



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 05:25 AM JST

PDB ID : 6KAD
EMDB ID : EMD-9956
Title : Cryo-EM structure of the C2S2M2L2-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Sheng, X.; Watanabe, A.; Li, A.J.; Kim, E.; Song, C.; Murata, K.; Song, D.F.; Minagawa, J.; Liu, Z.F.
Deposited on : 2019-06-21
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

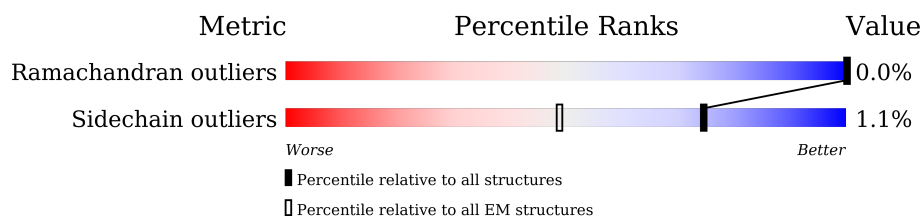
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	256	
1	1	256	
1	6	256	
1	7	256	
1	Y	256	
1	y	256	
2	2	257	
2	3	257	
2	5	257	

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Mol	Chain	Length	Quality of chain
2	8	257	
2	9	257	
2	N	257	
2	n	257	
2	p	257	
3	4	249	
3	G	249	
3	g	249	
3	q	249	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	461	
6	c	461	
7	D	352	
7	d	352	
8	E	82	
8	e	82	
9	F	44	
9	f	44	
10	H	88	
10	h	88	
11	I	37	
11	i	37	

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Mol	Chain	Length	Quality of chain
12	J	42	 5% 83% 17%
12	j	42	 5% 83% 17%
13	K	46	 5% 80% 20%
13	k	46	 5% 80% 20%
14	L	38	 95% . .
14	l	38	 95% . .
15	M	34	 5% 88% 12%
15	m	34	 5% 88% 12%
16	O	291	 9% 78% . 21%
16	o	291	 9% 78% . 21%
17	R	280	 5% 85% . 14%
17	r	280	 5% 85% . 14%
18	S	289	 5% 87% . 13%
18	s	289	 5% 87% . 13%
19	T	31	 94% . .
19	t	31	 94% . .
20	V	33	 5% 97% .
20	v	33	 5% 97% .
21	W	115	 49% 51%
21	w	115	 49% 51%
22	X	101	 34% 66%
22	x	101	 34% 66%
23	Z	62	 5% 98% .
23	z	62	 5% 97% . .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	0	601	X	-	-	-
24	CHL	0	605	X	-	-	-
24	CHL	0	606	X	-	-	-
24	CHL	0	607	X	-	-	-
24	CHL	0	608	X	-	-	-
24	CHL	0	609	X	-	-	-
24	CHL	1	601	X	-	-	-
24	CHL	1	605	X	-	-	-
24	CHL	1	606	X	-	-	-
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	605	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	605	X	-	-	-
24	CHL	8	606	X	-	-	-
24	CHL	8	607	X	-	-	-
24	CHL	8	608	X	-	-	-
24	CHL	8	609	X	-	-	-
24	CHL	9	601	X	-	-	-
24	CHL	9	605	X	-	-	-
24	CHL	9	606	X	-	-	-
24	CHL	9	607	X	-	-	-
24	CHL	9	608	X	-	-	-
24	CHL	9	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	p	601	X	-	-	-
24	CHL	p	605	X	-	-	-
24	CHL	p	606	X	-	-	-
24	CHL	p	607	X	-	-	-
24	CHL	p	608	X	-	-	-
24	CHL	p	609	X	-	-	-
24	CHL	q	601	X	-	-	-
24	CHL	q	605	X	-	-	-
24	CHL	q	606	X	-	-	-
24	CHL	q	607	X	-	-	-
24	CHL	q	608	X	-	-	-
24	CHL	q	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	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	0	602	X	-	-	-
25	CLA	0	603	X	-	-	-
25	CLA	0	604	X	-	-	-
25	CLA	0	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	0	611	X	-	-	-
25	CLA	0	612	X	-	-	-
25	CLA	0	614	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	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	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	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	4	613	X	-	-	-
25	CLA	4	614	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	-	-	-
25	CLA	5	613	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	612	X	-	-	-
25	CLA	6	614	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	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	604	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	8	614	X	-	-	-
25	CLA	9	602	X	-	-	-
25	CLA	9	603	X	-	-	-
25	CLA	9	604	X	-	-	-
25	CLA	9	610	X	-	-	-
25	CLA	9	611	X	-	-	-
25	CLA	9	612	X	-	-	-
25	CLA	9	613	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	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	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	C	513	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	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	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	605	X	-	-	-
25	CLA	S	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	610	X	-	-	-
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	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	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	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	505	X	-	-	-
25	CLA	c	506	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	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	403	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	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	p	602	X	-	-	-
25	CLA	p	603	X	-	-	-
25	CLA	p	604	X	-	-	-
25	CLA	p	610	X	-	-	-
25	CLA	p	611	X	-	-	-
25	CLA	p	612	X	-	-	-
25	CLA	p	613	X	-	-	-
25	CLA	q	602	X	-	-	-
25	CLA	q	603	X	-	-	-
25	CLA	q	610	X	-	-	-
25	CLA	q	611	X	-	-	-
25	CLA	q	612	X	-	-	-
25	CLA	q	613	X	-	-	-
25	CLA	q	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	s	603	X	-	-	-
25	CLA	s	604	X	-	-	-
25	CLA	s	605	X	-	-	-

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

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 105342 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	6	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
1	0	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	7	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	3	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	5	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
2	8	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	9	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	p	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
3	q	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		
6	c	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		
7	d	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			255	174	39	42		
12	j	35	Total	C	N	O	0	0
			255	174	39	42		

- 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
			297	209	43	45		

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

- 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
			306	205	50	51		
14	l	37	Total	C	N	O	0	0
			306	205	50	51		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	230	Total	C	N	O	S	0	0
			1742	1109	278	351	4		
16	o	230	Total	C	N	O	S	0	0
			1742	1109	278	351	4		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	240	Total	C	N	O	S	0	0
			1826	1156	313	352	5		
17	r	240	Total	C	N	O	S	0	0
			1826	1156	313	352	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	252	Total	C	N	O	S	0	0
			1907	1232	312	359	4		
18	s	252	Total	C	N	O	S	0	0
			1907	1232	312	359	4		

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

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

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	33	Total	C	N	O	S	0	0
			232	152	38	41	1		
20	v	33	Total	C	N	O	S	0	0
			232	152	38	41	1		

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

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

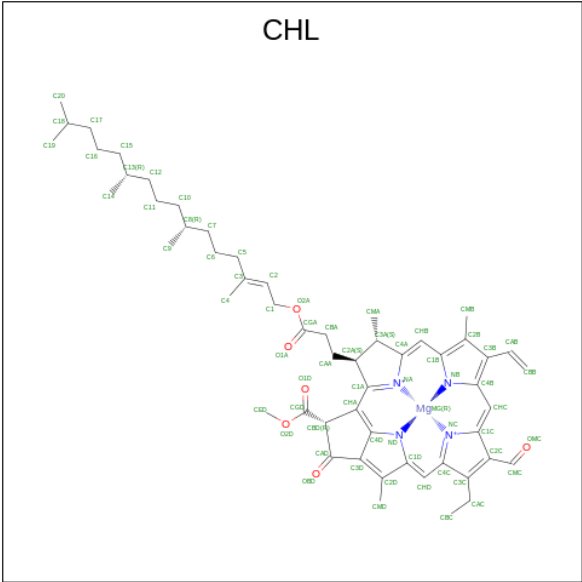
- Molecule 22 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	34	Total	C	N	O	0	0
			233	153	37	43		
22	x	34	Total	C	N	O	0	0
			233	153	37	43		

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

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

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	3	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			360	294	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0

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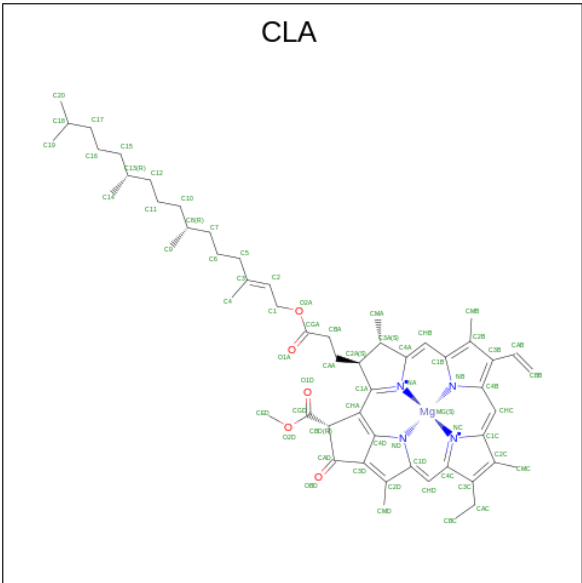
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
25	A	1	Total 239	C 199	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
25	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	a	1	Total 239	C 199	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
25	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
25	d	1	Total 130	C 110	Mg 2	N 8	O 10	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	g	1	Total 446	C 368	Mg 8	N 32	O 38	0

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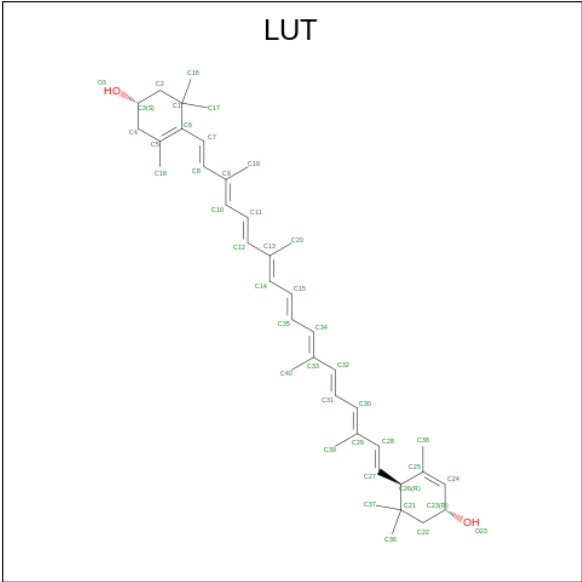
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	

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



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			84	80	4	
26	1	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	4	1	Total	C	O	0
			84	80	4	
26	4	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	G	1	Total	C	O	0
			84	80	4	
26	G	1	Total	C	O	0
			84	80	4	

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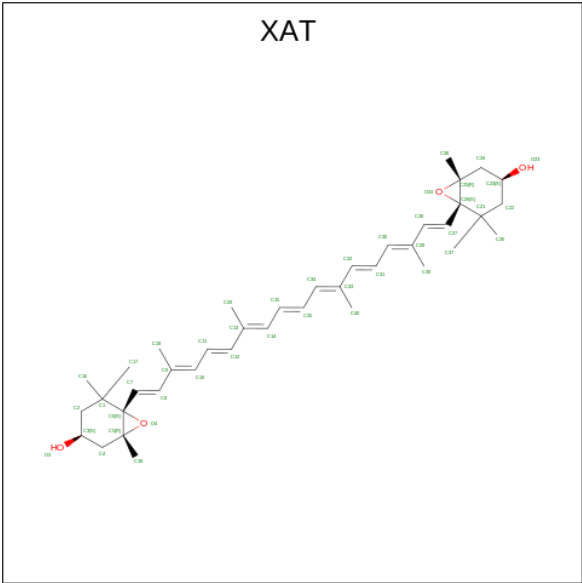
Mol	Chain	Residues	Atoms			AltConf
26	N	1	Total	C	O	0
			84	80	4	
26	N	1	Total	C	O	0
			84	80	4	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			84	80	4	
26	S	1	Total	C	O	0
			84	80	4	
26	Y	1	Total	C	O	0
			84	80	4	
26	Y	1	Total	C	O	0
			84	80	4	
26	0	1	Total	C	O	0
			84	80	4	
26	0	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	8	1	Total	C	O	0
			84	80	4	
26	8	1	Total	C	O	0
			84	80	4	
26	9	1	Total	C	O	0
			84	80	4	
26	9	1	Total	C	O	0
			84	80	4	
26	p	1	Total	C	O	0
			84	80	4	
26	p	1	Total	C	O	0
			84	80	4	
26	q	1	Total	C	O	0
			84	80	4	
26	q	1	Total	C	O	0
			84	80	4	
26	g	1	Total	C	O	0
			84	80	4	
26	g	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
26	n	1	Total	C	O	0
			84	80	4	
26	n	1	Total	C	O	0
			84	80	4	
26	s	1	Total	C	O	0
			84	80	4	
26	s	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	
26	r	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: C₄₀H₅₆O₄).



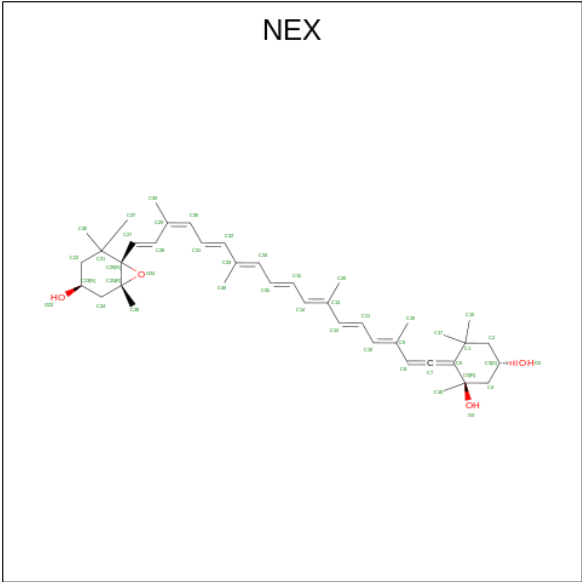
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	0	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	9	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	q	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	
27	y	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



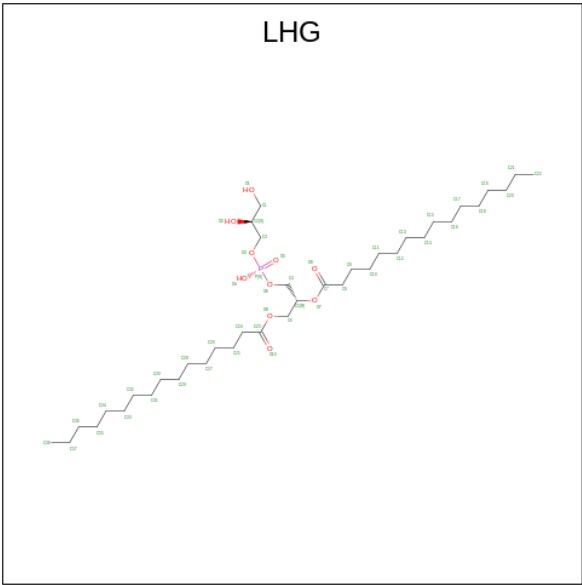
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			44	40	4	
28	S	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	
28	0	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	8	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
28	9	1	Total	C	O	0
			44	40	4	
28	p	1	Total	C	O	0
			44	40	4	
28	q	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	s	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
29	1	1	Total	C	O	P	0
			49	38	10	1	
29	2	1	Total	C	O	P	0
			49	38	10	1	
29	3	1	Total	C	O	P	0
			49	38	10	1	

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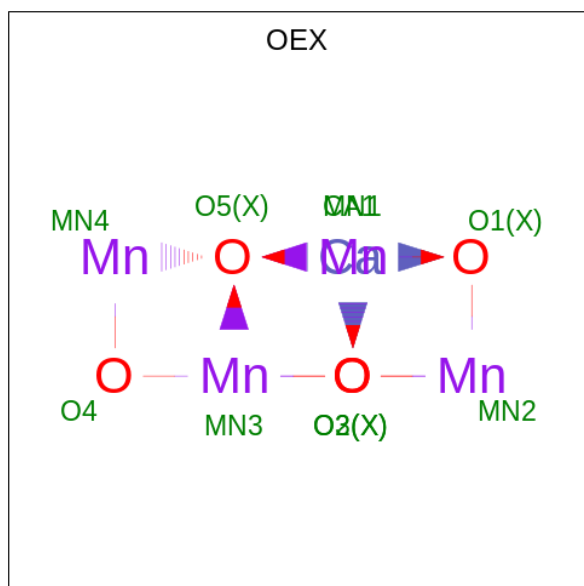
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total 49	C 38	O 10	P 1	0
29	5	1	Total 49	C 38	O 10	P 1	0
29	6	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 47	C 36	O 10	P 1	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	G	1	Total 49	C 38	O 10	P 1	0
29	L	1	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 38	C 27	O 10	P 1	0
29	S	1	Total 45	C 34	O 10	P 1	0
29	Y	1	Total 49	C 38	O 10	P 1	0
29	0	1	Total 49	C 38	O 10	P 1	0
29	7	1	Total 49	C 38	O 10	P 1	0
29	8	1	Total 49	C 38	O 10	P 1	0
29	9	1	Total 49	C 38	O 10	P 1	0
29	p	1	Total 49	C 38	O 10	P 1	0
29	q	1	Total 49	C 38	O 10	P 1	0
29	c	1	Total 47	C 36	O 10	P 1	0
29	d	1	Total 132	C 99	O 30	P 3	0

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Mol	Chain	Residues	Atoms				AltConf
29	d	1	Total	C	O	P	0
			132	99	30	3	
29	d	1	Total	C	O	P	0
			132	99	30	3	
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	s	1	Total	C	O	P	0
			45	34	10	1	
29	y	1	Total	C	O	P	0
			49	38	10	1	
29	r	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

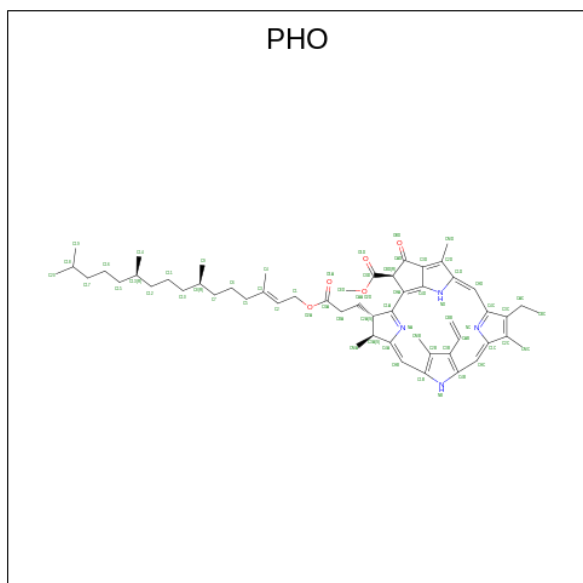
- Molecule 31 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

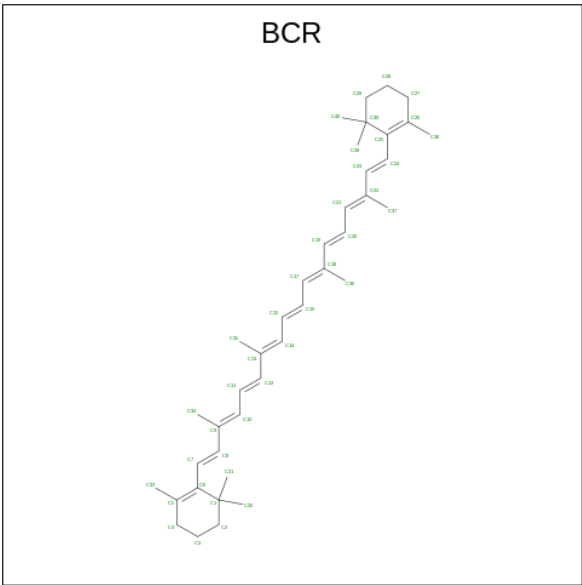
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Cl	0
			1	1	
32	a	1	Total	Cl	0
			1	1	

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 34 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



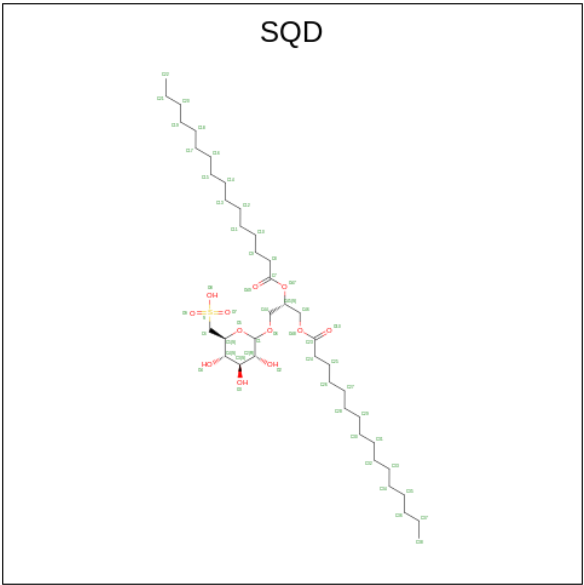
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	C	0
			40	40	
34	B	1	Total	C	0
			120	120	
34	B	1	Total	C	0
			120	120	
34	B	1	Total	C	0
			120	120	
34	C	1	Total	C	0
			160	160	
34	C	1	Total	C	0
			160	160	
34	C	1	Total	C	0
			160	160	
34	C	1	Total	C	0
			160	160	
34	D	1	Total	C	0
			40	40	
34	H	1	Total	C	0
			40	40	
34	a	1	Total	C	0
			40	40	
34	b	1	Total	C	0
			120	120	
34	b	1	Total	C	0
			120	120	
34	b	1	Total	C	0
			120	120	

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Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	d	1	Total	C	0
			40	40	
34	h	1	Total	C	0
			40	40	

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



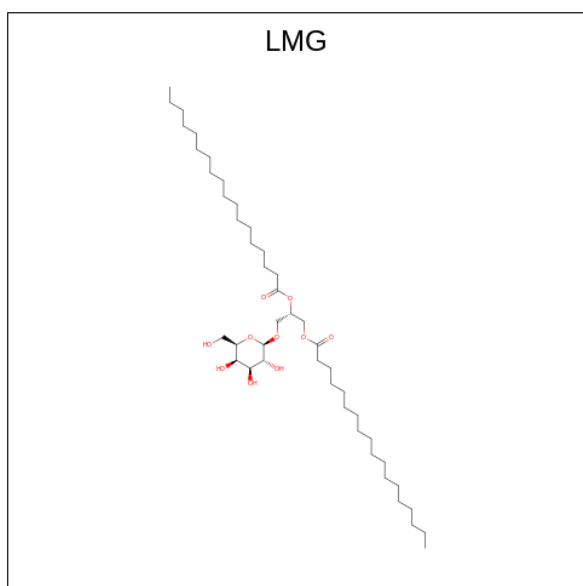
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			104	78	24	2	
35	B	1	Total	C	O	S	0
			104	78	24	2	
35	D	1	Total	C	O	S	0
			52	39	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	

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Mol	Chain	Residues	Atoms				AltConf
35	b	1	Total	C	O	S	0
			104	78	24	2	
35	b	1	Total	C	O	S	0
			104	78	24	2	
35	d	1	Total	C	O	S	0
			52	39	12	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



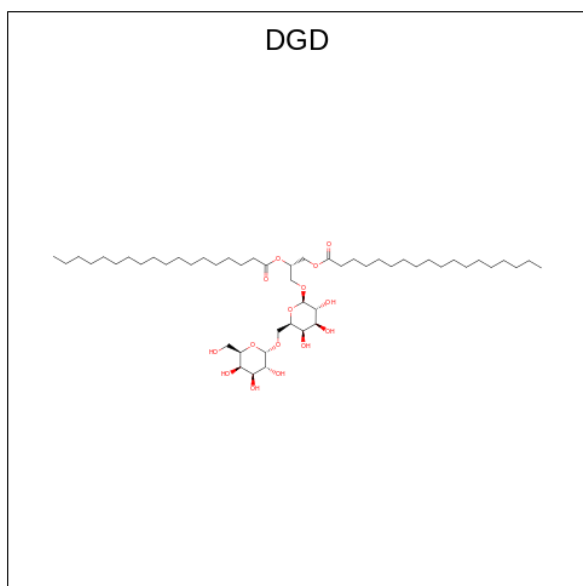
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O		0
			48	38	10		
36	B	1	Total	C	O		0
			51	41	10		
36	C	1	Total	C	O		0
			51	41	10		
36	D	1	Total	C	O		0
			92	72	20		
36	D	1	Total	C	O		0
			92	72	20		
36	H	1	Total	C	O		0
			48	38	10		
36	S	1	Total	C	O		0
			52	42	10		
36	a	1	Total	C	O		0
			48	38	10		

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Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	C	O	0
			51	41	10	
36	c	1	Total	C	O	0
			51	41	10	
36	d	1	Total	C	O	0
			92	72	20	
36	d	1	Total	C	O	0
			92	72	20	
36	h	1	Total	C	O	0
			48	38	10	
36	s	1	Total	C	O	0
			52	42	10	

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



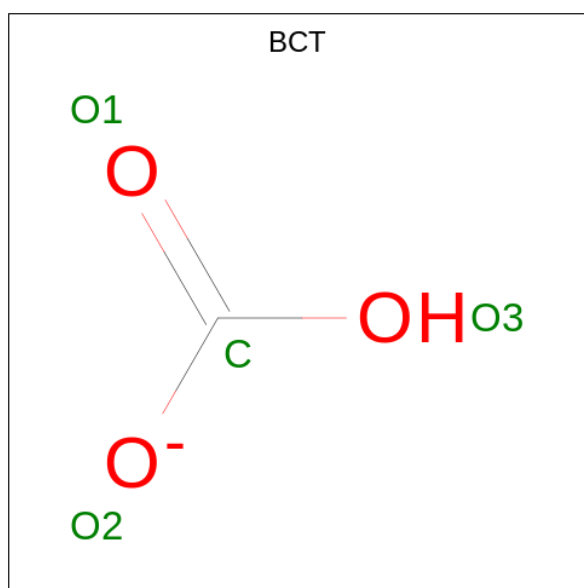
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	

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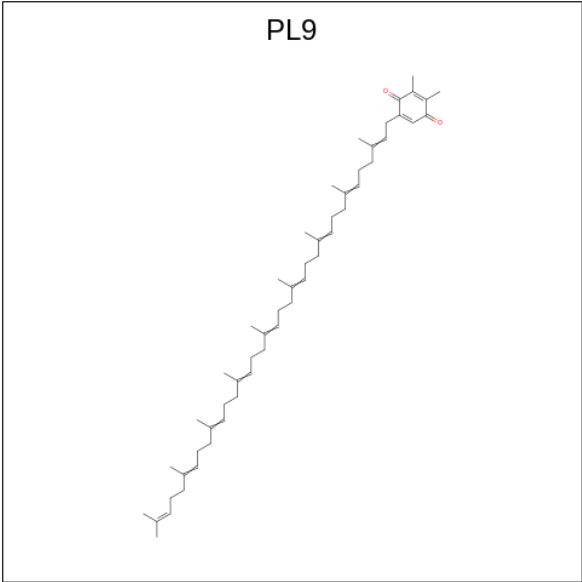
Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



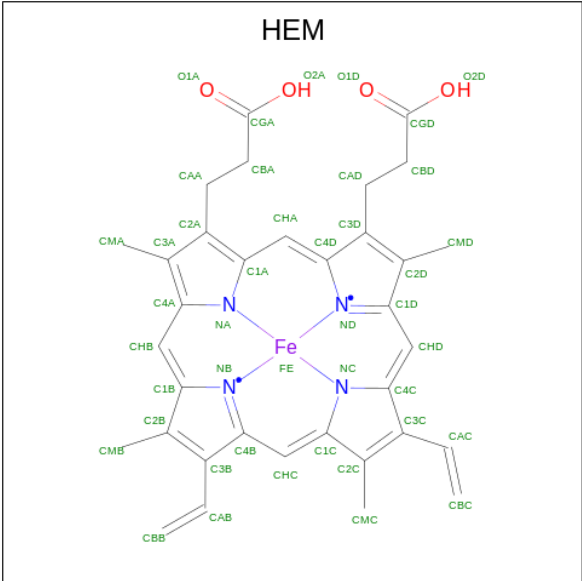
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			4	1	3	
38	d	1	Total	C	O	0
			4	1	3	

- Molecule 39 is 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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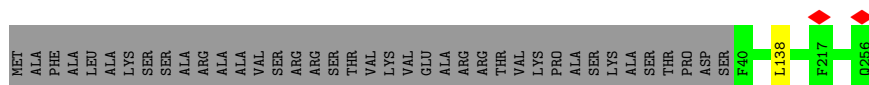
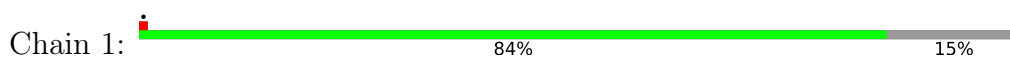
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
40	f	1	43	34	1	4	4	0

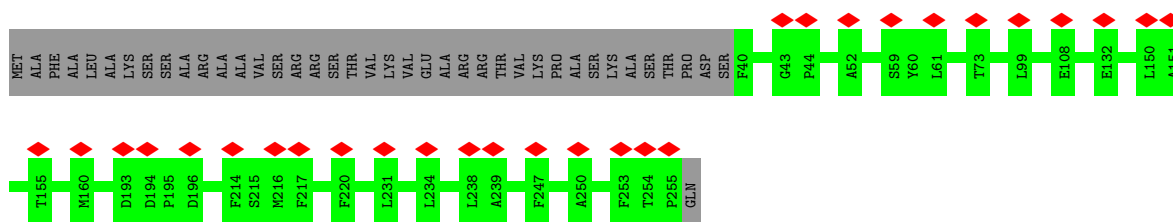
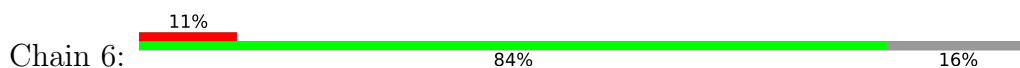
3 Residue-property plots [i](#)

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

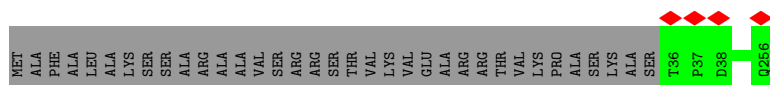
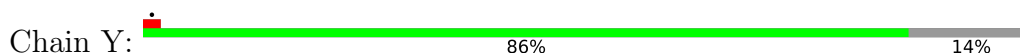
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



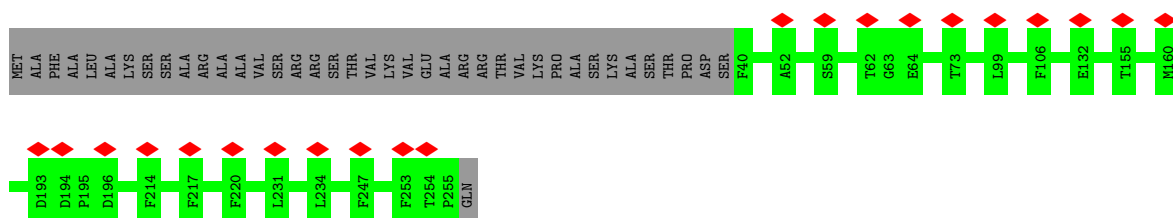
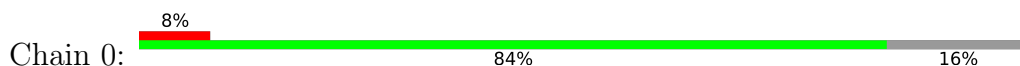
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic




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

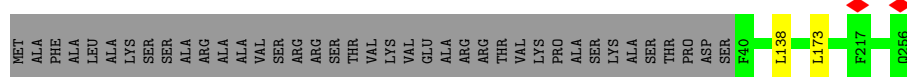


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic




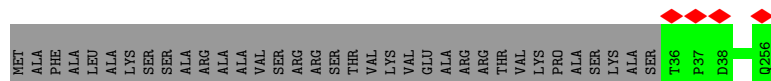
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  84% 15%




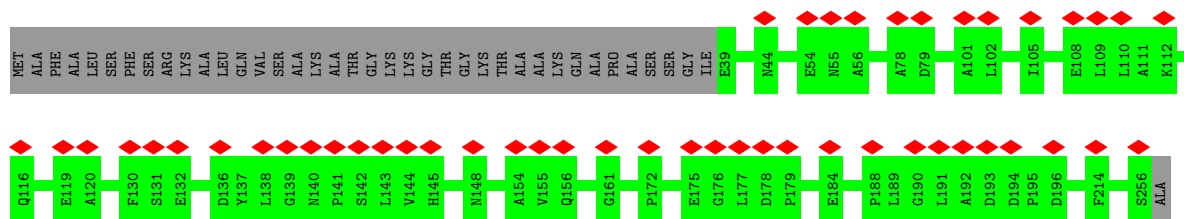
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain y:  86% 14%




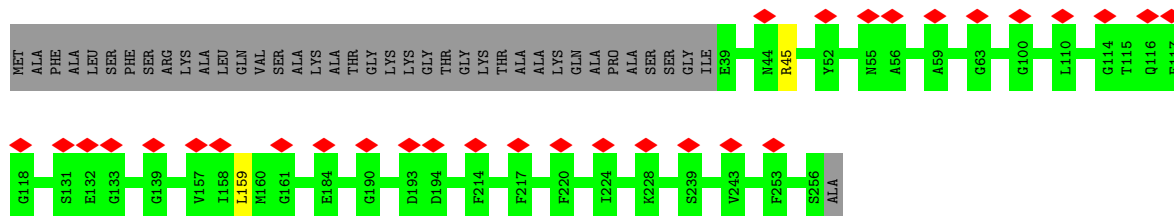
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  19% 85% 15%




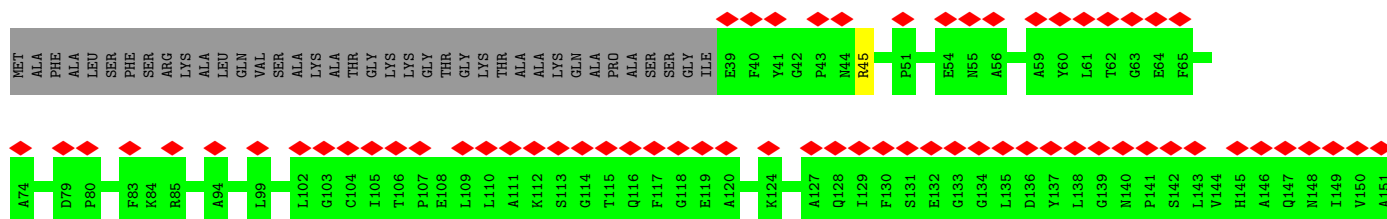
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

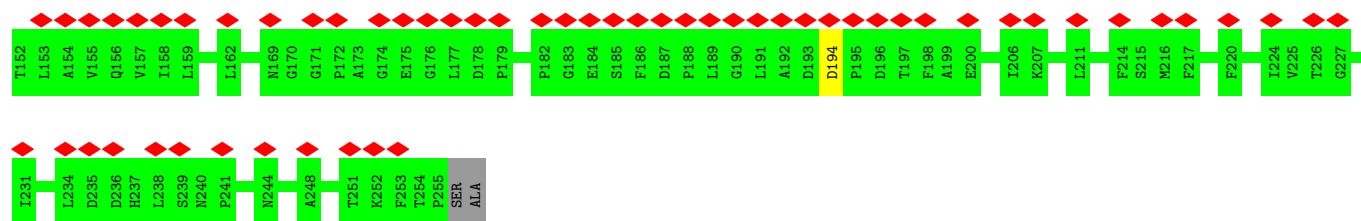
Chain 3:  12% 84% 15%



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

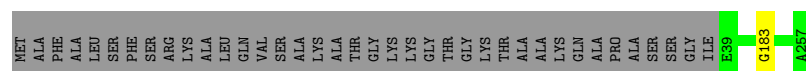
Chain 5:  48% 84% 16%





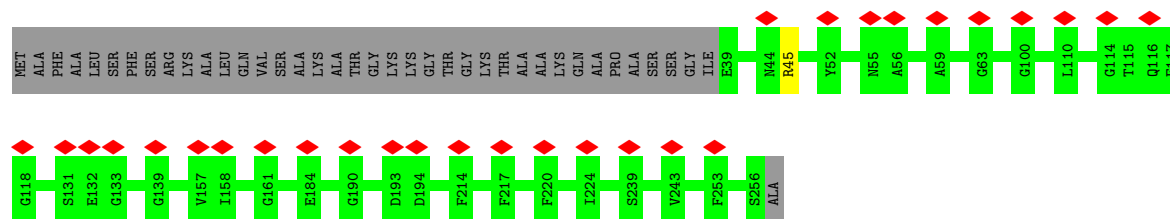
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain N: 85% 15%



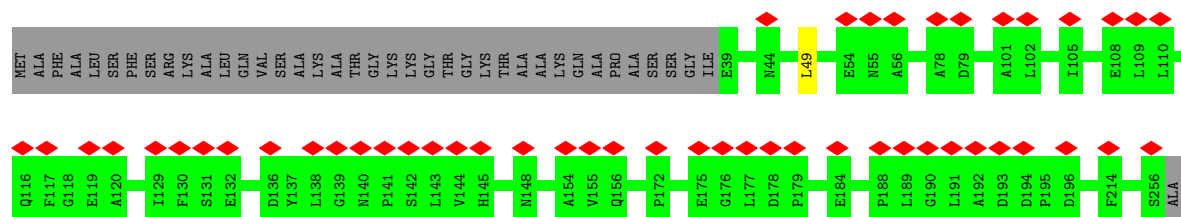
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 11% 84% 15%



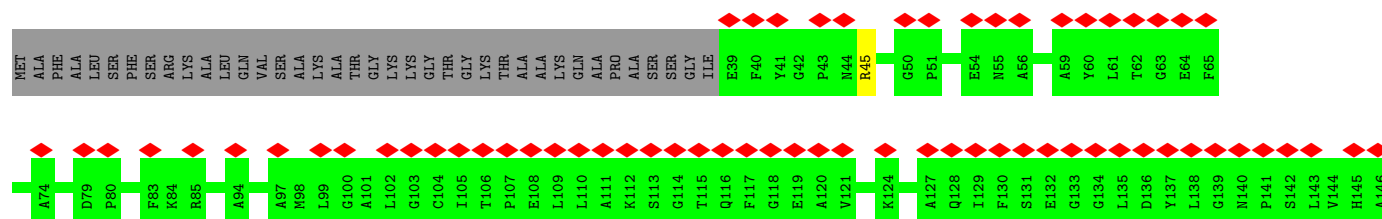
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

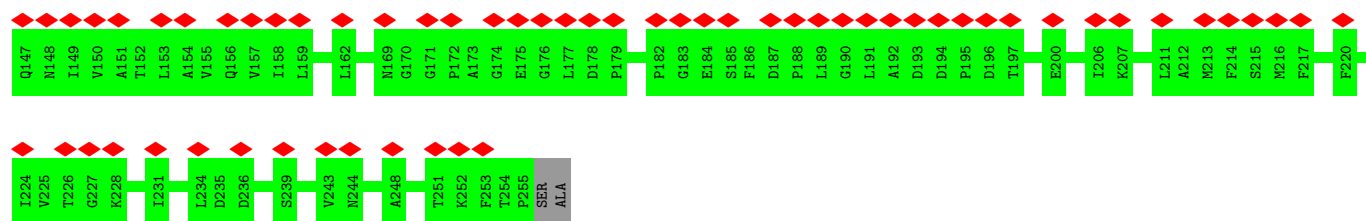
Chain 9: 19% 84% 15%



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

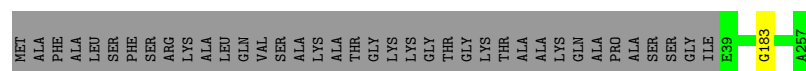
Chain p: 49% 84% 16%





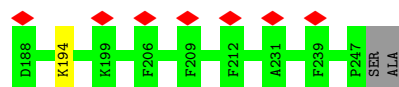
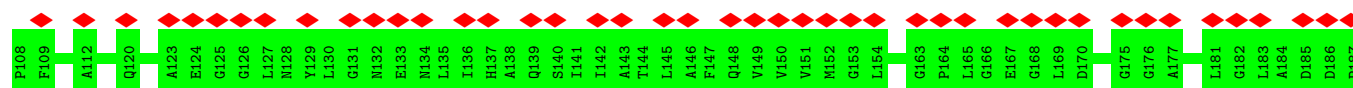
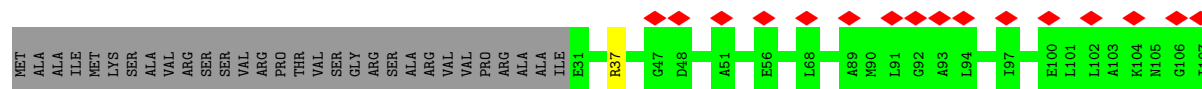
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain n: 85% 15%



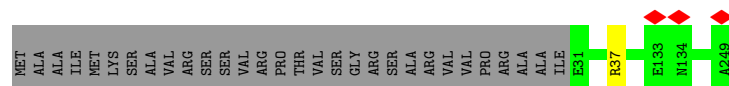
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 27% 86% 13%



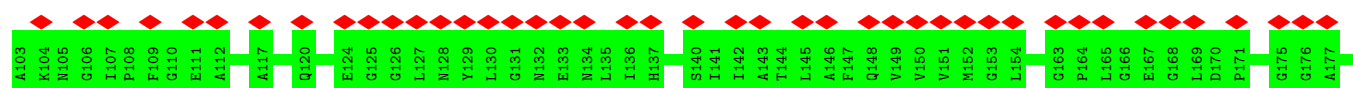
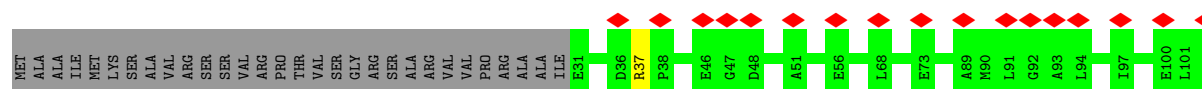
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

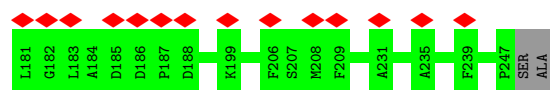
Chain G: 88% 12%



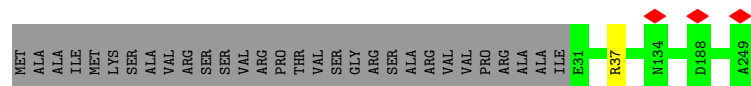
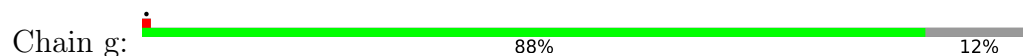
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain q: 30% 87% 13%





- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



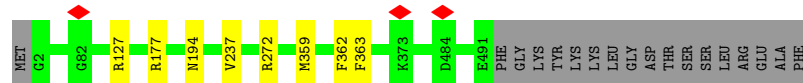
- Molecule 4: Photosystem II protein D1



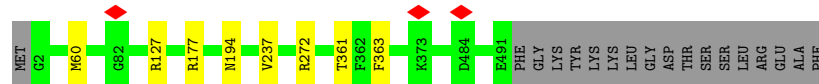
- Molecule 4: Photosystem II protein D1



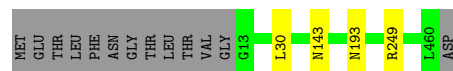
- Molecule 5: Photosystem II CP47 reaction center protein



- Molecule 5: Photosystem II CP47 reaction center protein

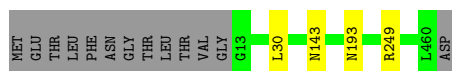


- Molecule 6: Photosystem II CP43 reaction center protein



- Molecule 6: Photosystem II CP43 reaction center protein

Chain c:  96% ..



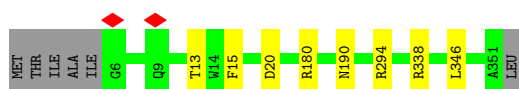
• Molecule 7: Photosystem II D2 protein

Chain D:  96% ..




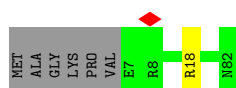
• Molecule 7: Photosystem II D2 protein

Chain d:  96% ..




• Molecule 8: Cytochrome b559 subunit alpha

Chain E:  91% • 7%



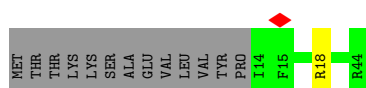
• Molecule 8: Cytochrome b559 subunit alpha

Chain e:  91% • 7%



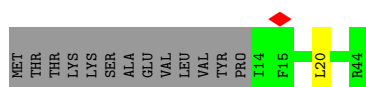
• Molecule 9: Cytochrome b559 subunit beta

Chain F:  68% • 30%



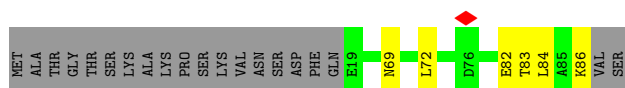
• Molecule 9: Cytochrome b559 subunit beta

Chain f:  68% • 30%



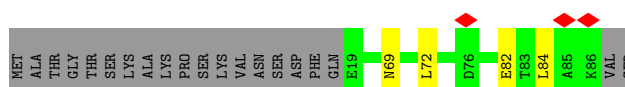
- Molecule 10: Photosystem II reaction center protein H

Chain H:  70% 7% 23%



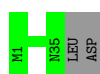
- Molecule 10: Photosystem II reaction center protein H

Chain h:  73% 5% 23%



- Molecule 11: Photosystem II reaction center protein I

Chain I:  95% 5%




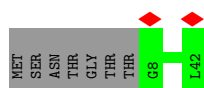
- Molecule 11: Photosystem II reaction center protein I

Chain i:  95% 5%




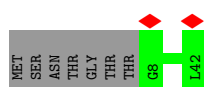
- Molecule 12: Photosystem II reaction center protein J

Chain J:  5% 83% 17%




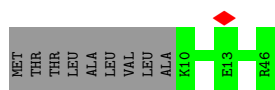
- Molecule 12: Photosystem II reaction center protein J

Chain j:  5% 83% 17%

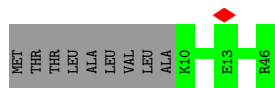
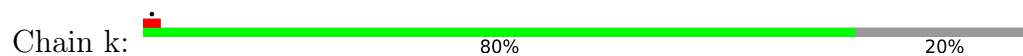


- Molecule 13: Photosystem II reaction center protein K

Chain K:  80% 20%



- Molecule 13: Photosystem II reaction center protein K



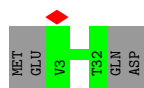
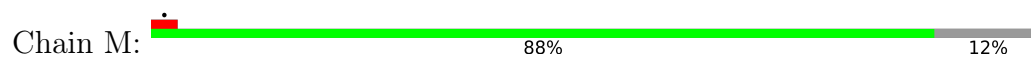
- Molecule 14: Photosystem II reaction center protein L



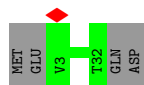
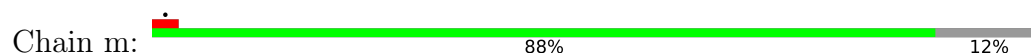
- Molecule 14: Photosystem II reaction center protein L



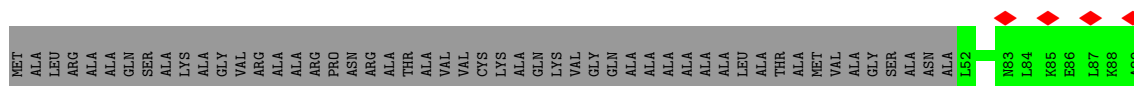
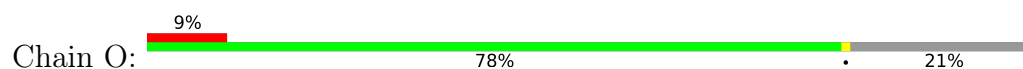
- Molecule 15: Photosystem II reaction center protein M



- Molecule 15: Photosystem II reaction center protein M



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







- Molecule 19: Photosystem II reaction center protein T

Chain t: 94%



- Molecule 20: Photosystem II reaction center protein Ycf12

Chain V: 97%



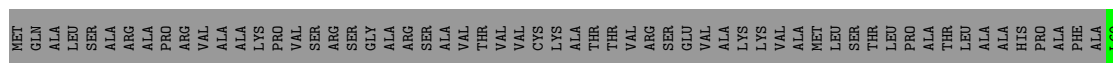
- Molecule 20: Photosystem II reaction center protein Ycf12

Chain v: 97%



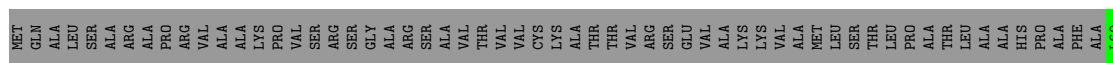
- Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W: 49%



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

Chain w: 49%



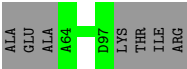
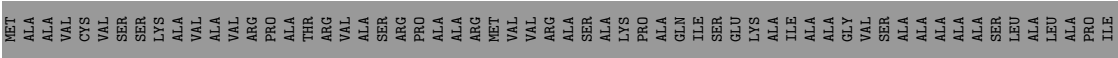
- Molecule 22: 4.1 kDa photosystem II subunit

Chain X: 34%

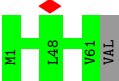




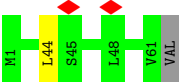
- Molecule 22: 4.1 kDa photosystem II subunit



- 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	118423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.31	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	0.082	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.32	0/1708	0.57	0/2322
1	1	0.37	0/1717	0.58	1/2334 (0.0%)
1	6	0.33	0/1708	0.56	0/2322
1	7	0.37	0/1717	0.57	1/2334 (0.0%)
1	Y	0.47	0/1746	0.55	0/2375
1	y	0.47	0/1746	0.56	0/2375
2	2	0.32	0/1715	0.52	0/2334
2	3	0.30	0/1715	0.52	0/2334
2	5	0.29	0/1709	0.54	1/2326 (0.0%)
2	8	0.30	0/1715	0.52	0/2334
2	9	0.32	0/1715	0.56	1/2334 (0.0%)
2	N	0.39	0/1720	0.54	0/2341
2	n	0.39	0/1720	0.53	0/2341
2	p	0.28	0/1709	0.51	0/2326
3	4	0.30	0/1706	0.52	0/2322
3	G	0.38	0/1717	0.54	0/2337
3	g	0.37	0/1717	0.53	0/2337
3	q	0.31	0/1706	0.54	0/2322
4	A	0.52	1/2718 (0.0%)	0.61	2/3706 (0.1%)
4	a	0.52	1/2718 (0.0%)	0.61	2/3706 (0.1%)
5	B	0.46	0/3964	0.56	0/5397
5	b	0.47	0/3964	0.56	1/5397 (0.0%)
6	C	0.46	0/3611	0.55	0/4920
6	c	0.46	0/3611	0.55	0/4920
7	D	0.51	0/2850	0.61	0/3887
7	d	0.51	0/2850	0.61	0/3887
8	E	0.36	0/637	0.54	0/869
8	e	0.36	0/637	0.55	0/869
9	F	0.39	0/258	0.58	0/349
9	f	0.40	0/258	0.60	0/349
10	H	0.45	0/530	0.64	1/725 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	h	0.44	0/530	0.64	1/725 (0.1%)
11	I	0.53	0/291	0.62	0/394
11	i	0.53	0/291	0.62	0/394
12	J	0.38	0/261	0.57	0/356
12	j	0.38	0/261	0.58	0/356
13	K	0.45	0/309	0.66	0/425
13	k	0.45	0/309	0.66	0/425
14	L	0.53	0/314	0.65	0/427
14	l	0.53	0/314	0.65	0/427
15	M	0.45	0/234	0.57	0/321
15	m	0.45	0/234	0.57	0/321
16	O	0.33	0/1771	0.59	1/2386 (0.0%)
16	o	0.33	0/1771	0.58	1/2386 (0.0%)
17	R	0.40	0/1866	0.59	1/2529 (0.0%)
17	r	0.40	0/1866	0.59	1/2529 (0.0%)
18	S	0.37	0/1961	0.54	0/2670
18	s	0.38	0/1961	0.55	0/2670
19	T	0.43	0/254	0.58	0/343
19	t	0.43	0/254	0.59	0/343
20	V	0.31	0/232	0.63	0/317
20	v	0.31	0/232	0.63	0/317
21	W	0.40	0/445	0.60	0/603
21	w	0.40	0/445	0.58	0/603
22	X	0.31	0/235	0.53	0/319
22	x	0.31	0/235	0.53	0/319
23	Z	0.33	0/469	0.58	0/644
23	z	0.33	0/469	0.62	1/644 (0.2%)
All	All	0.41	2/77326 (0.0%)	0.57	16/105224 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1
2	n	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	170	ASP	C-N	5.12	1.42	1.33
4	A	170	ASP	C-N	5.12	1.42	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	49	LEU	CA-CB-CG	7.09	131.60	115.30
5	b	60	MET	CG-SD-CE	-6.59	89.66	100.20
1	7	138	LEU	CA-CB-CG	6.33	129.87	115.30
17	r	113	ASP	CB-CG-OD1	5.98	123.68	118.30
17	R	113	ASP	CB-CG-OD1	5.93	123.64	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	183	GLY	Peptide
2	n	183	GLY	Peptide

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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	214/256 (84%)	201 (94%)	13 (6%)	0	100	100
1	1	215/256 (84%)	201 (94%)	14 (6%)	0	100	100
1	6	214/256 (84%)	198 (92%)	16 (8%)	0	100	100
1	7	215/256 (84%)	198 (92%)	17 (8%)	0	100	100
1	Y	219/256 (86%)	204 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
2	2	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	3	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	5	215/257 (84%)	195 (91%)	20 (9%)	0	100	100
2	8	216/257 (84%)	194 (90%)	22 (10%)	0	100	100
2	9	216/257 (84%)	196 (91%)	20 (9%)	0	100	100
2	N	217/257 (84%)	195 (90%)	22 (10%)	0	100	100
2	n	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
2	p	215/257 (84%)	199 (93%)	16 (7%)	0	100	100
3	4	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
3	G	217/249 (87%)	197 (91%)	20 (9%)	0	100	100
3	g	217/249 (87%)	199 (92%)	18 (8%)	0	100	100
3	q	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
4	A	334/352 (95%)	316 (95%)	18 (5%)	0	100	100
4	a	334/352 (95%)	318 (95%)	16 (5%)	0	100	100
5	B	488/508 (96%)	458 (94%)	30 (6%)	0	100	100
5	b	488/508 (96%)	460 (94%)	28 (6%)	0	100	100
6	C	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
6	c	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
7	D	344/352 (98%)	327 (95%)	17 (5%)	0	100	100
7	d	344/352 (98%)	326 (95%)	18 (5%)	0	100	100
8	E	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
8	e	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
9	F	29/44 (66%)	29 (100%)	0	0	100	100
9	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
10	H	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
10	h	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
11	I	33/37 (89%)	33 (100%)	0	0	100	100
11	i	33/37 (89%)	33 (100%)	0	0	100	100
12	J	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
12	j	33/42 (79%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
13	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
14	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
14	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
15	M	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
15	m	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
16	O	226/291 (78%)	201 (89%)	25 (11%)	0	100	100
16	o	226/291 (78%)	202 (89%)	24 (11%)	0	100	100
17	R	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	34	67
17	r	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	34	67
18	S	250/289 (86%)	224 (90%)	26 (10%)	0	100	100
18	s	250/289 (86%)	223 (89%)	27 (11%)	0	100	100
19	T	28/31 (90%)	28 (100%)	0	0	100	100
19	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
20	V	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
20	v	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
21	W	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
21	w	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
22	X	32/101 (32%)	32 (100%)	0	0	100	100
22	x	32/101 (32%)	32 (100%)	0	0	100	100
23	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
23	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	9614/11160 (86%)	8903 (93%)	709 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	R	100	ASN
17	r	100	ASN

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	0	165/196 (84%)	165 (100%)	0	100	100
1	1	166/196 (85%)	166 (100%)	0	100	100
1	6	165/196 (84%)	165 (100%)	0	100	100
1	7	166/196 (85%)	165 (99%)	1 (1%)	86	94
1	Y	170/196 (87%)	170 (100%)	0	100	100
1	y	170/196 (87%)	170 (100%)	0	100	100
2	2	169/194 (87%)	169 (100%)	0	100	100
2	3	169/194 (87%)	167 (99%)	2 (1%)	71	85
2	5	168/194 (87%)	167 (99%)	1 (1%)	86	94
2	8	169/194 (87%)	168 (99%)	1 (1%)	86	94
2	9	169/194 (87%)	169 (100%)	0	100	100
2	N	169/194 (87%)	169 (100%)	0	100	100
2	n	169/194 (87%)	169 (100%)	0	100	100
2	p	168/194 (87%)	167 (99%)	1 (1%)	86	94
3	4	163/187 (87%)	161 (99%)	2 (1%)	71	85
3	G	164/187 (88%)	163 (99%)	1 (1%)	86	94
3	g	164/187 (88%)	163 (99%)	1 (1%)	86	94
3	q	163/187 (87%)	162 (99%)	1 (1%)	86	94
4	A	274/289 (95%)	272 (99%)	2 (1%)	84	92
4	a	274/289 (95%)	272 (99%)	2 (1%)	84	92
5	B	392/407 (96%)	384 (98%)	8 (2%)	55	77
5	b	392/407 (96%)	385 (98%)	7 (2%)	59	79
6	C	351/362 (97%)	347 (99%)	4 (1%)	73	86
6	c	351/362 (97%)	347 (99%)	4 (1%)	73	86
7	D	276/281 (98%)	269 (98%)	7 (2%)	47	72
7	d	276/281 (98%)	268 (97%)	8 (3%)	42	69
8	E	67/71 (94%)	66 (98%)	1 (2%)	65	82
8	e	67/71 (94%)	66 (98%)	1 (2%)	65	82
9	F	25/37 (68%)	24 (96%)	1 (4%)	31	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	f	25/37 (68%)	24 (96%)	1 (4%)	31	60
10	H	58/75 (77%)	53 (91%)	5 (9%)	10	35
10	h	58/75 (77%)	55 (95%)	3 (5%)	23	53
11	I	32/34 (94%)	32 (100%)	0	100	100
11	i	32/34 (94%)	32 (100%)	0	100	100
12	J	26/32 (81%)	26 (100%)	0	100	100
12	j	26/32 (81%)	26 (100%)	0	100	100
13	K	31/38 (82%)	31 (100%)	0	100	100
13	k	31/38 (82%)	31 (100%)	0	100	100
14	L	34/35 (97%)	33 (97%)	1 (3%)	42	69
14	l	34/35 (97%)	33 (97%)	1 (3%)	42	69
15	M	26/30 (87%)	26 (100%)	0	100	100
15	m	26/30 (87%)	26 (100%)	0	100	100
16	O	190/222 (86%)	187 (98%)	3 (2%)	62	81
16	o	190/222 (86%)	187 (98%)	3 (2%)	62	81
17	R	187/218 (86%)	187 (100%)	0	100	100
17	r	187/218 (86%)	187 (100%)	0	100	100
18	S	189/217 (87%)	187 (99%)	2 (1%)	73	86
18	s	189/217 (87%)	187 (99%)	2 (1%)	73	86
19	T	27/28 (96%)	26 (96%)	1 (4%)	34	62
19	t	27/28 (96%)	26 (96%)	1 (4%)	34	62
20	V	27/27 (100%)	26 (96%)	1 (4%)	34	62
20	v	27/27 (100%)	26 (96%)	1 (4%)	34	62
21	W	44/87 (51%)	44 (100%)	0	100	100
21	w	44/87 (51%)	44 (100%)	0	100	100
22	X	24/67 (36%)	24 (100%)	0	100	100
22	x	24/67 (36%)	24 (100%)	0	100	100
23	Z	51/52 (98%)	51 (100%)	0	100	100
23	z	51/52 (98%)	51 (100%)	0	100	100
All	All	7668/8694 (88%)	7587 (99%)	81 (1%)	74	86

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	c	193	ASN
10	h	82	GLU
7	d	13	THR
7	d	338	ARG
18	s	161	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	0	233	ASN
16	o	233	ASN
4	a	304	GLN
17	r	94	GLN
14	l	5	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 560 ligands modelled in this entry, 4 are monoatomic - leaving 556 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
24	CHL	g	608	-	44,52,74	2.22	13 (29%)	46,87,114	3.13	18 (39%)
26	LUT	4	1621	-	42,43,43	0.76	0	51,60,60	1.50	11 (21%)
25	CLA	p	613	2	65,73,73	1.53	7 (10%)	76,113,113	1.31	7 (9%)
24	CHL	y	605	1	46,54,74	2.20	13 (28%)	49,90,114	3.06	20 (40%)
25	CLA	N	614	-	49,57,73	1.71	9 (18%)	55,93,113	1.43	7 (12%)
24	CHL	s	608	-	49,57,74	2.23	15 (30%)	52,93,114	3.06	20 (38%)
24	CHL	8	609	2	66,74,74	1.84	13 (19%)	73,114,114	2.64	22 (30%)
26	LUT	7	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	8 (15%)
24	CHL	3	601	2	66,74,74	1.89	13 (19%)	73,114,114	2.63	22 (30%)
24	CHL	6	608	-	50,58,74	2.15	14 (28%)	52,94,114	3.09	19 (36%)
25	CLA	3	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
25	CLA	7	610	1	65,73,73	1.46	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	5	612	2	45,53,73	1.82	9 (20%)	52,89,113	1.56	8 (15%)
25	CLA	B	610	-	65,73,73	1.44	10 (15%)	76,113,113	1.41	6 (7%)
25	CLA	n	614	-	49,57,73	1.70	9 (18%)	55,93,113	1.43	7 (12%)
25	CLA	N	612	2	45,53,73	1.81	10 (22%)	52,89,113	1.55	7 (13%)
25	CLA	6	611	29	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
25	CLA	S	611	29	49,57,73	1.65	10 (20%)	55,93,113	1.47	6 (10%)
25	CLA	8	603	-	65,73,73	1.47	10 (15%)	76,113,113	1.41	9 (11%)
25	CLA	c	506	-	65,73,73	1.52	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	D	402	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	9 (11%)
25	CLA	y	602	1	65,73,73	1.42	8 (12%)	76,113,113	1.37	7 (9%)
28	NEX	q	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.34	17 (34%)
24	CHL	y	601	1	66,74,74	1.87	14 (21%)	73,114,114	2.76	24 (32%)
25	CLA	B	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.21	5 (6%)
25	CLA	r	609	17	58,66,73	1.60	10 (17%)	67,104,113	1.44	6 (8%)
25	CLA	q	612	3	43,51,73	1.82	8 (18%)	49,86,113	1.62	9 (18%)
24	CHL	1	609	1	66,74,74	1.84	15 (22%)	73,114,114	2.65	21 (28%)
26	LUT	5	1620	-	42,43,43	0.76	0	51,60,60	1.83	13 (25%)
25	CLA	R	612	-	49,57,73	1.65	9 (18%)	55,93,113	1.54	8 (14%)
37	DGD	c	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
34	BCR	B	620	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	19 (33%)
24	CHL	1	607	-	66,74,74	1.89	14 (21%)	73,114,114	2.58	25 (34%)
25	CLA	4	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.48	9 (11%)
24	CHL	5	606	-	46,54,74	2.35	16 (34%)	49,90,114	2.95	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	G	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	c	511	6	65,73,73	1.45	10 (15%)	76,113,113	1.52	9 (11%)
25	CLA	6	602	1	65,73,73	1.49	8 (12%)	76,113,113	1.25	6 (7%)
25	CLA	C	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.40	7 (9%)
24	CHL	6	601	1	66,74,74	1.88	13 (19%)	73,114,114	2.68	25 (34%)
25	CLA	B	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.19	7 (9%)
25	CLA	p	611	29	49,57,73	1.72	6 (12%)	55,93,113	1.46	6 (10%)
24	CHL	q	606	-	50,58,74	2.34	16 (32%)	52,94,114	2.82	17 (32%)
25	CLA	a	406	-	65,73,73	1.42	11 (16%)	76,113,113	1.37	8 (10%)
25	CLA	7	612	1	65,73,73	1.49	10 (15%)	76,113,113	1.33	8 (10%)
25	CLA	B	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)
25	CLA	g	614	-	49,57,73	1.70	9 (18%)	55,93,113	1.33	8 (14%)
26	LUT	g	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.62	7 (13%)
25	CLA	G	610	3	65,73,73	1.44	9 (13%)	76,113,113	1.33	9 (11%)
25	CLA	Y	613	1	65,73,73	1.51	11 (16%)	76,113,113	1.28	7 (9%)
25	CLA	A	410	-	60,68,73	1.51	11 (18%)	70,107,113	1.50	9 (12%)
24	CHL	q	609	3	66,74,74	2.13	17 (25%)	73,114,114	2.68	21 (28%)
24	CHL	p	601	2	66,74,74	1.90	14 (21%)	73,114,114	2.70	23 (31%)
40	HEM	f	101	8,9	41,50,50	1.48	3 (7%)	45,82,82	1.30	3 (6%)
25	CLA	n	613	2	65,73,73	1.51	10 (15%)	76,113,113	1.44	7 (9%)
25	CLA	5	614	-	49,57,73	1.75	6 (12%)	55,93,113	1.43	8 (14%)
24	CHL	2	601	2	66,74,74	1.88	14 (21%)	73,114,114	2.57	23 (31%)
25	CLA	Y	614	-	54,62,73	1.60	9 (16%)	62,99,113	1.38	8 (12%)
24	CHL	7	605	1	46,54,74	2.30	14 (30%)	49,90,114	3.06	18 (36%)
25	CLA	r	610	17	65,73,73	1.47	9 (13%)	76,113,113	1.39	8 (10%)
33	PHO	a	408	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	9 (19%)
24	CHL	8	605	2	66,74,74	2.02	15 (22%)	73,114,114	2.61	21 (28%)
24	CHL	y	609	1	66,74,74	1.84	13 (19%)	73,114,114	2.76	24 (32%)
25	CLA	4	611	29	45,53,73	1.76	8 (17%)	52,89,113	1.50	6 (11%)
35	SQD	b	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
28	NEX	R	623	-	38,46,46	0.99	2 (5%)	50,70,70	2.39	15 (30%)
25	CLA	n	603	-	65,73,73	1.46	12 (18%)	76,113,113	1.43	8 (10%)
26	LUT	y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	17 (33%)
25	CLA	y	610	1	65,73,73	1.41	8 (12%)	76,113,113	1.33	8 (10%)
24	CHL	p	605	2	66,74,74	2.04	15 (22%)	73,114,114	2.70	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	616	-	65,73,73	1.51	11 (16%)	76,113,113	1.51	14 (18%)
24	CHL	9	607	-	50,58,74	2.23	15 (30%)	52,94,114	2.97	19 (36%)
25	CLA	B	614	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
24	CHL	3	608	-	50,58,74	2.16	13 (26%)	52,94,114	2.99	20 (38%)
24	CHL	q	605	3	48,56,74	2.34	15 (31%)	51,92,114	3.12	20 (39%)
27	XAT	q	1622	-	39,47,47	0.89	0	54,74,74	2.58	17 (31%)
24	CHL	1	605	1	46,54,74	2.30	14 (30%)	49,90,114	3.06	18 (36%)
24	CHL	0	607	-	66,74,74	1.85	13 (19%)	73,114,114	2.66	18 (24%)
25	CLA	0	610	1	65,73,73	1.48	9 (13%)	76,113,113	1.23	8 (10%)
25	CLA	p	604	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
25	CLA	s	612	18	45,53,73	1.81	11 (24%)	52,89,113	1.63	9 (17%)
24	CHL	N	608	-	50,58,74	2.05	14 (28%)	52,94,114	3.13	18 (34%)
29	LHG	2	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
37	DGD	C	520	-	60,60,67	0.85	2 (3%)	74,74,81	0.99	4 (5%)
24	CHL	s	607	-	43,51,74	2.33	13 (30%)	45,86,114	2.99	18 (40%)
25	CLA	p	602	2	65,73,73	1.53	7 (10%)	76,113,113	1.29	7 (9%)
26	LUT	6	1620	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
25	CLA	Y	603	-	65,73,73	1.46	11 (16%)	76,113,113	1.51	9 (11%)
25	CLA	b	608	-	65,73,73	1.48	11 (16%)	76,113,113	1.38	7 (9%)
25	CLA	N	603	-	65,73,73	1.46	12 (18%)	76,113,113	1.44	8 (10%)
24	CHL	r	607	-	56,64,74	1.97	12 (21%)	61,102,114	2.87	20 (32%)
25	CLA	A	405	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
29	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	9	611	29	45,53,73	1.77	9 (20%)	52,89,113	1.47	7 (13%)
26	LUT	8	1621	-	42,43,43	0.79	0	51,60,60	1.56	10 (19%)
24	CHL	R	607	-	56,64,74	1.98	13 (23%)	61,102,114	2.87	20 (32%)
34	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
25	CLA	4	602	3	65,73,73	1.50	7 (10%)	76,113,113	1.29	7 (9%)
27	XAT	2	1622	-	39,47,47	0.90	0	54,74,74	2.68	19 (35%)
36	LMG	h	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.22	5 (8%)
24	CHL	1	608	-	50,58,74	2.08	14 (28%)	52,94,114	3.17	19 (36%)
25	CLA	A	406	-	65,73,73	1.43	11 (16%)	76,113,113	1.37	8 (10%)
25	CLA	c	513	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	8 (10%)
36	LMG	s	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.11	4 (6%)
36	LMG	H	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.26	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	607	-	65,73,73	1.49	9 (13%)	76,113,113	1.44	10 (13%)
25	CLA	6	613	1	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
25	CLA	a	405	-	65,73,73	1.49	10 (15%)	76,113,113	1.47	7 (9%)
24	CHL	7	609	1	66,74,74	1.84	14 (21%)	73,114,114	2.67	19 (26%)
25	CLA	r	602	17	60,68,73	1.53	9 (15%)	70,107,113	1.41	8 (11%)
35	SQD	D	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
25	CLA	4	604	-	49,57,73	1.75	9 (18%)	55,93,113	1.38	7 (12%)
27	XAT	p	1622	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
25	CLA	G	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.58	8 (15%)
29	LHG	8	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
26	LUT	1	1621	-	42,43,43	0.82	0	51,60,60	1.71	16 (31%)
25	CLA	p	610	2	65,73,73	1.51	7 (10%)	76,113,113	1.26	7 (9%)
25	CLA	2	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.48	7 (13%)
25	CLA	5	602	2	65,73,73	1.52	7 (10%)	76,113,113	1.29	7 (9%)
25	CLA	7	603	-	65,73,73	1.53	11 (16%)	76,113,113	1.34	7 (9%)
25	CLA	B	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	9 (11%)
24	CHL	0	605	1	46,54,74	2.29	16 (34%)	49,90,114	3.06	21 (42%)
24	CHL	G	601	3	66,74,74	1.82	11 (16%)	73,114,114	2.78	27 (36%)
24	CHL	3	609	2	66,74,74	1.82	12 (18%)	73,114,114	2.65	22 (30%)
25	CLA	r	604	-	48,56,73	1.74	9 (18%)	55,92,113	1.55	7 (12%)
34	BCR	c	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)
36	LMG	d	412	-	46,46,55	0.94	2 (4%)	54,54,63	1.09	4 (7%)
24	CHL	n	608	-	50,58,74	2.03	13 (26%)	52,94,114	3.12	17 (32%)
25	CLA	q	602	3	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
24	CHL	0	609	1	66,74,74	1.95	16 (24%)	73,114,114	2.61	21 (28%)
25	CLA	a	407	-	49,57,73	1.64	11 (22%)	55,93,113	1.52	6 (10%)
24	CHL	q	608	-	44,52,74	2.40	14 (31%)	46,87,114	3.21	16 (34%)
24	CHL	y	606	-	66,74,74	1.82	14 (21%)	73,114,114	2.73	20 (27%)
25	CLA	8	610	2	65,73,73	1.50	7 (10%)	76,113,113	1.25	7 (9%)
25	CLA	B	617	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	9 (11%)
24	CHL	7	608	-	50,58,74	2.05	14 (28%)	52,94,114	3.16	17 (32%)
36	LMG	d	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.13	3 (5%)
25	CLA	S	613	18	49,57,73	1.74	11 (22%)	55,93,113	1.46	7 (12%)
24	CHL	Y	601	1	66,74,74	1.86	15 (22%)	73,114,114	2.71	25 (34%)
26	LUT	G	1620	-	42,43,43	0.78	0	51,60,60	1.48	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	N	1622	-	39,47,47	1.04	3 (7%)	54,74,74	2.85	21 (38%)
30	OEX	A	401	4,6	0,15,15	-	-	-		
26	LUT	y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.67	14 (27%)
24	CHL	G	606	-	50,58,74	2.13	14 (28%)	52,94,114	3.10	22 (42%)
24	CHL	9	609	2	66,74,74	1.99	15 (22%)	73,114,114	2.66	20 (27%)
25	CLA	8	602	2	65,73,73	1.49	7 (10%)	76,113,113	1.31	6 (7%)
25	CLA	p	612	2	45,53,73	1.81	7 (15%)	52,89,113	1.56	8 (15%)
25	CLA	G	604	-	49,57,73	1.69	10 (20%)	55,93,113	1.48	8 (14%)
25	CLA	n	610	2	65,73,73	1.46	9 (13%)	76,113,113	1.23	8 (10%)
24	CHL	S	607	-	43,51,74	2.33	13 (30%)	45,86,114	2.98	19 (42%)
28	NEX	S	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.46	16 (32%)
24	CHL	9	601	2	66,74,74	1.91	14 (21%)	73,114,114	2.55	24 (32%)
28	NEX	7	1623	-	38,46,46	1.03	2 (5%)	50,70,70	2.38	20 (40%)
25	CLA	0	614	-	54,62,73	1.65	5 (9%)	62,99,113	1.48	7 (11%)
25	CLA	2	613	2	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)
29	LHG	r	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
24	CHL	2	609	2	66,74,74	1.94	14 (21%)	73,114,114	2.70	19 (26%)
24	CHL	1	606	-	66,74,74	1.90	14 (21%)	73,114,114	2.61	20 (27%)
34	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
25	CLA	G	612	3	43,51,73	1.80	10 (23%)	49,86,113	1.47	7 (14%)
25	CLA	g	613	3	65,73,73	1.48	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	4	605	3	48,56,74	2.36	16 (33%)	51,92,114	3.06	21 (41%)
25	CLA	c	510	-	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
36	LMG	D	412	-	46,46,55	0.95	2 (4%)	54,54,63	1.08	4 (7%)
25	CLA	4	614	-	49,57,73	1.70	8 (16%)	55,93,113	1.41	7 (12%)
26	LUT	7	1621	-	42,43,43	0.77	0	51,60,60	1.60	11 (21%)
28	NEX	2	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.35	13 (26%)
25	CLA	b	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.60	8 (10%)
24	CHL	g	607	-	50,58,74	2.12	13 (26%)	52,94,114	3.14	23 (44%)
24	CHL	p	606	-	46,54,74	2.41	15 (32%)	49,90,114	2.85	18 (36%)
25	CLA	y	611	29	65,73,73	1.49	10 (15%)	76,113,113	1.32	6 (7%)
25	CLA	8	612	2	45,53,73	1.79	7 (15%)	52,89,113	1.62	8 (15%)
24	CHL	6	605	1	46,54,74	2.32	16 (34%)	49,90,114	3.00	21 (42%)
24	CHL	N	607	-	66,74,74	1.82	14 (21%)	73,114,114	2.84	25 (34%)
25	CLA	y	603	-	65,73,73	1.46	11 (16%)	76,113,113	1.50	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	p	1621	-	42,43,43	0.73	0	51,60,60	1.55	9 (17%)
34	BCR	c	515	-	41,41,41	0.91	2 (4%)	56,56,56	1.74	11 (19%)
29	LHG	y	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.18	5 (9%)
29	LHG	d	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
25	CLA	b	609	-	65,73,73	1.44	11 (16%)	76,113,113	1.43	7 (9%)
24	CHL	6	609	1	66,74,74	1.89	14 (21%)	73,114,114	2.61	22 (30%)
24	CHL	4	606	-	50,58,74	2.30	16 (32%)	52,94,114	2.86	19 (36%)
26	LUT	Y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	16 (31%)
25	CLA	c	502	-	65,73,73	1.52	12 (18%)	76,113,113	1.69	10 (13%)
25	CLA	1	612	1	65,73,73	1.47	10 (15%)	76,113,113	1.33	8 (10%)
34	BCR	C	515	-	41,41,41	0.92	2 (4%)	56,56,56	1.73	11 (19%)
25	CLA	6	603	-	65,73,73	1.46	9 (13%)	76,113,113	1.42	7 (9%)
25	CLA	c	512	-	65,73,73	1.50	10 (15%)	76,113,113	1.44	7 (9%)
25	CLA	C	502	-	65,73,73	1.51	12 (18%)	76,113,113	1.68	11 (14%)
24	CHL	N	605	2	66,74,74	1.87	12 (18%)	73,114,114	2.63	23 (31%)
25	CLA	r	613	17	60,68,73	1.53	10 (16%)	70,107,113	1.43	8 (11%)
38	BCT	d	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
24	CHL	q	607	-	50,58,74	2.30	16 (32%)	52,94,114	2.93	18 (34%)
25	CLA	B	608	-	65,73,73	1.47	11 (16%)	76,113,113	1.36	7 (9%)
24	CHL	7	607	-	66,74,74	1.89	14 (21%)	73,114,114	2.62	25 (34%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	1.03	3 (3%)
27	XAT	r	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.48	17 (31%)
25	CLA	b	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	11 (14%)
25	CLA	C	507	-	65,73,73	1.41	11 (16%)	76,113,113	1.45	11 (14%)
34	BCR	b	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)
34	BCR	d	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)
24	CHL	g	601	3	66,74,74	1.82	12 (18%)	73,114,114	2.77	29 (39%)
26	LUT	r	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
25	CLA	2	603	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	9 (11%)
25	CLA	9	602	2	65,73,73	1.44	8 (12%)	76,113,113	1.39	9 (11%)
24	CHL	R	608	-	61,69,74	1.93	13 (21%)	67,108,114	2.82	23 (34%)
35	SQD	B	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
27	XAT	7	1622	-	39,47,47	0.94	0	54,74,74	4.18	22 (40%)
26	LUT	R	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
24	CHL	5	601	2	66,74,74	1.90	13 (19%)	73,114,114	2.71	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	0	602	1	65,73,73	1.49	8 (12%)	76,113,113	1.26	6 (7%)
25	CLA	q	613	3	65,73,73	1.46	7 (10%)	76,113,113	1.47	6 (7%)
25	CLA	b	610	-	65,73,73	1.44	10 (15%)	76,113,113	1.40	6 (7%)
28	NEX	N	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.36	14 (28%)
25	CLA	9	613	2	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
28	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.40	16 (32%)
25	CLA	p	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	7 (9%)
24	CHL	0	608	-	50,58,74	2.16	14 (28%)	52,94,114	3.07	18 (34%)
25	CLA	0	604	-	65,73,73	1.50	9 (13%)	76,113,113	1.25	7 (9%)
34	BCR	B	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.97	17 (30%)
26	LUT	g	1620	-	42,43,43	0.78	0	51,60,60	1.47	6 (11%)
25	CLA	b	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.21	5 (6%)
24	CHL	5	608	-	50,58,74	2.14	14 (28%)	52,94,114	3.12	17 (32%)
29	LHG	3	2630	25	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
28	NEX	9	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.33	12 (24%)
24	CHL	S	601	18	46,54,74	2.32	14 (30%)	49,90,114	3.10	22 (44%)
24	CHL	Y	605	1	46,54,74	2.20	13 (28%)	49,90,114	3.05	20 (40%)
25	CLA	g	604	-	49,57,73	1.69	8 (16%)	55,93,113	1.48	8 (14%)
26	LUT	9	1621	-	42,43,43	0.77	0	51,60,60	1.74	13 (25%)
25	CLA	q	614	-	49,57,73	1.68	7 (14%)	55,93,113	1.41	6 (10%)
24	CHL	n	605	2	66,74,74	1.86	12 (18%)	73,114,114	2.64	26 (35%)
27	XAT	0	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.20	22 (40%)
26	LUT	6	1621	-	42,43,43	0.80	0	51,60,60	1.61	9 (17%)
27	XAT	9	1622	-	39,47,47	0.91	0	54,74,74	2.65	19 (35%)
24	CHL	2	606	-	50,58,74	2.23	15 (30%)	52,94,114	2.94	19 (36%)
25	CLA	R	613	17	60,68,73	1.53	10 (16%)	70,107,113	1.43	8 (11%)
29	LHG	p	2630	25	48,48,48	0.95	2 (4%)	51,54,54	1.04	3 (5%)
24	CHL	n	609	2	66,74,74	1.88	14 (21%)	73,114,114	2.66	25 (34%)
24	CHL	N	609	2	66,74,74	1.86	14 (21%)	73,114,114	2.68	24 (32%)
30	OEX	a	401	4,6	0,15,15	-	-	-	-	-
25	CLA	1	611	29	65,73,73	1.48	9 (13%)	76,113,113	1.31	6 (7%)
25	CLA	B	615	-	65,73,73	1.47	12 (18%)	76,113,113	1.29	6 (7%)
25	CLA	y	604	-	65,73,73	1.53	11 (16%)	76,113,113	1.36	7 (9%)
29	LHG	6	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	c	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	3	605	2	66,74,74	2.02	15 (22%)	73,114,114	2.60	21 (28%)
29	LHG	4	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)
34	BCR	A	411	-	41,41,41	0.82	0	56,56,56	1.70	12 (21%)
26	LUT	0	1621	-	42,43,43	0.79	0	51,60,60	1.61	10 (19%)
25	CLA	G	602	3	65,73,73	1.43	9 (13%)	76,113,113	1.40	8 (10%)
28	NEX	1	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.45	17 (34%)
25	CLA	7	604	-	65,73,73	1.51	11 (16%)	76,113,113	1.31	9 (11%)
35	SQD	a	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.79	9 (15%)
25	CLA	q	610	3	65,73,73	1.49	8 (12%)	76,113,113	1.26	8 (10%)
26	LUT	s	1621	-	42,43,43	0.82	0	51,60,60	1.80	14 (27%)
25	CLA	C	511	6	65,73,73	1.44	11 (16%)	76,113,113	1.53	10 (13%)
27	XAT	y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.30	23 (42%)
26	LUT	q	1621	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
25	CLA	3	613	2	65,73,73	1.48	7 (10%)	76,113,113	1.49	8 (10%)
25	CLA	D	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.32	8 (10%)
26	LUT	S	1621	-	42,43,43	0.81	0	51,60,60	1.79	14 (27%)
34	BCR	D	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)
28	NEX	s	1623	-	38,46,46	1.03	3 (7%)	50,70,70	2.55	18 (36%)
35	SQD	d	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
24	CHL	g	609	3	66,74,74	1.90	15 (22%)	73,114,114	2.61	20 (27%)
25	CLA	r	611	29	49,57,73	1.69	11 (22%)	55,93,113	1.48	6 (10%)
25	CLA	S	610	18	49,57,73	1.70	10 (20%)	55,93,113	1.37	8 (14%)
25	CLA	G	614	-	49,57,73	1.67	9 (18%)	55,93,113	1.33	8 (14%)
24	CHL	7	601	1	66,74,74	1.88	12 (18%)	73,114,114	2.83	25 (34%)
24	CHL	Y	609	1	66,74,74	1.84	14 (21%)	73,114,114	2.76	24 (32%)
27	XAT	6	1622	-	39,47,47	0.92	2 (5%)	54,74,74	4.25	21 (38%)
25	CLA	S	602	18	49,57,73	1.71	9 (18%)	55,93,113	1.57	7 (12%)
25	CLA	2	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.48	8 (14%)
25	CLA	Y	611	29	65,73,73	1.49	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	5	607	-	66,74,74	1.90	14 (21%)	73,114,114	2.61	21 (28%)
25	CLA	s	611	29	49,57,73	1.66	10 (20%)	55,93,113	1.47	6 (10%)
25	CLA	8	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
28	NEX	5	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.54	15 (30%)
25	CLA	b	614	-	65,73,73	1.43	9 (13%)	76,113,113	1.44	7 (9%)
25	CLA	2	610	2	65,73,73	1.48	7 (10%)	76,113,113	1.31	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	504	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	7 (9%)
28	NEX	3	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.35	13 (26%)
37	DGD	c	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
26	LUT	3	1621	-	42,43,43	0.77	0	51,60,60	1.56	11 (21%)
29	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	4 (7%)
28	NEX	y	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.44	17 (34%)
33	PHO	A	408	-	51,69,69	1.14	8 (15%)	47,99,99	1.28	9 (19%)
25	CLA	c	501	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
27	XAT	8	1622	-	39,47,47	0.92	0	54,74,74	2.62	19 (35%)
29	LHG	s	2630	25	44,44,48	0.95	2 (4%)	47,50,54	1.12	3 (6%)
24	CHL	6	606	-	66,74,74	1.92	15 (22%)	73,114,114	2.64	21 (28%)
25	CLA	l	613	1	65,73,73	1.44	8 (12%)	76,113,113	1.48	7 (9%)
29	LHG	C	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.02	3 (6%)
25	CLA	d	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.32	8 (10%)
36	LMG	A	413	-	48,48,55	0.93	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	r	601	17	49,57,73	1.68	10 (20%)	55,93,113	1.74	10 (18%)
25	CLA	N	602	2	65,73,73	1.47	10 (15%)	76,113,113	1.29	8 (10%)
24	CHL	Y	606	-	66,74,74	1.82	16 (24%)	73,114,114	2.72	20 (27%)
25	CLA	b	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.27	7 (9%)
24	CHL	Y	608	-	50,58,74	2.06	14 (28%)	52,94,114	3.23	19 (36%)
27	XAT	4	1622	-	39,47,47	0.89	0	54,74,74	2.60	16 (29%)
25	CLA	R	601	17	49,57,73	1.68	10 (20%)	55,93,113	1.72	10 (18%)
25	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.39	8 (10%)
25	CLA	c	508	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.32	12 (24%)
24	CHL	8	606	-	46,54,74	2.42	15 (32%)	49,90,114	2.99	19 (38%)
27	XAT	1	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.22	24 (44%)
25	CLA	5	613	2	65,73,73	1.51	7 (10%)	76,113,113	1.47	7 (9%)
25	CLA	1	610	1	65,73,73	1.45	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	R	602	17	60,68,73	1.53	9 (15%)	70,107,113	1.41	8 (11%)
25	CLA	y	612	1	65,73,73	1.50	11 (16%)	76,113,113	1.38	9 (11%)
25	CLA	2	612	2	43,51,73	1.81	9 (20%)	49,86,113	1.59	7 (14%)
24	CHL	9	605	2	48,56,74	2.34	16 (33%)	51,92,114	2.98	21 (41%)
28	NEX	p	1623	-	38,46,46	0.88	1 (2%)	50,70,70	2.39	16 (32%)
26	LUT	n	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	1	602	1	65,73,73	1.48	7 (10%)	76,113,113	1.28	6 (7%)
25	CLA	C	513	-	65,73,73	1.44	10 (15%)	76,113,113	1.35	8 (10%)
25	CLA	g	612	3	43,51,73	1.79	10 (23%)	49,86,113	1.47	7 (14%)
24	CHL	2	605	2	48,56,74	2.34	16 (33%)	51,92,114	2.98	21 (41%)
36	LMG	D	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.12	3 (5%)
26	LUT	N	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.58	9 (17%)
24	CHL	S	608	-	49,57,74	2.22	15 (30%)	52,93,114	3.05	20 (38%)
25	CLA	3	610	2	65,73,73	1.50	7 (10%)	76,113,113	1.25	7 (9%)
24	CHL	q	601	3	66,74,74	1.93	14 (21%)	73,114,114	2.67	25 (34%)
24	CHL	G	608	-	44,52,74	2.24	13 (29%)	46,87,114	3.10	18 (39%)
25	CLA	7	602	1	65,73,73	1.48	9 (13%)	76,113,113	1.29	8 (10%)
25	CLA	1	604	-	65,73,73	1.50	11 (16%)	76,113,113	1.20	7 (9%)
25	CLA	r	612	-	49,57,73	1.67	9 (18%)	55,93,113	1.56	8 (14%)
26	LUT	2	1620	-	42,43,43	0.77	0	51,60,60	1.55	10 (19%)
26	LUT	8	1620	-	42,43,43	0.72	0	51,60,60	1.62	12 (23%)
24	CHL	5	605	2	66,74,74	2.00	16 (24%)	73,114,114	2.78	25 (34%)
25	CLA	s	613	18	49,57,73	1.74	11 (22%)	55,93,113	1.46	7 (12%)
27	XAT	3	1622	-	39,47,47	0.92	0	54,74,74	2.60	20 (37%)
29	LHG	S	2630	25	44,44,48	0.94	2 (4%)	47,50,54	1.12	3 (6%)
25	CLA	y	614	-	54,62,73	1.60	9 (16%)	62,99,113	1.39	8 (12%)
27	XAT	n	1622	-	39,47,47	1.05	3 (7%)	54,74,74	2.82	22 (40%)
25	CLA	7	613	1	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
25	CLA	s	605	18	50,58,73	1.70	8 (16%)	58,95,113	1.37	7 (12%)
25	CLA	C	512	-	65,73,73	1.50	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	B	605	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	11 (14%)
34	BCR	B	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)
26	LUT	p	1620	-	42,43,43	0.75	0	51,60,60	1.76	9 (17%)
25	CLA	R	609	17	58,66,73	1.60	10 (17%)	67,104,113	1.44	6 (8%)
25	CLA	9	614	-	49,57,73	1.73	8 (16%)	55,93,113	1.37	7 (12%)
25	CLA	b	617	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	9 (11%)
25	CLA	N	611	29	49,57,73	1.67	10 (20%)	55,93,113	1.46	6 (10%)
25	CLA	C	506	-	65,73,73	1.51	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	s	609	18	41,49,73	1.85	7 (17%)	47,84,113	1.53	9 (19%)
24	CHL	p	608	-	50,58,74	2.15	15 (30%)	52,94,114	3.12	17 (32%)
36	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	610	1	65,73,73	1.47	9 (13%)	76,113,113	1.22	8 (10%)
24	CHL	5	609	2	66,74,74	1.96	14 (21%)	73,114,114	2.65	20 (27%)
25	CLA	2	614	-	49,57,73	1.72	8 (16%)	55,93,113	1.37	7 (12%)
29	LHG	D	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
25	CLA	R	604	-	48,56,73	1.73	9 (18%)	55,92,113	1.55	7 (12%)
25	CLA	R	616	17	65,73,73	1.50	9 (13%)	76,113,113	1.29	9 (11%)
25	CLA	3	612	2	45,53,73	1.79	7 (15%)	52,89,113	1.64	8 (15%)
39	PL9	D	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.54	11 (16%)
26	LUT	Y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.66	14 (27%)
25	CLA	B	609	-	65,73,73	1.44	11 (16%)	76,113,113	1.43	7 (9%)
25	CLA	R	610	17	65,73,73	1.47	9 (13%)	76,113,113	1.40	8 (10%)
25	CLA	q	603	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	8 (10%)
29	LHG	N	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	3 (5%)
36	LMG	a	413	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	n	612	2	45,53,73	1.82	10 (22%)	52,89,113	1.54	9 (17%)
24	CHL	Y	607	-	66,74,74	1.84	14 (21%)	73,114,114	2.89	24 (32%)
24	CHL	8	601	2	66,74,74	1.90	12 (18%)	73,114,114	2.65	21 (28%)
24	CHL	4	608	-	44,52,74	2.31	14 (31%)	46,87,114	3.22	17 (36%)
29	LHG	q	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)
25	CLA	p	614	-	49,57,73	1.76	6 (12%)	55,93,113	1.41	8 (14%)
25	CLA	8	614	-	49,57,73	1.72	5 (10%)	55,93,113	1.33	8 (14%)
24	CHL	n	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.82	25 (34%)
24	CHL	9	606	-	50,58,74	2.24	15 (30%)	52,94,114	2.91	20 (38%)
28	NEX	4	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.36	18 (36%)
25	CLA	b	615	-	65,73,73	1.46	11 (16%)	76,113,113	1.29	6 (7%)
28	NEX	n	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.37	15 (30%)
25	CLA	S	603	-	42,50,73	1.82	9 (21%)	48,85,113	1.65	8 (16%)
25	CLA	g	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.57	8 (15%)
25	CLA	7	611	29	65,73,73	1.47	9 (13%)	76,113,113	1.32	6 (7%)
27	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.65	18 (33%)
27	XAT	Y	1622	-	39,47,47	0.97	2 (5%)	54,74,74	4.30	23 (42%)
35	SQD	b	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.14	4 (6%)
25	CLA	C	504	-	65,73,73	1.50	11 (16%)	76,113,113	1.31	7 (9%)
24	CHL	y	607	-	66,74,74	1.84	14 (21%)	73,114,114	2.88	24 (32%)
34	BCR	a	411	-	41,41,41	0.82	0	56,56,56	1.71	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	510	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	8 (10%)
34	BCR	b	620	-	41,41,41	0.83	1 (2%)	56,56,56	1.87	19 (33%)
37	DGD	C	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
24	CHL	1	601	1	66,74,74	1.89	12 (18%)	73,114,114	2.82	25 (34%)
24	CHL	4	607	-	50,58,74	2.27	15 (30%)	52,94,114	3.00	19 (36%)
25	CLA	1	614	-	54,62,73	1.64	8 (14%)	62,99,113	1.35	6 (9%)
25	CLA	6	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.29	9 (11%)
29	LHG	g	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
29	LHG	7	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	4 (7%)
25	CLA	3	602	2	65,73,73	1.49	6 (9%)	76,113,113	1.30	6 (7%)
24	CHL	r	606	-	66,74,74	1.80	14 (21%)	73,114,114	2.76	23 (31%)
25	CLA	4	612	3	43,51,73	1.83	8 (18%)	49,86,113	1.63	10 (20%)
25	CLA	S	609	18	41,49,73	1.85	8 (19%)	47,84,113	1.53	9 (19%)
24	CHL	R	606	-	66,74,74	1.80	13 (19%)	73,114,114	2.76	23 (31%)
40	HEM	F	101	8,9	41,50,50	1.46	3 (7%)	45,82,82	1.24	4 (8%)
25	CLA	n	611	29	49,57,73	1.66	10 (20%)	55,93,113	1.48	6 (10%)
24	CHL	0	606	-	66,74,74	1.95	15 (22%)	73,114,114	2.62	21 (28%)
24	CHL	6	607	-	66,74,74	1.88	15 (22%)	73,114,114	2.60	19 (26%)
34	BCR	H	101	-	41,41,41	0.81	0	56,56,56	2.03	16 (28%)
25	CLA	Y	612	1	65,73,73	1.50	11 (16%)	76,113,113	1.37	9 (11%)
25	CLA	s	610	18	49,57,73	1.69	10 (20%)	55,93,113	1.37	8 (14%)
25	CLA	N	613	2	65,73,73	1.51	10 (15%)	76,113,113	1.44	8 (10%)
24	CHL	9	608	-	44,52,74	2.22	15 (34%)	46,87,114	3.21	17 (36%)
24	CHL	s	606	-	44,52,74	2.17	14 (31%)	46,87,114	3.29	20 (43%)
25	CLA	C	508	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
25	CLA	g	610	3	65,73,73	1.44	9 (13%)	76,113,113	1.33	9 (11%)
37	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
28	NEX	Y	1623	-	38,46,46	1.04	3 (7%)	50,70,70	2.39	16 (32%)
24	CHL	p	607	-	66,74,74	1.94	15 (22%)	73,114,114	2.56	22 (30%)
25	CLA	G	613	3	65,73,73	1.48	10 (15%)	76,113,113	1.33	6 (7%)
25	CLA	d	402	-	65,73,73	1.53	11 (16%)	76,113,113	1.43	7 (9%)
36	LMG	c	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
24	CHL	8	607	-	66,74,74	1.88	14 (21%)	73,114,114	2.77	23 (31%)
34	BCR	b	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.98	16 (28%)
25	CLA	S	614	-	48,56,73	1.67	7 (14%)	55,92,113	1.47	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	1	603	-	65,73,73	1.52	11 (16%)	76,113,113	1.35	7 (9%)
25	CLA	2	602	2	65,73,73	1.45	8 (12%)	76,113,113	1.35	7 (9%)
38	BCT	D	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
24	CHL	3	606	-	46,54,74	2.42	15 (32%)	49,90,114	2.99	18 (36%)
24	CHL	G	607	-	50,58,74	2.11	13 (26%)	52,94,114	3.14	22 (42%)
28	NEX	G	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.42	19 (38%)
25	CLA	b	611	-	65,73,73	1.51	11 (16%)	76,113,113	1.54	8 (10%)
24	CHL	2	608	-	44,52,74	2.20	17 (38%)	46,87,114	3.25	19 (41%)
24	CHL	8	608	-	50,58,74	2.15	14 (28%)	52,94,114	3.01	21 (40%)
25	CLA	r	603	-	60,68,73	1.52	11 (18%)	70,107,113	1.53	7 (10%)
33	PHO	a	409	-	51,69,69	1.08	6 (11%)	47,99,99	1.37	7 (14%)
29	LHG	D	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
24	CHL	0	601	1	66,74,74	1.90	14 (21%)	73,114,114	2.62	21 (28%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	8	611	29	49,57,73	1.71	7 (14%)	55,93,113	1.44	8 (14%)
25	CLA	R	603	-	60,68,73	1.51	11 (18%)	70,107,113	1.53	7 (10%)
25	CLA	5	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.28	8 (10%)
24	CHL	s	601	18	46,54,74	2.32	14 (30%)	49,90,114	3.11	21 (42%)
39	PL9	d	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.55	10 (14%)
29	LHG	d	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
26	LUT	5	1621	-	42,43,43	0.74	0	51,60,60	1.58	11 (21%)
25	CLA	q	604	-	49,57,73	1.73	9 (18%)	55,93,113	1.49	8 (14%)
29	LHG	1	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	5 (9%)
25	CLA	s	602	18	49,57,73	1.70	9 (18%)	55,93,113	1.56	7 (12%)
34	BCR	h	101	-	41,41,41	0.81	0	56,56,56	2.03	17 (30%)
25	CLA	C	509	-	65,73,73	1.40	11 (16%)	76,113,113	1.55	10 (13%)
24	CHL	G	605	3	48,56,74	2.27	15 (31%)	51,92,114	3.07	20 (39%)
29	LHG	9	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	2 (3%)
27	XAT	R	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.47	16 (29%)
25	CLA	s	604	-	49,57,73	1.66	7 (14%)	55,93,113	1.50	8 (14%)
25	CLA	6	604	-	65,73,73	1.55	9 (13%)	76,113,113	1.29	6 (7%)
25	CLA	S	604	-	49,57,73	1.67	8 (16%)	55,93,113	1.50	8 (14%)
29	LHG	0	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
36	LMG	C	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
24	CHL	G	609	3	66,74,74	1.92	15 (22%)	73,114,114	2.61	21 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	3	607	-	66,74,74	1.88	14 (21%)	73,114,114	2.78	22 (30%)
26	LUT	q	1620	-	42,43,43	0.72	0	51,60,60	1.57	13 (25%)
25	CLA	5	611	29	49,57,73	1.72	7 (14%)	55,93,113	1.39	6 (10%)
26	LUT	2	1621	-	42,43,43	0.76	0	51,60,60	1.78	11 (21%)
25	CLA	B	607	-	65,73,73	1.50	9 (13%)	76,113,113	1.43	10 (13%)
35	SQD	A	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.78	9 (15%)
26	LUT	9	1620	-	42,43,43	0.77	0	51,60,60	1.61	13 (25%)
25	CLA	7	614	-	54,62,73	1.66	8 (14%)	62,99,113	1.37	7 (11%)
25	CLA	9	610	2	65,73,73	1.48	7 (10%)	76,113,113	1.28	8 (10%)
24	CHL	n	606	-	46,54,74	2.18	13 (28%)	49,90,114	3.24	19 (38%)
29	LHG	R	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
28	NEX	g	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.41	21 (42%)
25	CLA	q	611	29	45,53,73	1.75	8 (17%)	52,89,113	1.54	6 (11%)
25	CLA	N	604	-	65,73,73	1.52	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	y	608	-	50,58,74	2.06	14 (28%)	52,94,114	3.24	19 (36%)
29	LHG	5	2630	25	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	R	611	29	49,57,73	1.68	11 (22%)	55,93,113	1.47	6 (10%)
26	LUT	s	1620	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.98	4 (5%)
25	CLA	C	501	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
25	CLA	b	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.20	7 (9%)
24	CHL	S	606	-	44,52,74	2.18	14 (31%)	46,87,114	3.30	20 (43%)
25	CLA	5	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.35	7 (9%)
33	PHO	A	409	-	51,69,69	1.08	6 (11%)	47,99,99	1.37	8 (17%)
25	CLA	S	605	18	50,58,73	1.70	9 (18%)	58,95,113	1.37	8 (13%)
34	BCR	C	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)
24	CHL	r	608	-	61,69,74	1.93	15 (24%)	67,108,114	2.81	23 (34%)
24	CHL	4	609	3	66,74,74	2.10	17 (25%)	73,114,114	2.58	19 (26%)
37	DGD	C	523	-	67,67,67	0.82	2 (2%)	81,81,81	1.02	4 (4%)
24	CHL	g	606	-	50,58,74	2.13	14 (28%)	52,94,114	3.11	22 (42%)
24	CHL	4	601	3	66,74,74	1.95	15 (22%)	73,114,114	2.58	23 (31%)
24	CHL	n	601	2	66,74,74	1.83	11 (16%)	73,114,114	2.78	28 (38%)
25	CLA	9	612	2	43,51,73	1.83	8 (18%)	49,86,113	1.58	8 (16%)
25	CLA	3	611	29	49,57,73	1.73	7 (14%)	55,93,113	1.44	9 (16%)
25	CLA	Y	602	1	65,73,73	1.42	8 (12%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.55	11 (21%)
25	CLA	a	410	-	60,68,73	1.52	11 (18%)	70,107,113	1.50	9 (12%)
24	CHL	N	606	-	46,54,74	2.17	13 (28%)	49,90,114	3.21	19 (38%)
26	LUT	0	1620	-	42,43,43	0.76	0	51,60,60	1.59	11 (21%)
25	CLA	n	602	2	65,73,73	1.47	10 (15%)	76,113,113	1.29	8 (10%)
25	CLA	g	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.36	8 (10%)
25	CLA	b	616	-	65,73,73	1.49	11 (16%)	76,113,113	1.52	14 (18%)
25	CLA	Y	604	-	65,73,73	1.54	11 (16%)	76,113,113	1.37	7 (9%)
25	CLA	3	604	-	65,73,73	1.50	7 (10%)	76,113,113	1.41	7 (9%)
25	CLA	n	604	-	65,73,73	1.52	10 (15%)	76,113,113	1.33	6 (7%)
25	CLA	b	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	9 (11%)
24	CHL	2	607	-	50,58,74	2.25	16 (32%)	52,94,114	2.94	20 (38%)
34	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
25	CLA	r	616	17	65,73,73	1.51	9 (13%)	76,113,113	1.29	8 (10%)
25	CLA	b	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)
24	CHL	p	609	2	66,74,74	1.94	14 (21%)	73,114,114	2.67	21 (28%)
35	SQD	B	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.13	4 (6%)
25	CLA	c	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.40	9 (11%)
24	CHL	N	601	2	66,74,74	1.84	11 (16%)	73,114,114	2.76	26 (35%)
36	LMG	S	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.10	4 (6%)
25	CLA	0	613	1	65,73,73	1.47	8 (12%)	76,113,113	1.33	9 (11%)
24	CHL	g	605	3	48,56,74	2.27	15 (31%)	51,92,114	3.09	21 (41%)
25	CLA	y	613	1	65,73,73	1.52	11 (16%)	76,113,113	1.29	7 (9%)
27	XAT	g	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	19 (35%)
25	CLA	0	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.31	8 (10%)
24	CHL	7	606	-	66,74,74	1.90	14 (21%)	73,114,114	2.59	22 (30%)
25	CLA	B	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.60	8 (10%)
25	CLA	B	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.27	7 (9%)
25	CLA	c	509	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	10 (13%)
25	CLA	s	614	-	48,56,73	1.68	7 (14%)	55,92,113	1.47	8 (14%)
28	NEX	0	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.38	12 (24%)
25	CLA	6	614	-	54,62,73	1.66	5 (9%)	62,99,113	1.47	7 (11%)
25	CLA	9	603	-	65,73,73	1.50	9 (13%)	76,113,113	1.36	9 (11%)
26	LUT	3	1620	-	42,43,43	0.73	0	51,60,60	1.67	12 (23%)
26	LUT	4	1620	-	42,43,43	0.74	0	51,60,60	1.61	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	n	1620	-	42,43,43	0.78	0	51,60,60	1.53	10 (19%)
29	LHG	d	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	4	610	3	65,73,73	1.49	8 (12%)	76,113,113	1.30	7 (9%)
27	XAT	G	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	20 (37%)
29	LHG	c	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.04	3 (6%)
26	LUT	1	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	9 (17%)
29	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
36	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
25	CLA	G	603	-	65,73,73	1.48	11 (16%)	76,113,113	1.36	8 (10%)
25	CLA	8	613	2	65,73,73	1.49	7 (10%)	76,113,113	1.48	8 (10%)
34	BCR	c	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
37	DGD	C	518	-	56,56,67	0.89	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	9	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.48	7 (12%)
29	LHG	Y	2630	25	48,48,48	0.88	2 (4%)	51,54,54	1.21	5 (9%)
28	NEX	8	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.31	12 (24%)
25	CLA	4	613	3	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
25	CLA	0	611	29	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
29	LHG	n	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.10	3 (5%)
25	CLA	5	610	2	65,73,73	1.51	7 (10%)	76,113,113	1.21	7 (9%)
25	CLA	Y	610	1	65,73,73	1.43	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	3	614	-	49,57,73	1.72	6 (12%)	55,93,113	1.34	8 (14%)
25	CLA	c	507	-	65,73,73	1.40	11 (16%)	76,113,113	1.45	12 (15%)
26	LUT	N	1620	-	42,43,43	0.77	0	51,60,60	1.49	8 (15%)
25	CLA	B	611	-	65,73,73	1.51	11 (16%)	76,113,113	1.55	9 (11%)
25	CLA	N	610	2	65,73,73	1.46	9 (13%)	76,113,113	1.25	8 (10%)
25	CLA	S	612	18	45,53,73	1.83	11 (24%)	52,89,113	1.63	9 (17%)
25	CLA	0	603	-	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
25	CLA	g	602	3	65,73,73	1.43	8 (12%)	76,113,113	1.38	8 (10%)
26	LUT	G	1621	-	42,43,43	0.78	0	51,60,60	1.65	11 (21%)
25	CLA	s	603	-	42,50,73	1.81	9 (21%)	48,85,113	1.64	7 (14%)
25	CLA	A	407	-	49,57,73	1.65	11 (22%)	55,93,113	1.52	6 (10%)

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
24	CHL	g	608	-	3/3/15/26	3/13/111/137	-
26	LUT	4	1621	-	-	7/29/67/67	0/2/2/2
25	CLA	p	613	2	1/1/15/20	11/37/115/115	-
24	CHL	y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	N	614	-	1/1/11/20	6/18/96/115	-
24	CHL	s	608	-	3/3/16/26	11/19/117/137	-
24	CHL	8	609	2	3/3/20/26	20/39/137/137	-
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	3	601	2	3/3/20/26	24/39/137/137	-
24	CHL	6	608	-	3/3/16/26	8/20/118/137	-
25	CLA	3	603	-	1/1/15/20	13/37/115/115	-
25	CLA	7	610	1	1/1/15/20	15/37/115/115	-
25	CLA	5	612	2	1/1/11/20	6/13/91/115	-
25	CLA	B	610	-	1/1/15/20	8/37/115/115	-
25	CLA	n	614	-	1/1/11/20	6/18/96/115	-
25	CLA	N	612	2	1/1/11/20	6/13/91/115	-
25	CLA	6	611	29	1/1/15/20	12/37/115/115	-
25	CLA	S	611	29	1/1/11/20	6/18/96/115	-
25	CLA	8	603	-	1/1/15/20	14/37/115/115	-
25	CLA	c	506	-	1/1/15/20	20/37/115/115	-
25	CLA	D	402	-	1/1/15/20	14/37/115/115	-
25	CLA	y	602	1	1/1/15/20	12/37/115/115	-
28	NEX	q	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	y	601	1	3/3/20/26	14/39/137/137	-
25	CLA	B	602	-	1/1/15/20	17/37/115/115	-
25	CLA	r	609	17	1/1/13/20	6/29/107/115	-
25	CLA	q	612	3	1/1/10/20	7/11/89/115	-
24	CHL	1	609	1	3/3/20/26	17/39/137/137	-
26	LUT	5	1620	-	-	4/29/67/67	0/2/2/2
25	CLA	R	612	-	1/1/11/20	8/18/96/115	-
37	DGD	c	519	-	-	20/51/91/95	0/2/2/2
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
24	CHL	1	607	-	3/3/20/26	19/39/137/137	-
25	CLA	4	603	-	1/1/15/20	18/37/115/115	-
24	CHL	5	606	-	3/3/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	G	2630	25	-	12/53/53/53	-
25	CLA	c	511	6	-	14/37/115/115	-
25	CLA	6	602	1	1/1/15/20	12/37/115/115	-
25	CLA	C	503	-	1/1/15/20	10/37/115/115	-
24	CHL	6	601	1	3/3/20/26	10/39/137/137	-
25	CLA	B	606	-	1/1/15/20	12/37/115/115	-
25	CLA	p	611	29	1/1/11/20	6/18/96/115	-
24	CHL	q	606	-	3/3/16/26	5/20/118/137	-
25	CLA	a	406	-	1/1/15/20	3/37/115/115	-
25	CLA	7	612	1	1/1/15/20	13/37/115/115	-
25	CLA	B	612	-	1/1/15/20	9/37/115/115	-
25	CLA	g	614	-	1/1/11/20	9/18/96/115	-
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	G	610	3	1/1/15/20	10/37/115/115	-
25	CLA	Y	613	1	-	9/37/115/115	-
25	CLA	A	410	-	1/1/14/20	6/31/109/115	-
24	CHL	q	609	3	3/3/20/26	20/39/137/137	-
24	CHL	p	601	2	3/3/20/26	16/39/137/137	-
40	HEM	f	101	8,9	-	3/12/54/54	-
25	CLA	n	613	2	1/1/15/20	14/37/115/115	-
25	CLA	5	614	-	-	8/18/96/115	-
24	CHL	2	601	2	3/3/20/26	24/39/137/137	-
25	CLA	Y	614	-	1/1/12/20	10/24/102/115	-
24	CHL	7	605	1	3/3/16/26	8/15/113/137	-
25	CLA	r	610	17	1/1/15/20	14/37/115/115	-
33	PHO	a	408	-	-	10/37/103/103	0/5/6/6
24	CHL	8	605	2	3/3/20/26	15/39/137/137	-
24	CHL	y	609	1	3/3/20/26	17/39/137/137	-
25	CLA	4	611	29	1/1/11/20	7/13/91/115	-
35	SQD	b	623	-	-	14/45/65/69	0/1/1/1
28	NEX	R	623	-	-	2/27/83/83	0/3/3/3
25	CLA	n	603	-	1/1/15/20	7/37/115/115	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	y	610	1	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	p	605	2	3/3/20/26	17/39/137/137	-
25	CLA	B	616	-	1/1/15/20	10/37/115/115	-
24	CHL	9	607	-	3/3/16/26	11/20/118/137	-
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
24	CHL	3	608	-	3/3/16/26	11/20/118/137	-
24	CHL	q	605	3	3/3/16/26	8/18/116/137	-
27	XAT	q	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
24	CHL	0	607	-	3/3/20/26	24/39/137/137	-
25	CLA	0	610	1	1/1/15/20	6/37/115/115	-
25	CLA	p	604	-	1/1/15/20	15/37/115/115	-
25	CLA	s	612	18	1/1/11/20	4/13/91/115	-
24	CHL	N	608	-	3/3/16/26	6/20/118/137	-
29	LHG	2	2630	25	-	22/53/53/53	-
37	DGD	C	520	-	-	10/48/88/95	0/2/2/2
24	CHL	s	607	-	3/3/15/26	4/12/110/137	-
25	CLA	p	602	2	1/1/15/20	12/37/115/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
25	CLA	b	608	-	1/1/15/20	18/37/115/115	-
25	CLA	N	603	-	1/1/15/20	6/37/115/115	-
24	CHL	r	607	-	3/3/18/26	17/27/125/137	-
25	CLA	A	405	-	1/1/15/20	11/37/115/115	-
29	LHG	L	101	-	-	17/53/53/53	-
25	CLA	9	611	29	1/1/11/20	8/13/91/115	-
26	LUT	8	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	R	607	-	3/3/18/26	17/27/125/137	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	4	602	3	1/1/15/20	10/37/115/115	-
27	XAT	2	1622	-	-	2/31/93/93	0/4/4/4
36	LMG	h	102	-	-	14/43/63/70	0/1/1/1
24	CHL	1	608	-	3/3/16/26	9/20/118/137	-
25	CLA	A	406	-	1/1/15/20	3/37/115/115	-
25	CLA	c	513	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	s	2631	-	-	10/47/67/70	0/1/1/1
36	LMG	H	102	-	-	15/43/63/70	0/1/1/1
25	CLA	b	607	-	-	15/37/115/115	-
25	CLA	6	613	1	-	20/37/115/115	-
25	CLA	a	405	-	1/1/15/20	11/37/115/115	-
24	CHL	7	609	1	3/3/20/26	17/39/137/137	-
25	CLA	r	602	17	1/1/14/20	6/31/109/115	-
35	SQD	D	413	-	-	10/47/67/69	0/1/1/1
25	CLA	4	604	-	1/1/11/20	13/18/96/115	-
27	XAT	p	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	G	611	29	1/1/11/20	6/13/91/115	-
29	LHG	8	2630	25	-	10/53/53/53	-
26	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	p	610	2	1/1/15/20	9/37/115/115	-
25	CLA	2	611	29	1/1/11/20	8/13/91/115	-
25	CLA	5	602	2	1/1/15/20	16/37/115/115	-
25	CLA	7	603	-	1/1/15/20	15/37/115/115	-
25	CLA	B	603	-	1/1/15/20	13/37/115/115	-
24	CHL	0	605	1	3/3/16/26	7/15/113/137	-
24	CHL	G	601	3	3/3/20/26	18/39/137/137	-
24	CHL	3	609	2	3/3/20/26	18/39/137/137	-
25	CLA	r	604	-	1/1/11/20	8/17/95/115	-
34	BCR	c	517	-	-	0/29/63/63	0/2/2/2
36	LMG	d	412	-	-	5/41/61/70	0/1/1/1
24	CHL	n	608	-	3/3/16/26	12/20/118/137	-
25	CLA	q	602	3	1/1/15/20	15/37/115/115	-
24	CHL	0	609	1	3/3/20/26	19/39/137/137	-
25	CLA	a	407	-	1/1/11/20	6/18/96/115	-
24	CHL	q	608	-	3/3/15/26	6/13/111/137	-
24	CHL	y	606	-	3/3/20/26	21/39/137/137	-
25	CLA	8	610	2	1/1/15/20	9/37/115/115	-
25	CLA	B	617	-	1/1/15/20	10/37/115/115	-
24	CHL	7	608	-	3/3/16/26	12/20/118/137	-
36	LMG	d	411	-	-	8/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	613	18	-	9/18/96/115	-
24	CHL	Y	601	1	3/3/20/26	13/39/137/137	-
26	LUT	G	1620	-	-	3/29/67/67	0/2/2/2
27	XAT	N	1622	-	-	0/31/93/93	0/4/4/4
26	LUT	y	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	G	606	-	3/3/16/26	5/20/118/137	-
24	CHL	9	609	2	3/3/20/26	19/39/137/137	-
25	CLA	8	602	2	1/1/15/20	11/37/115/115	-
25	CLA	p	612	2	1/1/11/20	4/13/91/115	-
25	CLA	G	604	-	1/1/11/20	7/18/96/115	-
25	CLA	n	610	2	1/1/15/20	6/37/115/115	-
24	CHL	S	607	-	3/3/15/26	4/12/110/137	-
28	NEX	S	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	9	601	2	3/3/20/26	21/39/137/137	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	0	614	-	1/1/12/20	9/24/102/115	-
25	CLA	2	613	2	1/1/15/20	8/37/115/115	-
29	LHG	r	2630	25	-	16/42/42/53	-
24	CHL	2	609	2	3/3/20/26	20/39/137/137	-
24	CHL	1	606	-	3/3/20/26	19/39/137/137	-
34	BCR	C	516	-	-	9/29/63/63	0/2/2/2
25	CLA	G	612	3	1/1/10/20	4/11/89/115	-
25	CLA	g	613	3	1/1/15/20	13/37/115/115	-
24	CHL	4	605	3	3/3/16/26	12/18/116/137	-
25	CLA	c	510	-	1/1/15/20	10/37/115/115	-
36	LMG	D	412	-	-	5/41/61/70	0/1/1/1
25	CLA	4	614	-	1/1/11/20	8/18/96/115	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	b	613	-	1/1/15/20	14/37/115/115	-
24	CHL	g	607	-	3/3/16/26	10/20/118/137	-
24	CHL	p	606	-	3/3/16/26	5/15/113/137	-
25	CLA	y	611	29	1/1/15/20	8/37/115/115	-
25	CLA	8	612	2	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	6	605	1	3/3/16/26	5/15/113/137	-
24	CHL	N	607	-	3/3/20/26	14/39/137/137	-
25	CLA	y	603	-	1/1/15/20	15/37/115/115	-
26	LUT	p	1621	-	-	4/29/67/67	0/2/2/2
34	BCR	c	515	-	-	4/29/63/63	0/2/2/2
29	LHG	y	2630	25	-	24/53/53/53	-
29	LHG	d	408	-	-	10/48/48/53	-
25	CLA	b	609	-	1/1/15/20	12/37/115/115	-
24	CHL	6	609	1	3/3/20/26	19/39/137/137	-
24	CHL	4	606	-	3/3/16/26	8/20/118/137	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	c	502	-	1/1/15/20	17/37/115/115	-
25	CLA	1	612	1	1/1/15/20	15/37/115/115	-
34	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	6	603	-	1/1/15/20	10/37/115/115	-
25	CLA	c	512	-	1/1/15/20	13/37/115/115	-
25	CLA	C	502	-	1/1/15/20	18/37/115/115	-
24	CHL	N	605	2	3/3/20/26	23/39/137/137	-
25	CLA	r	613	17	-	15/31/109/115	-
24	CHL	q	607	-	3/3/16/26	13/20/118/137	-
25	CLA	B	608	-	1/1/15/20	16/37/115/115	-
24	CHL	7	607	-	3/3/20/26	19/39/137/137	-
37	DGD	c	523	-	-	12/55/95/95	0/2/2/2
27	XAT	r	622	-	-	0/31/93/93	0/4/4/4
25	CLA	b	605	-	1/1/15/20	15/37/115/115	-
25	CLA	C	507	-	1/1/15/20	11/37/115/115	-
34	BCR	b	618	-	-	5/29/63/63	0/2/2/2
34	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CHL	g	601	3	3/3/20/26	19/39/137/137	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
25	CLA	2	603	-	1/1/15/20	20/37/115/115	-
25	CLA	9	602	2	1/1/15/20	16/37/115/115	-
24	CHL	R	608	-	3/3/19/26	15/33/131/137	-
35	SQD	B	623	-	-	11/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
24	CHL	5	601	2	3/3/20/26	18/39/137/137	-
25	CLA	0	602	1	1/1/15/20	11/37/115/115	-
25	CLA	q	613	3	1/1/15/20	16/37/115/115	-
25	CLA	b	610	-	1/1/15/20	8/37/115/115	-
28	NEX	N	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	9	613	2	1/1/15/20	8/37/115/115	-
28	NEX	r	623	-	-	2/27/83/83	0/3/3/3
25	CLA	p	603	-	1/1/15/20	14/37/115/115	-
24	CHL	0	608	-	3/3/16/26	6/20/118/137	-
25	CLA	0	604	-	1/1/15/20	17/37/115/115	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	LUT	g	1620	-	-	3/29/67/67	0/2/2/2
25	CLA	b	602	-	1/1/15/20	17/37/115/115	-
24	CHL	5	608	-	3/3/16/26	11/20/118/137	-
29	LHG	3	2630	25	-	12/53/53/53	-
28	NEX	9	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	S	601	18	3/3/16/26	9/15/113/137	-
24	CHL	Y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	g	604	-	1/1/11/20	8/18/96/115	-
26	LUT	9	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	q	614	-	1/1/11/20	8/18/96/115	-
24	CHL	n	605	2	3/3/20/26	20/39/137/137	-
27	XAT	0	1622	-	-	2/31/93/93	0/4/4/4
26	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
27	XAT	9	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	2	606	-	3/3/16/26	9/20/118/137	-
25	CLA	R	613	17	-	15/31/109/115	-
29	LHG	p	2630	25	-	12/53/53/53	-
24	CHL	n	609	2	3/3/20/26	20/39/137/137	-
24	CHL	N	609	2	3/3/20/26	19/39/137/137	-
25	CLA	1	611	29	1/1/15/20	8/37/115/115	-
25	CLA	B	615	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	y	604	-	-	18/37/115/115	-
29	LHG	6	2630	25	-	19/53/53/53	-
25	CLA	c	503	-	1/1/15/20	14/37/115/115	-
24	CHL	3	605	2	3/3/20/26	17/39/137/137	-
29	LHG	4	2630	25	-	19/53/53/53	-
34	BCR	A	411	-	-	2/29/63/63	0/2/2/2
26	LUT	0	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	G	602	3	1/1/15/20	11/37/115/115	-
28	NEX	1	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	7	604	-	1/1/15/20	17/37/115/115	-
35	SQD	a	412	-	-	18/46/66/69	0/1/1/1
25	CLA	q	610	3	1/1/15/20	9/37/115/115	-
26	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	C	511	6	-	14/37/115/115	-
27	XAT	y	1622	-	-	0/31/93/93	0/4/4/4
26	LUT	q	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	3	613	2	-	15/37/115/115	-
25	CLA	D	403	-	1/1/15/20	12/37/115/115	-
26	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
34	BCR	D	404	-	-	4/29/63/63	0/2/2/2
28	NEX	s	1623	-	-	4/27/83/83	0/3/3/3
35	SQD	d	413	-	-	9/47/67/69	0/1/1/1
24	CHL	g	609	3	3/3/20/26	15/39/137/137	-
25	CLA	r	611	29	1/1/11/20	10/18/96/115	-
25	CLA	S	610	18	1/1/11/20	9/18/96/115	-
25	CLA	G	614	-	1/1/11/20	9/18/96/115	-
24	CHL	7	601	1	3/3/20/26	16/39/137/137	-
24	CHL	Y	609	1	3/3/20/26	17/39/137/137	-
27	XAT	6	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	S	602	18	-	10/18/96/115	-
25	CLA	2	604	-	1/1/11/20	9/18/96/115	-
25	CLA	Y	611	29	1/1/15/20	8/37/115/115	-
24	CHL	5	607	-	3/3/20/26	19/39/137/137	-
25	CLA	s	611	29	1/1/11/20	6/18/96/115	-
25	CLA	8	604	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	5	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	b	614	-	1/1/15/20	10/37/115/115	-
25	CLA	2	610	2	1/1/15/20	4/37/115/115	-
25	CLA	c	504	-	1/1/15/20	15/37/115/115	-
28	NEX	3	1623	-	-	5/27/83/83	0/3/3/3
37	DGD	c	524	-	-	9/55/95/95	0/2/2/2
26	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
29	LHG	l	101	-	-	18/53/53/53	-
28	NEX	y	1623	-	-	5/27/83/83	0/3/3/3
33	PHO	A	408	-	-	10/37/103/103	0/5/6/6
25	CLA	c	501	-	1/1/15/20	14/37/115/115	-
27	XAT	8	1622	-	-	1/31/93/93	0/4/4/4
29	LHG	s	2630	25	-	18/49/49/53	-
24	CHL	6	606	-	3/3/20/26	22/39/137/137	-
25	CLA	1	613	1	-	14/37/115/115	-
29	LHG	C	2630	-	-	19/51/51/53	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
36	LMG	A	413	-	-	12/43/63/70	0/1/1/1
25	CLA	r	601	17	1/1/11/20	8/18/96/115	-
25	CLA	N	602	2	1/1/15/20	6/37/115/115	-
24	CHL	Y	606	-	3/3/20/26	21/39/137/137	-
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
24	CHL	Y	608	-	3/3/16/26	4/20/118/137	-
27	XAT	4	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	R	601	17	1/1/11/20	8/18/96/115	-
25	CLA	C	505	-	1/1/15/20	18/37/115/115	-
25	CLA	c	508	-	1/1/15/20	13/37/115/115	-
28	NEX	6	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	8	606	-	3/3/16/26	8/15/113/137	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	5	613	2	1/1/15/20	12/37/115/115	-
25	CLA	1	610	1	1/1/15/20	14/37/115/115	-
25	CLA	R	602	17	1/1/14/20	6/31/109/115	-
25	CLA	y	612	1	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	2	612	2	1/1/10/20	4/11/89/115	-
24	CHL	9	605	2	3/3/16/26	6/18/116/137	-
28	NEX	p	1623	-	-	4/27/83/83	0/3/3/3
26	LUT	n	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	1	602	1	1/1/15/20	11/37/115/115	-
25	CLA	C	513	-	1/1/15/20	17/37/115/115	-
25	CLA	g	612	3	1/1/10/20	4/11/89/115	-
24	CHL	2	605	2	3/3/16/26	6/18/116/137	-
36	LMG	D	411	-	-	8/41/61/70	0/1/1/1
26	LUT	N	1621	-	-	5/29/67/67	0/2/2/2
24	CHL	S	608	-	3/3/16/26	11/19/117/137	-
25	CLA	3	610	2	1/1/15/20	6/37/115/115	-
24	CHL	q	601	3	3/3/20/26	19/39/137/137	-
24	CHL	G	608	-	3/3/15/26	6/13/111/137	-
25	CLA	7	602	1	1/1/15/20	13/37/115/115	-
25	CLA	1	604	-	1/1/15/20	15/37/115/115	-
25	CLA	r	612	-	1/1/11/20	8/18/96/115	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
26	LUT	8	1620	-	-	4/29/67/67	0/2/2/2
24	CHL	5	605	2	3/3/20/26	20/39/137/137	-
25	CLA	s	613	18	-	9/18/96/115	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
29	LHG	S	2630	25	-	16/49/49/53	-
25	CLA	y	614	-	1/1/12/20	10/24/102/115	-
27	XAT	n	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	7	613	1	-	15/37/115/115	-
25	CLA	s	605	18	1/1/12/20	8/19/97/115	-
25	CLA	C	512	-	1/1/15/20	15/37/115/115	-
25	CLA	B	605	-	1/1/15/20	15/37/115/115	-
34	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	LUT	p	1620	-	-	6/29/67/67	0/2/2/2
25	CLA	R	609	17	1/1/13/20	6/29/107/115	-
25	CLA	9	614	-	-	8/18/96/115	-
25	CLA	b	617	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	N	611	29	1/1/11/20	9/18/96/115	-
25	CLA	C	506	-	1/1/15/20	20/37/115/115	-
25	CLA	s	609	18	1/1/10/20	4/8/86/115	-
24	CHL	p	608	-	3/3/16/26	13/20/118/137	-
36	LMG	B	622	-	-	9/46/66/70	0/1/1/1
25	CLA	6	610	1	1/1/15/20	6/37/115/115	-
24	CHL	5	609	2	3/3/20/26	19/39/137/137	-
25	CLA	2	614	-	-	7/18/96/115	-
29	LHG	D	408	-	-	10/48/48/53	-
25	CLA	R	604	-	1/1/11/20	8/17/95/115	-
25	CLA	R	616	17	-	22/37/115/115	-
25	CLA	3	612	2	1/1/11/20	8/13/91/115	-
39	PL9	D	405	-	-	14/53/73/73	0/1/1/1
26	LUT	Y	1621	-	-	4/29/67/67	0/2/2/2
25	CLA	B	609	-	1/1/15/20	12/37/115/115	-
25	CLA	R	610	17	1/1/15/20	14/37/115/115	-
25	CLA	q	603	-	1/1/15/20	17/37/115/115	-
29	LHG	N	2630	25	-	15/53/53/53	-
36	LMG	a	413	-	-	12/43/63/70	0/1/1/1
25	CLA	n	612	2	1/1/11/20	6/13/91/115	-
24	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
24	CHL	8	601	2	3/3/20/26	24/39/137/137	-
24	CHL	4	608	-	3/3/15/26	4/13/111/137	-
29	LHG	q	2630	25	-	17/53/53/53	-
25	CLA	p	614	-	-	7/18/96/115	-
25	CLA	8	614	-	1/1/11/20	8/18/96/115	-
24	CHL	n	607	-	3/3/20/26	14/39/137/137	-
24	CHL	9	606	-	3/3/16/26	10/20/118/137	-
28	NEX	4	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	b	615	-	1/1/15/20	14/37/115/115	-
28	NEX	n	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	S	603	-	1/1/10/20	5/10/88/115	-
25	CLA	g	611	29	1/1/11/20	6/13/91/115	-
25	CLA	7	611	29	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	5	1622	-	-	0/31/93/93	0/4/4/4
27	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
35	SQD	b	621	-	-	17/49/69/69	0/1/1/1
25	CLA	C	504	-	1/1/15/20	15/37/115/115	-
24	CHL	y	607	-	3/3/20/26	18/39/137/137	-
34	BCR	a	411	-	-	2/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	10/37/115/115	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
37	DGD	C	524	-	-	9/55/95/95	0/2/2/2
24	CHL	1	601	1	3/3/20/26	14/39/137/137	-
24	CHL	4	607	-	3/3/16/26	13/20/118/137	-
25	CLA	1	614	-	1/1/12/20	13/24/102/115	-
25	CLA	6	612	1	1/1/15/20	11/37/115/115	-
29	LHG	g	2630	25	-	12/53/53/53	-
29	LHG	7	2630	25	-	18/53/53/53	-
25	CLA	3	602	2	1/1/15/20	11/37/115/115	-
24	CHL	r	606	-	3/3/20/26	22/39/137/137	-
25	CLA	4	612	3	1/1/10/20	7/11/89/115	-
25	CLA	S	609	18	1/1/10/20	4/8/86/115	-
24	CHL	R	606	-	3/3/20/26	22/39/137/137	-
40	HEM	F	101	8,9	-	4/12/54/54	-
25	CLA	n	611	29	1/1/11/20	9/18/96/115	-
24	CHL	0	606	-	3/3/20/26	21/39/137/137	-
24	CHL	6	607	-	3/3/20/26	25/39/137/137	-
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	Y	612	1	1/1/15/20	15/37/115/115	-
25	CLA	s	610	18	1/1/11/20	9/18/96/115	-
25	CLA	N	613	2	1/1/15/20	14/37/115/115	-
24	CHL	9	608	-	3/3/15/26	4/13/111/137	-
24	CHL	s	606	-	3/3/15/26	10/13/111/137	-
25	CLA	C	508	-	1/1/15/20	15/37/115/115	-
25	CLA	g	610	3	1/1/15/20	10/37/115/115	-
37	DGD	C	519	-	-	20/51/91/95	0/2/2/2
28	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	p	607	-	3/3/20/26	22/39/137/137	-
25	CLA	G	613	3	1/1/15/20	14/37/115/115	-
25	CLA	d	402	-	1/1/15/20	14/37/115/115	-
36	LMG	c	521	-	-	10/46/66/70	0/1/1/1
24	CHL	8	607	-	3/3/20/26	24/39/137/137	-
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	CLA	S	614	-	1/1/11/20	7/17/95/115	-
25	CLA	1	603	-	1/1/15/20	17/37/115/115	-
25	CLA	2	602	2	-	12/37/115/115	-
24	CHL	3	606	-	3/3/16/26	8/15/113/137	-
24	CHL	G	607	-	3/3/16/26	7/20/118/137	-
28	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	b	611	-	1/1/15/20	8/37/115/115	-
24	CHL	2	608	-	3/3/15/26	5/13/111/137	-
24	CHL	8	608	-	3/3/16/26	11/20/118/137	-
25	CLA	r	603	-	1/1/14/20	10/31/109/115	-
33	PHO	a	409	-	-	9/37/103/103	0/5/6/6
29	LHG	D	410	-	-	10/43/43/53	-
24	CHL	0	601	1	3/3/20/26	11/39/137/137	-
37	DGD	c	518	-	-	7/44/84/95	0/2/2/2
25	CLA	8	611	29	1/1/11/20	8/18/96/115	-
25	CLA	R	603	-	1/1/14/20	10/31/109/115	-
25	CLA	5	604	-	1/1/15/20	16/37/115/115	-
24	CHL	s	601	18	3/3/16/26	9/15/113/137	-
39	PL9	d	405	-	-	14/53/73/73	0/1/1/1
29	LHG	d	410	-	-	12/43/43/53	-
26	LUT	5	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	q	604	-	-	12/18/96/115	-
29	LHG	1	2630	25	-	16/53/53/53	-
25	CLA	s	602	18	-	7/18/96/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	4/37/115/115	-
24	CHL	G	605	3	3/3/16/26	10/18/116/137	-
29	LHG	9	2630	25	-	20/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	R	622	-	-	0/31/93/93	0/4/4/4
25	CLA	s	604	-	1/1/11/20	10/18/96/115	-
25	CLA	6	604	-	-	18/37/115/115	-
25	CLA	S	604	-	1/1/11/20	10/18/96/115	-
29	LHG	0	2630	25	-	18/53/53/53	-
36	LMG	C	521	-	-	10/46/66/70	0/1/1/1
24	CHL	G	609	3	3/3/20/26	14/39/137/137	-
24	CHL	3	607	-	3/3/20/26	24/39/137/137	-
26	LUT	q	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	5	611	29	1/1/11/20	11/18/96/115	-
26	LUT	2	1621	-	-	6/29/67/67	0/2/2/2
25	CLA	B	607	-	-	15/37/115/115	-
35	SQD	A	412	-	-	18/46/66/69	0/1/1/1
26	LUT	9	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	7	614	-	1/1/12/20	13/24/102/115	-
25	CLA	9	610	2	1/1/15/20	4/37/115/115	-
24	CHL	n	606	-	3/3/16/26	9/15/113/137	-
29	LHG	R	2630	25	-	16/42/42/53	-
28	NEX	g	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	q	611	29	1/1/11/20	7/13/91/115	-
25	CLA	N	604	-	1/1/15/20	9/37/115/115	-
24	CHL	y	608	-	3/3/16/26	4/20/118/137	-
29	LHG	5	2630	25	-	13/53/53/53	-
25	CLA	R	611	29	1/1/11/20	9/18/96/115	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
37	DGD	c	520	-	-	10/48/88/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	14/37/115/115	-
25	CLA	b	606	-	1/1/15/20	12/37/115/115	-
24	CHL	S	606	-	3/3/15/26	10/13/111/137	-
25	CLA	5	603	-	1/1/15/20	13/37/115/115	-
33	PHO	A	409	-	-	9/37/103/103	0/5/6/6
25	CLA	S	605	18	1/1/12/20	9/19/97/115	-
34	BCR	C	517	-	-	0/29/63/63	0/2/2/2
24	CHL	r	608	-	3/3/19/26	15/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	4	609	3	3/3/20/26	18/39/137/137	-
37	DGD	C	523	-	-	12/55/95/95	0/2/2/2
24	CHL	g	606	-	3/3/16/26	5/20/118/137	-
24	CHL	4	601	3	3/3/20/26	18/39/137/137	-
24	CHL	n	601	2	3/3/20/26	8/39/137/137	-
25	CLA	9	612	2	1/1/10/20	4/11/89/115	-
25	CLA	3	611	29	1/1/11/20	8/18/96/115	-
25	CLA	Y	602	1	1/1/15/20	12/37/115/115	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	a	410	-	1/1/14/20	6/31/109/115	-
24	CHL	N	606	-	3/3/16/26	9/15/113/137	-
26	LUT	0	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	n	602	2	1/1/15/20	6/37/115/115	-
25	CLA	g	603	-	1/1/15/20	7/37/115/115	-
25	CLA	b	616	-	1/1/15/20	10/37/115/115	-
25	CLA	Y	604	-	-	18/37/115/115	-
25	CLA	3	604	-	1/1/15/20	8/37/115/115	-
25	CLA	n	604	-	1/1/15/20	9/37/115/115	-
25	CLA	b	603	-	1/1/15/20	13/37/115/115	-
24	CHL	2	607	-	3/3/16/26	10/20/118/137	-
34	BCR	C	514	-	-	4/29/63/63	0/2/2/2
25	CLA	r	616	17	-	22/37/115/115	-
25	CLA	b	612	-	1/1/15/20	9/37/115/115	-
24	CHL	p	609	2	3/3/20/26	19/39/137/137	-
35	SQD	B	621	-	-	17/49/69/69	0/1/1/1
25	CLA	c	505	-	1/1/15/20	18/37/115/115	-
24	CHL	N	601	2	3/3/20/26	8/39/137/137	-
36	LMG	S	2631	-	-	12/47/67/70	0/1/1/1
25	CLA	0	613	1	-	16/37/115/115	-
24	CHL	g	605	3	3/3/16/26	9/18/116/137	-
25	CLA	y	613	1	-	9/37/115/115	-
27	XAT	g	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	0	612	1	1/1/15/20	11/37/115/115	-
24	CHL	7	606	-	3/3/20/26	20/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	-	1/1/15/20	14/37/115/115	-
25	CLA	B	604	-	1/1/15/20	11/37/115/115	-
25	CLA	c	509	-	1/1/15/20	5/37/115/115	-
25	CLA	s	614	-	1/1/11/20	7/17/95/115	-
28	NEX	0	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	6	614	-	1/1/12/20	9/24/102/115	-
25	CLA	9	603	-	1/1/15/20	21/37/115/115	-
26	LUT	3	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	4	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	d	409	-	-	12/53/53/53	-
25	CLA	4	610	3	1/1/15/20	12/37/115/115	-
27	XAT	G	1622	-	-	0/31/93/93	0/4/4/4
29	LHG	c	2630	-	-	15/51/51/53	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	D	409	-	-	12/53/53/53	-
36	LMG	b	622	-	-	8/46/66/70	0/1/1/1
25	CLA	G	603	-	1/1/15/20	7/37/115/115	-
25	CLA	8	613	2	-	15/37/115/115	-
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
37	DGD	C	518	-	-	7/44/84/95	0/2/2/2
25	CLA	9	604	-	1/1/11/20	8/18/96/115	-
29	LHG	Y	2630	25	-	23/53/53/53	-
28	NEX	8	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	4	613	3	1/1/15/20	17/37/115/115	-
25	CLA	0	611	29	1/1/15/20	7/37/115/115	-
29	LHG	n	2630	25	-	15/53/53/53	-
25	CLA	5	610	2	1/1/15/20	8/37/115/115	-
25	CLA	Y	610	1	1/1/15/20	11/37/115/115	-
25	CLA	3	614	-	1/1/11/20	8/18/96/115	-
25	CLA	c	507	-	1/1/15/20	12/37/115/115	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	611	-	1/1/15/20	8/37/115/115	-
25	CLA	N	610	2	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	612	18	1/1/11/20	4/13/91/115	-
25	CLA	0	603	-	1/1/15/20	11/37/115/115	-
25	CLA	g	602	3	1/1/15/20	11/37/115/115	-
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	s	603	-	1/1/10/20	5/10/88/115	-
25	CLA	A	407	-	1/1/11/20	6/18/96/115	-

The worst 5 of 4330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	614	CLA	C4B-NB	7.88	1.42	1.35
25	p	602	CLA	C4B-NB	7.84	1.42	1.35
25	0	614	CLA	C4B-NB	7.80	1.42	1.35
25	p	614	CLA	C4B-NB	7.80	1.42	1.35
25	4	612	CLA	C4B-NB	7.79	1.42	1.35

The worst 5 of 6324 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	412	SQD	O9-S-C6	-19.98	83.20	106.94
35	A	412	SQD	O9-S-C6	-19.85	83.34	106.94
27	Y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	6	1622	XAT	C37-C21-C36	-17.56	81.47	107.37

5 of 591 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 5618 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	C1A-C2A-CAA-CBA

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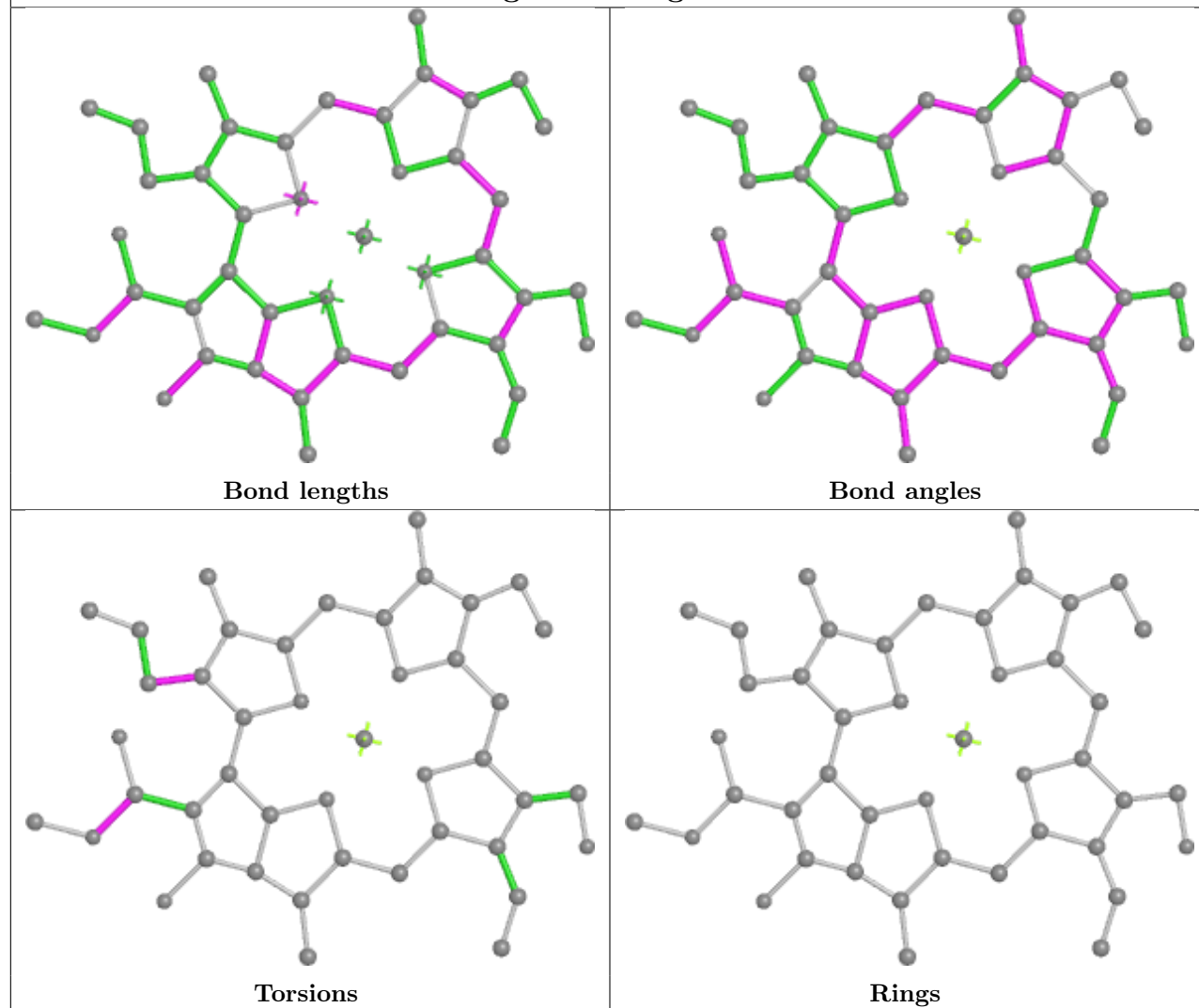
Mol	Chain	Res	Type	Atoms
24	1	606	CHL	C1C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

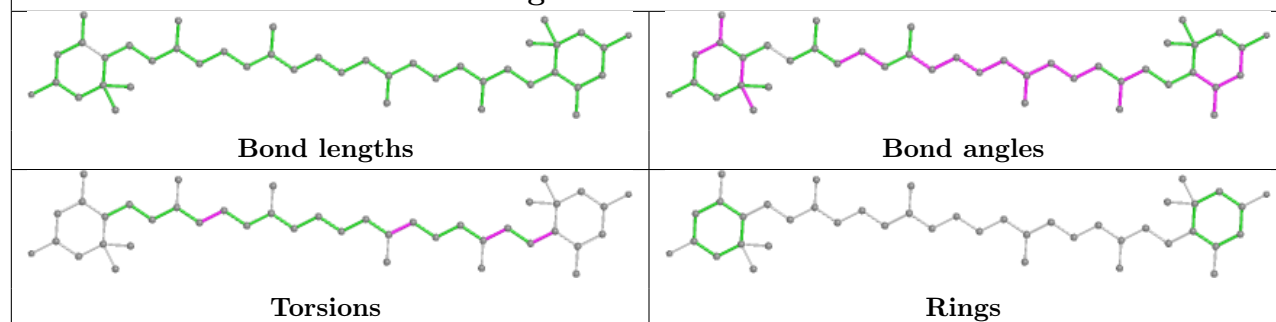
No monomer is involved in short contacts.

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.

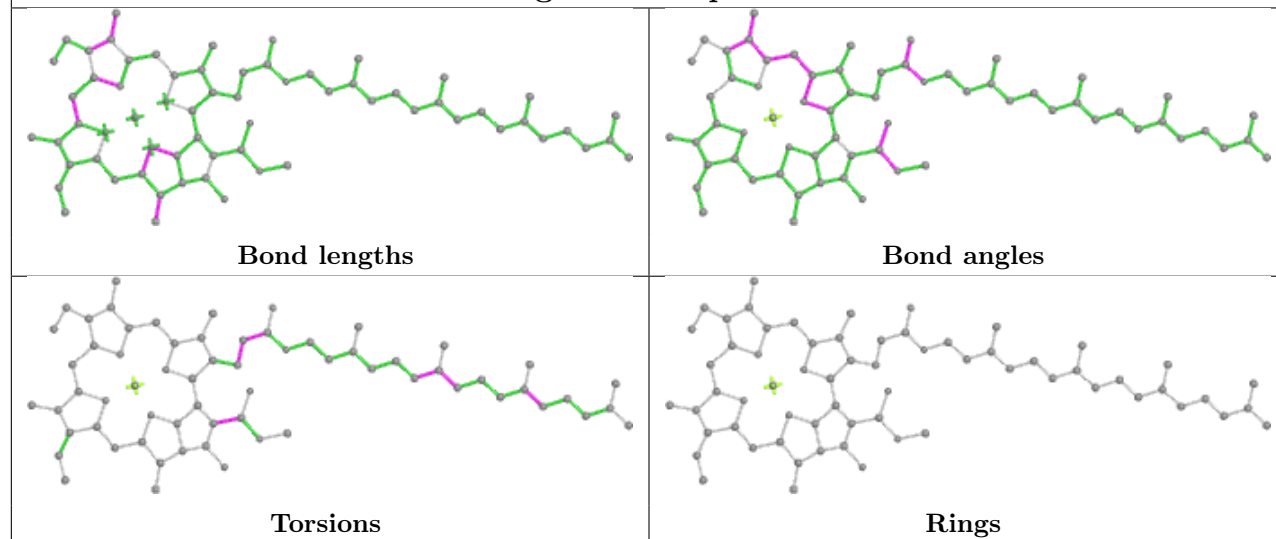
Ligand CHL g 608



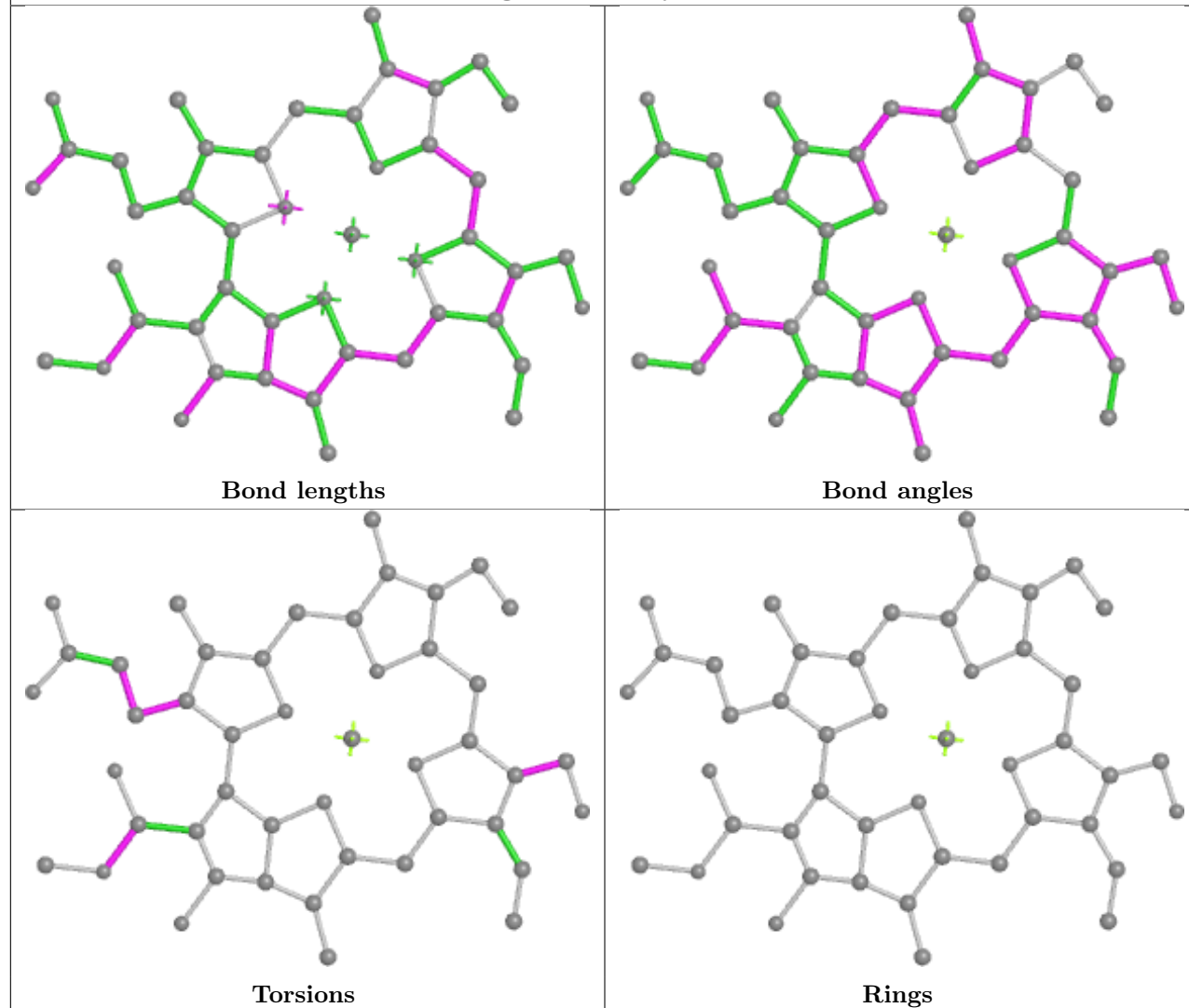
Ligand LUT 4 1621

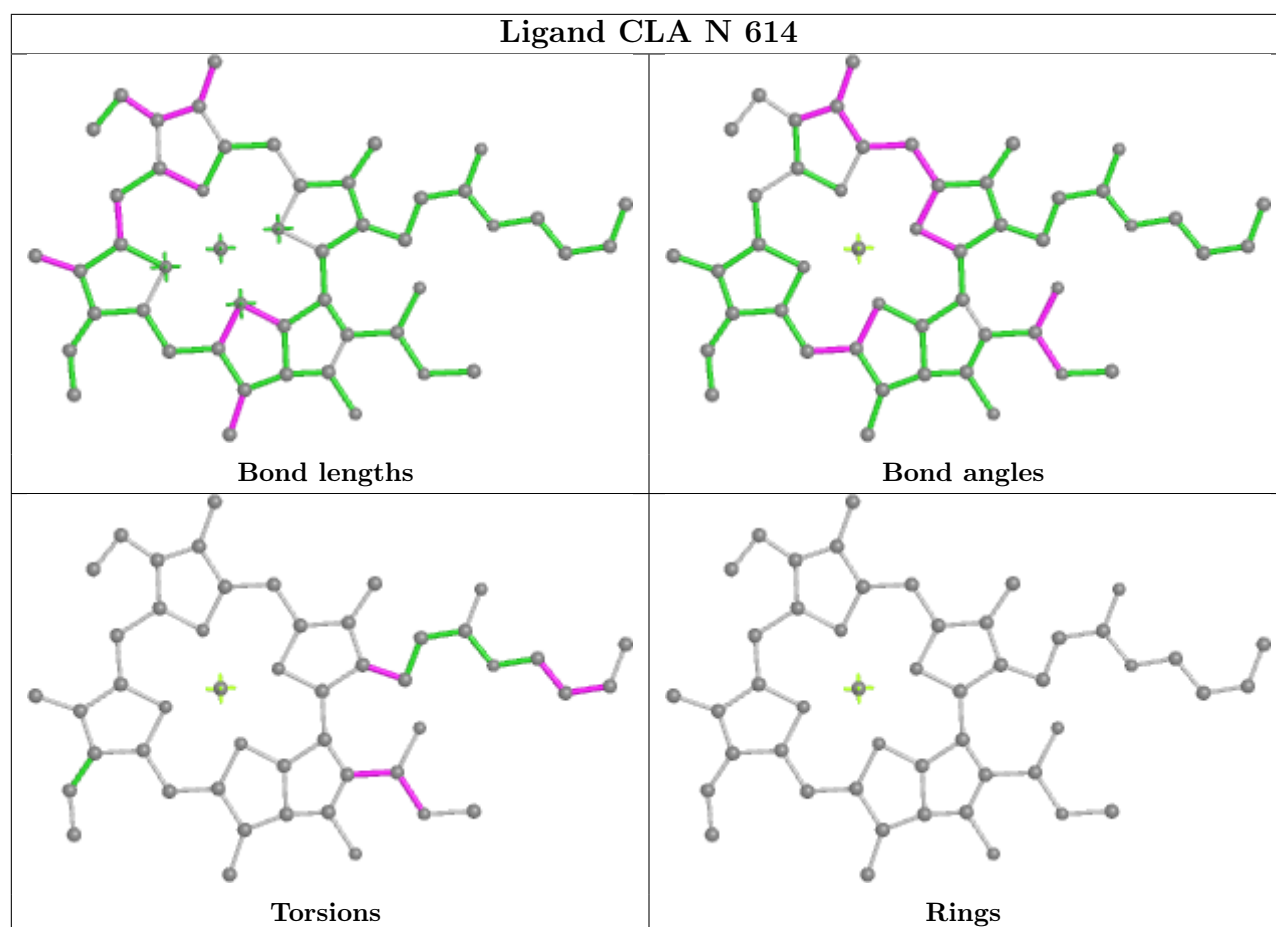


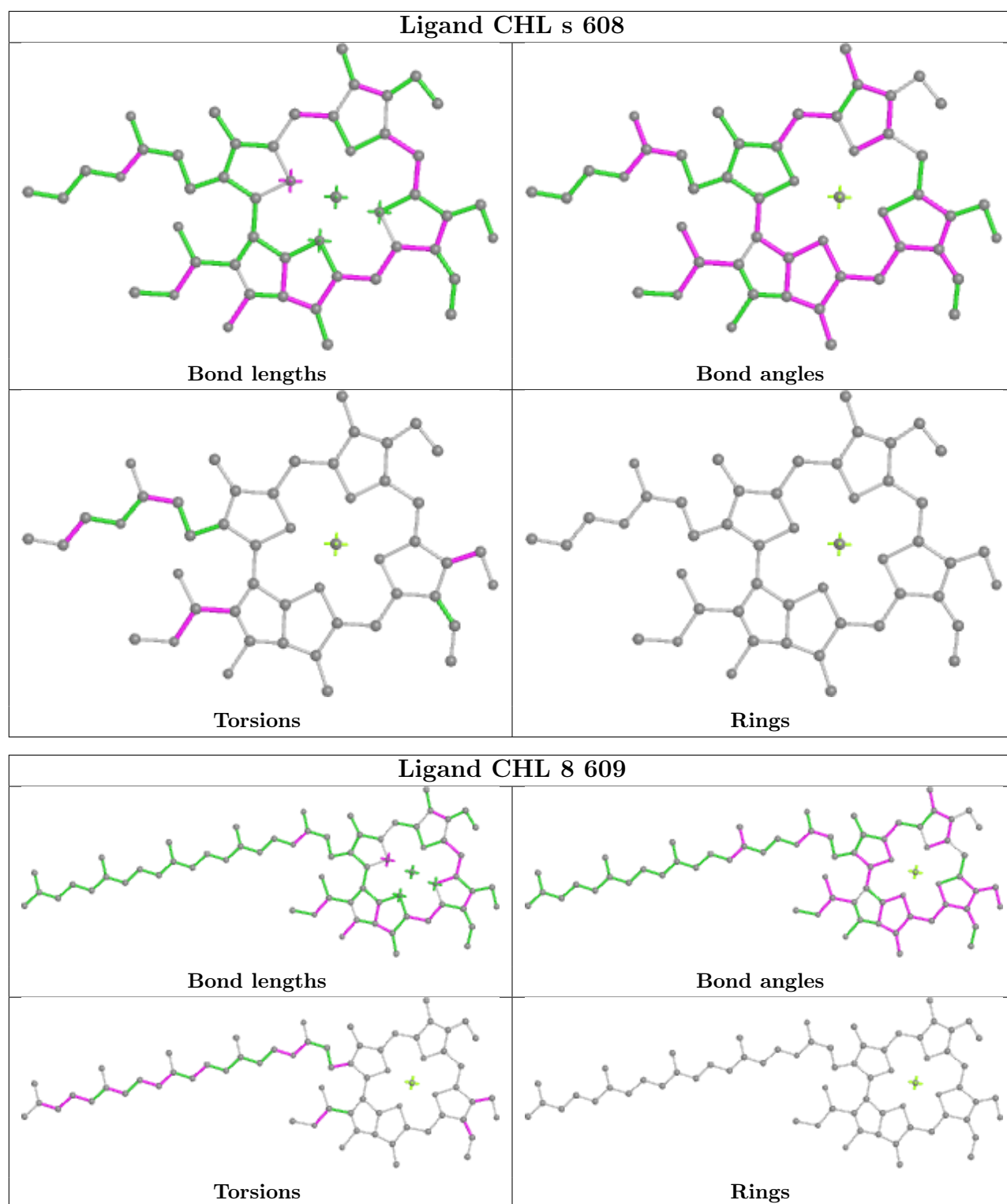
Ligand CLA p 613

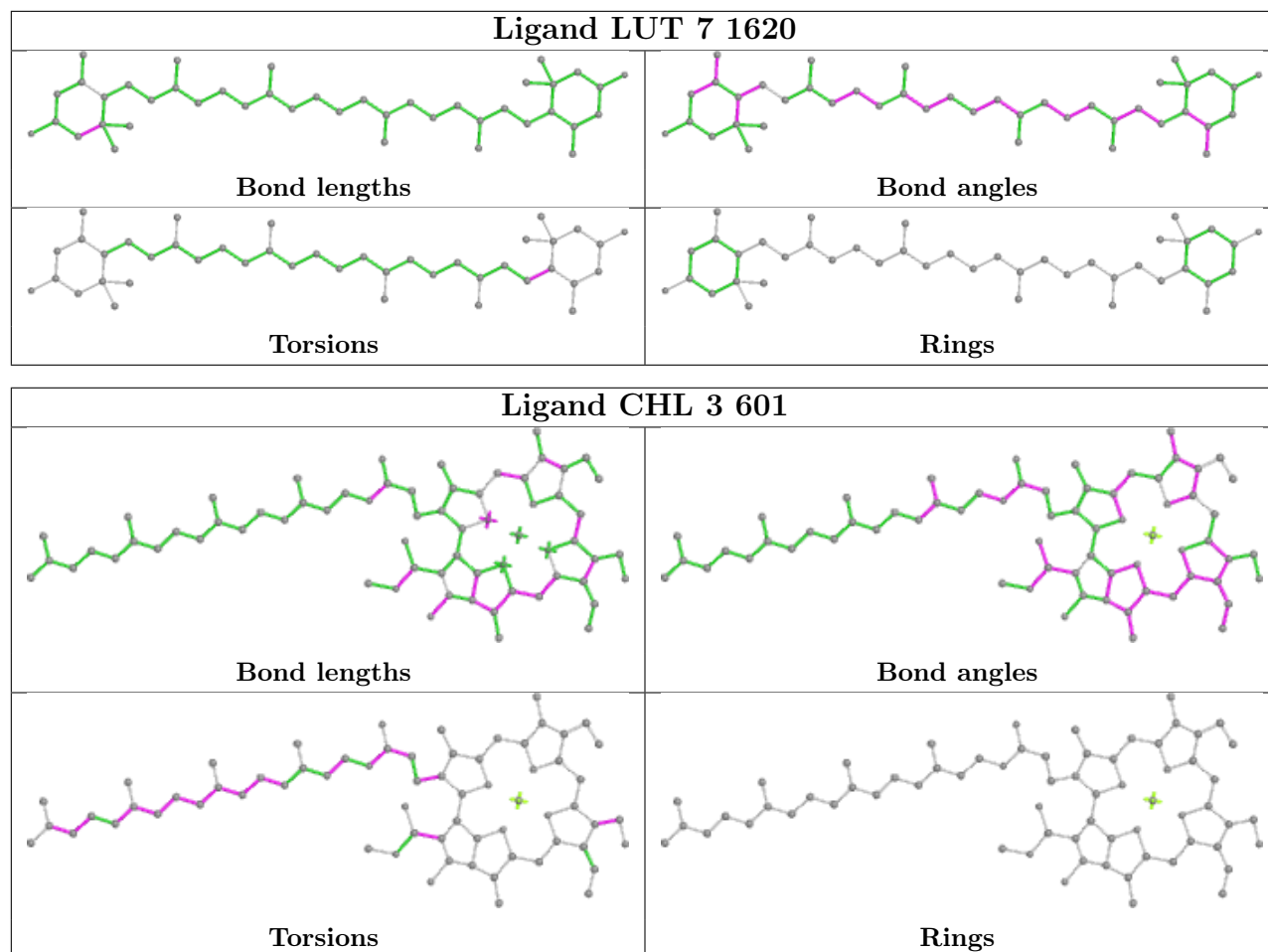


Ligand CHL y 605

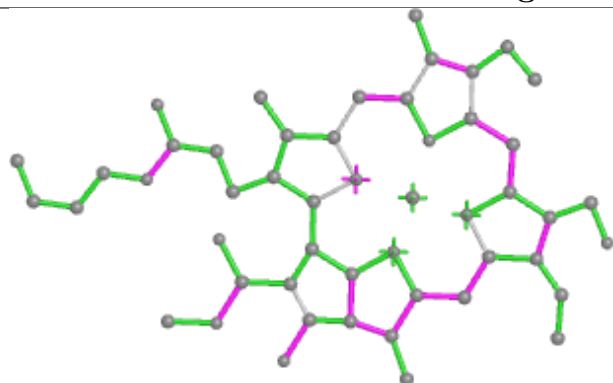




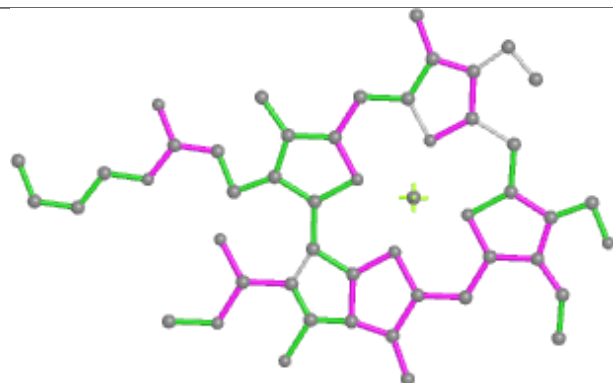




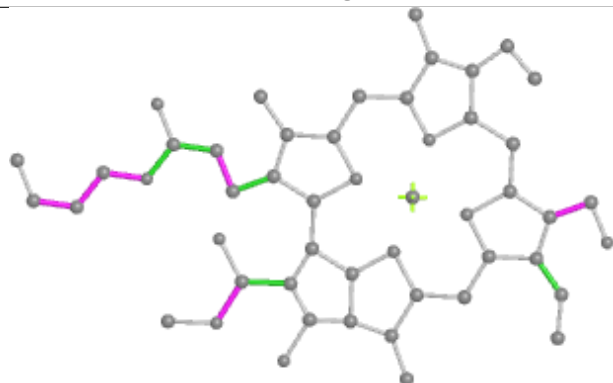
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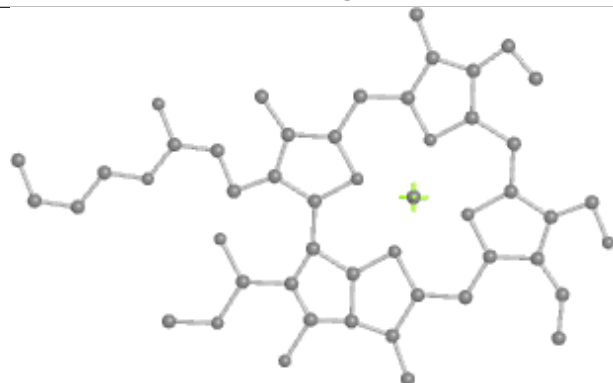
Bond lengths



Bond angles

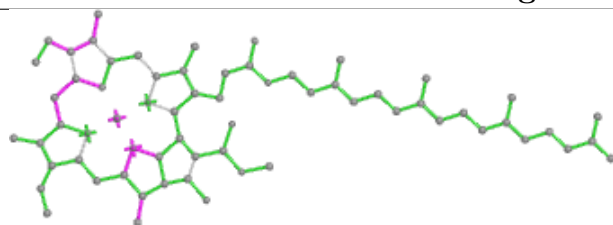


Torsions

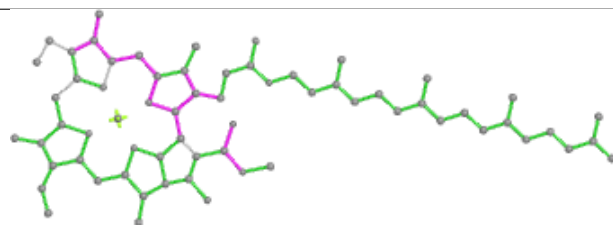


Rings

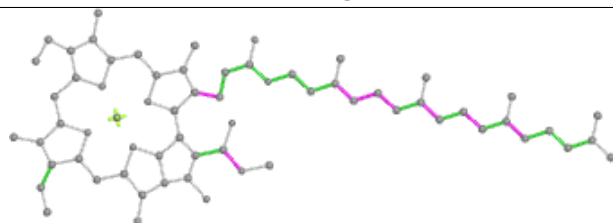
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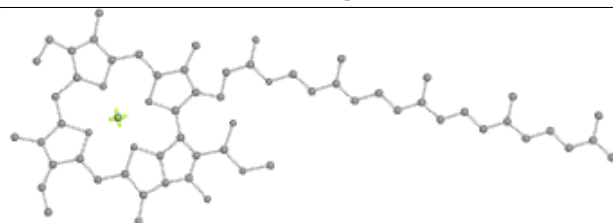
Bond lengths



Bond angles

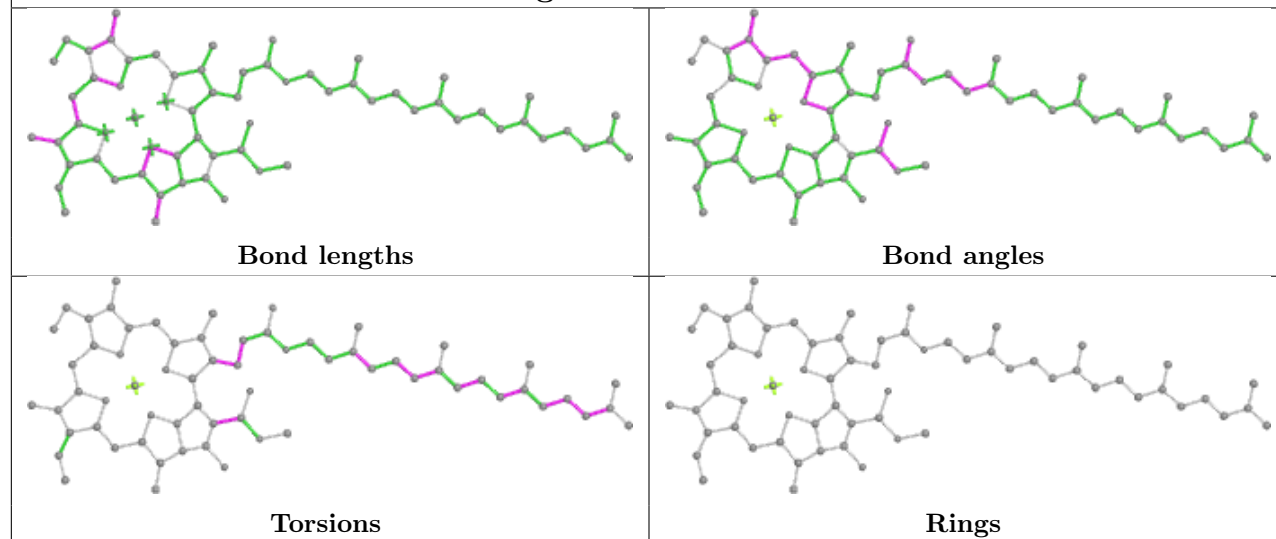


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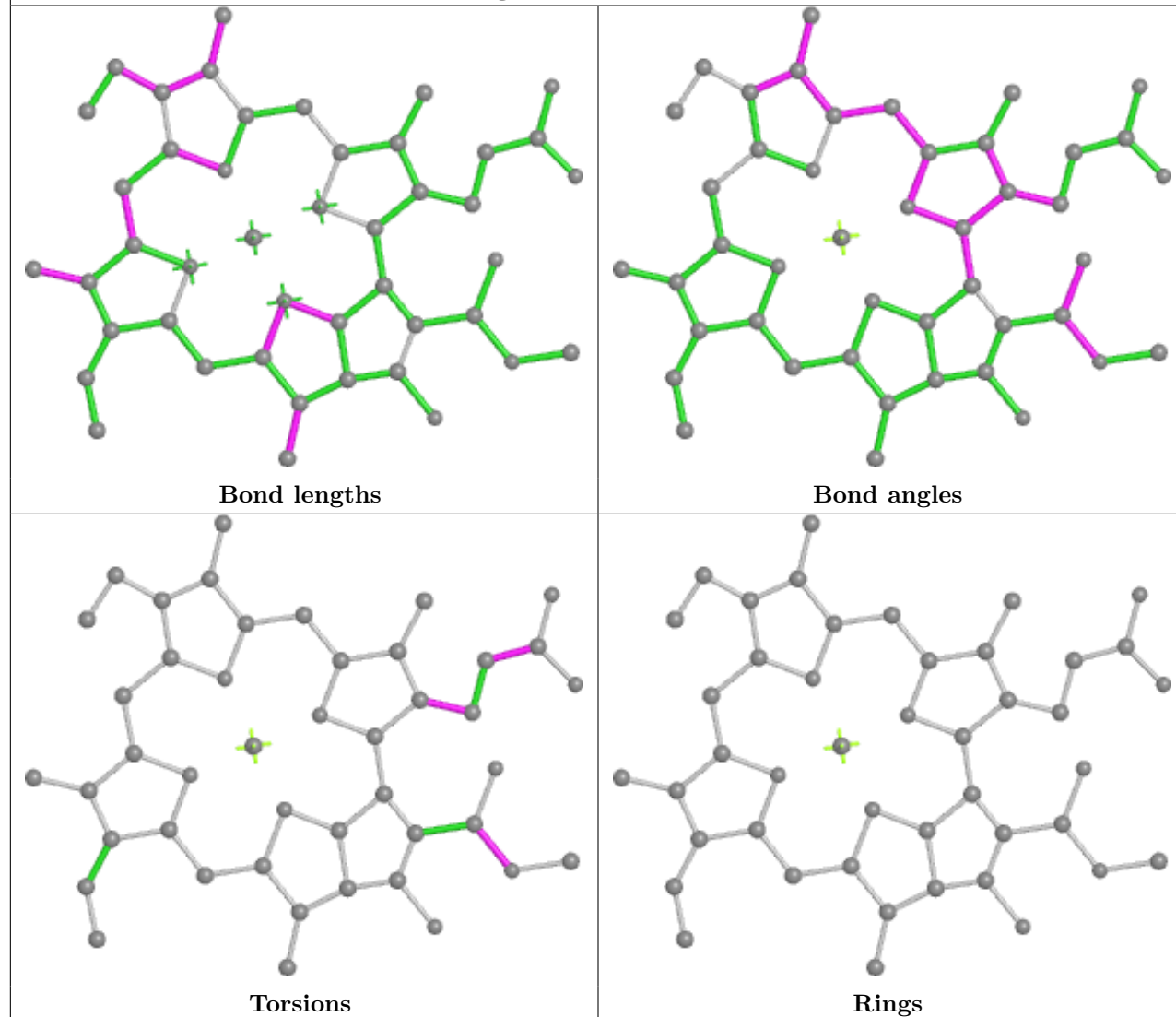


Rings

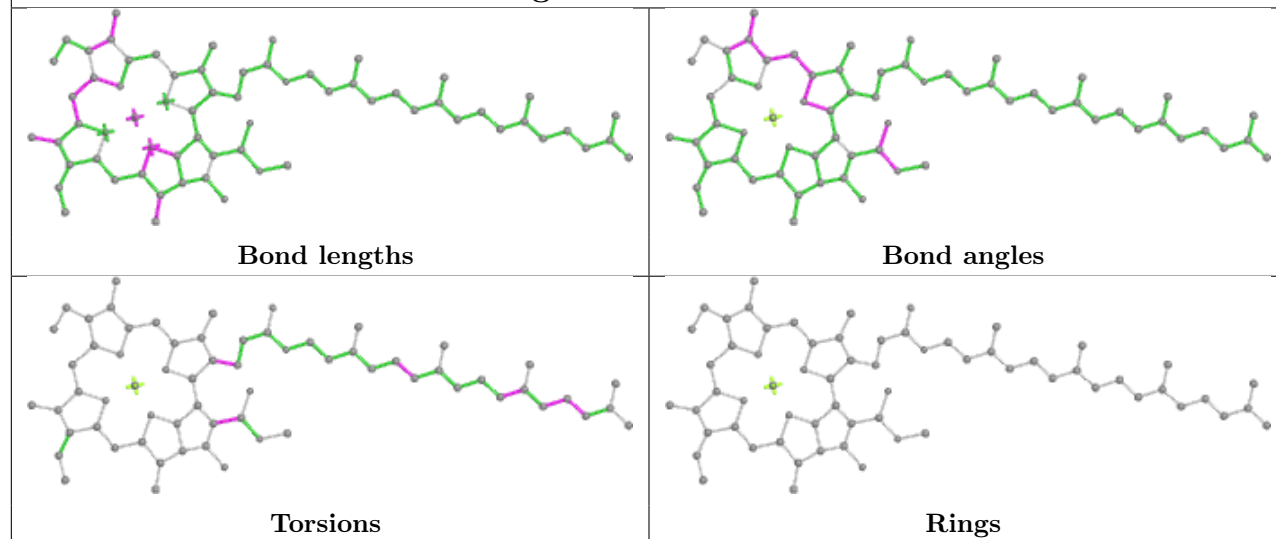
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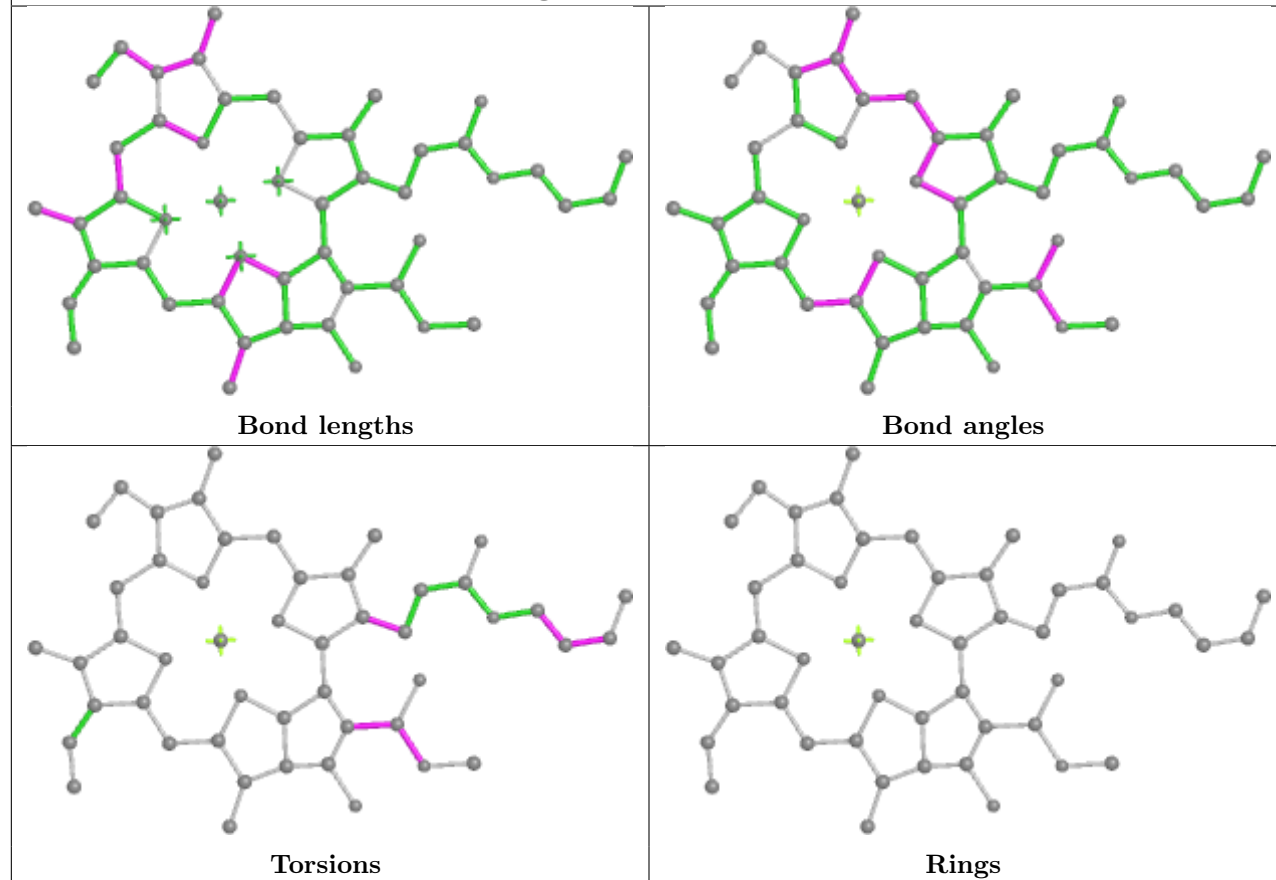
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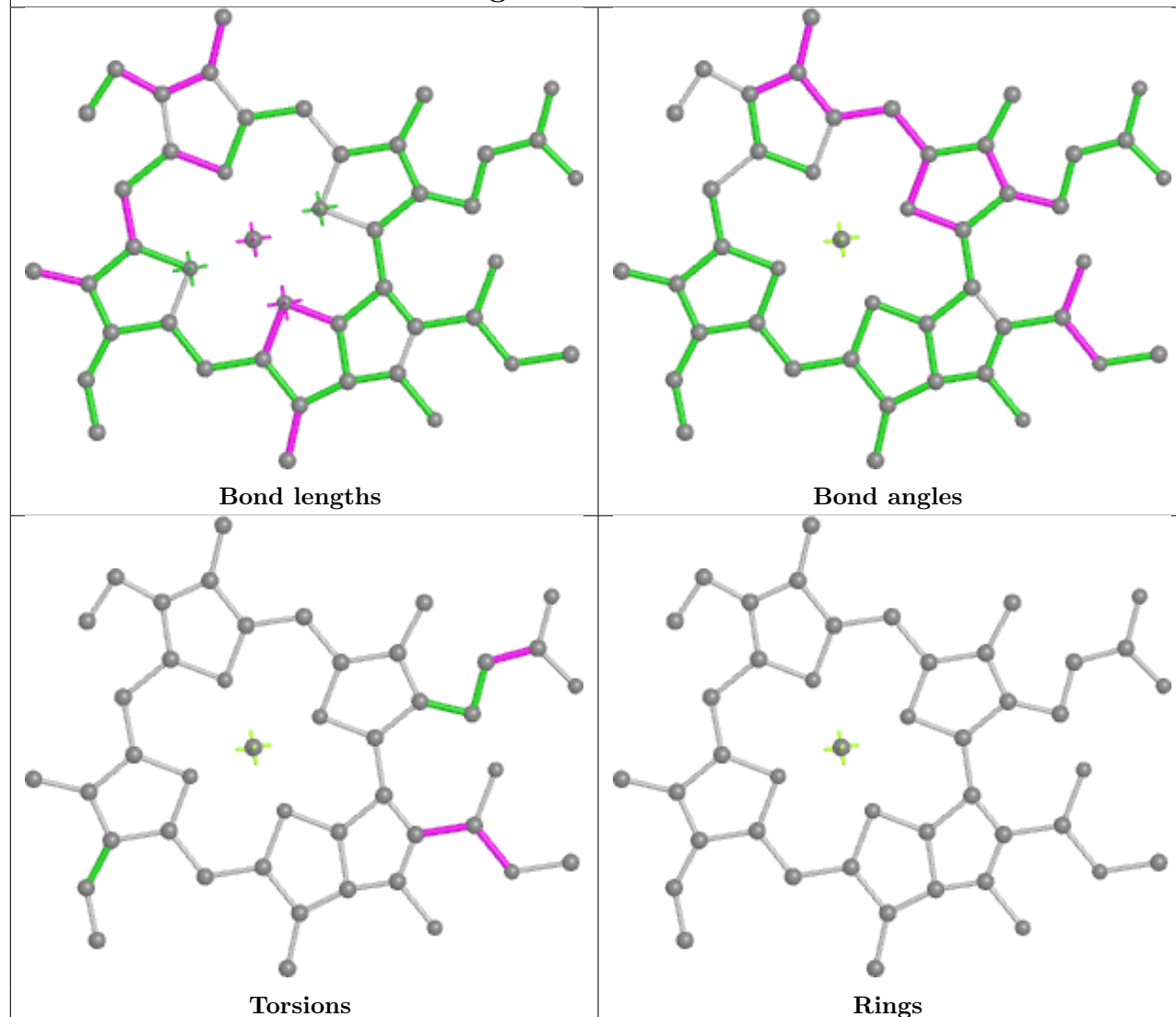
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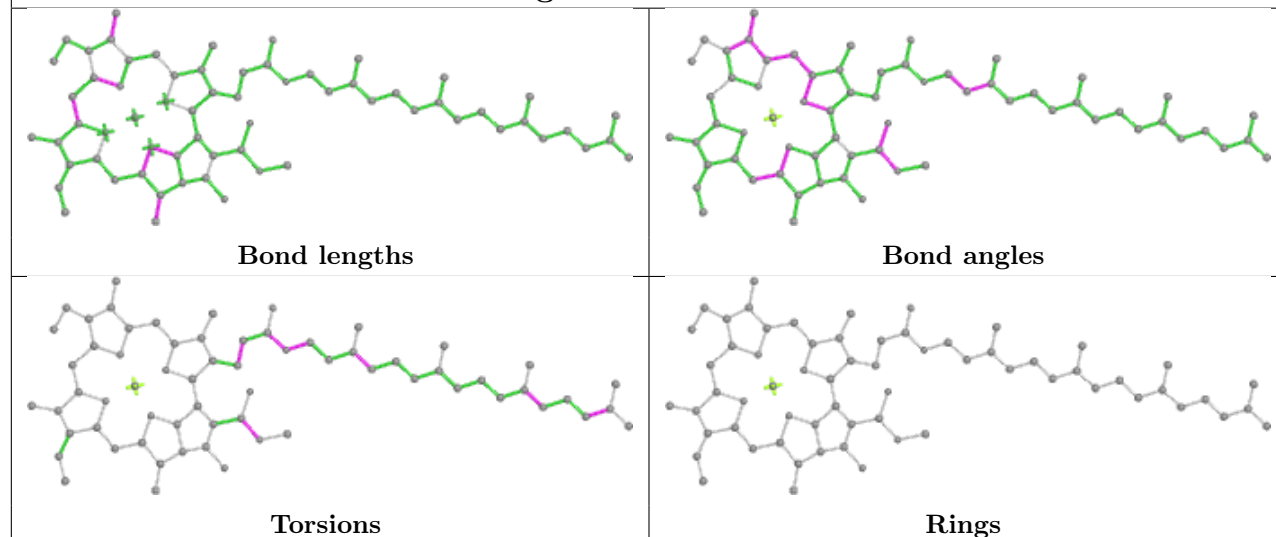
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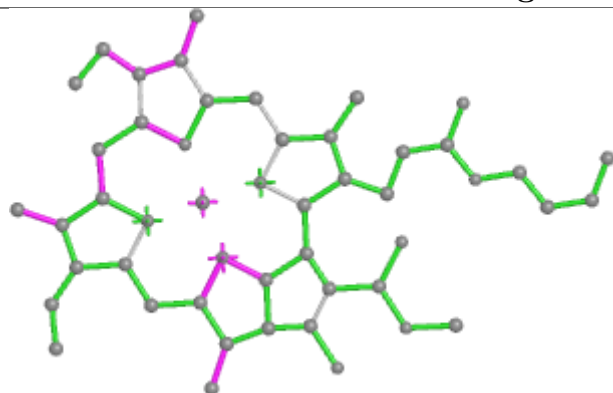
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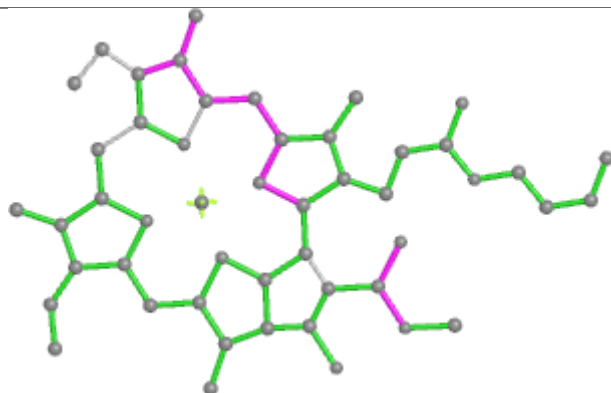
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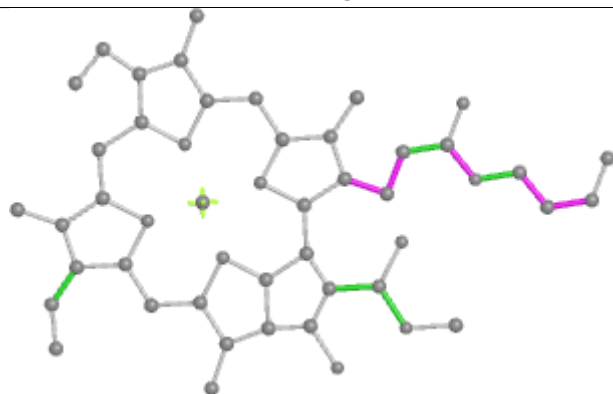
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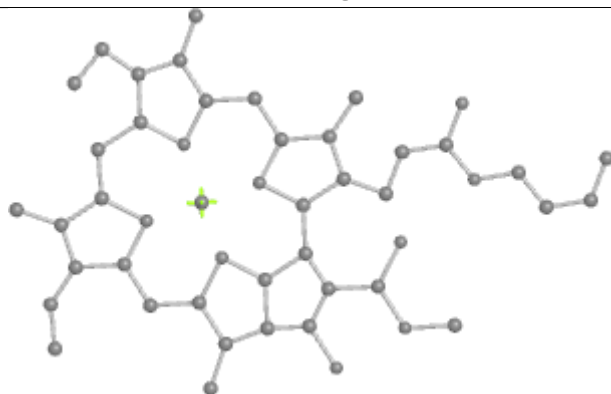
Bond lengths



