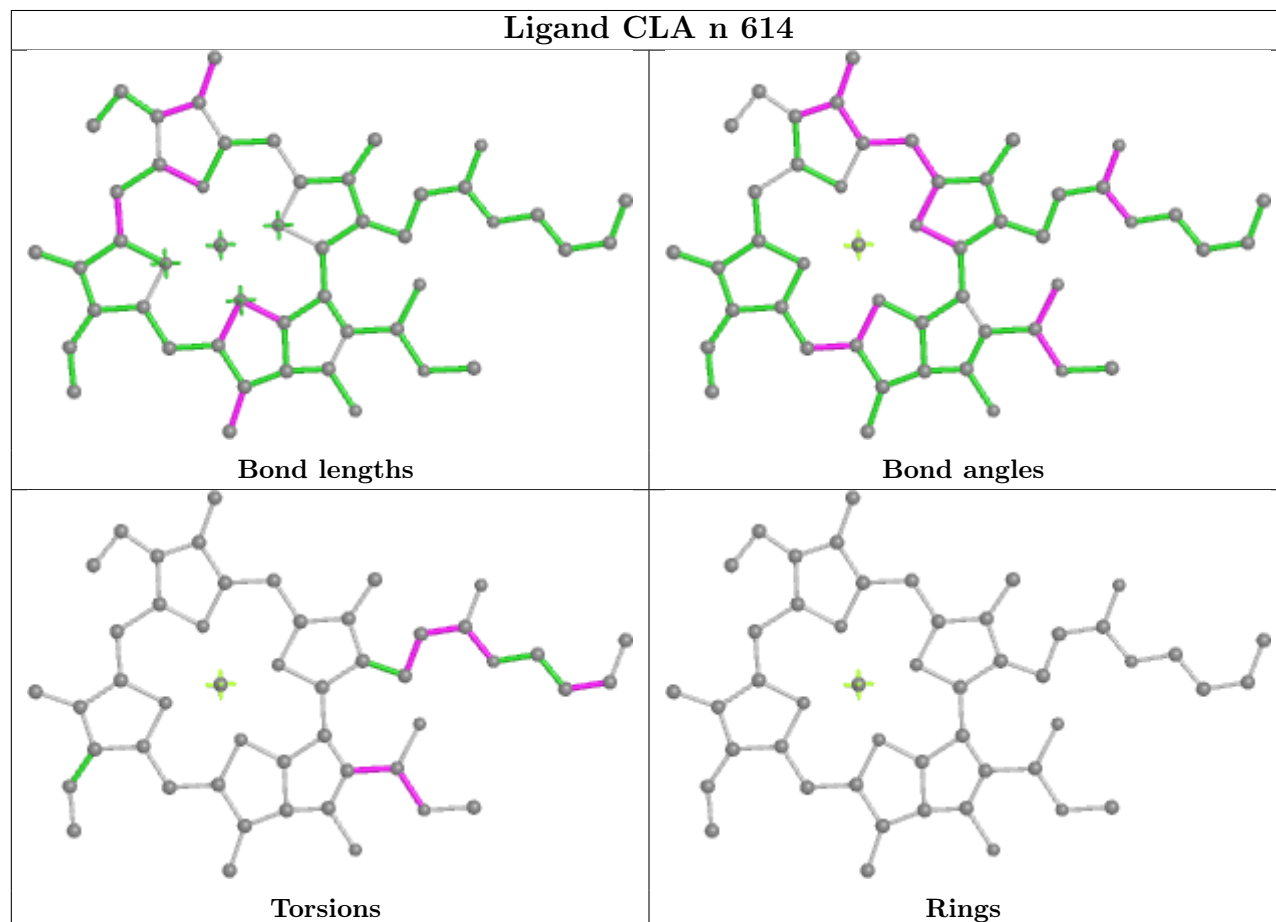
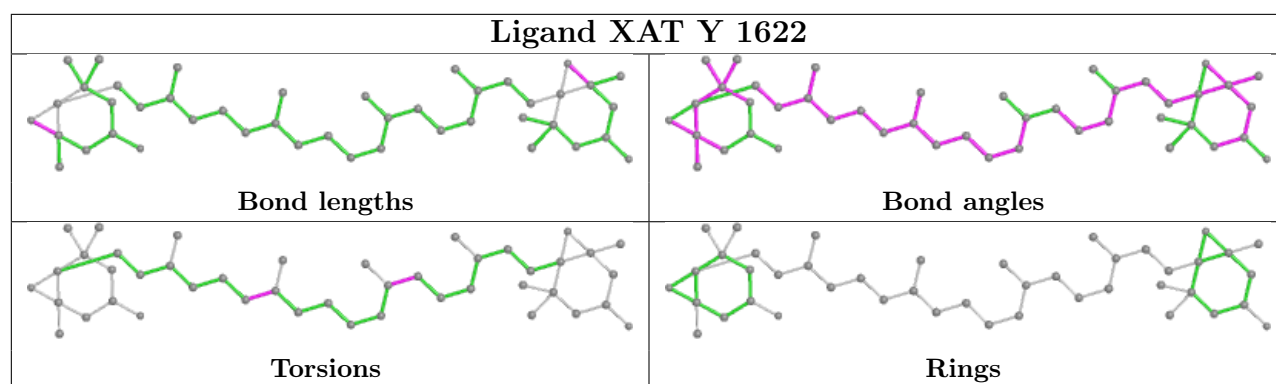
Ligand CLA y 611

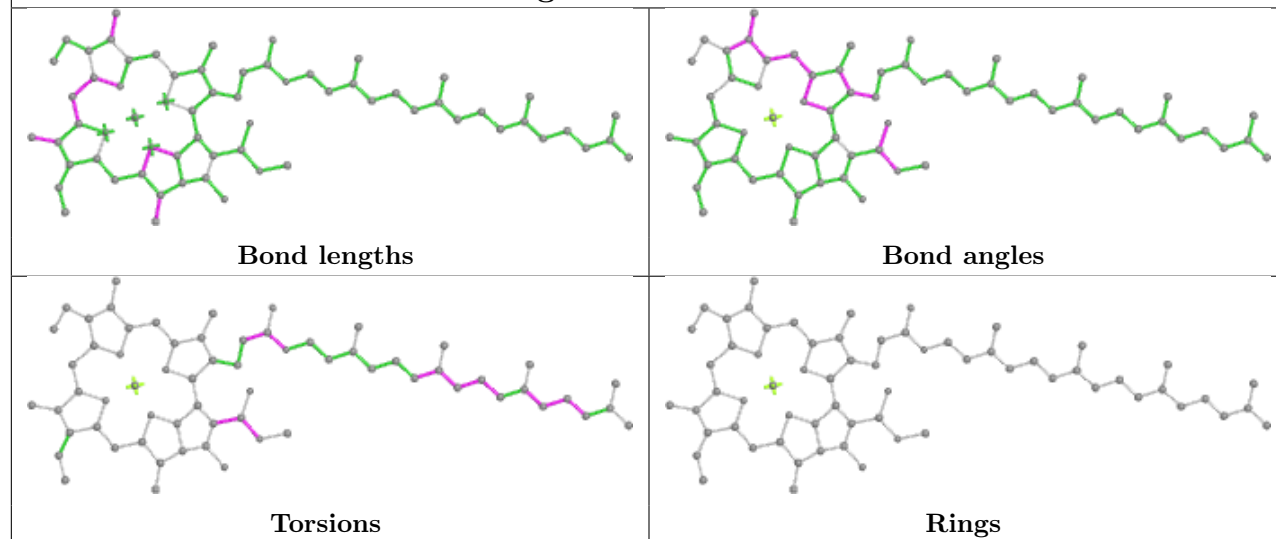
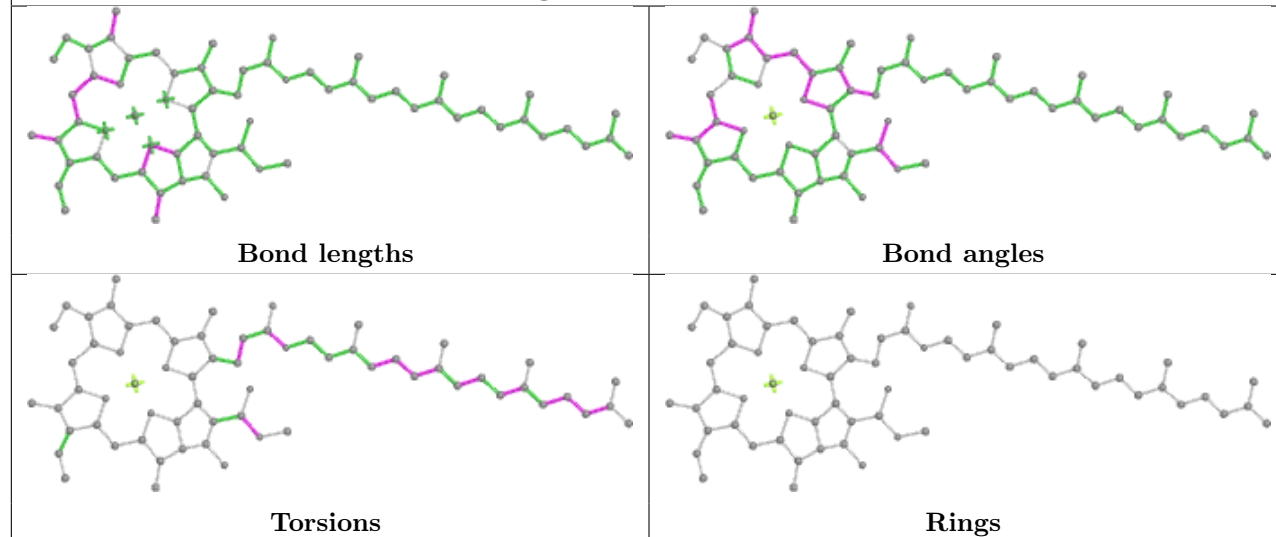
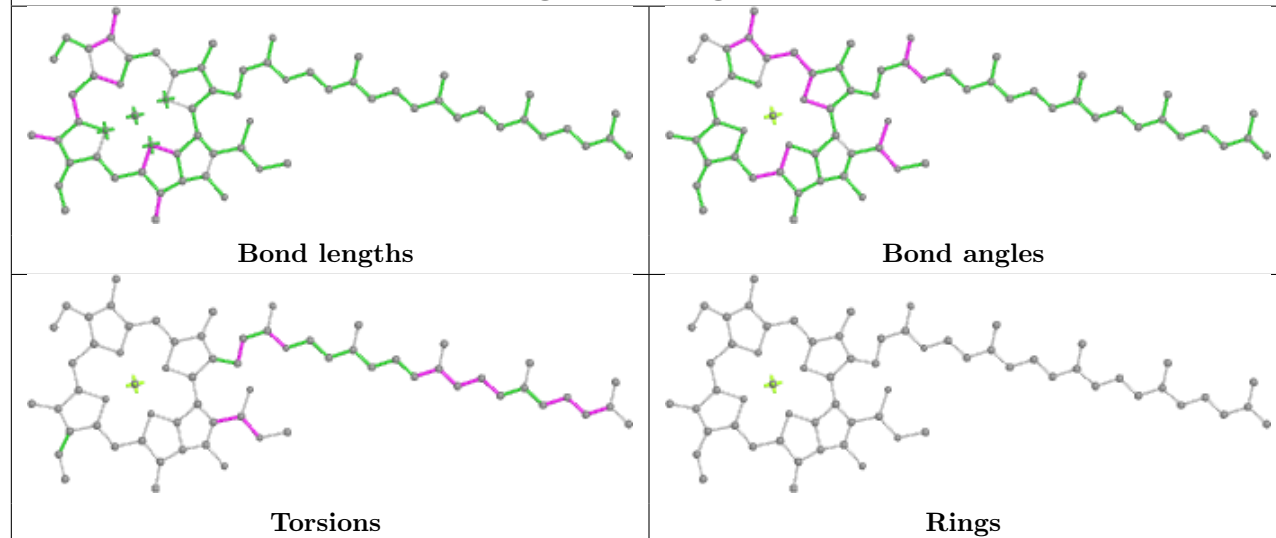


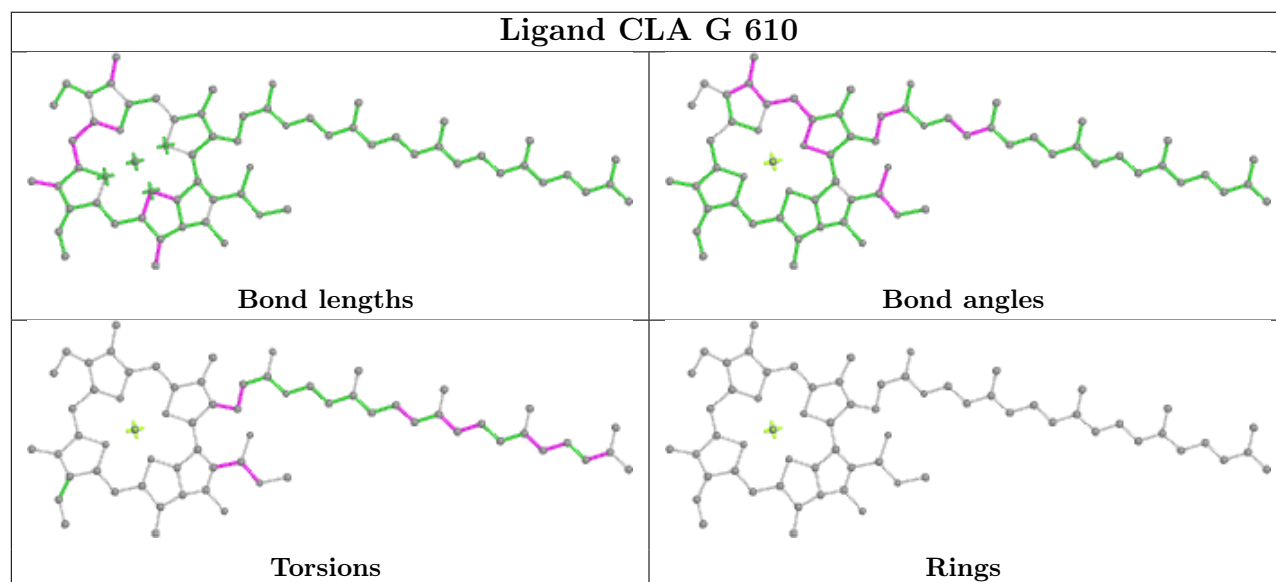
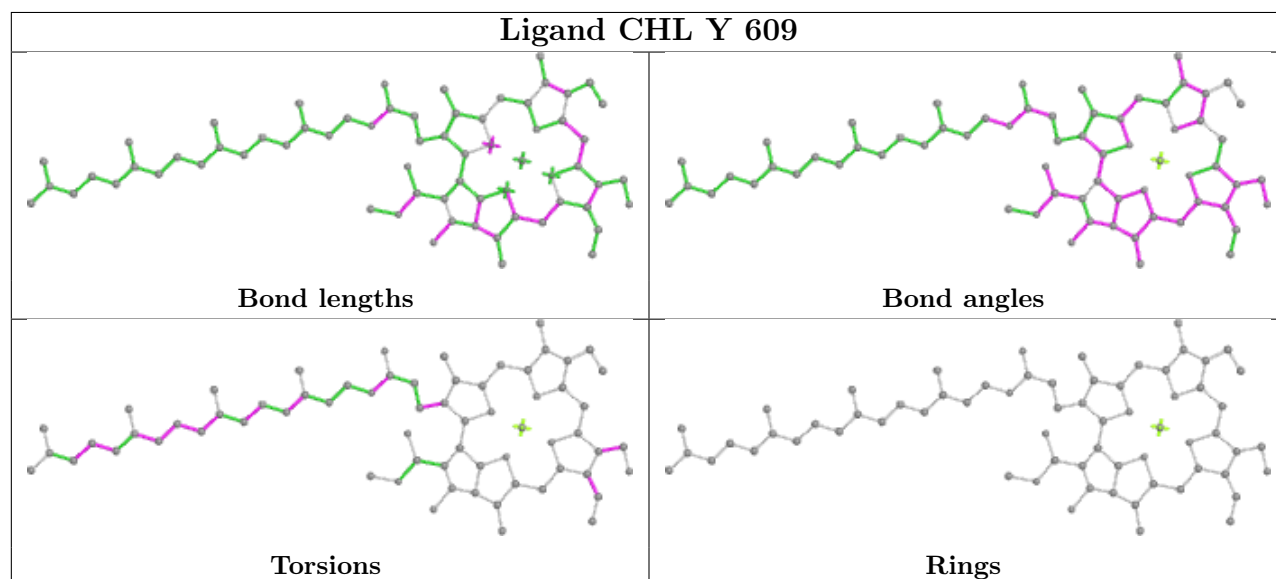
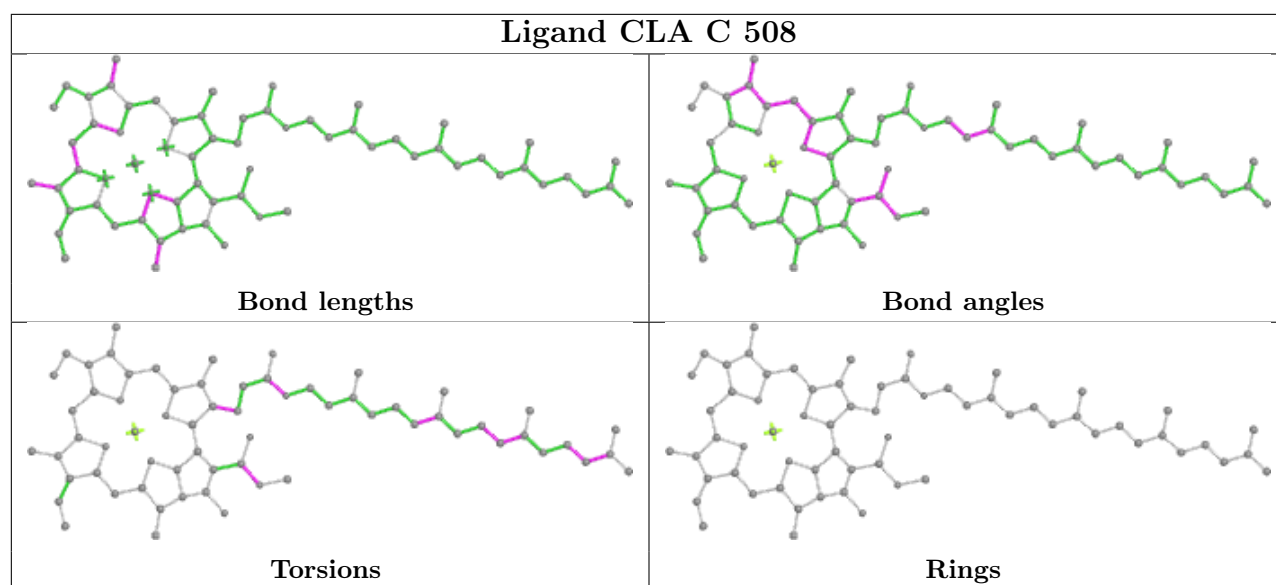




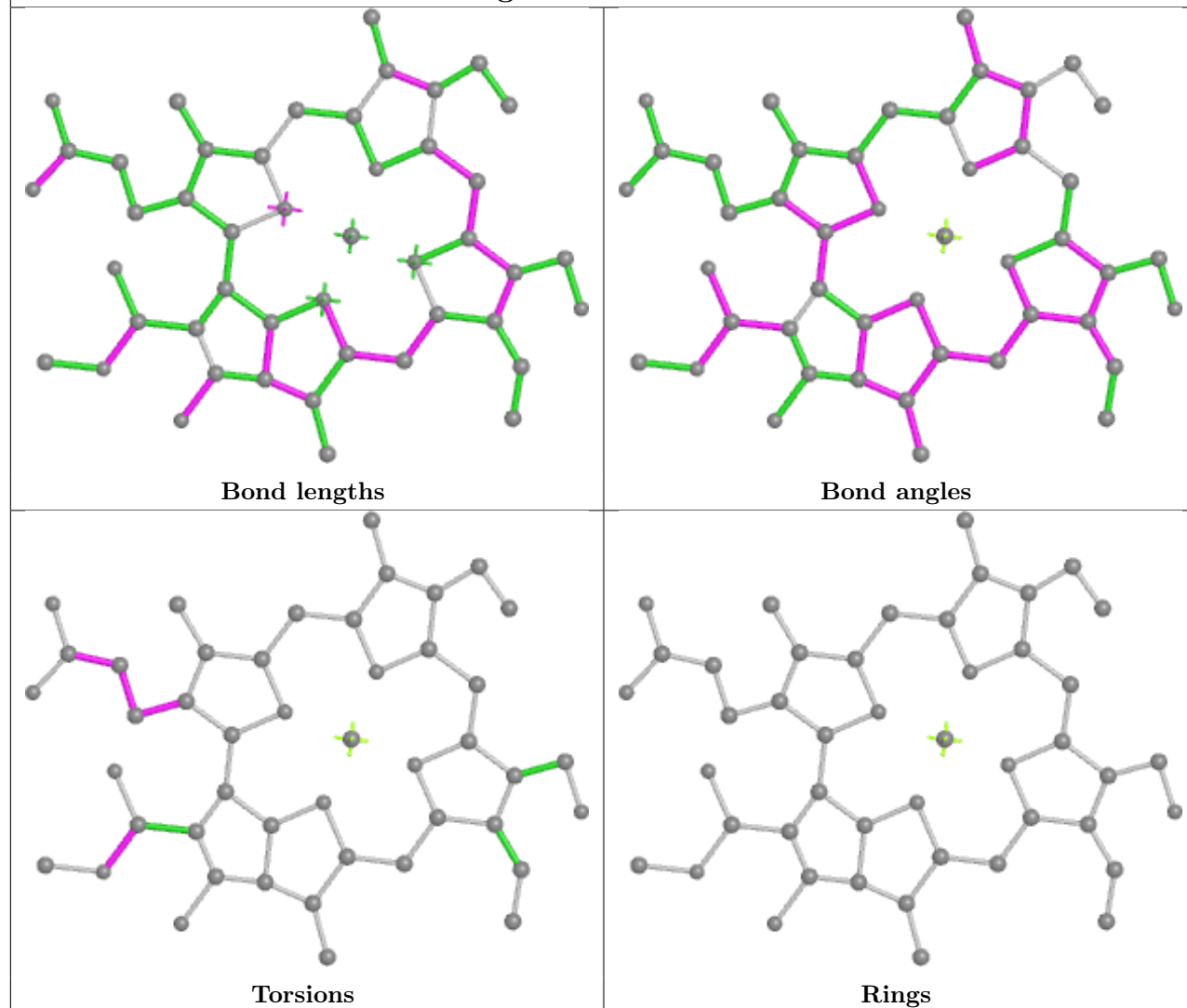


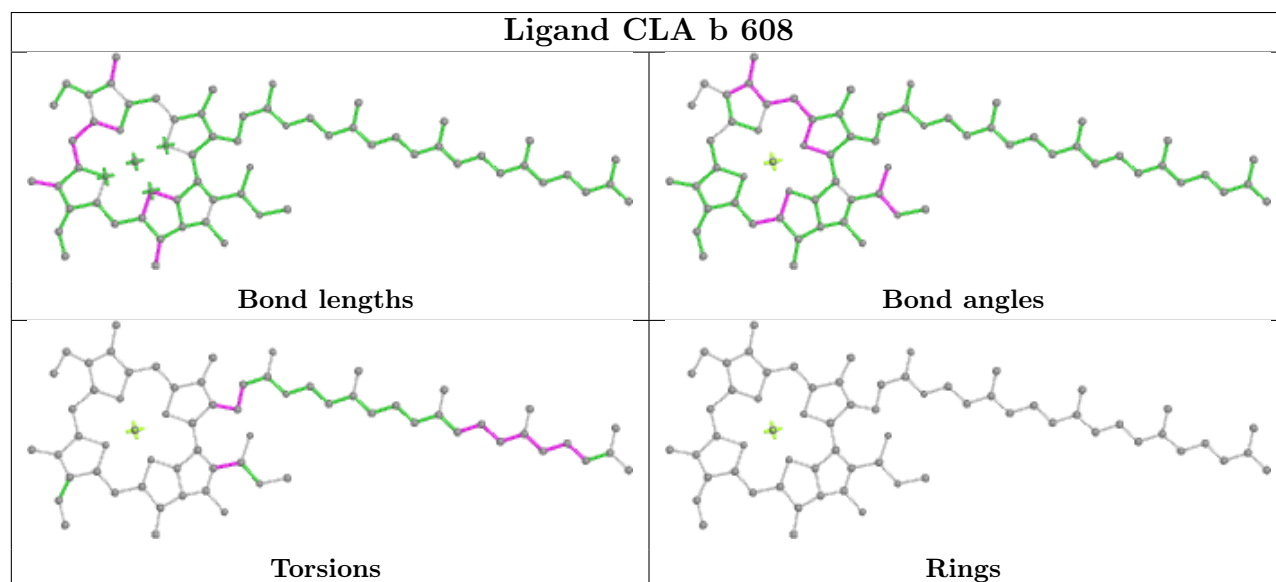
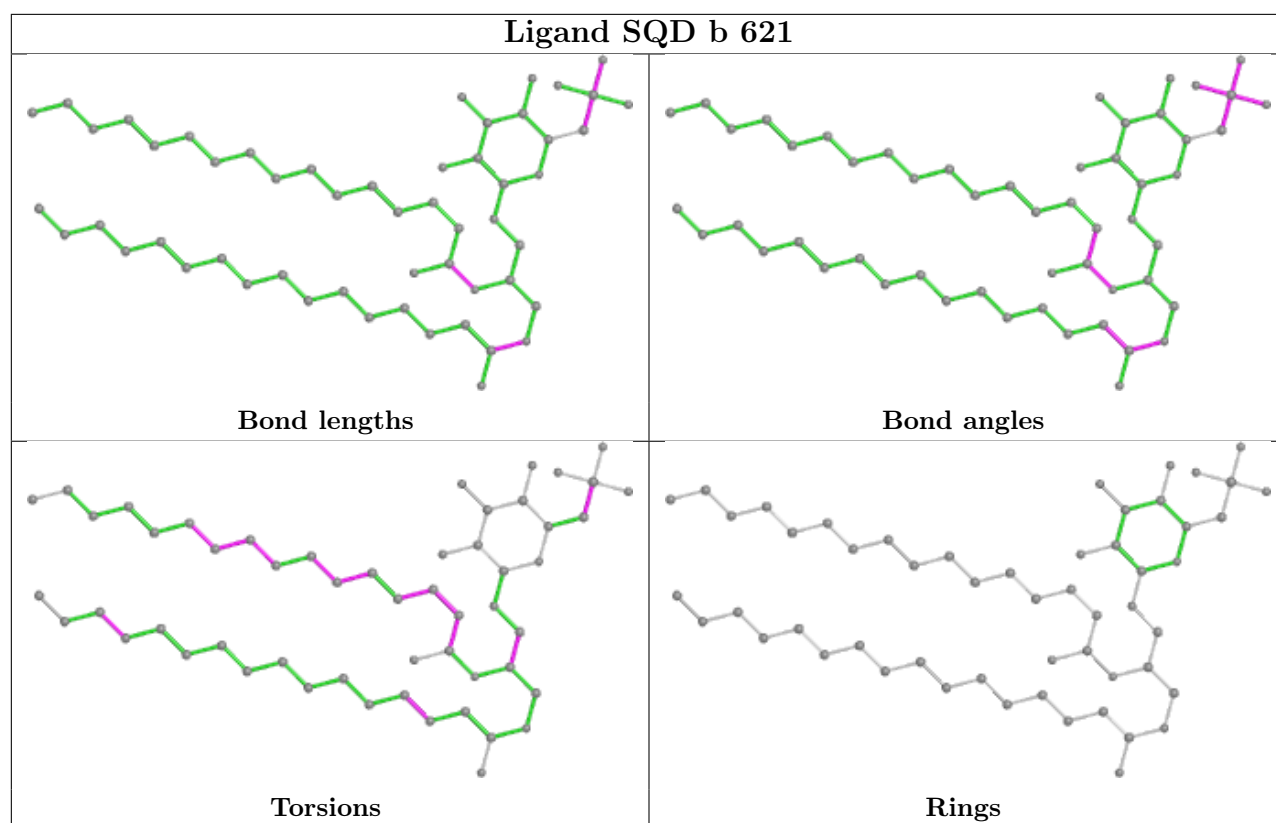


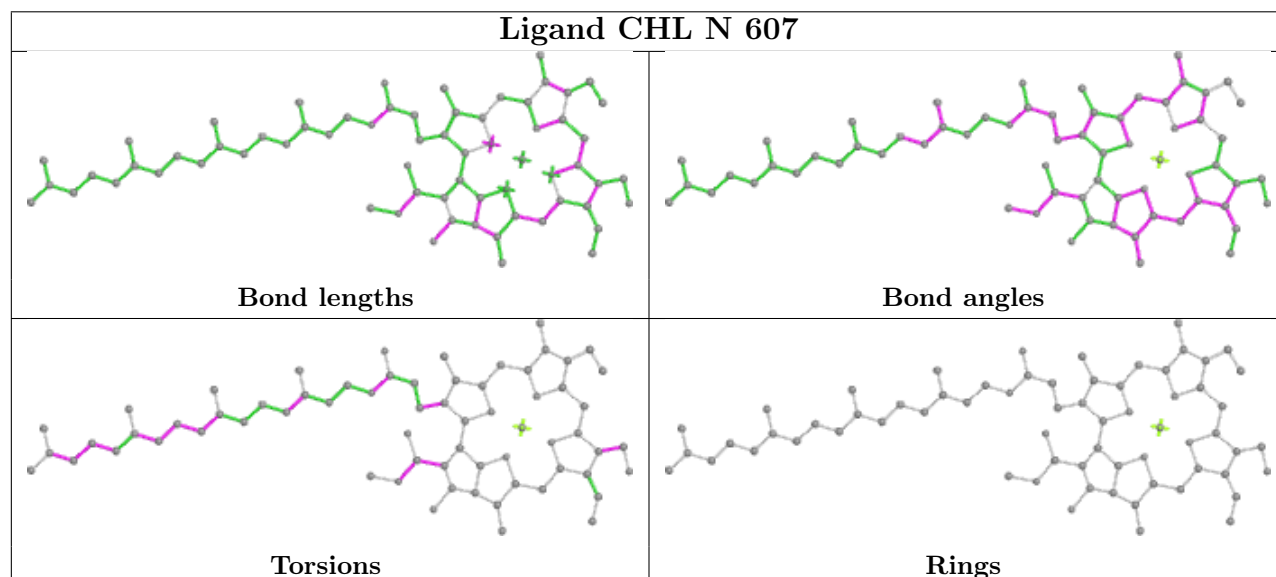
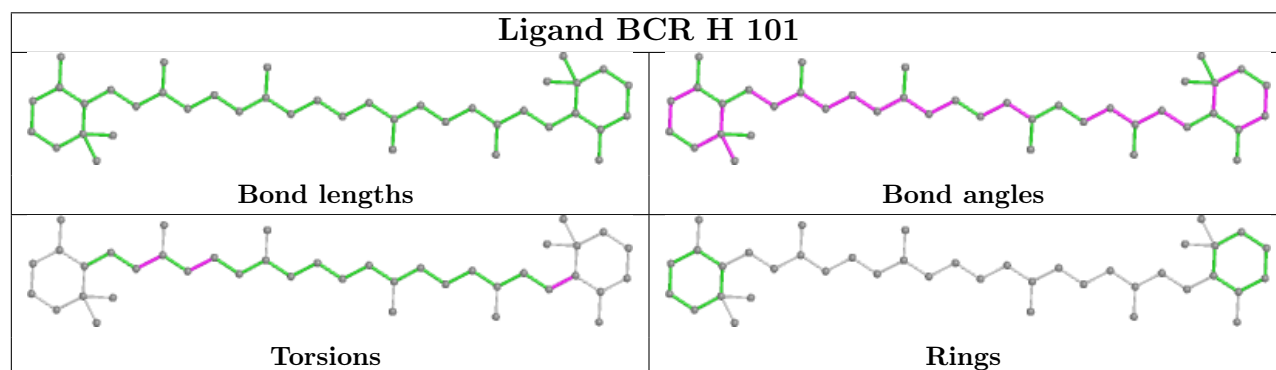
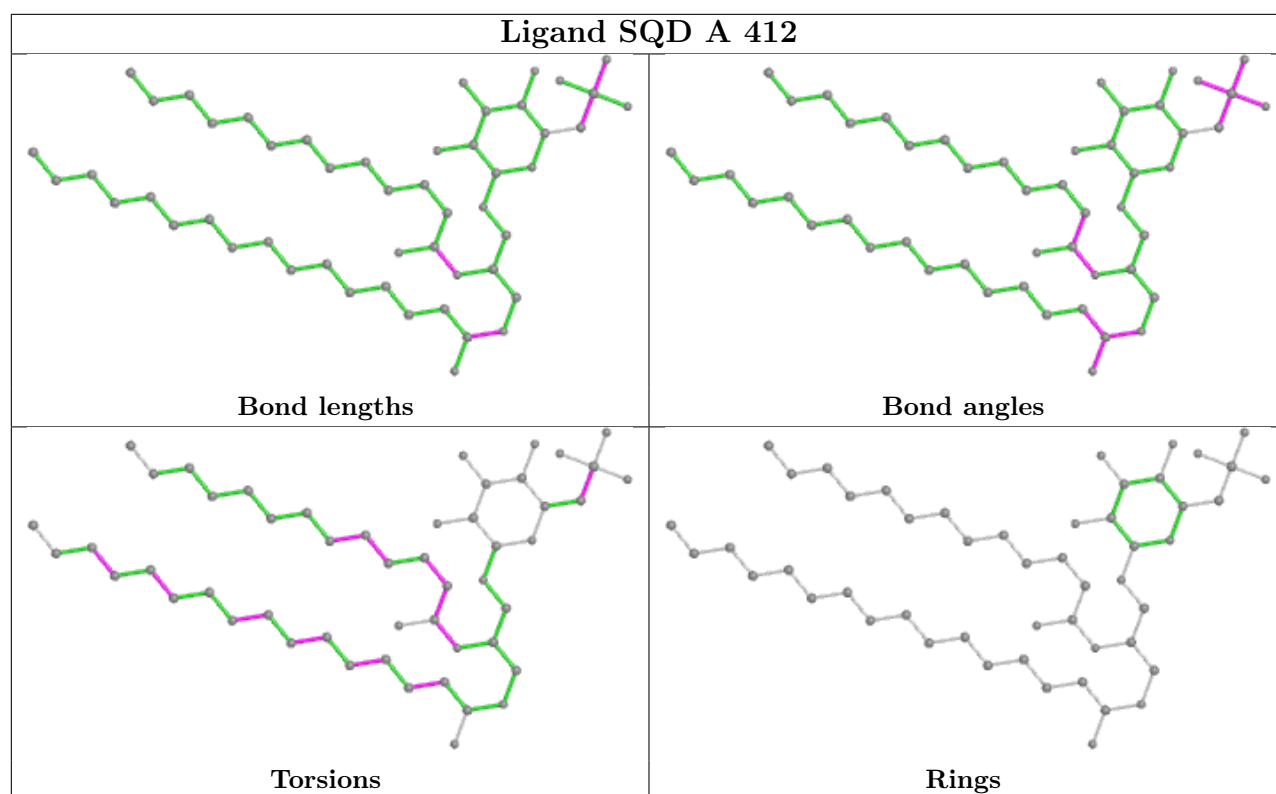
Ligand CLA c 510**Ligand CLA b 617****Ligand CLA g 602**

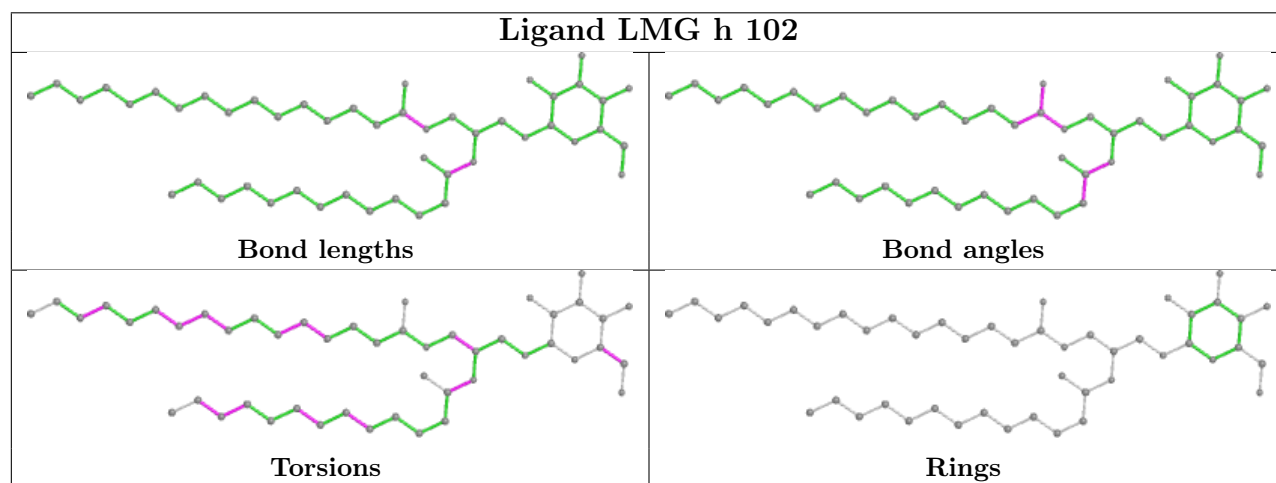
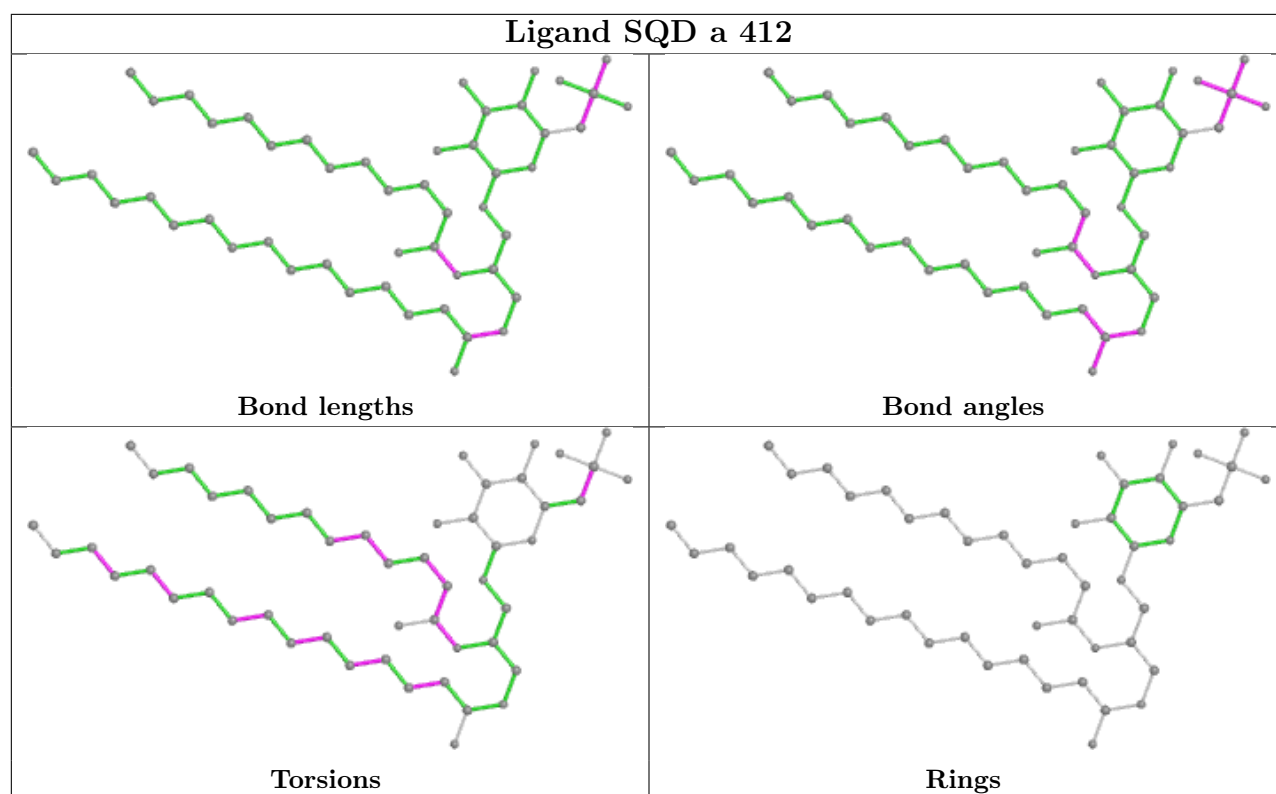


Ligand CHL n 606

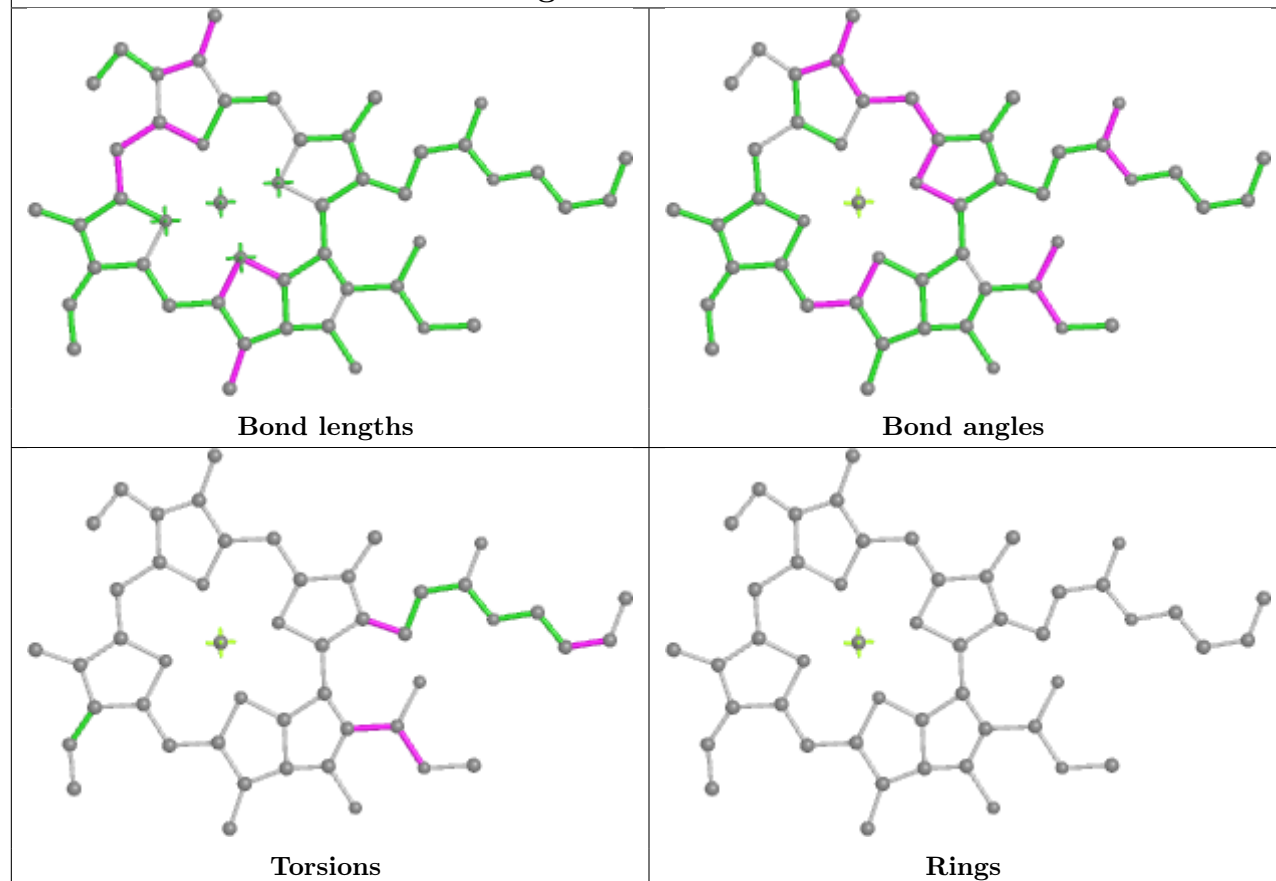




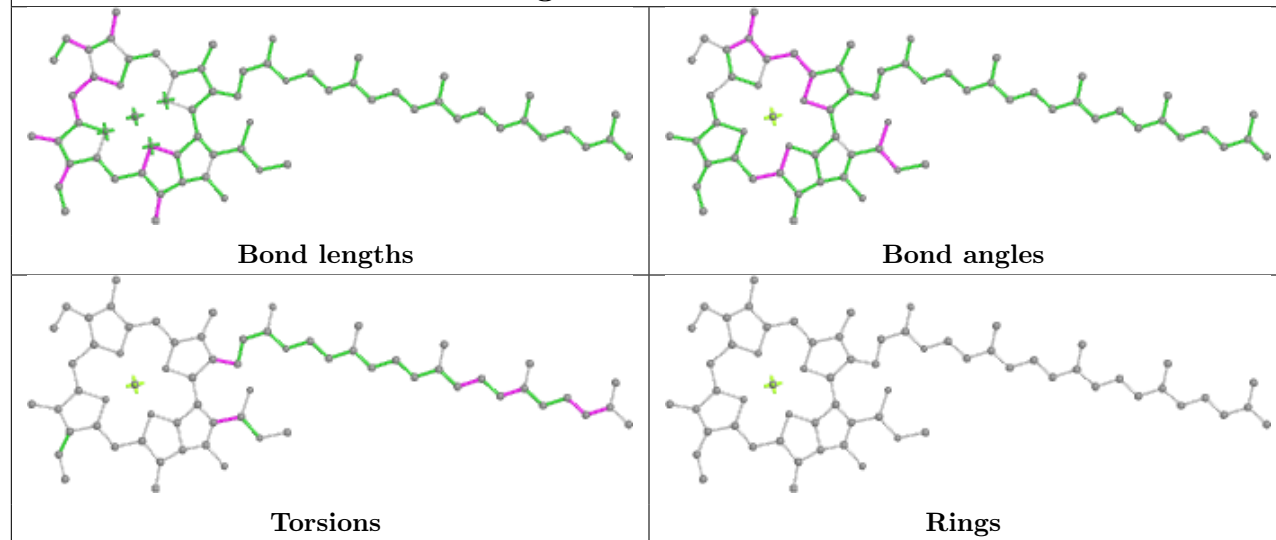




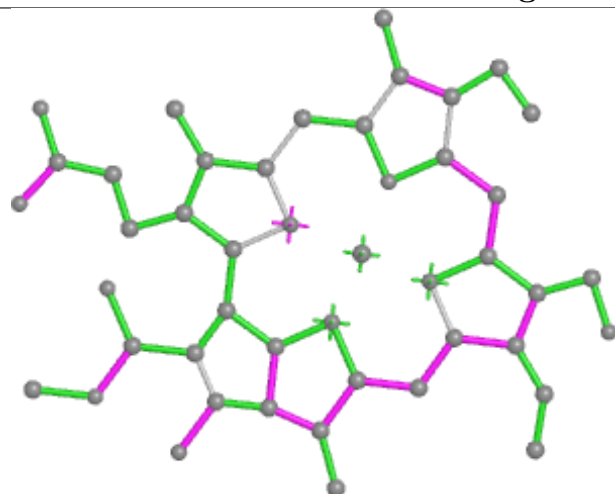
Ligand CLA s 604



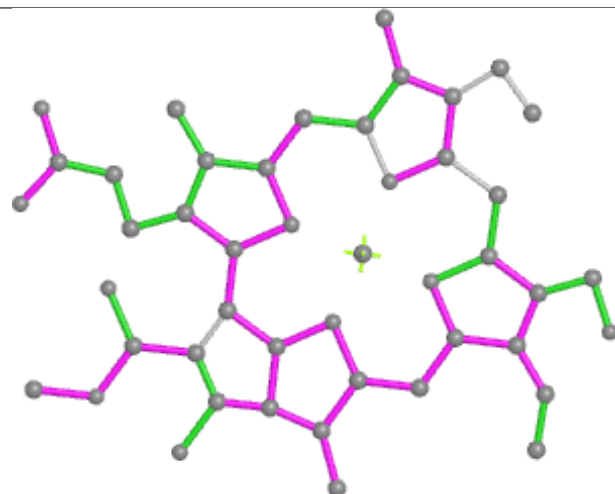
Ligand CLA a 406



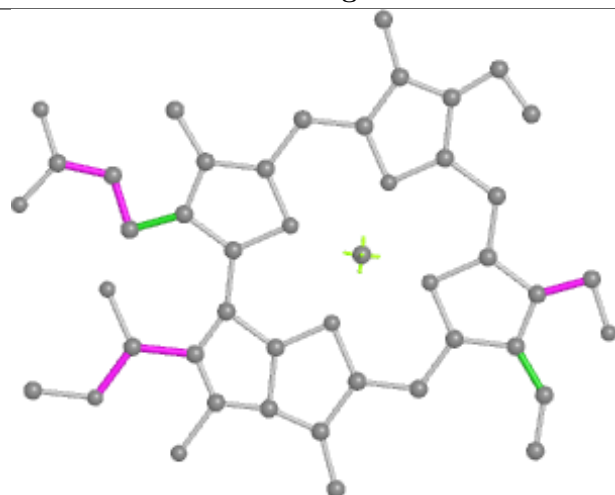
Ligand CHL S 601



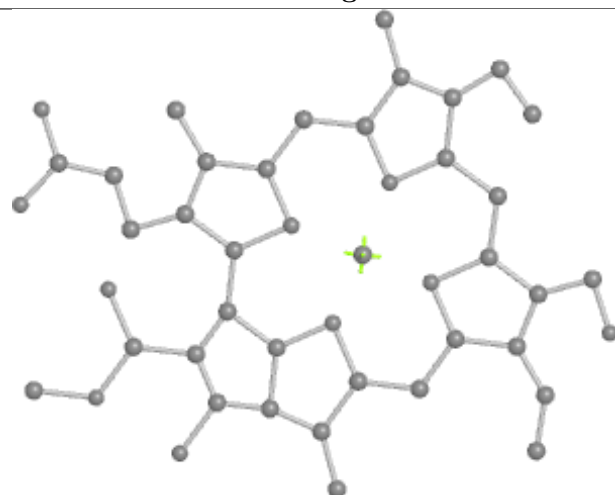
Bond lengths



Bond angles

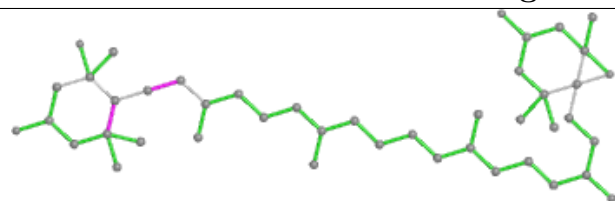


Torsions

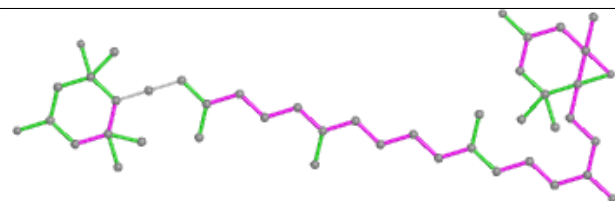


Rings

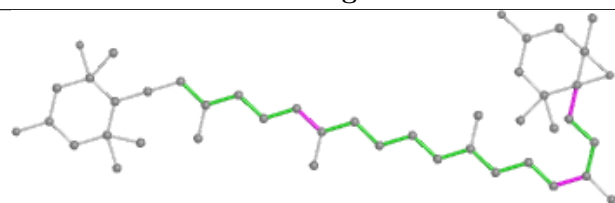
Ligand NEX r 625



Bond lengths



Bond angles

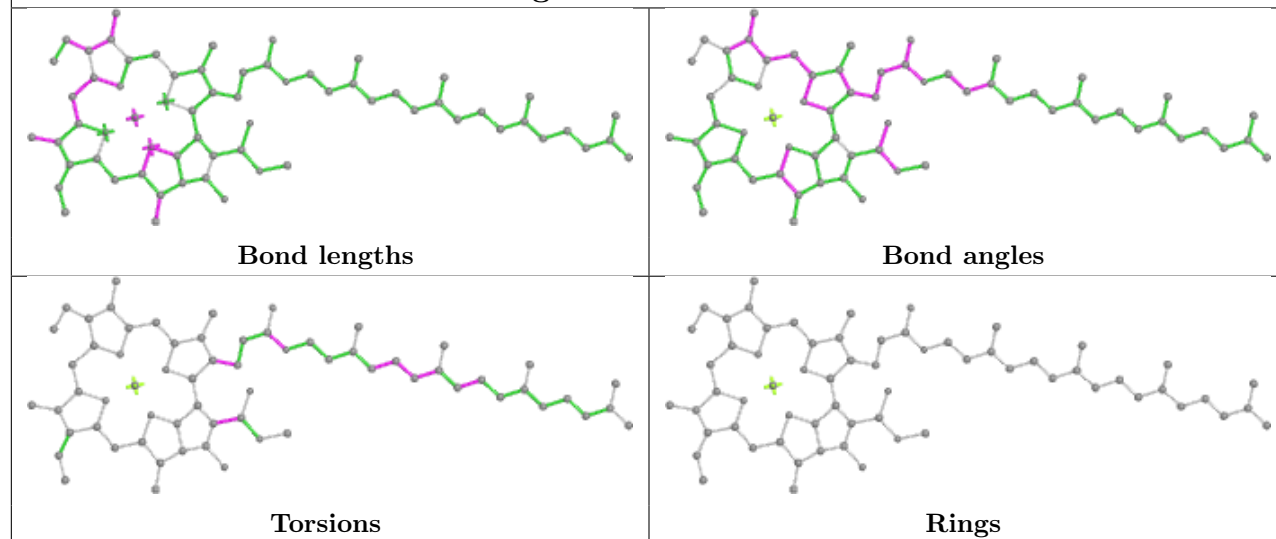


Torsions

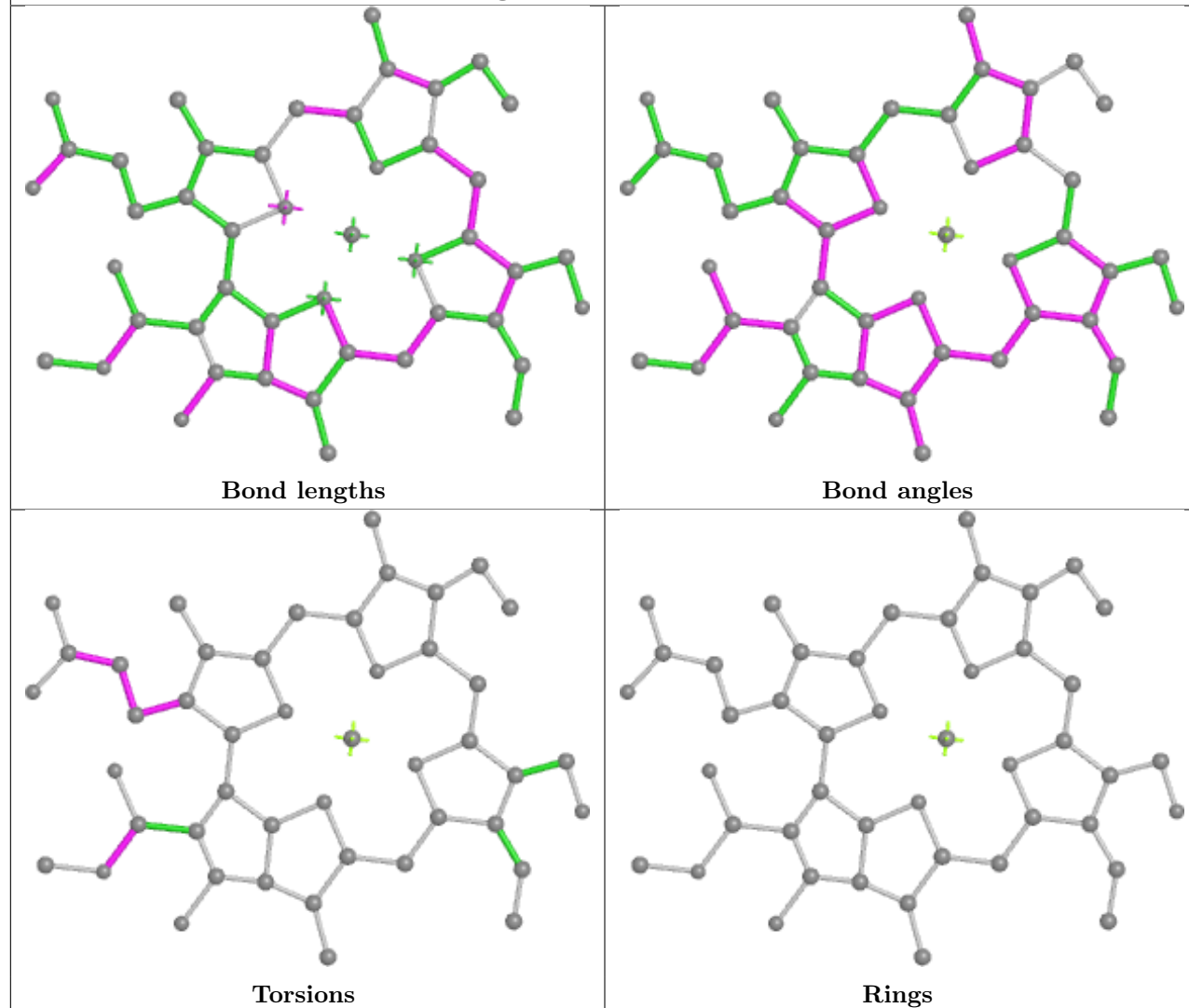


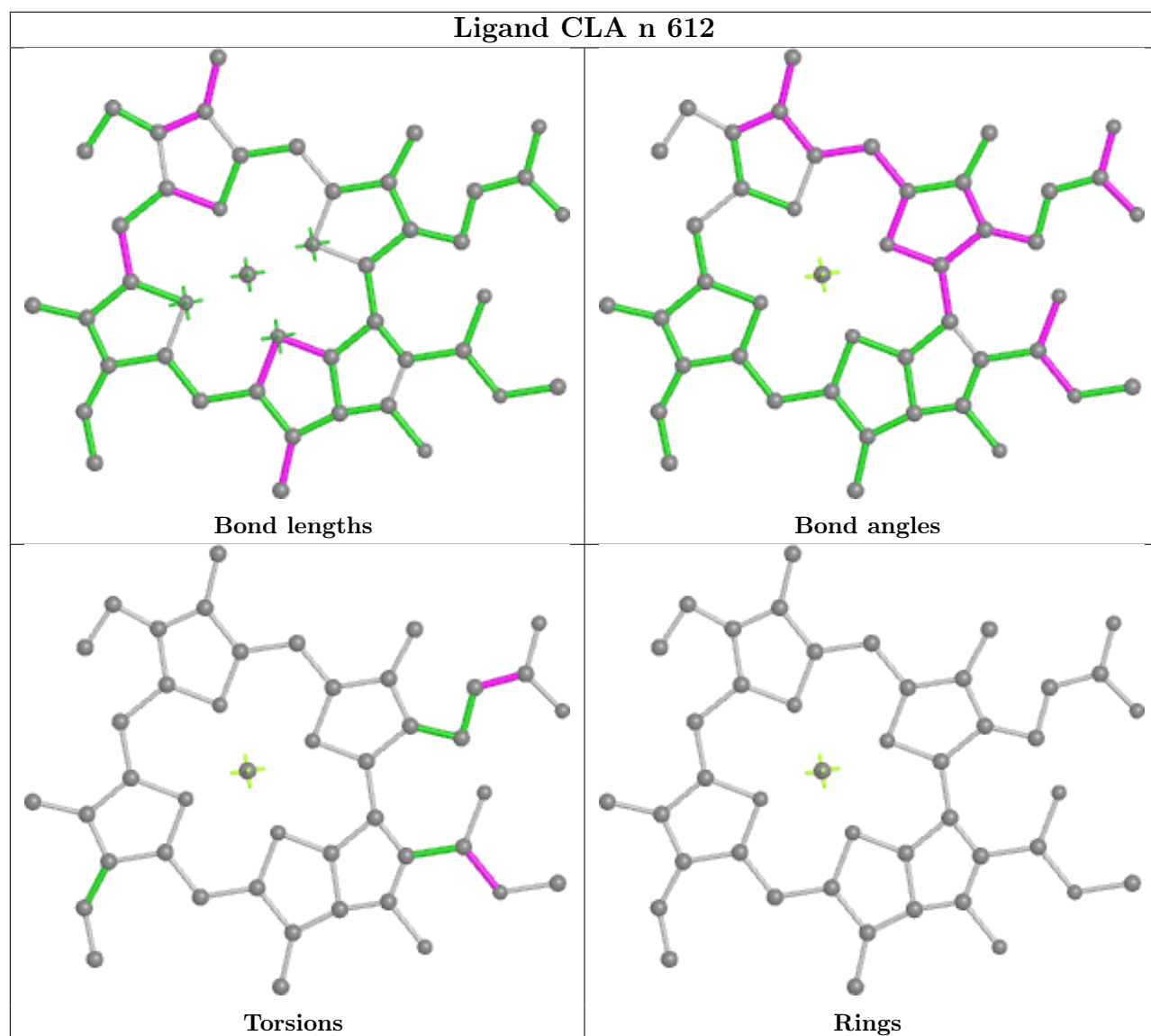
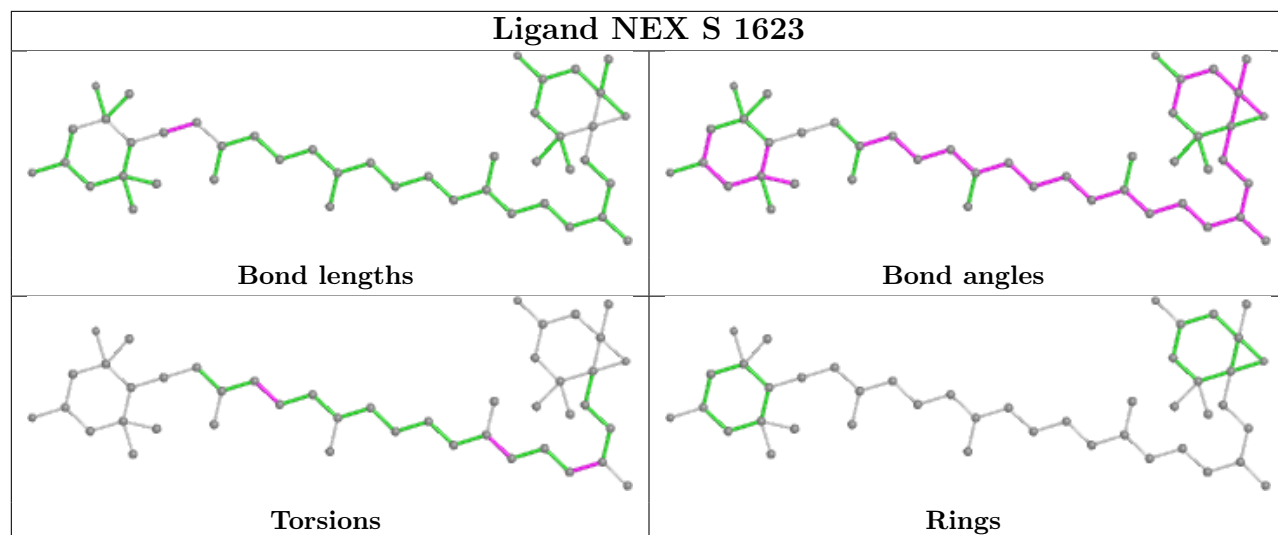
Rings

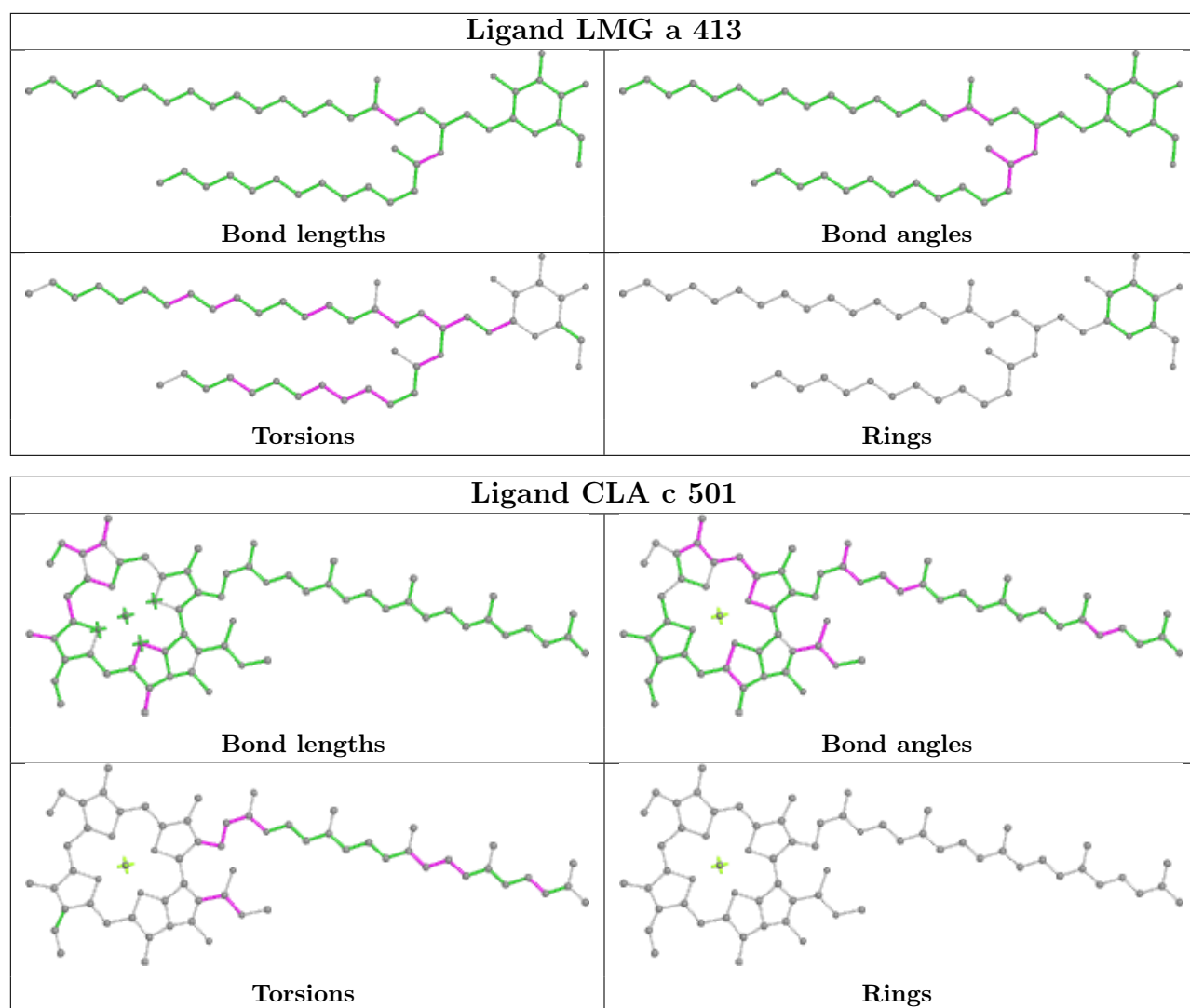
Ligand CLA B 605

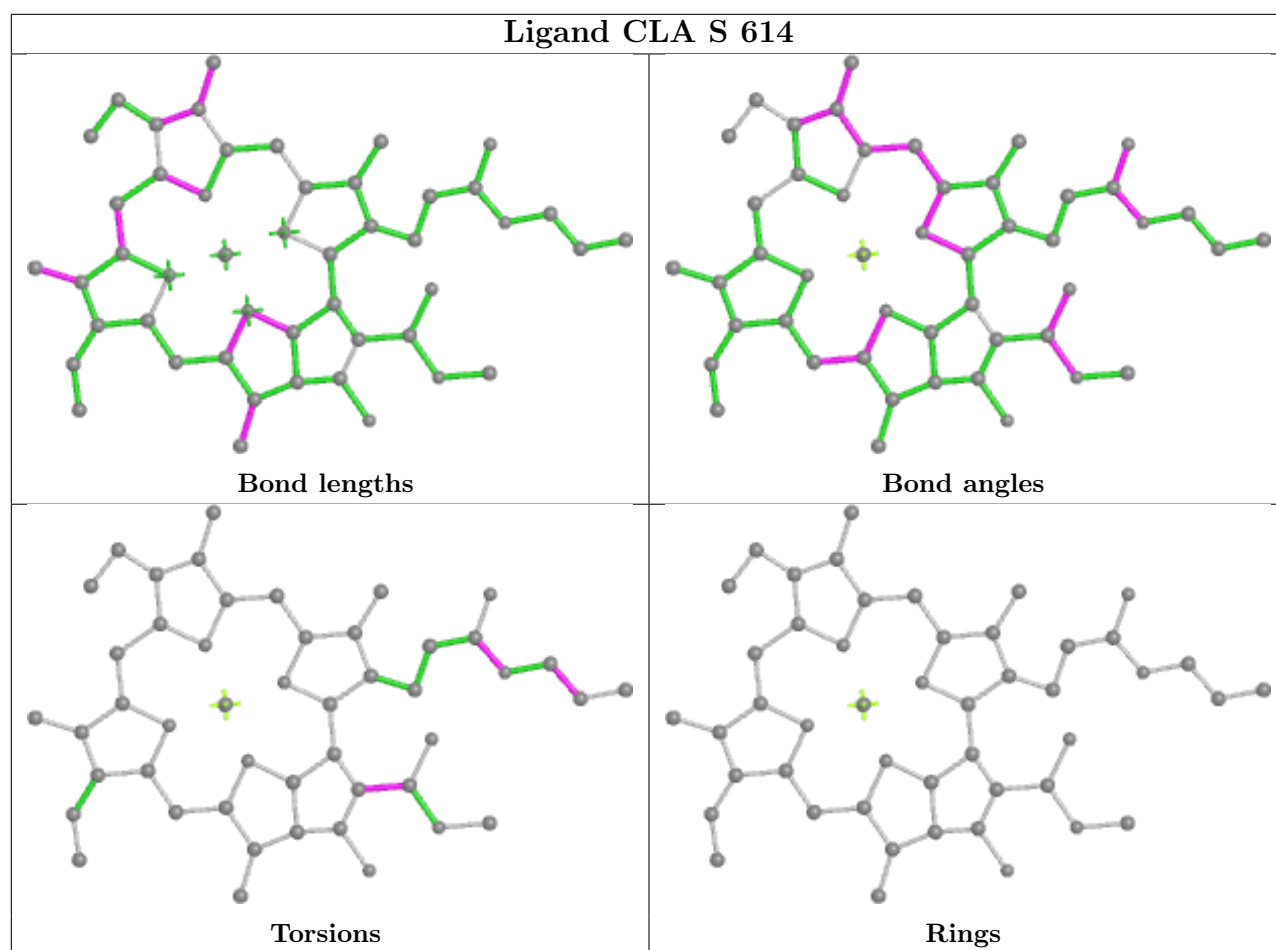


Ligand CHL N 606

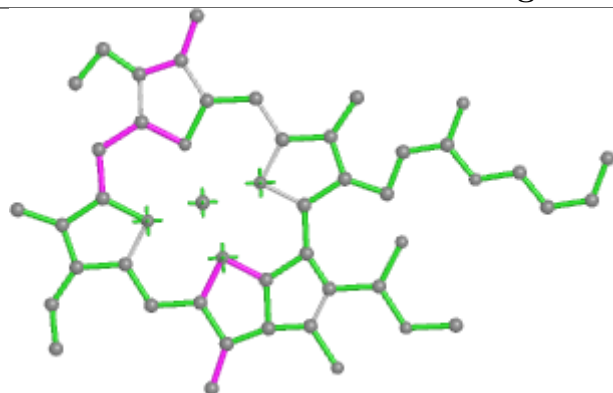




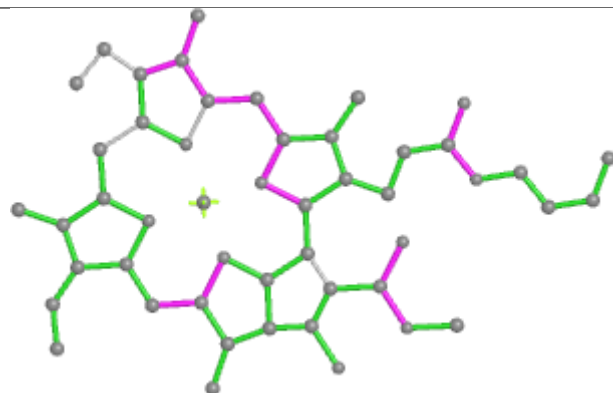




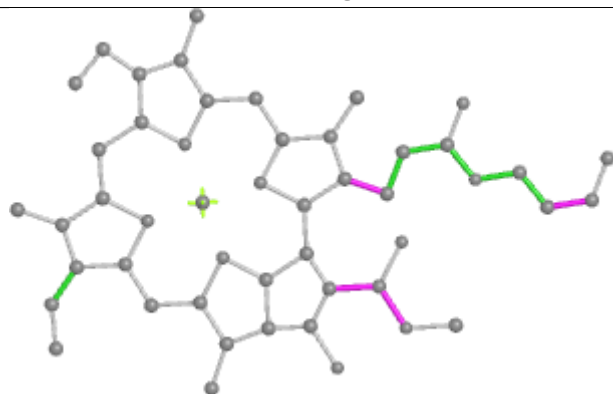
Ligand CLA S 604



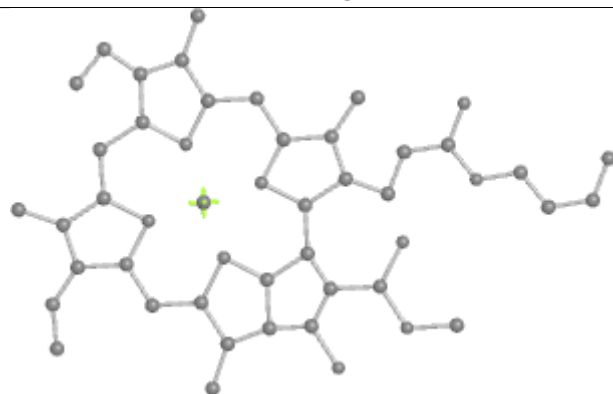
Bond lengths



Bond angles

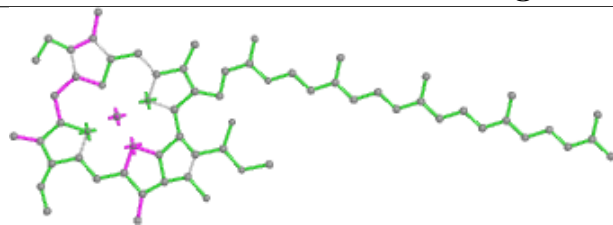


Torsions

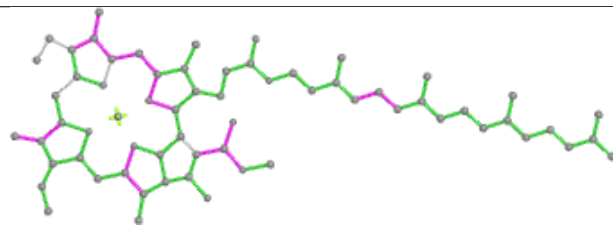


Rings

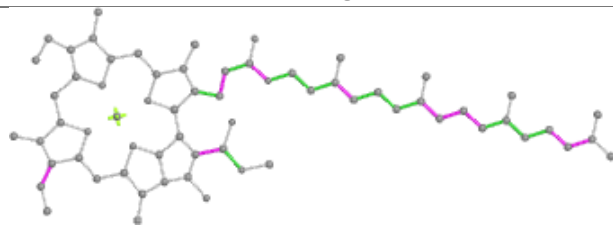
Ligand CLA C 505



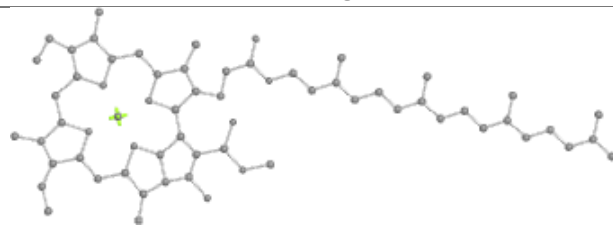
Bond lengths



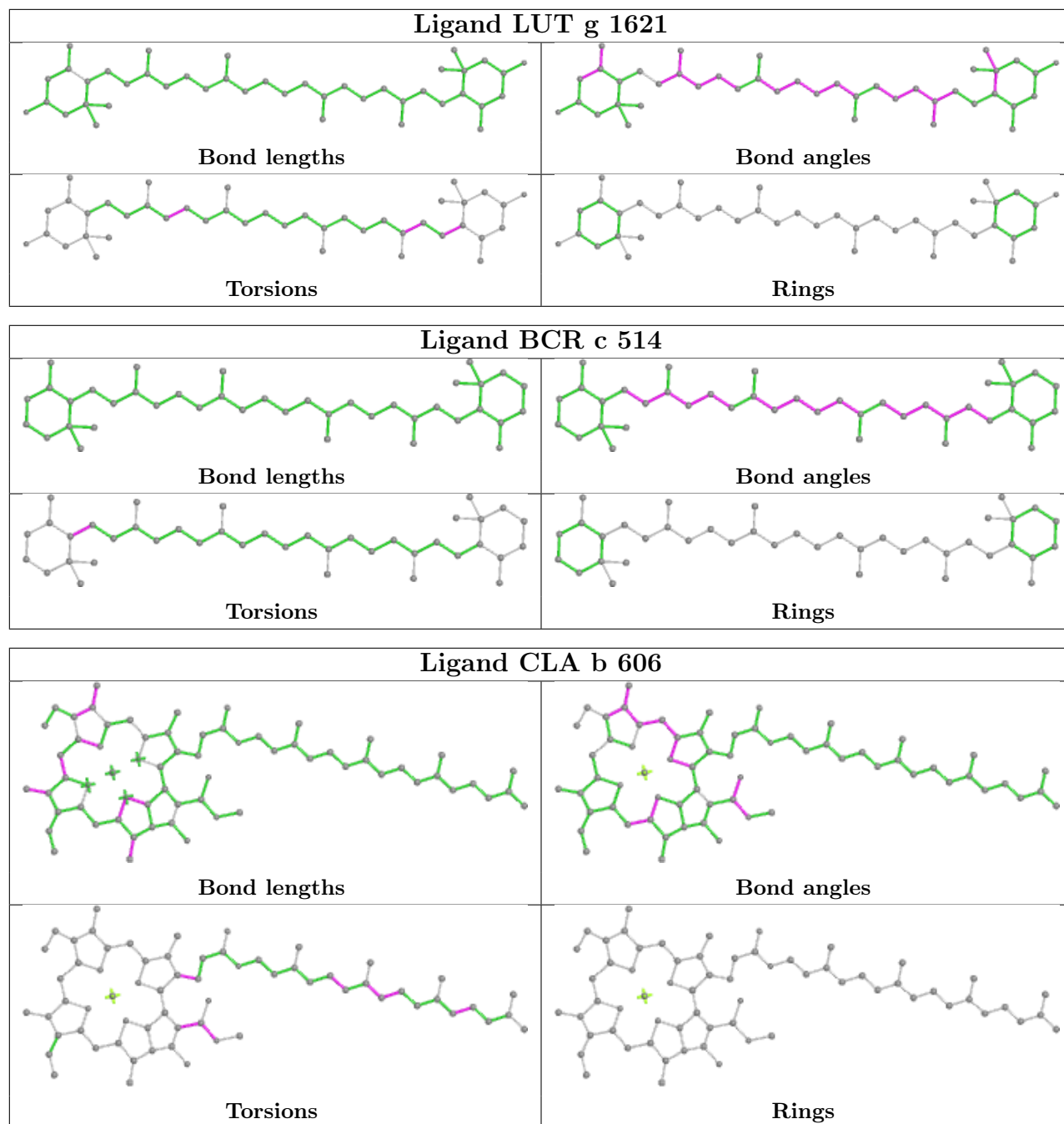
Bond angles

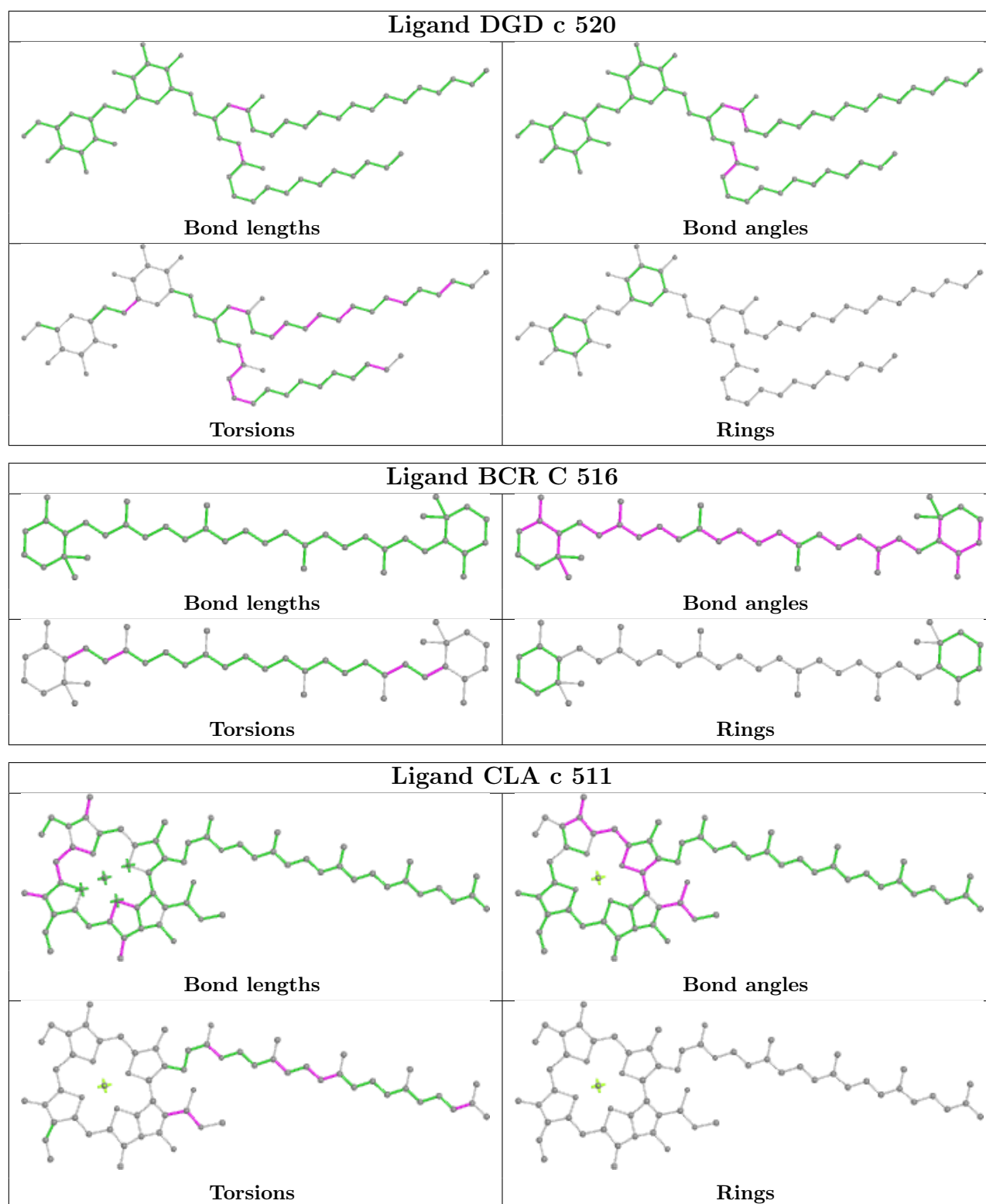


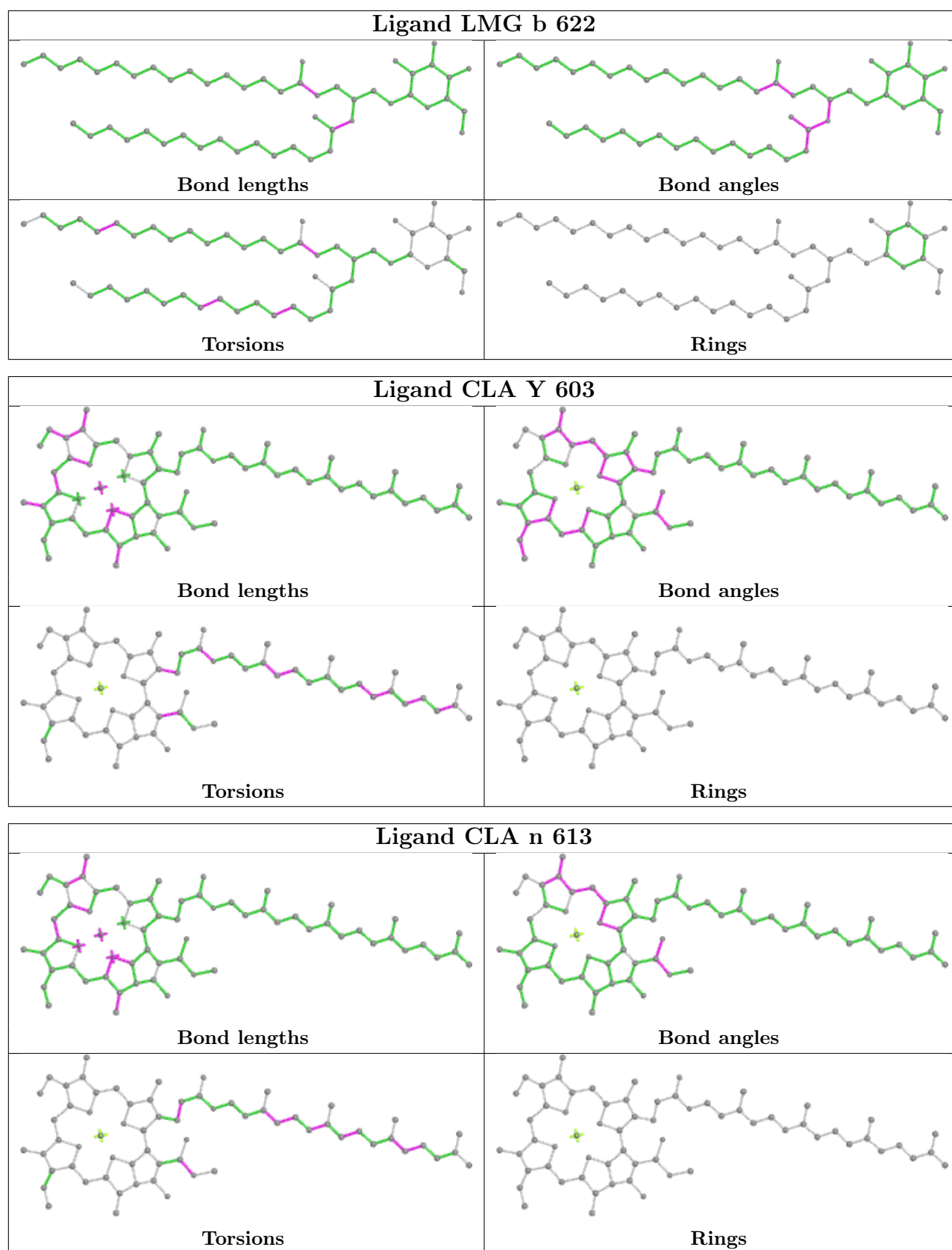
Torsions

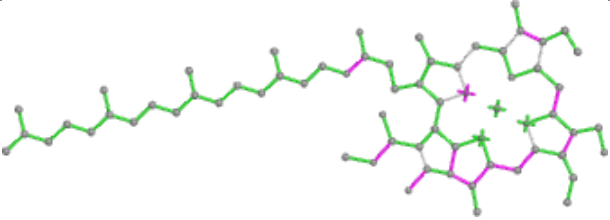
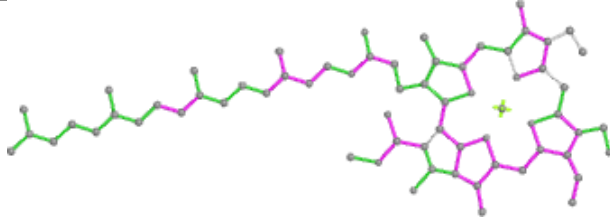
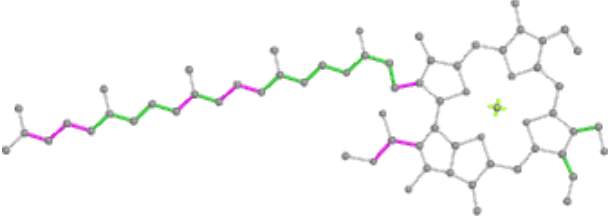
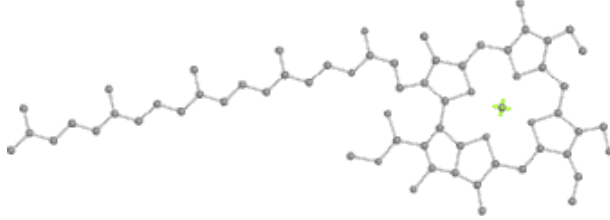
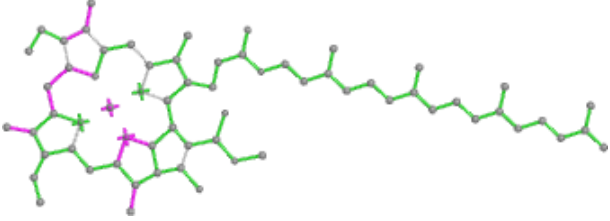
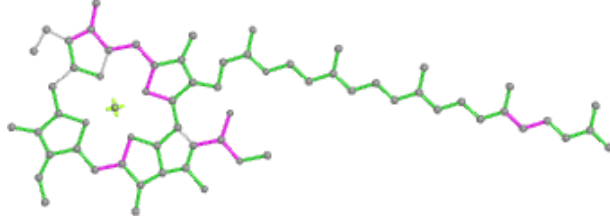
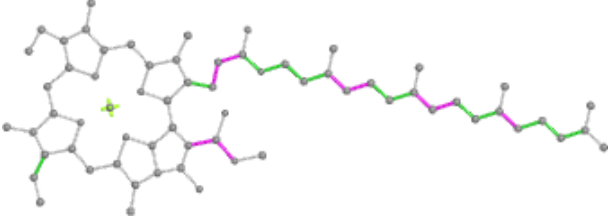
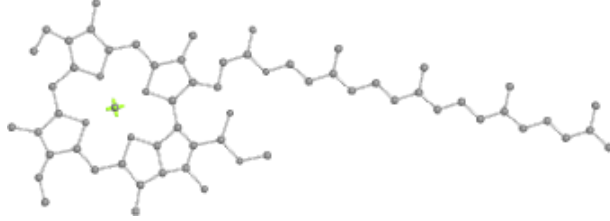
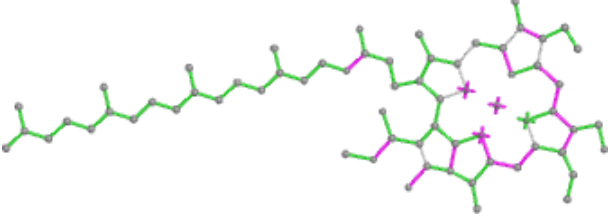
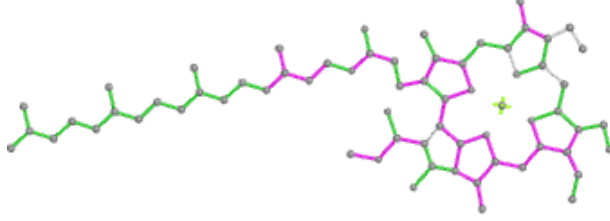
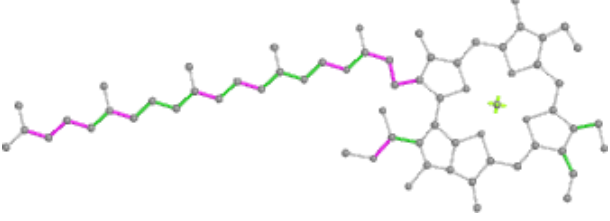
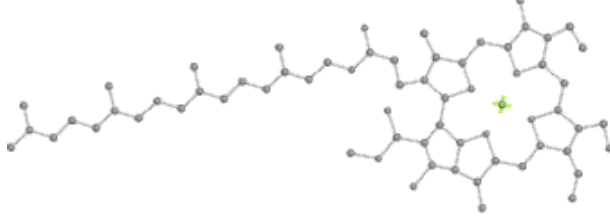


