



## wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 12:39 PM JST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

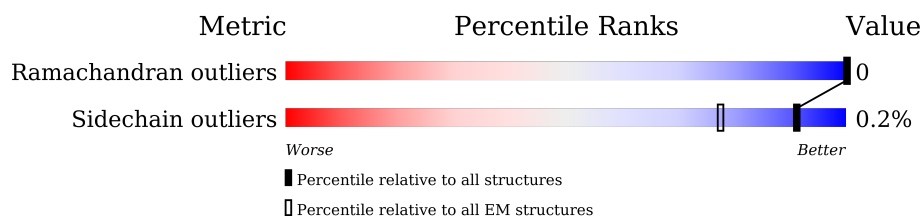
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

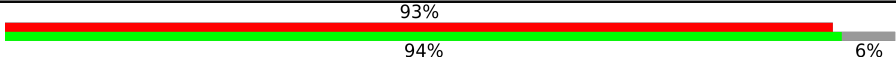
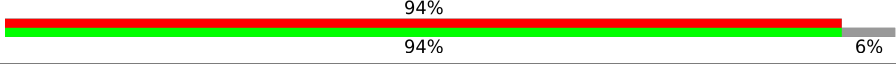
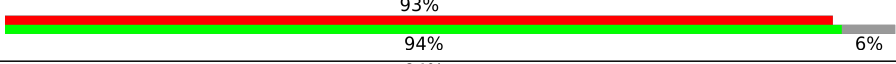
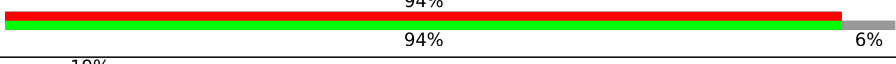
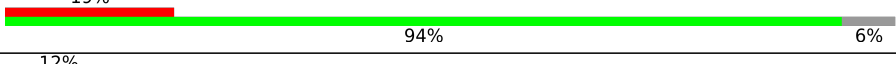
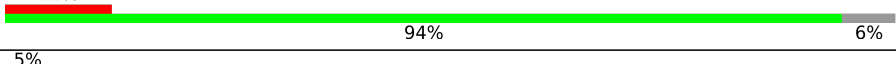
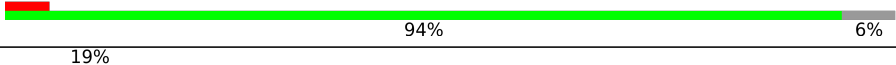
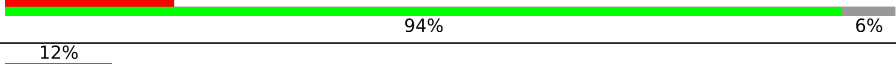
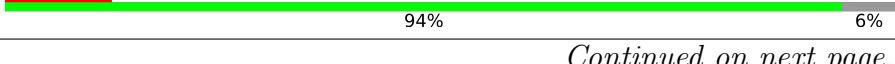
The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	232	
1	2	232	
1	5	232	
1	6	232	
1	G	232	
1	N	232	
1	Y	232	
1	g	232	
1	n	232	

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Mol	Chain	Length	Quality of chain
1	y	232	
2	3	243	
2	7	243	
3	4	210	
3	8	210	
4	A	344	
4	a	344	
5	B	507	
5	b	507	
6	C	473	
6	c	473	
7	D	353	
7	d	353	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	73	
10	h	73	
11	I	36	
11	i	36	
12	J	40	
12	j	40	
13	K	61	
13	k	61	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	1	601	X	-	-	-
24	CHL	1	605	X	-	-	-
24	CHL	1	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	1	607	X	-	-	-
24	CHL	1	608	X	-	-	-
24	CHL	1	609	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	606	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	608	X	-	-	-
24	CHL	2	609	X	-	-	-
24	CHL	3	601	X	-	-	-
24	CHL	3	605	X	-	-	-
24	CHL	3	606	X	-	-	-
24	CHL	3	607	X	-	-	-
24	CHL	3	608	X	-	-	-
24	CHL	3	609	X	-	-	-
24	CHL	4	601	X	-	-	-
24	CHL	4	606	X	-	-	-
24	CHL	4	607	X	-	-	-
24	CHL	4	608	X	-	-	-
24	CHL	4	609	X	-	-	-
24	CHL	5	601	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	5	606	X	-	-	-
24	CHL	5	607	X	-	-	-
24	CHL	5	608	X	-	-	-
24	CHL	5	609	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	6	607	X	-	-	-
24	CHL	6	608	X	-	-	-
24	CHL	6	609	X	-	-	-
24	CHL	7	601	X	-	-	-
24	CHL	7	605	X	-	-	-
24	CHL	7	606	X	-	-	-
24	CHL	7	607	X	-	-	-
24	CHL	7	608	X	-	-	-
24	CHL	7	609	X	-	-	-
24	CHL	8	601	X	-	-	-
24	CHL	8	606	X	-	-	-
24	CHL	8	607	X	-	-	-
24	CHL	8	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	8	609	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	R	614	X	-	-	-
24	CHL	S	601	X	-	-	-
24	CHL	S	606	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	S	608	X	-	-	-
24	CHL	Y	601	X	-	-	-
24	CHL	Y	605	X	-	-	-
24	CHL	Y	606	X	-	-	-
24	CHL	Y	607	X	-	-	-
24	CHL	Y	608	X	-	-	-
24	CHL	Y	609	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	r	614	X	-	-	-
24	CHL	s	601	X	-	-	-
24	CHL	s	606	X	-	-	-
24	CHL	s	607	X	-	-	-
24	CHL	s	608	X	-	-	-
24	CHL	y	601	X	-	-	-
24	CHL	y	605	X	-	-	-
24	CHL	y	606	X	-	-	-
24	CHL	y	607	X	-	-	-
24	CHL	y	608	X	-	-	-
24	CHL	y	609	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	604	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	614	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	611	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	7	613	X	-	-	-
25	CLA	7	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	407	X	-	-	-
25	CLA	A	410	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	604	X	-	-	-
25	CLA	Y	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	X	-	-	-
25	CLA	Y	613	X	-	-	-
25	CLA	Y	614	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	407	X	-	-	-
25	CLA	a	410	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	613	X	-	-	-
25	CLA	s	602	X	-	-	-
25	CLA	s	603	X	-	-	-
25	CLA	s	604	X	-	-	-
25	CLA	s	609	X	-	-	-
25	CLA	s	610	X	-	-	-
25	CLA	s	611	X	-	-	-
25	CLA	s	612	X	-	-	-
25	CLA	s	613	X	-	-	-
25	CLA	s	614	X	-	-	-
25	CLA	y	602	X	-	-	-
25	CLA	y	603	X	-	-	-
25	CLA	y	604	X	-	-	-
25	CLA	y	610	X	-	-	-
25	CLA	y	611	X	-	-	-
25	CLA	y	612	X	-	-	-
25	CLA	y	613	X	-	-	-
25	CLA	y	614	X	-	-	-

## 2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

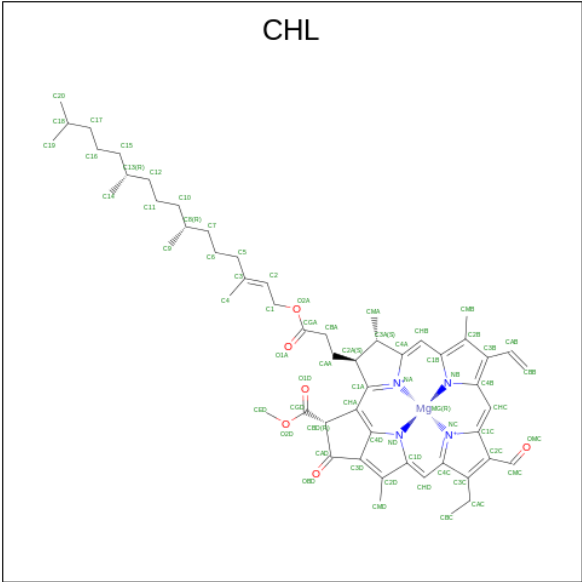
- Molecule 22 is a protein called Photosystem II reaction center protein X.

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

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

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

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

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

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

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

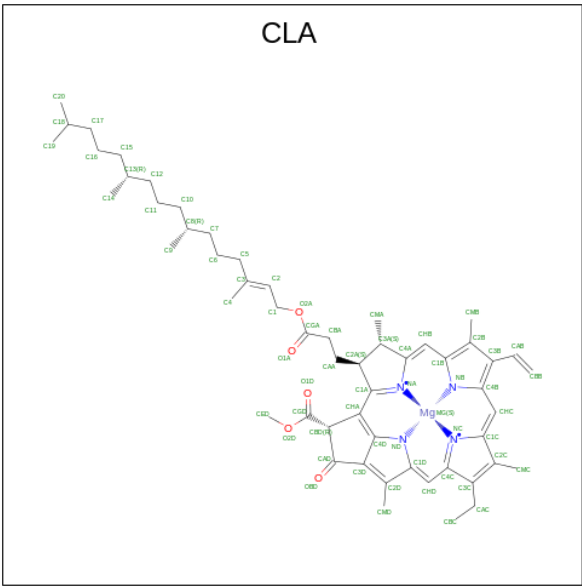
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Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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

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

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

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

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

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

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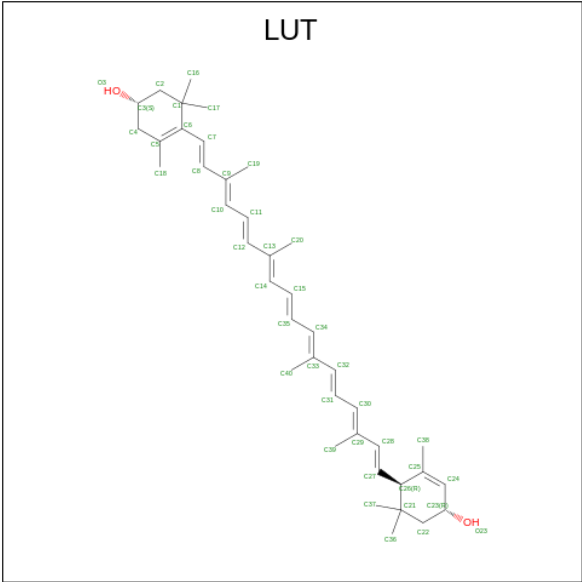
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total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

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

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



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

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

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).

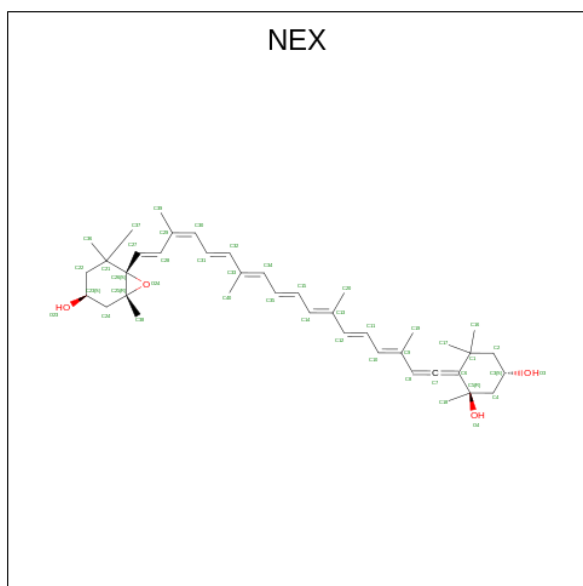


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Mol	Chain	Residues	Atoms			AltConf
27	r	1	Total	C	O	0
			44	40	4	
27	y	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



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

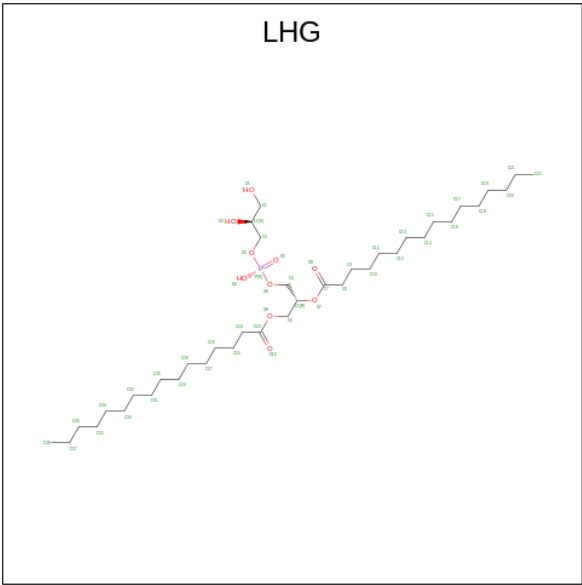
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Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	
28	s	1	Total	C	O	0
			44	40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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



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

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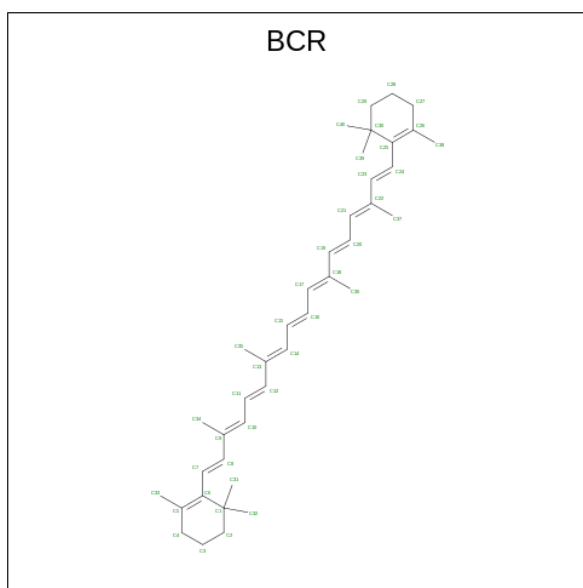
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total 21	C 10	O 10	P 1	0
29	B	1	Total 47	C 36	O 10	P 1	0
29	B	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 49	C 38	O 10	P 1	0
29	D	1	Total 46	C 35	O 10	P 1	0
29	D	1	Total 49	C 38	O 10	P 1	0
29	D	1	Total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

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

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



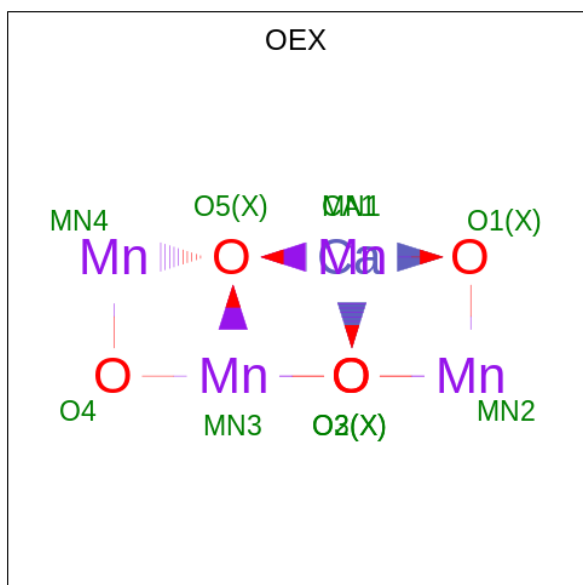
Mol	Chain	Residues	Atoms	AltConf
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	T	1	Total C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

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

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).

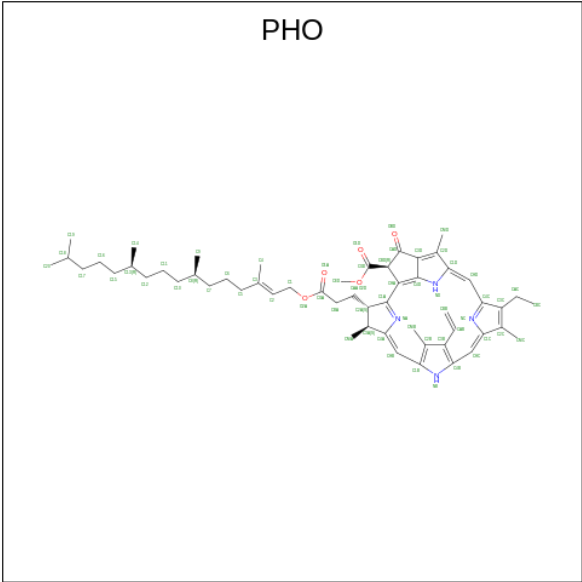


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Ca Mn O 10 1 4 5	0
31	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 32 is FE (II) ION (three-letter code: FE2) (formula: Fe).

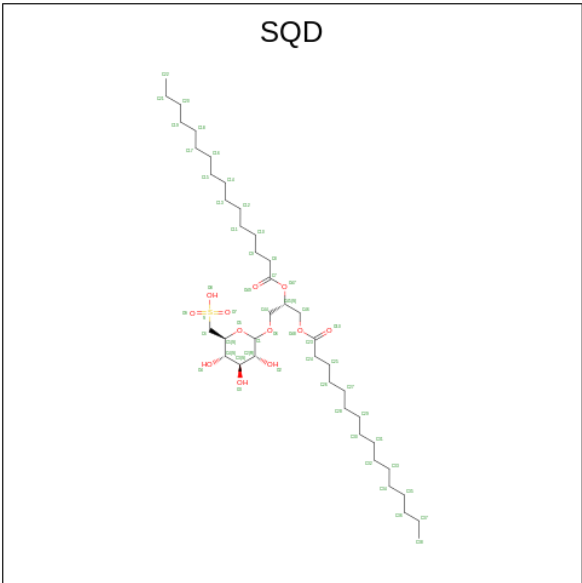
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Fe 1 1	0
32	a	1	Total Fe 1 1	0

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



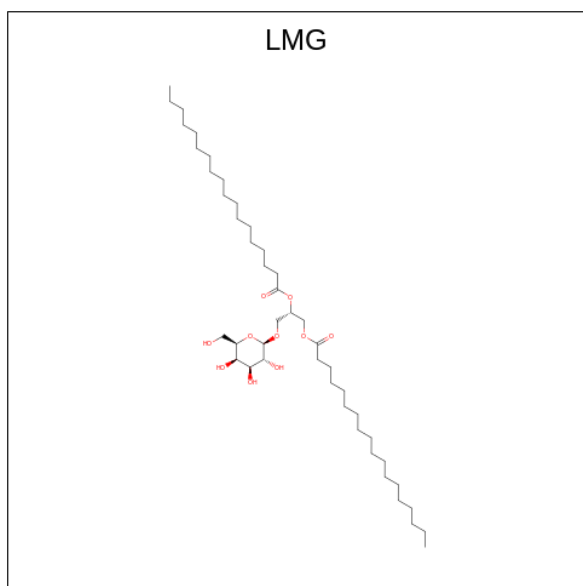
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			50	37	12	1	
34	A	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			54	41	12	1	
34	B	1	Total	C	O	S	0
			42	29	12	1	
34	a	1	Total	C	O	S	0
			50	37	12	1	
34	a	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			54	41	12	1	
34	b	1	Total	C	O	S	0
			42	29	12	1	

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



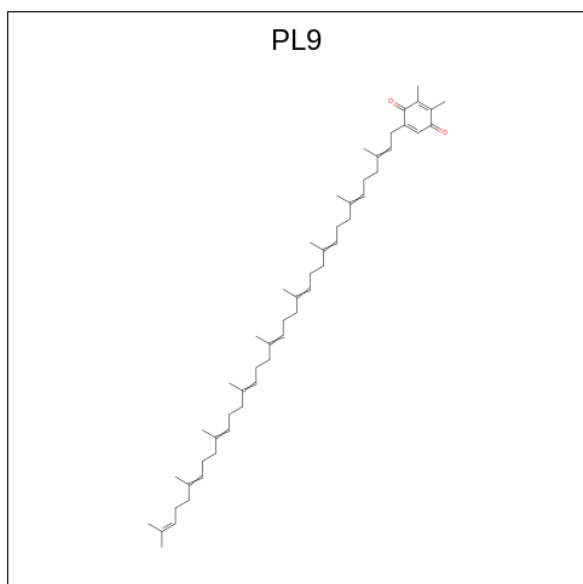
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	
35	A	1	Total	C	O	0
			40	30	10	
35	B	1	Total	C	O	0
			51	41	10	

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

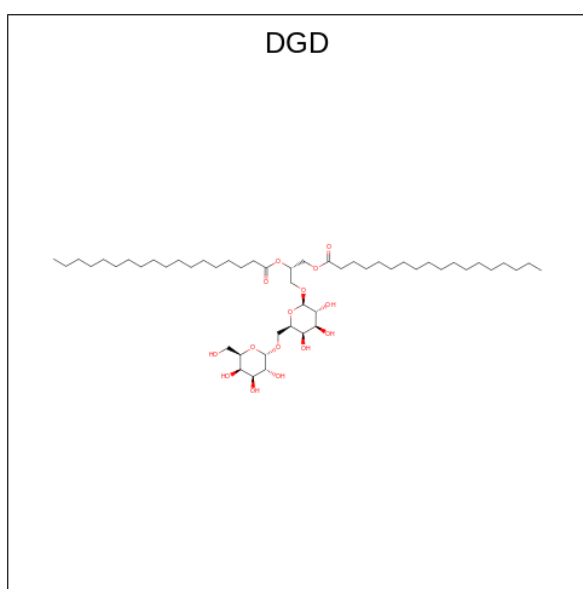
- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).





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

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



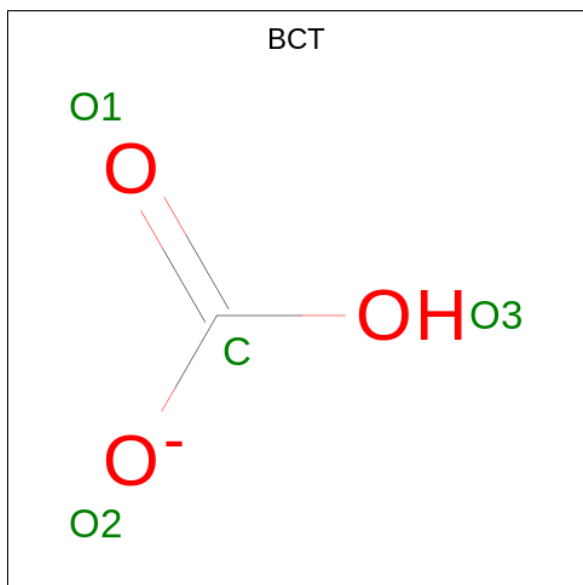
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			55	40	15	
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			60	45	15	
37	H	1	Total	C	O	0
			62	47	15	
37	b	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			55	40	15	

*Continued on next page...*

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

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

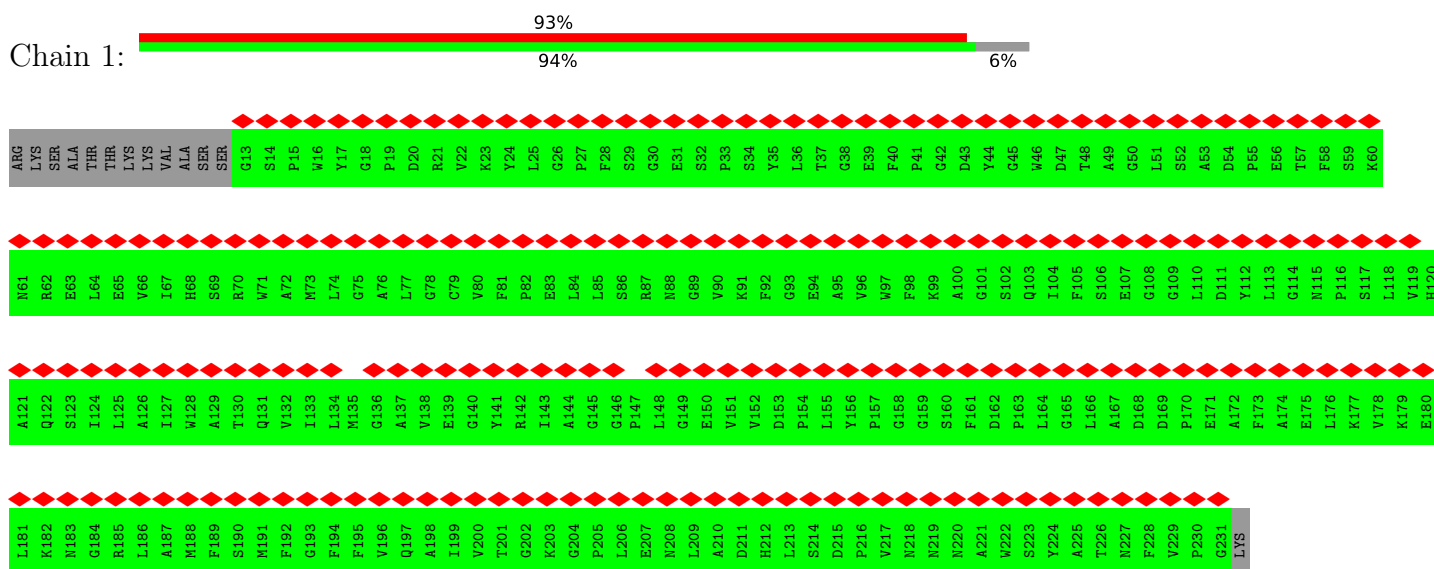
- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).

	AltConf
O 4	0
O 4	0

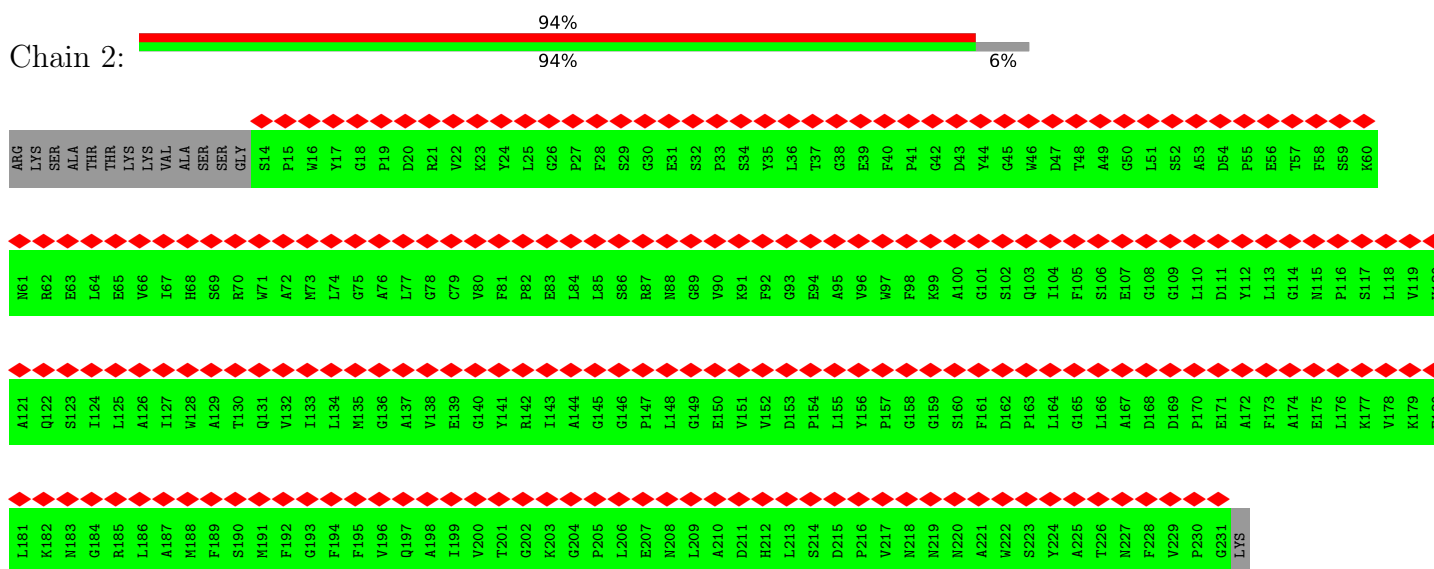
### 3 Residue-property plots

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

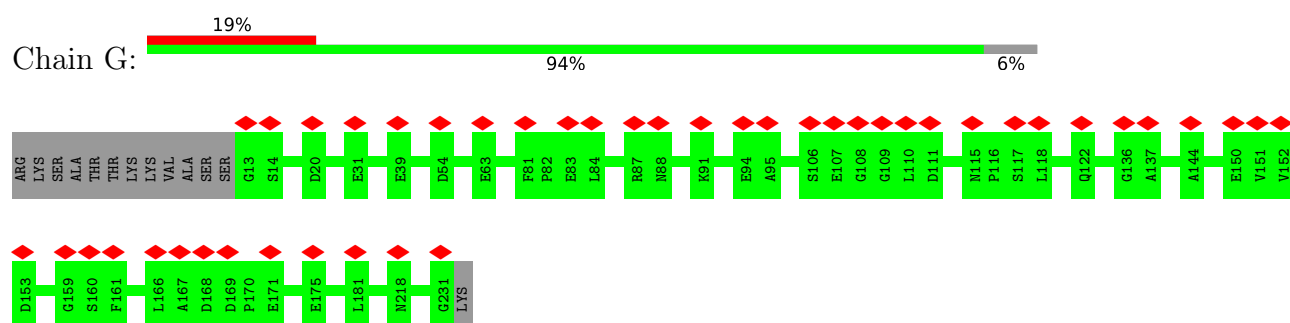
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



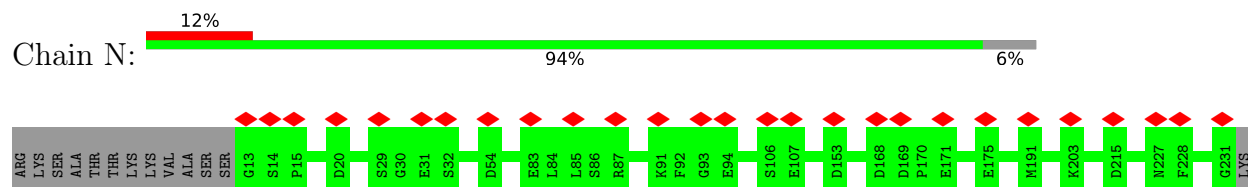
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



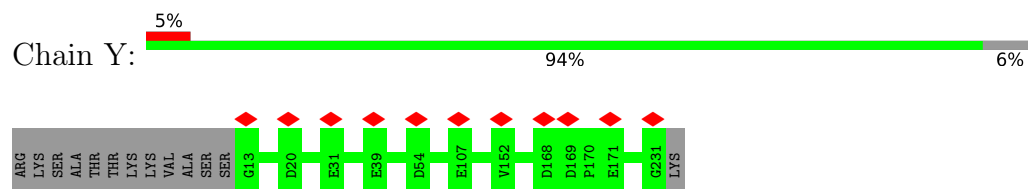
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



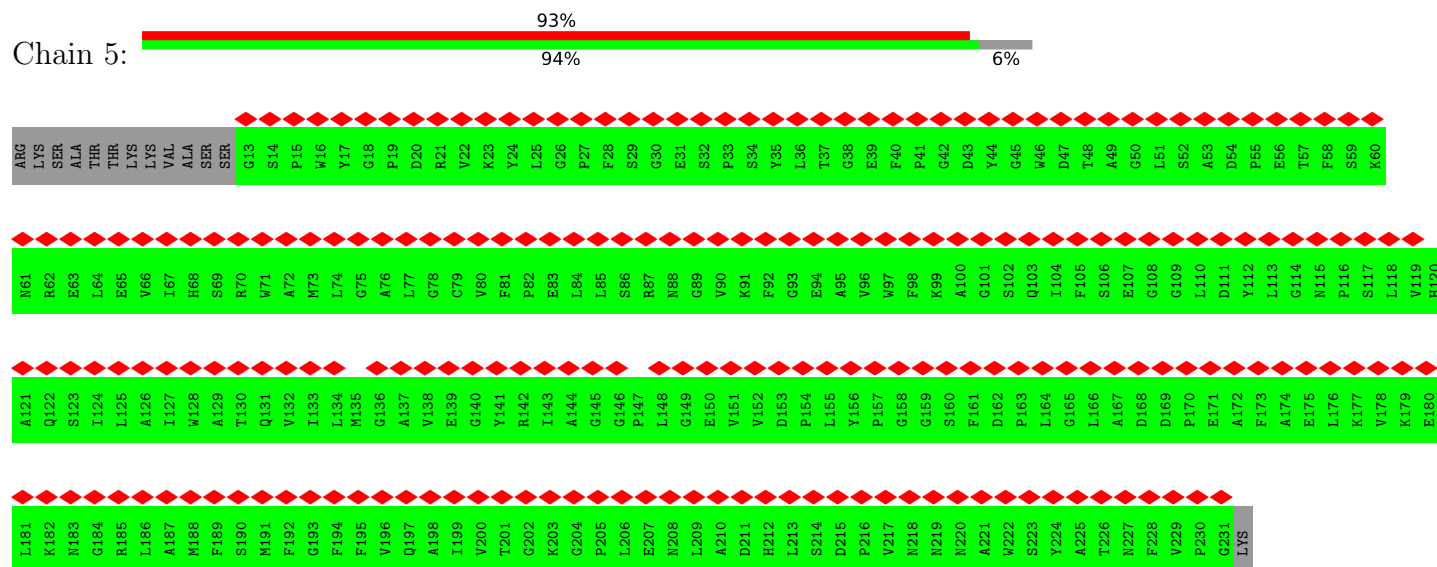
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



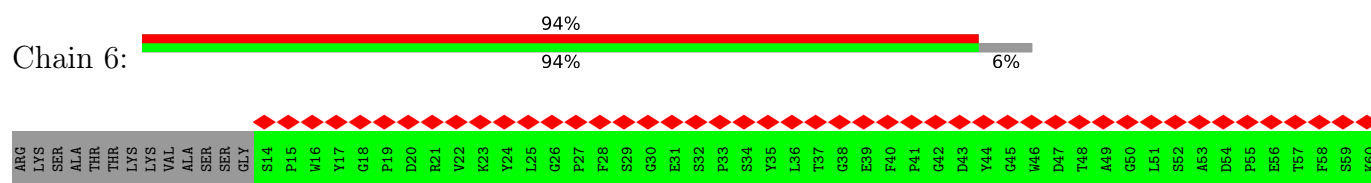
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

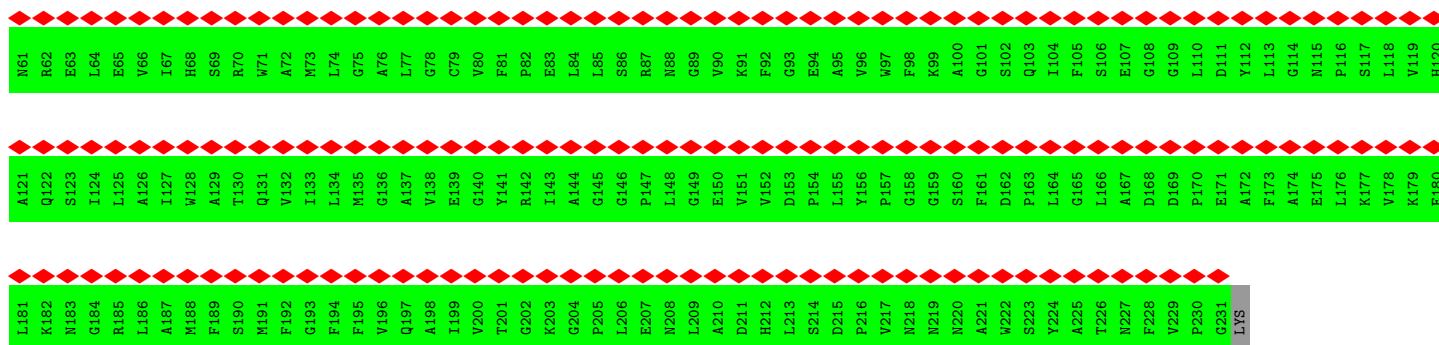


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

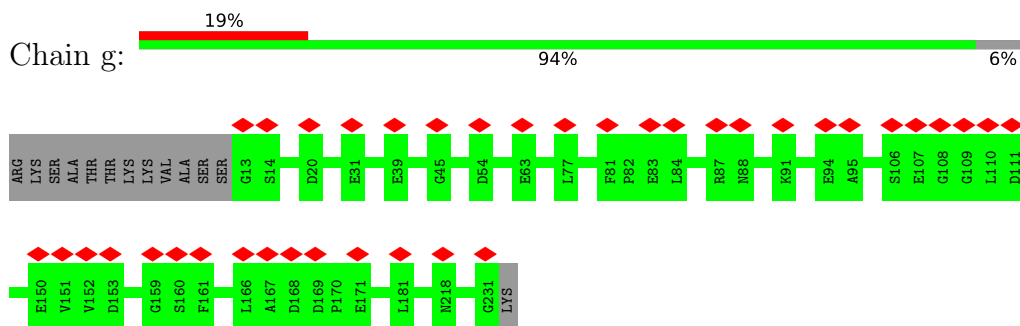


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

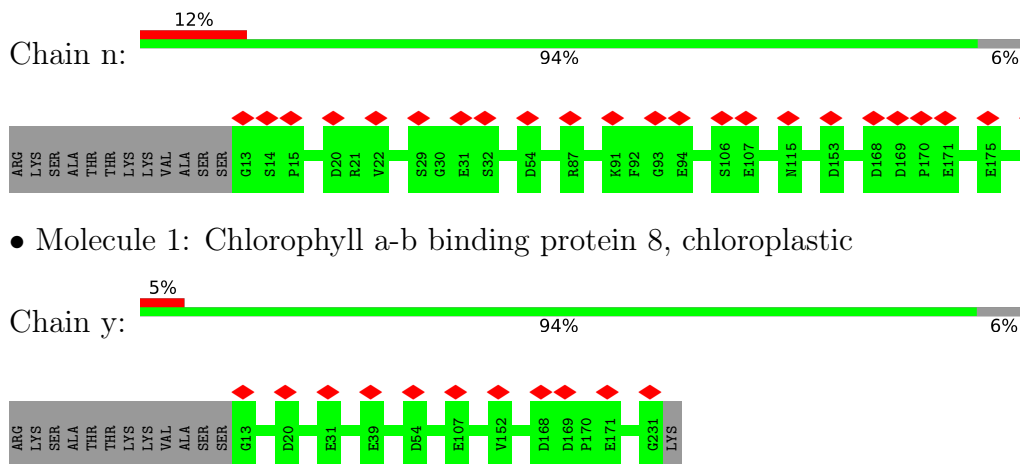




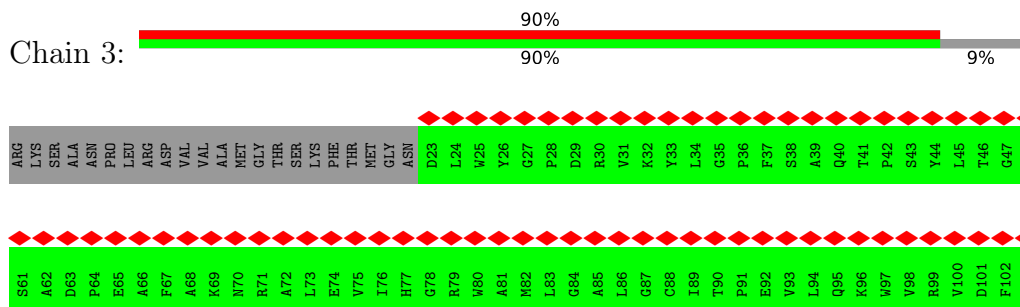
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

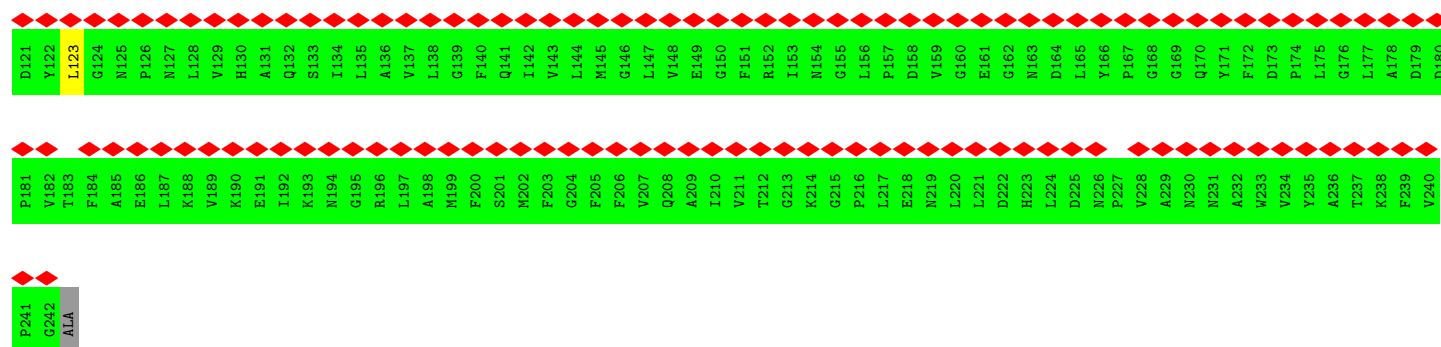


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



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





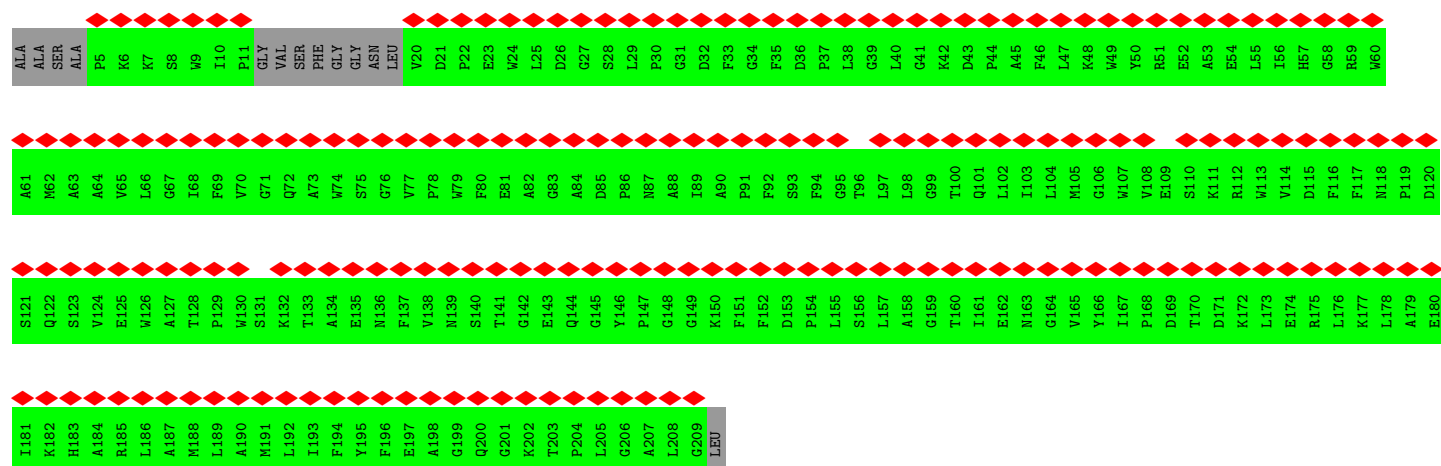
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 90%  
90% 9%

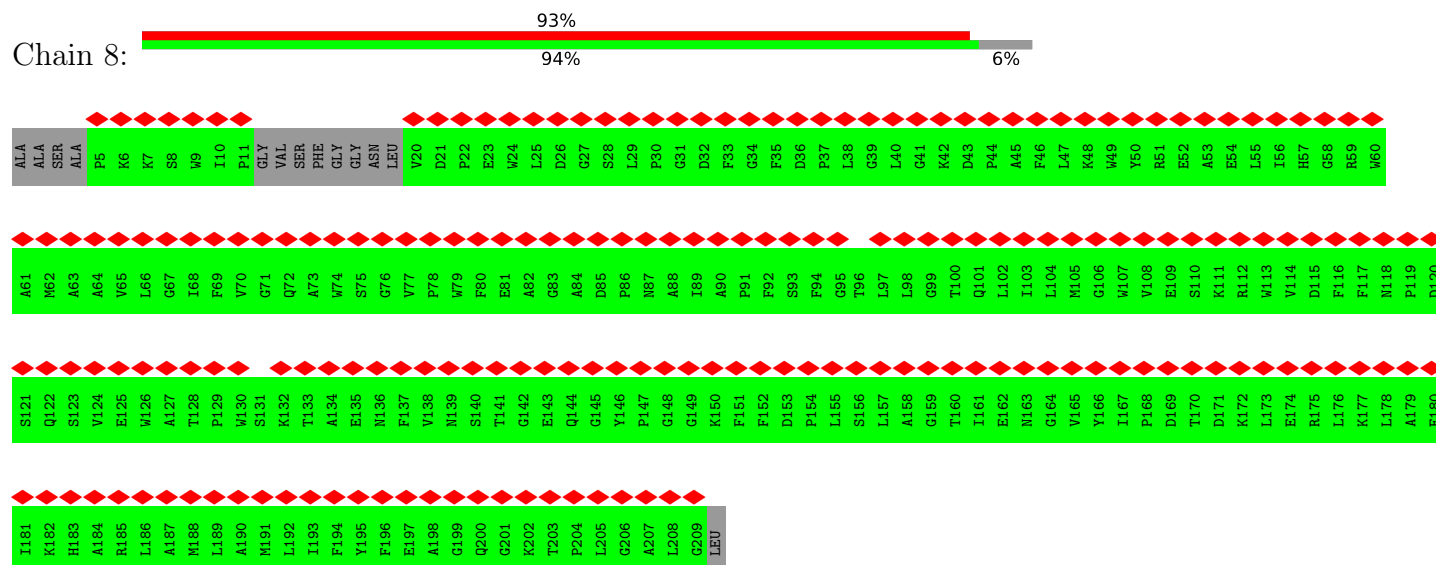


- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

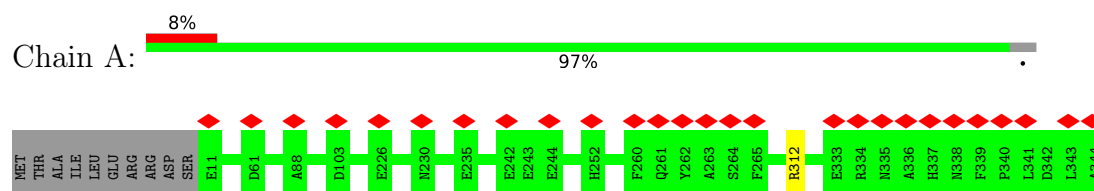
Chain 4: 92%  
94% 6%



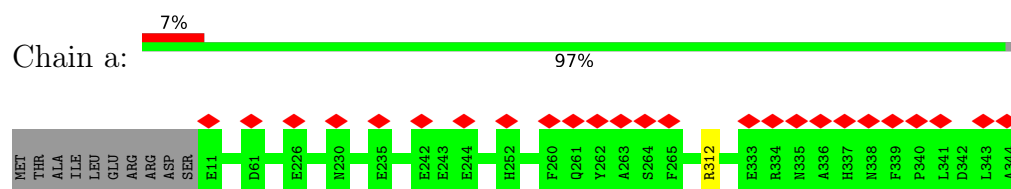
- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



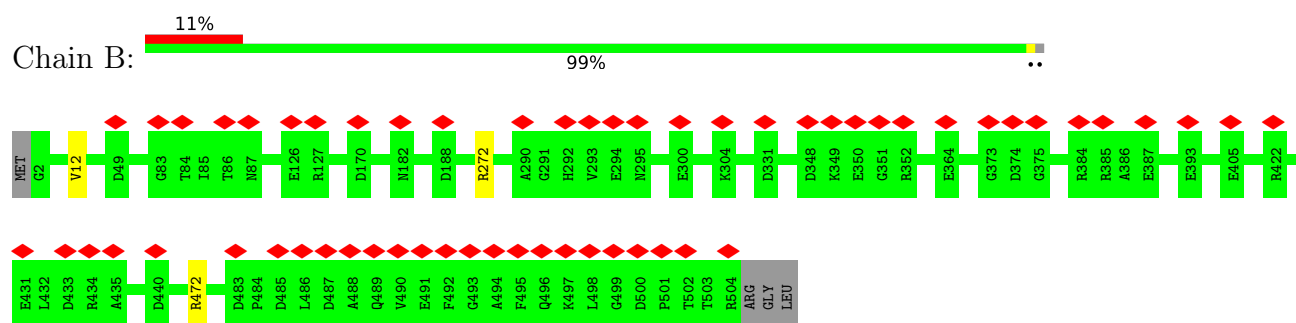
- Molecule 4: Photosystem II protein D1



- Molecule 4: Photosystem II protein D1



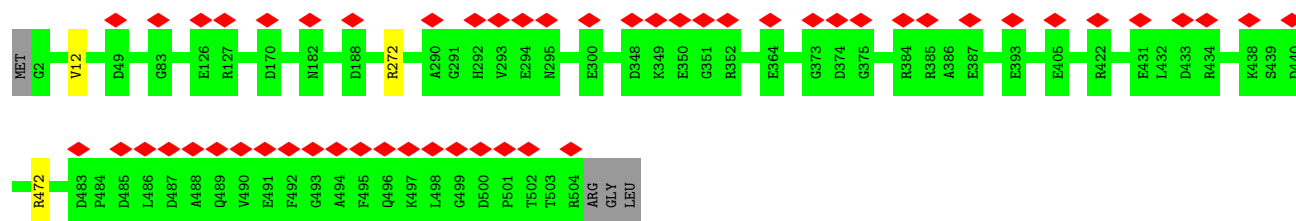
- Molecule 5: Photosystem II CP47 reaction center protein



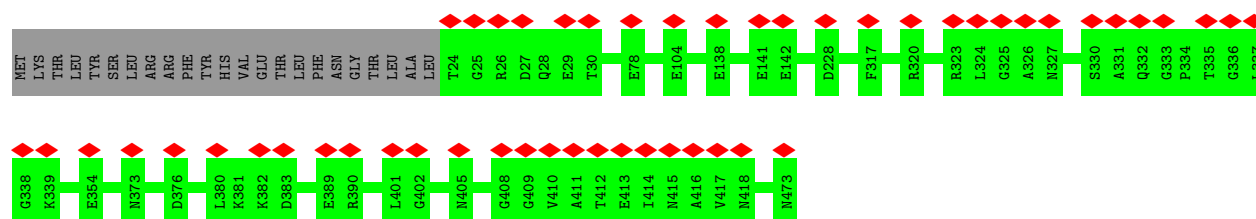
- Molecule 5: Photosystem II CP47 reaction center protein



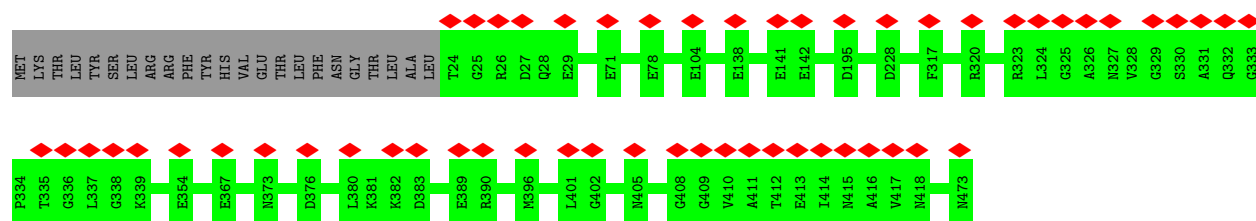
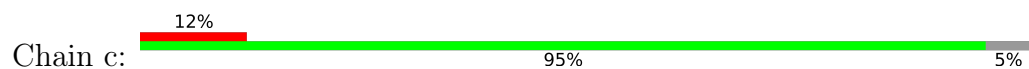




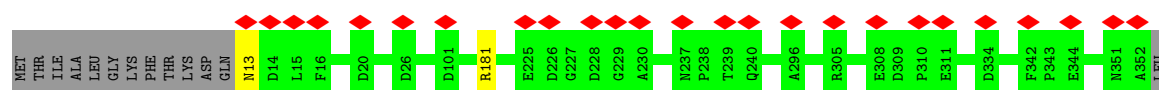
• Molecule 6: Photosystem II CP43 reaction center protein



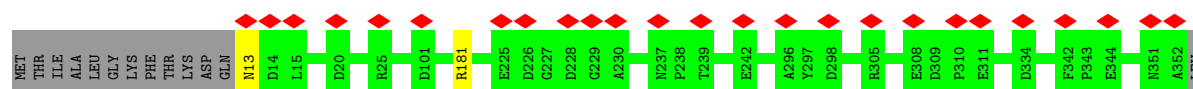
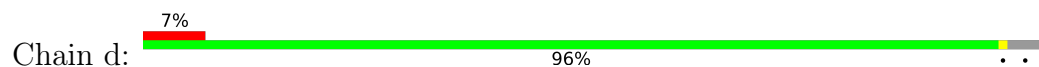
• Molecule 6: Photosystem II CP43 reaction center protein



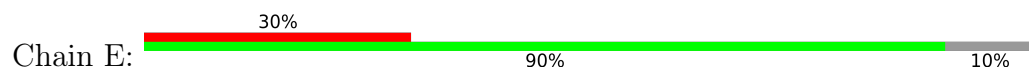
• Molecule 7: Photosystem II D2 protein

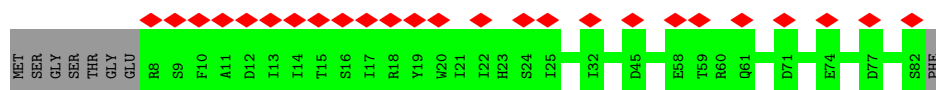


• Molecule 7: Photosystem II D2 protein

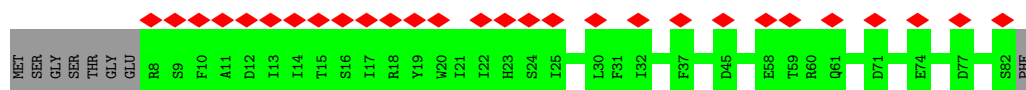
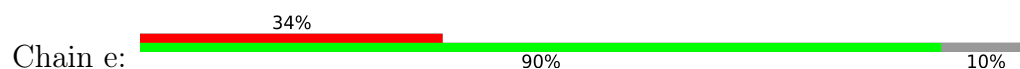


• Molecule 8: Cytochrome b559 subunit alpha

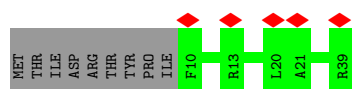
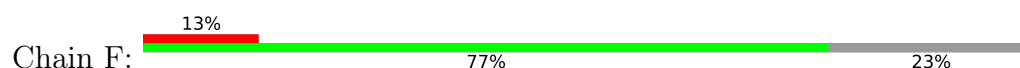




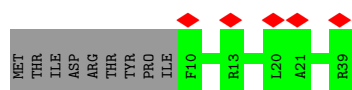
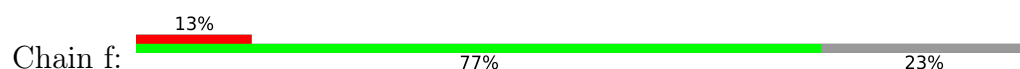
- Molecule 8: Cytochrome b559 subunit alpha



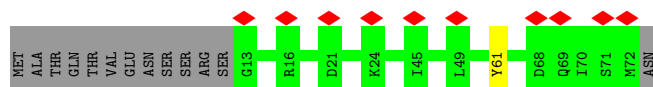
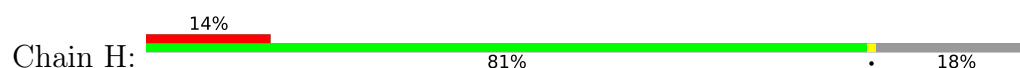
- Molecule 9: Cytochrome b559 subunit beta, PsbF



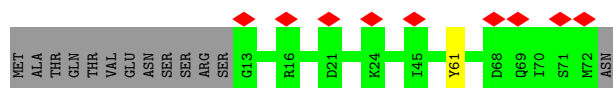
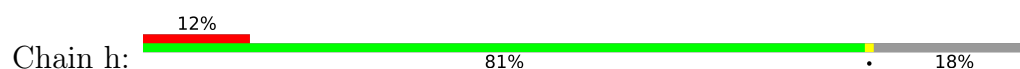
- Molecule 9: Cytochrome b559 subunit beta, PsbF



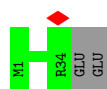
- Molecule 10: Photosystem II reaction center protein H



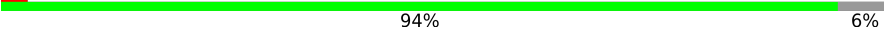
- Molecule 10: Photosystem II reaction center protein H

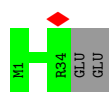


- Molecule 11: Photosystem II reaction center protein I, PsbI




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

Chain i:  94% 6%




- Molecule 12: Photosystem II reaction center protein J

Chain J:  85% 15%



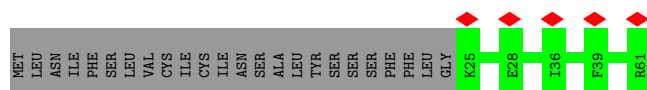
- Molecule 12: Photosystem II reaction center protein J

Chain j:  82% 85% 15%



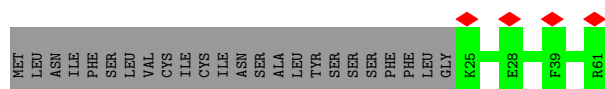
- Molecule 13: Photosystem II reaction center protein K

Chain K:  8% 61% 39%



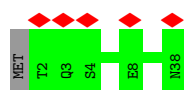
- Molecule 13: Photosystem II reaction center protein K

Chain k:  7% 61% 39%



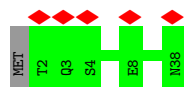
- Molecule 14: Photosystem II reaction center protein L

Chain L:  13% 97%

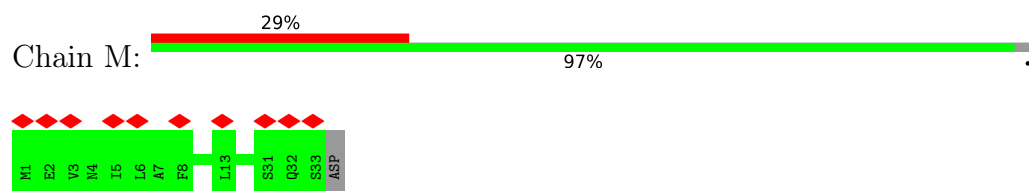


- Molecule 14: Photosystem II reaction center protein L

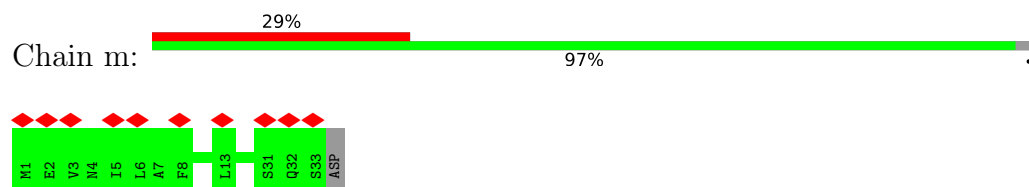
Chain l:  13% 97%



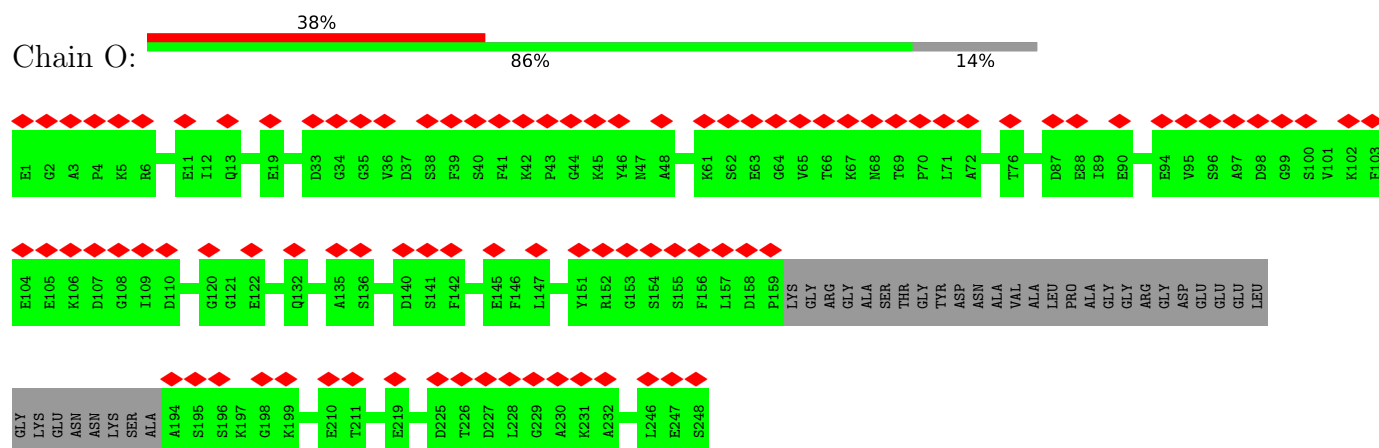
- Molecule 15: Photosystem II reaction center protein M



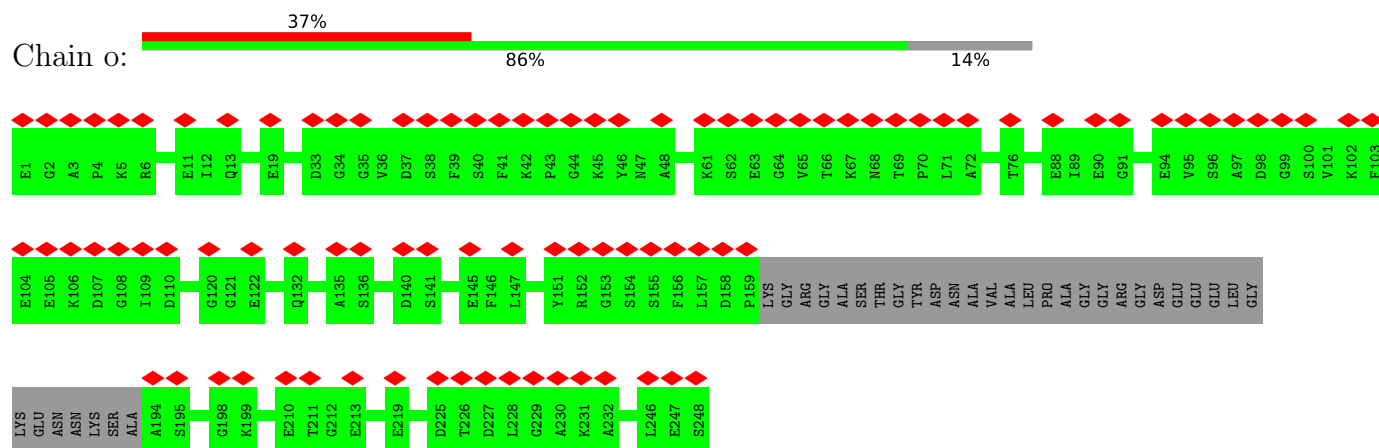
- Molecule 15: Photosystem II reaction center protein M



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

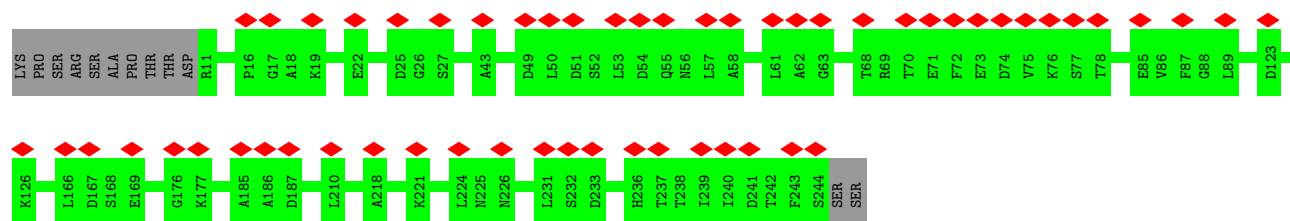


- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



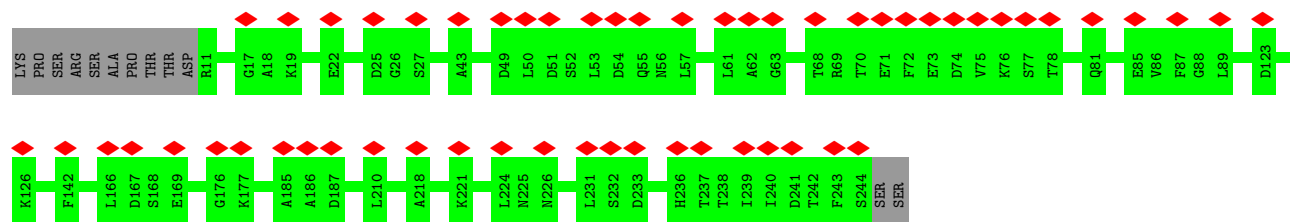
- Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29





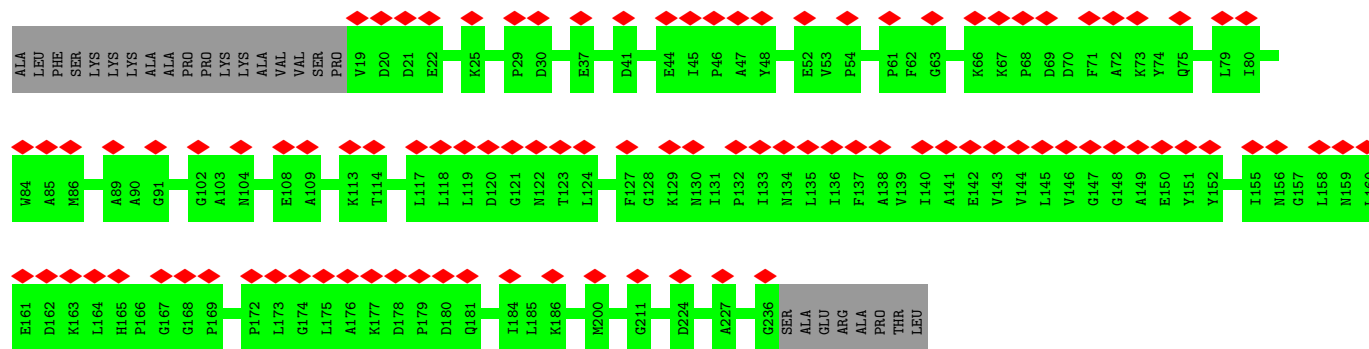
- Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain r: 23% 95% 5%



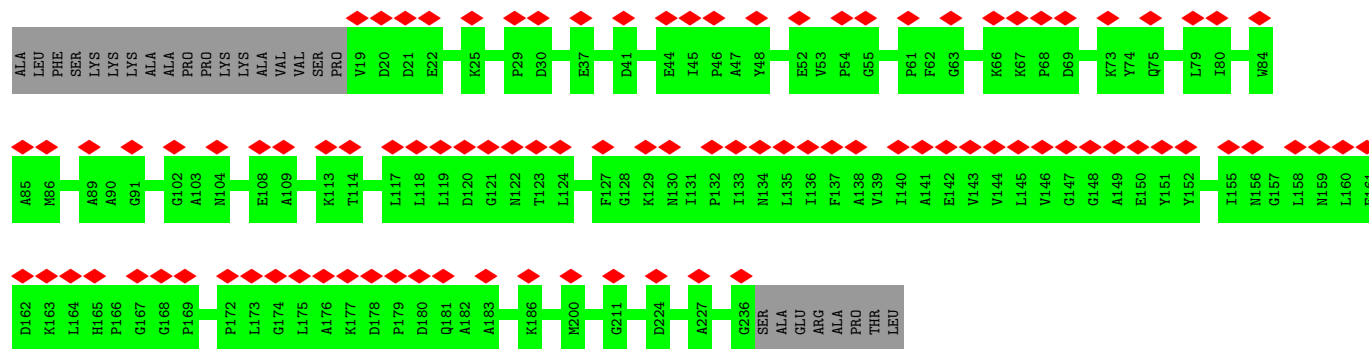
- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S: 41% 89% 11%

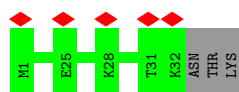


- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

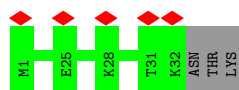
Chain s: 40% 89% 11%



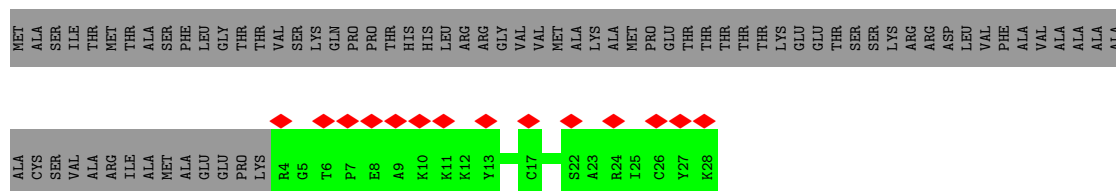
- Molecule 19: Photosystem II reaction center protein T



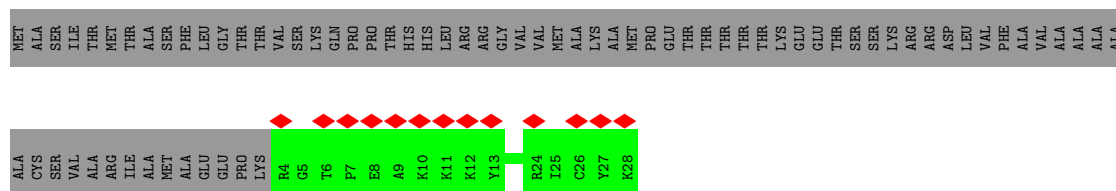
- Molecule 19: Photosystem II reaction center protein T



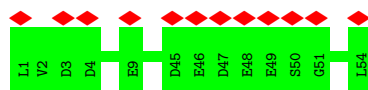
- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



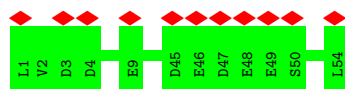
- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn



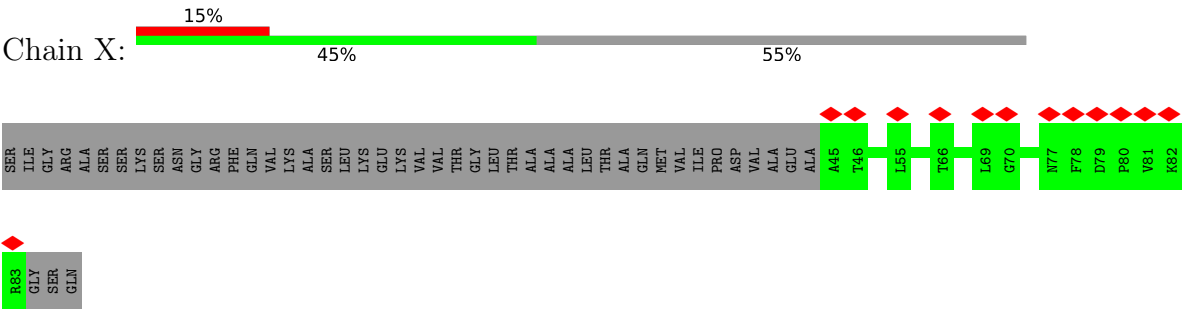
- Molecule 21: Photosystem II reaction center protein W, PSBW



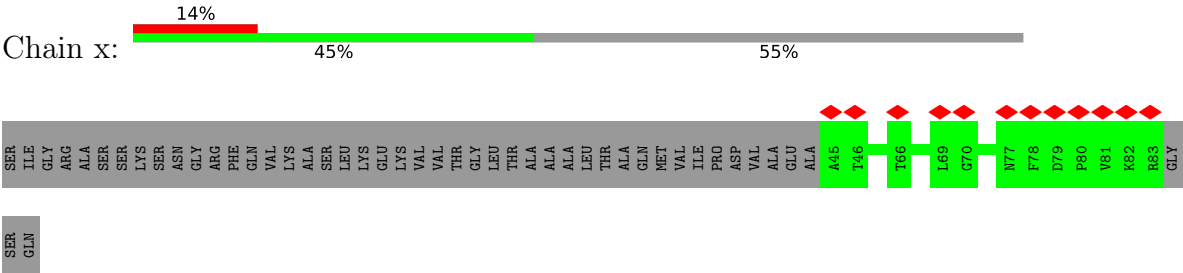
- Molecule 21: Photosystem II reaction center protein W, PSBW



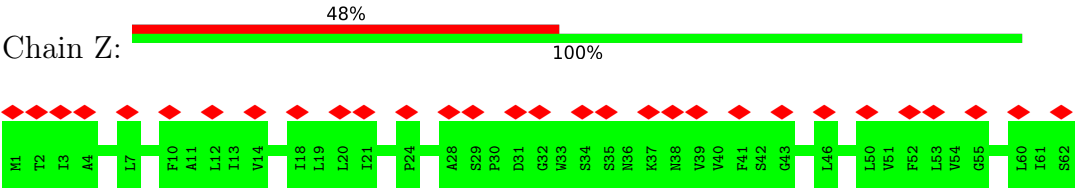
- Molecule 22: Photosystem II reaction center protein X



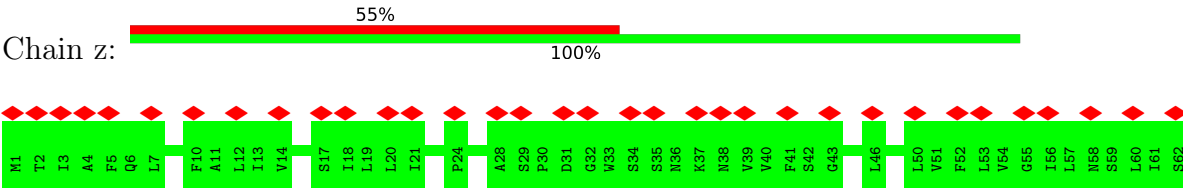
• Molecule 22: Photosystem II reaction center protein X



• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z



## 4 Experimental information

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



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.48	0/1720	0.55	0/2342
1	2	0.43	0/1716	0.54	0/2337
1	5	0.48	0/1720	0.55	0/2342
1	6	0.43	0/1716	0.54	0/2337
1	G	0.44	0/1720	0.53	0/2342
1	N	0.45	0/1720	0.53	0/2342
1	Y	0.52	0/1720	0.55	0/2342
1	g	0.44	0/1720	0.53	0/2342
1	n	0.45	0/1720	0.53	0/2342
1	y	0.52	0/1720	0.55	0/2342
2	3	0.49	0/1759	0.59	1/2396 (0.0%)
2	7	0.49	0/1759	0.59	1/2396 (0.0%)
3	4	0.42	0/1586	0.59	0/2158
3	8	0.42	0/1586	0.59	0/2158
4	A	0.47	0/2697	0.57	0/3677
4	a	0.47	0/2697	0.57	0/3677
5	B	0.56	0/4081	0.59	0/5556
5	b	0.56	0/4081	0.59	0/5556
6	C	0.36	0/3614	0.54	0/4922
6	c	0.36	0/3614	0.54	0/4922
7	D	0.62	0/2795	0.65	0/3812
7	d	0.62	0/2795	0.65	0/3812
8	E	0.33	0/630	0.50	0/857
8	e	0.33	0/630	0.50	0/857
9	F	0.34	0/248	0.51	0/335
9	f	0.34	0/248	0.51	0/335
10	H	0.47	0/461	0.58	0/626
10	h	0.47	0/461	0.58	0/626
11	I	0.61	0/286	0.69	0/386
11	i	0.61	0/286	0.69	0/386
12	J	0.30	0/253	0.59	0/343
12	j	0.30	0/253	0.60	0/343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
13	K	0.55	0/318	0.64	0/434
13	k	0.55	0/318	0.64	0/434
14	L	0.48	0/319	0.56	0/434
14	l	0.48	0/319	0.56	0/434
15	M	0.54	0/260	0.65	0/355
15	m	0.54	0/260	0.65	0/355
16	O	0.41	0/1664	0.56	0/2250
16	o	0.41	0/1664	0.56	0/2250
17	R	0.43	0/1886	0.57	0/2569
17	r	0.43	0/1886	0.57	0/2569
18	S	0.32	0/1736	0.54	0/2359
18	s	0.32	0/1736	0.54	0/2359
19	T	0.51	0/269	0.50	0/365
19	t	0.51	0/269	0.50	0/365
20	U	0.36	0/197	0.56	0/264
20	u	0.36	0/197	0.57	0/264
21	W	0.48	0/429	0.60	0/581
21	w	0.48	0/429	0.60	0/581
22	X	0.49	0/279	0.56	0/380
22	x	0.48	0/279	0.56	0/380
23	Z	0.42	0/474	0.53	0/648
23	z	0.42	0/474	0.53	0/648
All	All	0.47	0/69674	0.57	2/94824 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	123	LEU	CA-CB-CG	6.24	129.66	115.30
2	3	123	LEU	CA-CB-CG	6.24	129.64	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	171 (100%)	0	100	100
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100
1	y	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	269 (100%)	1 (0%)	89	94
4	a	270/279 (97%)	269 (100%)	1 (0%)	89	94
5	B	400/403 (99%)	397 (99%)	3 (1%)	79	90
5	b	400/403 (99%)	397 (99%)	3 (1%)	79	90
6	C	352/373 (94%)	352 (100%)	0	100	100
6	c	352/373 (94%)	352 (100%)	0	100	100
7	D	274/285 (96%)	272 (99%)	2 (1%)	81	92
7	d	274/285 (96%)	272 (99%)	2 (1%)	81	92
8	E	67/73 (92%)	67 (100%)	0	100	100
8	e	67/73 (92%)	67 (100%)	0	100	100
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	49/61 (80%)	48 (98%)	1 (2%)	50	75
10	h	49/61 (80%)	48 (98%)	1 (2%)	50	75
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	25/30 (83%)	25 (100%)	0	100	100
12	j	25/30 (83%)	25 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	182/204 (89%)	182 (100%)	0	100	100
16	o	182/204 (89%)	182 (100%)	0	100	100
17	R	191/202 (95%)	191 (100%)	0	100	100
17	r	191/202 (95%)	191 (100%)	0	100	100
18	S	170/190 (90%)	170 (100%)	0	100	100
18	s	170/190 (90%)	170 (100%)	0	100	100
19	T	29/32 (91%)	29 (100%)	0	100	100
19	t	29/32 (91%)	29 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/44 (100%)	44 (100%)	0	100	100
21	w	44/44 (100%)	44 (100%)	0	100	100
22	X	32/67 (48%)	32 (100%)	0	100	100
22	x	32/67 (48%)	32 (100%)	0	100	100
23	Z	54/54 (100%)	54 (100%)	0	100	100
23	z	54/54 (100%)	54 (100%)	0	100	100
All	All	6992/7658 (91%)	6978 (100%)	14 (0%)	91	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	a	312	ARG
5	b	12	VAL
10	h	61	TYR
7	d	13	ASN
7	d	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	7	95	GLN
5	b	216	HIS
1	y	88	ASN
2	7	219	ASN
4	a	301	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 486 ligands modelled in this entry, 2 are monoatomic - leaving 484 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LUT	Y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.87	17 (33%)
37	DGD	H	102	-	63,63,67	1.21	6 (9%)	77,77,81	1.52	10 (12%)
24	CHL	g	607	-	66,74,74	1.83	12 (18%)	73,114,114	2.67	19 (26%)
26	LUT	Y	1620	-	42,43,43	1.08	5 (11%)	51,60,60	1.92	20 (39%)
25	CLA	n	614	1	48,56,73	1.64	9 (18%)	55,92,113	1.55	8 (14%)
24	CHL	8	601	3	44,53,74	2.44	16 (36%)	46,89,114	3.07	17 (36%)
25	CLA	r	601	17	49,57,73	1.71	9 (18%)	55,93,113	1.73	10 (18%)
29	LHG	7	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.31	4 (8%)
25	CLA	6	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.26	6 (10%)
25	CLA	n	602	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
26	LUT	1	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.87	14 (27%)
25	CLA	B	603	5	65,73,73	1.46	10 (15%)	76,113,113	1.26	6 (7%)
34	SQD	b	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
25	CLA	6	613	1	45,53,73	1.80	10 (22%)	52,89,113	1.46	8 (15%)
25	CLA	B	615	5	65,73,73	1.42	11 (16%)	76,113,113	1.35	9 (11%)
25	CLA	b	612	5	65,73,73	1.59	11 (16%)	76,113,113	1.69	12 (15%)
28	NEX	S	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	16 (32%)
25	CLA	1	612	1	45,53,73	1.81	11 (24%)	52,89,113	1.61	12 (23%)
25	CLA	6	612	1	45,53,73	1.83	9 (20%)	52,89,113	1.48	9 (17%)
28	NEX	n	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	17 (34%)
25	CLA	N	603	1	65,73,73	1.51	10 (15%)	76,113,113	1.44	11 (14%)
39	HEM	f	101	8,9	41,50,50	1.44	4 (9%)	45,82,82	1.26	4 (8%)
25	CLA	7	612	2	45,53,73	1.76	11 (24%)	52,89,113	1.52	9 (17%)
30	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
24	CHL	1	606	-	46,54,74	2.21	15 (32%)	49,90,114	3.06	18 (36%)
25	CLA	a	405	4	65,73,73	1.46	9 (13%)	76,113,113	1.43	6 (7%)
25	CLA	n	604	-	50,58,73	1.73	10 (20%)	58,95,113	1.59	9 (15%)
34	SQD	b	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
24	CHL	2	607	-	61,69,74	2.05	15 (24%)	67,108,114	2.60	22 (32%)
30	BCR	B	619	-	41,41,41	0.87	1 (2%)	56,56,56	1.86	17 (30%)
25	CLA	3	613	2	58,66,73	1.60	12 (20%)	67,104,113	1.42	7 (10%)
24	CHL	N	607	-	66,74,74	1.81	13 (19%)	73,114,114	2.77	19 (26%)
33	PHO	A	408	-	51,69,69	1.09	8 (15%)	47,99,99	1.19	6 (12%)
25	CLA	C	501	6	65,73,73	1.55	8 (12%)	76,113,113	1.22	7 (9%)
25	CLA	b	603	5	65,73,73	1.46	10 (15%)	76,113,113	1.26	6 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	SQD	A	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.67	13 (20%)
24	CHL	y	605	1	48,56,74	2.14	12 (25%)	51,92,114	3.03	18 (35%)
25	CLA	Y	614	1	48,56,73	1.73	11 (22%)	55,92,113	1.42	7 (12%)
25	CLA	3	602	2	60,68,73	1.49	9 (15%)	70,107,113	1.40	8 (11%)
24	CHL	7	607	-	53,61,74	2.09	16 (30%)	57,98,114	2.96	20 (35%)
29	LHG	d	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
25	CLA	8	610	3	45,53,73	1.75	10 (22%)	52,89,113	1.44	7 (13%)
25	CLA	A	405	4	65,73,73	1.46	9 (13%)	76,113,113	1.44	6 (7%)
25	CLA	s	610	18	55,63,73	1.65	8 (14%)	64,101,113	1.42	8 (12%)
25	CLA	R	604	-	48,56,73	1.68	10 (20%)	55,92,113	1.65	10 (18%)
25	CLA	4	603	3	45,53,73	1.77	9 (20%)	52,89,113	1.60	7 (13%)
25	CLA	R	610	17	65,73,73	1.46	9 (13%)	76,113,113	1.40	8 (10%)
25	CLA	r	610	17	65,73,73	1.46	9 (13%)	76,113,113	1.40	8 (10%)
27	XAT	2	1622	-	39,47,47	1.03	0	54,74,74	2.98	22 (40%)
25	CLA	2	614	1	45,53,73	1.75	9 (20%)	52,89,113	1.50	7 (13%)
24	CHL	Y	605	1	48,56,74	2.14	12 (25%)	51,92,114	3.03	18 (35%)
24	CHL	s	601	18	46,54,74	2.23	13 (28%)	49,90,114	3.21	22 (44%)
24	CHL	n	601	1	66,74,74	1.89	14 (21%)	73,114,114	2.70	23 (31%)
24	CHL	y	601	1	66,74,74	1.81	11 (16%)	73,114,114	2.83	23 (31%)
30	BCR	C	517	-	41,41,41	0.80	0	56,56,56	2.10	13 (23%)
30	BCR	b	619	-	41,41,41	0.87	2 (4%)	56,56,56	1.86	17 (30%)
25	CLA	R	616	17	45,53,73	1.76	10 (22%)	52,89,113	1.53	7 (13%)
27	XAT	g	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.86	22 (40%)
29	LHG	8	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
30	BCR	4	623	-	41,41,41	0.78	0	56,56,56	2.18	15 (26%)
24	CHL	5	607	-	63,71,74	1.90	14 (22%)	69,110,114	2.88	23 (33%)
25	CLA	R	602	17	60,68,73	1.48	10 (16%)	70,107,113	1.52	10 (14%)
24	CHL	4	608	-	46,54,74	2.16	13 (28%)	49,90,114	3.24	24 (48%)
25	CLA	7	603	2	55,63,73	1.59	12 (21%)	64,101,113	1.57	10 (15%)
25	CLA	3	614	2	48,56,73	1.79	7 (14%)	55,92,113	1.48	7 (12%)
24	CHL	S	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.12	17 (34%)
26	LUT	S	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
24	CHL	Y	601	1	66,74,74	1.81	11 (16%)	73,114,114	2.83	23 (31%)
27	XAT	R	622	-	39,47,47	1.05	2 (5%)	54,74,74	2.72	19 (35%)
25	CLA	g	610	1	64,72,73	1.44	10 (15%)	74,111,113	1.39	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LHG	B	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
37	DGD	c	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)
24	CHL	G	605	1	46,54,74	2.26	15 (32%)	49,90,114	3.09	20 (40%)
30	BCR	B	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
26	LUT	g	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	b	604	5	65,73,73	1.54	11 (16%)	76,113,113	1.37	9 (11%)
26	LUT	n	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
25	CLA	G	611	29	60,68,73	1.52	10 (16%)	70,107,113	1.38	6 (8%)
25	CLA	b	610	5	65,73,73	1.41	10 (15%)	76,113,113	1.48	10 (13%)
33	PHO	a	408	-	51,69,69	1.09	8 (15%)	47,99,99	1.19	7 (14%)
25	CLA	8	603	3	45,53,73	1.76	9 (20%)	52,89,113	1.60	7 (13%)
24	CHL	2	609	1	61,69,74	1.95	13 (21%)	67,108,114	2.78	22 (32%)
24	CHL	1	605	1	46,54,74	2.28	15 (32%)	49,90,114	3.15	17 (34%)
29	LHG	R	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.34	6 (13%)
26	LUT	7	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
25	CLA	N	614	1	48,56,73	1.64	9 (18%)	55,92,113	1.55	8 (14%)
24	CHL	7	608	-	46,54,74	2.22	14 (30%)	49,90,114	3.27	19 (38%)
24	CHL	R	606	-	66,74,74	1.86	13 (19%)	73,114,114	2.72	24 (32%)
25	CLA	A	410	4	60,68,73	1.50	10 (16%)	70,107,113	1.44	9 (12%)
25	CLA	n	613	1	60,68,73	1.59	7 (11%)	70,107,113	1.69	7 (10%)
29	LHG	D	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
25	CLA	C	511	6	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
30	BCR	c	515	-	41,41,41	0.77	0	56,56,56	1.90	17 (30%)
35	LMG	A	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
24	CHL	N	608	-	66,74,74	1.80	13 (19%)	73,114,114	2.73	22 (30%)
24	CHL	s	607	-	58,66,74	2.00	16 (27%)	63,104,114	2.77	21 (33%)
25	CLA	y	611	29	60,68,73	1.61	9 (15%)	70,107,113	1.33	9 (12%)
26	LUT	6	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
28	NEX	Y	1623	-	38,46,46	1.12	2 (5%)	50,70,70	2.70	22 (44%)
25	CLA	2	612	1	45,53,73	1.82	10 (22%)	52,89,113	1.48	9 (17%)
26	LUT	7	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
25	CLA	7	602	2	60,68,73	1.50	10 (16%)	70,107,113	1.39	8 (11%)
25	CLA	R	609	17	58,66,73	1.53	11 (18%)	67,104,113	1.40	7 (10%)
35	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	6	604	-	45,53,73	1.73	11 (24%)	52,89,113	1.64	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	n	612	1	60,68,73	1.51	10 (16%)	70,107,113	1.41	8 (11%)
25	CLA	4	604	-	45,53,73	1.77	11 (24%)	52,89,113	1.57	8 (15%)
24	CHL	g	601	1	66,74,74	1.83	13 (19%)	73,114,114	2.72	24 (32%)
25	CLA	7	611	29	55,63,73	1.67	11 (20%)	64,101,113	1.45	9 (14%)
25	CLA	C	505	6	65,73,73	1.46	8 (12%)	76,113,113	1.51	8 (10%)
25	CLA	Y	611	29	60,68,73	1.60	9 (15%)	70,107,113	1.33	9 (12%)
24	CHL	N	601	1	66,74,74	1.89	14 (21%)	73,114,114	2.70	23 (31%)
29	LHG	6	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
25	CLA	s	603	18	45,53,73	1.83	7 (15%)	52,89,113	1.56	8 (15%)
25	CLA	A	406	-	65,73,73	1.49	10 (15%)	76,113,113	1.53	9 (11%)
25	CLA	N	604	-	50,58,73	1.73	10 (20%)	58,95,113	1.59	9 (15%)
25	CLA	3	612	2	45,53,73	1.76	11 (24%)	52,89,113	1.51	9 (17%)
28	NEX	3	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.46	16 (32%)
27	XAT	3	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.06	27 (50%)
36	PL9	D	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
29	LHG	y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)
30	BCR	c	516	-	41,41,41	0.68	0	56,56,56	1.94	14 (25%)
25	CLA	B	604	5	65,73,73	1.54	11 (16%)	76,113,113	1.37	8 (10%)
30	BCR	8	623	-	41,41,41	0.79	0	56,56,56	2.18	15 (26%)
29	LHG	S	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
24	CHL	2	606	-	46,54,74	2.23	14 (30%)	49,90,114	3.10	20 (40%)
24	CHL	s	608	-	46,54,74	2.29	15 (32%)	49,90,114	3.05	17 (34%)
25	CLA	2	613	1	45,53,73	1.81	10 (22%)	52,89,113	1.46	8 (15%)
25	CLA	B	613	5	65,73,73	1.48	11 (16%)	76,113,113	1.68	12 (15%)
25	CLA	a	407	-	50,58,73	1.69	11 (22%)	58,95,113	1.48	8 (13%)
25	CLA	b	609	5	65,73,73	1.37	9 (13%)	76,113,113	1.61	9 (11%)
25	CLA	b	615	5	65,73,73	1.42	11 (16%)	76,113,113	1.35	9 (11%)
25	CLA	a	410	4	60,68,73	1.50	10 (16%)	70,107,113	1.44	9 (12%)
25	CLA	b	607	5	65,73,73	1.52	11 (16%)	76,113,113	1.43	8 (10%)
26	LUT	R	620	-	42,43,43	0.99	4 (9%)	51,60,60	1.95	18 (35%)
25	CLA	5	610	1	56,64,73	1.53	10 (17%)	65,102,113	1.36	6 (9%)
27	XAT	4	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	19 (35%)
28	NEX	5	1623	-	38,46,46	1.13	3 (7%)	50,70,70	2.62	18 (36%)
25	CLA	5	604	-	50,58,73	1.73	11 (22%)	58,95,113	1.51	9 (15%)
34	SQD	a	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	r	614	17	42,50,74	2.39	15 (35%)	44,85,114	3.37	18 (40%)
26	LUT	N	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
24	CHL	r	608	-	61,69,74	1.82	10 (16%)	67,108,114	2.88	19 (28%)
27	XAT	5	1622	-	39,47,47	0.96	2 (5%)	54,74,74	2.84	22 (40%)
25	CLA	A	407	-	50,58,73	1.69	11 (22%)	58,95,113	1.48	8 (13%)
24	CHL	n	605	1	48,56,74	2.18	13 (27%)	51,92,114	3.12	23 (45%)
25	CLA	c	508	6	65,73,73	1.46	8 (12%)	76,113,113	1.54	8 (10%)
35	LMG	a	415	-	40,40,55	0.88	0	48,48,63	1.31	6 (12%)
30	BCR	A	411	-	41,41,41	0.81	0	56,56,56	1.85	12 (21%)
34	SQD	a	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.66	13 (20%)
25	CLA	c	503	6	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
25	CLA	c	507	-	65,73,73	1.44	8 (12%)	76,113,113	1.54	10 (13%)
24	CHL	4	606	-	46,54,74	2.24	13 (28%)	49,90,114	3.17	20 (40%)
24	CHL	7	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.20	22 (44%)
25	CLA	2	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.26	6 (10%)
35	LMG	C	521	-	51,51,55	0.76	0	59,59,63	1.31	6 (10%)
25	CLA	c	510	6	65,73,73	1.46	7 (10%)	76,113,113	1.45	9 (11%)
33	PHO	a	409	-	51,69,69	1.02	5 (9%)	47,99,99	1.30	5 (10%)
25	CLA	2	603	1	55,63,73	1.62	11 (20%)	64,101,113	1.53	10 (15%)
25	CLA	g	612	1	60,68,73	1.53	9 (15%)	70,107,113	1.38	9 (12%)
26	LUT	5	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
24	CHL	y	607	-	66,74,74	1.81	12 (18%)	73,114,114	2.70	17 (23%)
24	CHL	7	609	2	61,69,74	2.03	16 (26%)	67,108,114	2.69	21 (31%)
25	CLA	N	613	1	60,68,73	1.59	7 (11%)	70,107,113	1.68	7 (10%)
25	CLA	s	612	18	49,57,73	1.68	7 (14%)	55,93,113	1.52	7 (12%)
29	LHG	5	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
25	CLA	C	507	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	10 (13%)
25	CLA	y	612	1	60,68,73	1.59	11 (18%)	70,107,113	1.38	9 (12%)
26	LUT	3	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
24	CHL	n	608	-	66,74,74	1.80	12 (18%)	73,114,114	2.73	23 (31%)
24	CHL	4	609	3	46,54,74	2.19	14 (30%)	49,90,114	3.29	20 (40%)
26	LUT	5	1620	-	42,43,43	0.94	2 (4%)	51,60,60	1.87	14 (27%)
29	LHG	d	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
24	CHL	S	607	-	58,66,74	1.99	16 (27%)	63,104,114	2.78	22 (34%)
37	DGD	c	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	c	513	6	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
25	CLA	Y	613	1	65,73,73	1.54	10 (15%)	76,113,113	1.68	8 (10%)
25	CLA	c	501	6	65,73,73	1.54	8 (12%)	76,113,113	1.22	7 (9%)
25	CLA	R	613	17	60,68,73	1.56	8 (13%)	70,107,113	1.49	9 (12%)
24	CHL	1	609	1	62,70,74	2.02	15 (24%)	68,109,114	2.73	20 (29%)
26	LUT	S	1621	-	42,43,43	0.80	0	51,60,60	1.74	15 (29%)
25	CLA	Y	612	1	60,68,73	1.59	11 (18%)	70,107,113	1.38	9 (12%)
25	CLA	1	611	29	45,53,73	1.75	12 (26%)	52,89,113	1.61	7 (13%)
25	CLA	6	611	29	45,53,73	1.74	9 (20%)	52,89,113	1.58	7 (13%)
25	CLA	G	612	1	60,68,73	1.53	9 (15%)	70,107,113	1.38	9 (12%)
24	CHL	G	608	-	66,74,74	1.85	13 (19%)	73,114,114	2.74	21 (28%)
28	NEX	r	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.52	21 (42%)
25	CLA	n	611	29	60,68,73	1.52	9 (15%)	70,107,113	1.44	8 (11%)
25	CLA	c	502	6	65,73,73	1.44	6 (9%)	76,113,113	1.57	8 (10%)
25	CLA	a	406	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	9 (11%)
29	LHG	D	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	7 (13%)
25	CLA	8	602	3	45,53,73	1.71	9 (20%)	52,89,113	1.68	8 (15%)
25	CLA	N	610	1	65,73,73	1.41	10 (15%)	76,113,113	1.39	8 (10%)
25	CLA	S	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.62	8 (13%)
35	LMG	B	2633	-	55,55,55	0.74	2 (3%)	63,63,63	1.36	6 (9%)
25	CLA	C	506	6	65,73,73	1.52	10 (15%)	76,113,113	1.40	7 (9%)
25	CLA	r	602	17	60,68,73	1.49	10 (16%)	70,107,113	1.52	10 (14%)
25	CLA	N	612	1	60,68,73	1.52	10 (16%)	70,107,113	1.42	8 (11%)
37	DGD	C	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)
34	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
24	CHL	Y	607	-	66,74,74	1.81	12 (18%)	73,114,114	2.70	17 (23%)
24	CHL	y	608	-	66,74,74	1.78	12 (18%)	73,114,114	2.80	18 (24%)
25	CLA	B	610	5	65,73,73	1.42	10 (15%)	76,113,113	1.48	10 (13%)
25	CLA	g	614	1	48,56,73	1.70	10 (20%)	55,92,113	1.34	6 (10%)
27	XAT	r	622	-	39,47,47	1.06	2 (5%)	54,74,74	2.72	19 (35%)
36	PL9	d	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
24	CHL	7	605	2	46,54,74	2.23	13 (28%)	49,90,114	3.18	22 (44%)
25	CLA	1	613	1	55,63,73	1.62	11 (20%)	64,101,113	1.47	6 (9%)
29	LHG	b	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
30	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.89	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	D	403	7	65,73,73	1.43	10 (15%)	76,113,113	1.43	9 (11%)
25	CLA	c	509	6	65,73,73	1.45	8 (12%)	76,113,113	1.44	8 (10%)
25	CLA	3	603	2	55,63,73	1.59	12 (21%)	64,101,113	1.57	10 (15%)
26	LUT	2	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
24	CHL	G	601	1	66,74,74	1.83	13 (19%)	73,114,114	2.72	24 (32%)
25	CLA	y	602	1	65,73,73	1.46	11 (16%)	76,113,113	1.42	11 (14%)
30	BCR	d	404	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
25	CLA	5	603	1	55,63,73	1.60	12 (21%)	64,101,113	1.57	11 (17%)
26	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
28	NEX	2	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.41	14 (28%)
29	LHG	c	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	B	616	5	65,73,73	1.49	10 (15%)	76,113,113	1.42	11 (14%)
25	CLA	7	614	2	48,56,73	1.79	7 (14%)	55,92,113	1.48	7 (12%)
24	CHL	6	601	1	46,54,74	2.25	14 (30%)	49,90,114	3.23	21 (42%)
29	LHG	4	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
25	CLA	B	602	-	65,73,73	1.47	11 (16%)	76,113,113	1.38	10 (13%)
25	CLA	b	605	5	65,73,73	1.52	14 (21%)	76,113,113	1.85	18 (23%)
28	NEX	s	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	15 (30%)
25	CLA	2	604	-	45,53,73	1.73	10 (22%)	52,89,113	1.64	10 (19%)
25	CLA	S	614	18	49,57,73	1.64	6 (12%)	55,93,113	1.60	8 (14%)
37	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
25	CLA	S	613	18	55,63,73	1.61	7 (12%)	64,101,113	1.41	6 (9%)
25	CLA	g	604	-	50,58,73	1.75	11 (22%)	58,95,113	1.54	7 (12%)
25	CLA	c	505	6	65,73,73	1.47	8 (12%)	76,113,113	1.51	8 (10%)
26	LUT	3	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
24	CHL	6	605	1	46,54,74	2.29	14 (30%)	49,90,114	3.11	19 (38%)
24	CHL	3	608	-	46,54,74	2.22	14 (30%)	49,90,114	3.29	19 (38%)
25	CLA	Y	602	1	65,73,73	1.47	11 (16%)	76,113,113	1.42	11 (14%)
25	CLA	5	612	1	45,53,73	1.81	11 (24%)	52,89,113	1.62	12 (23%)
25	CLA	B	611	-	65,73,73	1.50	10 (15%)	76,113,113	1.48	12 (15%)
35	LMG	D	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.38	6 (11%)
25	CLA	s	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.62	8 (13%)
24	CHL	1	601	1	46,54,74	2.26	14 (30%)	49,90,114	3.19	20 (40%)
25	CLA	8	612	3	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
25	CLA	y	610	1	60,68,73	1.54	9 (15%)	70,107,113	1.34	8 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	n	606	-	50,58,74	2.10	14 (28%)	52,94,114	3.10	18 (34%)
24	CHL	N	605	1	48,56,74	2.17	13 (27%)	51,92,114	3.11	23 (45%)
29	LHG	1	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
24	CHL	r	606	-	66,74,74	1.86	12 (18%)	73,114,114	2.71	24 (32%)
29	LHG	d	409	-	48,48,48	0.80	1 (2%)	51,54,54	1.33	7 (13%)
25	CLA	C	503	6	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
25	CLA	Y	610	1	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
24	CHL	7	601	2	64,72,74	1.88	13 (20%)	70,111,114	2.77	24 (34%)
26	LUT	N	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
24	CHL	8	607	-	46,54,74	2.27	15 (32%)	49,90,114	3.11	19 (38%)
24	CHL	n	609	1	66,74,74	1.85	16 (24%)	73,114,114	2.62	23 (31%)
26	LUT	1	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
34	SQD	B	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
34	SQD	A	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)
25	CLA	C	512	6	65,73,73	1.46	6 (9%)	76,113,113	1.33	8 (10%)
29	LHG	D	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
24	CHL	r	607	-	56,64,74	2.04	12 (21%)	61,102,114	2.93	25 (40%)
26	LUT	n	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
29	LHG	b	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
29	LHG	B	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
24	CHL	g	608	-	66,74,74	1.86	14 (21%)	73,114,114	2.75	21 (28%)
25	CLA	G	602	1	65,73,73	1.46	8 (12%)	76,113,113	1.56	11 (14%)
25	CLA	R	603	17	60,68,73	1.52	10 (16%)	70,107,113	1.45	8 (11%)
24	CHL	g	605	1	46,54,74	2.26	14 (30%)	49,90,114	3.09	21 (42%)
27	XAT	G	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.85	22 (40%)
24	CHL	5	608	-	46,54,74	2.19	13 (28%)	49,90,114	3.25	19 (38%)
25	CLA	4	611	29	45,53,73	1.77	9 (20%)	52,89,113	1.41	8 (15%)
24	CHL	g	609	1	61,69,74	1.92	15 (24%)	67,108,114	2.71	22 (32%)
31	OEX	A	401	6,4	0,15,15	-	-	-	-	-
25	CLA	y	614	1	48,56,73	1.73	10 (20%)	55,92,113	1.43	7 (12%)
25	CLA	s	602	18	61,69,73	1.58	7 (11%)	71,108,113	1.39	8 (11%)
24	CHL	R	607	-	56,64,74	2.04	12 (21%)	61,102,114	2.93	25 (40%)
25	CLA	S	611	29	56,64,73	1.60	7 (12%)	65,102,113	1.35	6 (9%)
26	LUT	G	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.81	12 (23%)
26	LUT	g	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	S	601	18	46,54,74	2.23	13 (28%)	49,90,114	3.20	22 (44%)
25	CLA	N	602	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
25	CLA	r	603	17	60,68,73	1.52	10 (16%)	70,107,113	1.45	8 (11%)
24	CHL	1	607	-	63,71,74	1.90	14 (22%)	69,110,114	2.88	23 (33%)
27	XAT	y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.99	20 (37%)
39	HEM	F	101	8,9	41,50,50	1.44	4 (9%)	45,82,82	1.26	4 (8%)
30	BCR	b	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.02	15 (26%)
25	CLA	G	610	1	64,72,73	1.43	10 (15%)	74,111,113	1.39	9 (12%)
26	LUT	s	1621	-	42,43,43	0.80	0	51,60,60	1.73	15 (29%)
37	DGD	B	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
35	LMG	c	521	-	51,51,55	0.76	1 (1%)	59,59,63	1.31	6 (10%)
25	CLA	5	611	29	45,53,73	1.74	12 (26%)	52,89,113	1.62	7 (13%)
30	BCR	T	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.63	23 (41%)
25	CLA	C	509	6	65,73,73	1.45	8 (12%)	76,113,113	1.44	8 (10%)
30	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.94	14 (25%)
25	CLA	1	610	1	56,64,73	1.53	10 (17%)	65,102,113	1.36	7 (10%)
25	CLA	s	609	18	45,53,73	1.86	5 (11%)	52,89,113	1.45	9 (17%)
25	CLA	C	510	6	65,73,73	1.46	7 (10%)	76,113,113	1.45	9 (11%)
24	CHL	G	606	-	50,58,74	2.14	13 (26%)	52,94,114	3.15	20 (38%)
30	BCR	h	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
25	CLA	7	604	-	45,53,73	1.80	11 (24%)	52,89,113	1.48	6 (11%)
26	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
25	CLA	Y	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.41	12 (15%)
25	CLA	s	613	18	55,63,73	1.61	6 (10%)	64,101,113	1.41	6 (9%)
27	XAT	Y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.98	19 (35%)
29	LHG	G	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
35	LMG	Z	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.29	5 (8%)
28	NEX	y	1623	-	38,46,46	1.12	3 (7%)	50,70,70	2.70	22 (44%)
24	CHL	8	608	-	46,54,74	2.16	13 (28%)	49,90,114	3.24	23 (46%)
25	CLA	b	617	5	65,73,73	1.42	9 (13%)	76,113,113	1.47	9 (11%)
25	CLA	2	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.37	8 (11%)
25	CLA	1	603	1	55,63,73	1.60	12 (21%)	64,101,113	1.57	11 (17%)
24	CHL	s	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.12	17 (34%)
25	CLA	d	403	7	65,73,73	1.42	10 (15%)	76,113,113	1.43	9 (11%)
24	CHL	y	606	-	50,58,74	2.06	15 (30%)	52,94,114	3.04	19 (36%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	R	601	17	49,57,73	1.71	9 (18%)	55,93,113	1.73	10 (18%)
27	XAT	1	1622	-	39,47,47	0.95	2 (5%)	54,74,74	2.85	22 (40%)
24	CHL	3	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.19	22 (44%)
37	DGD	h	102	-	63,63,67	1.21	7 (11%)	77,77,81	1.52	10 (12%)
37	DGD	b	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
25	CLA	c	512	6	65,73,73	1.46	6 (9%)	76,113,113	1.34	8 (10%)
29	LHG	3	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.30	4 (8%)
25	CLA	y	604	-	50,58,73	1.75	9 (18%)	58,95,113	1.61	8 (13%)
25	CLA	B	612	5	65,73,73	1.59	11 (16%)	76,113,113	1.70	13 (17%)
25	CLA	2	611	29	45,53,73	1.73	9 (20%)	52,89,113	1.58	7 (13%)
25	CLA	C	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.41	7 (9%)
25	CLA	B	607	5	65,73,73	1.52	11 (16%)	76,113,113	1.43	8 (10%)
30	BCR	a	411	-	41,41,41	0.81	0	56,56,56	1.84	12 (21%)
24	CHL	8	609	3	46,54,74	2.19	14 (30%)	49,90,114	3.28	20 (40%)
25	CLA	r	612	17	49,57,73	1.70	9 (18%)	55,93,113	1.55	7 (12%)
25	CLA	b	613	5	65,73,73	1.49	11 (16%)	76,113,113	1.68	11 (14%)
25	CLA	B	608	-	65,73,73	1.50	11 (16%)	76,113,113	1.46	7 (9%)
25	CLA	C	513	6	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
25	CLA	B	605	5	65,73,73	1.52	13 (20%)	76,113,113	1.86	18 (23%)
24	CHL	y	609	1	66,74,74	1.87	14 (21%)	73,114,114	2.68	26 (35%)
25	CLA	C	502	6	65,73,73	1.43	6 (9%)	76,113,113	1.56	8 (10%)
24	CHL	Y	606	-	50,58,74	2.06	15 (30%)	52,94,114	3.04	19 (36%)
25	CLA	G	603	1	65,73,73	1.56	10 (15%)	76,113,113	1.43	10 (13%)
35	LMG	d	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.37	6 (11%)
38	BCT	D	401	32	2,3,3	1.30	0	2,3,3	4.21	2 (100%)
25	CLA	s	614	18	49,57,73	1.64	6 (12%)	55,93,113	1.59	8 (14%)
33	PHO	A	409	-	51,69,69	1.02	5 (9%)	47,99,99	1.30	5 (10%)
25	CLA	6	603	1	55,63,73	1.62	11 (20%)	64,101,113	1.53	10 (15%)
29	LHG	N	2630	25	48,48,48	0.75	1 (2%)	51,54,54	1.32	7 (13%)
27	XAT	6	1622	-	39,47,47	1.03	0	54,74,74	2.97	23 (42%)
25	CLA	b	614	5	65,73,73	1.50	11 (16%)	76,113,113	1.51	9 (11%)
24	CHL	Y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.68	26 (35%)
24	CHL	5	606	-	46,54,74	2.22	15 (32%)	49,90,114	3.06	18 (36%)
24	CHL	G	607	-	66,74,74	1.83	12 (18%)	73,114,114	2.67	20 (27%)
29	LHG	c	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	6	602	1	61,69,73	1.51	8 (13%)	71,108,113	1.37	8 (11%)
25	CLA	g	613	1	65,73,73	1.53	11 (16%)	76,113,113	1.45	5 (6%)
25	CLA	y	603	1	65,73,73	1.53	11 (16%)	76,113,113	1.42	12 (15%)
24	CHL	N	609	1	66,74,74	1.85	15 (22%)	73,114,114	2.62	23 (31%)
25	CLA	b	608	-	65,73,73	1.49	11 (16%)	76,113,113	1.46	7 (9%)
24	CHL	6	607	-	61,69,74	2.05	15 (24%)	67,108,114	2.59	22 (32%)
25	CLA	7	613	2	58,66,73	1.61	12 (20%)	67,104,113	1.42	7 (10%)
25	CLA	8	604	-	45,53,73	1.77	11 (24%)	52,89,113	1.58	9 (17%)
25	CLA	S	610	18	55,63,73	1.65	8 (14%)	64,101,113	1.43	9 (14%)
24	CHL	6	608	-	46,54,74	2.21	14 (30%)	49,90,114	3.22	17 (34%)
25	CLA	R	611	29	49,57,73	1.72	9 (18%)	55,93,113	1.37	8 (14%)
25	CLA	4	612	3	45,53,73	1.74	8 (17%)	52,89,113	1.61	7 (13%)
25	CLA	r	604	-	48,56,73	1.69	10 (20%)	55,92,113	1.65	9 (16%)
24	CHL	3	609	2	61,69,74	2.03	16 (26%)	67,108,114	2.69	21 (31%)
24	CHL	2	601	1	46,54,74	2.26	14 (30%)	49,90,114	3.23	21 (42%)
29	LHG	C	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	3	611	29	55,63,73	1.67	11 (20%)	64,101,113	1.45	9 (14%)
24	CHL	4	607	-	46,54,74	2.28	14 (30%)	49,90,114	3.11	19 (38%)
30	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
31	OEX	a	401	6,4	0,15,15	-	-	-	-	-
25	CLA	S	612	18	49,57,73	1.69	7 (14%)	55,93,113	1.52	7 (12%)
35	LMG	b	2633	-	55,55,55	0.75	2 (3%)	63,63,63	1.36	6 (9%)
27	XAT	8	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	21 (38%)
24	CHL	2	605	1	46,54,74	2.29	14 (30%)	49,90,114	3.11	19 (38%)
25	CLA	n	610	1	65,73,73	1.41	10 (15%)	76,113,113	1.40	8 (10%)
28	NEX	g	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
25	CLA	r	616	17	45,53,73	1.76	10 (22%)	52,89,113	1.52	7 (13%)
25	CLA	S	602	18	61,69,73	1.58	7 (11%)	71,108,113	1.39	8 (11%)
24	CHL	3	601	2	64,72,74	1.88	13 (20%)	70,111,114	2.78	24 (34%)
25	CLA	6	614	1	45,53,73	1.75	9 (20%)	52,89,113	1.50	7 (13%)
25	CLA	7	610	2	60,68,73	1.54	10 (16%)	70,107,113	1.25	10 (14%)
30	BCR	c	517	-	41,41,41	0.80	0	56,56,56	2.11	13 (23%)
24	CHL	g	606	-	50,58,74	2.13	13 (26%)	52,94,114	3.14	20 (38%)
27	XAT	N	1622	-	39,47,47	0.96	1 (2%)	54,74,74	3.00	23 (42%)
25	CLA	1	604	-	50,58,73	1.73	11 (22%)	58,95,113	1.51	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	3	605	2	46,54,74	2.23	13 (28%)	49,90,114	3.19	22 (44%)
25	CLA	y	613	1	65,73,73	1.54	10 (15%)	76,113,113	1.67	7 (9%)
36	PL9	a	414	-	13,13,55	0.74	0	17,17,69	2.09	4 (23%)
25	CLA	S	609	18	45,53,73	1.86	5 (11%)	52,89,113	1.45	9 (17%)
29	LHG	s	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
25	CLA	g	611	29	60,68,73	1.51	10 (16%)	70,107,113	1.38	6 (8%)
29	LHG	r	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.33	6 (13%)
25	CLA	g	602	1	65,73,73	1.46	9 (13%)	76,113,113	1.56	11 (14%)
29	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
29	LHG	C	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
30	BCR	B	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	15 (26%)
24	CHL	4	601	3	44,53,74	2.45	16 (36%)	46,89,114	3.07	17 (36%)
26	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
37	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
35	LMG	a	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
25	CLA	b	616	5	65,73,73	1.49	10 (15%)	76,113,113	1.42	11 (14%)
25	CLA	c	504	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	7 (9%)
27	XAT	7	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.07	27 (50%)
24	CHL	Y	608	-	66,74,74	1.78	12 (18%)	73,114,114	2.80	18 (24%)
24	CHL	5	609	1	62,70,74	2.02	15 (24%)	68,109,114	2.73	20 (29%)
25	CLA	d	402	7	65,73,73	1.51	12 (18%)	76,113,113	1.50	12 (15%)
25	CLA	b	602	-	65,73,73	1.46	11 (16%)	76,113,113	1.38	9 (11%)
25	CLA	1	602	1	61,69,73	1.54	10 (16%)	71,108,113	1.32	9 (12%)
29	LHG	Y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)
28	NEX	G	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
25	CLA	5	614	1	45,53,73	1.77	9 (20%)	52,89,113	1.53	8 (15%)
24	CHL	8	606	-	46,54,74	2.23	13 (28%)	49,90,114	3.16	20 (40%)
25	CLA	r	609	17	58,66,73	1.53	11 (18%)	67,104,113	1.40	7 (10%)
28	NEX	1	1623	-	38,46,46	1.13	4 (10%)	50,70,70	2.62	18 (36%)
38	BCT	d	401	32	2,3,3	1.31	0	2,3,3	4.20	2 (100%)
25	CLA	D	402	7	65,73,73	1.51	12 (18%)	76,113,113	1.50	12 (15%)
24	CHL	6	609	1	61,69,74	1.95	13 (21%)	67,108,114	2.78	22 (32%)
29	LHG	n	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	7 (13%)
30	BCR	t	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.62	23 (41%)
28	NEX	7	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.46	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	s	611	29	56,64,73	1.60	6 (10%)	65,102,113	1.34	6 (9%)
24	CHL	5	605	1	46,54,74	2.28	15 (32%)	49,90,114	3.15	17 (34%)
25	CLA	3	604	-	45,53,73	1.80	11 (24%)	52,89,113	1.48	7 (13%)
25	CLA	b	611	-	65,73,73	1.50	10 (15%)	76,113,113	1.48	12 (15%)
26	LUT	4	620	-	42,43,43	0.95	2 (4%)	51,60,60	2.09	15 (29%)
24	CHL	n	607	-	66,74,74	1.81	13 (19%)	73,114,114	2.77	19 (26%)
25	CLA	8	611	29	45,53,73	1.76	8 (17%)	52,89,113	1.40	8 (15%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.42	14 (28%)
35	LMG	A	415	-	40,40,55	0.88	0	48,48,63	1.32	6 (12%)
30	BCR	H	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
25	CLA	r	611	29	49,57,73	1.73	10 (20%)	55,93,113	1.37	8 (14%)
25	CLA	r	613	17	60,68,73	1.56	8 (13%)	70,107,113	1.50	9 (12%)
25	CLA	c	506	6	65,73,73	1.52	10 (15%)	76,113,113	1.41	7 (9%)
25	CLA	B	606	5	65,73,73	1.53	12 (18%)	76,113,113	1.57	12 (15%)
25	CLA	B	614	5	65,73,73	1.51	11 (16%)	76,113,113	1.51	9 (11%)
24	CHL	1	608	-	46,54,74	2.19	13 (28%)	49,90,114	3.25	19 (38%)
29	LHG	2	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
25	CLA	S	603	18	45,53,73	1.82	7 (15%)	52,89,113	1.56	8 (15%)
25	CLA	4	602	3	45,53,73	1.71	9 (20%)	52,89,113	1.68	8 (15%)
25	CLA	B	609	5	65,73,73	1.38	9 (13%)	76,113,113	1.61	9 (11%)
25	CLA	R	612	17	49,57,73	1.70	9 (18%)	55,93,113	1.55	7 (12%)
28	NEX	N	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	16 (32%)
25	CLA	n	603	1	65,73,73	1.51	10 (15%)	76,113,113	1.45	11 (14%)
24	CHL	5	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.19	20 (40%)
25	CLA	G	604	-	50,58,73	1.75	11 (22%)	58,95,113	1.54	7 (12%)
30	BCR	b	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
25	CLA	1	614	1	45,53,73	1.77	9 (20%)	52,89,113	1.54	8 (15%)
25	CLA	3	610	2	60,68,73	1.54	10 (16%)	70,107,113	1.25	9 (12%)
26	LUT	8	620	-	42,43,43	0.94	2 (4%)	51,60,60	2.09	15 (29%)
28	NEX	R	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.53	19 (38%)
35	LMG	z	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.29	5 (8%)
25	CLA	B	617	5	65,73,73	1.42	9 (13%)	76,113,113	1.47	8 (10%)
26	LUT	r	620	-	42,43,43	0.98	4 (9%)	51,60,60	1.95	18 (35%)
29	LHG	g	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
29	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	c	511	6	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
25	CLA	5	613	1	55,63,73	1.61	11 (20%)	64,101,113	1.46	6 (9%)
27	XAT	n	1622	-	39,47,47	0.97	1 (2%)	54,74,74	3.01	23 (42%)
24	CHL	S	608	-	46,54,74	2.30	15 (32%)	49,90,114	3.06	17 (34%)
30	BCR	D	404	-	41,41,41	0.76	0	56,56,56	1.93	14 (25%)
25	CLA	4	610	3	45,53,73	1.75	10 (22%)	52,89,113	1.44	7 (13%)
25	CLA	b	606	5	65,73,73	1.52	12 (18%)	76,113,113	1.57	12 (15%)
25	CLA	Y	604	-	50,58,73	1.75	9 (18%)	58,95,113	1.61	8 (13%)
25	CLA	5	602	1	61,69,73	1.54	10 (16%)	71,108,113	1.32	8 (11%)
29	LHG	C	523	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	6 (11%)
36	PL9	A	414	-	13,13,55	0.75	0	17,17,69	2.08	4 (23%)
24	CHL	6	606	-	46,54,74	2.23	14 (30%)	49,90,114	3.10	20 (40%)
24	CHL	3	607	-	53,61,74	2.09	15 (28%)	57,98,114	2.95	20 (35%)
25	CLA	N	611	29	60,68,73	1.52	8 (13%)	70,107,113	1.44	8 (11%)
37	DGD	C	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)
24	CHL	2	608	-	46,54,74	2.21	14 (30%)	49,90,114	3.23	17 (34%)
26	LUT	y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.86	17 (33%)
24	CHL	R	614	17	42,50,74	2.39	15 (35%)	44,85,114	3.37	18 (40%)
35	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	G	614	1	48,56,73	1.70	10 (20%)	55,92,113	1.34	6 (10%)
24	CHL	G	609	1	61,69,74	1.92	15 (24%)	67,108,114	2.70	22 (32%)
25	CLA	C	508	6	65,73,73	1.46	8 (12%)	76,113,113	1.54	8 (10%)
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
25	CLA	g	603	1	65,73,73	1.56	10 (15%)	76,113,113	1.43	10 (13%)
26	LUT	y	1620	-	42,43,43	1.09	5 (11%)	51,60,60	1.91	20 (39%)
24	CHL	R	608	-	61,69,74	1.82	10 (16%)	67,108,114	2.88	19 (28%)
24	CHL	N	606	-	50,58,74	2.10	14 (28%)	52,94,114	3.10	18 (34%)
25	CLA	G	613	1	65,73,73	1.53	11 (16%)	76,113,113	1.45	5 (6%)
26	LUT	G	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)

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
26	LUT	Y	1621	-	-	2/29/67/67	0/2/2/2
37	DGD	H	102	-	-	25/51/91/95	0/2/2/2
24	CHL	g	607	-	4/4/20/26	13/39/137/137	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	n	614	1	1/1/11/20	7/17/95/115	-
24	CHL	8	601	3	3/3/16/26	4/13/111/137	-
25	CLA	r	601	17	1/1/11/20	9/18/96/115	-
29	LHG	7	2630	25	-	25/51/51/53	-
25	CLA	6	610	1	1/1/12/20	3/19/97/115	-
25	CLA	n	602	1	1/1/15/20	14/37/115/115	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	603	5	1/1/15/20	10/37/115/115	-
34	SQD	b	623	-	-	17/37/57/69	0/1/1/1
25	CLA	6	613	1	-	5/13/91/115	-
25	CLA	B	615	5	1/1/15/20	15/37/115/115	-
25	CLA	b	612	5	1/1/15/20	12/37/115/115	-
28	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	1	612	1	1/1/11/20	4/13/91/115	-
25	CLA	6	612	1	1/1/11/20	6/13/91/115	-
28	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	N	603	1	1/1/15/20	14/37/115/115	-
39	HEM	f	101	8,9	-	1/12/54/54	-
25	CLA	7	612	2	1/1/11/20	6/13/91/115	-
30	BCR	C	514	-	-	2/29/63/63	0/2/2/2
24	CHL	1	606	-	3/3/16/26	7/15/113/137	-
25	CLA	a	405	4	1/1/15/20	10/37/115/115	-
25	CLA	n	604	-	1/1/12/20	4/19/97/115	-
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
24	CHL	2	607	-	4/4/19/26	18/33/131/137	-
30	BCR	B	619	-	-	2/29/63/63	0/2/2/2
25	CLA	3	613	2	1/1/13/20	8/29/107/115	-
24	CHL	N	607	-	4/4/20/26	17/39/137/137	-
33	PHO	A	408	-	-	6/37/103/103	0/5/6/6
25	CLA	C	501	6	1/1/15/20	15/37/115/115	-
25	CLA	b	603	5	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SQD	A	418	-	-	22/49/69/69	0/1/1/1
24	CHL	y	605	1	3/3/16/26	6/18/116/137	-
25	CLA	Y	614	1	1/1/11/20	3/17/95/115	-
25	CLA	3	602	2	1/1/14/20	15/31/109/115	-
24	CHL	7	607	-	3/3/17/26	12/24/122/137	-
29	LHG	d	408	-	-	17/50/50/53	-
25	CLA	8	610	3	1/1/11/20	6/13/91/115	-
25	CLA	A	405	4	1/1/15/20	10/37/115/115	-
25	CLA	s	610	18	1/1/13/20	4/25/103/115	-
25	CLA	R	604	-	1/1/11/20	4/17/95/115	-
25	CLA	4	603	3	1/1/11/20	4/13/91/115	-
25	CLA	R	610	17	1/1/15/20	12/37/115/115	-
25	CLA	r	610	17	1/1/15/20	12/37/115/115	-
27	XAT	2	1622	-	-	4/31/93/93	0/4/4/4
25	CLA	2	614	1	-	6/13/91/115	-
24	CHL	Y	605	1	3/3/16/26	6/18/116/137	-
24	CHL	s	601	18	3/3/16/26	8/15/113/137	-
24	CHL	n	601	1	4/4/20/26	17/39/137/137	-
24	CHL	y	601	1	4/4/20/26	15/39/137/137	-
30	BCR	C	517	-	-	6/29/63/63	0/2/2/2
30	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CLA	R	616	17	-	6/13/91/115	-
27	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
29	LHG	8	2630	25	-	8/23/23/53	-
30	BCR	4	623	-	-	12/29/63/63	0/2/2/2
24	CHL	5	607	-	4/4/19/26	19/36/134/137	-
25	CLA	R	602	17	1/1/14/20	7/31/109/115	-
24	CHL	4	608	-	3/3/16/26	8/15/113/137	-
25	CLA	7	603	2	1/1/13/20	9/25/103/115	-
25	CLA	3	614	2	1/1/11/20	5/17/95/115	-
24	CHL	S	606	-	3/3/16/26	10/15/113/137	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	Y	601	1	4/4/20/26	15/39/137/137	-
27	XAT	R	622	-	-	5/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	610	1	1/1/14/20	13/36/114/115	-
29	LHG	B	2631	-	-	20/53/53/53	-
37	DGD	c	520	-	-	28/49/89/95	0/2/2/2
24	CHL	G	605	1	3/3/16/26	9/15/113/137	-
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
26	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	b	604	5	1/1/15/20	9/37/115/115	-
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	G	611	29	1/1/14/20	11/31/109/115	-
25	CLA	b	610	5	-	7/37/115/115	-
33	PHO	a	408	-	-	6/37/103/103	0/5/6/6
25	CLA	8	603	3	1/1/11/20	4/13/91/115	-
24	CHL	2	609	1	4/4/19/26	15/33/131/137	-
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
29	LHG	R	2630	25	-	16/46/46/53	-
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	N	614	1	1/1/11/20	7/17/95/115	-
24	CHL	7	608	-	3/3/16/26	6/15/113/137	-
24	CHL	R	606	-	4/4/20/26	22/39/137/137	-
25	CLA	A	410	4	1/1/14/20	6/31/109/115	-
25	CLA	n	613	1	1/1/14/20	6/31/109/115	-
29	LHG	D	410	-	-	24/47/47/53	-
25	CLA	C	511	6	-	13/37/115/115	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
35	LMG	A	413	-	-	17/43/63/70	0/1/1/1
24	CHL	N	608	-	4/4/20/26	14/39/137/137	-
24	CHL	s	607	-	4/4/18/26	11/30/128/137	-
25	CLA	y	611	29	1/1/14/20	8/31/109/115	-
26	LUT	6	1621	-	-	1/29/67/67	0/2/2/2
28	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	2	612	1	1/1/11/20	6/13/91/115	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	7	602	2	1/1/14/20	14/31/109/115	-
25	CLA	R	609	17	1/1/13/20	2/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	B	622	-	-	22/46/66/70	0/1/1/1
25	CLA	6	604	-	-	9/13/91/115	-
25	CLA	n	612	1	1/1/14/20	9/31/109/115	-
25	CLA	4	604	-	-	9/13/91/115	-
24	CHL	g	601	1	4/4/20/26	17/39/137/137	-
25	CLA	7	611	29	1/1/13/20	10/25/103/115	-
25	CLA	Y	611	29	1/1/14/20	8/31/109/115	-
25	CLA	C	505	6	-	13/37/115/115	-
24	CHL	N	601	1	4/4/20/26	17/39/137/137	-
29	LHG	6	2630	25	-	14/41/41/53	-
25	CLA	s	603	18	1/1/11/20	3/13/91/115	-
25	CLA	A	406	-	1/1/15/20	4/37/115/115	-
25	CLA	N	604	-	1/1/12/20	4/19/97/115	-
25	CLA	3	612	2	1/1/11/20	6/13/91/115	-
28	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
36	PL9	D	405	-	-	8/53/73/73	0/1/1/1
29	LHG	y	2630	25	-	20/53/53/53	-
30	BCR	c	516	-	-	9/29/63/63	0/2/2/2
25	CLA	B	604	5	1/1/15/20	9/37/115/115	-
30	BCR	8	623	-	-	12/29/63/63	0/2/2/2
29	LHG	S	2630	25	-	24/53/53/53	-
24	CHL	2	606	-	3/3/16/26	3/15/113/137	-
24	CHL	s	608	-	3/3/16/26	3/15/113/137	-
25	CLA	a	407	-	1/1/12/20	5/19/97/115	-
25	CLA	B	613	5	1/1/15/20	15/37/115/115	-
25	CLA	b	609	5	1/1/15/20	5/37/115/115	-
25	CLA	2	613	1	-	5/13/91/115	-
25	CLA	b	615	5	1/1/15/20	15/37/115/115	-
25	CLA	a	410	4	1/1/14/20	6/31/109/115	-
25	CLA	b	607	5	1/1/15/20	11/37/115/115	-
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
25	CLA	5	610	1	1/1/13/20	3/27/105/115	-
27	XAT	4	622	-	-	3/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	5	1623	-	-	9/27/83/83	0/3/3/3
25	CLA	5	604	-	1/1/12/20	10/19/97/115	-
34	SQD	a	412	-	-	18/45/65/69	0/1/1/1
24	CHL	r	614	17	3/3/15/26	6/10/108/137	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	r	608	-	4/4/19/26	16/33/131/137	-
27	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	A	407	-	1/1/12/20	5/19/97/115	-
24	CHL	n	605	1	3/3/16/26	10/18/116/137	-
25	CLA	c	508	6	1/1/15/20	8/37/115/115	-
35	LMG	a	415	-	-	11/35/55/70	0/1/1/1
30	BCR	A	411	-	-	2/29/63/63	0/2/2/2
34	SQD	a	418	-	-	22/49/69/69	0/1/1/1
25	CLA	c	503	6	1/1/15/20	10/37/115/115	-
25	CLA	c	507	-	1/1/15/20	21/37/115/115	-
24	CHL	4	606	-	3/3/16/26	7/15/113/137	-
24	CHL	7	606	-	3/3/16/26	5/15/113/137	-
25	CLA	2	610	1	1/1/12/20	3/19/97/115	-
35	LMG	C	521	-	-	21/46/66/70	0/1/1/1
25	CLA	c	510	6	1/1/15/20	17/37/115/115	-
33	PHO	a	409	-	-	8/37/103/103	0/5/6/6
25	CLA	2	603	1	1/1/13/20	13/25/103/115	-
25	CLA	g	612	1	1/1/14/20	11/31/109/115	-
26	LUT	5	1621	-	-	5/29/67/67	0/2/2/2
24	CHL	y	607	-	4/4/20/26	15/39/137/137	-
24	CHL	7	609	2	4/4/19/26	14/33/131/137	-
25	CLA	N	613	1	1/1/14/20	6/31/109/115	-
25	CLA	s	612	18	1/1/11/20	3/18/96/115	-
29	LHG	5	2630	25	-	9/45/45/53	-
25	CLA	C	507	-	1/1/15/20	21/37/115/115	-
25	CLA	y	612	1	1/1/14/20	13/31/109/115	-
26	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	n	608	-	4/4/20/26	14/39/137/137	-
24	CHL	4	609	3	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	d	410	-	-	24/47/47/53	-
24	CHL	S	607	-	4/4/18/26	11/30/128/137	-
37	DGD	c	519	-	-	25/51/91/95	0/2/2/2
25	CLA	c	513	6	-	12/37/115/115	-
25	CLA	Y	613	1	1/1/15/20	9/37/115/115	-
25	CLA	c	501	6	1/1/15/20	15/37/115/115	-
25	CLA	R	613	17	1/1/14/20	11/31/109/115	-
24	CHL	1	609	1	4/4/19/26	11/35/133/137	-
26	LUT	S	1621	-	-	4/29/67/67	0/2/2/2
25	CLA	Y	612	1	1/1/14/20	13/31/109/115	-
25	CLA	1	611	29	1/1/11/20	5/13/91/115	-
25	CLA	6	611	29	1/1/11/20	3/13/91/115	-
25	CLA	G	612	1	1/1/14/20	11/31/109/115	-
24	CHL	G	608	-	4/4/20/26	18/39/137/137	-
28	NEX	r	623	-	-	4/27/83/83	0/3/3/3
25	CLA	n	611	29	1/1/14/20	7/31/109/115	-
25	CLA	c	502	6	1/1/15/20	20/37/115/115	-
25	CLA	a	406	-	1/1/15/20	4/37/115/115	-
29	LHG	D	409	-	-	20/53/53/53	-
25	CLA	8	602	3	1/1/11/20	3/13/91/115	-
25	CLA	N	610	1	1/1/15/20	11/37/115/115	-
25	CLA	S	604	-	1/1/12/20	6/19/97/115	-
35	LMG	B	2633	-	-	21/50/70/70	0/1/1/1
25	CLA	C	506	6	-	16/37/115/115	-
25	CLA	r	602	17	1/1/14/20	7/31/109/115	-
25	CLA	N	612	1	1/1/14/20	9/31/109/115	-
37	DGD	C	520	-	-	28/49/89/95	0/2/2/2
34	SQD	B	623	-	-	17/37/57/69	0/1/1/1
24	CHL	Y	607	-	4/4/20/26	15/39/137/137	-
24	CHL	y	608	-	4/4/20/26	16/39/137/137	-
25	CLA	B	610	5	-	7/37/115/115	-
25	CLA	g	614	1	1/1/11/20	5/17/95/115	-
27	XAT	r	622	-	-	5/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PL9	d	405	-	-	8/53/73/73	0/1/1/1
24	CHL	7	605	2	3/3/16/26	10/15/113/137	-
25	CLA	1	613	1	-	7/25/103/115	-
29	LHG	b	2630	-	-	30/51/51/53	-
30	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	D	403	7	-	13/37/115/115	-
25	CLA	c	509	6	1/1/15/20	8/37/115/115	-
25	CLA	3	603	2	1/1/13/20	9/25/103/115	-
26	LUT	2	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	G	601	1	4/4/20/26	17/39/137/137	-
25	CLA	y	602	1	1/1/15/20	14/37/115/115	-
30	BCR	d	404	-	-	5/29/63/63	0/2/2/2
25	CLA	5	603	1	1/1/13/20	10/25/103/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
29	LHG	c	522	-	-	20/53/53/53	-
25	CLA	B	616	5	1/1/15/20	12/37/115/115	-
25	CLA	7	614	2	1/1/11/20	5/17/95/115	-
24	CHL	6	601	1	3/3/16/26	8/15/113/137	-
29	LHG	4	2630	25	-	8/23/23/53	-
25	CLA	B	602	-	1/1/15/20	15/37/115/115	-
25	CLA	b	605	5	1/1/15/20	14/37/115/115	-
28	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	S	614	18	1/1/11/20	5/18/96/115	-
25	CLA	2	604	-	-	9/13/91/115	-
37	DGD	C	518	-	-	16/44/84/95	0/2/2/2
25	CLA	S	613	18	1/1/13/20	6/25/103/115	-
25	CLA	g	604	-	-	5/19/97/115	-
25	CLA	c	505	6	-	13/37/115/115	-
26	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
24	CHL	6	605	1	3/3/16/26	8/15/113/137	-
24	CHL	3	608	-	3/3/16/26	6/15/113/137	-
25	CLA	Y	602	1	1/1/15/20	14/37/115/115	-
25	CLA	5	612	1	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	611	-	1/1/15/20	9/37/115/115	-
35	LMG	D	411	-	-	15/41/61/70	0/1/1/1
25	CLA	s	604	-	1/1/12/20	6/19/97/115	-
24	CHL	1	601	1	3/3/16/26	5/15/113/137	-
25	CLA	8	612	3	1/1/11/20	8/13/91/115	-
25	CLA	y	610	1	1/1/14/20	7/31/109/115	-
24	CHL	n	606	-	3/3/16/26	8/20/118/137	-
24	CHL	N	605	1	3/3/16/26	10/18/116/137	-
29	LHG	1	2630	25	-	9/45/45/53	-
24	CHL	r	606	-	4/4/20/26	22/39/137/137	-
29	LHG	d	409	-	-	20/53/53/53	-
25	CLA	C	503	6	1/1/15/20	10/37/115/115	-
25	CLA	Y	610	1	1/1/14/20	7/31/109/115	-
24	CHL	7	601	2	4/4/19/26	13/37/135/137	-
26	LUT	N	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	8	607	-	3/3/16/26	8/15/113/137	-
24	CHL	n	609	1	4/4/20/26	15/39/137/137	-
26	LUT	1	1621	-	-	5/29/67/67	0/2/2/2
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
34	SQD	A	412	-	-	18/45/65/69	0/1/1/1
25	CLA	C	512	6	1/1/15/20	9/37/115/115	-
29	LHG	D	408	-	-	17/50/50/53	-
24	CHL	r	607	-	4/4/18/26	8/27/125/137	-
26	LUT	n	1621	-	-	1/29/67/67	0/2/2/2
29	LHG	b	2631	-	-	20/53/53/53	-
29	LHG	B	2630	-	-	30/51/51/53	-
24	CHL	g	608	-	4/4/20/26	18/39/137/137	-
25	CLA	G	602	1	1/1/15/20	11/37/115/115	-
25	CLA	R	603	17	1/1/14/20	13/31/109/115	-
24	CHL	g	605	1	3/3/16/26	10/15/113/137	-
27	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	5	608	-	3/3/16/26	3/15/113/137	-
25	CLA	4	611	29	1/1/11/20	6/13/91/115	-
24	CHL	g	609	1	4/4/19/26	11/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	y	614	1	1/1/11/20	3/17/95/115	-
25	CLA	s	602	18	1/1/14/20	14/33/111/115	-
24	CHL	R	607	-	4/4/18/26	8/27/125/137	-
25	CLA	S	611	29	1/1/13/20	9/27/105/115	-
26	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
24	CHL	S	601	18	3/3/16/26	8/15/113/137	-
25	CLA	N	602	1	1/1/15/20	14/37/115/115	-
25	CLA	r	603	17	1/1/14/20	13/31/109/115	-
24	CHL	l	607	-	4/4/19/26	19/36/134/137	-
27	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
39	HEM	F	101	8,9	-	1/12/54/54	-
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2
25	CLA	G	610	1	1/1/14/20	13/36/114/115	-
26	LUT	s	1621	-	-	4/29/67/67	0/2/2/2
37	DGD	B	626	-	-	22/48/88/95	0/2/2/2
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
25	CLA	5	611	29	1/1/11/20	5/13/91/115	-
30	BCR	T	101	-	-	13/29/63/63	0/2/2/2
25	CLA	C	509	6	1/1/15/20	8/37/115/115	-
30	BCR	C	516	-	-	9/29/63/63	0/2/2/2
25	CLA	l	610	1	1/1/13/20	3/27/105/115	-
25	CLA	s	609	18	1/1/11/20	7/13/91/115	-
25	CLA	C	510	6	1/1/15/20	17/37/115/115	-
24	CHL	G	606	-	3/3/16/26	8/20/118/137	-
30	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	7	604	-	1/1/11/20	9/13/91/115	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	Y	603	1	1/1/15/20	14/37/115/115	-
25	CLA	s	613	18	1/1/13/20	6/25/103/115	-
27	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
29	LHG	G	2630	25	-	24/53/53/53	-
35	LMG	Z	101	-	-	22/46/66/70	0/1/1/1
28	NEX	y	1623	-	-	3/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	8	608	-	3/3/16/26	8/15/113/137	-
25	CLA	b	617	5	1/1/15/20	17/37/115/115	-
25	CLA	2	602	1	1/1/14/20	15/33/111/115	-
25	CLA	1	603	1	1/1/13/20	10/25/103/115	-
24	CHL	s	606	-	3/3/16/26	10/15/113/137	-
25	CLA	d	403	7	-	13/37/115/115	-
24	CHL	y	606	-	3/3/16/26	5/20/118/137	-
25	CLA	R	601	17	1/1/11/20	9/18/96/115	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	3	606	-	3/3/16/26	5/15/113/137	-
37	DGD	h	102	-	-	25/51/91/95	0/2/2/2
37	DGD	b	626	-	-	22/48/88/95	0/2/2/2
25	CLA	c	512	6	1/1/15/20	9/37/115/115	-
29	LHG	3	2630	25	-	25/51/51/53	-
25	CLA	y	604	-	1/1/12/20	5/19/97/115	-
25	CLA	B	612	5	1/1/15/20	12/37/115/115	-
25	CLA	2	611	29	1/1/11/20	3/13/91/115	-
25	CLA	C	504	-	1/1/15/20	12/37/115/115	-
25	CLA	B	607	5	1/1/15/20	11/37/115/115	-
30	BCR	a	411	-	-	2/29/63/63	0/2/2/2
24	CHL	8	609	3	3/3/16/26	7/15/113/137	-
25	CLA	r	612	17	1/1/11/20	6/18/96/115	-
25	CLA	b	613	5	1/1/15/20	15/37/115/115	-
25	CLA	B	608	-	1/1/15/20	13/37/115/115	-
25	CLA	C	513	6	-	12/37/115/115	-
25	CLA	B	605	5	1/1/15/20	14/37/115/115	-
24	CHL	y	609	1	4/4/20/26	14/39/137/137	-
25	CLA	C	502	6	1/1/15/20	20/37/115/115	-
24	CHL	Y	606	-	3/3/16/26	5/20/118/137	-
25	CLA	G	603	1	1/1/15/20	11/37/115/115	-
35	LMG	d	411	-	-	15/41/61/70	0/1/1/1
25	CLA	s	614	18	1/1/11/20	5/18/96/115	-
33	PHO	A	409	-	-	8/37/103/103	0/5/6/6
25	CLA	6	603	1	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	N	2630	25	-	23/53/53/53	-
27	XAT	6	1622	-	-	4/31/93/93	0/4/4/4
25	CLA	b	614	5	1/1/15/20	15/37/115/115	-
24	CHL	Y	609	1	4/4/20/26	14/39/137/137	-
24	CHL	5	606	-	3/3/16/26	7/15/113/137	-
24	CHL	G	607	-	4/4/20/26	13/39/137/137	-
29	LHG	c	2630	-	-	27/53/53/53	-
25	CLA	6	602	1	1/1/14/20	15/33/111/115	-
25	CLA	y	603	1	1/1/15/20	14/37/115/115	-
25	CLA	g	613	1	-	11/37/115/115	-
24	CHL	N	609	1	4/4/20/26	15/39/137/137	-
25	CLA	b	608	-	1/1/15/20	13/37/115/115	-
24	CHL	6	607	-	4/4/19/26	18/33/131/137	-
25	CLA	7	613	2	1/1/13/20	8/29/107/115	-
25	CLA	8	604	-	-	9/13/91/115	-
25	CLA	S	610	18	1/1/13/20	4/25/103/115	-
24	CHL	6	608	-	3/3/16/26	8/15/113/137	-
25	CLA	R	611	29	1/1/11/20	9/18/96/115	-
25	CLA	4	612	3	1/1/11/20	8/13/91/115	-
25	CLA	r	604	-	1/1/11/20	4/17/95/115	-
24	CHL	3	609	2	4/4/19/26	14/33/131/137	-
24	CHL	2	601	1	3/3/16/26	8/15/113/137	-
29	LHG	C	522	-	-	20/53/53/53	-
25	CLA	3	611	29	1/1/13/20	10/25/103/115	-
24	CHL	4	607	-	3/3/16/26	8/15/113/137	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2
25	CLA	S	612	18	1/1/11/20	3/18/96/115	-
35	LMG	b	2633	-	-	21/50/70/70	0/1/1/1
27	XAT	8	622	-	-	3/31/93/93	0/4/4/4
24	CHL	2	605	1	3/3/16/26	8/15/113/137	-
25	CLA	n	610	1	1/1/15/20	11/37/115/115	-
28	NEX	g	1623	-	-	6/27/83/83	0/3/3/3
25	CLA	r	616	17	-	6/13/91/115	-
25	CLA	S	602	18	1/1/14/20	14/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	3	601	2	4/4/19/26	13/37/135/137	-
25	CLA	6	614	1	-	6/13/91/115	-
25	CLA	7	610	2	1/1/14/20	4/31/109/115	-
30	BCR	c	517	-	-	6/29/63/63	0/2/2/2
24	CHL	g	606	-	3/3/16/26	8/20/118/137	-
27	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	1	604	-	1/1/12/20	10/19/97/115	-
24	CHL	3	605	2	3/3/16/26	10/15/113/137	-
25	CLA	y	613	1	1/1/15/20	9/37/115/115	-
36	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CLA	S	609	18	1/1/11/20	7/13/91/115	-
29	LHG	s	2630	25	-	24/53/53/53	-
25	CLA	g	611	29	1/1/14/20	11/31/109/115	-
29	LHG	r	2630	25	-	16/46/46/53	-
25	CLA	g	602	1	1/1/15/20	11/37/115/115	-
29	LHG	l	101	-	-	21/53/53/53	-
29	LHG	C	2630	-	-	27/53/53/53	-
30	BCR	B	620	-	-	6/29/63/63	0/2/2/2
24	CHL	4	601	3	3/3/16/26	4/13/111/137	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
37	DGD	c	518	-	-	16/44/84/95	0/2/2/2
35	LMG	a	413	-	-	17/43/63/70	0/1/1/1
25	CLA	b	616	5	1/1/15/20	12/37/115/115	-
25	CLA	c	504	-	1/1/15/20	12/37/115/115	-
27	XAT	7	1622	-	-	1/31/93/93	0/4/4/4
24	CHL	Y	608	-	4/4/20/26	16/39/137/137	-
24	CHL	5	609	1	4/4/19/26	11/35/133/137	-
25	CLA	d	402	7	1/1/15/20	5/37/115/115	-
25	CLA	b	602	-	1/1/15/20	15/37/115/115	-
25	CLA	1	602	1	1/1/14/20	9/33/111/115	-
29	LHG	Y	2630	25	-	20/53/53/53	-
28	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	5	614	1	1/1/11/20	4/13/91/115	-
24	CHL	8	606	-	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	609	17	1/1/13/20	2/29/107/115	-
28	NEX	1	1623	-	-	9/27/83/83	0/3/3/3
25	CLA	D	402	7	1/1/15/20	5/37/115/115	-
24	CHL	6	609	1	4/4/19/26	15/33/131/137	-
29	LHG	n	2630	25	-	23/53/53/53	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	s	611	29	1/1/13/20	9/27/105/115	-
24	CHL	5	605	1	3/3/16/26	8/15/113/137	-
25	CLA	3	604	-	1/1/11/20	9/13/91/115	-
25	CLA	b	611	-	1/1/15/20	9/37/115/115	-
26	LUT	4	620	-	-	5/29/67/67	0/2/2/2
24	CHL	n	607	-	4/4/20/26	17/39/137/137	-
25	CLA	8	611	29	1/1/11/20	6/13/91/115	-
28	NEX	6	1623	-	-	4/27/83/83	0/3/3/3
35	LMG	A	415	-	-	11/35/55/70	0/1/1/1
30	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	r	611	29	1/1/11/20	9/18/96/115	-
25	CLA	r	613	17	1/1/14/20	11/31/109/115	-
25	CLA	c	506	6	-	16/37/115/115	-
25	CLA	B	606	5	1/1/15/20	15/37/115/115	-
25	CLA	B	614	5	1/1/15/20	15/37/115/115	-
24	CHL	1	608	-	3/3/16/26	3/15/113/137	-
29	LHG	2	2630	25	-	14/41/41/53	-
25	CLA	S	603	18	1/1/11/20	3/13/91/115	-
25	CLA	4	602	3	1/1/11/20	3/13/91/115	-
25	CLA	B	609	5	1/1/15/20	5/37/115/115	-
25	CLA	R	612	17	1/1/11/20	6/18/96/115	-
28	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	n	603	1	1/1/15/20	14/37/115/115	-
24	CHL	5	601	1	3/3/16/26	5/15/113/137	-
25	CLA	G	604	-	-	5/19/97/115	-
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	1	614	1	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	3	610	2	1/1/14/20	4/31/109/115	-
26	LUT	8	620	-	-	5/29/67/67	0/2/2/2
28	NEX	R	623	-	-	4/27/83/83	0/3/3/3
35	LMG	z	101	-	-	22/46/66/70	0/1/1/1
25	CLA	B	617	5	1/1/15/20	17/37/115/115	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
29	LHG	g	2630	25	-	24/53/53/53	-
29	LHG	c	523	-	-	21/53/53/53	-
25	CLA	c	511	6	-	13/37/115/115	-
25	CLA	5	613	1	-	7/25/103/115	-
27	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	S	608	-	3/3/16/26	3/15/113/137	-
30	BCR	D	404	-	-	5/29/63/63	0/2/2/2
25	CLA	4	610	3	1/1/11/20	6/13/91/115	-
25	CLA	b	606	5	1/1/15/20	15/37/115/115	-
25	CLA	Y	604	-	1/1/12/20	5/19/97/115	-
25	CLA	5	602	1	1/1/14/20	9/33/111/115	-
29	LHG	C	523	-	-	21/53/53/53	-
36	PL9	A	414	-	-	1/5/18/73	0/1/1/1
24	CHL	6	606	-	3/3/16/26	3/15/113/137	-
24	CHL	3	607	-	3/3/17/26	12/24/122/137	-
25	CLA	N	611	29	1/1/14/20	7/31/109/115	-
37	DGD	C	519	-	-	25/51/91/95	0/2/2/2
24	CHL	2	608	-	3/3/16/26	8/15/113/137	-
26	LUT	y	1621	-	-	2/29/67/67	0/2/2/2
24	CHL	R	614	17	3/3/15/26	6/10/108/137	-
35	LMG	b	622	-	-	22/46/66/70	0/1/1/1
25	CLA	G	614	1	1/1/11/20	5/17/95/115	-
24	CHL	G	609	1	4/4/19/26	11/33/131/137	-
25	CLA	C	508	6	1/1/15/20	8/37/115/115	-
29	LHG	L	101	-	-	21/53/53/53	-
25	CLA	g	603	1	1/1/15/20	11/37/115/115	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	R	608	-	4/4/19/26	16/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	N	606	-	3/3/16/26	8/20/118/137	-
25	CLA	G	613	1	-	11/37/115/115	-
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2

The worst 5 of 3737 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	614	CLA	C4B-NB	8.15	1.42	1.35
25	7	614	CLA	C4B-NB	8.11	1.42	1.35
25	C	501	CLA	C4B-NB	7.90	1.42	1.35
25	s	602	CLA	C4B-NB	7.88	1.42	1.35
25	S	602	CLA	C4B-NB	7.88	1.42	1.35

The worst 5 of 5869 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	1622	XAT	O24-C25-C24	10.52	121.28	113.38
27	1	1622	XAT	O24-C25-C24	10.51	121.28	113.38
24	y	601	CHL	CMD-C2D-C1D	10.18	142.65	124.71
24	Y	601	CHL	CMD-C2D-C1D	10.16	142.62	124.71
24	2	601	CHL	CMD-C2D-C1D	9.95	142.25	124.71

5 of 526 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	ND
24	1	601	CHL	NC
24	1	601	CHL	NA
24	1	605	CHL	ND
24	1	605	CHL	NC

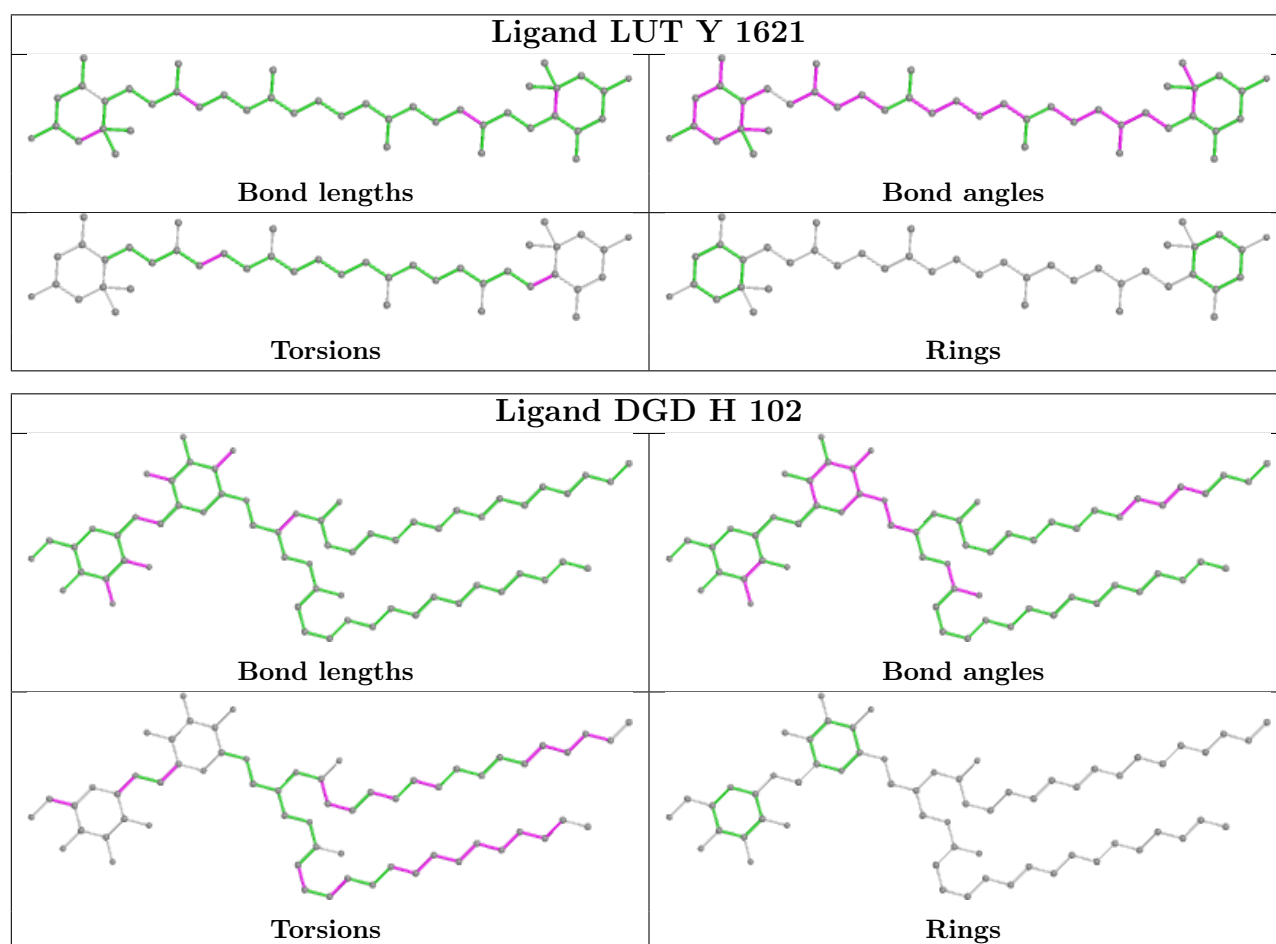
5 of 4767 torsion outliers are listed below:

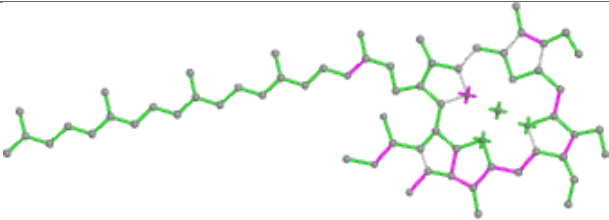
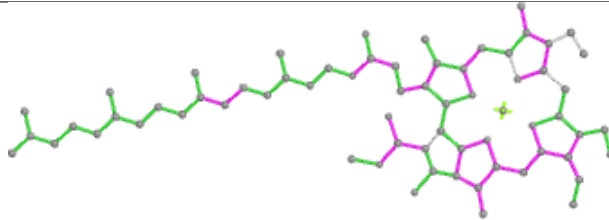
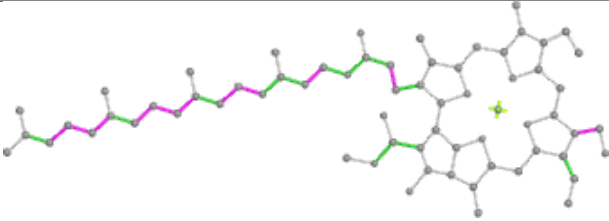
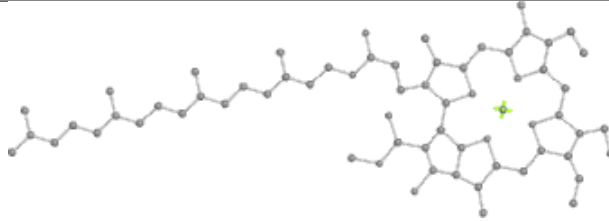
Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	CBD-CGD-O2D-CED
24	1	607	CHL	C1C-C2C-CMC-OMC

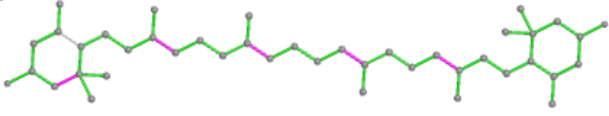
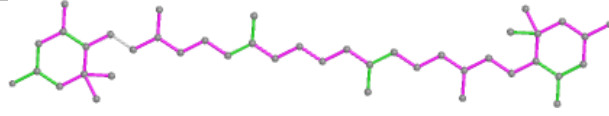
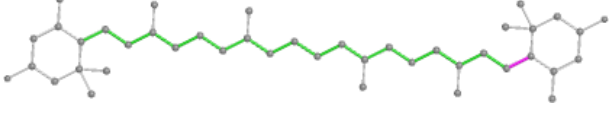
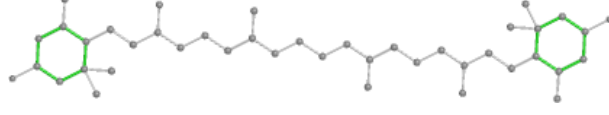
There are no ring outliers.

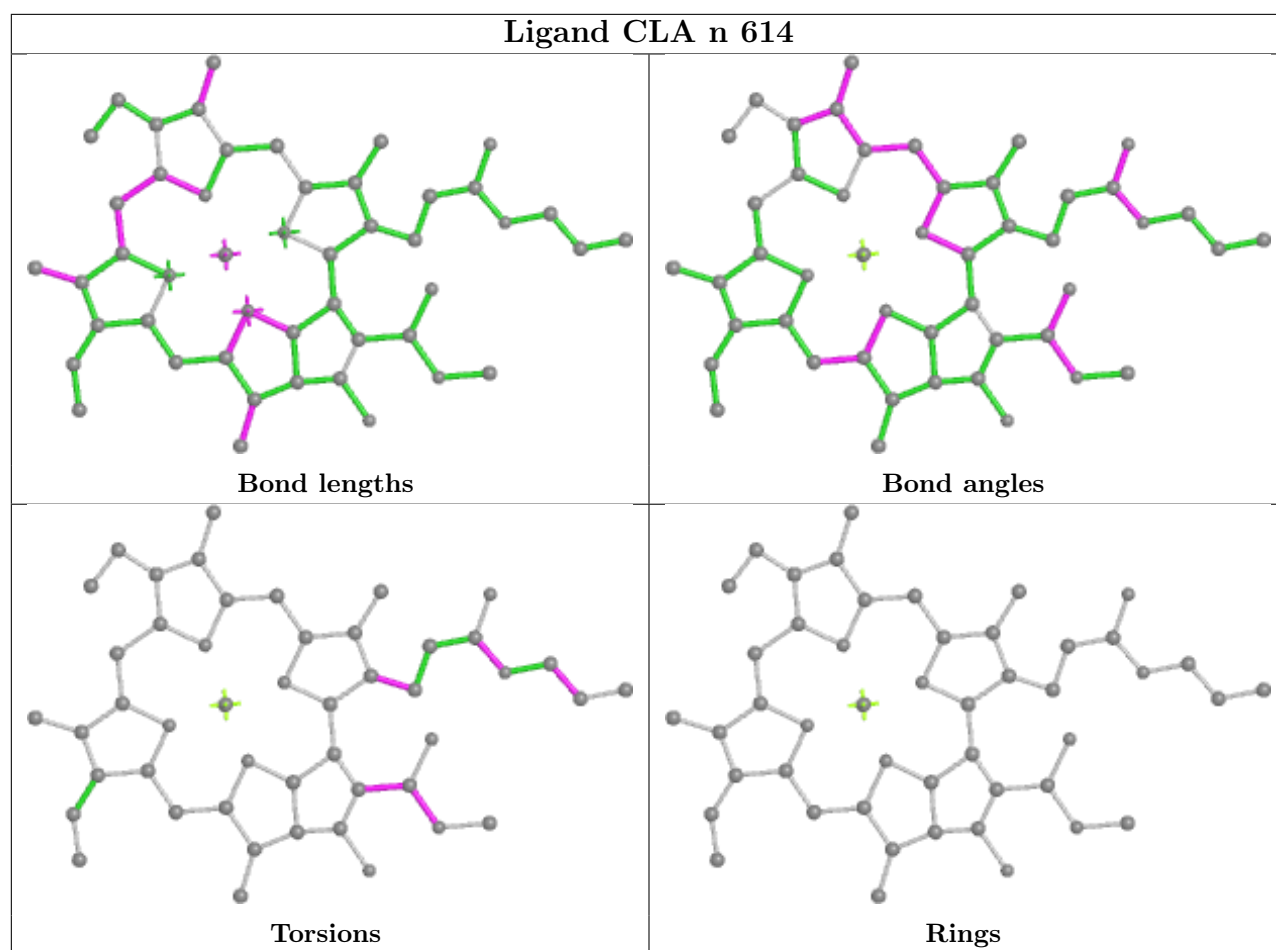
No monomer is involved in short contacts.

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.

