



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:27 PM UTC

PDB ID : 6KAD / pdb_00006kad
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

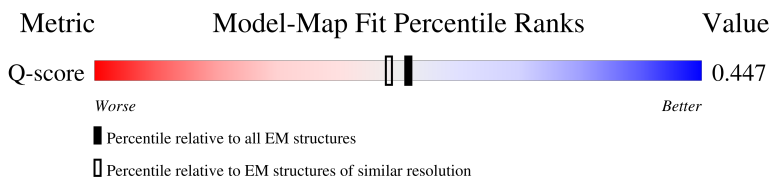
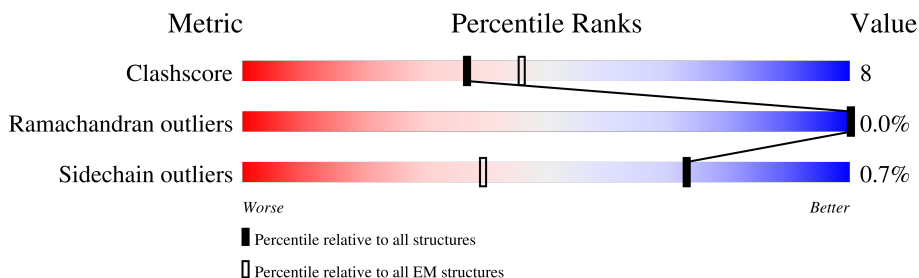
1 Overall quality at a glance

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.



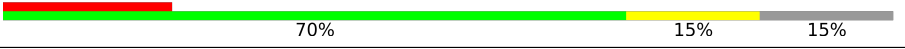
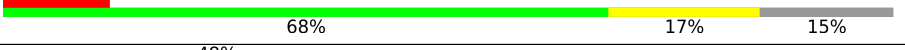
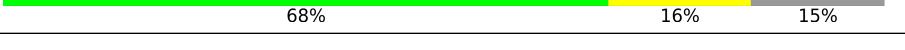
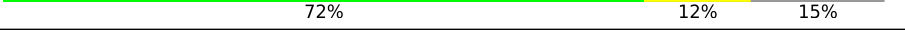
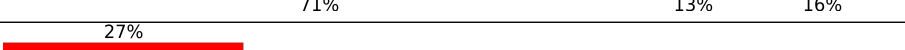
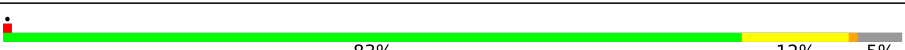
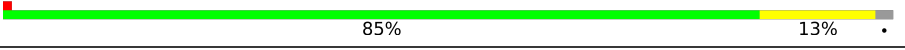
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	8% 63% 21% 16%
1	1	256	76% 9% 15%
1	6	256	11% 62% 23% 16%
1	7	256	74% 11% 15%

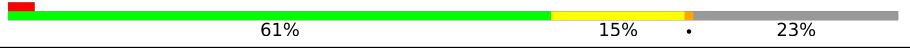
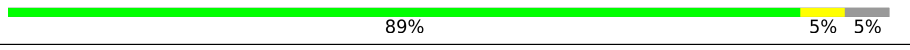
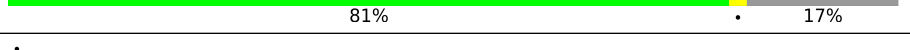
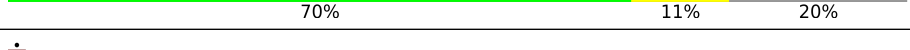
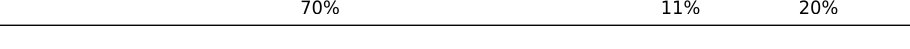
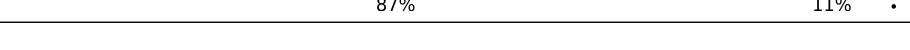
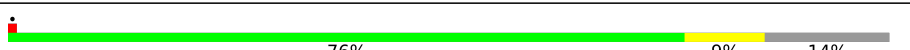
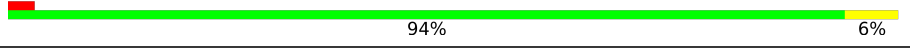
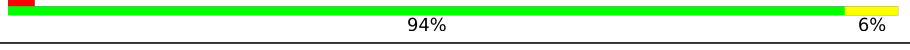
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Mol	Chain	Length	Quality of chain
1	Y	256	
1	y	256	
2	2	257	
2	3	257	
2	5	257	
2	8	257	
2	9	257	
2	N	257	
2	n	257	
2	p	257	
3	4	249	
3	G	249	
3	g	249	
3	q	249	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	461	
6	c	461	
7	D	352	
7	d	352	
8	E	82	
8	e	82	
9	F	44	