Bond angles

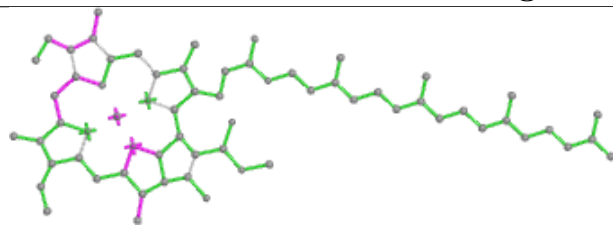


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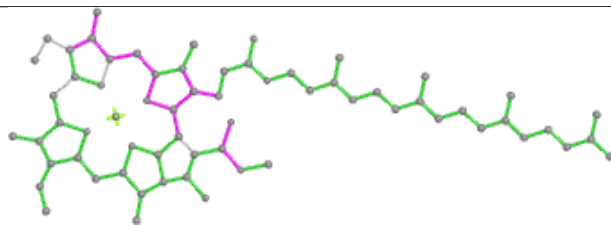


Rings

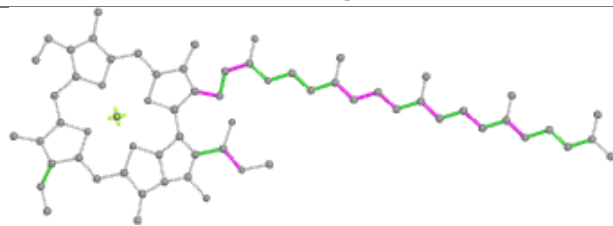
Ligand CLA 8 603



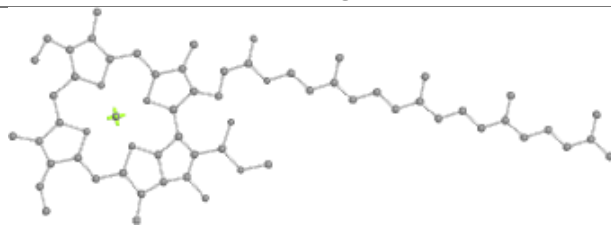
Bond lengths



Bond angles

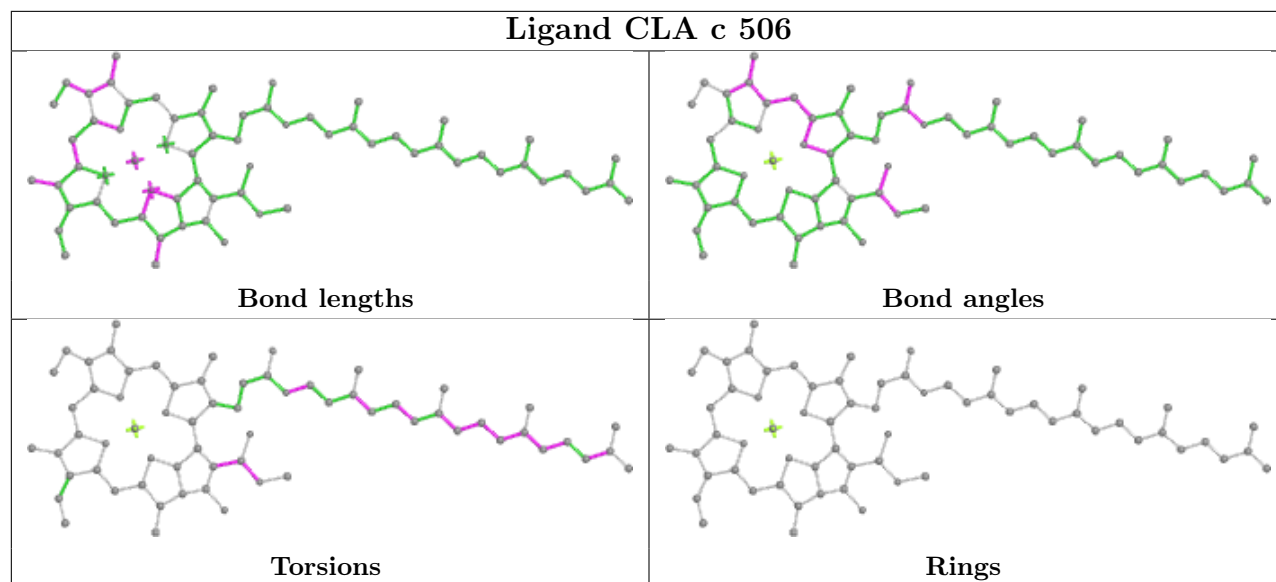


Torsions

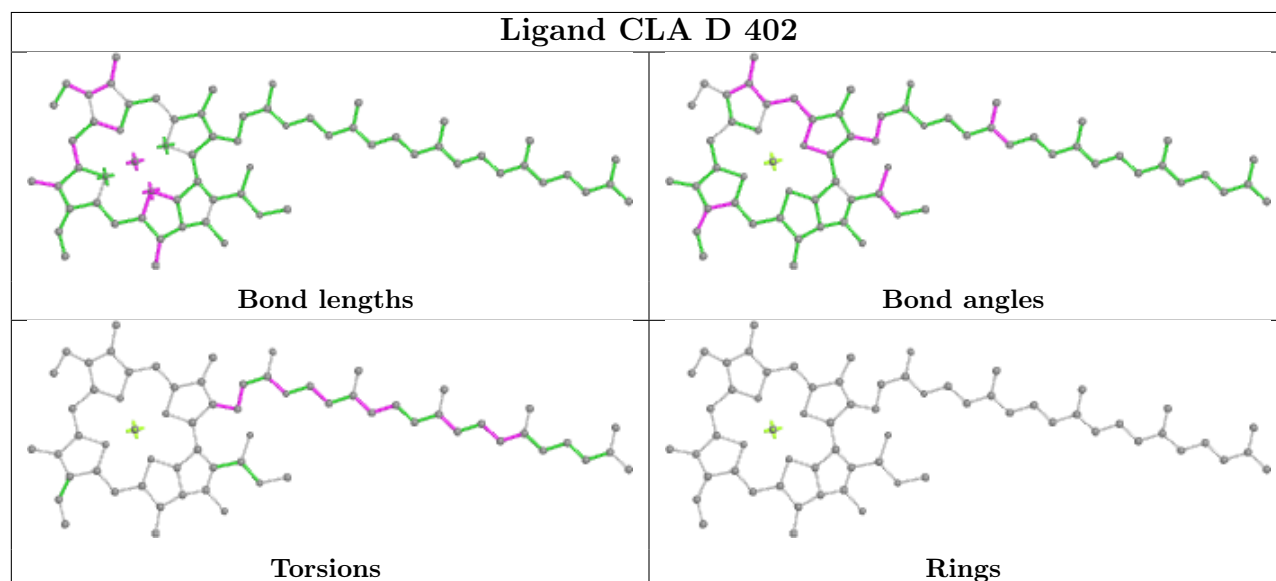


Rings

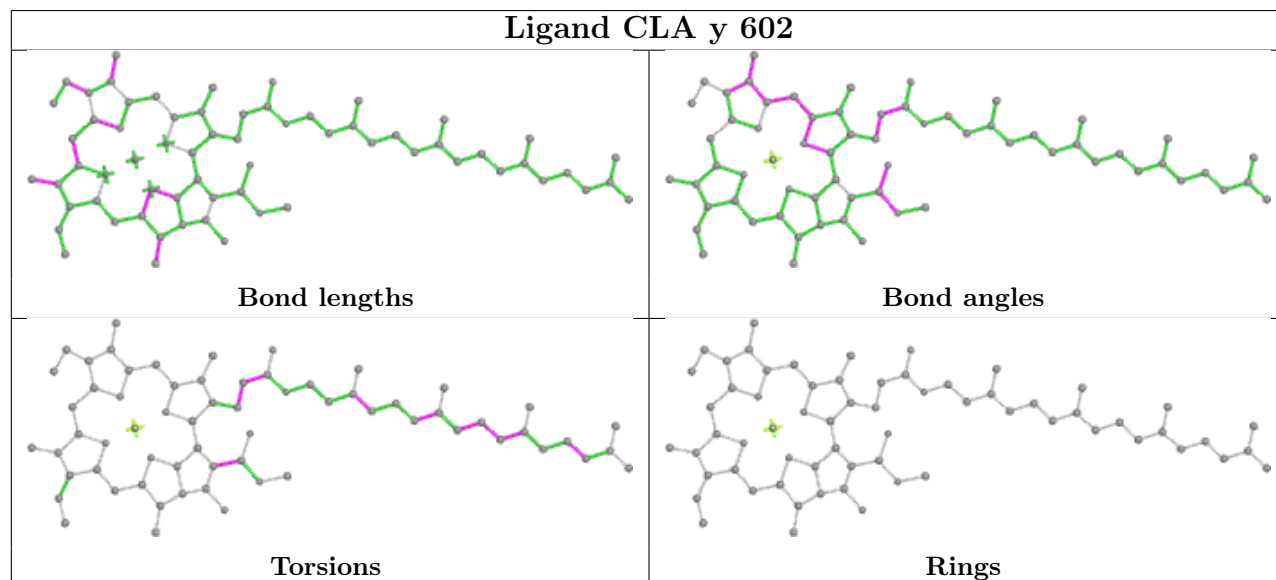
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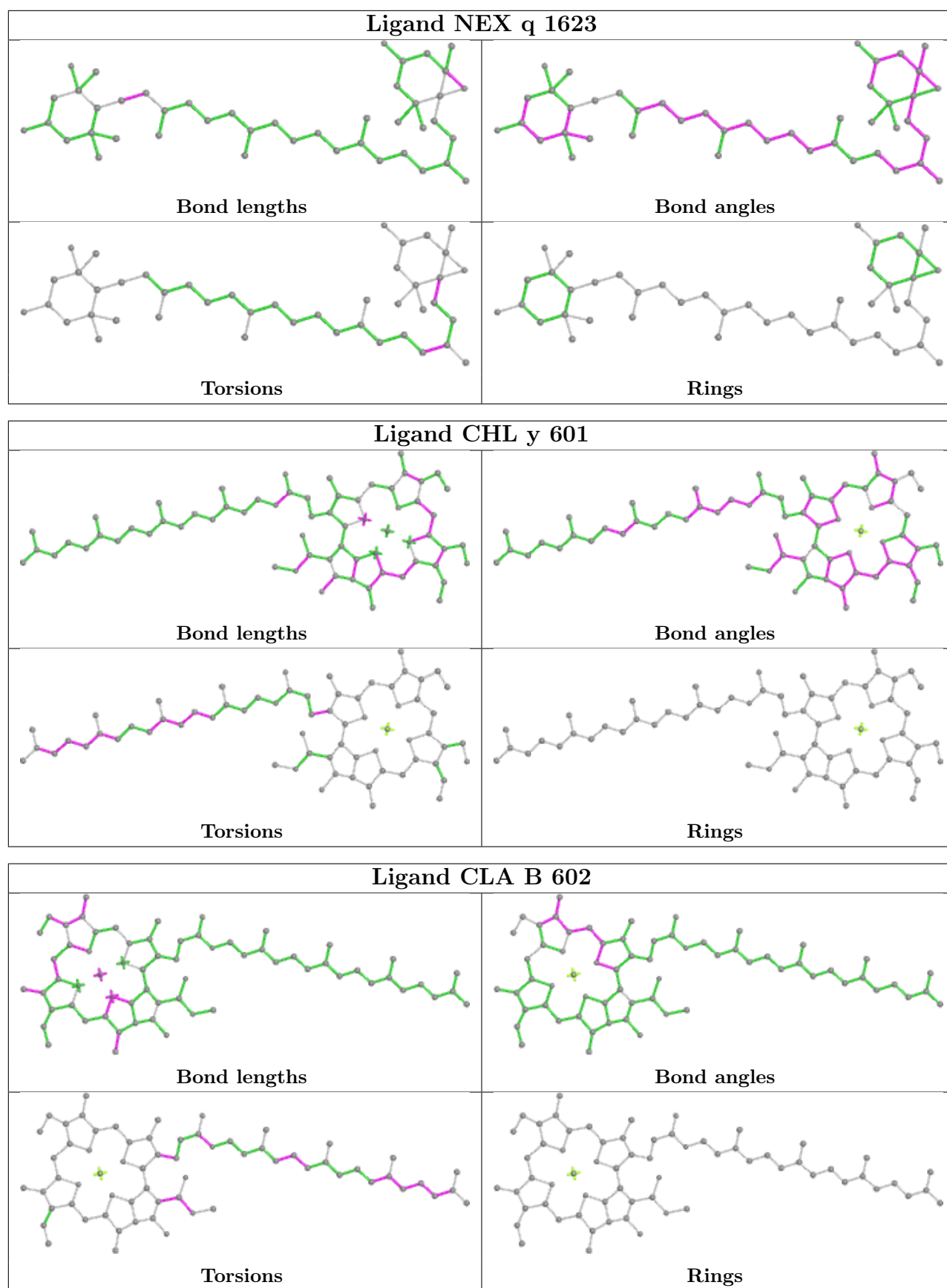


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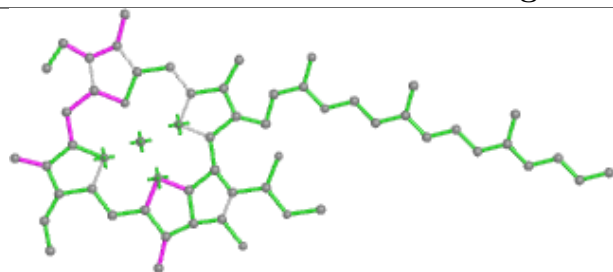


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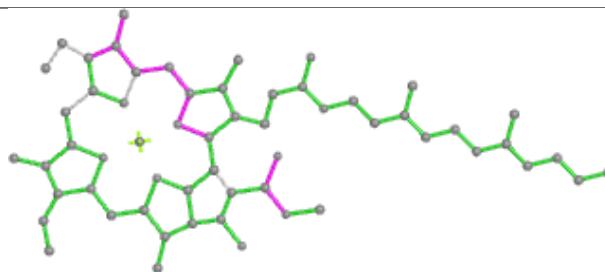




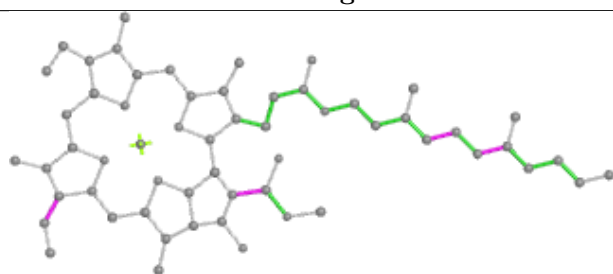
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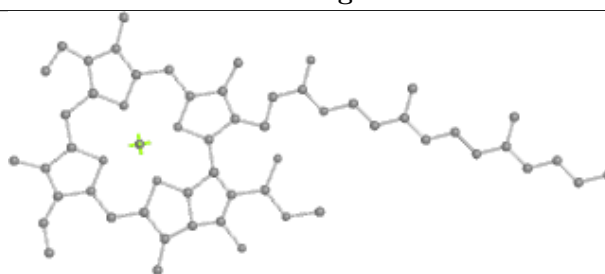
Bond lengths



Bond angles

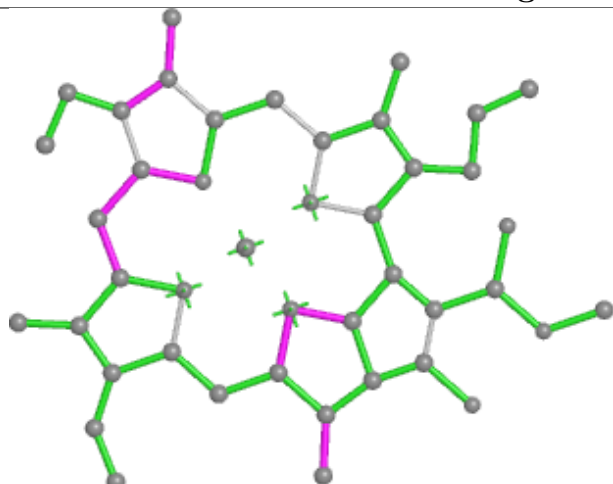


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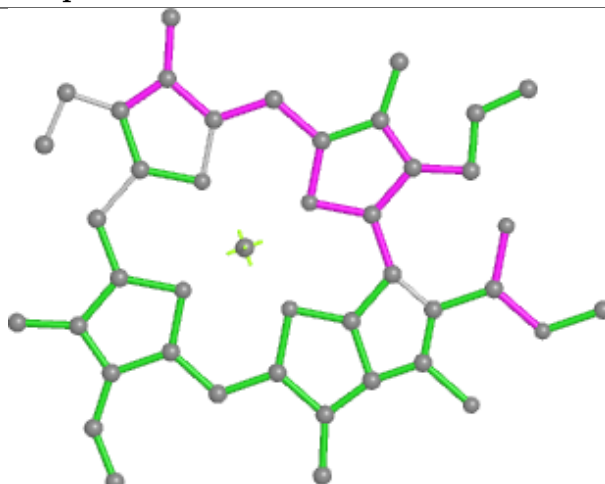


Rings

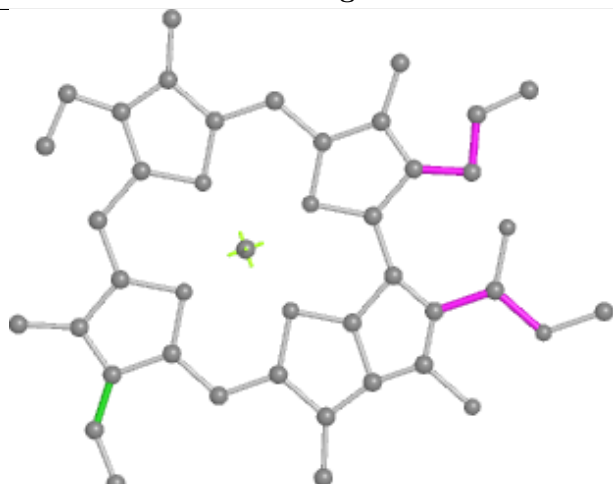
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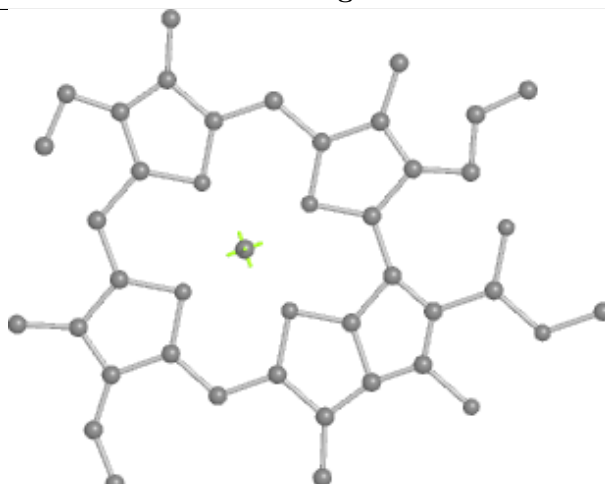
Bond lengths



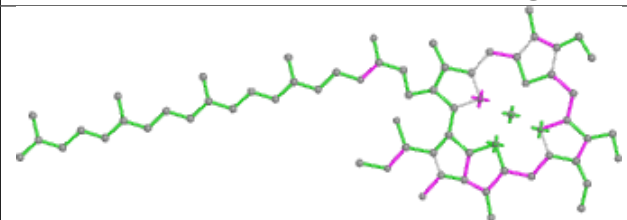
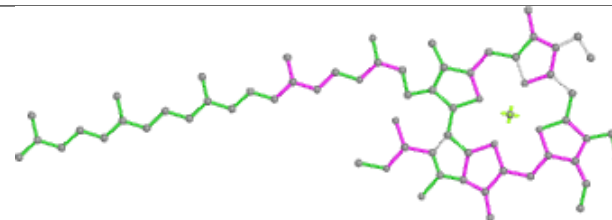
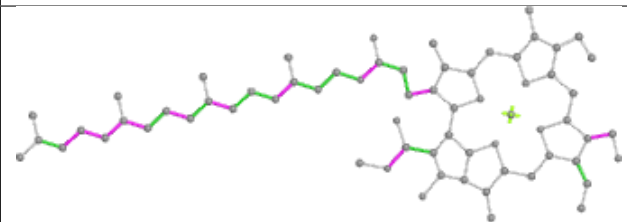
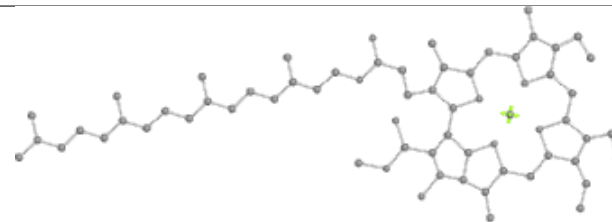
Bond angles

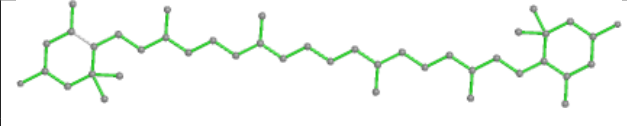
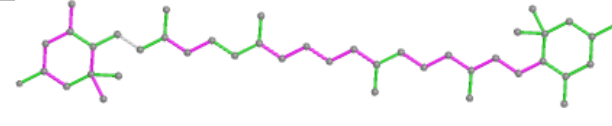
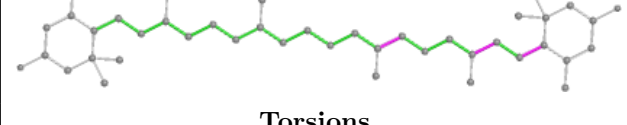



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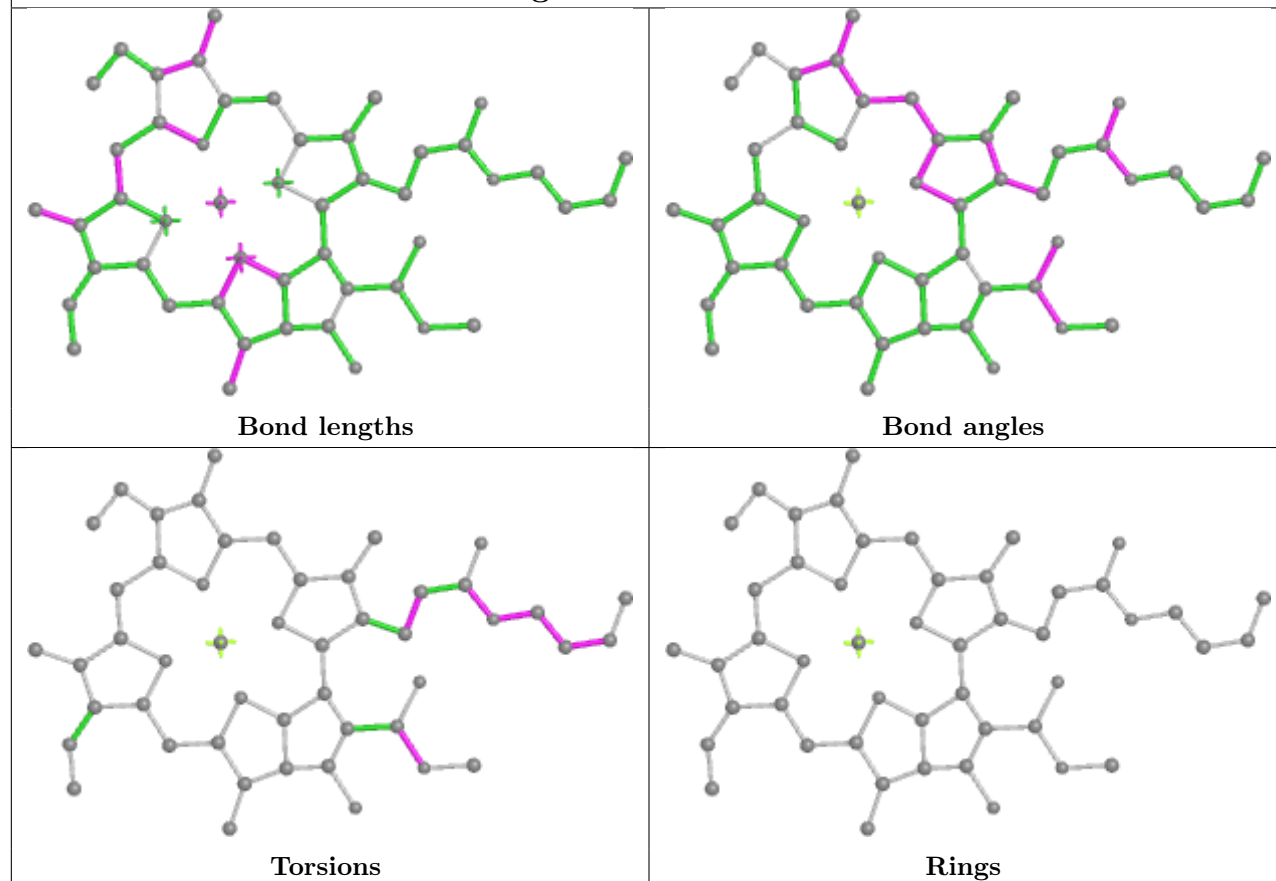


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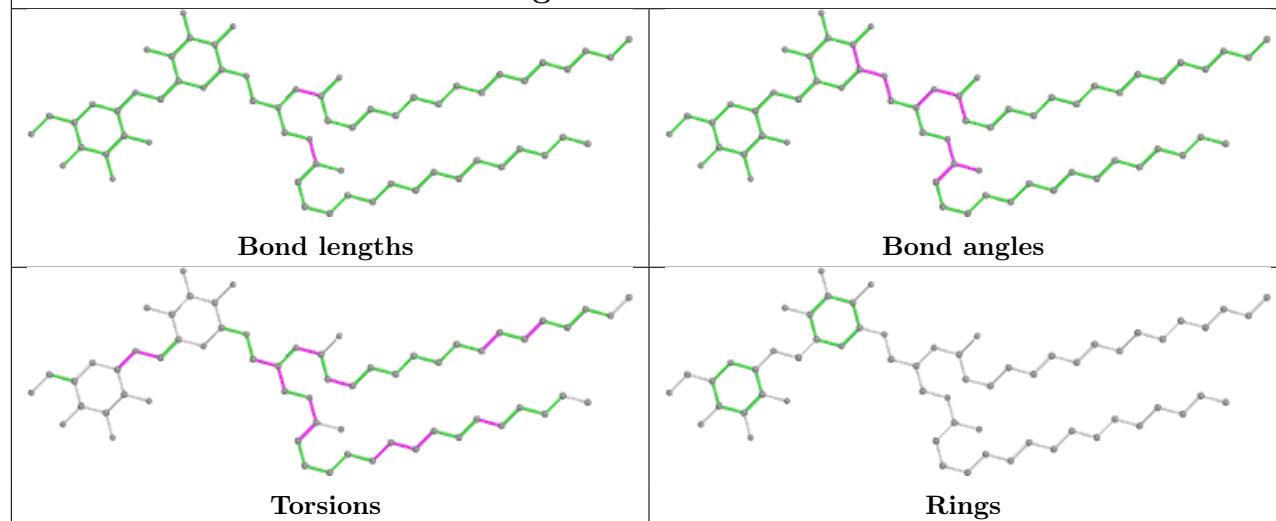
Ligand CHL 1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

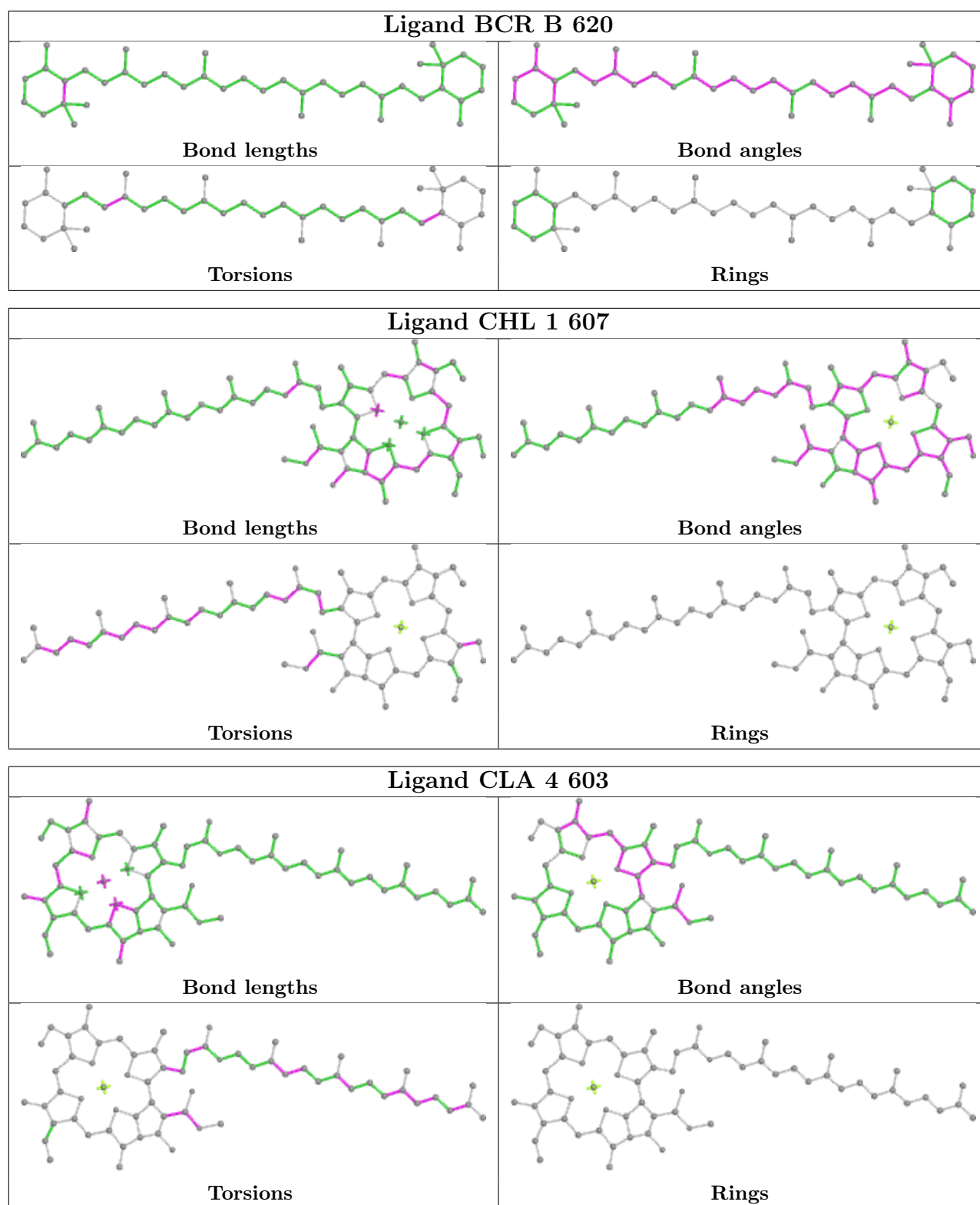
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 612

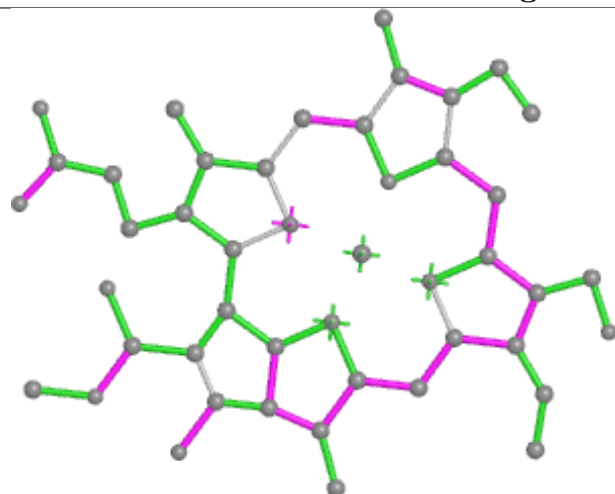


Ligand DGD c 519

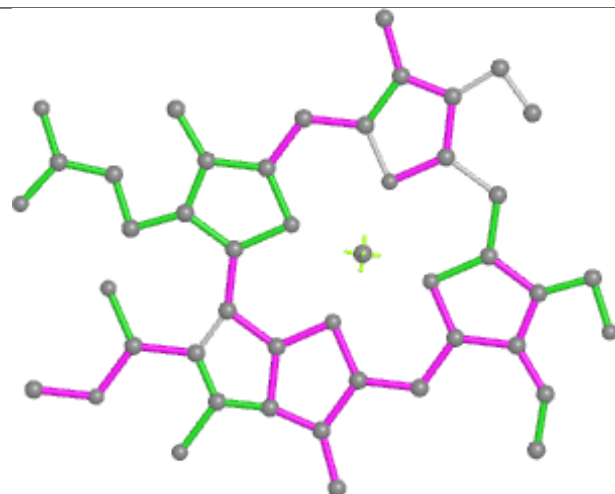




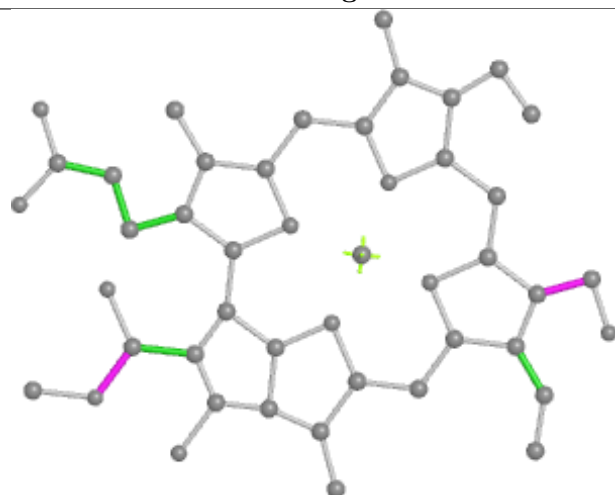
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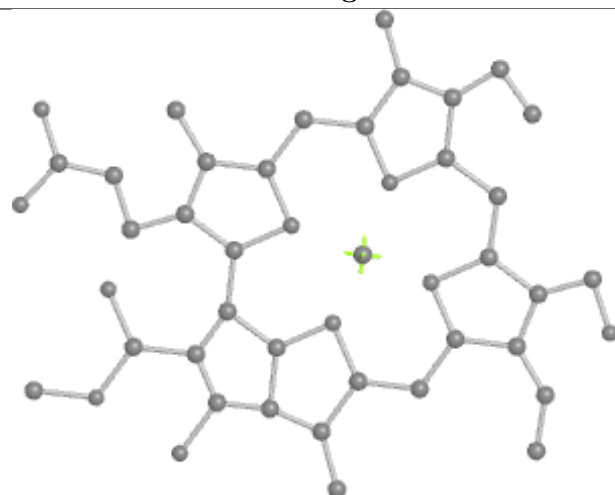
Bond lengths



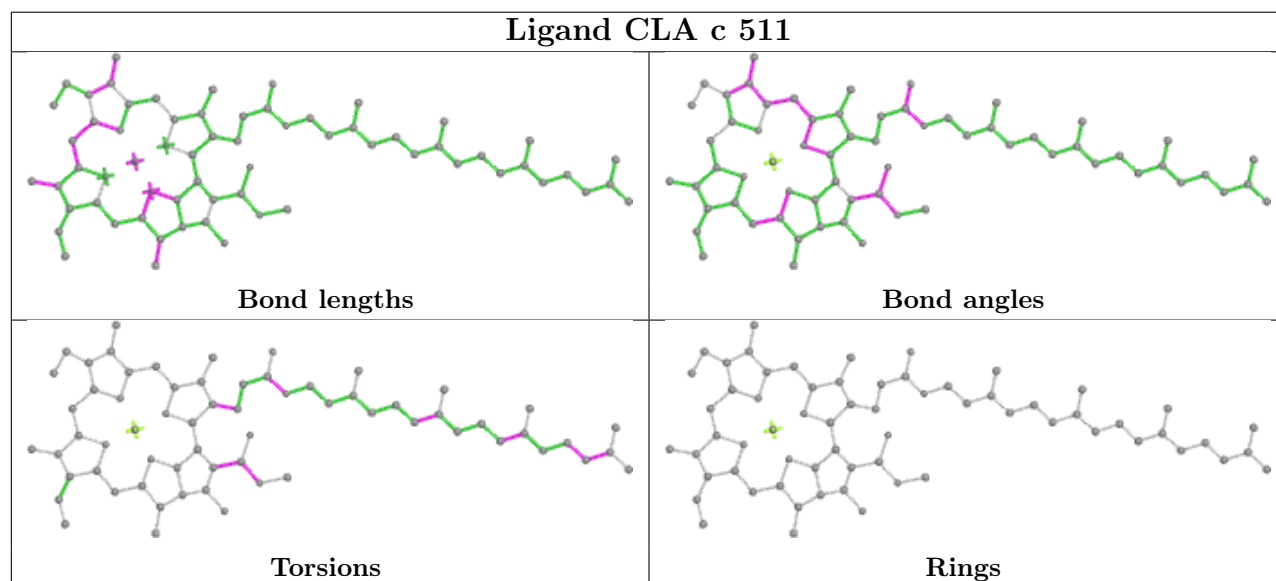
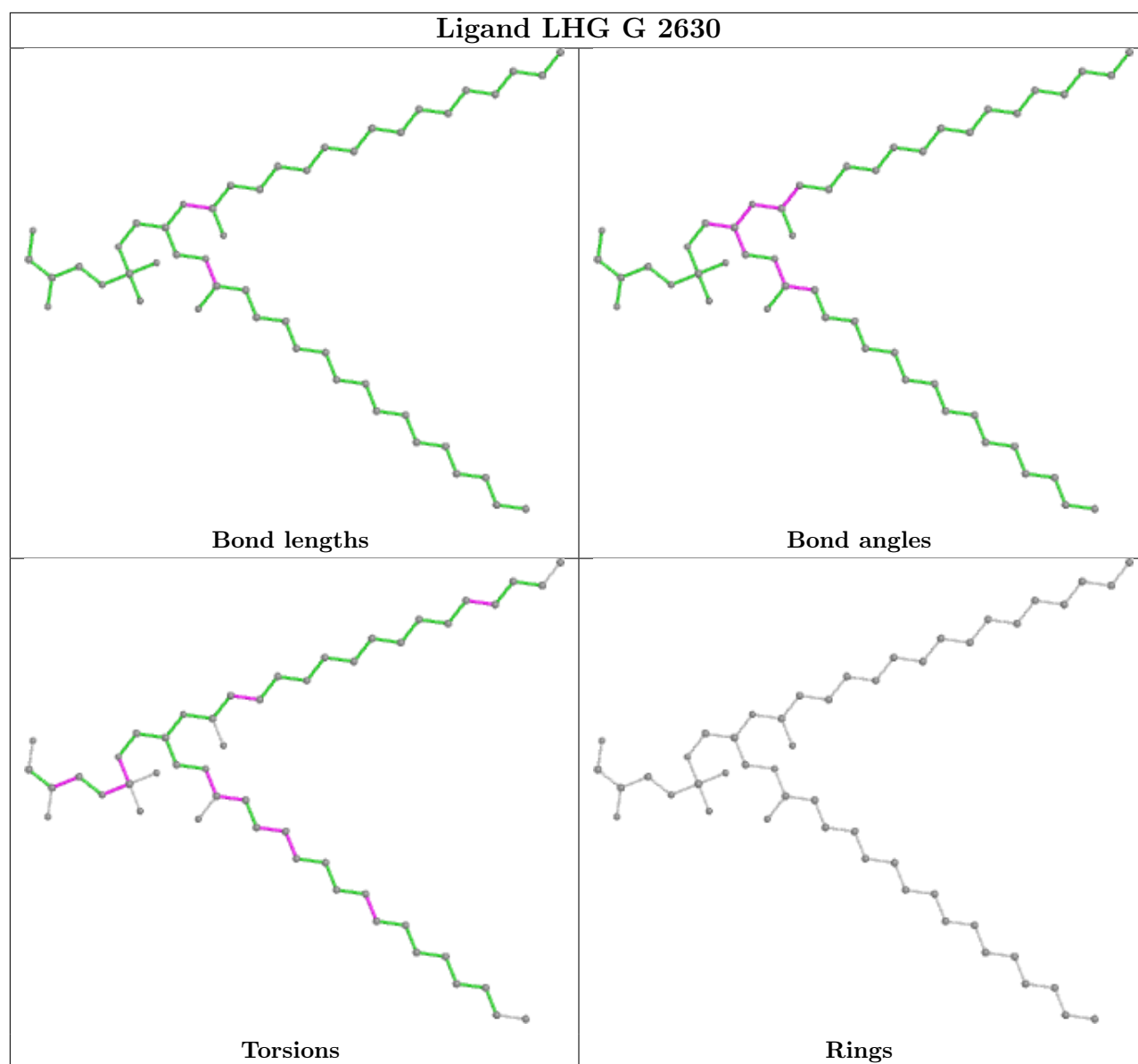
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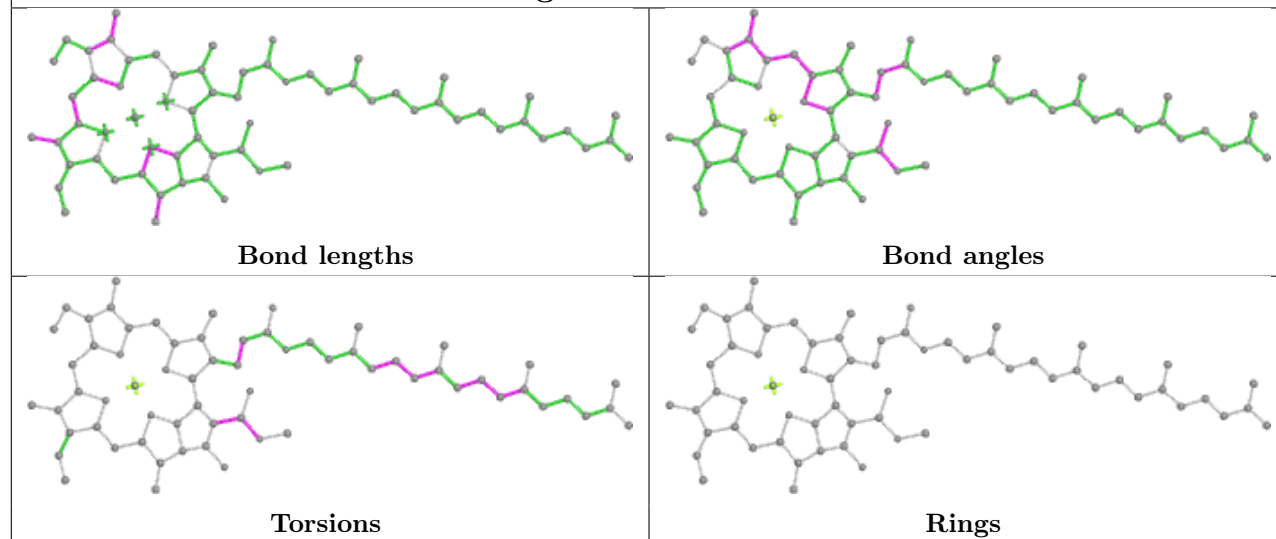
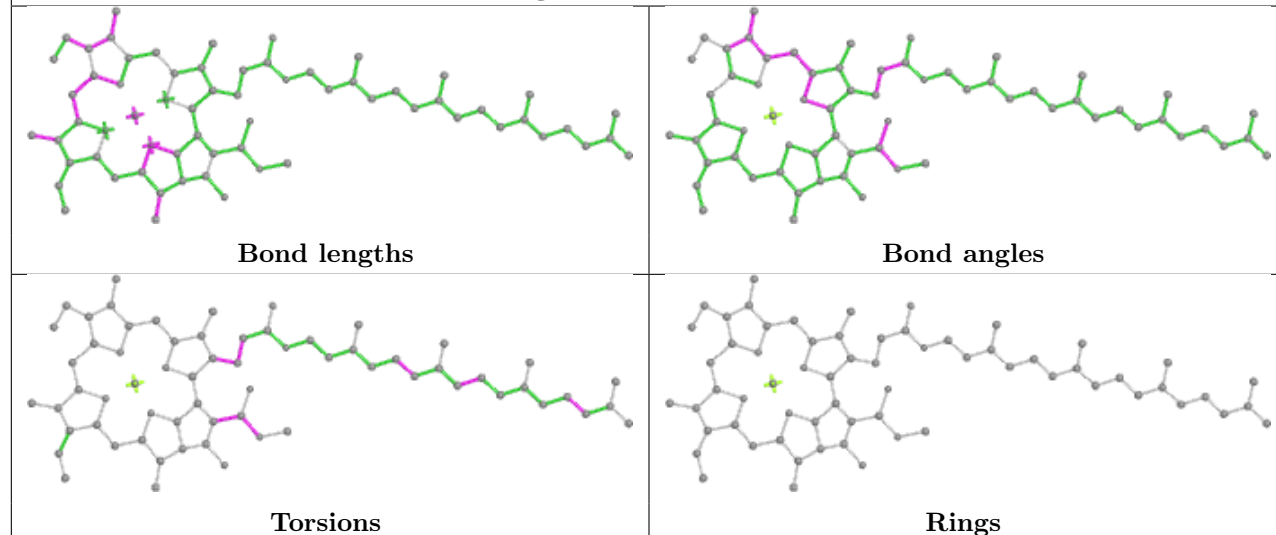
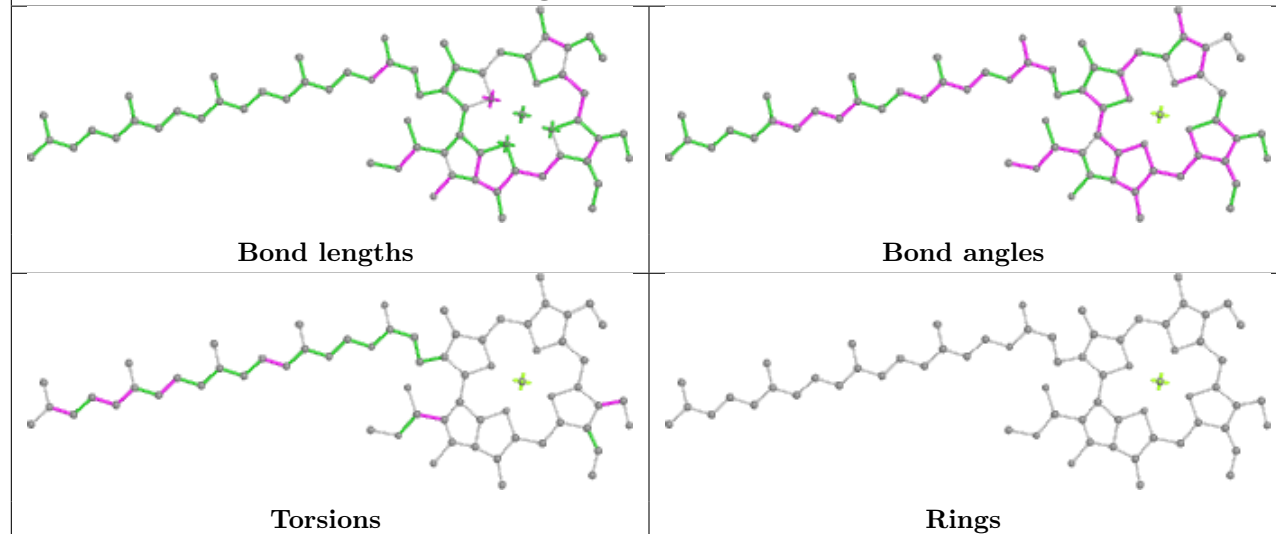


Torsions

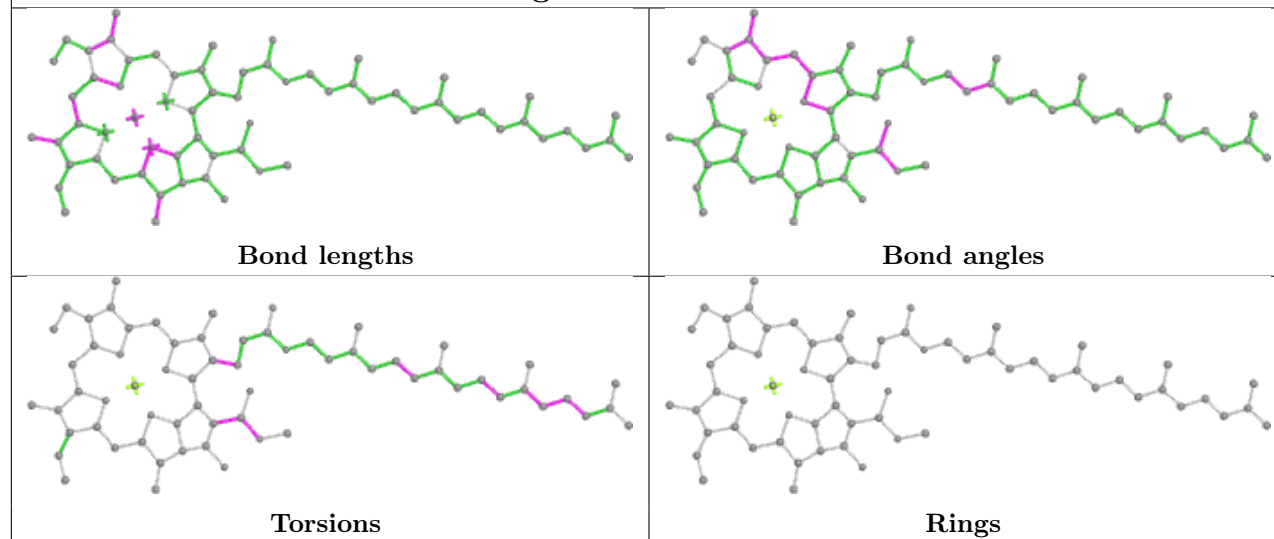


Rings

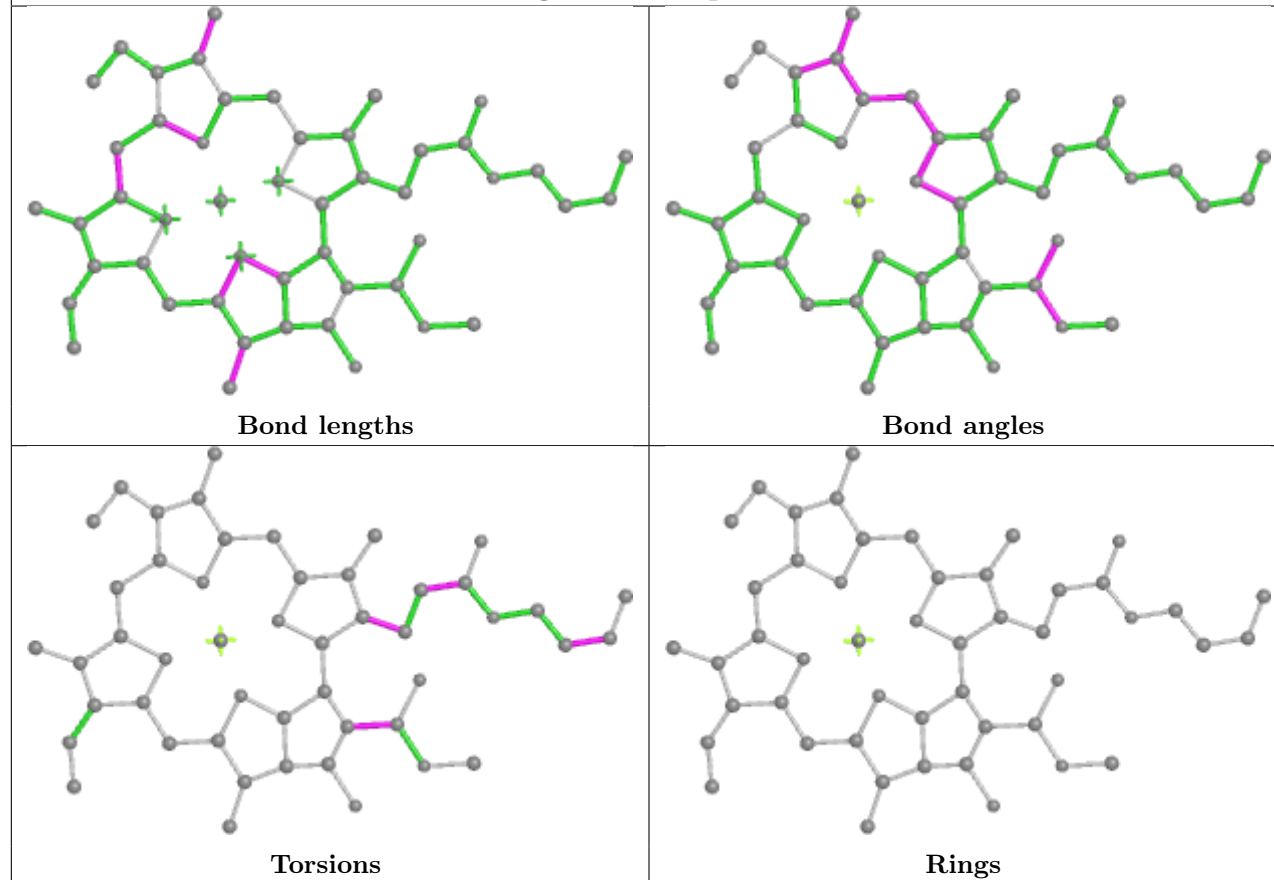


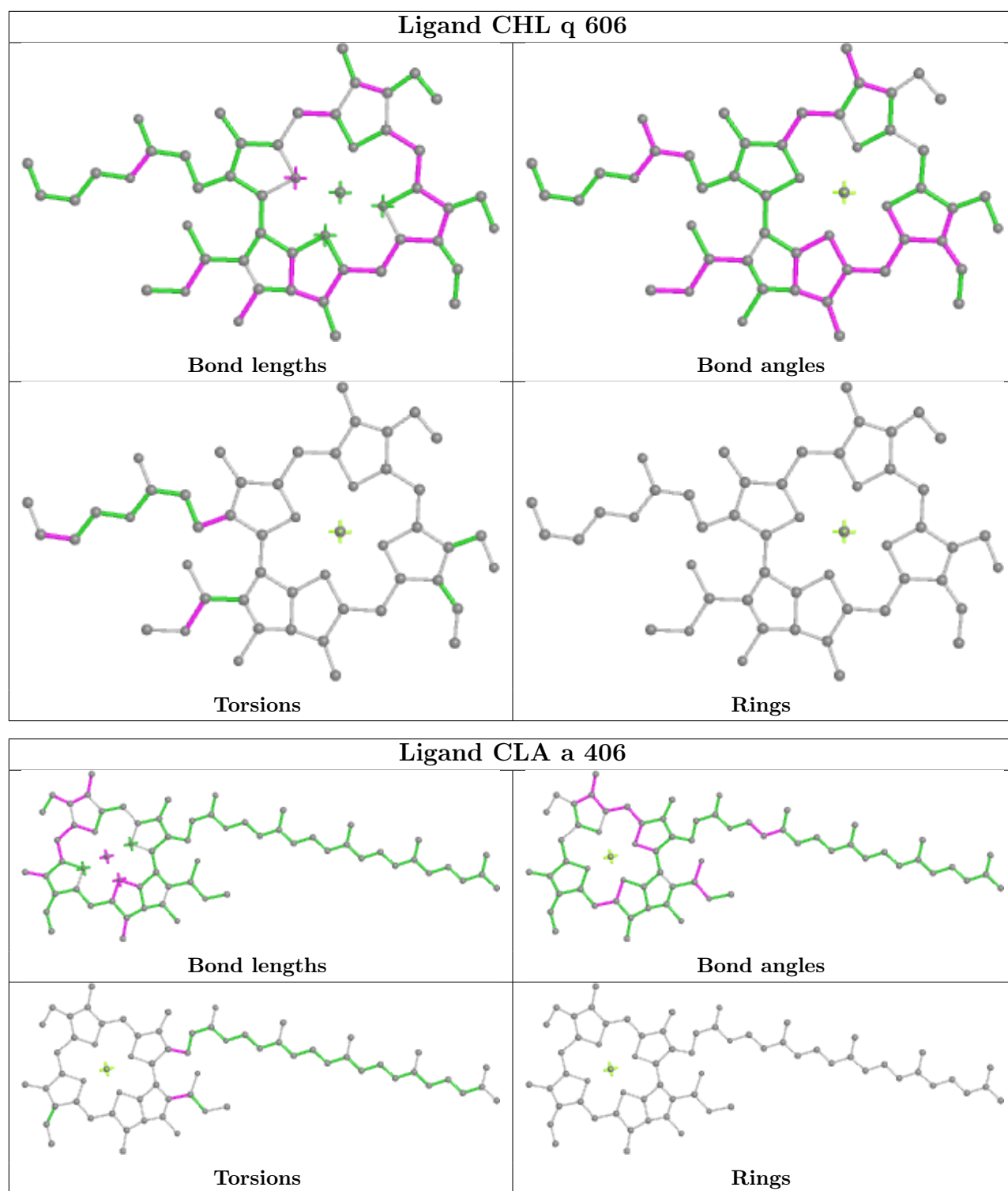
Ligand CLA 6 602**Ligand CLA C 503****Ligand CHL 6 601**

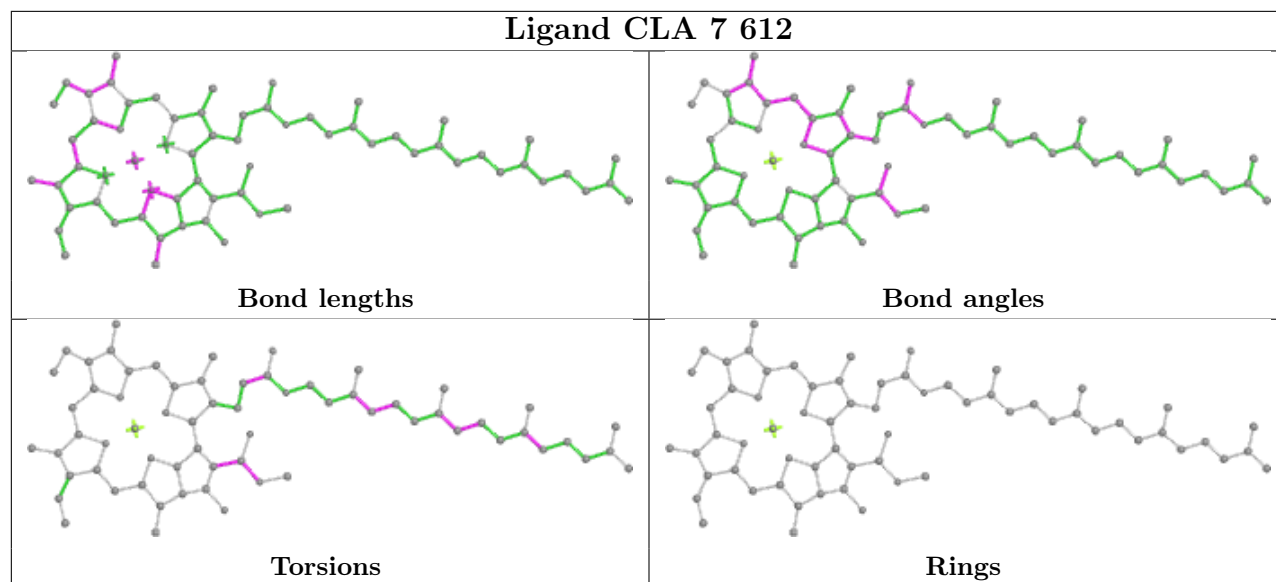
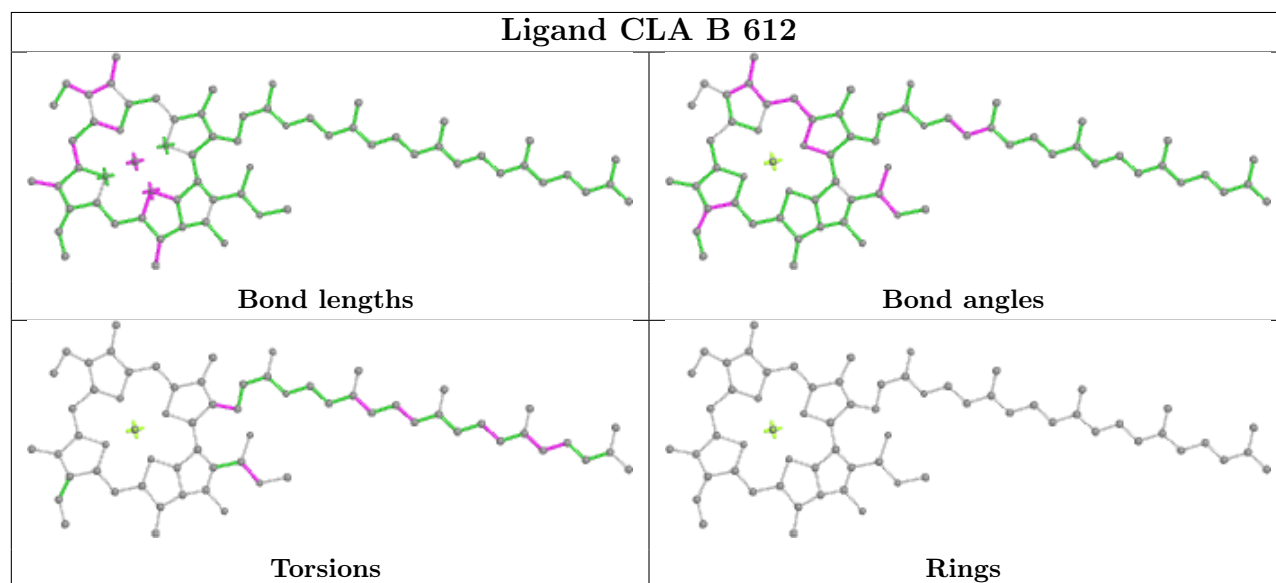
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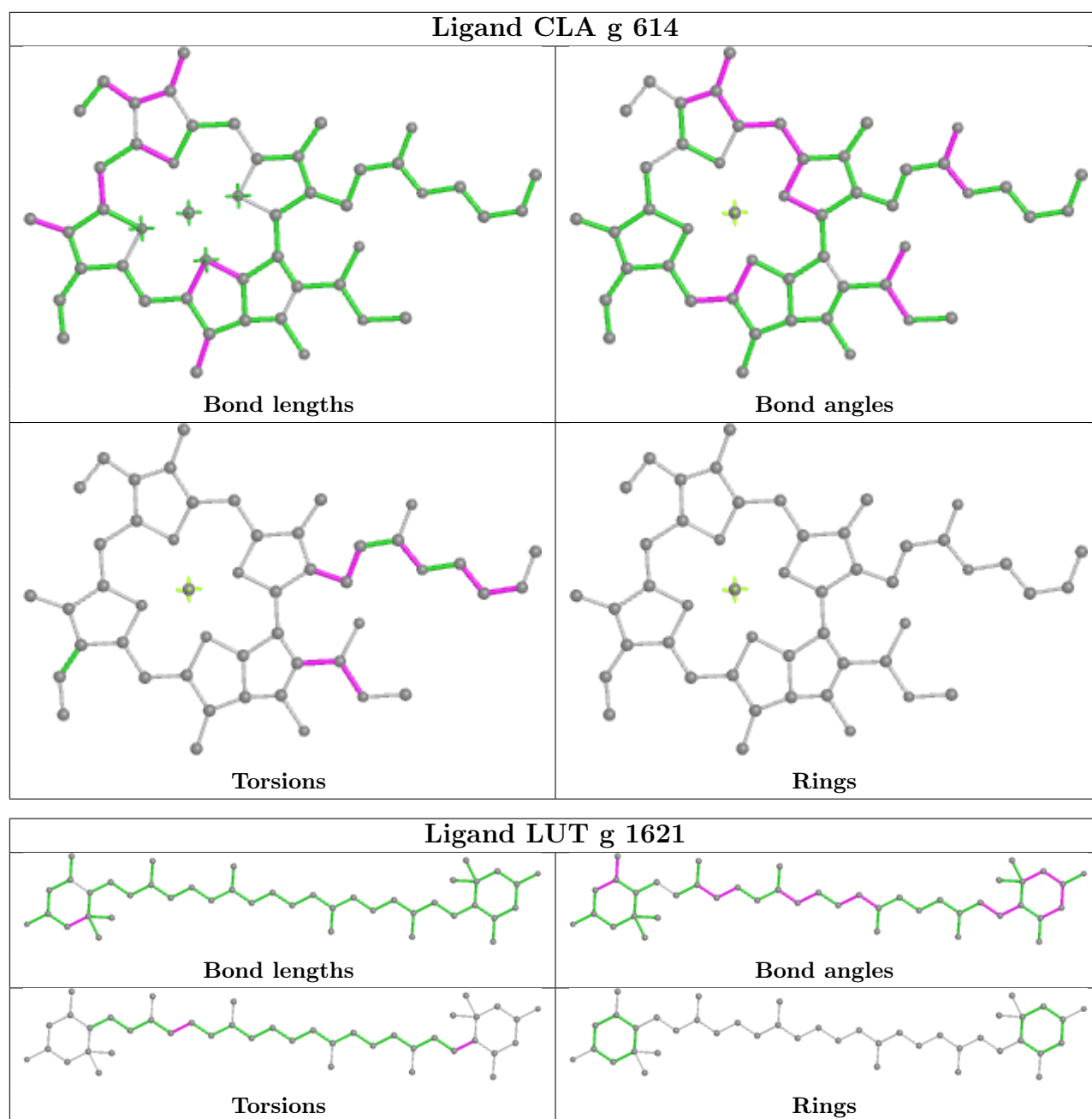


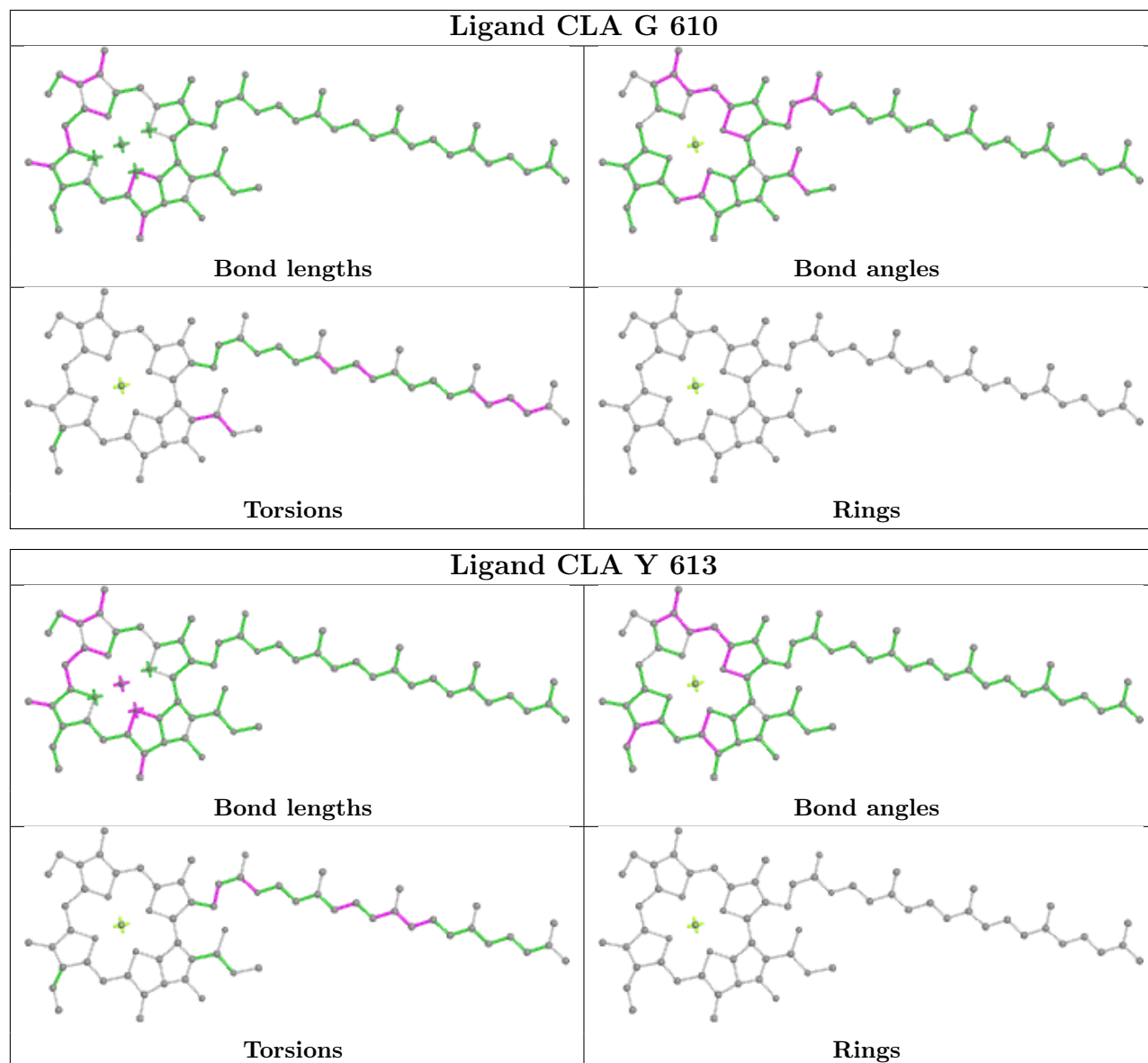
Ligand CLA p 611

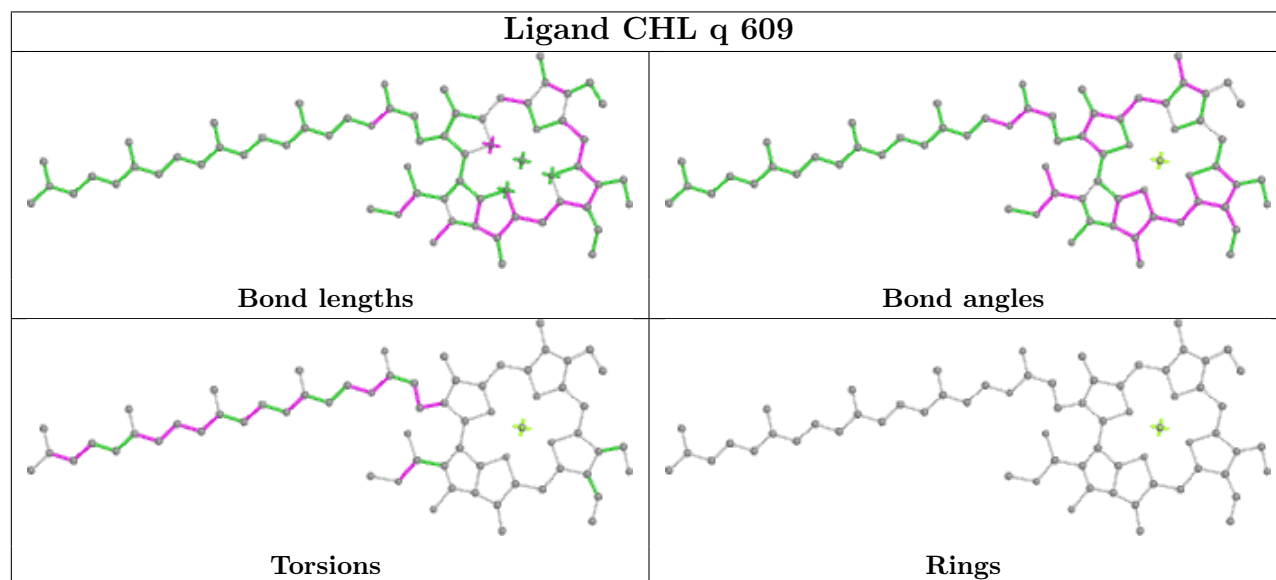
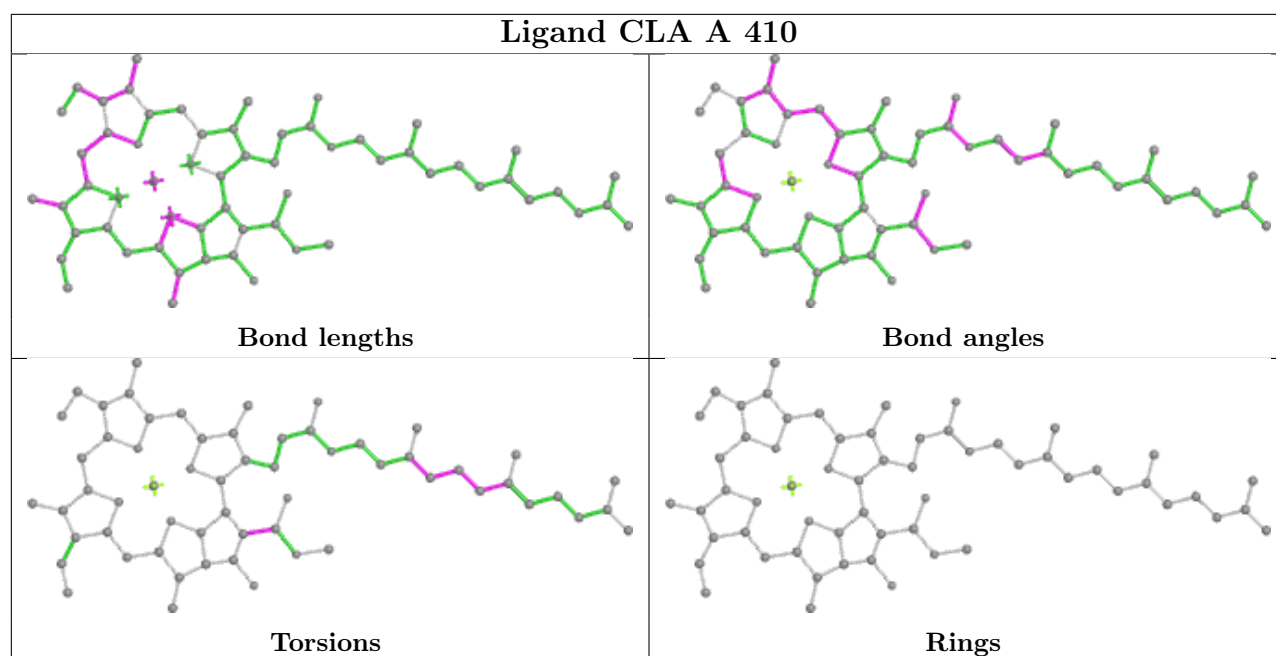


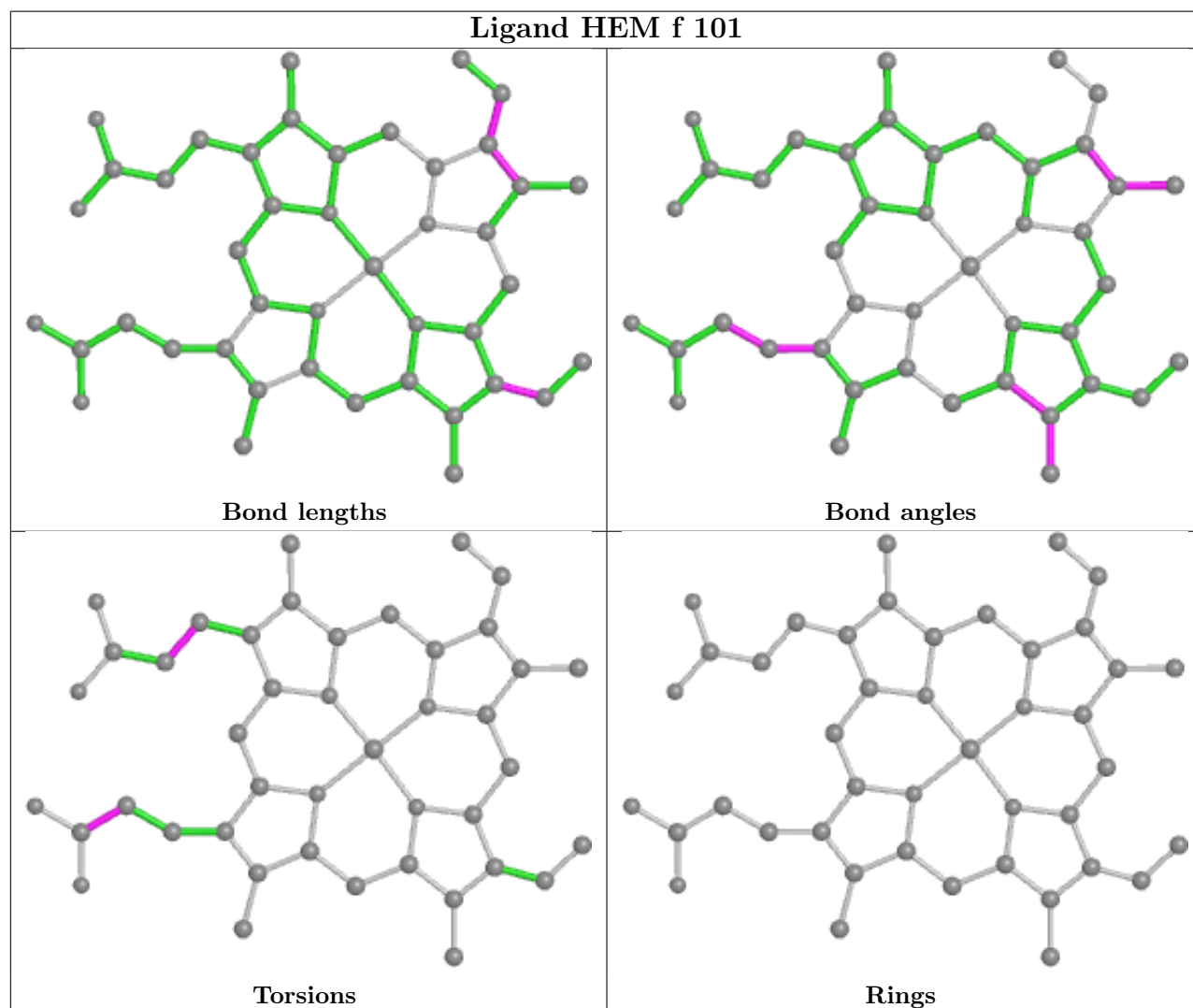
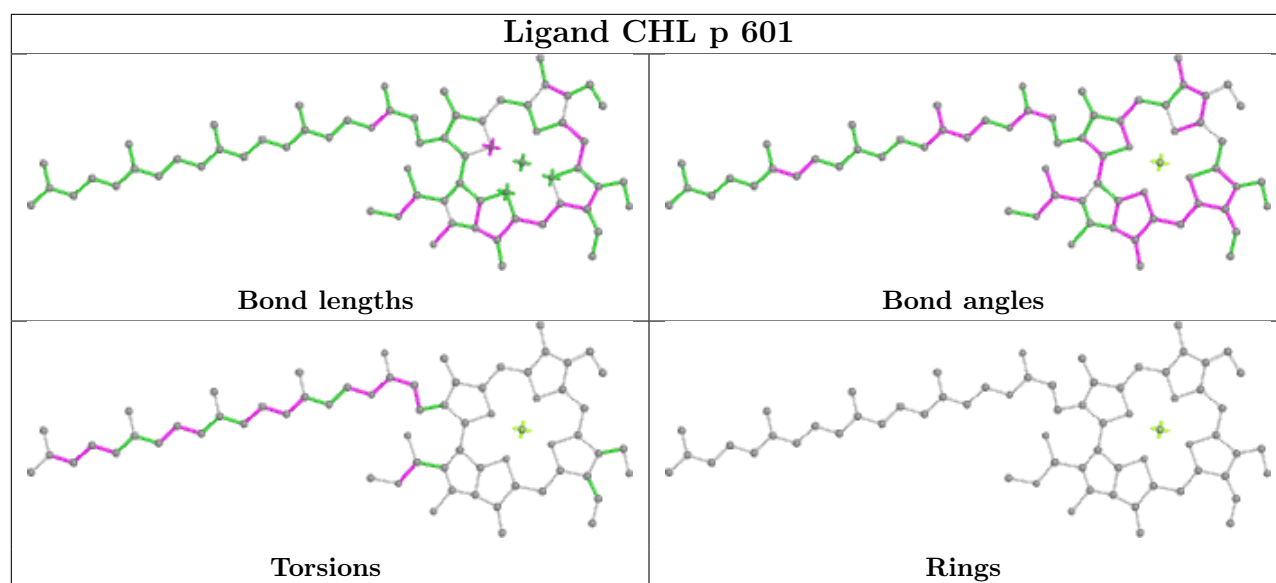


Ligand CLA 7 612**Ligand CLA B 612**

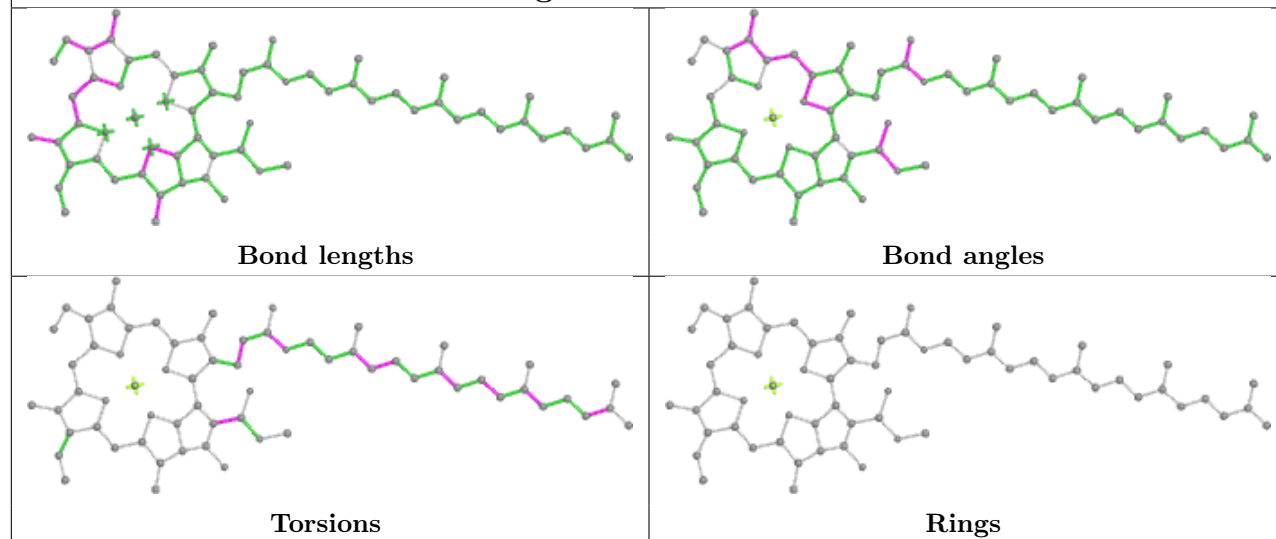




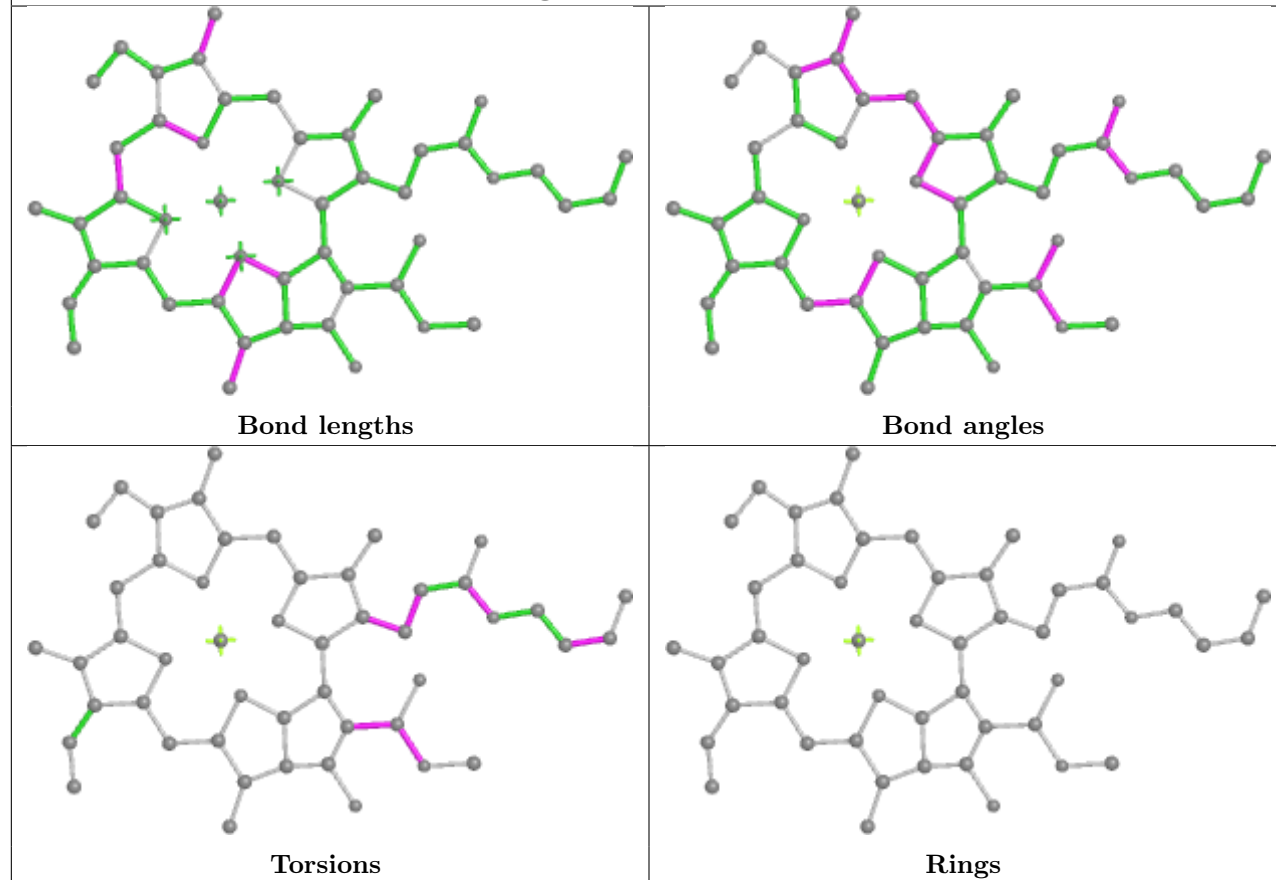


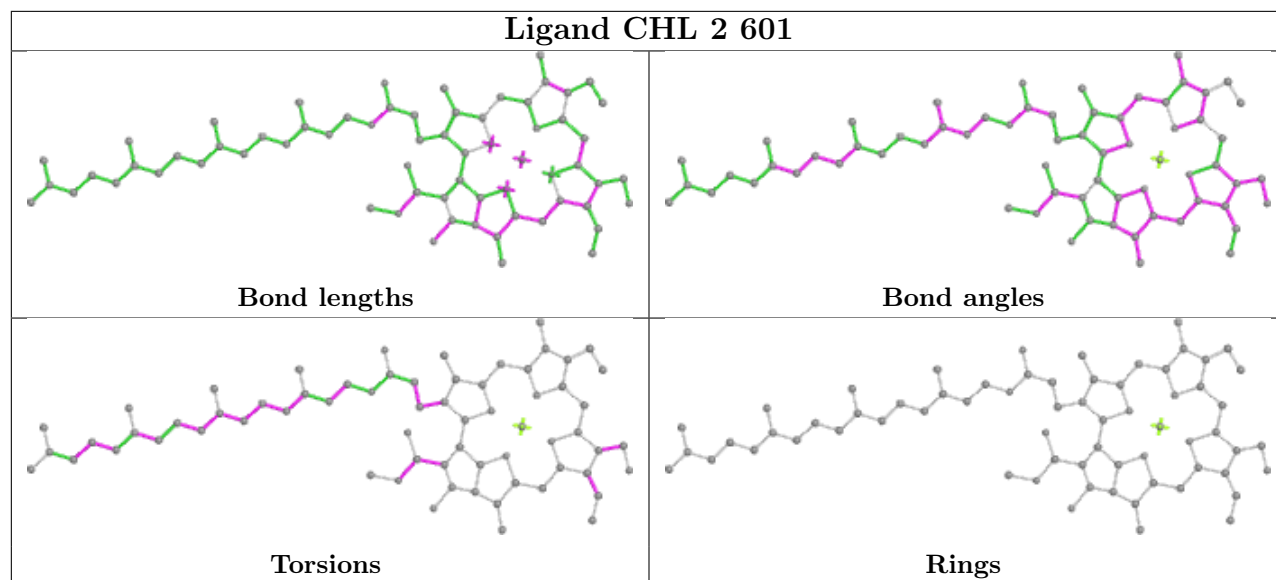
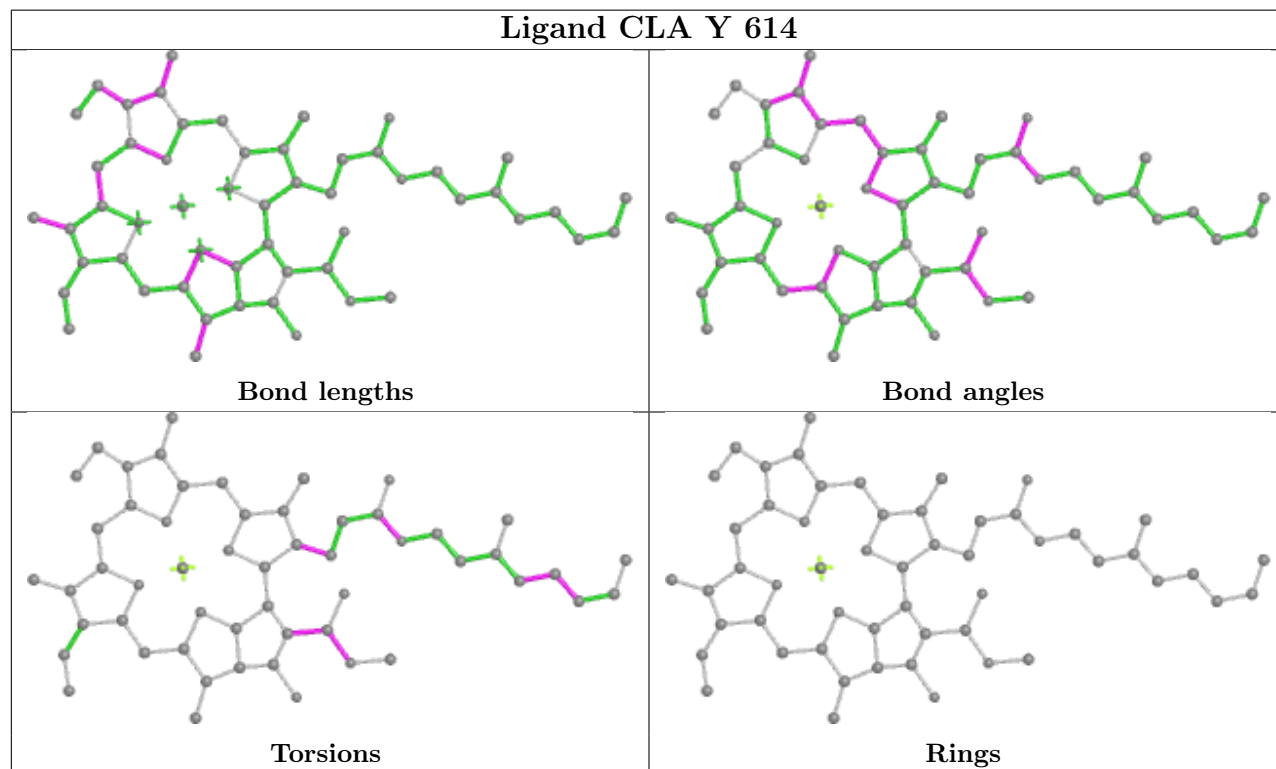


Ligand CLA n 613

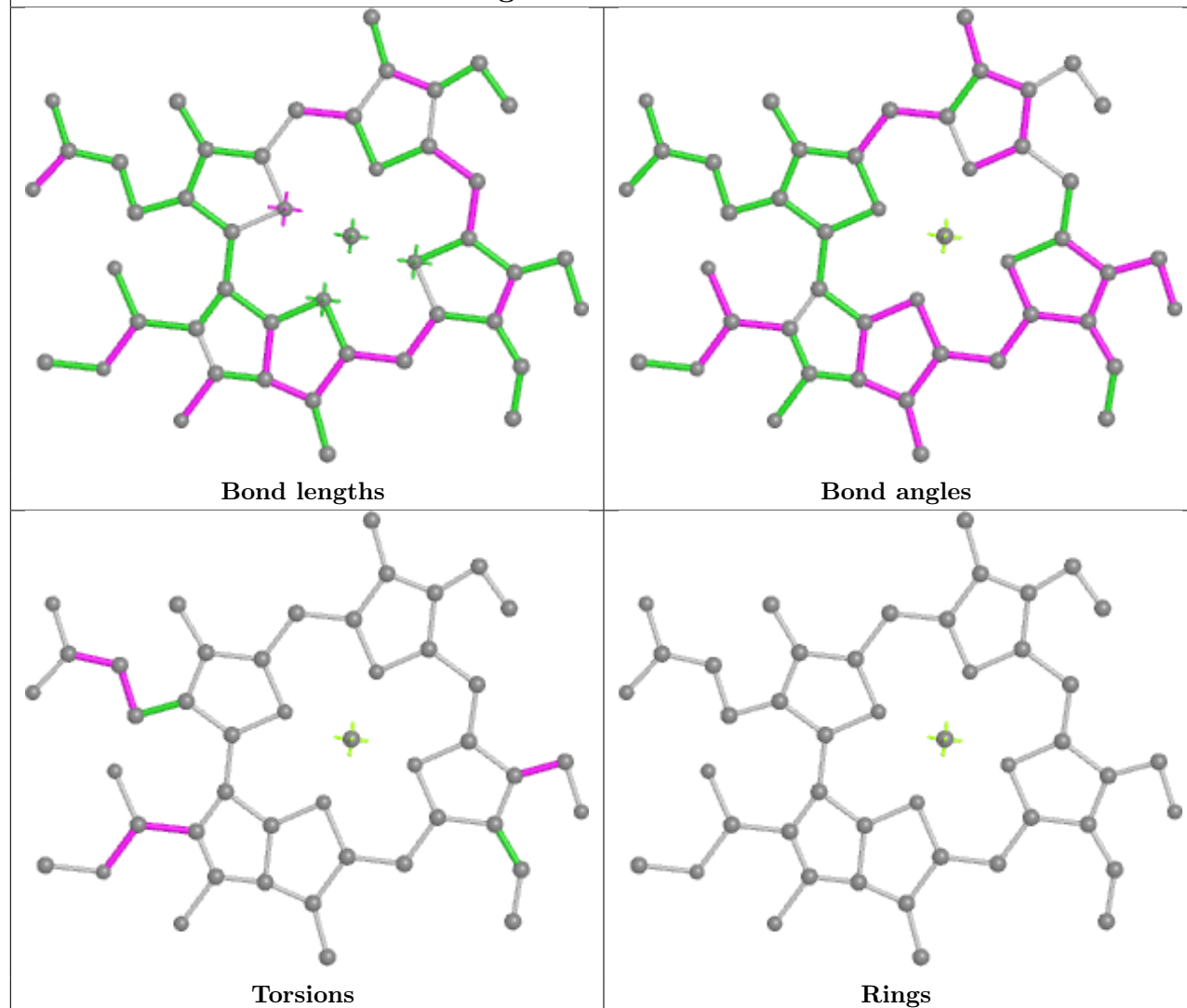


Ligand CLA 5 614

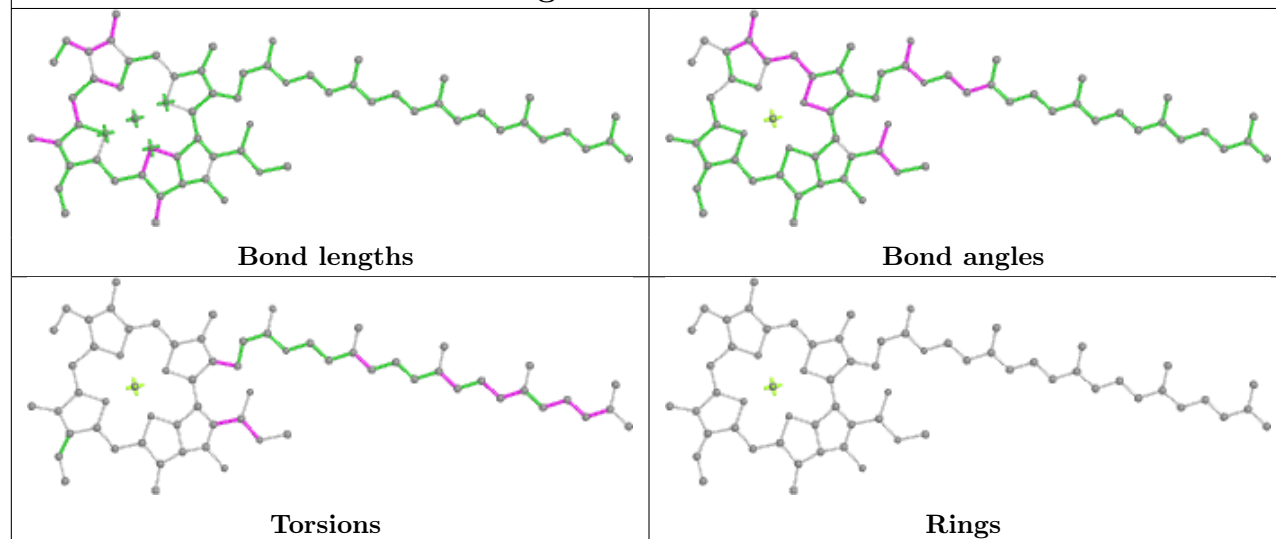


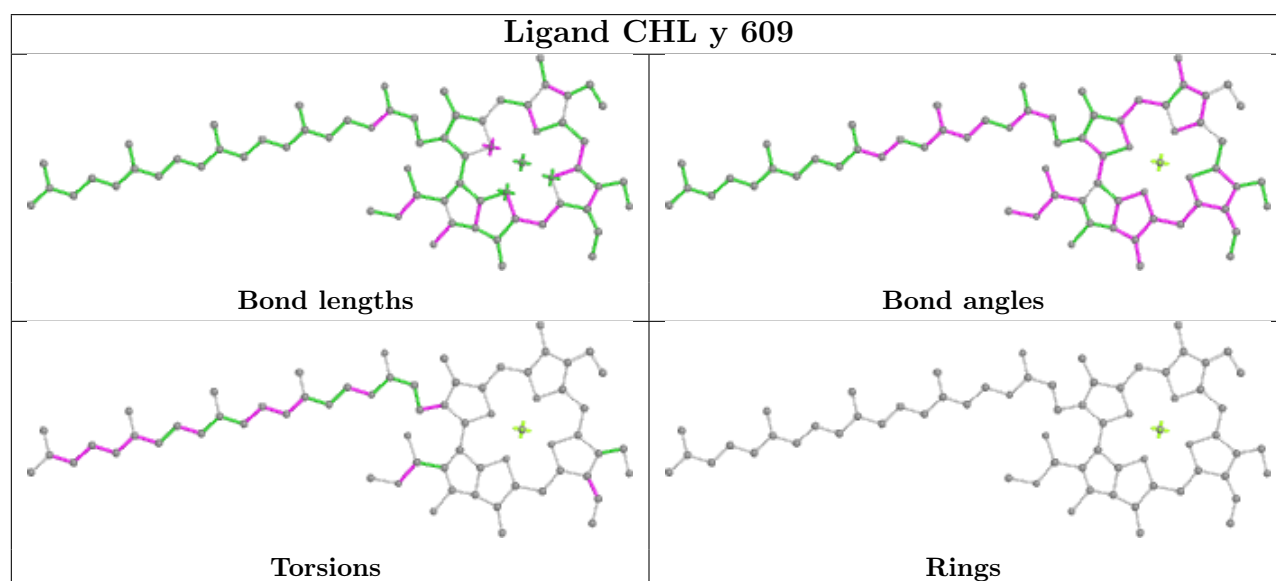
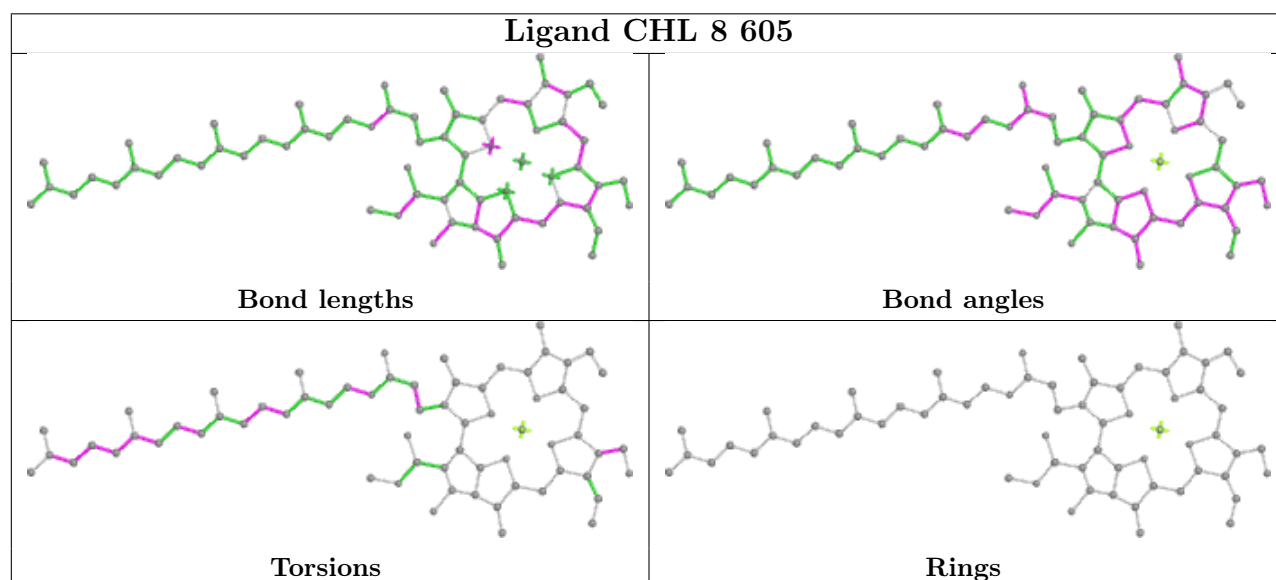
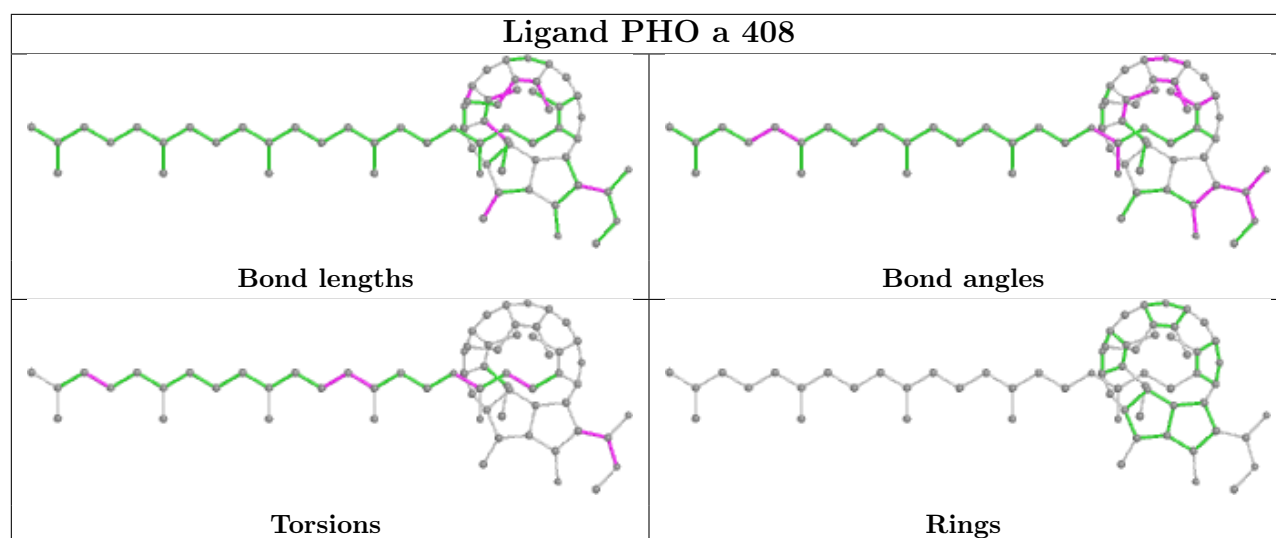
Ligand CHL 2 601**Ligand CLA Y 614**

Ligand CHL 7 605

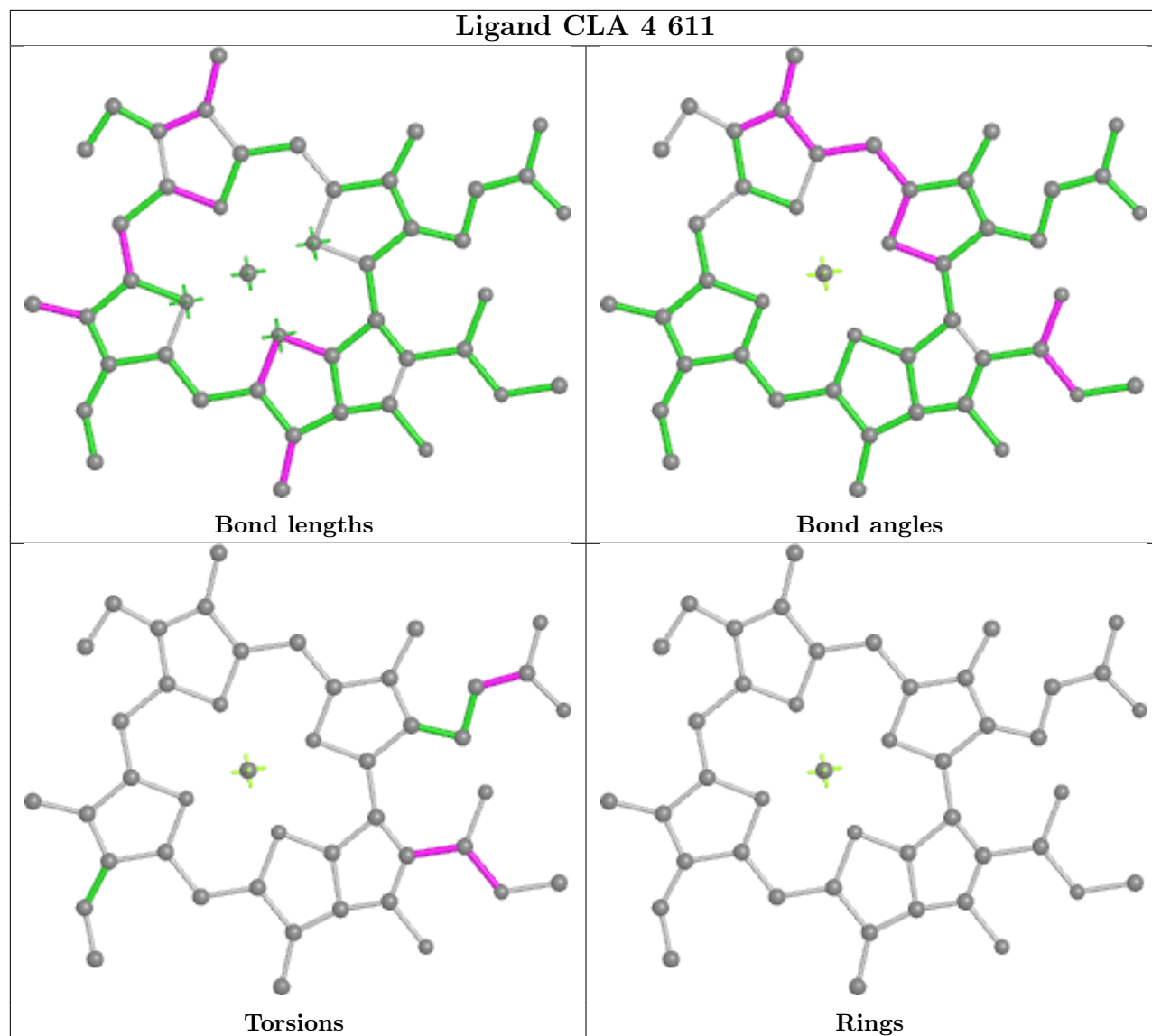


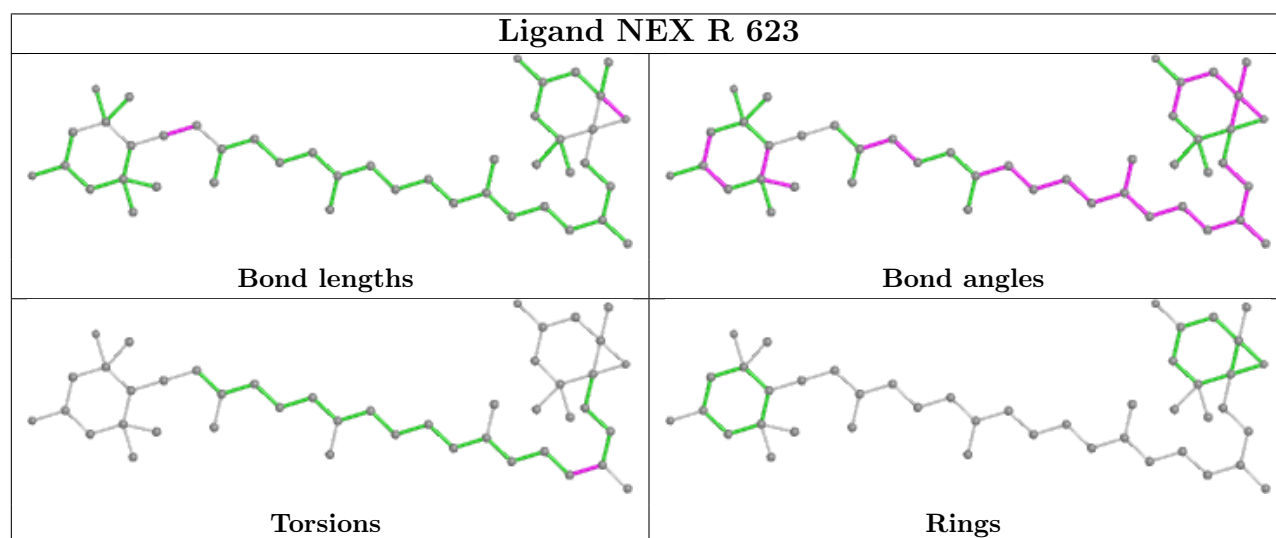
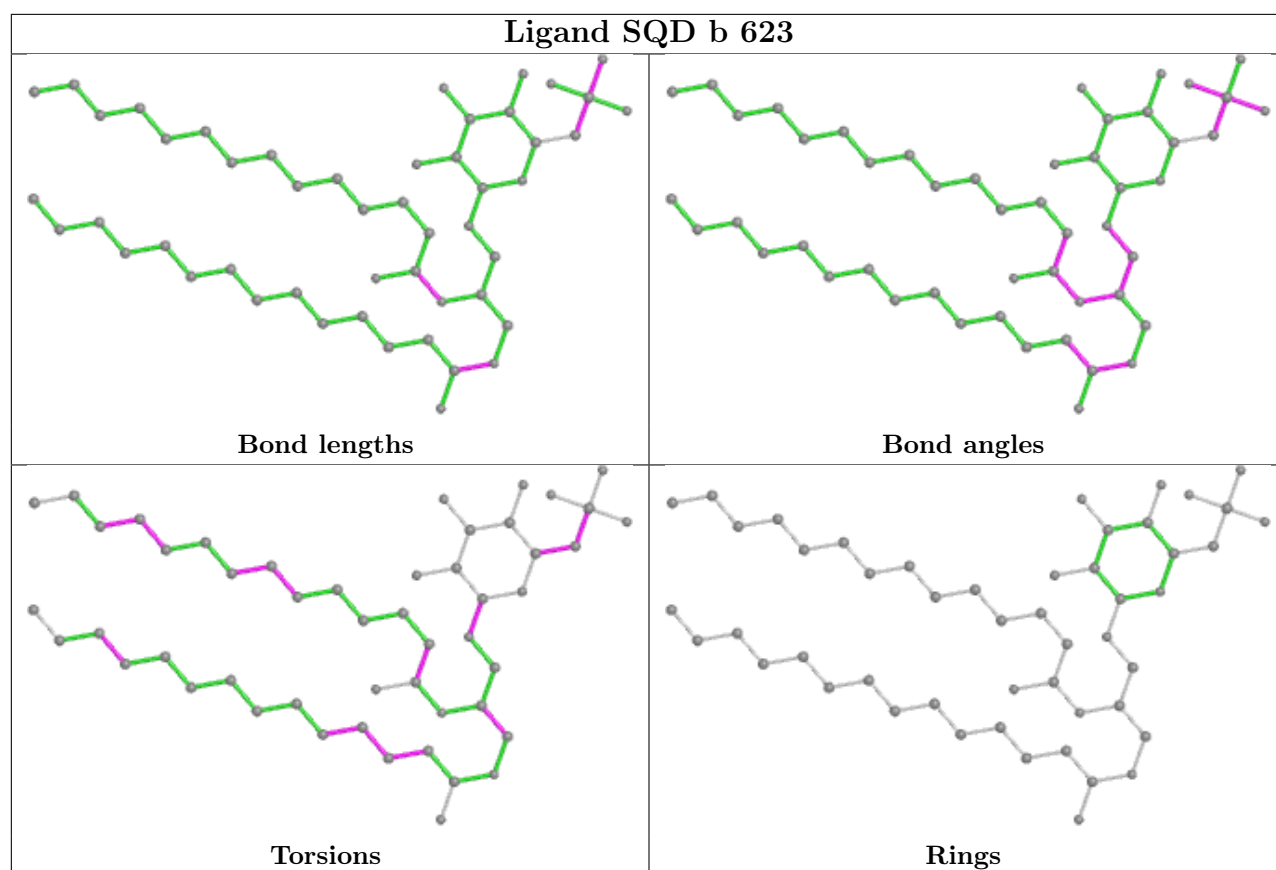
Ligand CLA r 610

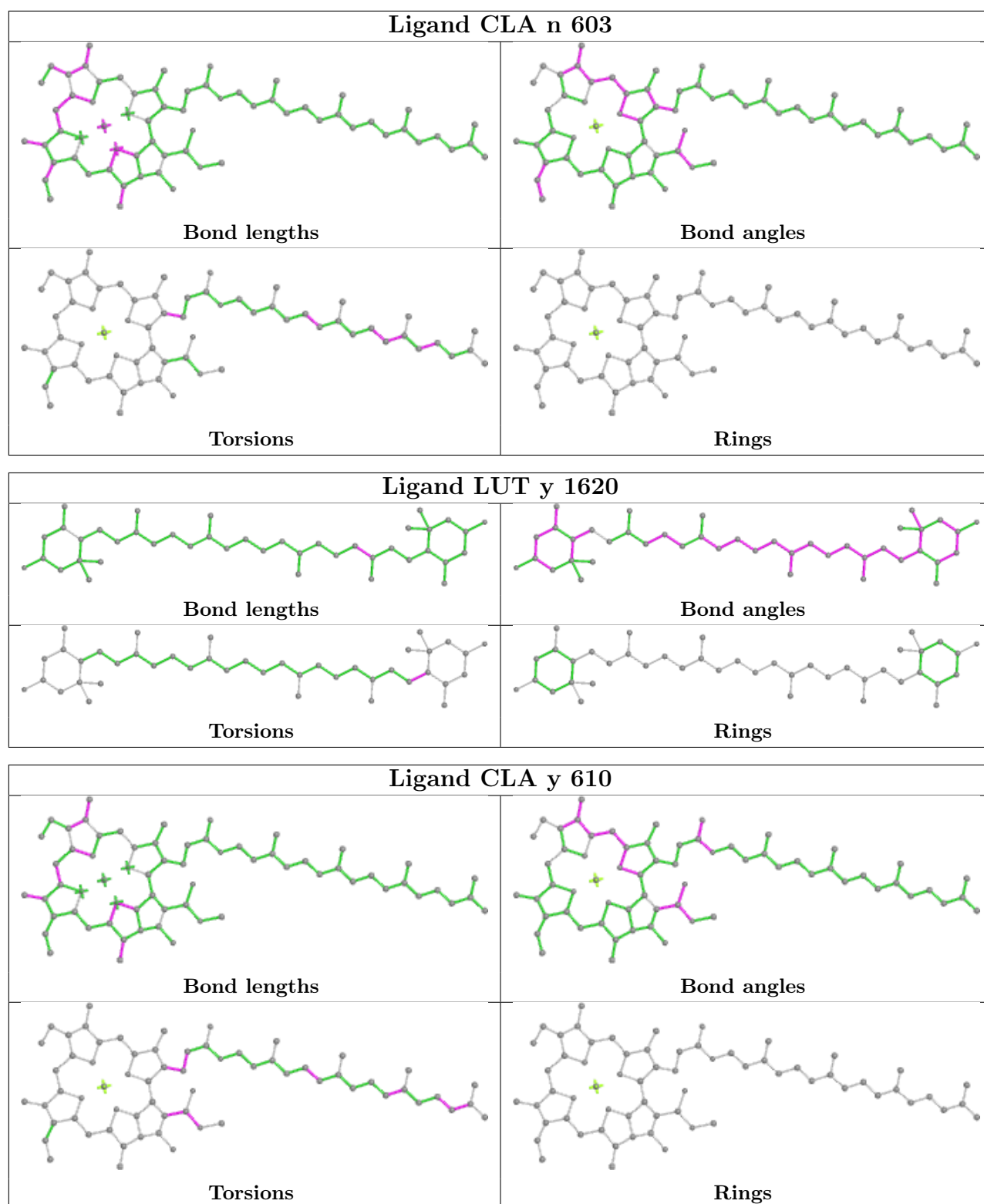


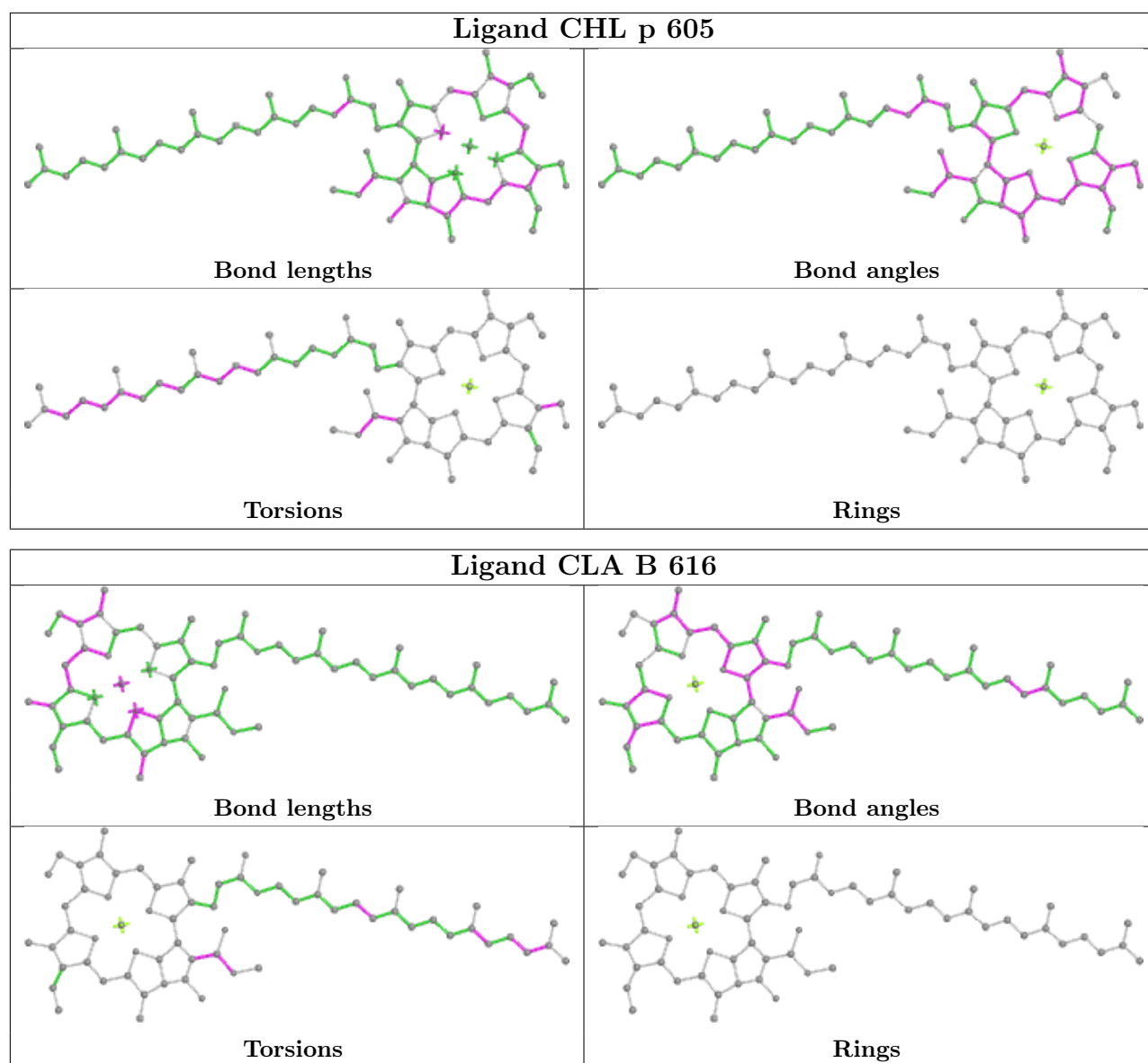


Ligand CLA 4 611

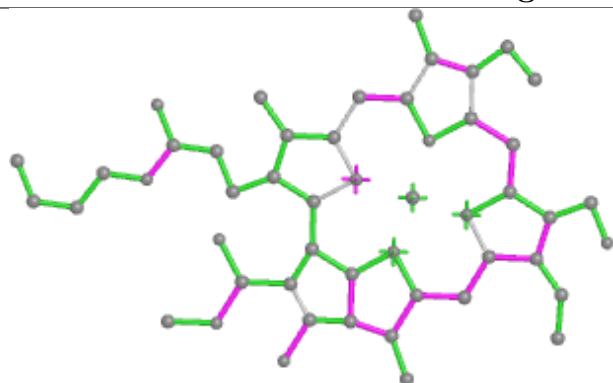




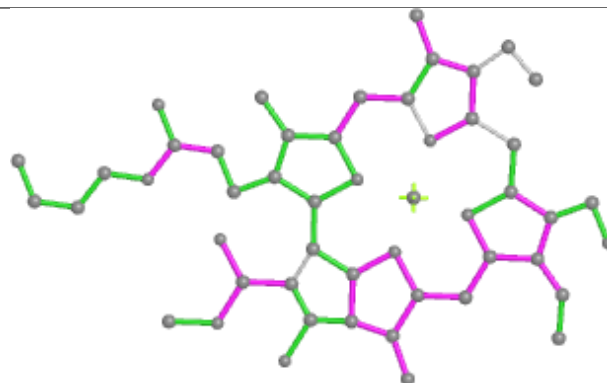




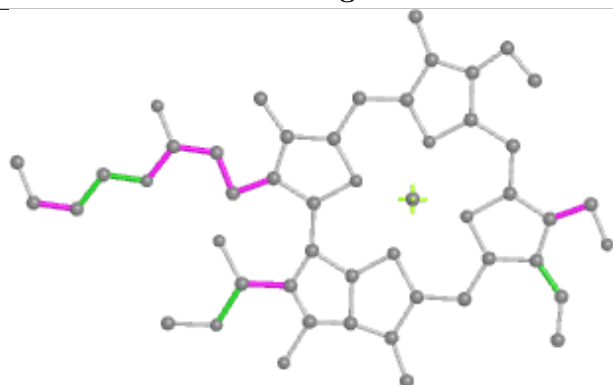
Ligand CHL 9 607



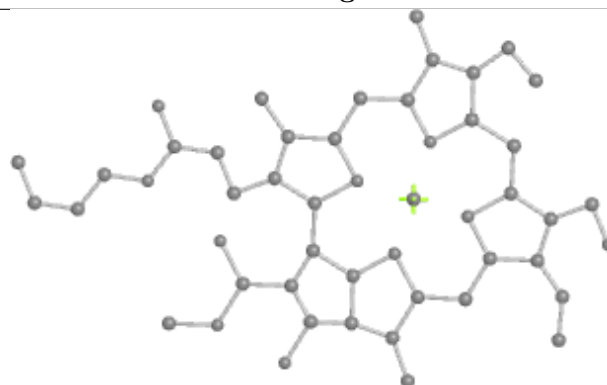
Bond lengths



Bond angles

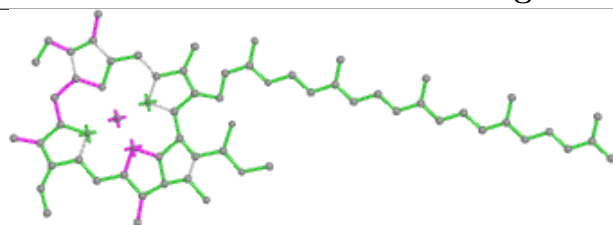


Torsions

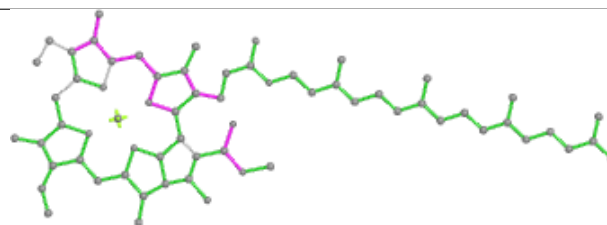


Rings

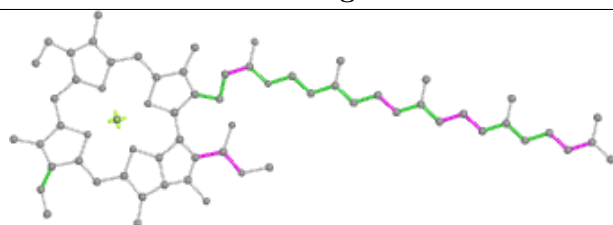
Ligand CLA B 614



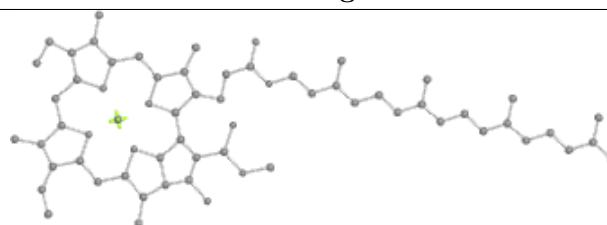
Bond lengths



Bond angles

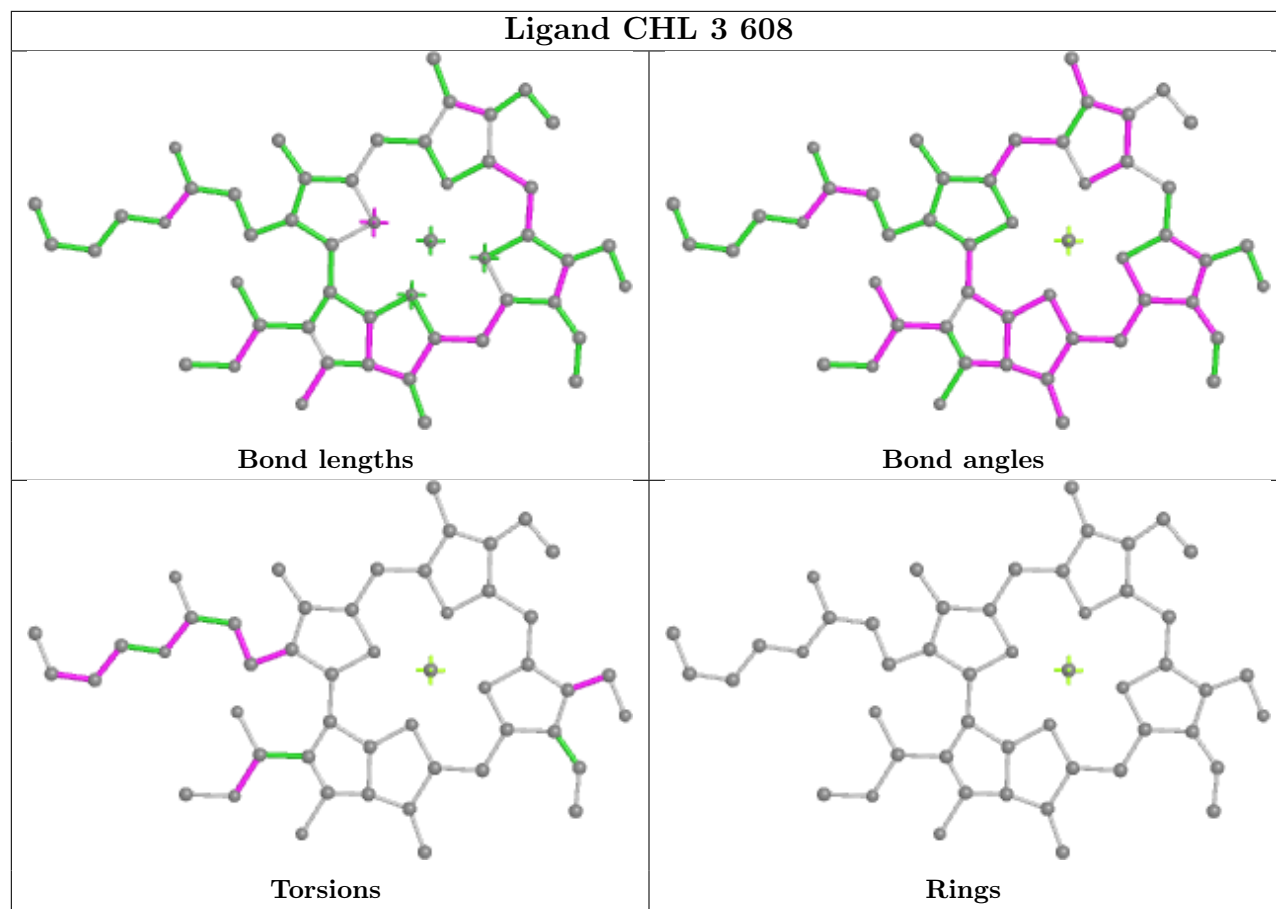


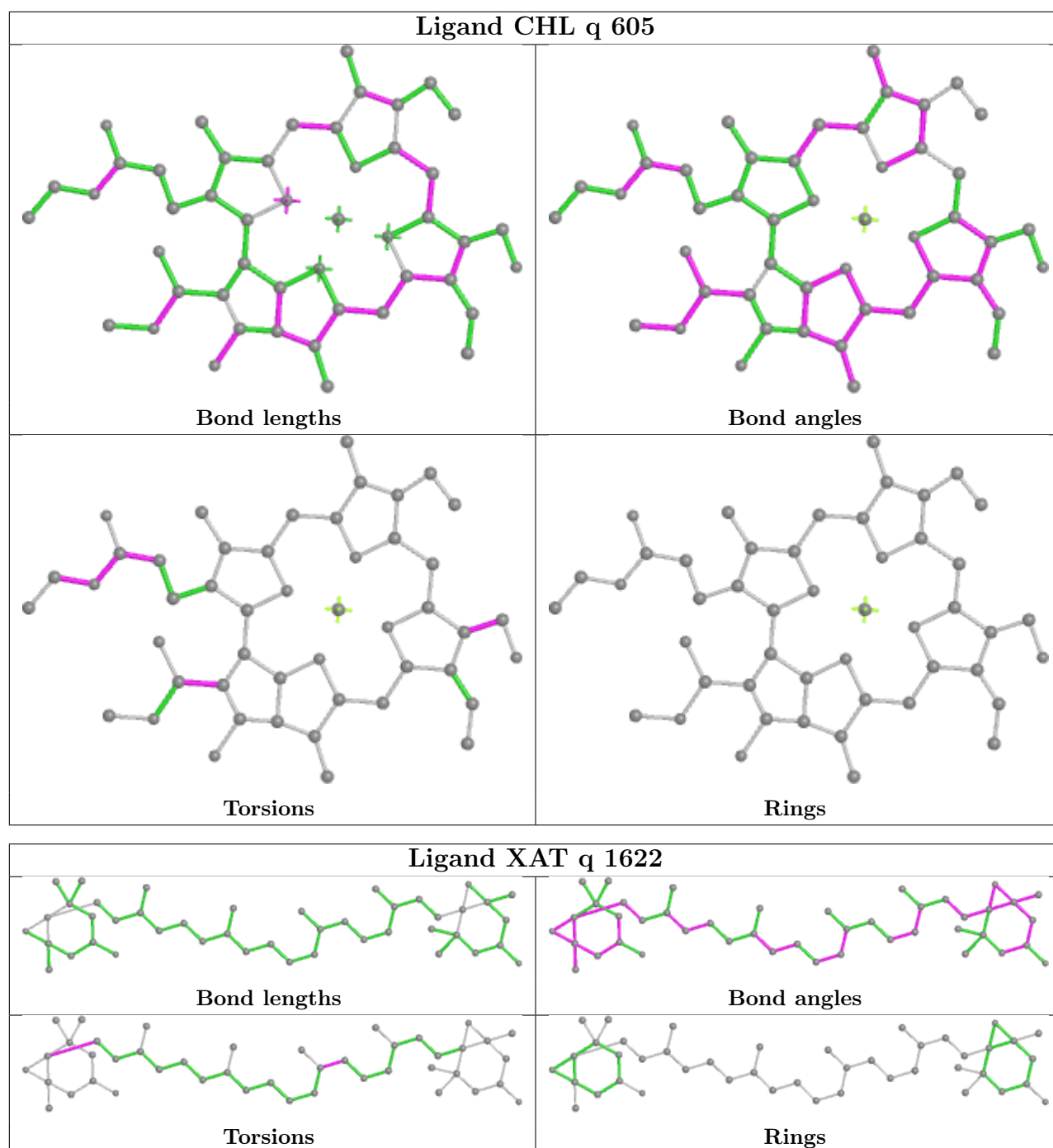
Torsions



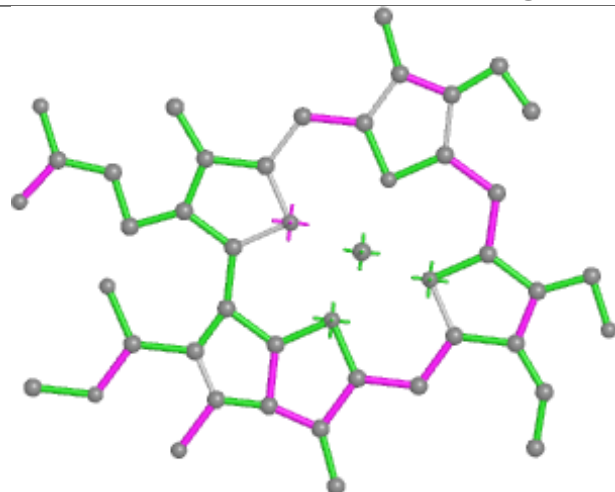
Rings

Ligand CHL 3 608

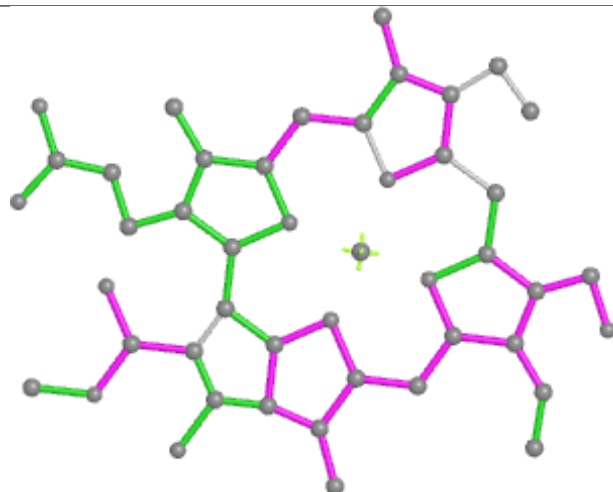




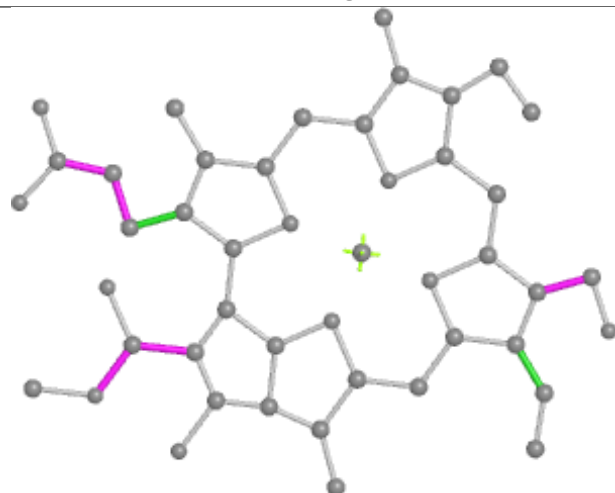
Ligand CHL 1 605



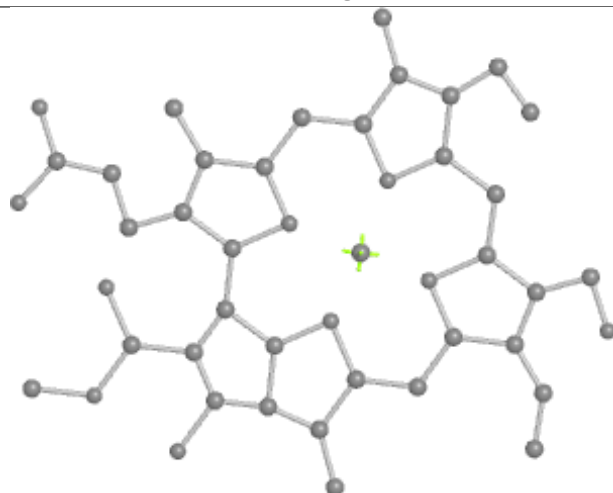
Bond lengths



Bond angles

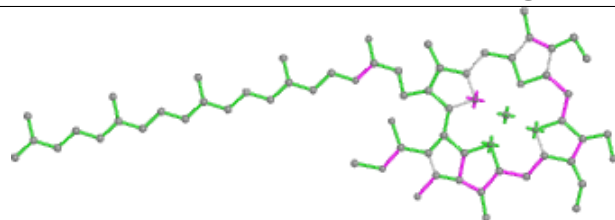


Torsions

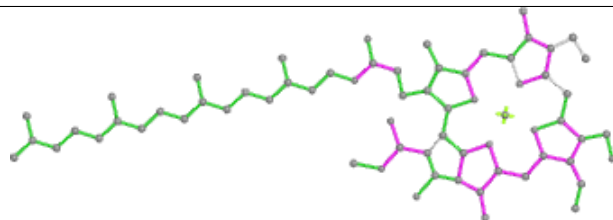


Rings

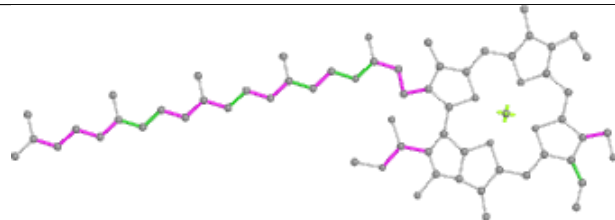
Ligand CHL 0 607



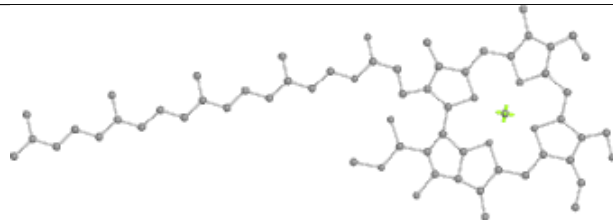
Bond lengths



Bond angles

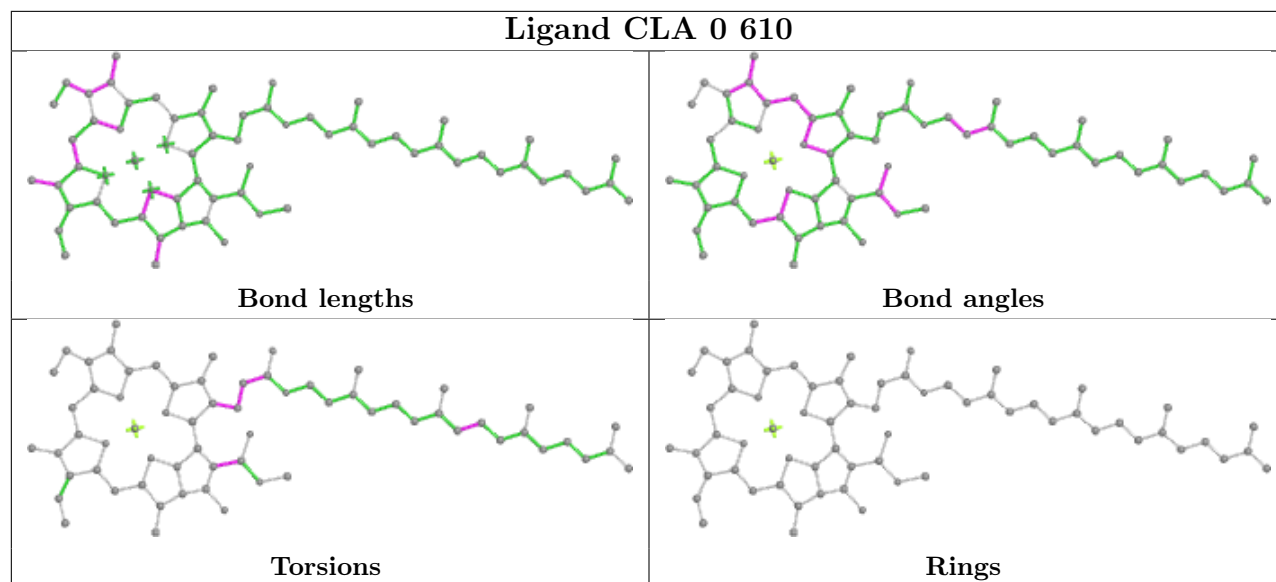


Torsions

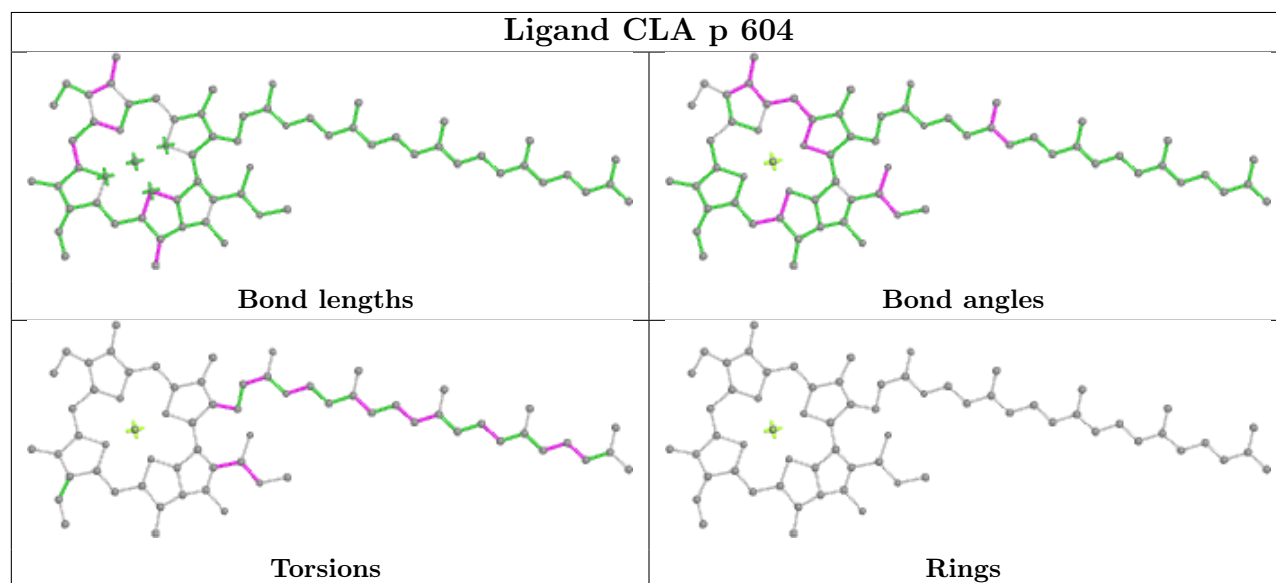


Rings

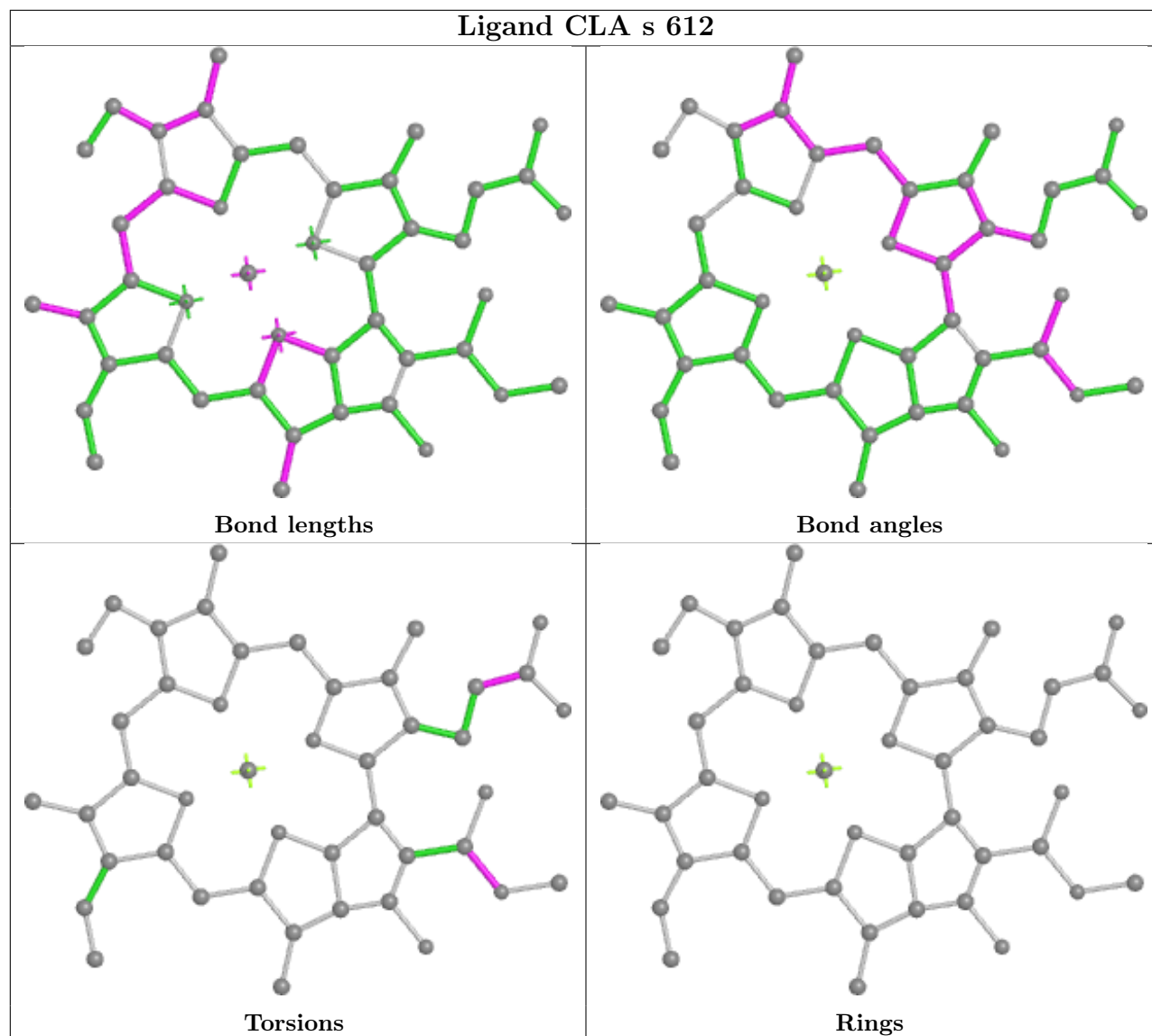
Ligand CLA 0 610

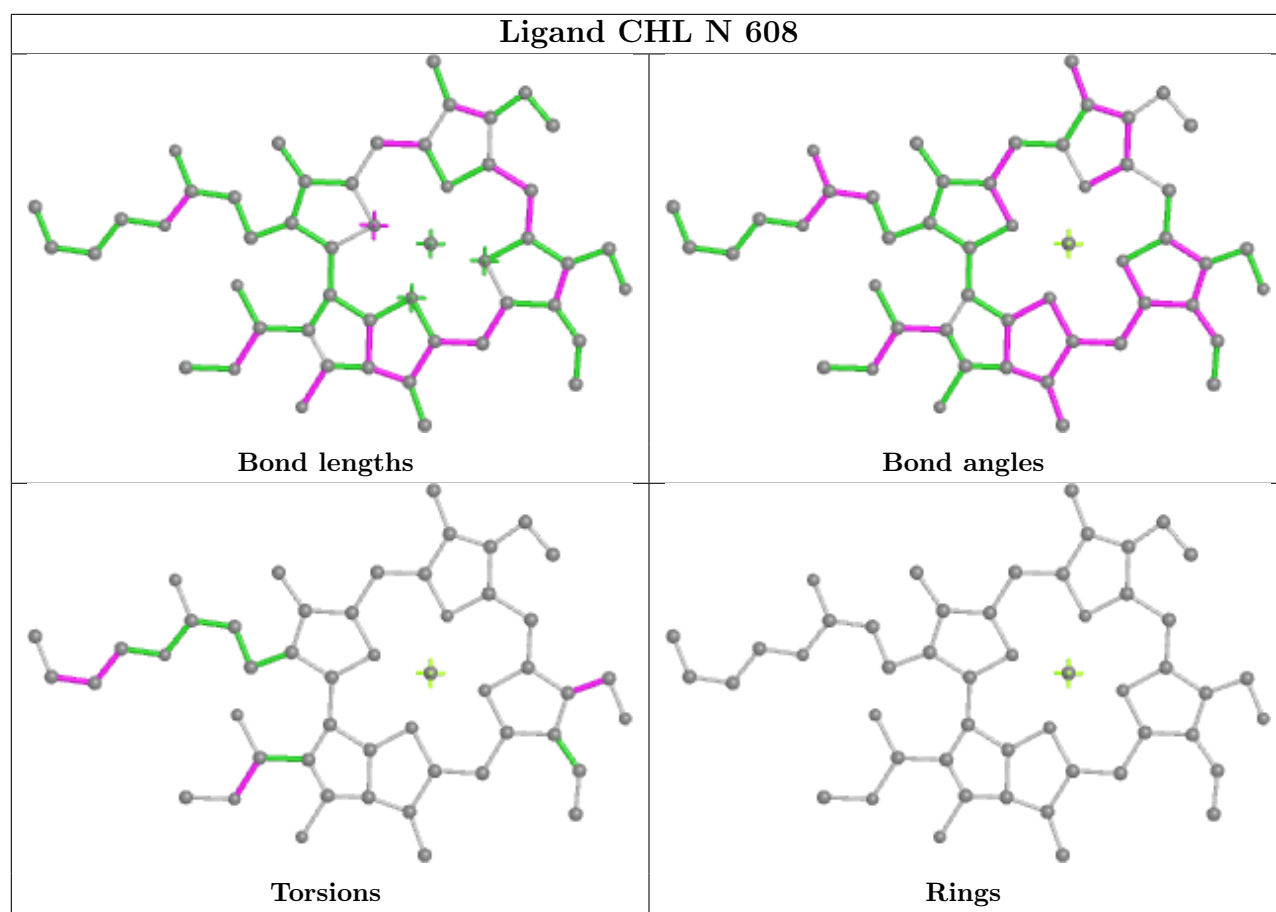


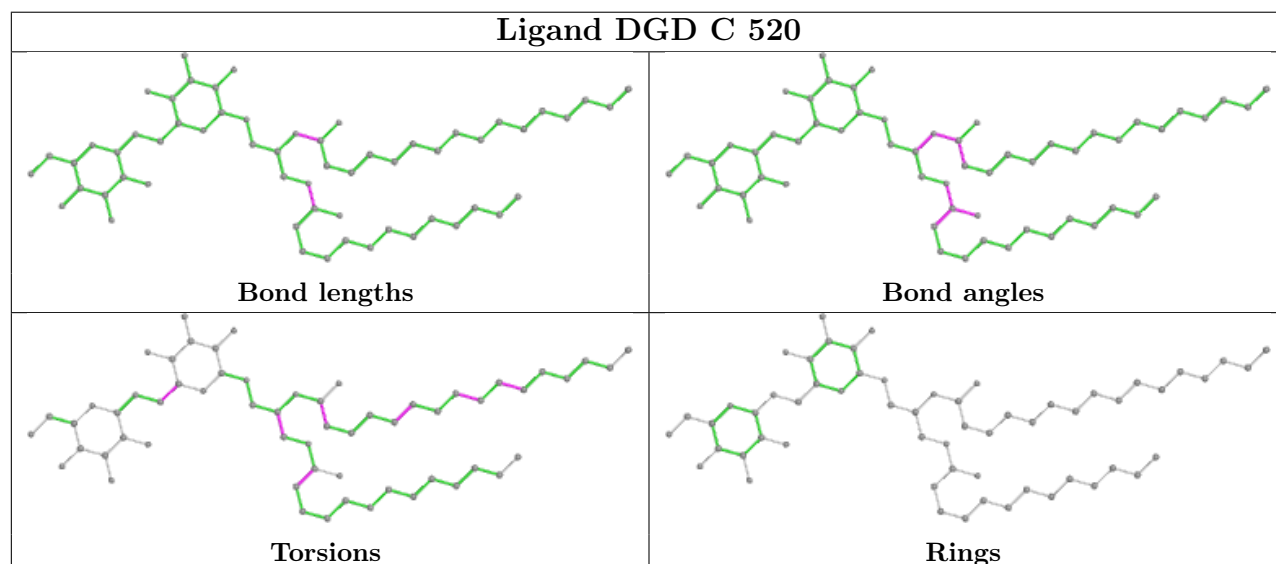
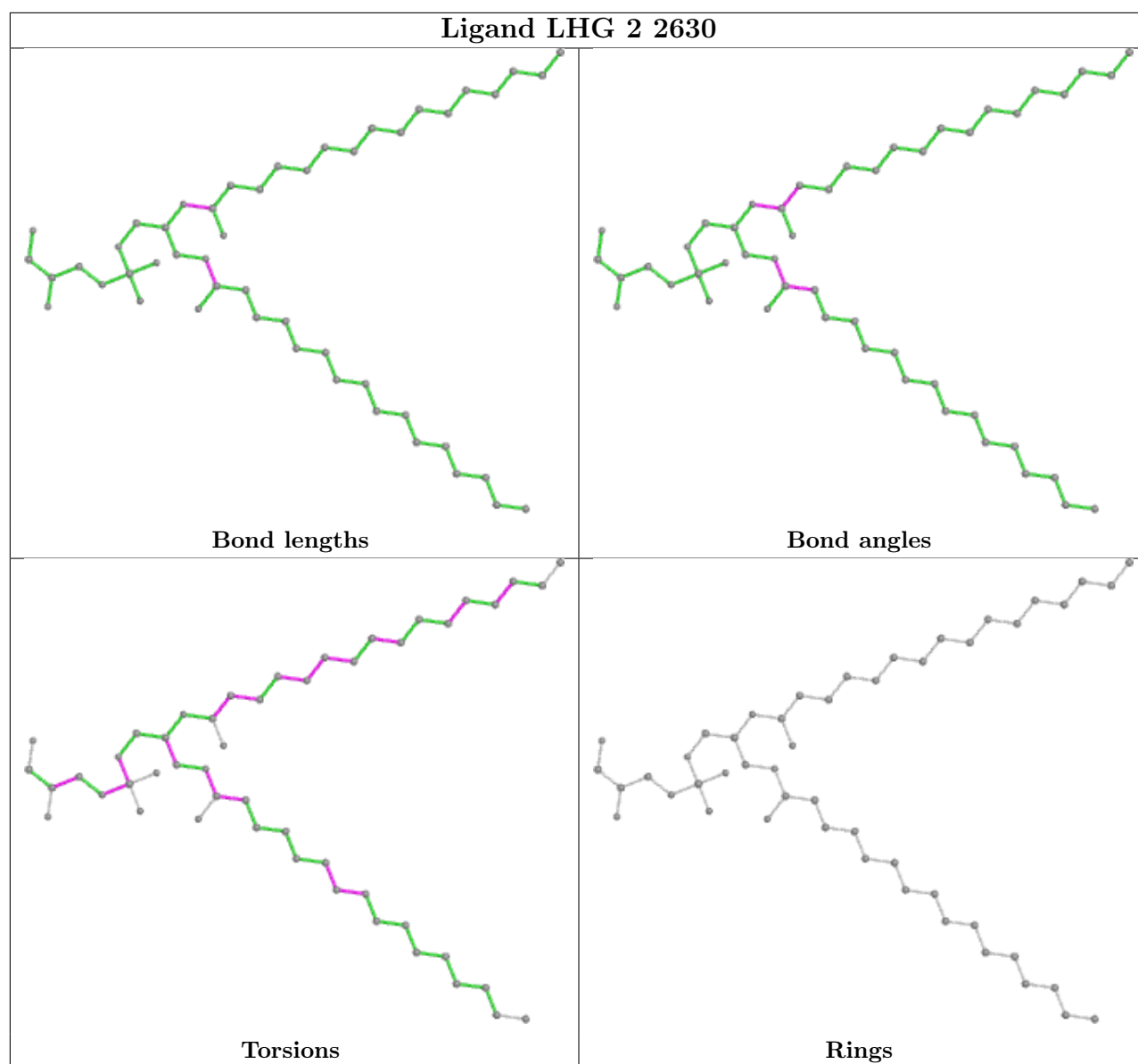
Ligand CLA p 604



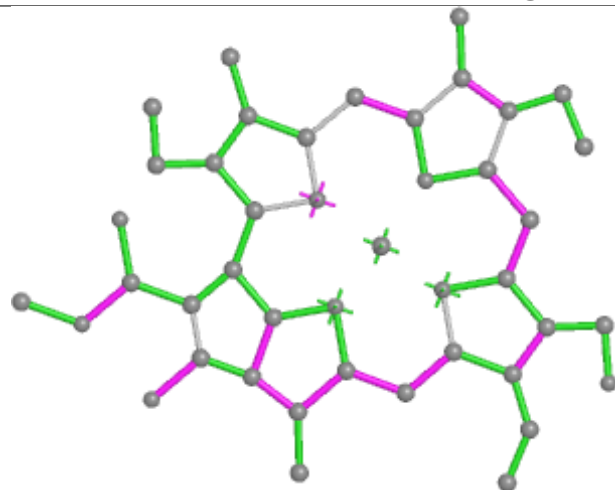
Ligand CLA s 612



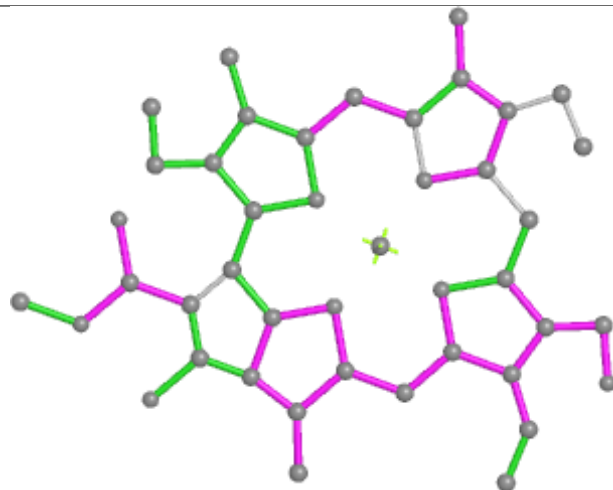




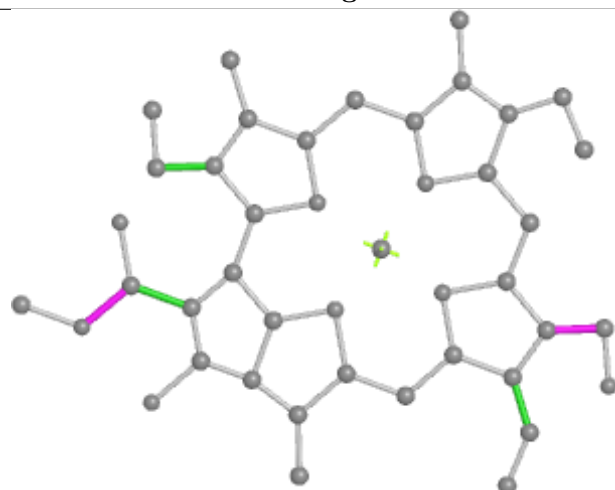
Ligand CHL s 607



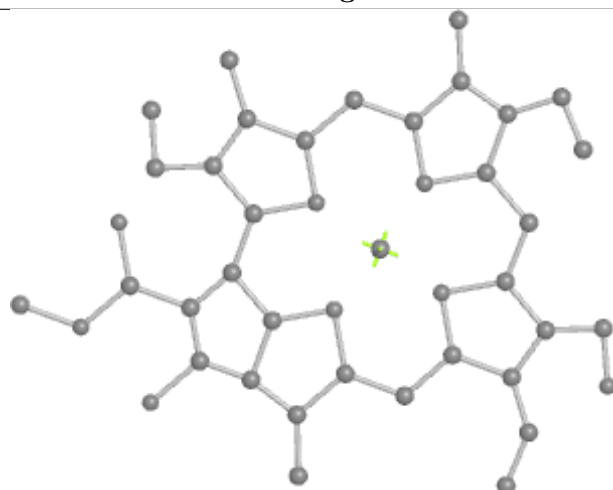
Bond lengths



Bond angles

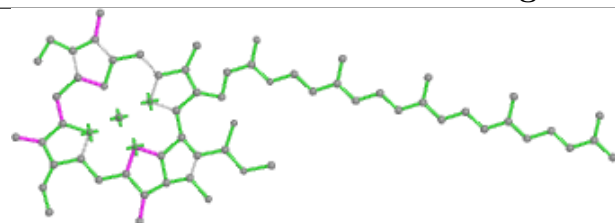


Torsions

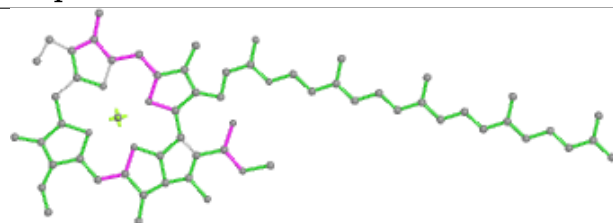


Rings

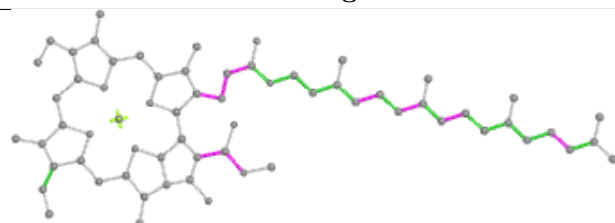
Ligand CLA p 602



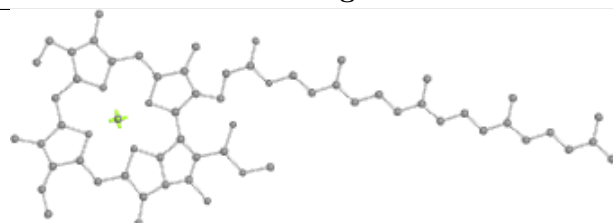
Bond lengths



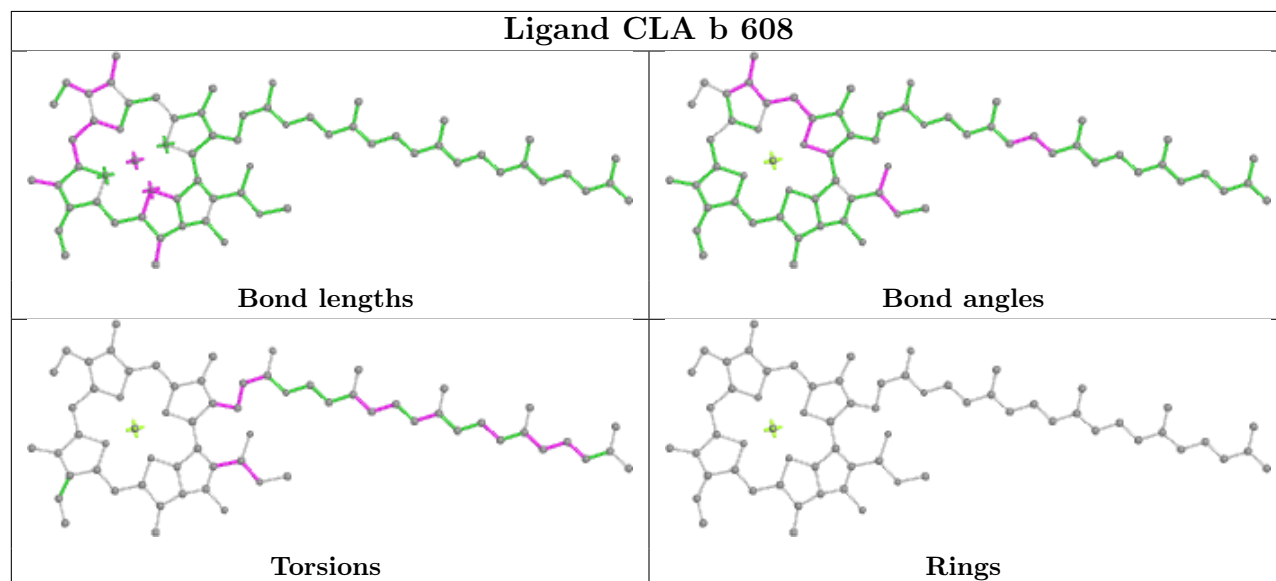
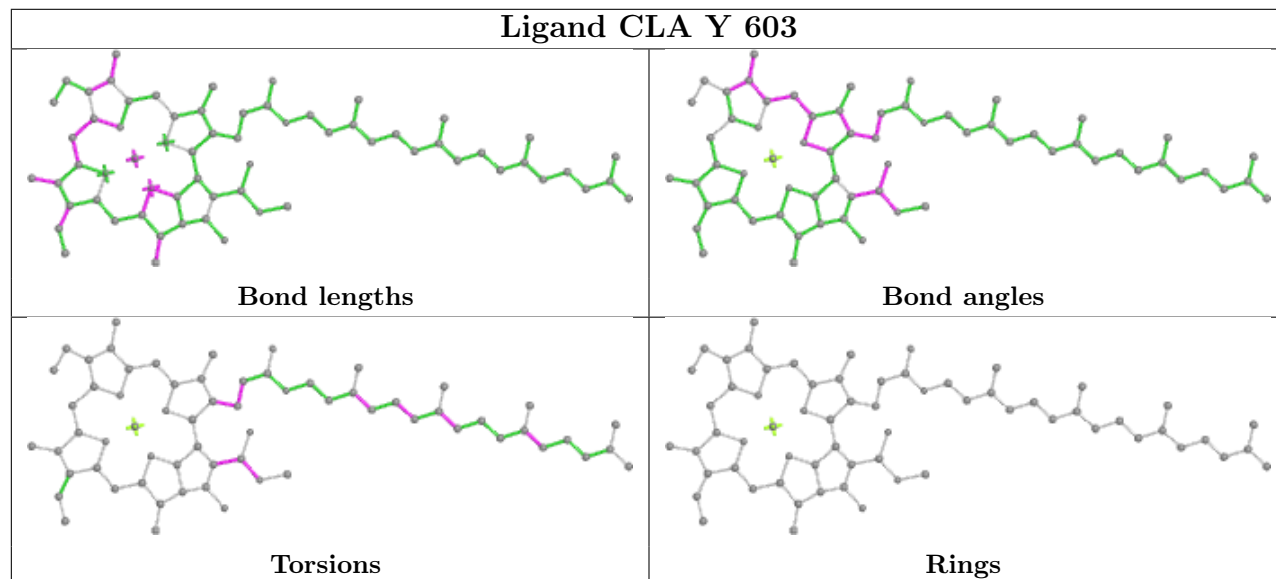
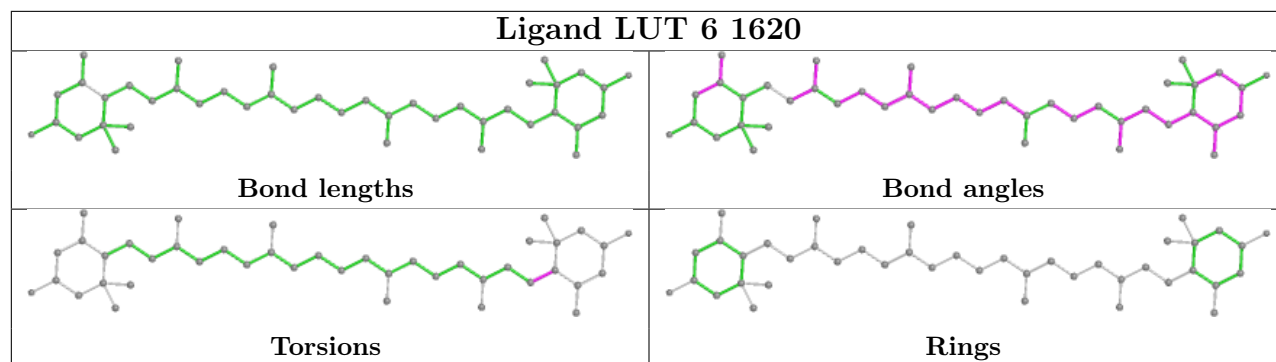
Bond angles

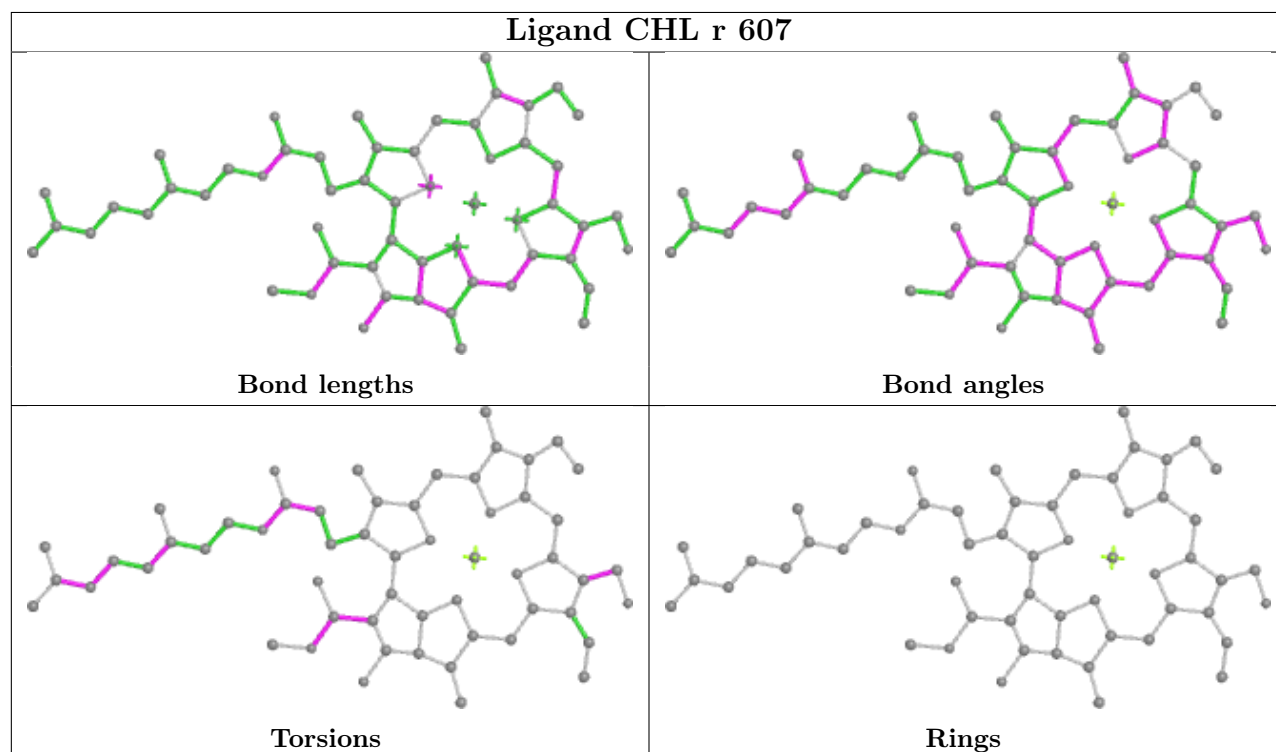
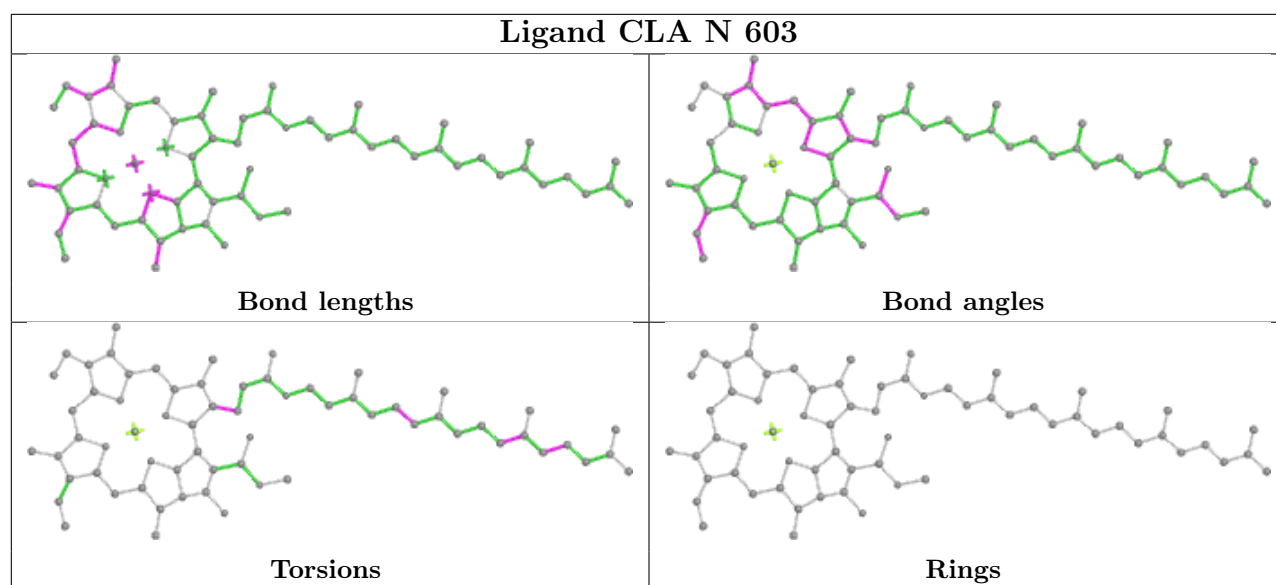


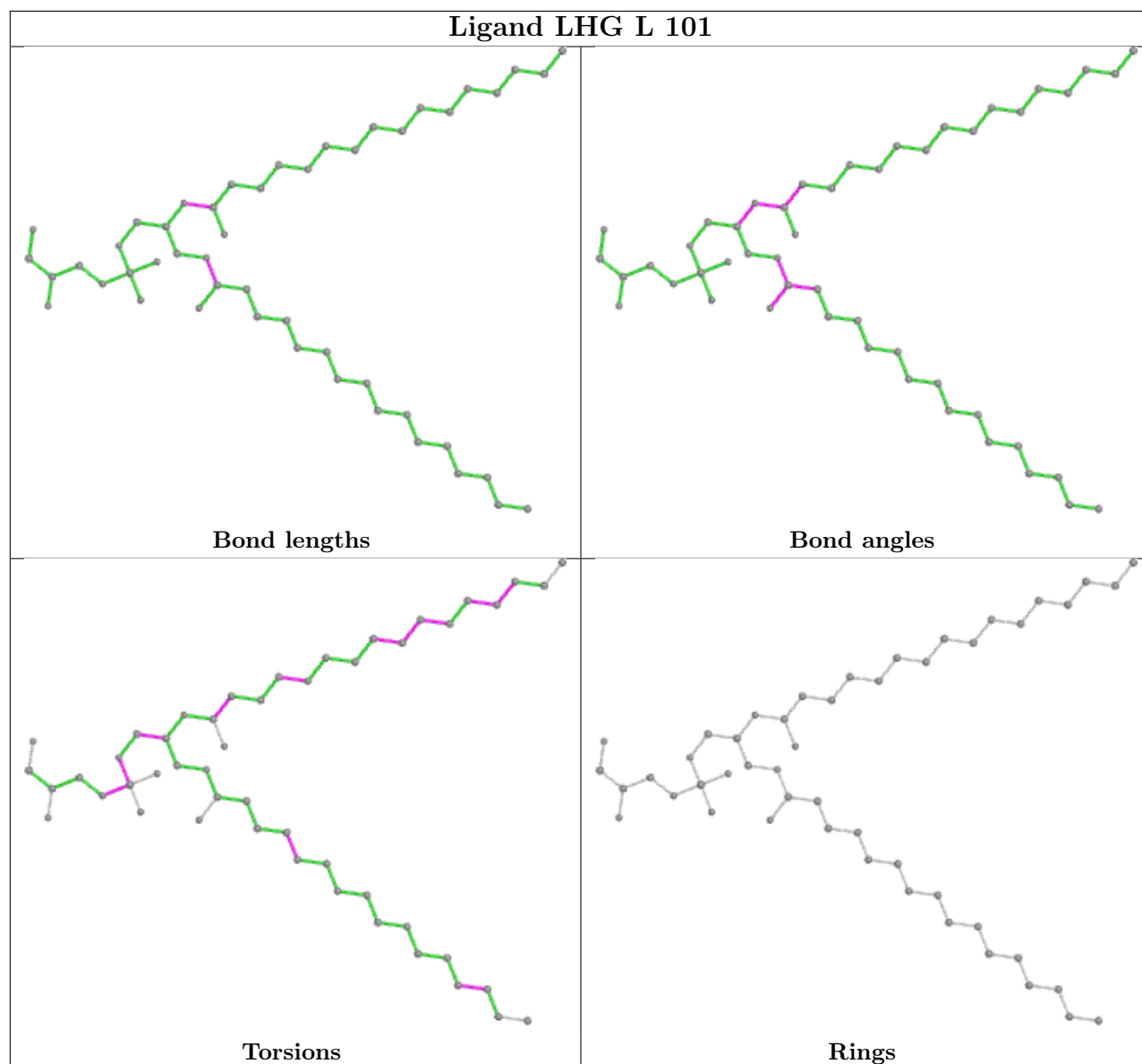
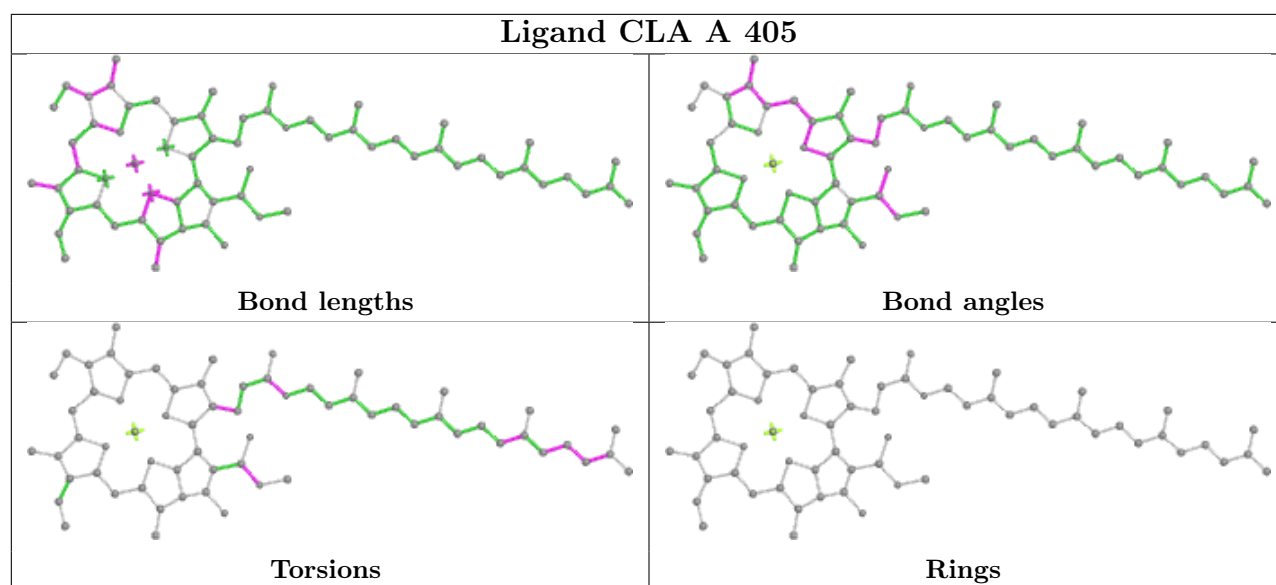
Torsions