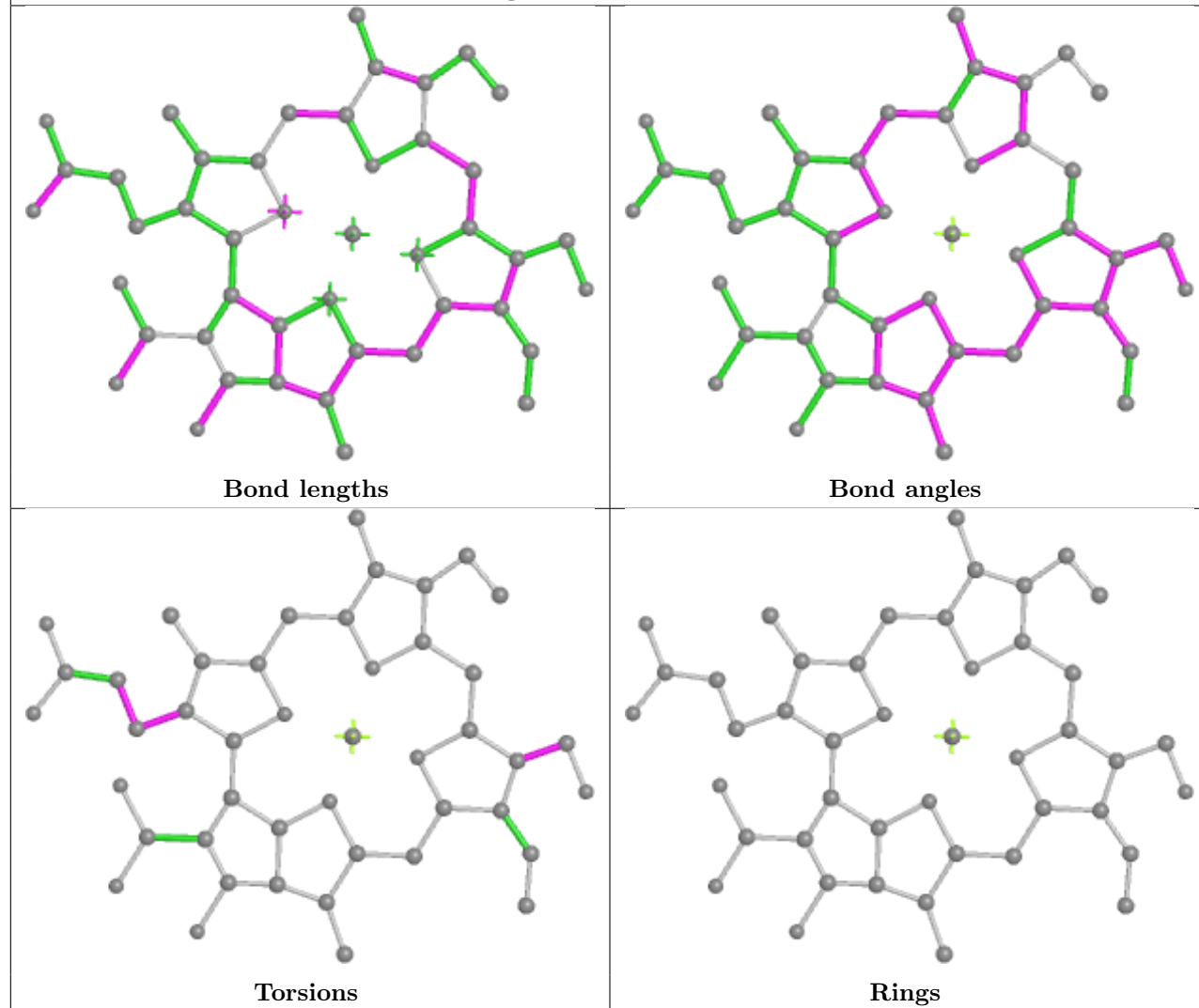


Ligand CHL g 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT Y 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

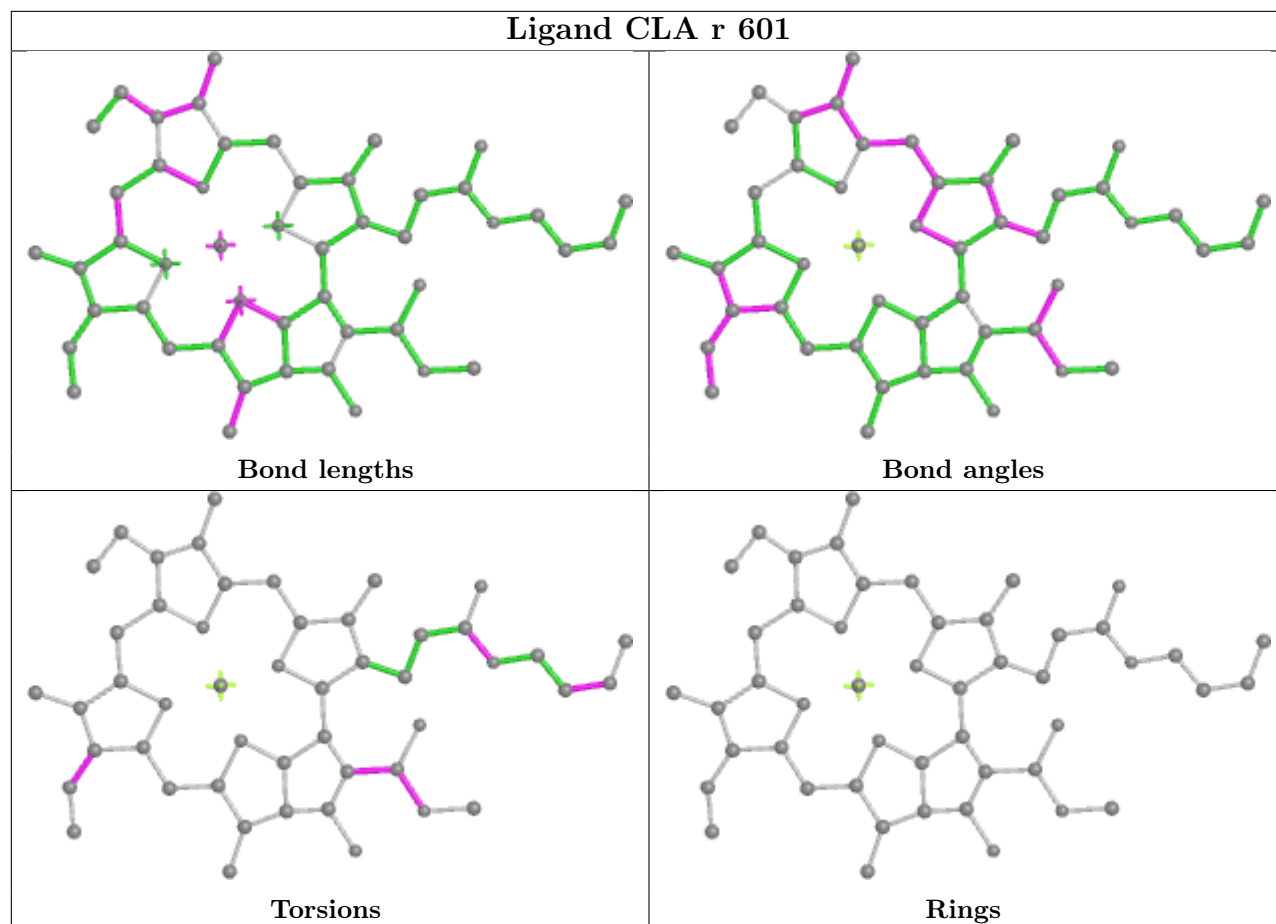


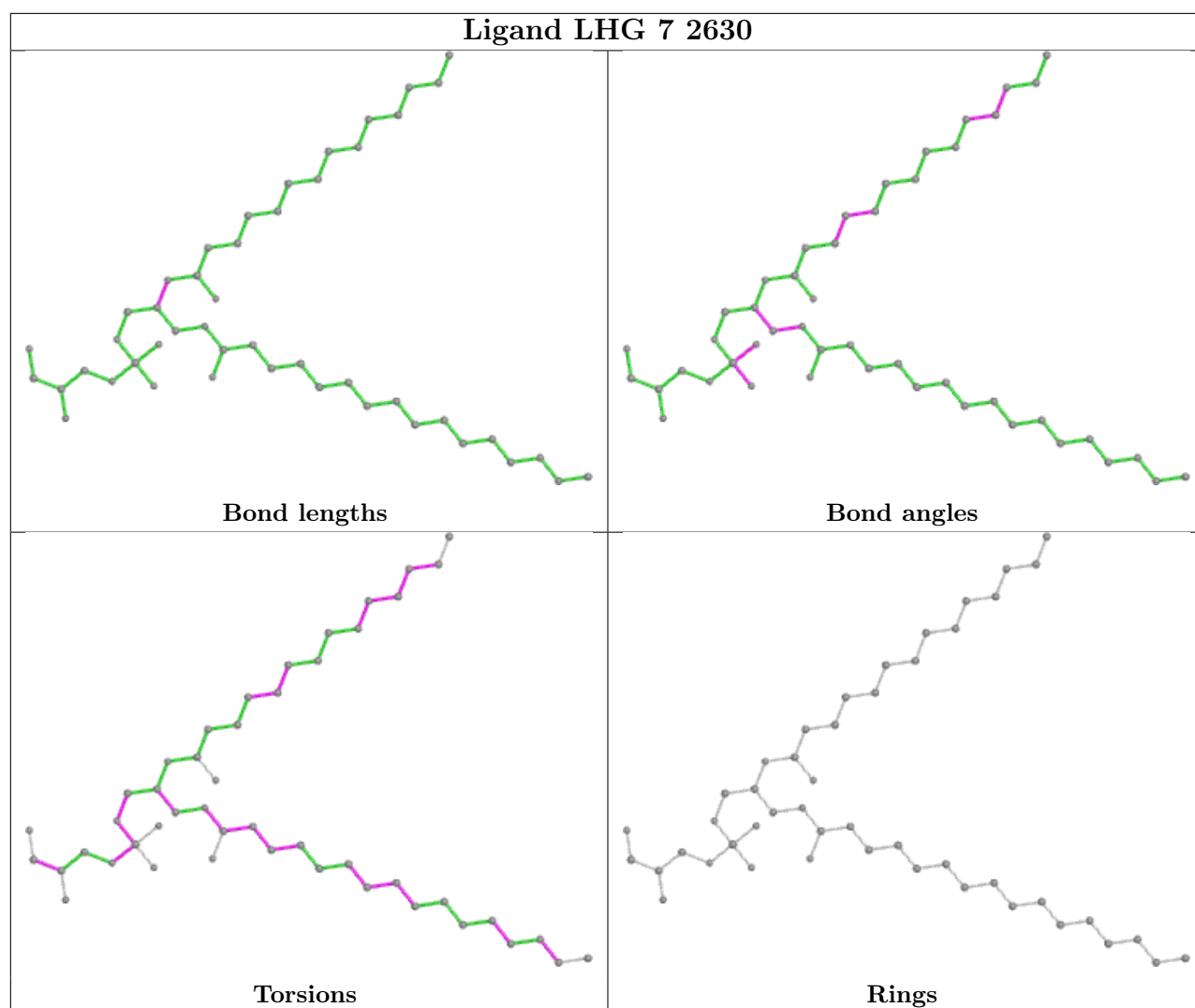
## Ligand CHL 8 601



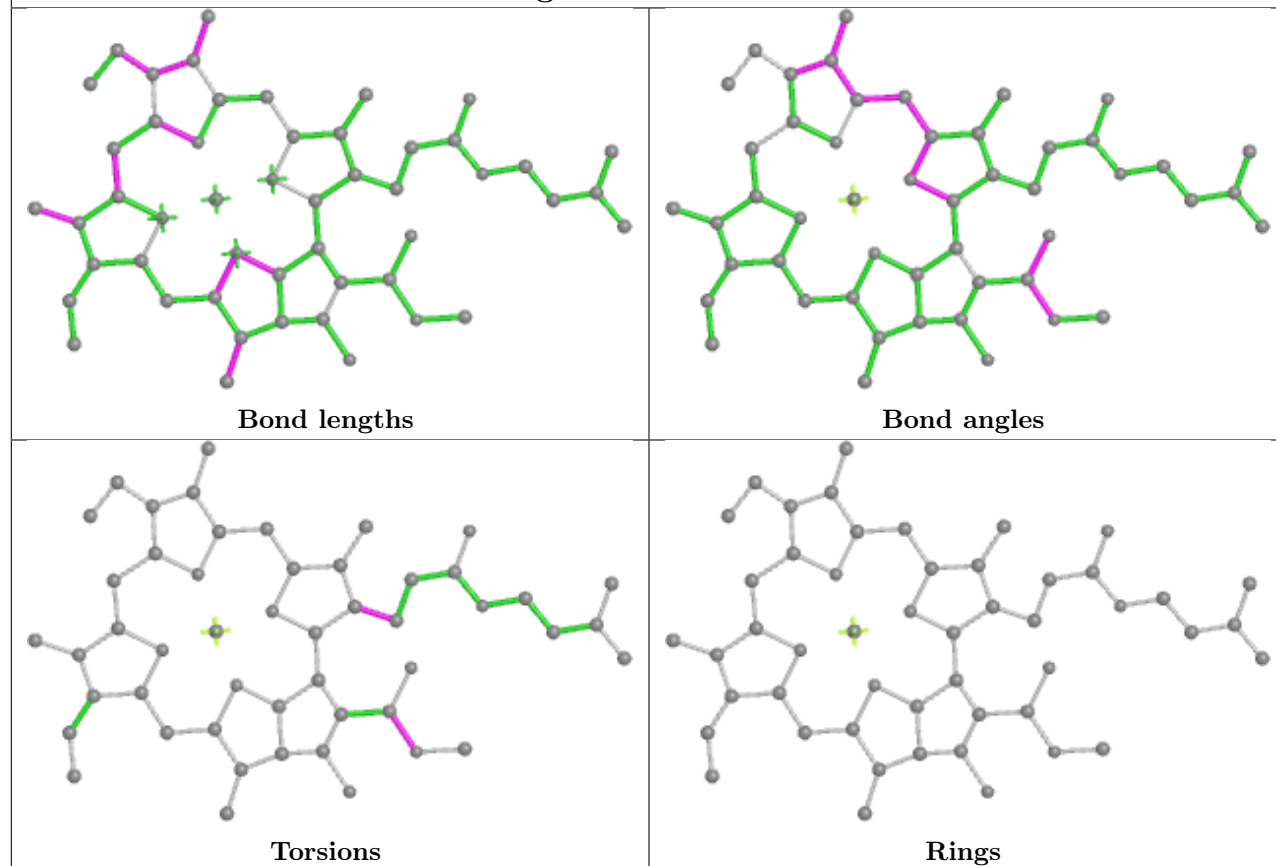


## Ligand CLA r 601

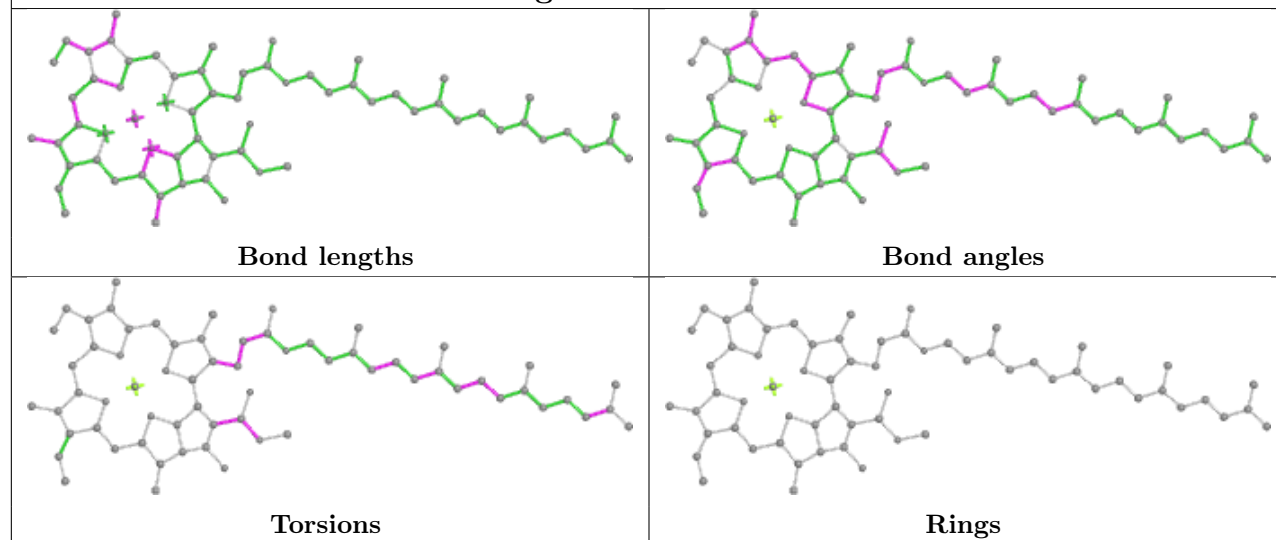


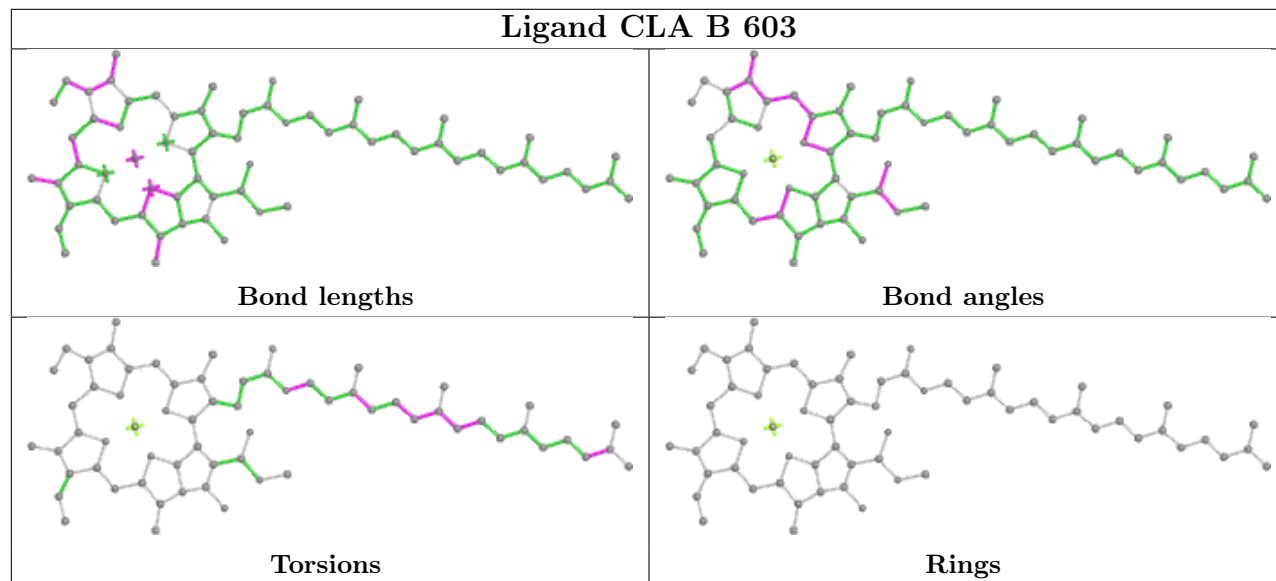
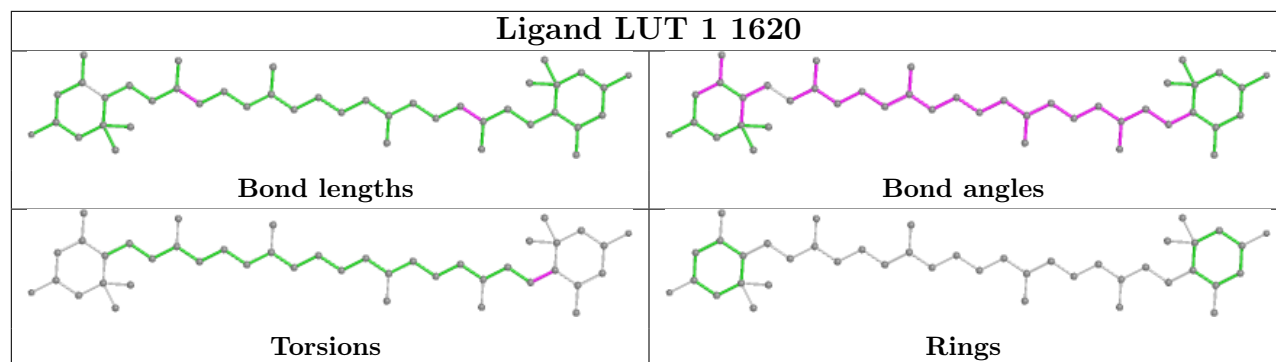


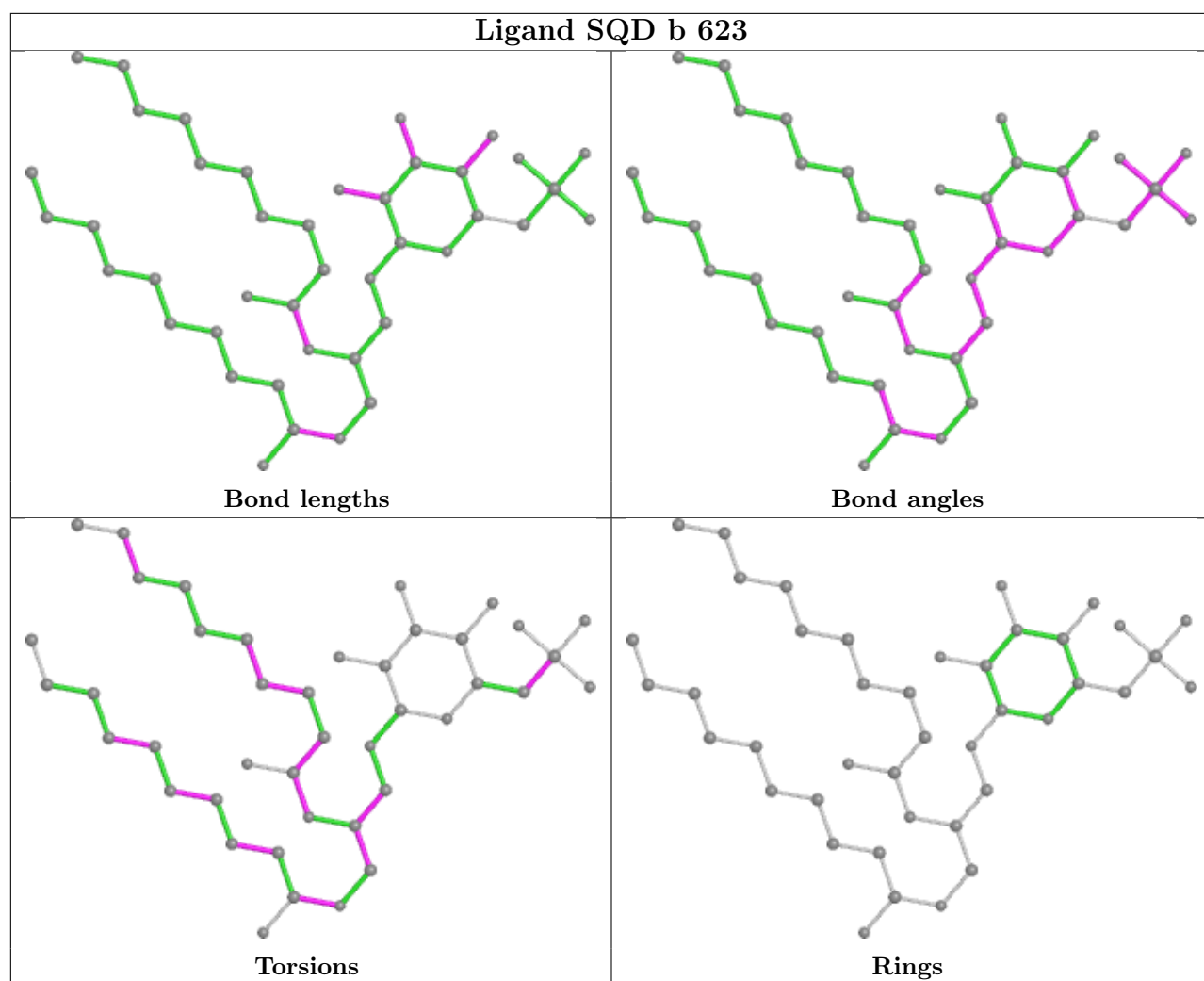
## Ligand CLA 6 610



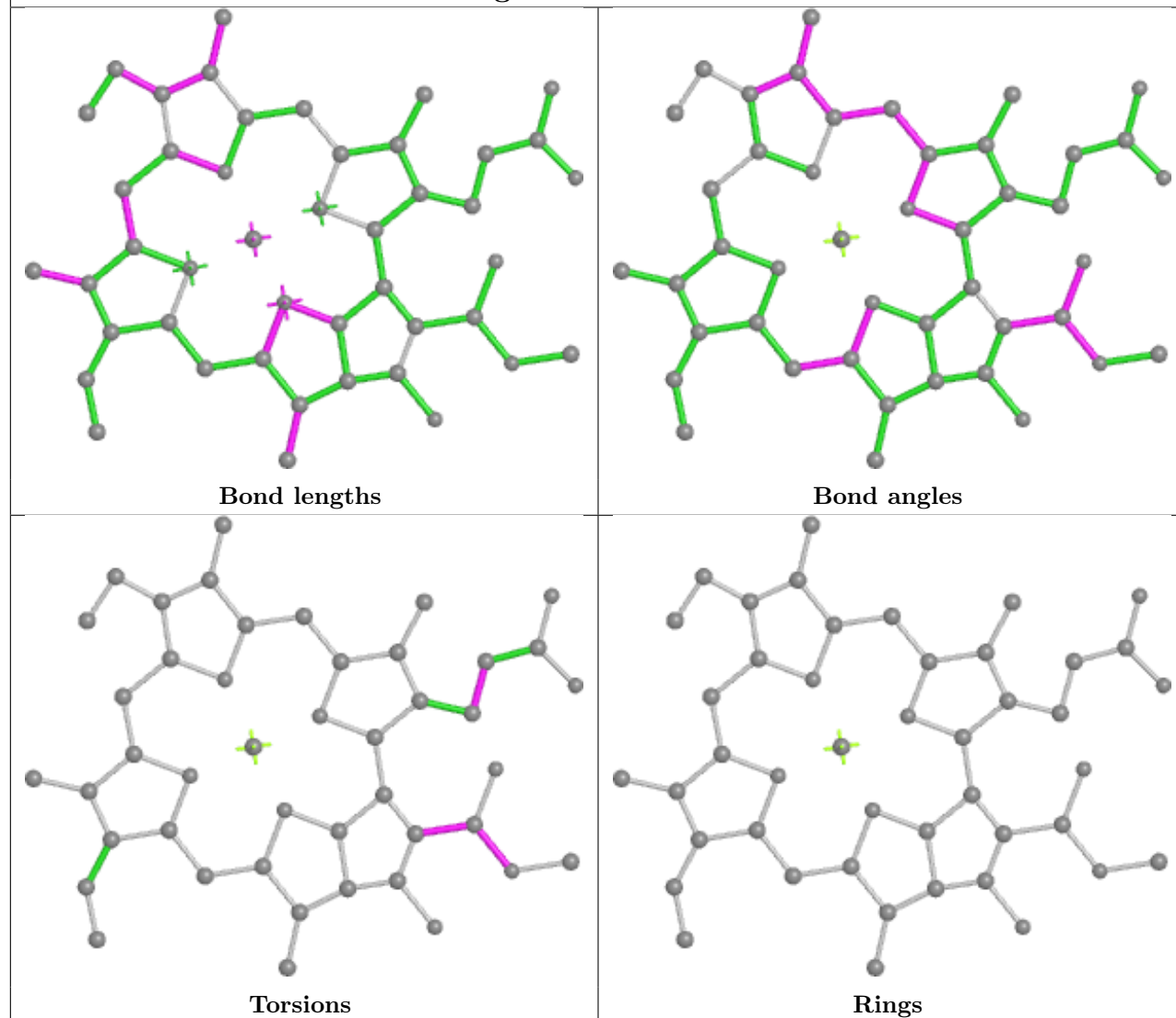
## Ligand CLA n 602



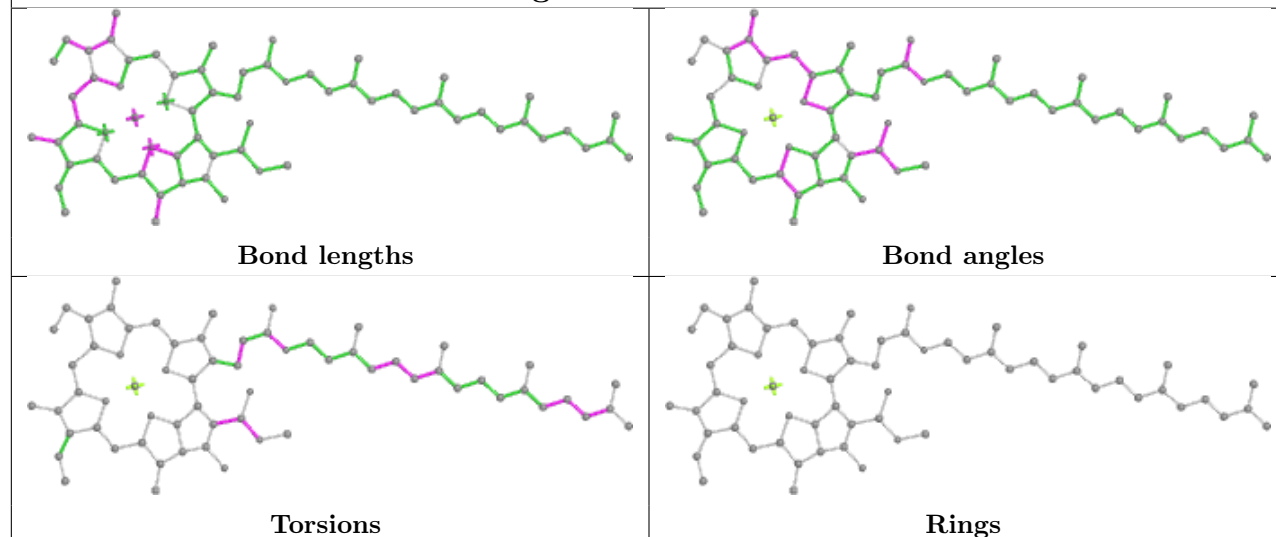


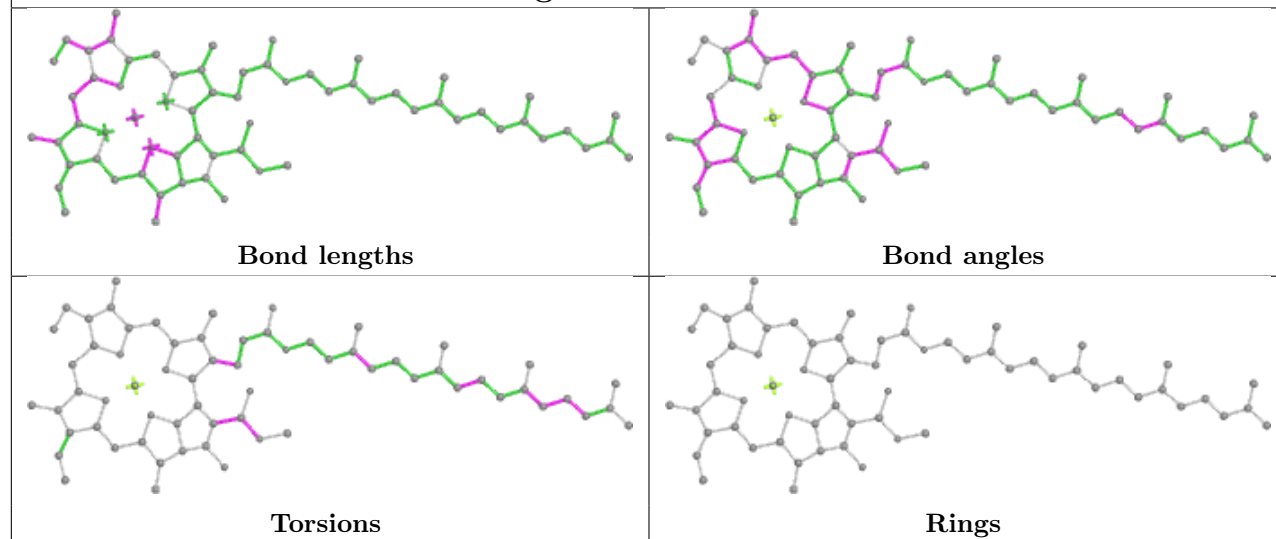
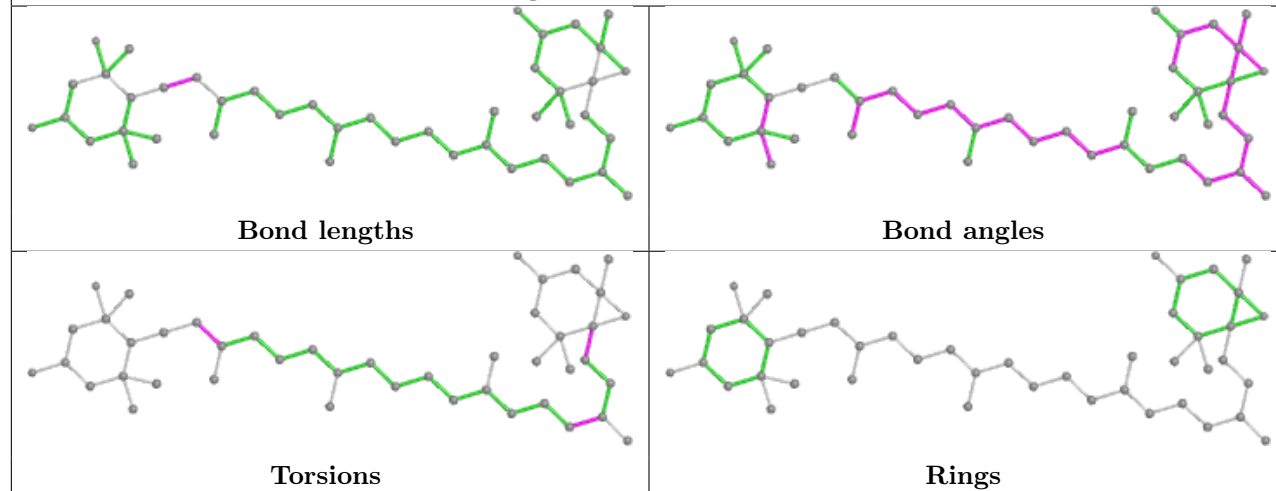


## Ligand CLA 6 613

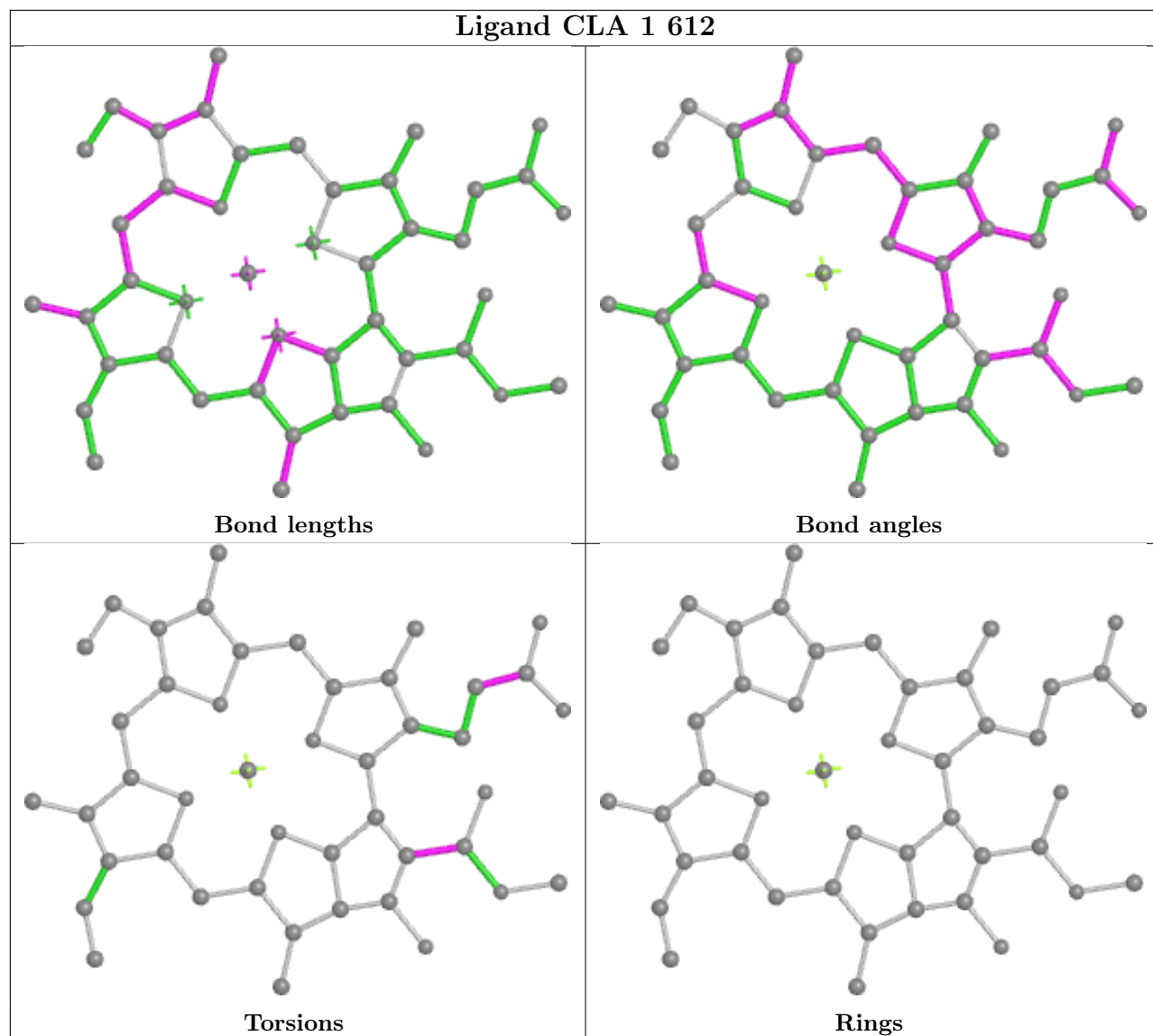


## Ligand CLA B 615



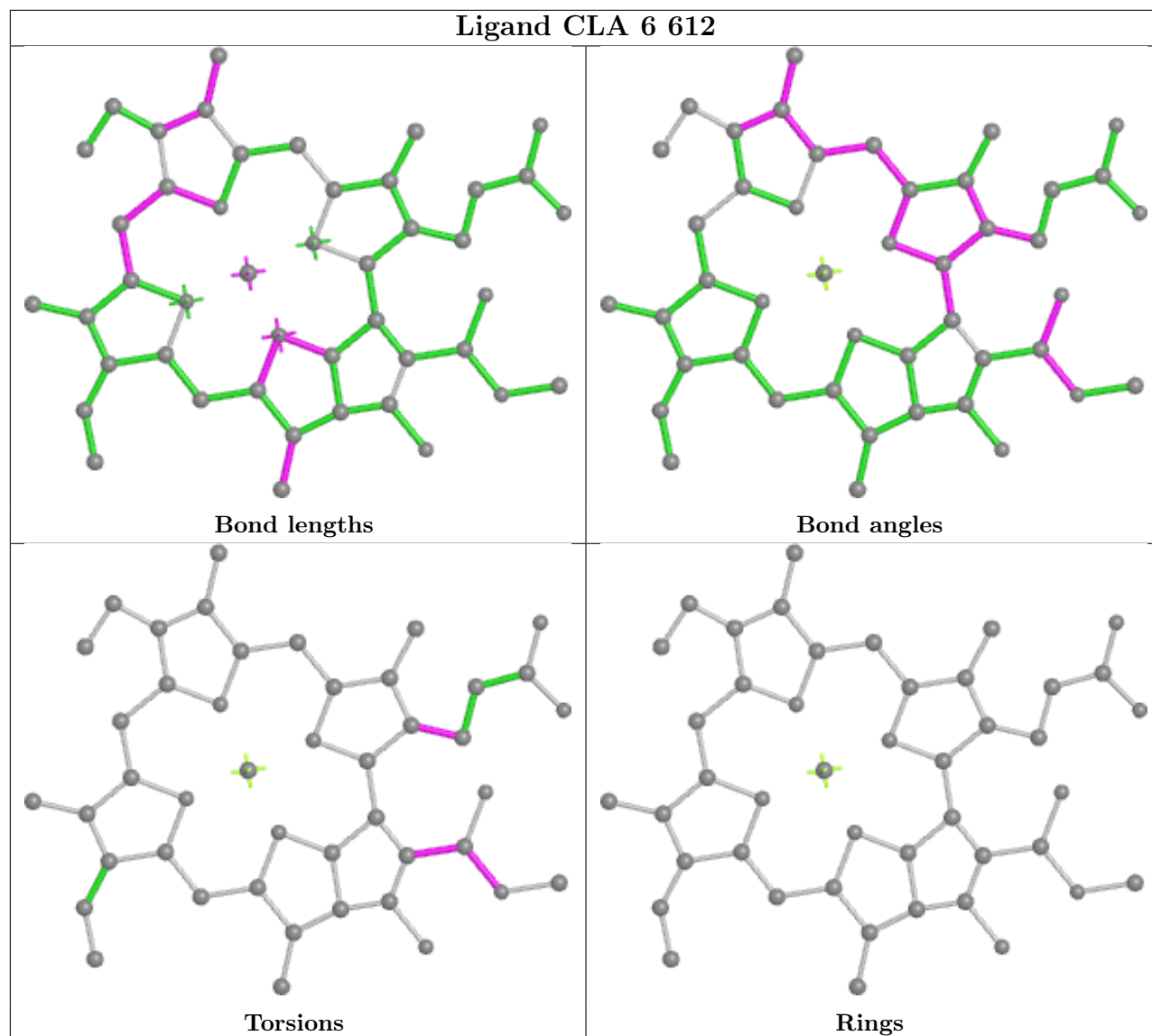
**Ligand CLA b 612****Ligand NEX S 1623**

## Ligand CLA 1 612

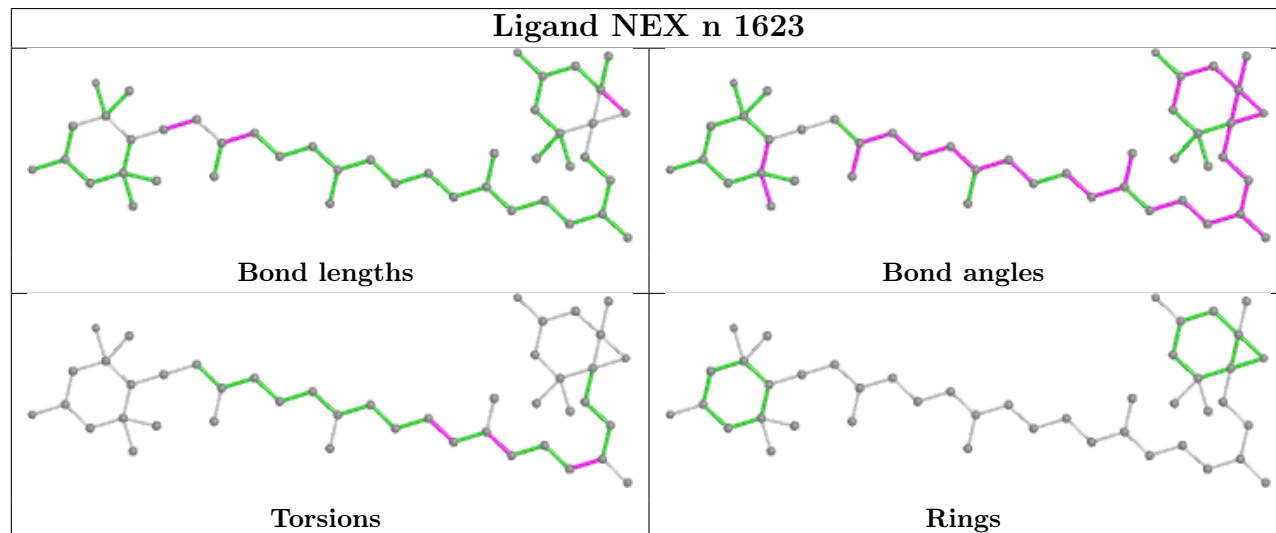


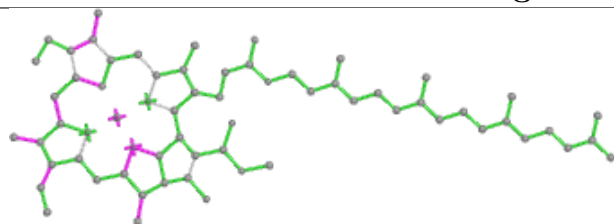
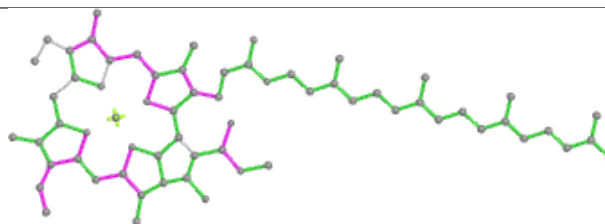
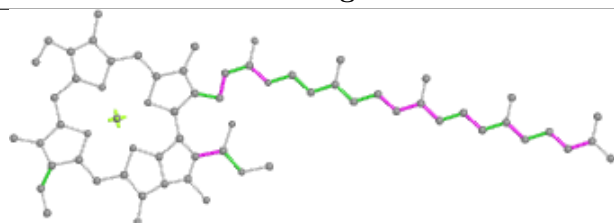
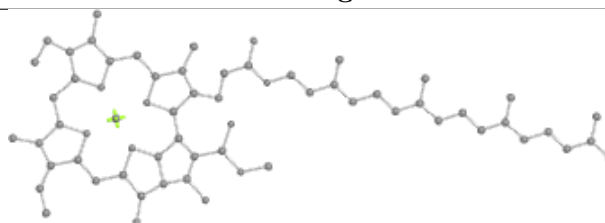
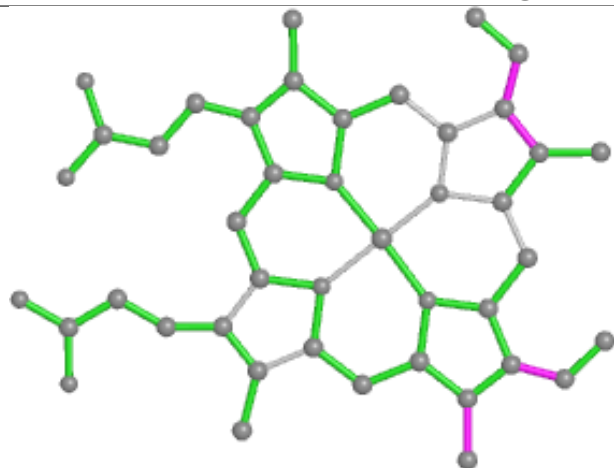
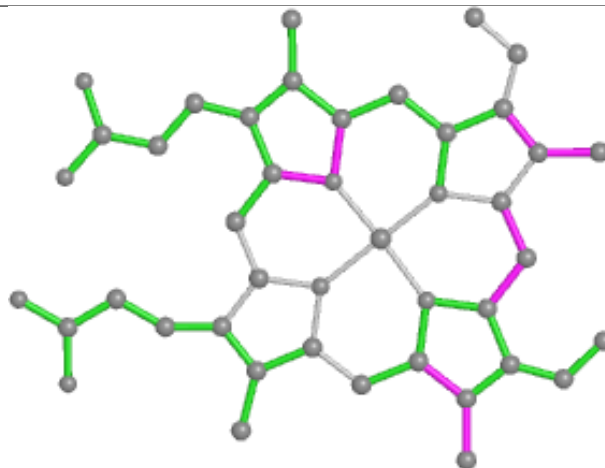
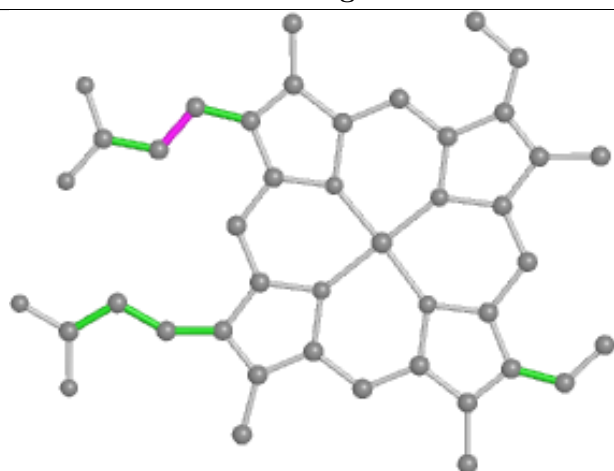
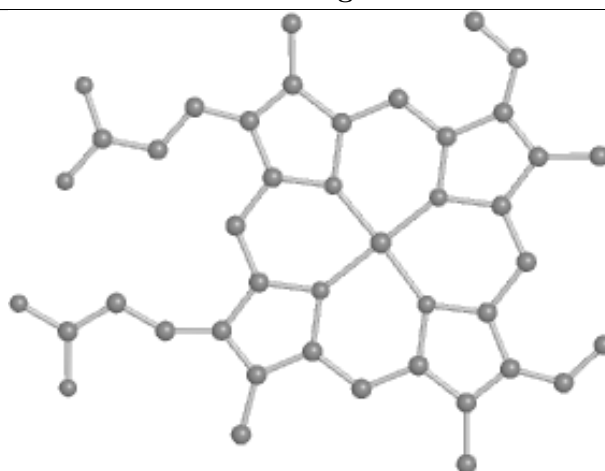


## Ligand CLA 6 612

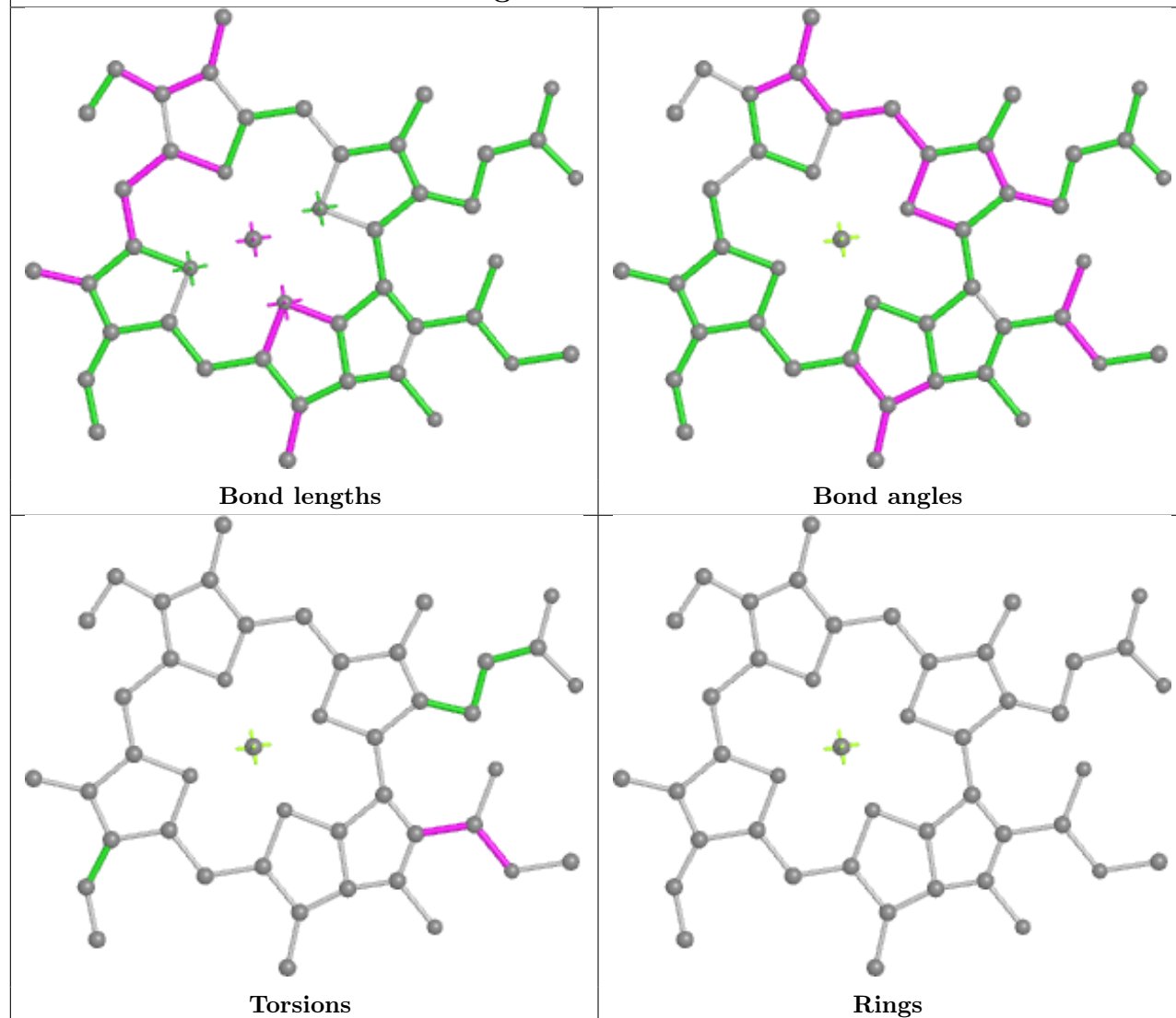


## Ligand NEX n 1623

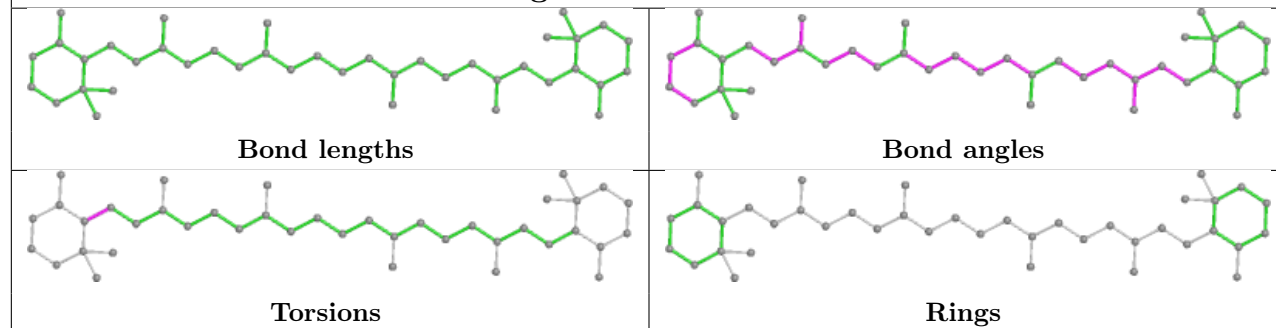


**Ligand CLA N 603****Bond lengths****Bond angles****Torsions****Rings****Ligand HEM f 101****Bond lengths****Bond angles****Torsions****Rings**

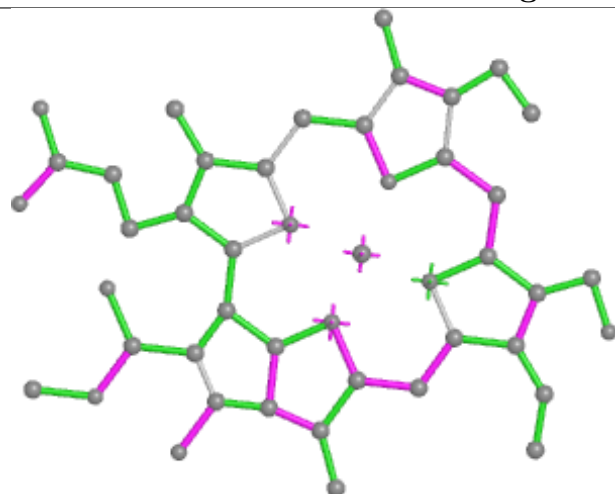
## Ligand CLA 7 612



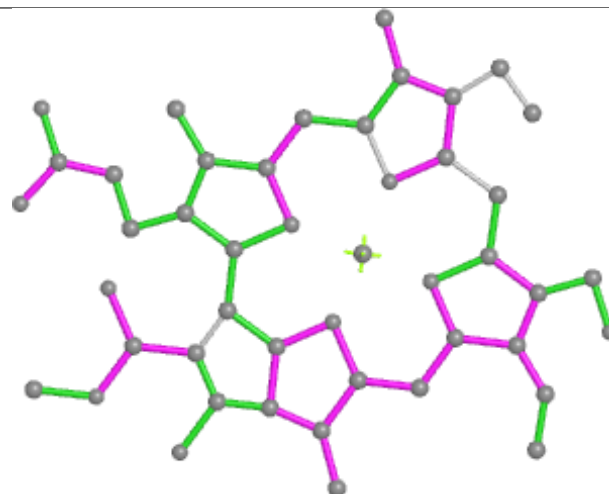
## Ligand BCR C 514



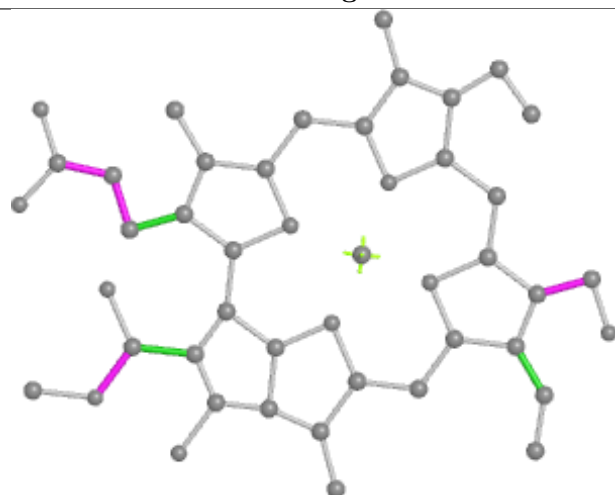
## Ligand CHL 1 606



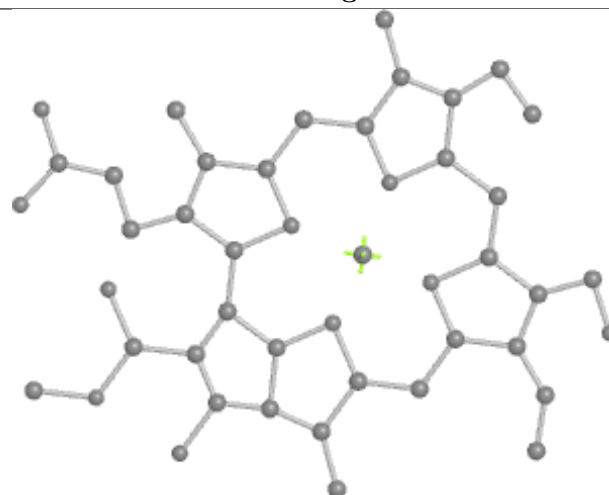
Bond lengths



Bond angles

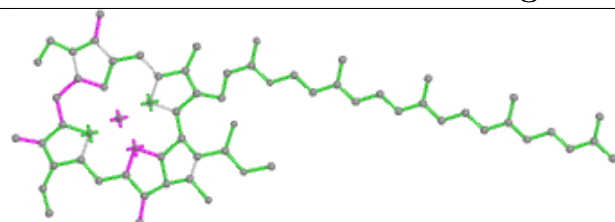


Torsions

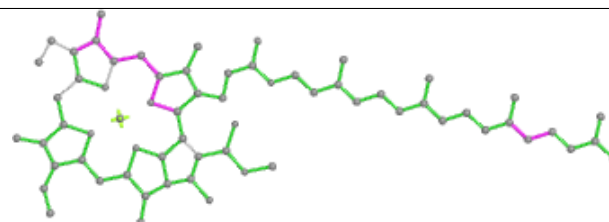


Rings

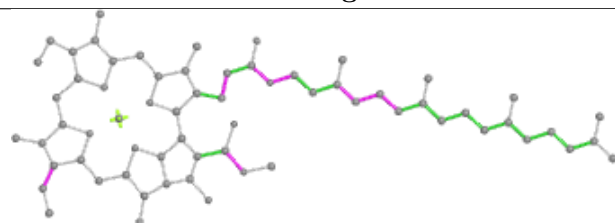
## Ligand CLA a 405



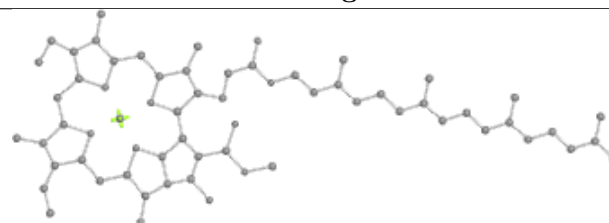
Bond lengths



Bond angles

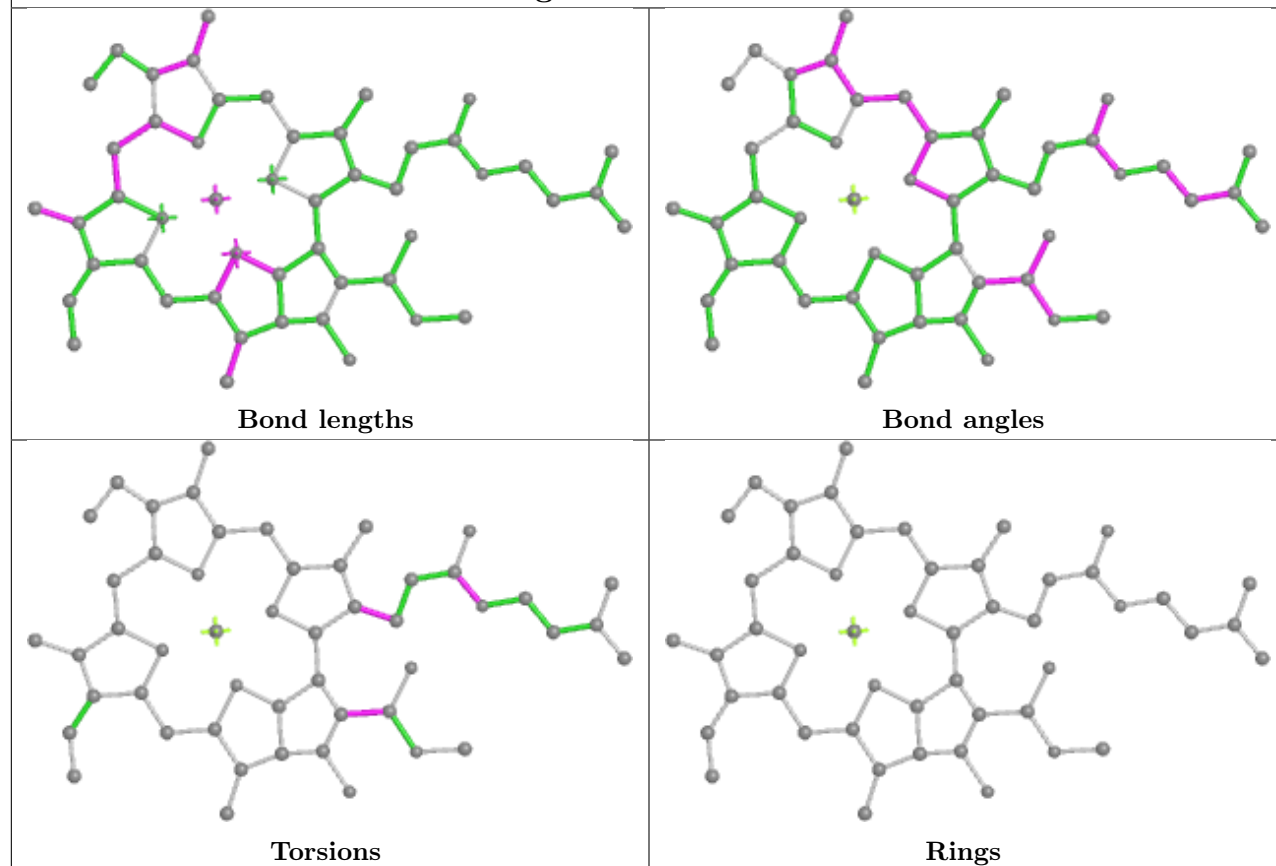


Torsions

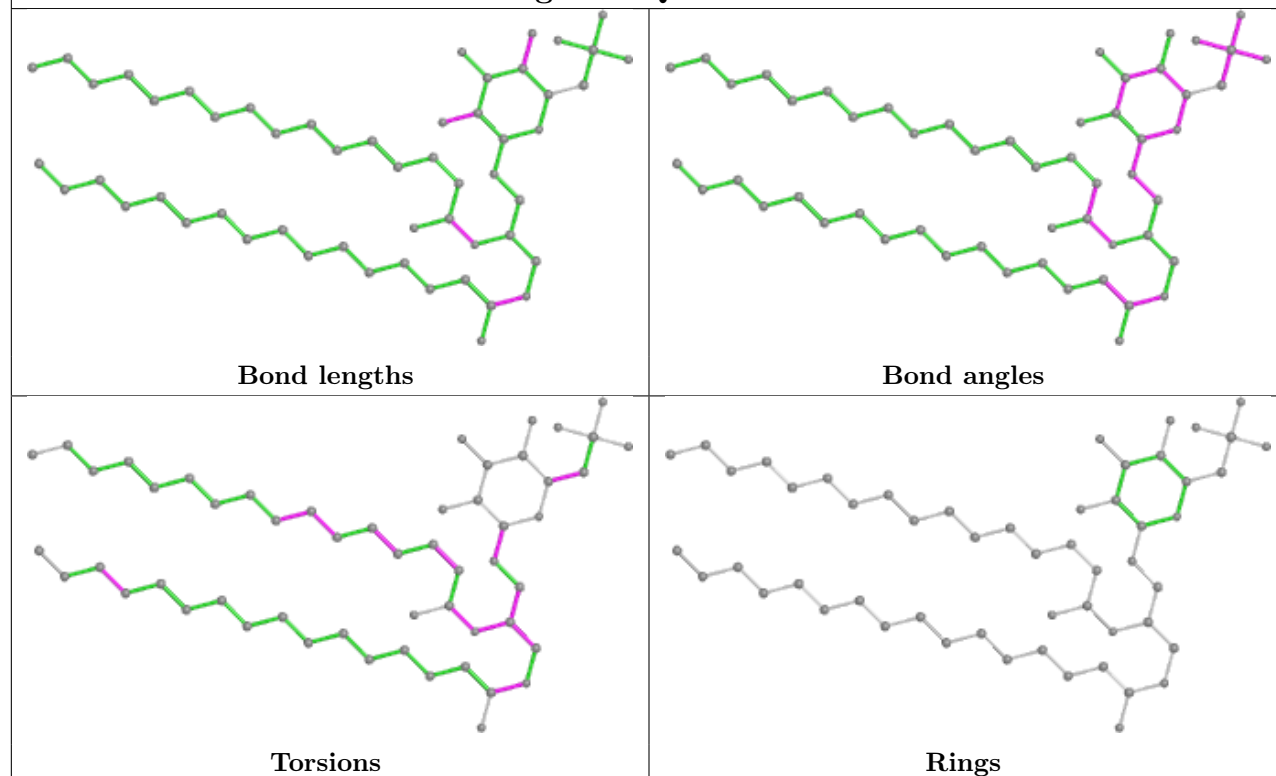


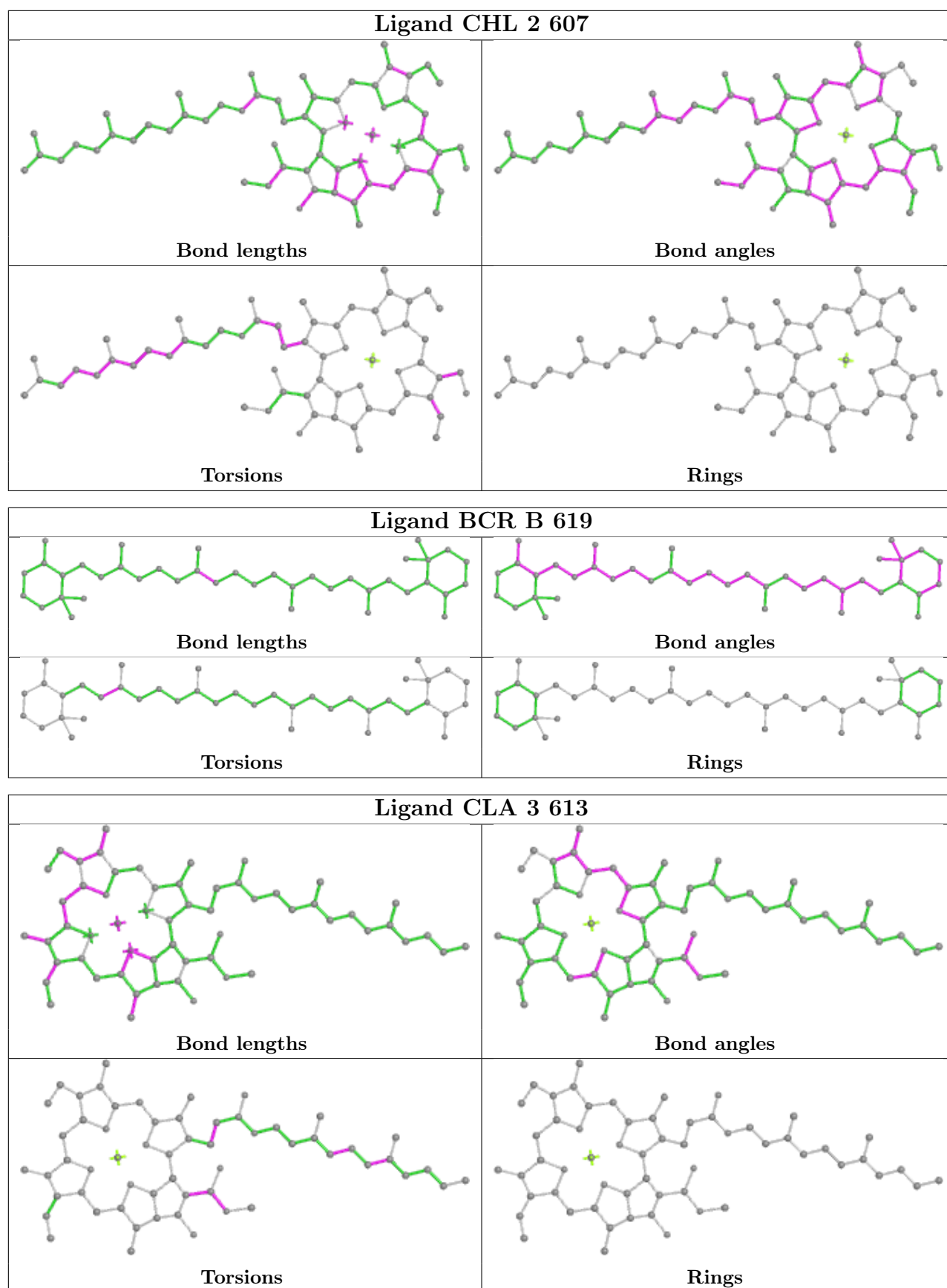
Rings

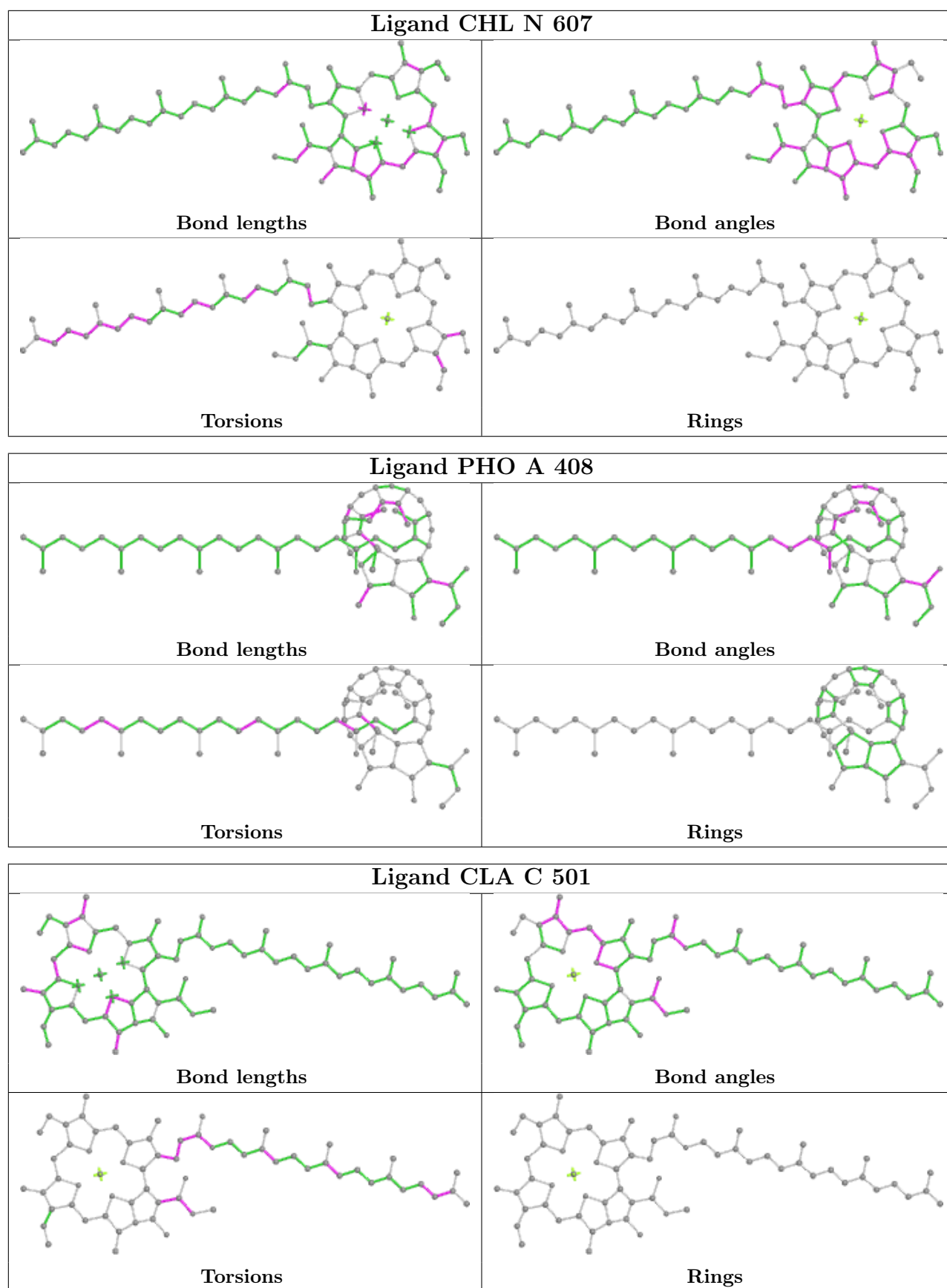
## Ligand CLA n 604

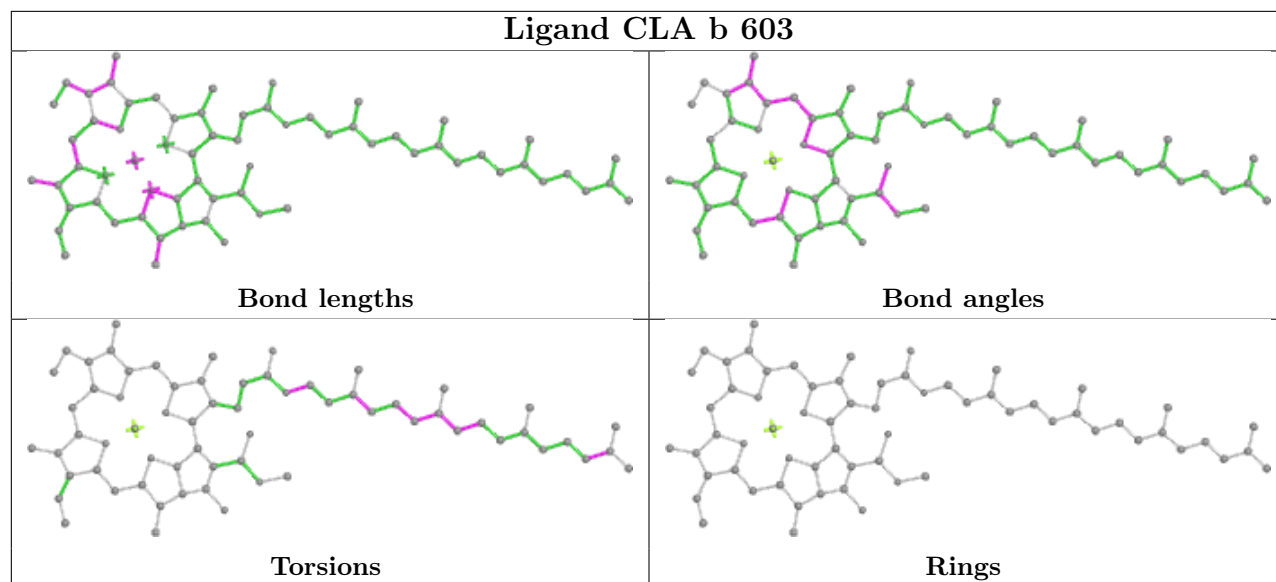
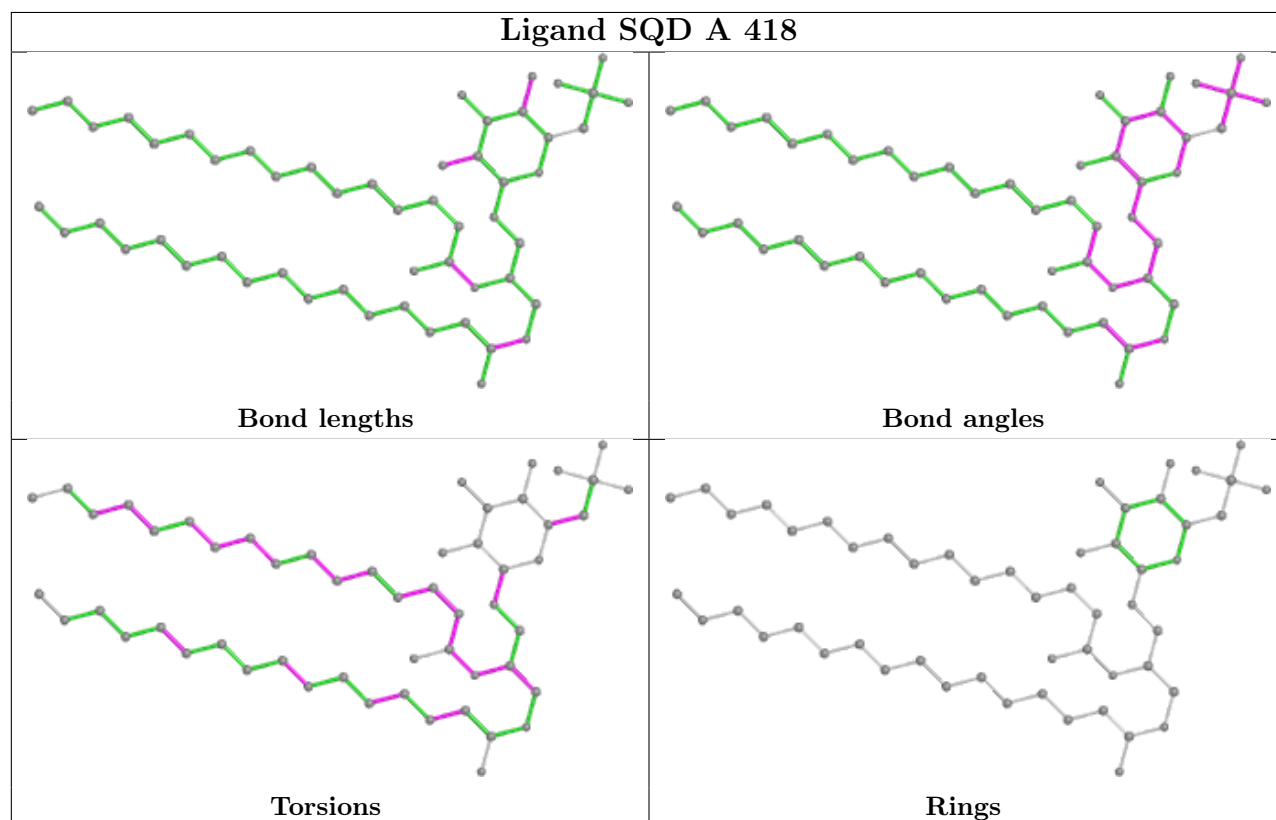


## Ligand SQD b 621

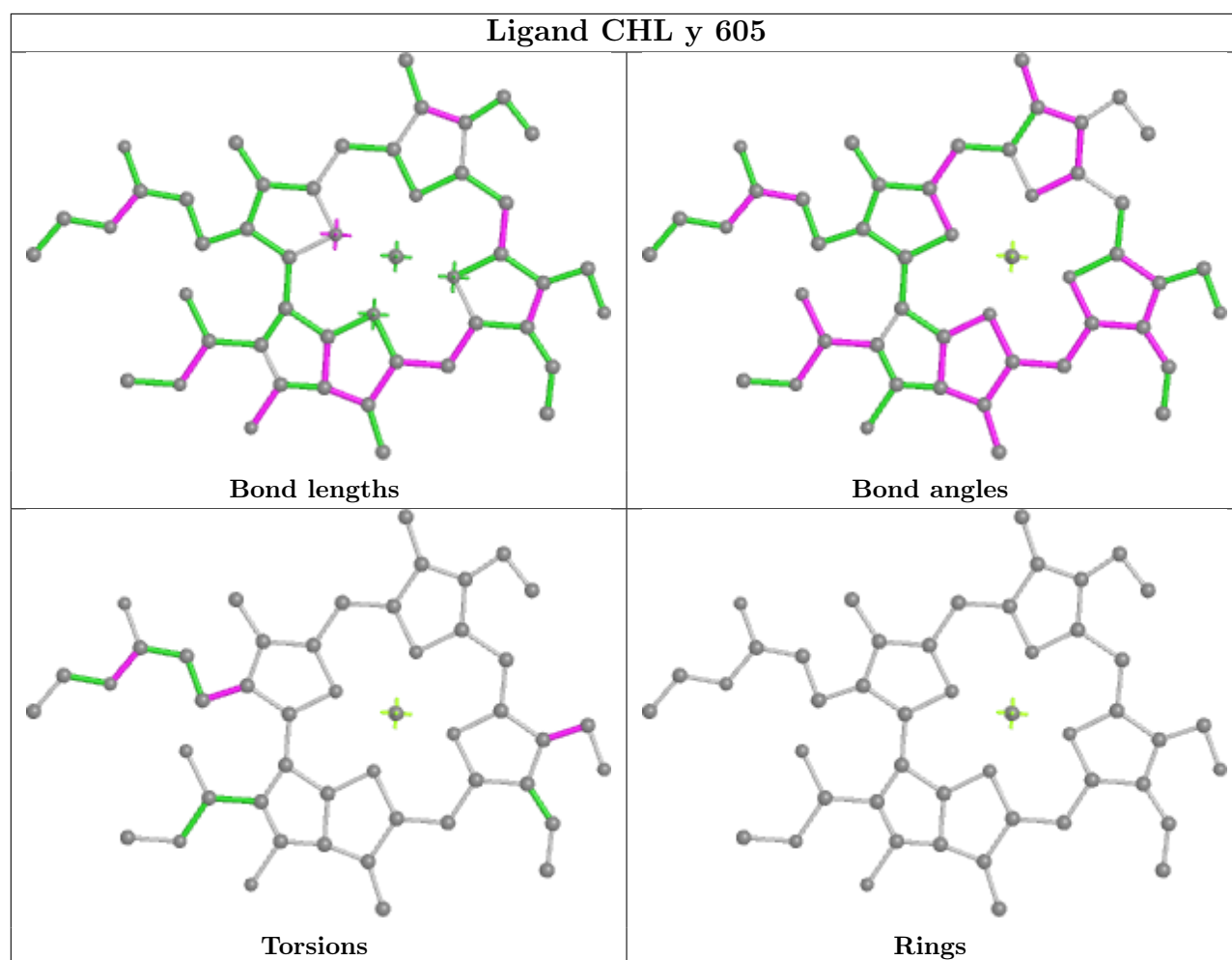




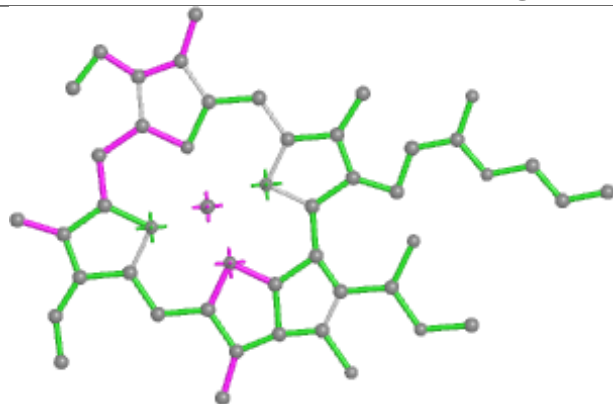


**Ligand CLA b 603****Ligand SQD A 418**

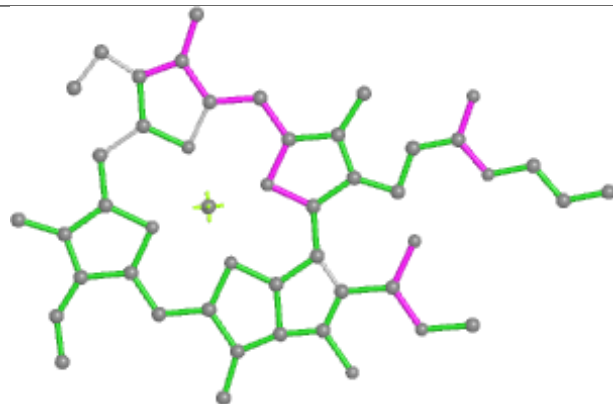




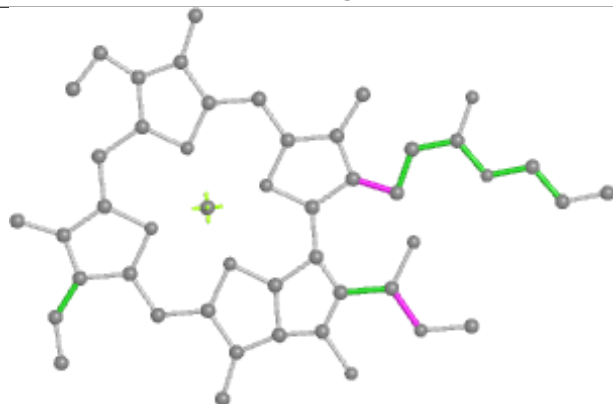
## Ligand CLA Y 614



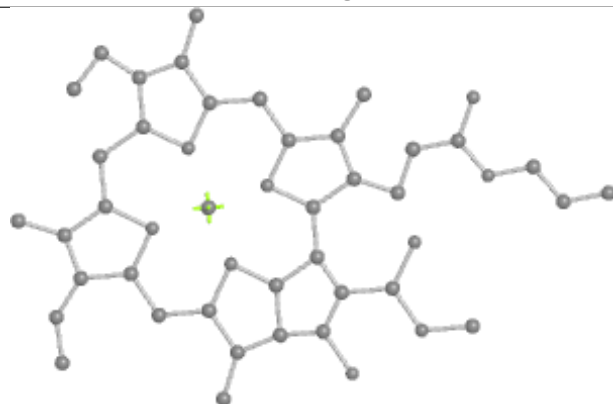
Bond lengths



Bond angles

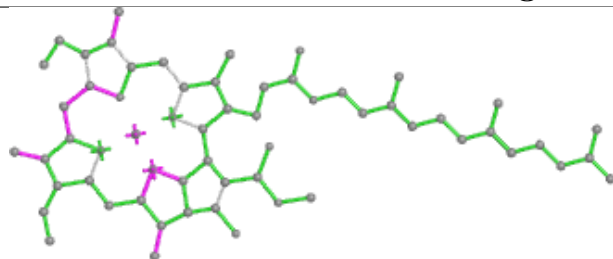


Torsions

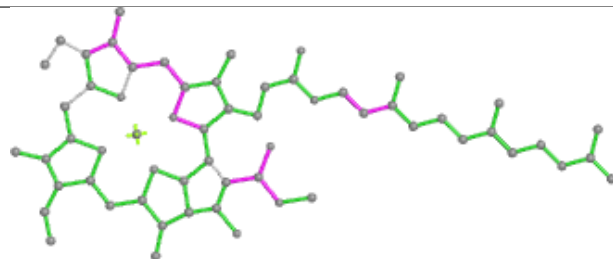


Rings

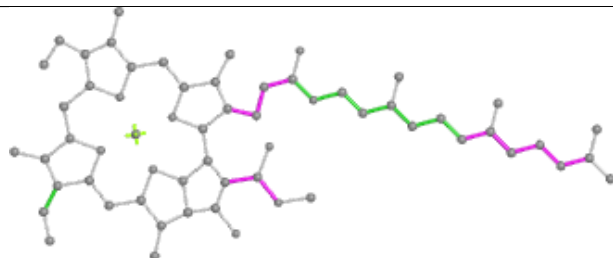
## Ligand CLA 3 602



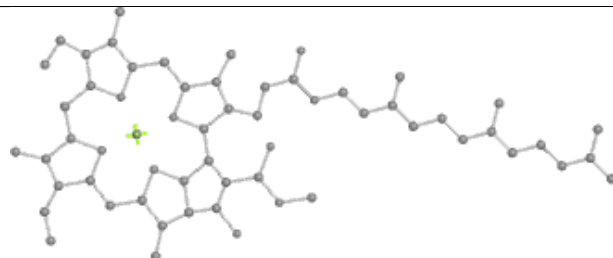
Bond lengths



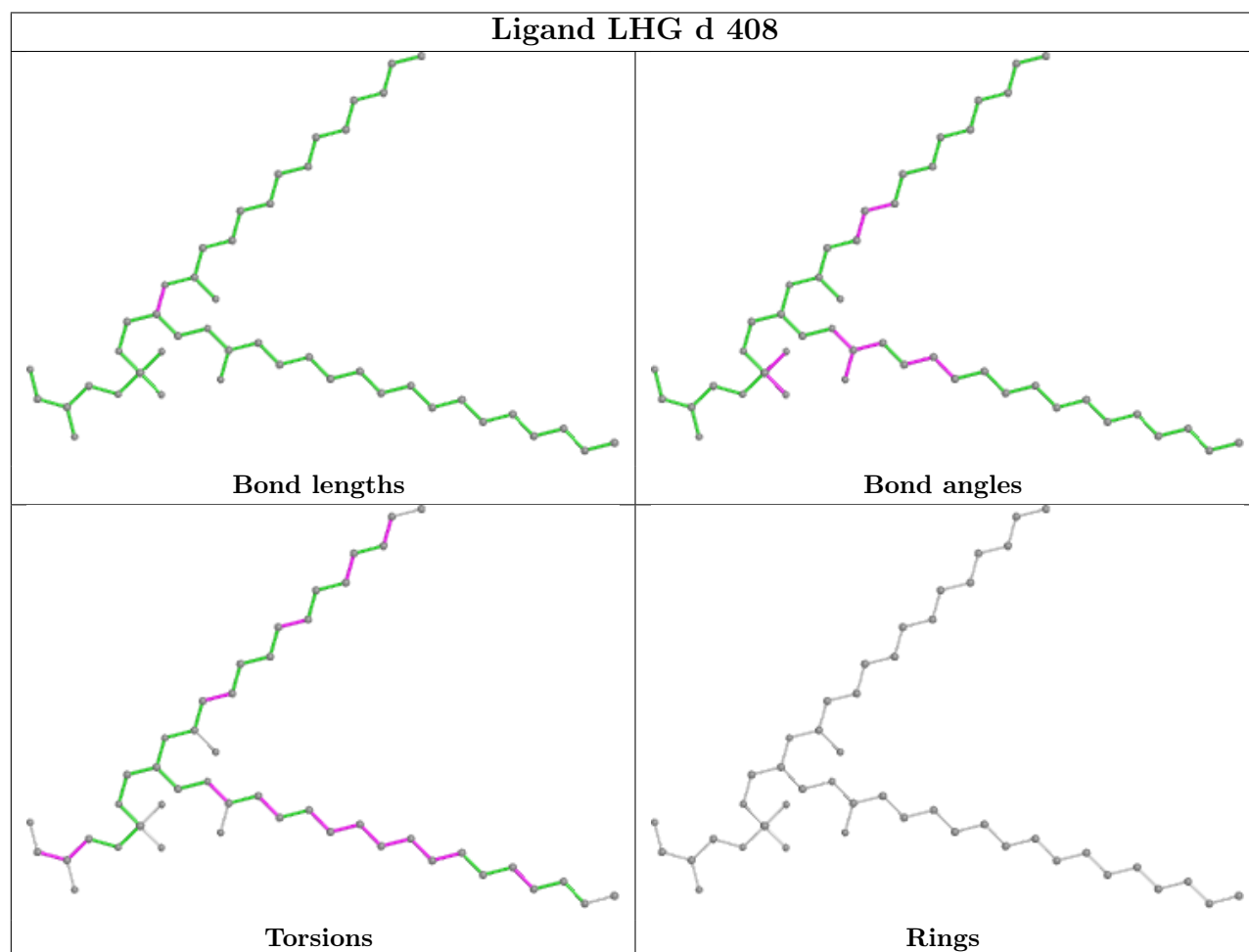
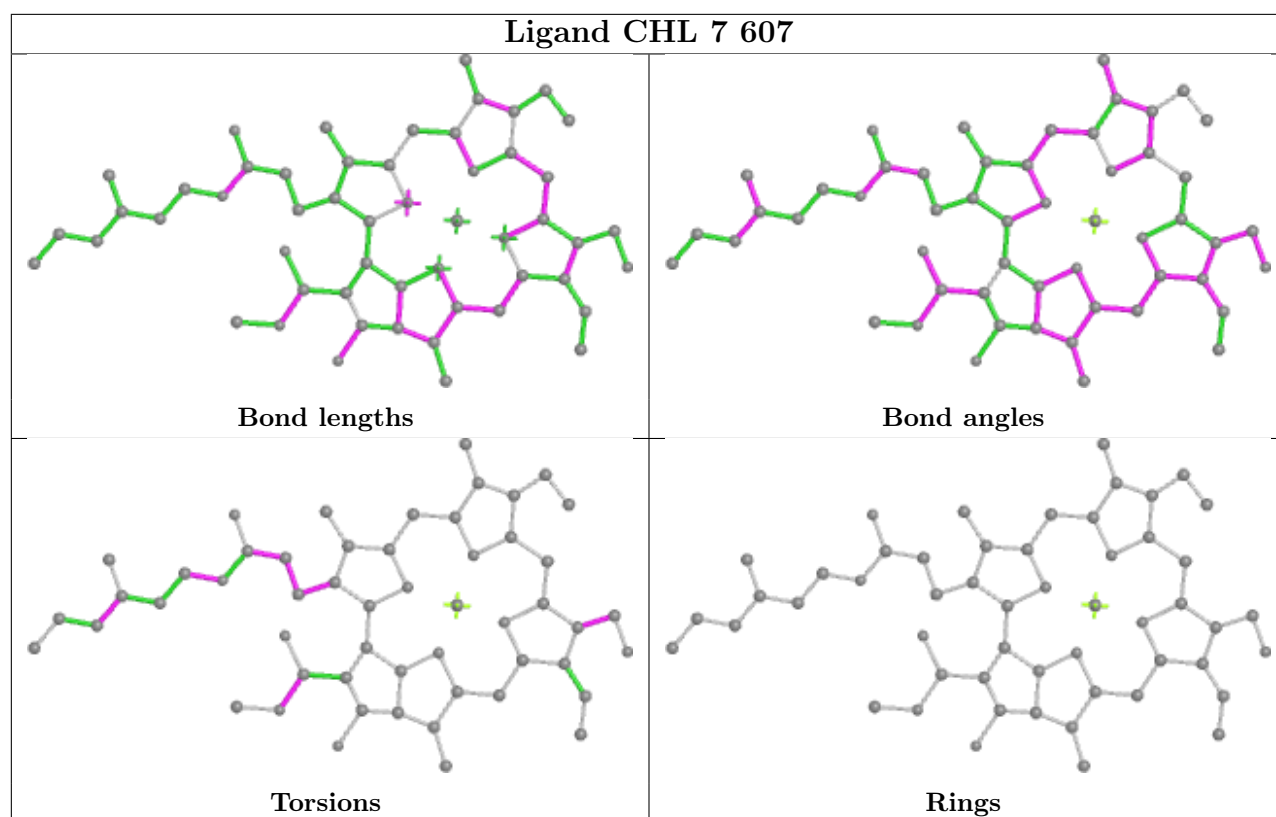
Bond angles



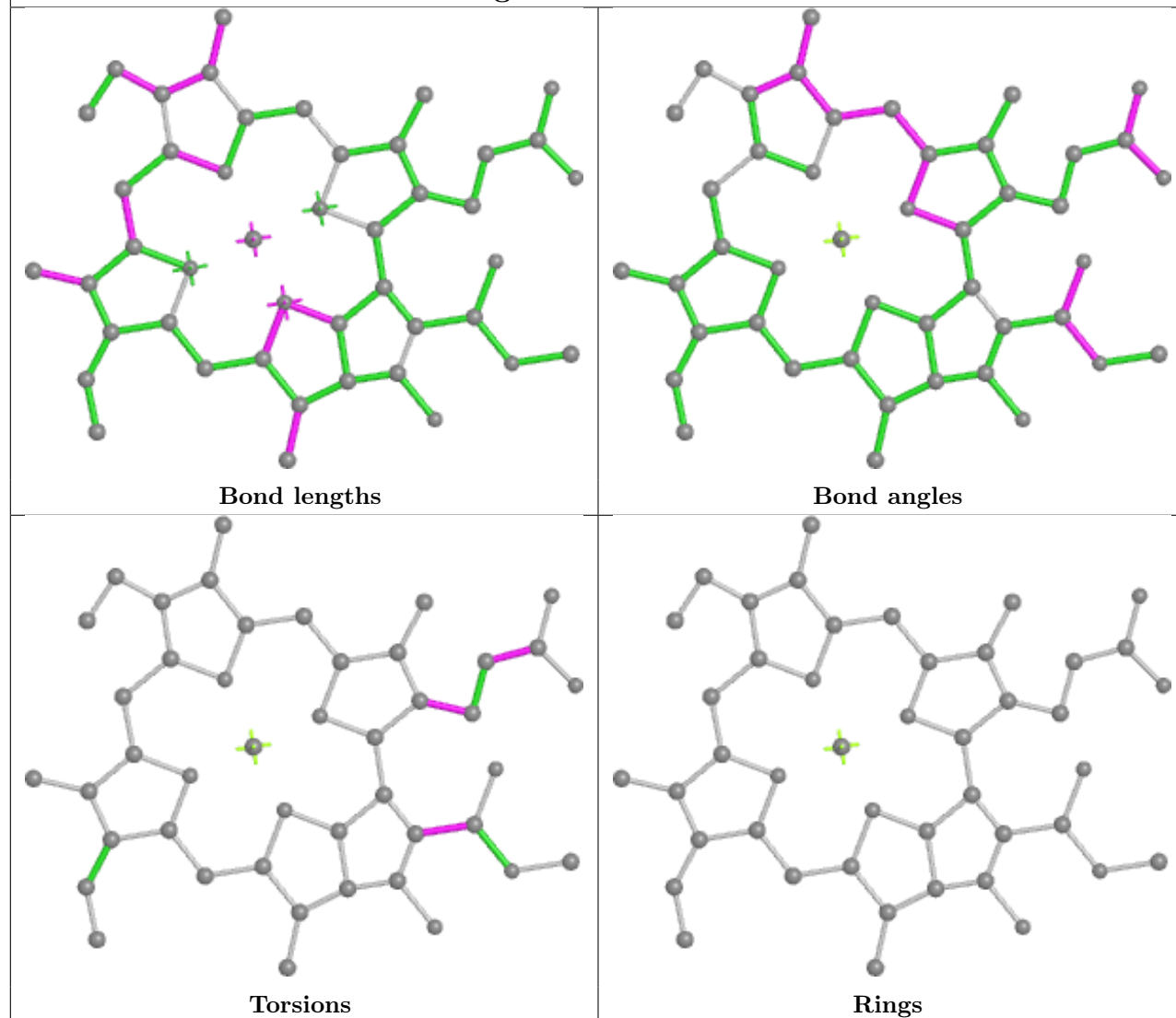
Torsions



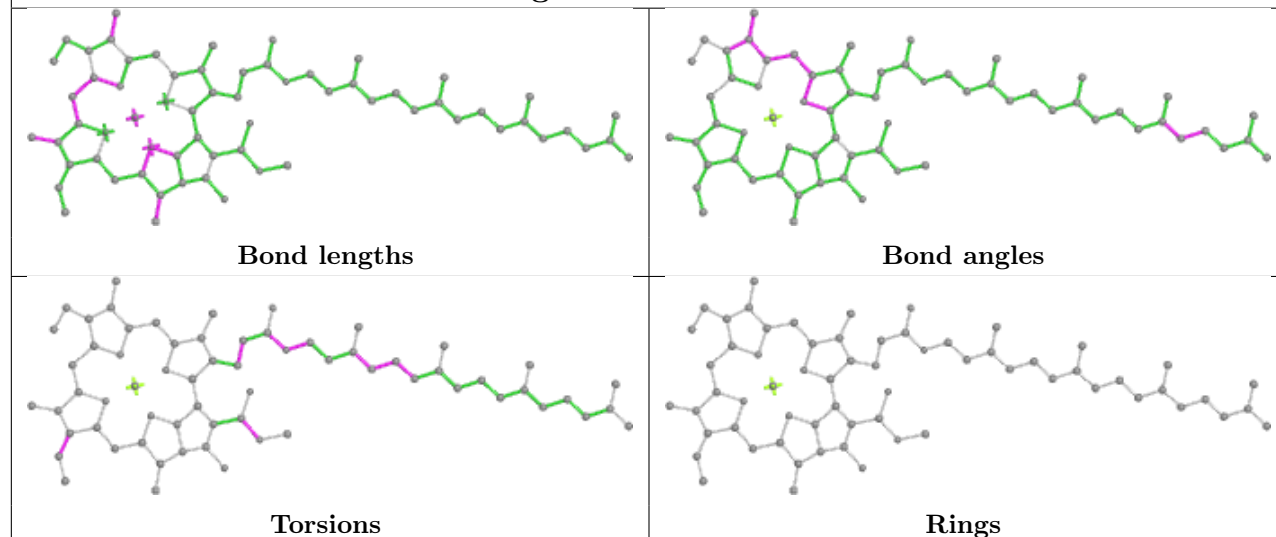
Rings



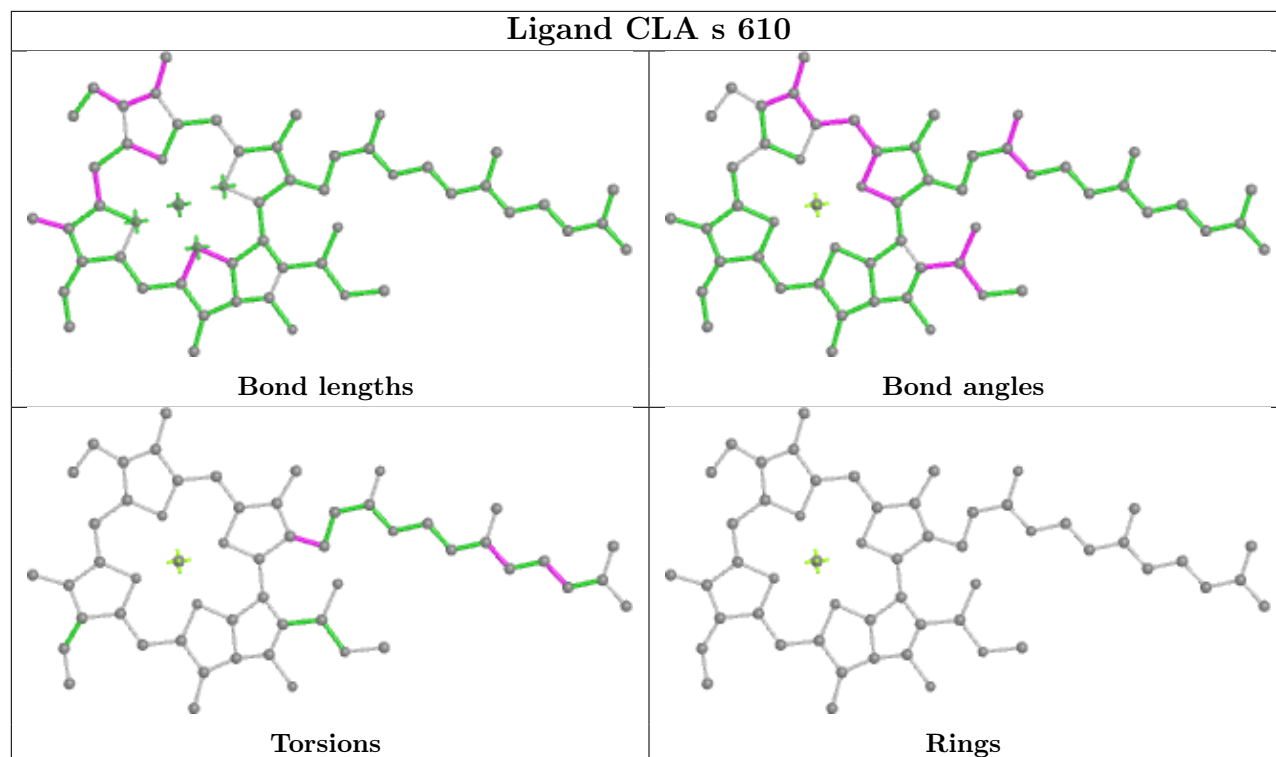
## Ligand CLA 8 610



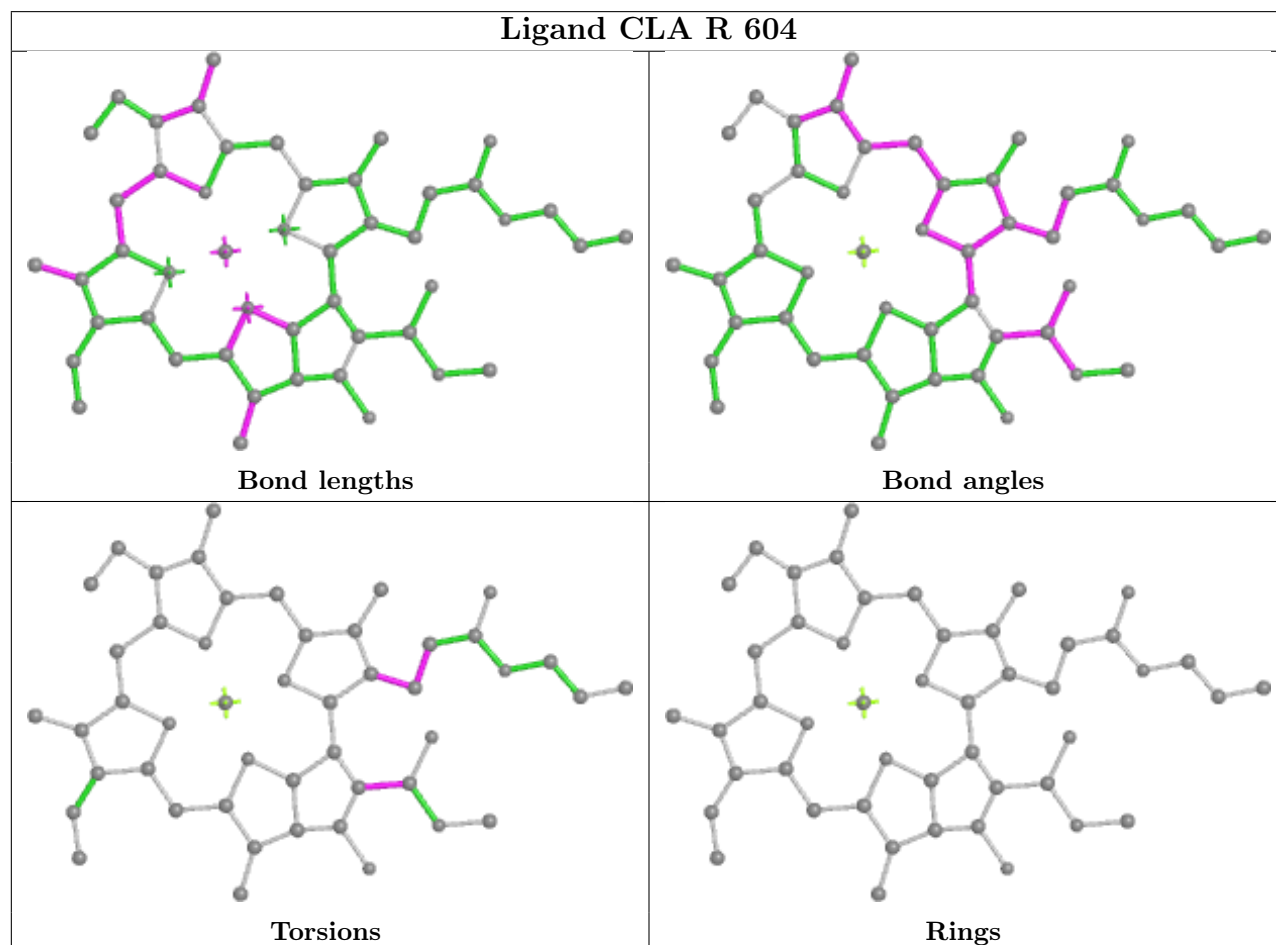
## Ligand CLA A 405



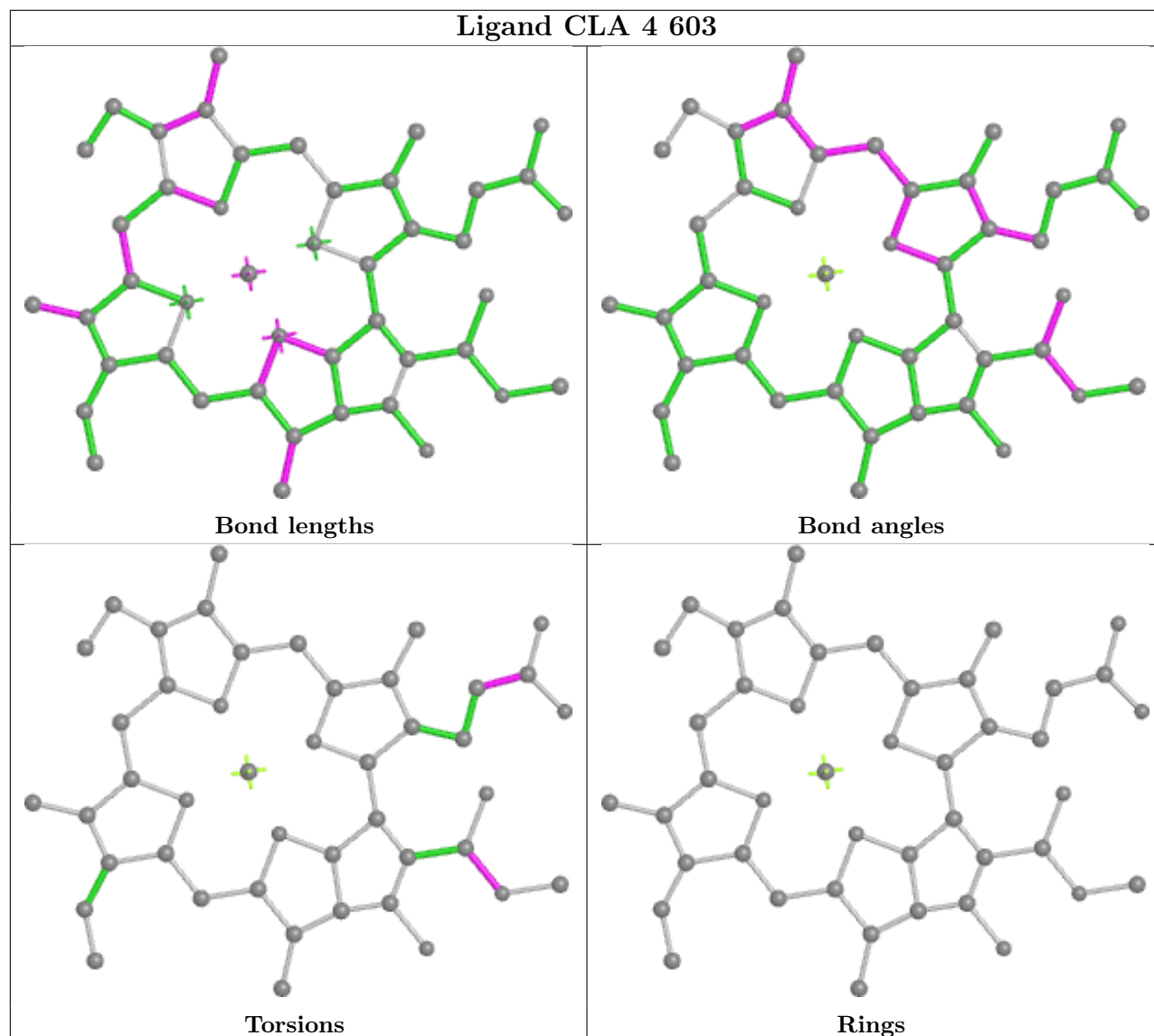
## Ligand CLA s 610



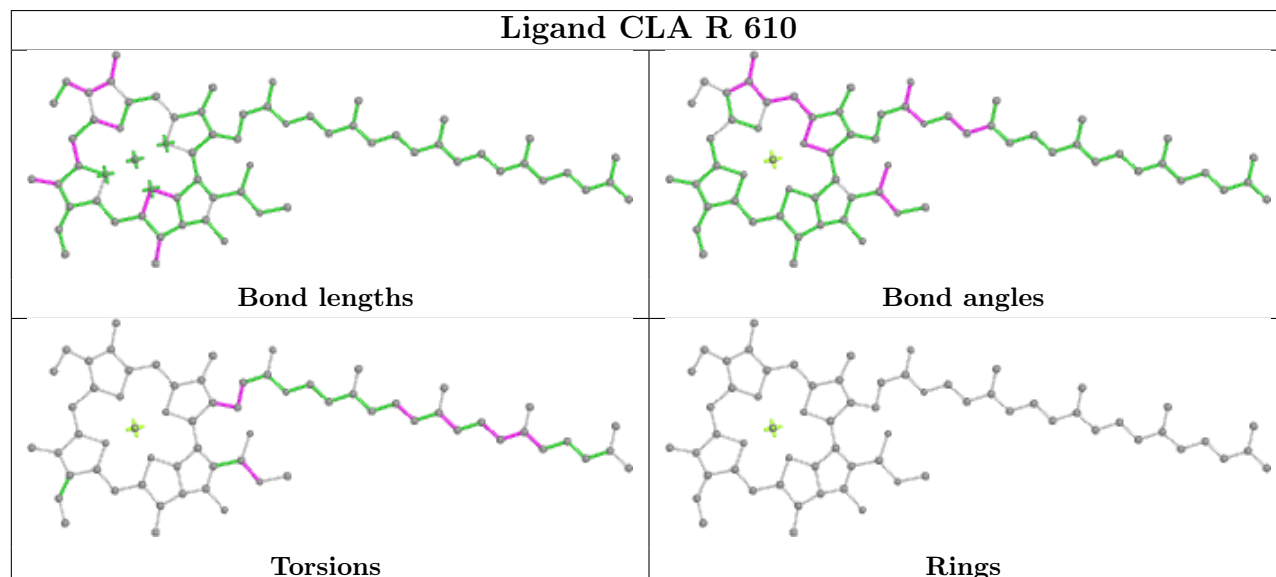
## Ligand CLA R 604

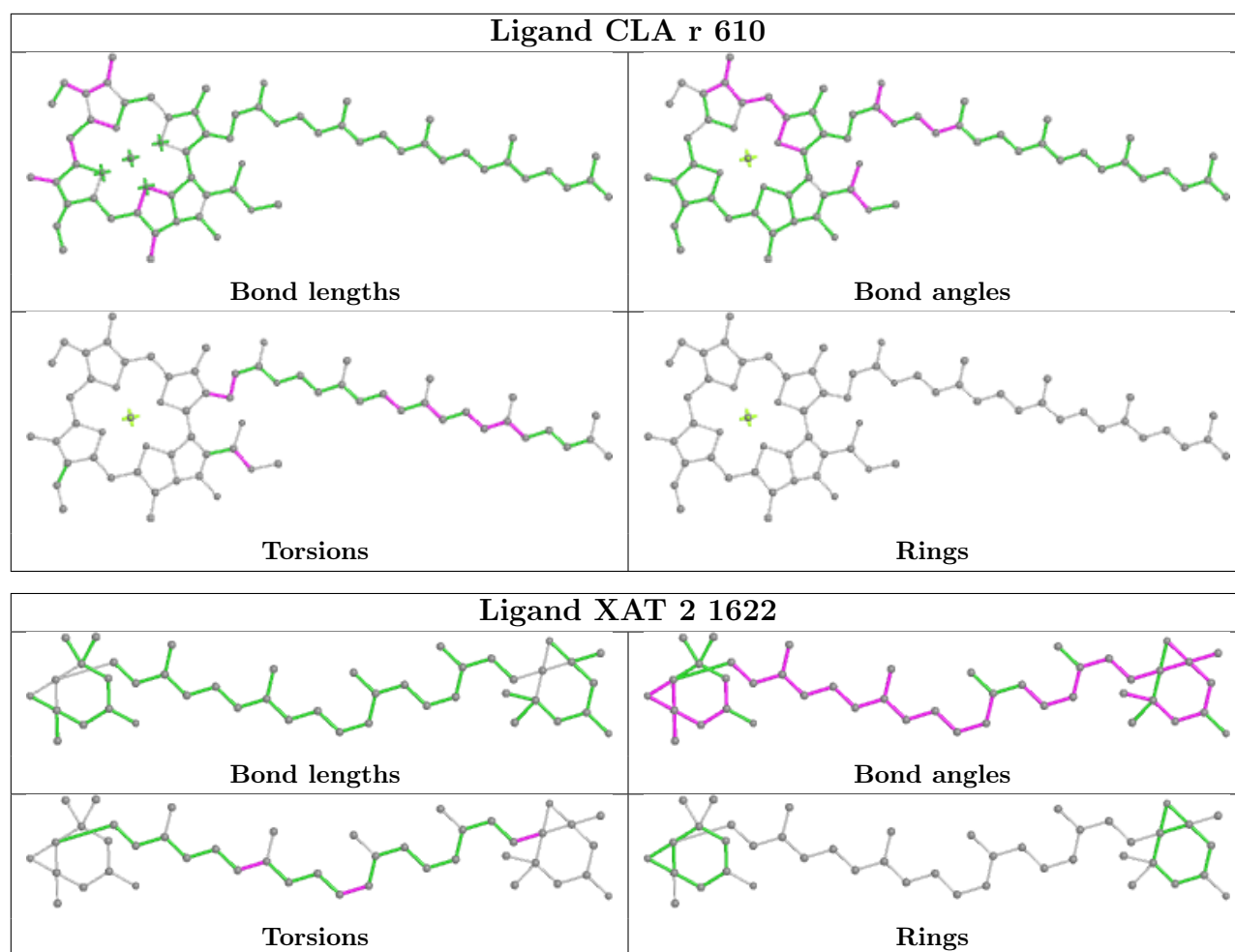


## Ligand CLA 4 603

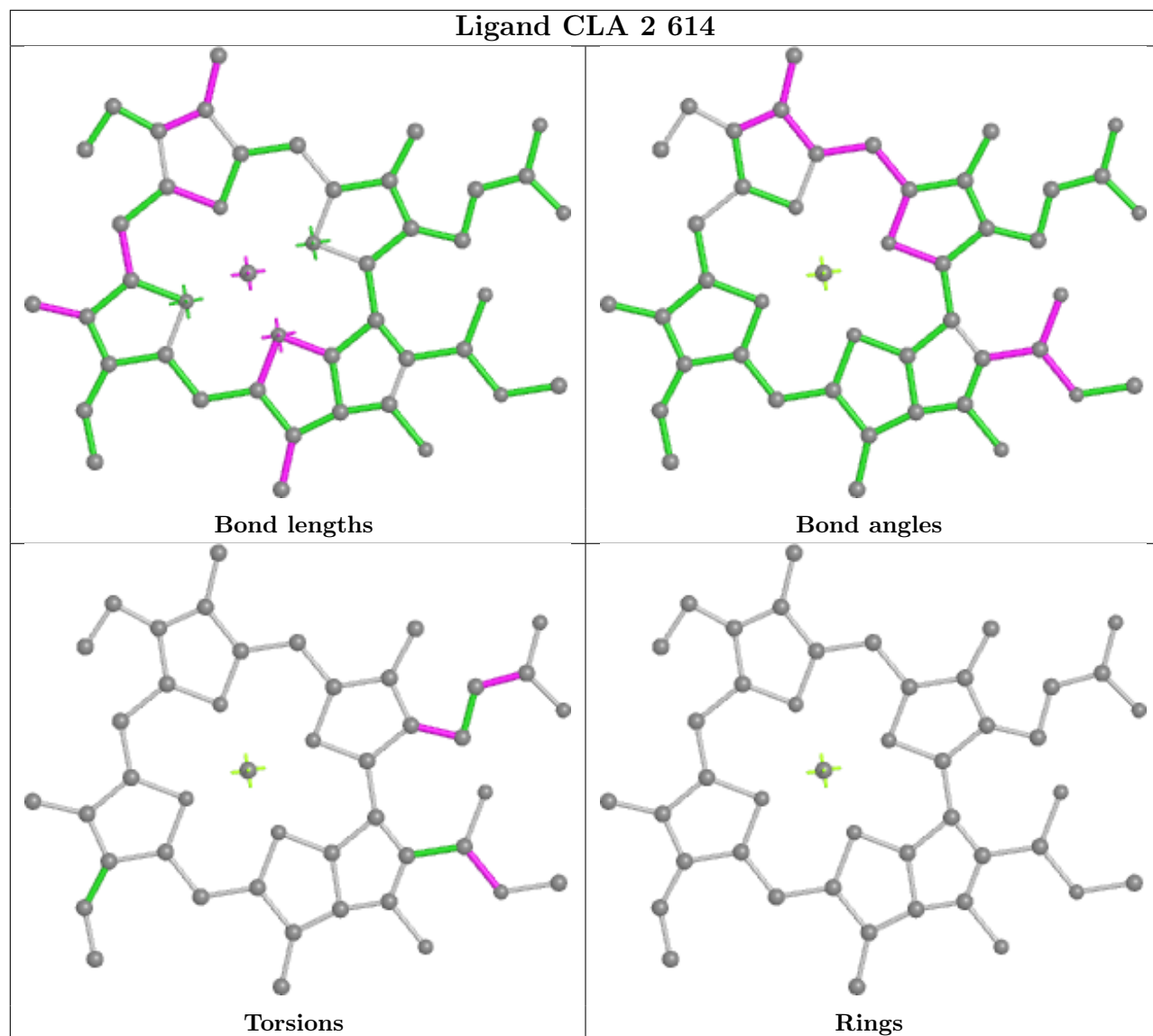


## Ligand CLA R 610

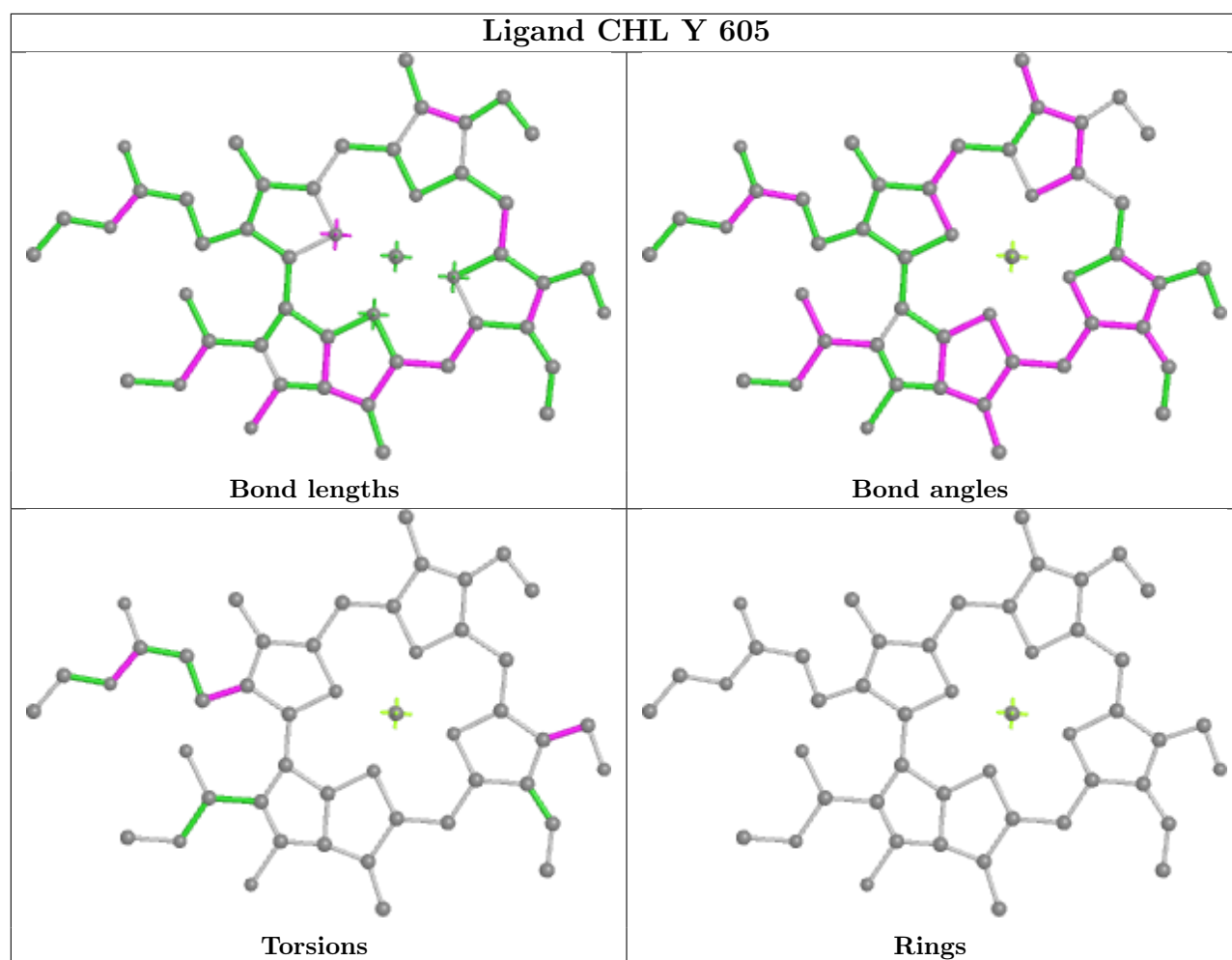


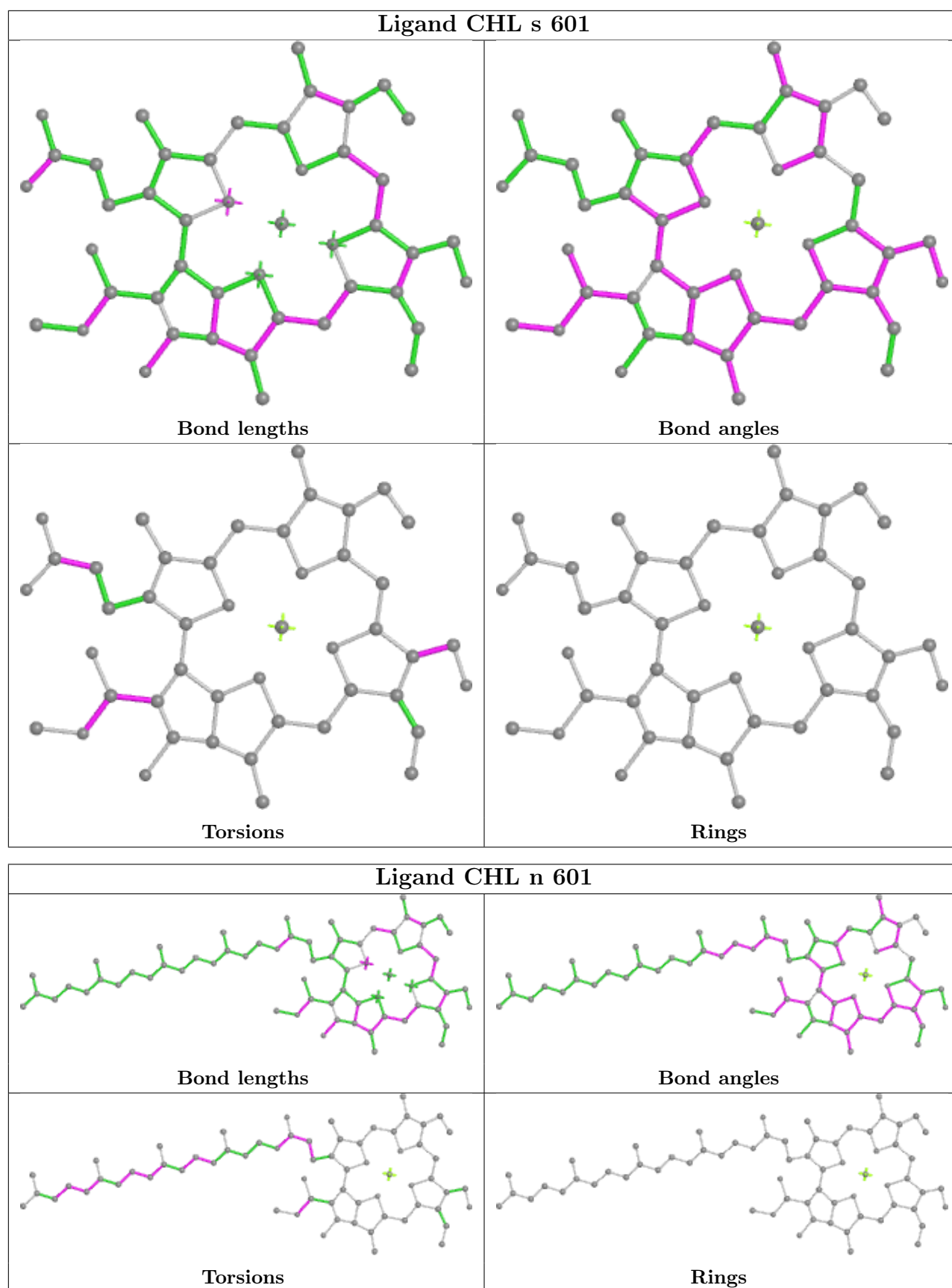


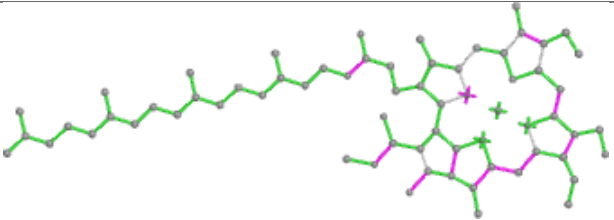
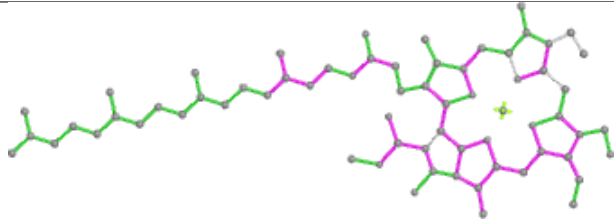
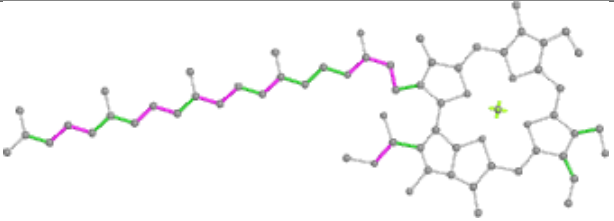
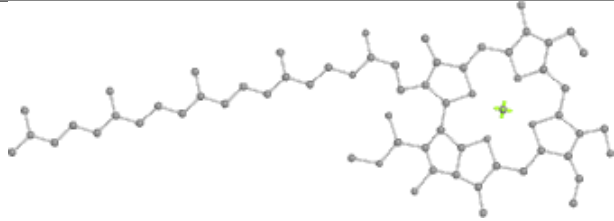
## Ligand CLA 2 614

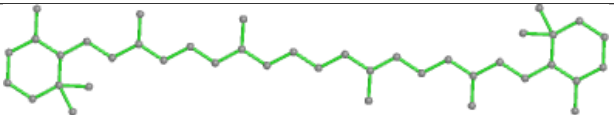
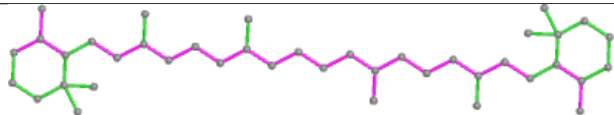
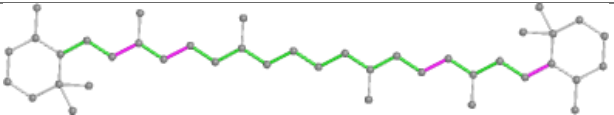
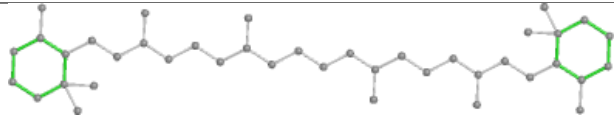


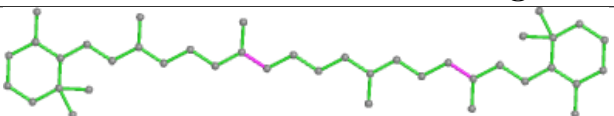
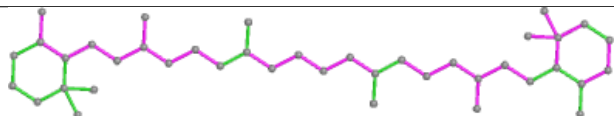
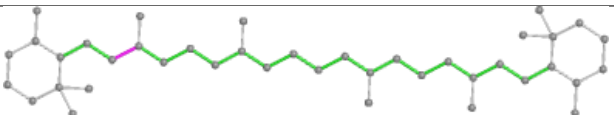
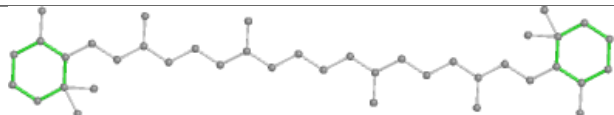




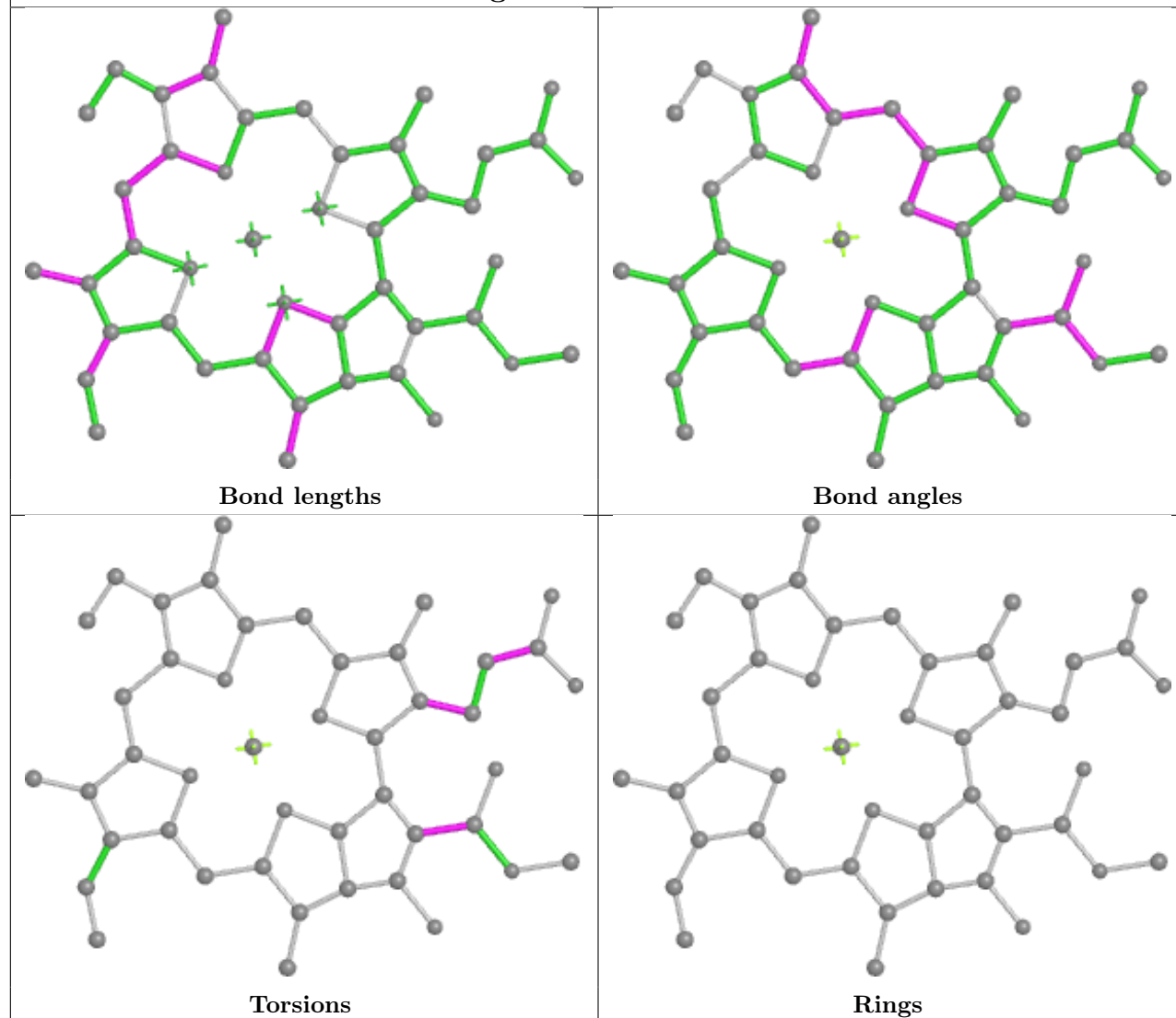


Ligand CHL y 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

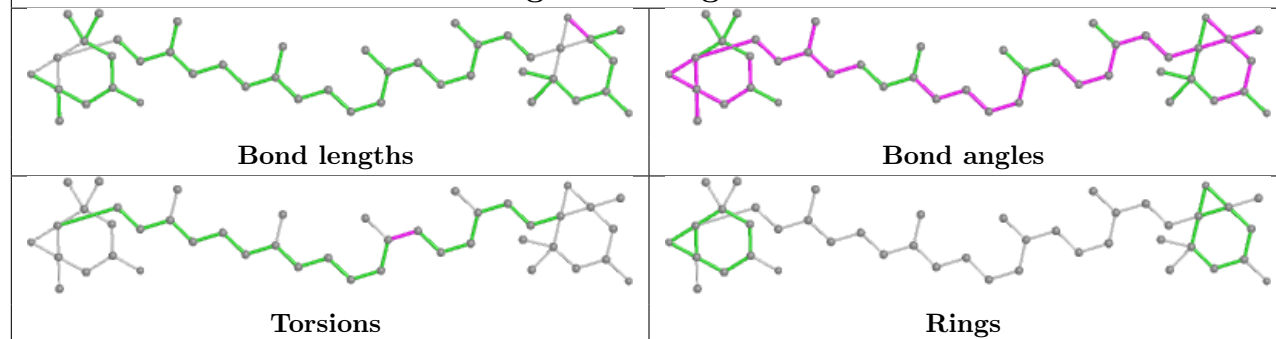
Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

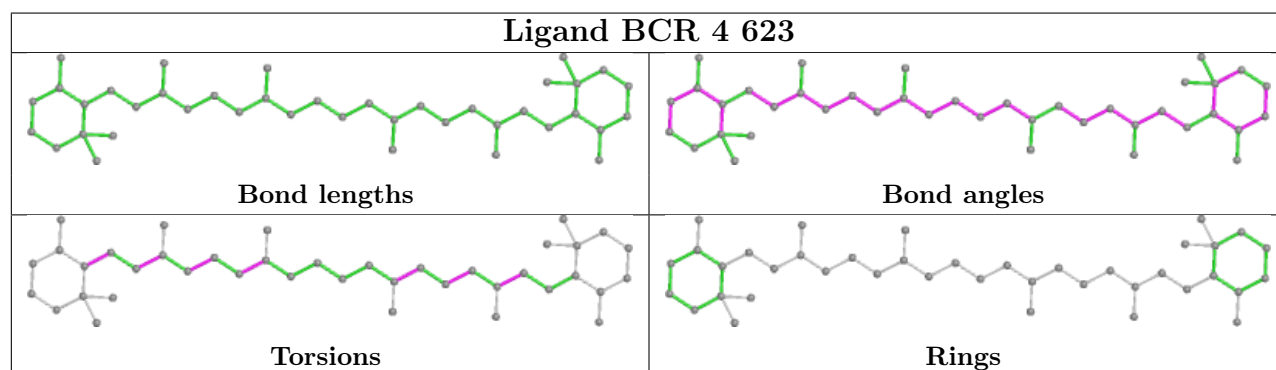
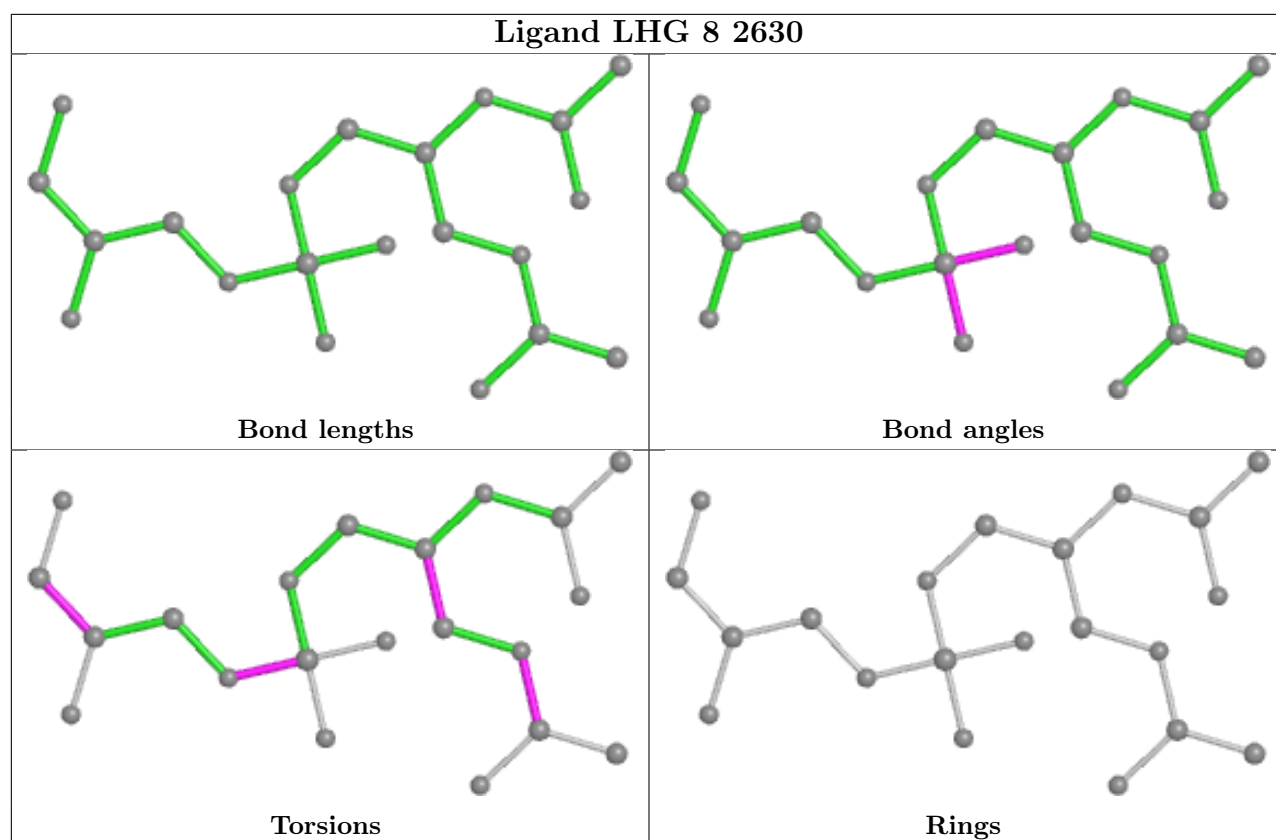
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

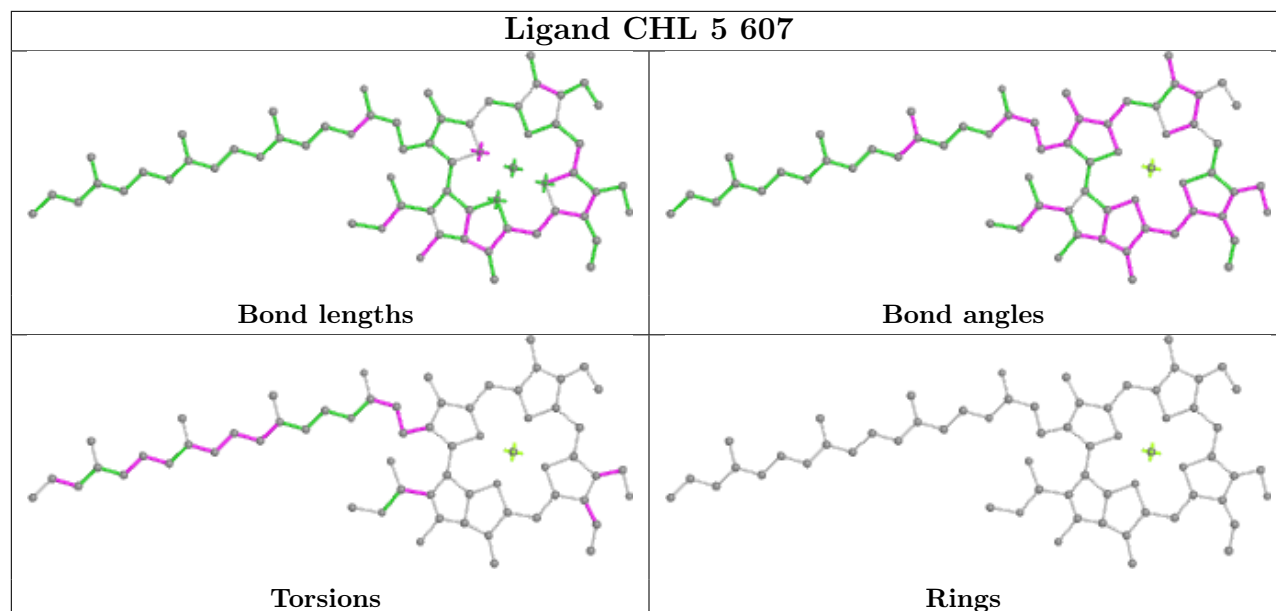
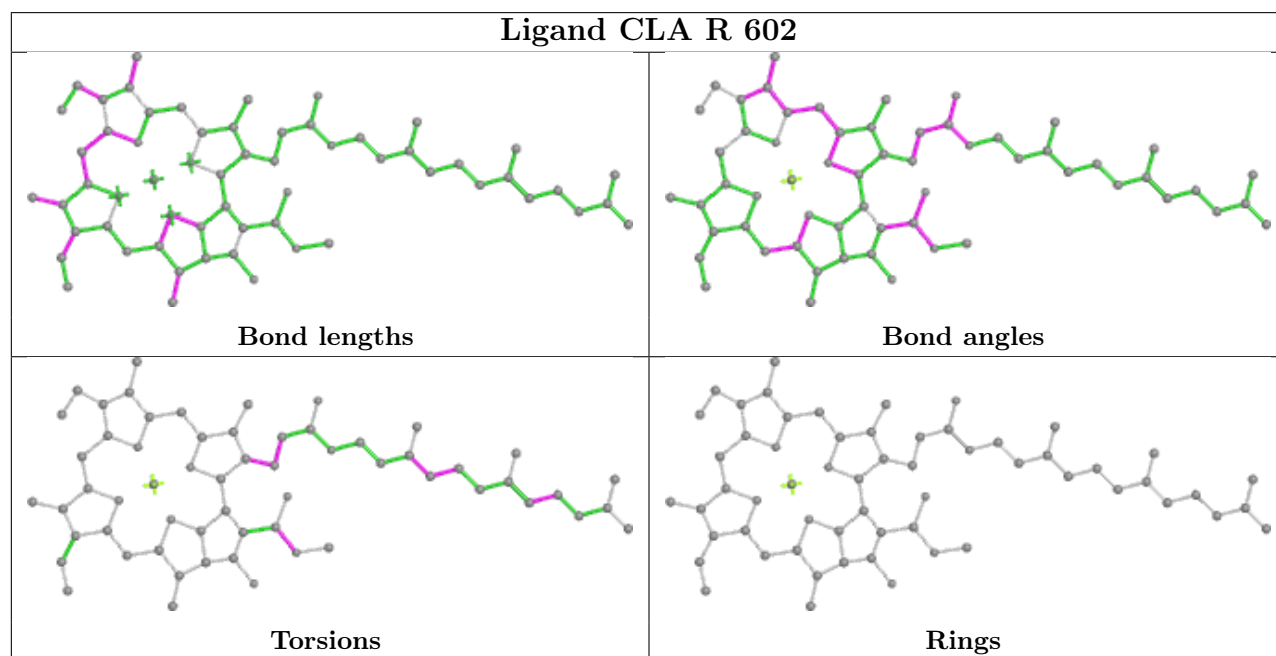
## Ligand CLA R 616



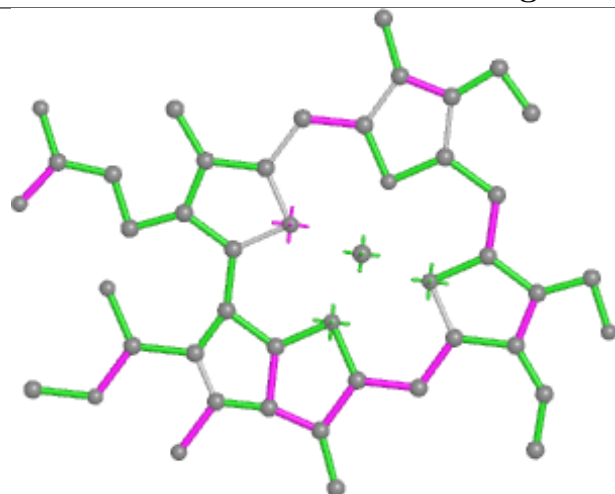
## Ligand XAT g 1622



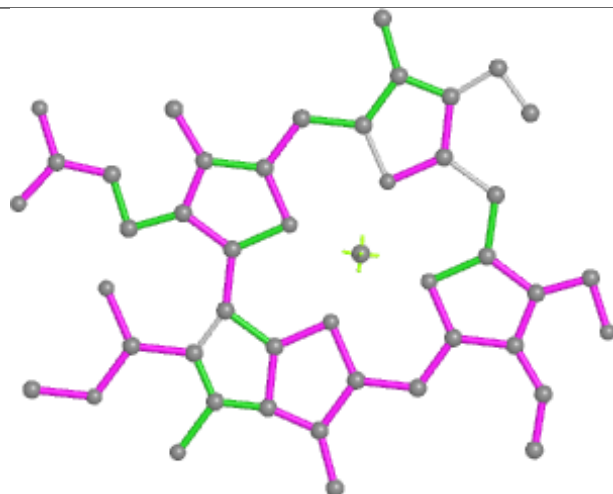


**Ligand CHL 5 607****Ligand CLA R 602**

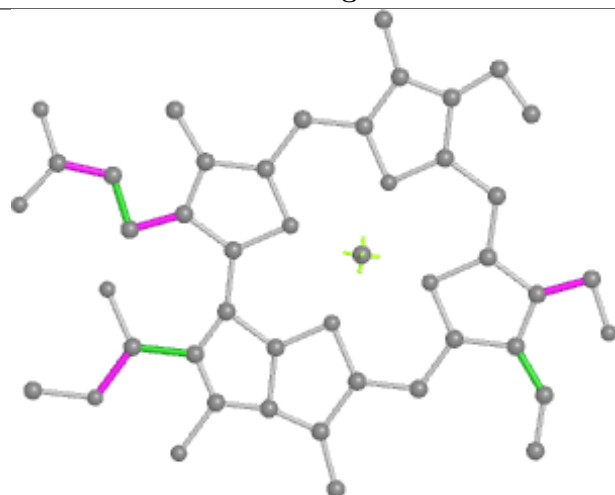
## Ligand CHL 4 608



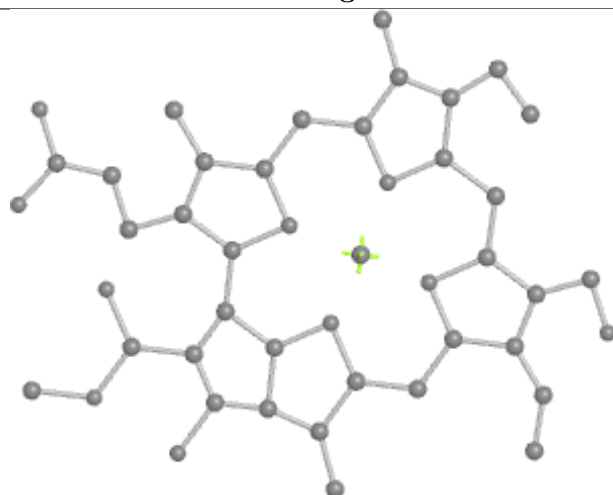
Bond lengths



Bond angles

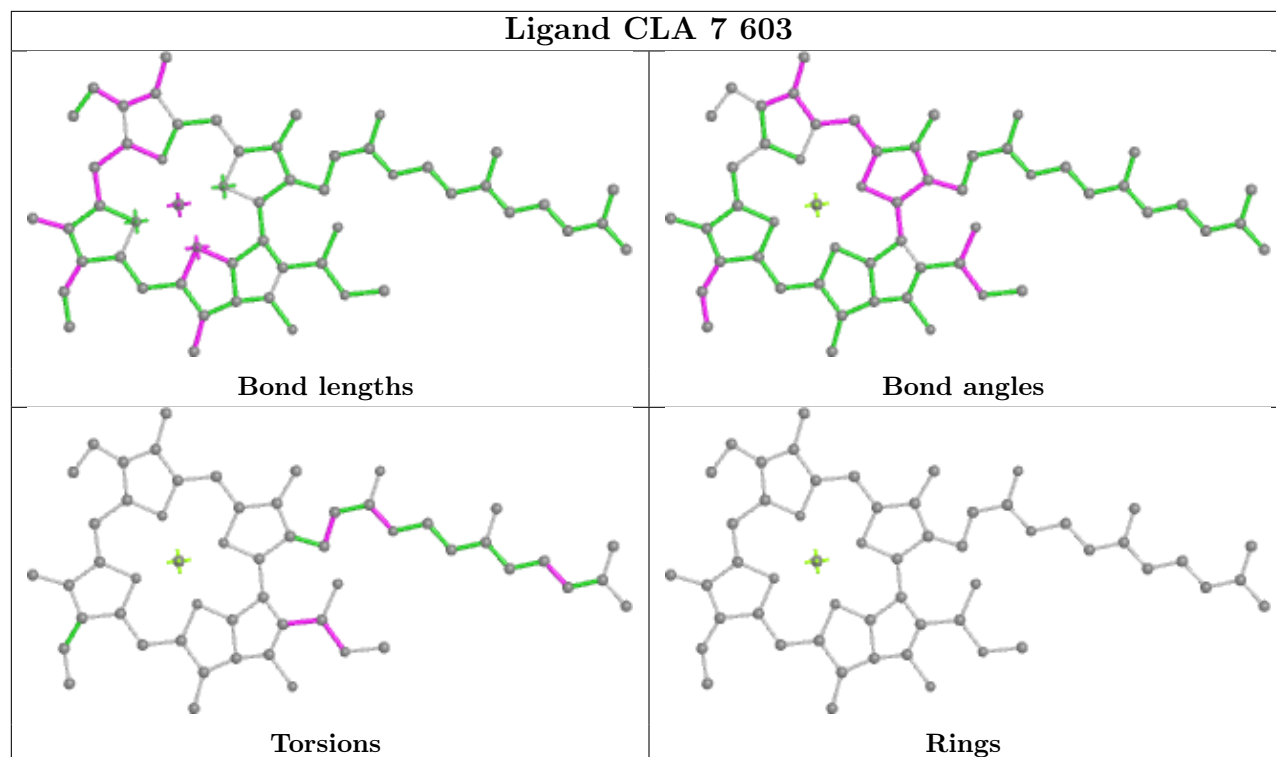


Torsions

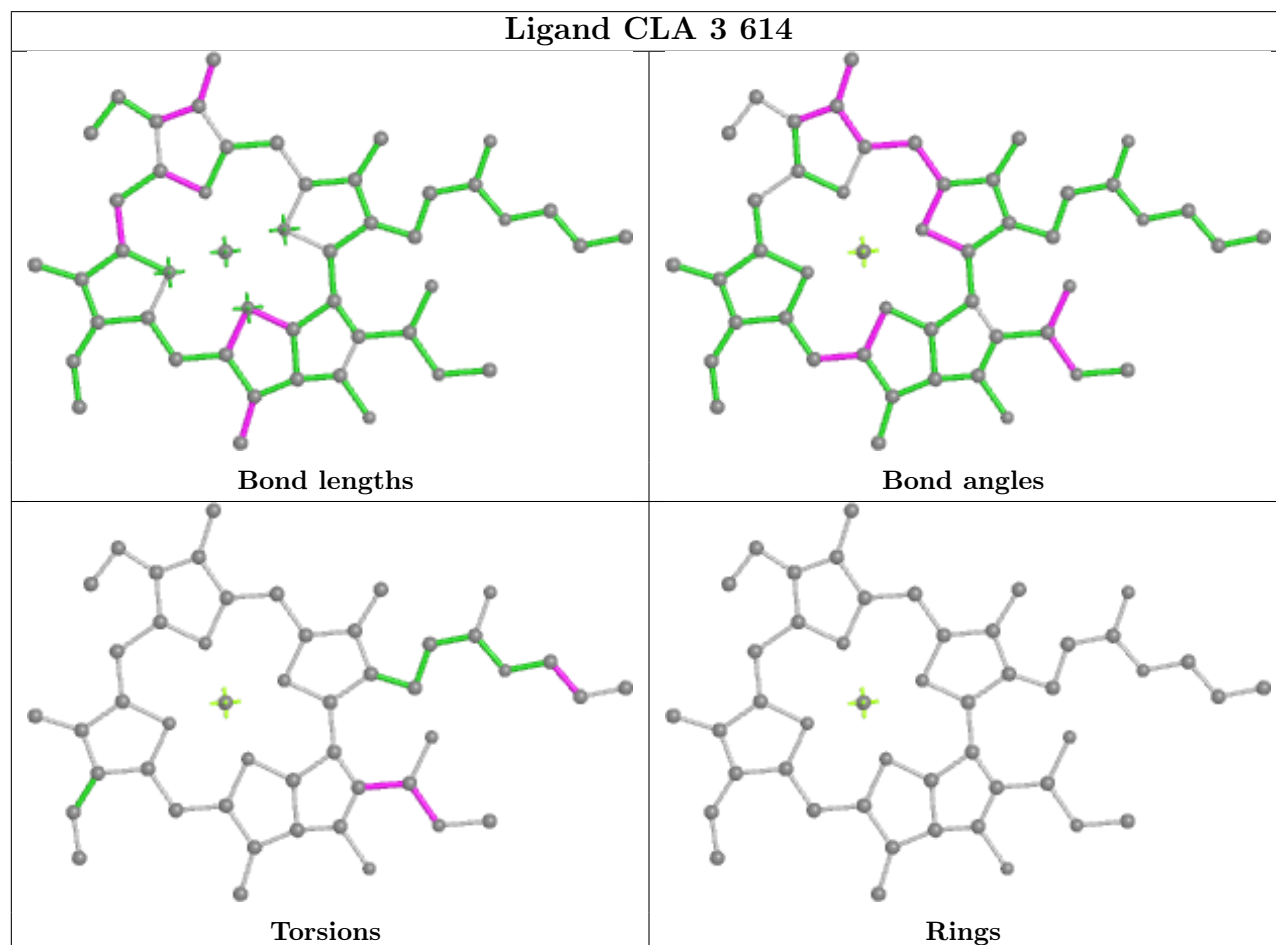


Rings

## Ligand CLA 7 603

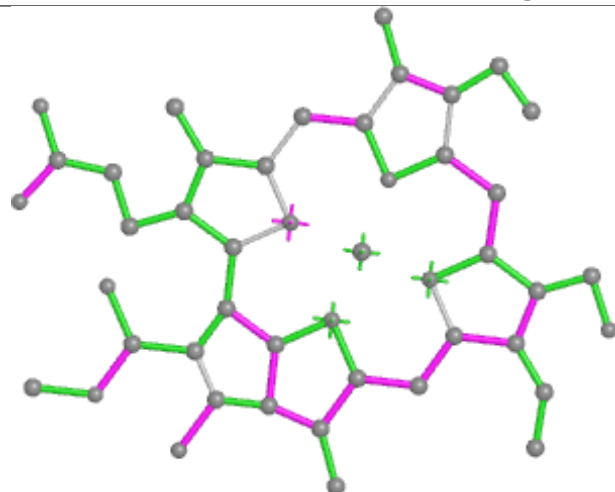


## Ligand CLA 3 614

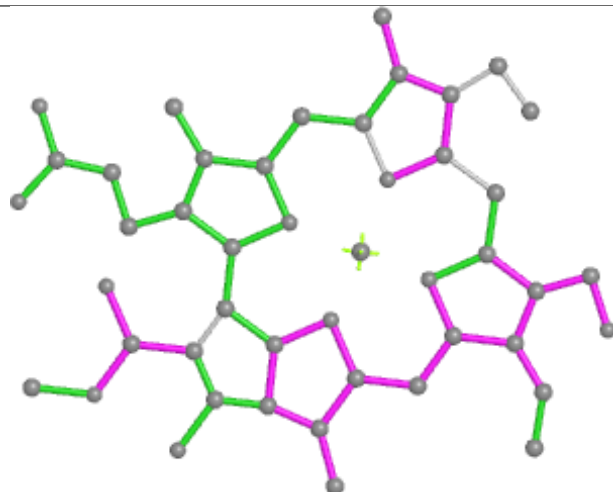




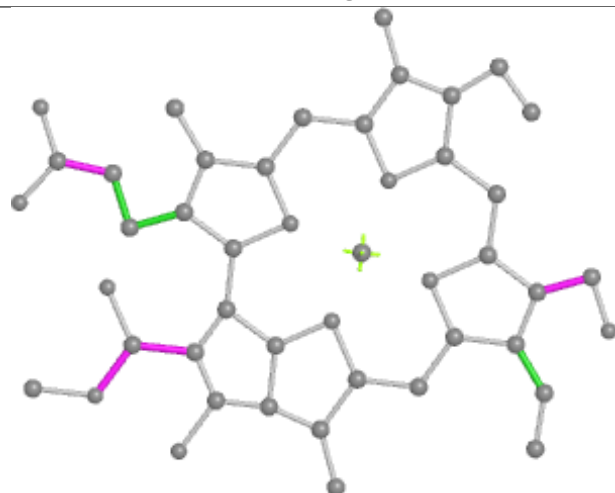
## Ligand CHL S 606



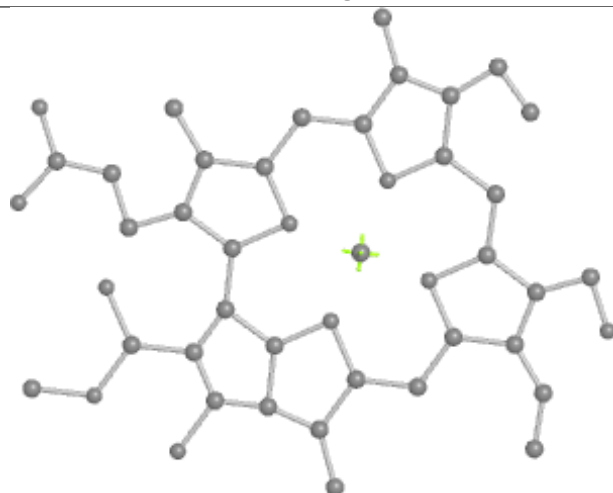
Bond lengths



Bond angles

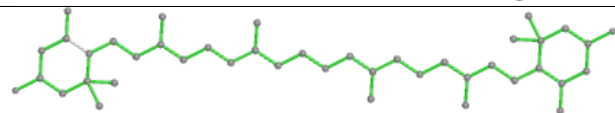


Torsions

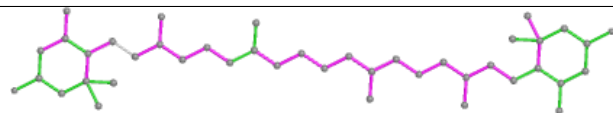


Rings

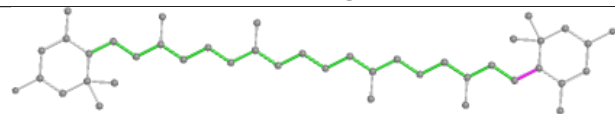
## Ligand LUT S 1620



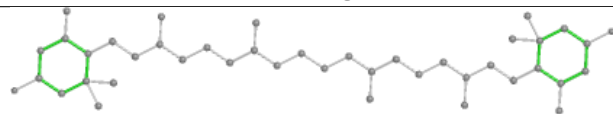
Bond lengths



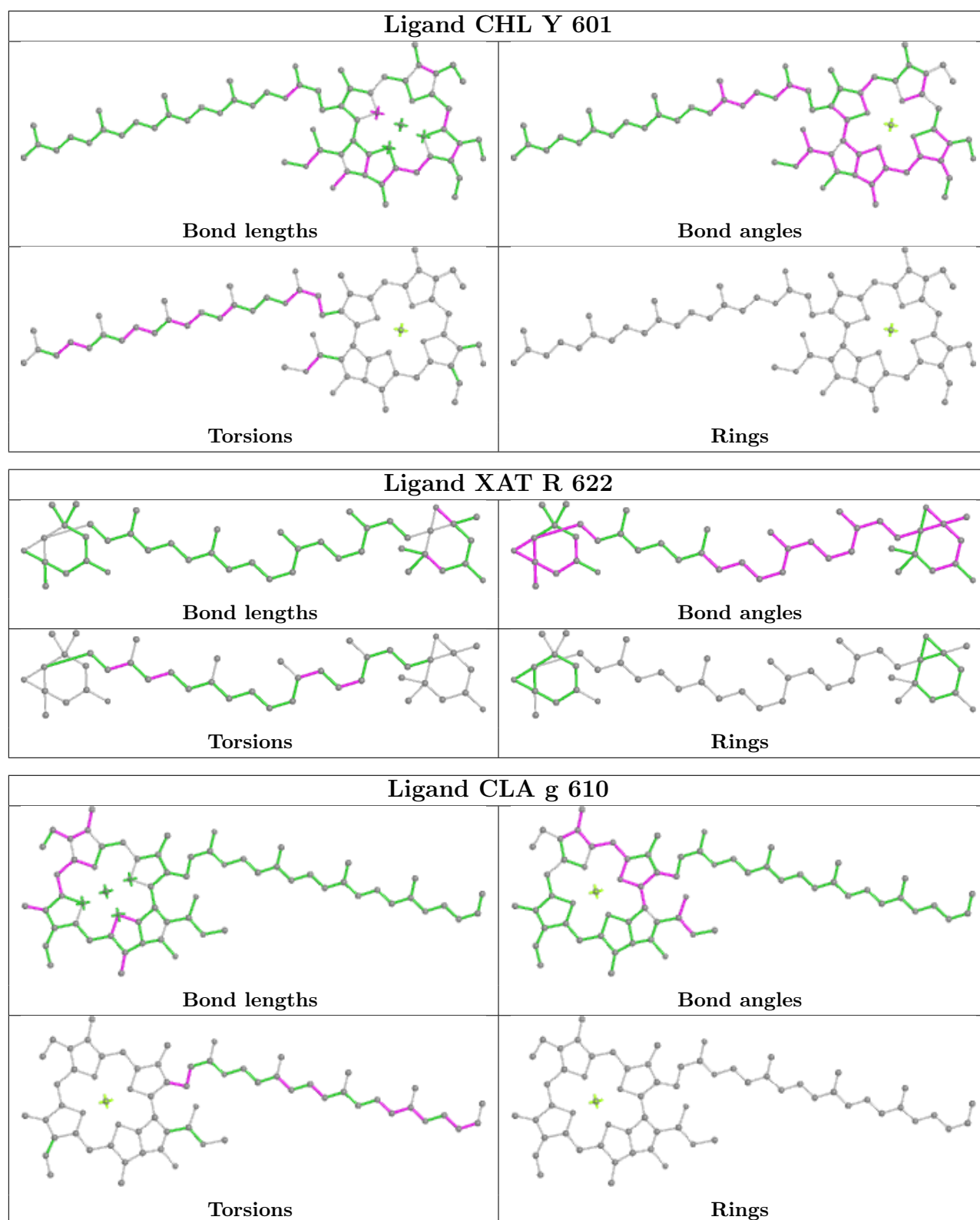
Bond angles

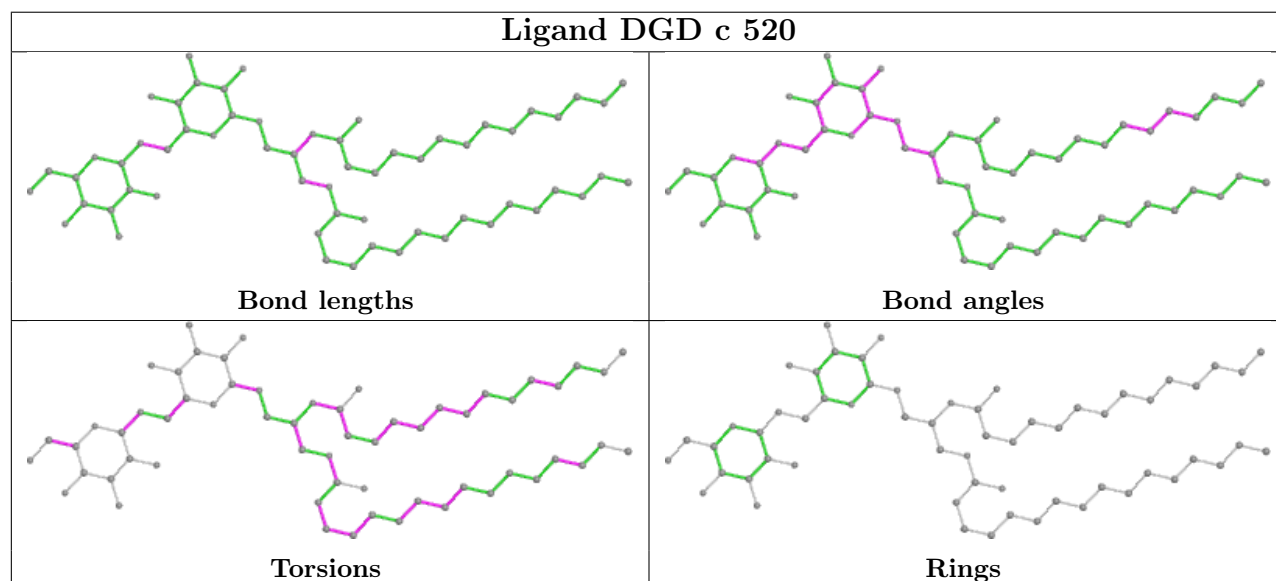
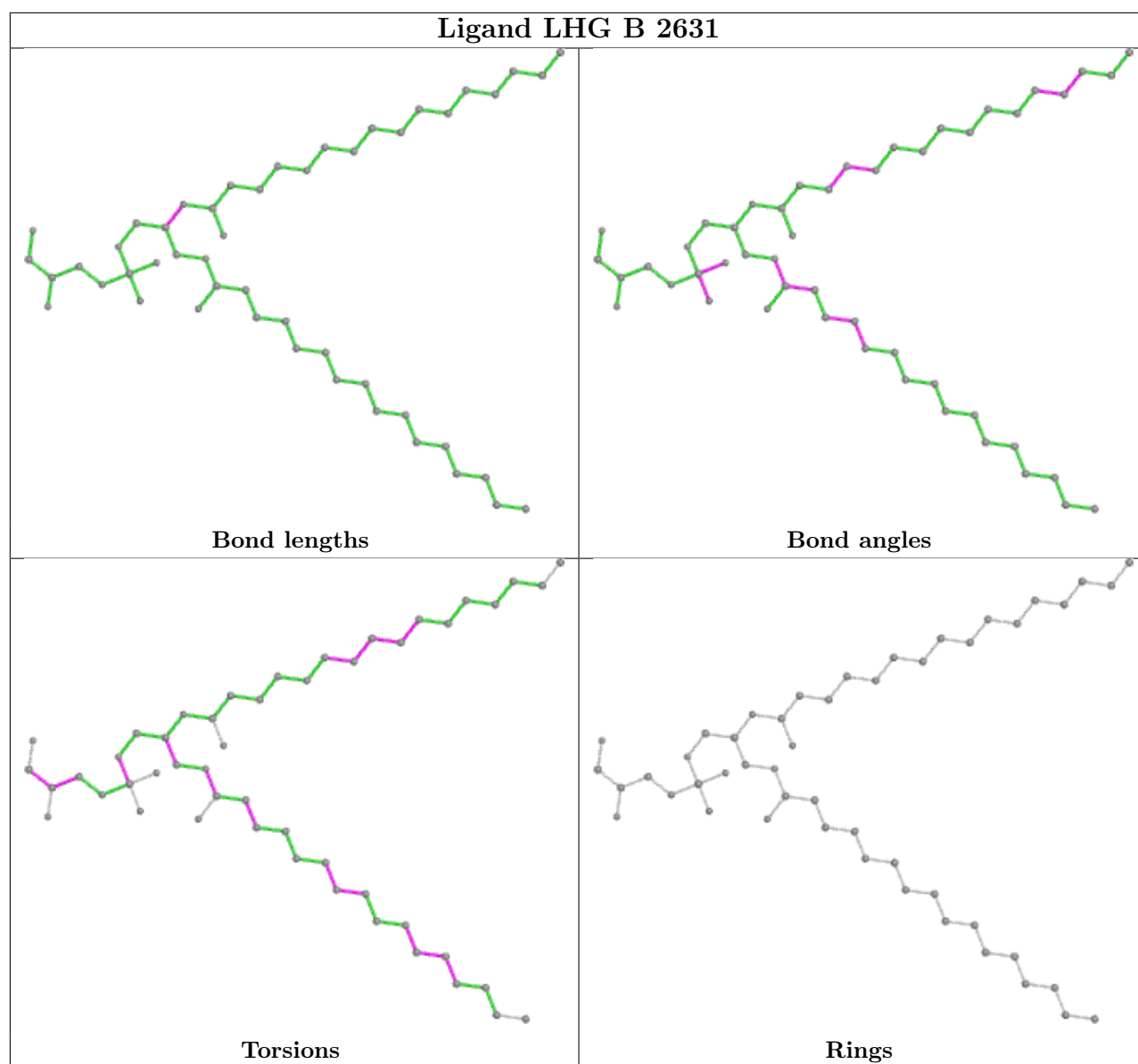


Torsions

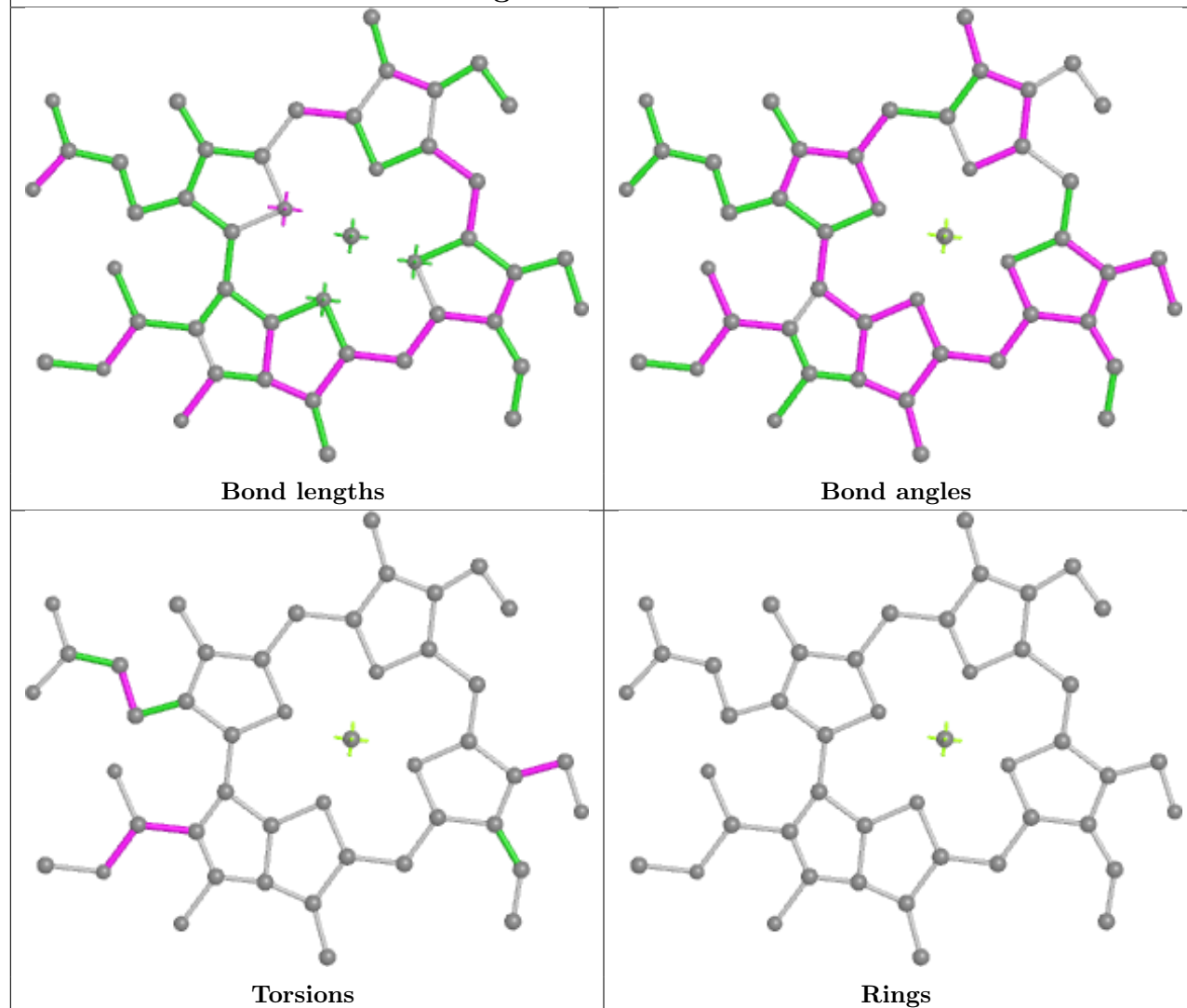


Rings

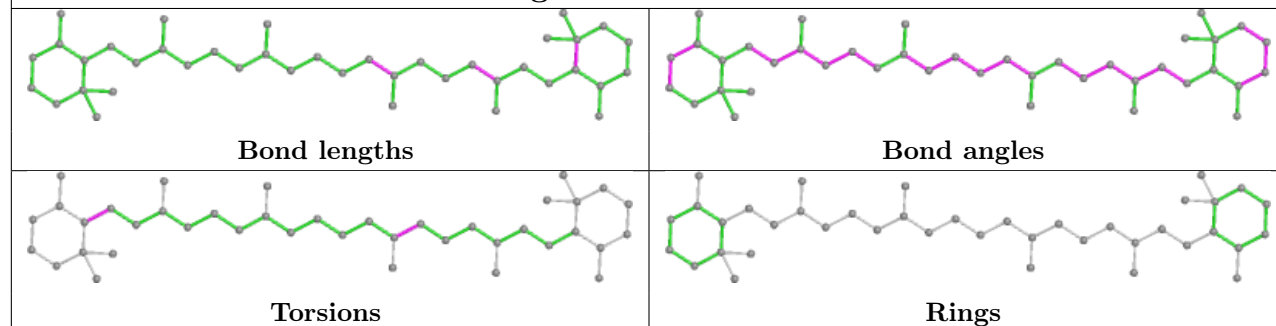


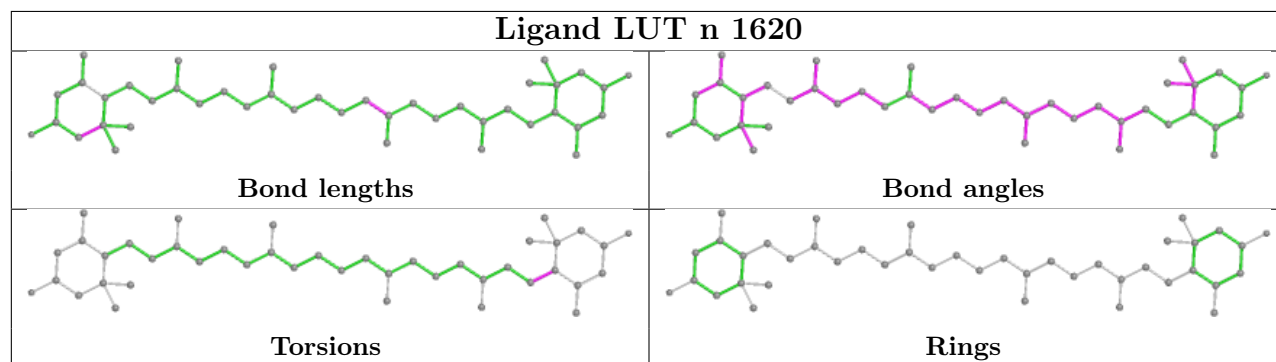
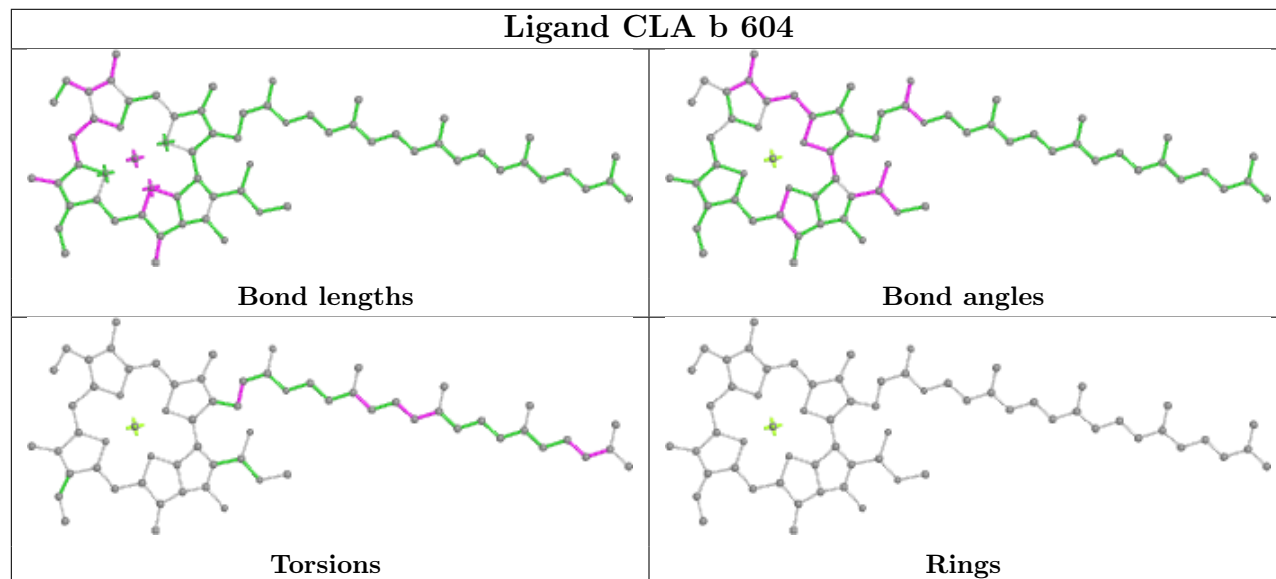
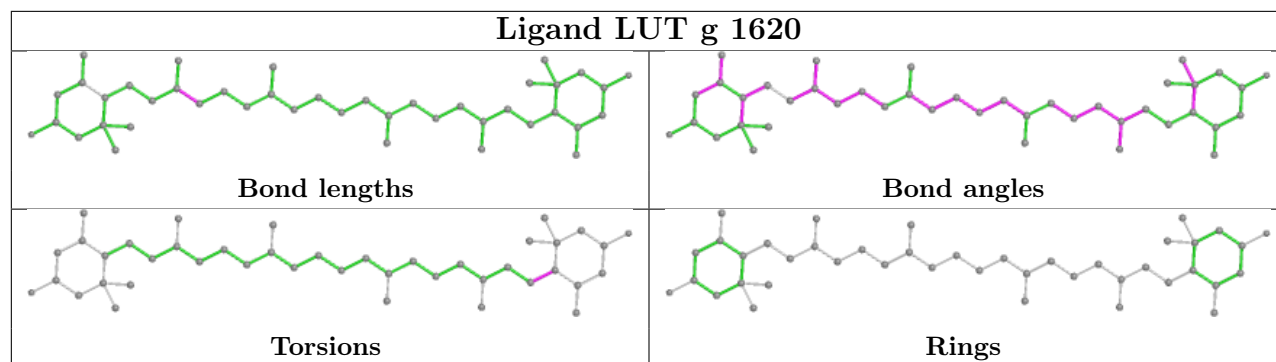