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Mol	Chain	Length	Quality of chain
9	f	44	
10	H	88	
10	h	88	
11	I	37	
11	i	37	
12	J	42	
12	j	42	
13	K	46	
13	k	46	
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	291	
16	o	291	
17	R	280	
17	r	280	
18	S	289	
18	s	289	
19	T	31	
19	t	31	
20	V	33	
20	v	33	
21	W	115	
21	w	115	

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Mol	Chain	Length	Quality of chain
22	X	101	
22	x	101	
23	Z	62	
23	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	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	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-
38	BCT	D	401	-	-	X	-
38	BCT	d	401	-	-	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		

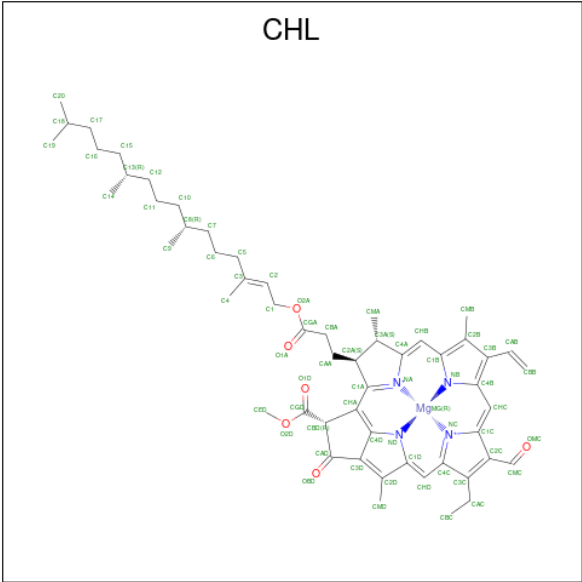
- Molecule 22 is a protein called 4.1 kDa photosystem II subunit.

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 (CCD ID: 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
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	3	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	4	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	4	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	4	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	4	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	5	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	6	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
24	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	0	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	0	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	7	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	8	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	8	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	9	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
24	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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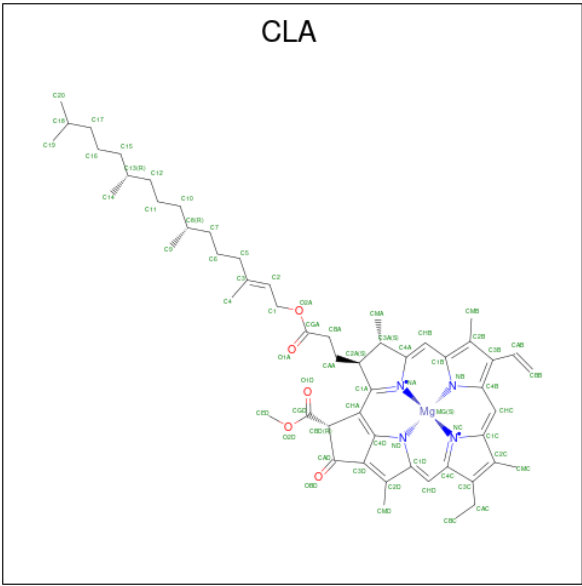
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
24	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	n	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	0	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	0	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	9	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	9	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	9	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	9	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	p	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	p	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	q	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	q	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	q	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 49	C 39	Mg 1	N 4	O 5	0