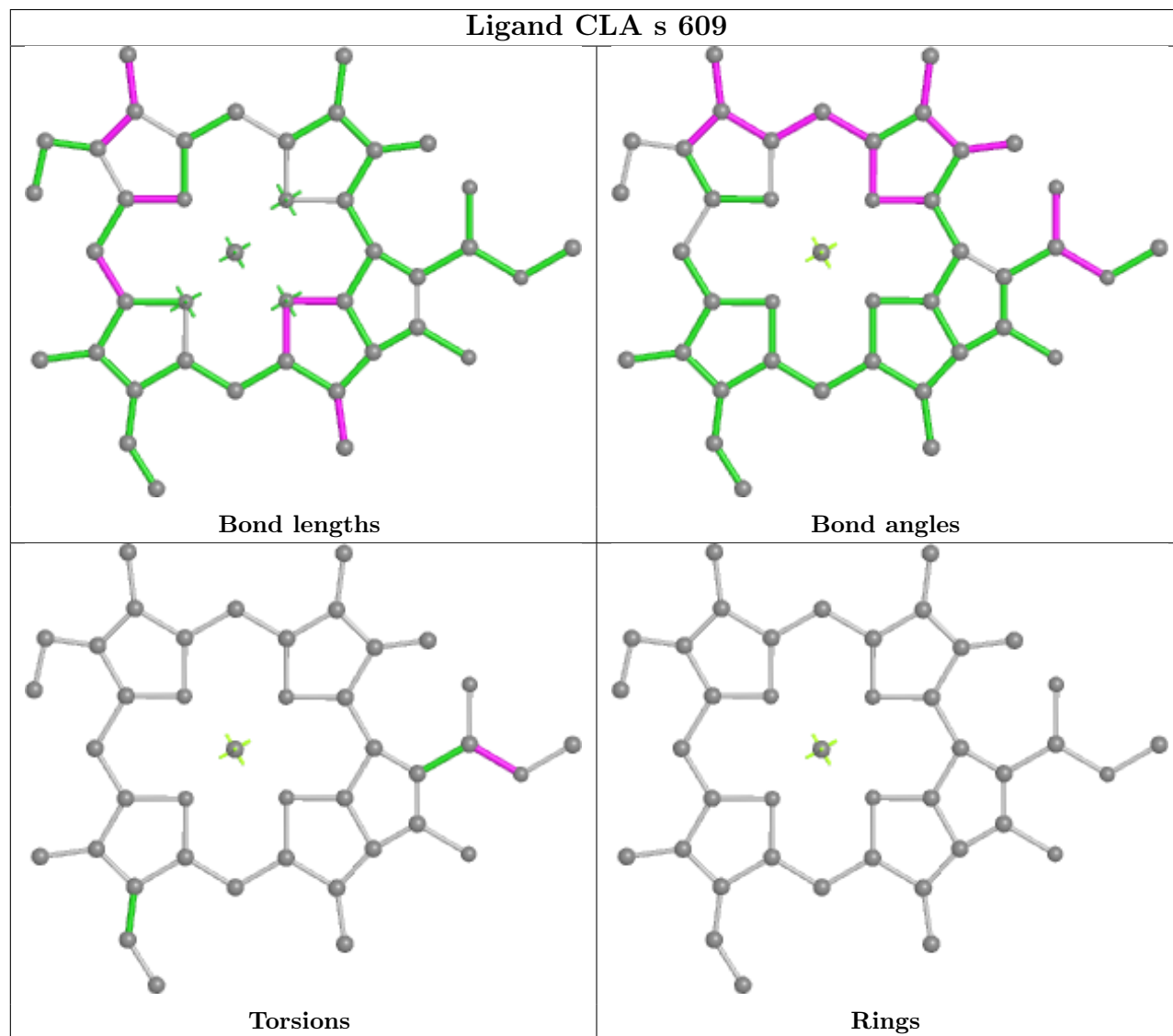
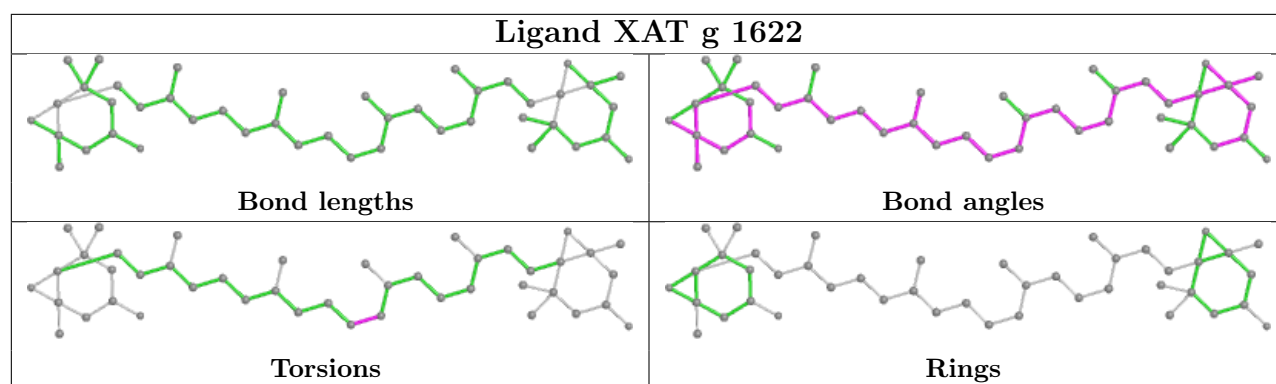
Rings

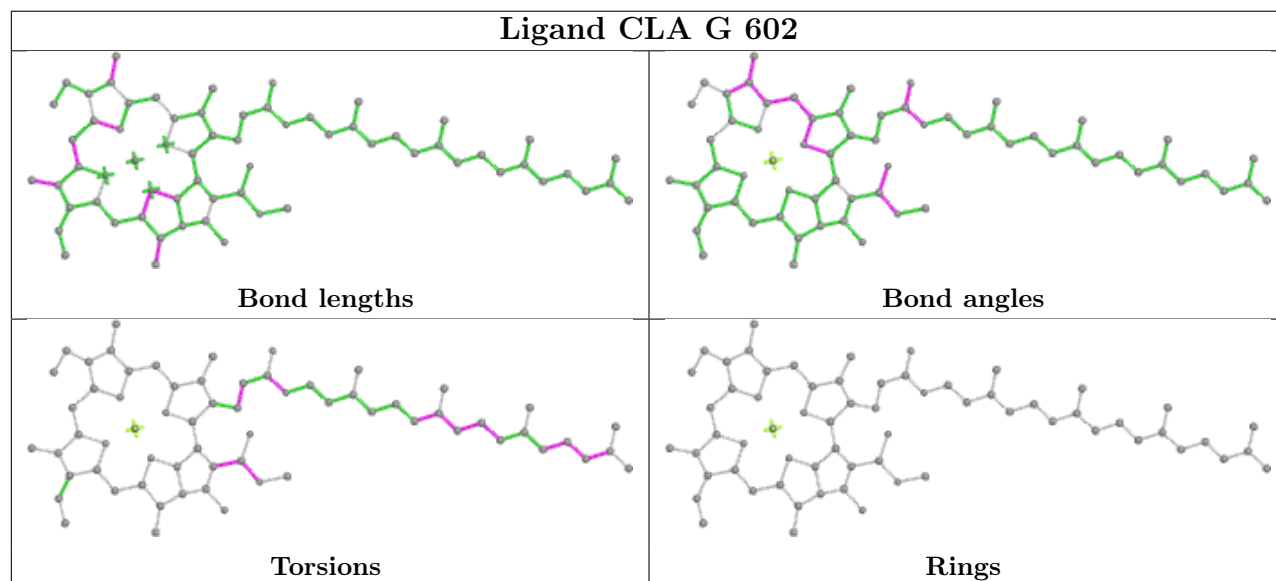
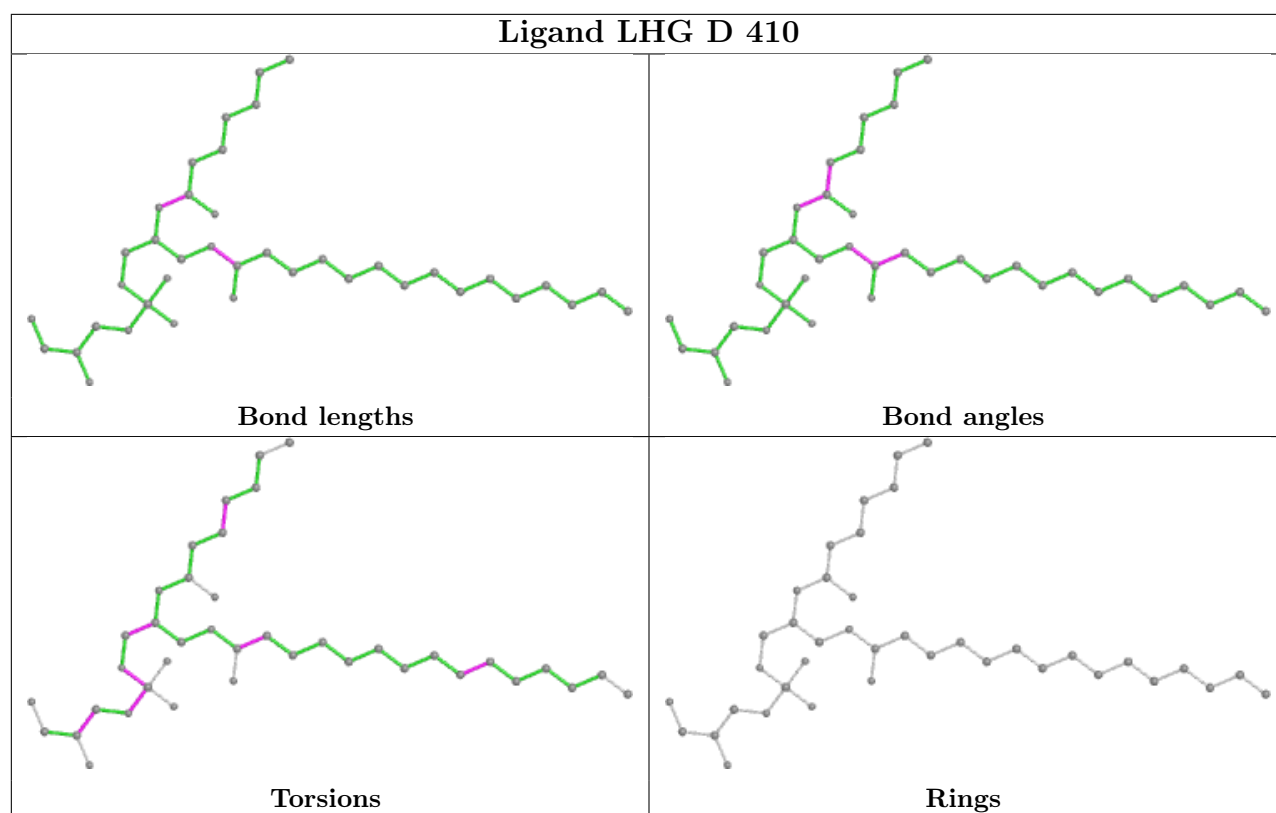


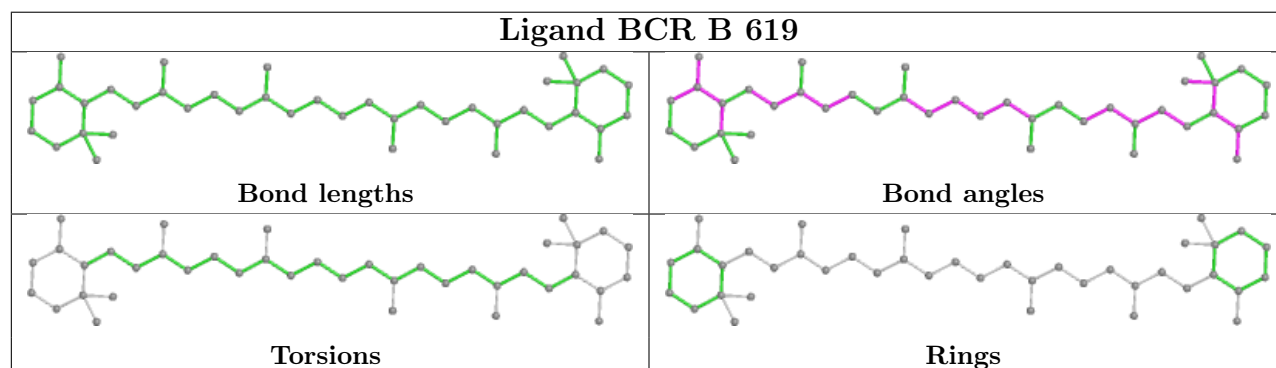
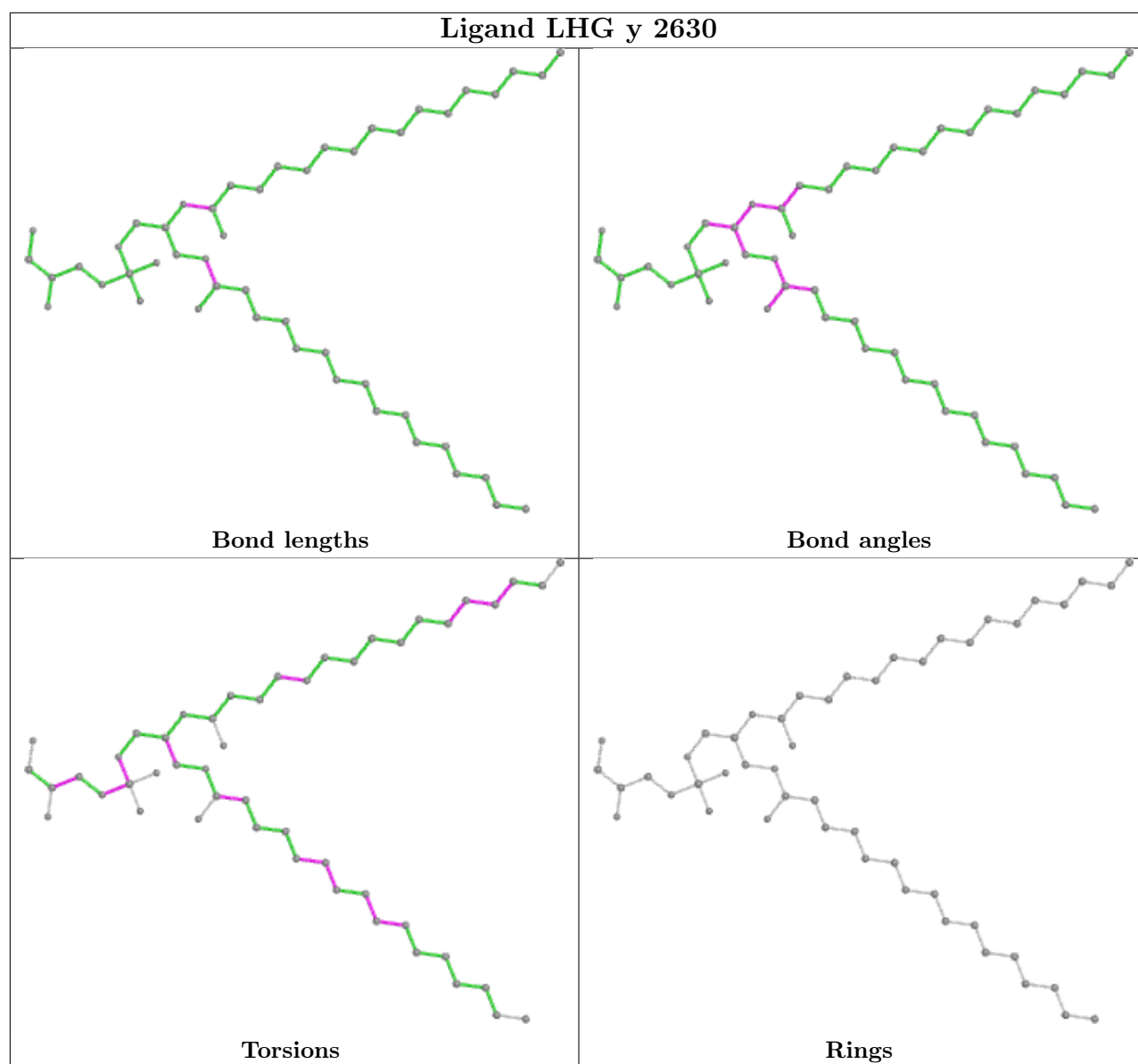


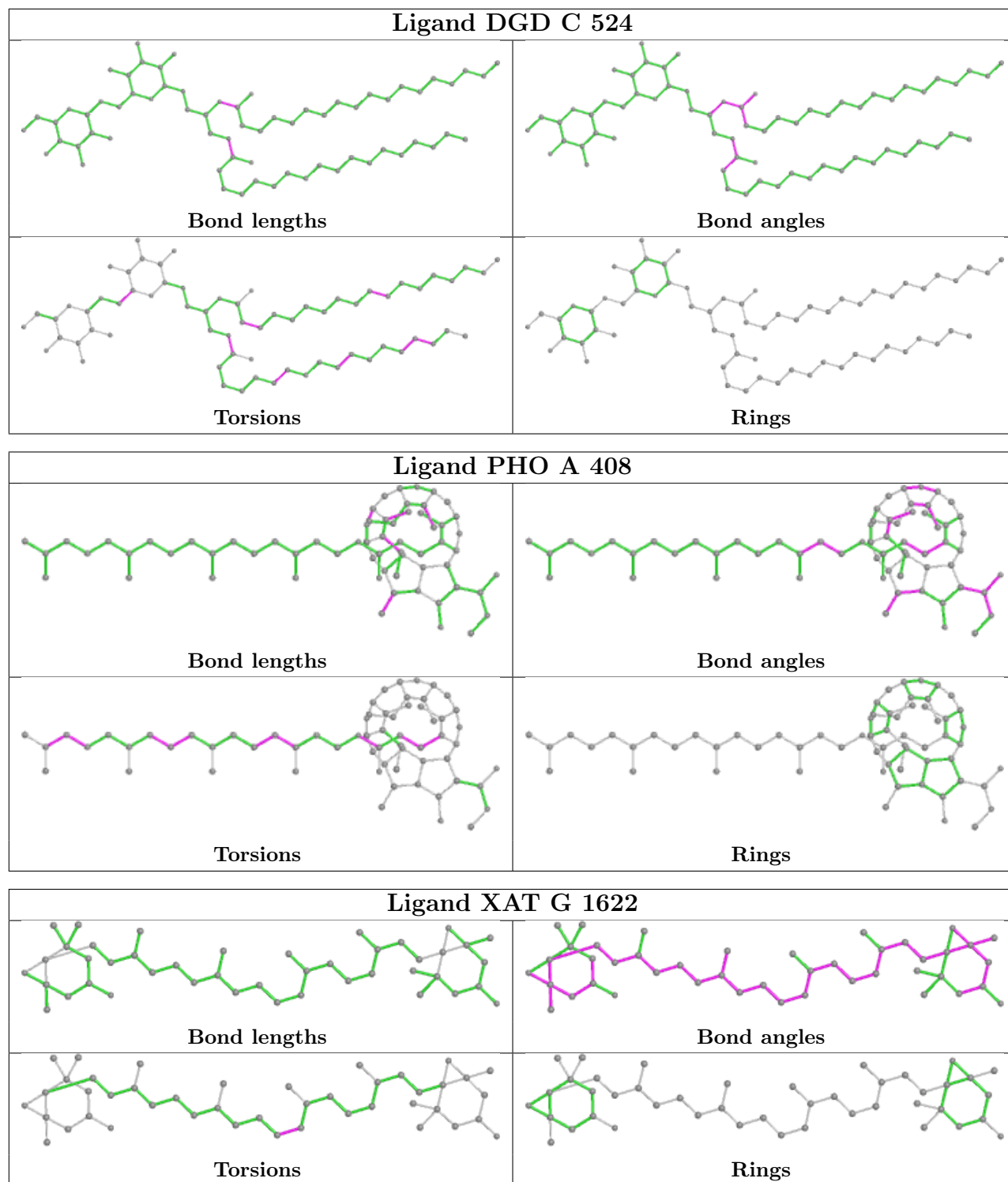


Ligand CHL G 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA Y 613	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL Y 606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

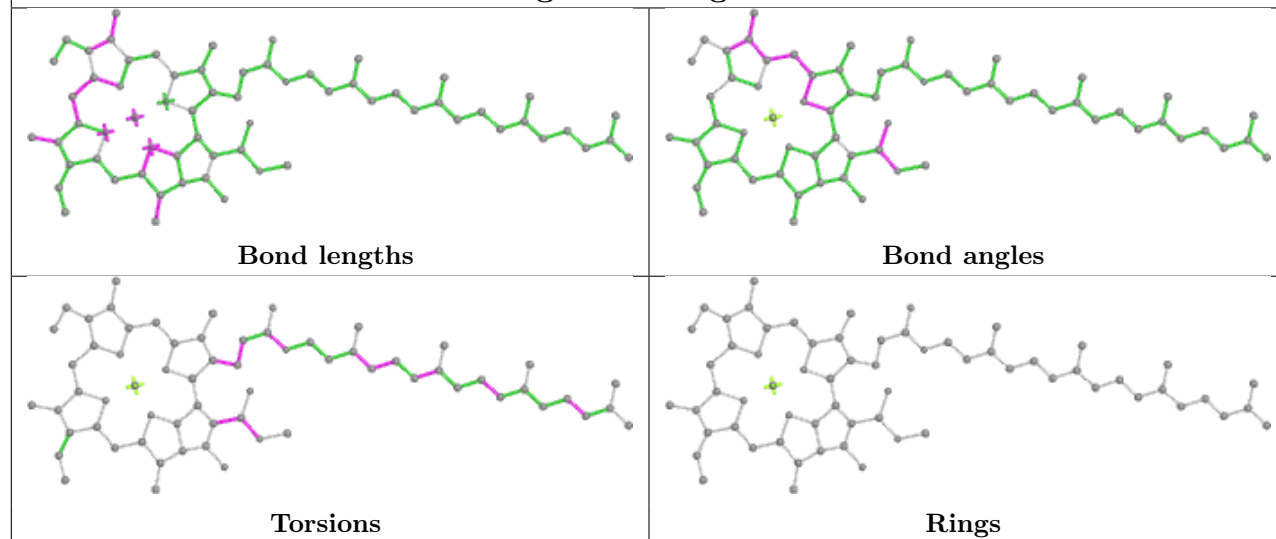




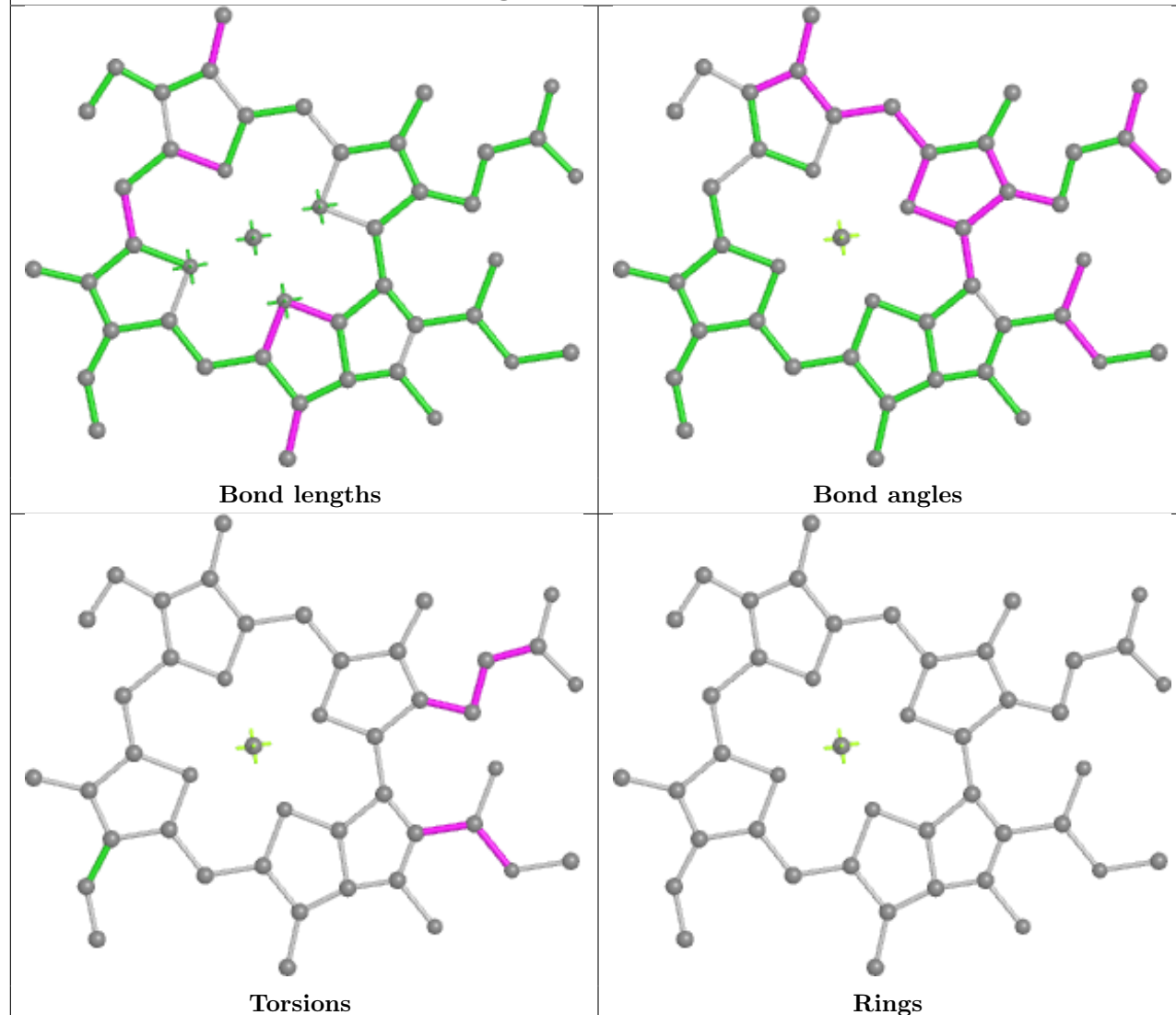




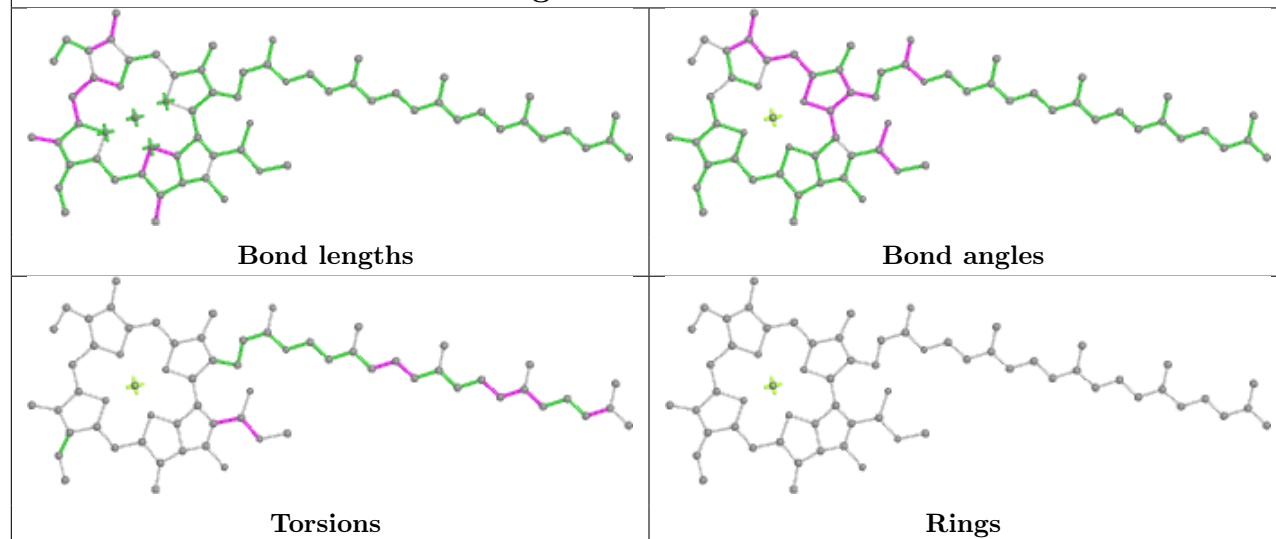
Ligand CLA g 613



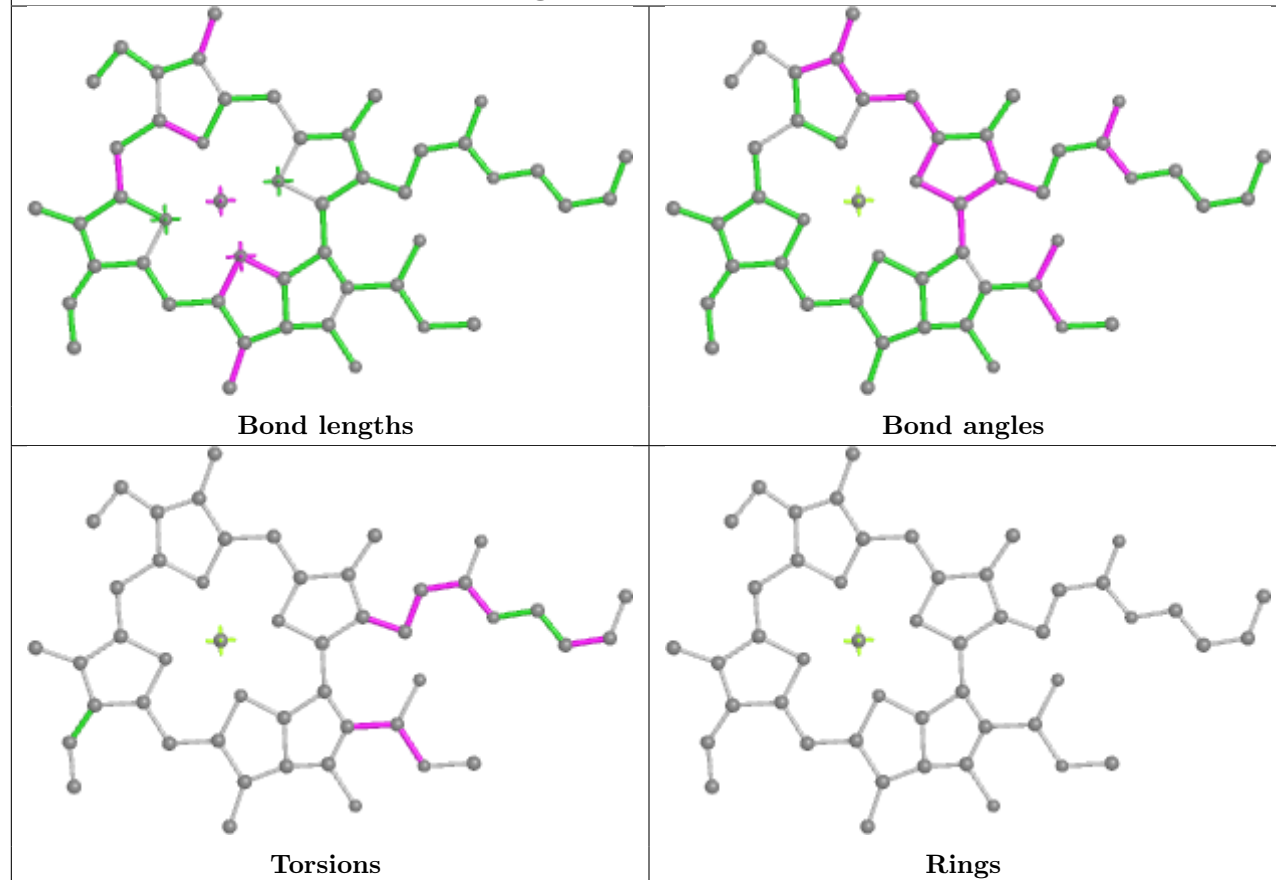
Ligand CLA r 609

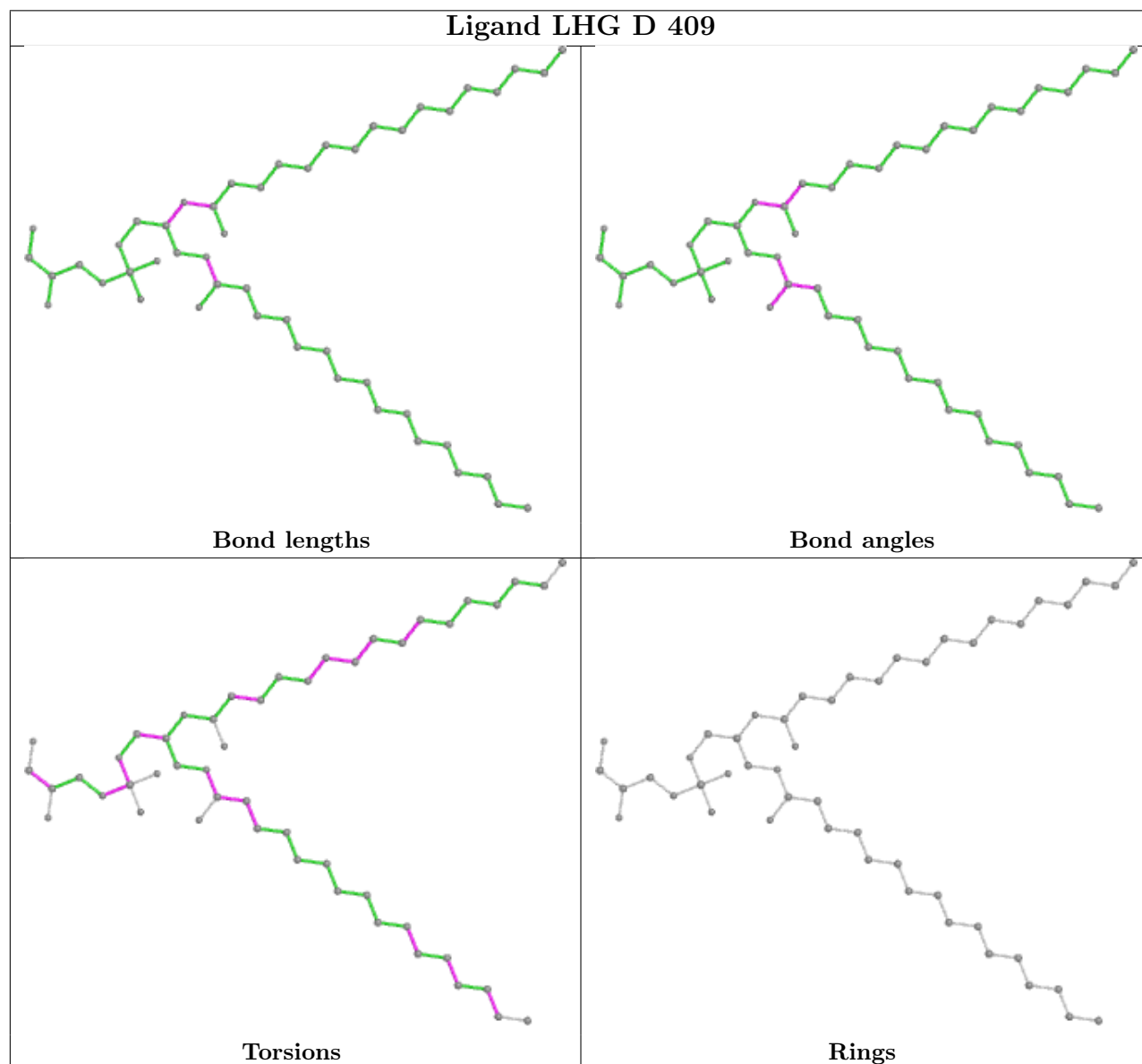
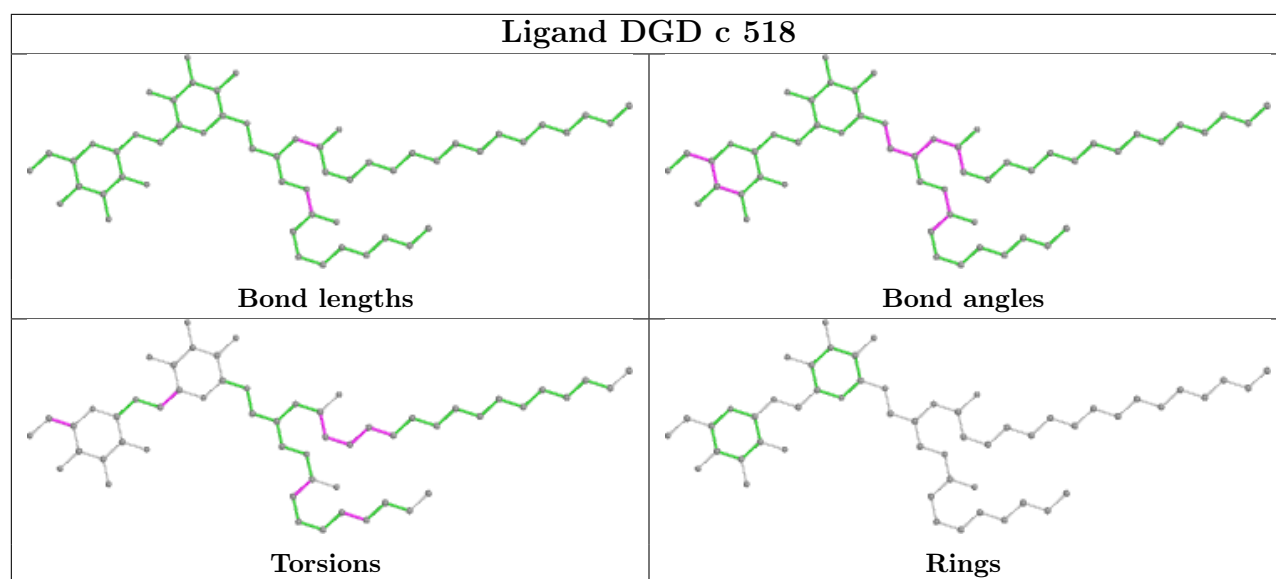


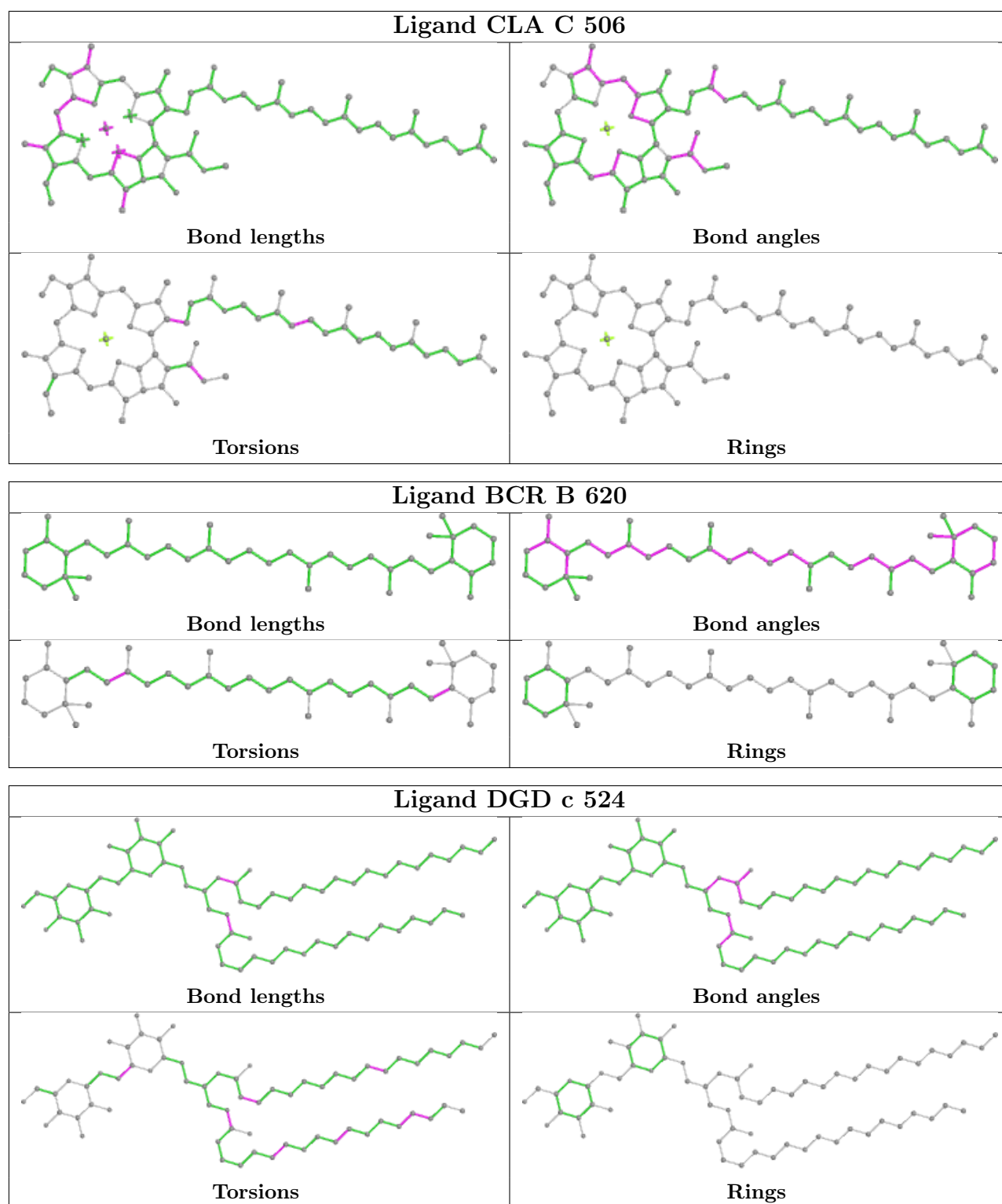
Ligand CLA B 616



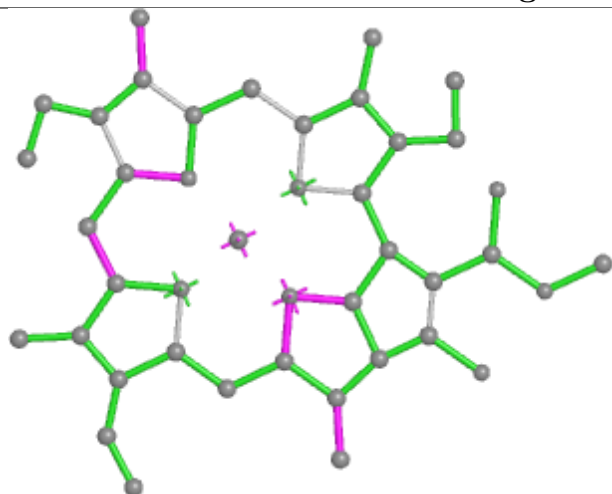
Ligand CLA R 603



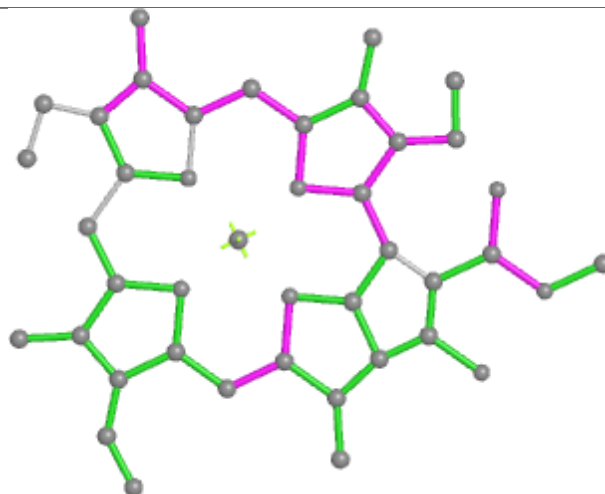




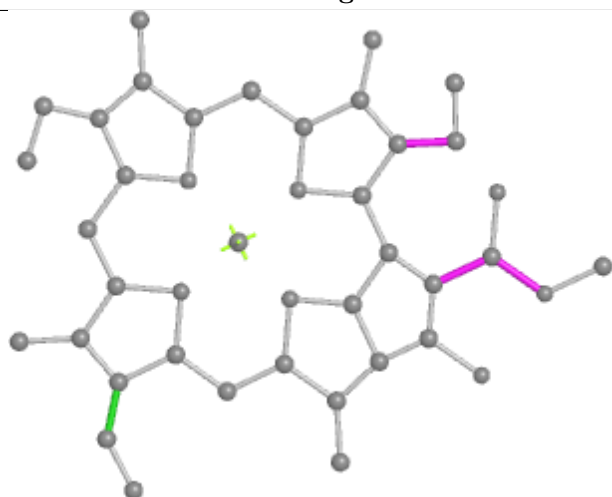
Ligand CLA s 603



Bond lengths



Bond angles

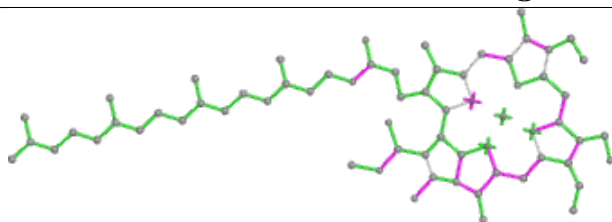


Torsions

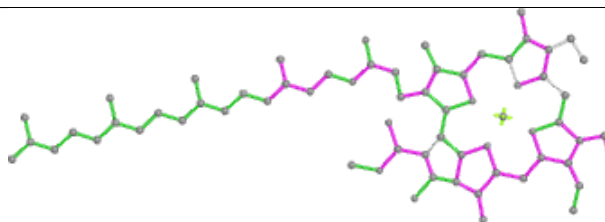


Rings

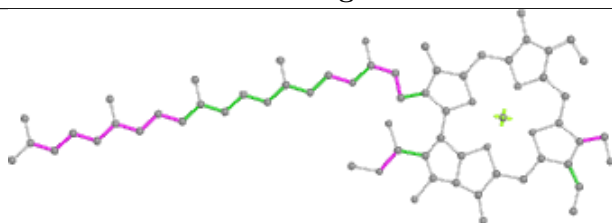
Ligand CHL n 605



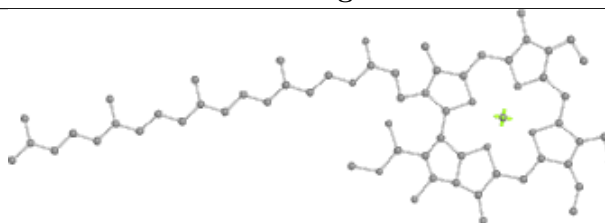
Bond lengths



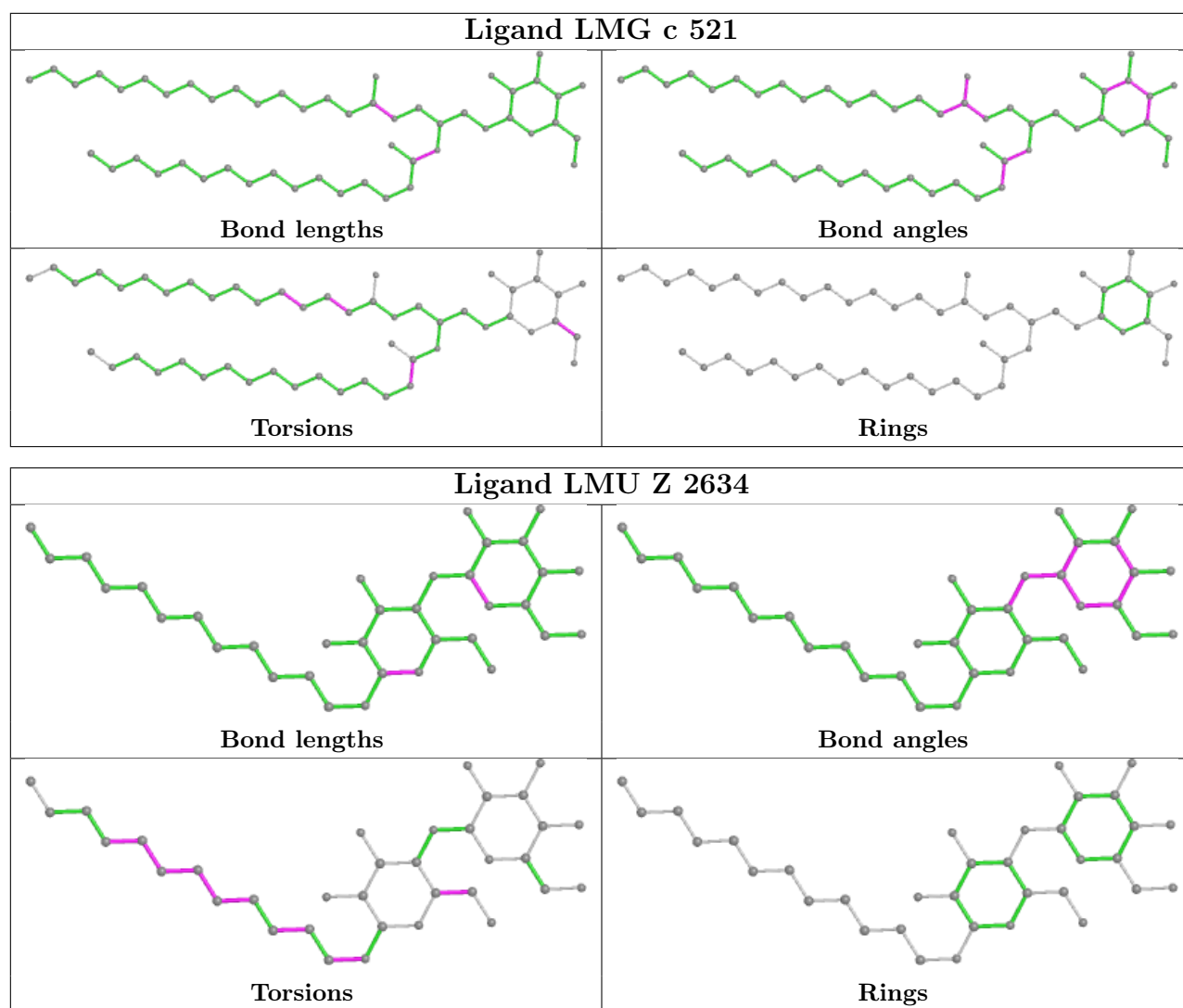
Bond angles

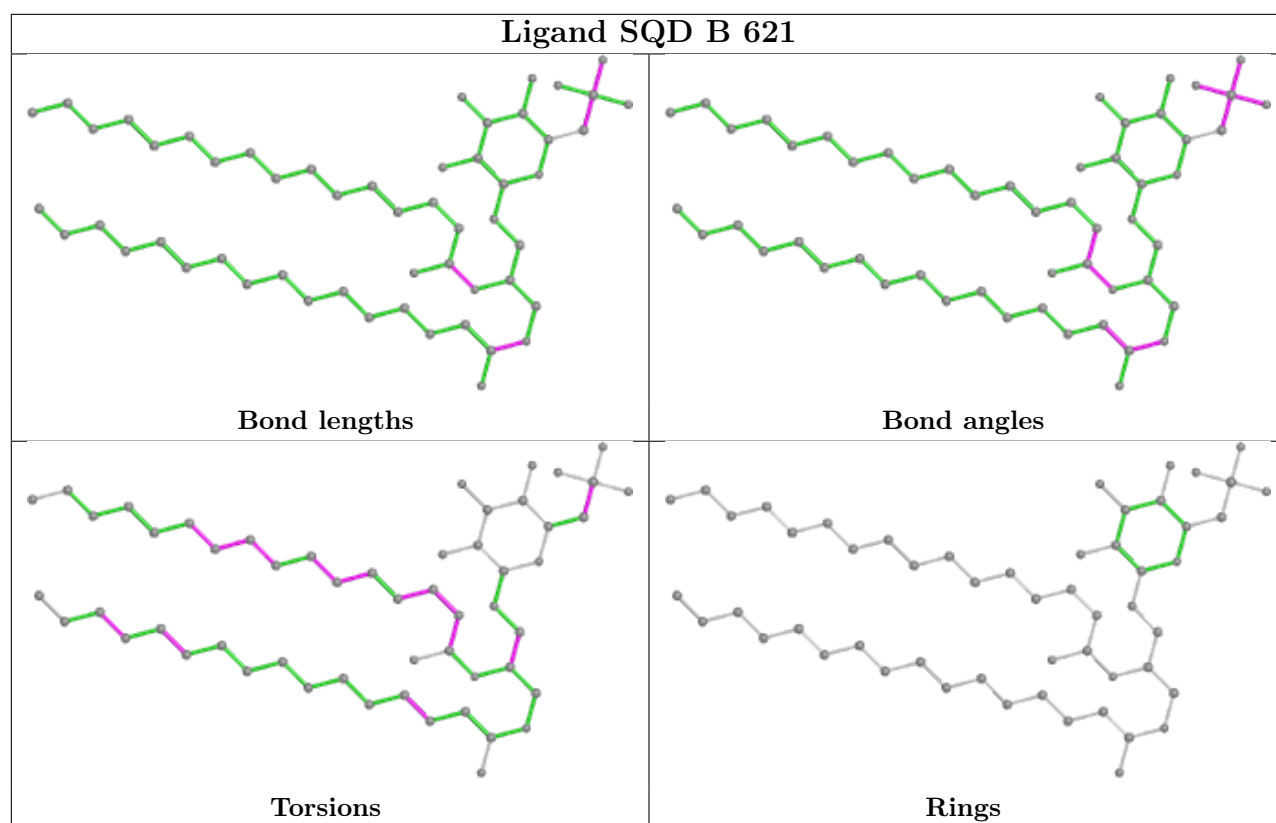


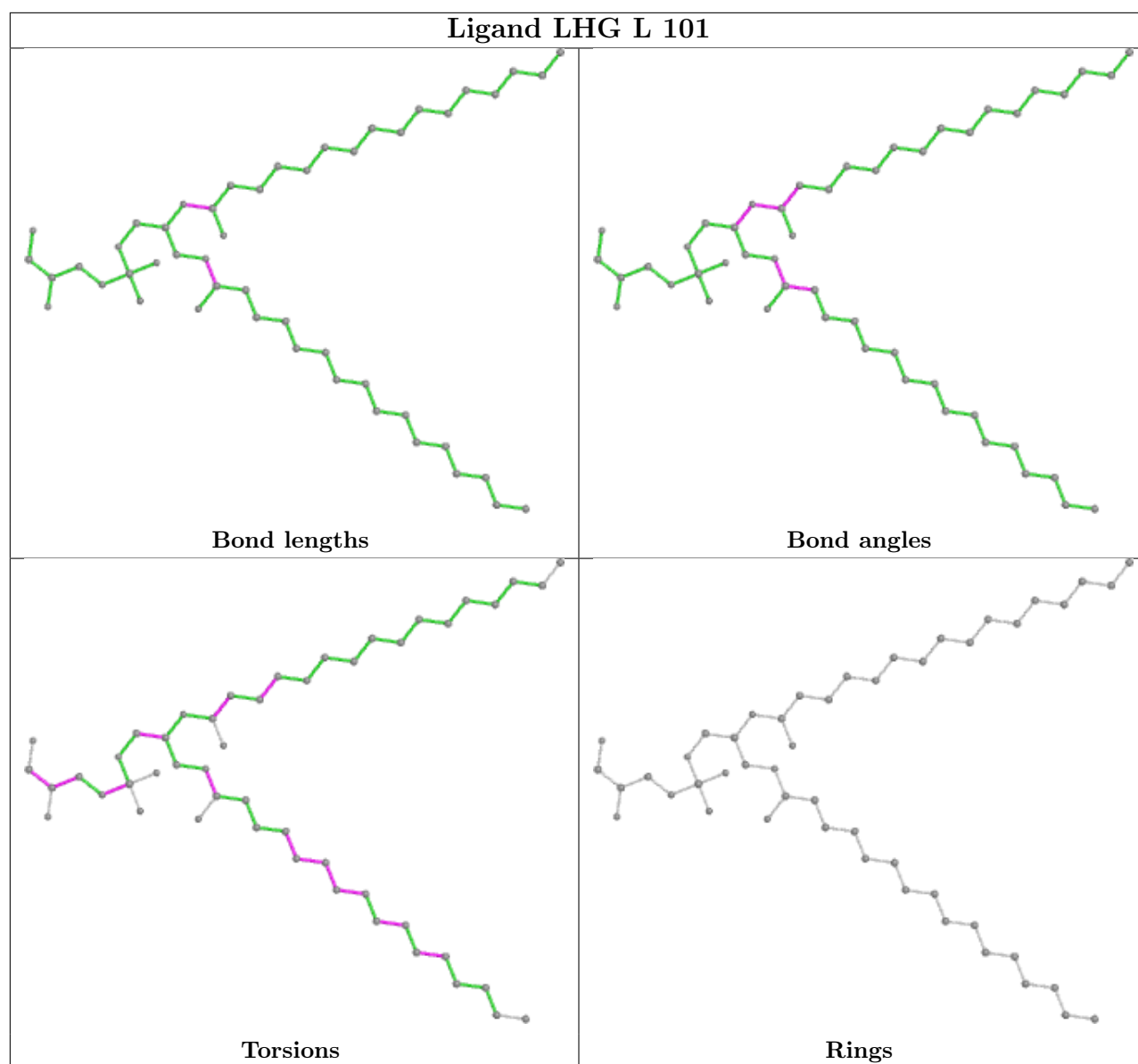
Torsions

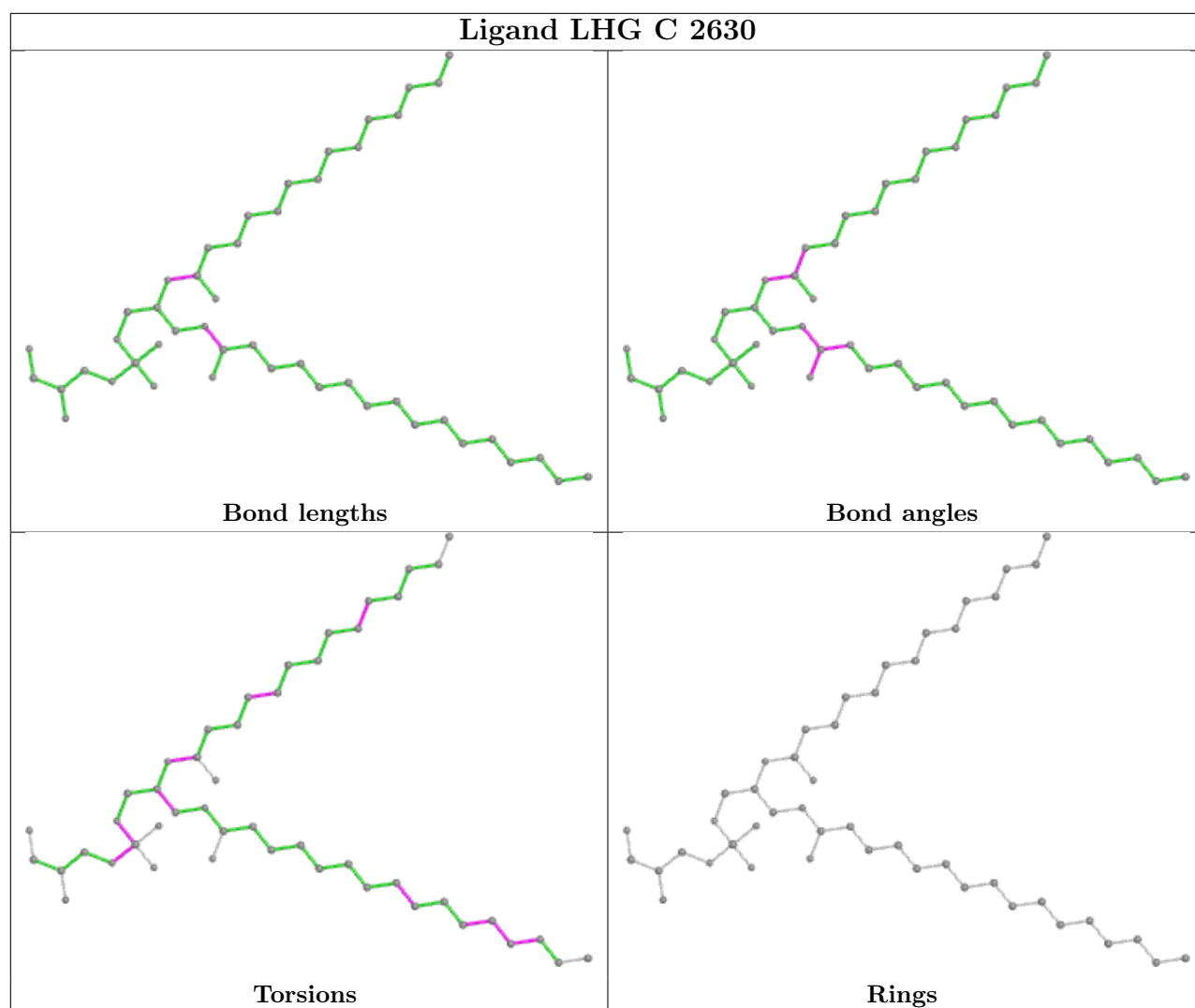


Rings

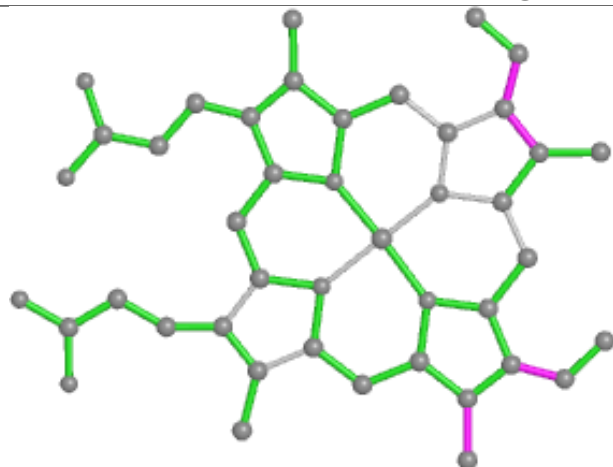




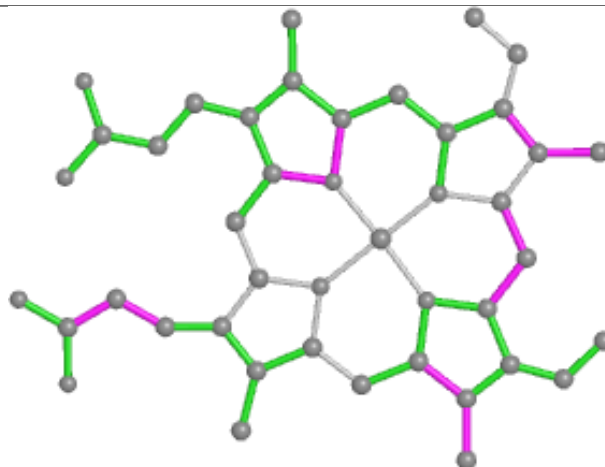




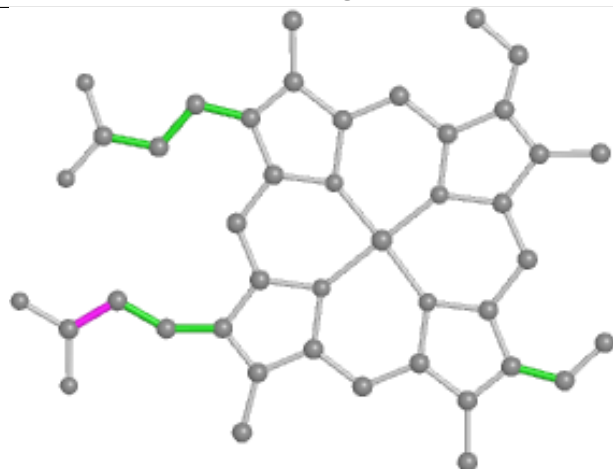
Ligand HEM f 101



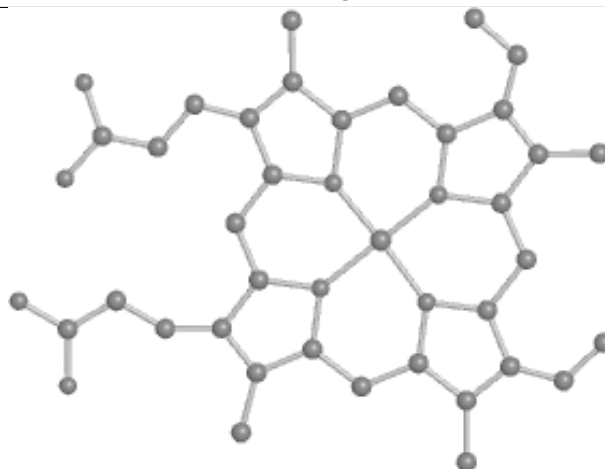
Bond lengths



Bond angles

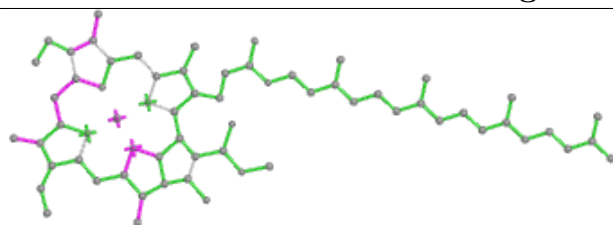


Torsions

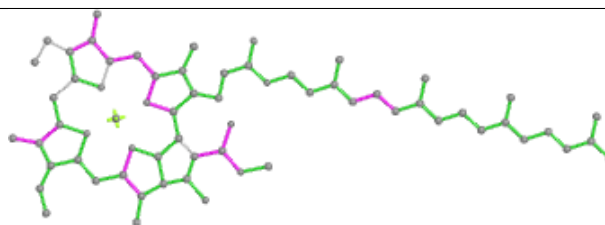


Rings

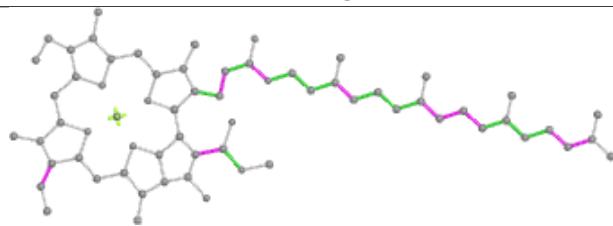
Ligand CLA c 505



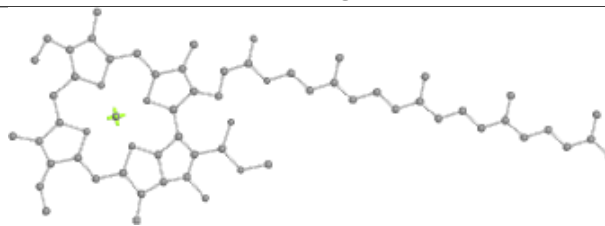
Bond lengths



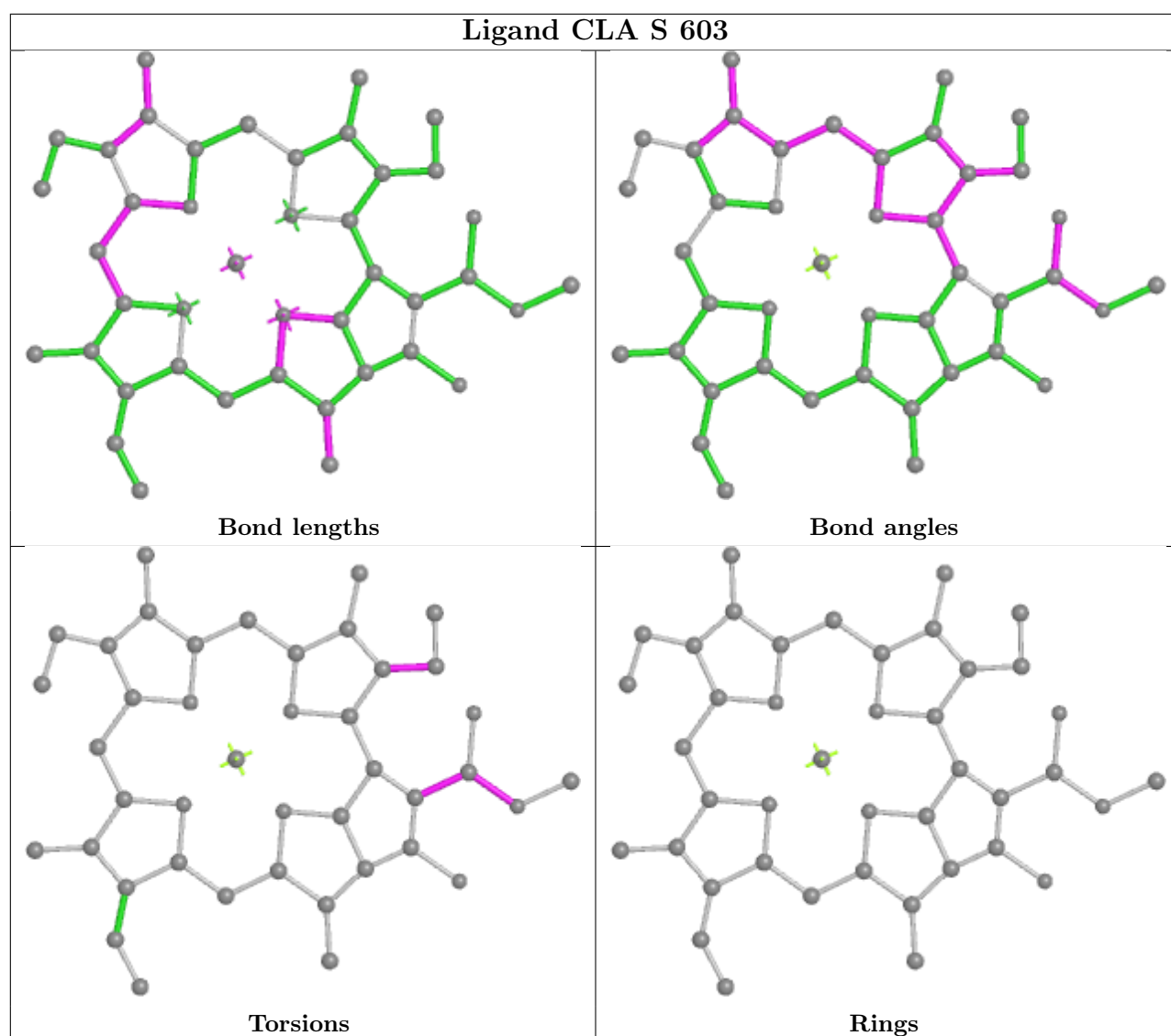
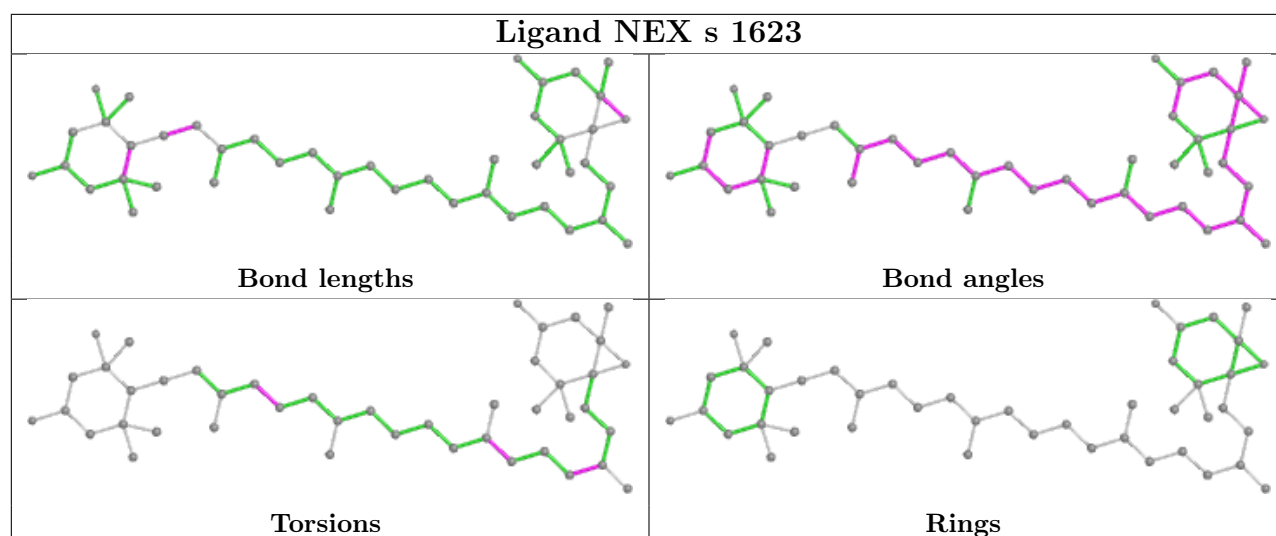
Bond angles