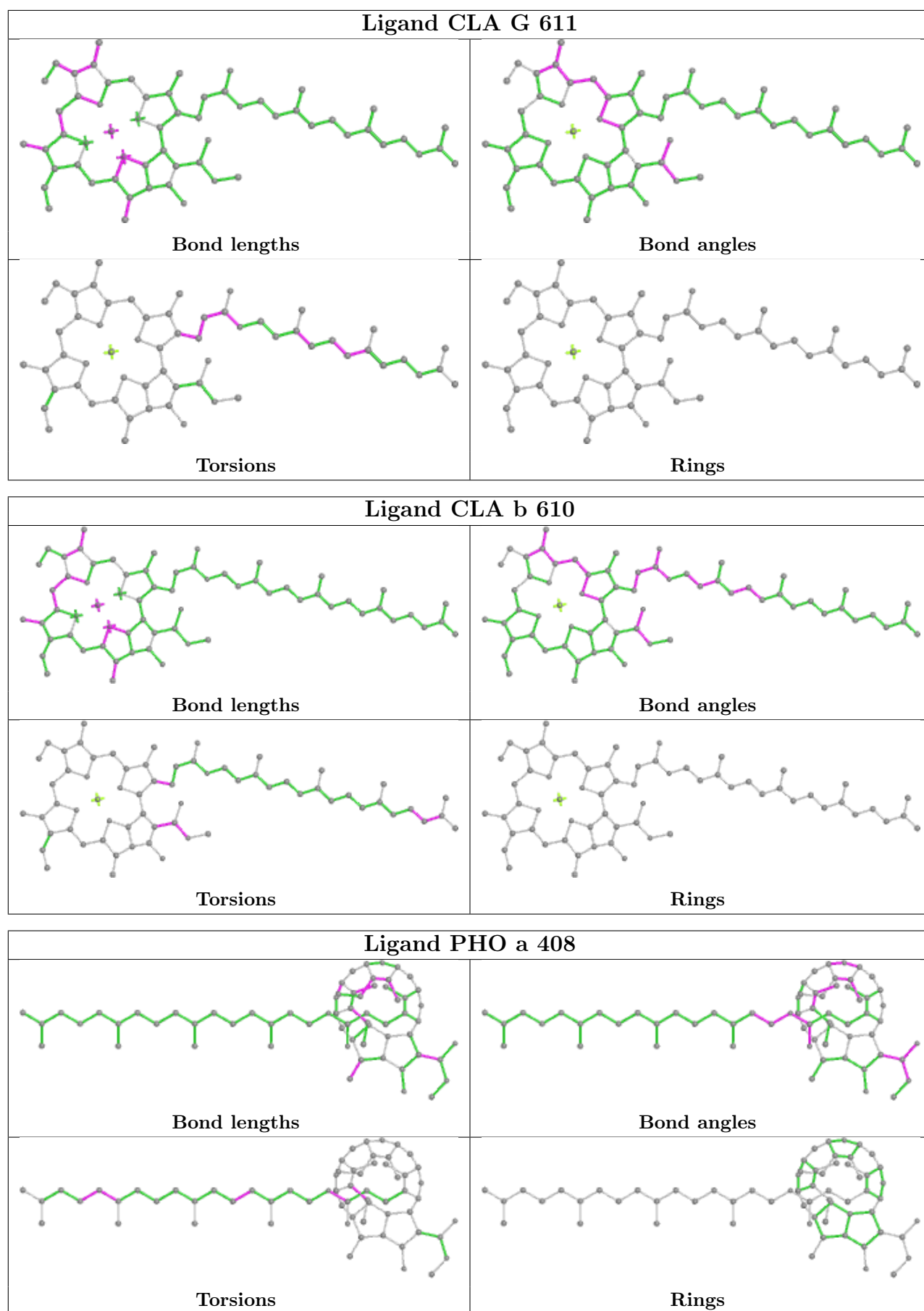
## Ligand CHL G 605



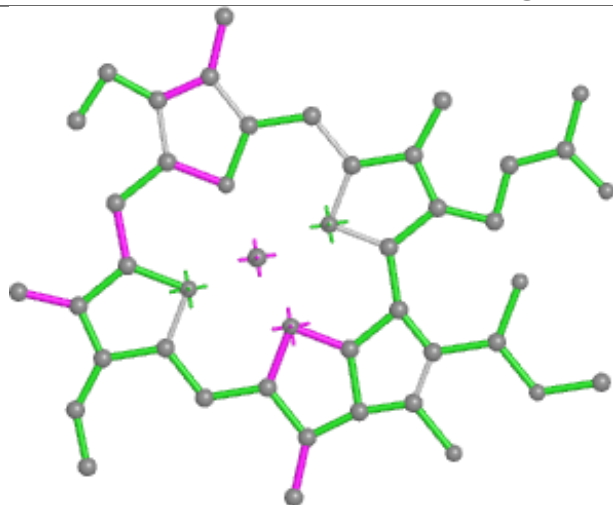
## Ligand BCR B 618



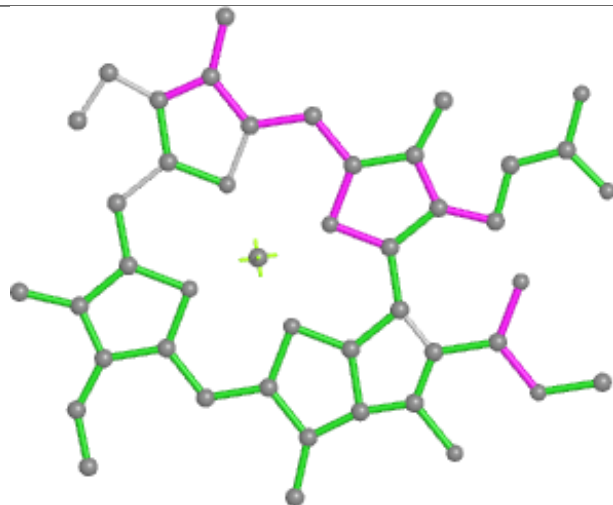




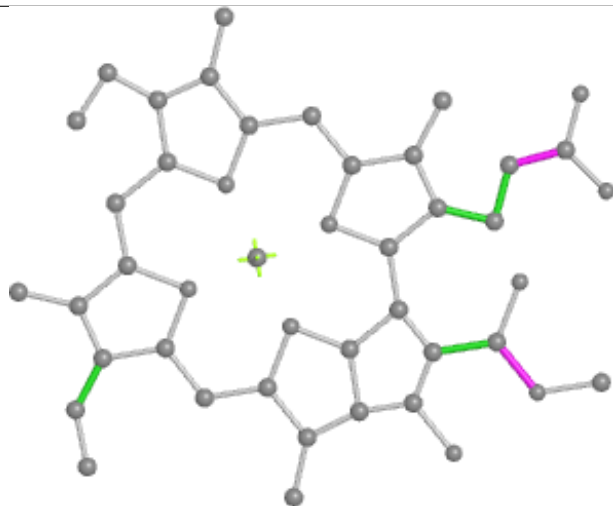
## Ligand CLA 8 603



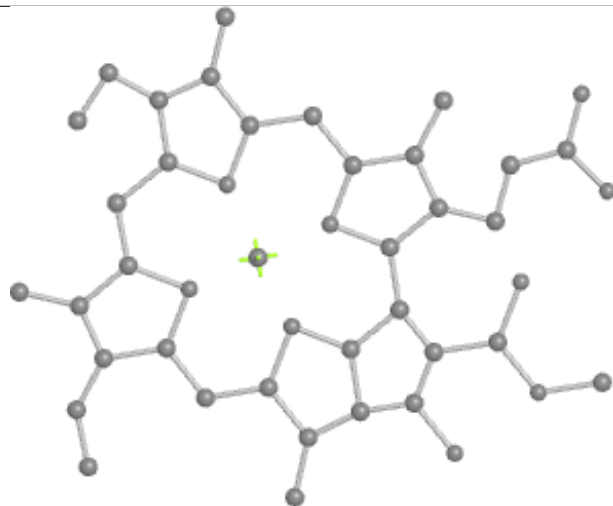
Bond lengths



Bond angles

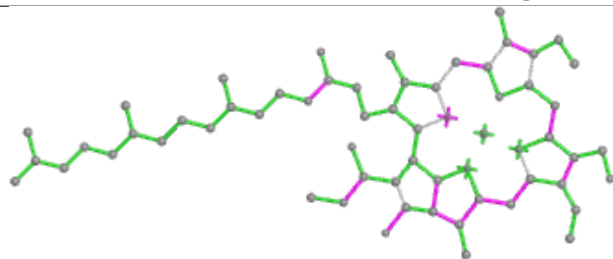


Torsions

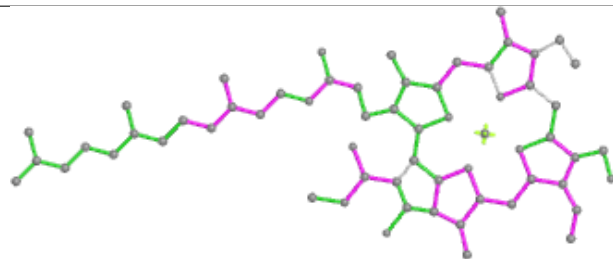


Rings

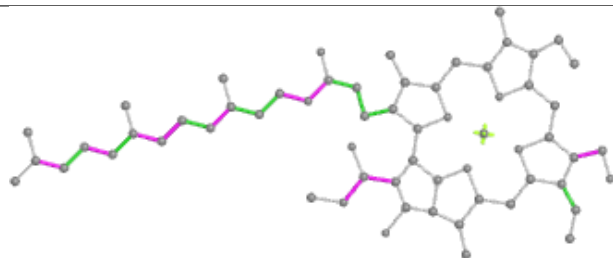
## Ligand CHL 2 609



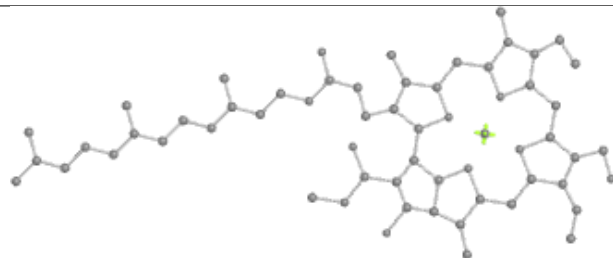
Bond lengths



Bond angles

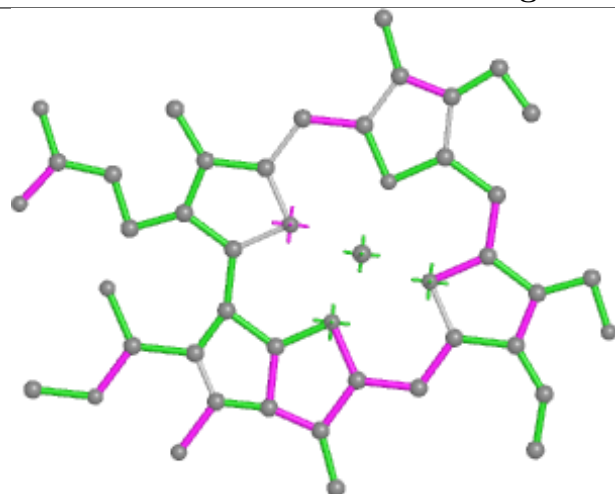


Torsions

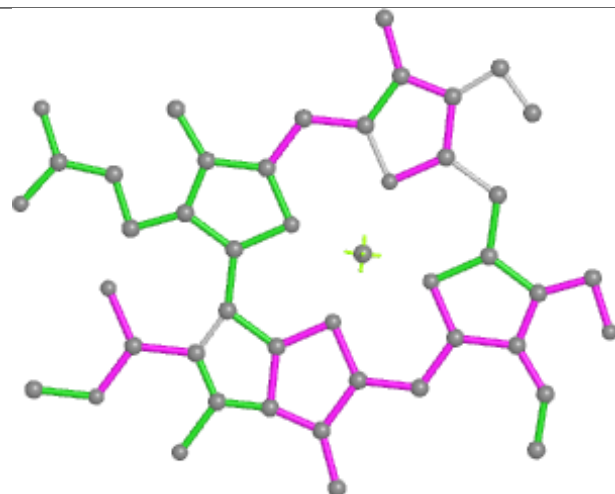


Rings

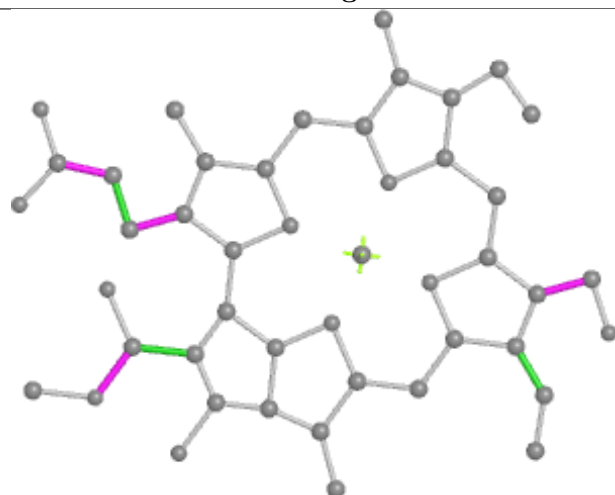
## Ligand CHL 1 605



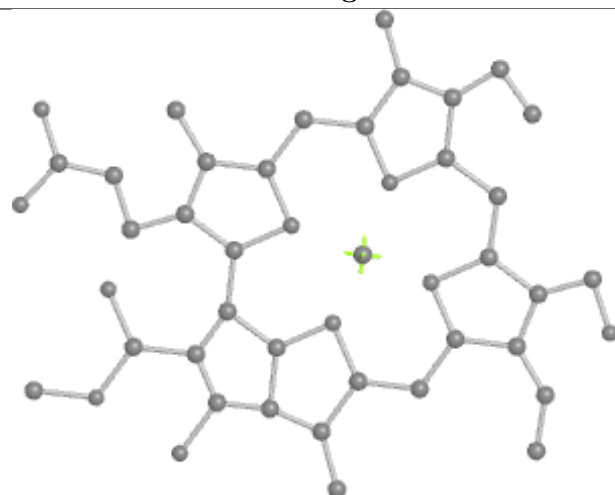
Bond lengths



Bond angles

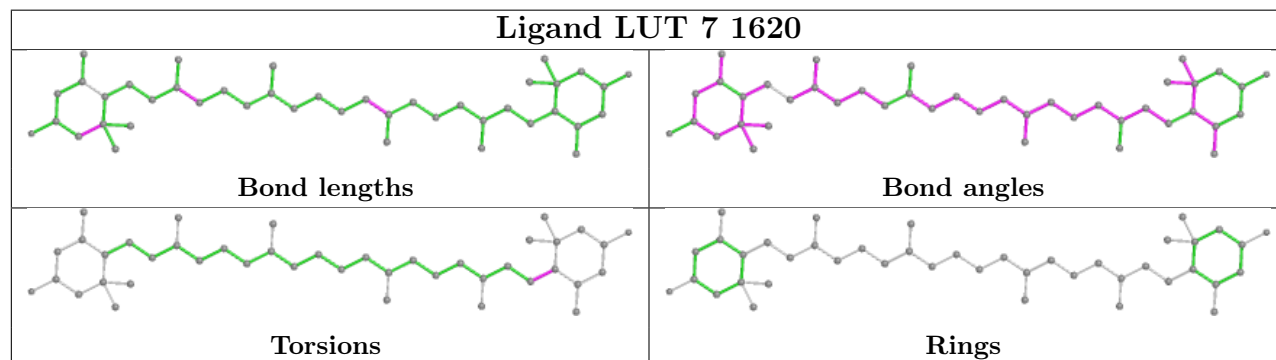
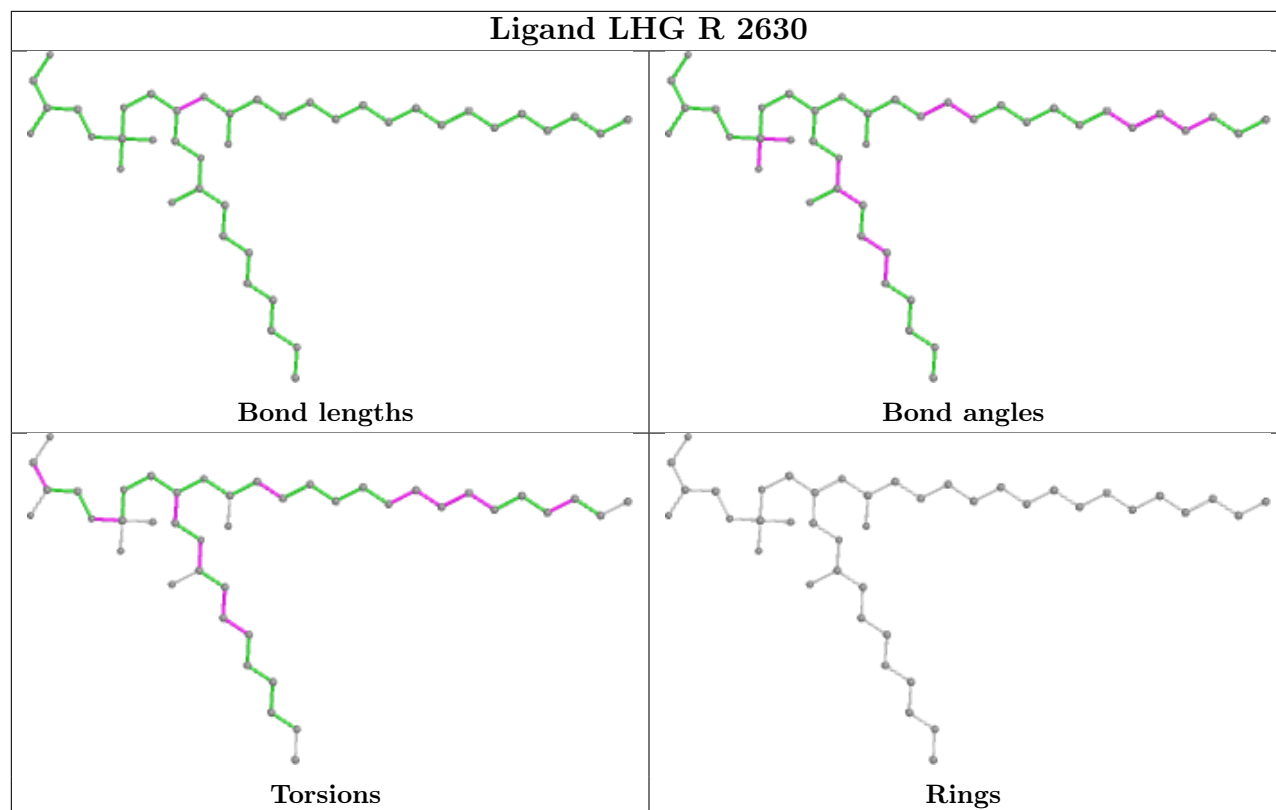


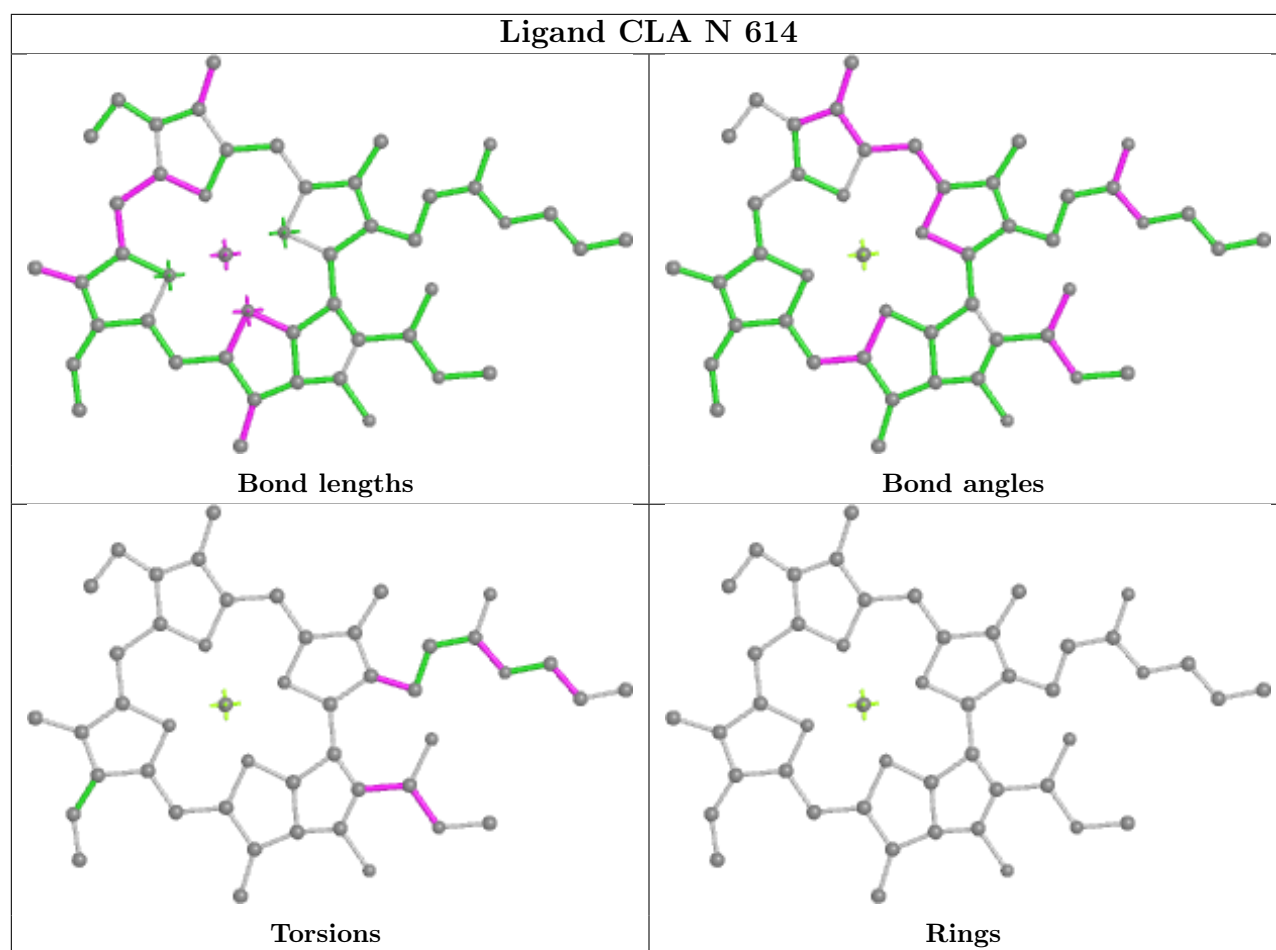
Torsions



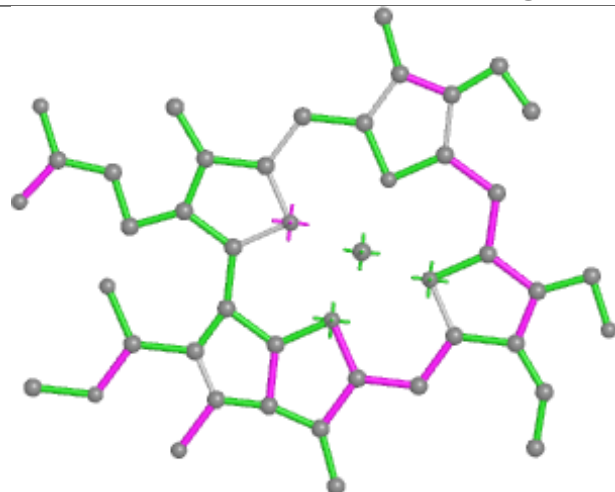
Rings



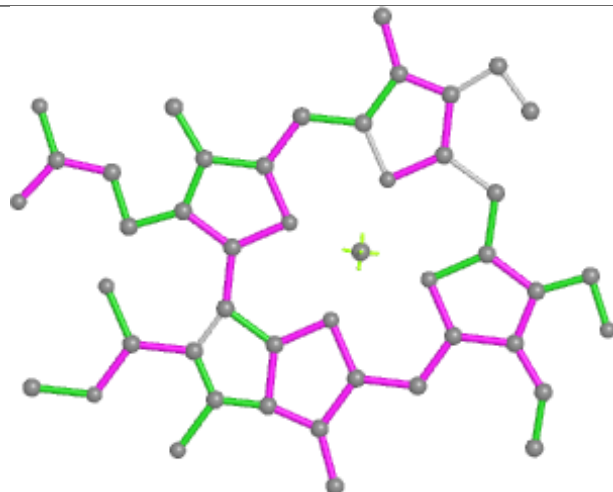




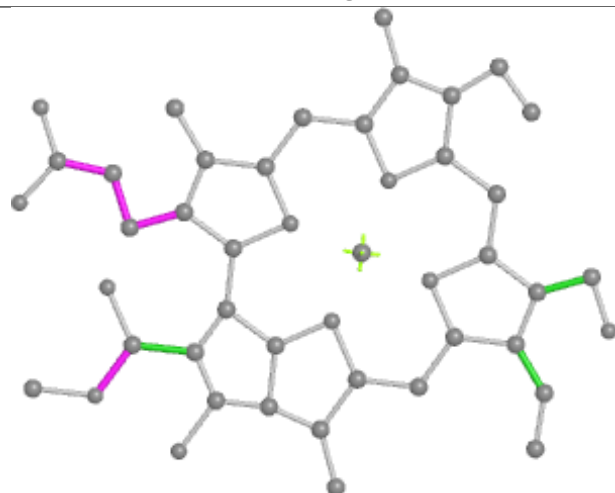
## Ligand CHL 7 608



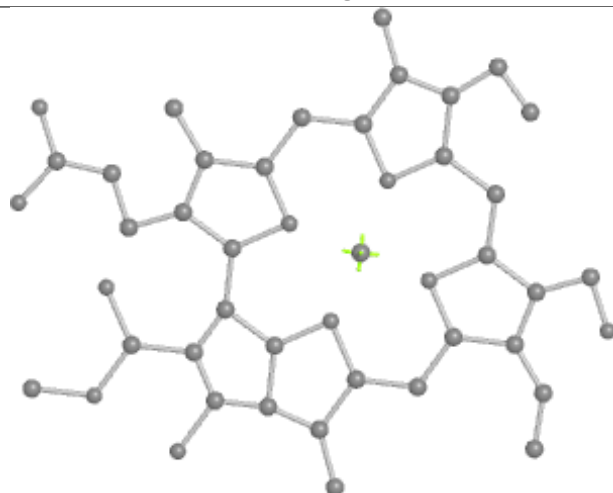
Bond lengths



Bond angles

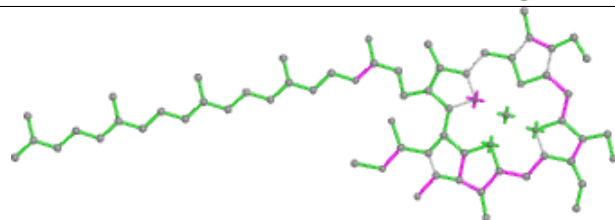


Torsions

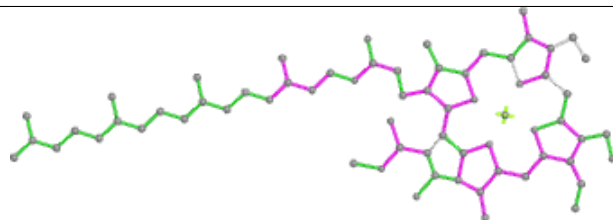


Rings

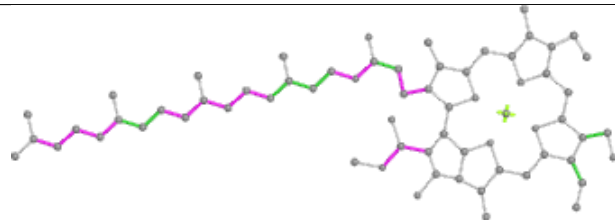
## Ligand CHL R 606



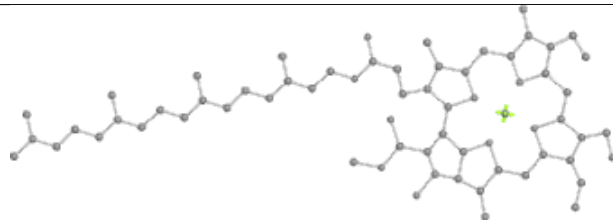
Bond lengths



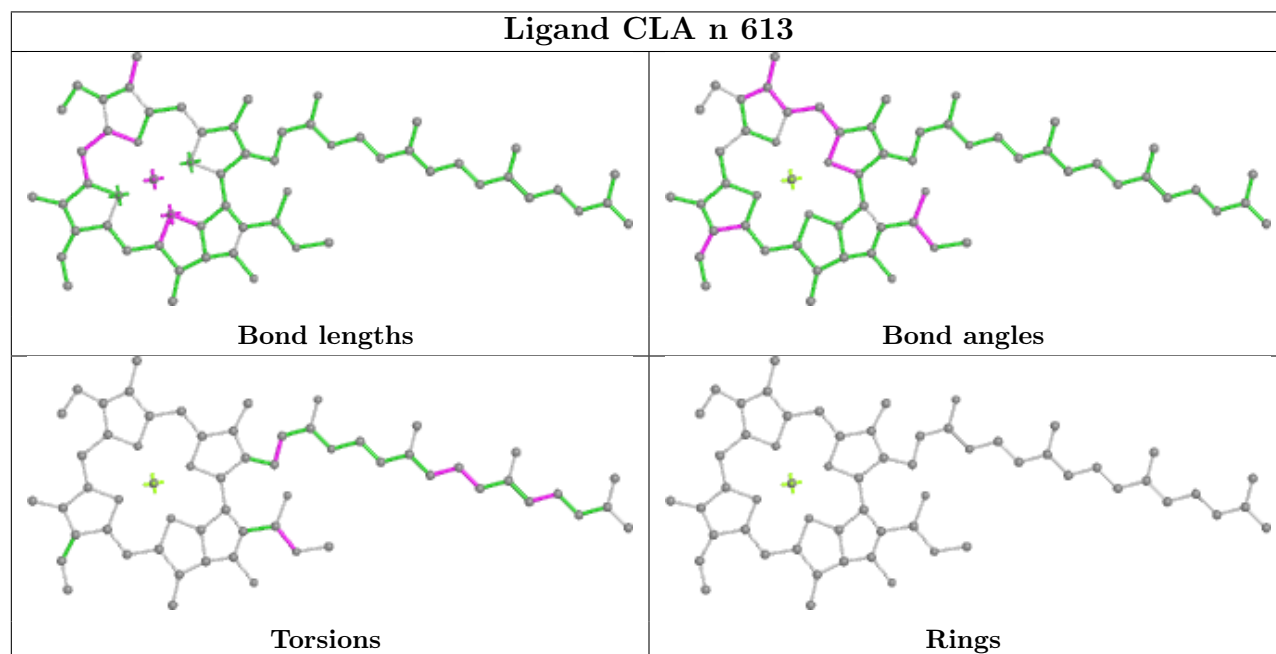
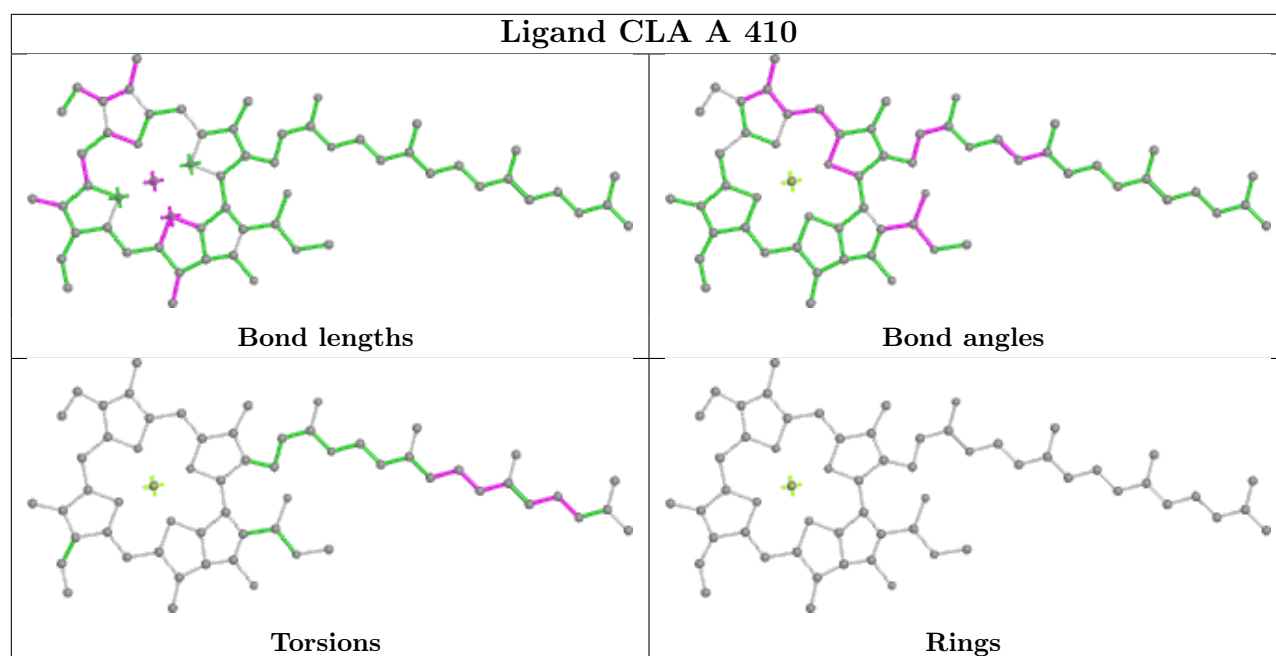
Bond angles

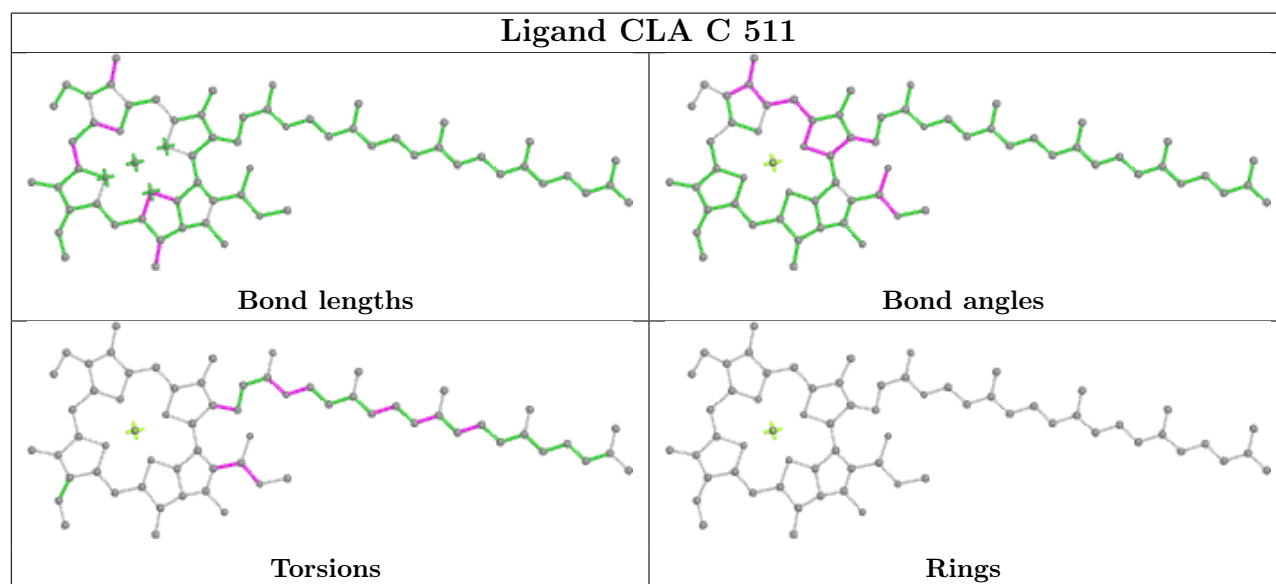
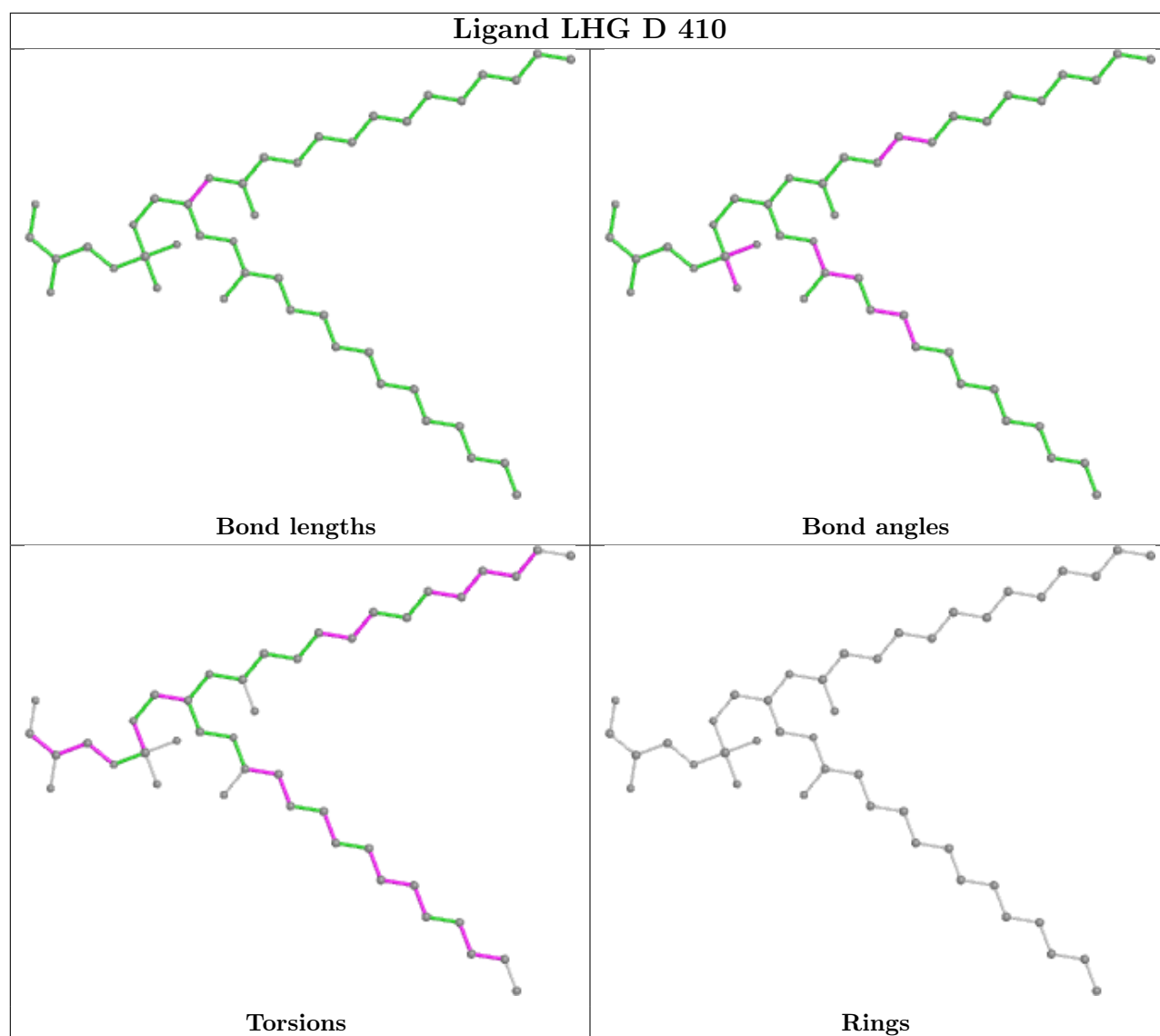


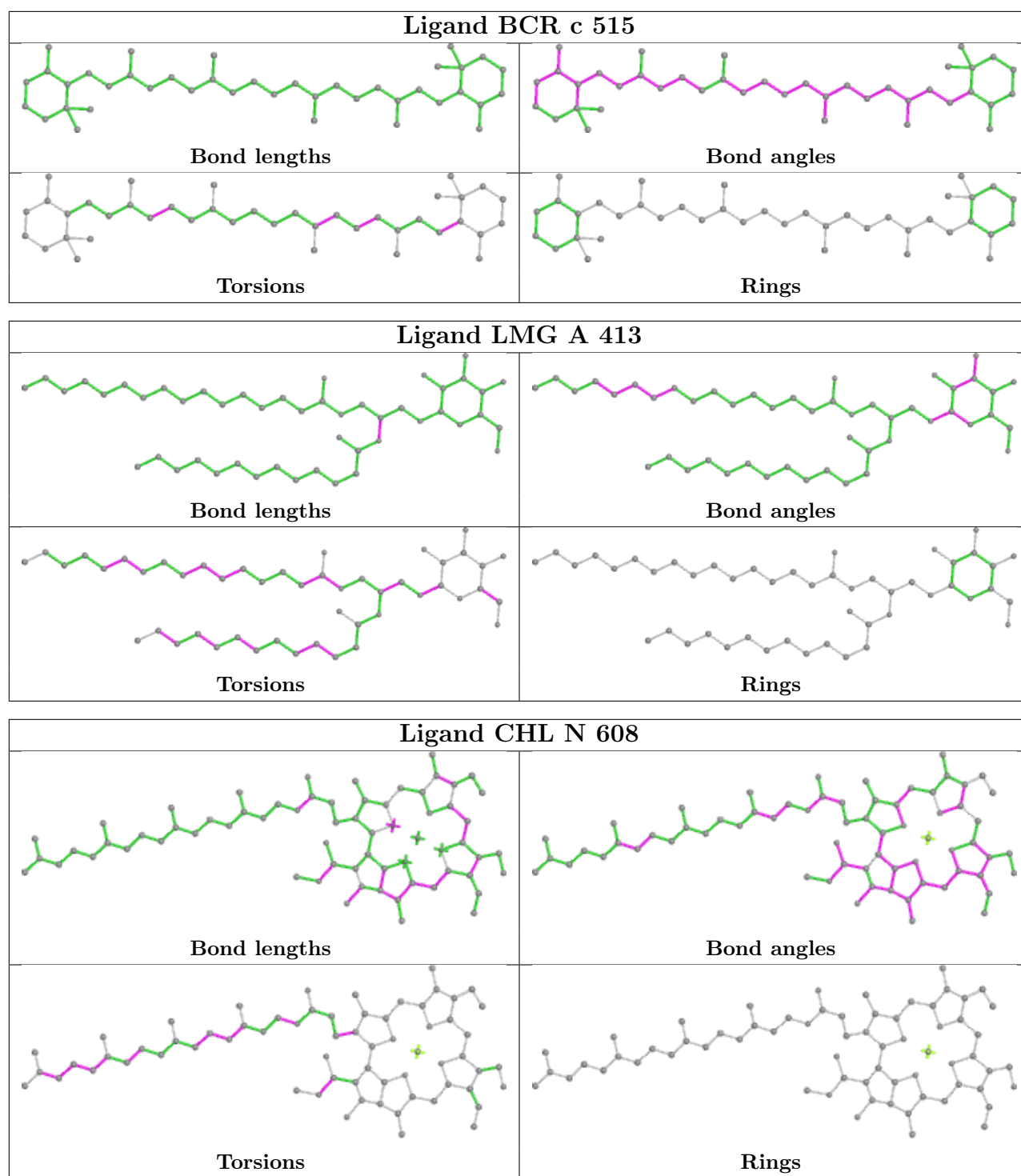
Torsions

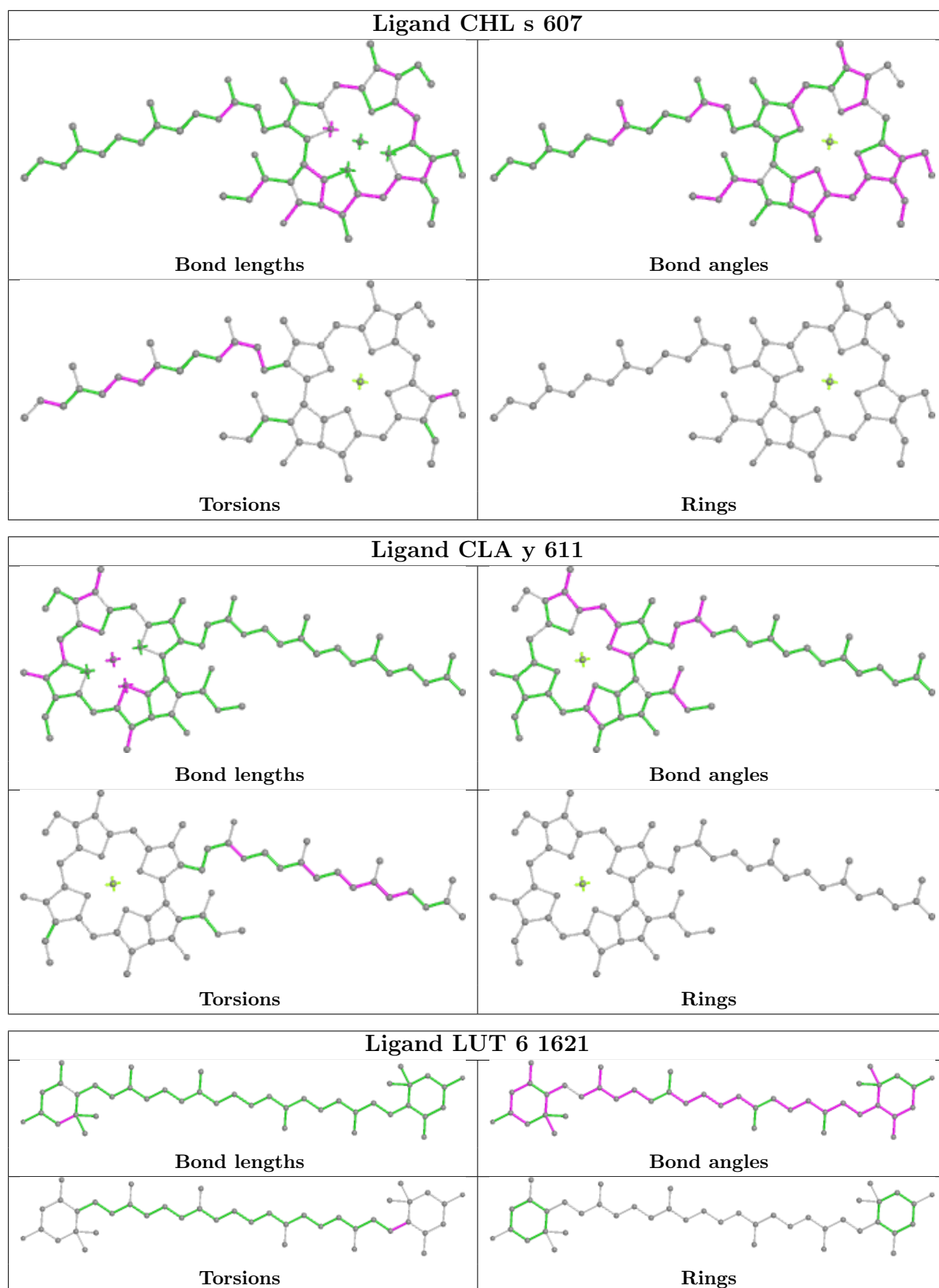


Rings

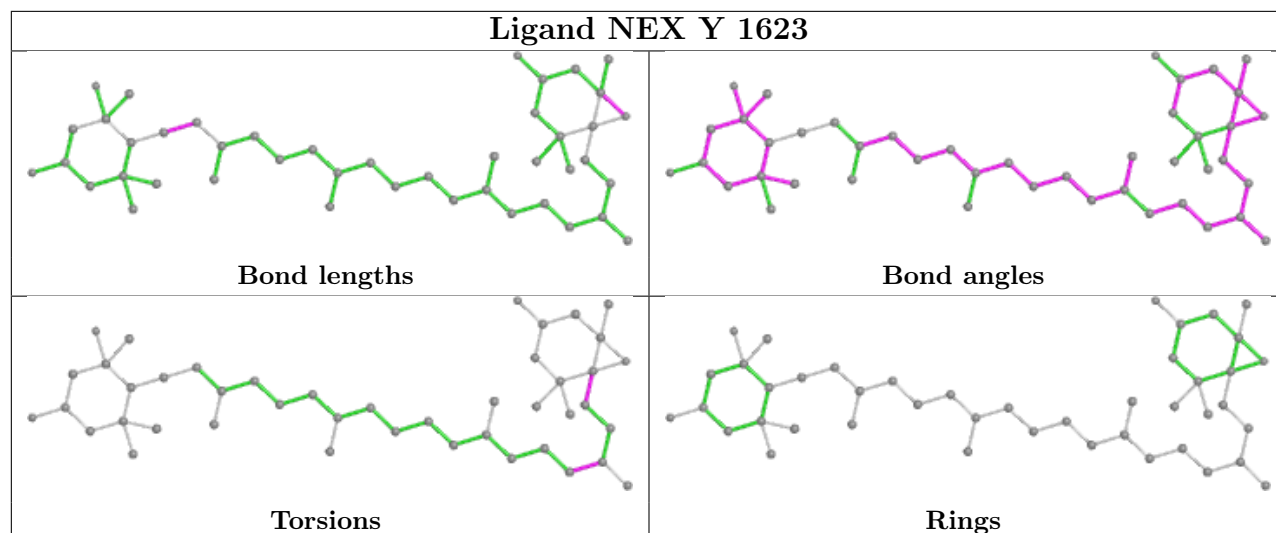




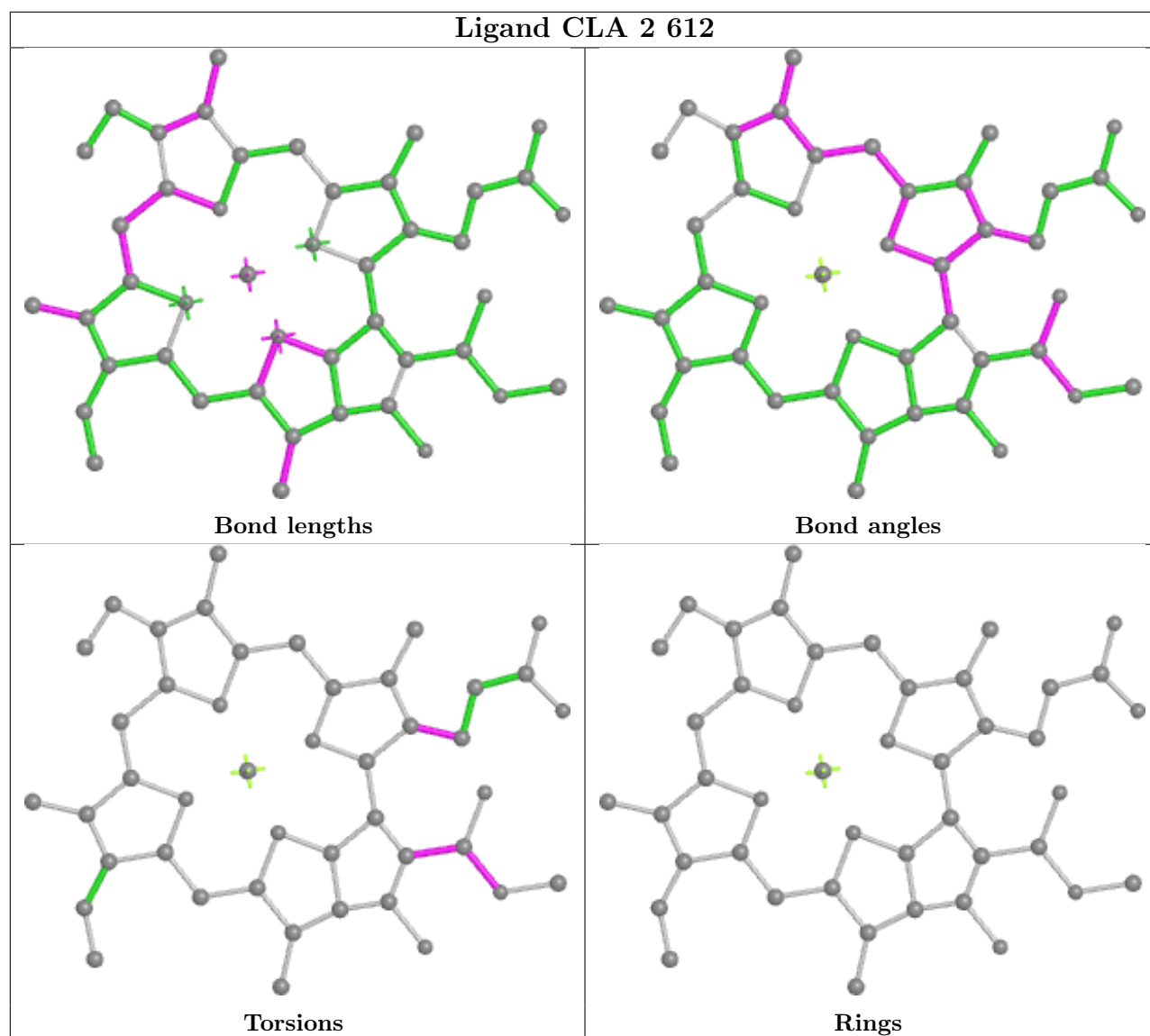




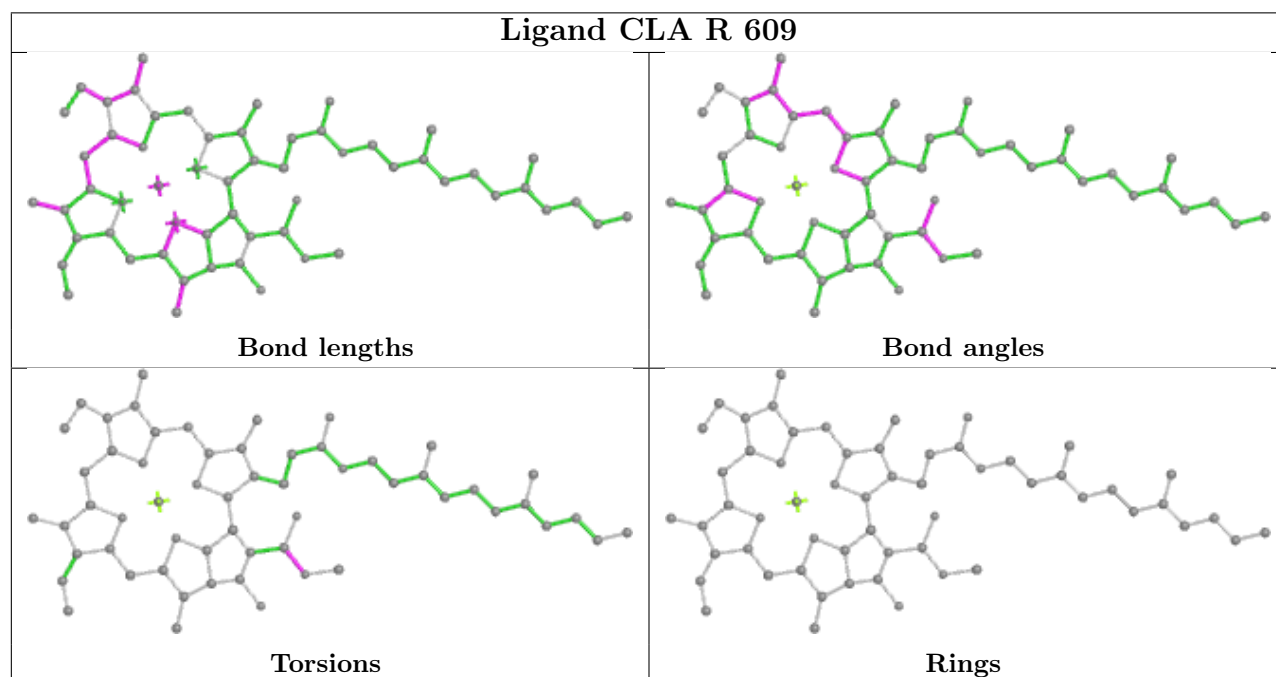
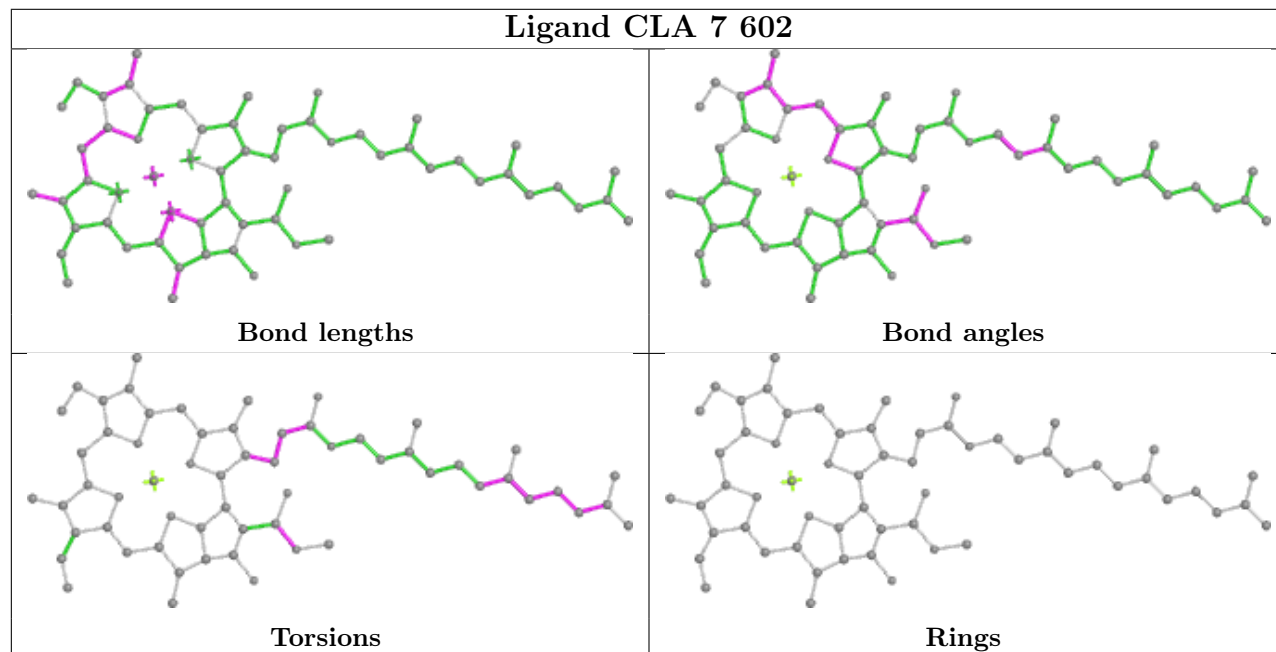
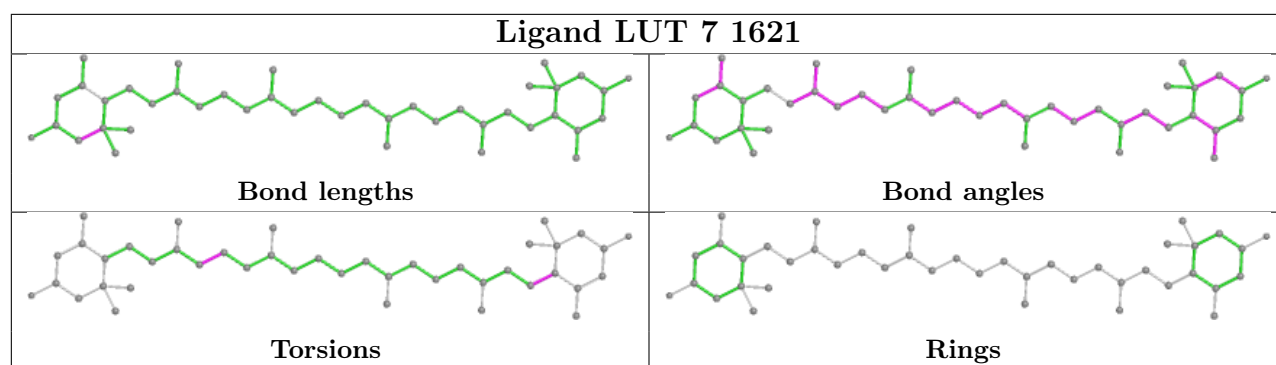
## Ligand NEX Y 1623

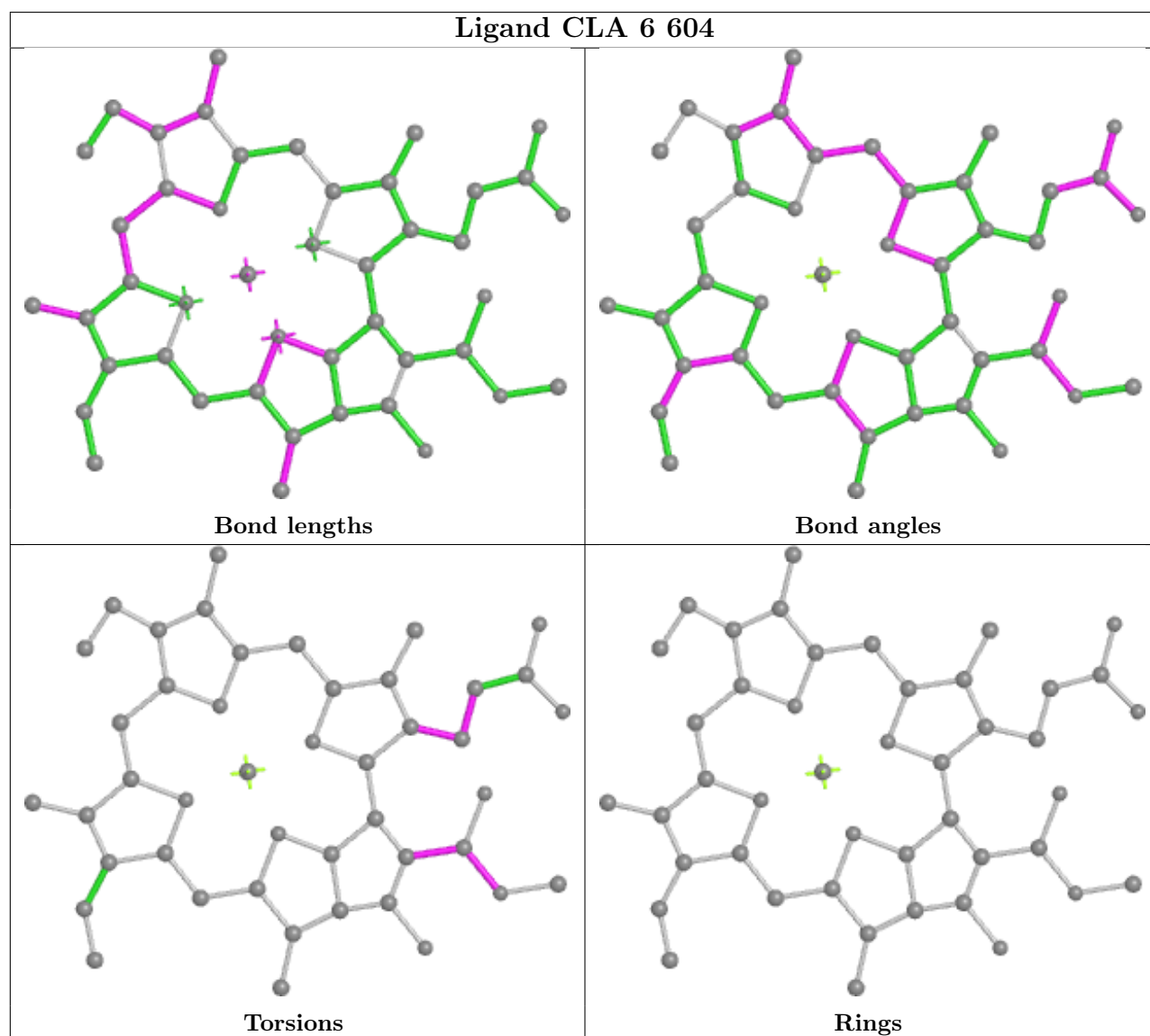
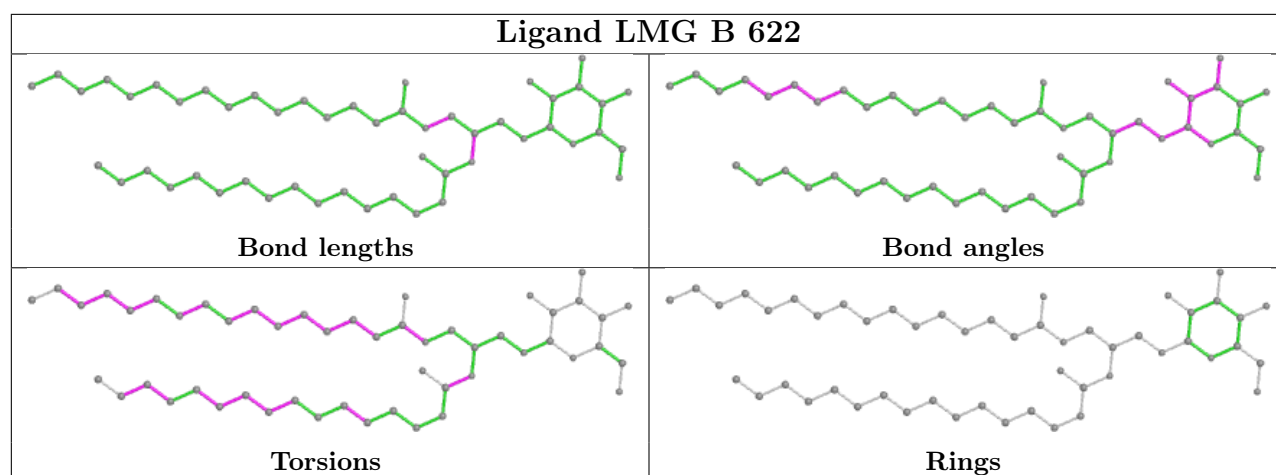


## Ligand CLA 2 612

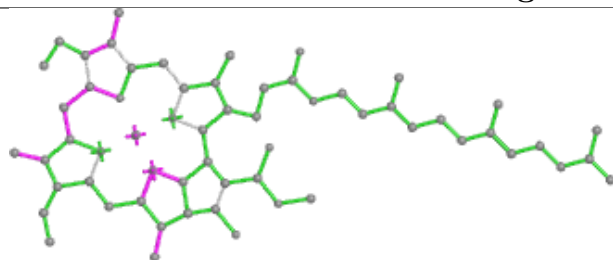




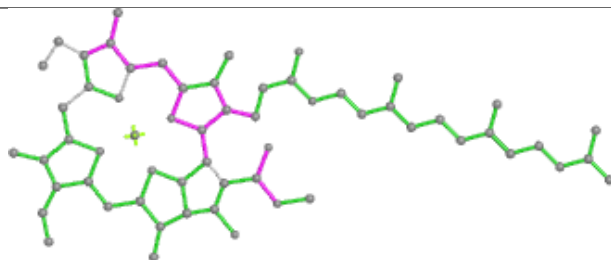




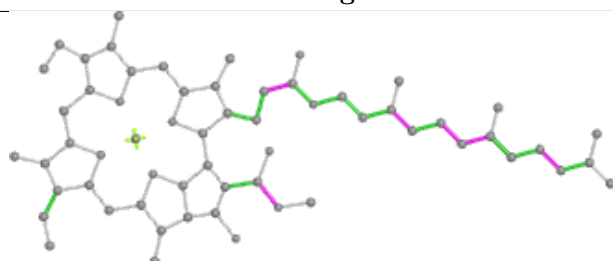
## Ligand CLA n 612



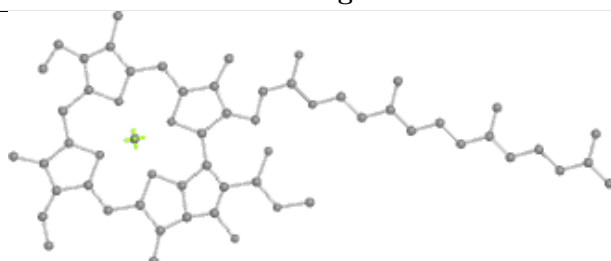
Bond lengths



Bond angles

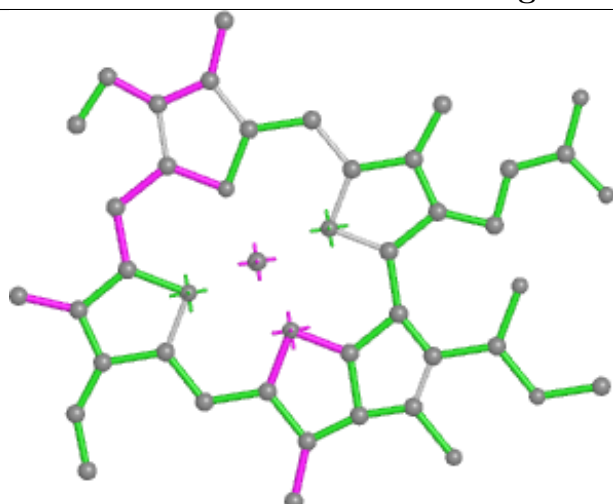


Torsions

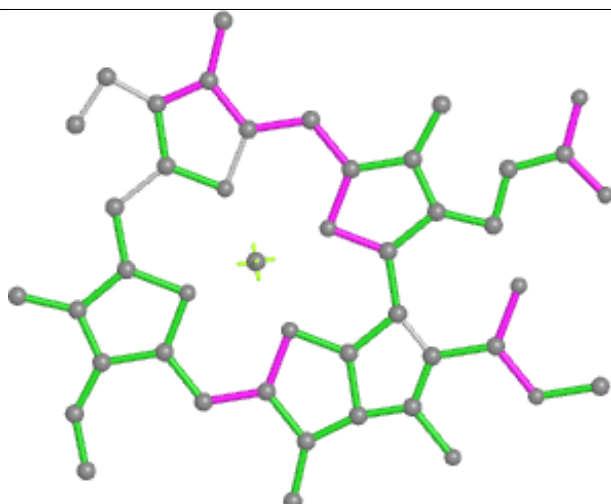


Rings

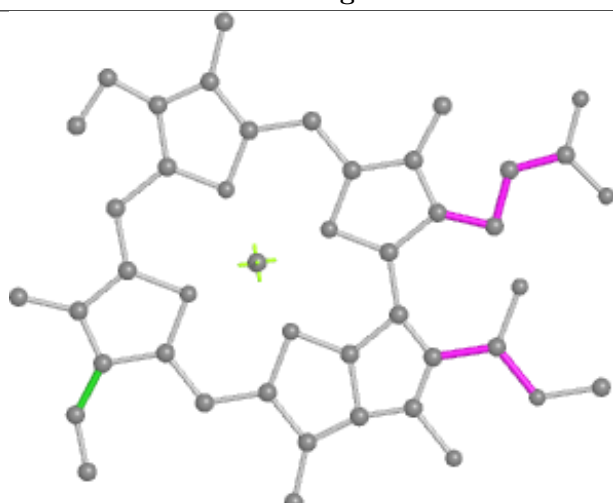
## Ligand CLA 4 604



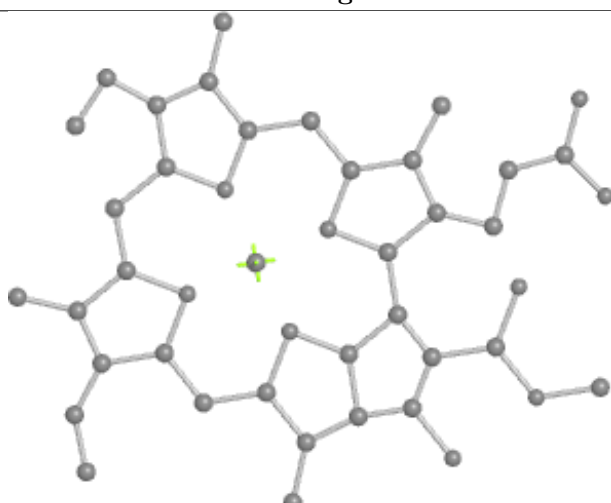
Bond lengths



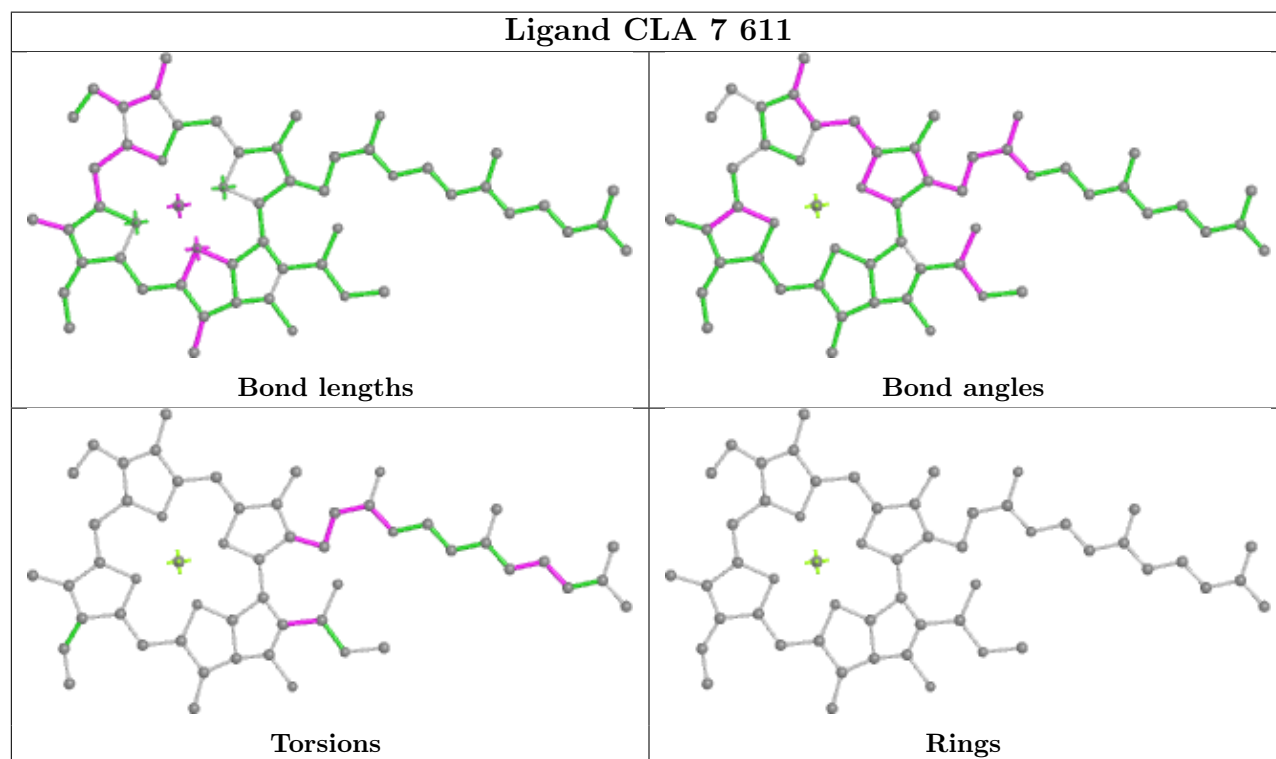
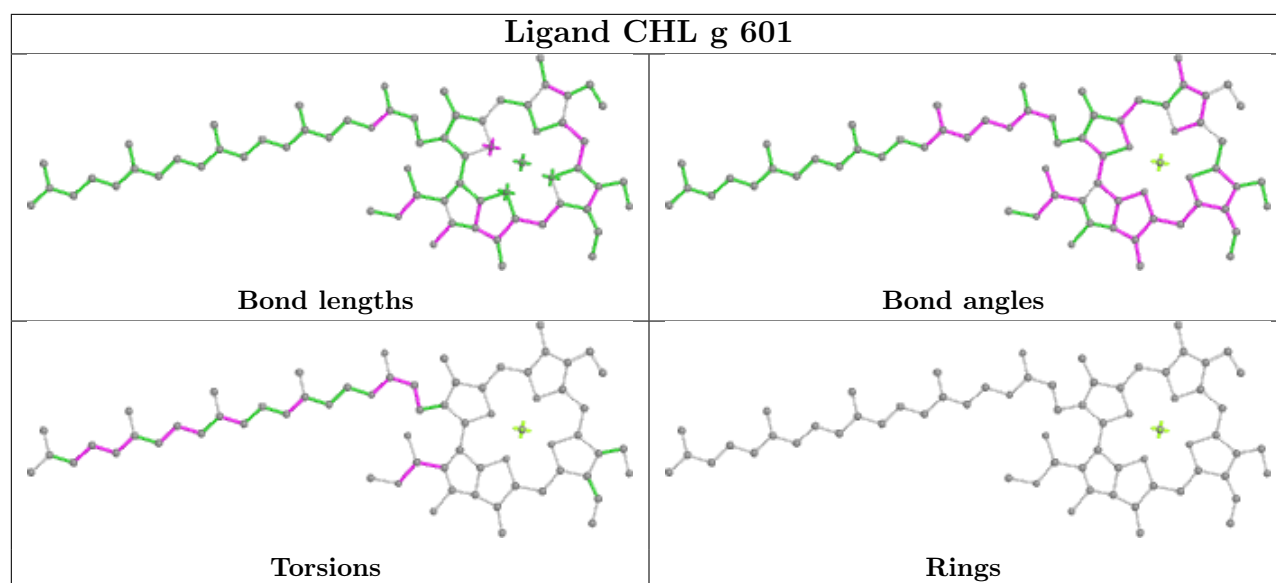
Bond angles



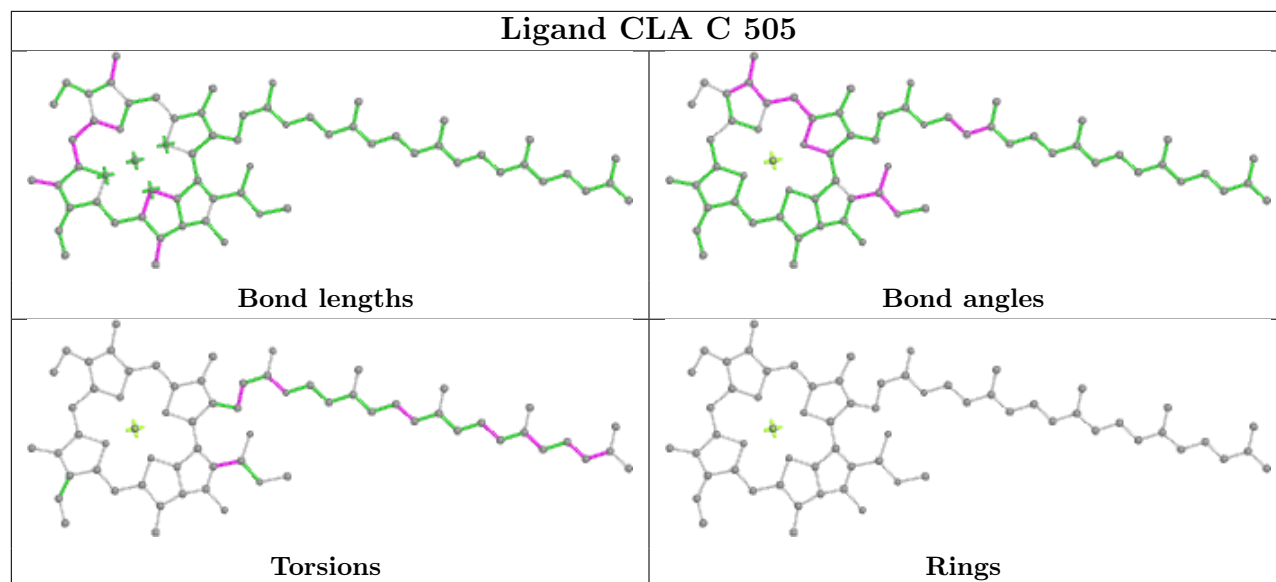
Torsions



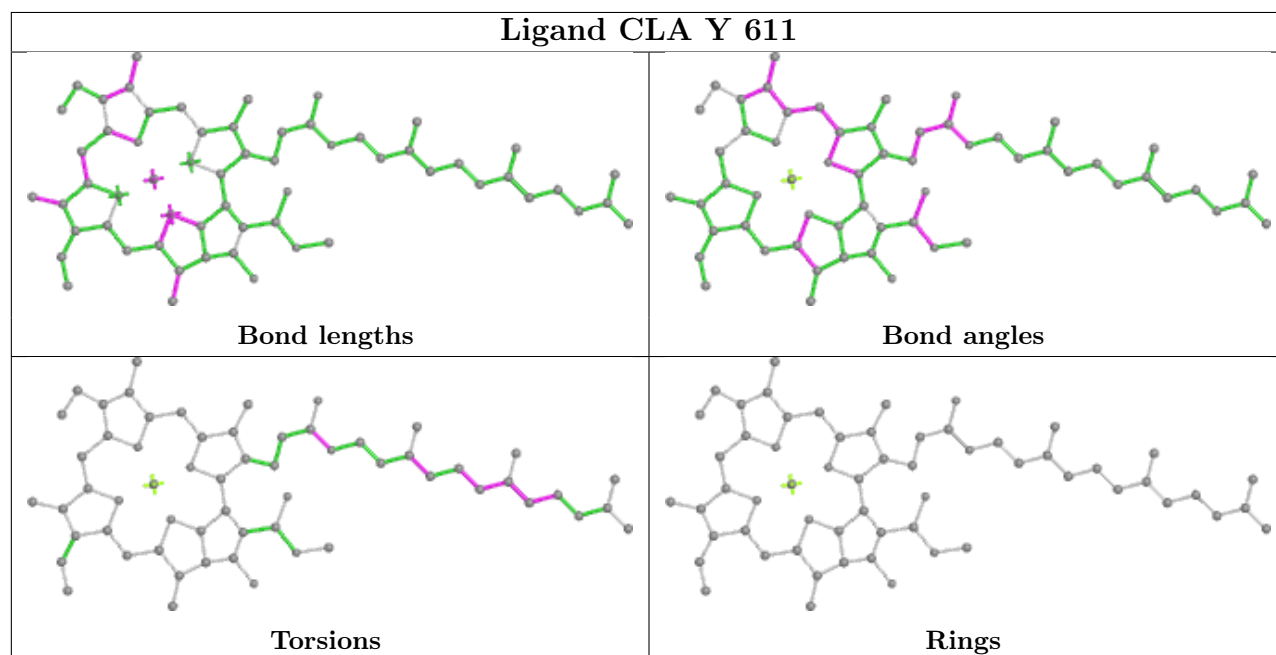
Rings

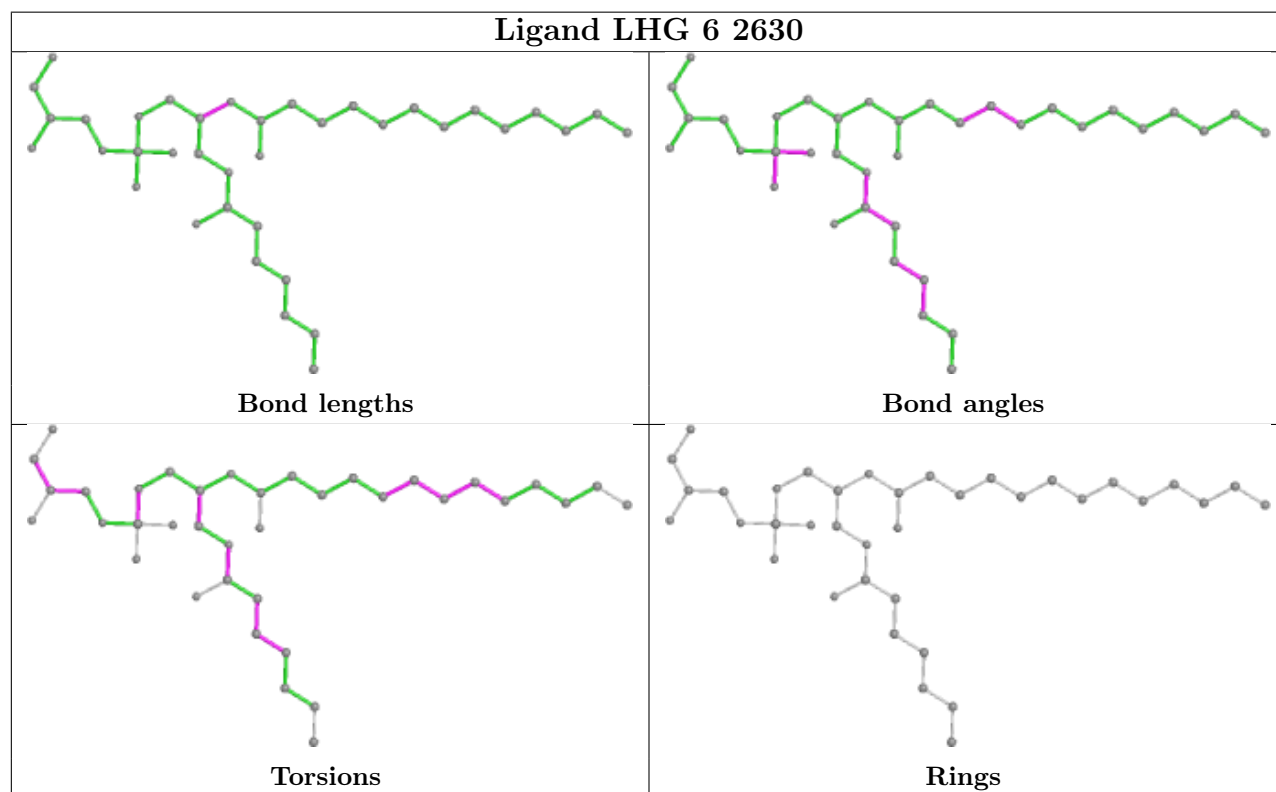
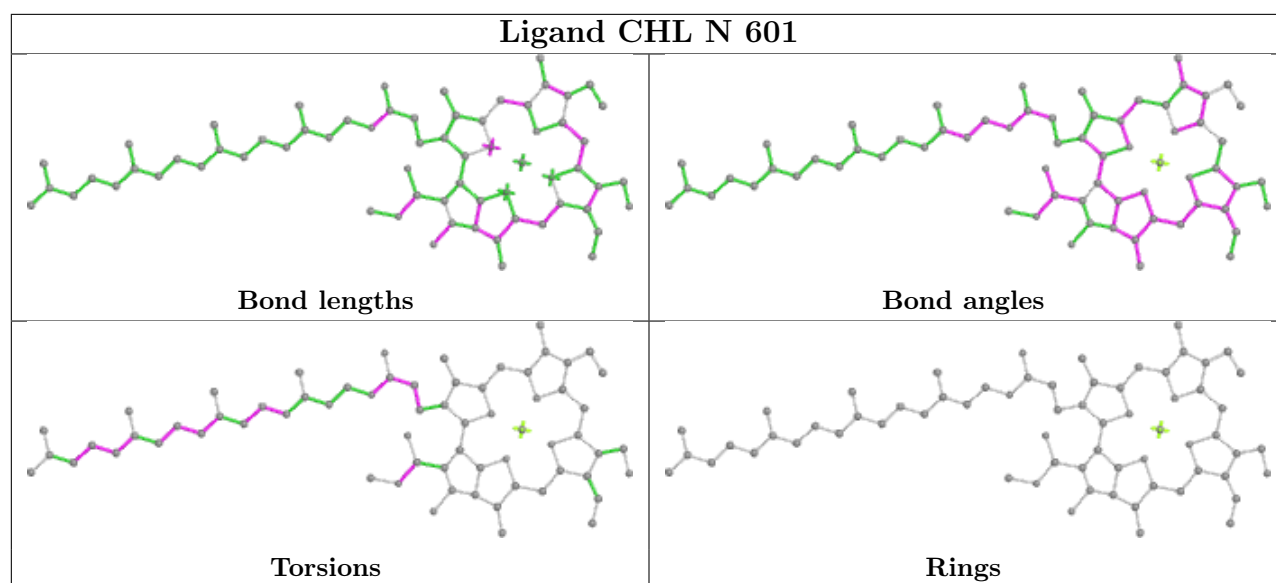


## Ligand CLA C 505

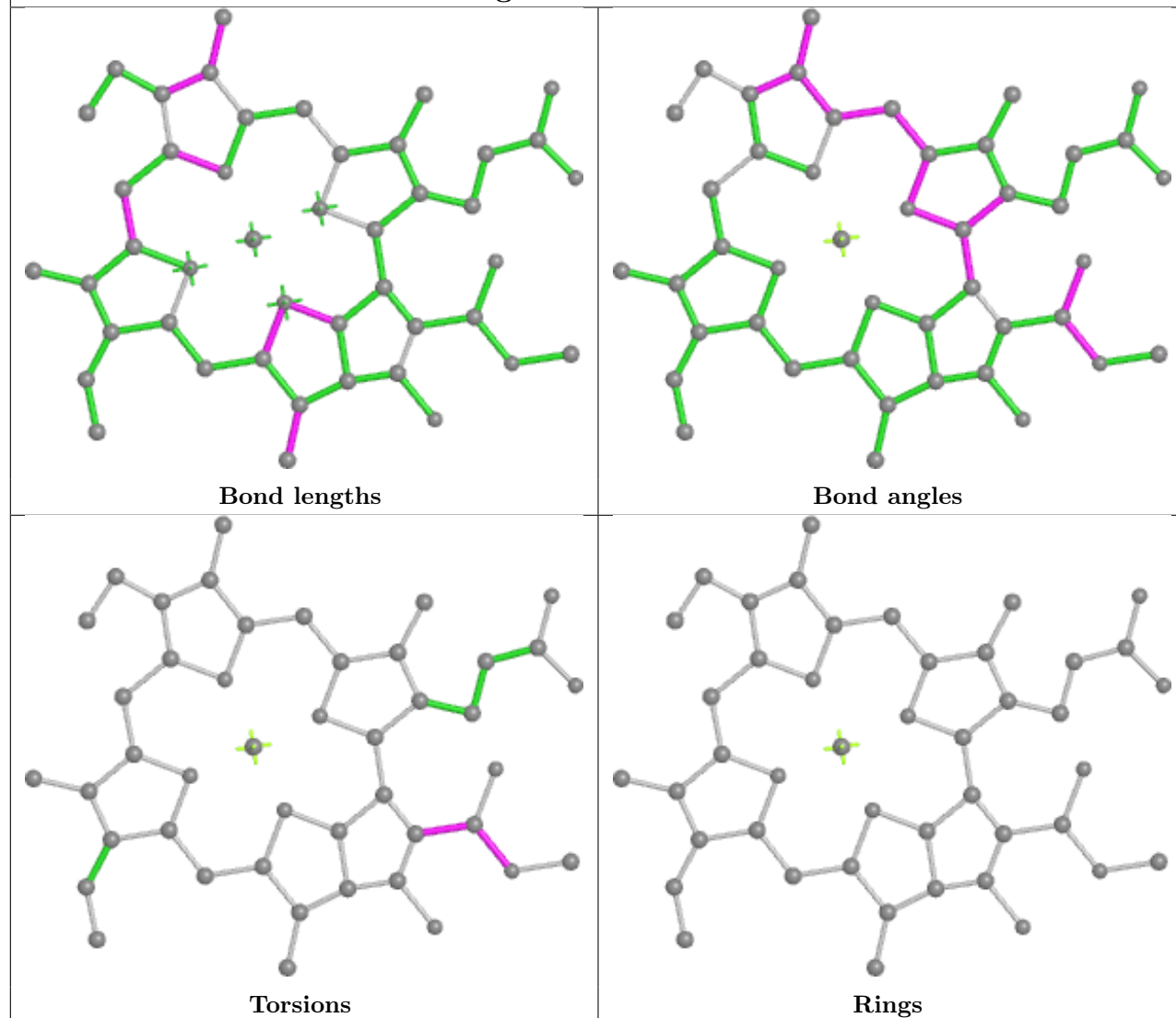


## Ligand CLA Y 611

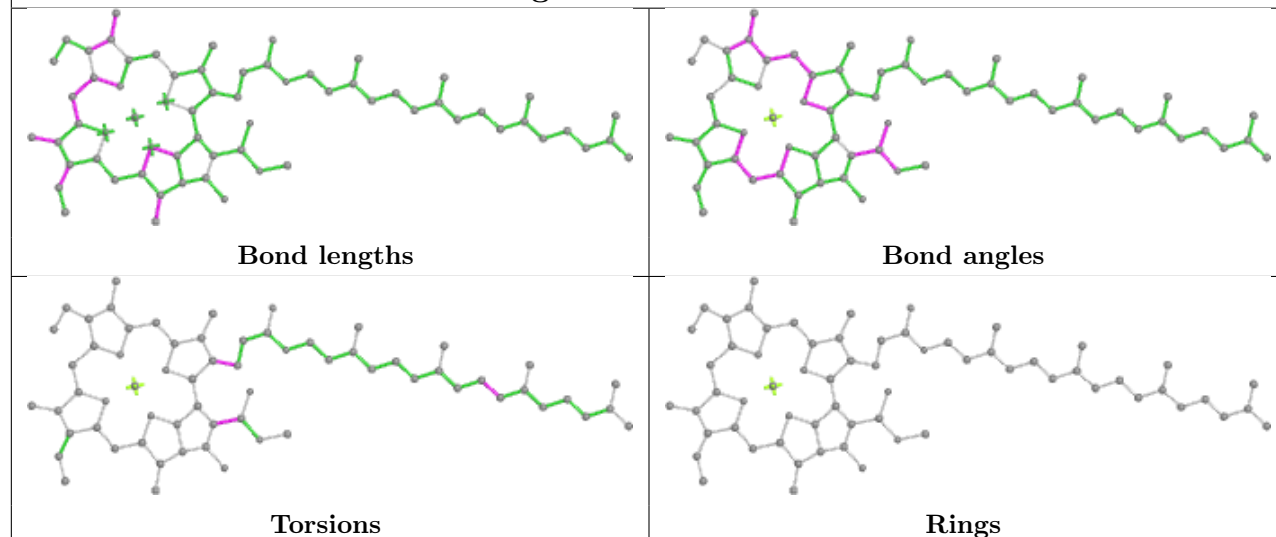


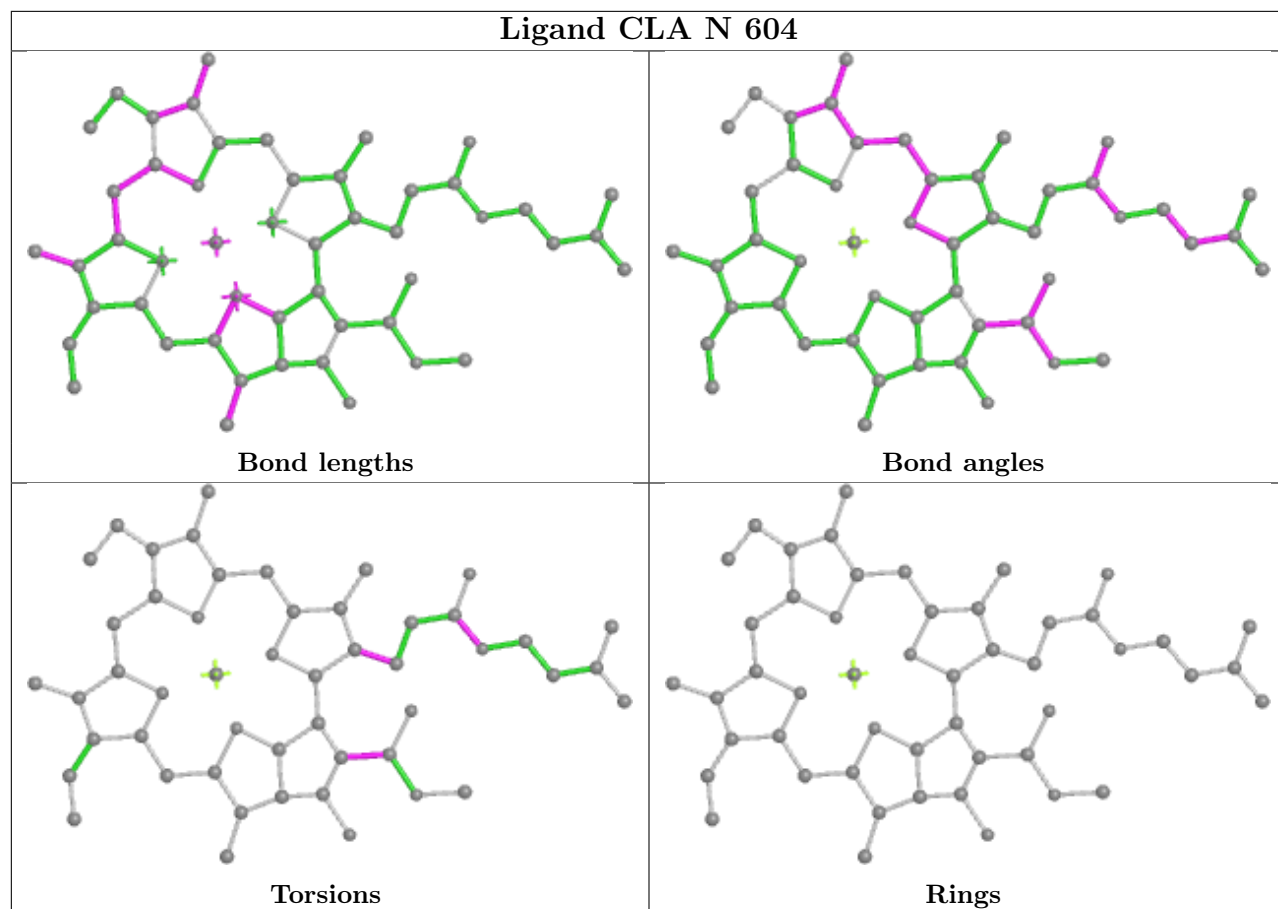


## Ligand CLA s 603



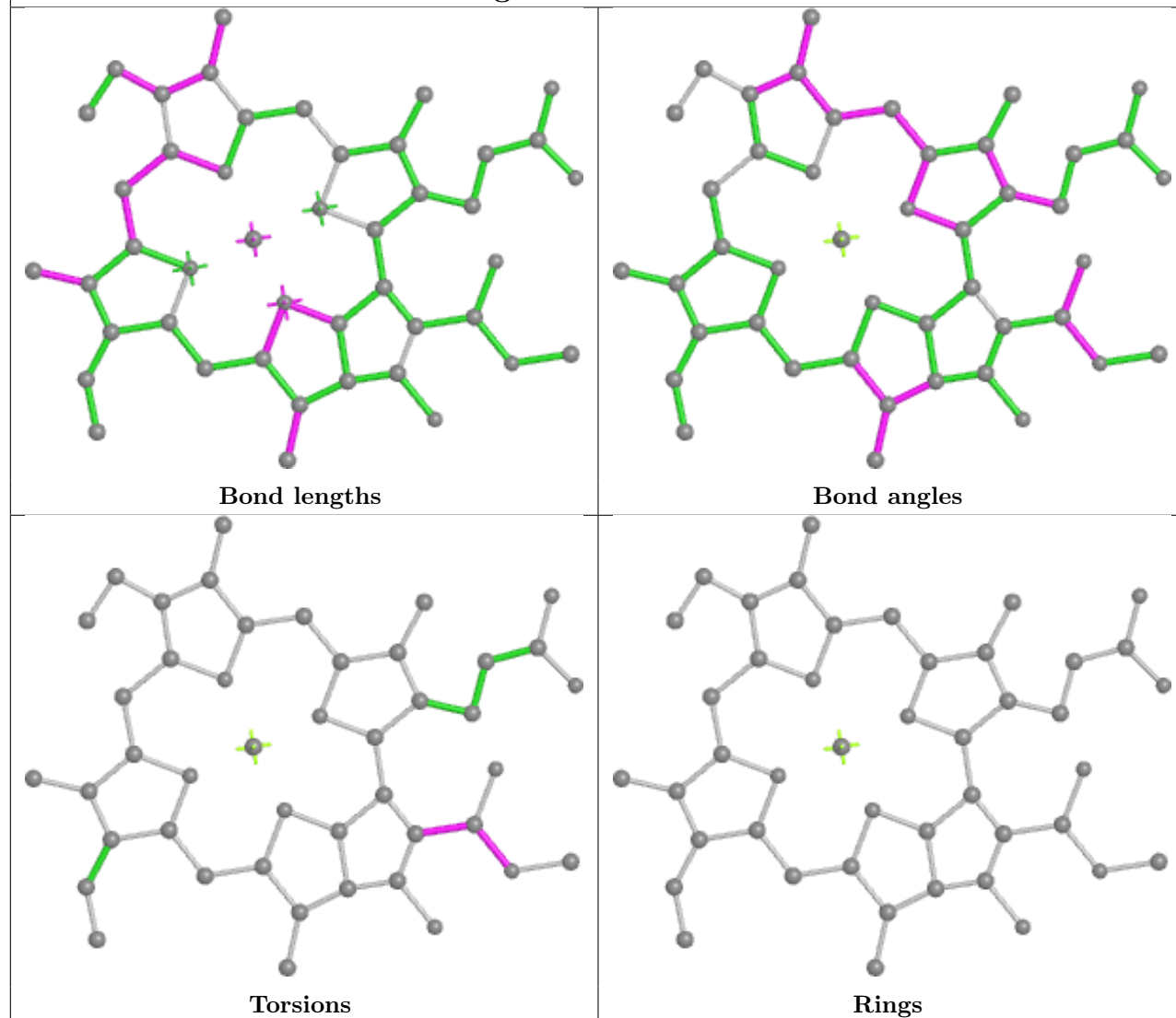
## Ligand CLA A 406



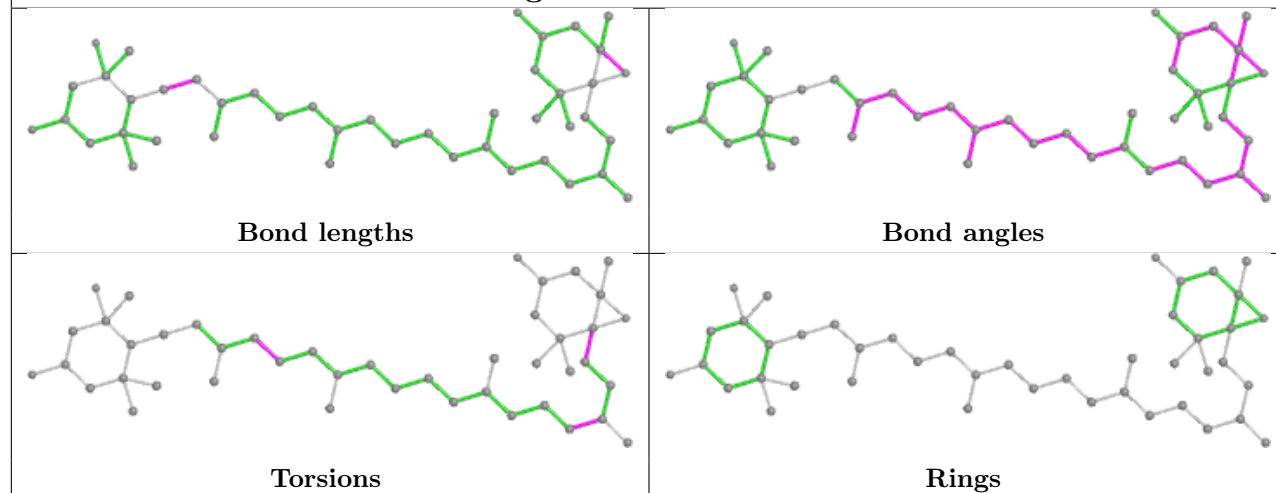


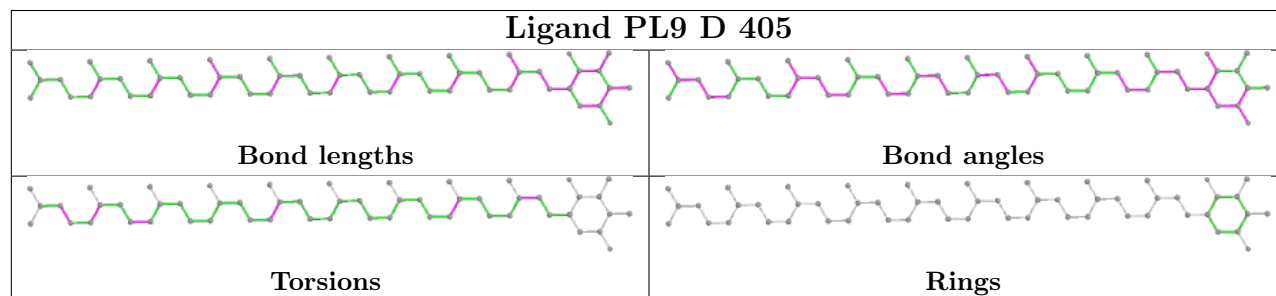
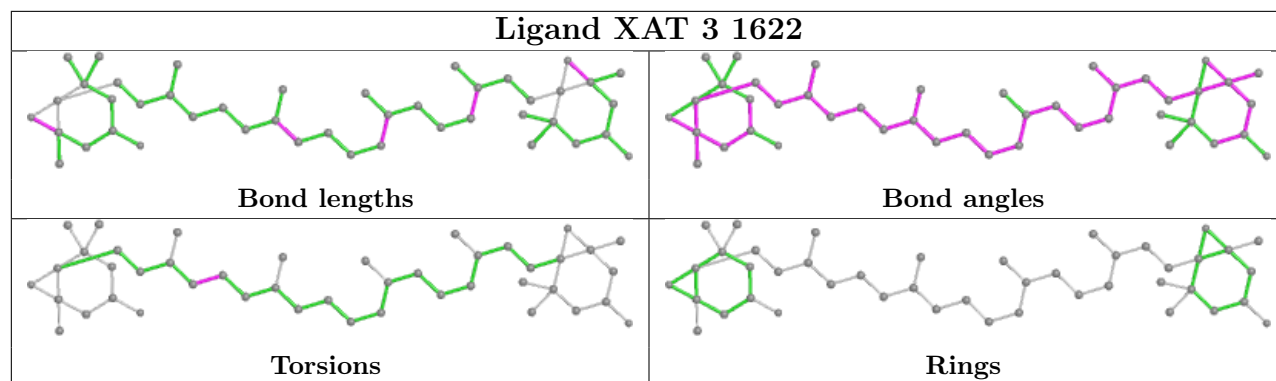


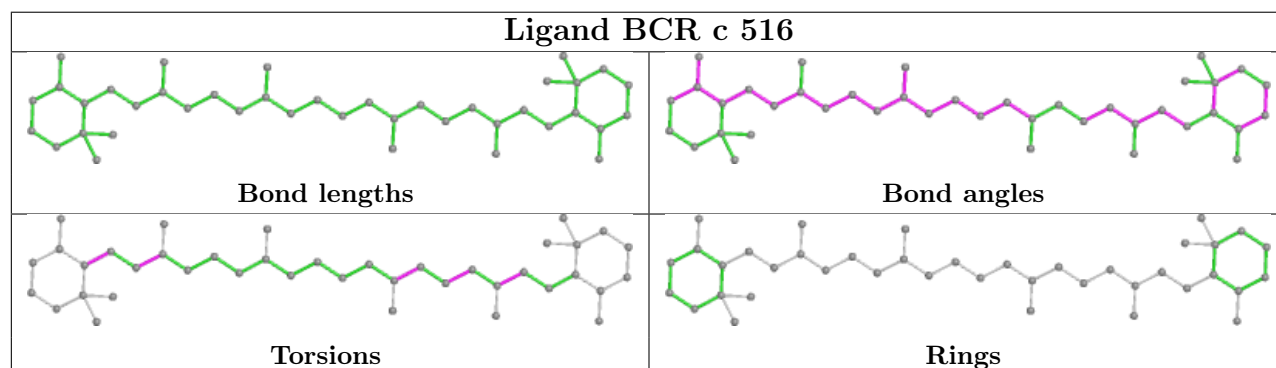
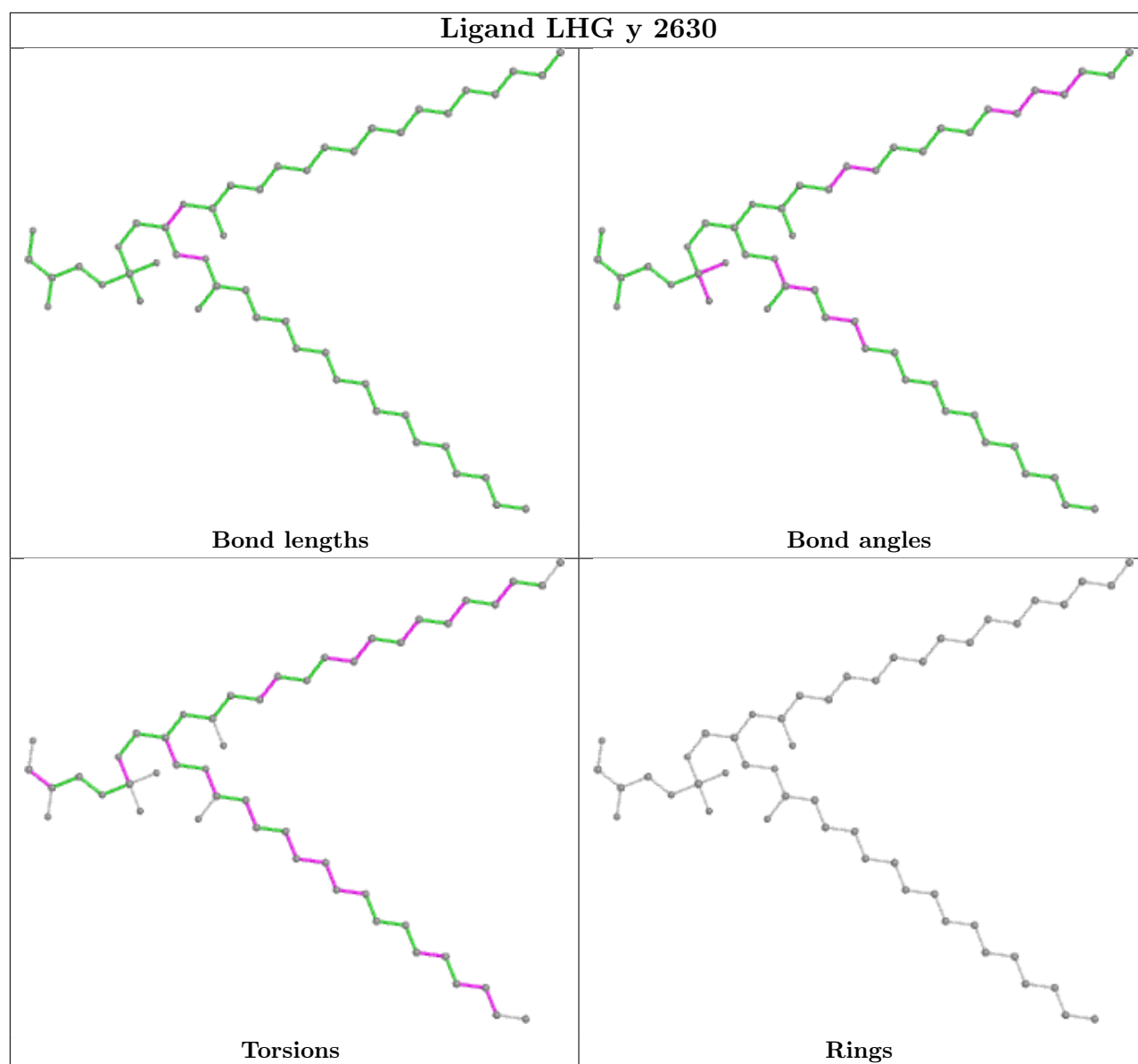
## Ligand CLA 3 612

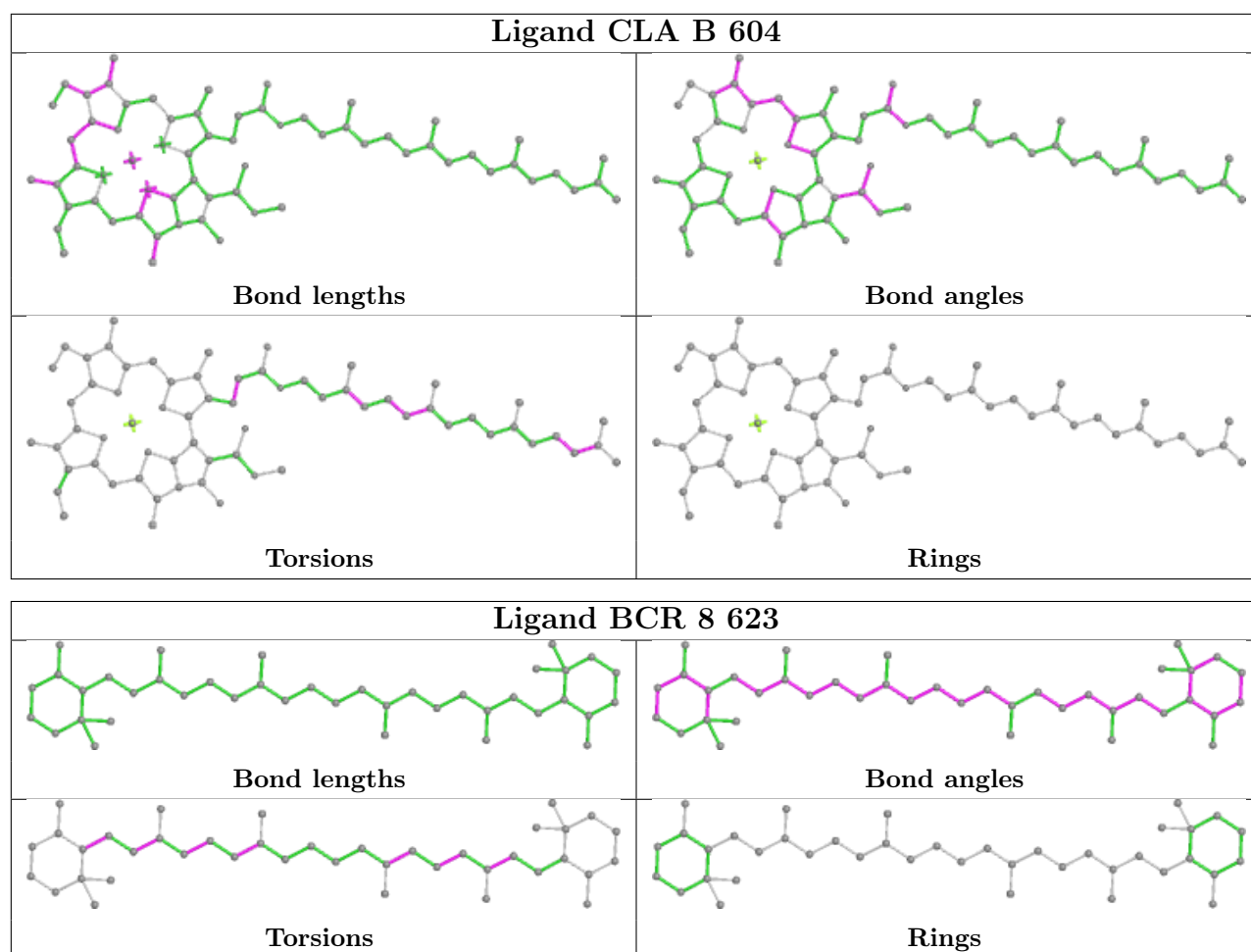


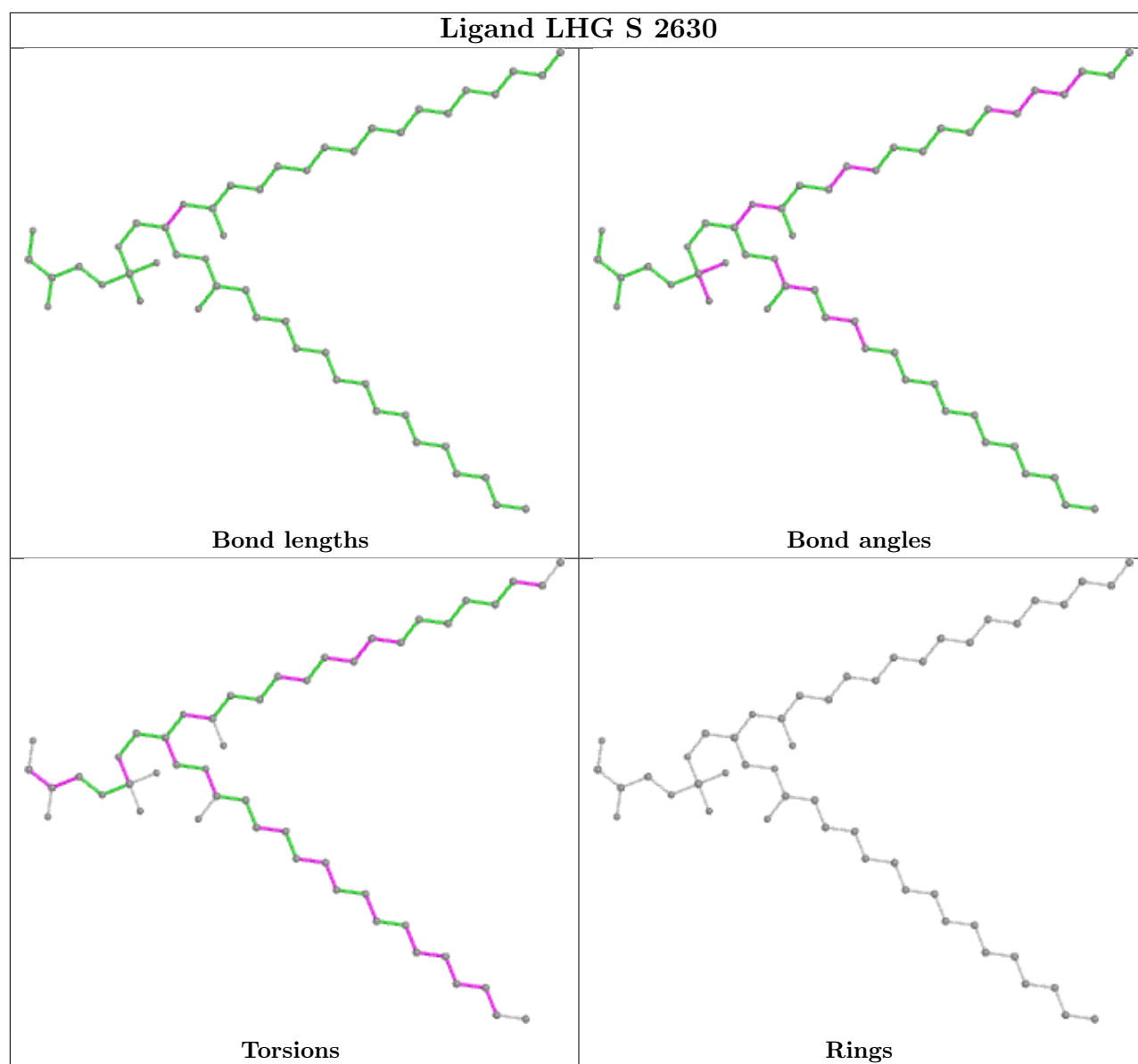
## Ligand NEX 3 1623



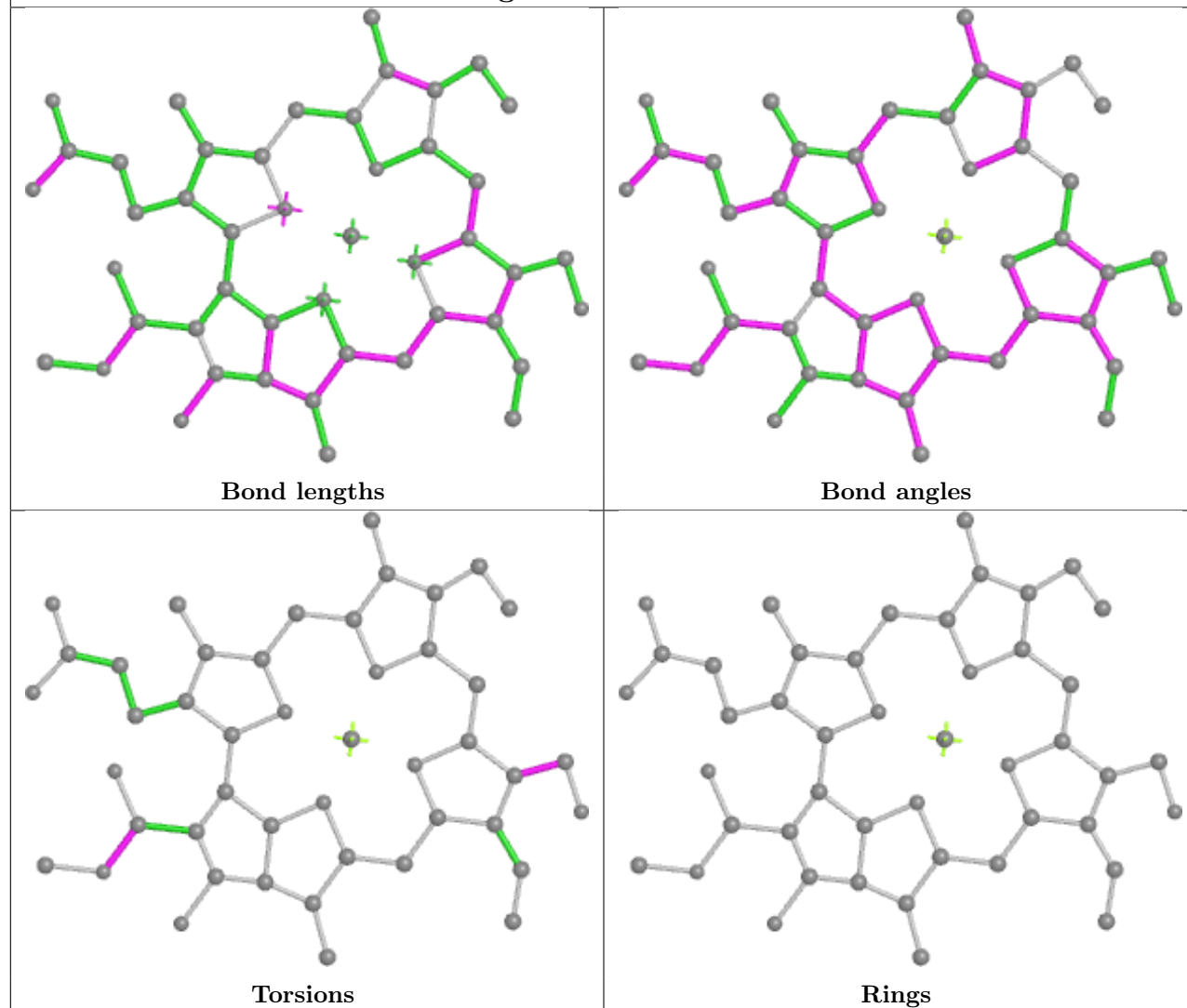




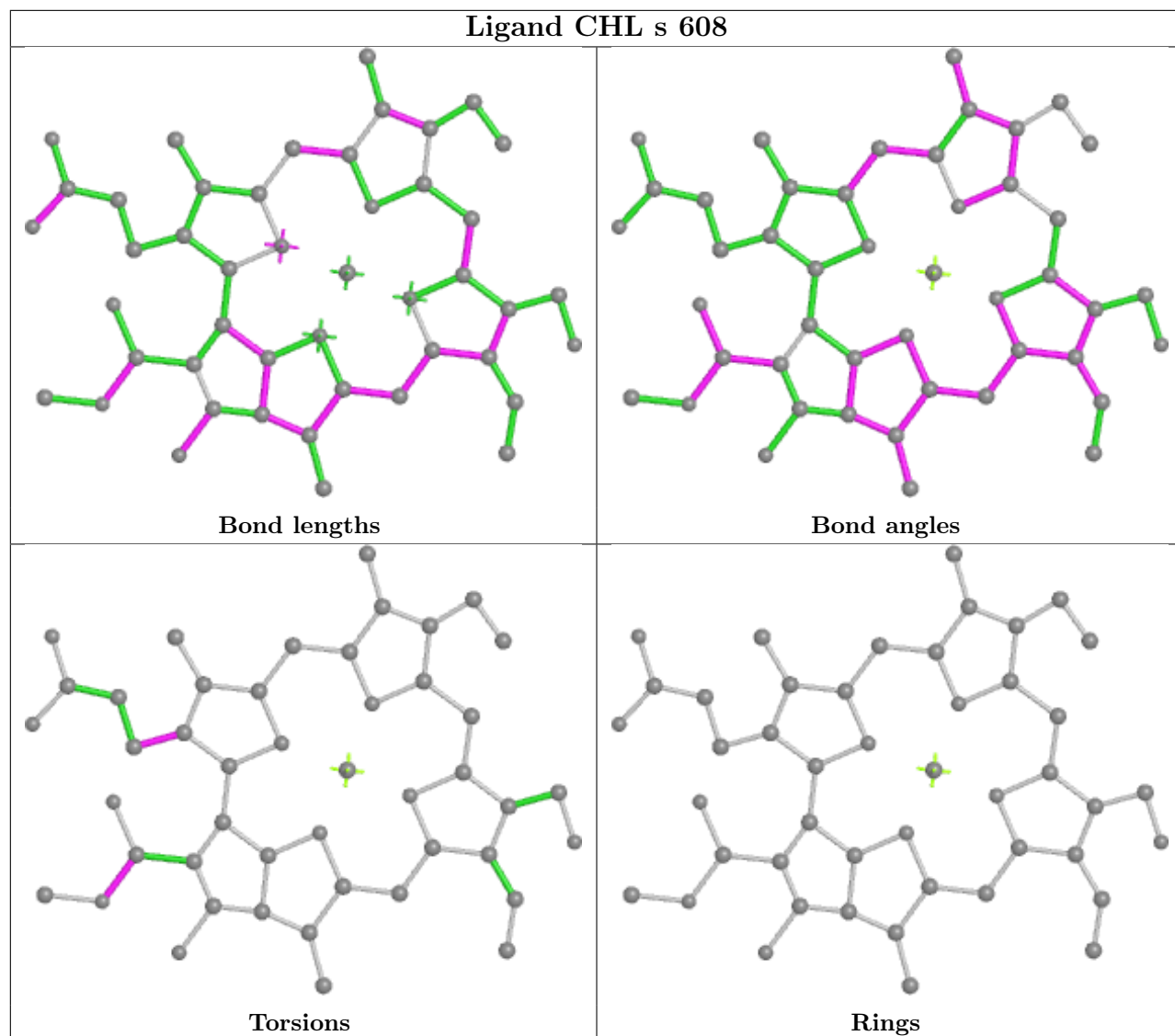




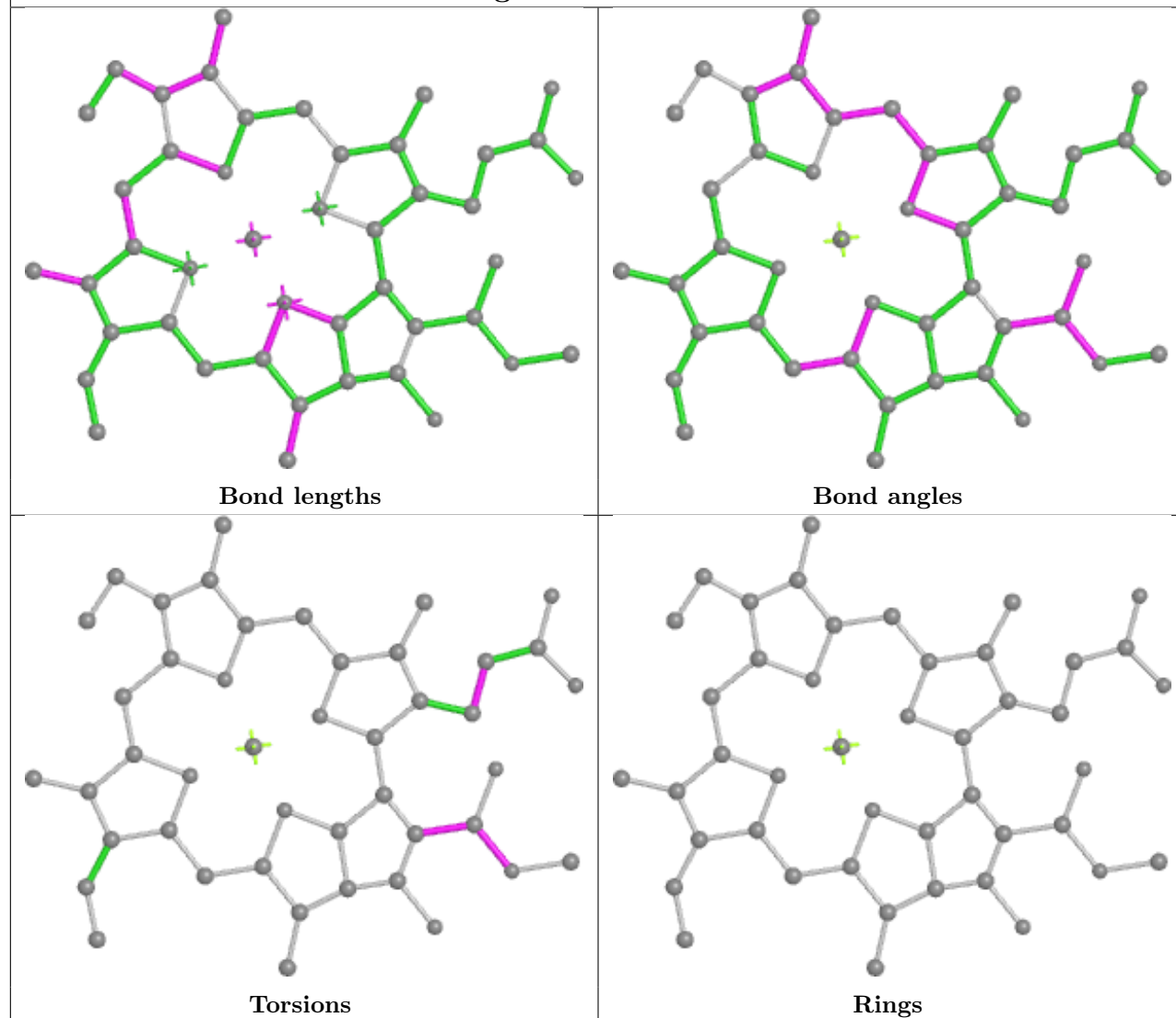
## Ligand CHL 2 606



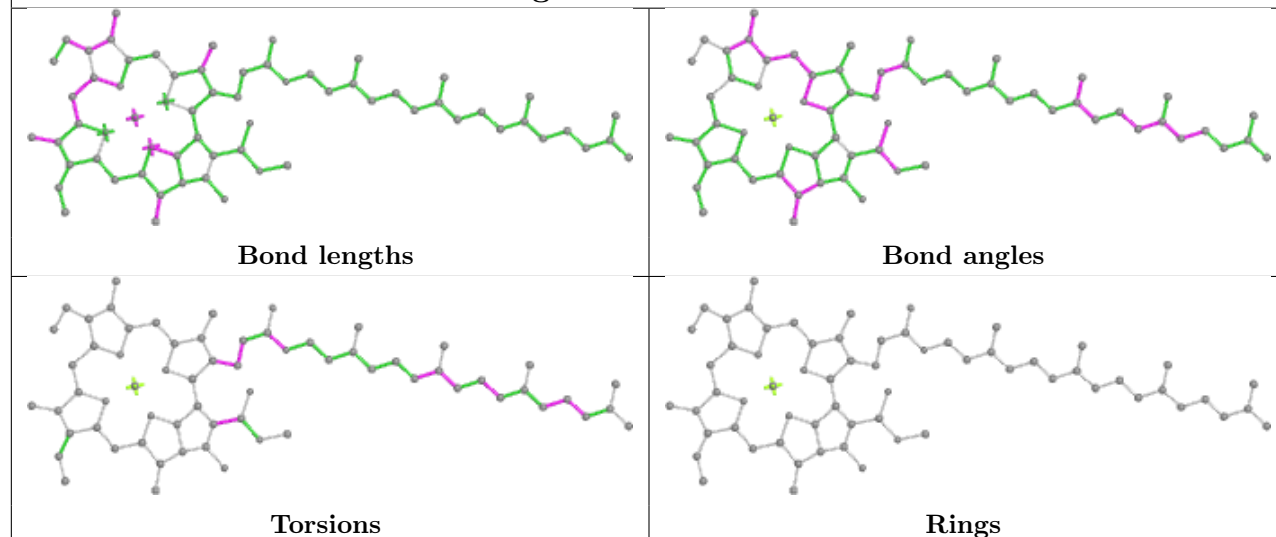
## Ligand CHL s 608



## Ligand CLA 2 613

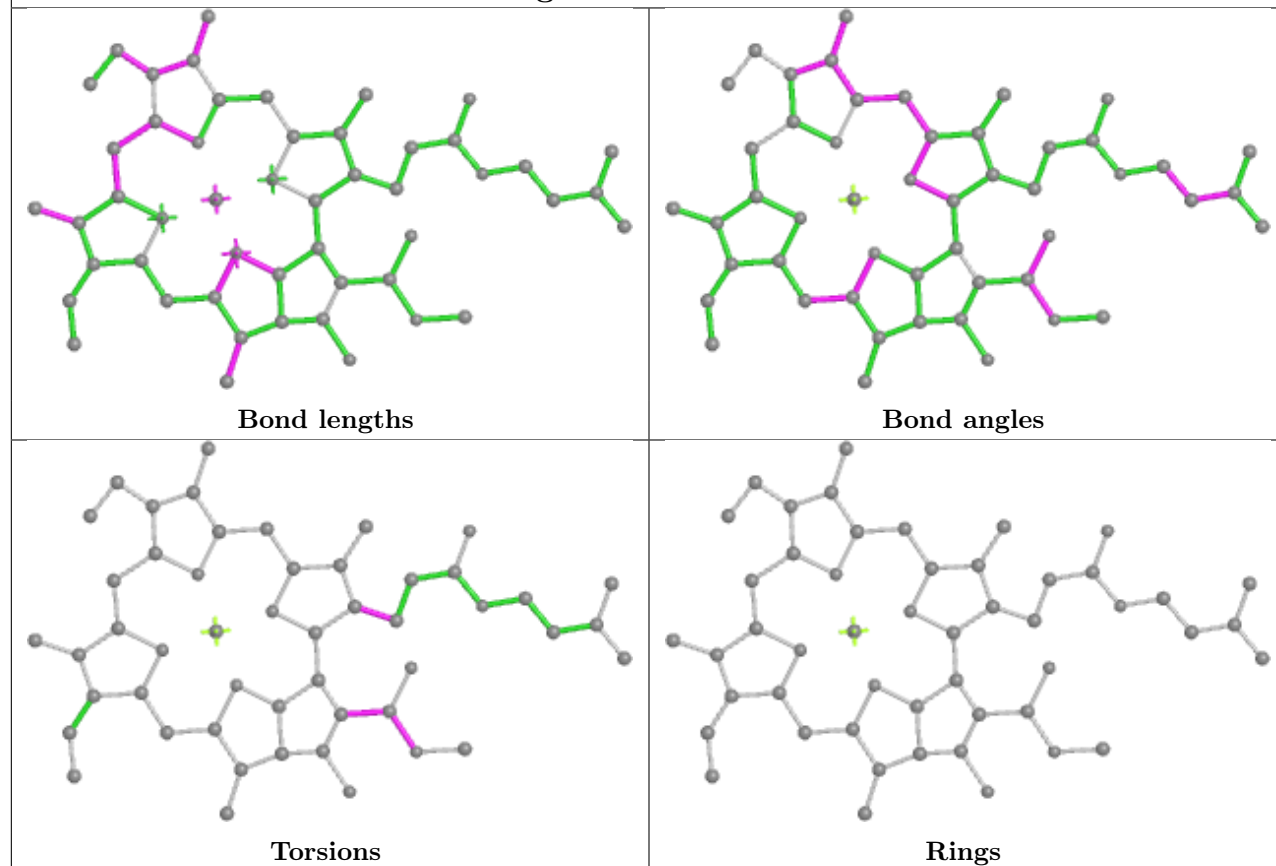


## Ligand CLA B 613

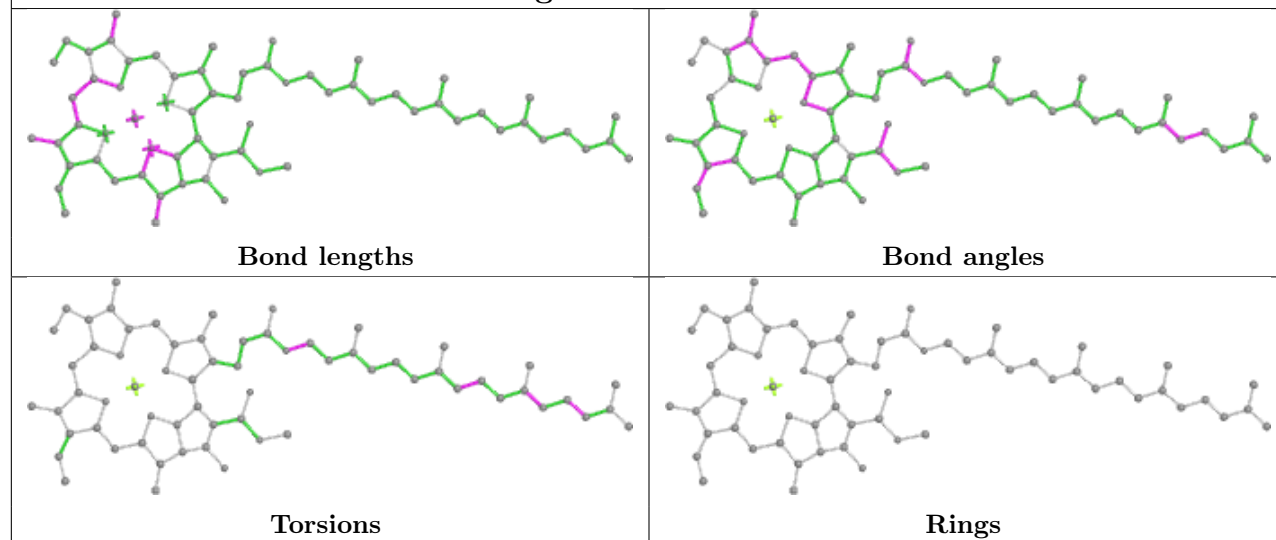


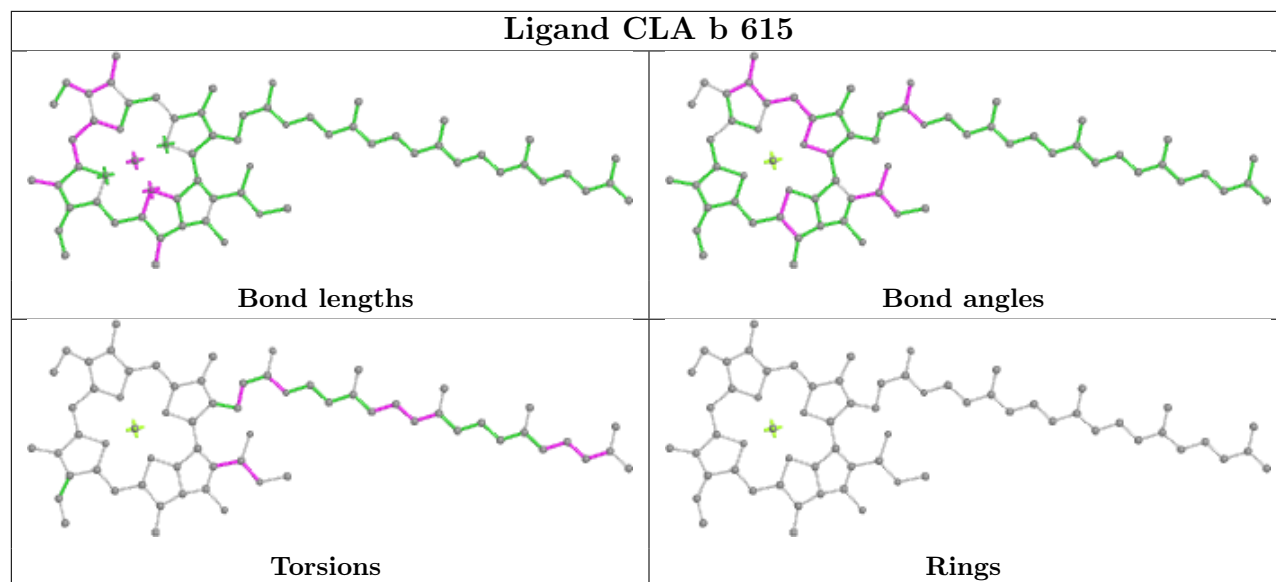
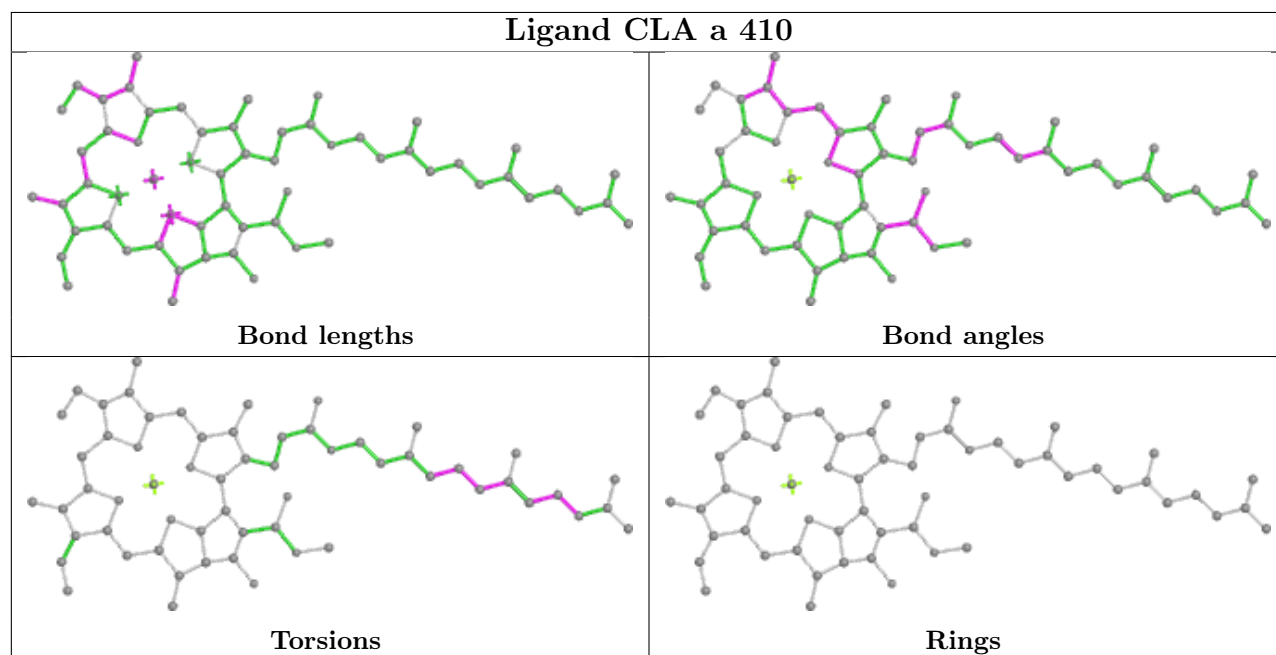


## Ligand CLA a 407

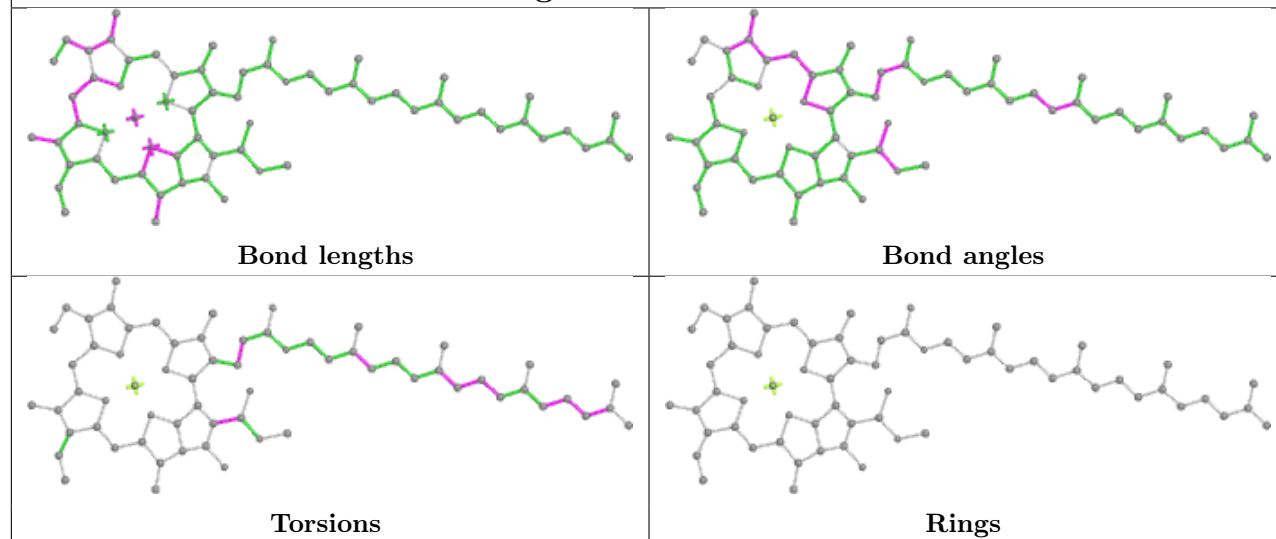


## Ligand CLA b 609

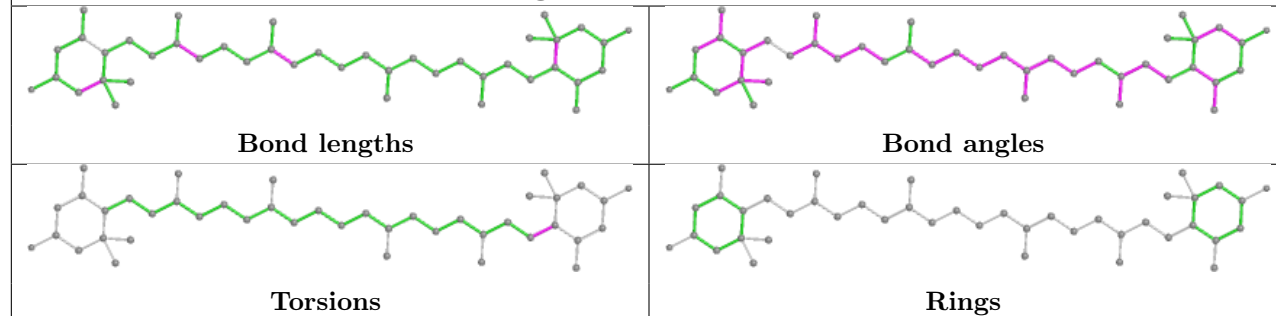


**Ligand CLA b 615****Ligand CLA a 410**

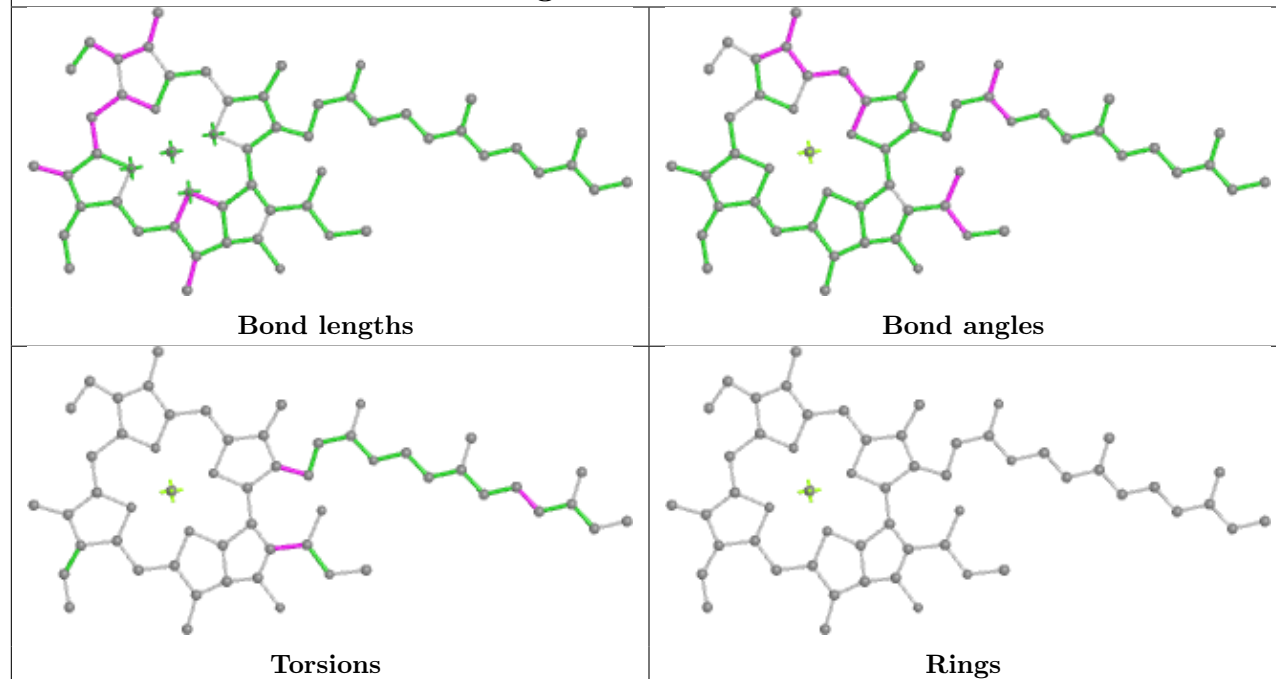
## Ligand CLA b 607

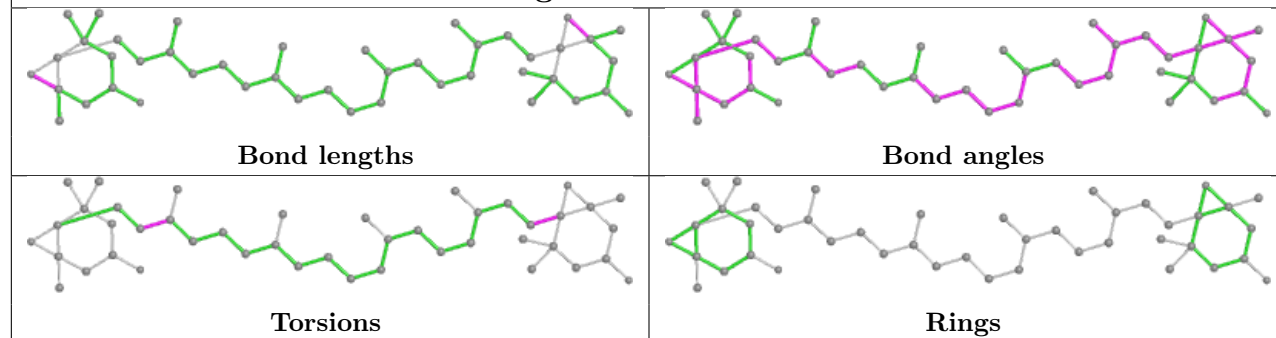
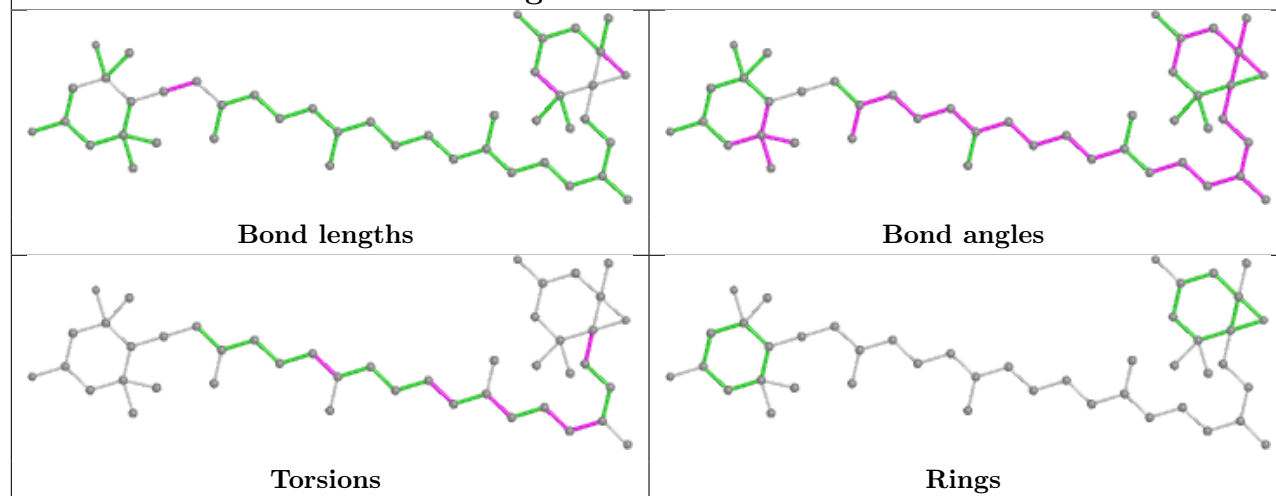


## Ligand LUT R 620

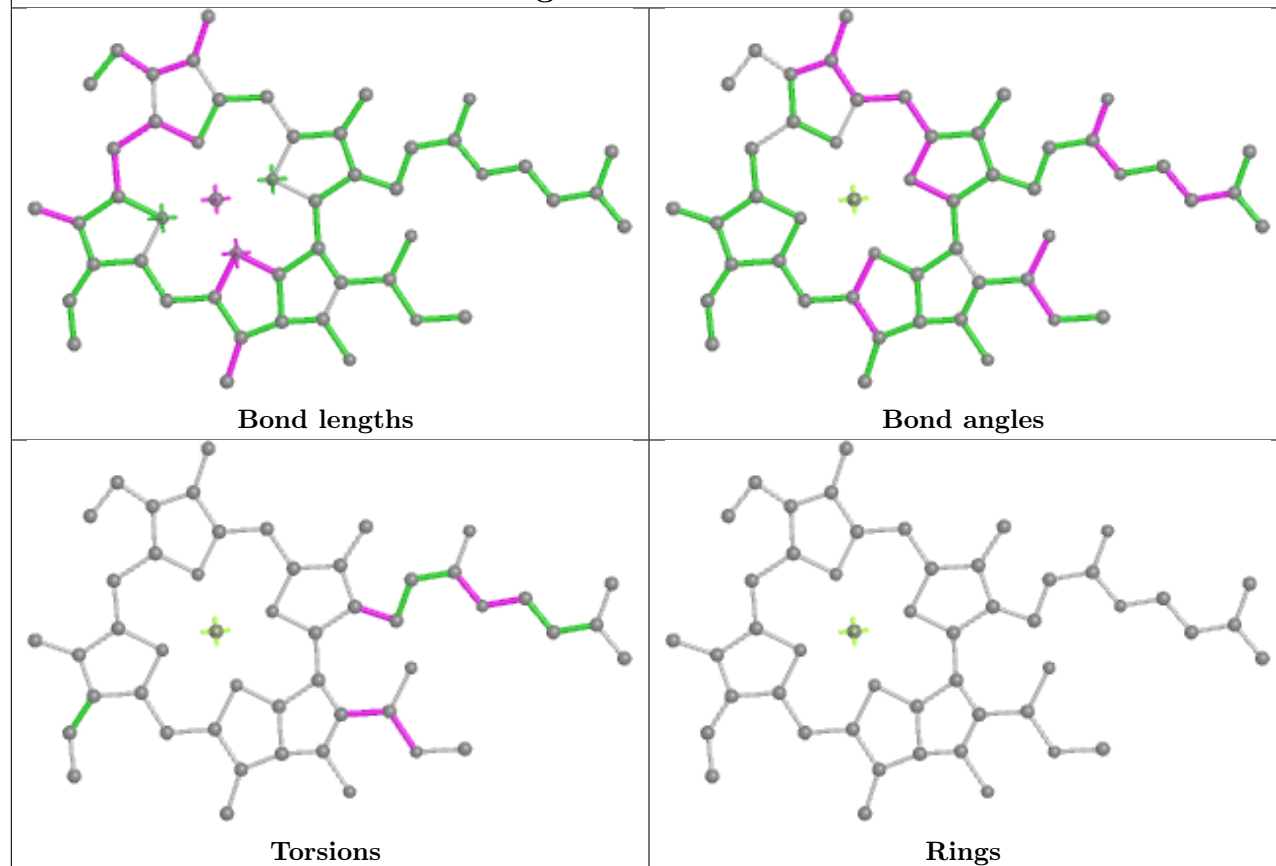


## Ligand CLA 5 610

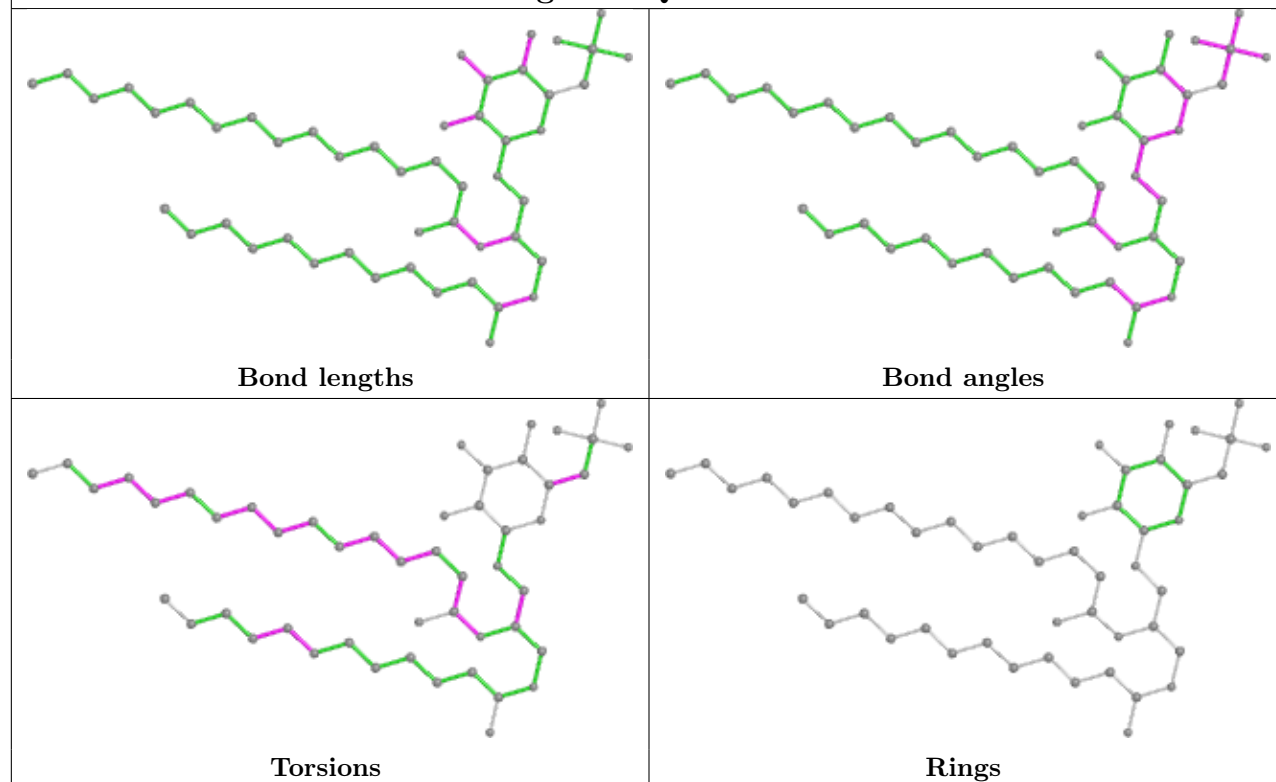


**Ligand XAT 4 622****Ligand NEX 5 1623**

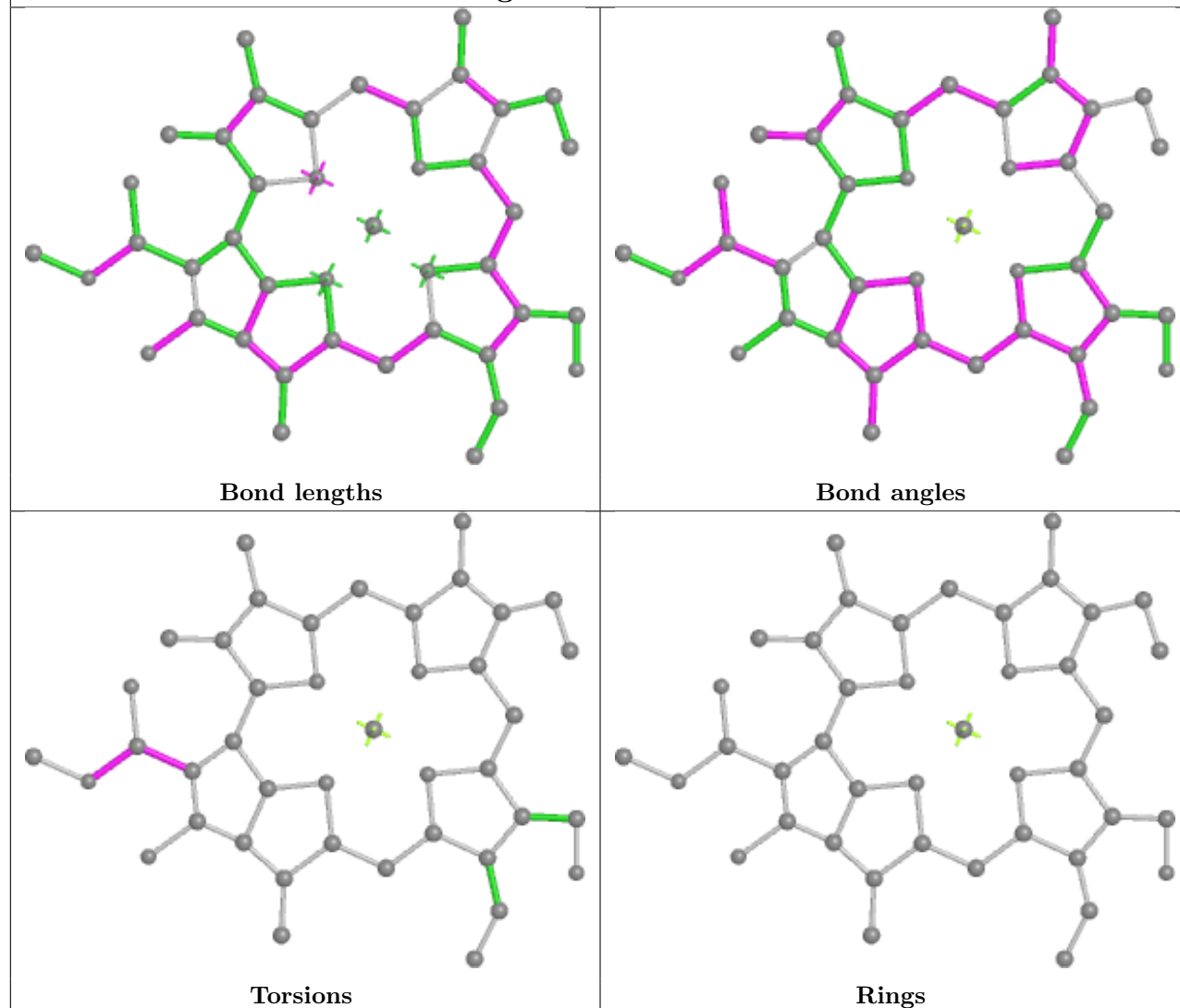
## Ligand CLA 5 604



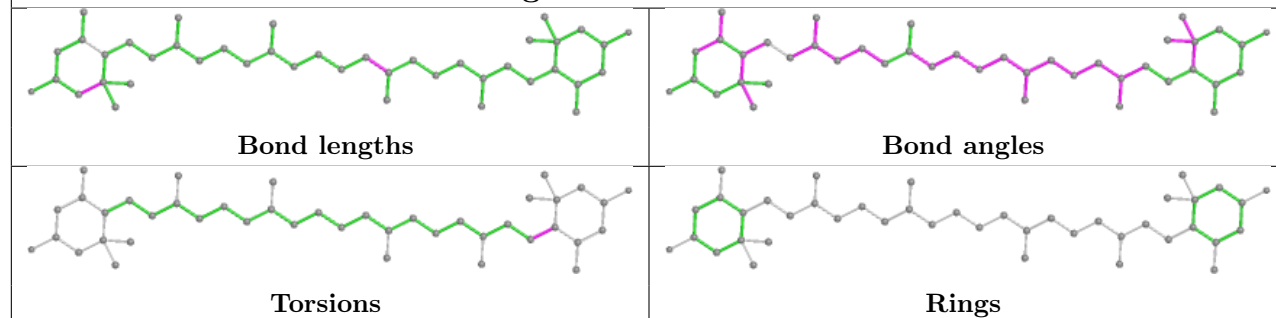
## Ligand SQD a 412

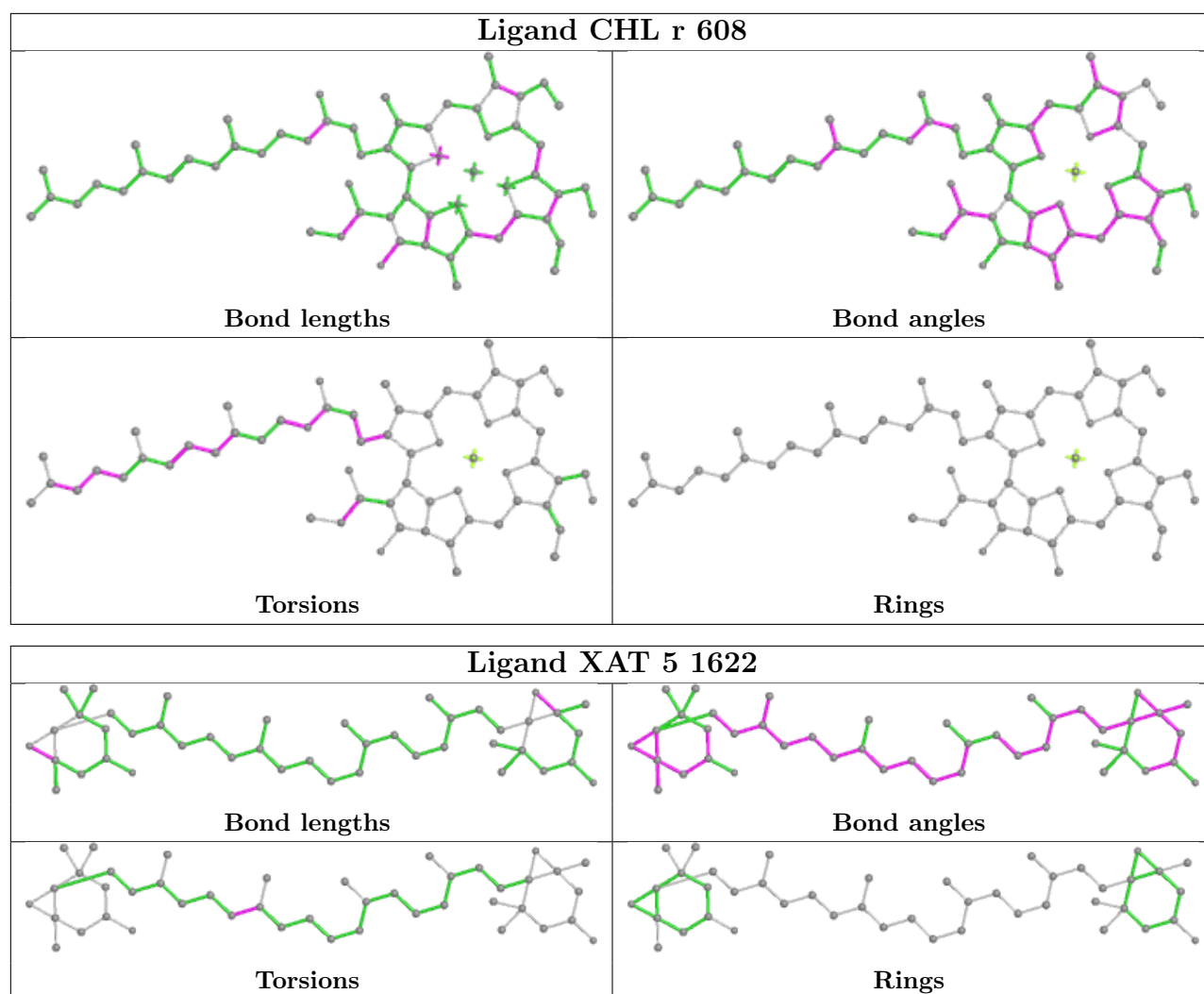


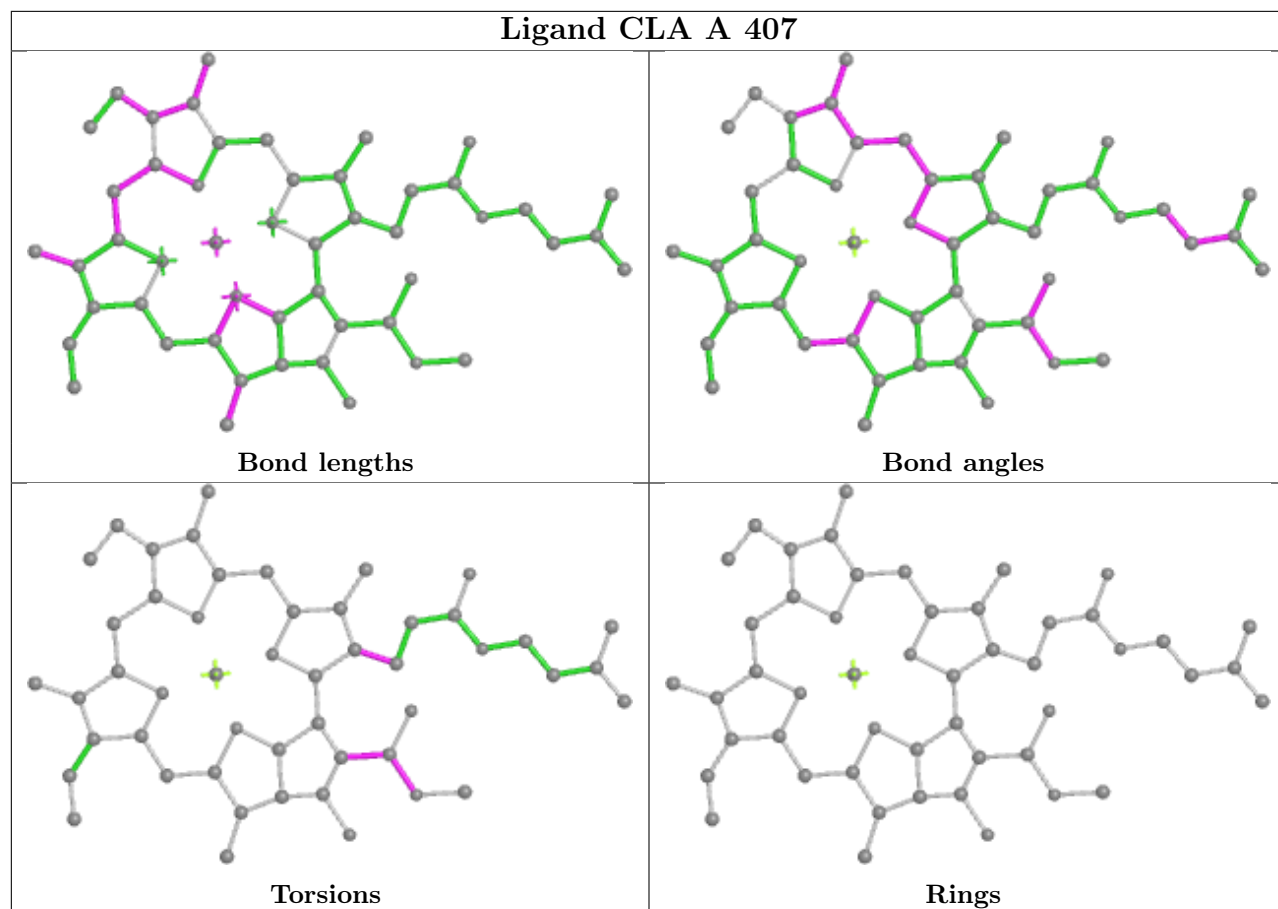
## Ligand CHL r 614



## Ligand LUT N 1620

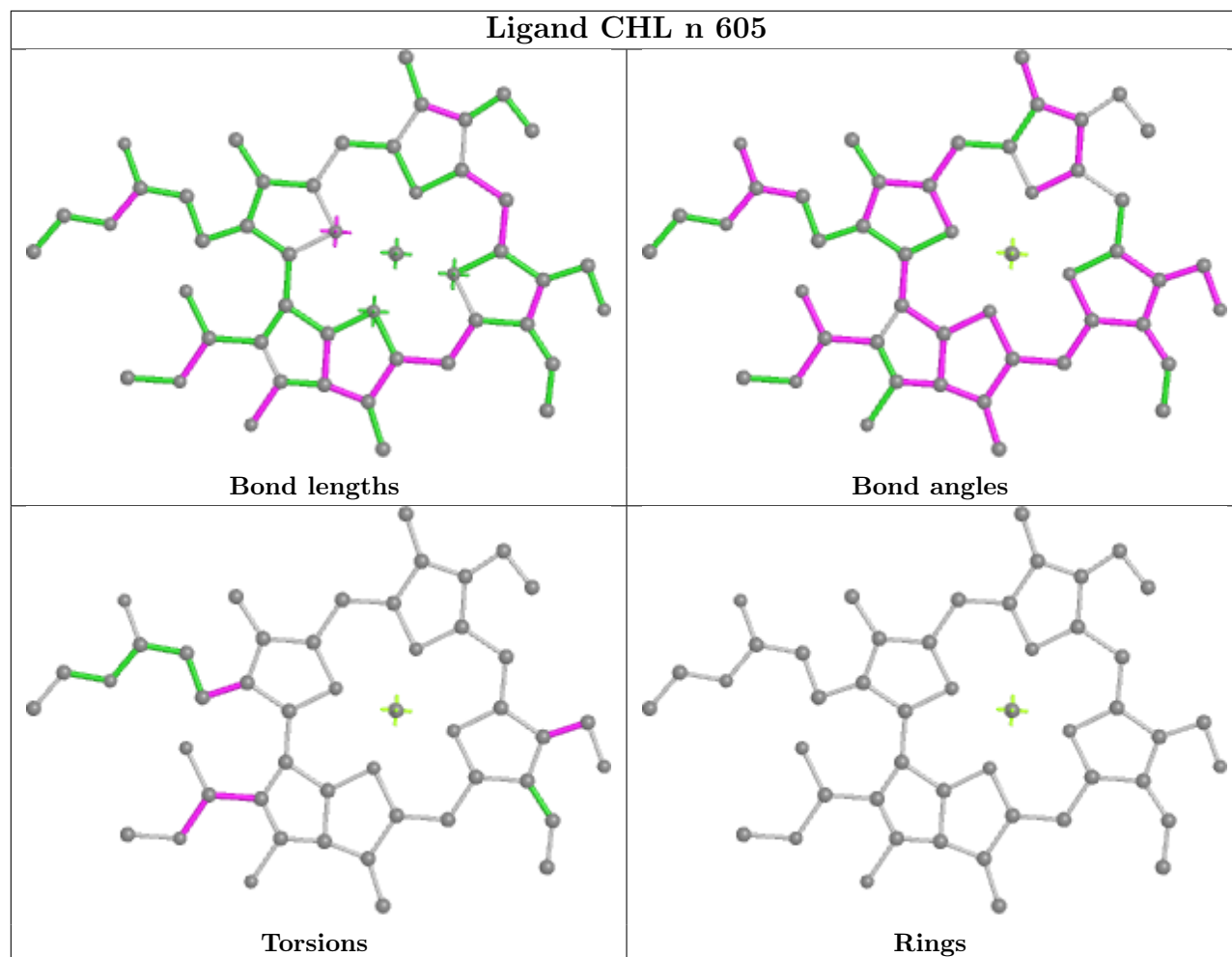




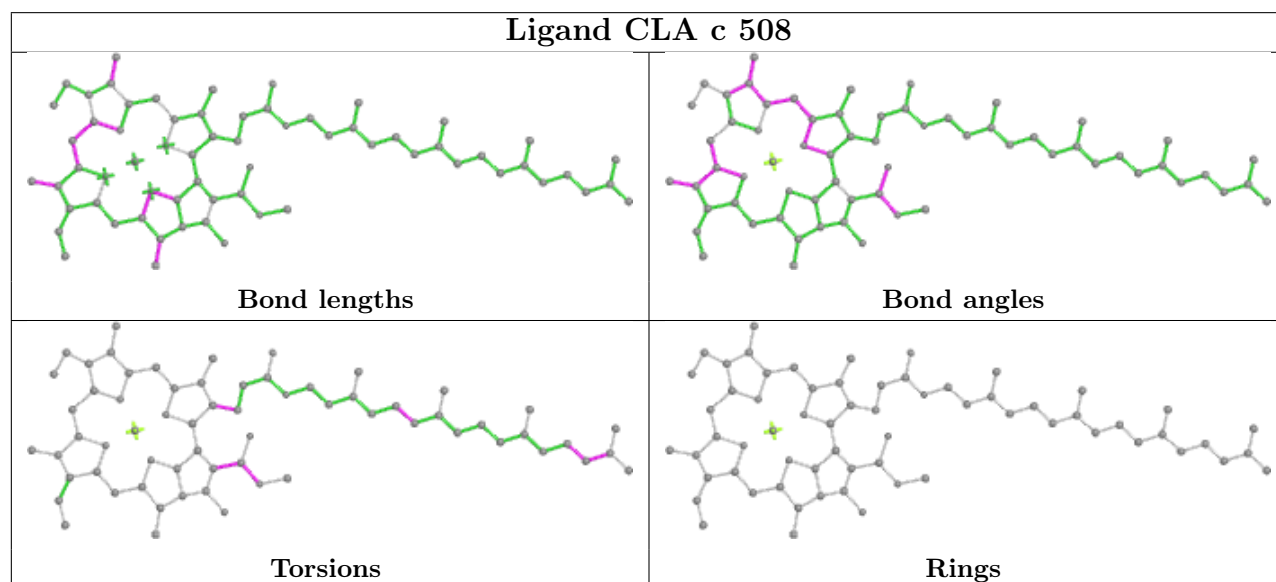


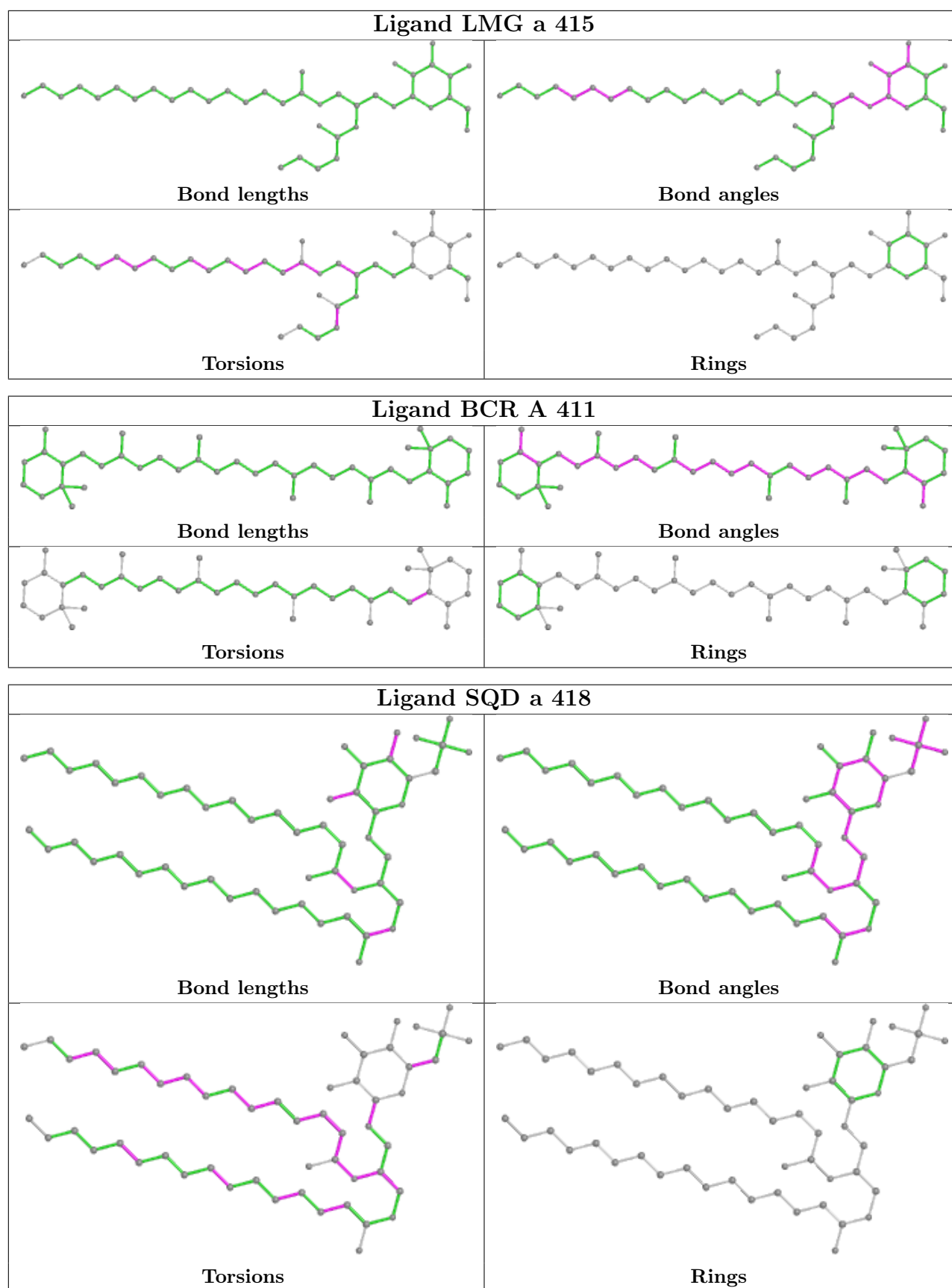


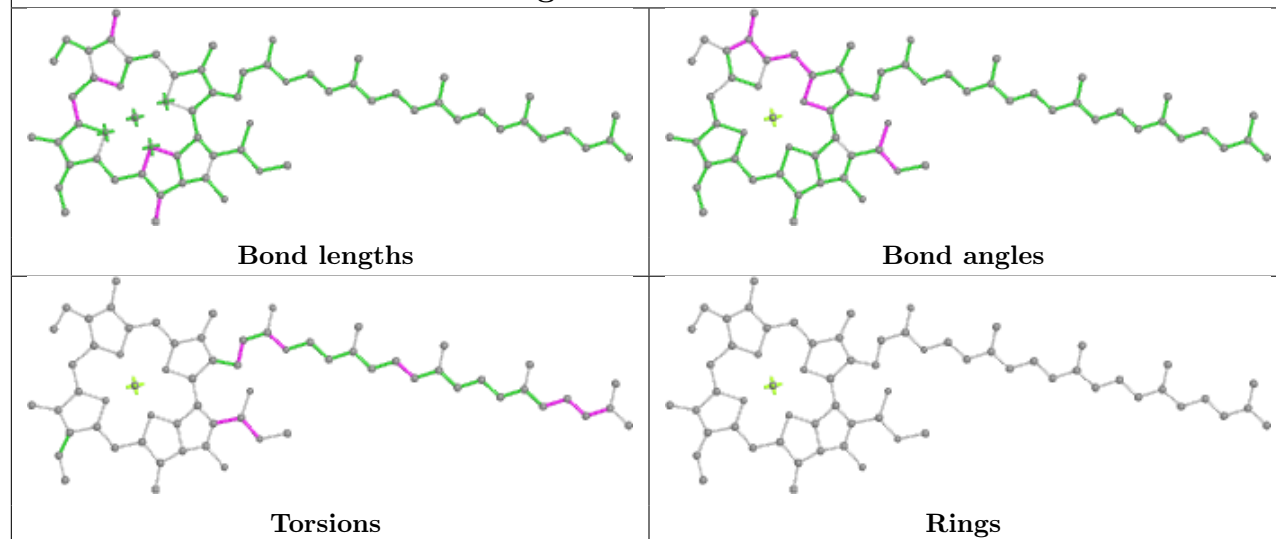
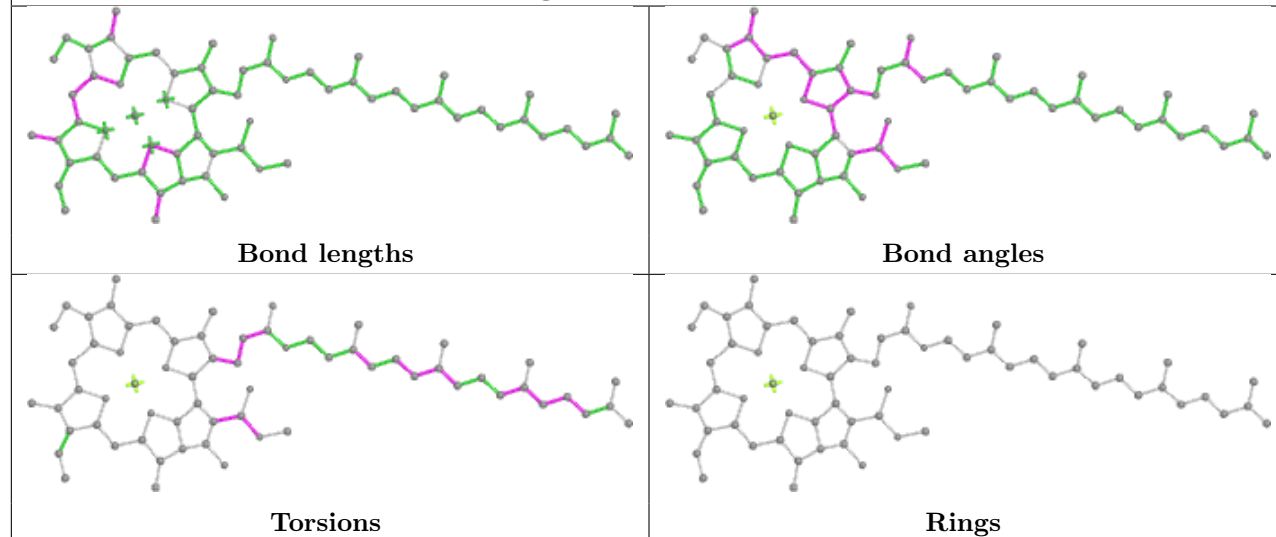
## Ligand CHL n 605