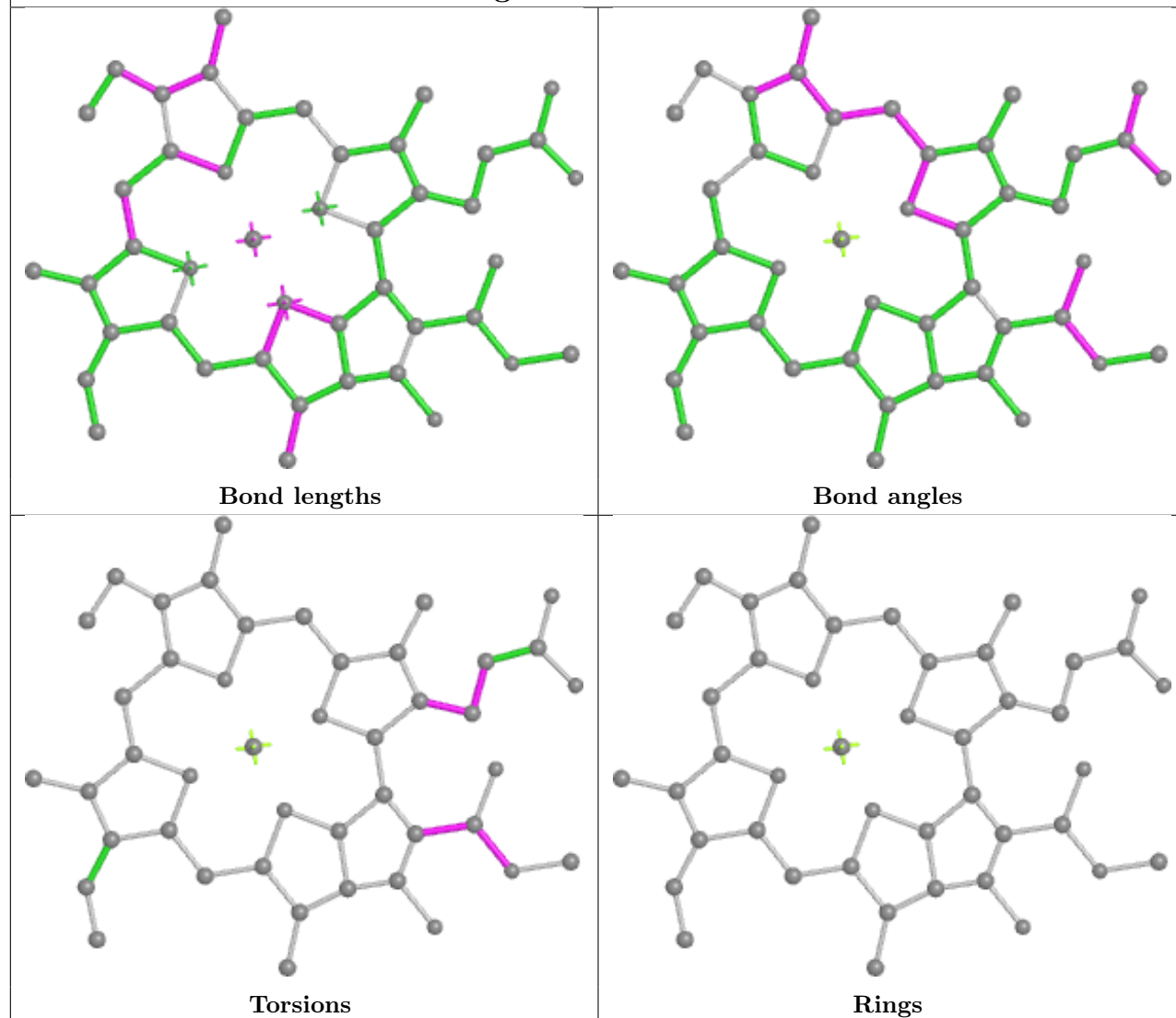
Rings



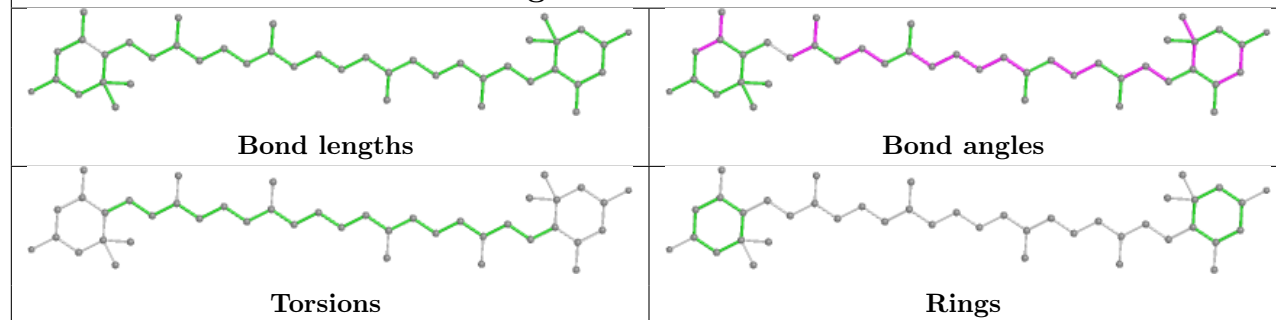


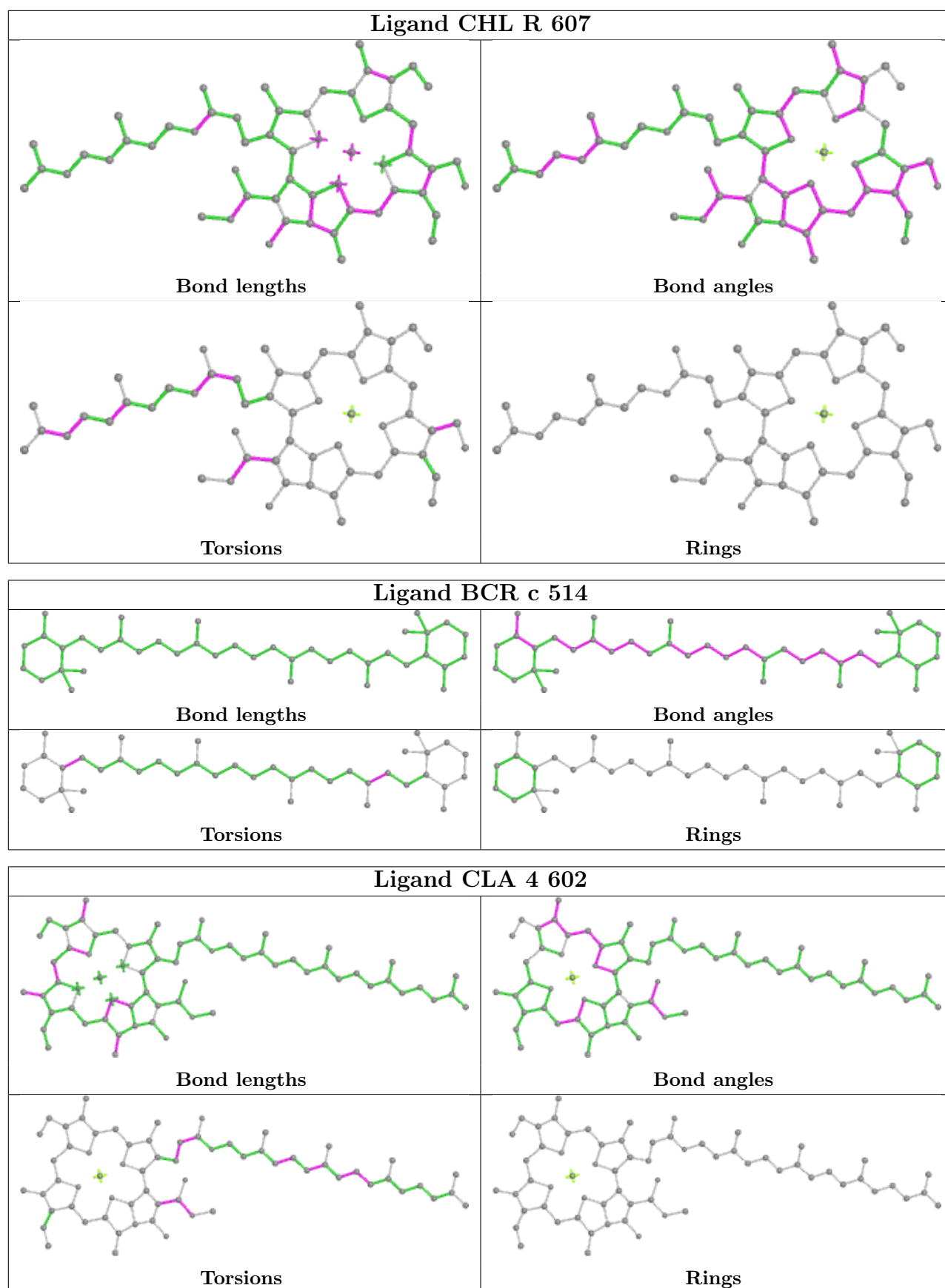


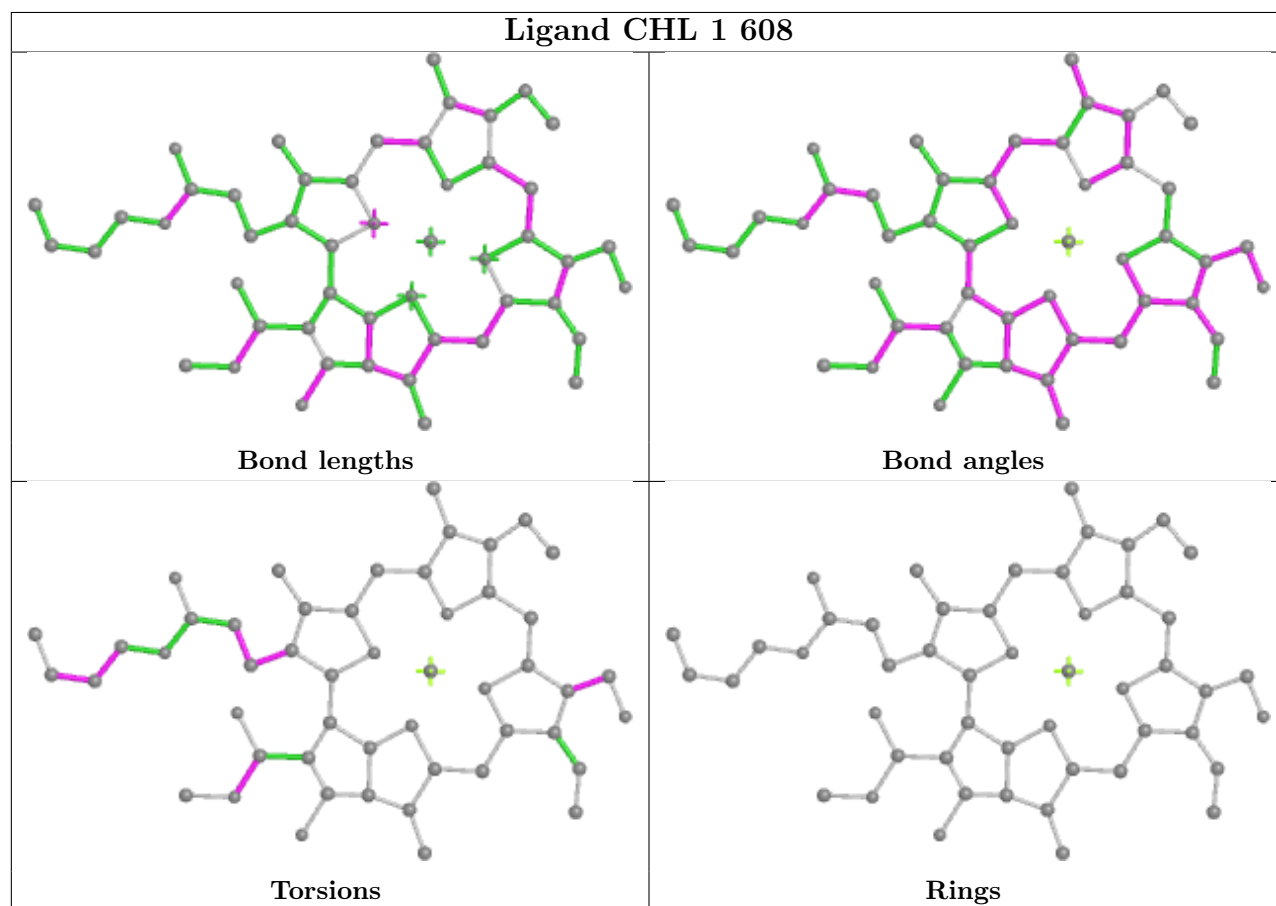
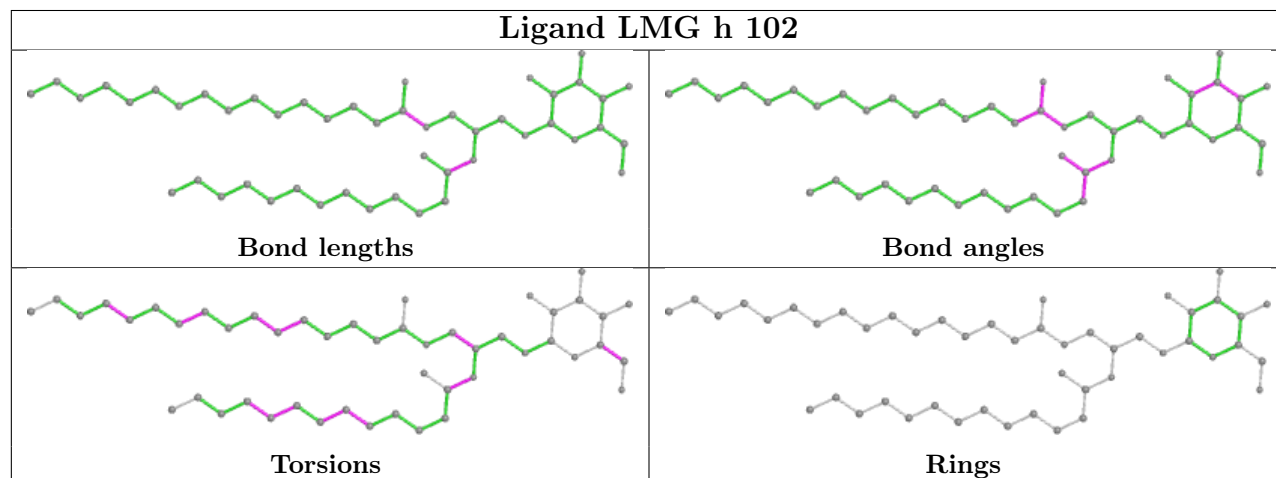
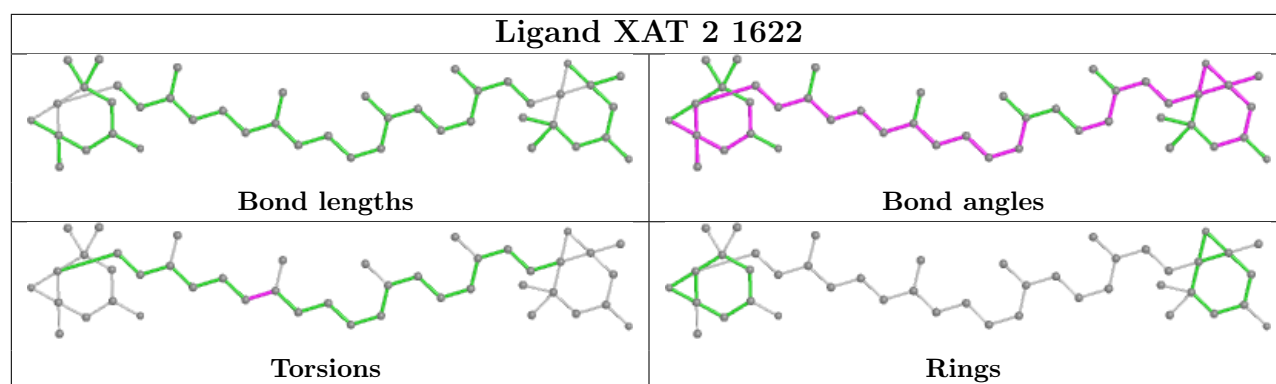
Ligand CLA 9 611

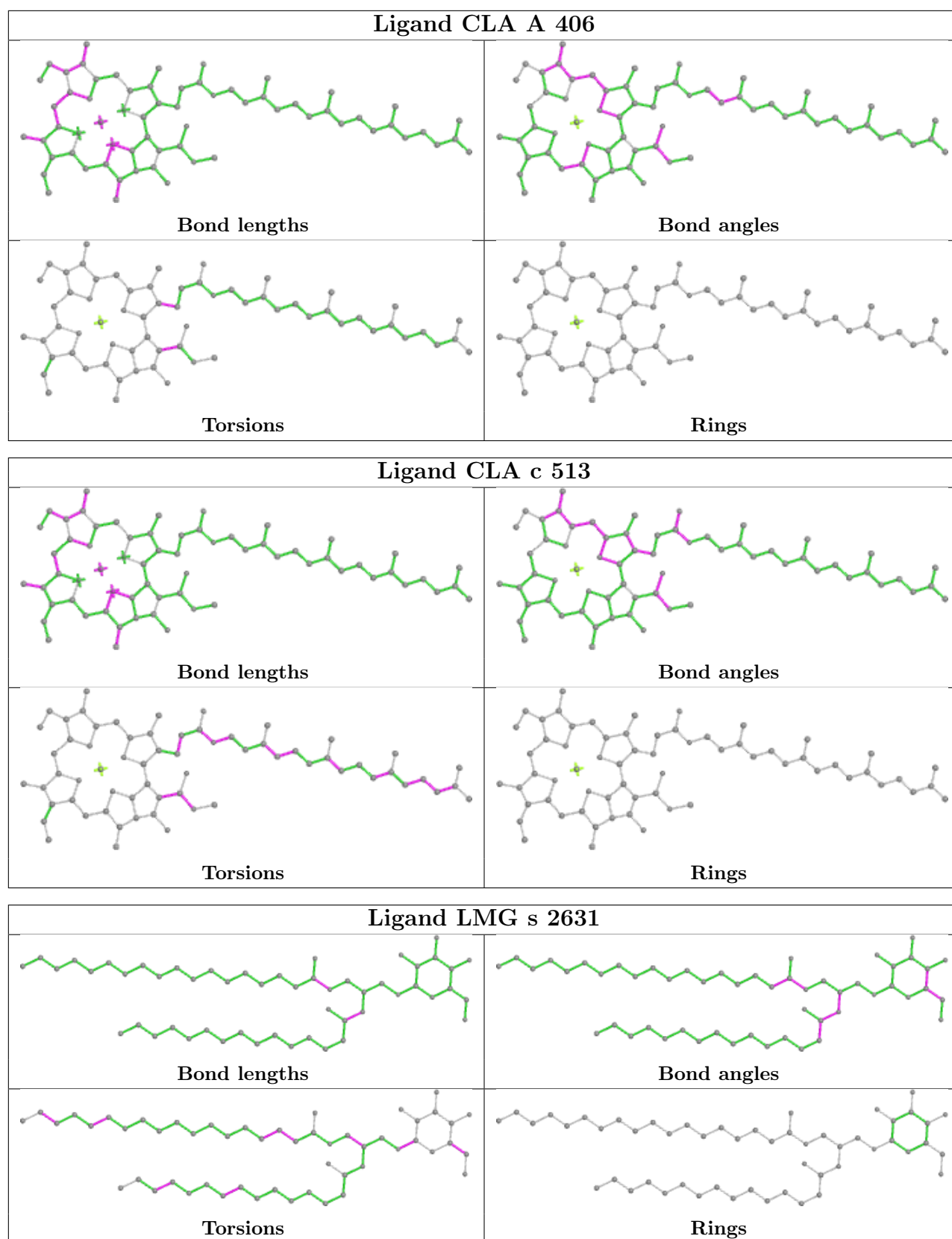


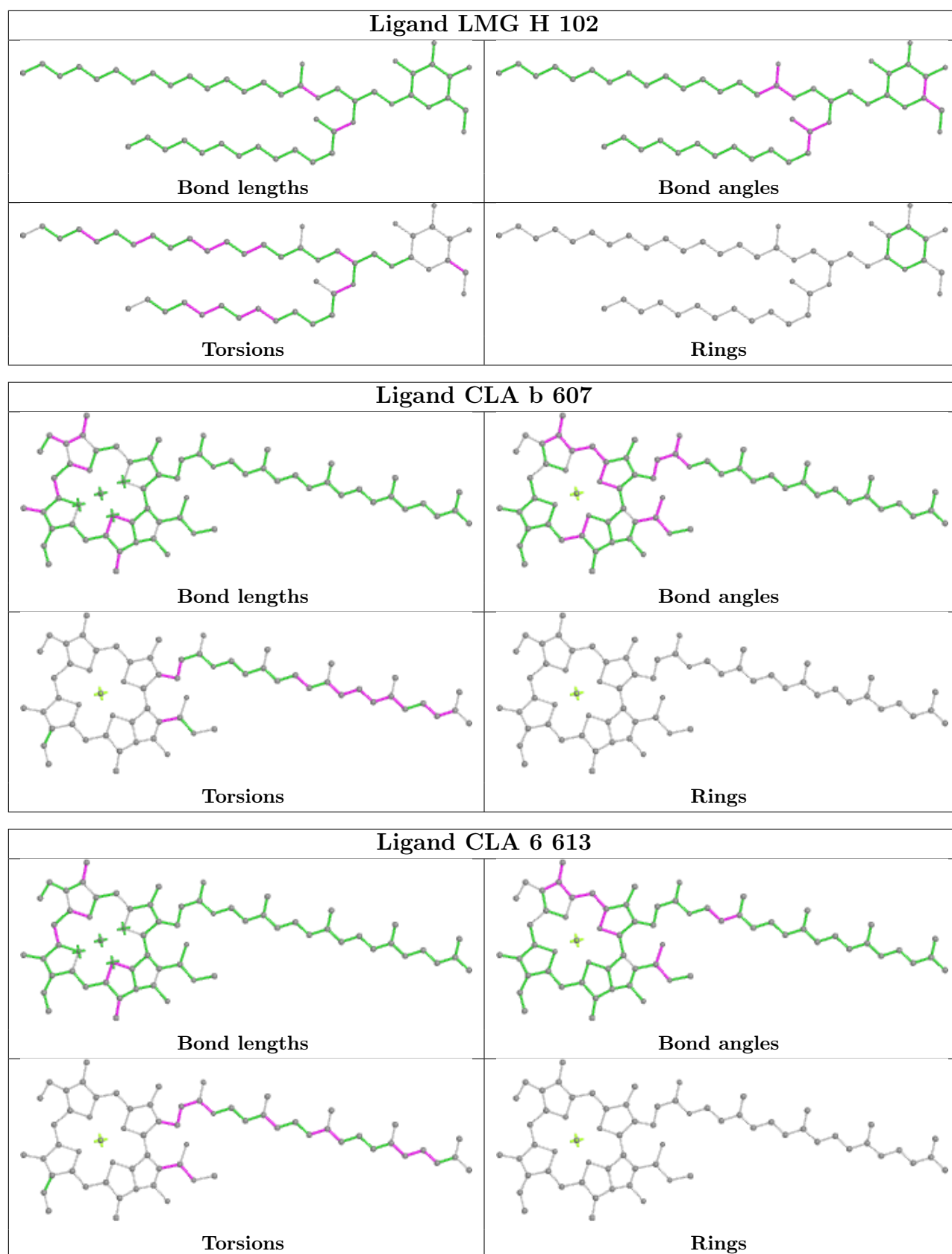
Ligand LUT 8 1621

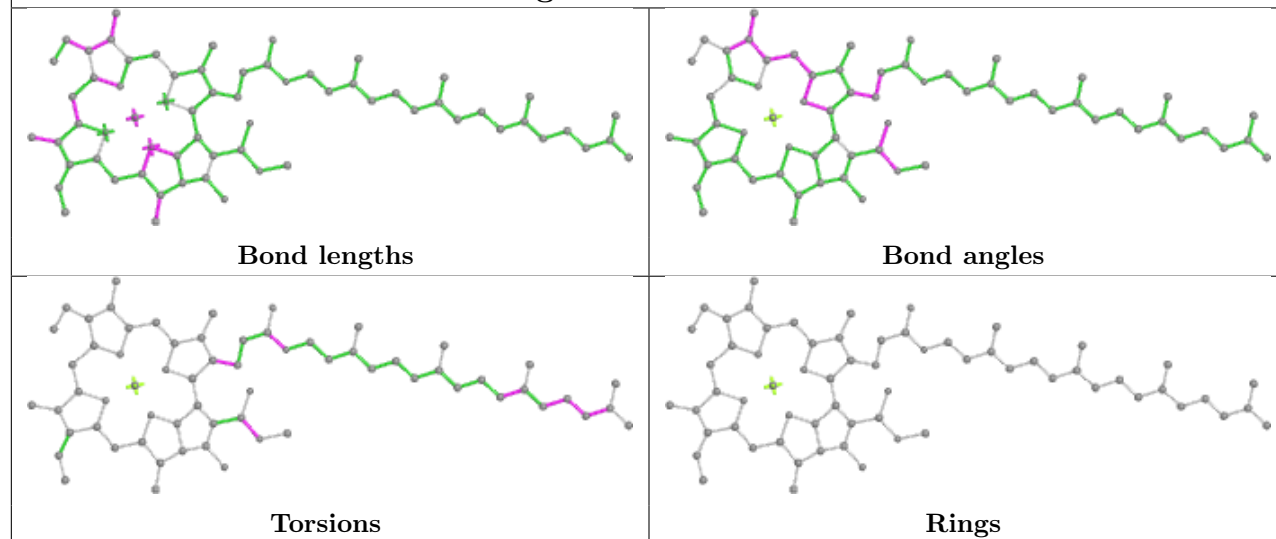
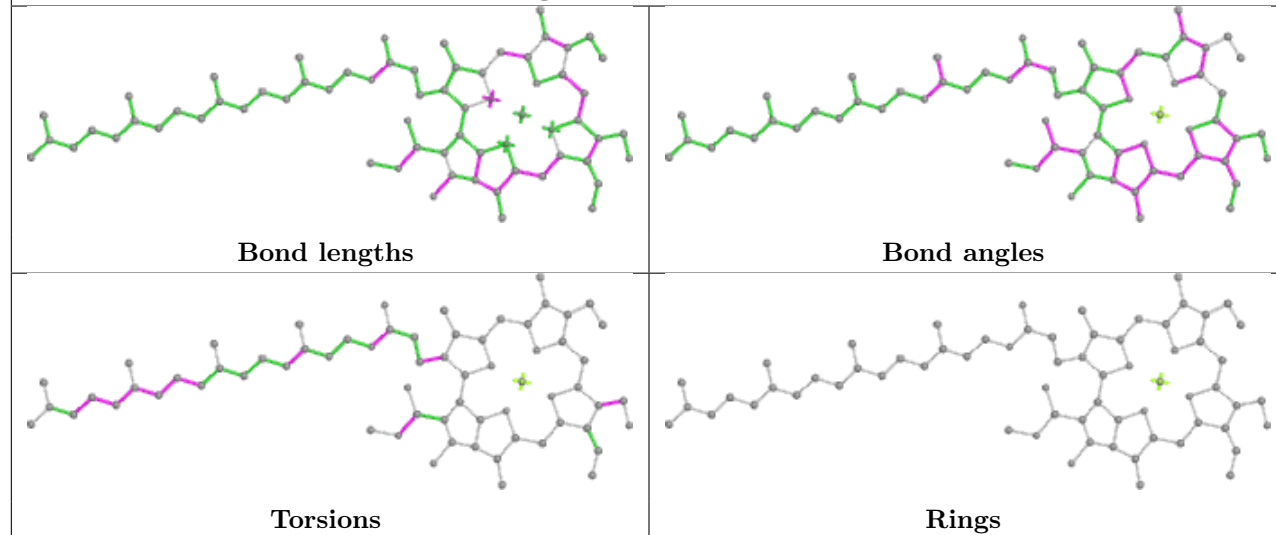


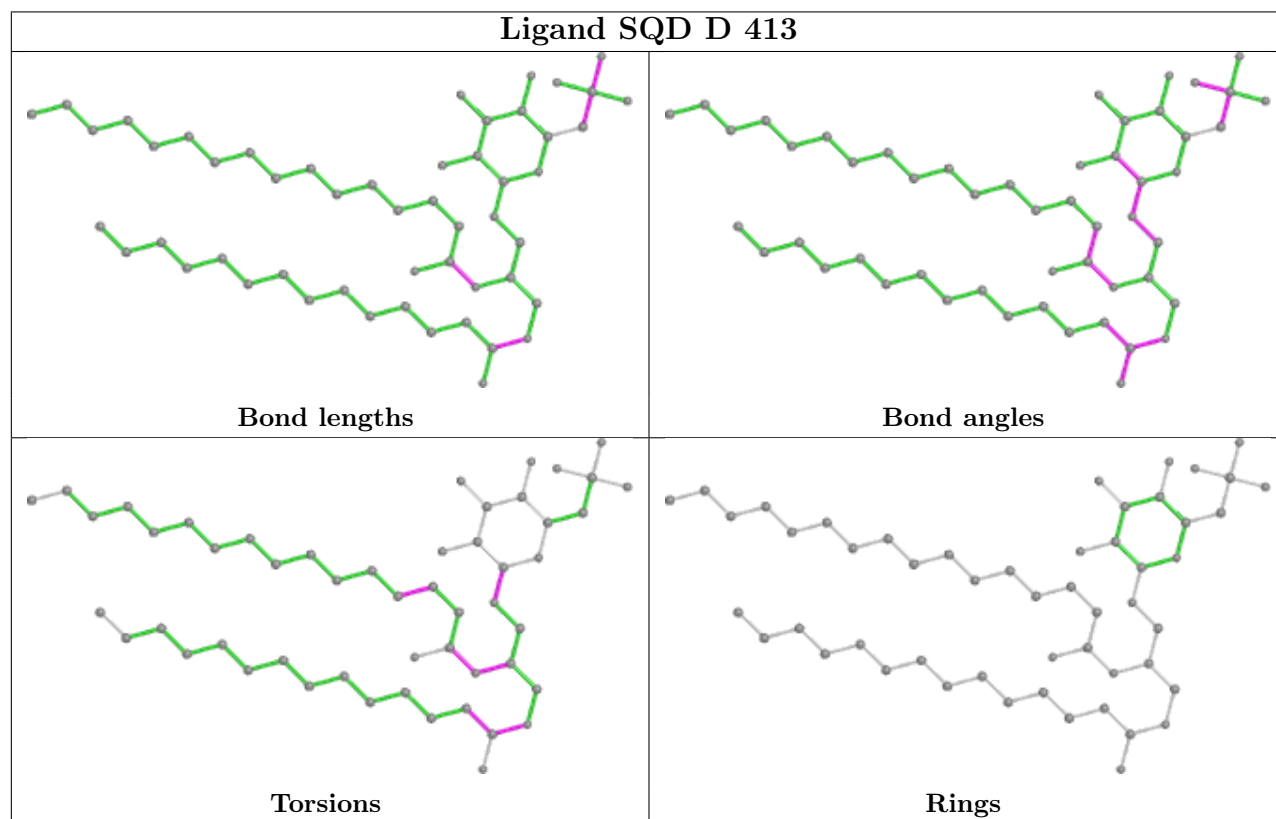
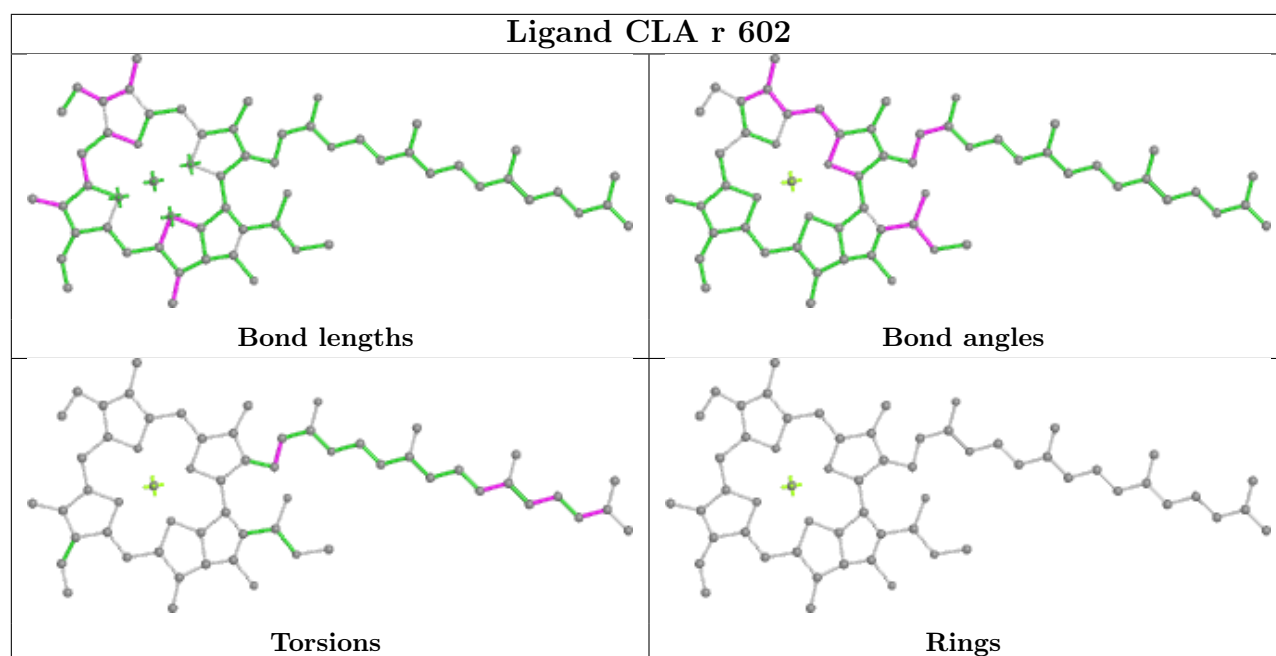


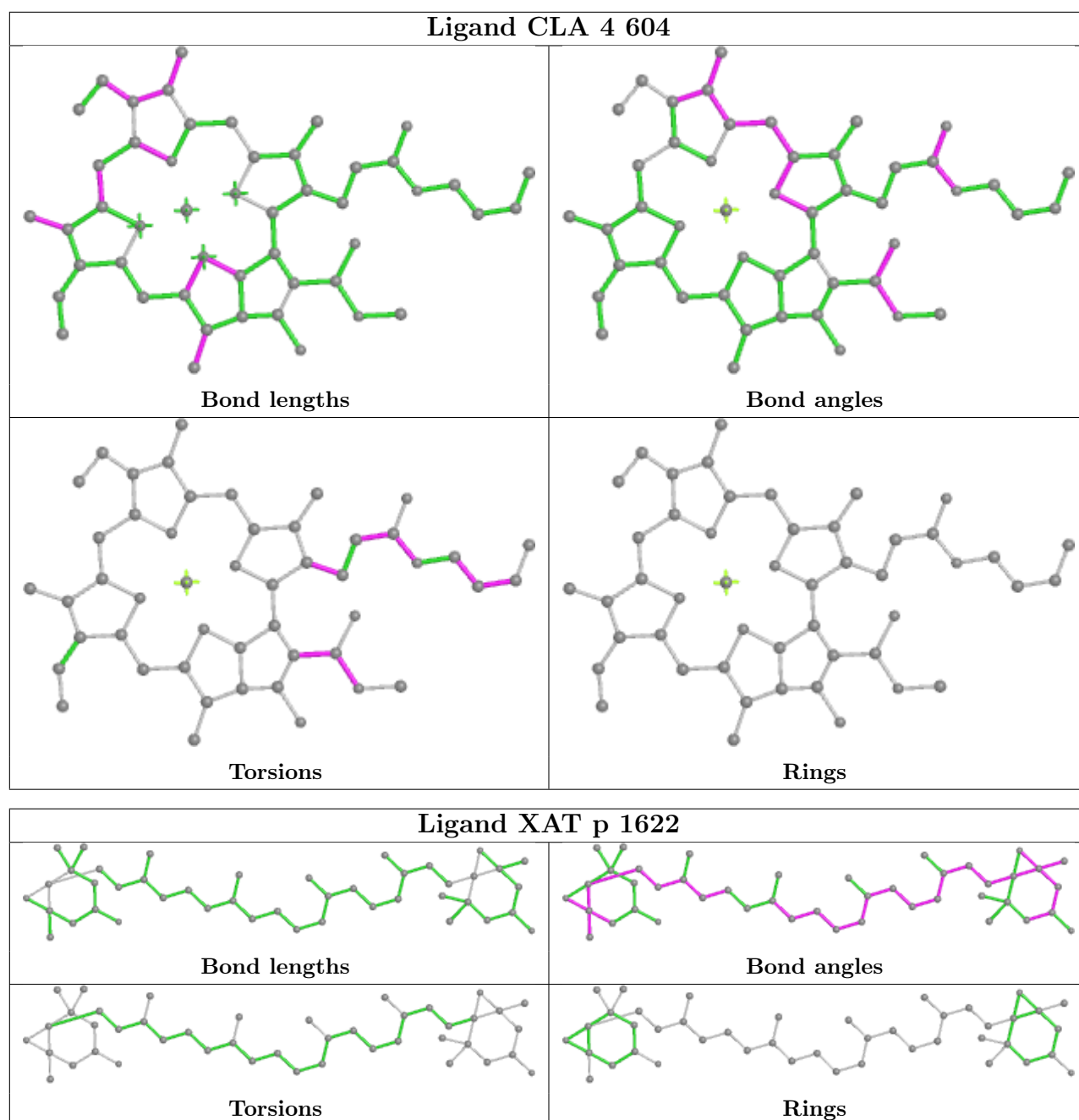




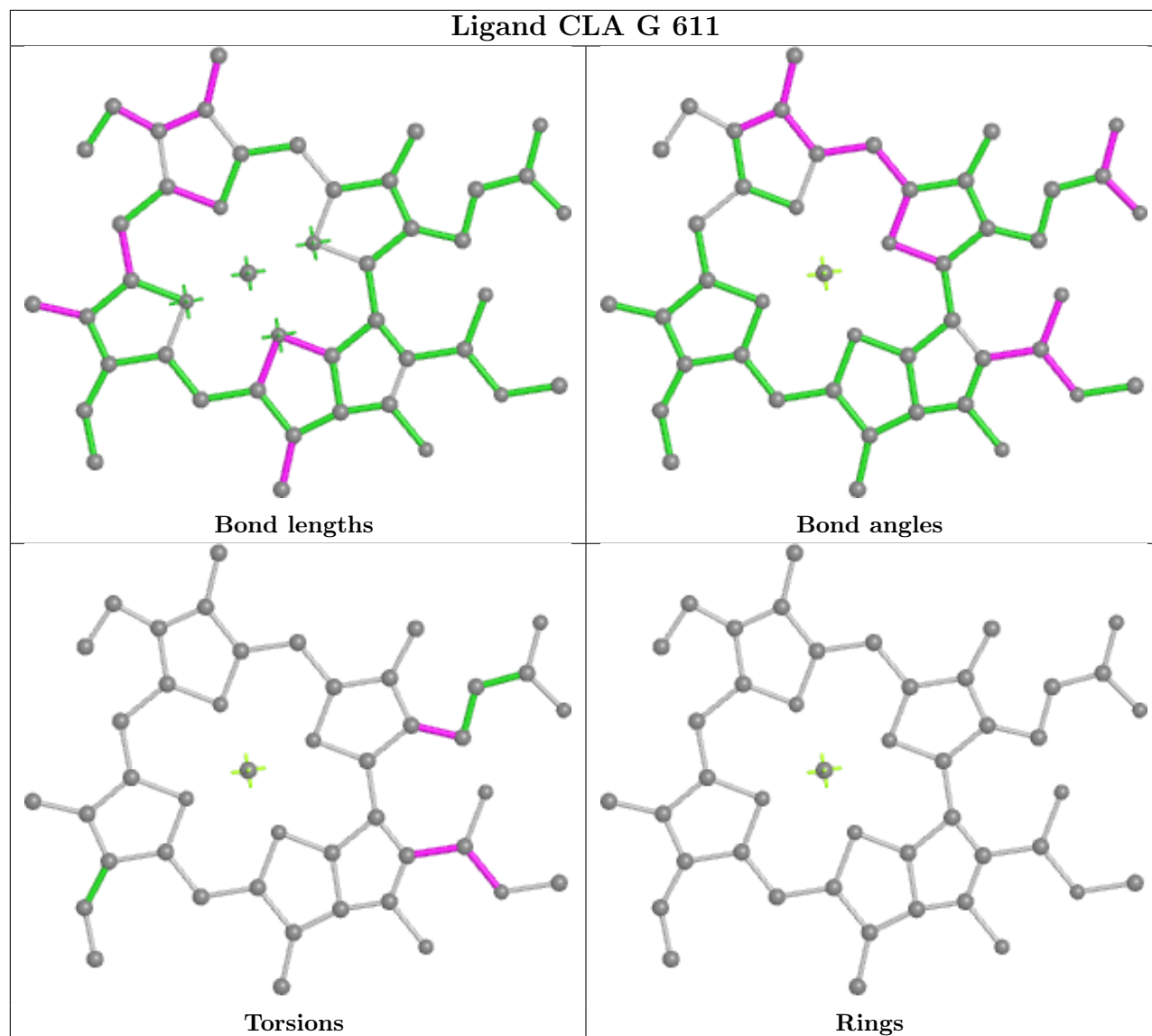


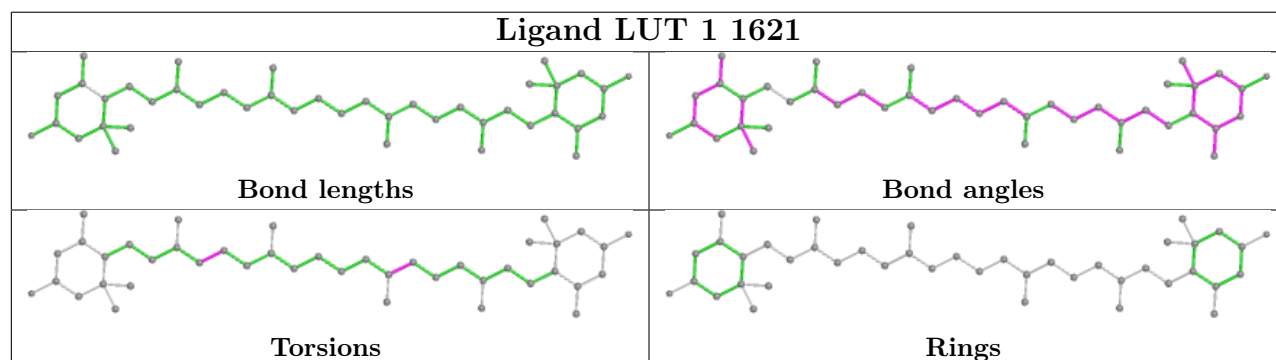
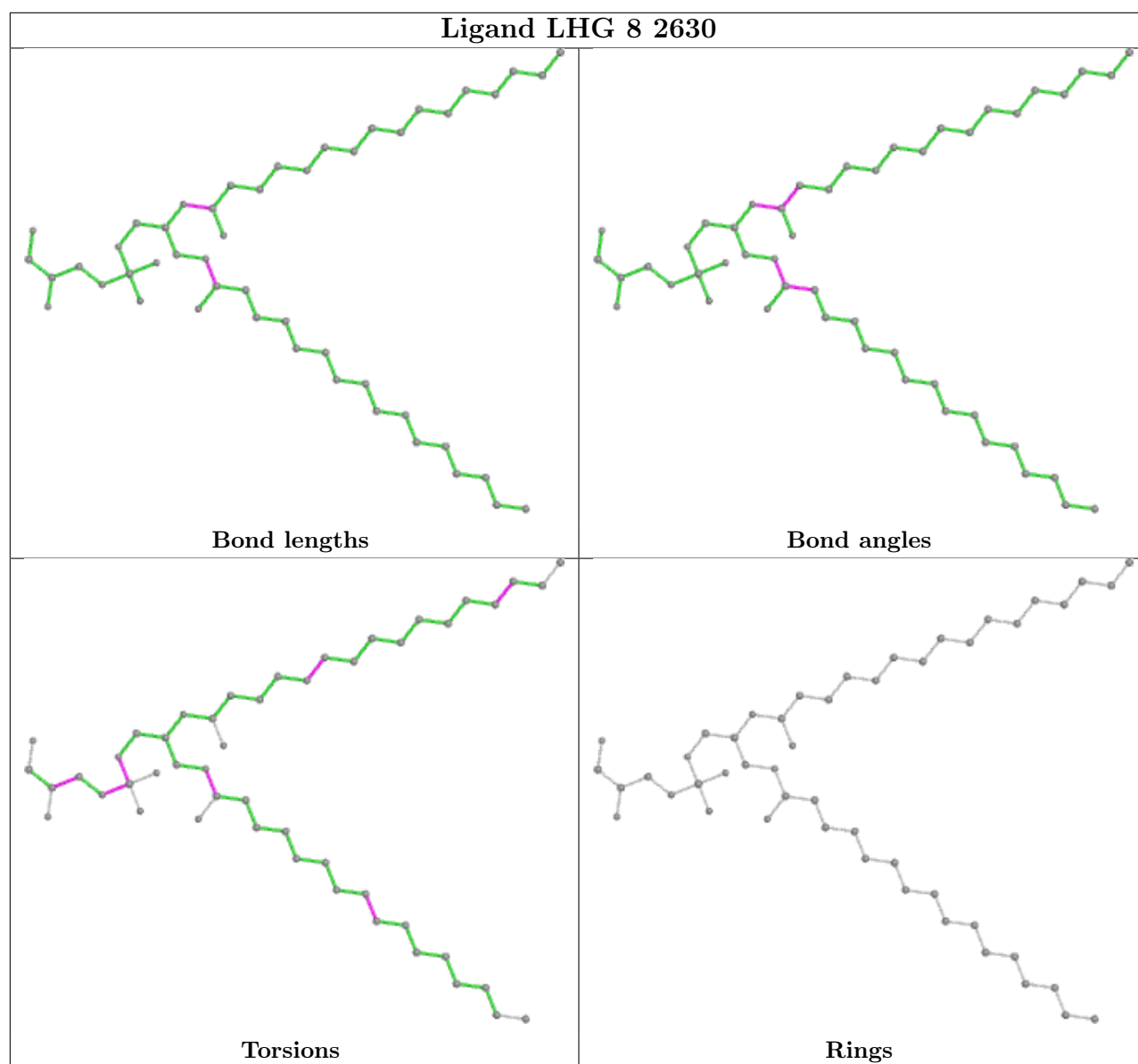
Ligand CLA a 405**Ligand CHL 7 609**



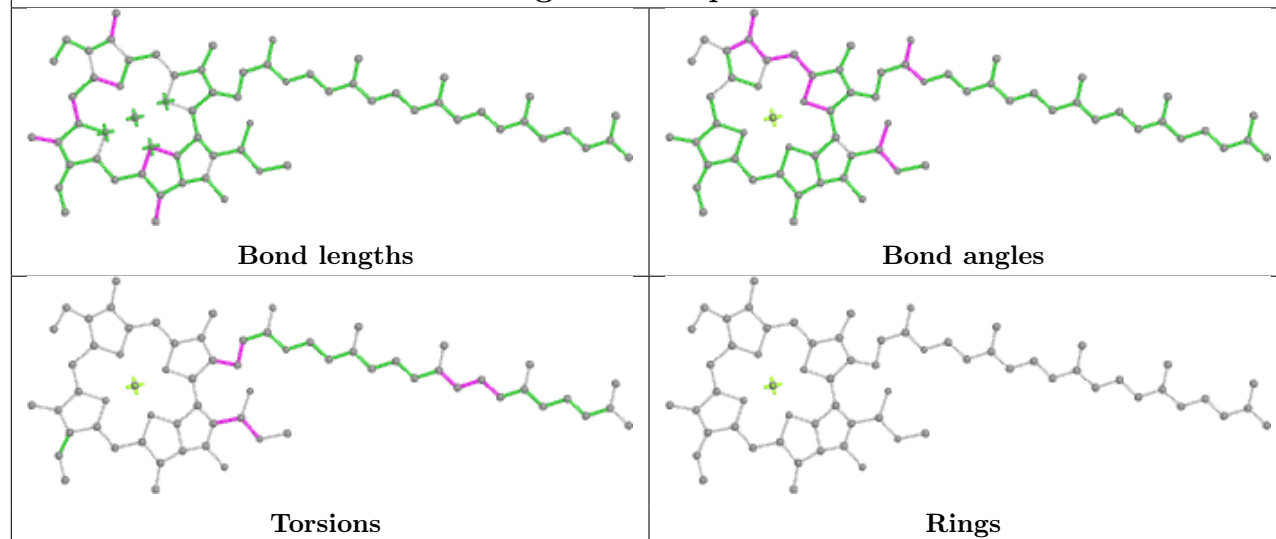


Ligand CLA G 611

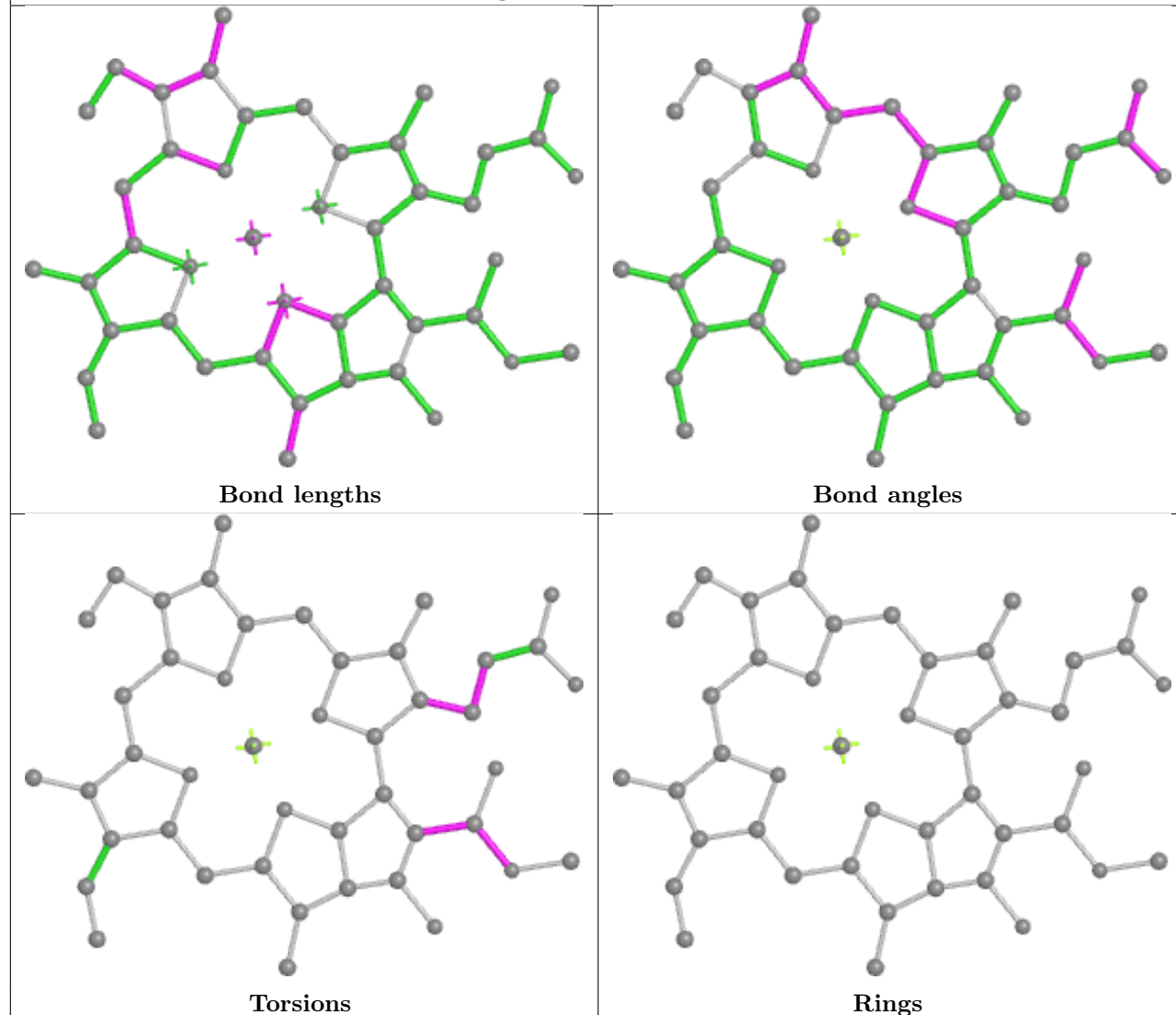


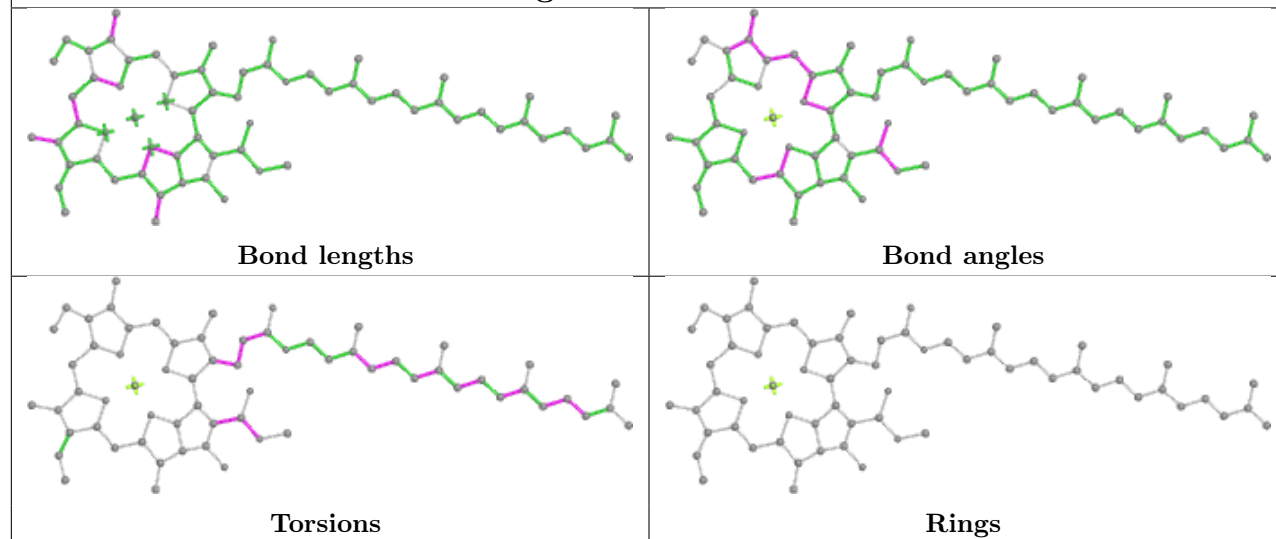
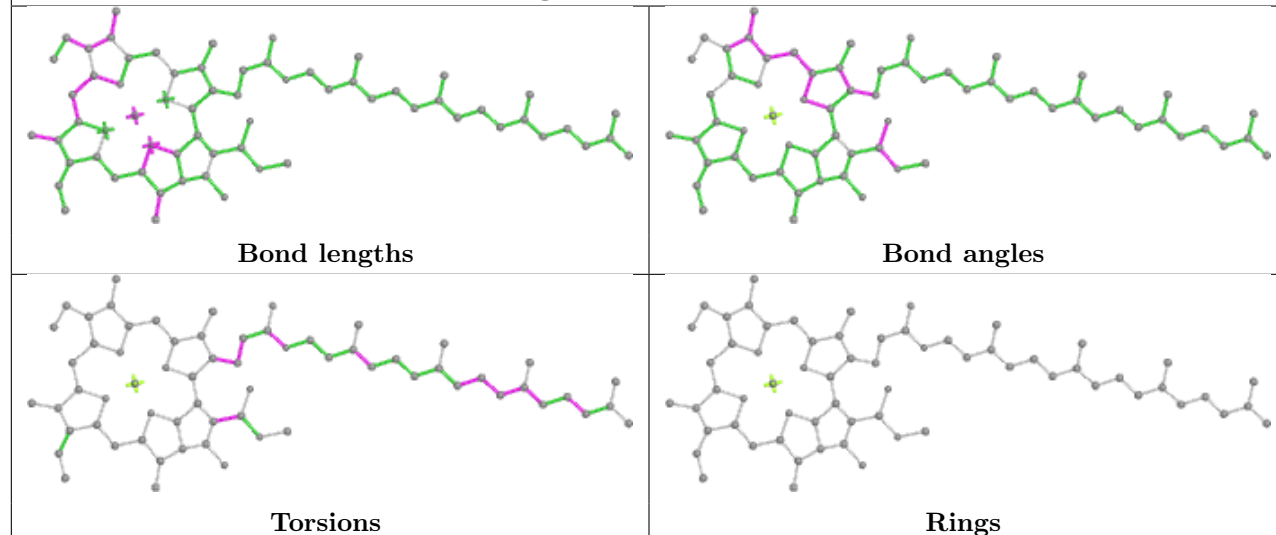
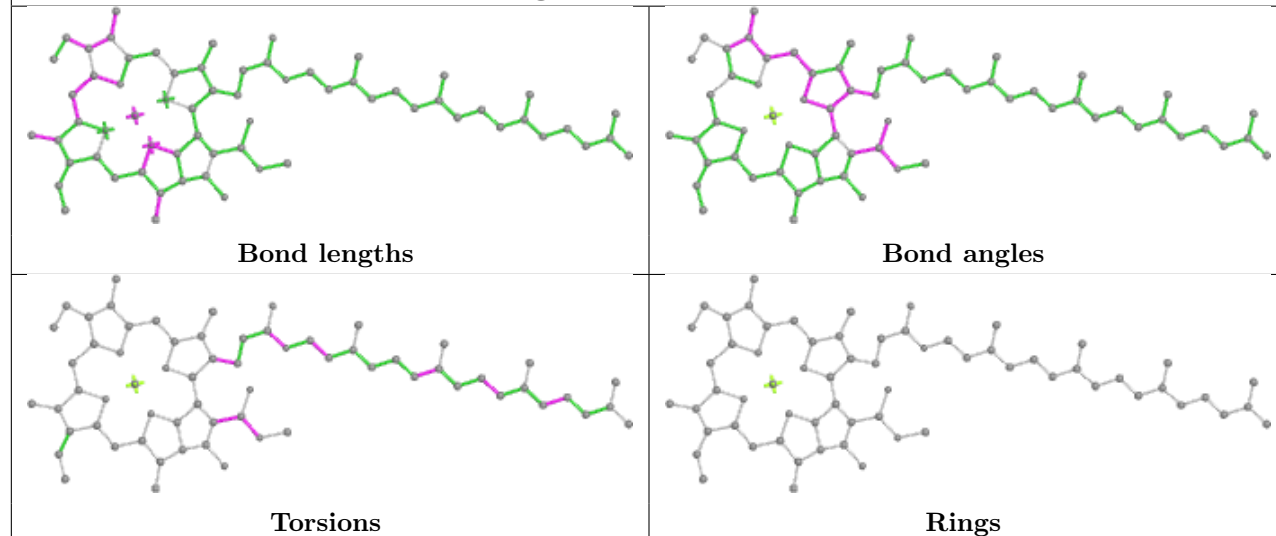


Ligand CLA p 610

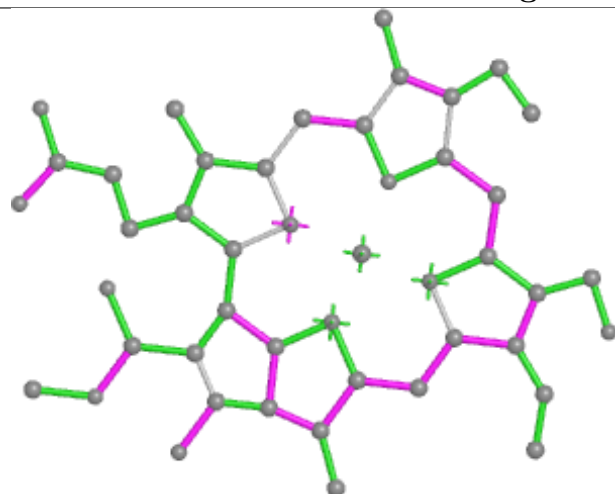


Ligand CLA 2 611

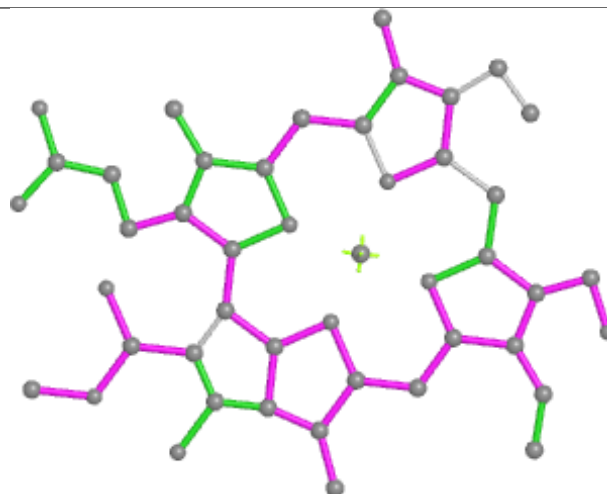


Ligand CLA 5 602**Ligand CLA 7 603****Ligand CLA B 603**

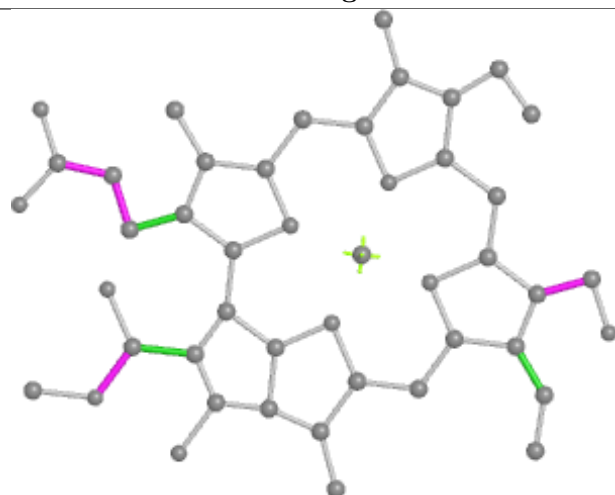
Ligand CHL 0 605



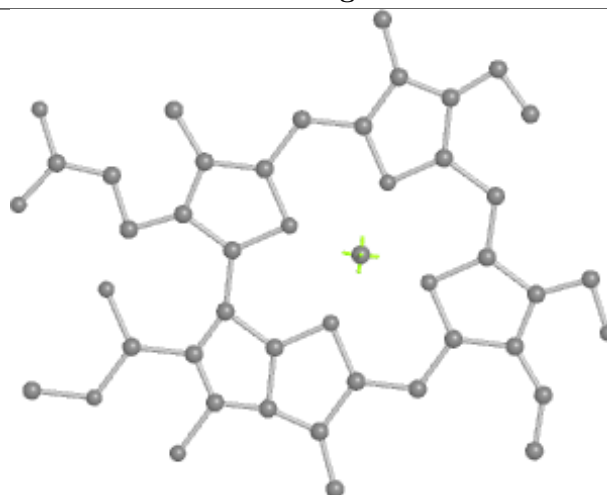
Bond lengths



Bond angles

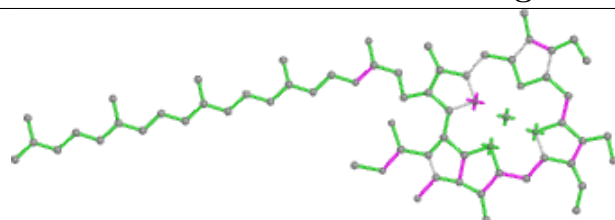


Torsions

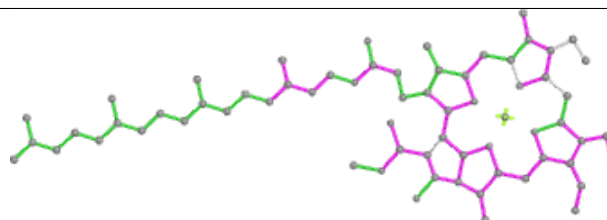


Rings

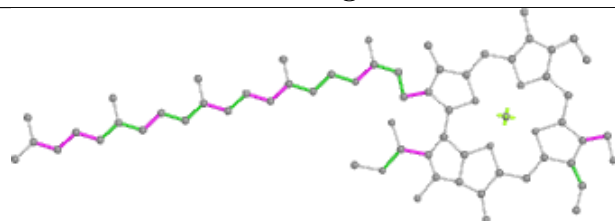
Ligand CHL G 601



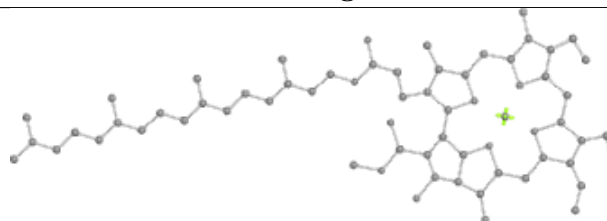
Bond lengths



Bond angles

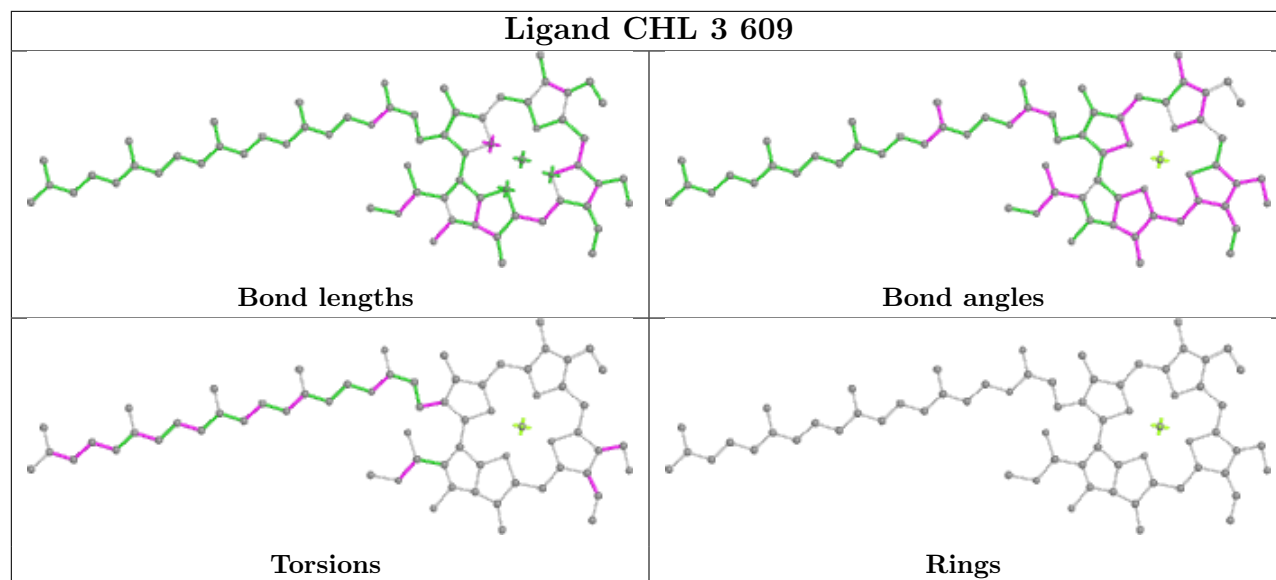


Torsions

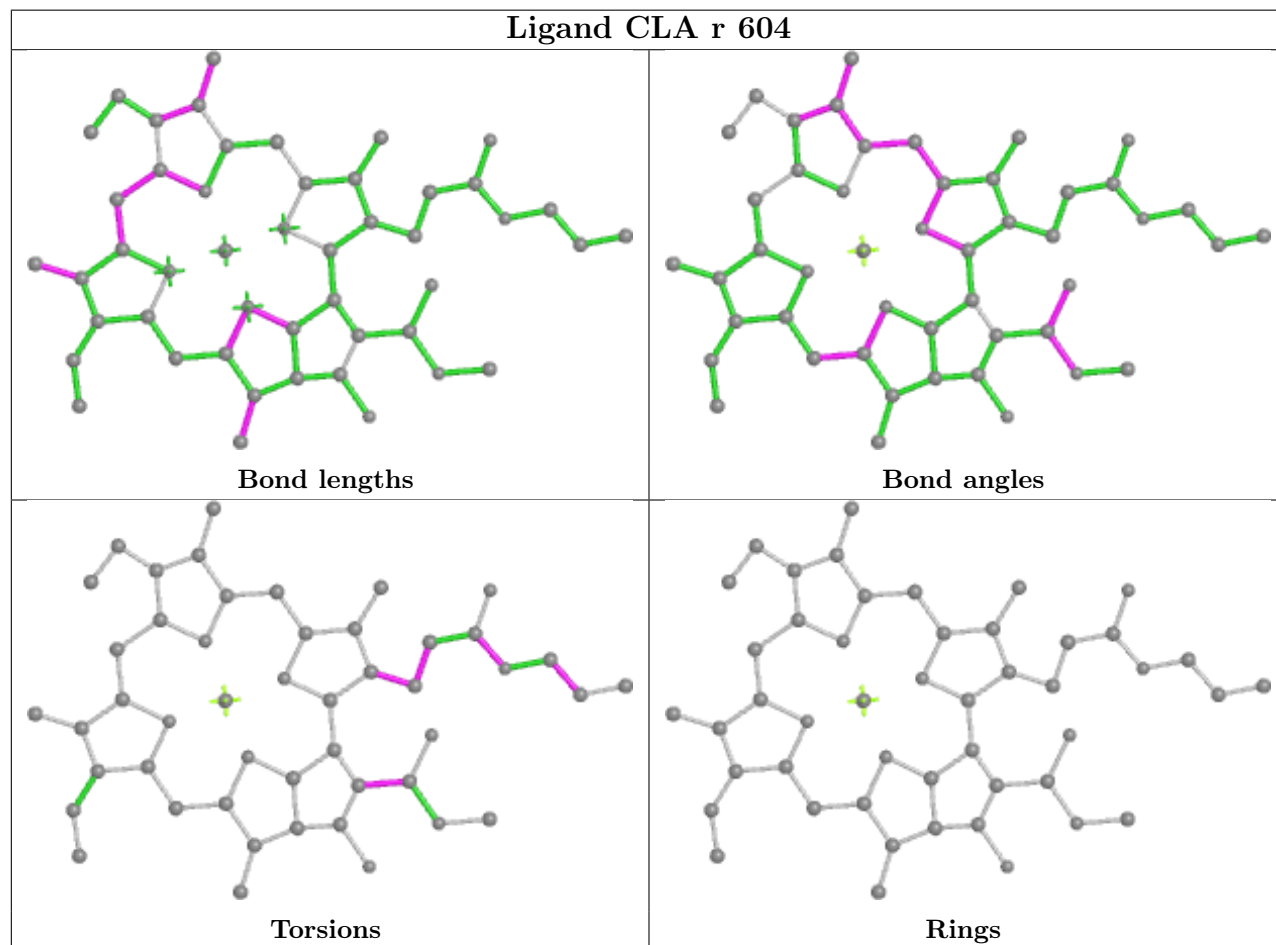


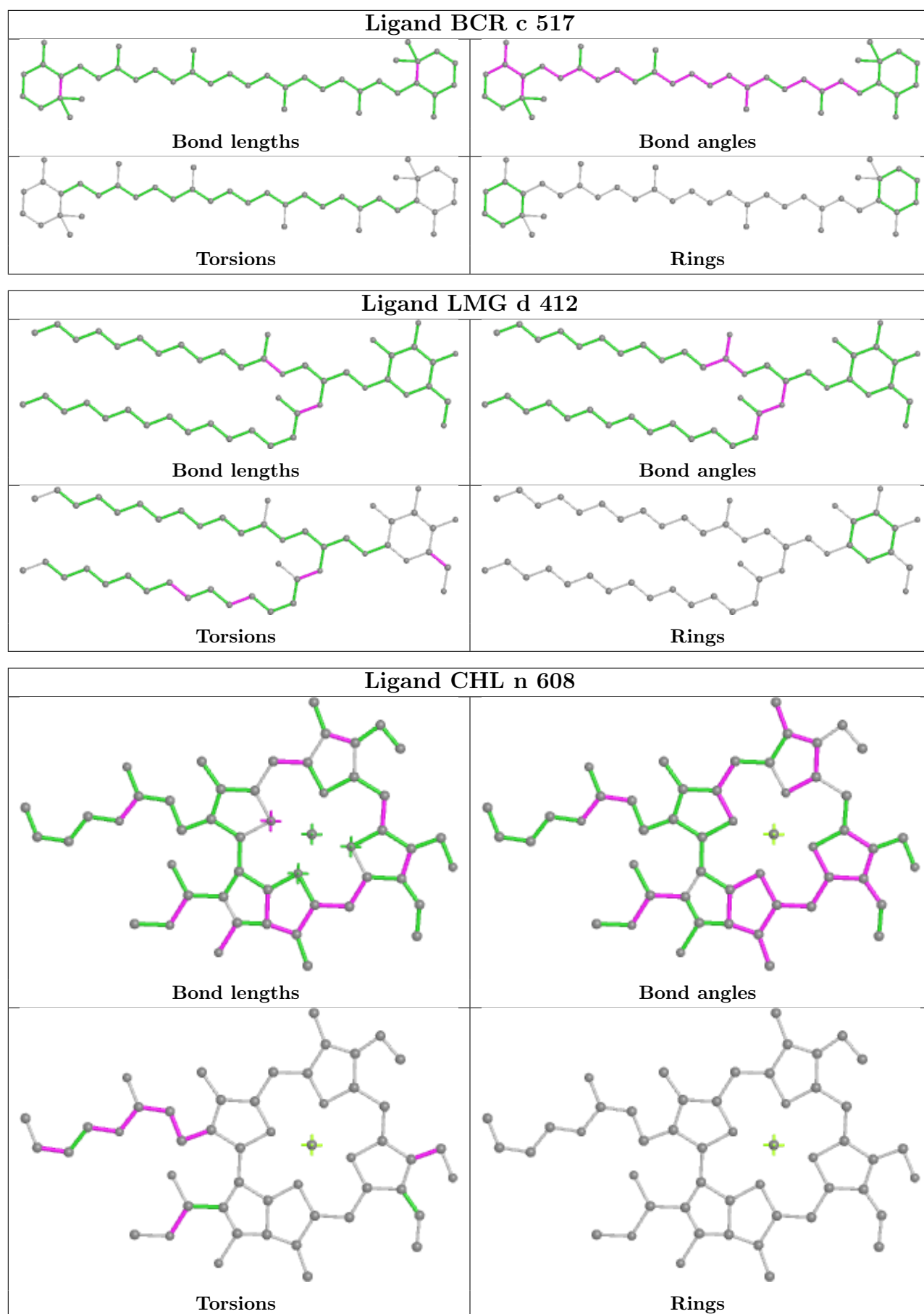
Rings

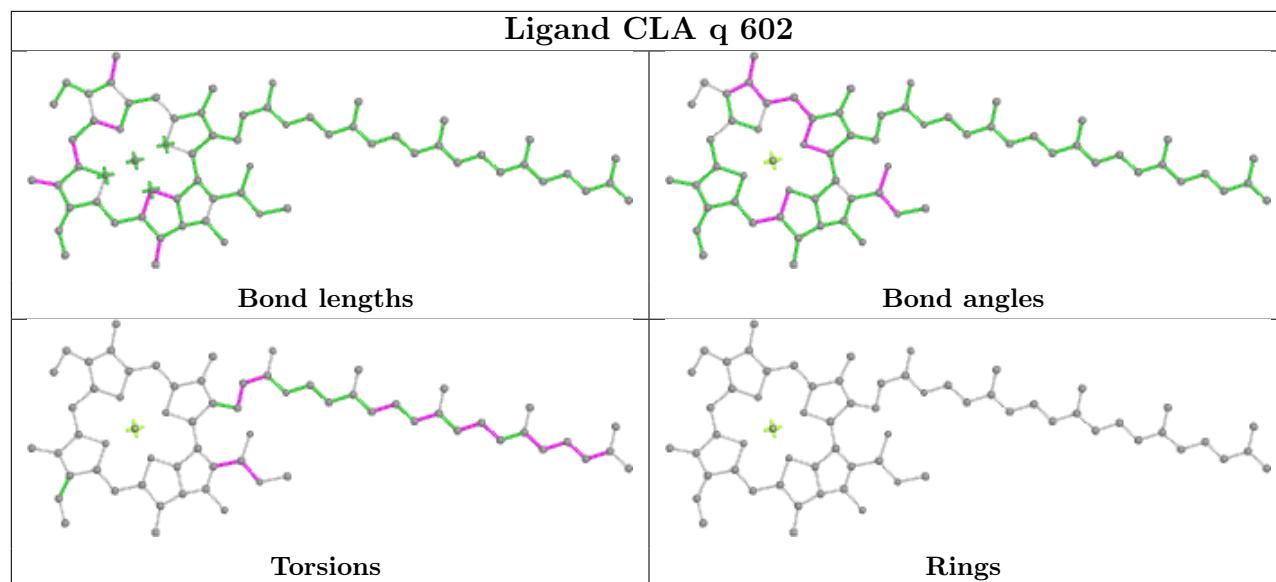
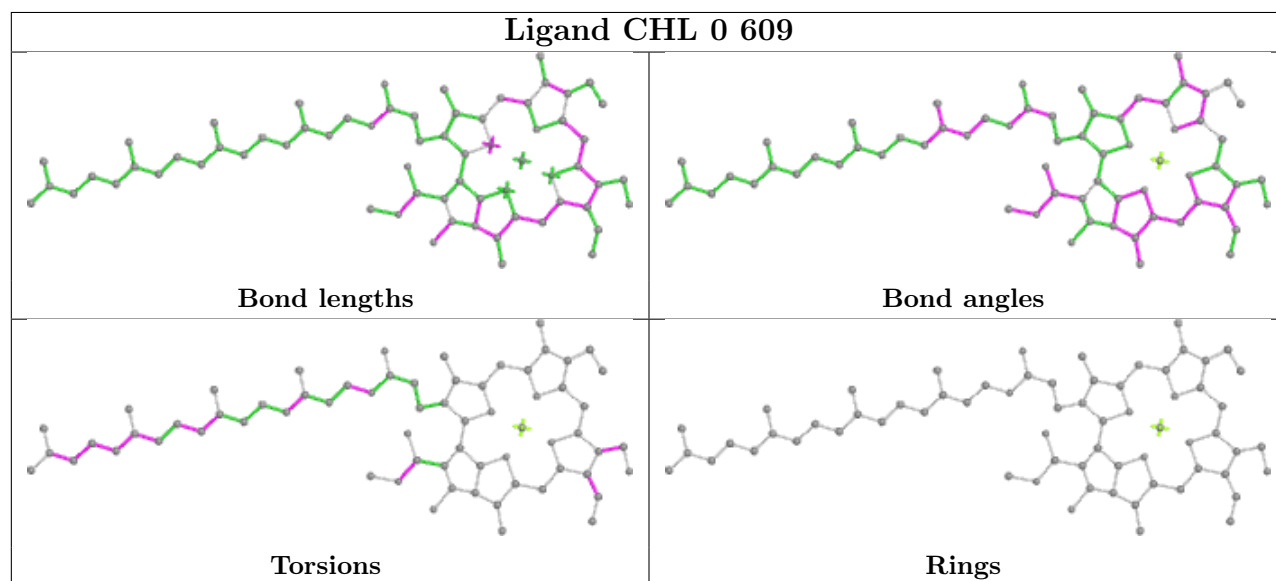
Ligand CHL 3 609



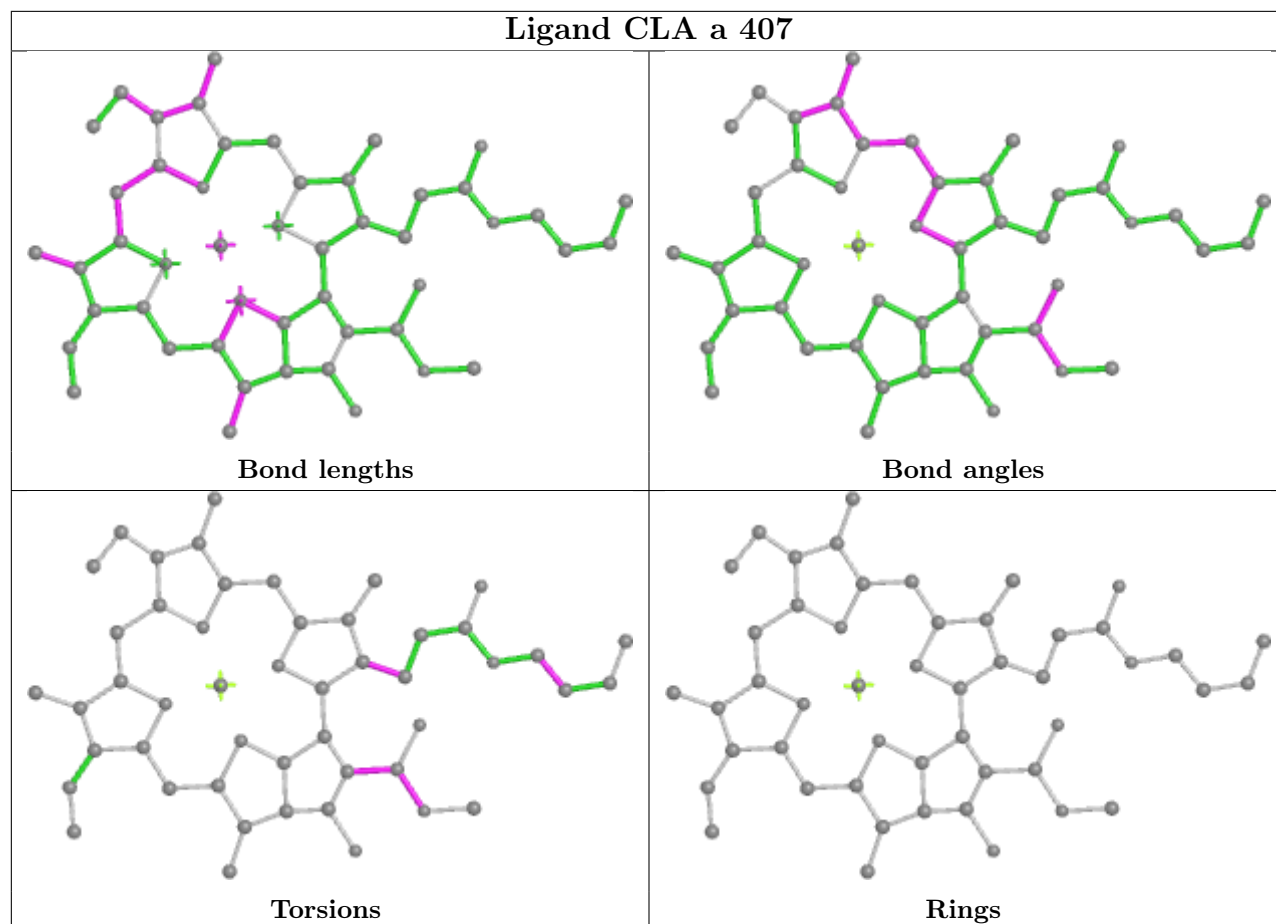
Ligand CLA r 604

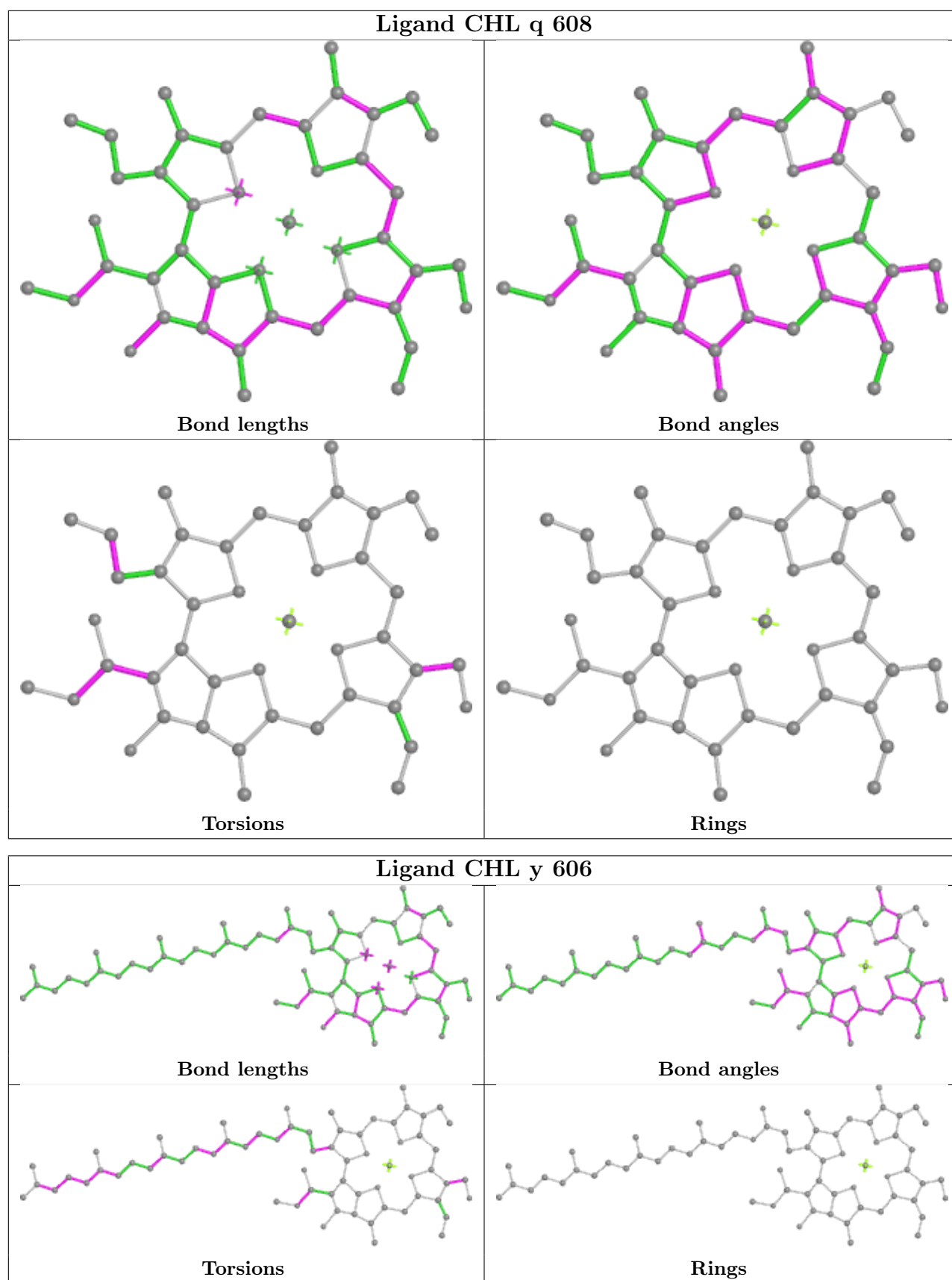


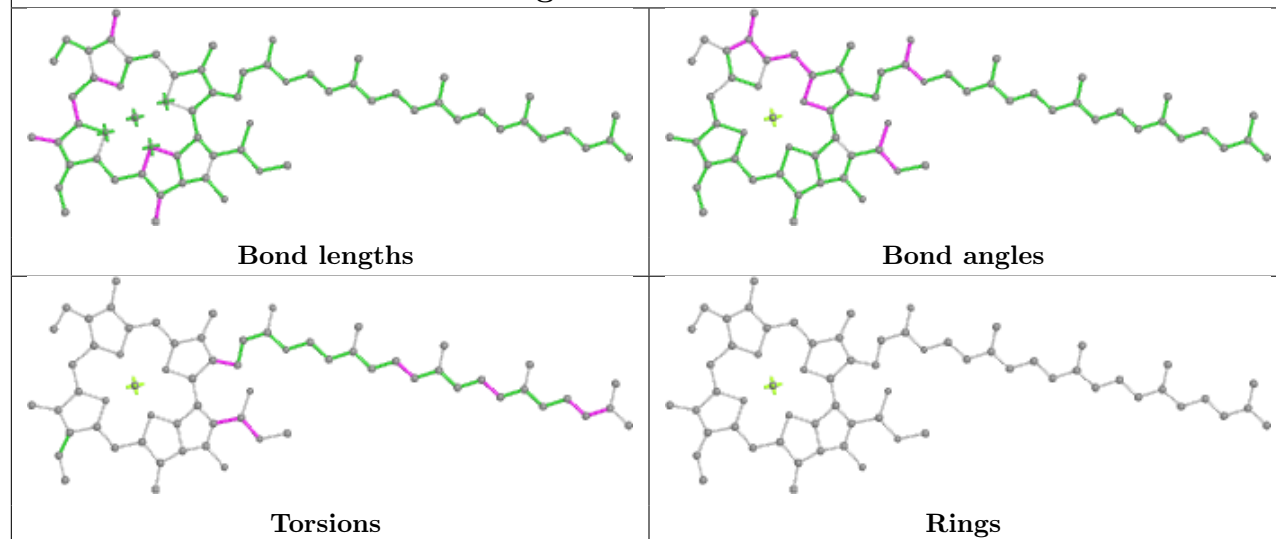
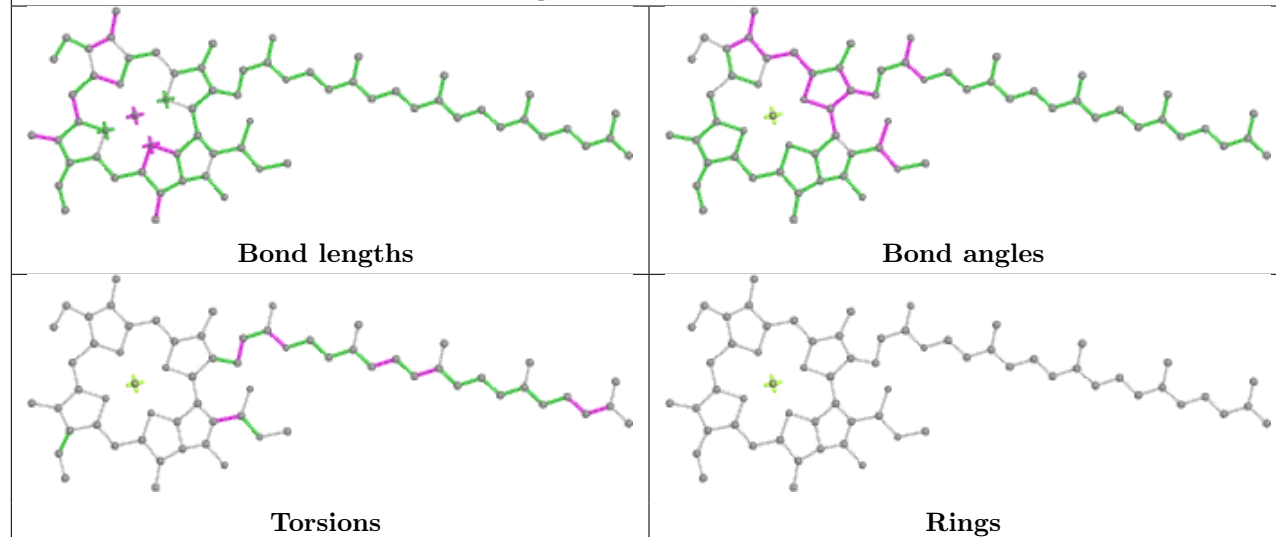


Ligand CLA q 602**Ligand CHL 0 609**

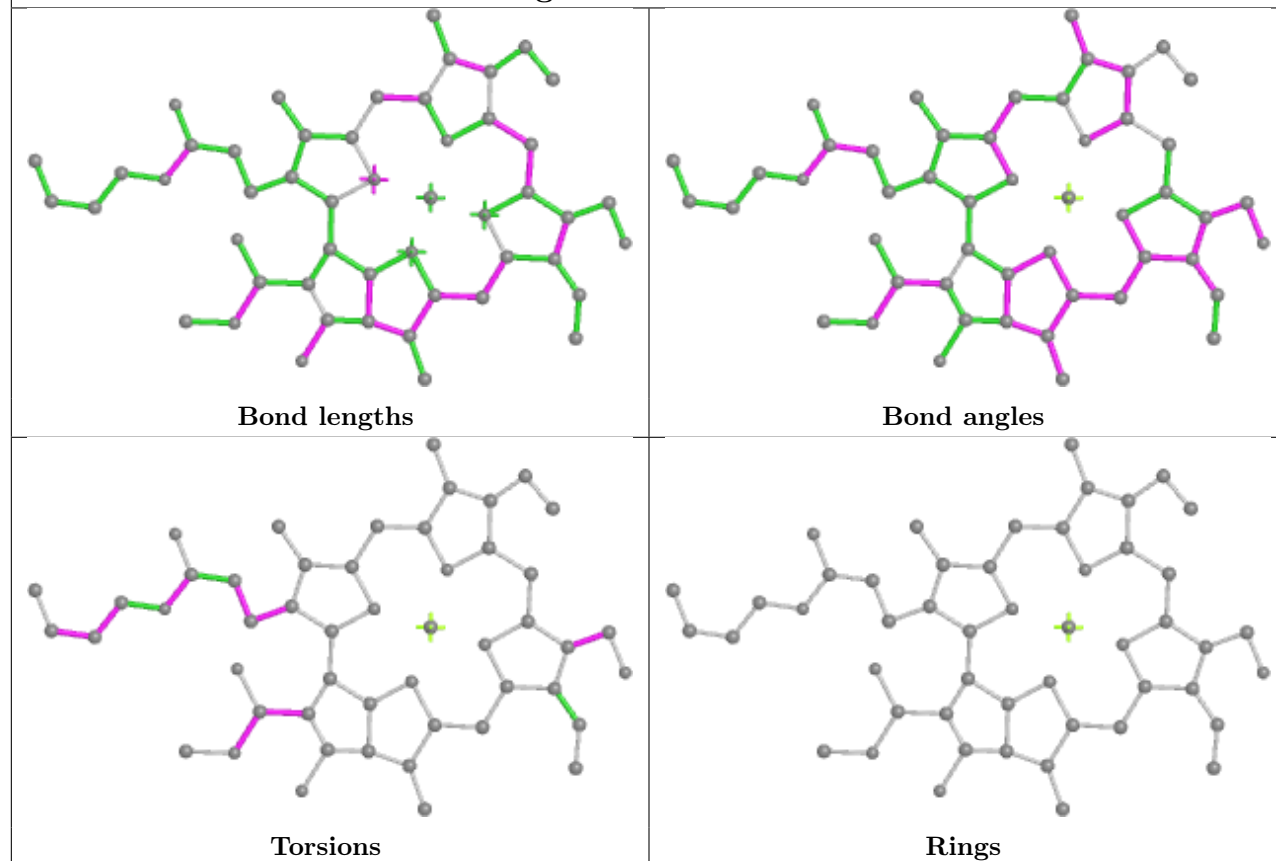
Ligand CLA a 407



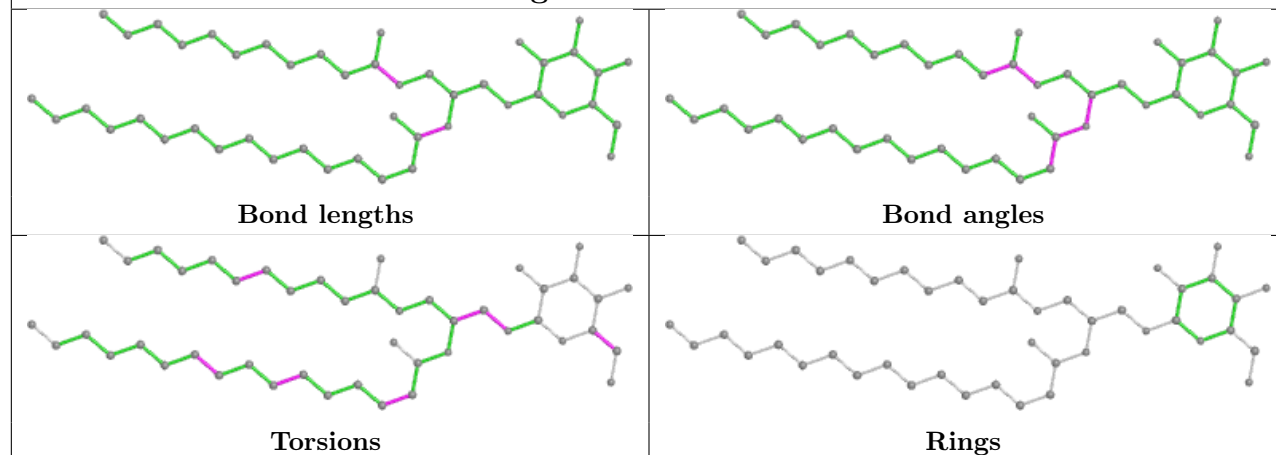


Ligand CLA 8 610**Ligand CLA B 617**

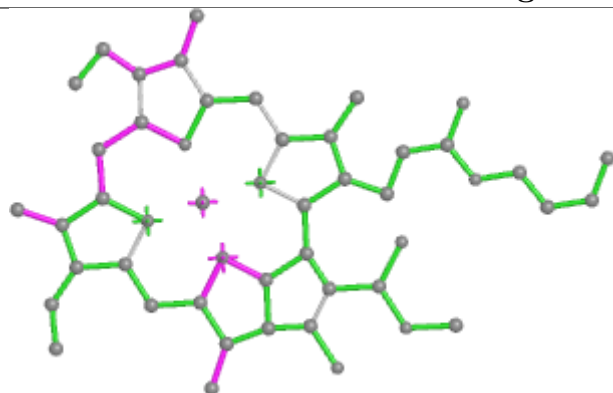
Ligand CHL 7 608



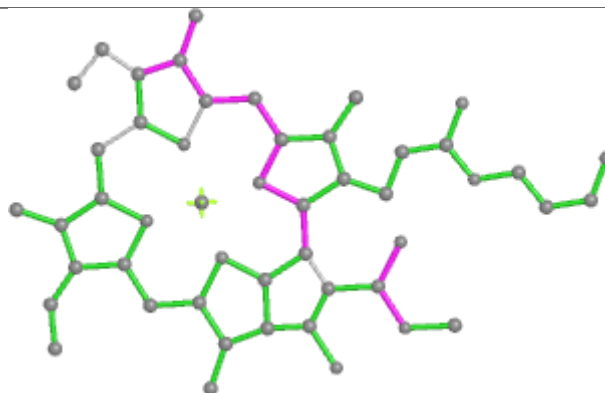
Ligand LMG d 411



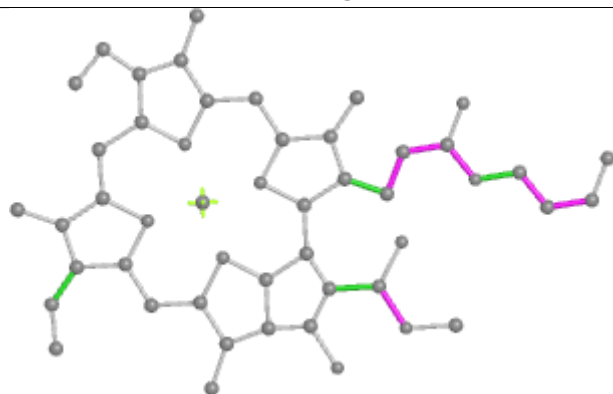
Ligand CLA S 613



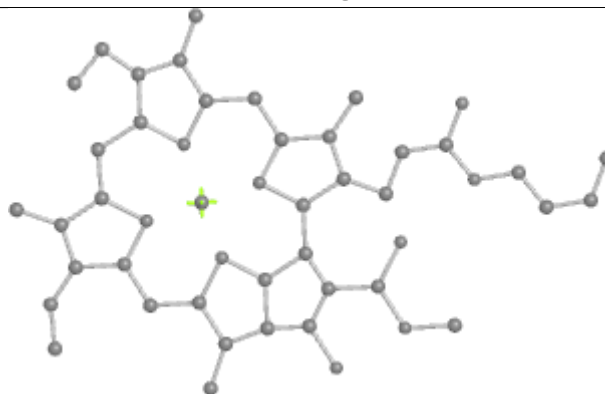
Bond lengths



Bond angles

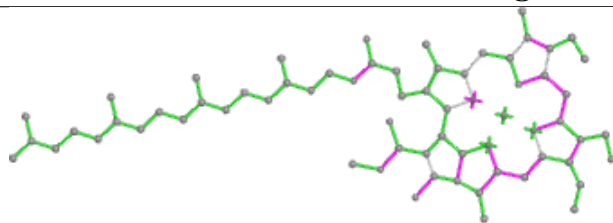


Torsions

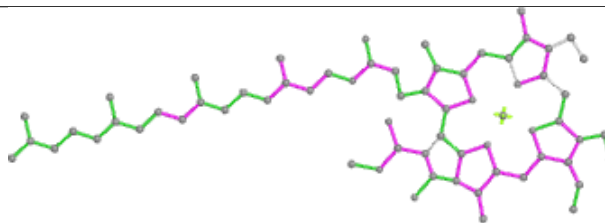


Rings

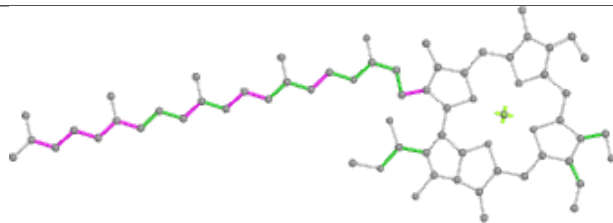
Ligand CHL Y 601



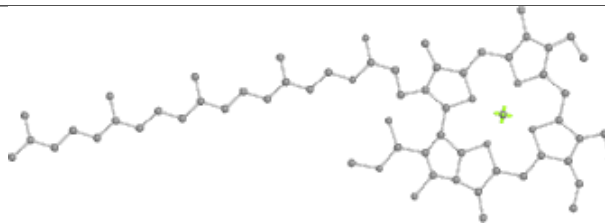
Bond lengths



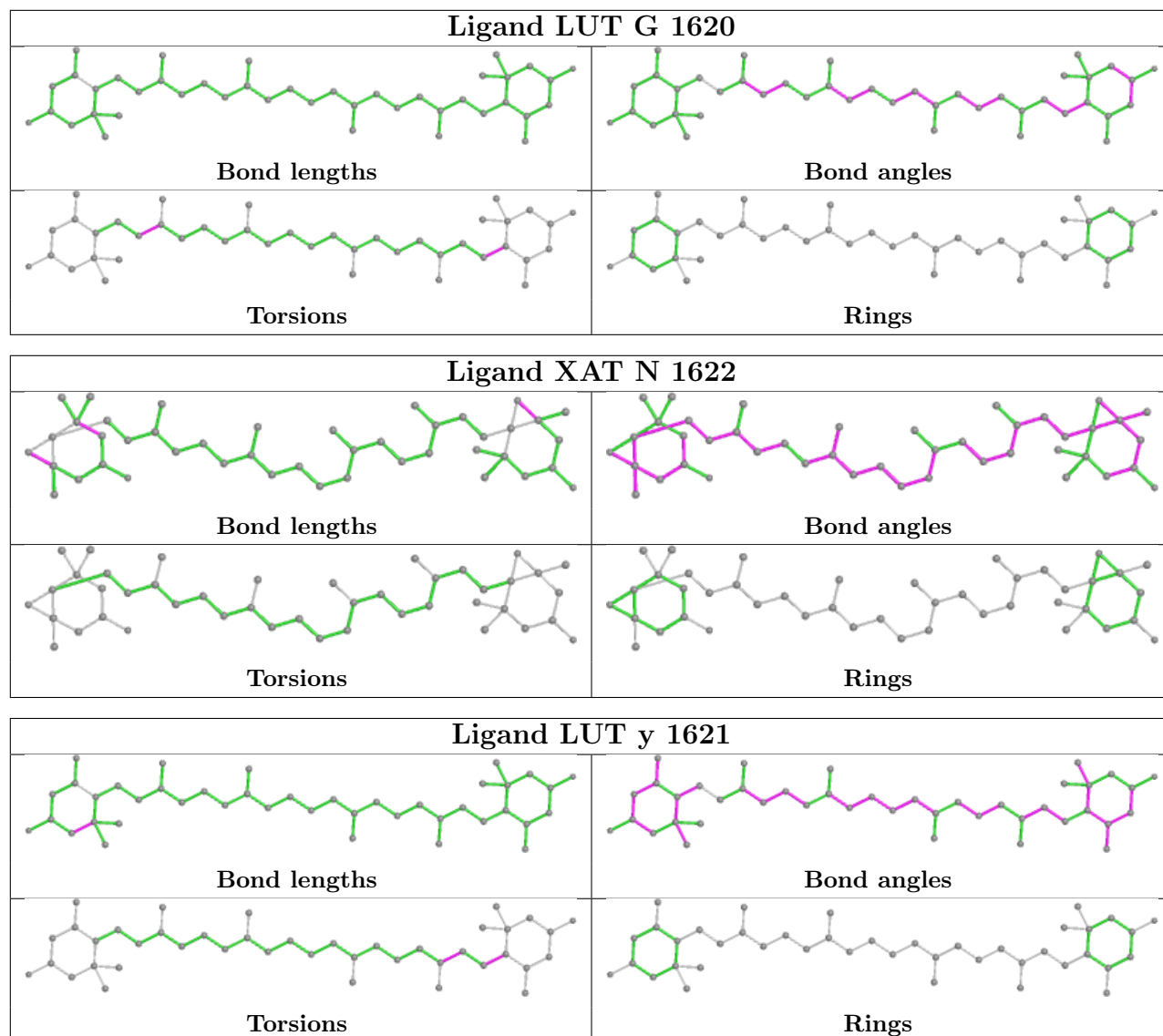
Bond angles

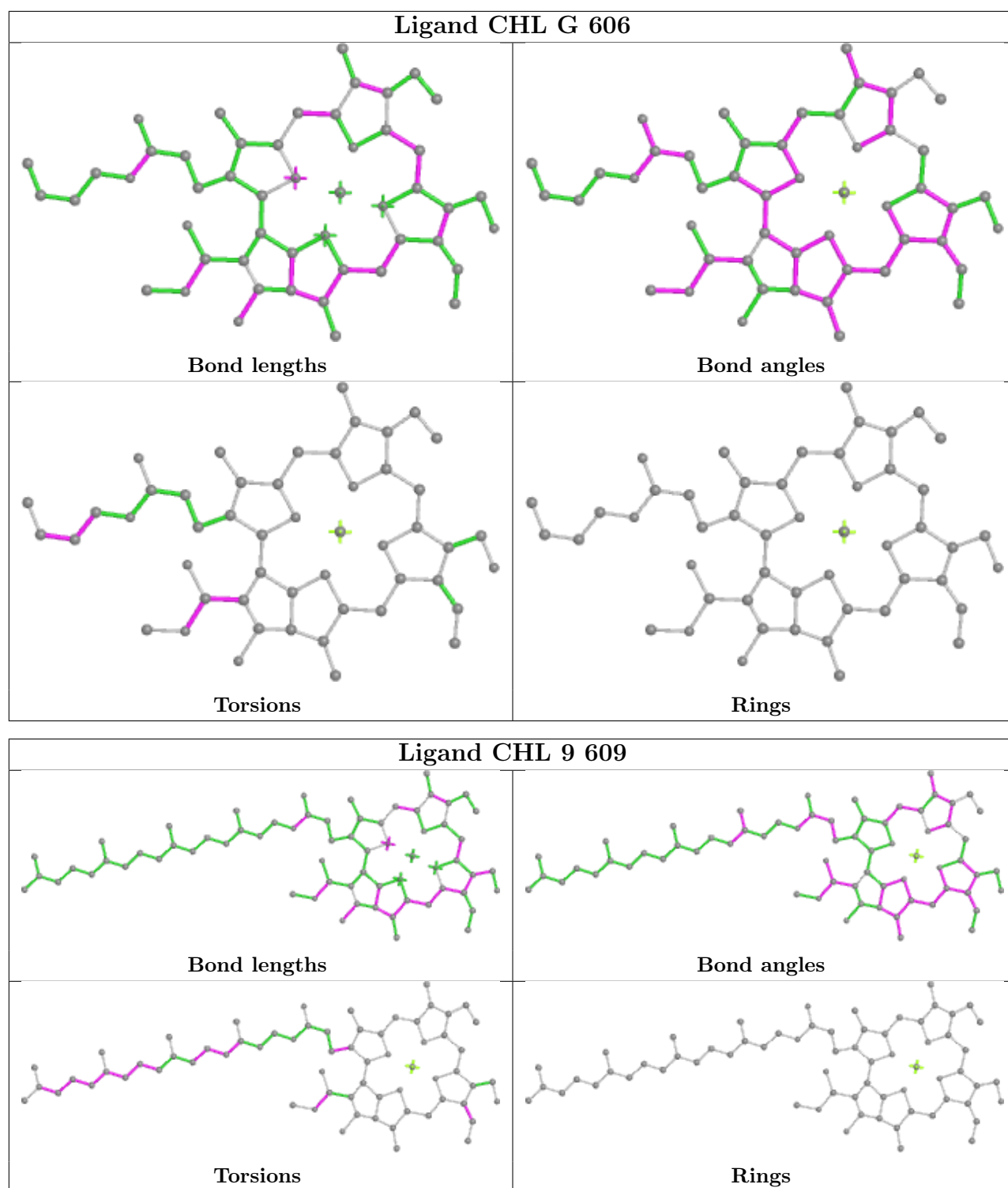


Torsions

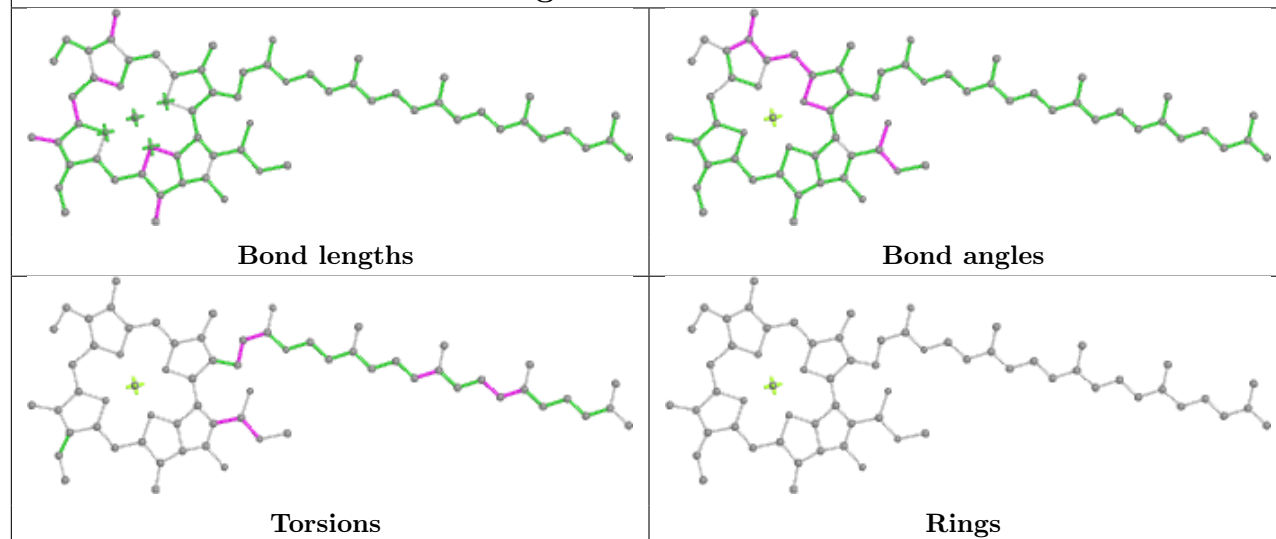


Rings

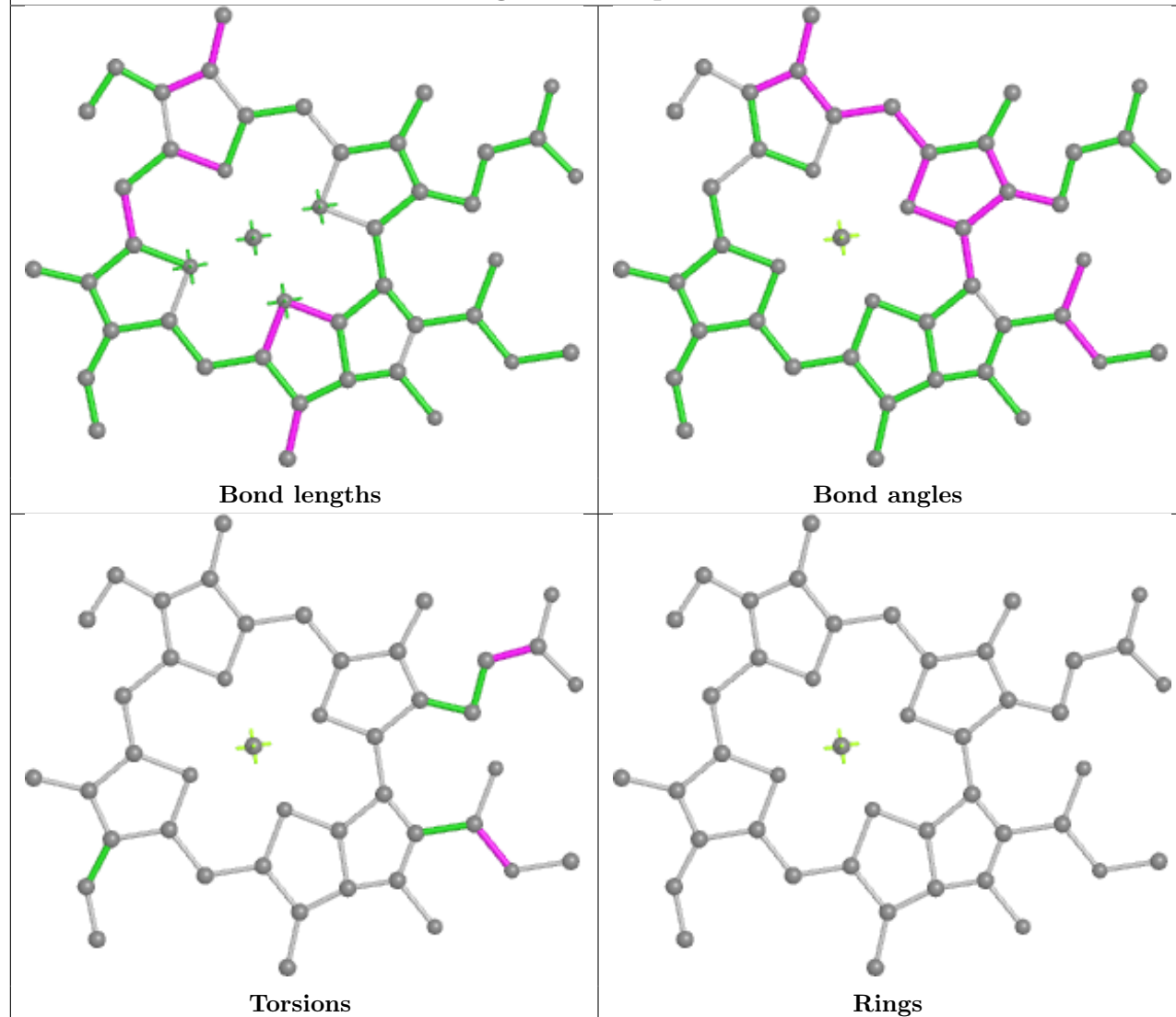


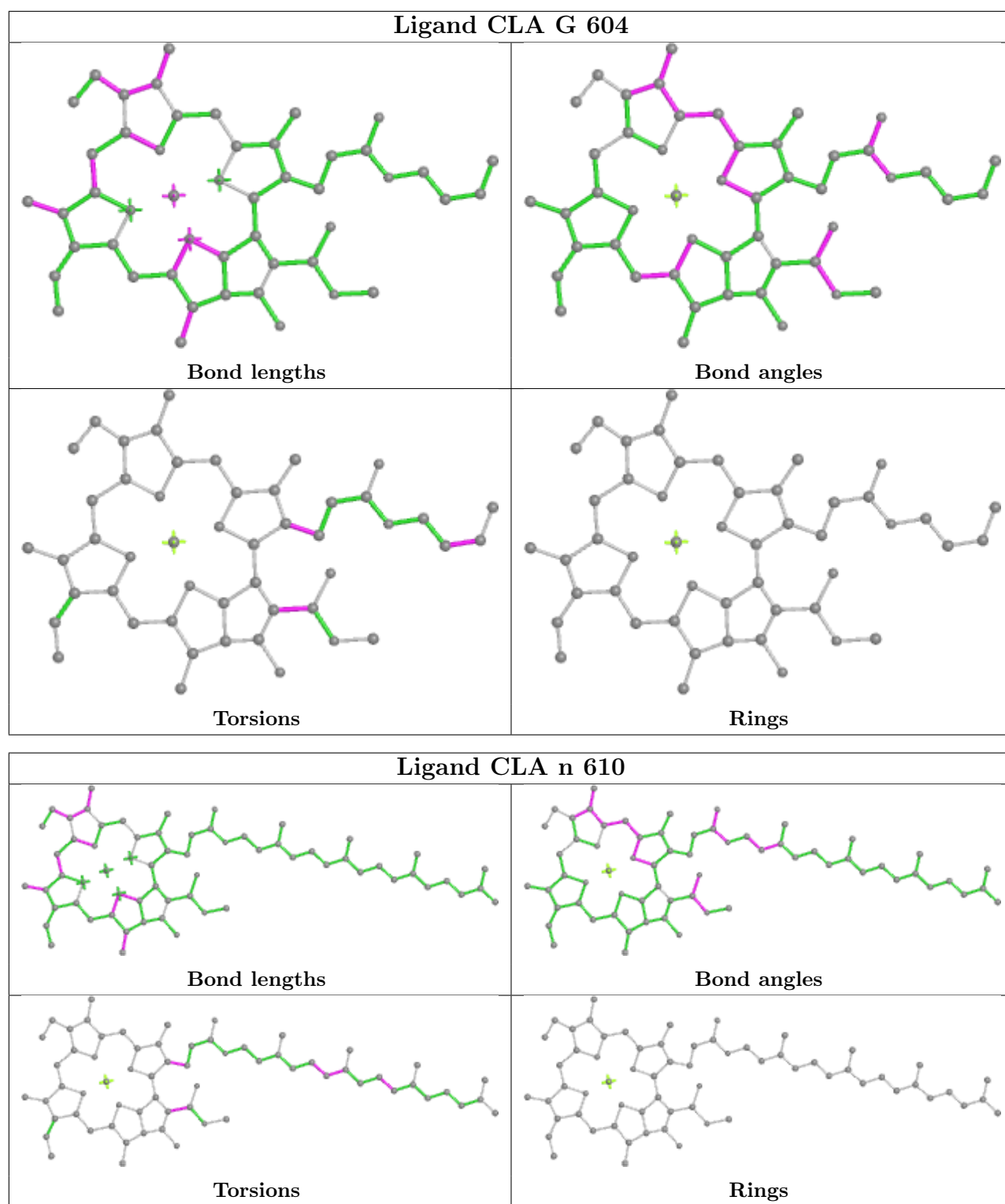


Ligand CLA 8 602

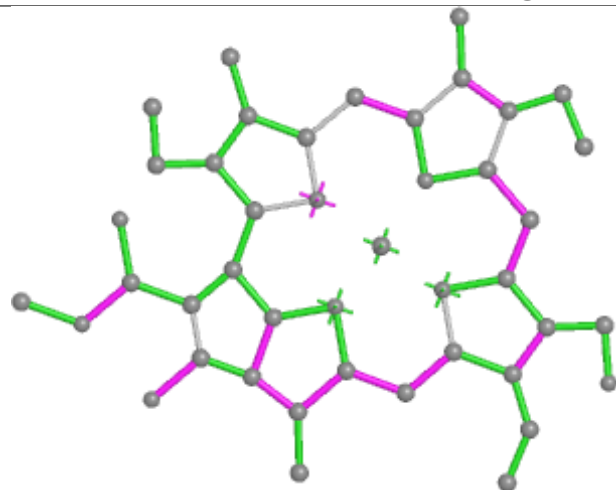


Ligand CLA p 612

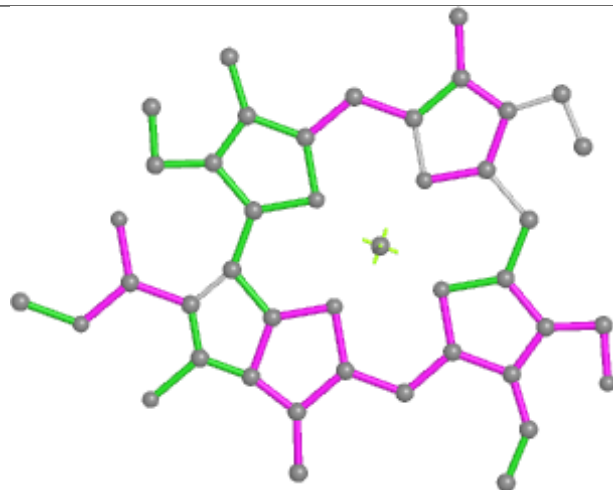




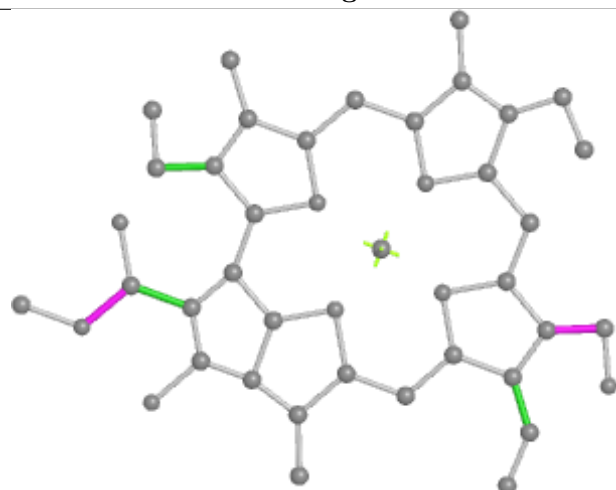
Ligand CHL S 607



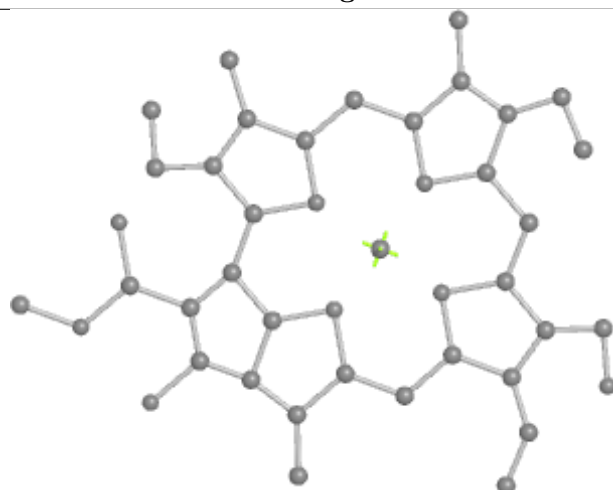
Bond lengths



Bond angles

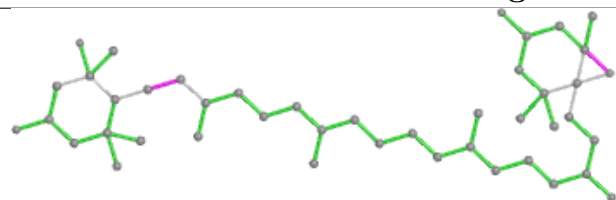


Torsions

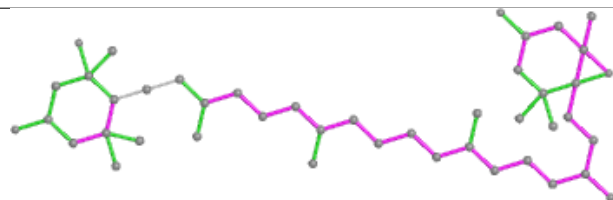


Rings

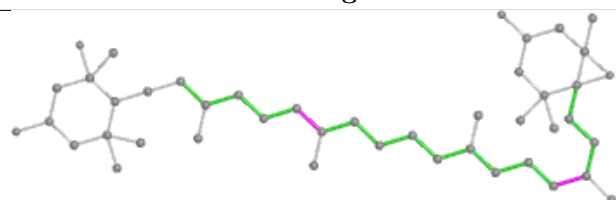
Ligand NEX S 1623



Bond lengths



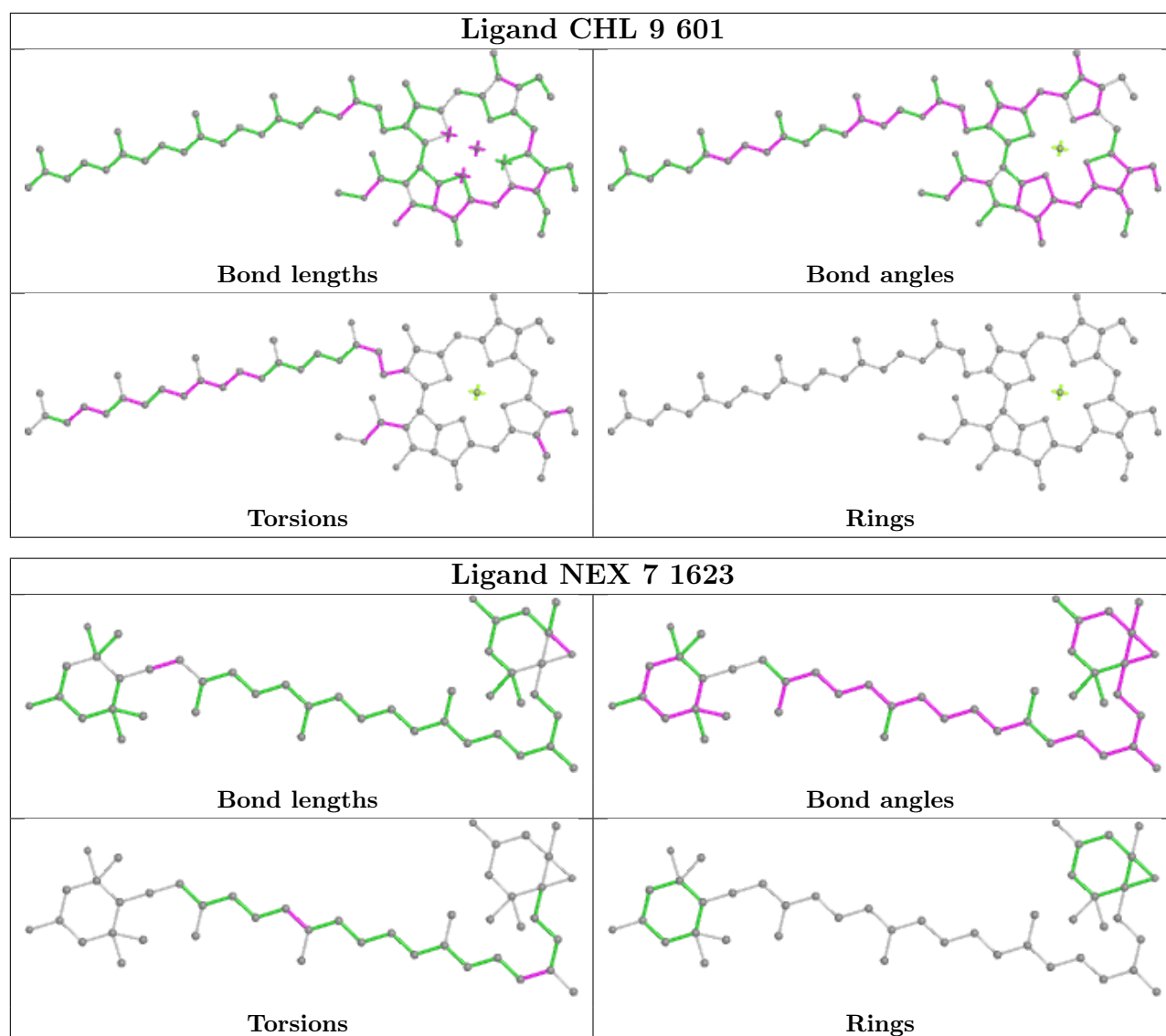
Bond angles



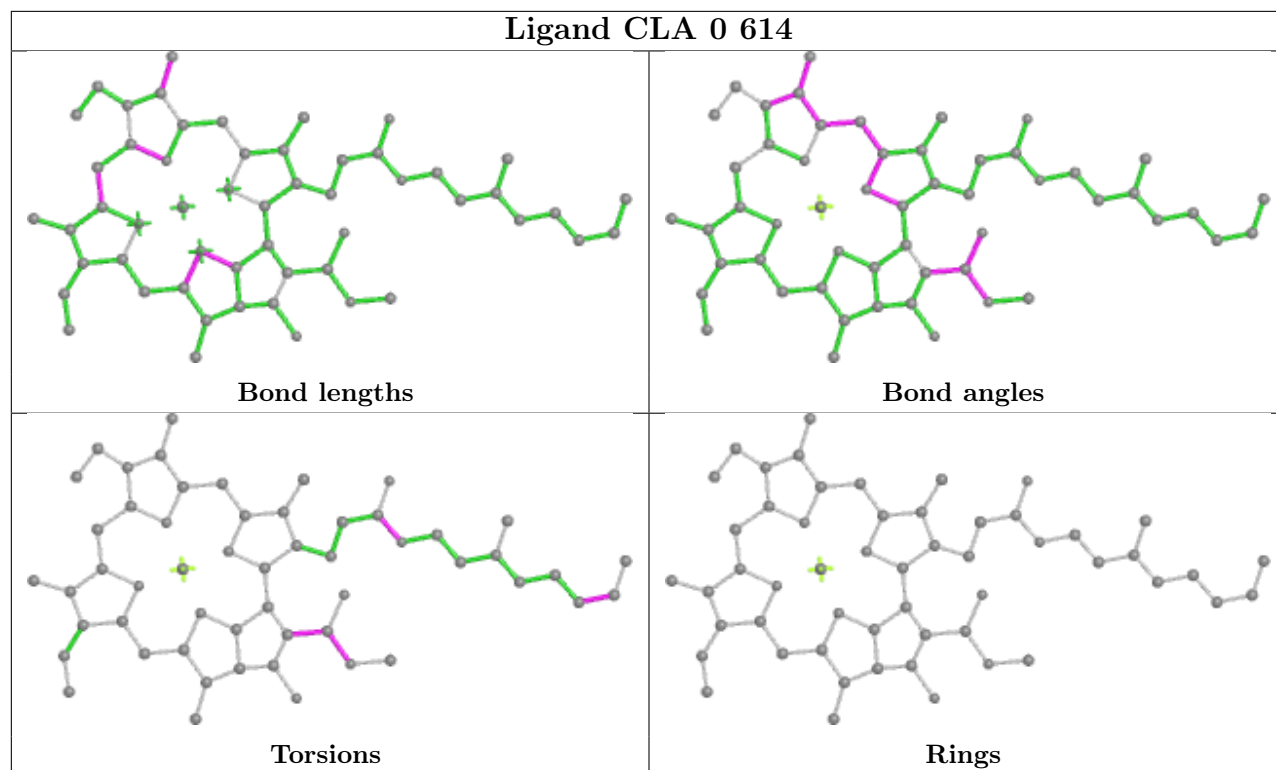
Torsions



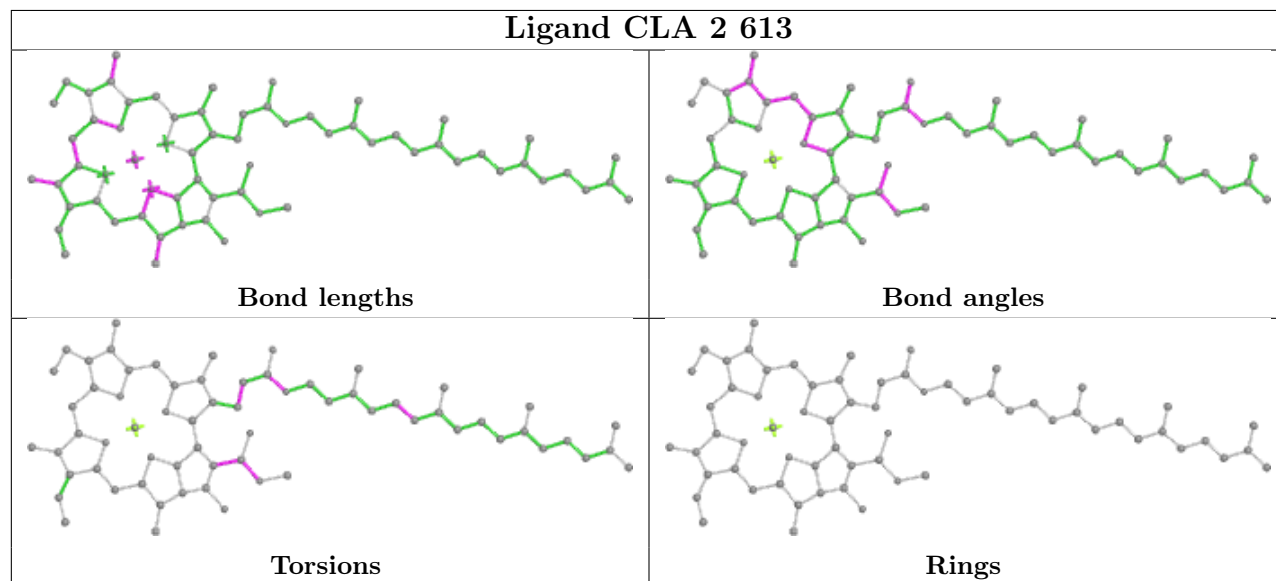
Rings

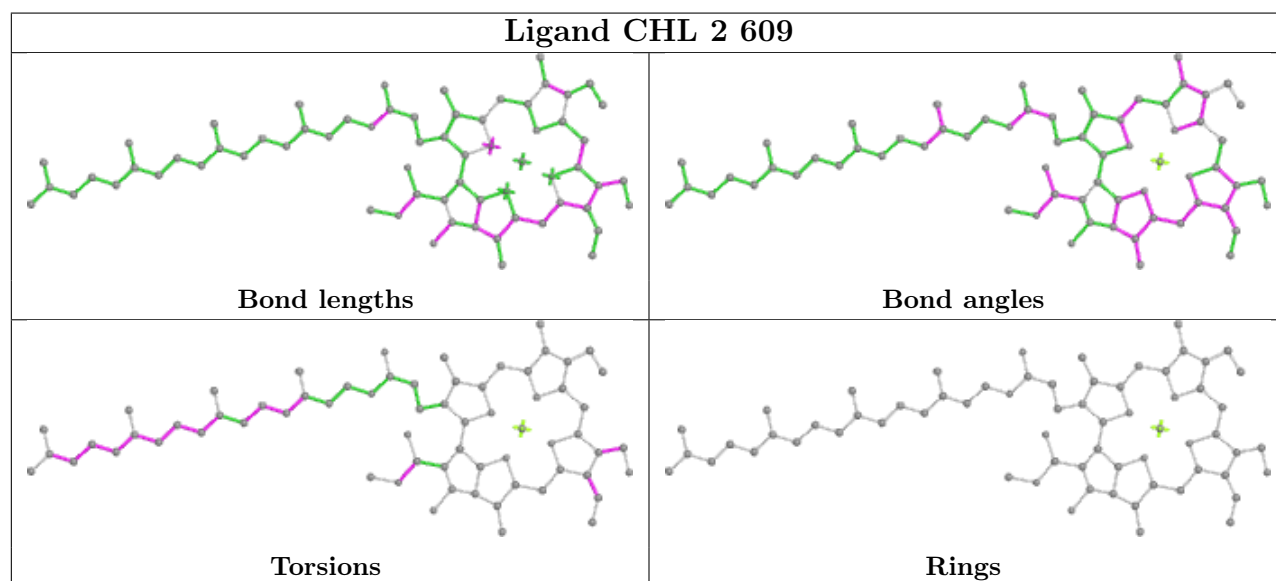
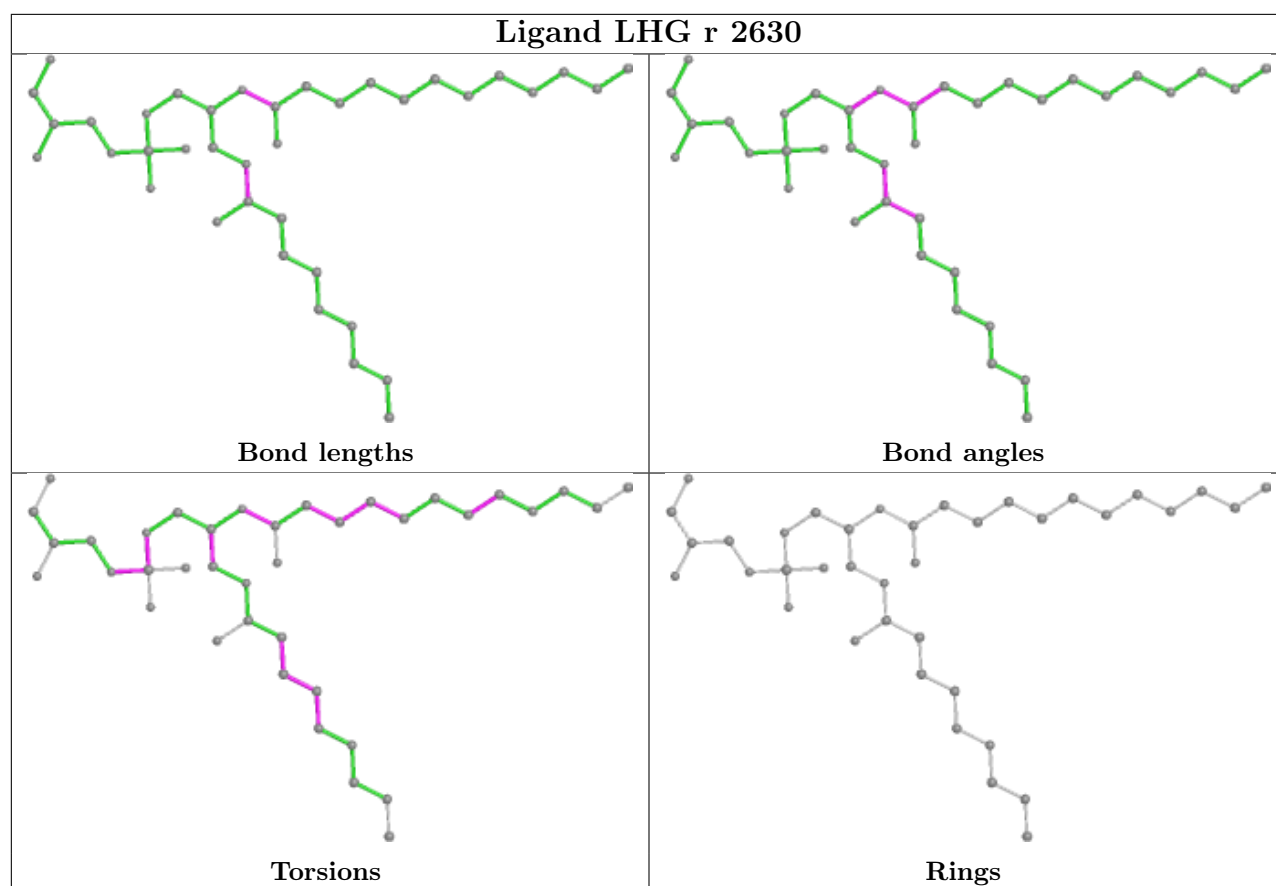


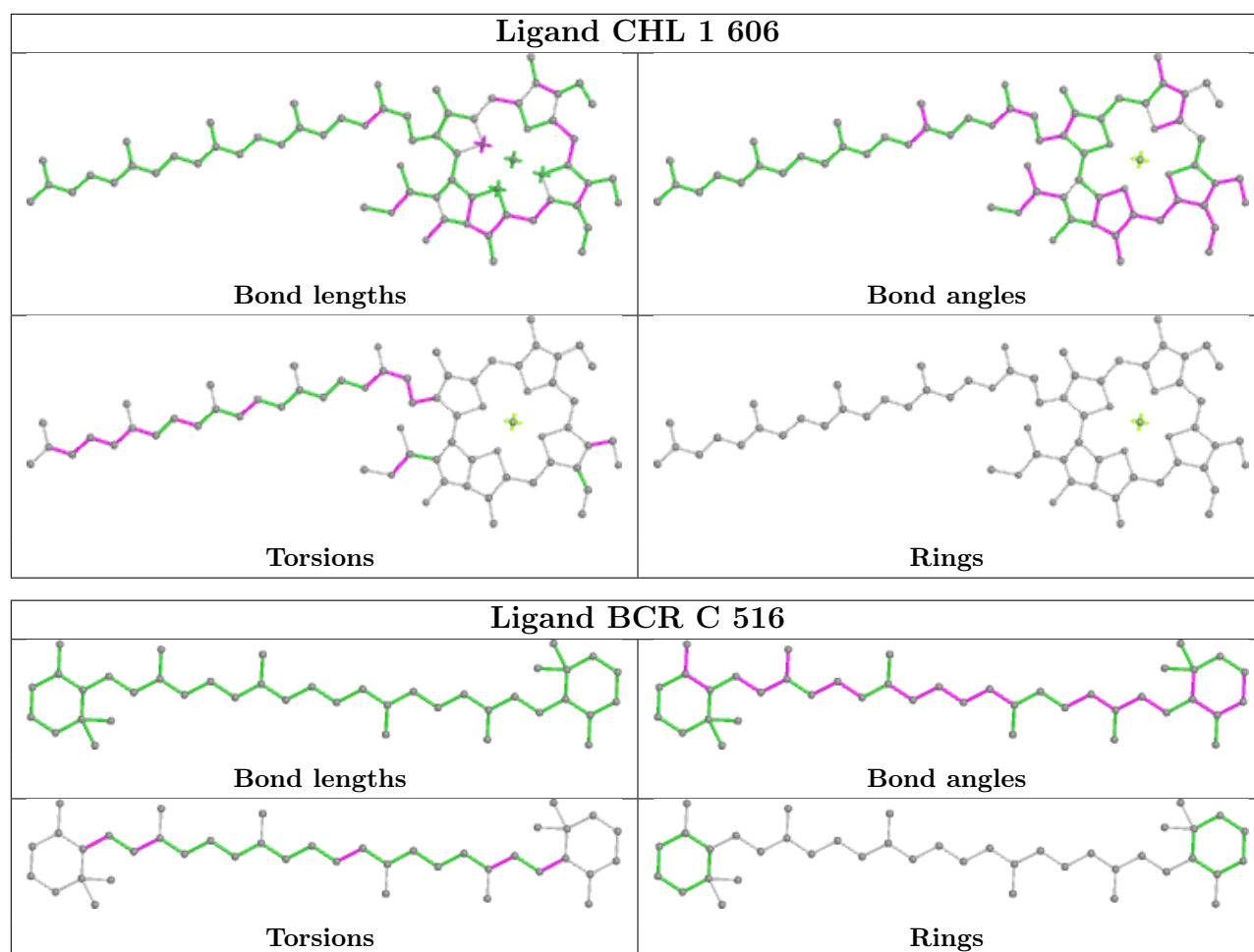
Ligand CLA 0 614

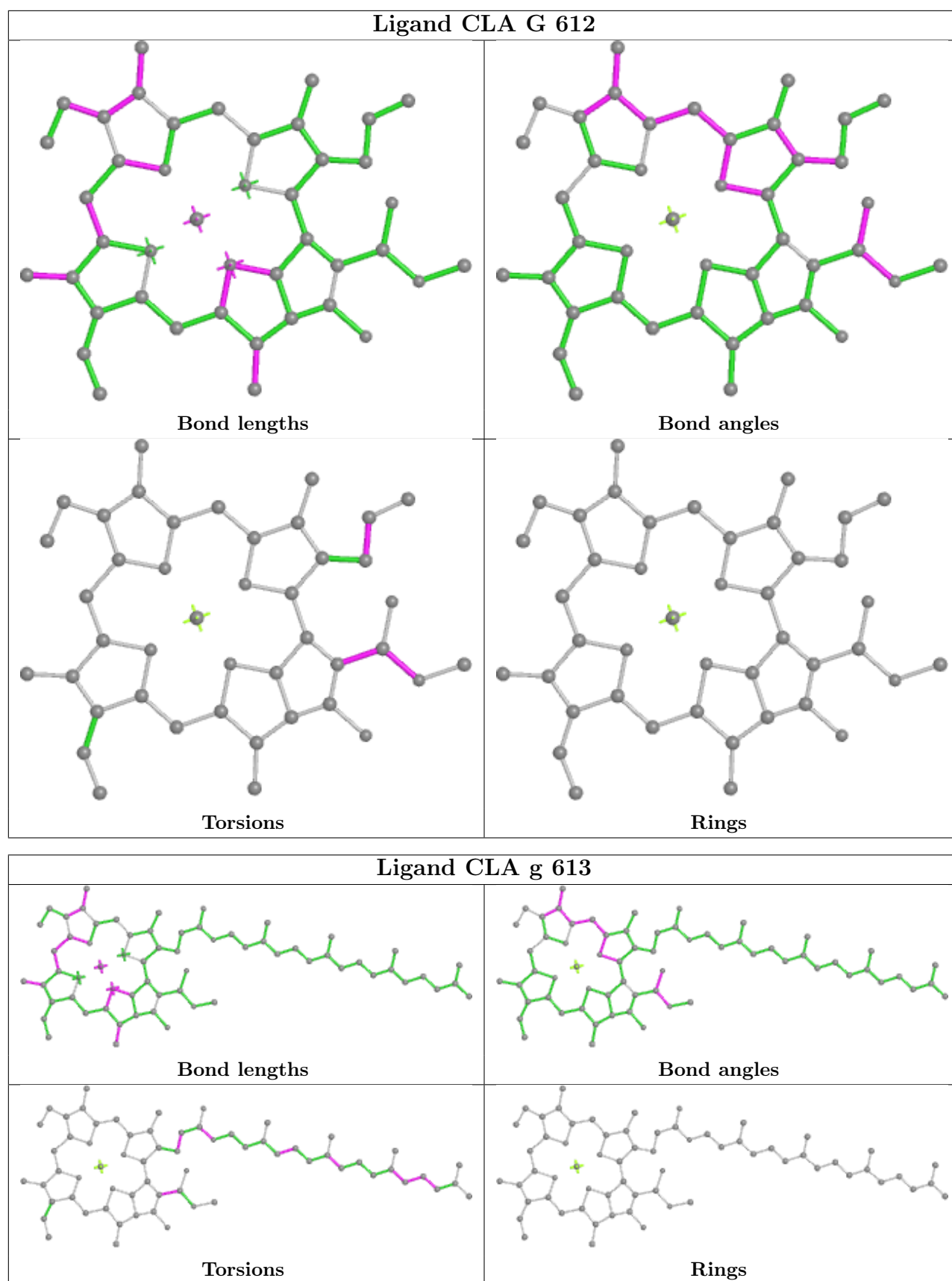


Ligand CLA 2 613

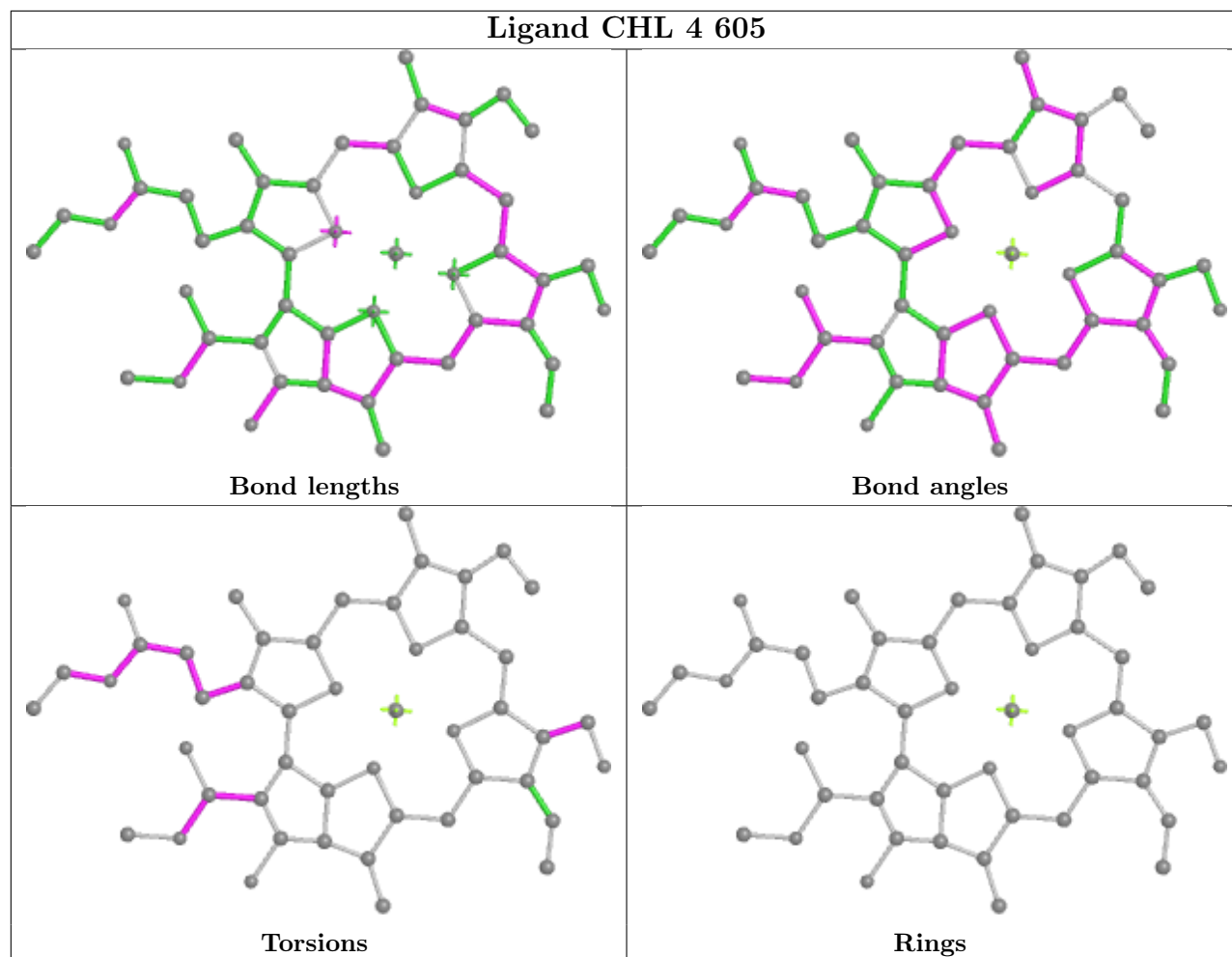




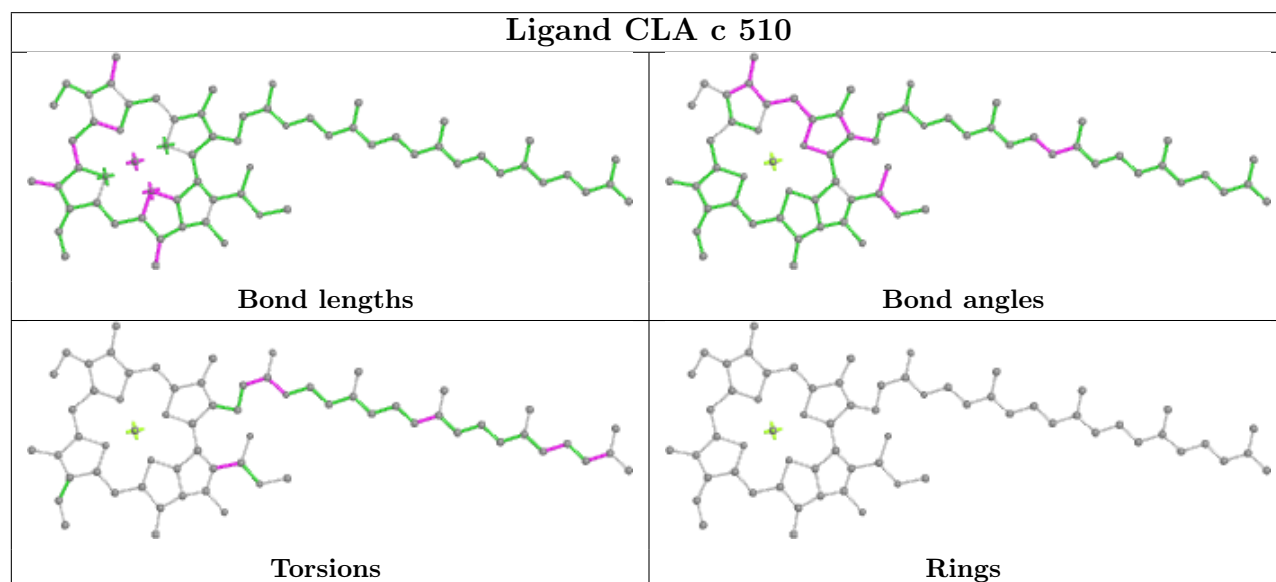


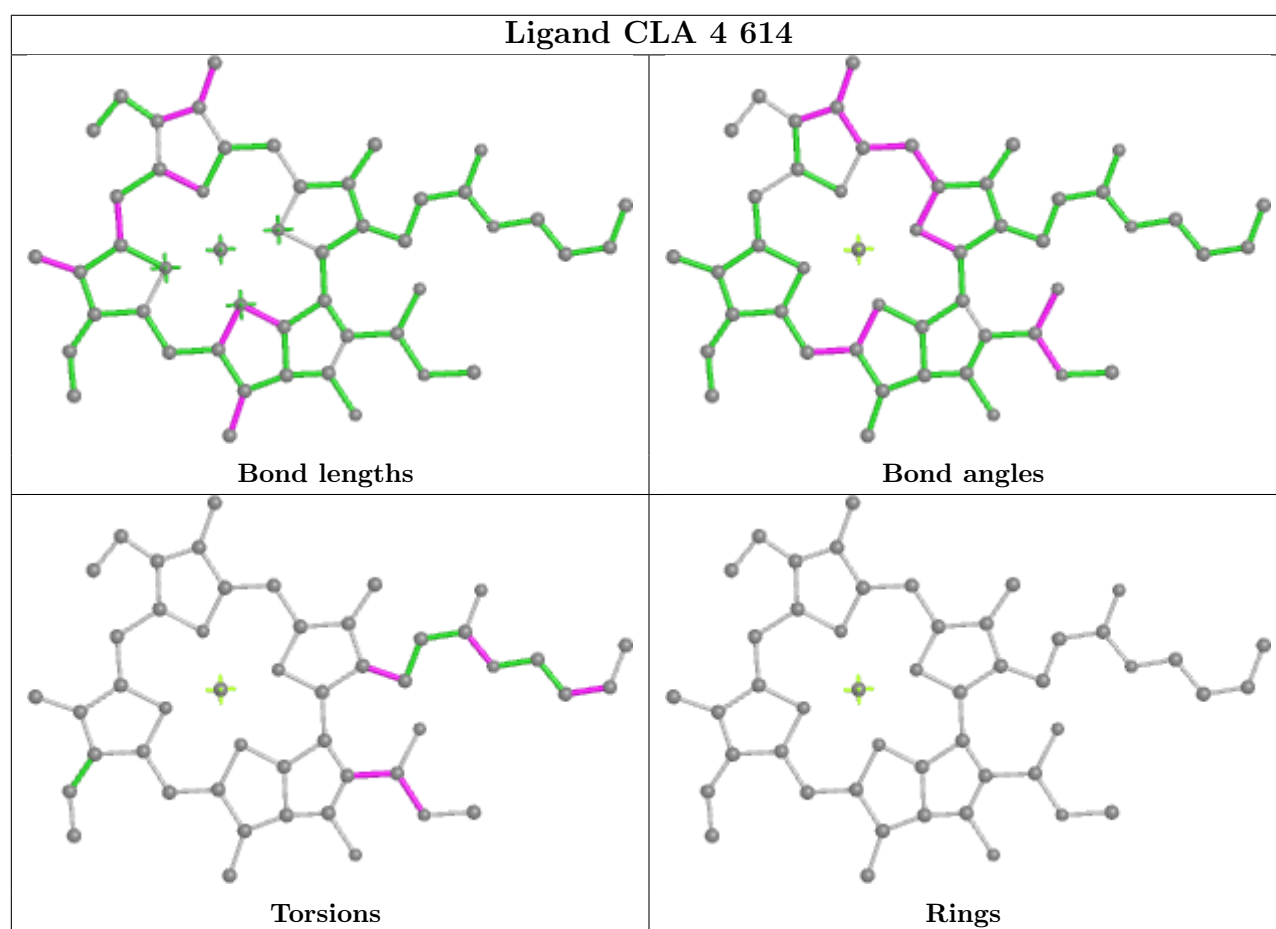
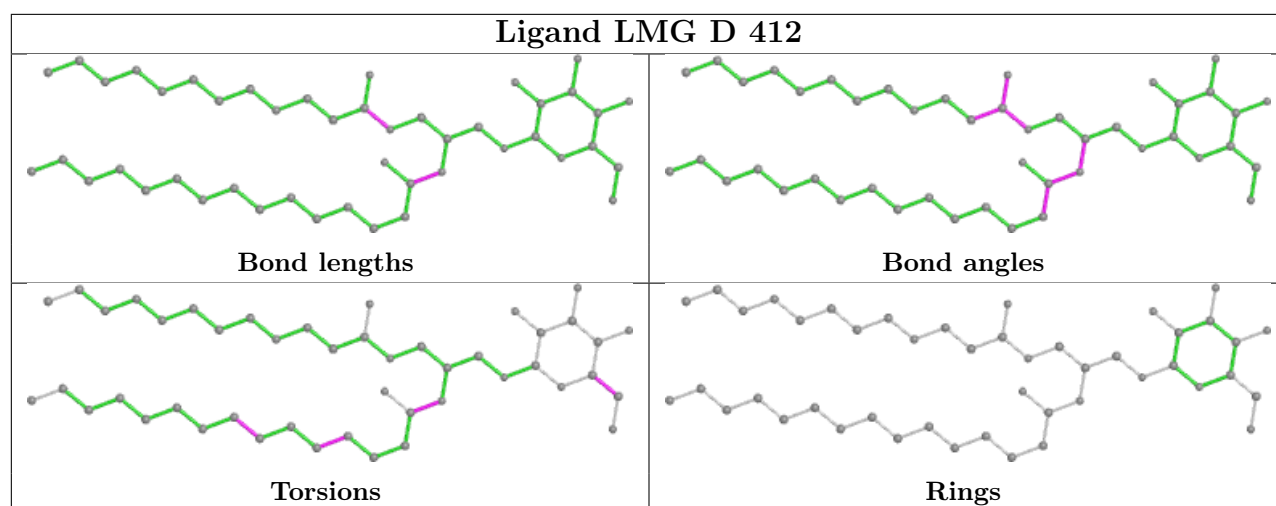


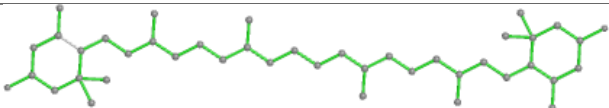
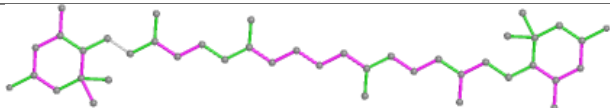
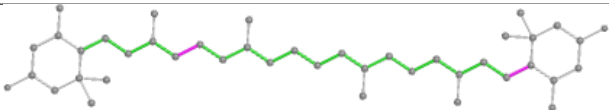
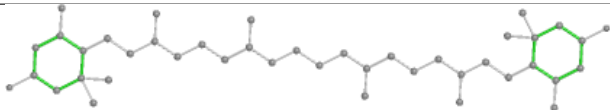
Ligand CHL 4 605

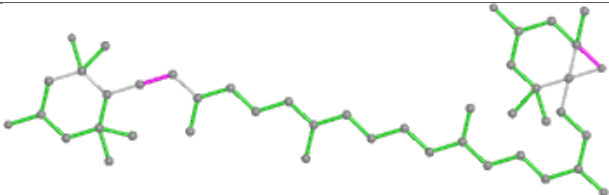
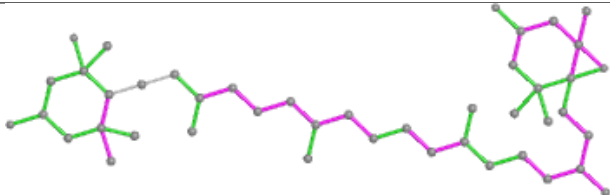
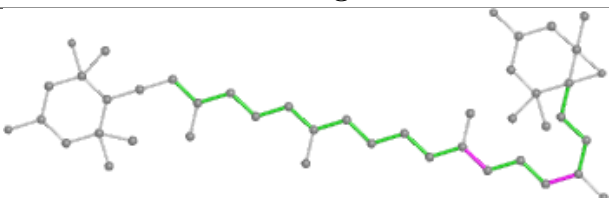



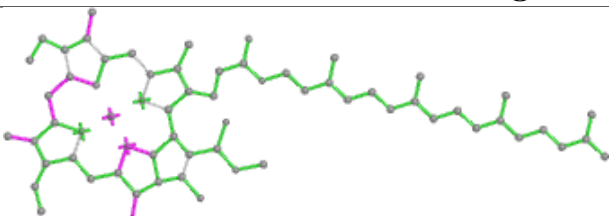
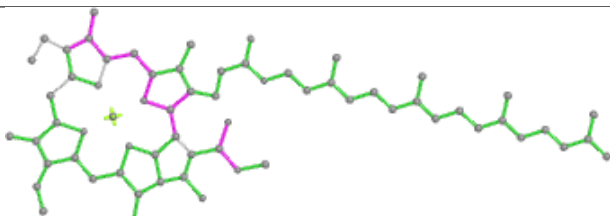
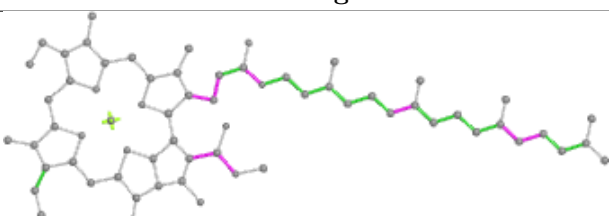
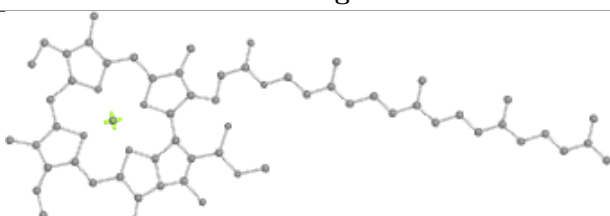
Ligand CLA c 510

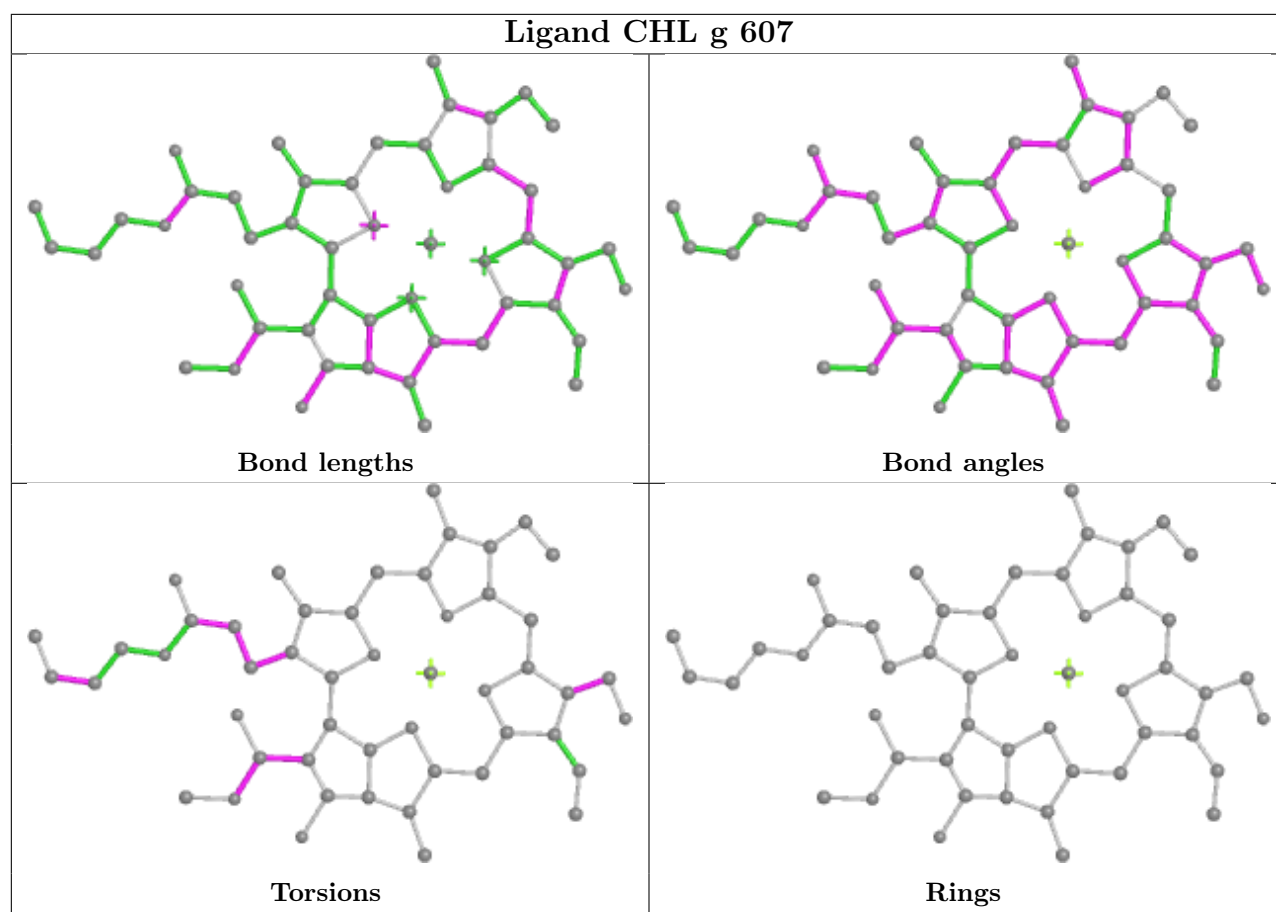




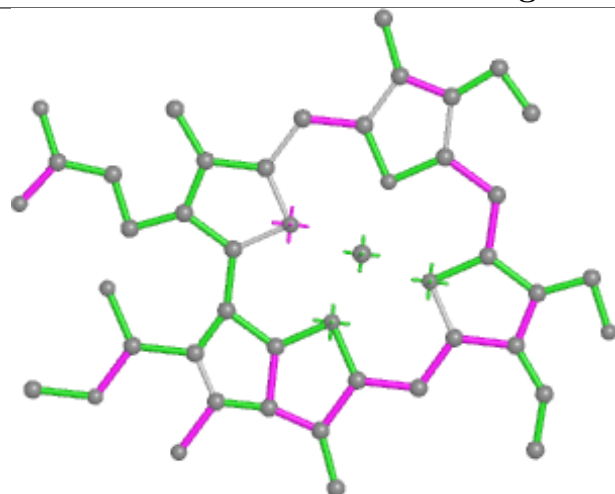
Ligand LUT 7 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX 2 1623	
	
Bond lengths	Bond angles
	
Torsions	Rings

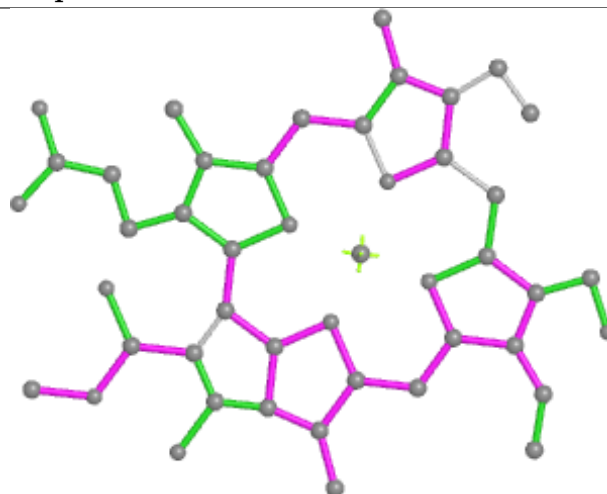
Ligand CLA b 613	
	
Bond lengths	Bond angles
	
Torsions	Rings



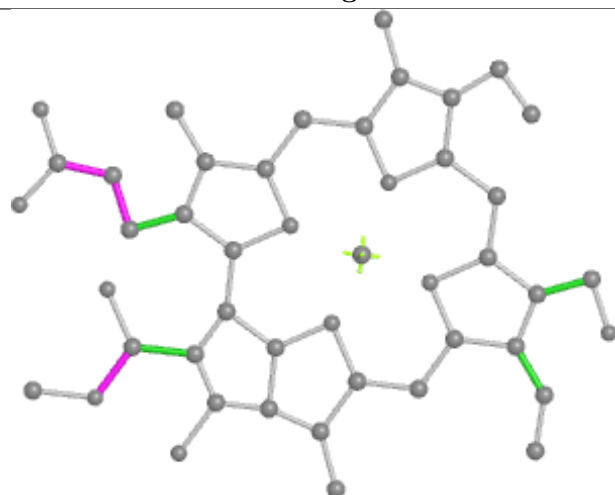
Ligand CHL p 606



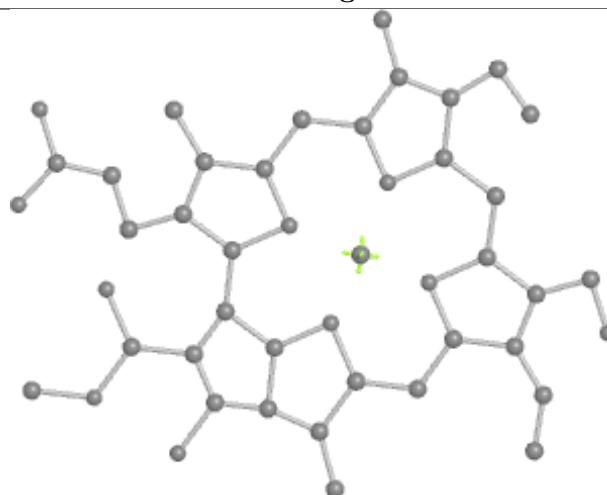
Bond lengths



Bond angles

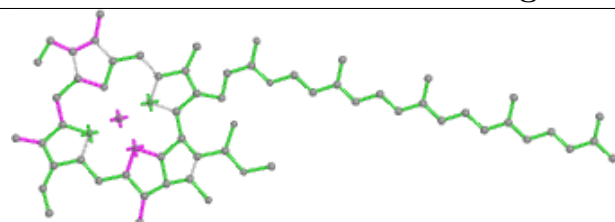


Torsions

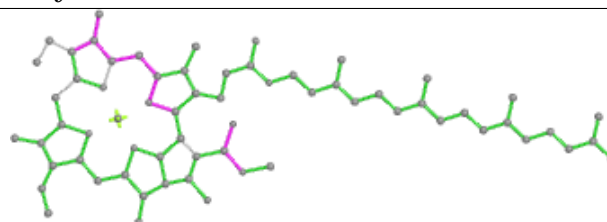


Rings

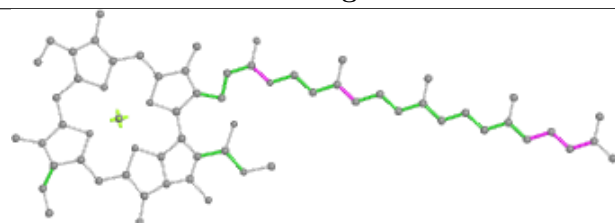
Ligand CLA y 611



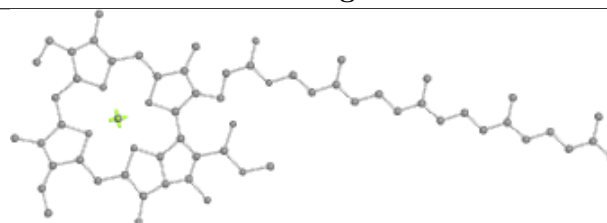
Bond lengths



Bond angles

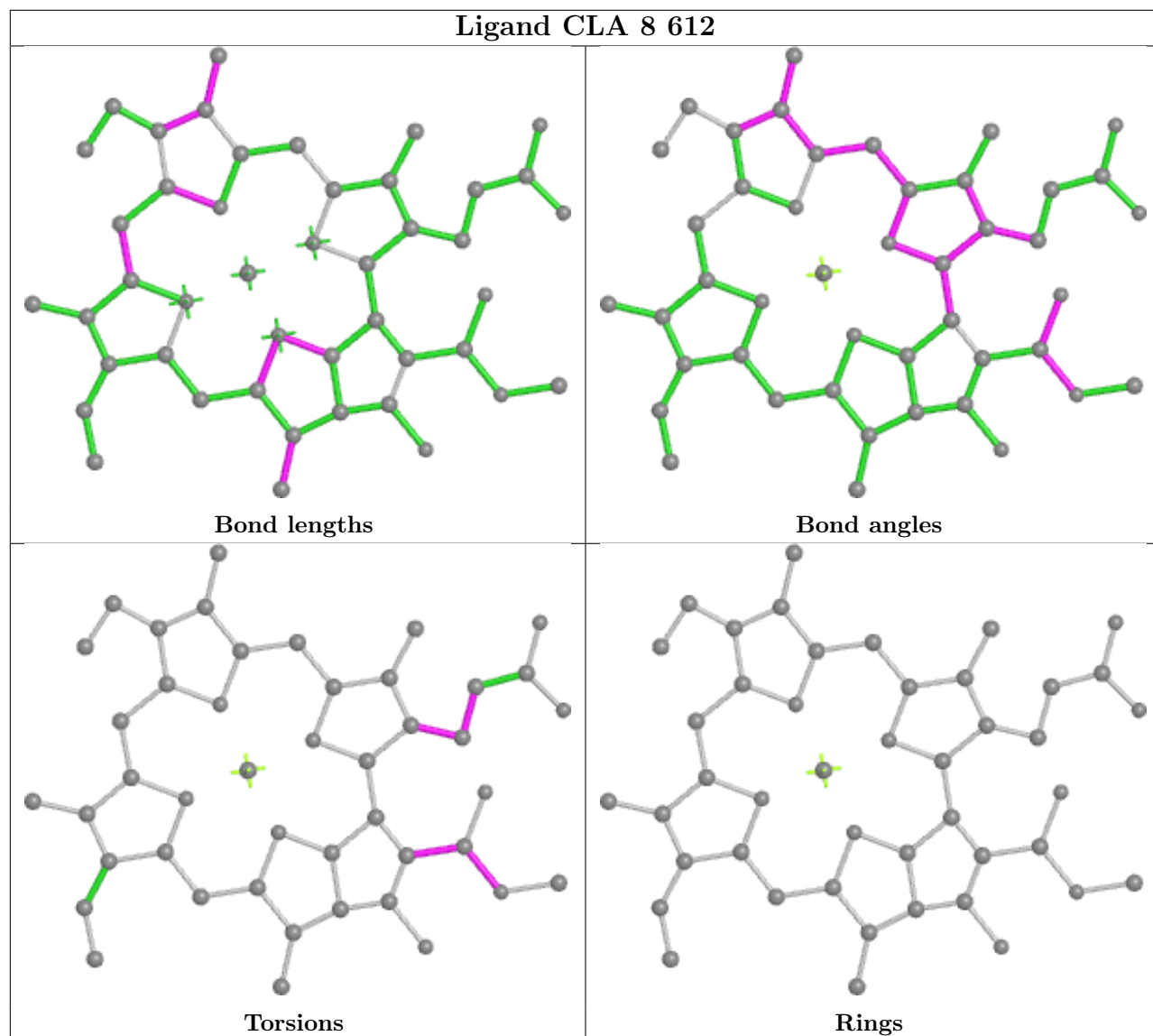


Torsions

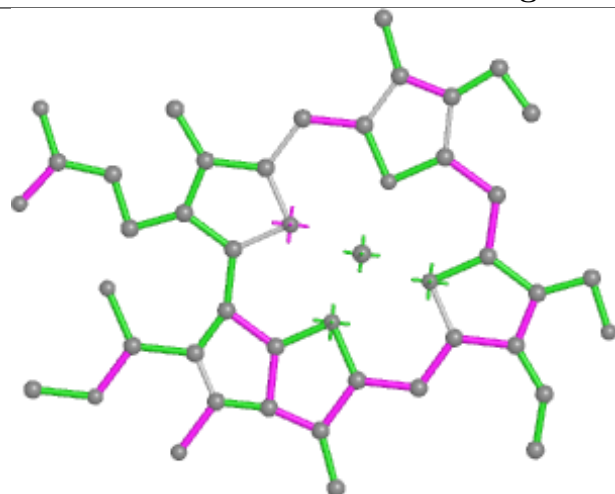


Rings

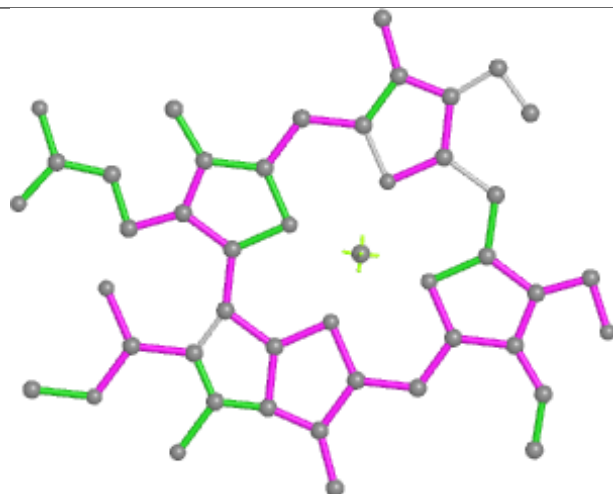
Ligand CLA 8 612



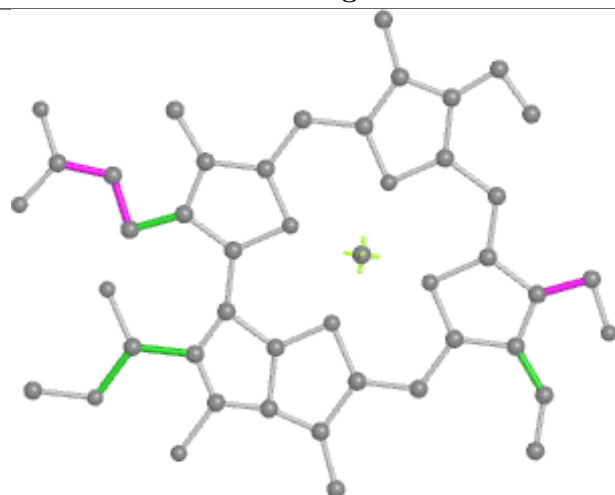
Ligand CHL 6 605



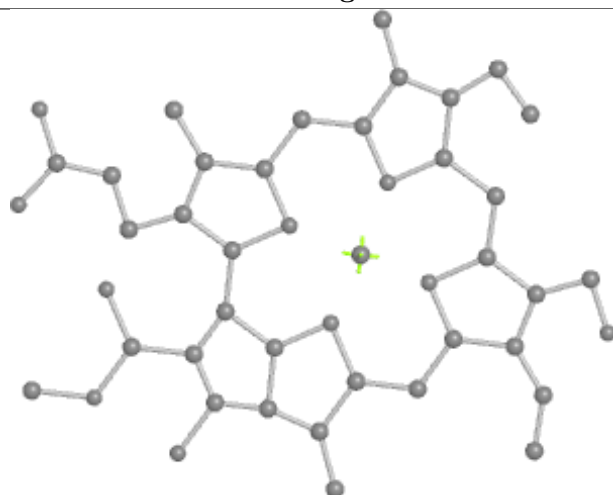
Bond lengths



Bond angles

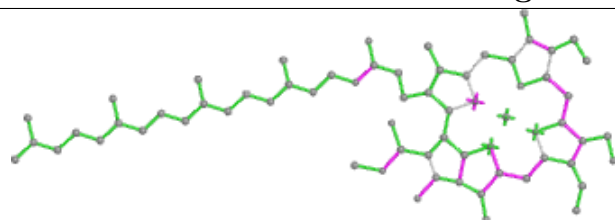


Torsions

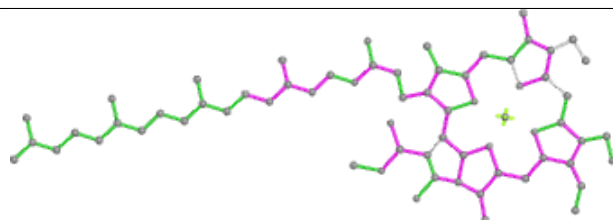


Rings

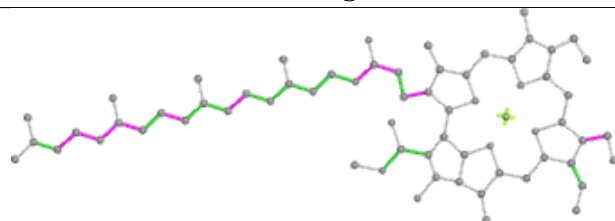
Ligand CHL N 607



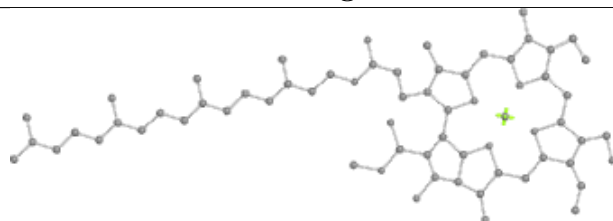
Bond lengths



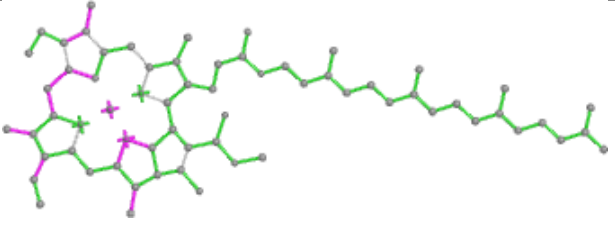
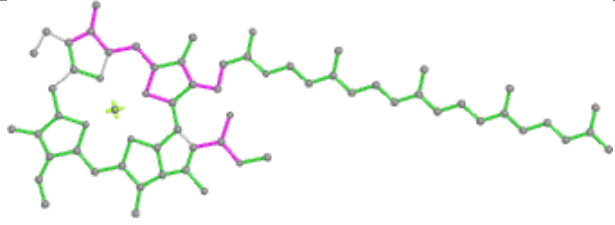
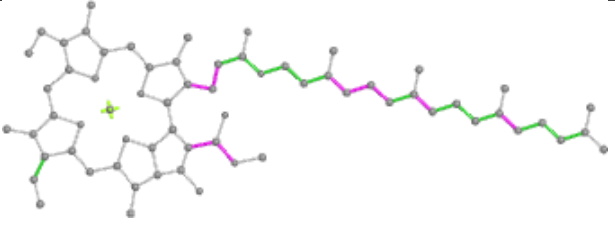
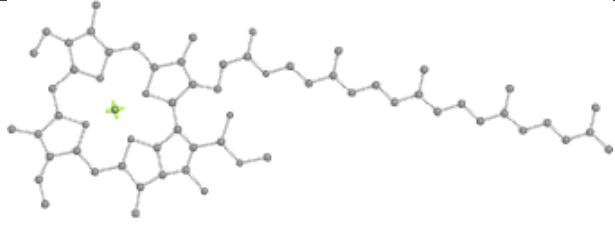
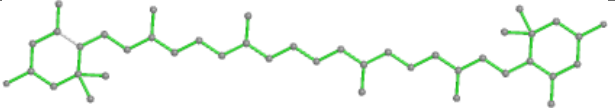
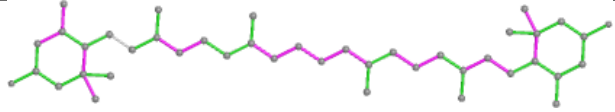
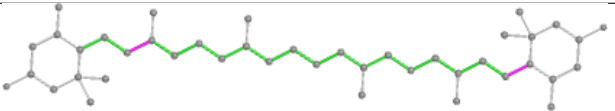
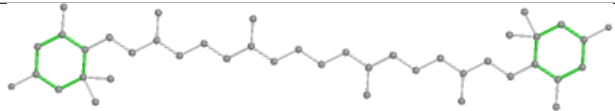
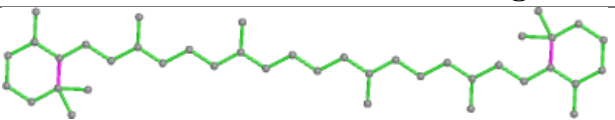
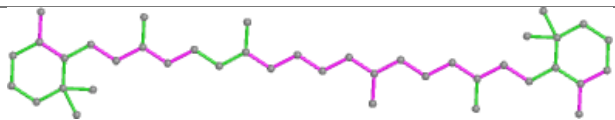
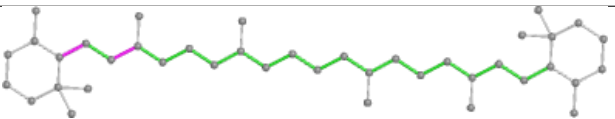
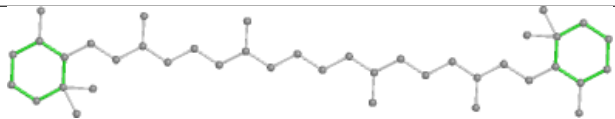
Bond angles