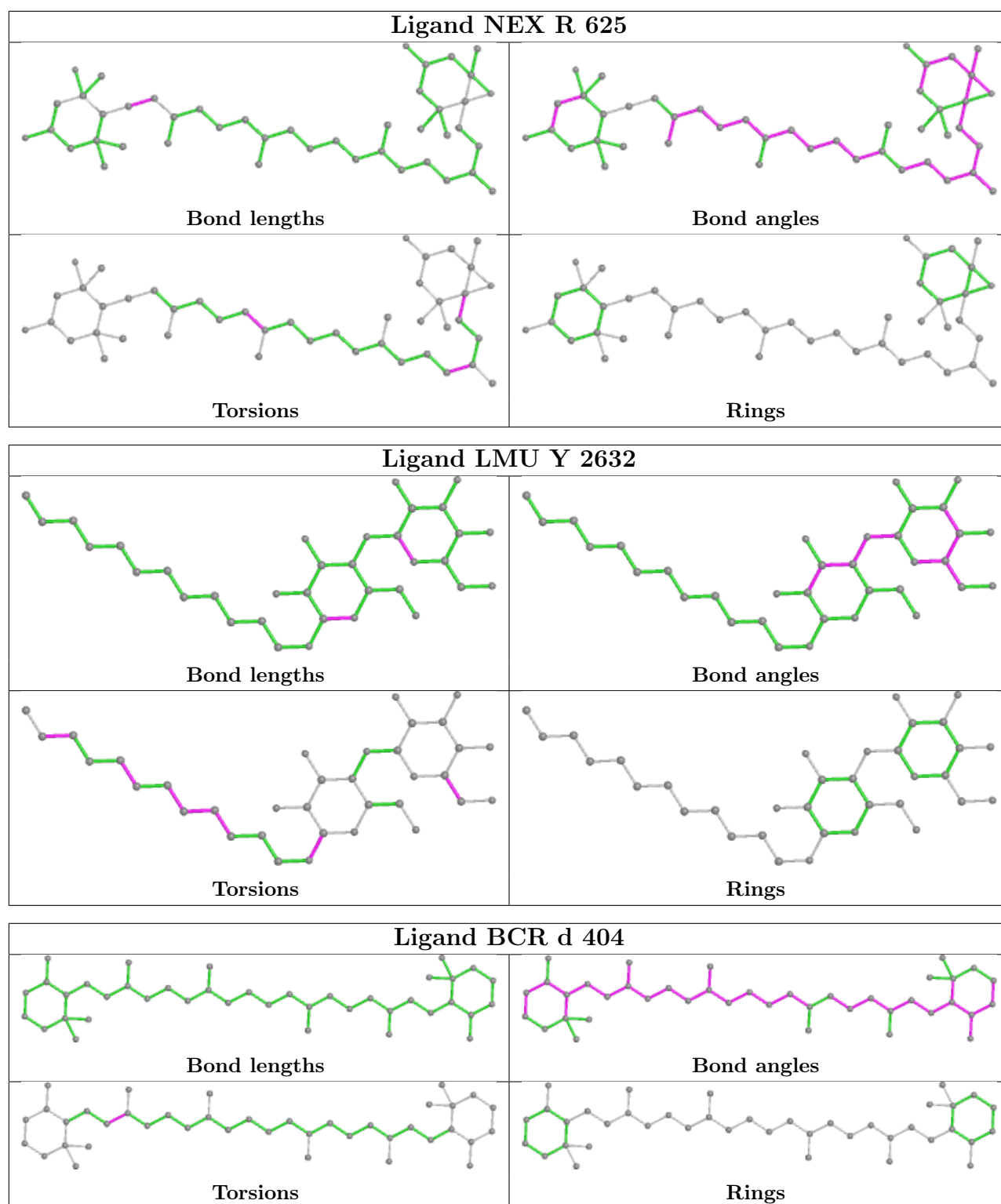


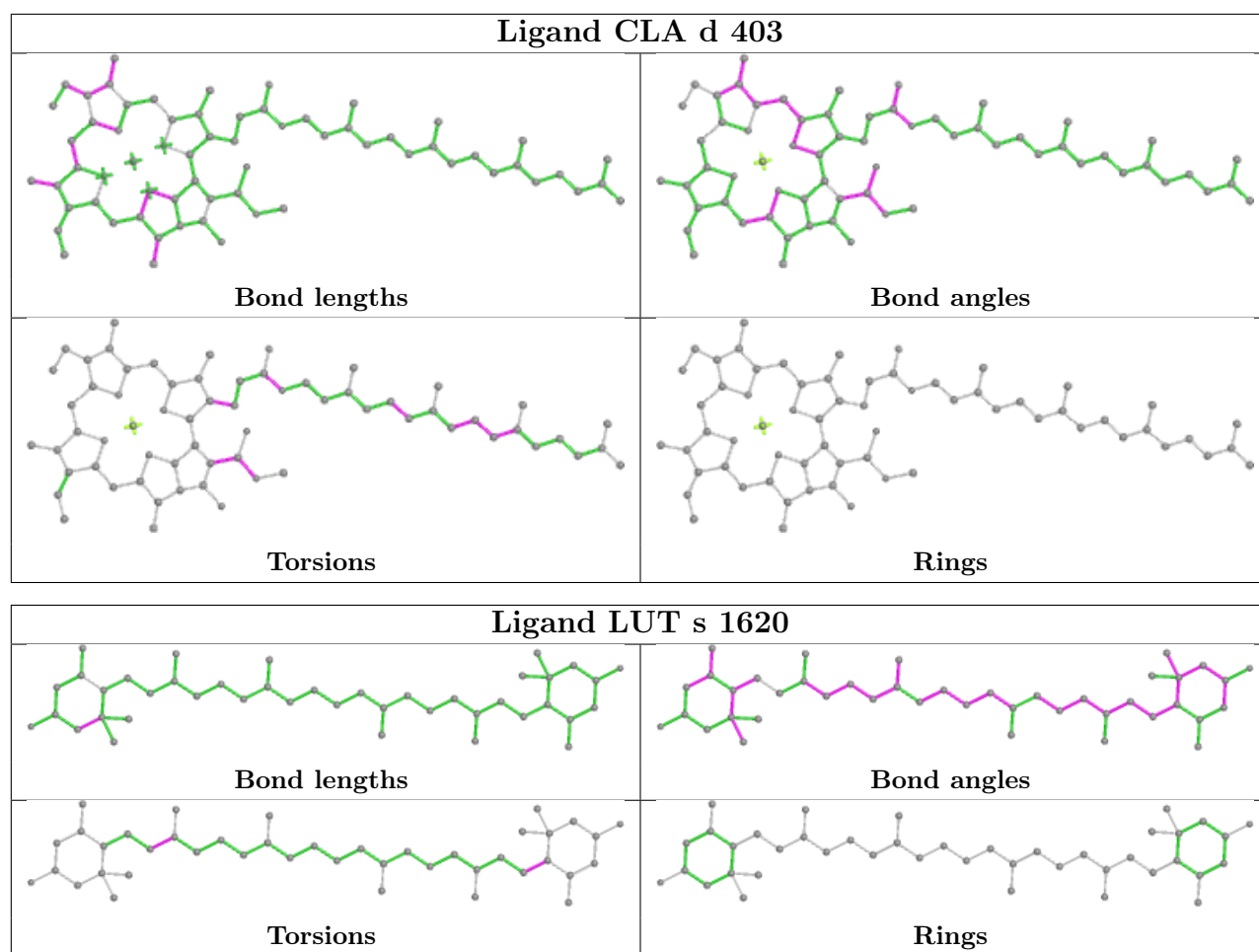
Torsions



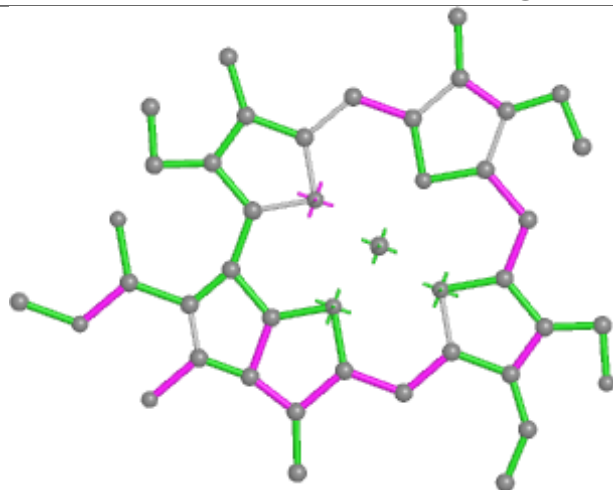
Rings



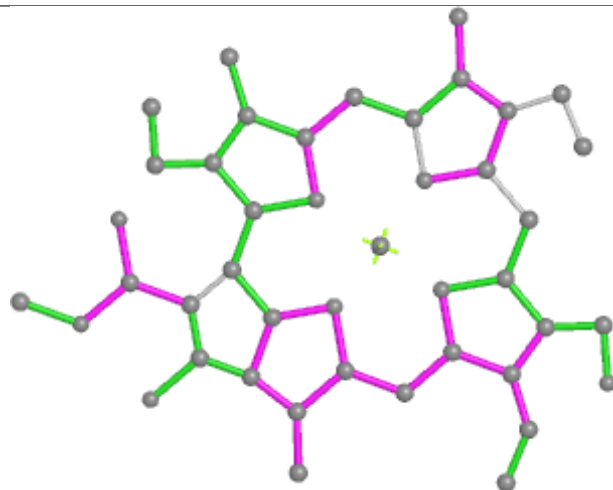




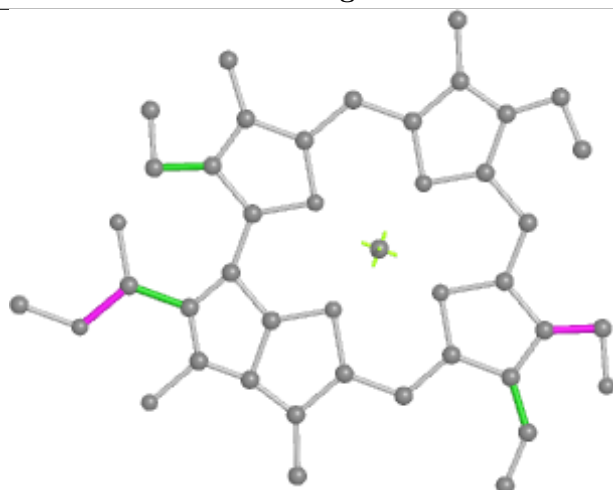
Ligand CHL S 607



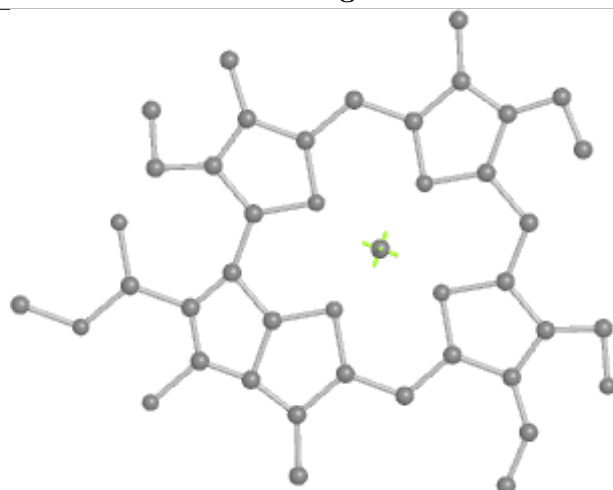
Bond lengths



Bond angles

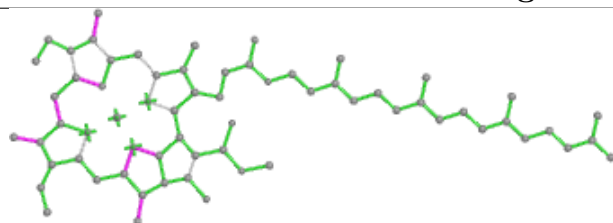


Torsions

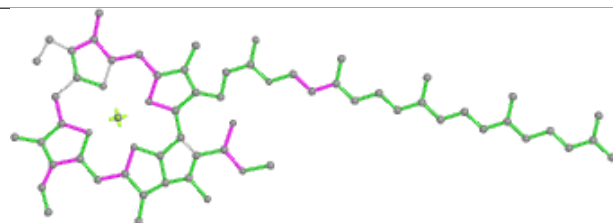


Rings

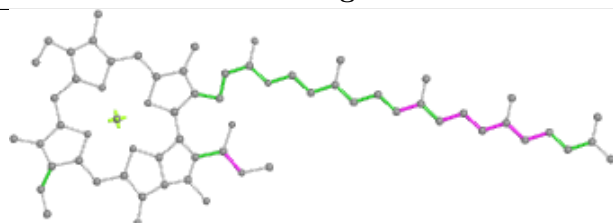
Ligand CLA b 612



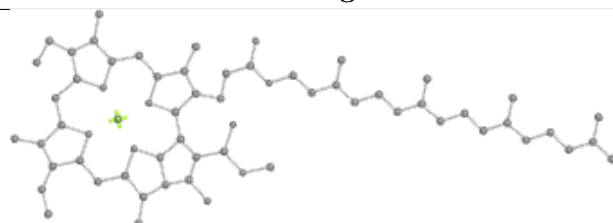
Bond lengths



Bond angles

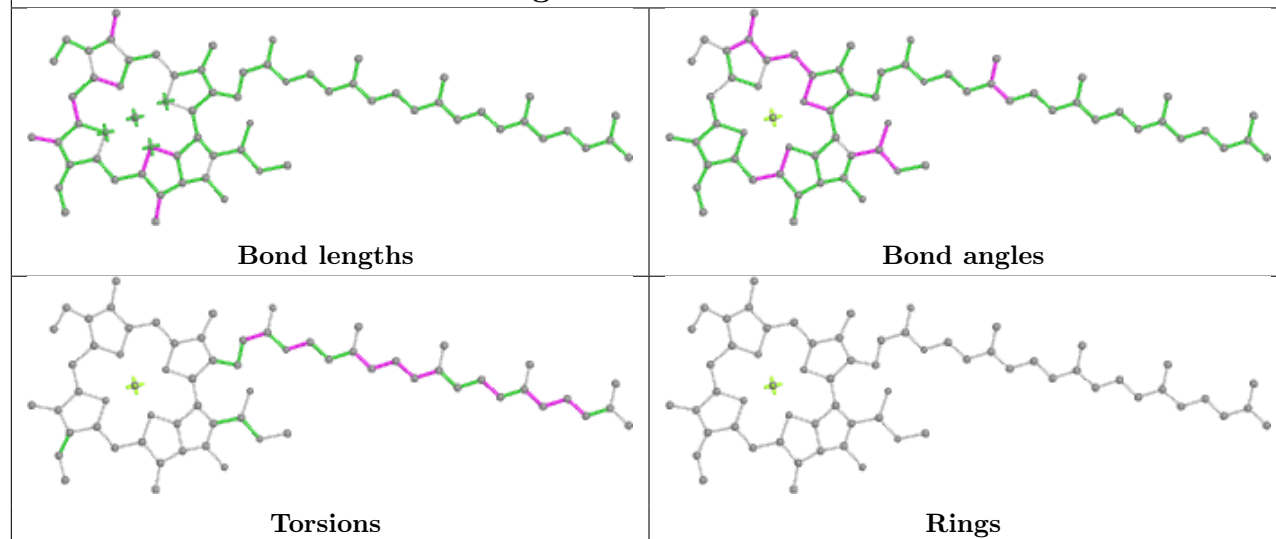


Torsions

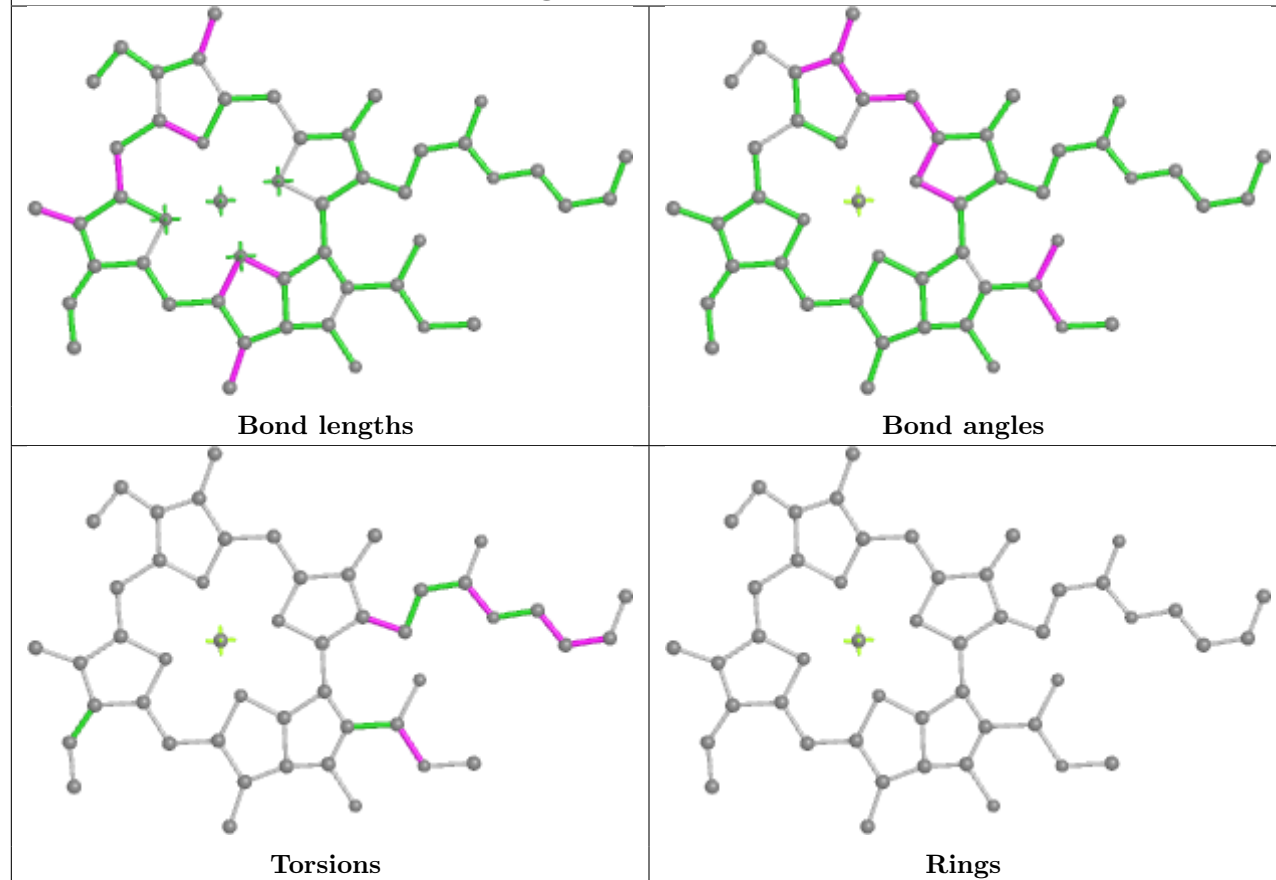


Rings

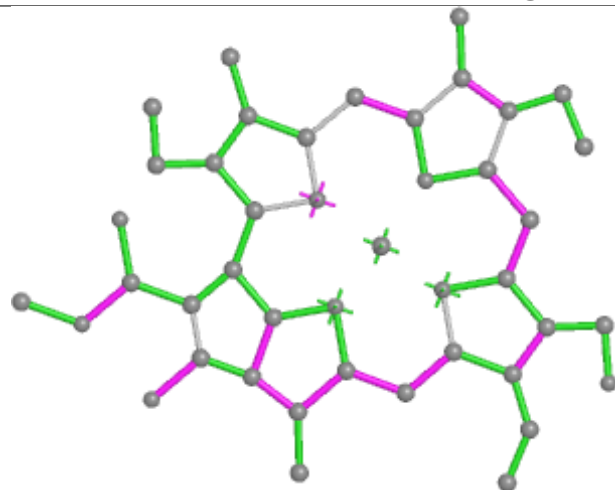
Ligand CLA B 603



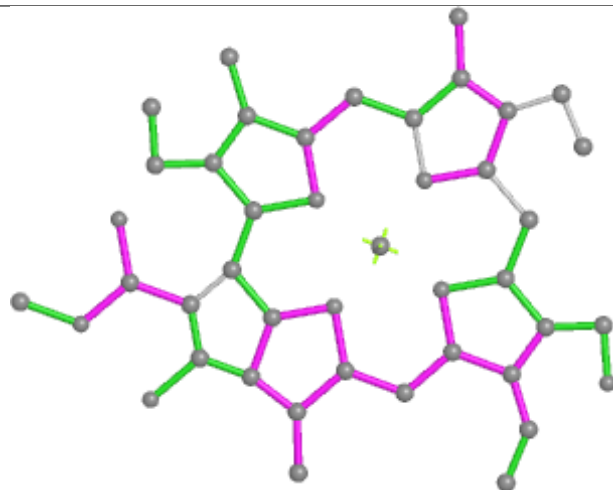
Ligand CLA s 611



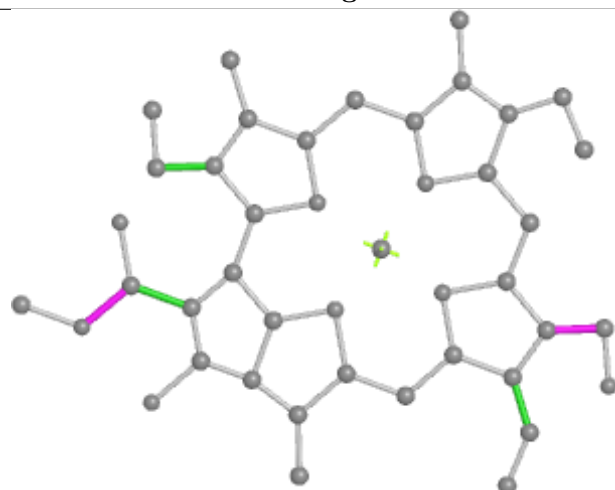
Ligand CHL s 607



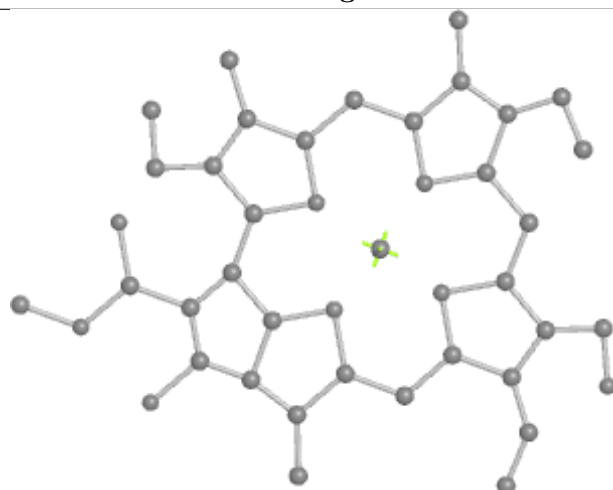
Bond lengths



Bond angles

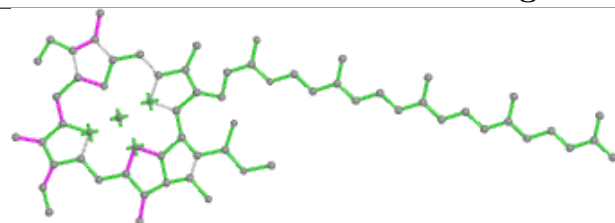


Torsions

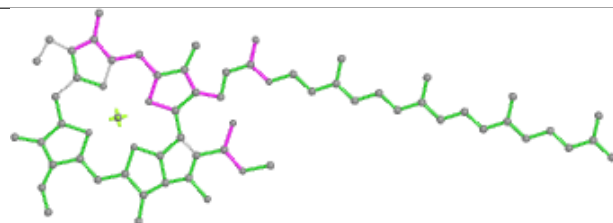


Rings

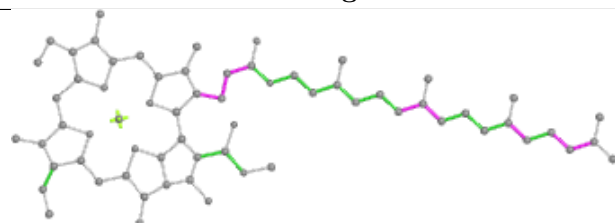
Ligand CLA n 603



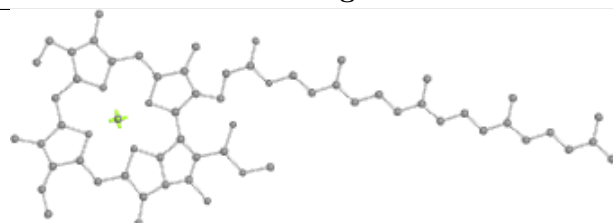
Bond lengths



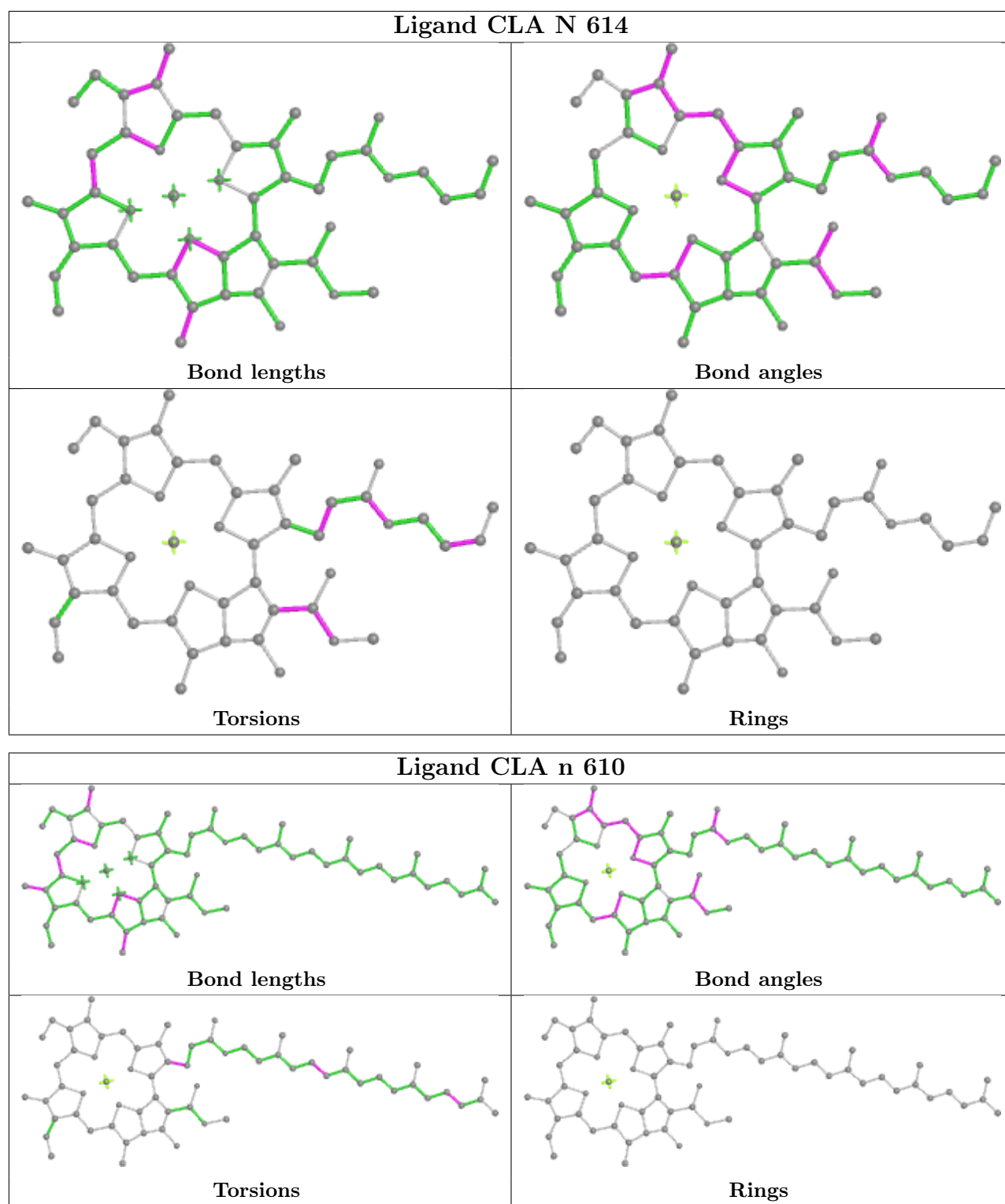
Bond angles



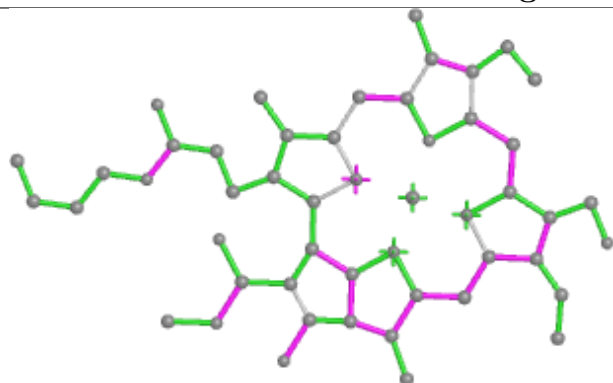
Torsions



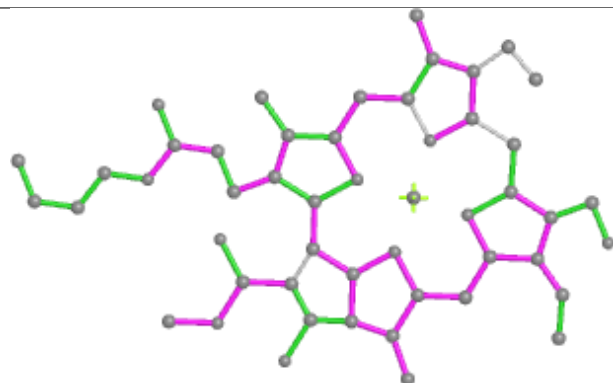
Rings



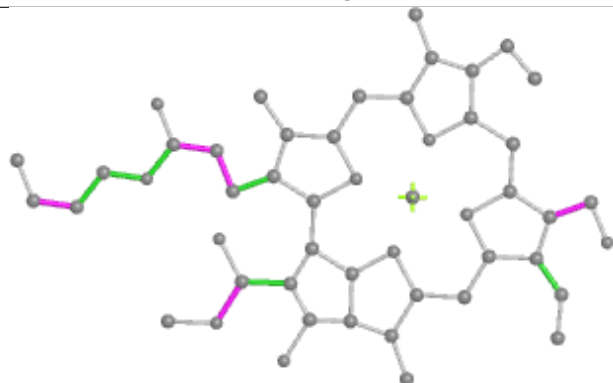
Ligand CHL r 607



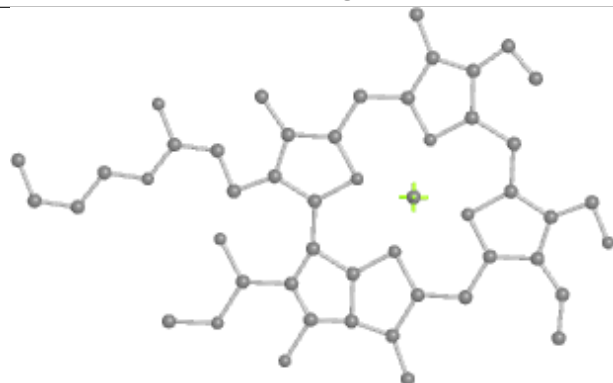
Bond lengths



Bond angles

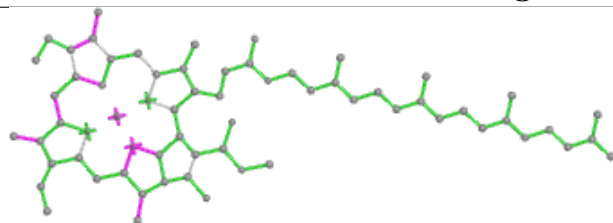


Torsions

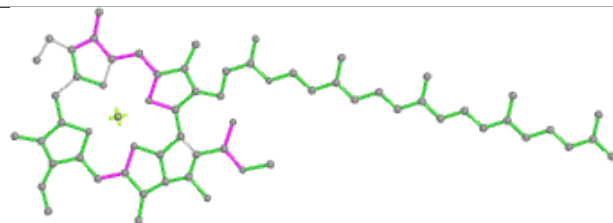


Rings

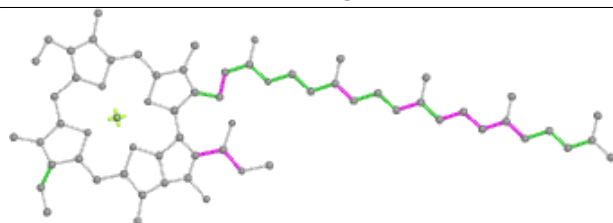
Ligand CLA Y 604



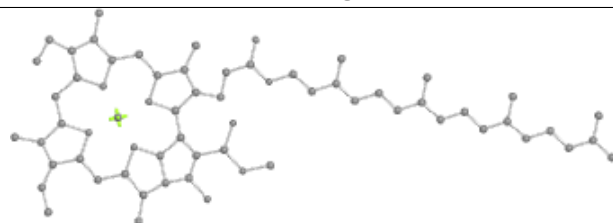
Bond lengths



Bond angles

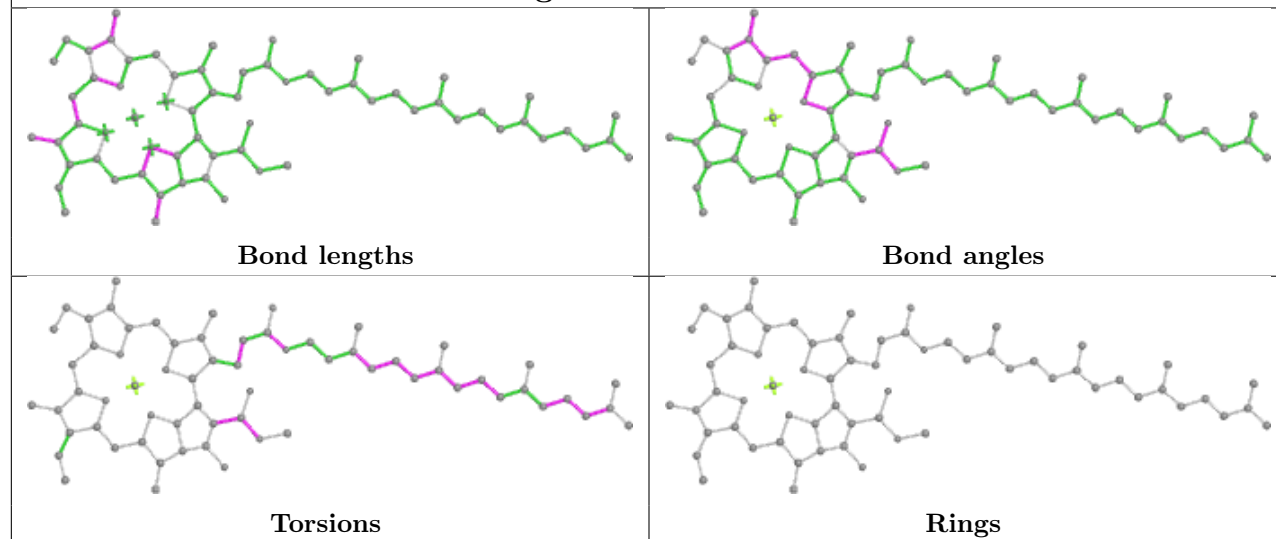


Torsions

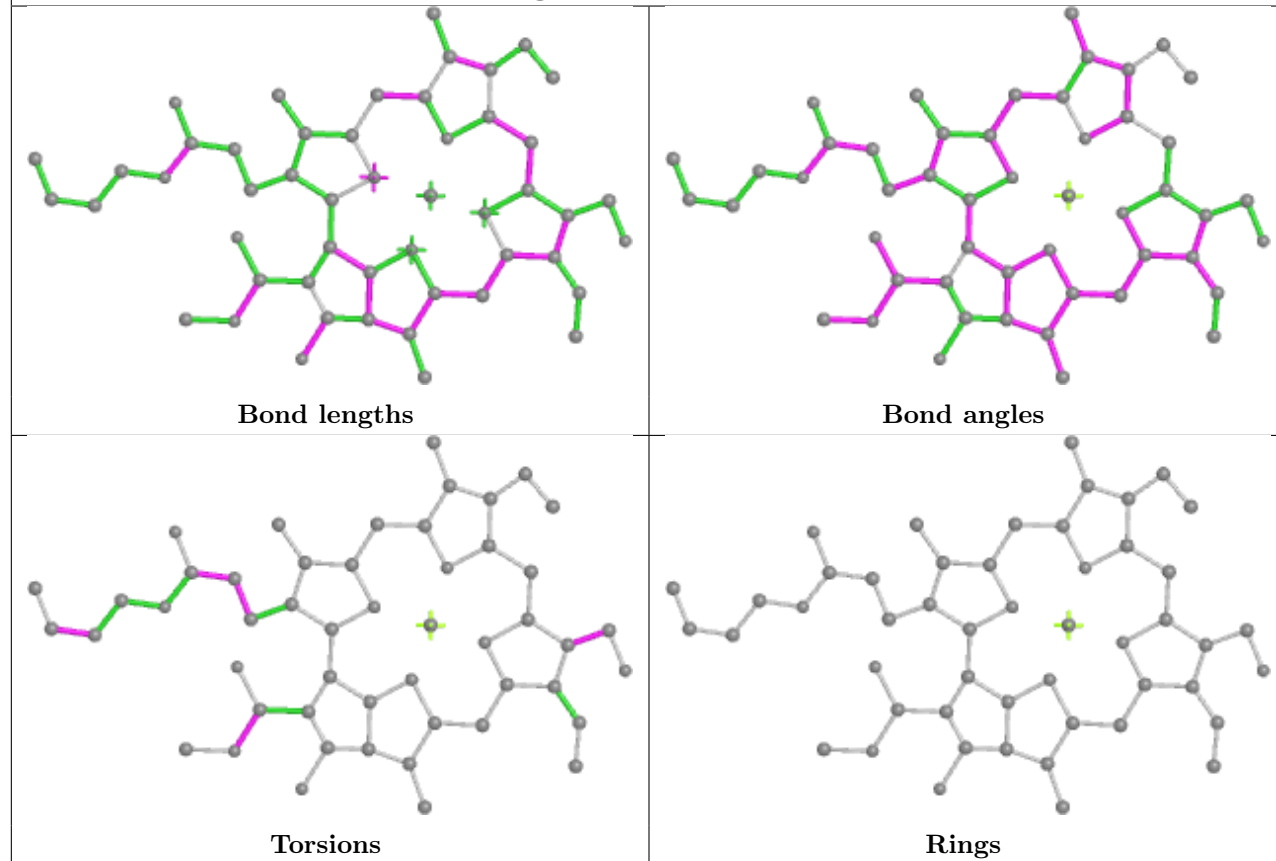


Rings

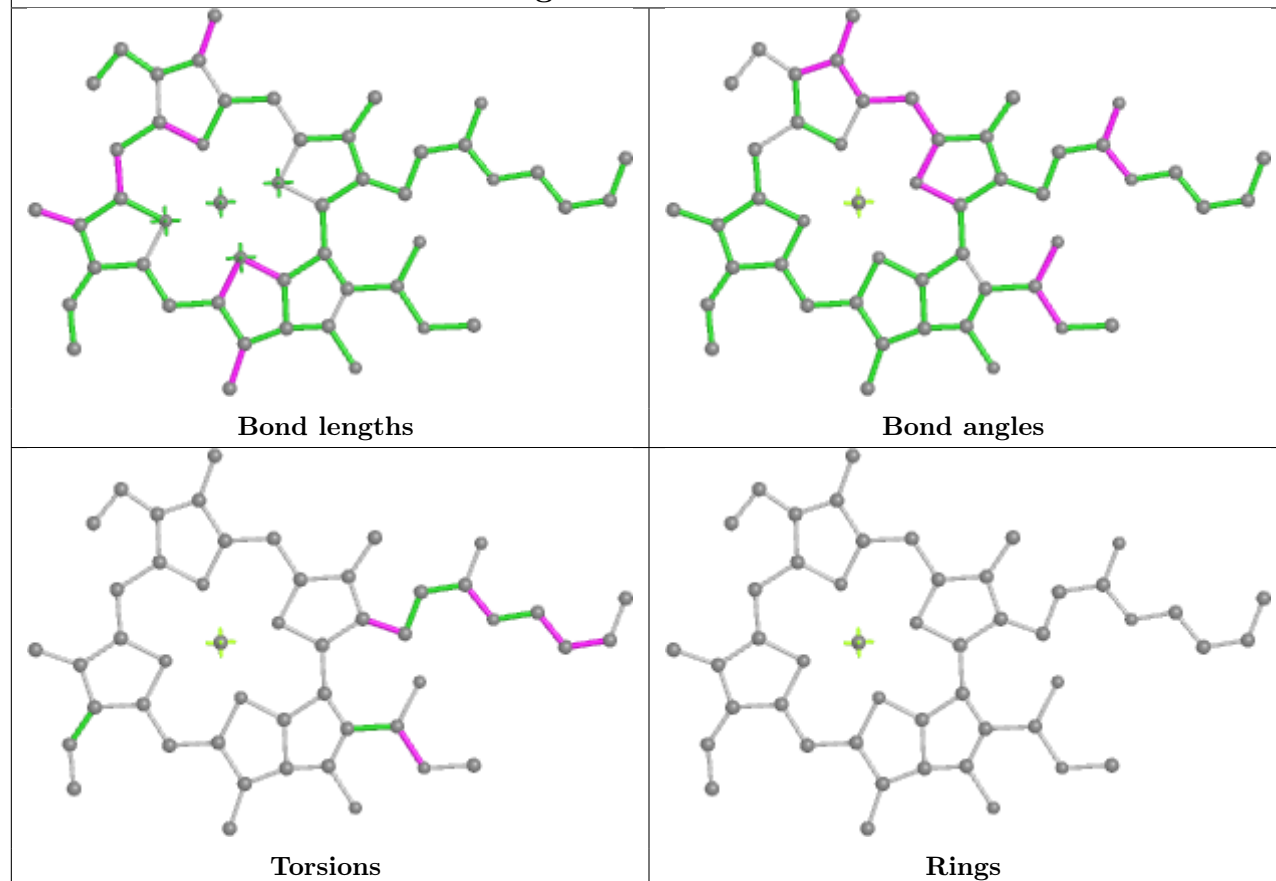
Ligand CLA b 615



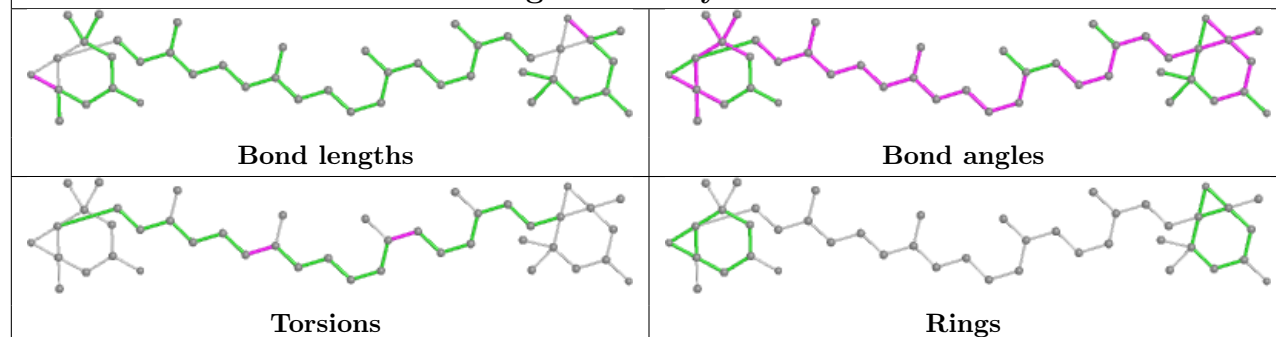
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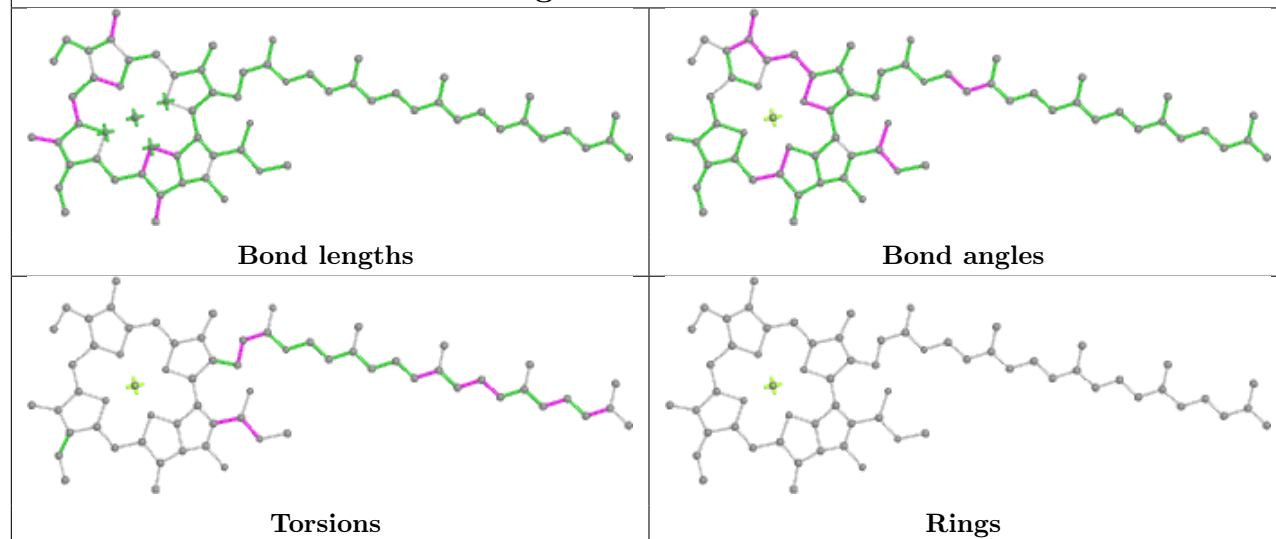
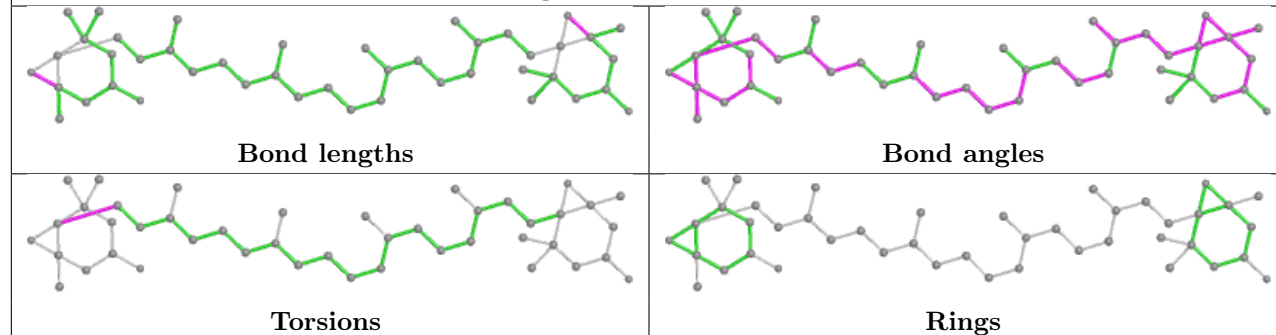
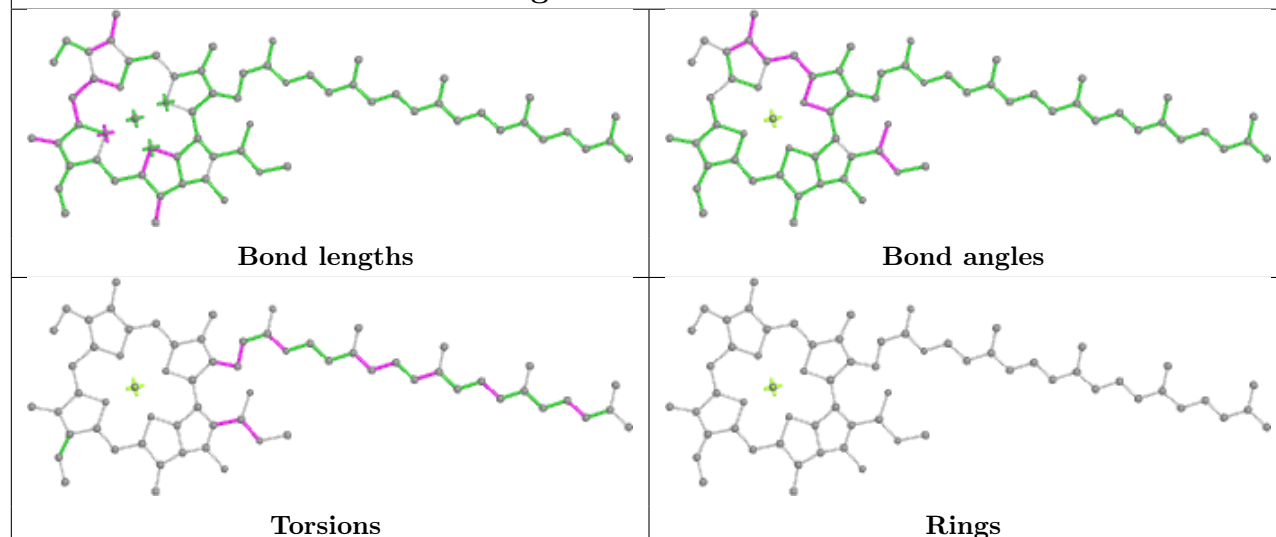


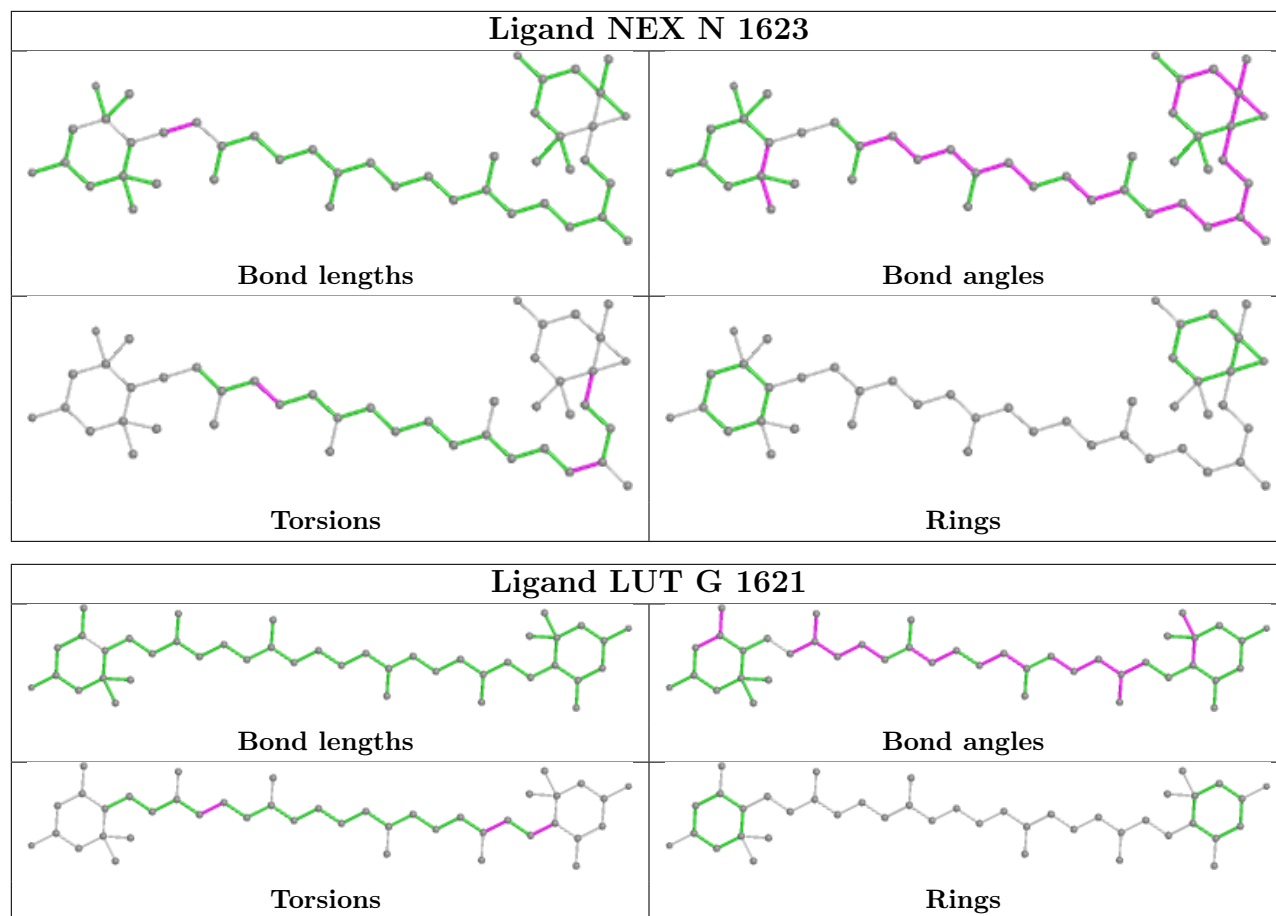
Ligand CLA S 611



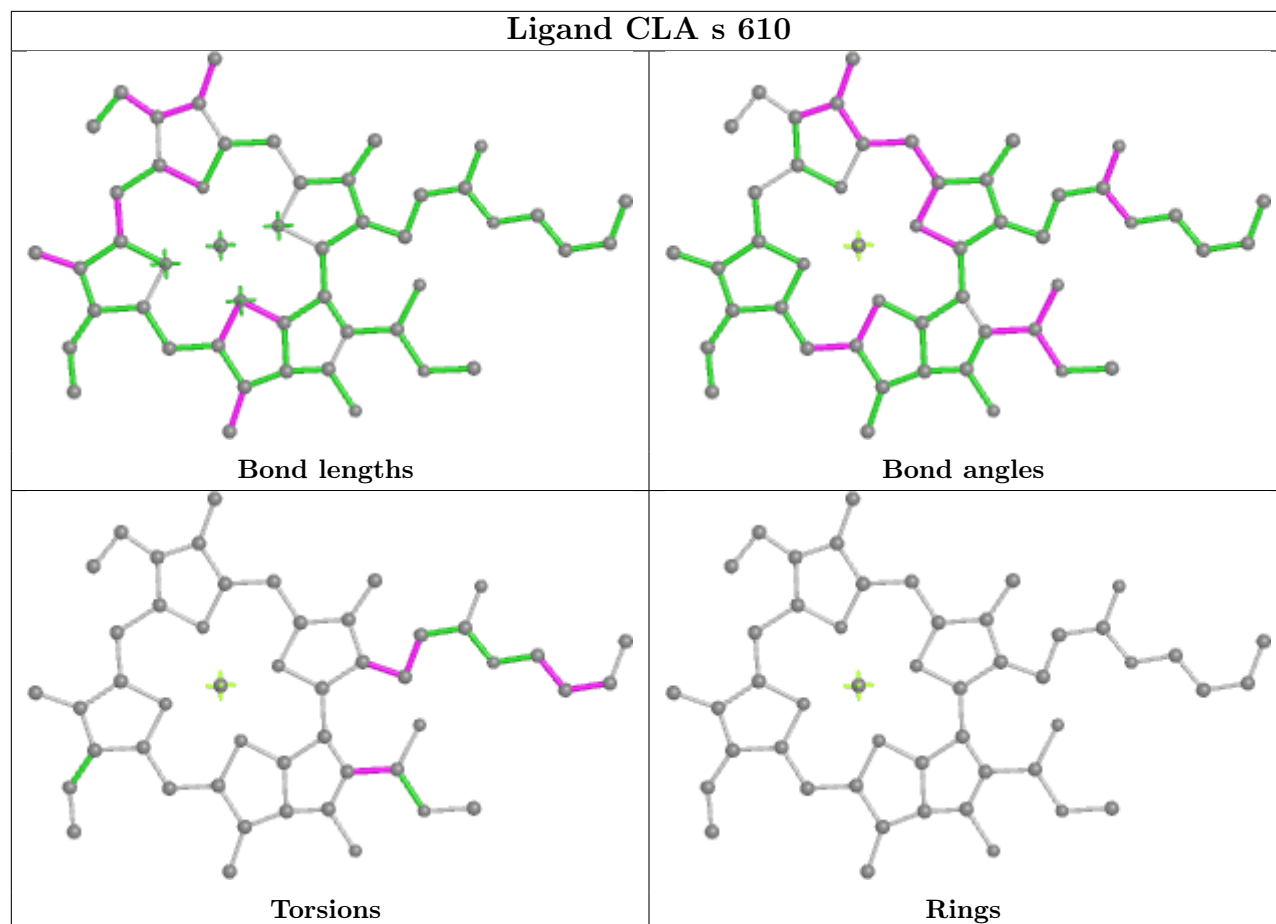
Ligand XAT y 1622



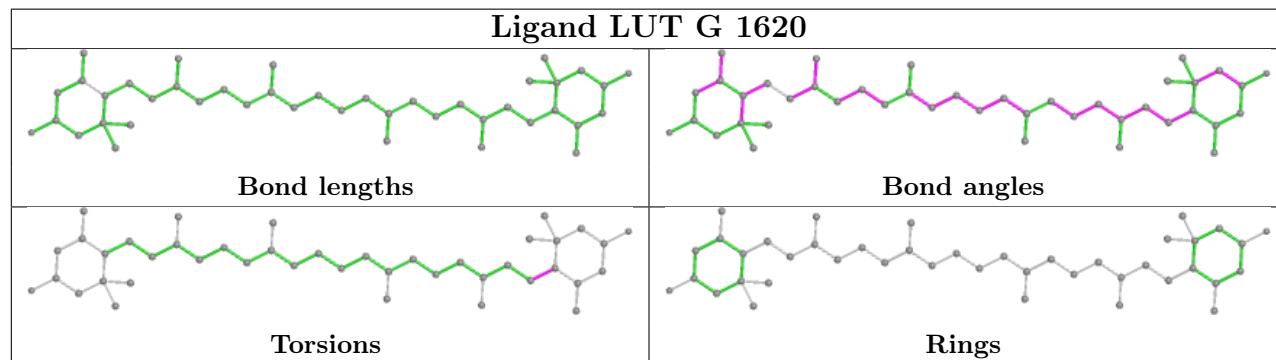
Ligand CLA n 602**Ligand XAT r 624****Ligand CLA G 613**



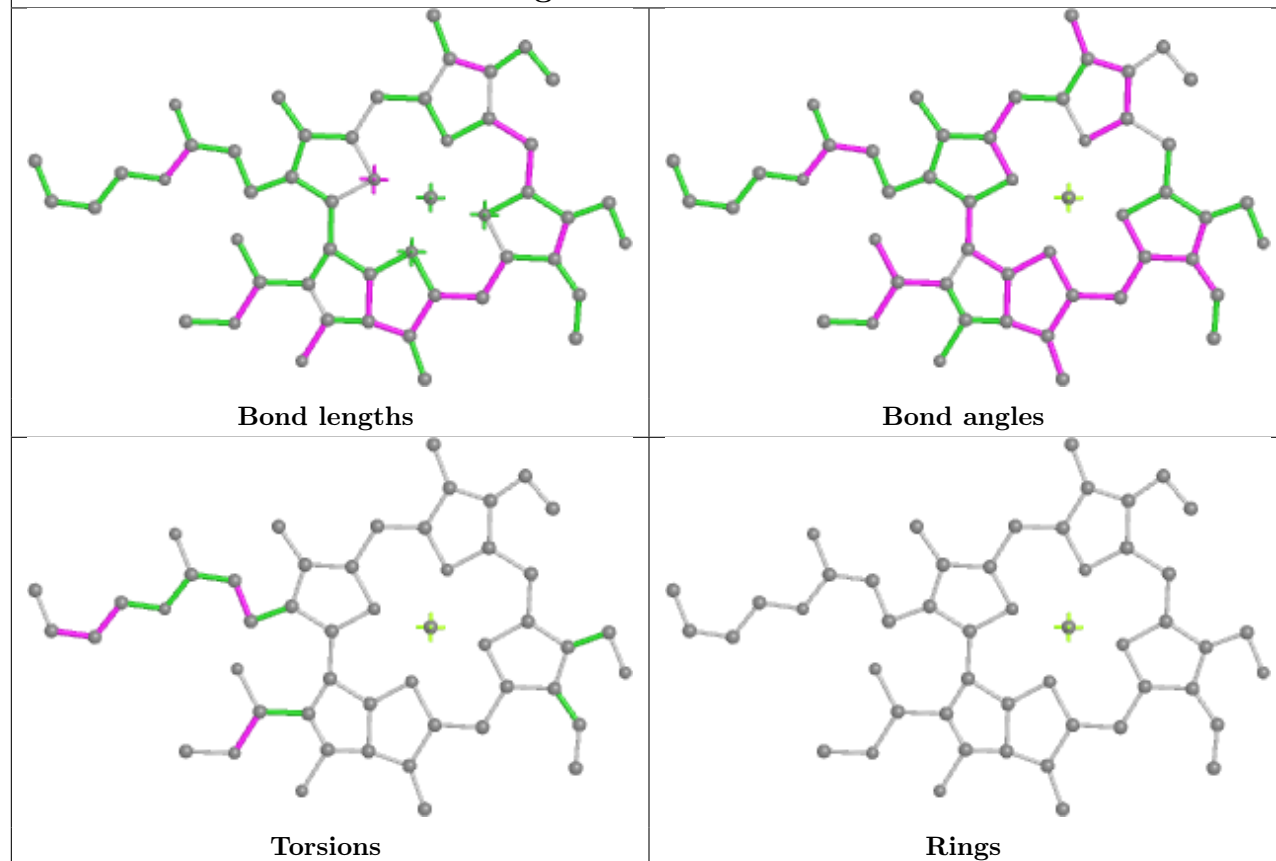
Ligand CLA s 610



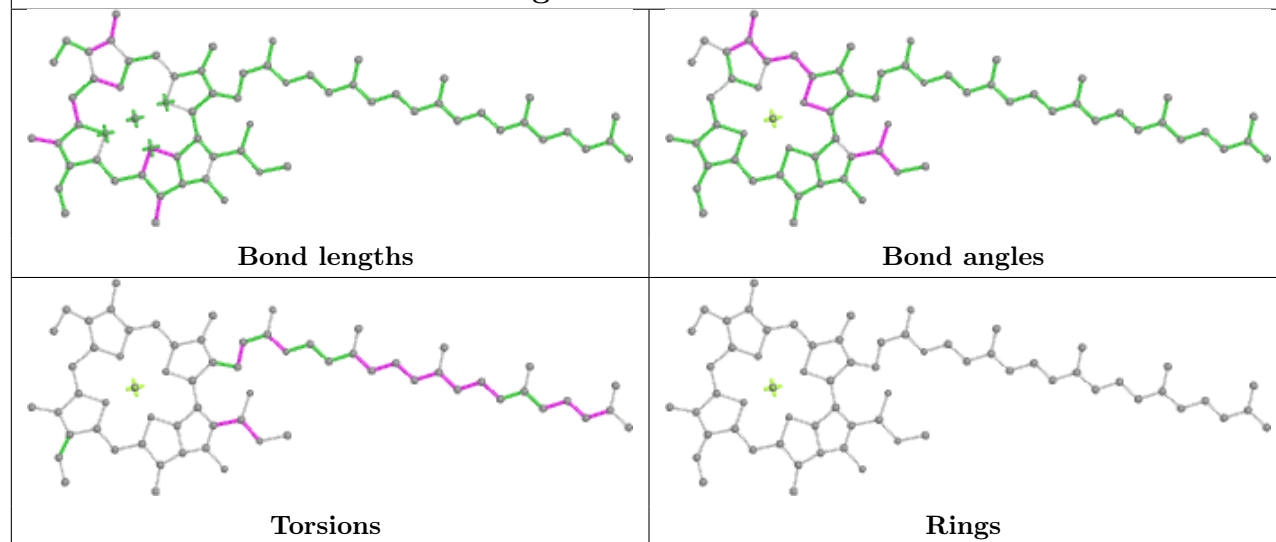
Ligand LUT G 1620



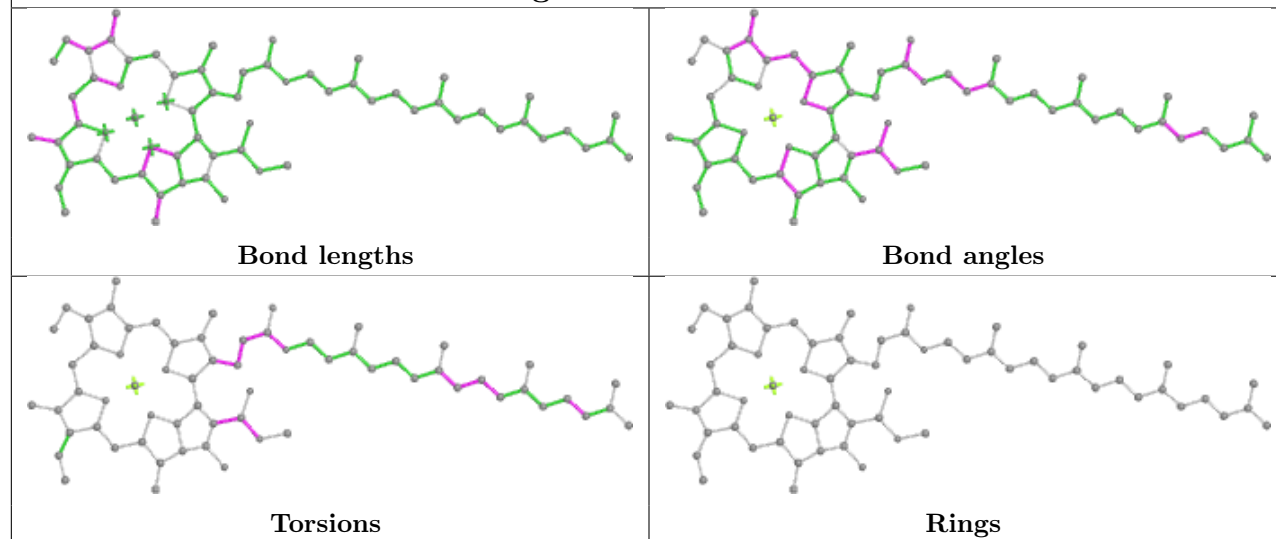
Ligand CHL n 608



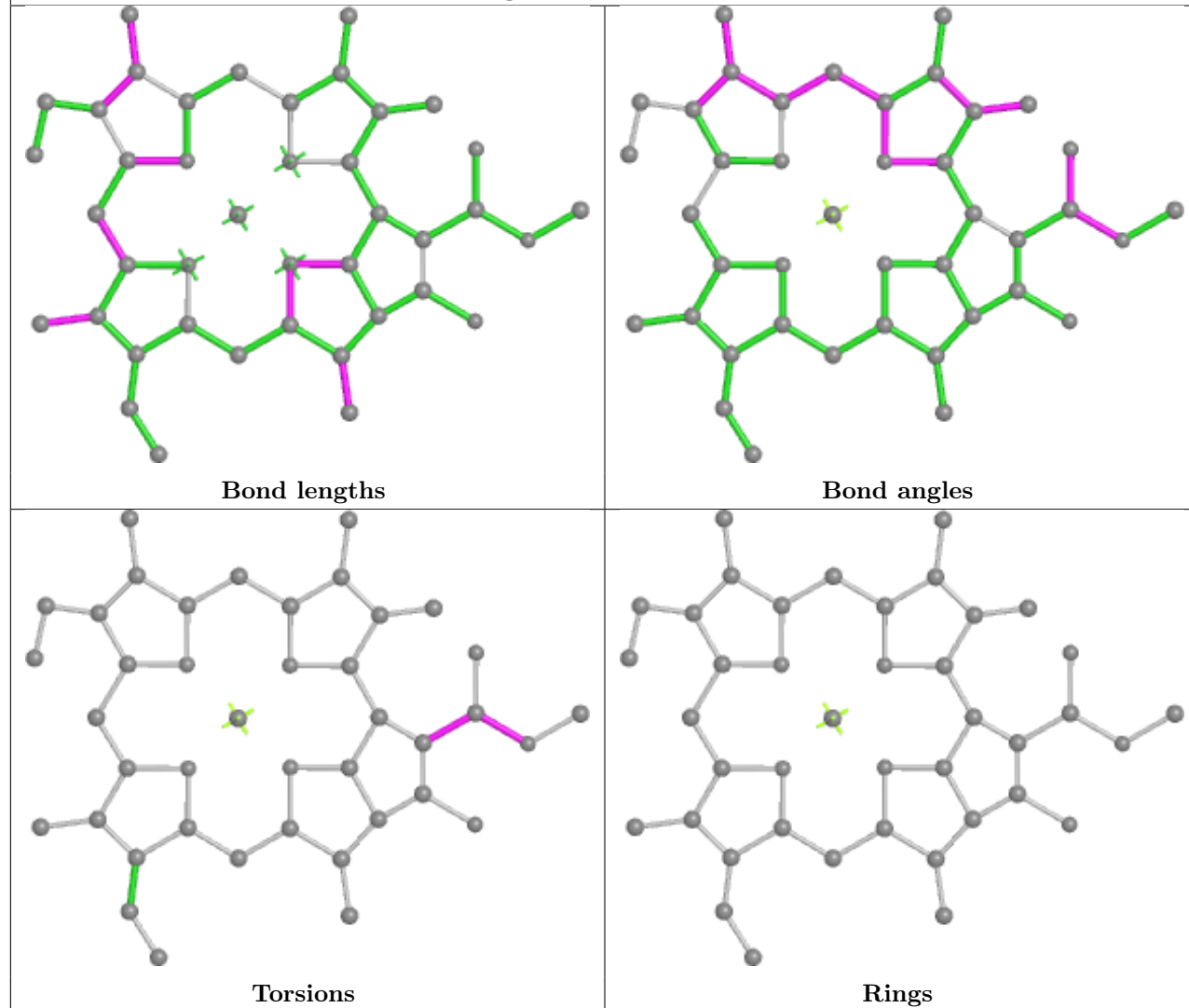
Ligand CLA B 615

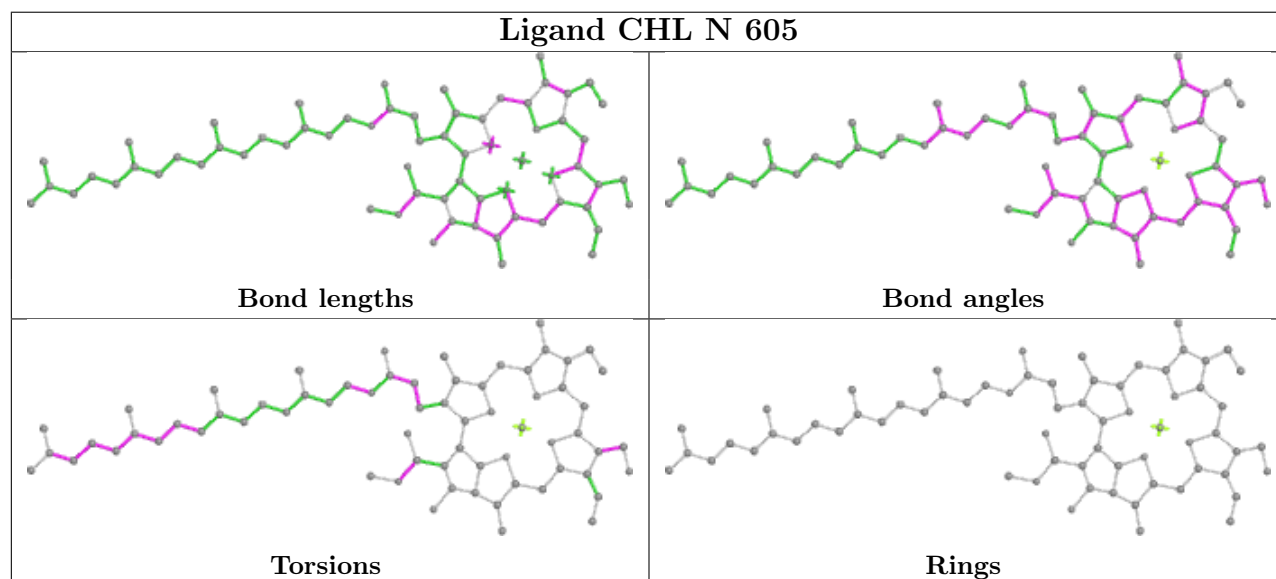
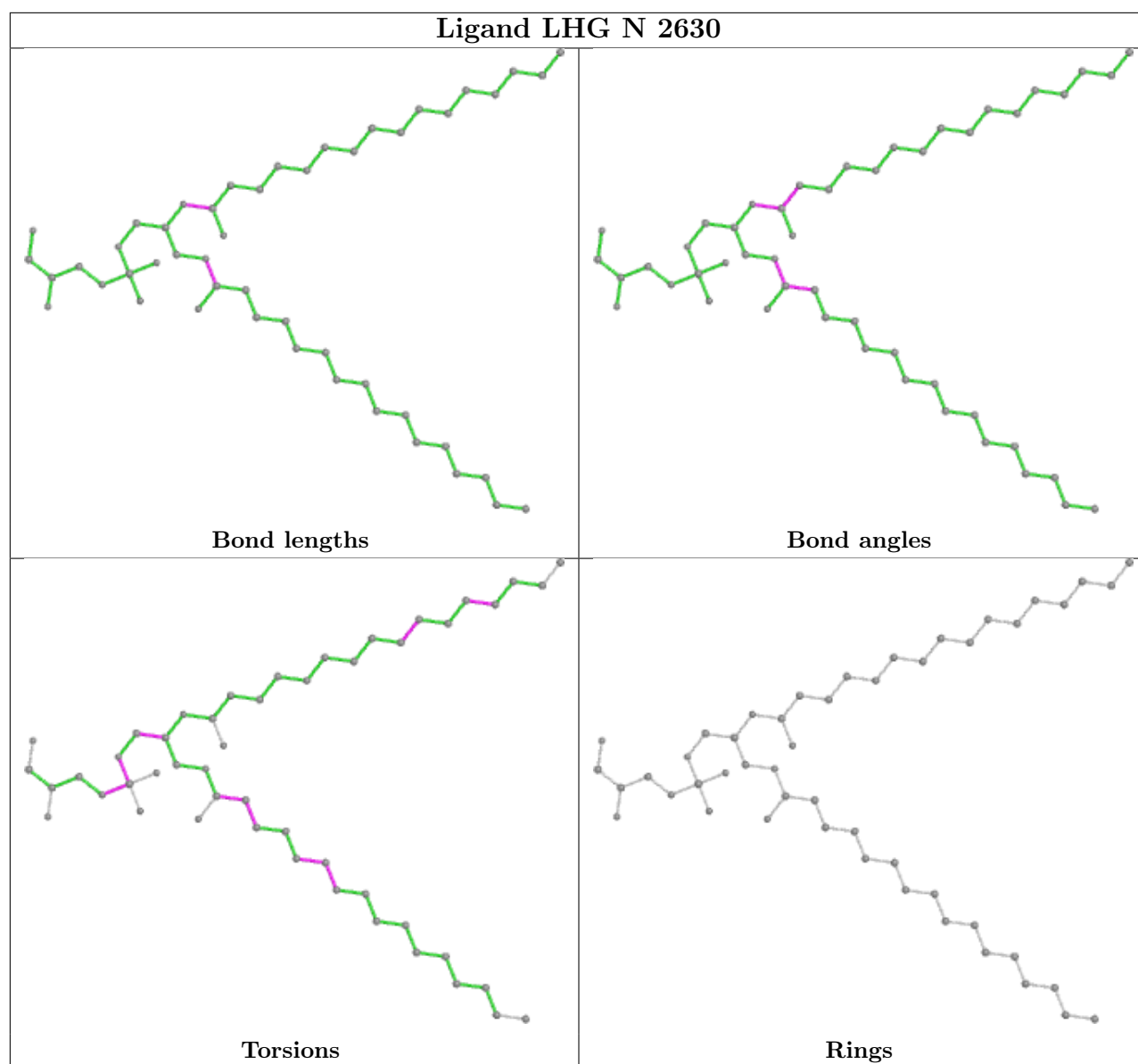


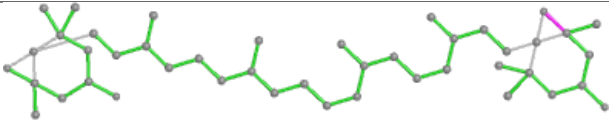
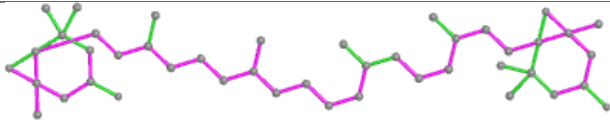
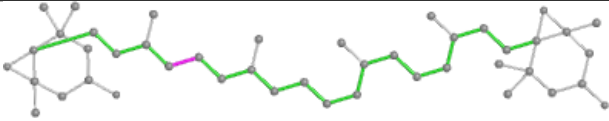
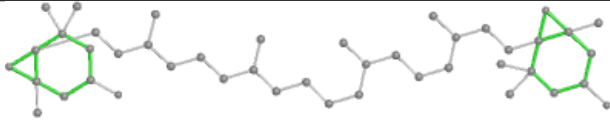
Ligand CLA C 501

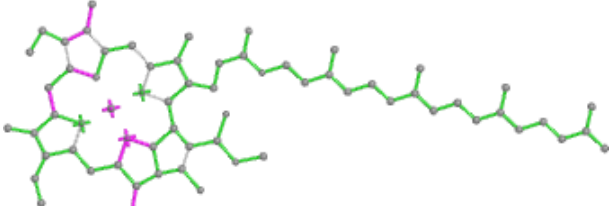
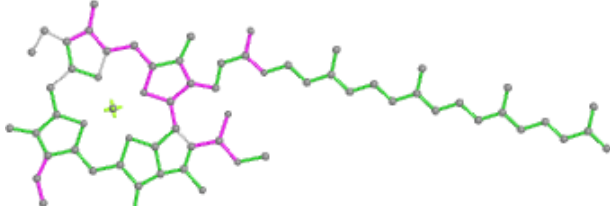
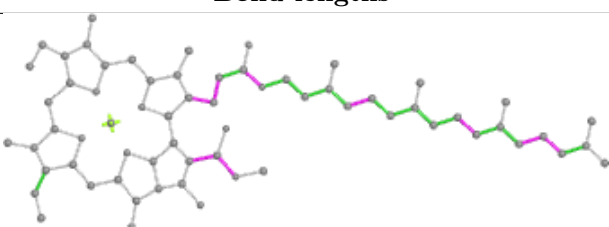
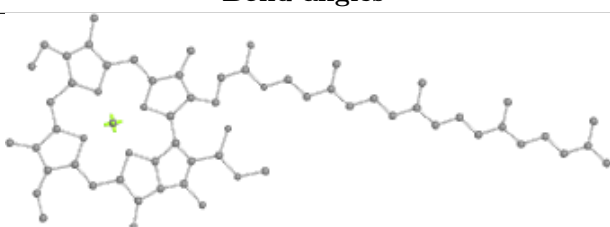


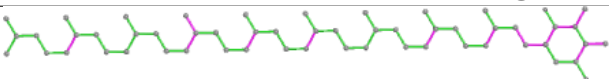
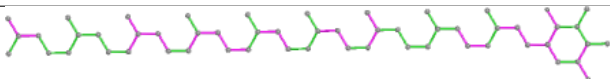
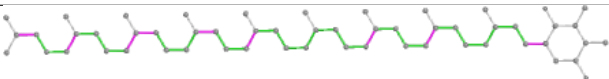
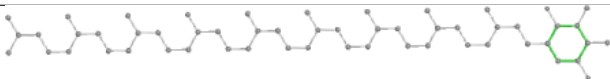
Ligand CLA r 610



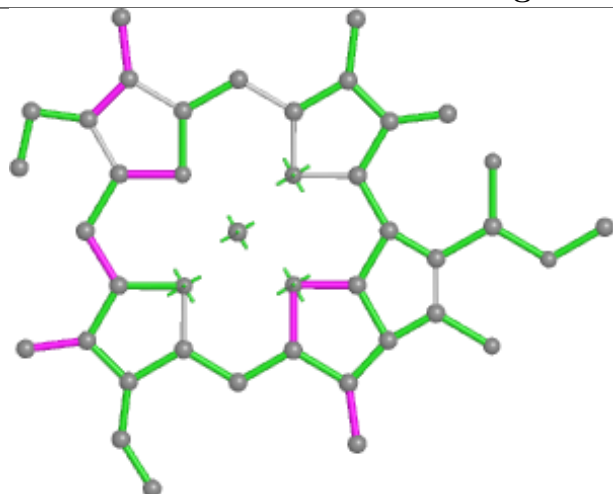


Ligand XAT n 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

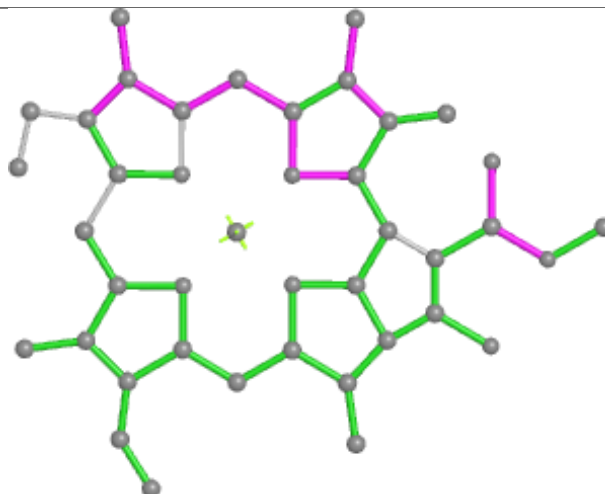
Ligand CLA g 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