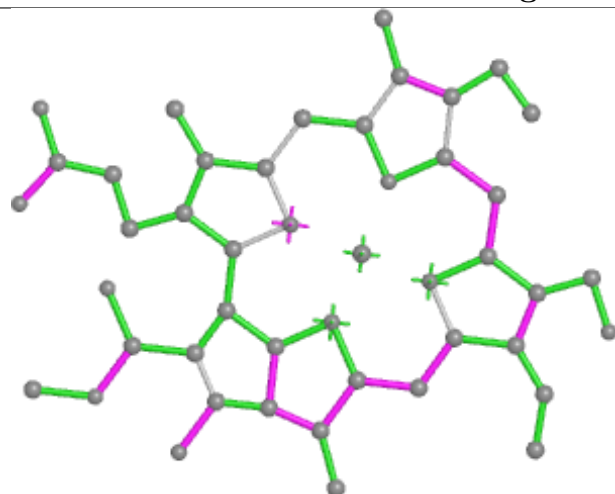
## Ligand CLA c 508



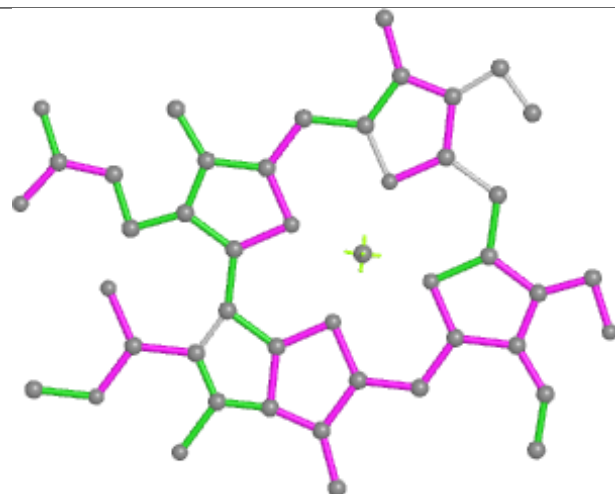


**Ligand CLA c 503****Ligand CLA c 507**

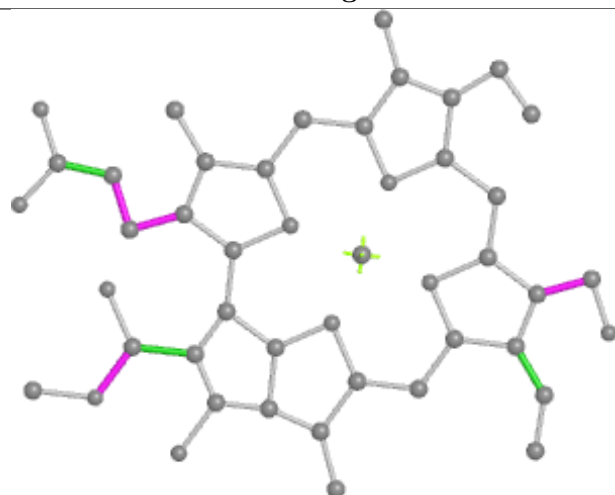
## Ligand CHL 4 606



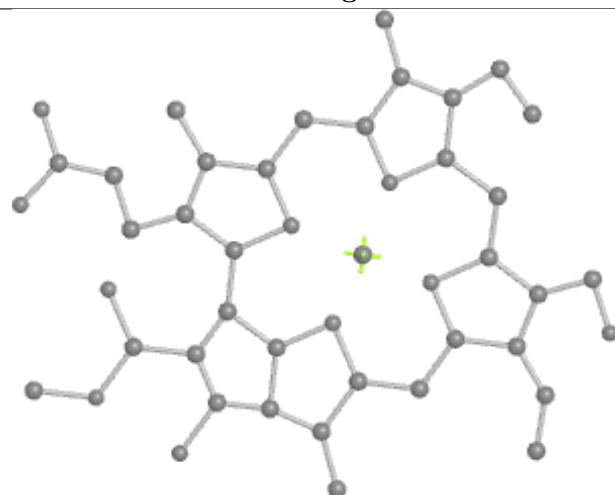
Bond lengths



Bond angles

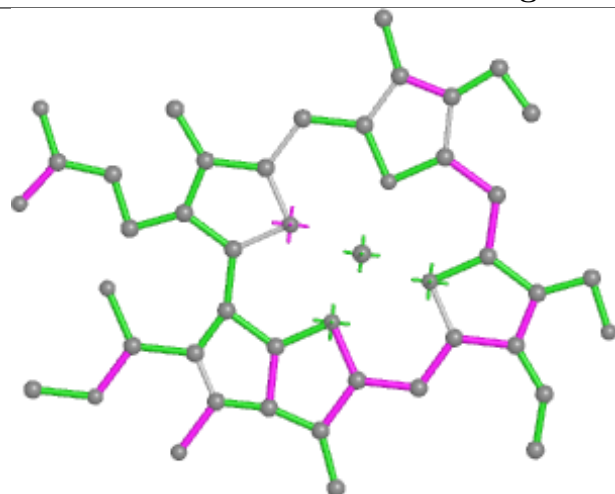


Torsions

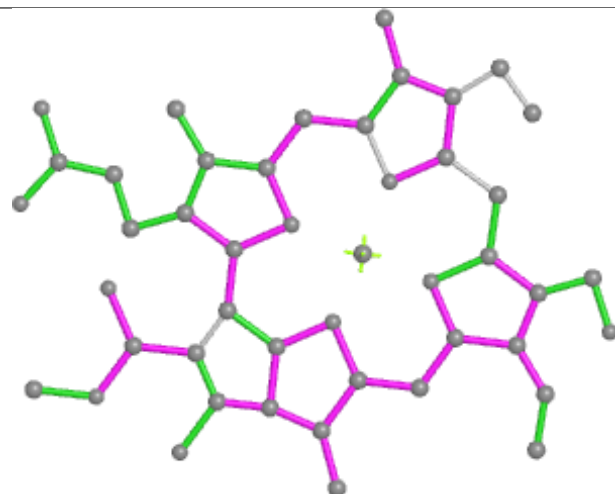


Rings

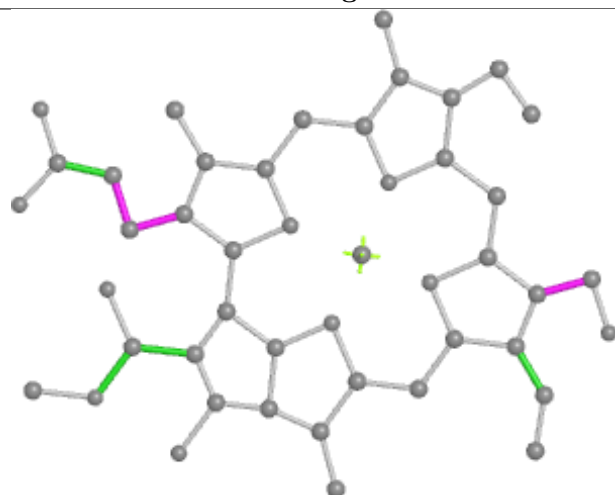
## Ligand CHL 7 606



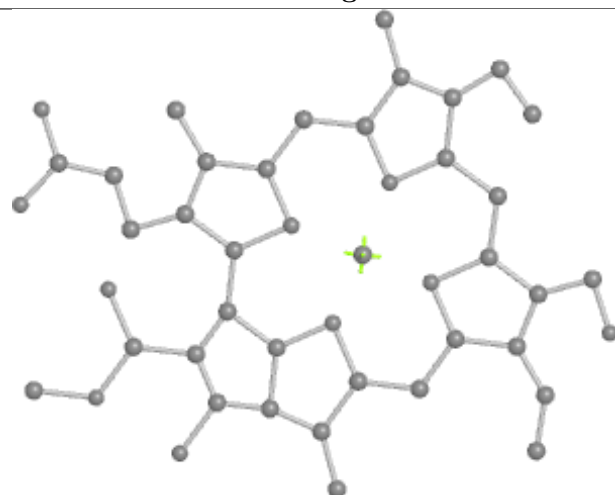
Bond lengths



Bond angles

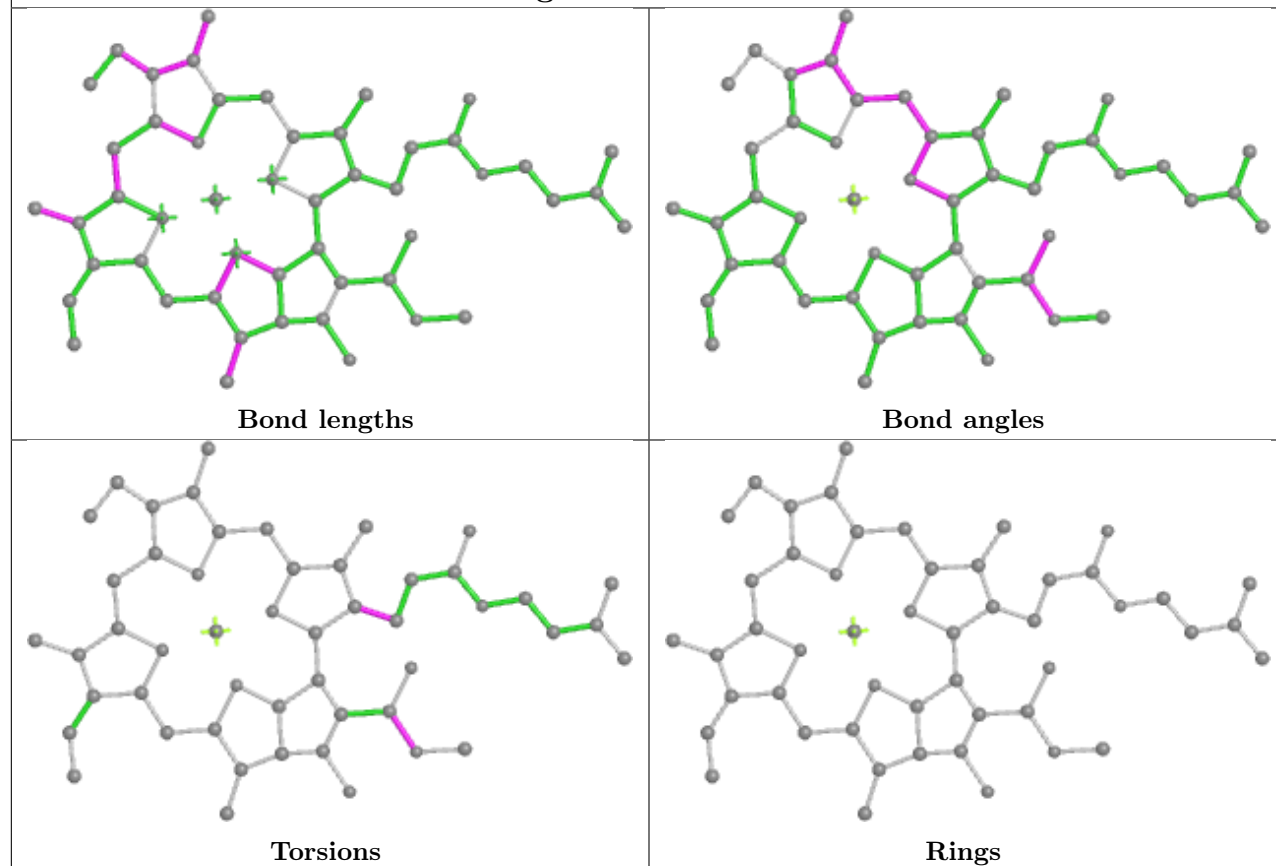


Torsions

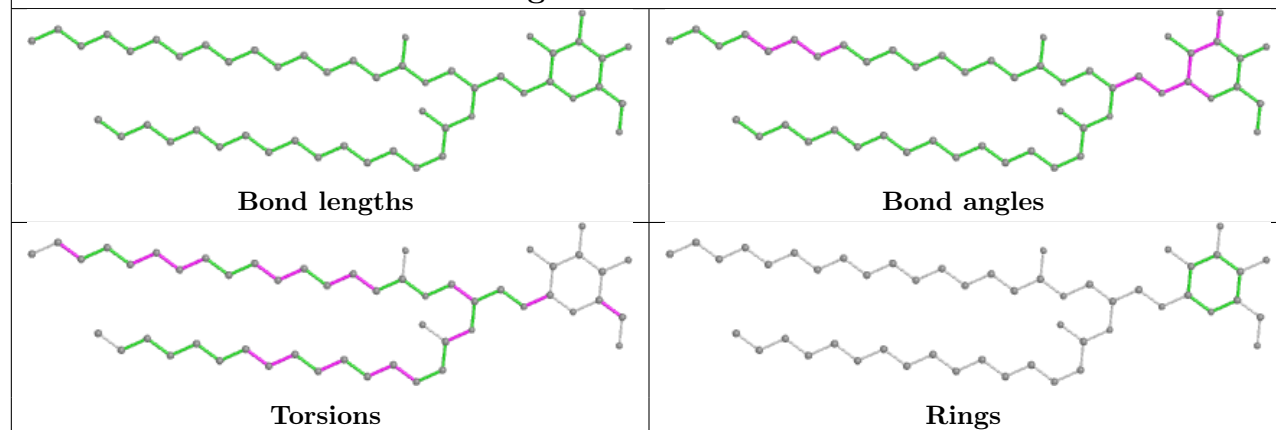


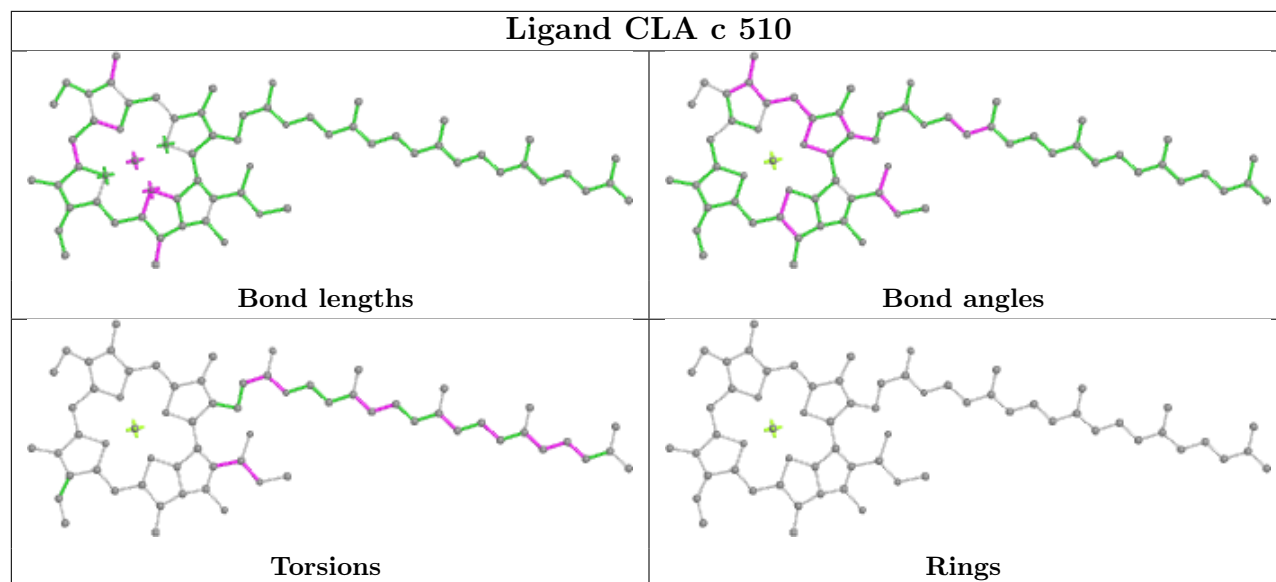
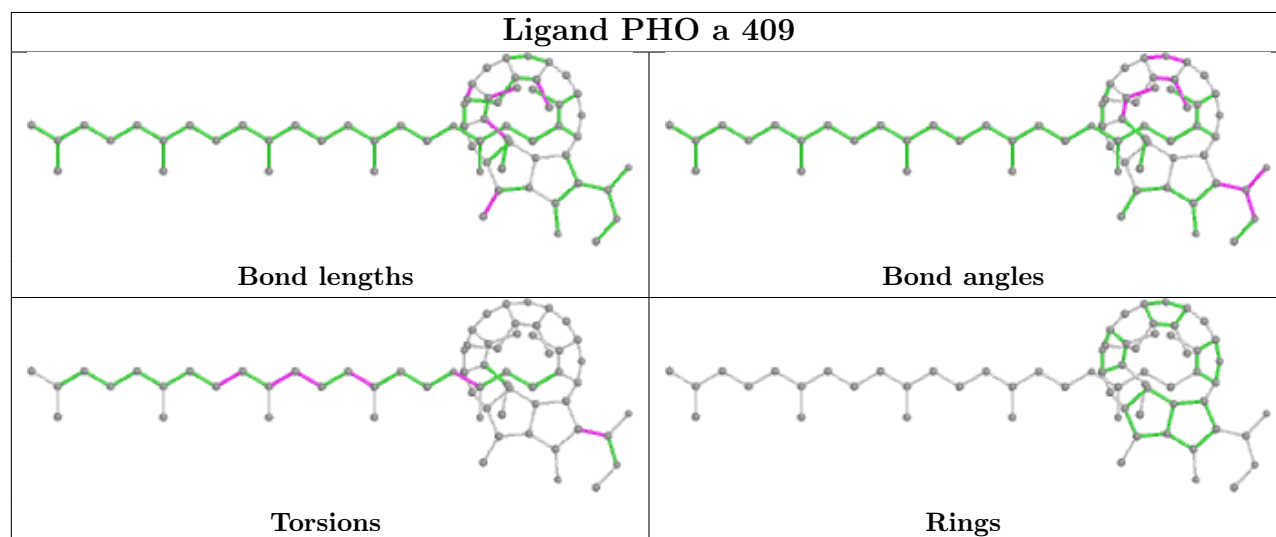
Rings

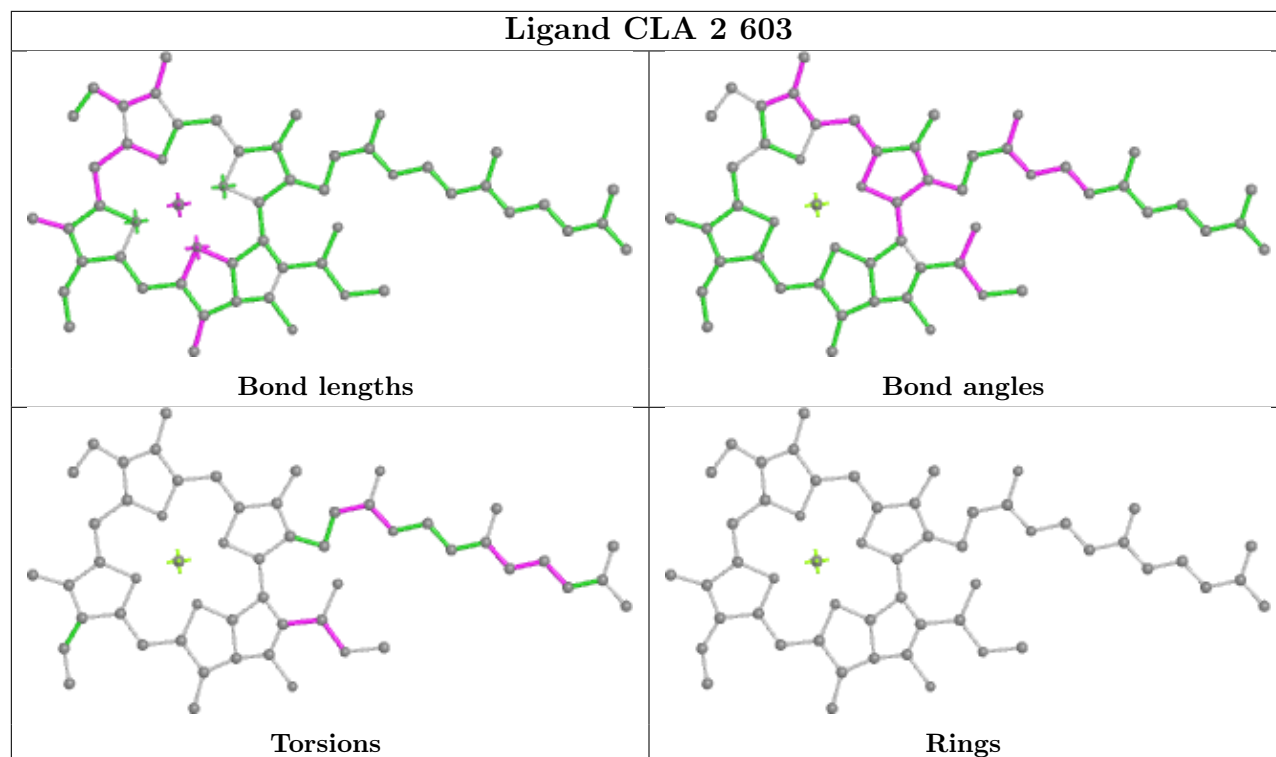
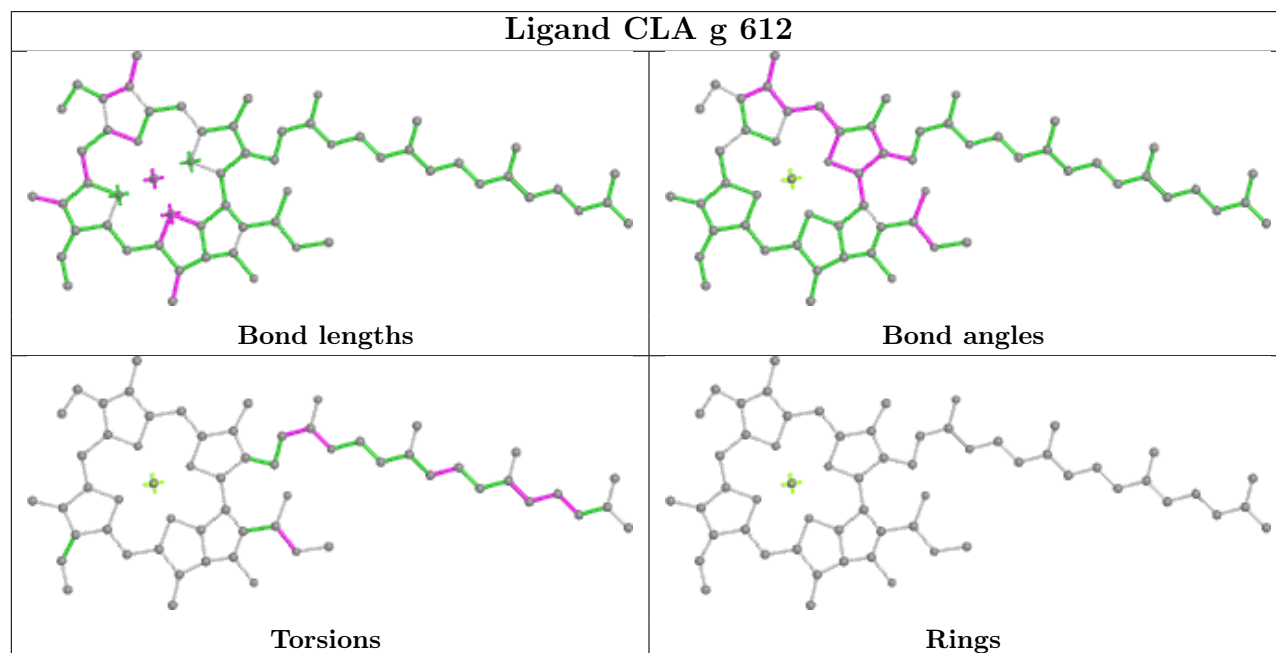
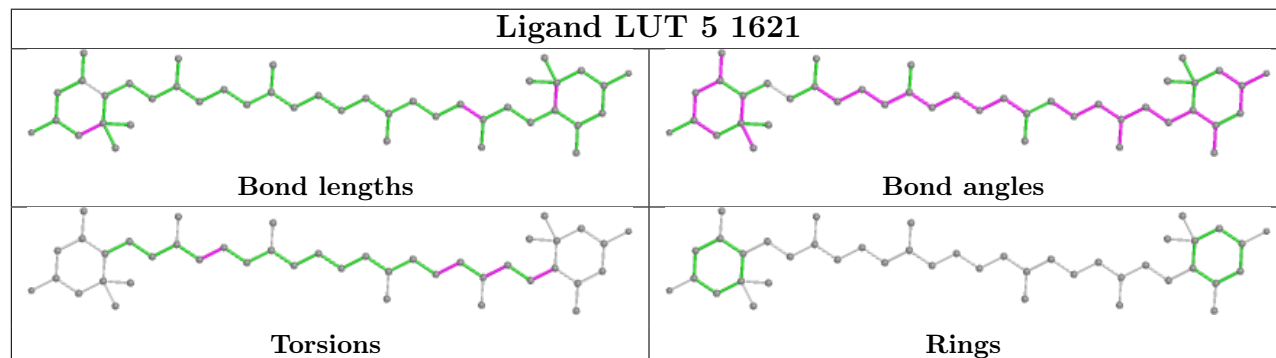
## Ligand CLA 2 610



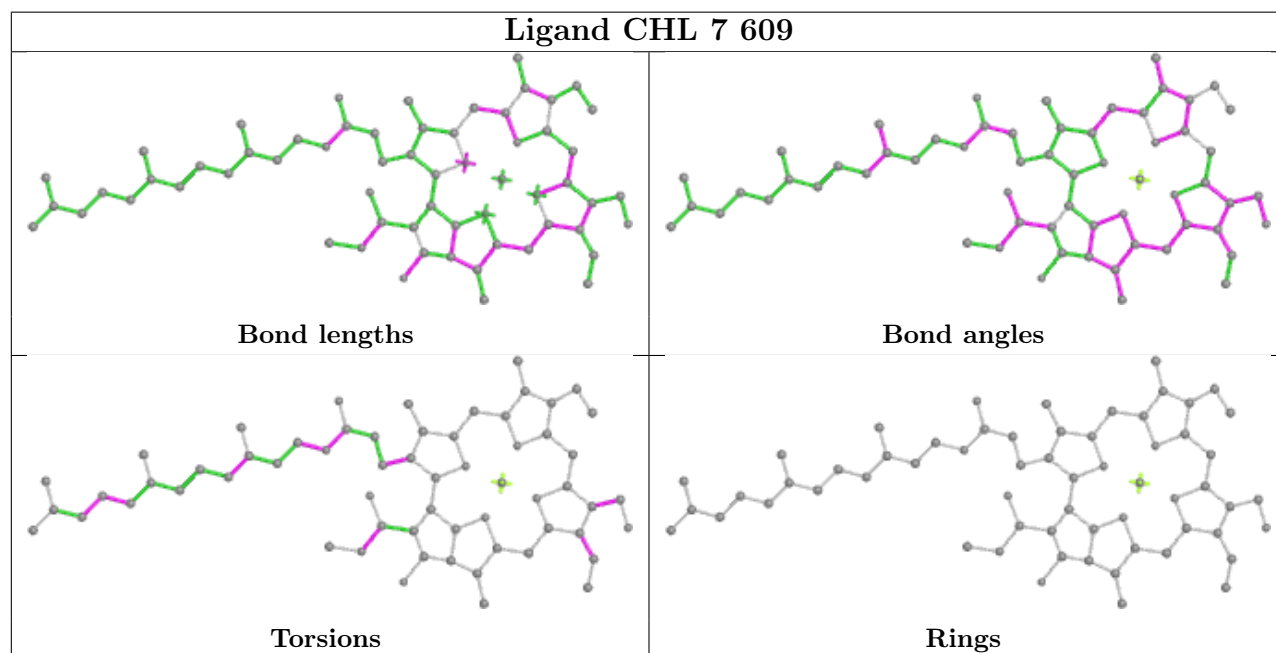
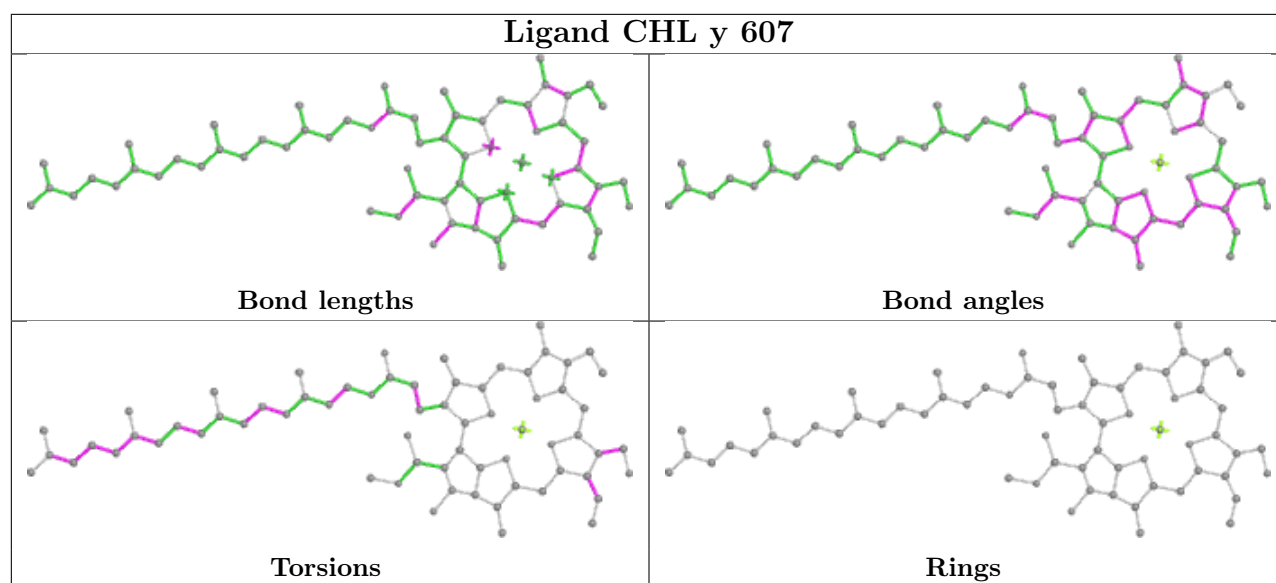
## Ligand LMG C 521

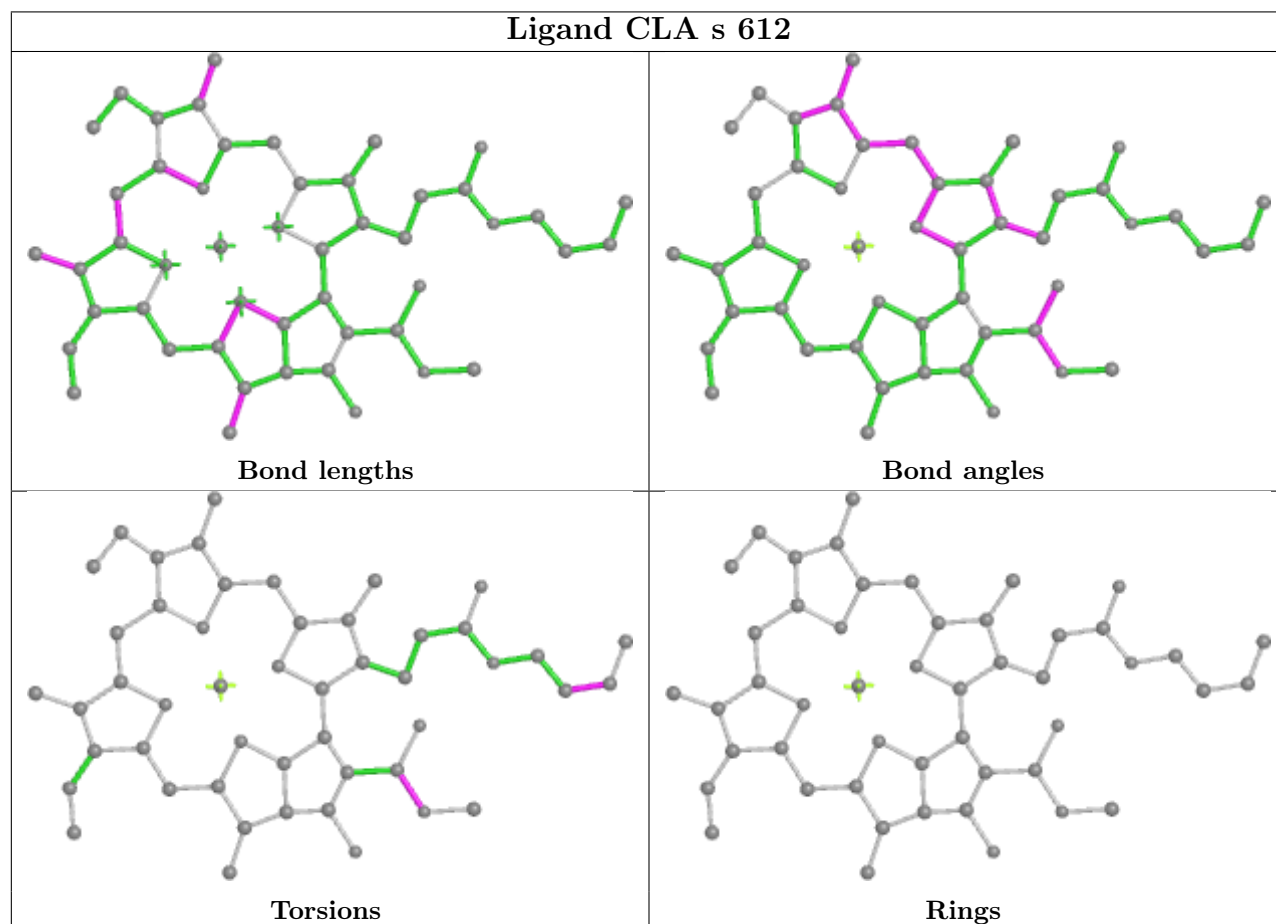
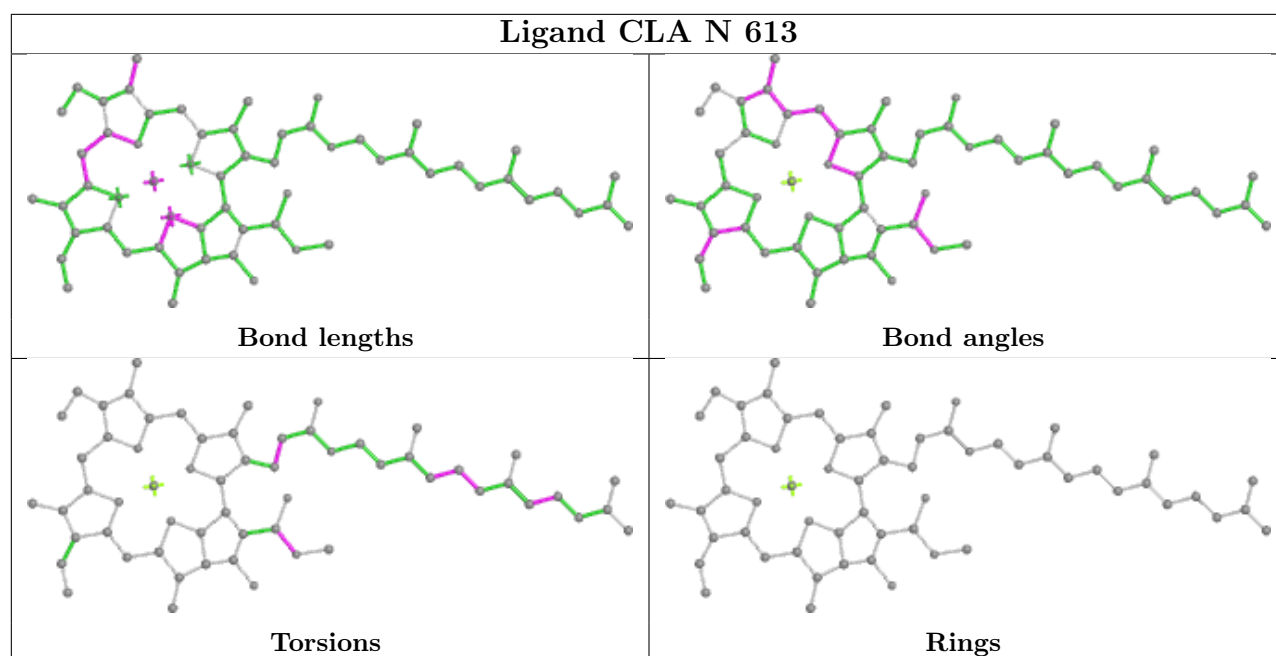


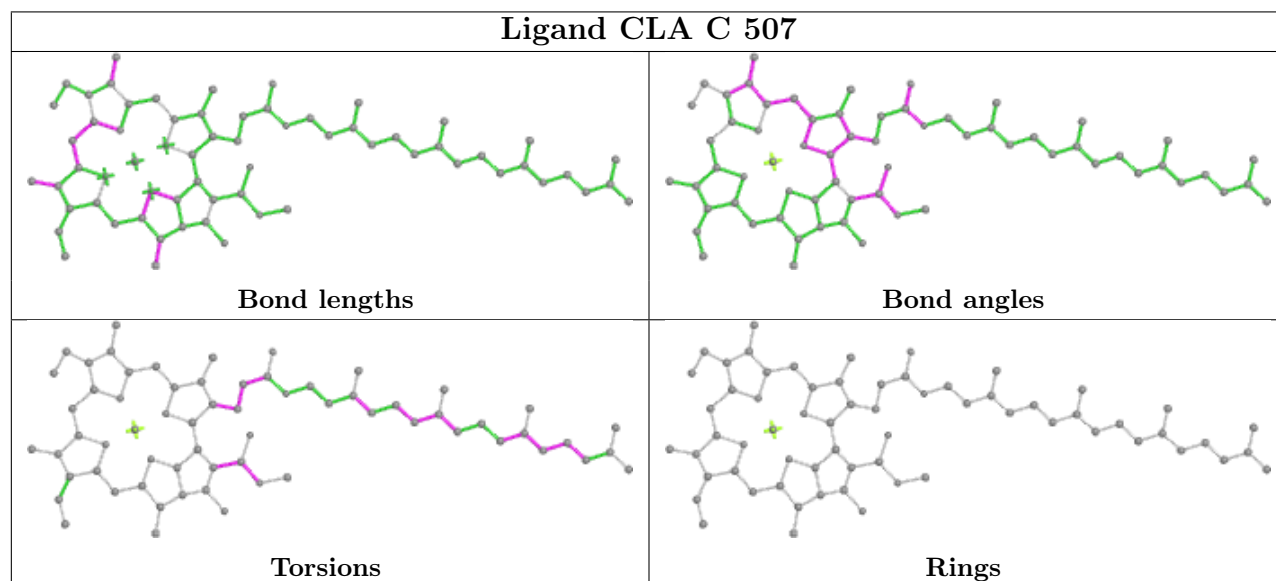
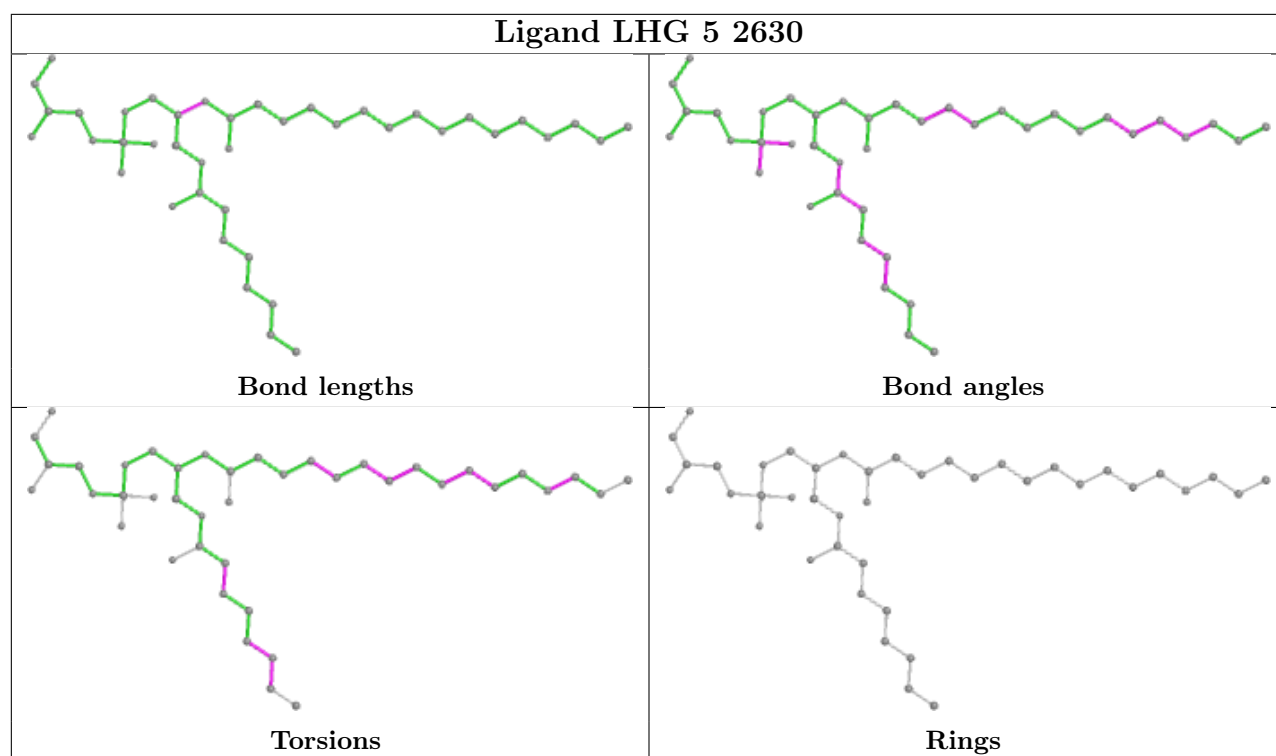
**Ligand CLA c 510****Ligand PHO a 409**

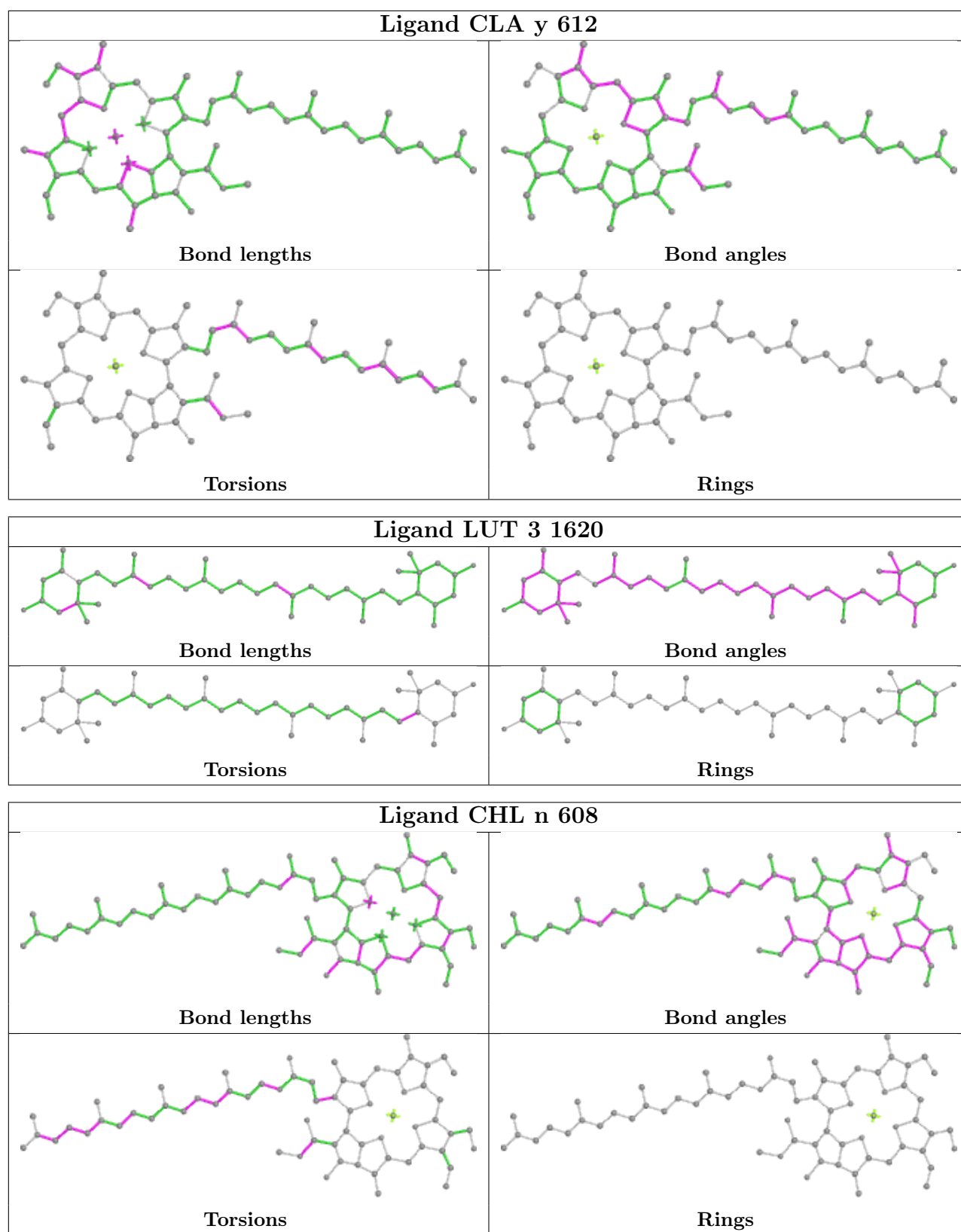
**Ligand CLA 2 603****Ligand CLA g 612****Ligand LUT 5 1621**



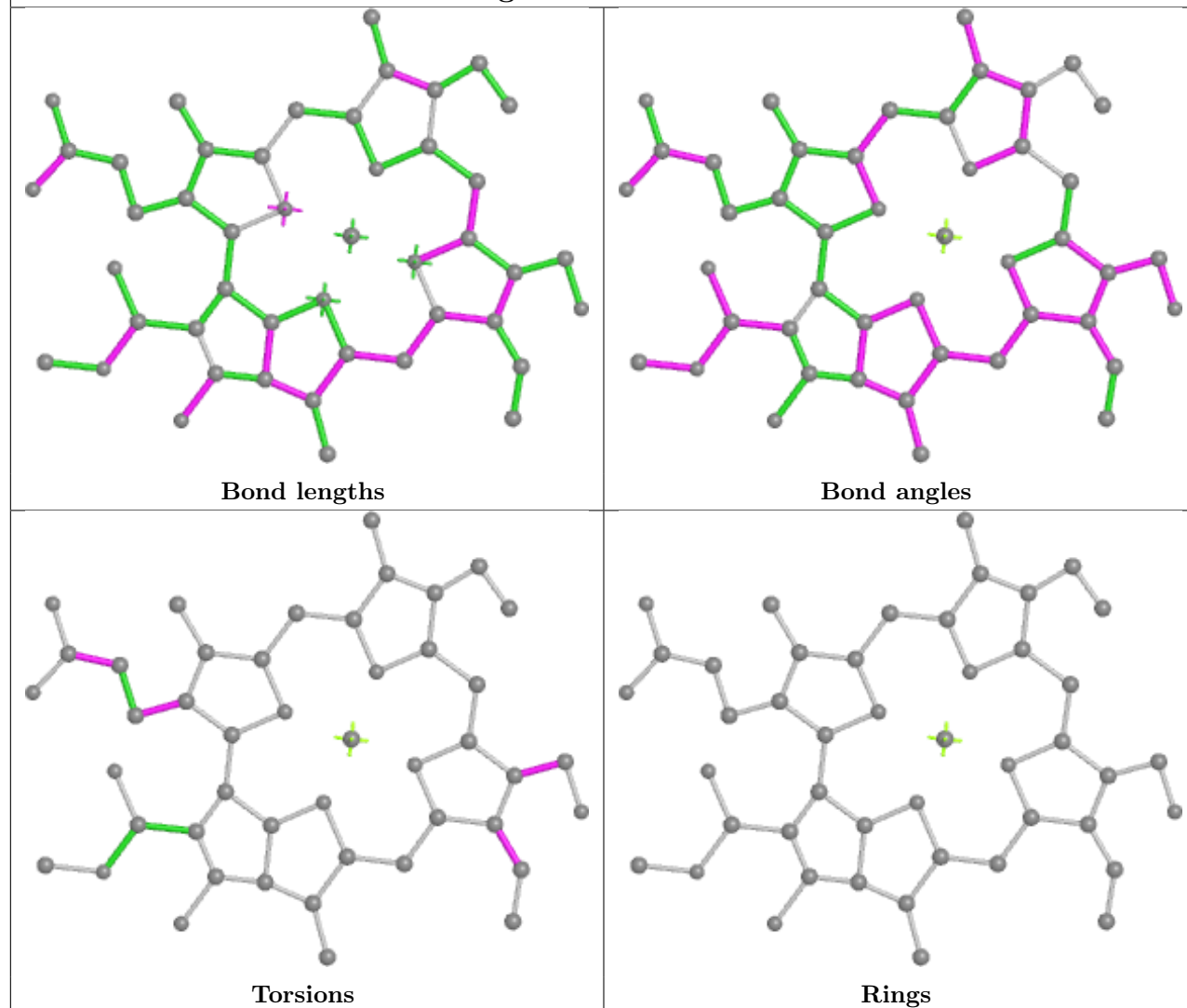




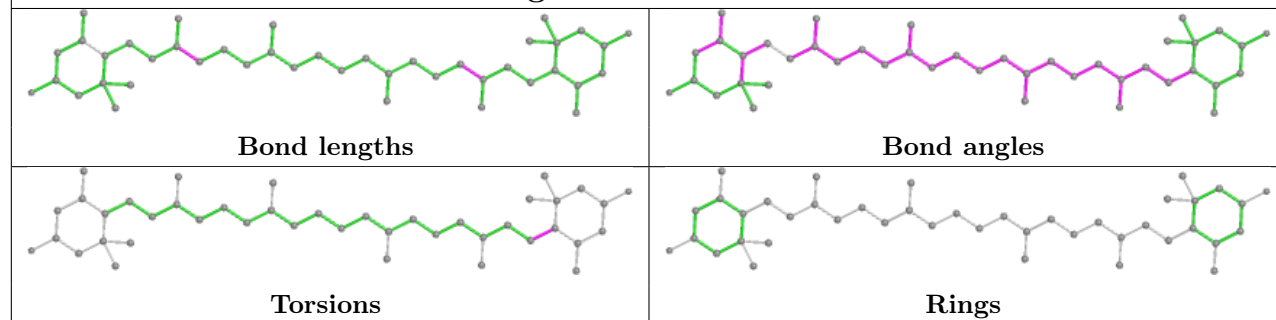


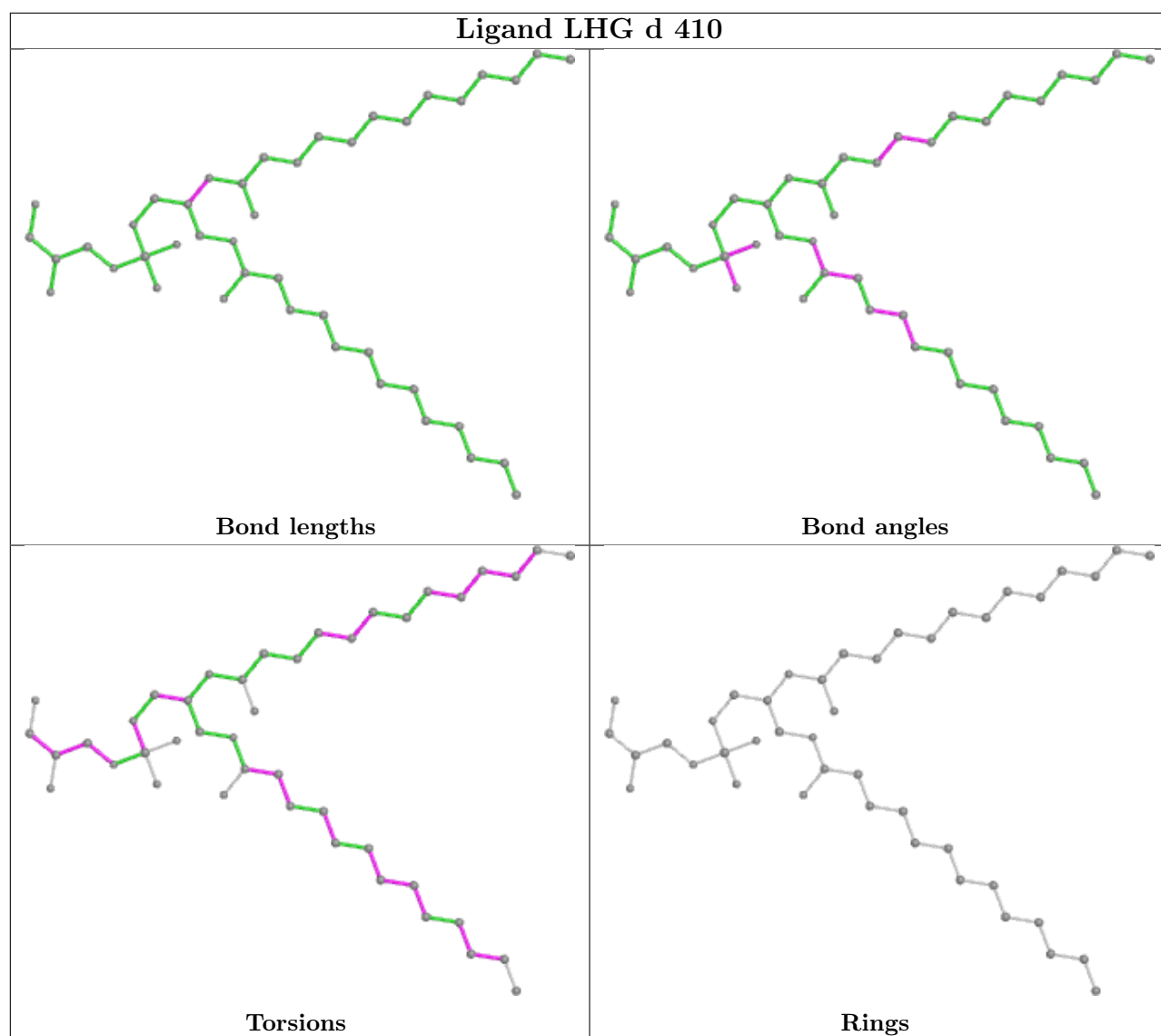


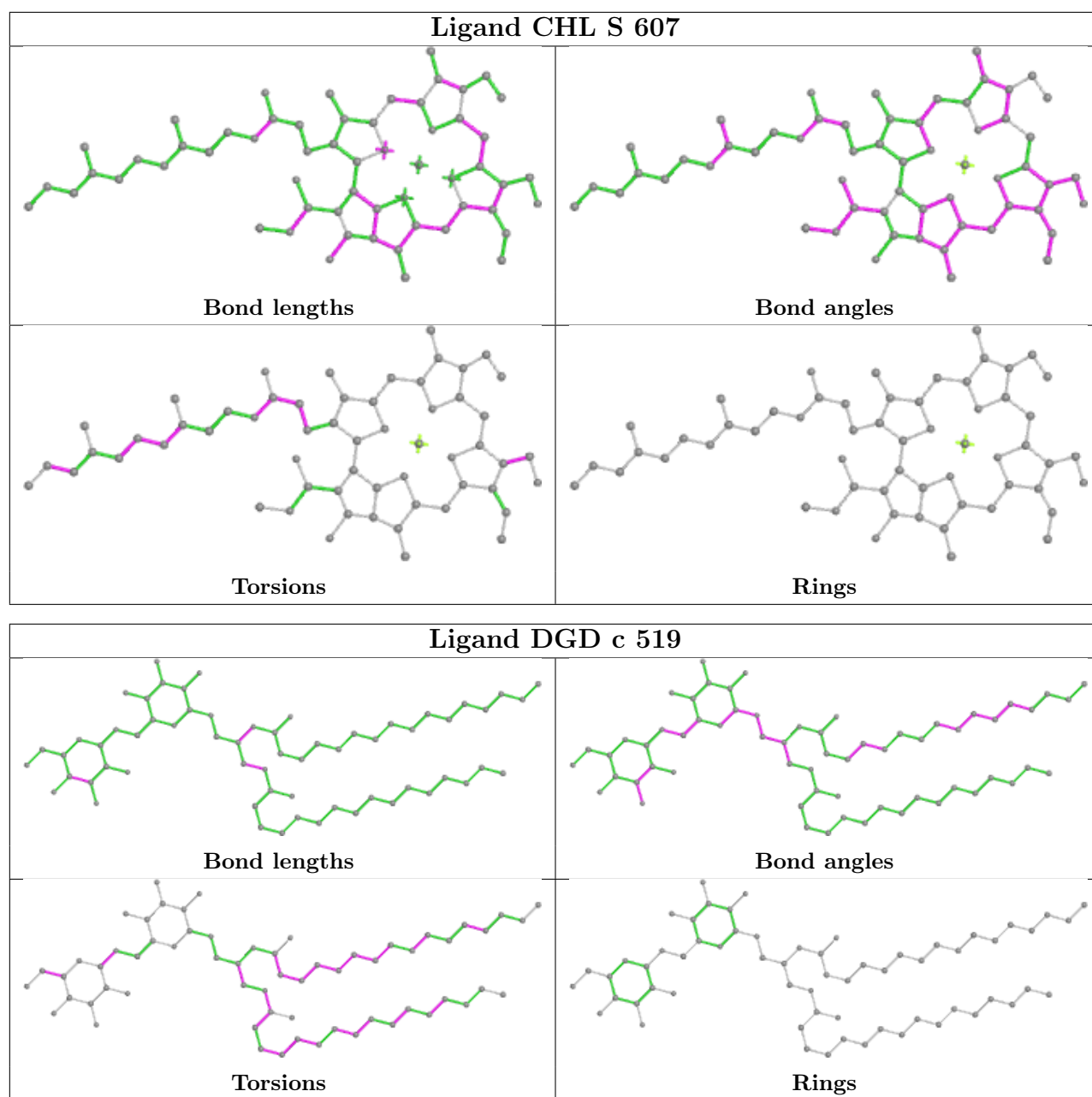
## Ligand CHL 4 609

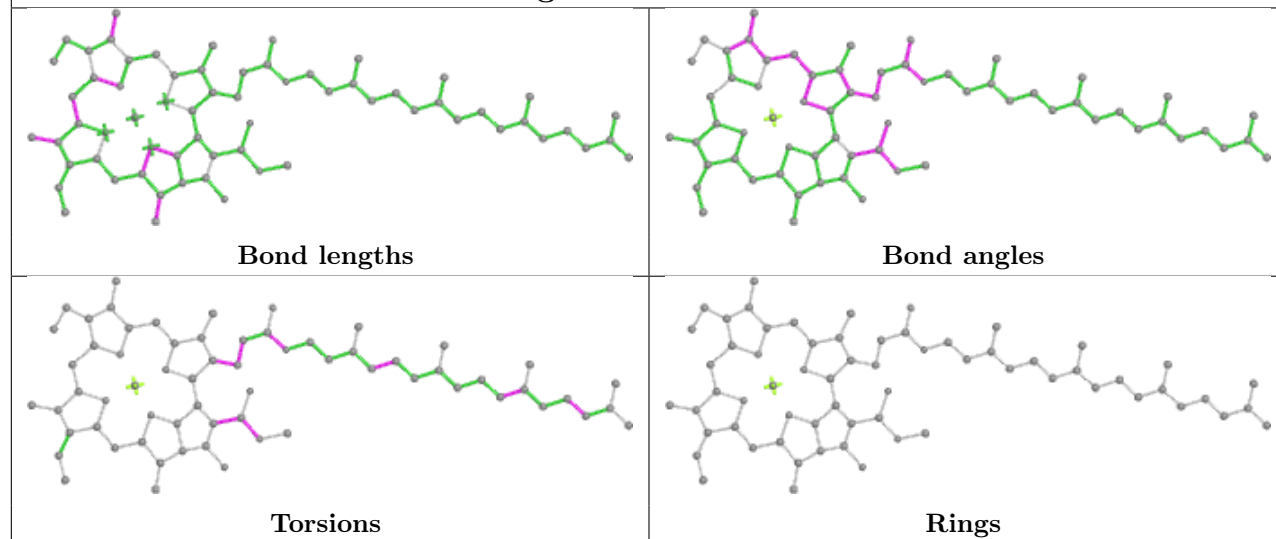
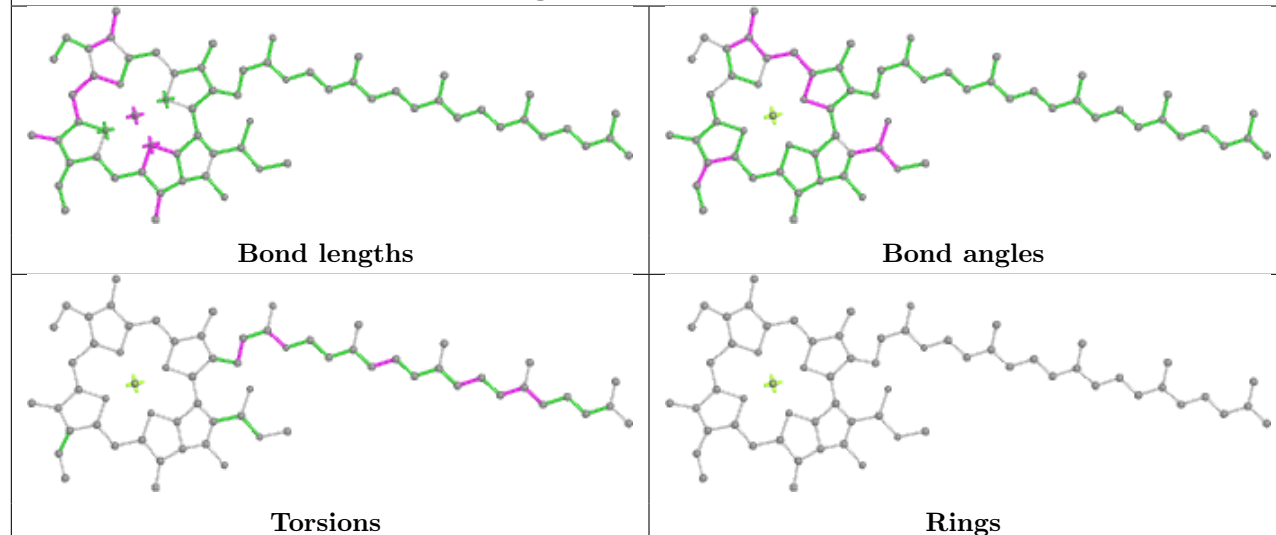
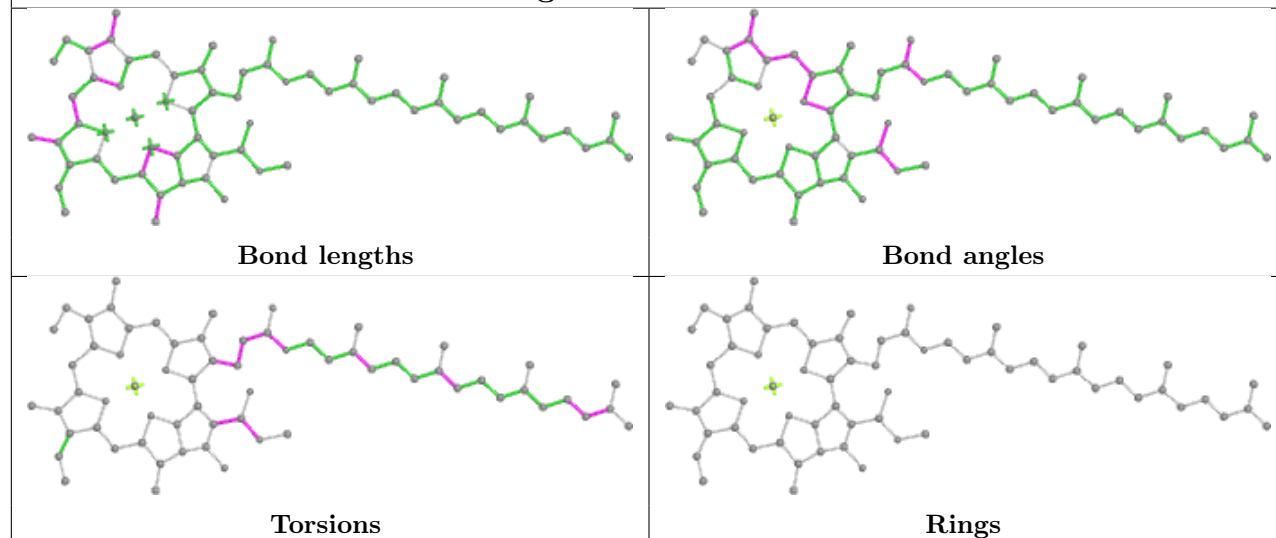


## Ligand LUT 5 1620

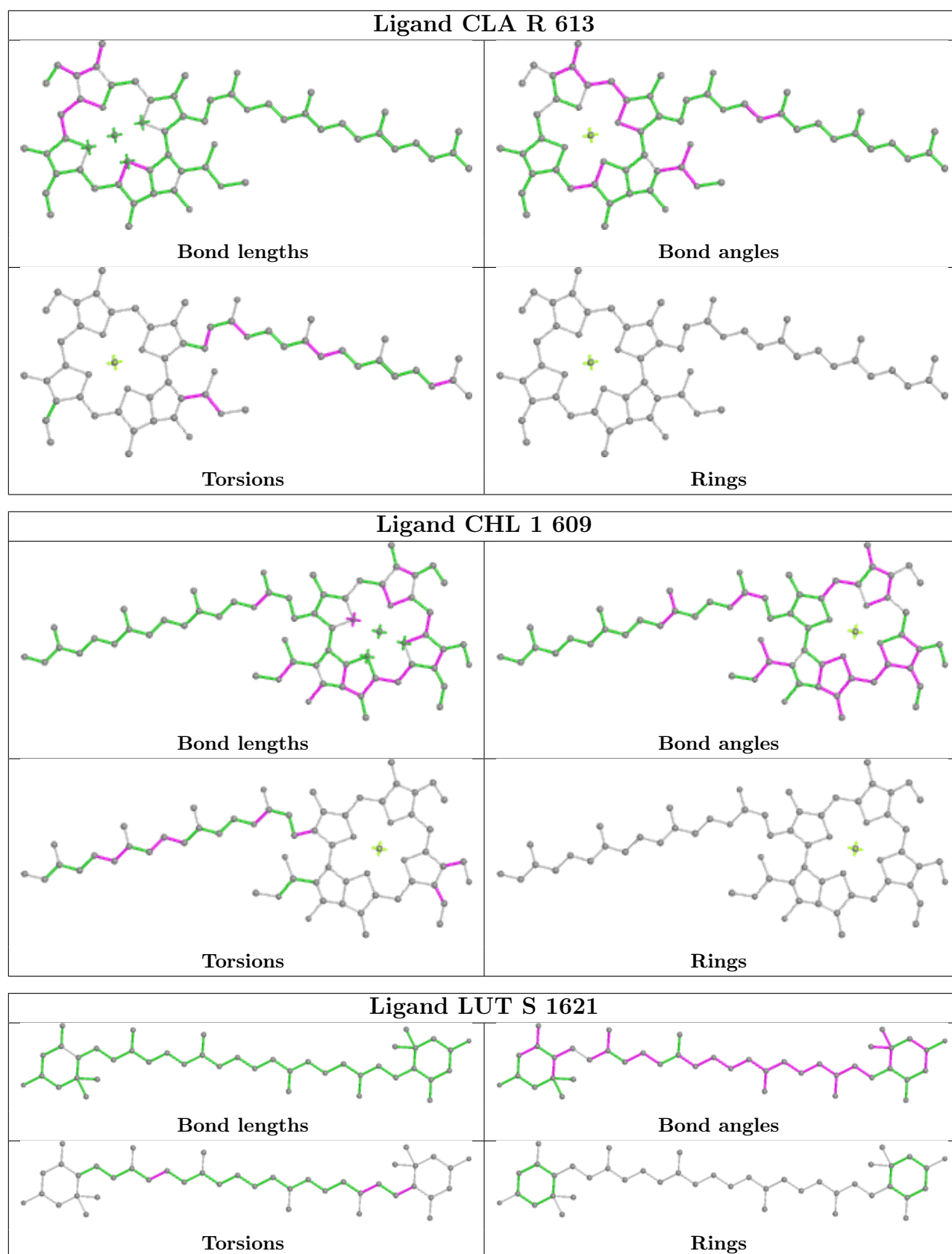




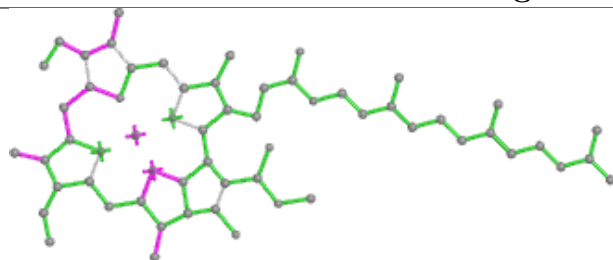


**Ligand CLA c 513****Ligand CLA Y 613****Ligand CLA c 501**

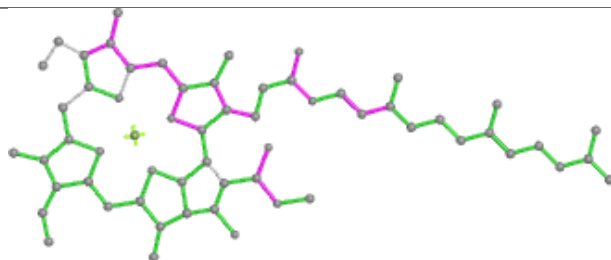




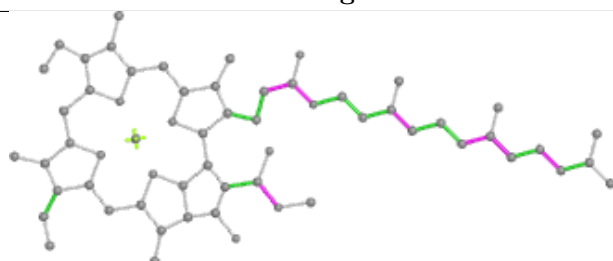
## Ligand CLA Y 612



Bond lengths



Bond angles

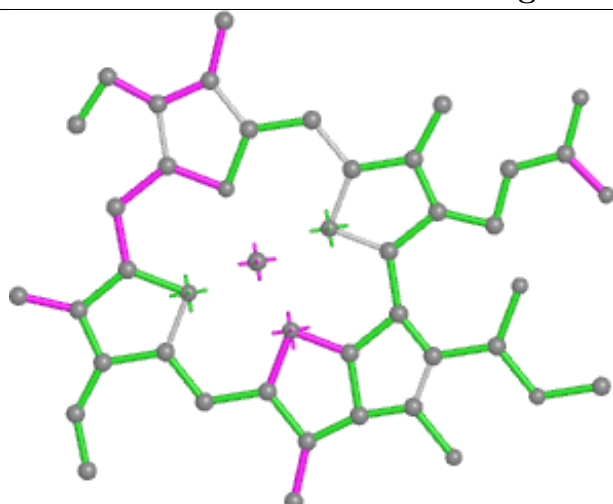


Torsions

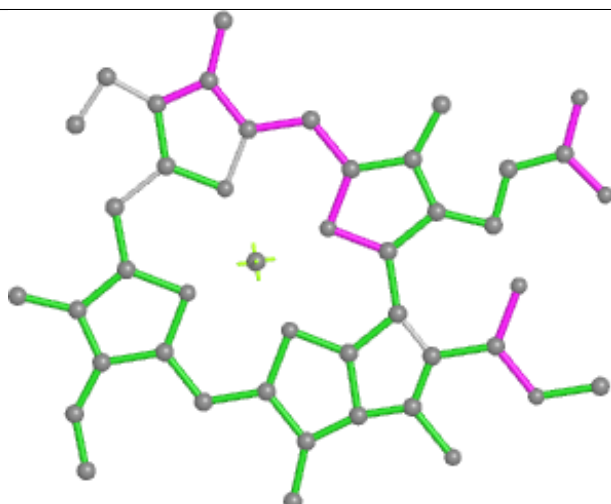


Rings

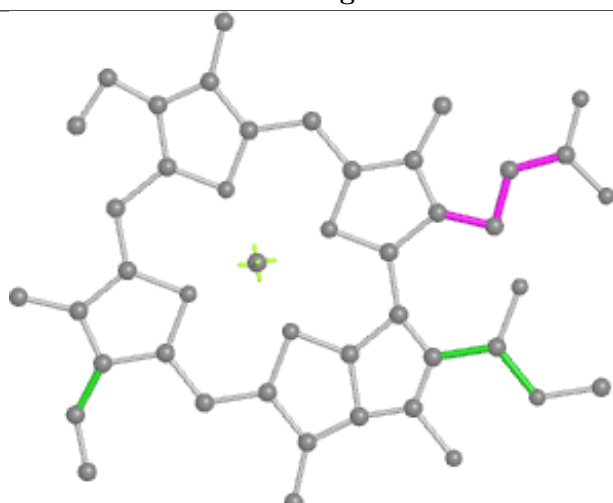
## Ligand CLA 1 611



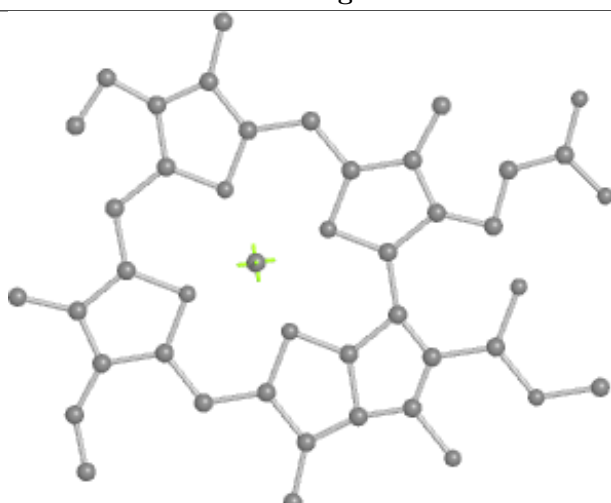
Bond lengths



Bond angles

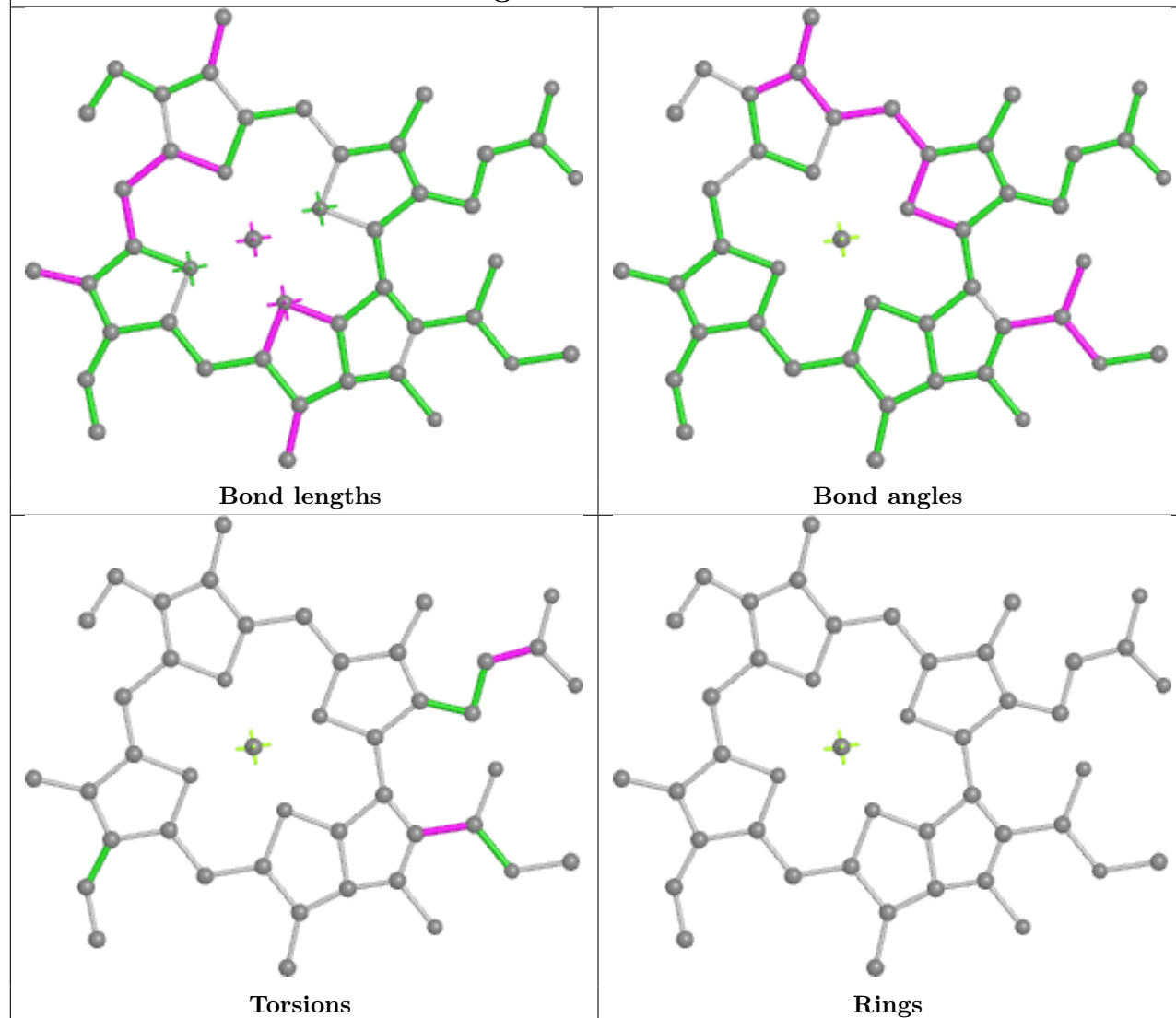


Torsions

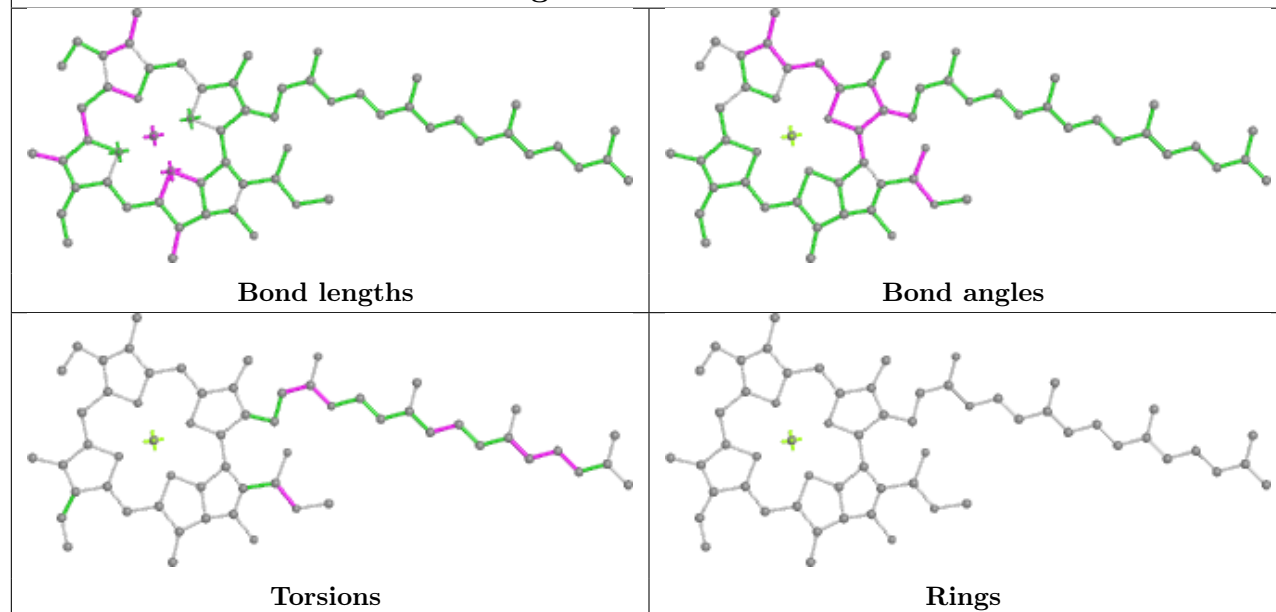


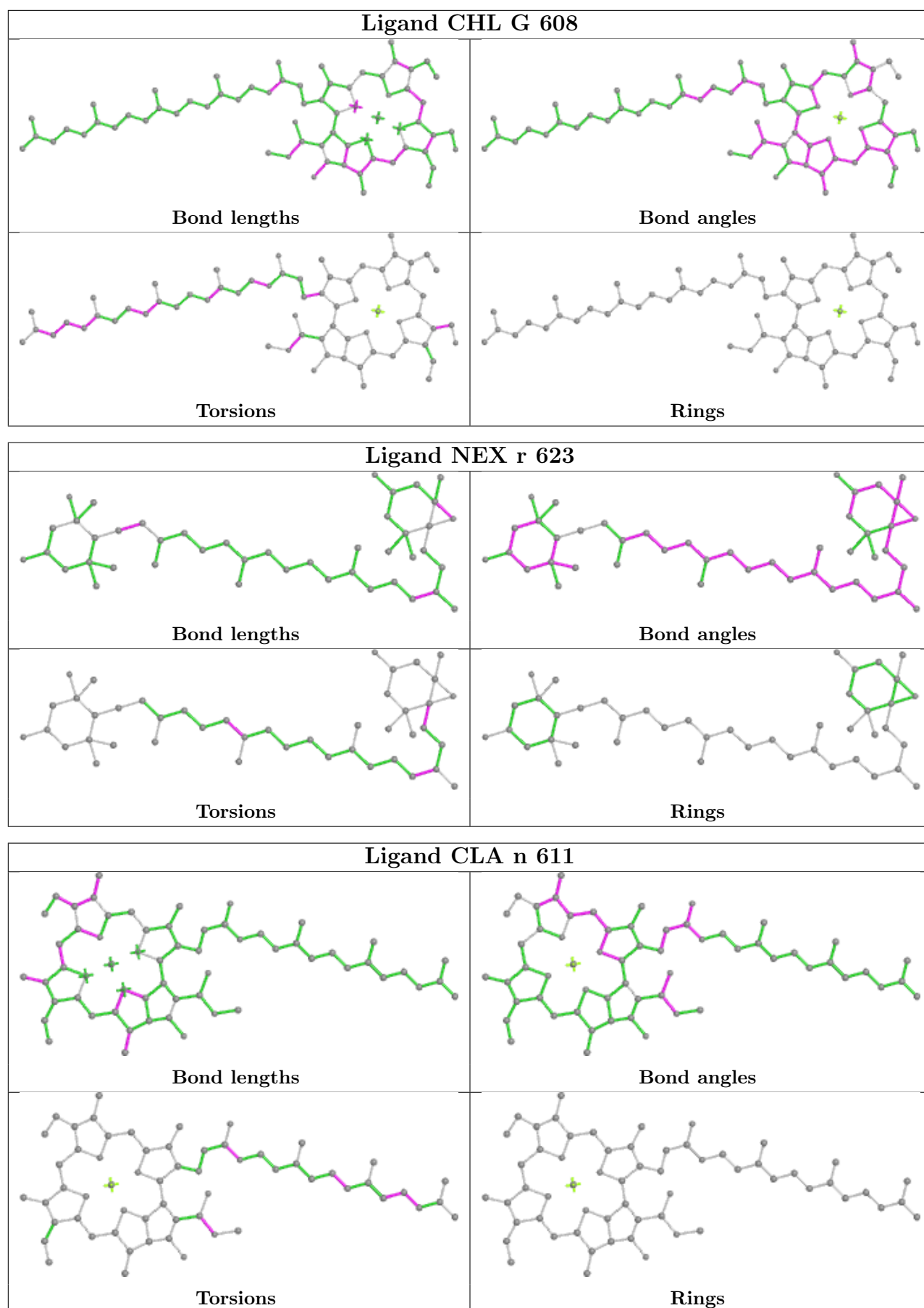
Rings

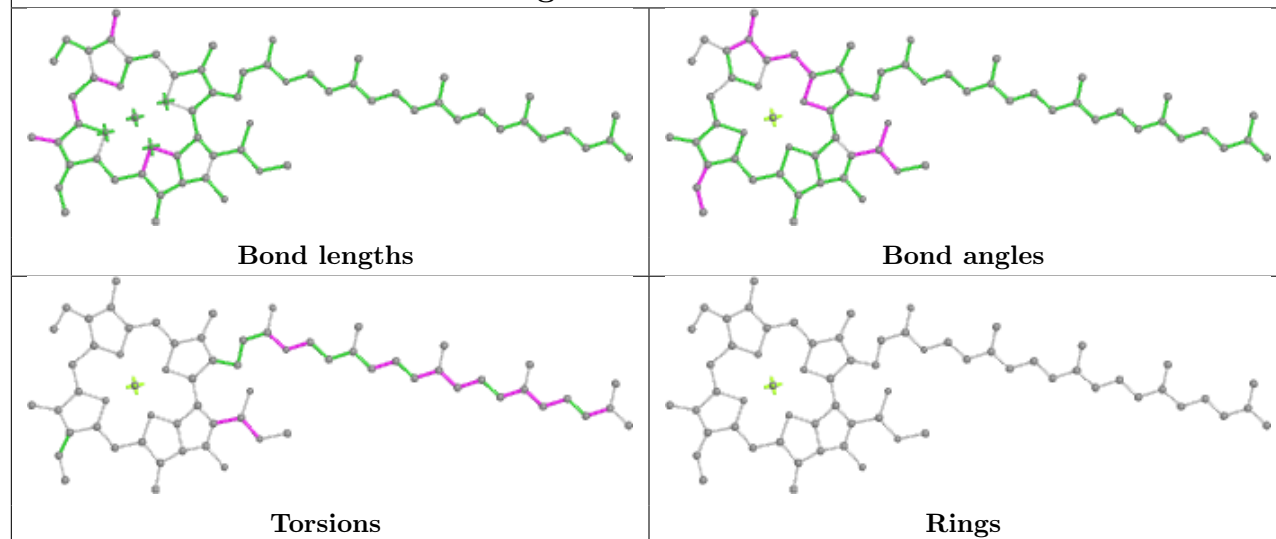
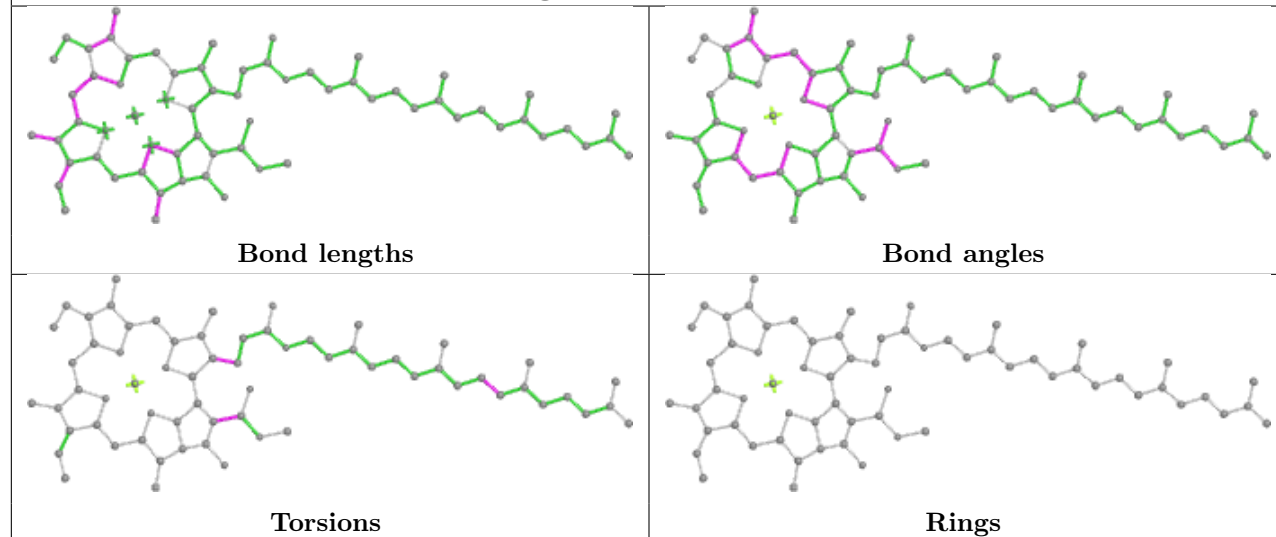
## Ligand CLA 6 611

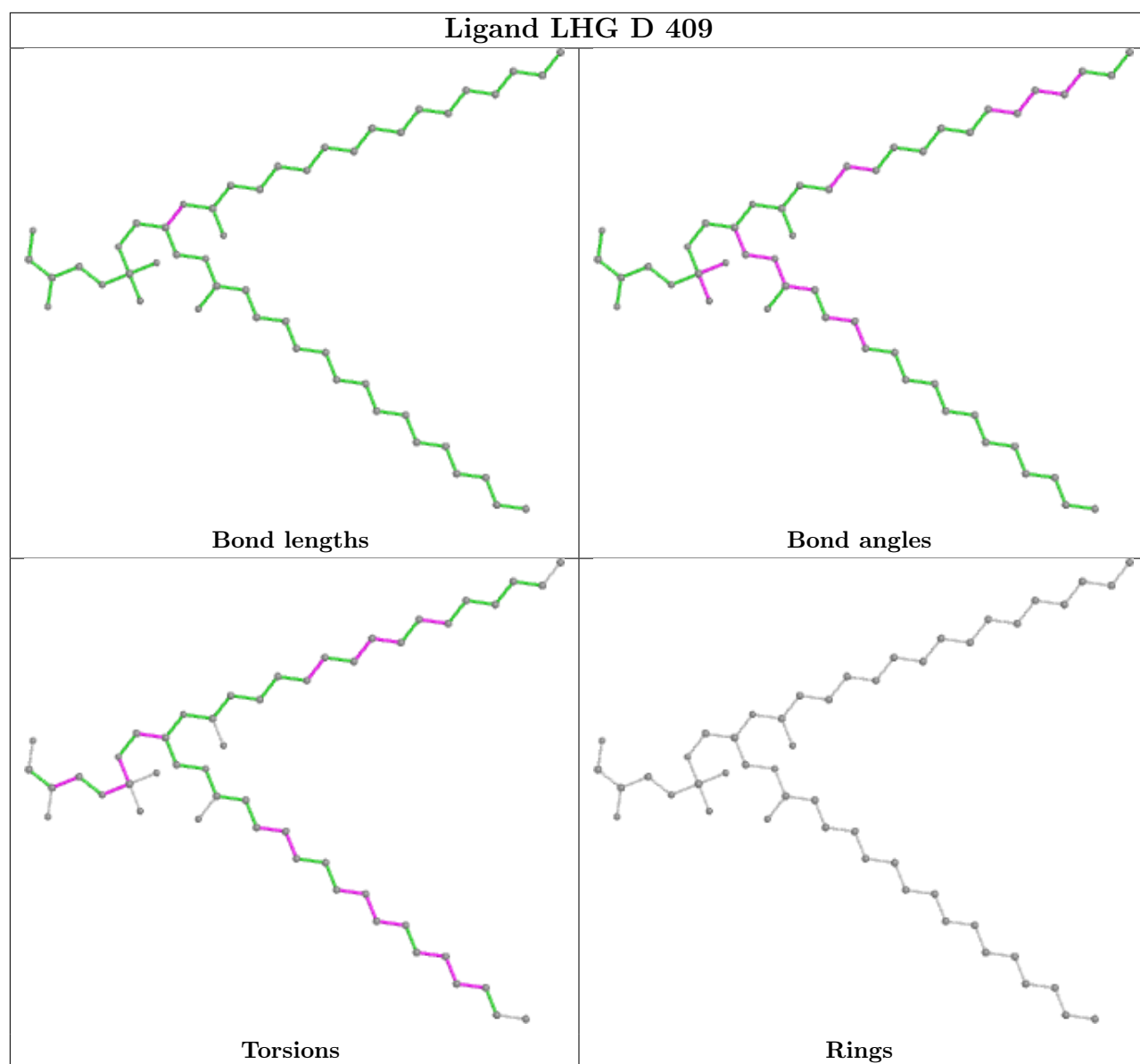


## Ligand CLA G 612

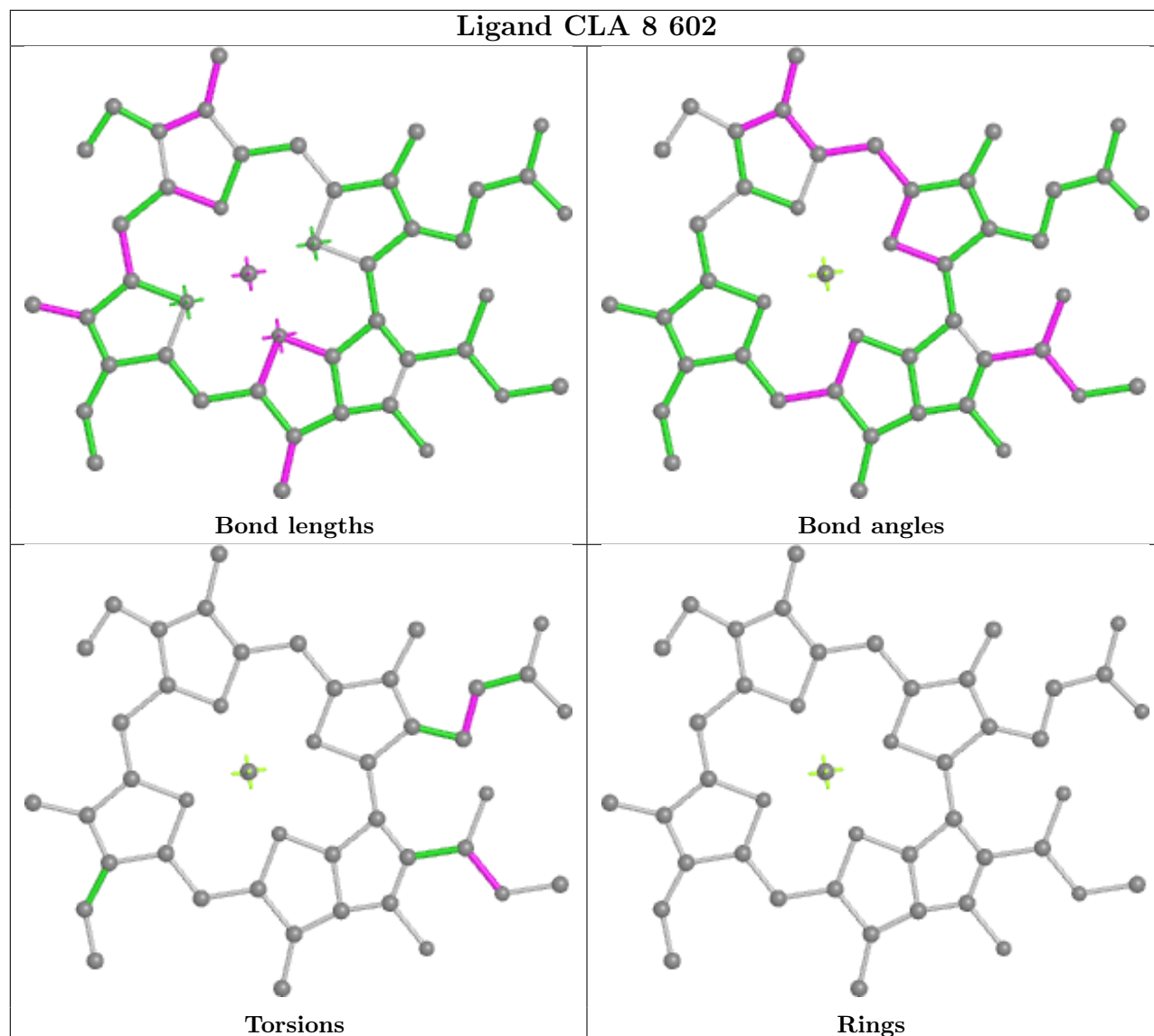




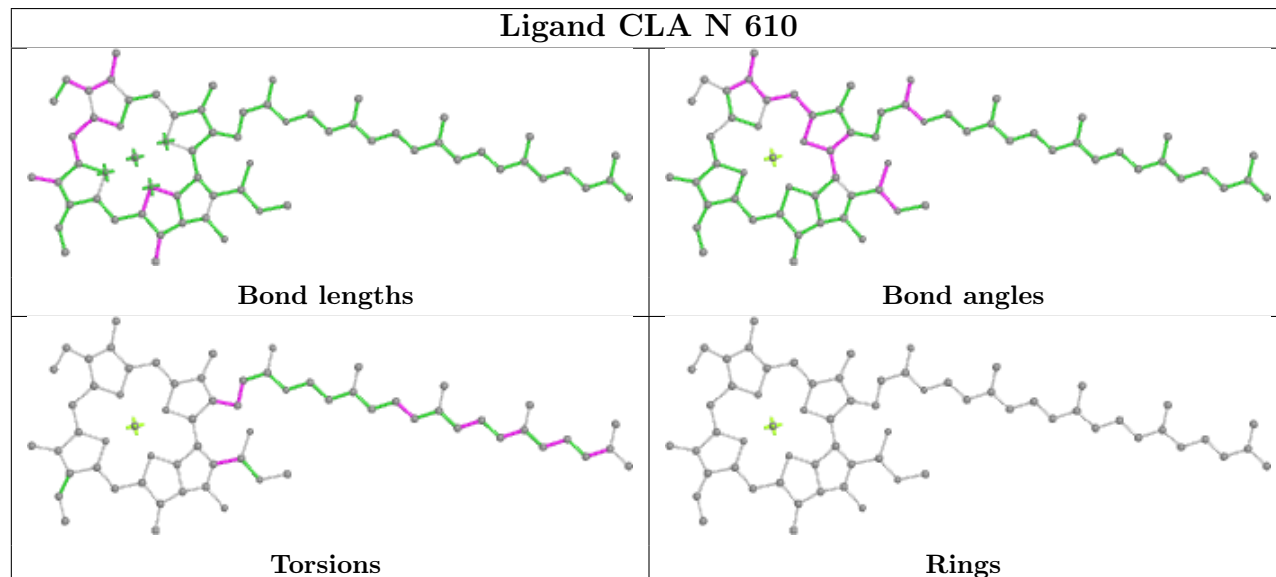
**Ligand CLA c 502****Ligand CLA a 406**



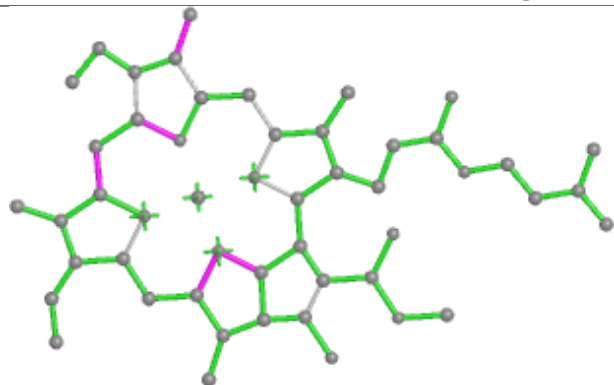
## Ligand CLA 8 602



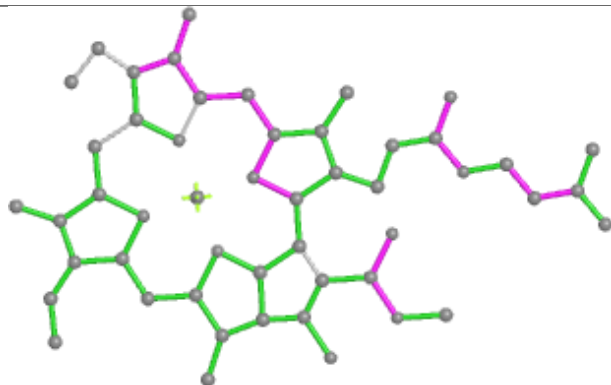
## Ligand CLA N 610



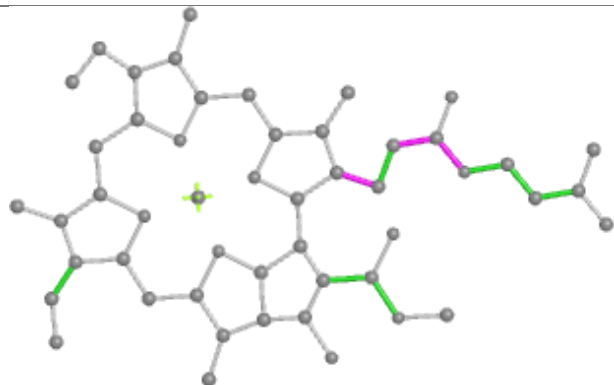
## Ligand CLA S 604



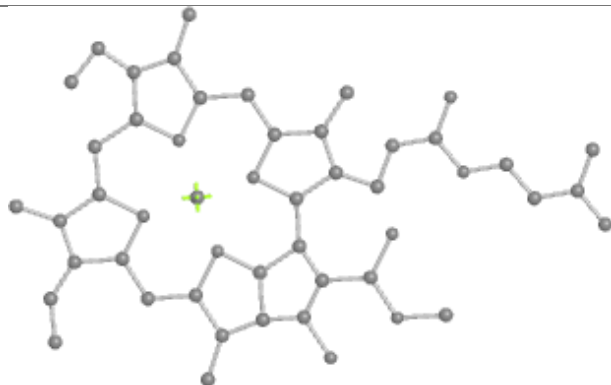
Bond lengths



Bond angles

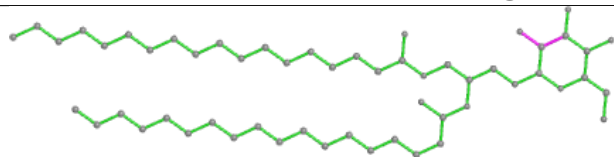


Torsions

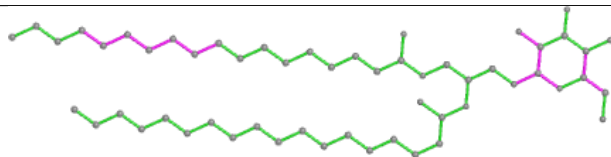


Rings

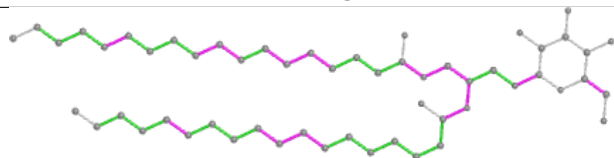
## Ligand LMG B 2633



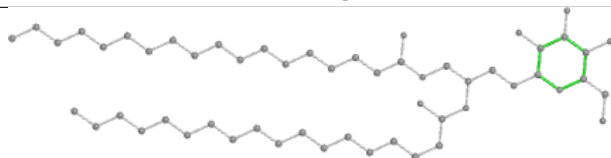
Bond lengths



Bond angles

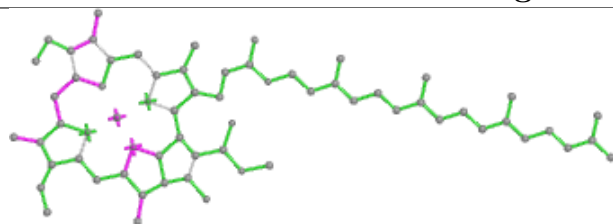


Torsions

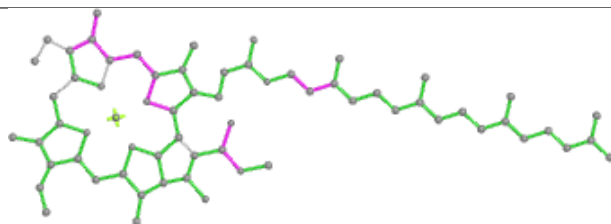


Rings

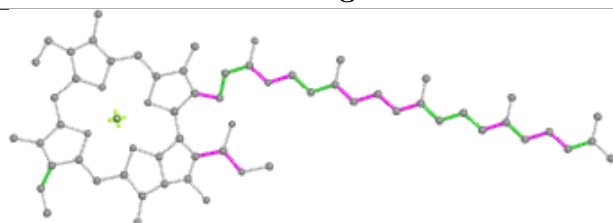


**Ligand CLA C 506**

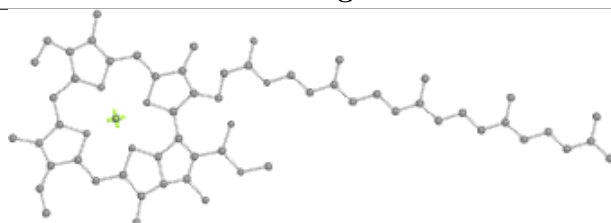
Bond lengths



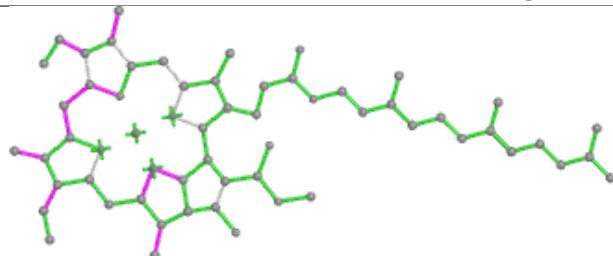
Bond angles



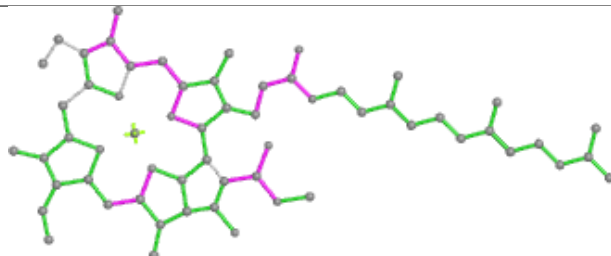
Torsions



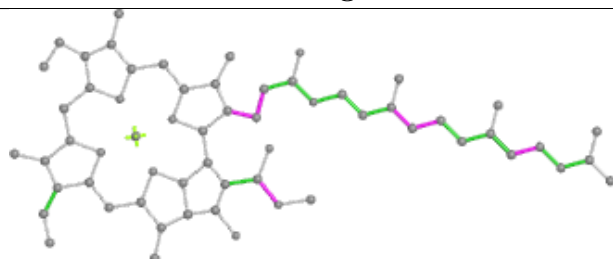
Rings

**Ligand CLA r 602**

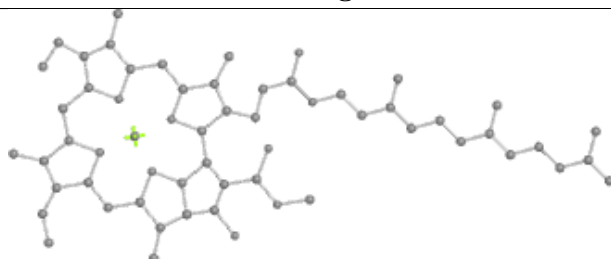
Bond lengths



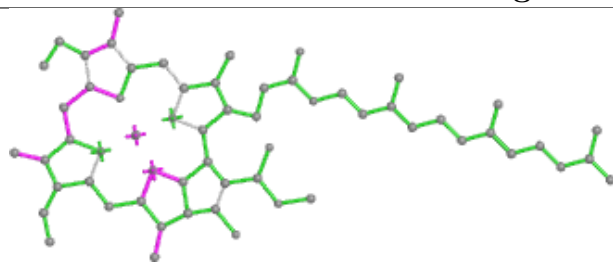
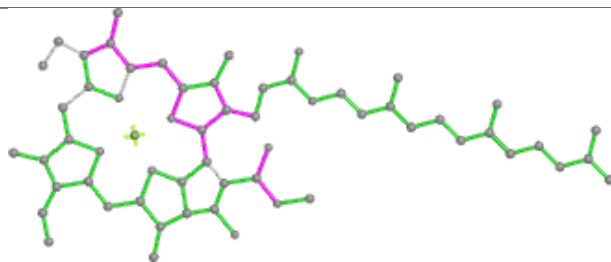
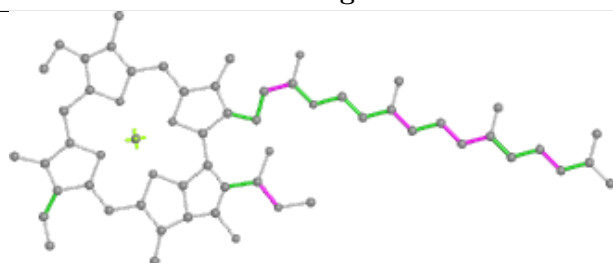
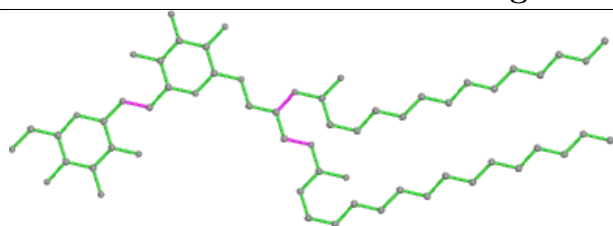
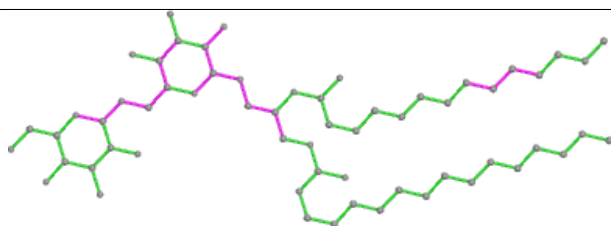
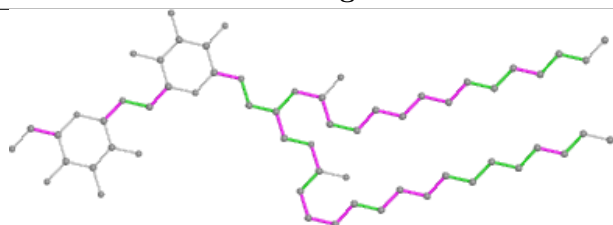
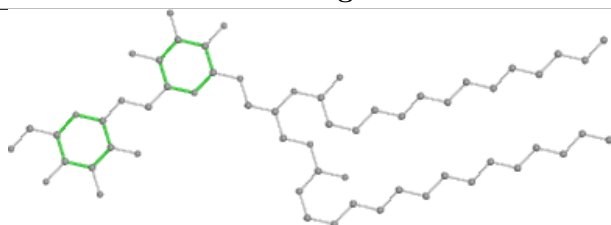
Bond angles



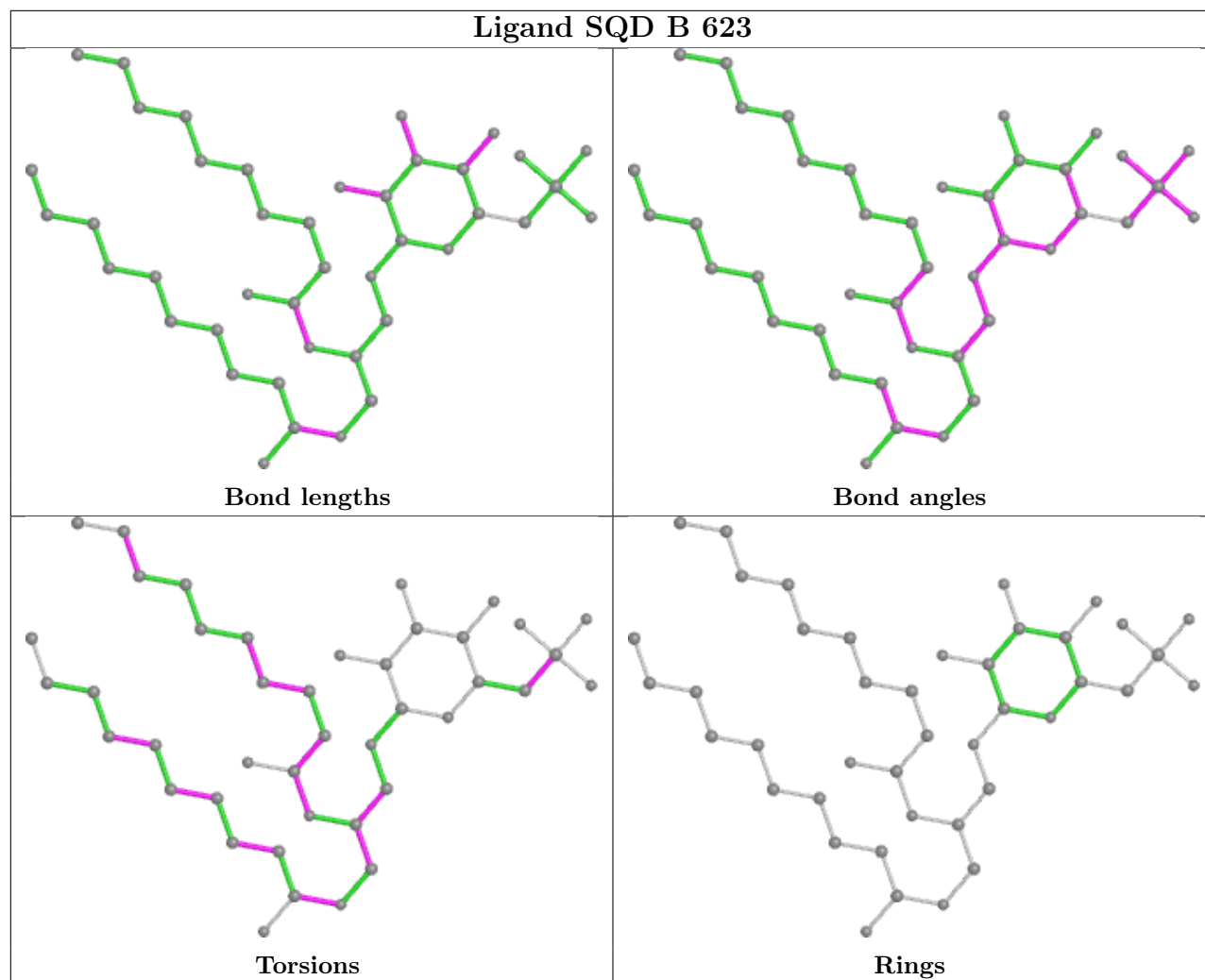
Torsions



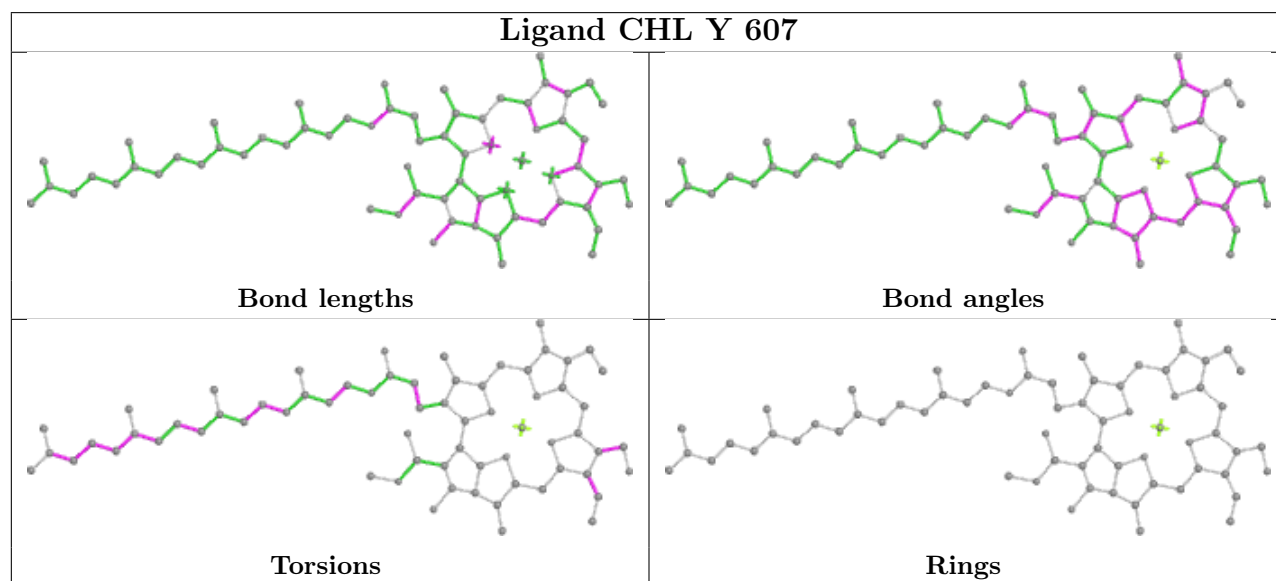
Rings

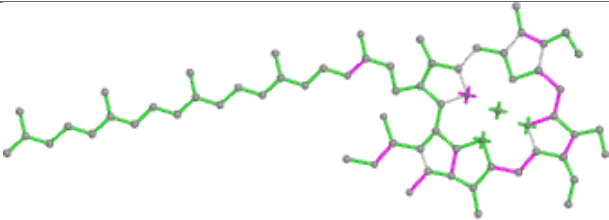
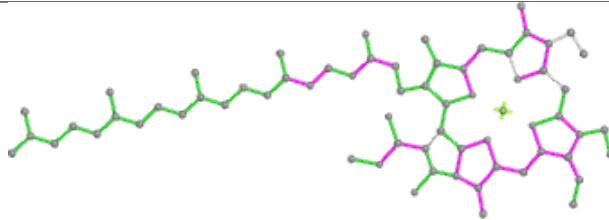
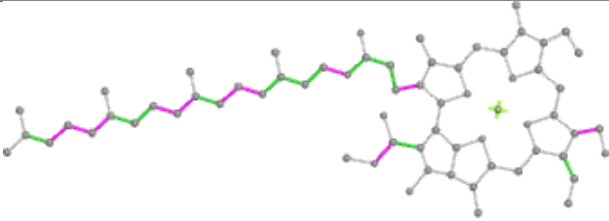
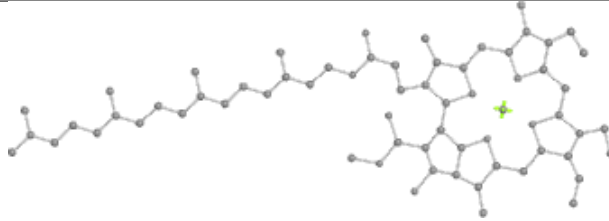
**Ligand CLA N 612****Bond lengths****Bond angles****Torsions****Rings****Ligand DGD C 520****Bond lengths****Bond angles****Torsions****Rings**

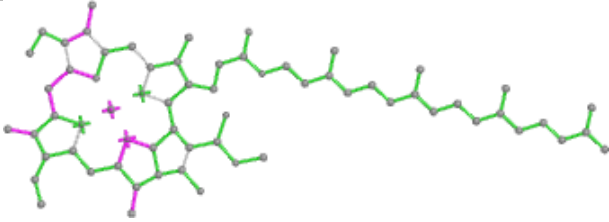
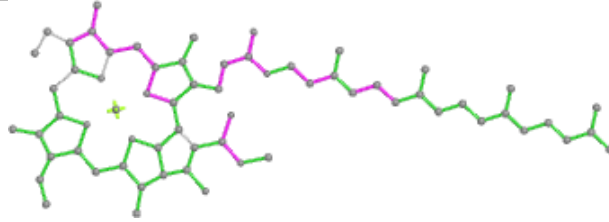
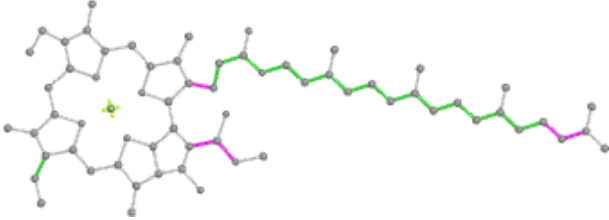
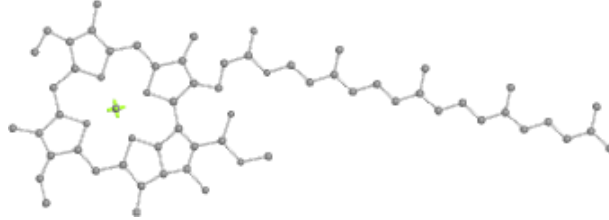
## Ligand SQD B 623

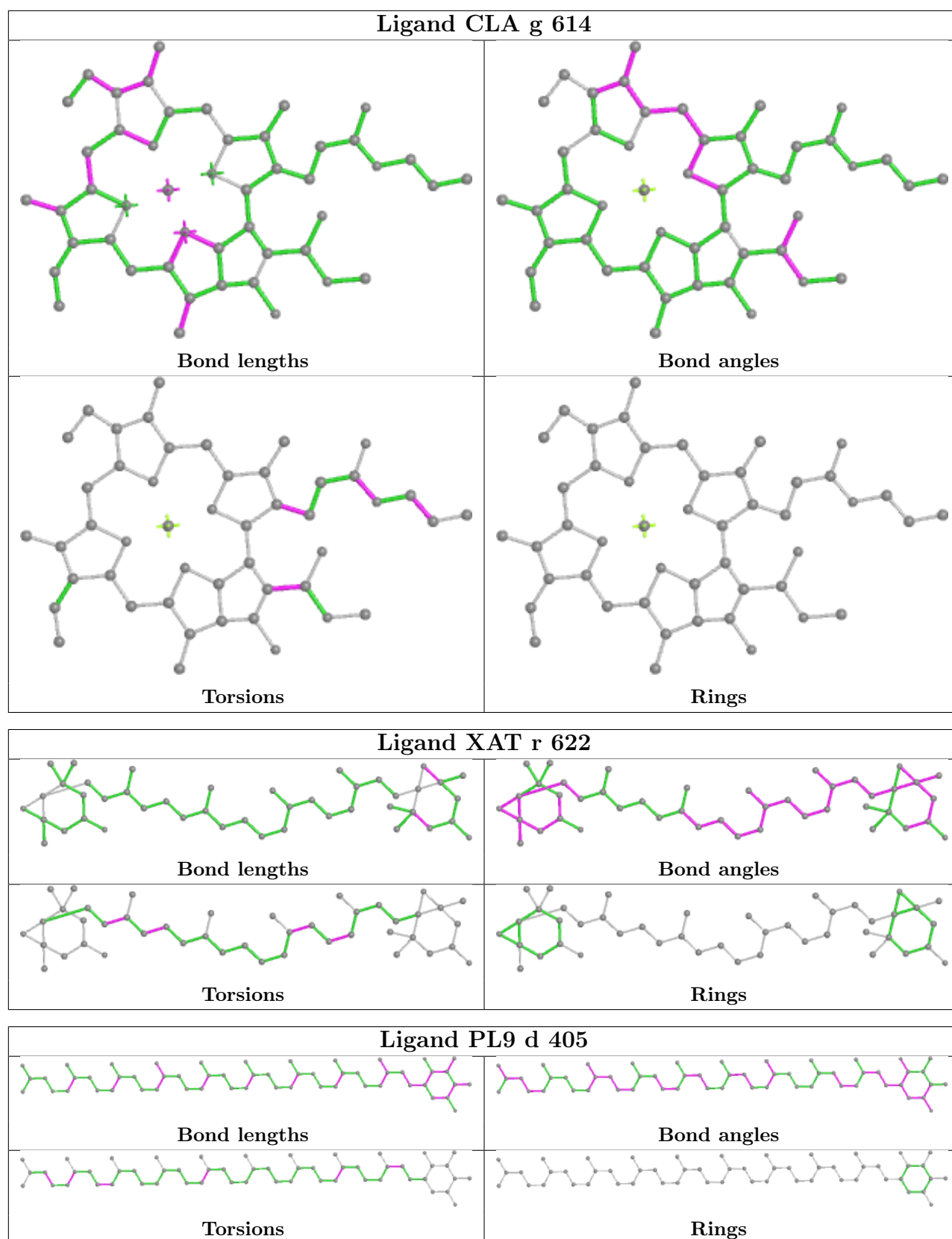


## Ligand CHL Y 607

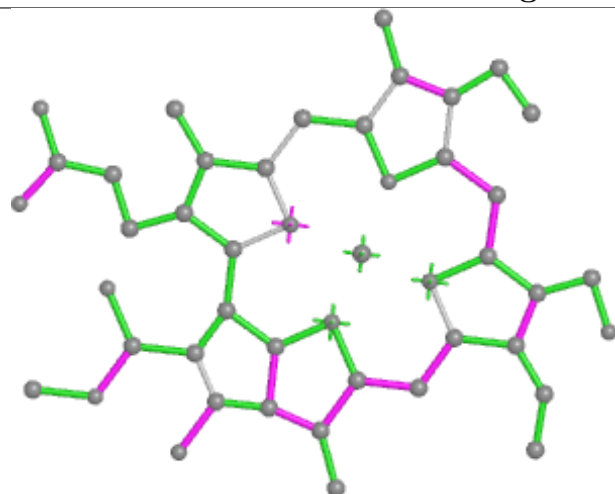


Ligand CHL y 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

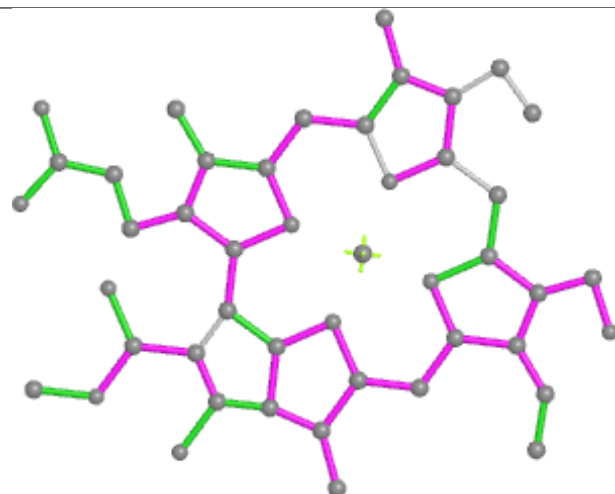
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



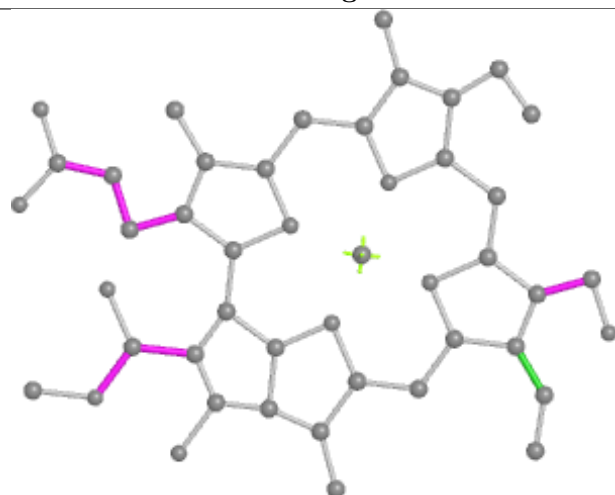
## Ligand CHL 7 605



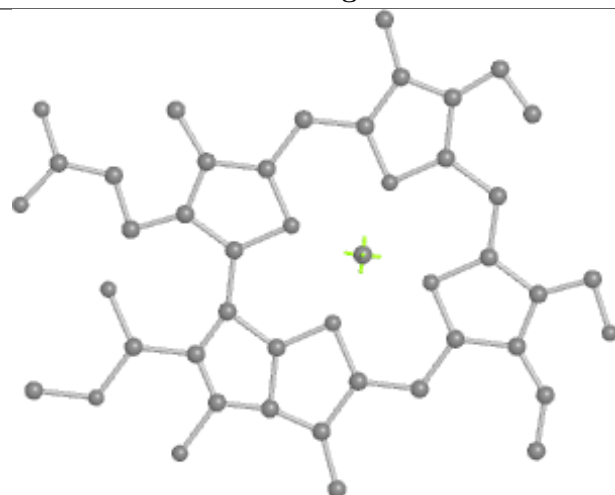
Bond lengths



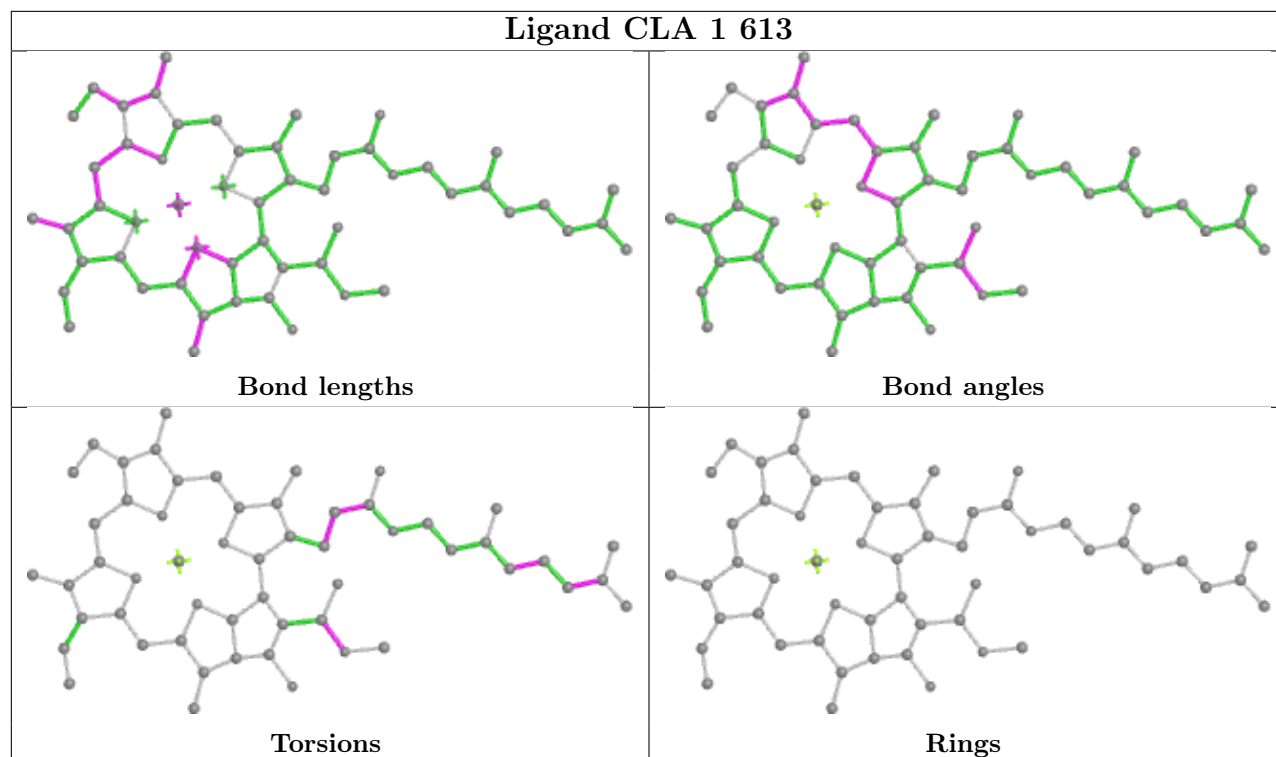
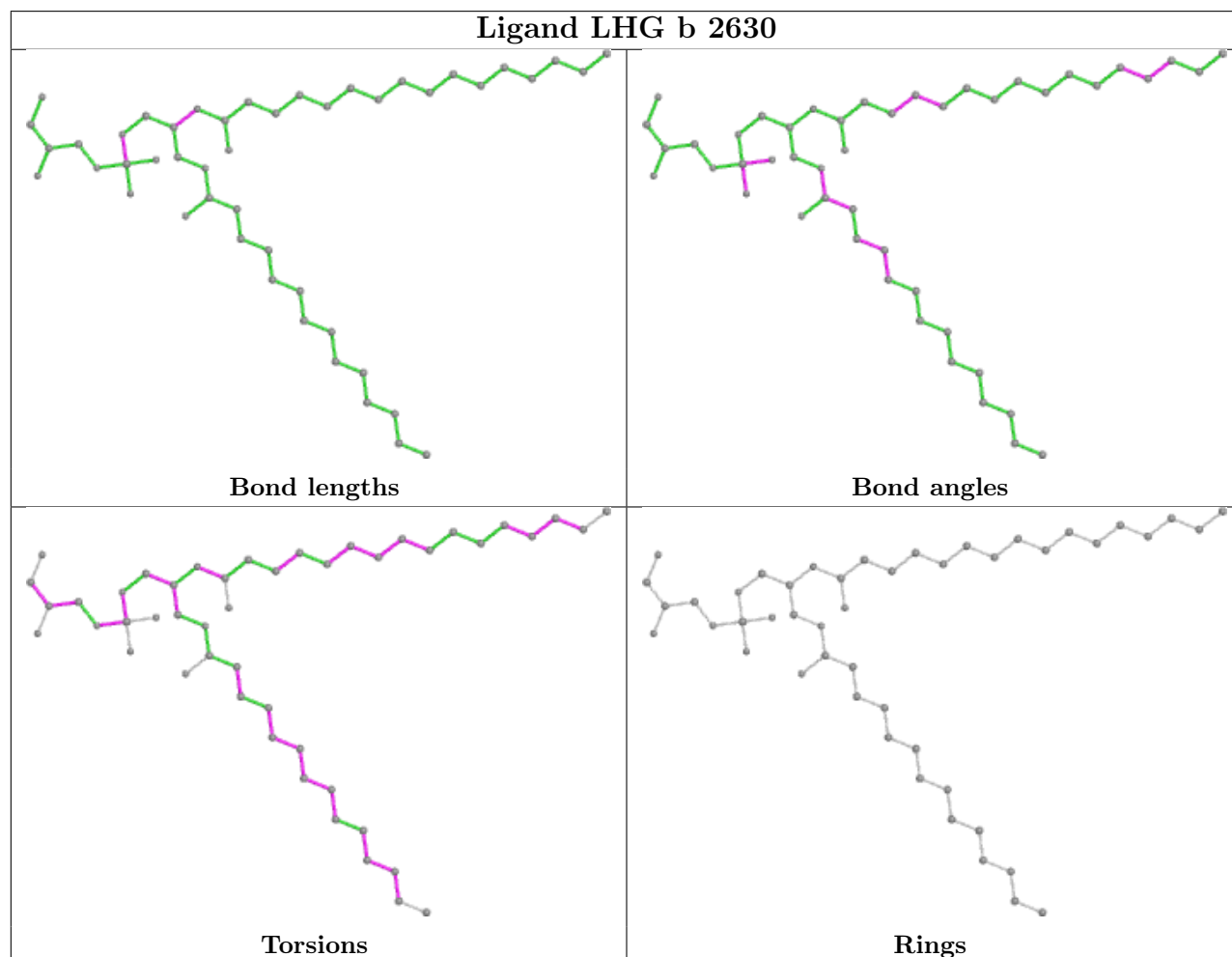
Bond angles

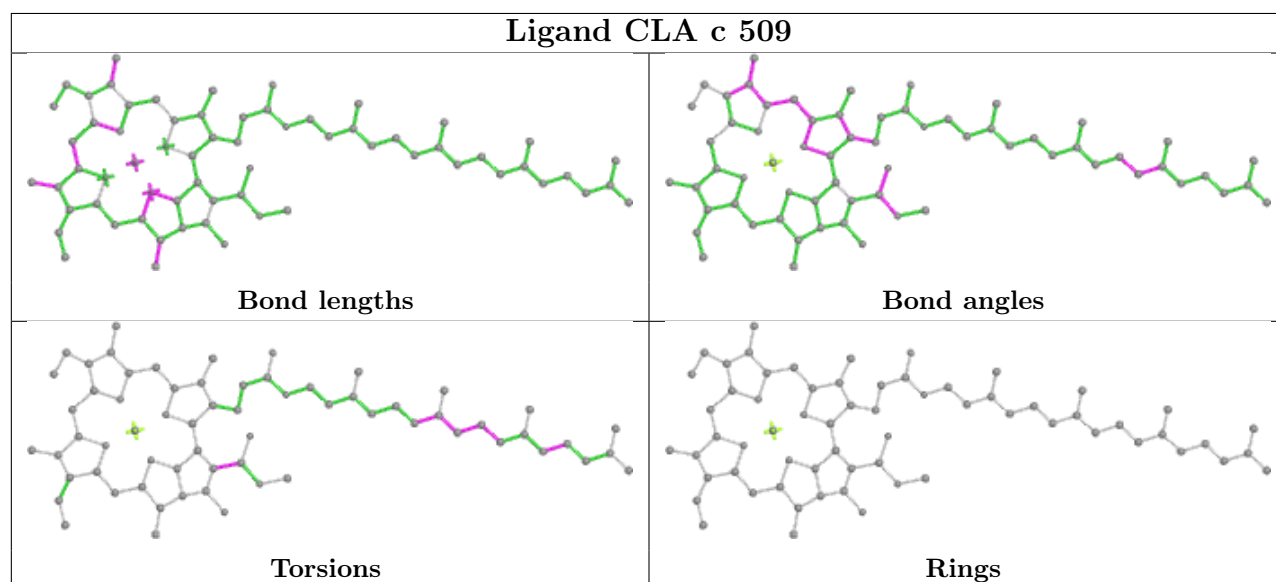
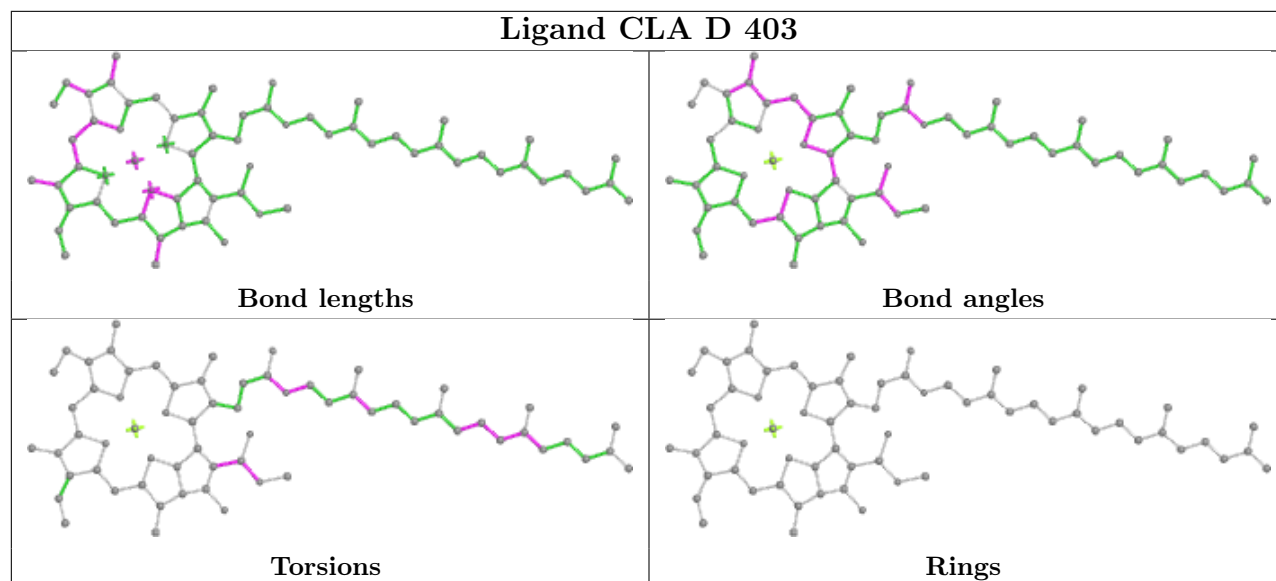
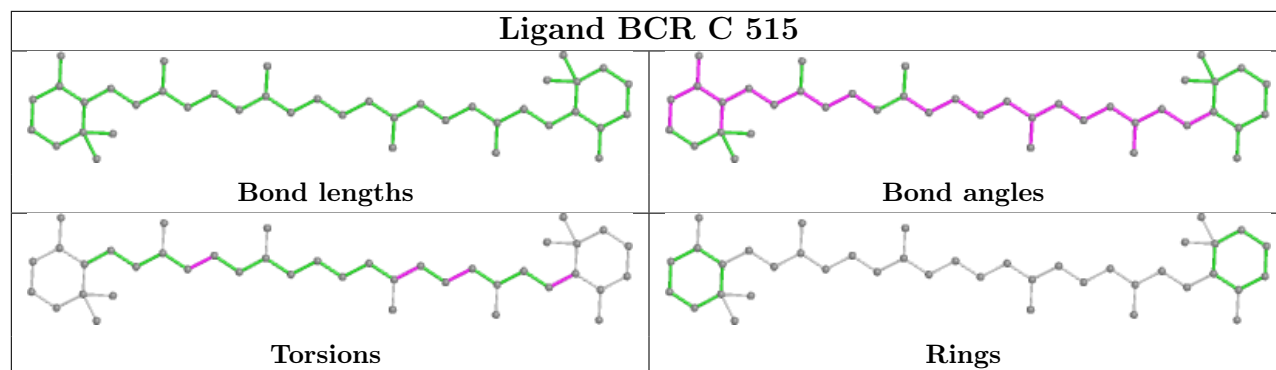


Torsions

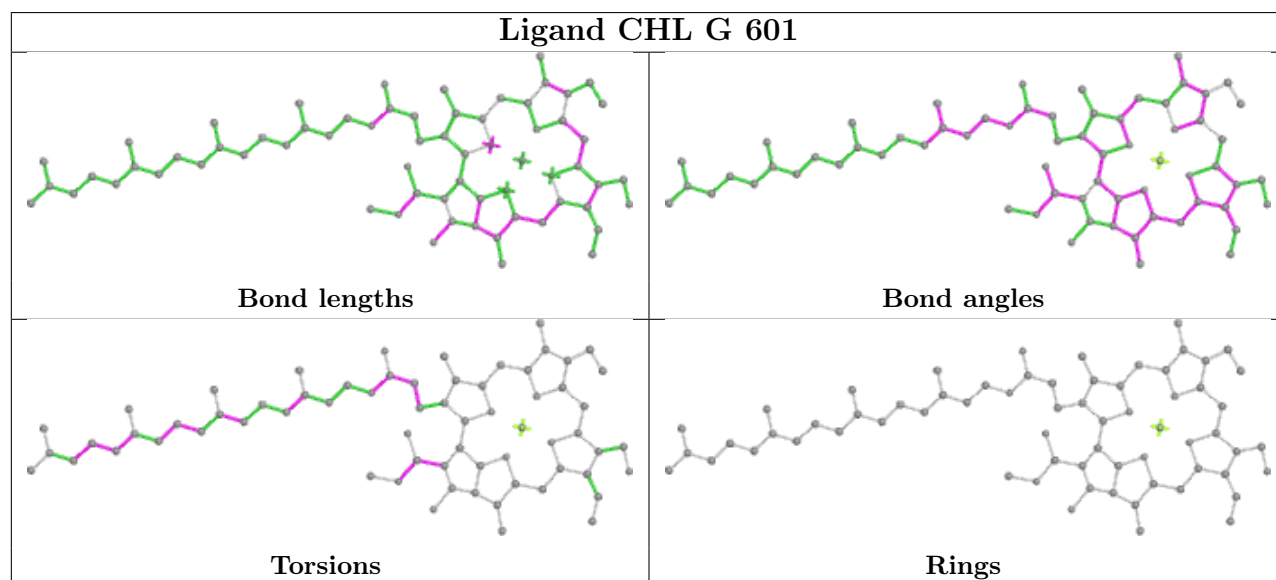
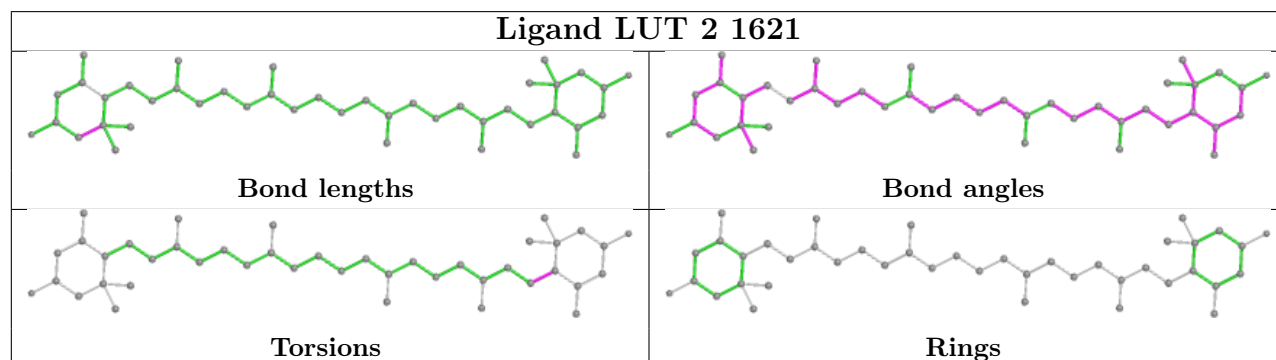
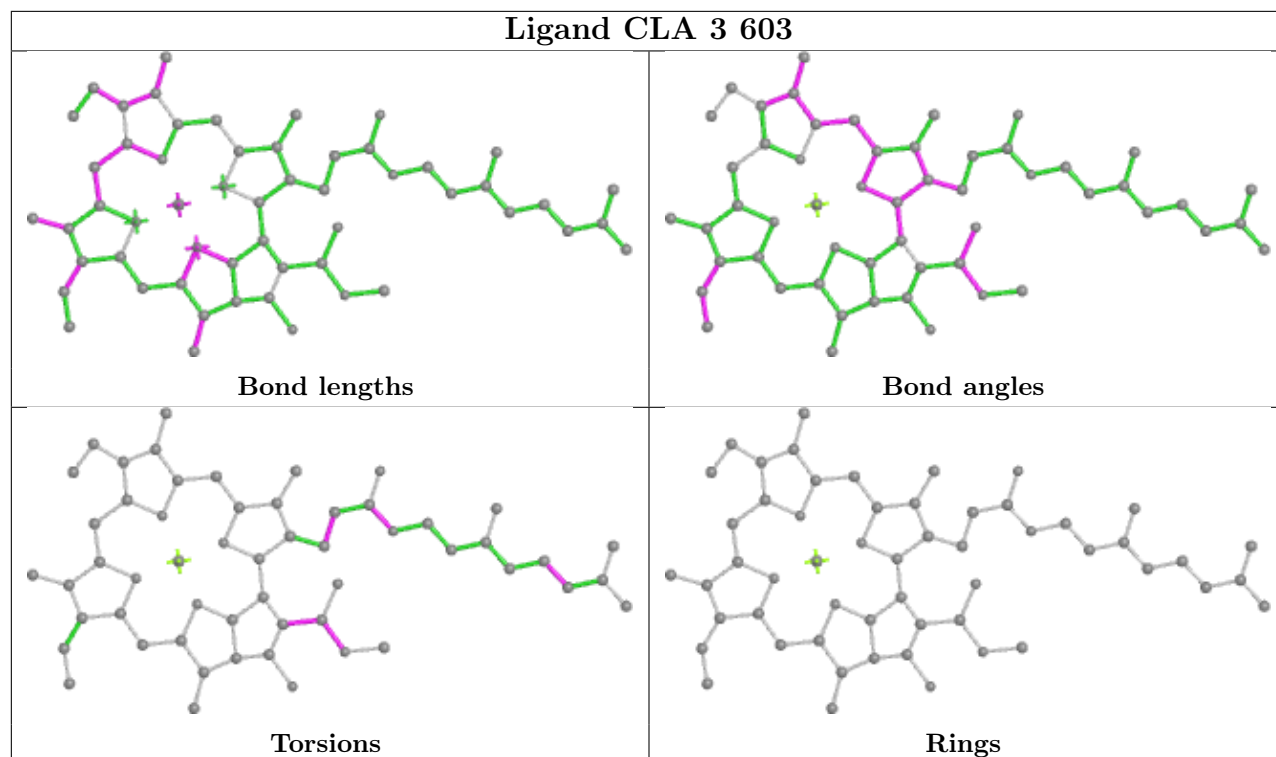


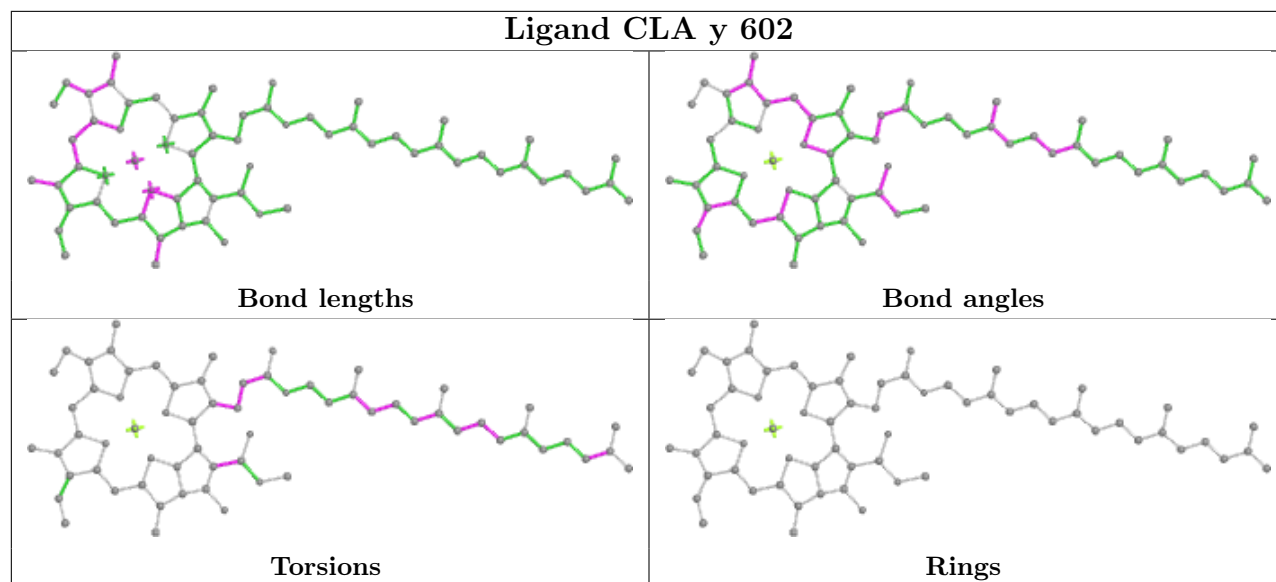
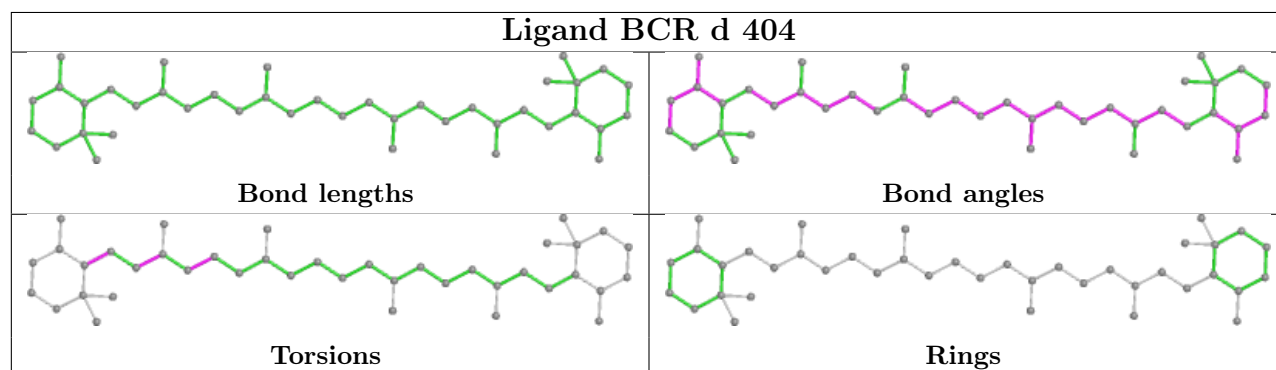
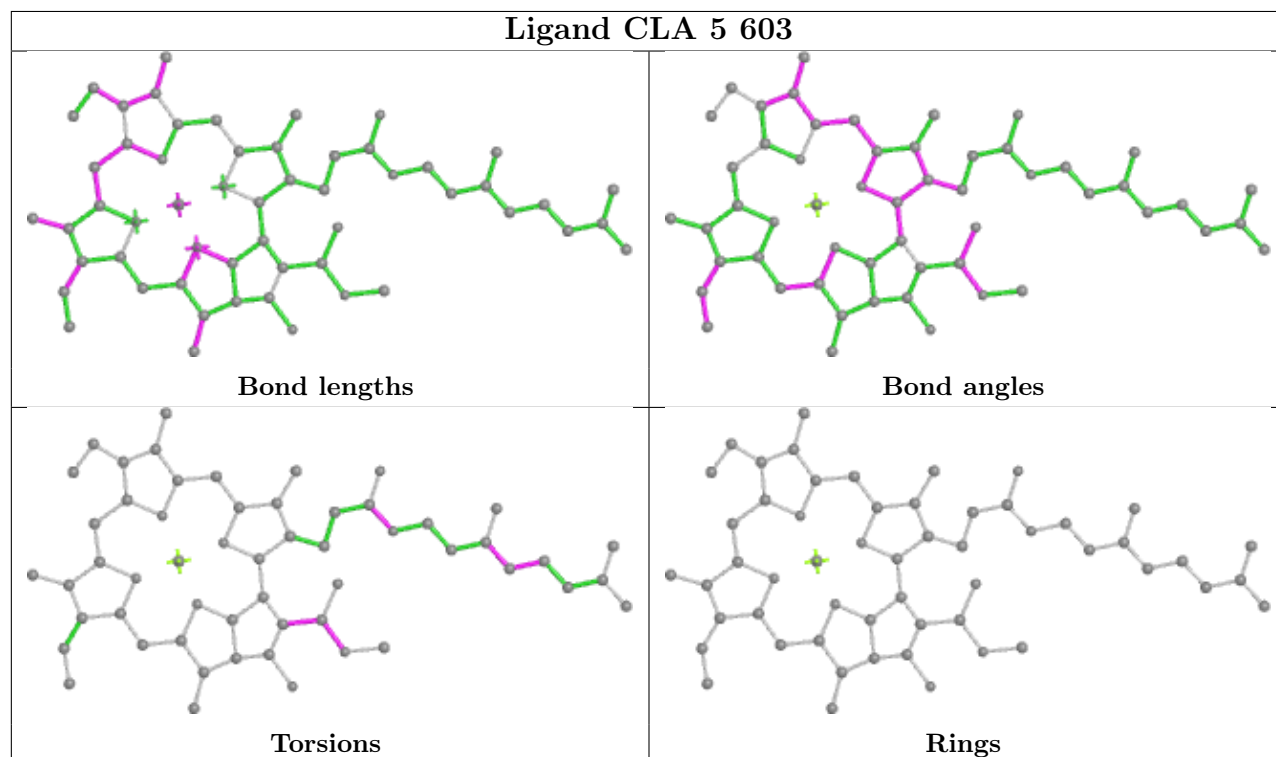
Rings

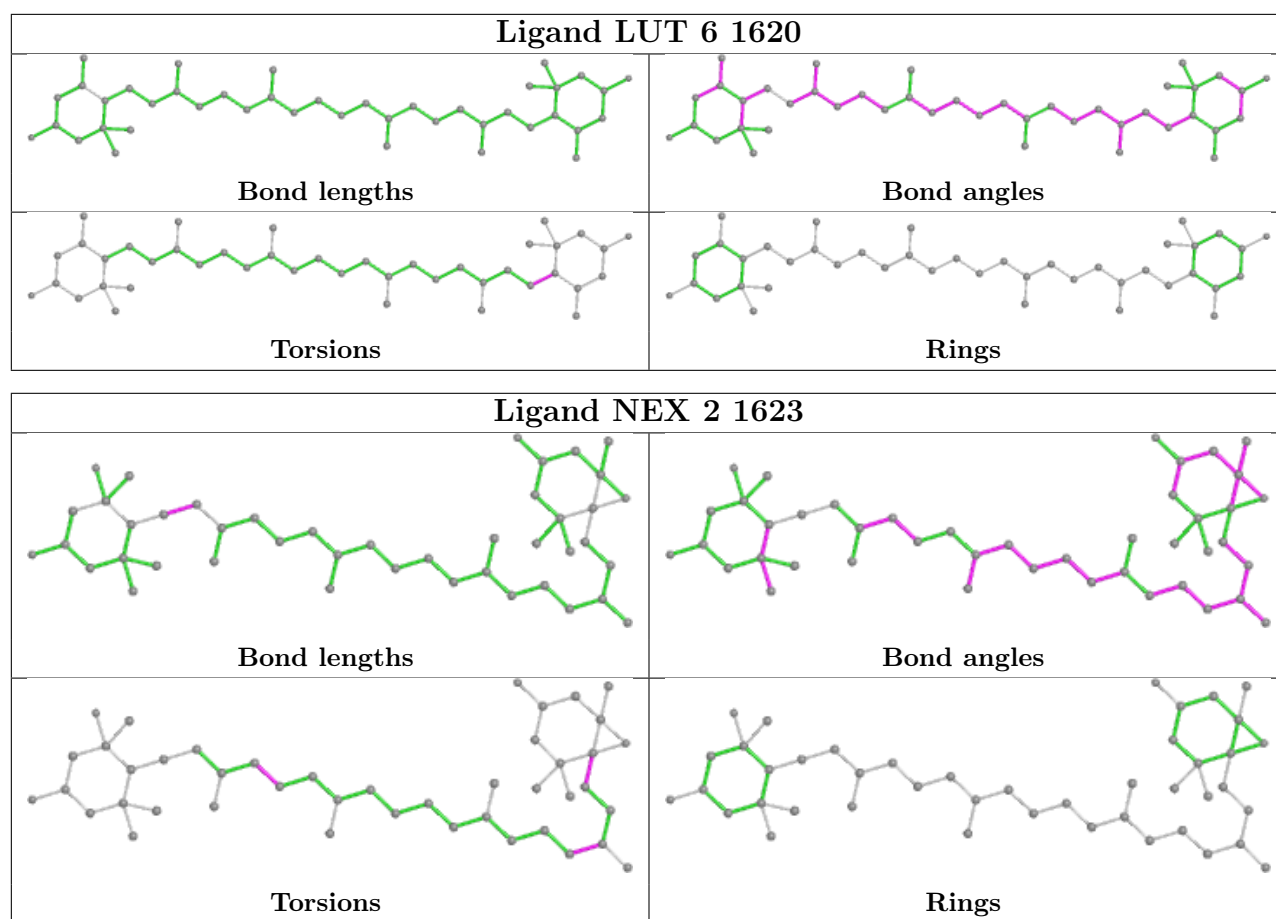
**Ligand CLA 1 613****Ligand LHG b 2630**

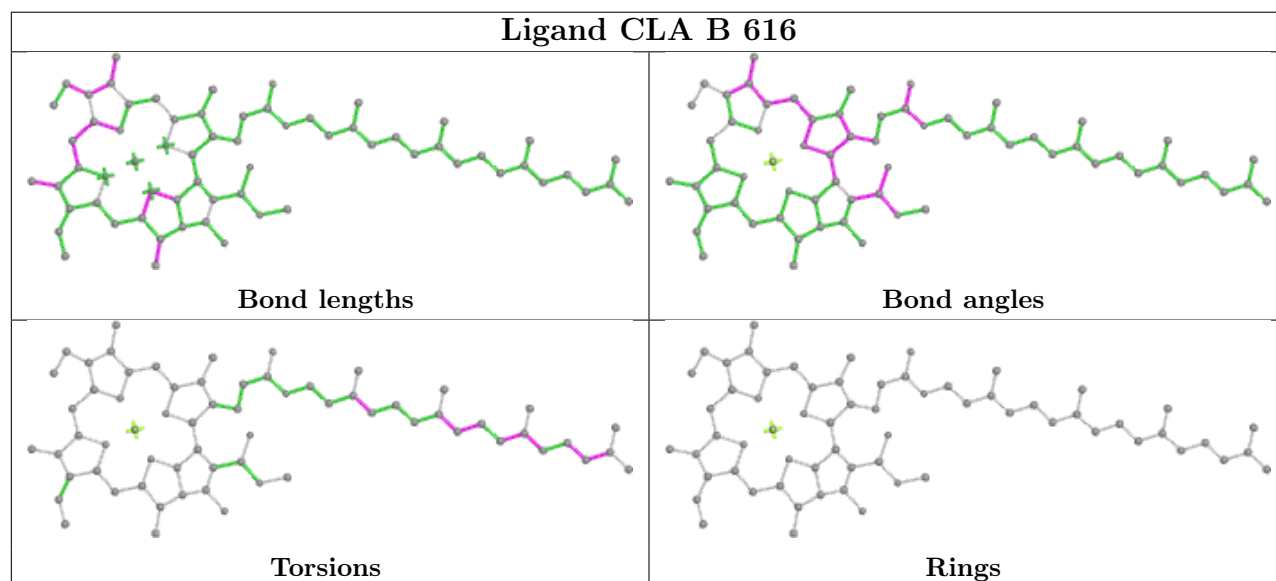
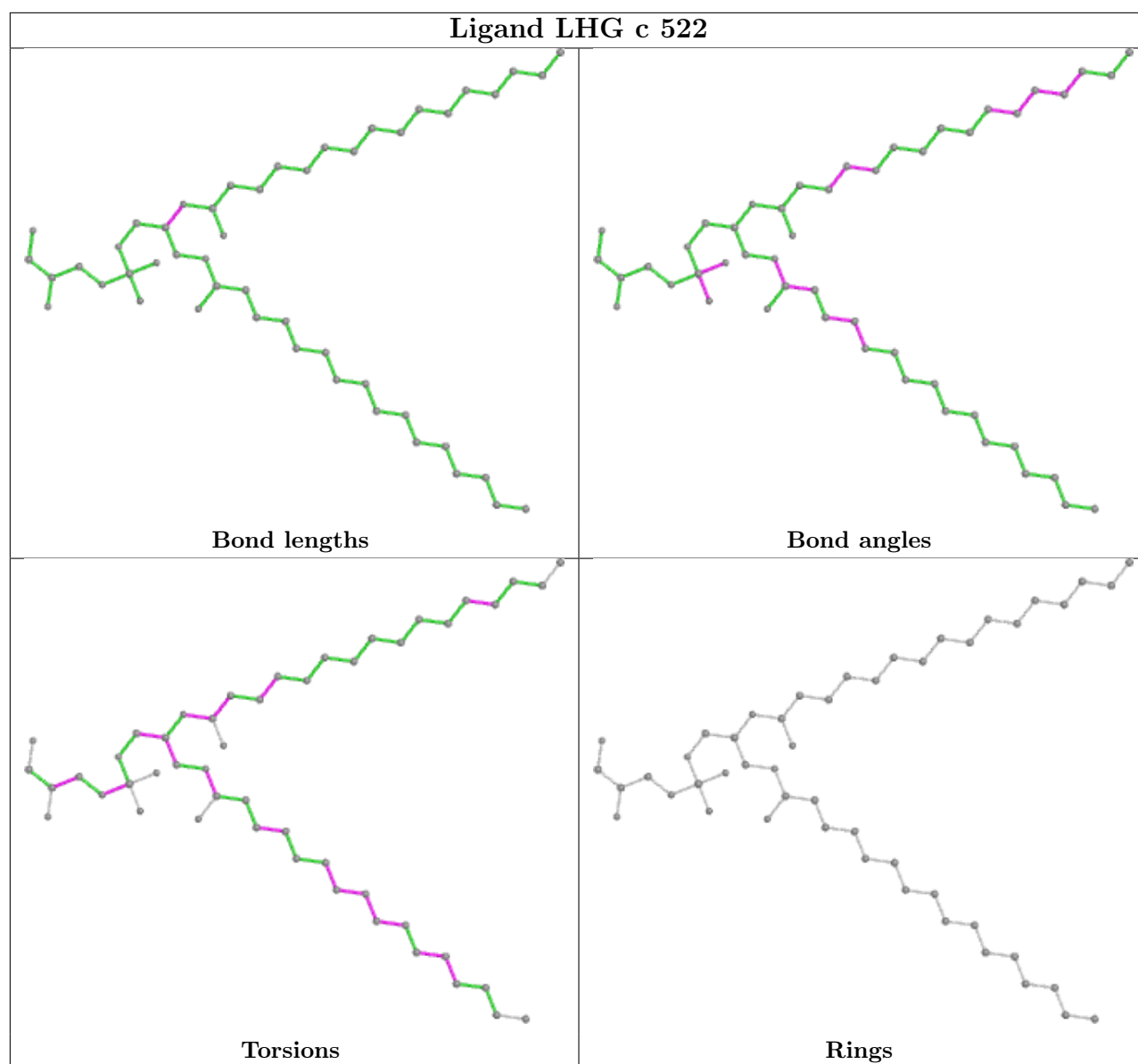


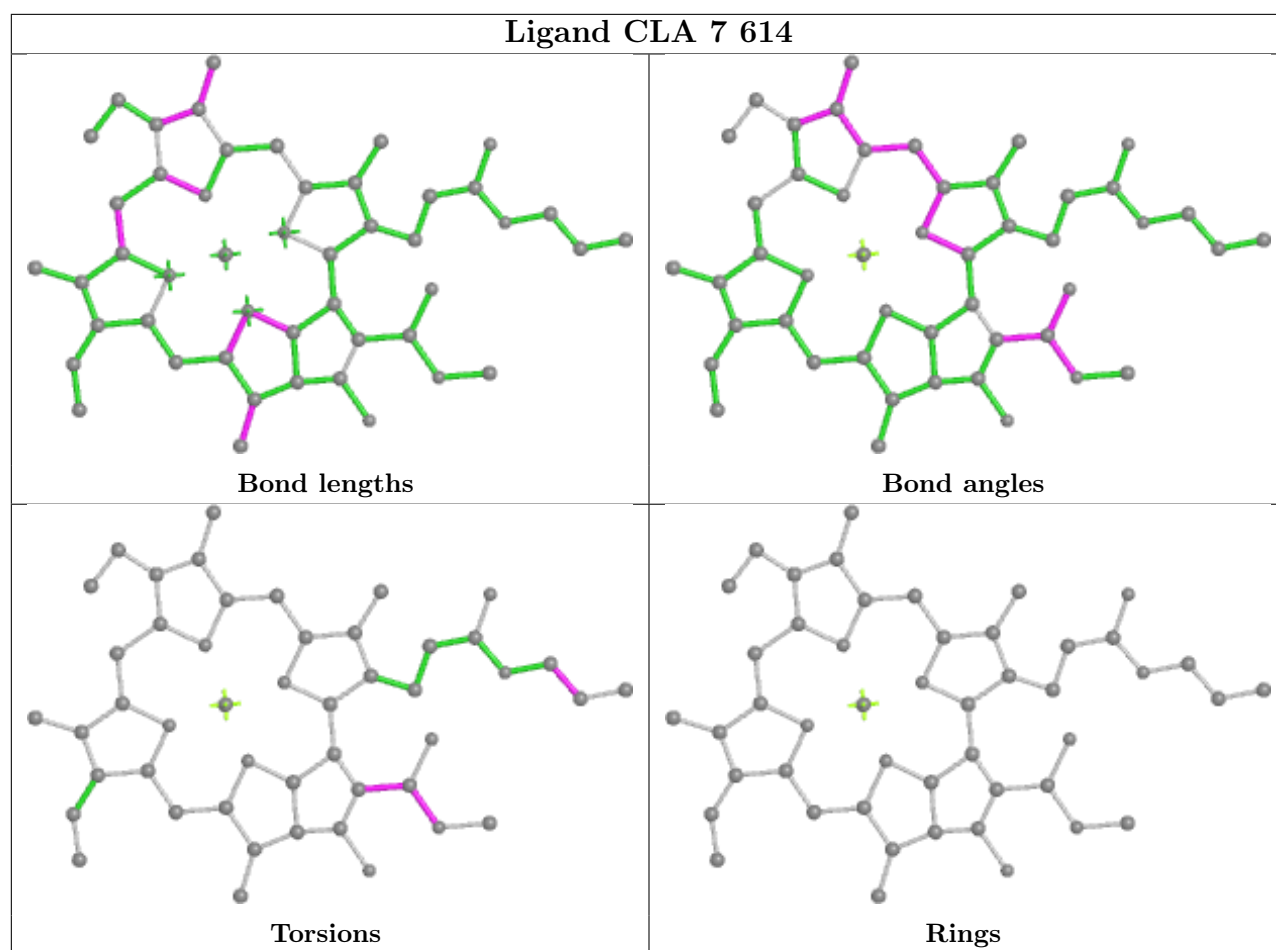




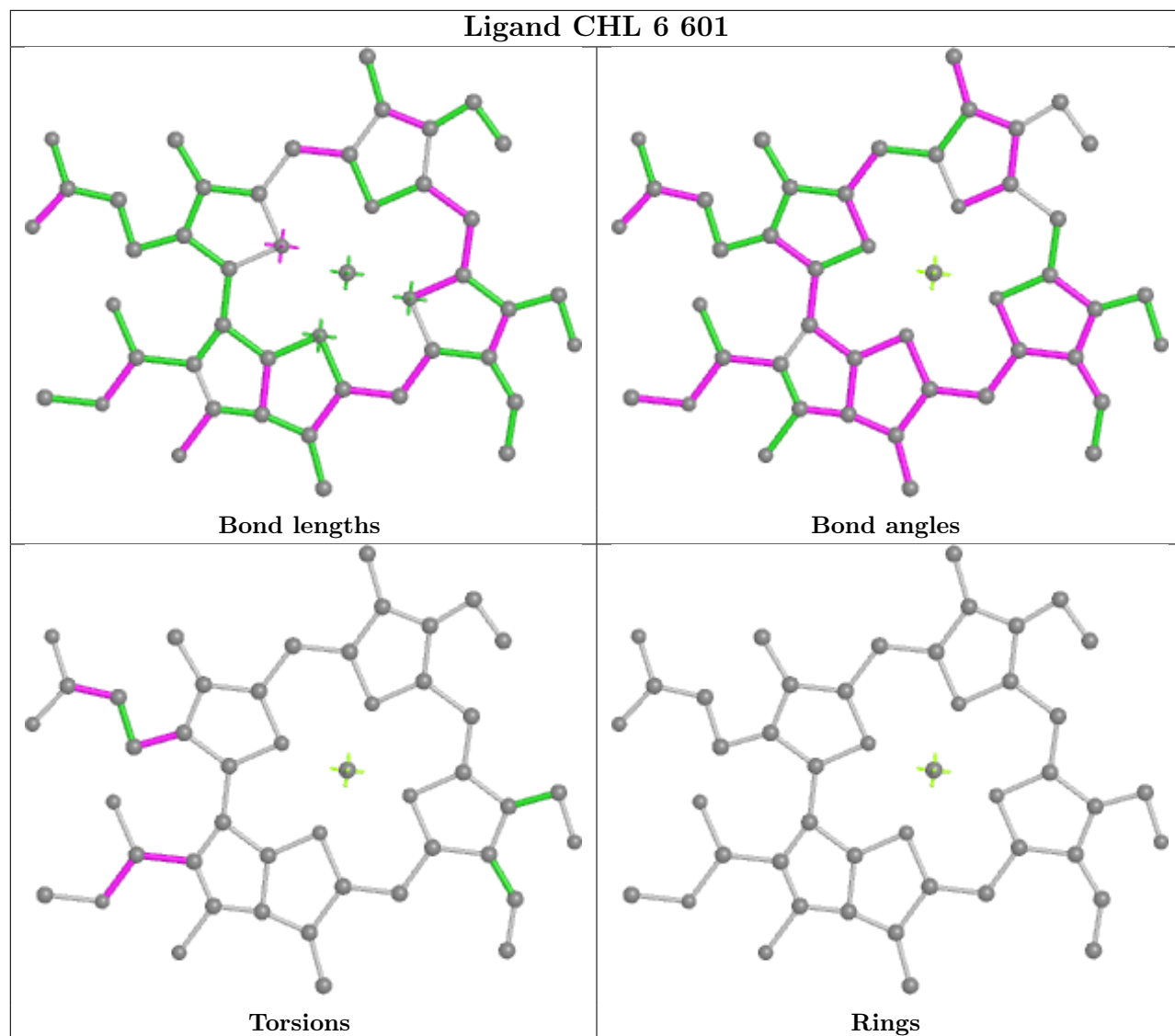
**Ligand CLA y 602****Ligand BCR d 404****Ligand CLA 5 603**