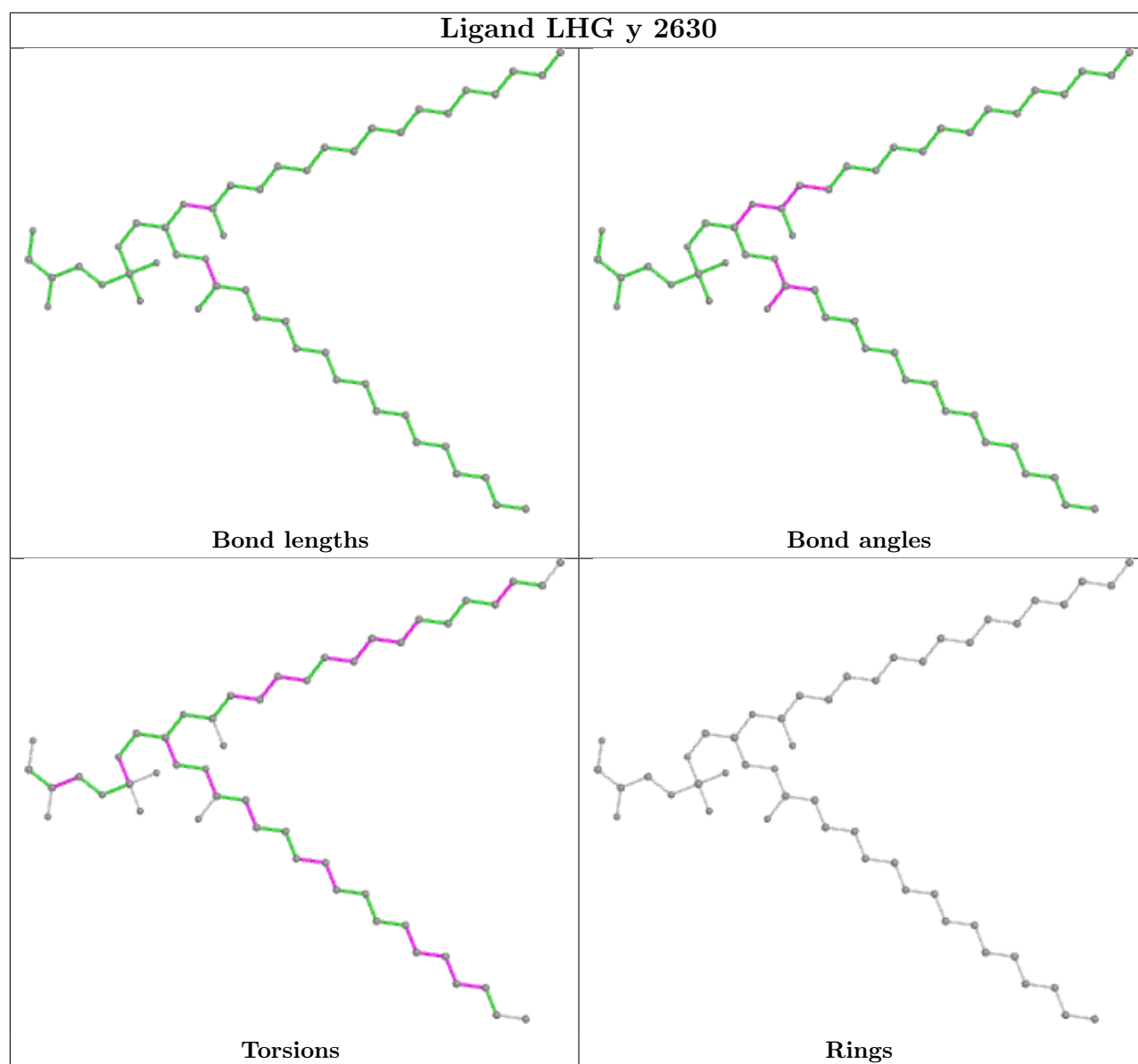


Torsions

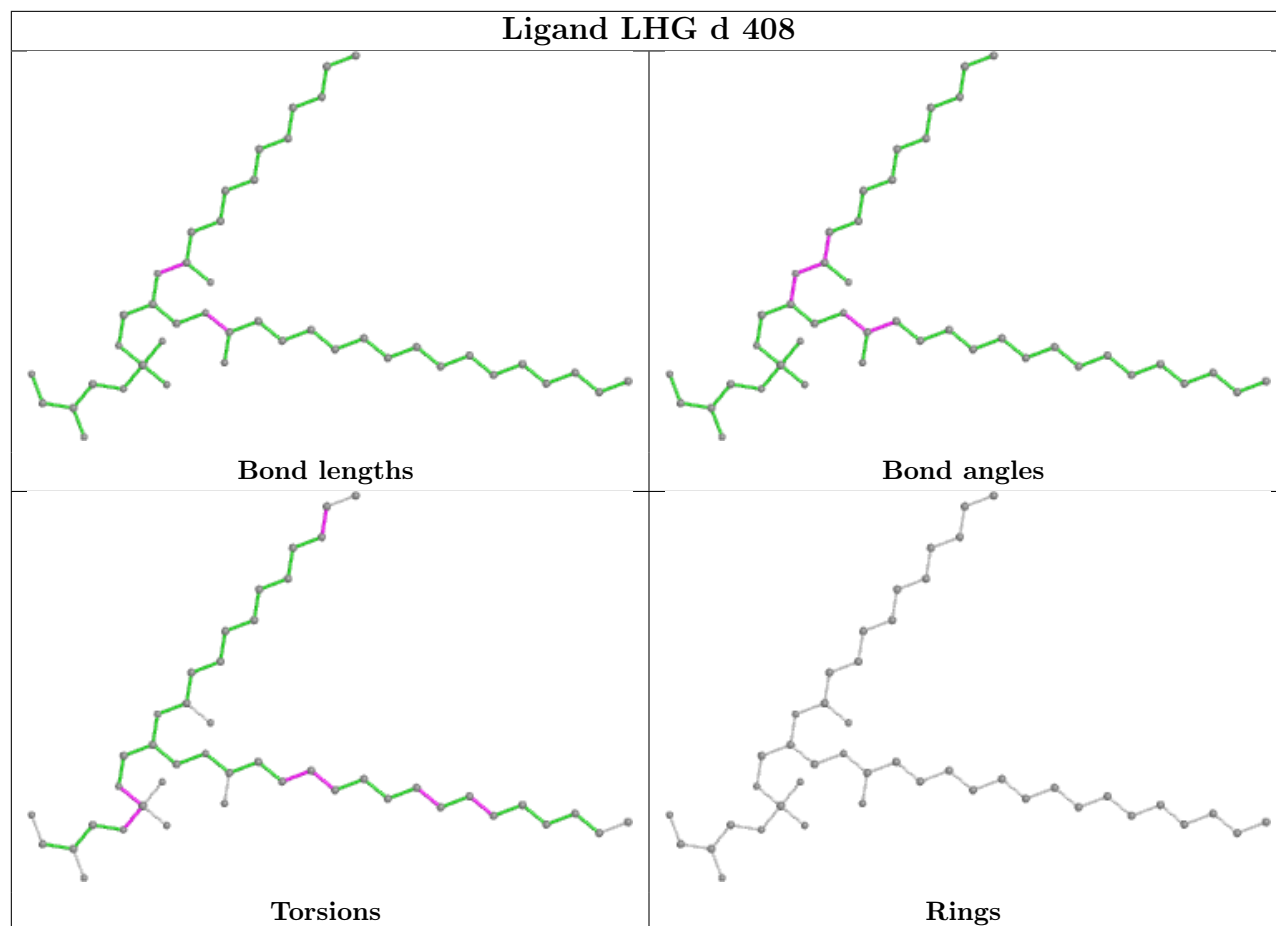


Rings

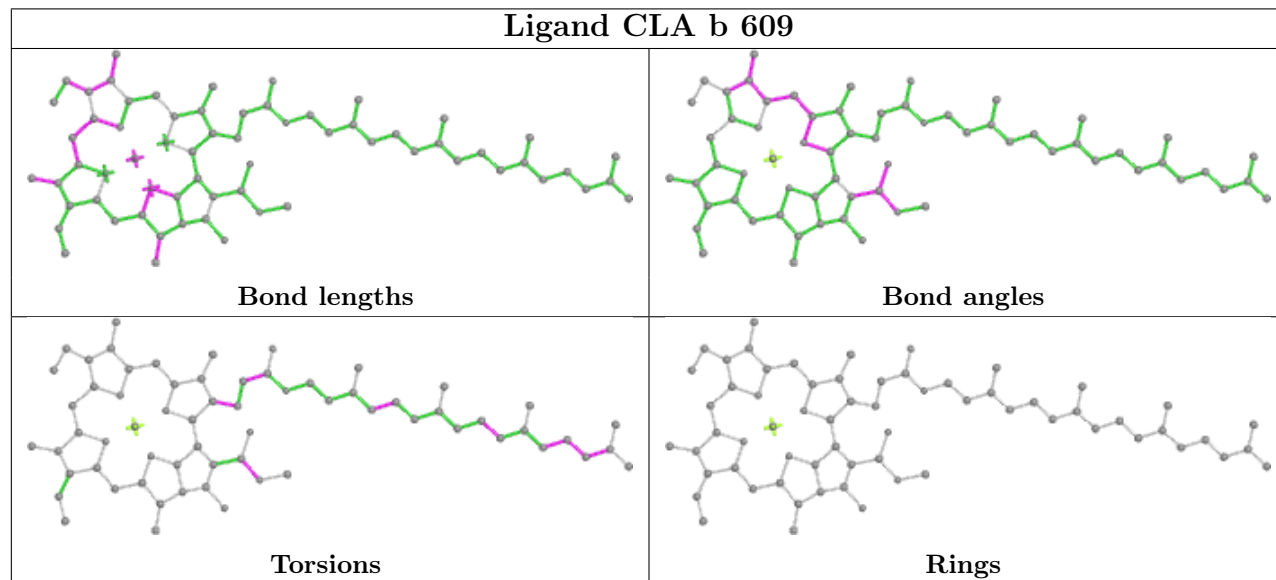
Ligand CLA y 603	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT p 1621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

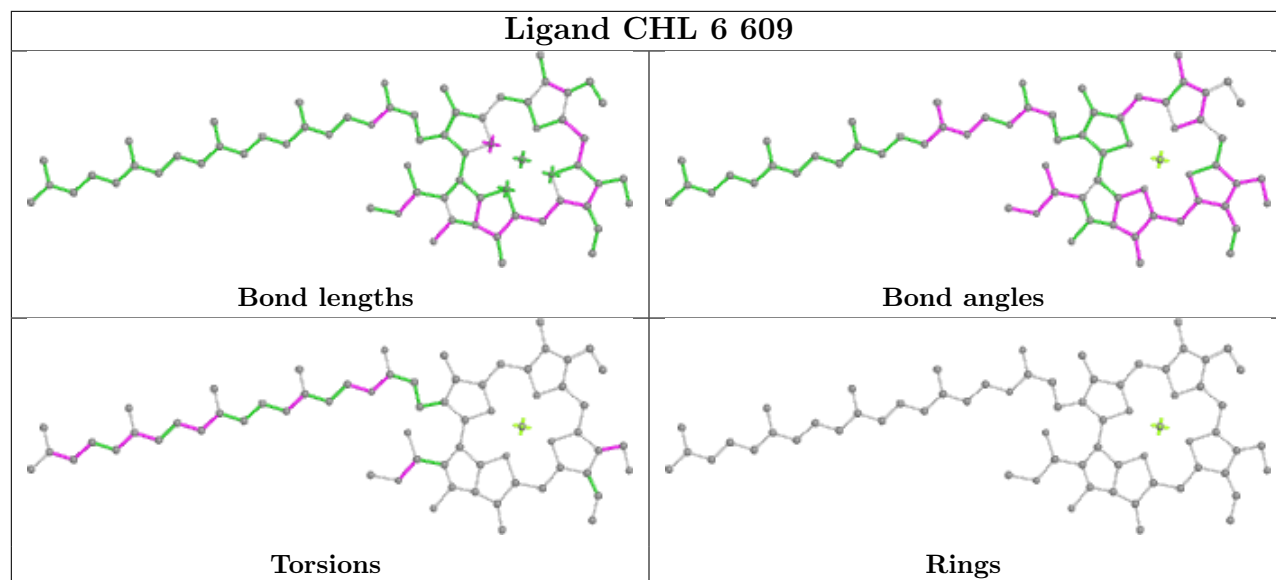
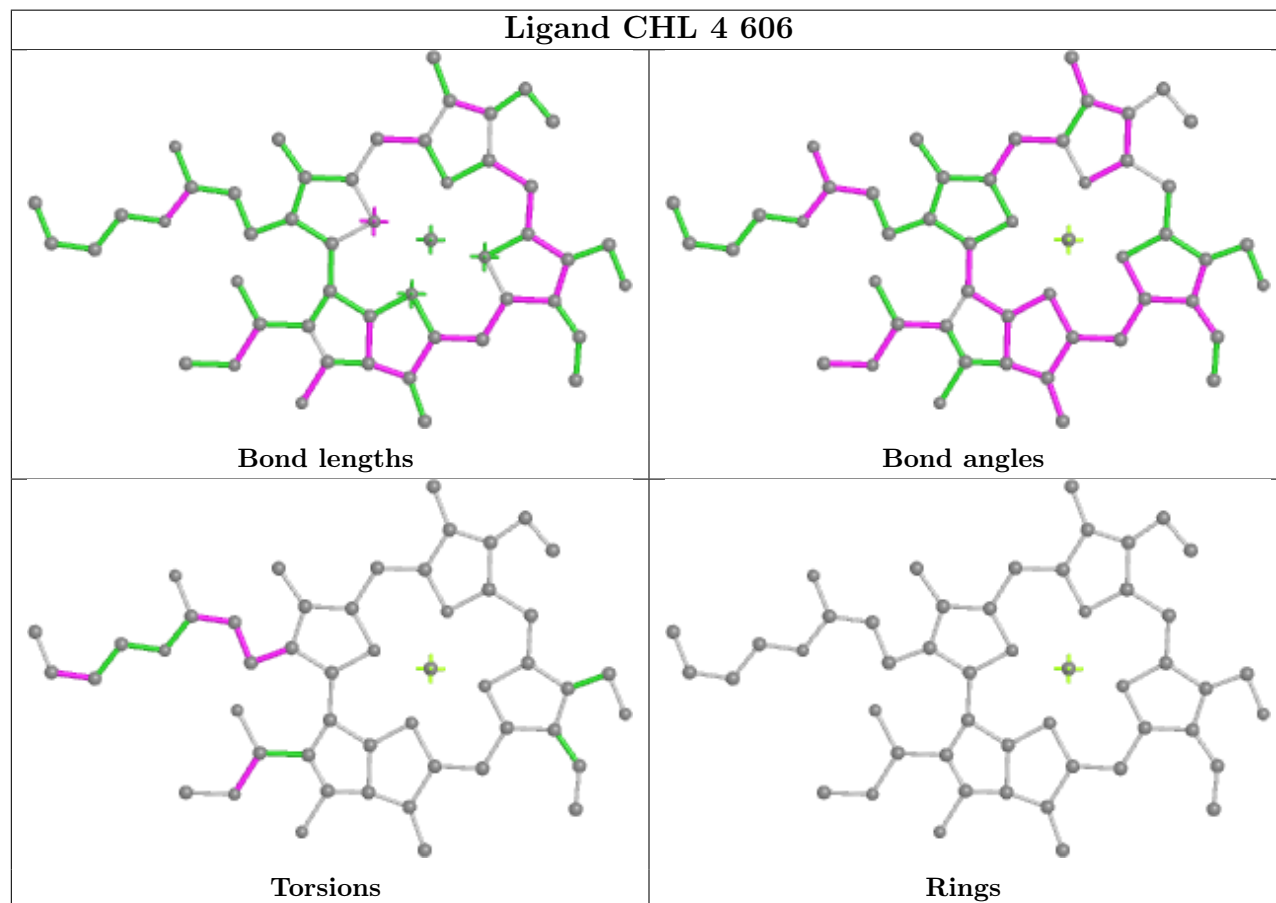


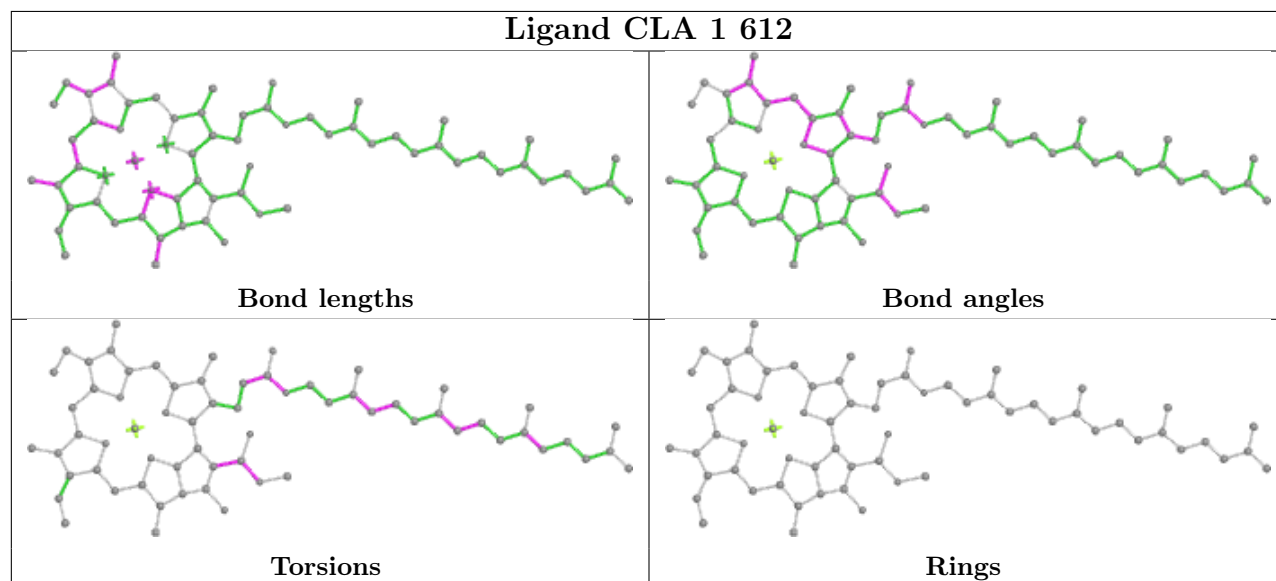
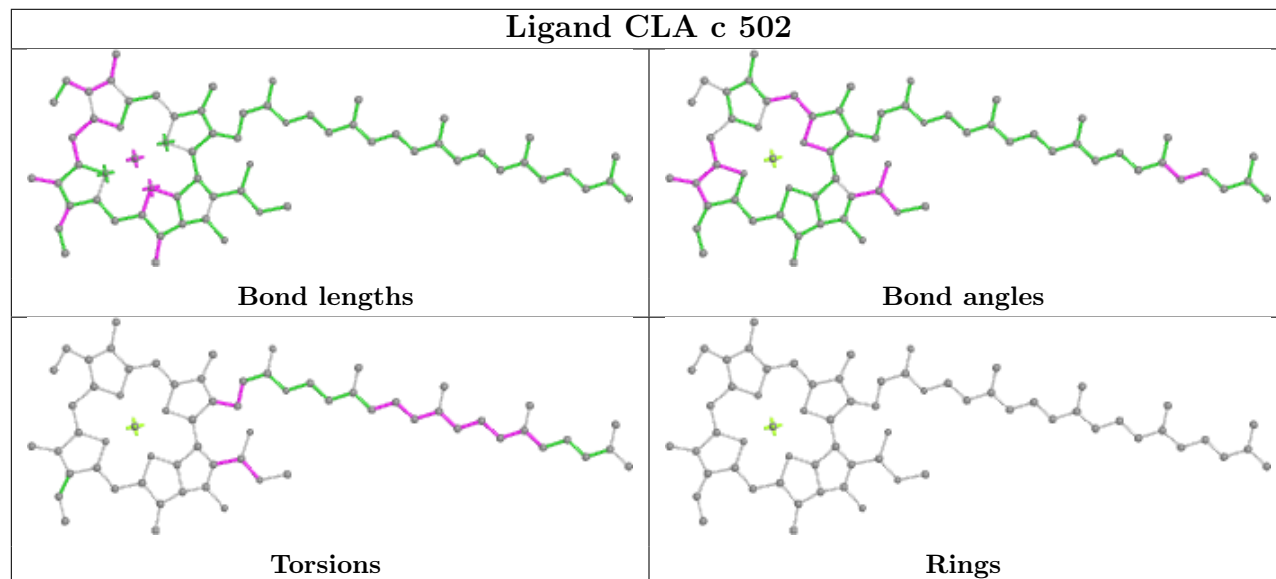
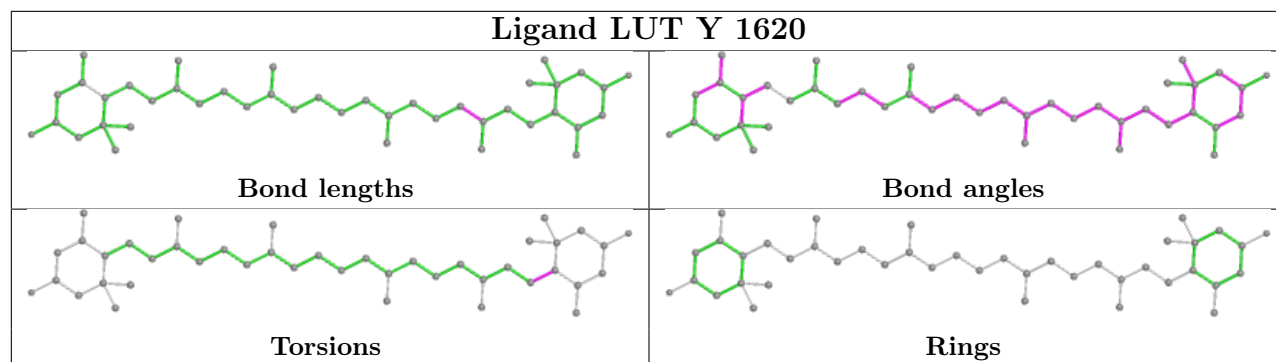
Ligand LHG d 408

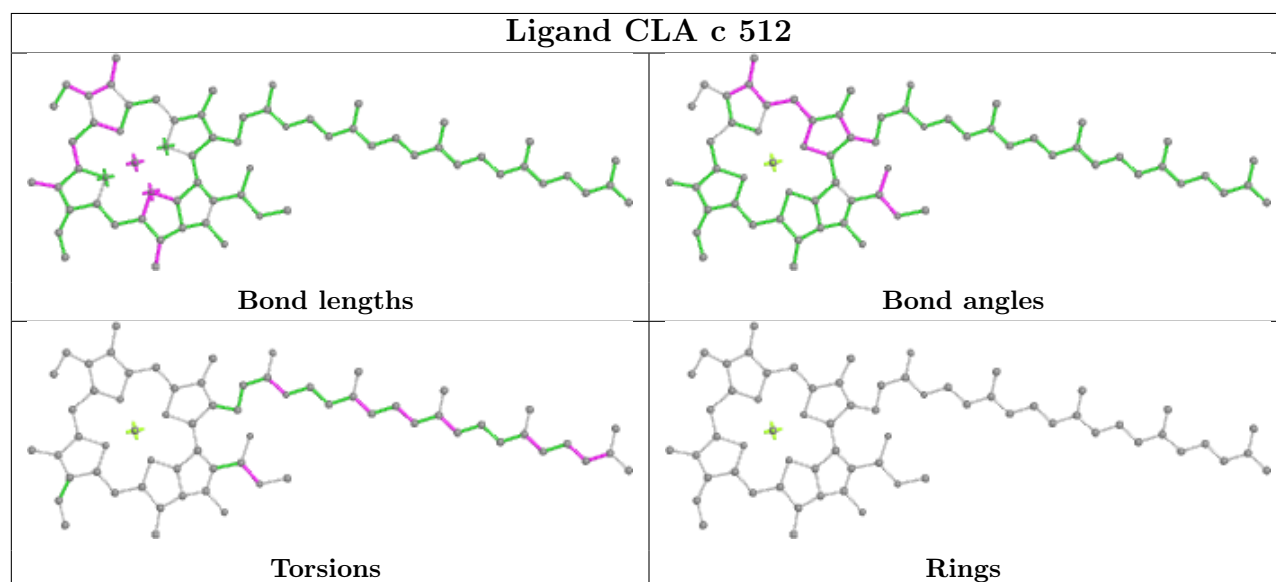
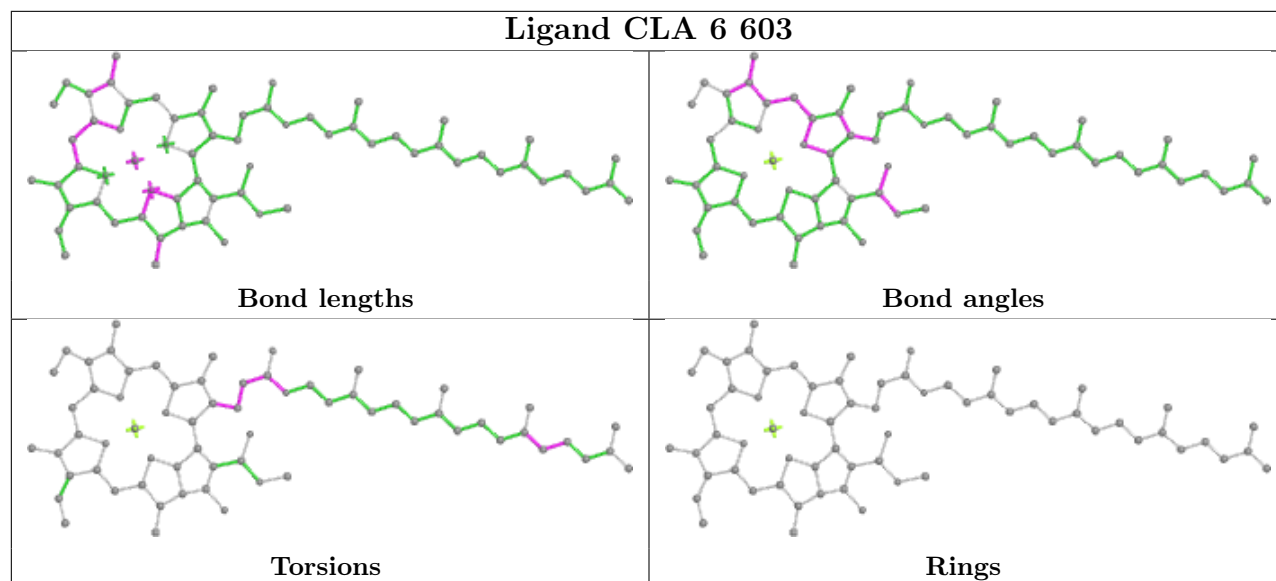
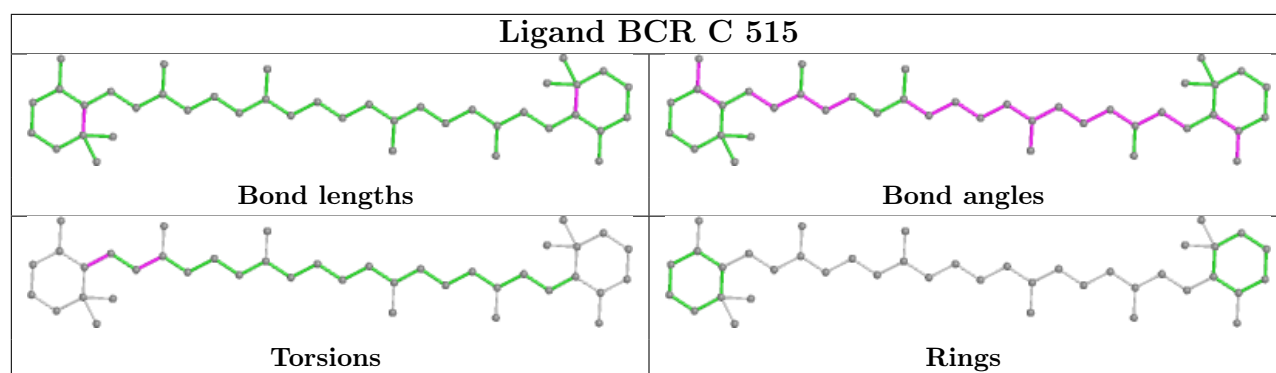


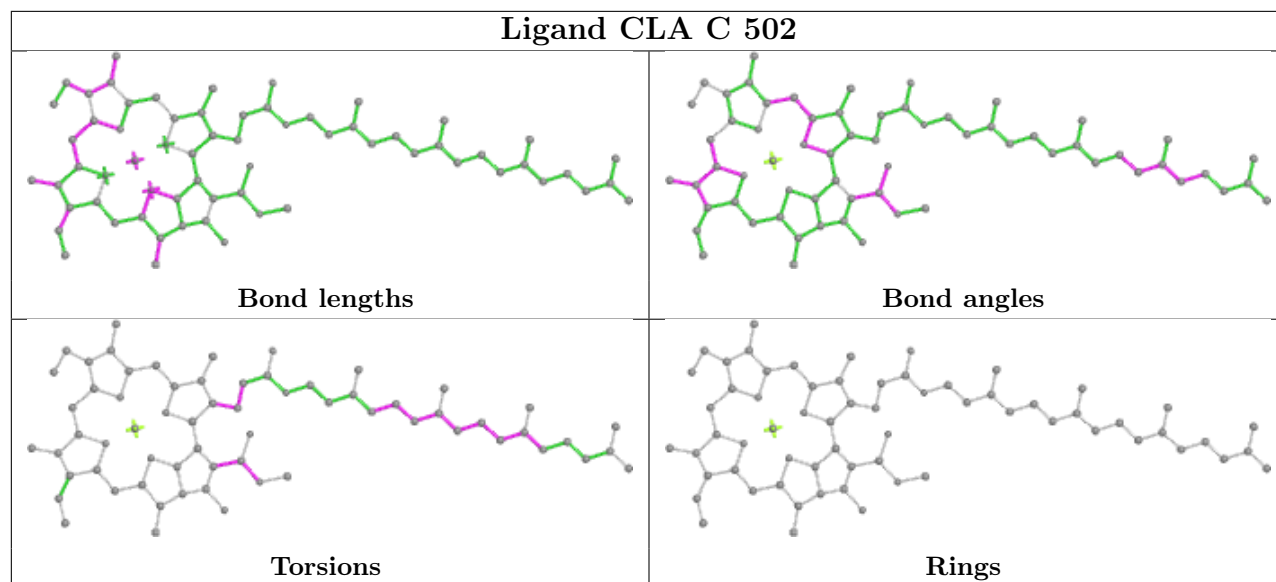
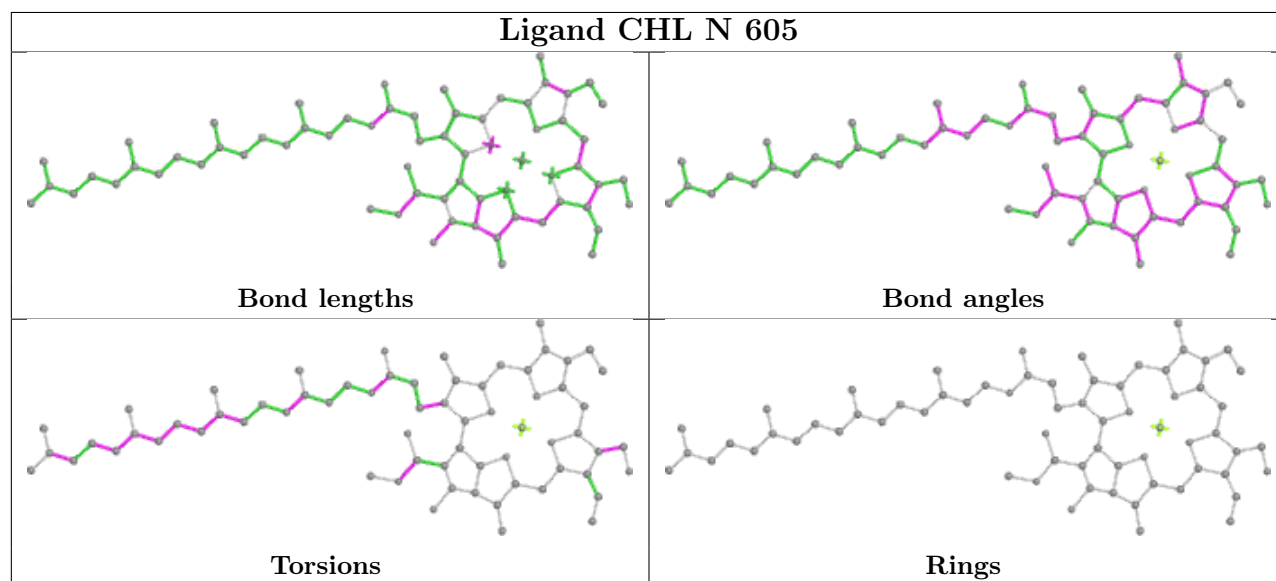
Ligand CLA b 609



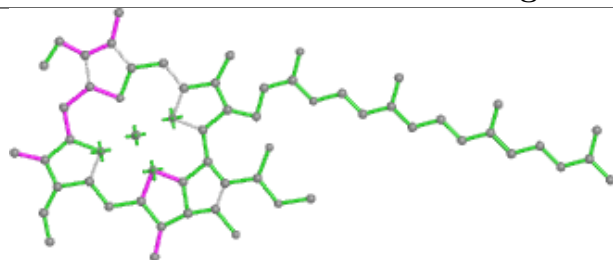
Ligand CHL 6 609**Ligand CHL 4 606**



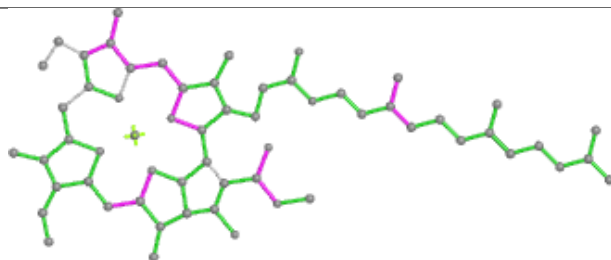


Ligand CLA C 502**Ligand CHL N 605**

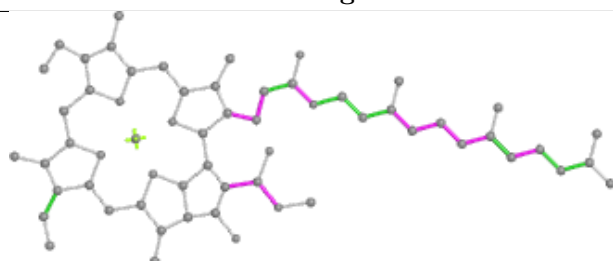
Ligand CLA r 613



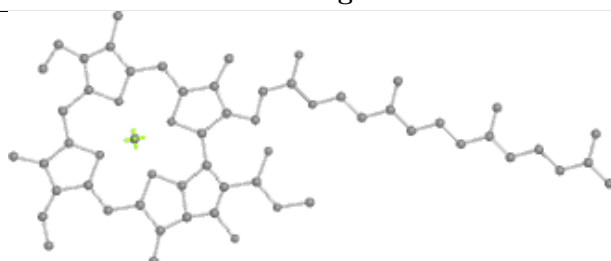
Bond lengths



Bond angles

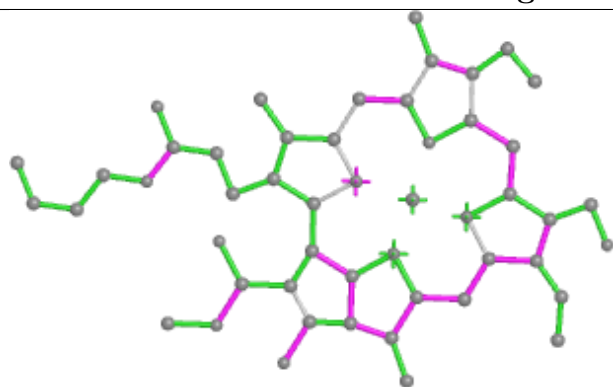


Torsions

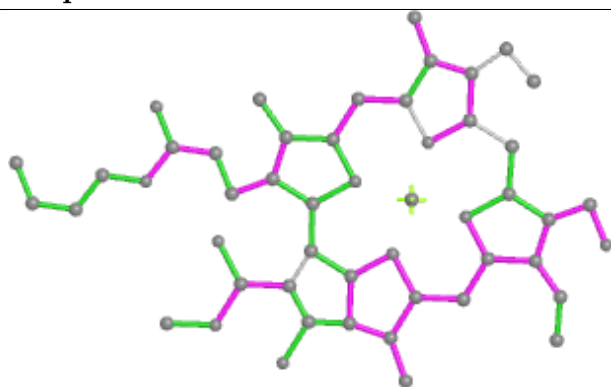


Rings

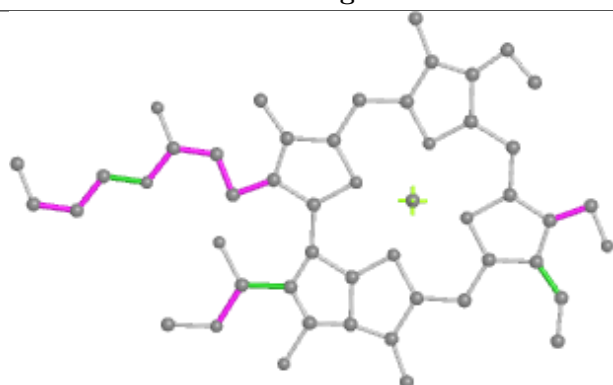
Ligand CHL q 607



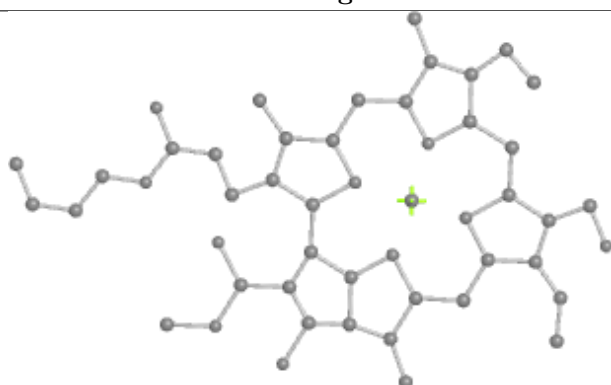
Bond lengths



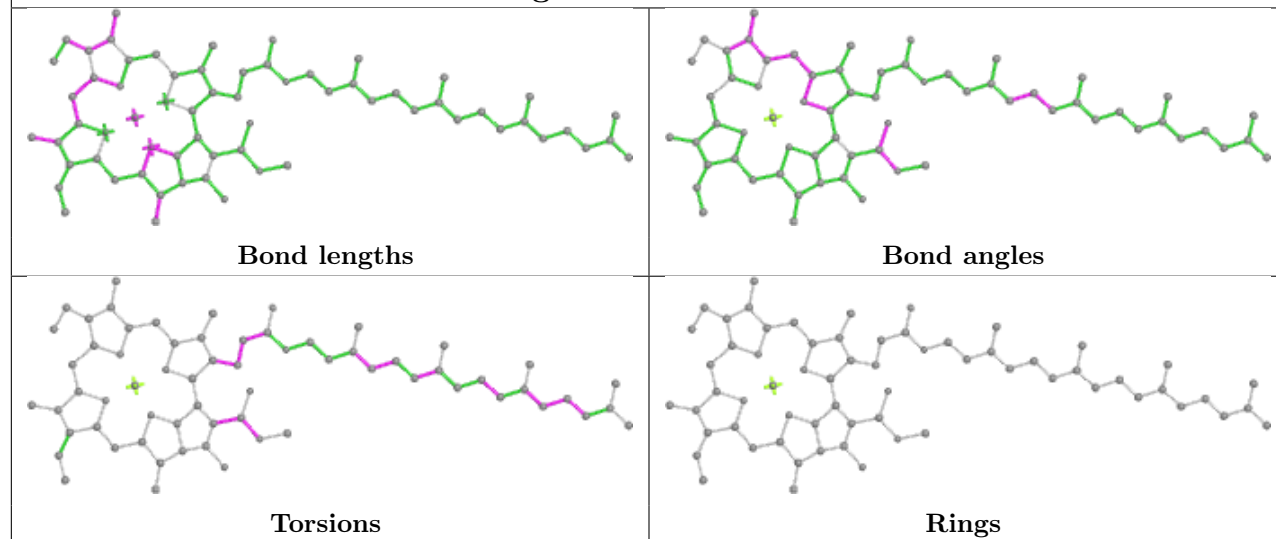
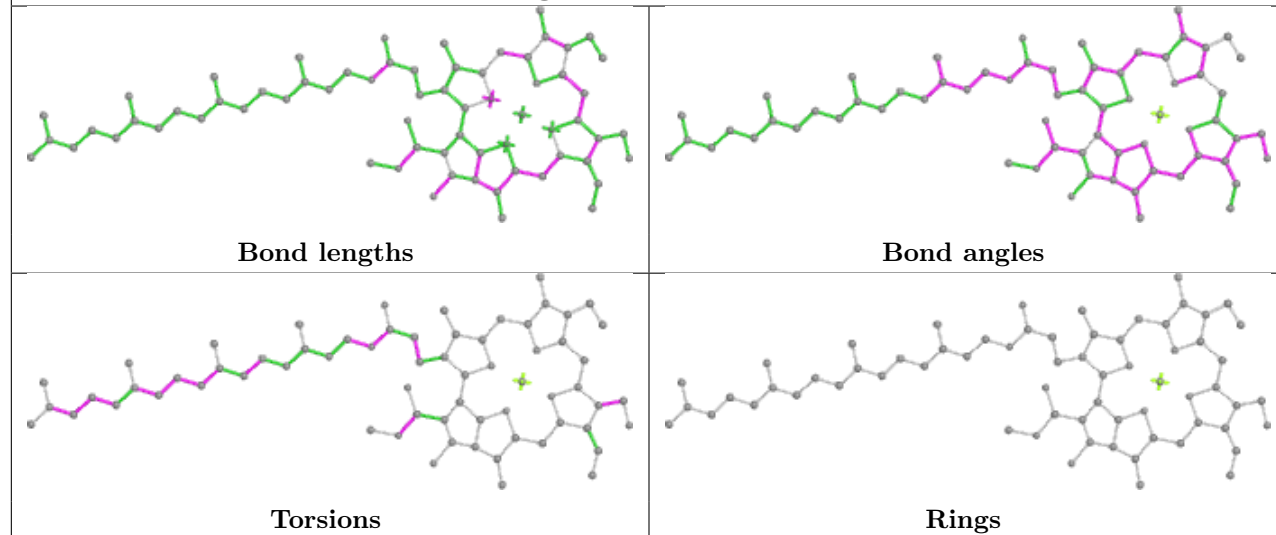
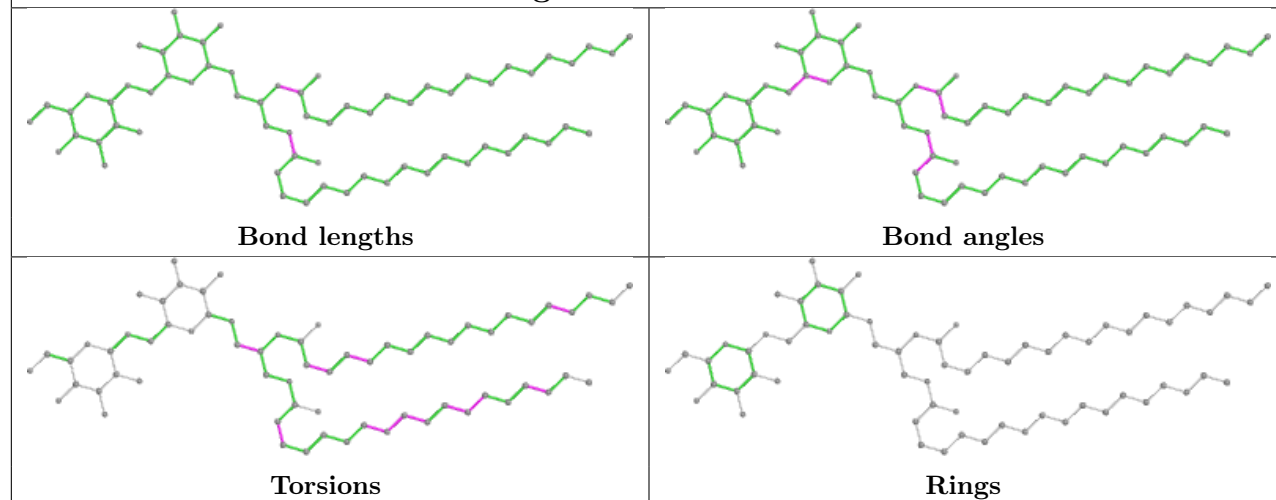
Bond angles

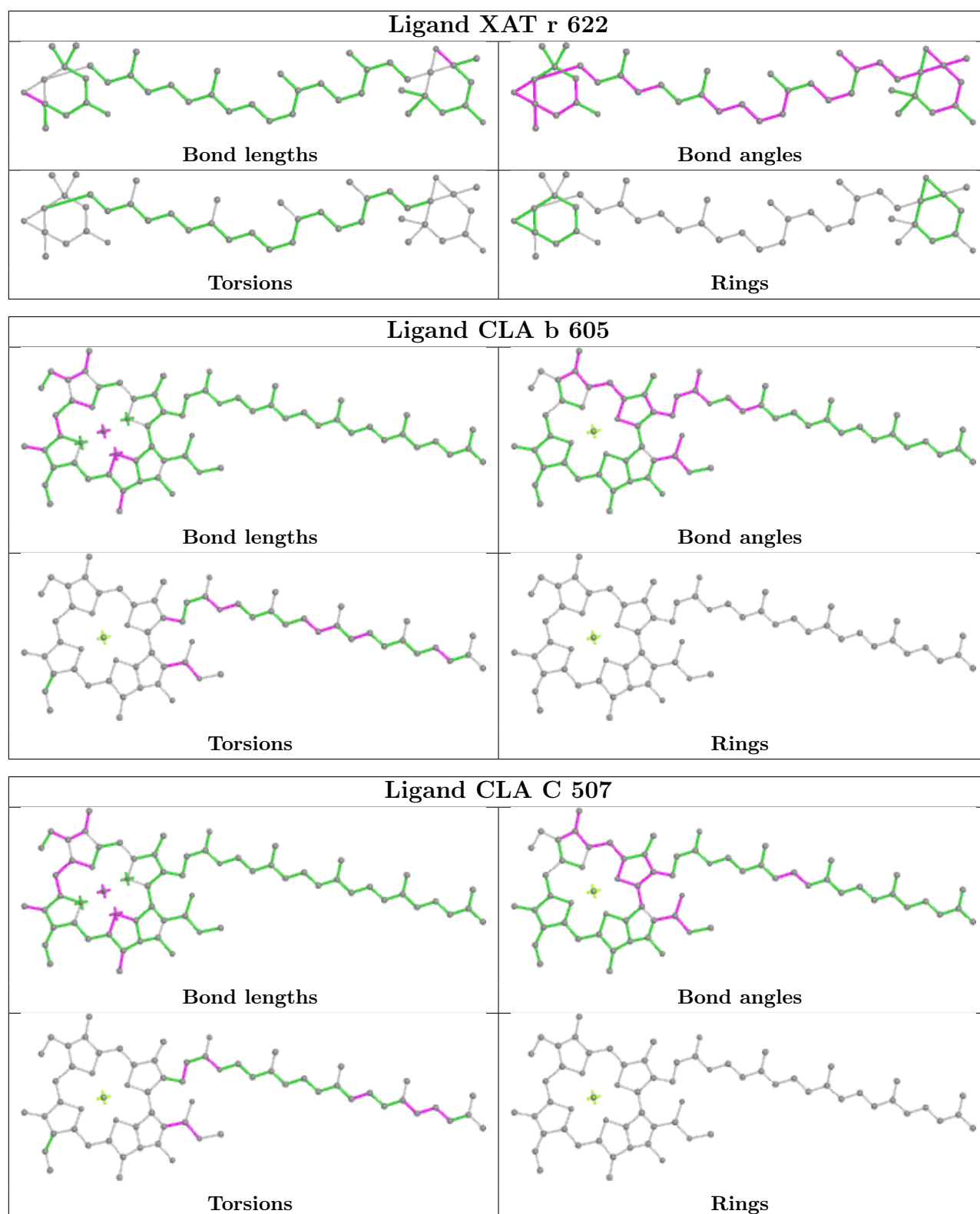


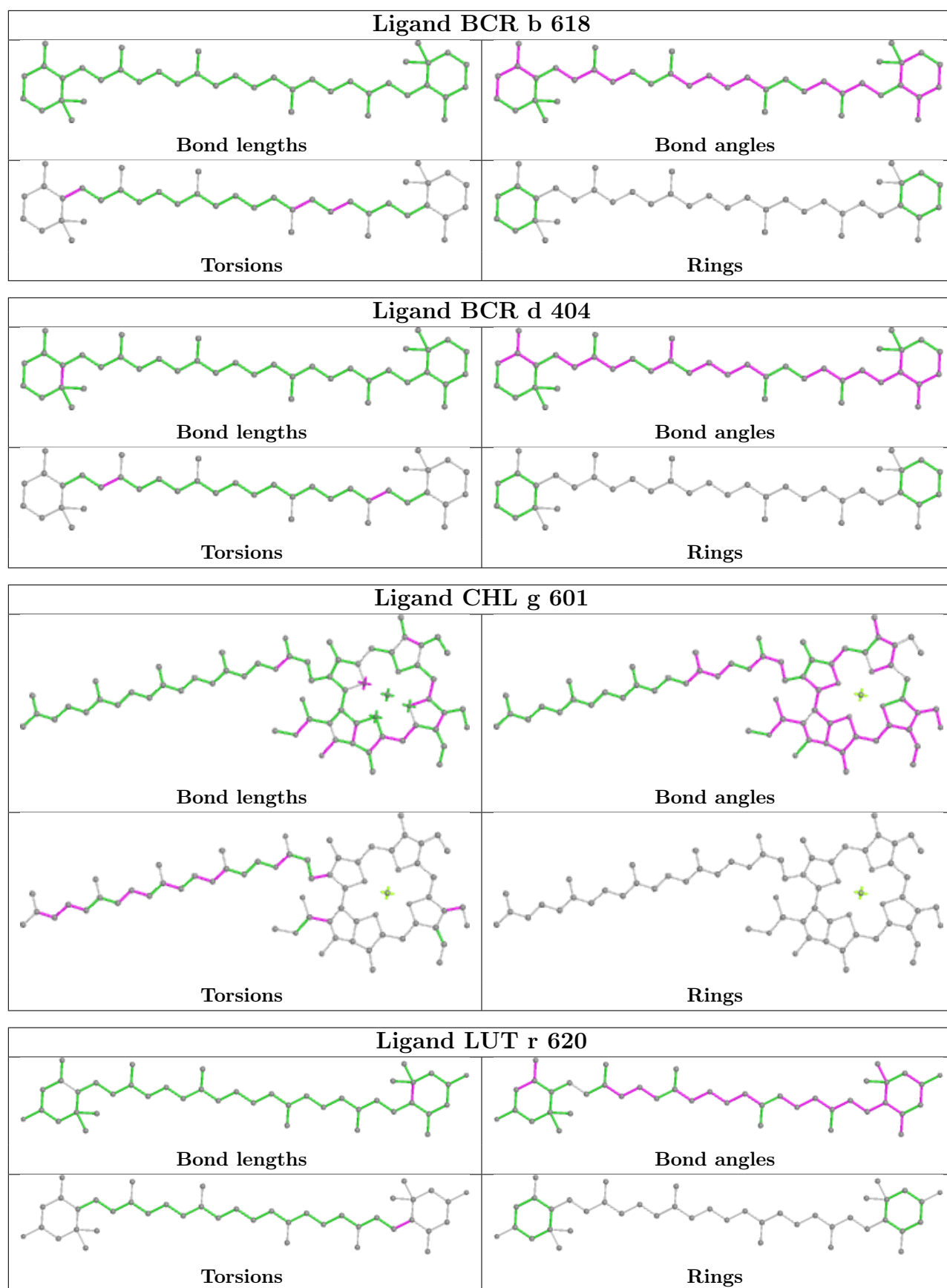
Torsions

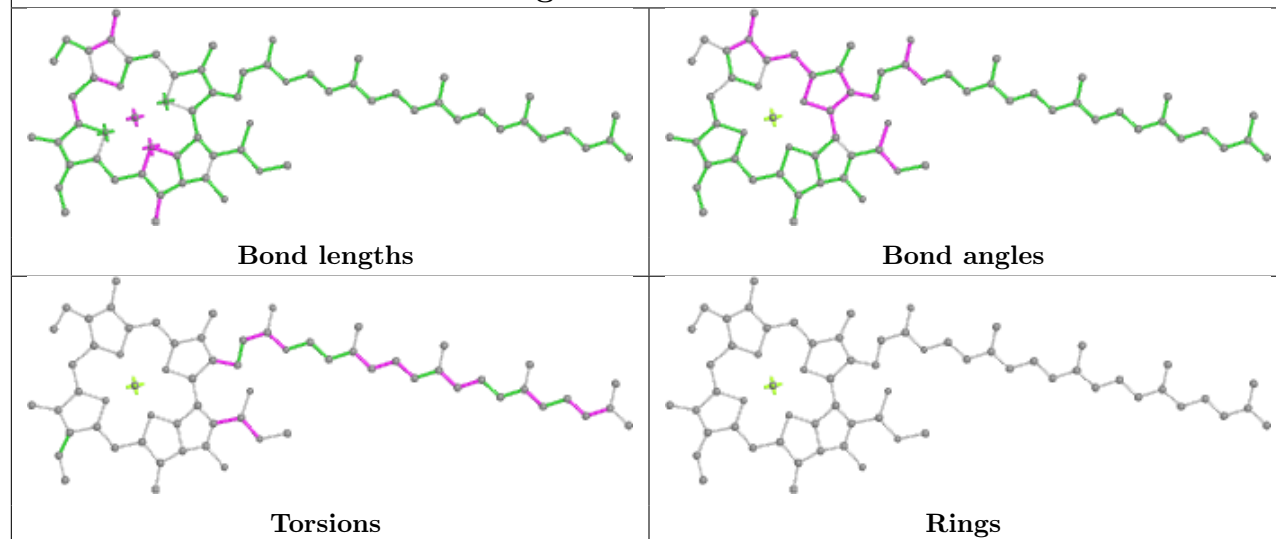
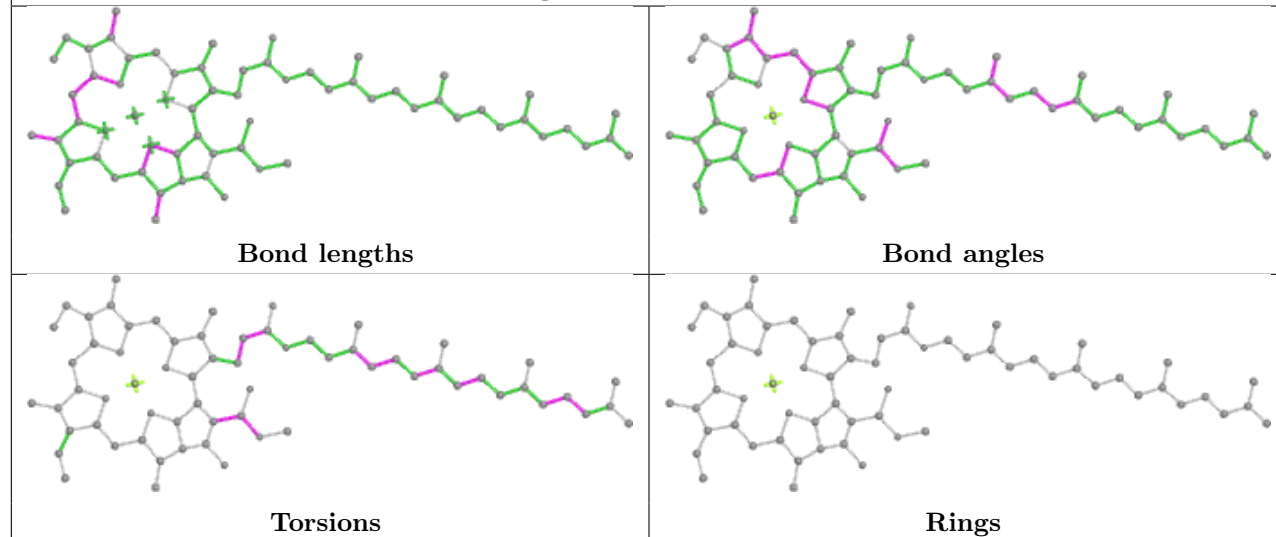


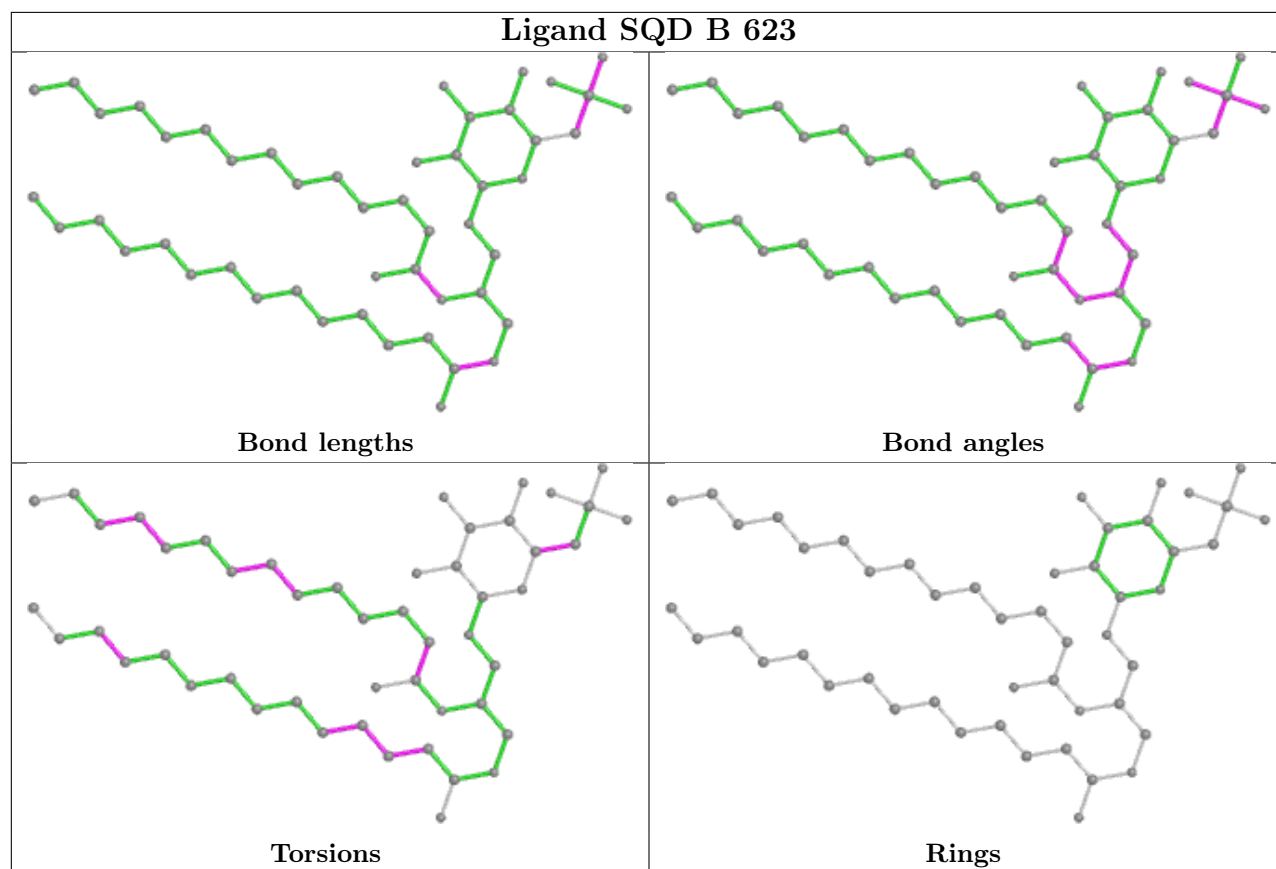
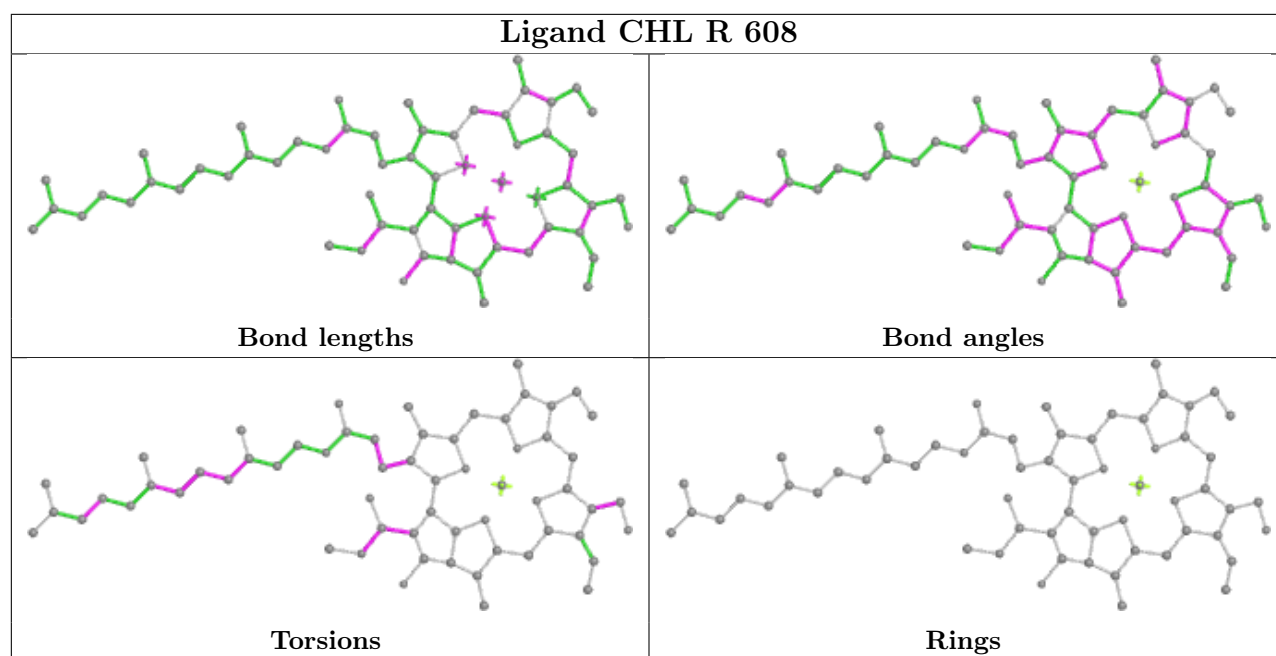
Rings

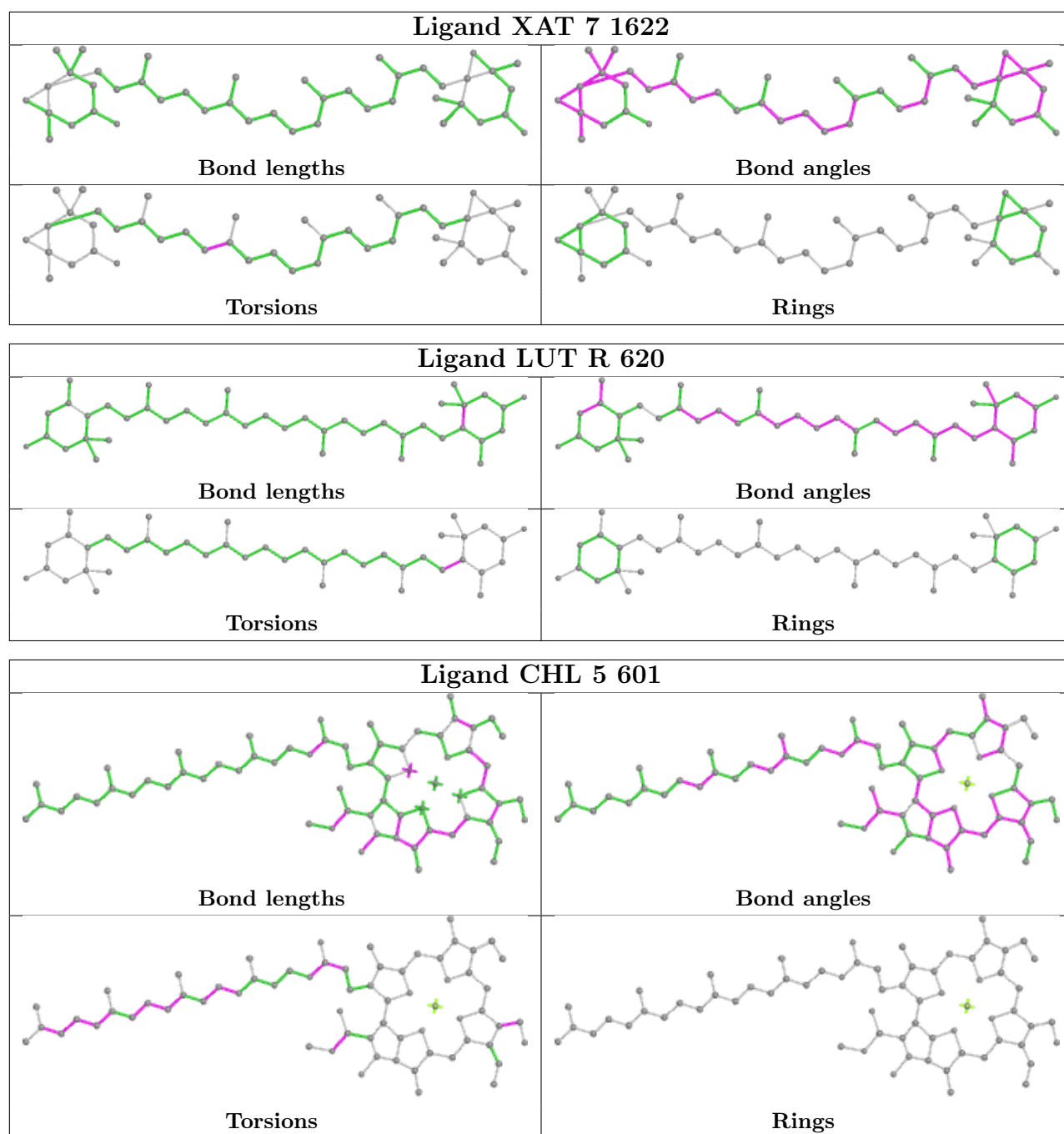
Ligand CLA B 608**Ligand CHL 7 607****Ligand DGD c 523**



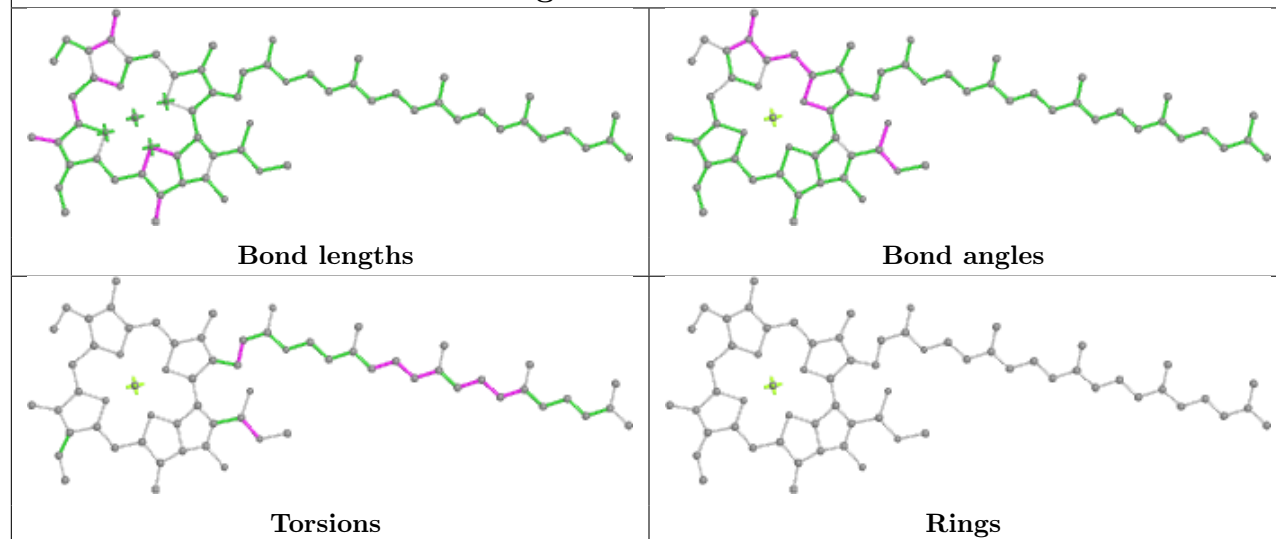


Ligand CLA 2 603**Ligand CLA 9 602**

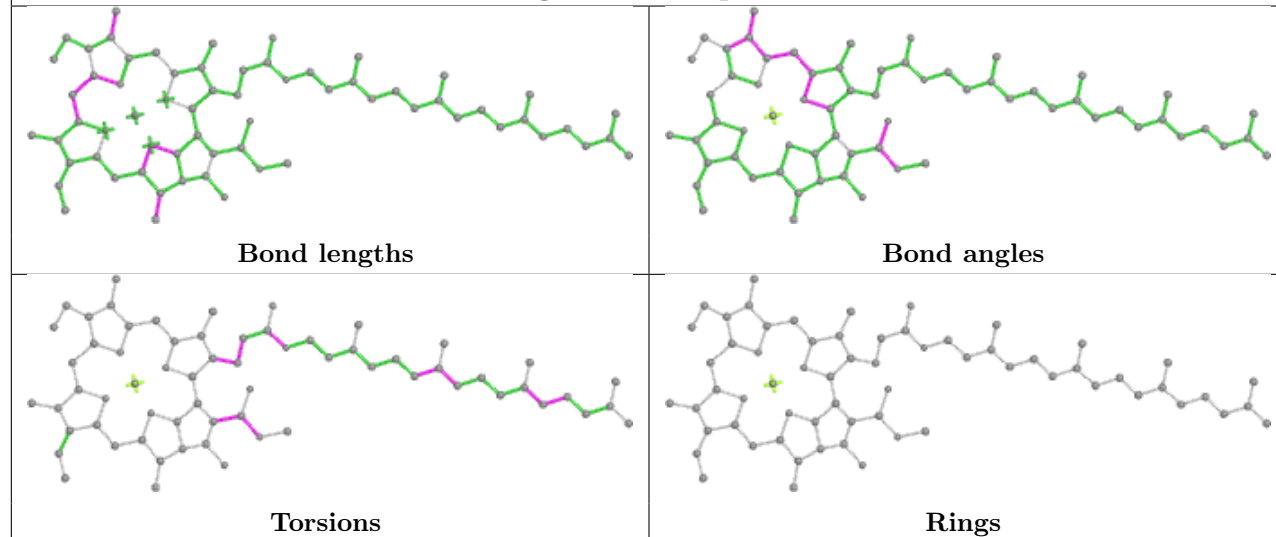




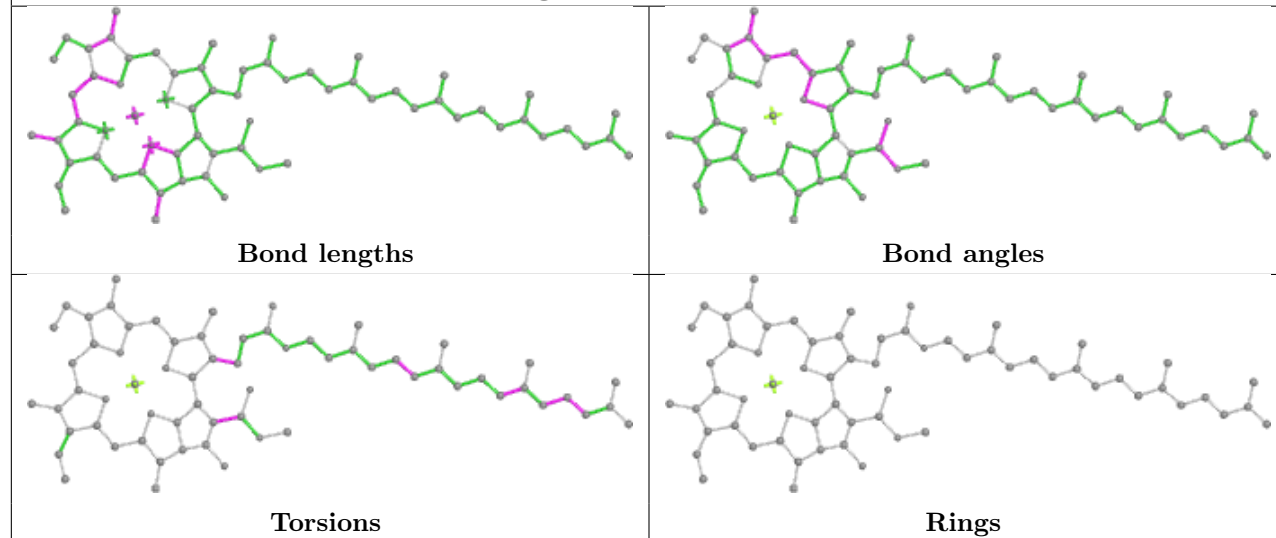
Ligand CLA 0 602

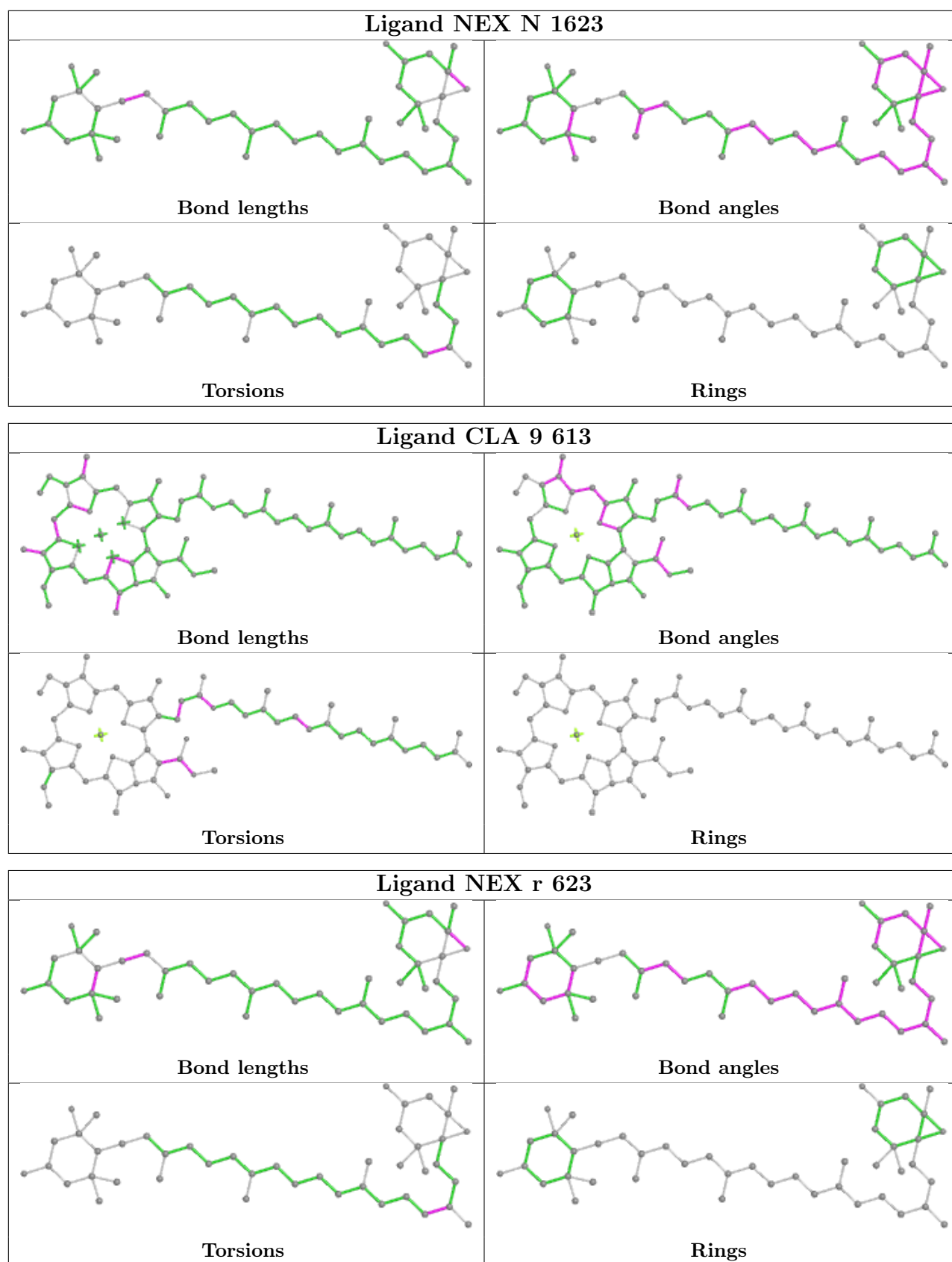


Ligand CLA q 613

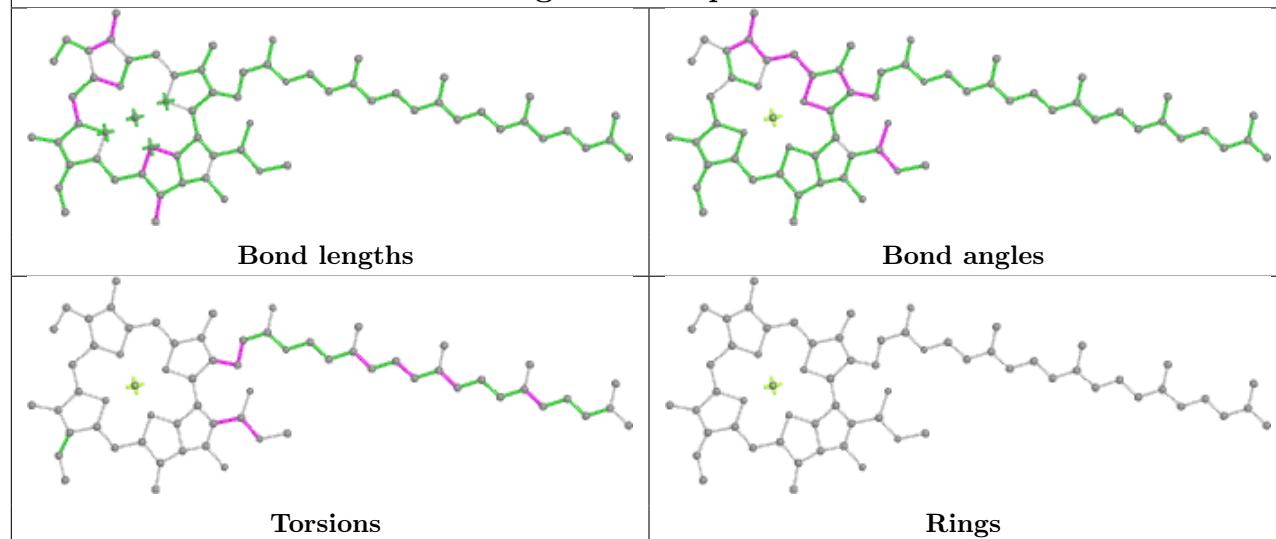


Ligand CLA b 610

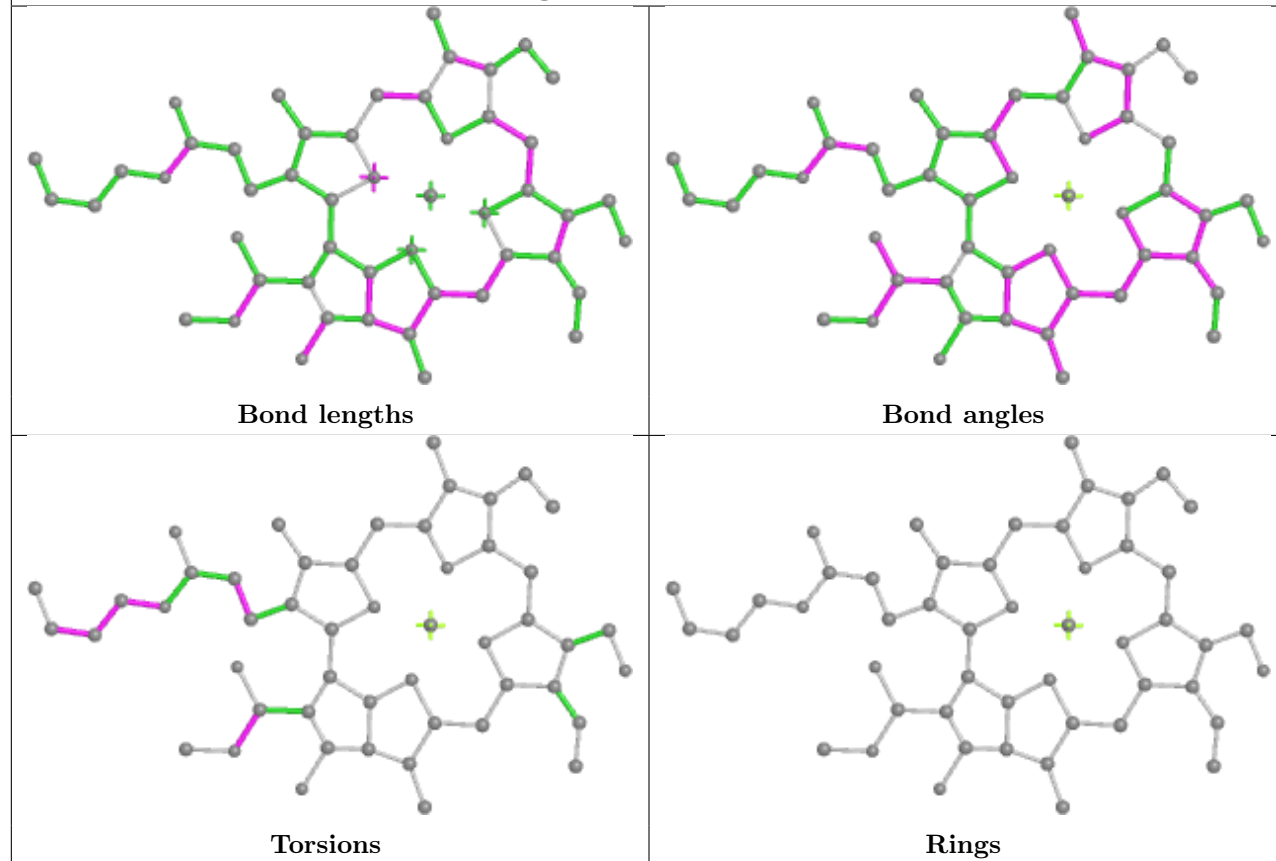


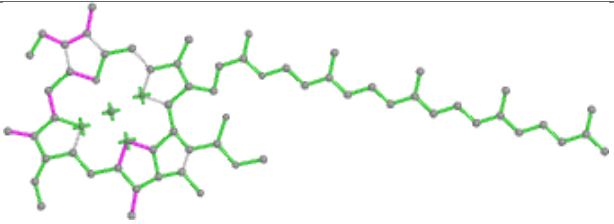
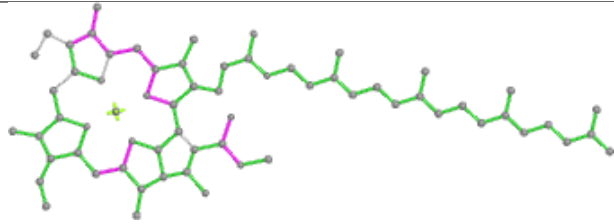
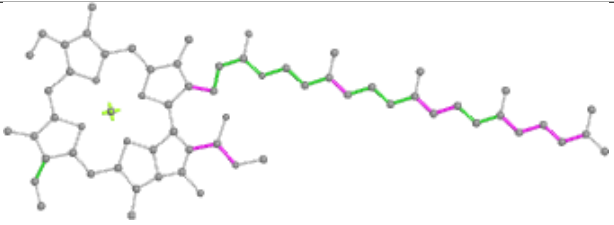
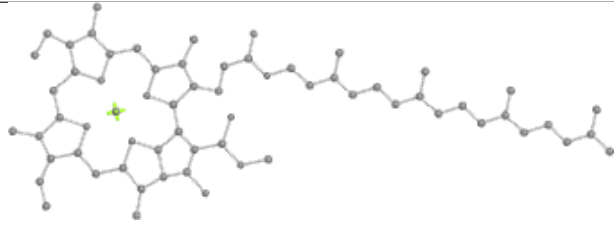
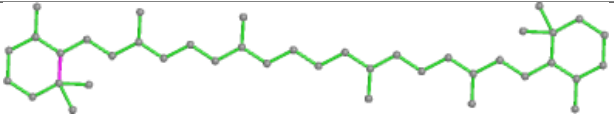
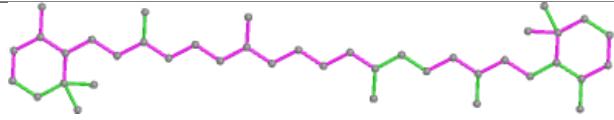
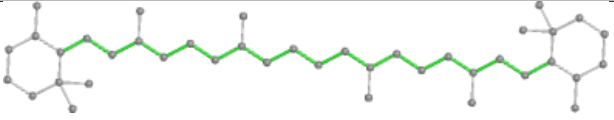
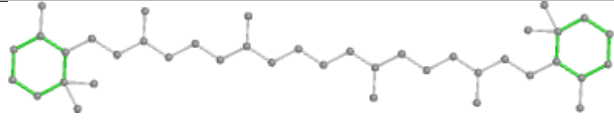
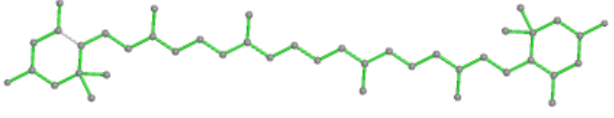
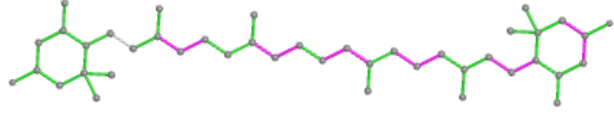
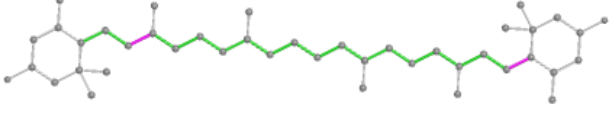
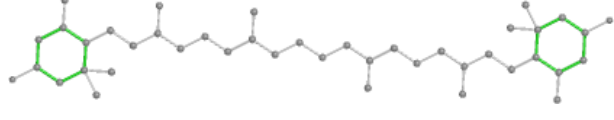


Ligand CLA p 603

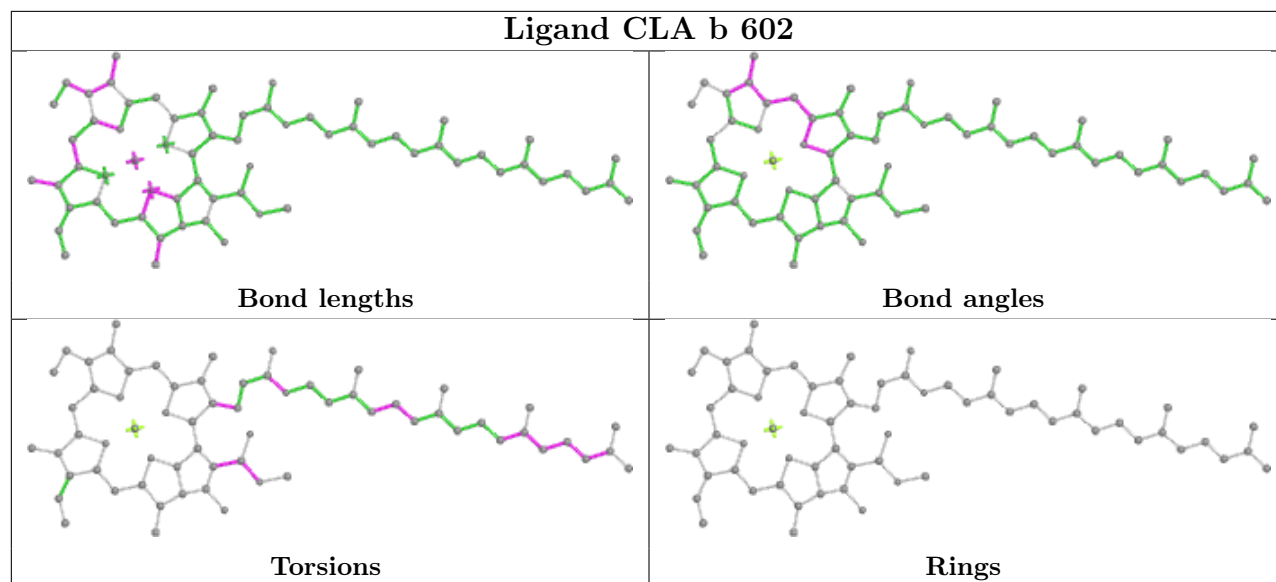


Ligand CHL 0 608

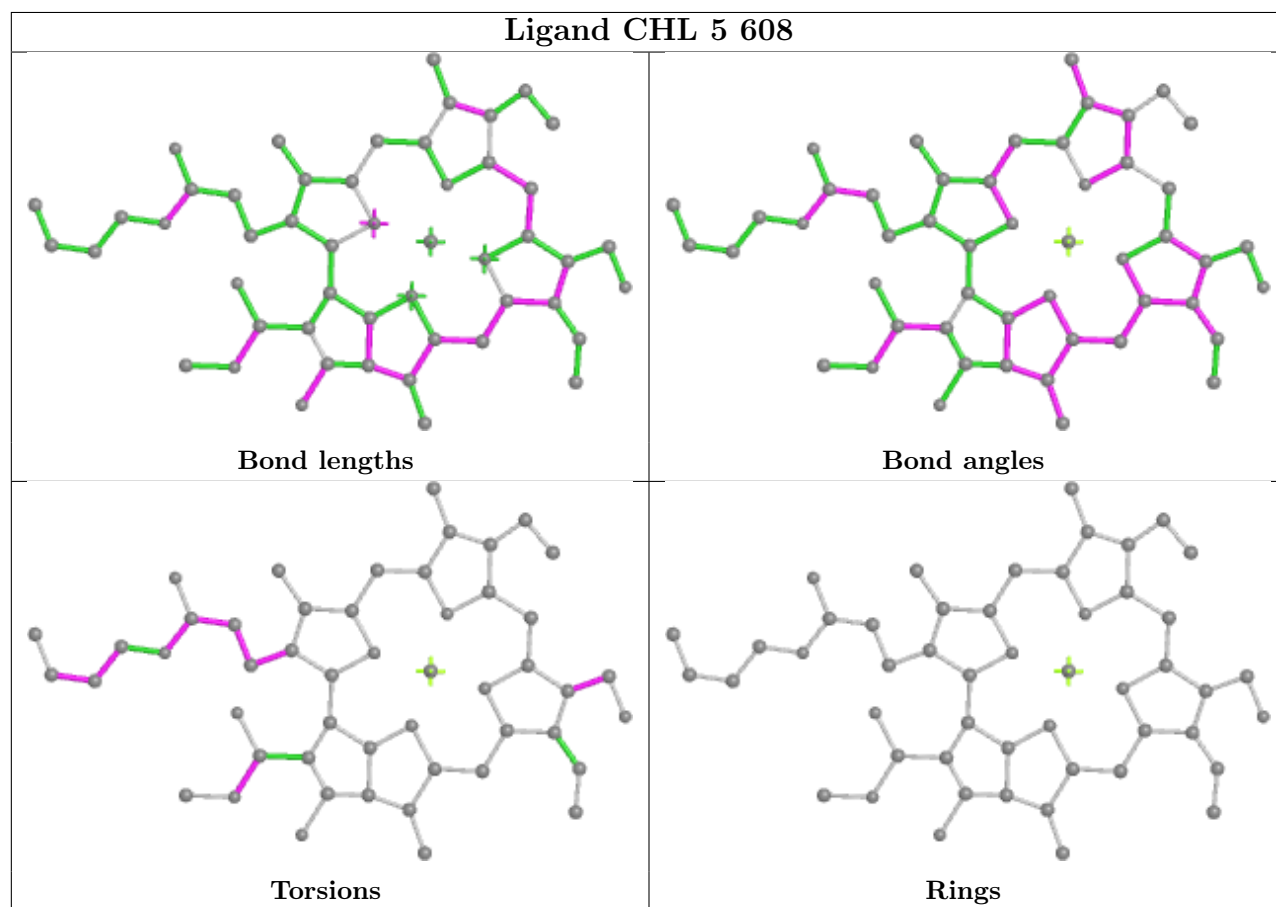


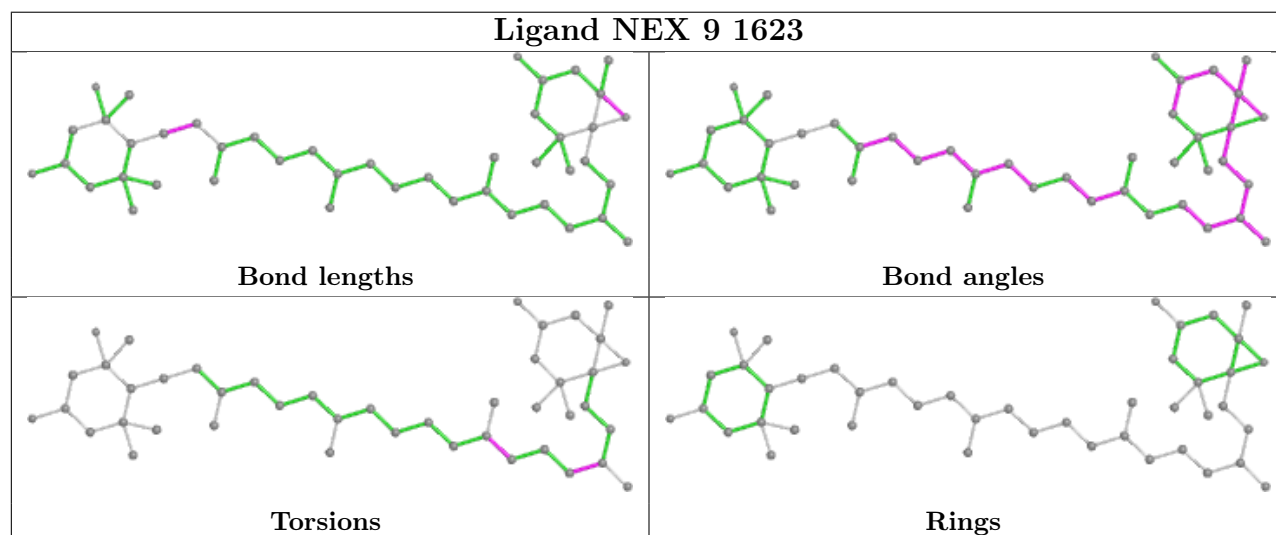
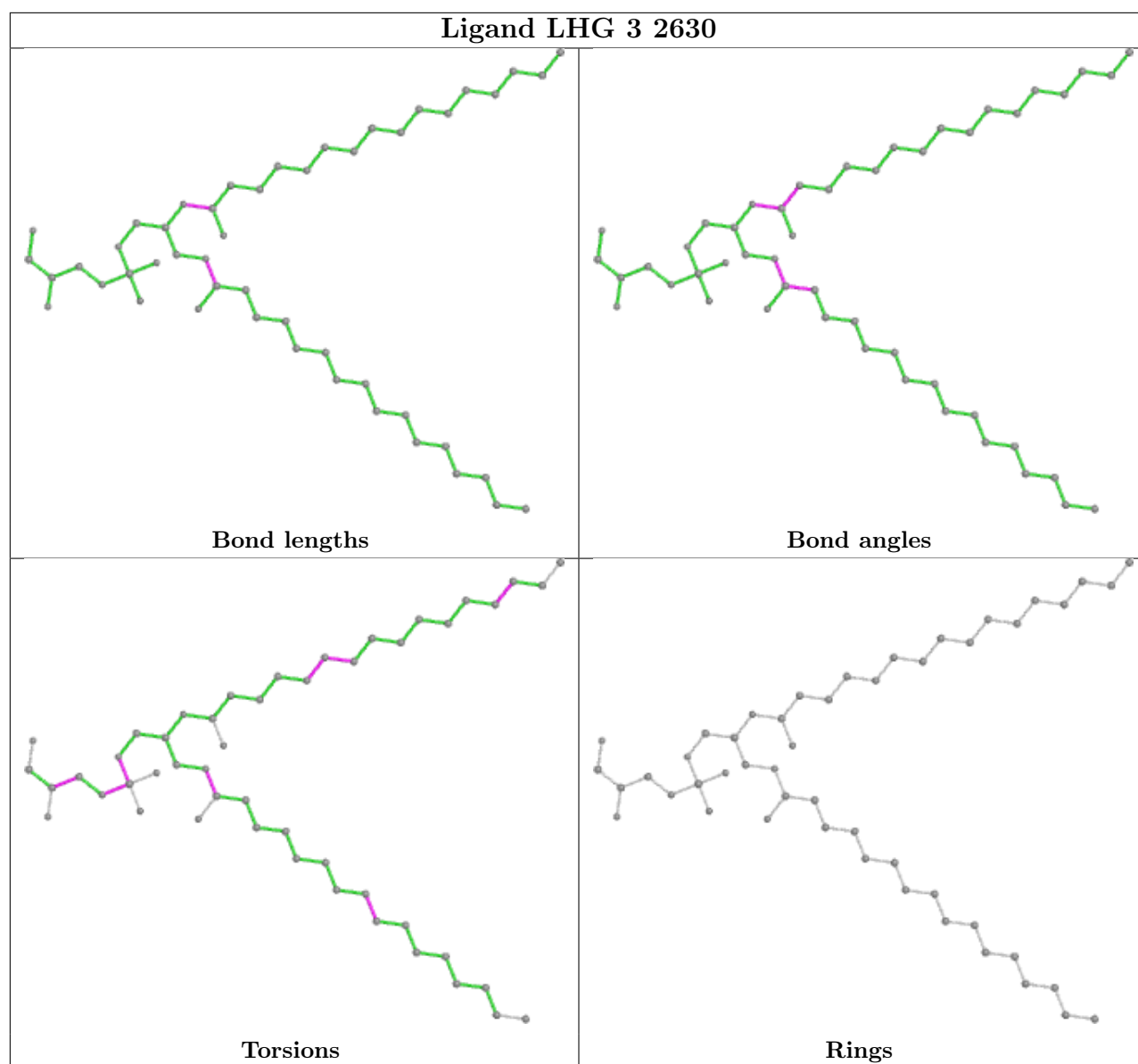
Ligand CLA 0 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT g 1620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA b 602

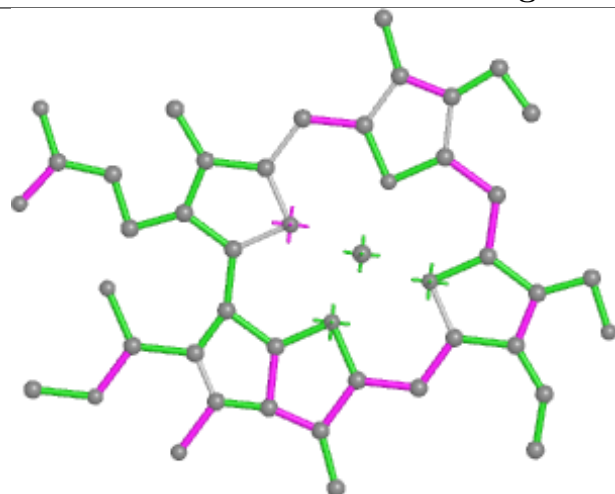


Ligand CHL 5 608

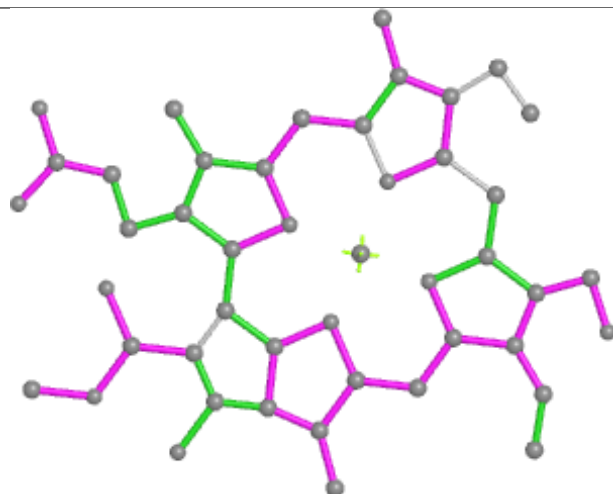




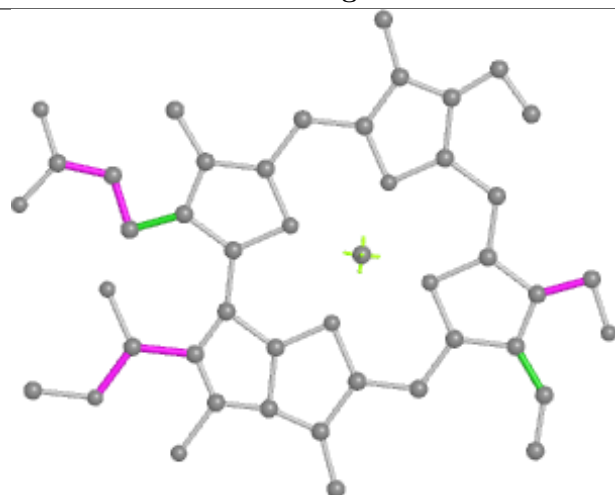
Ligand CHL S 601



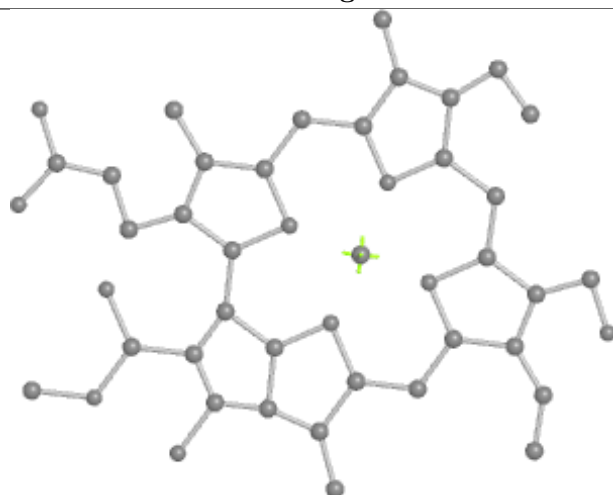
Bond lengths



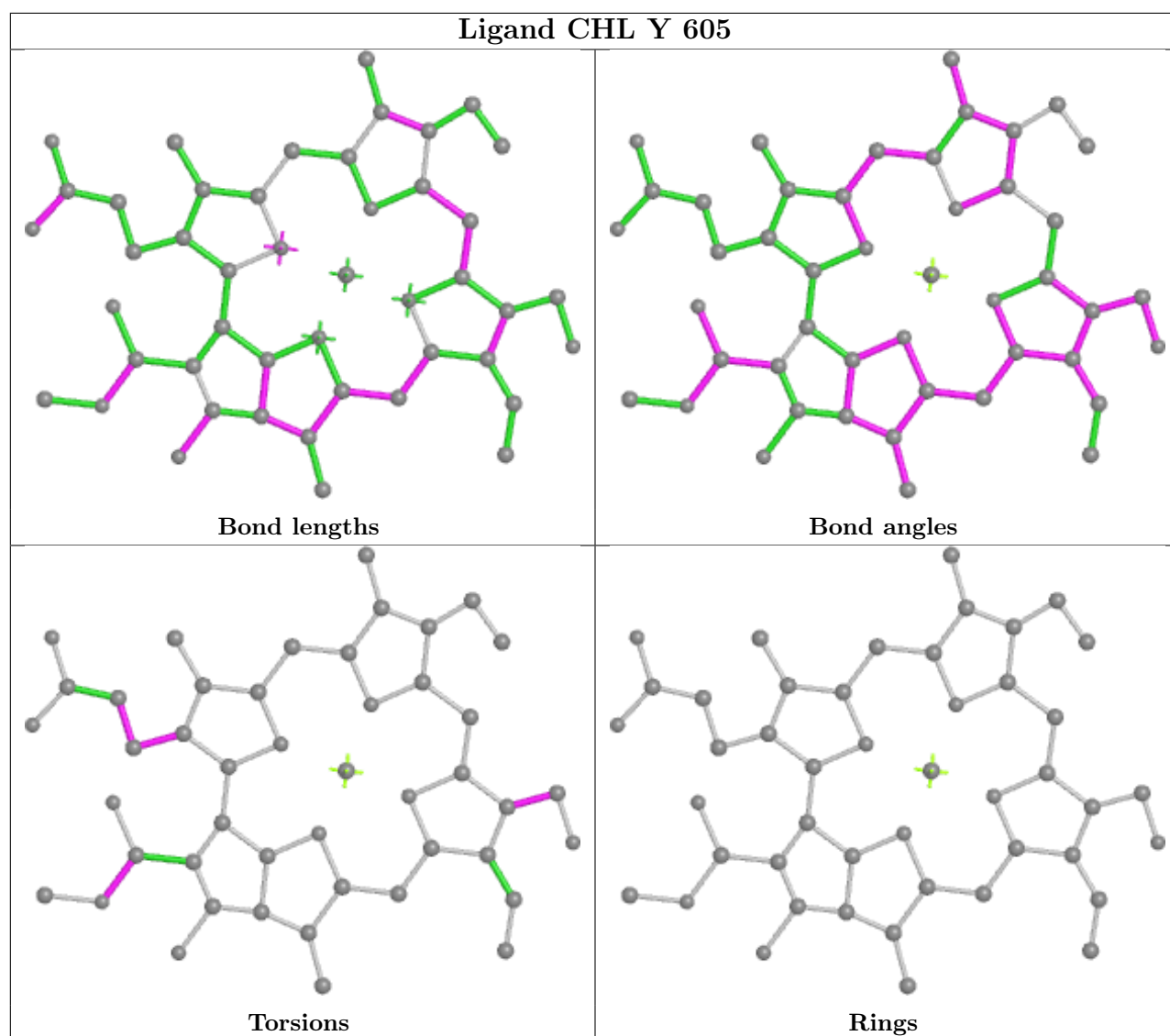
Bond angles



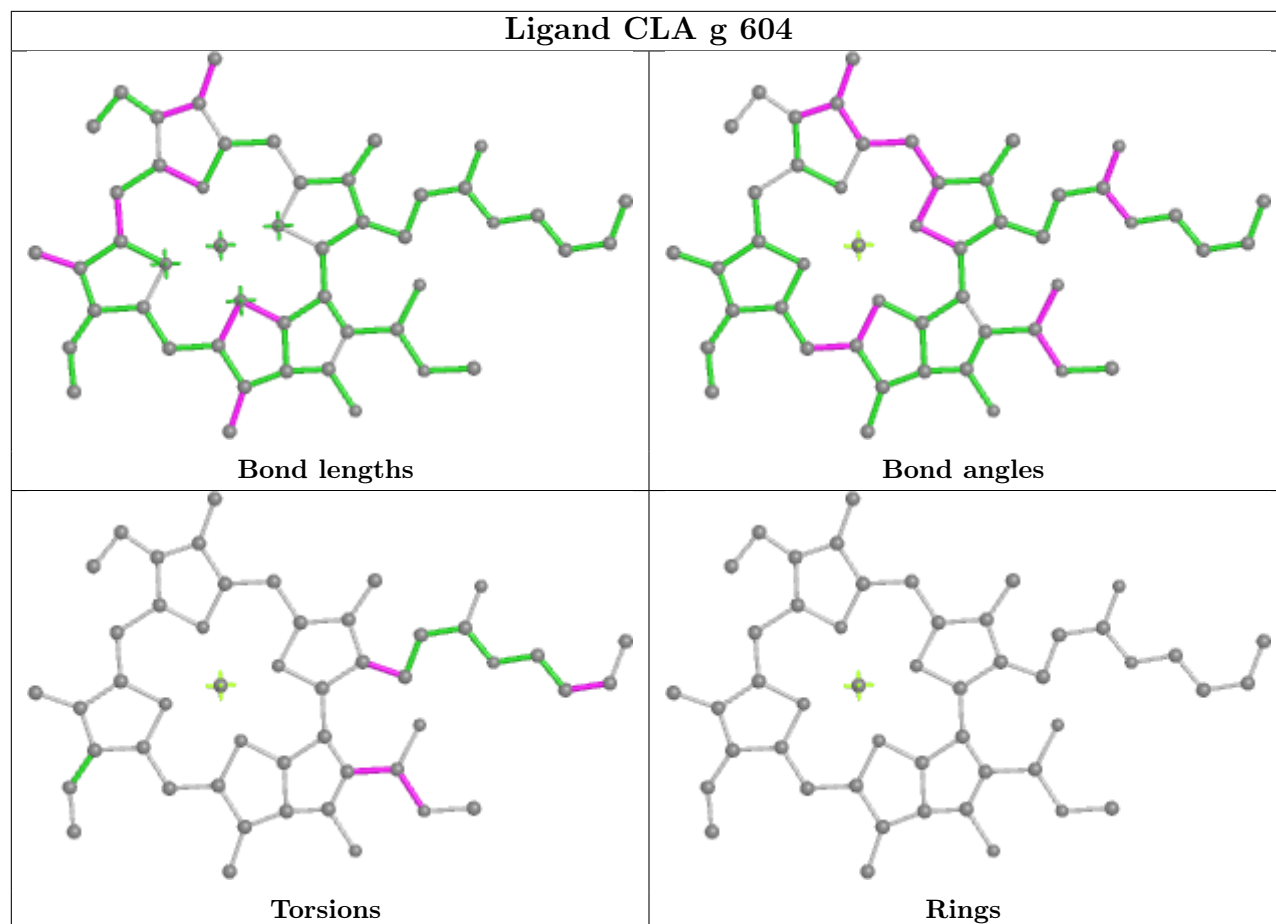
Torsions



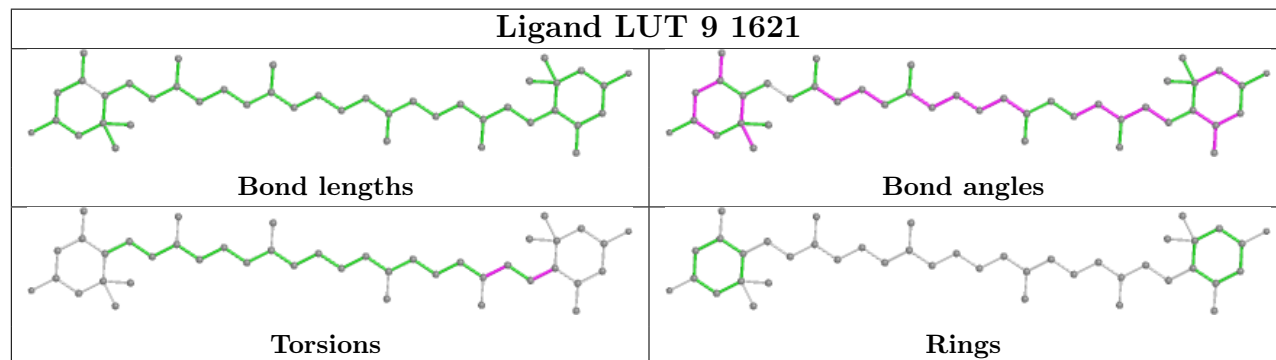
Rings

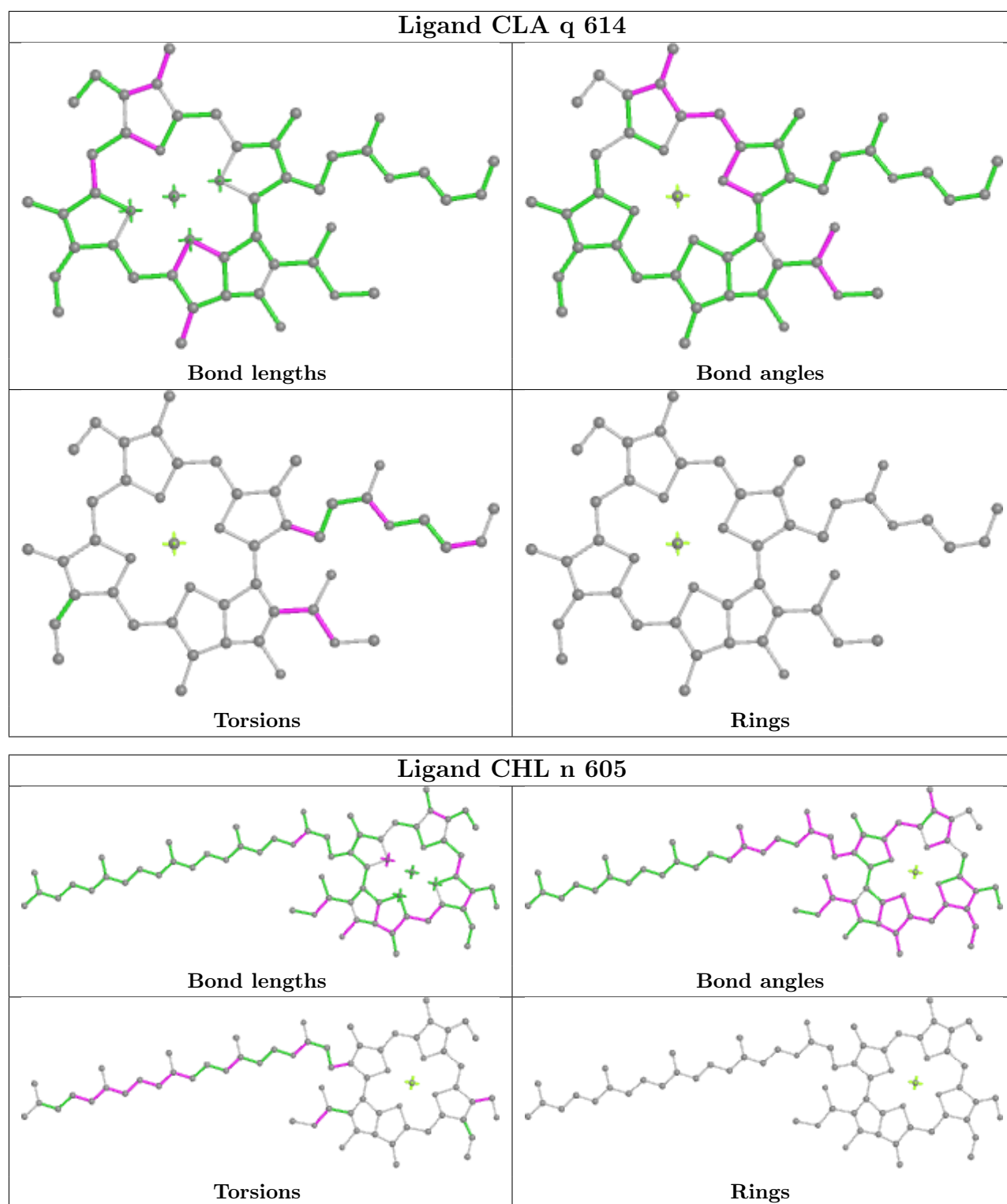


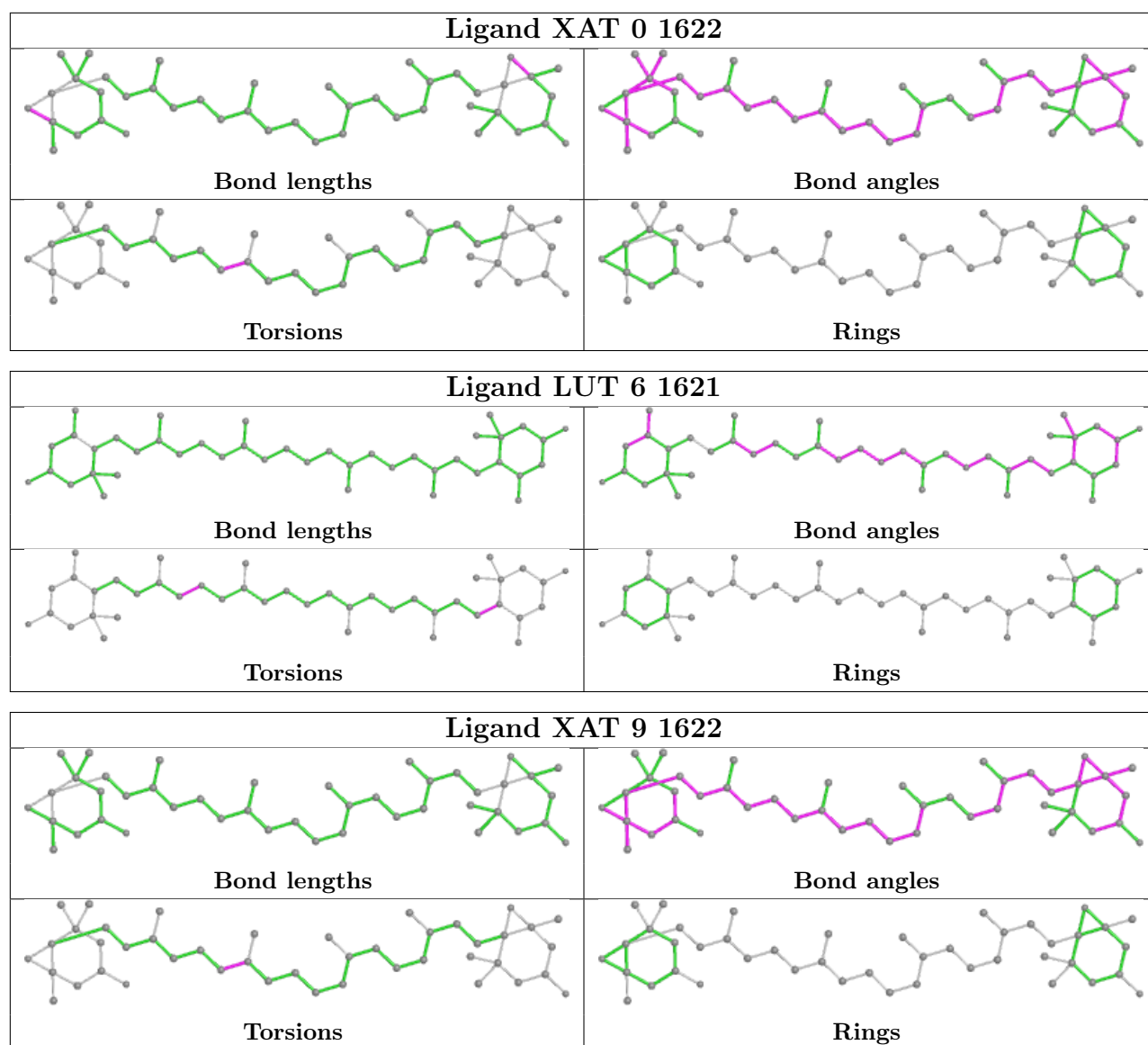
Ligand CLA g 604



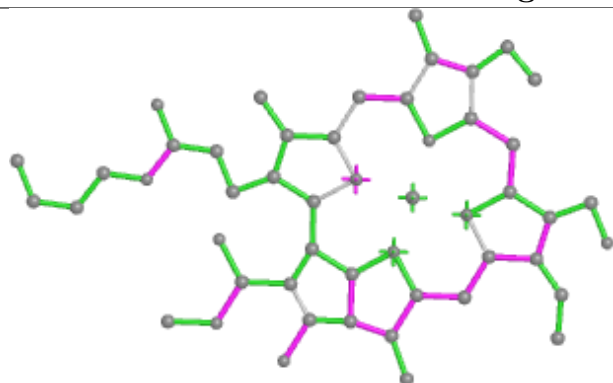
Ligand LUT 9 1621



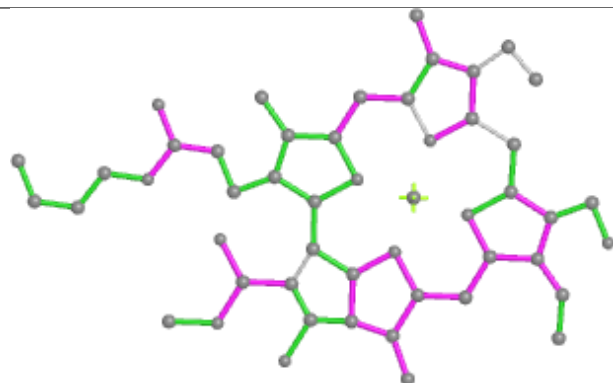




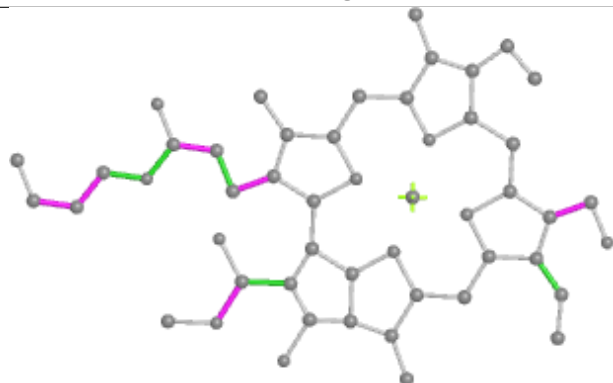
Ligand CHL 2 606



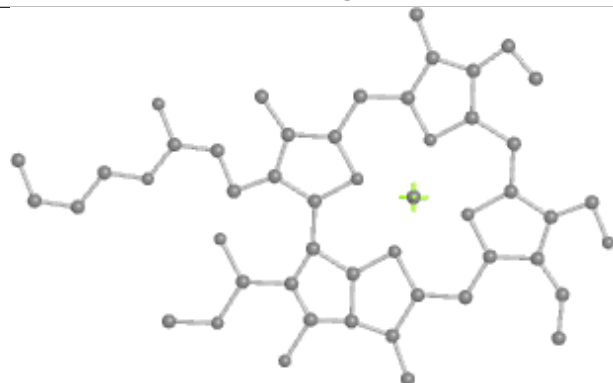
Bond lengths



Bond angles

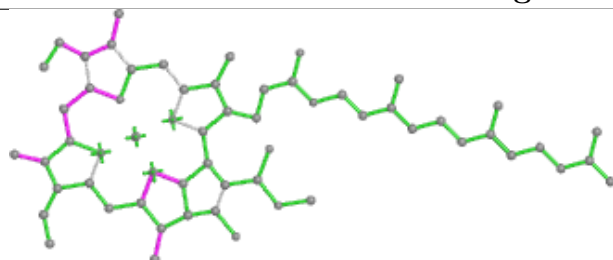


Torsions

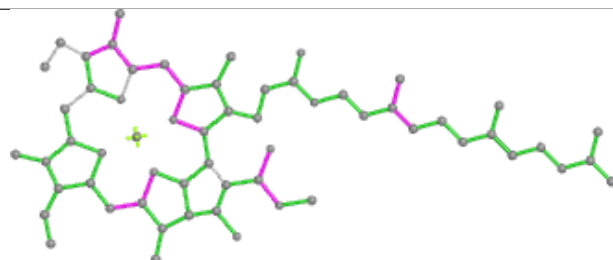


Rings

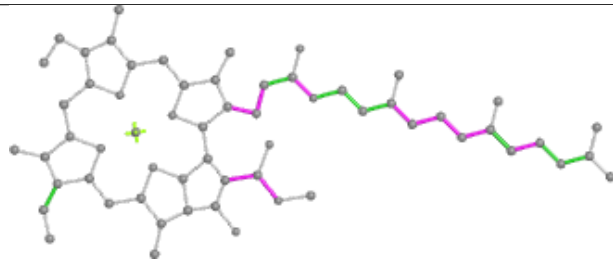
Ligand CLA R 613



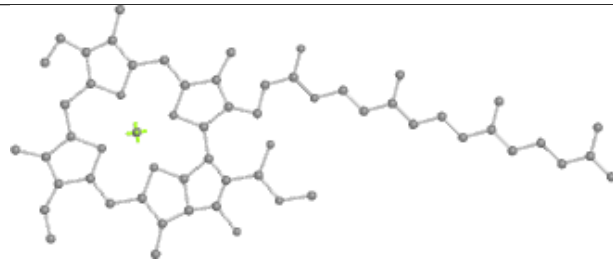
Bond lengths



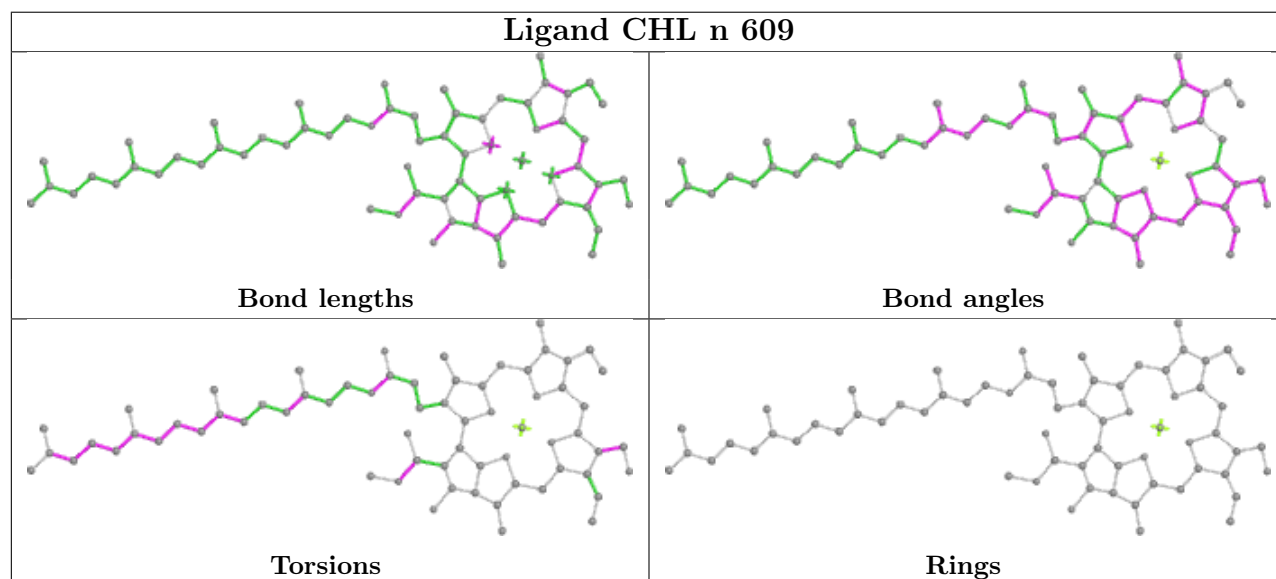
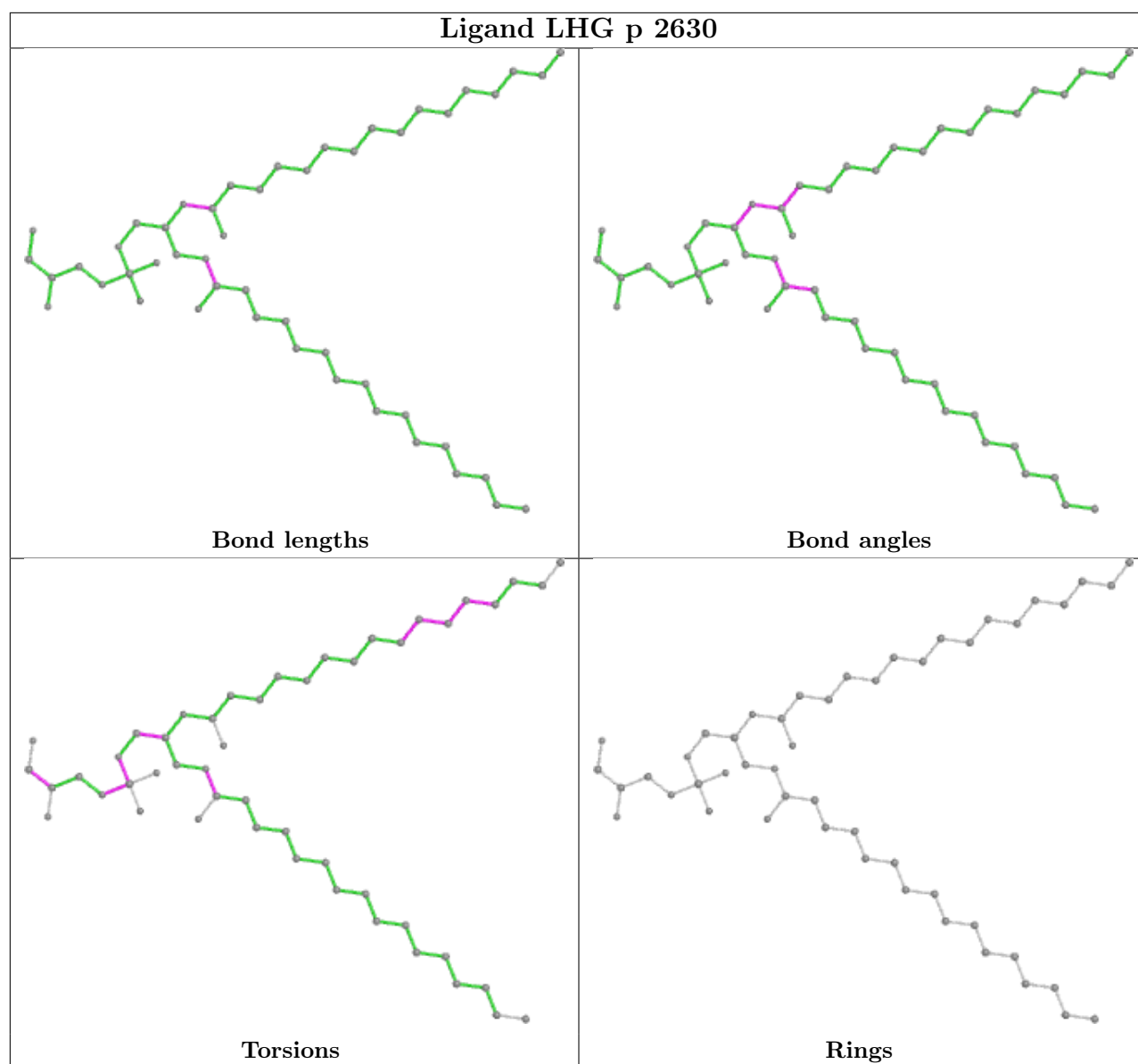
Bond angles

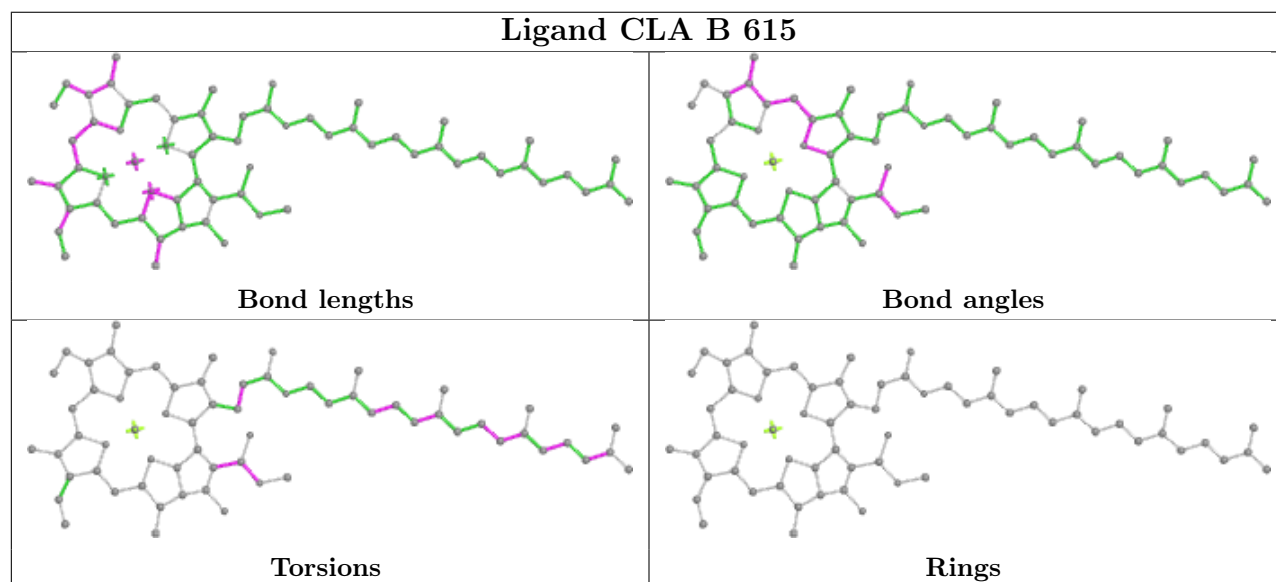
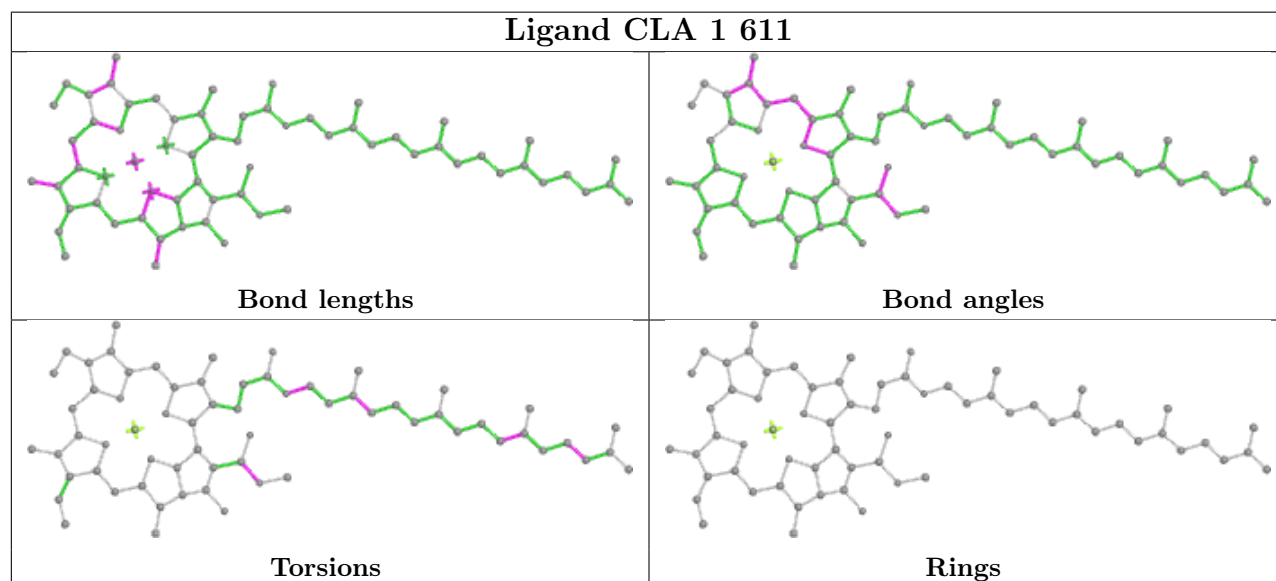
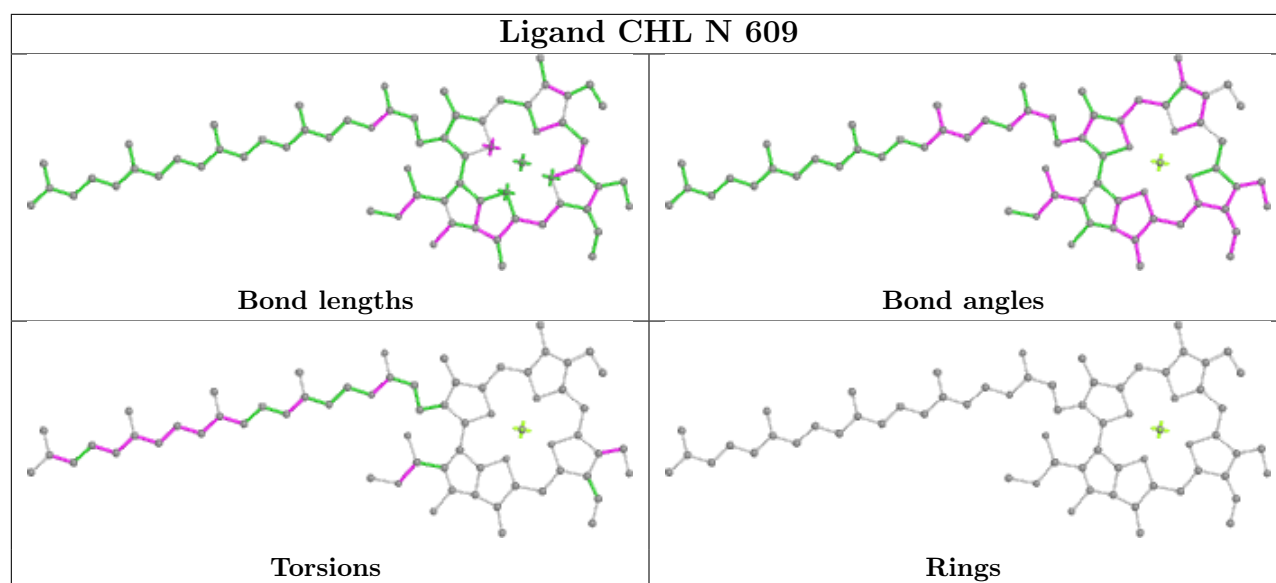


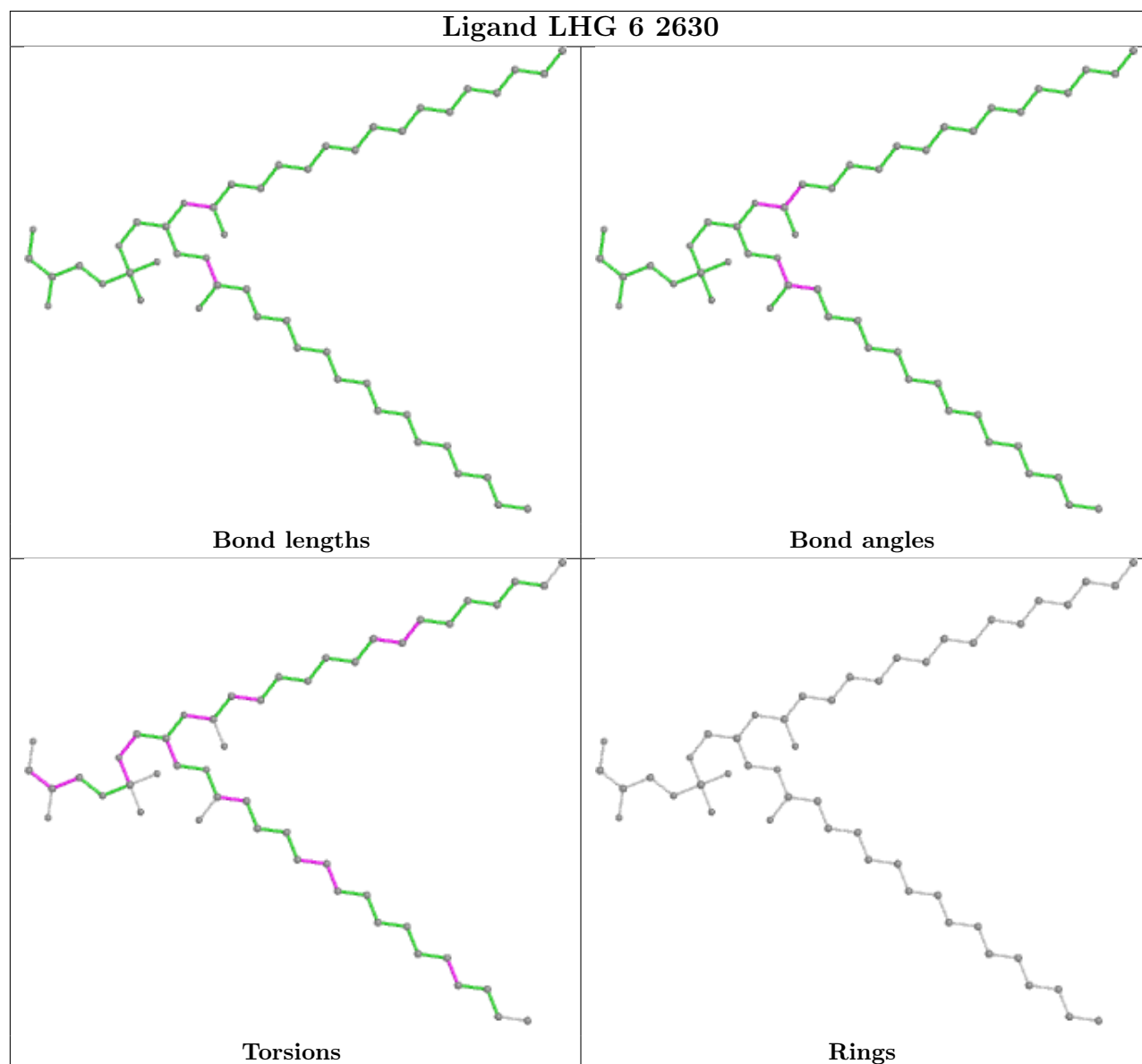
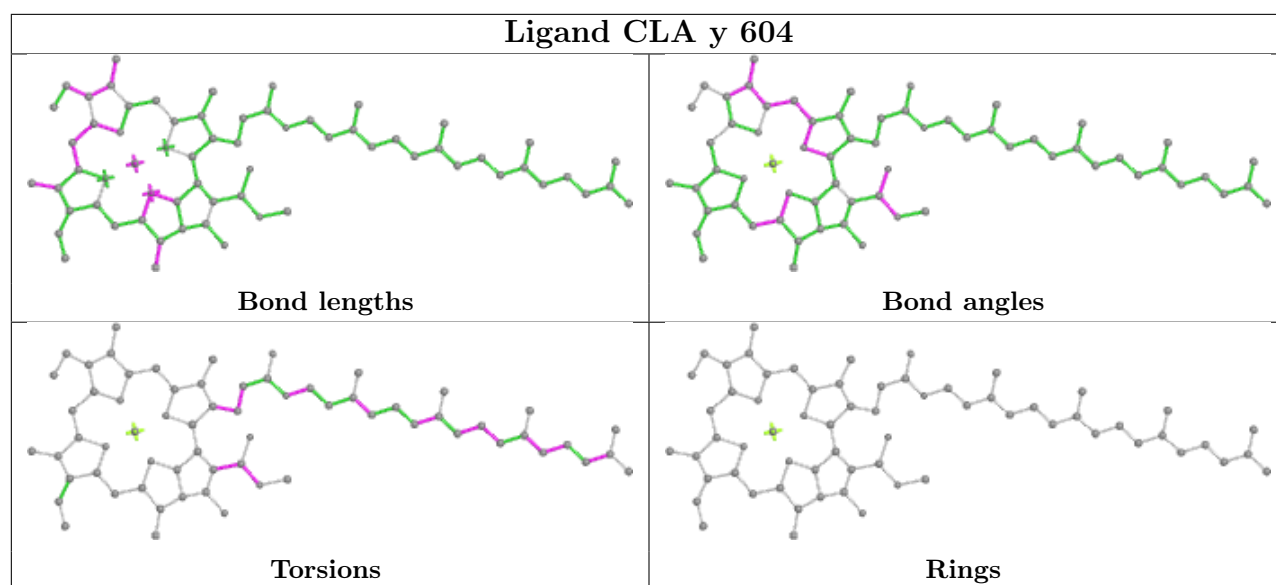
Torsions

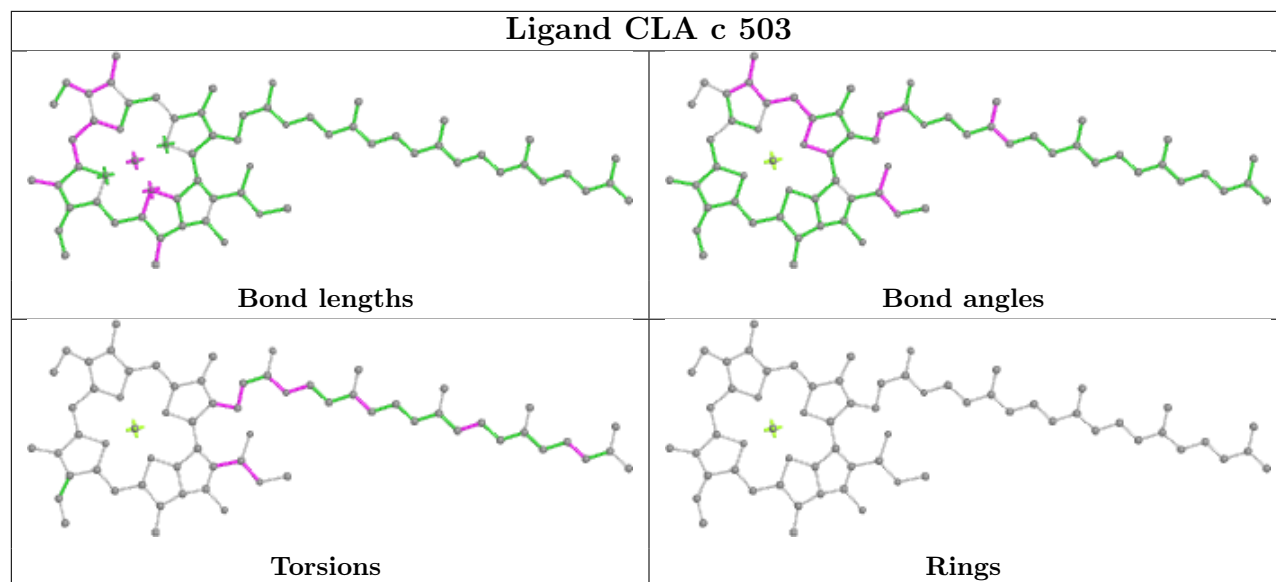
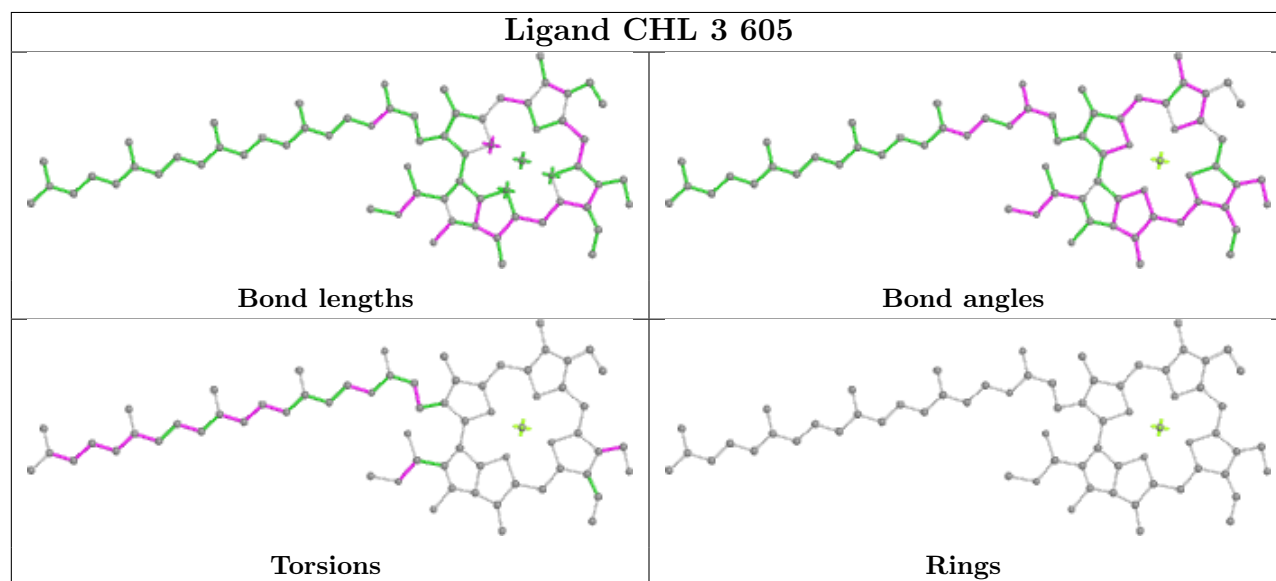


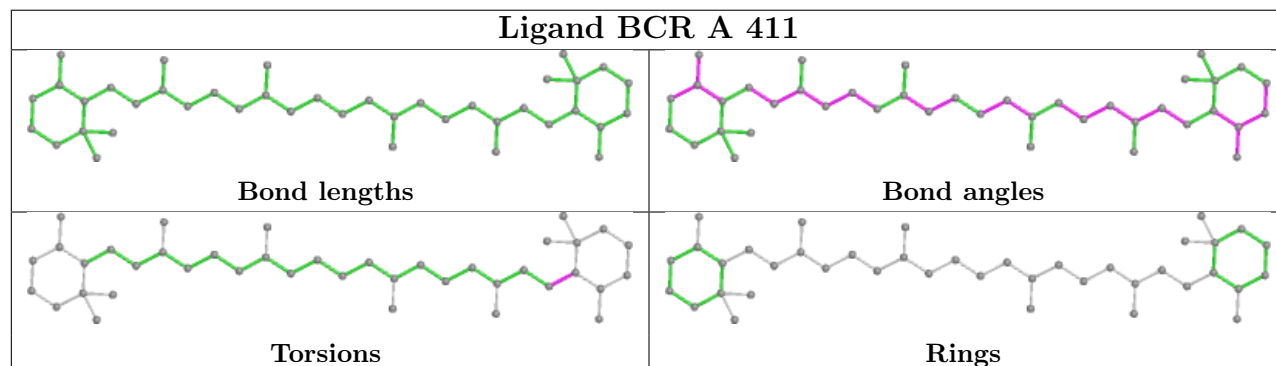
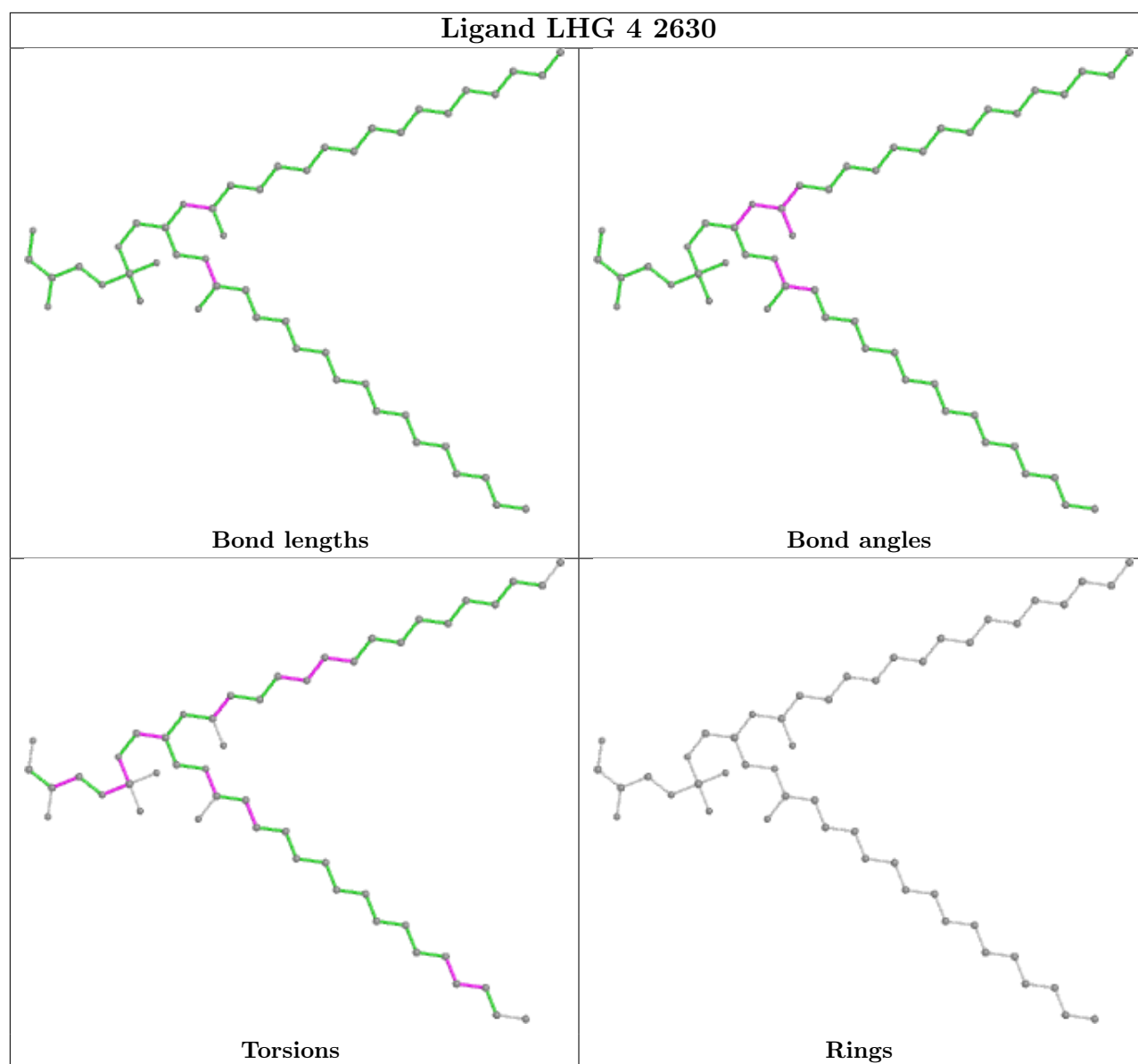
Rings

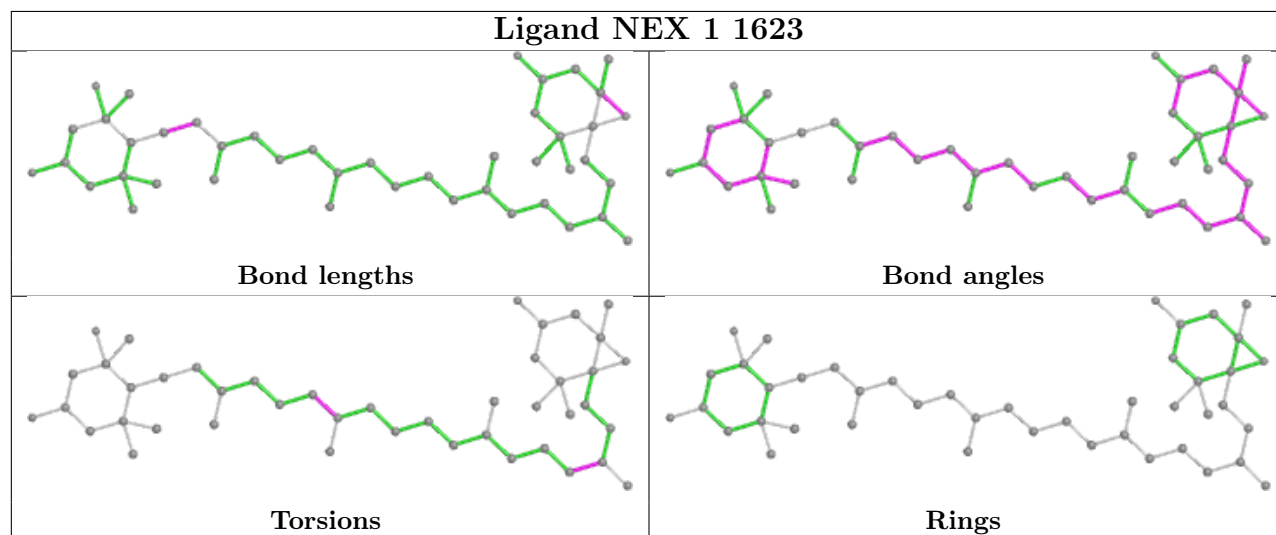
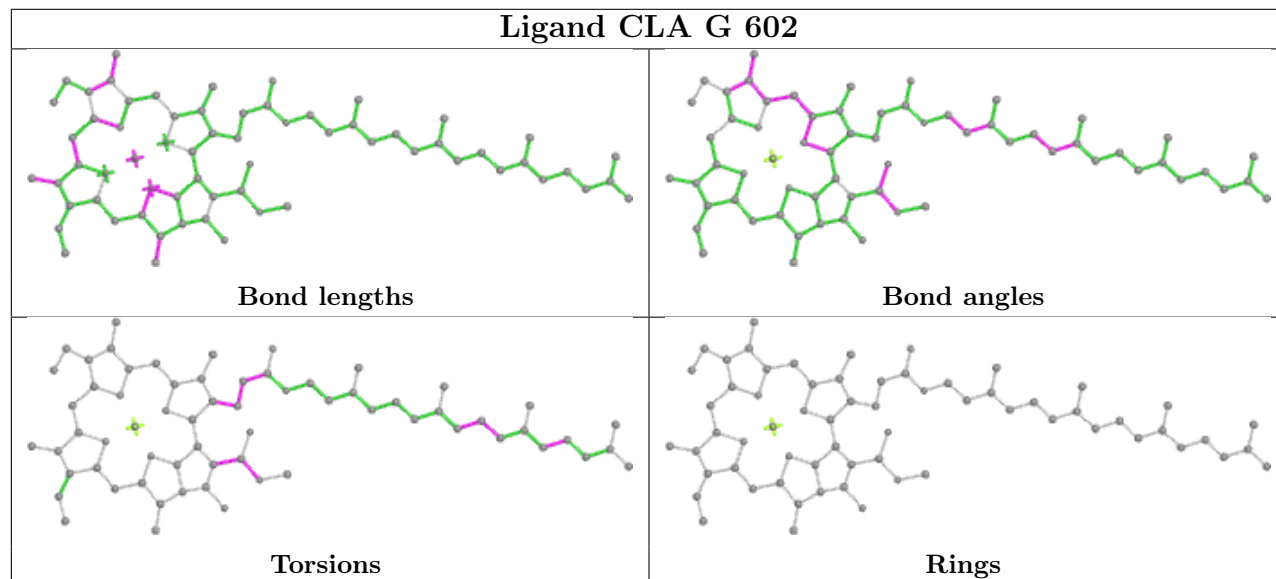
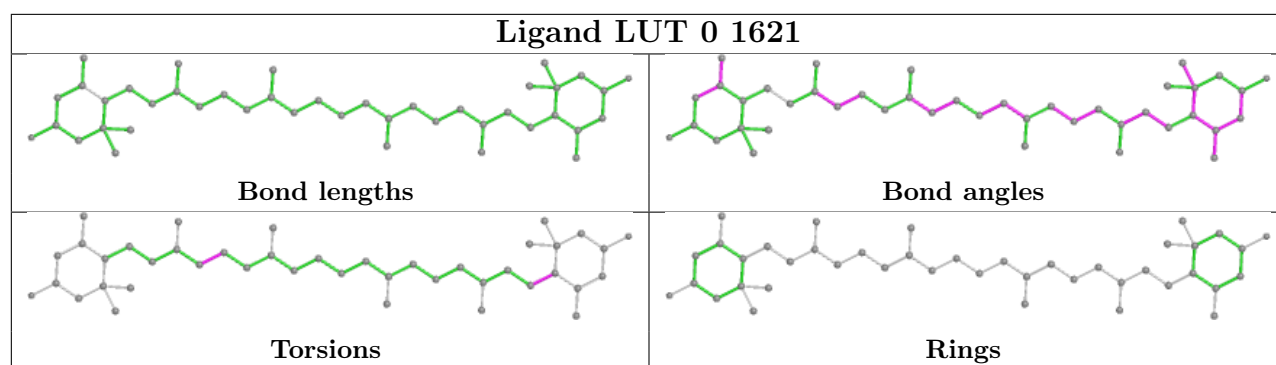


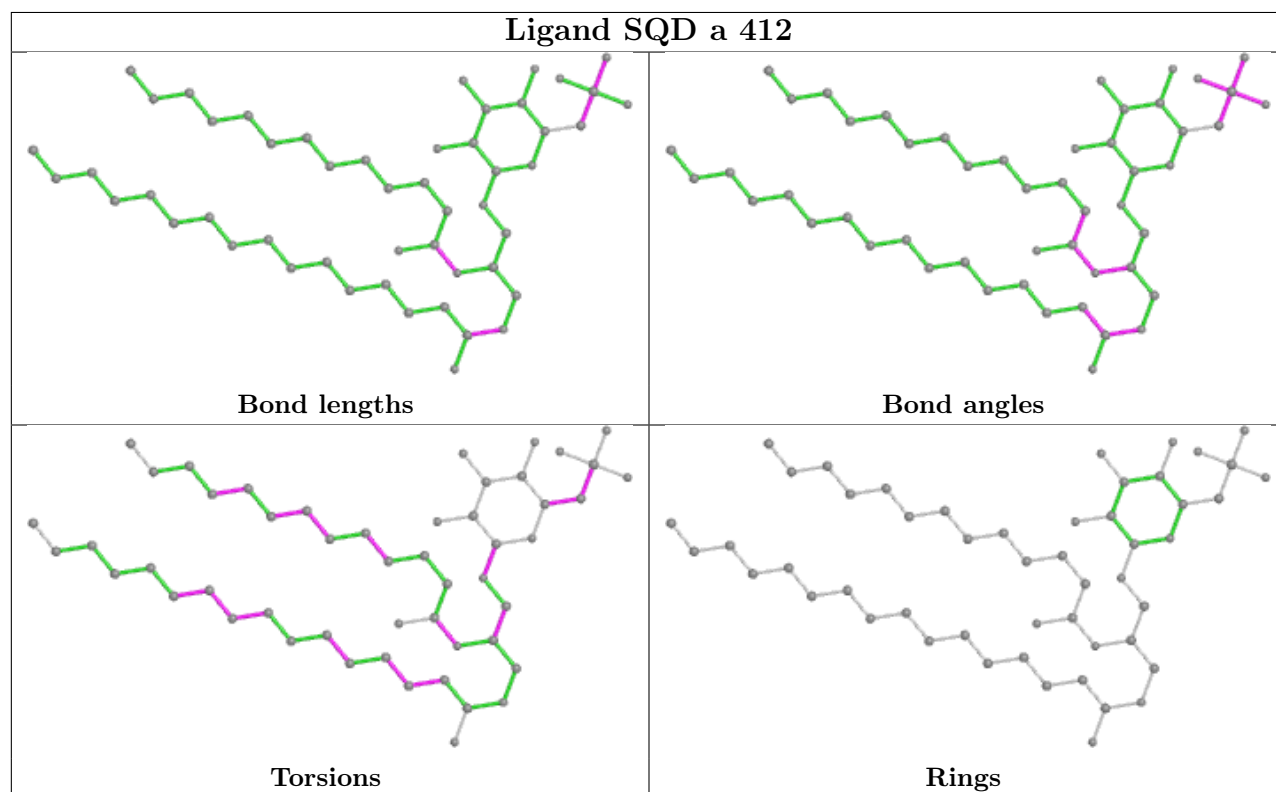
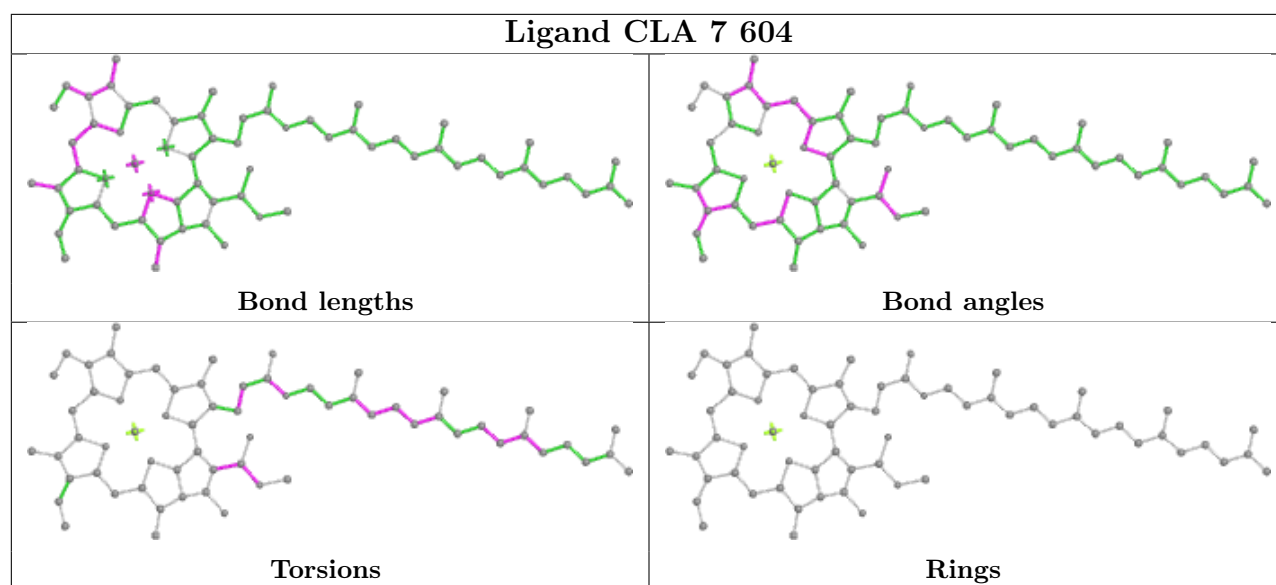


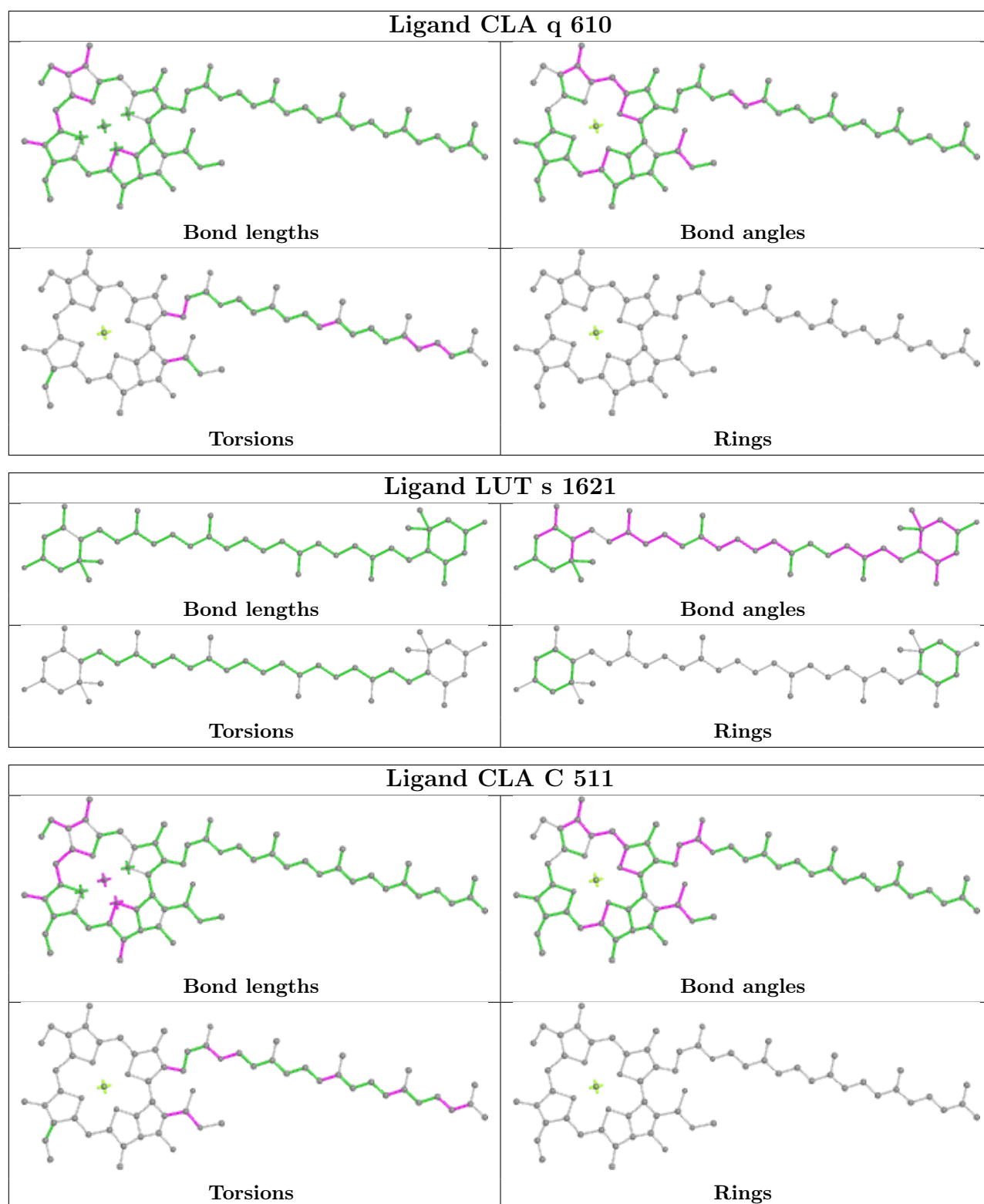


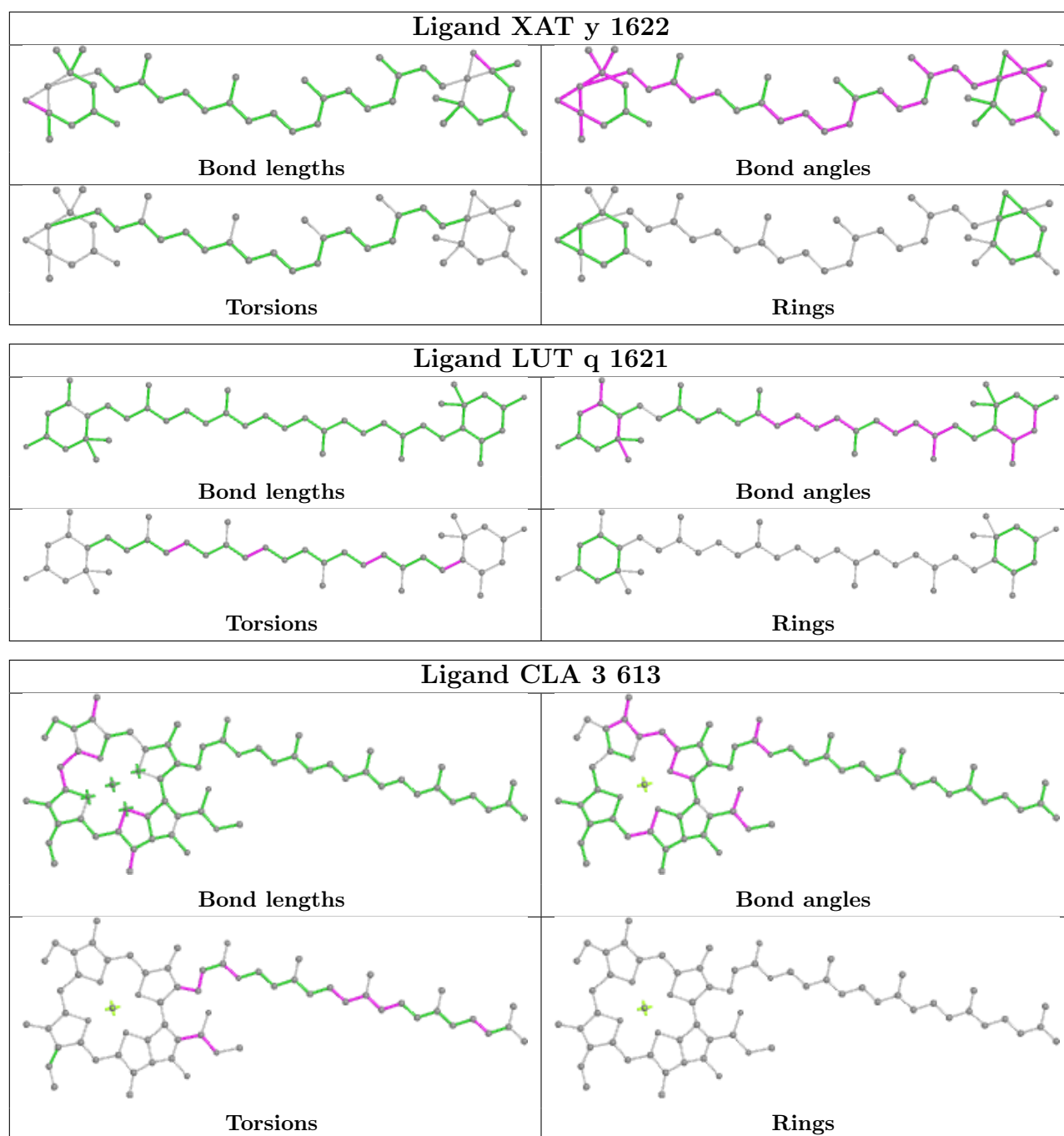
Ligand CLA c 503**Ligand CHL 3 605**

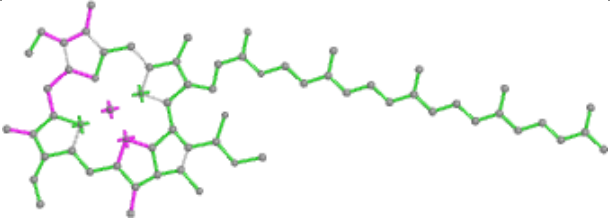
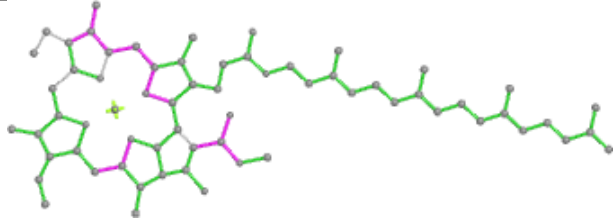
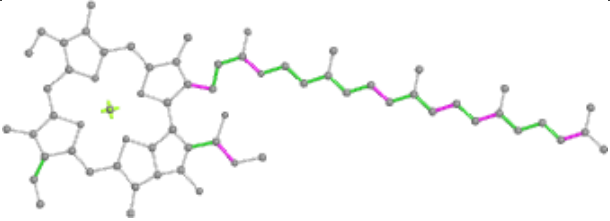
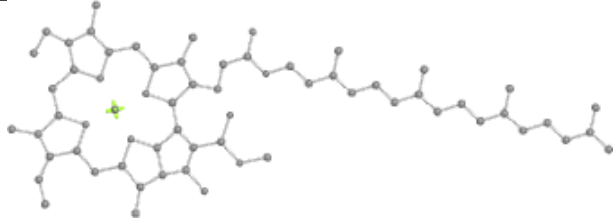
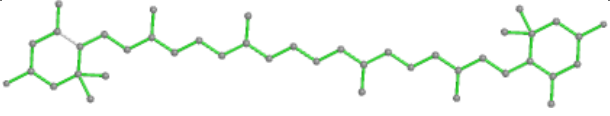
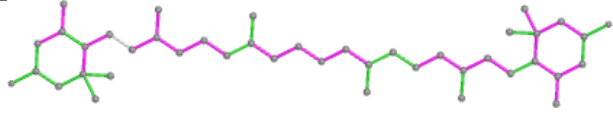
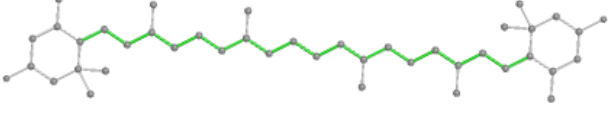
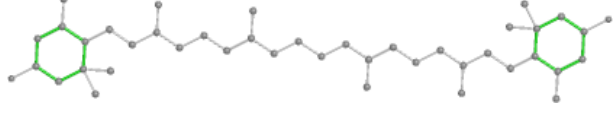
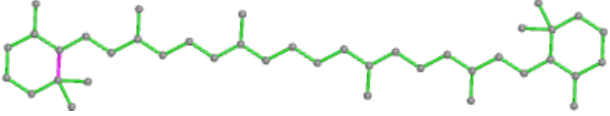
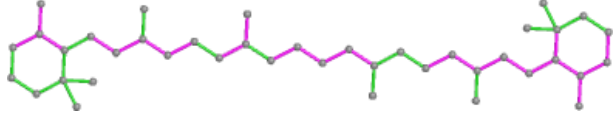
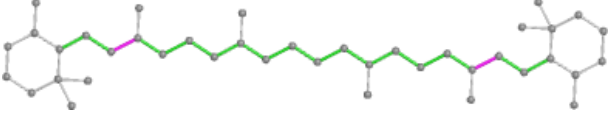
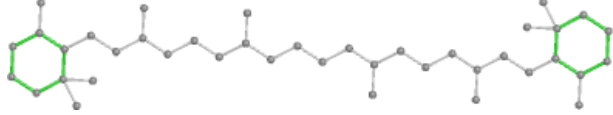


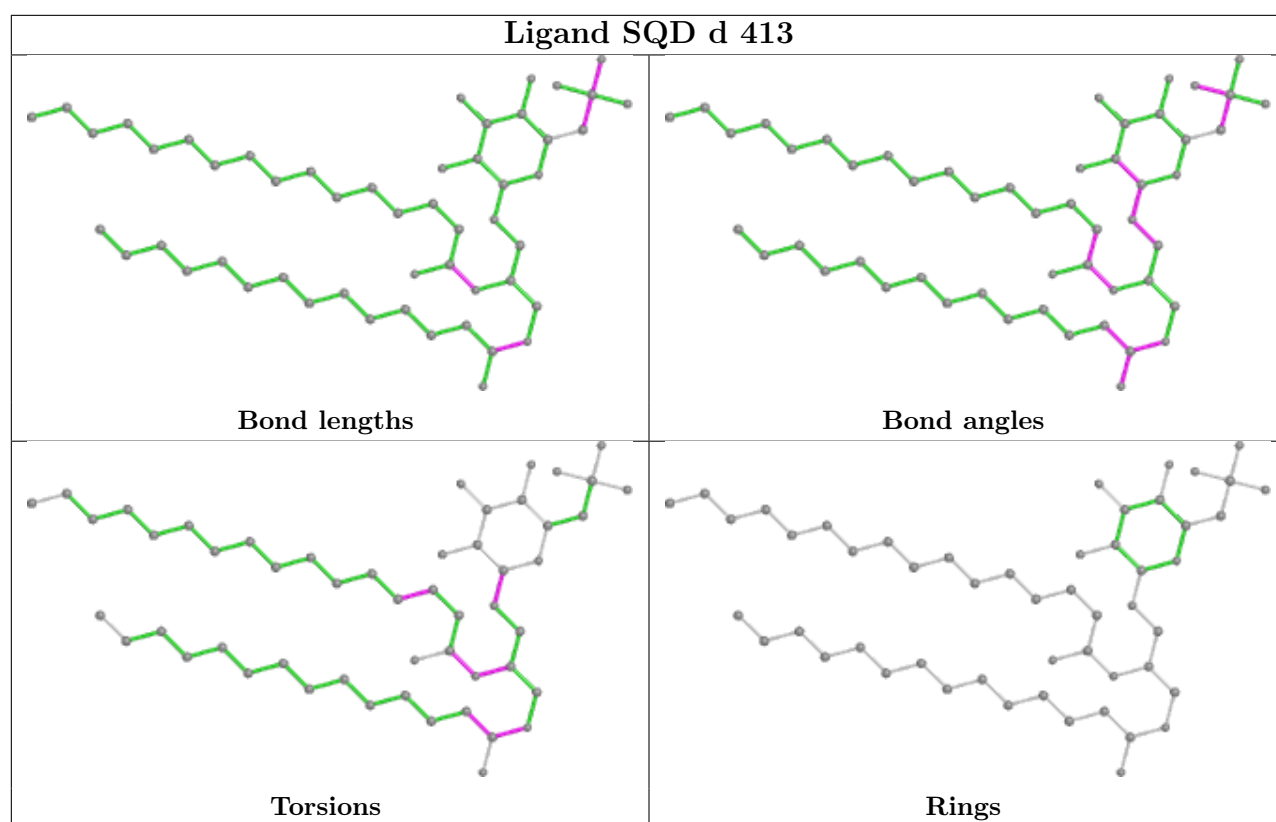
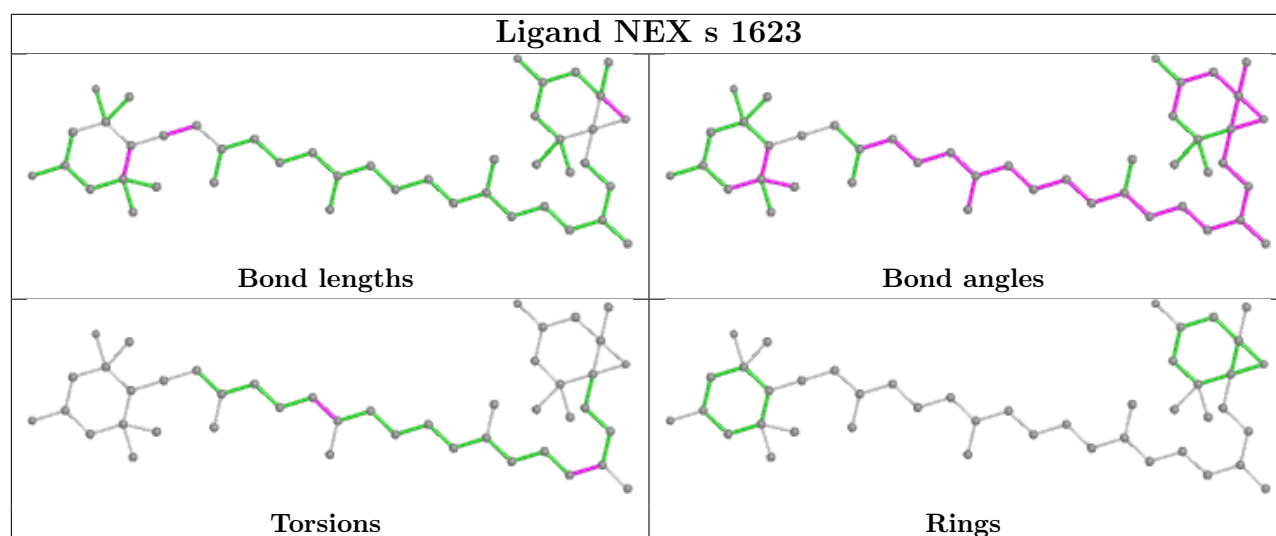




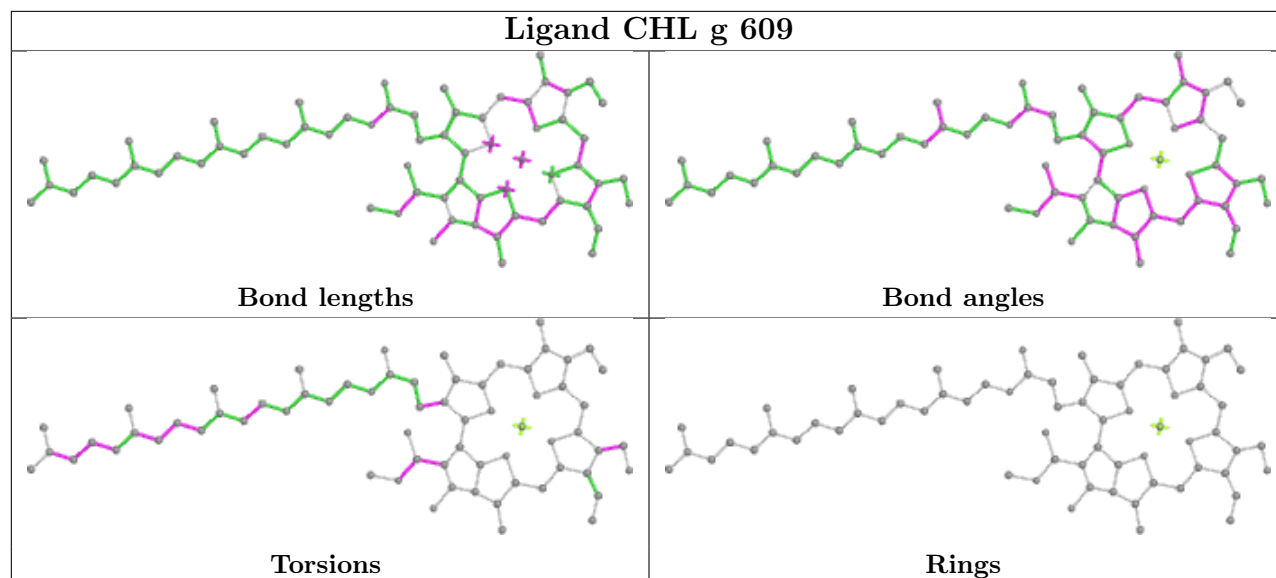




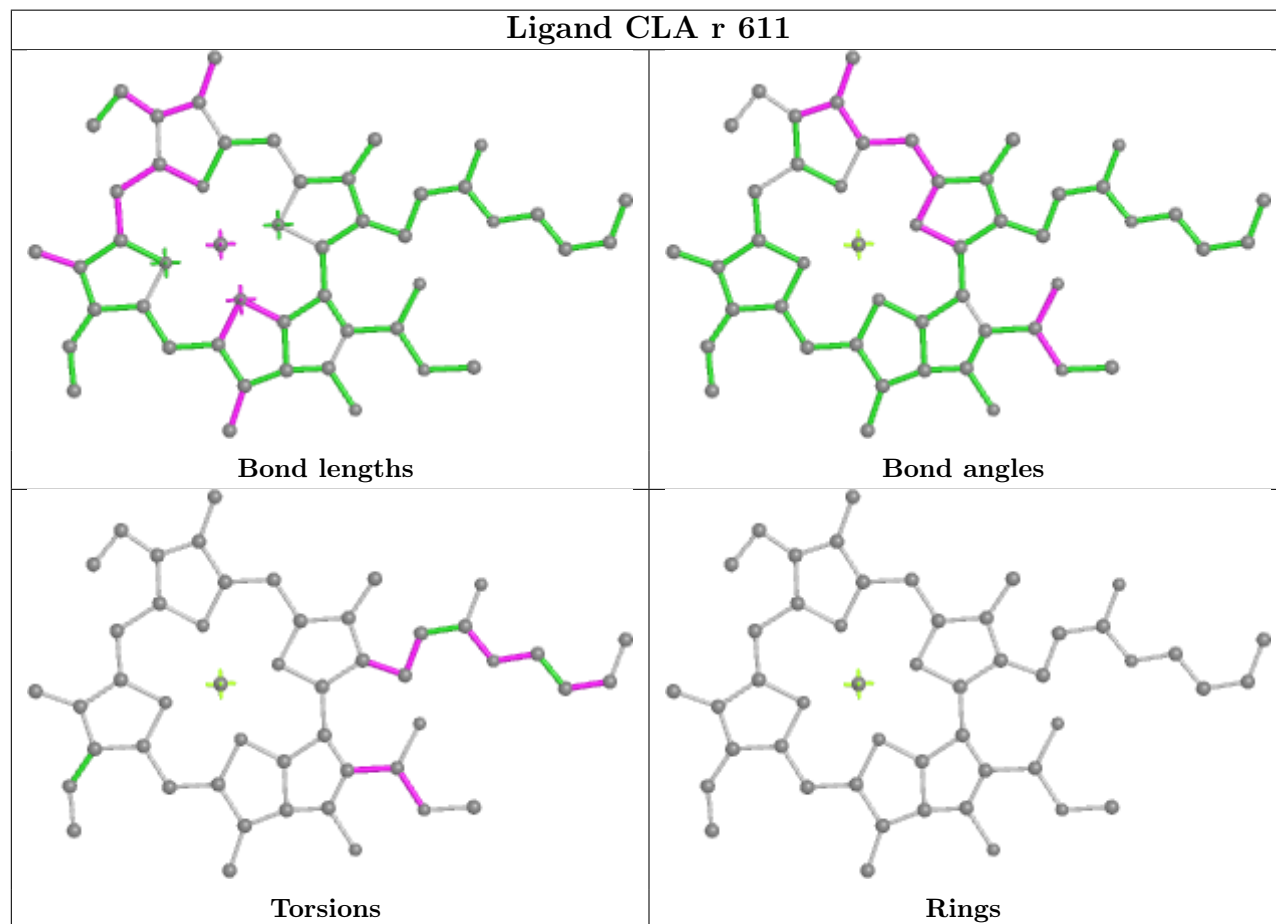
Ligand CLA D 403	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S 1621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR D 404	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