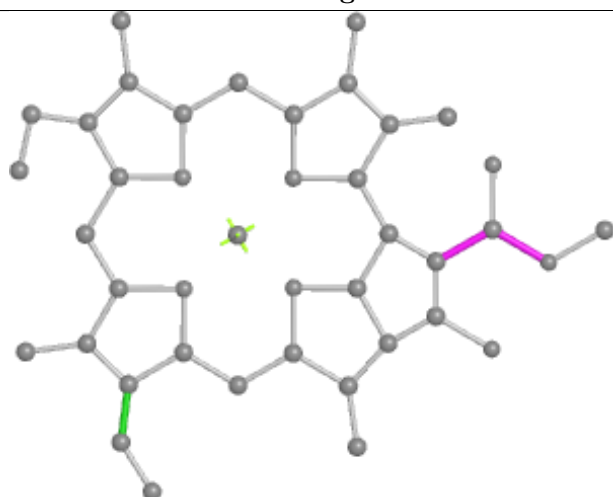
Ligand CLA R 610



Bond lengths



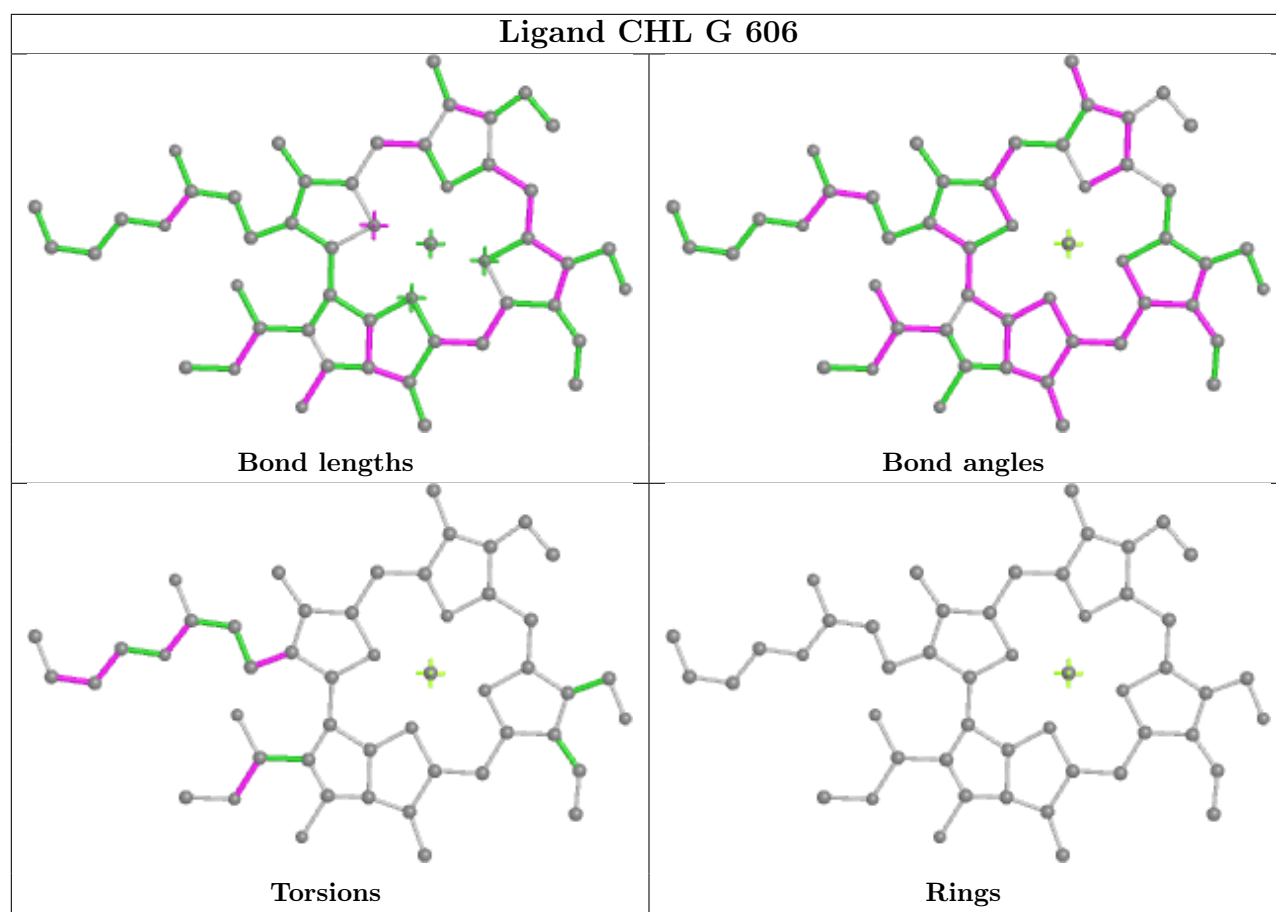
Bond angles



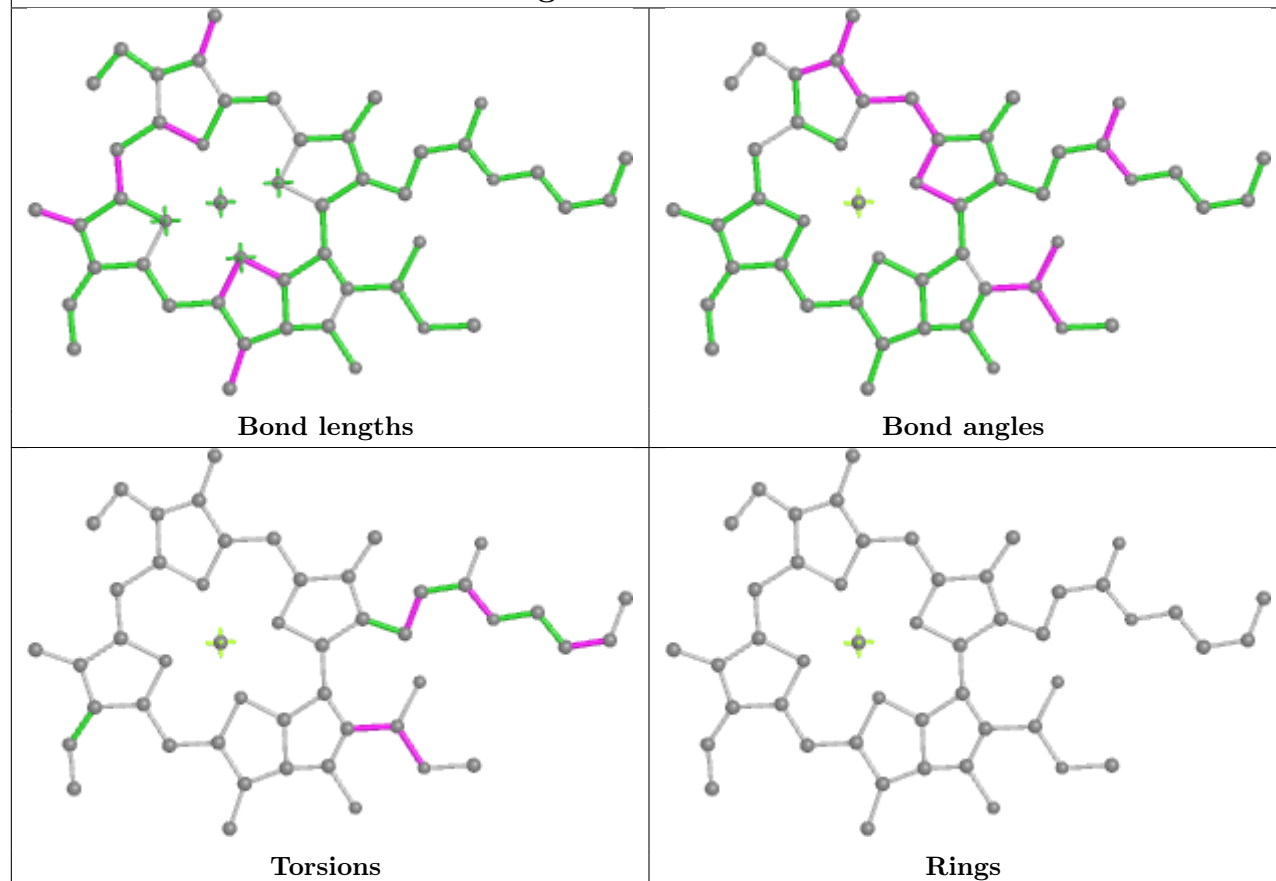
Torsions



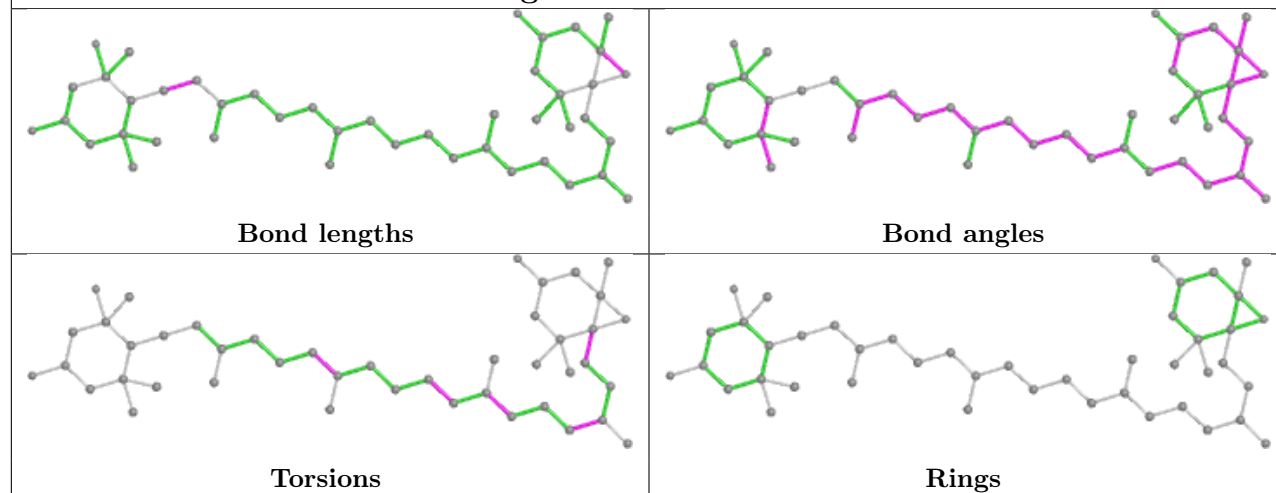
Rings

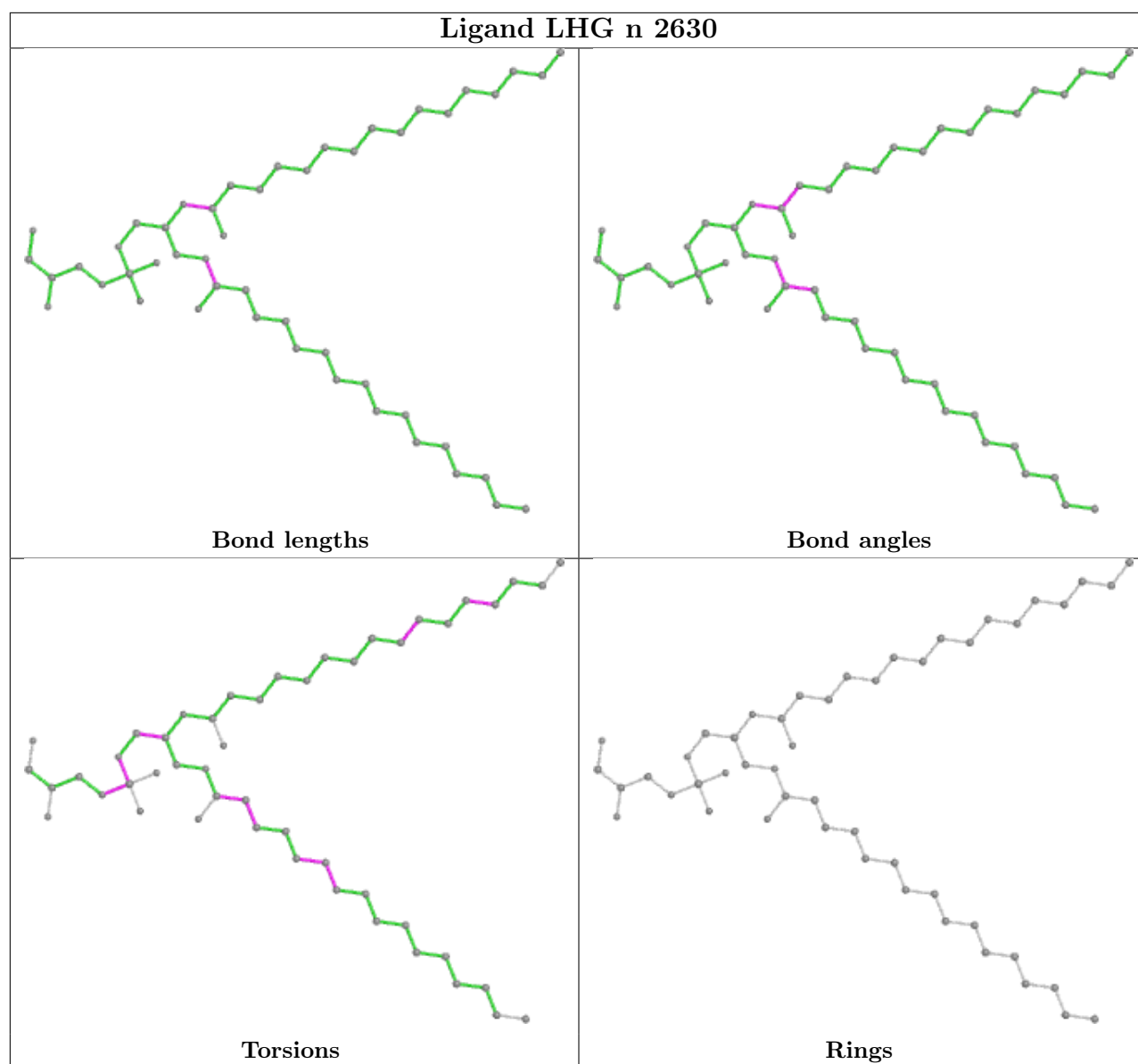


Ligand CLA s 602

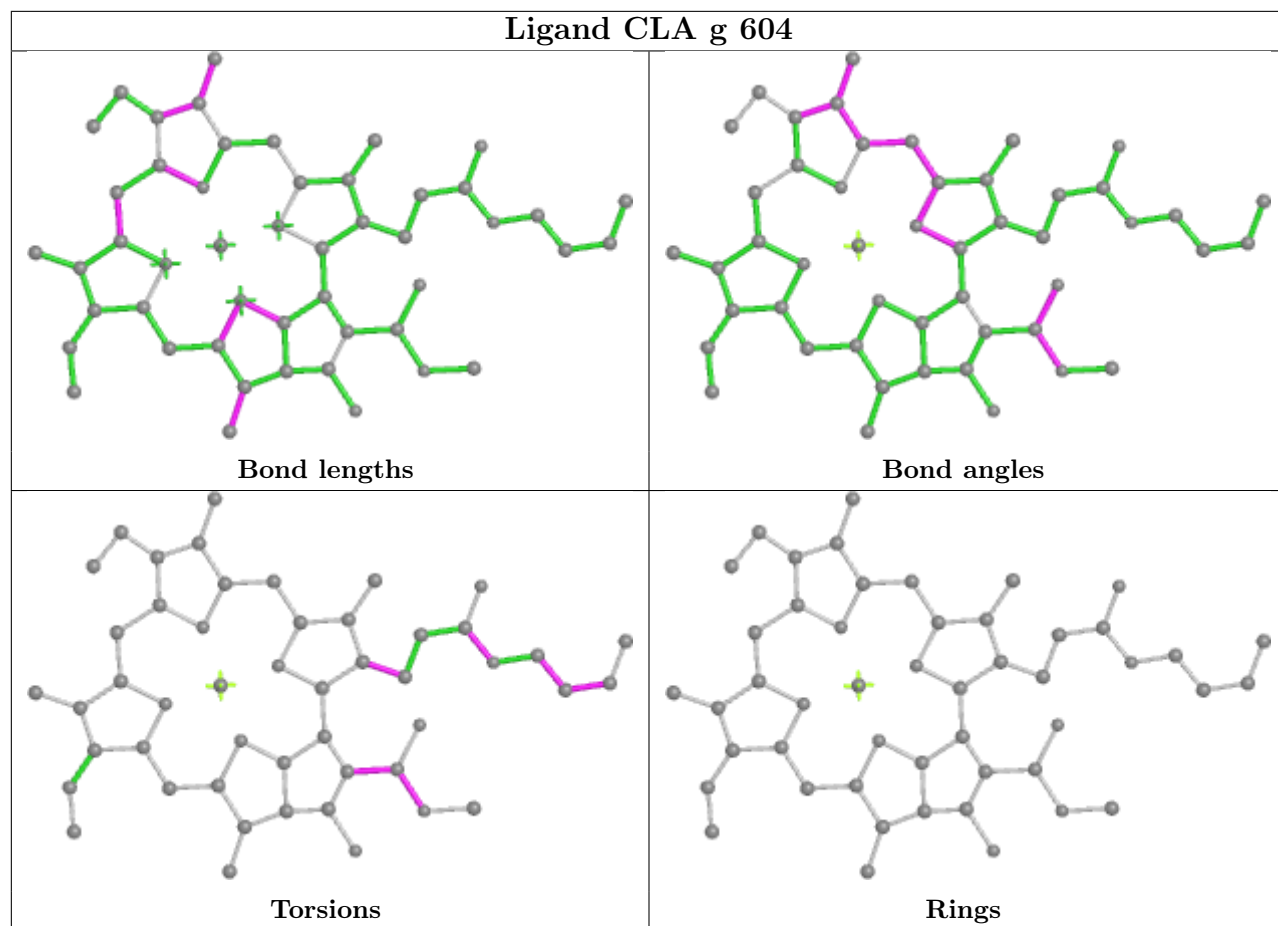


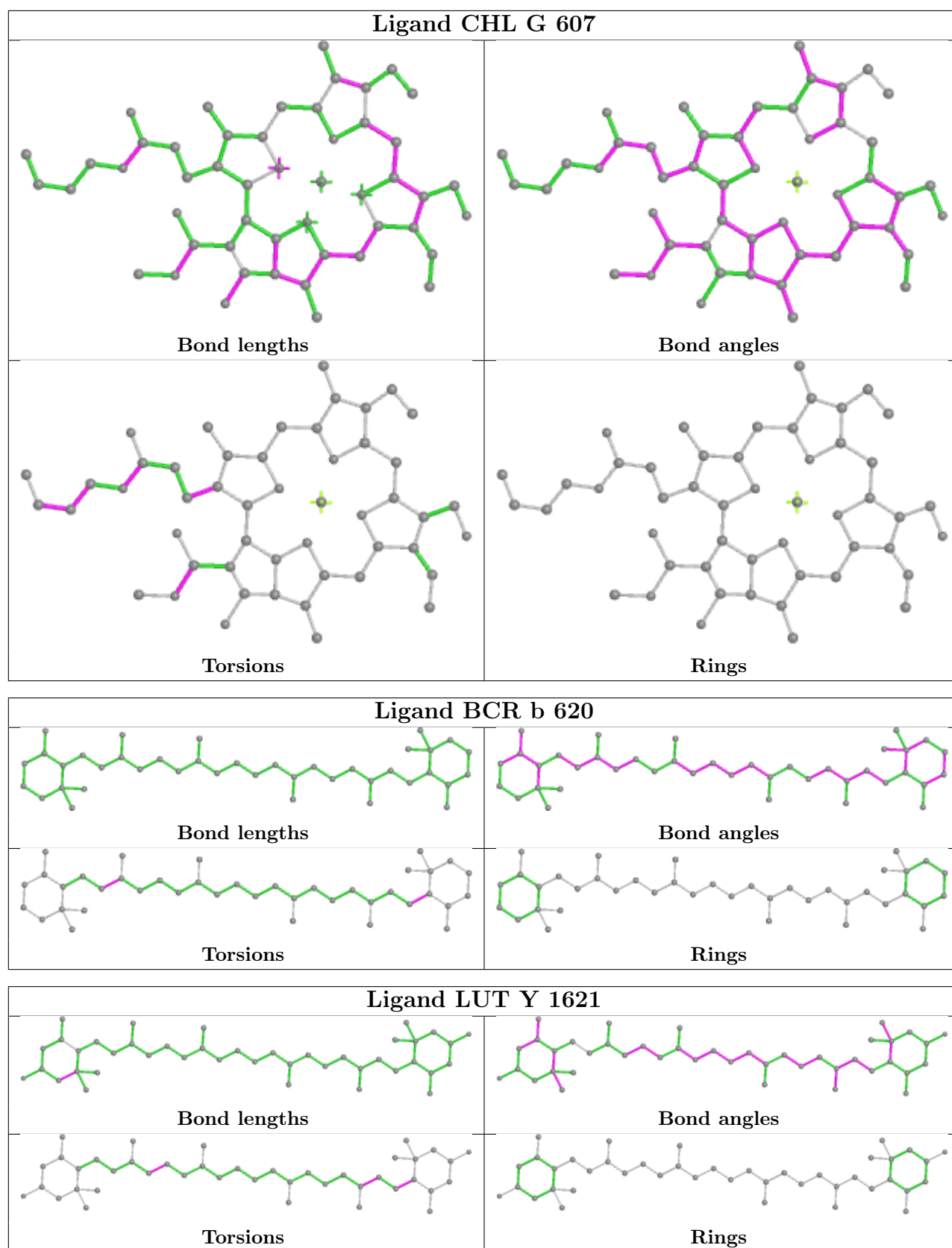
Ligand NEX Y 1623

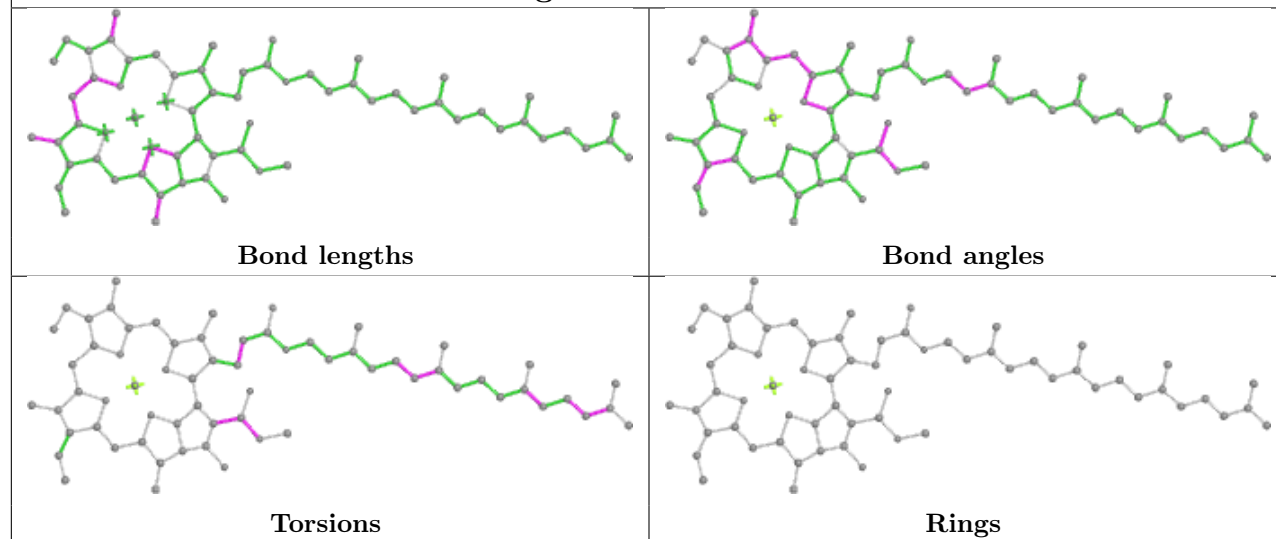
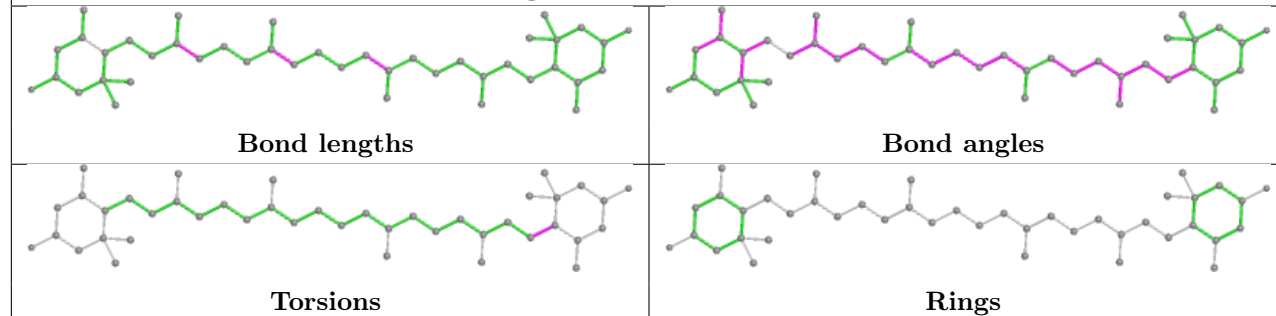




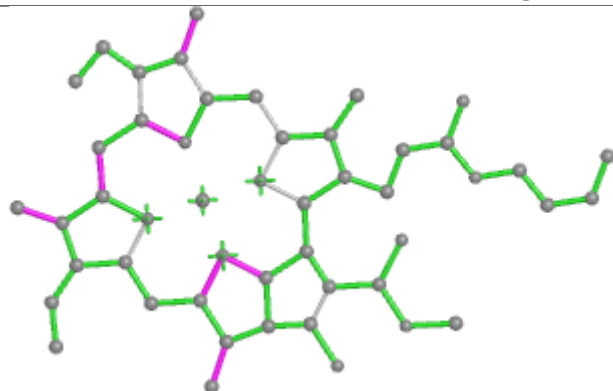
Ligand CLA g 604



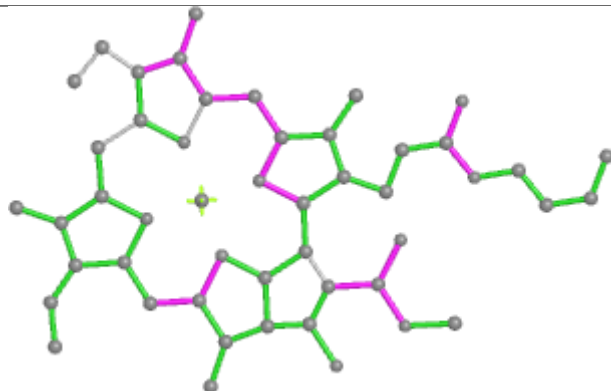


Ligand CLA b 607**Ligand LUT Y 1620**

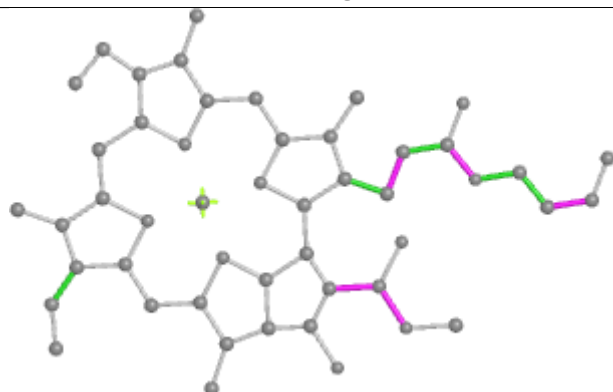
Ligand CLA S 602



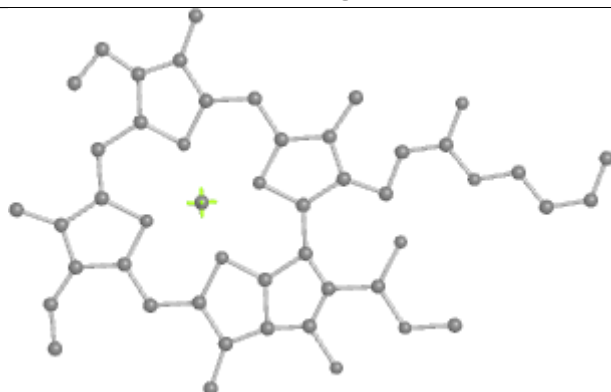
Bond lengths



Bond angles

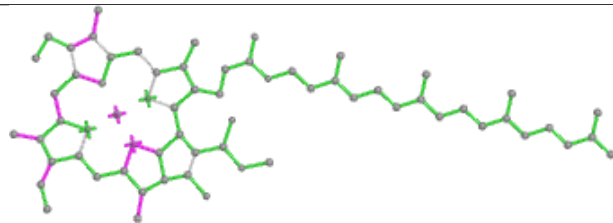


Torsions

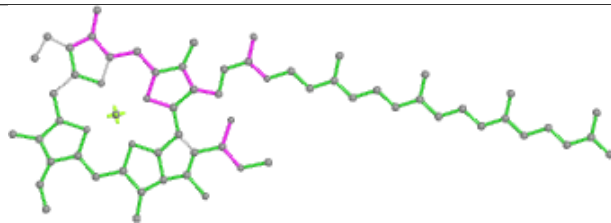


Rings

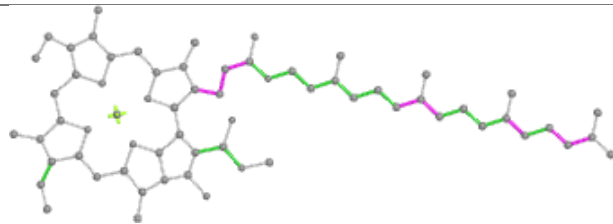
Ligand CLA N 603



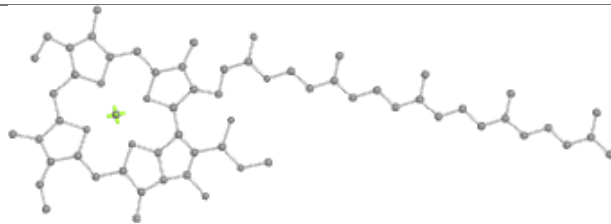
Bond lengths



Bond angles

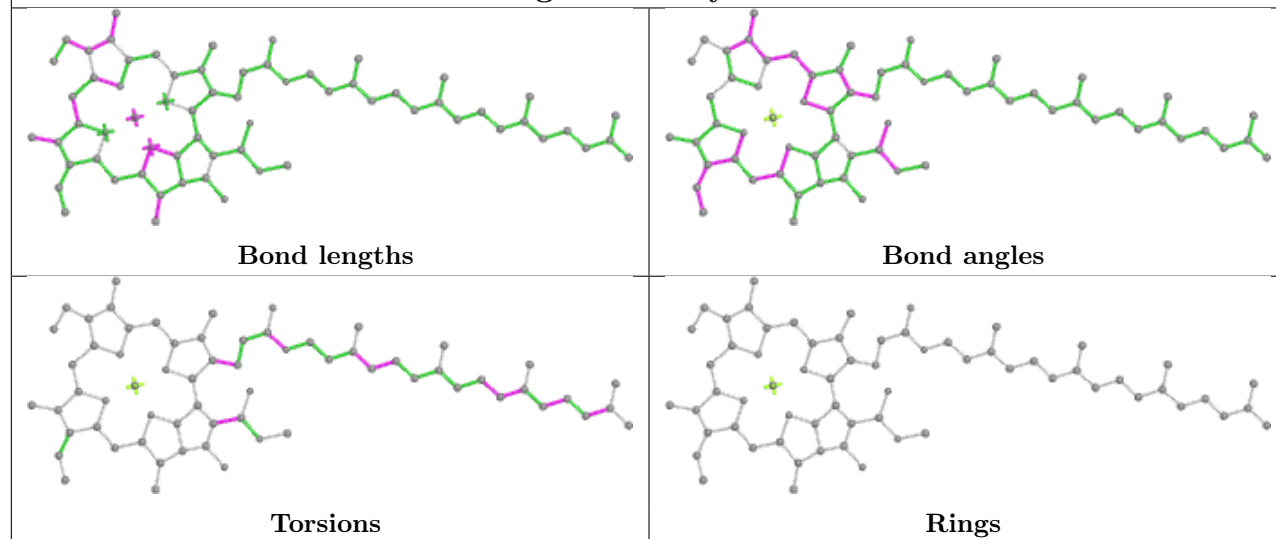


Torsions

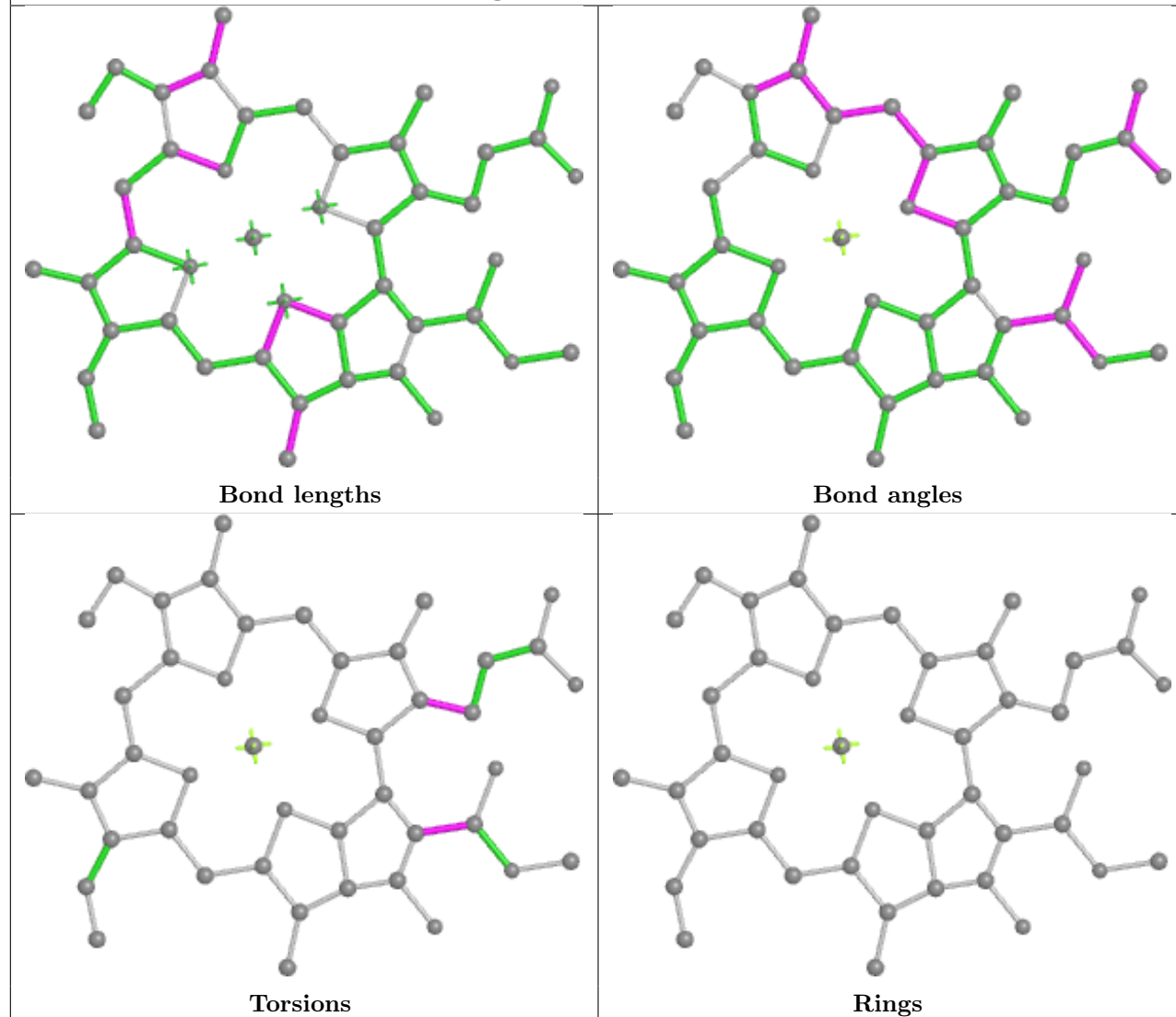


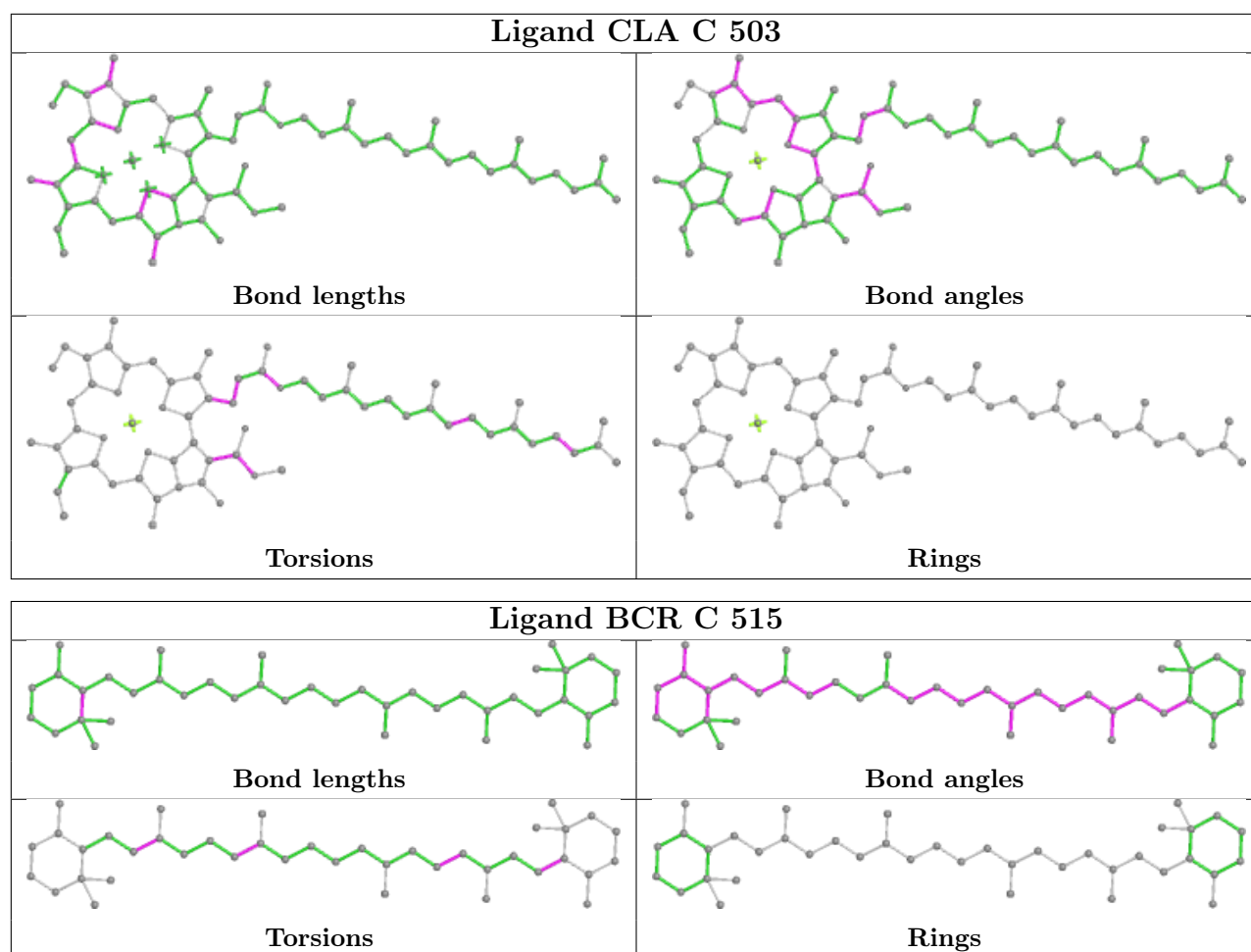
Rings

Ligand CLA y 603

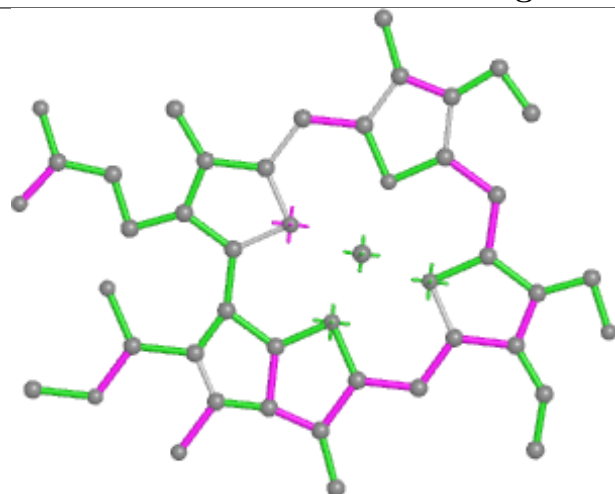


Ligand CLA G 611

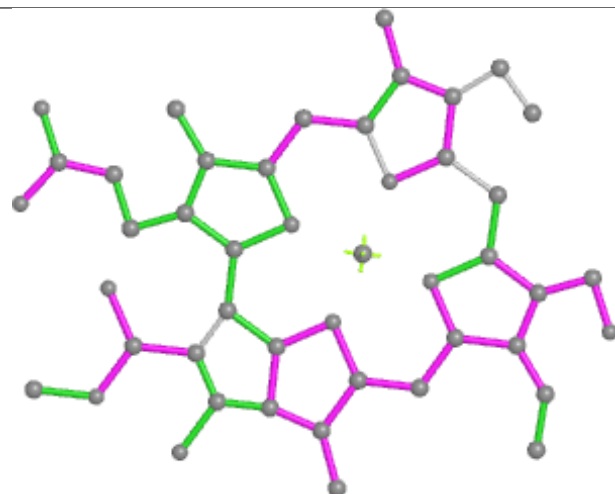




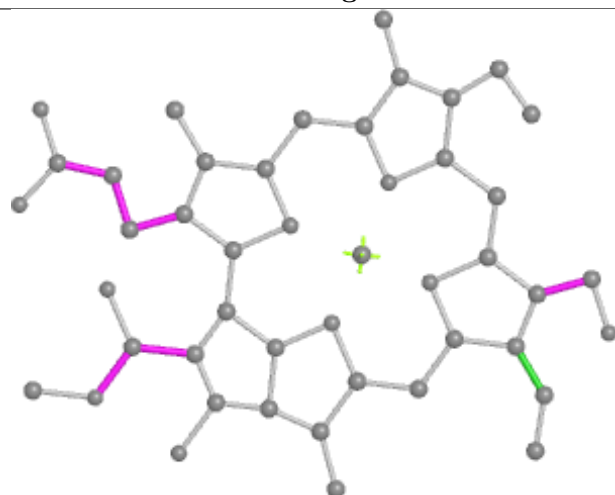
Ligand CHL Y 605



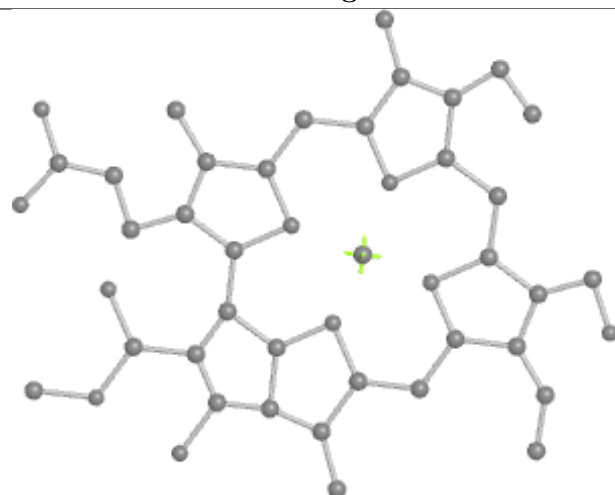
Bond lengths



Bond angles

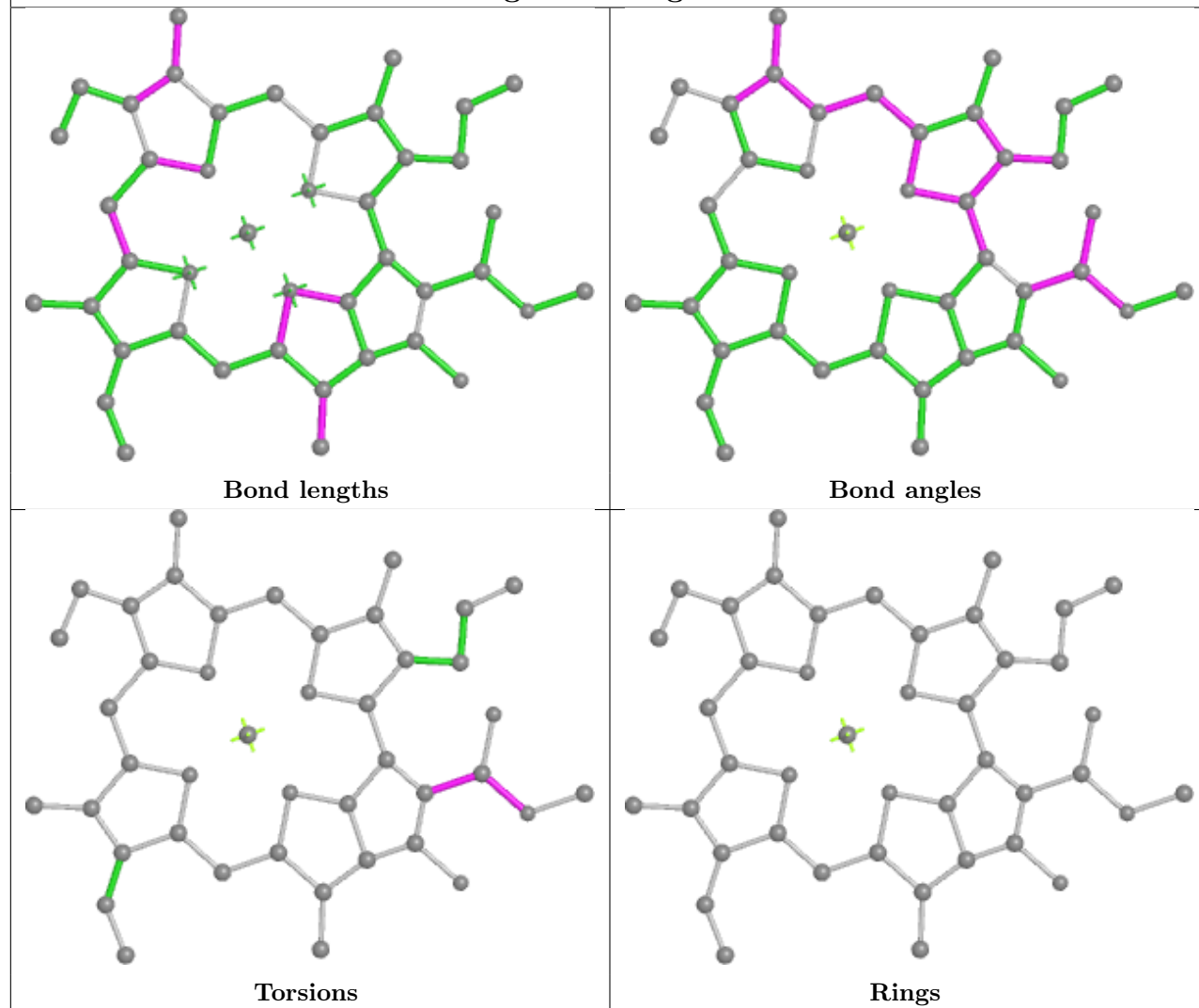


Torsions

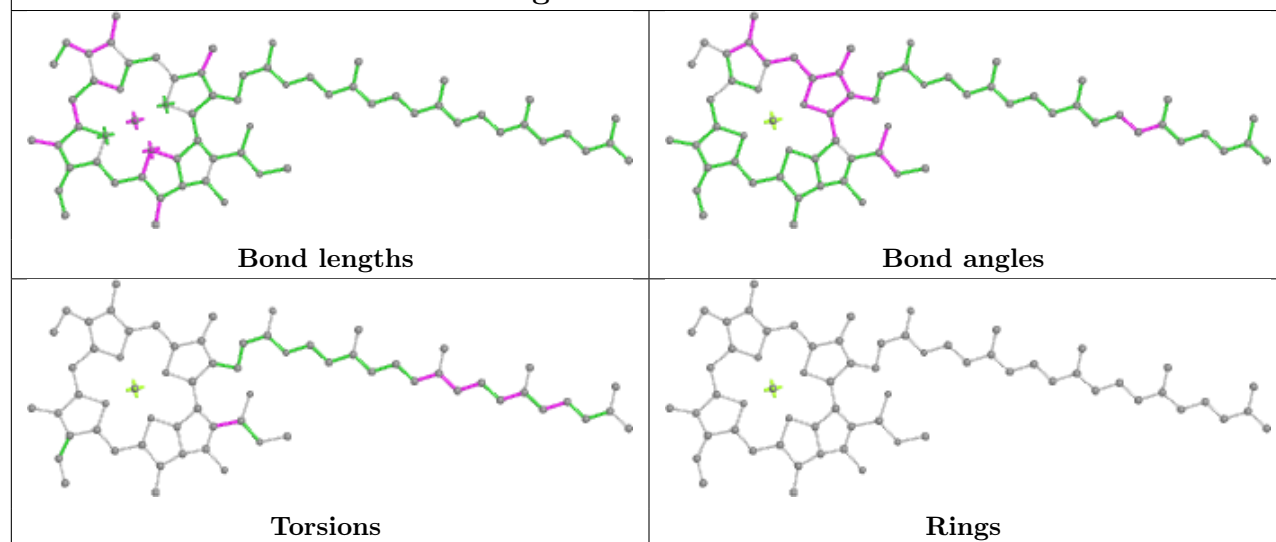


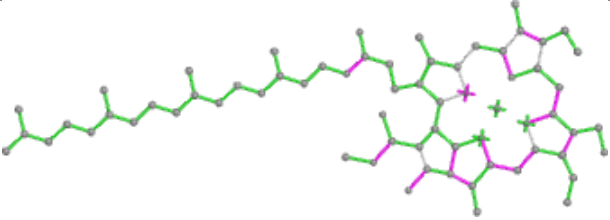
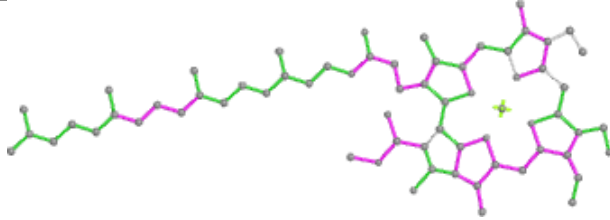
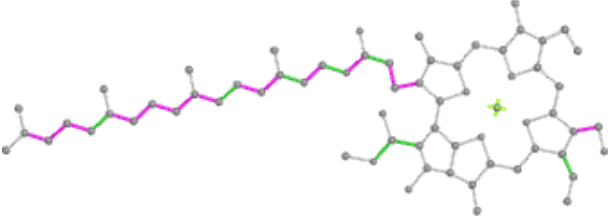
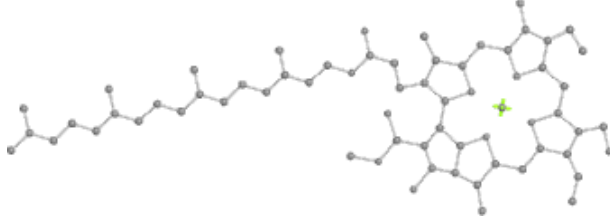
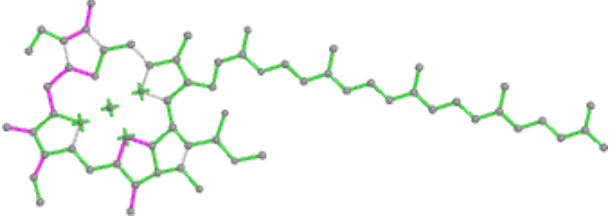
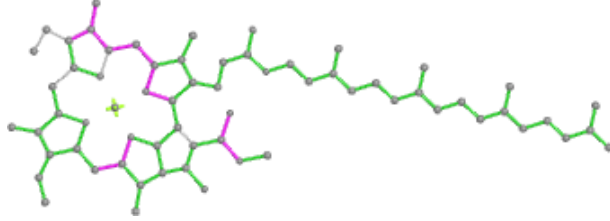
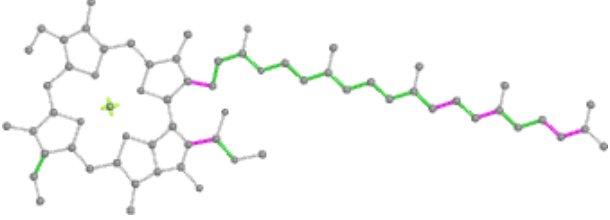
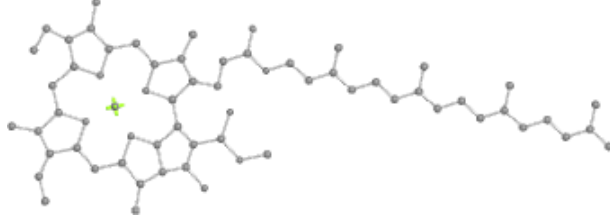
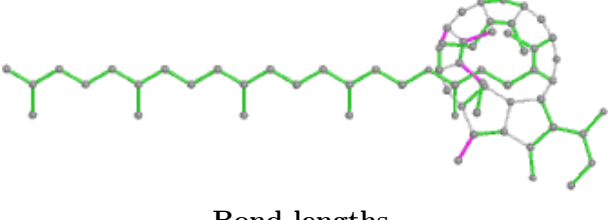
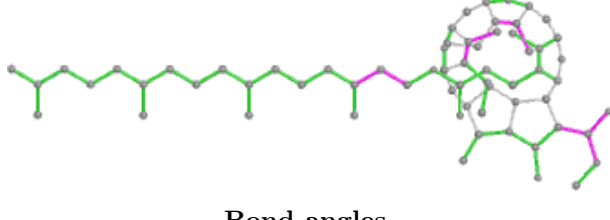
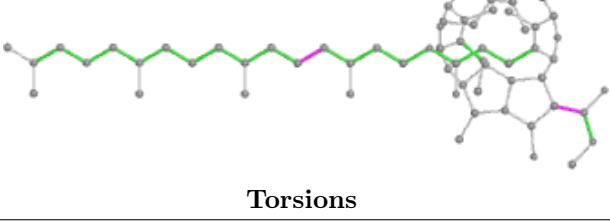
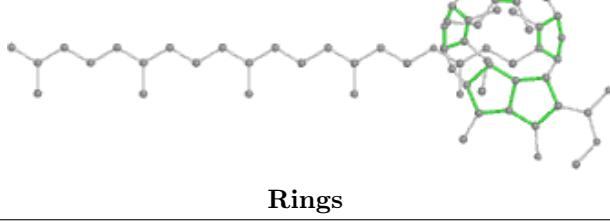
Rings

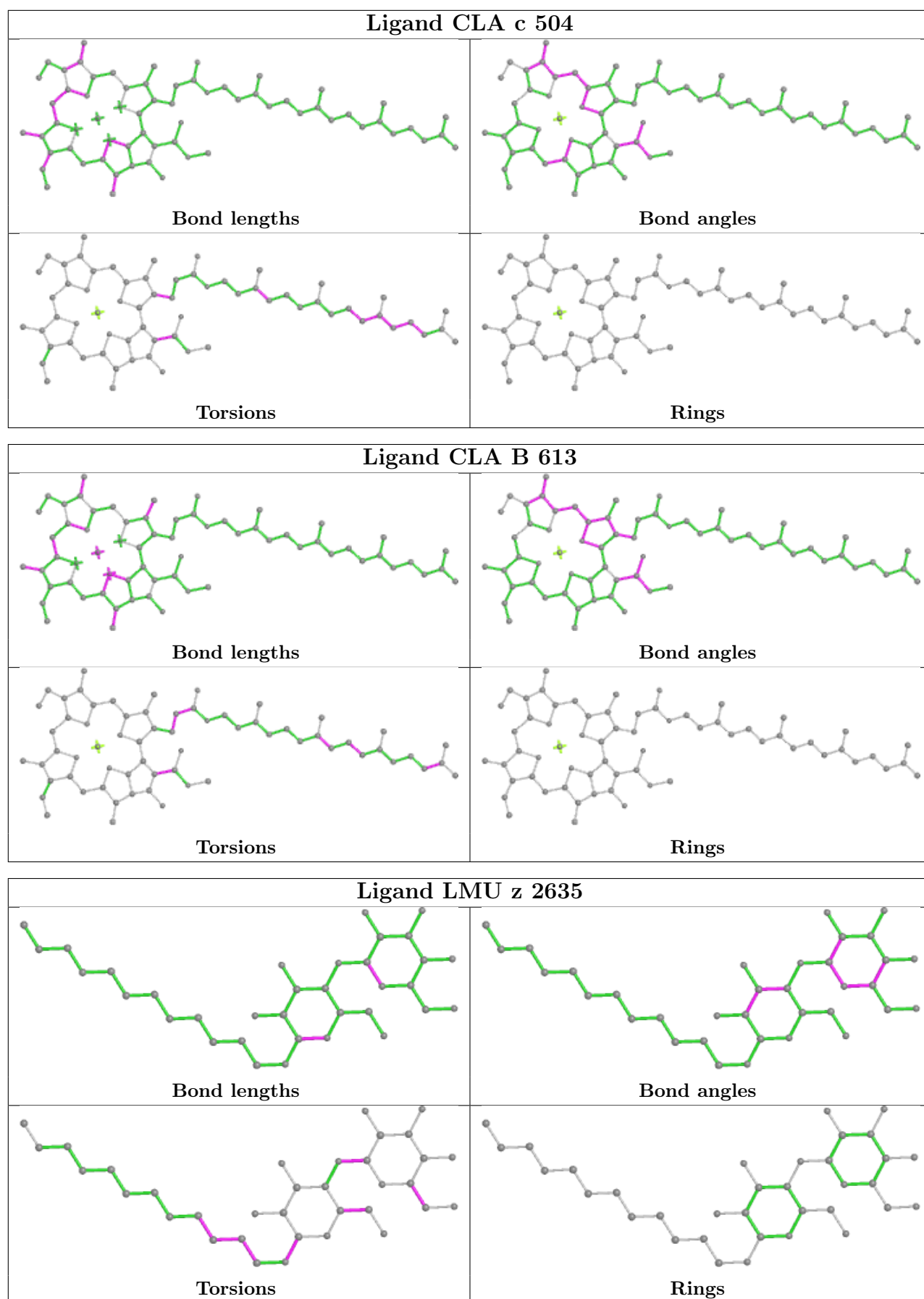
Ligand CLA g 612



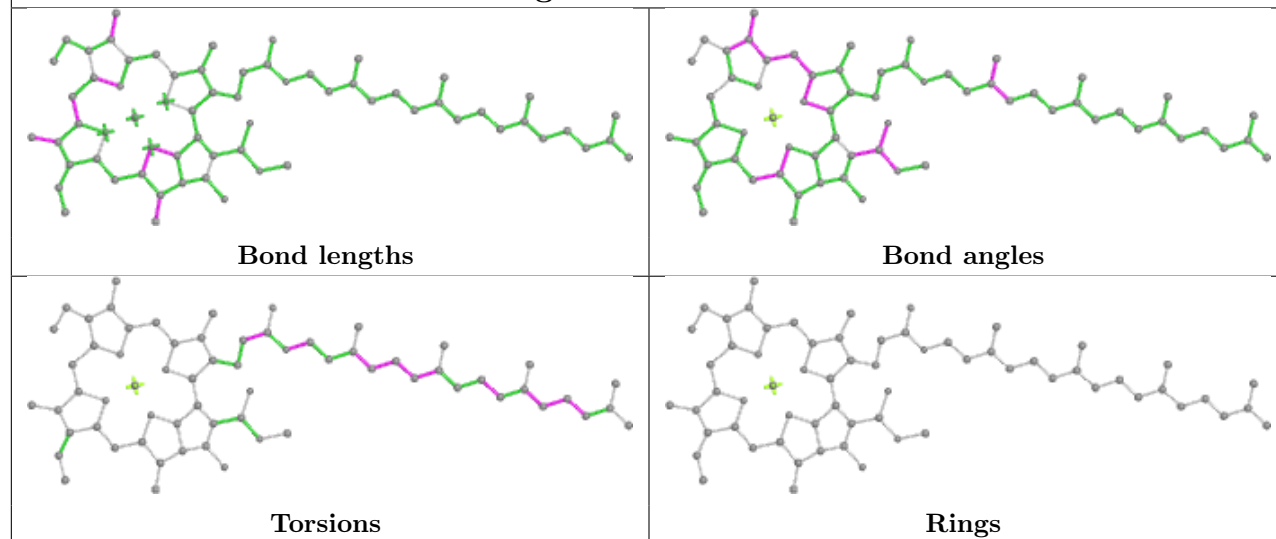
Ligand CLA C 509



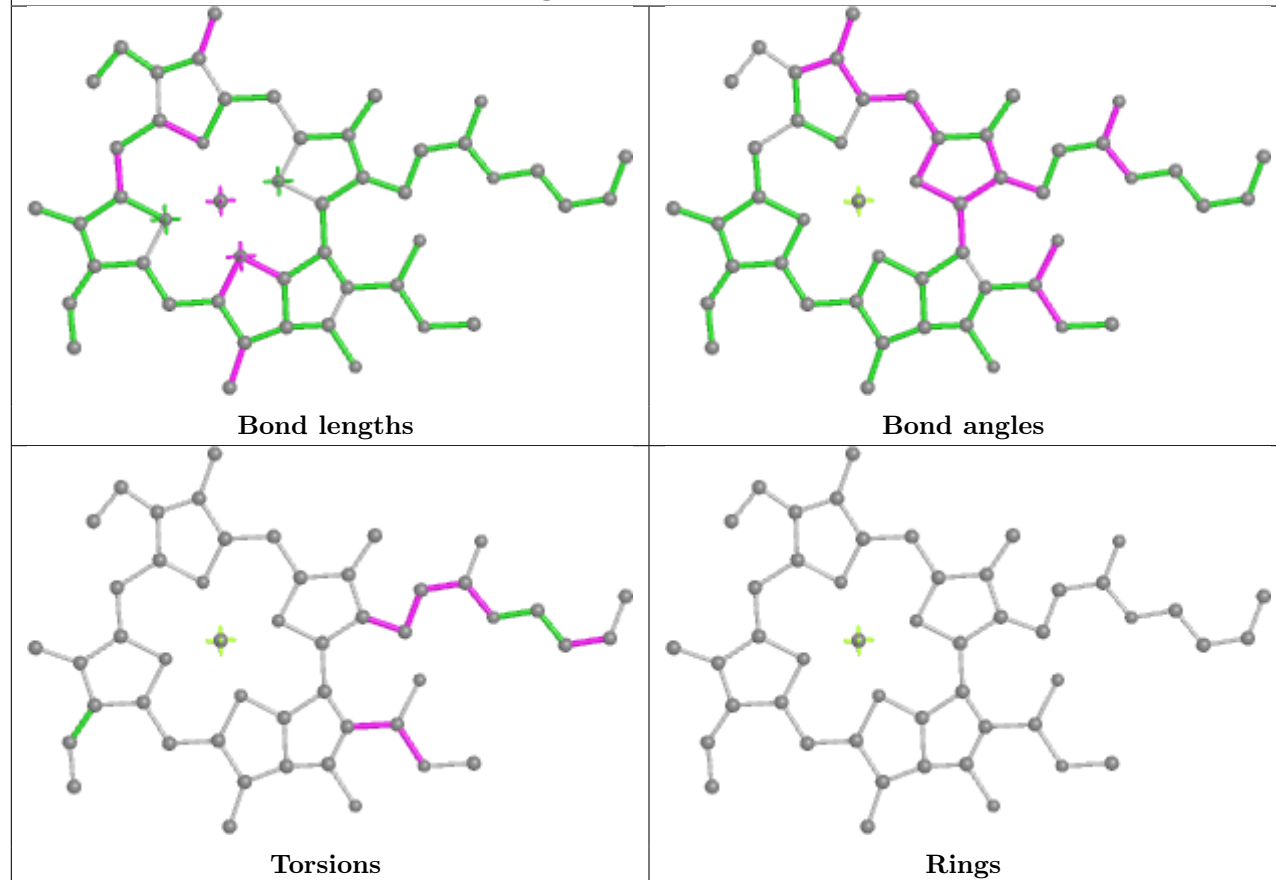
Ligand CHL Y 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO a 409	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



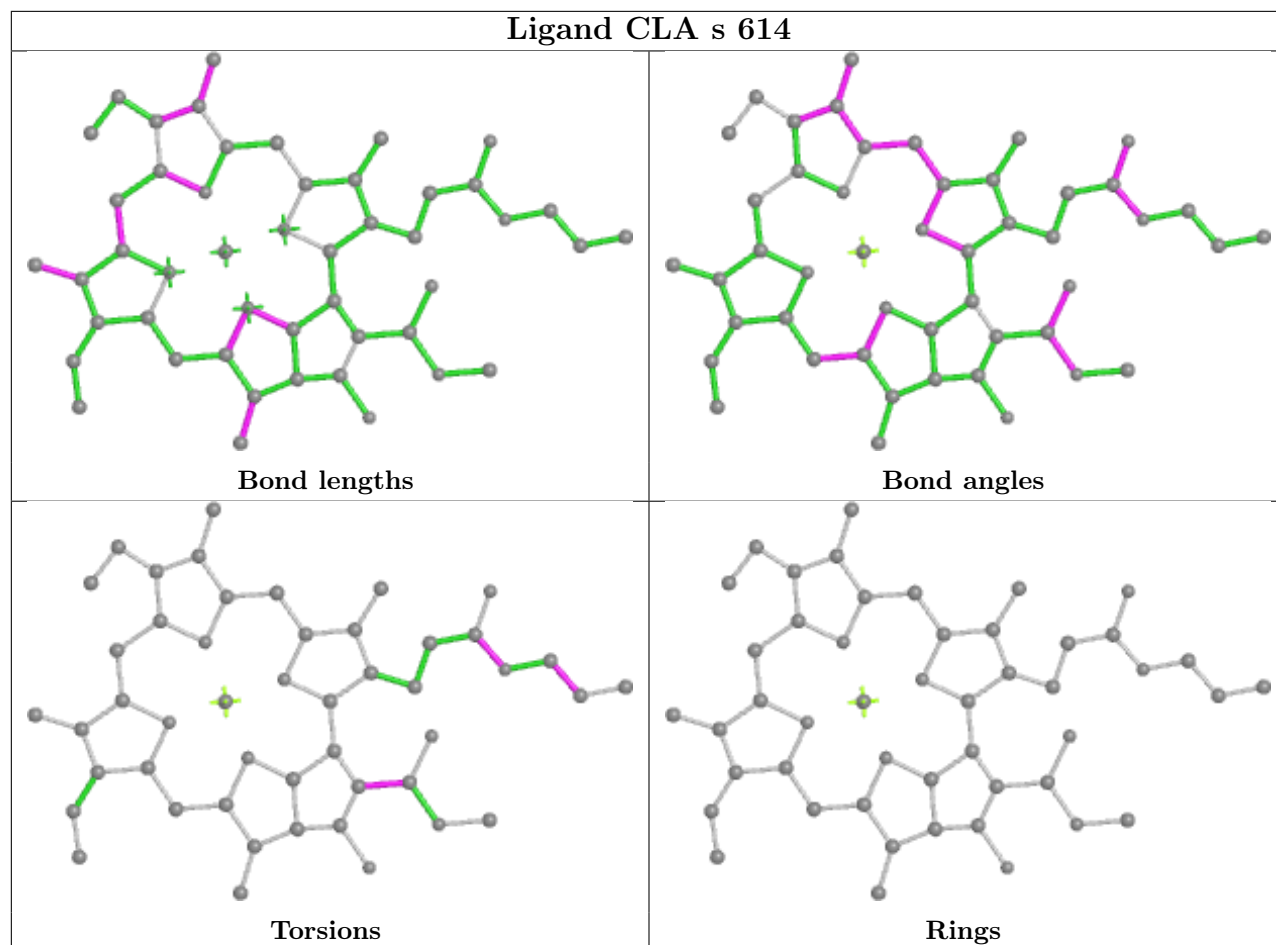
Ligand CLA b 603

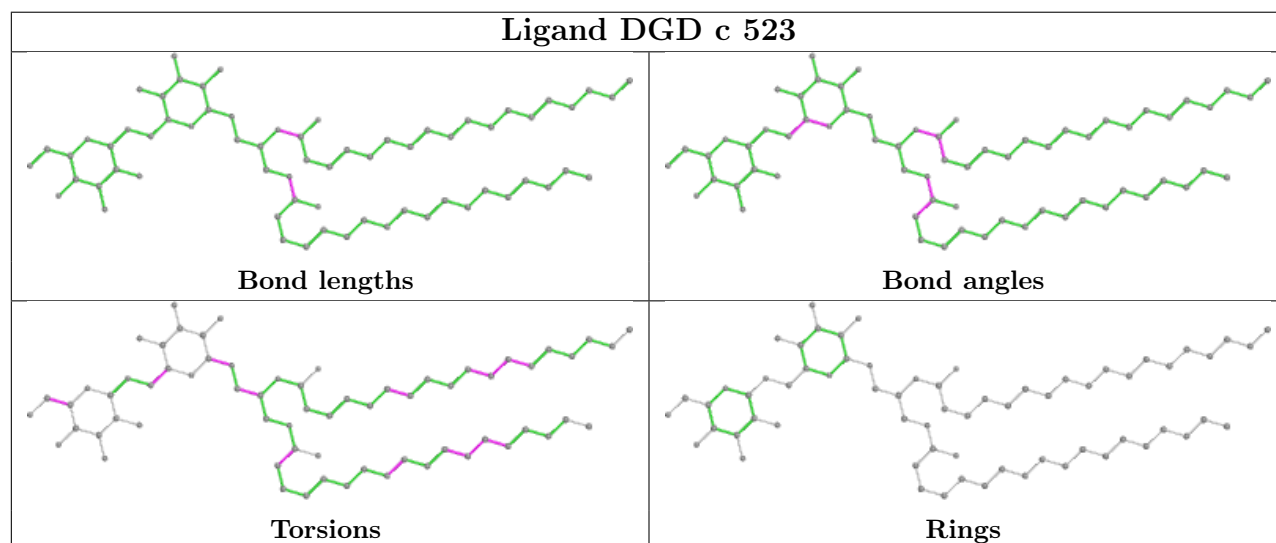
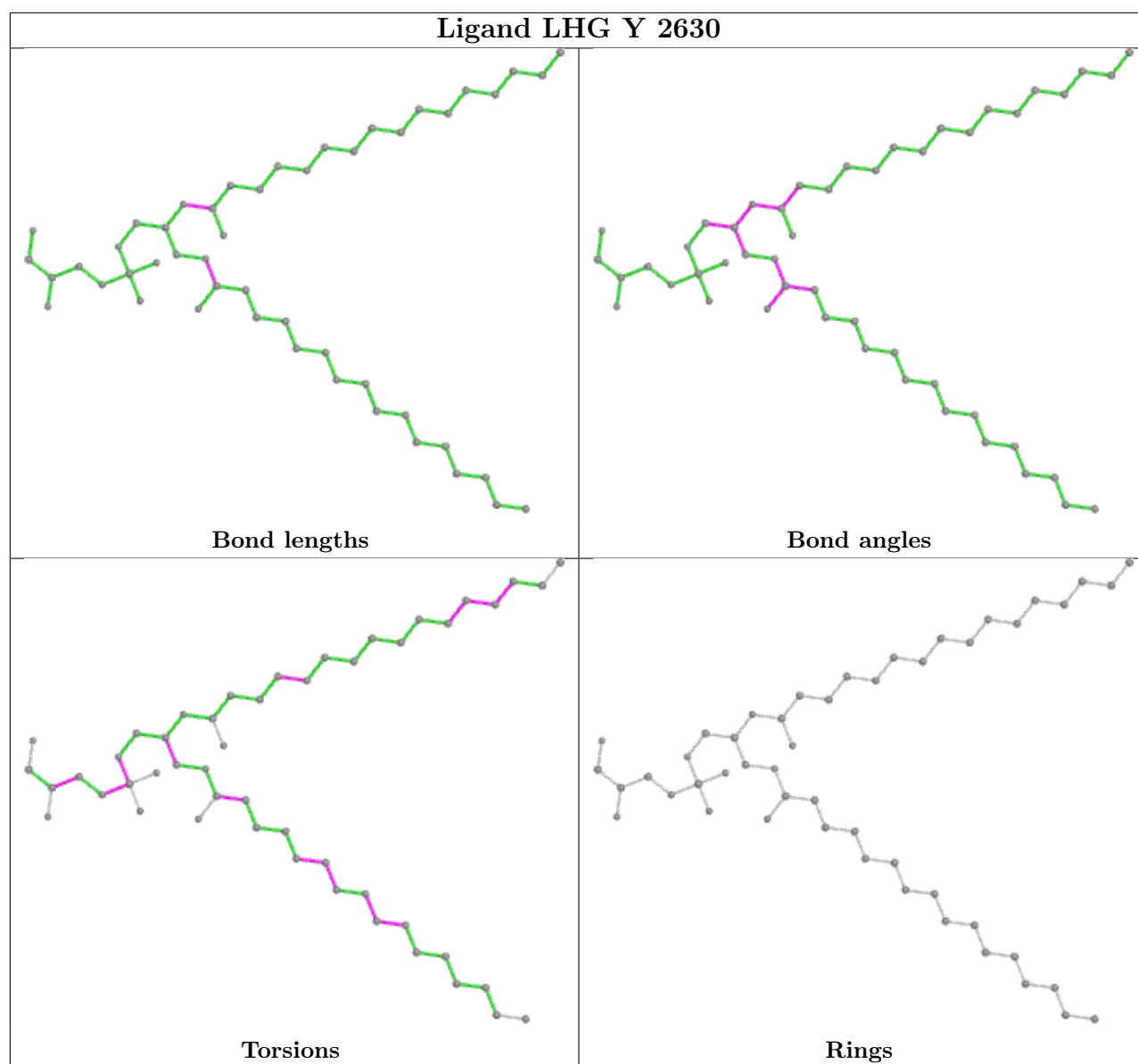


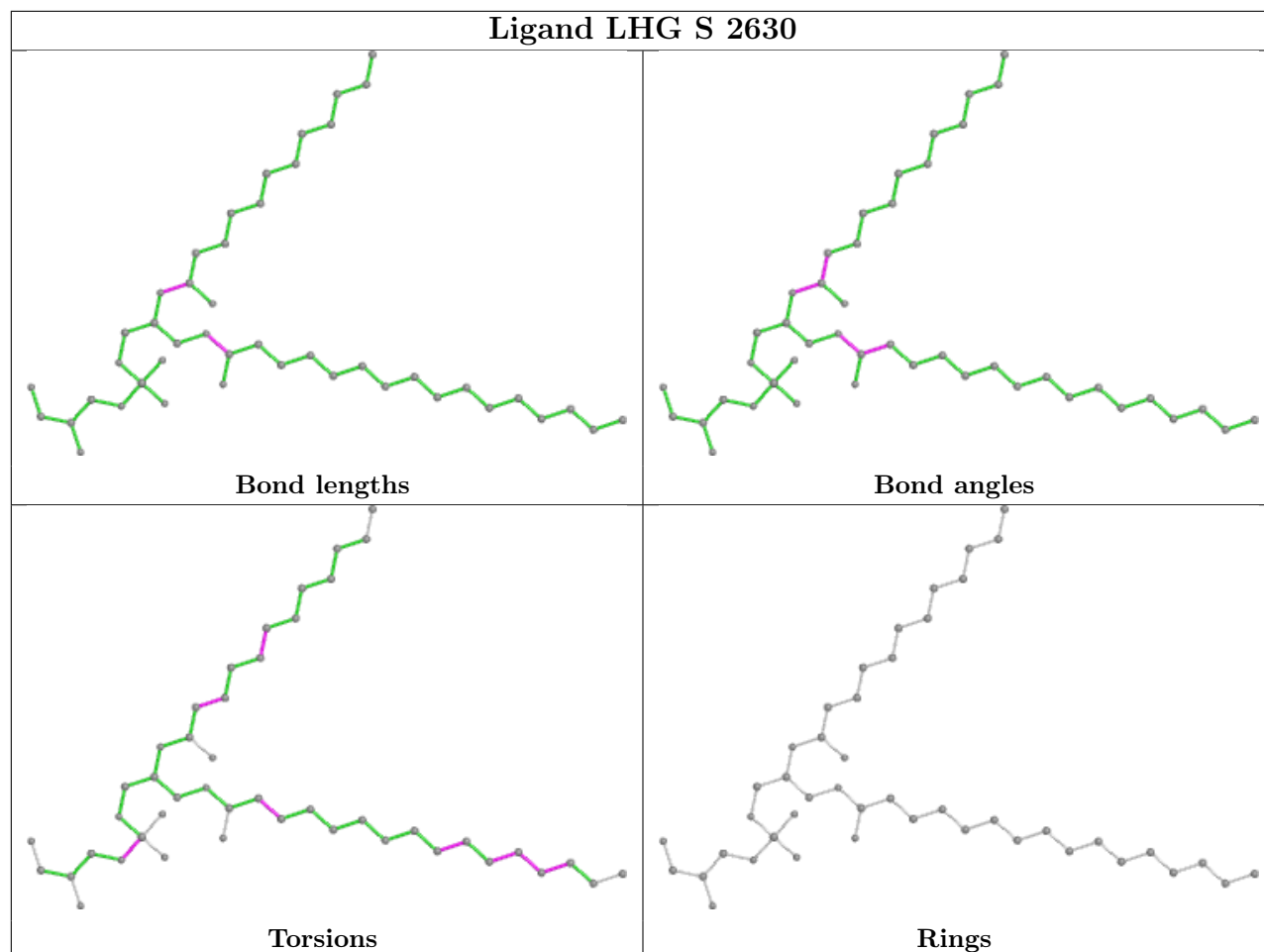
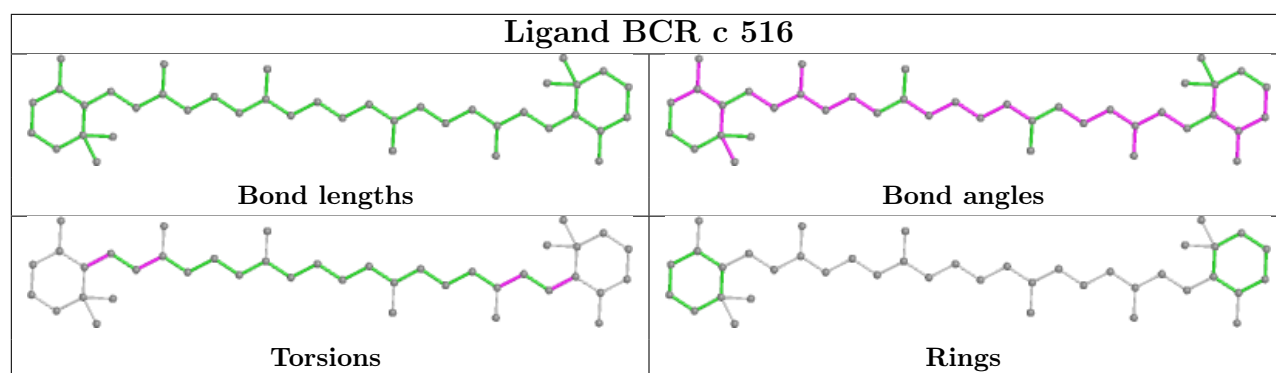
Ligand CLA r 603

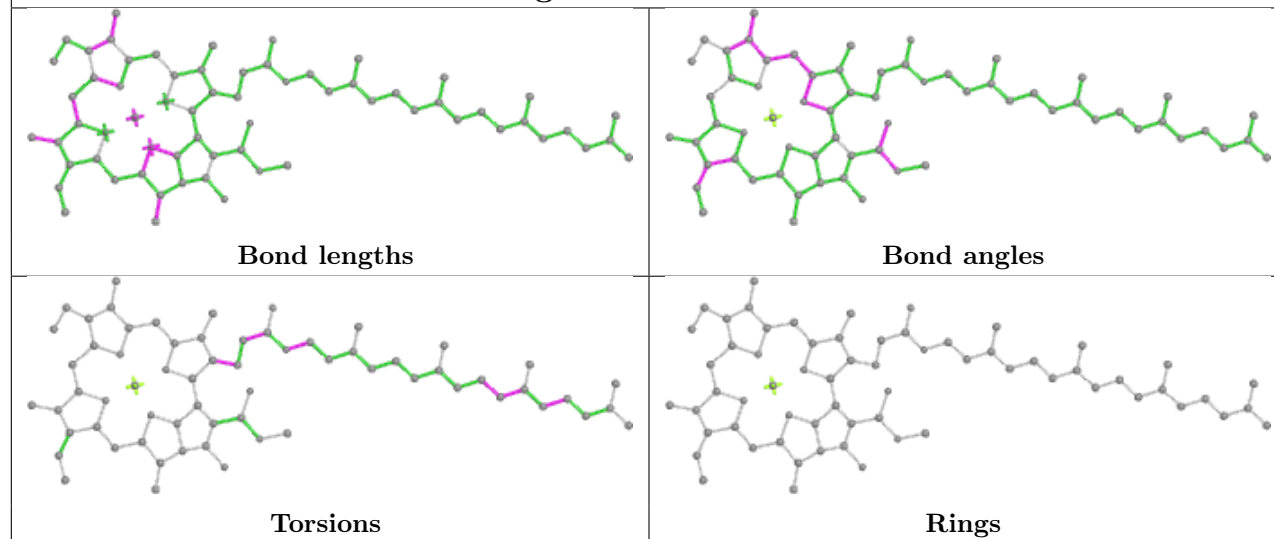
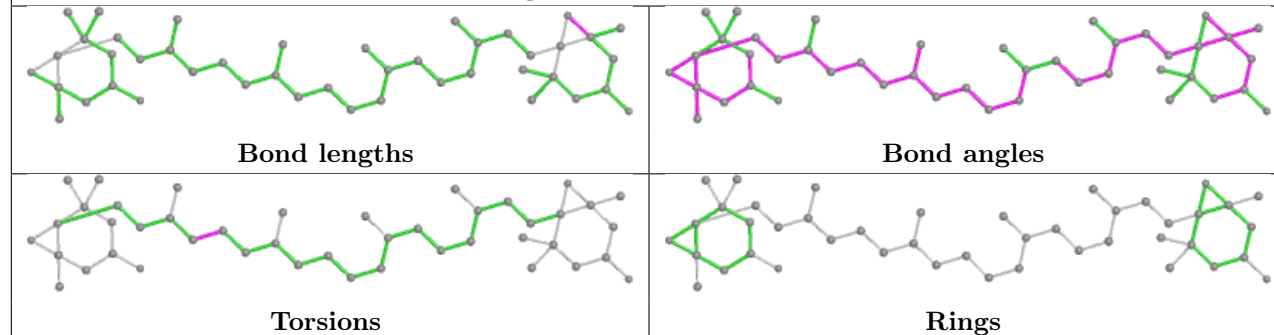
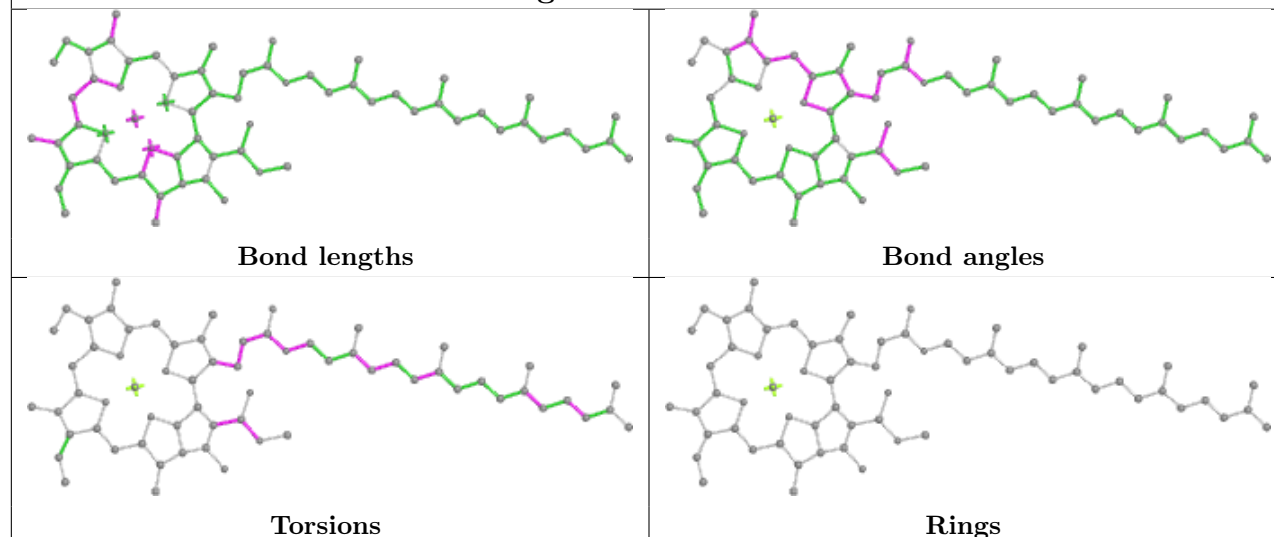