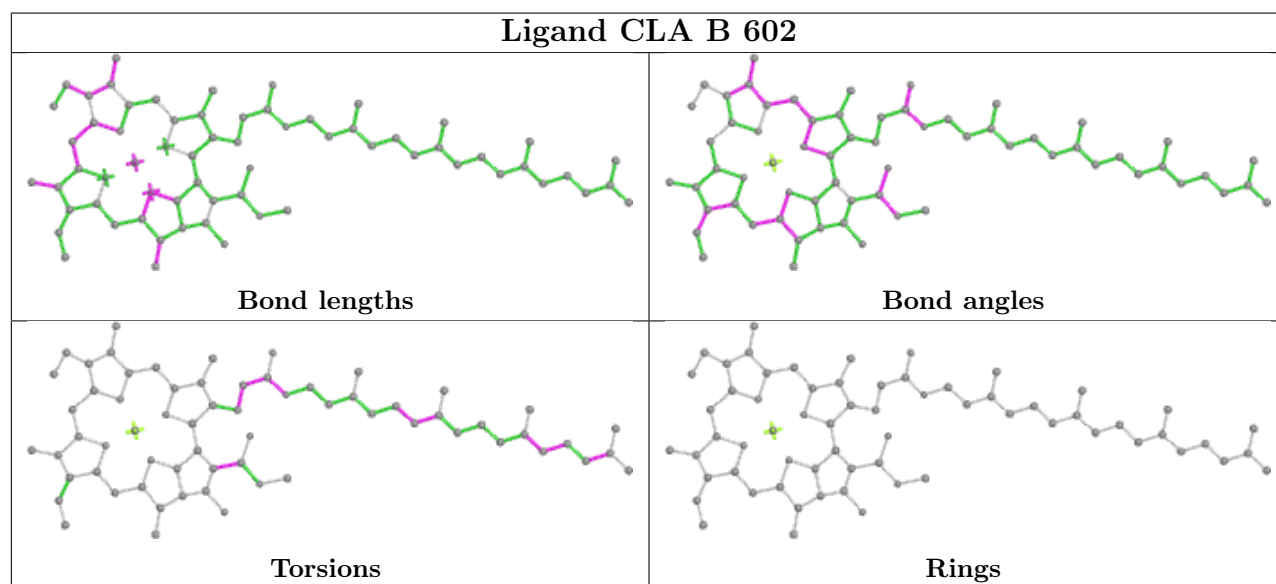
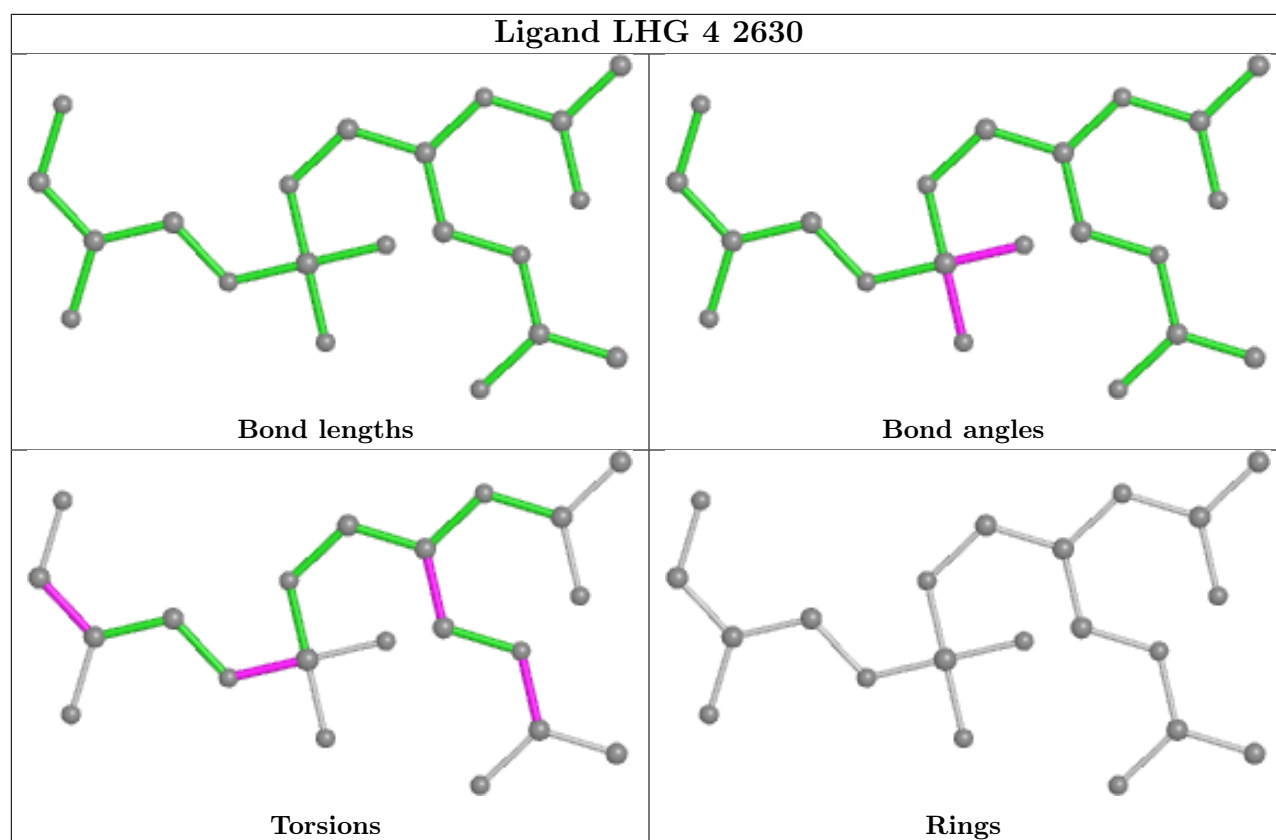


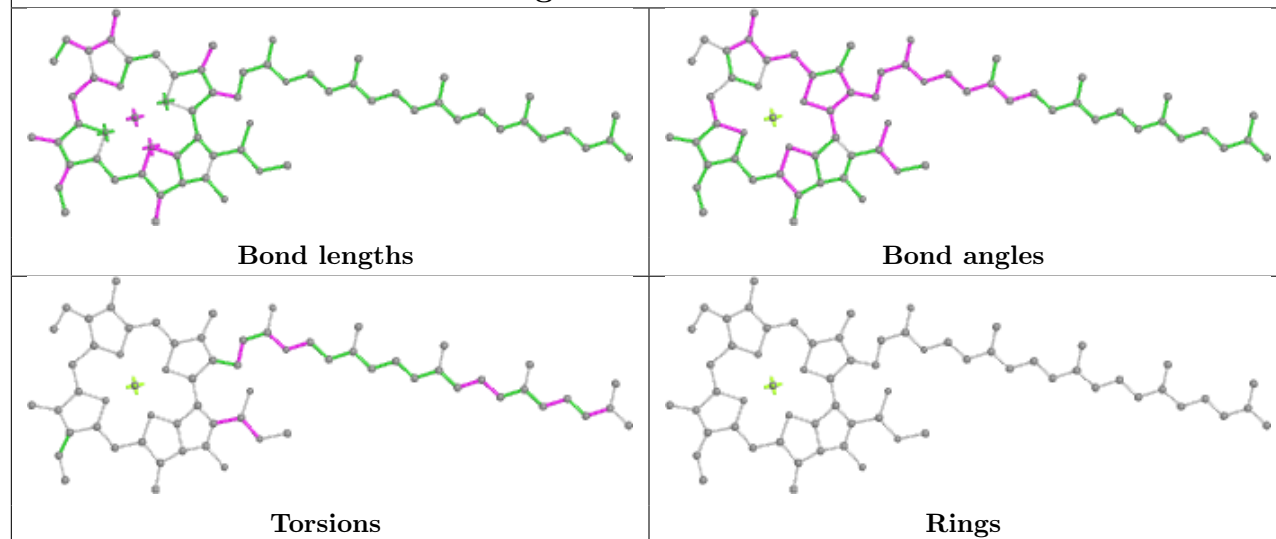
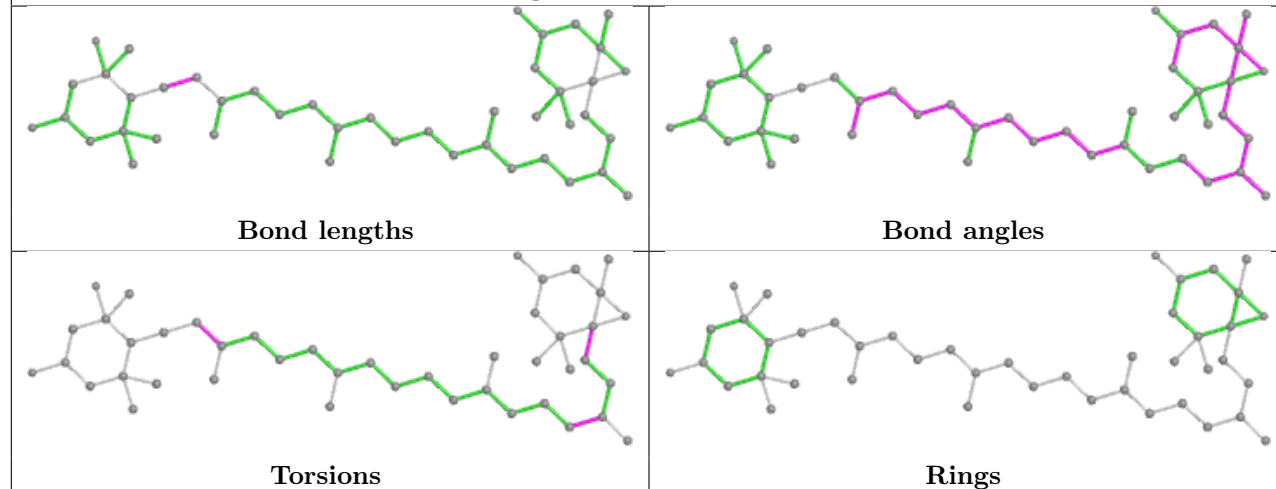




## Ligand CHL 6 601

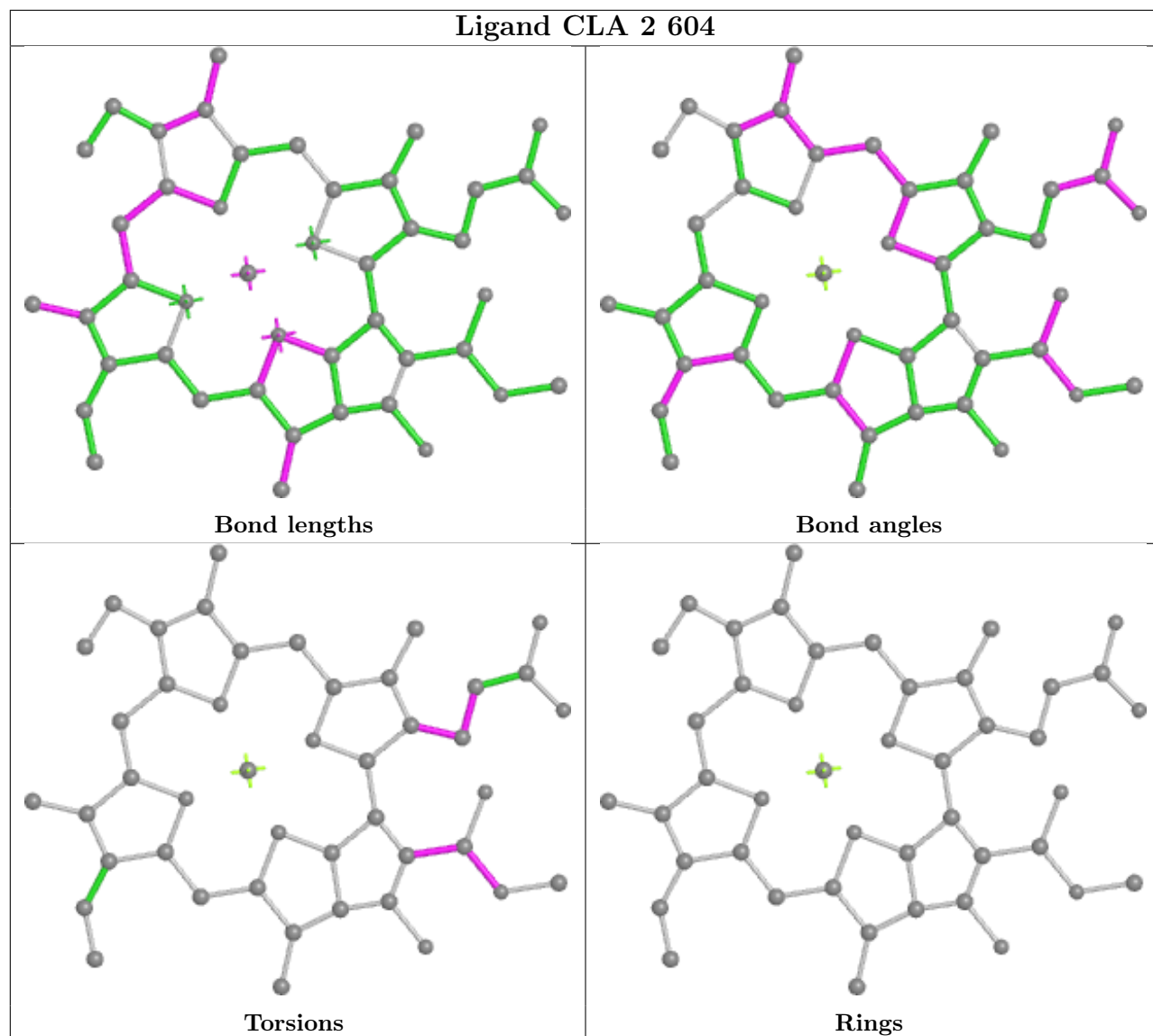




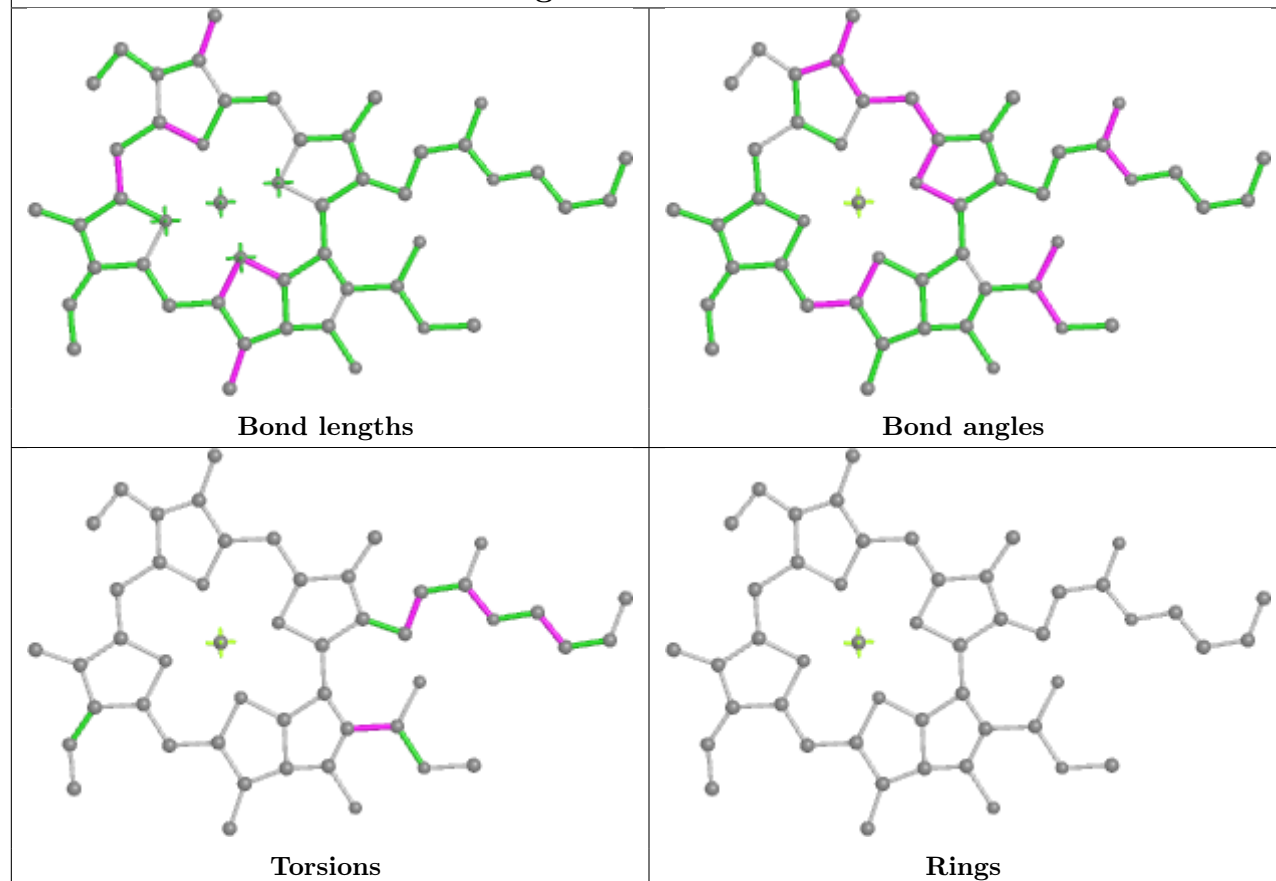
**Ligand CLA b 605****Ligand NEX s 1623**



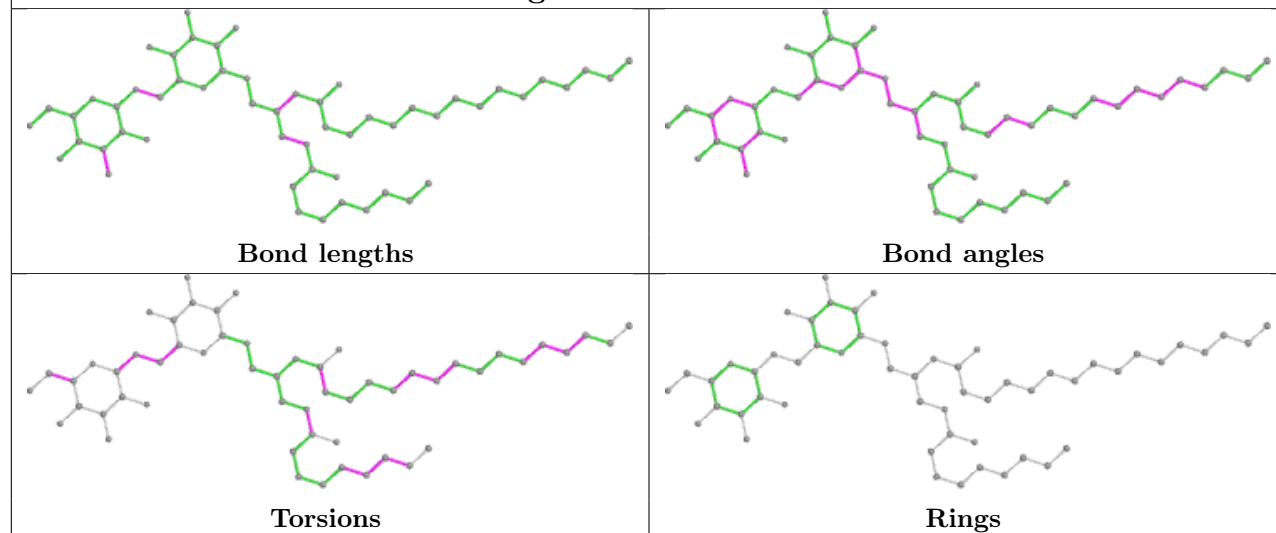
## Ligand CLA 2 604



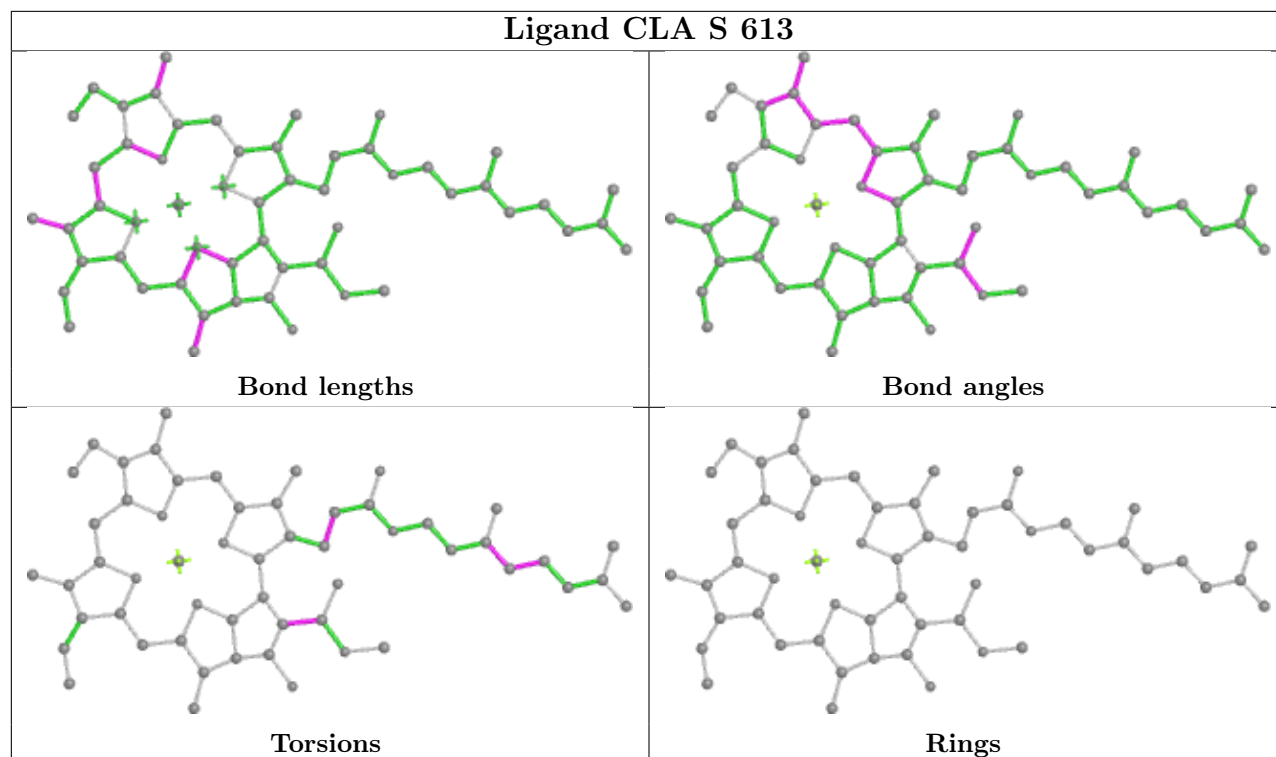
## Ligand CLA S 614



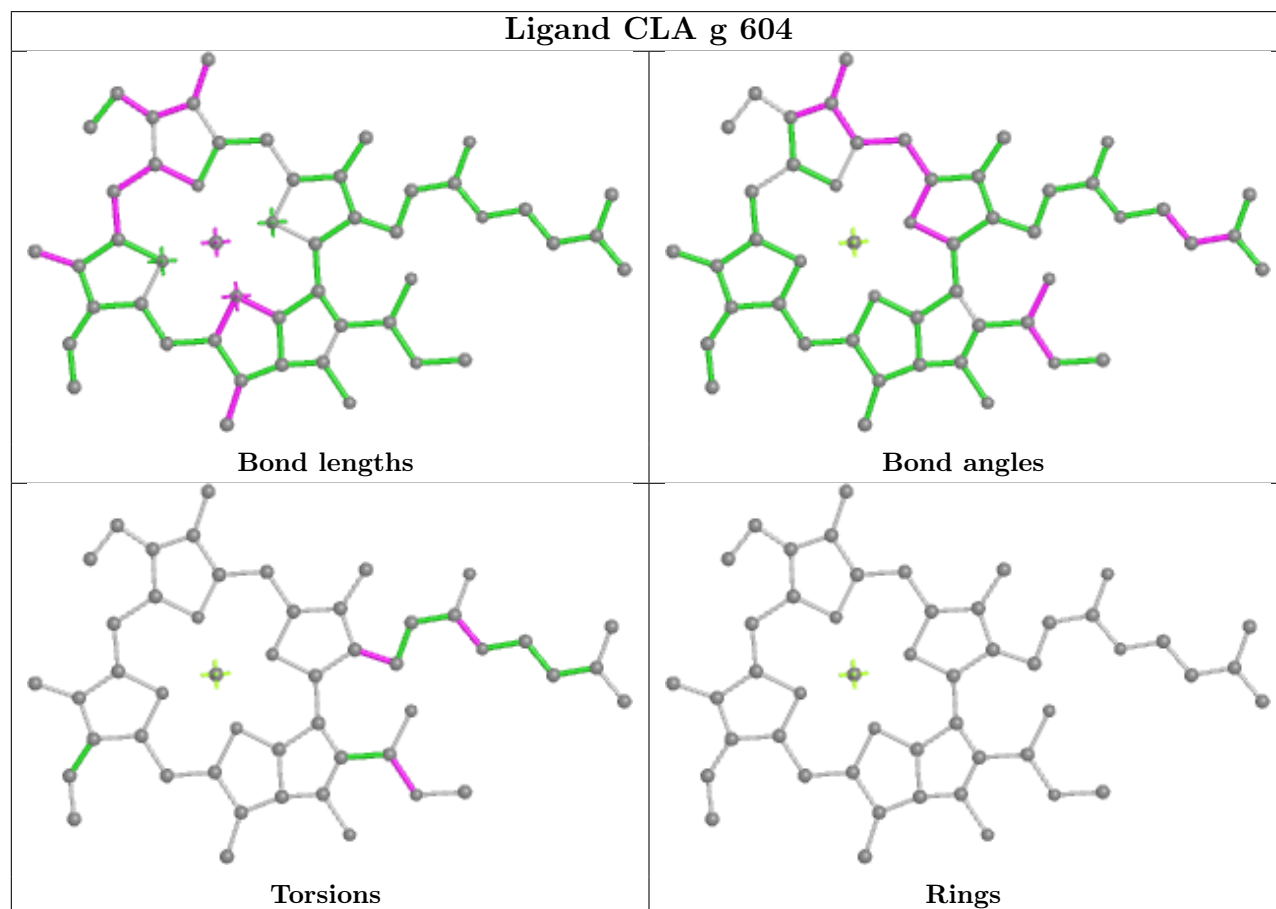
## Ligand DGD C 518

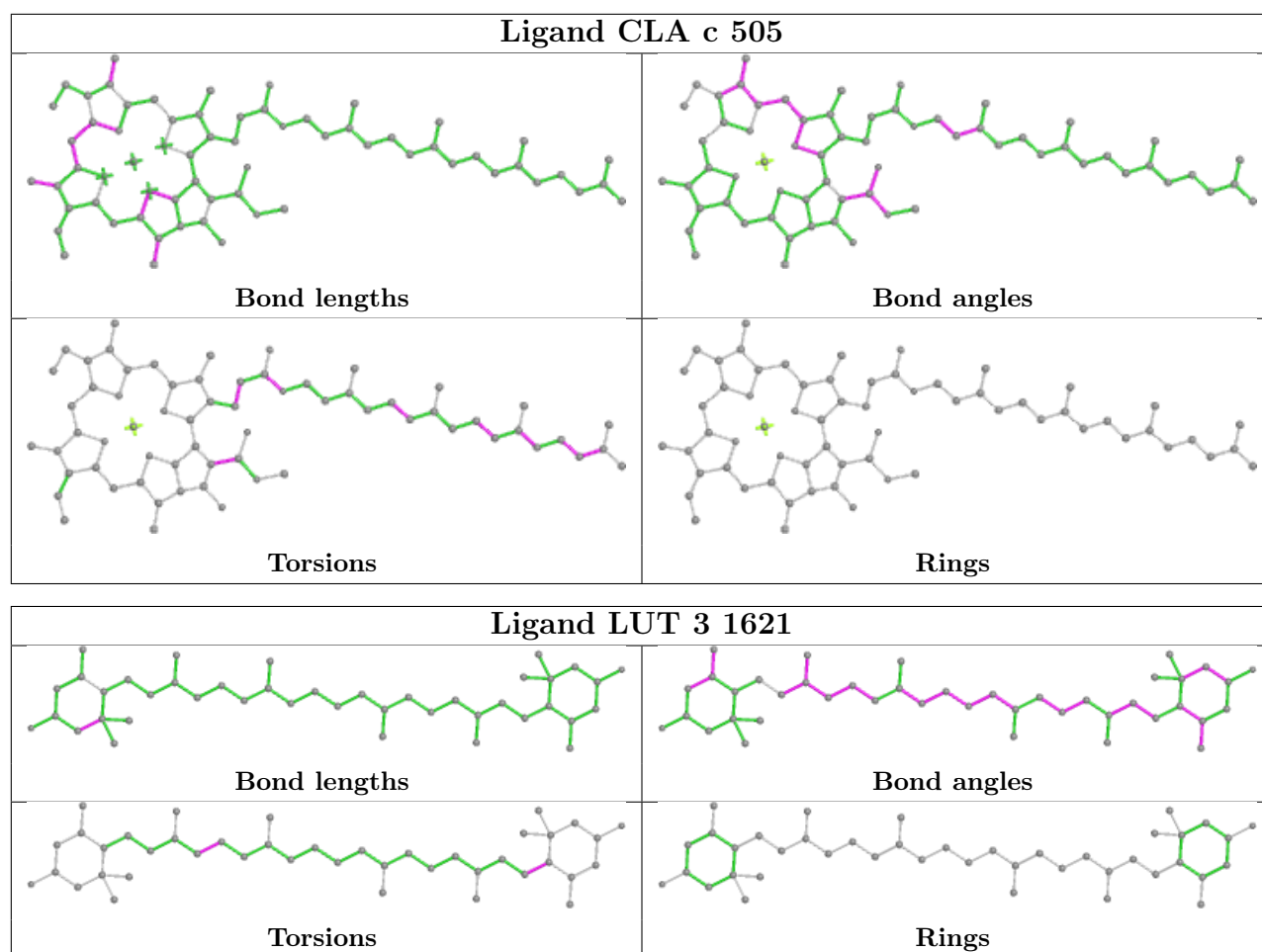


## Ligand CLA S 613

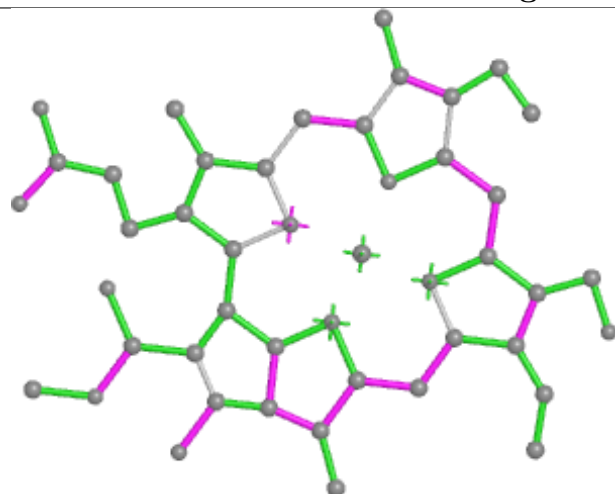


## Ligand CLA g 604

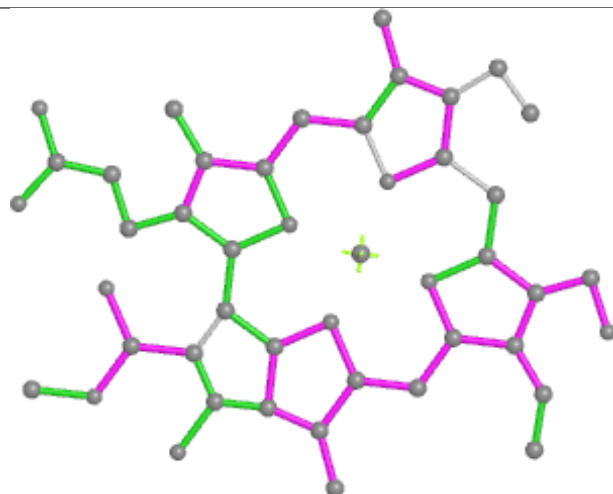




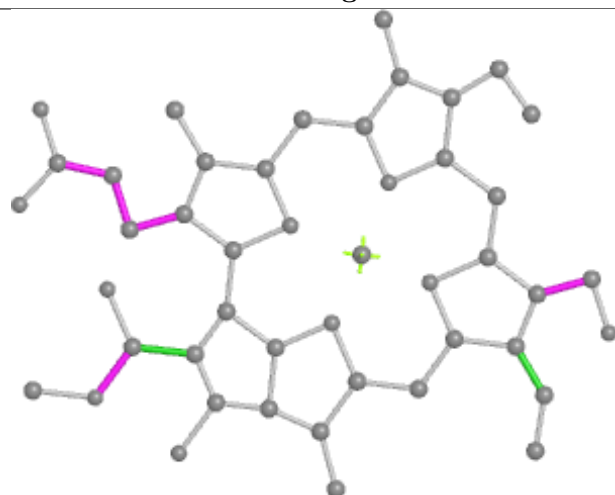
## Ligand CHL 6 605



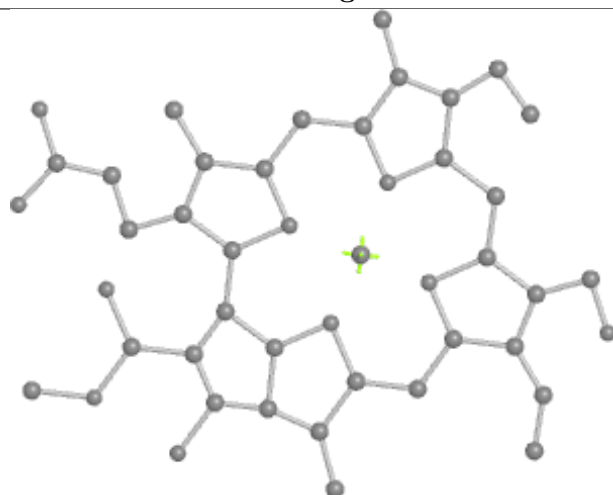
Bond lengths



Bond angles

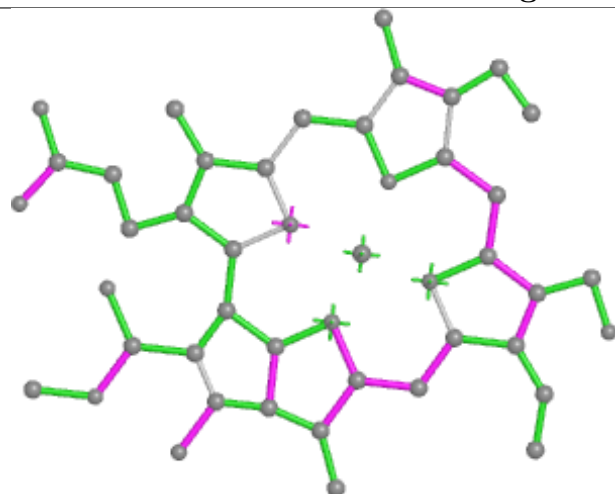


Torsions

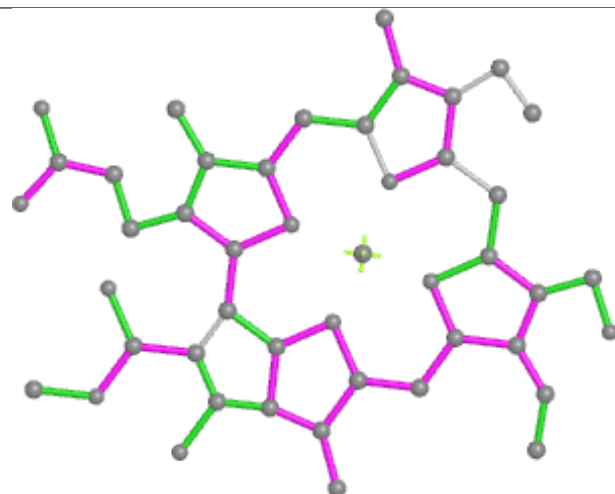


Rings

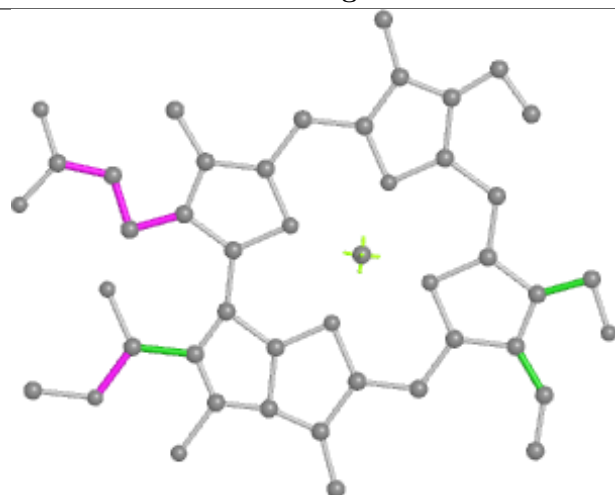
## Ligand CHL 3 608



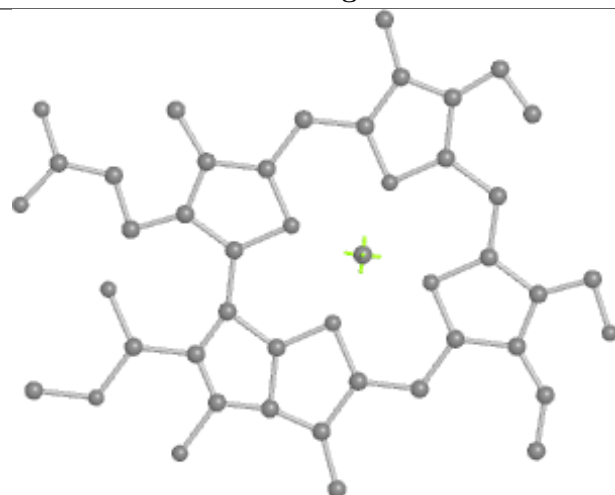
Bond lengths



Bond angles

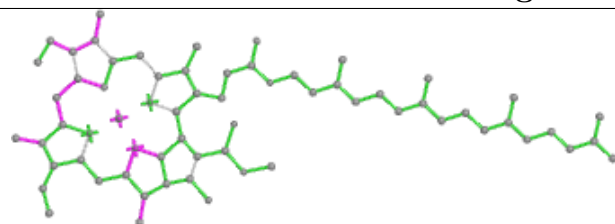


Torsions

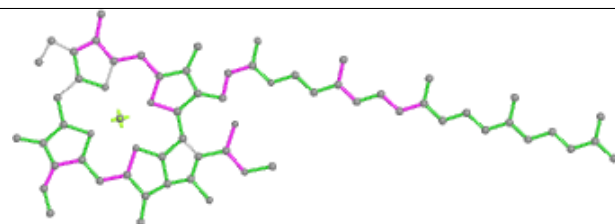


Rings

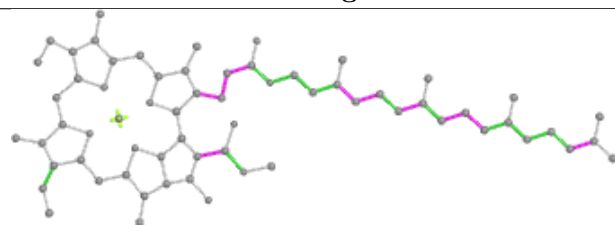
## Ligand CLA Y 602



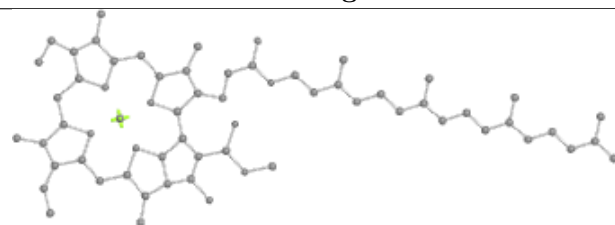
Bond lengths



Bond angles

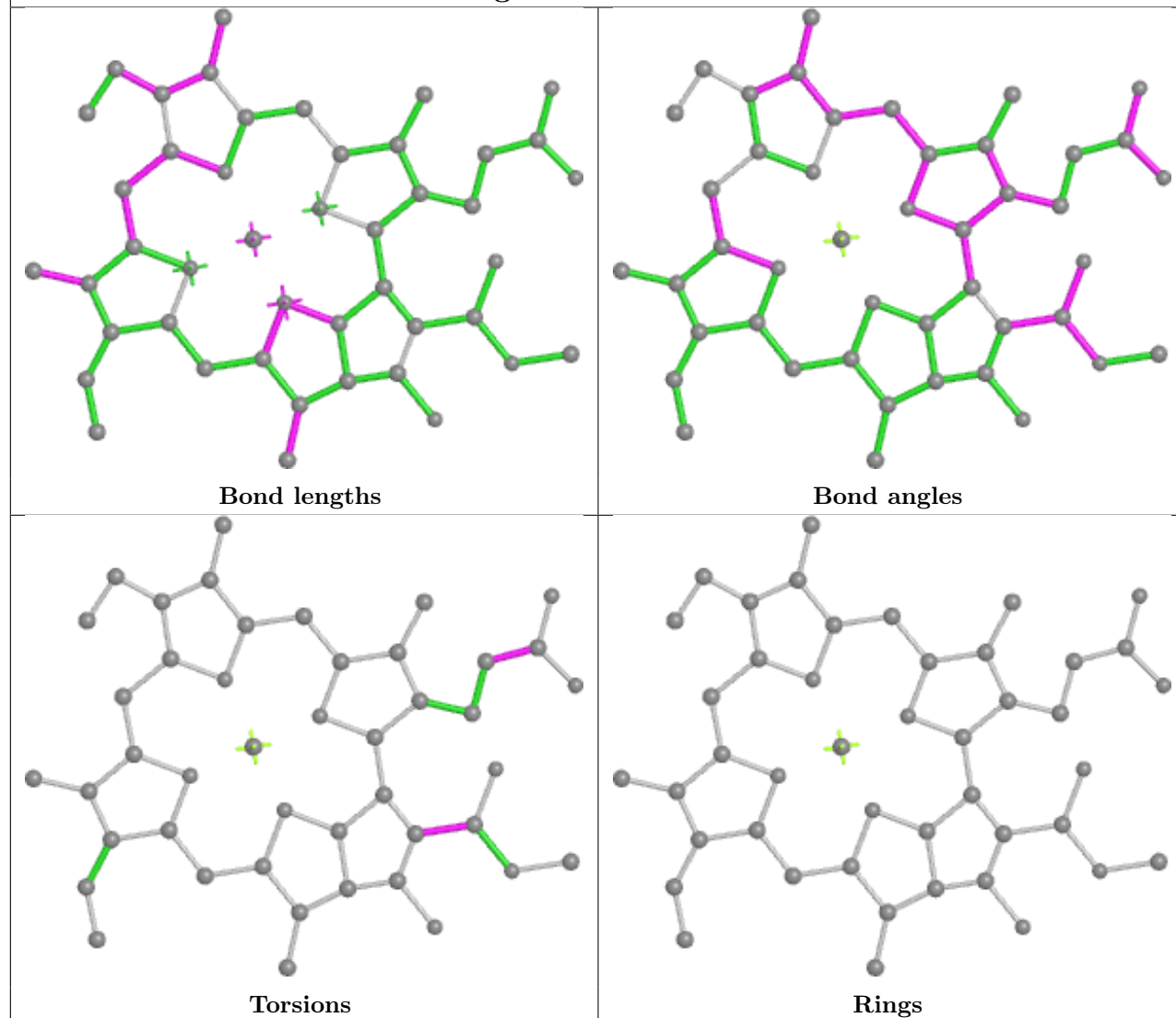


Torsions

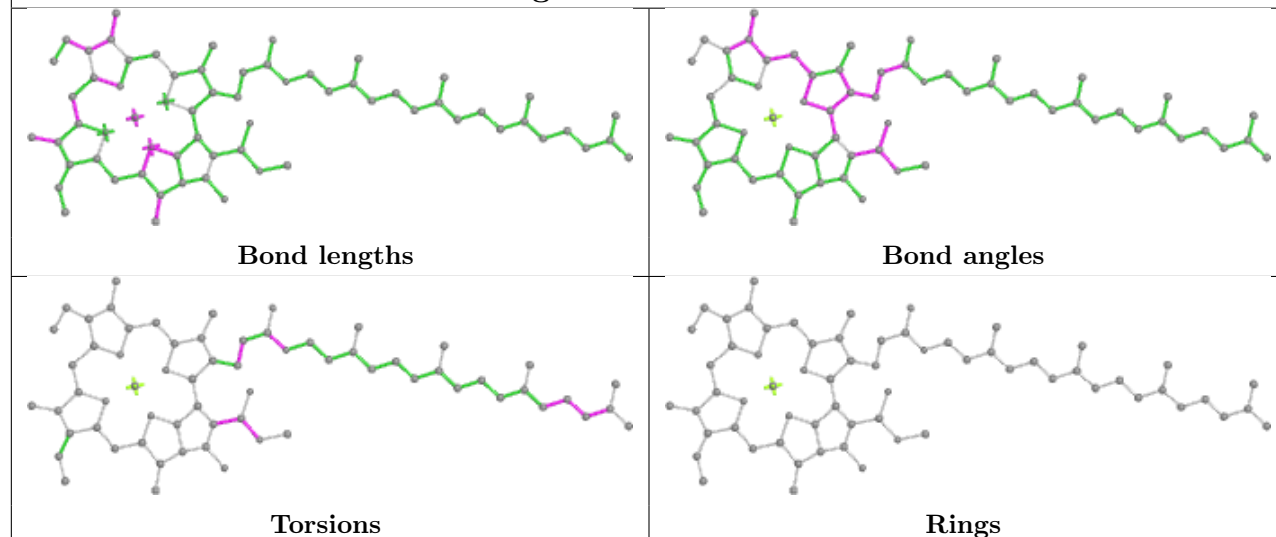


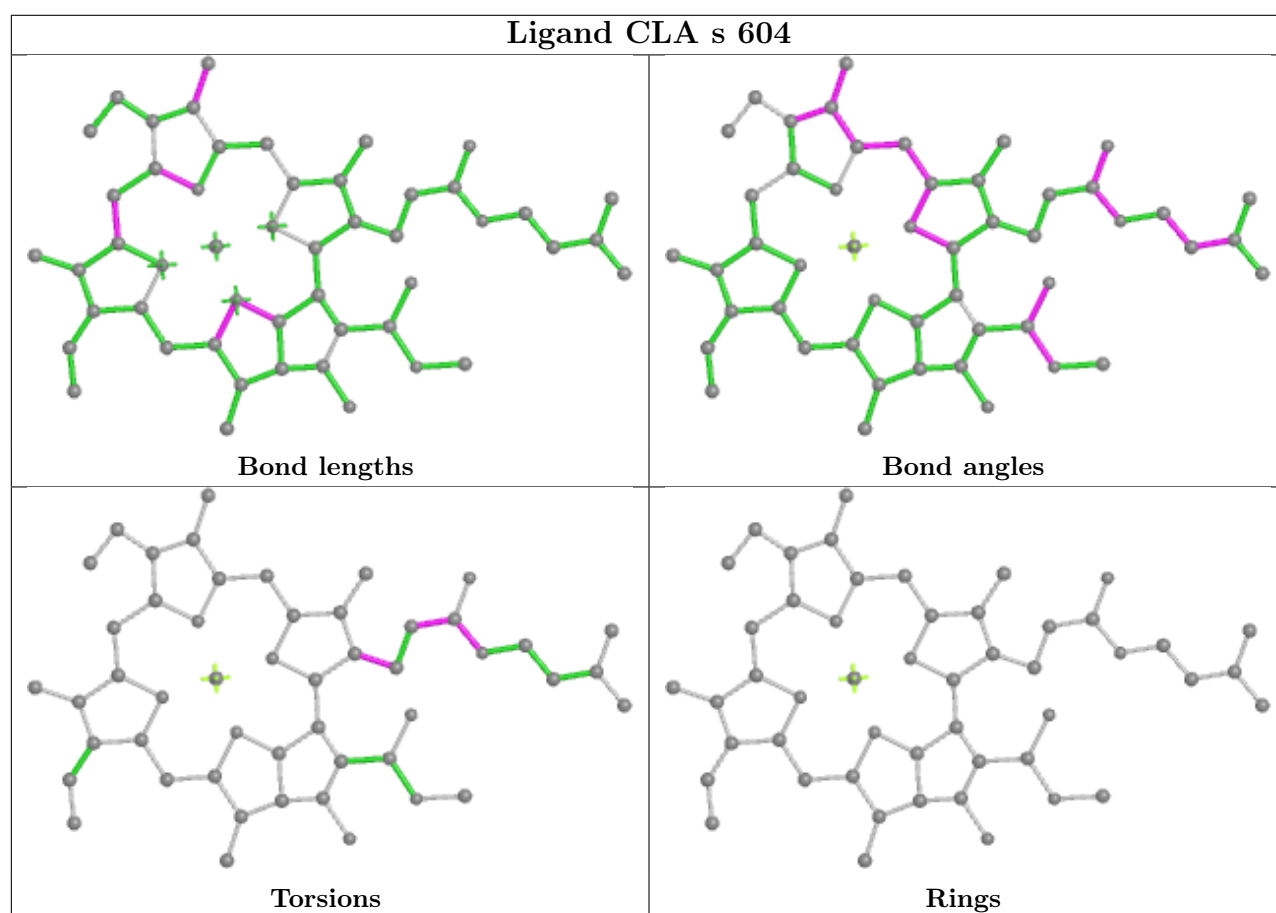
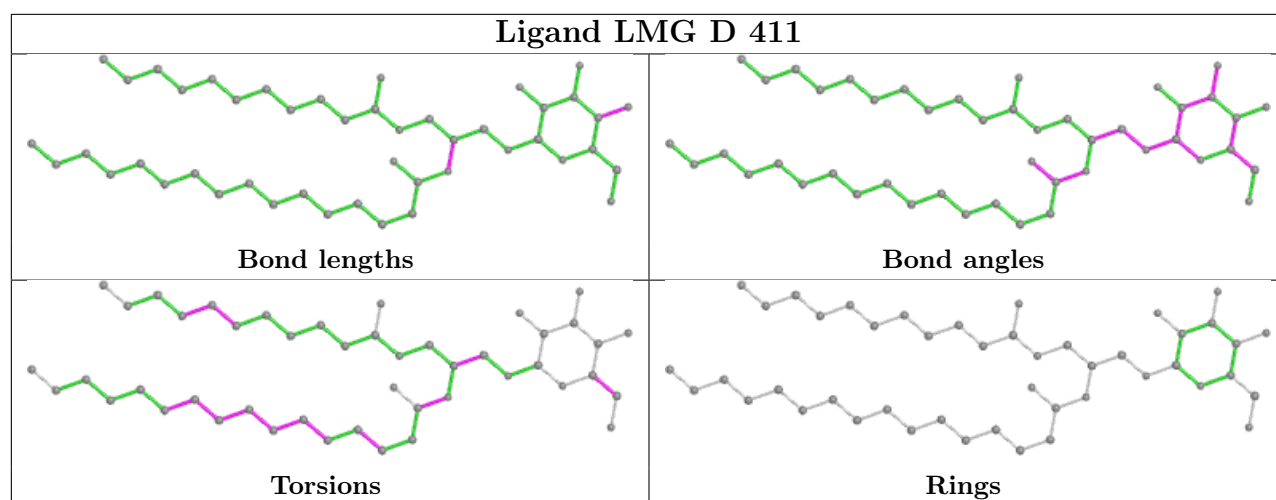
Rings

## Ligand CLA 5 612



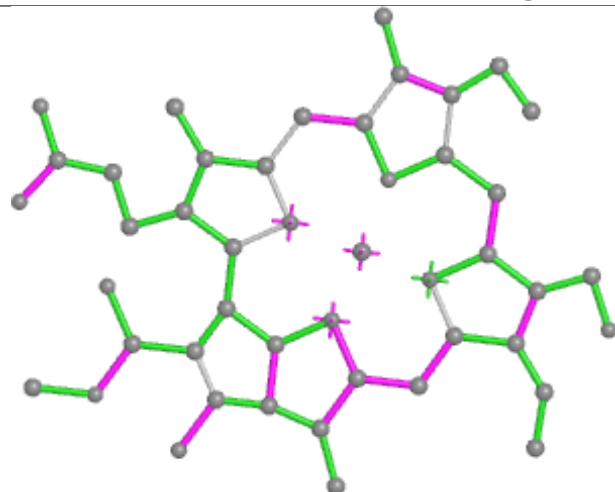
## Ligand CLA B 611



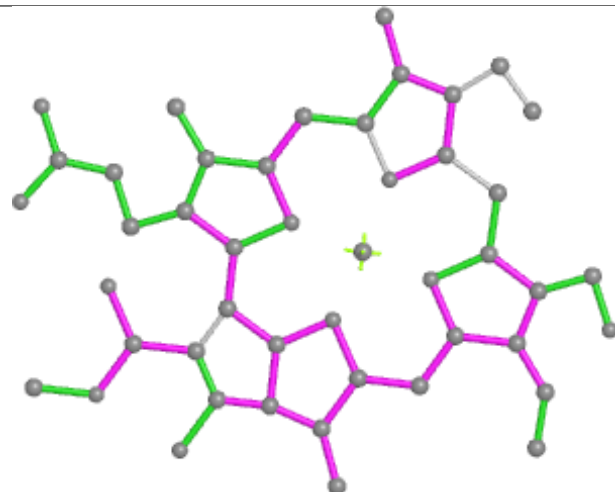




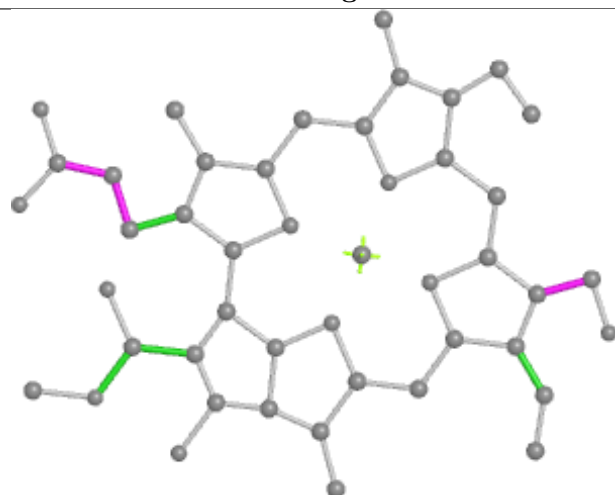
## Ligand CHL 1 601



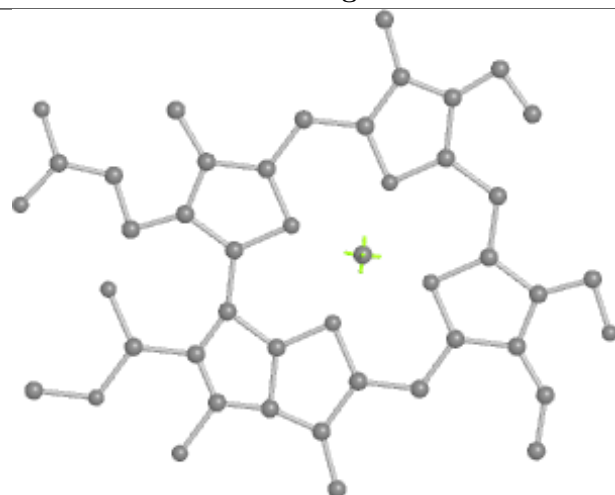
Bond lengths



Bond angles

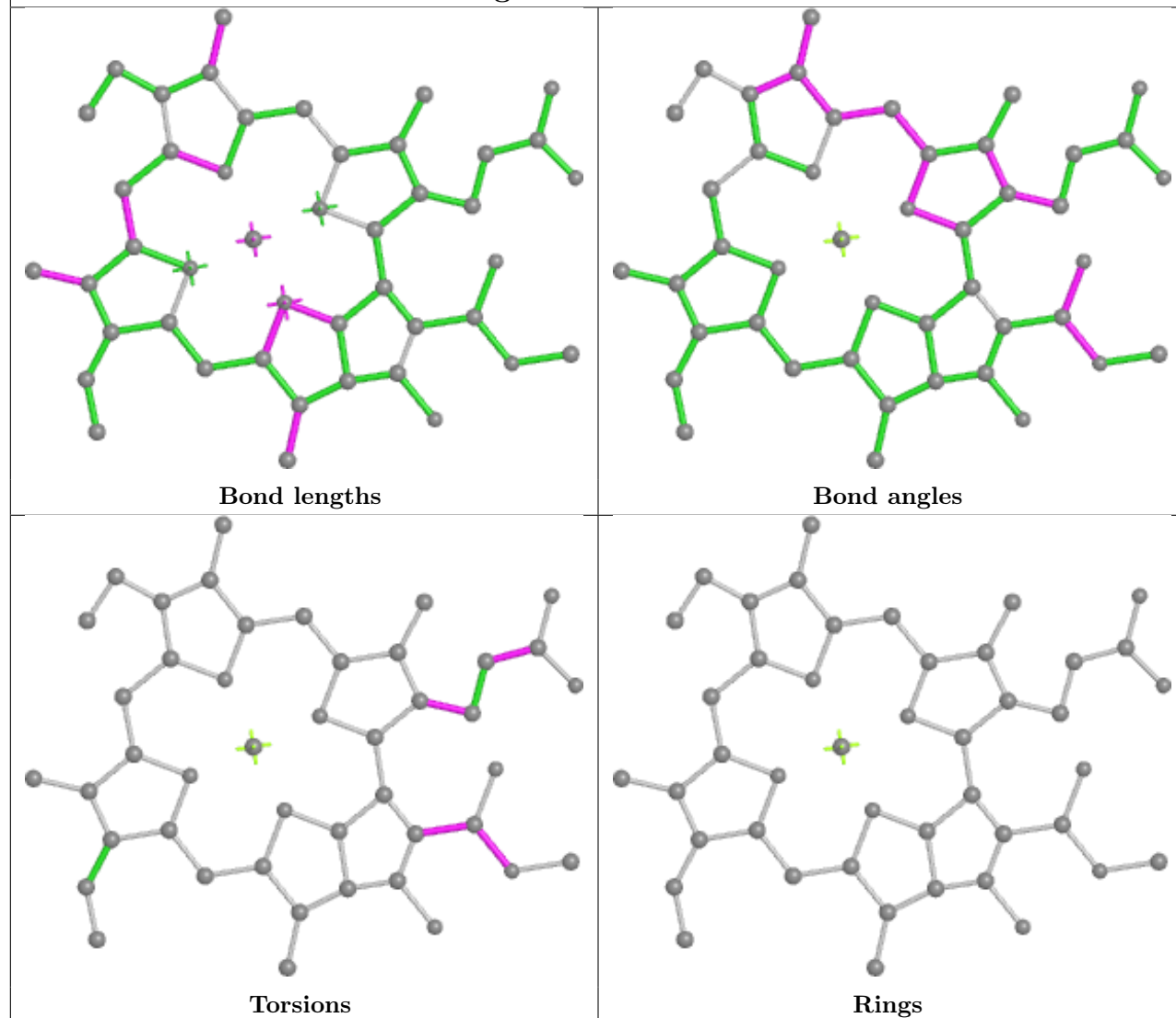


Torsions

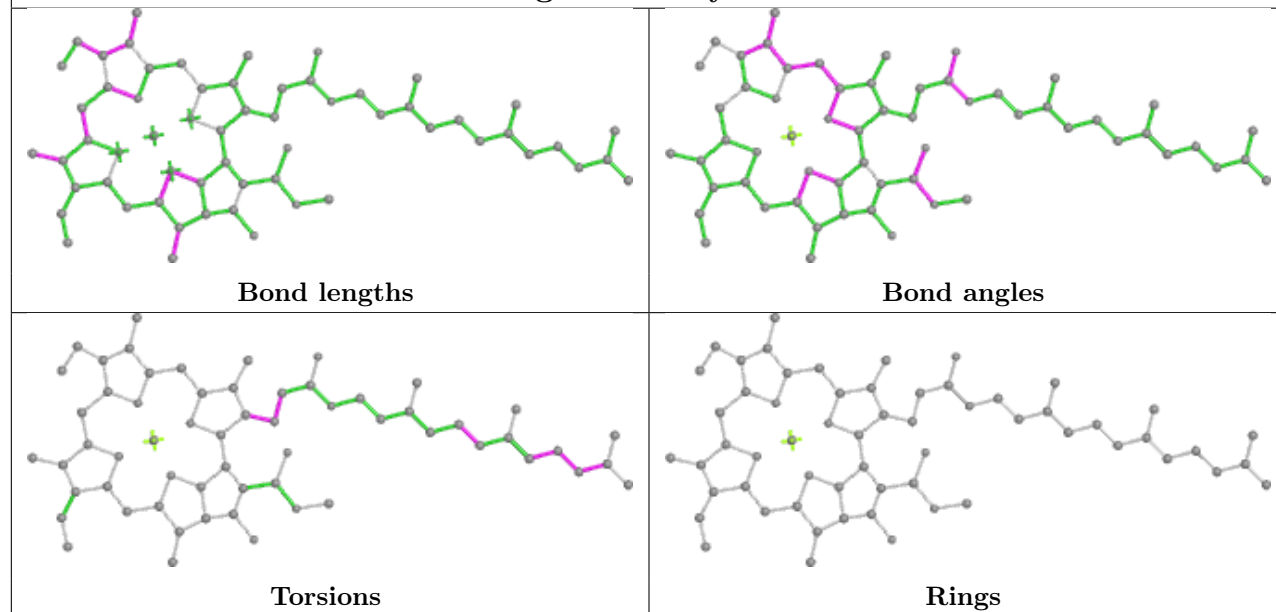


Rings

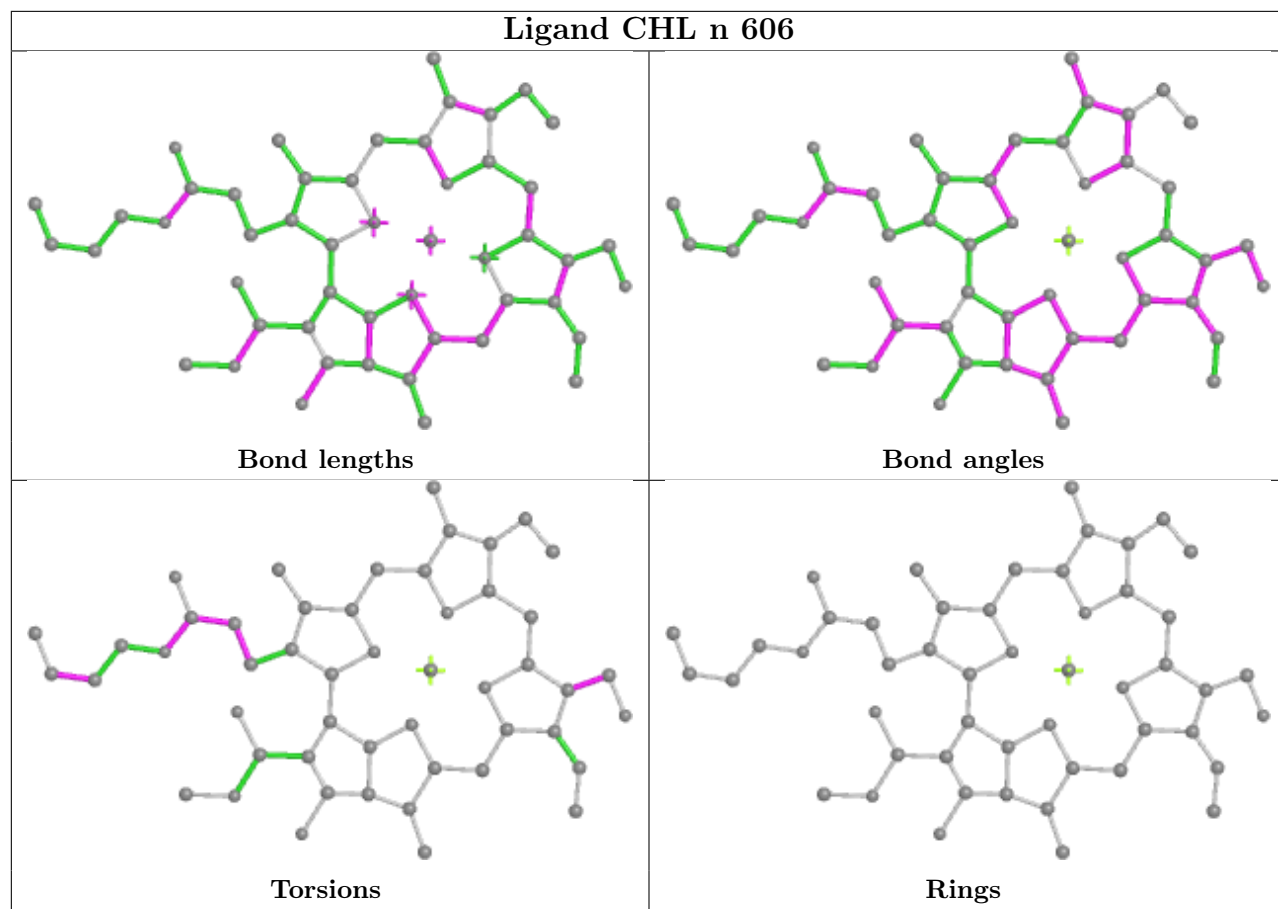
## Ligand CLA 8 612

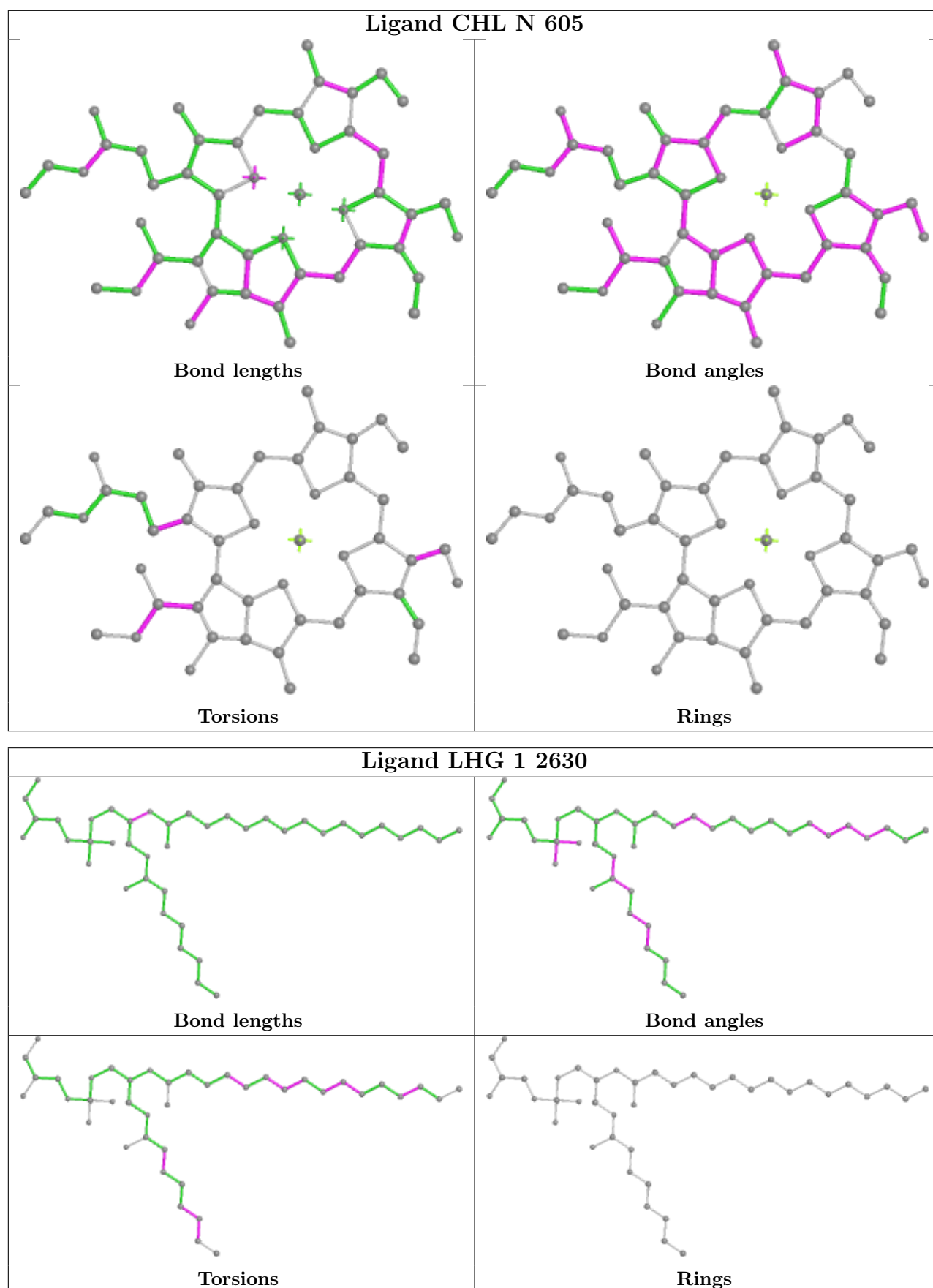


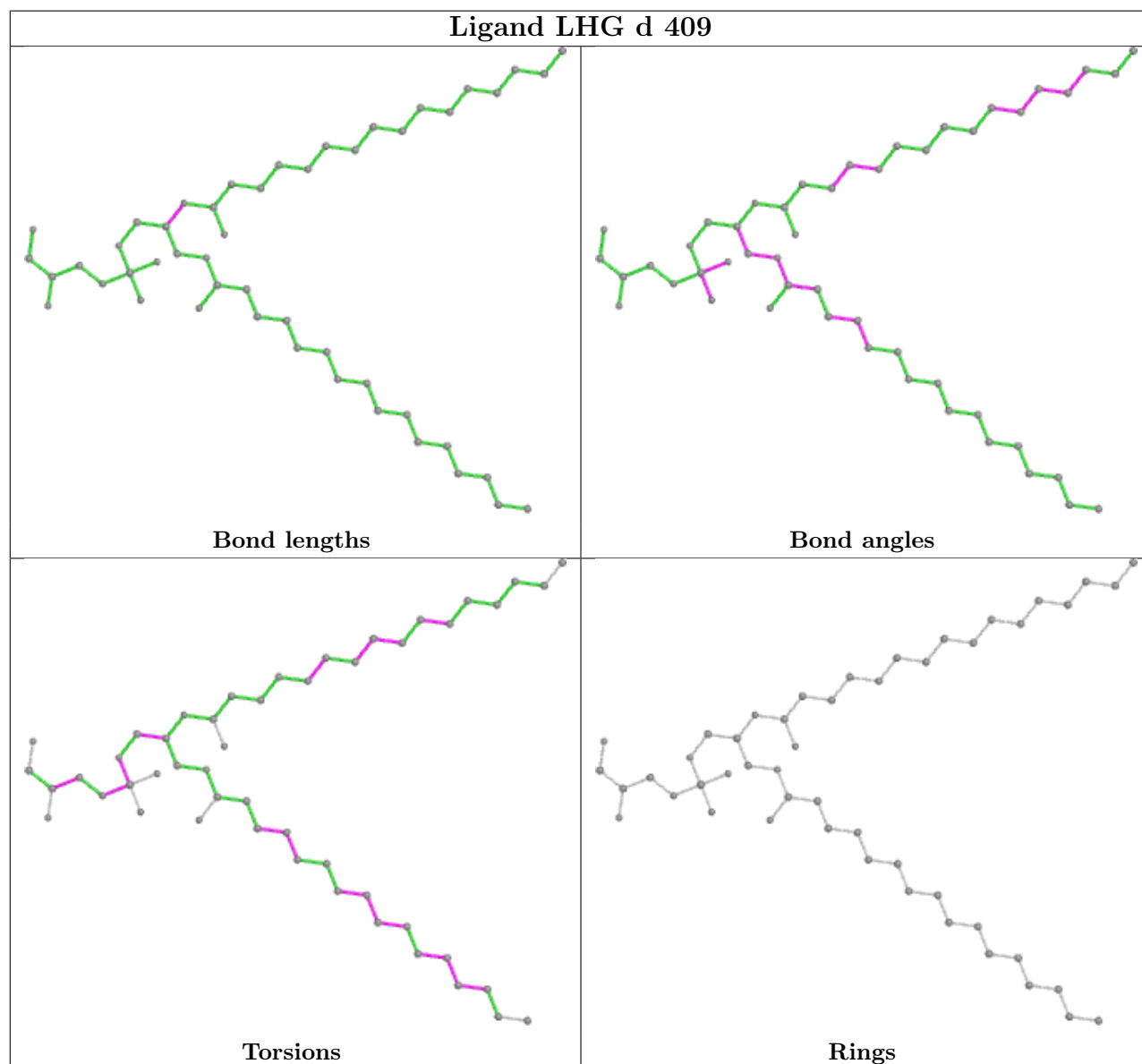
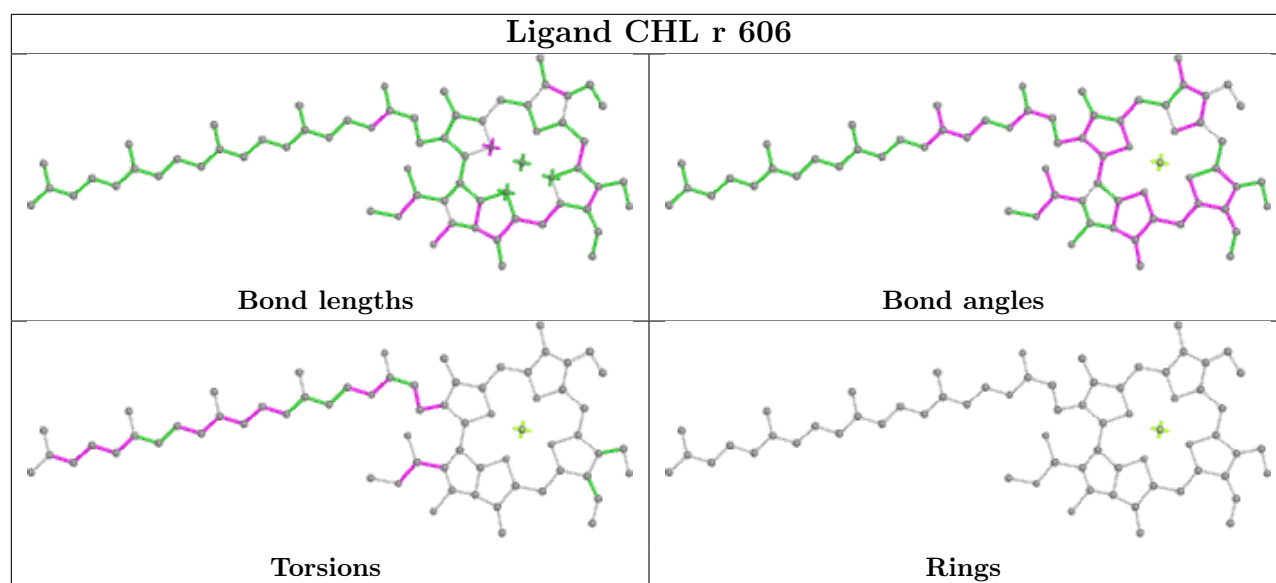
## Ligand CLA y 610

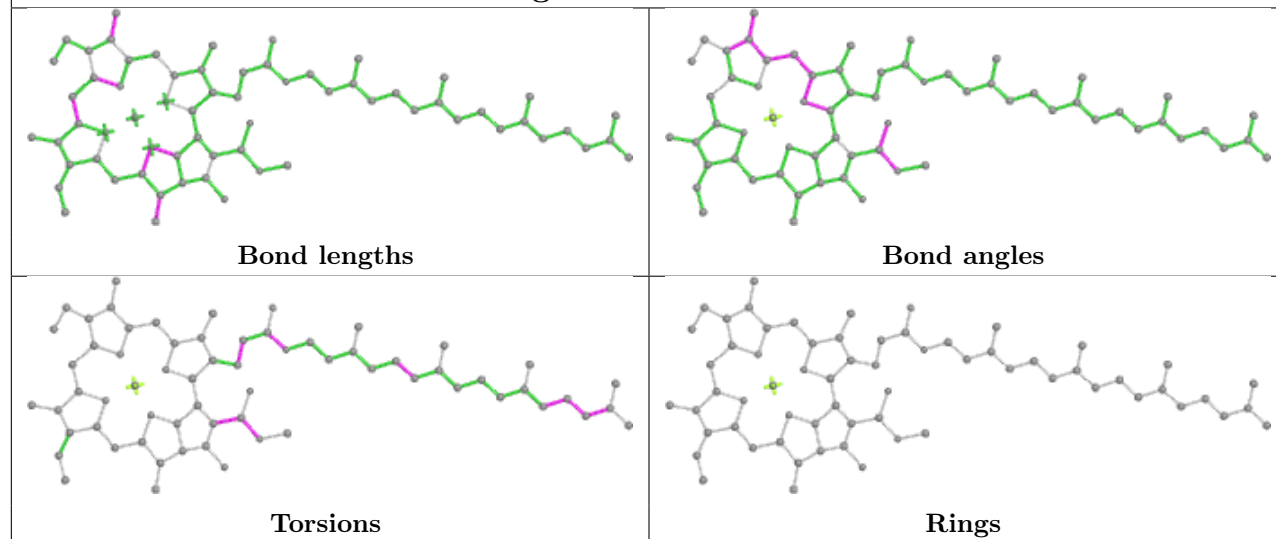
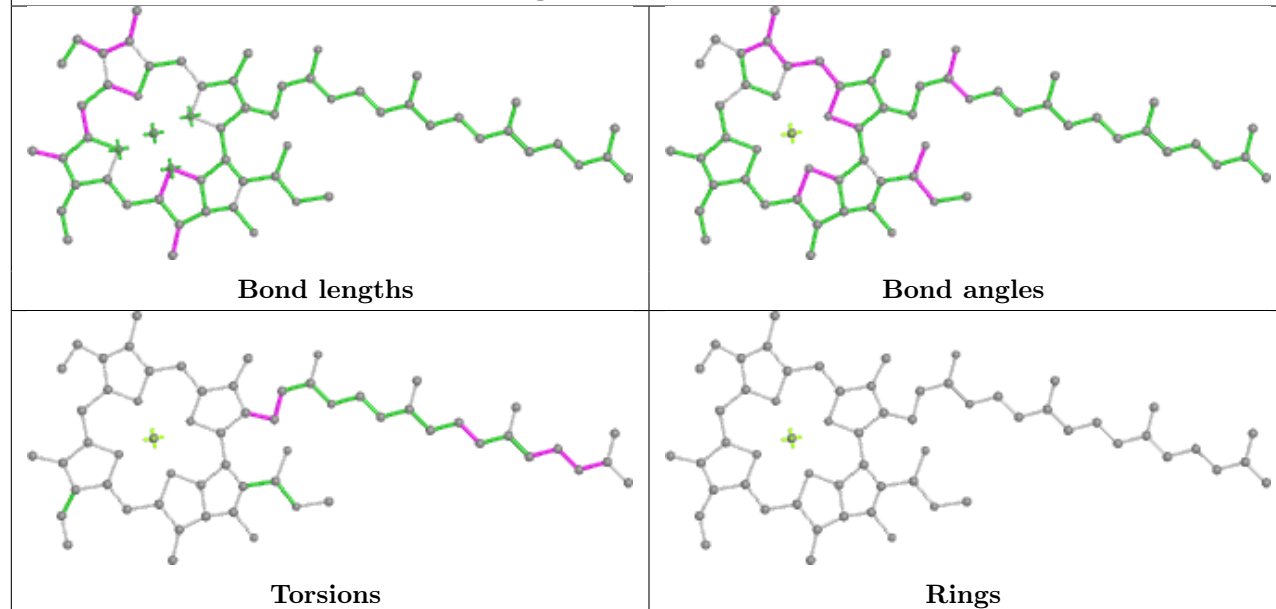


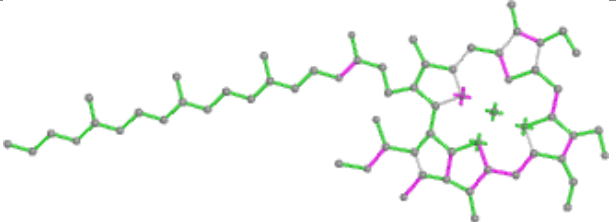
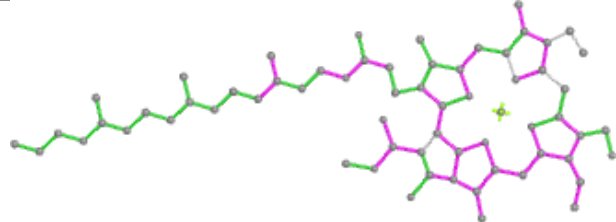
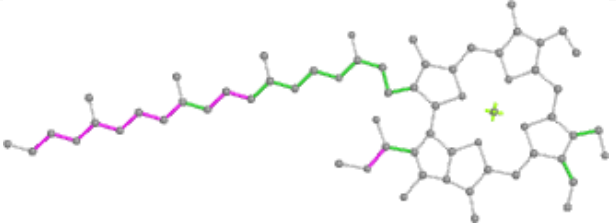
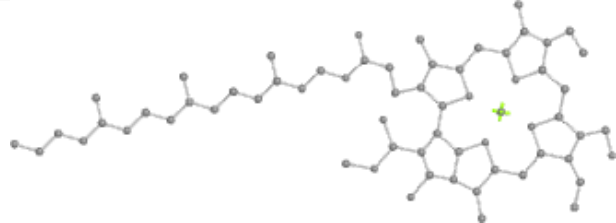
## Ligand CHL n 606

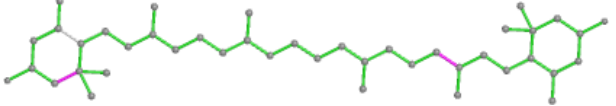
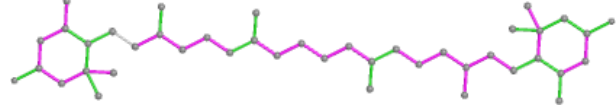
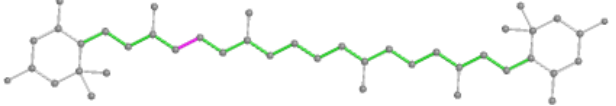
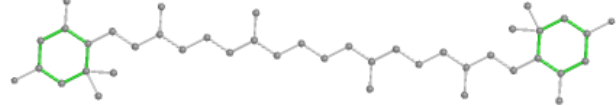




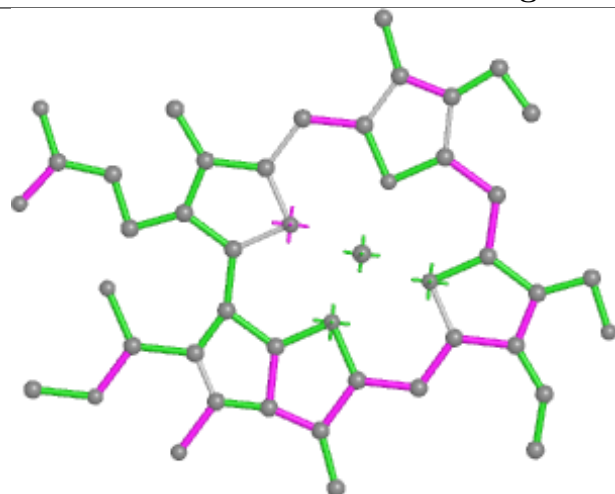


**Ligand CLA C 503****Ligand CLA Y 610**

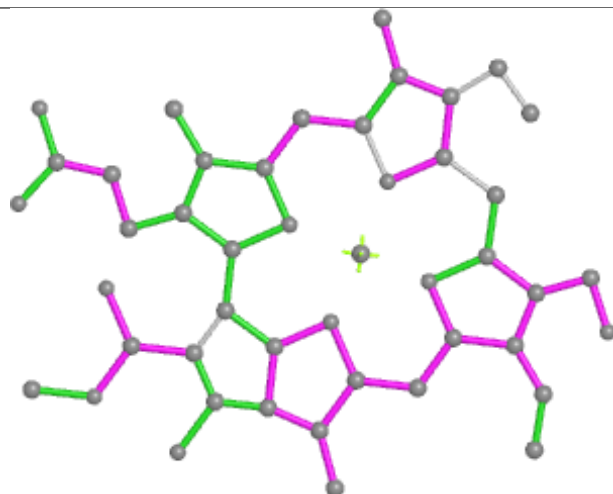
Ligand CHL 7 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT N 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

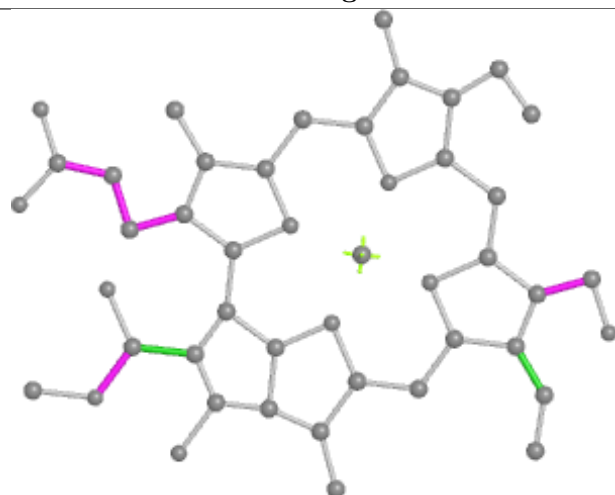
## Ligand CHL 8 607



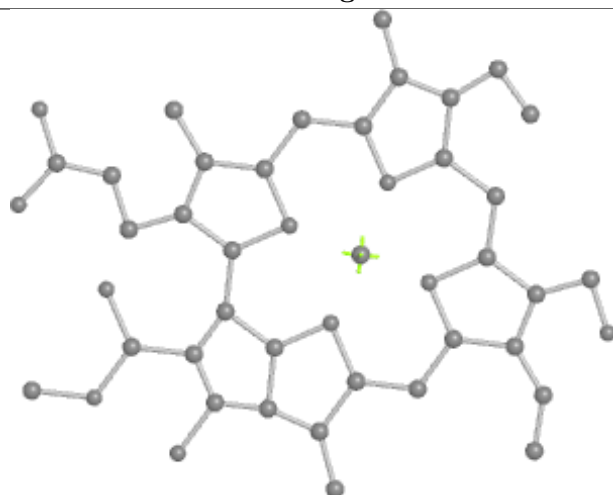
Bond lengths



Bond angles

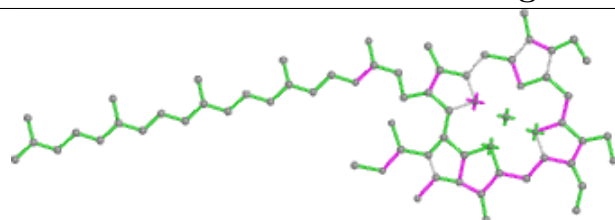


Torsions

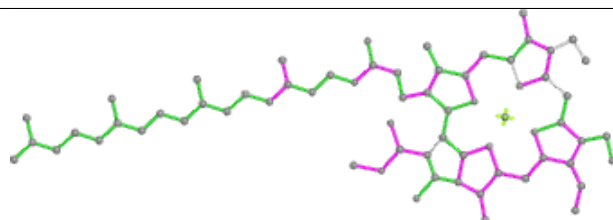


Rings

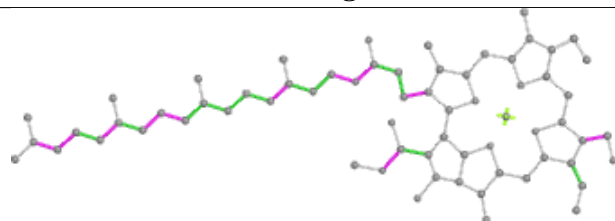
## Ligand CHL n 609



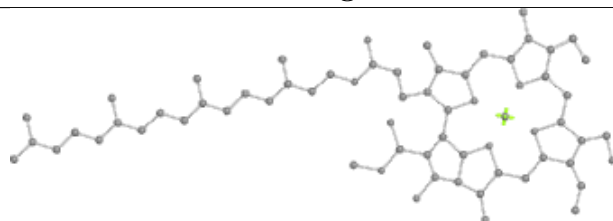
Bond lengths



Bond angles

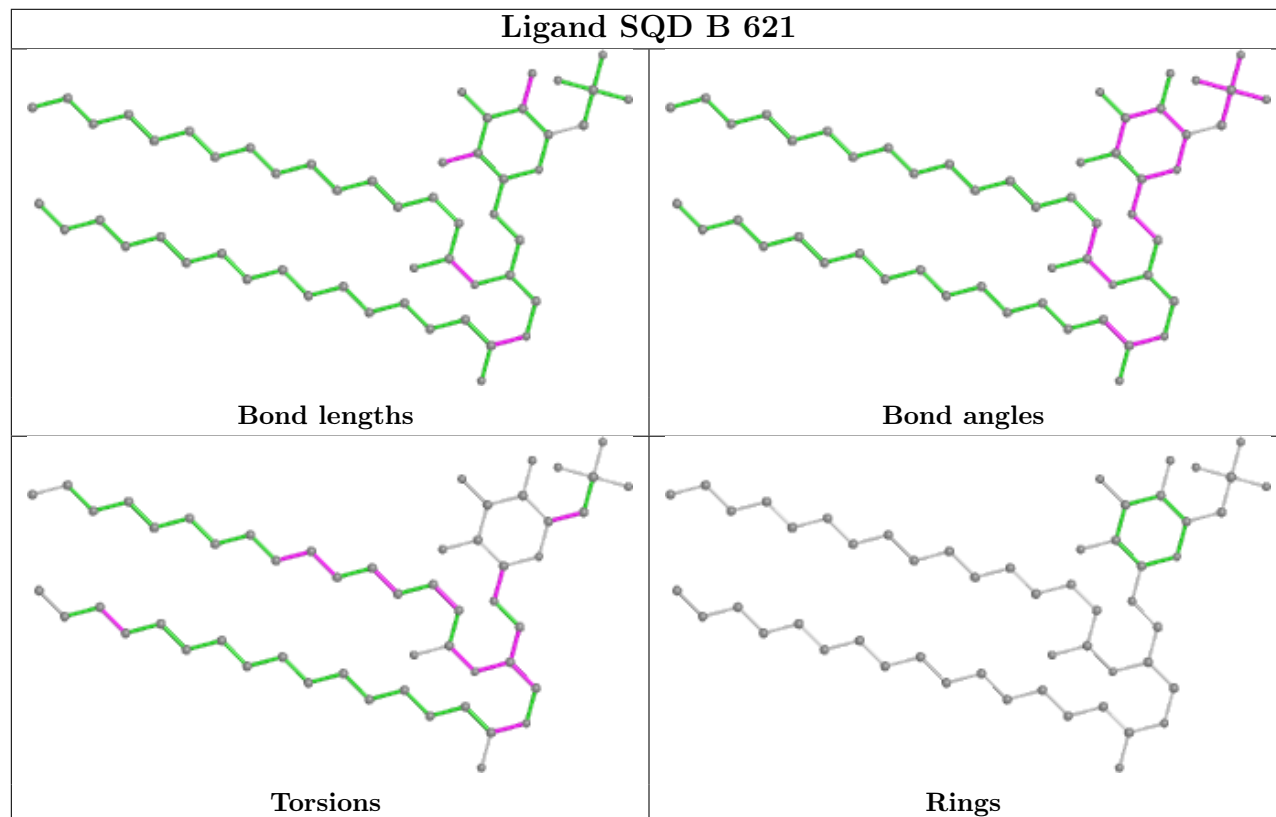
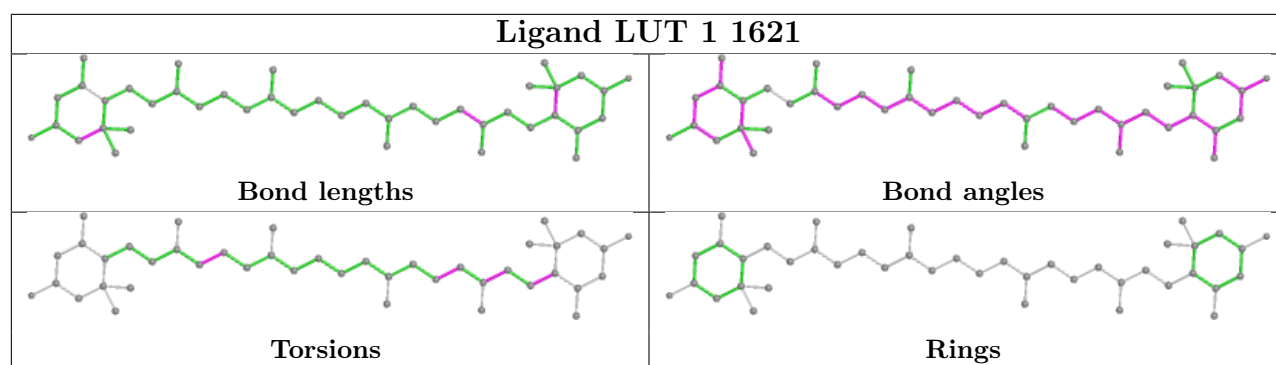


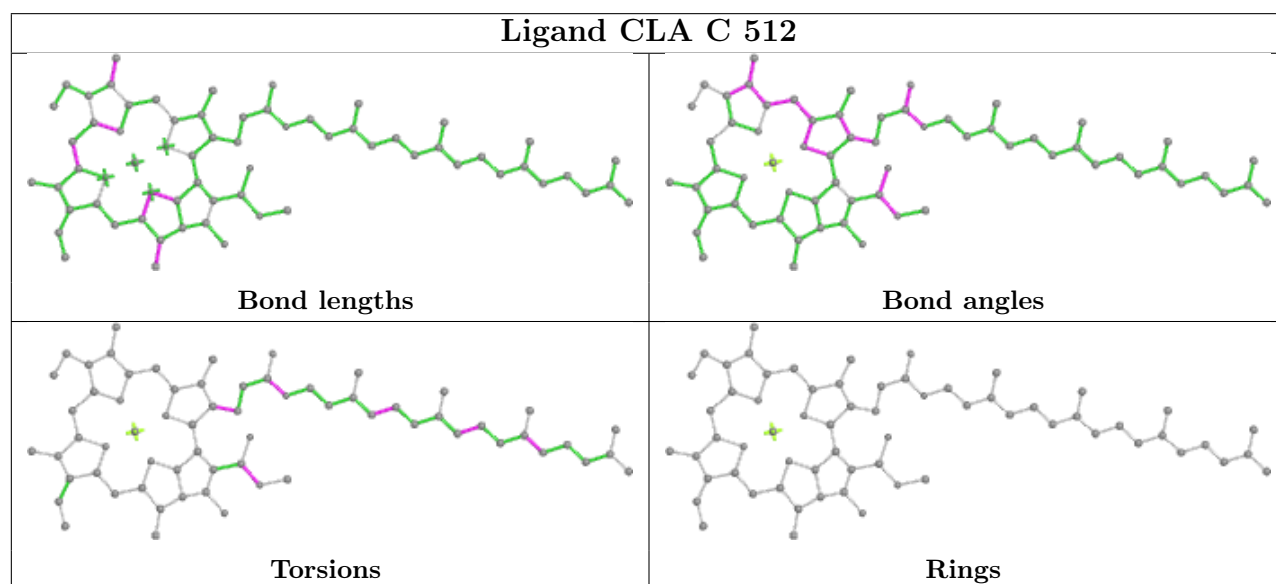
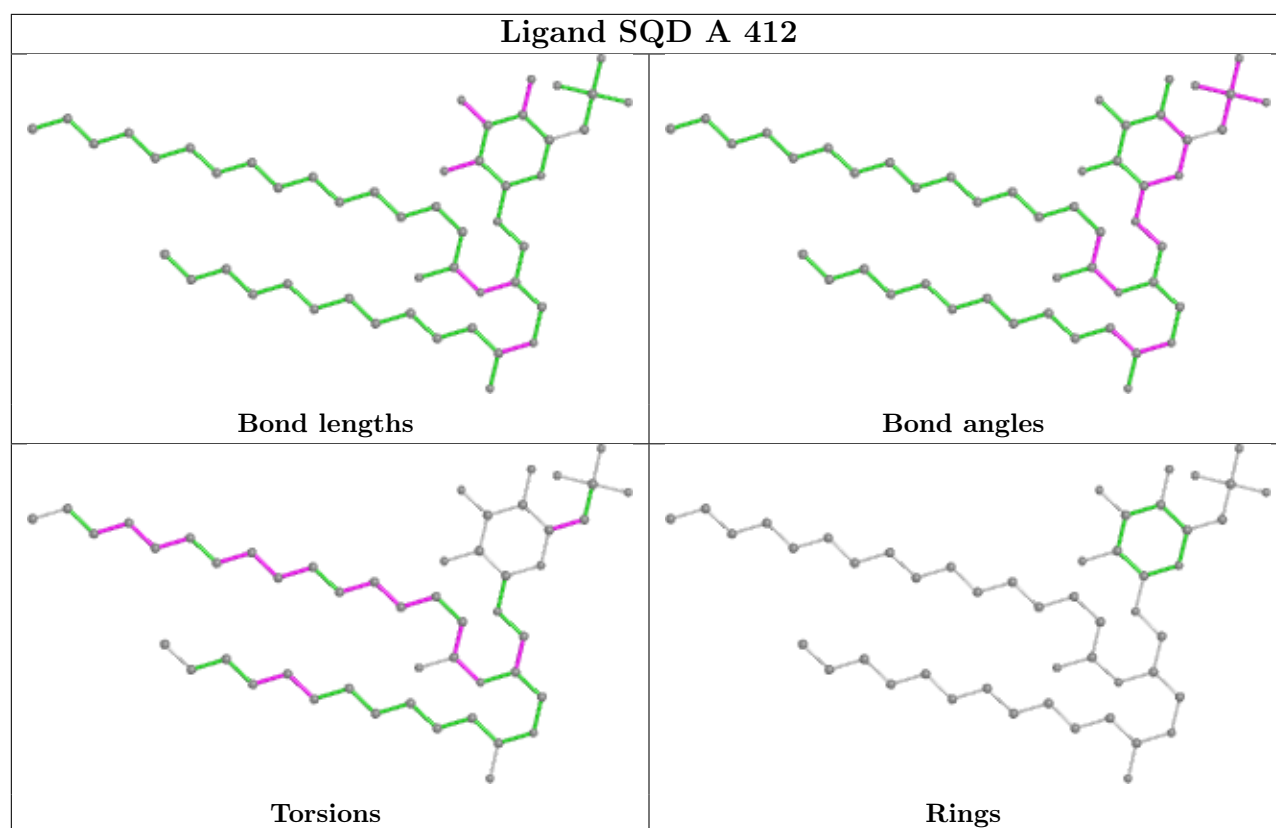
Torsions

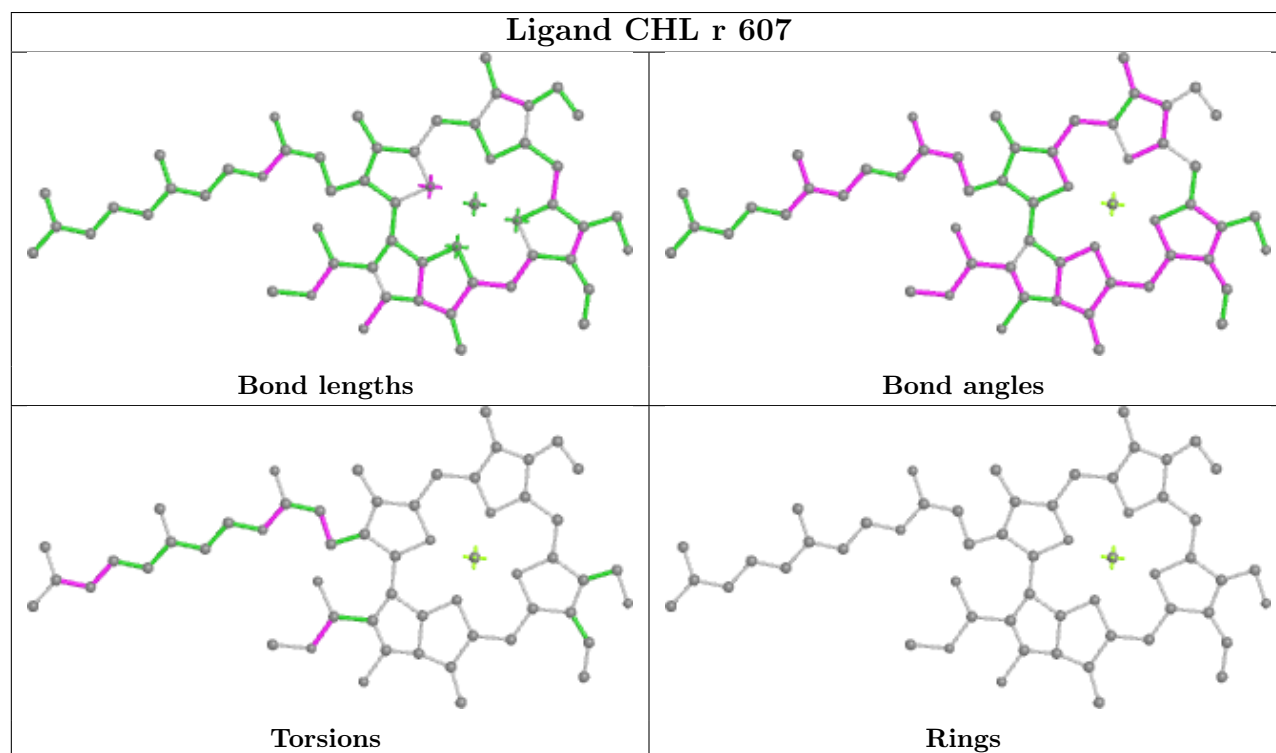
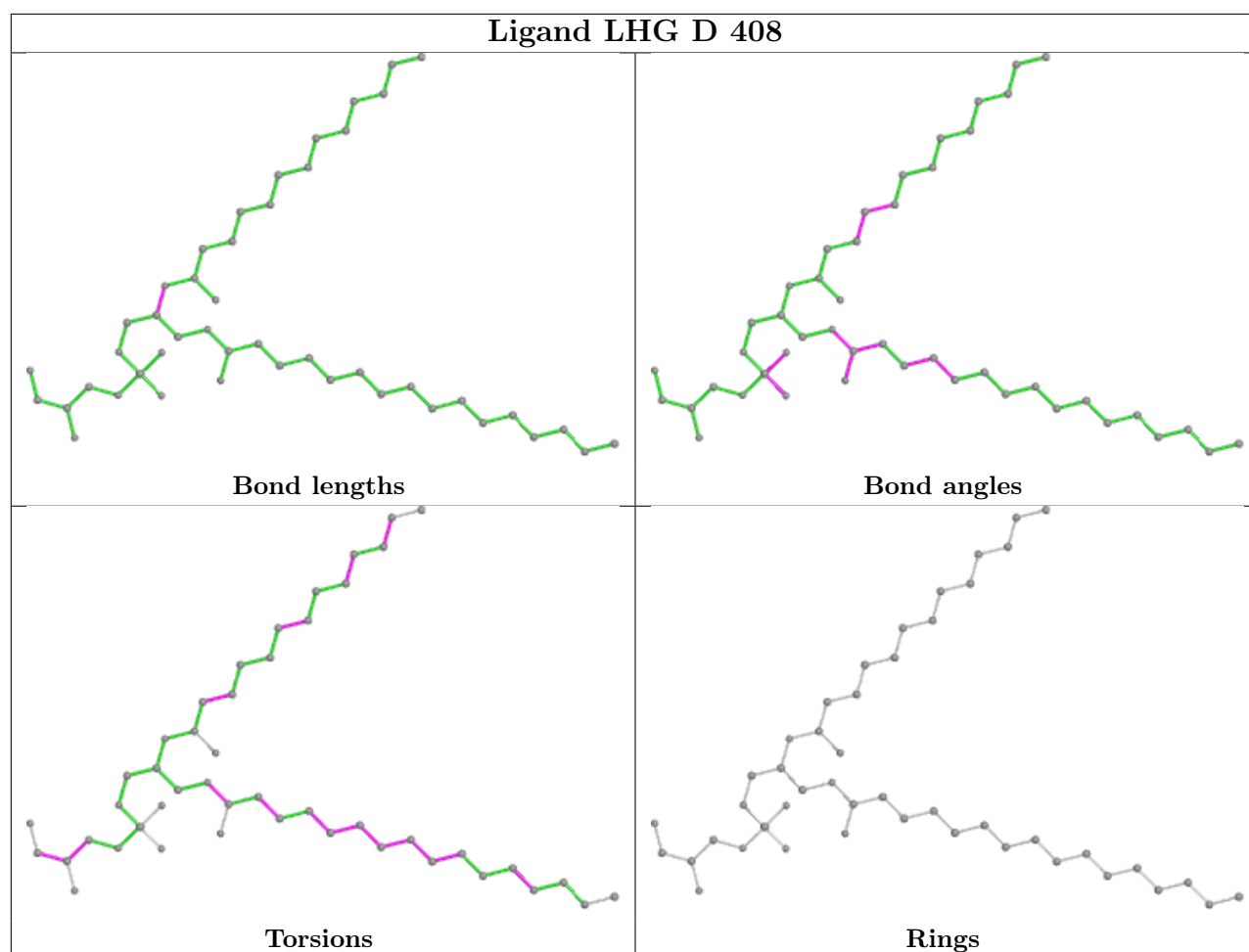


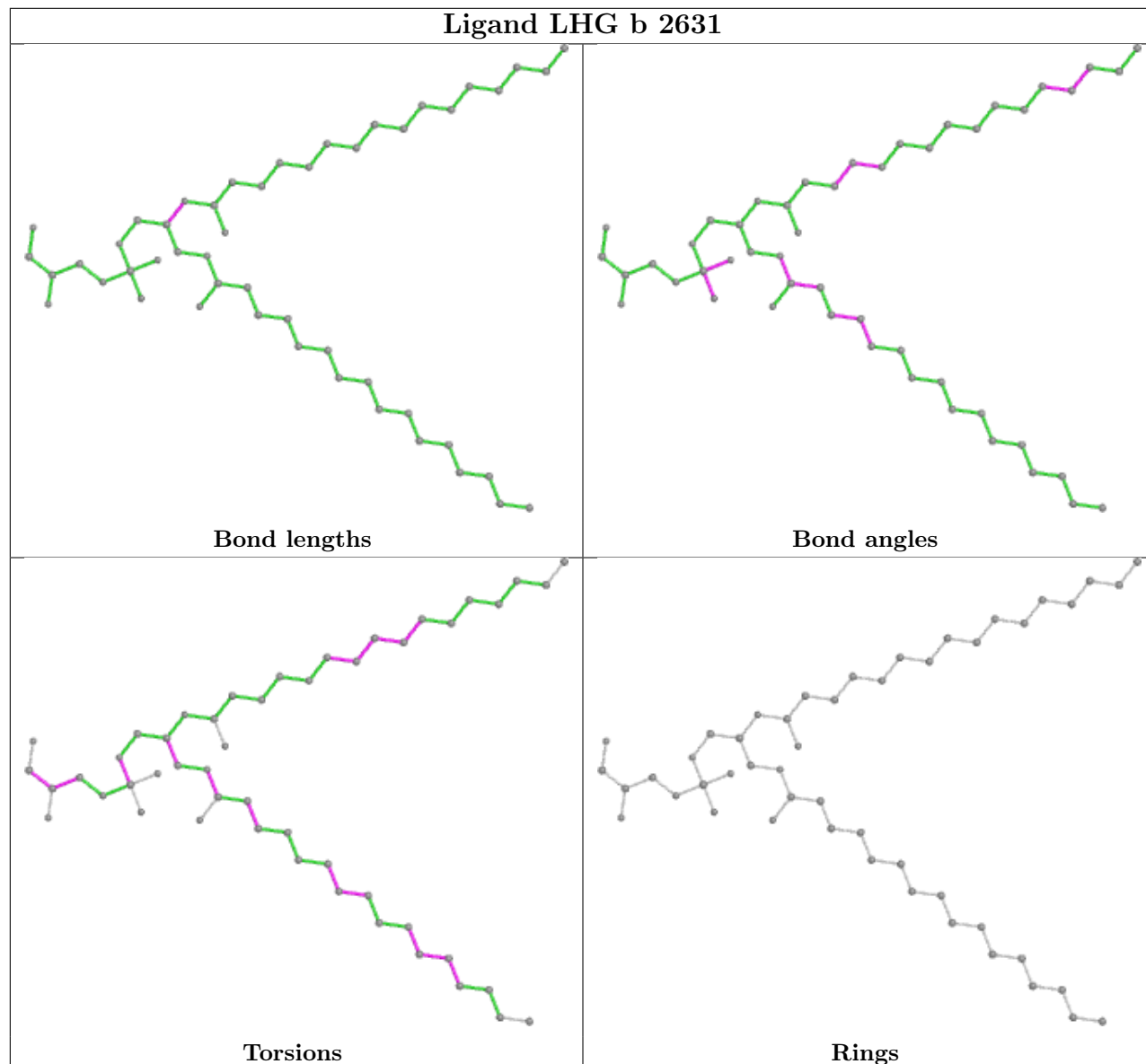
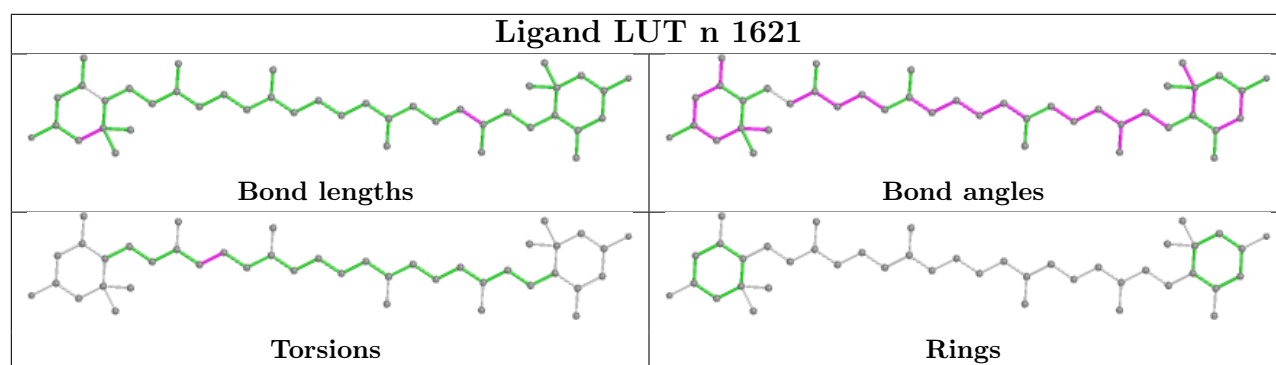
Rings



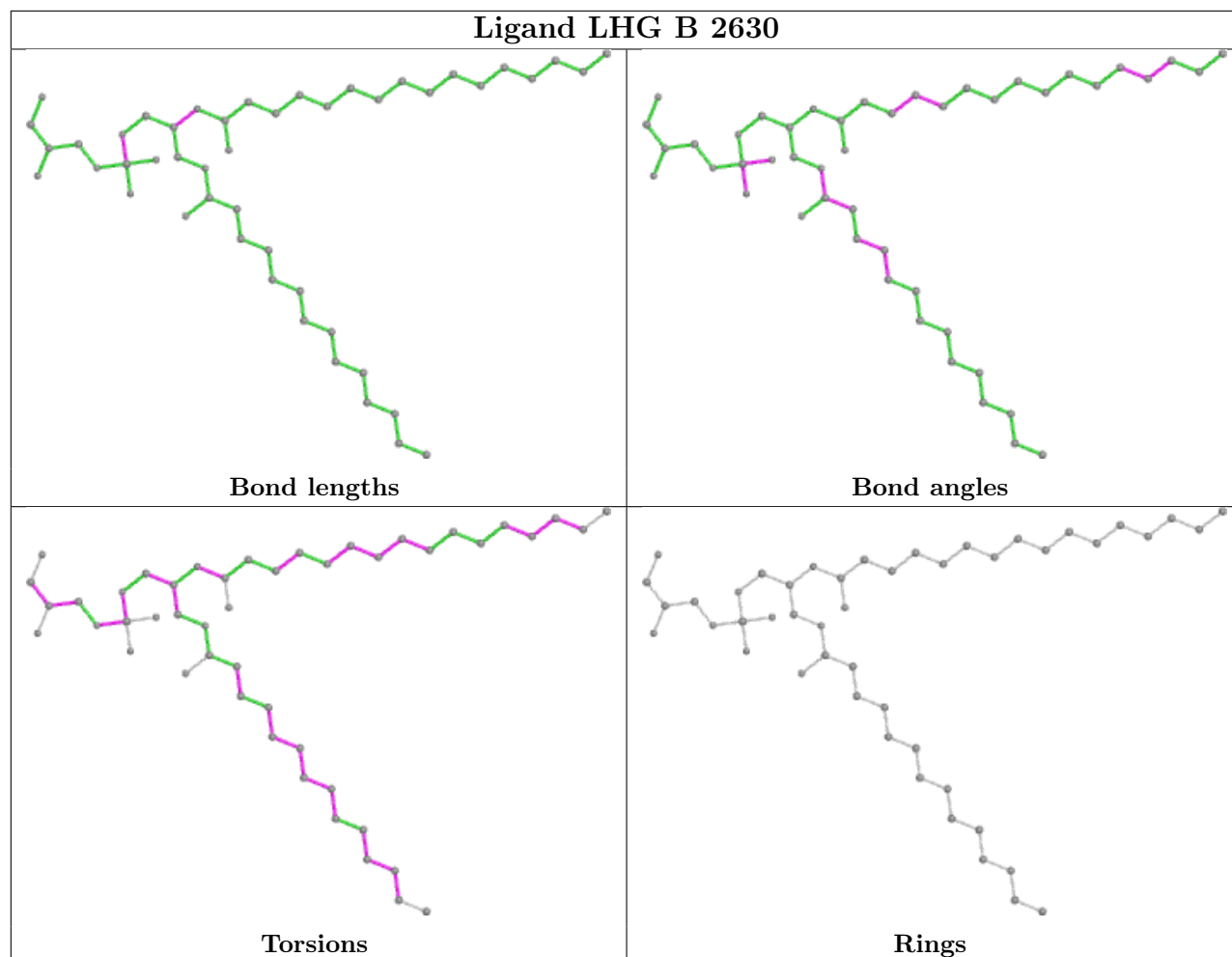




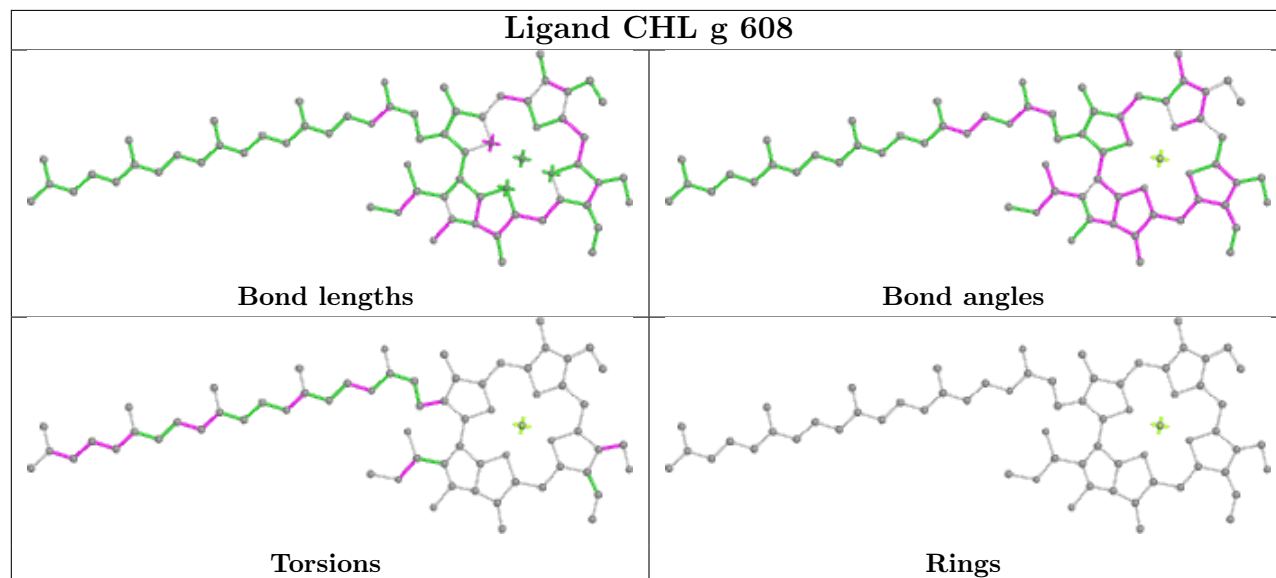


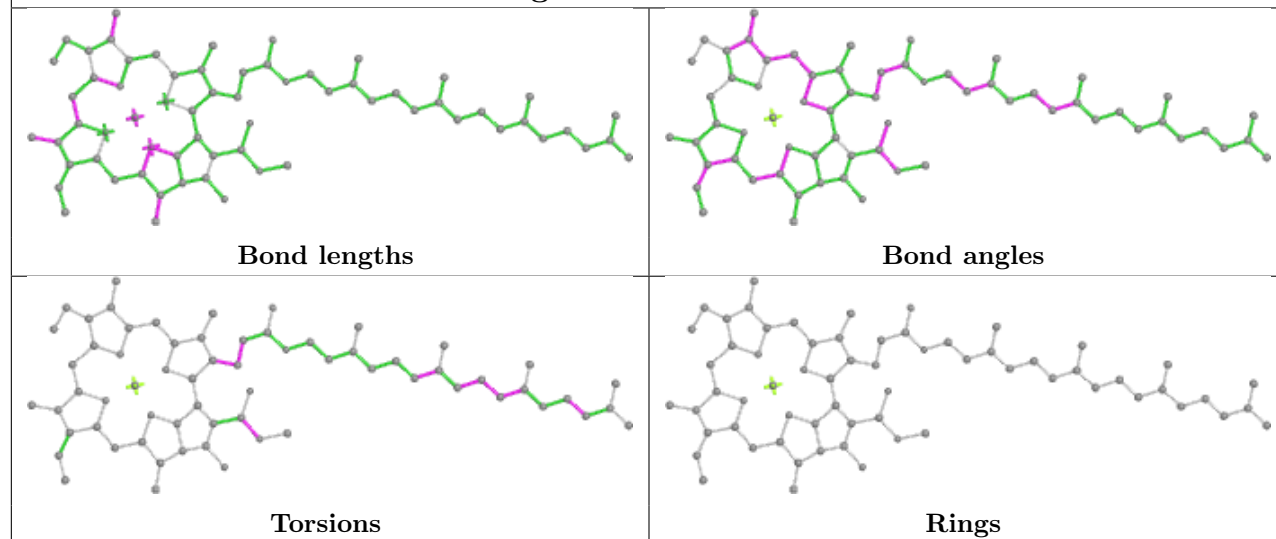
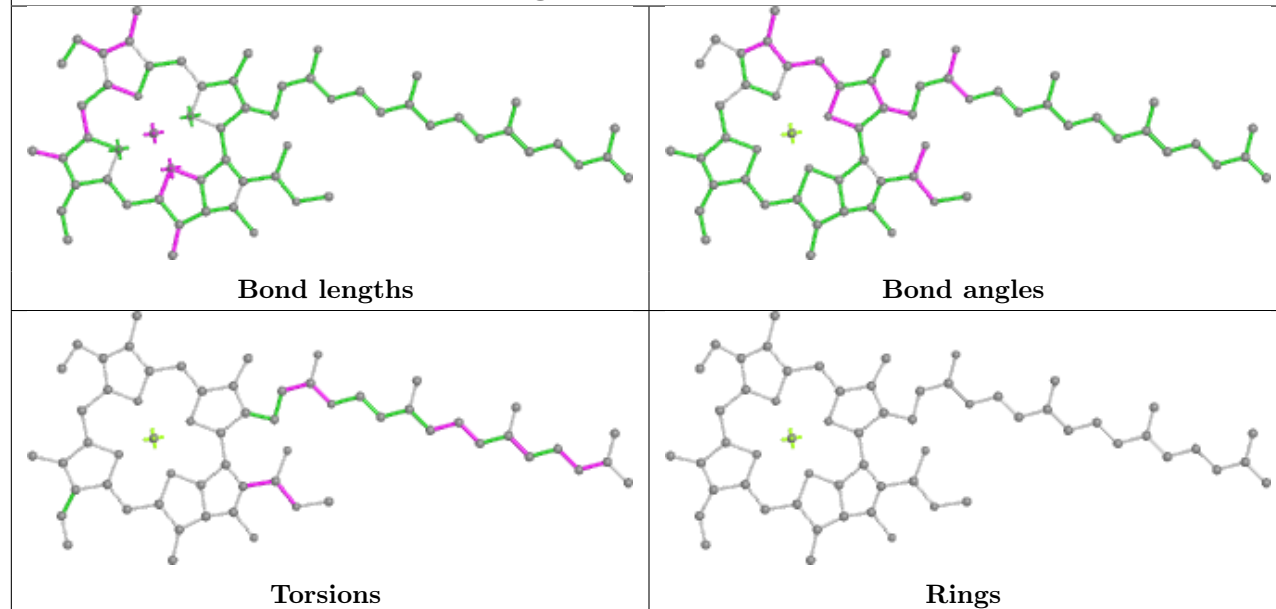


## Ligand LHG B 2630

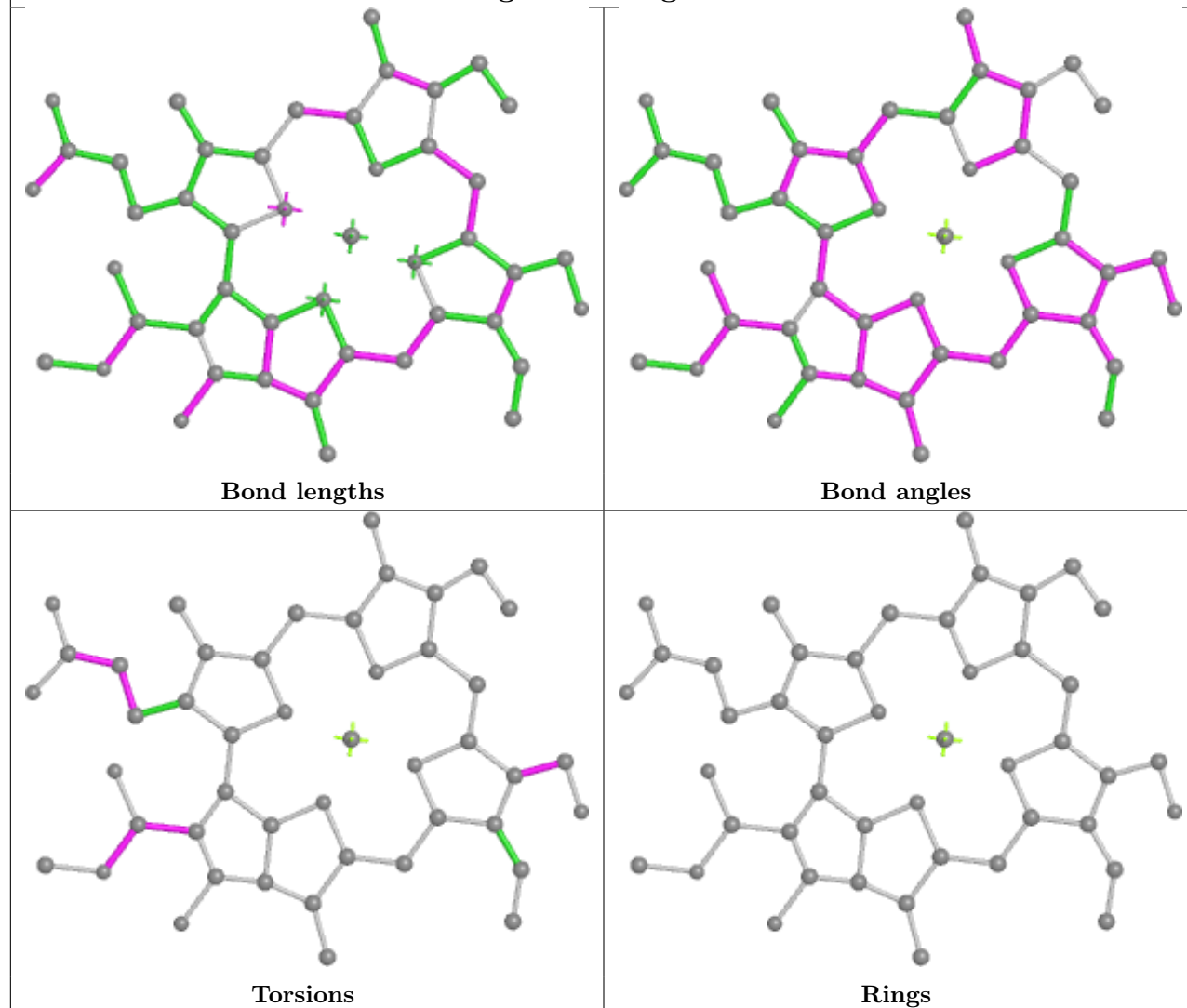


## Ligand CHL g 608

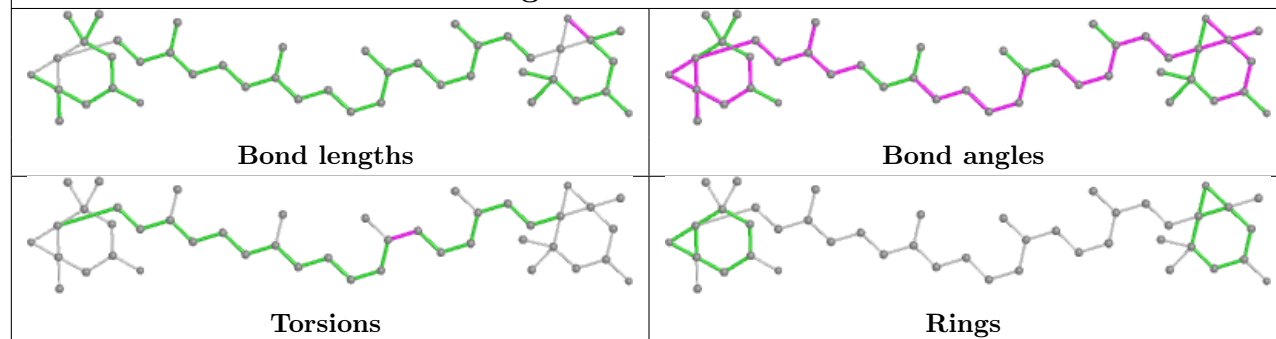


**Ligand CLA G 602****Ligand CLA R 603**

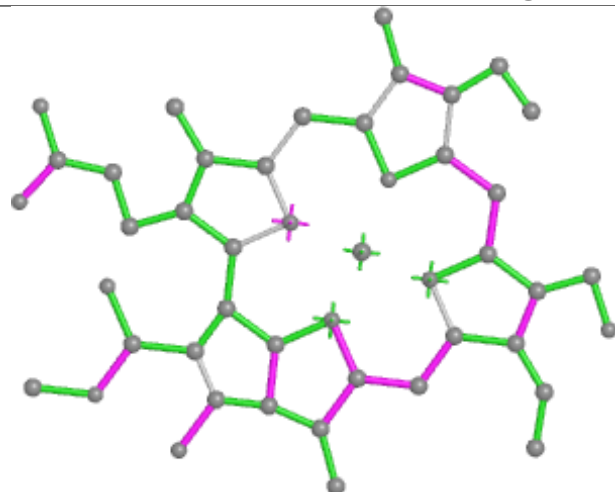
## Ligand CHL g 605



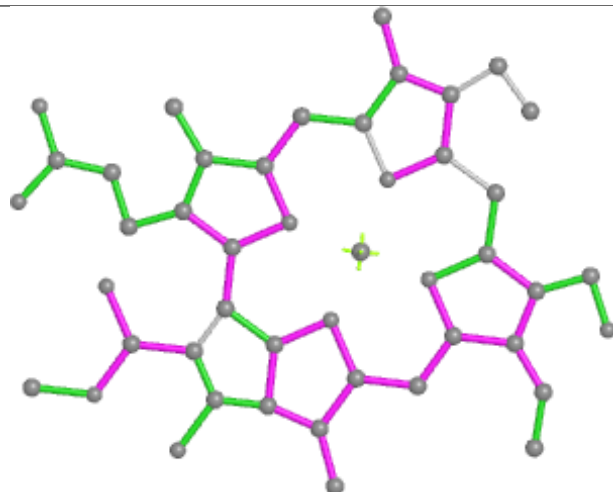
## Ligand XAT G 1622



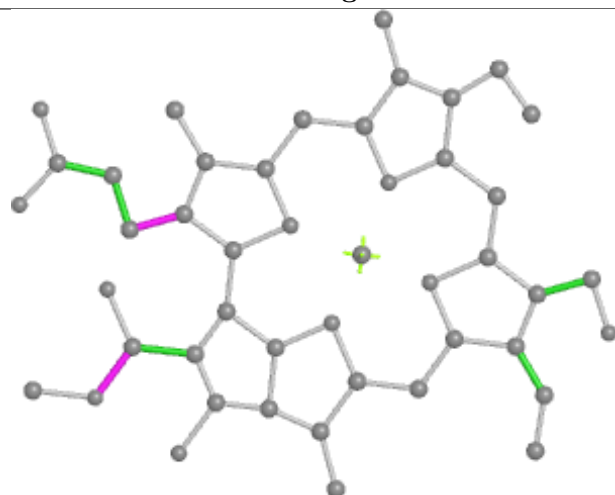
## Ligand CHL 5 608



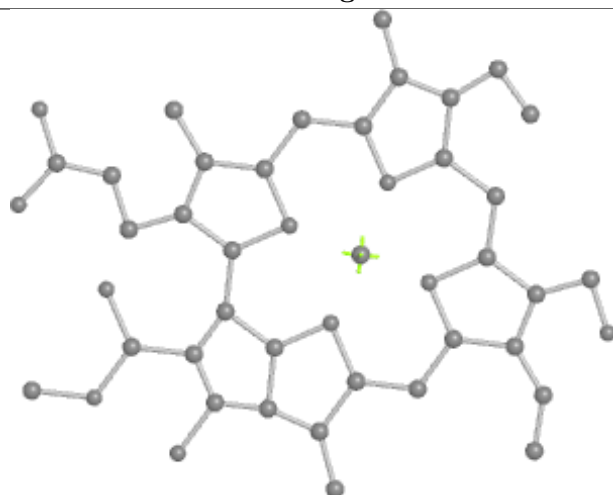
Bond lengths



Bond angles



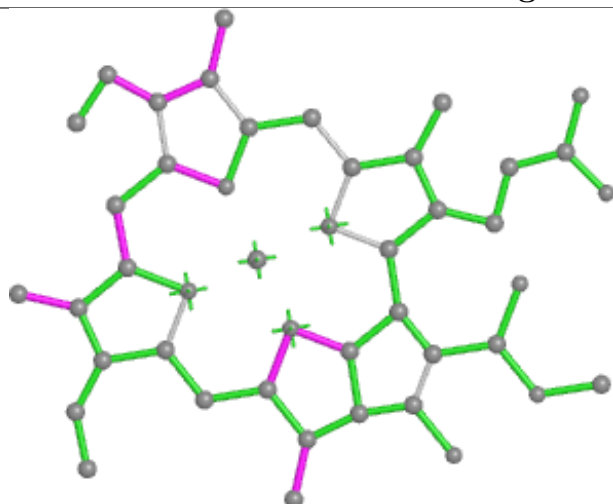
Torsions



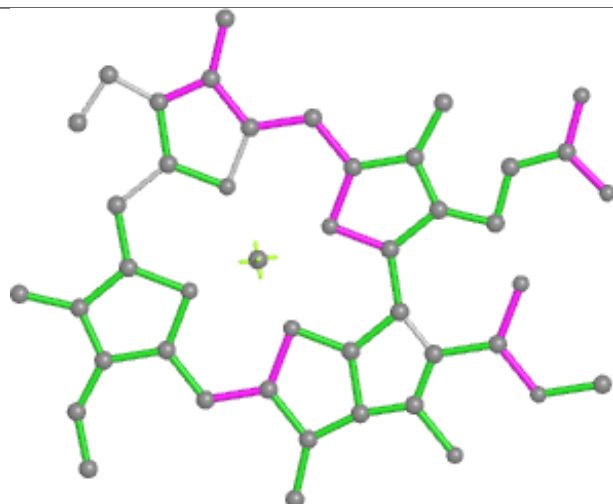
Rings



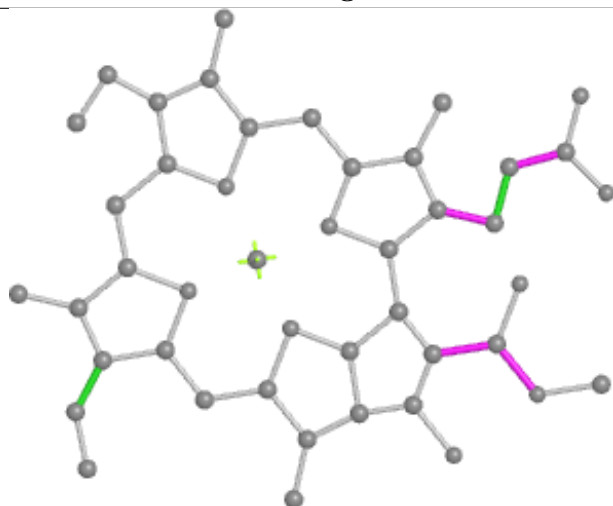
## Ligand CLA 4 611



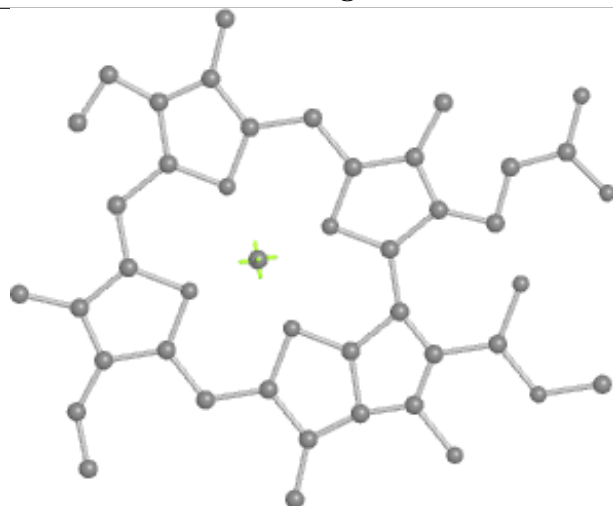
Bond lengths



Bond angles

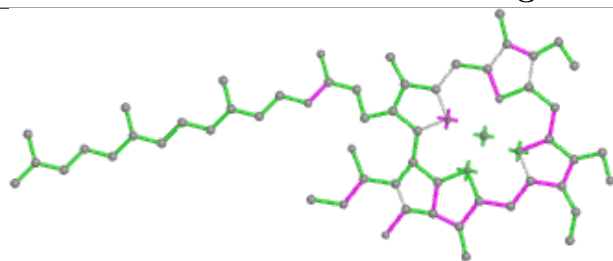


Torsions

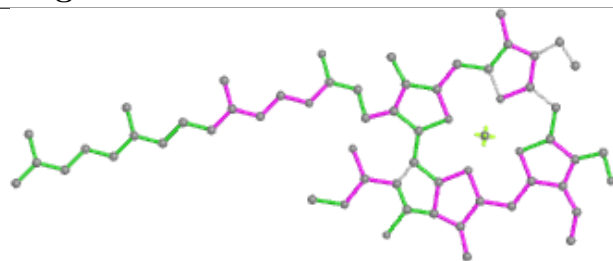


Rings

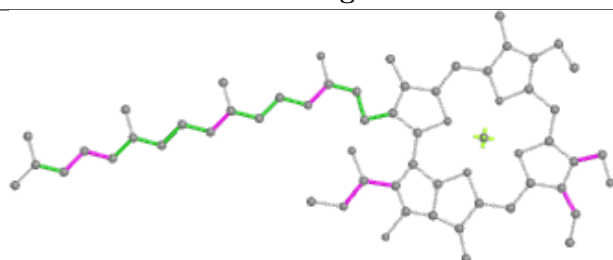
## Ligand CHL g 609



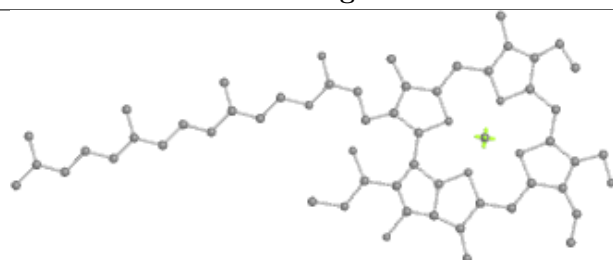
Bond lengths



Bond angles

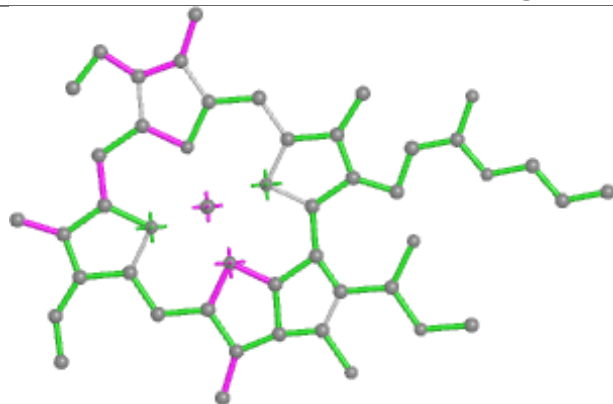


Torsions

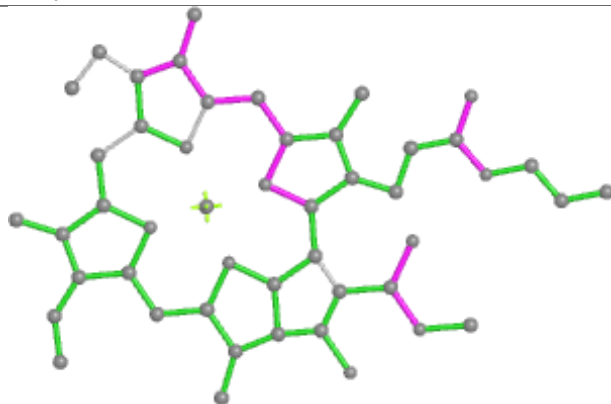


Rings

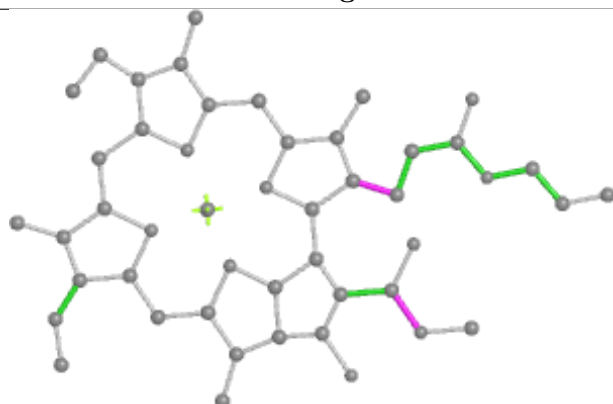
## Ligand CLA y 614



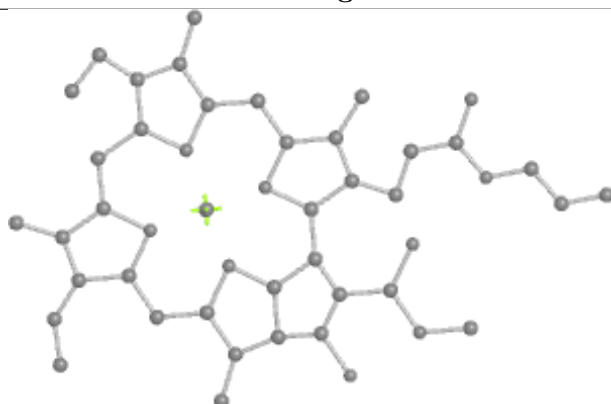
Bond lengths



Bond angles

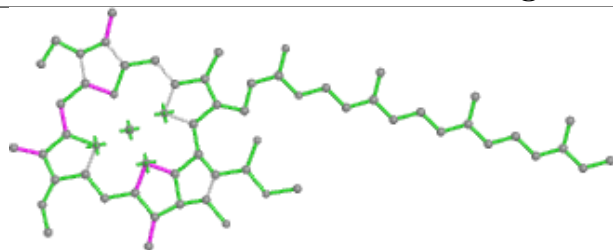


Torsions

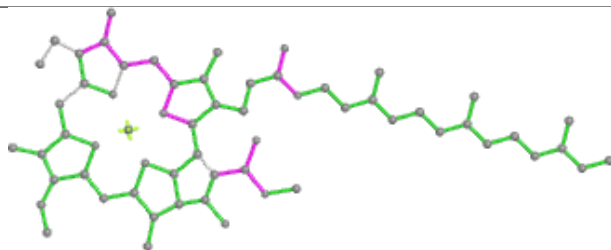


Rings

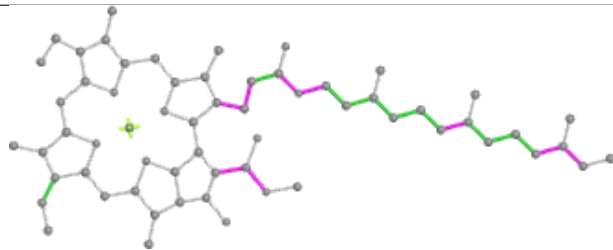
## Ligand CLA s 602



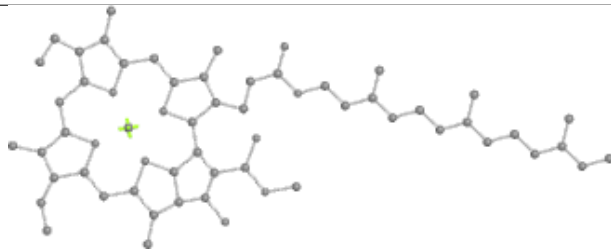
Bond lengths



Bond angles

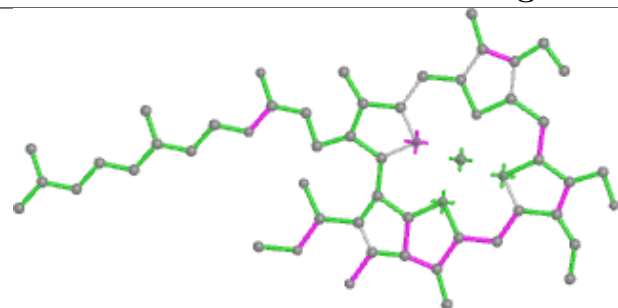


Torsions

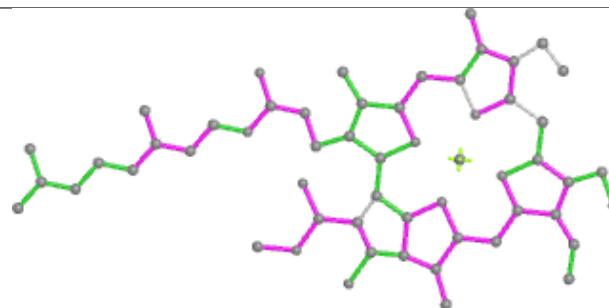


Rings

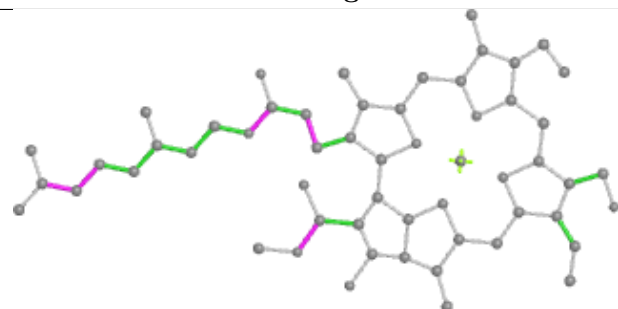
## Ligand CHL R 607



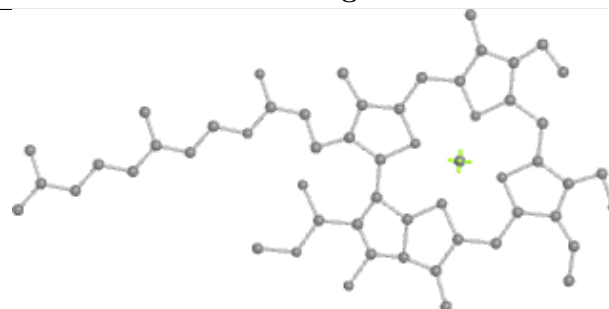
Bond lengths



Bond angles

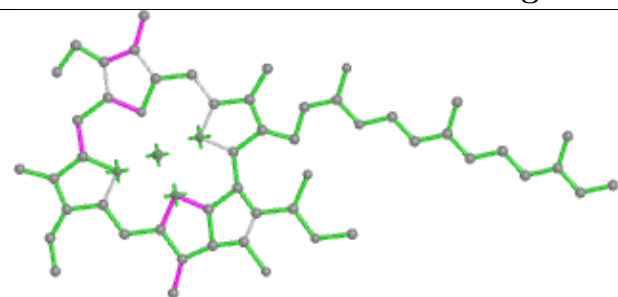


Torsions

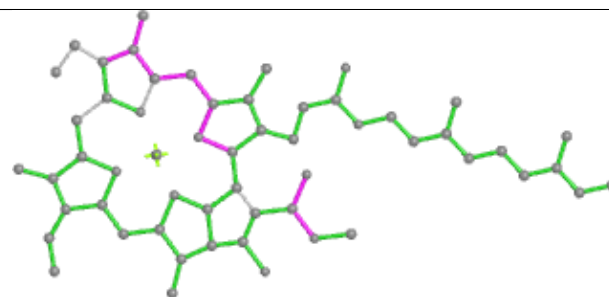


Rings

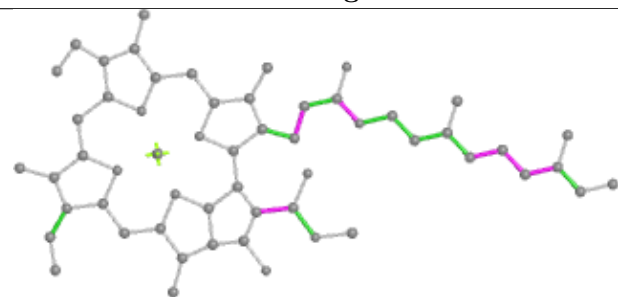
## Ligand CLA S 611



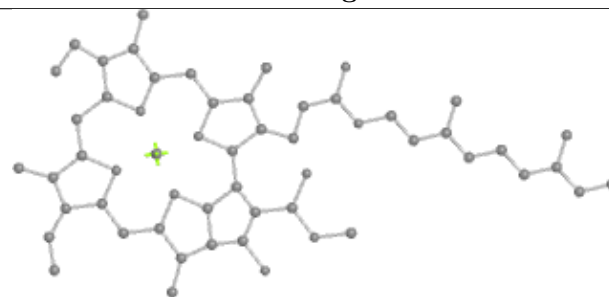
Bond lengths



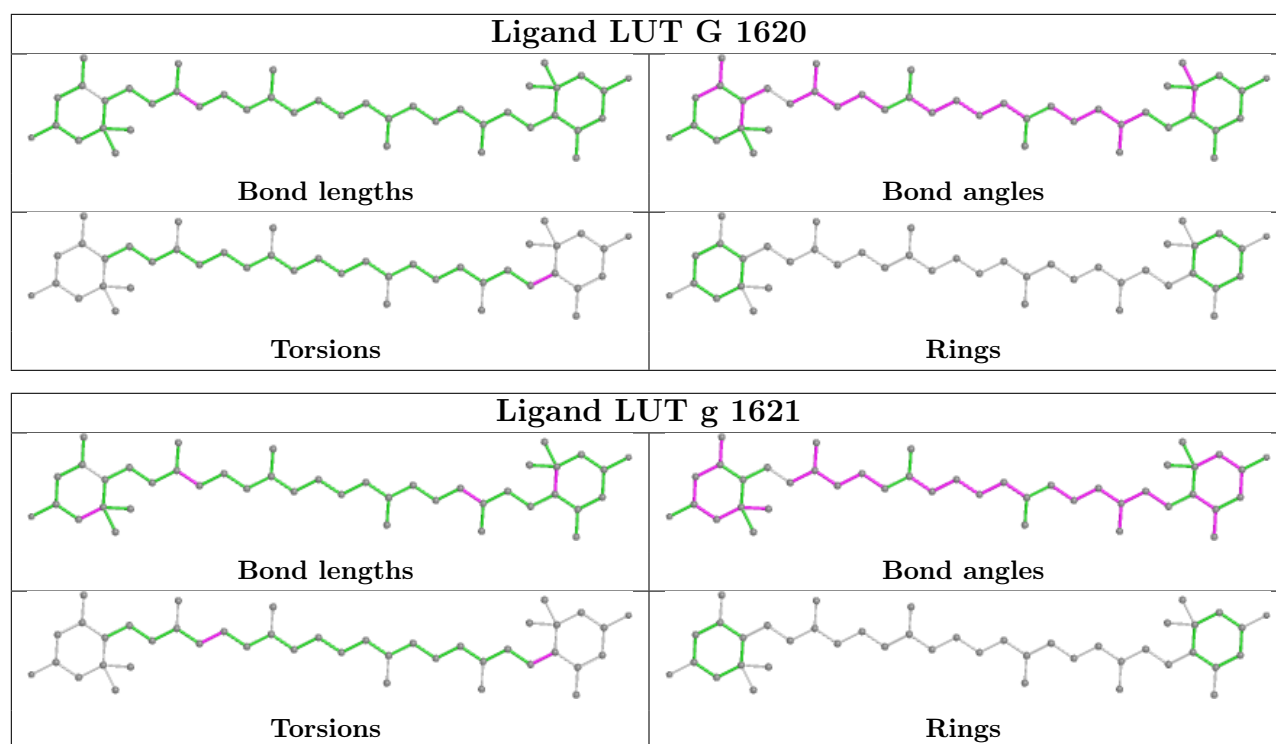
Bond angles



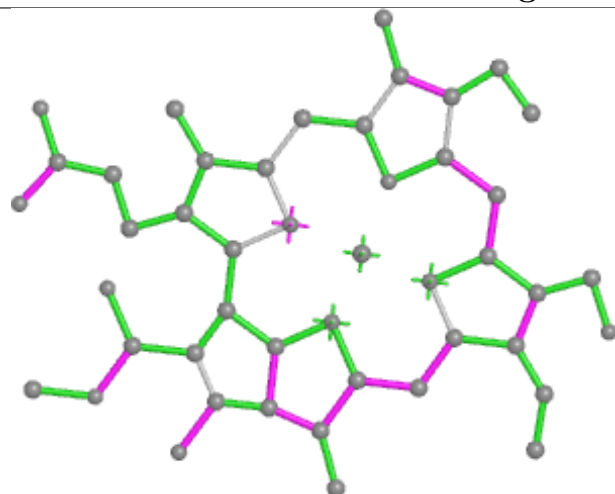
Torsions



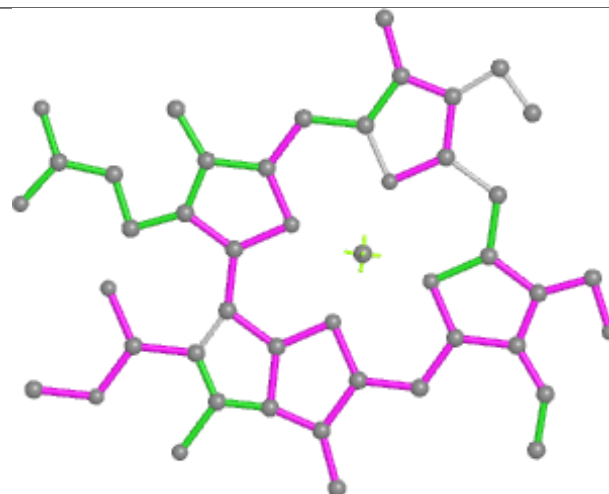
Rings



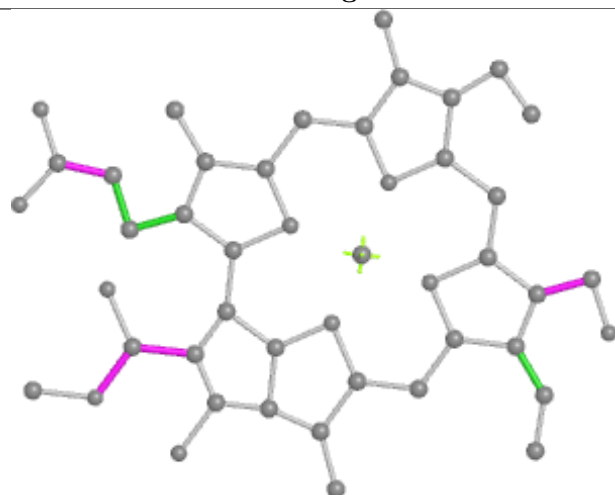
## Ligand CHL S 601



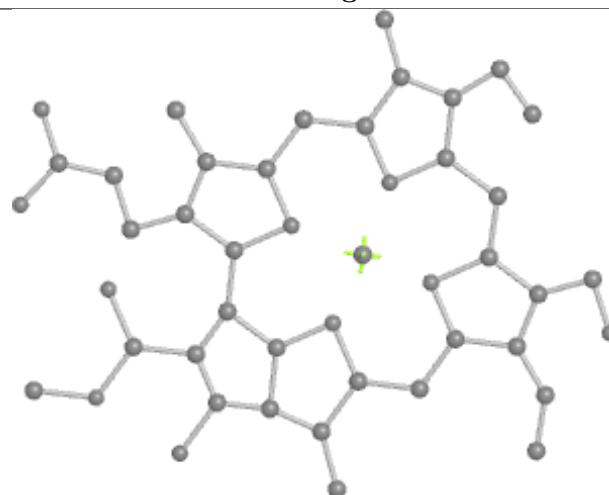
Bond lengths



Bond angles

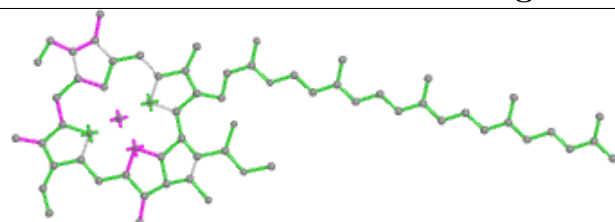


Torsions

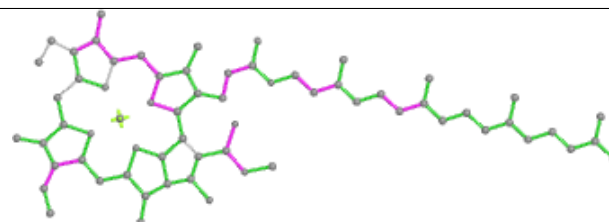


Rings

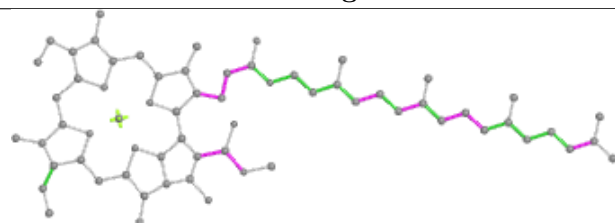
## Ligand CLA N 602



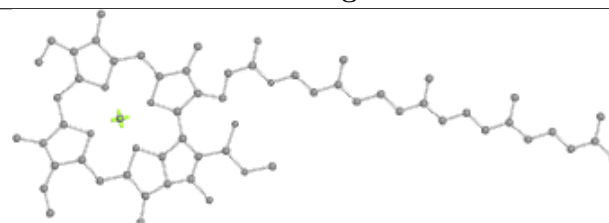
Bond lengths



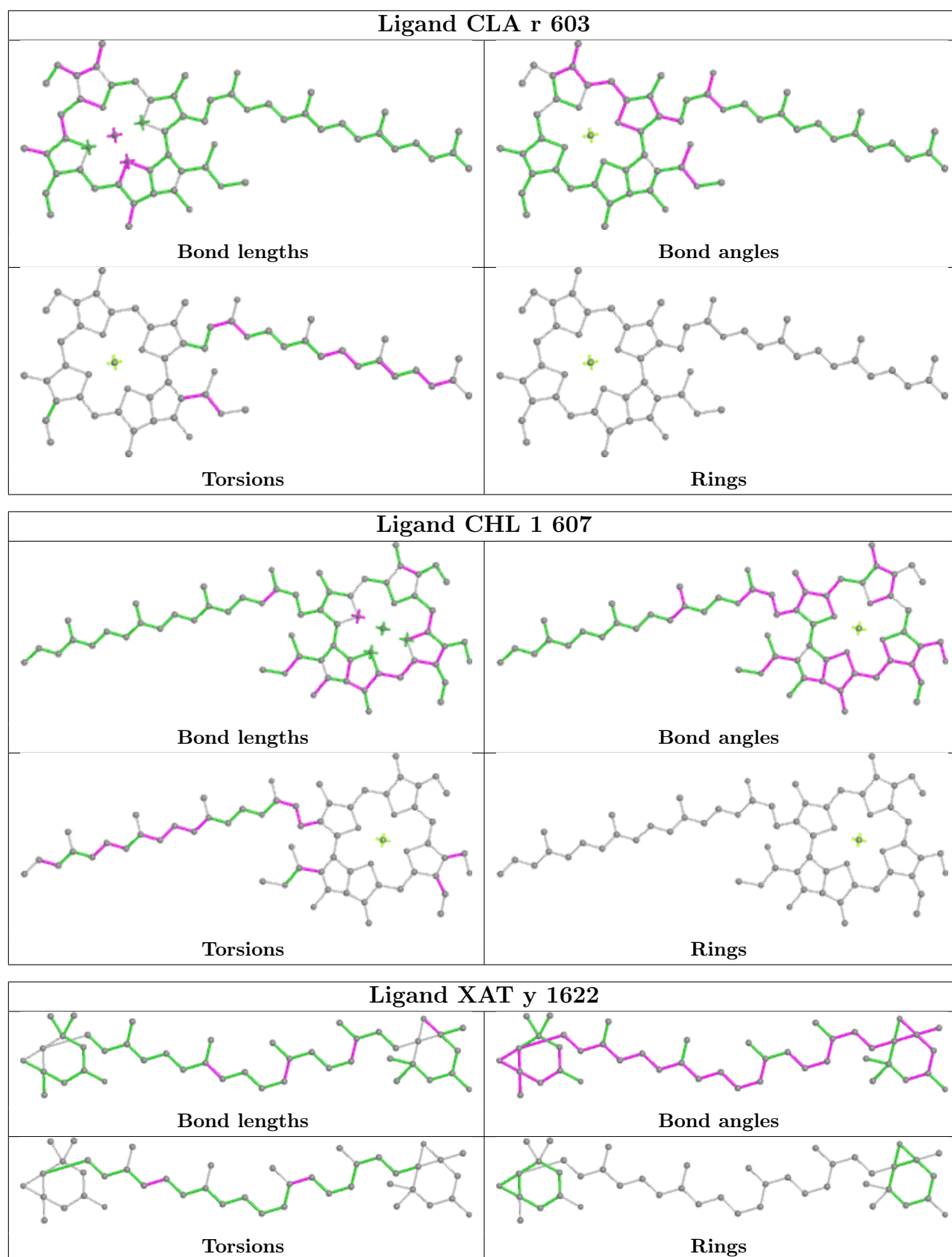
Bond angles

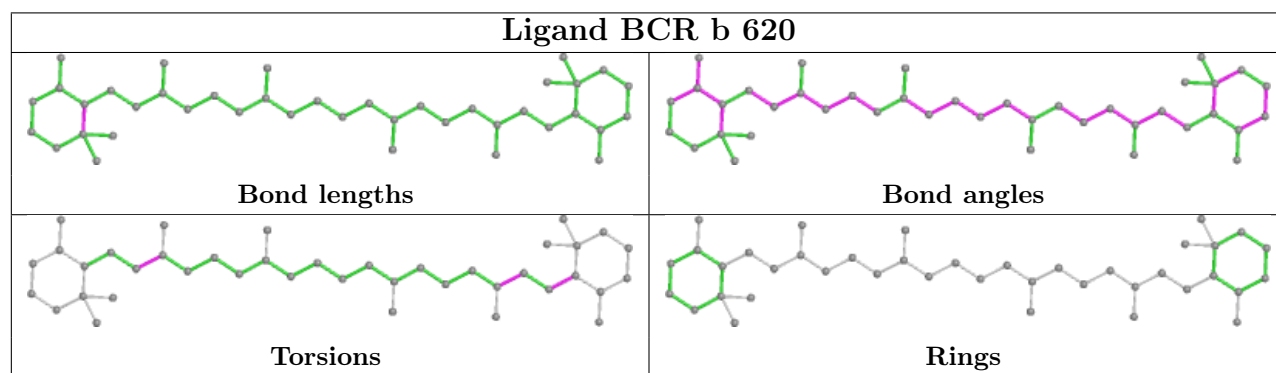
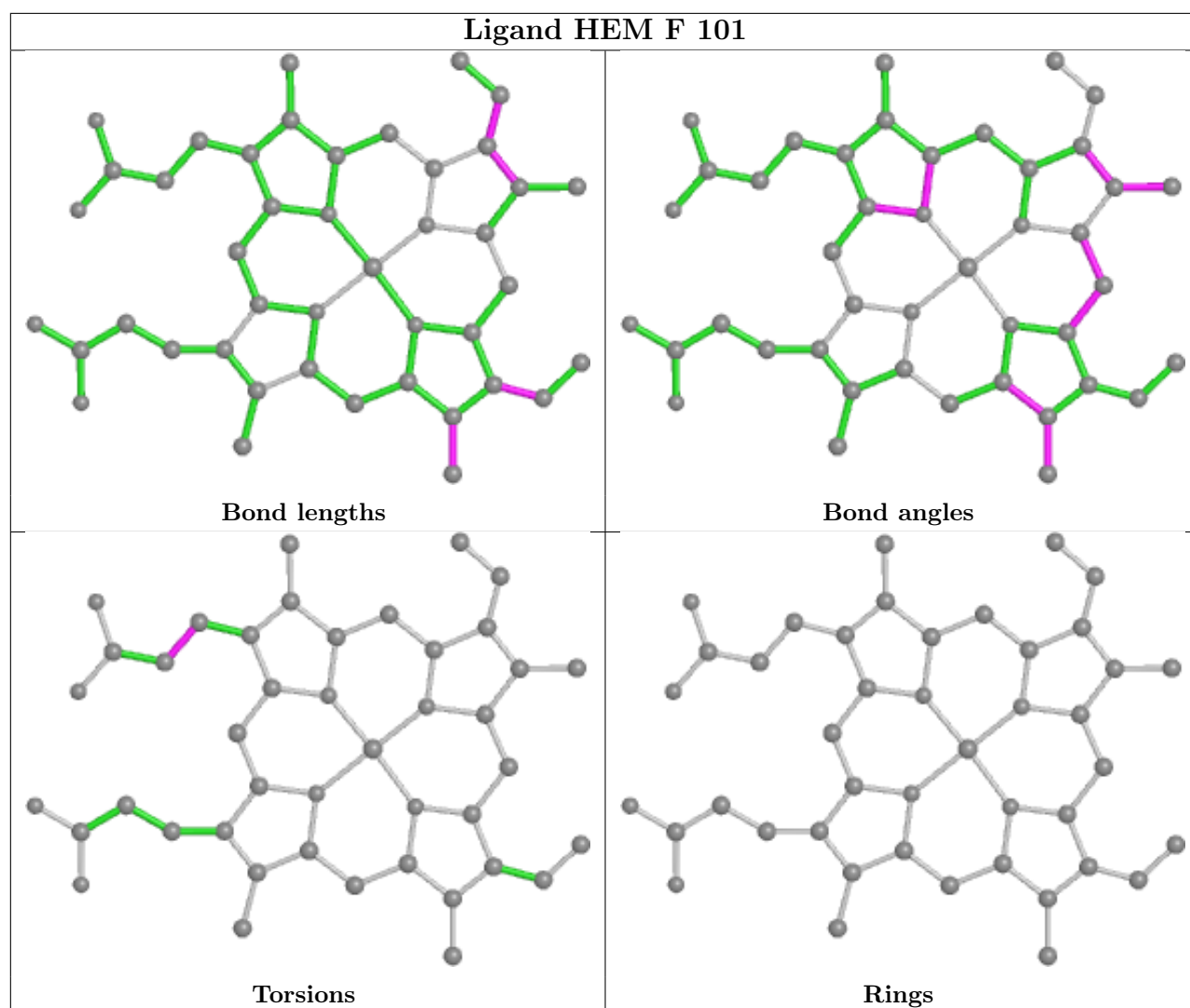


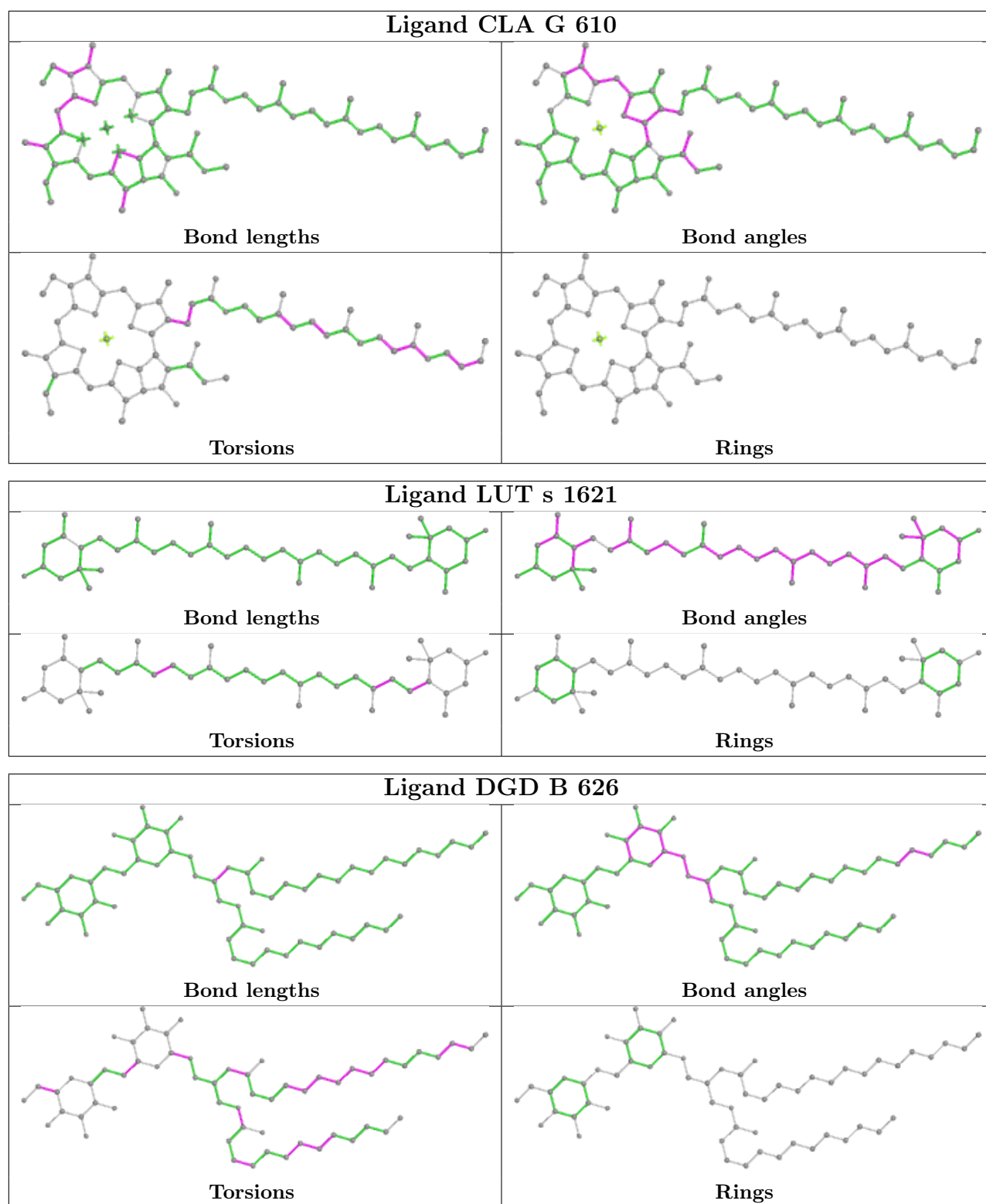
Torsions



Rings

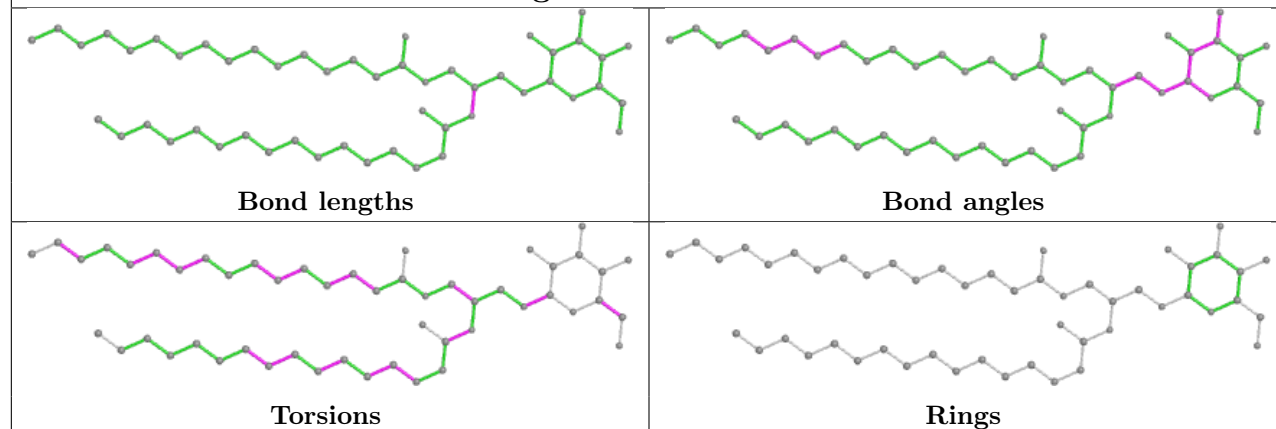




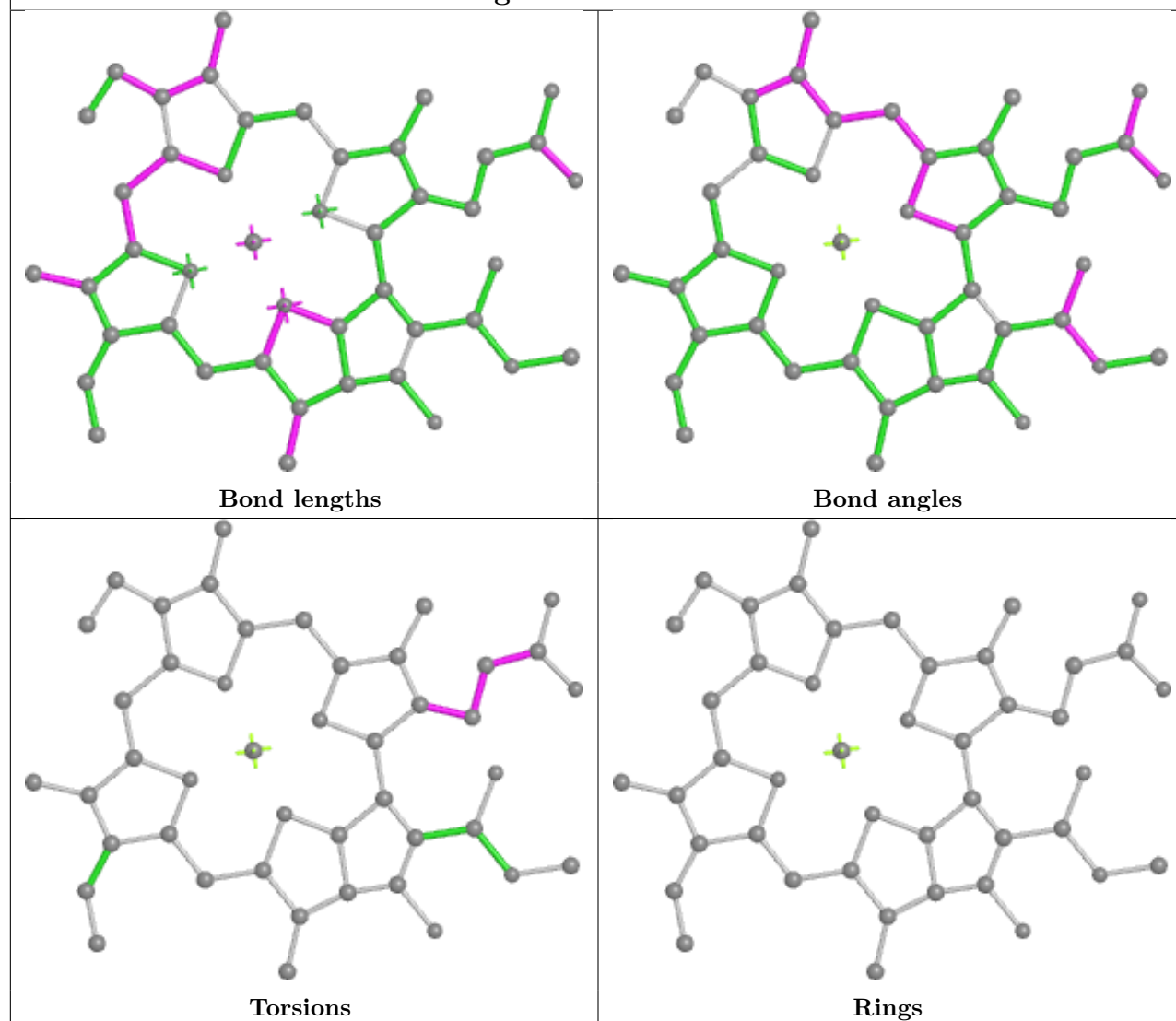


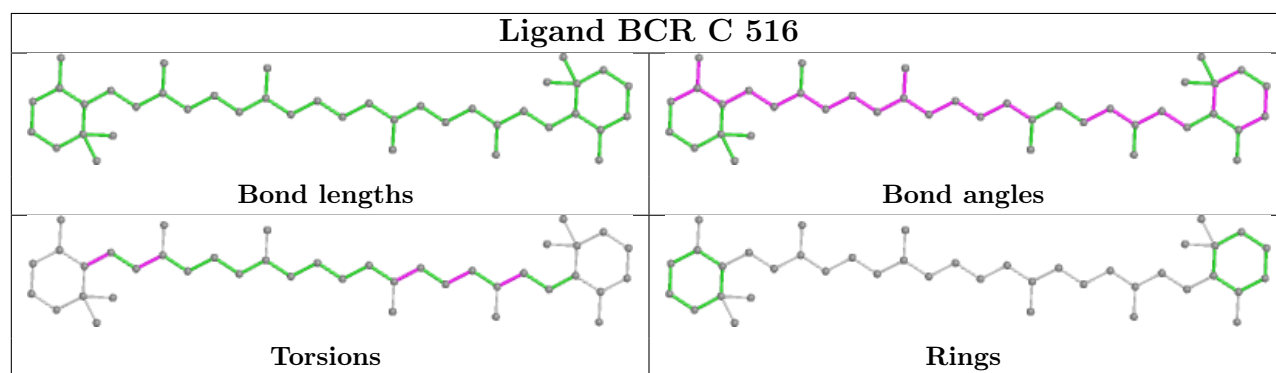
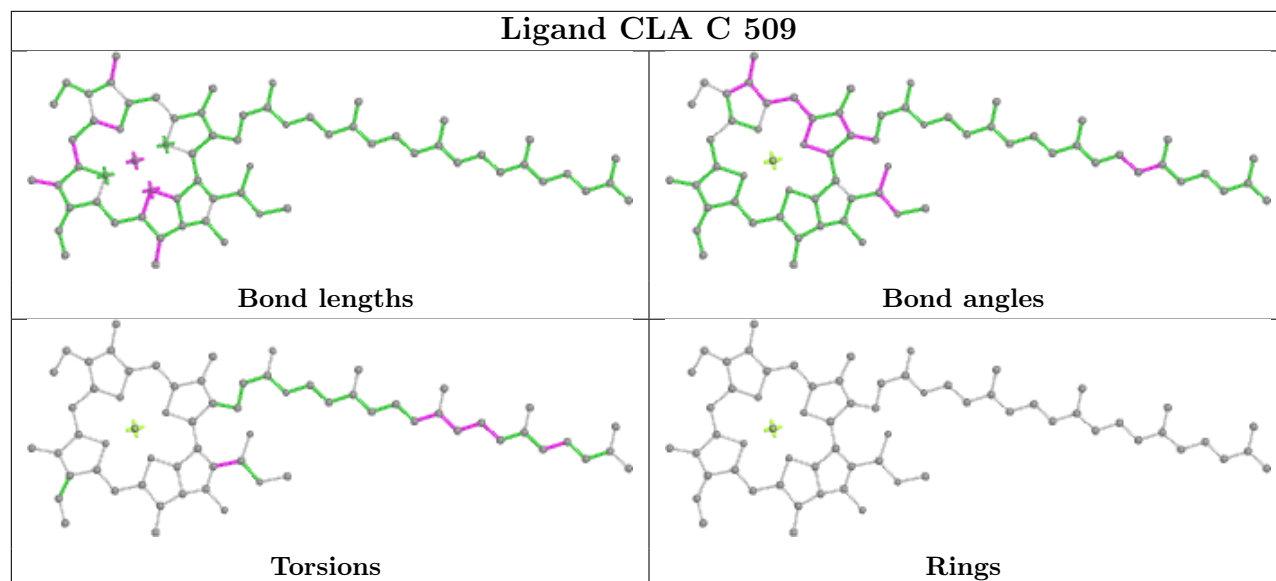
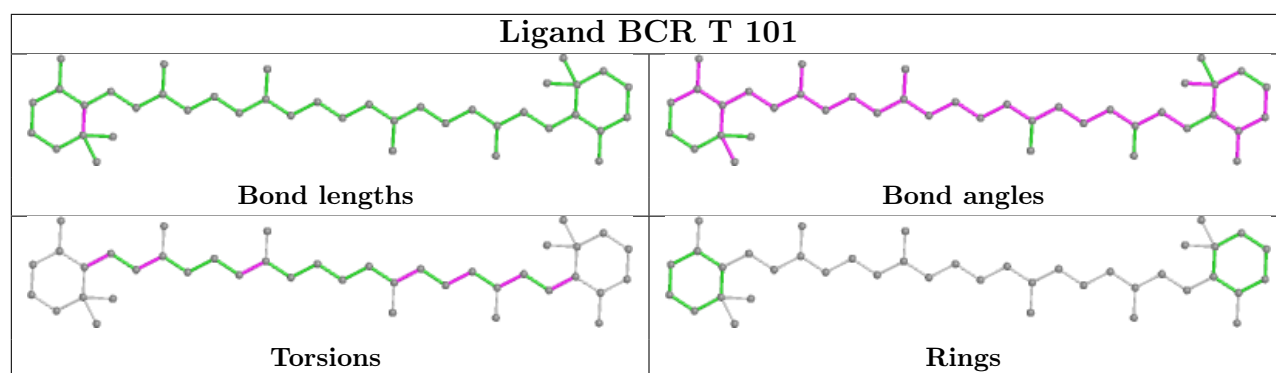