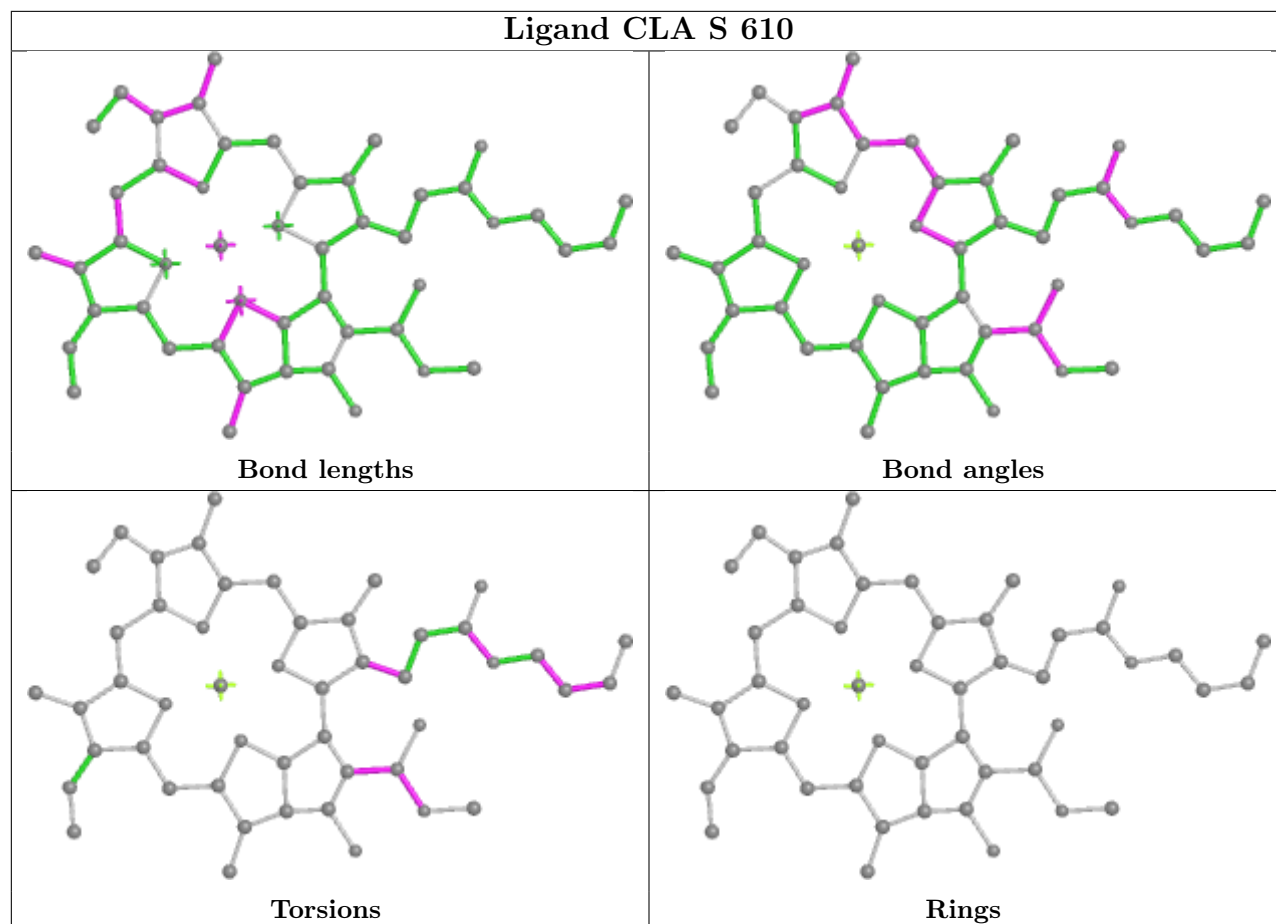
Ligand CHL g 609

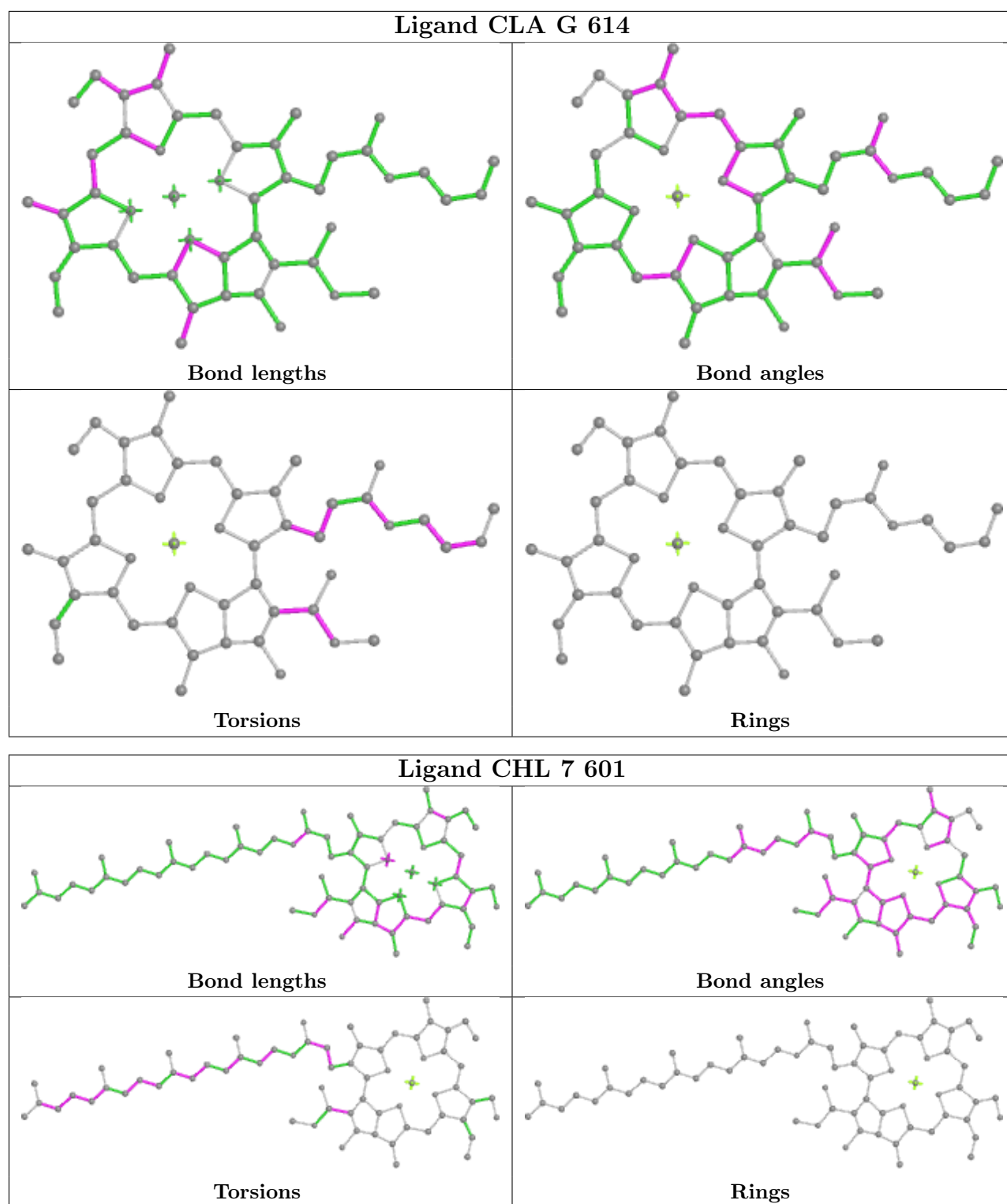


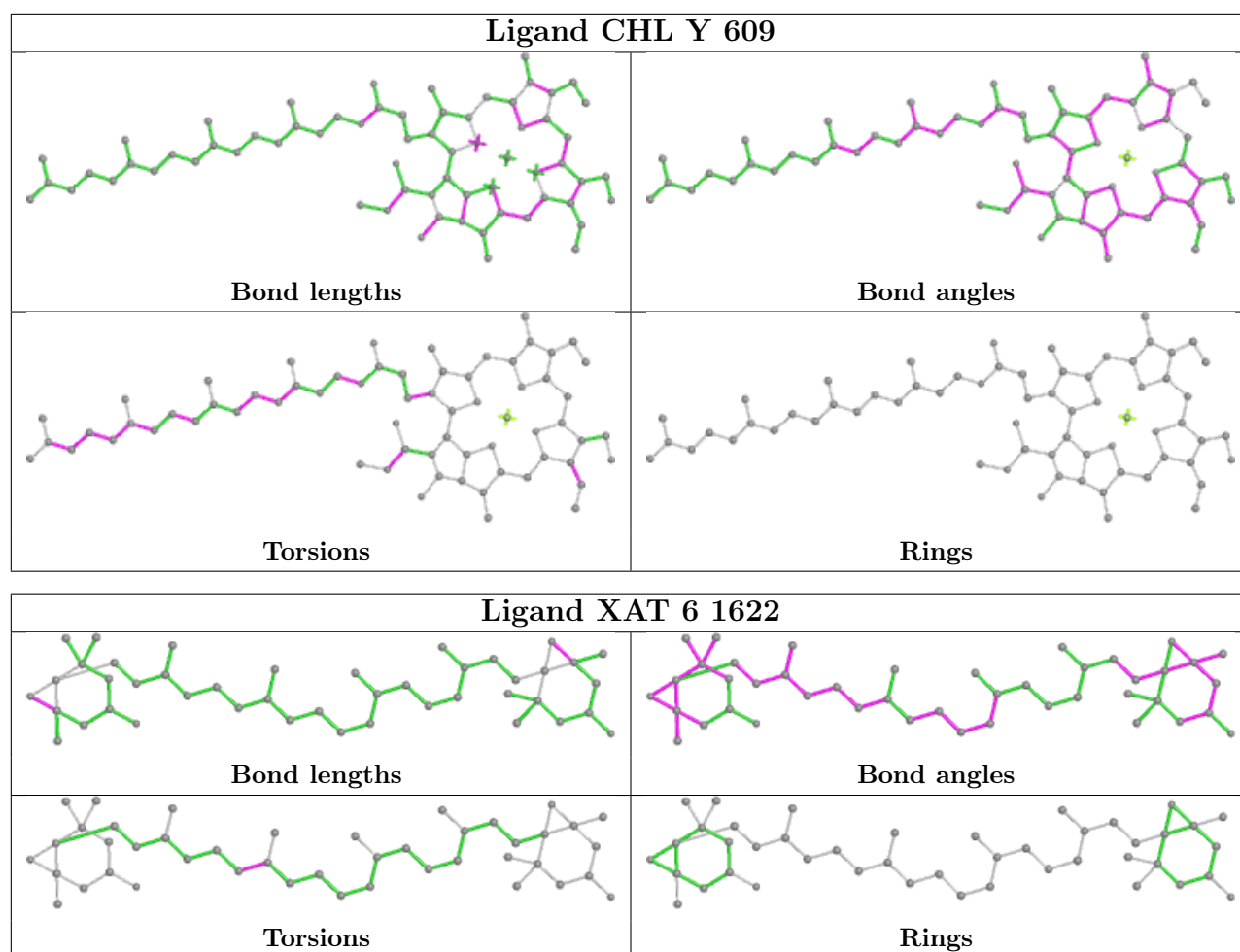
Ligand CLA r 611

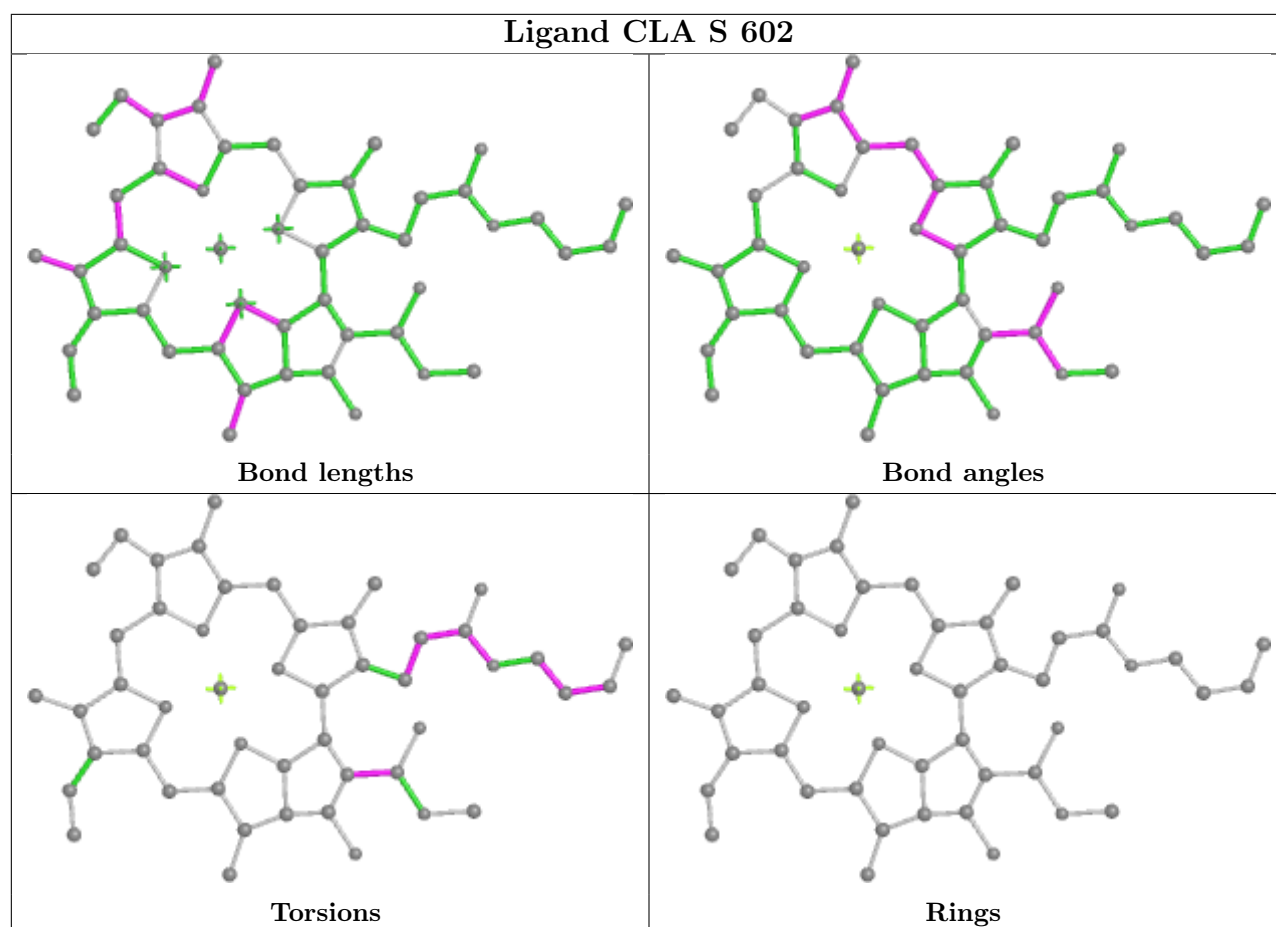


Ligand CLA S 610

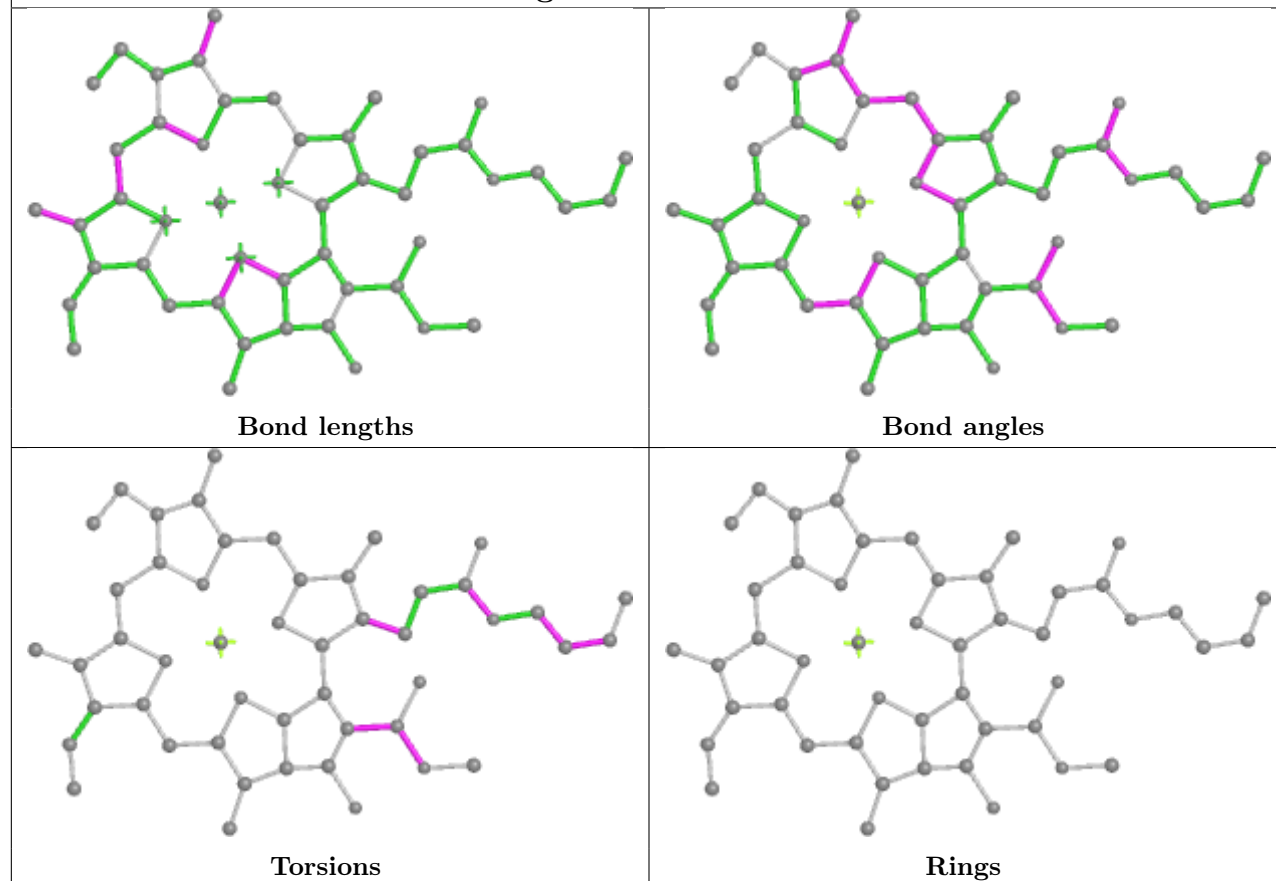




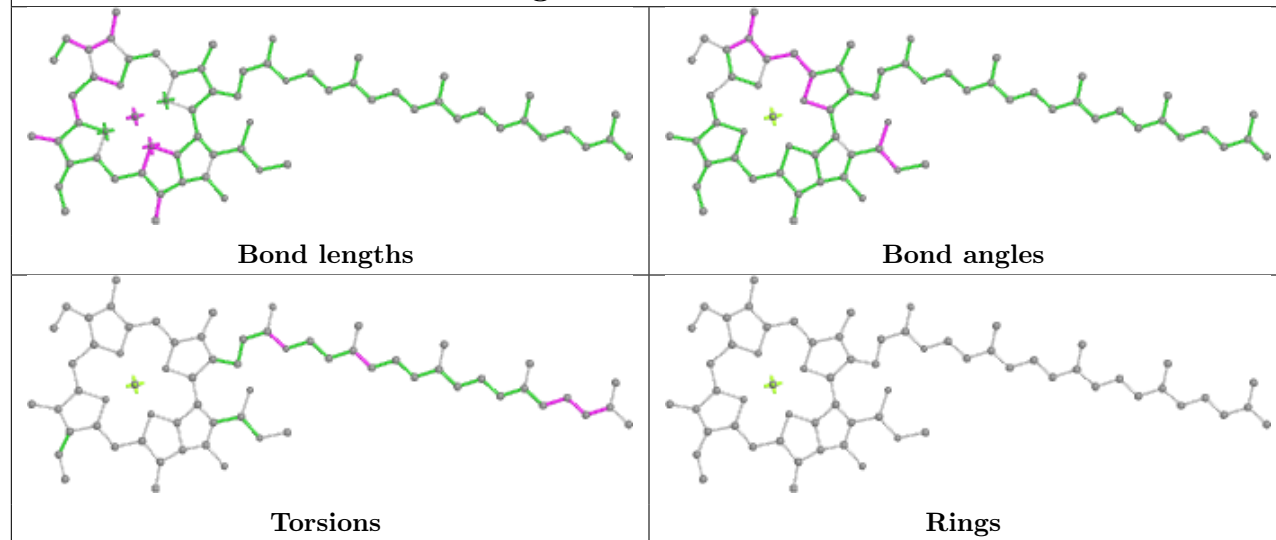




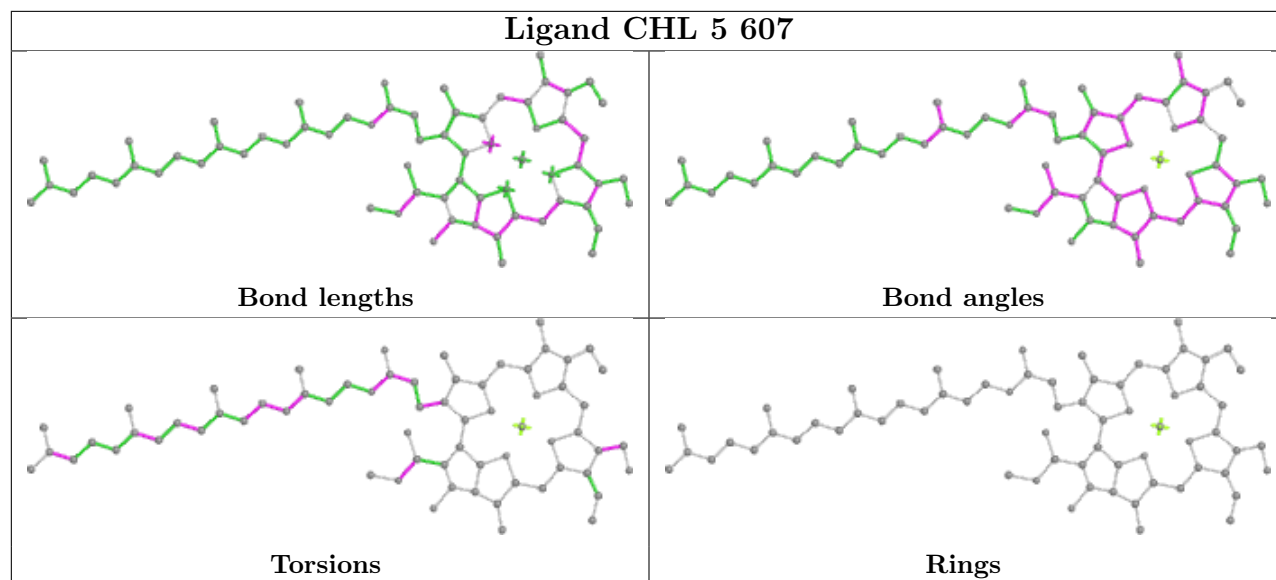
Ligand CLA 2 604



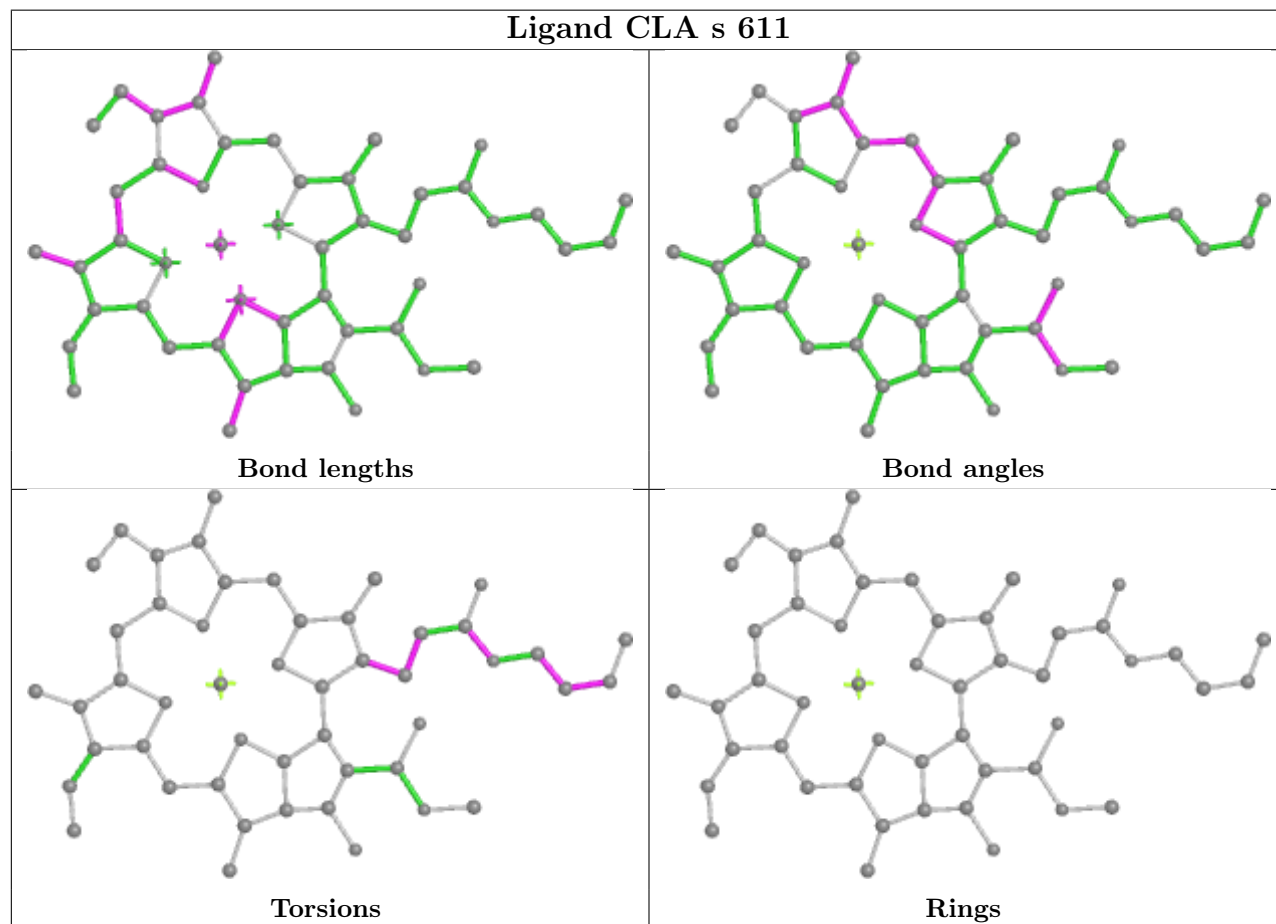
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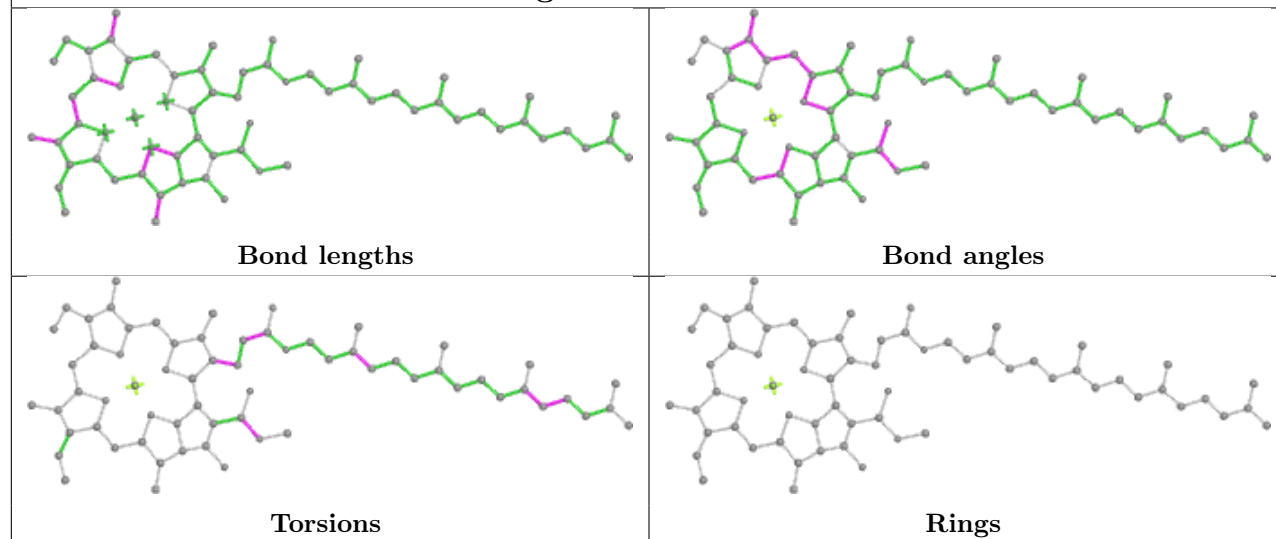
Ligand CHL 5 607



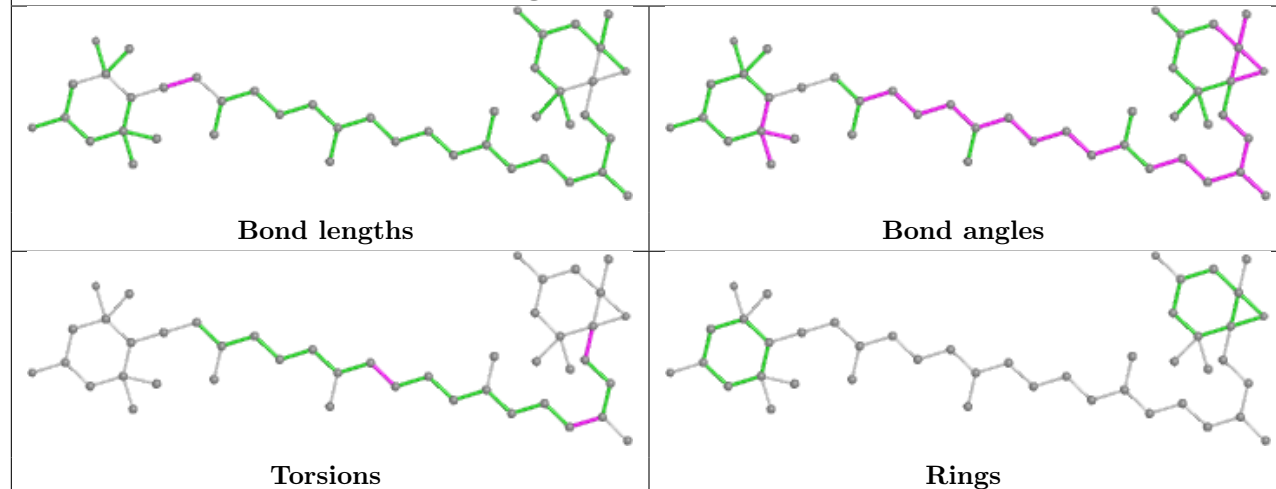
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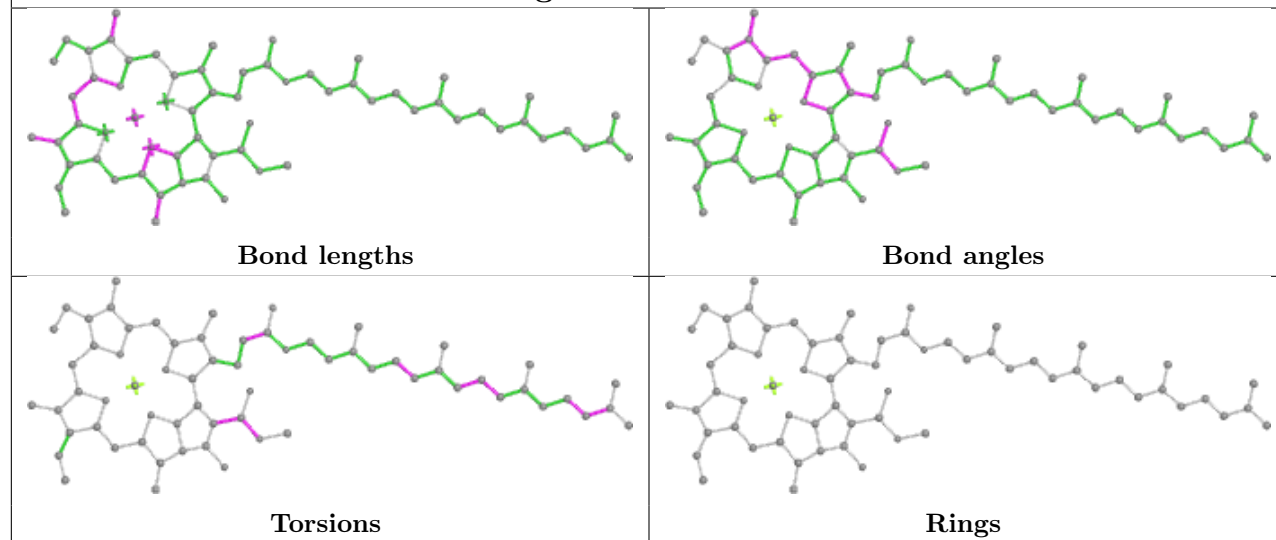
Ligand CLA 8 604

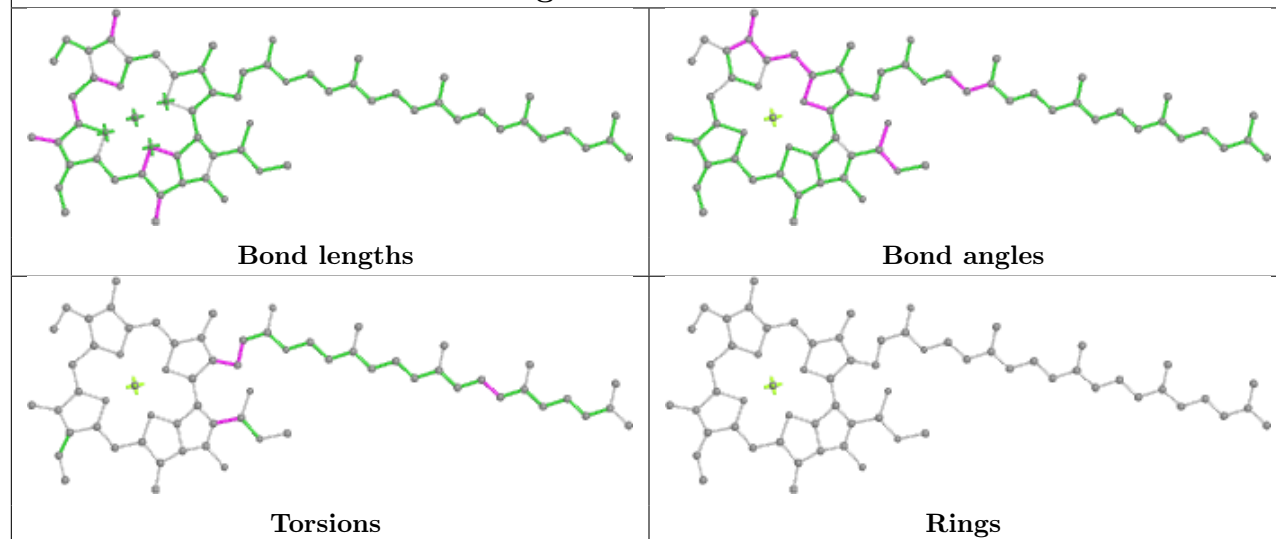
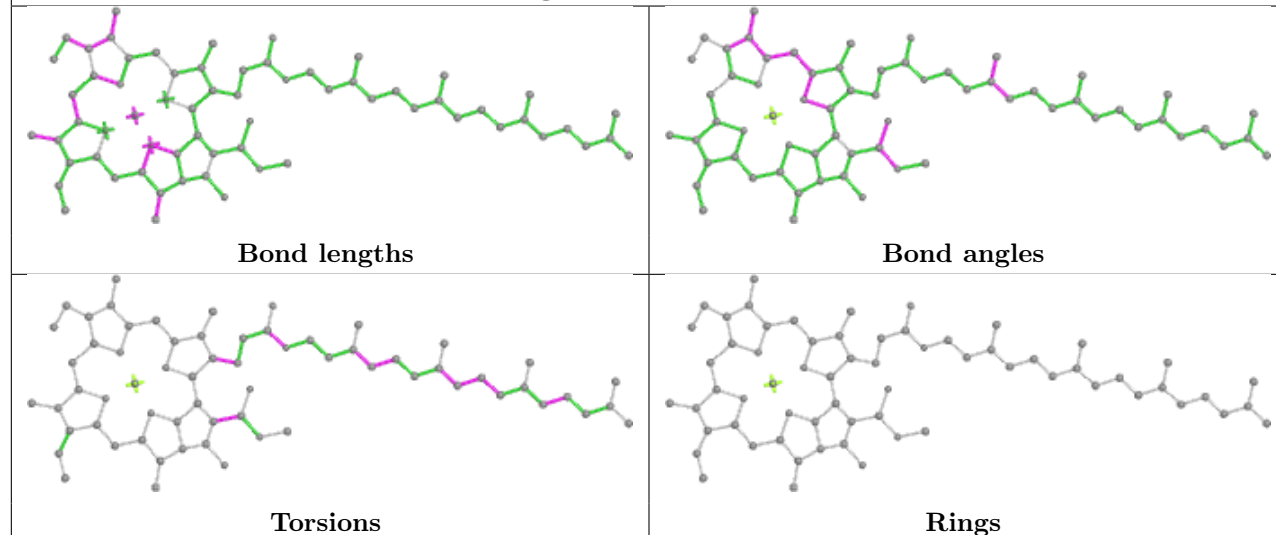
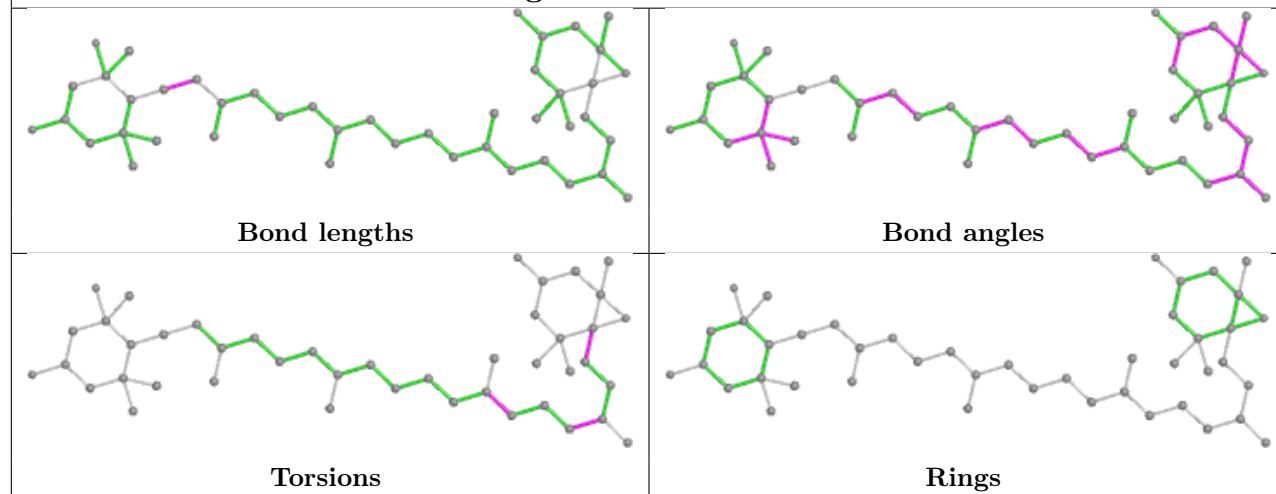


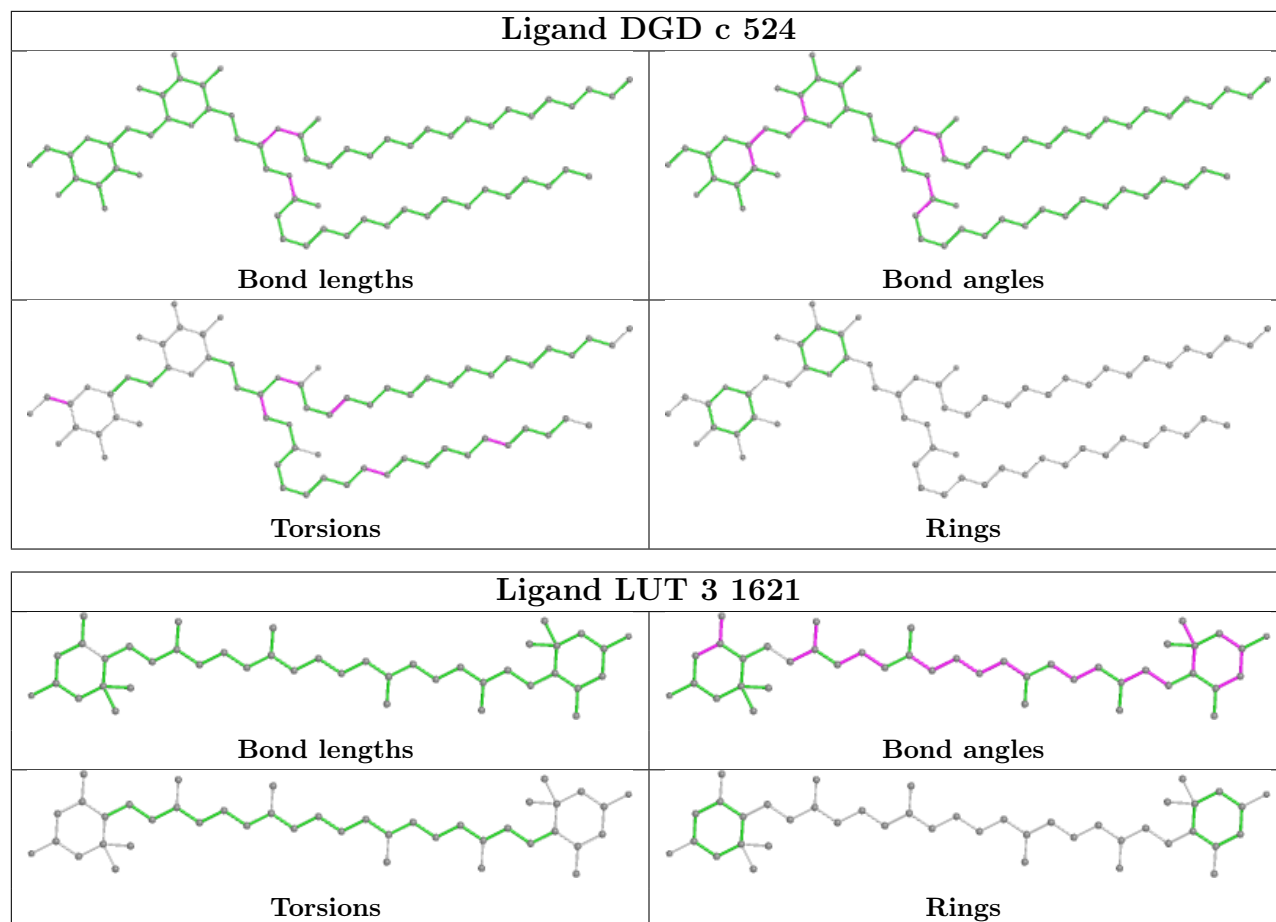
Ligand NEX 5 1623

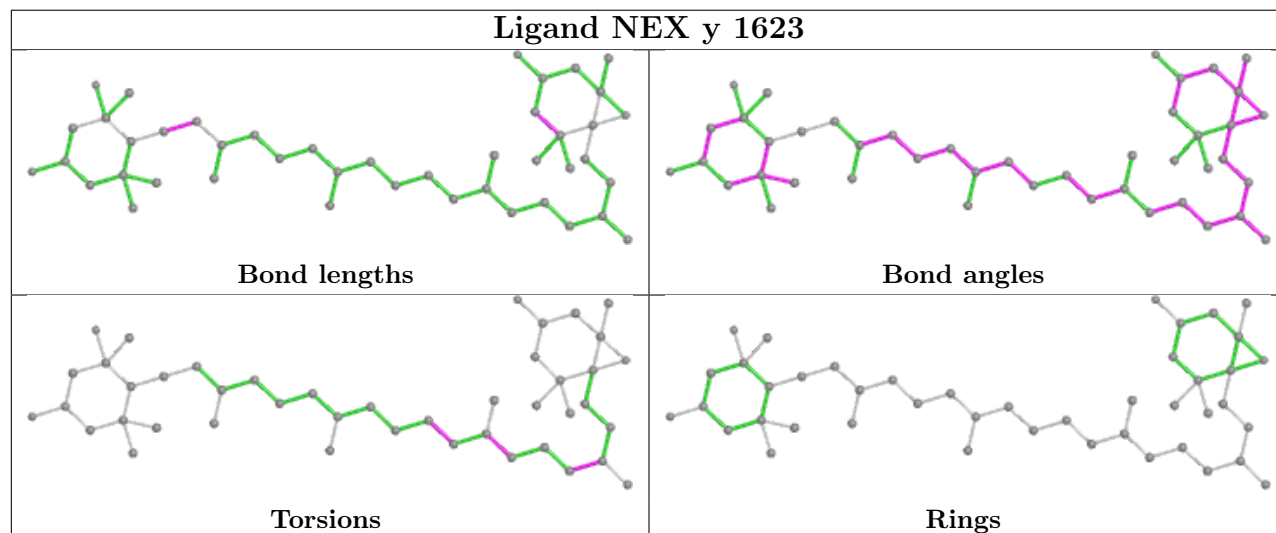
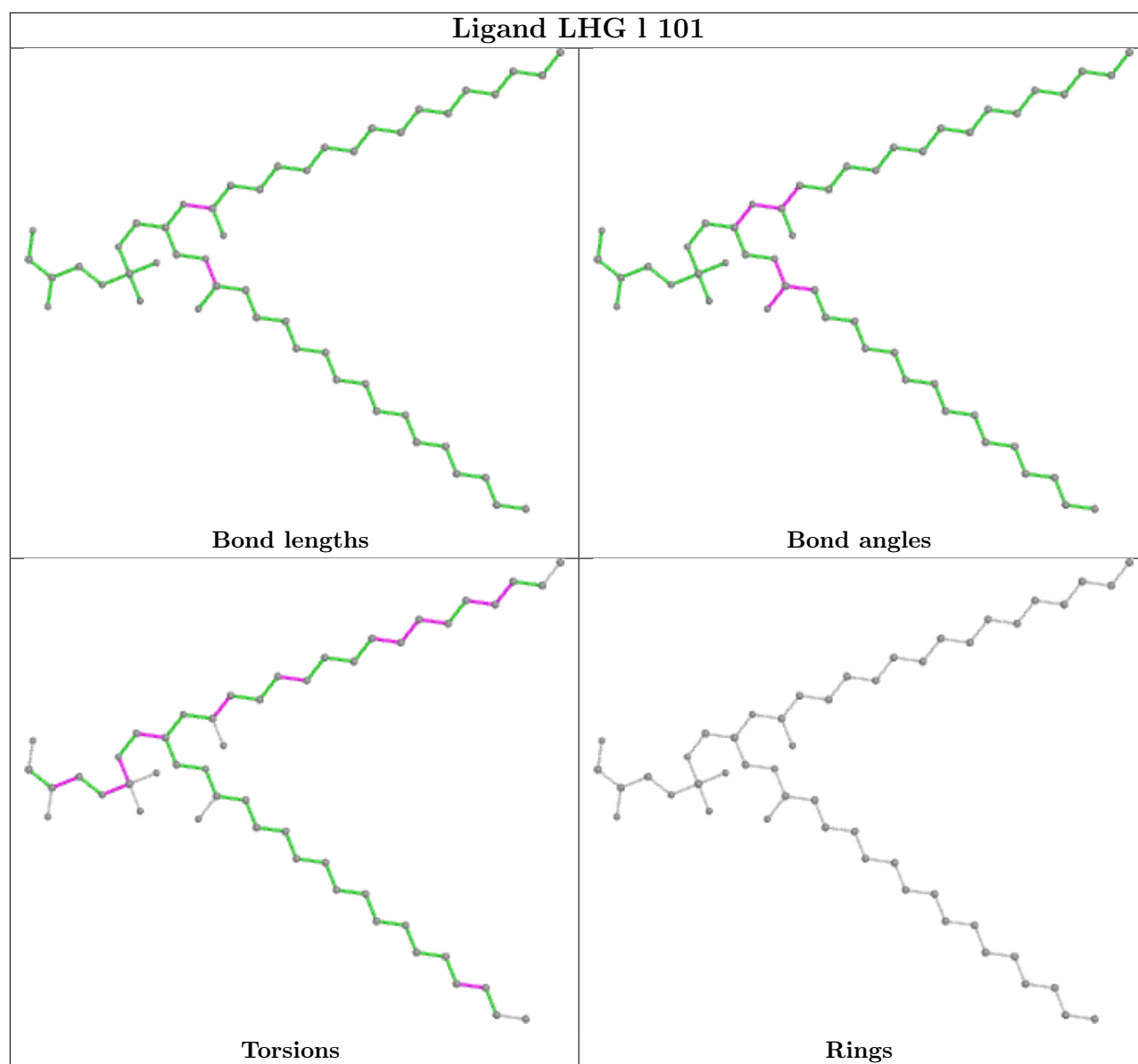


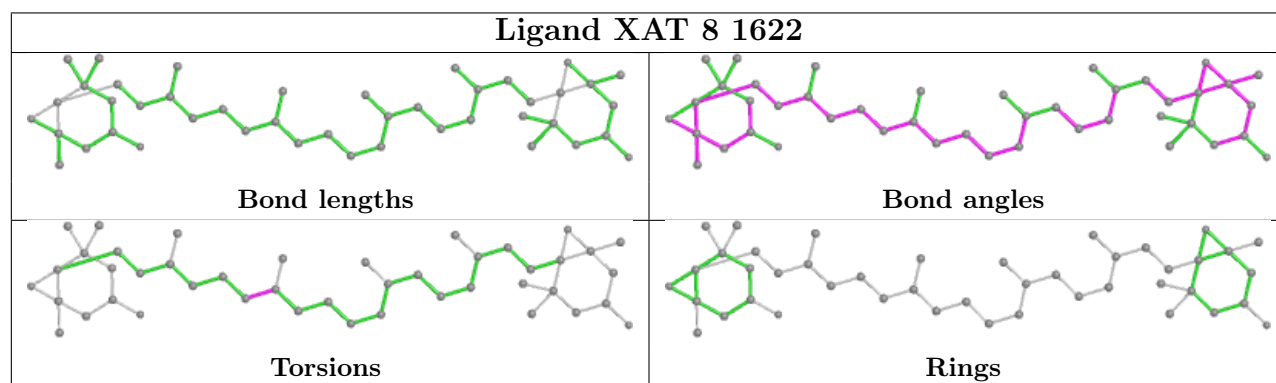
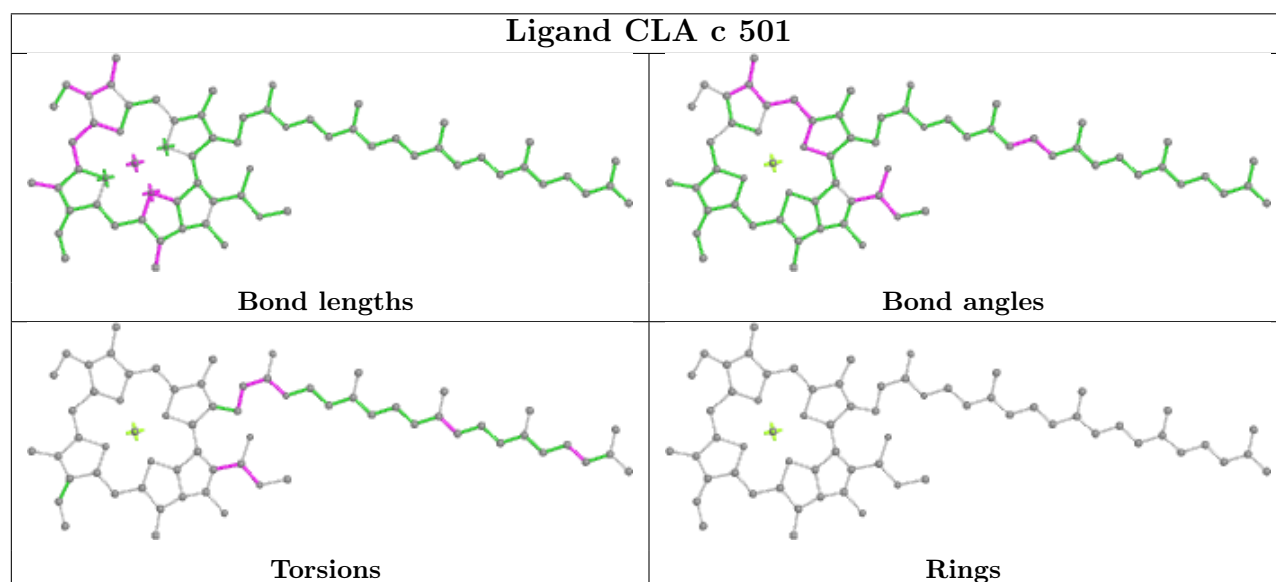
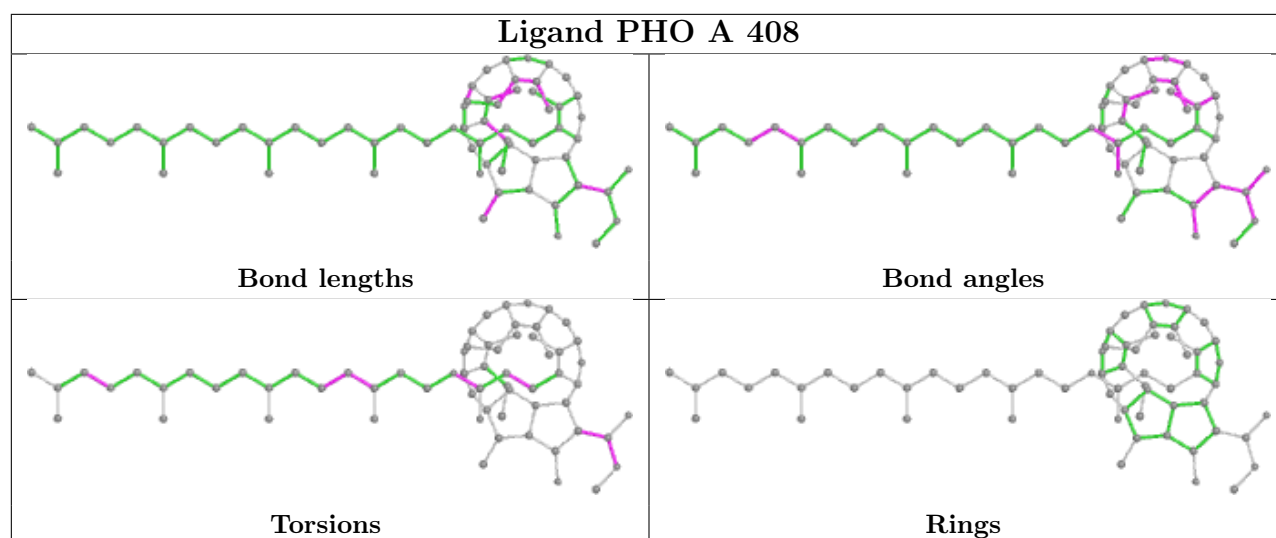
Ligand CLA b 614

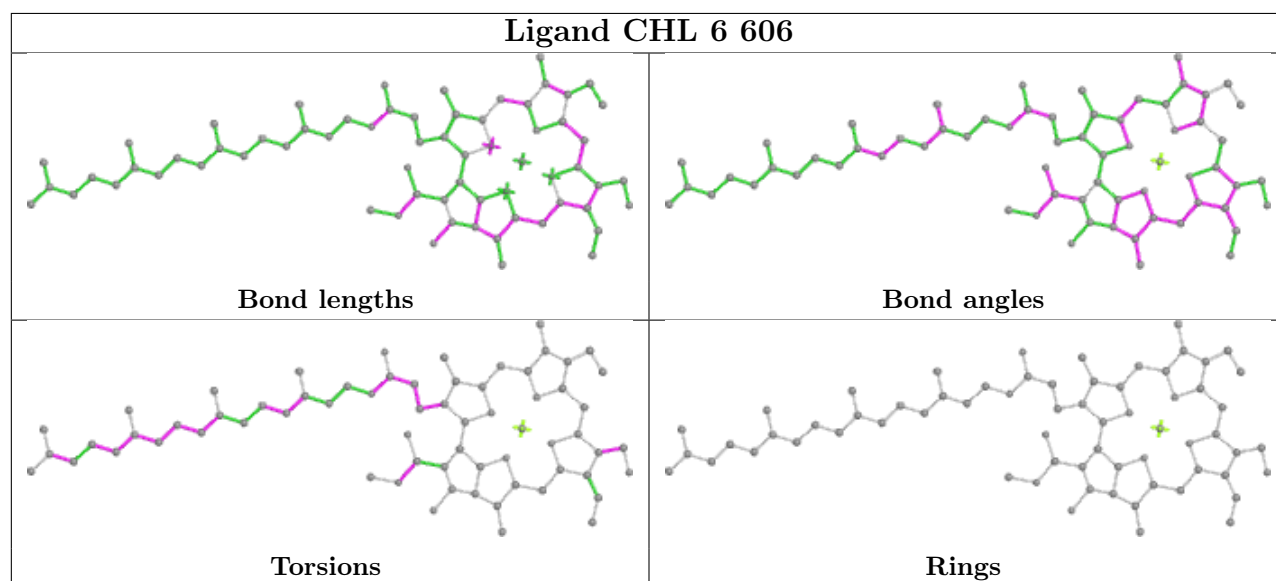
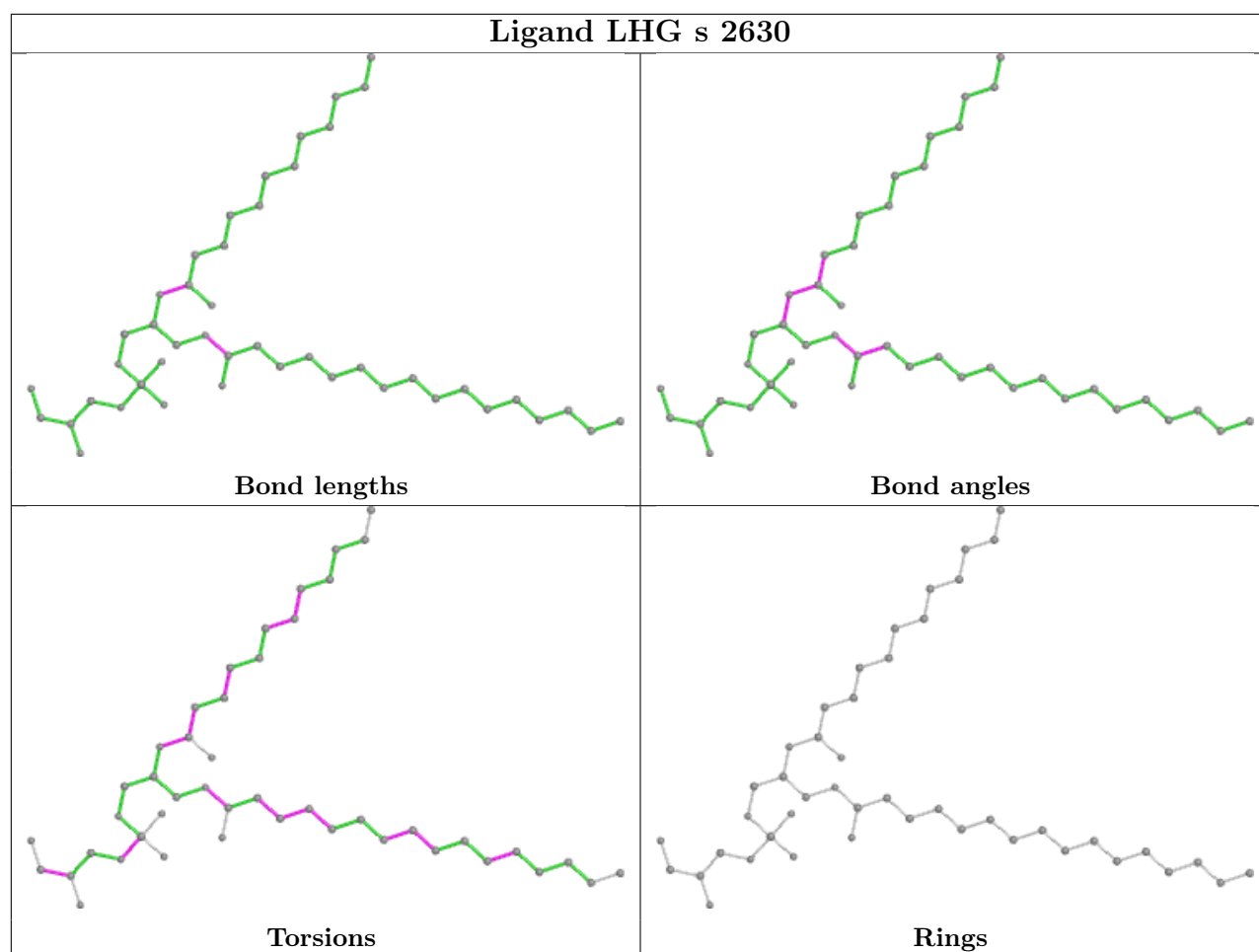


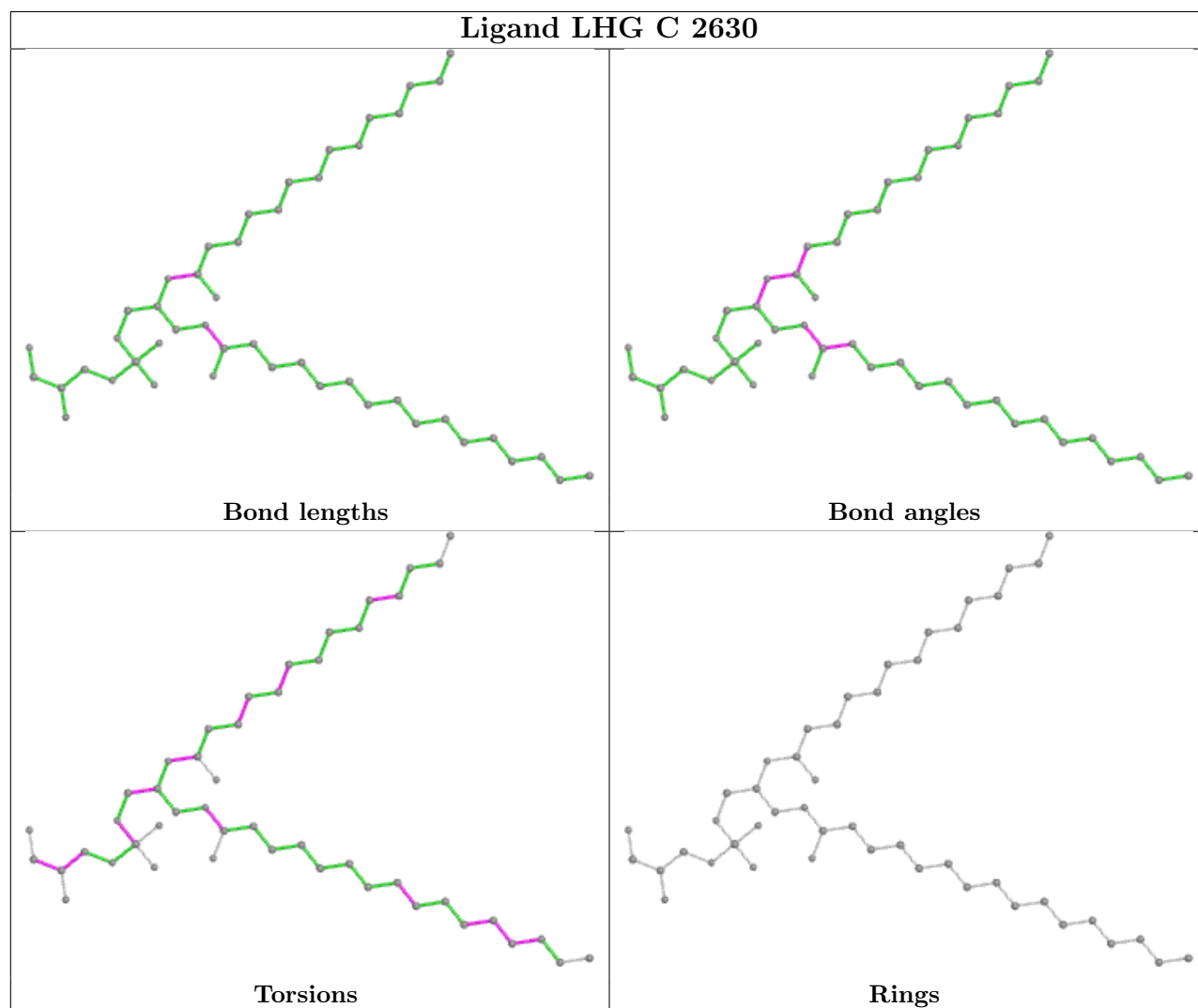
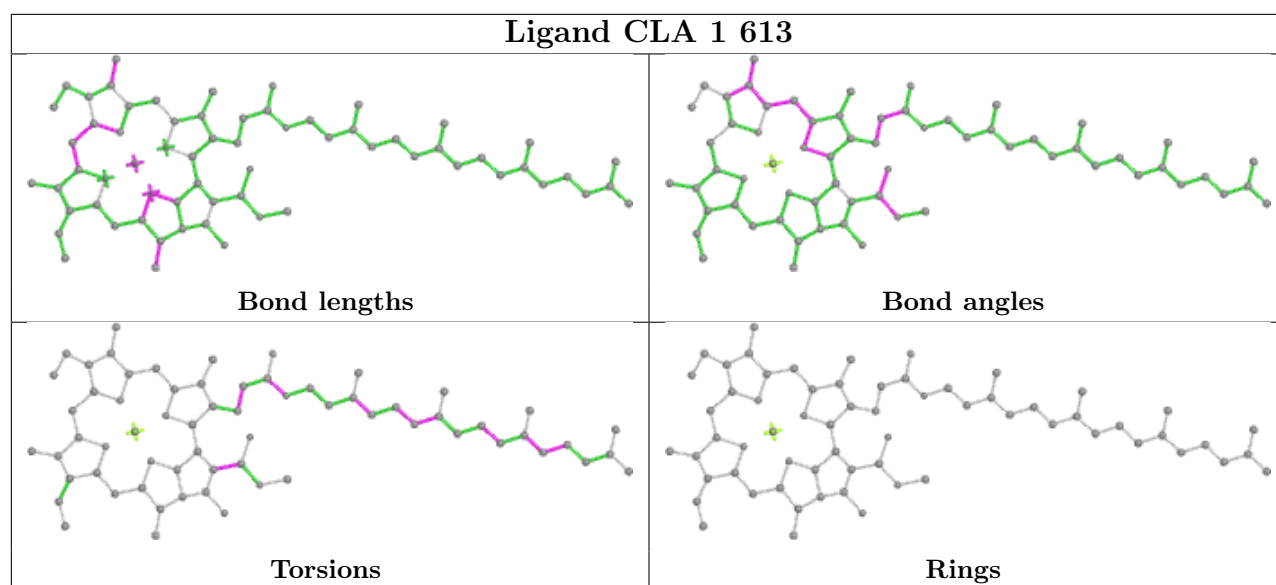
Ligand CLA 2 610**Ligand CLA c 504****Ligand NEX 3 1623**

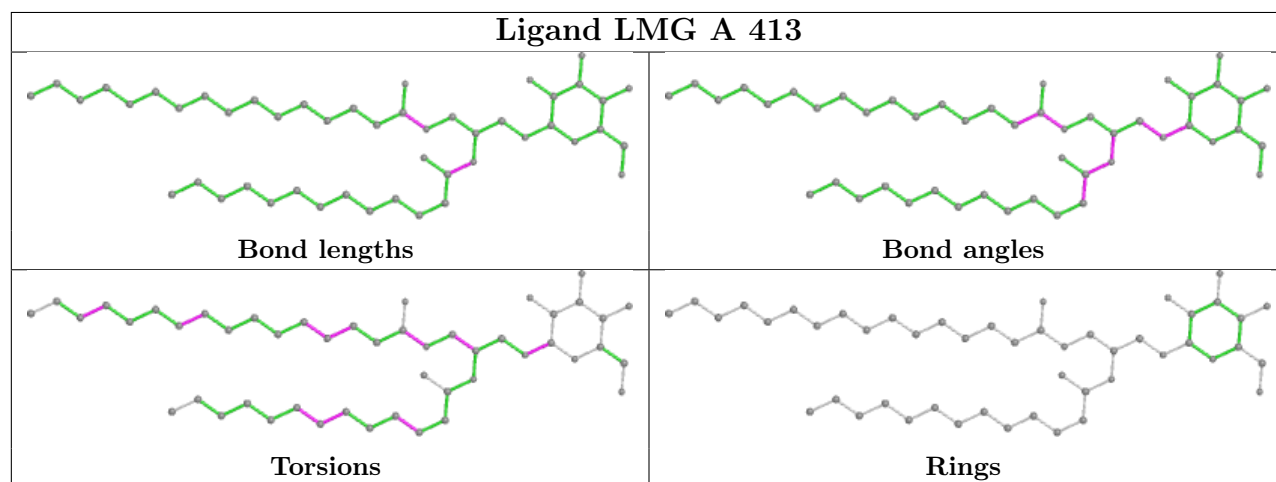
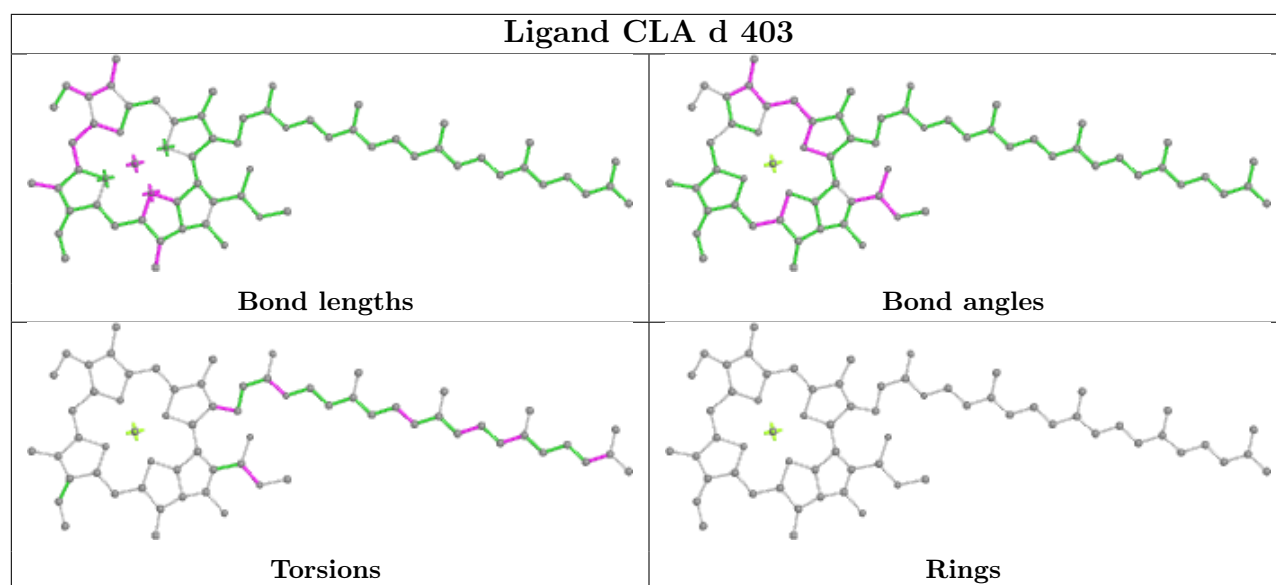




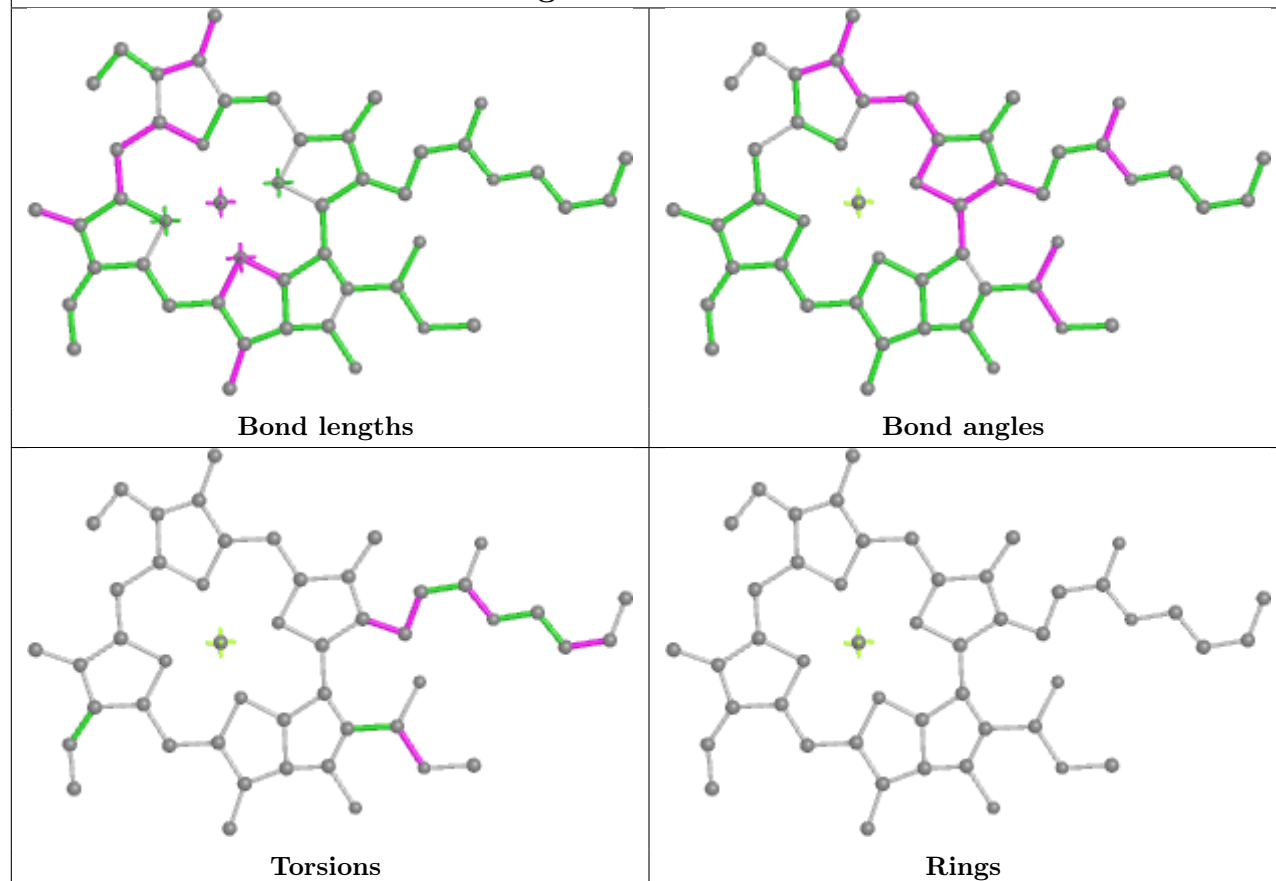




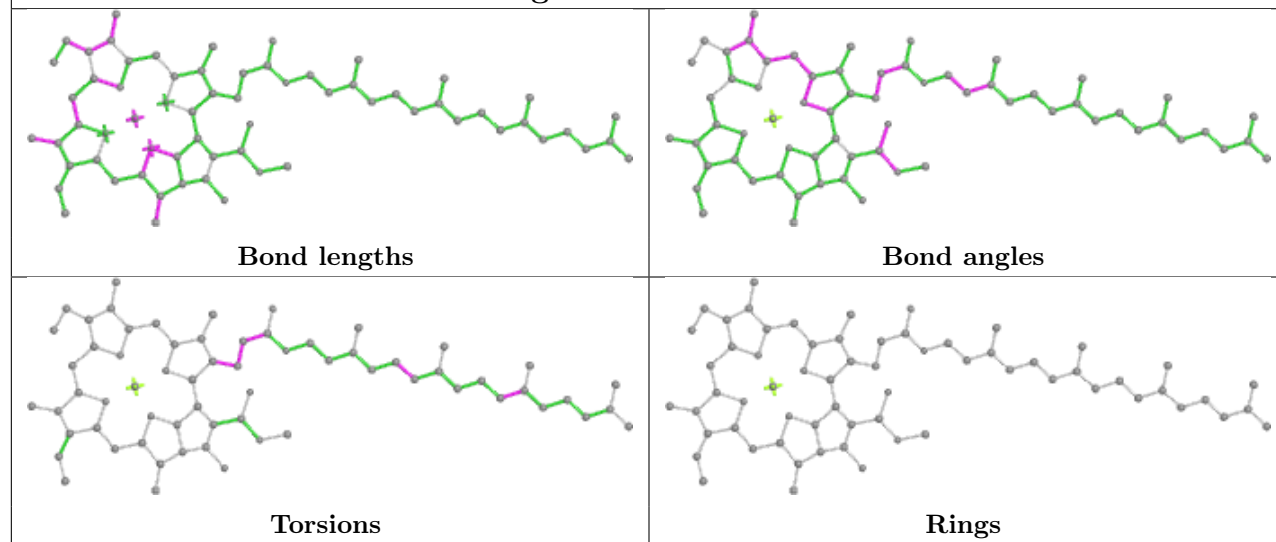


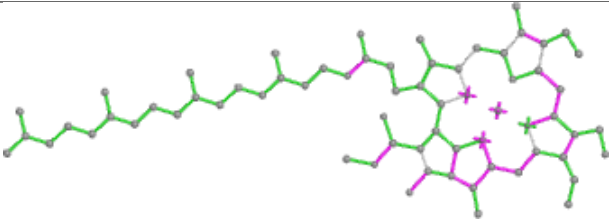
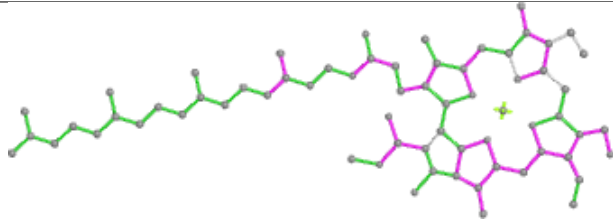
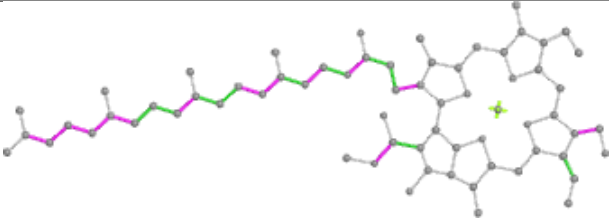
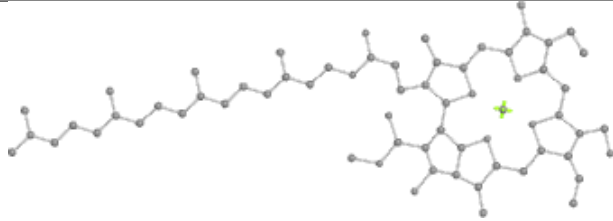
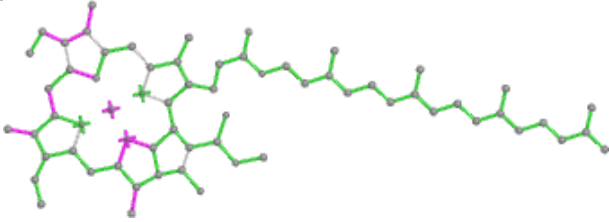
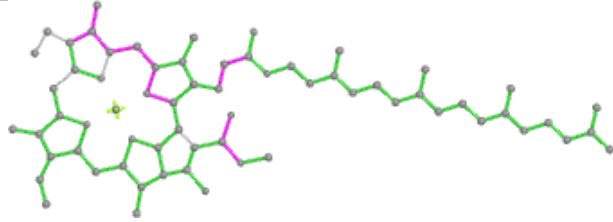
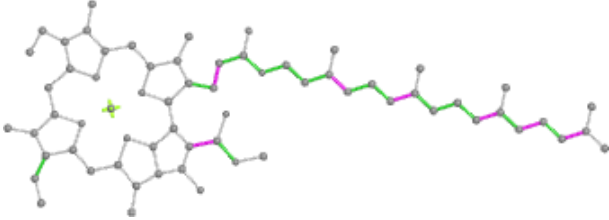
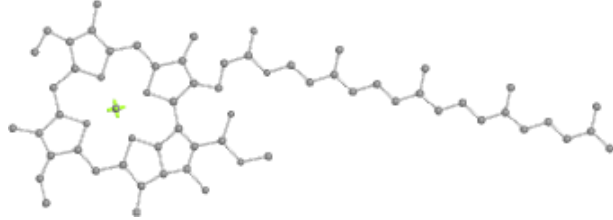


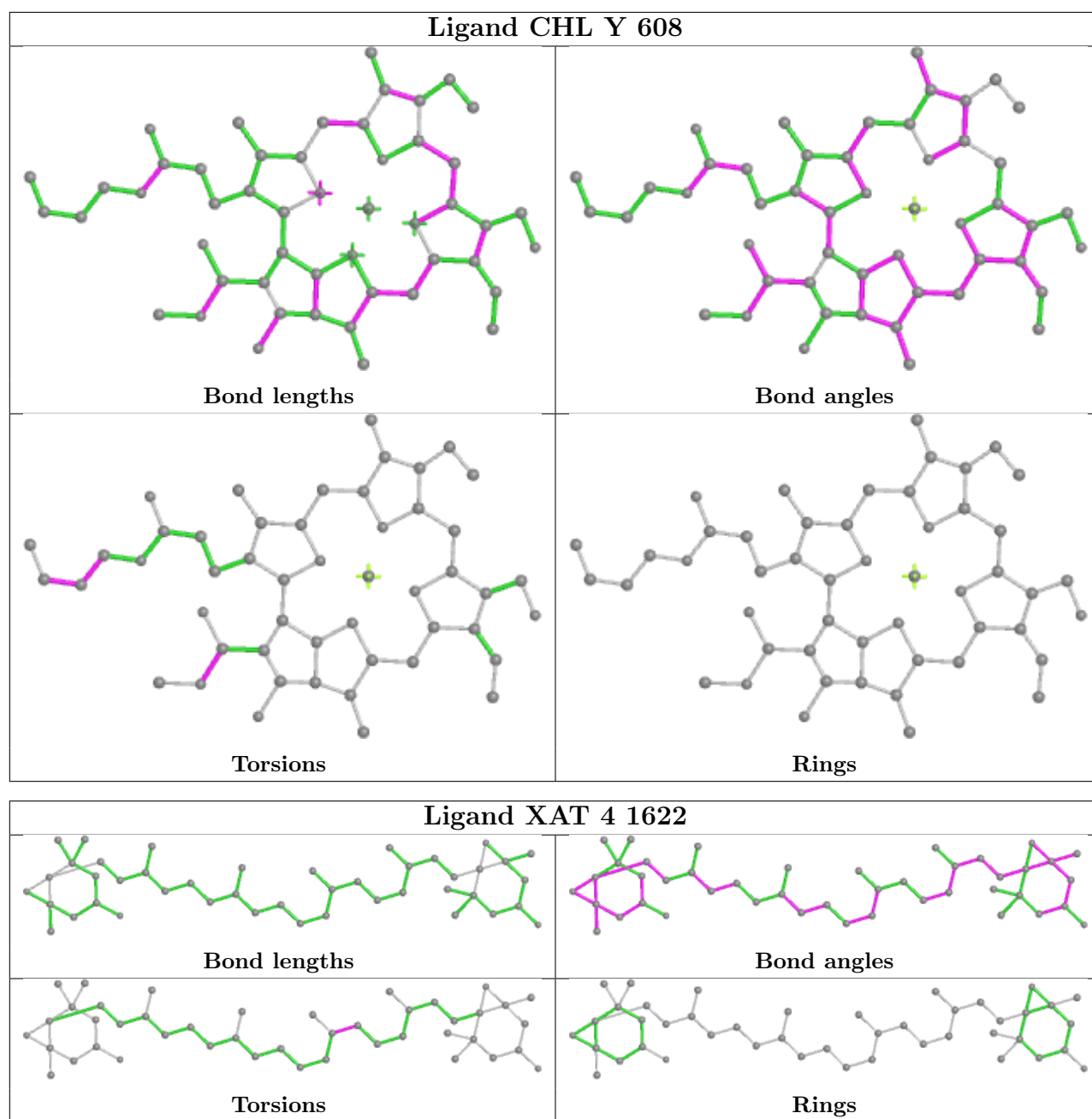
Ligand CLA r 601



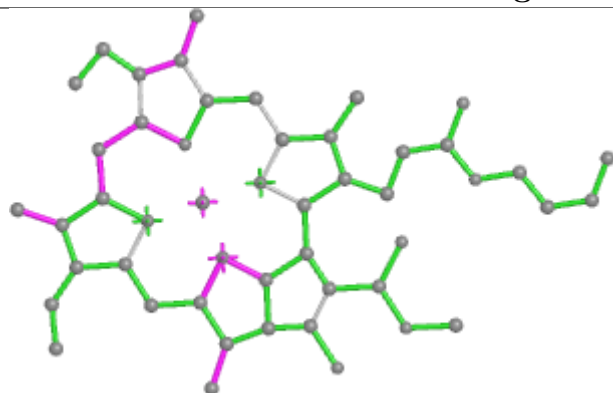
Ligand CLA N 602



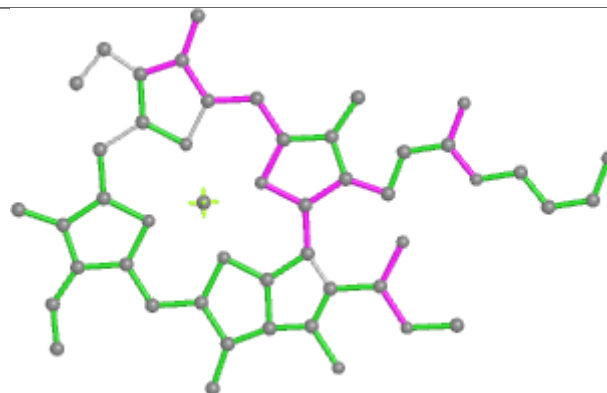
Ligand CHL Y 606	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA b 604	
	
Bond lengths	Bond angles
	
Torsions	Rings



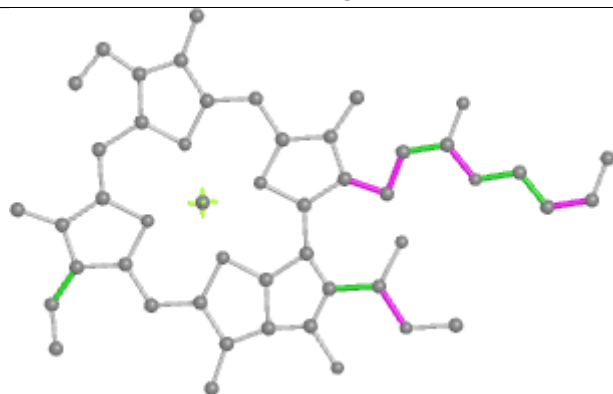
Ligand CLA R 601



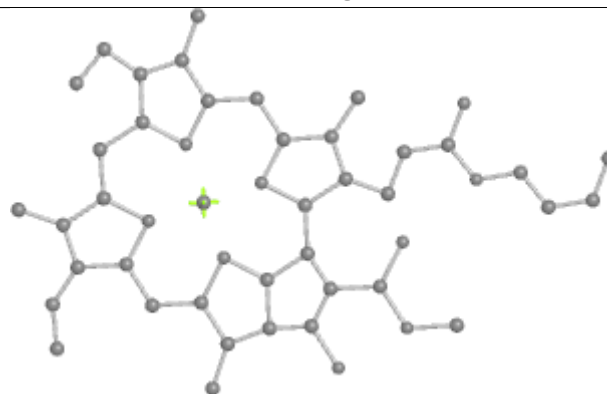
Bond lengths



Bond angles

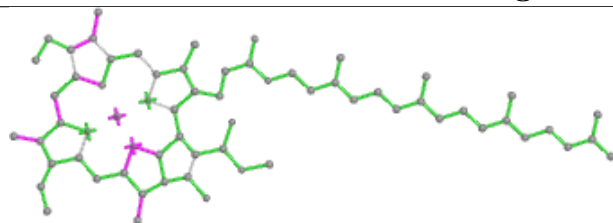


Torsions

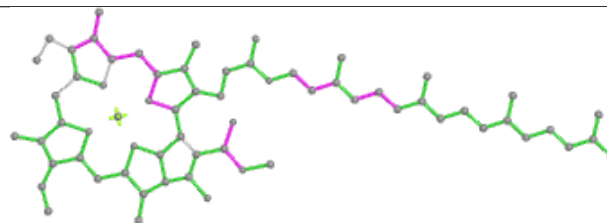


Rings

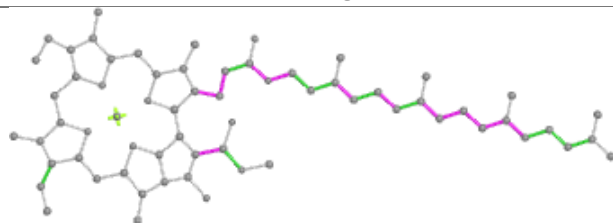
Ligand CLA C 505



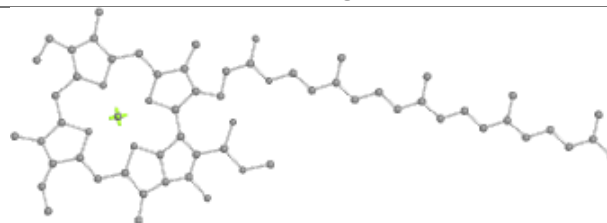
Bond lengths



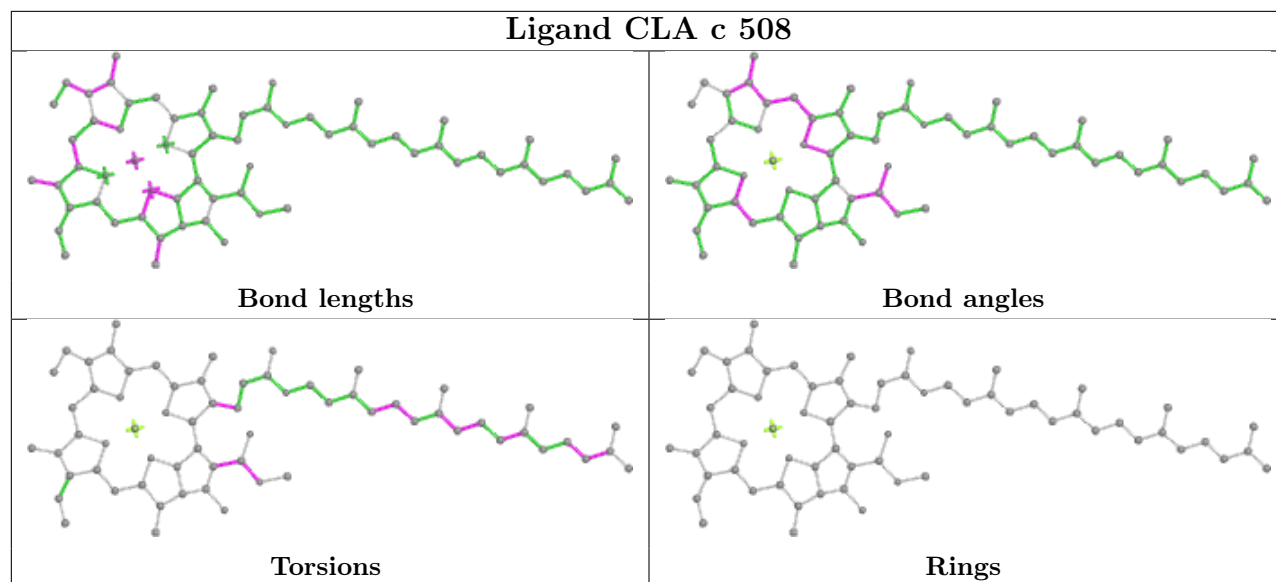
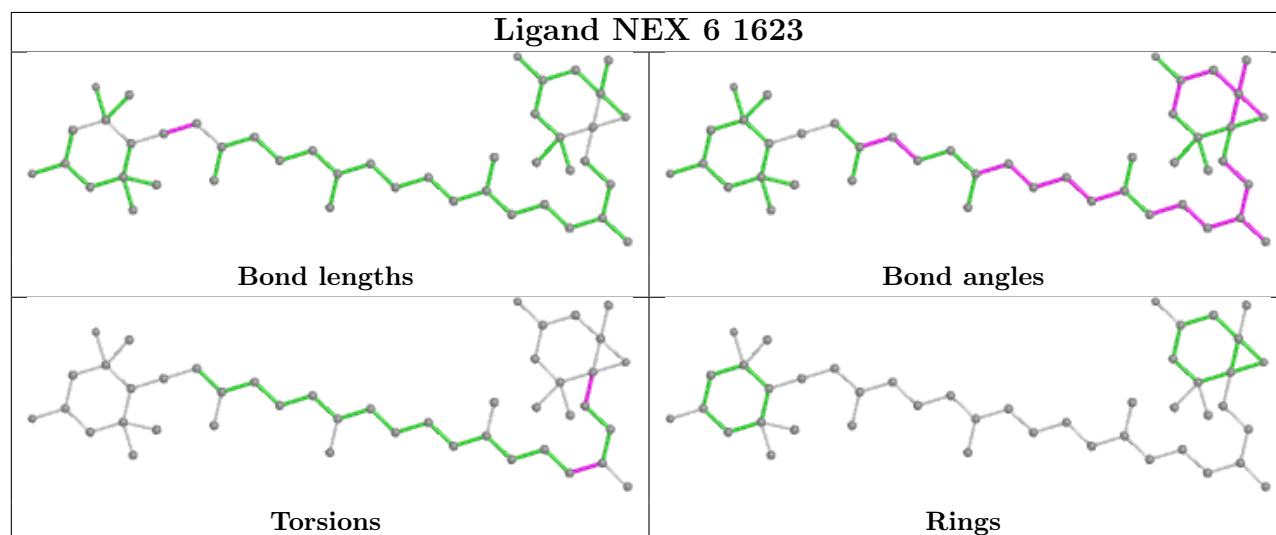
Bond angles



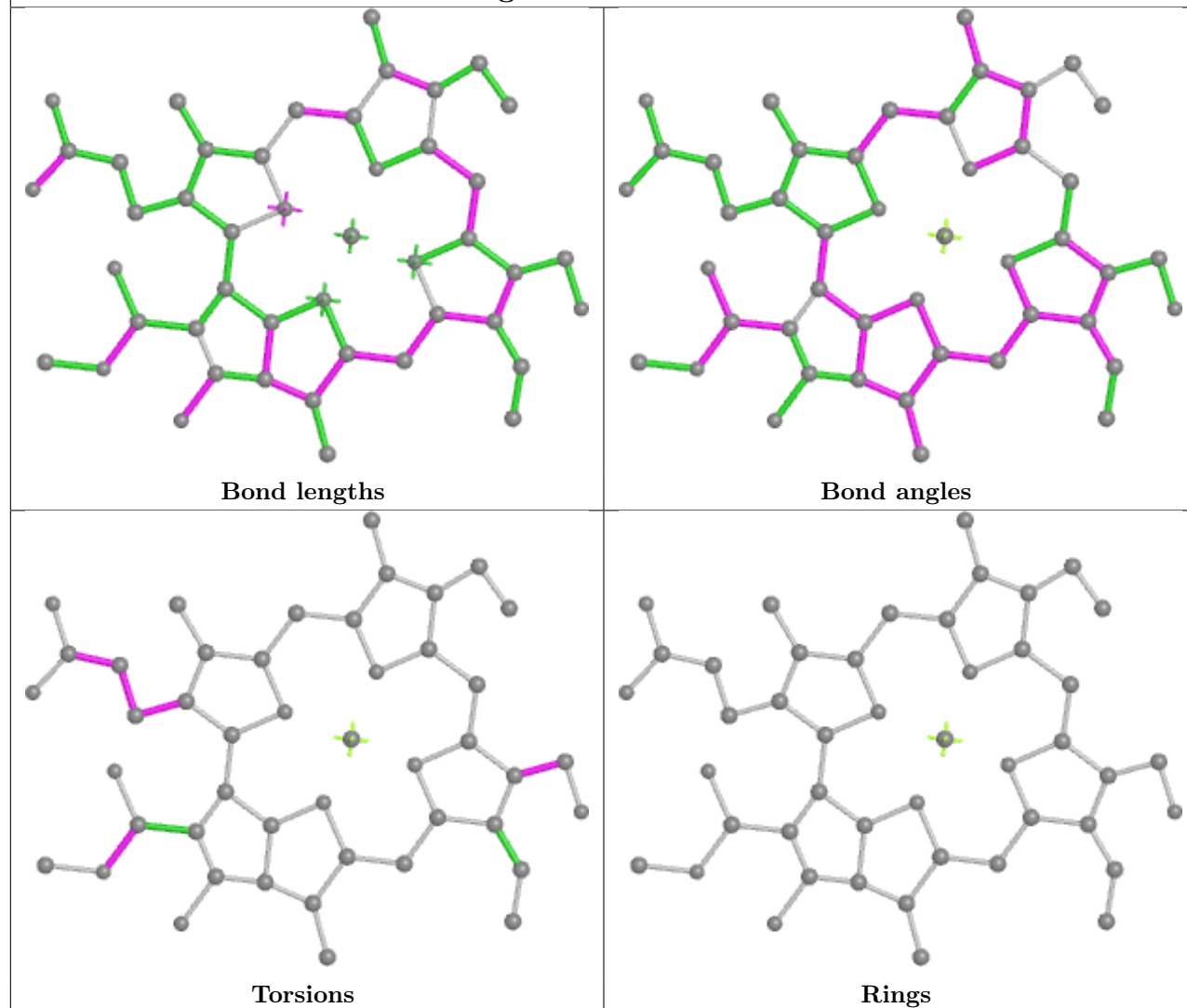
Torsions



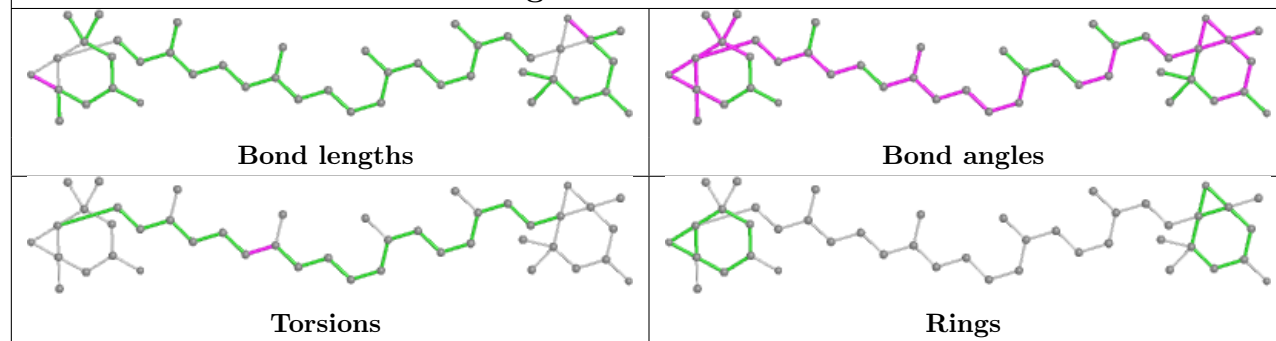
Rings

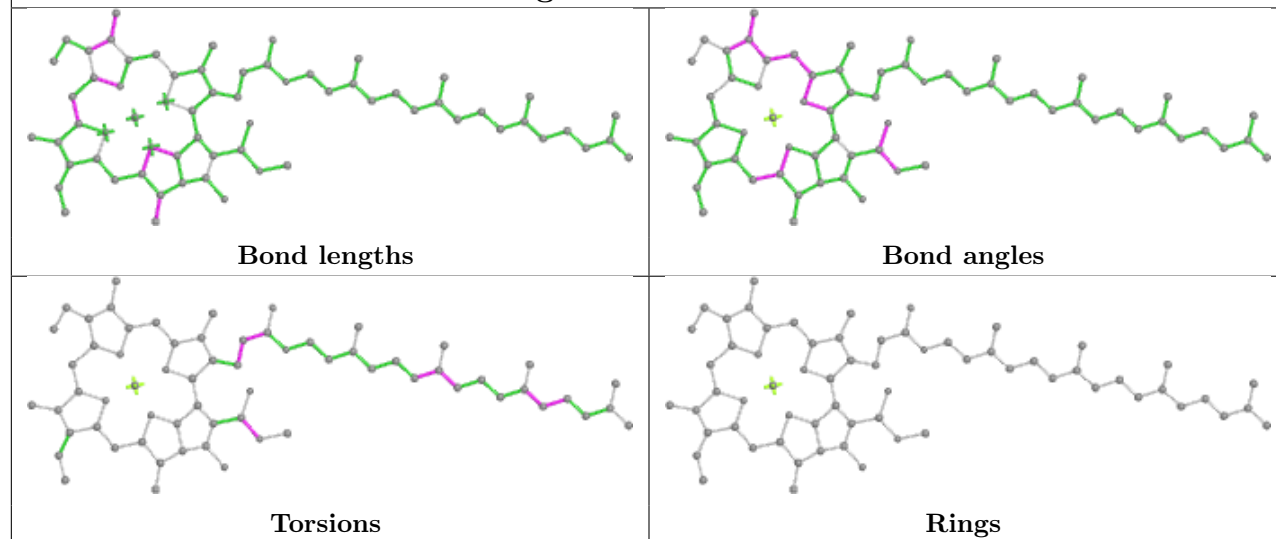
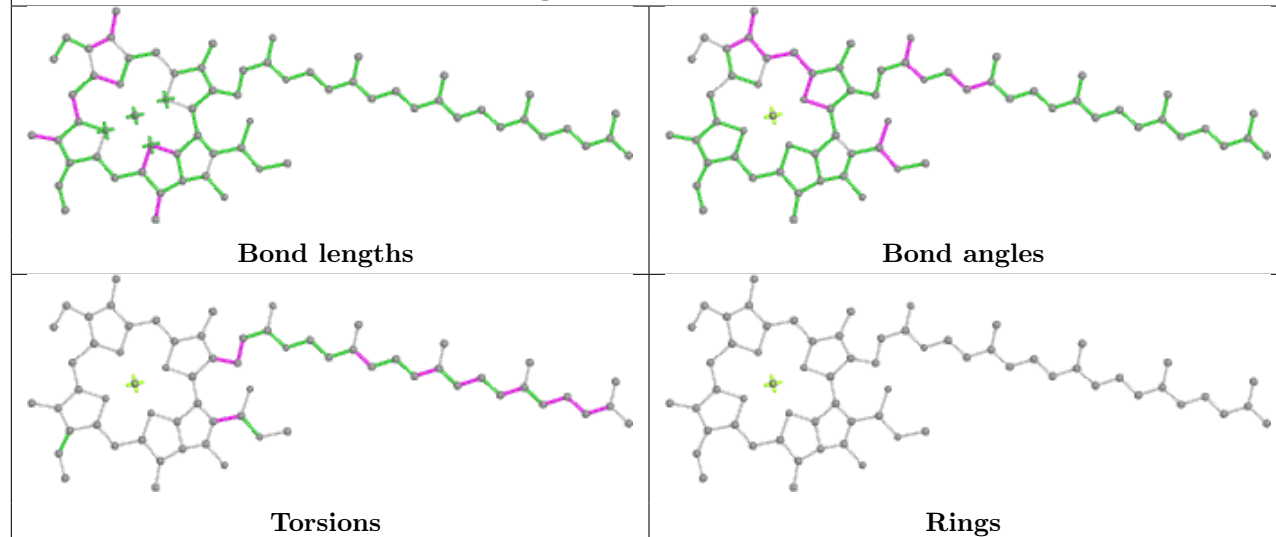
Ligand CLA c 508**Ligand NEX 6 1623**

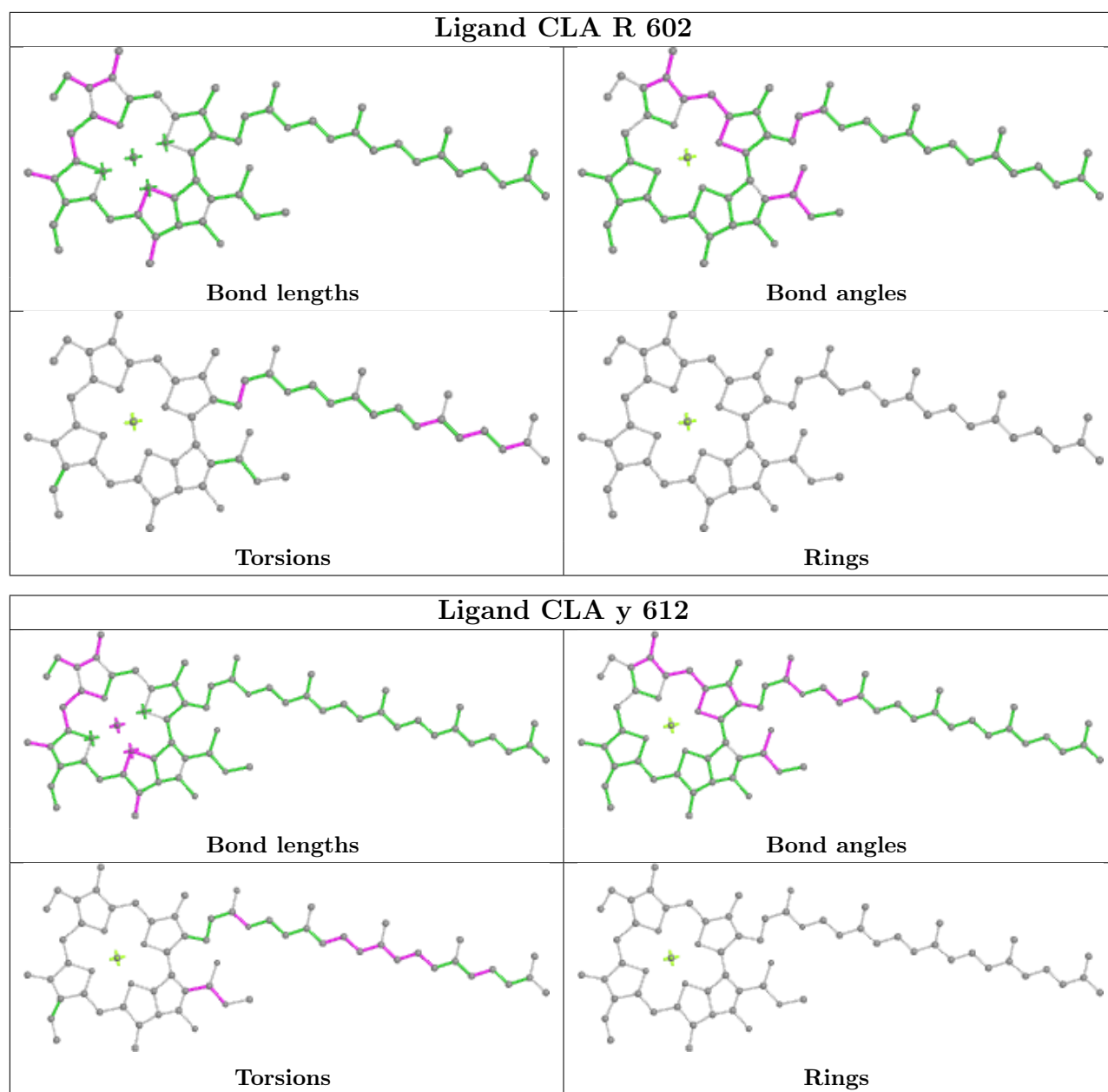
Ligand CHL 8 606



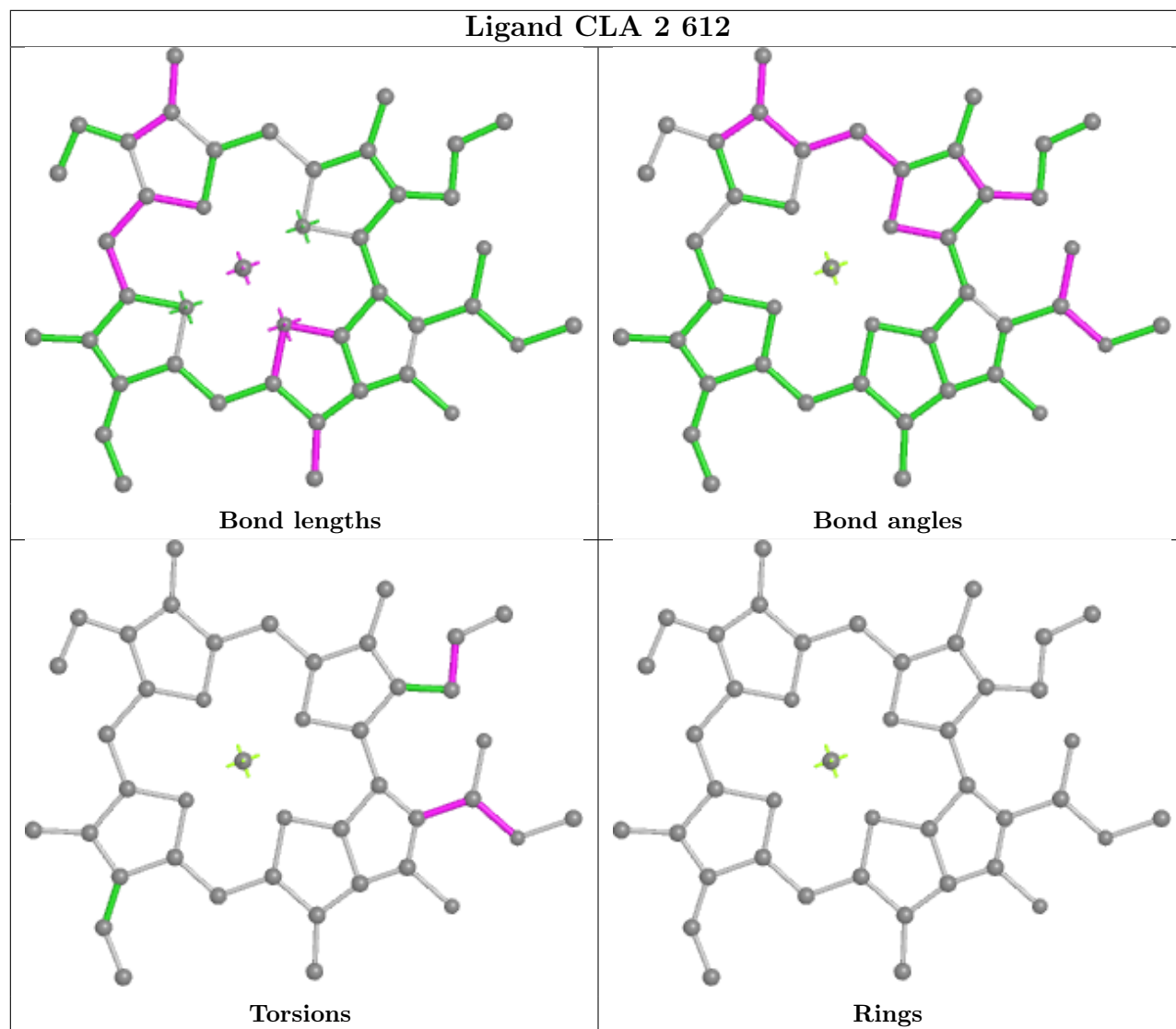
Ligand XAT 1 1622



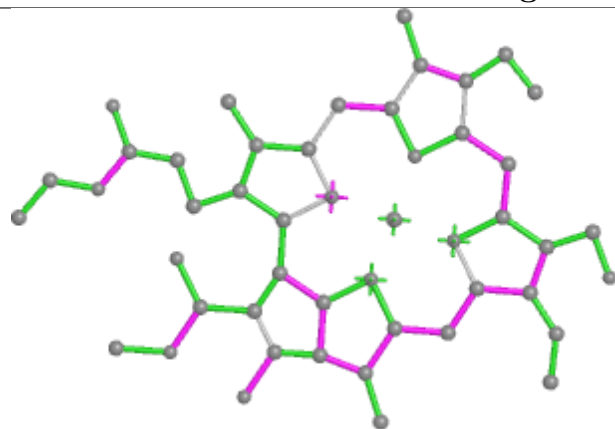
Ligand CLA 5 613**Ligand CLA 1 610**



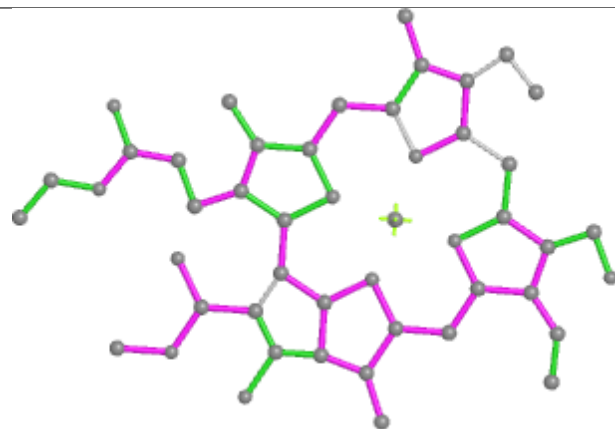
Ligand CLA 2 612



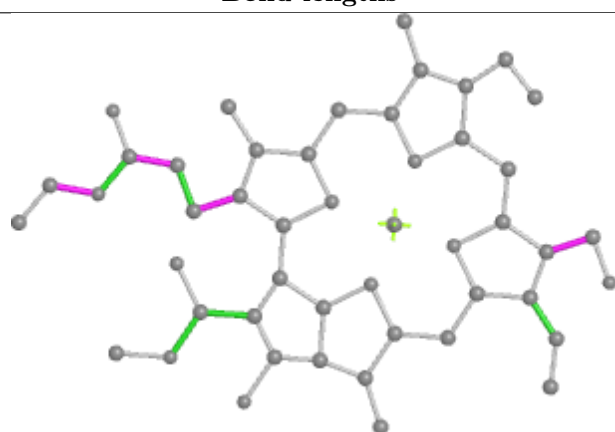
Ligand CHL 9 605



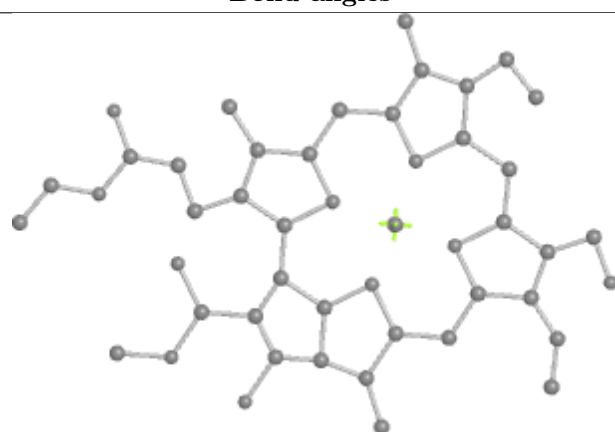
Bond lengths



Bond angles

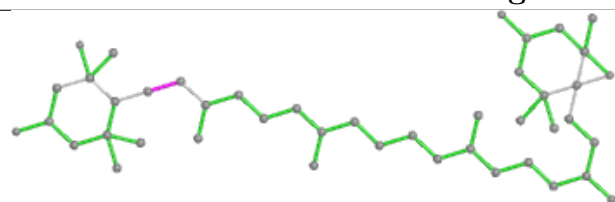


Torsions

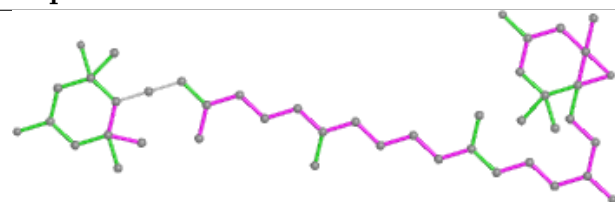


Rings

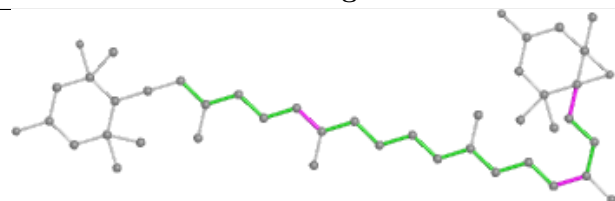
Ligand NEX p 1623



Bond lengths



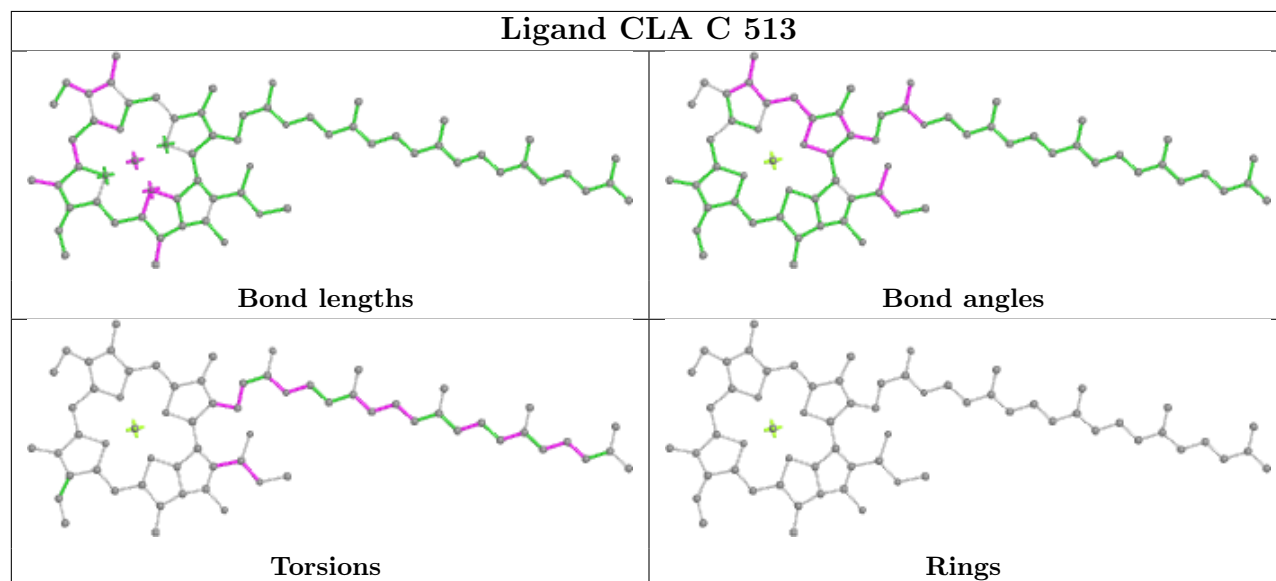
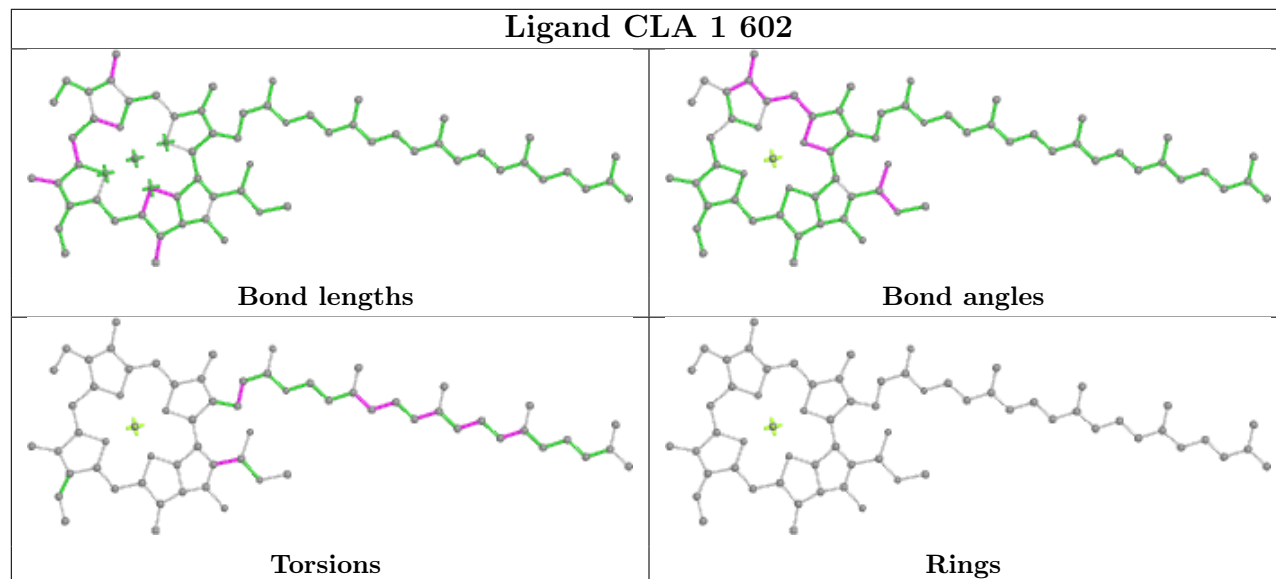
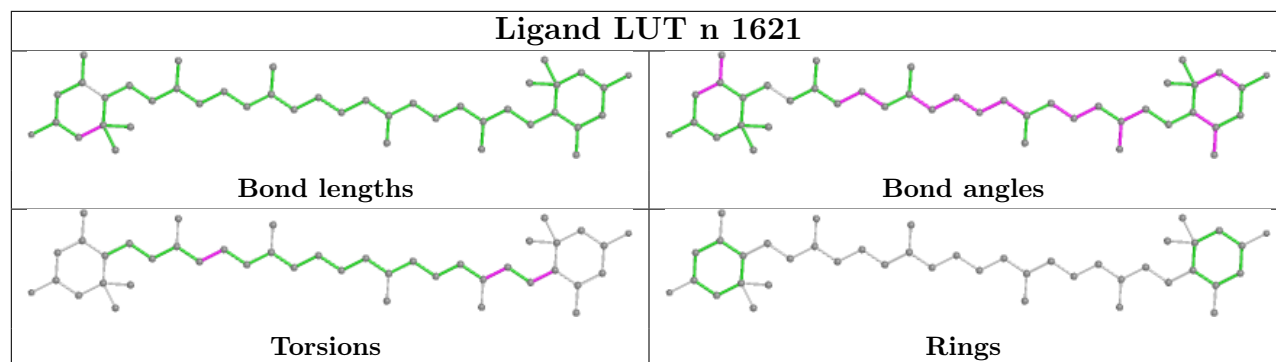
Bond angles



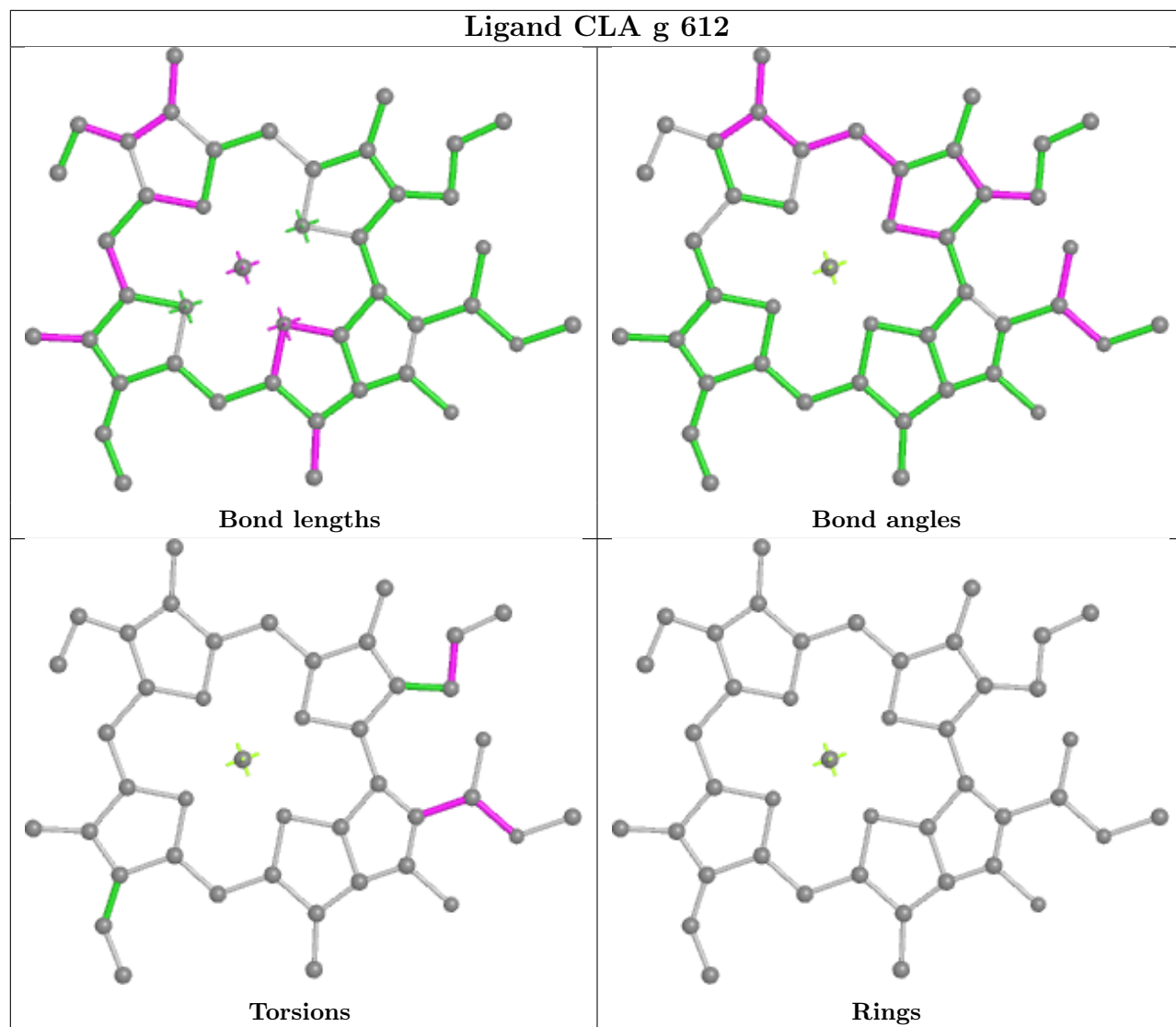
Torsions



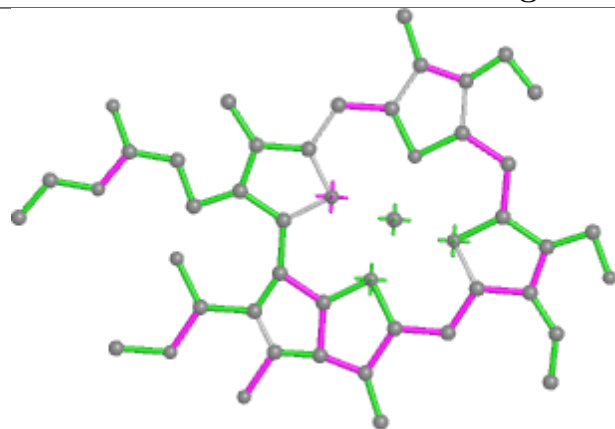
Rings



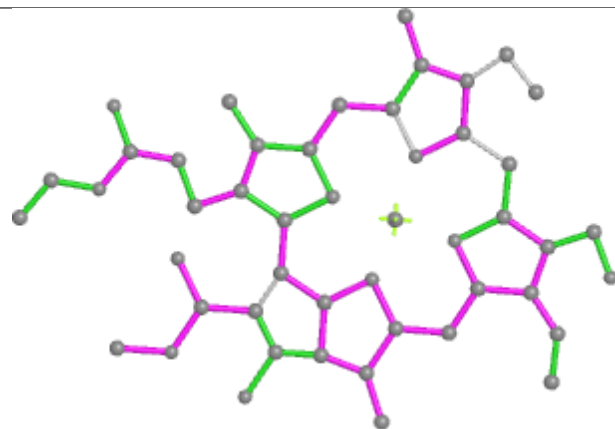
Ligand CLA g 612



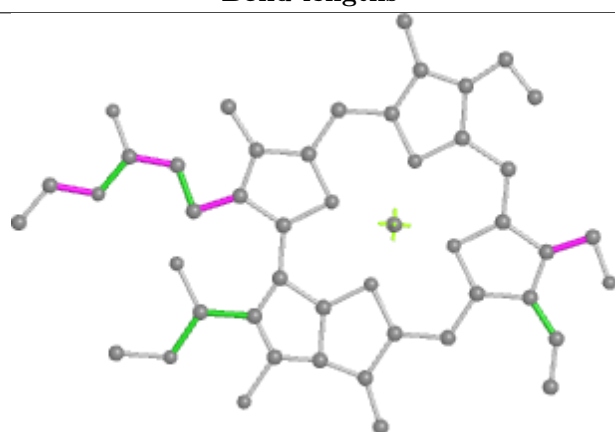
Ligand CHL 2 605



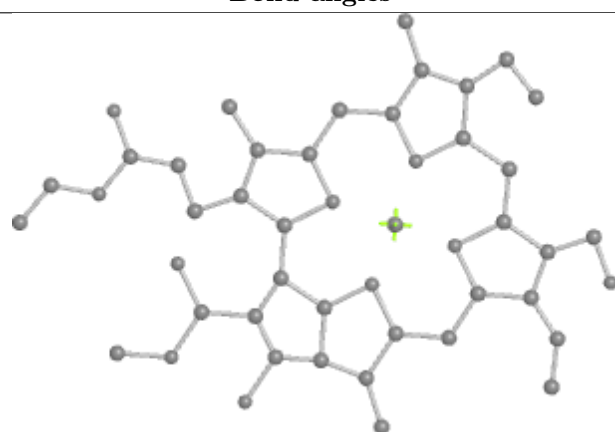
Bond lengths



Bond angles

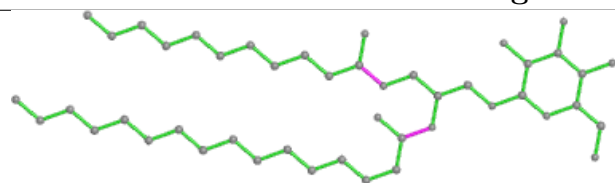


Torsions

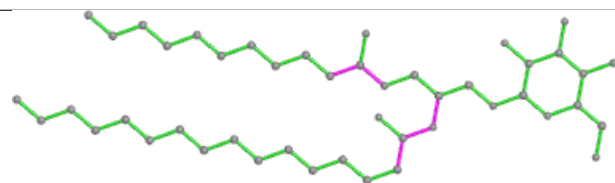


Rings

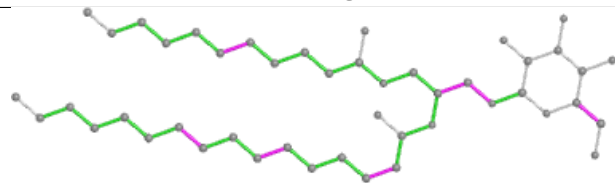
Ligand LMG D 411



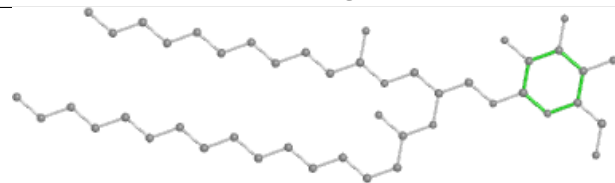
Bond lengths



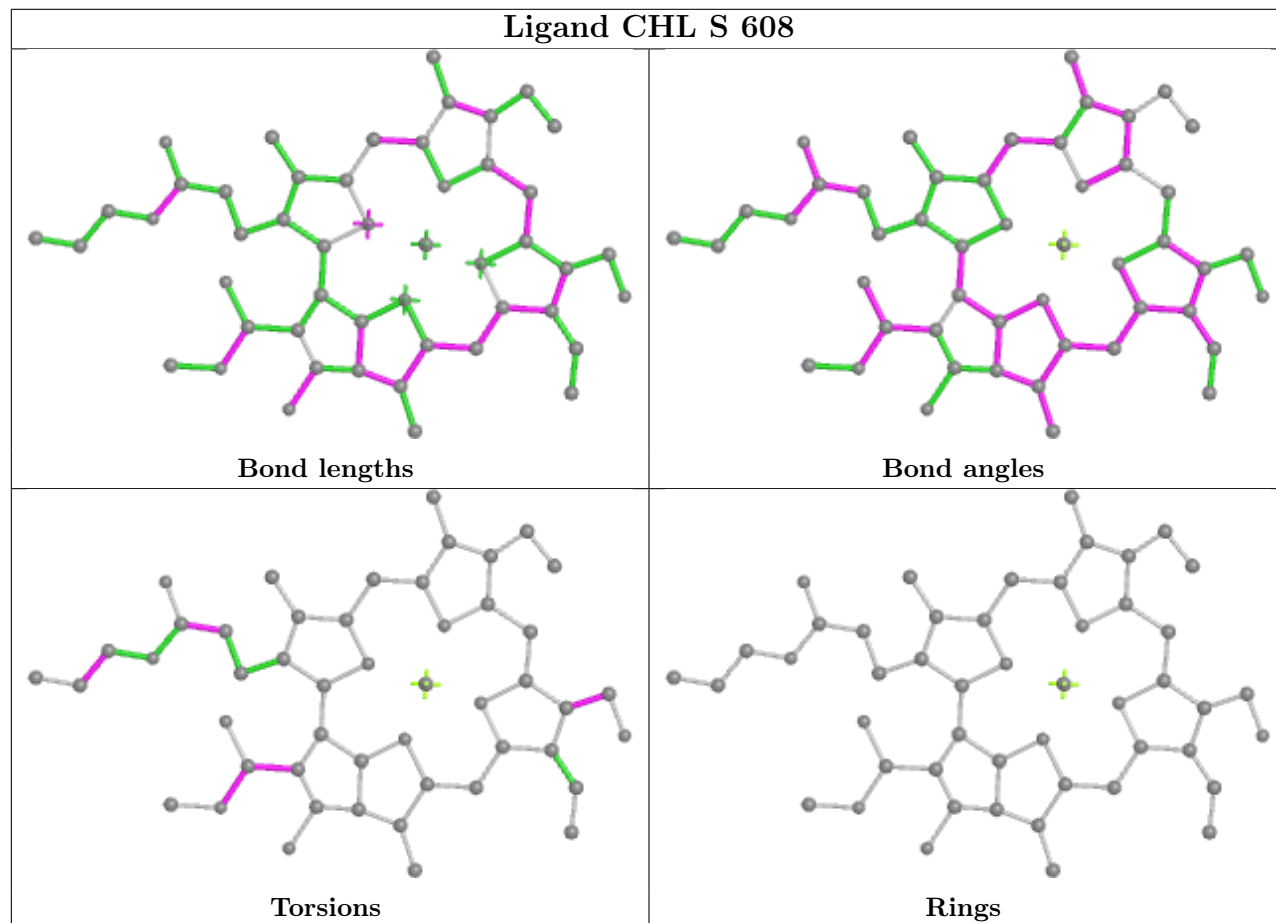
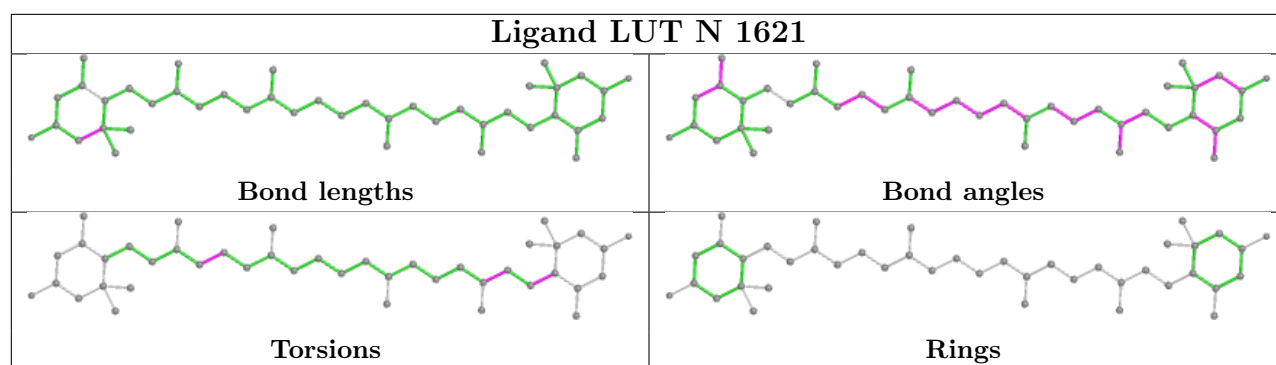
Bond angles

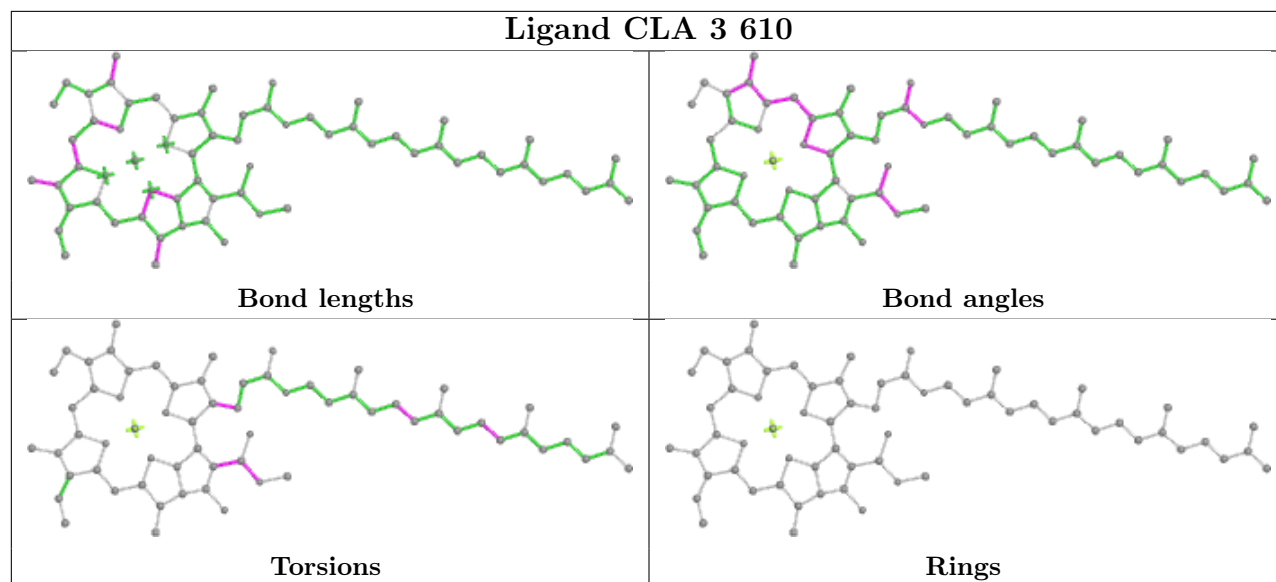
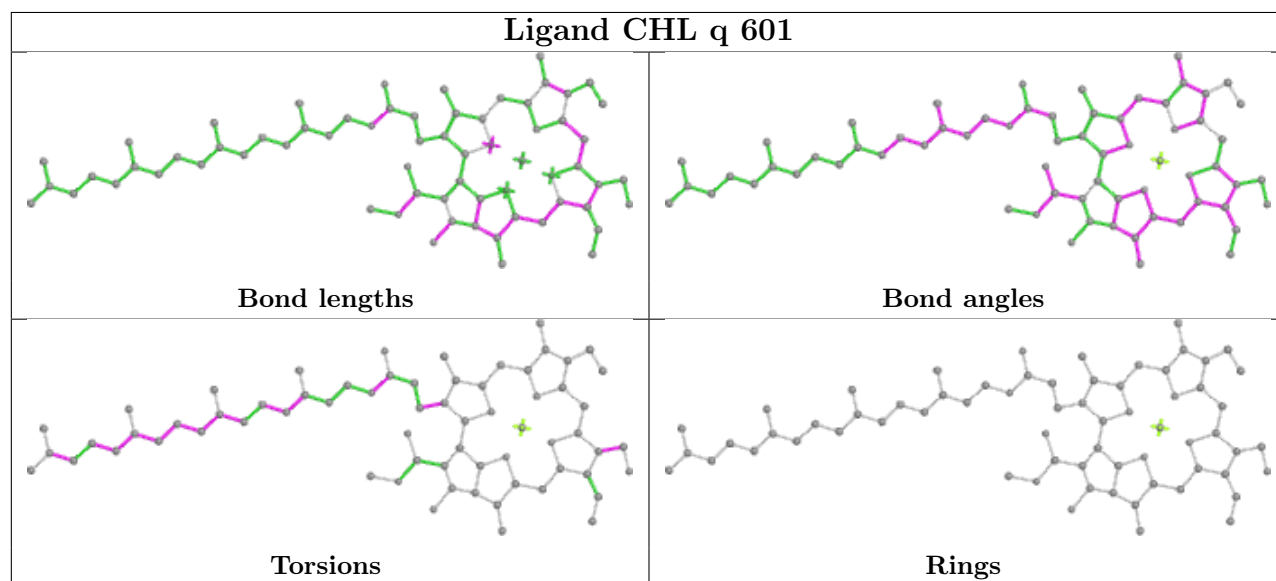


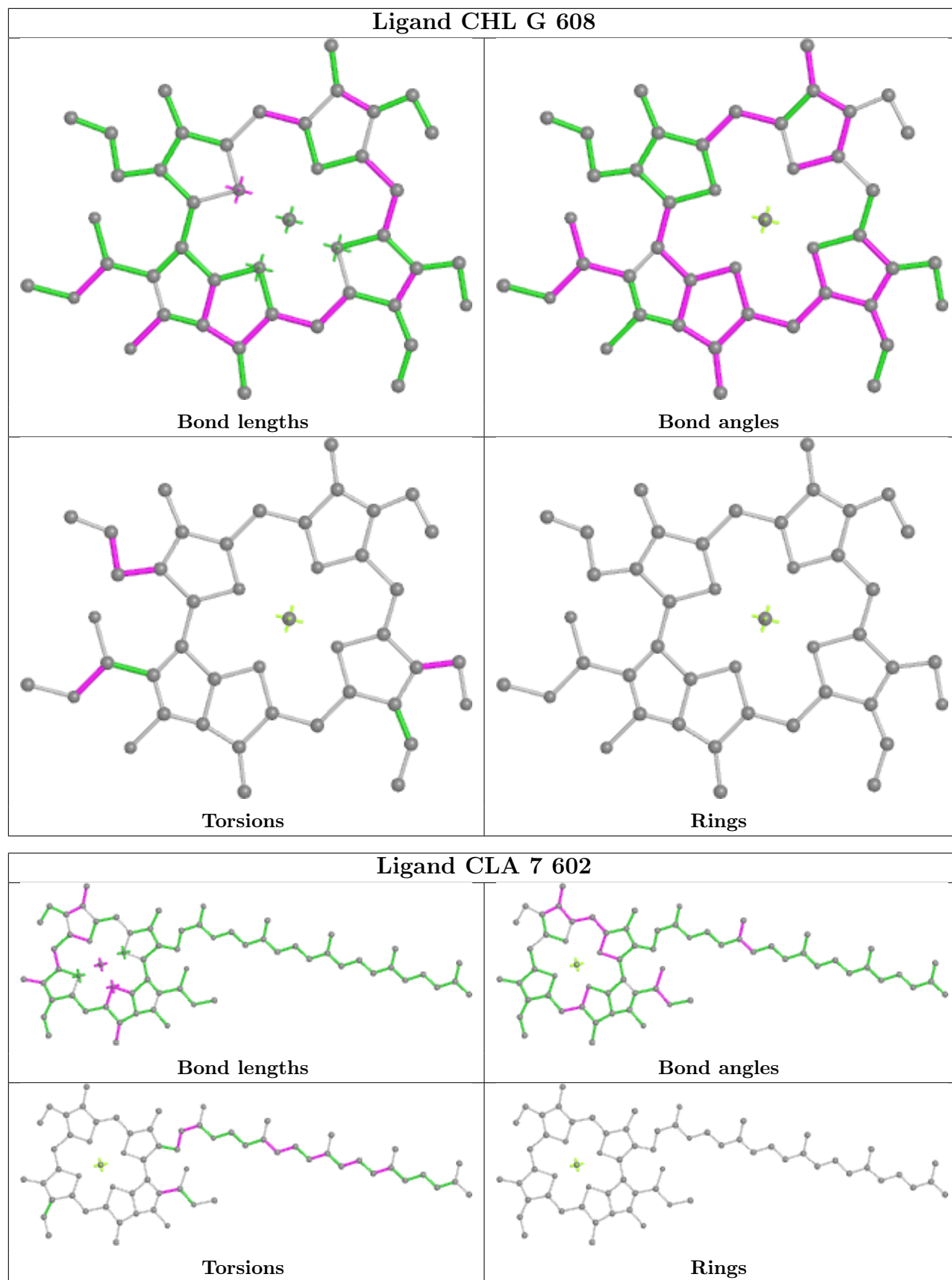
Torsions



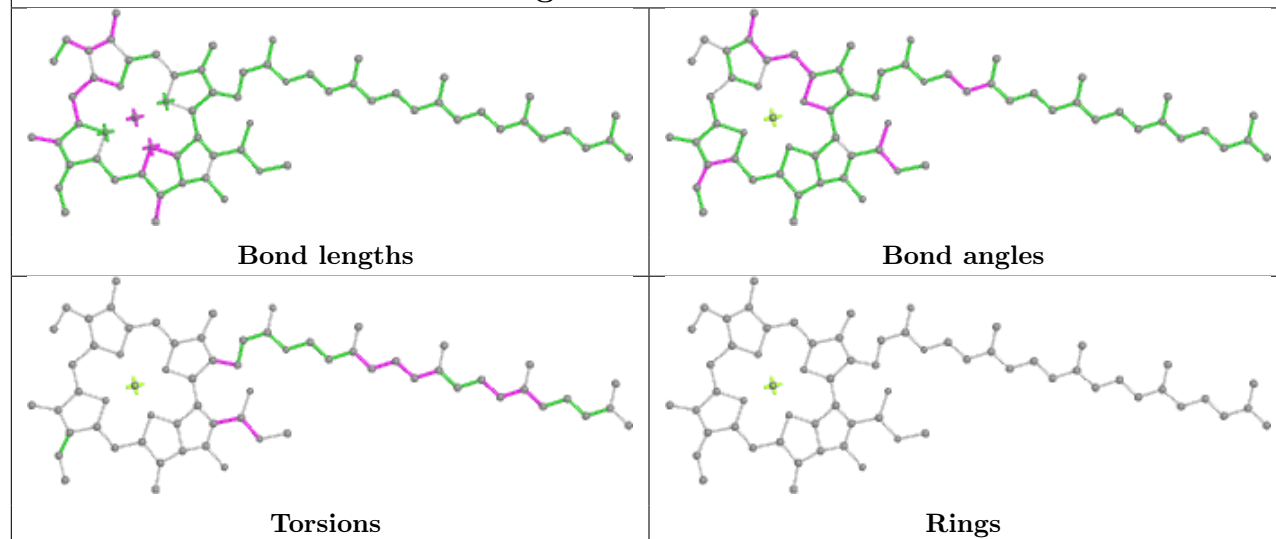
Rings



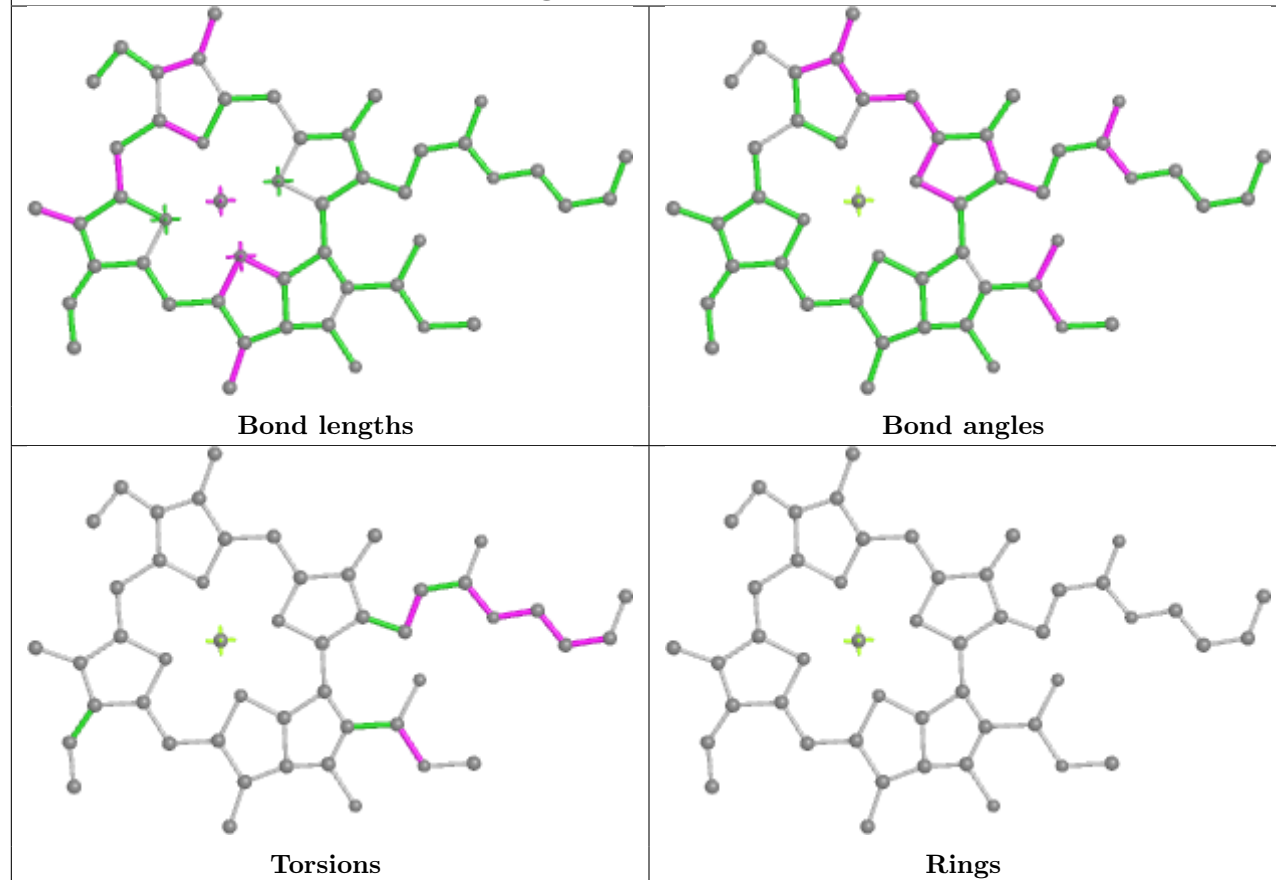
Ligand CLA 3 610**Ligand CHL q 601**

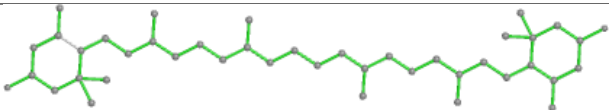
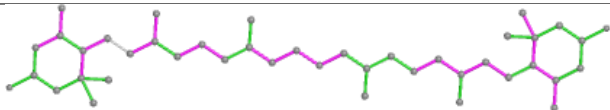
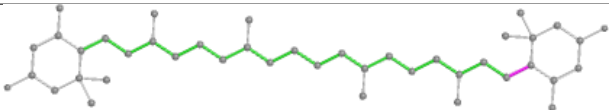
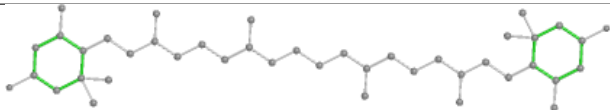


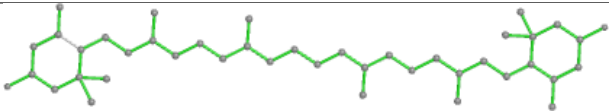
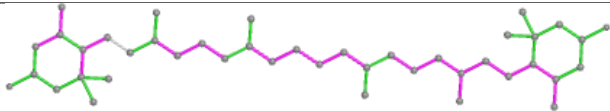
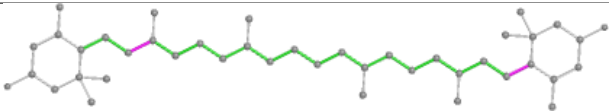
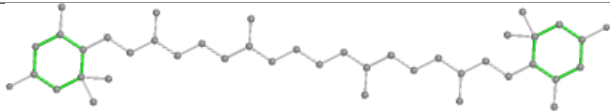
Ligand CLA 1 604

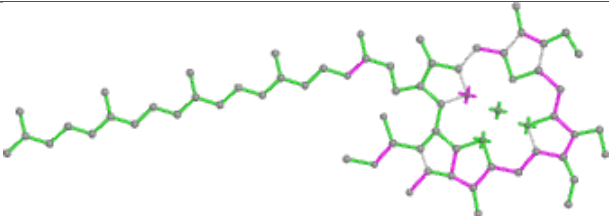
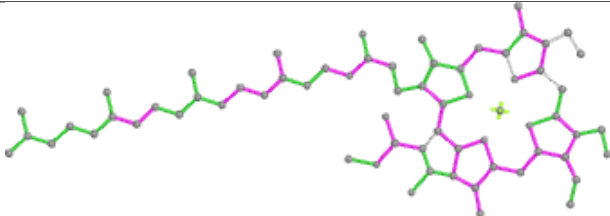
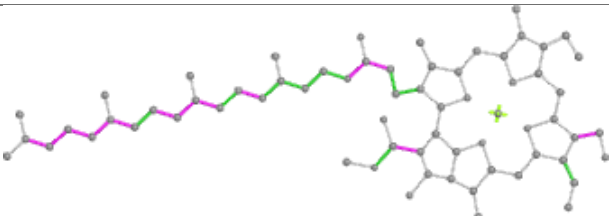
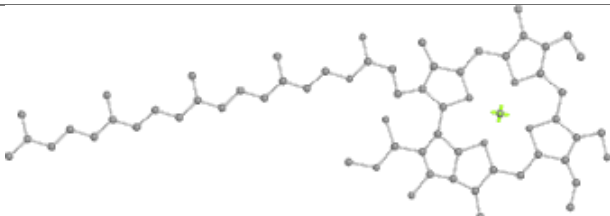


Ligand CLA r 612

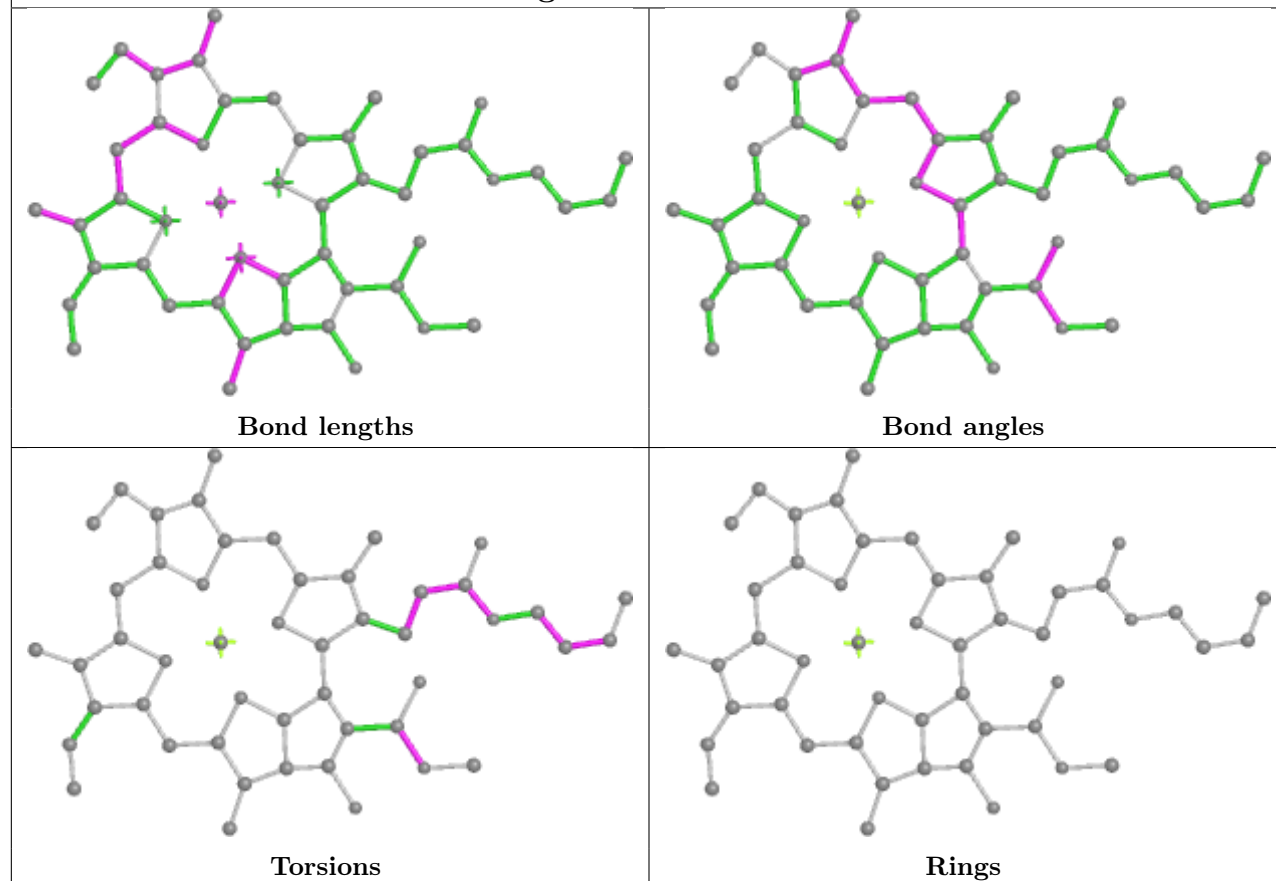


Ligand LUT 2 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

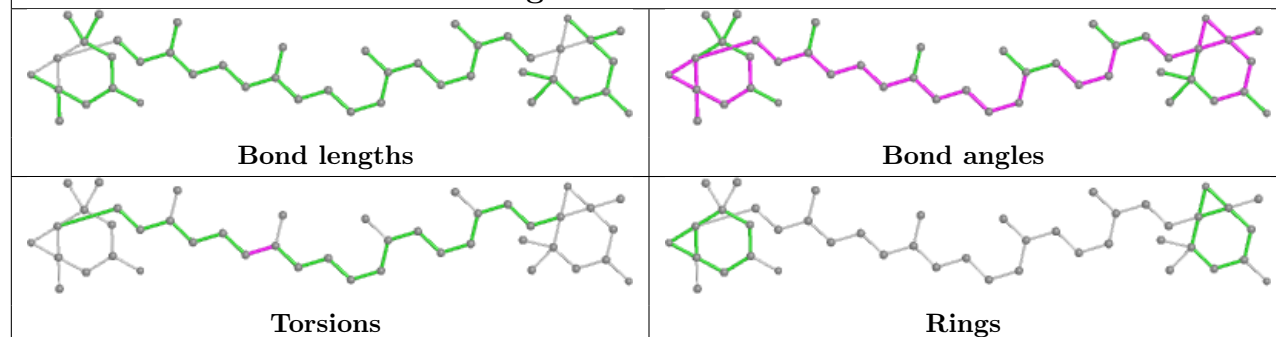
Ligand LUT 8 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

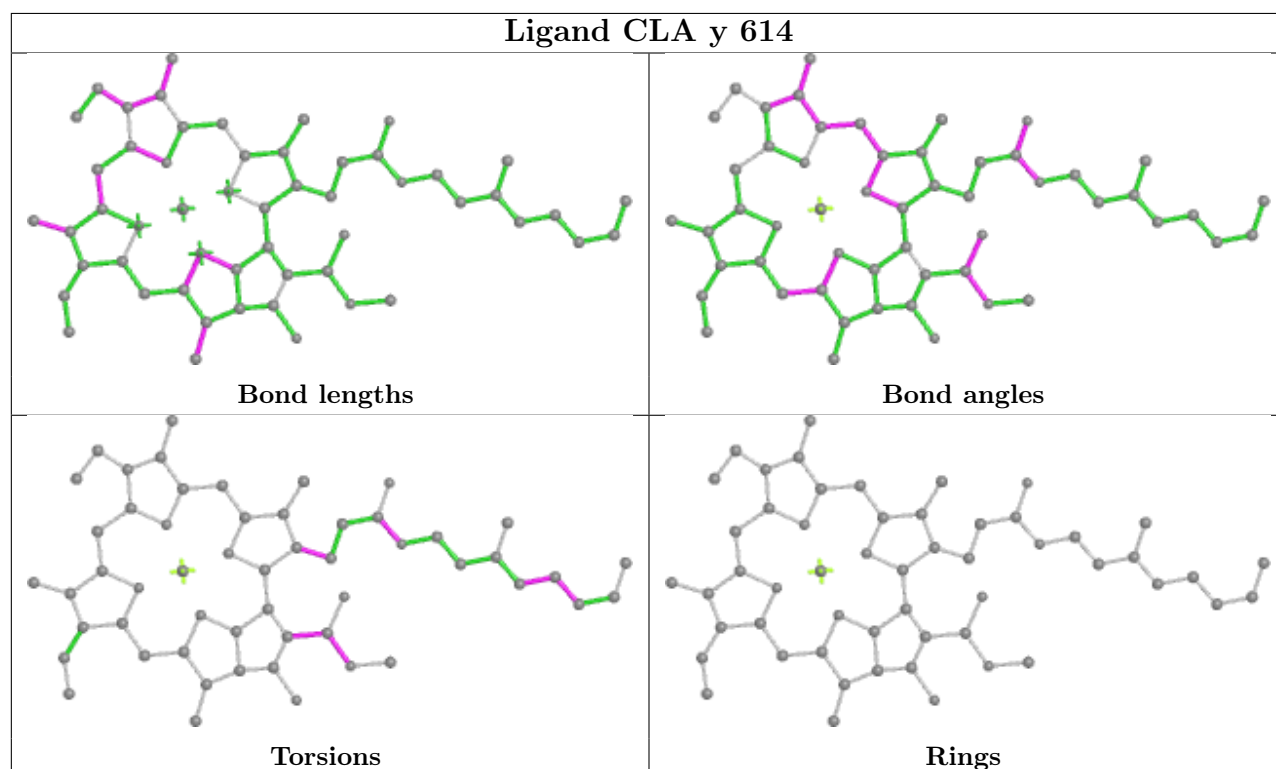
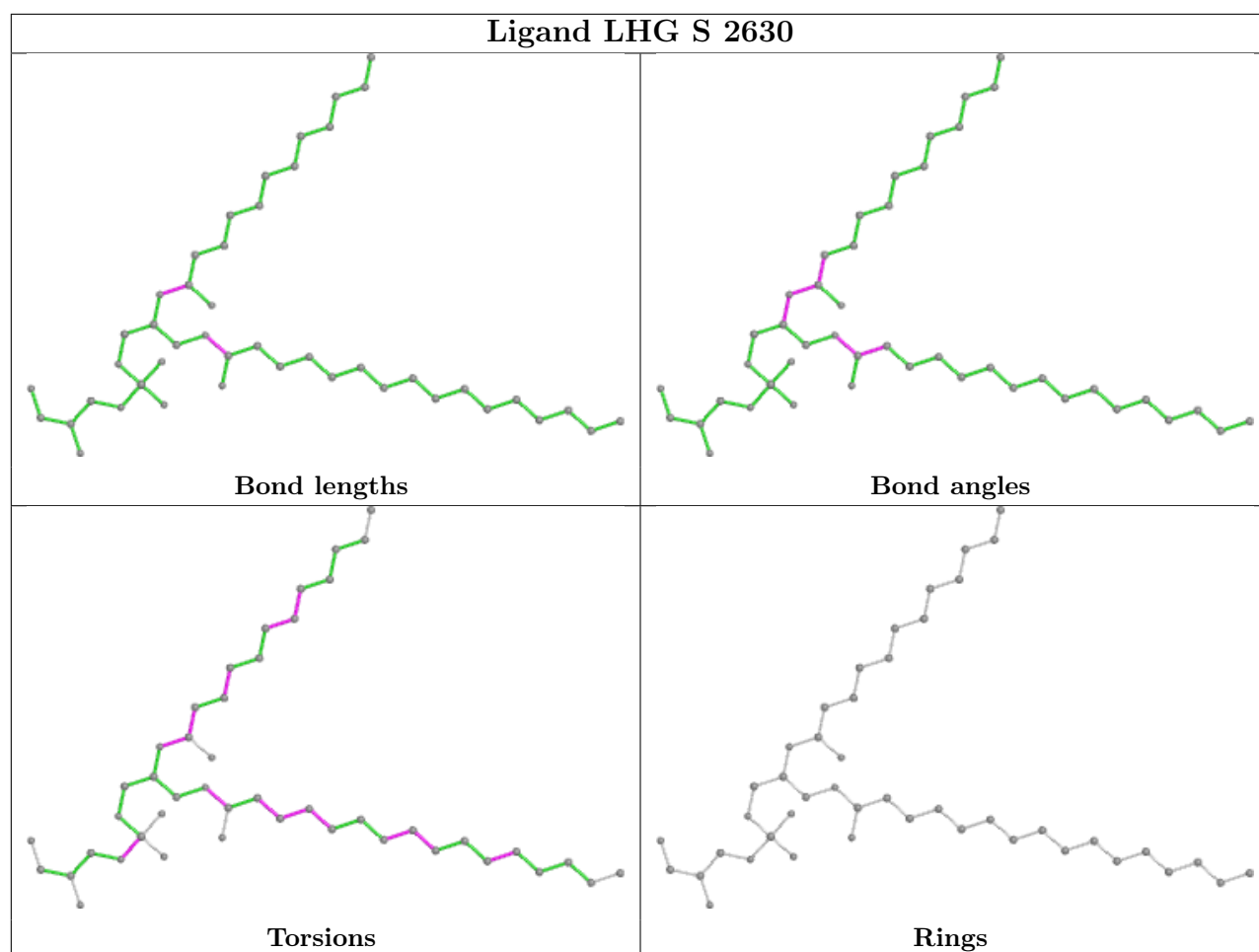
Ligand CHL 5 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