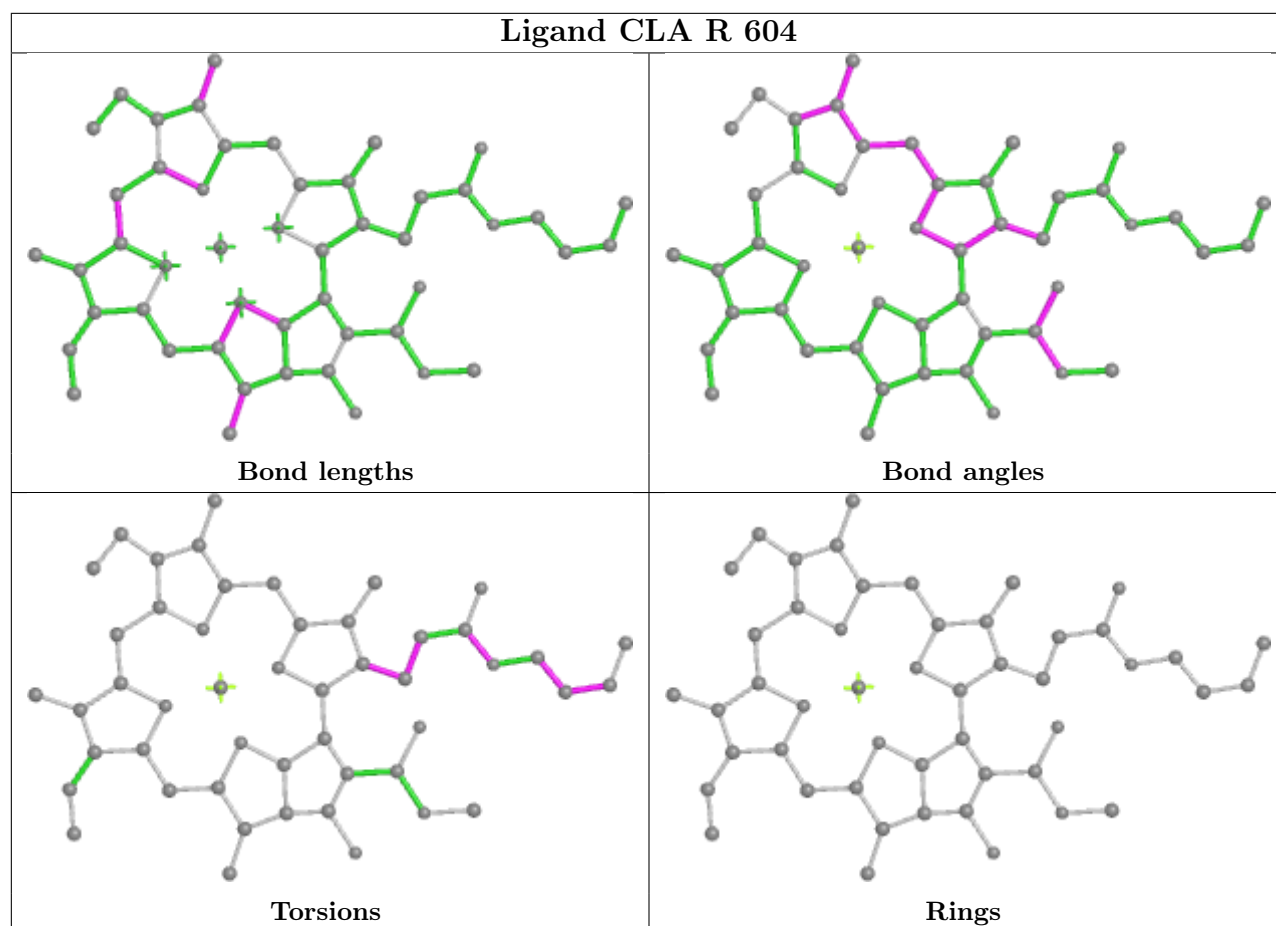
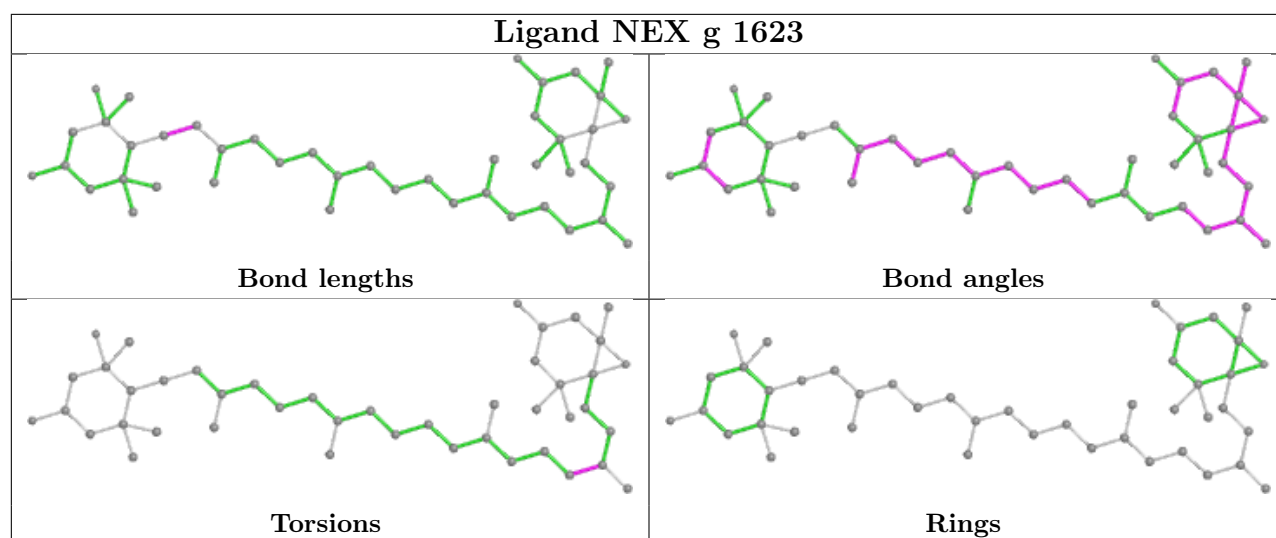
Ligand CLA s 614

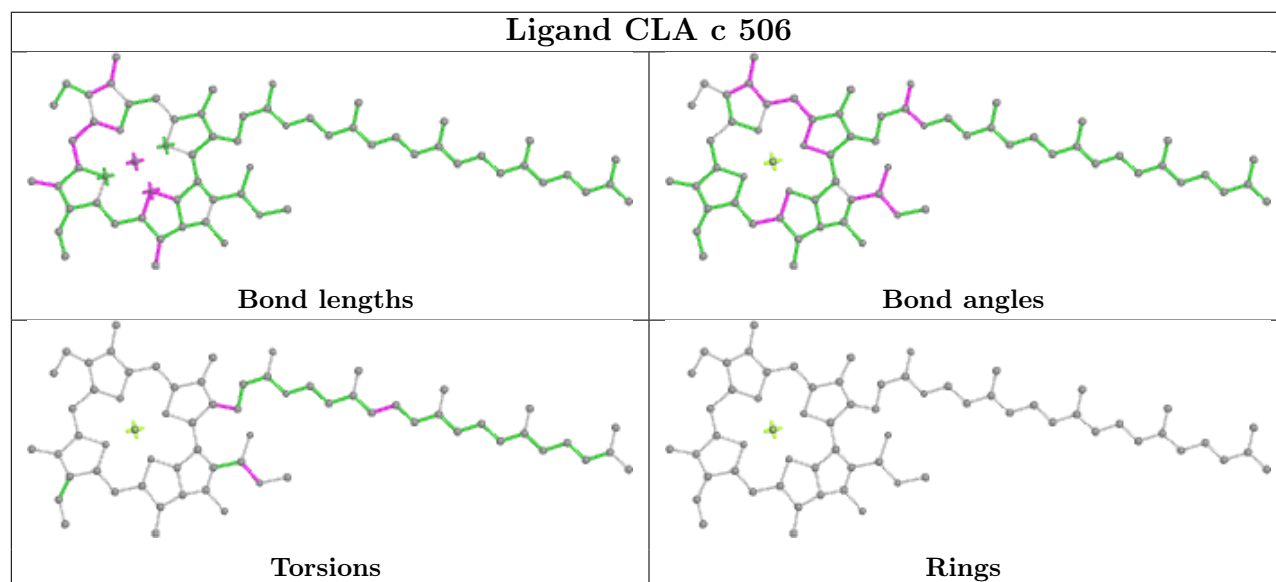
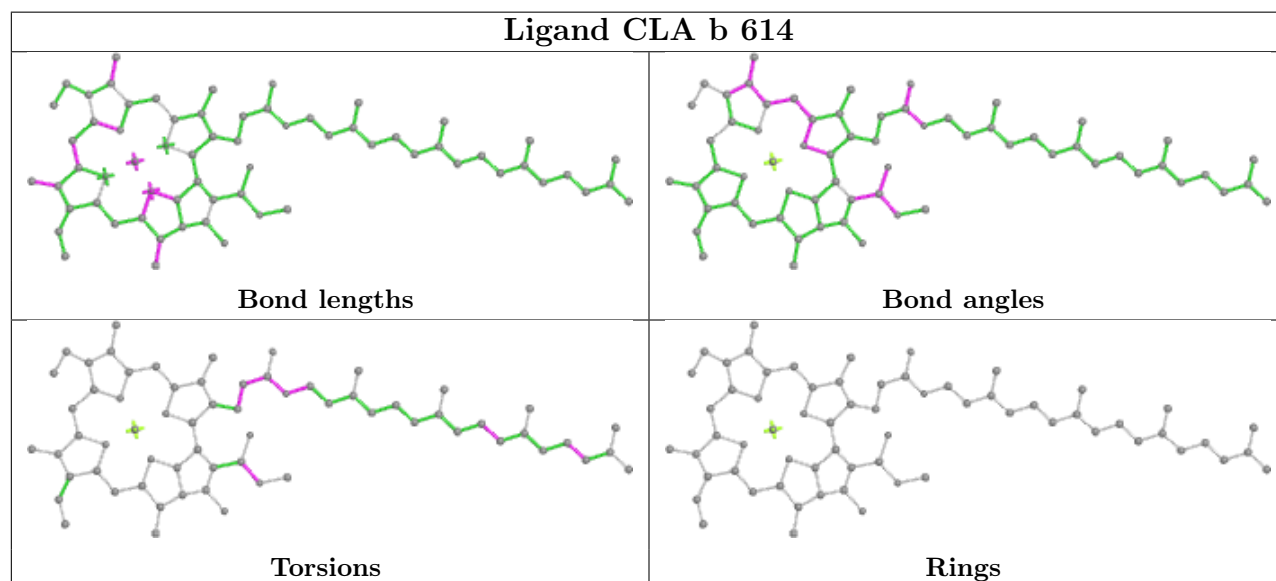
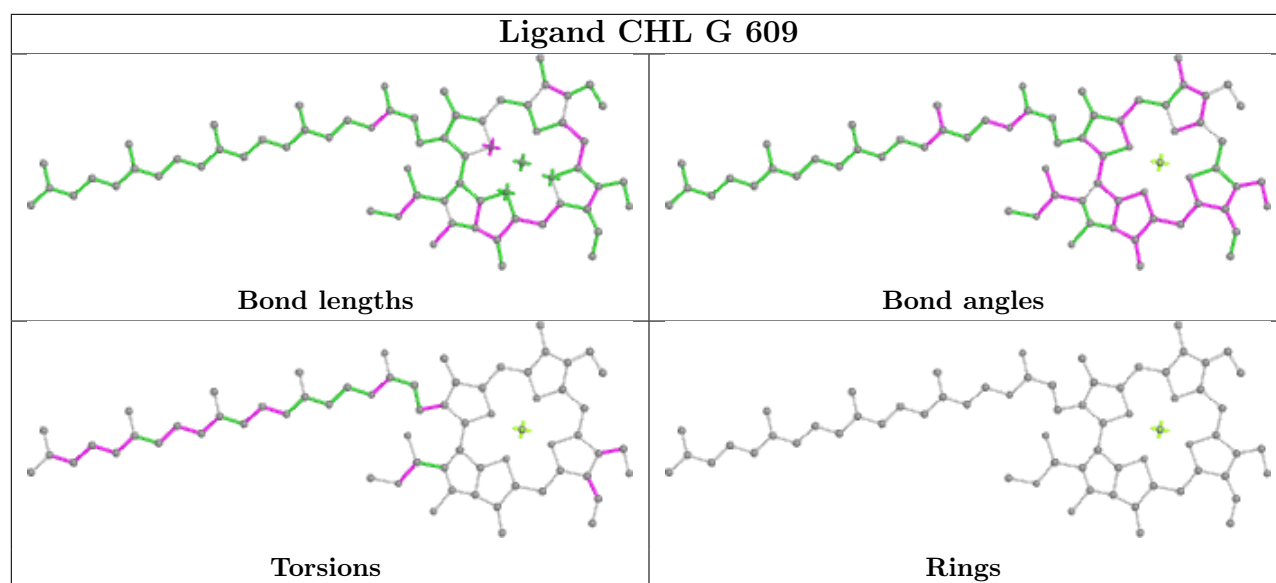


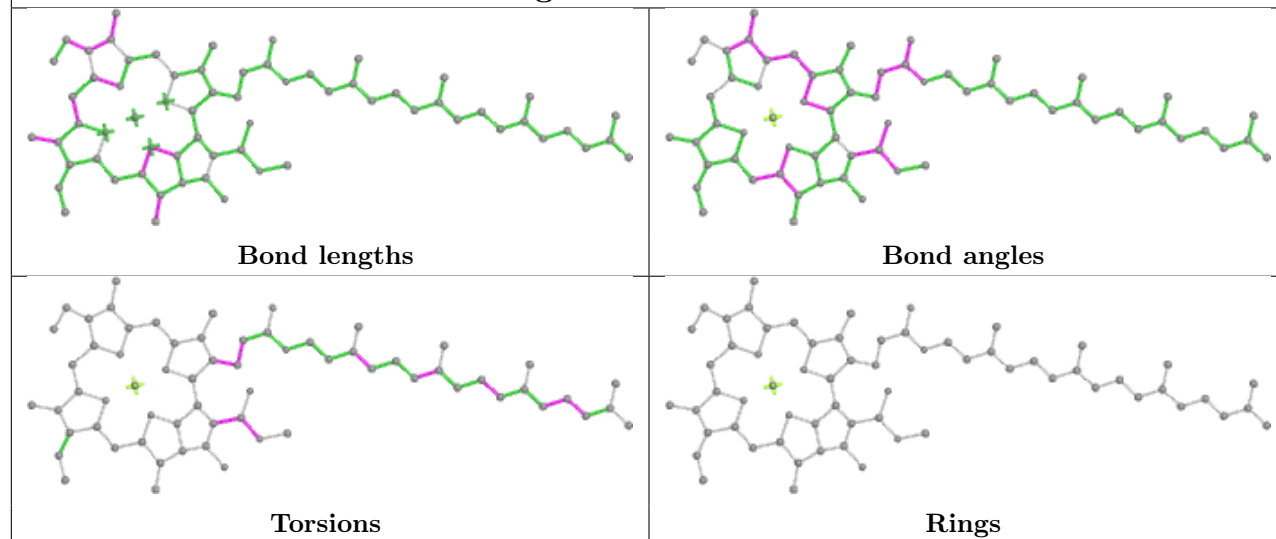
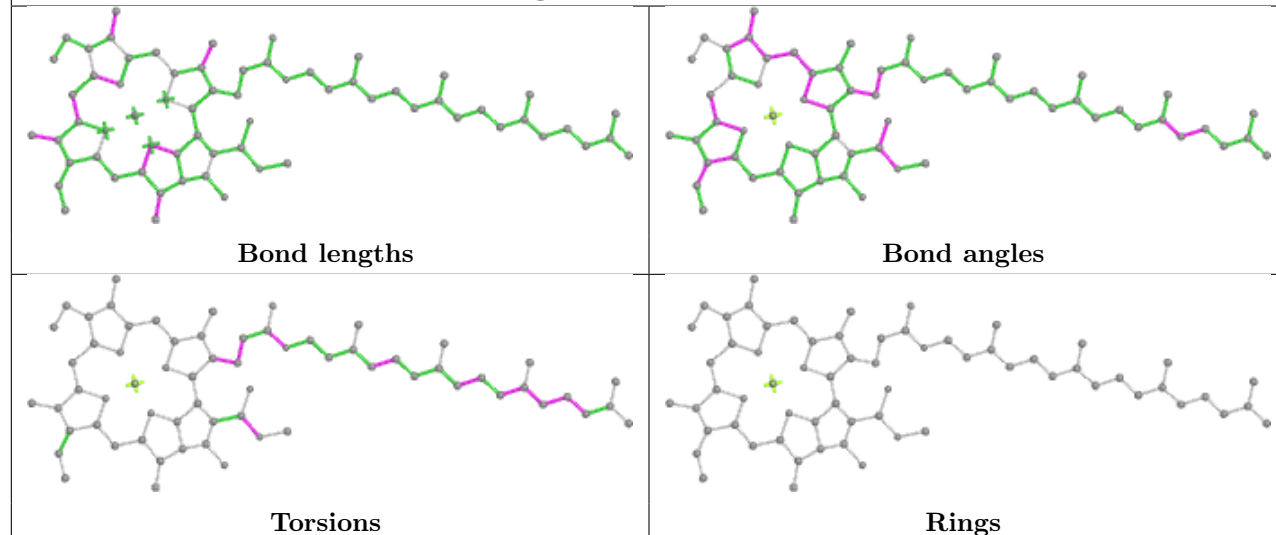
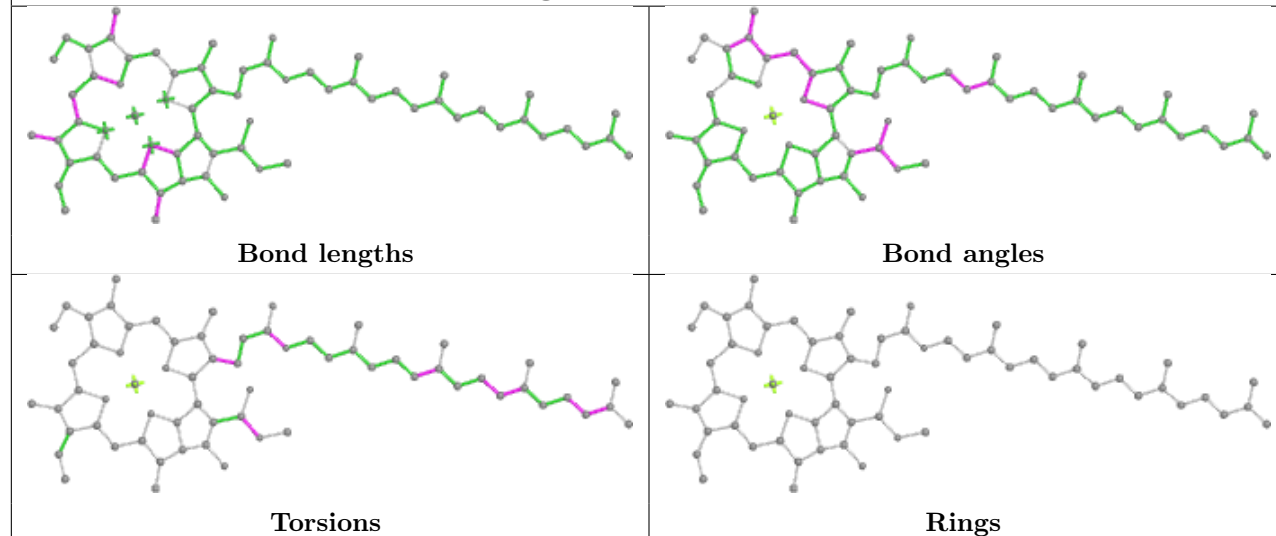


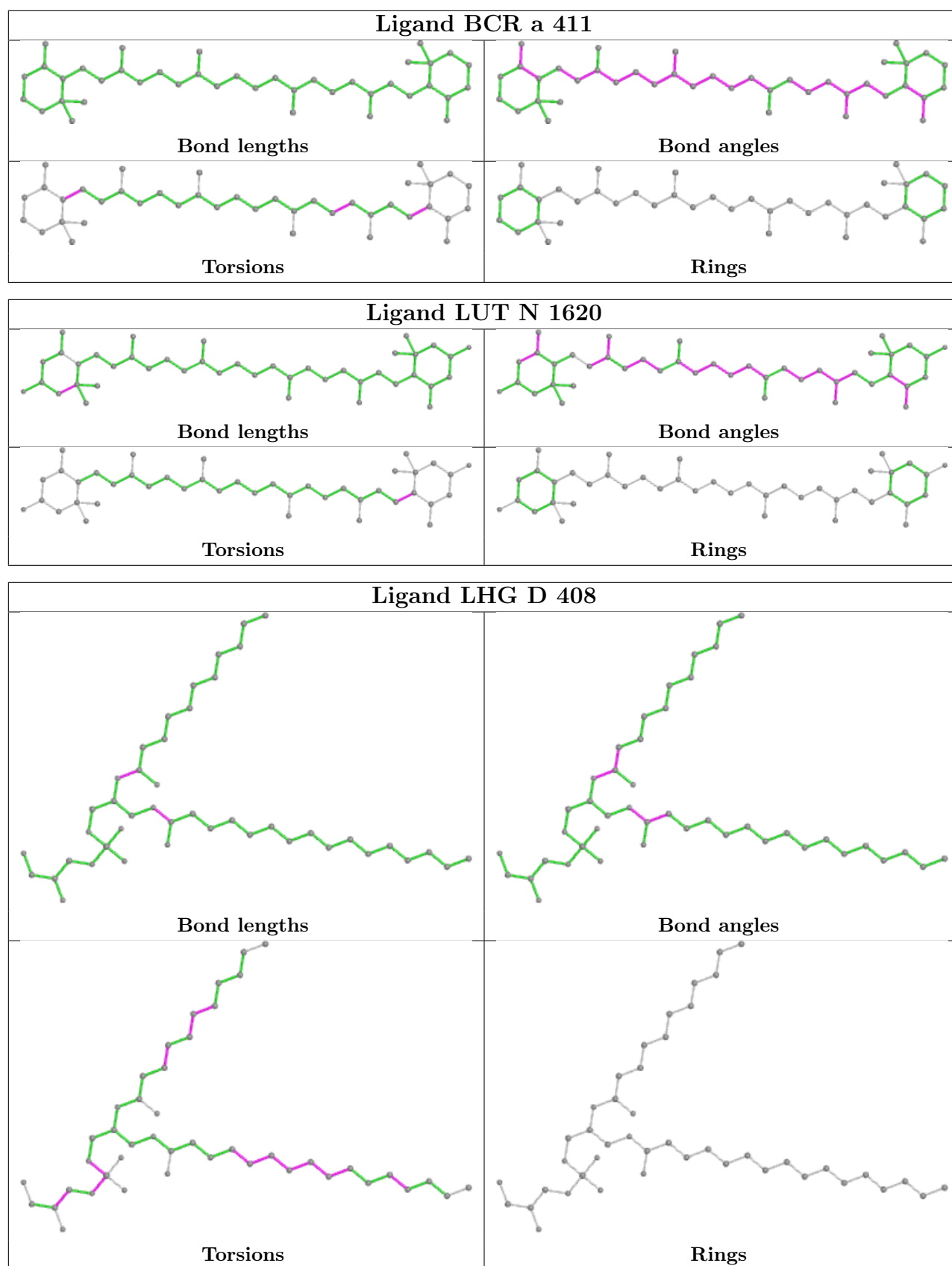


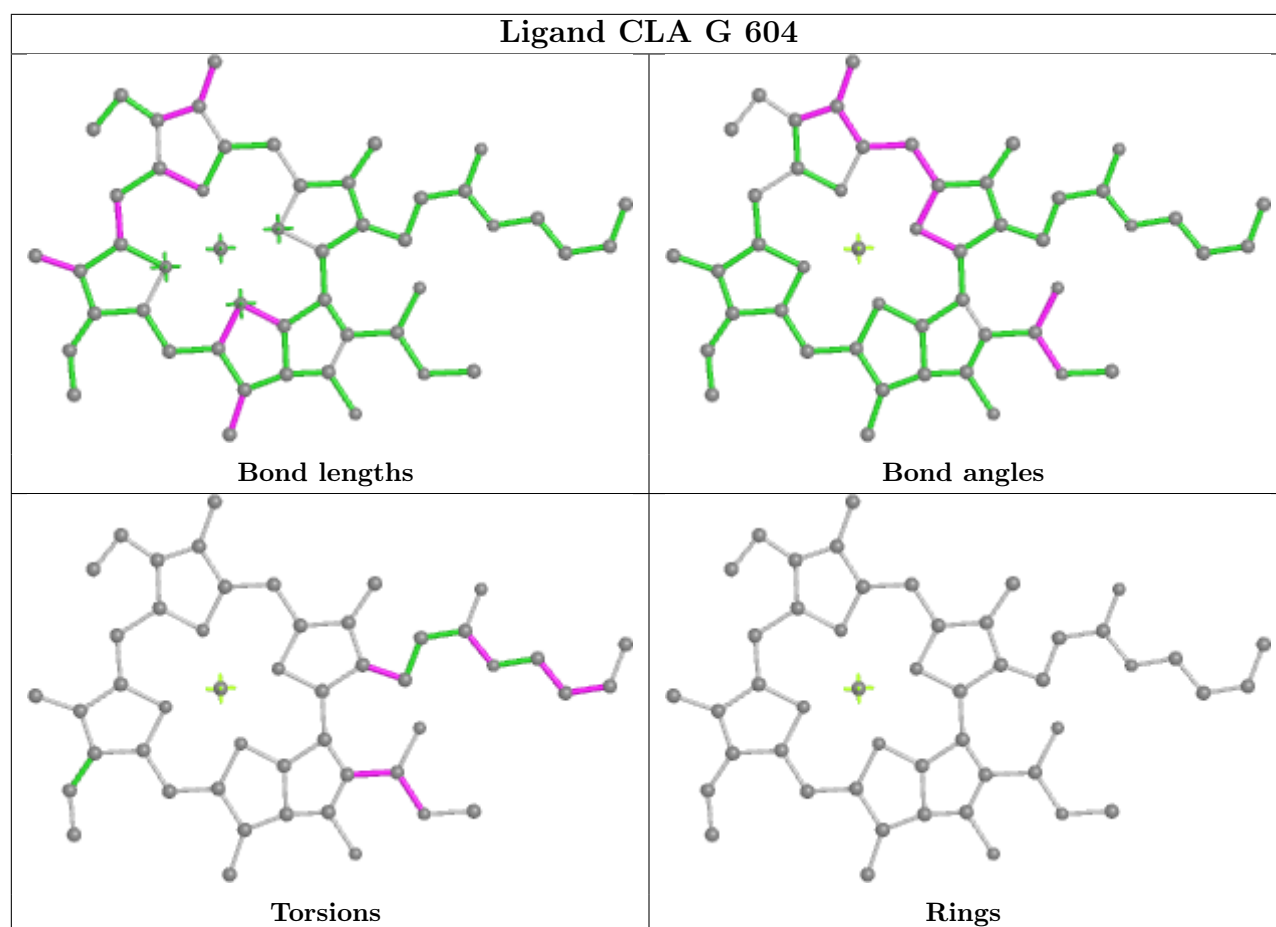
Ligand CLA d 402**Ligand XAT N 1622****Ligand CLA c 513**



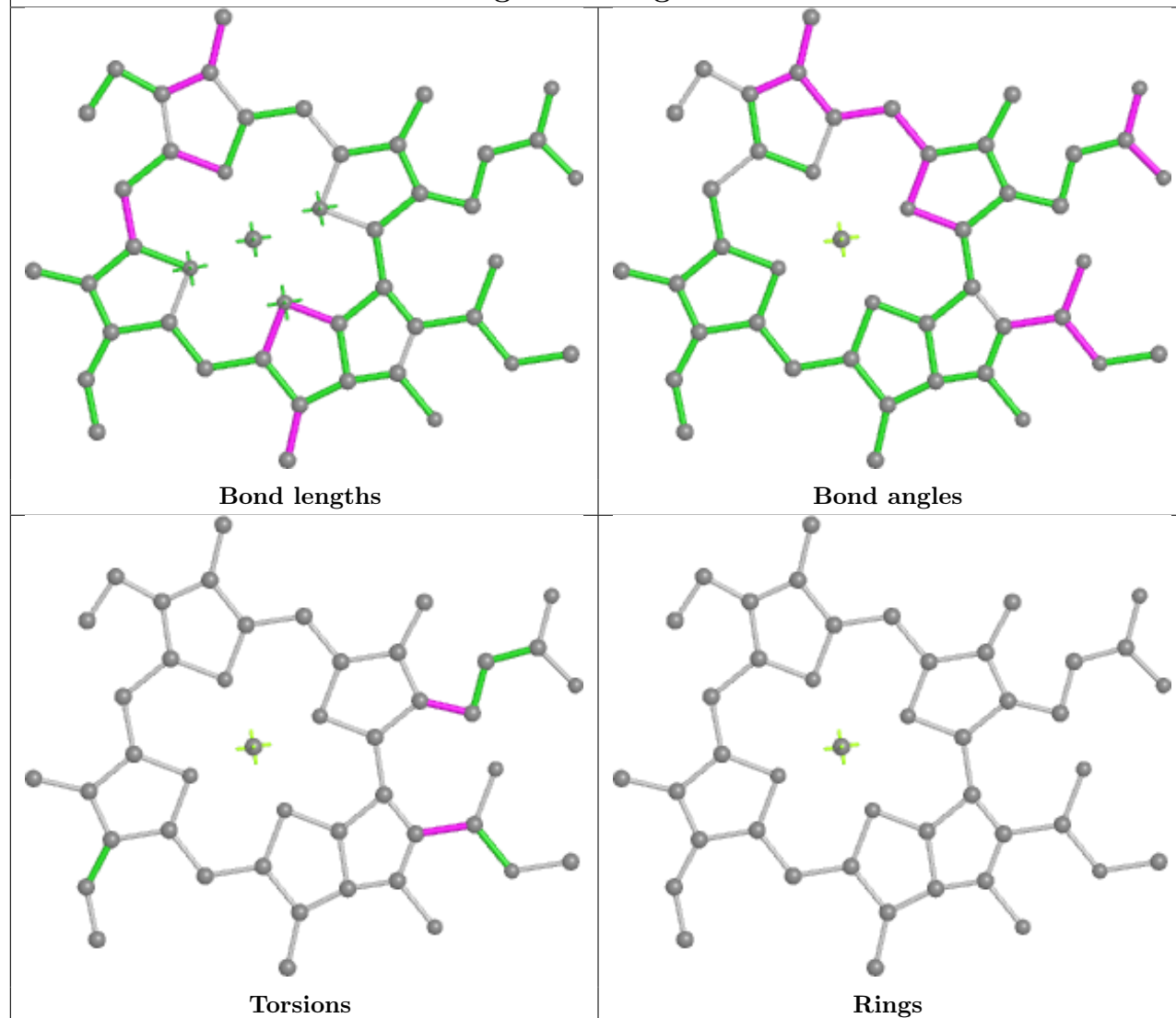


Ligand CLA b 604**Ligand CLA A 405****Ligand CLA c 508**

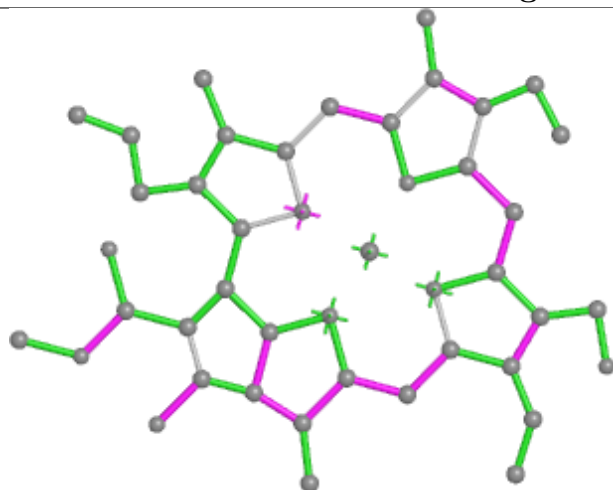




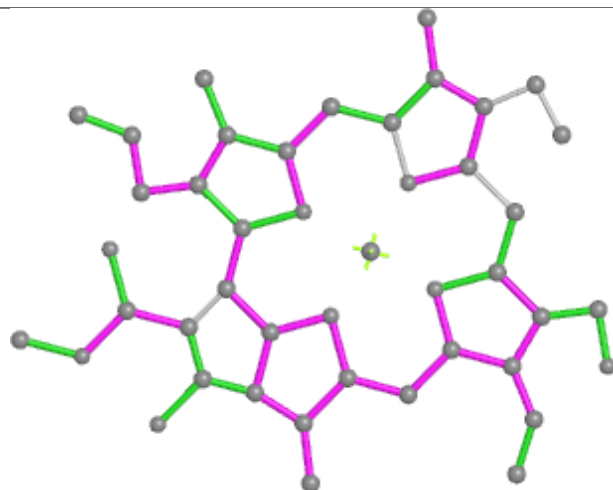
Ligand CLA g 611



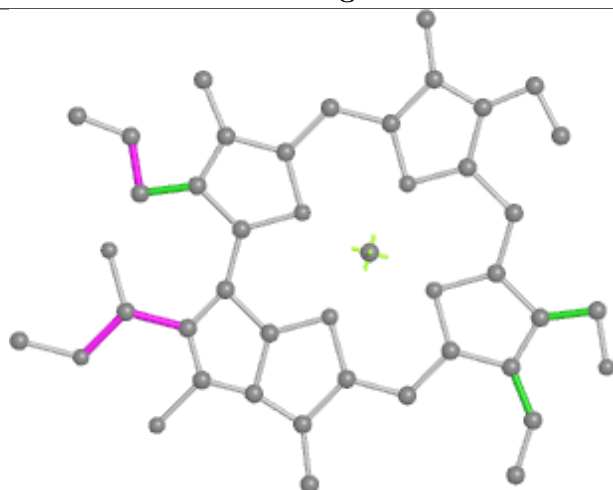
Ligand CHL s 606



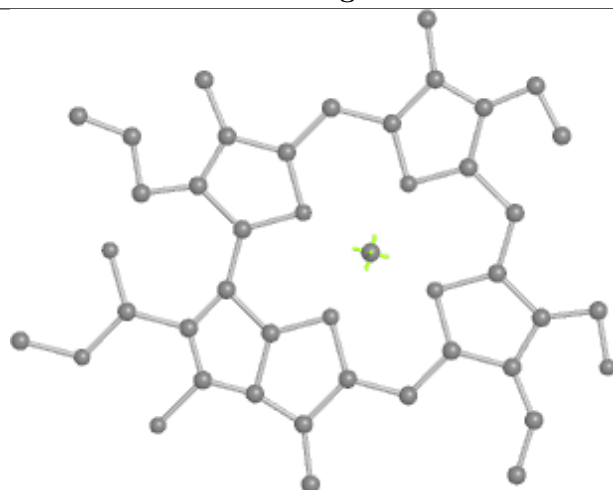
Bond lengths



Bond angles

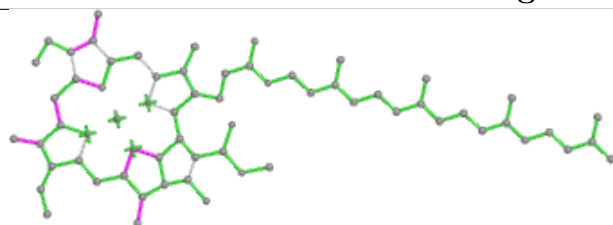


Torsions

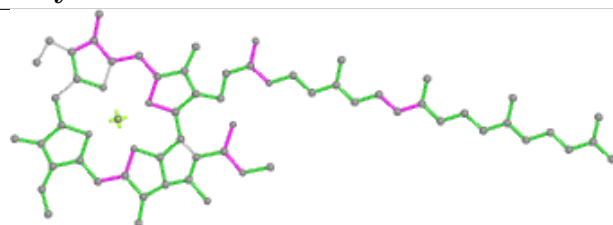


Rings

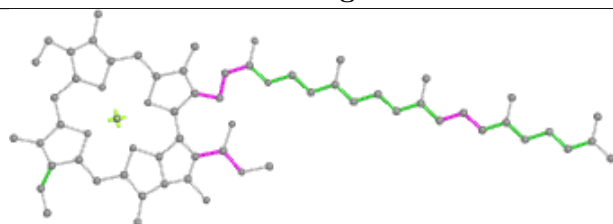
Ligand CLA y 602



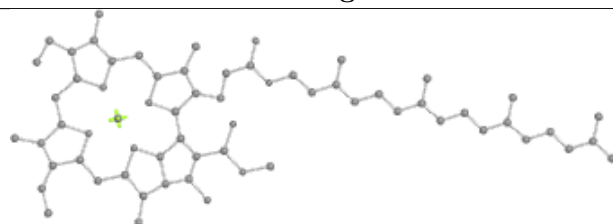
Bond lengths



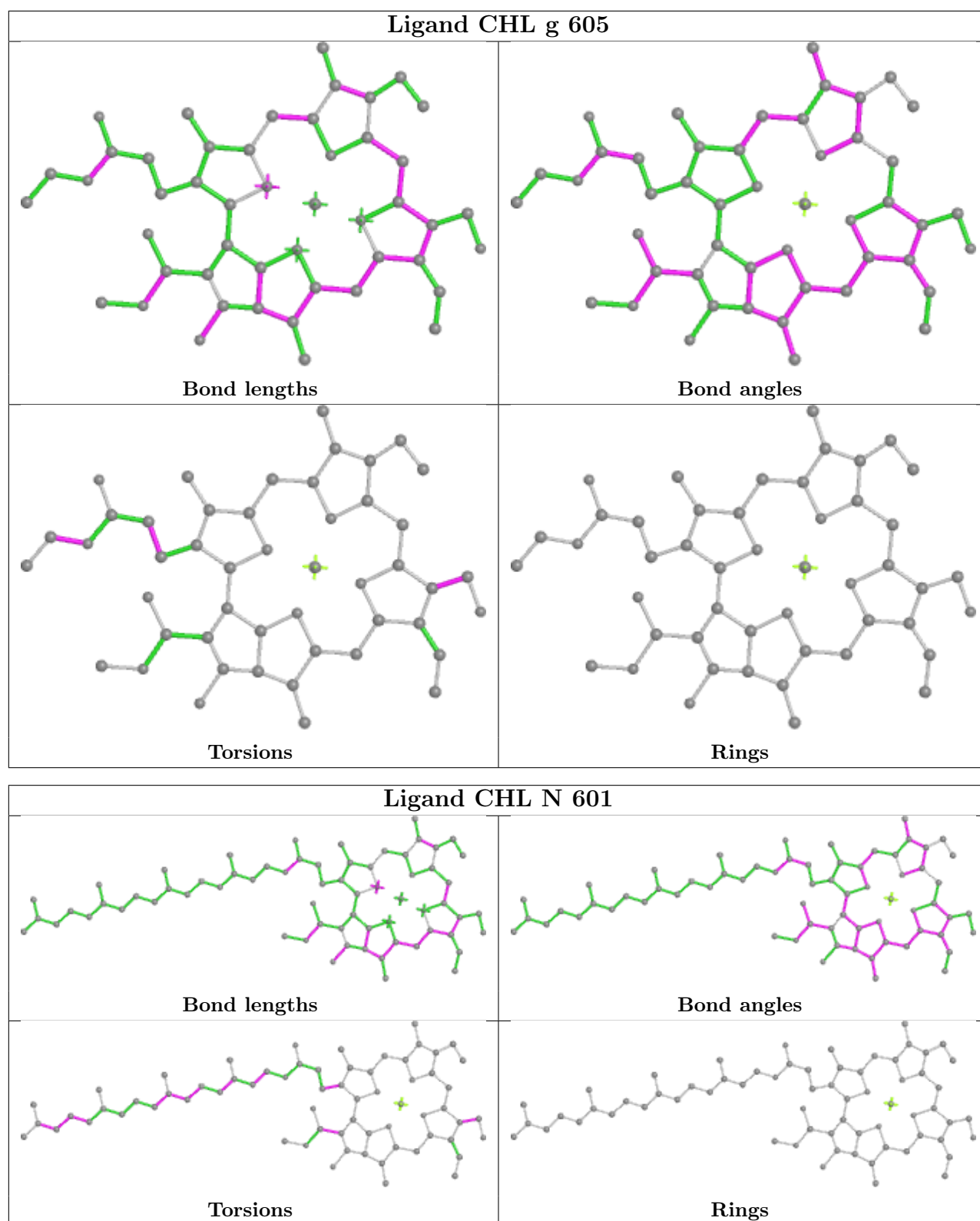
Bond angles



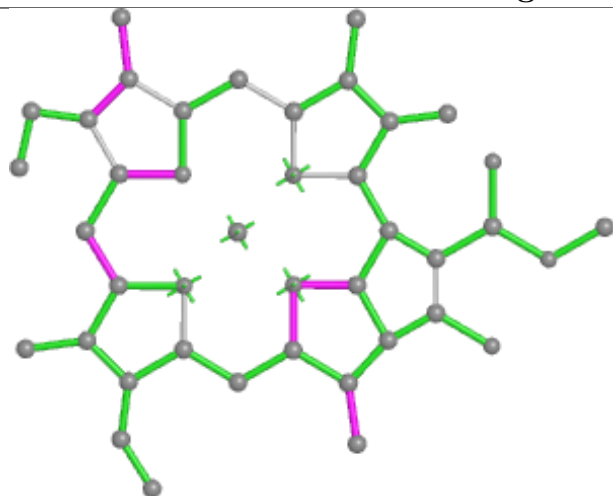
Torsions



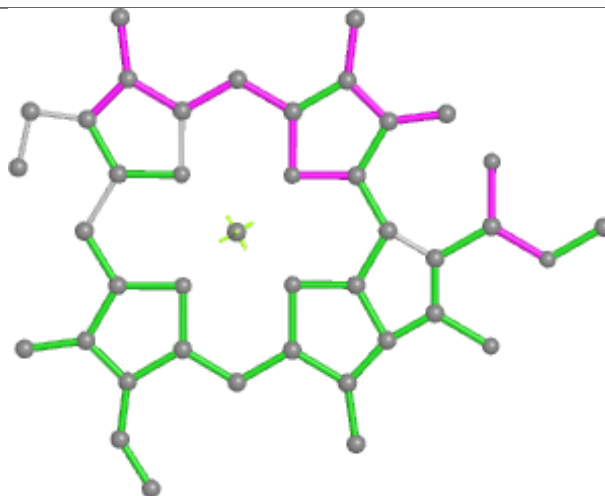
Rings



Ligand CLA S 609



Bond lengths



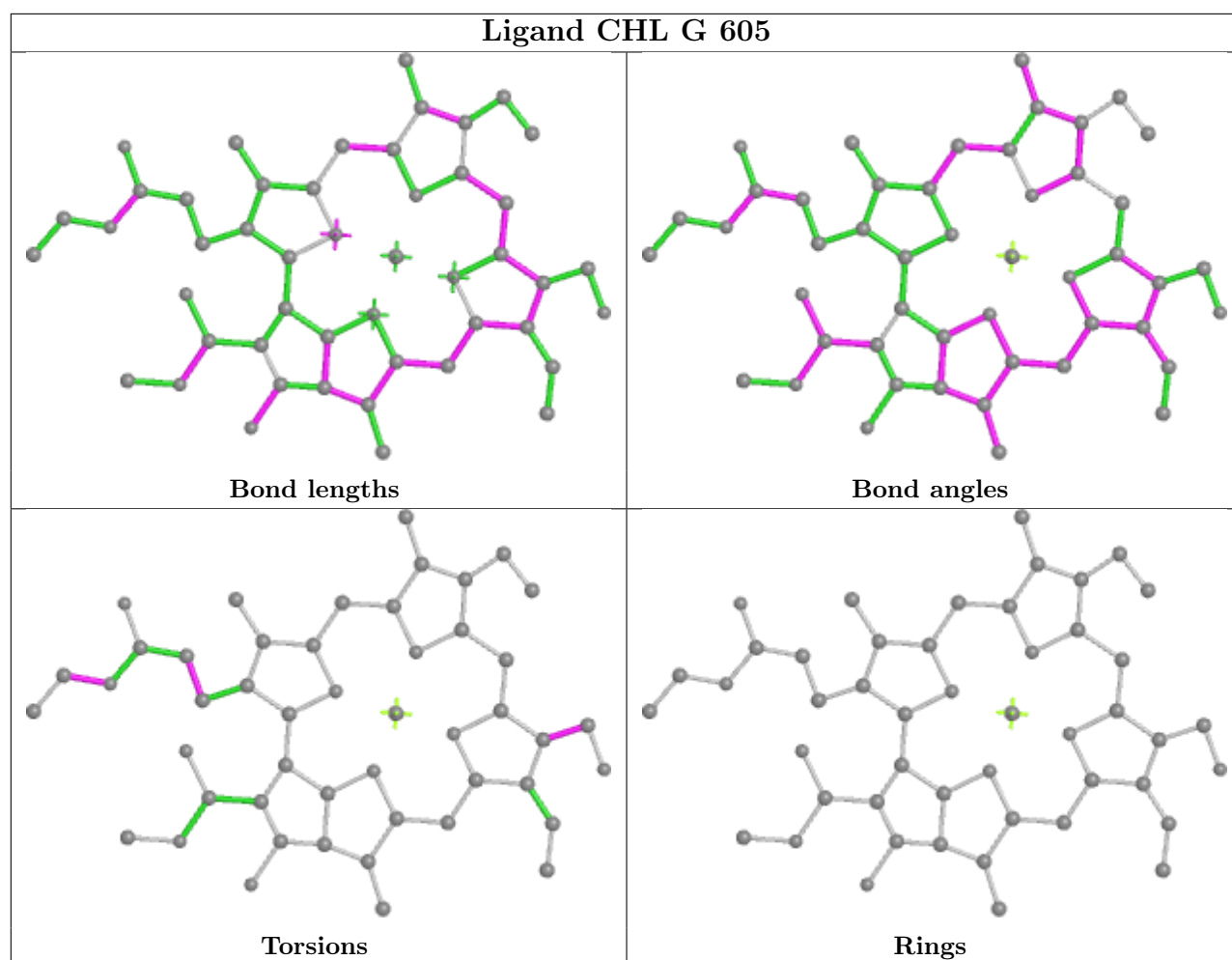
Bond angles

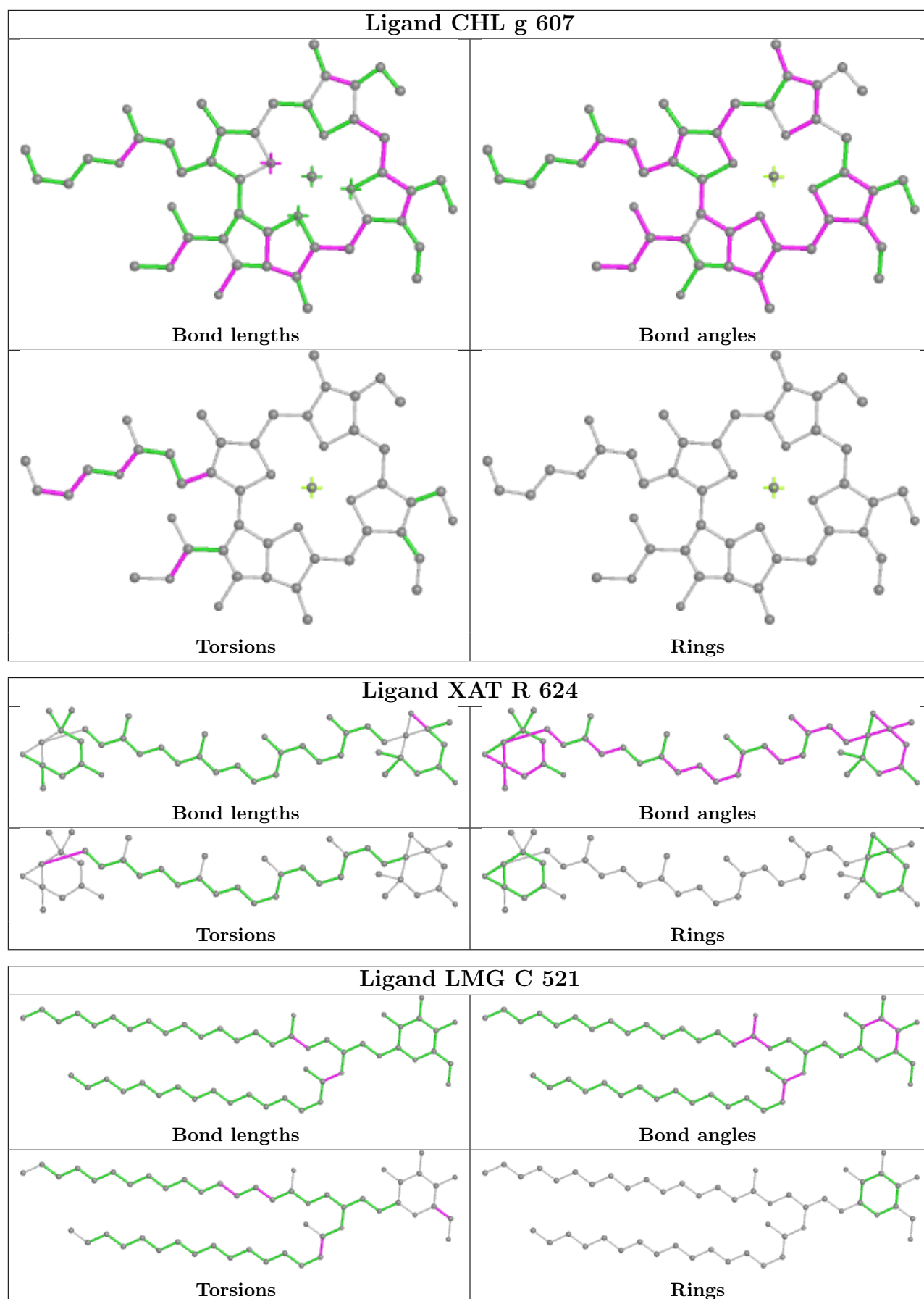


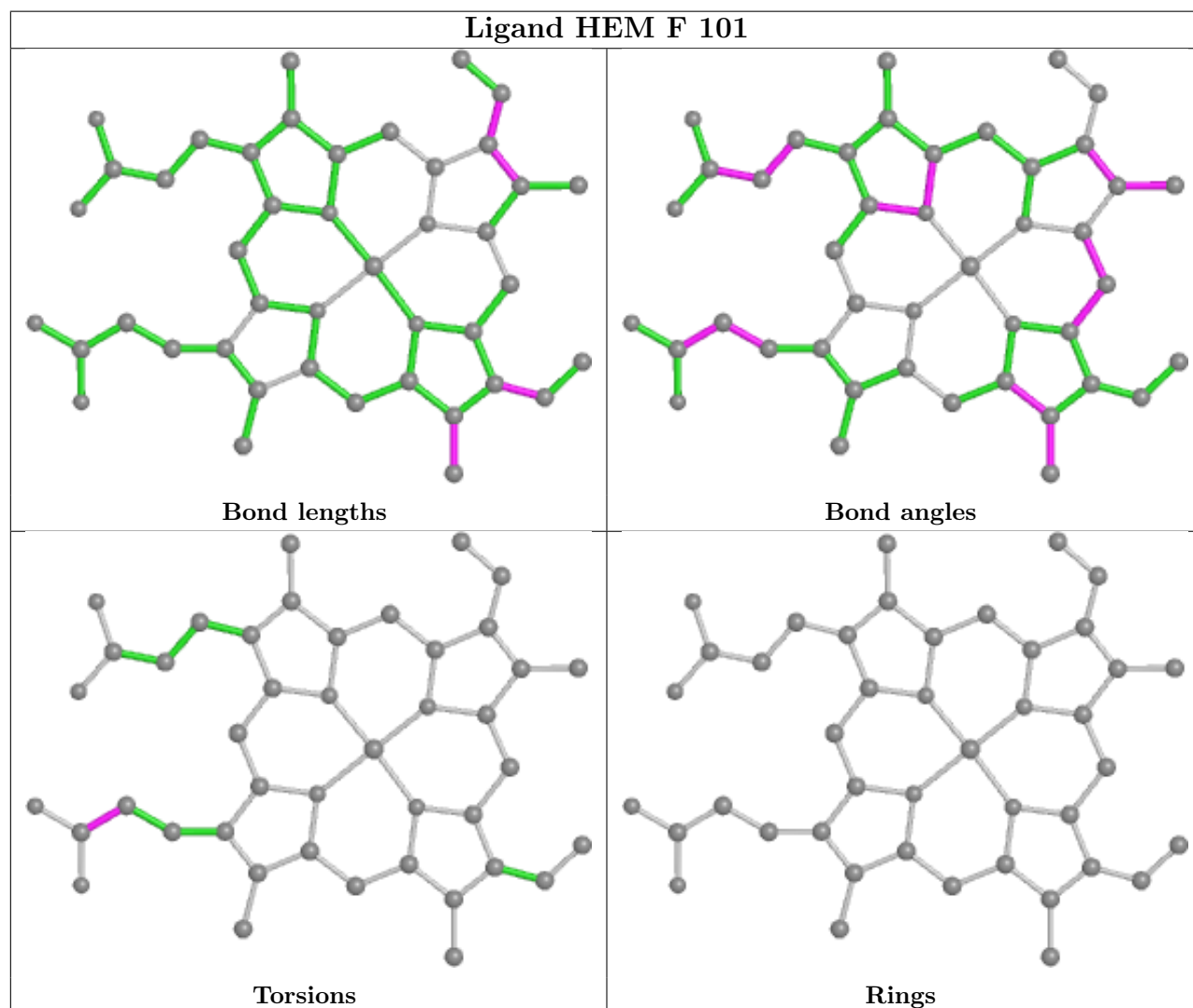
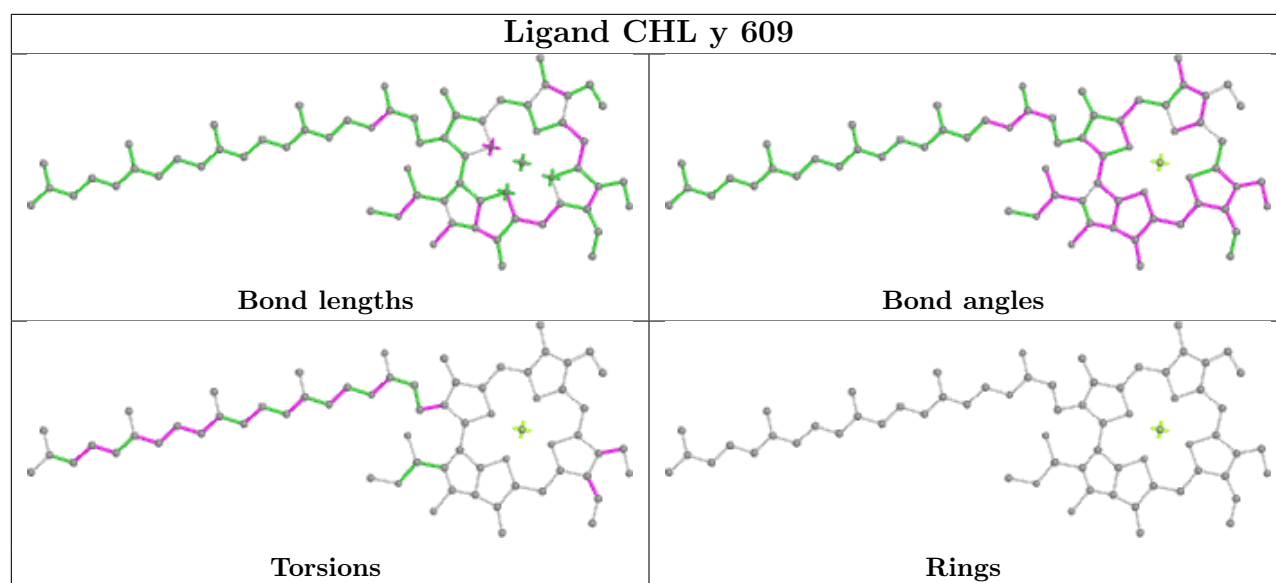
Torsions

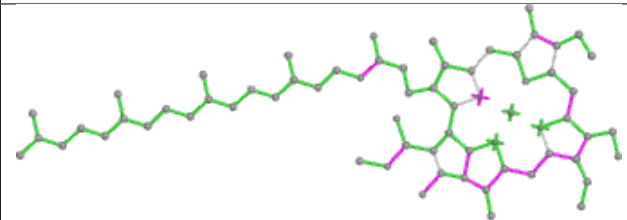
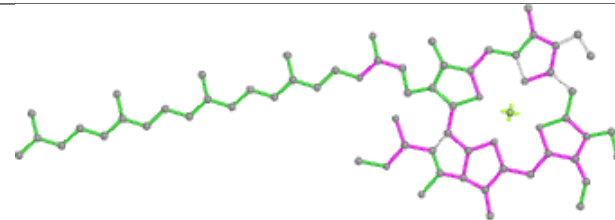
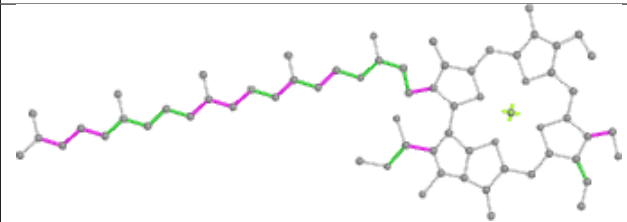
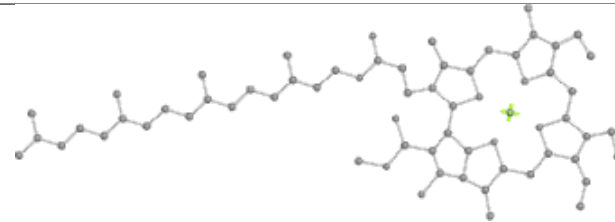


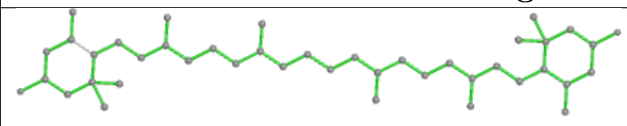
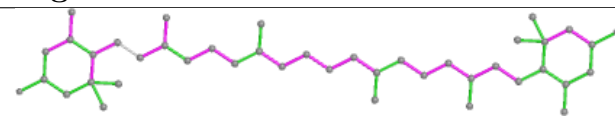
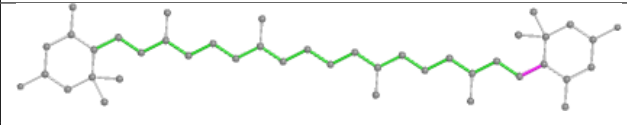
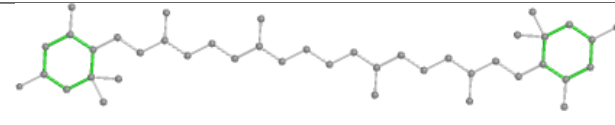
Rings



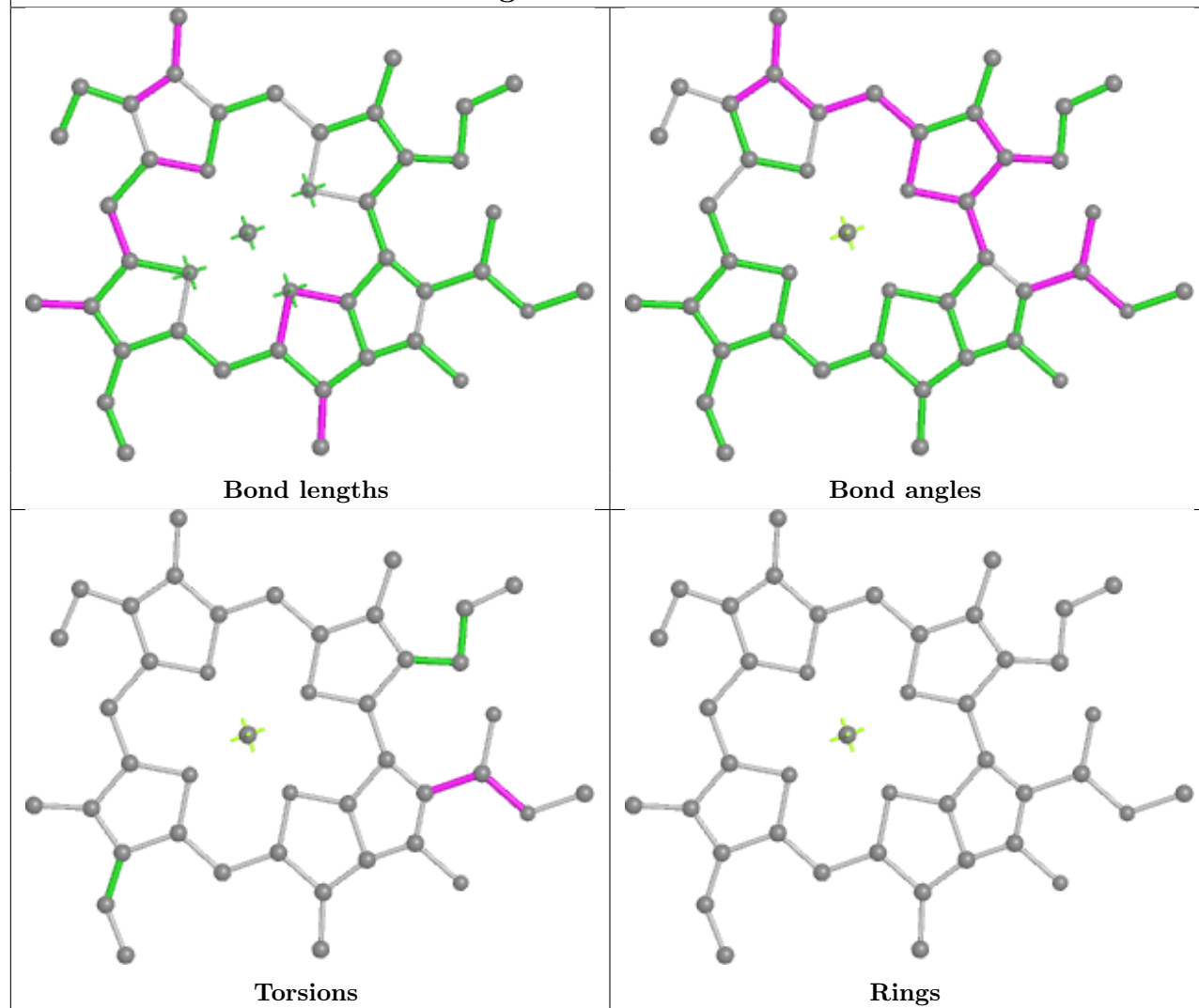




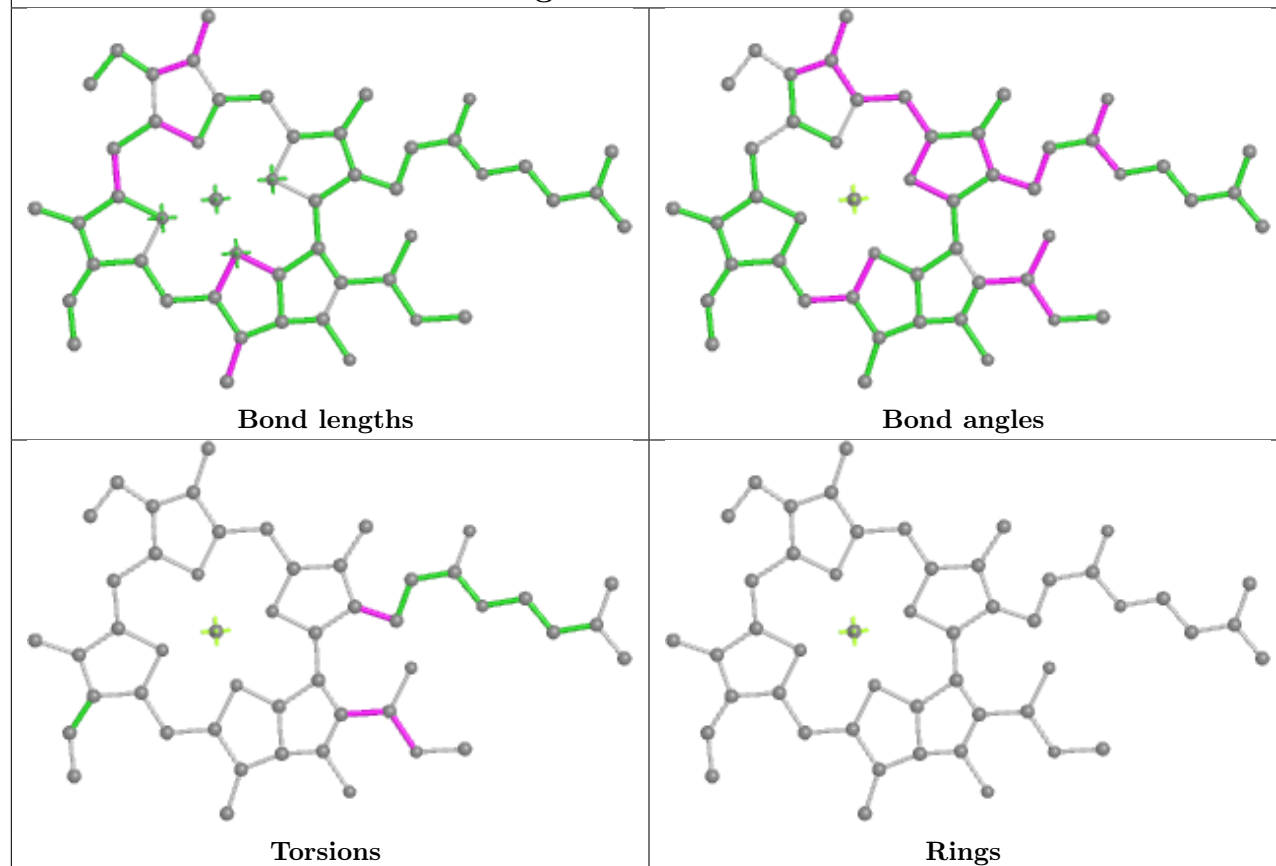
Ligand CHL n 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT g 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

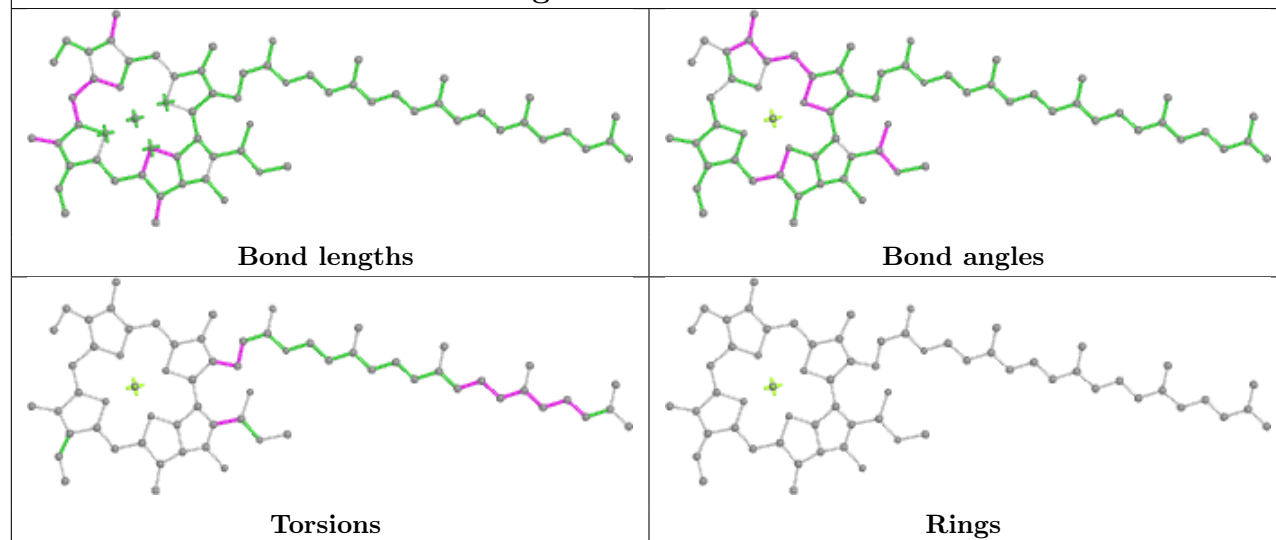
Ligand CLA G 612



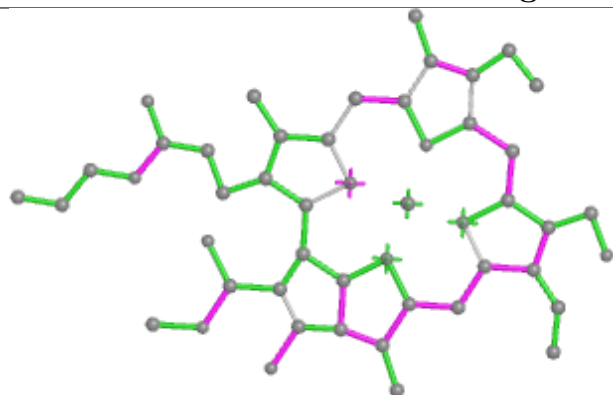
Ligand CLA S 605



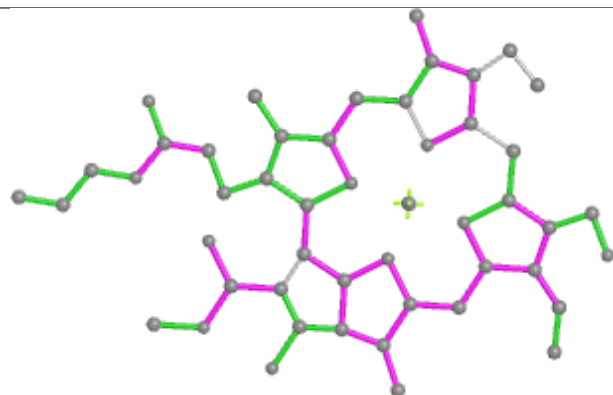
Ligand CLA B 608



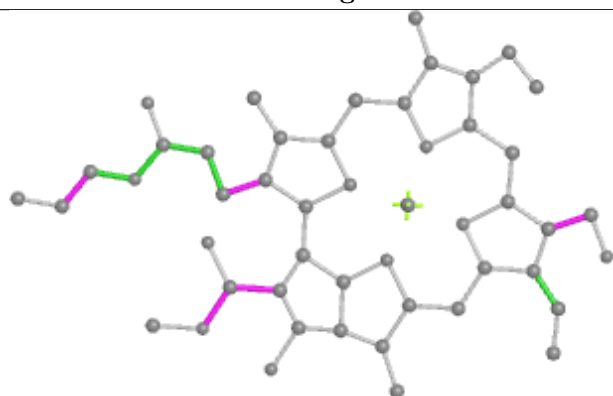
Ligand CHL s 608



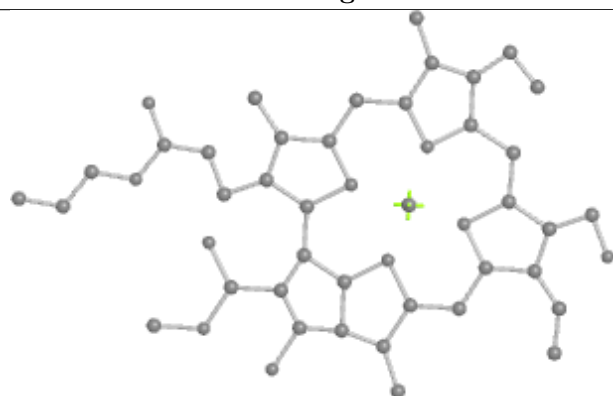
Bond lengths



Bond angles

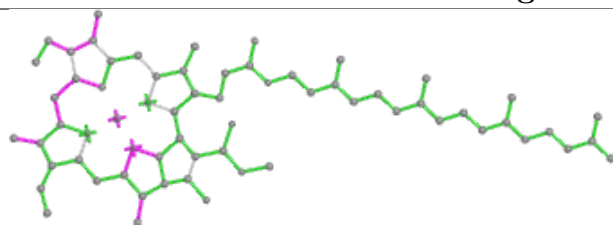


Torsions

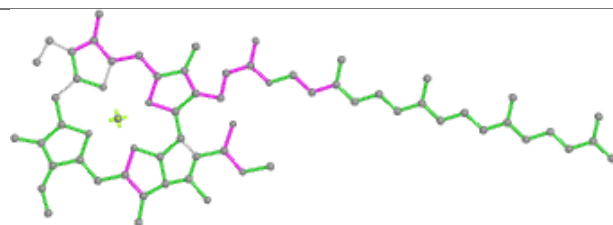


Rings

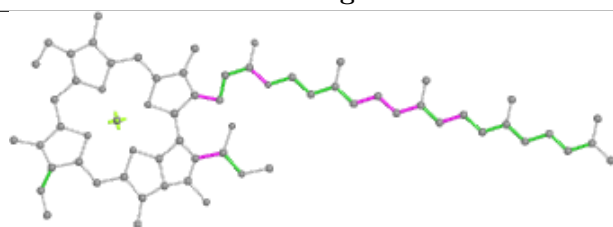
Ligand CLA b 605



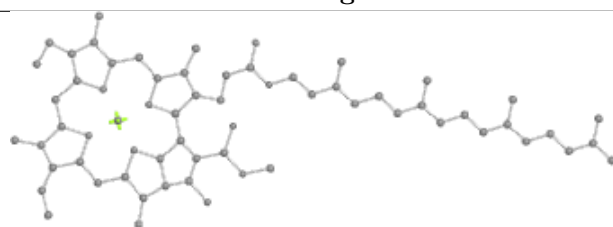
Bond lengths



Bond angles

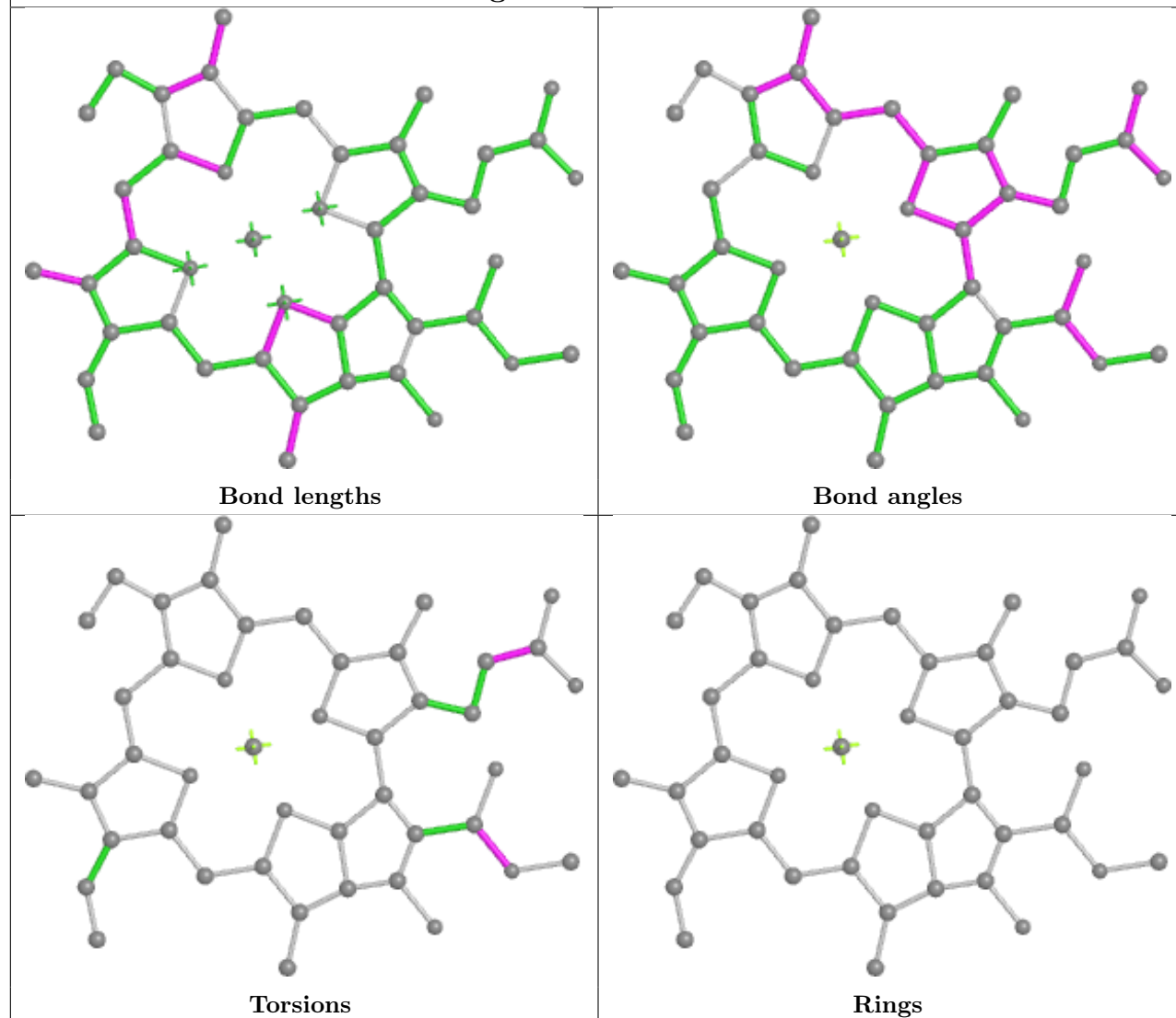


Torsions

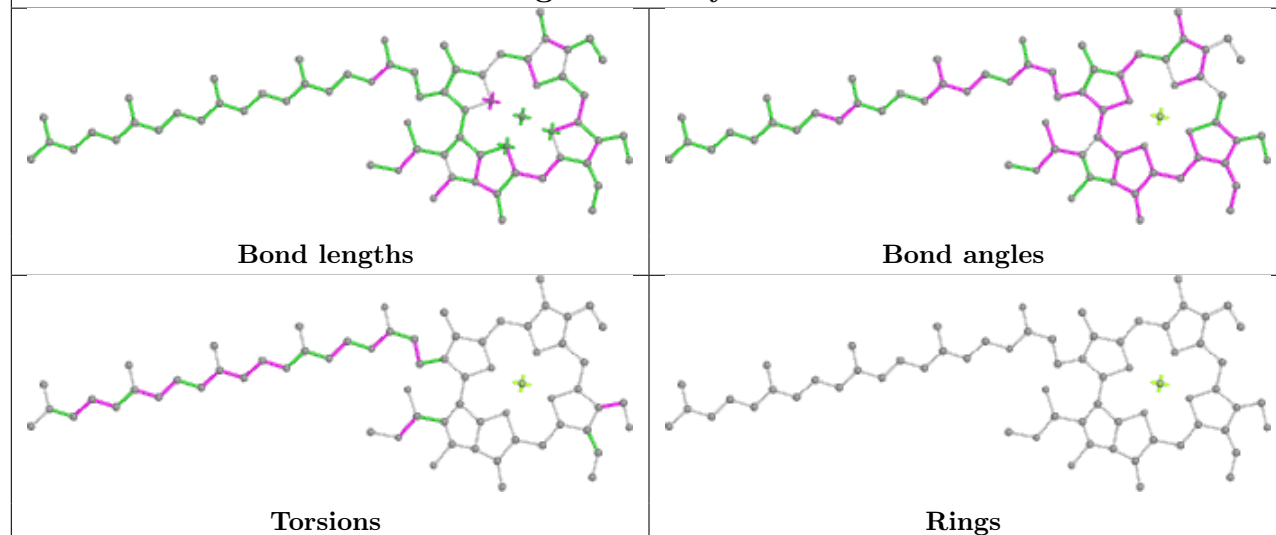


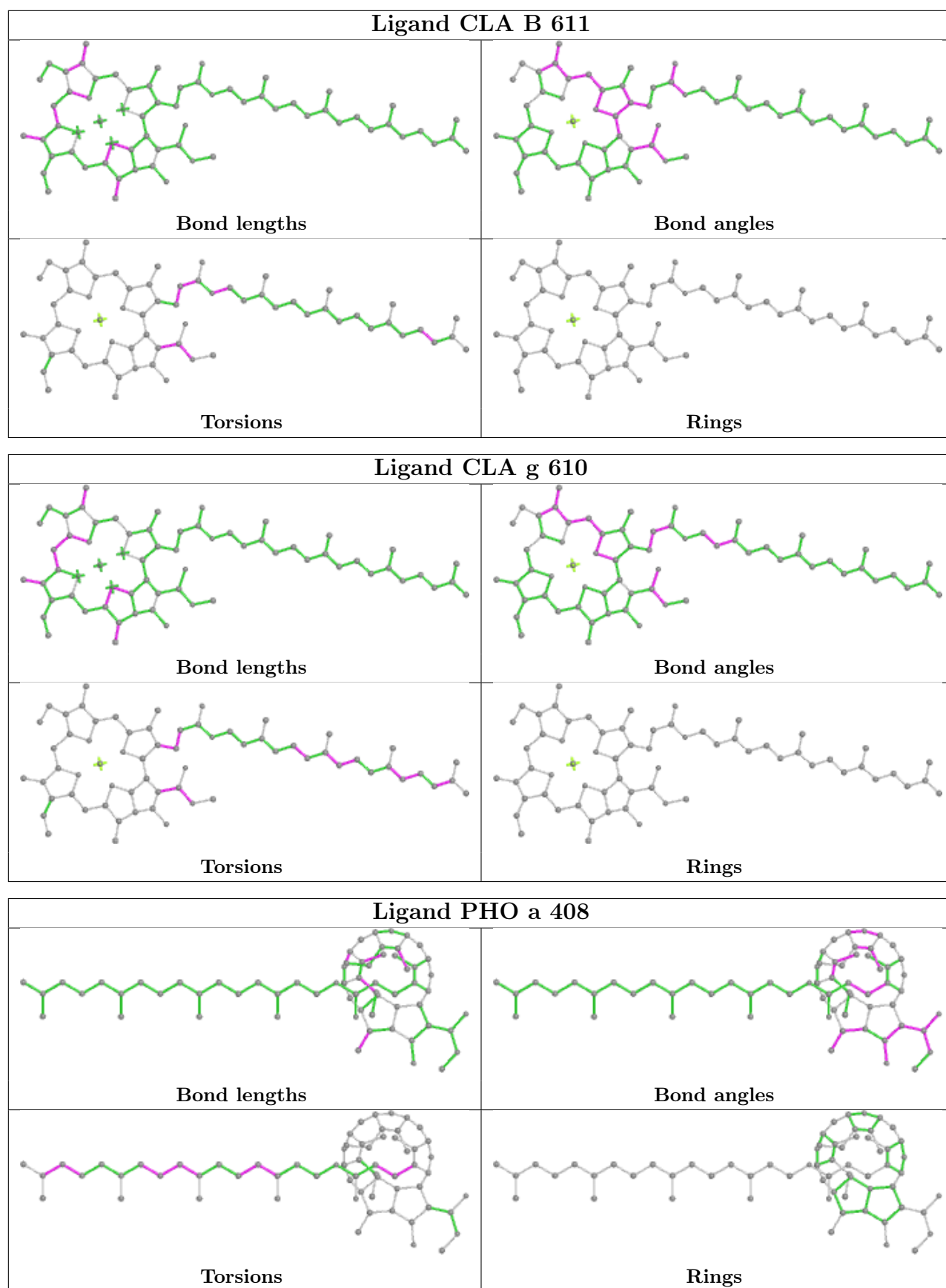
Rings

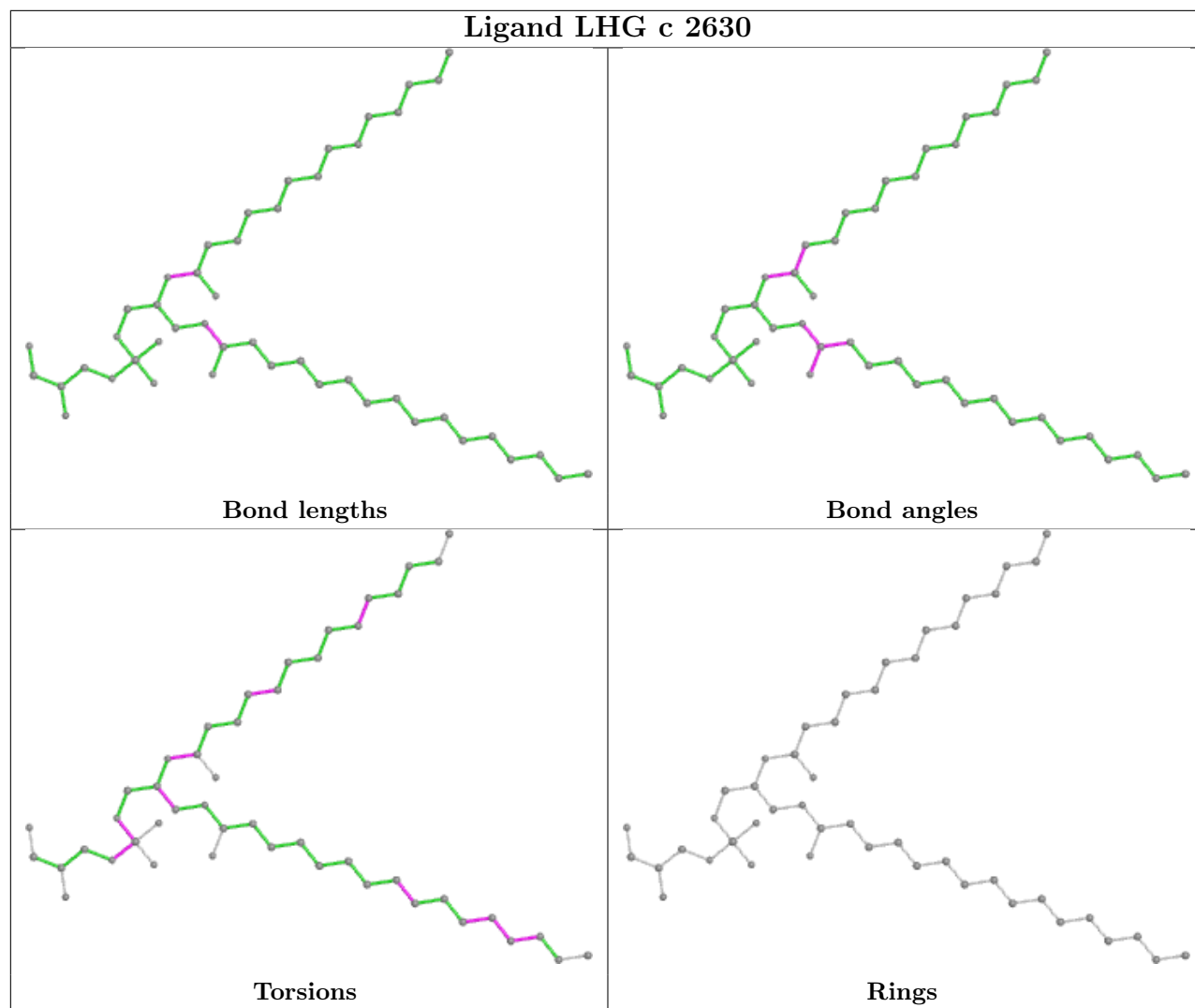
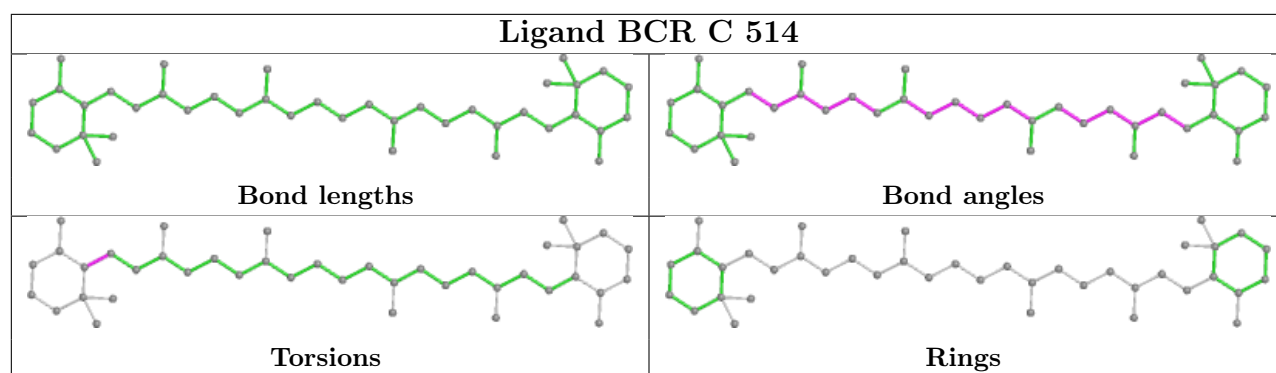
Ligand CLA N 612