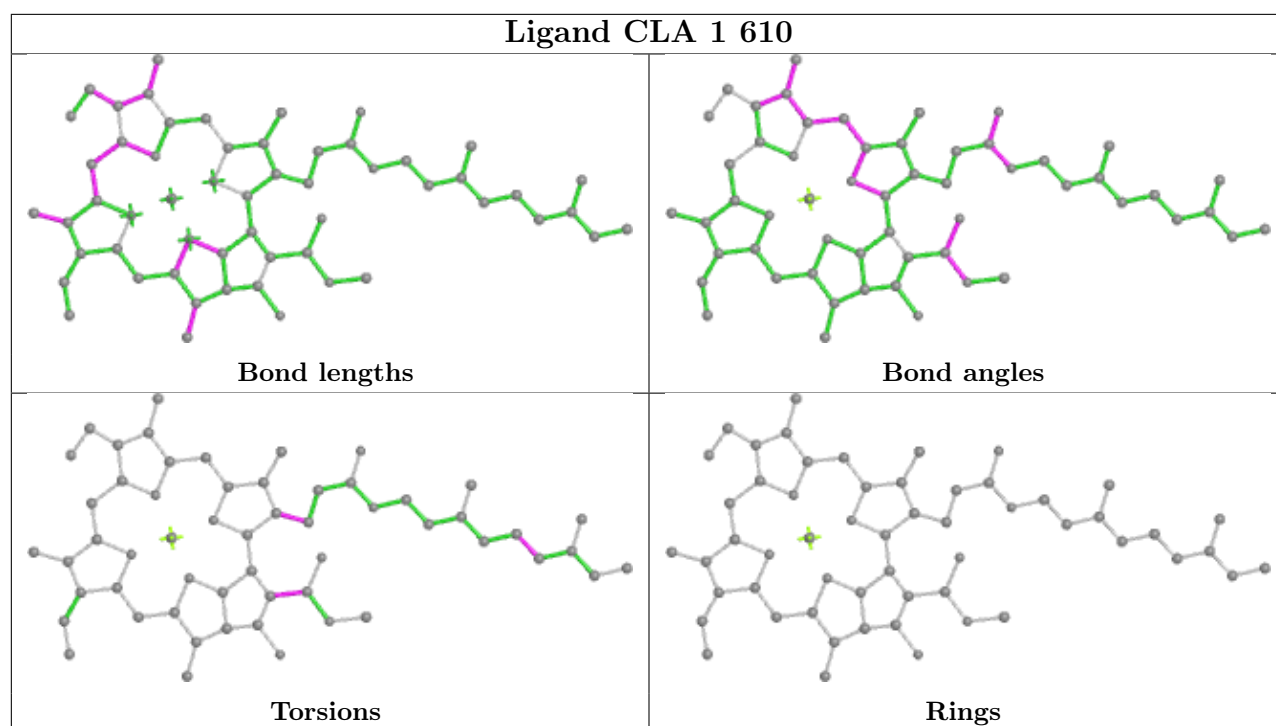
## Ligand LMG c 521



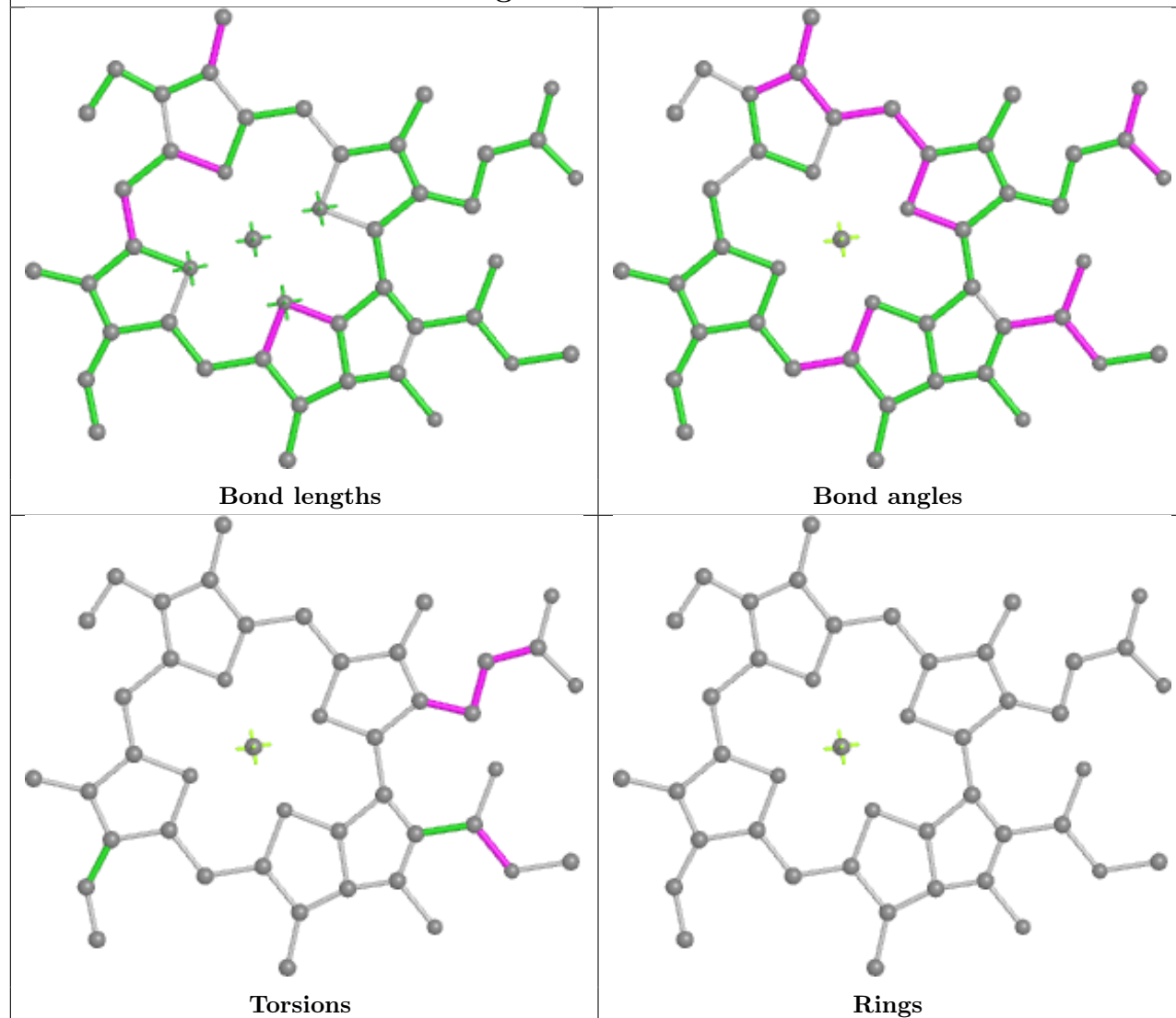
## Ligand CLA 5 611



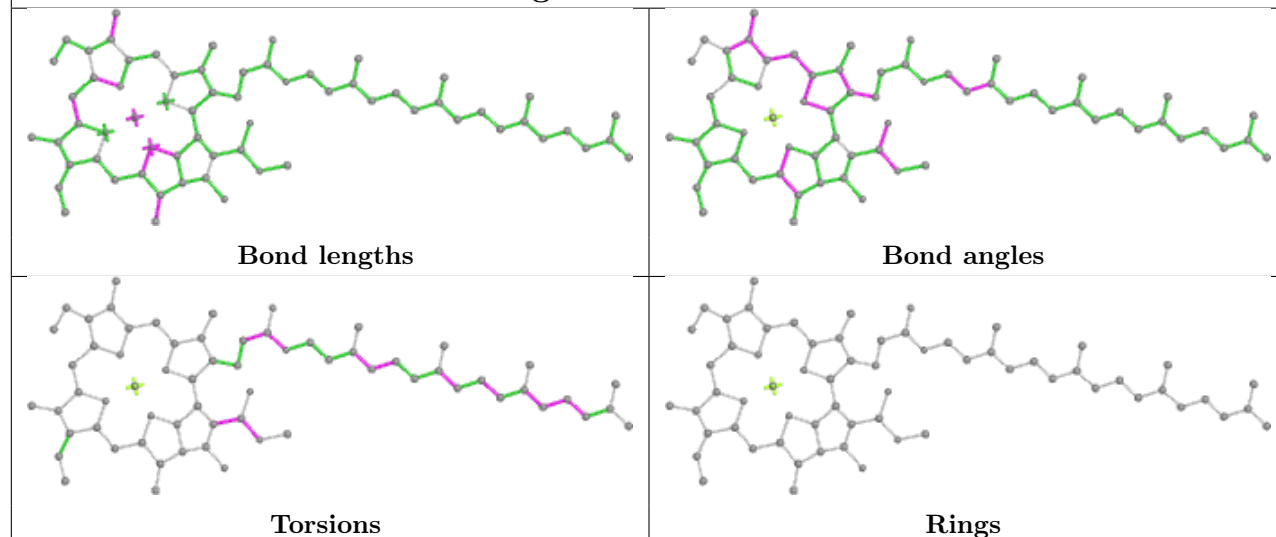


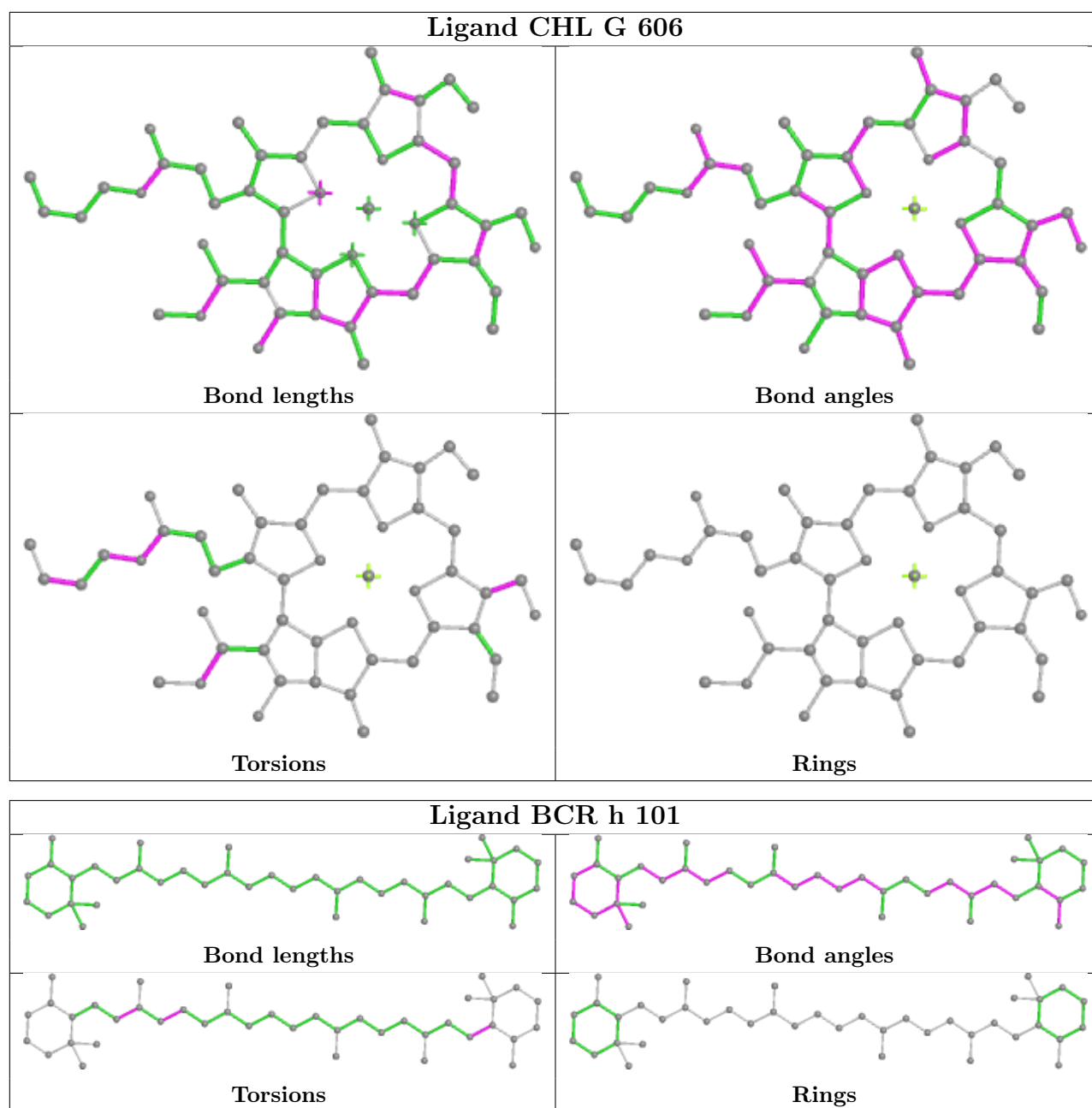


## Ligand CLA s 609

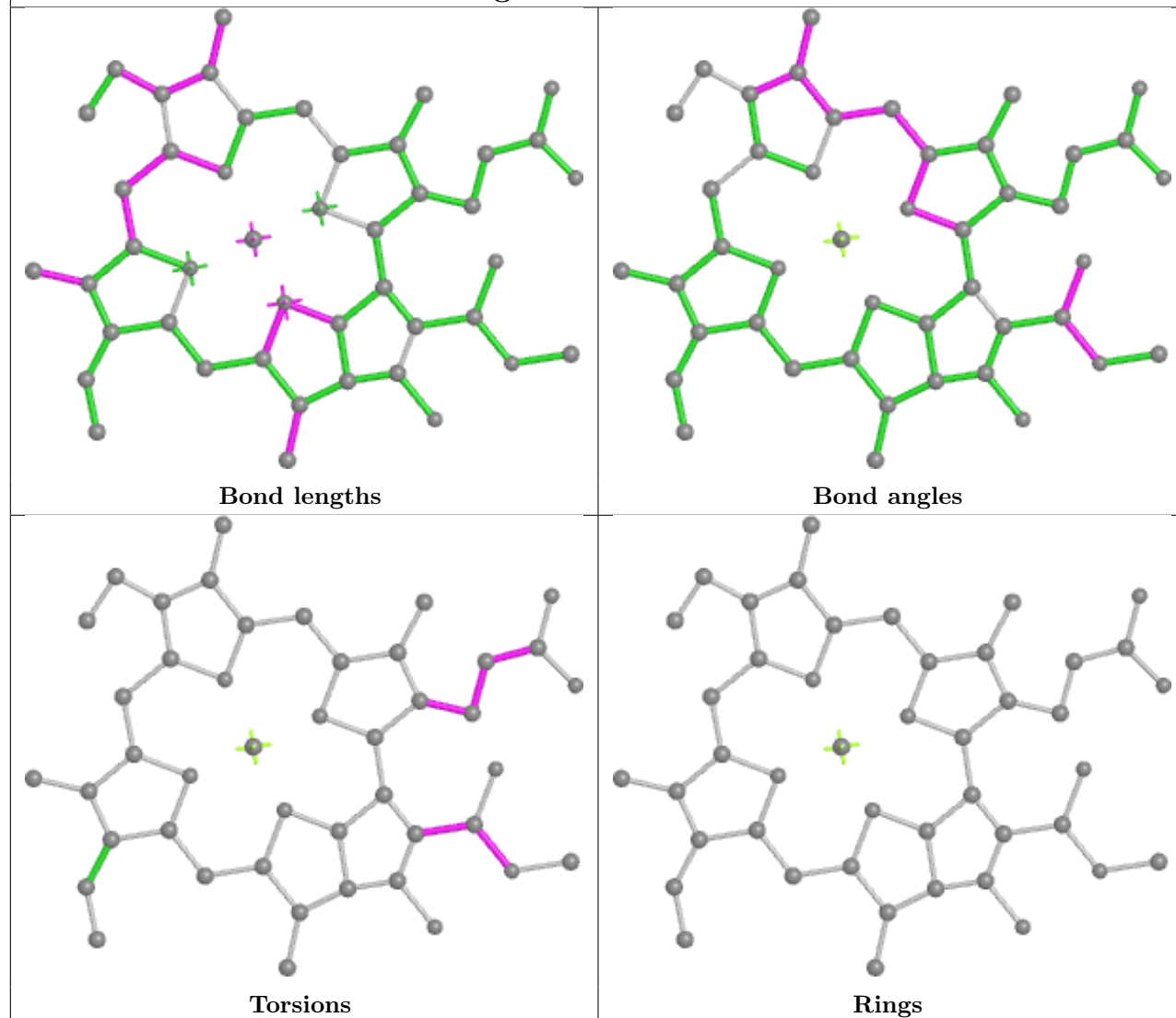


## Ligand CLA C 510

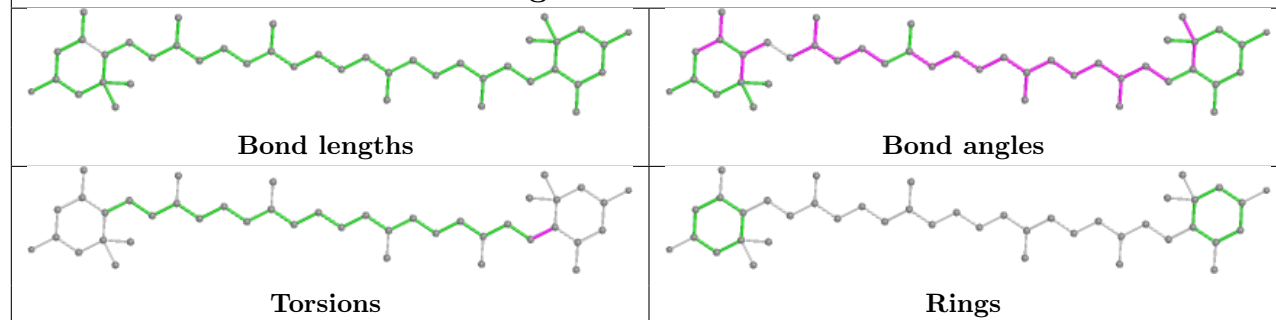


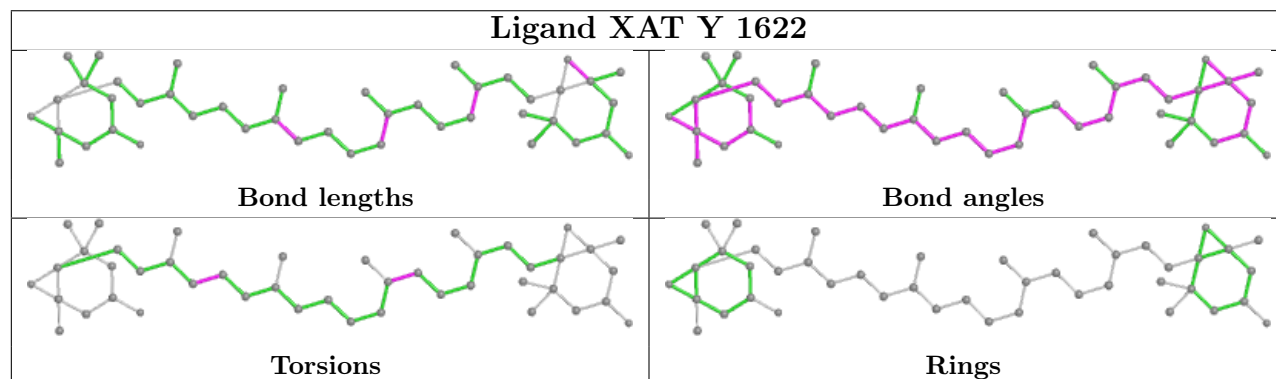
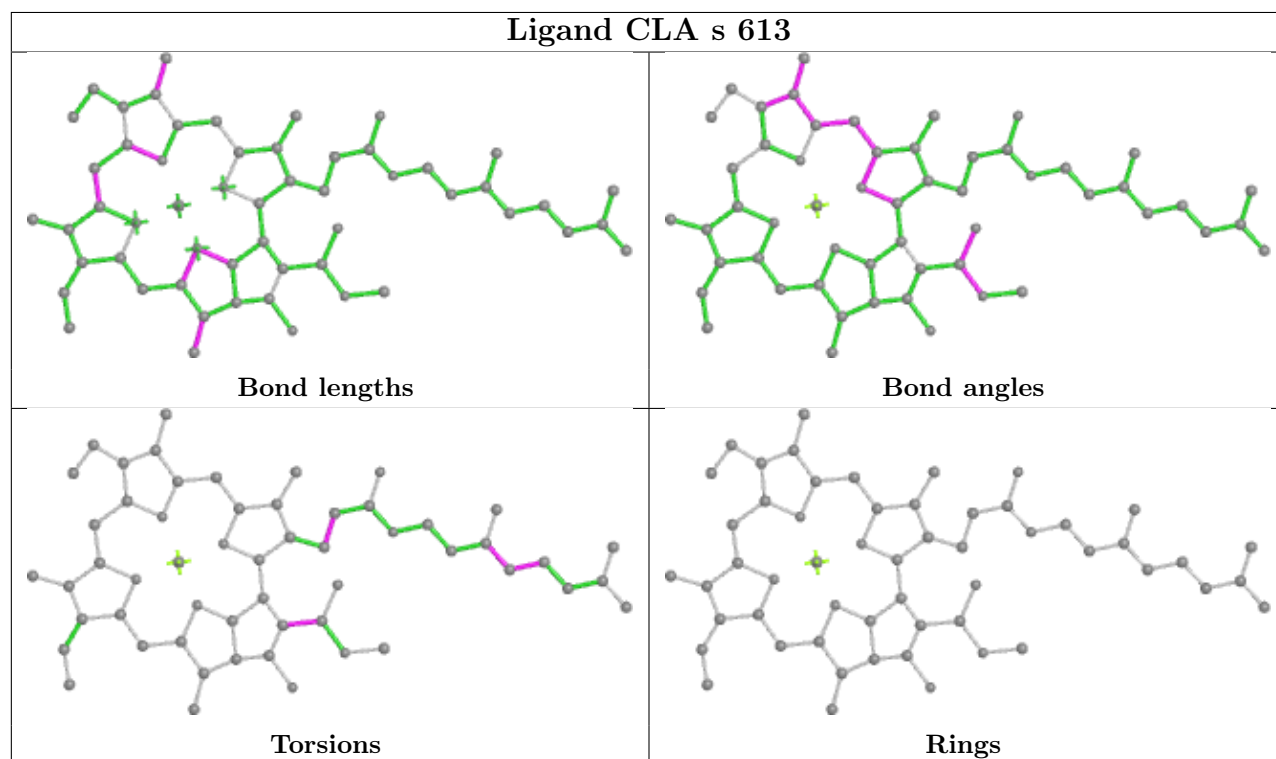
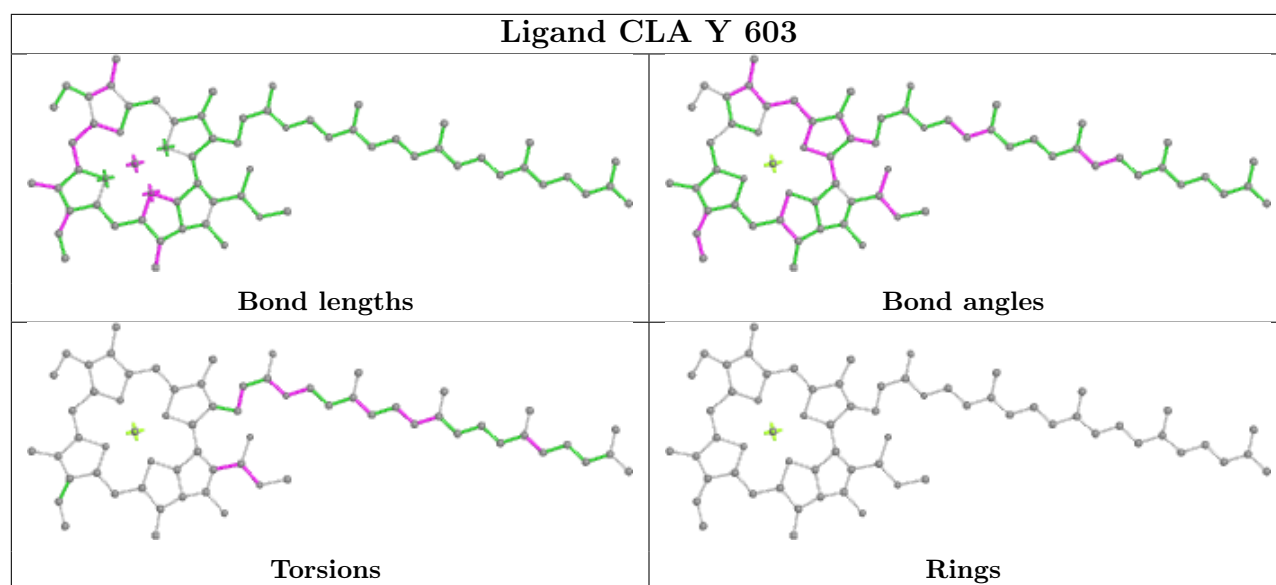


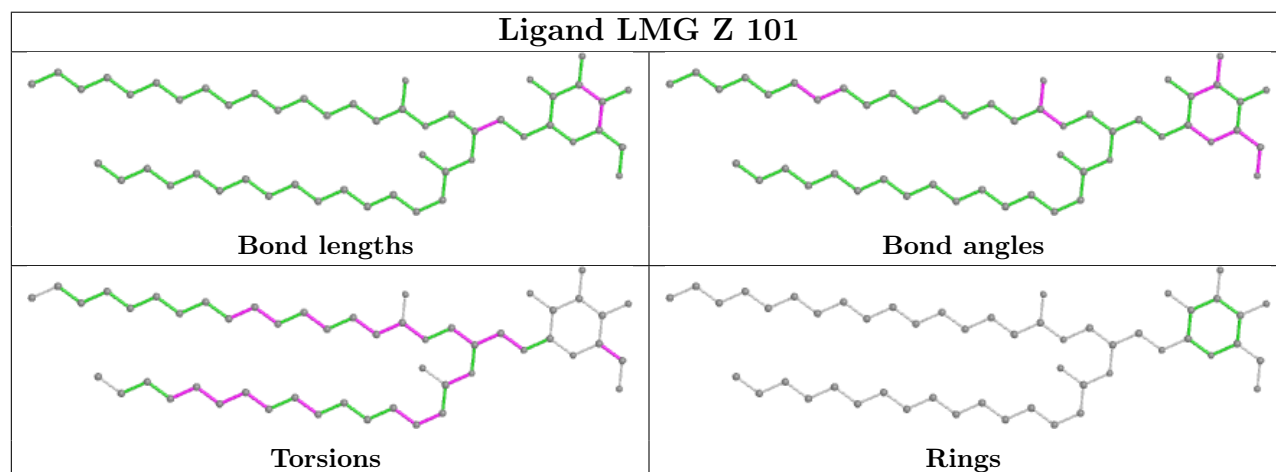
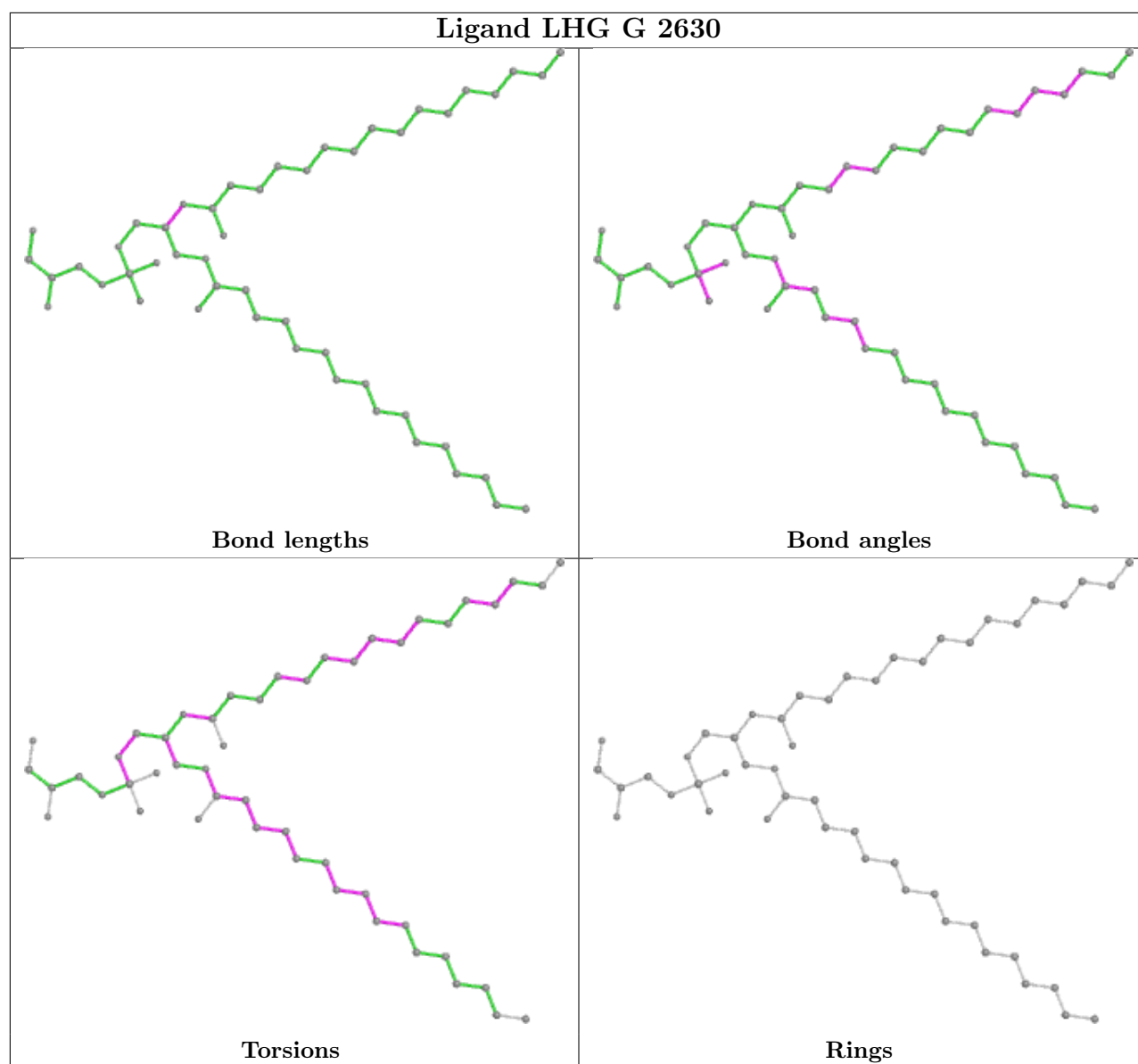
## Ligand CLA 7 604



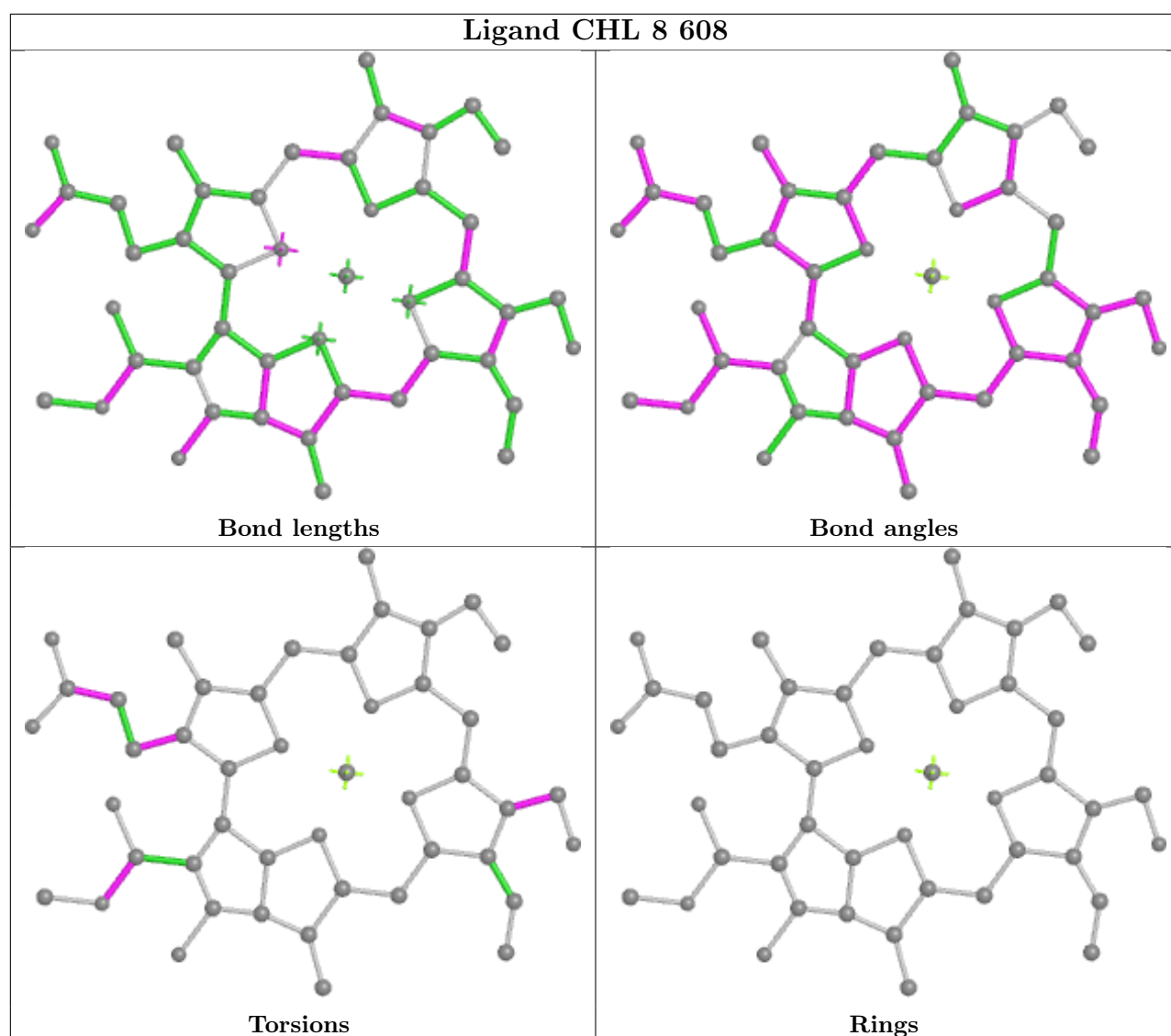
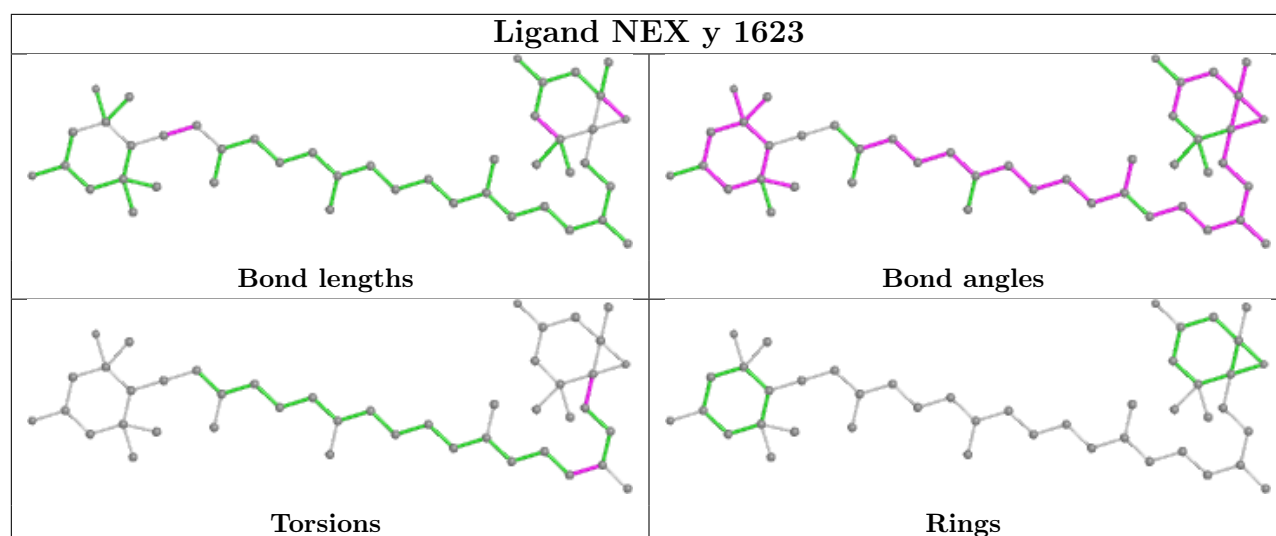
## Ligand LUT s 1620



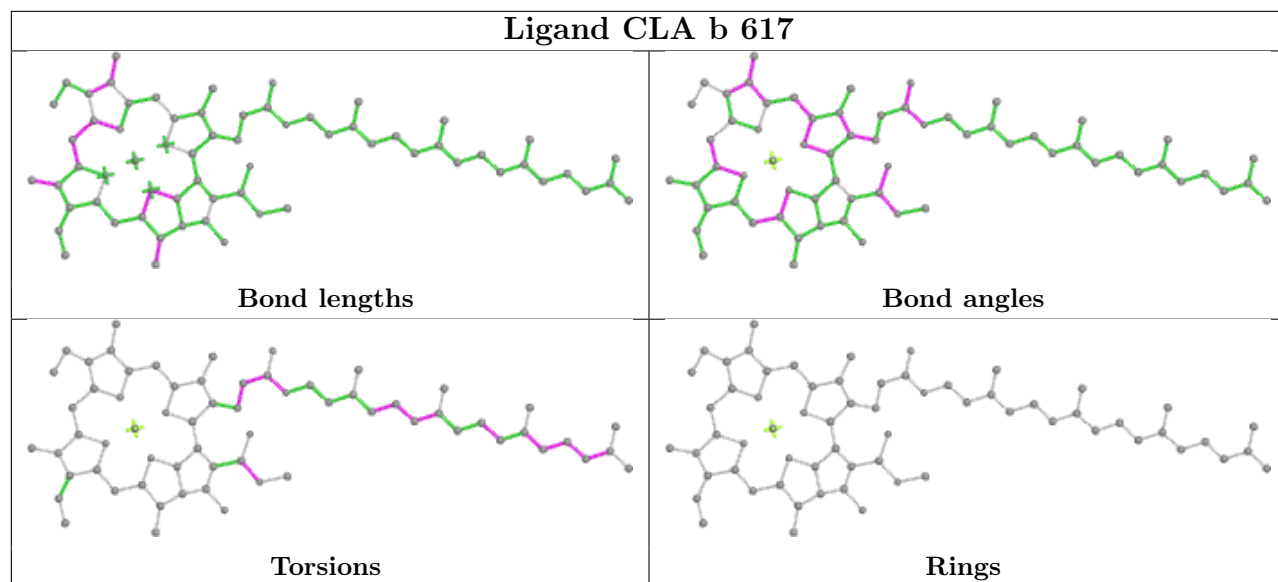




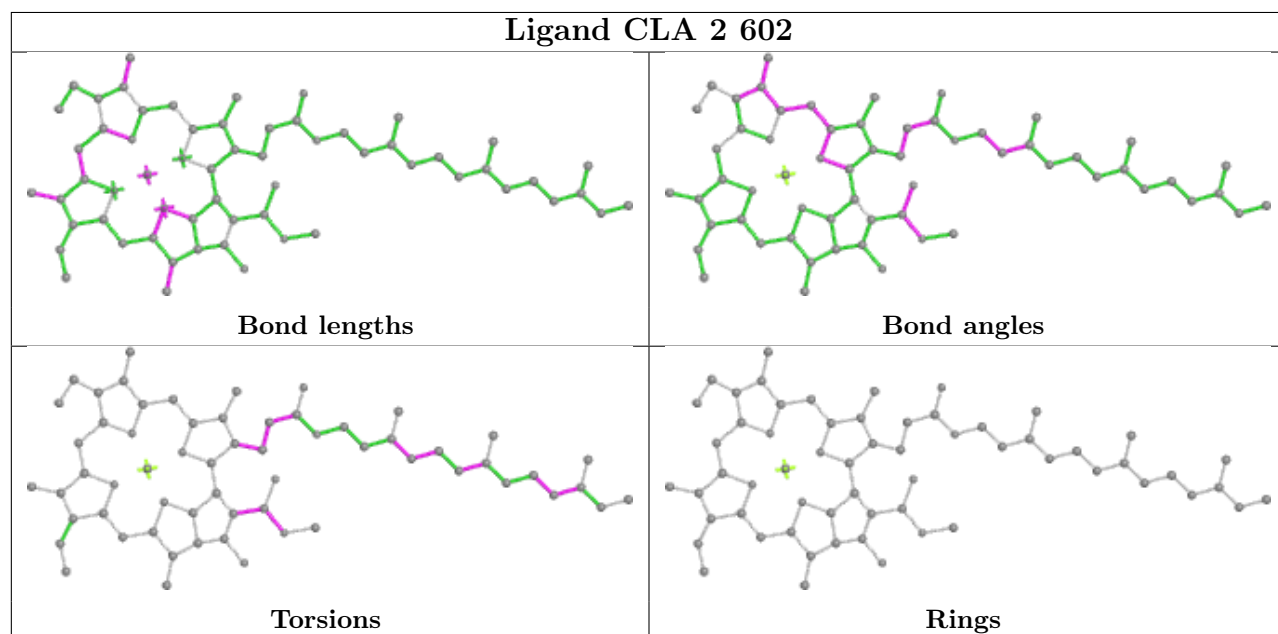


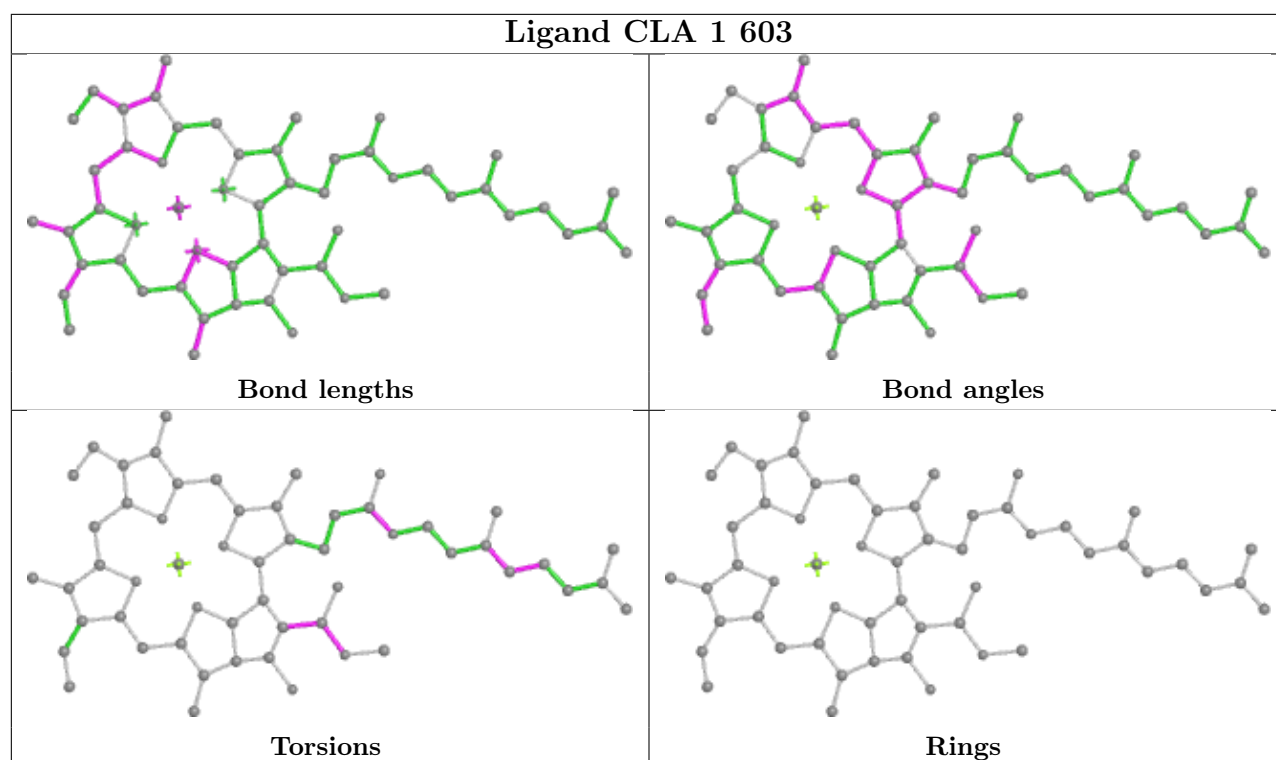


## Ligand CLA b 617

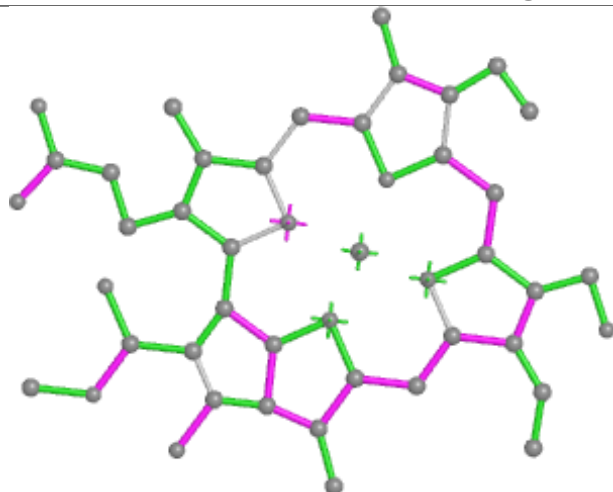


## Ligand CLA 2 602

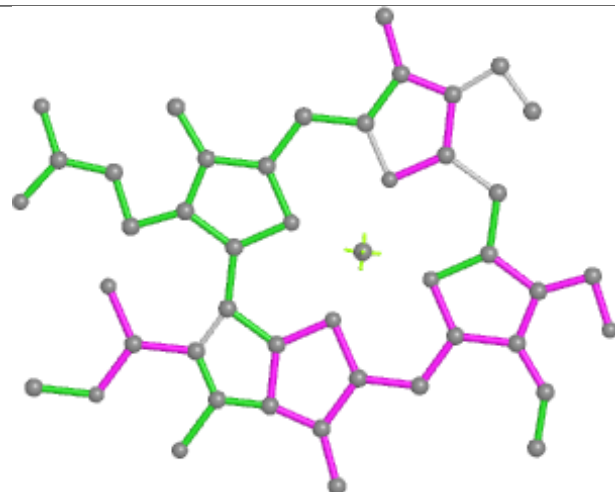




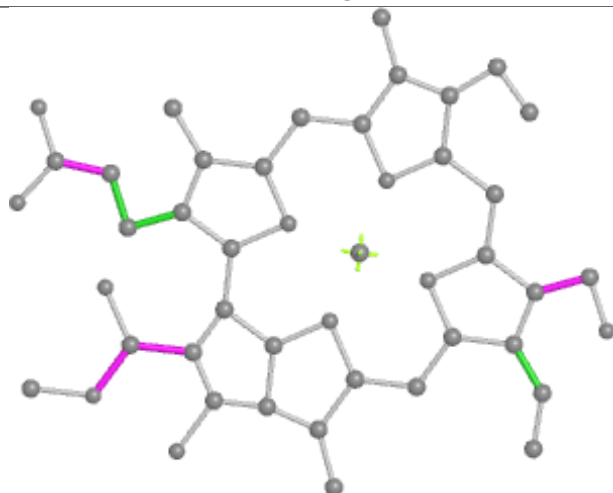
## Ligand CHL s 606



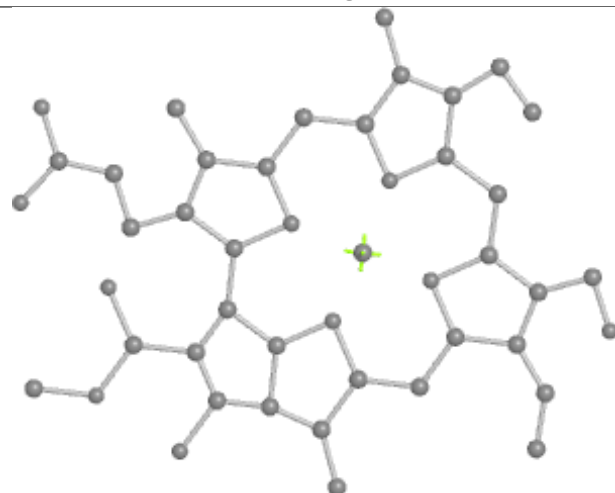
Bond lengths



Bond angles

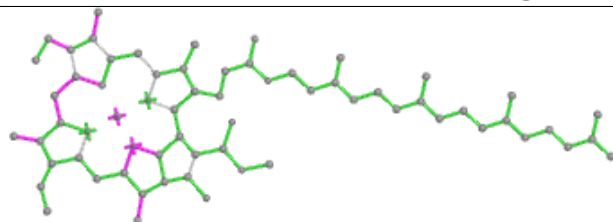


Torsions

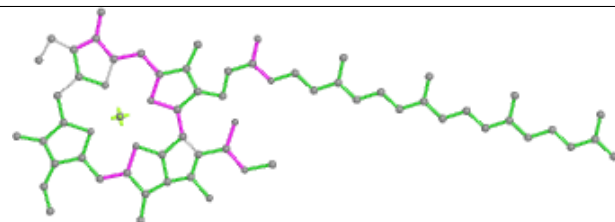


Rings

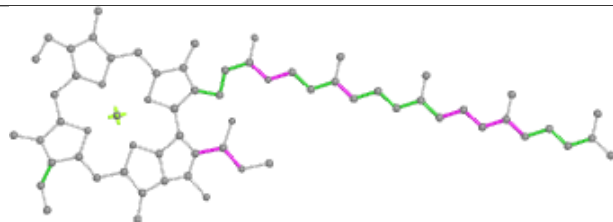
## Ligand CLA d 403



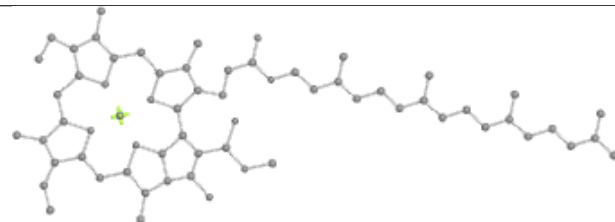
Bond lengths



Bond angles

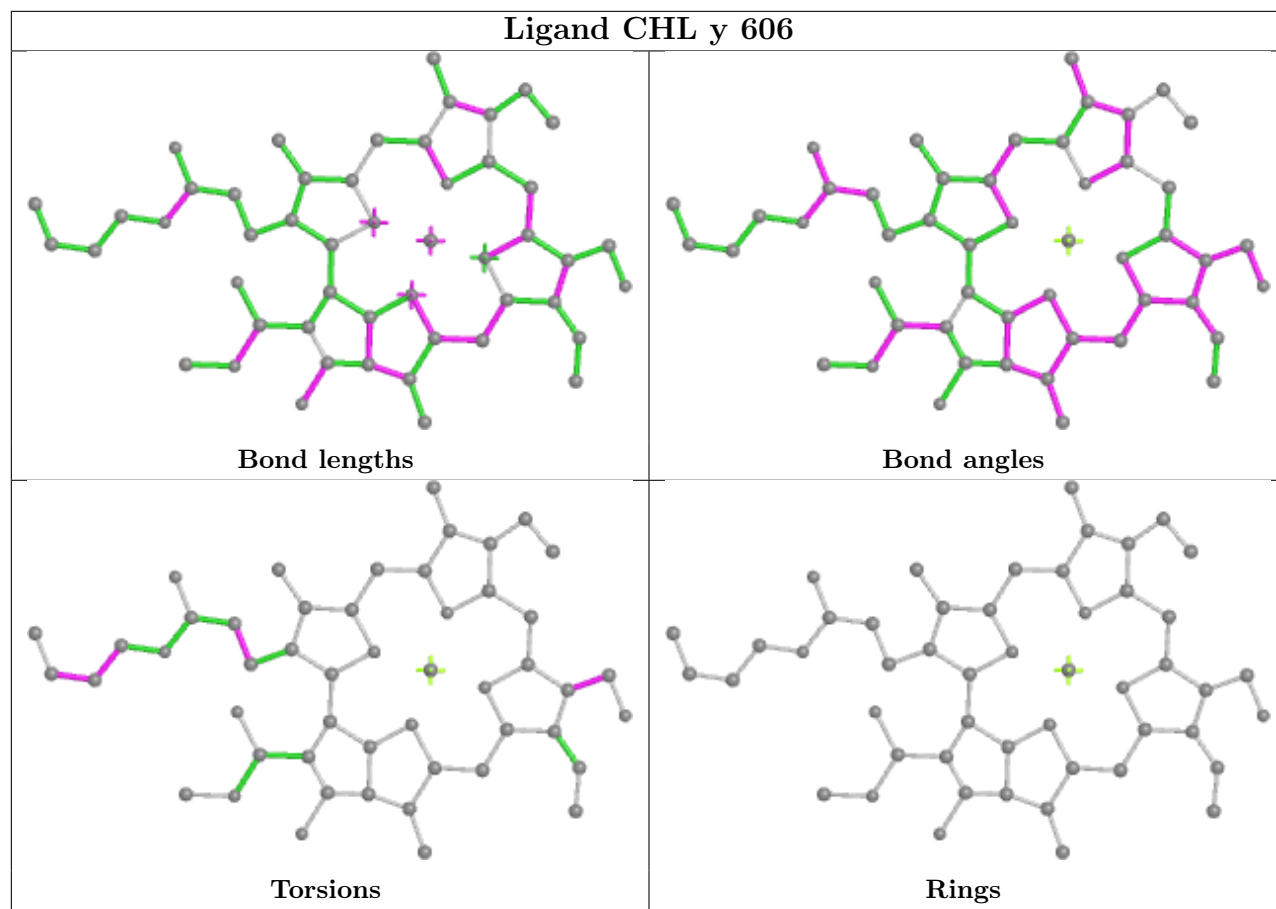


Torsions

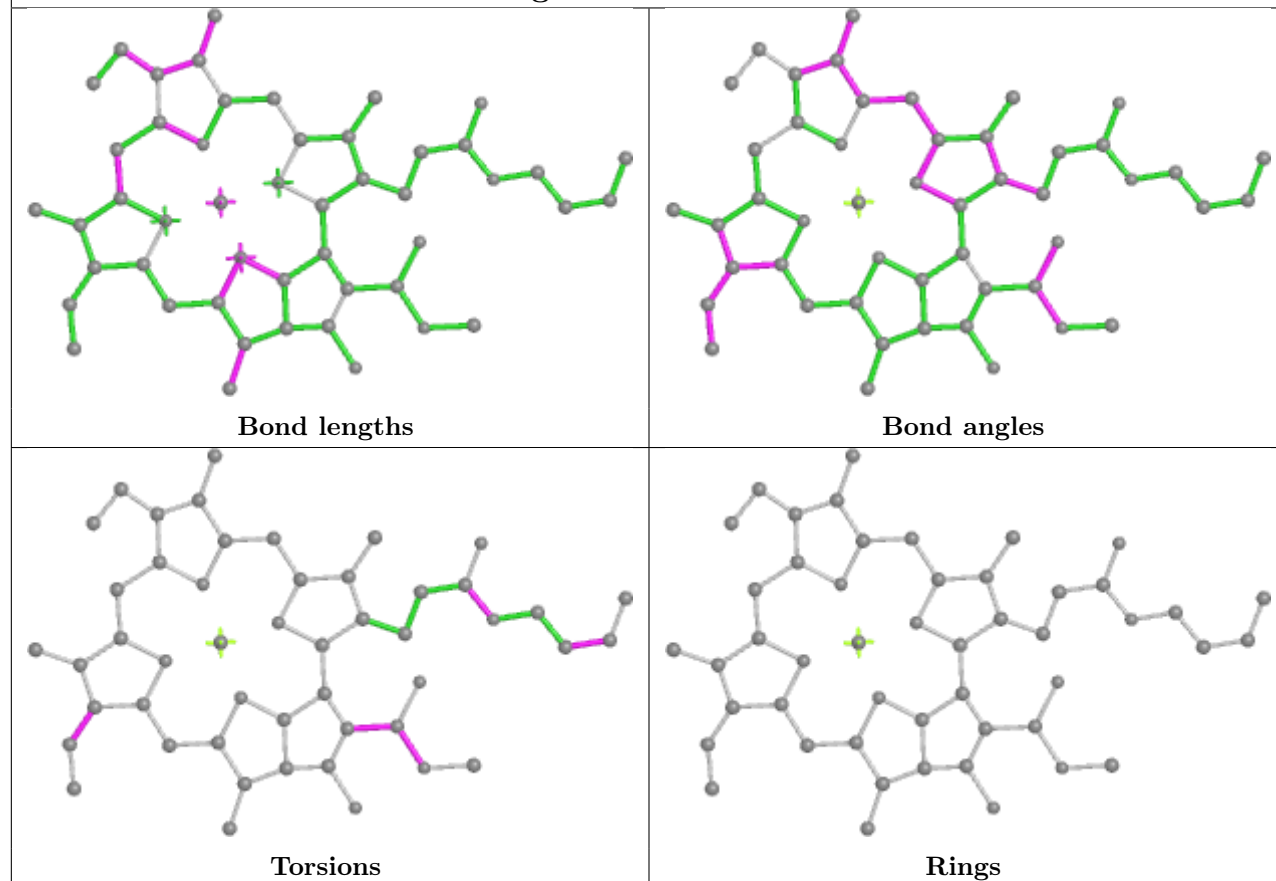


Rings

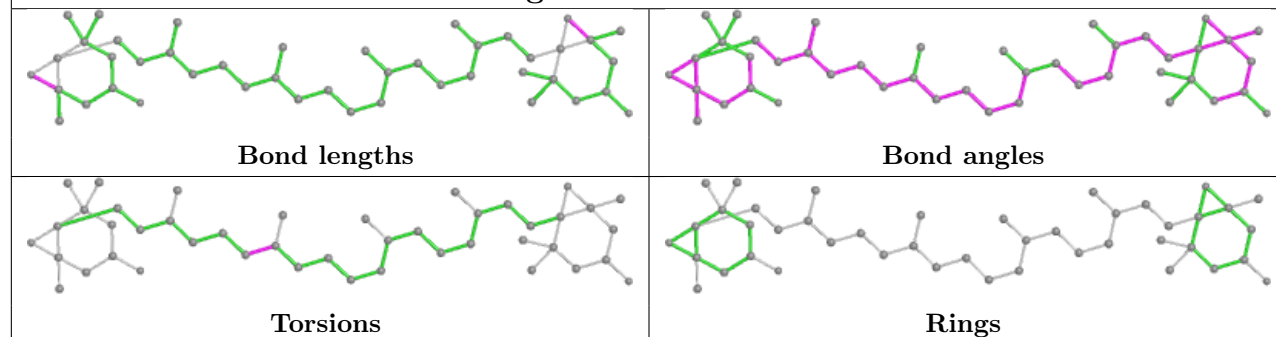
## Ligand CHL y 606



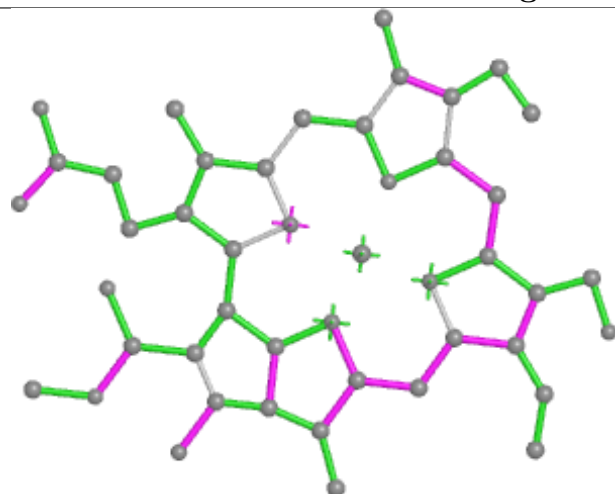
## Ligand CLA R 601



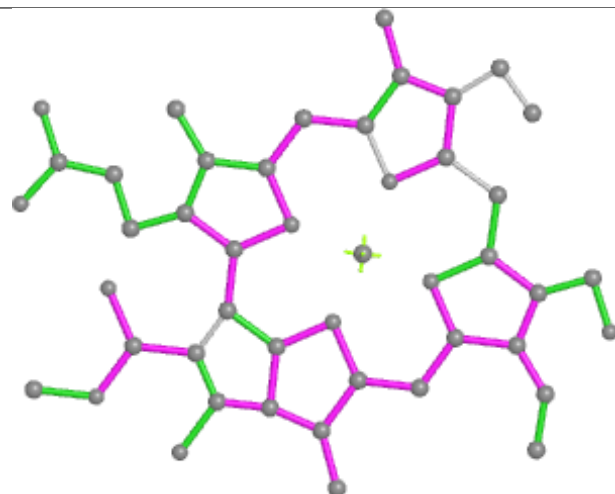
## Ligand XAT 1 1622



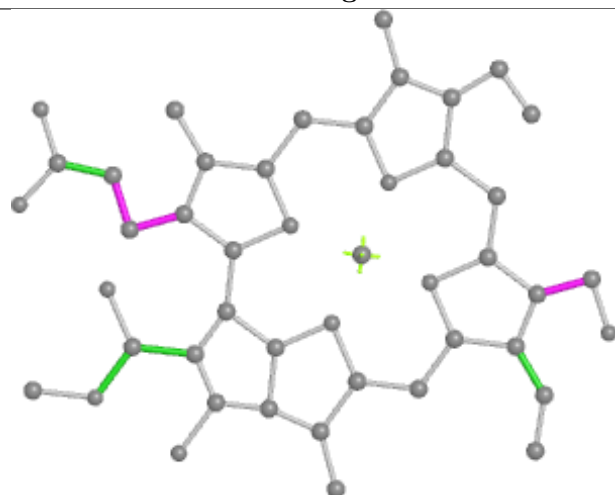
## Ligand CHL 3 606



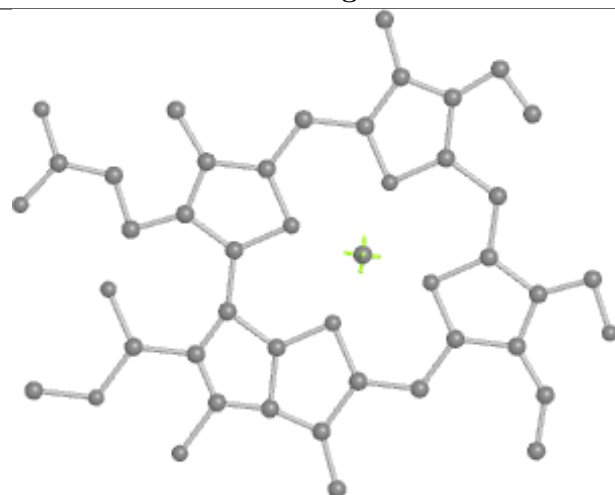
Bond lengths



Bond angles

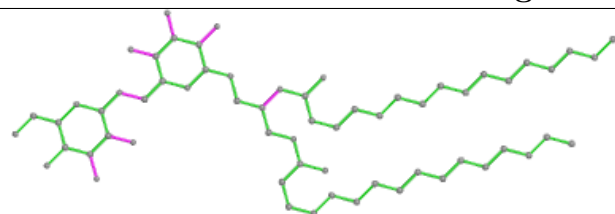


Torsions

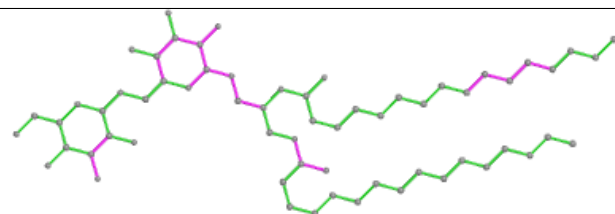


Rings

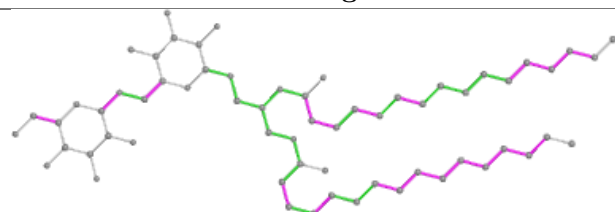
## Ligand DGD h 102



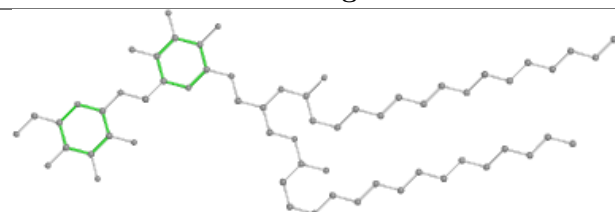
Bond lengths



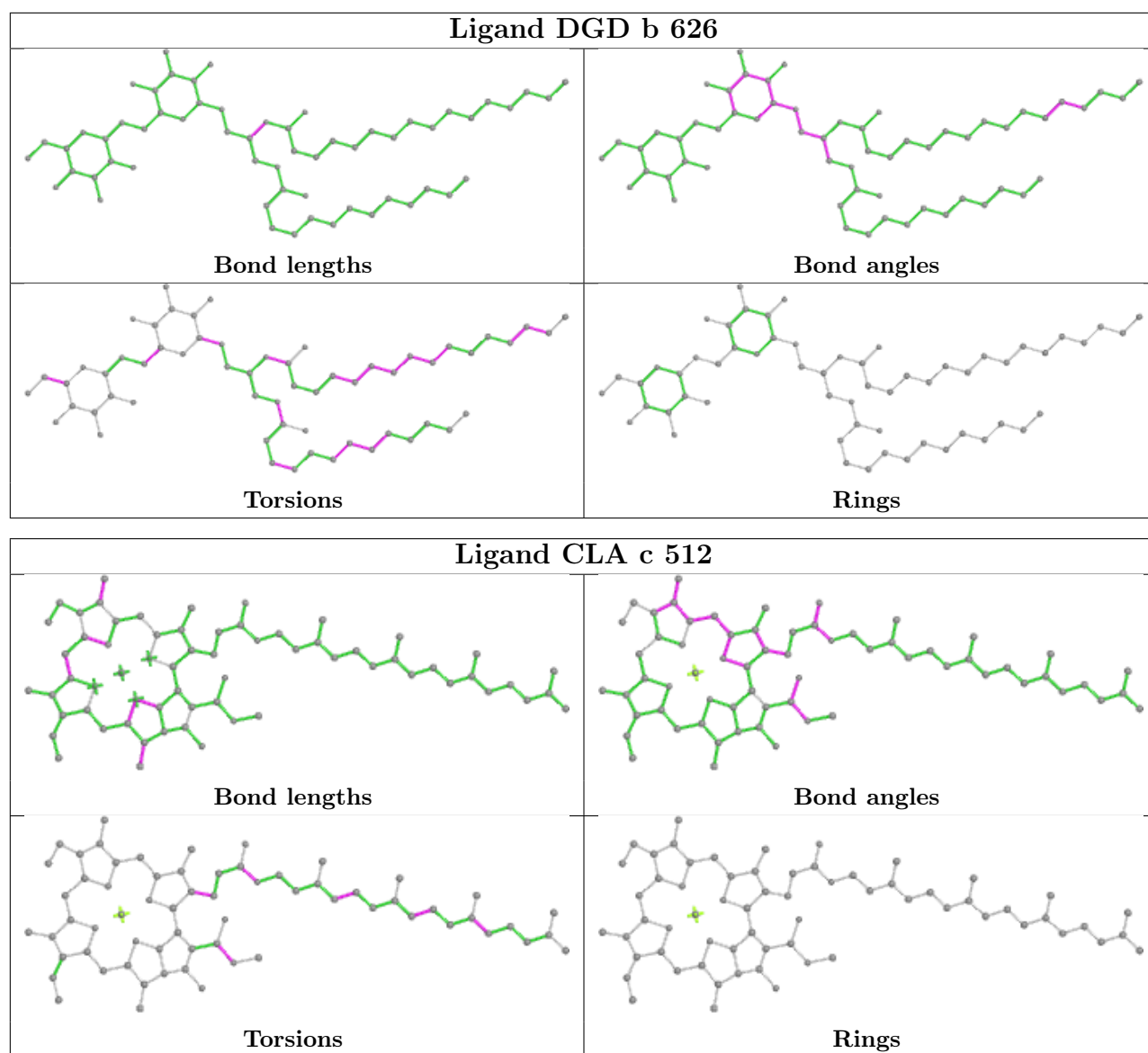
Bond angles



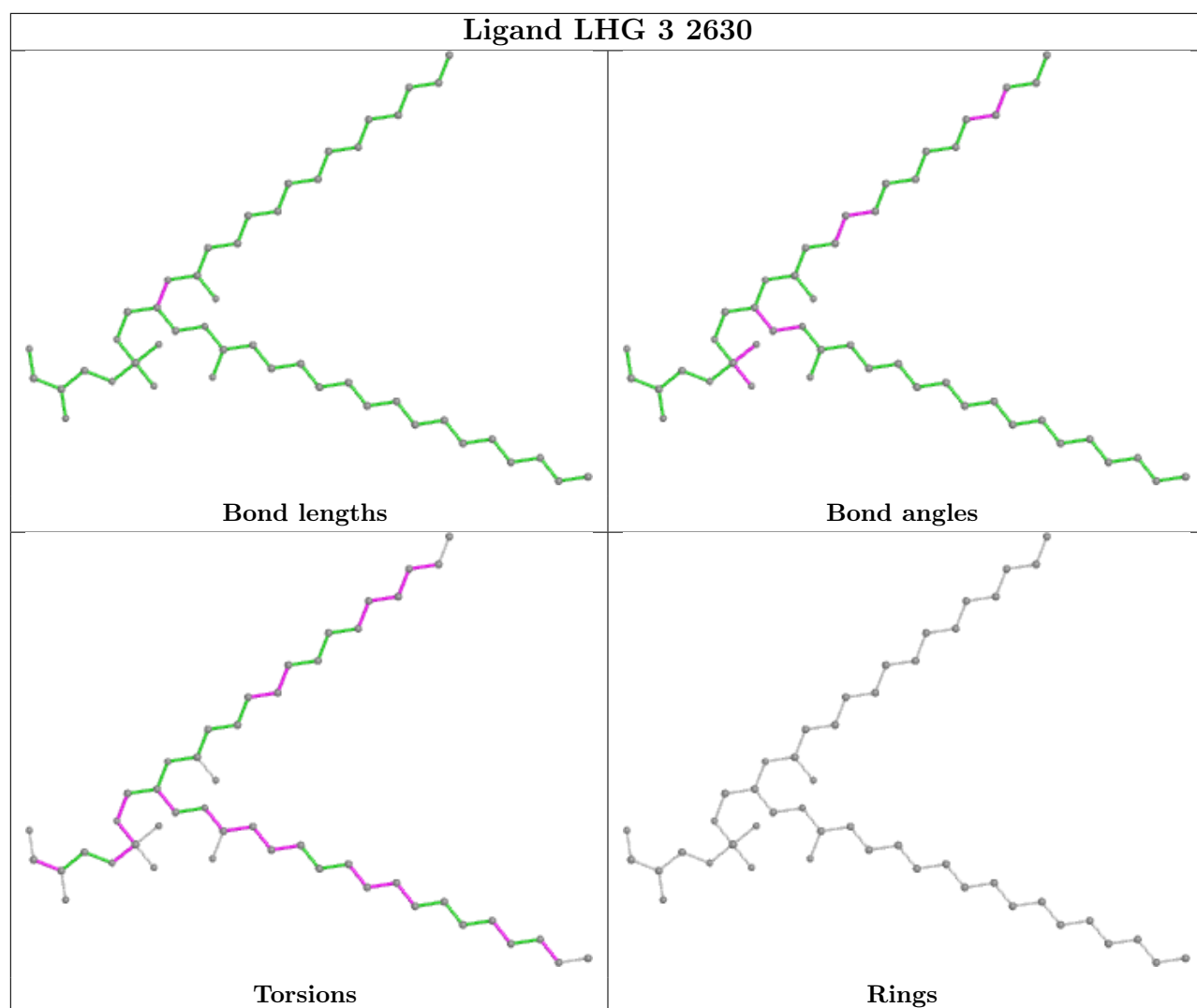
Torsions

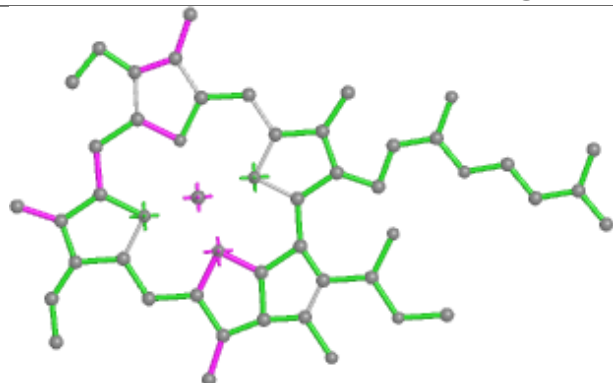


Rings

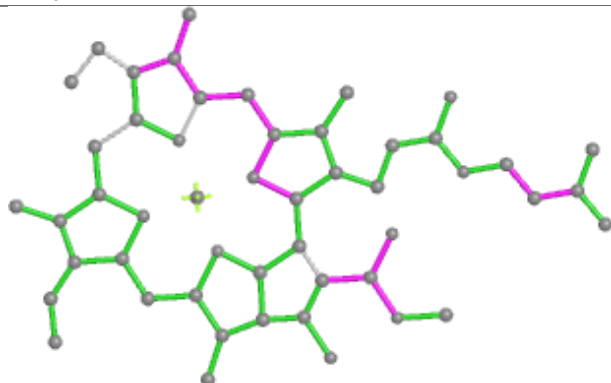




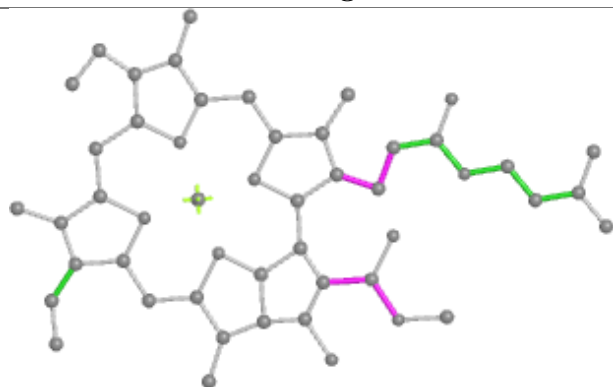


**Ligand CLA y 604**

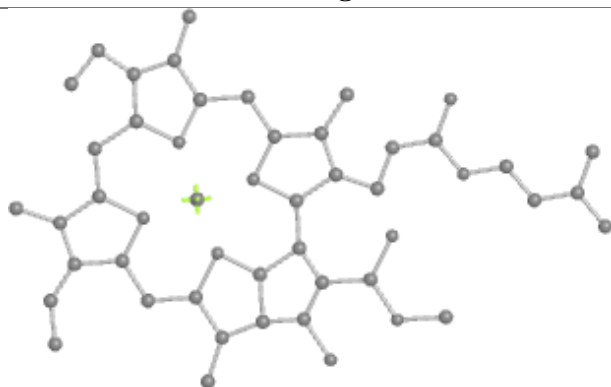
Bond lengths



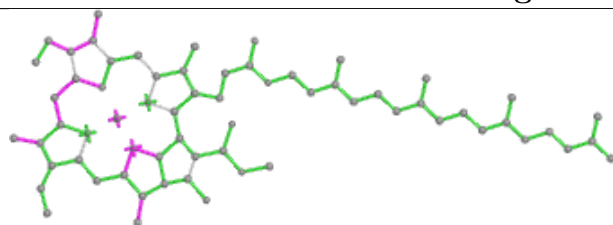
Bond angles



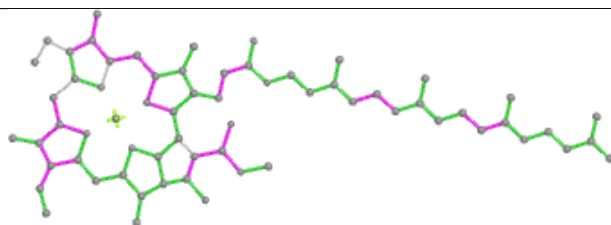
Torsions



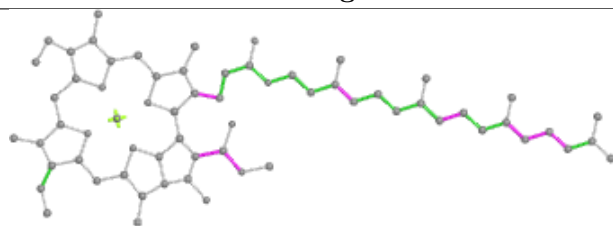
Rings

**Ligand CLA B 612**

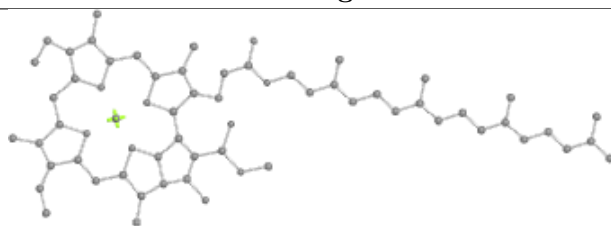
Bond lengths



Bond angles

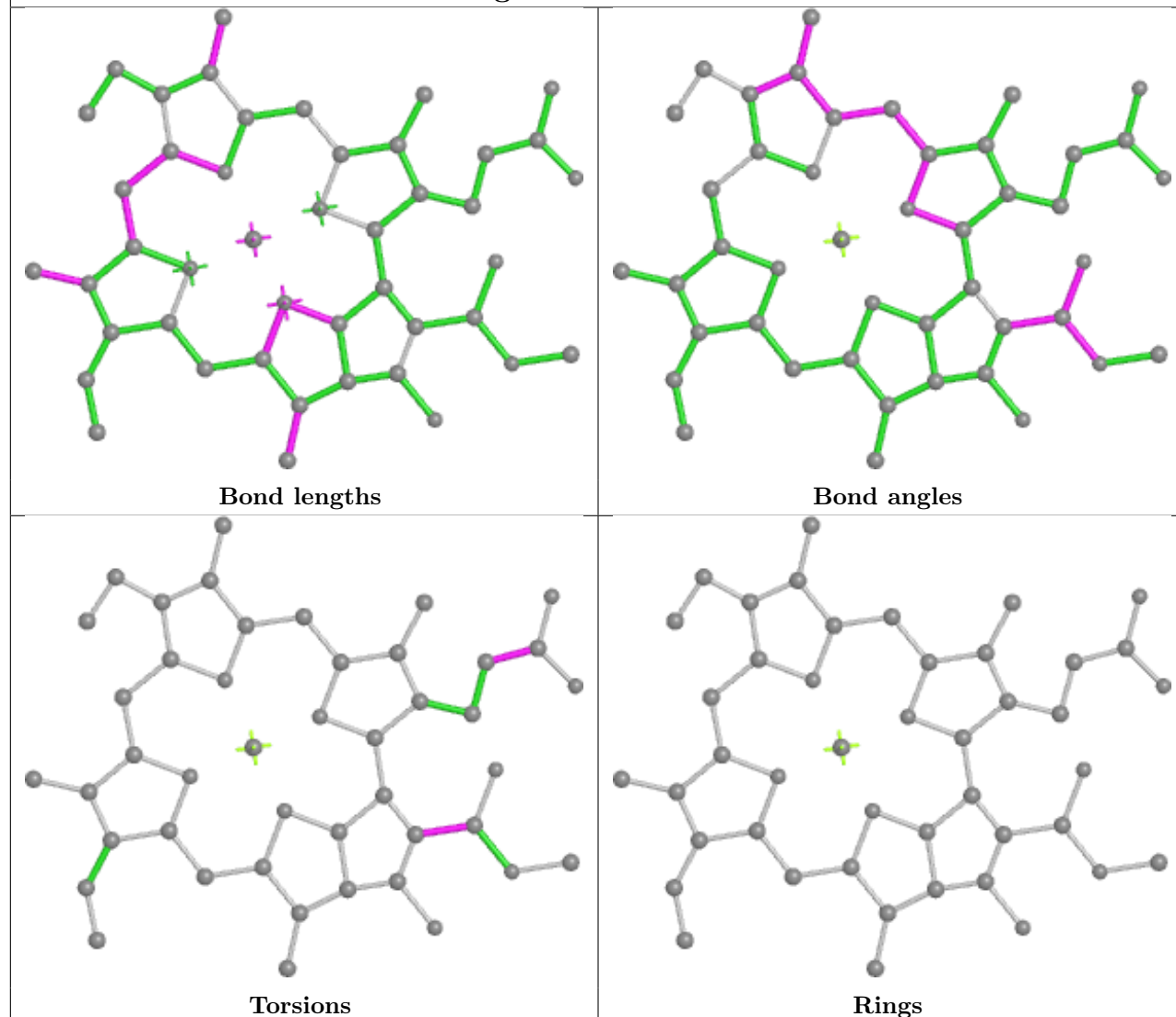


Torsions

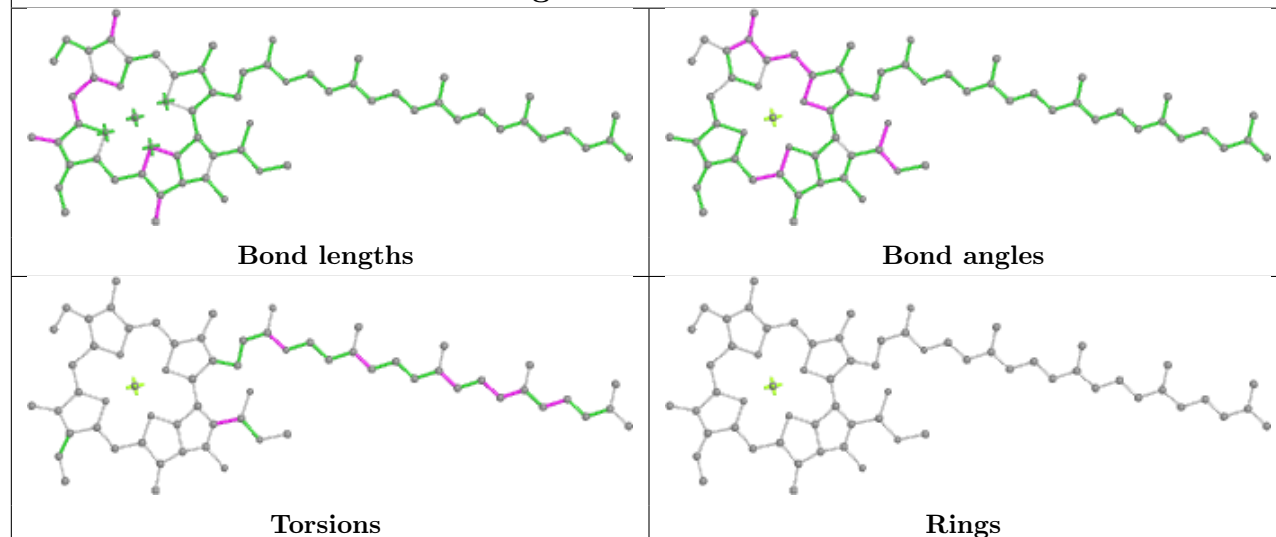


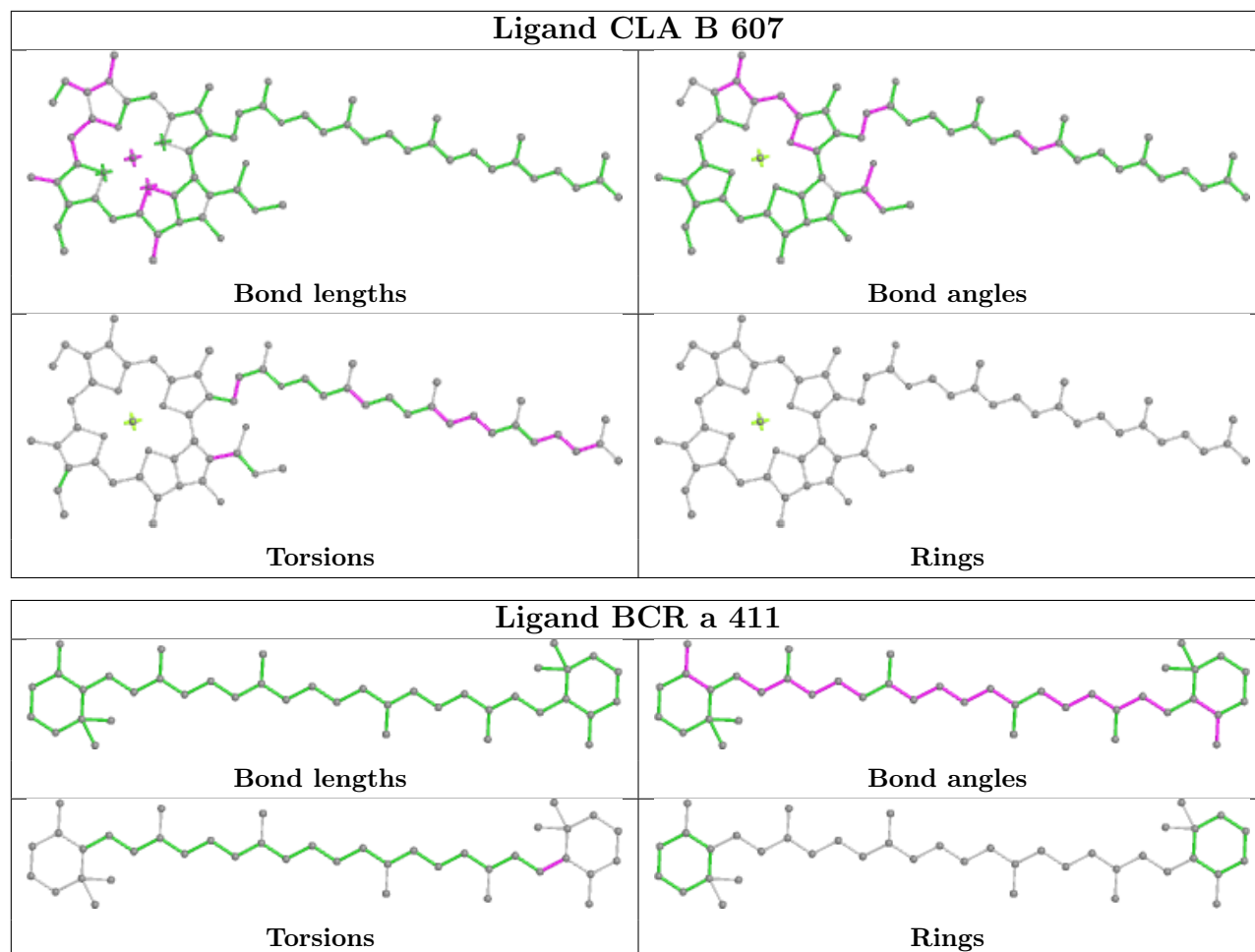
Rings

## Ligand CLA 2 611

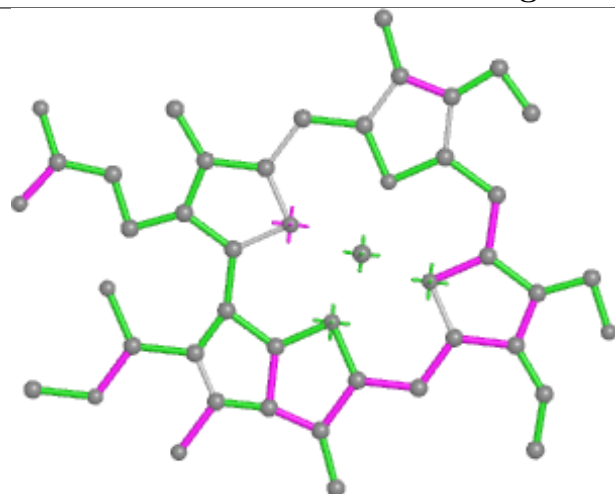


## Ligand CLA C 504

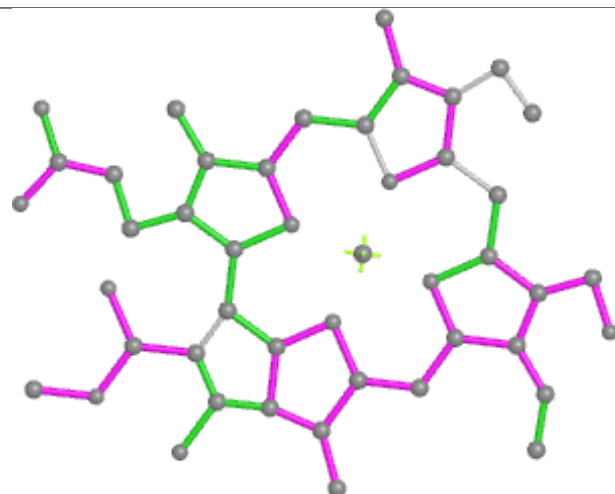




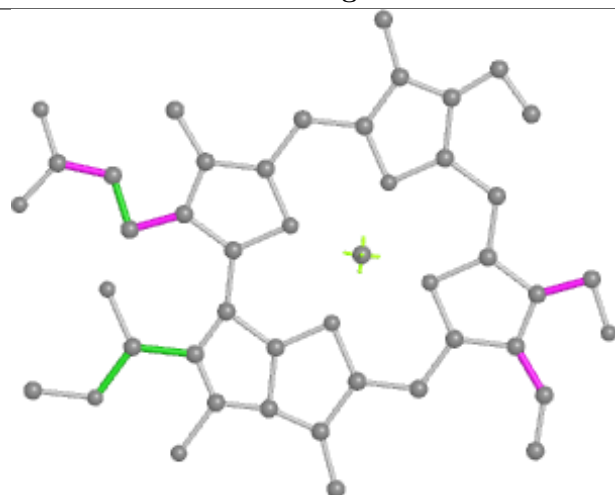
## Ligand CHL 8 609



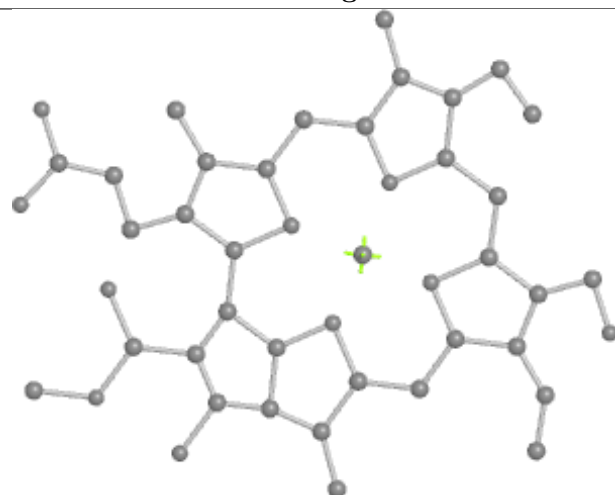
Bond lengths



Bond angles

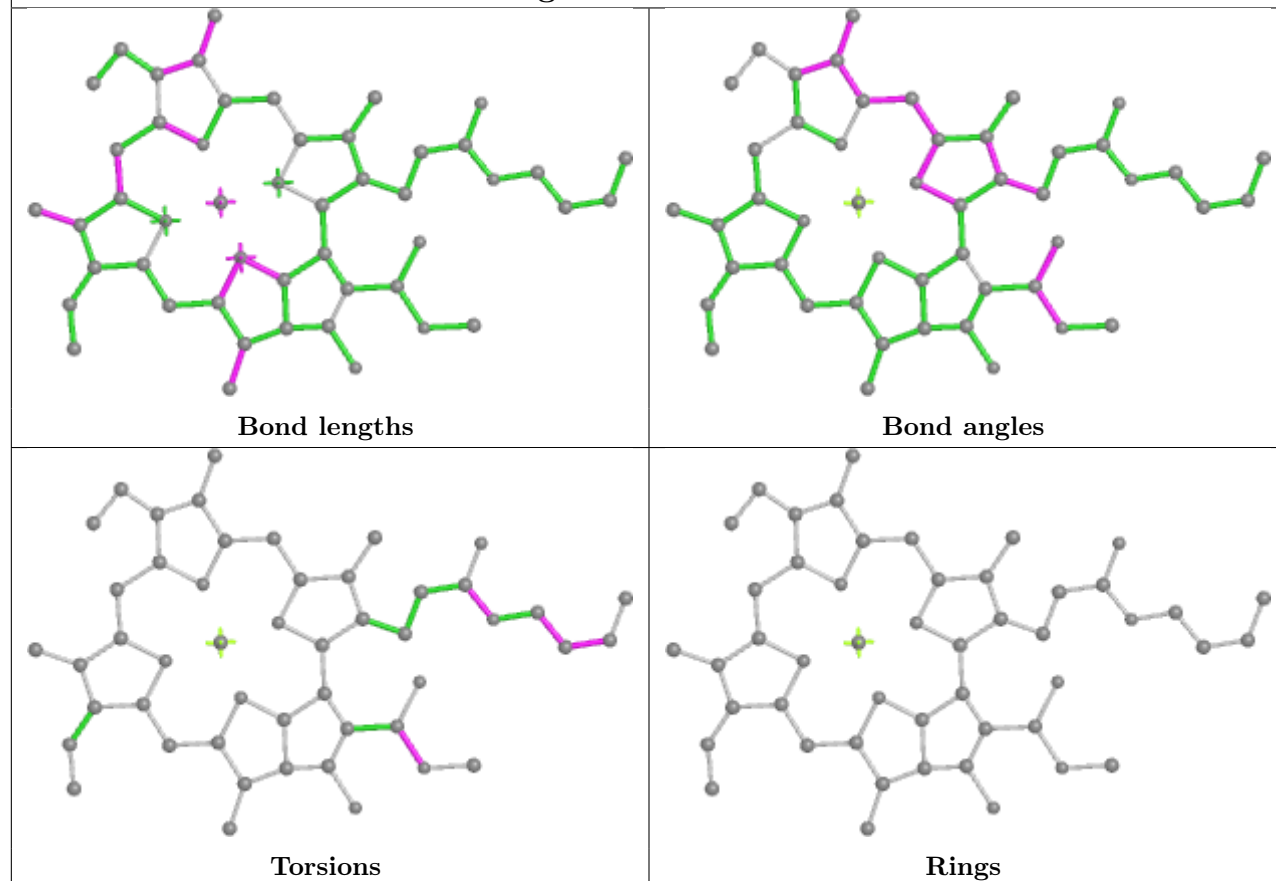


Torsions

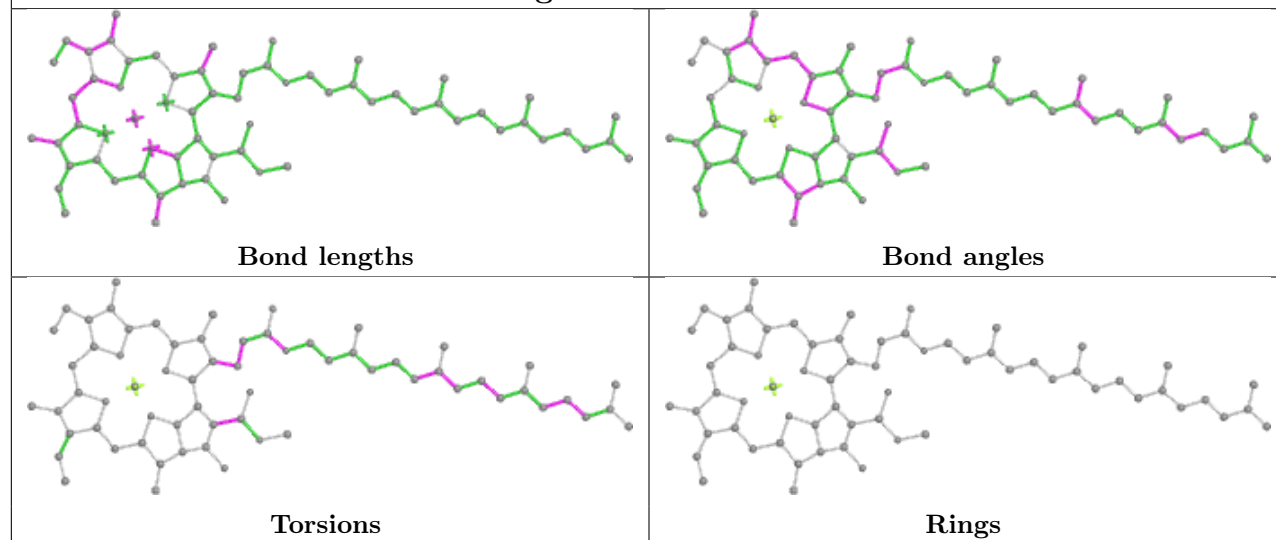


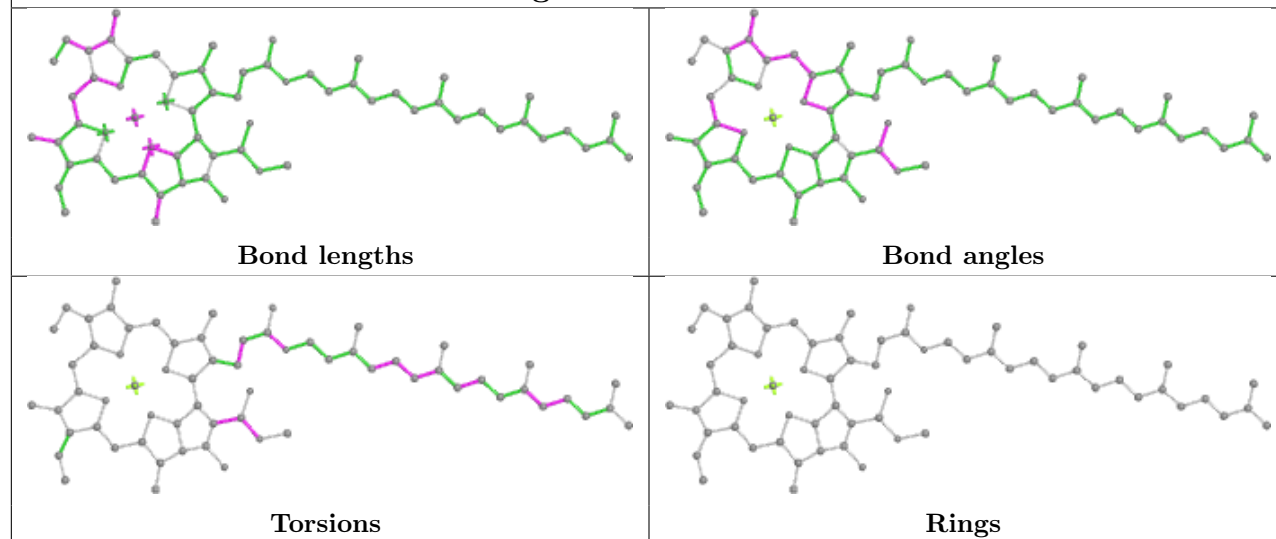
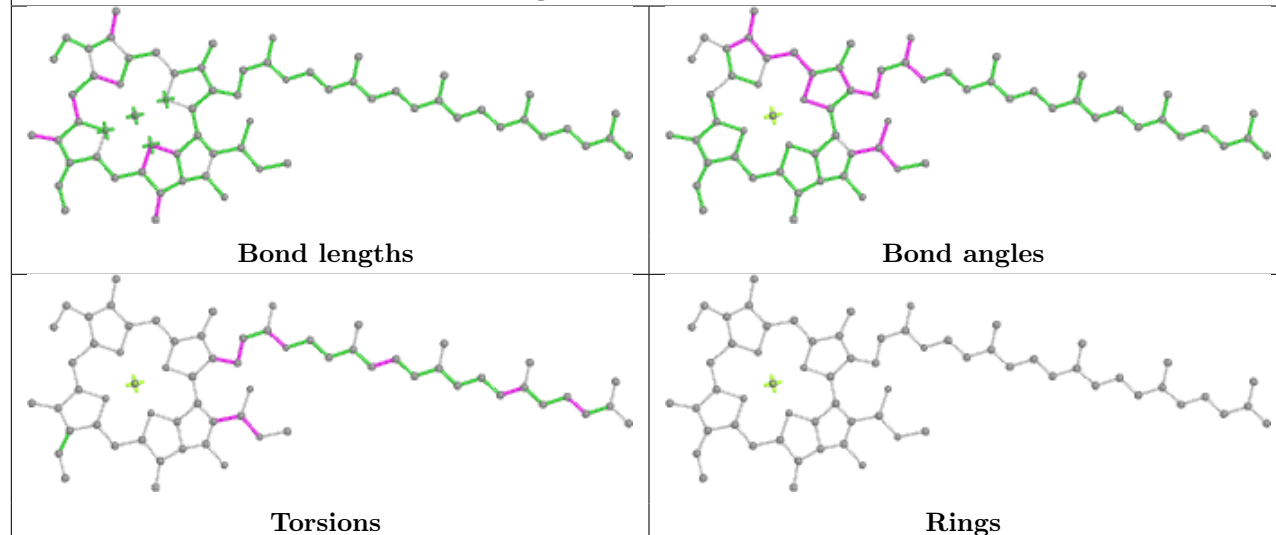
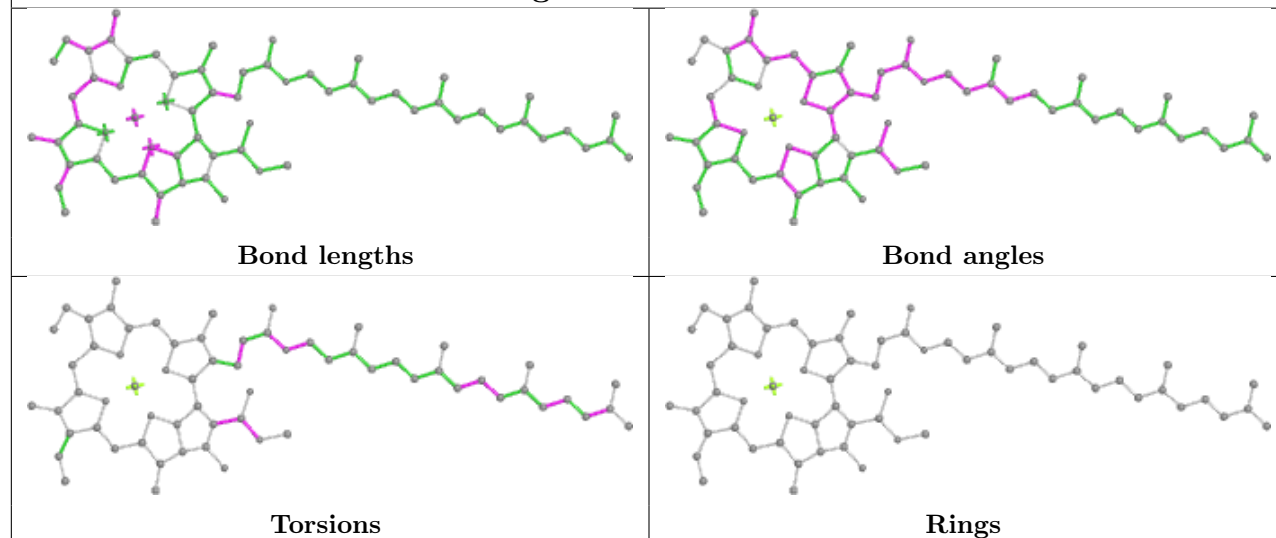
Rings

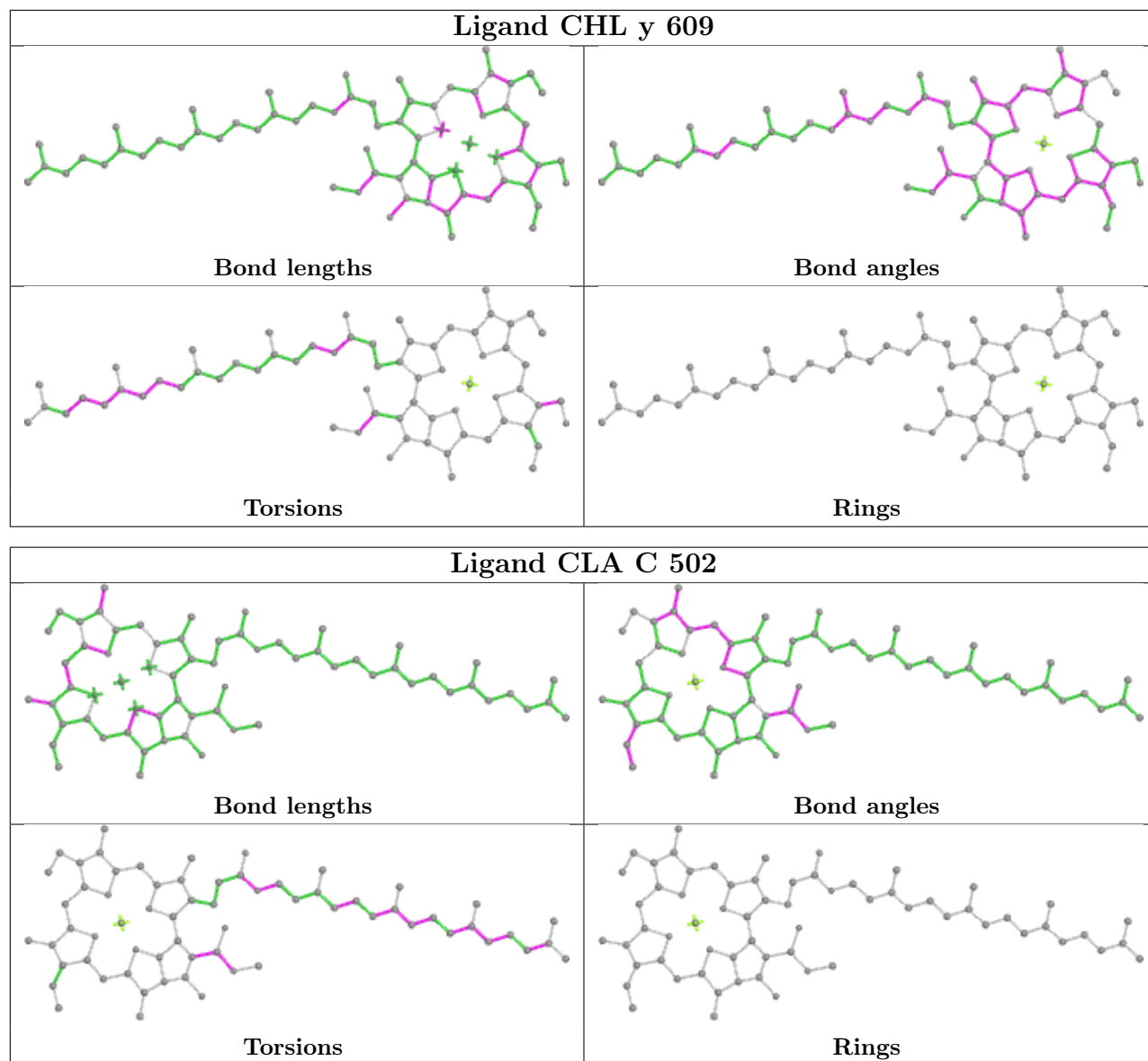
## Ligand CLA r 612



## Ligand CLA b 613

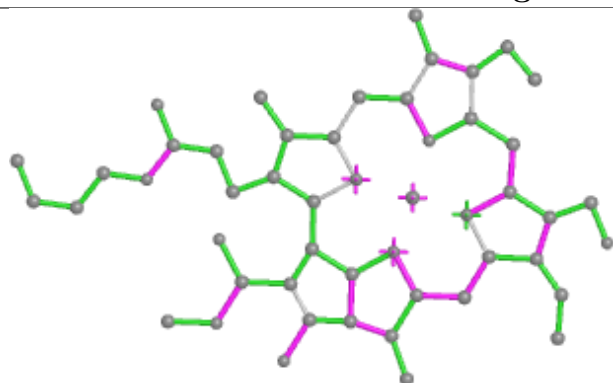


**Ligand CLA B 608****Ligand CLA C 513****Ligand CLA B 605**

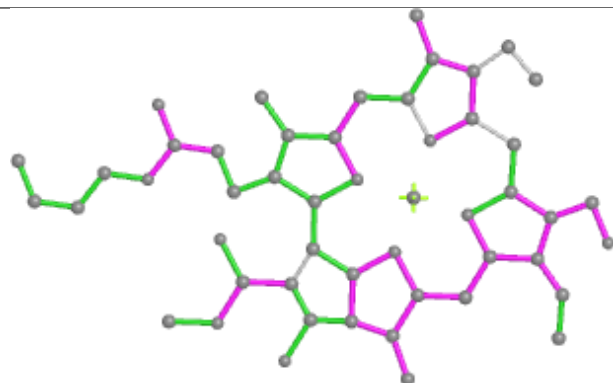




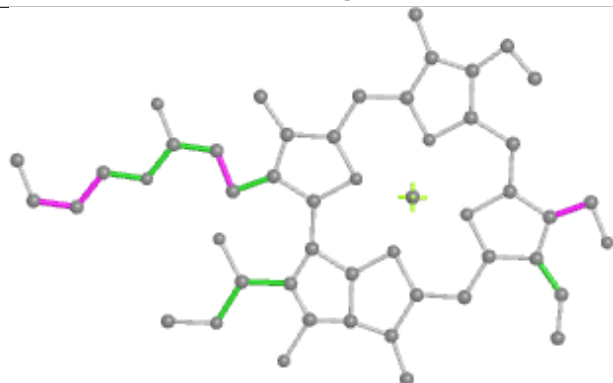
## Ligand CHL Y 606



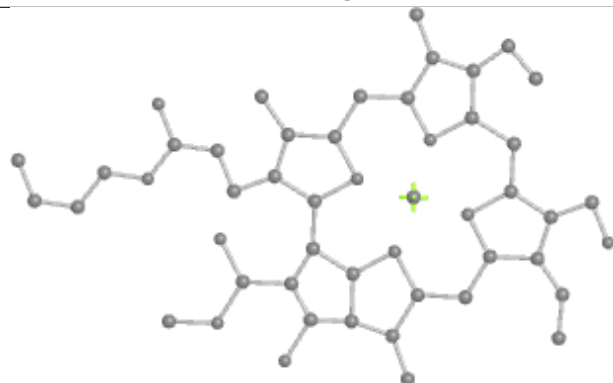
Bond lengths



Bond angles

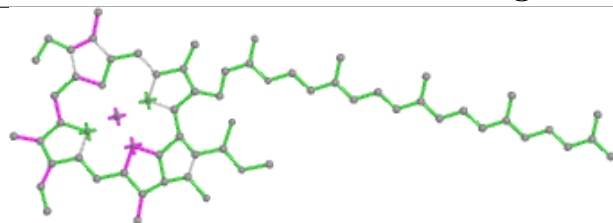


Torsions

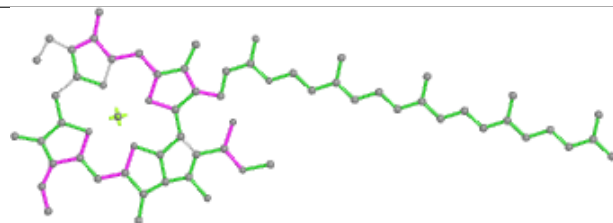


Rings

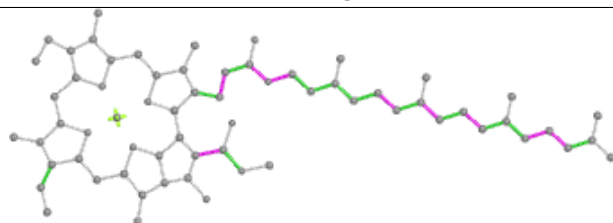
## Ligand CLA G 603



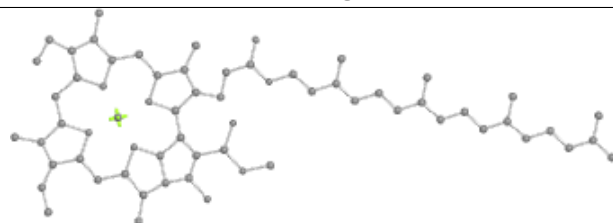
Bond lengths



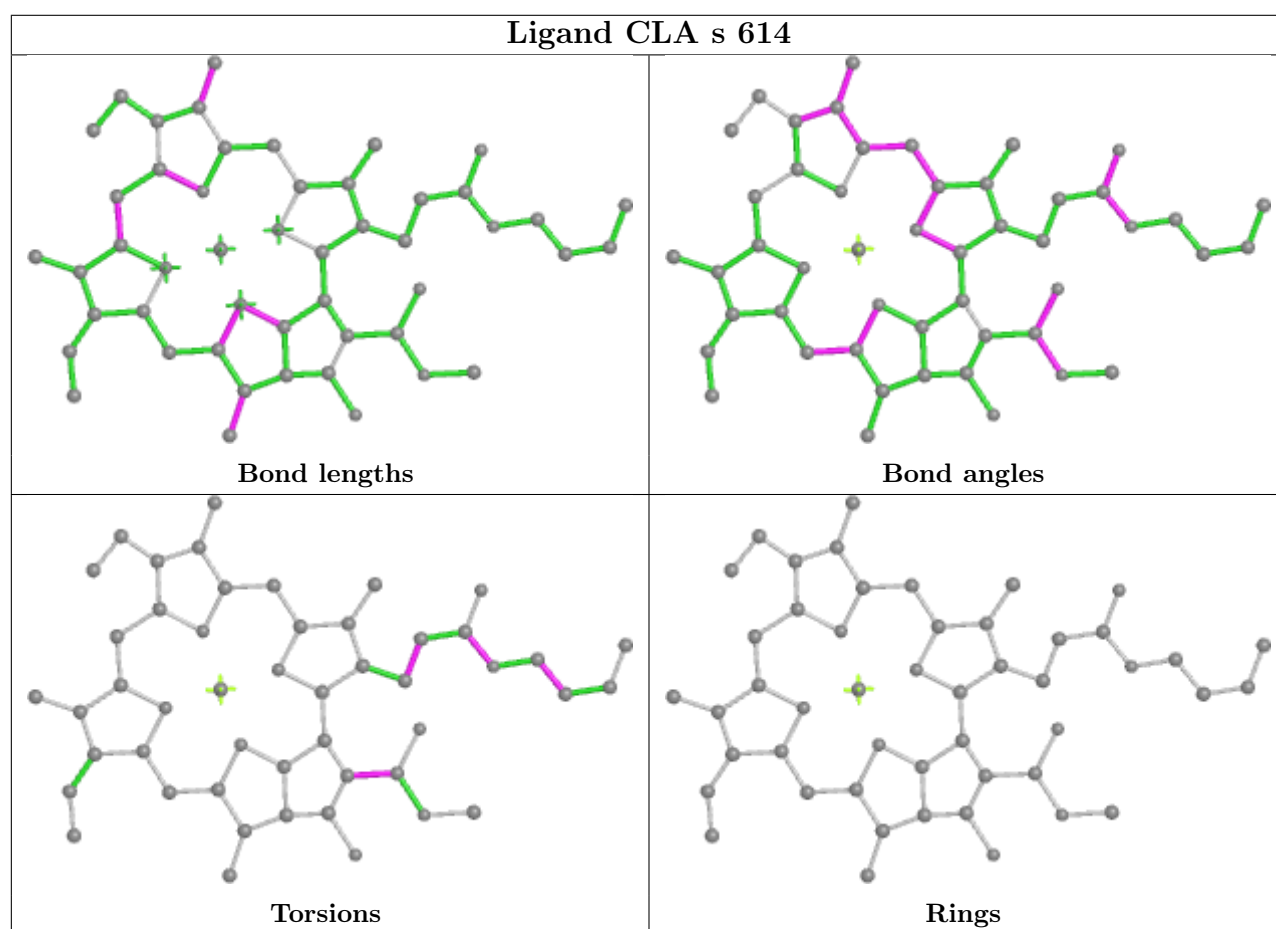
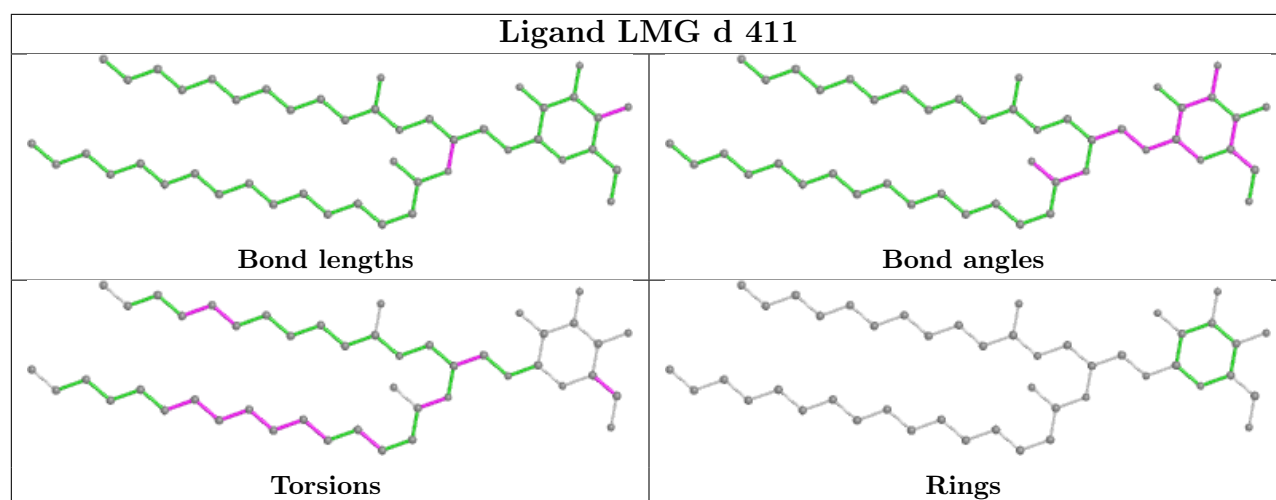
Bond angles

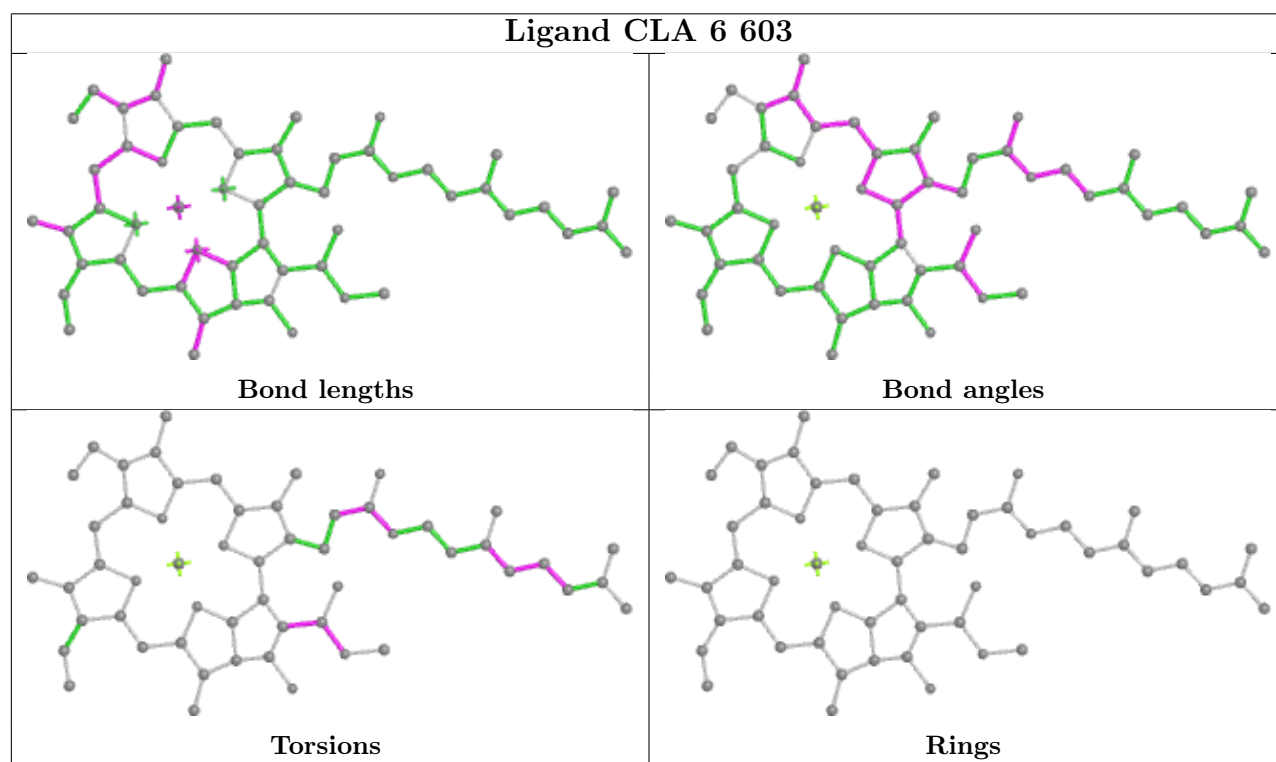
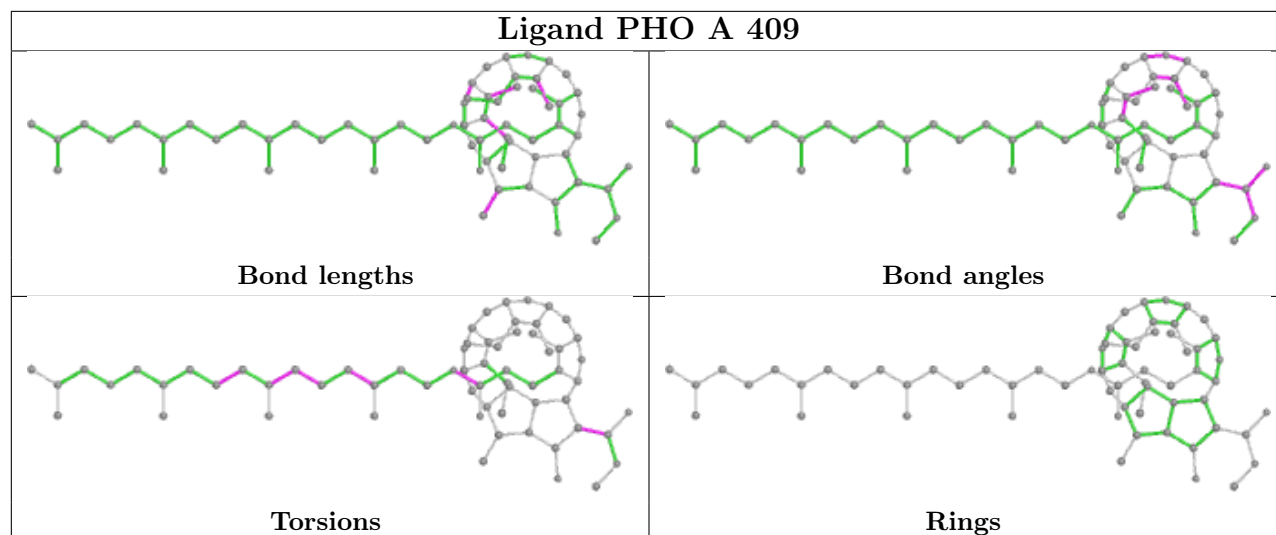


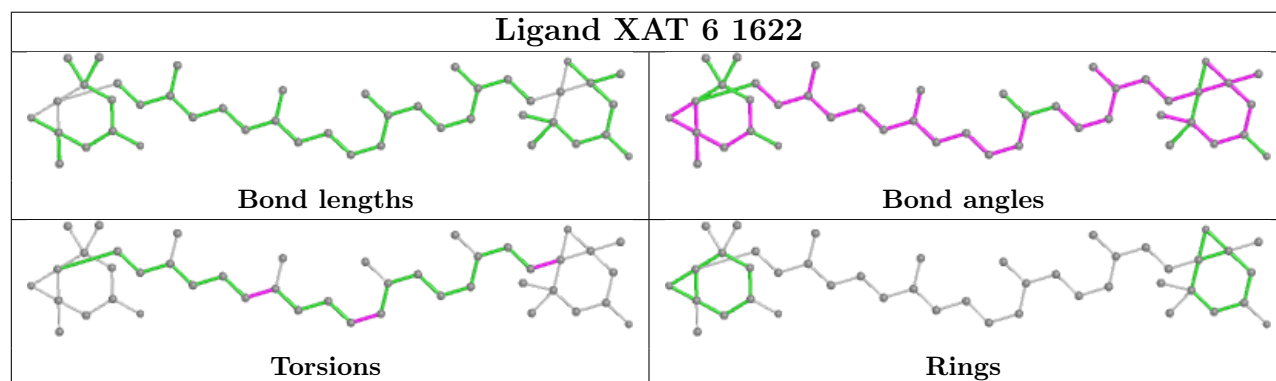
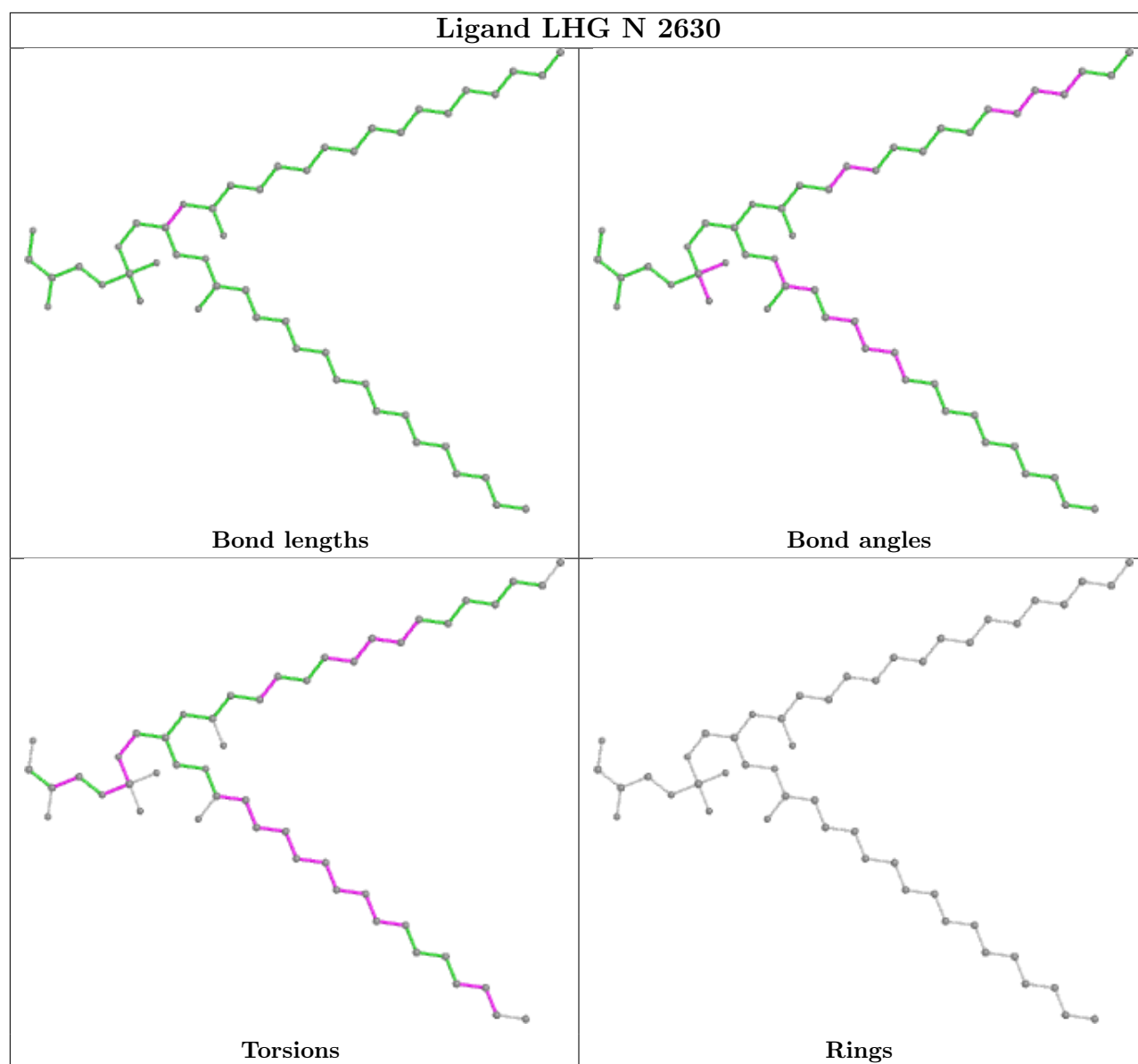
Torsions

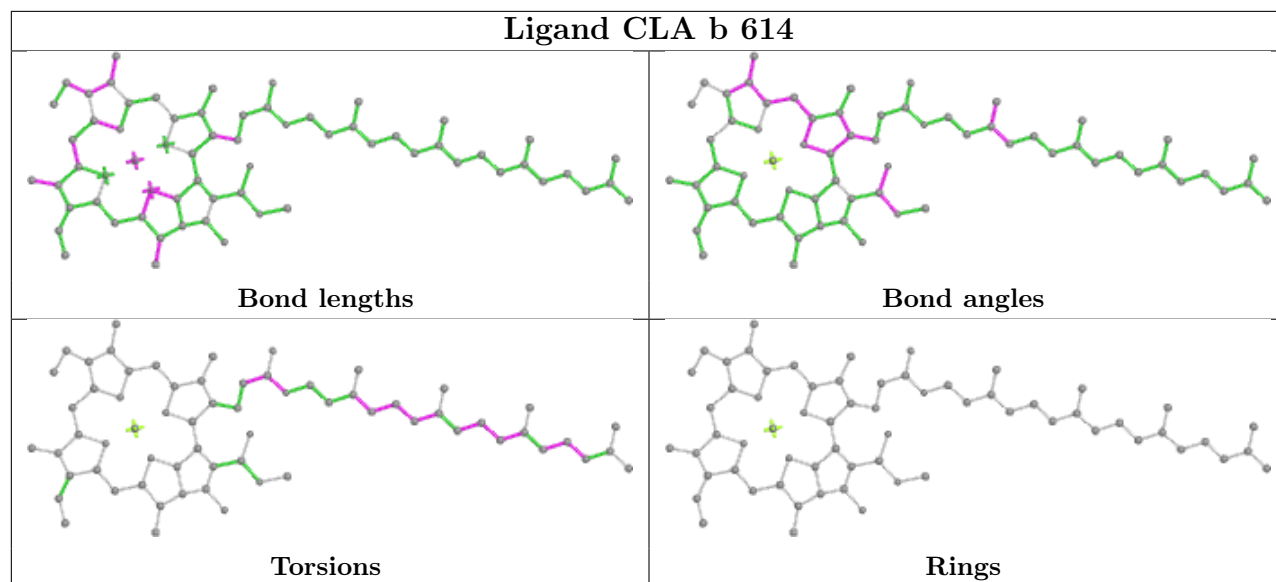
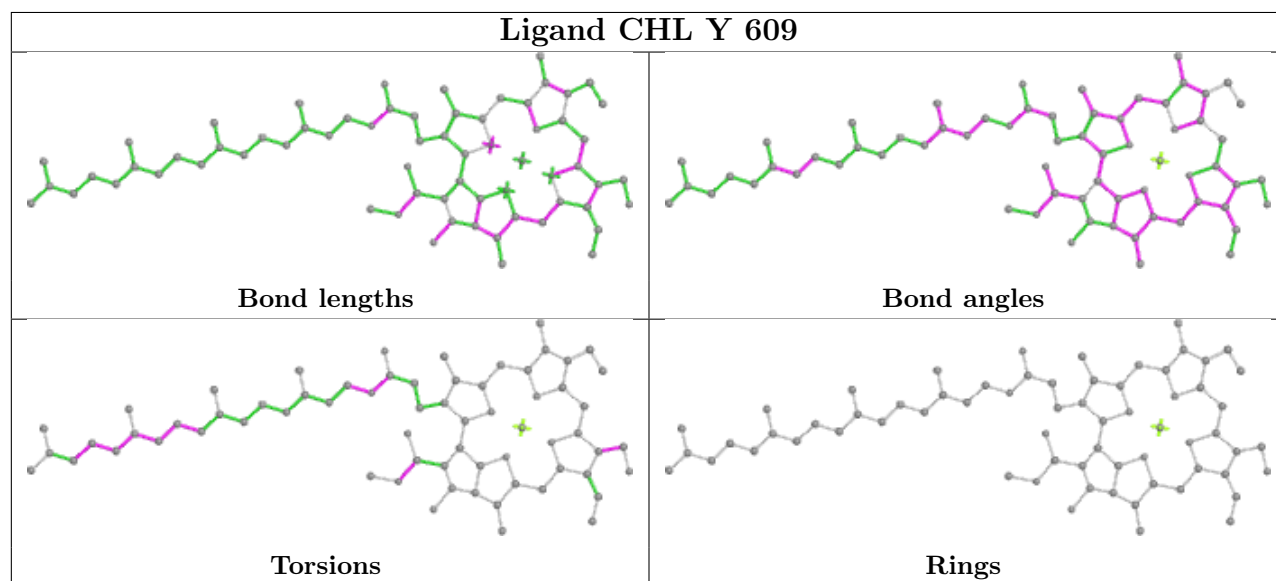


Rings

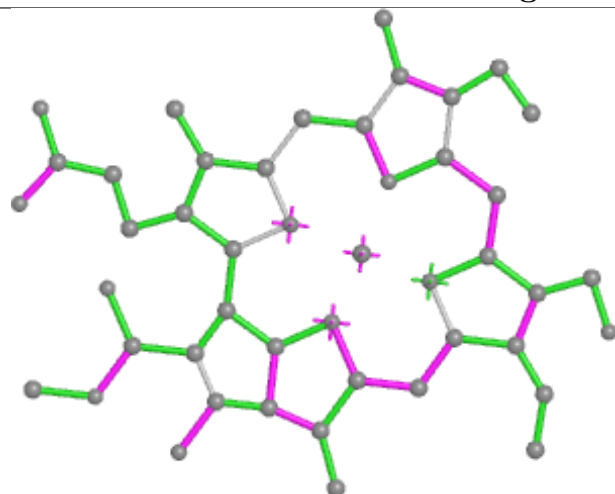




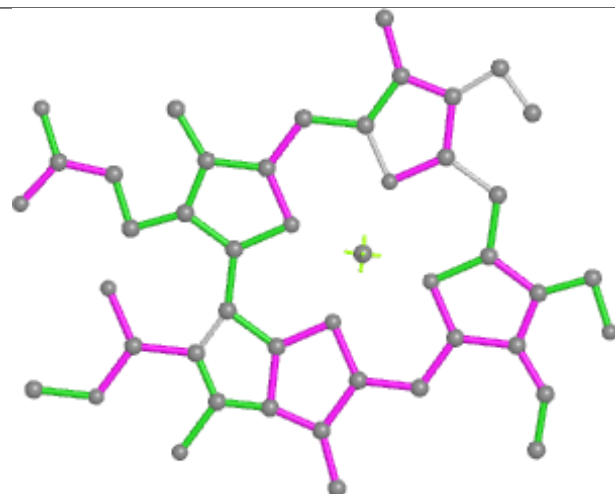


**Ligand CLA b 614****Ligand CHL Y 609**

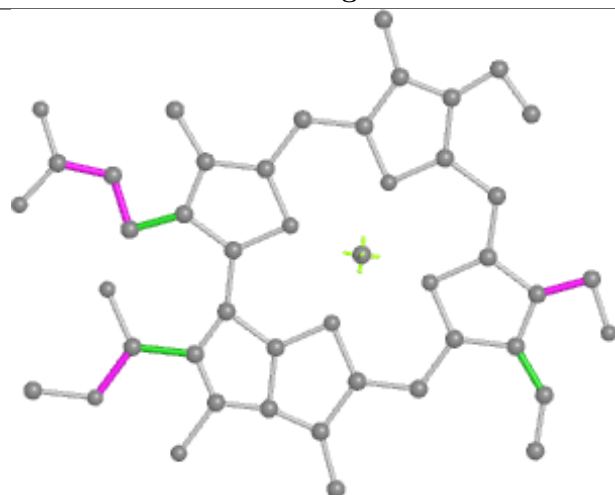
## Ligand CHL 5 606



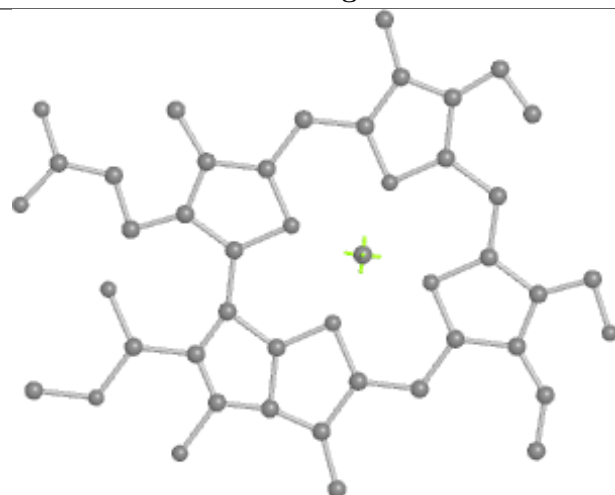
Bond lengths



Bond angles

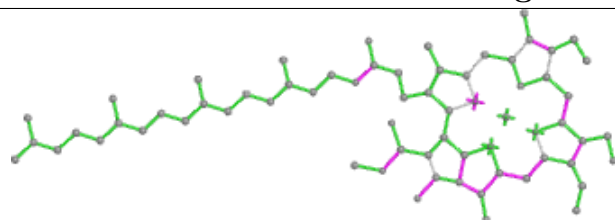


Torsions

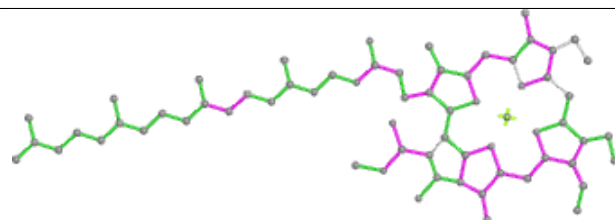


Rings

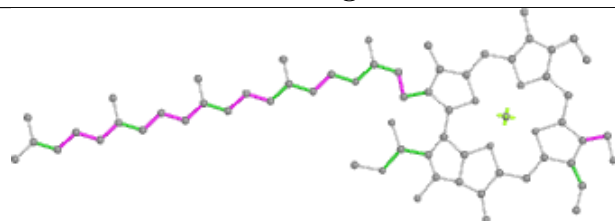
## Ligand CHL G 607



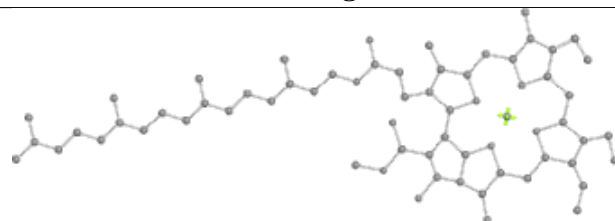
Bond lengths



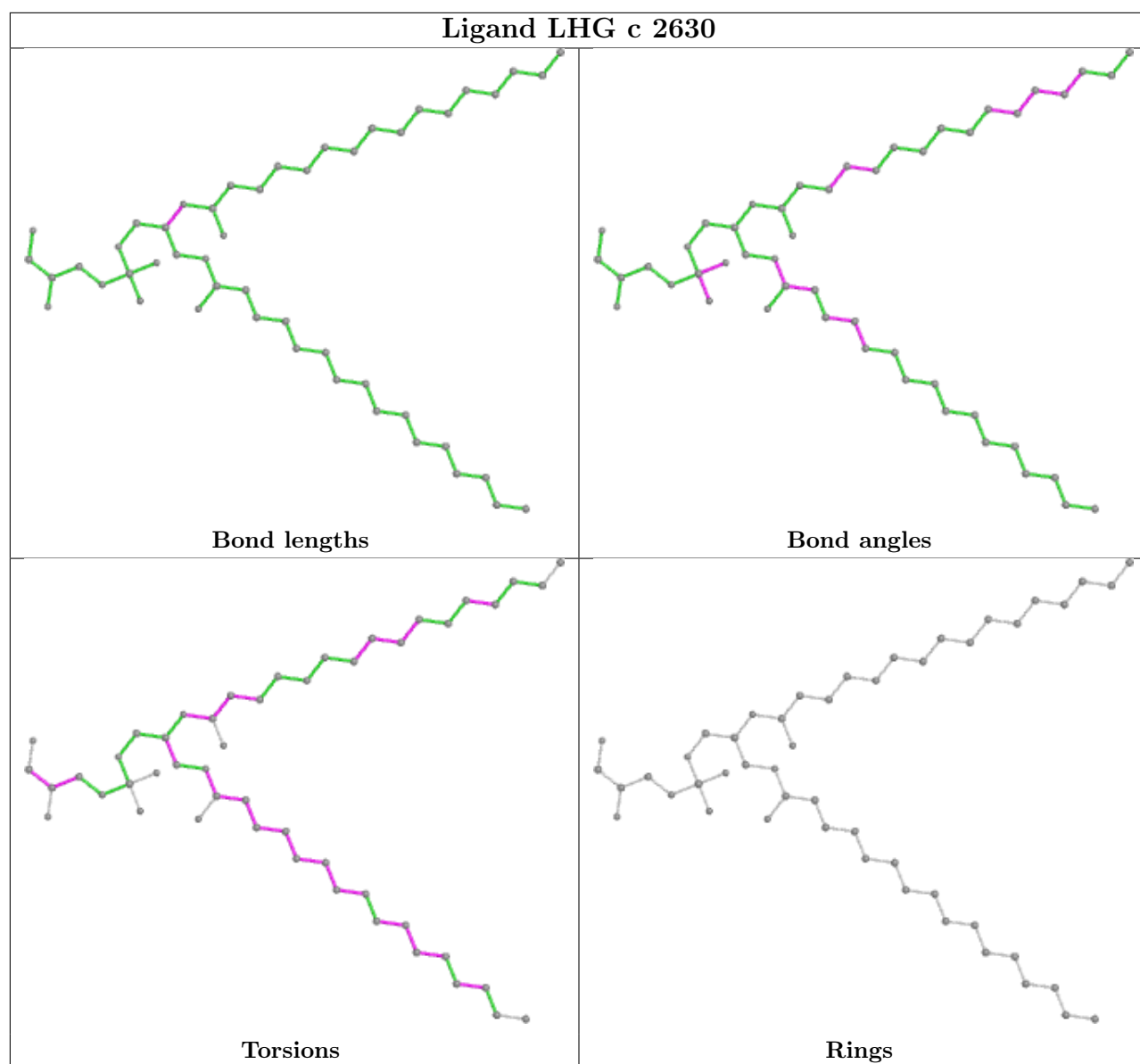
Bond angles

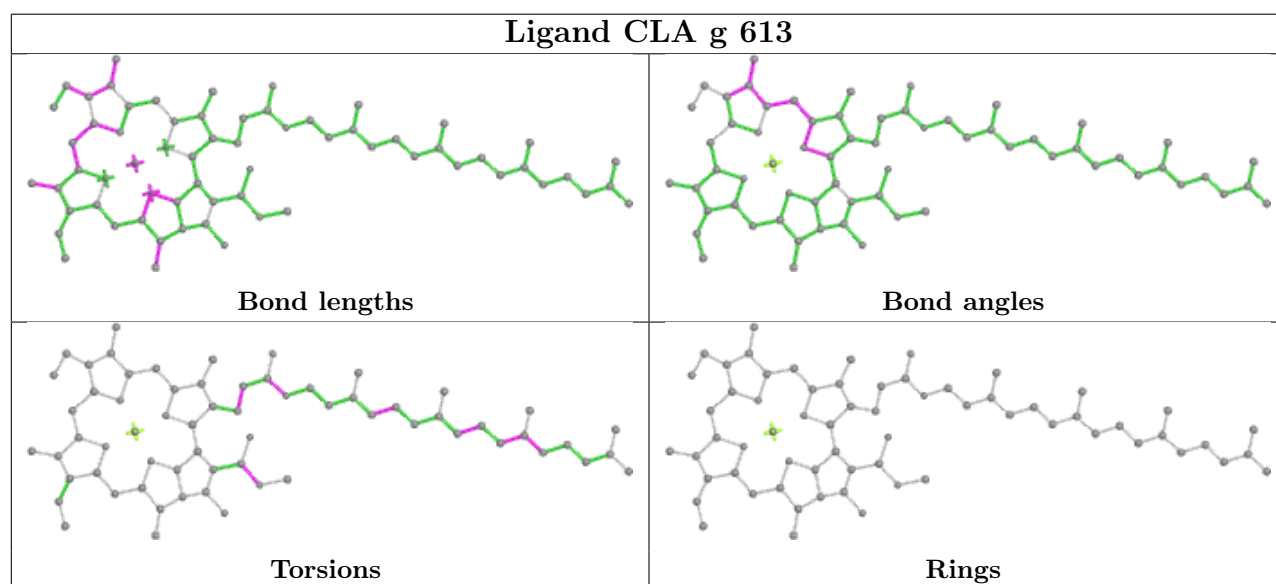
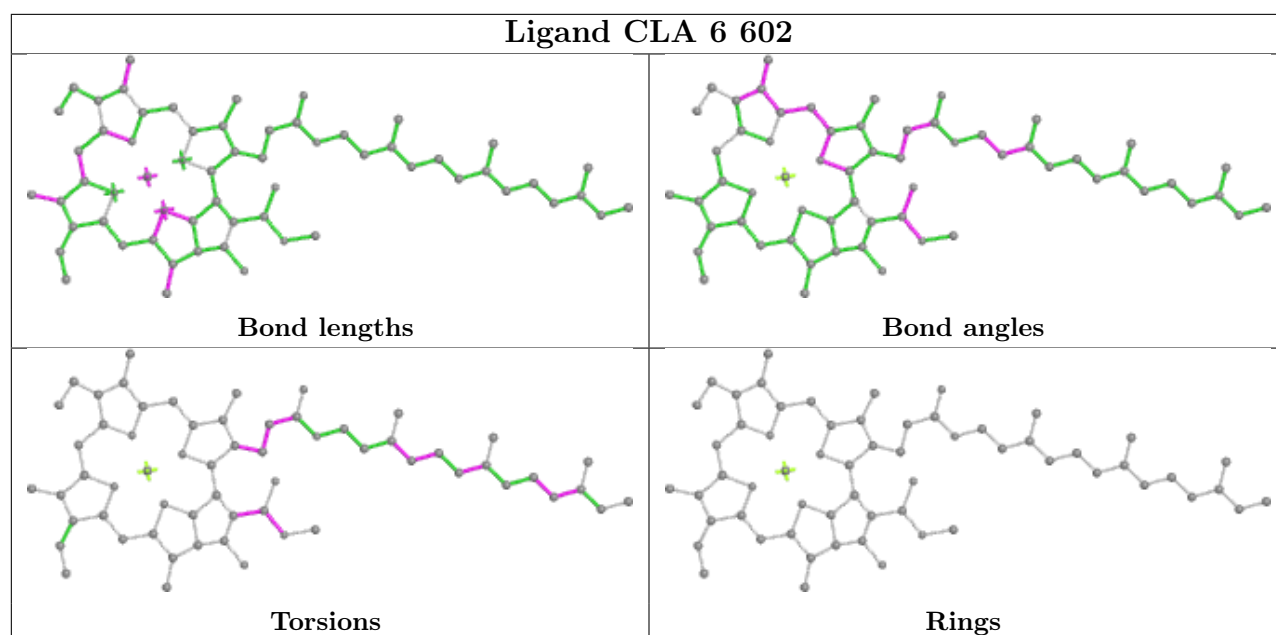


Torsions

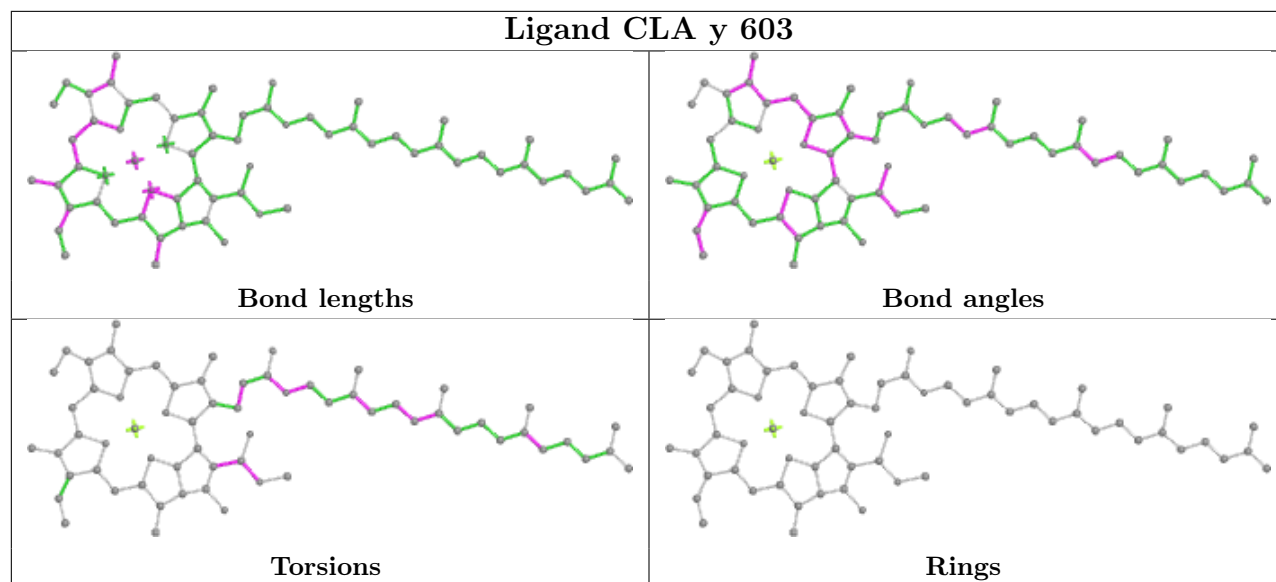
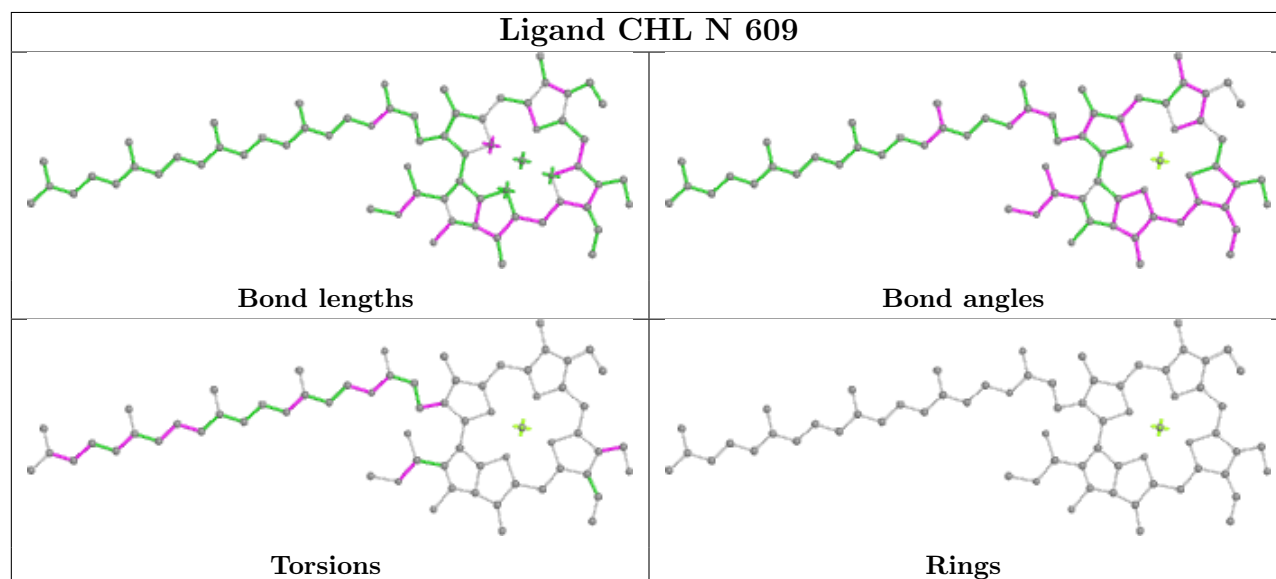
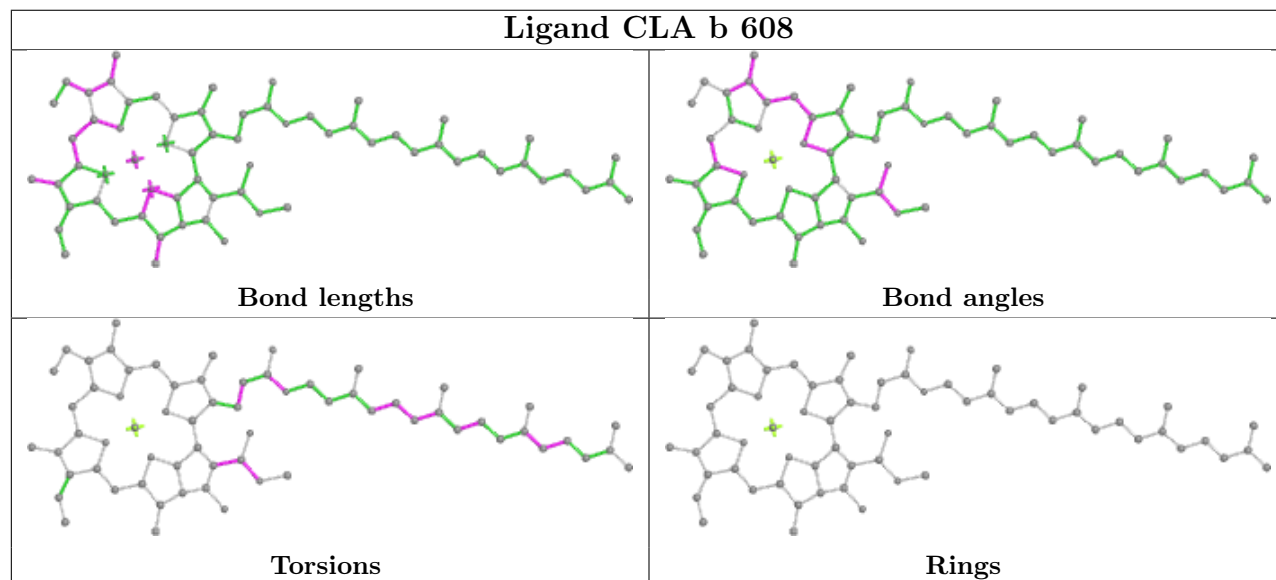


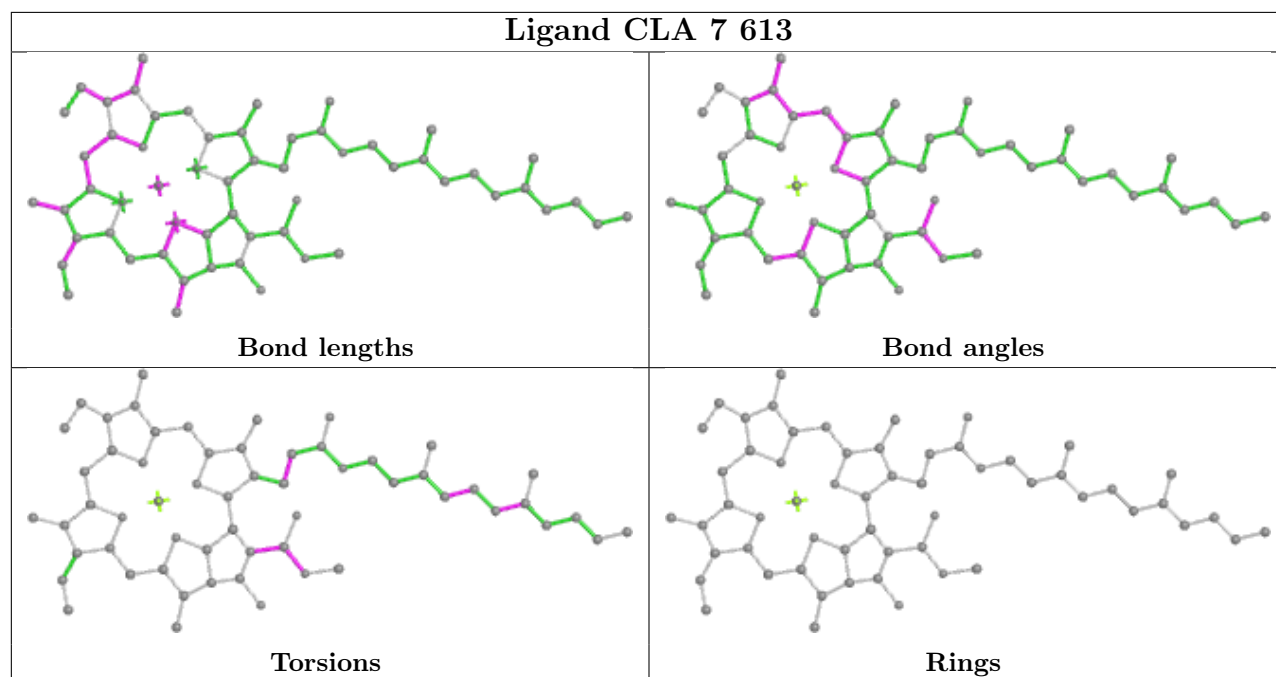
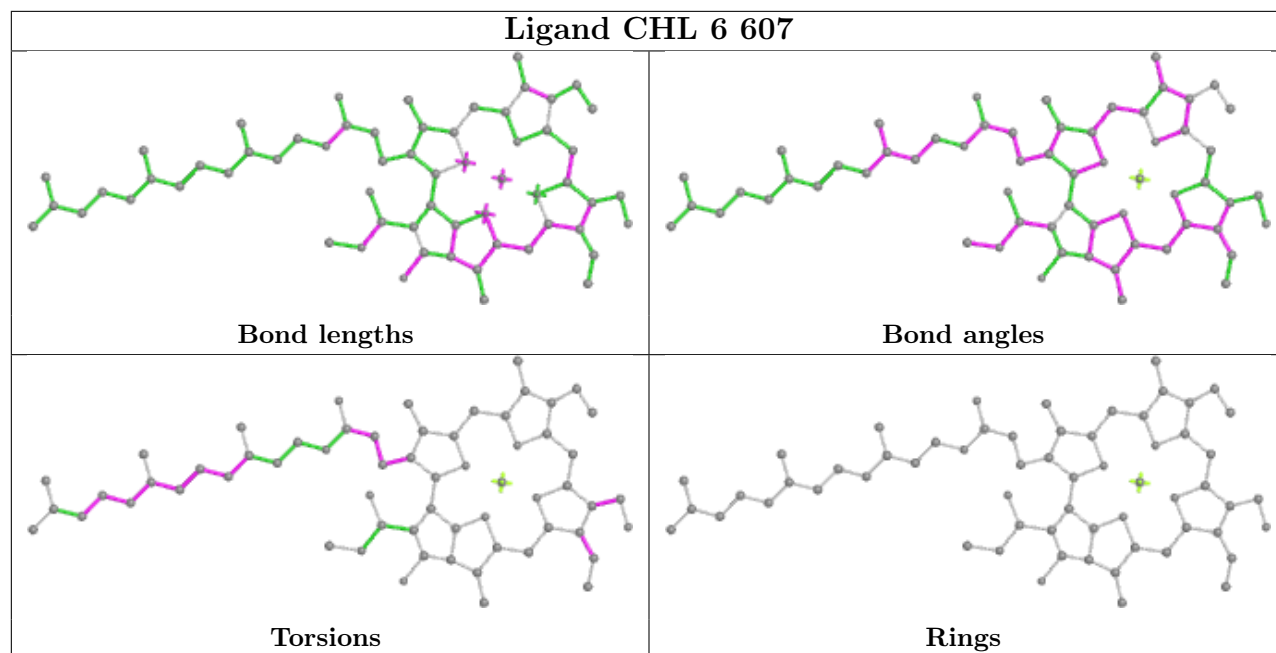
Rings