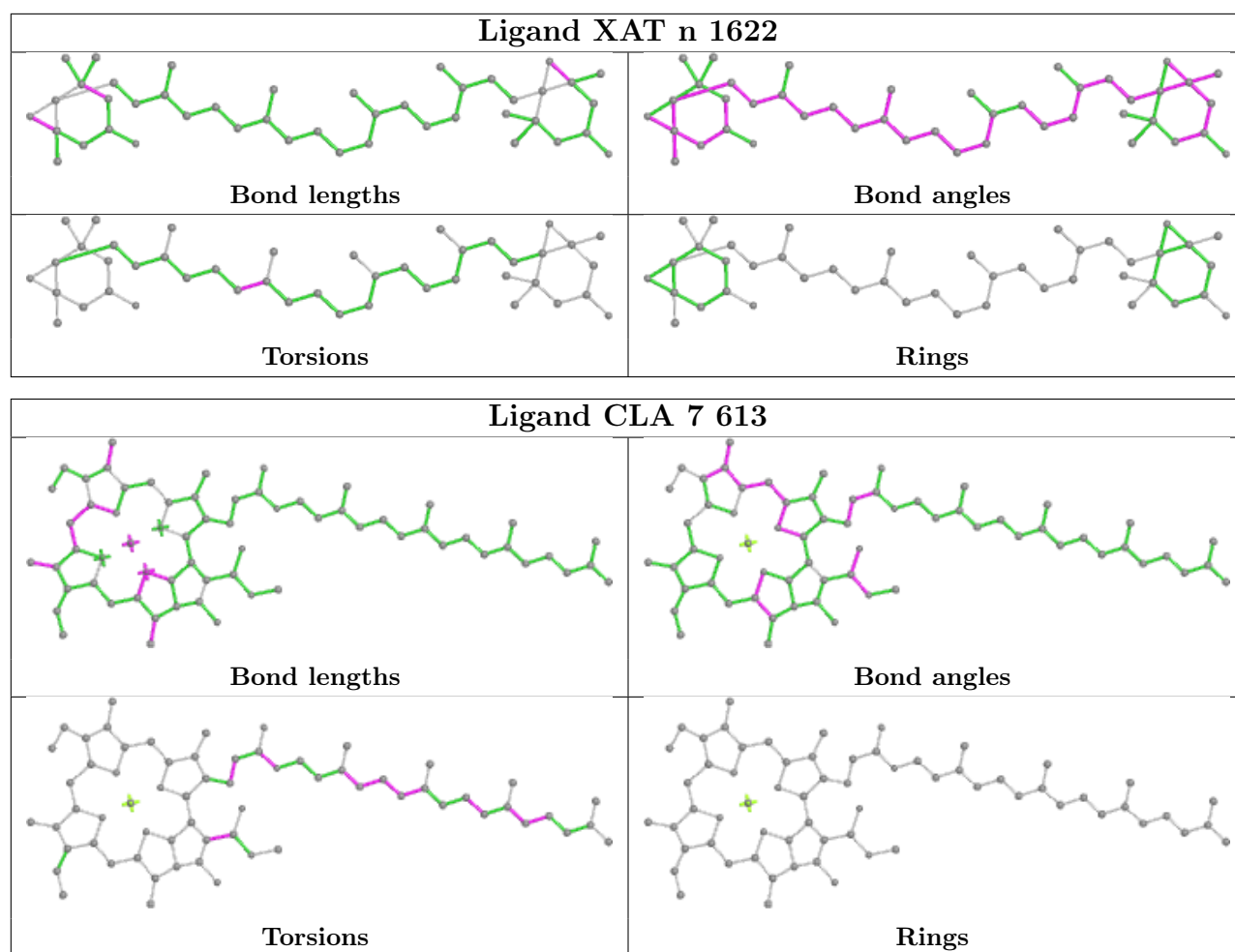
Ligand CLA s 613



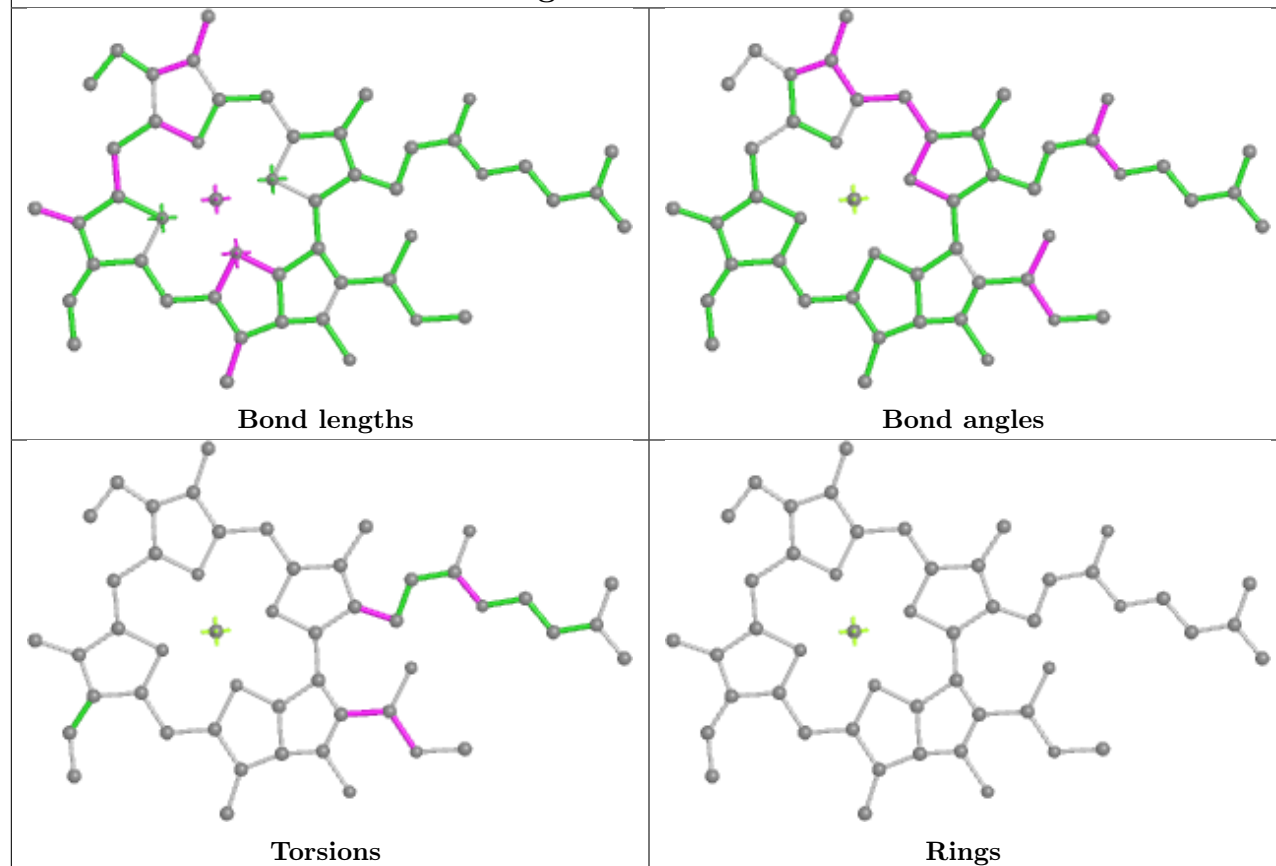
Ligand XAT 3 1622



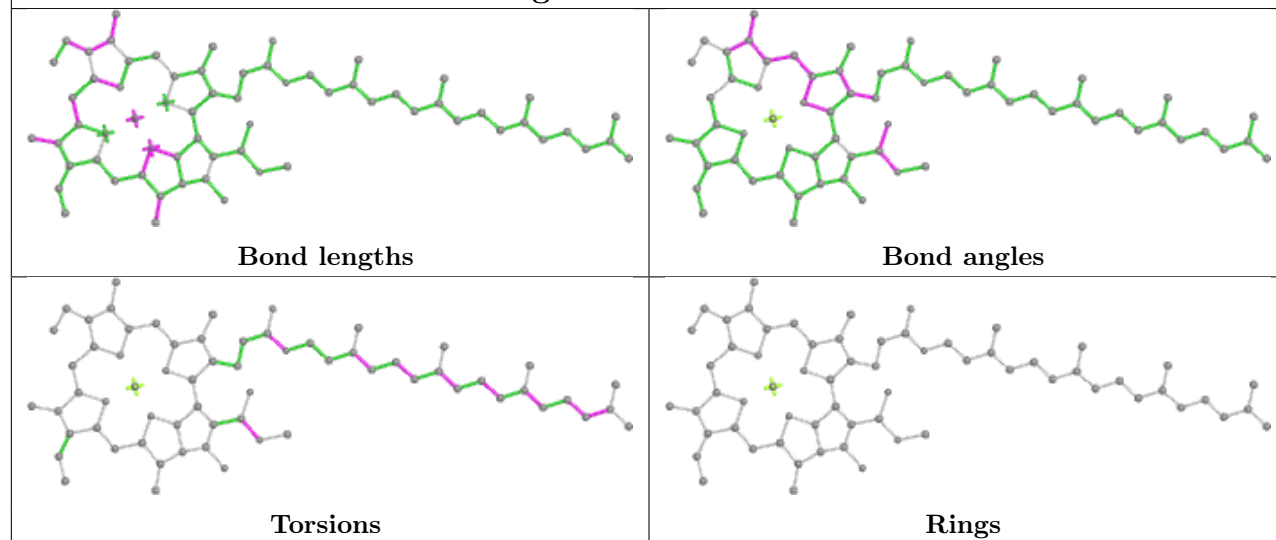


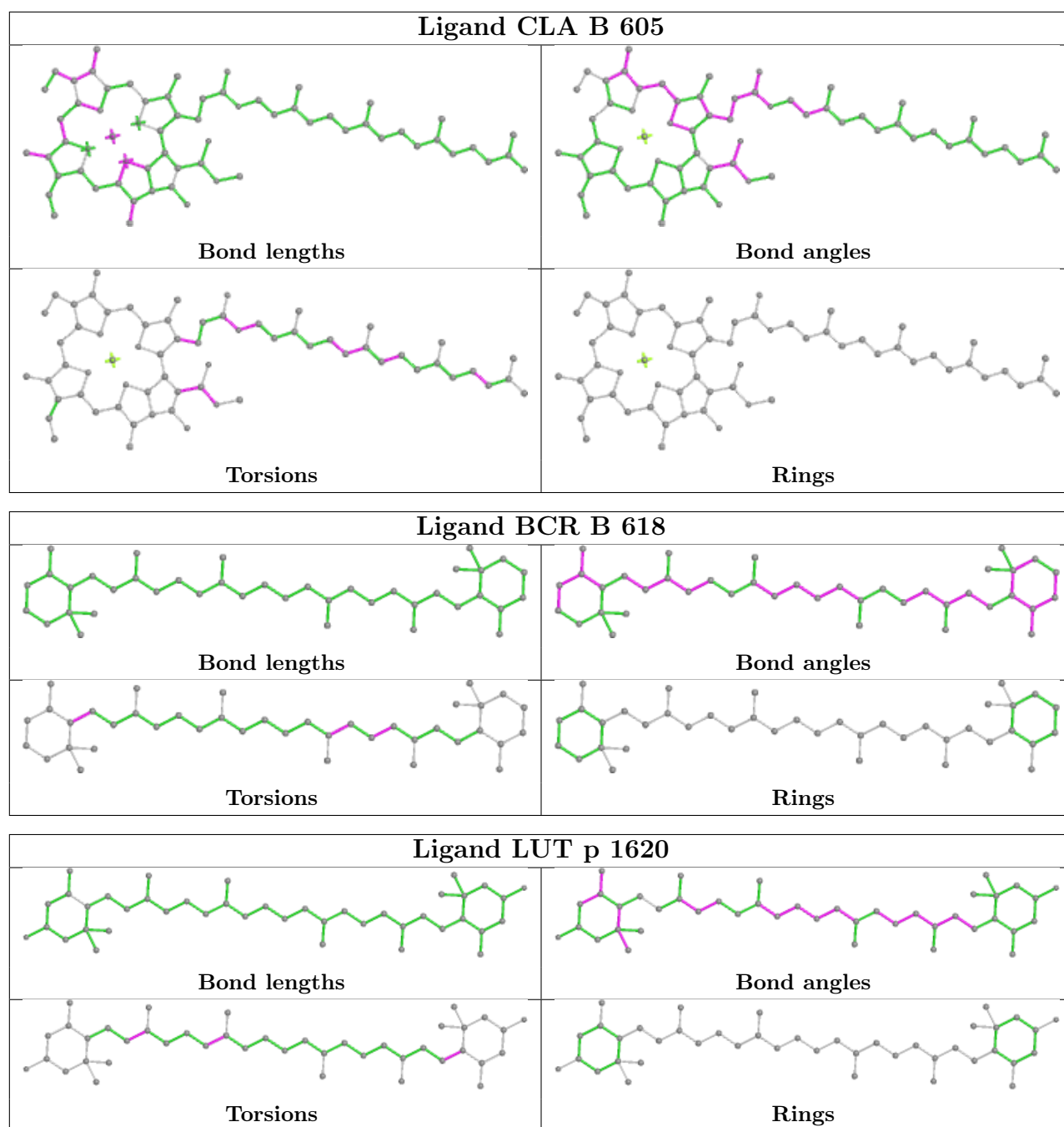


Ligand CLA s 605

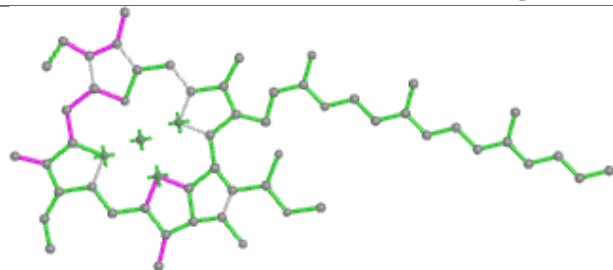


Ligand CLA C 512

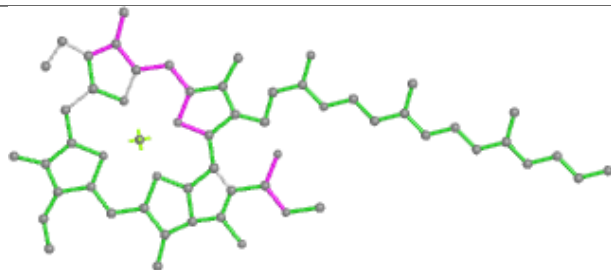




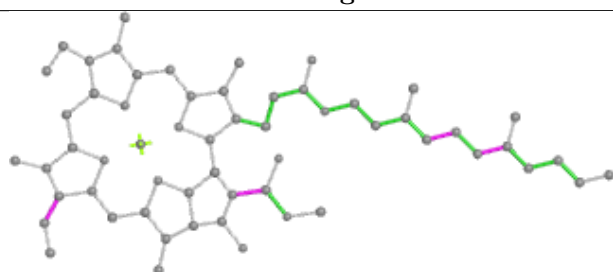
Ligand CLA R 609



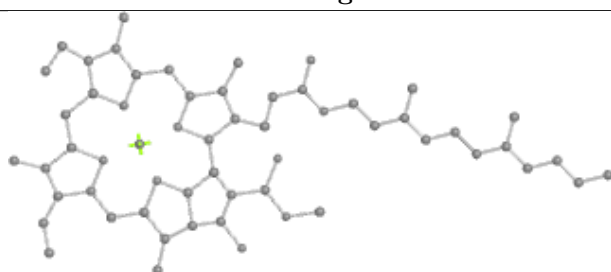
Bond lengths



Bond angles

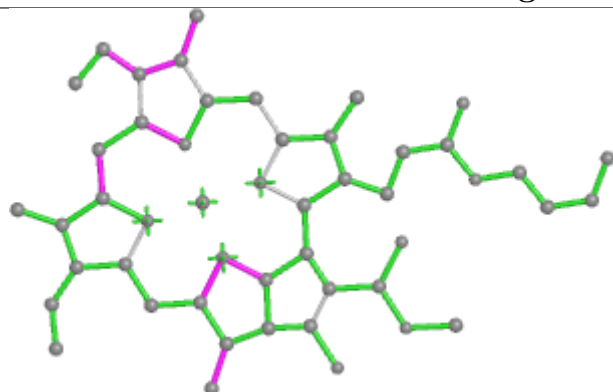


Torsions

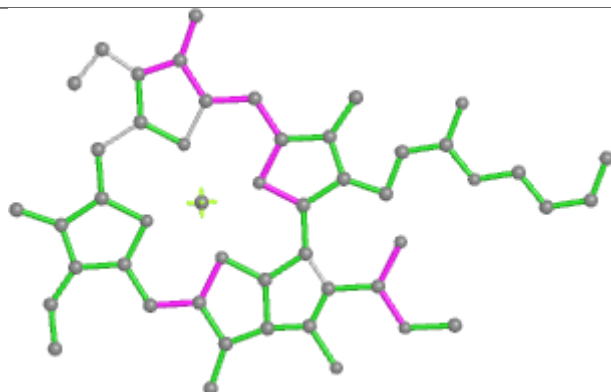


Rings

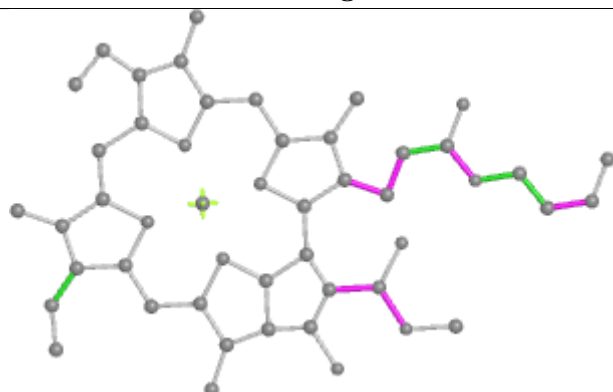
Ligand CLA 9 614



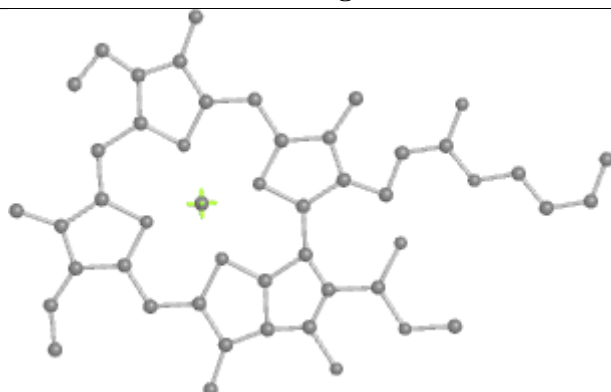
Bond lengths



Bond angles

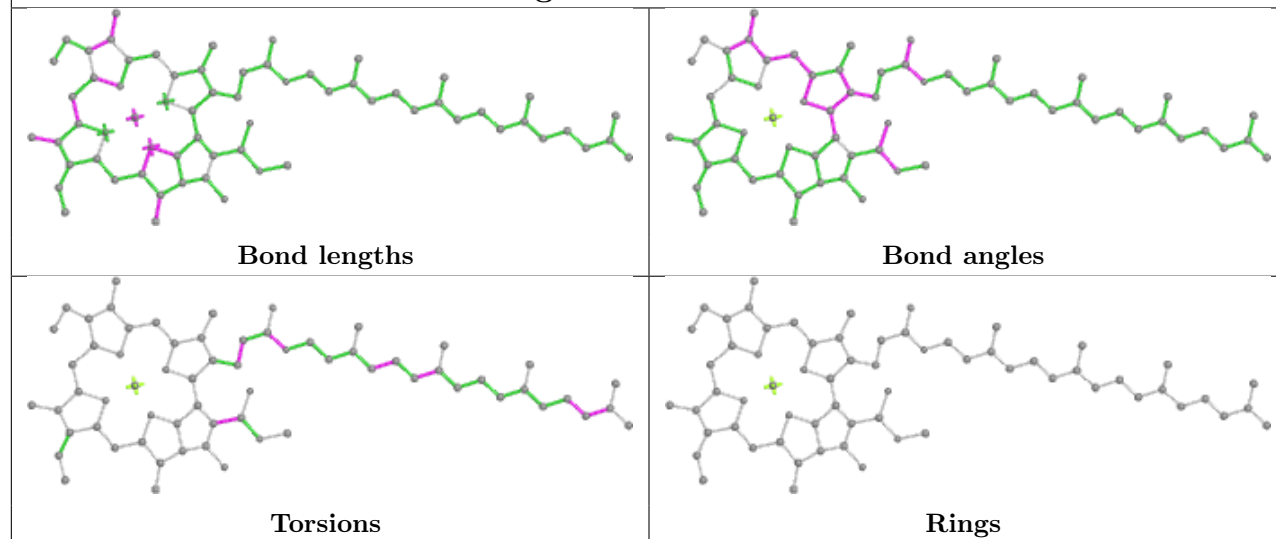


Torsions

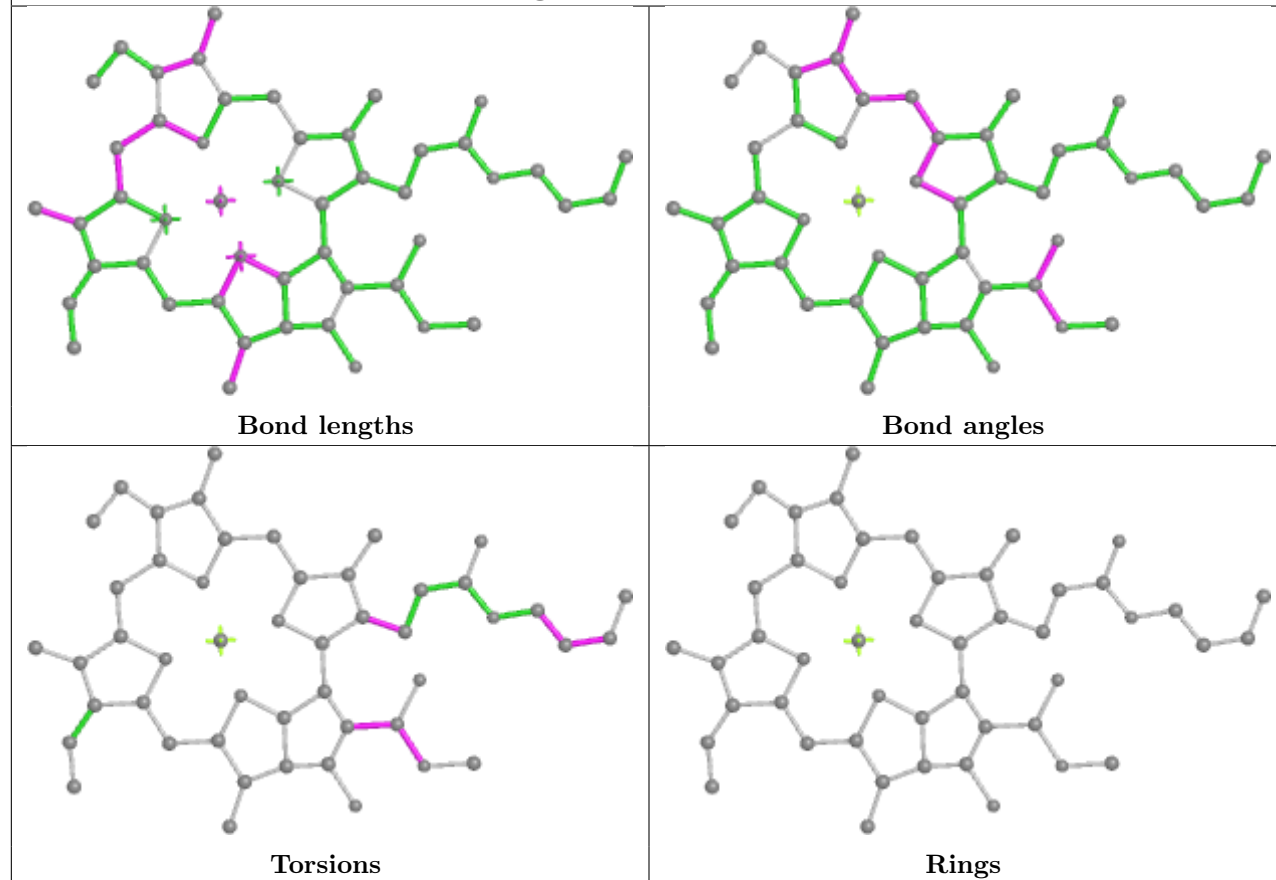


Rings

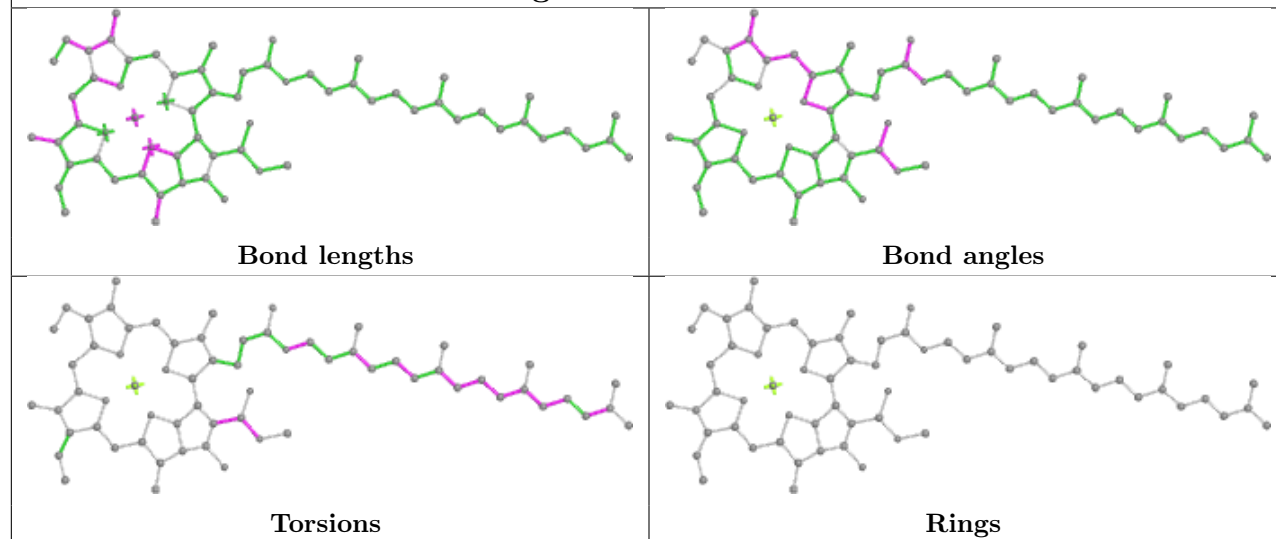
Ligand CLA b 617



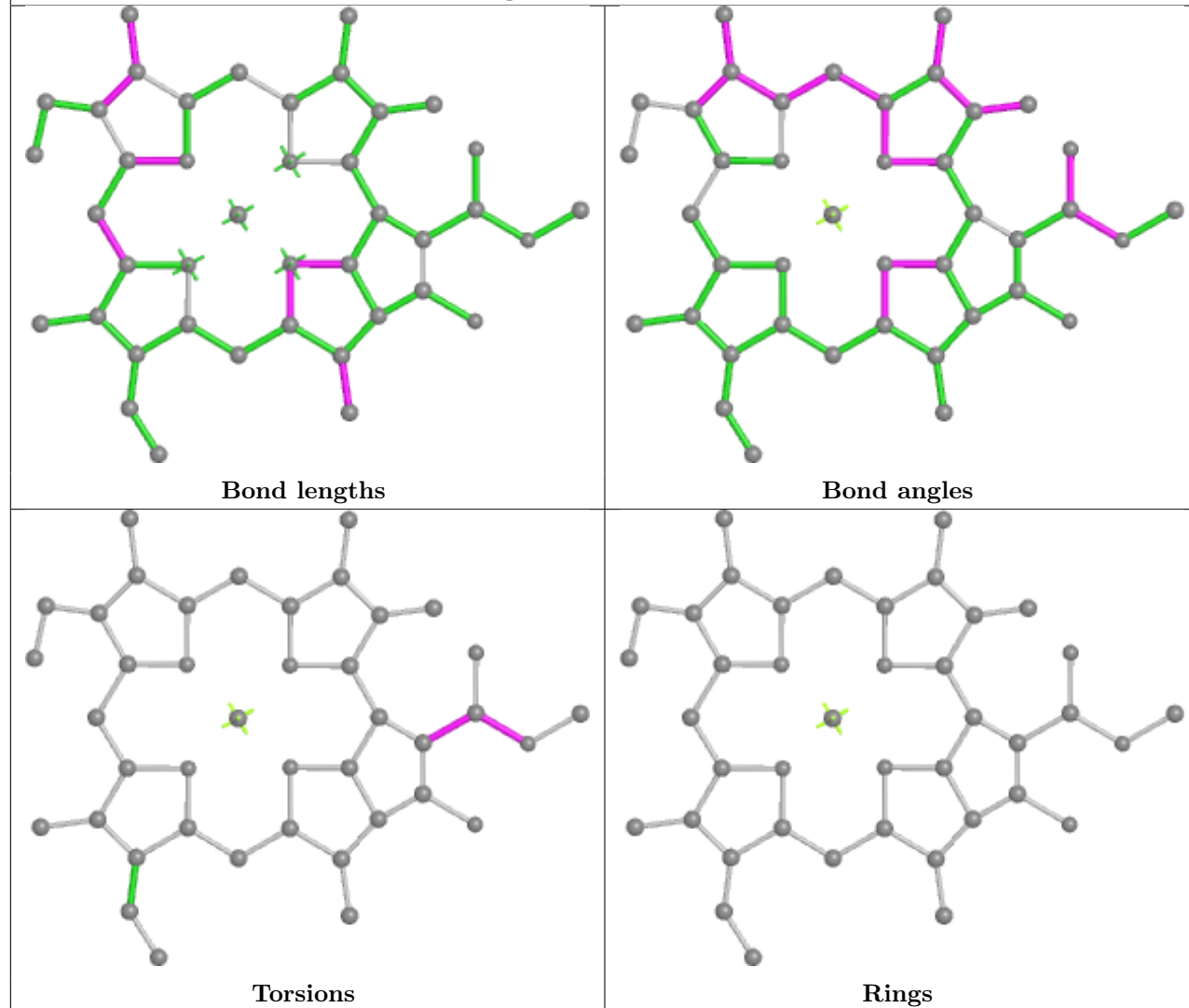
Ligand CLA N 611

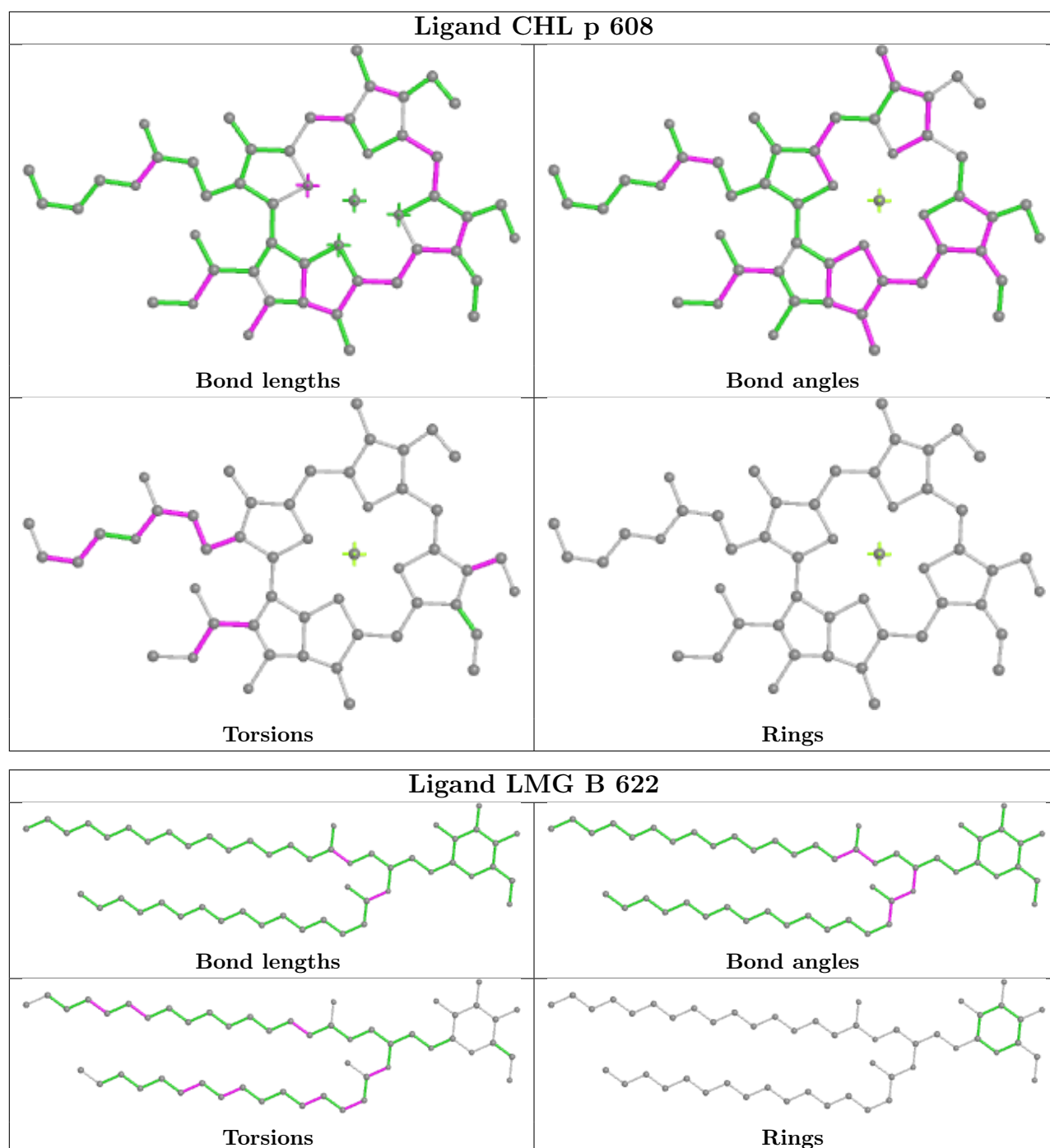


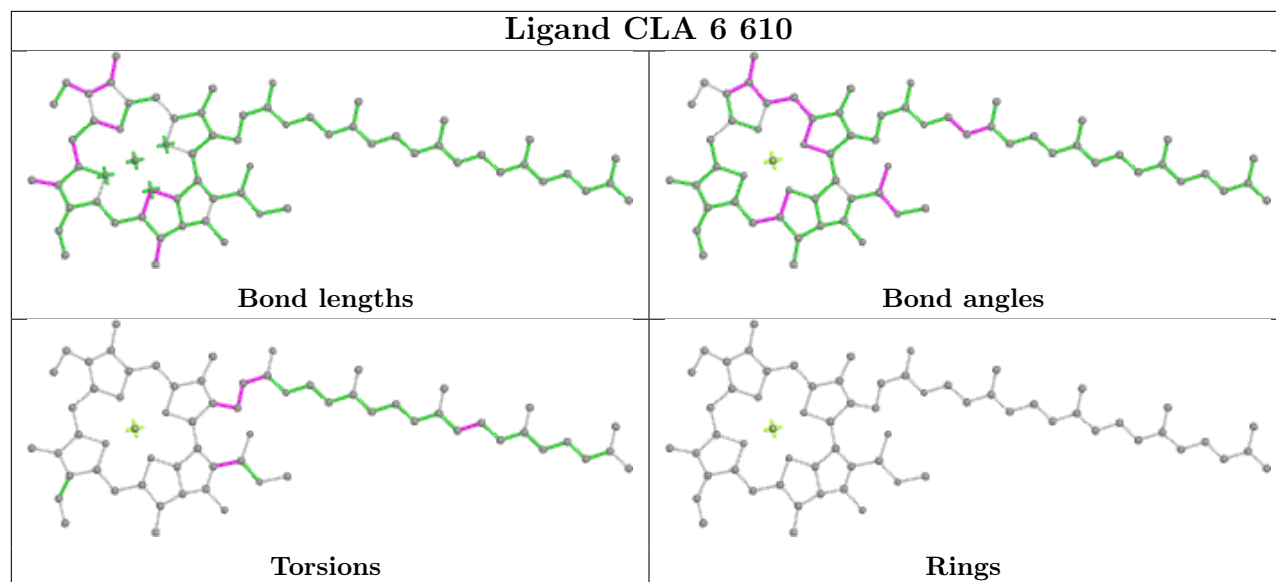
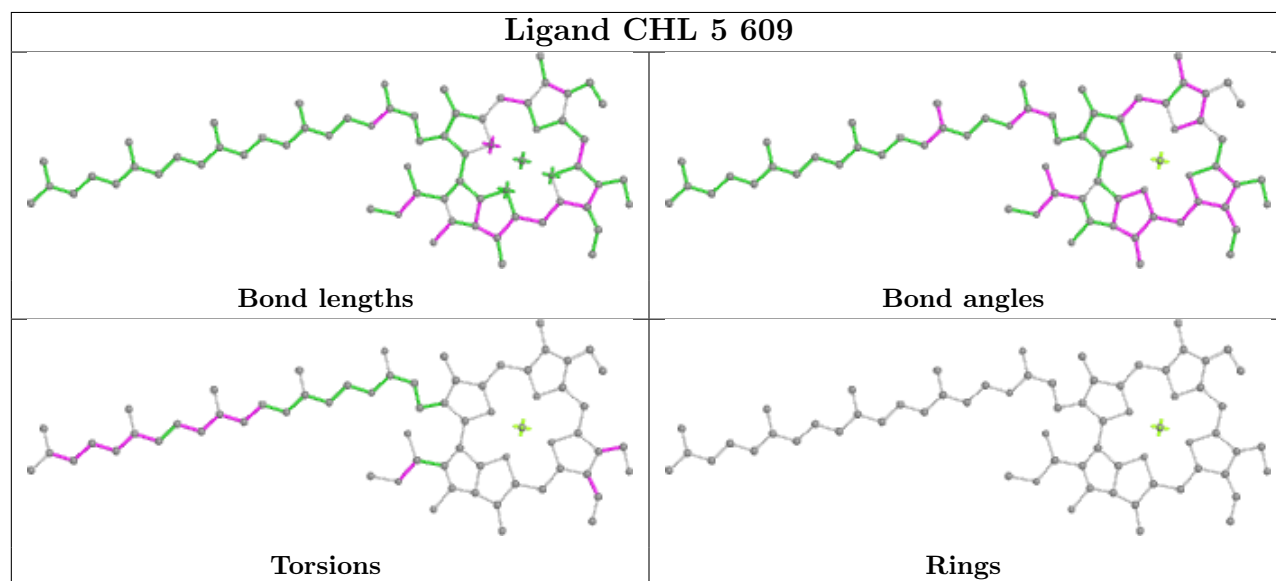
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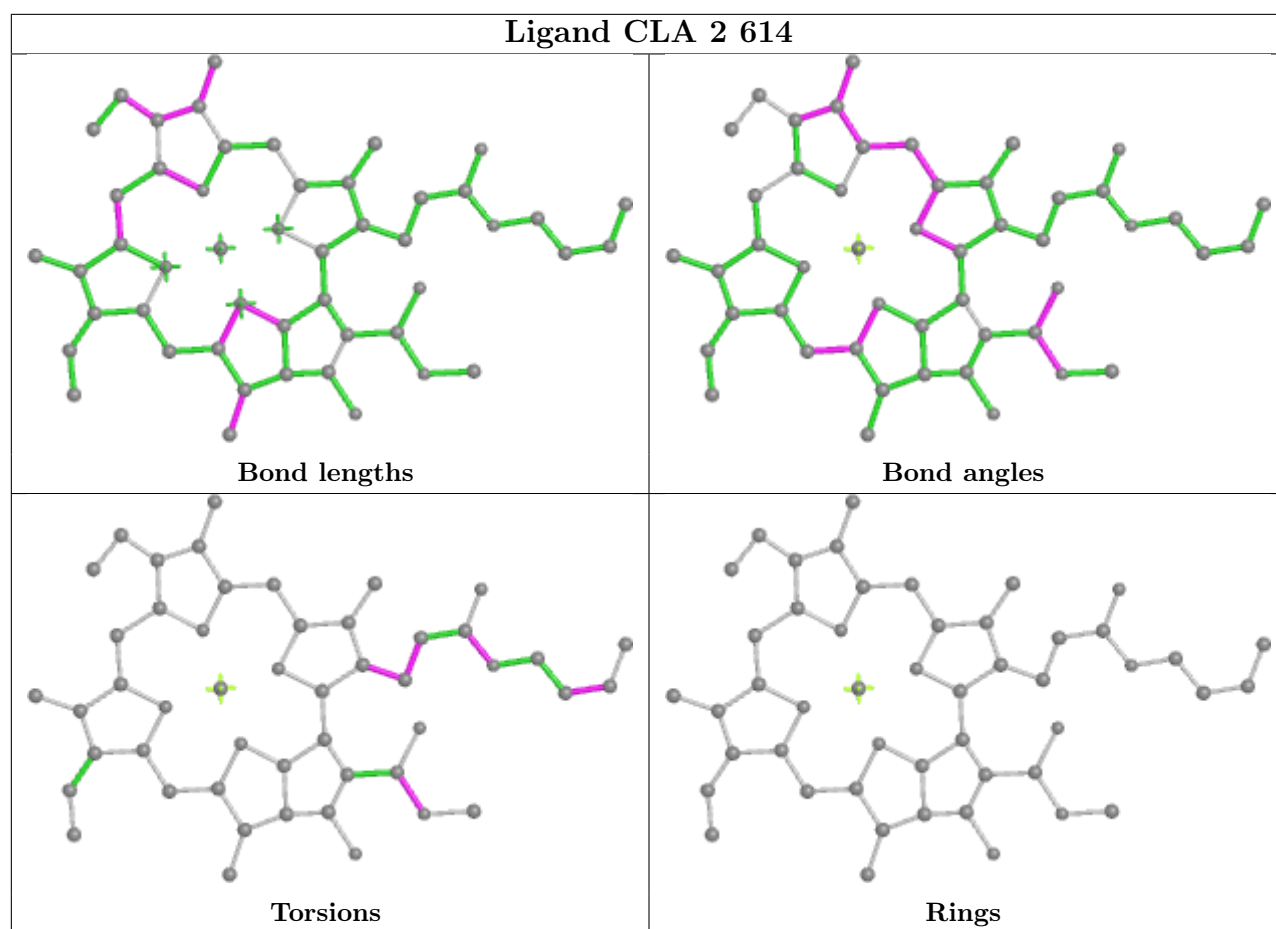


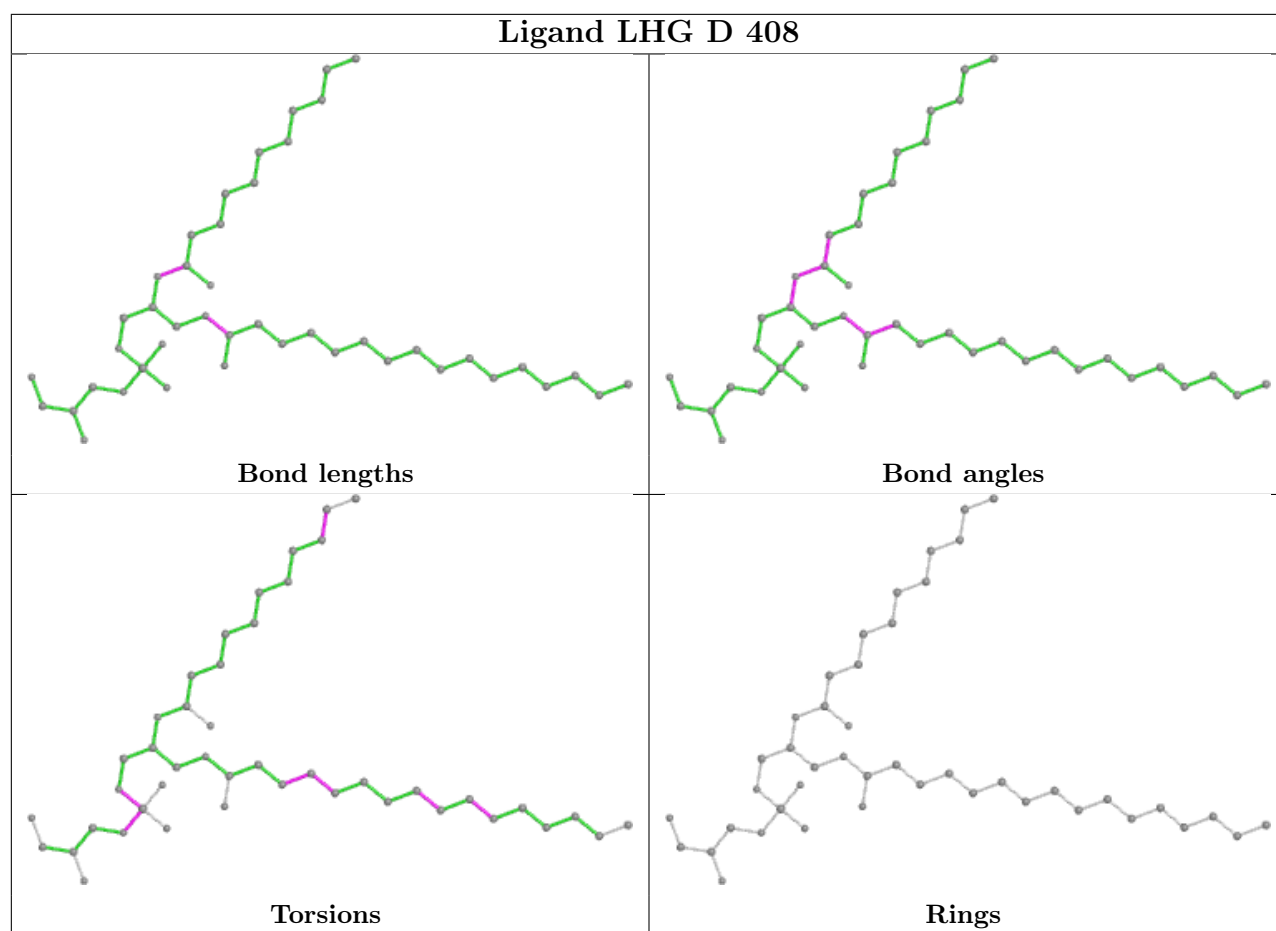
Ligand CLA s 609



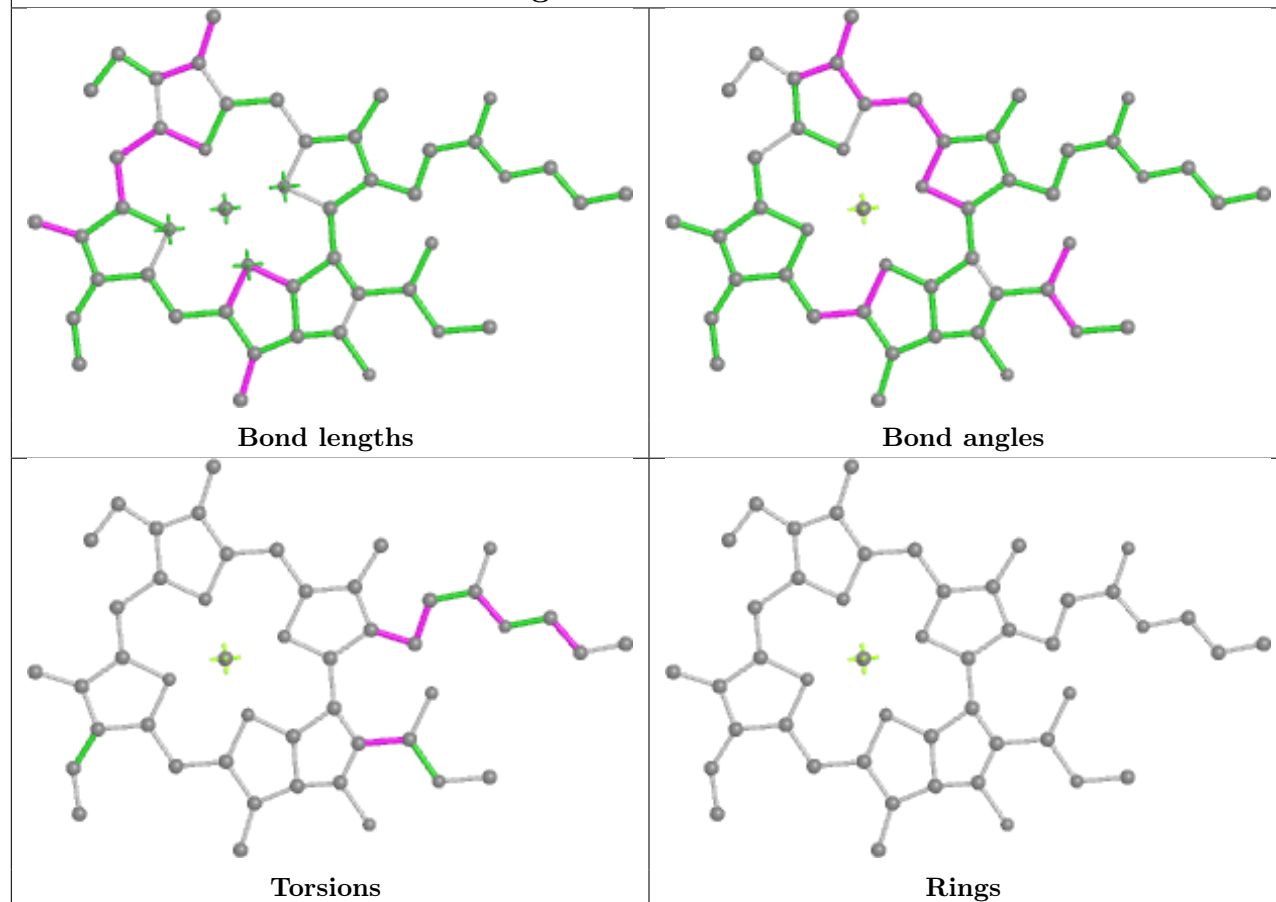


Ligand CLA 6 610**Ligand CHL 5 609**

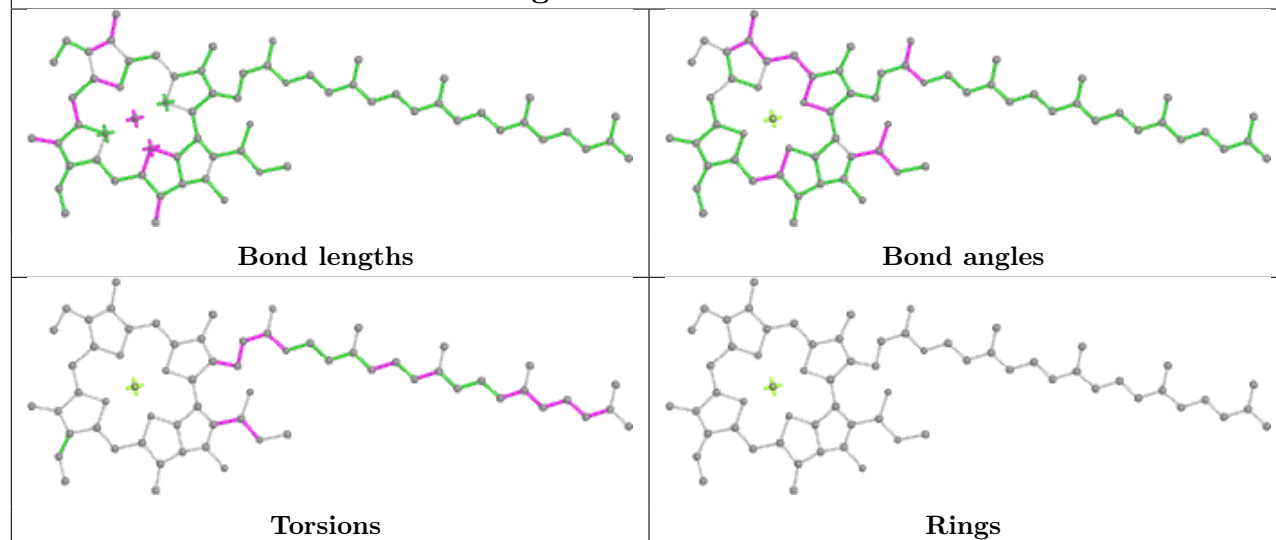




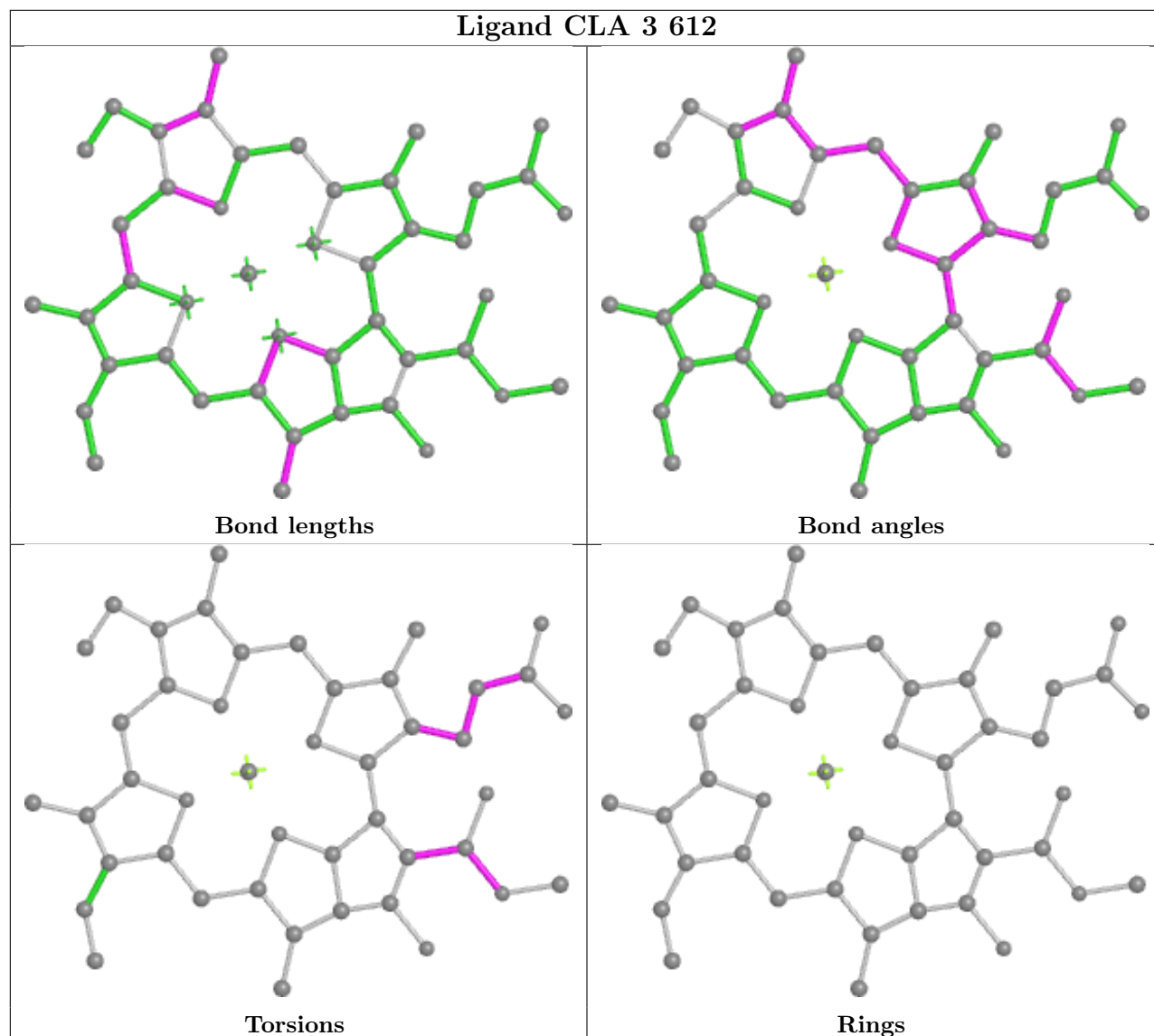
Ligand CLA R 604



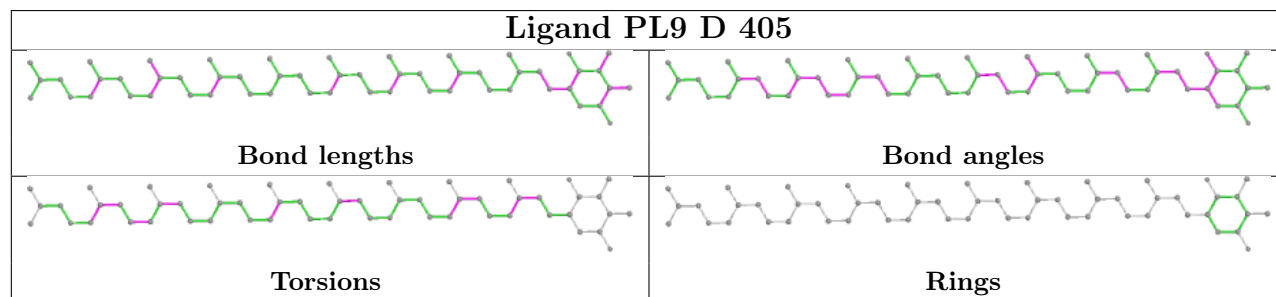
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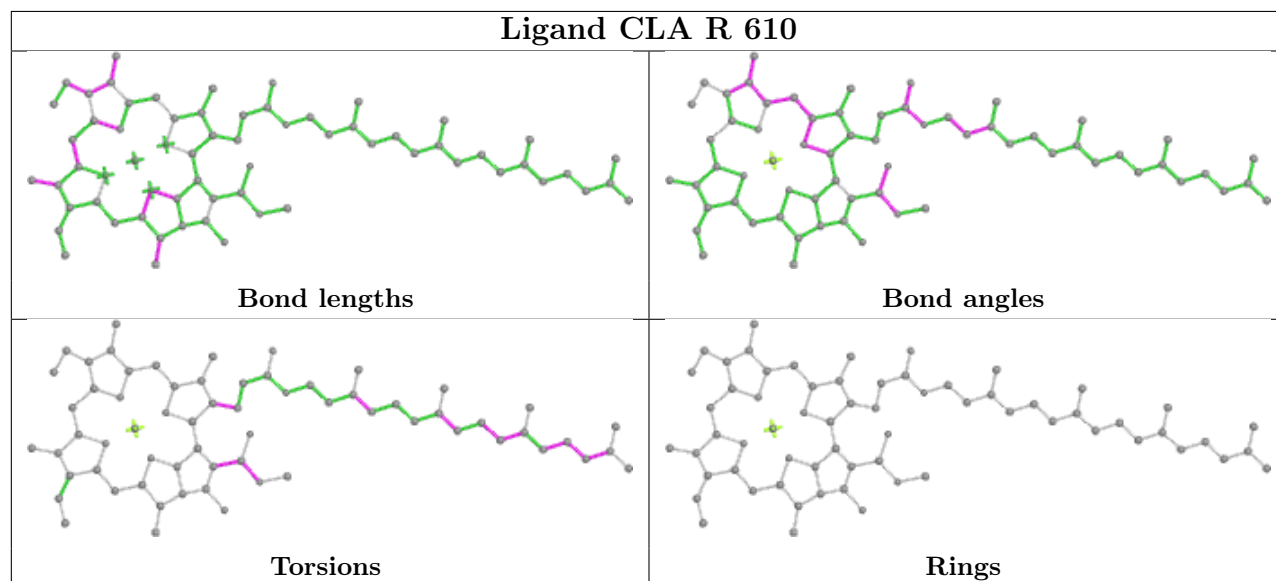
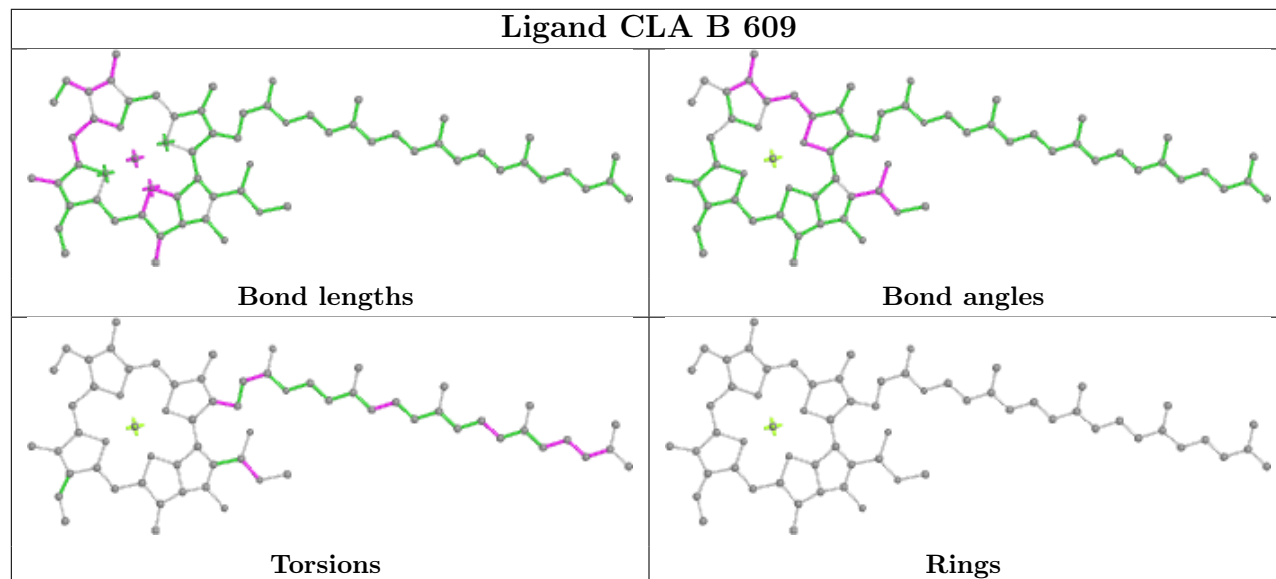
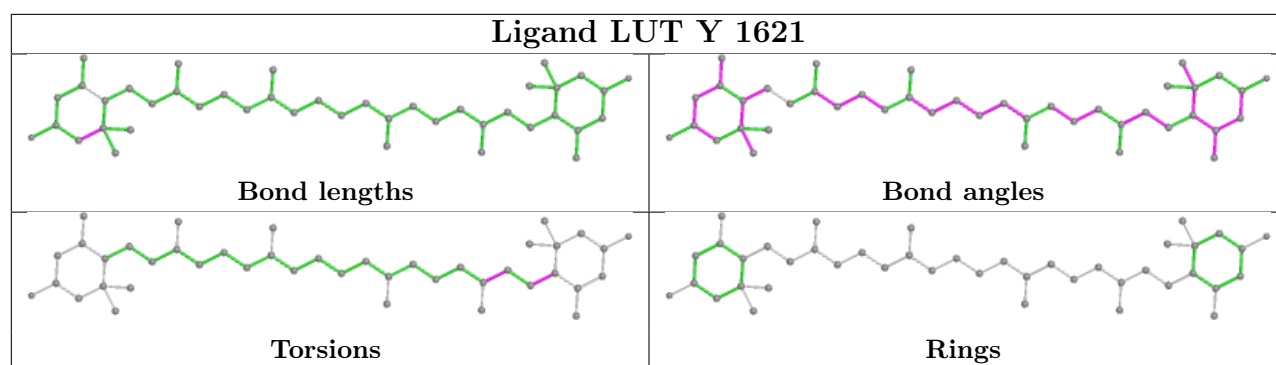


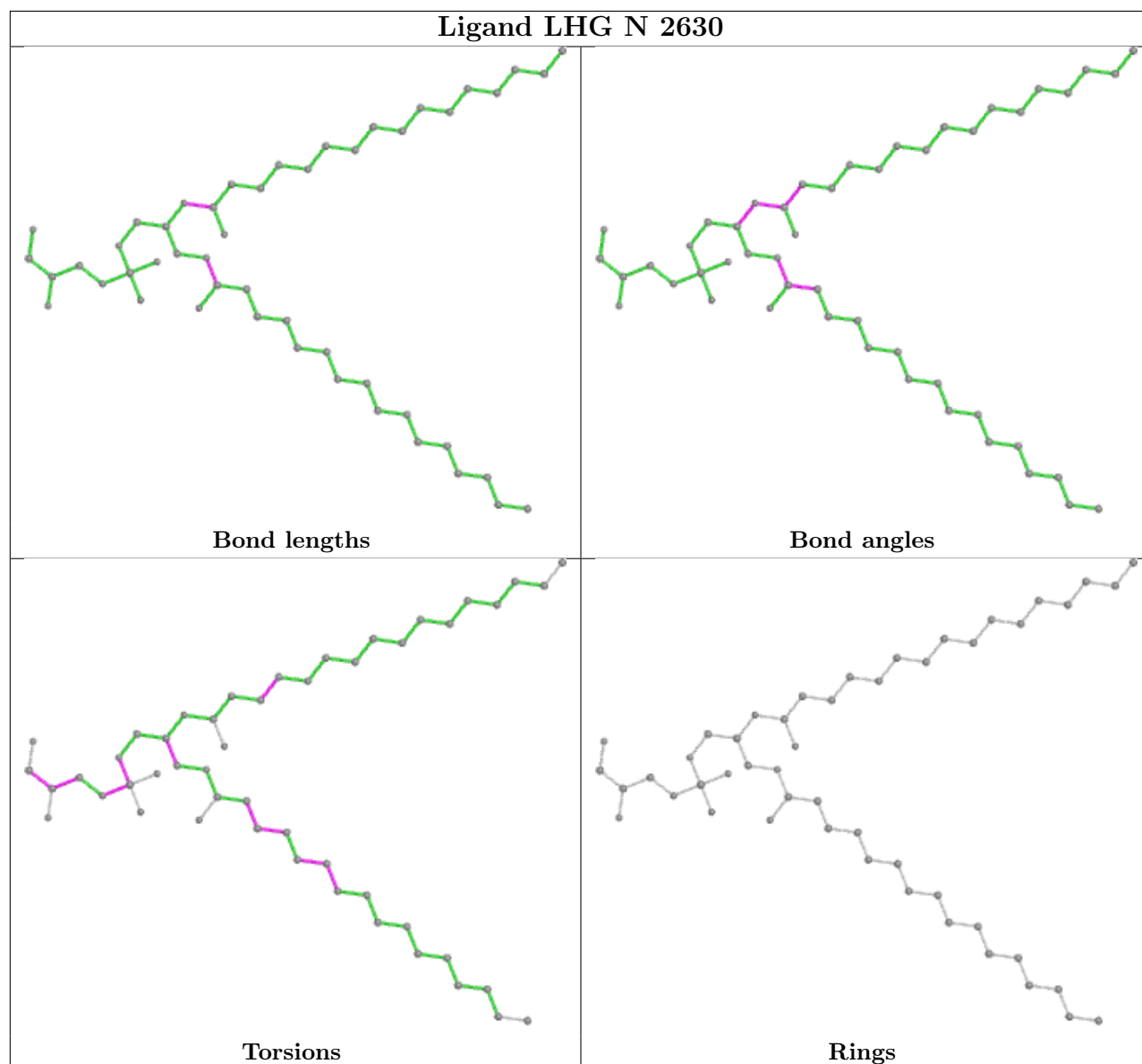
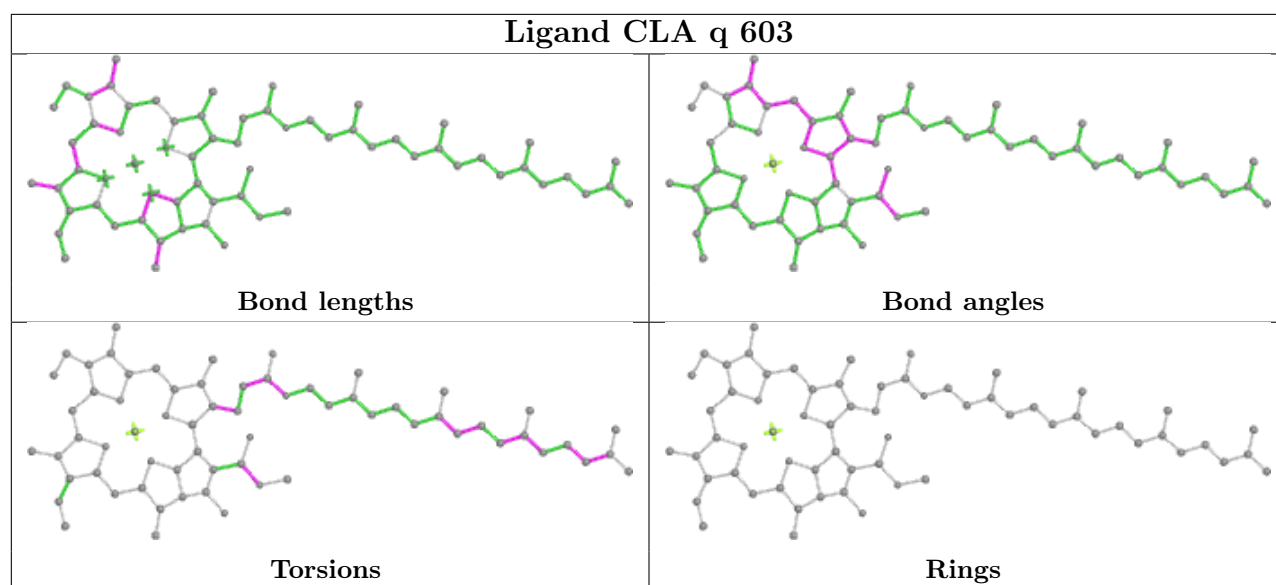
Ligand CLA 3 612

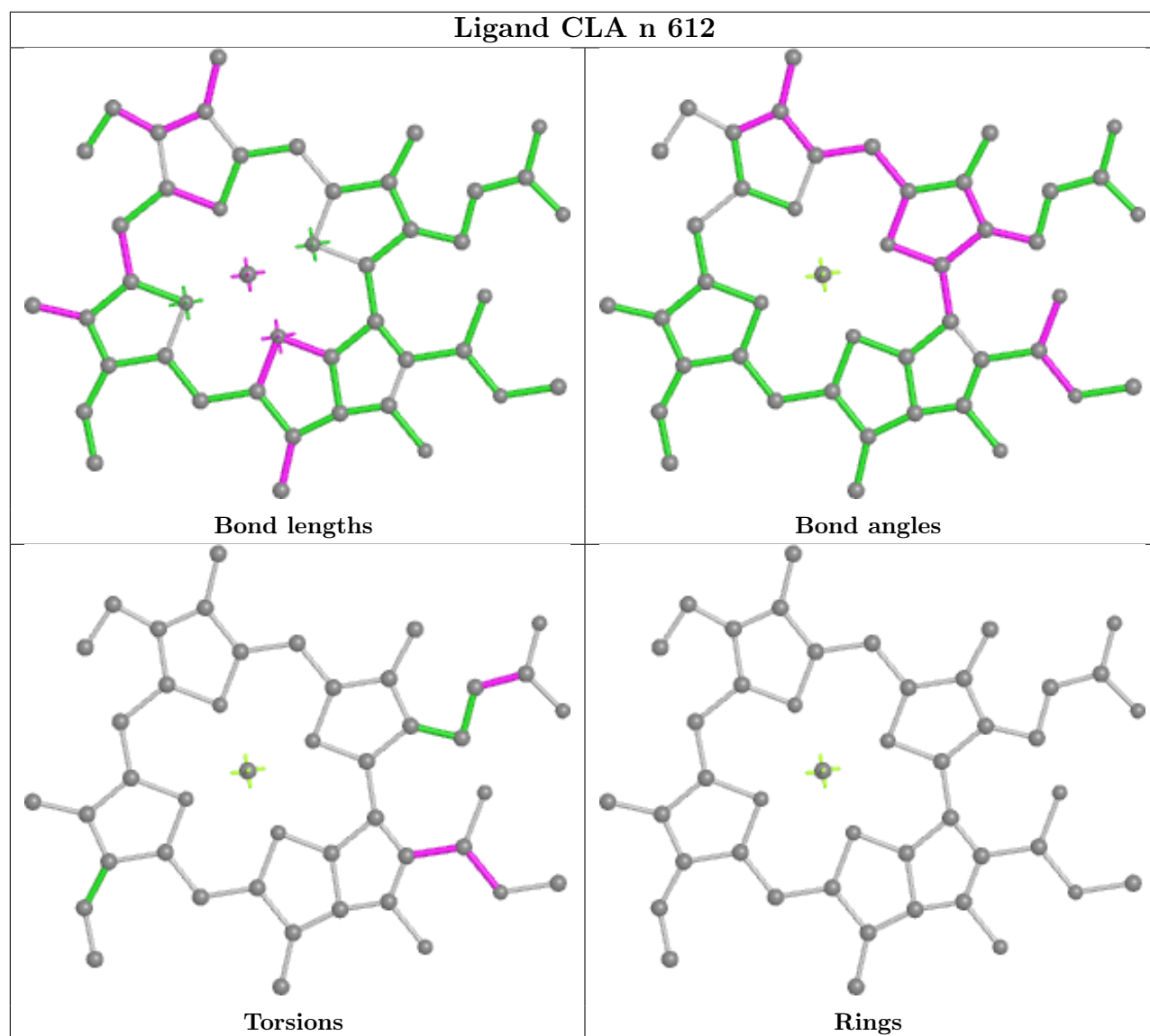
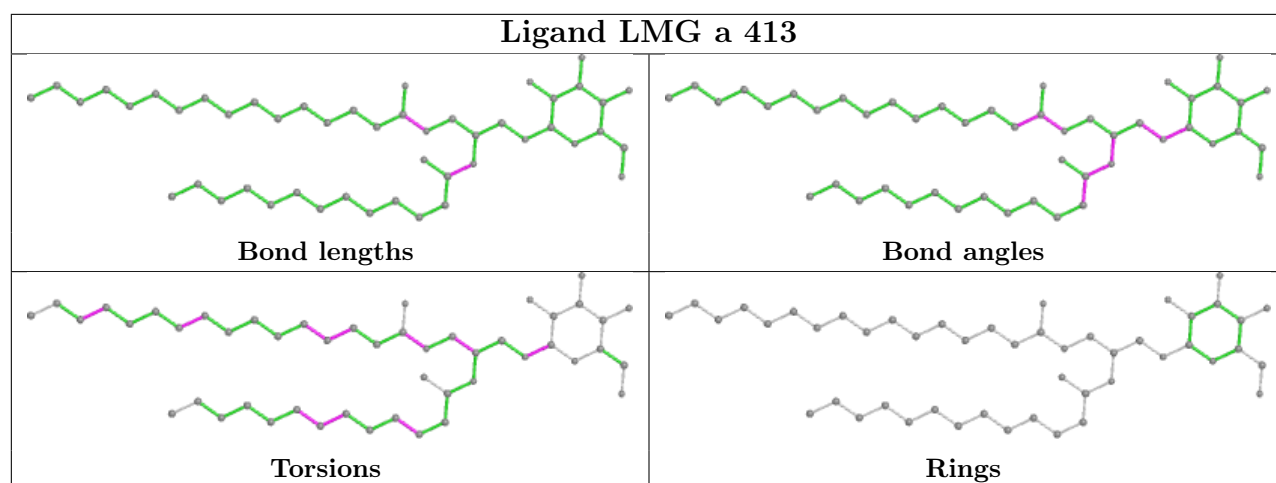


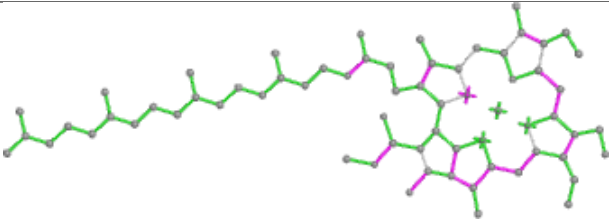
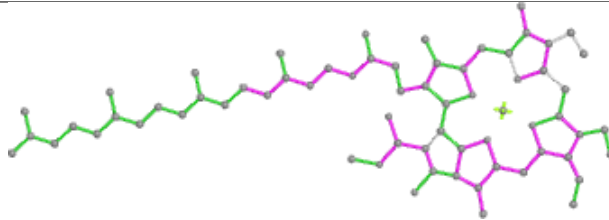
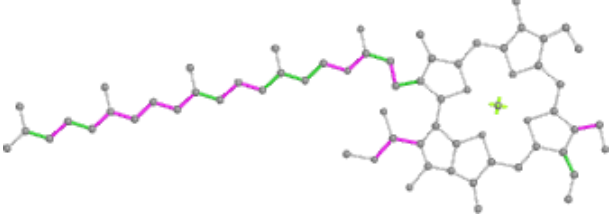
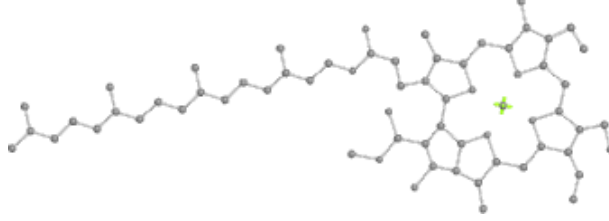
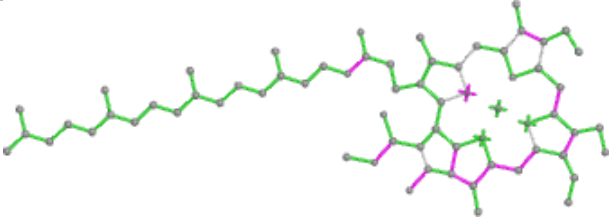
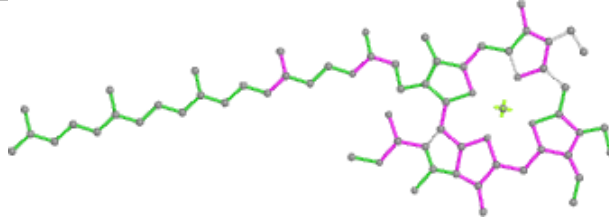
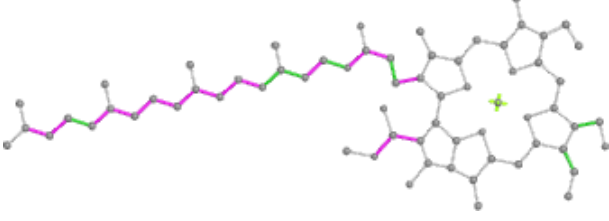
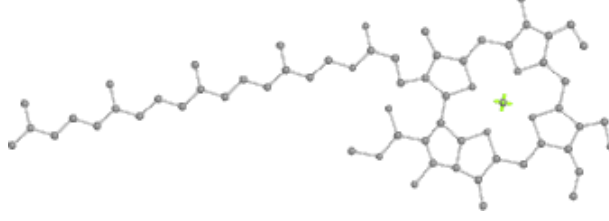
Ligand PL9 D 405



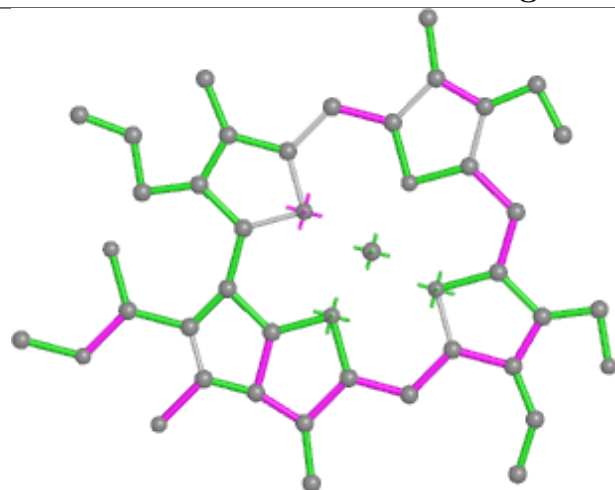




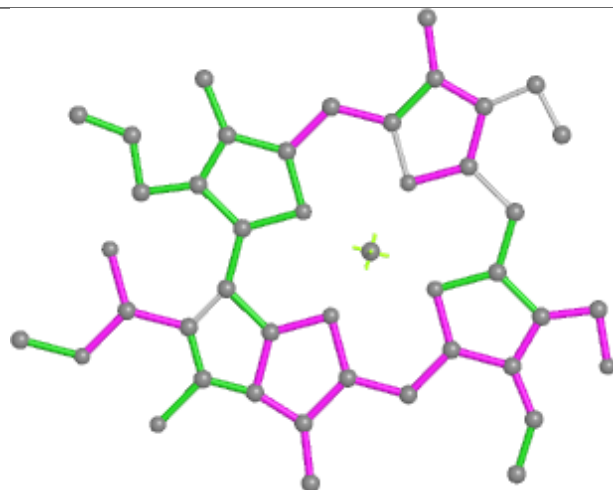


Ligand CHL Y 607	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL 8 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

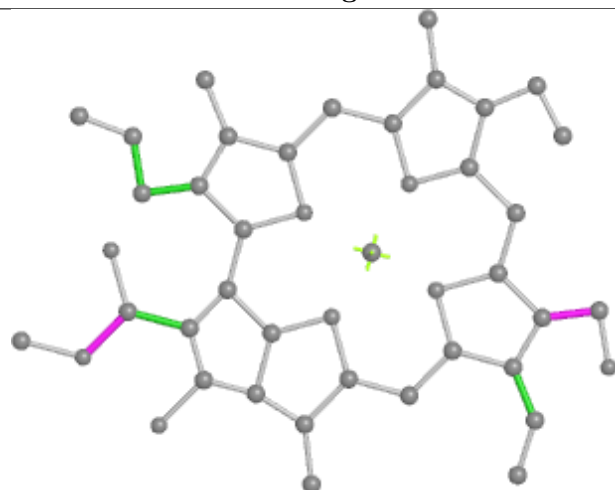
Ligand CHL 4 608



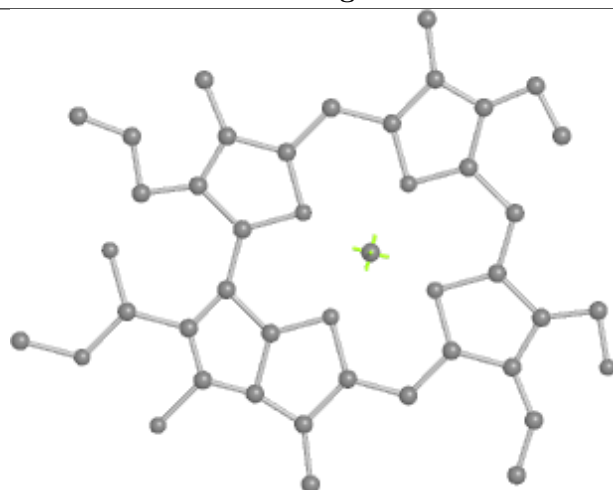
Bond lengths



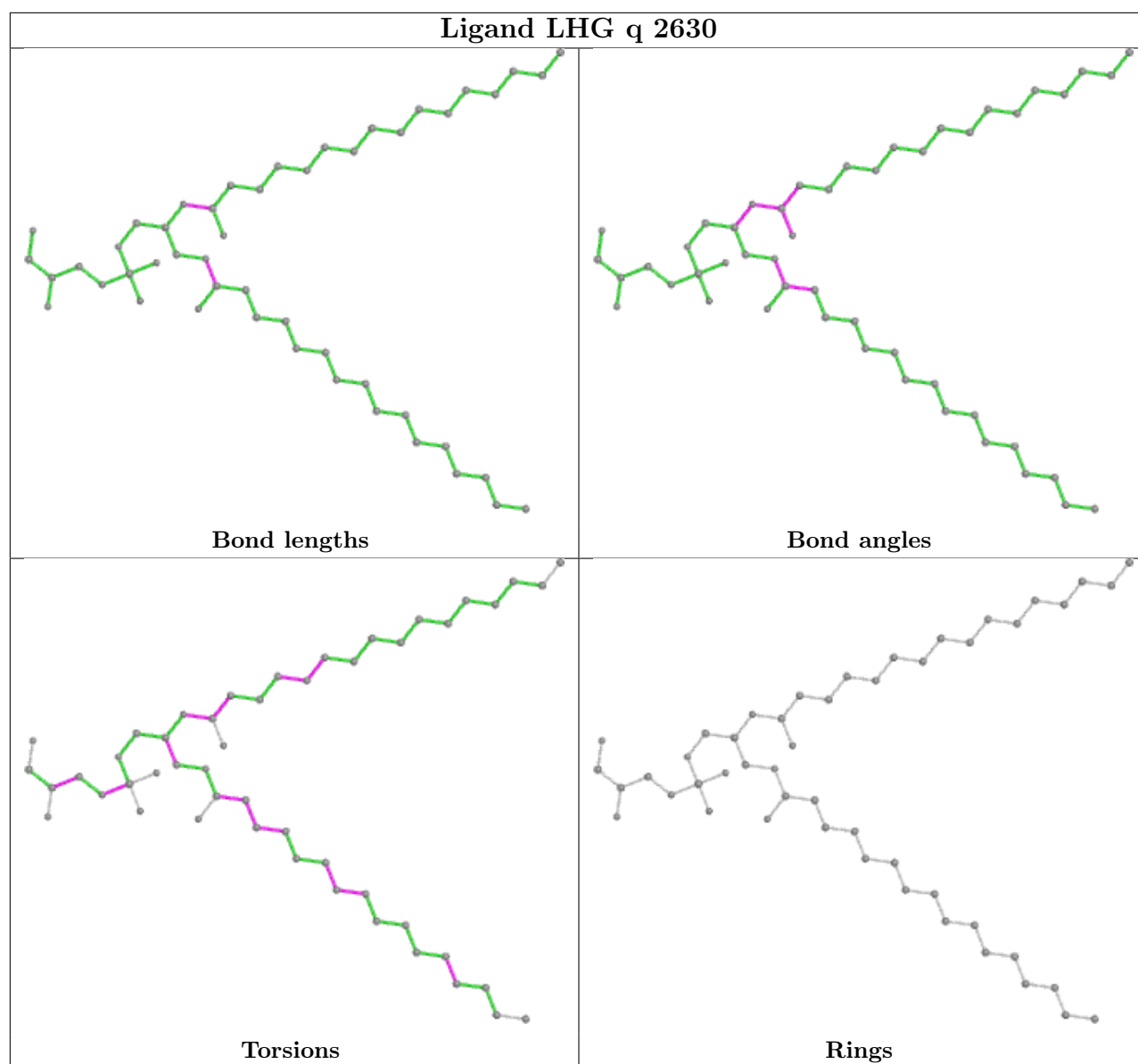
Bond angles



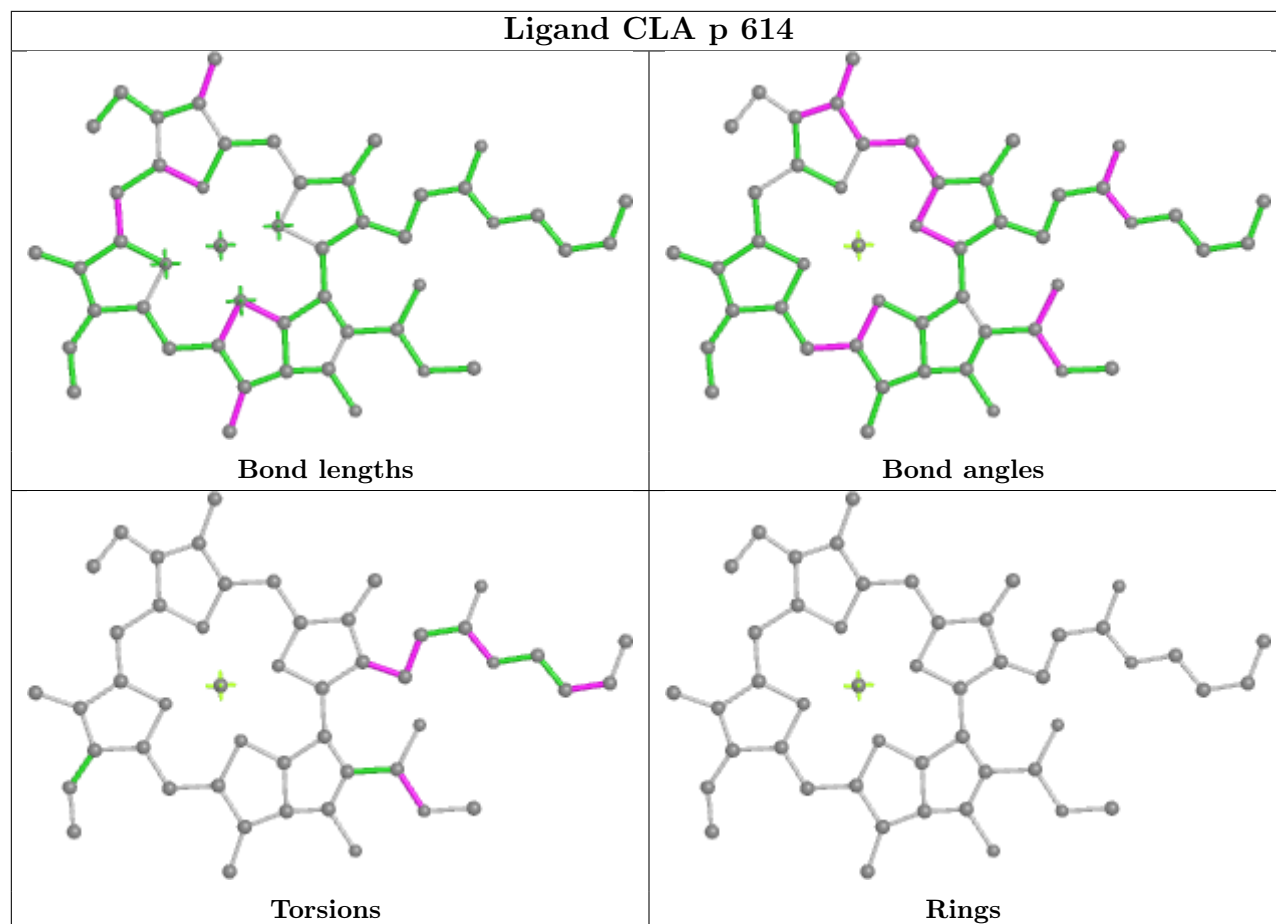
Torsions



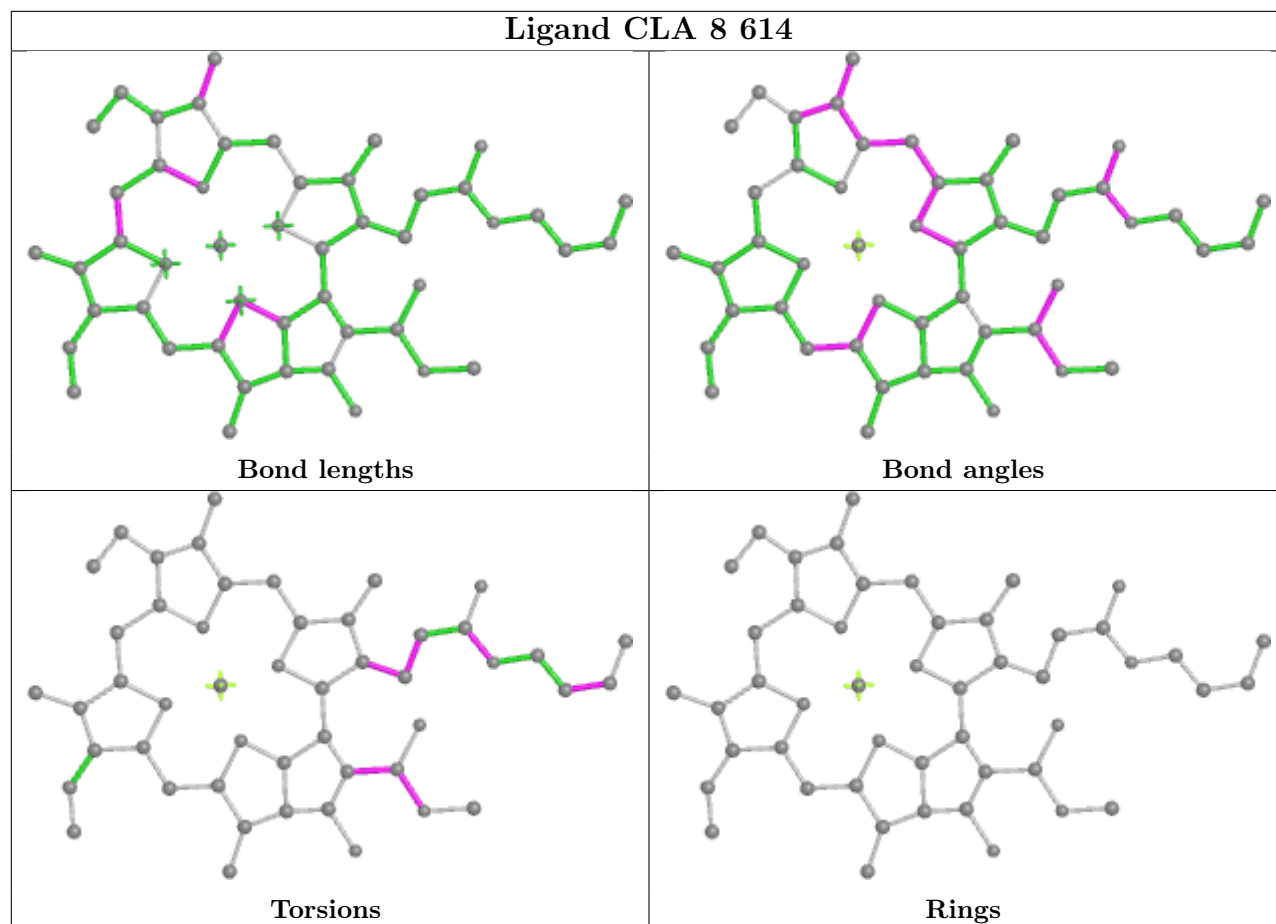
Rings



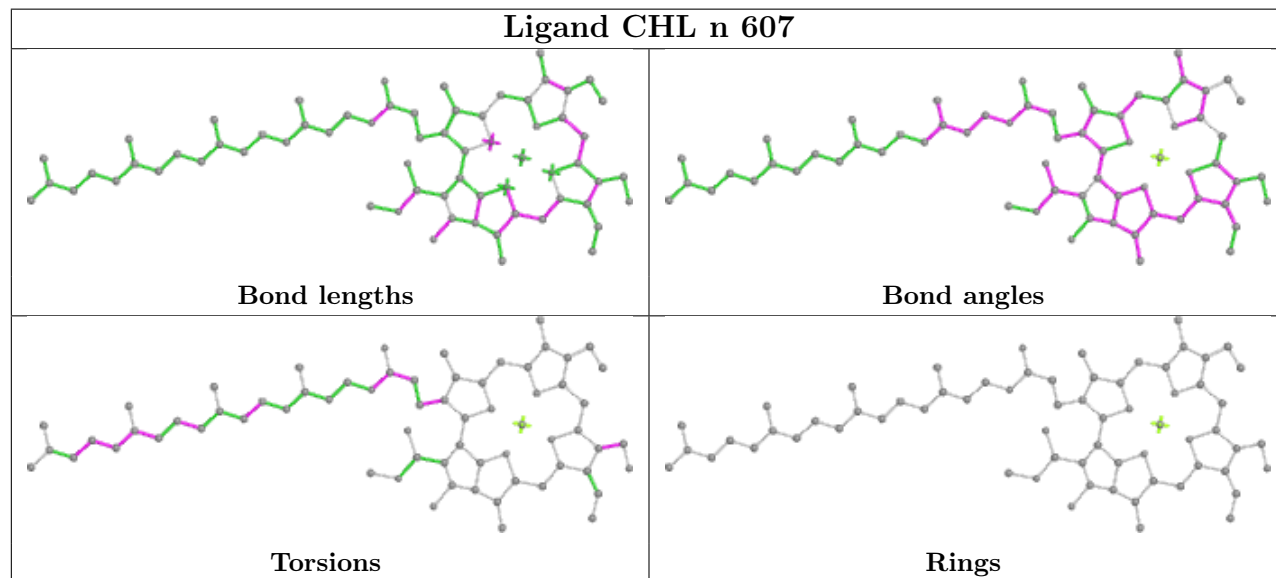
Ligand CLA p 614



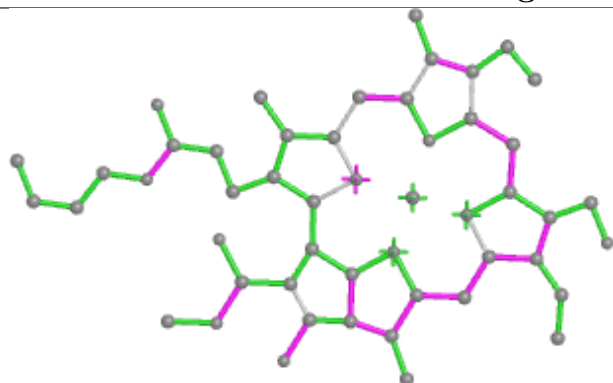
Ligand CLA 8 614



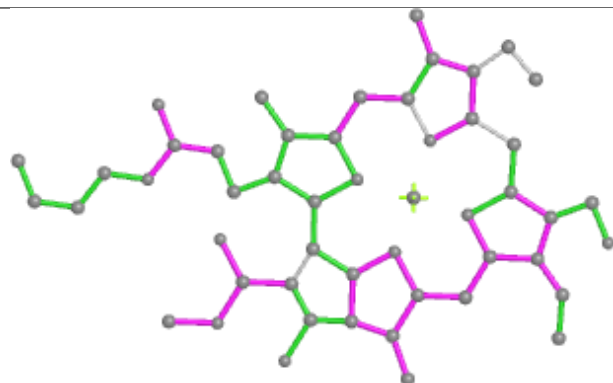
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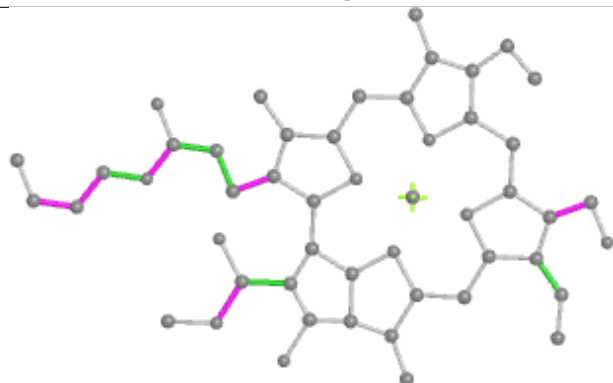
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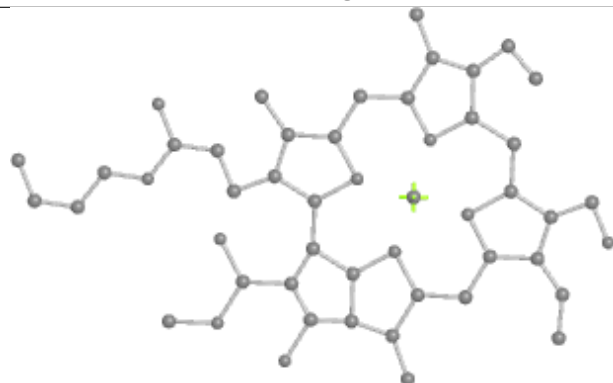
Bond lengths



Bond angles

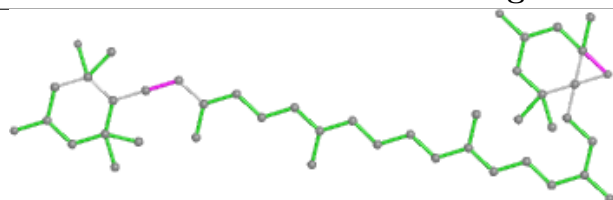


Torsions

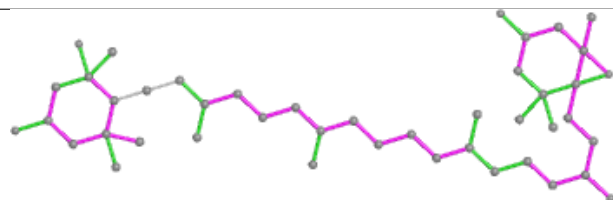


Rings

Ligand NEX 4 1623



Bond lengths



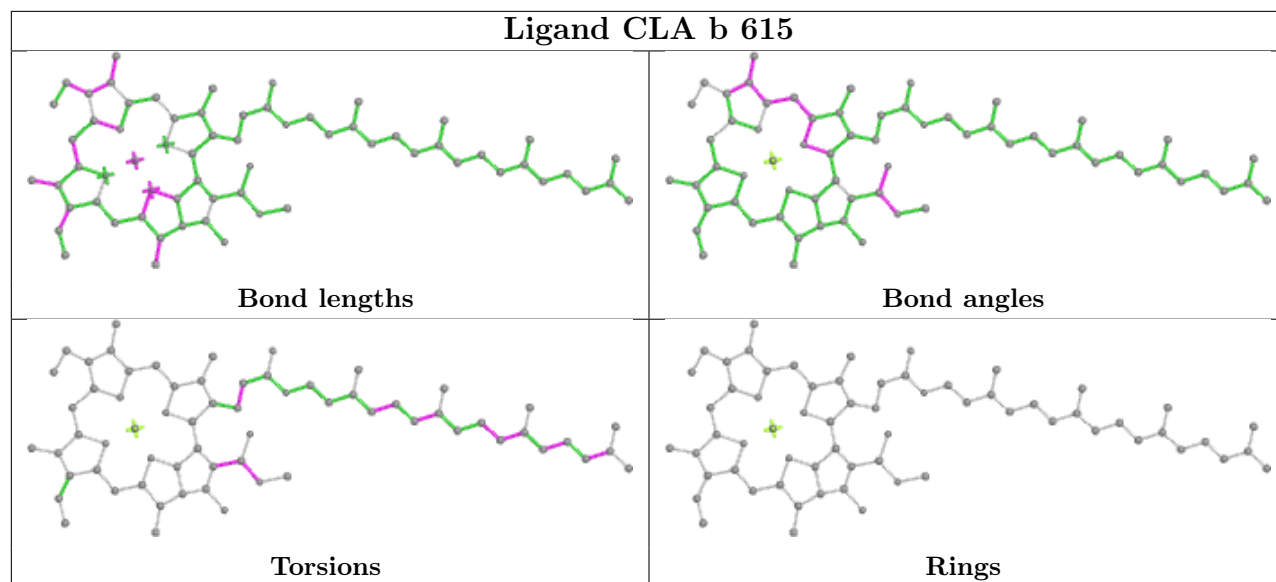
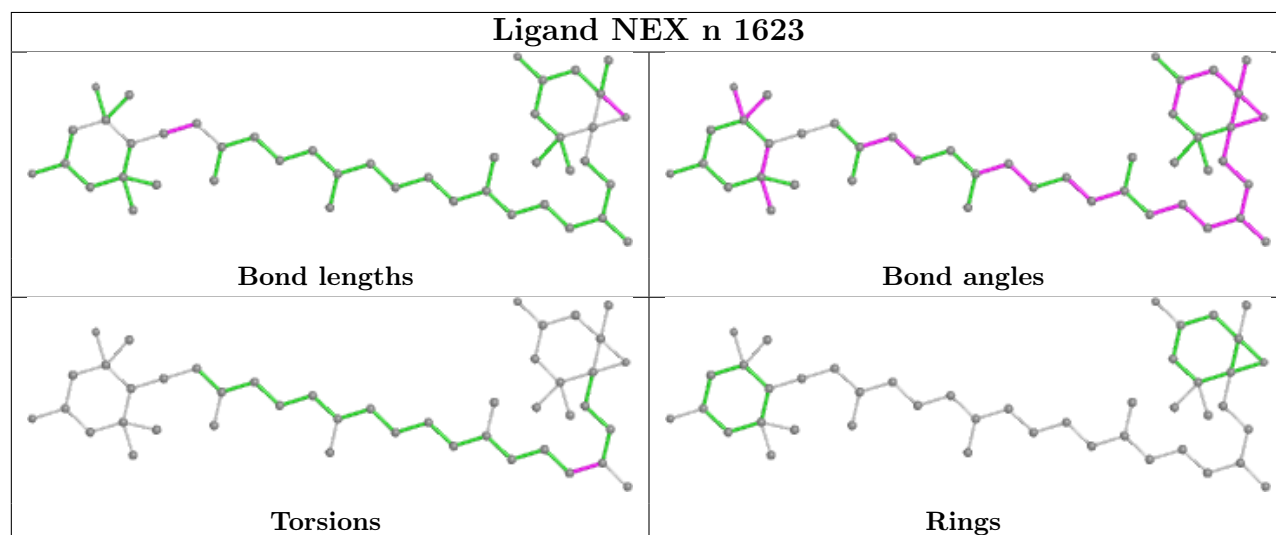
Bond angles



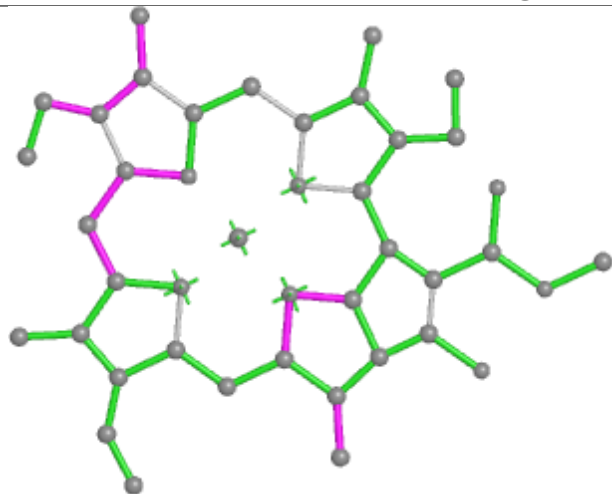
Torsions



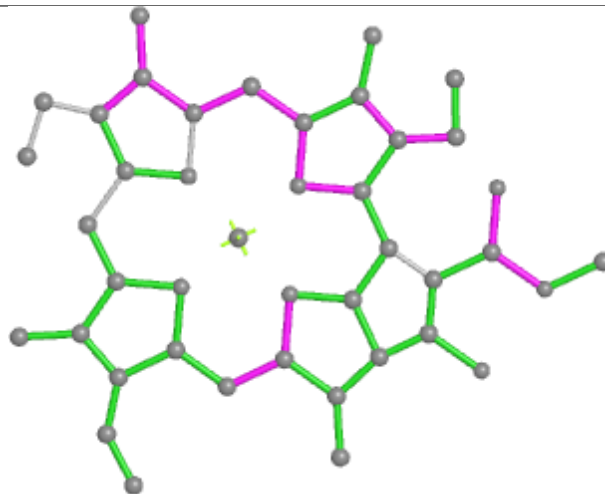
Rings

Ligand CLA b 615**Ligand NEX n 1623**

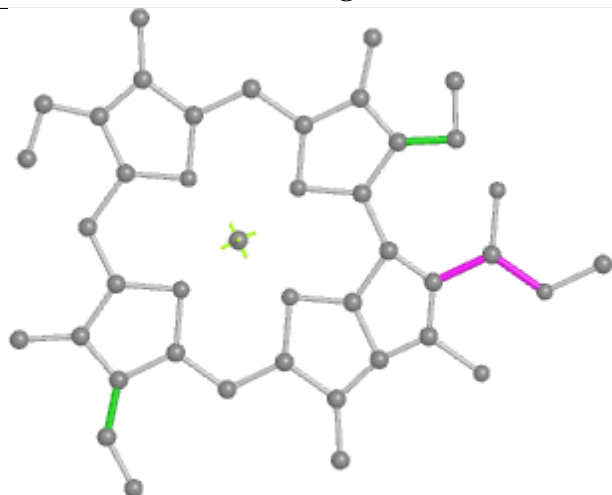
Ligand CLA S 603



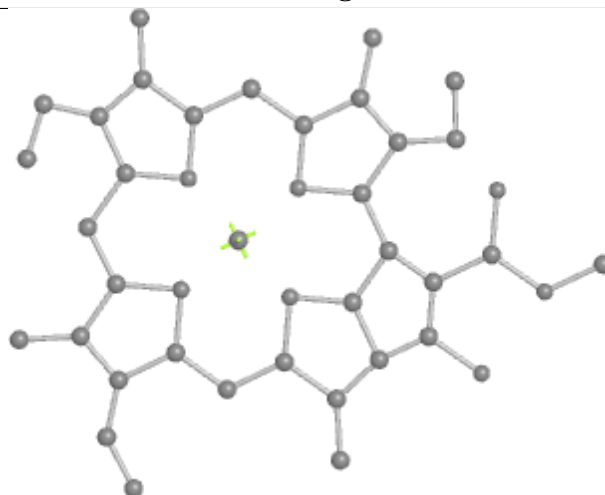
Bond lengths



Bond angles

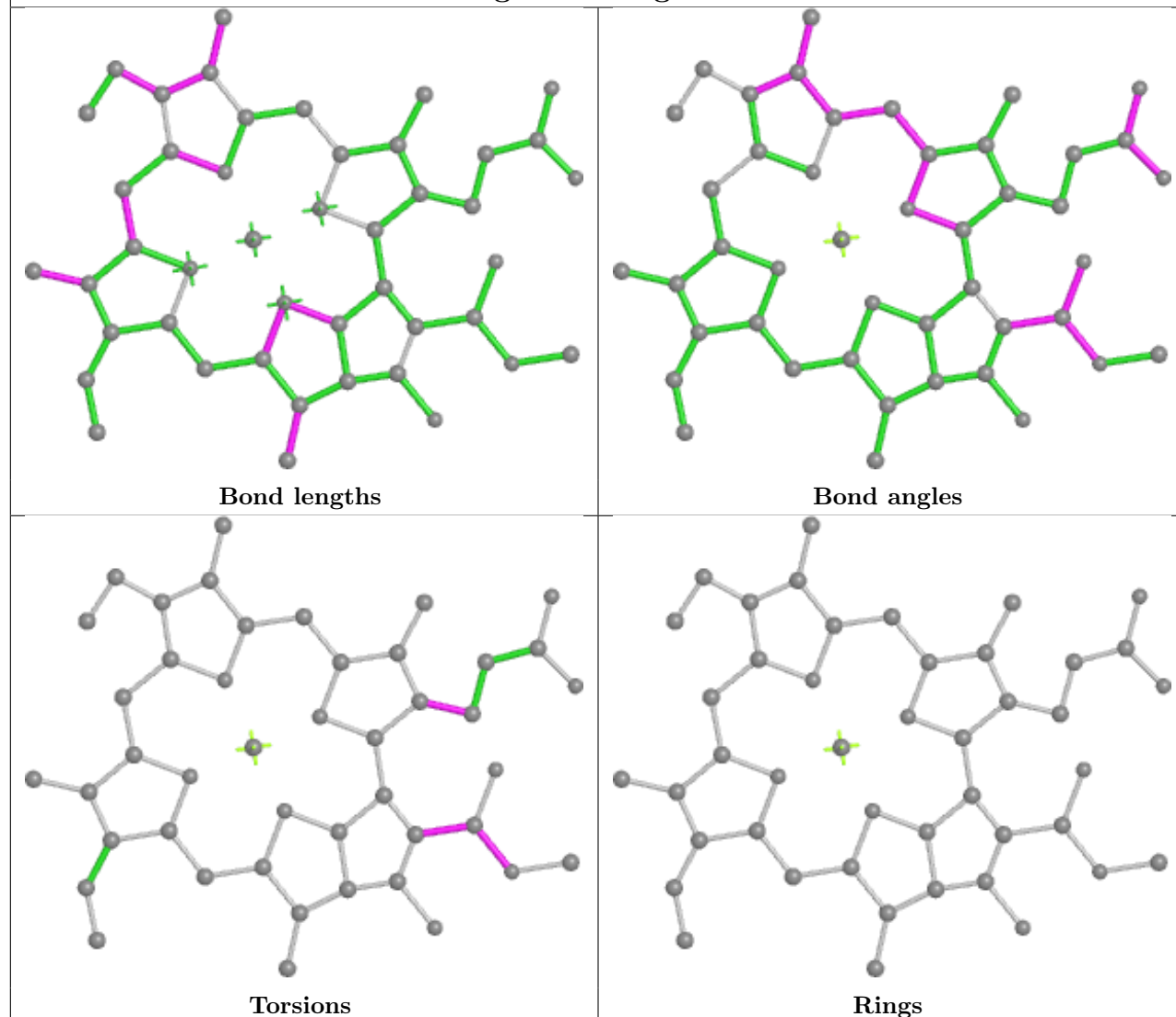


Torsions

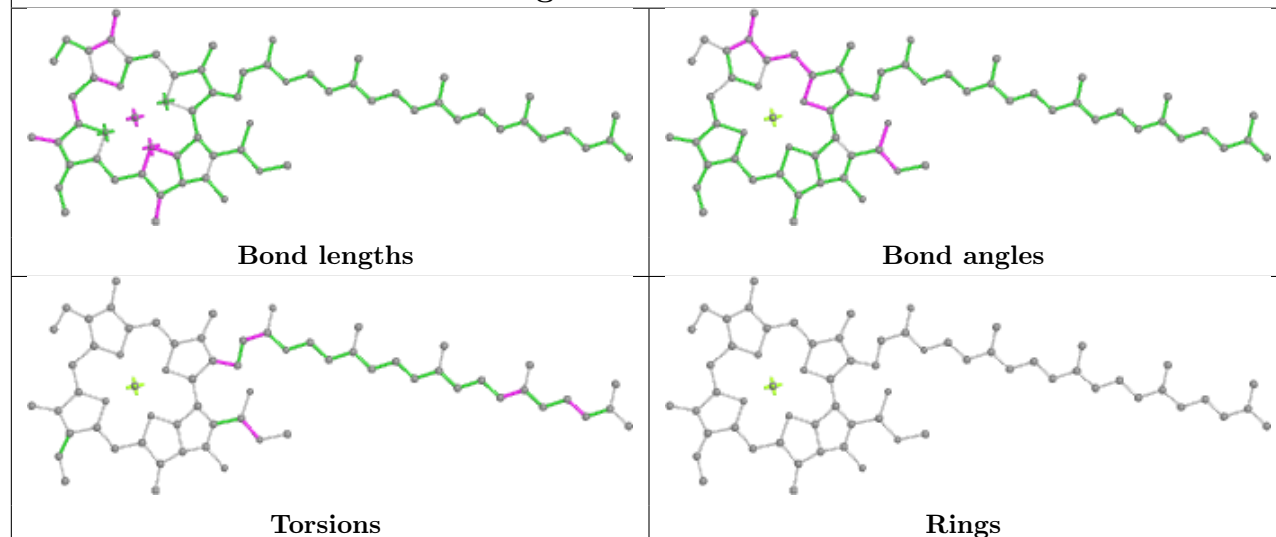


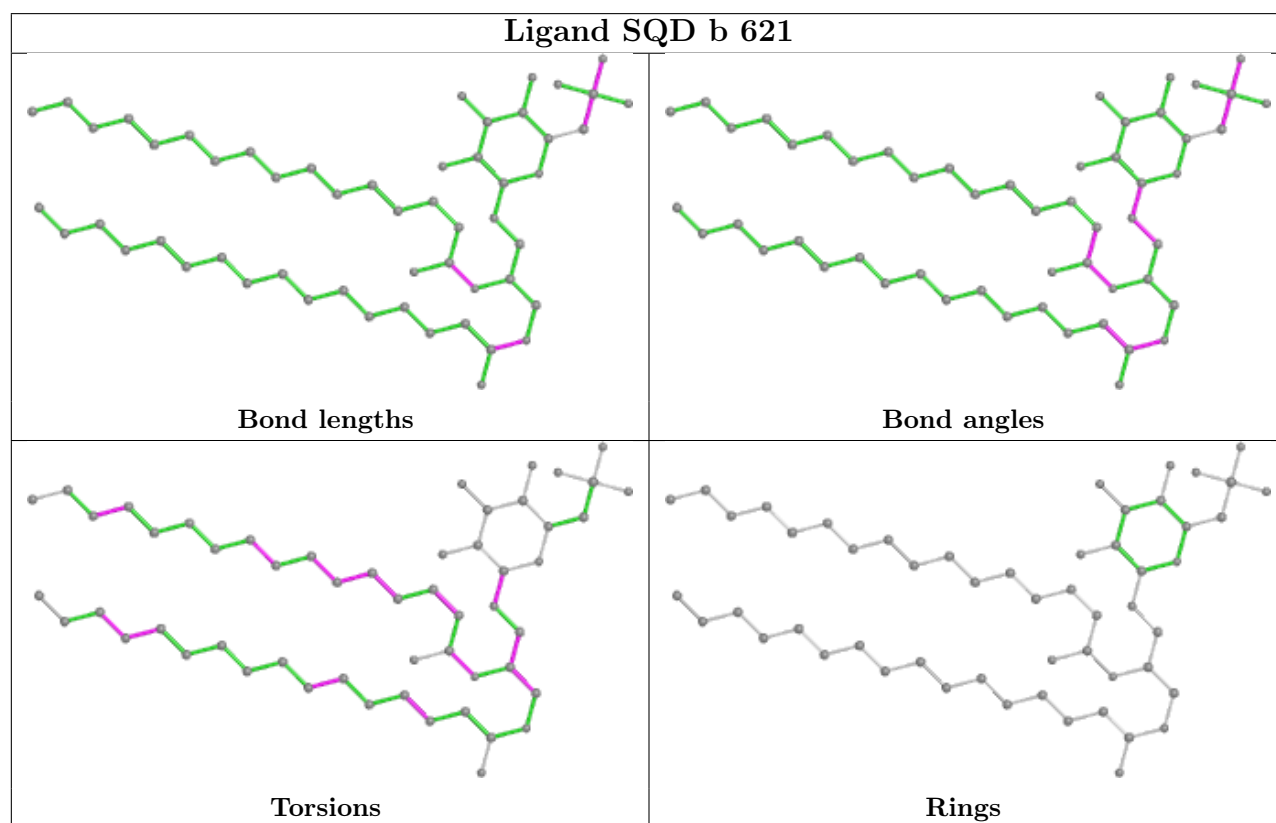
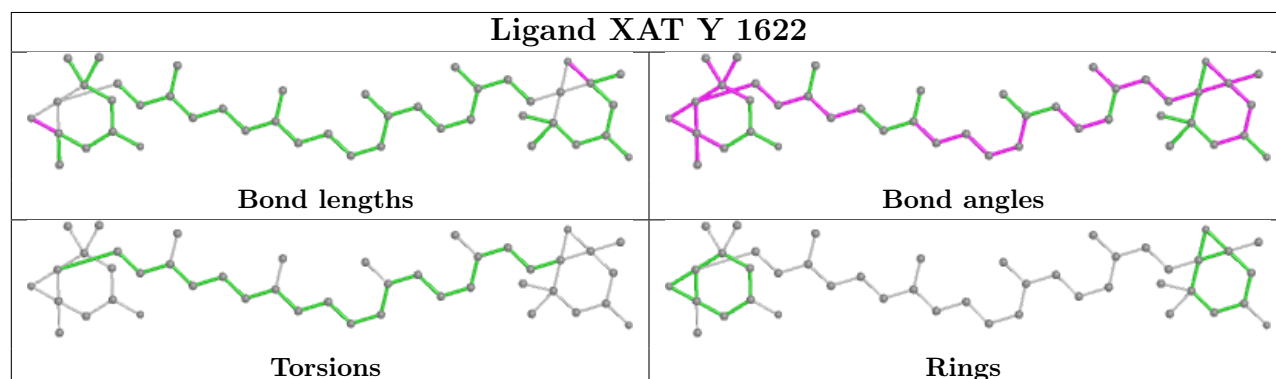
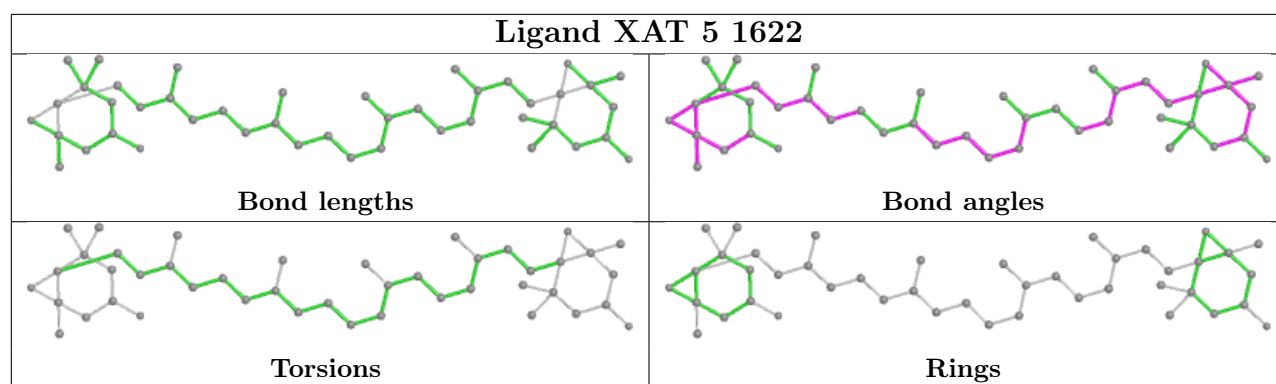
Rings

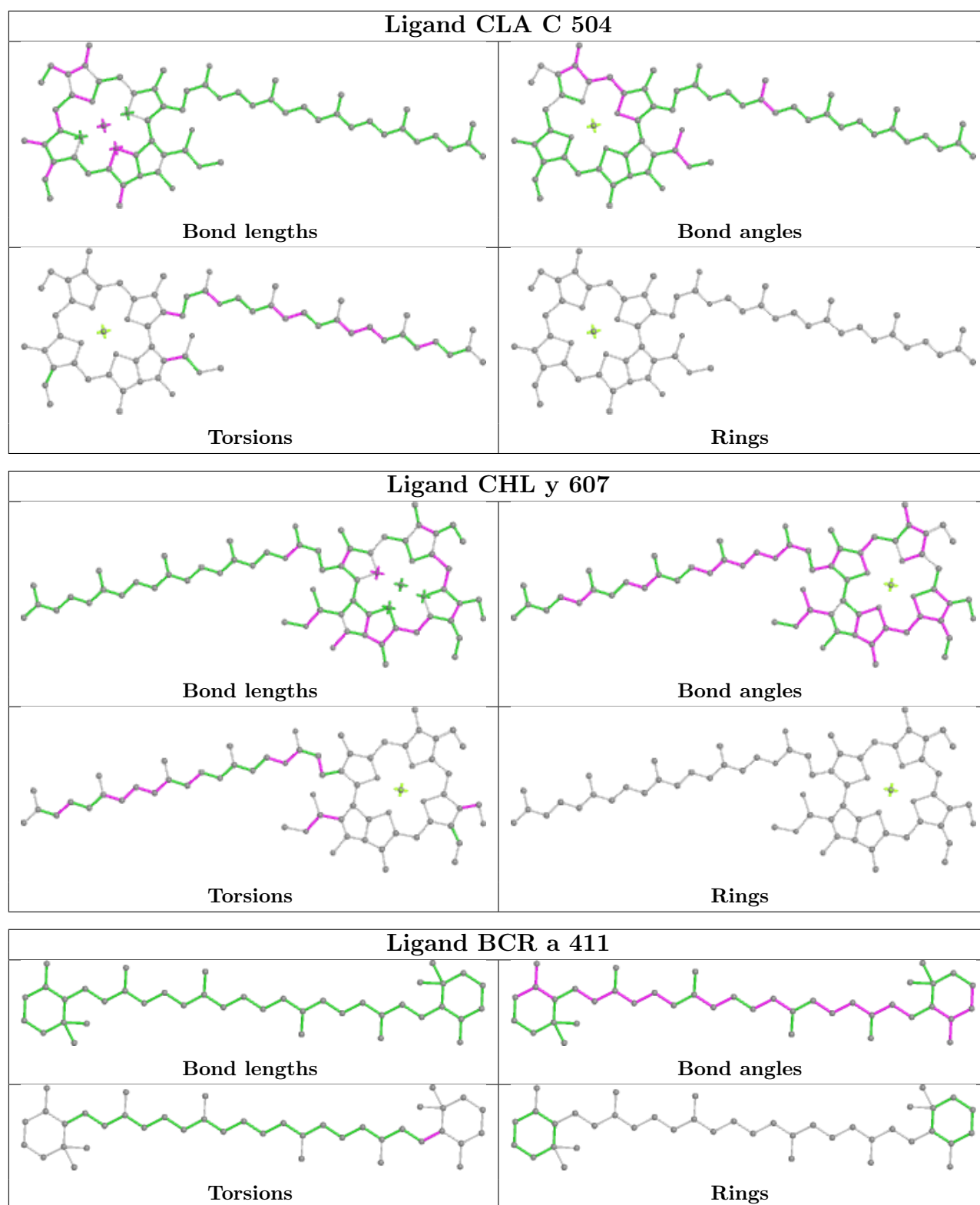
Ligand CLA g 611

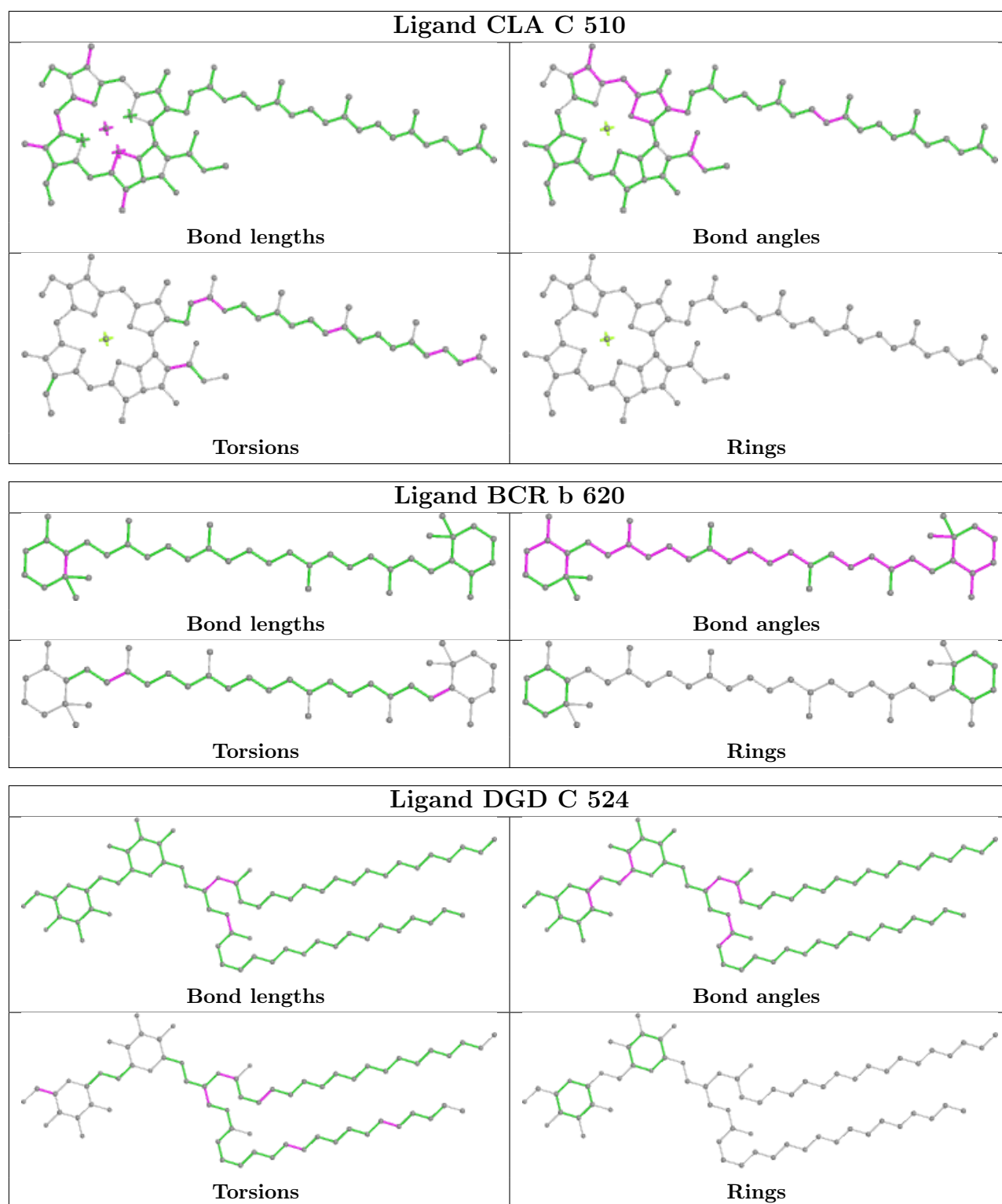


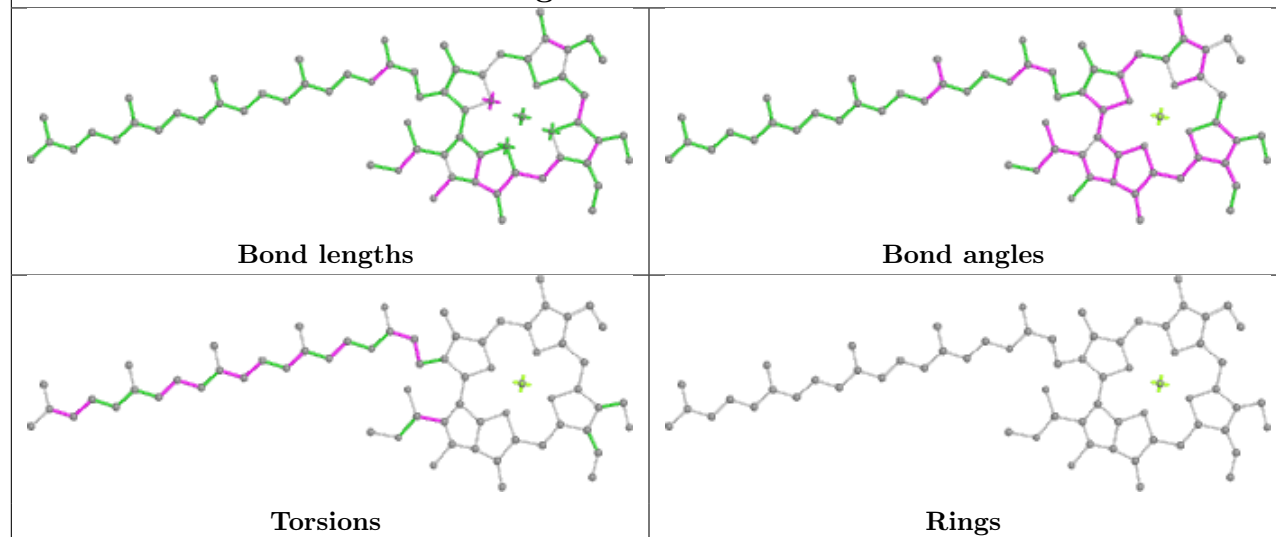
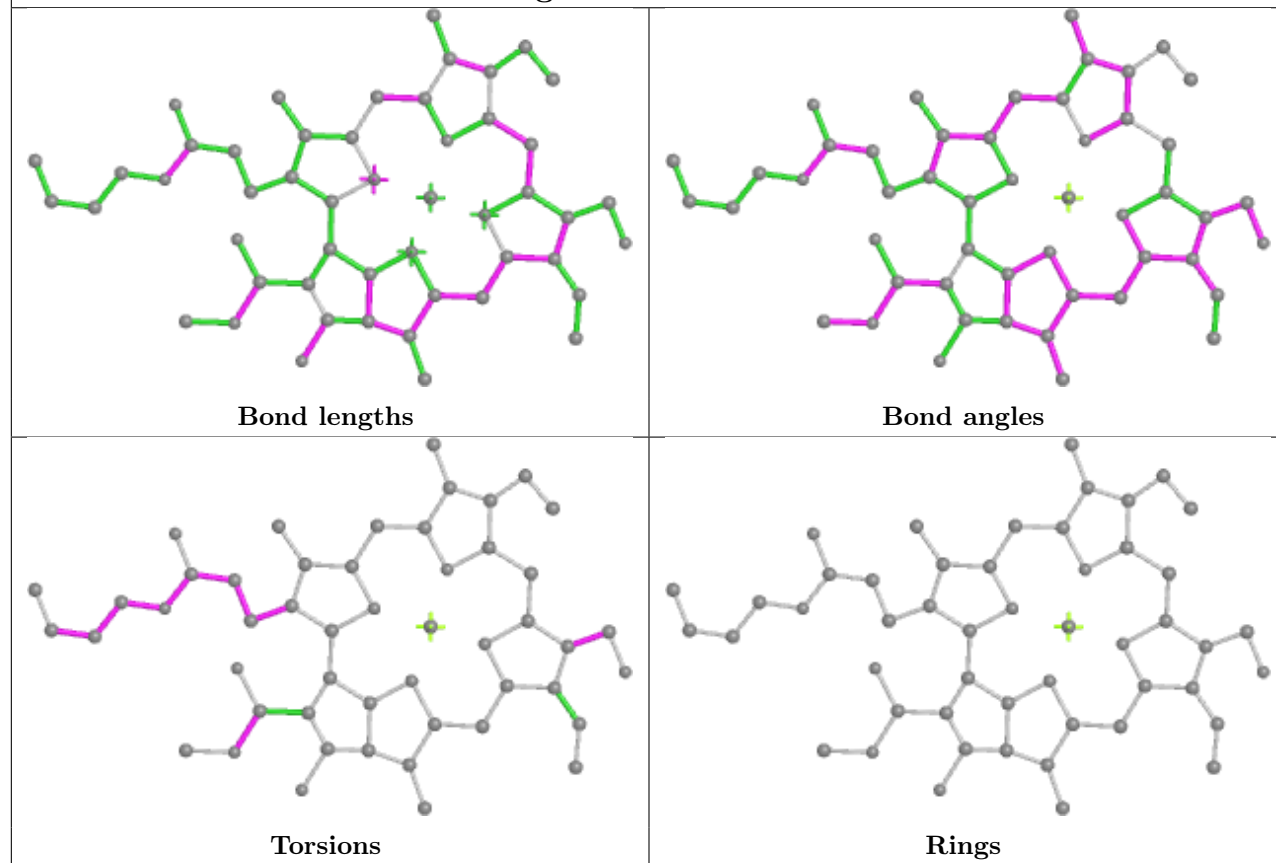
Ligand CLA 7 611



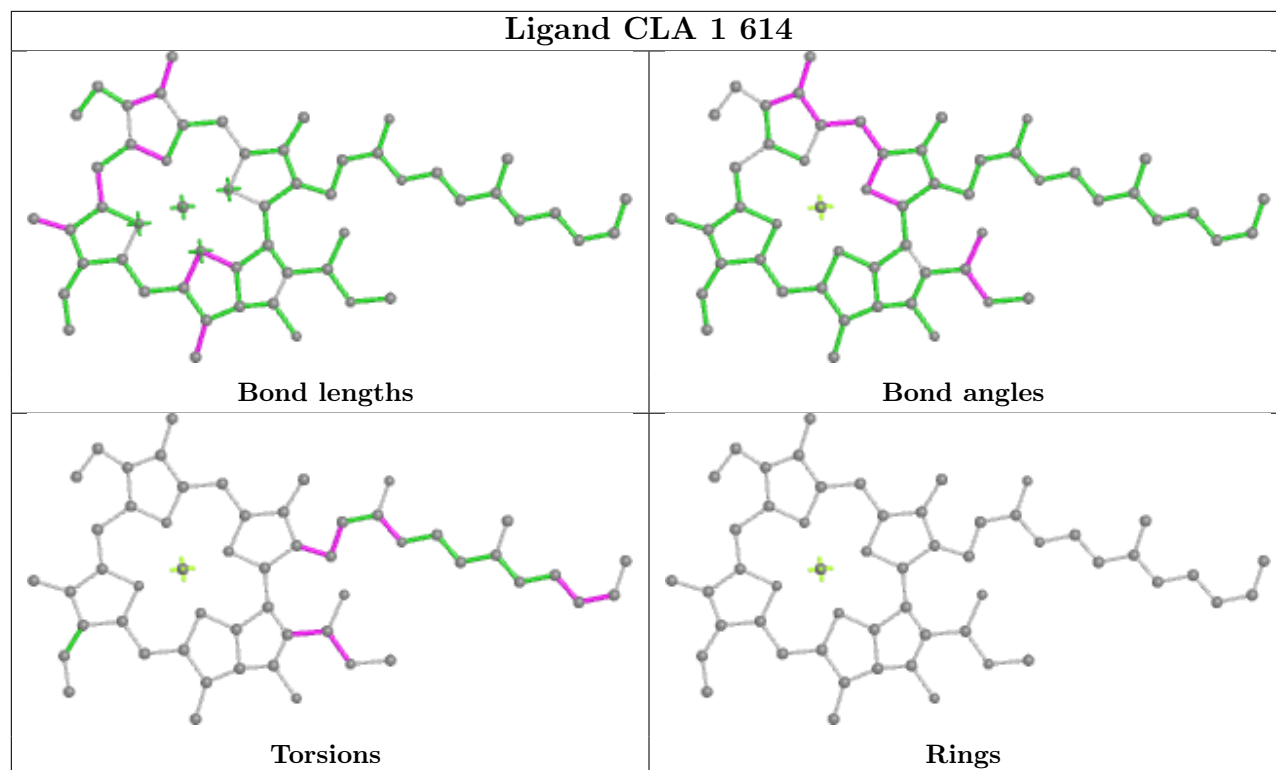




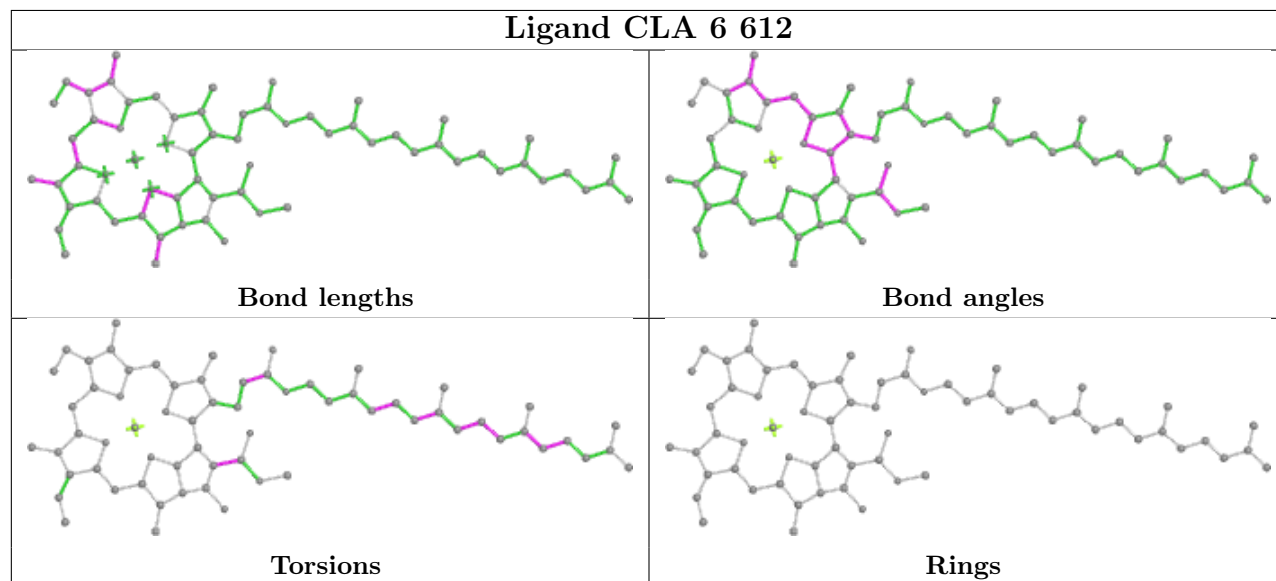


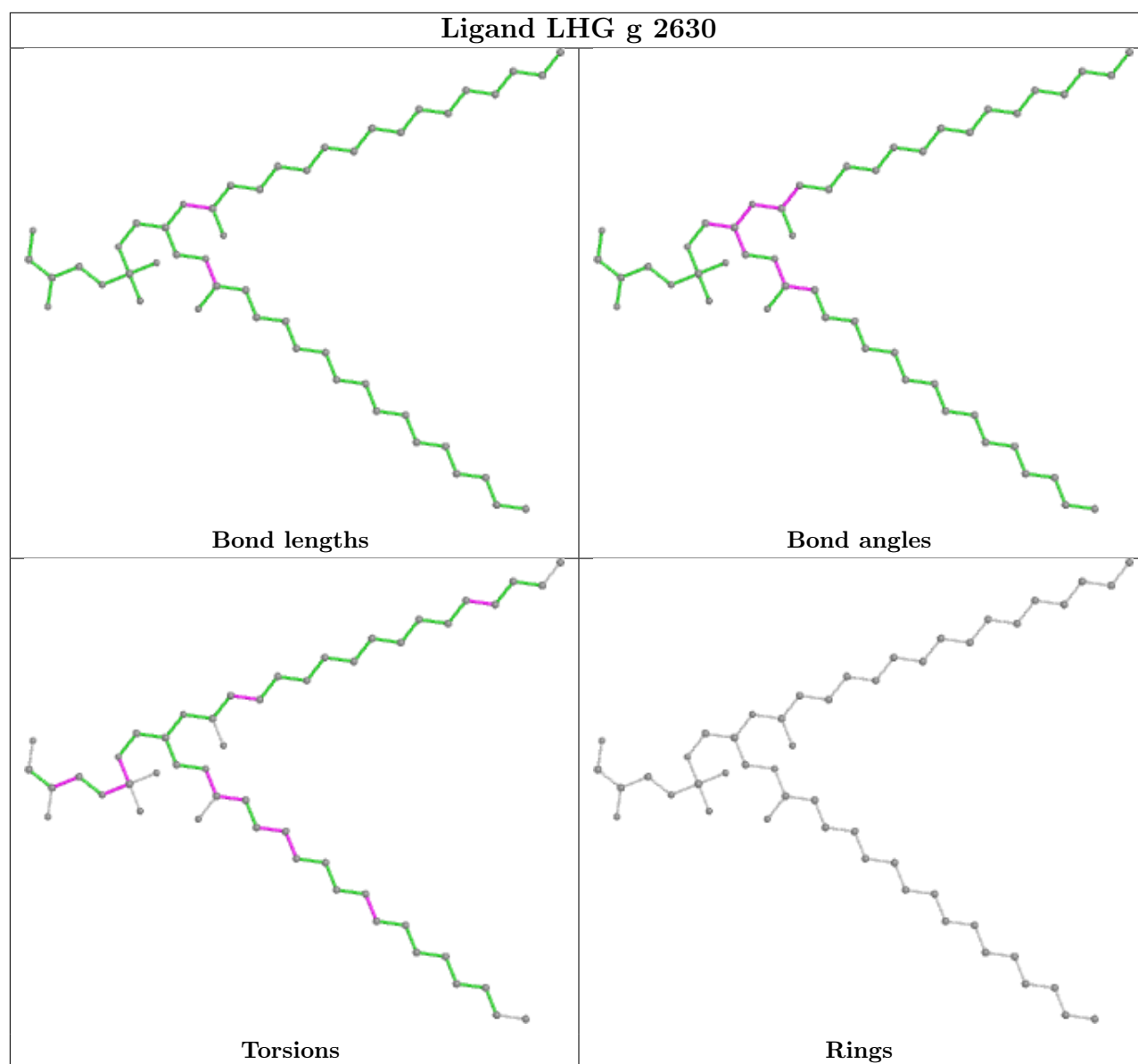
Ligand CHL 1 601**Ligand CHL 4 607**

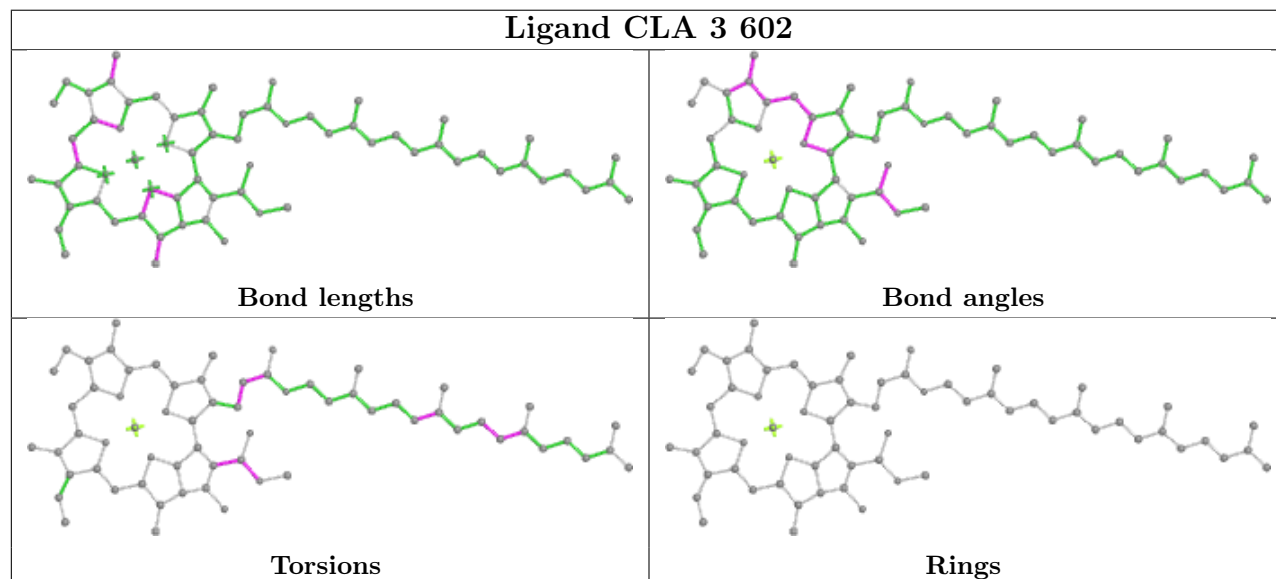
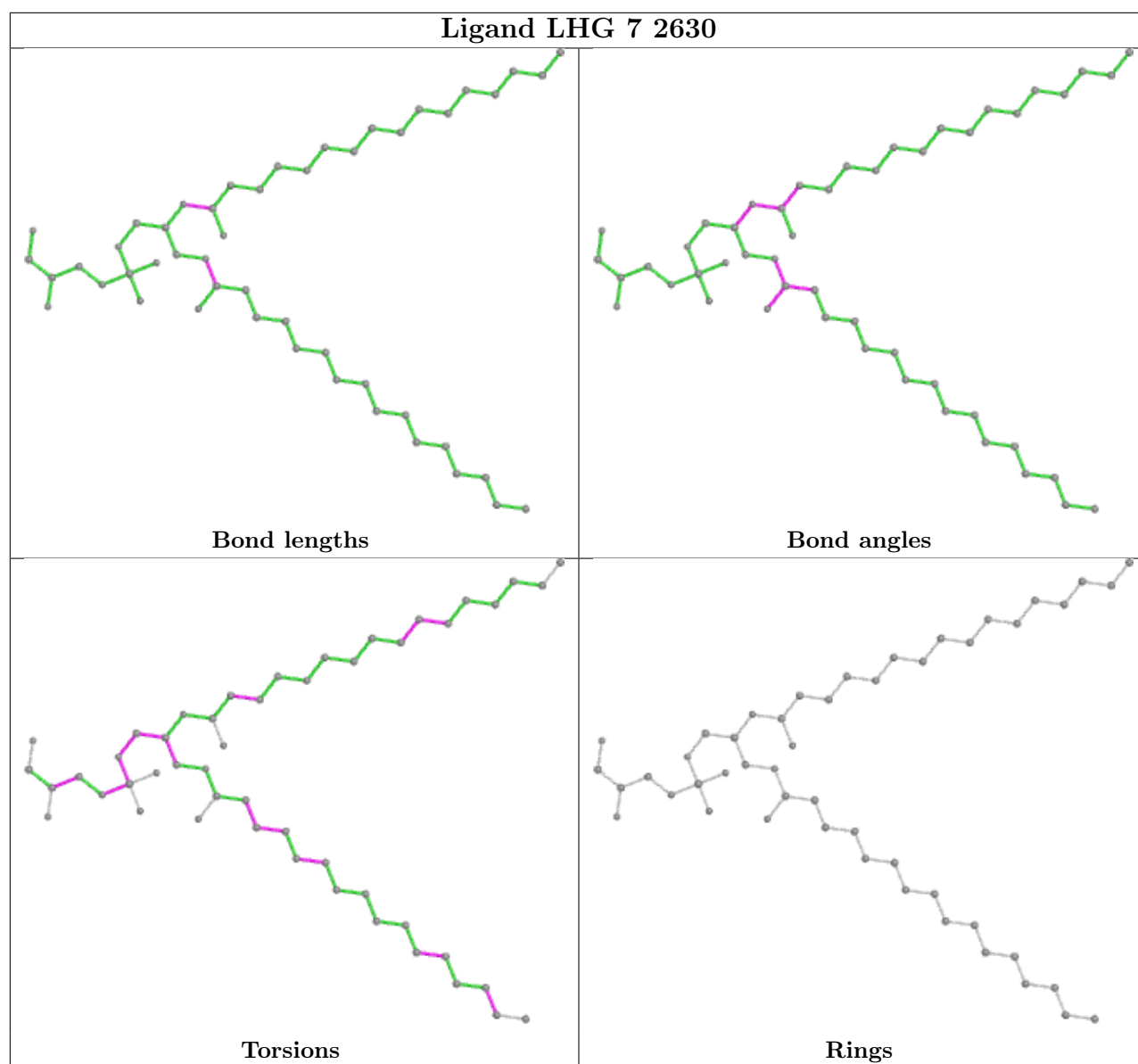
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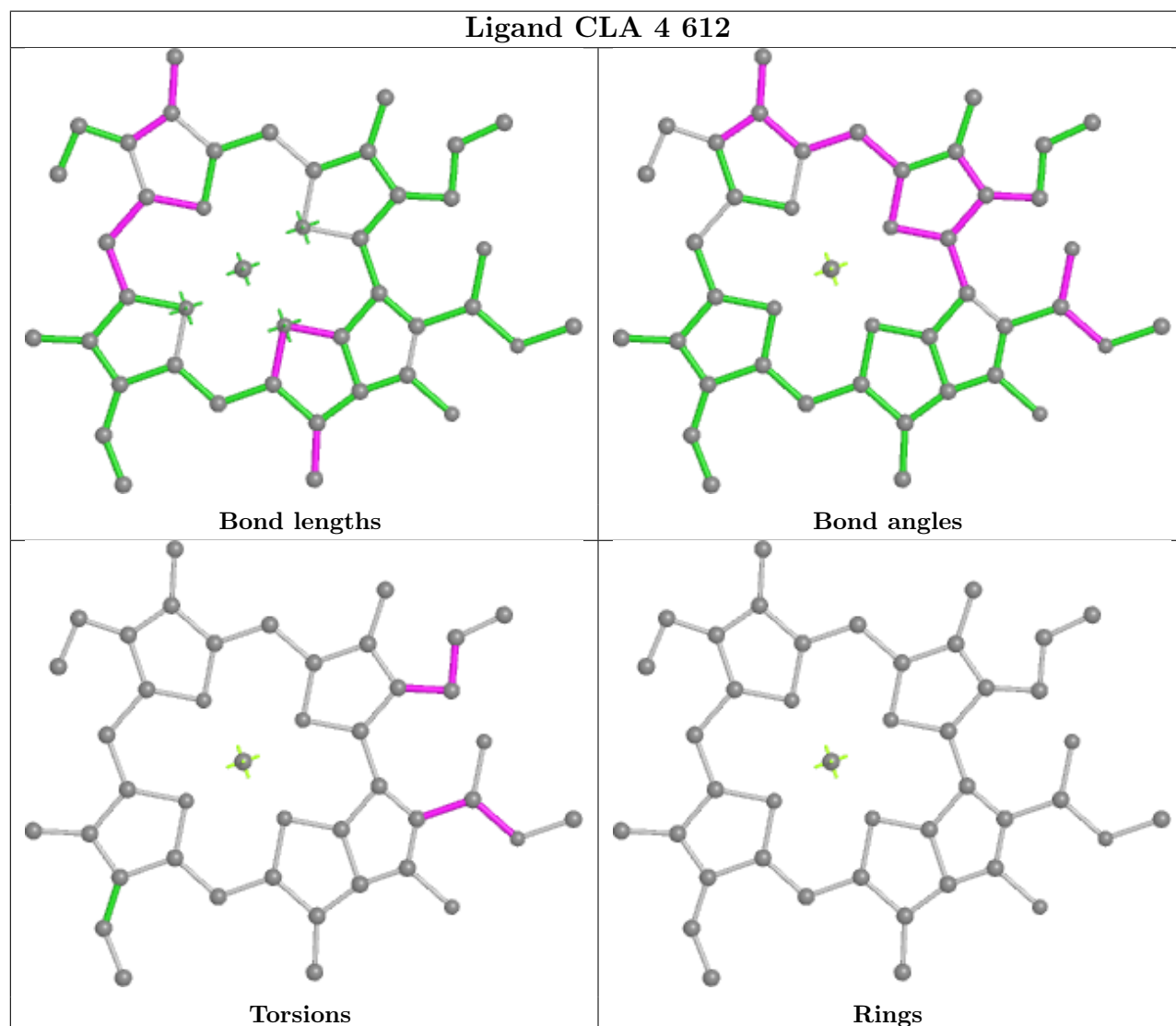
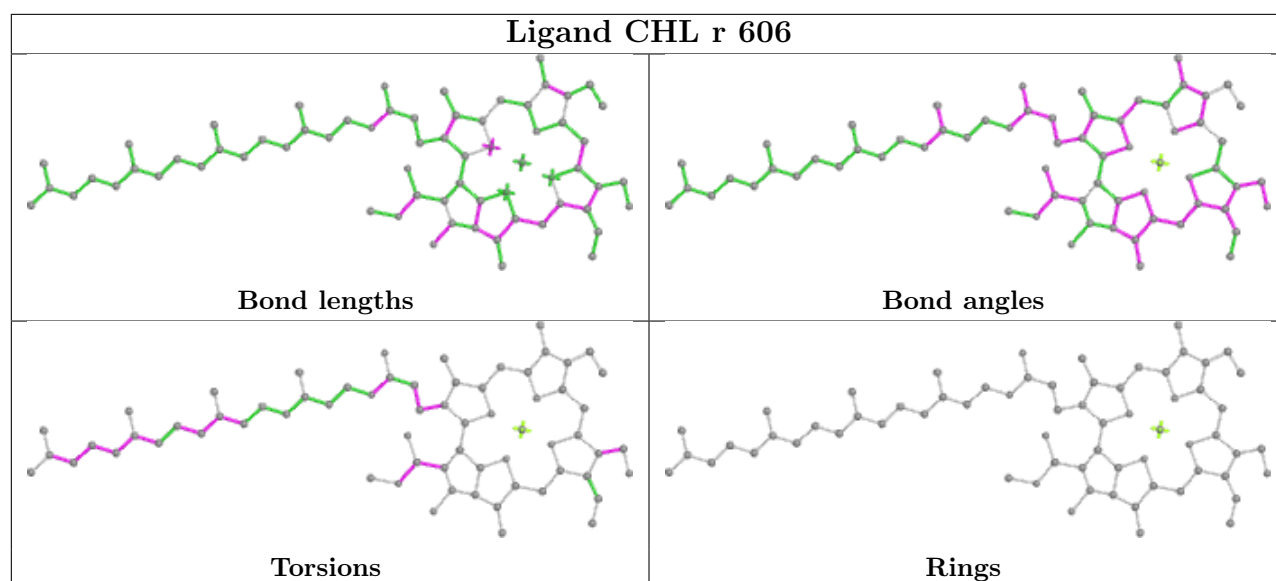


Ligand CLA 6 612

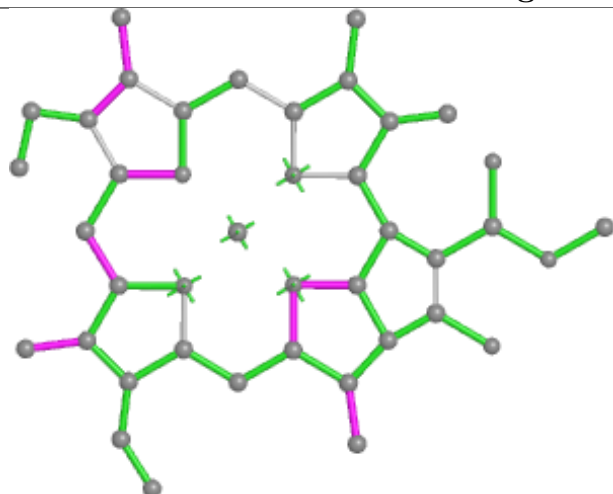




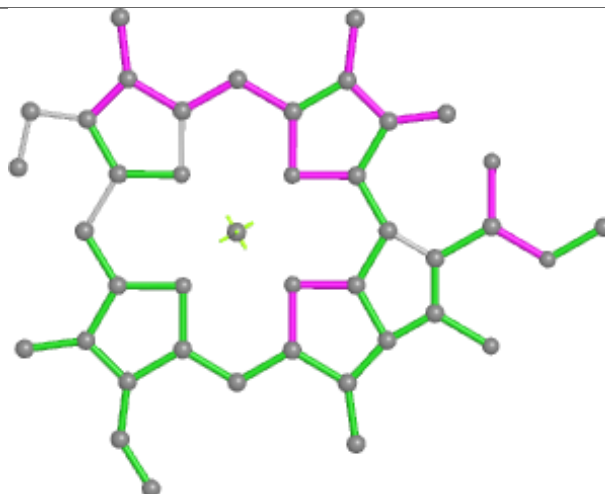




Ligand CLA S 609



Bond lengths



Bond angles

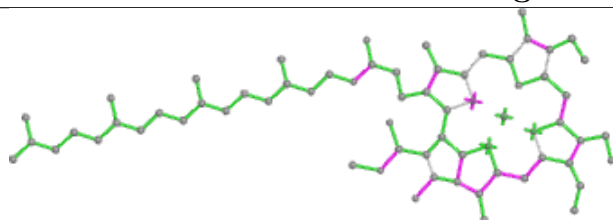


Torsions

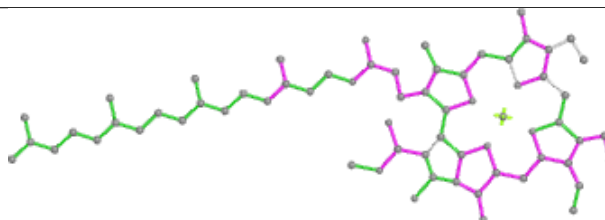


Rings

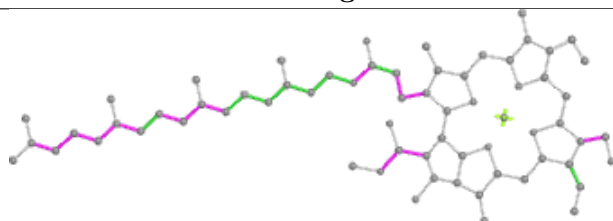
Ligand CHL R 606



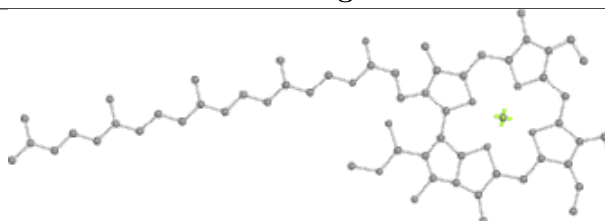
Bond lengths



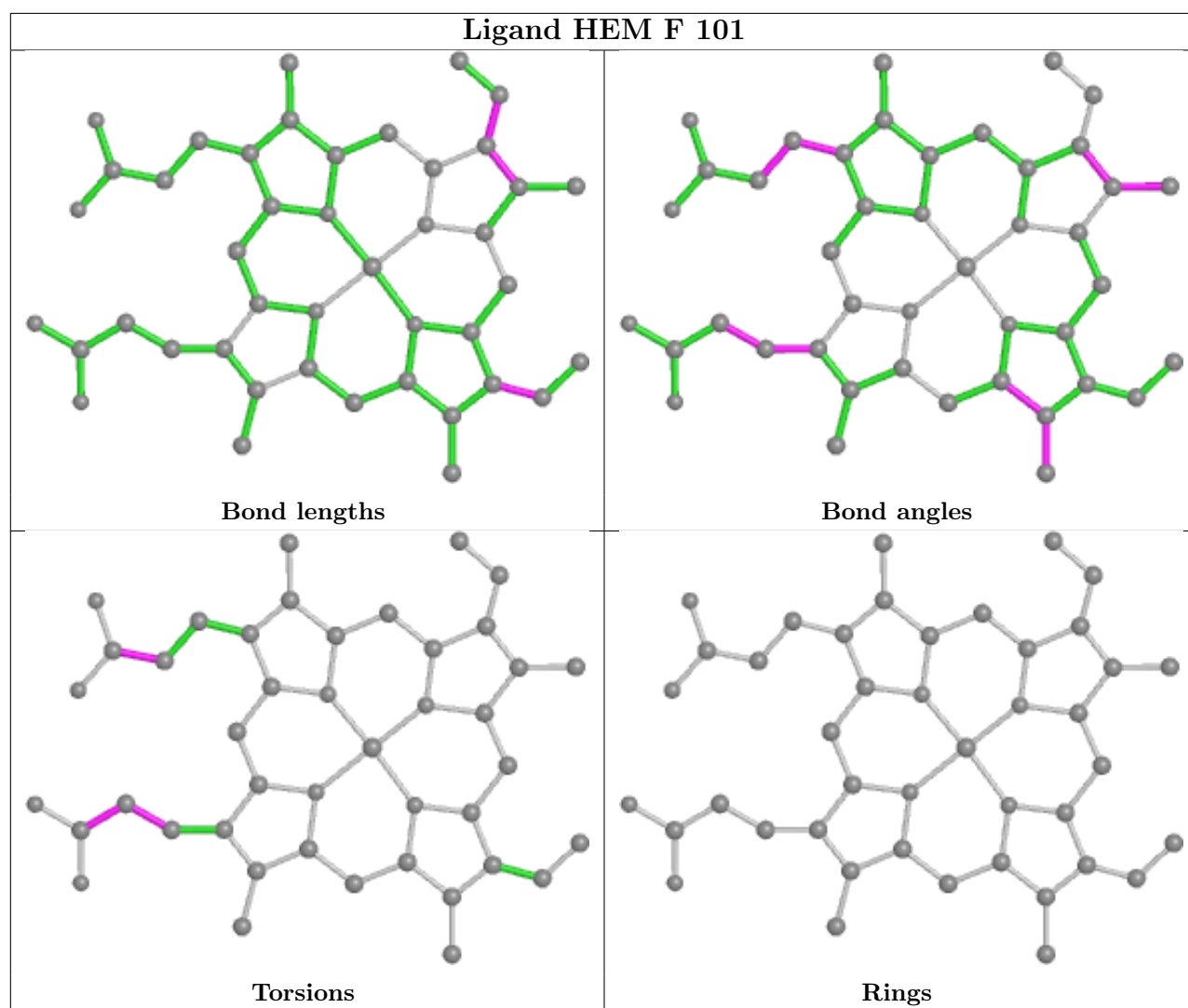
Bond angles



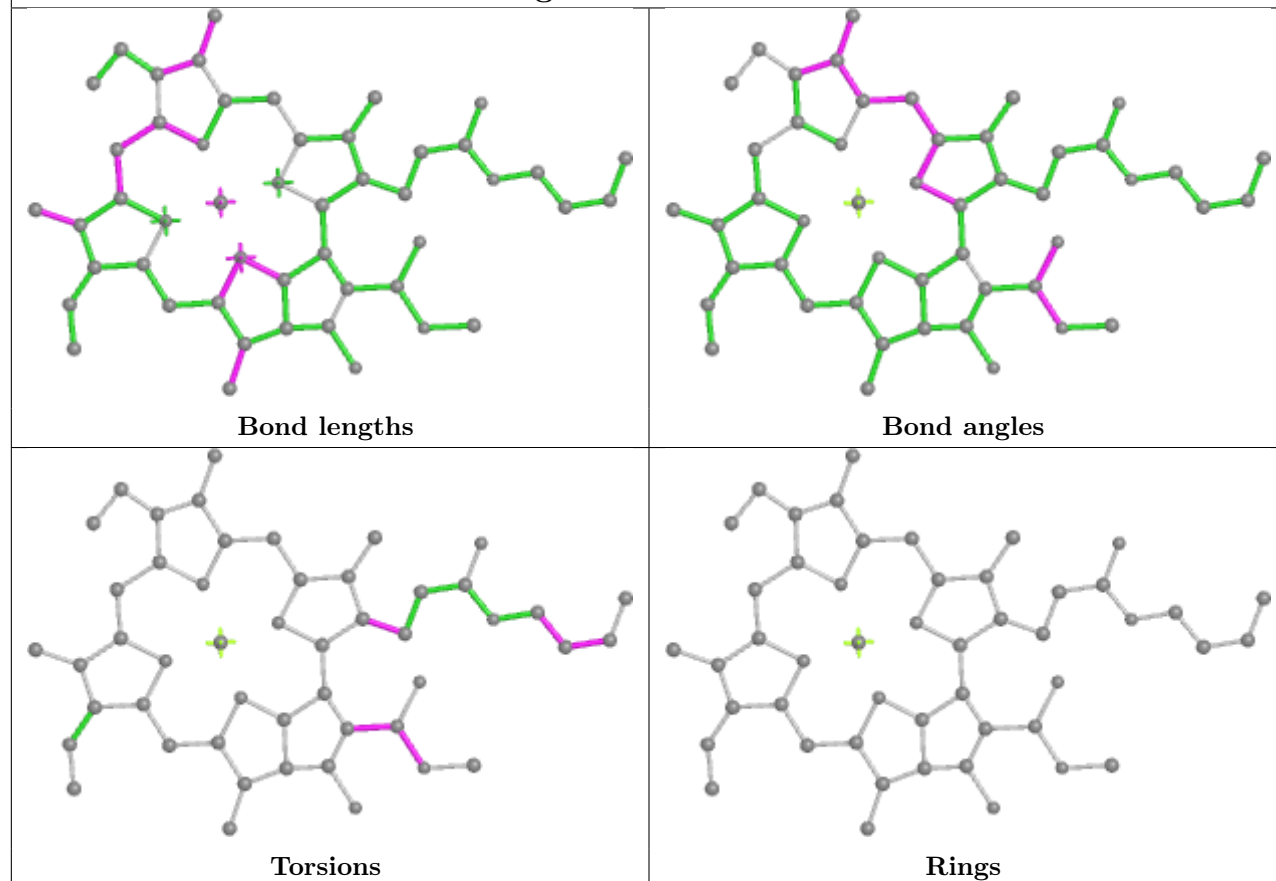
Torsions



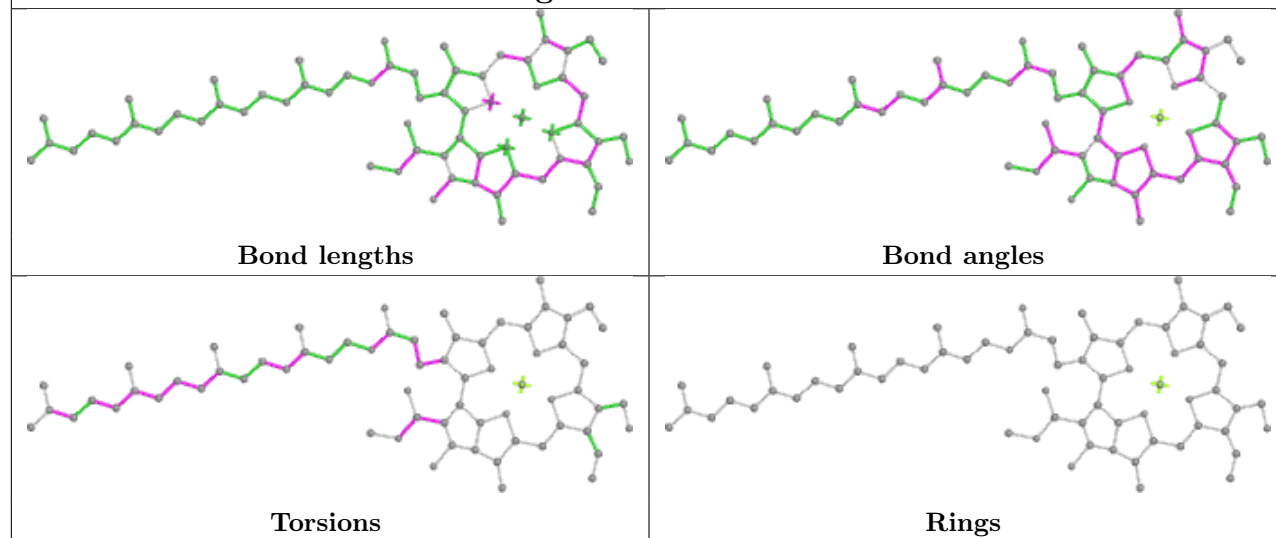
Rings

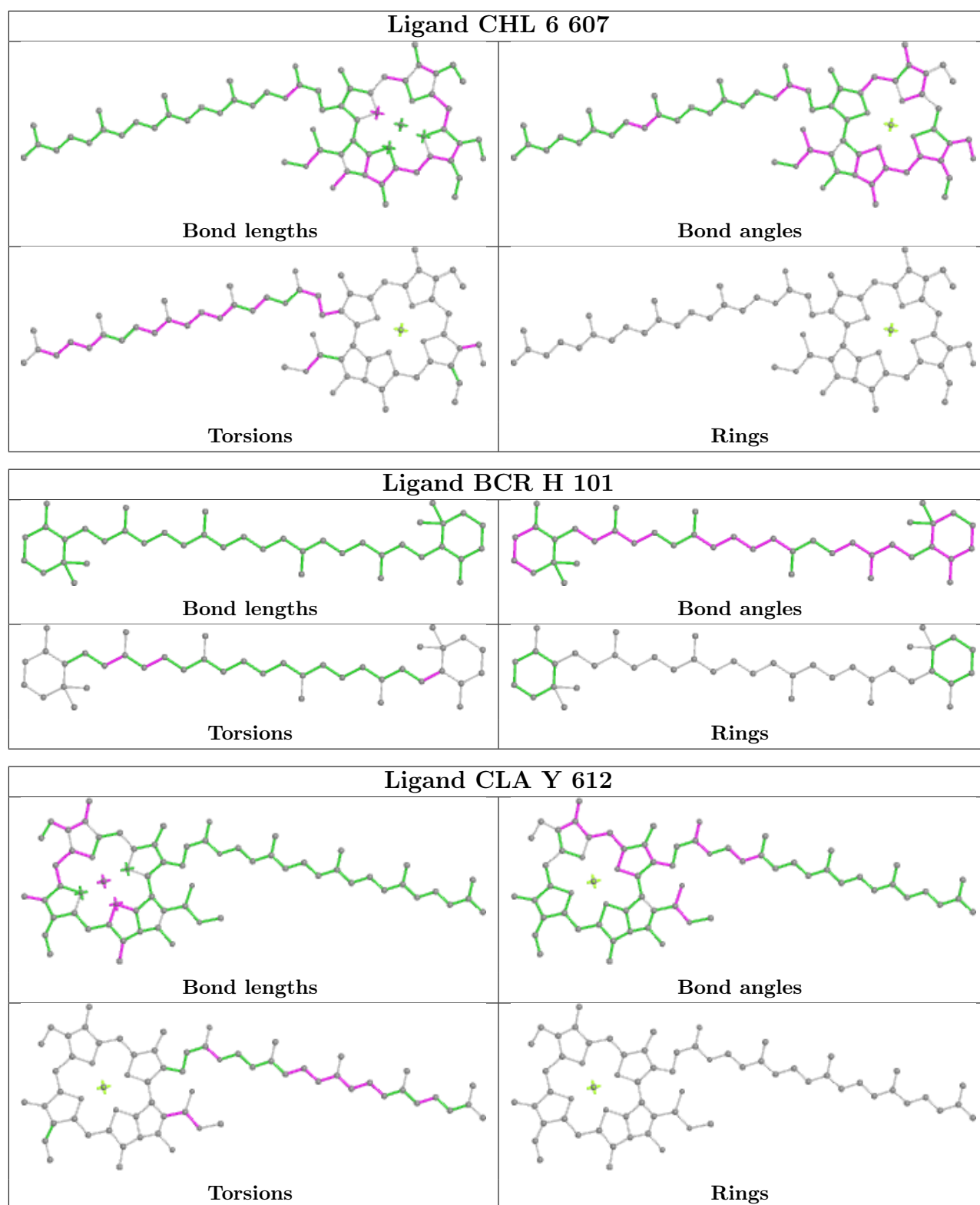


Ligand CLA n 611

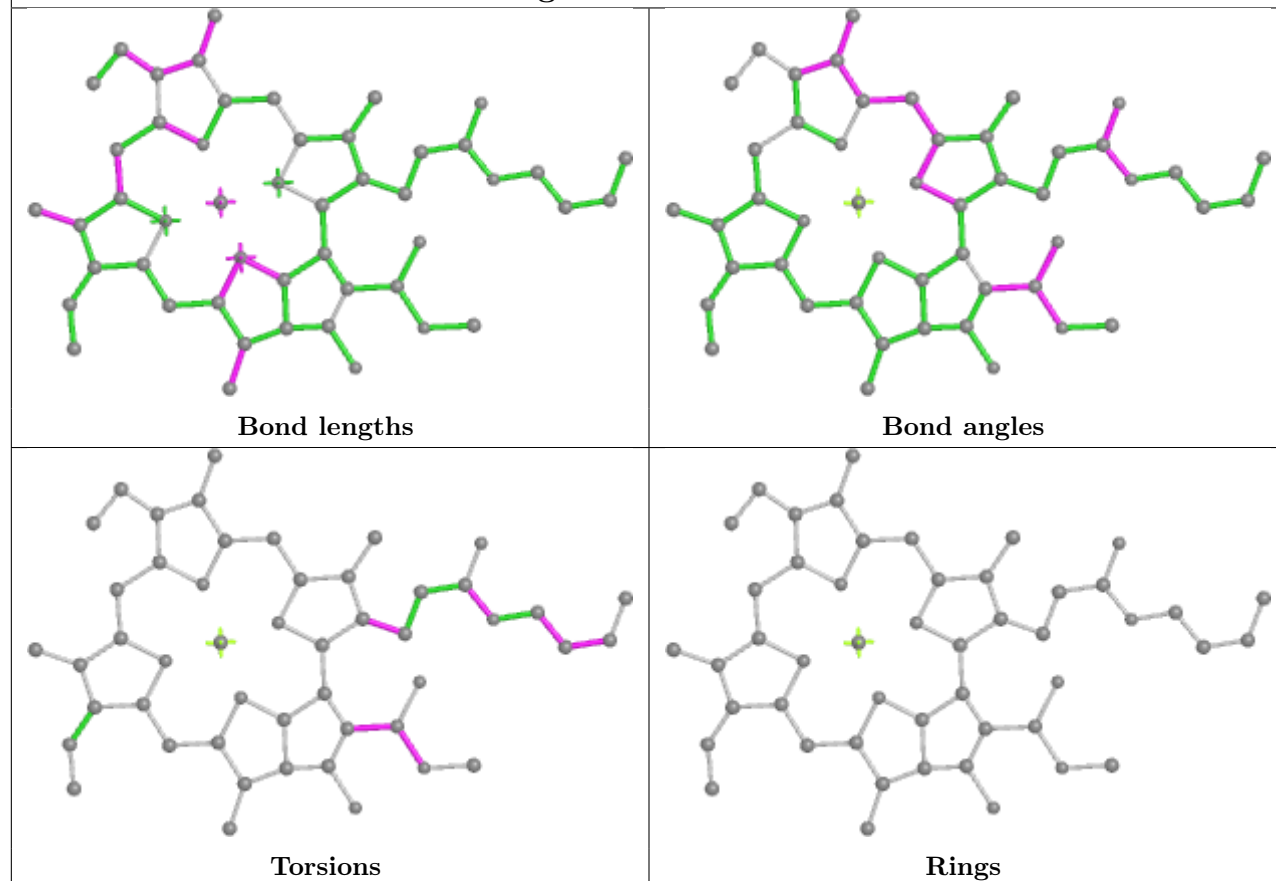


Ligand CHL 0 606

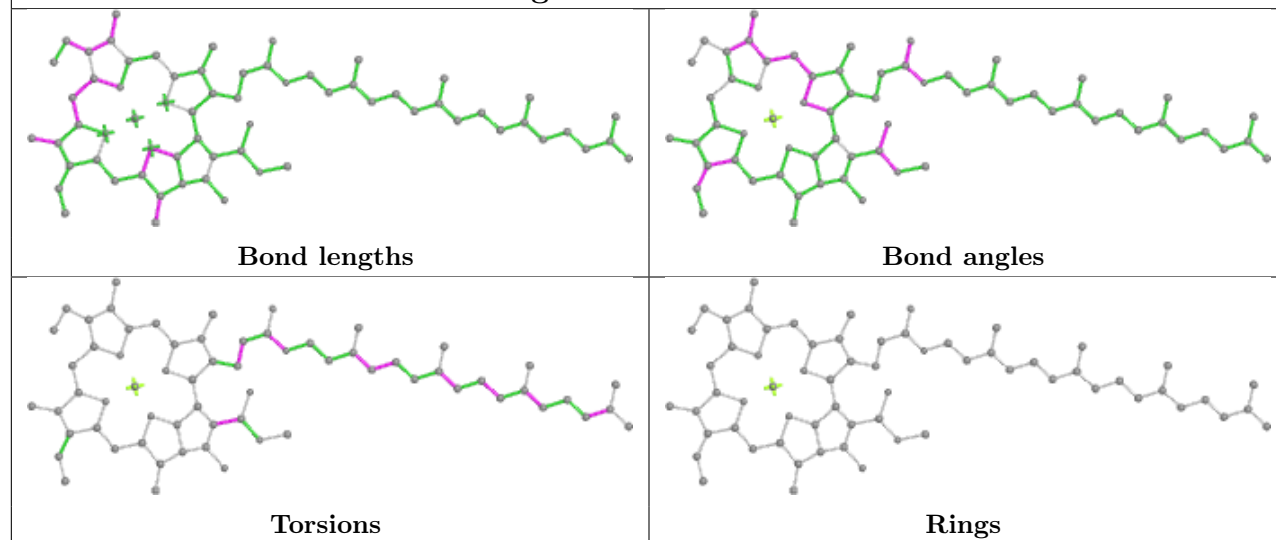




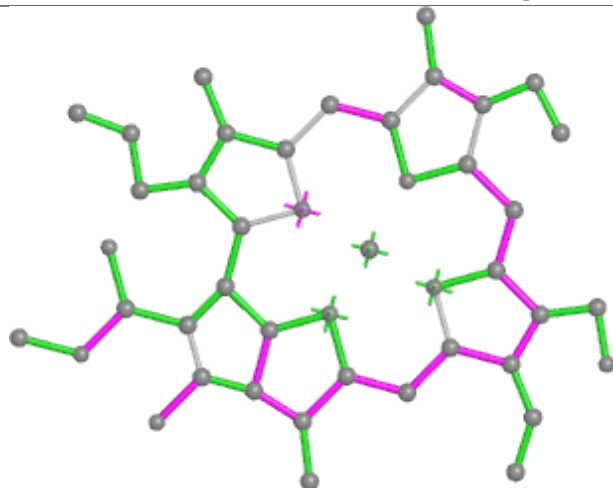
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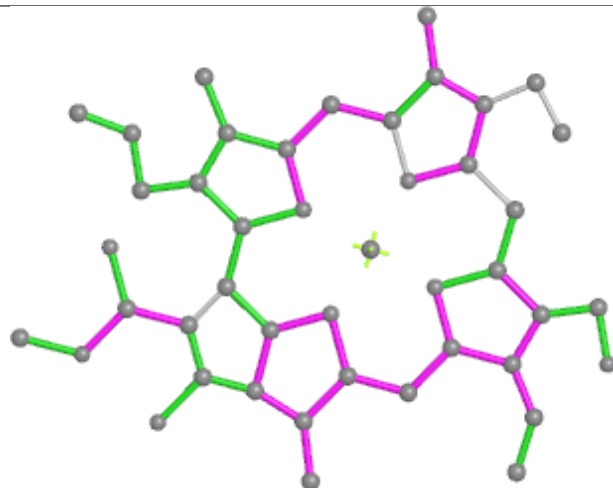
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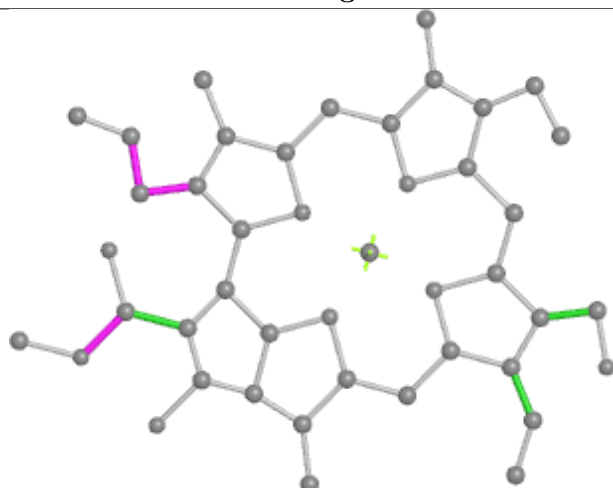
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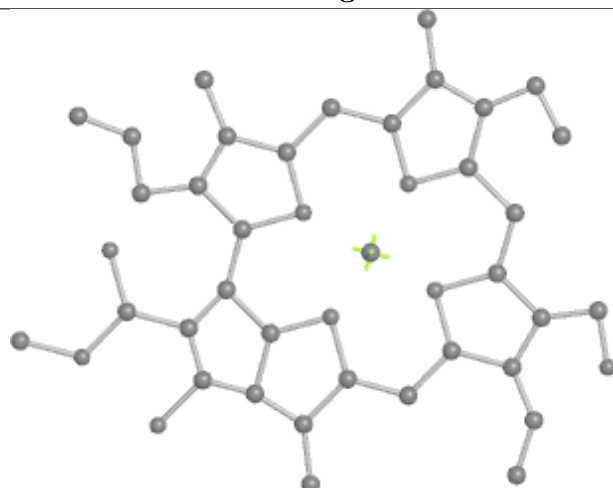
Bond lengths



Bond angles

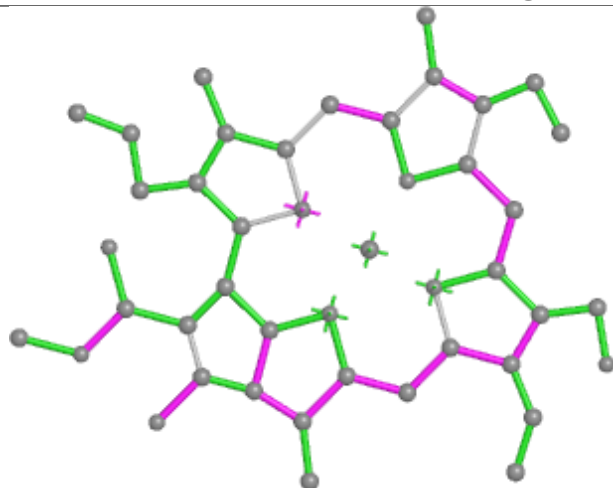


Torsions

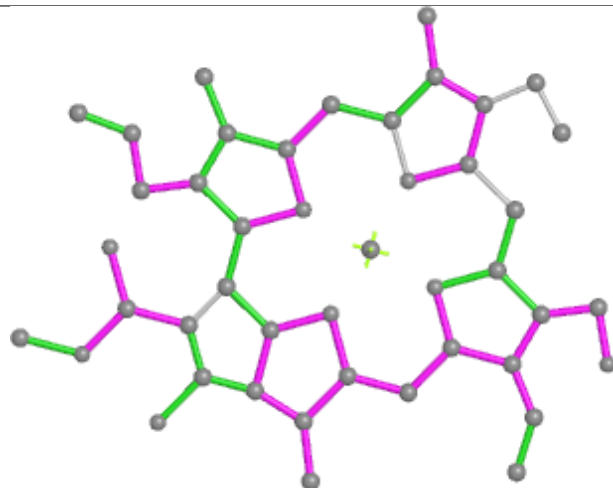


Rings

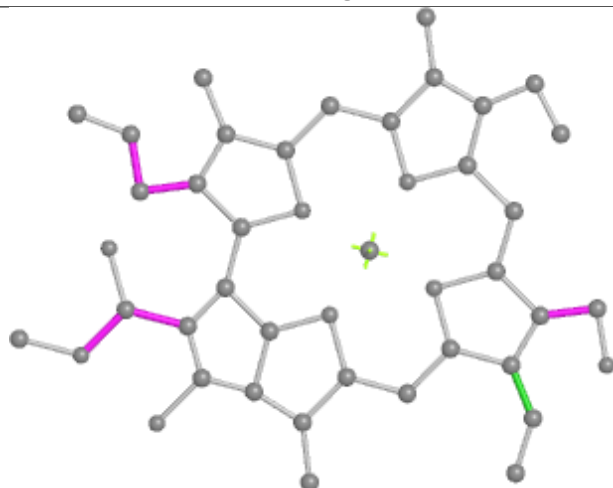
Ligand CHL s 606



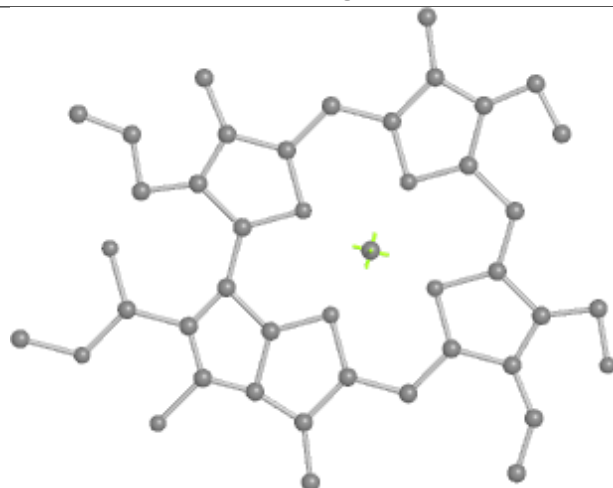
Bond lengths



Bond angles

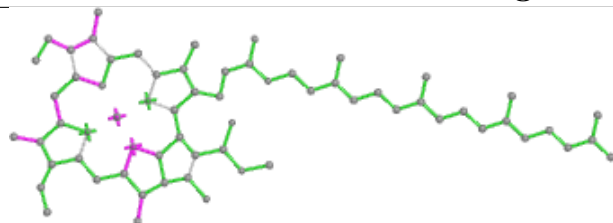


Torsions

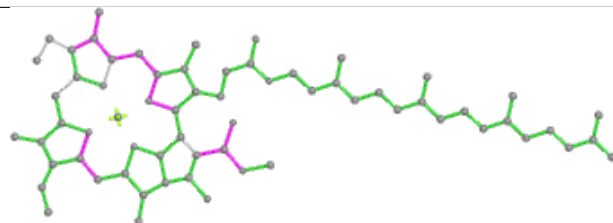


Rings

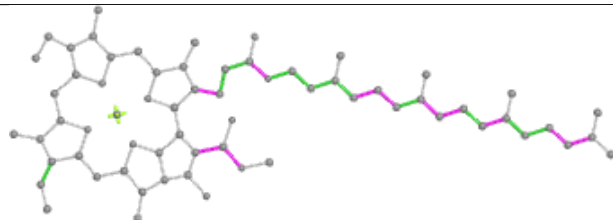
Ligand CLA C 508



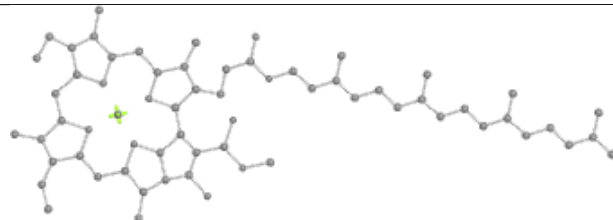
Bond lengths



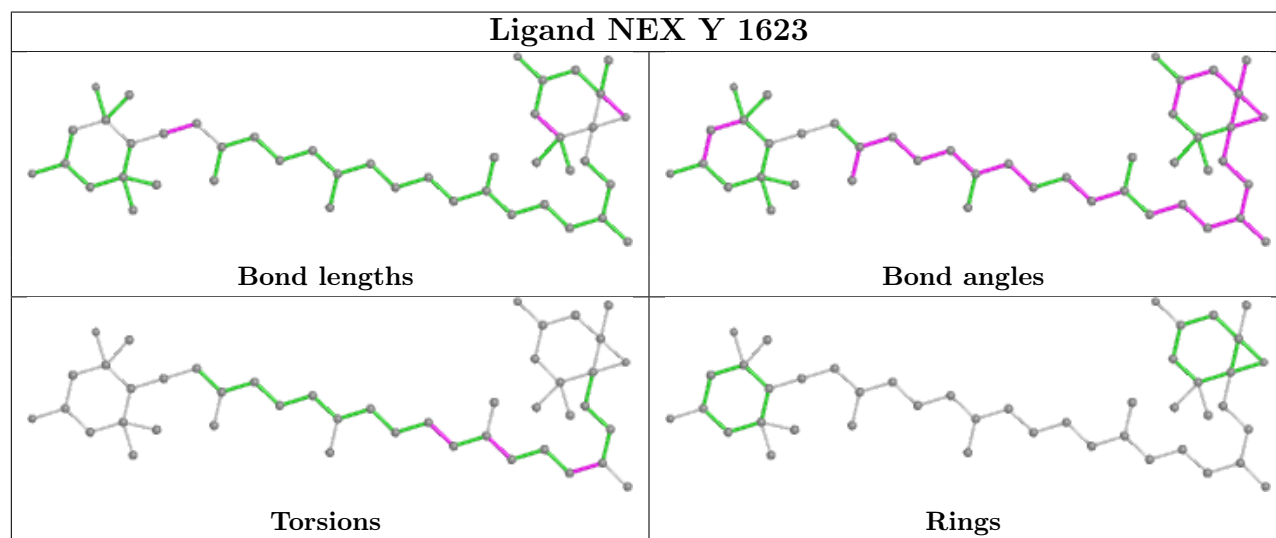
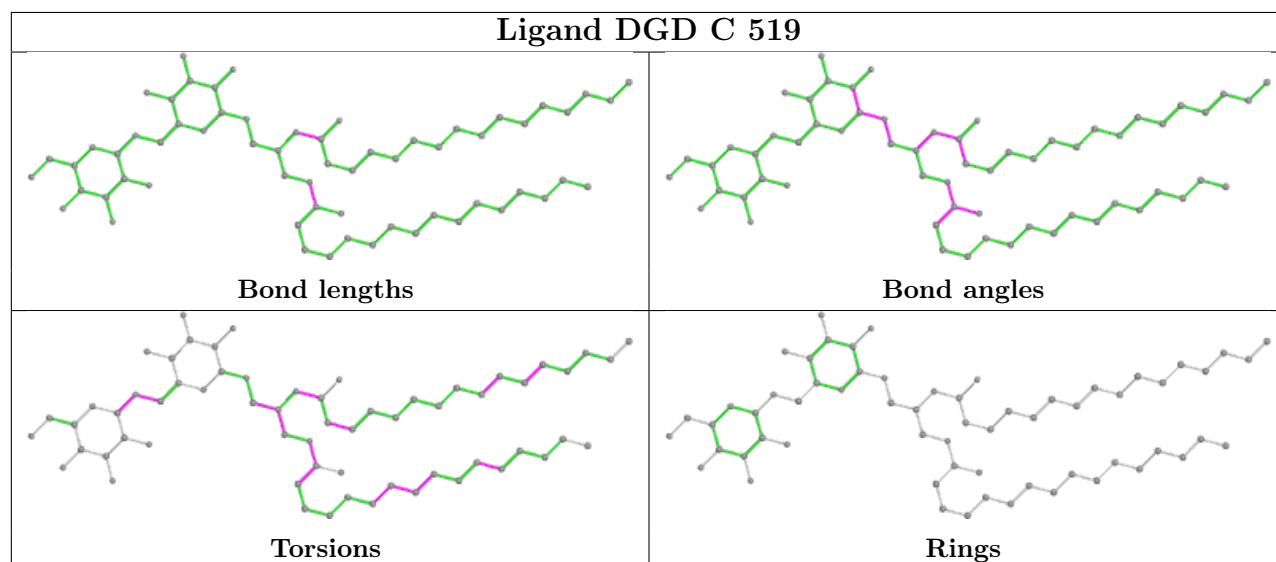
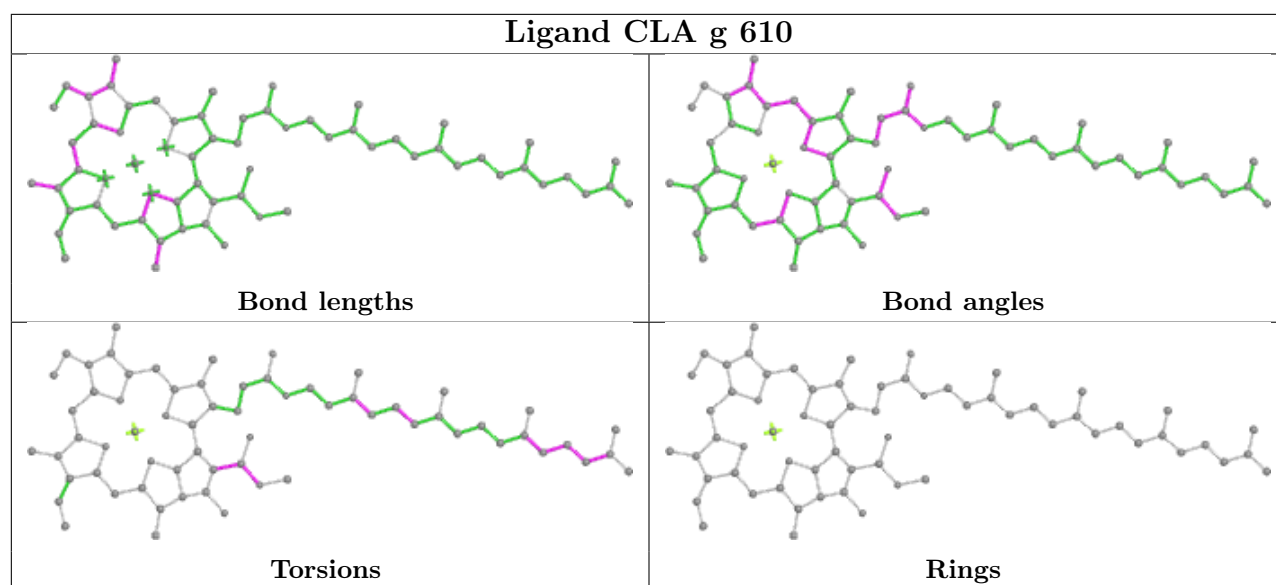
Bond angles

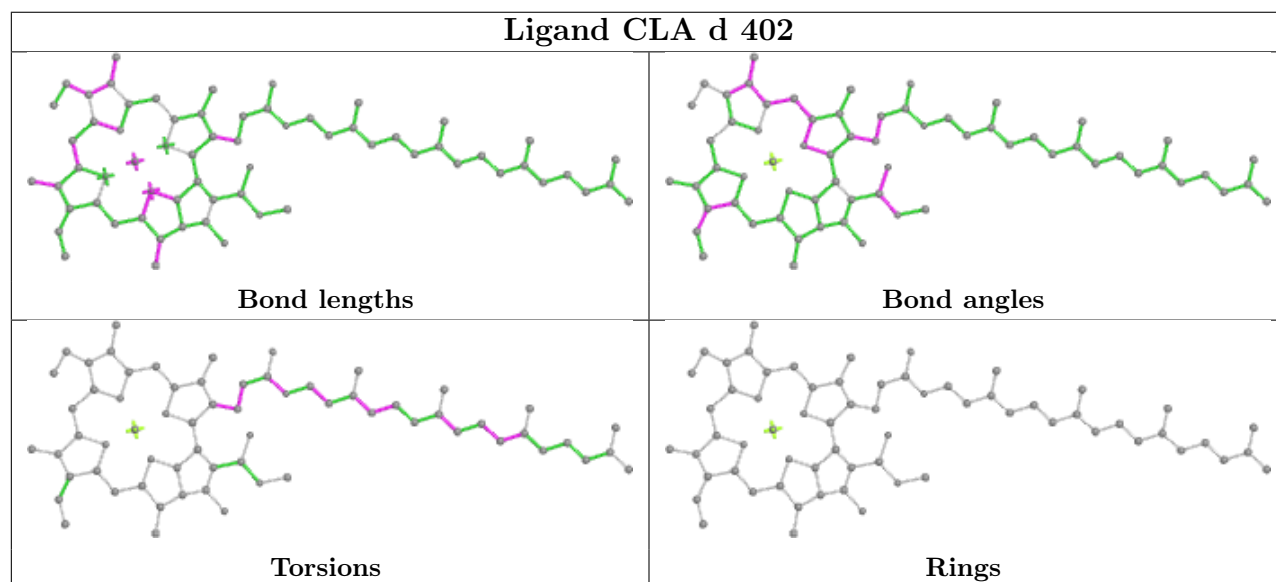
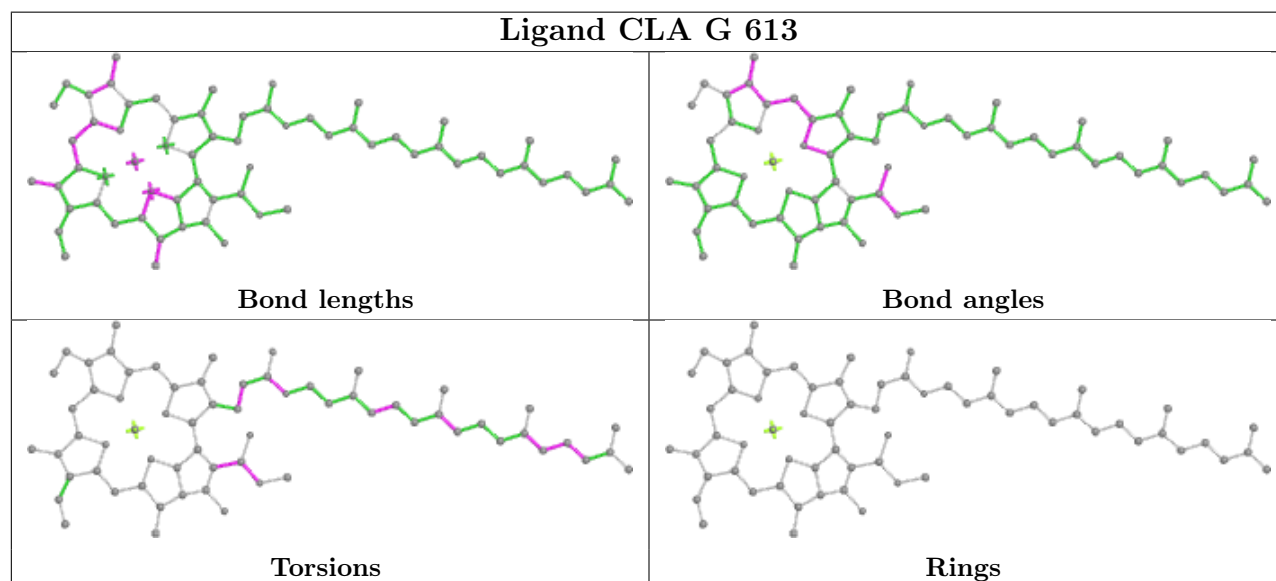
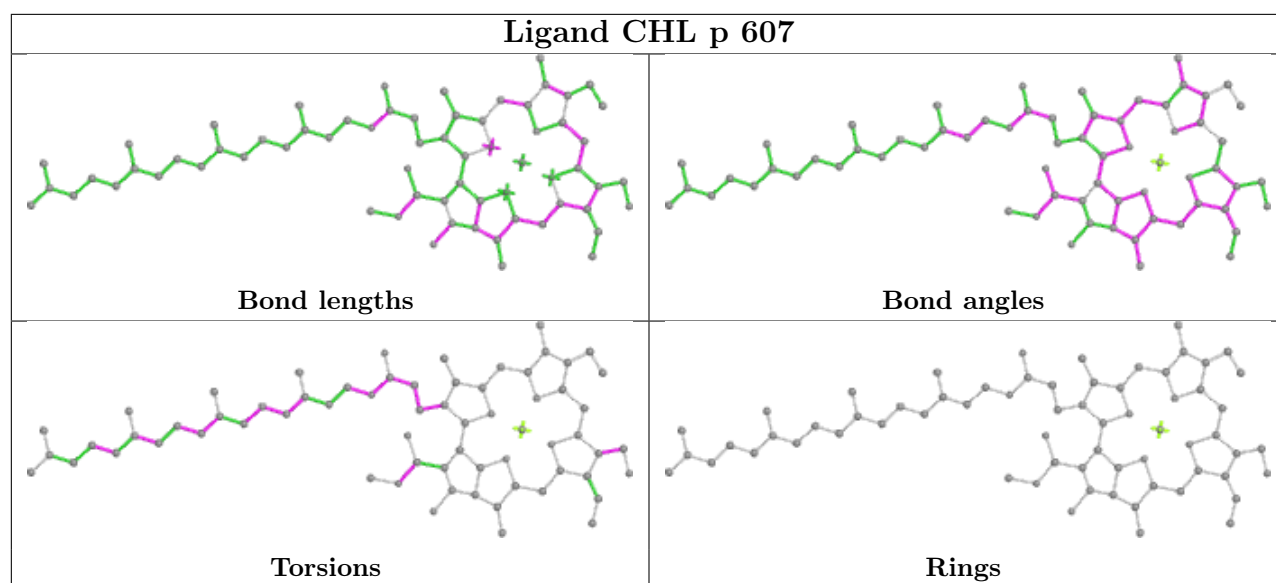