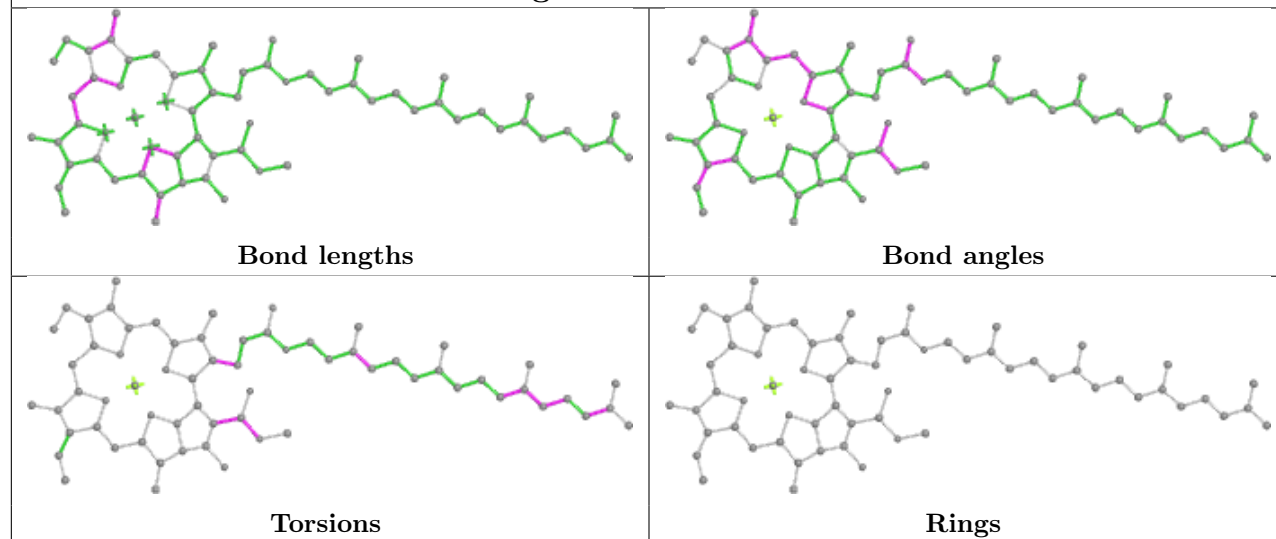
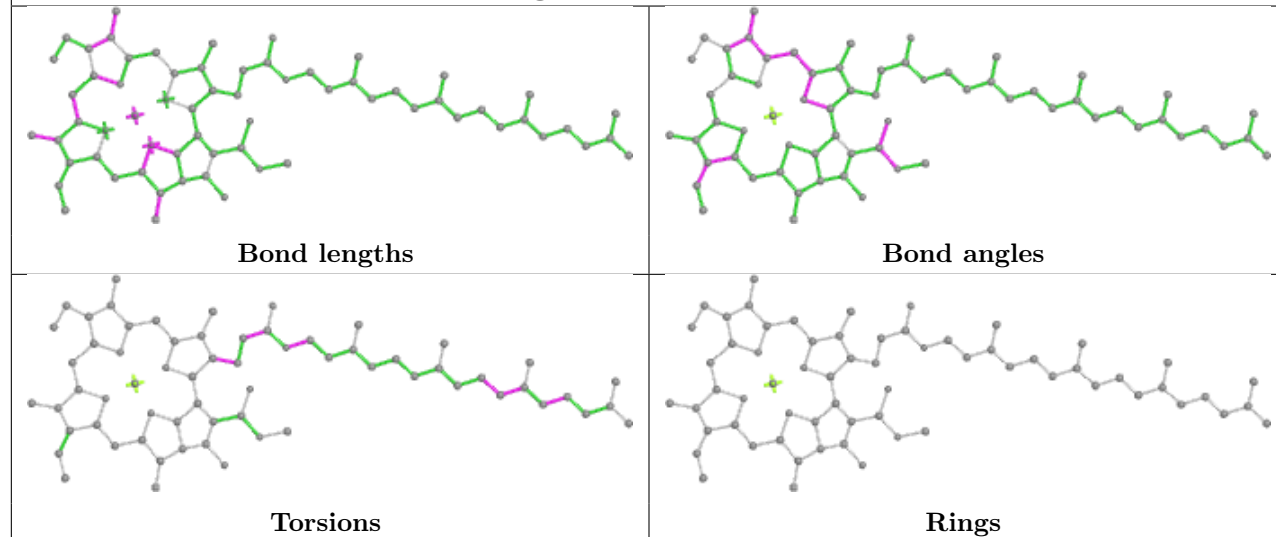
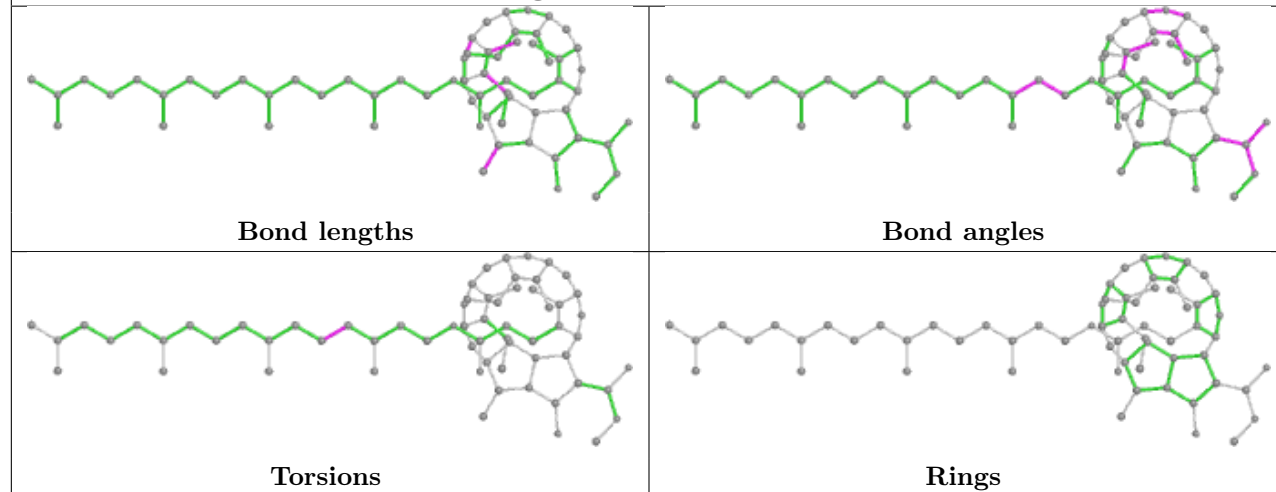


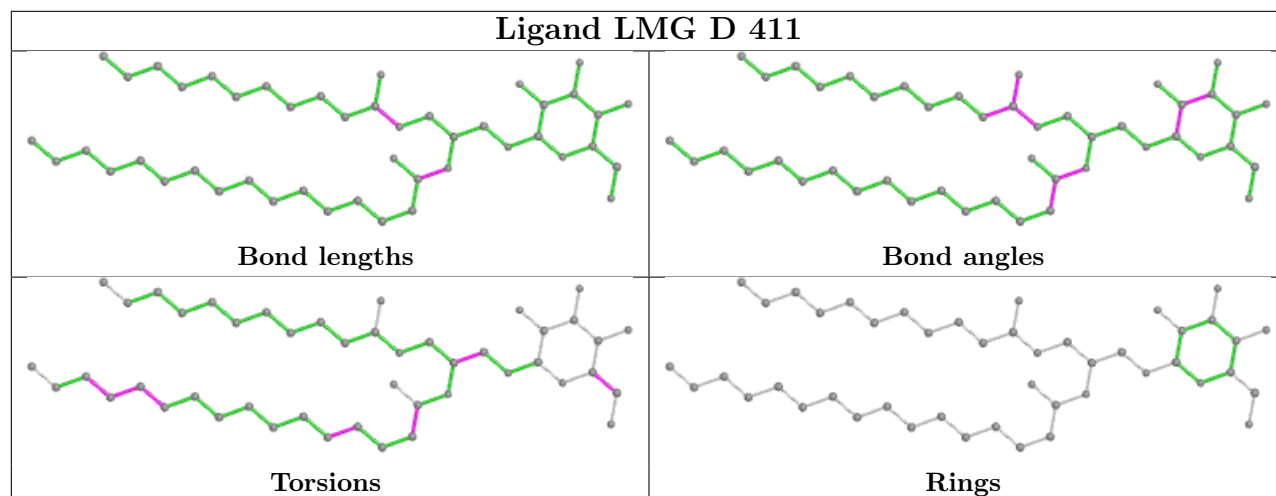
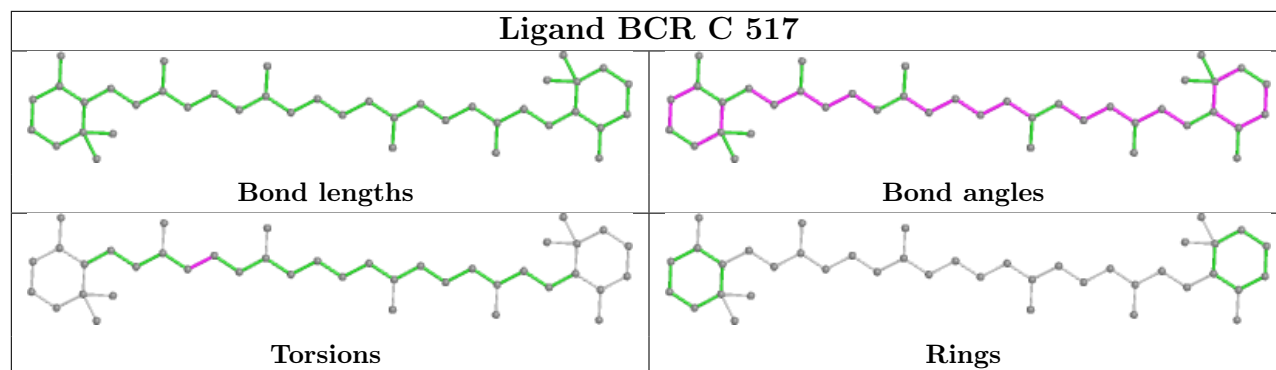
Ligand CHL y 601



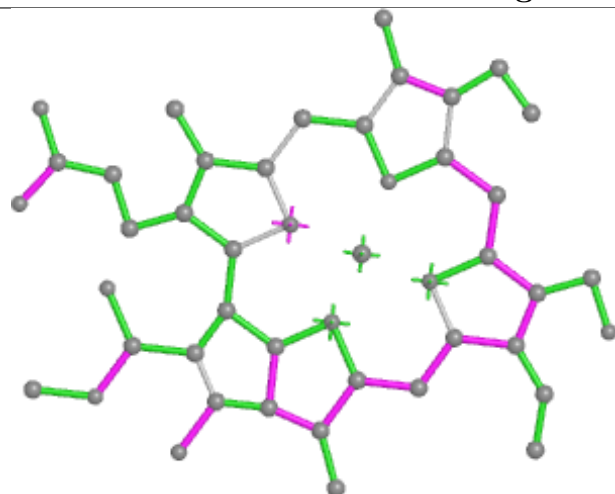




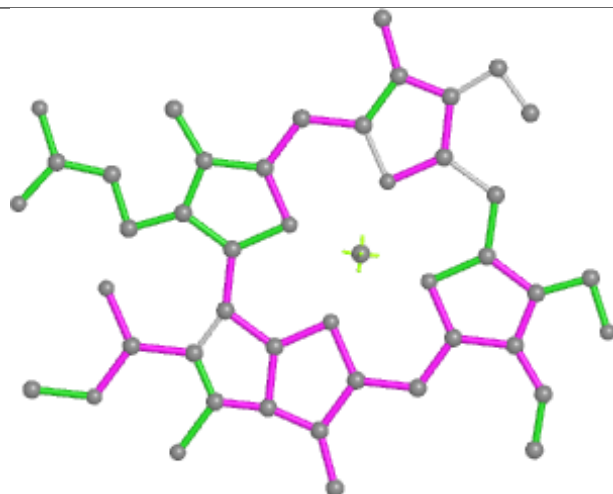
Ligand CLA B 610**Ligand CLA D 402****Ligand PHO A 409**



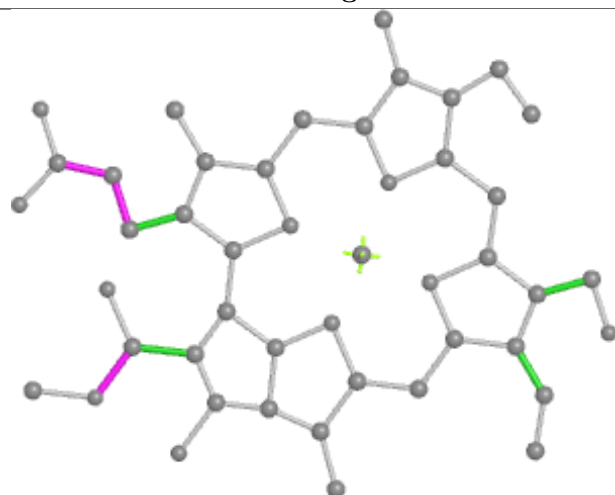
Ligand CHL R 608



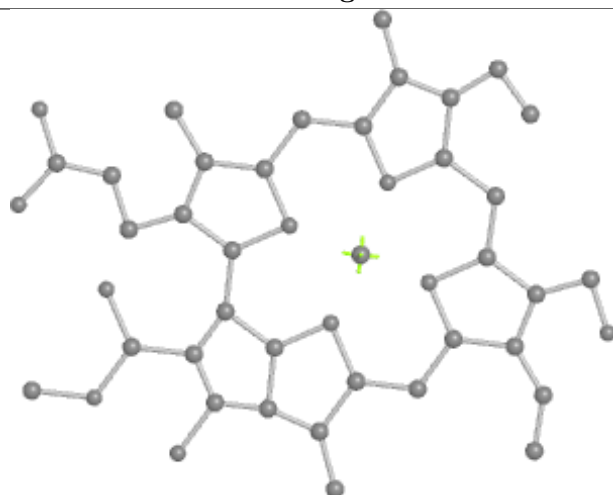
Bond lengths



Bond angles

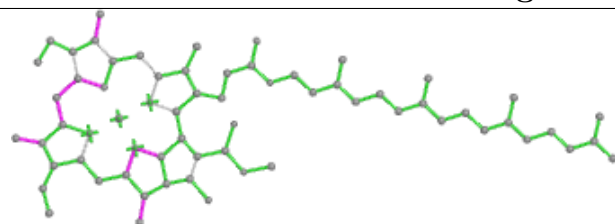


Torsions

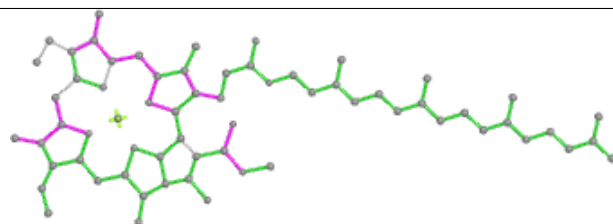


Rings

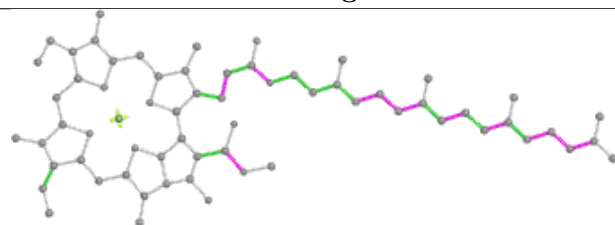
Ligand CLA B 617



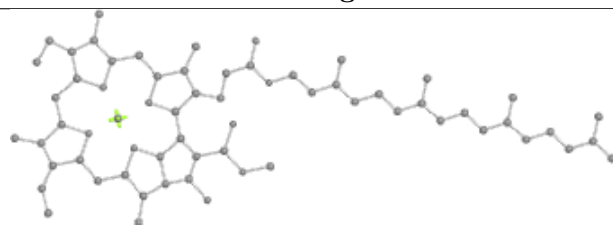
Bond lengths



Bond angles

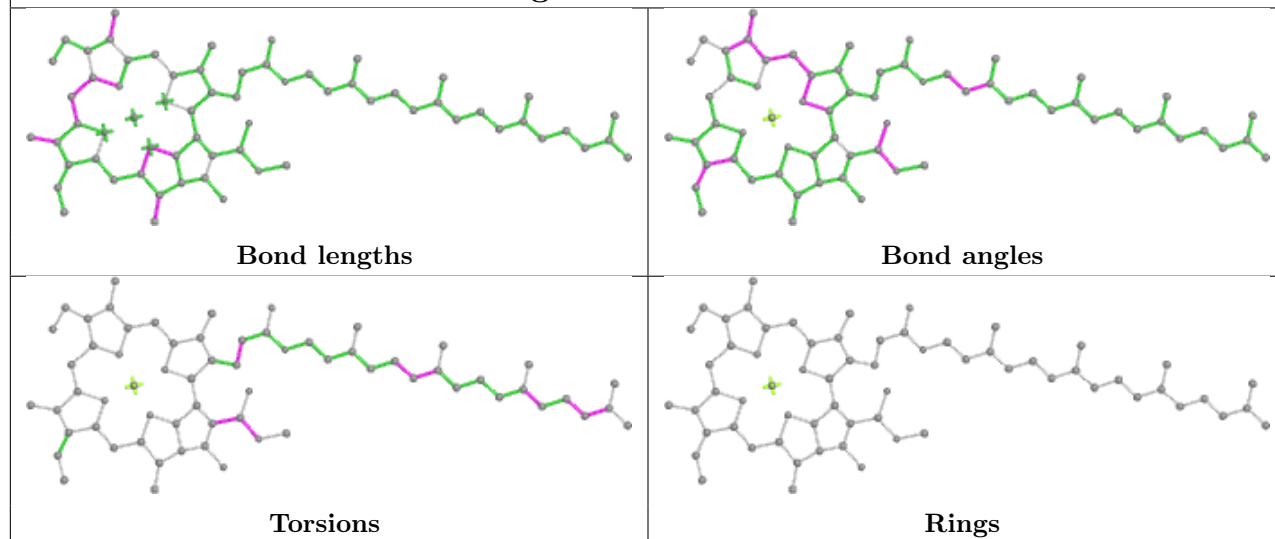


Torsions

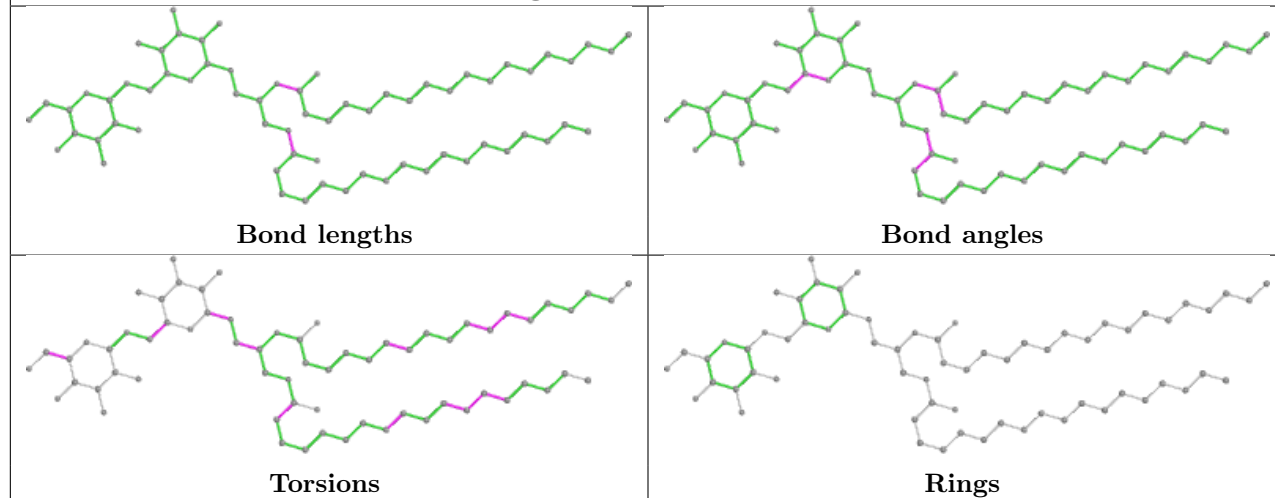


Rings

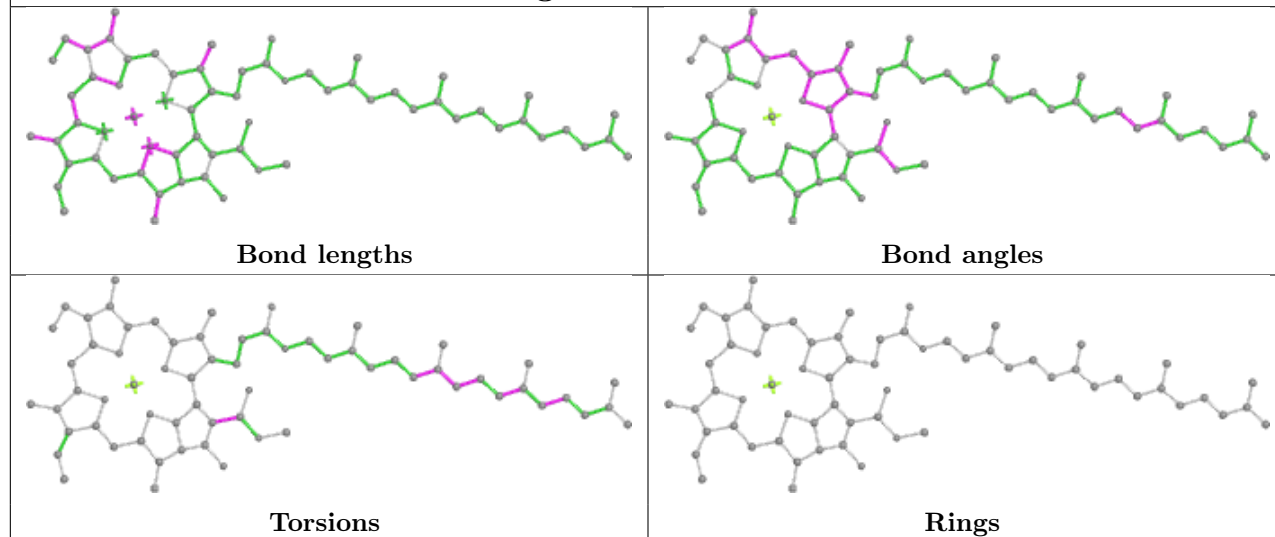
Ligand CLA B 607

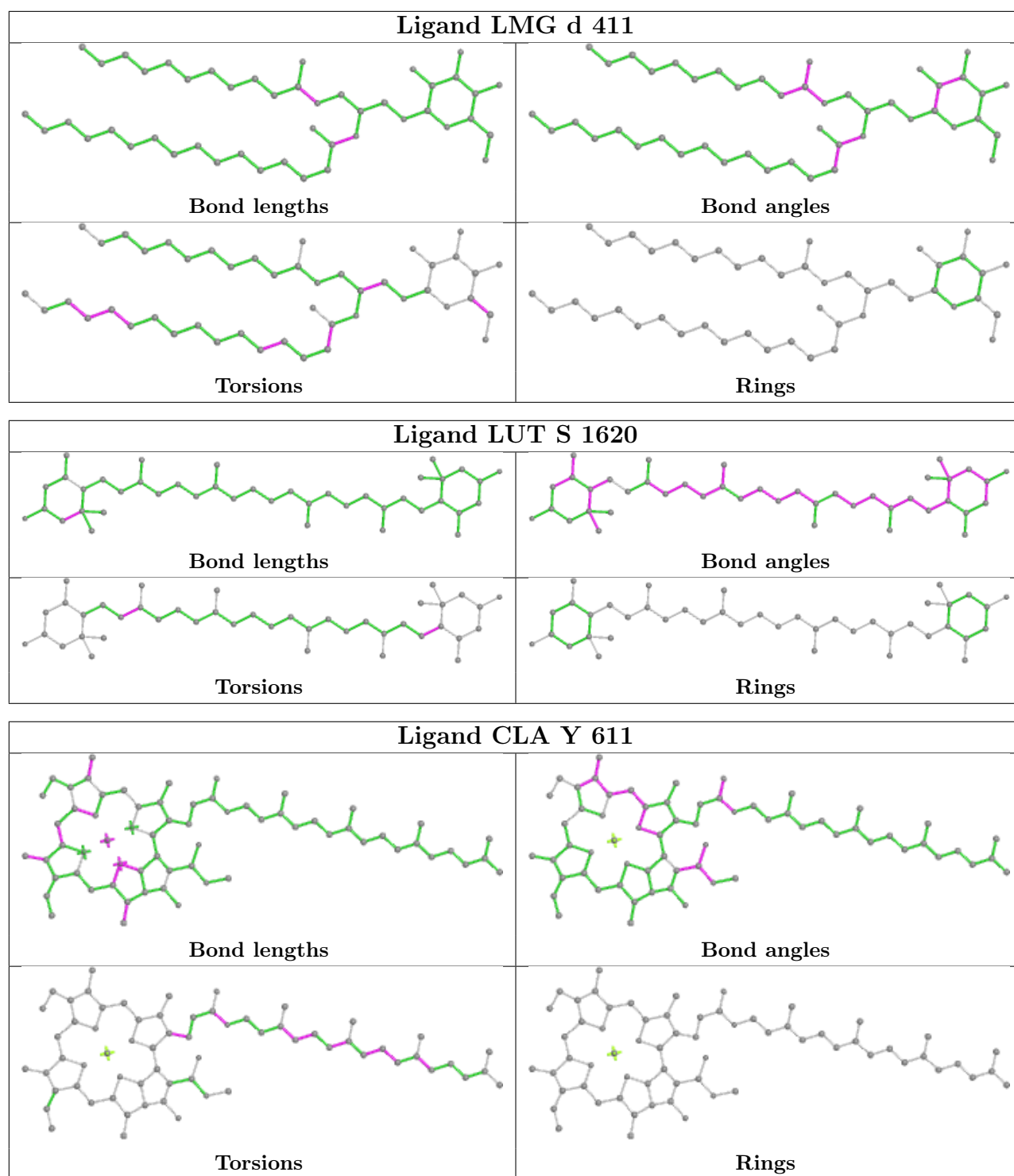


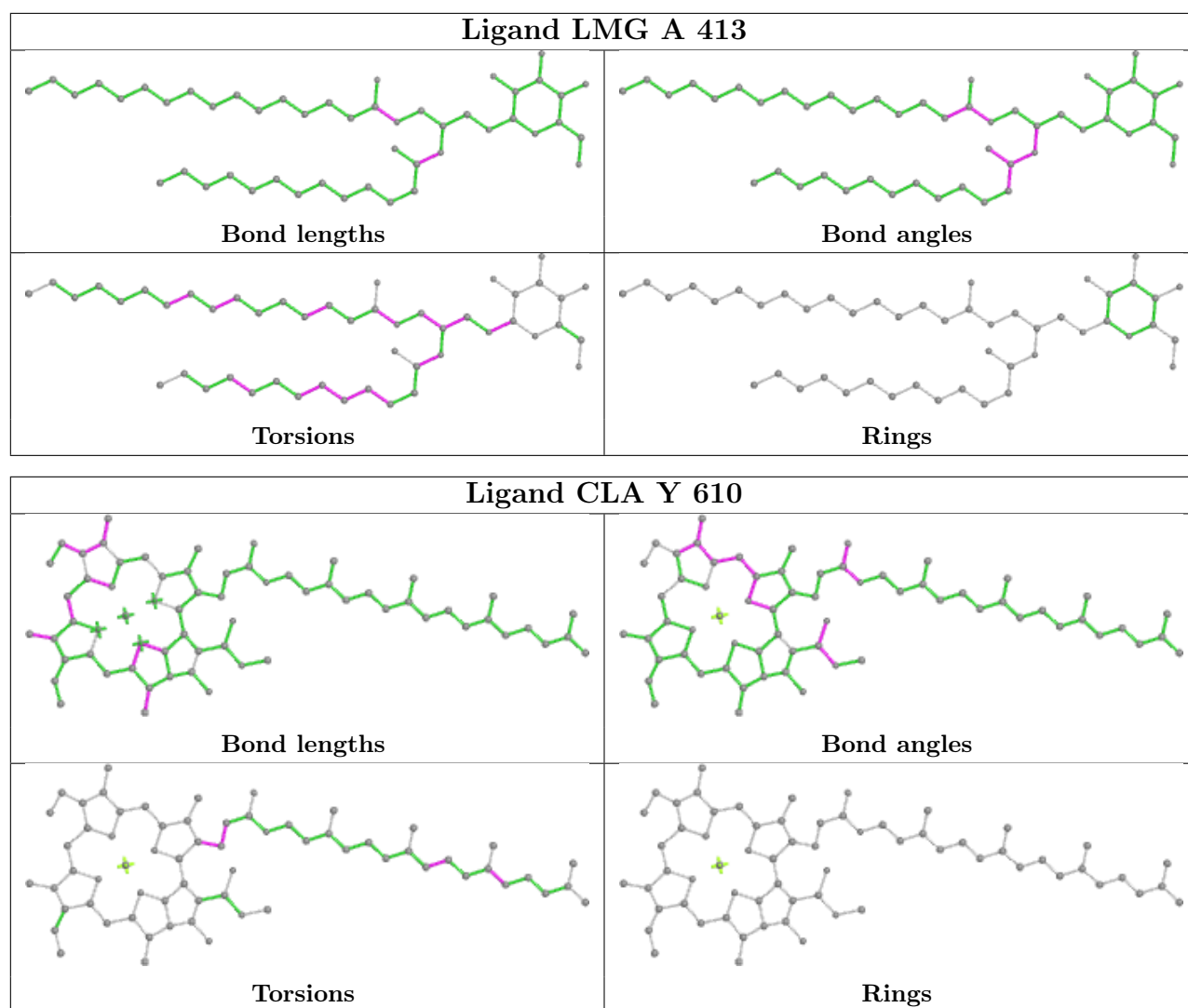
Ligand DGD C 523

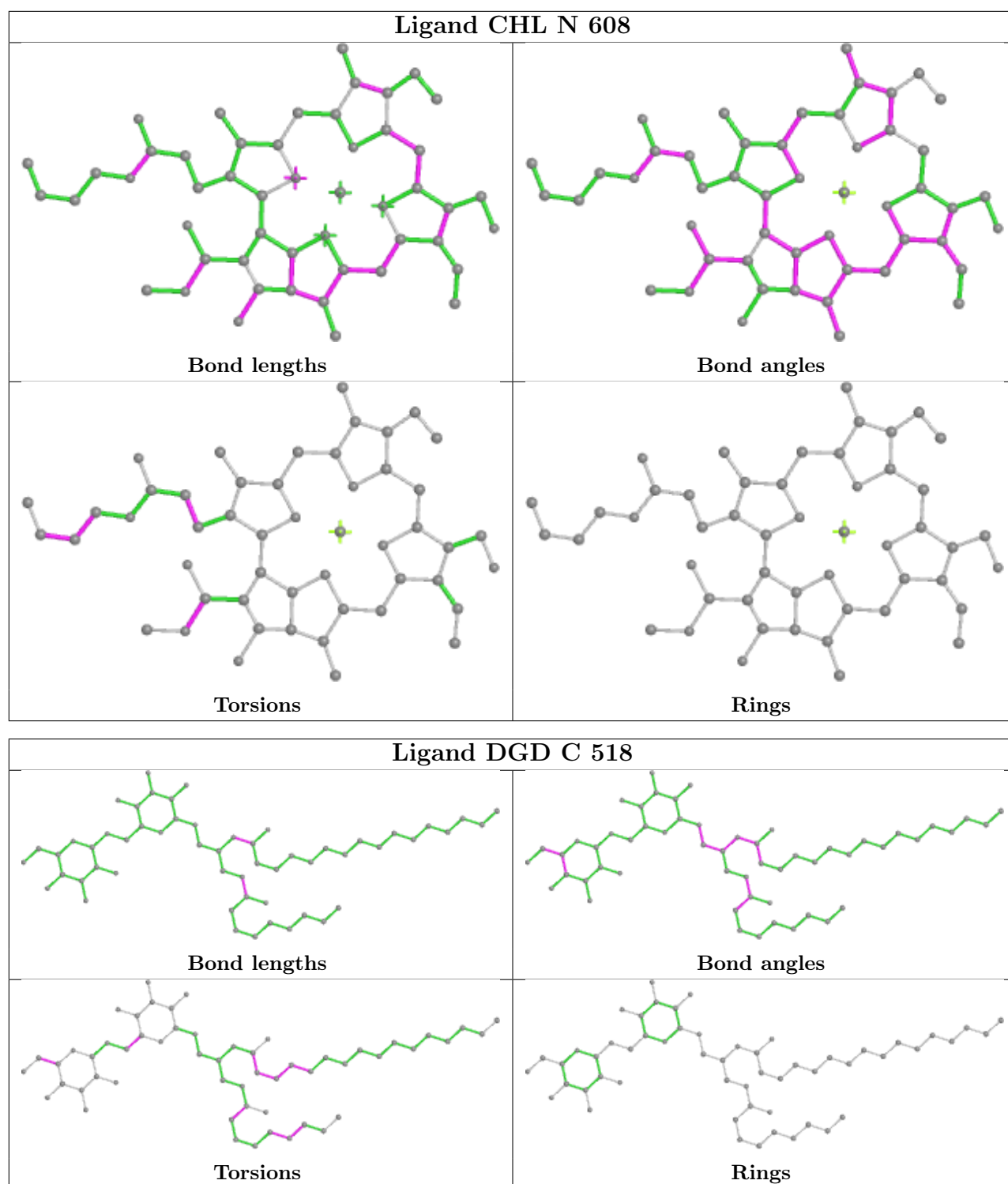


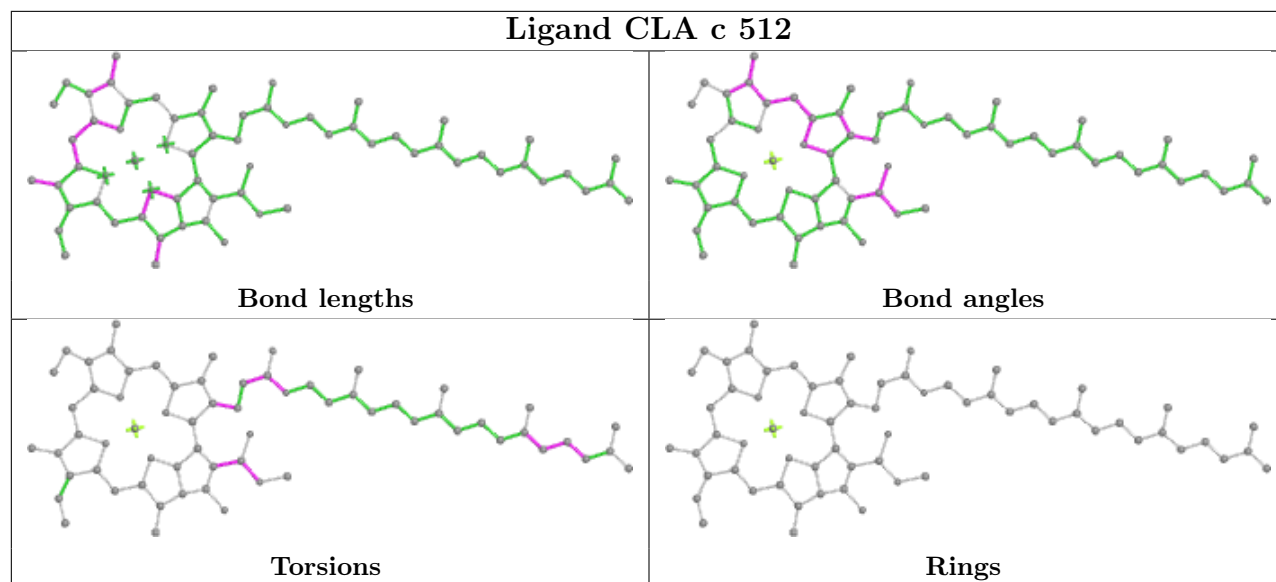
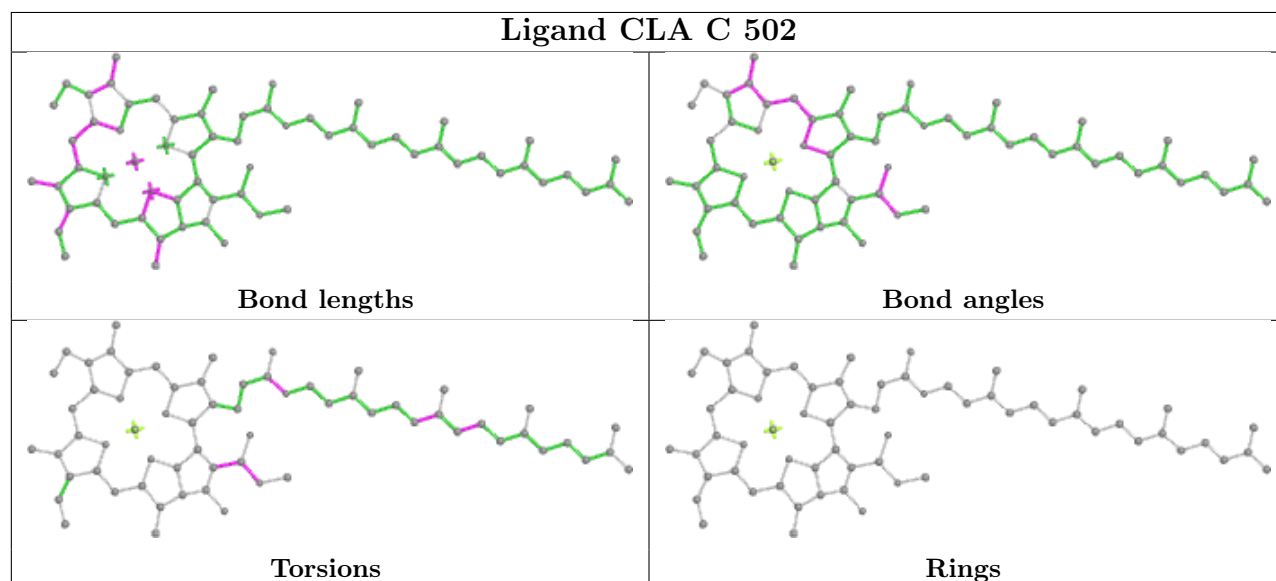
Ligand CLA c 509



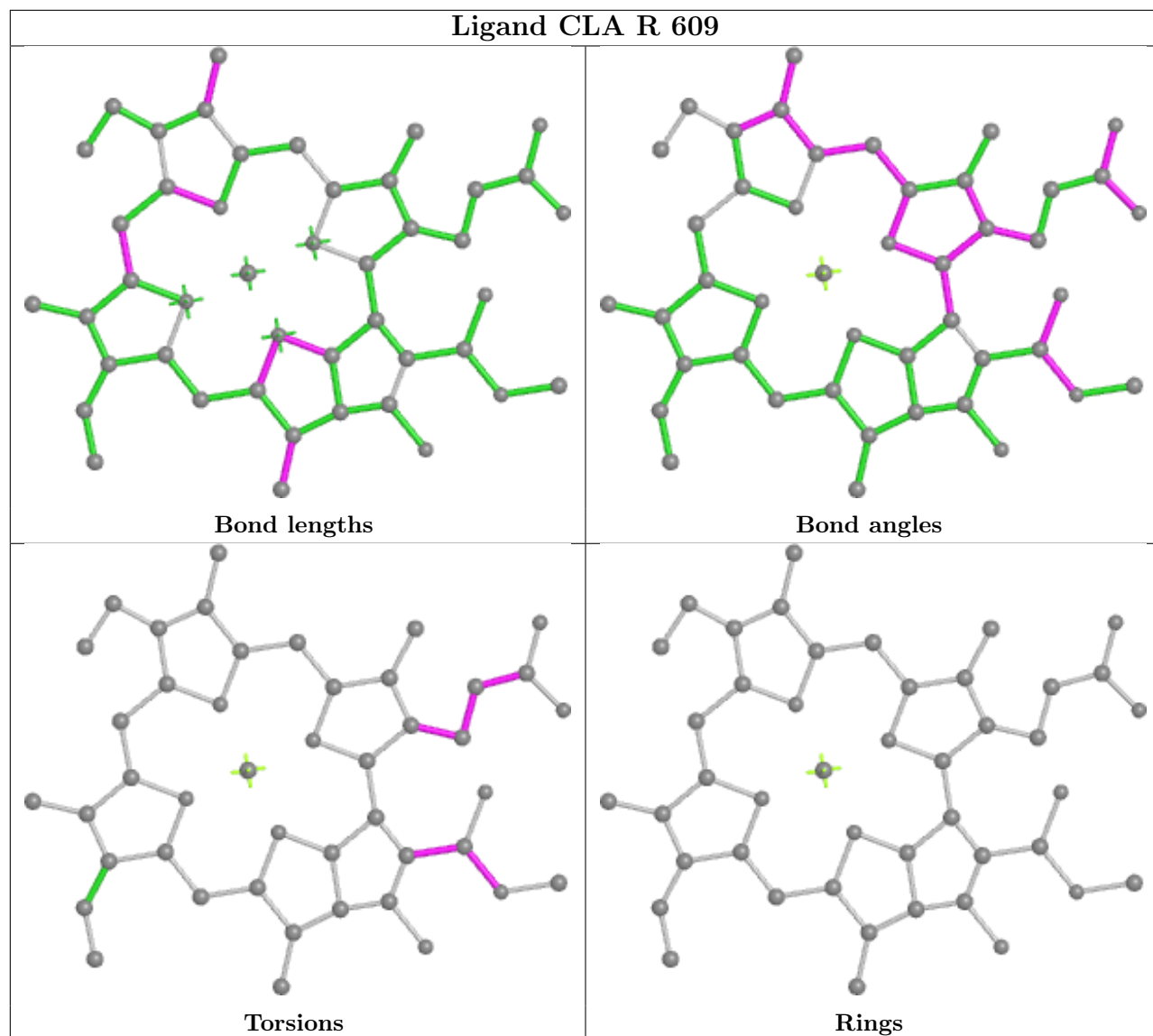


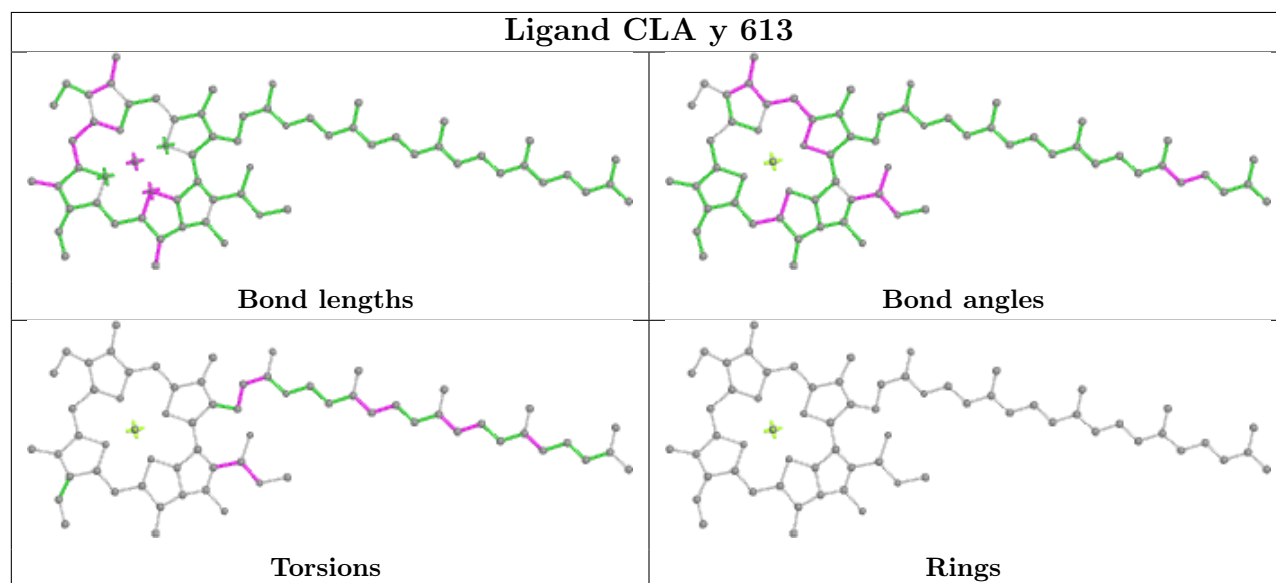
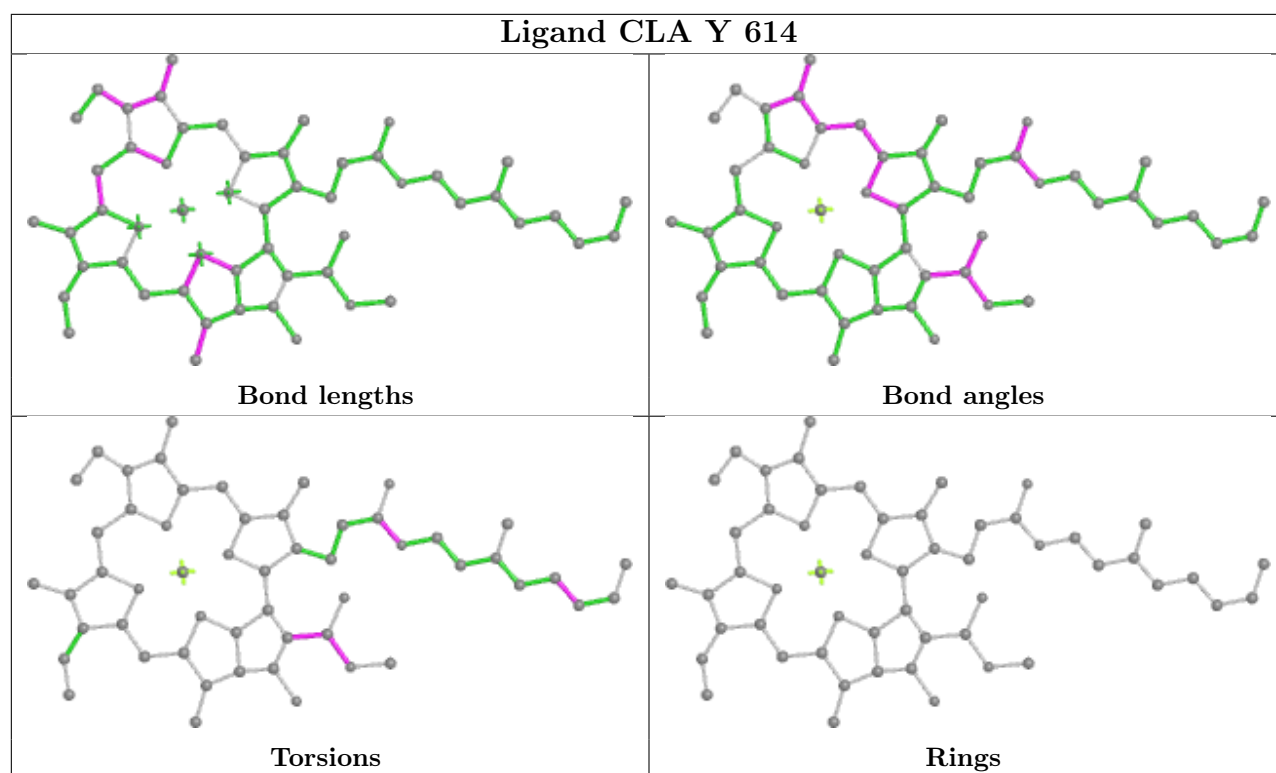


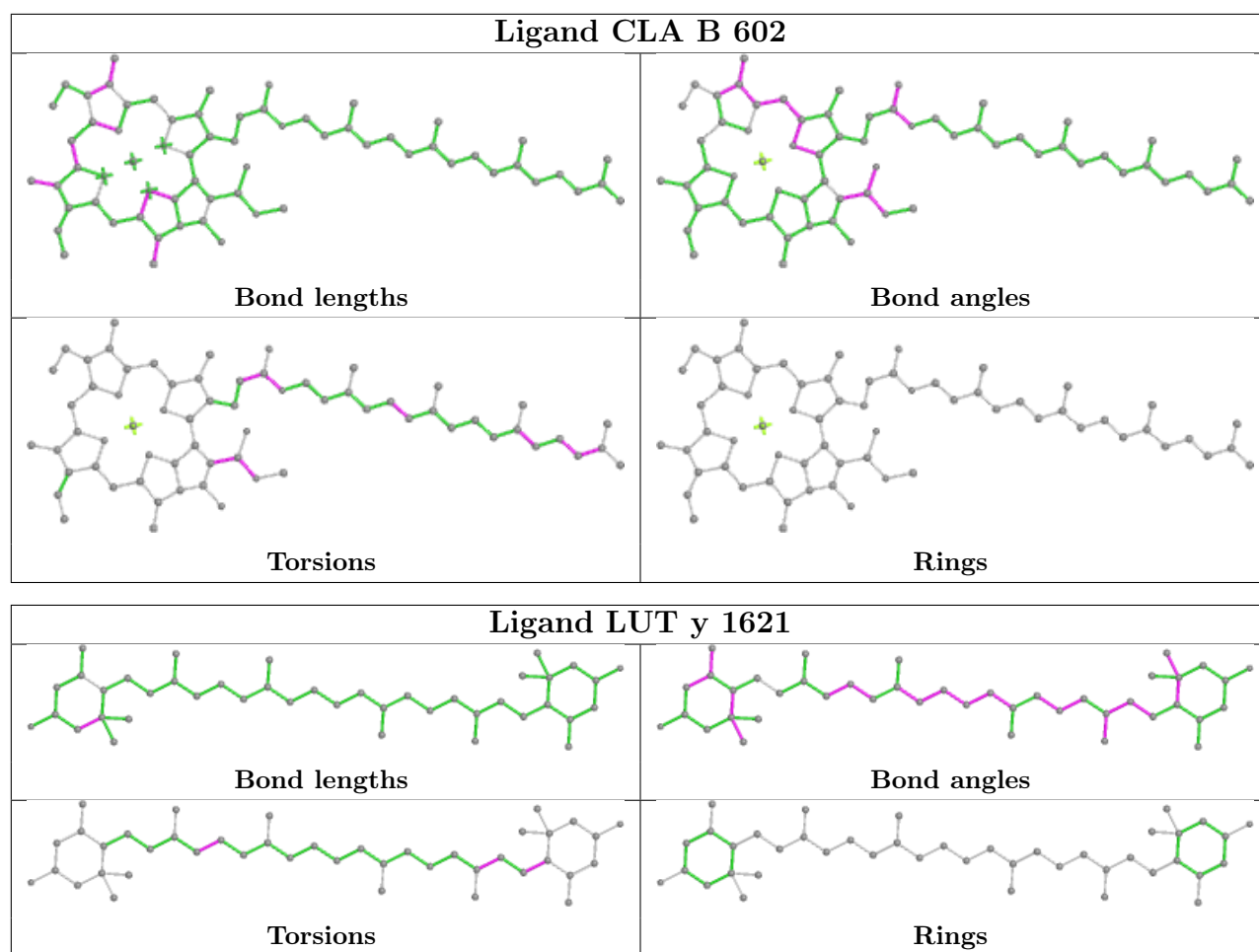


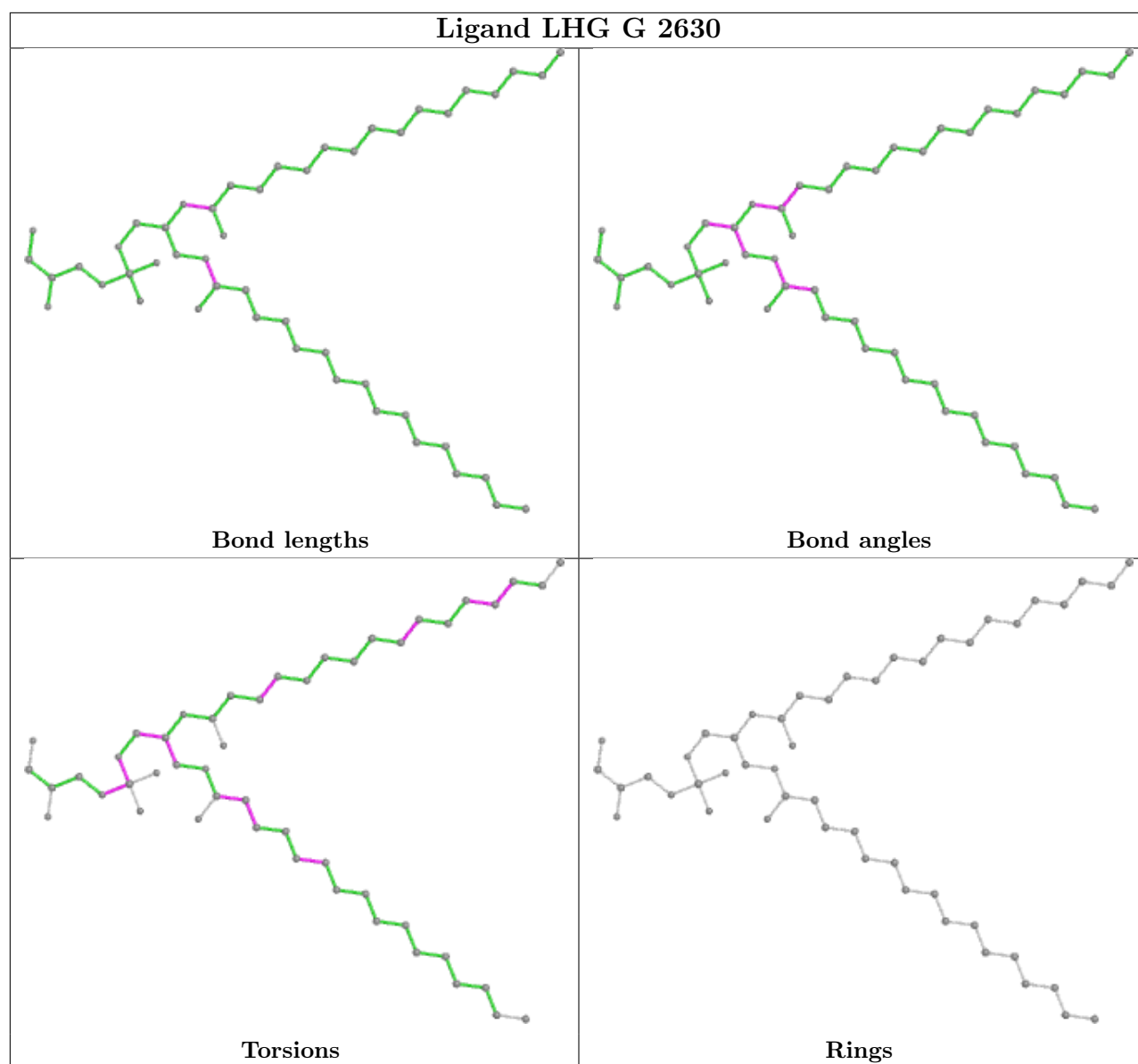
Ligand CLA c 512**Ligand CLA C 502**

Ligand CLA R 609

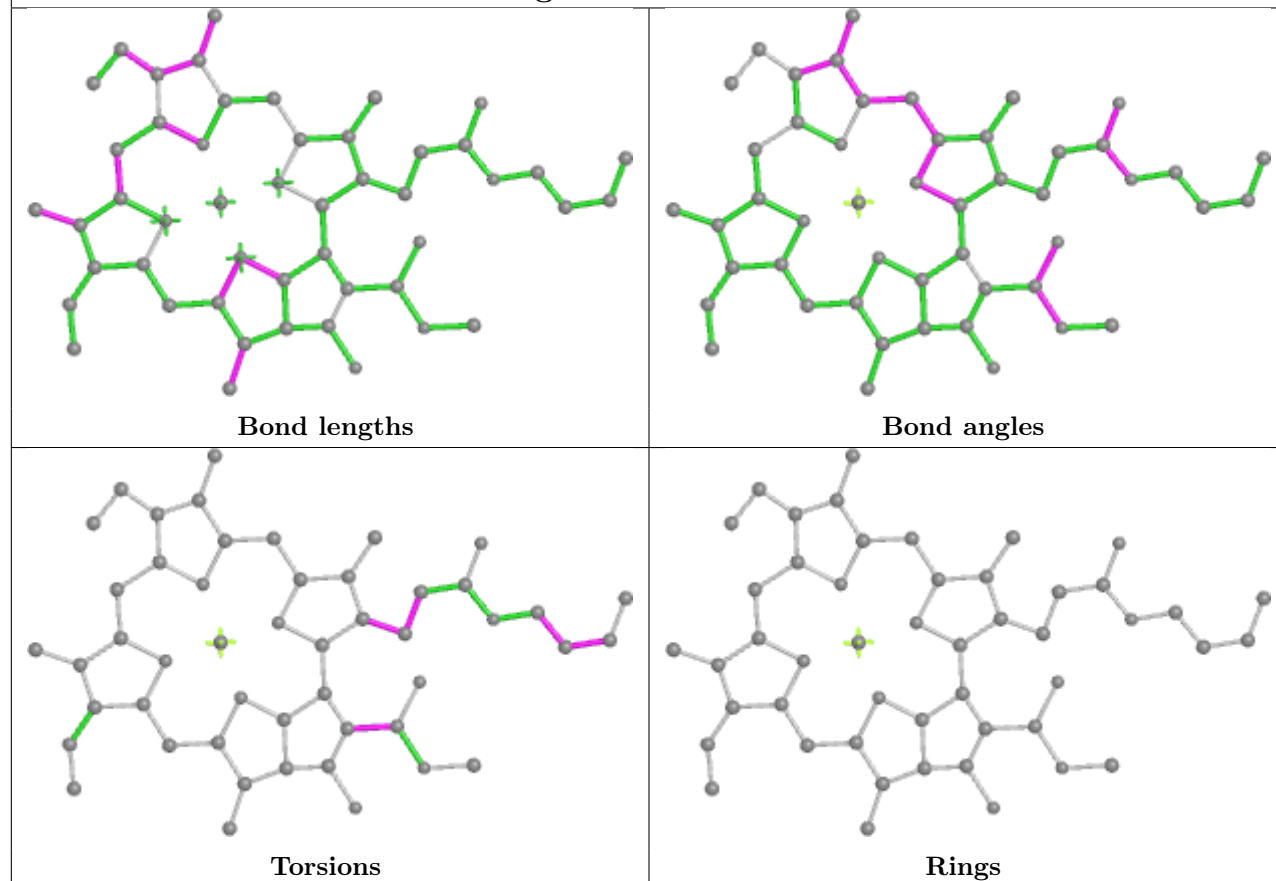




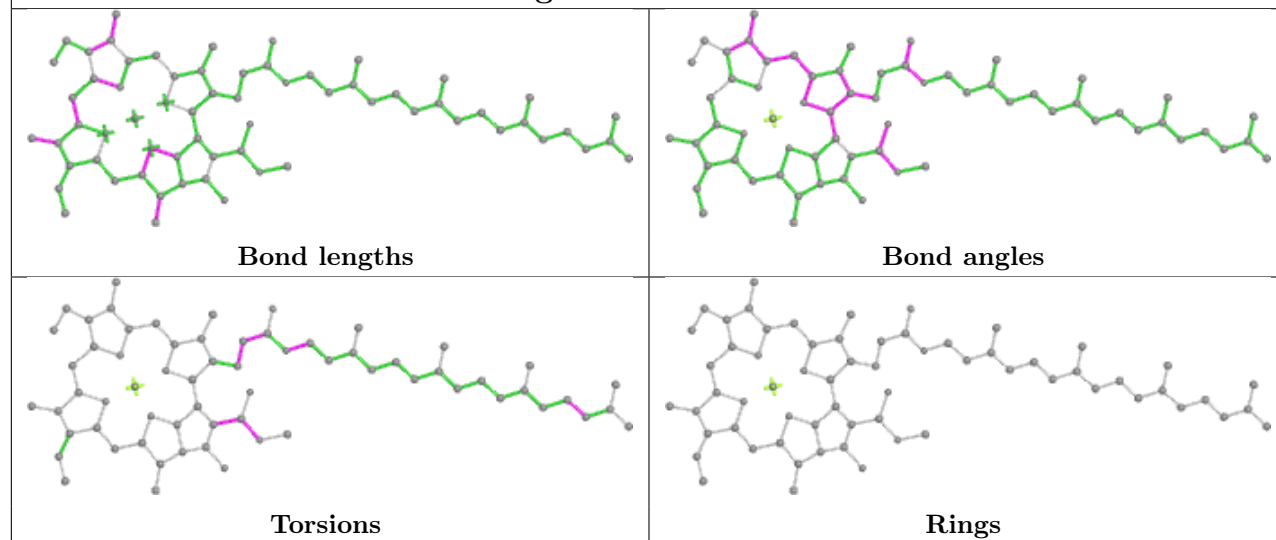




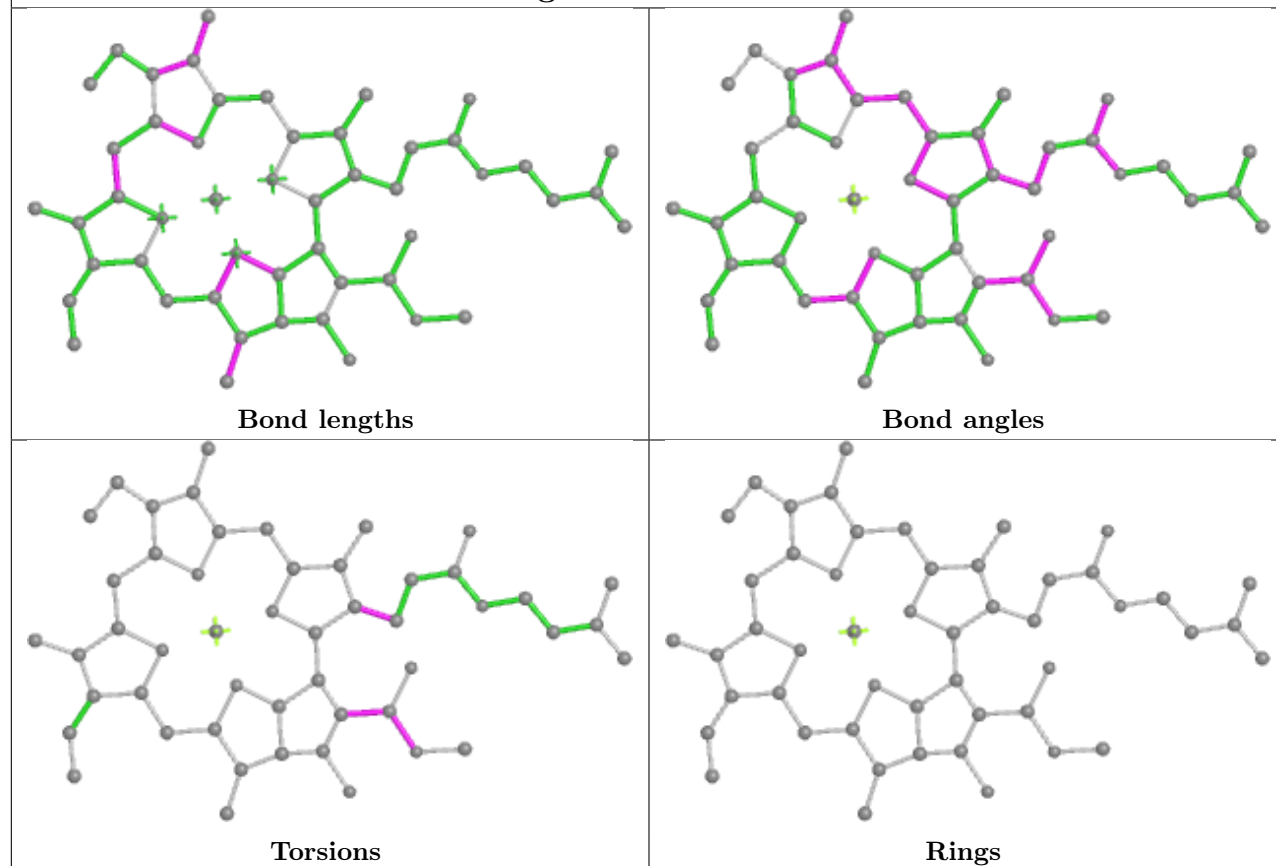
Ligand CLA S 610



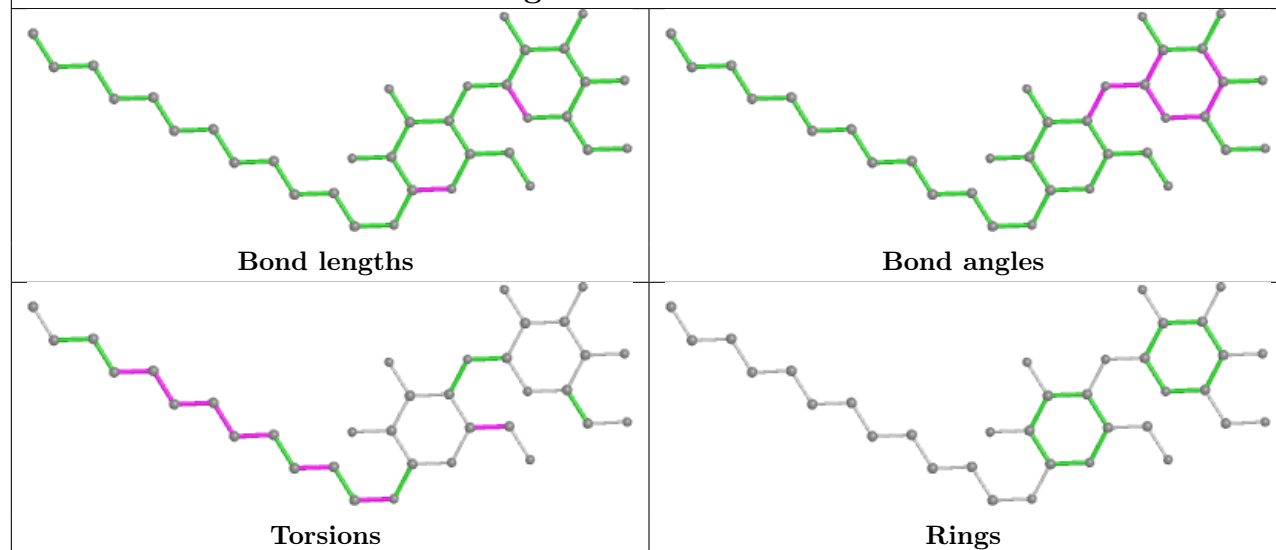
Ligand CLA b 611

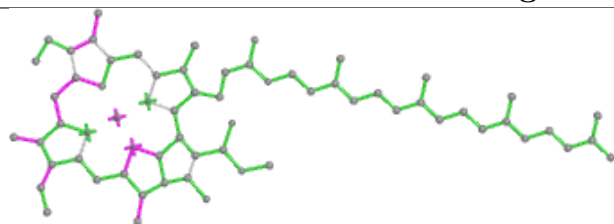


Ligand CLA s 605

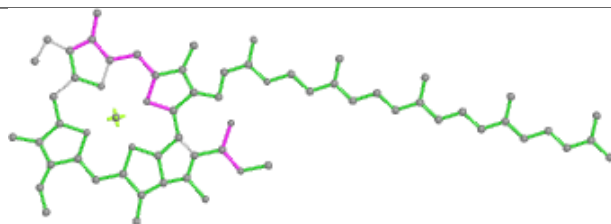


Ligand LMU z 2634

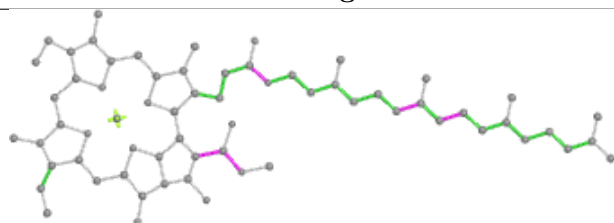


Ligand CLA c 502

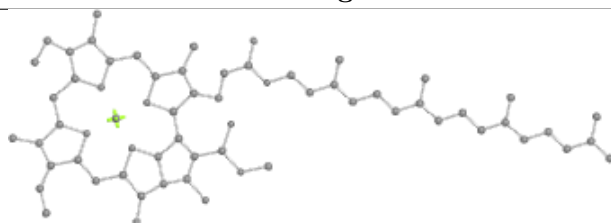
Bond lengths



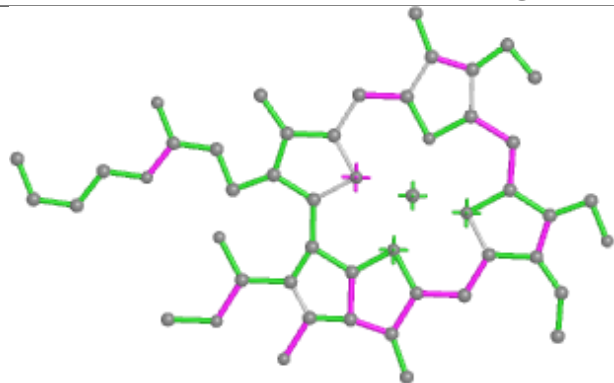
Bond angles



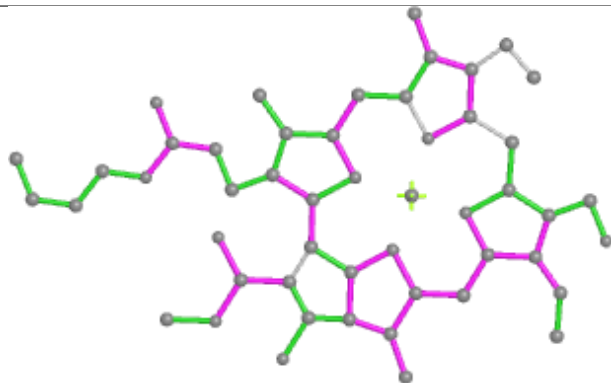
Torsions



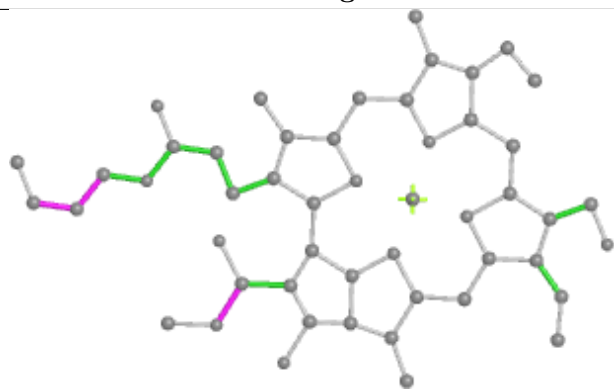
Rings

Ligand CHL Y 608

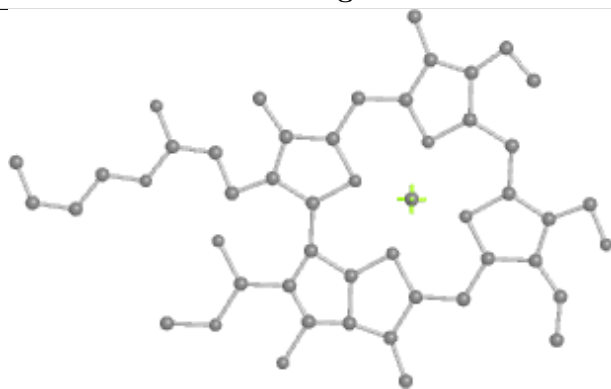
Bond lengths



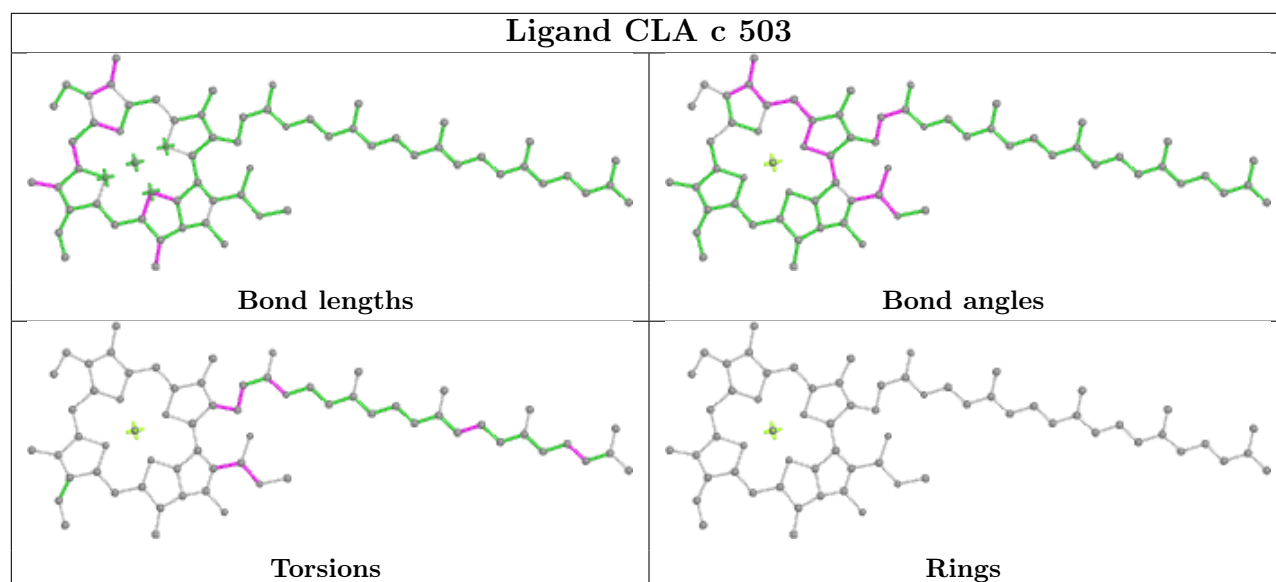
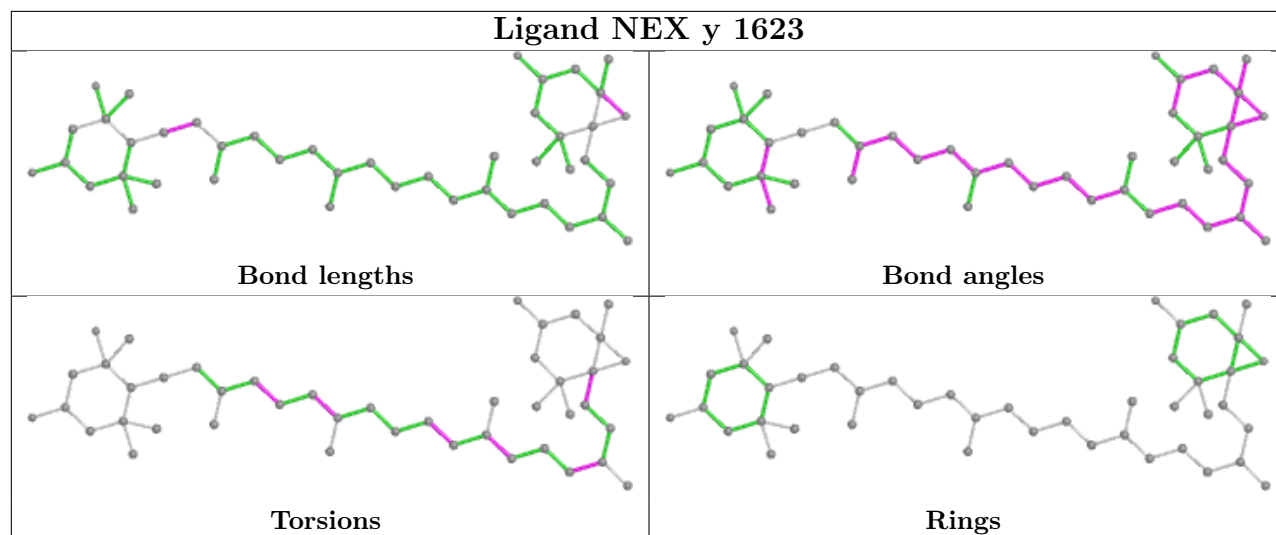
Bond angles