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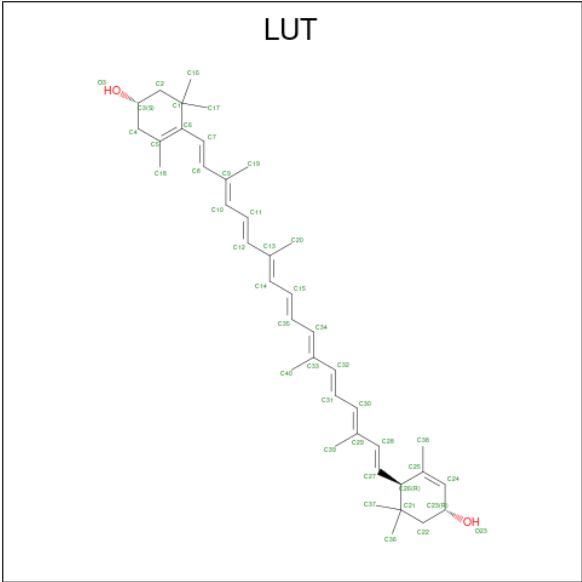
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	r	1	Total 65	C 55	Mg 1	N 4	O 5	0

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



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			42	40	2	

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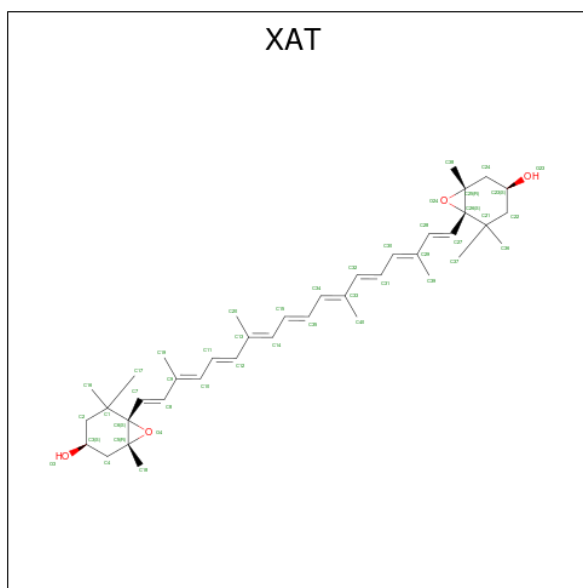
Mol	Chain	Residues	Atoms			AltConf
26	N	1	Total 42	C 40	O 2	0
26	N	1	Total 42	C 40	O 2	0
26	R	1	Total 42	C 40	O 2	0
26	S	1	Total 42	C 40	O 2	0
26	S	1	Total 42	C 40	O 2	0
26	Y	1	Total 42	C 40	O 2	0
26	Y	1	Total 42	C 40	O 2	0
26	0	1	Total 42	C 40	O 2	0
26	0	1	Total 42	C 40	O 2	0
26	7	1	Total 42	C 40	O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

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Mol	Chain	Residues	Atoms			AltConf
26	n	1	Total	C	O	0
			42	40	2	
26	n	1	Total	C	O	0
			42	40	2	
26	s	1	Total	C	O	0
			42	40	2	
26	s	1	Total	C	O	0
			42	40	2	
26	y	1	Total	C	O	0
			42	40	2	
26	y	1	Total	C	O	0
			42	40	2	
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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



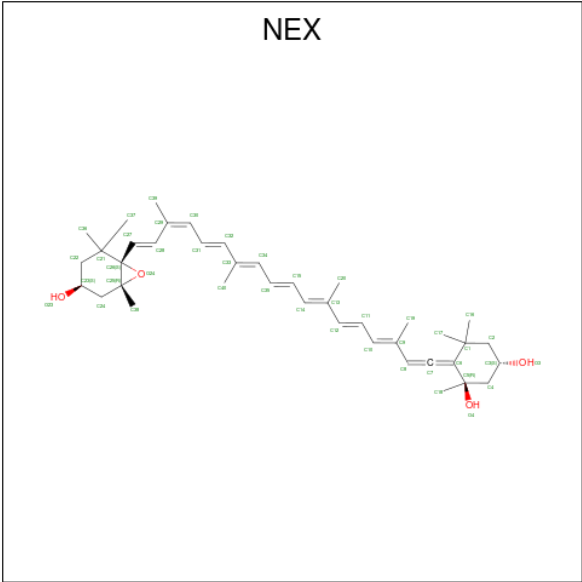
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	

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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 (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