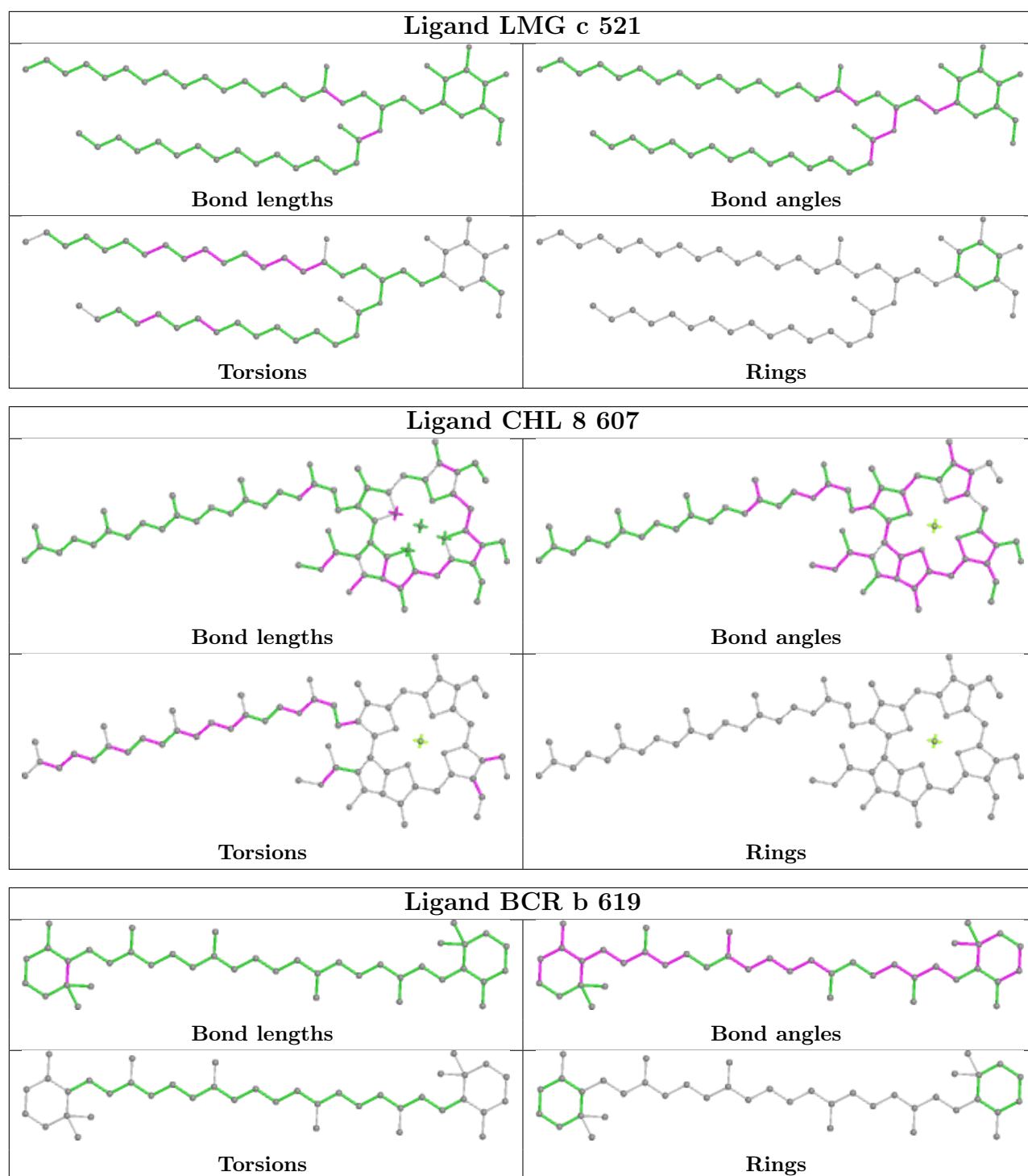
Torsions



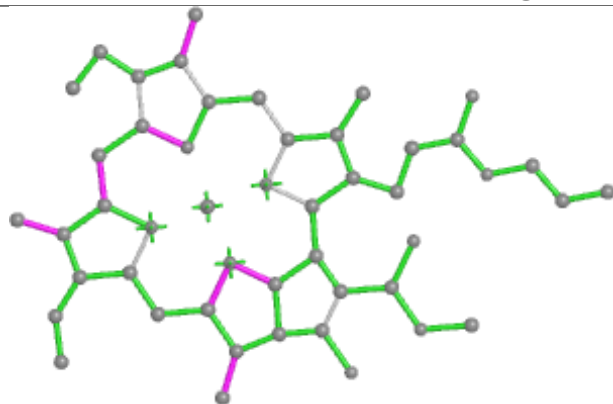
Rings



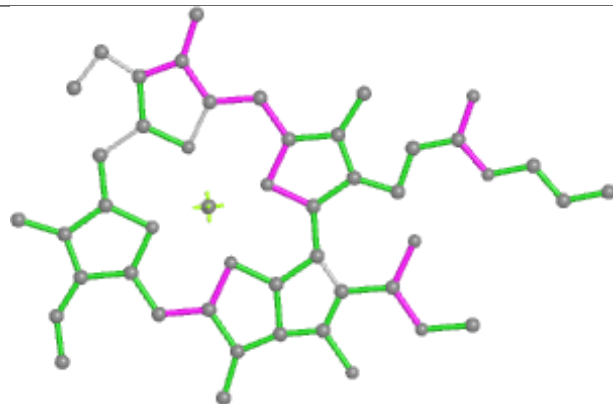




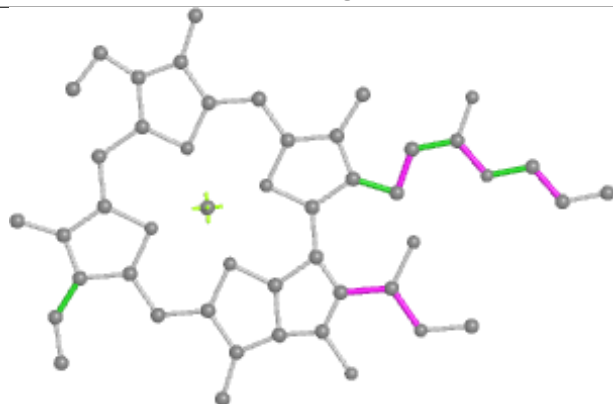
Ligand CLA S 614



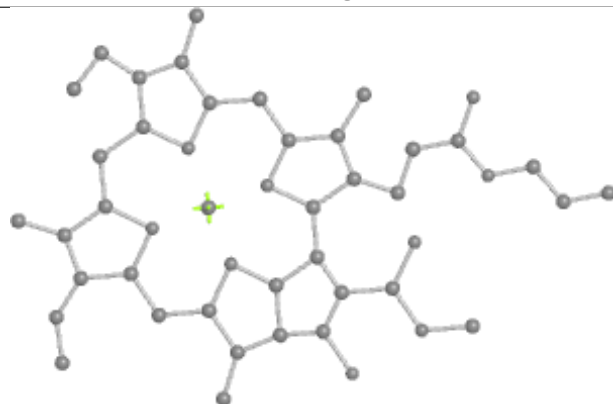
Bond lengths



Bond angles

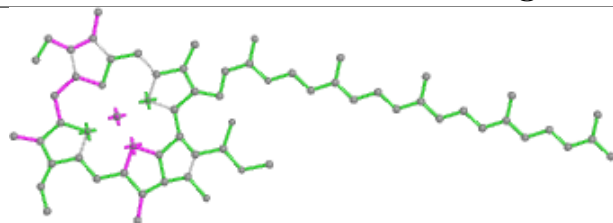


Torsions

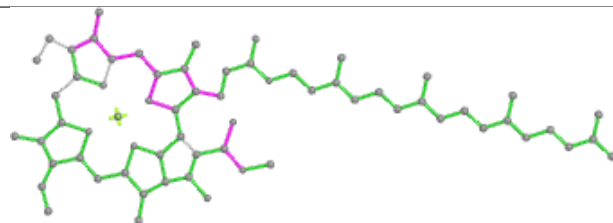


Rings

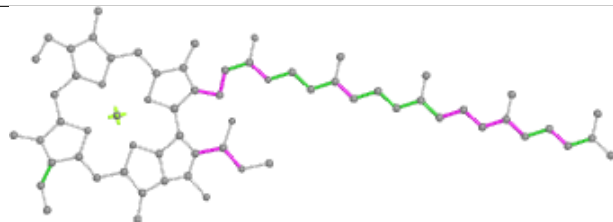
Ligand CLA 1 603



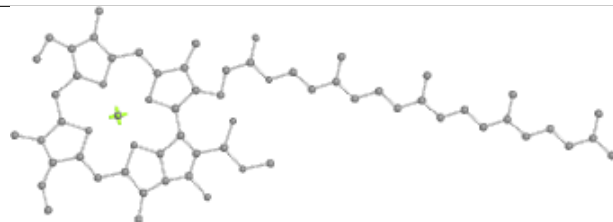
Bond lengths



Bond angles

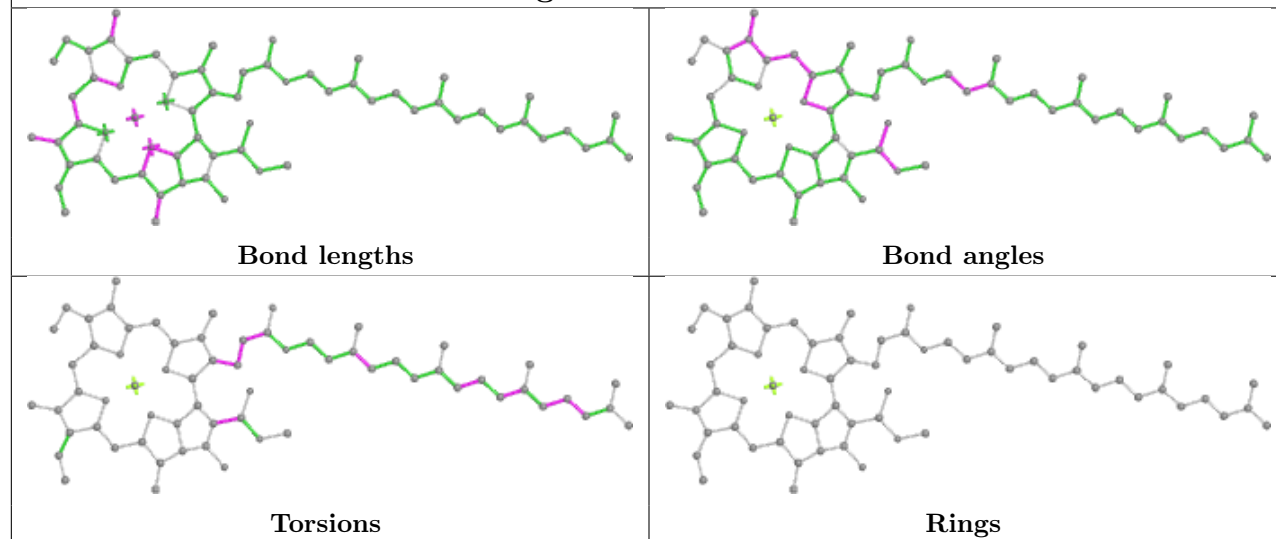


Torsions

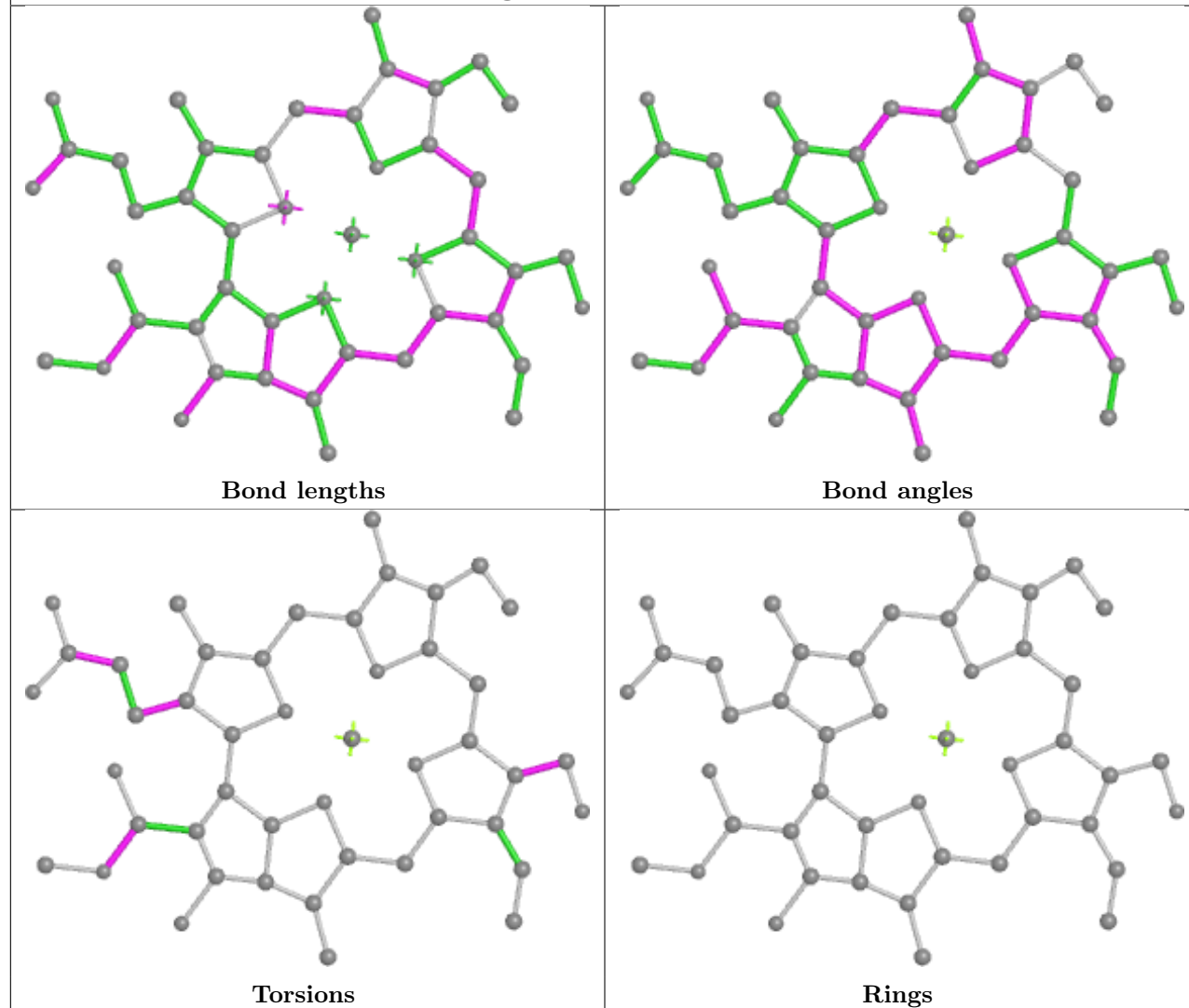


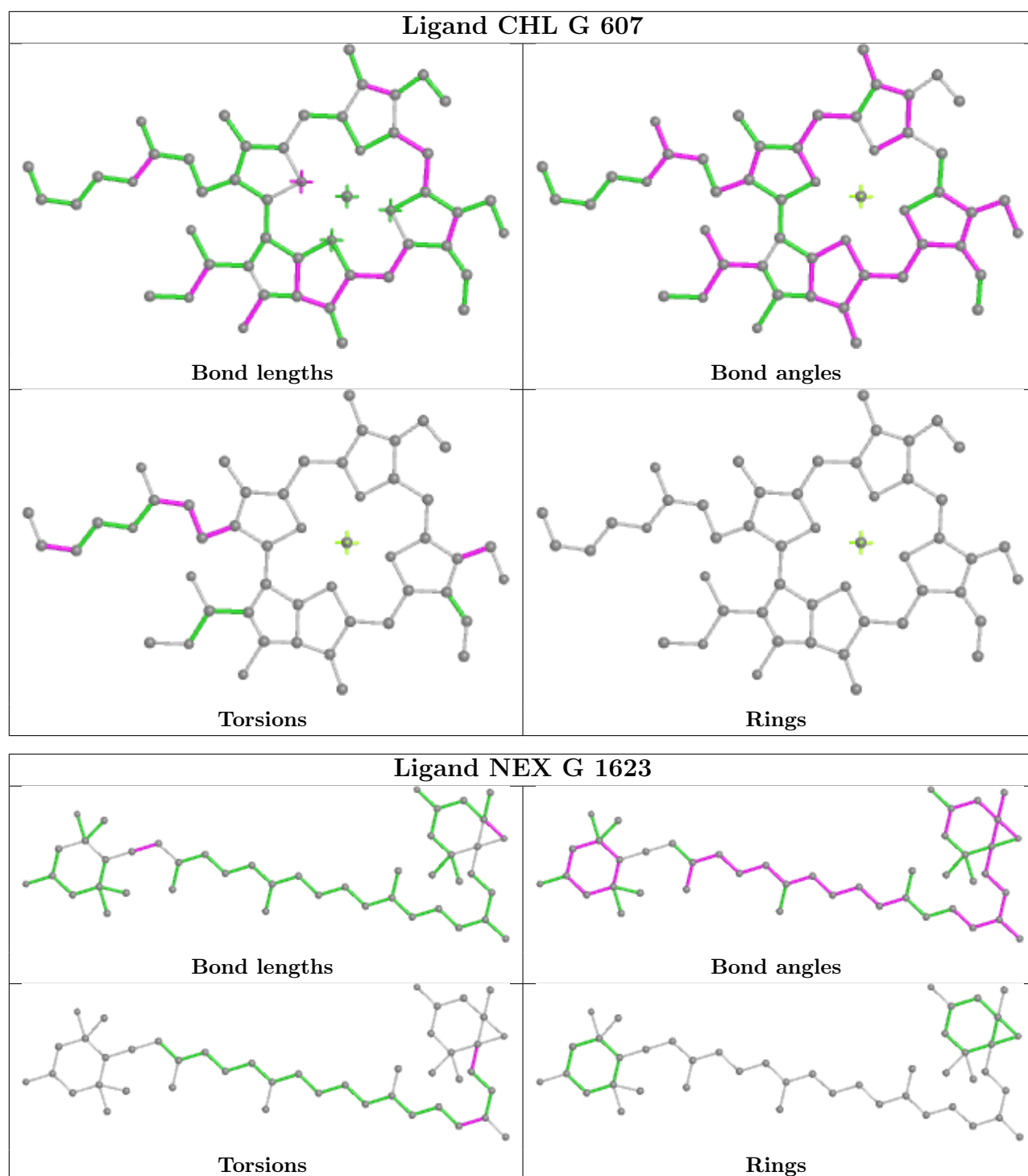
Rings

Ligand CLA 2 602

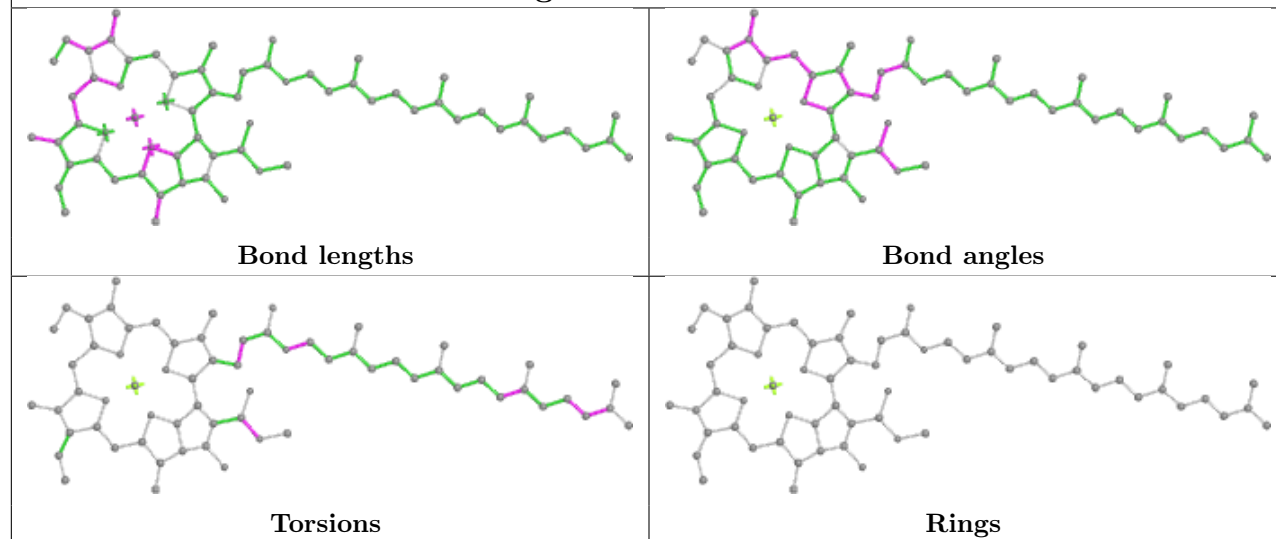


Ligand CHL 3 606

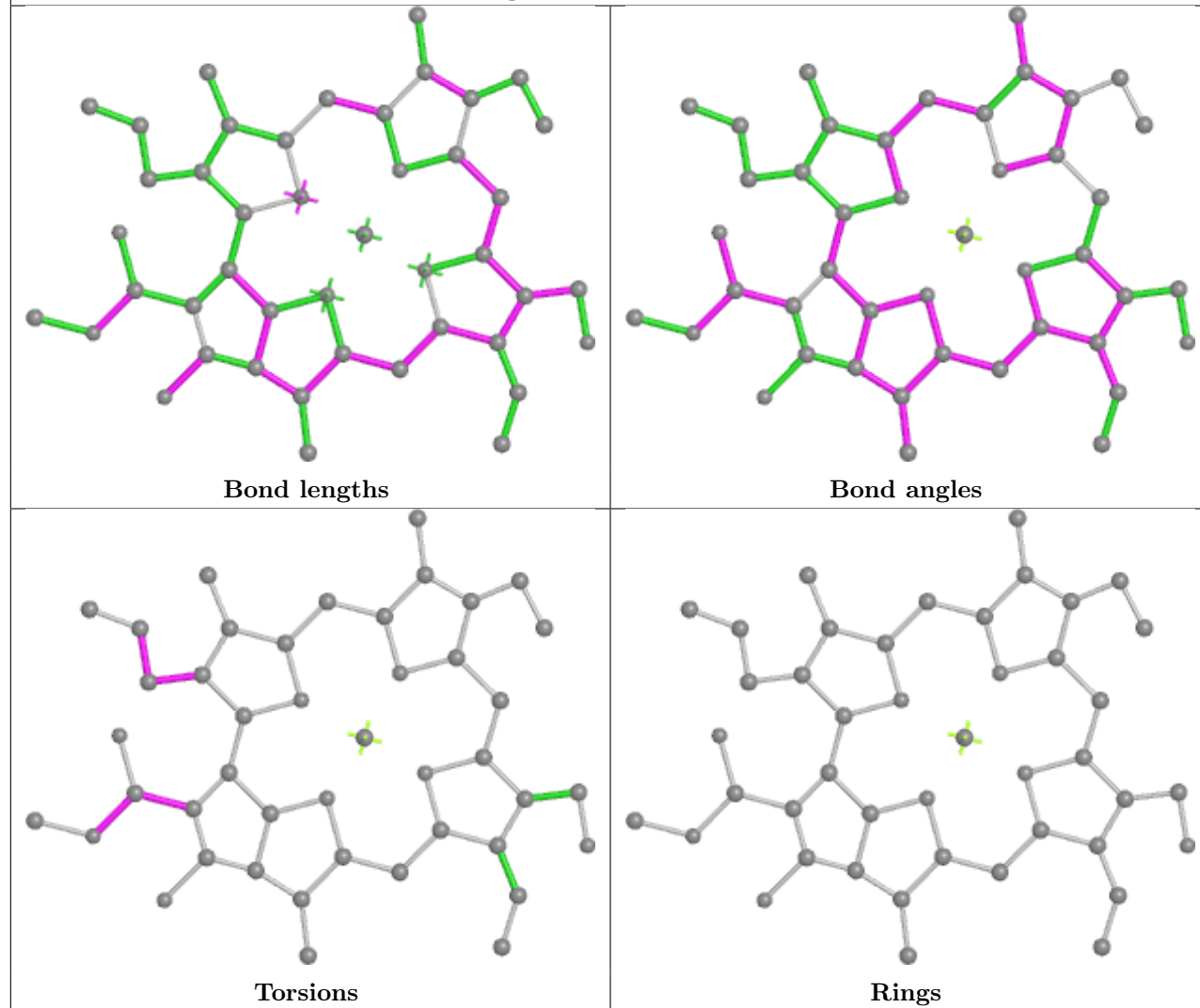




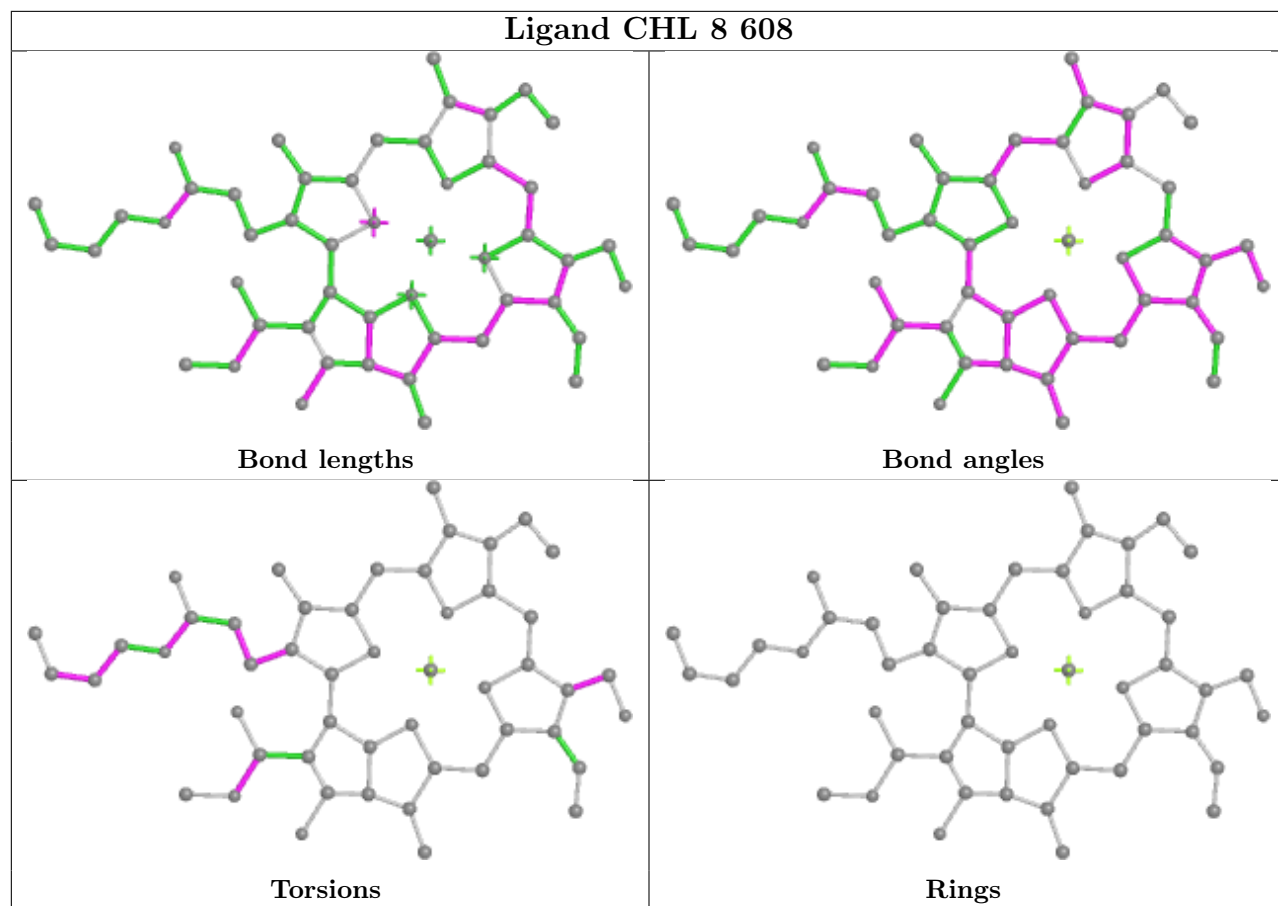
Ligand CLA b 611



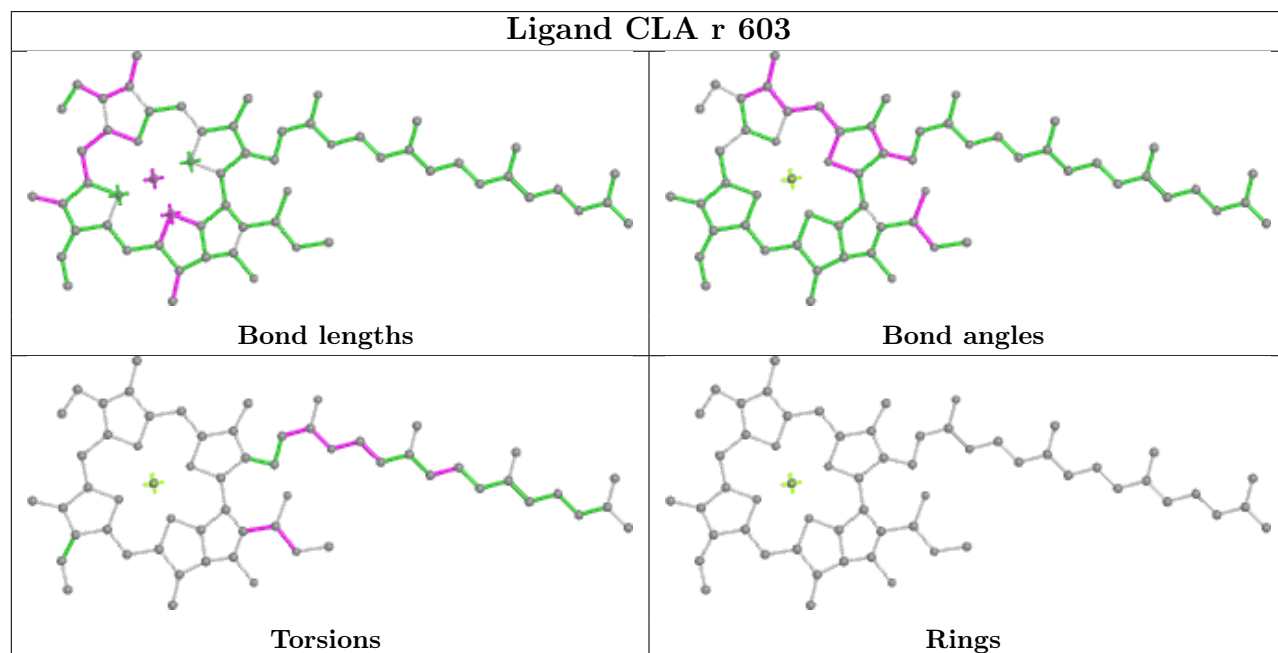
Ligand CHL 2 608

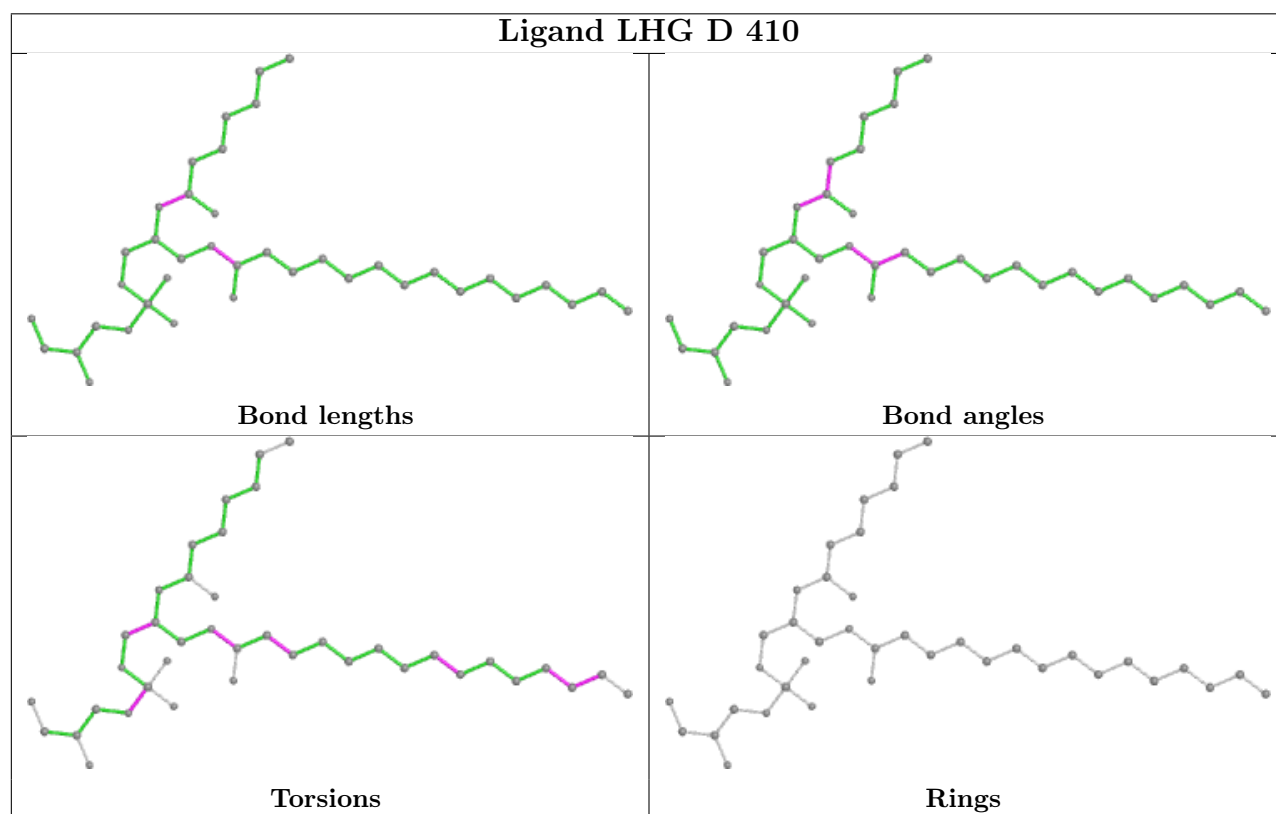
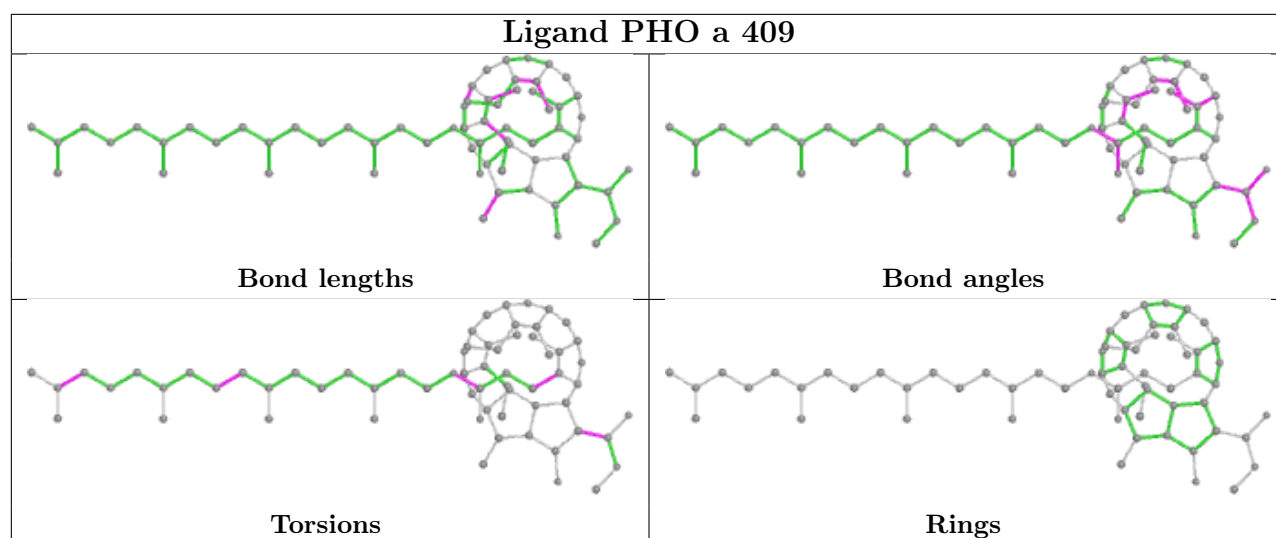


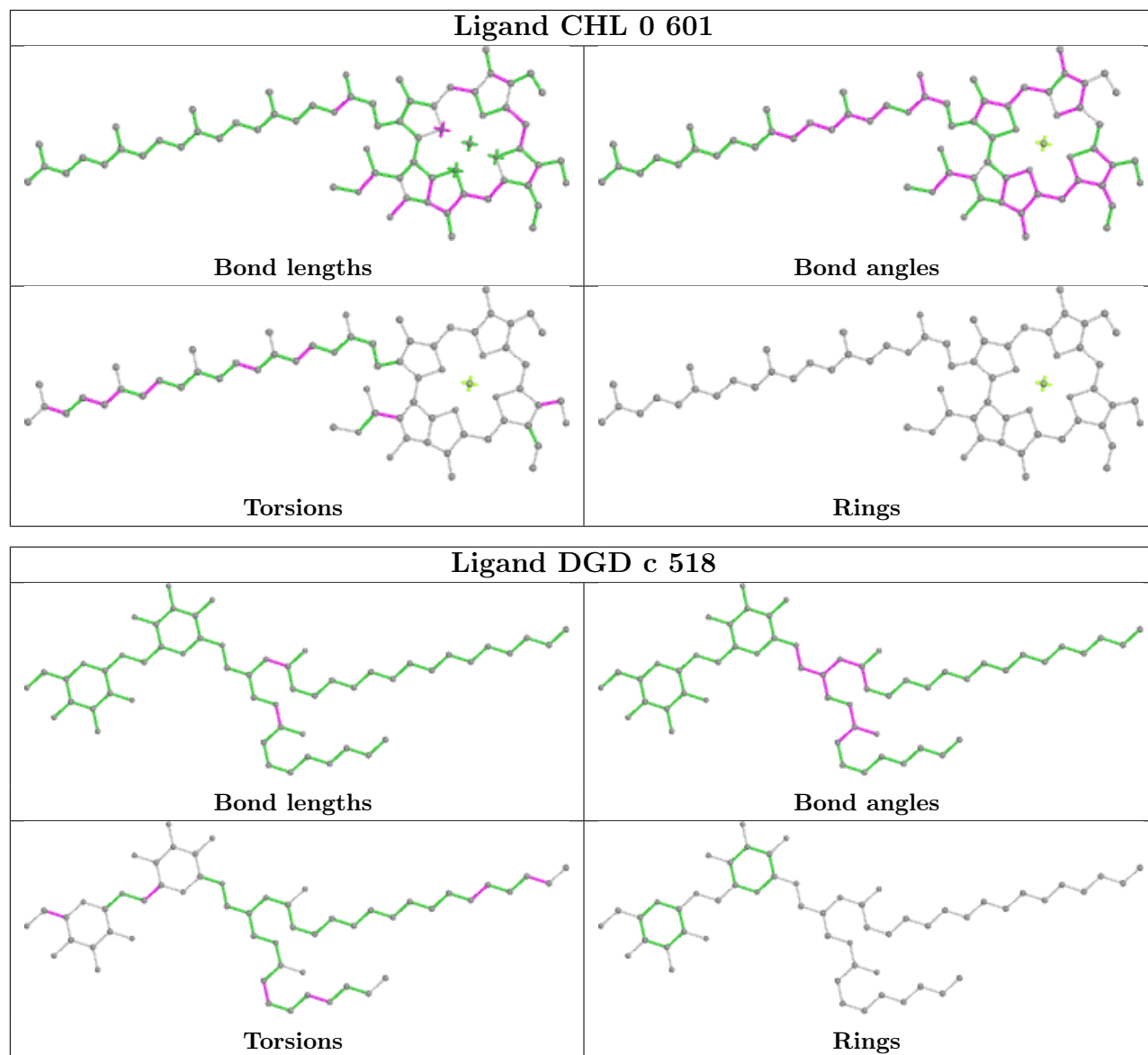
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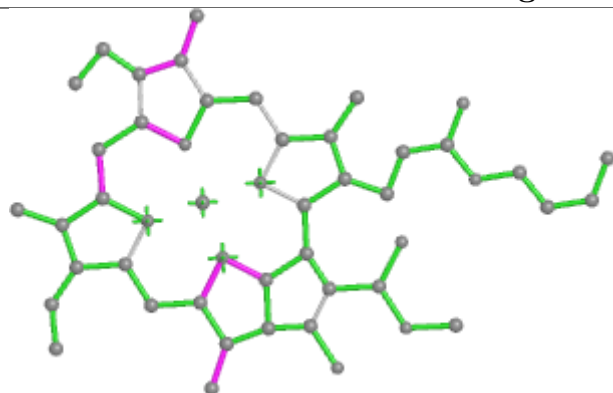
Ligand CLA r 603



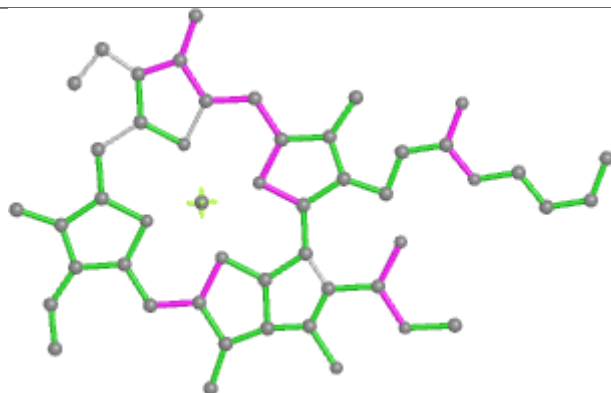




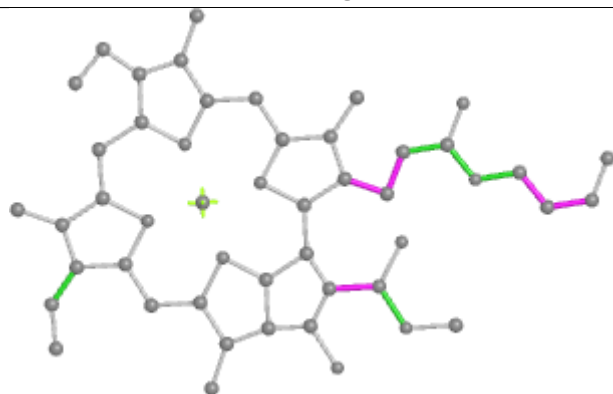
Ligand CLA 8 611



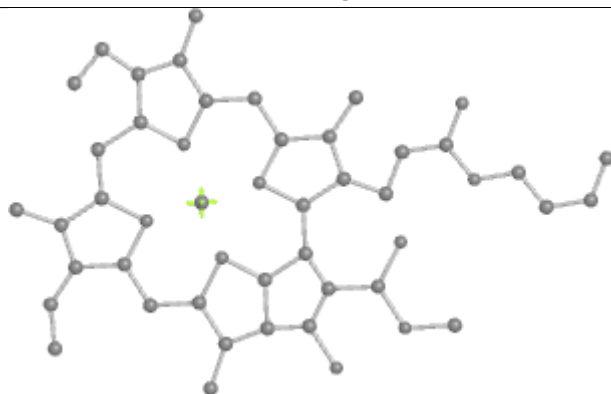
Bond lengths



Bond angles

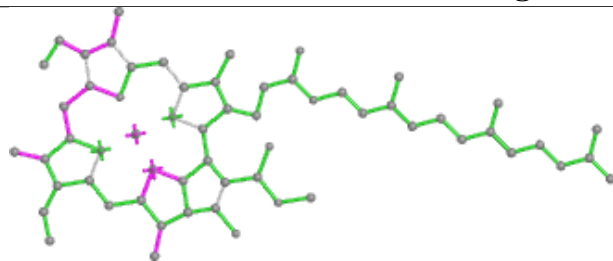


Torsions

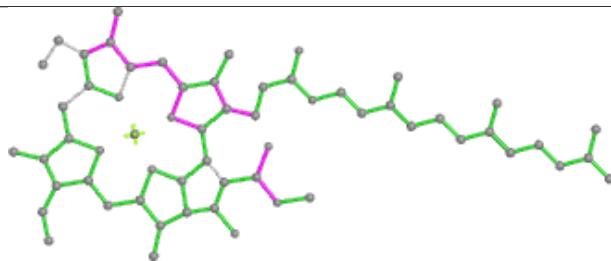


Rings

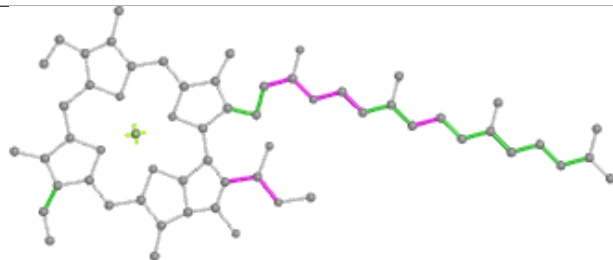
Ligand CLA R 603



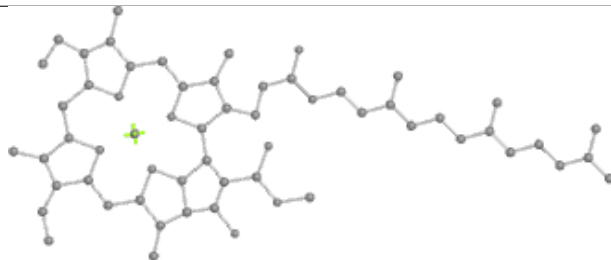
Bond lengths



Bond angles

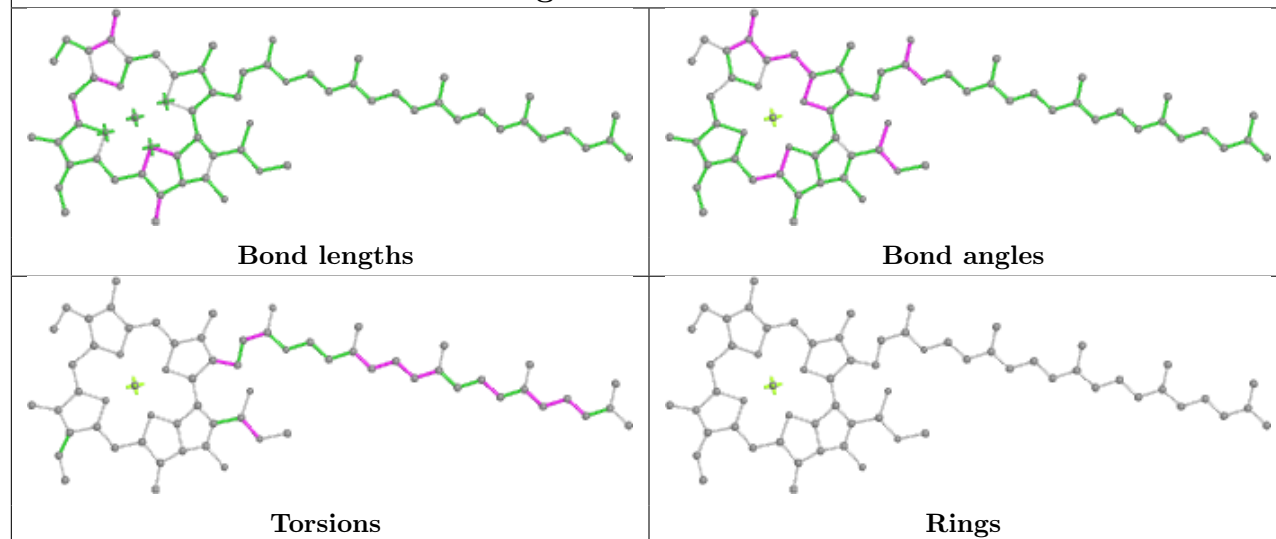


Torsions

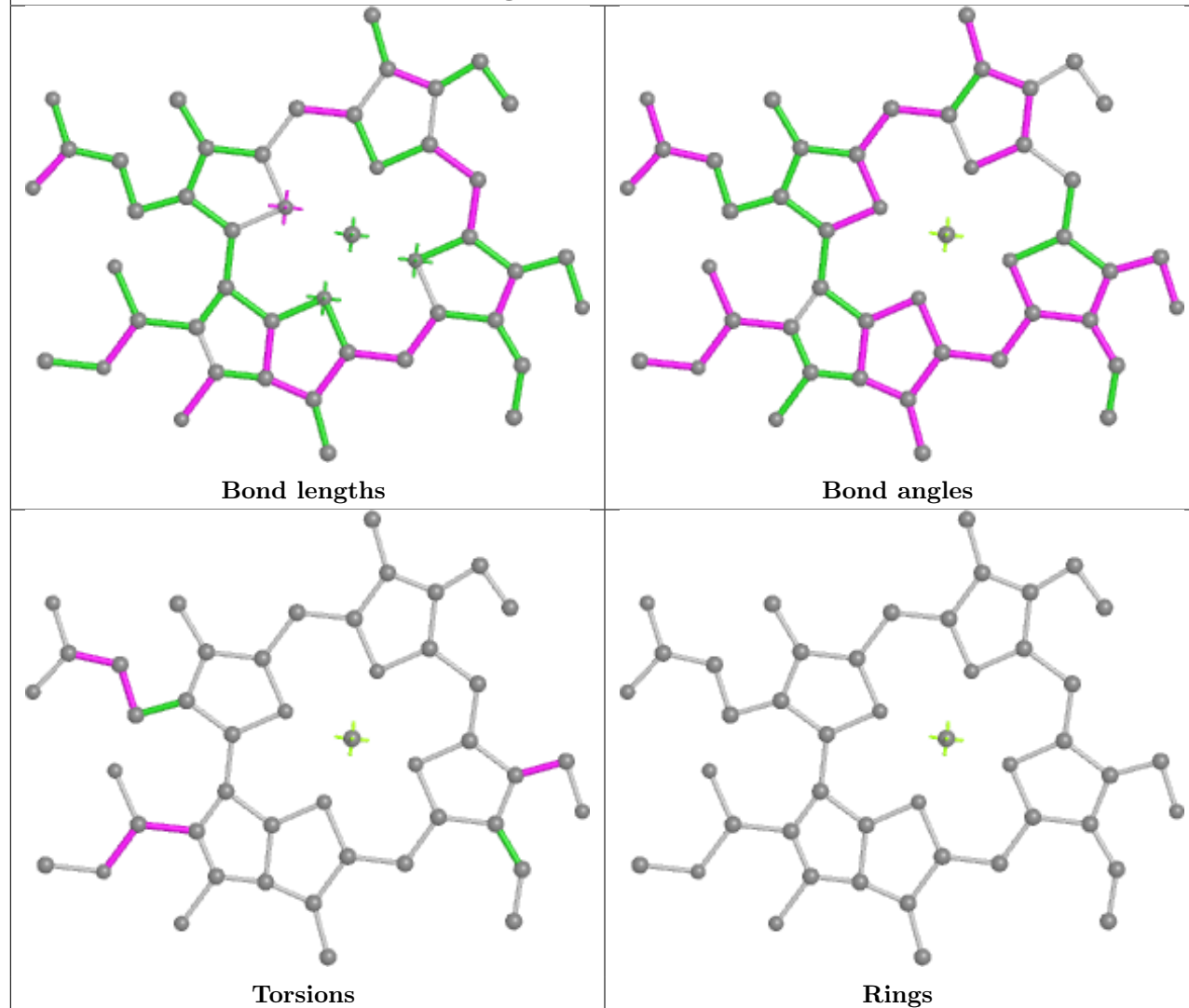


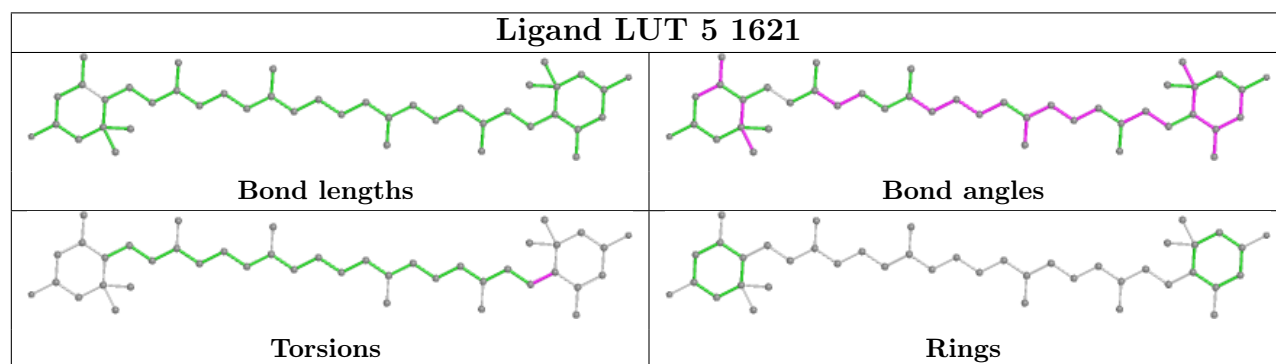
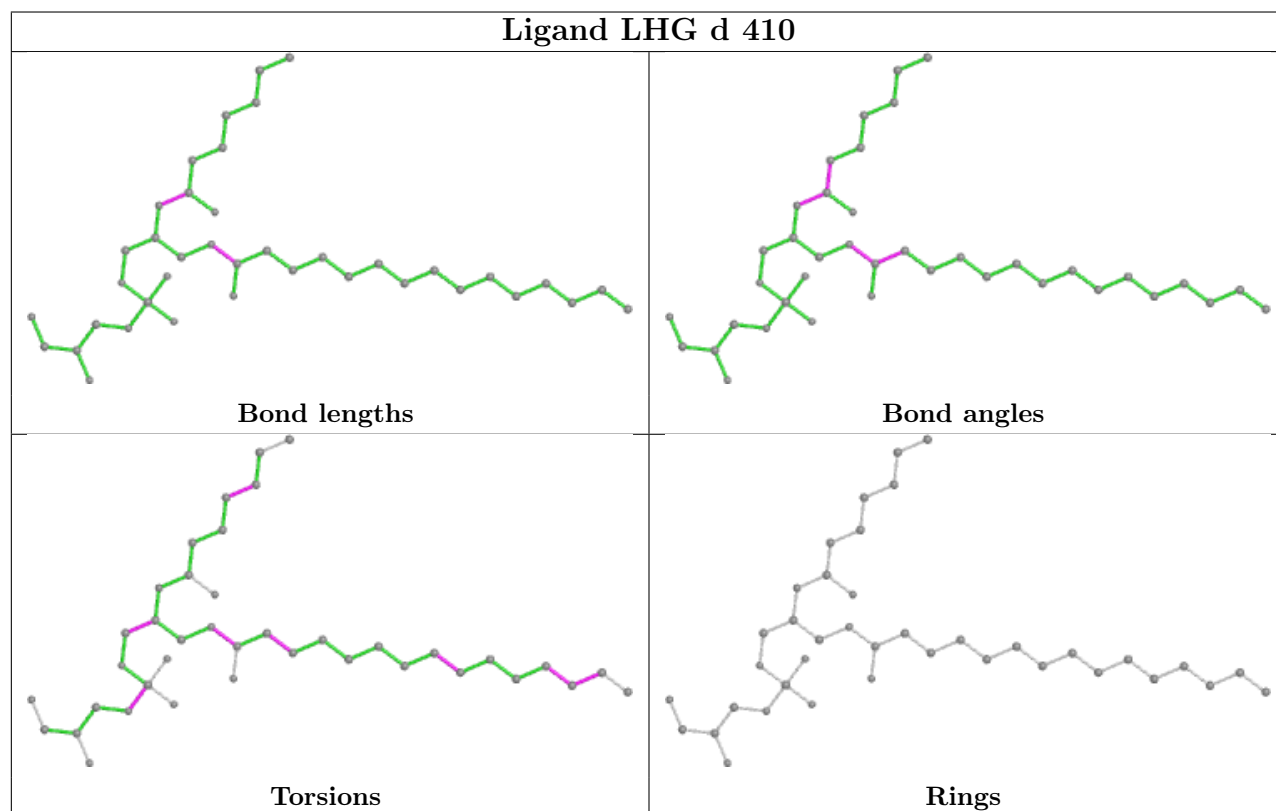
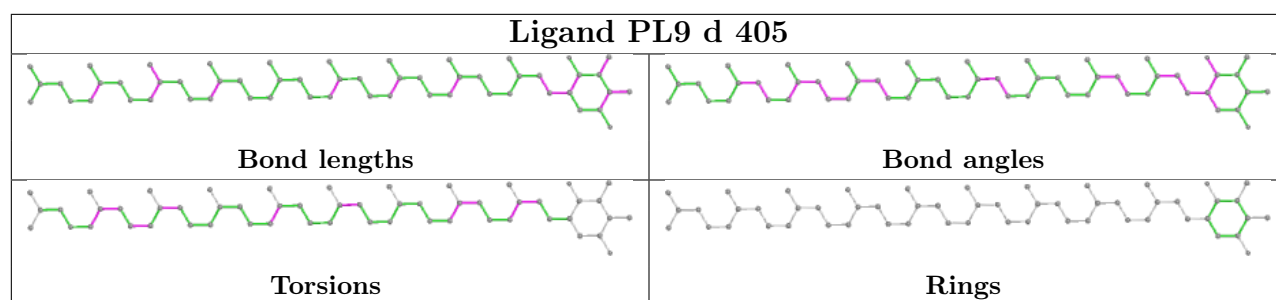
Rings

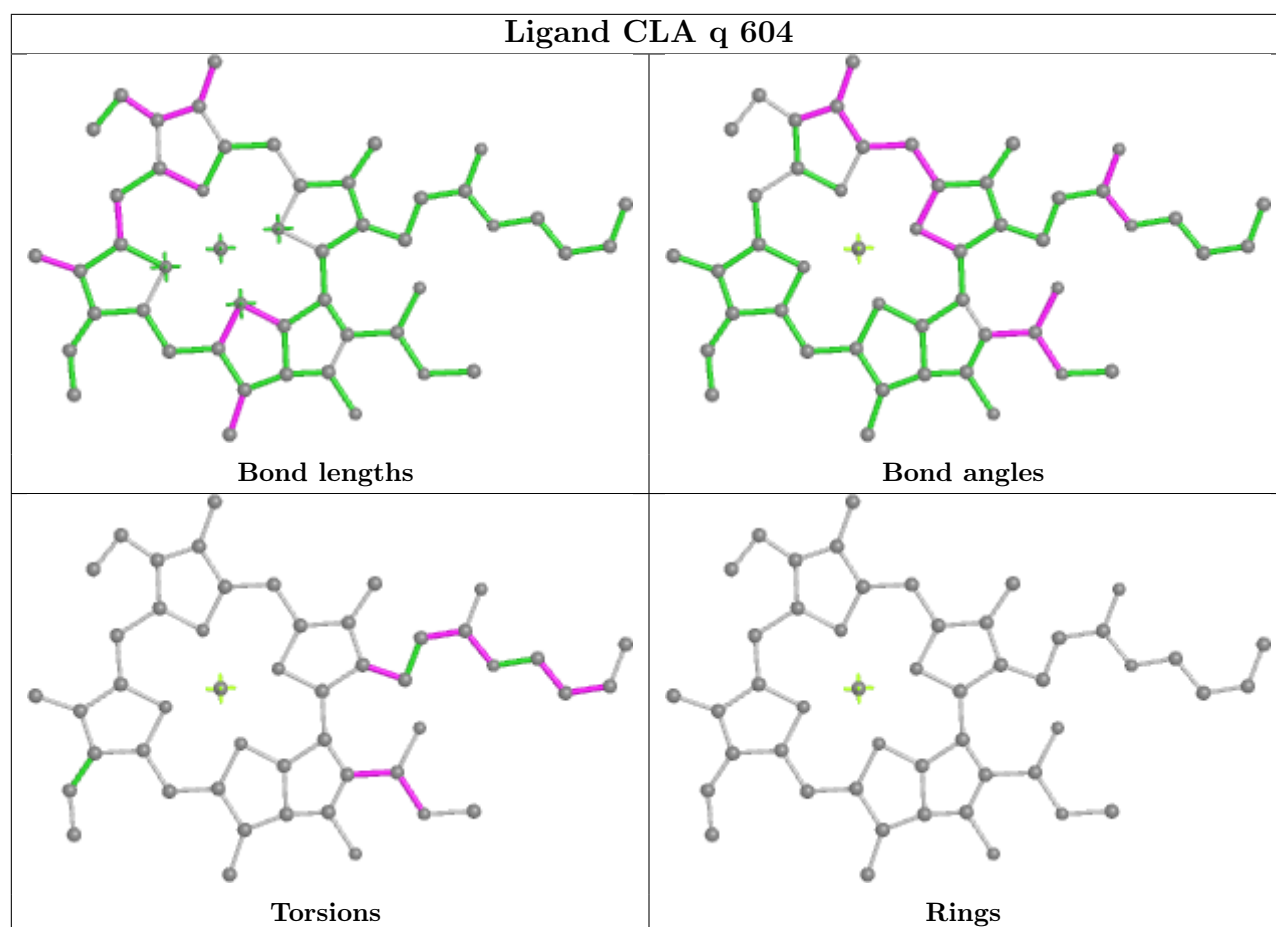
Ligand CLA 5 604

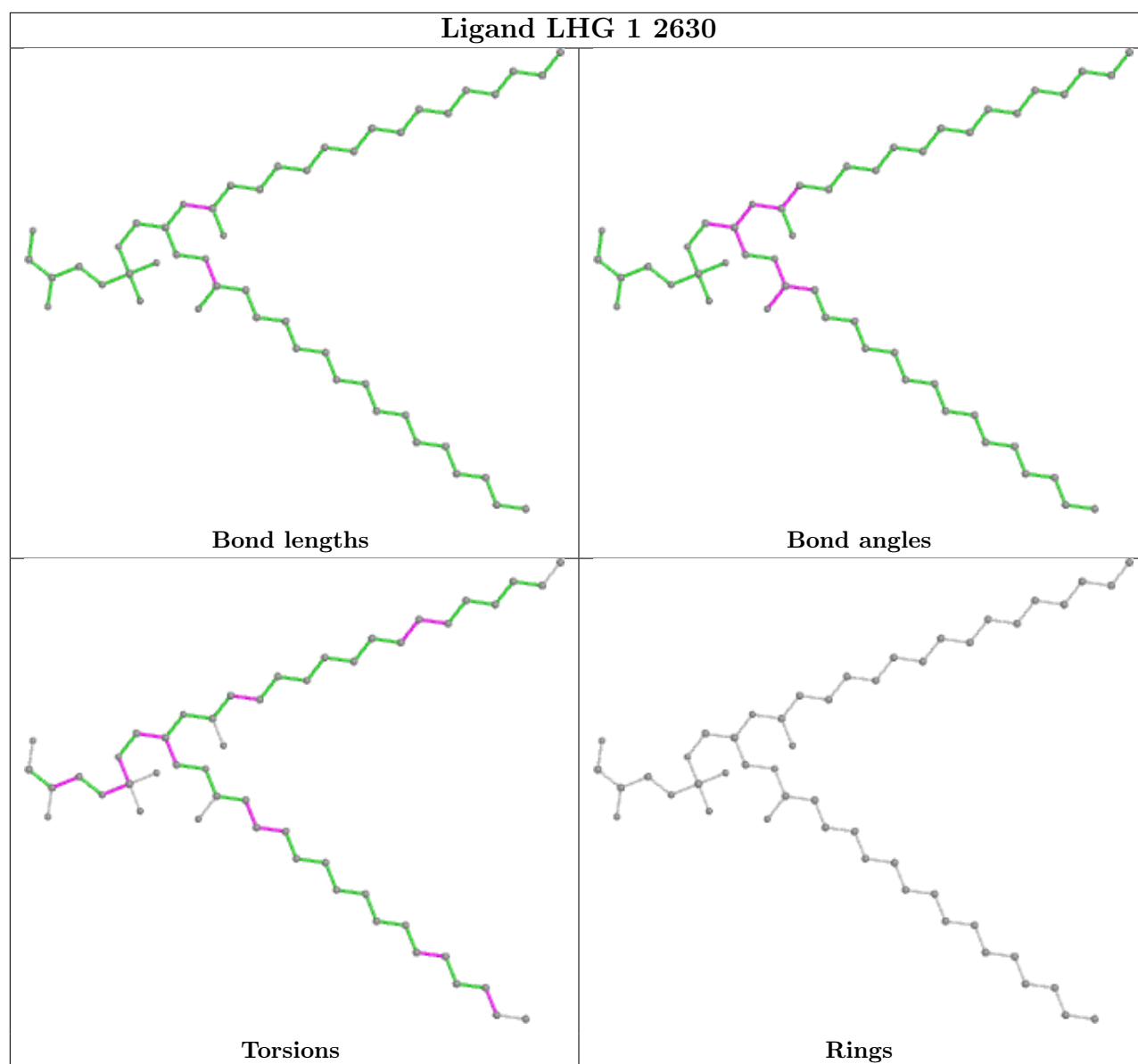


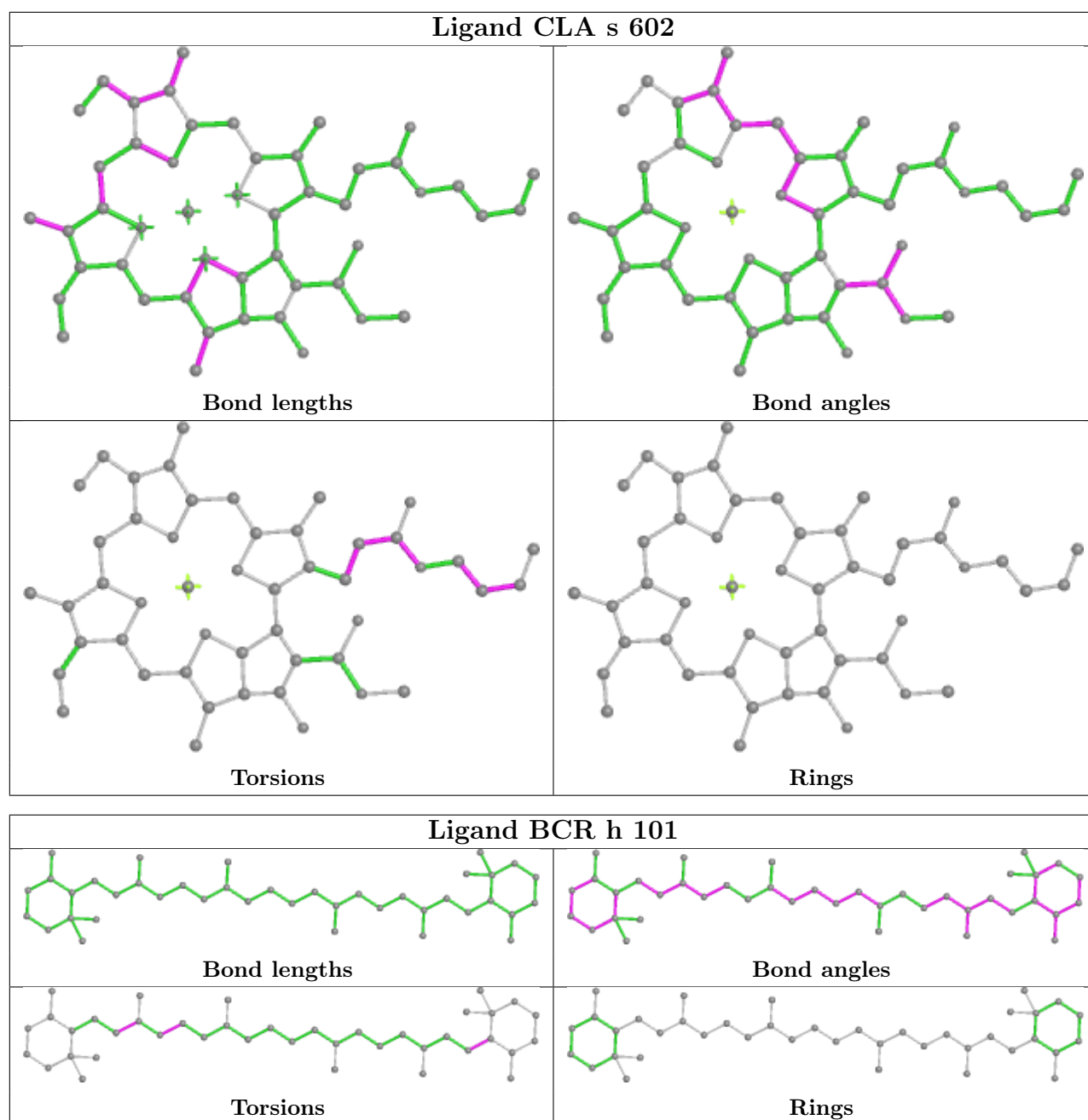
Ligand CHL s 601



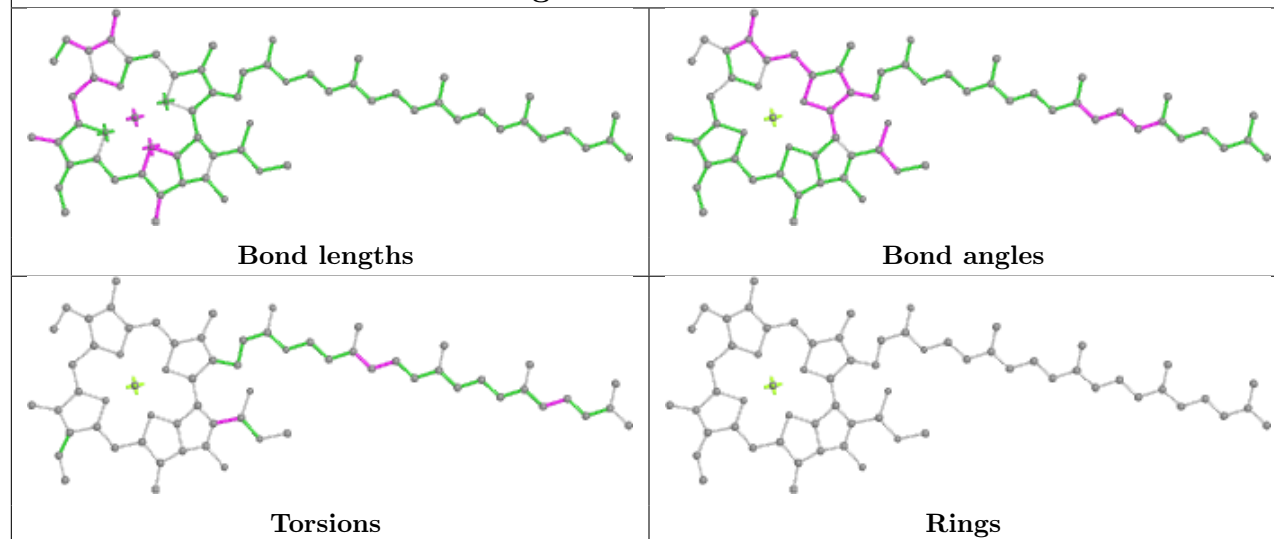




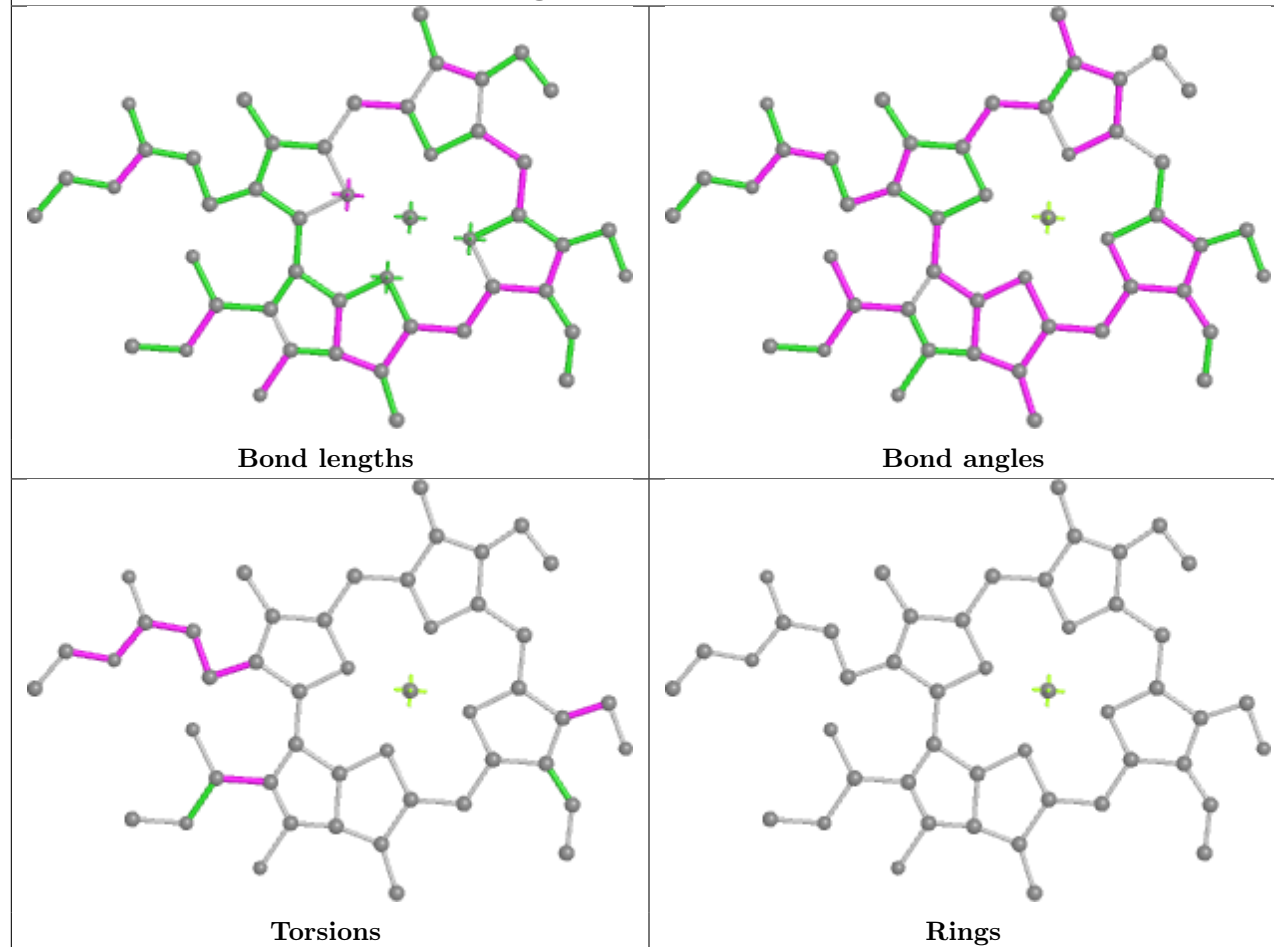


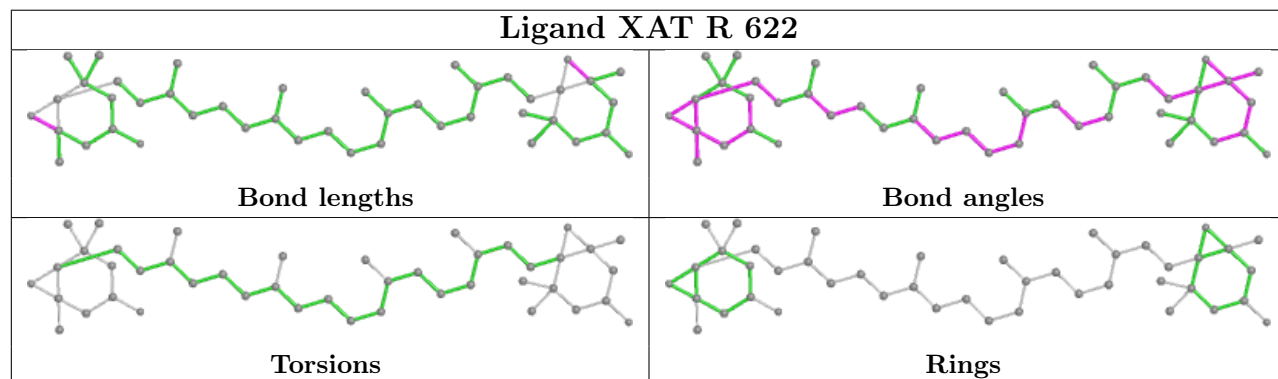
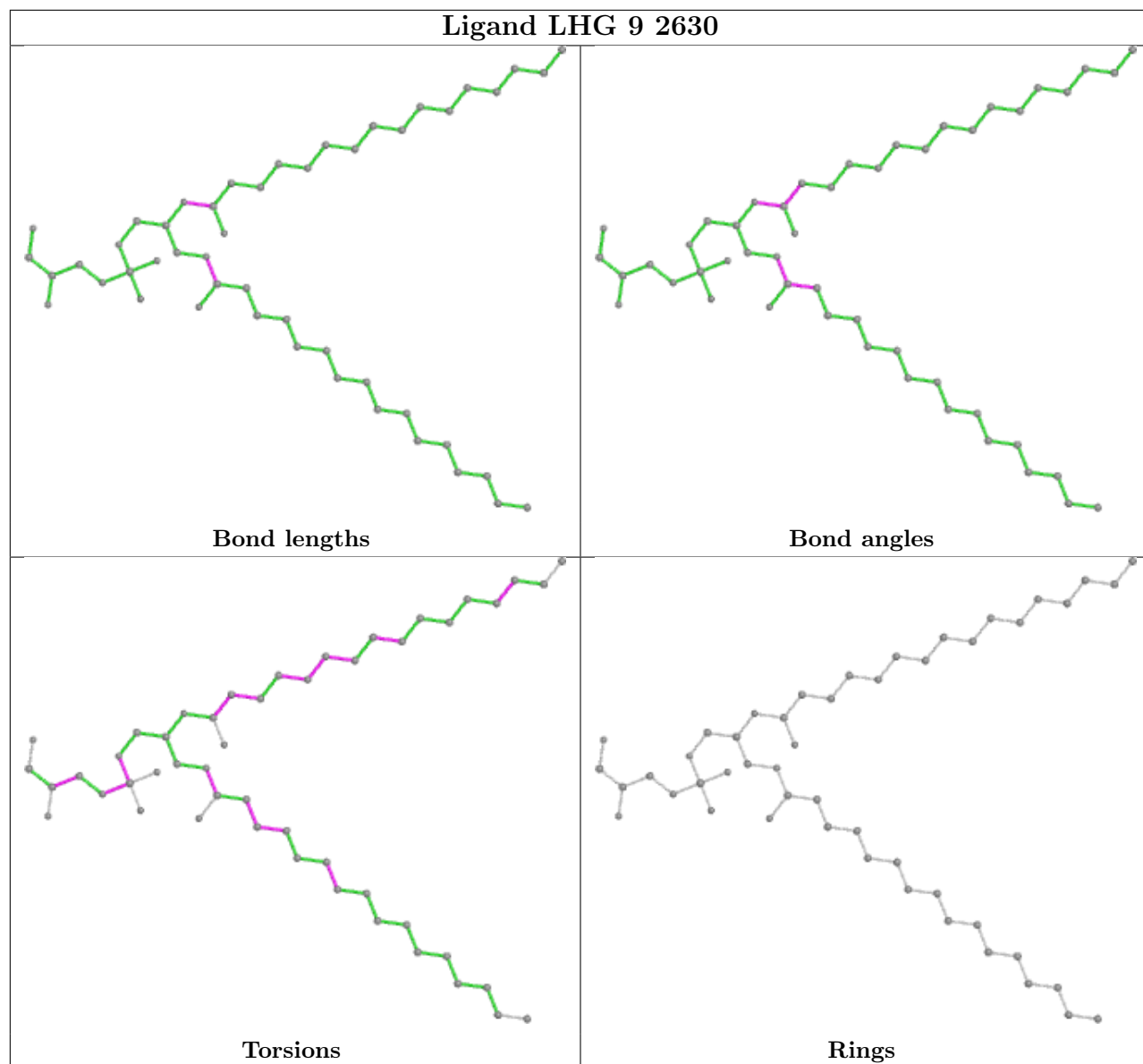


Ligand CLA C 509

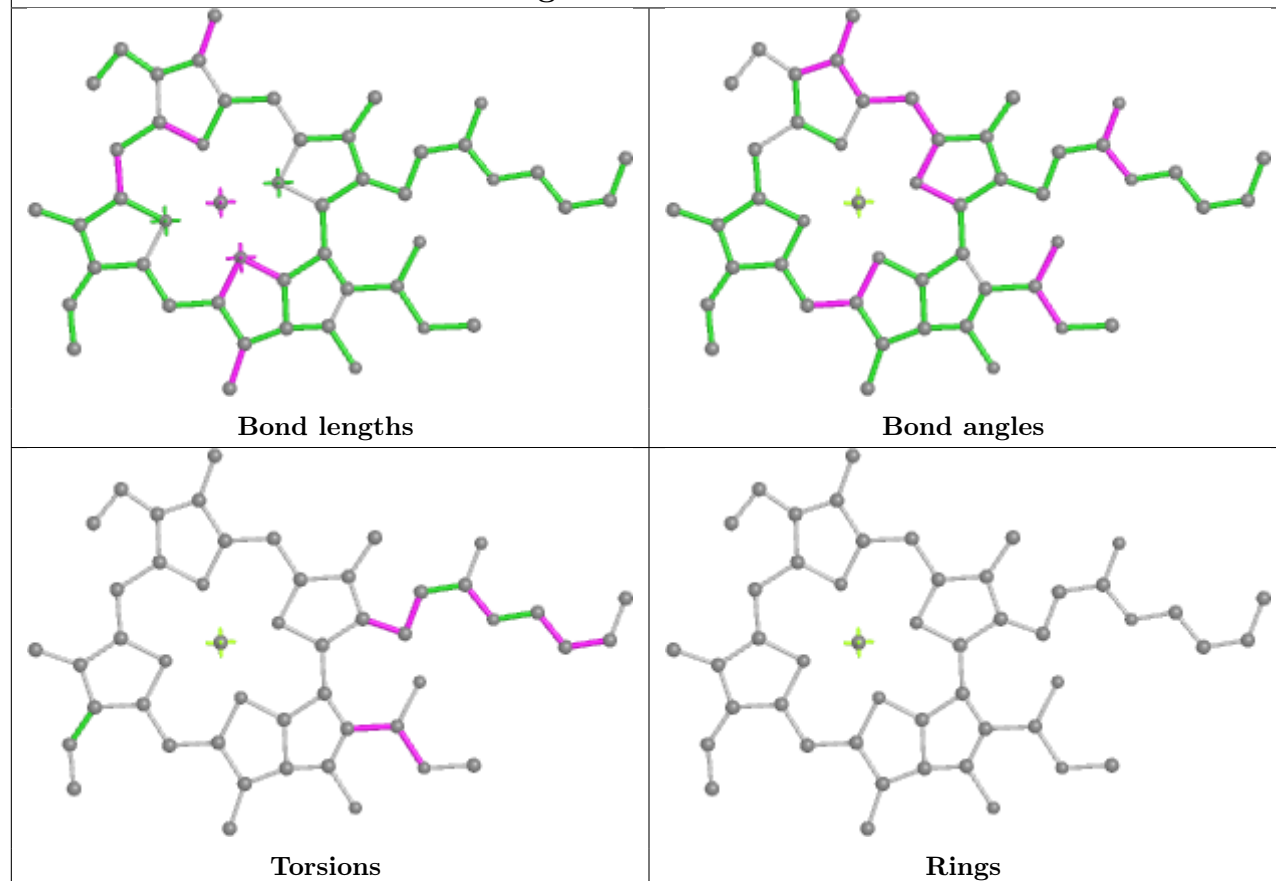


Ligand CHL G 605

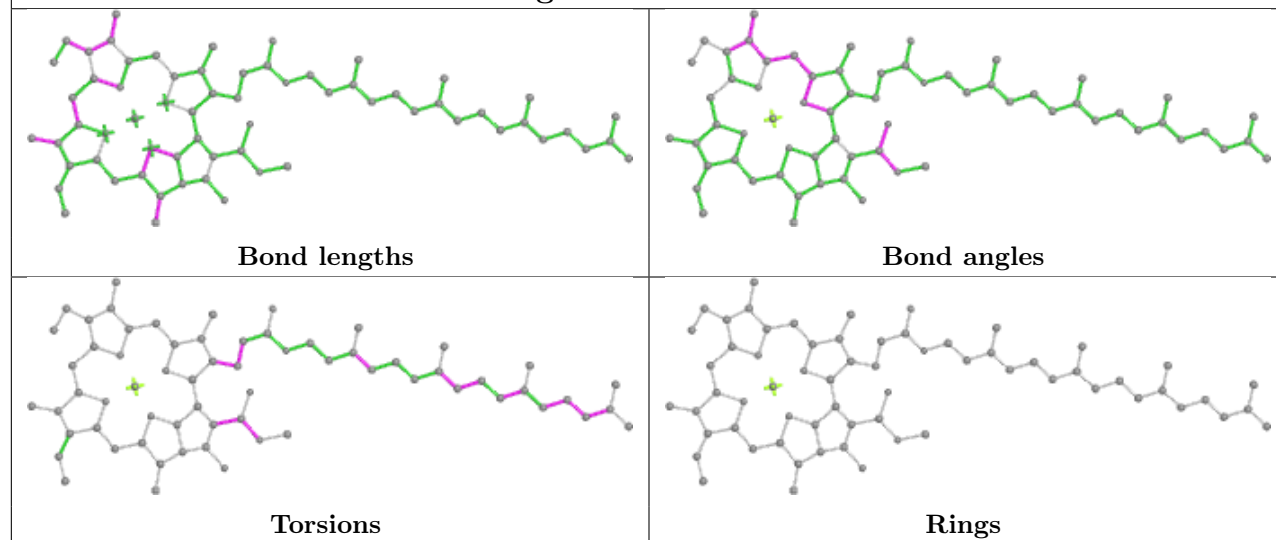




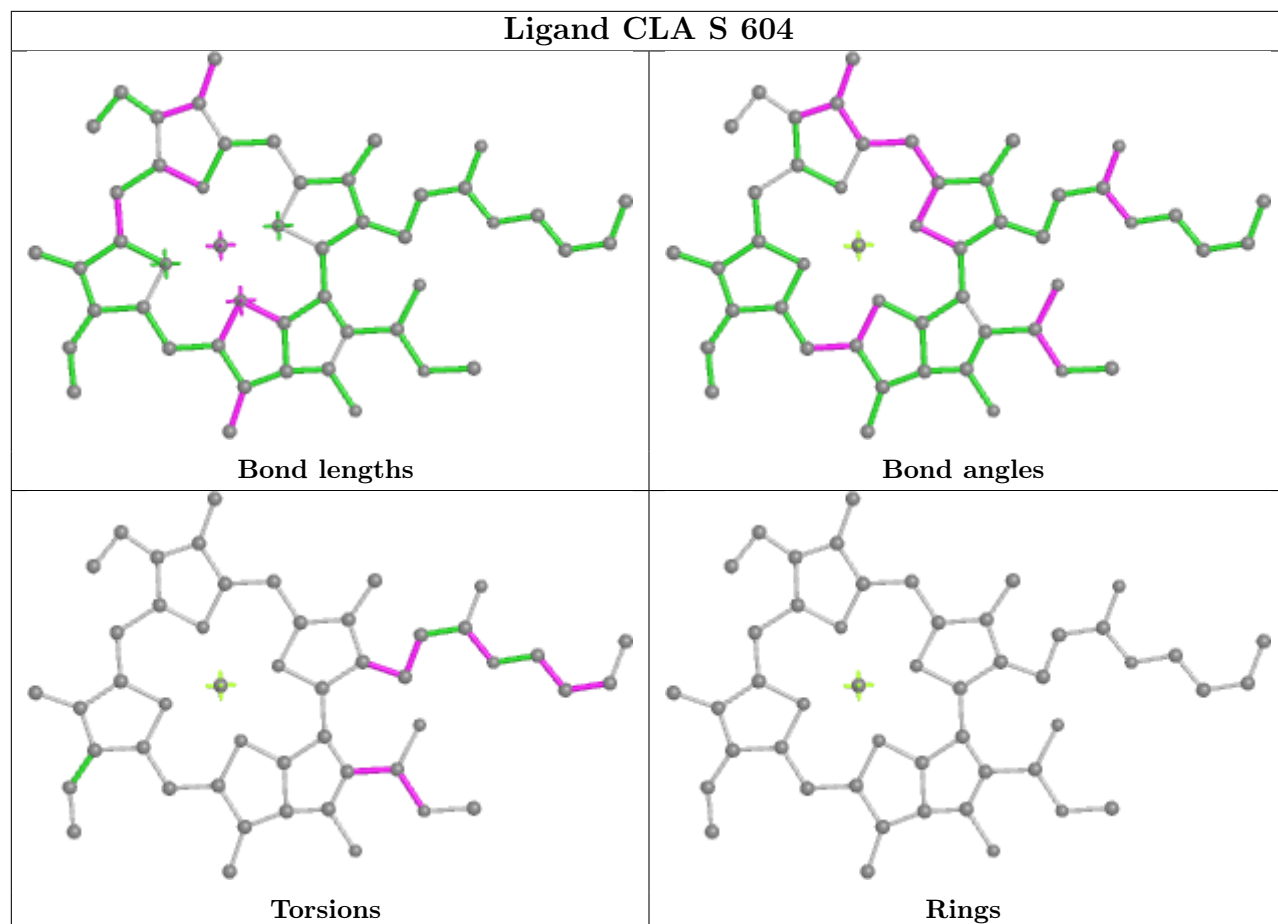
Ligand CLA s 604

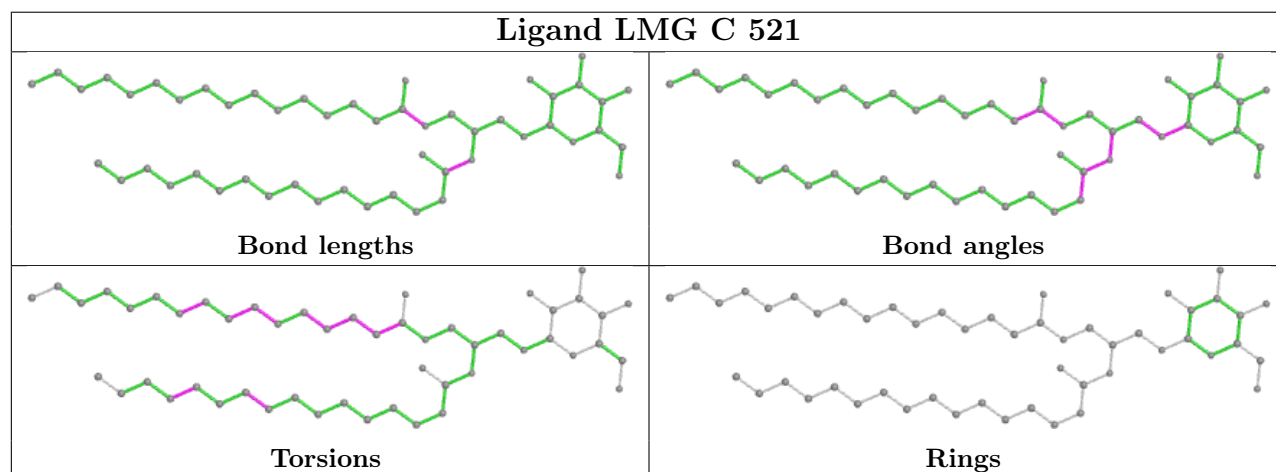
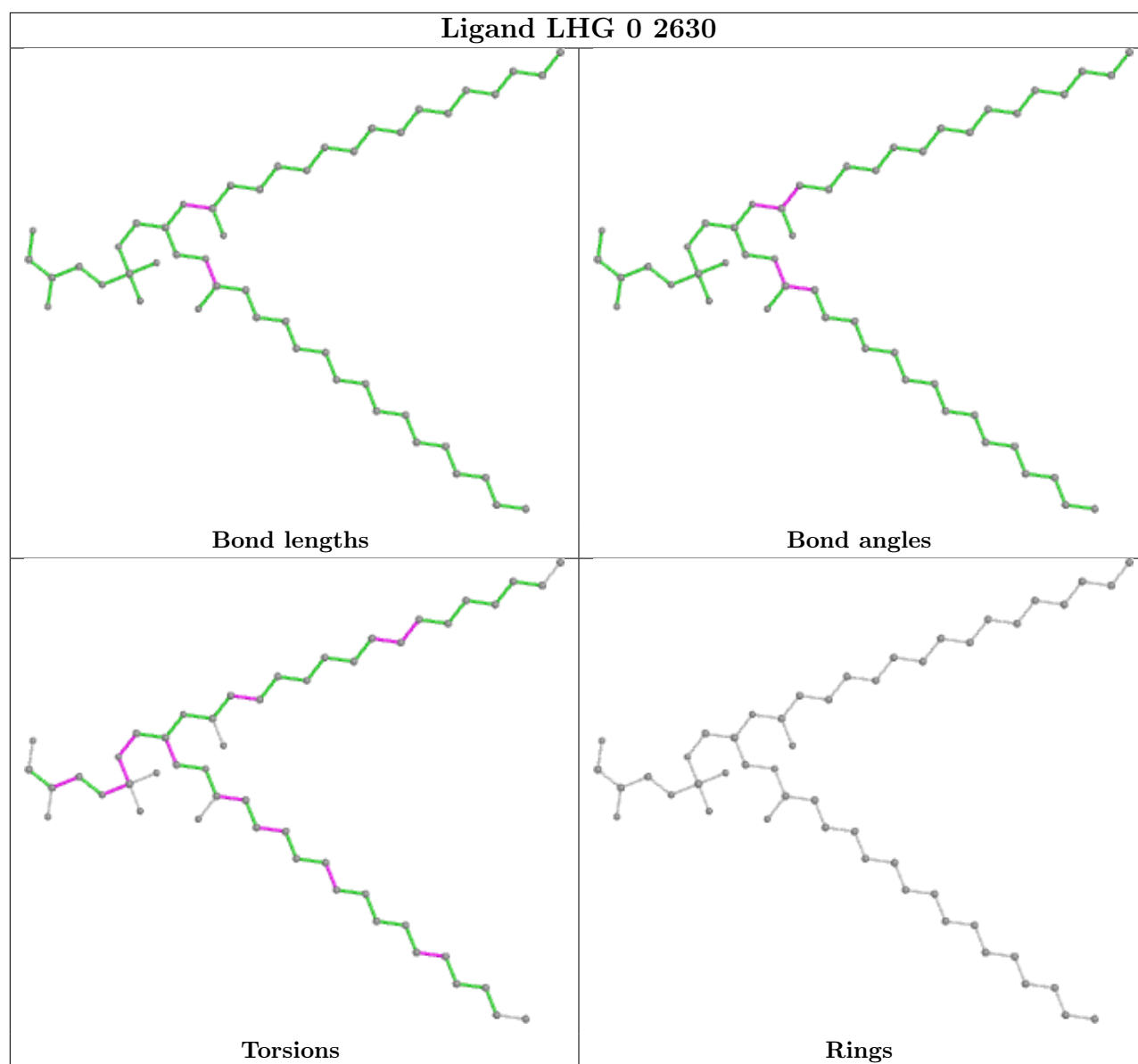


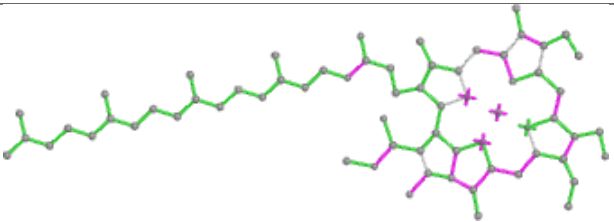
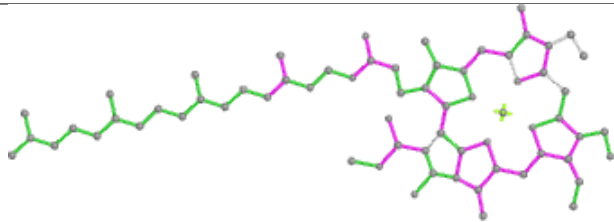
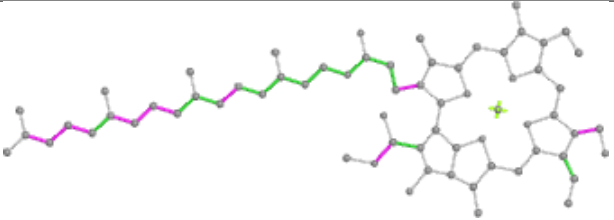
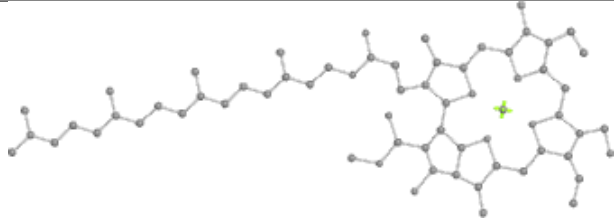
Ligand CLA 6 604

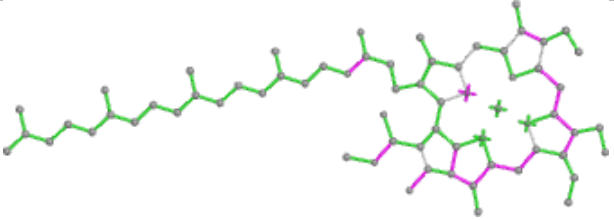
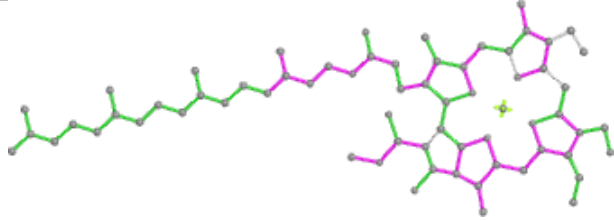
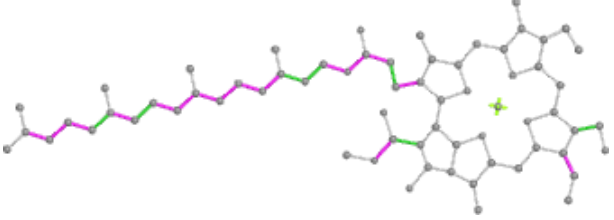
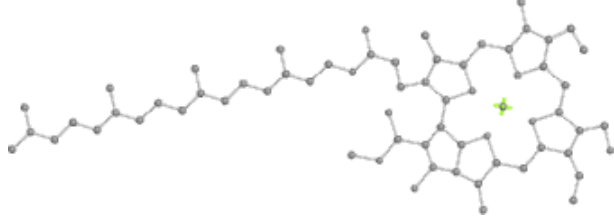


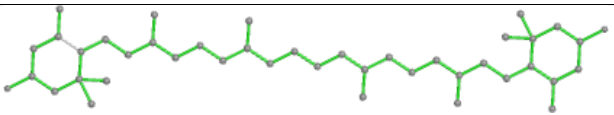
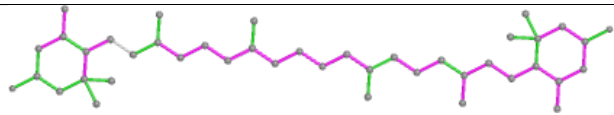
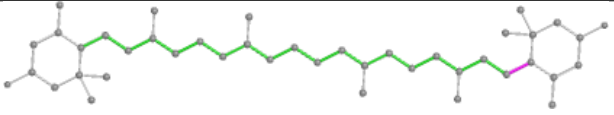
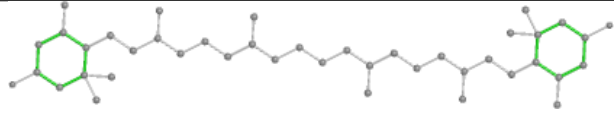
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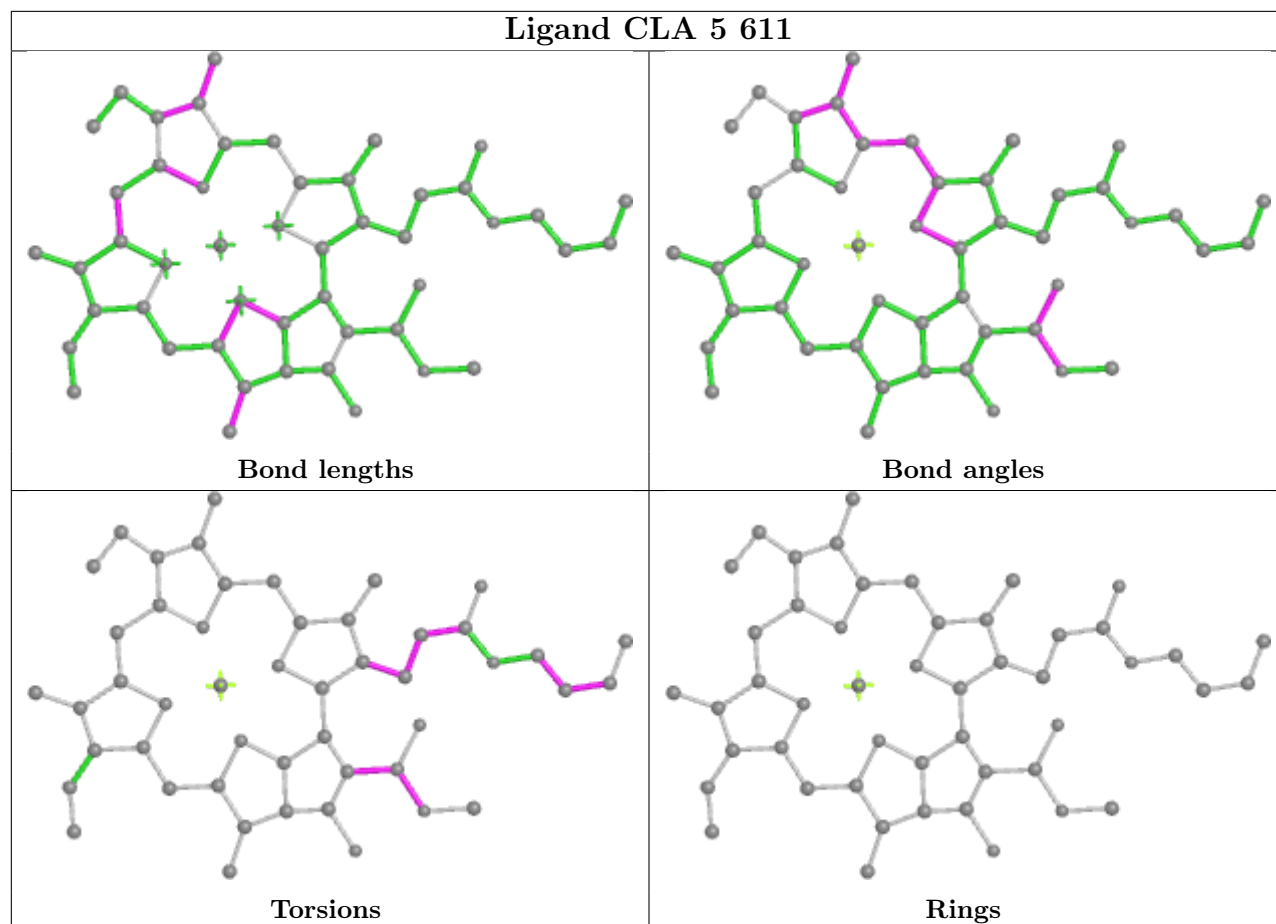


Ligand CHL G 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

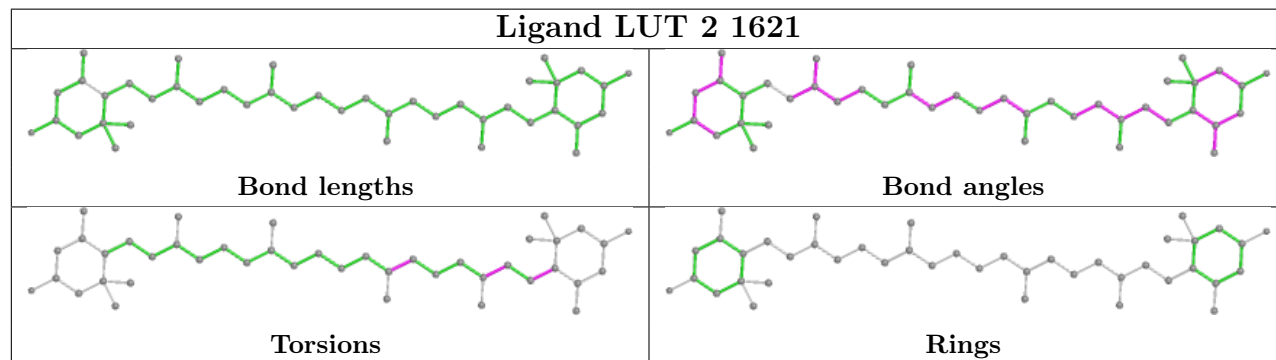
Ligand CHL 3 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

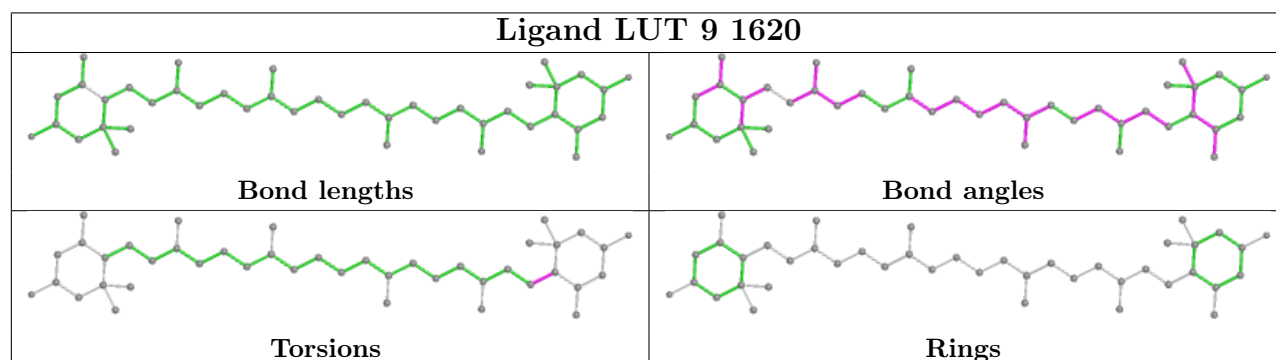
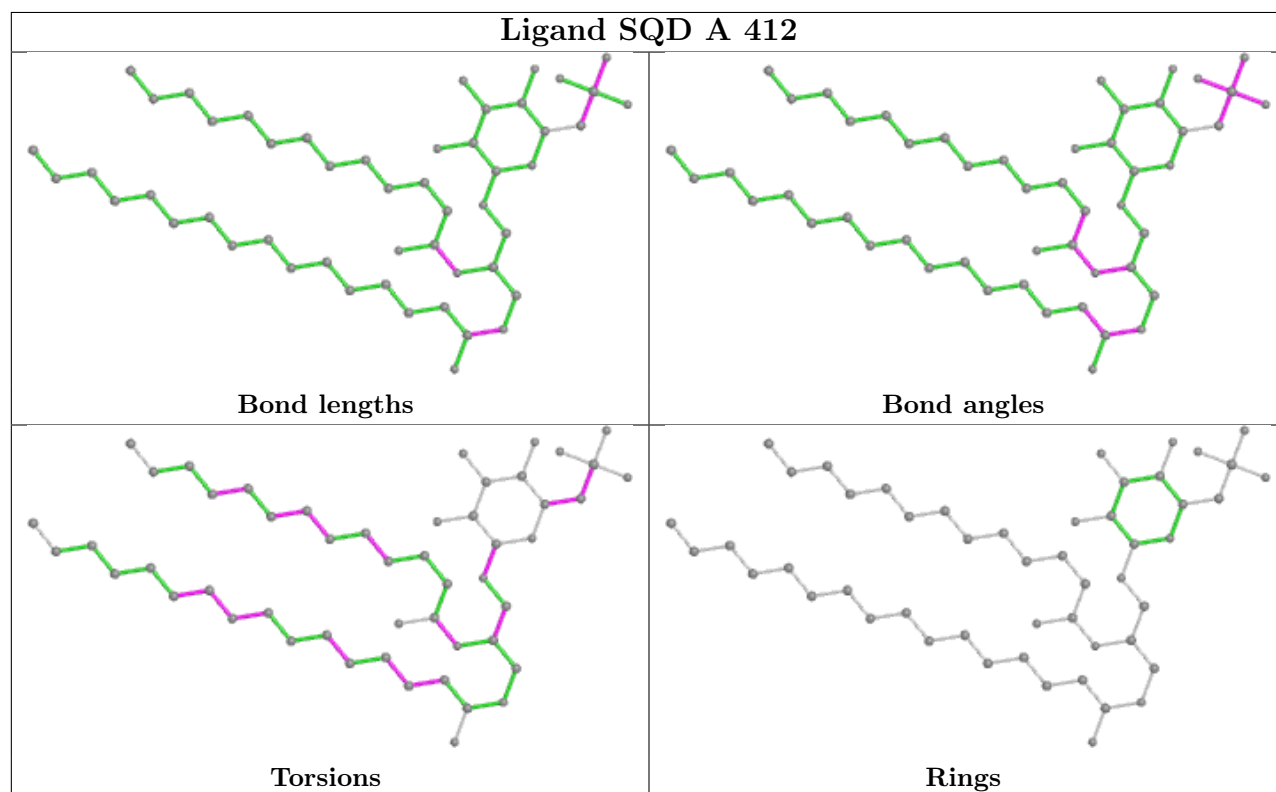
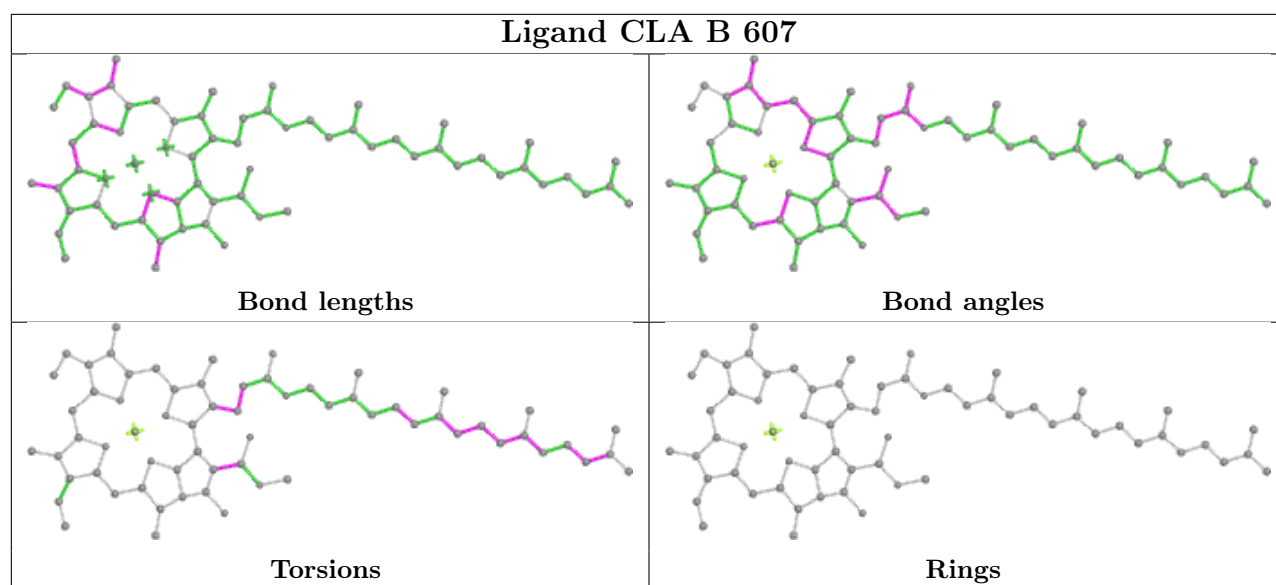
Ligand LUT q 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 611

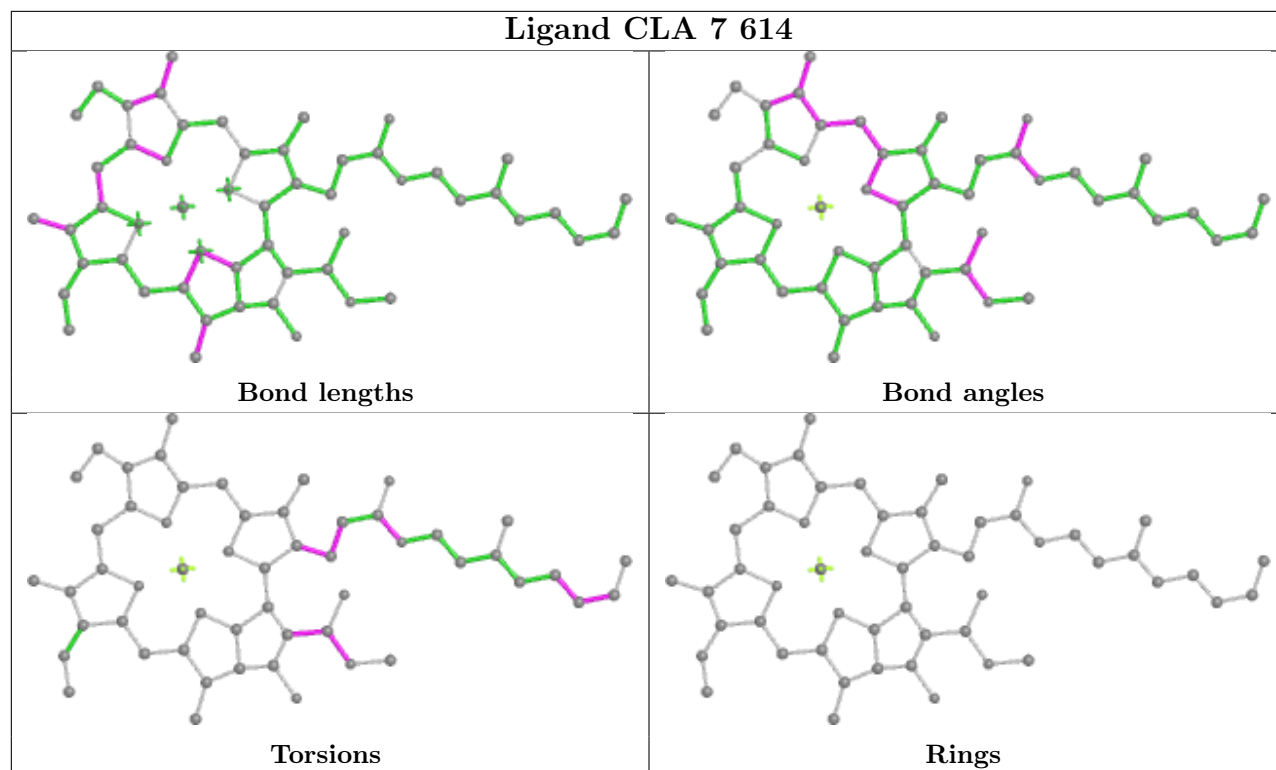


Ligand LUT 2 1621

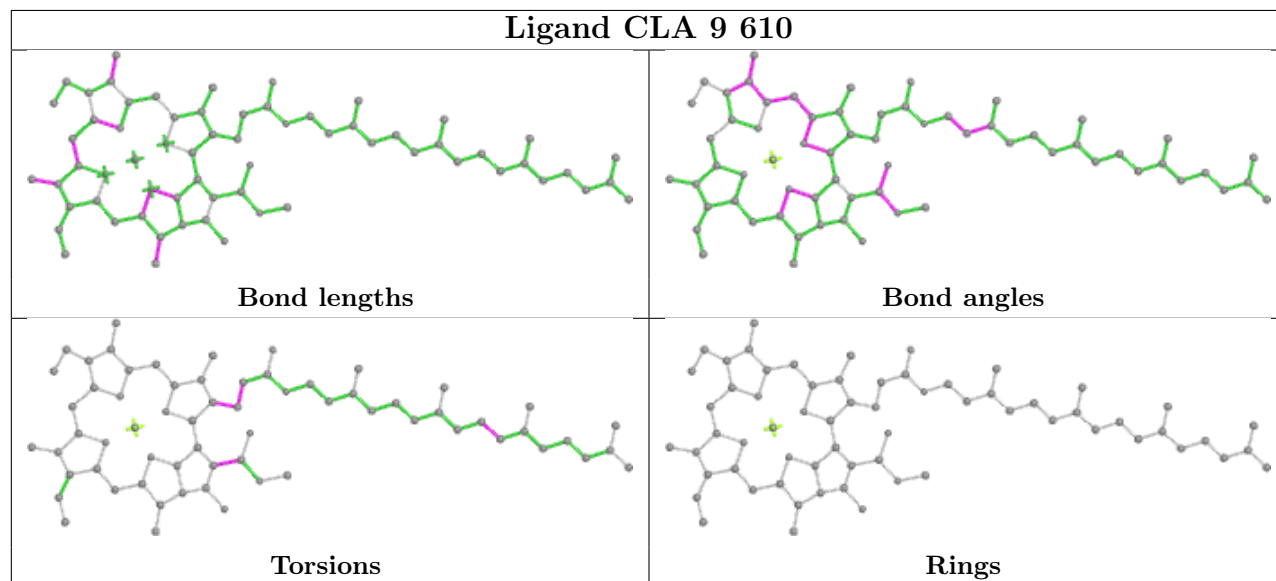




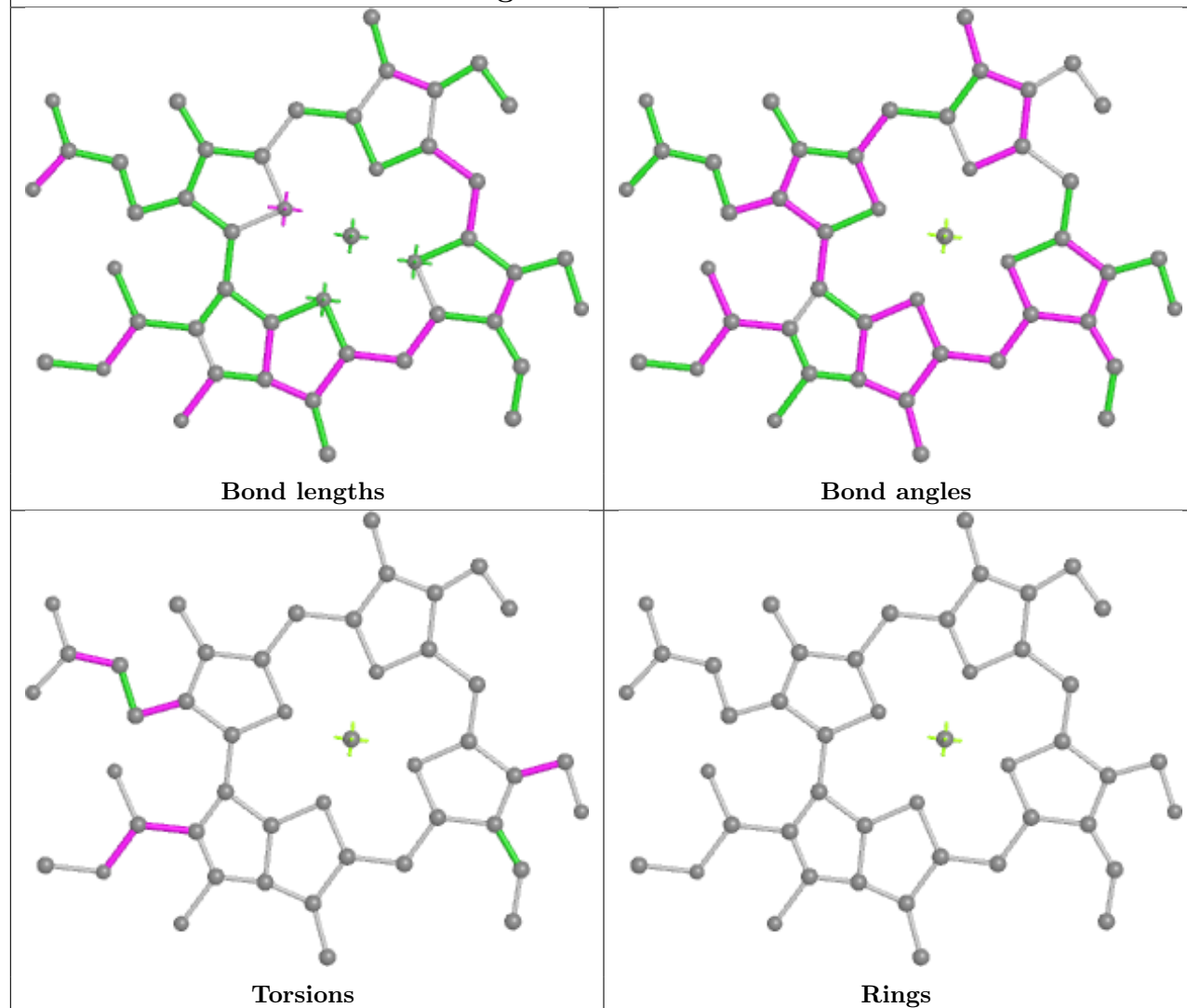
Ligand CLA 7 614

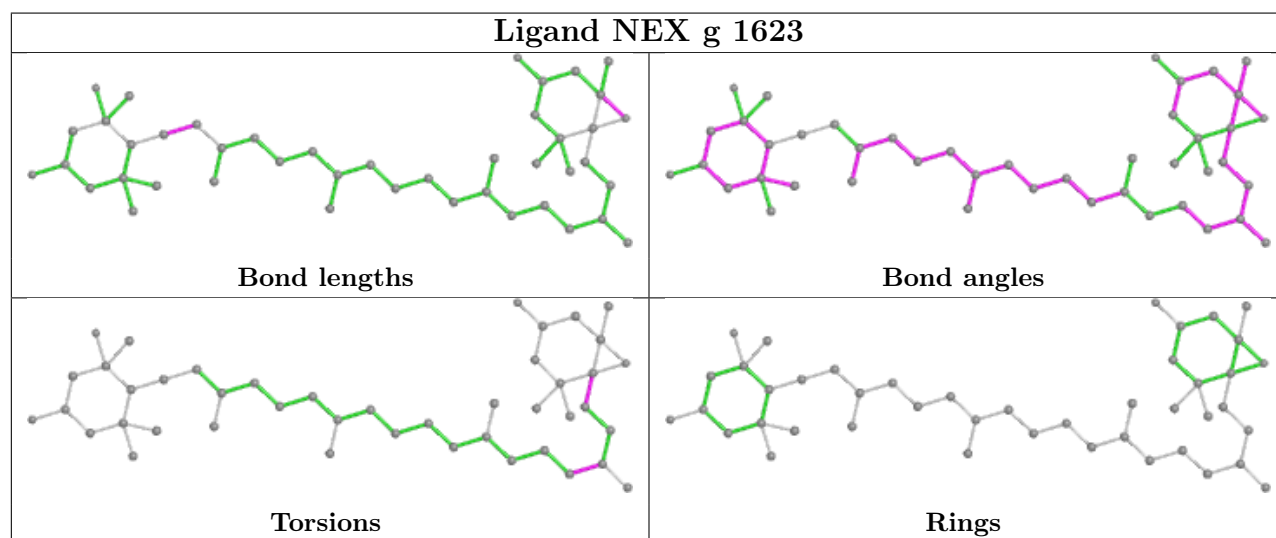
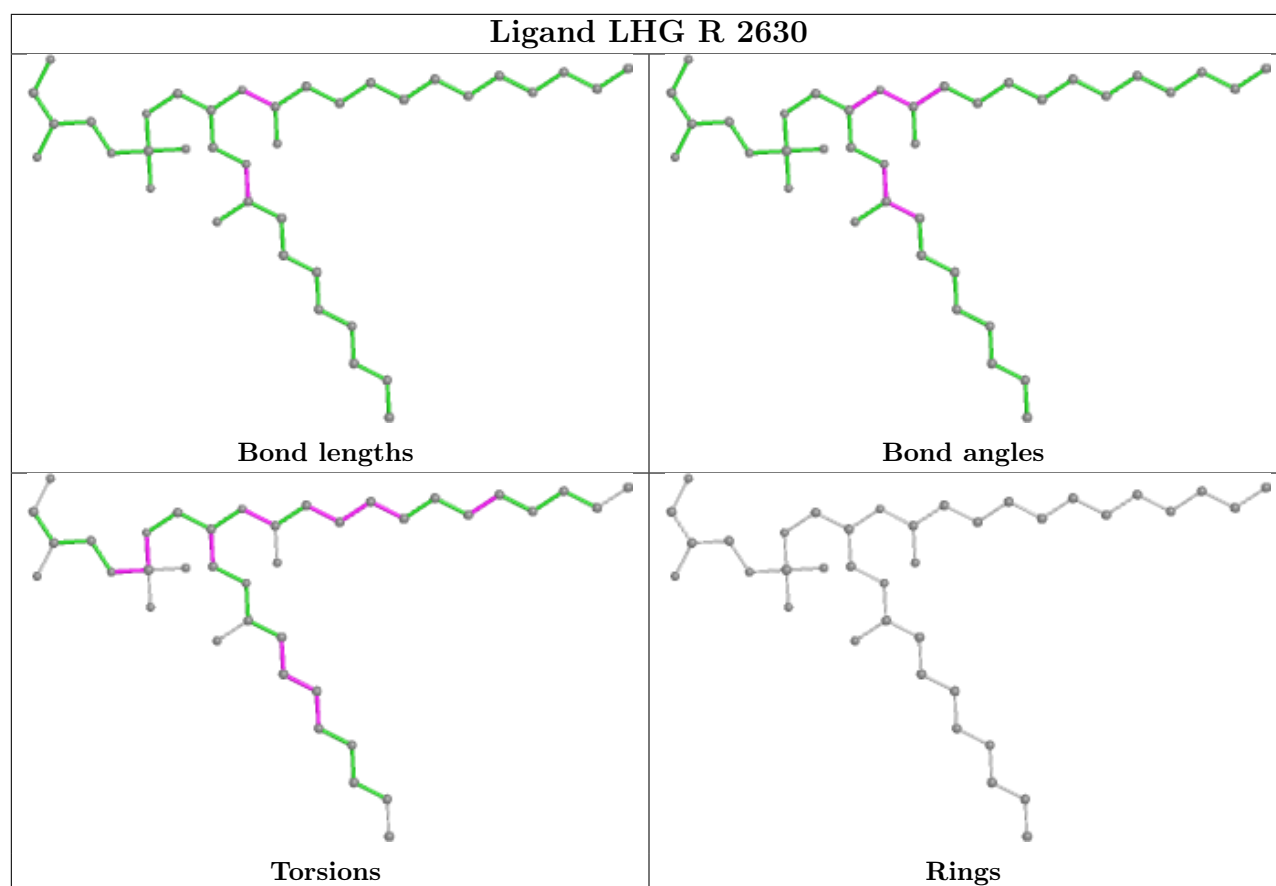


Ligand CLA 9 610

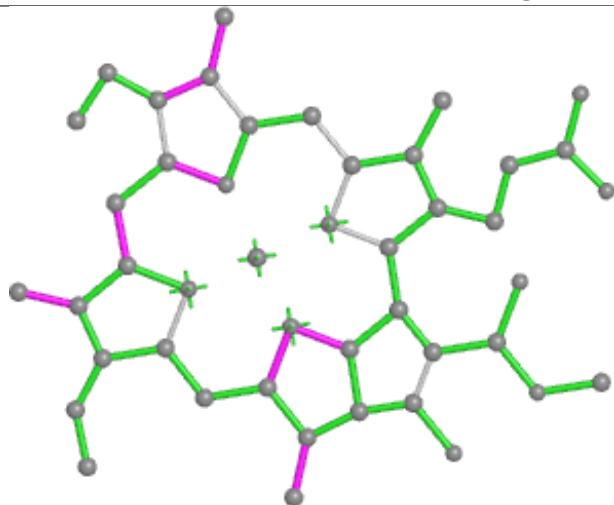


Ligand CHL n 606

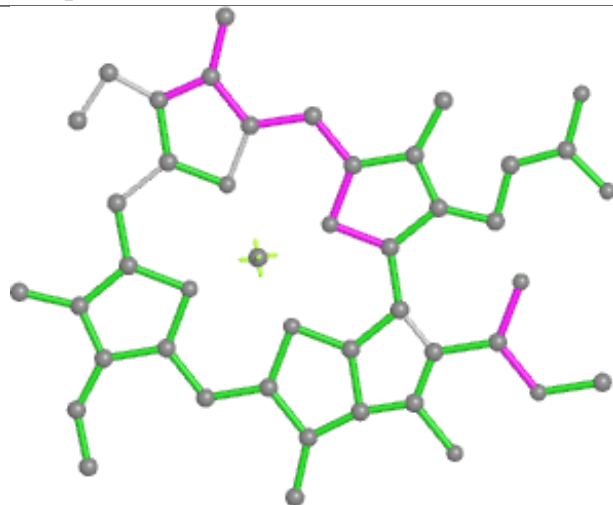




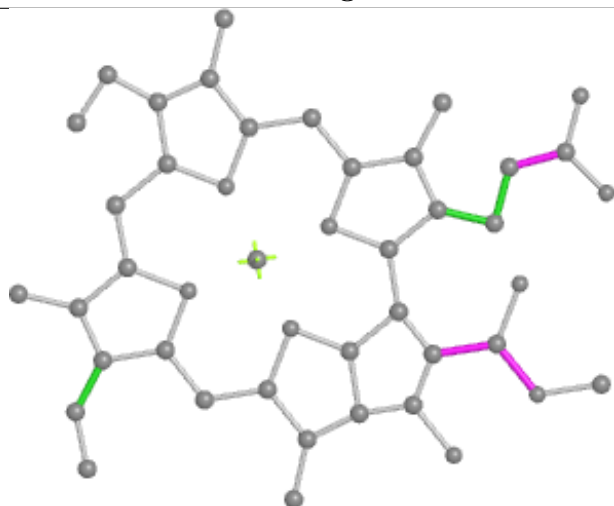
Ligand CLA q 611



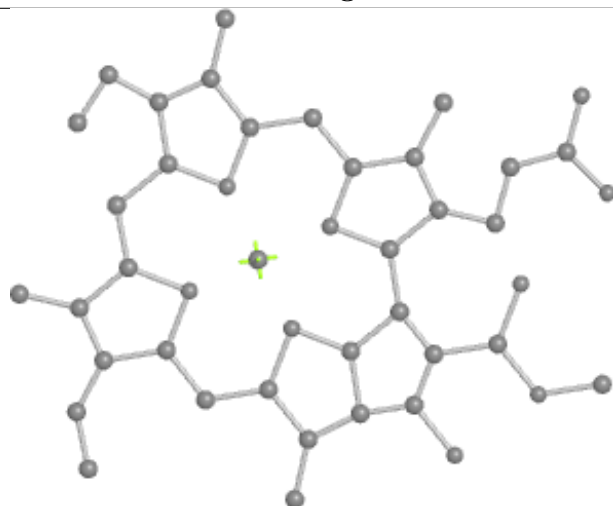
Bond lengths



Bond angles

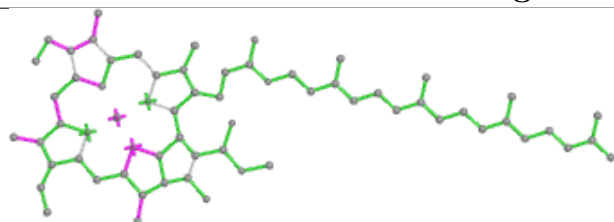


Torsions

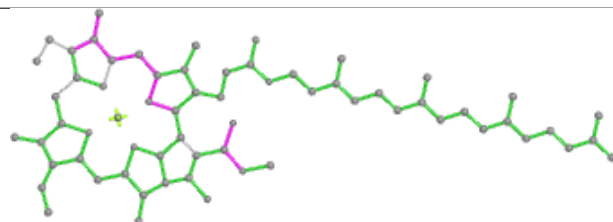


Rings

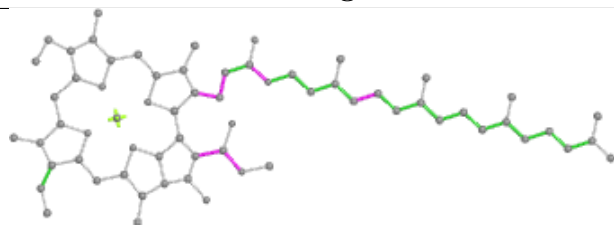
Ligand CLA N 604



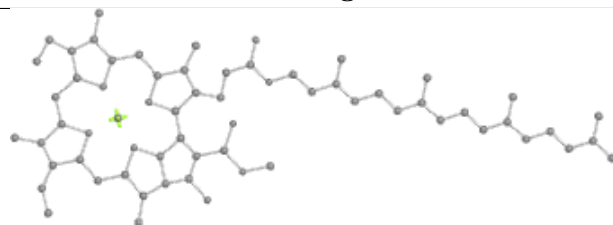
Bond lengths



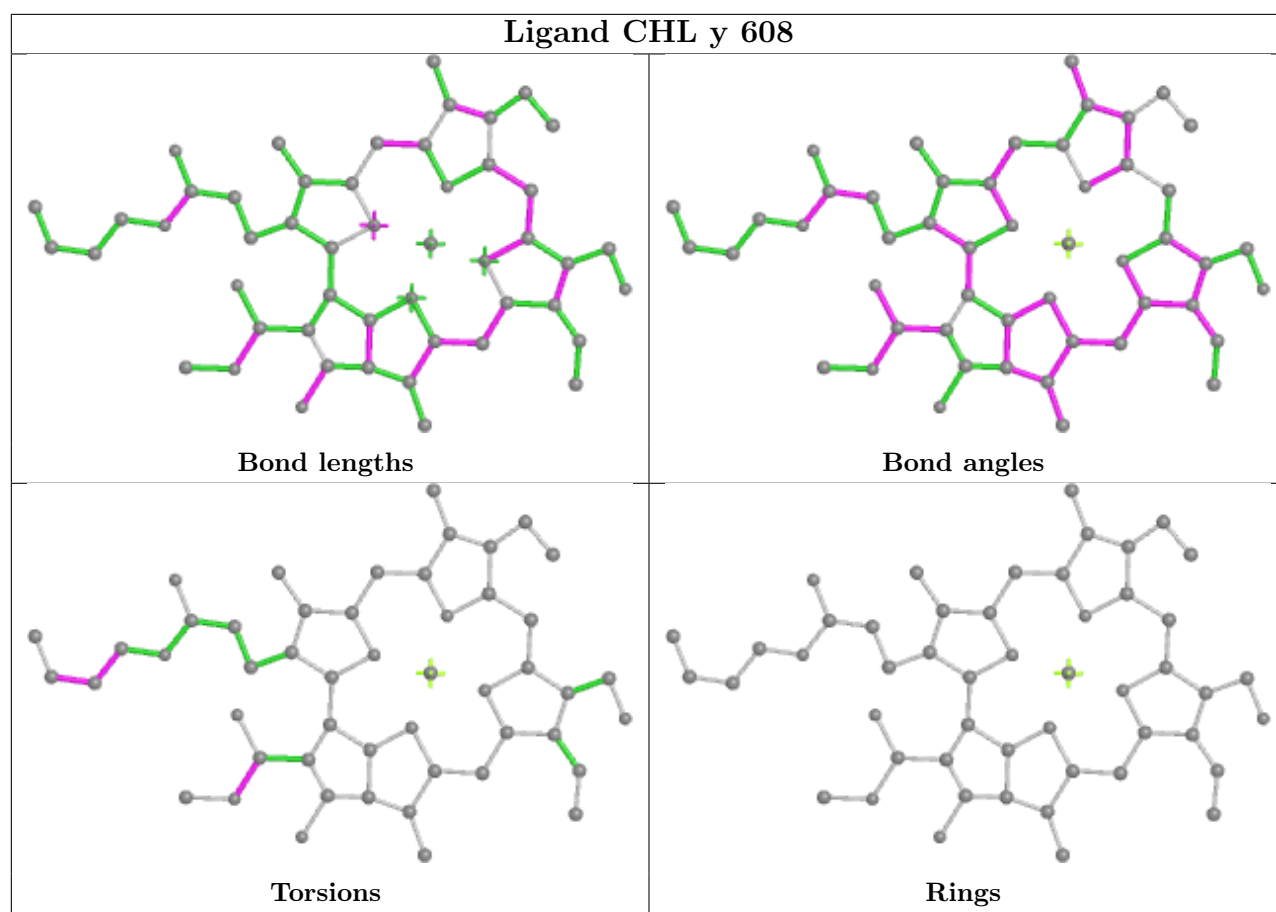
Bond angles

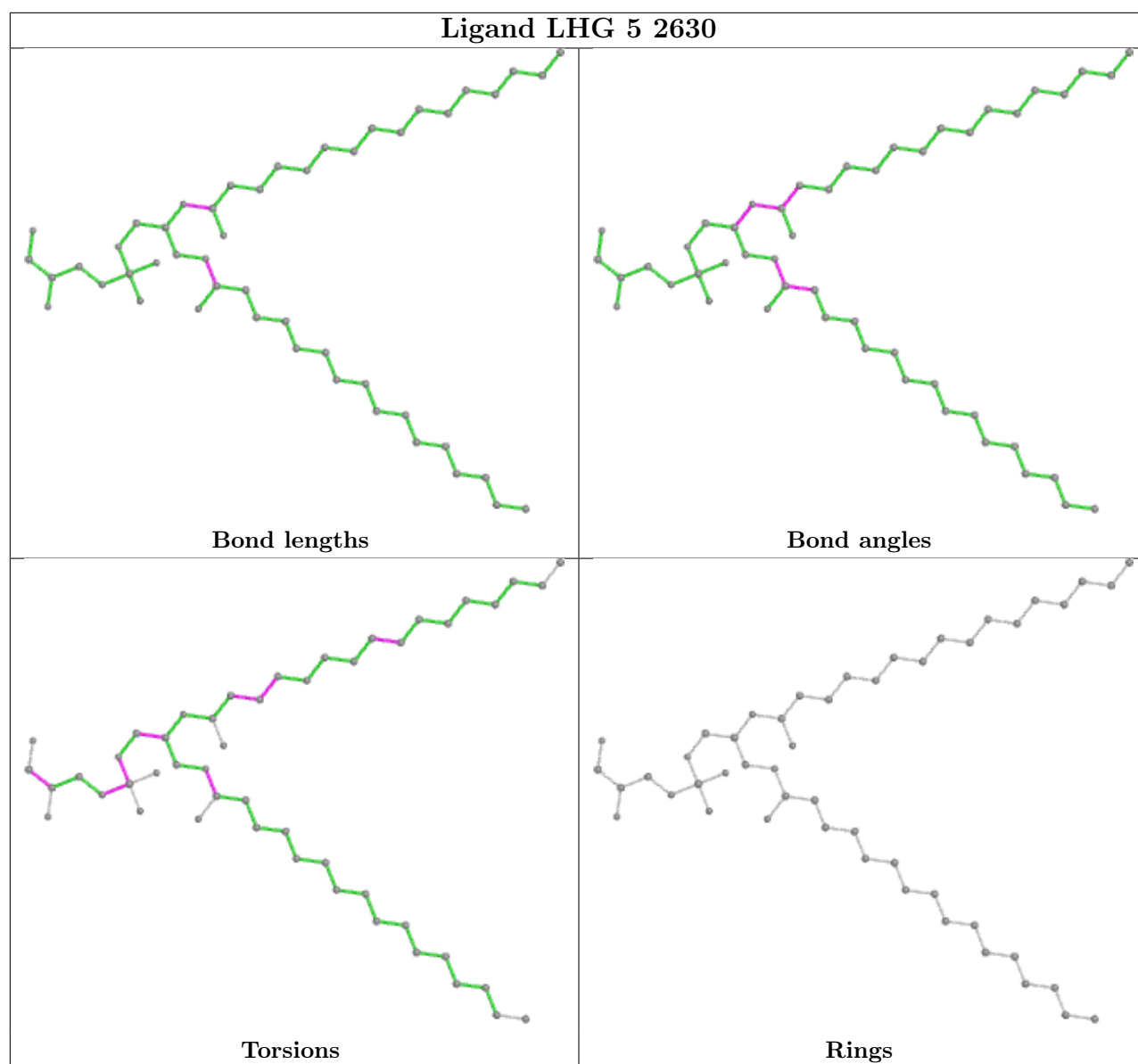


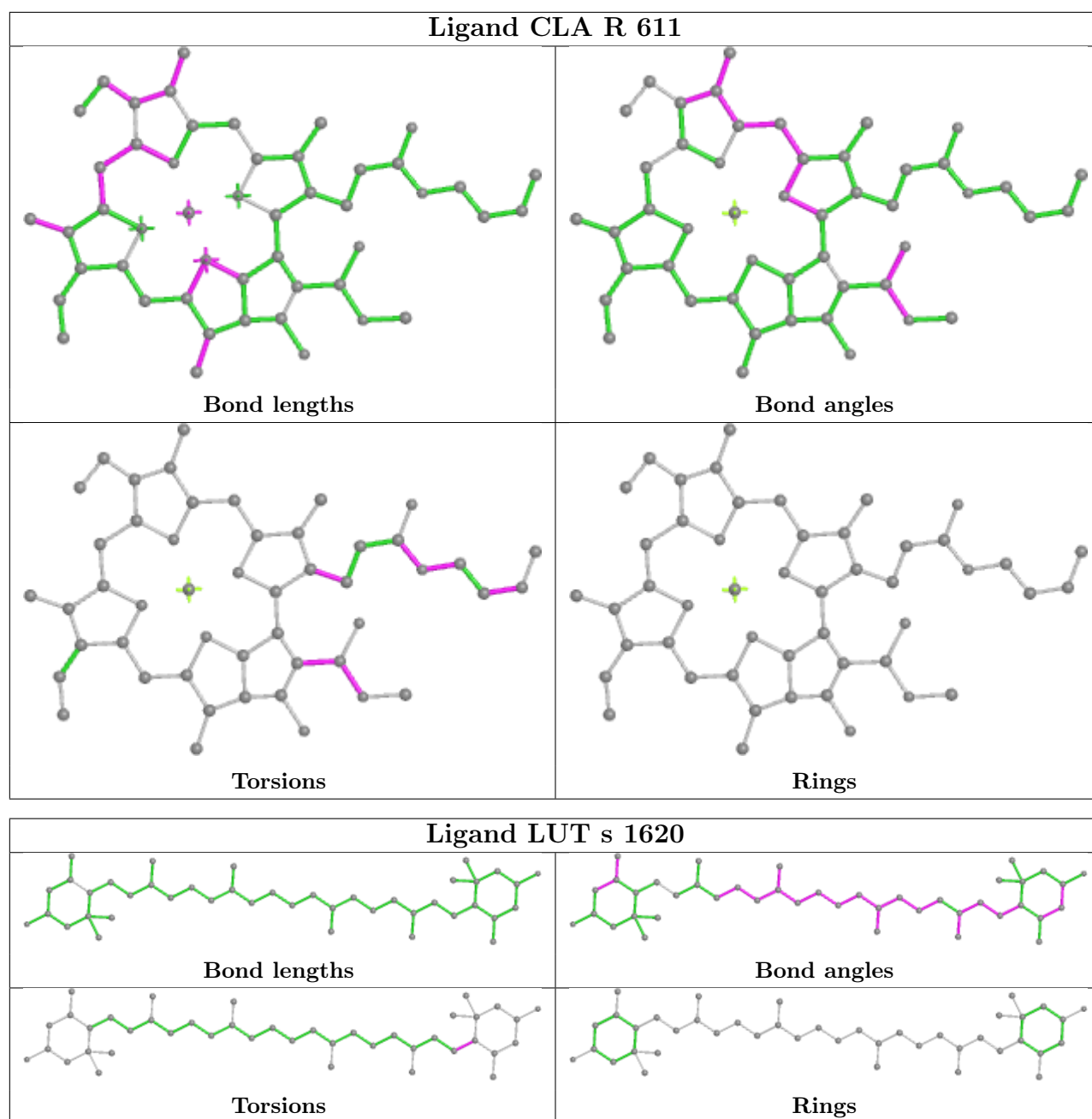
Torsions

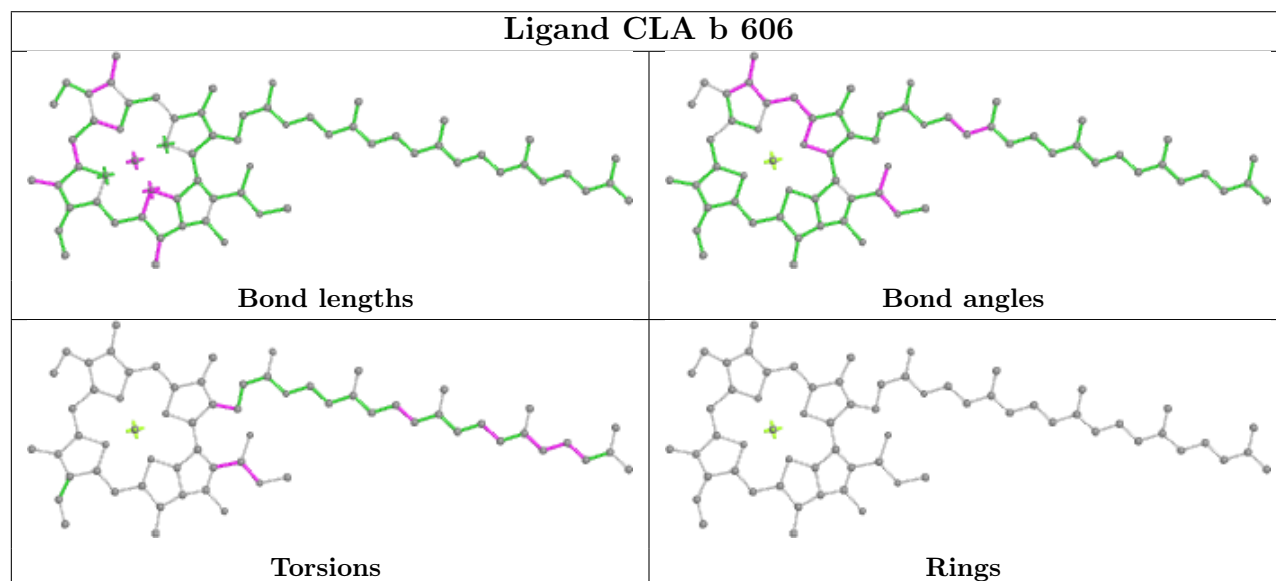
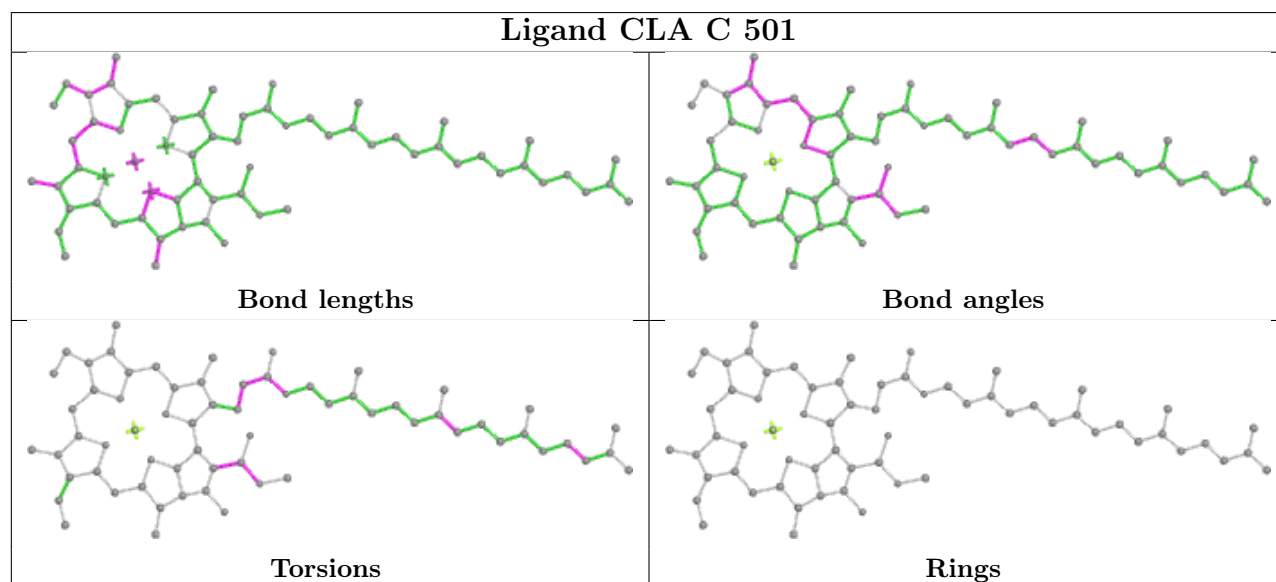
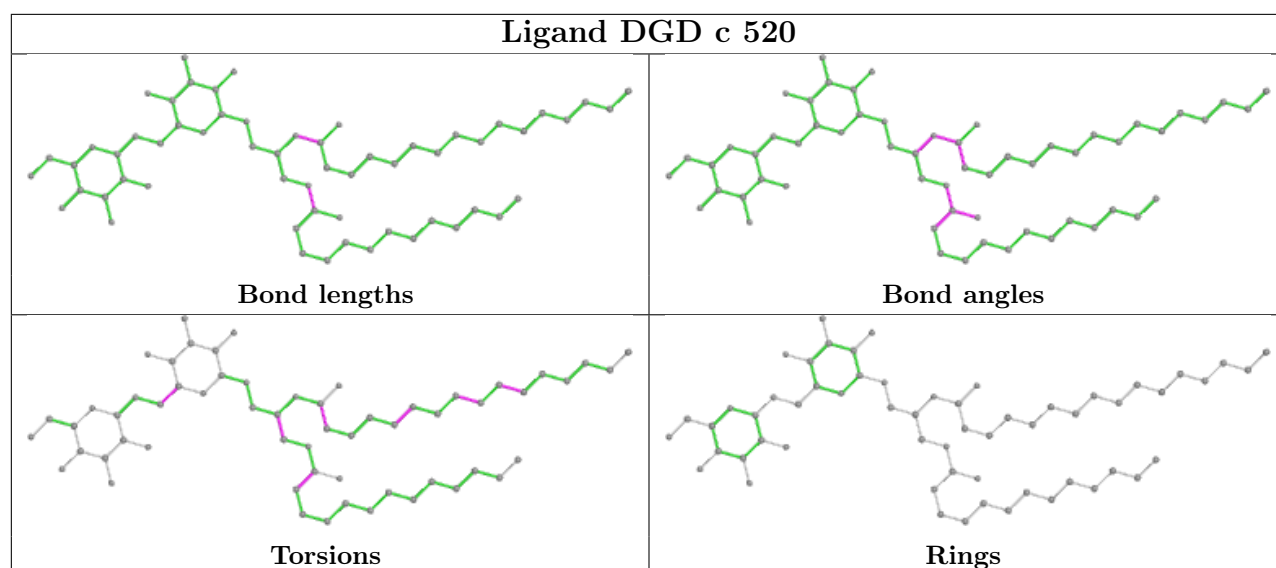


Rings

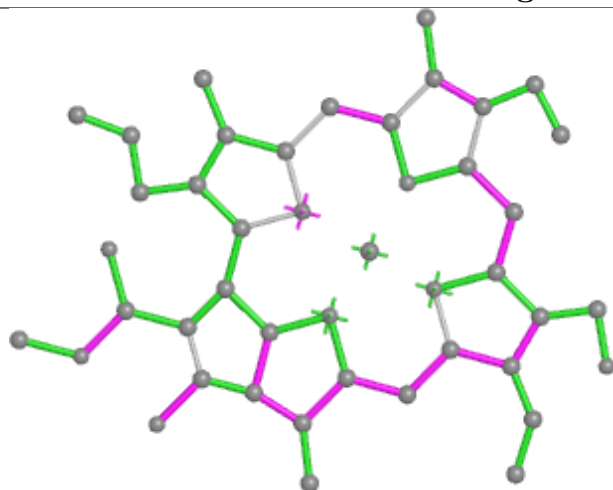




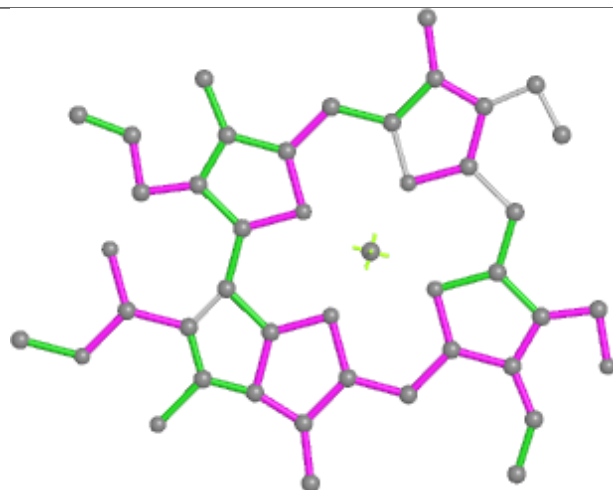




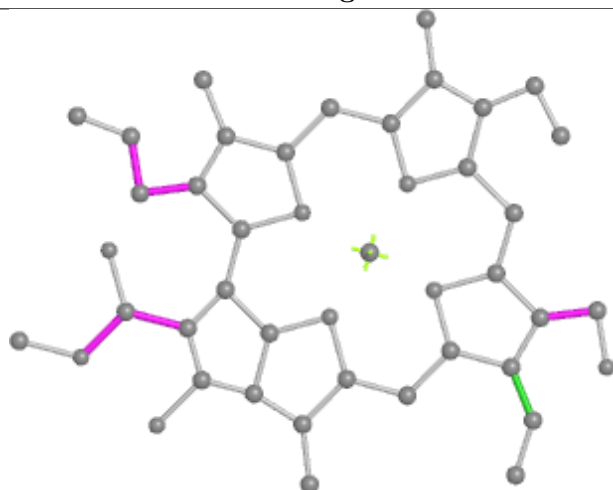
Ligand CHL S 606



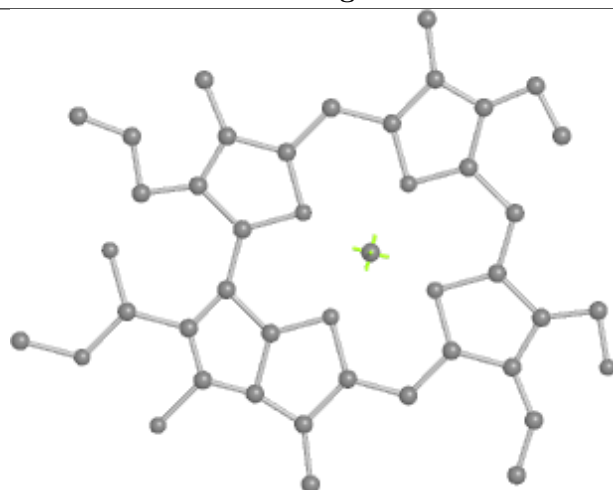
Bond lengths



Bond angles

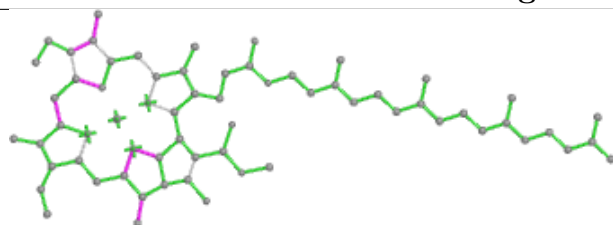


Torsions

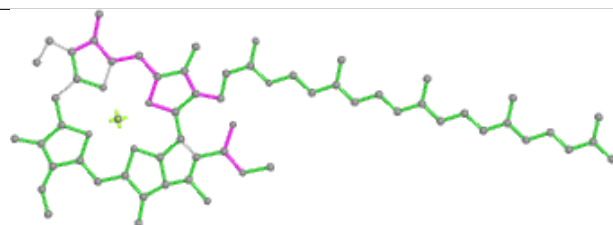


Rings

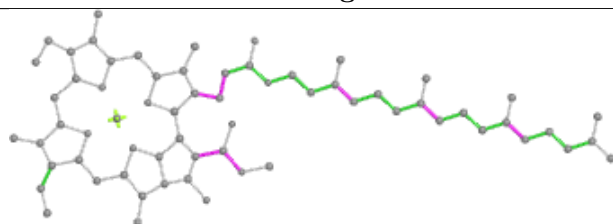
Ligand CLA 5 603



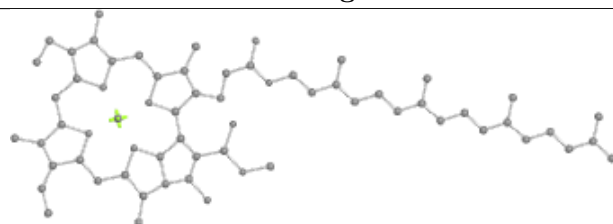
Bond lengths



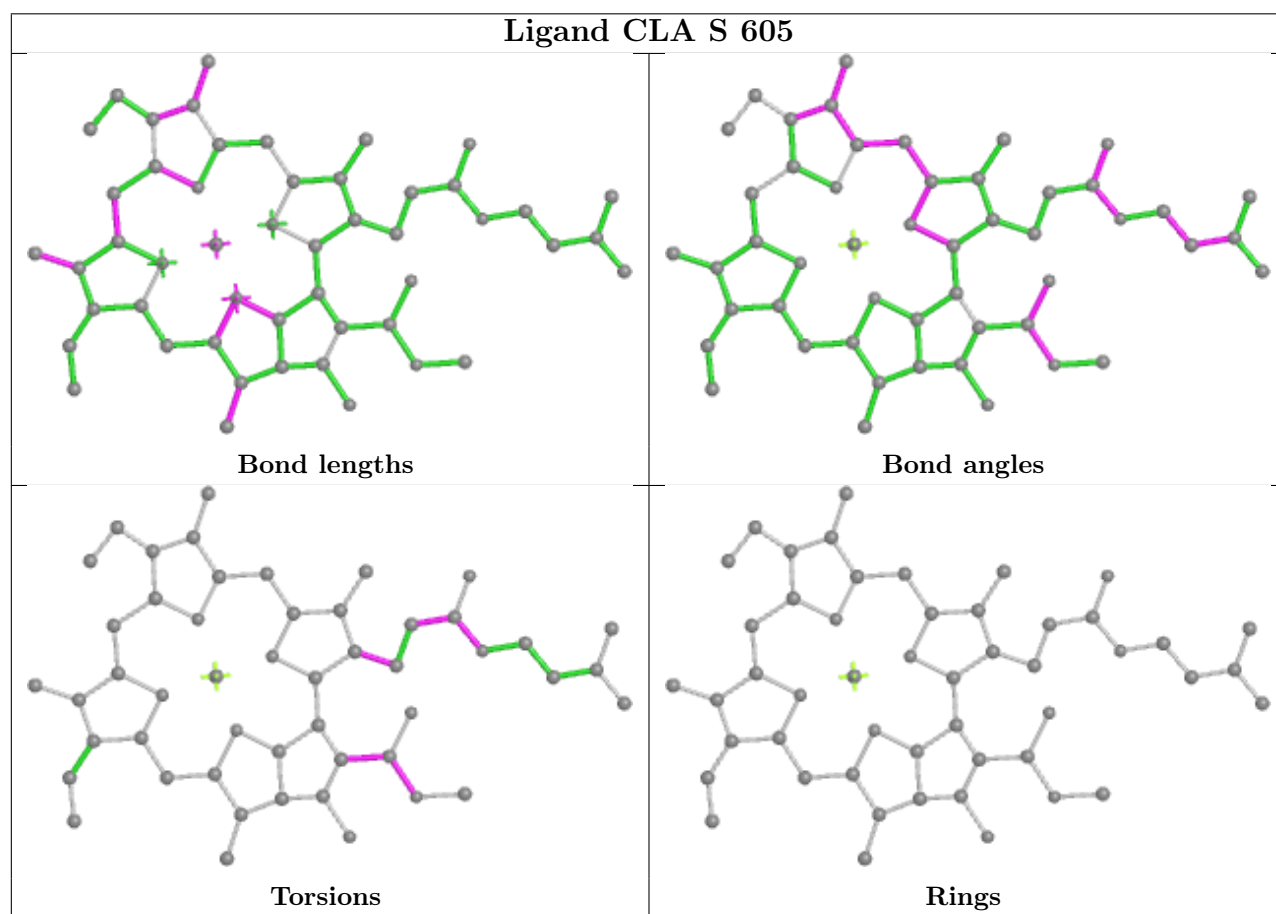
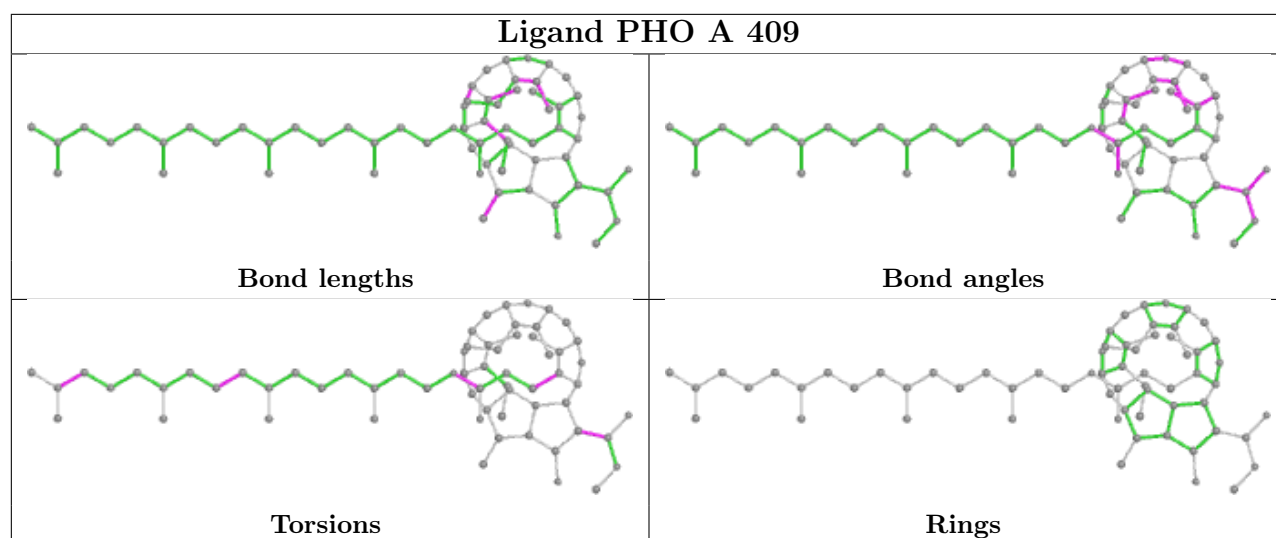
Bond angles

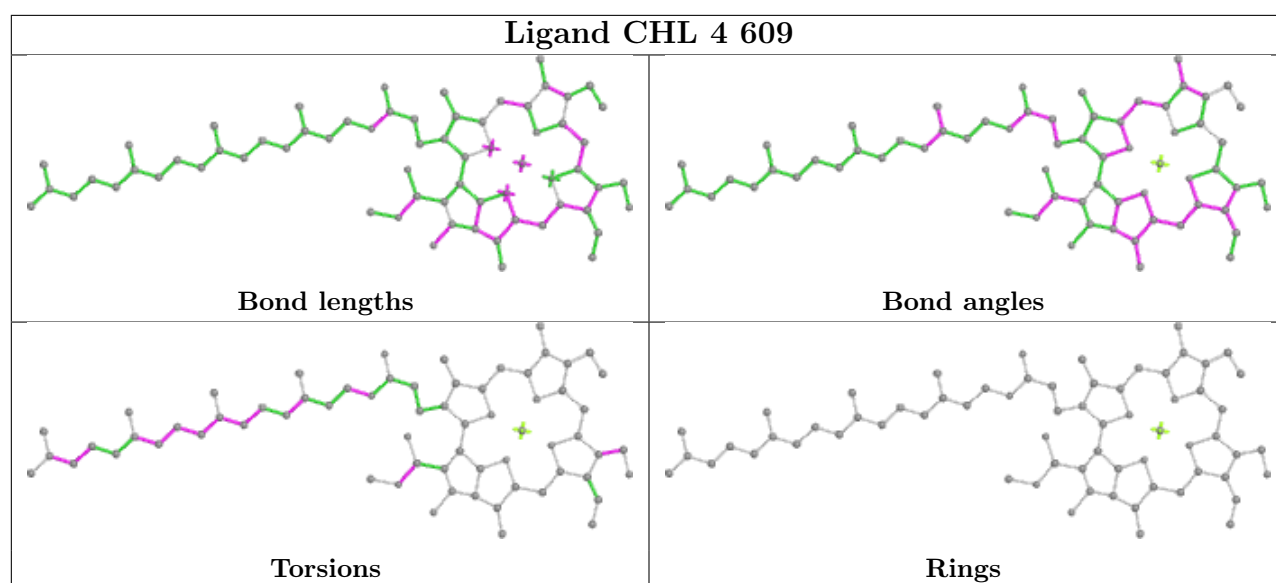
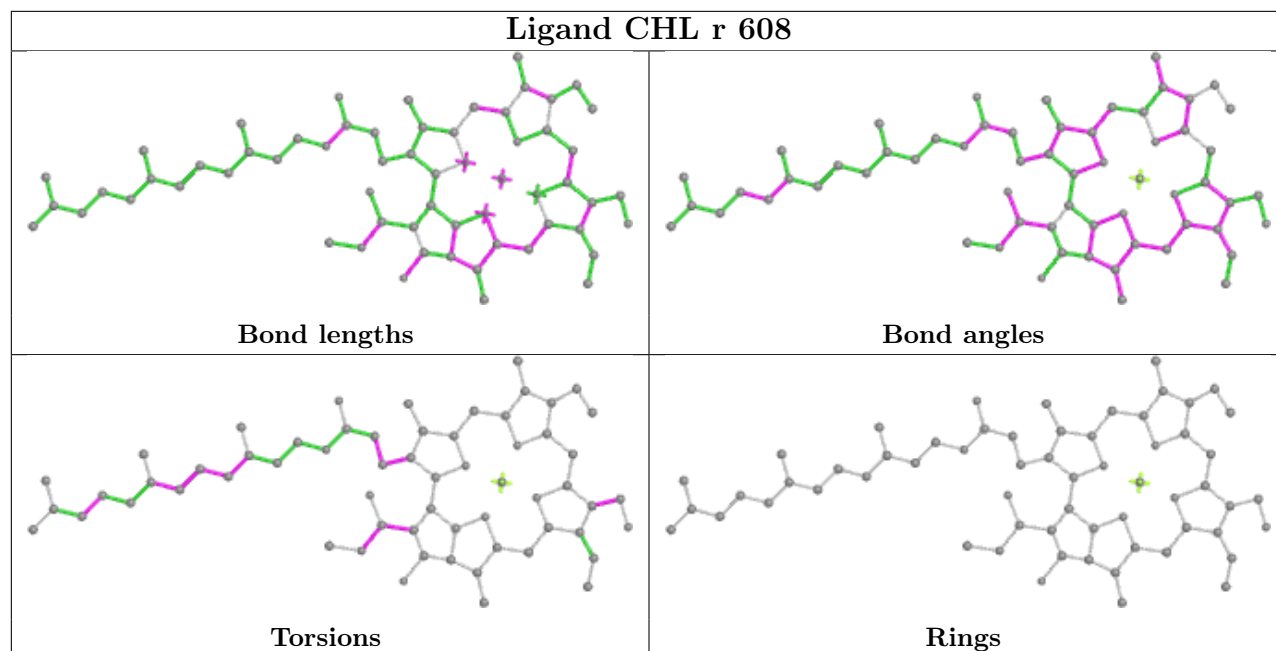
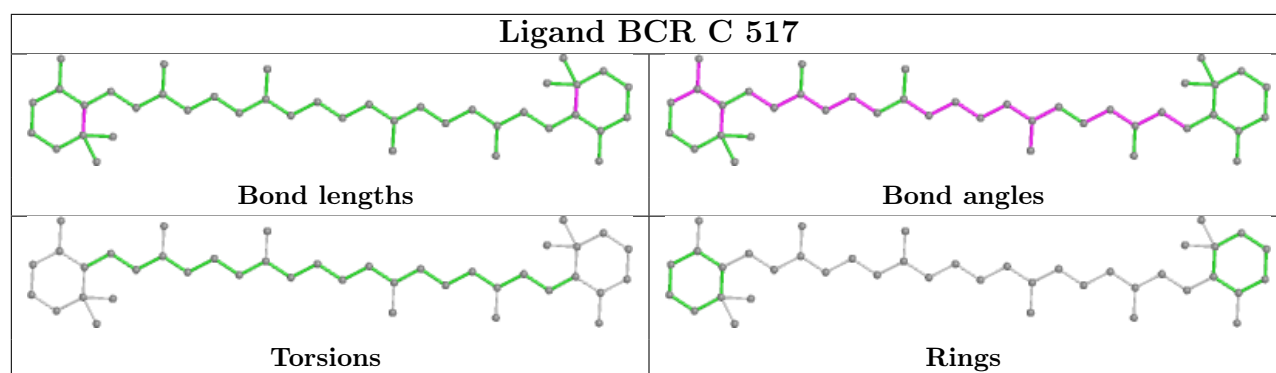


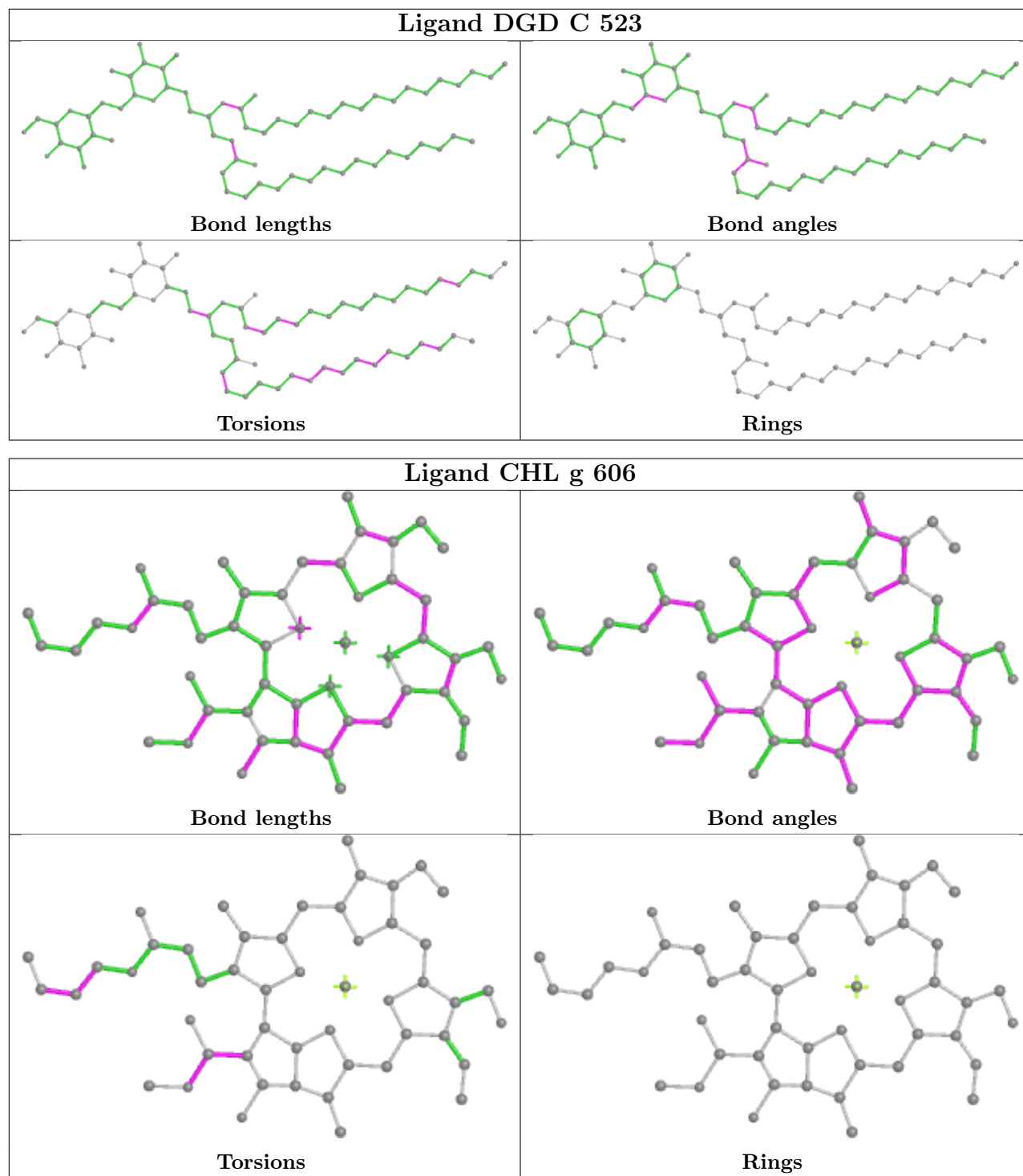
Torsions

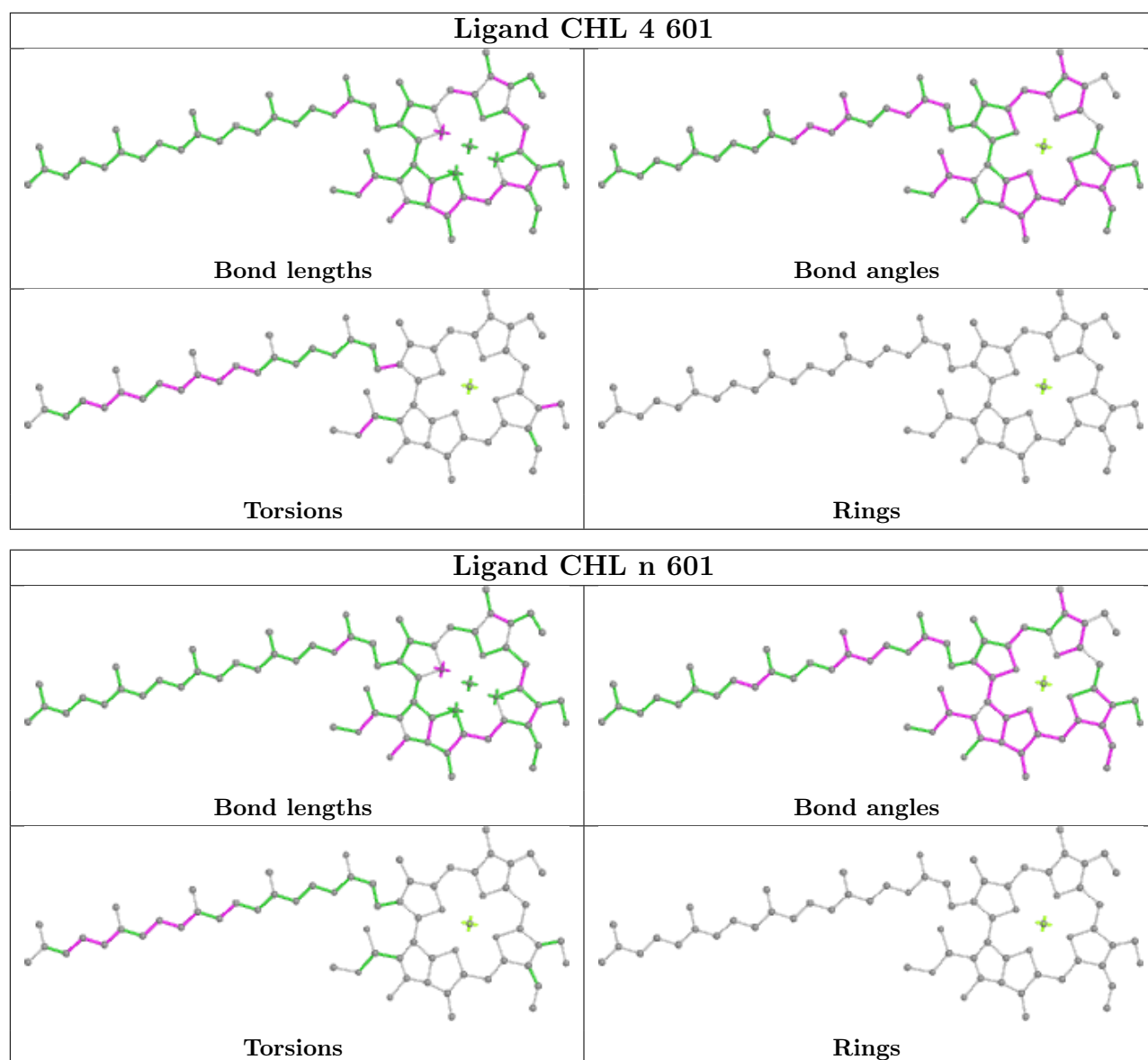


Rings

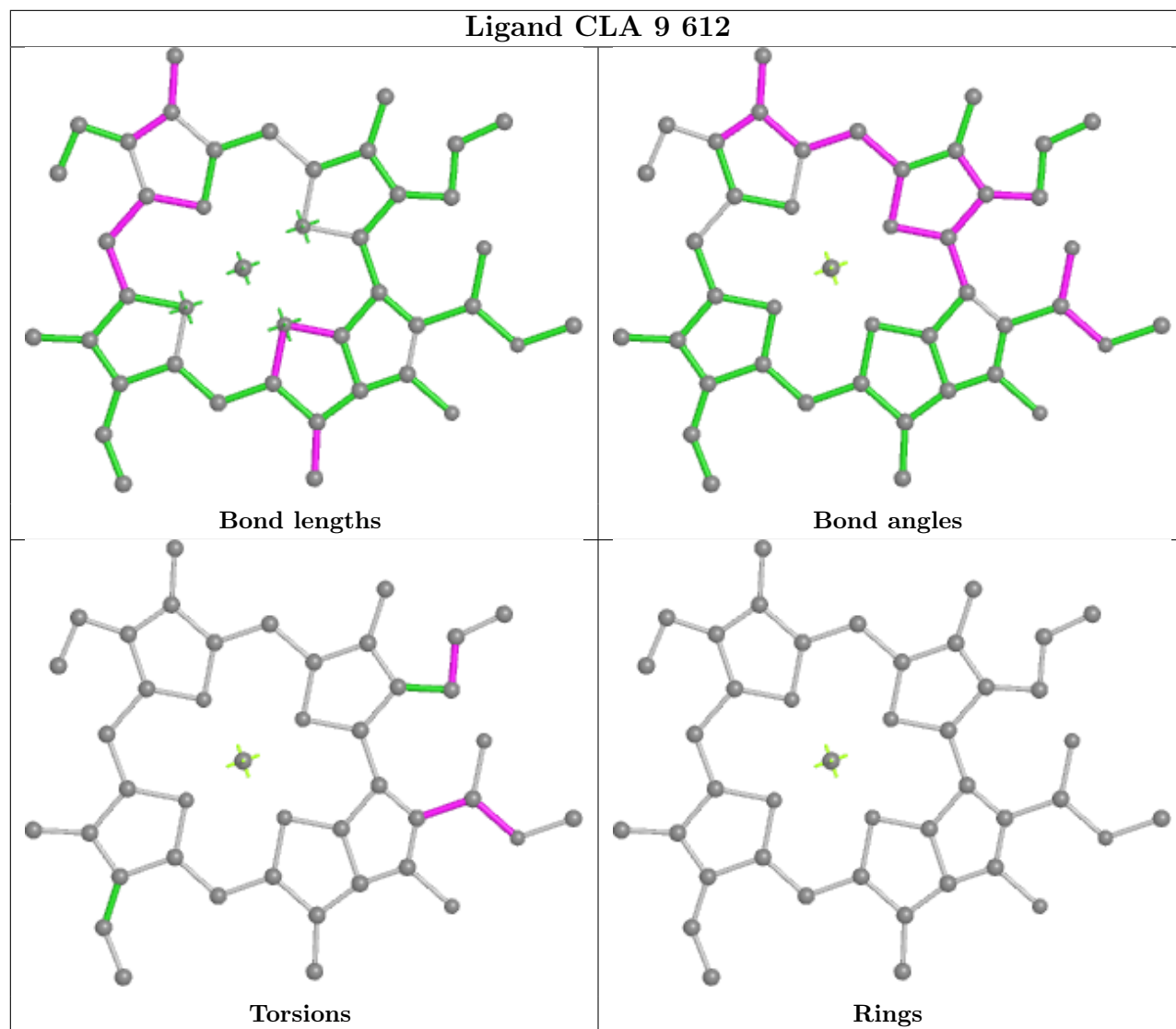




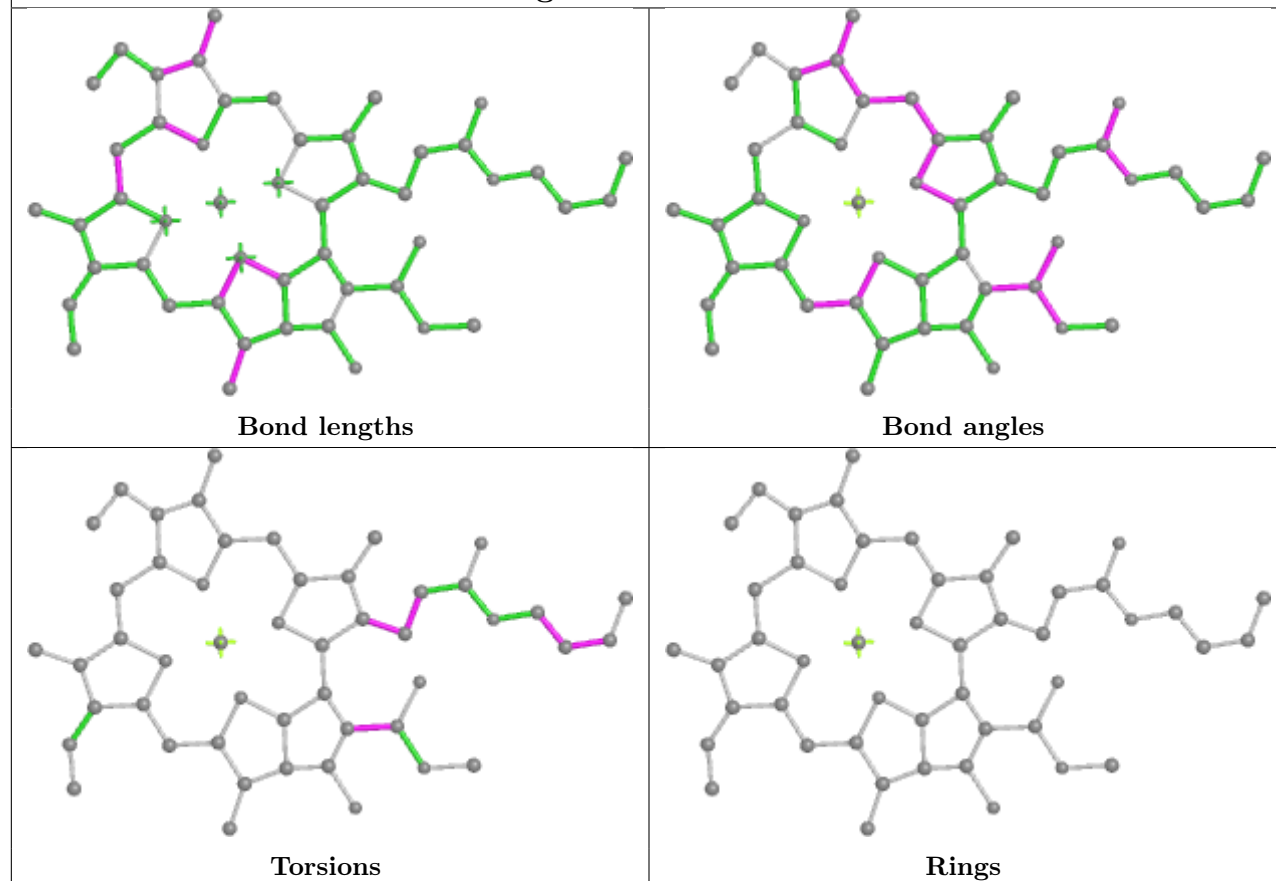




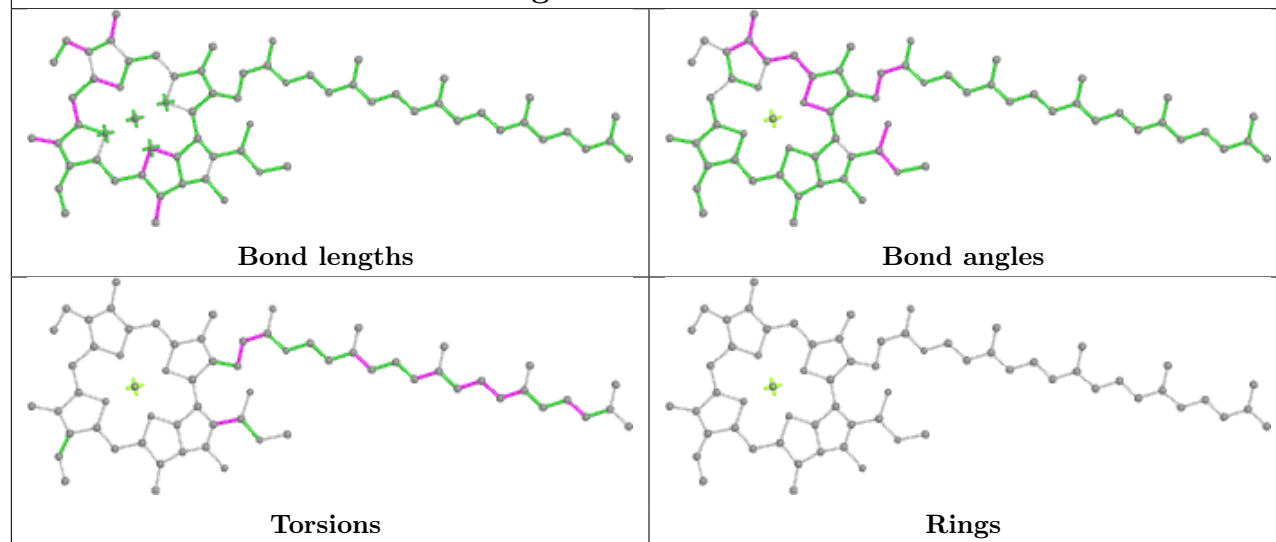
Ligand CLA 9 612

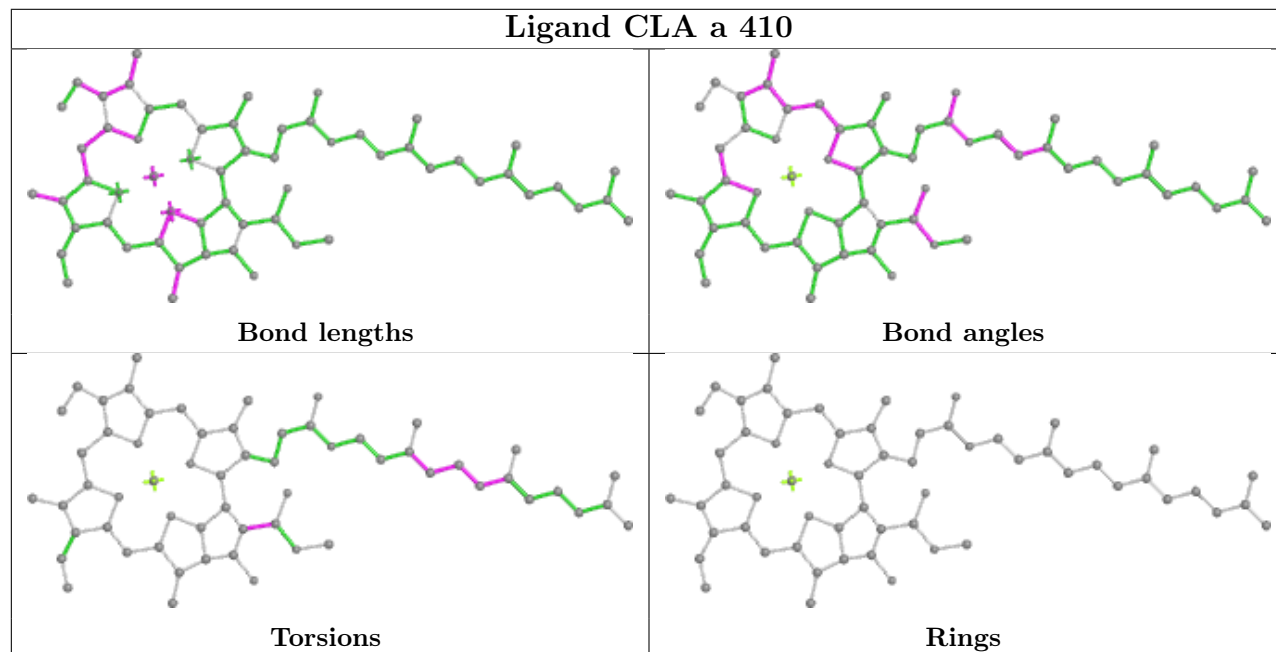
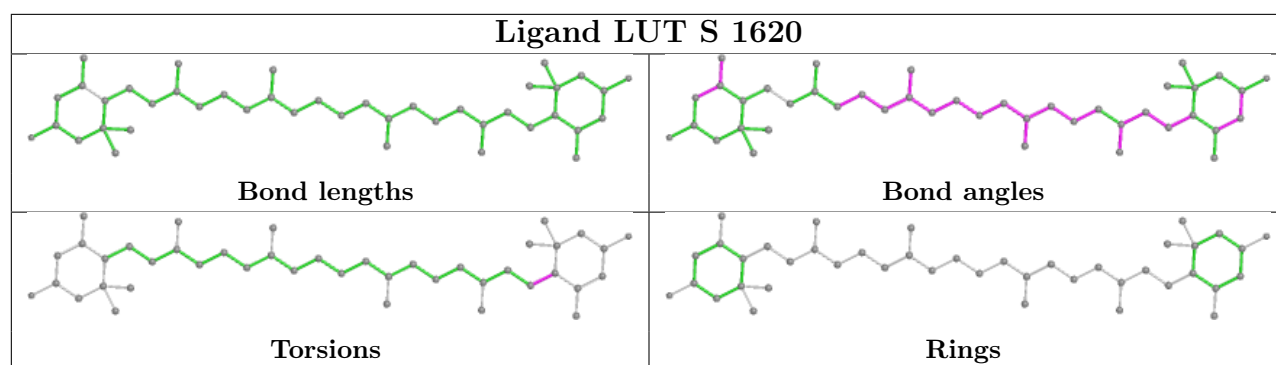