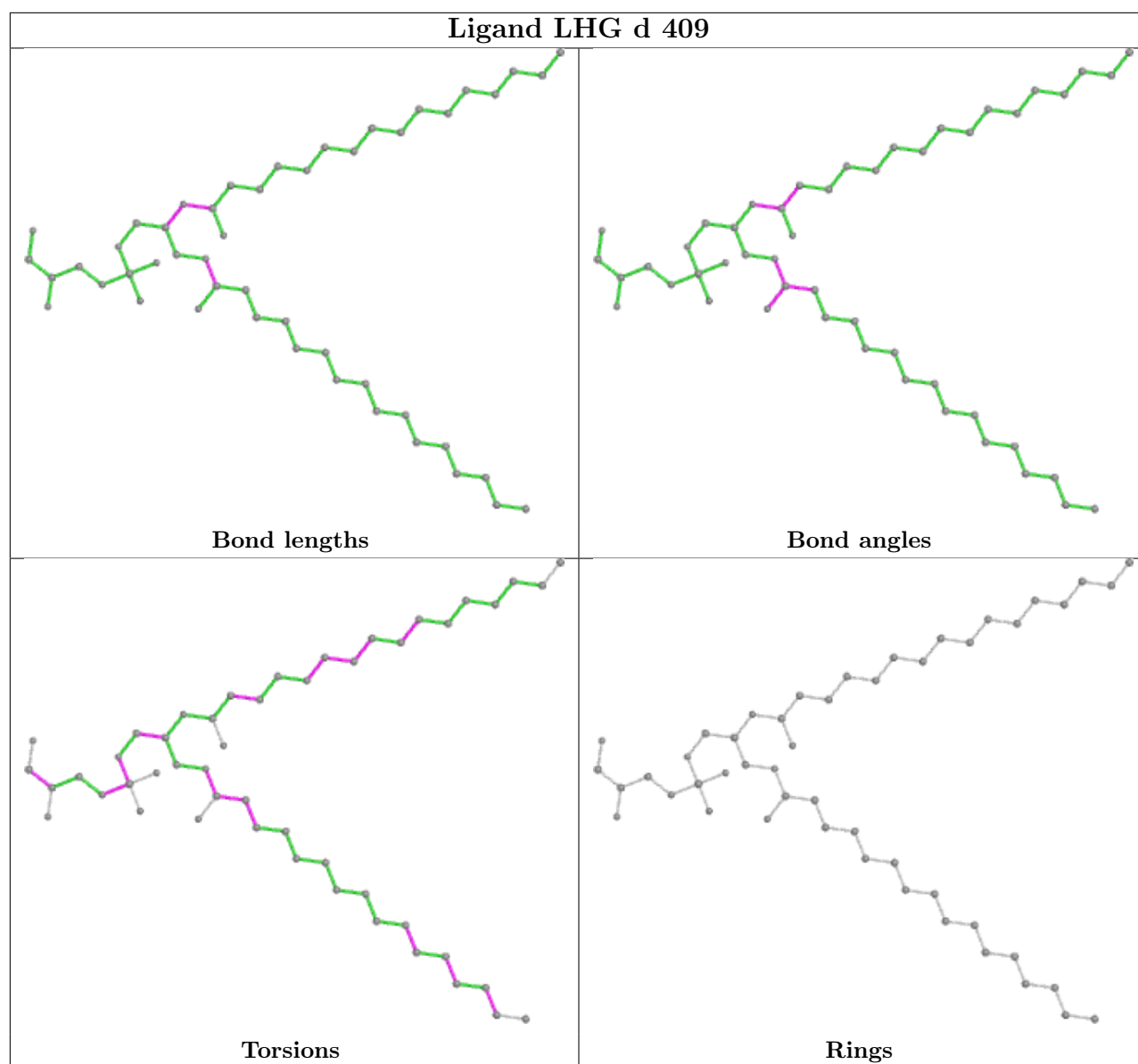


Torsions

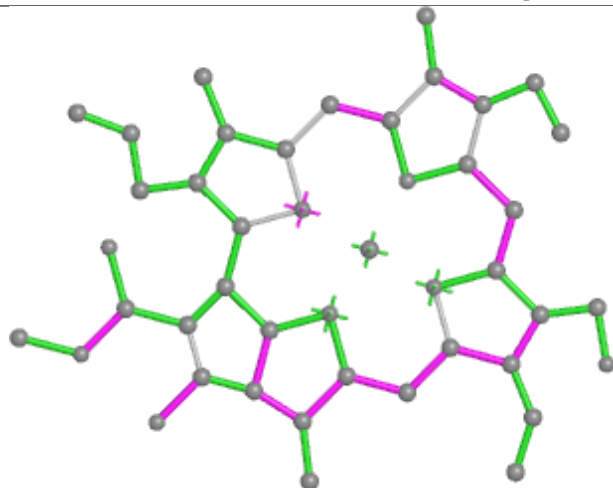


Rings

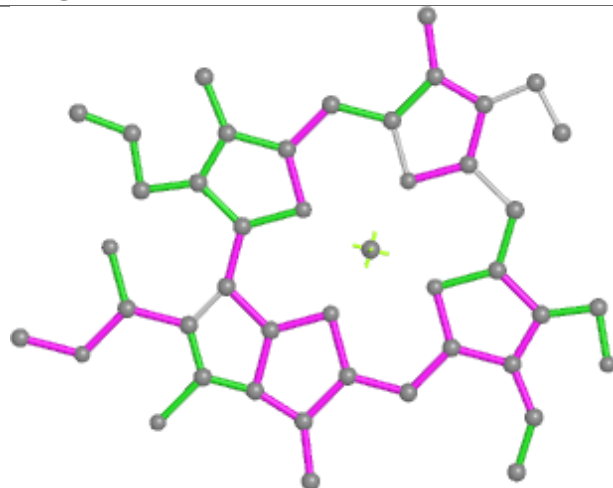




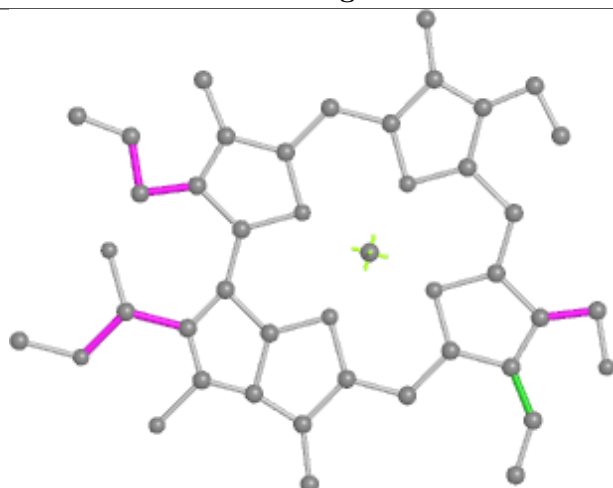
Ligand CHL g 608



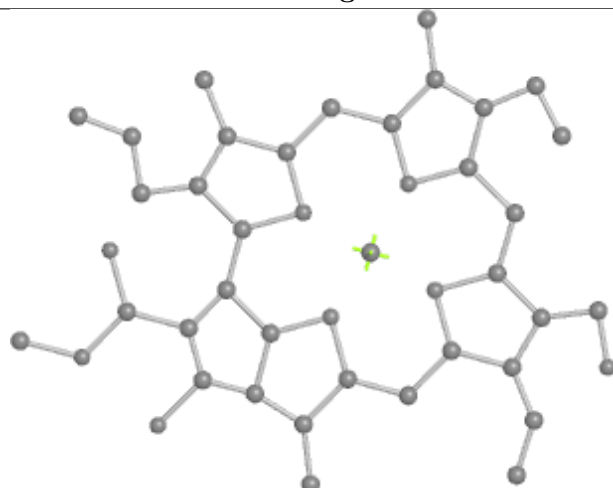
Bond lengths



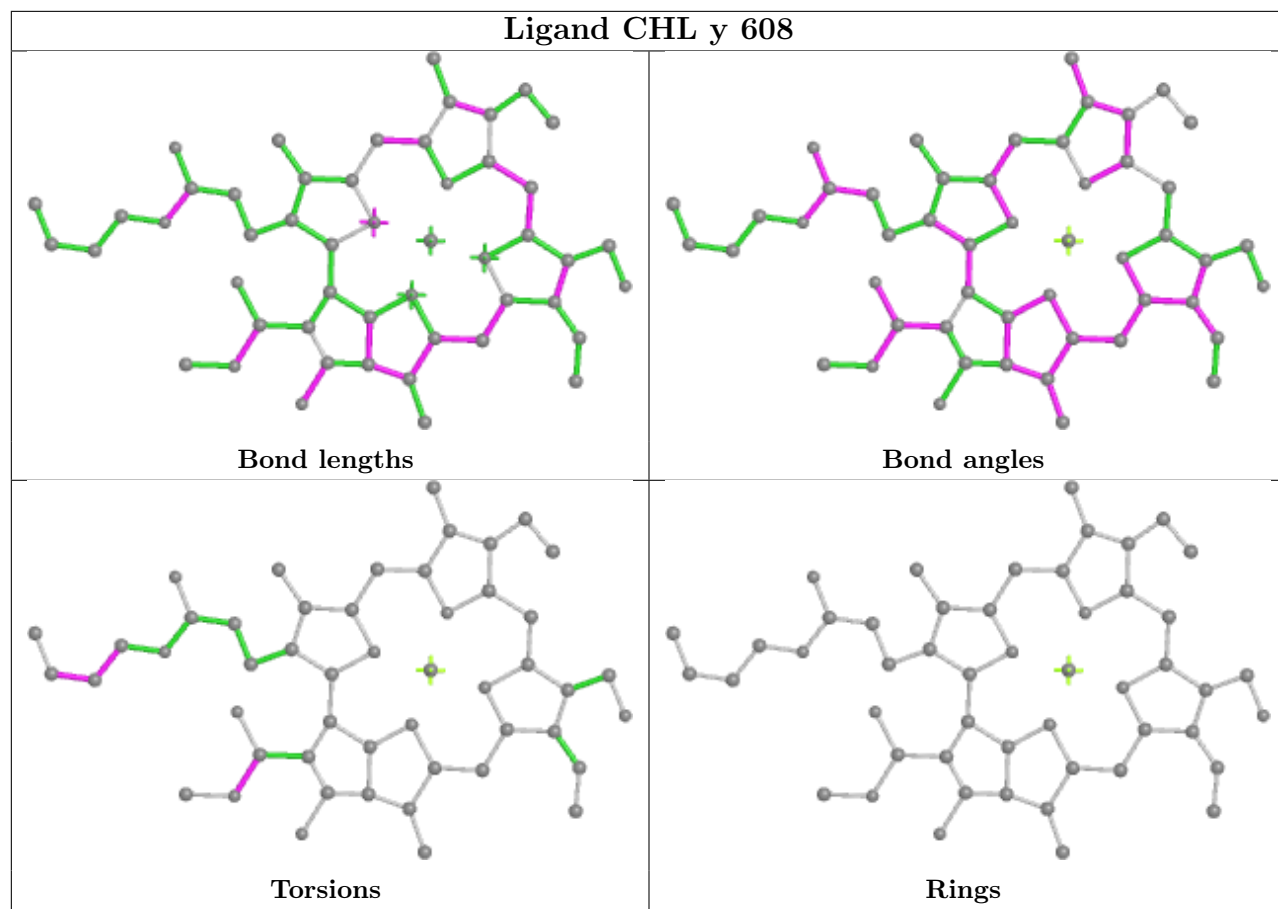
Bond angles



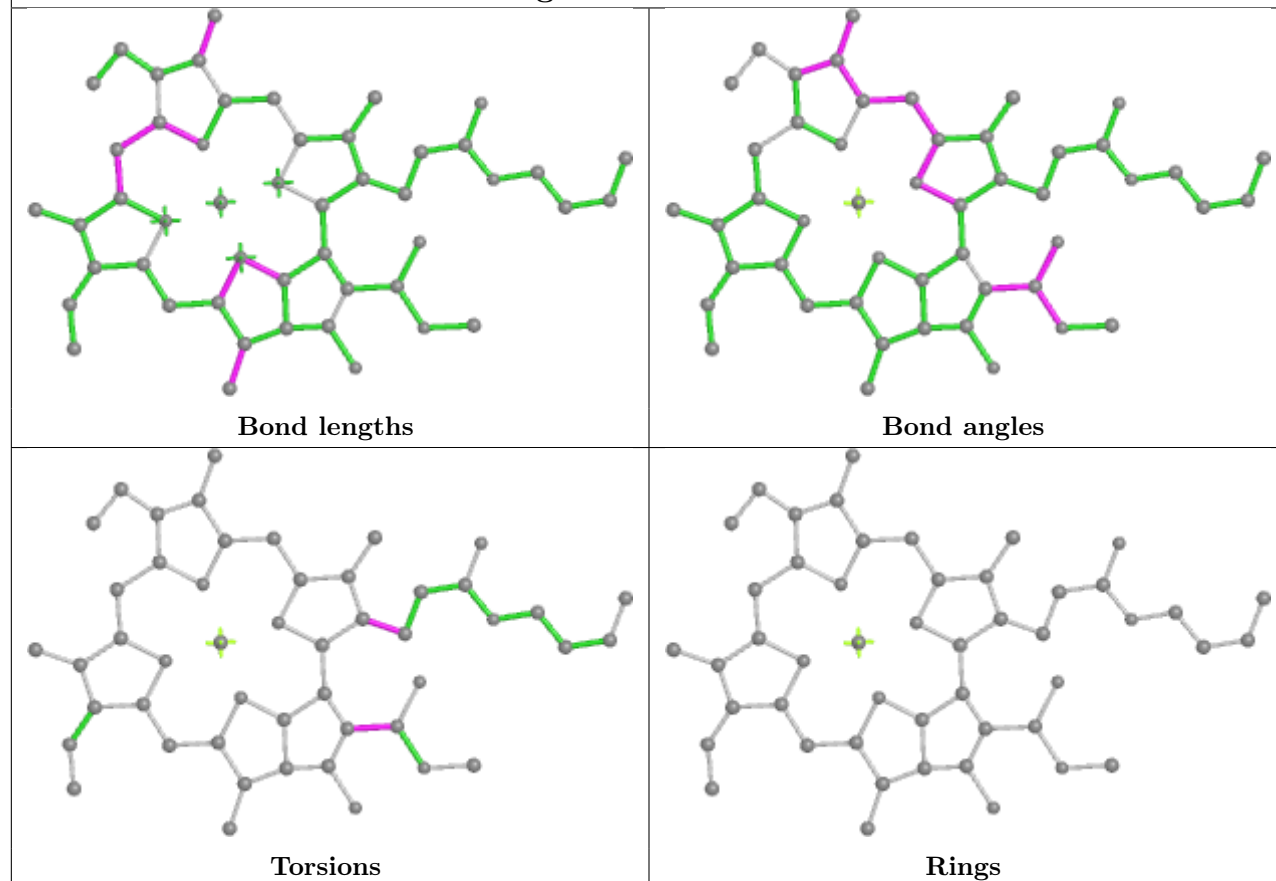
Torsions



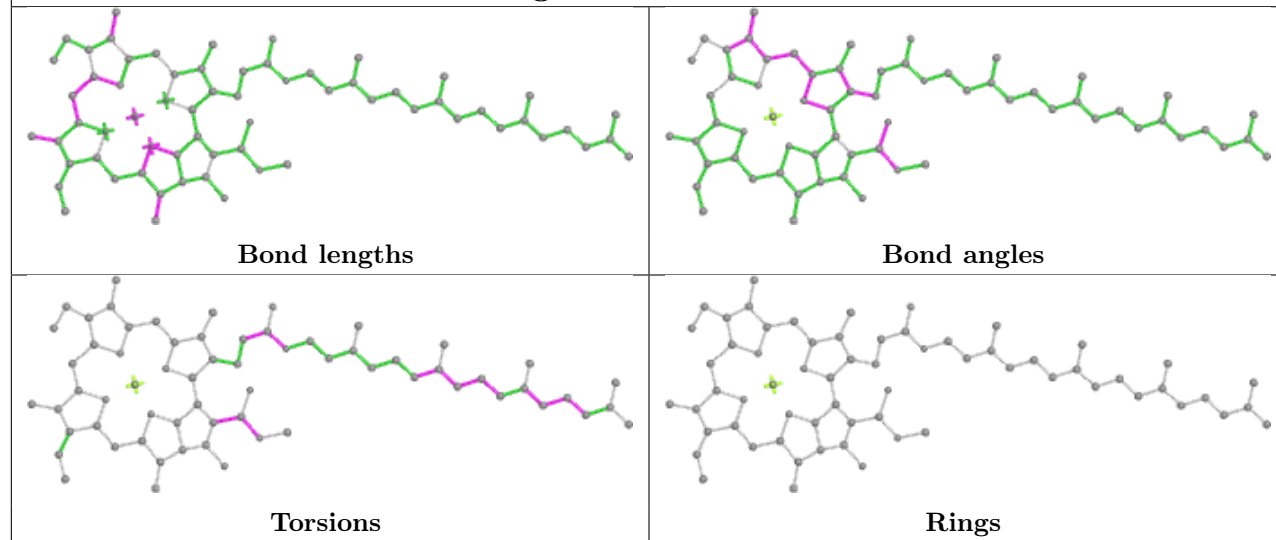
Rings

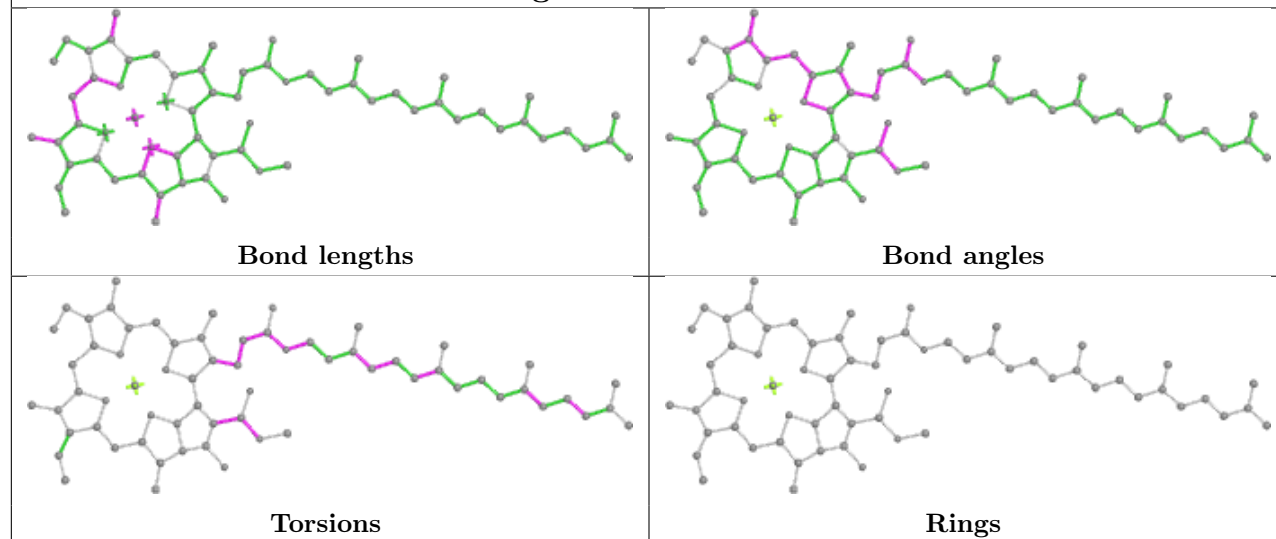
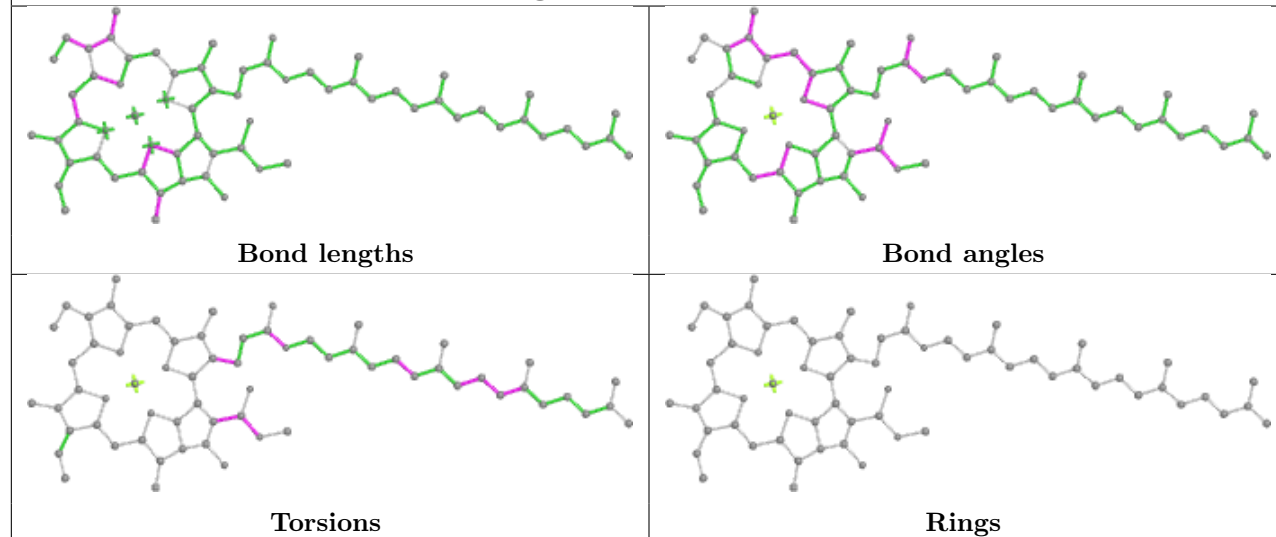
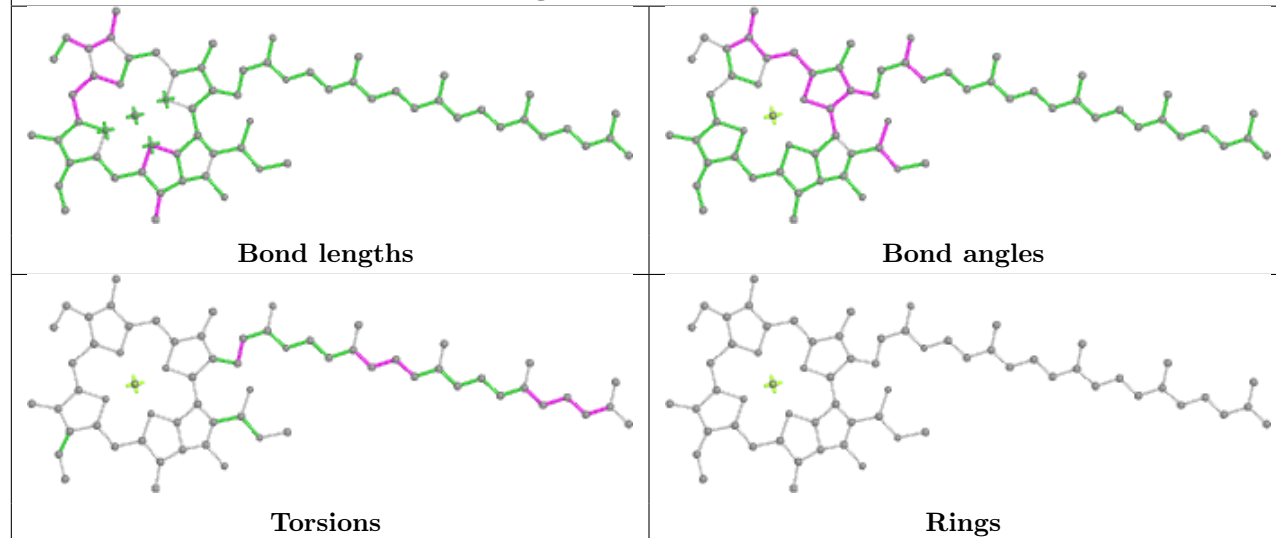


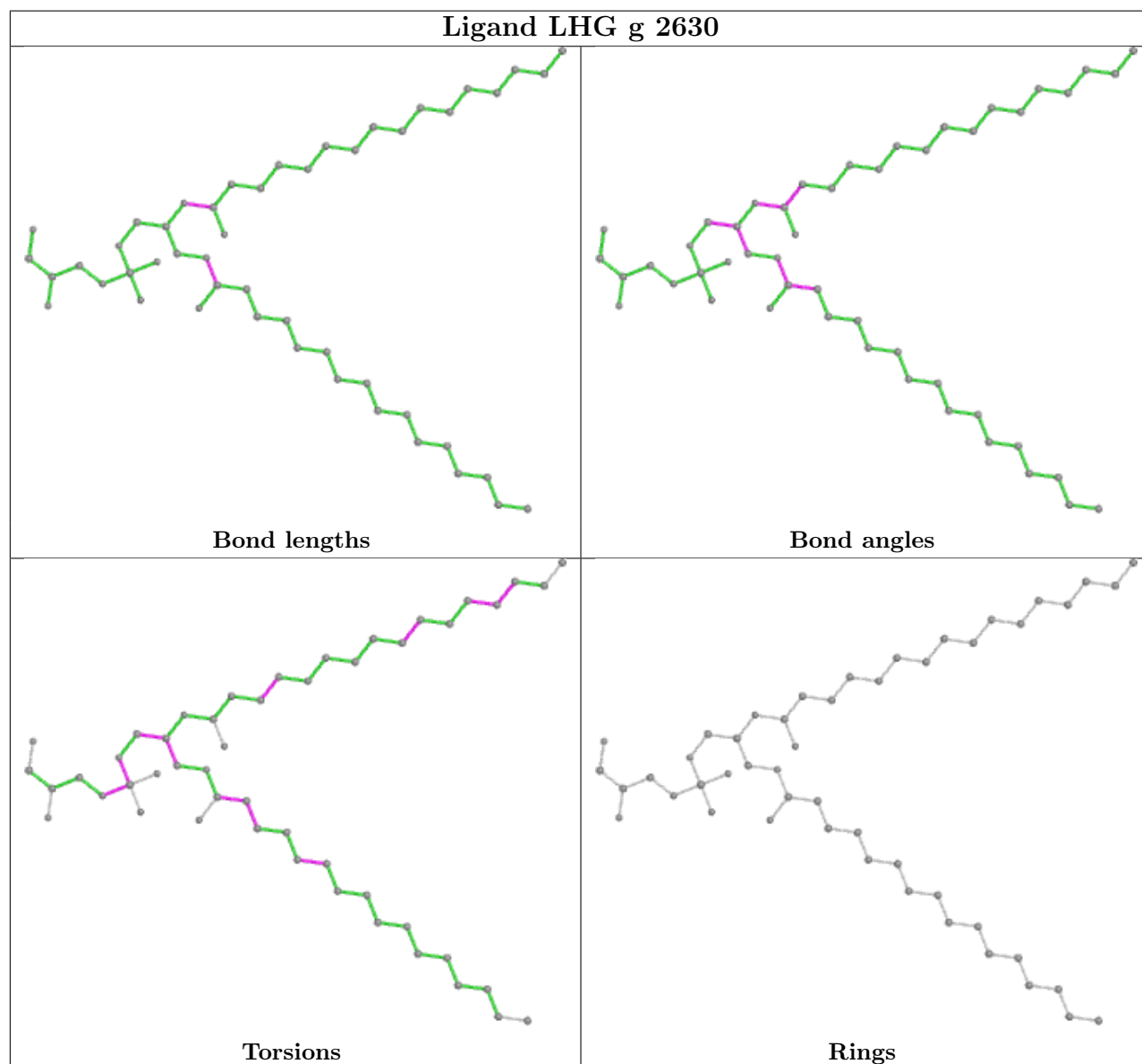
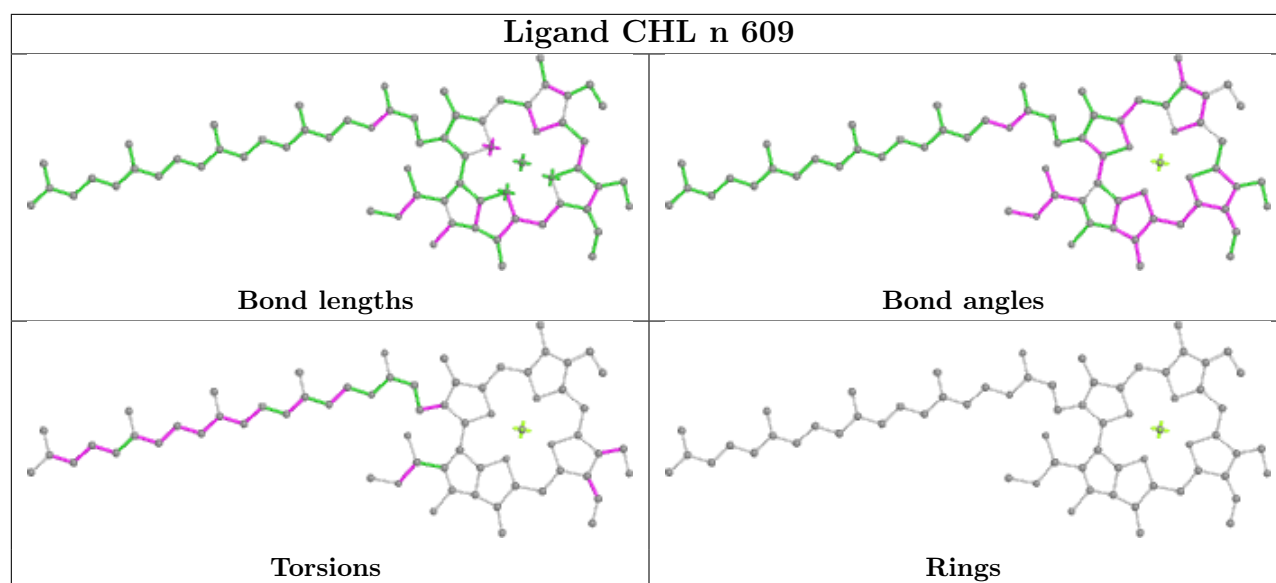
Ligand CLA a 407

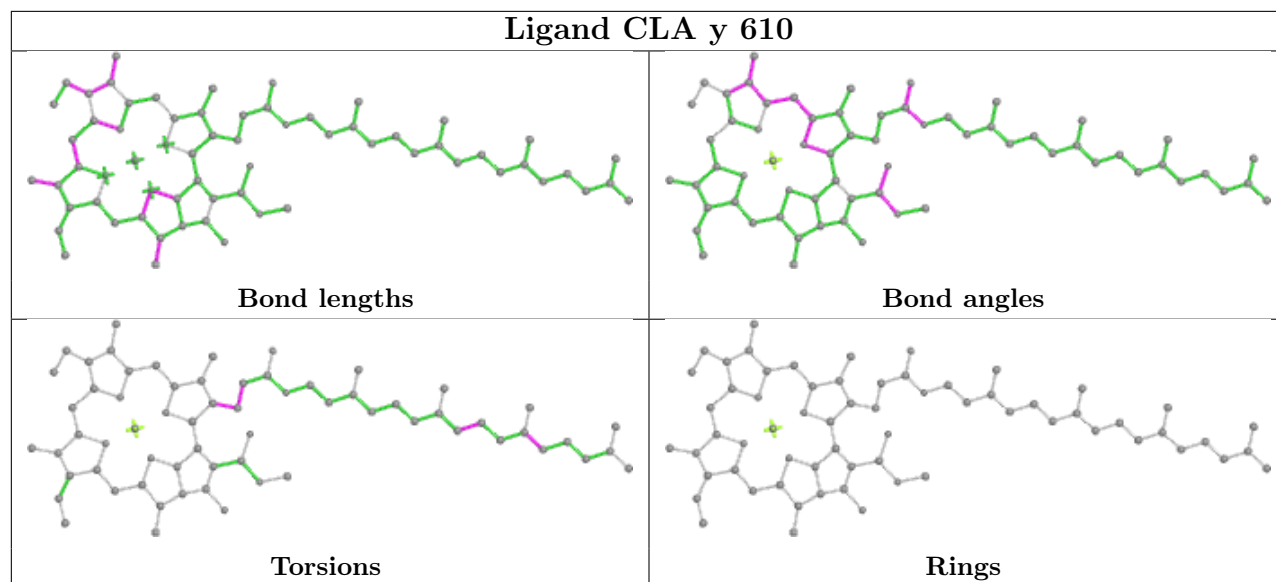
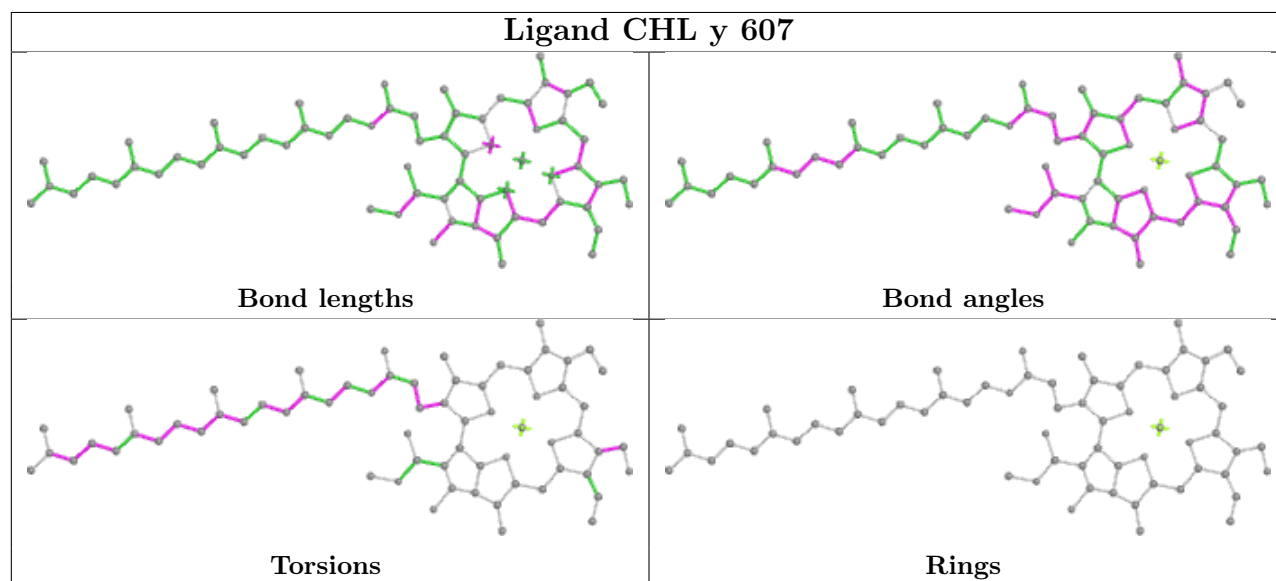


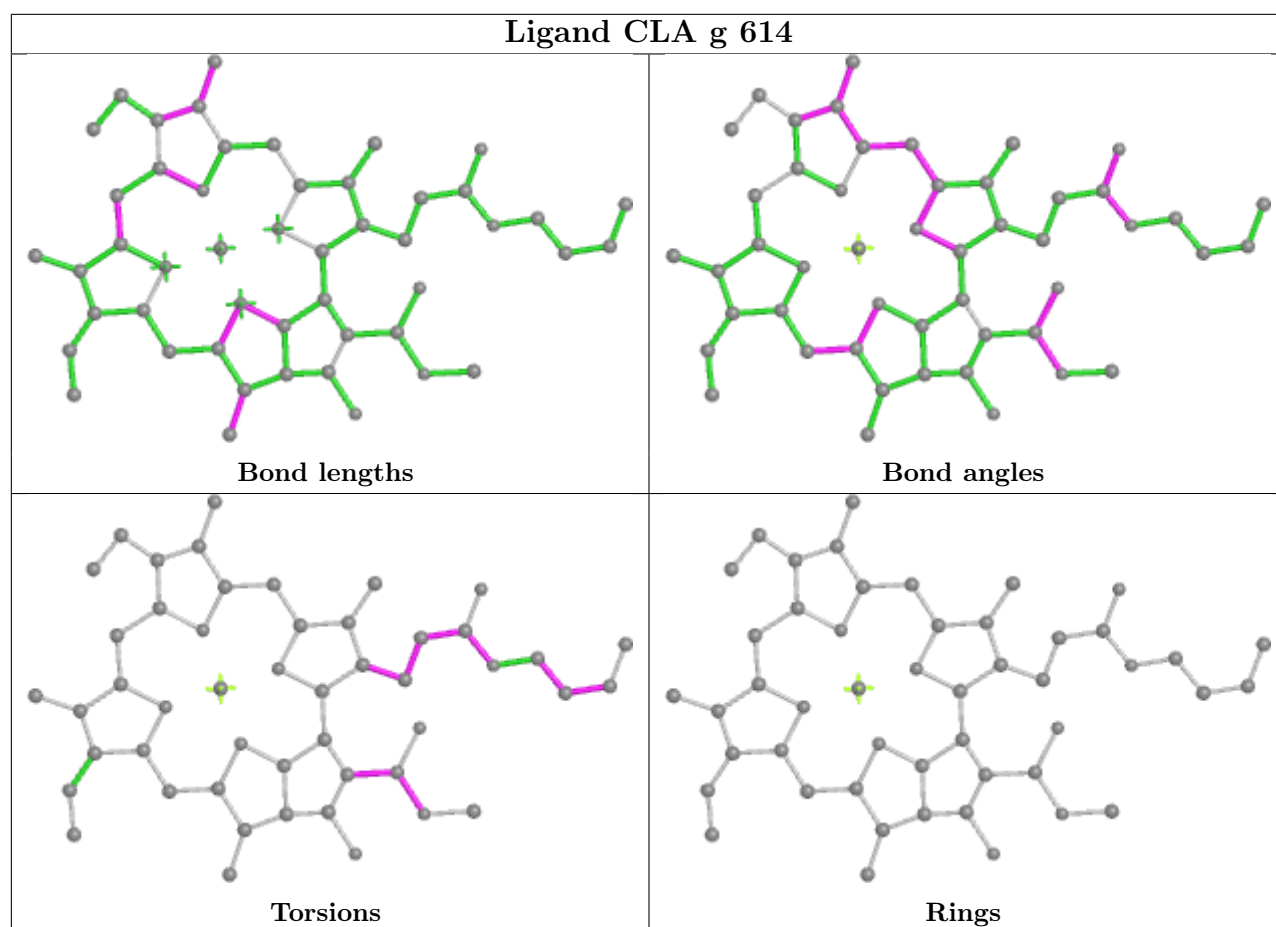
Ligand CLA C 510



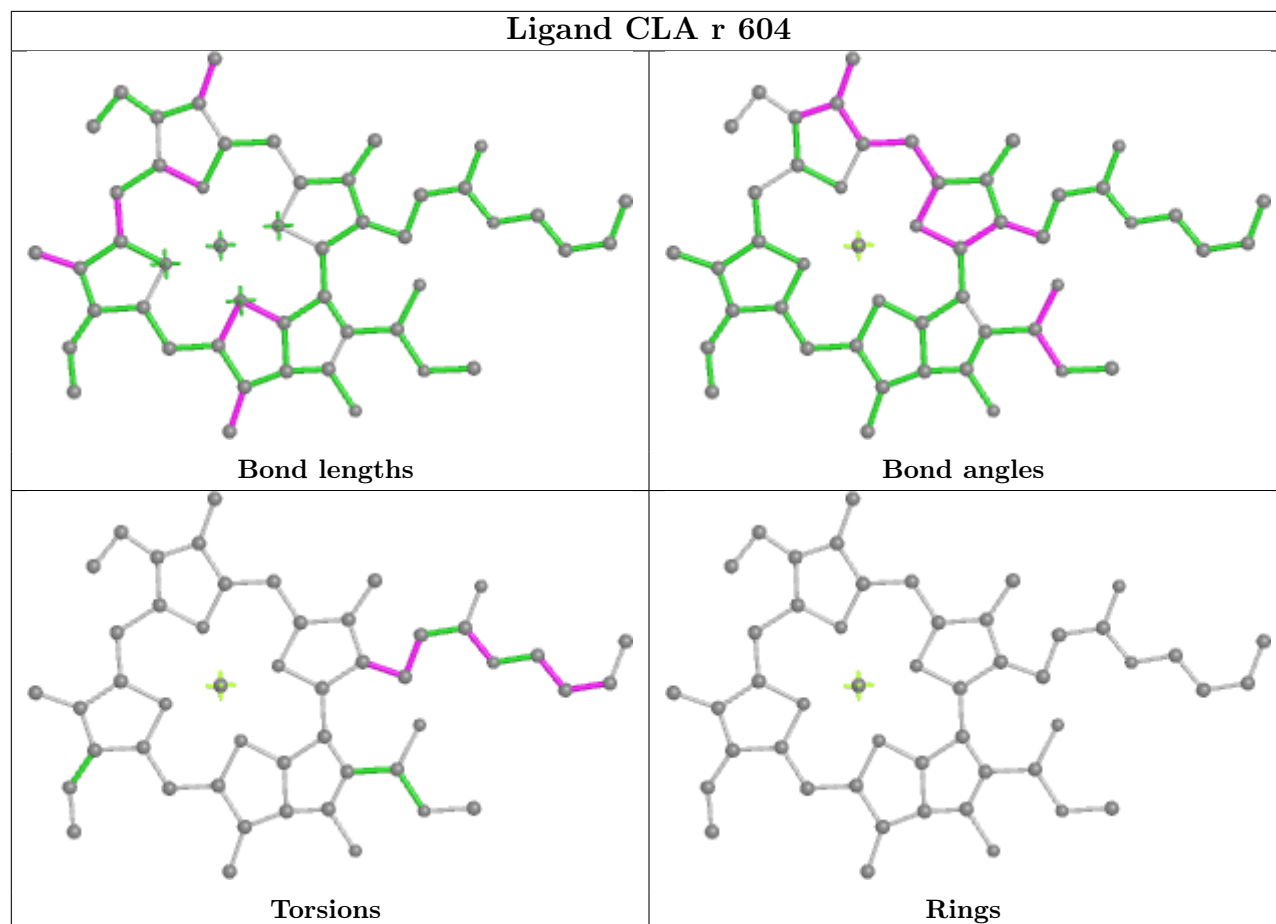
Ligand CLA C 513**Ligand CLA D 403****Ligand CLA C 507**



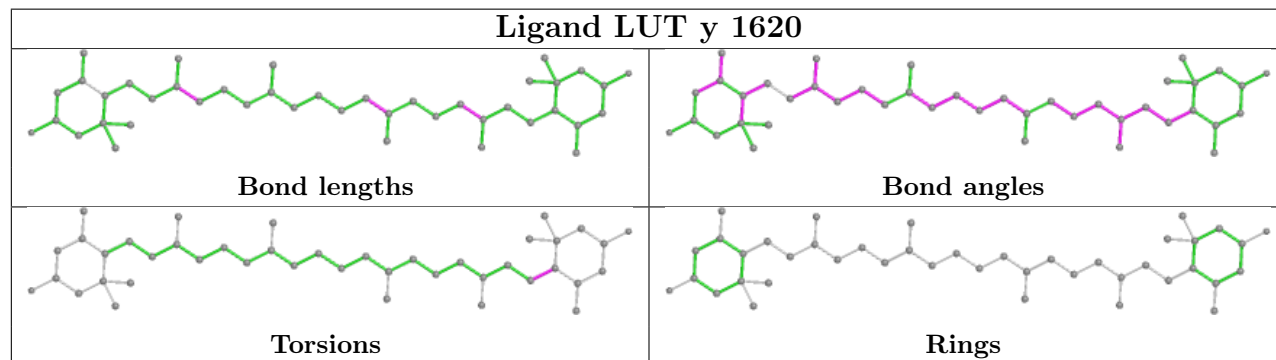
Ligand CLA y 610**Ligand CHL y 607**



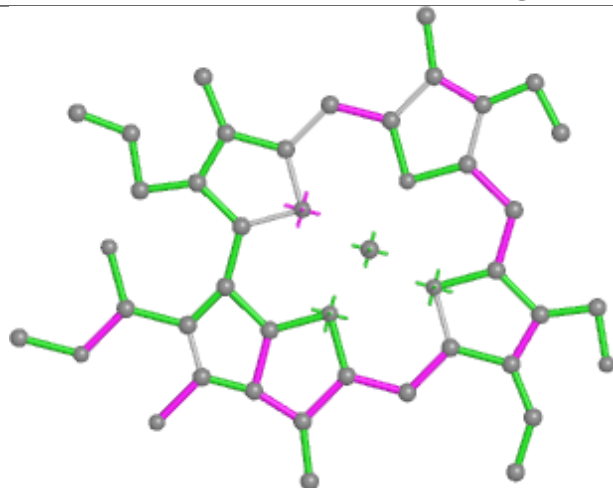
Ligand CLA r 604



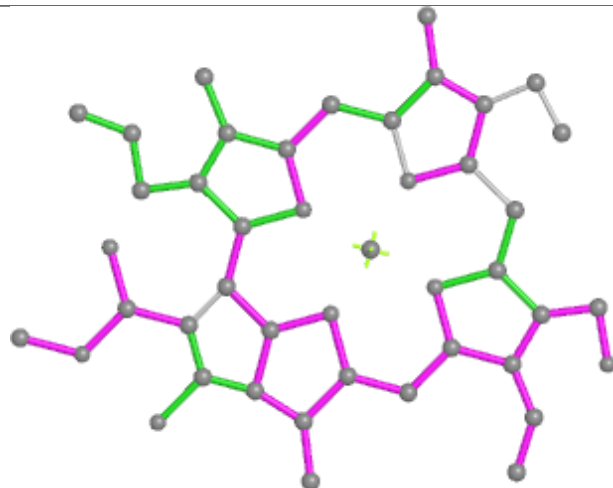
Ligand LUT y 1620



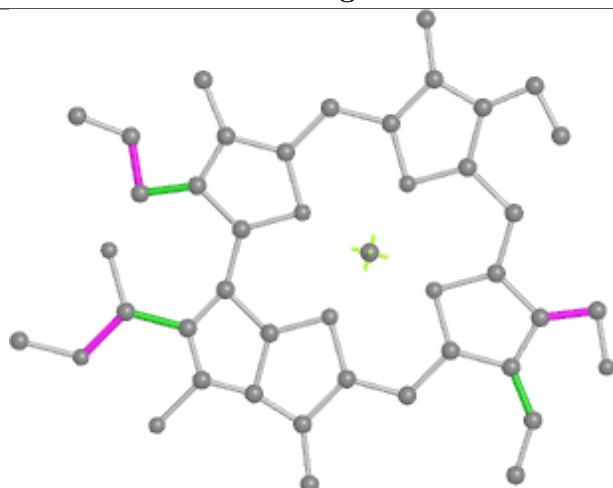
Ligand CHL R 606



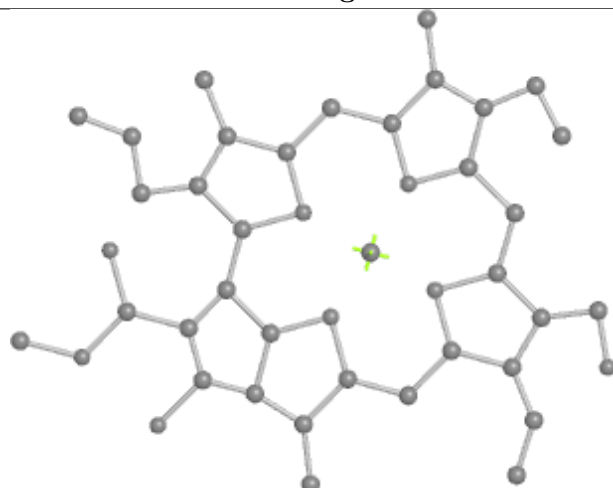
Bond lengths



Bond angles

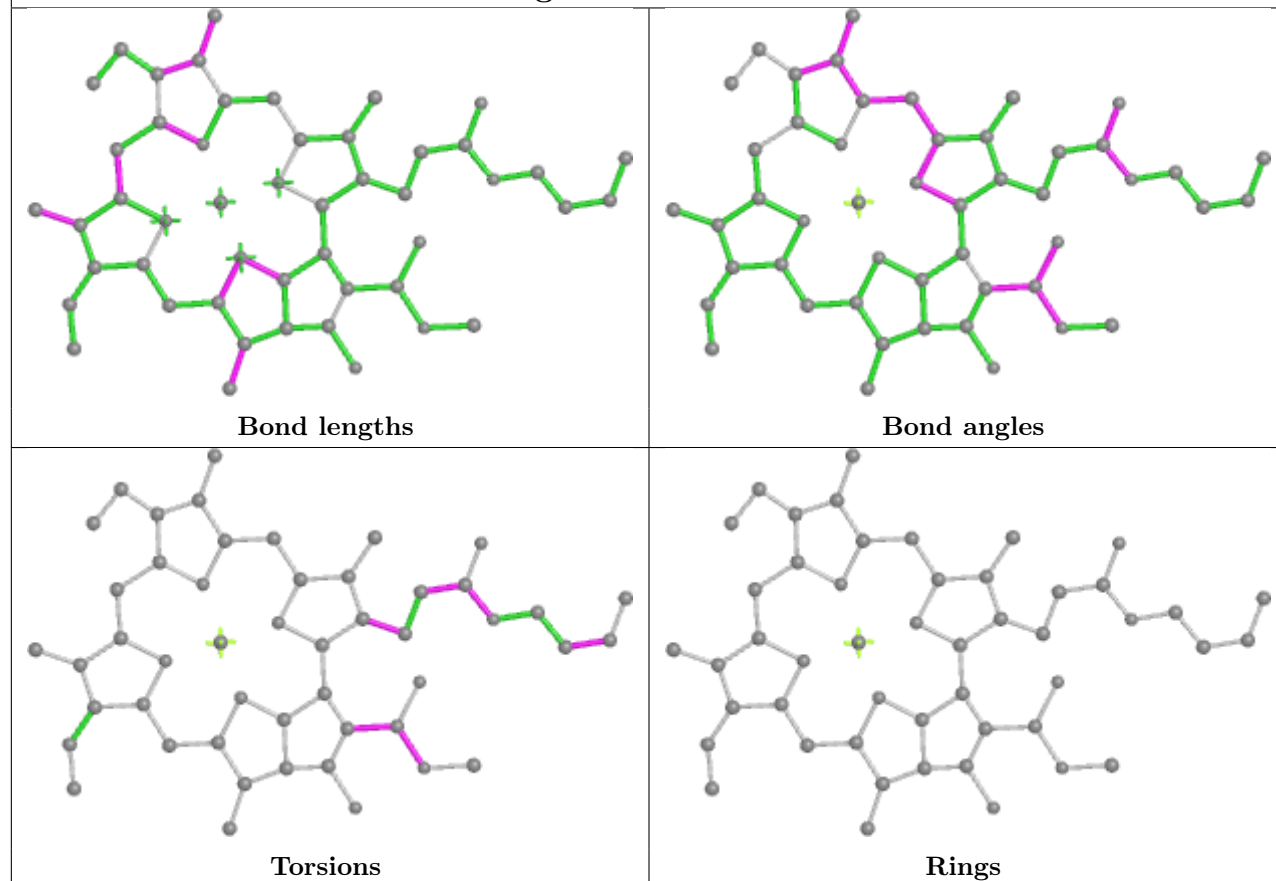


Torsions

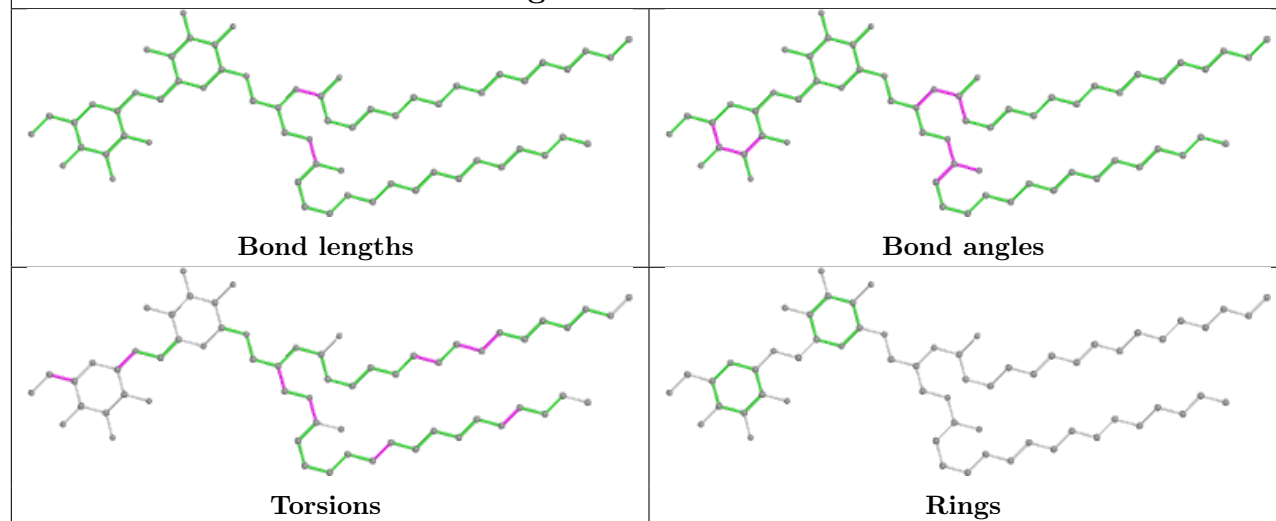


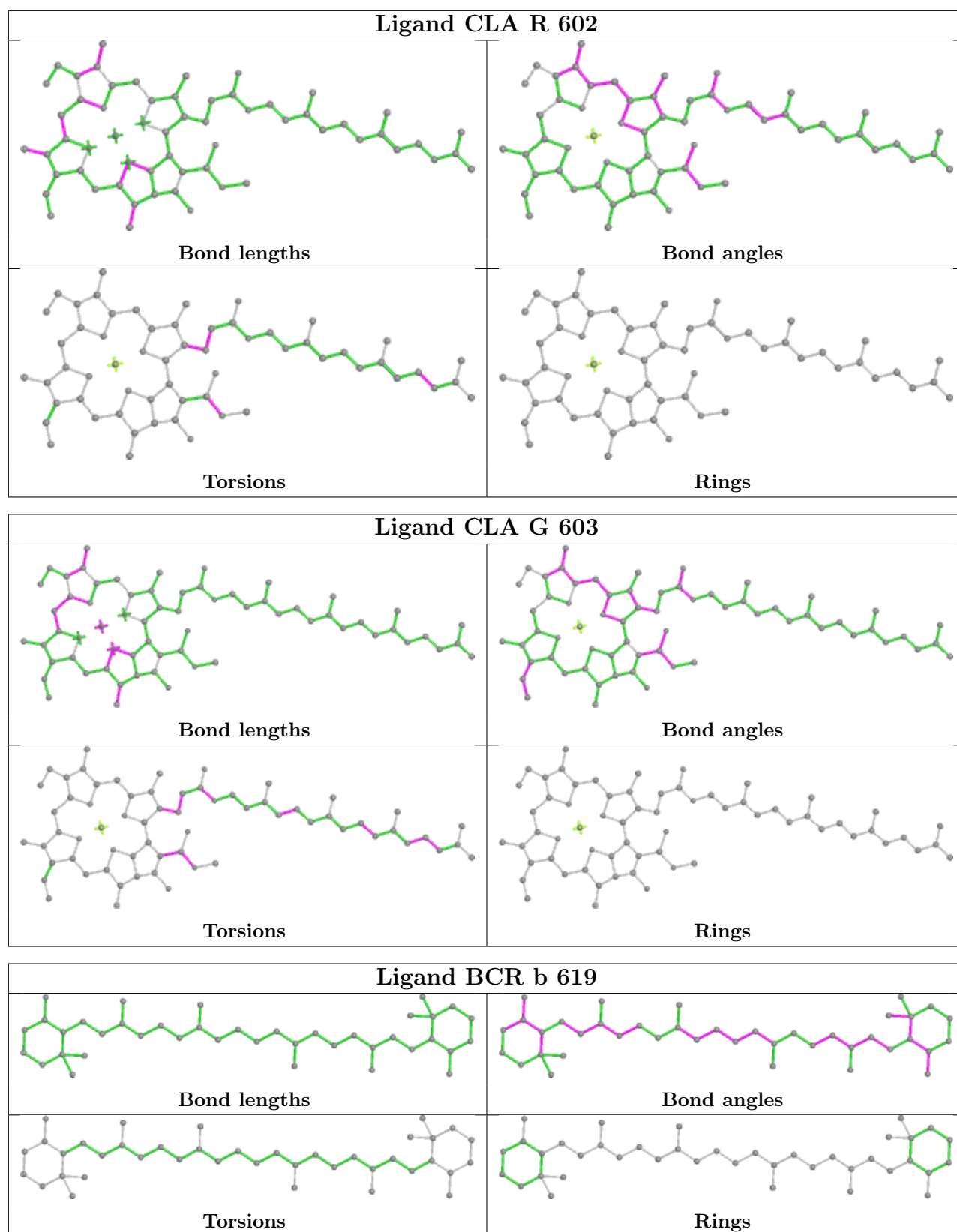
Rings

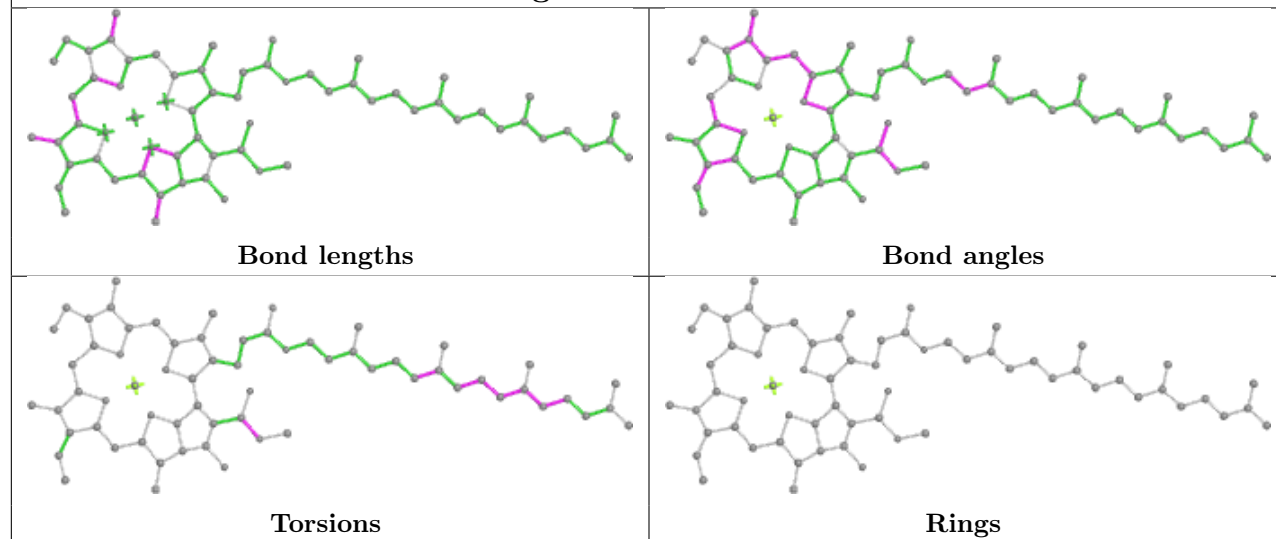
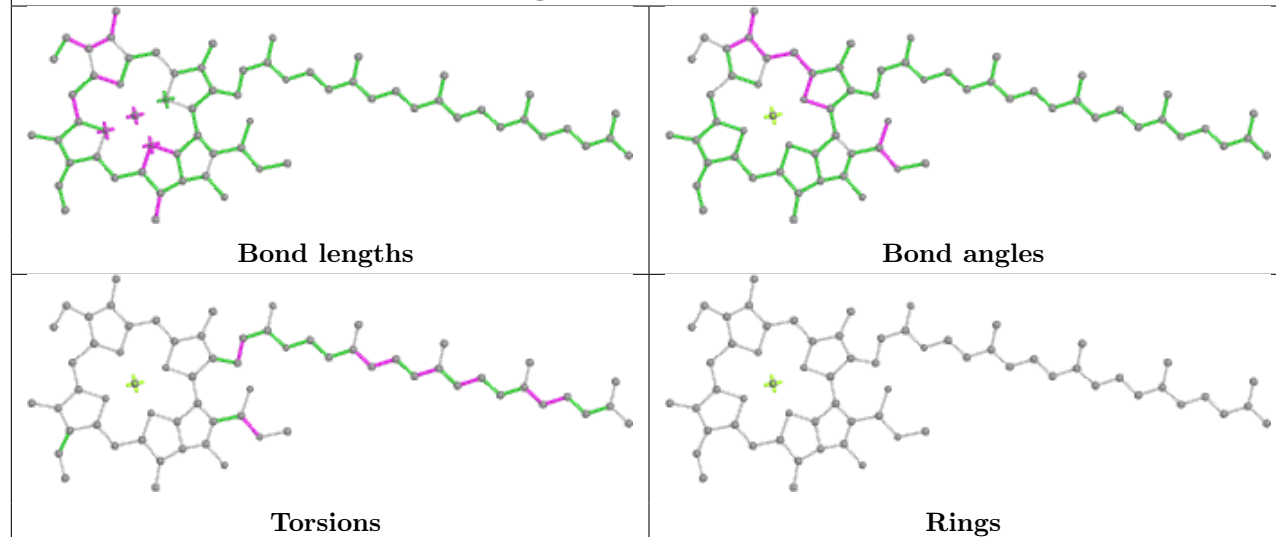
Ligand CLA n 611



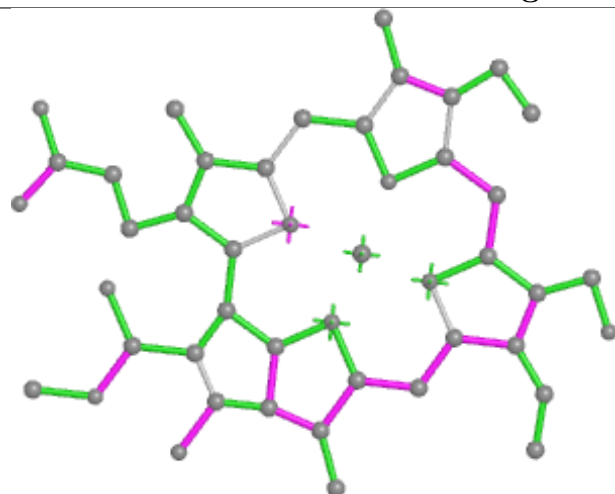
Ligand DGD C 519



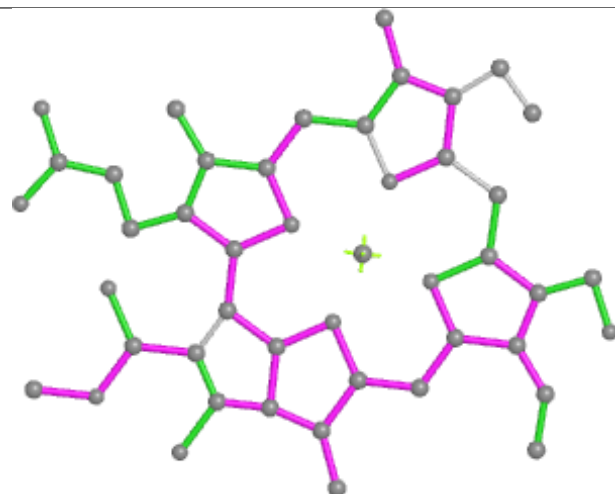


Ligand CLA B 612**Ligand CLA N 613**

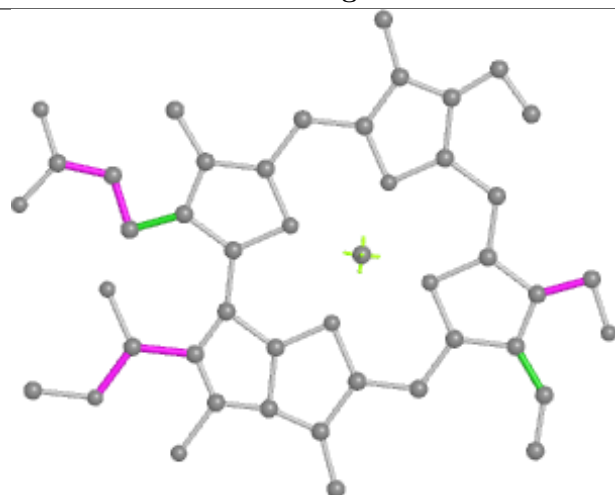
Ligand CHL s 601



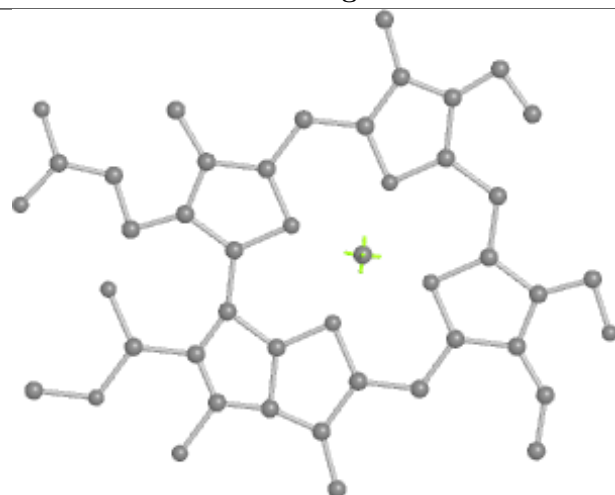
Bond lengths



Bond angles

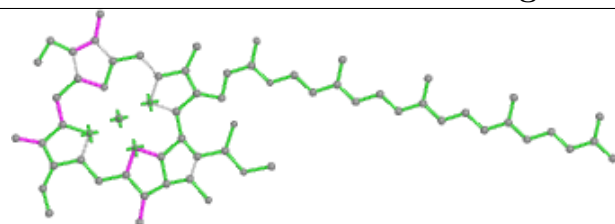


Torsions

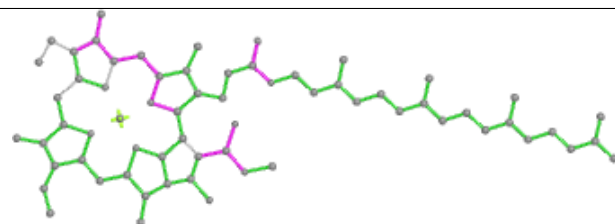


Rings

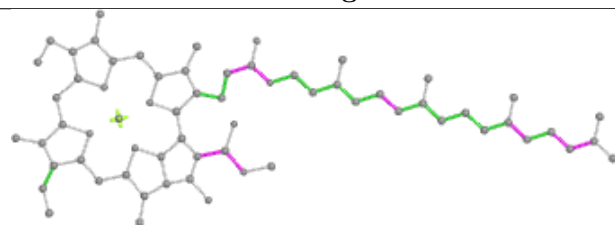
Ligand CLA b 602



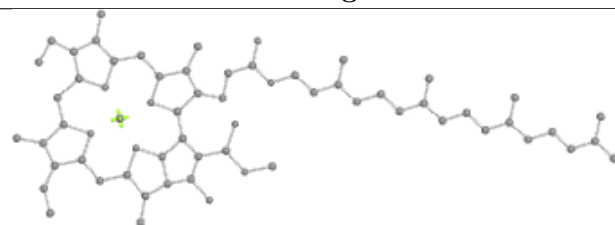
Bond lengths



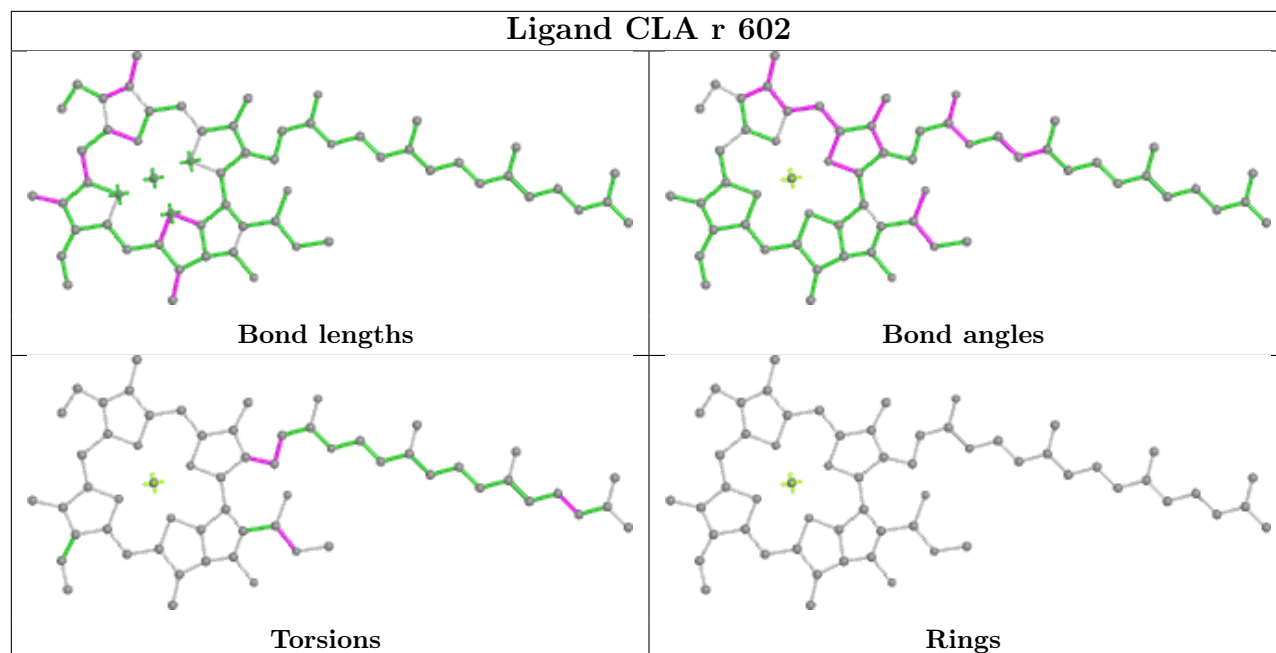
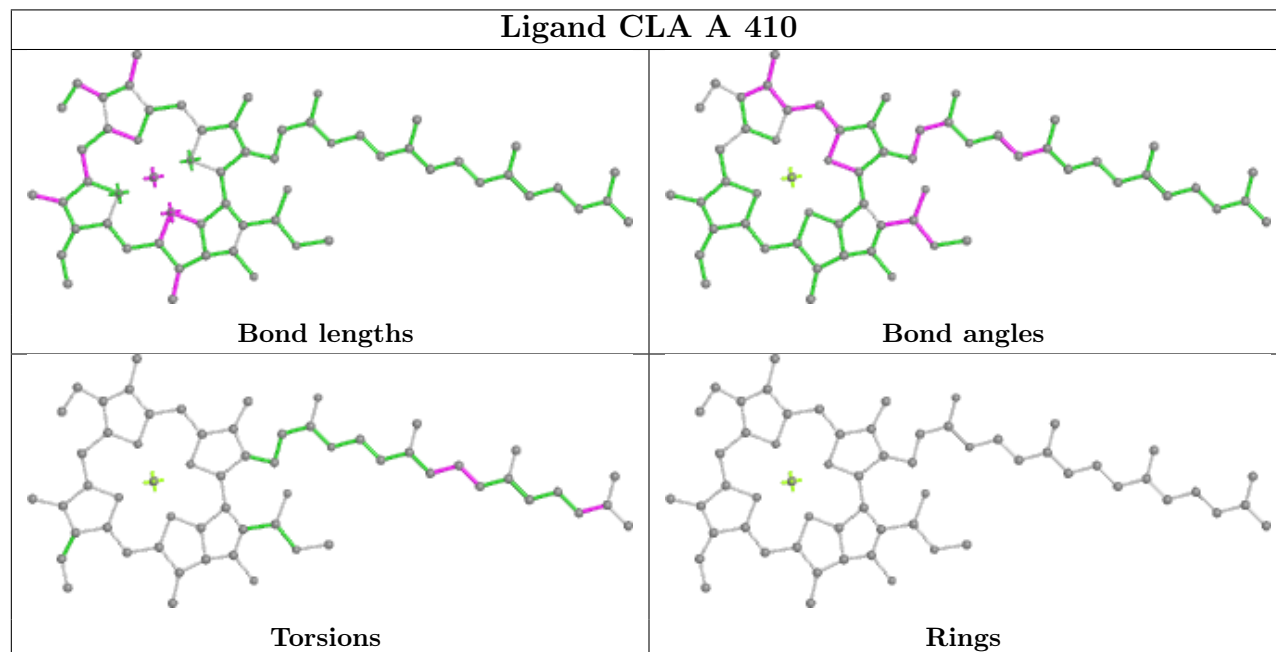
Bond angles