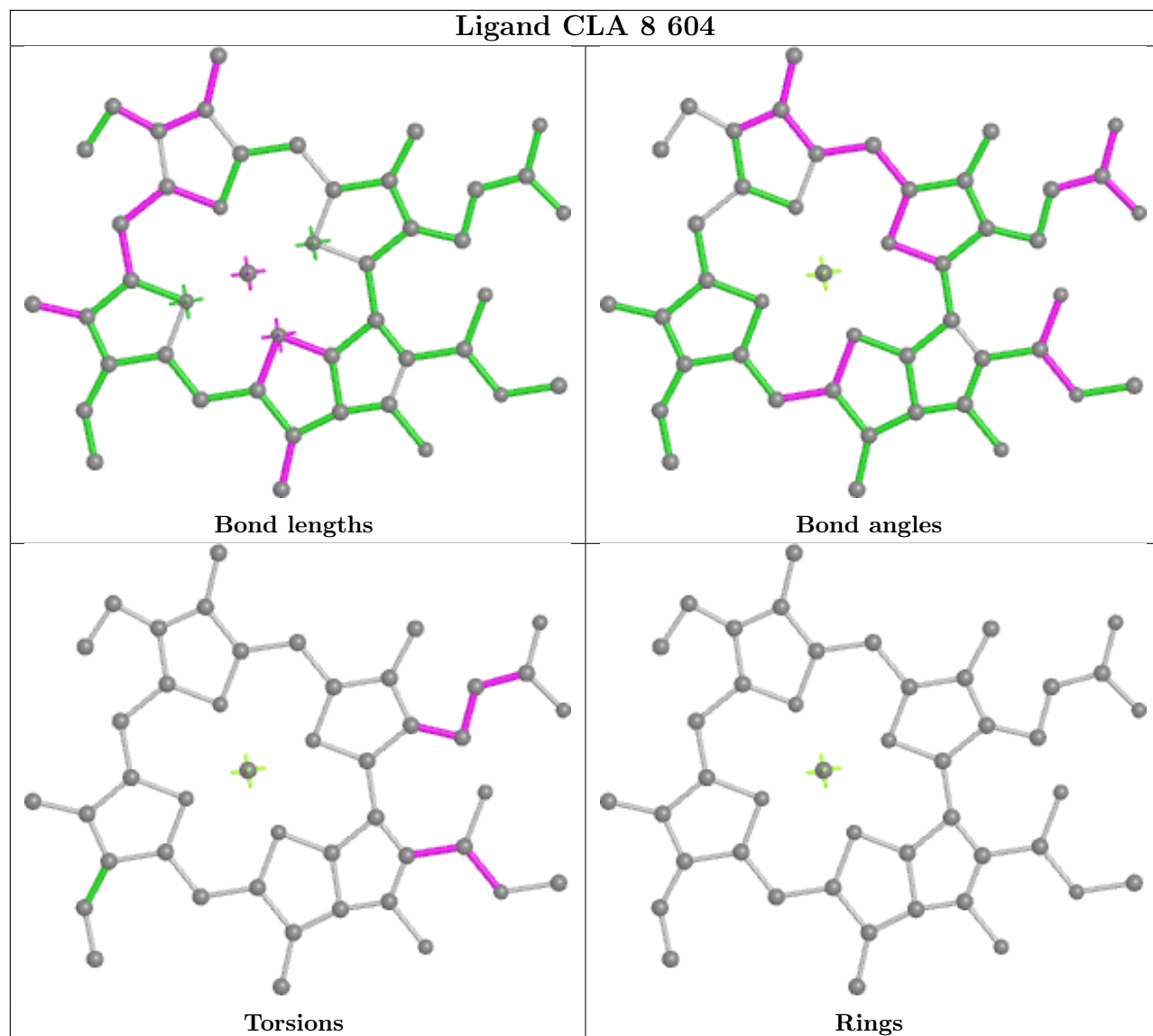


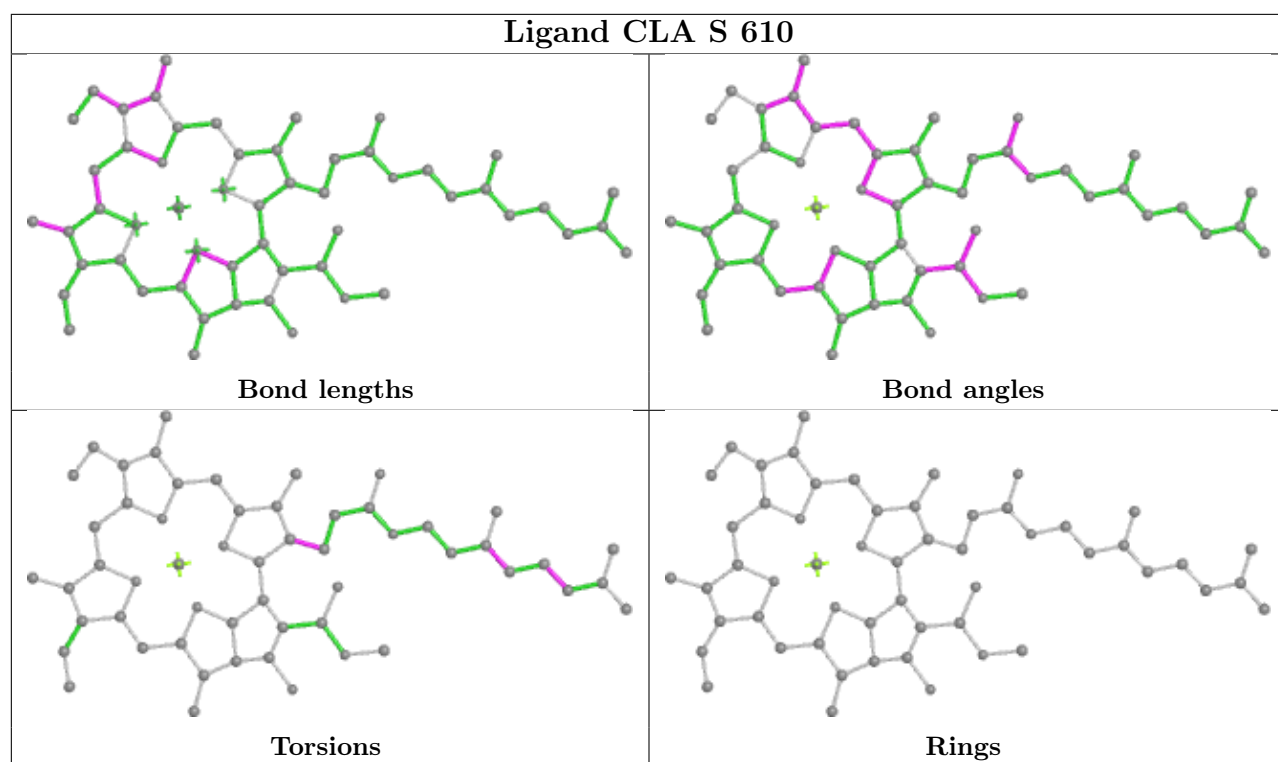


**Ligand CLA y 603****Ligand CHL N 609****Ligand CLA b 608**

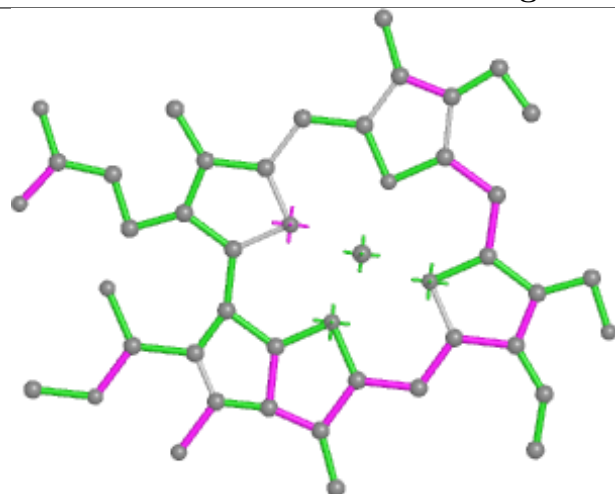


## Ligand CLA 8 604

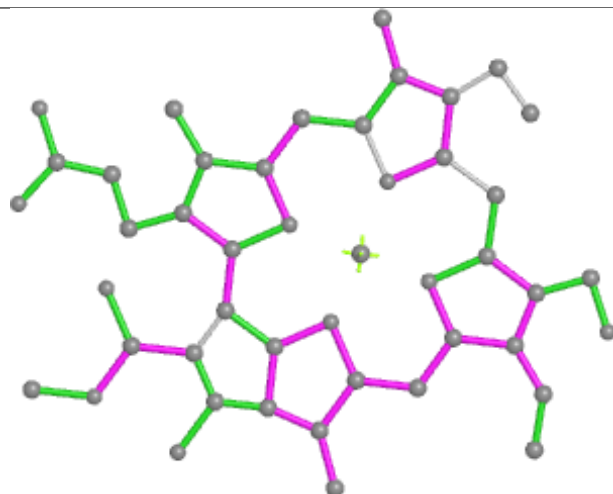




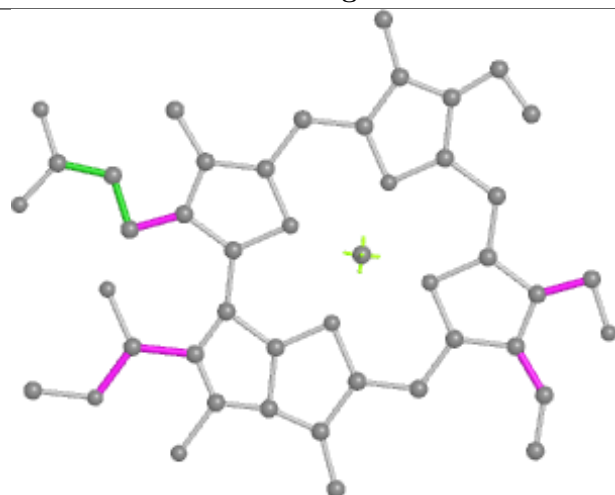
## Ligand CHL 6 608



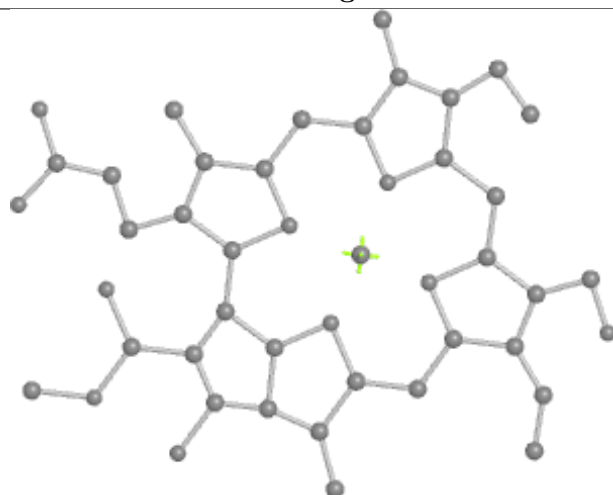
Bond lengths



Bond angles

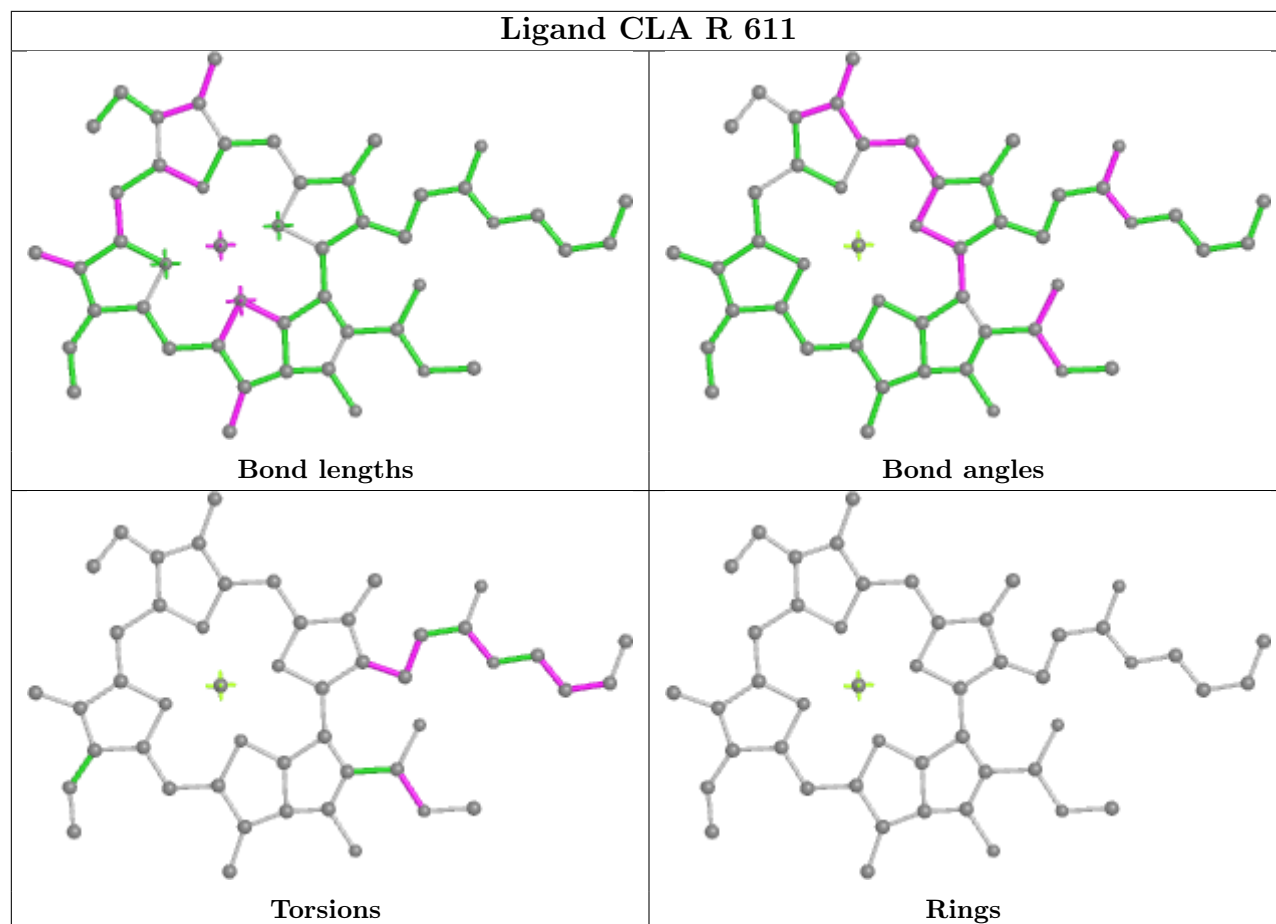


Torsions

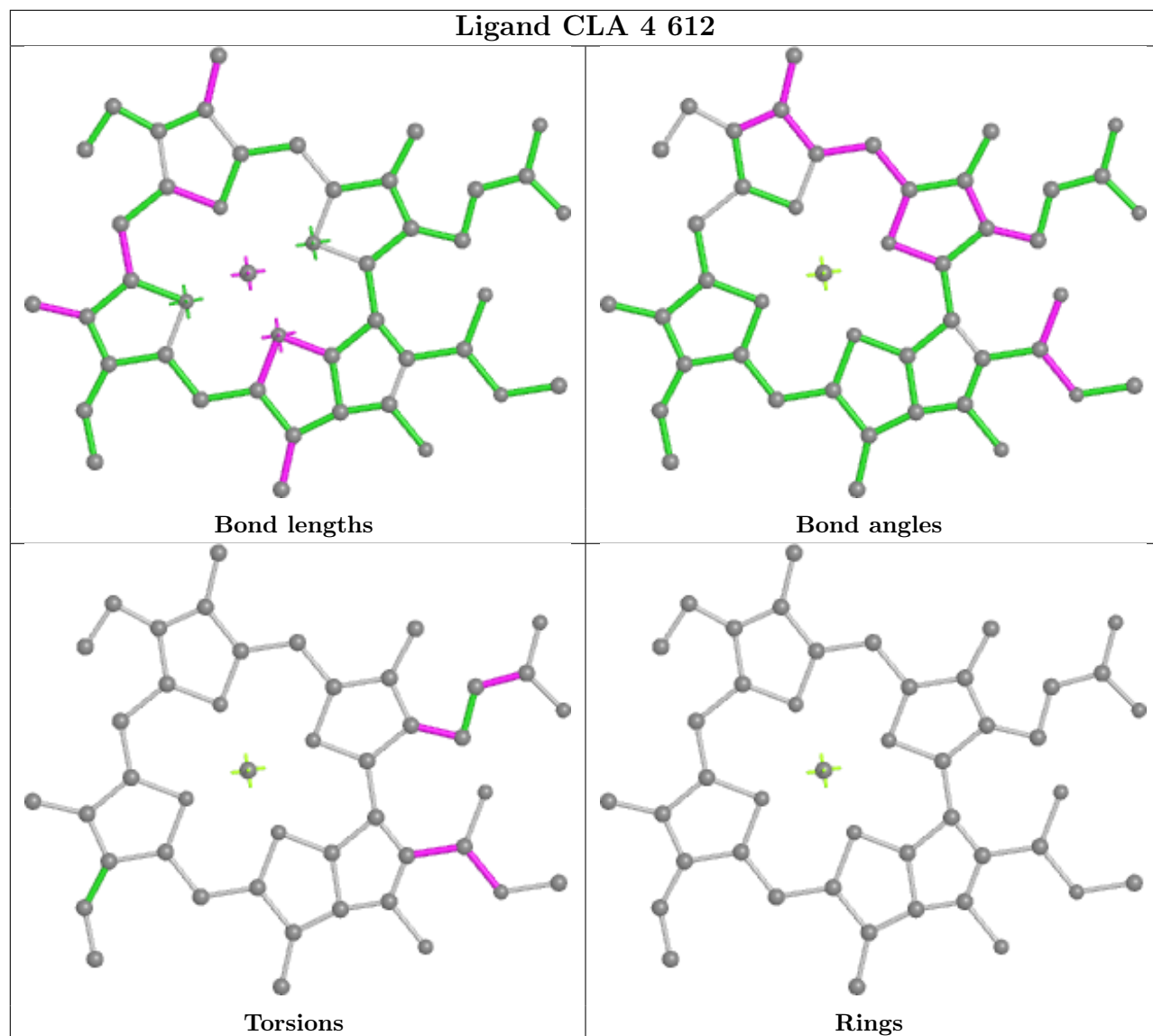


Rings

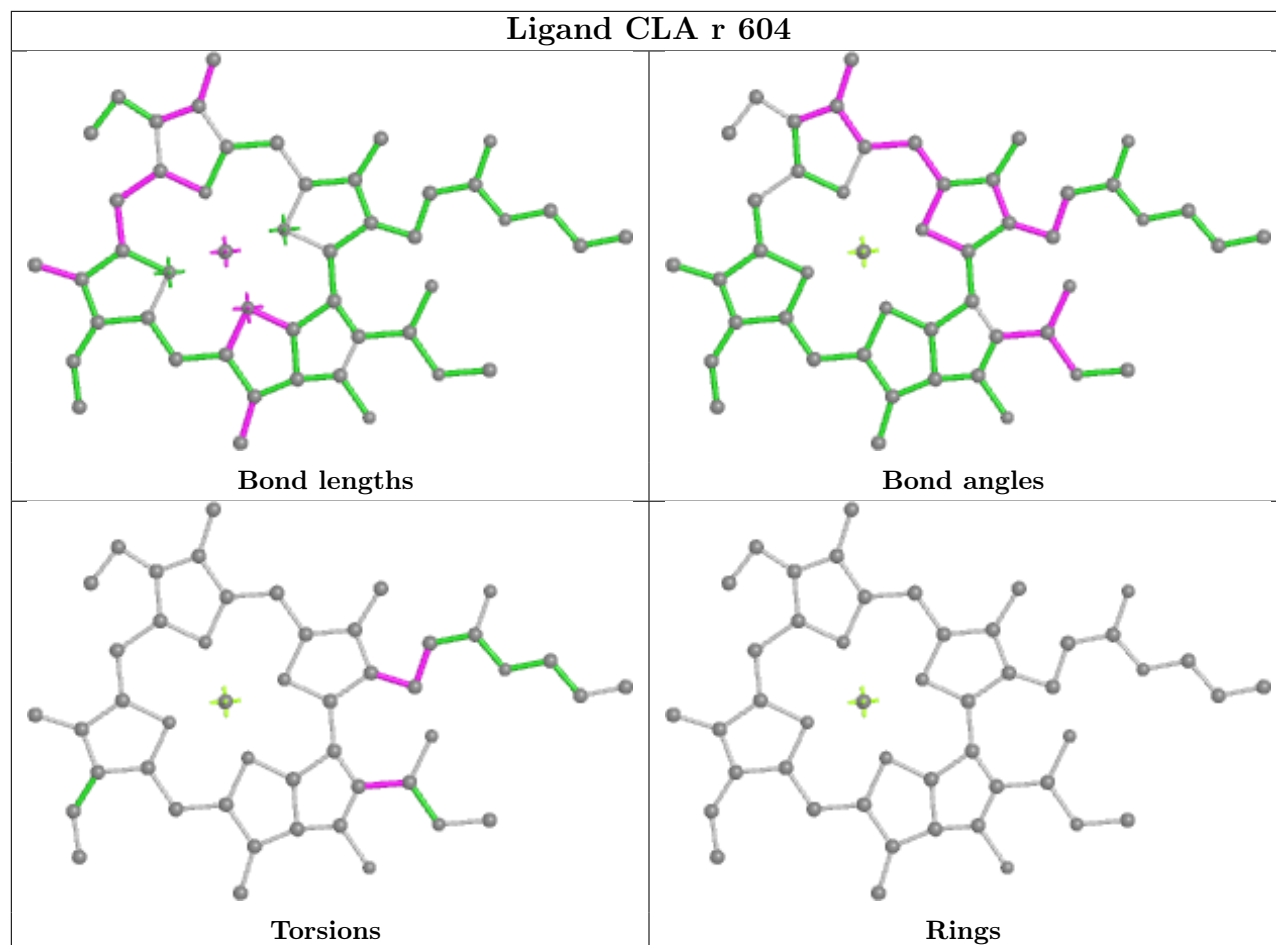
## Ligand CLA R 611



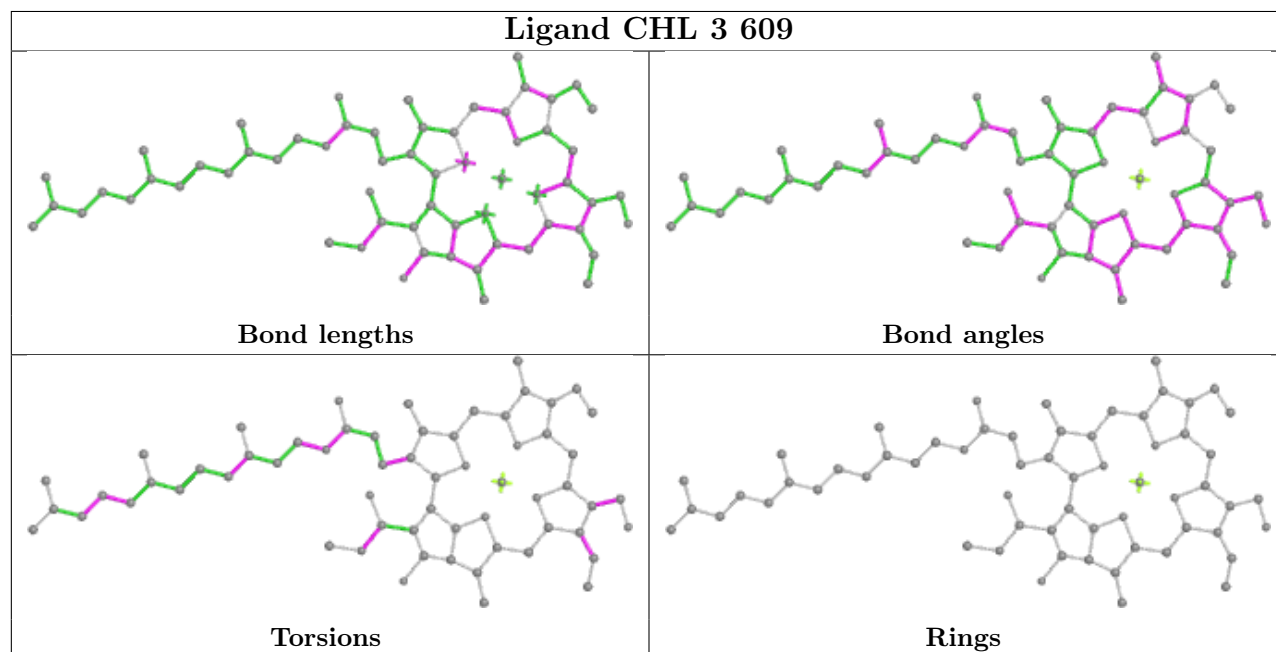
## Ligand CLA 4 612



## Ligand CLA r 604

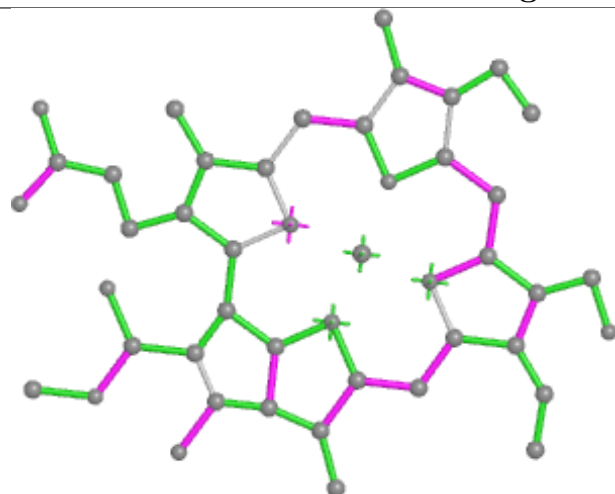


## Ligand CHL 3 609

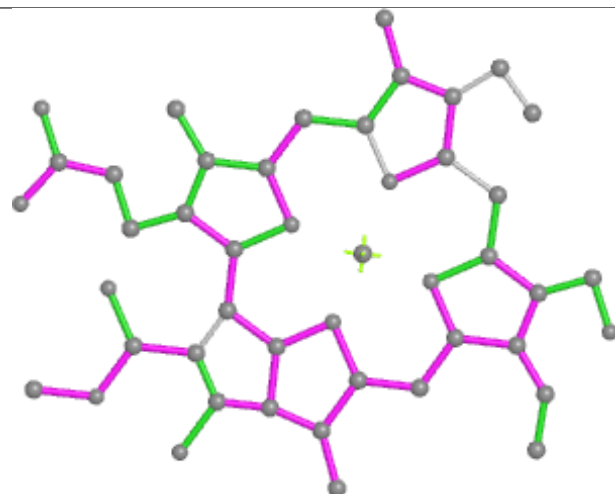




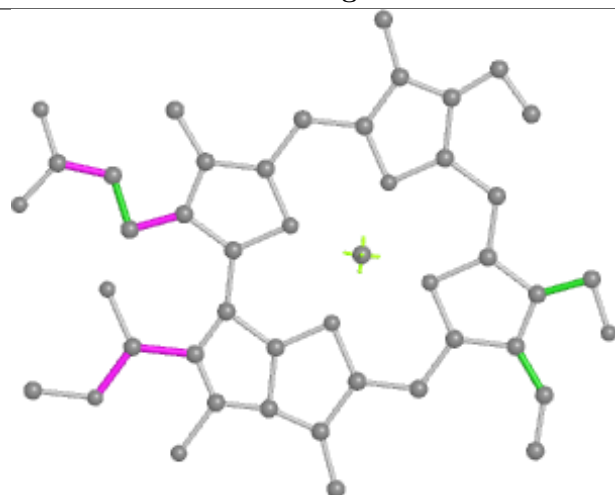
## Ligand CHL 2 601



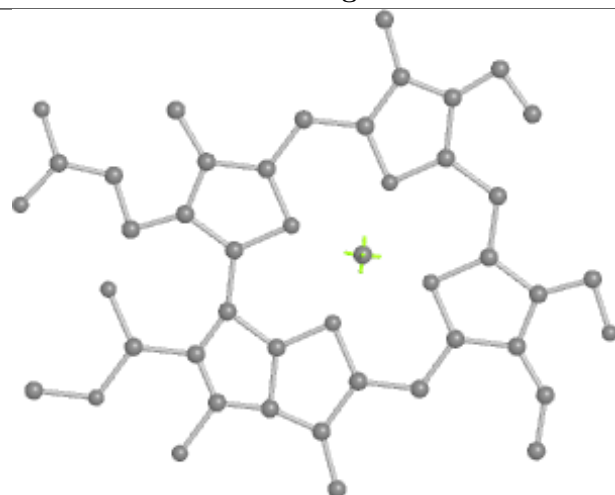
Bond lengths



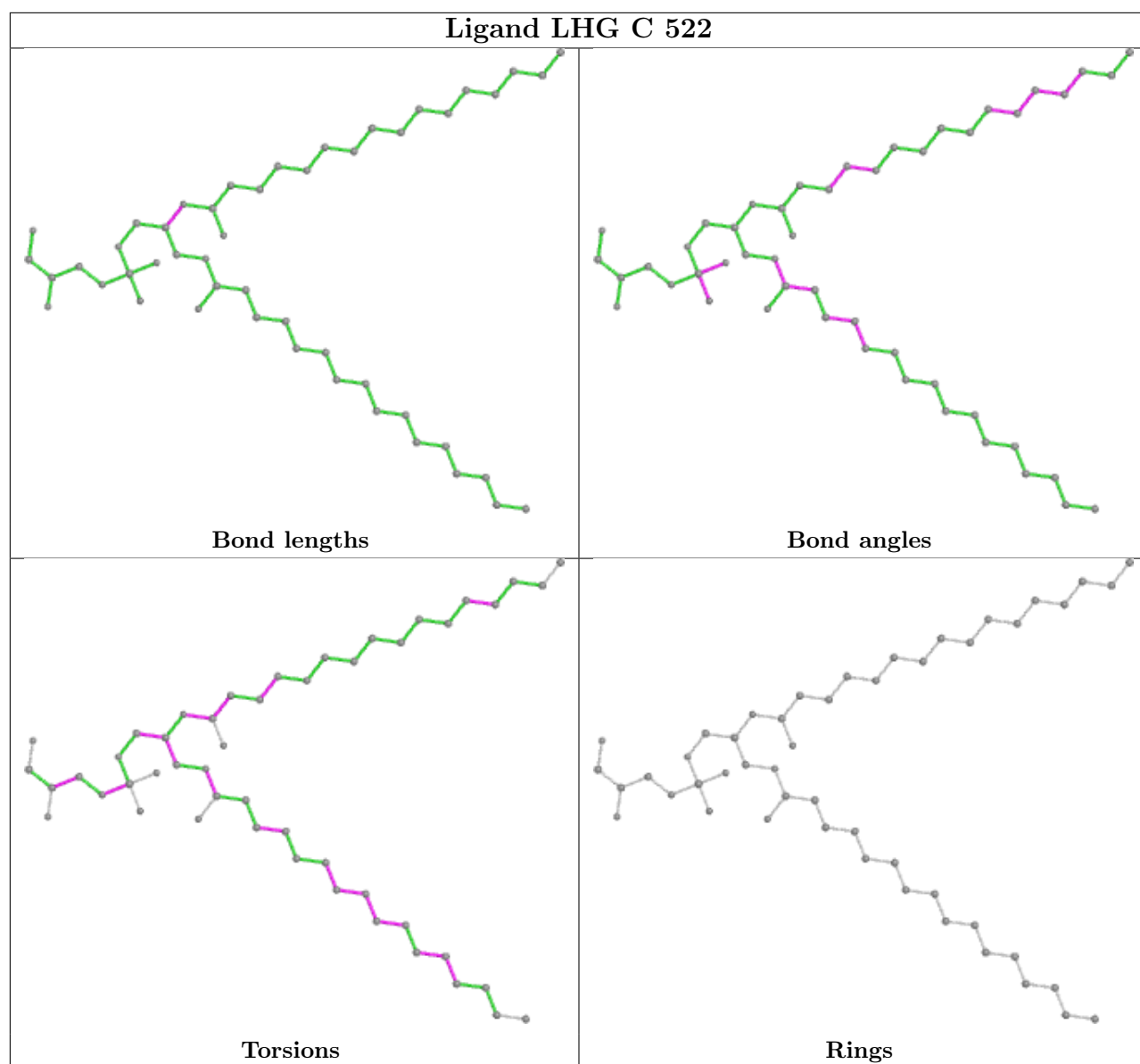
Bond angles

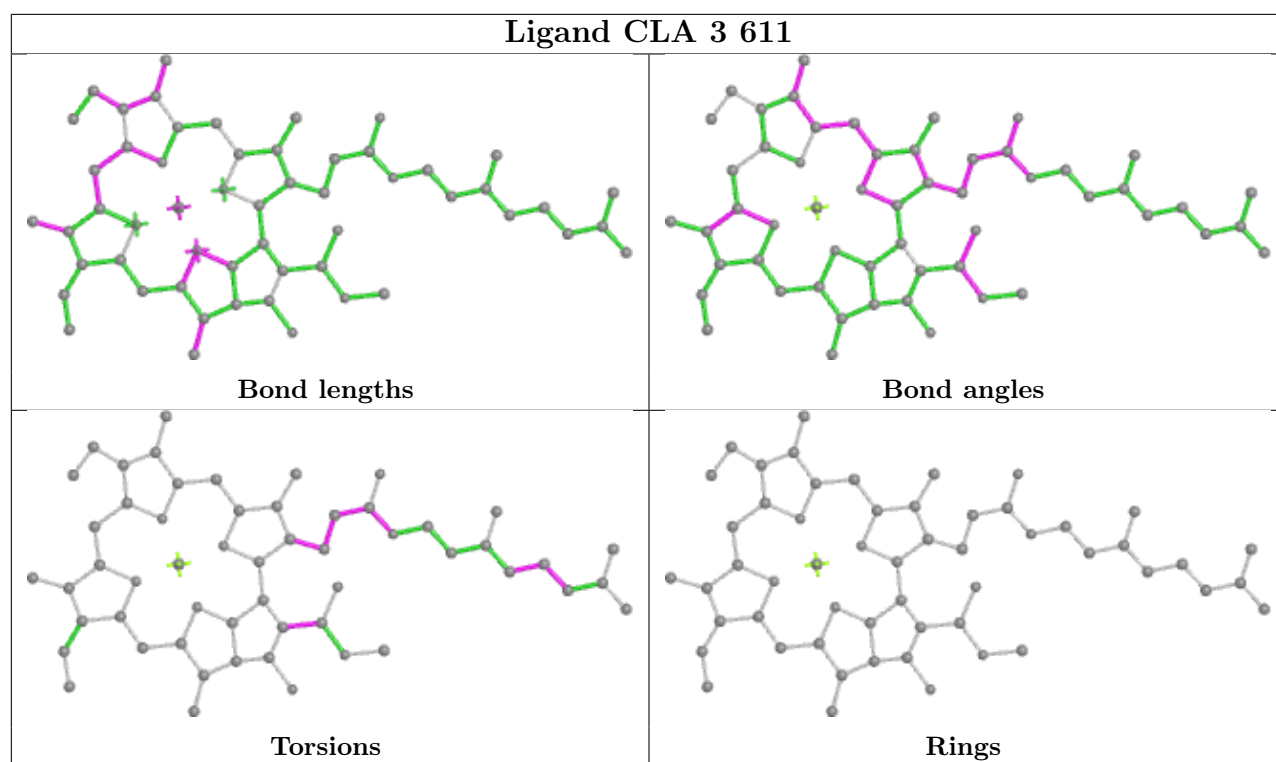


Torsions

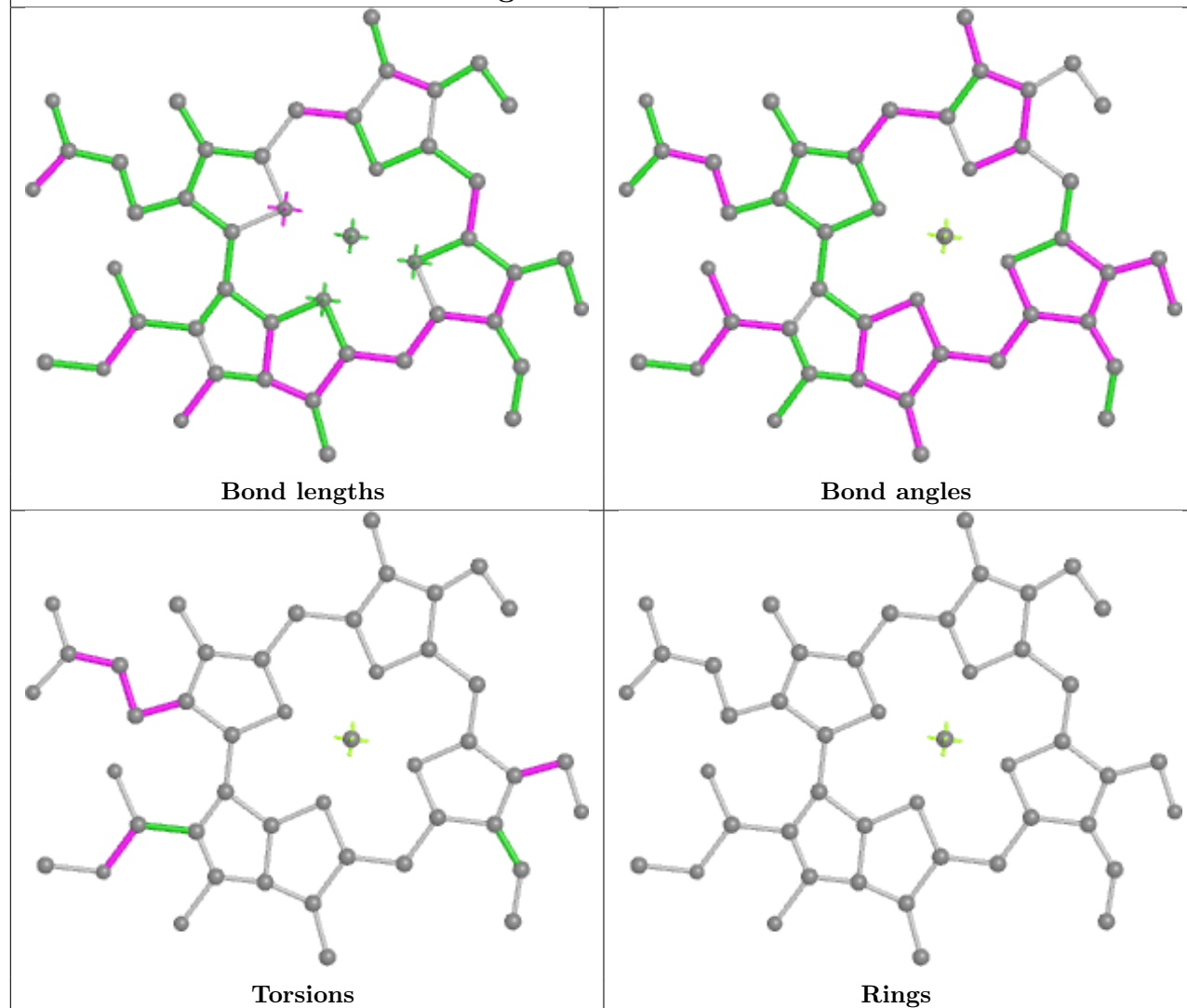


Rings

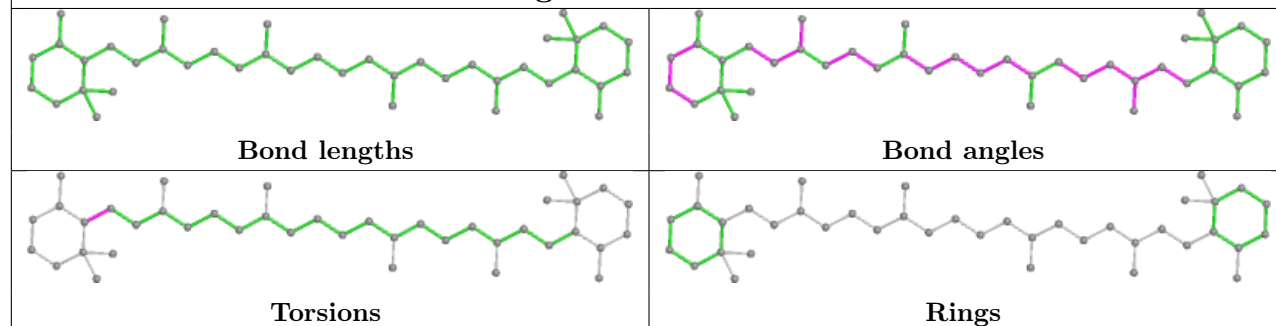




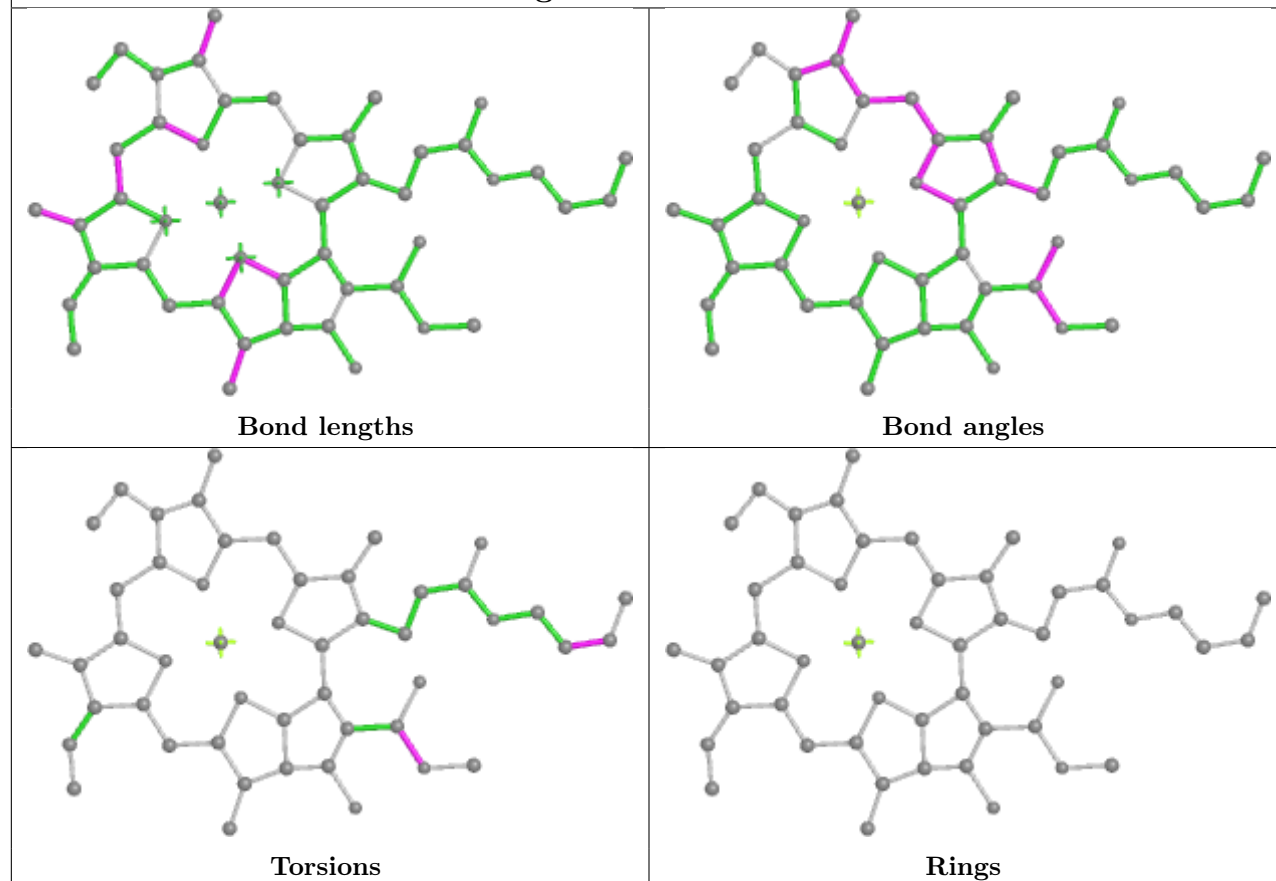
## Ligand CHL 4 607



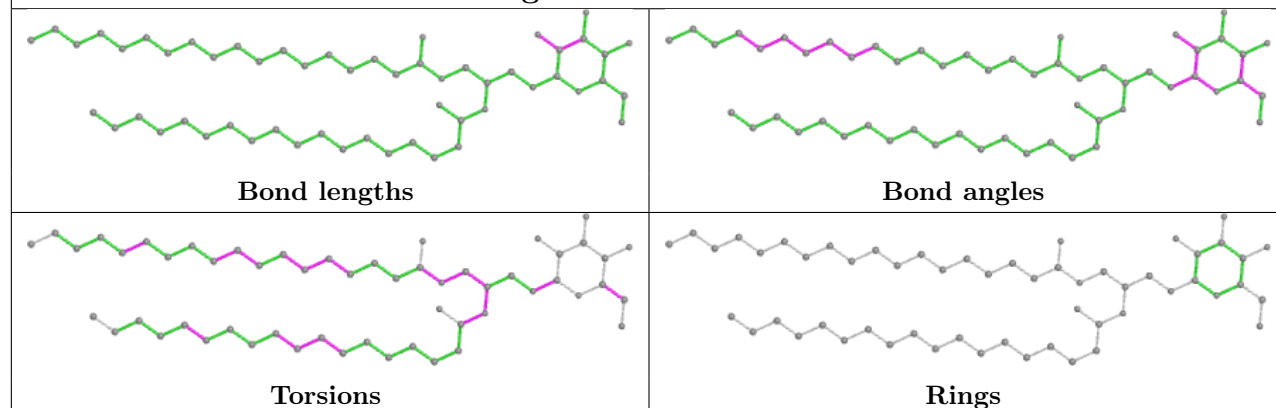
## Ligand BCR c 514



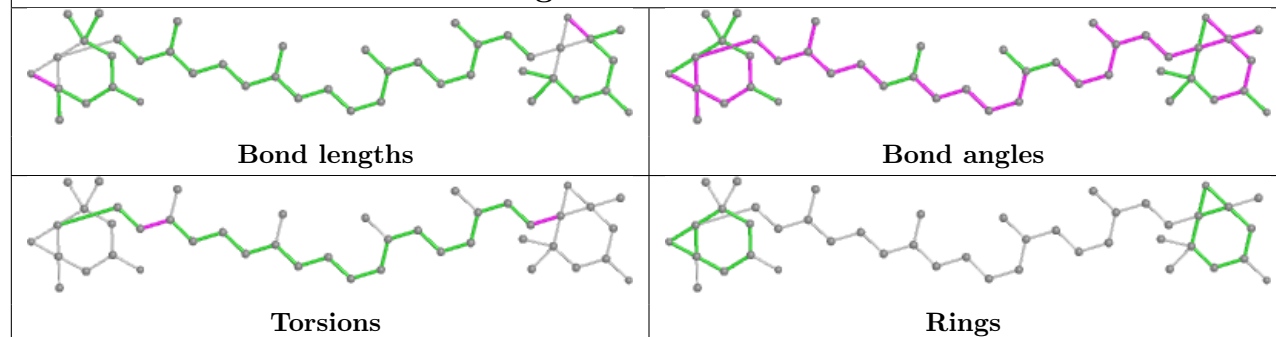
## Ligand CLA S 612



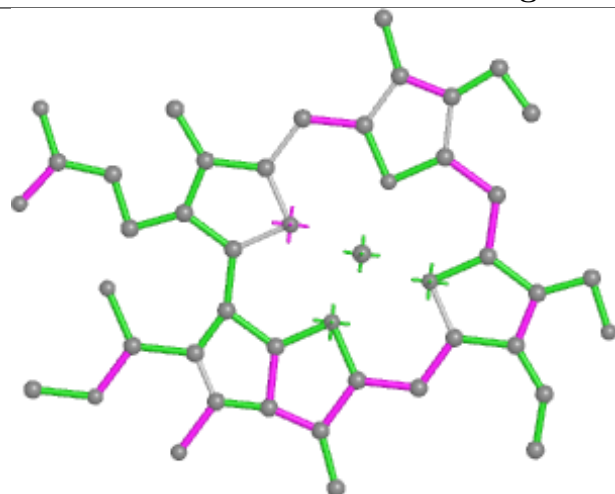
## Ligand LMG b 2633



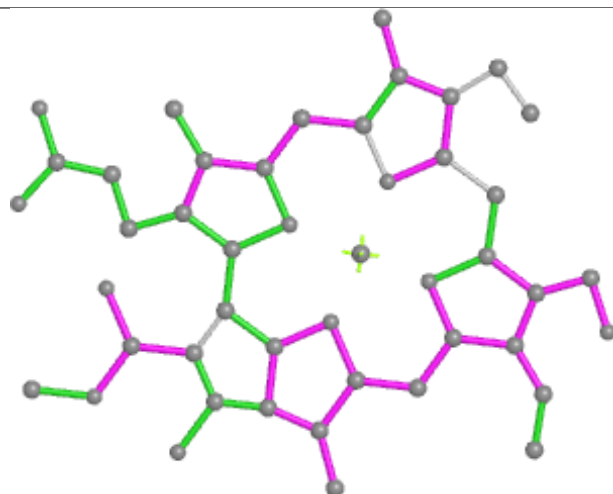
## Ligand XAT 8 622



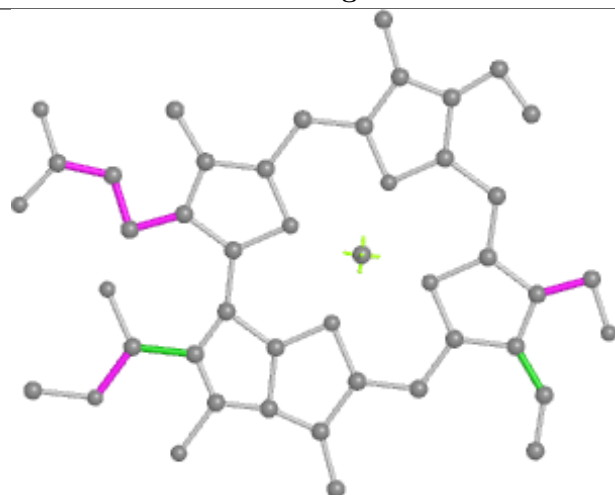
## Ligand CHL 2 605



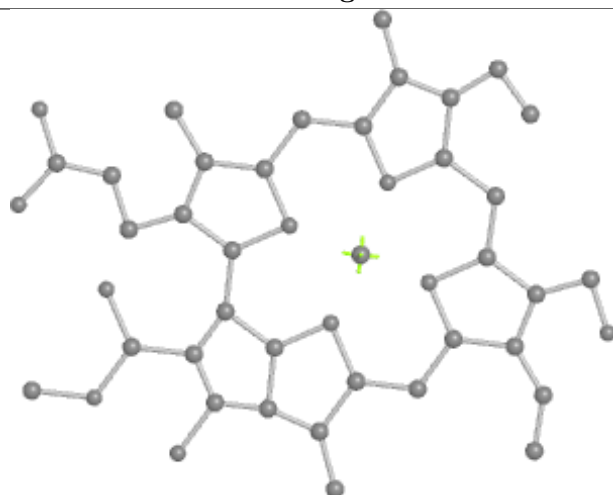
Bond lengths



Bond angles

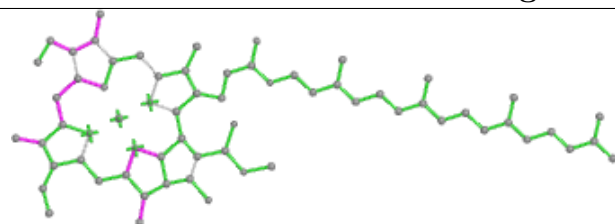


Torsions

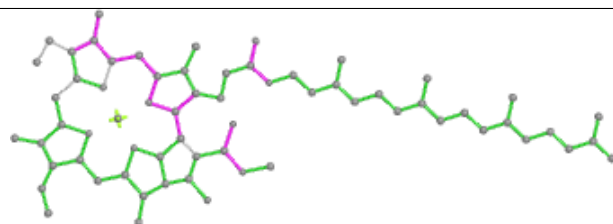


Rings

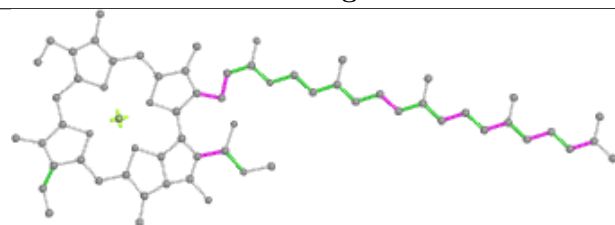
## Ligand CLA n 610



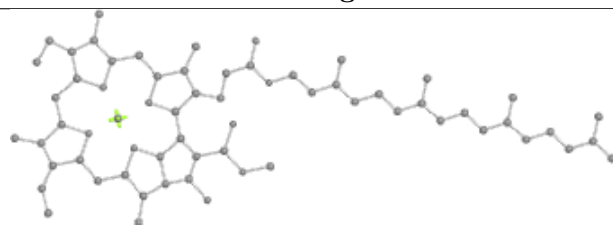
Bond lengths



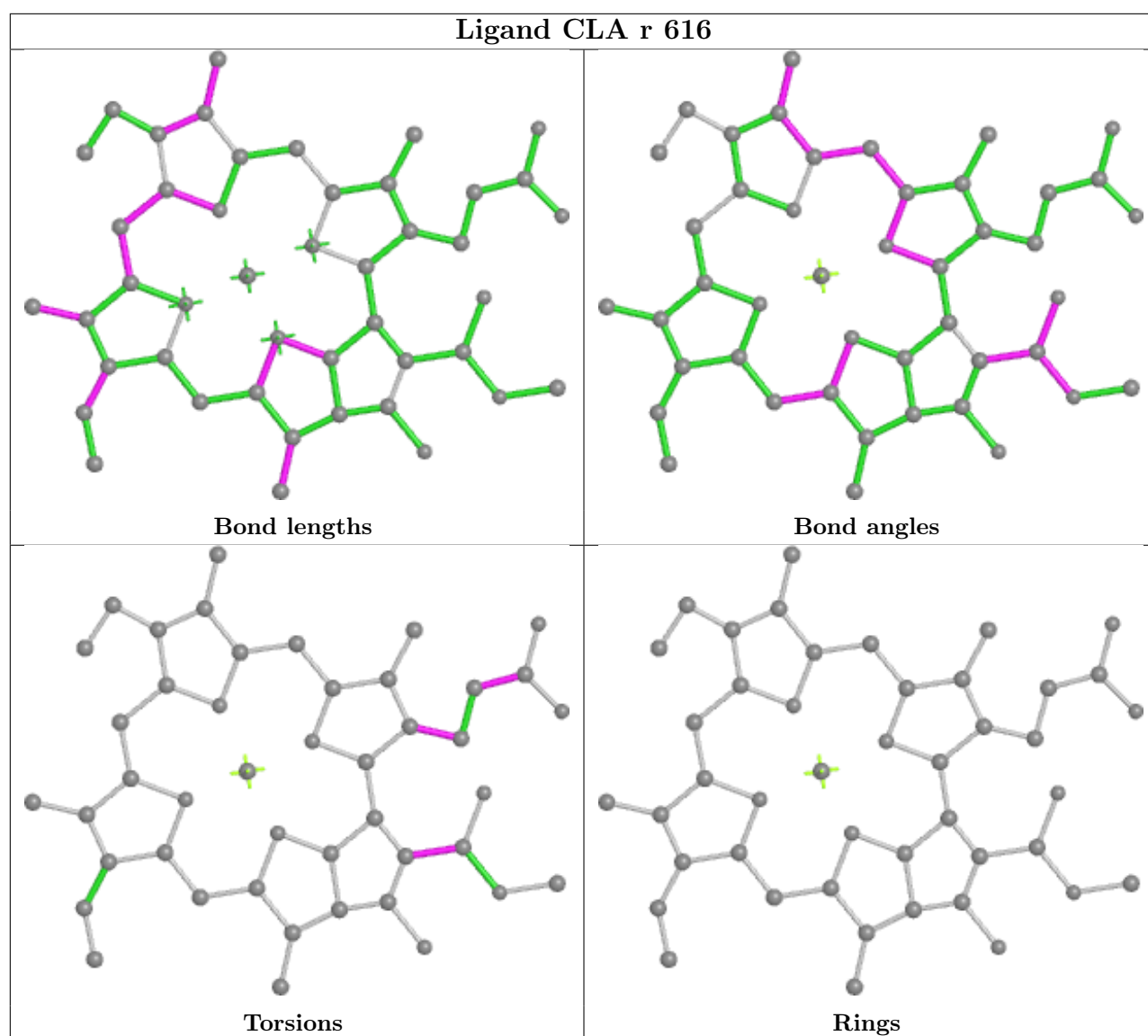
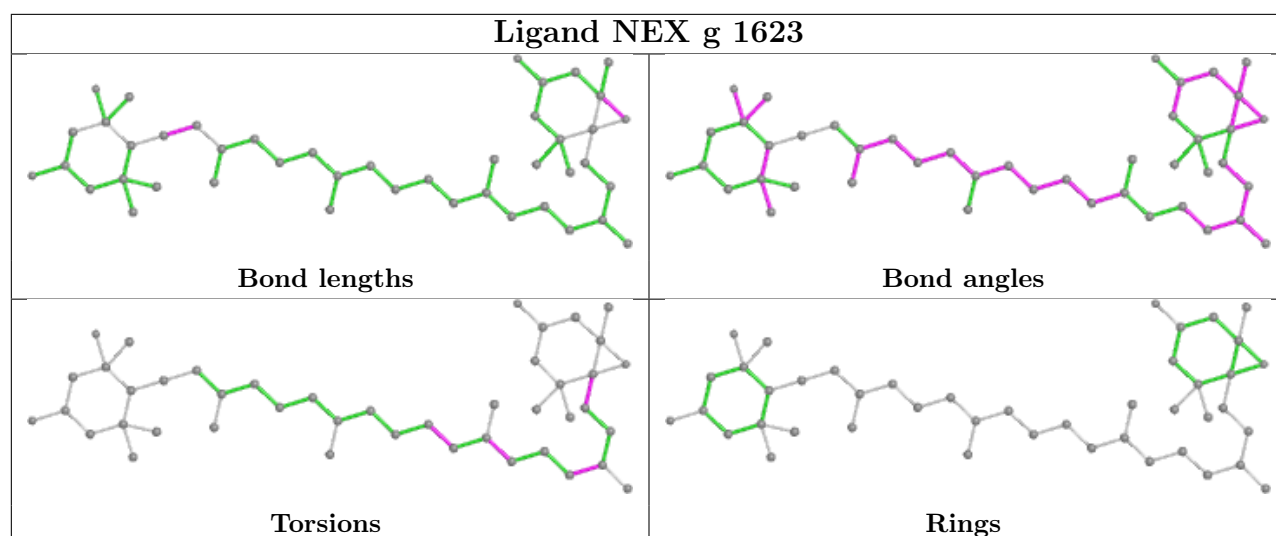
Bond angles

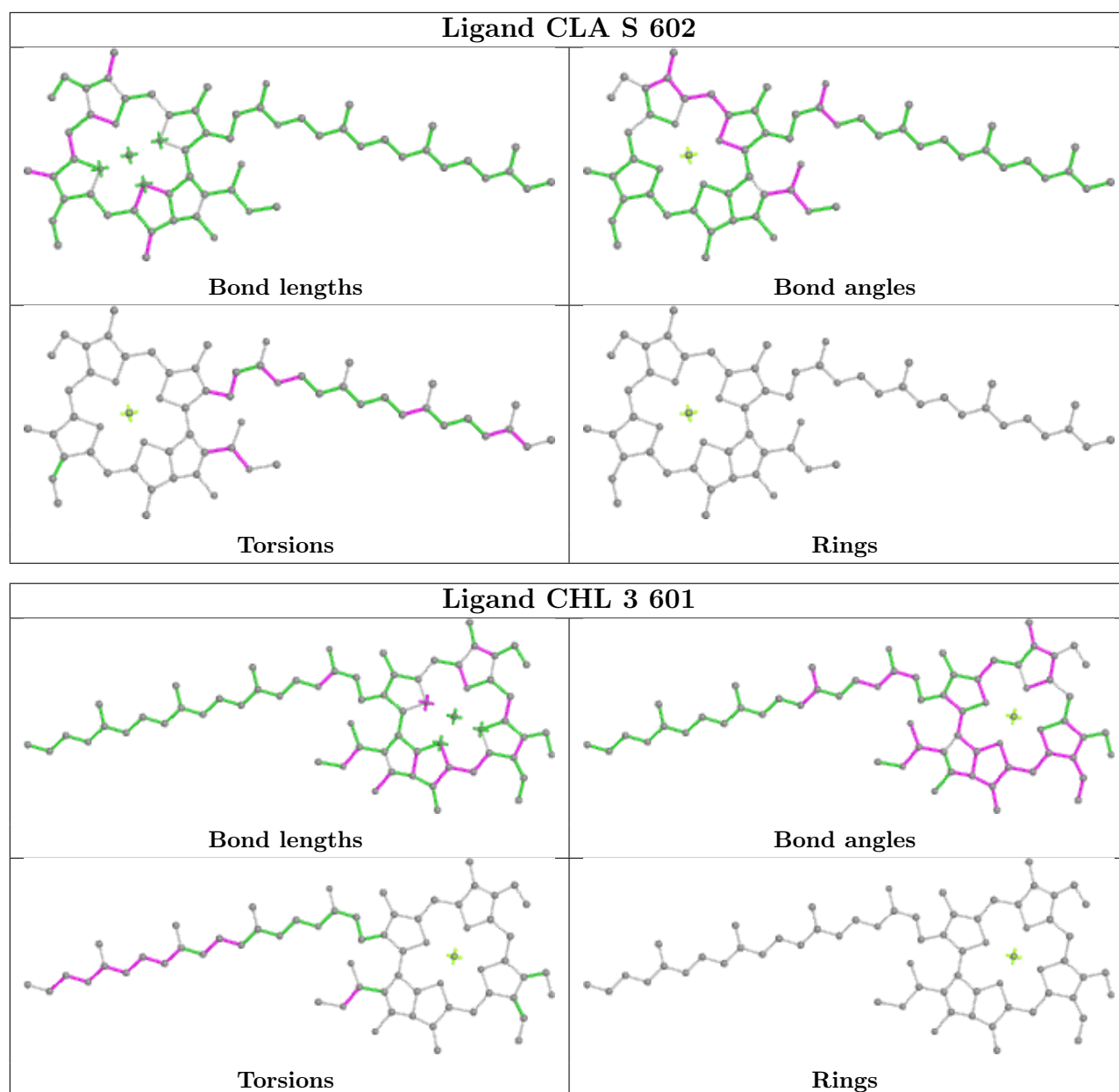


Torsions



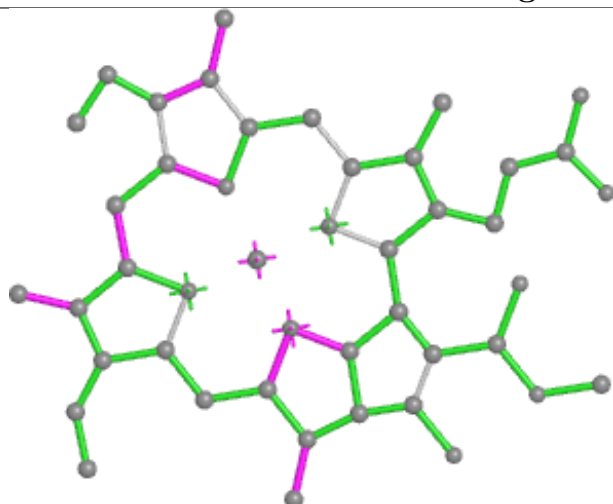
Rings



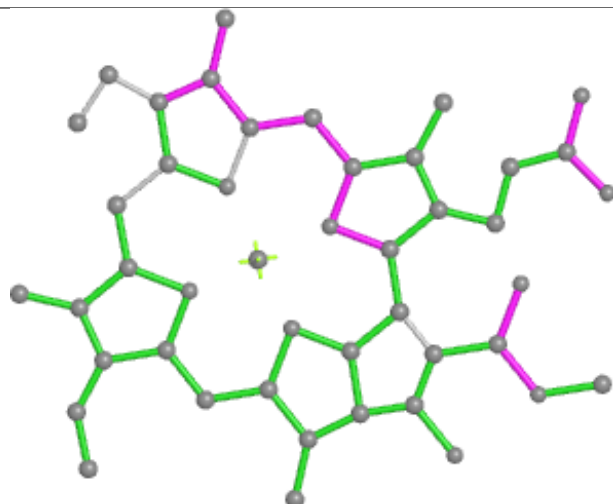




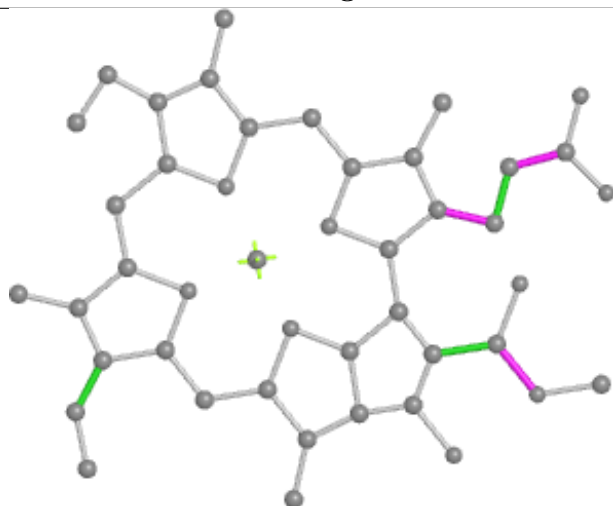
## Ligand CLA 6 614



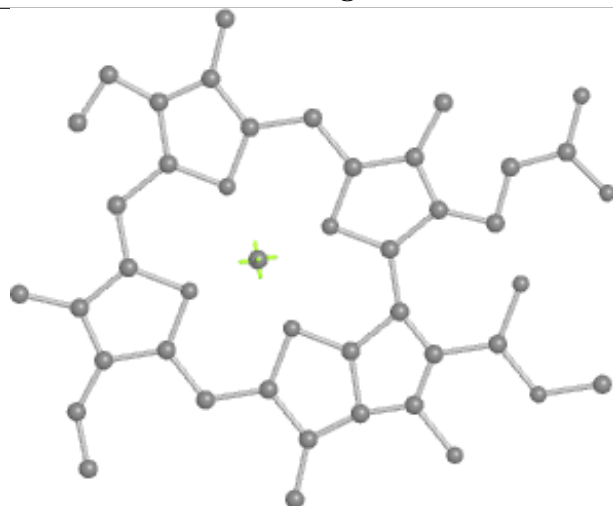
Bond lengths



Bond angles

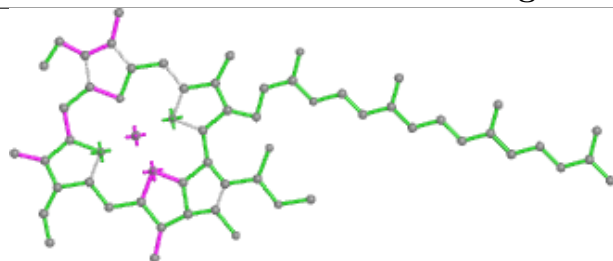


Torsions

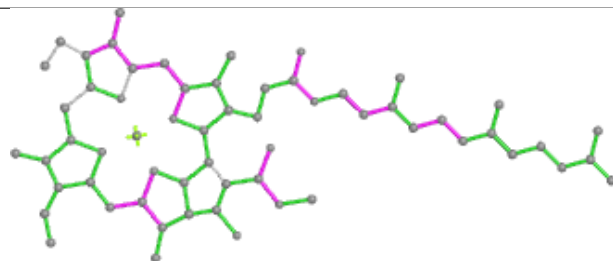


Rings

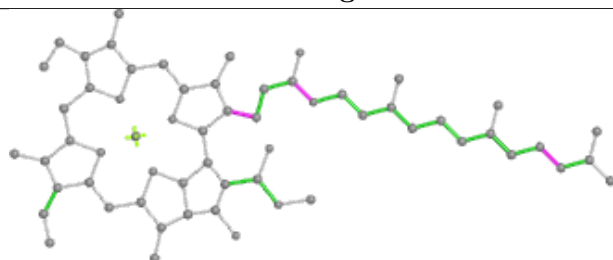
## Ligand CLA 7 610



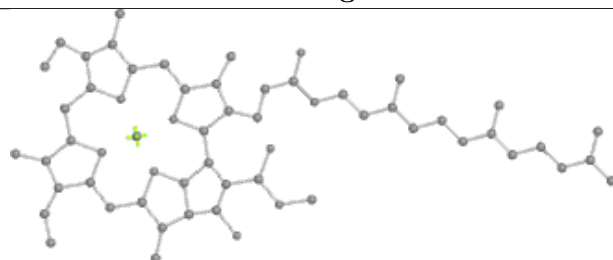
Bond lengths



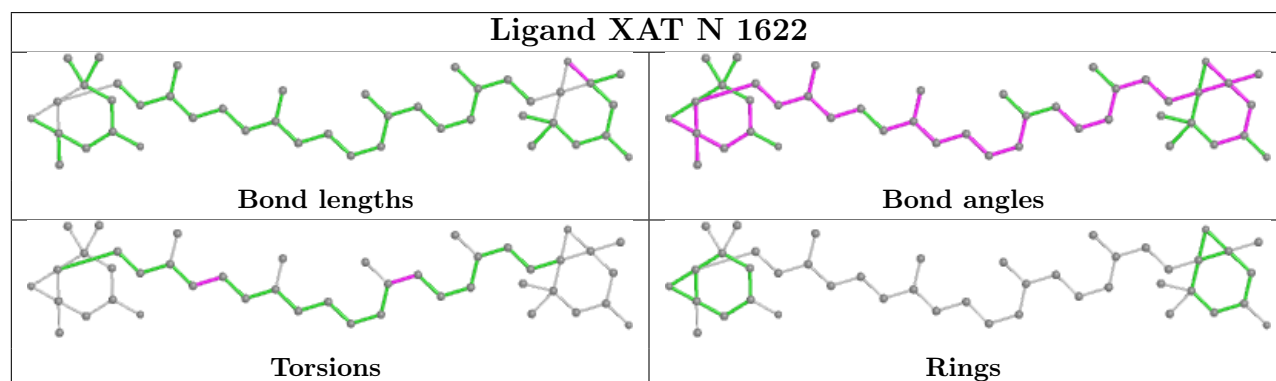
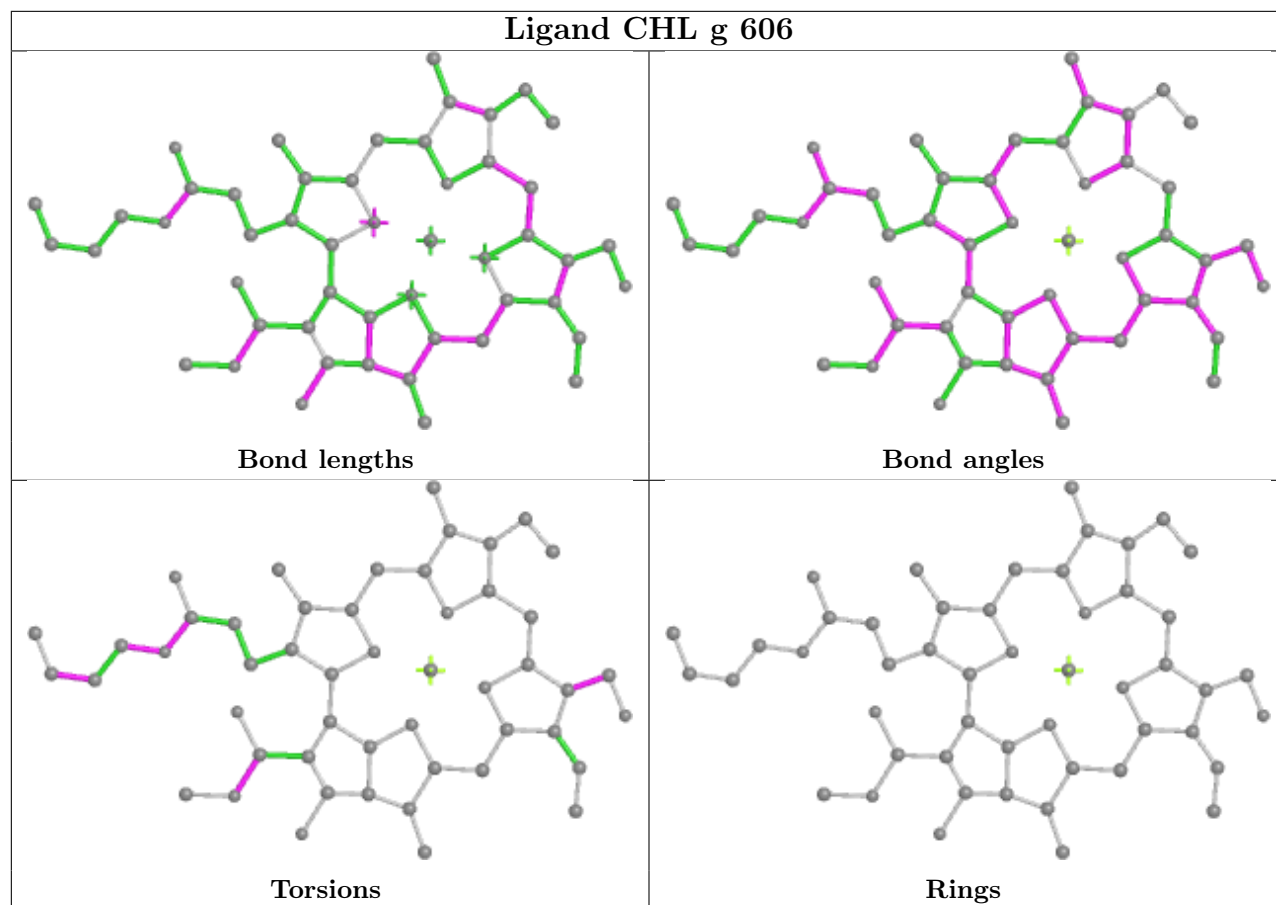
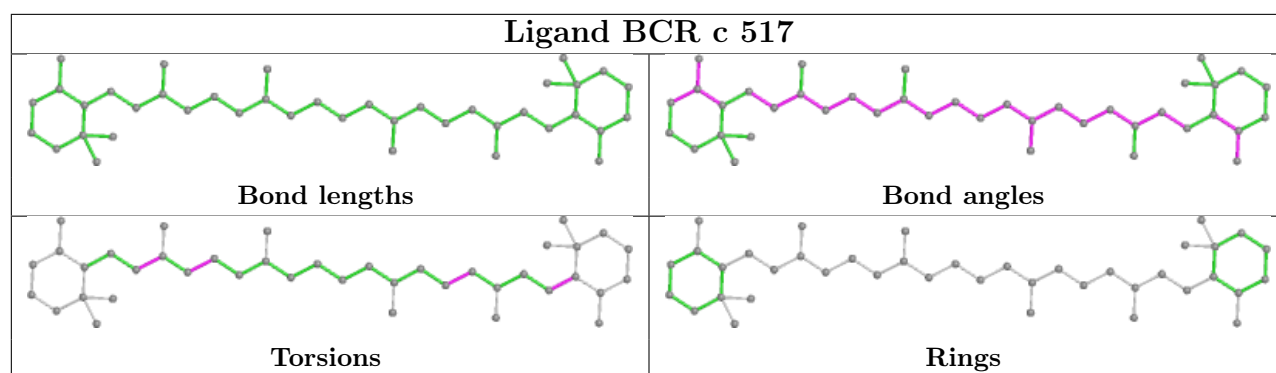
Bond angles



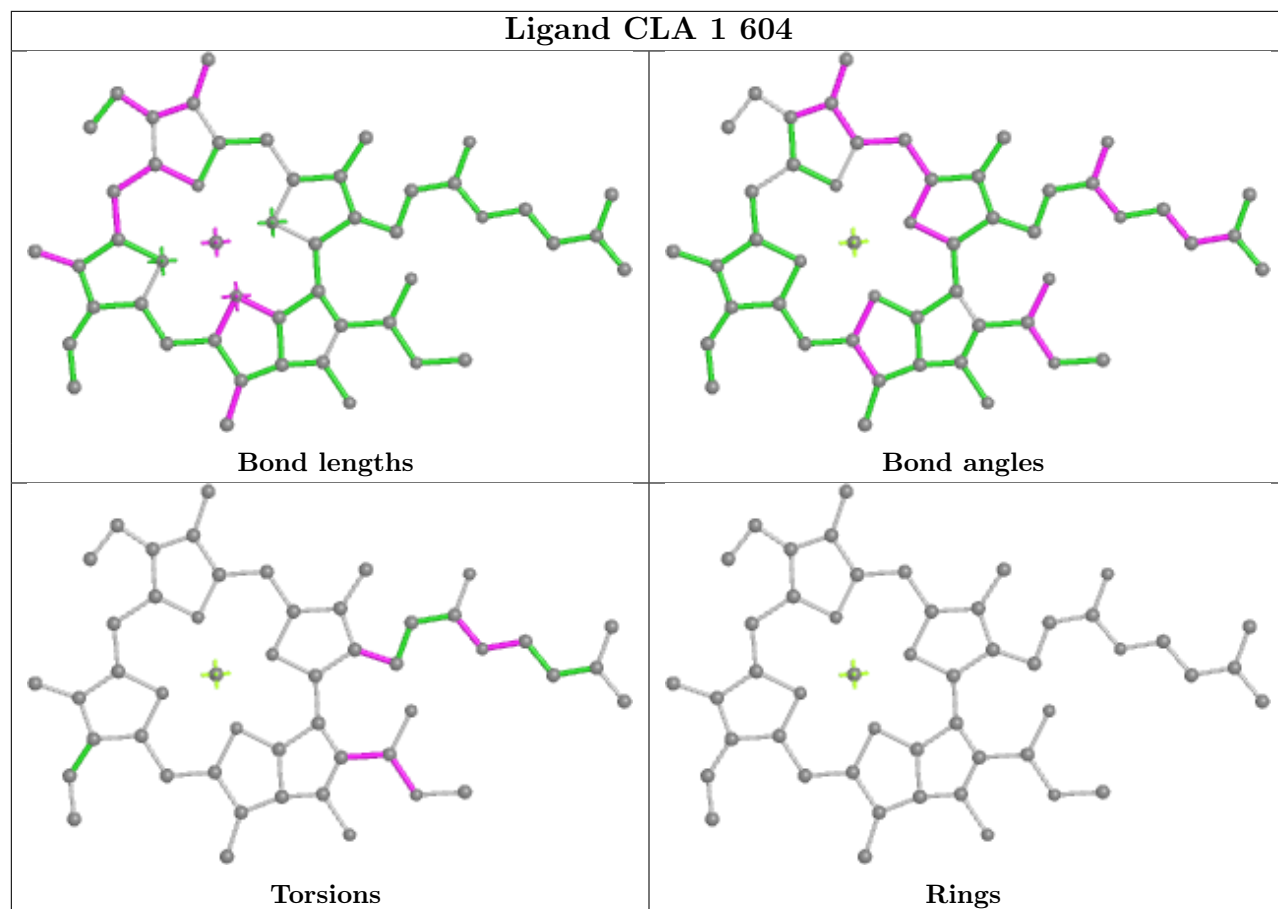
Torsions



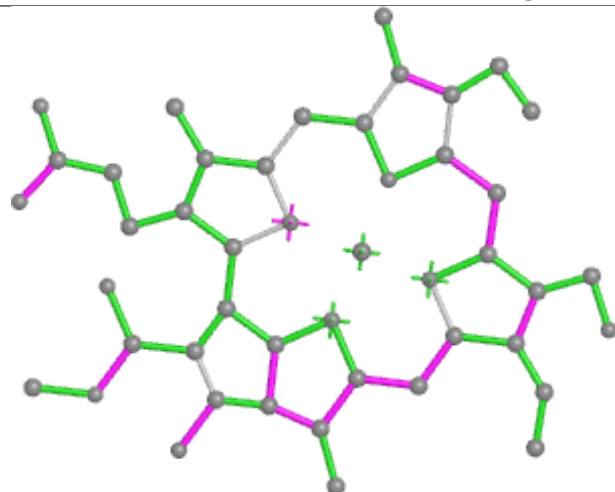
Rings



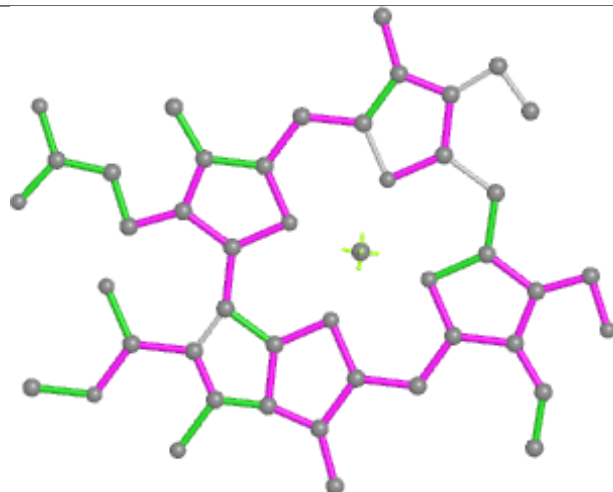
## Ligand CLA 1 604



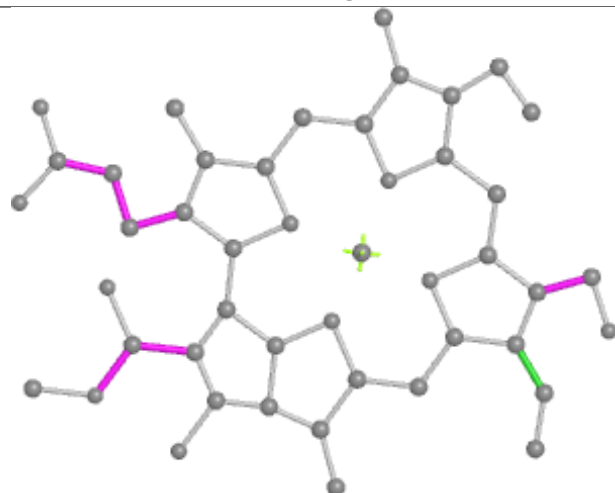
## Ligand CHL 3 605



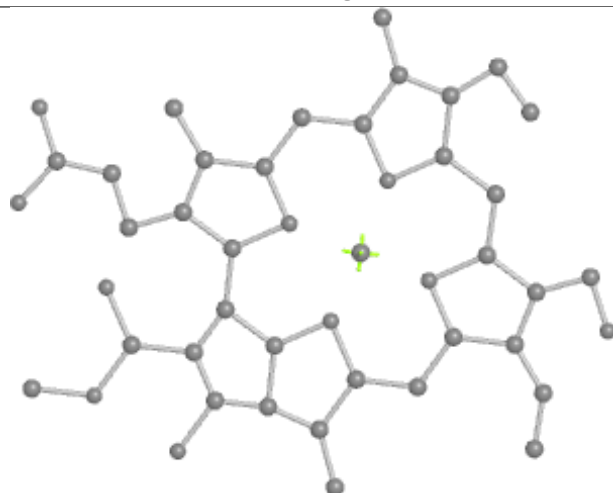
Bond lengths



Bond angles

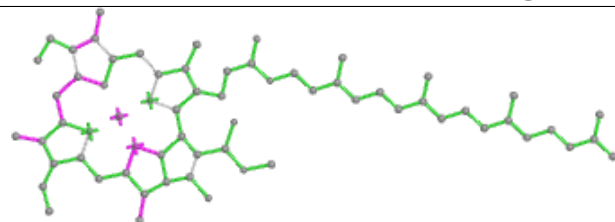


Torsions

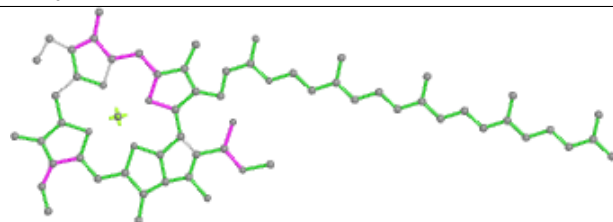


Rings

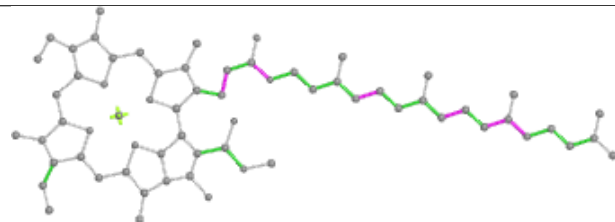
## Ligand CLA y 613



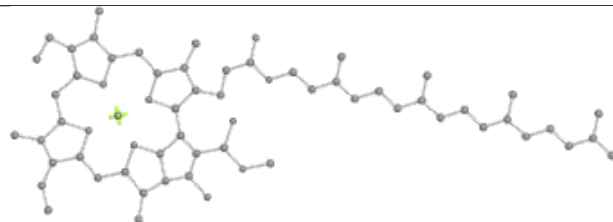
Bond lengths



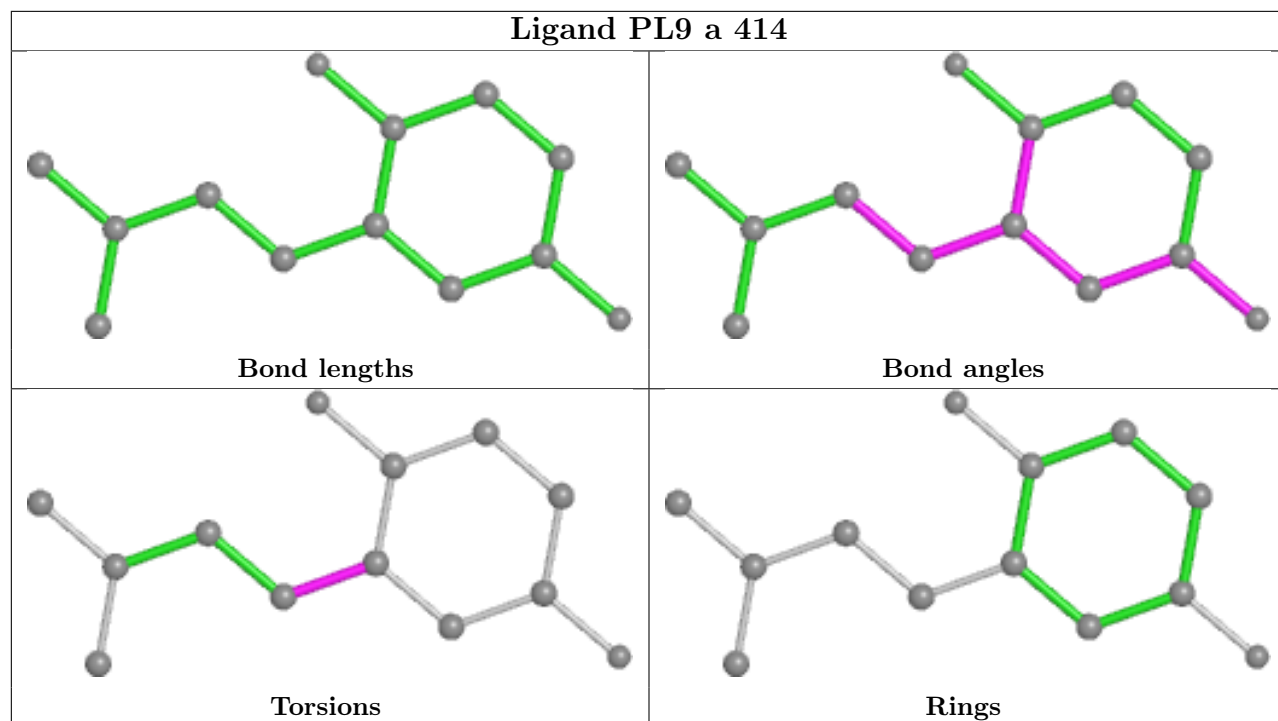
Bond angles



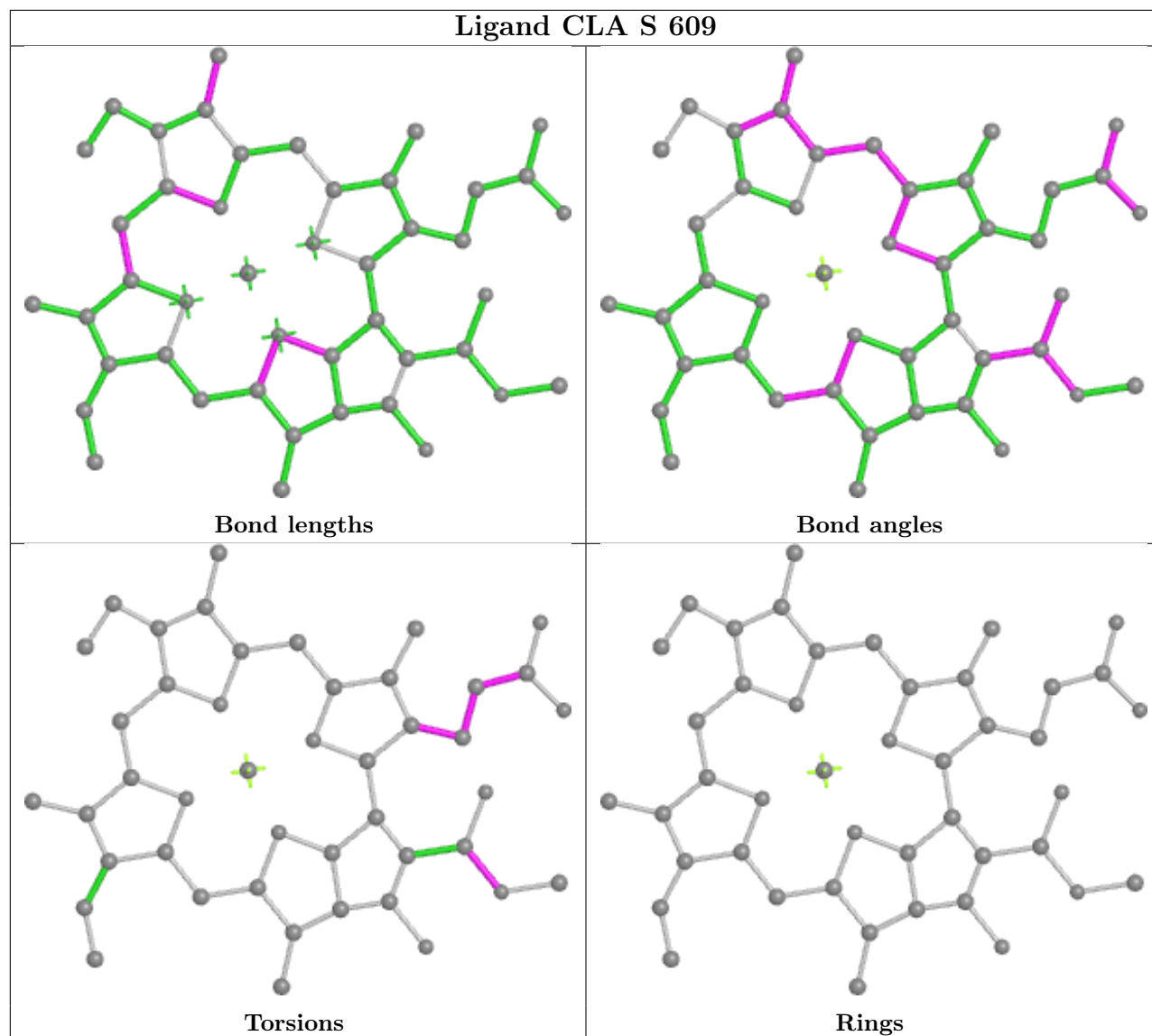
Torsions

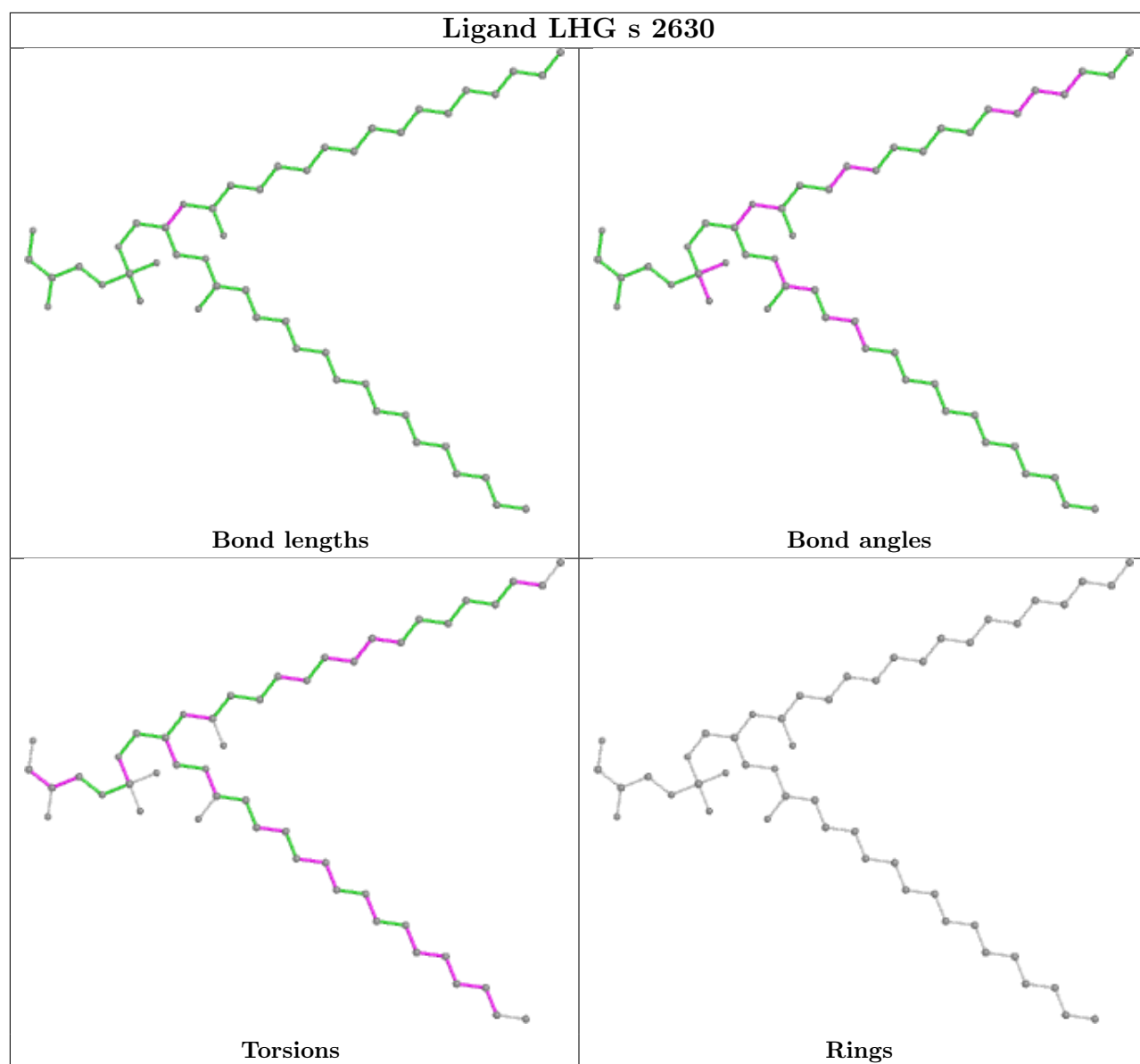


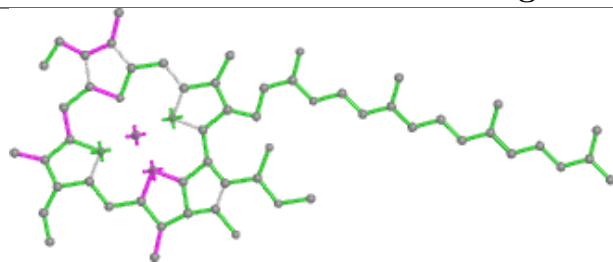
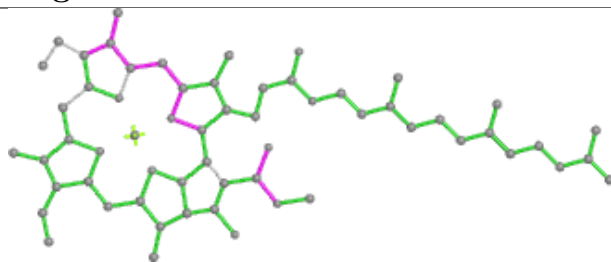
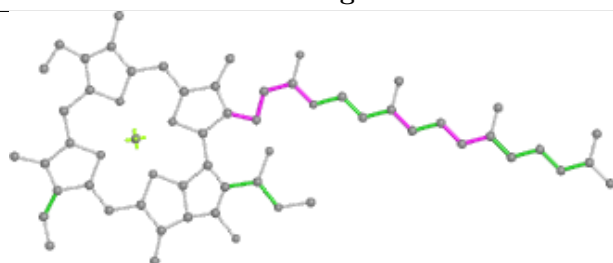
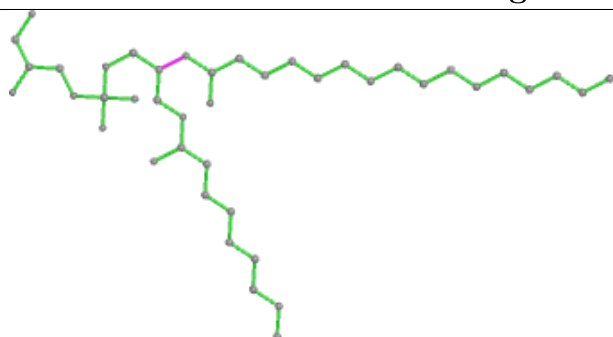
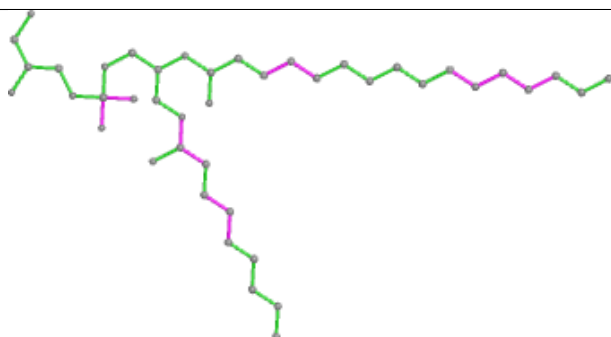
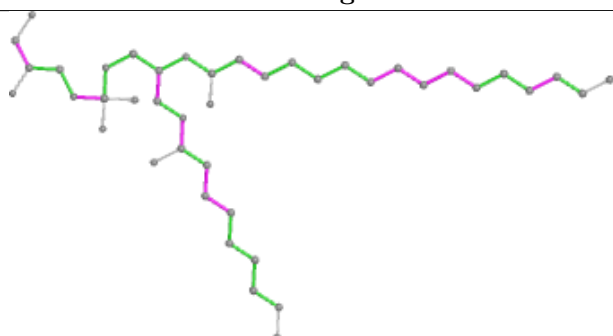
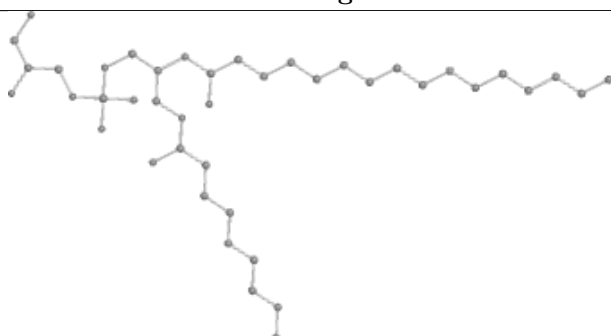
Rings



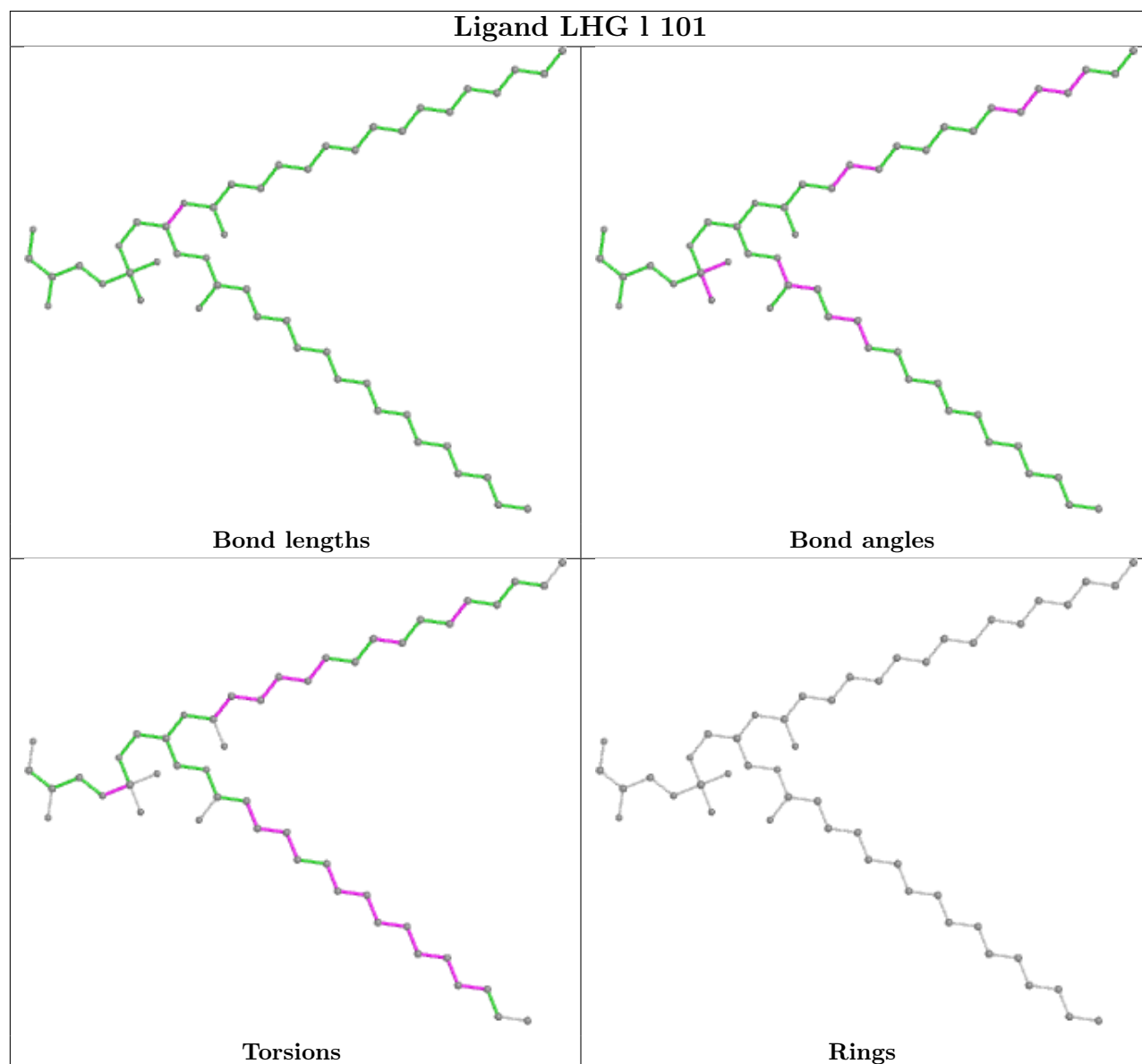
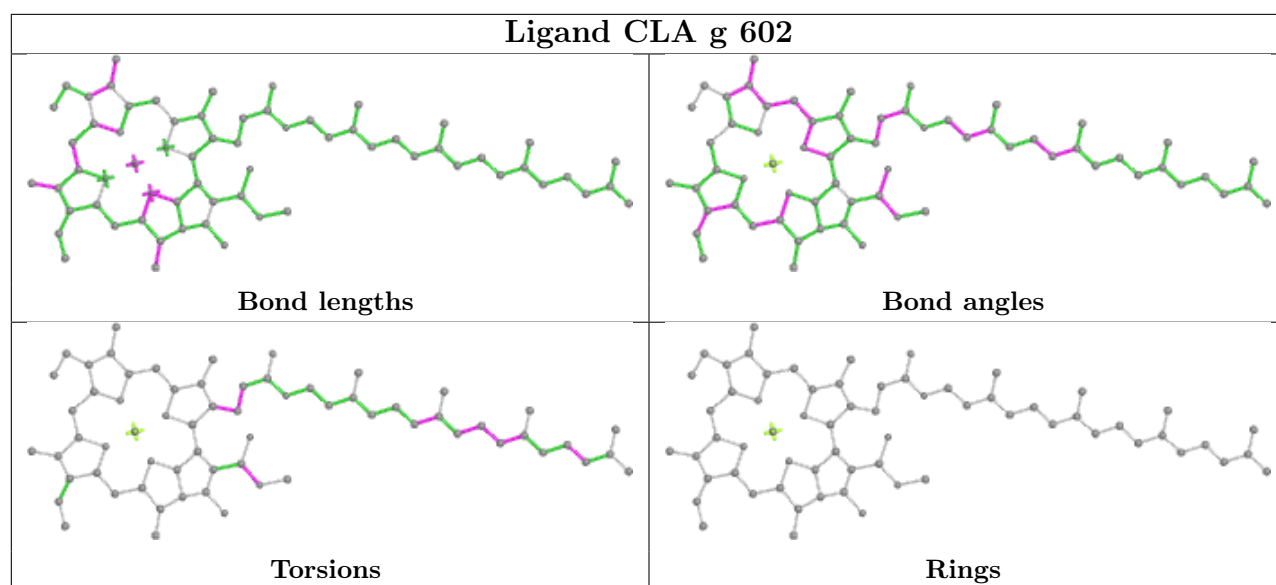
## Ligand CLA S 609

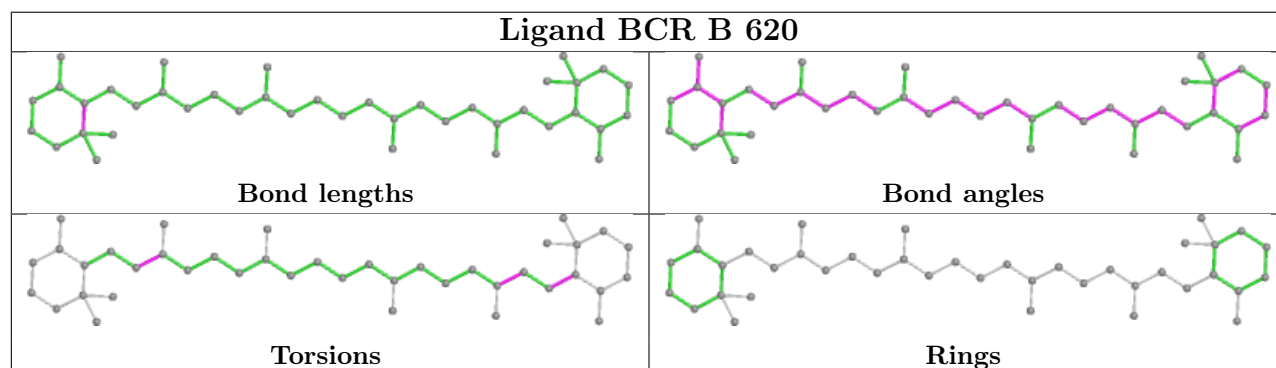
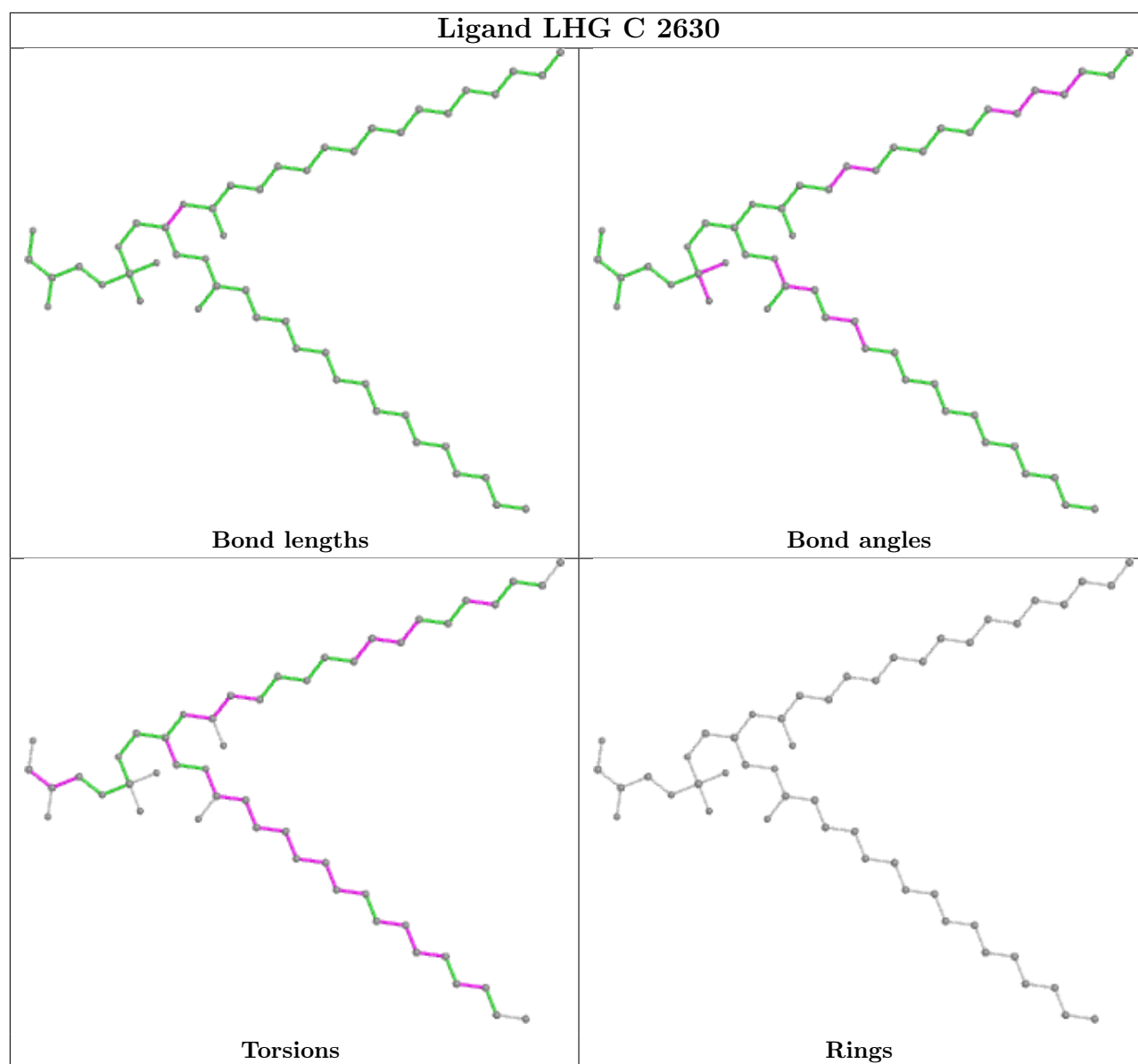




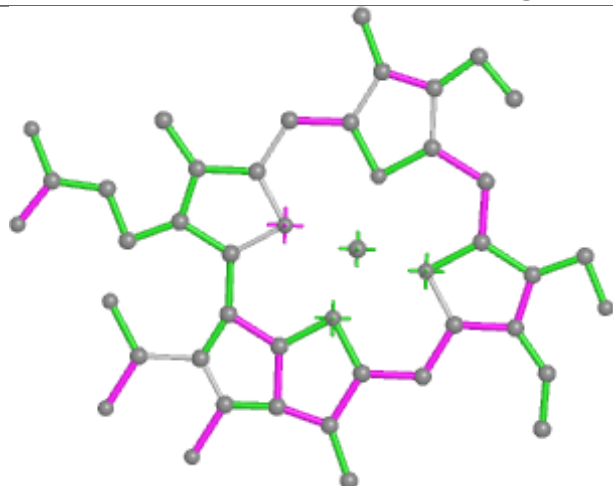
**Ligand CLA g 611****Bond lengths****Bond angles****Torsions****Rings****Ligand LHG r 2630****Bond lengths****Bond angles****Torsions****Rings**



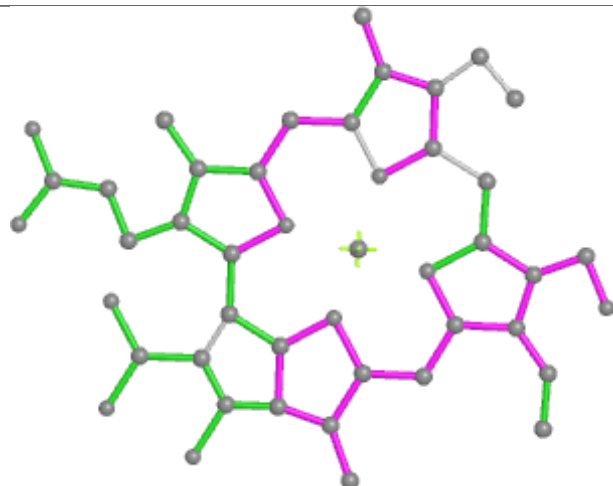




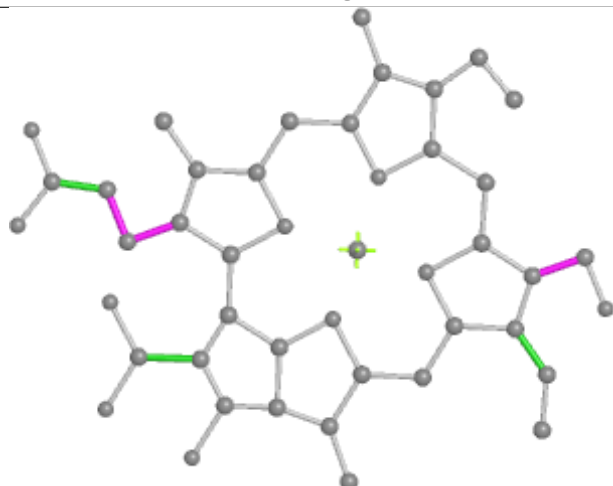
## Ligand CHL 4 601



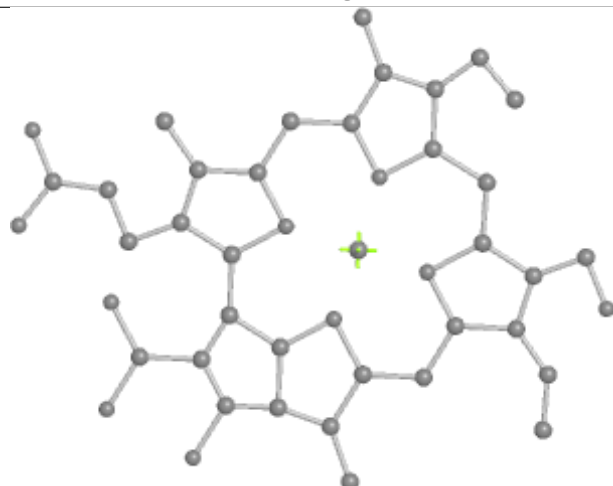
Bond lengths



Bond angles

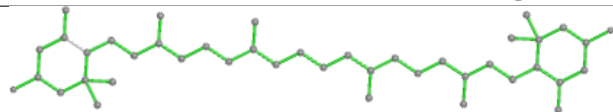


Torsions

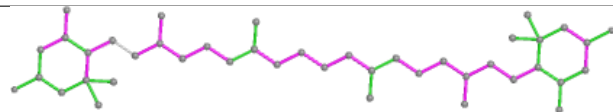


Rings

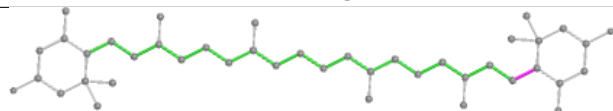
## Ligand LUT 2 1620



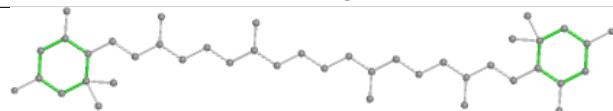
Bond lengths



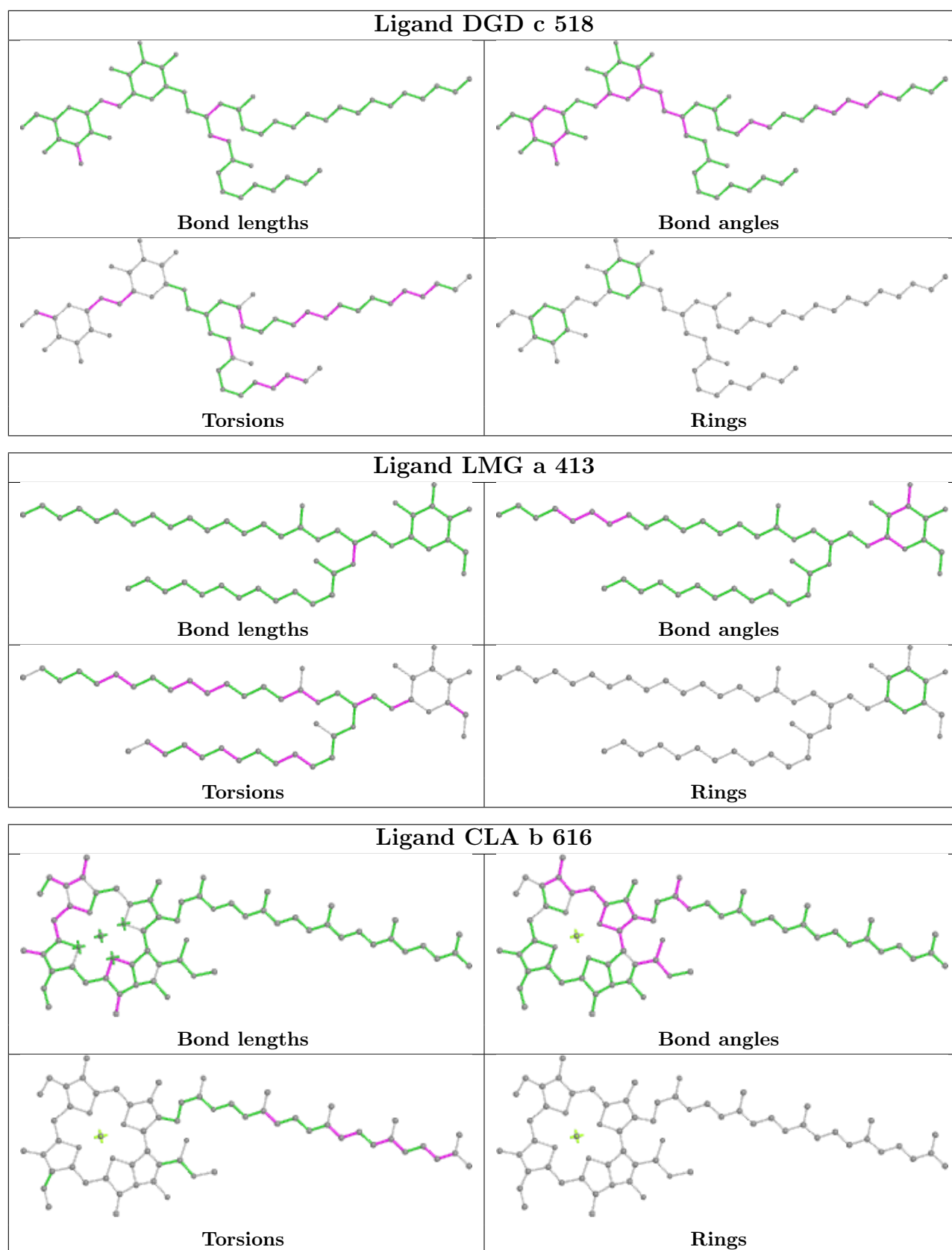
Bond angles



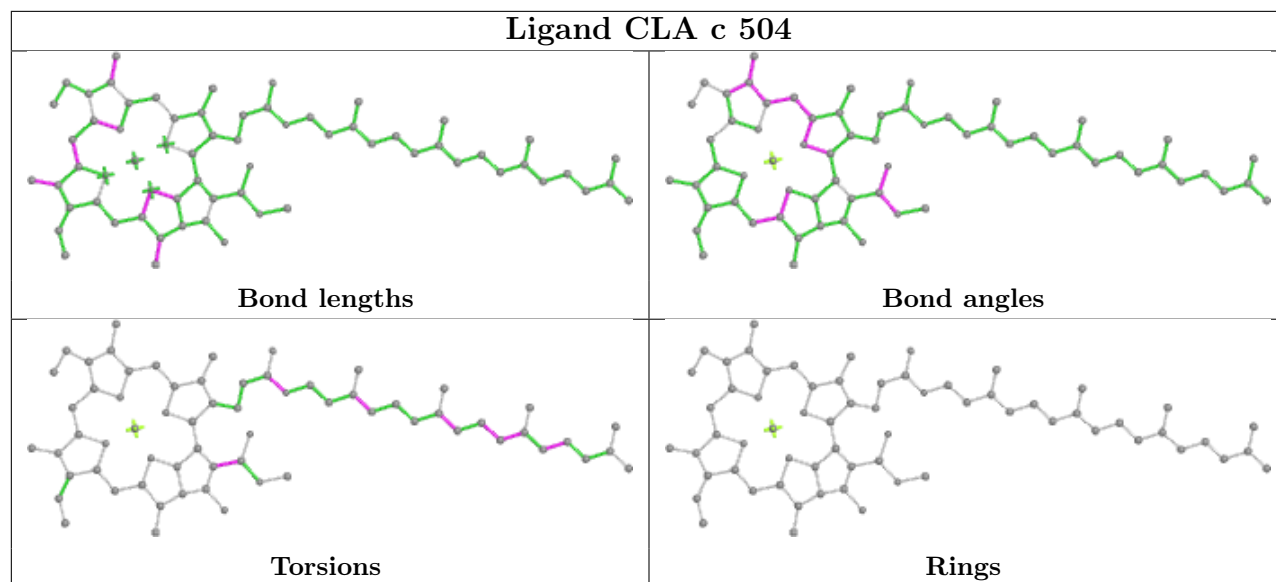
Torsions



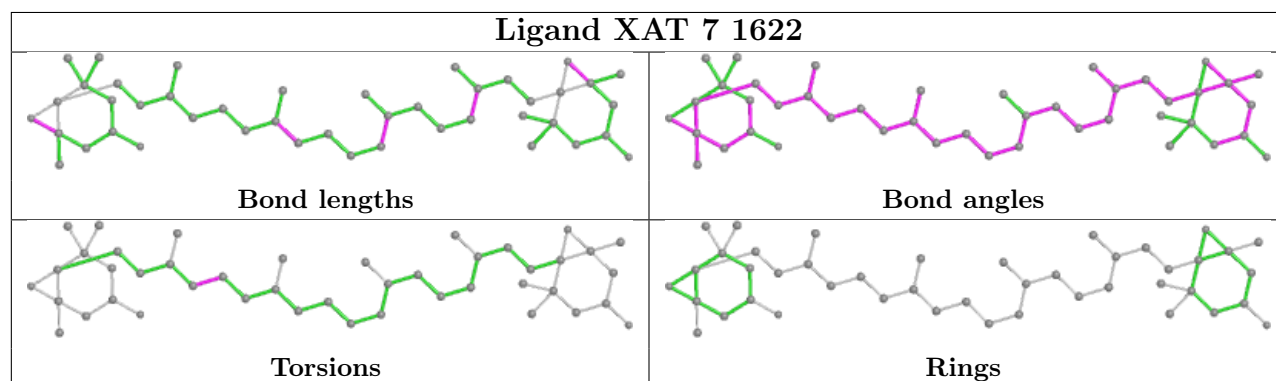
Rings



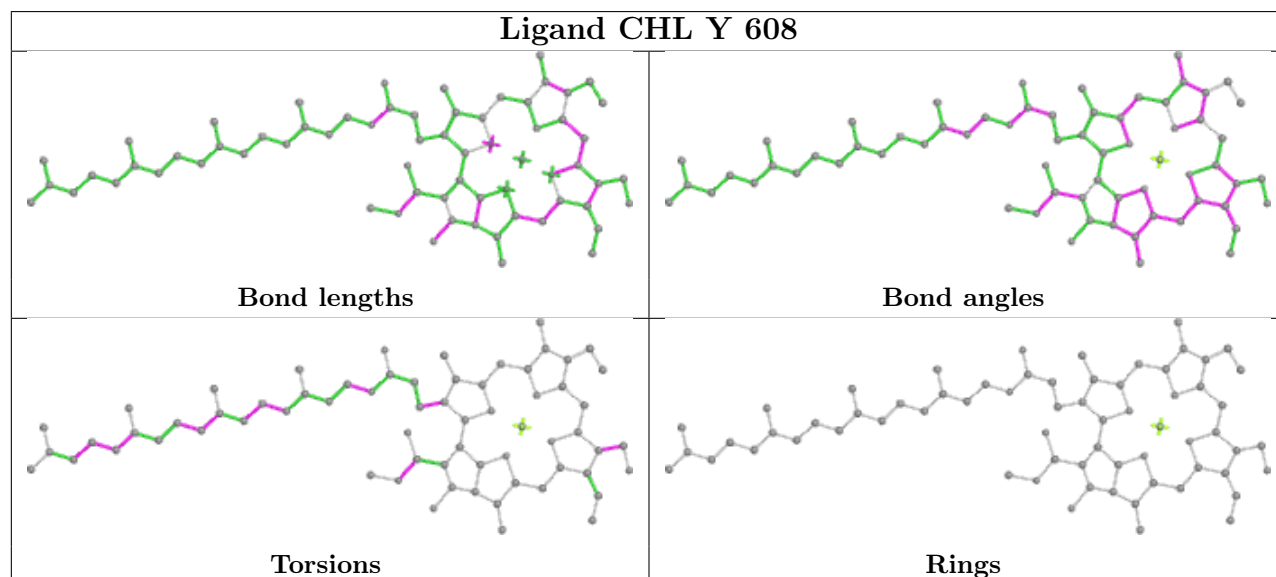
## Ligand CLA c 504

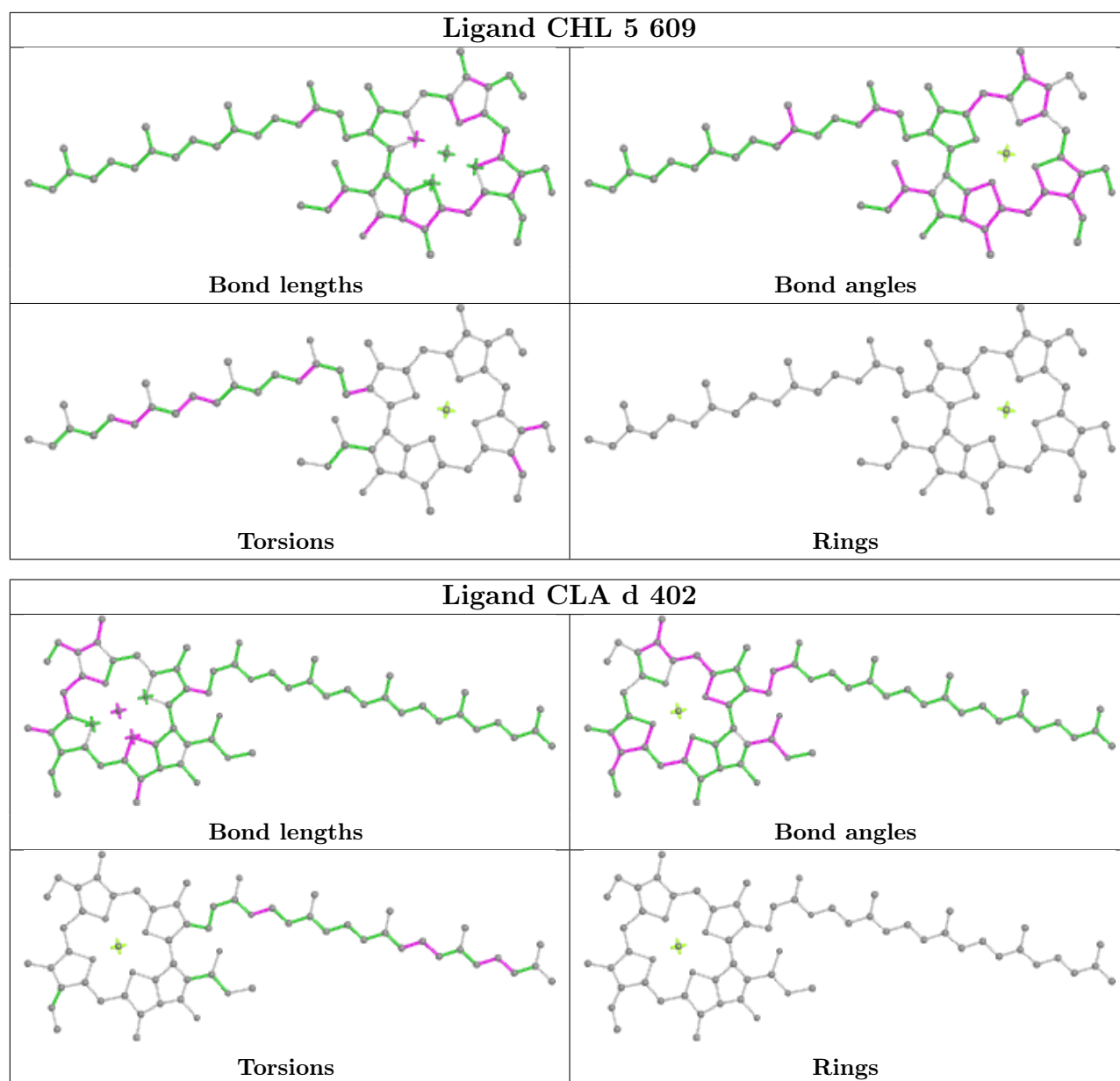


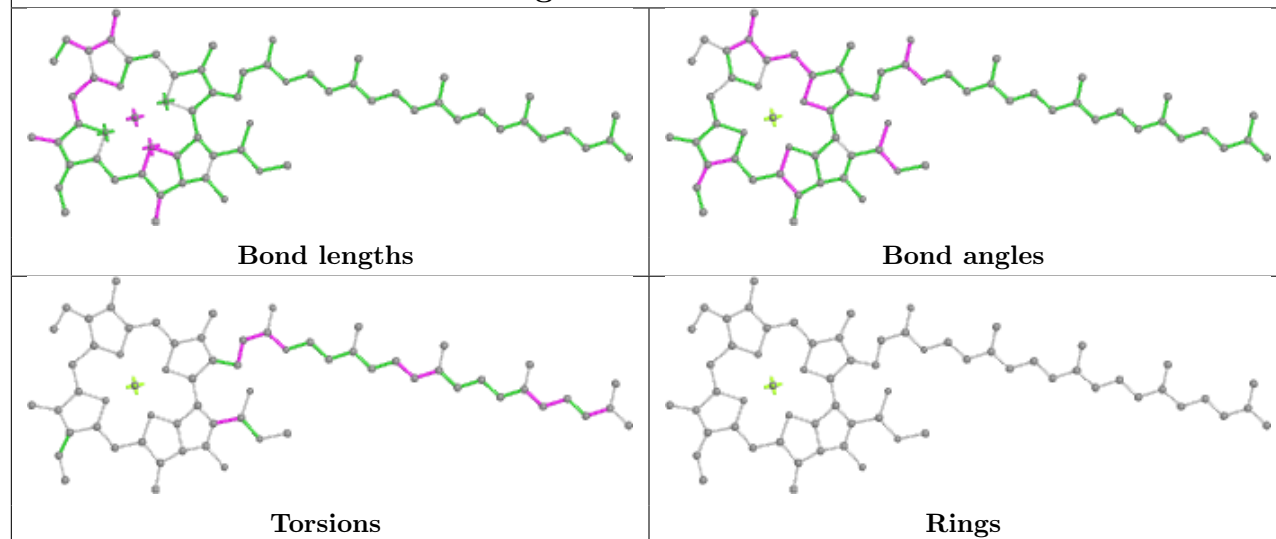
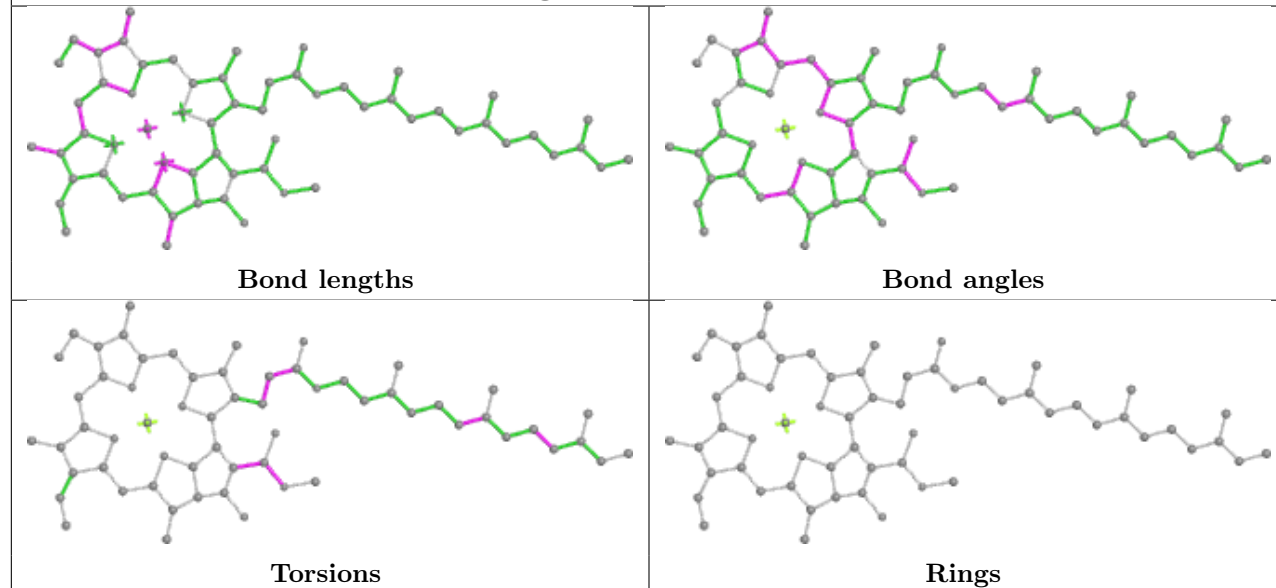
## Ligand XAT 7 1622

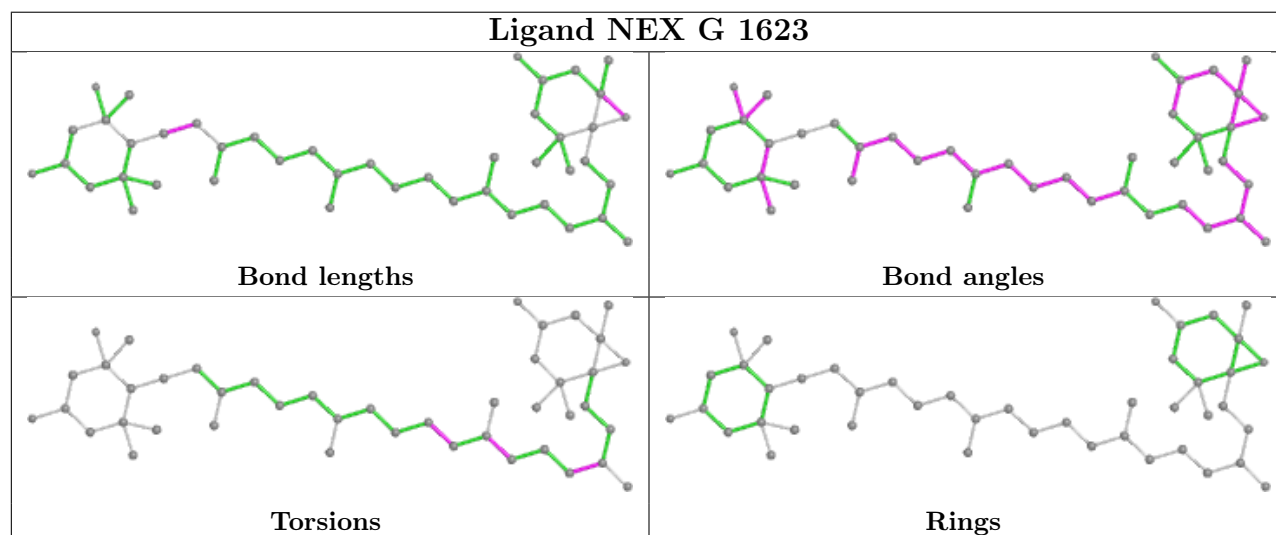
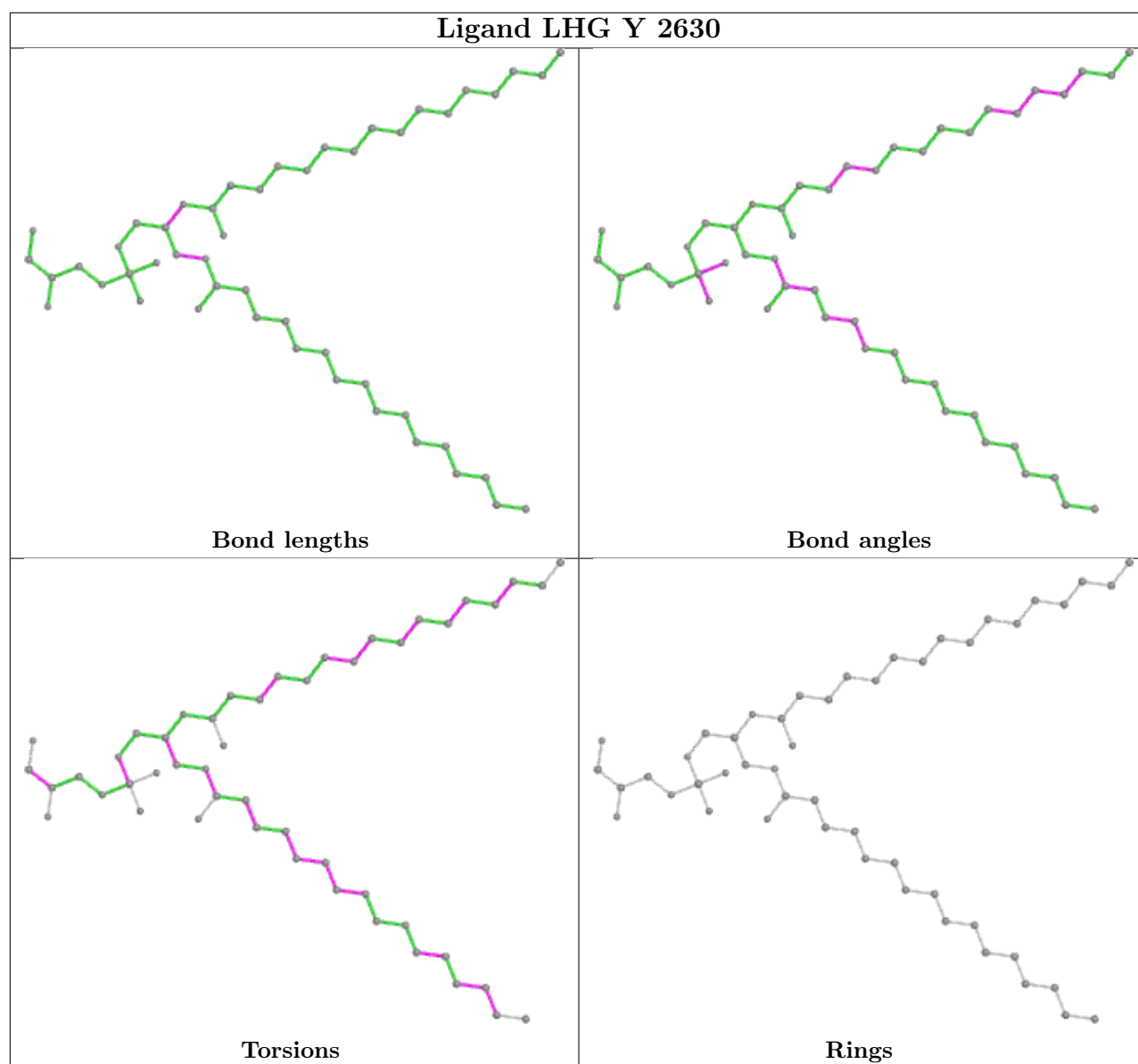


## Ligand CHL Y 608



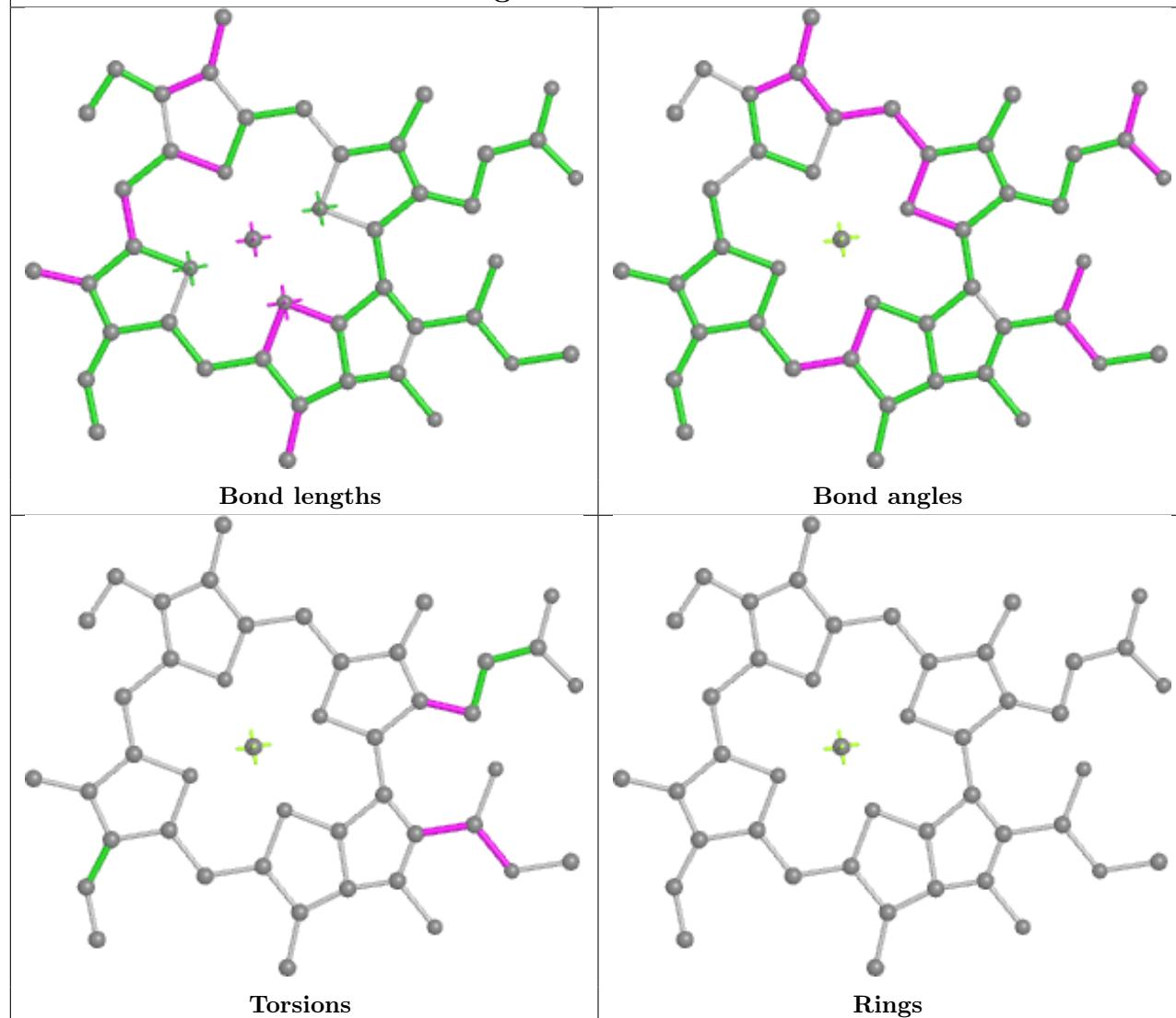


**Ligand CLA b 602****Ligand CLA 1 602**

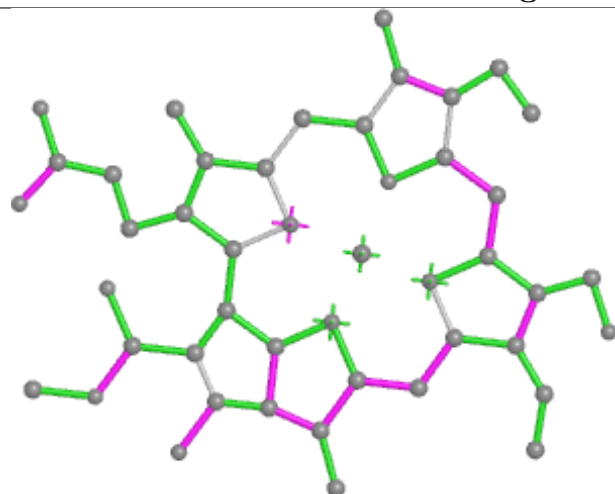




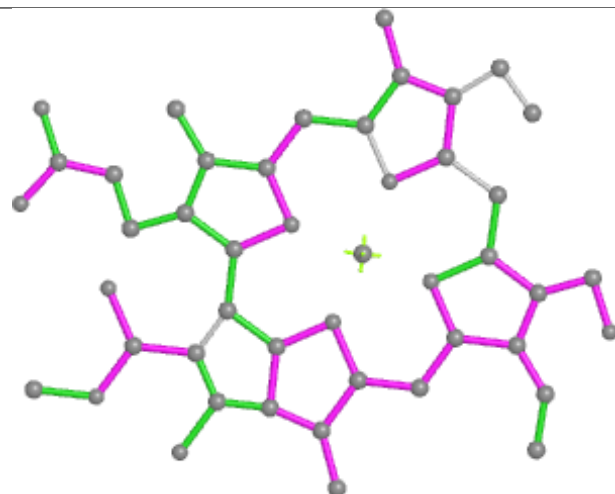
## Ligand CLA 5 614



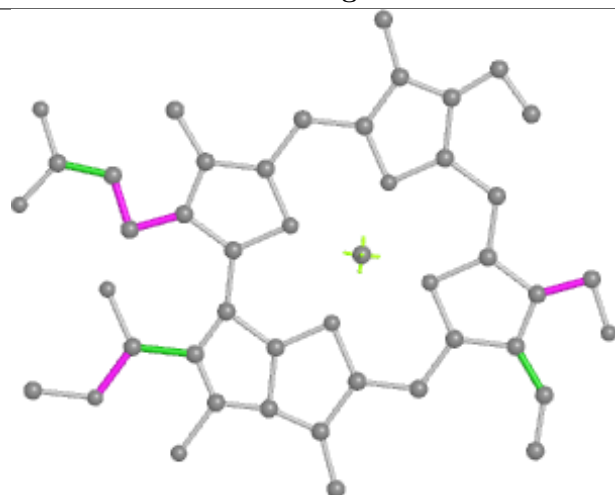
## Ligand CHL 8 606



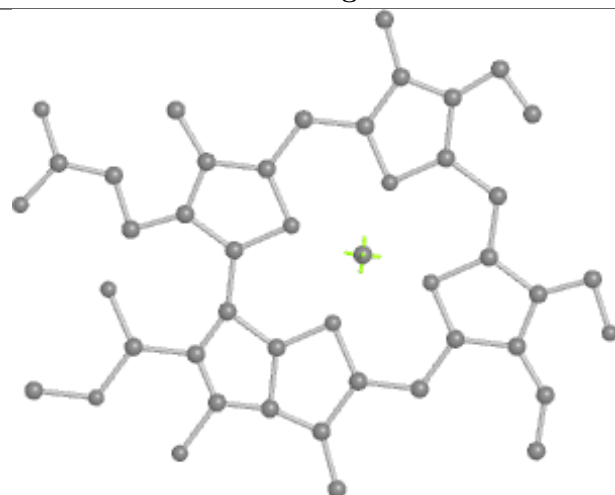
Bond lengths



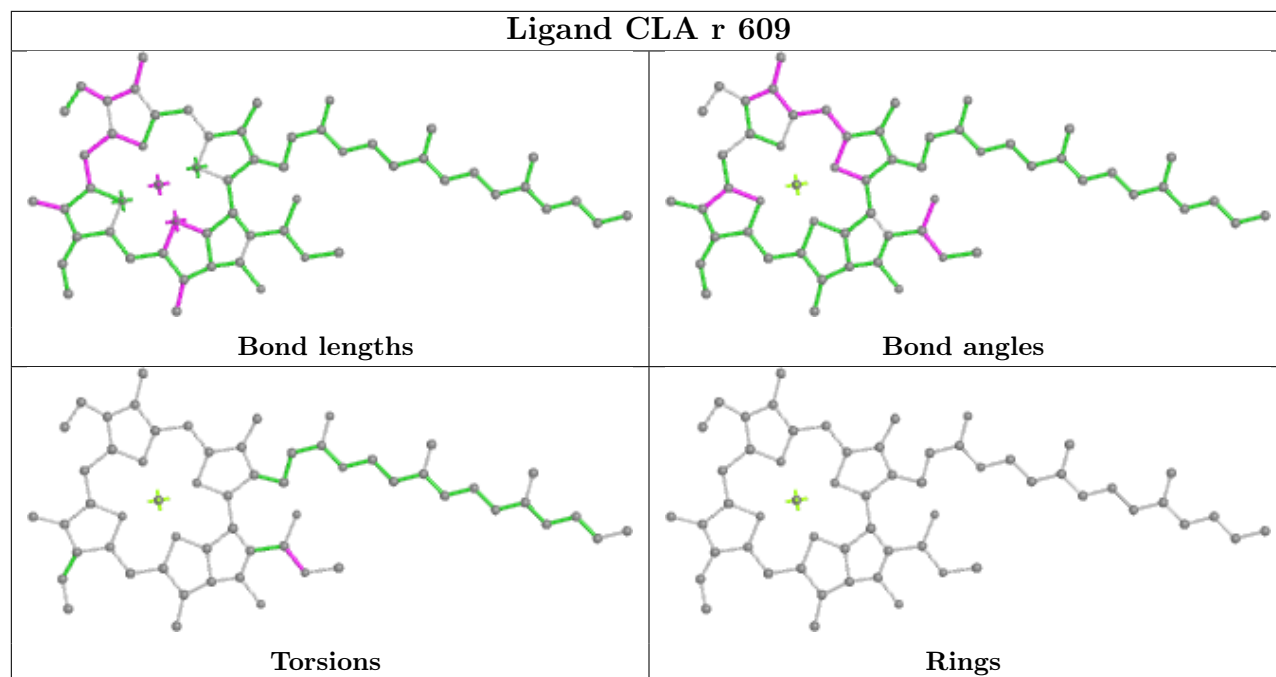
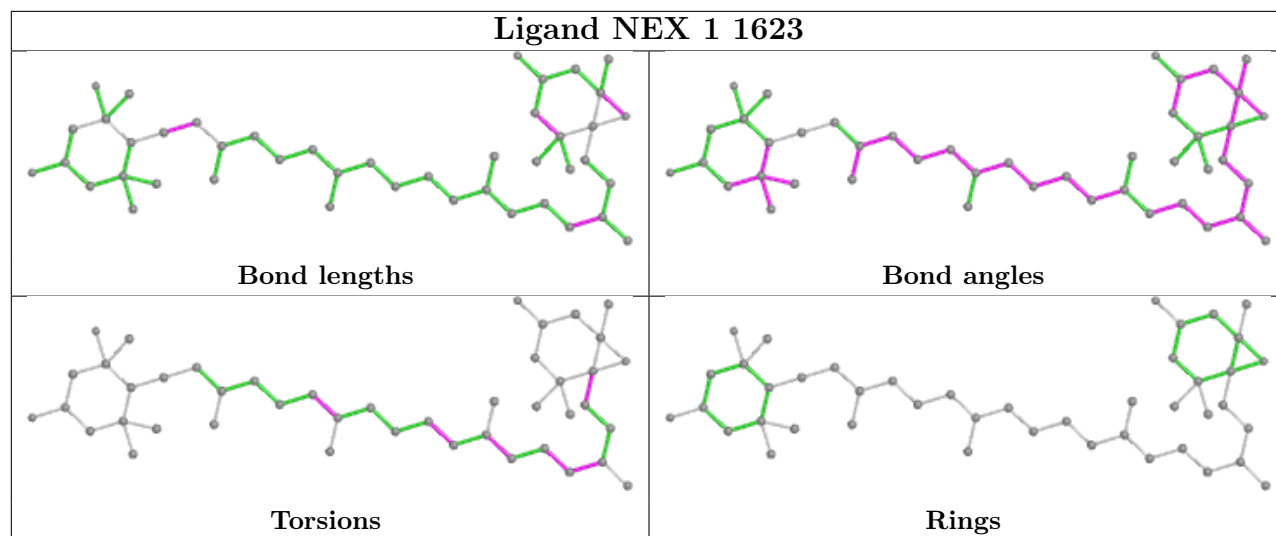
Bond angles

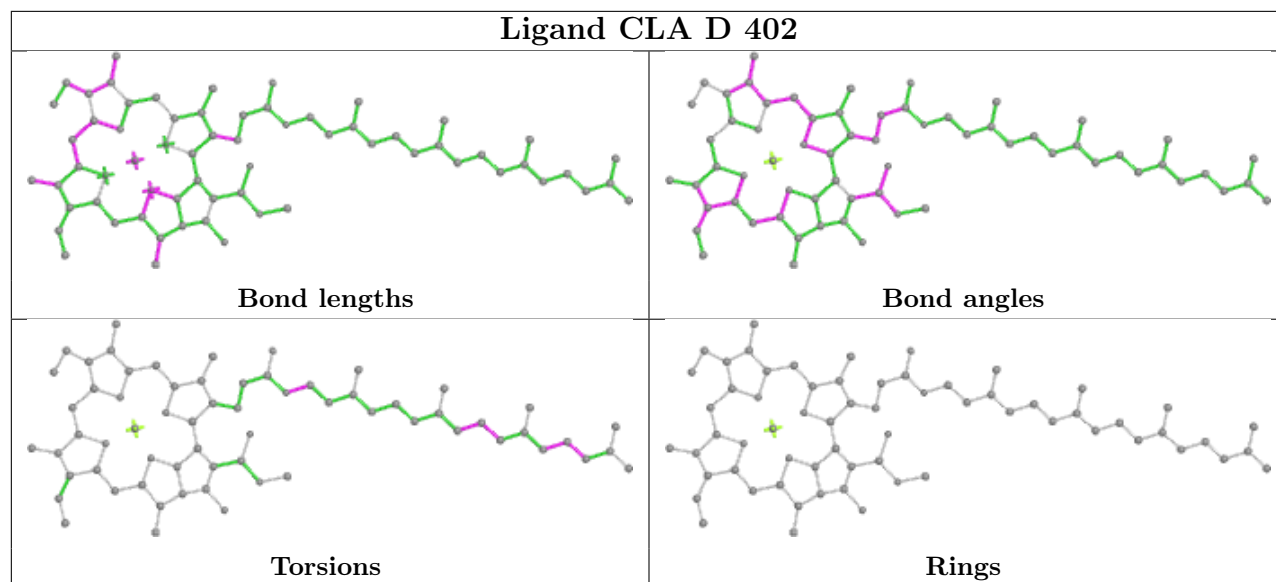
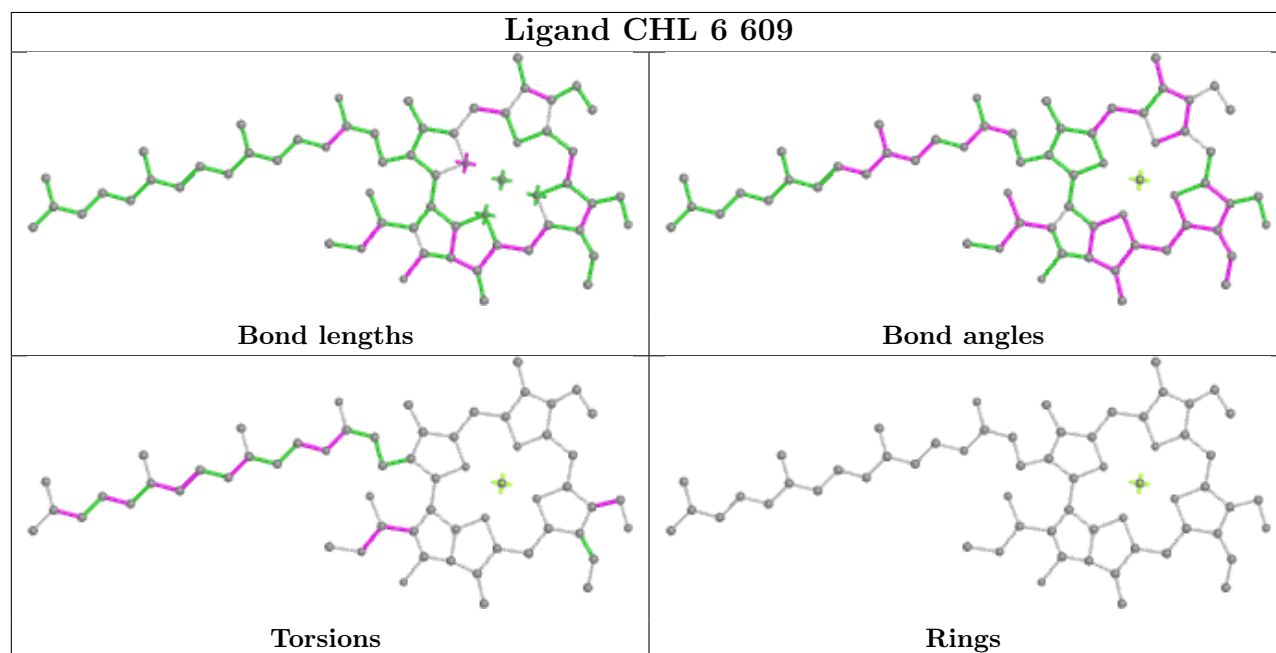


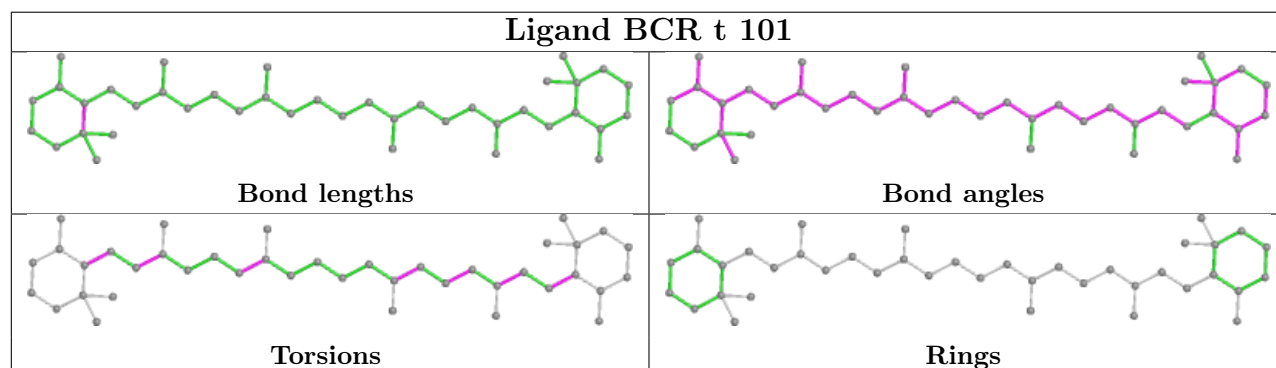
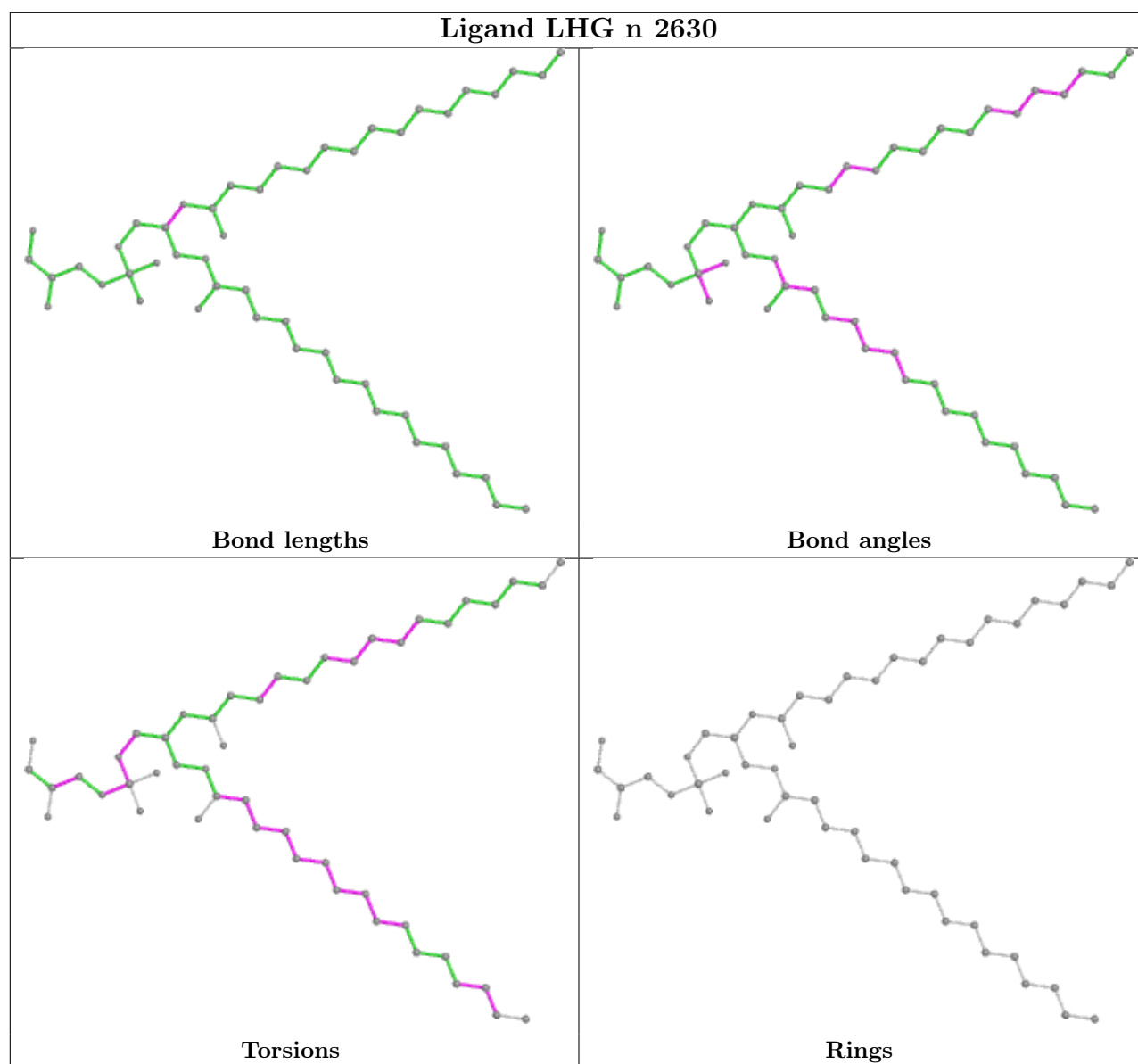
Torsions

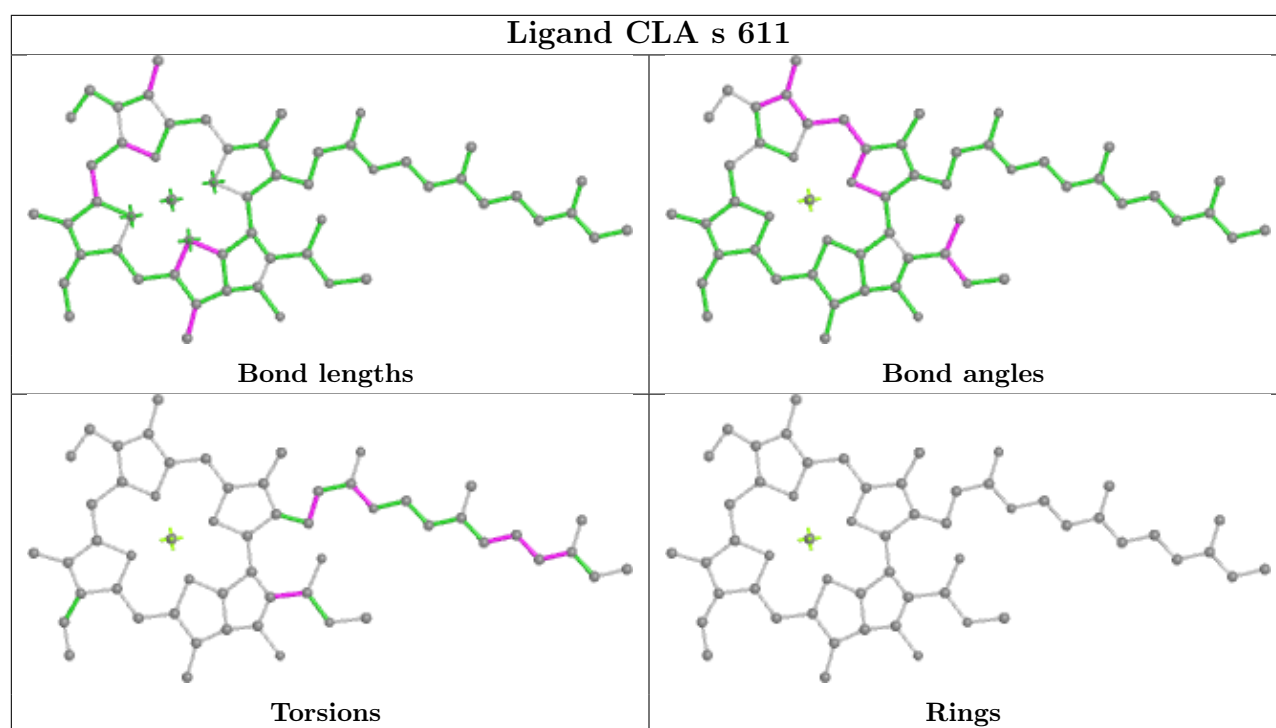
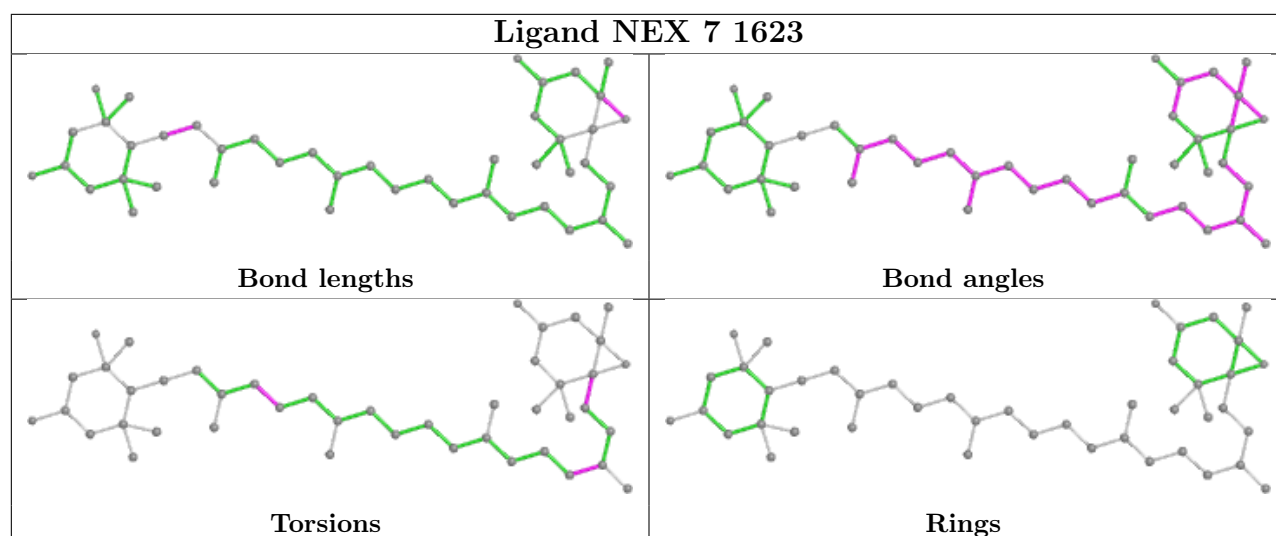


Rings

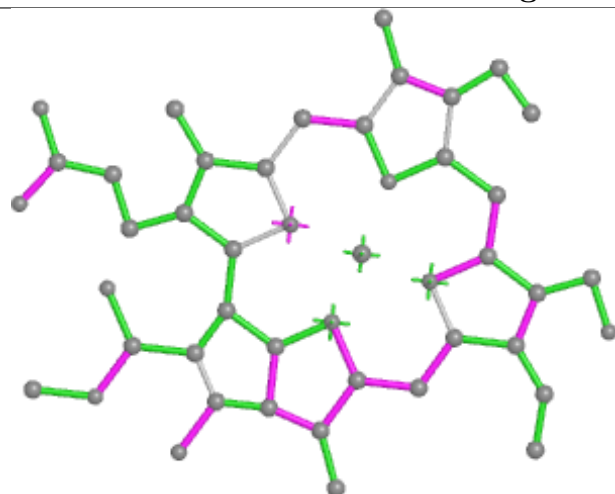
**Ligand CLA r 609****Ligand NEX 1 1623**

**Ligand CLA D 402****Ligand CHL 6 609**

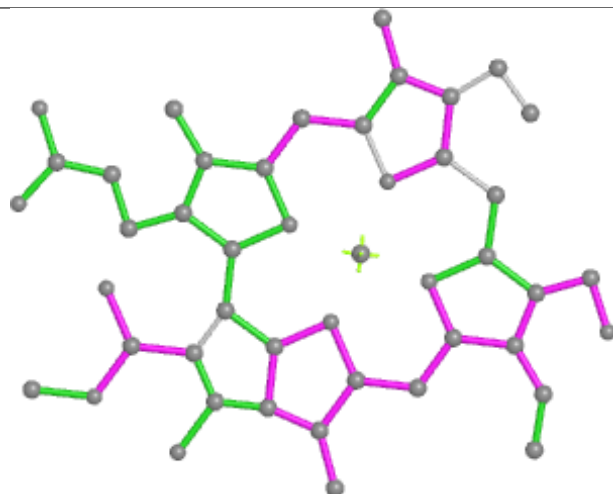




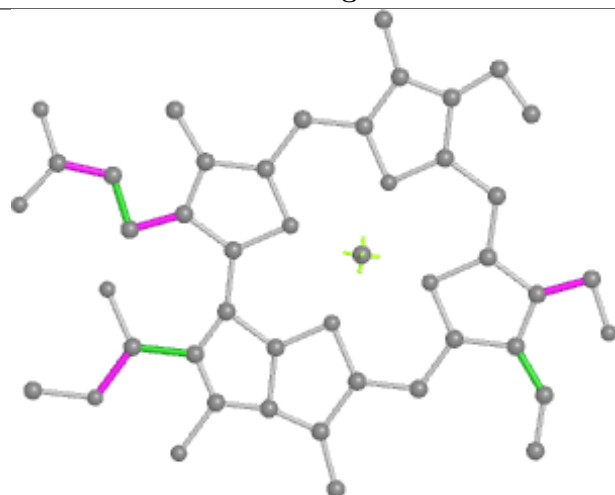
## Ligand CHL 5 605



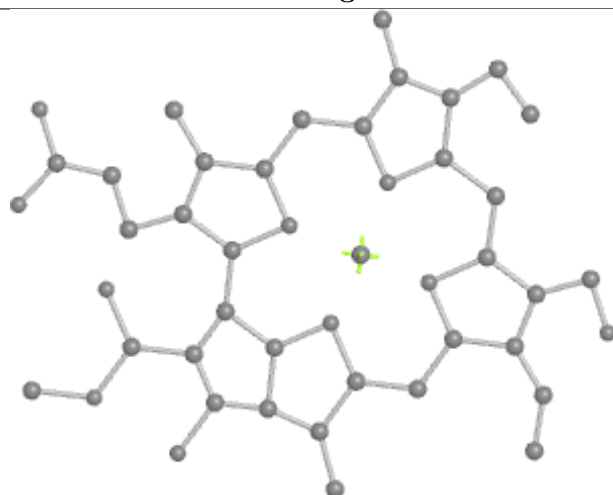
Bond lengths



Bond angles

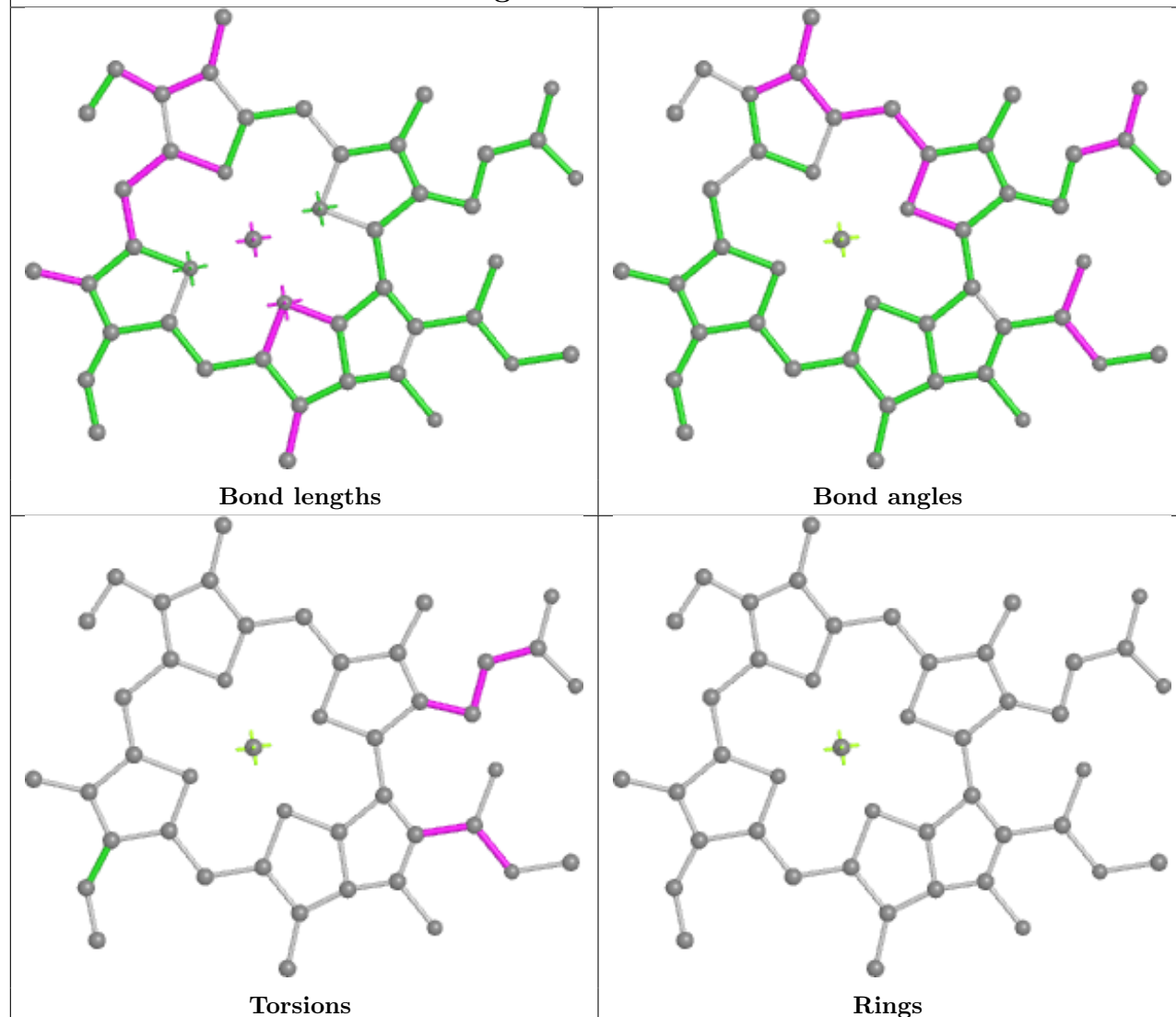


Torsions

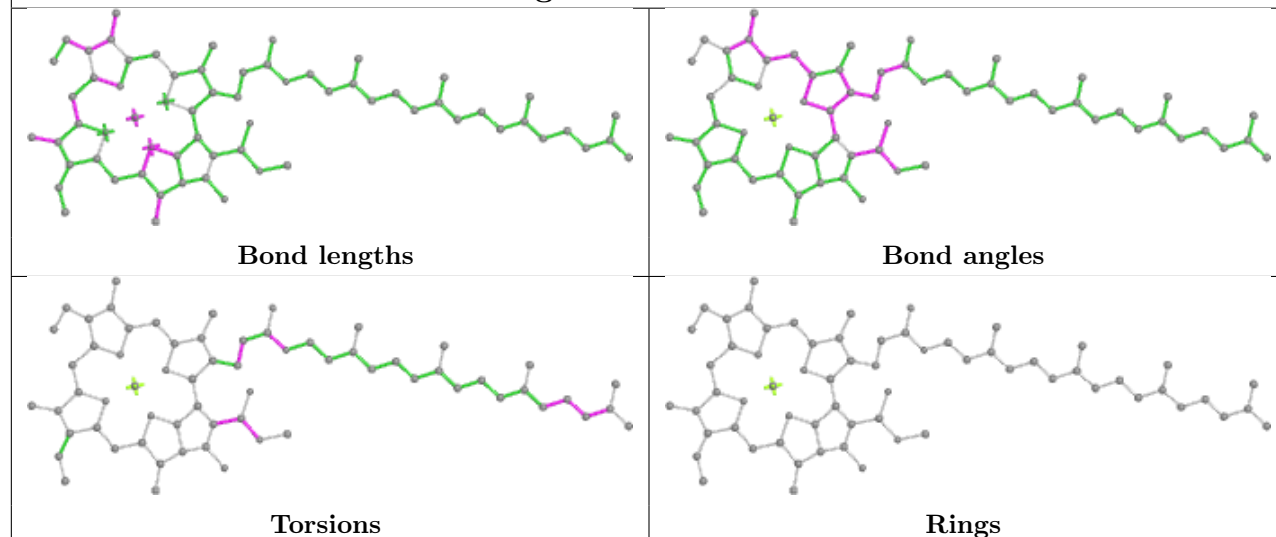


Rings

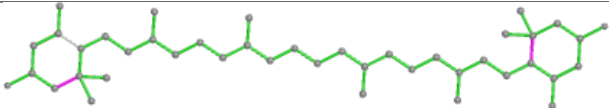
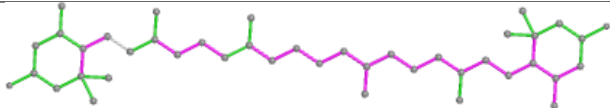
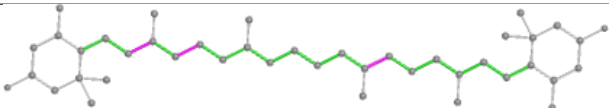
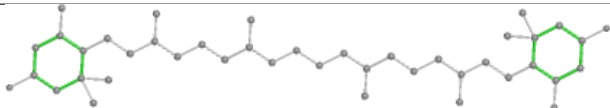
## Ligand CLA 3 604

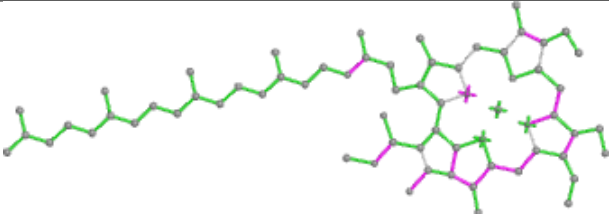
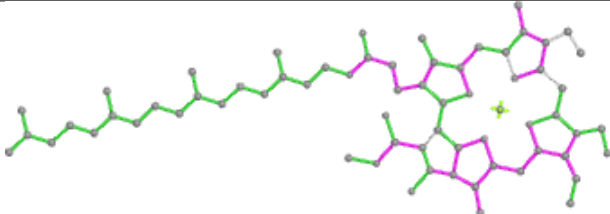
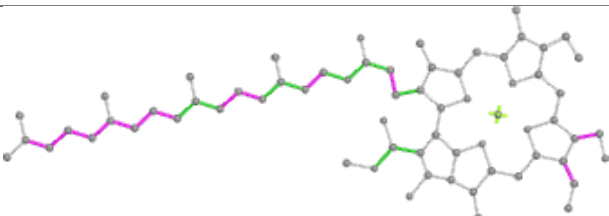
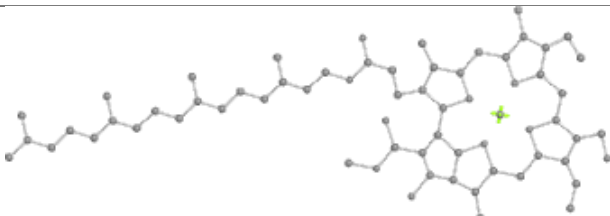


## Ligand CLA b 611

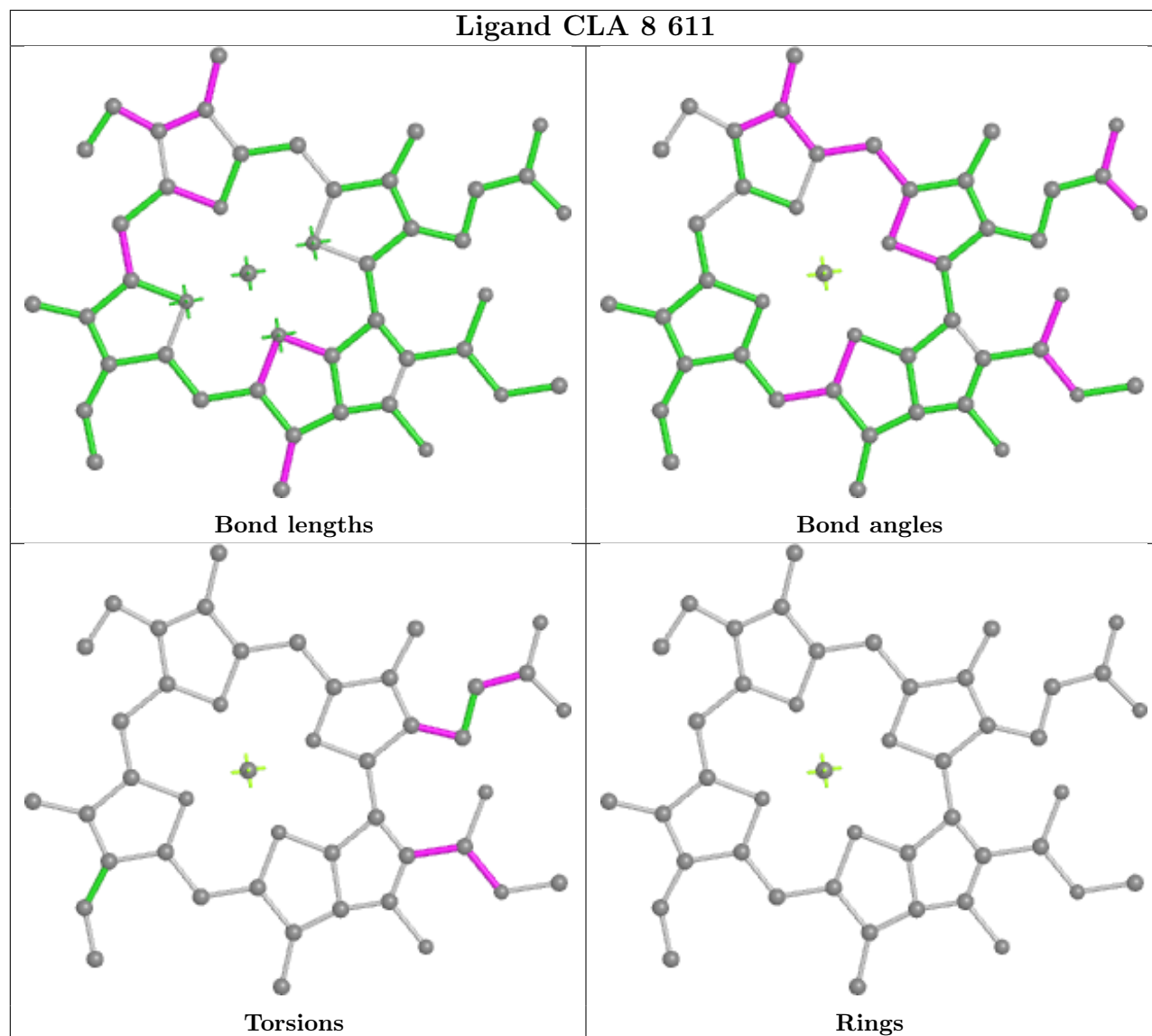




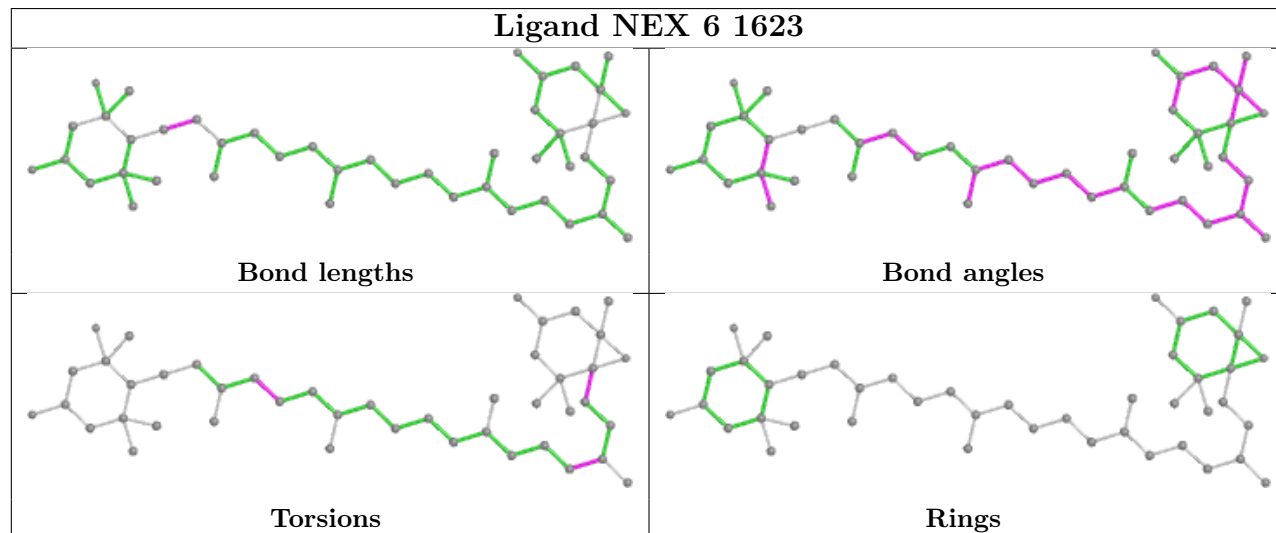
Ligand LUT 4 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