Ligand CLA 3 611

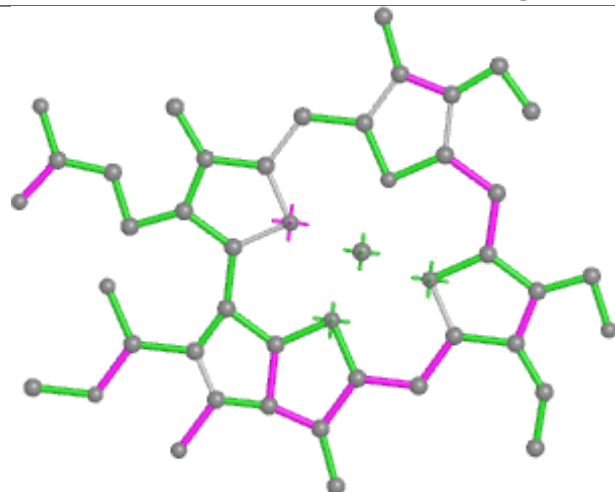


Ligand CLA Y 602

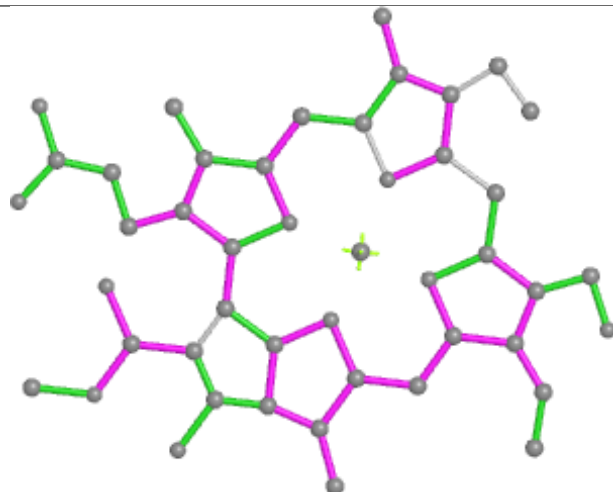




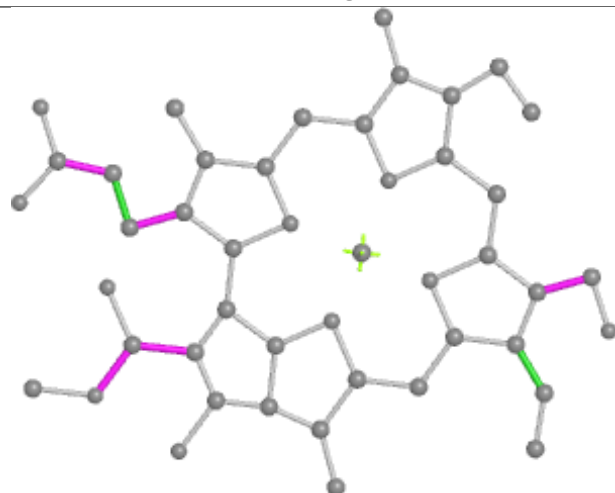
Ligand CHL N 606



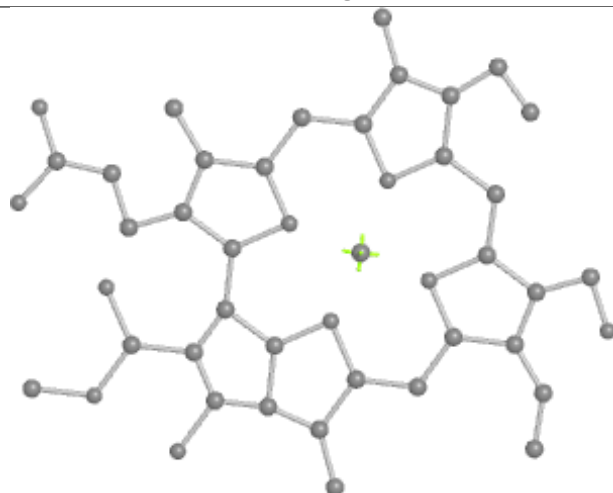
Bond lengths



Bond angles

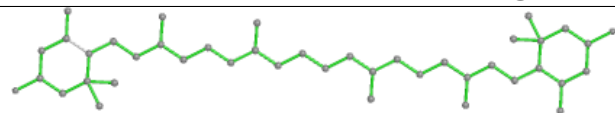


Torsions

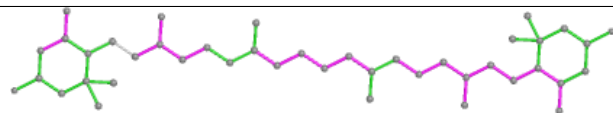


Rings

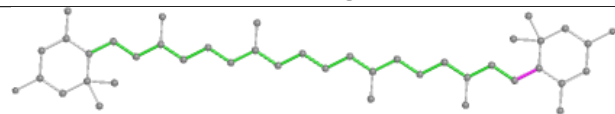
Ligand LUT 0 1620



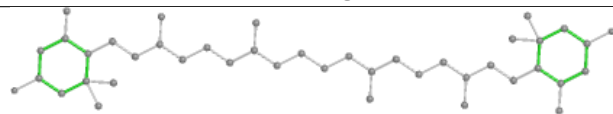
Bond lengths



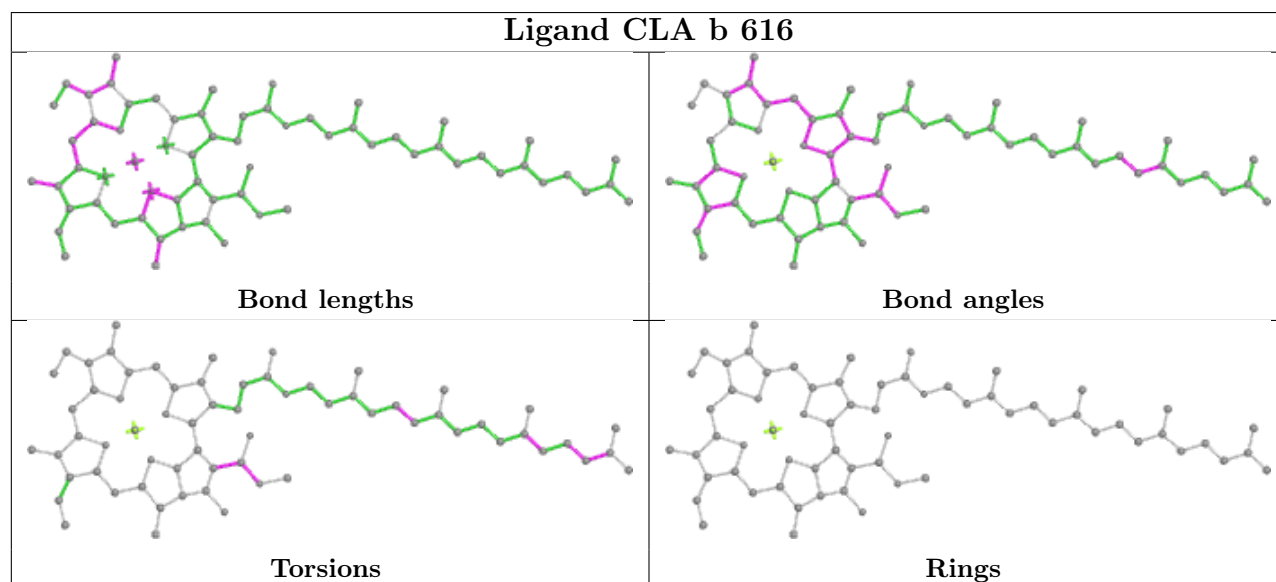
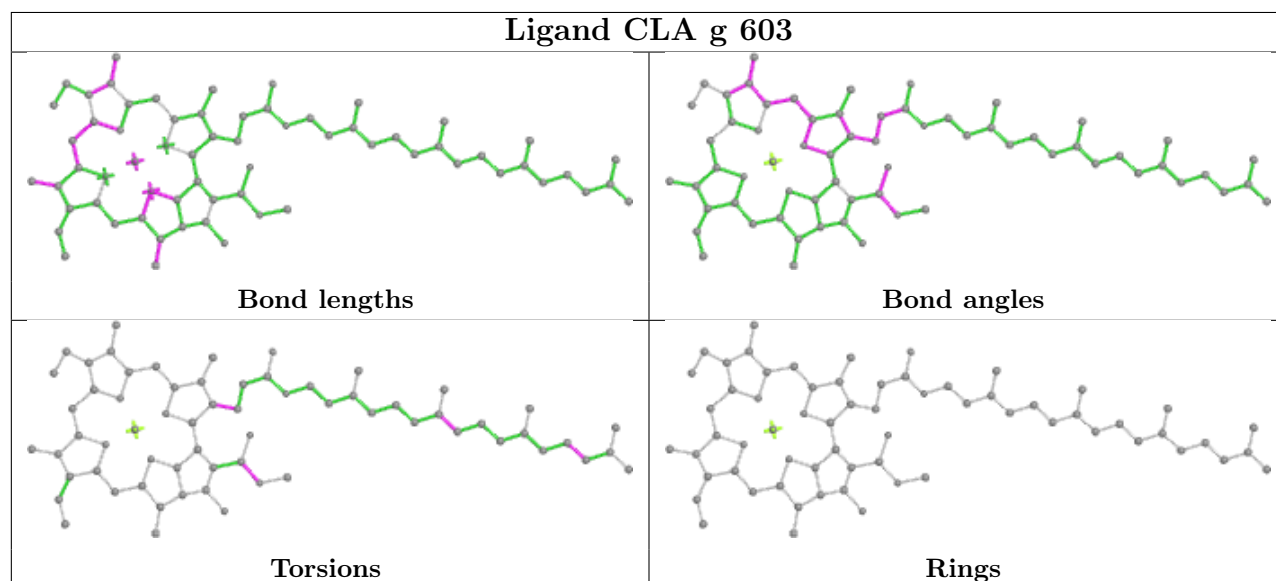
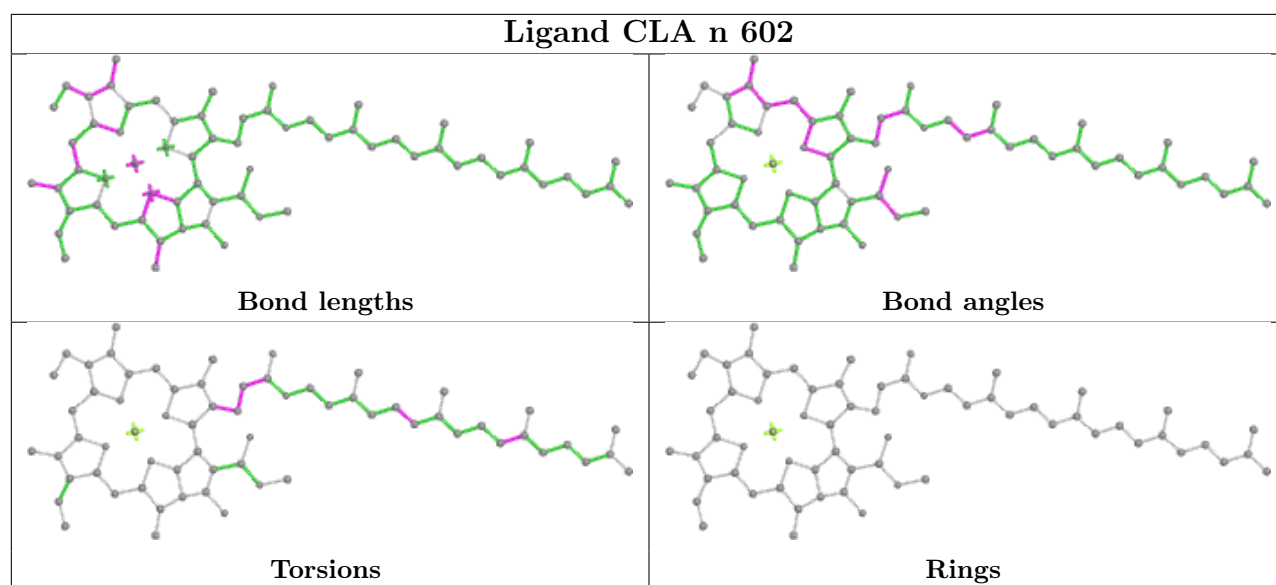
Bond angles

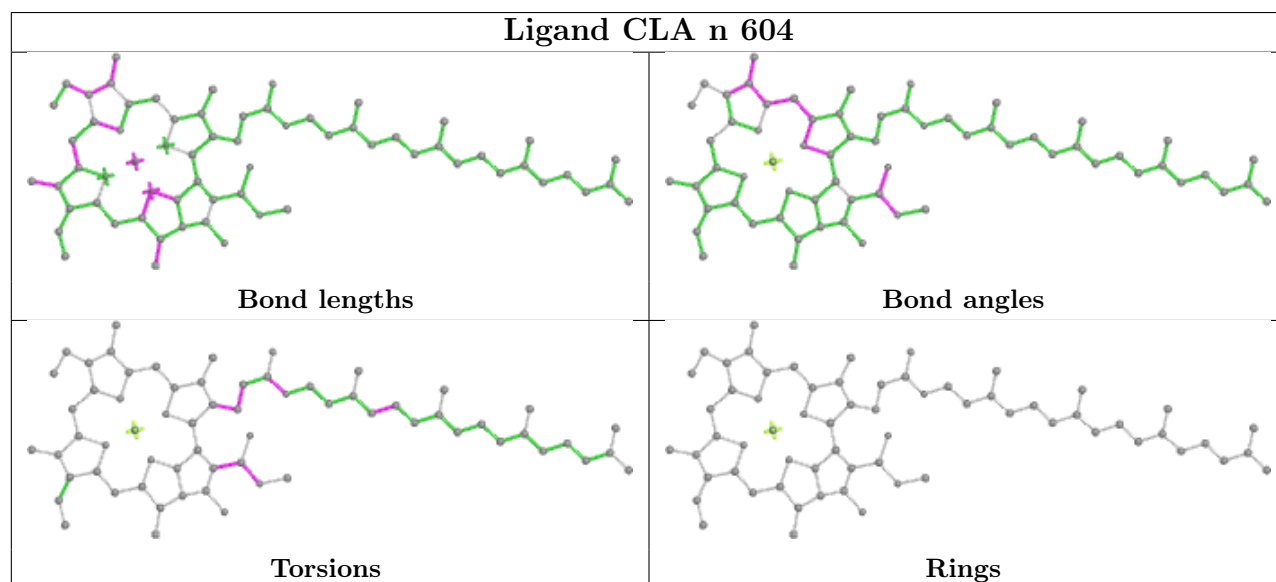
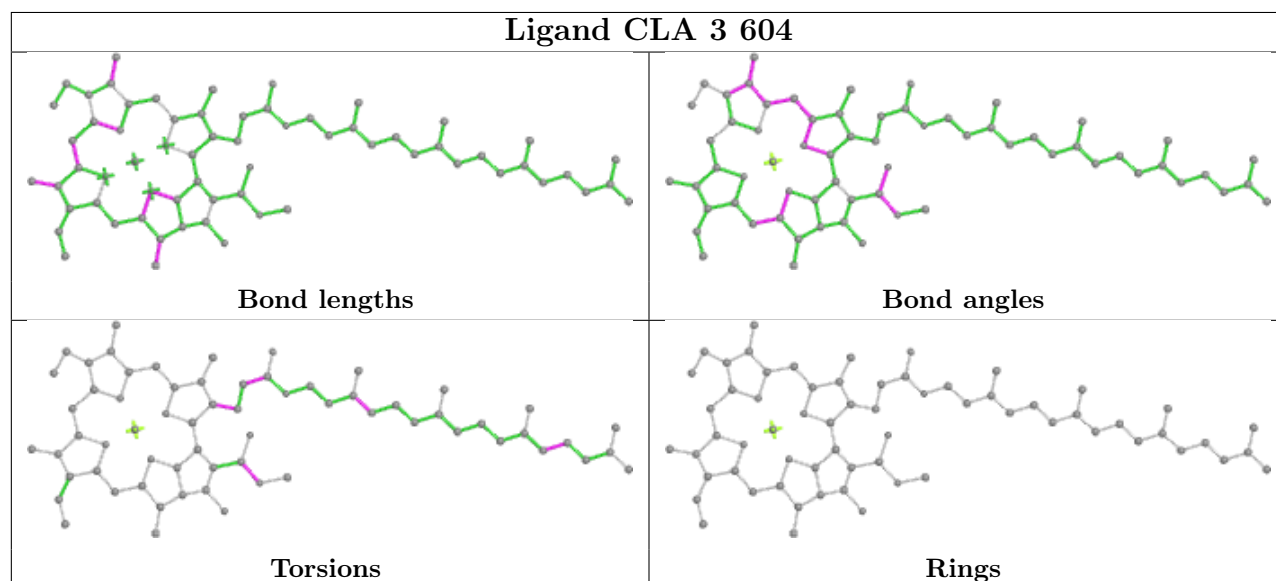
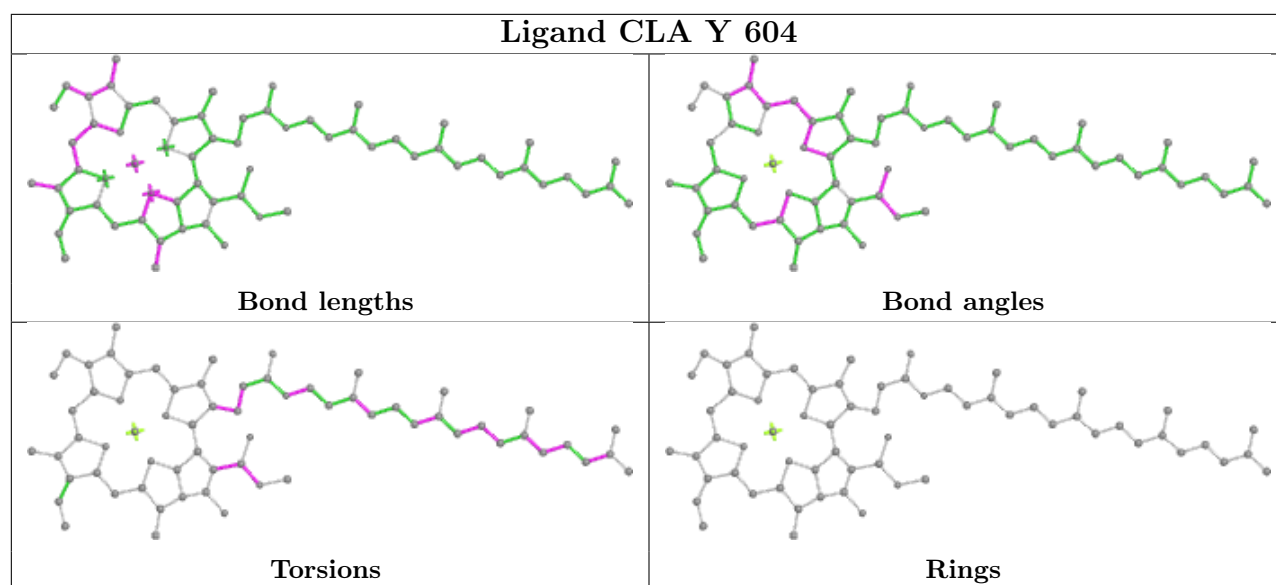


Torsions

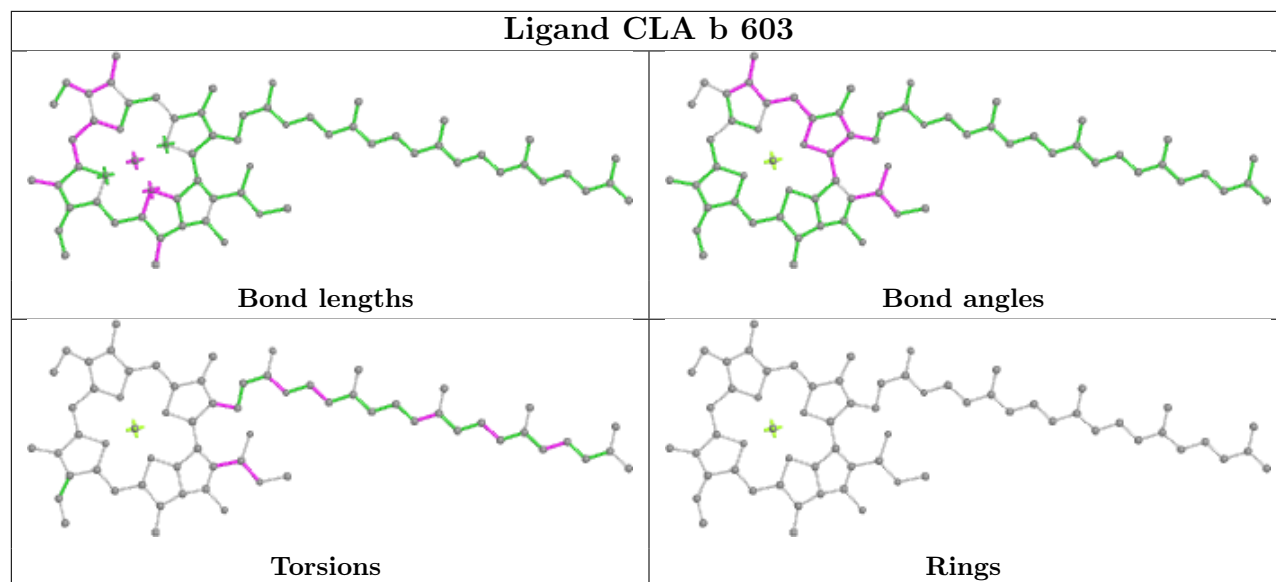


Rings

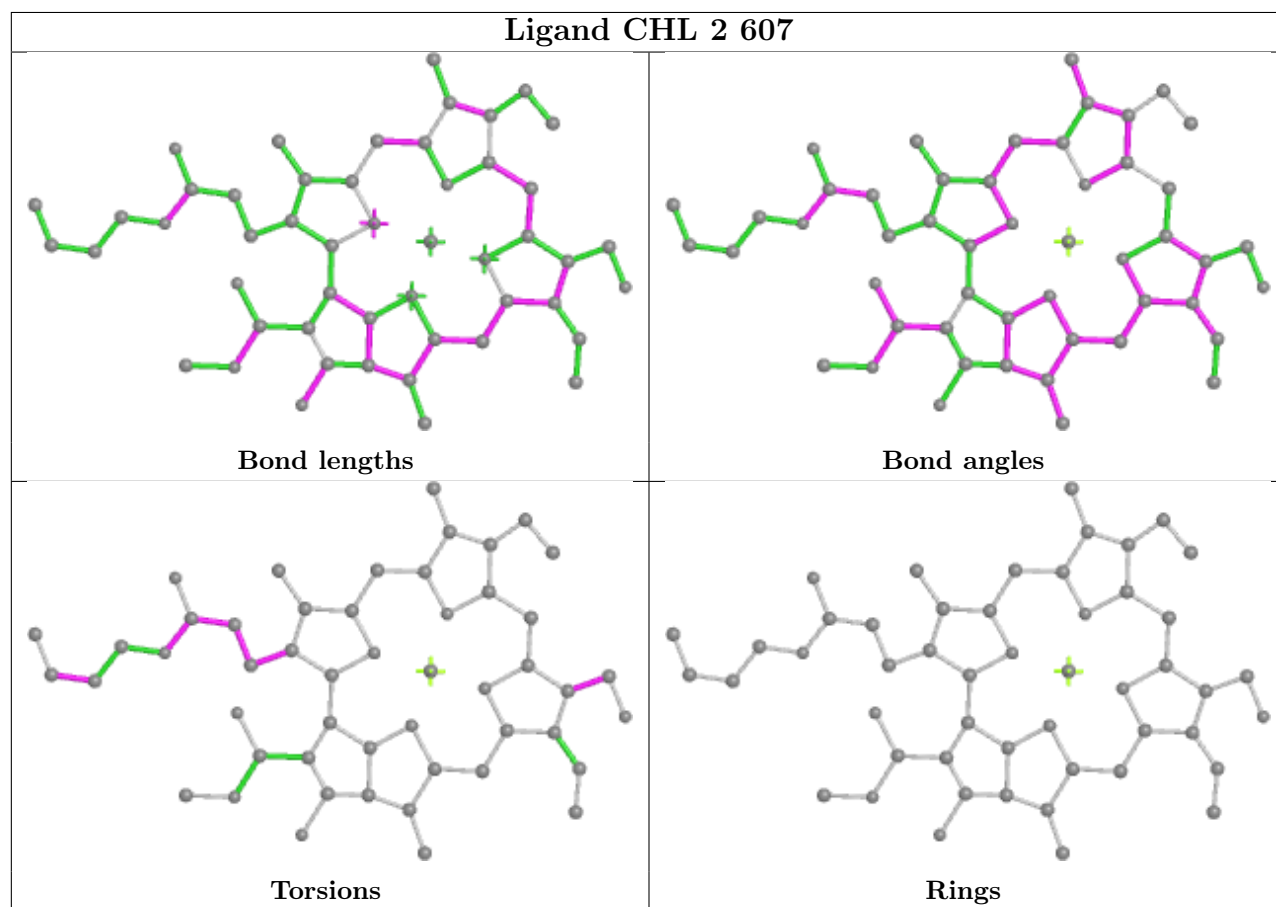


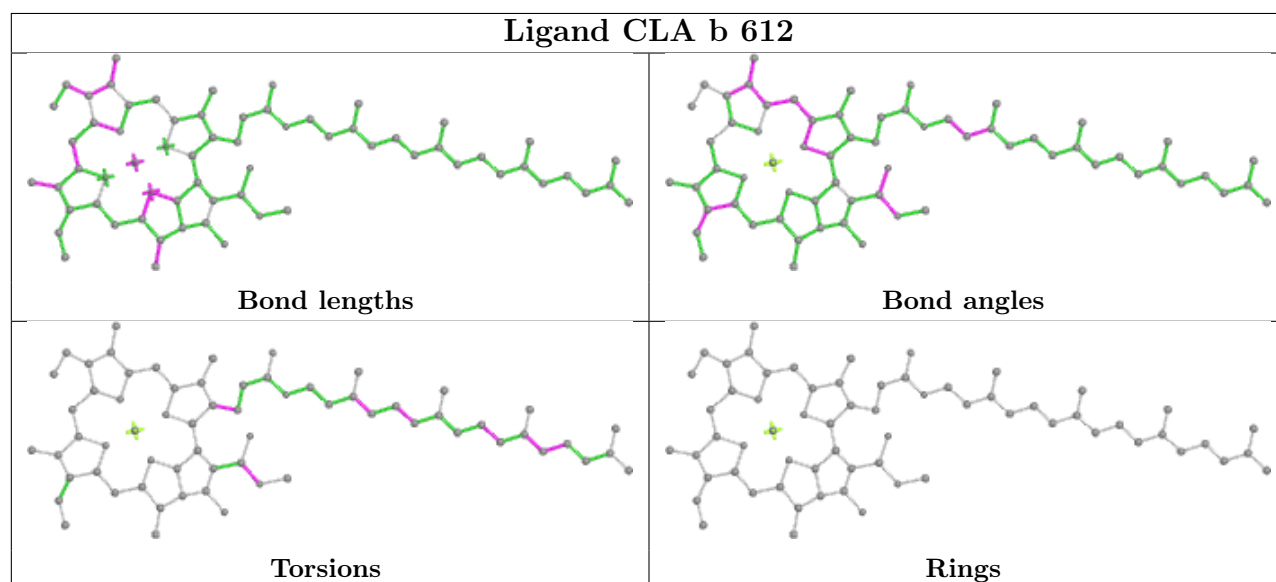
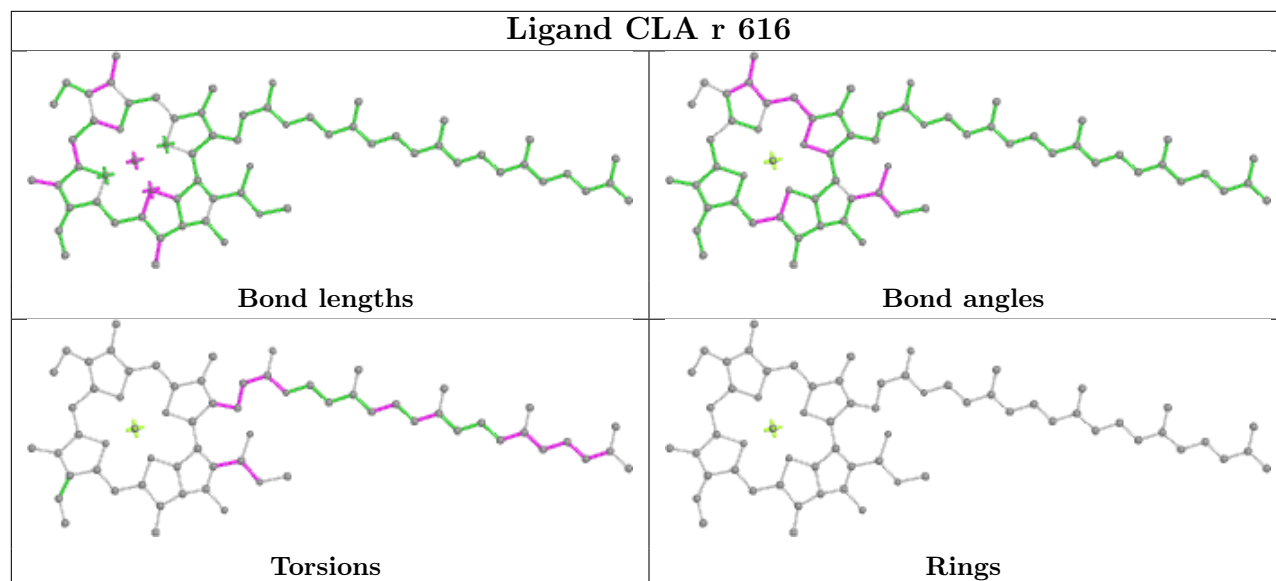
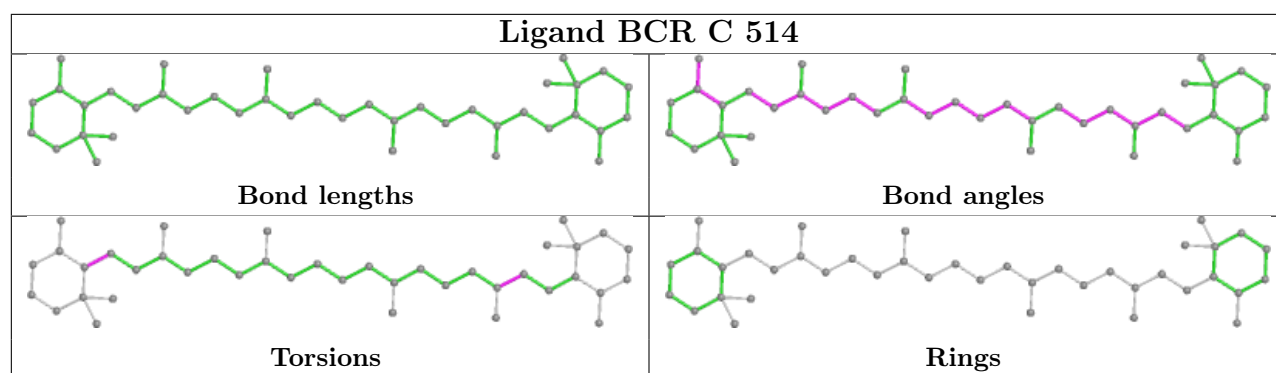


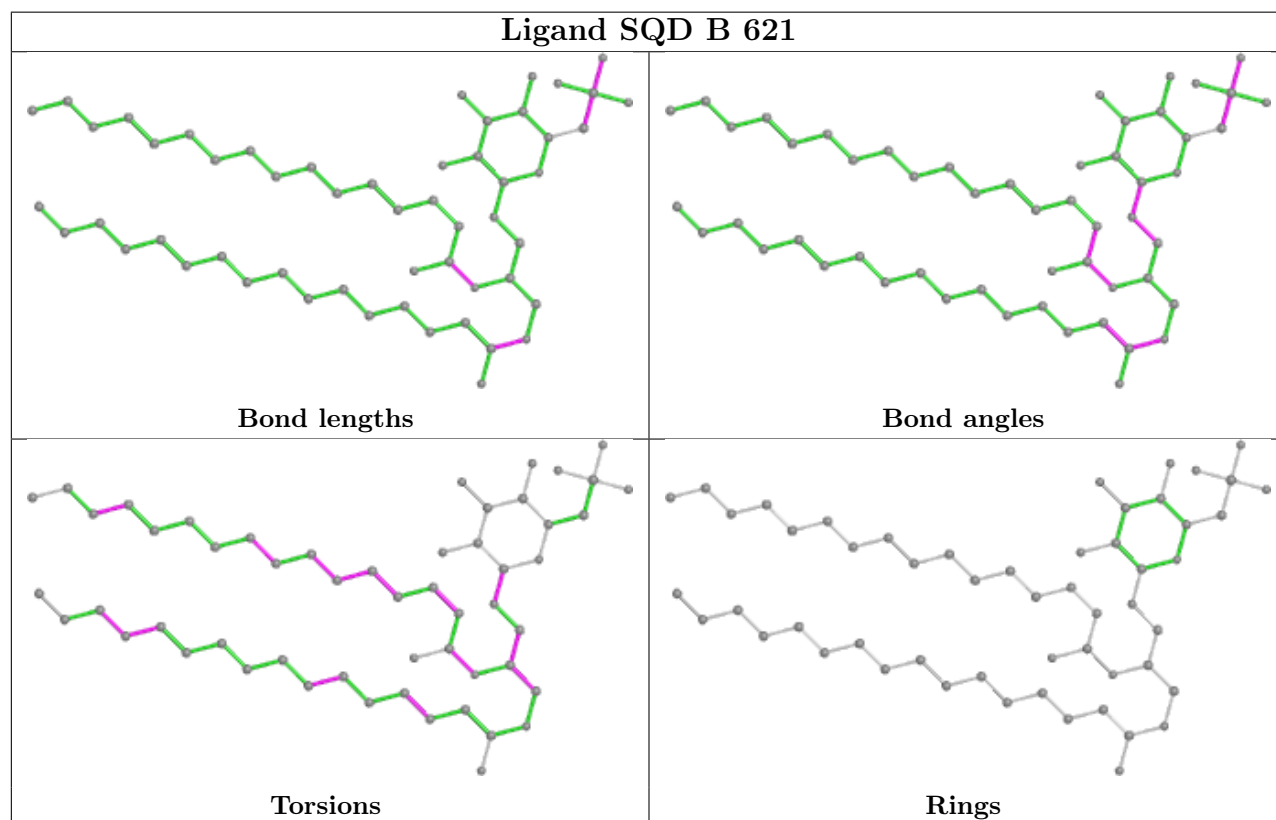
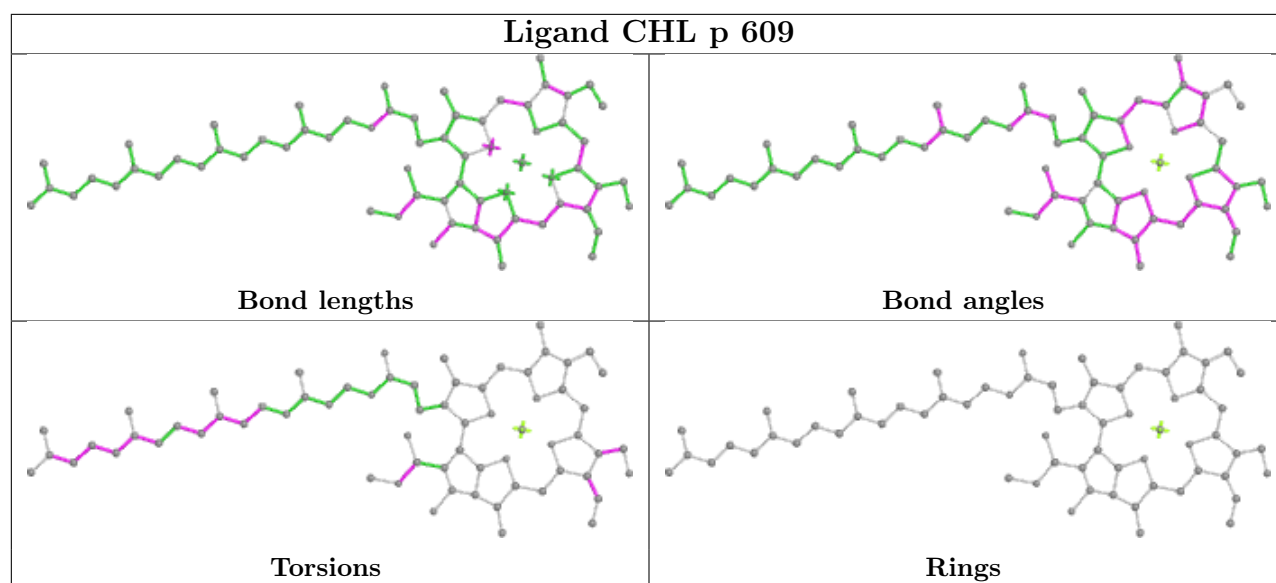
Ligand CLA b 603

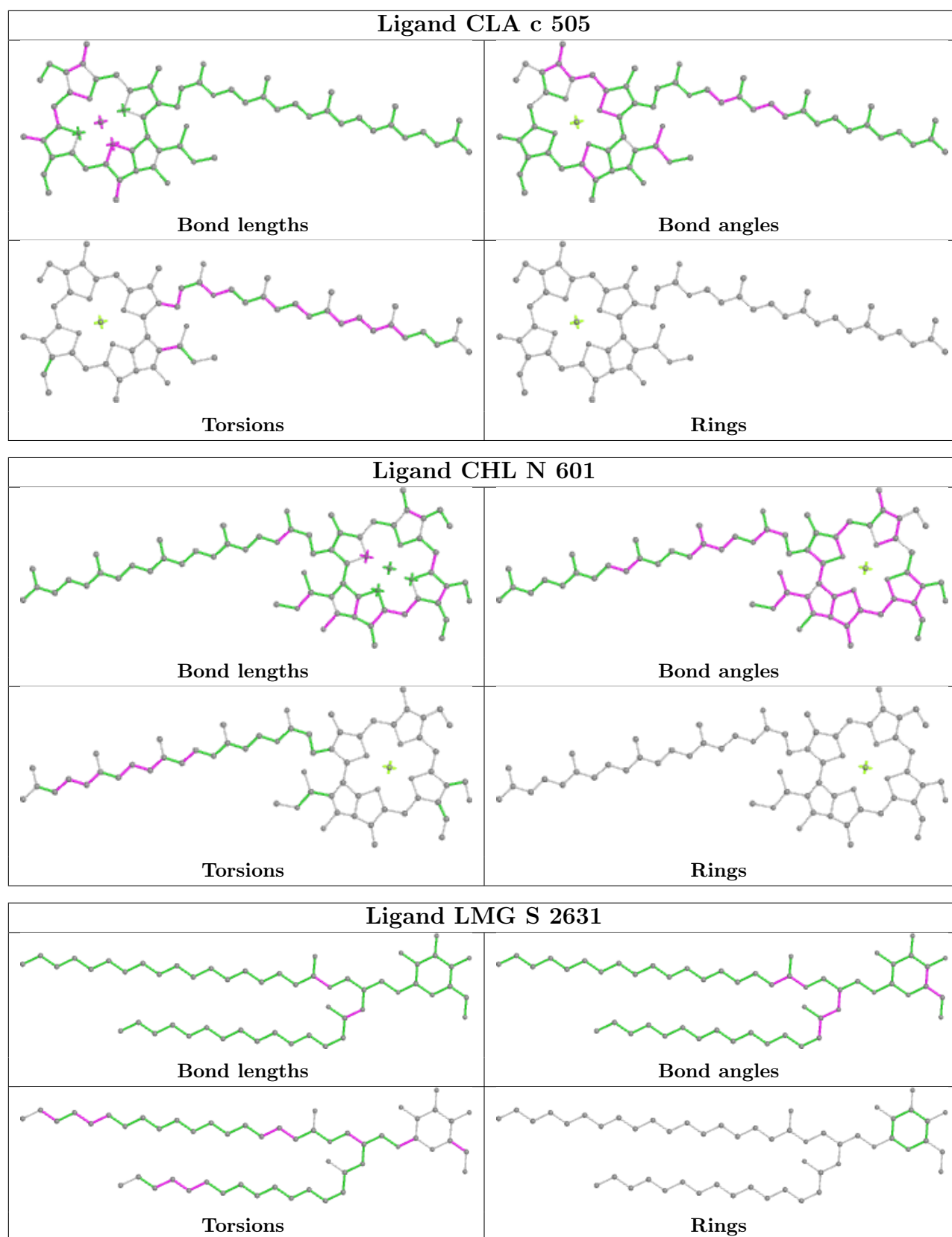


Ligand CHL 2 607

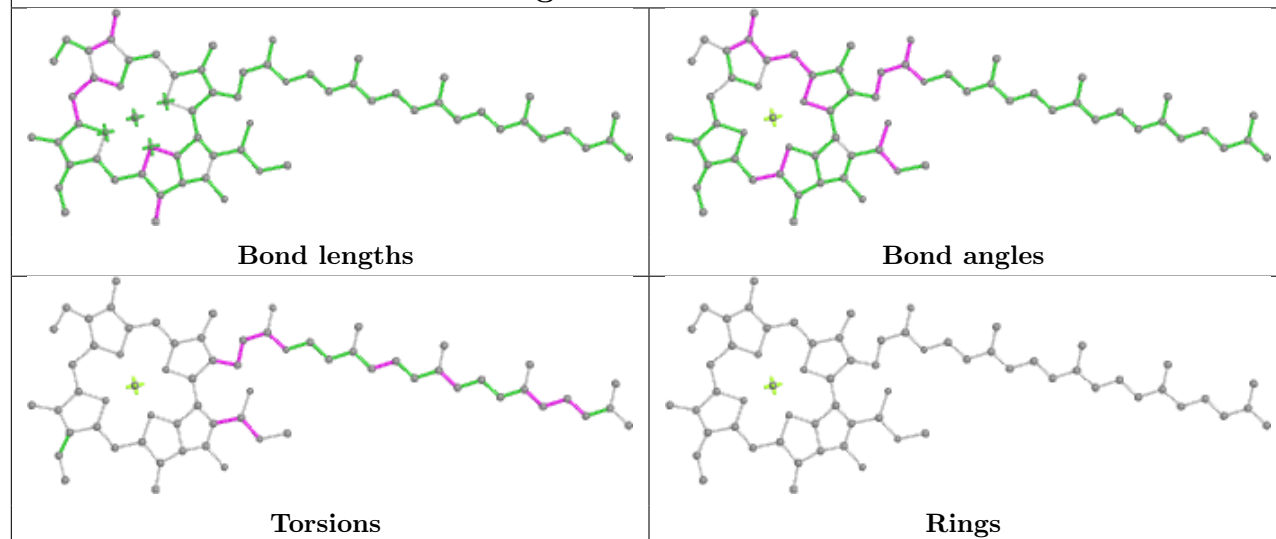




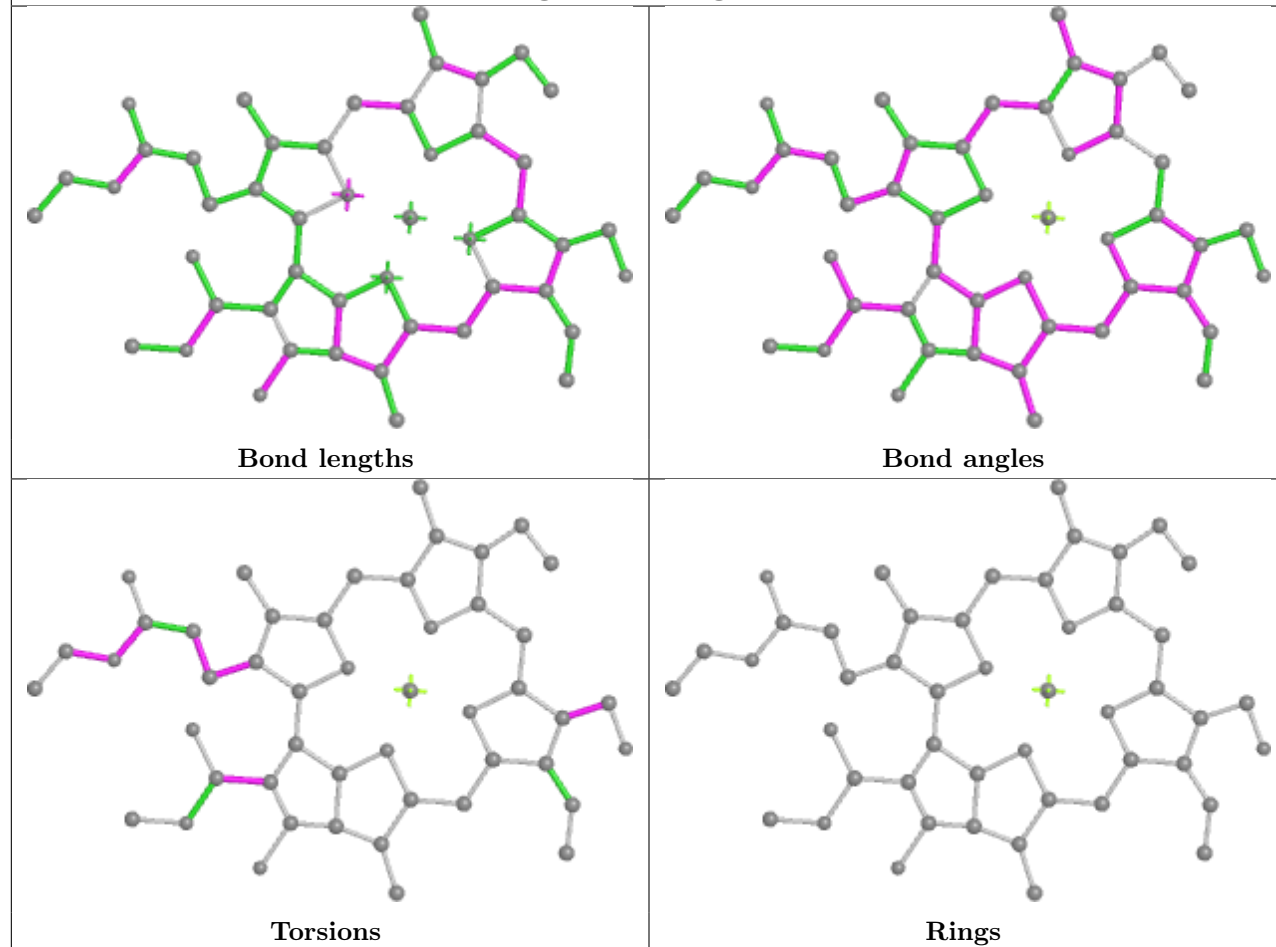


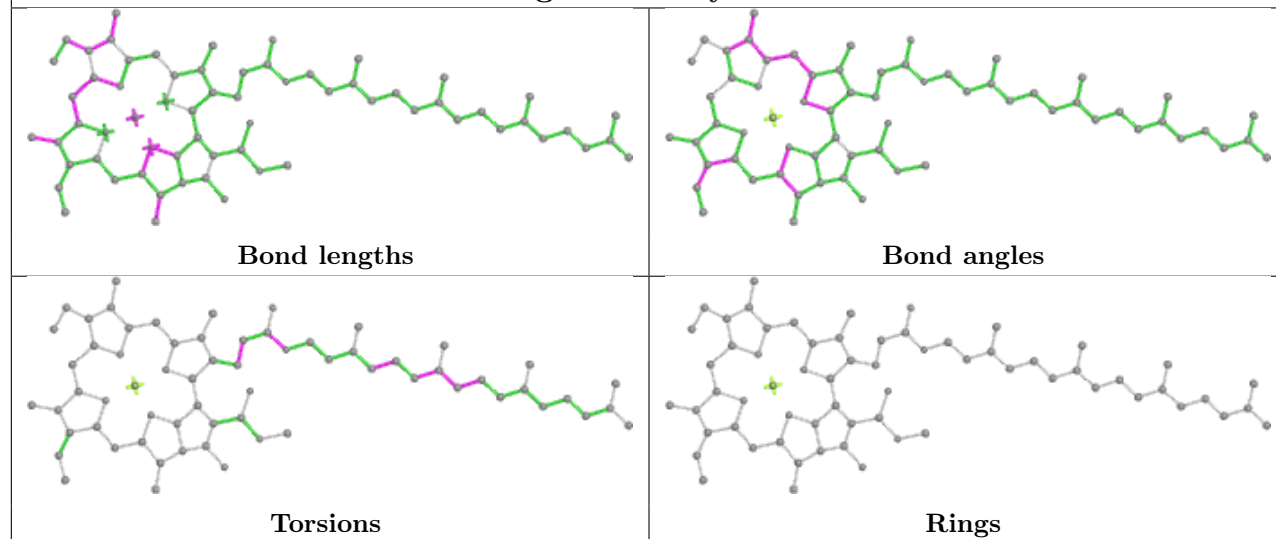
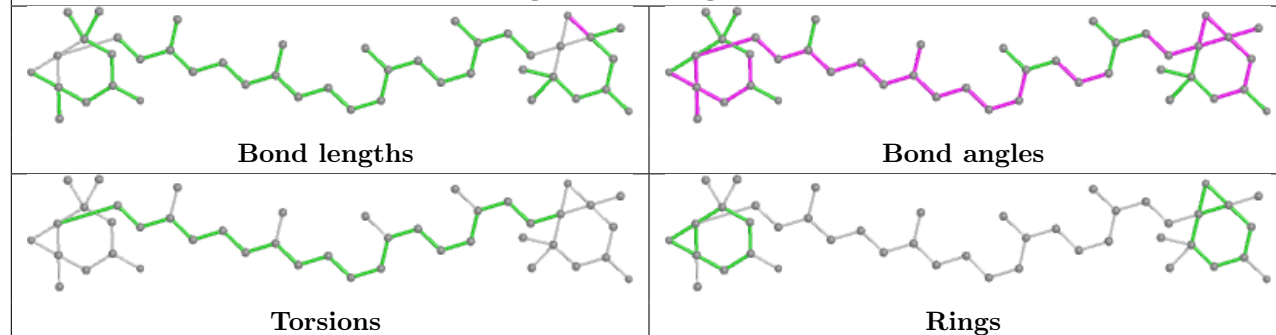
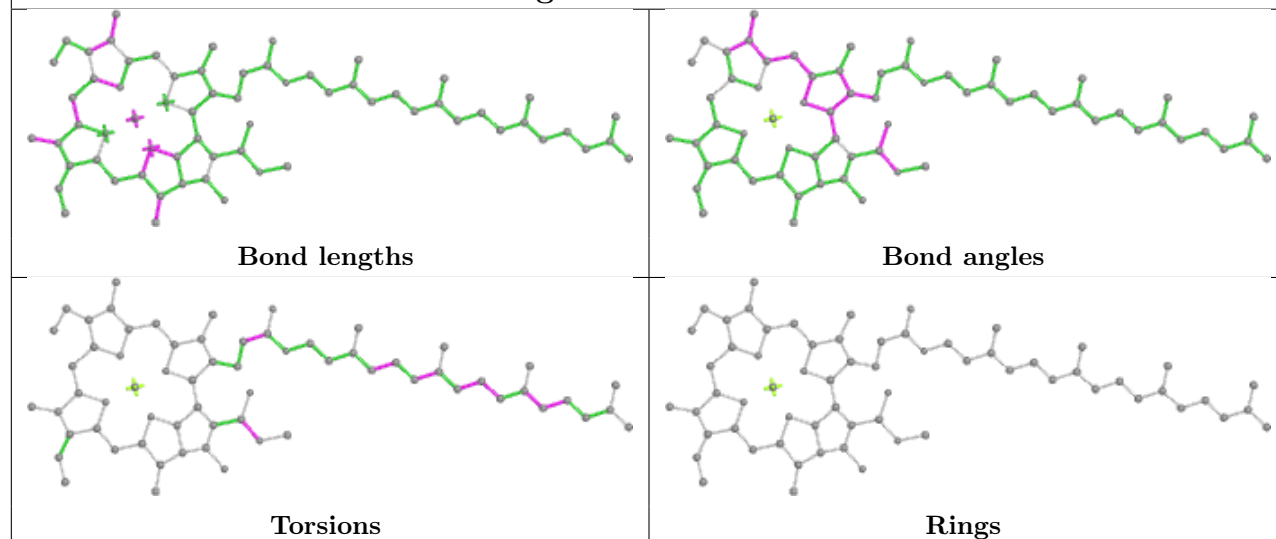


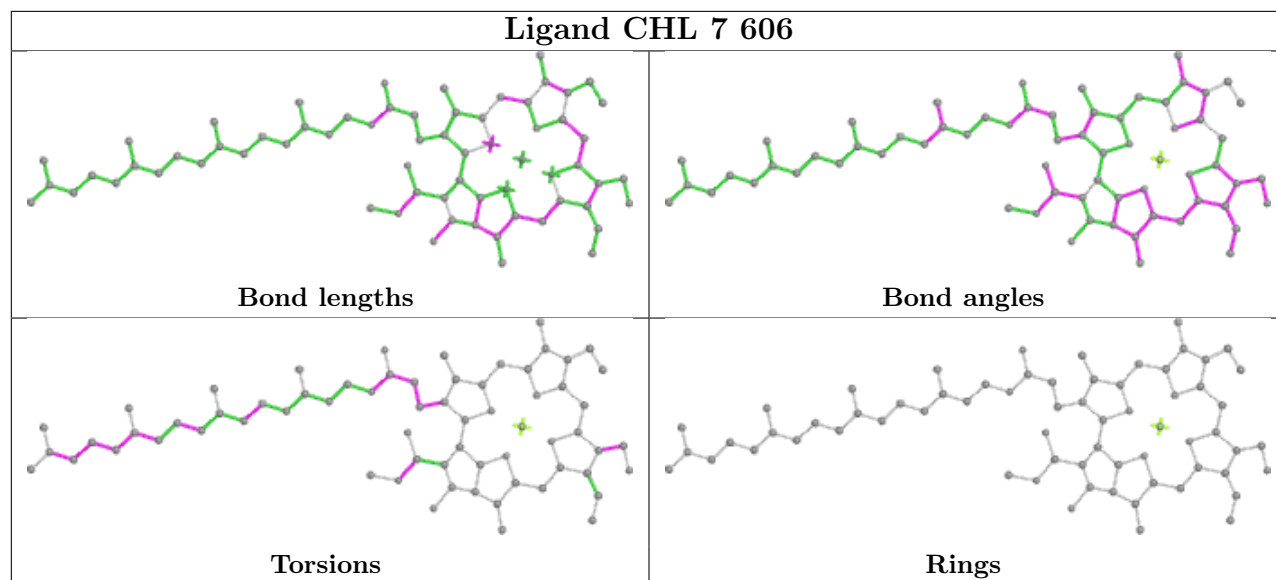
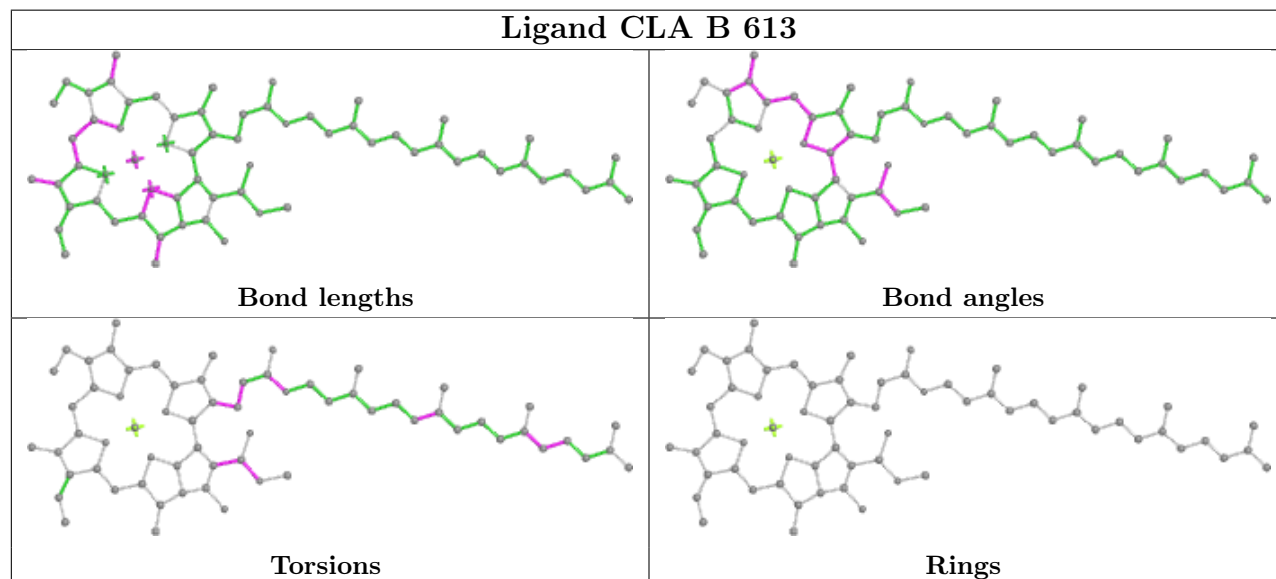
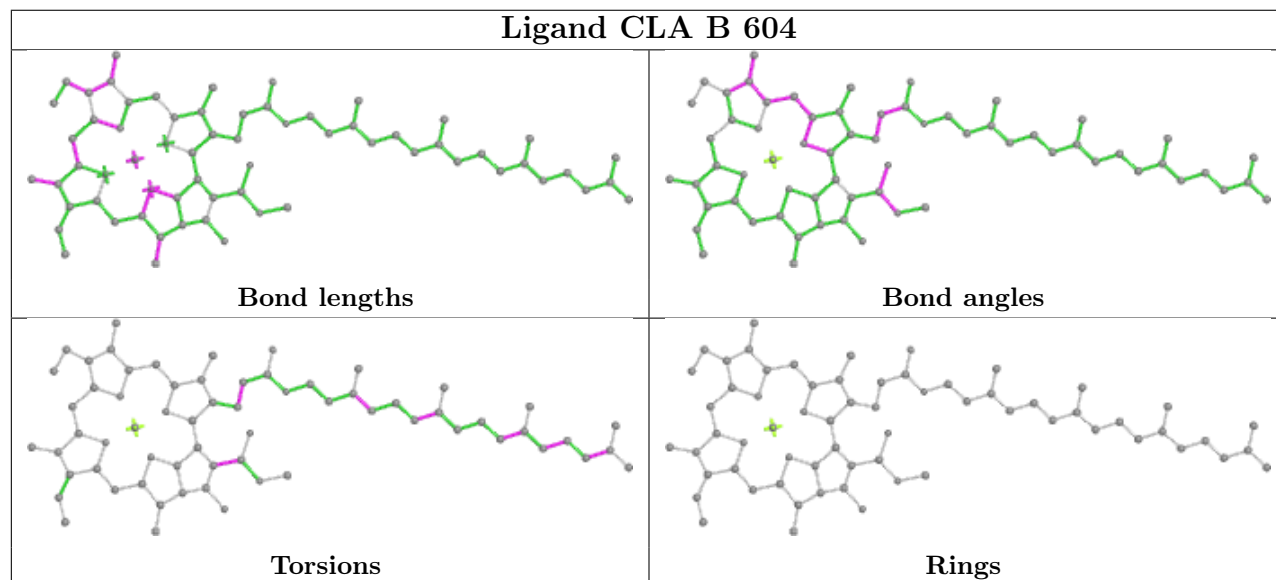
Ligand CLA 0 613



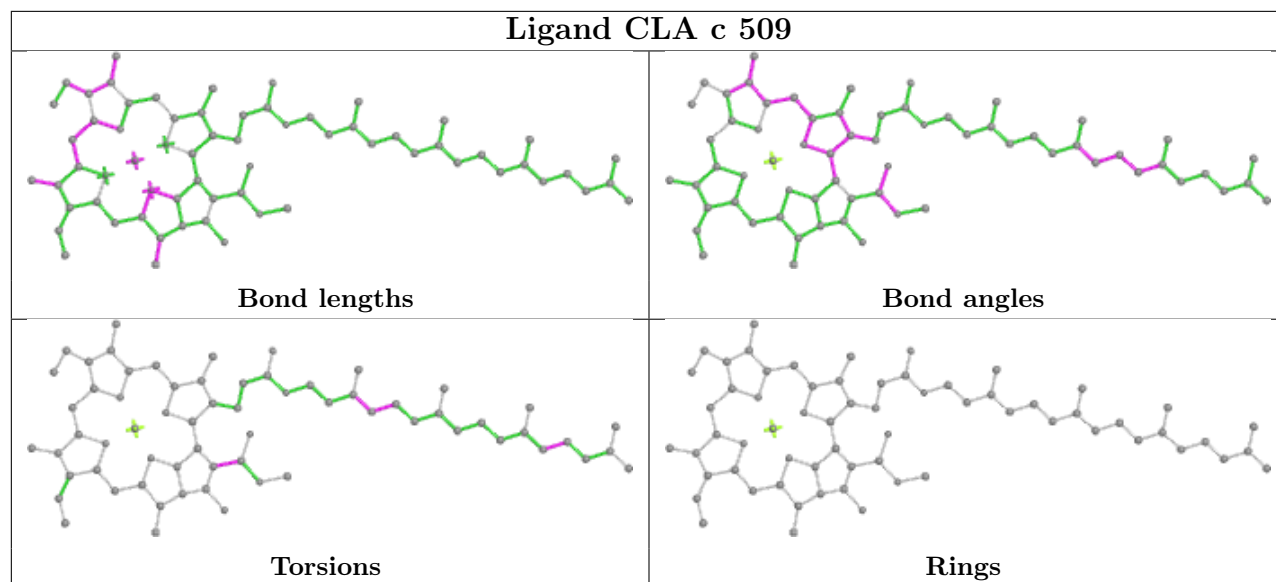
Ligand CHL g 605



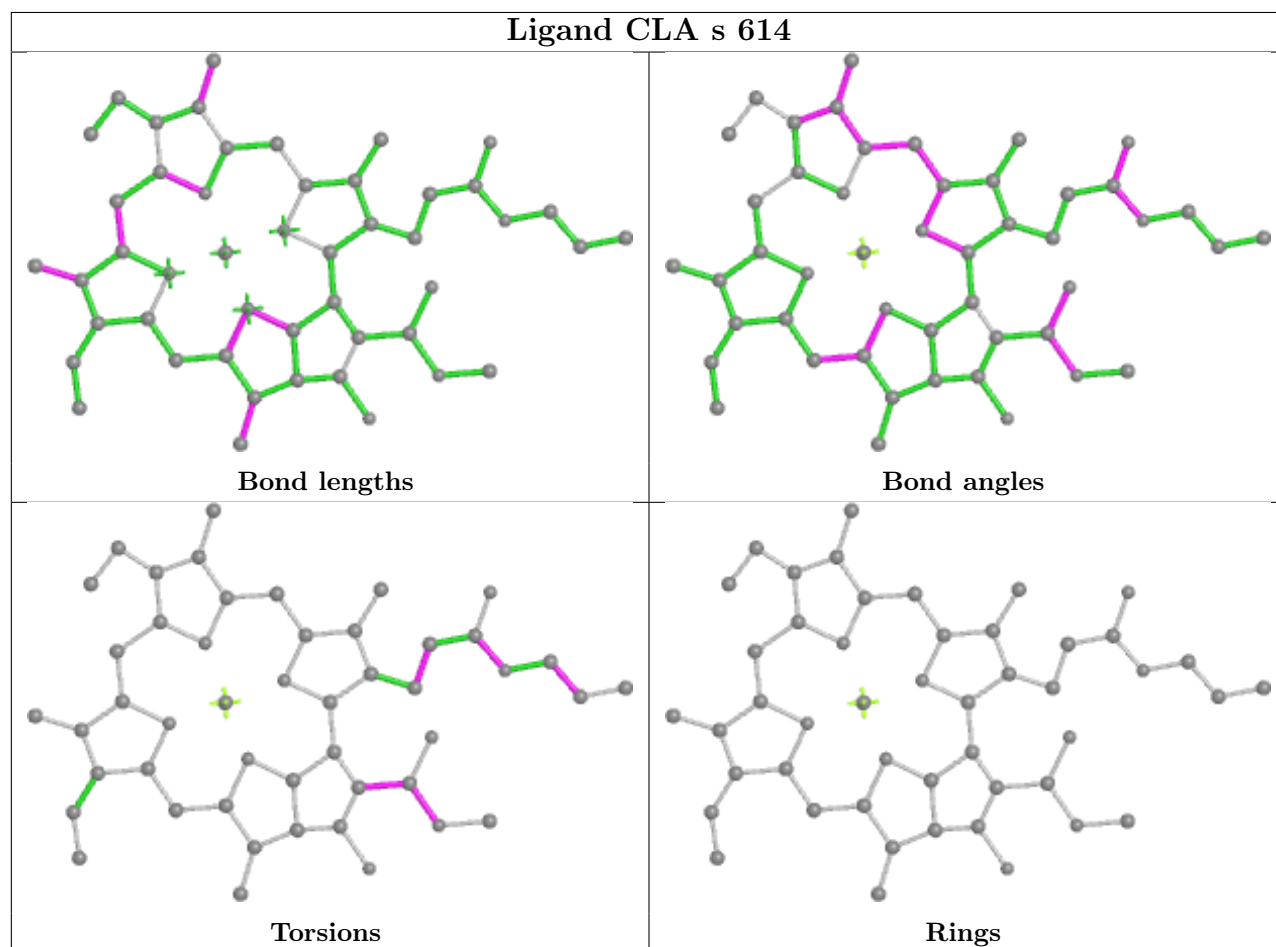
Ligand CLA y 613**Ligand XAT g 1622****Ligand CLA 0 612**

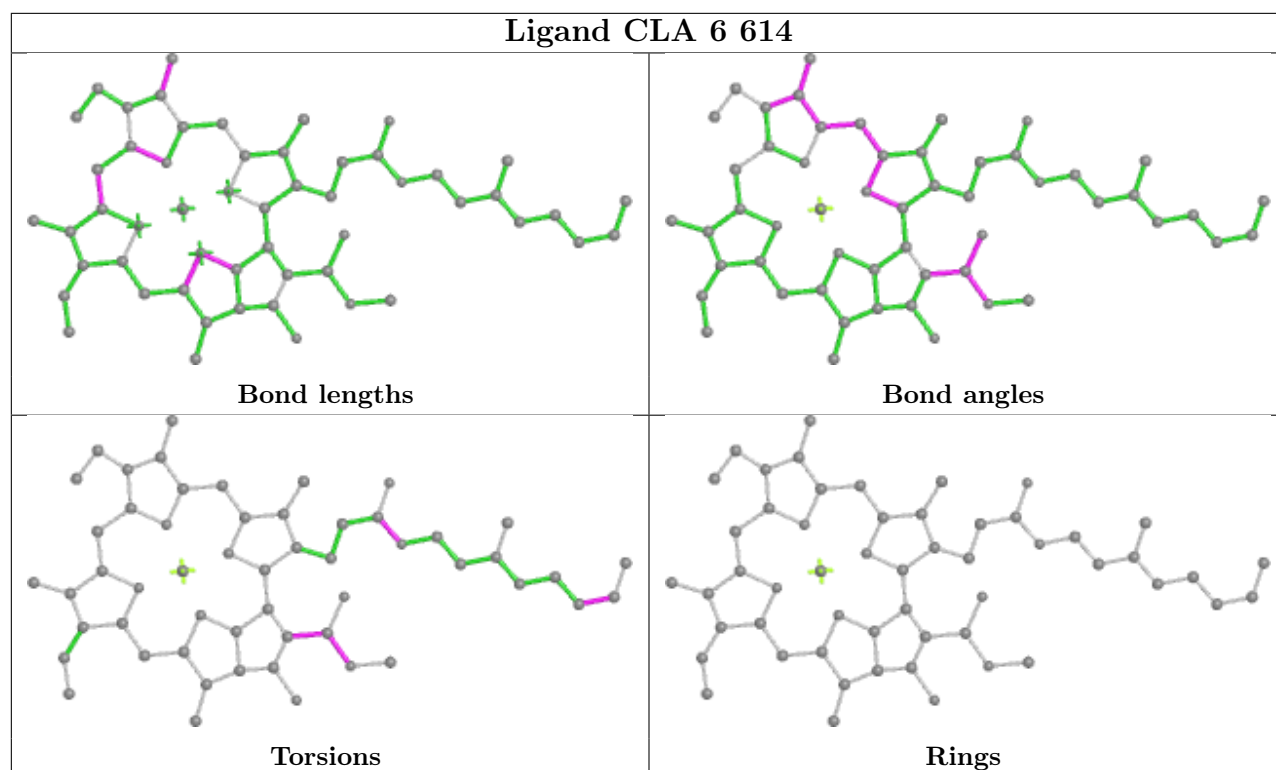
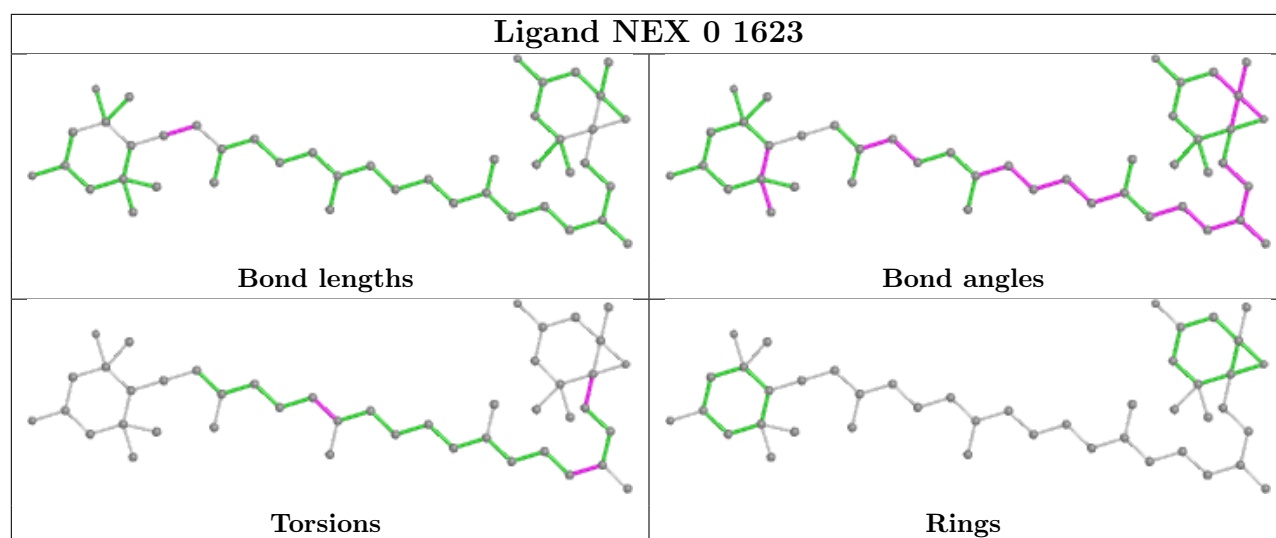
Ligand CHL 7 606**Ligand CLA B 613****Ligand CLA B 604**

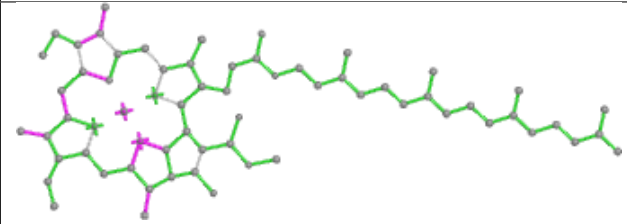
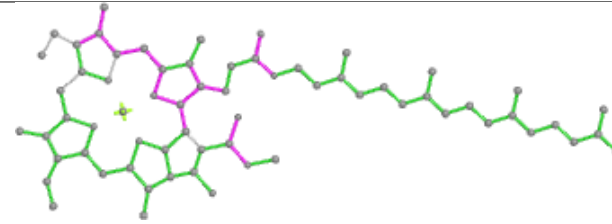
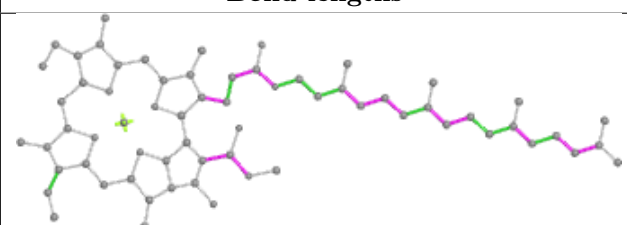
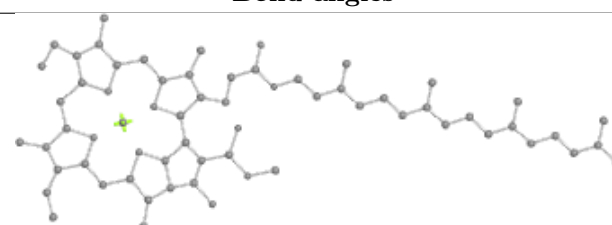
Ligand CLA c 509

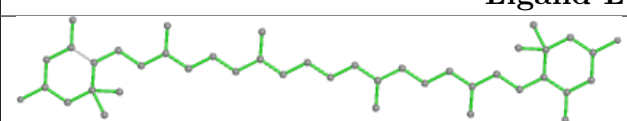
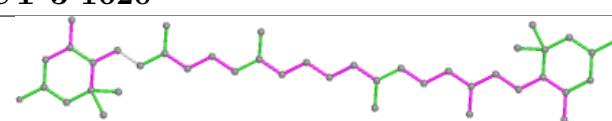
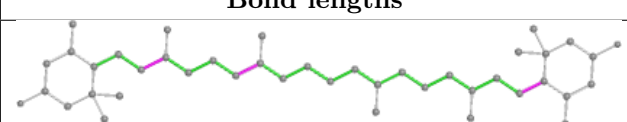
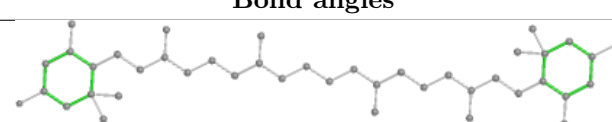


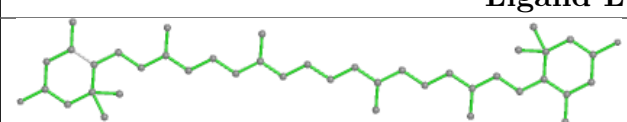
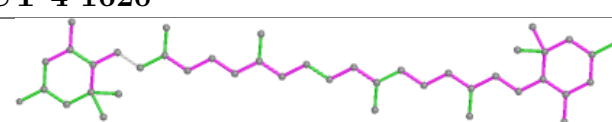
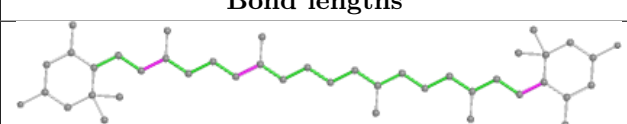
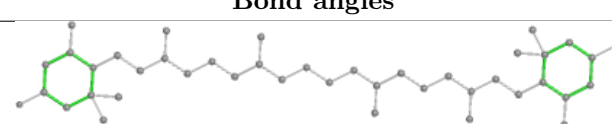
Ligand CLA s 614

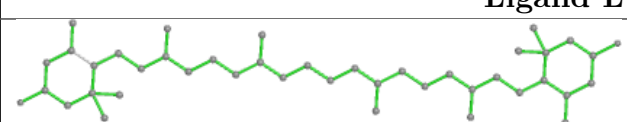
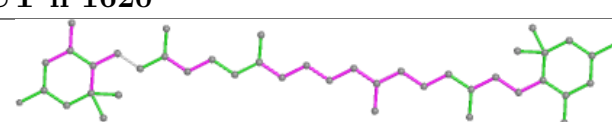
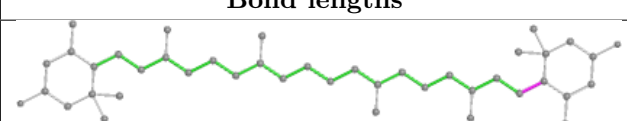
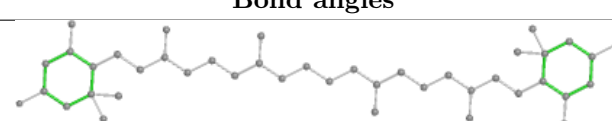


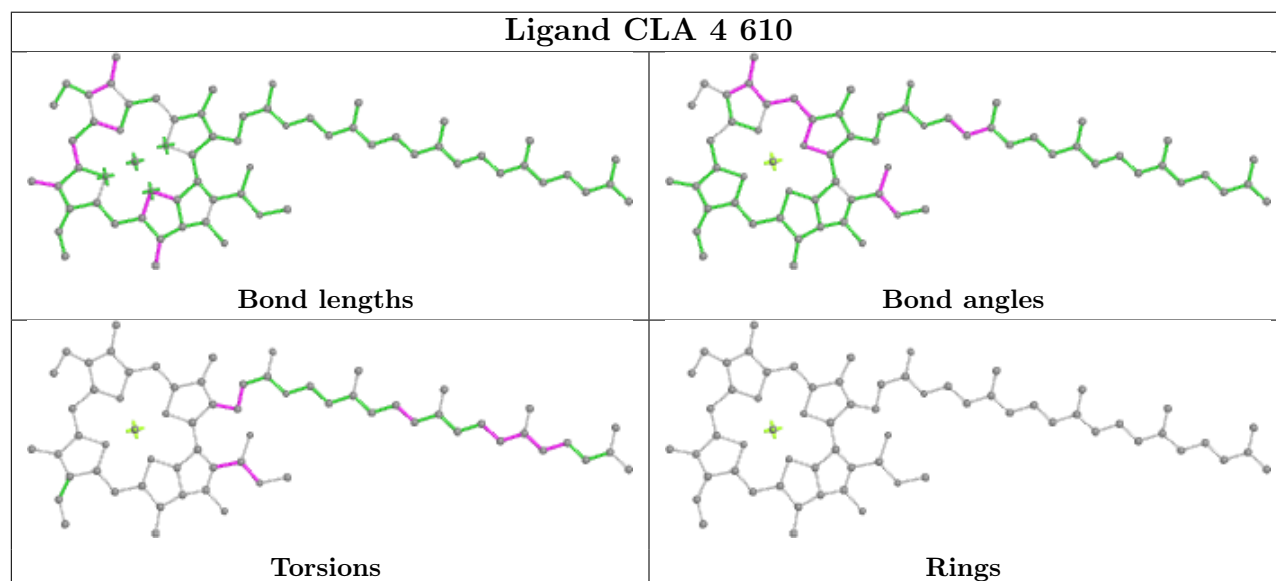
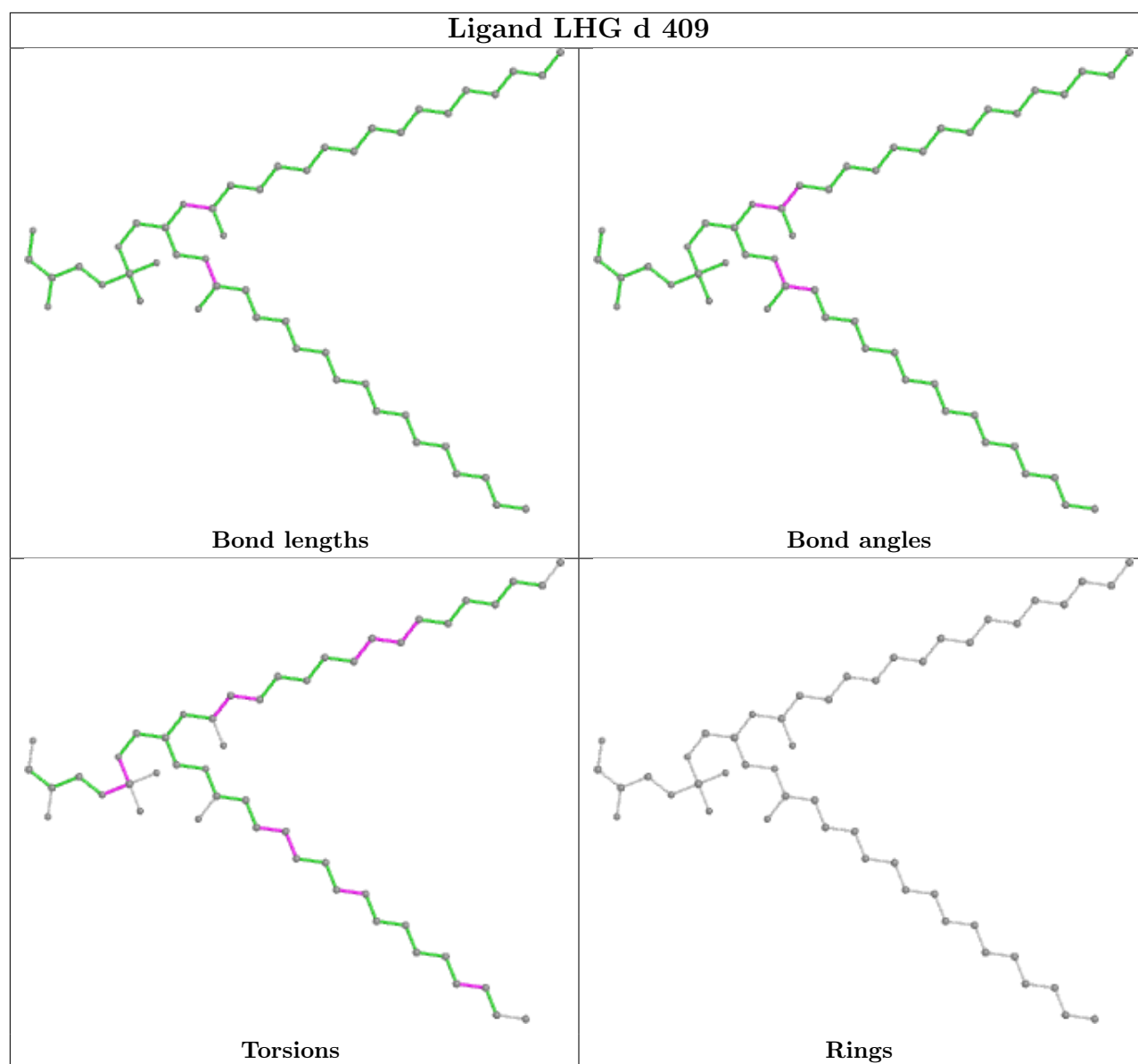


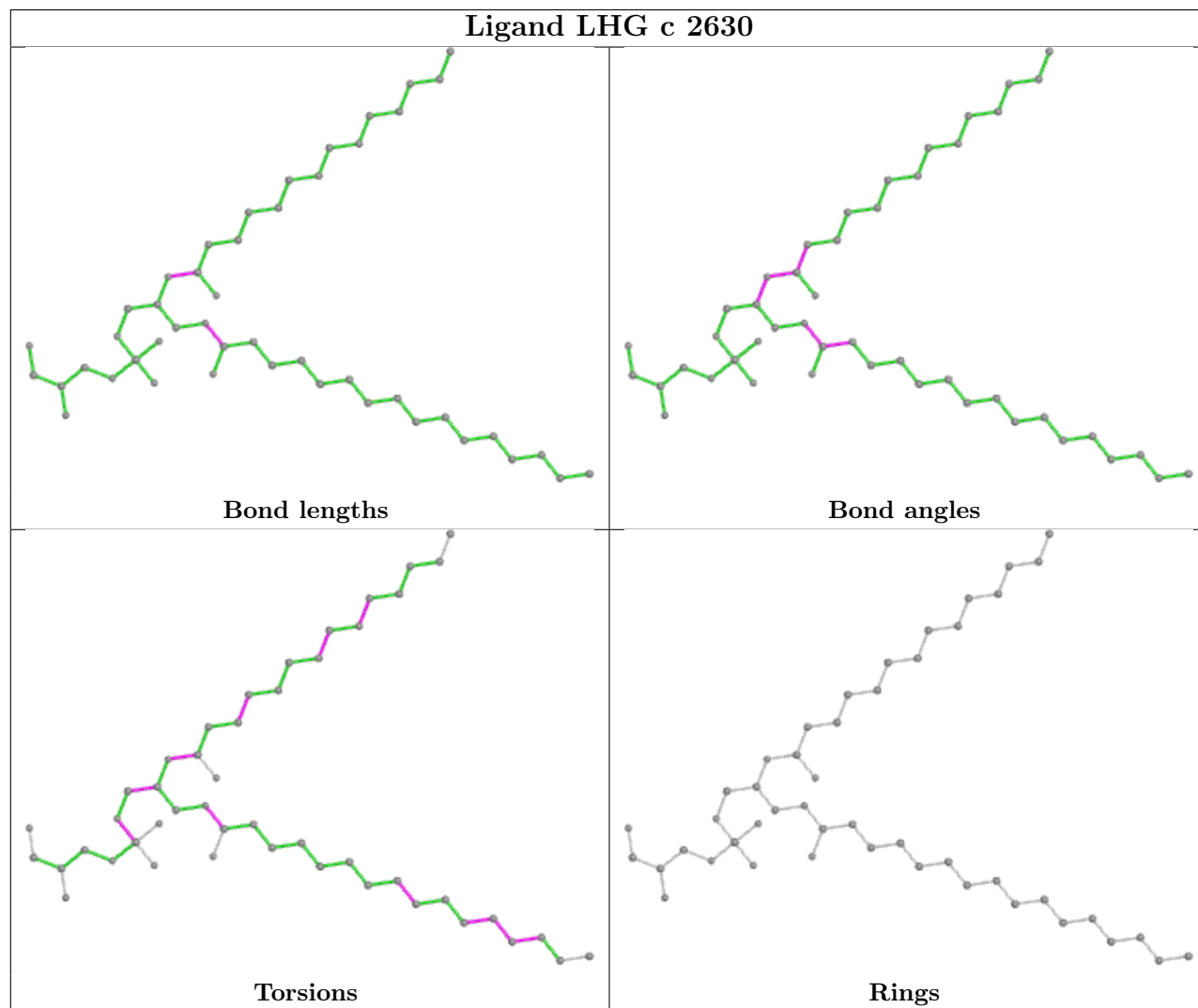
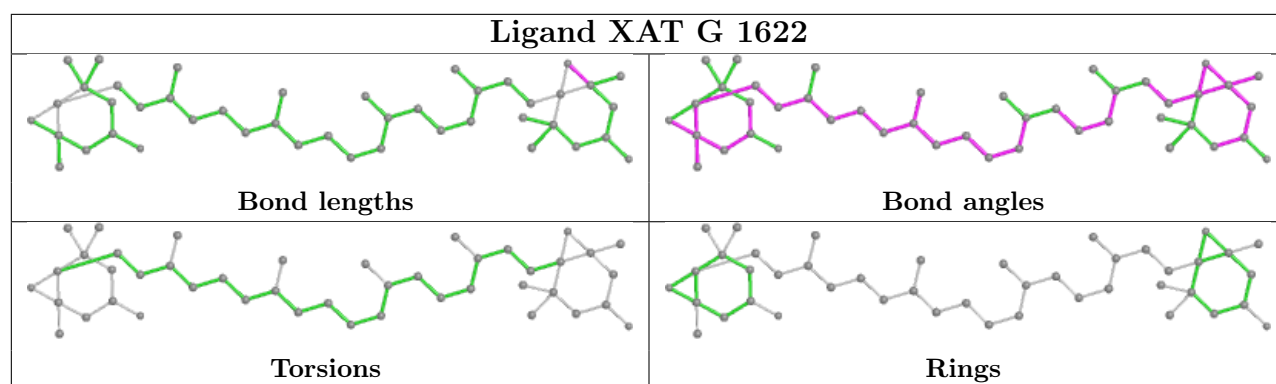
Ligand CLA 9 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

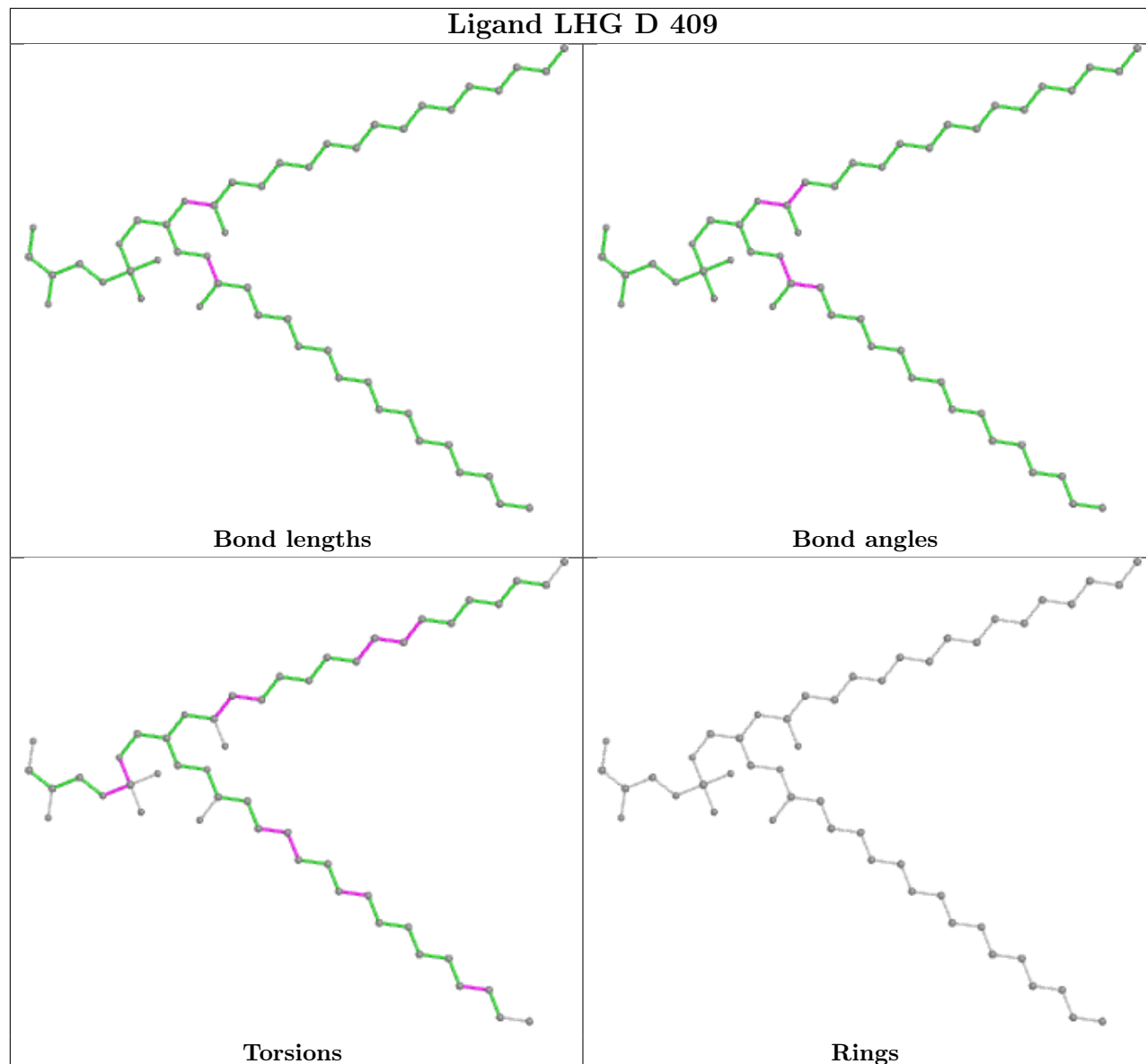
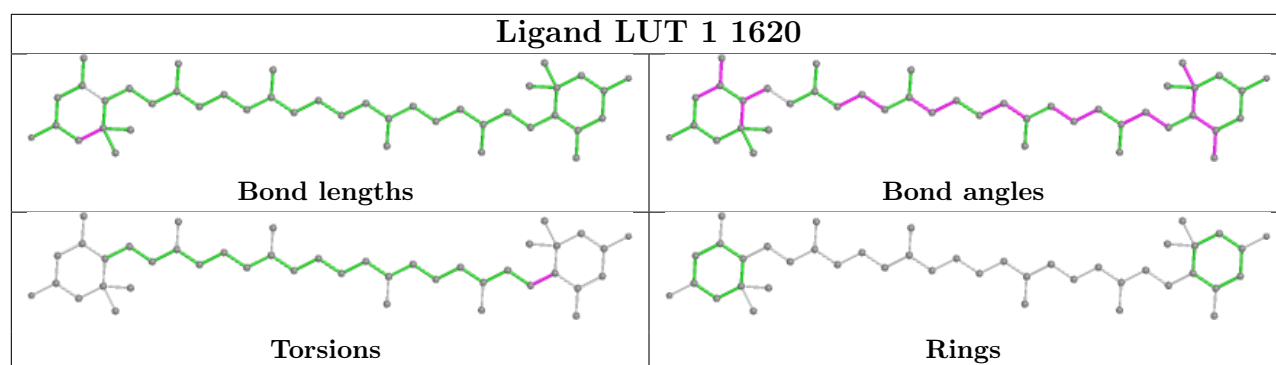
Ligand LUT 3 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

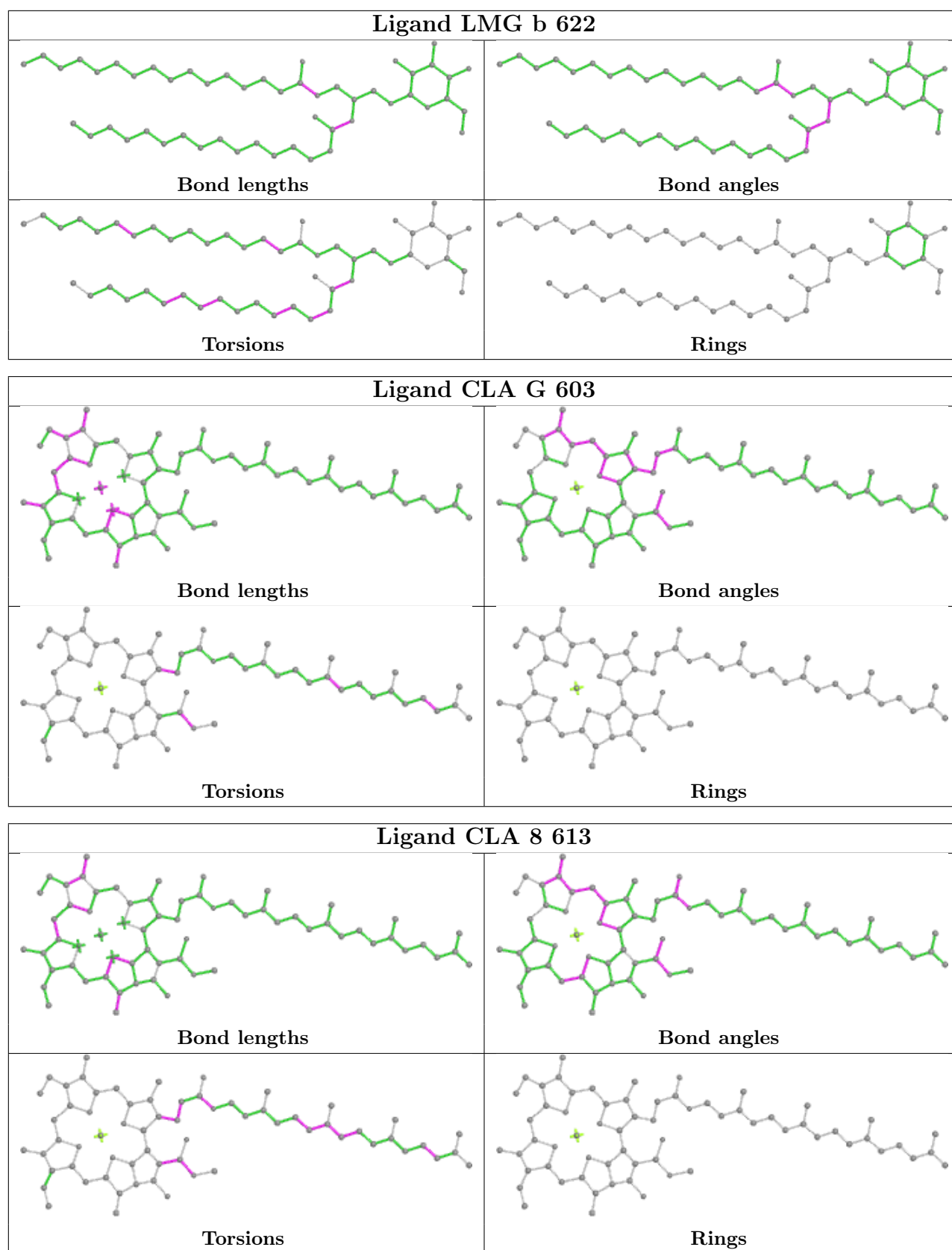
Ligand LUT 4 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

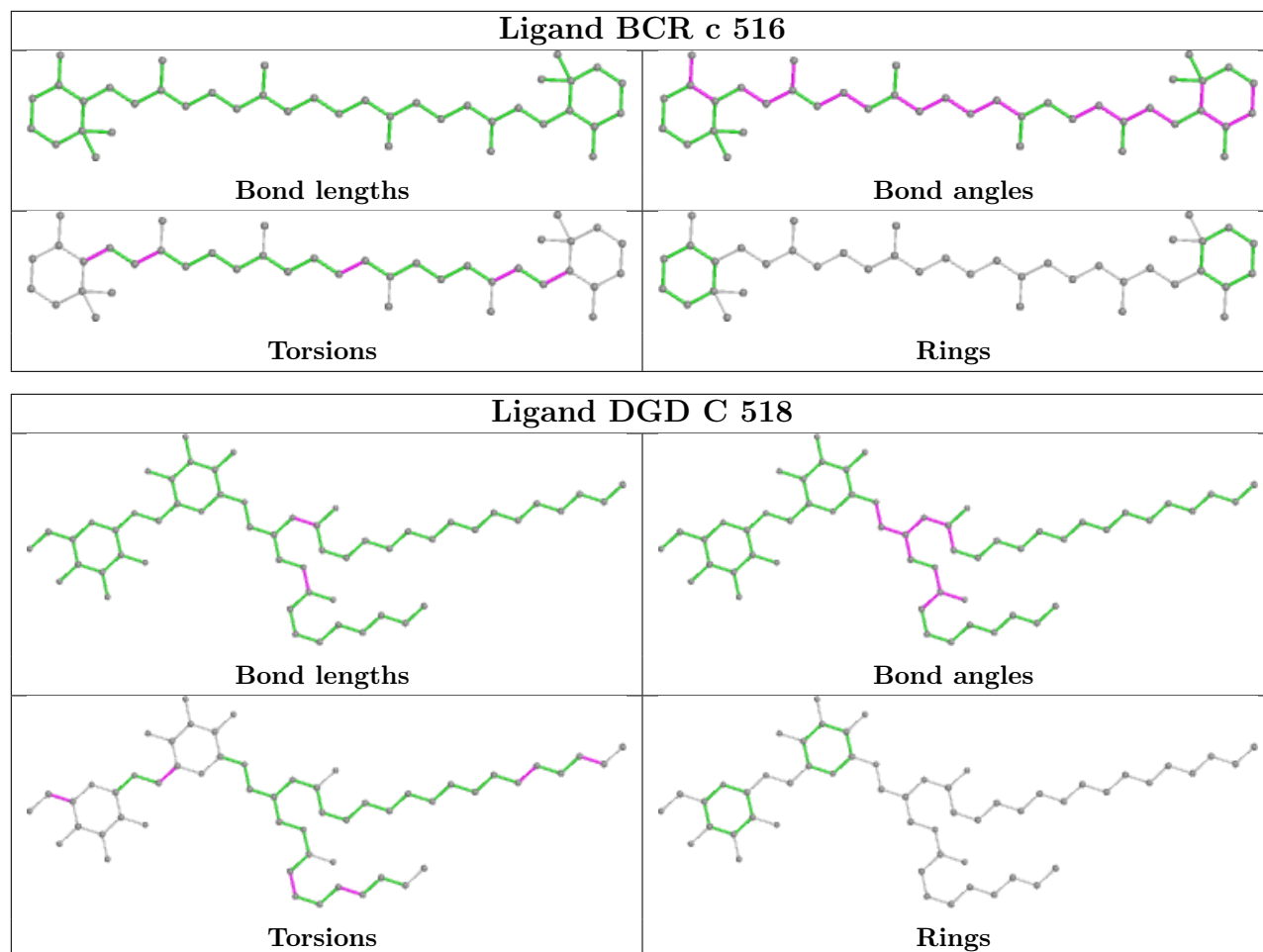
Ligand LUT n 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

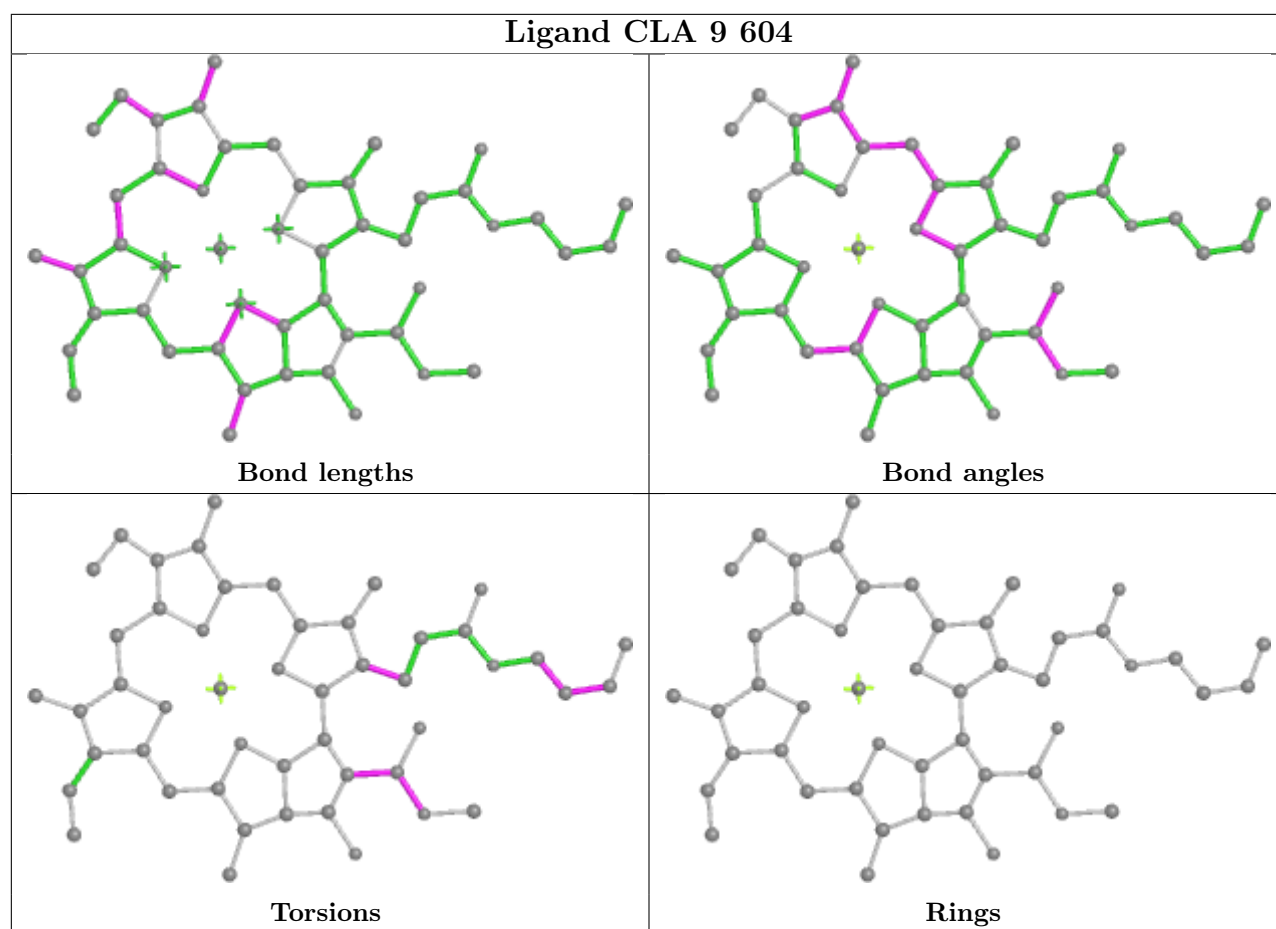


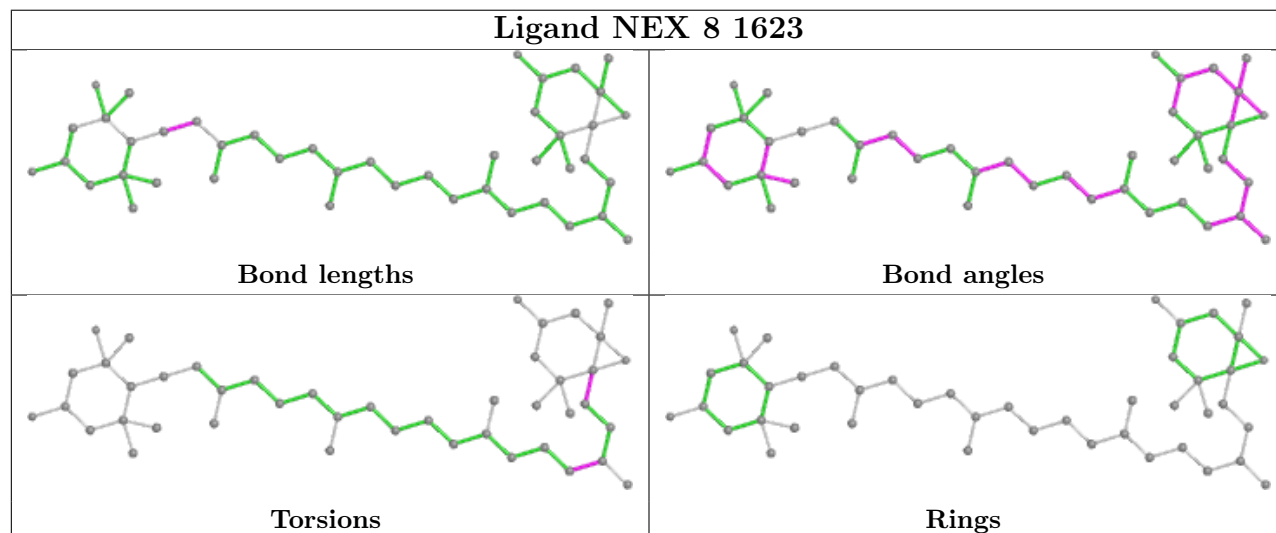
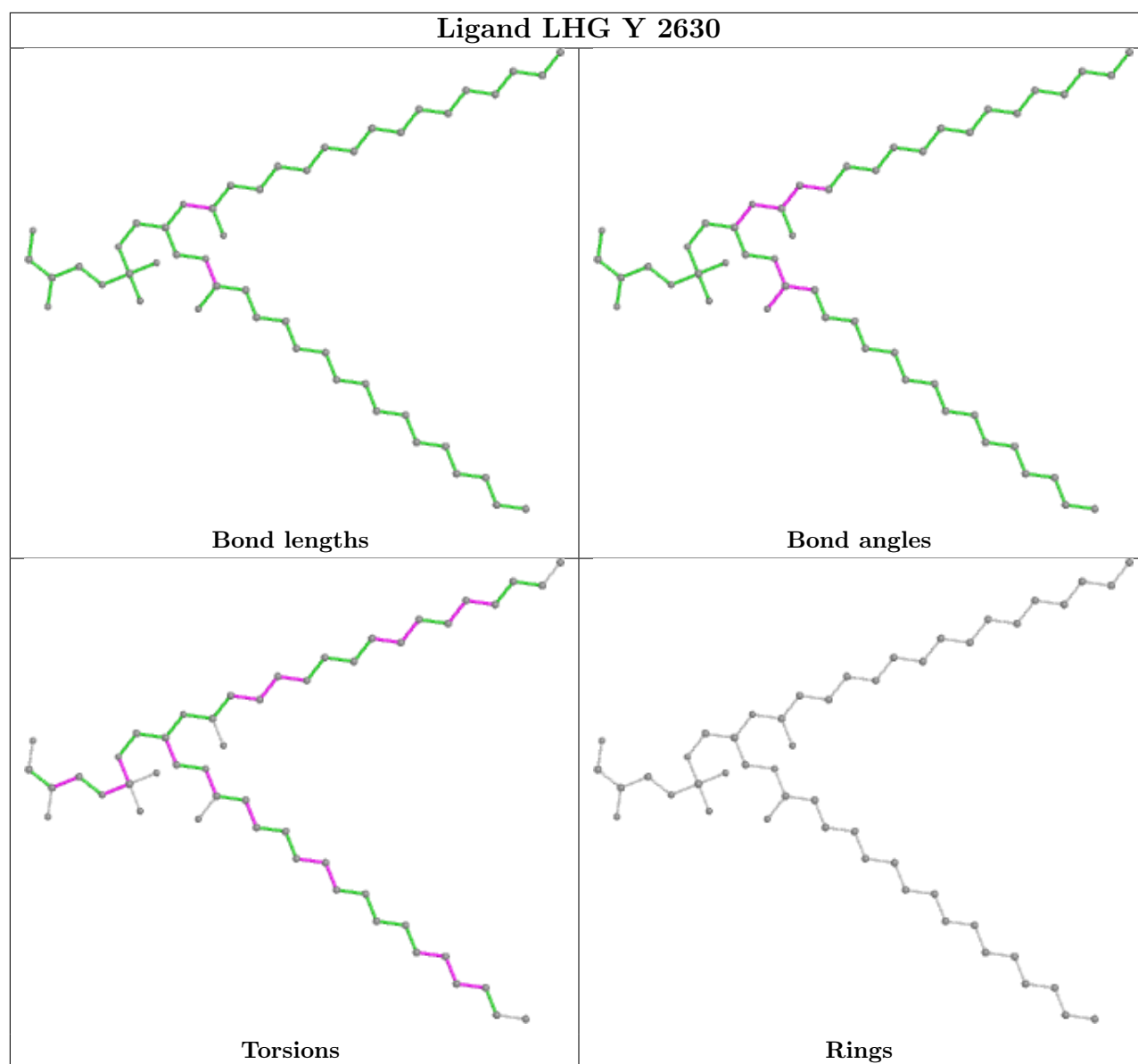


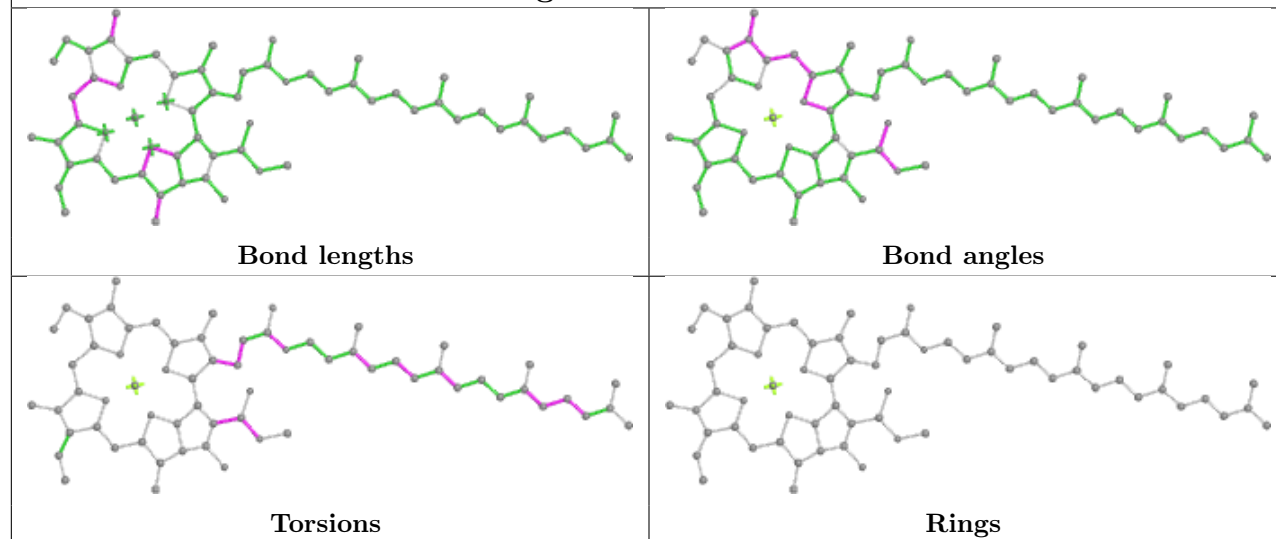
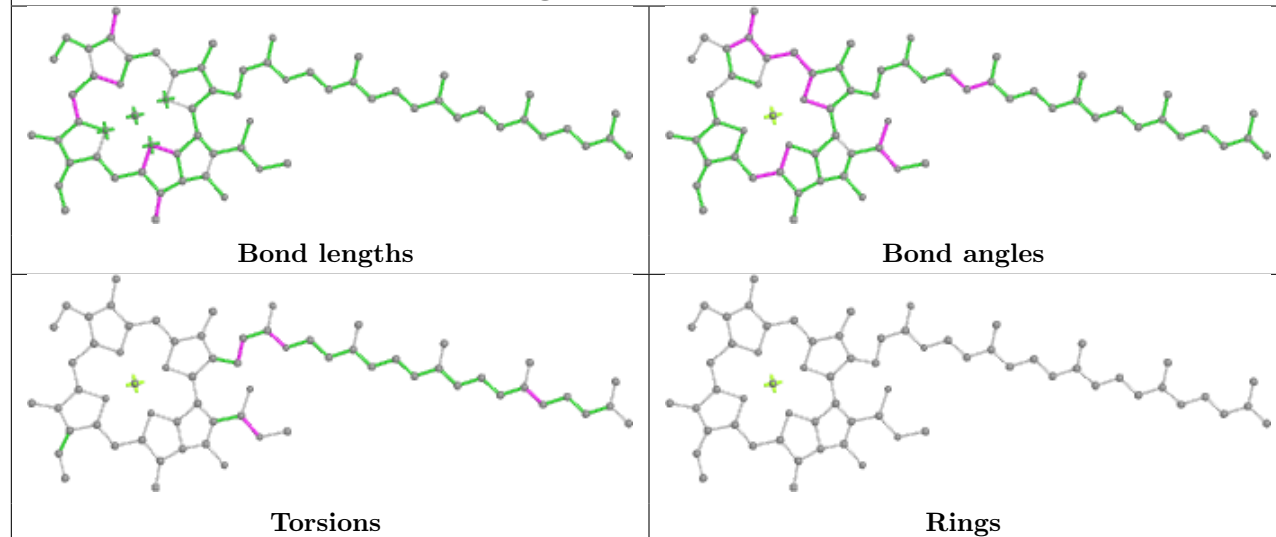


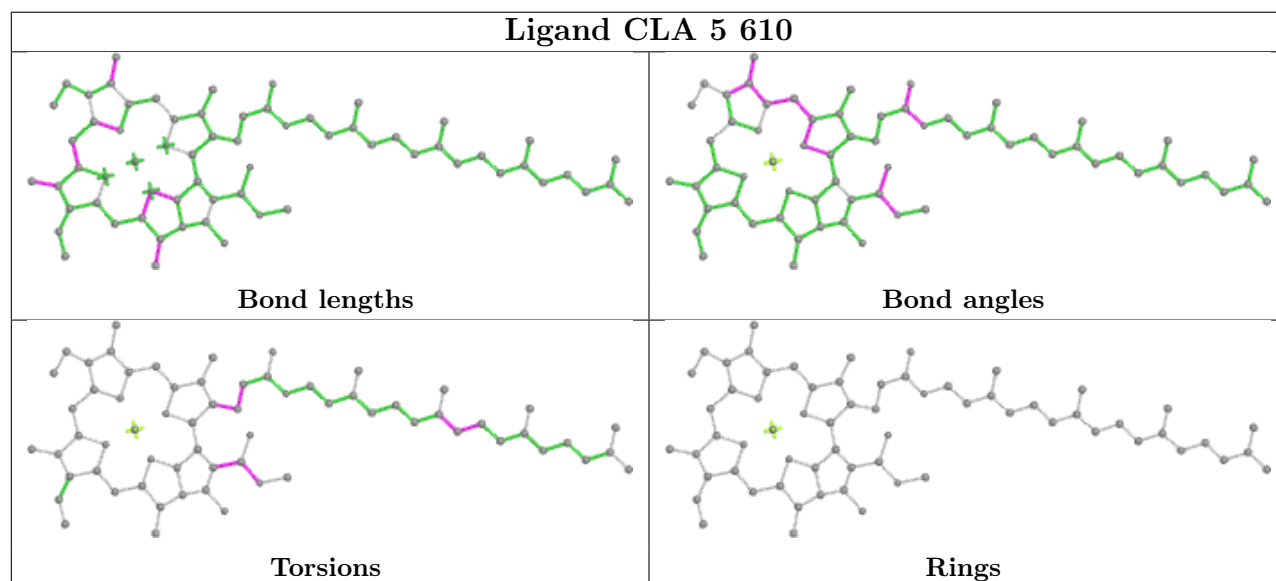
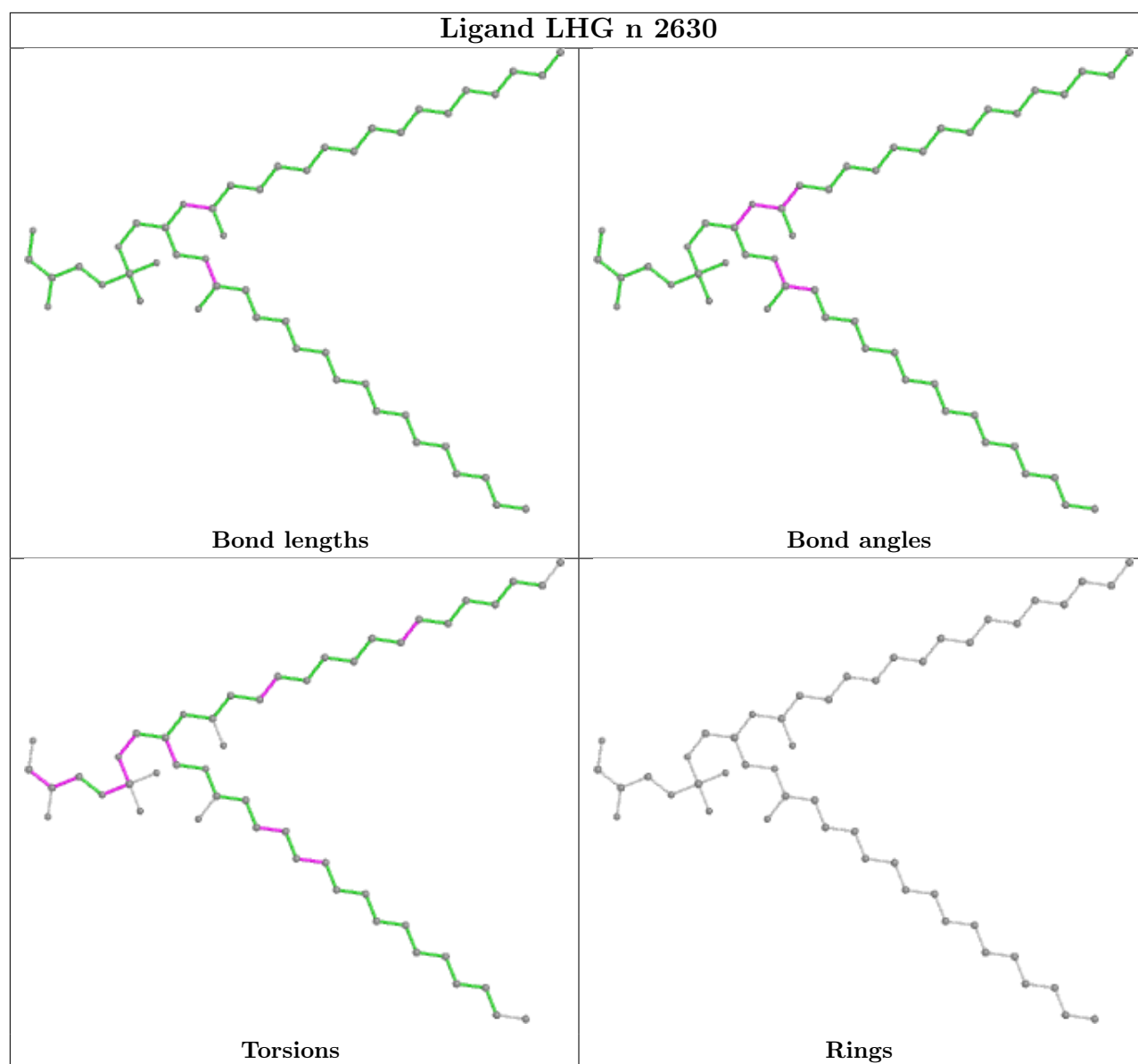




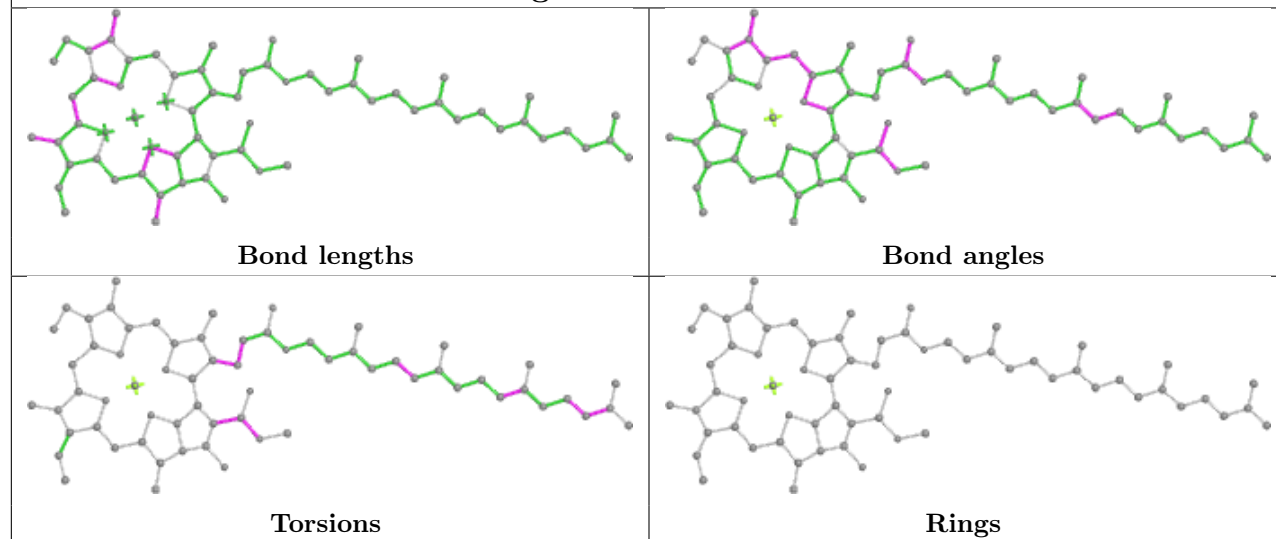




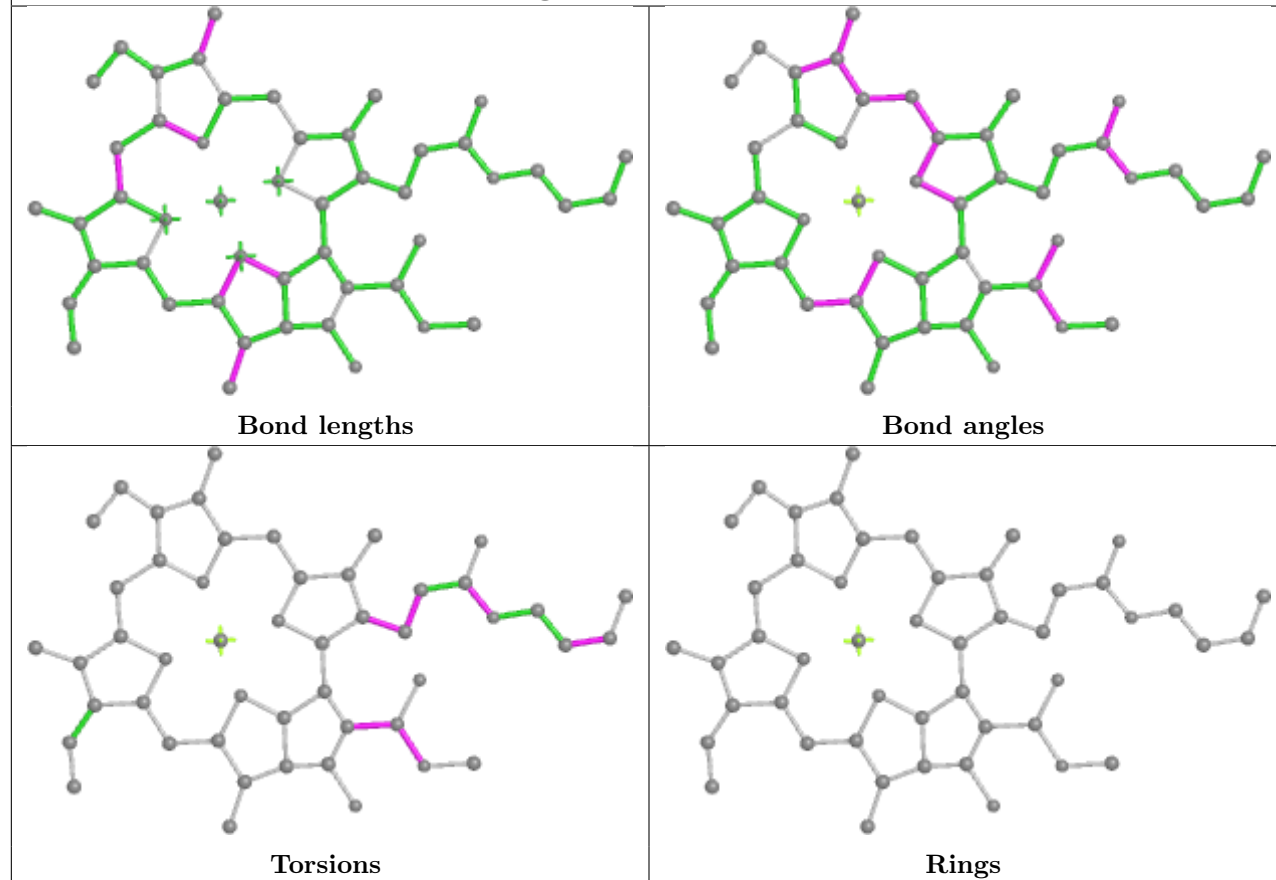
Ligand CLA 4 613**Ligand CLA 0 611**



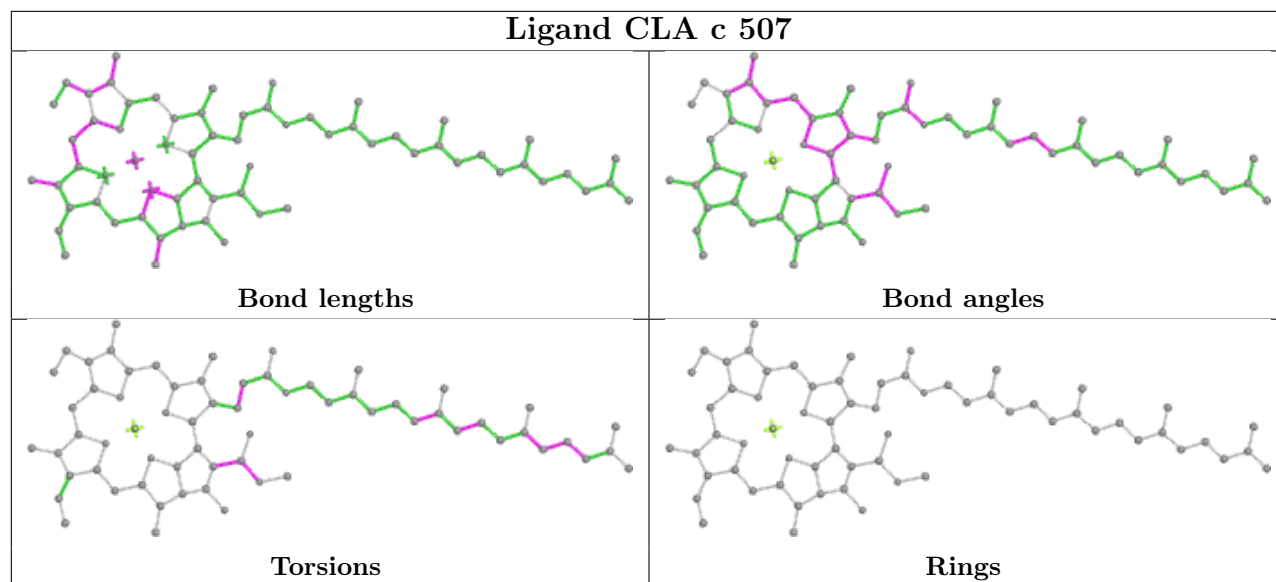
Ligand CLA Y 610



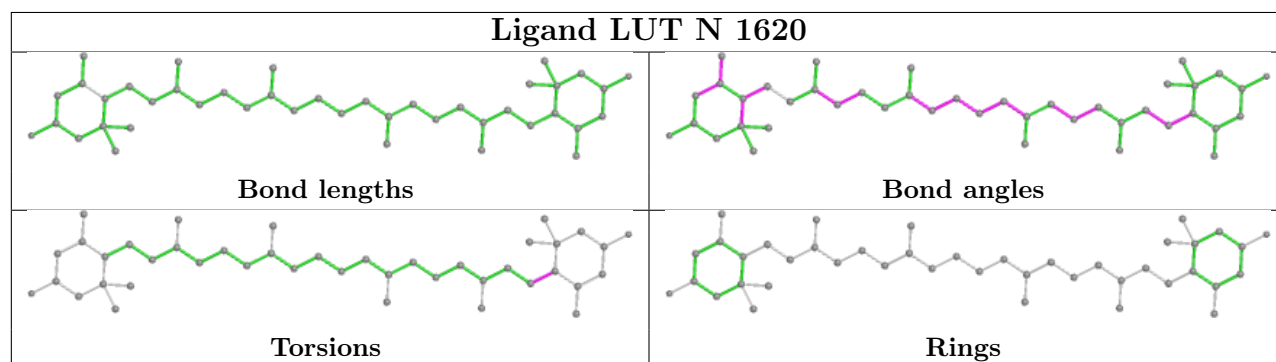
Ligand CLA 3 614



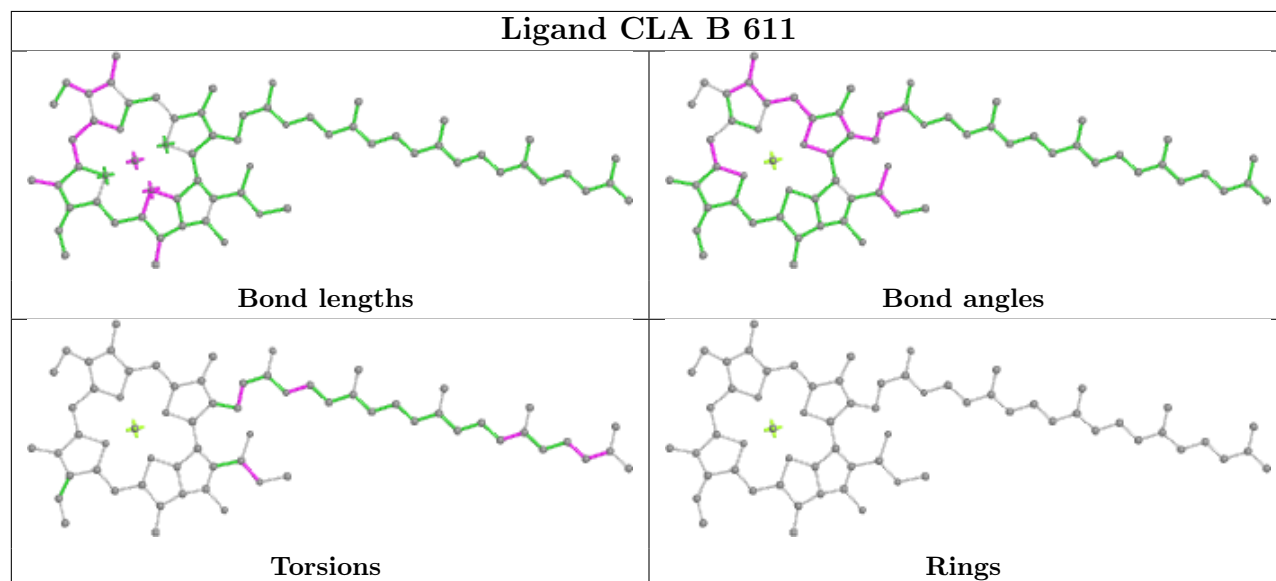
Ligand CLA c 507



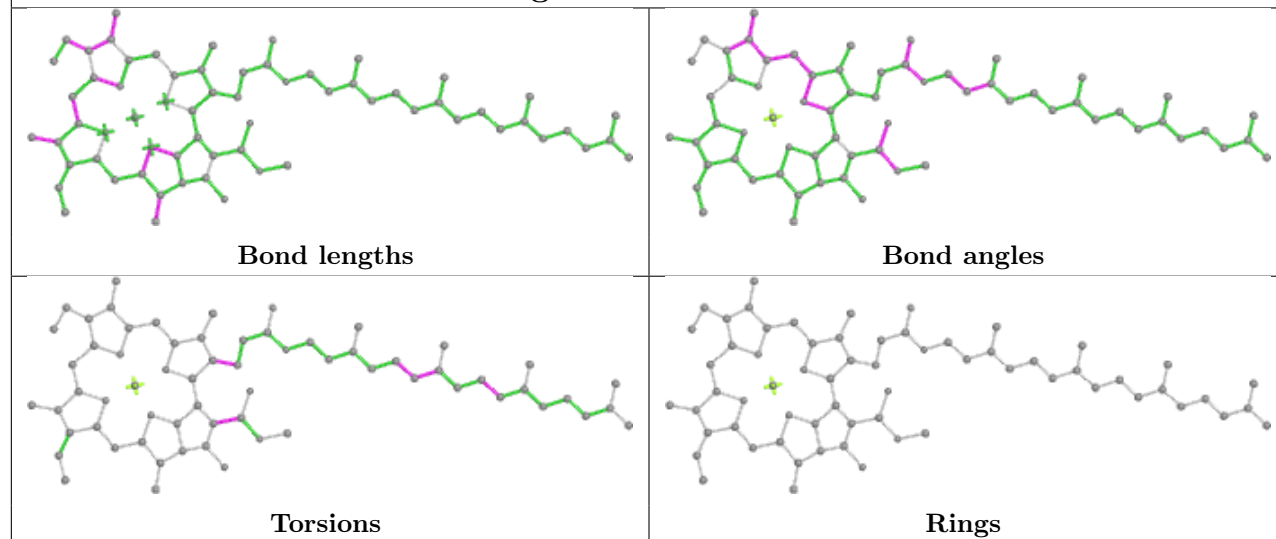
Ligand LUT N 1620



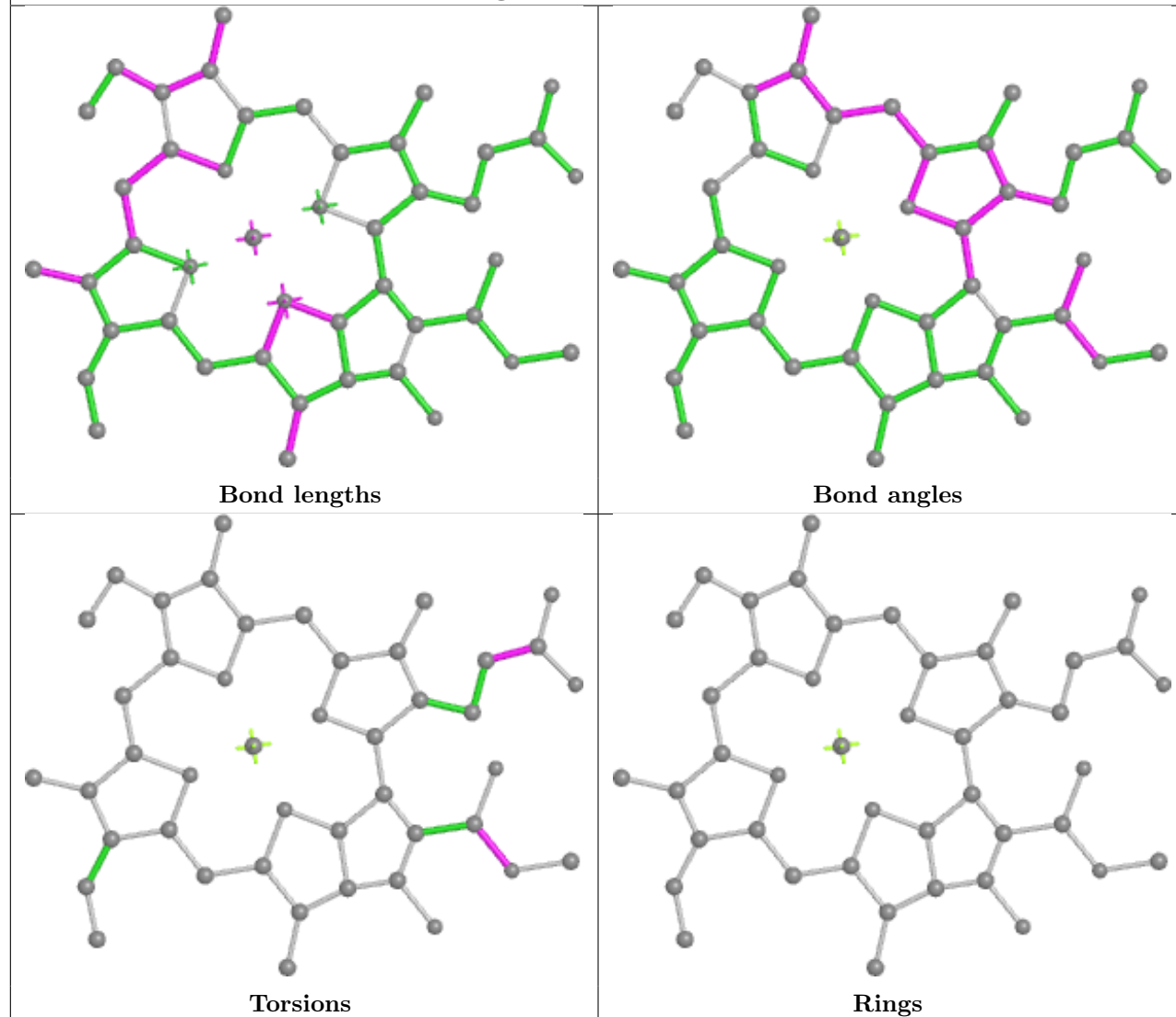
Ligand CLA B 611

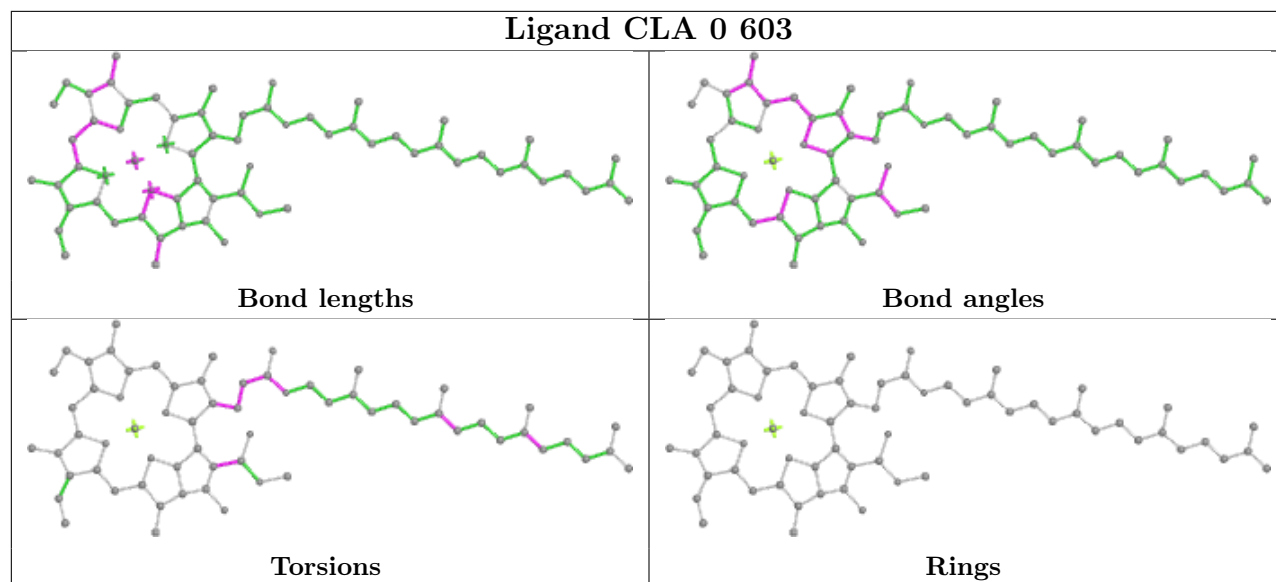
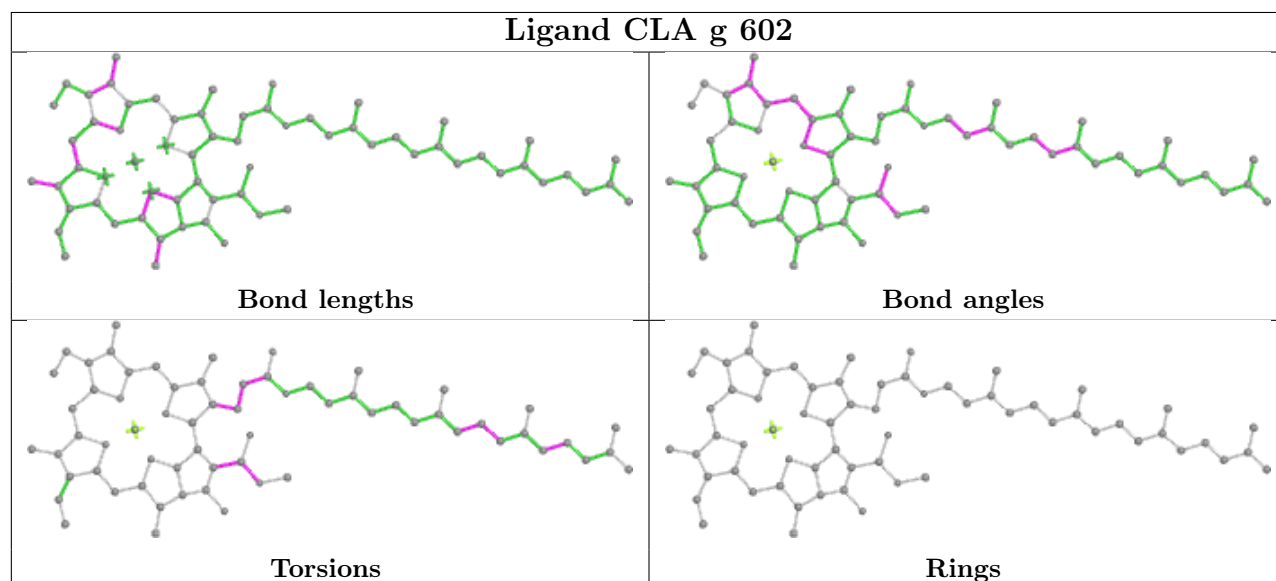
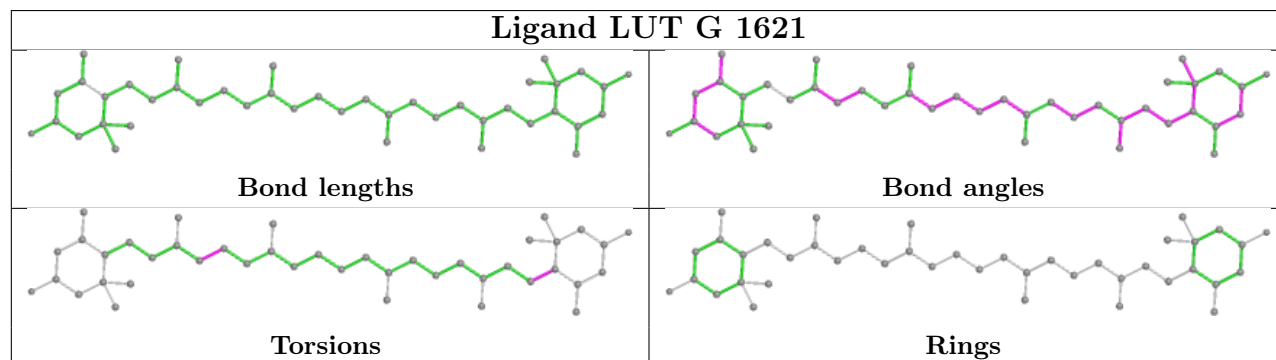


Ligand CLA N 610

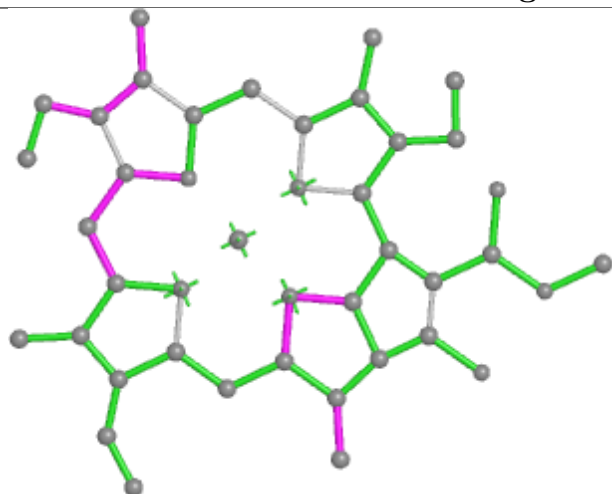


Ligand CLA S 612

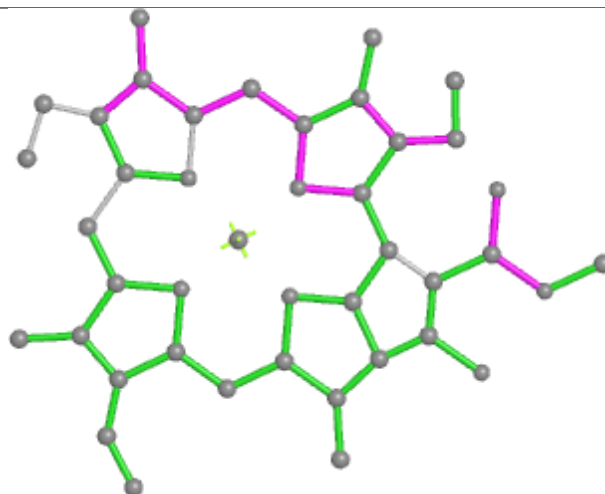


Ligand CLA 0 603**Ligand CLA g 602****Ligand LUT G 1621**

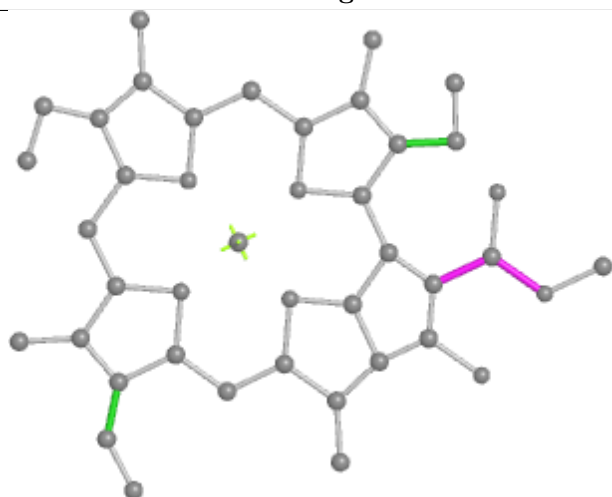
Ligand CLA s 603



Bond lengths



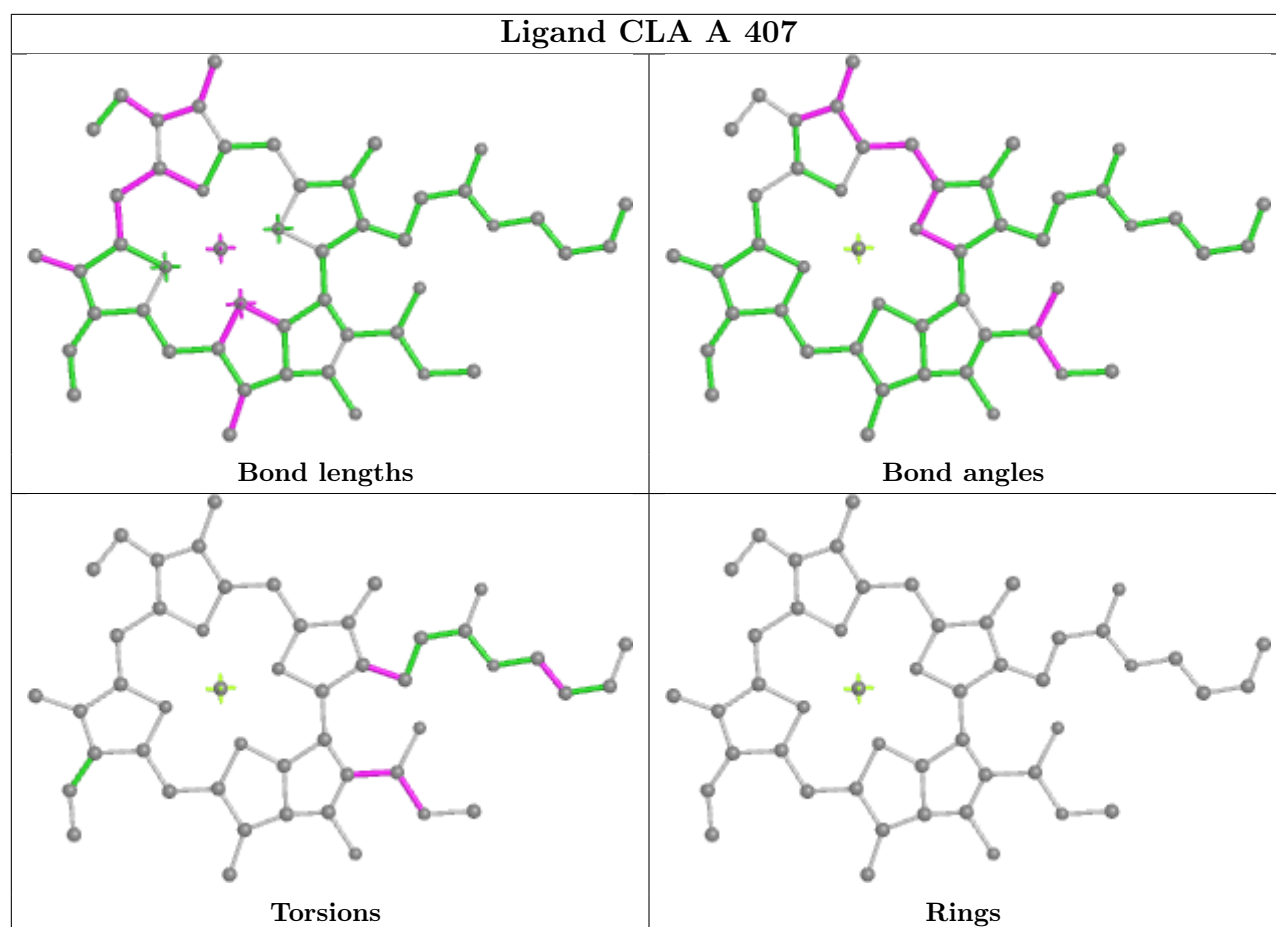
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

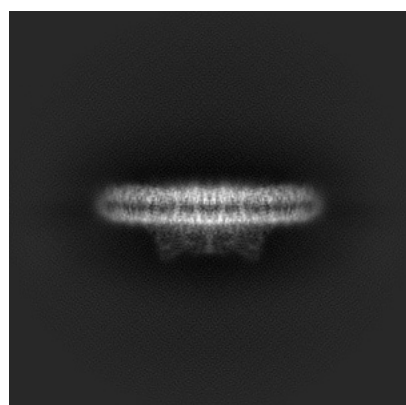
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9956. These allow visual inspection of the internal detail of the map and identification of artifacts.

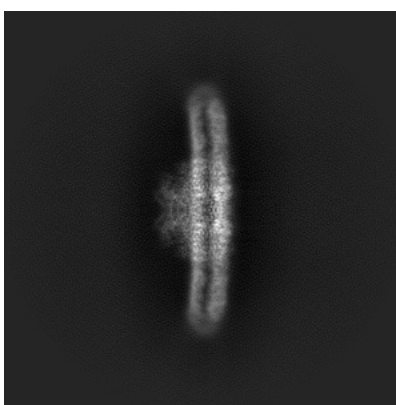
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

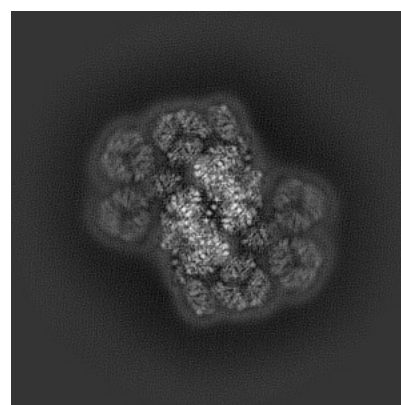
6.1.1 Primary map



X



Y

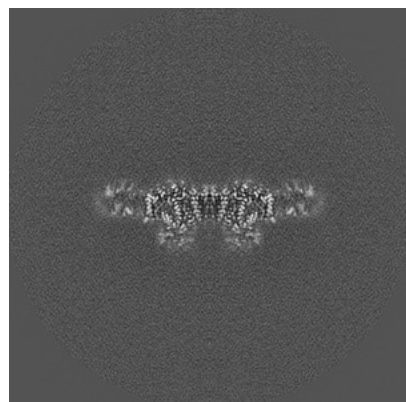


Z

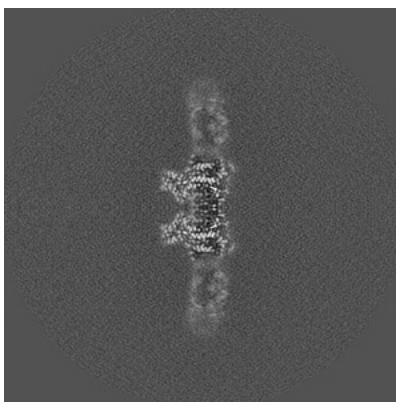
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

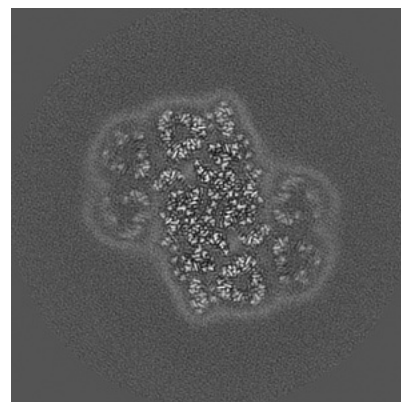
6.2.1 Primary map



X Index: 192



Y Index: 192

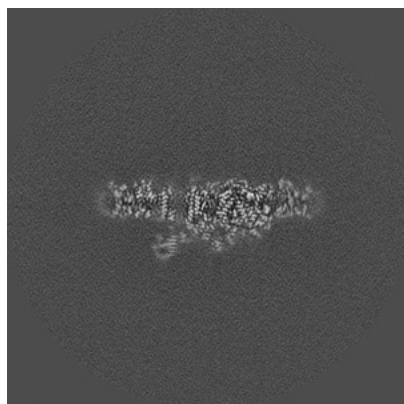


Z Index: 192

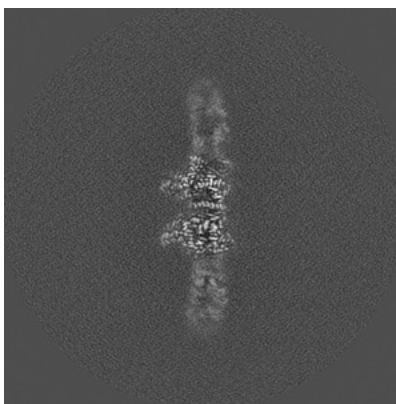
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

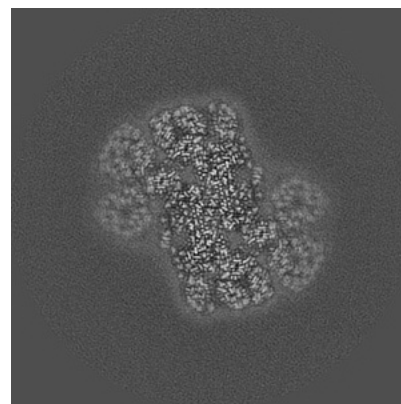
6.3.1 Primary map



X Index: 207



Y Index: 196



Z Index: 204

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

6.4 Orthogonal surface views [i](#)

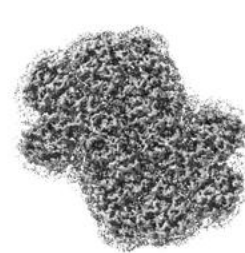
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

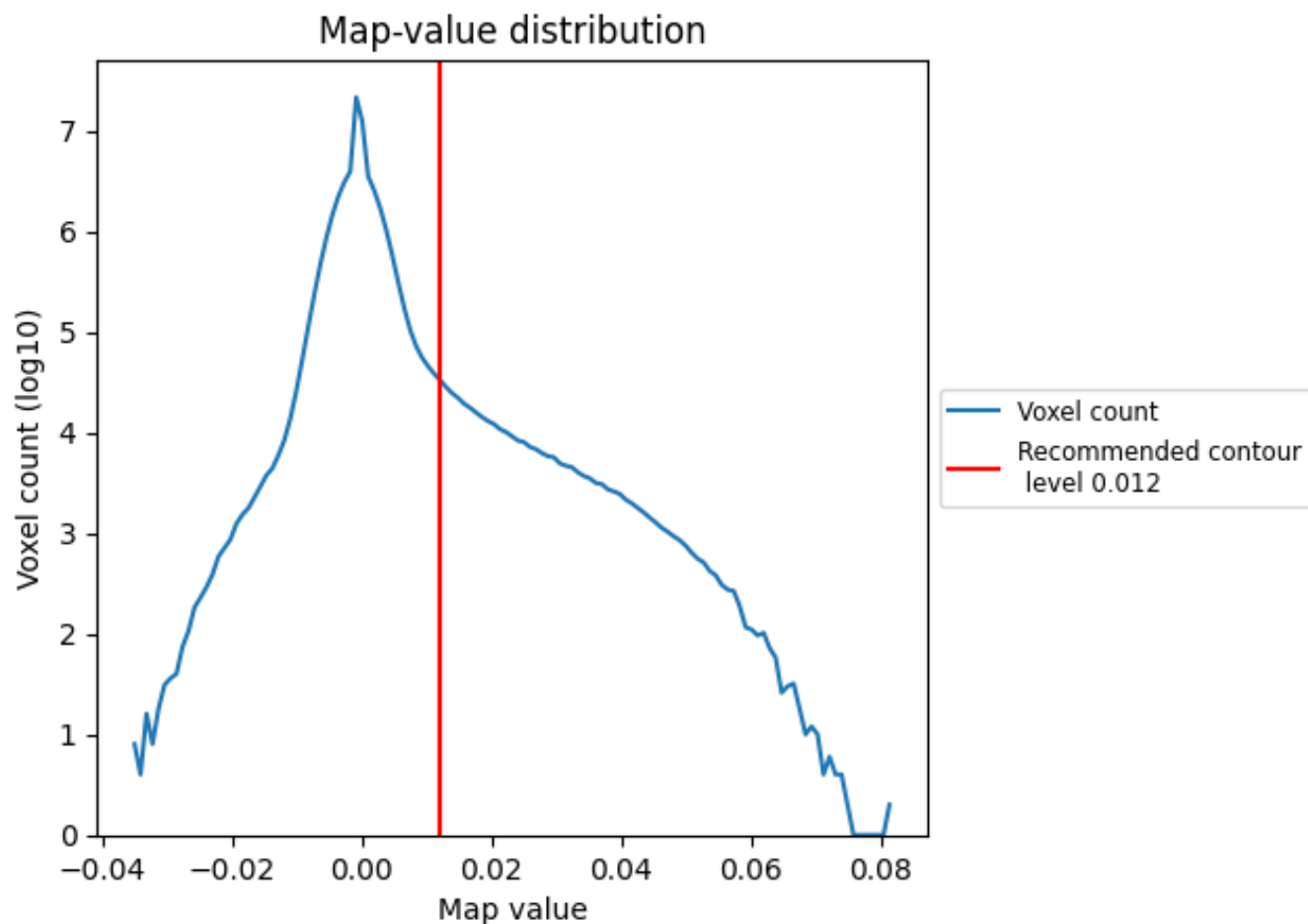
6.5 Mask visualisation

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

7 Map analysis [i](#)

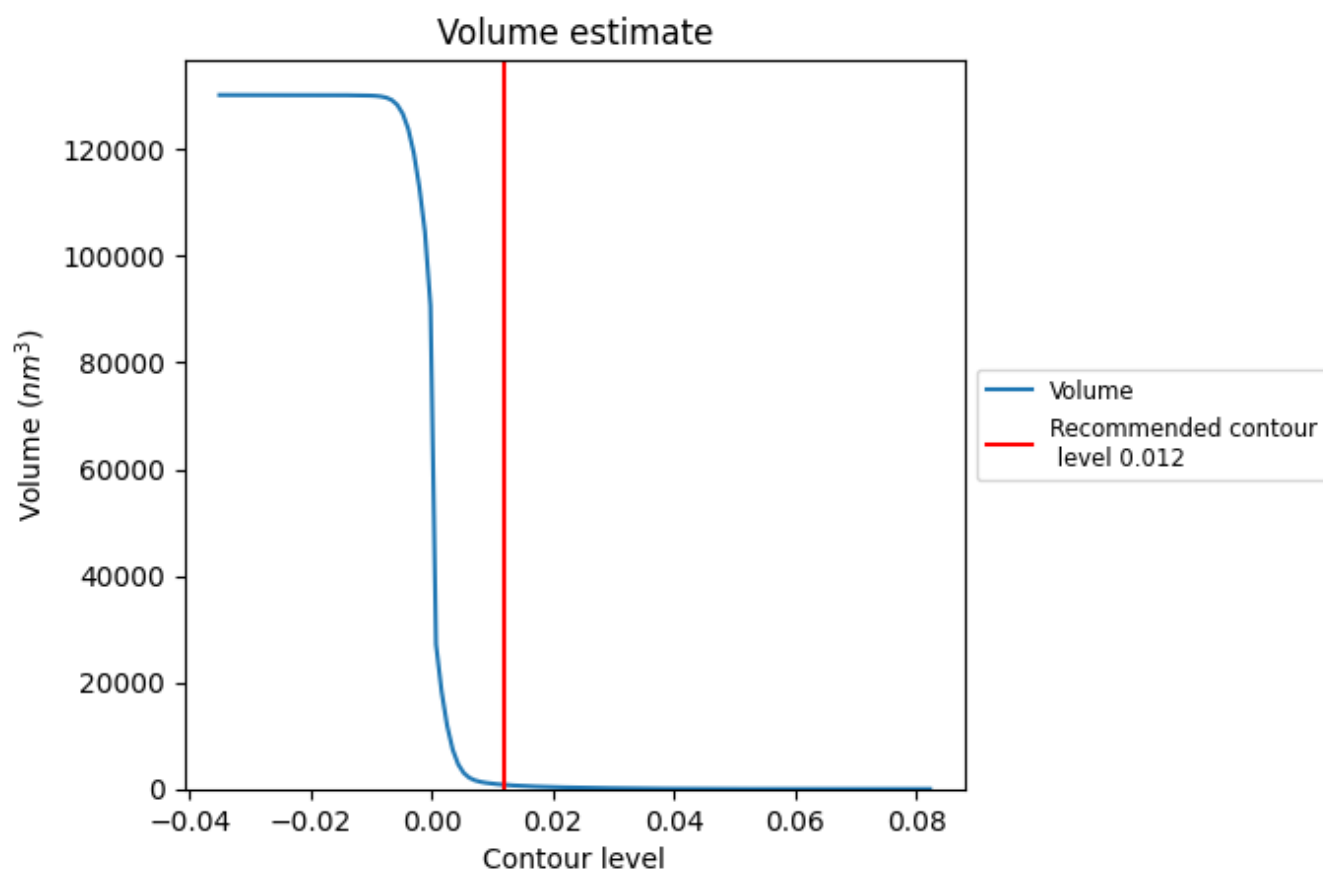
This section contains the results of statistical analysis of the map.

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.

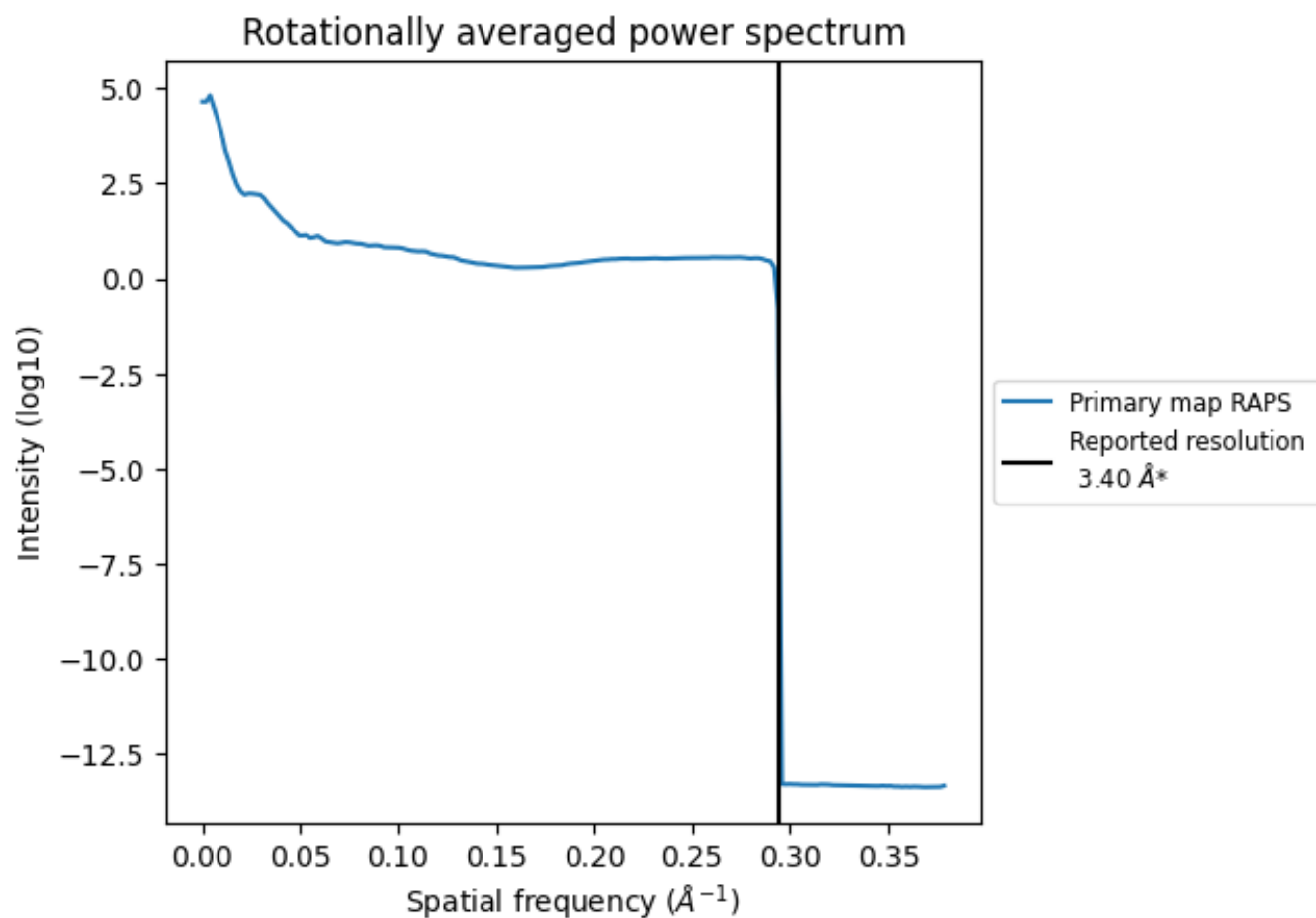
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm³; this corresponds to an approximate mass of 703 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 ⓘ

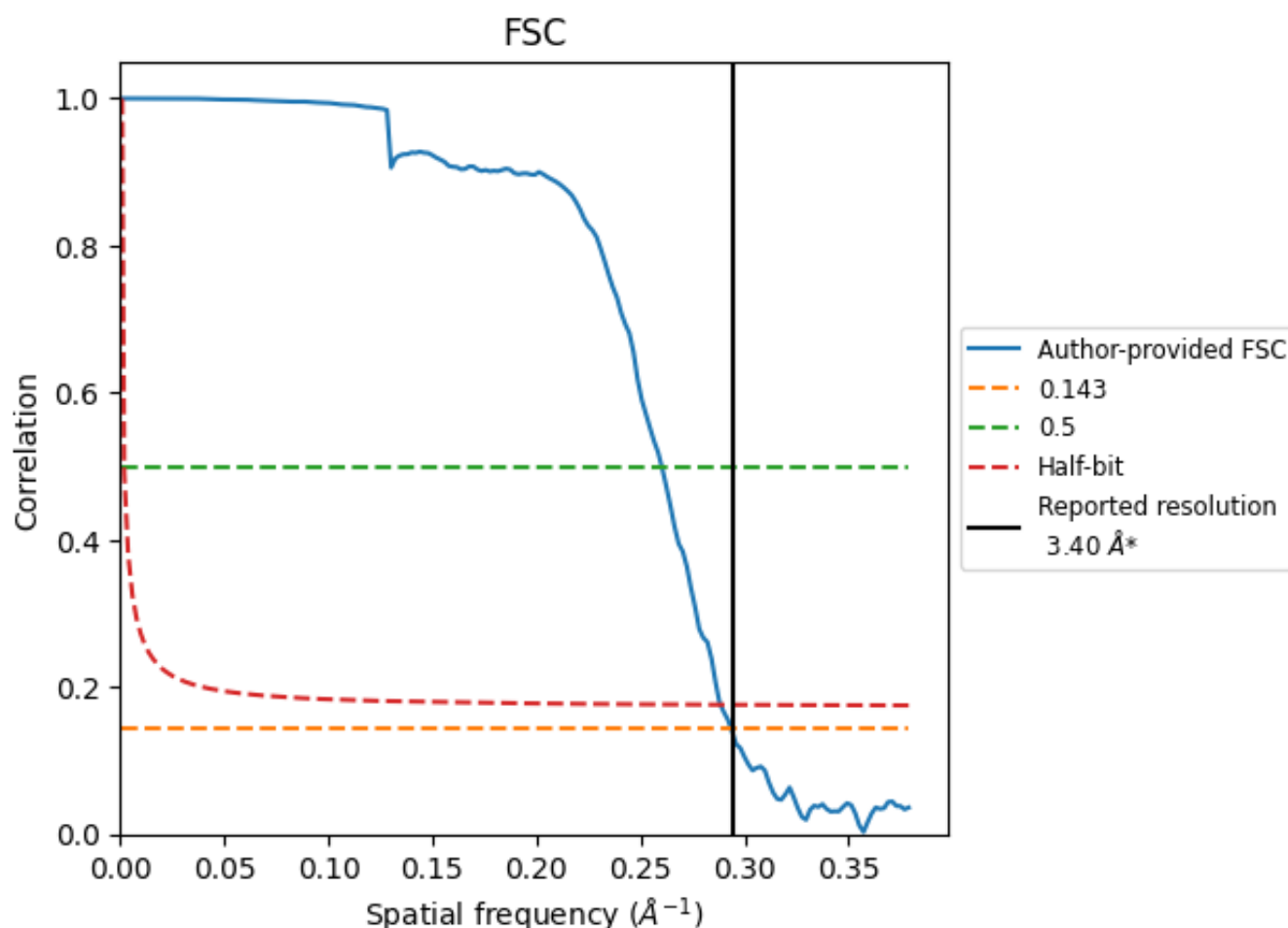


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

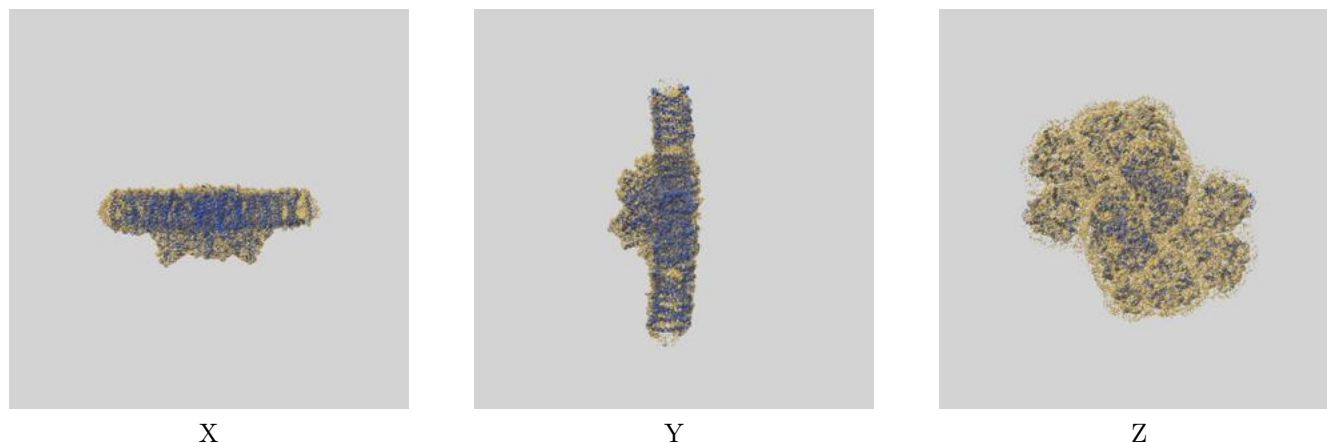
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.84	3.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

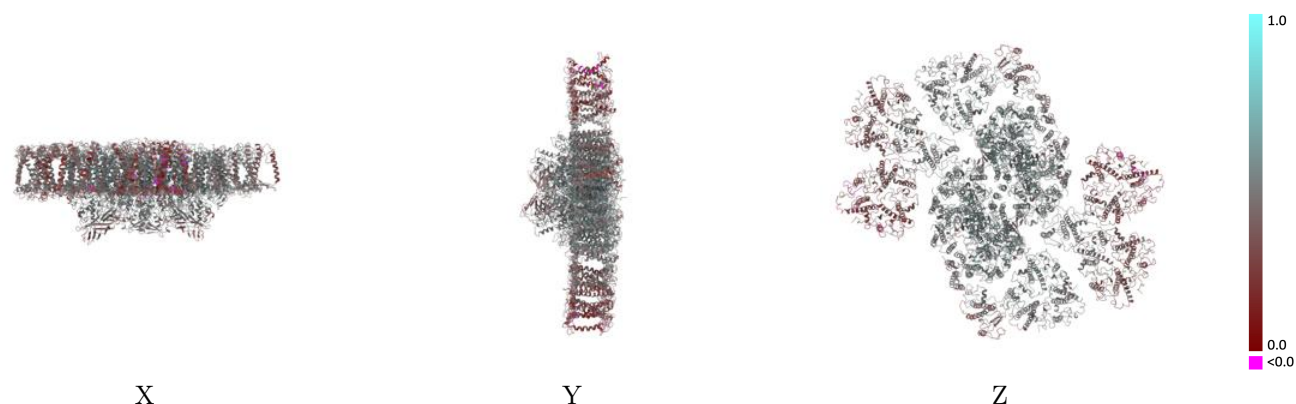
This section contains information regarding the fit between EMDB map EMD-9956 and PDB model 6KAD. Per-residue inclusion information can be found in section [3](#) on page [54](#).

9.1 Map-model overlay [i](#)



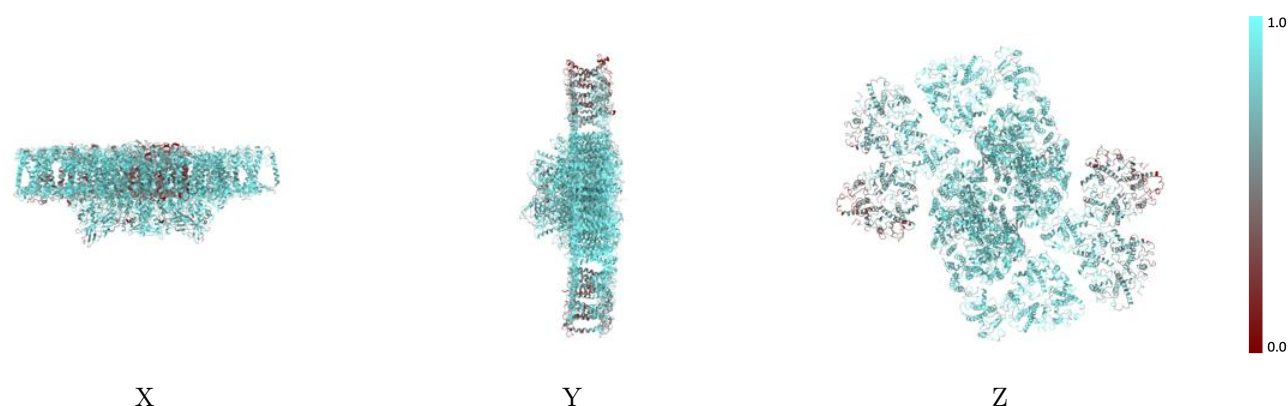
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



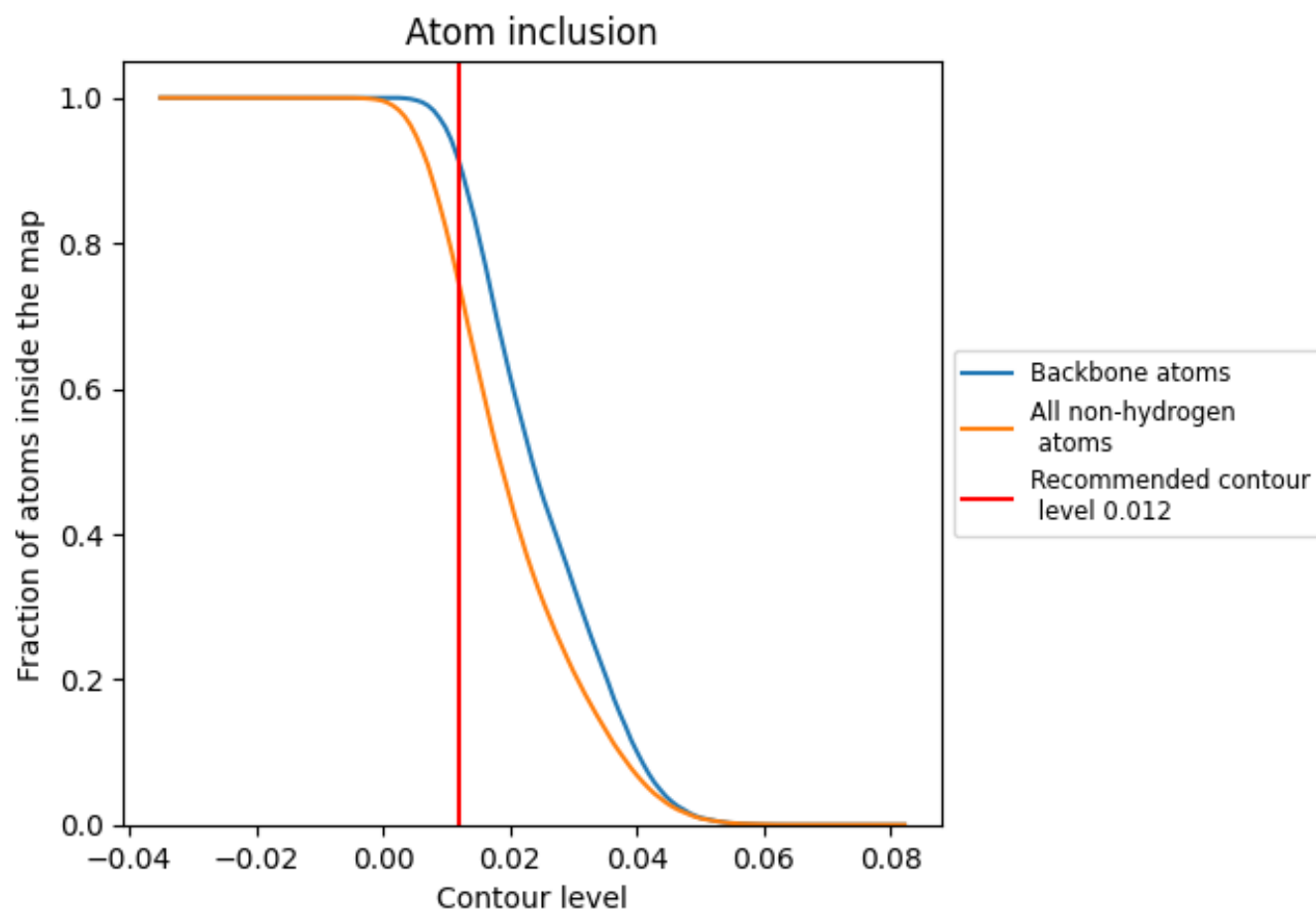
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 74% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7441	 0.4470
0	 0.5846	 0.3510
1	 0.7049	 0.4440
2	 0.5555	 0.3430
3	 0.5778	 0.3480
4	 0.4720	 0.2850
5	 0.3433	 0.2540
6	 0.5790	 0.3470
7	 0.7087	 0.4440
8	 0.5770	 0.3480
9	 0.5535	 0.3450
A	 0.8909	 0.5300
B	 0.8702	 0.5130
C	 0.8510	 0.5210
D	 0.8758	 0.5310
E	 0.8361	 0.4570
F	 0.8246	 0.4730
G	 0.8135	 0.4810
H	 0.8671	 0.5040
I	 0.9179	 0.5410
J	 0.8200	 0.4730
K	 0.8191	 0.4820
L	 0.8621	 0.5240
M	 0.8246	 0.4920
N	 0.8129	 0.4780
O	 0.7010	 0.4070
R	 0.8072	 0.4930
S	 0.7665	 0.4230
T	 0.8264	 0.5120
V	 0.7174	 0.4120
W	 0.8642	 0.5140
X	 0.8455	 0.4760
Y	 0.8583	 0.5270
Z	 0.7478	 0.4270
a	 0.8919	 0.5310



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Chain	Atom inclusion	Q-score
b	 0.8710	 0.5120
c	 0.8506	 0.5200
d	 0.8727	 0.5330
e	 0.8328	 0.4510
f	 0.8211	 0.4720
g	 0.8154	 0.4810
h	 0.8455	 0.5020
i	 0.9107	 0.5400
j	 0.8160	 0.4750
k	 0.8225	 0.4810
l	 0.8621	 0.5230
m	 0.8246	 0.4950
n	 0.8152	 0.4800
o	 0.7022	 0.4060
p	 0.3399	 0.2440
q	 0.4669	 0.2820
r	 0.8079	 0.4940
s	 0.7687	 0.4240
t	 0.8264	 0.5120
v	 0.7174	 0.4140
w	 0.8665	 0.5090
x	 0.8412	 0.4710
y	 0.8586	 0.5250
z	 0.7325	 0.4220