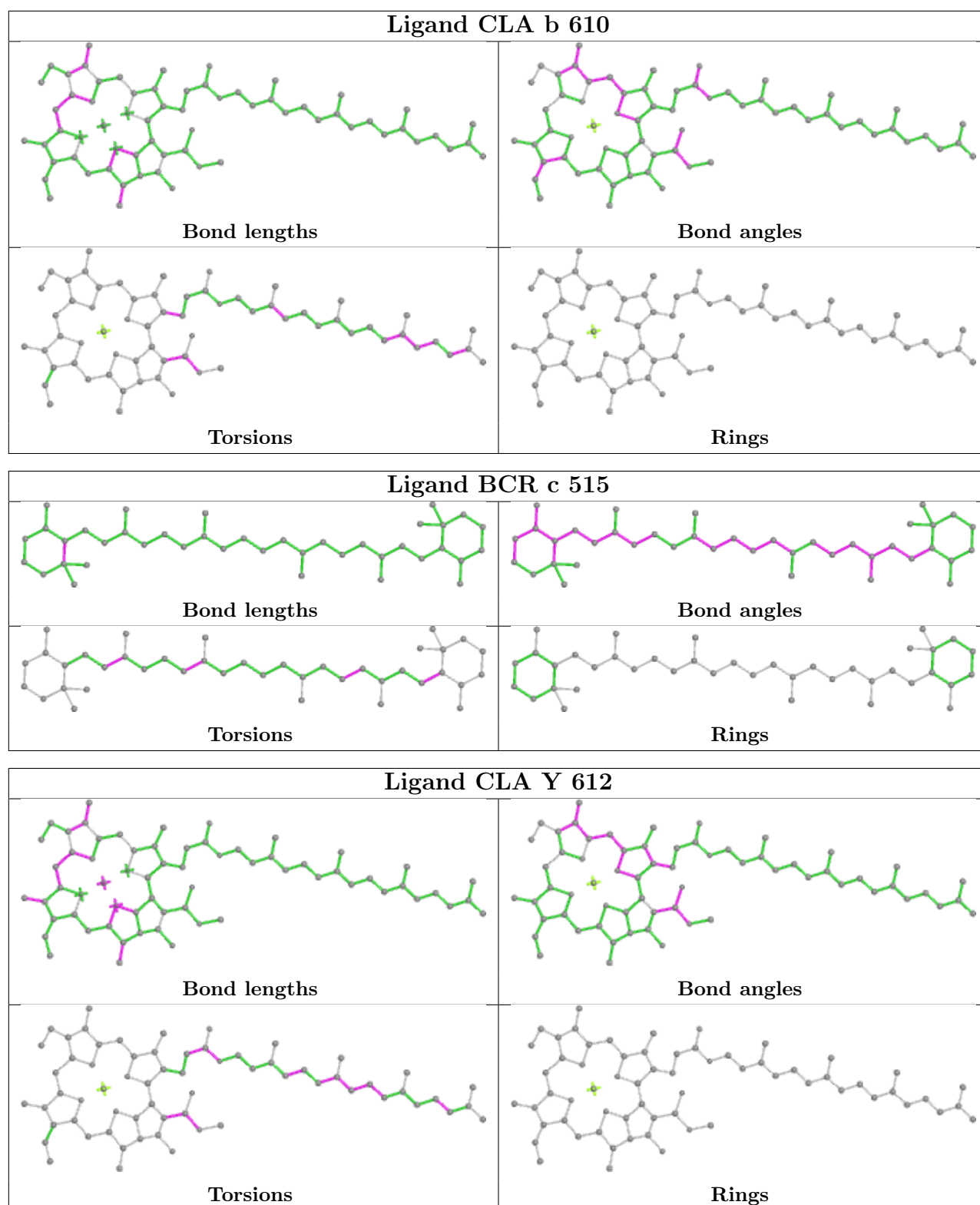


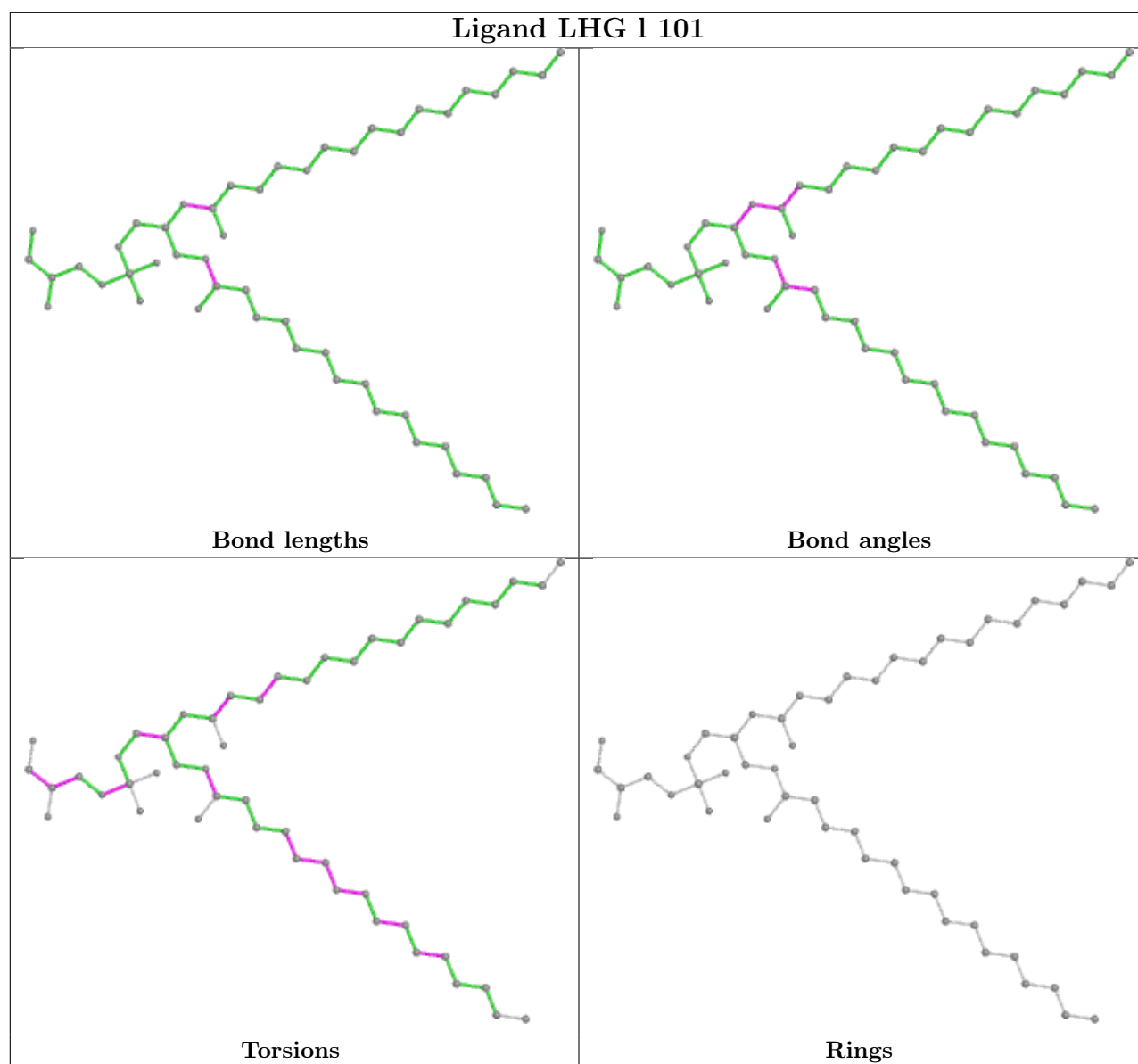
Torsions



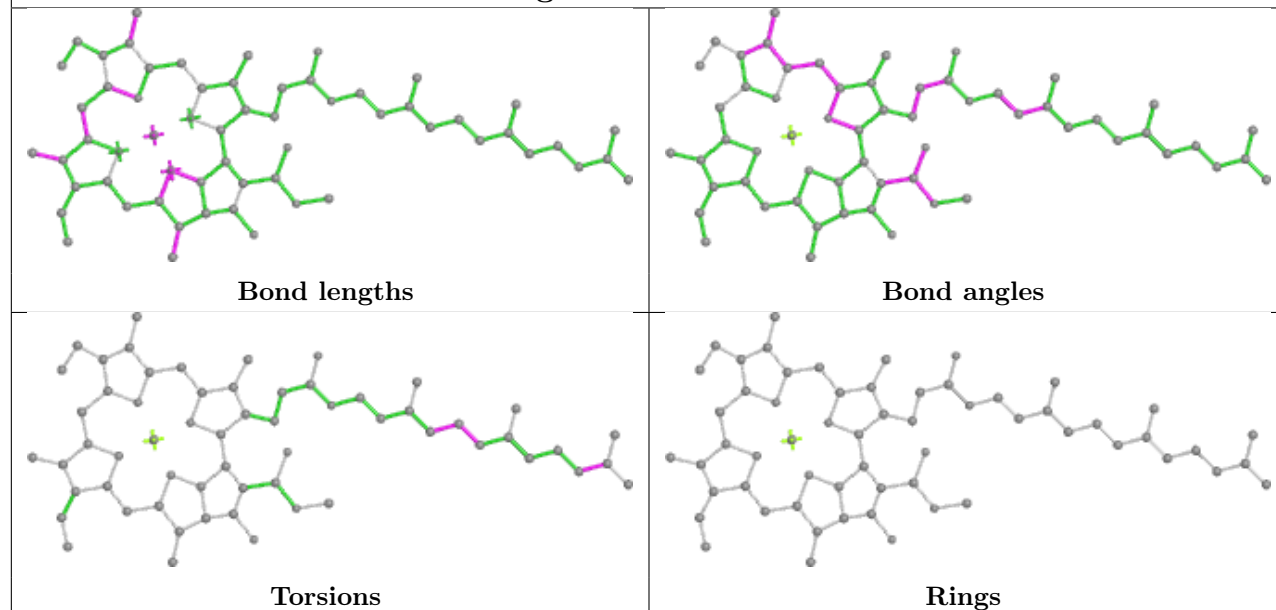
Rings

Ligand CLA r 602**Ligand CLA A 410**

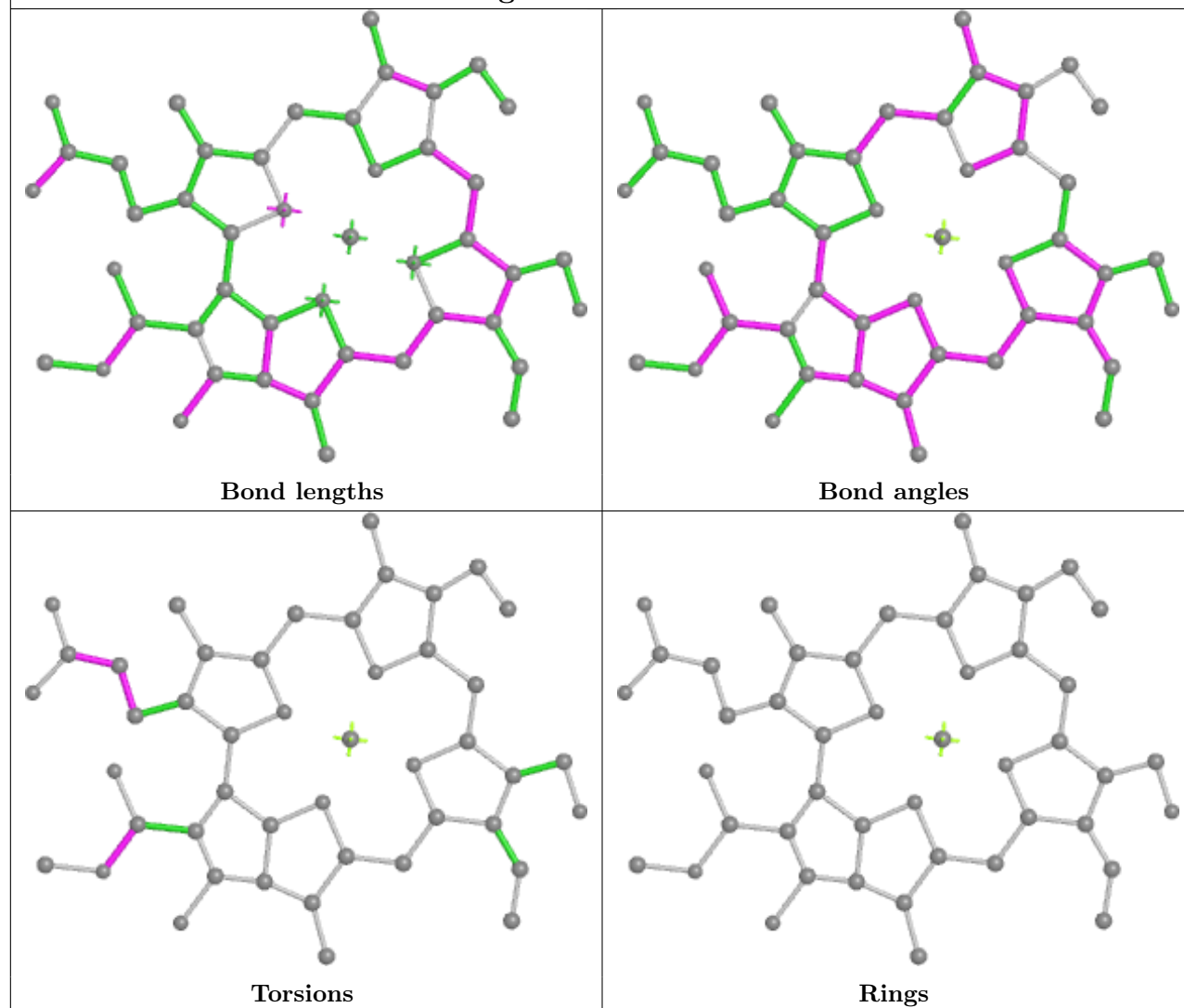




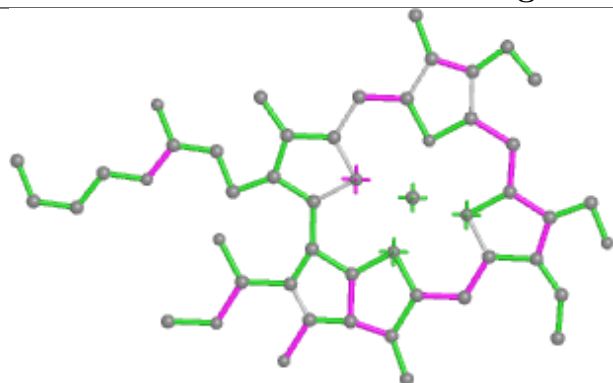
Ligand CLA a 410



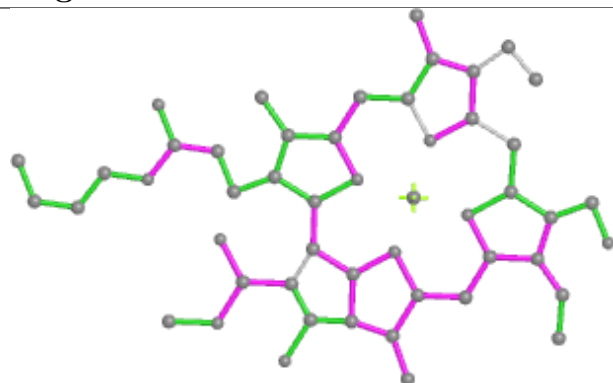
Ligand CHL r 608



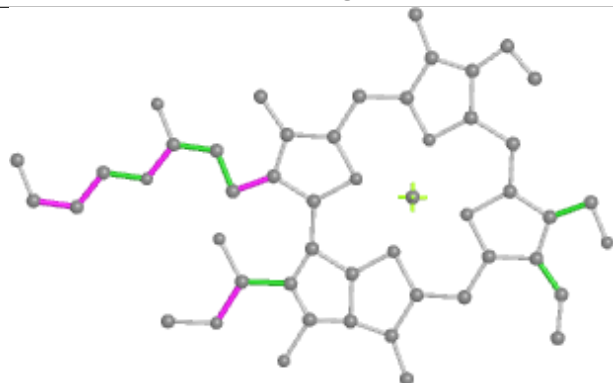
Ligand CHL g 606



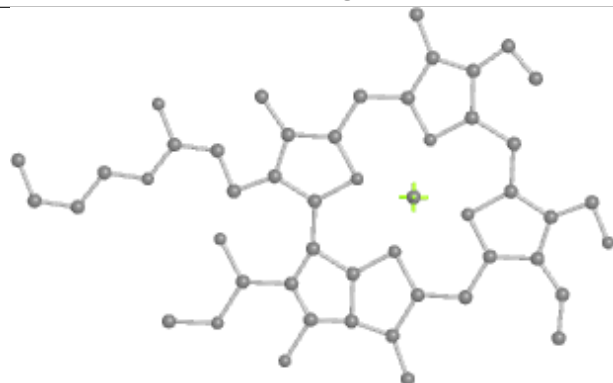
Bond lengths



Bond angles

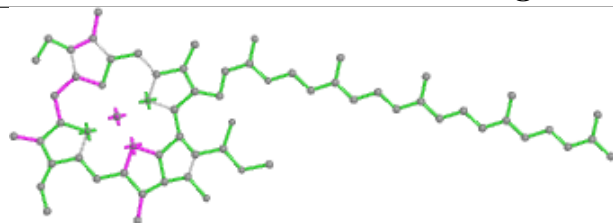


Torsions

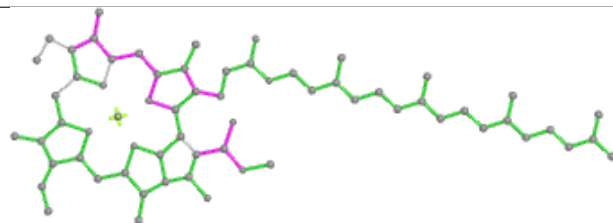


Rings

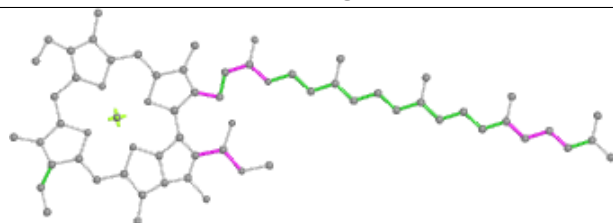
Ligand CLA C 512



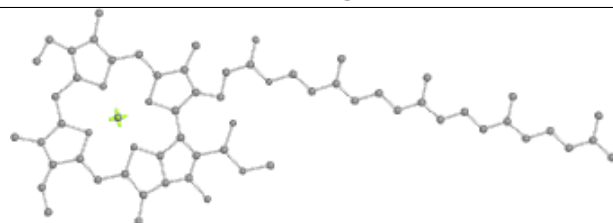
Bond lengths



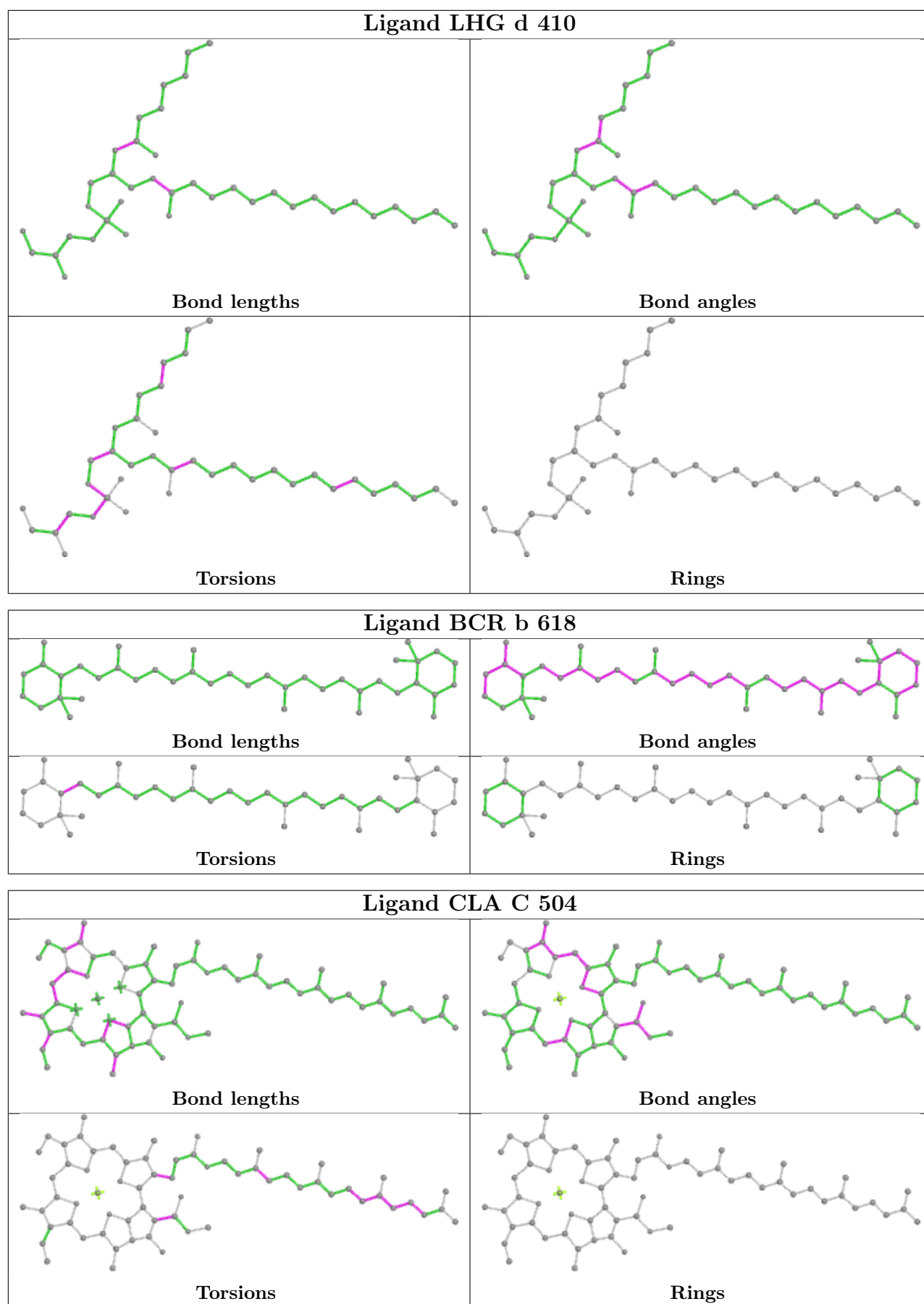
Bond angles

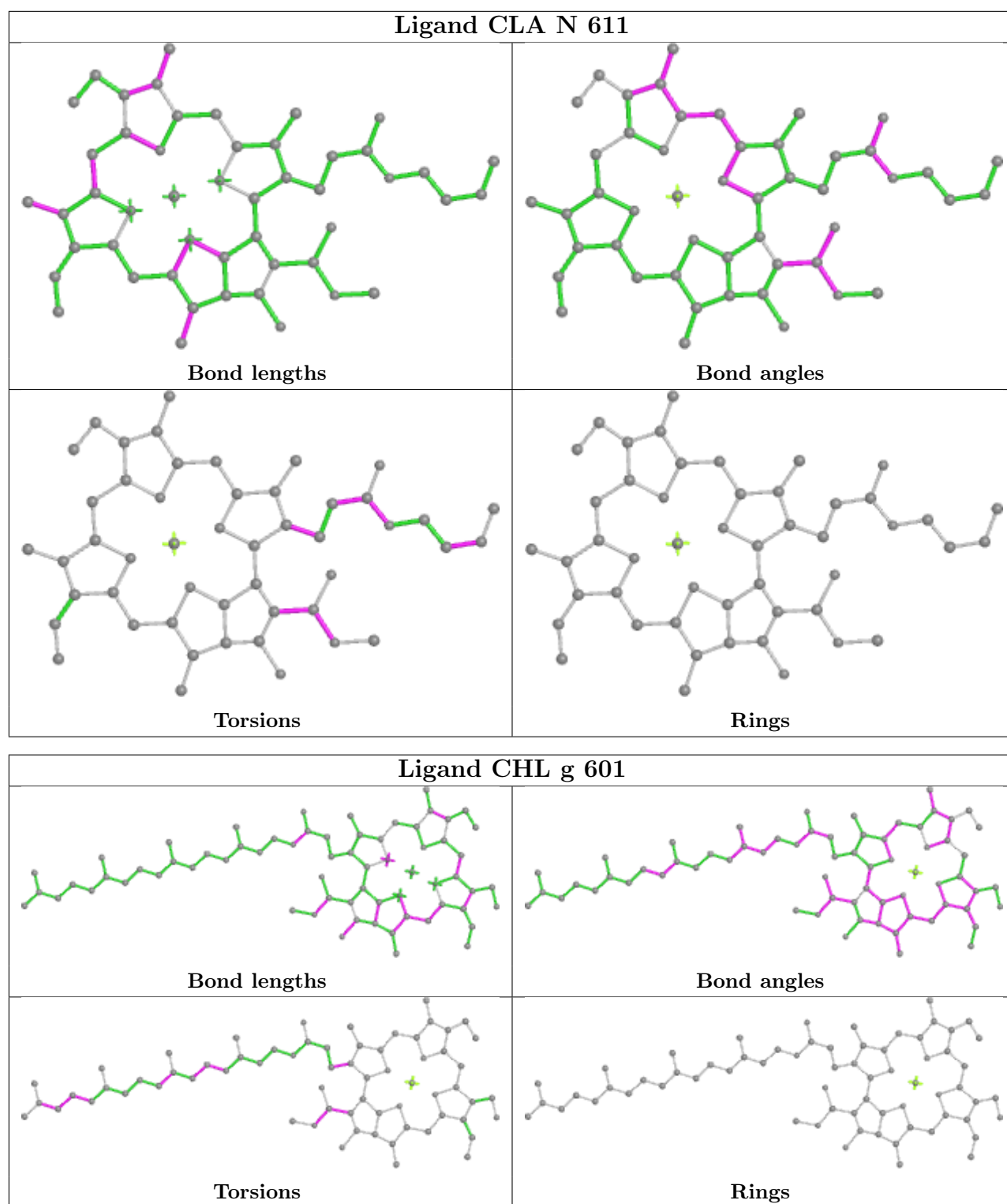


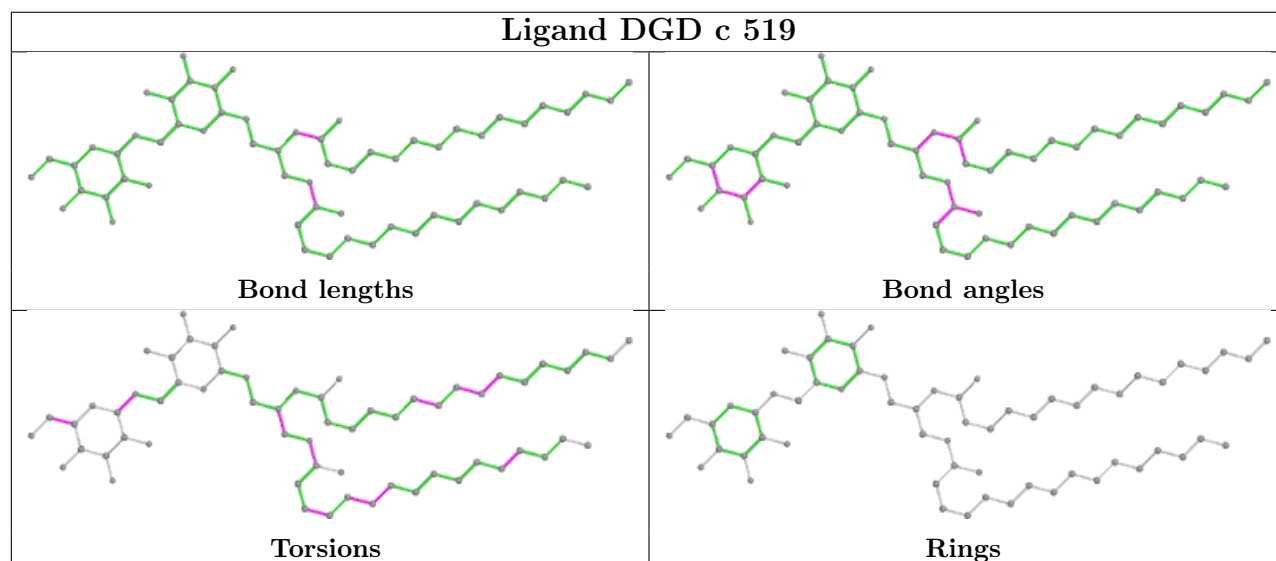
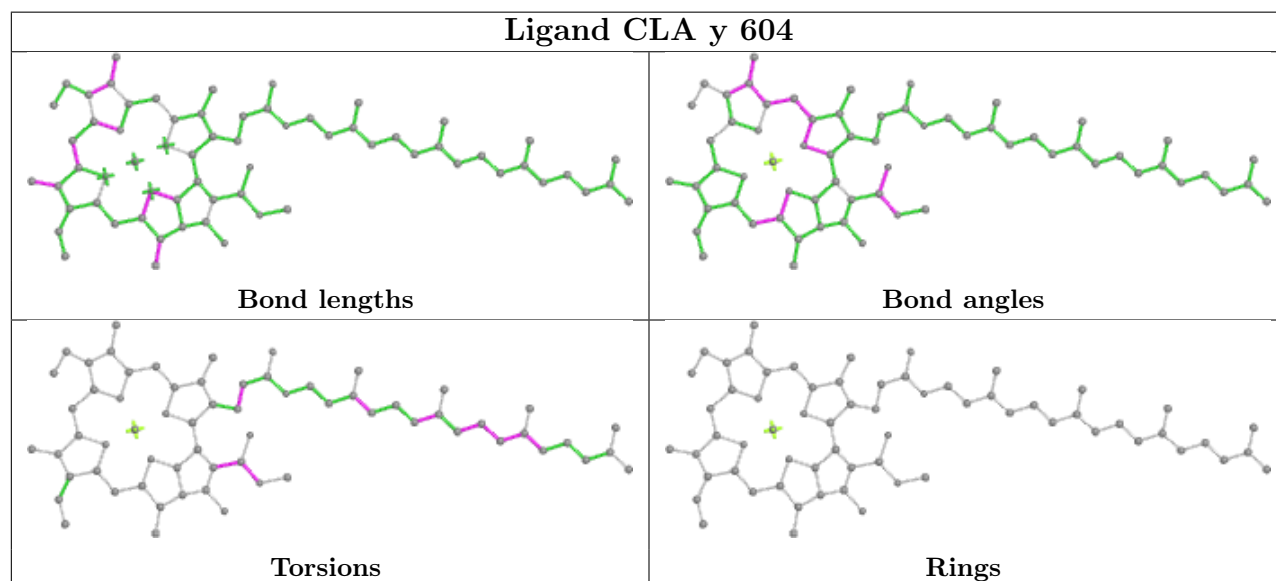
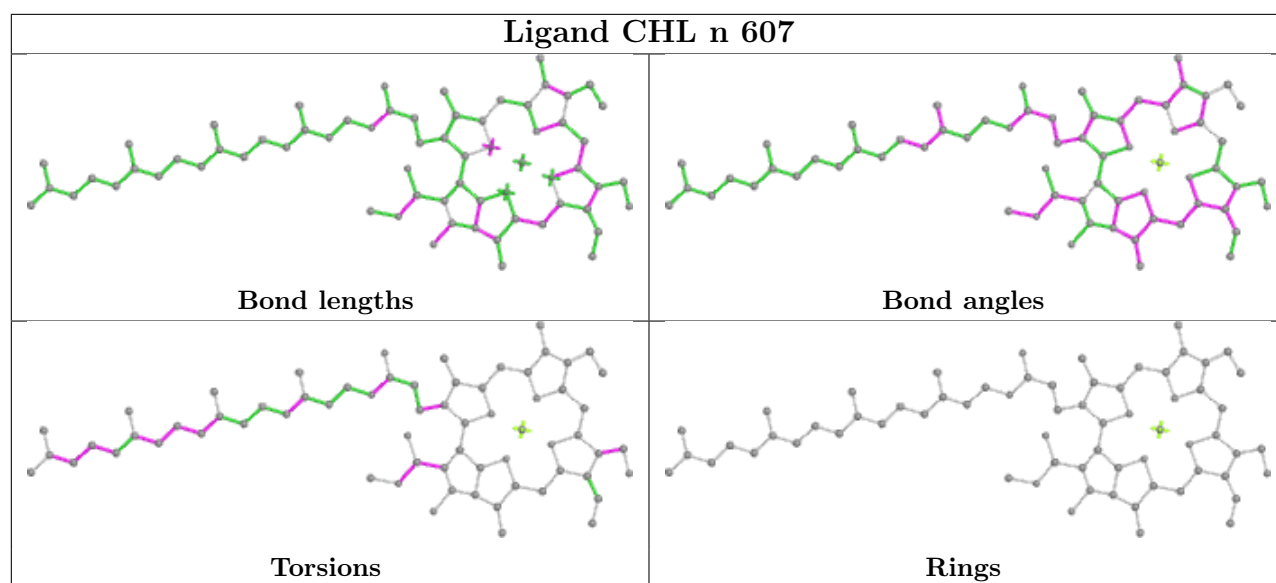
Torsions



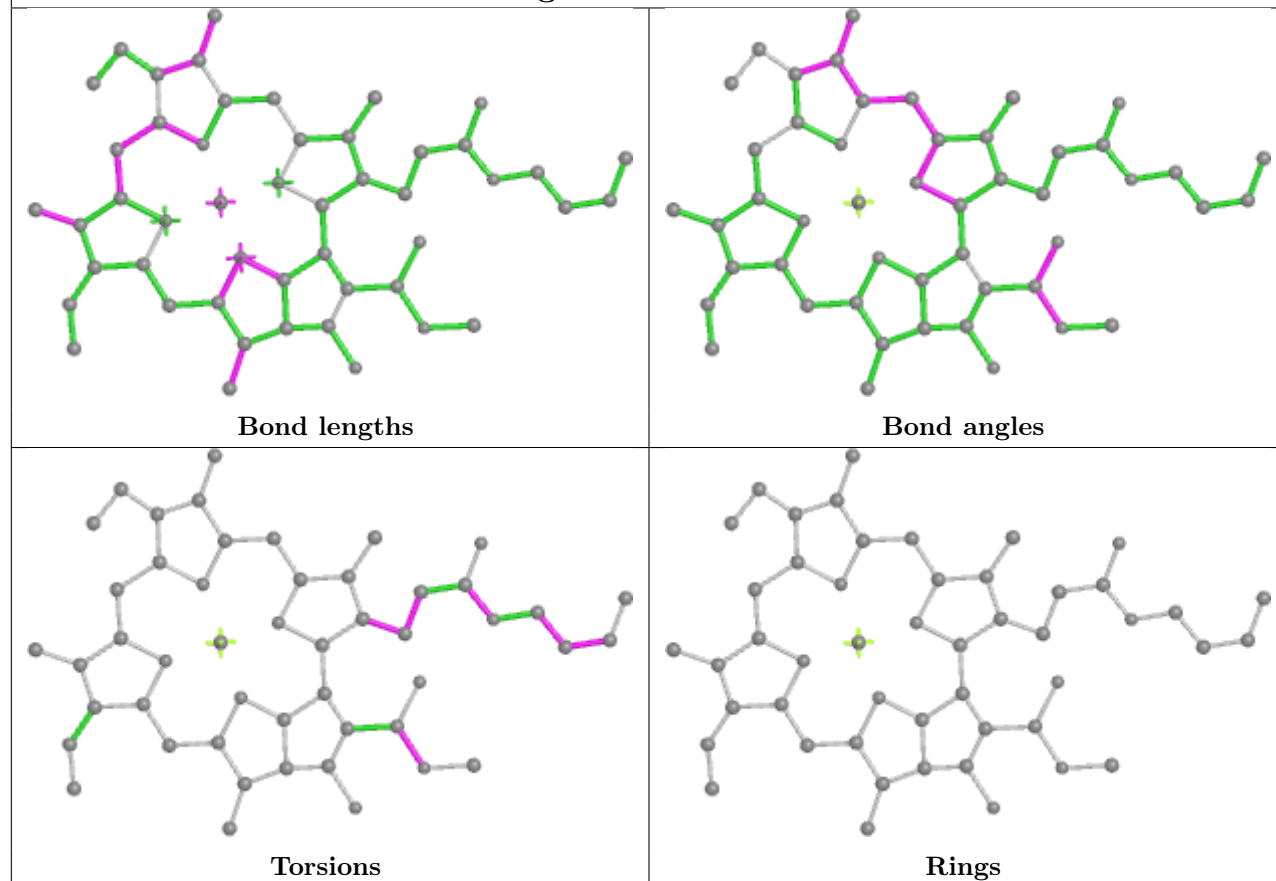
Rings



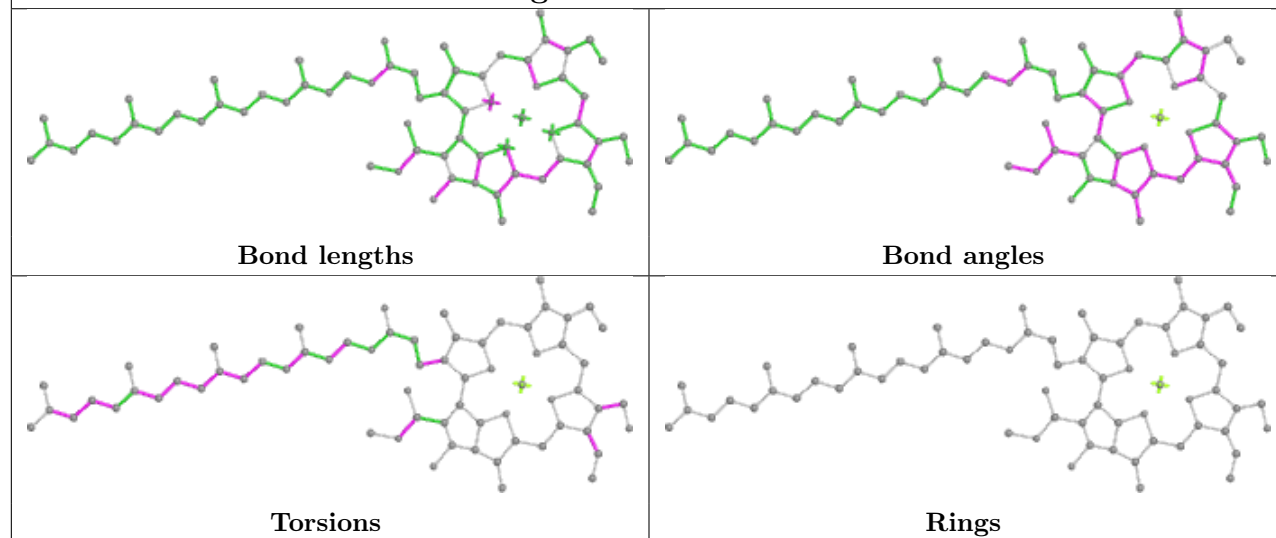


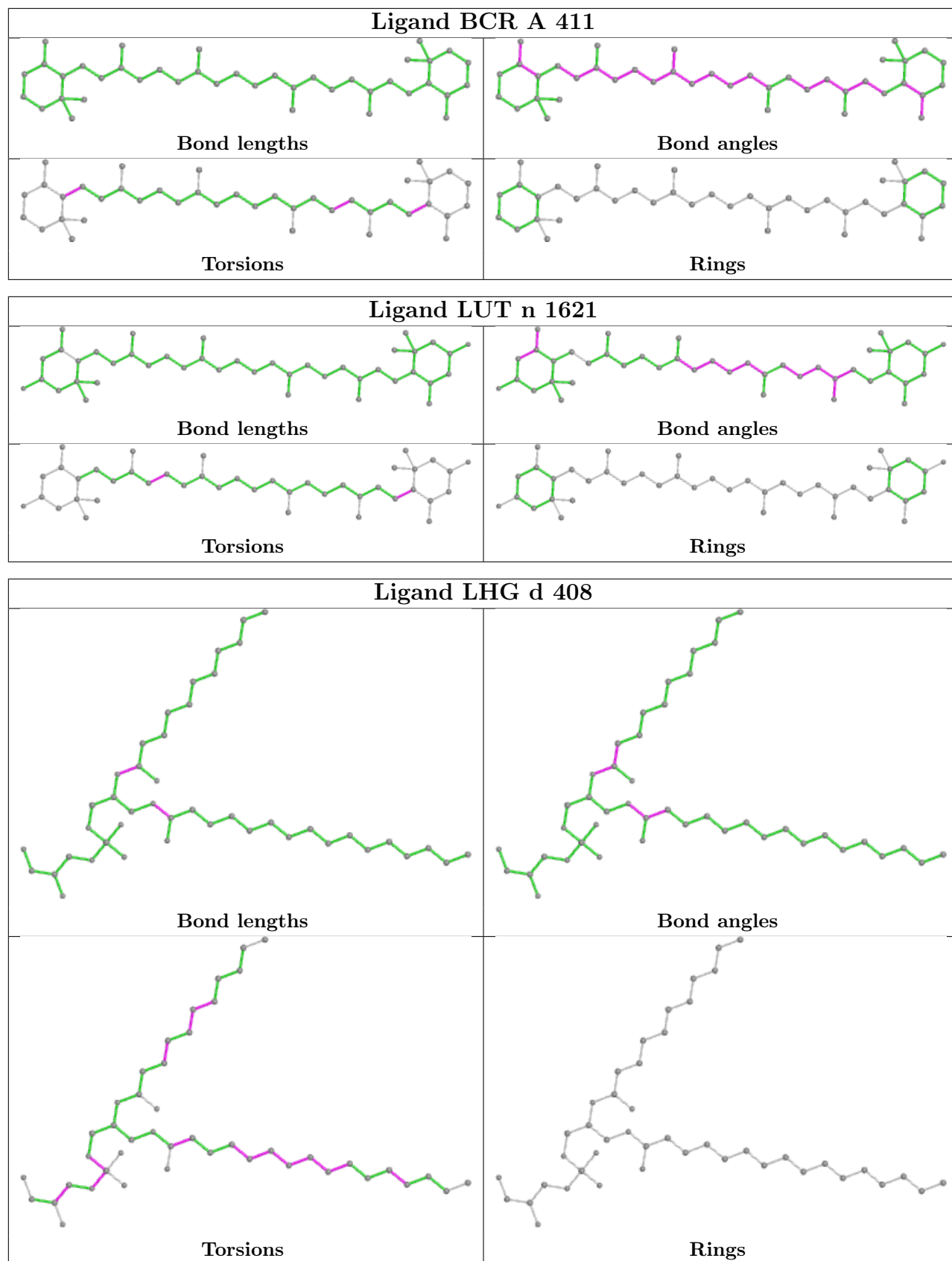


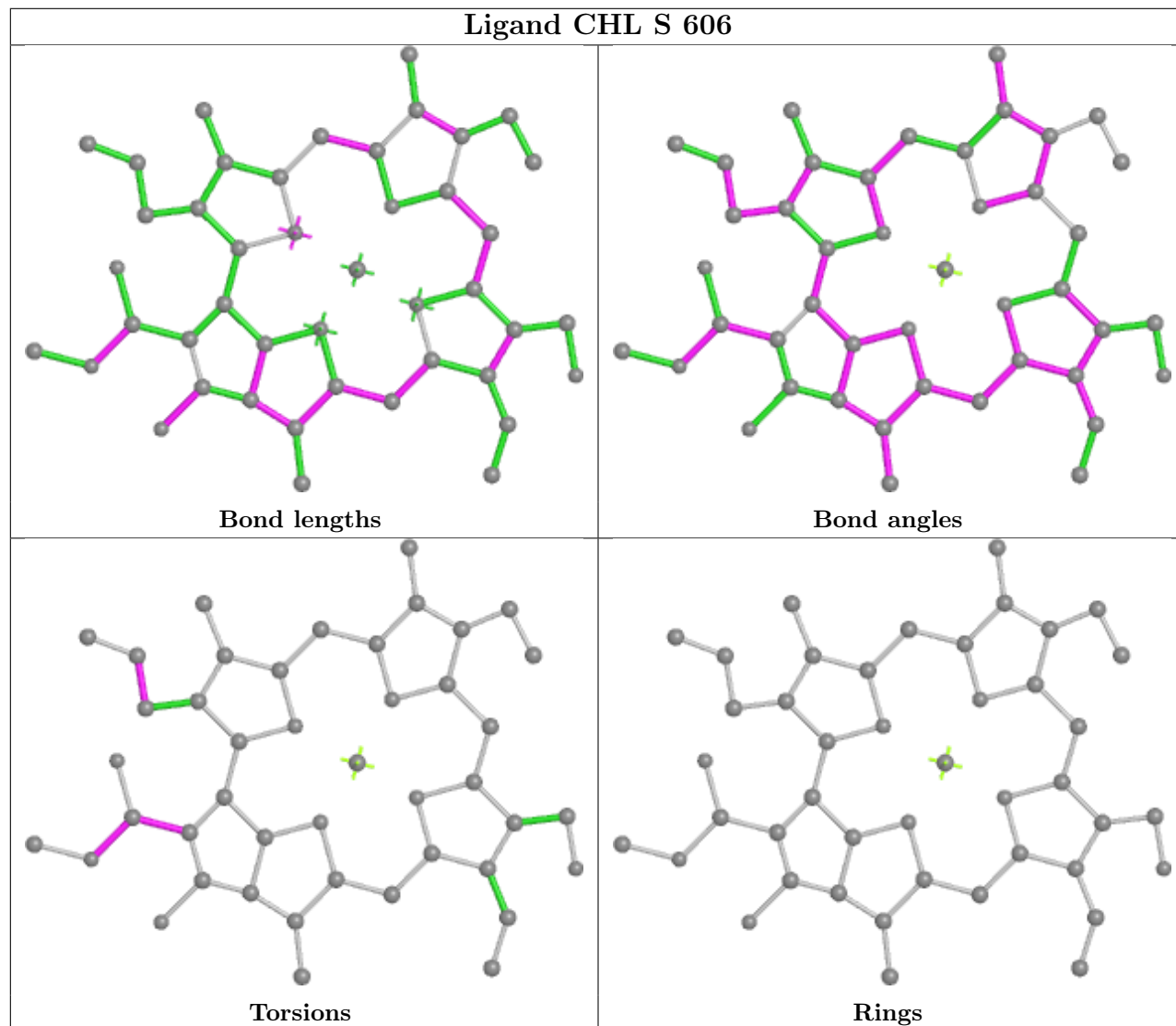
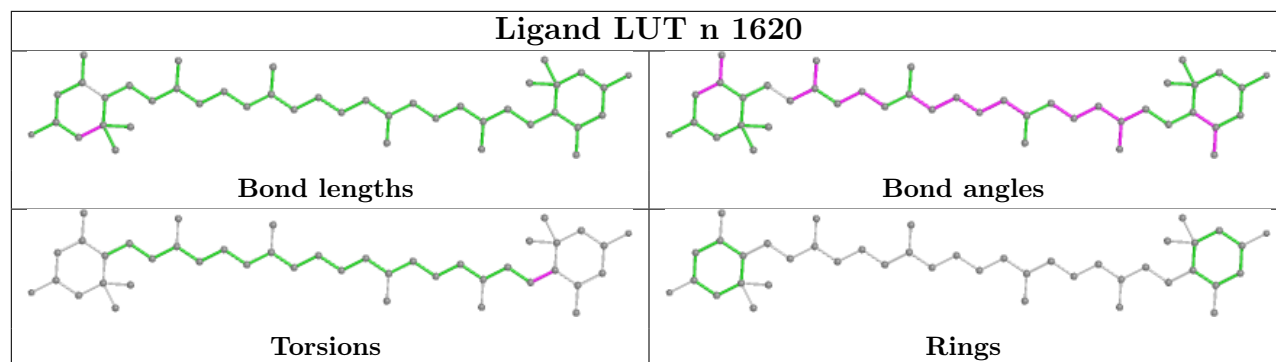
Ligand CLA s 613

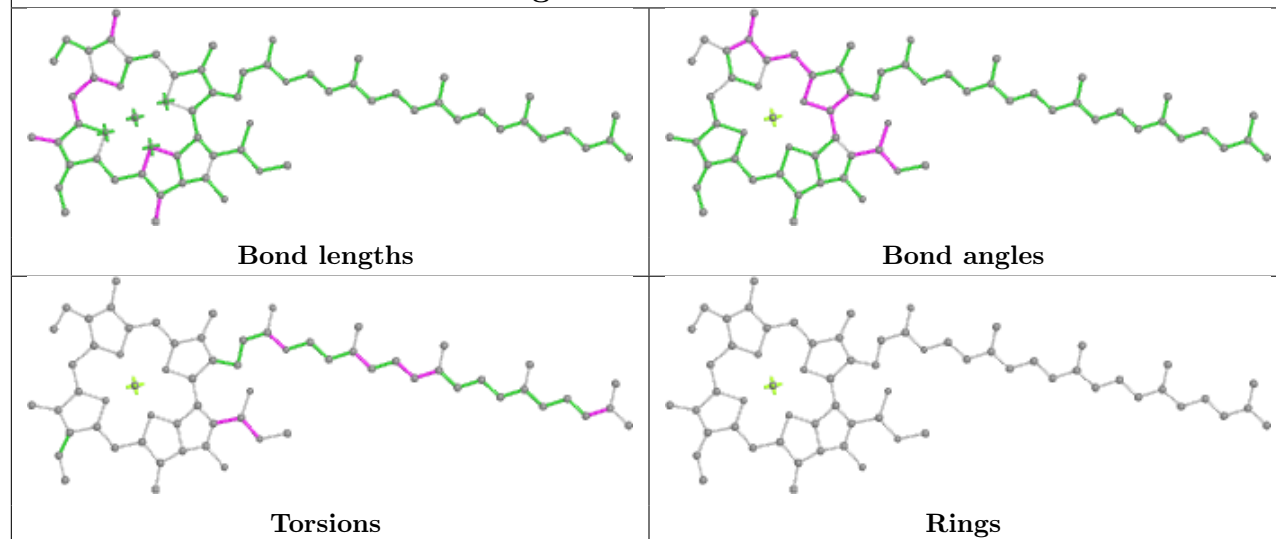
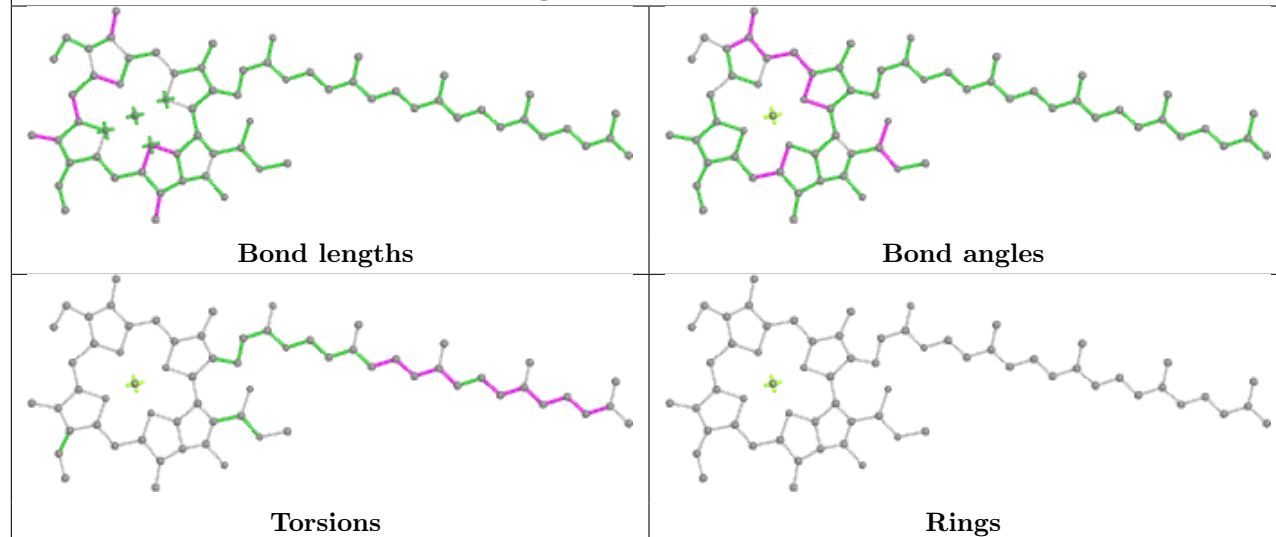


Ligand CHL N 609

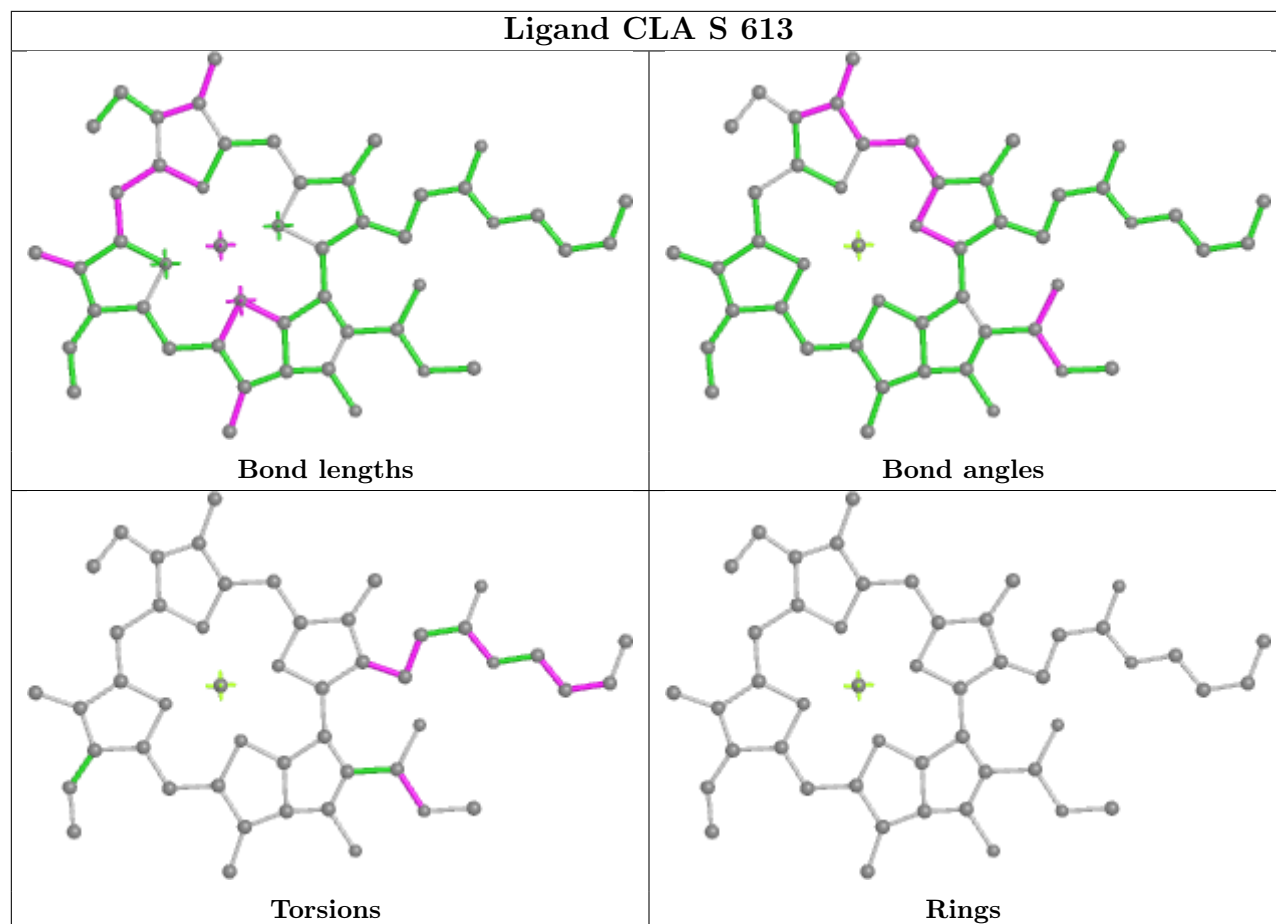




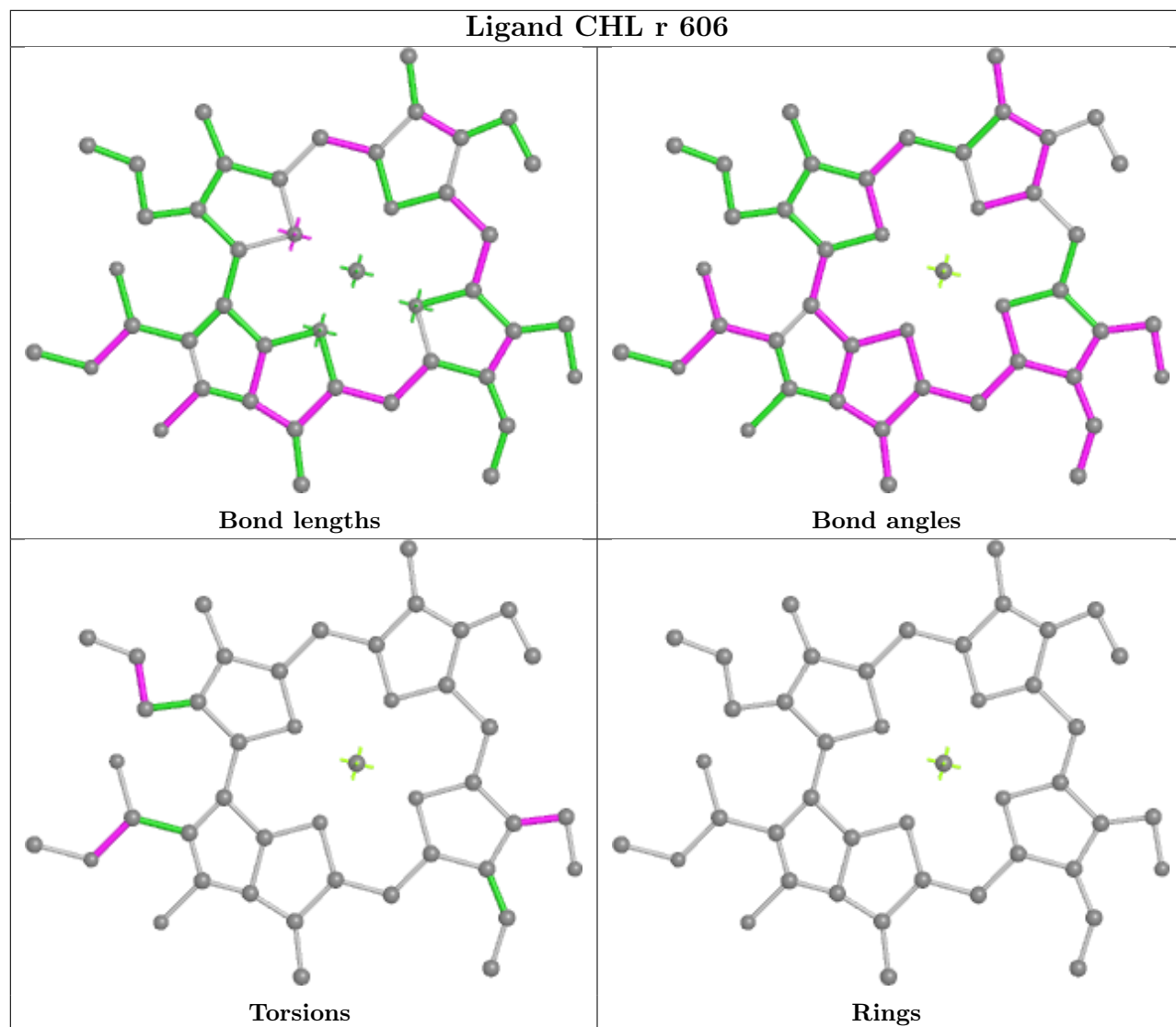


Ligand CLA C 511**Ligand CLA b 609**

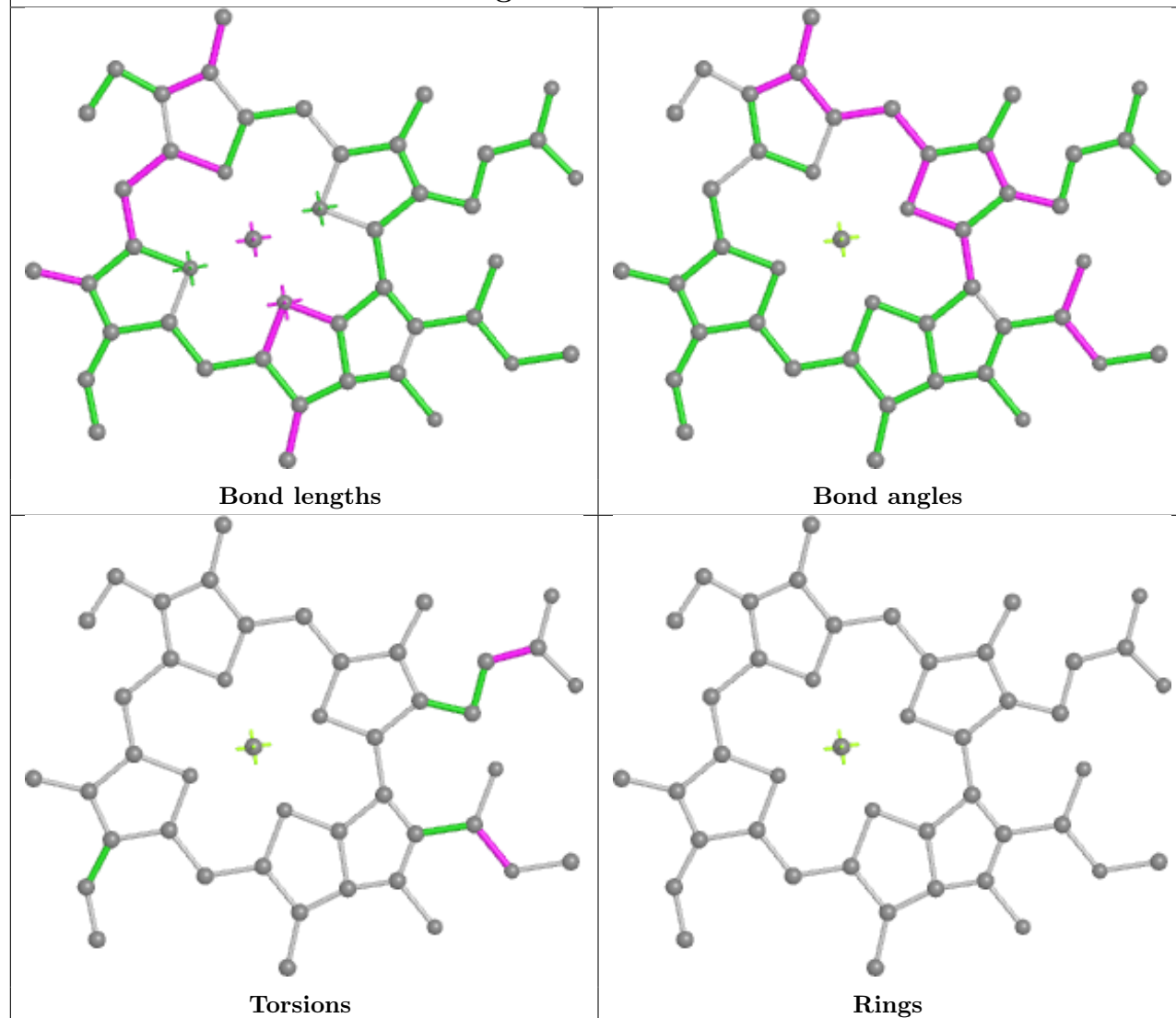
Ligand CLA S 613



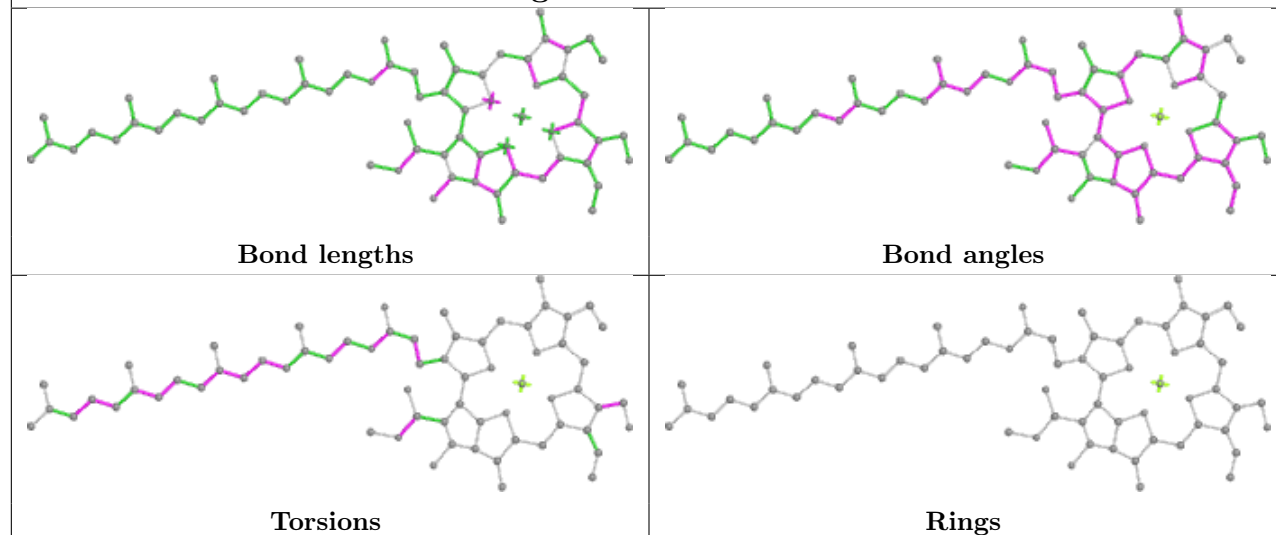
Ligand CHL r 606

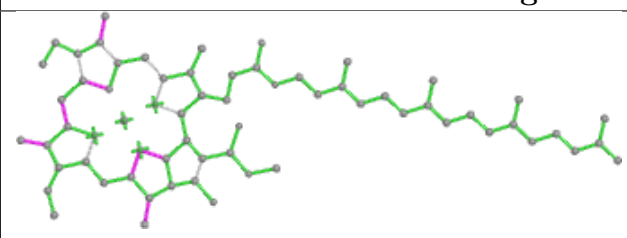
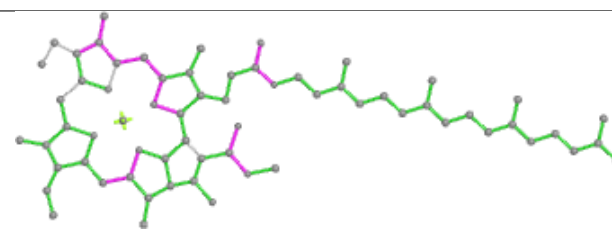
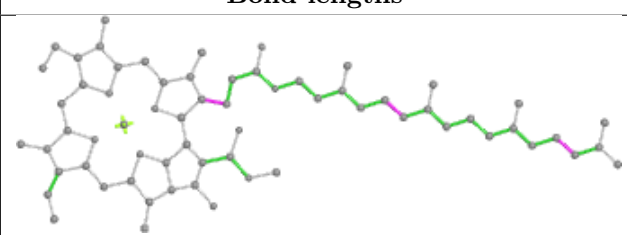
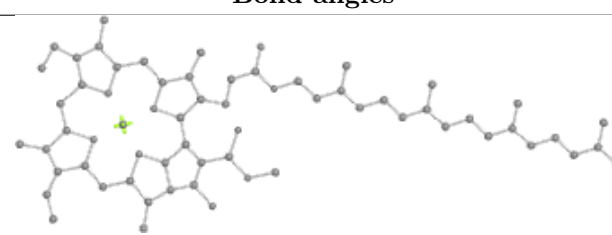


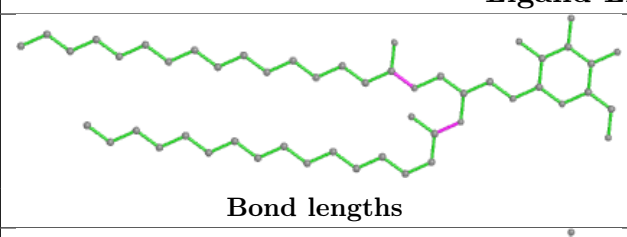
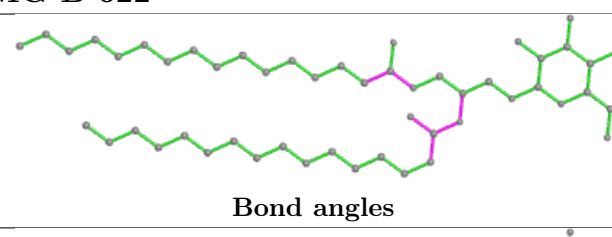
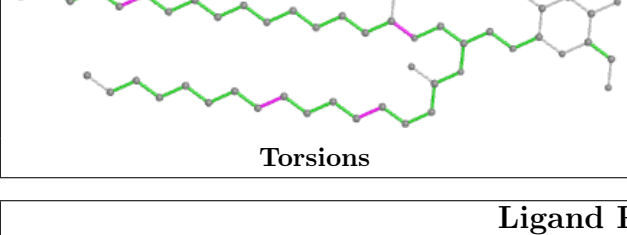

Ligand CLA s 612

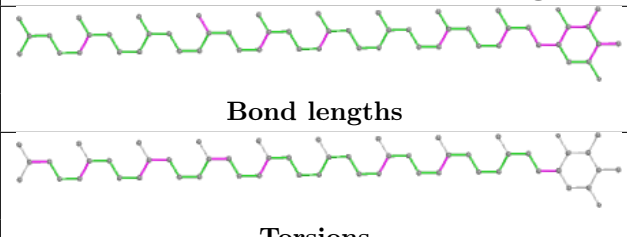
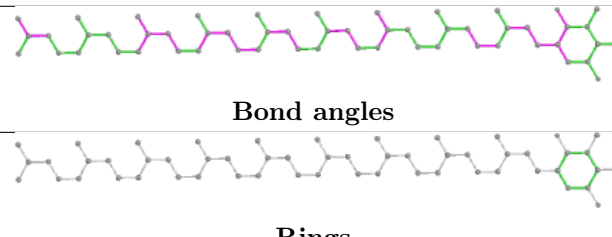
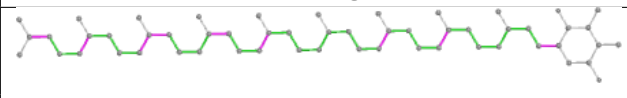
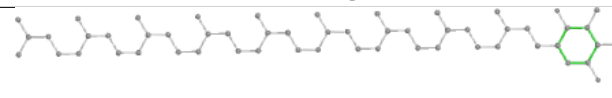


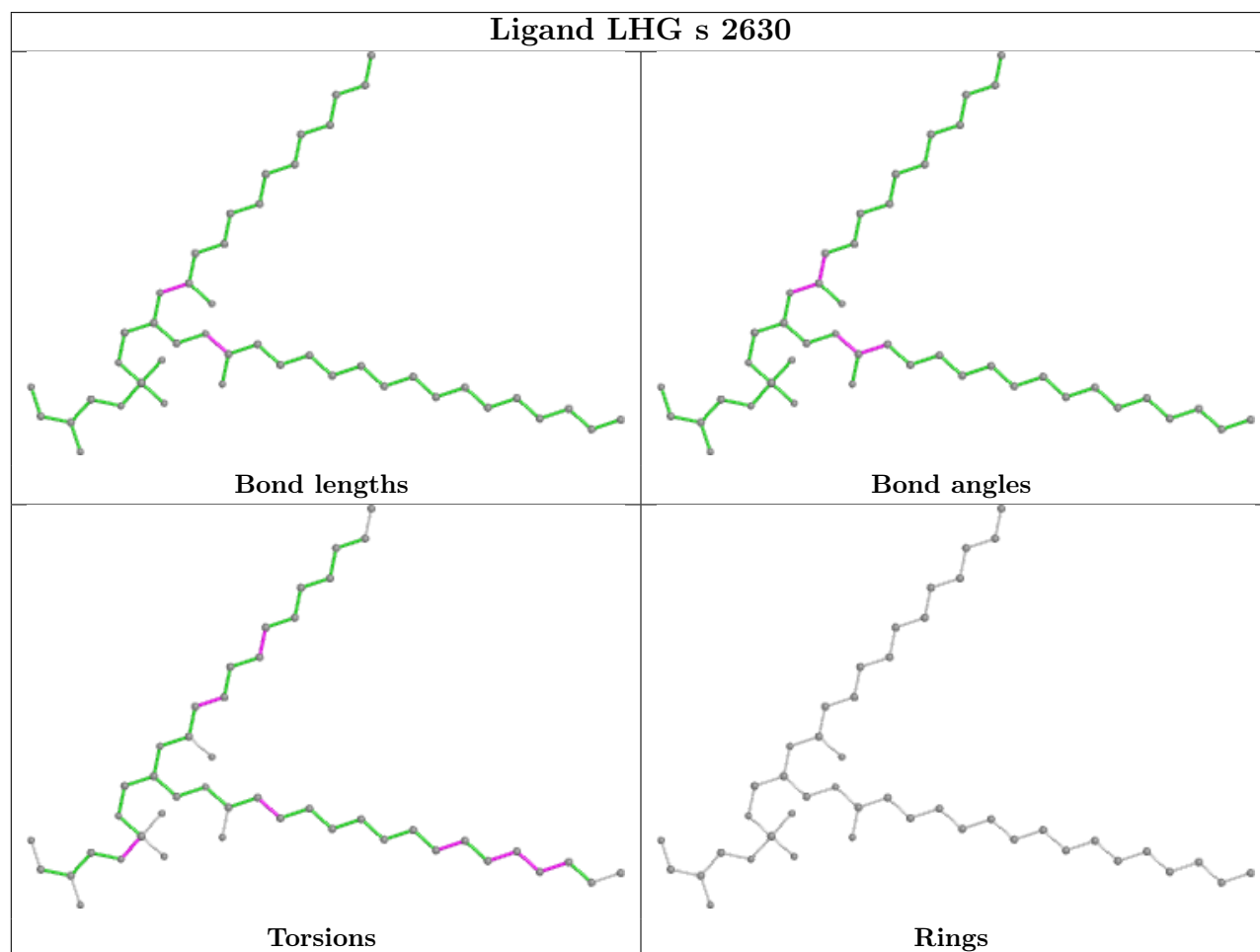
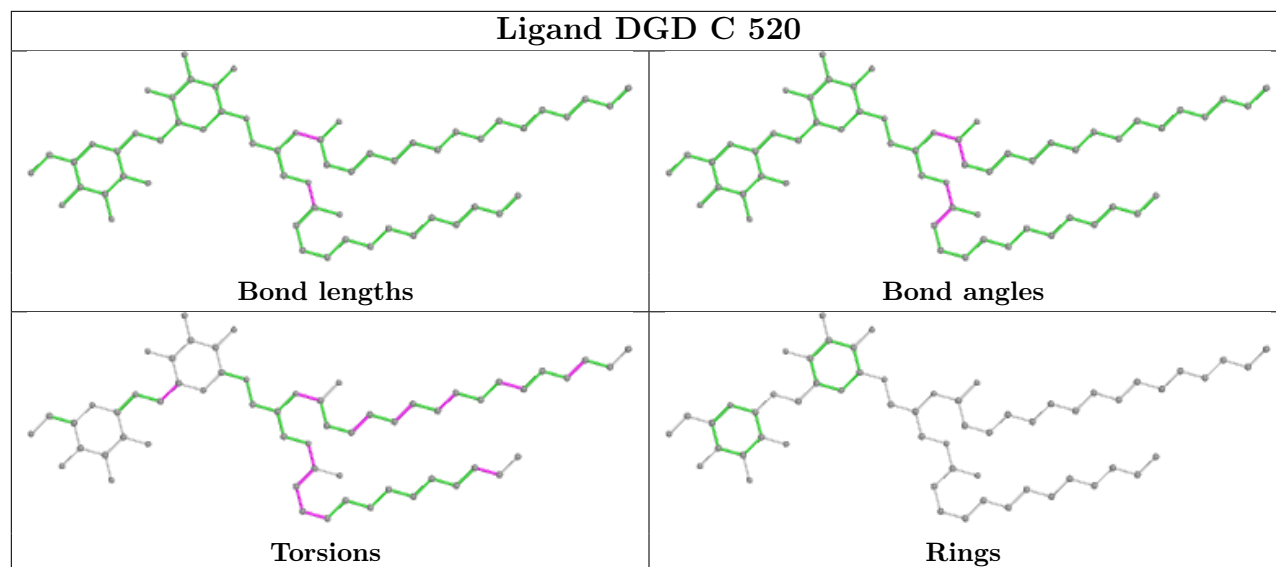
Ligand CHL Y 601

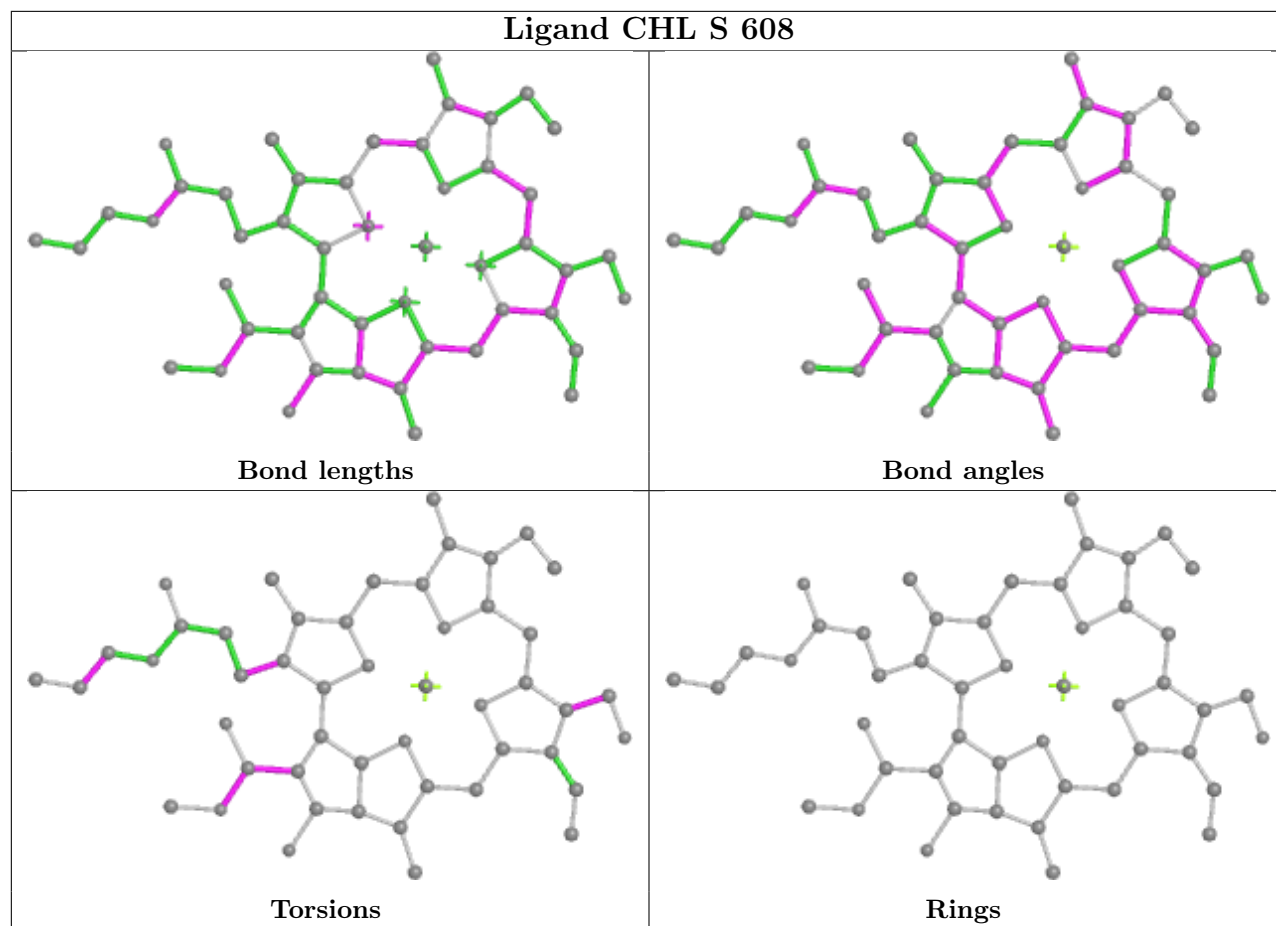


Ligand CLA N 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

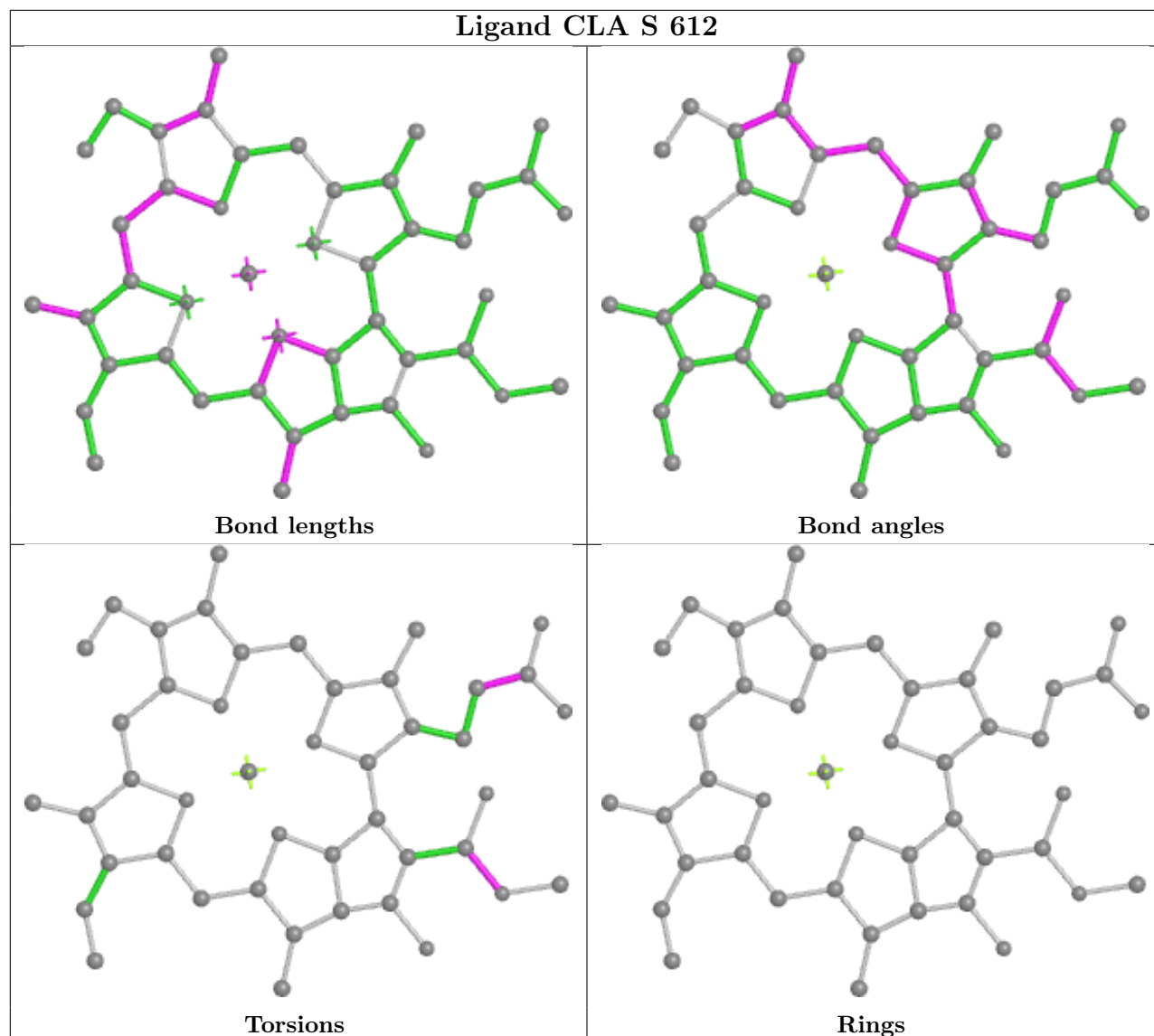
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

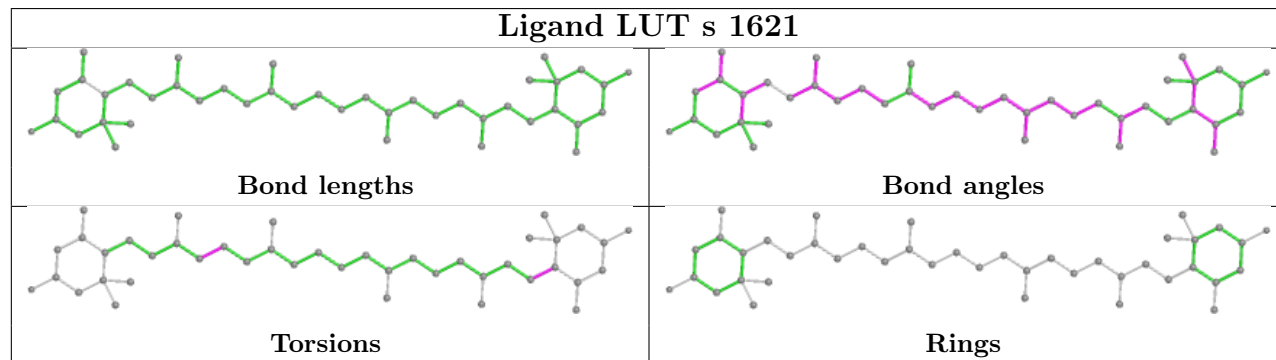


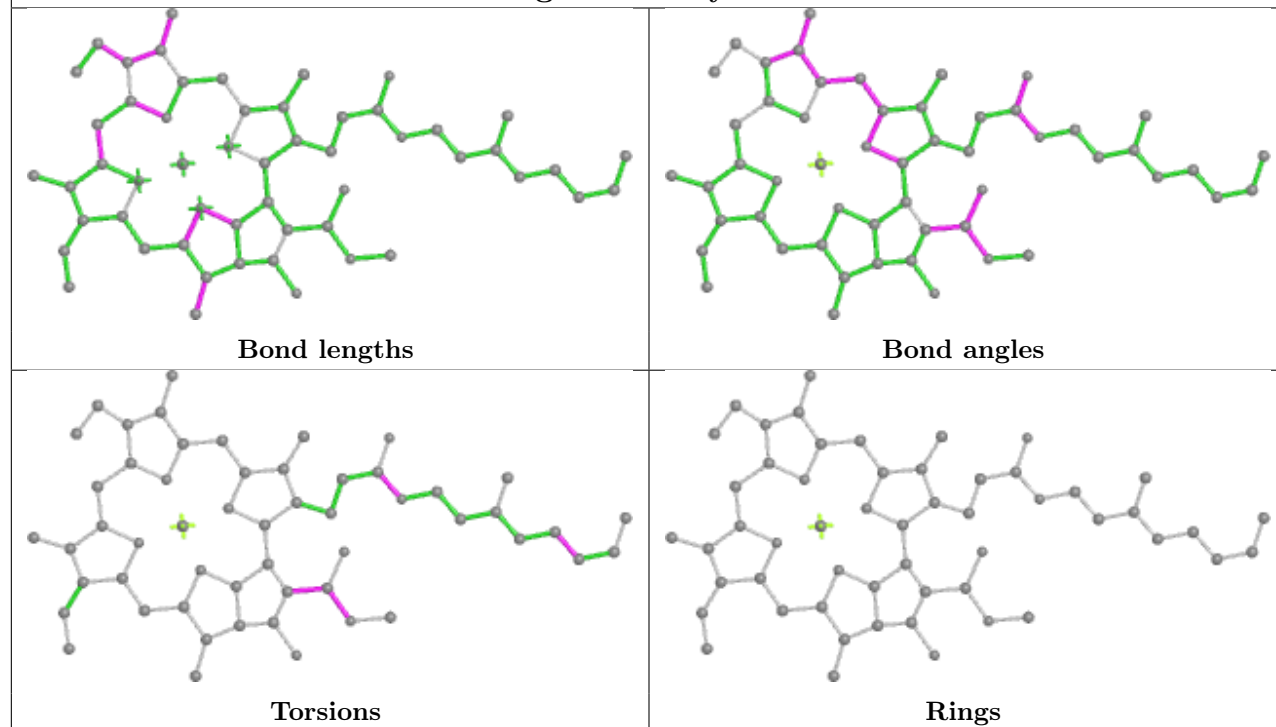
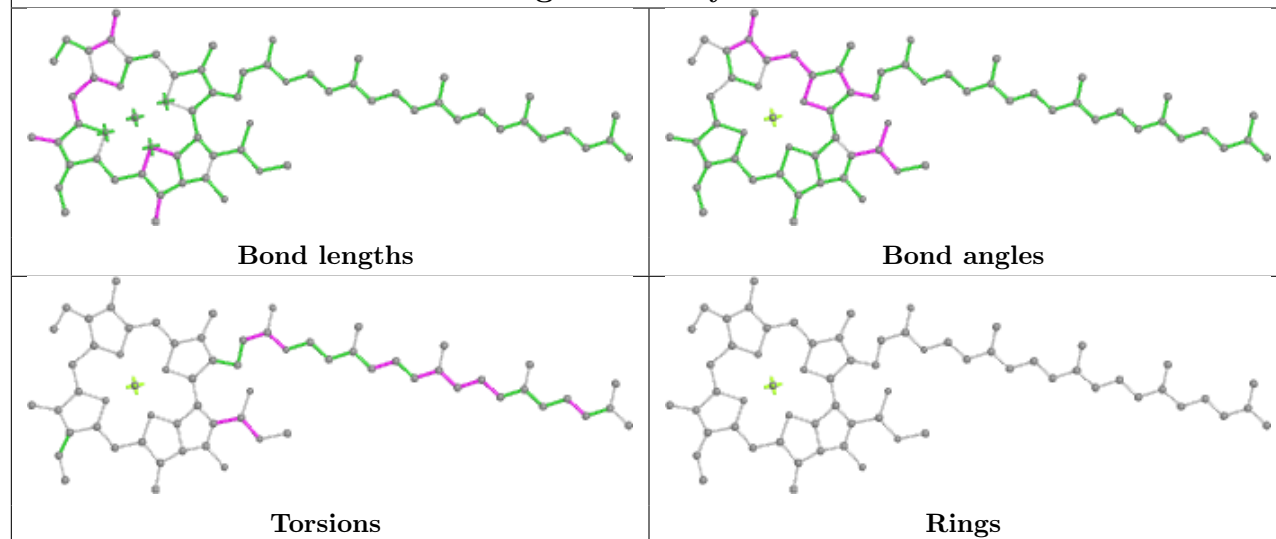


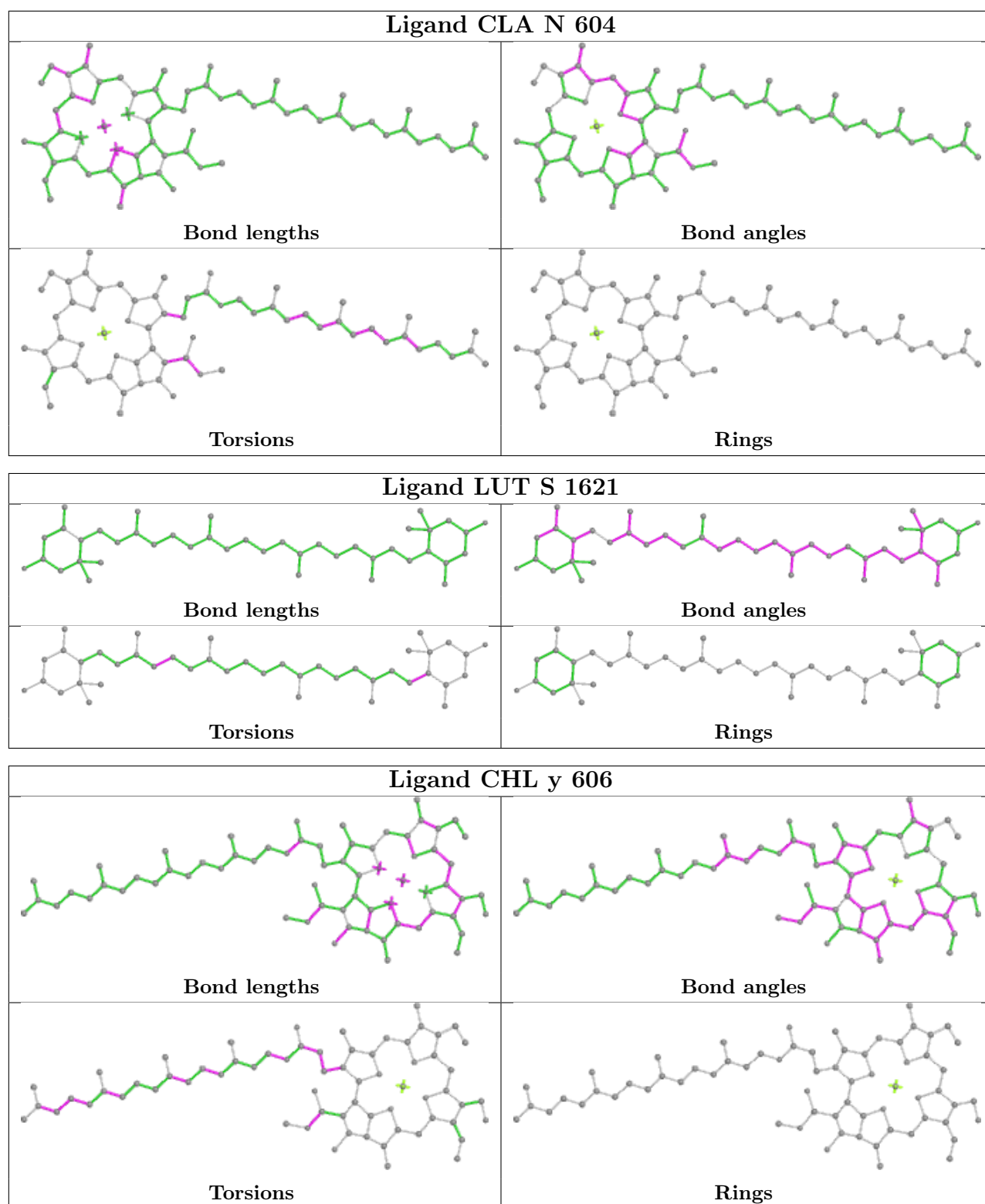
Ligand CLA S 612



Ligand LUT s 1621



Ligand CLA y 614**Ligand CLA y 612**



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

This section contains visualisations of the EMDB entry EMD-9955. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.