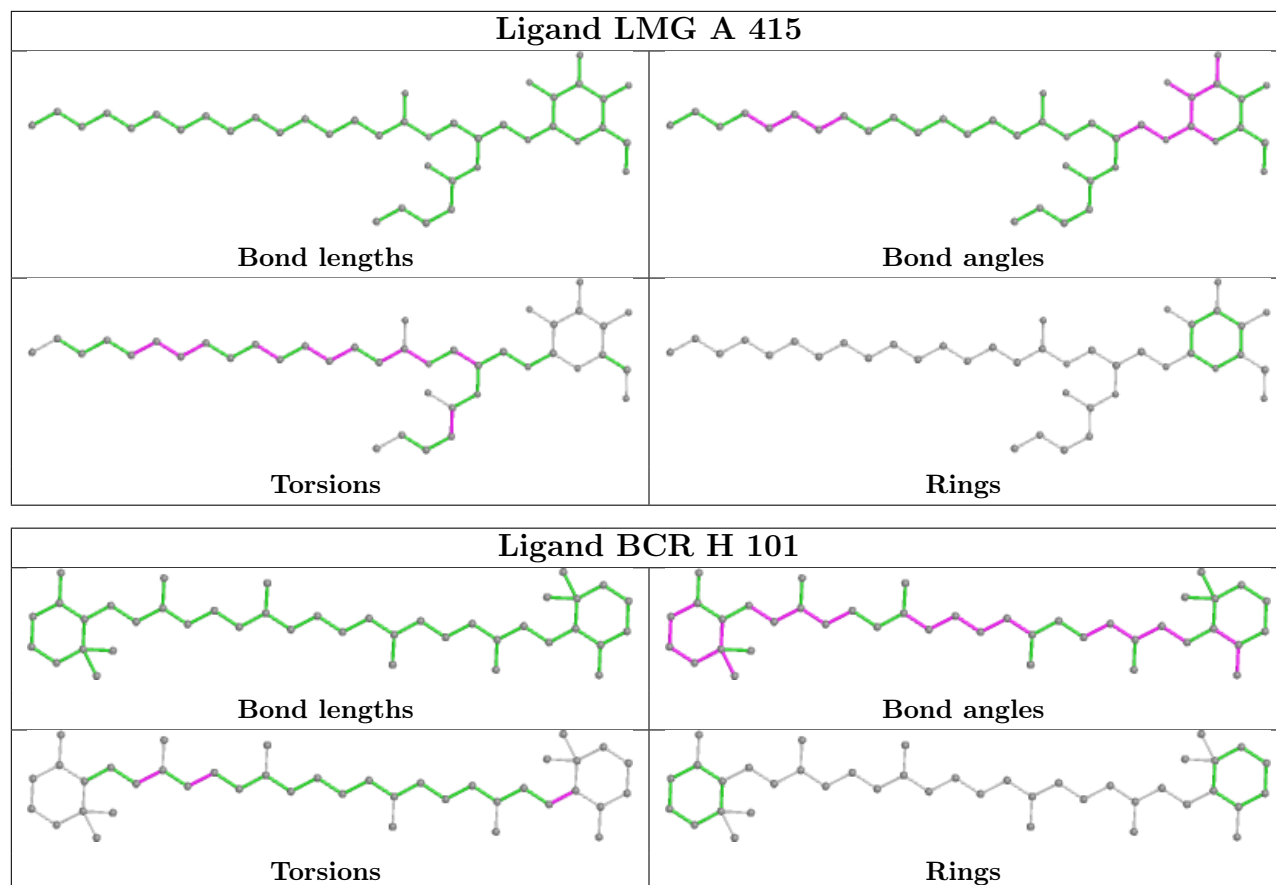
Ligand CHL n 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA 8 611

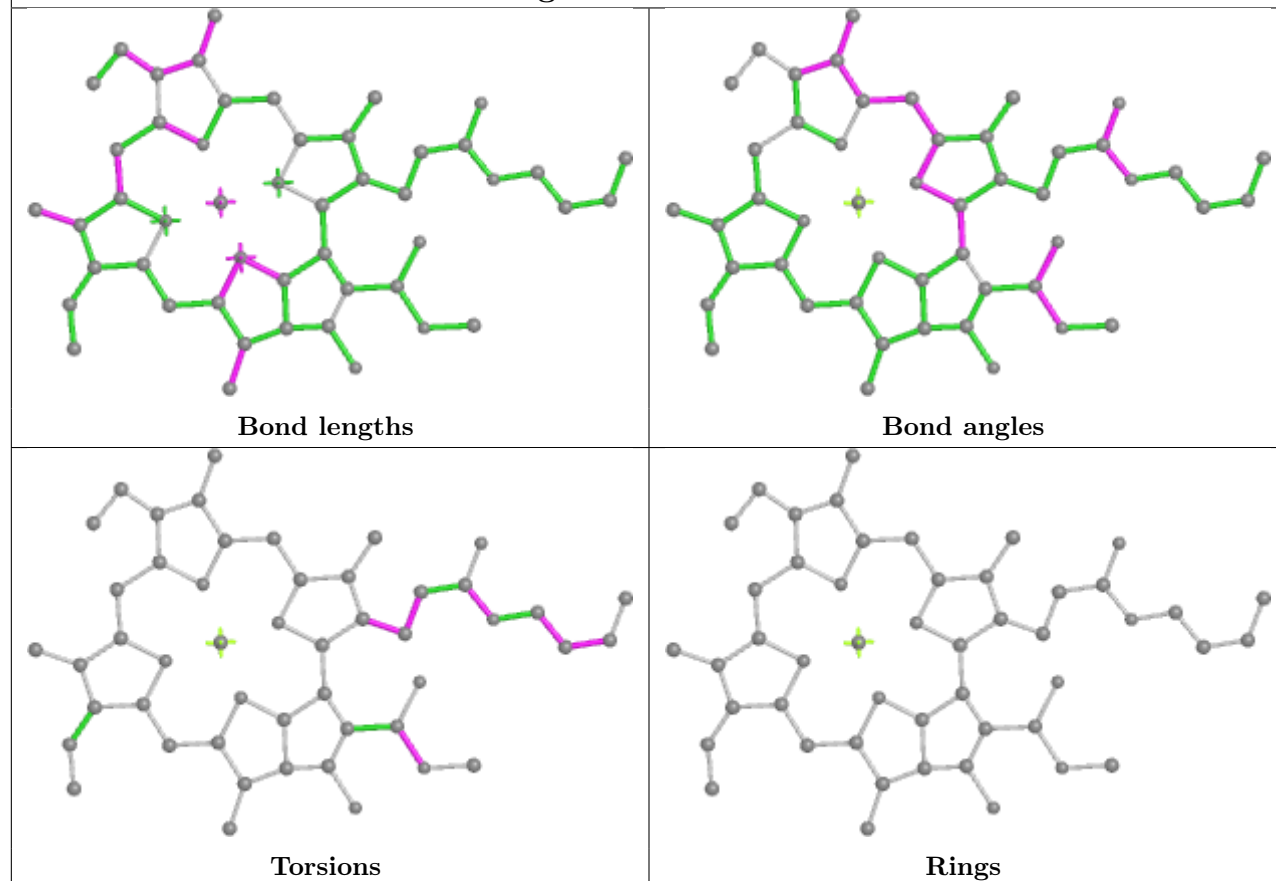


## Ligand NEX 6 1623

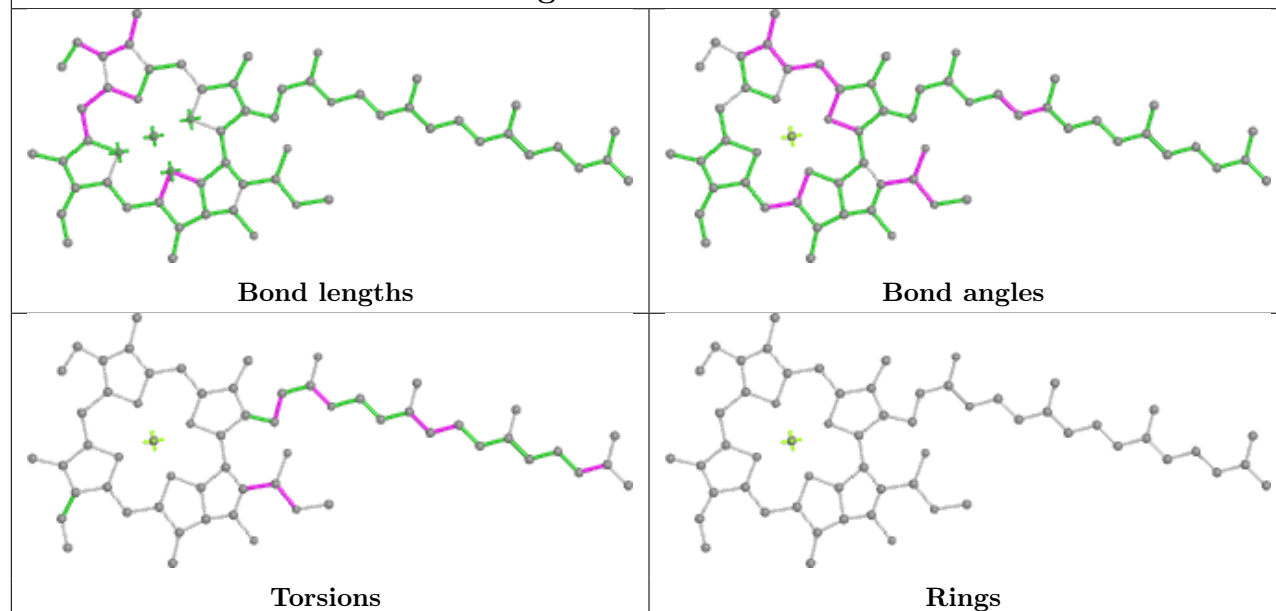


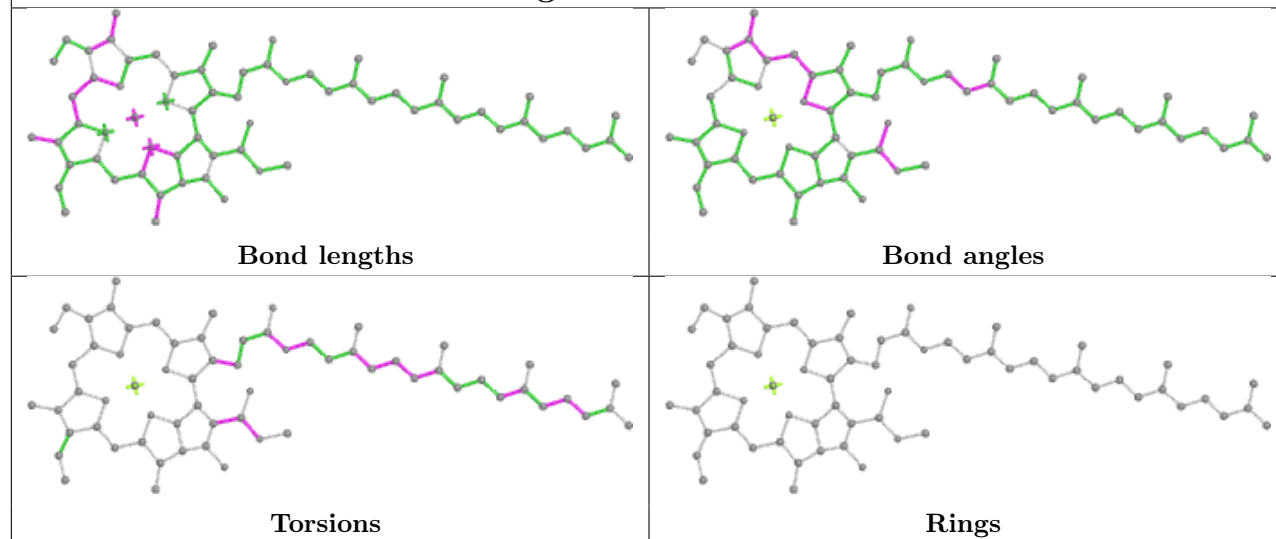
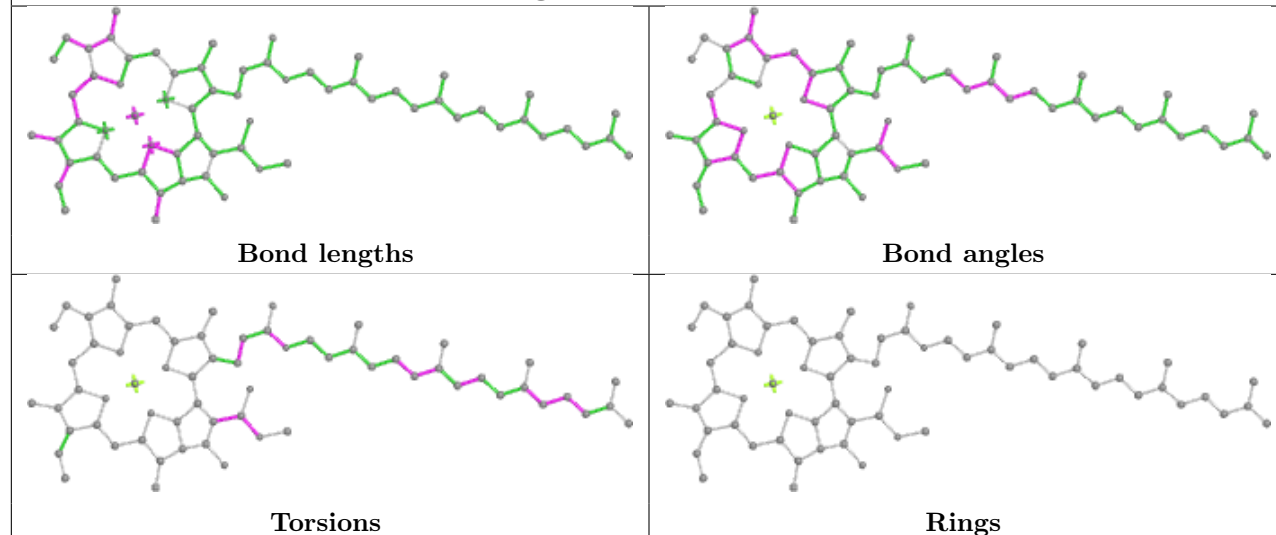
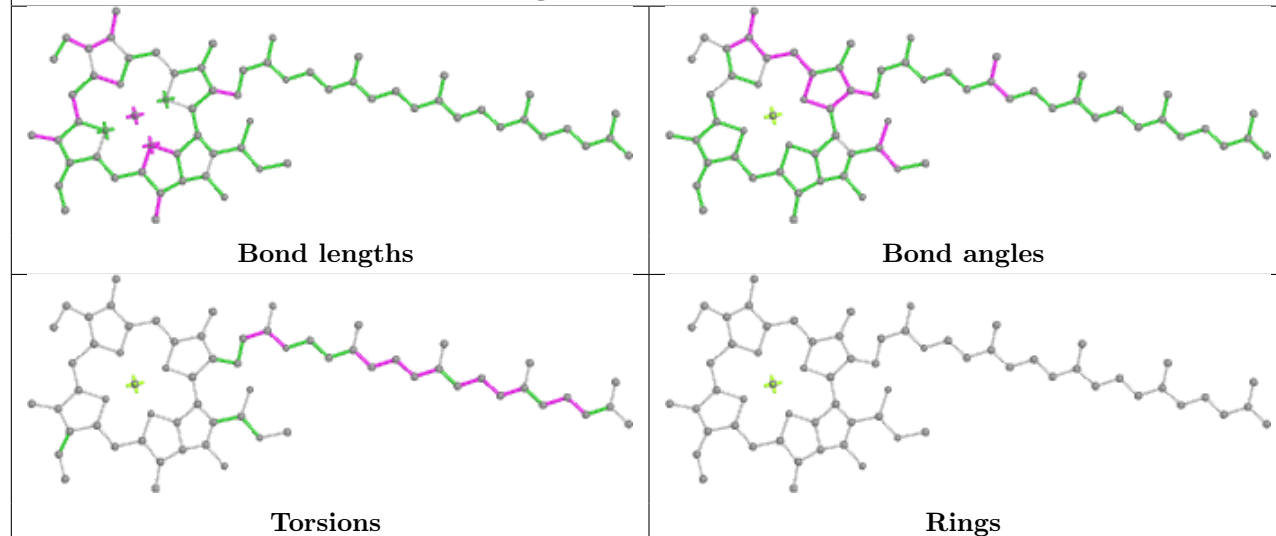


## Ligand CLA r 611

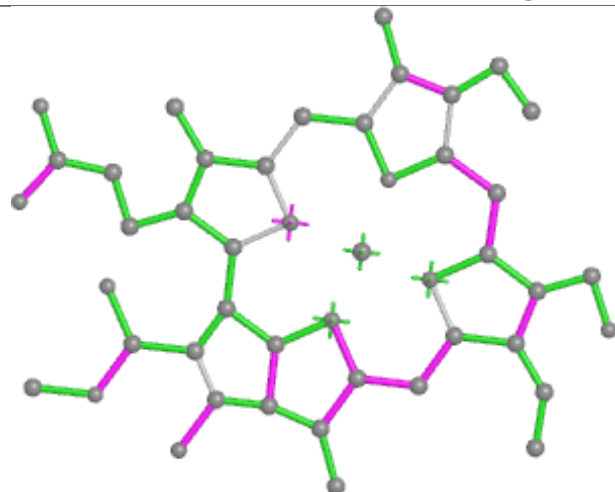


## Ligand CLA r 613

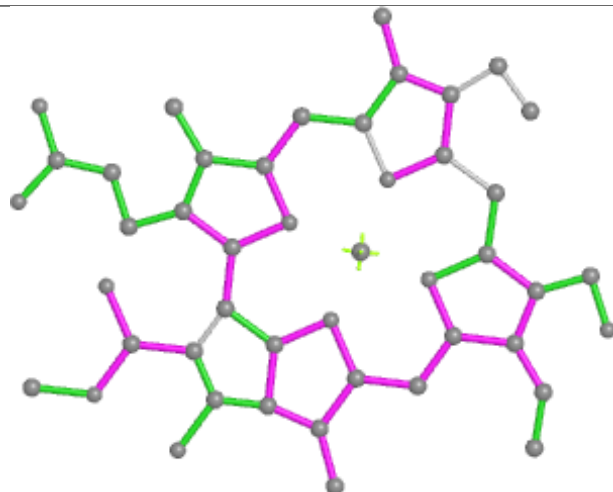


**Ligand CLA c 506****Ligand CLA B 606****Ligand CLA B 614**

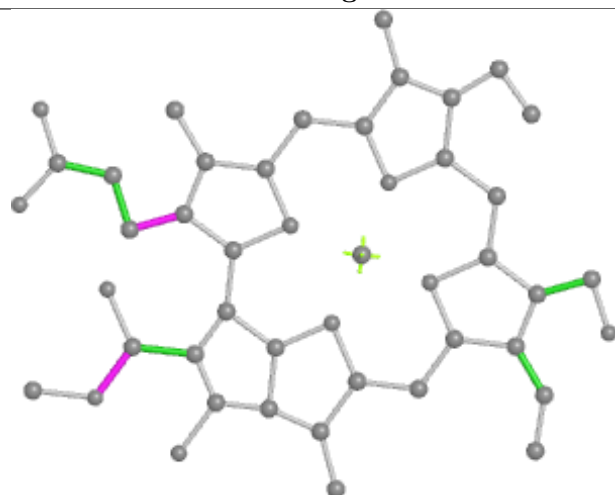
## Ligand CHL 1 608



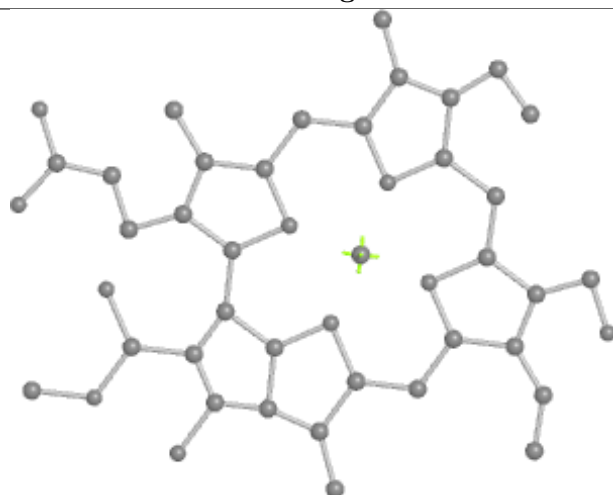
Bond lengths



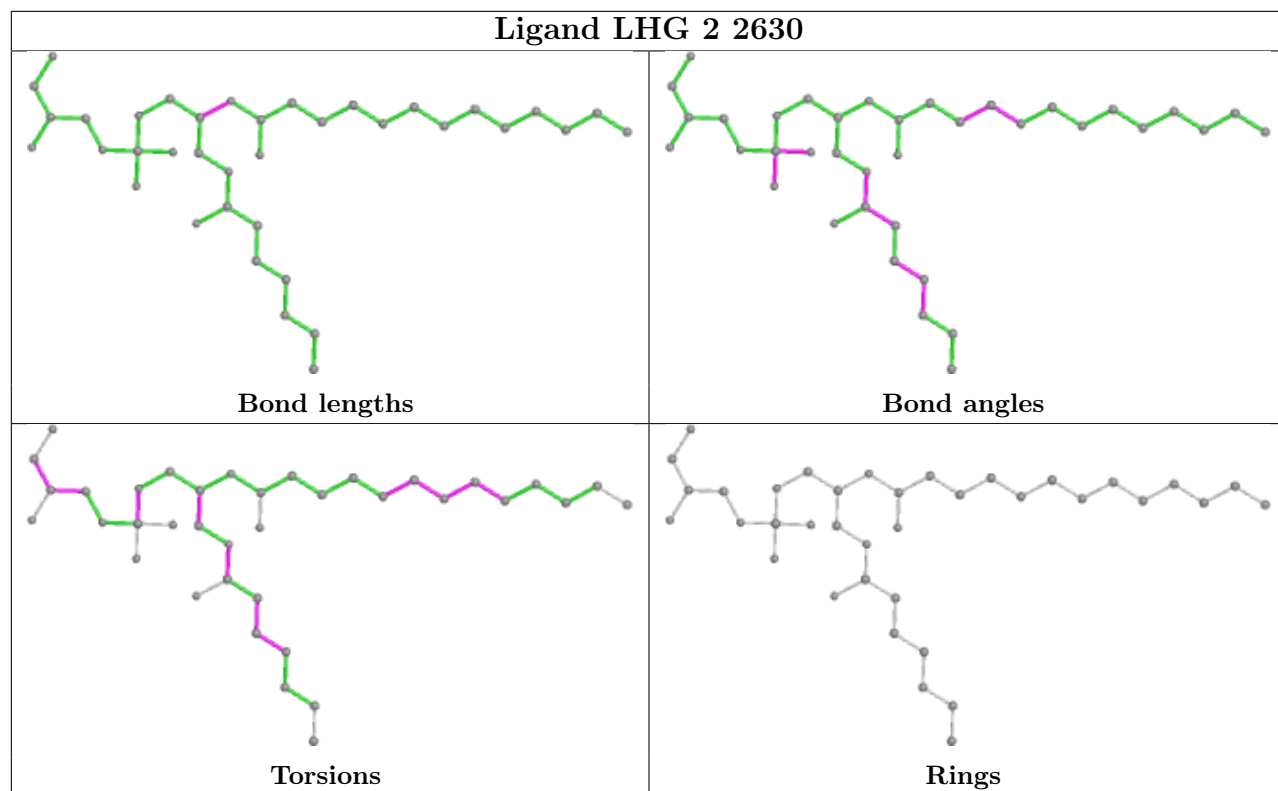
Bond angles



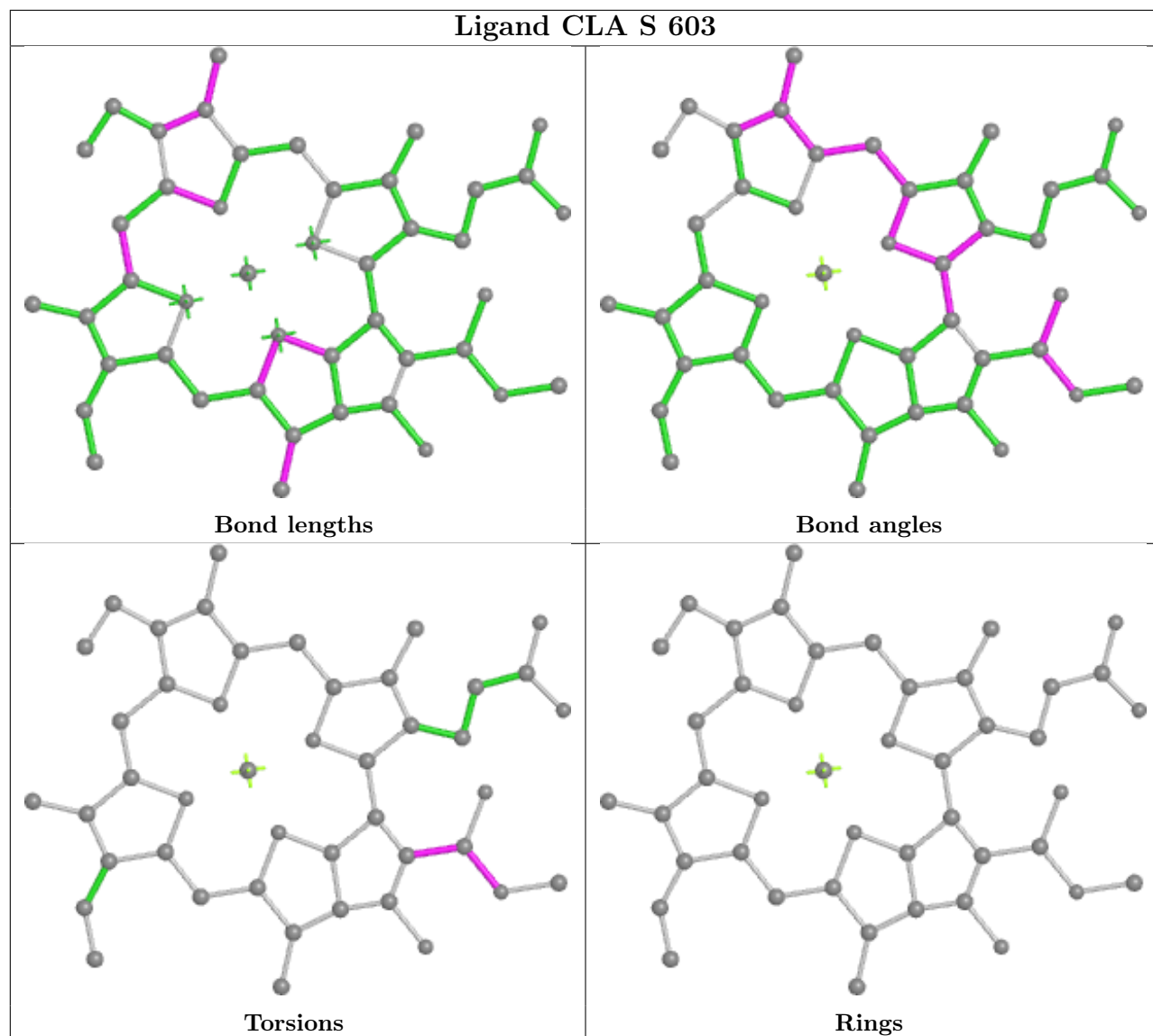
Torsions



Rings

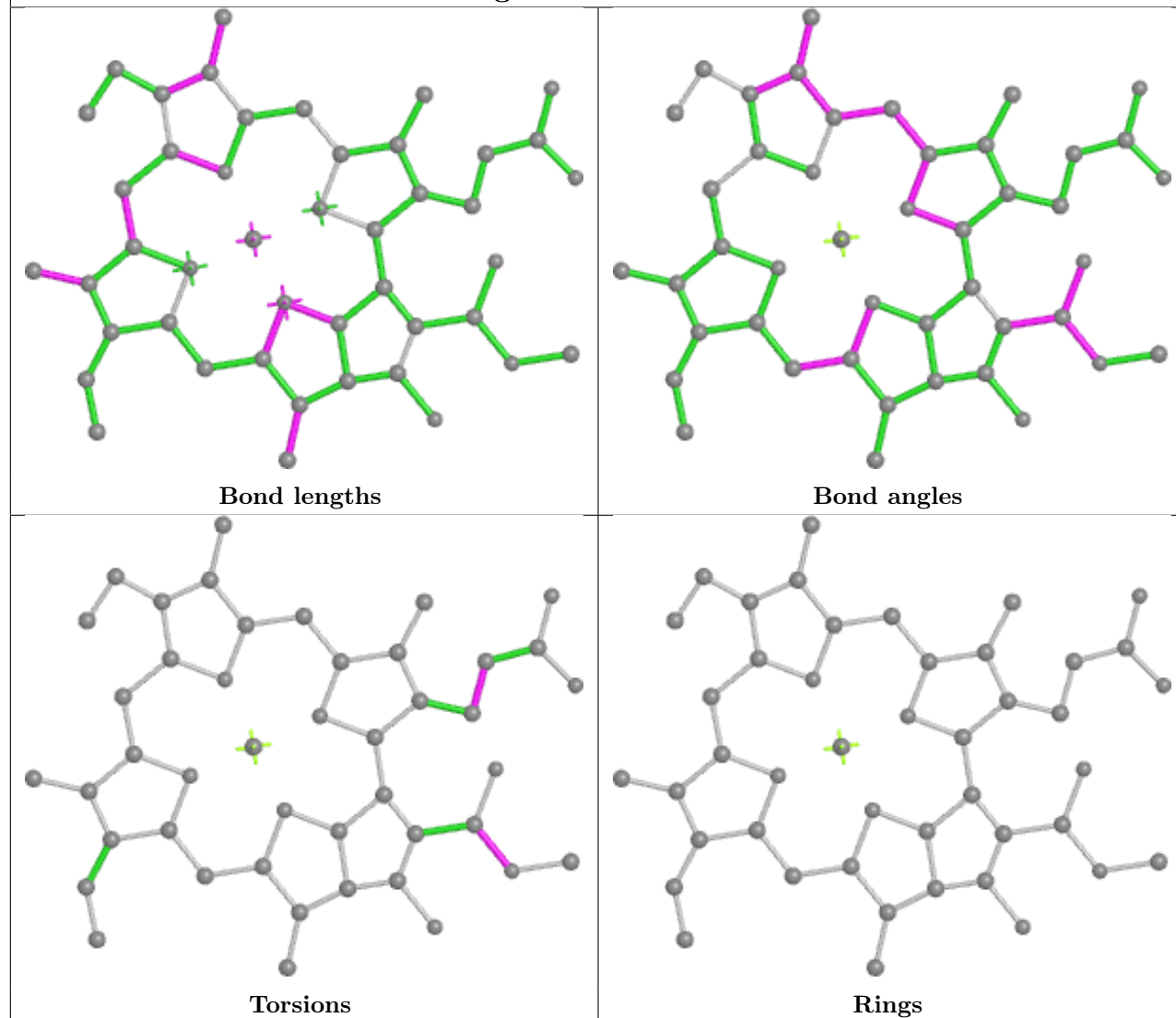


## Ligand CLA S 603

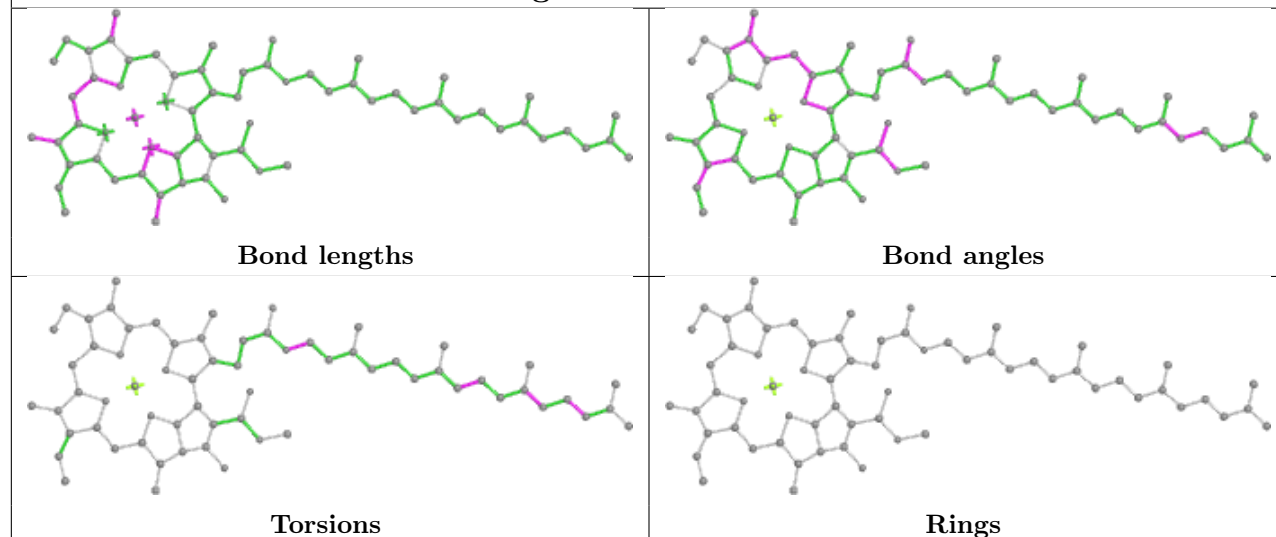




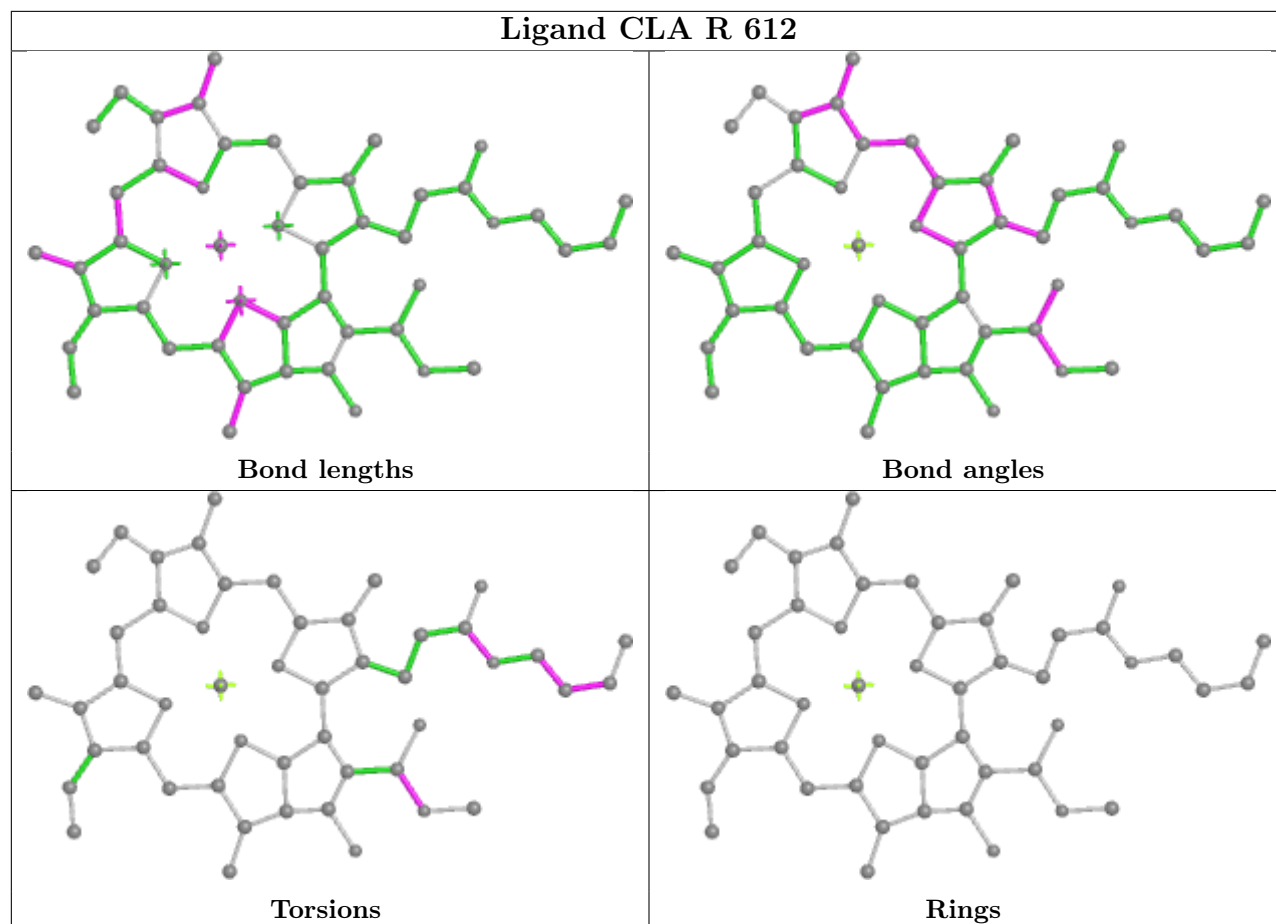
## Ligand CLA 4 602



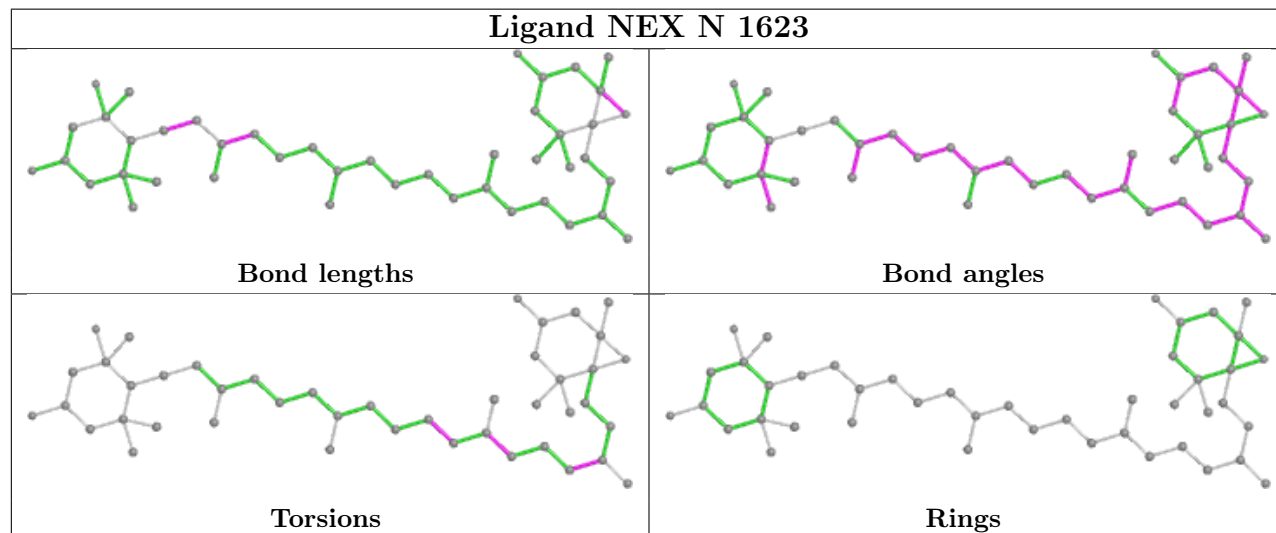
## Ligand CLA B 609



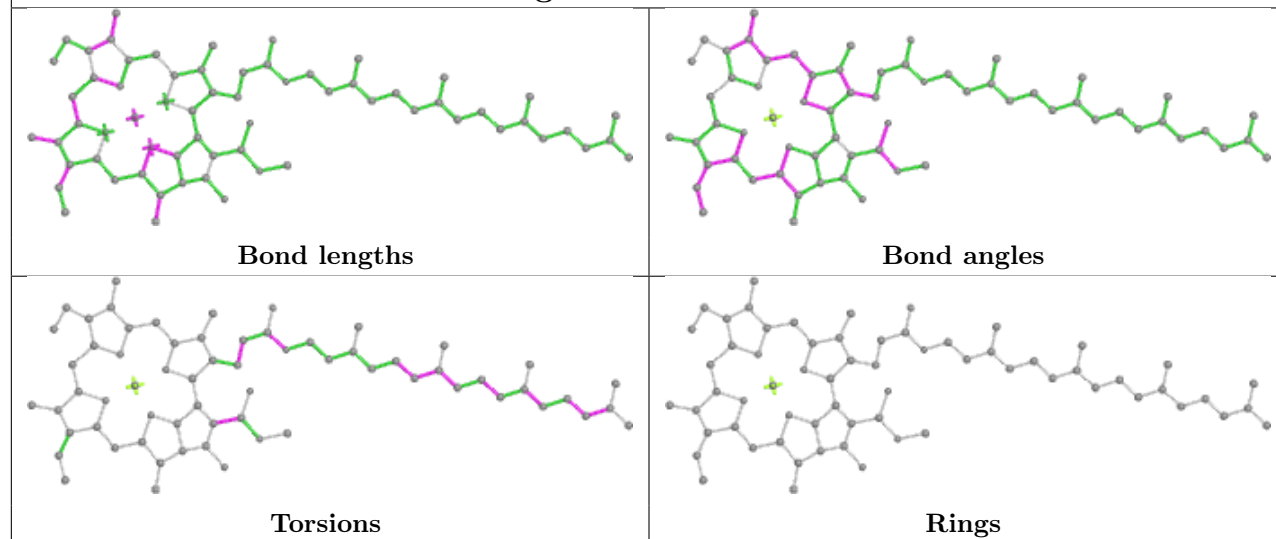
## Ligand CLA R 612



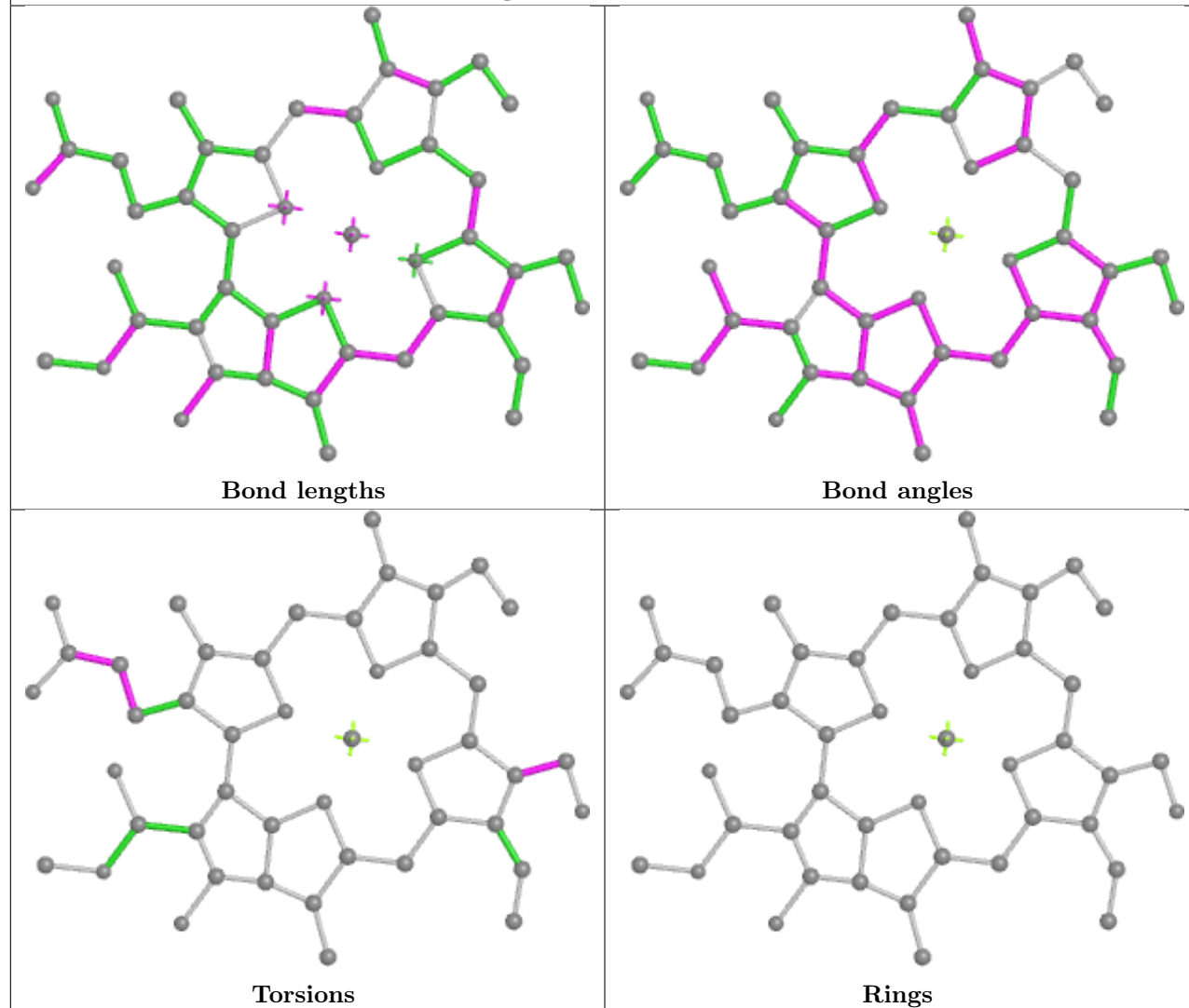
## Ligand NEX N 1623

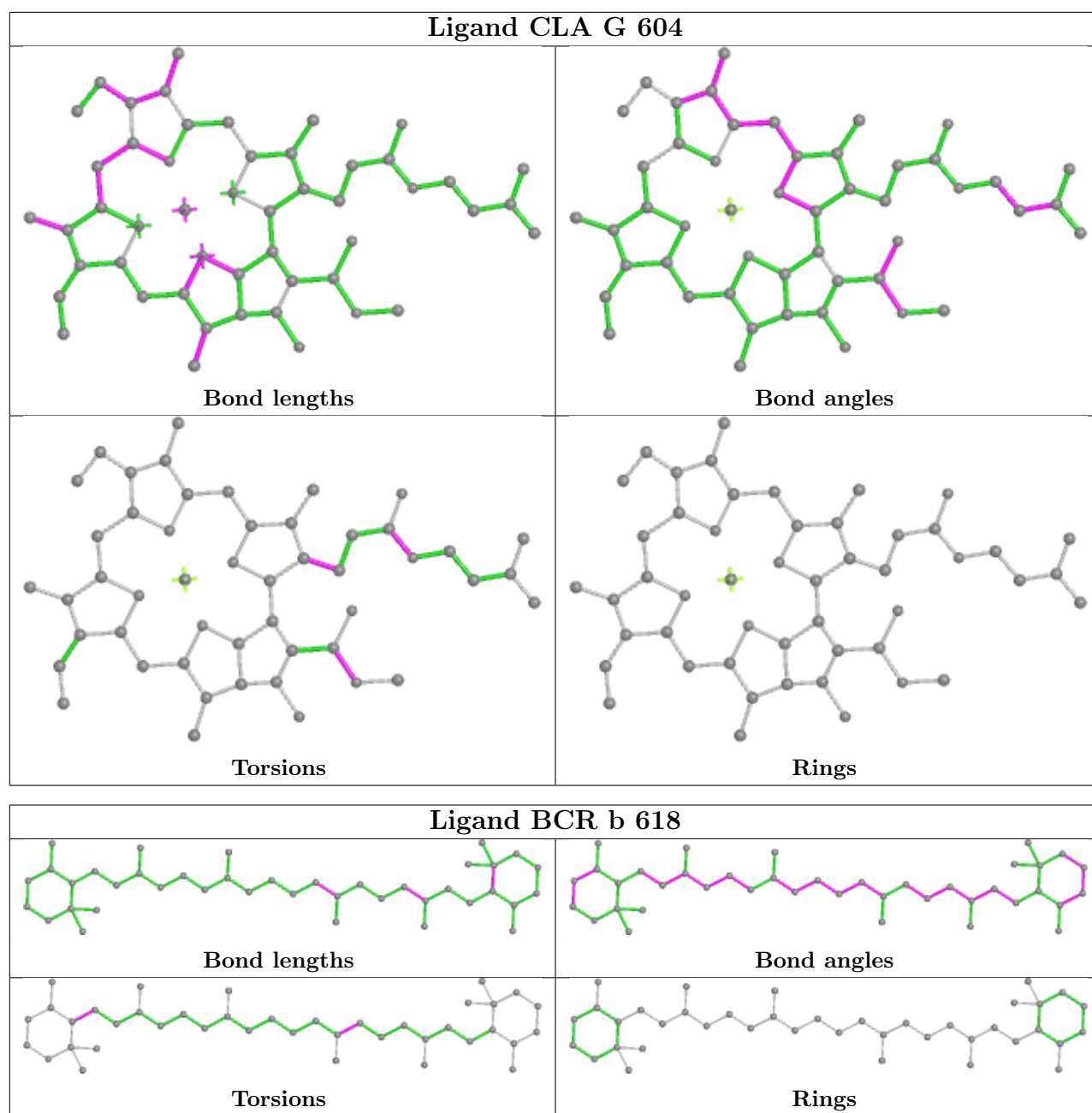


## Ligand CLA n 603

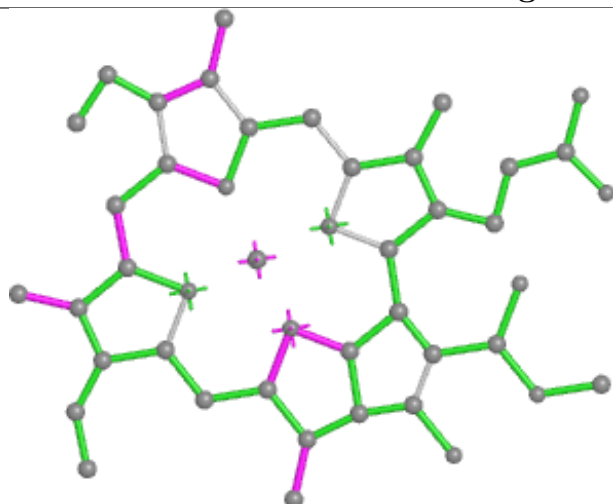


## Ligand CHL 5 601

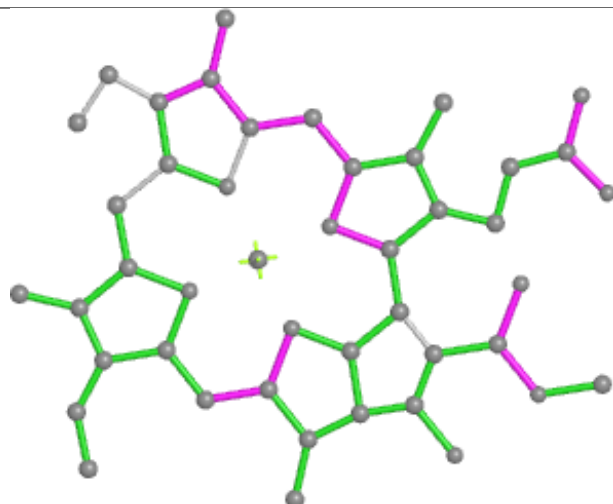




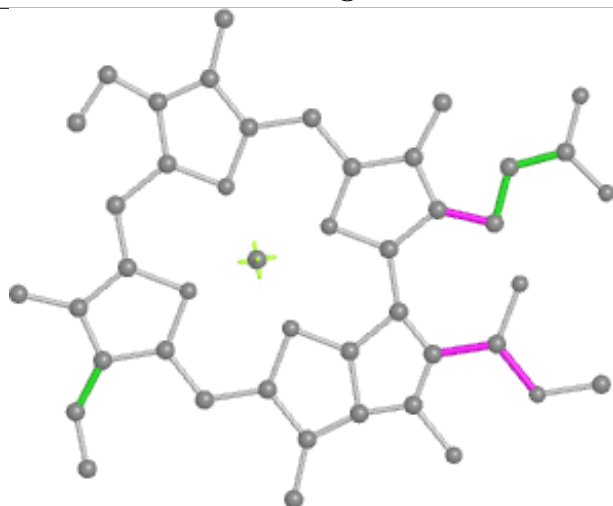
## Ligand CLA 1 614



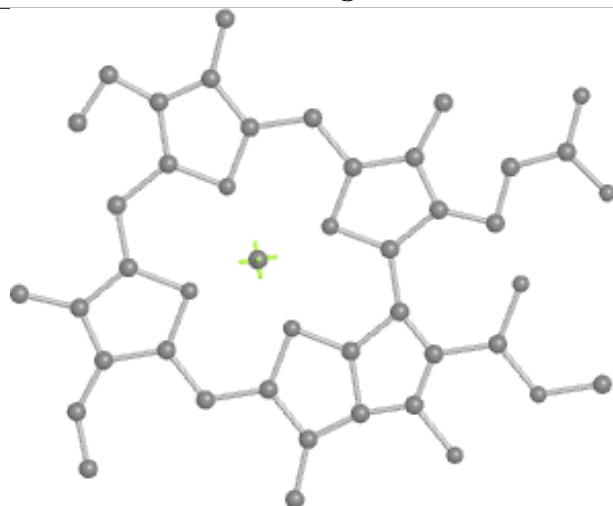
Bond lengths



Bond angles

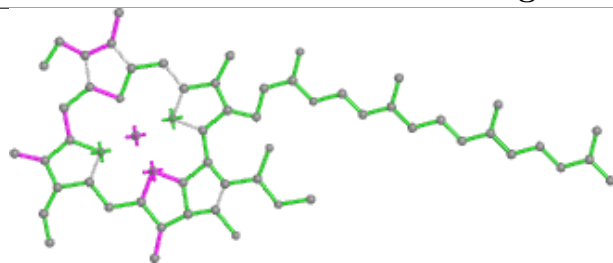


Torsions

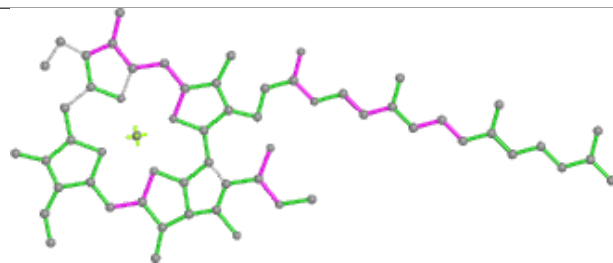


Rings

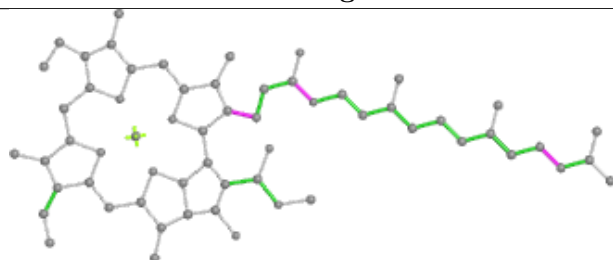
## Ligand CLA 3 610



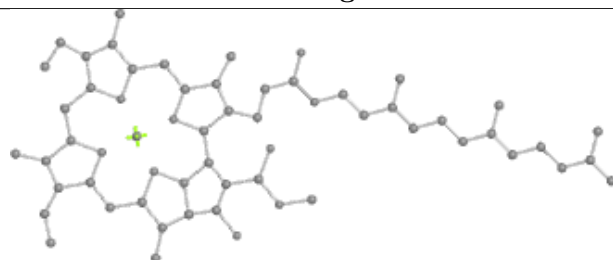
Bond lengths



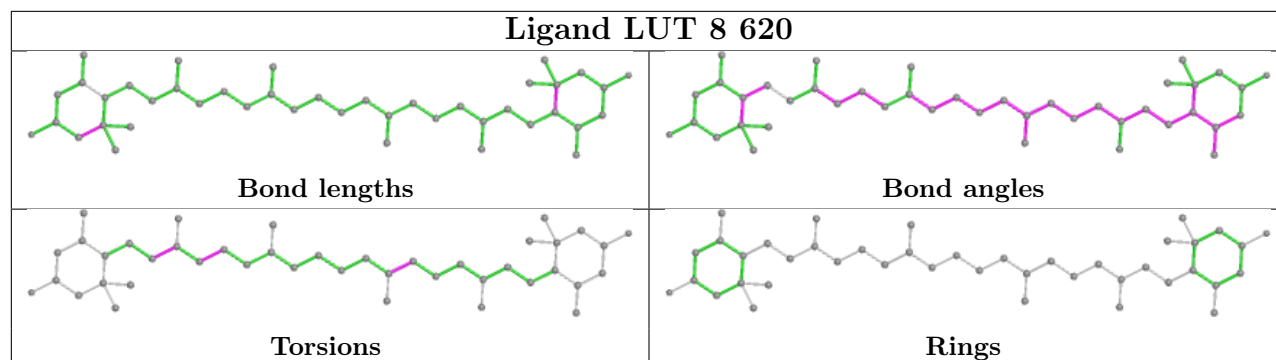
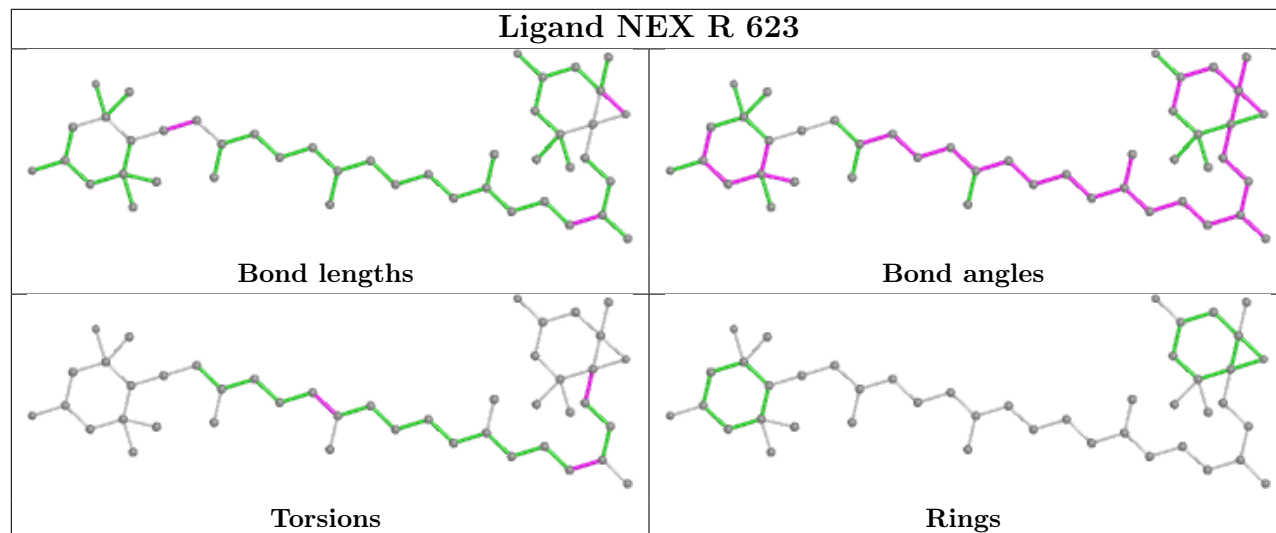
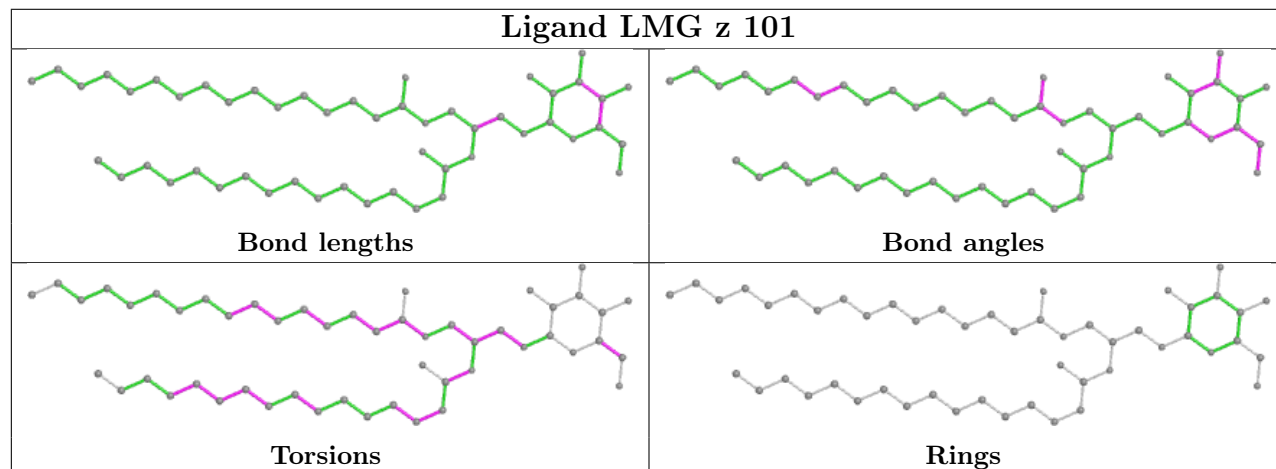
Bond angles

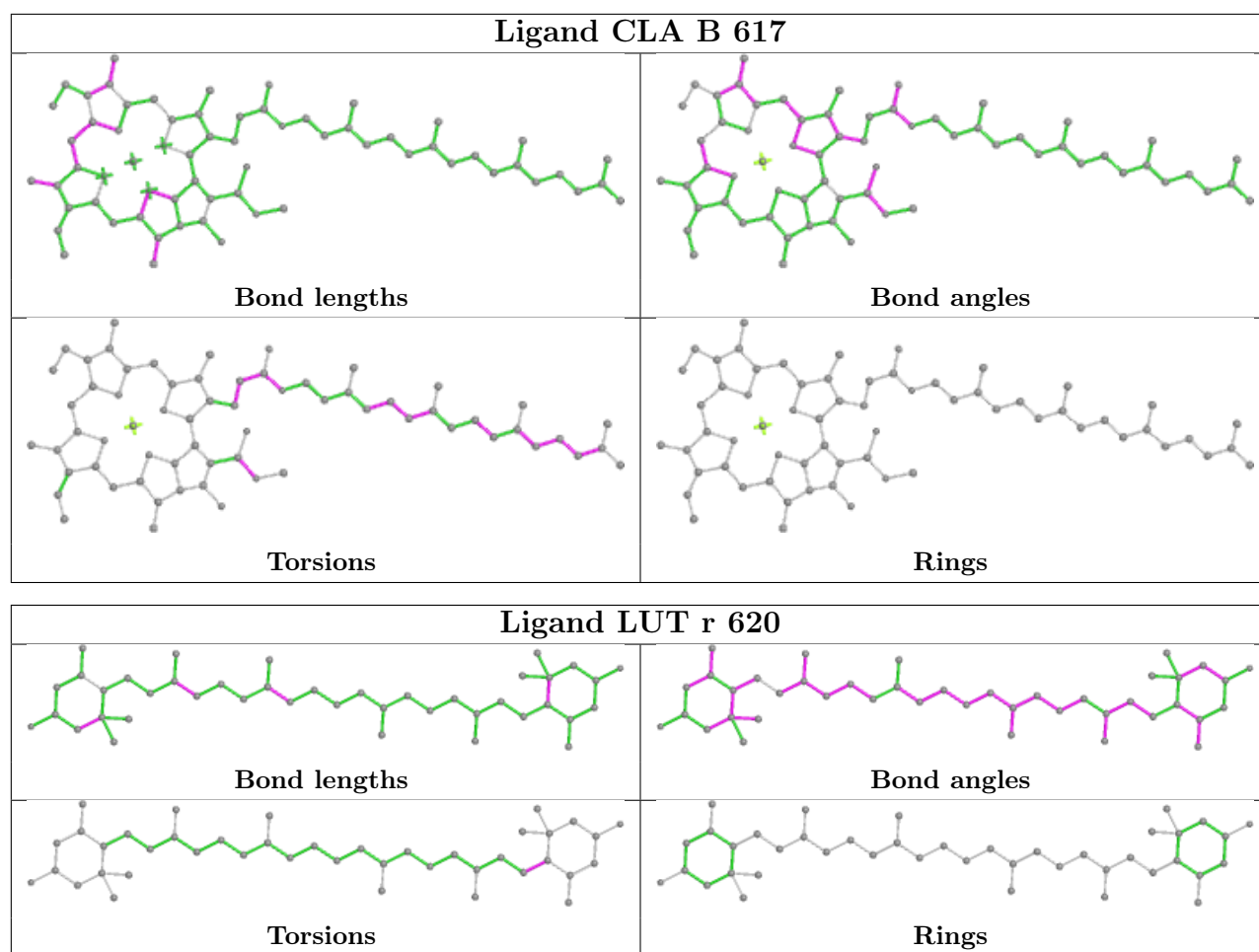


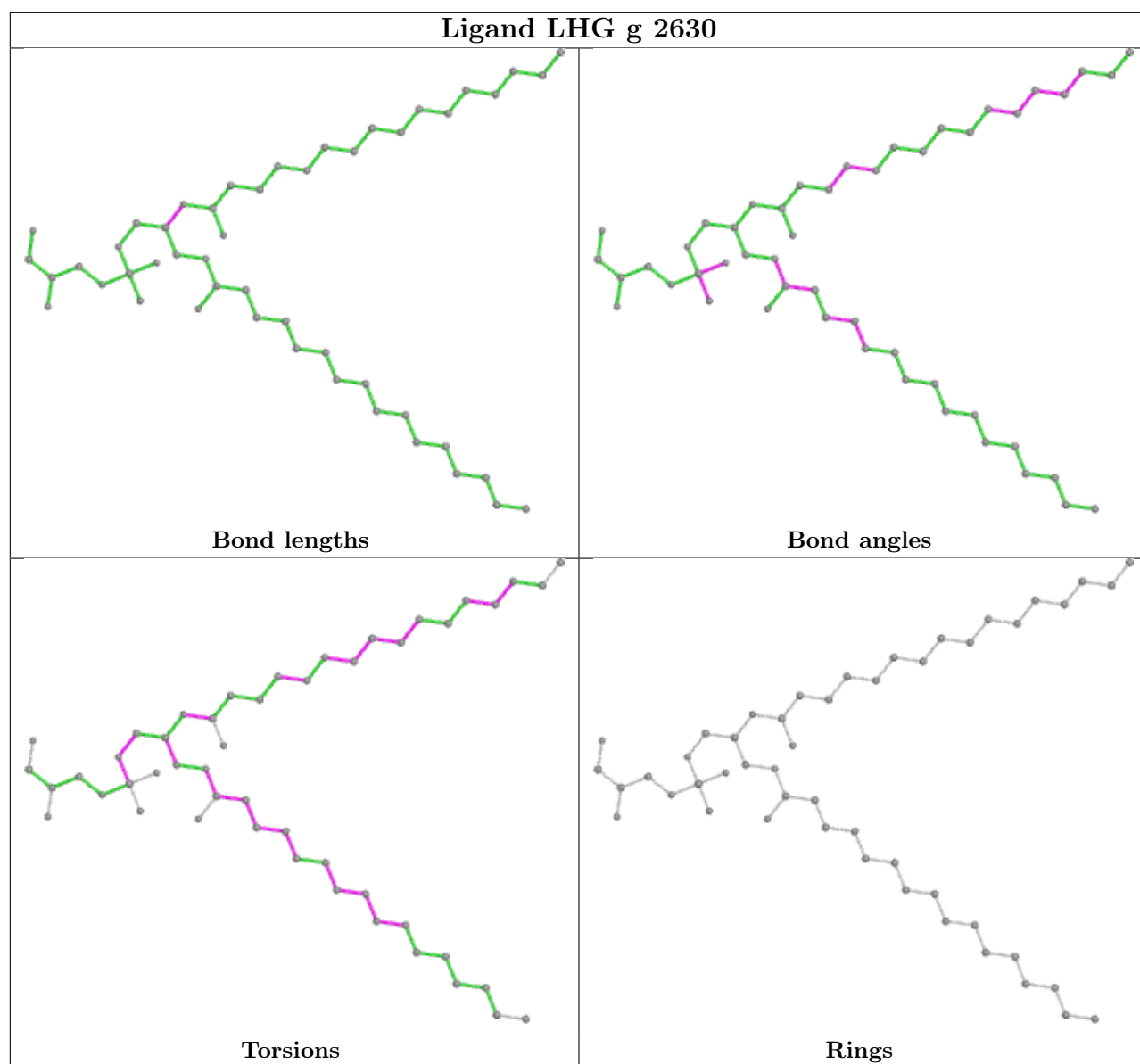
Torsions



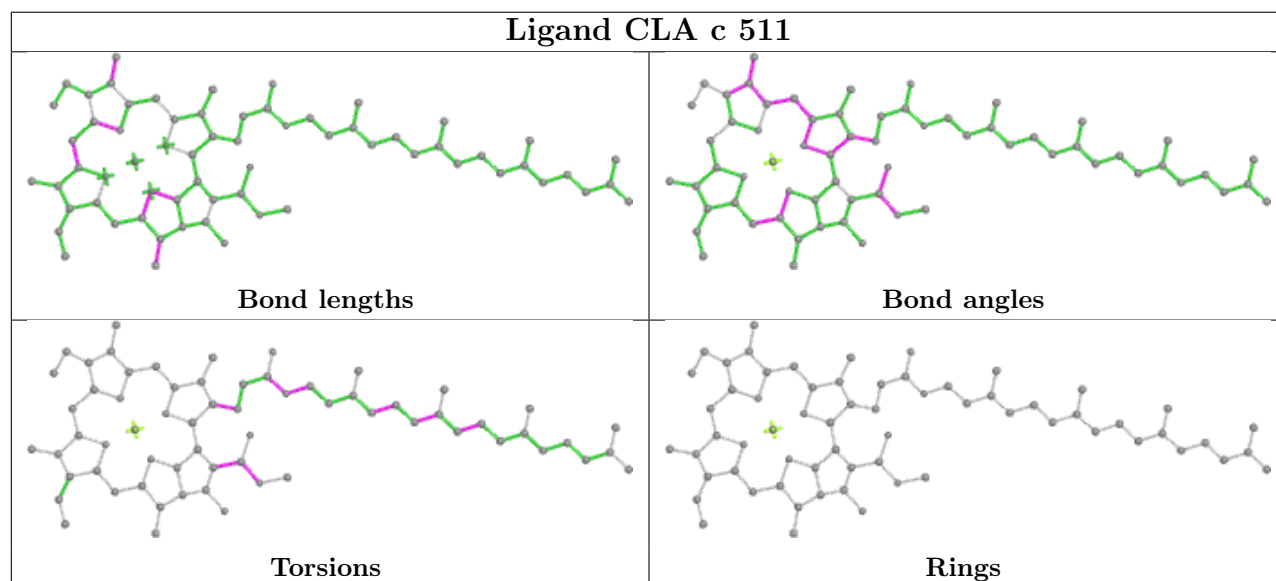
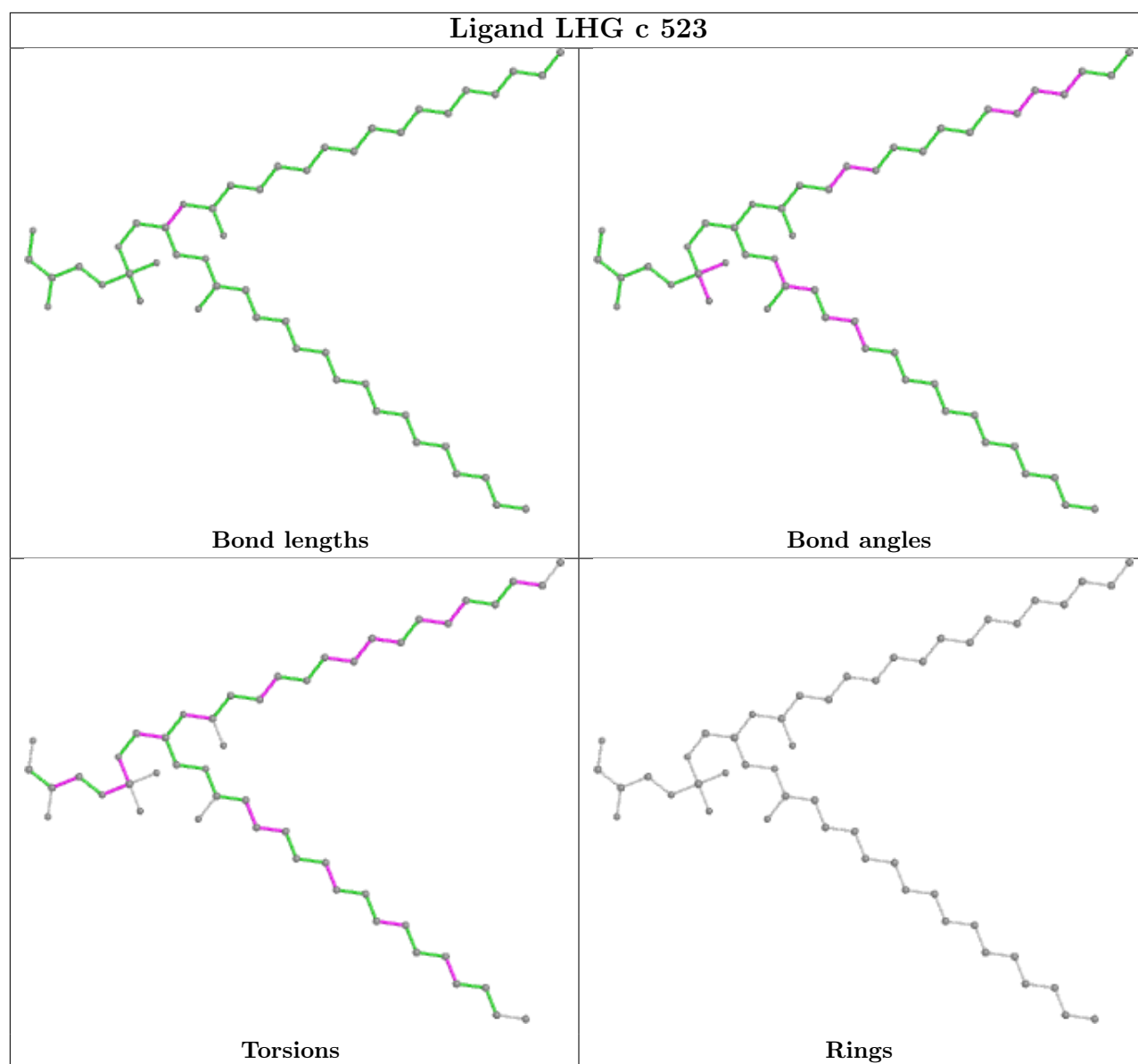
Rings

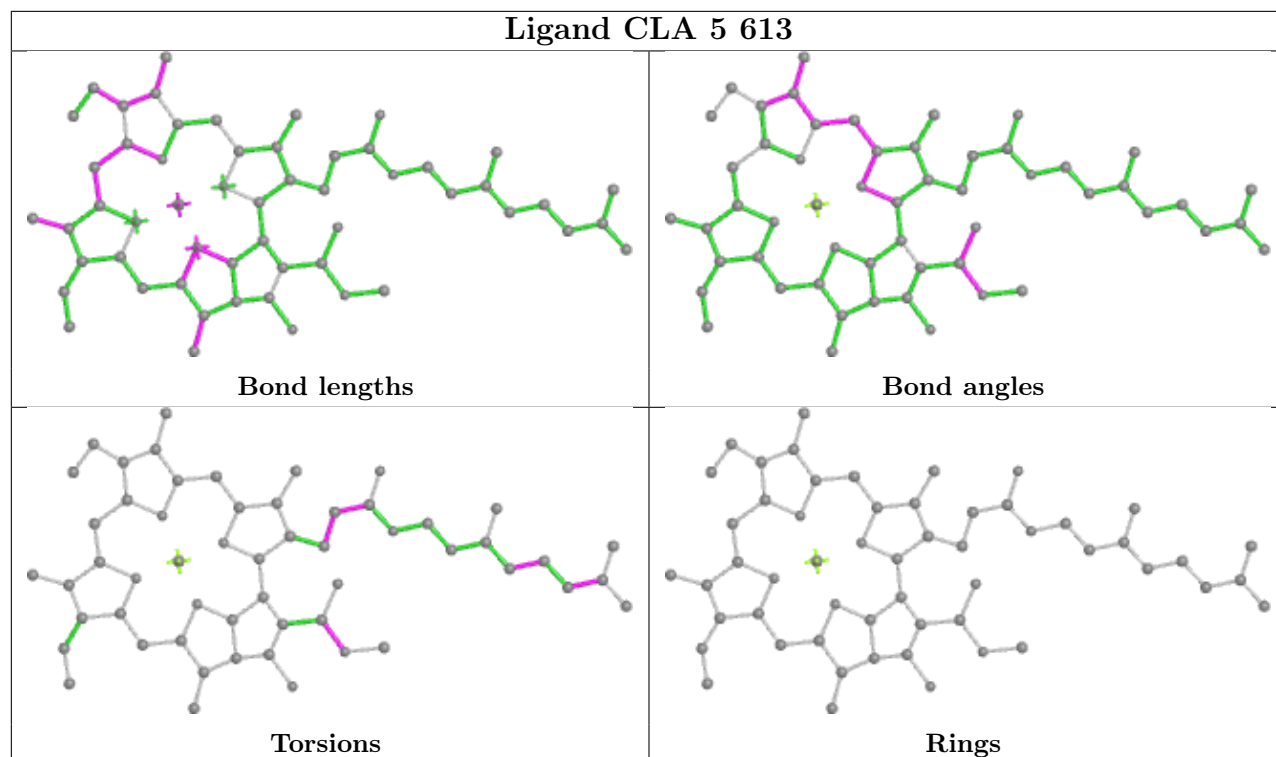
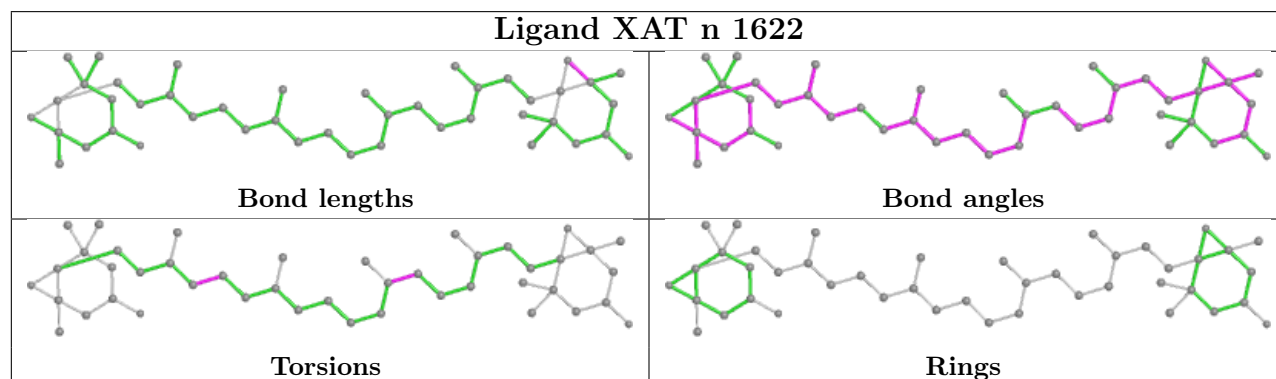
**Ligand LUT 8 620****Ligand NEX R 623****Ligand LMG z 101**



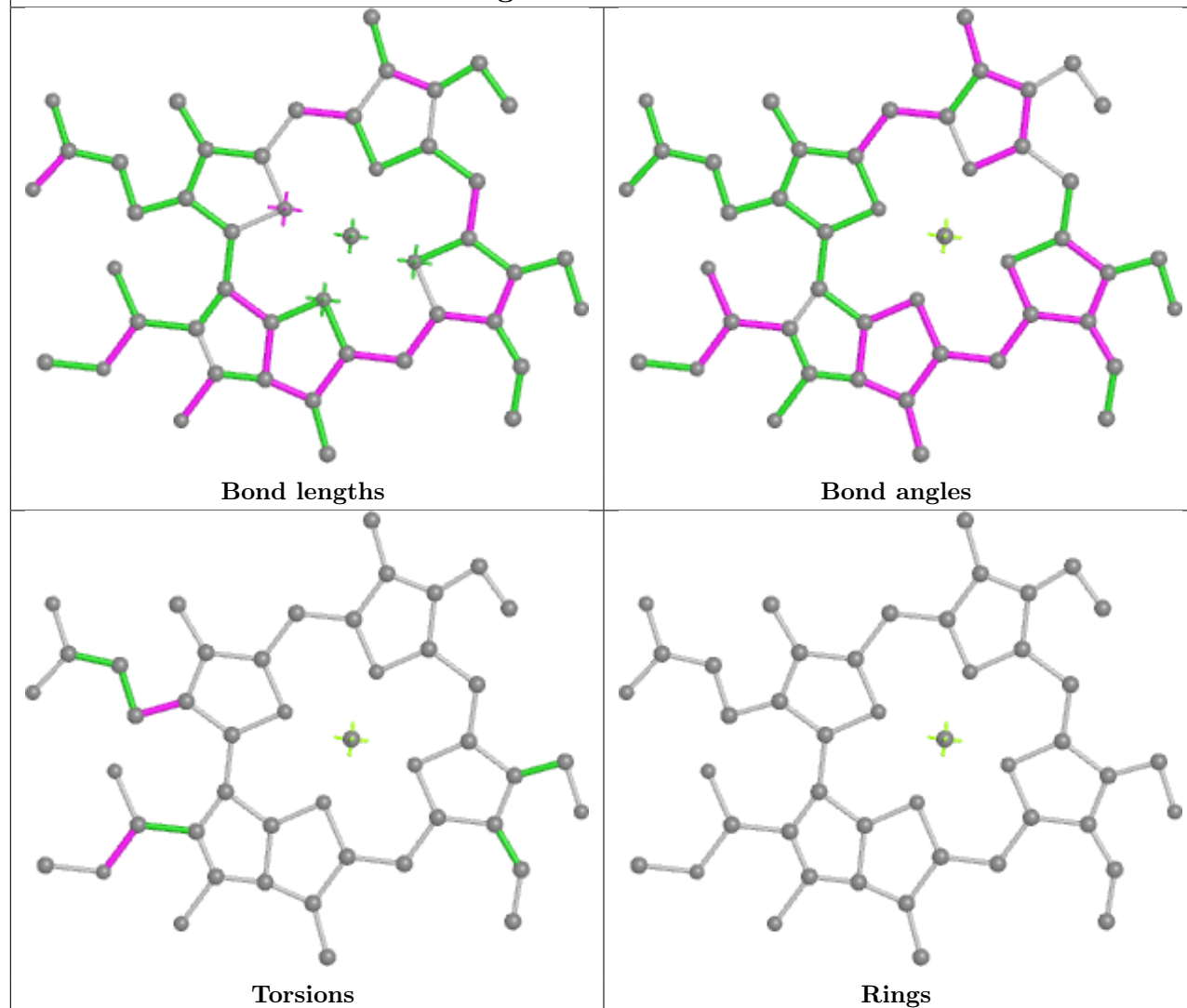




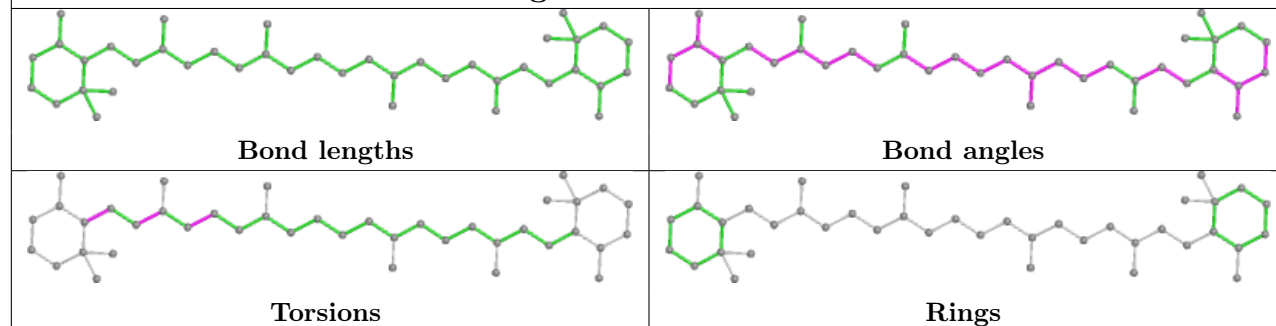


**Ligand CLA 5 613****Ligand XAT n 1622**

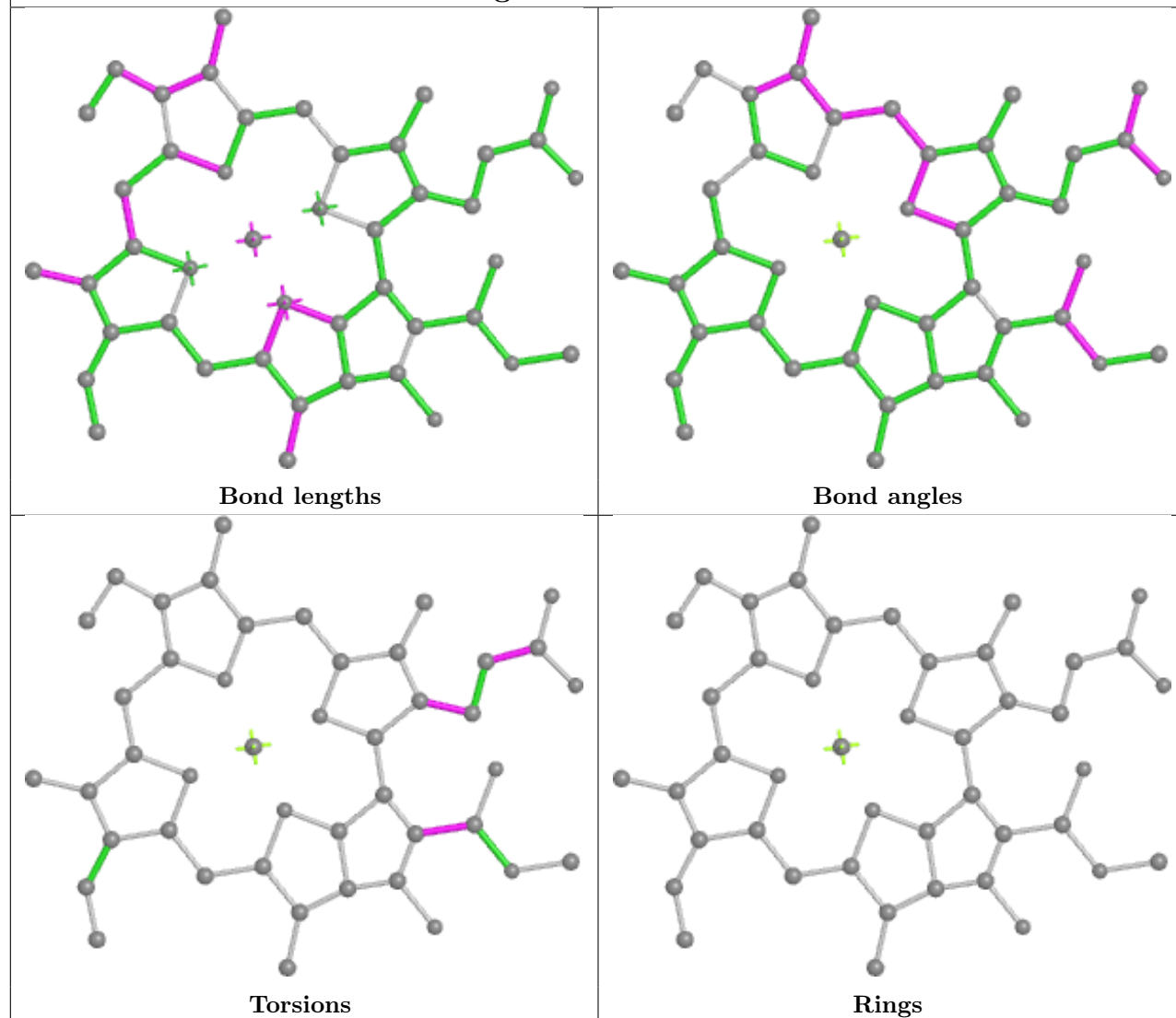
## Ligand CHL S 608



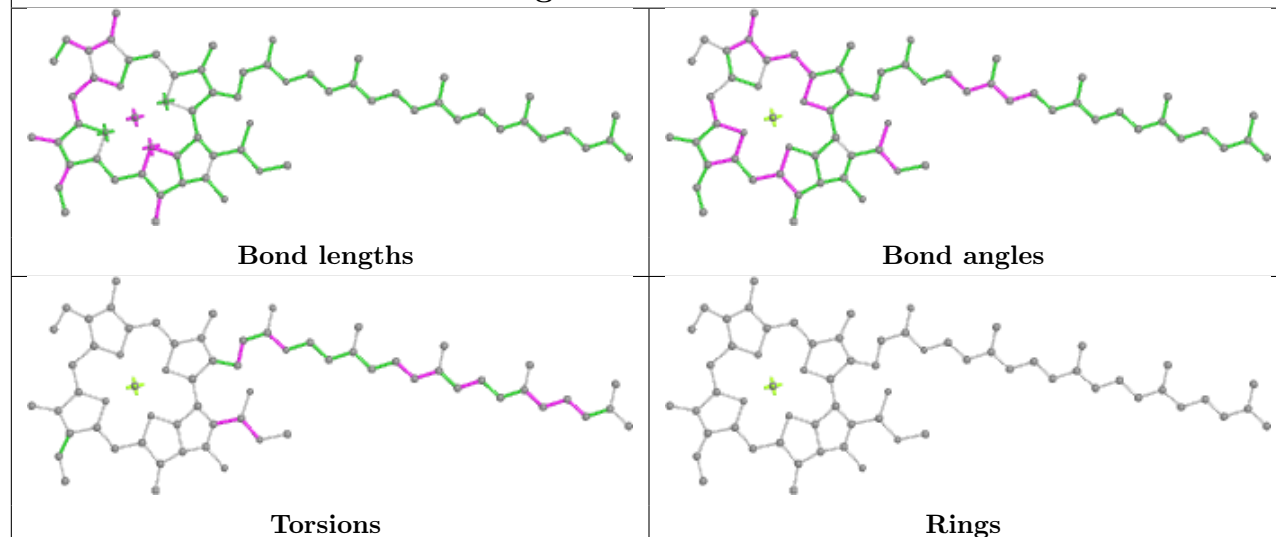
## Ligand BCR D 404



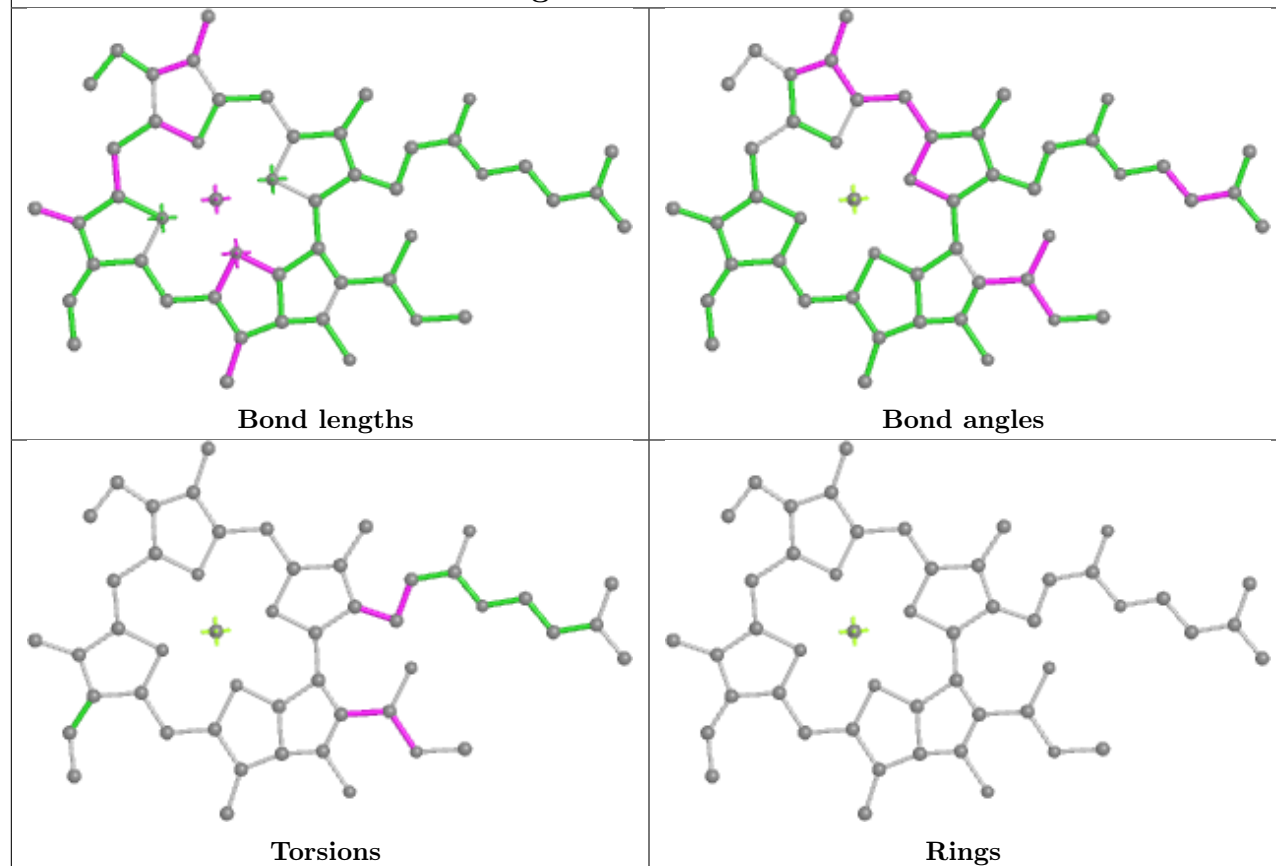
## Ligand CLA 4 610



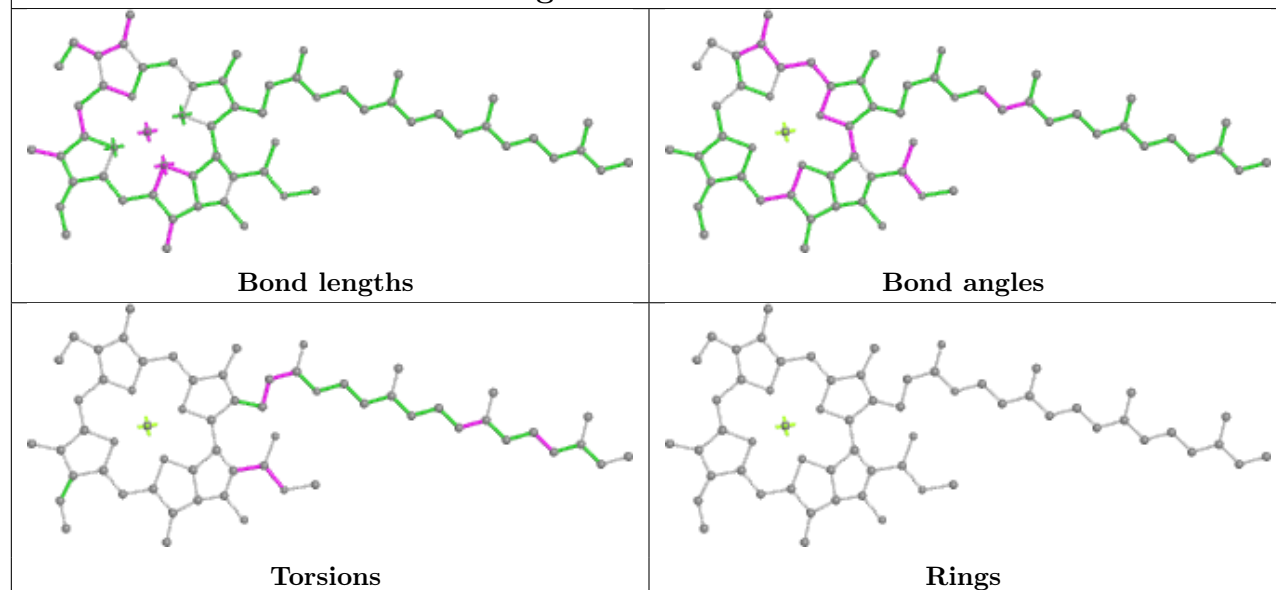
## Ligand CLA b 606

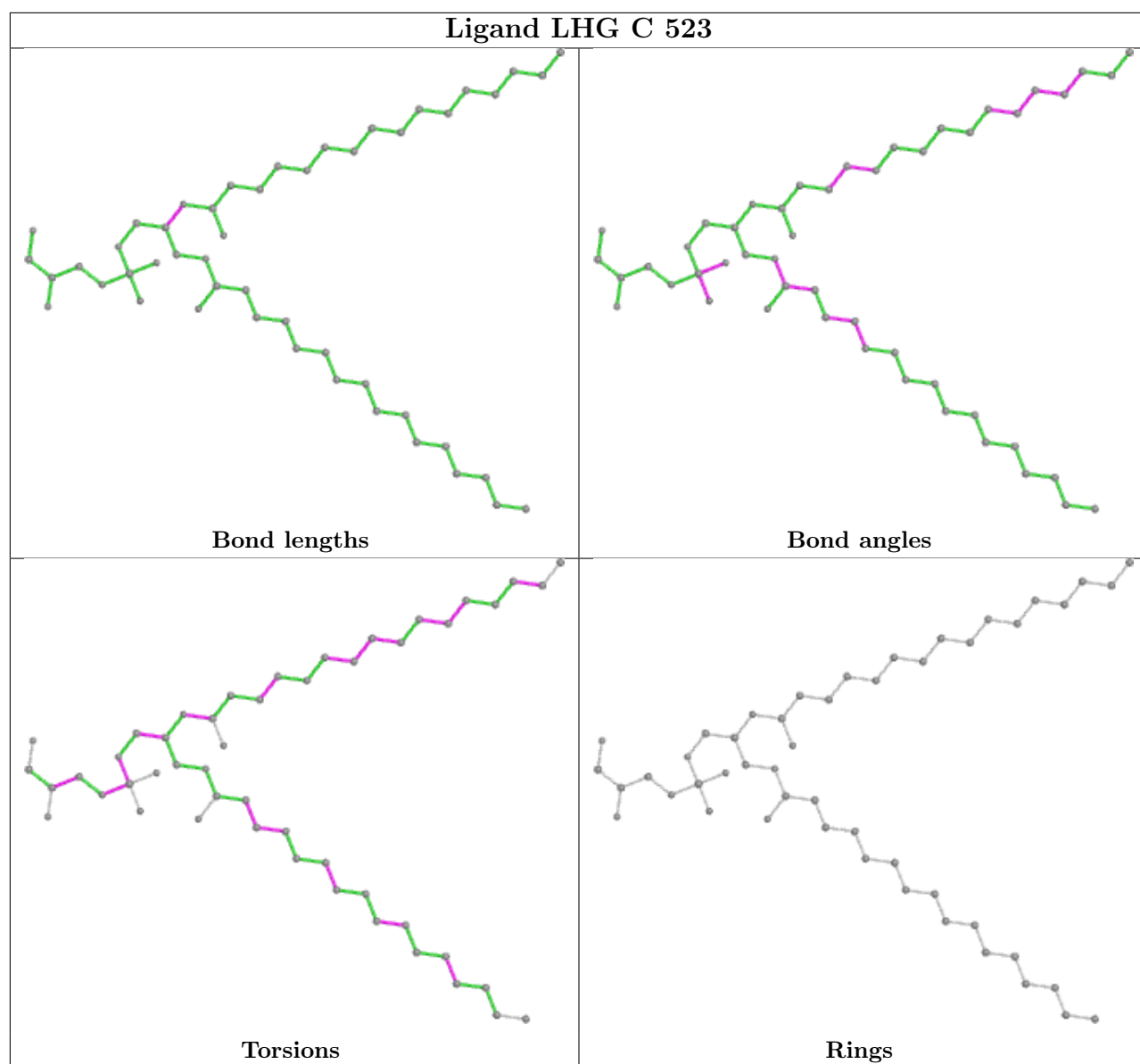


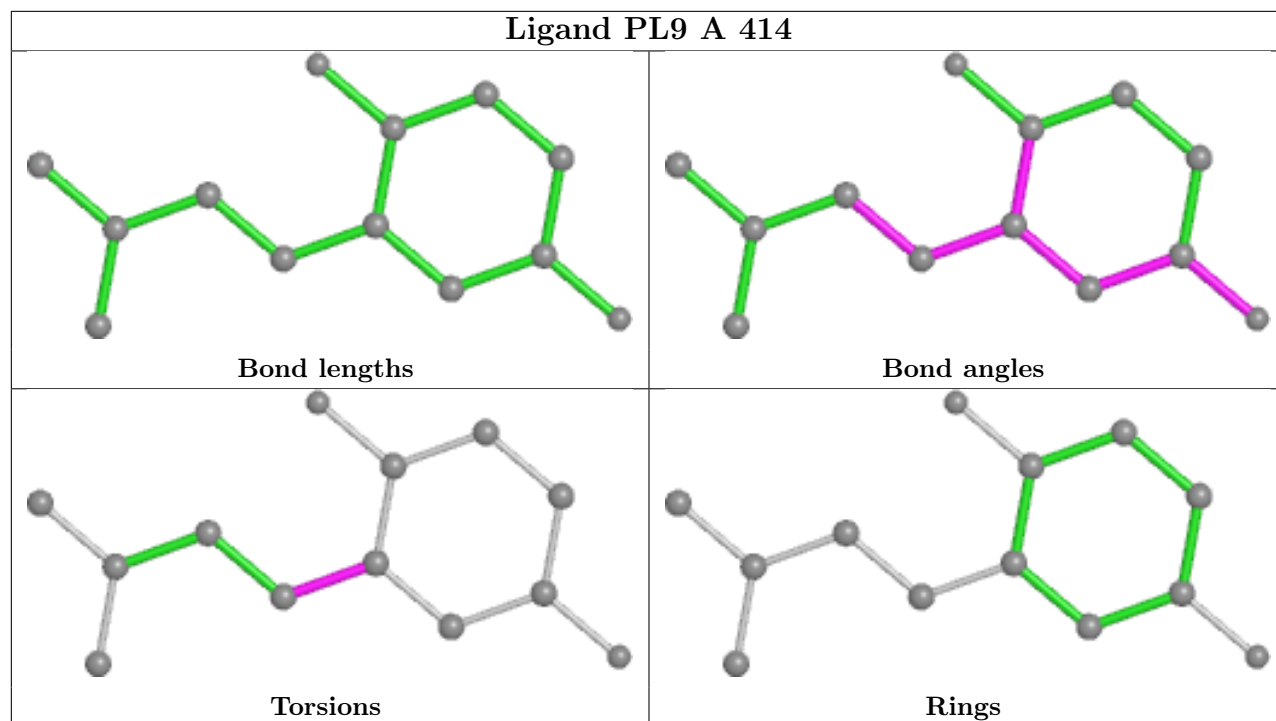
## Ligand CLA Y 604



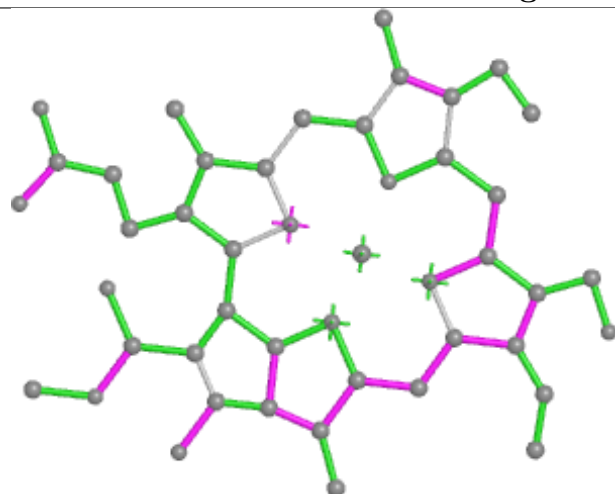
## Ligand CLA 5 602



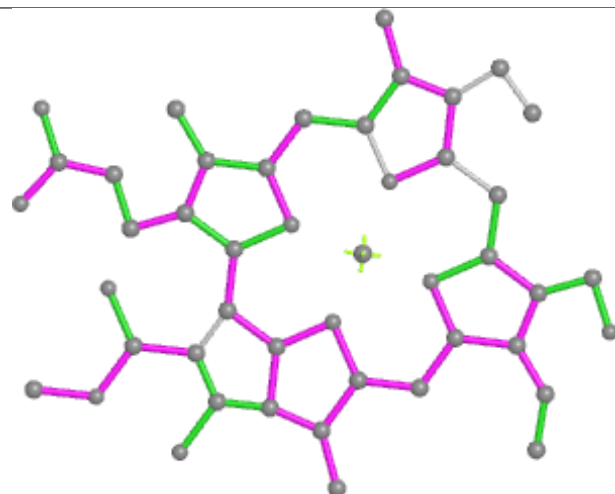




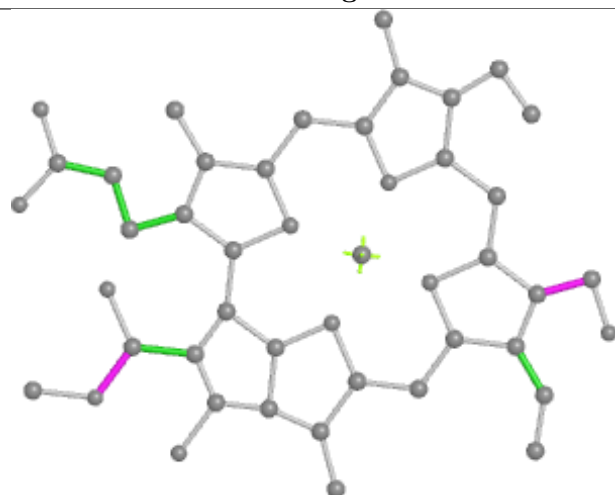
## Ligand CHL 6 606



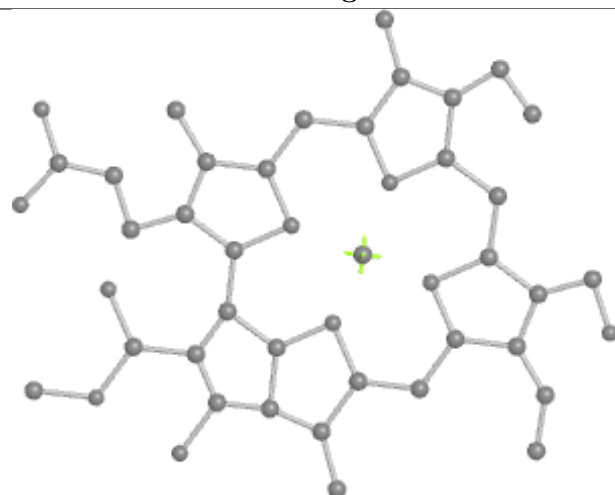
Bond lengths



Bond angles



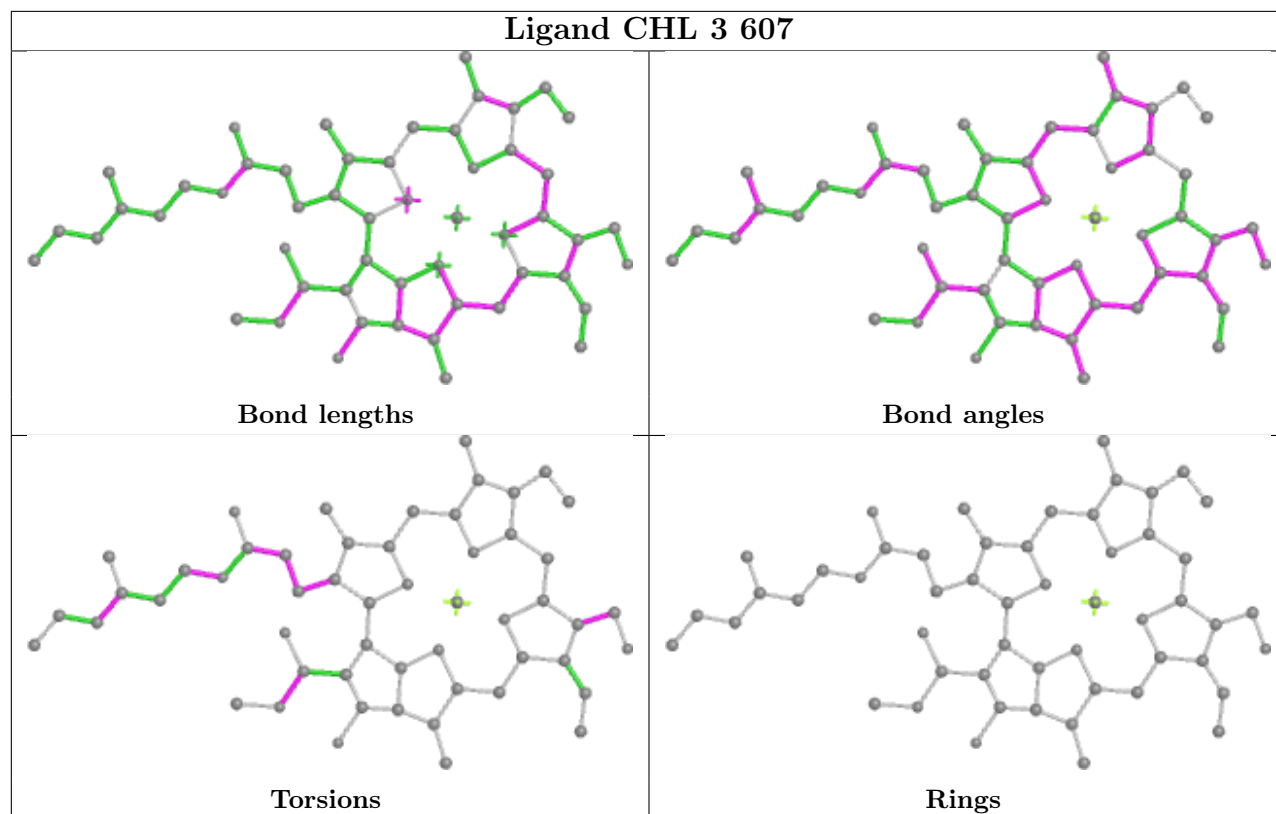
Torsions



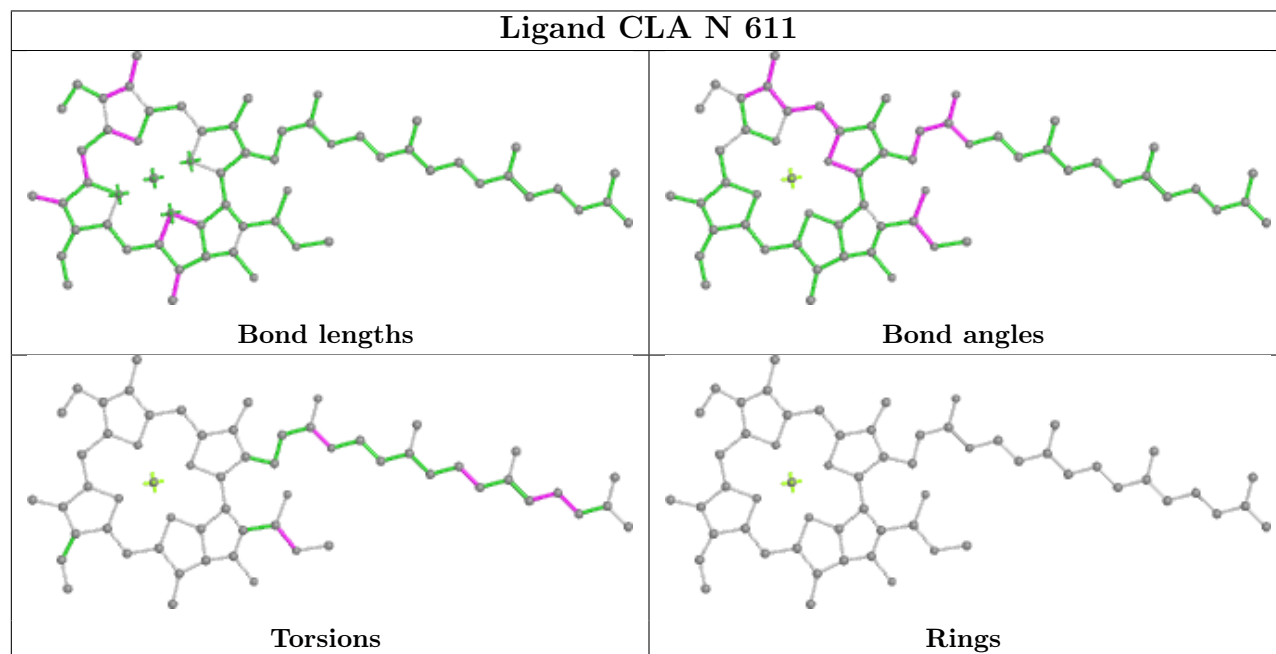
Rings

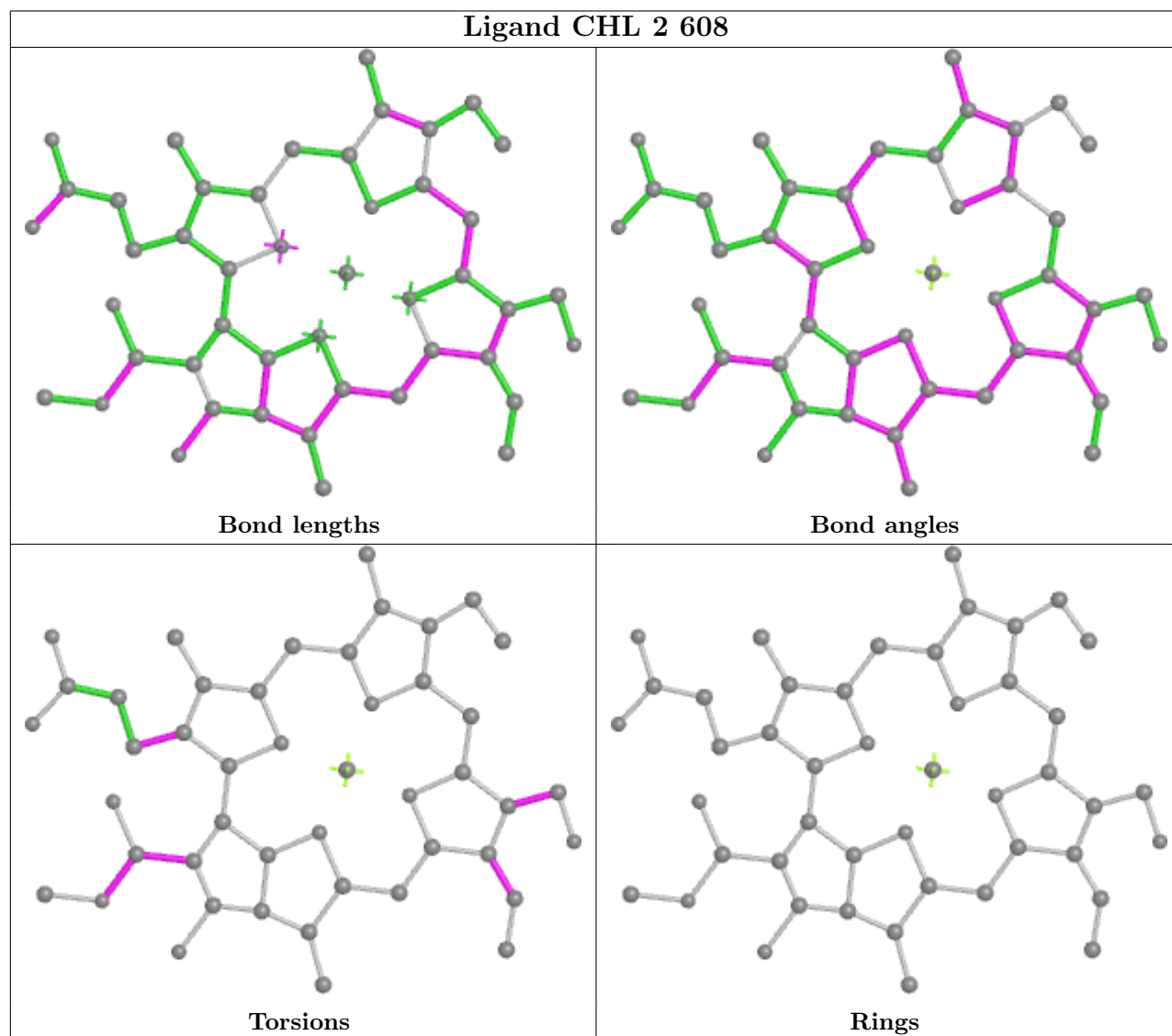
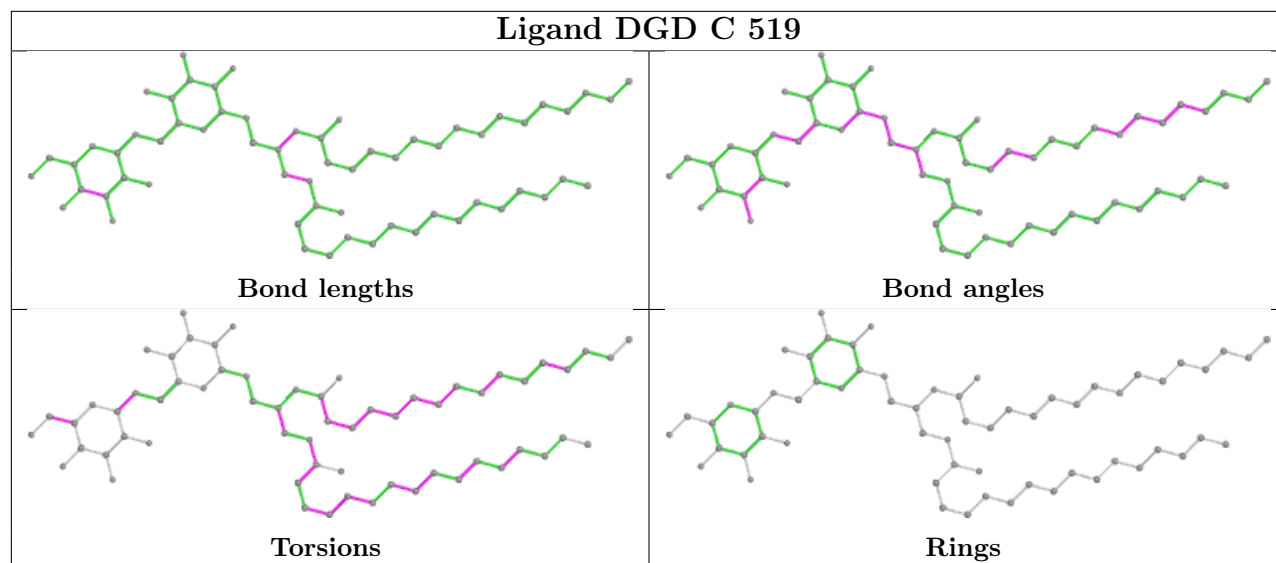


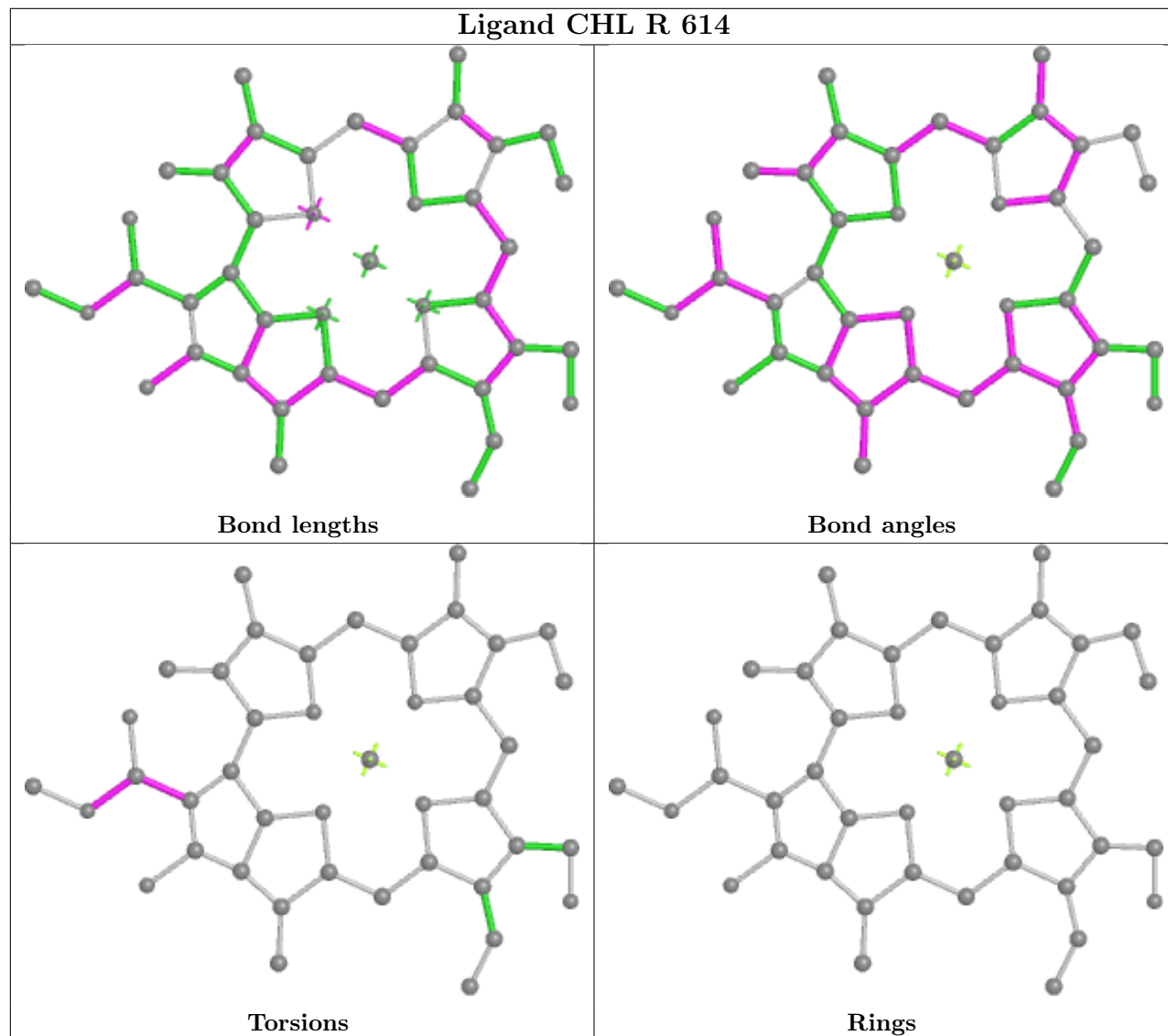
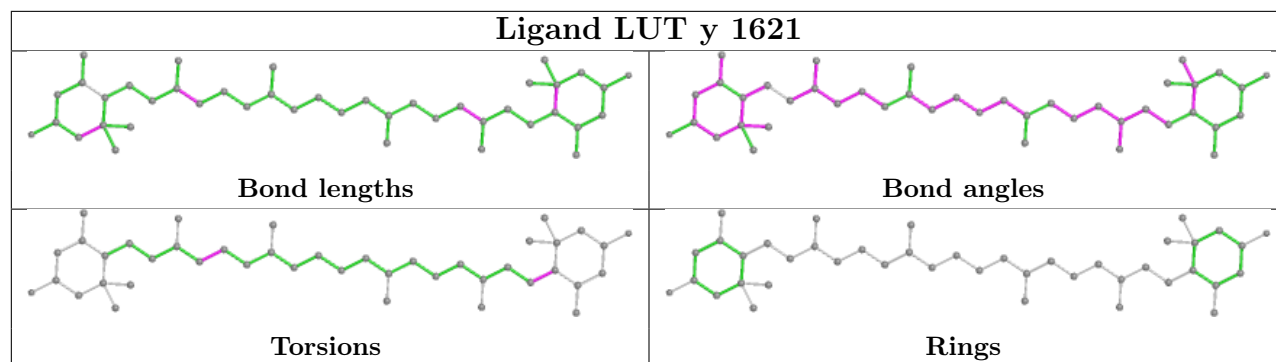
## Ligand CHL 3 607

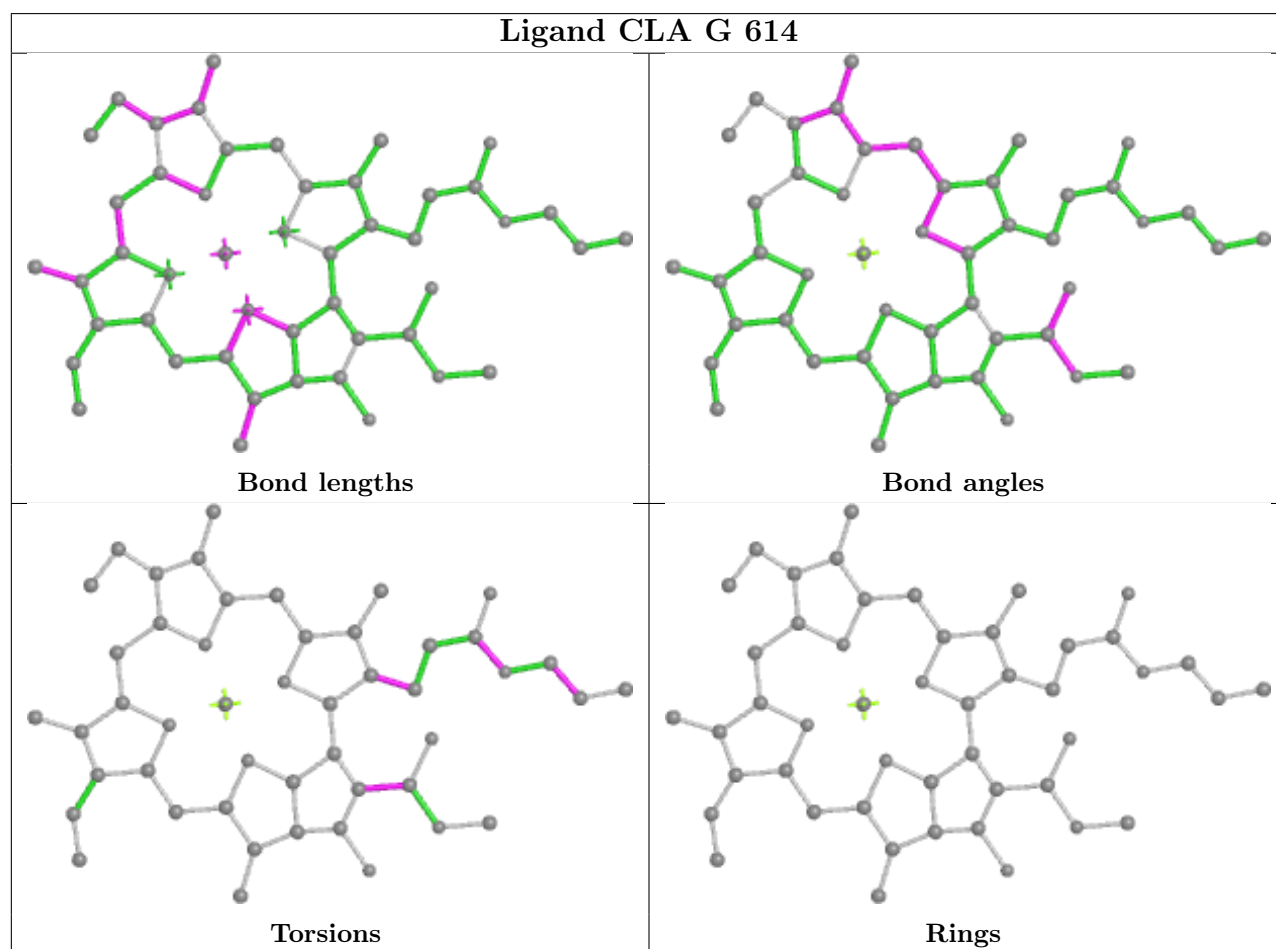
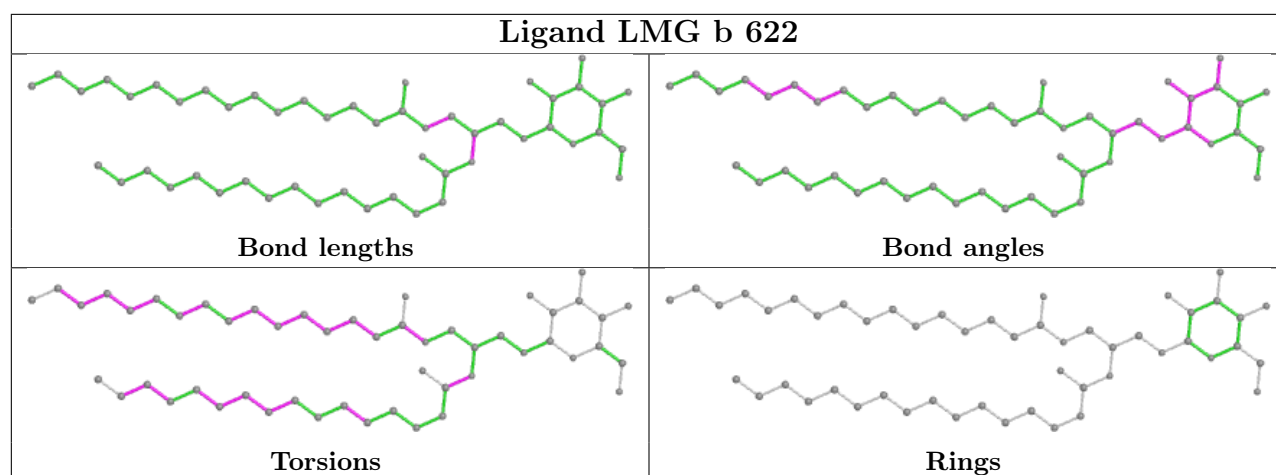


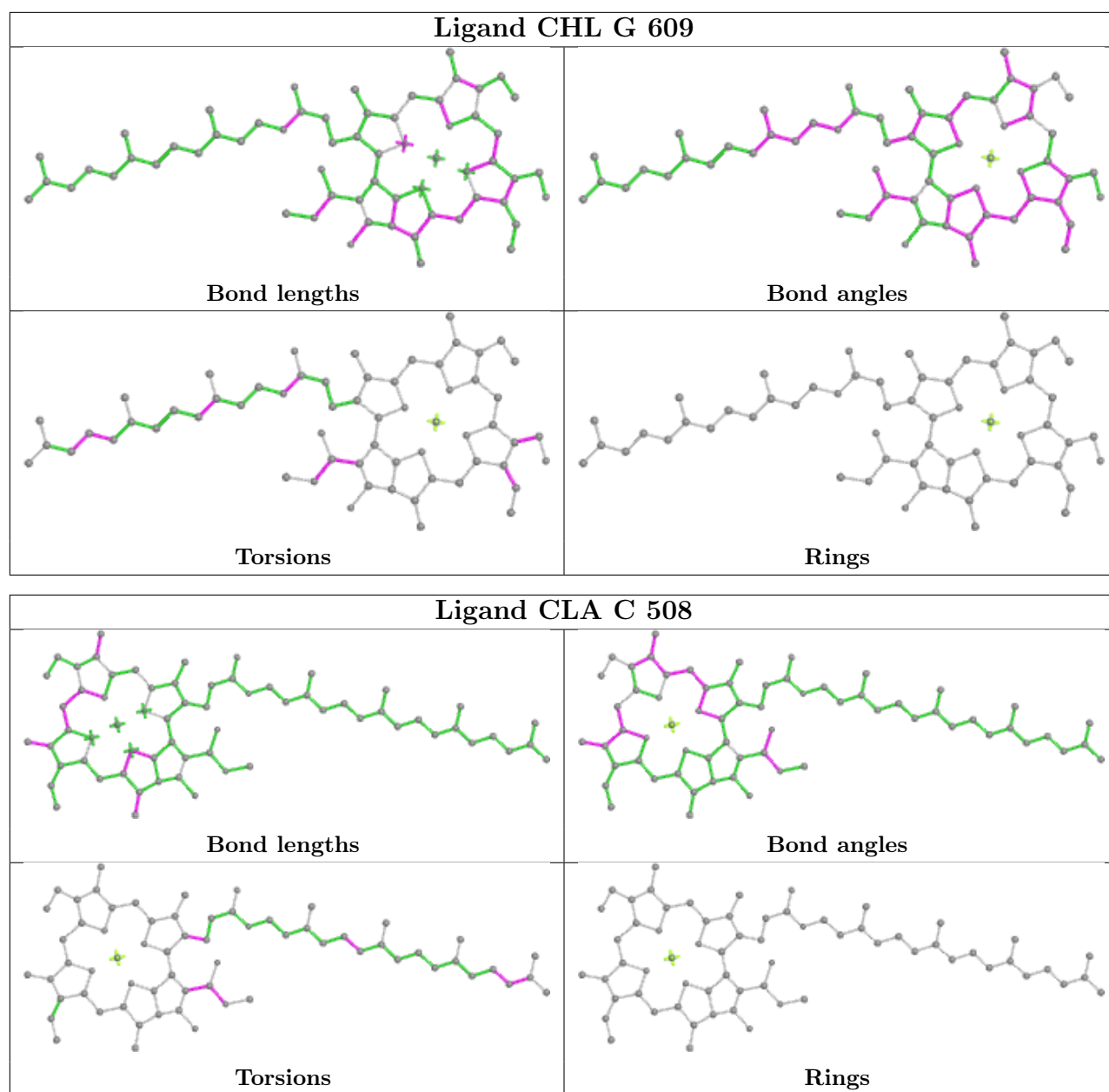
## Ligand CLA N 611

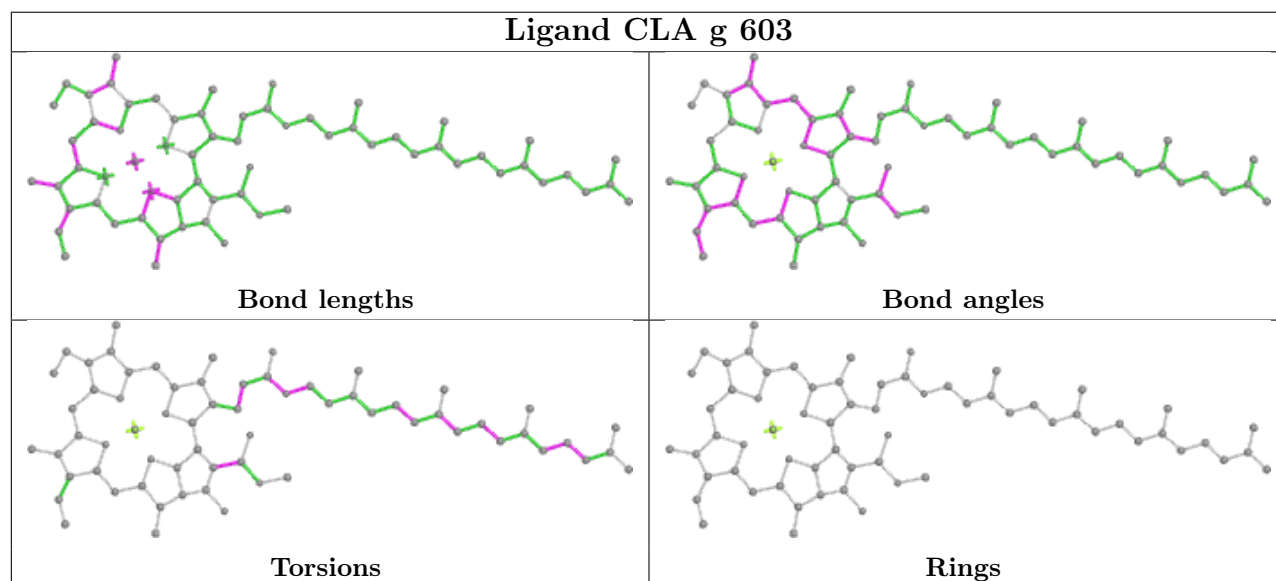
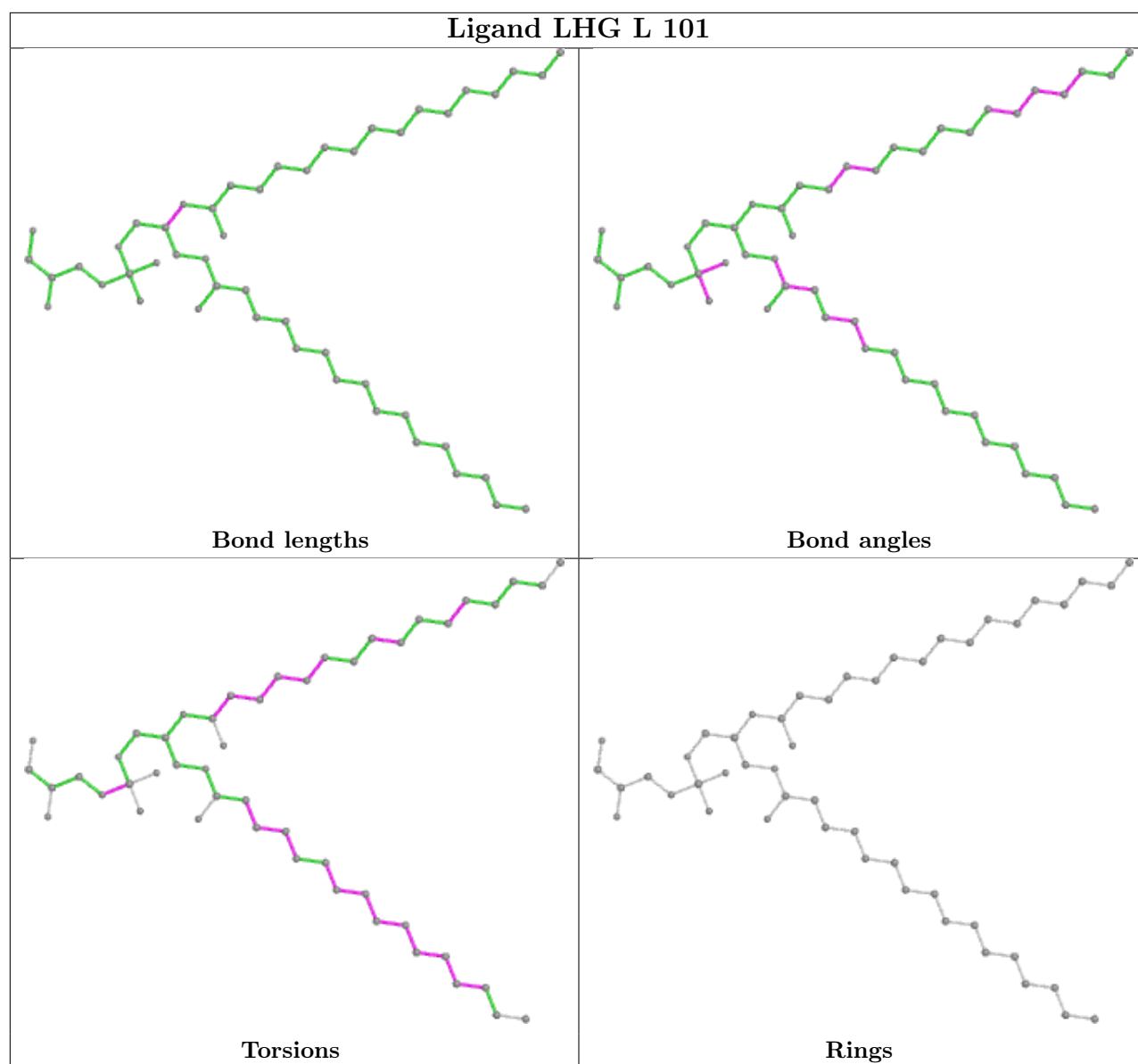


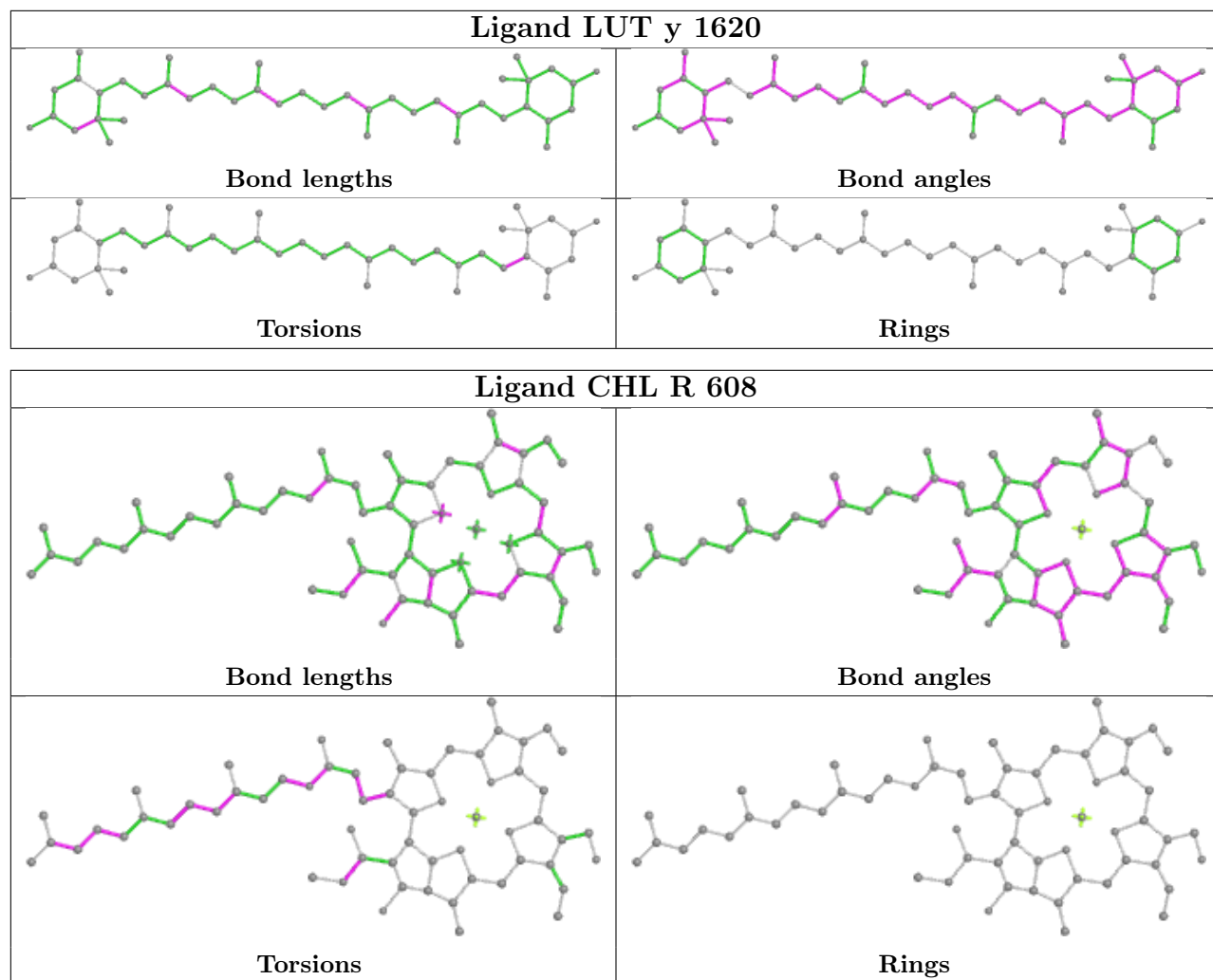


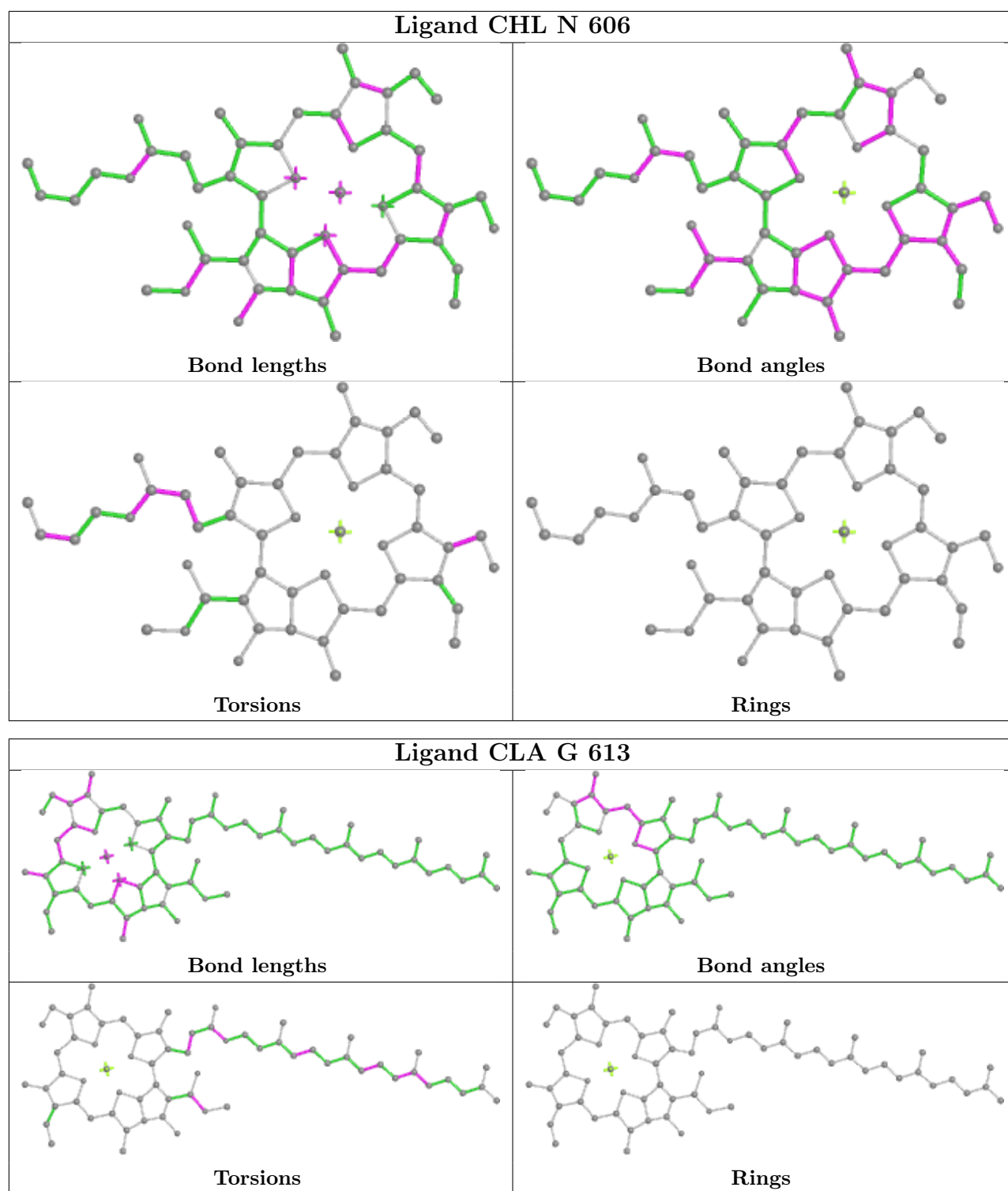




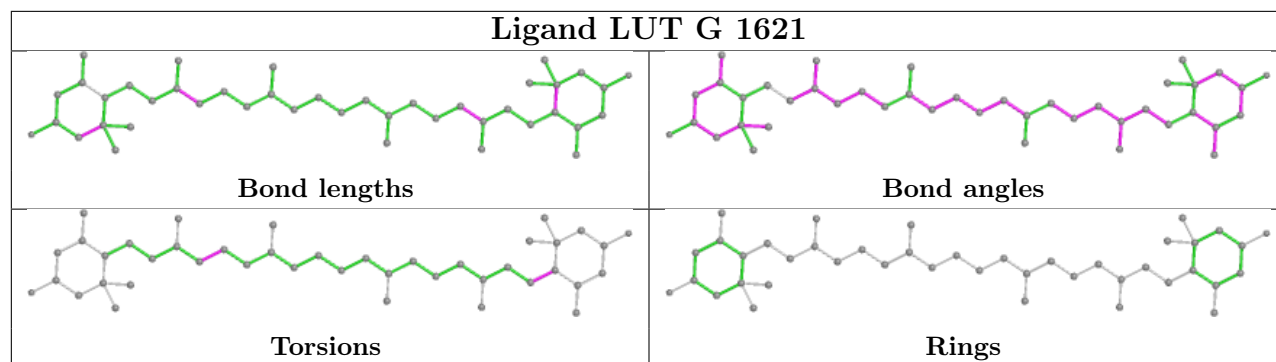












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

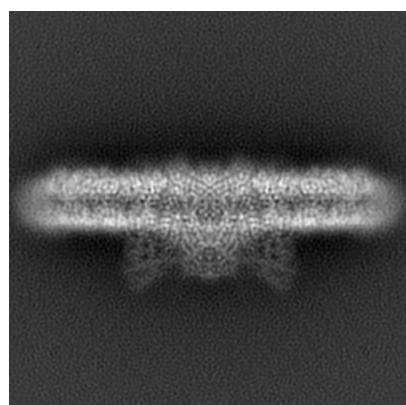
## 6 Map visualisation [i](#)

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

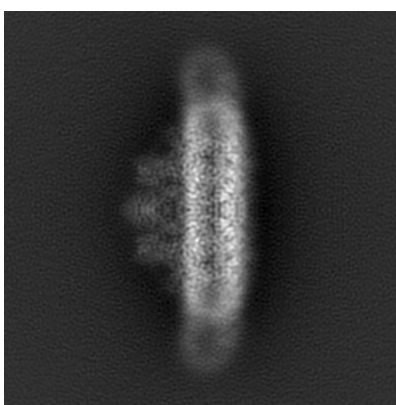
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

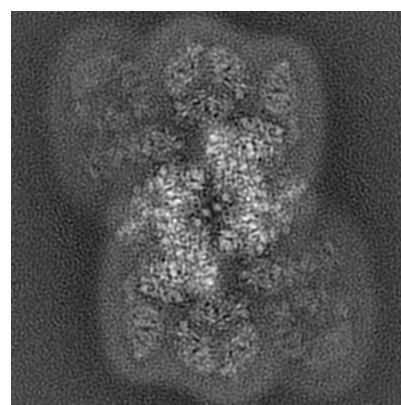
#### 6.1.1 Primary map



X



Y

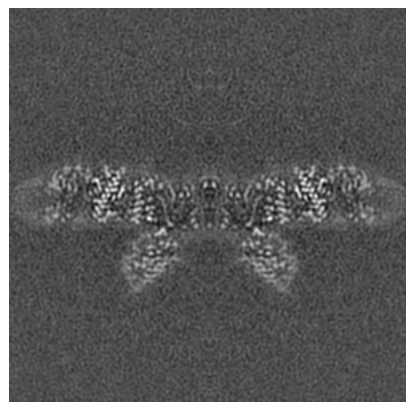


Z

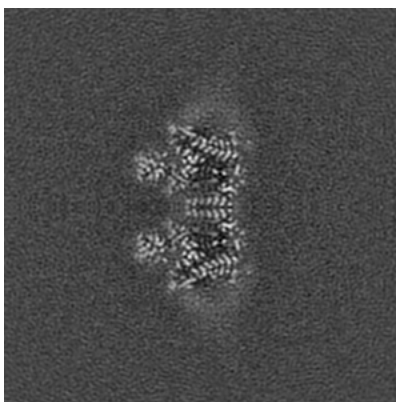
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

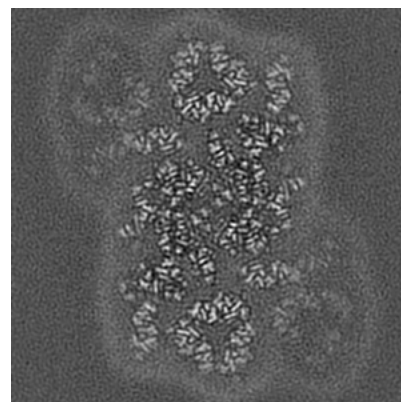
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

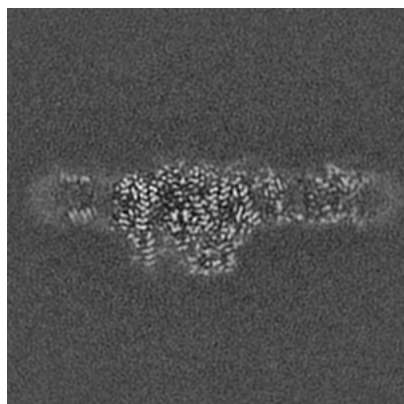


Z Index: 150

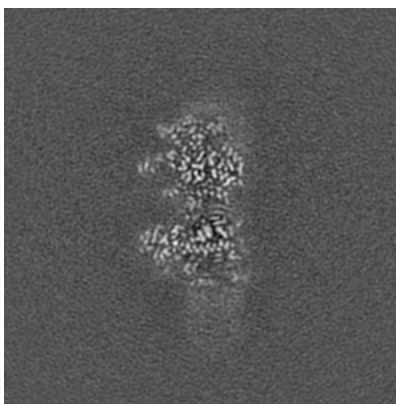
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

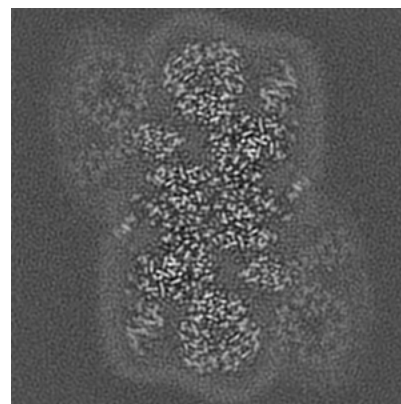
### 6.3.1 Primary map



X Index: 122



Y Index: 162

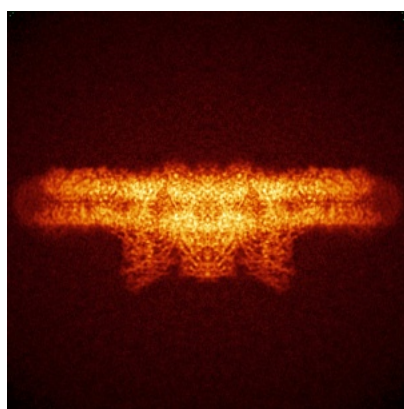


Z Index: 164

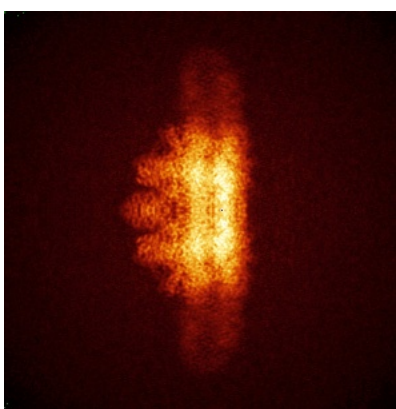
The images above show the largest variance slices of the map in three orthogonal directions.

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

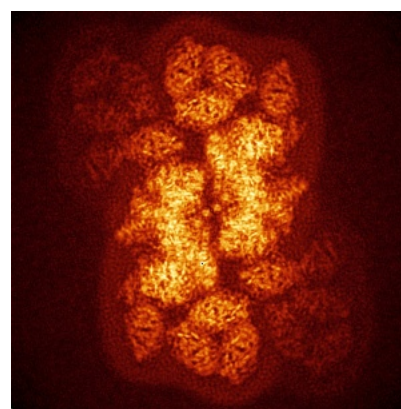
### 6.4.1 Primary map



X



Y

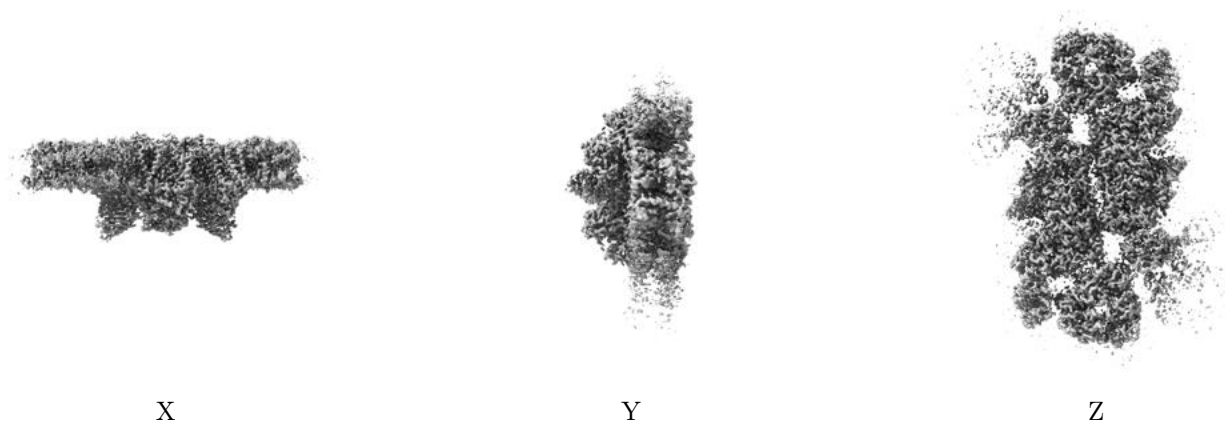


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

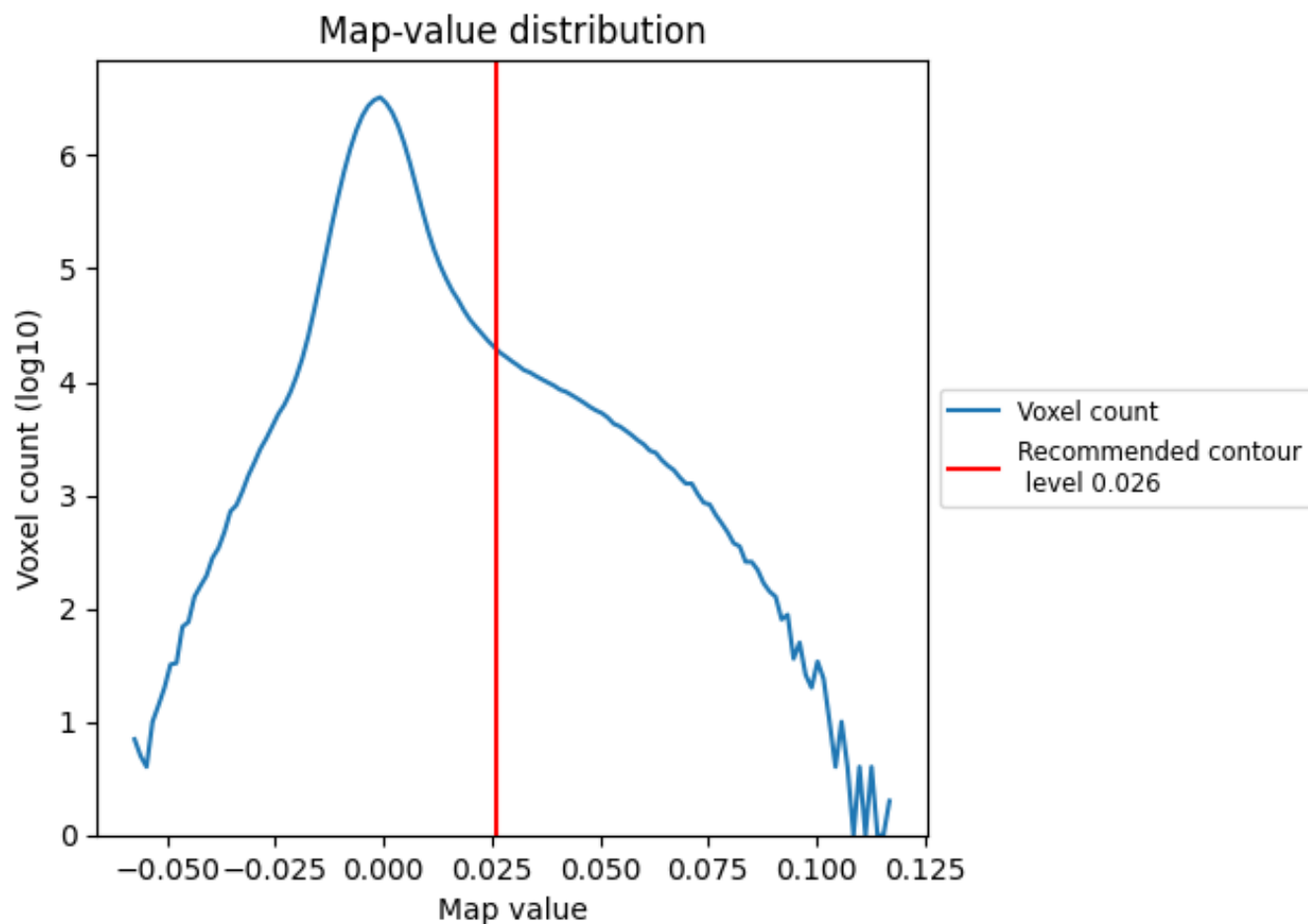
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

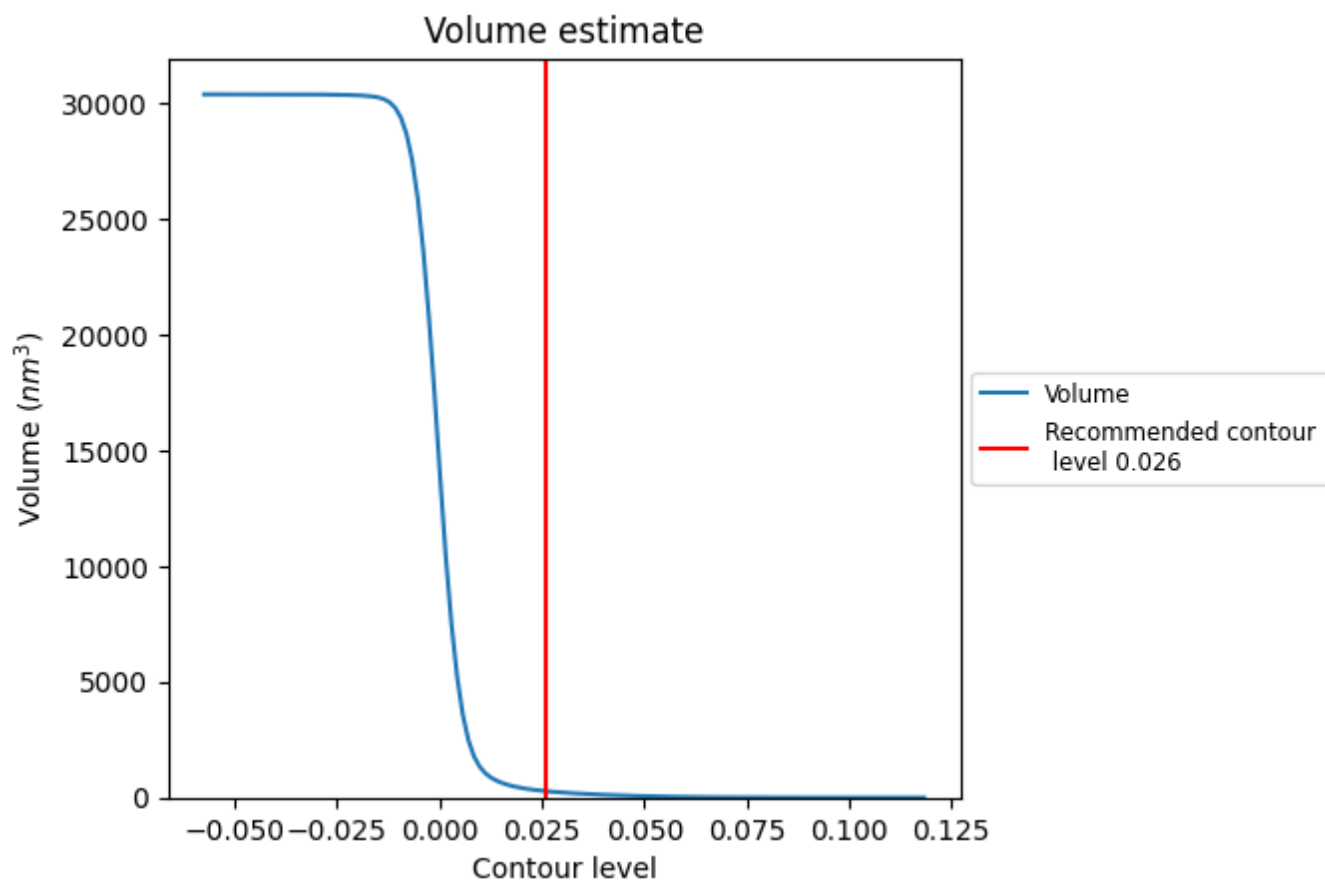
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

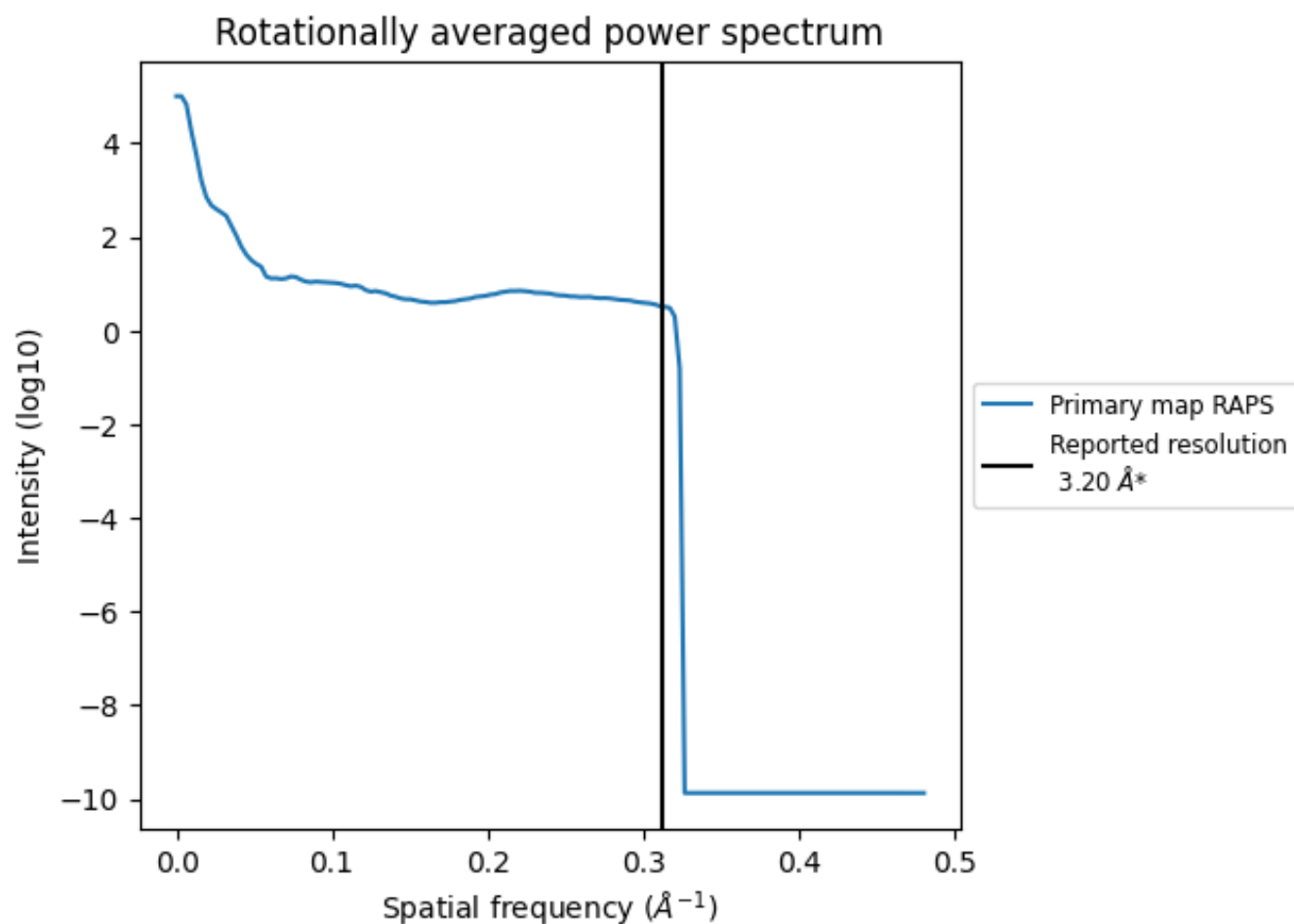
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm<sup>3</sup>; this corresponds to an approximate mass of 249 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

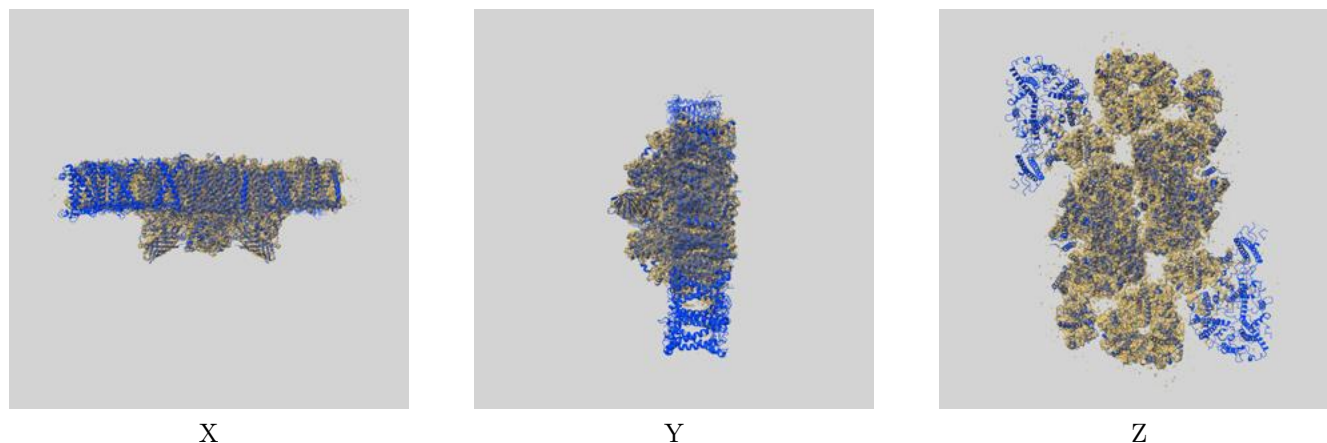
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

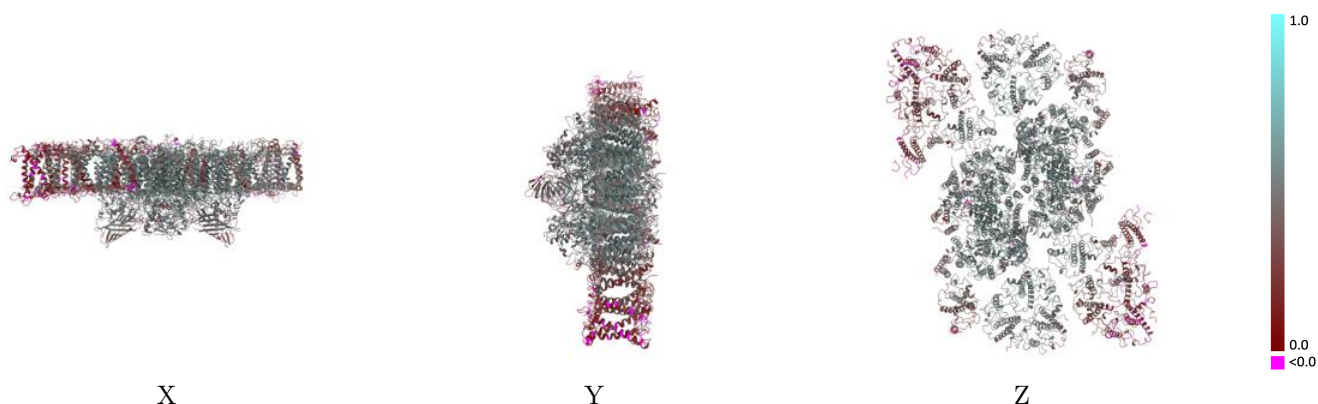
This section contains information regarding the fit between EMDB map EMD-6742 and PDB model 5XNM. Per-residue inclusion information can be found in section [3](#) on page [48](#).

### 9.1 Map-model overlay [i](#)



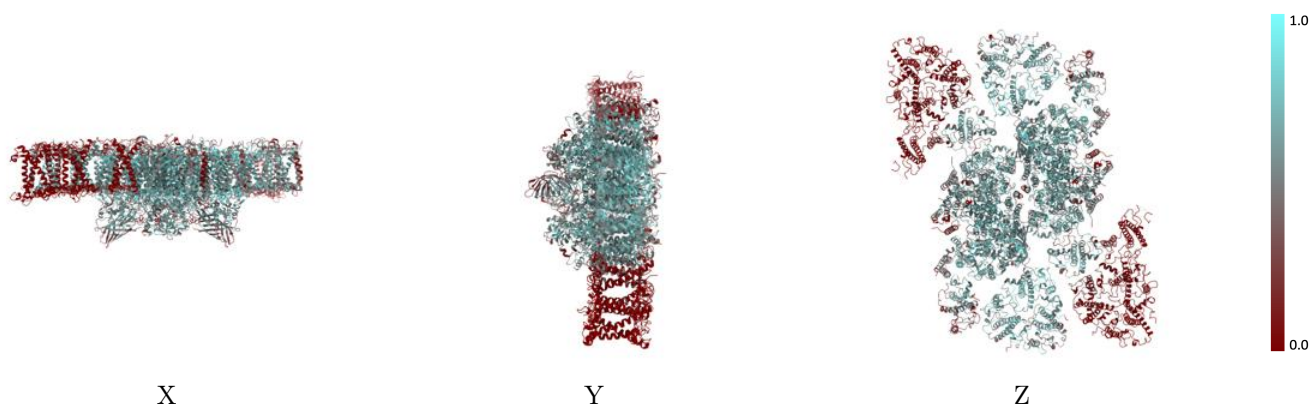
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



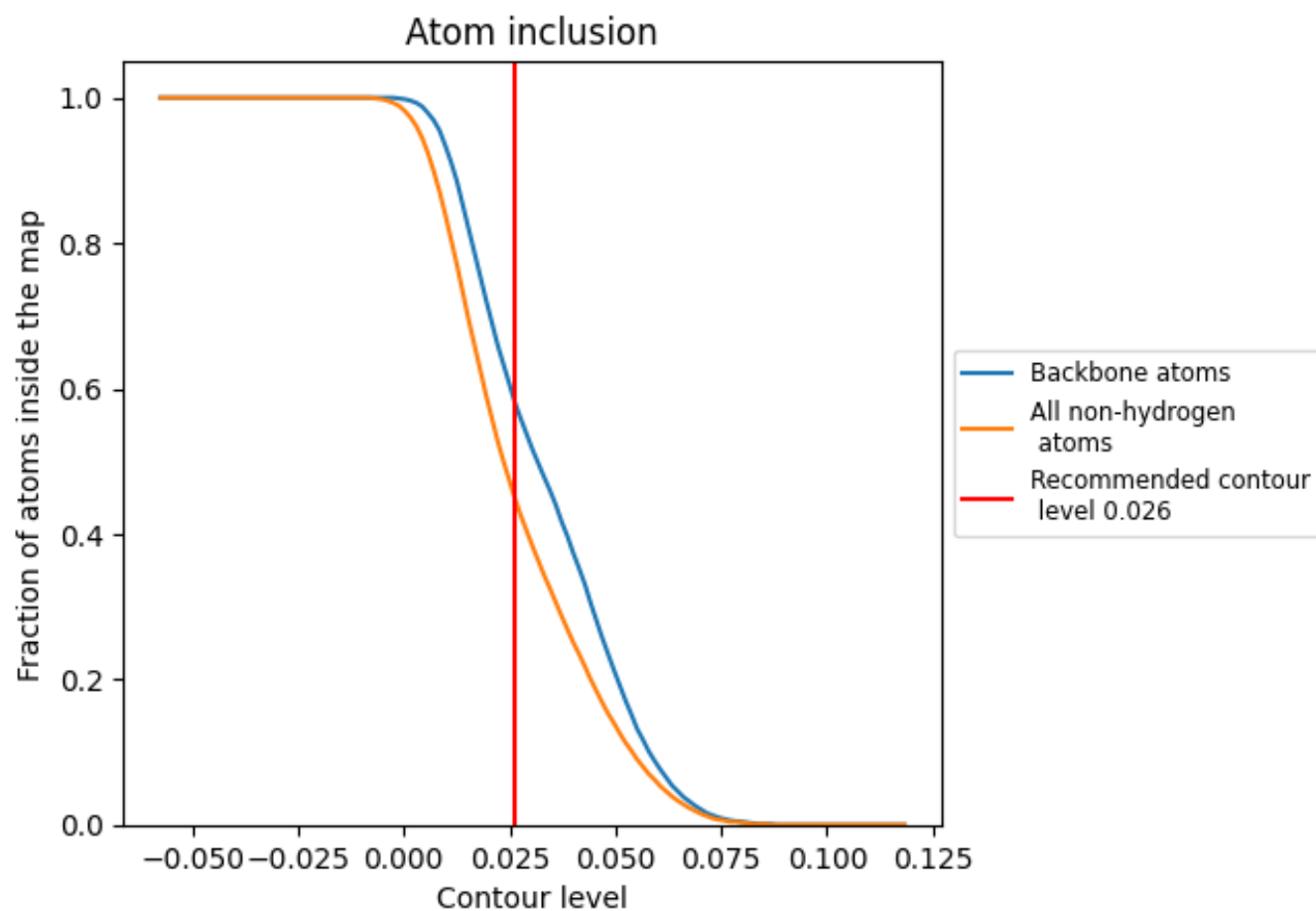
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



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

## 9.5 Map-model fit summary ⓘ









































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

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



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*Continued from previous page...*

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