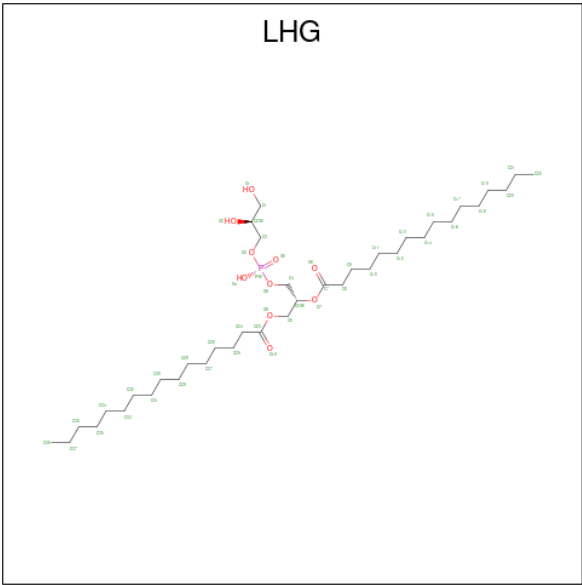
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			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 (CCD ID: 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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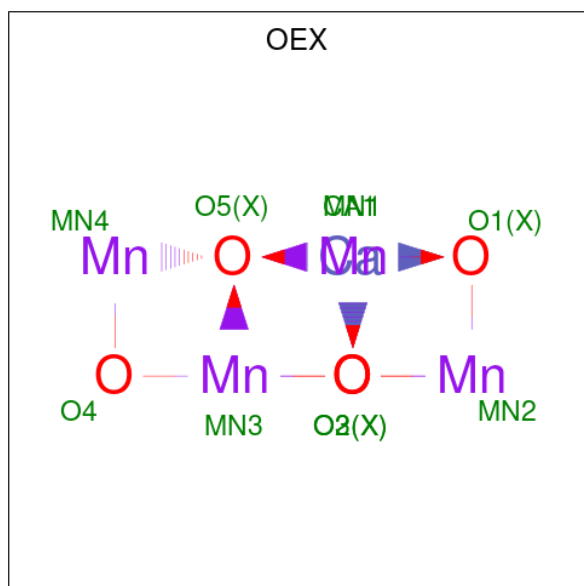
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total 49	C 38	O 10	P 1	0
29	5	1	Total 49	C 38	O 10	P 1	0
29	6	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 47	C 36	O 10	P 1	0
29	D	1	Total 44	C 33	O 10	P 1	0
29	D	1	Total 49	C 38	O 10	P 1	0
29	D	1	Total 39	C 28	O 10	P 1	0
29	G	1	Total 49	C 38	O 10	P 1	0
29	L	1	Total 49	C 38	O 10	P 1	0
29	N	1	Total 49	C 38	O 10	P 1	0
29	R	1	Total 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 44	C 33	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	d	1	Total	C	O	P	0
			49	38	10	1	
29	d	1	Total	C	O	P	0
			39	28	10	1	
29	g	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	
29	n	1	Total	C	O	P	0
			49	38	10	1	
29	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 (CCD ID: 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	

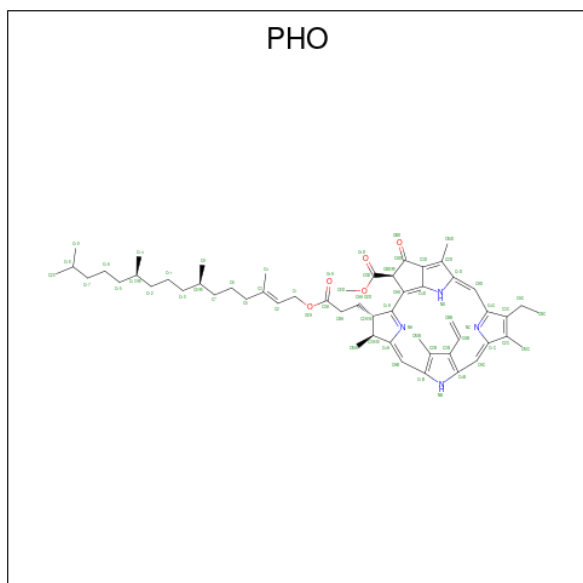
- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: CL) (formula: Cl).

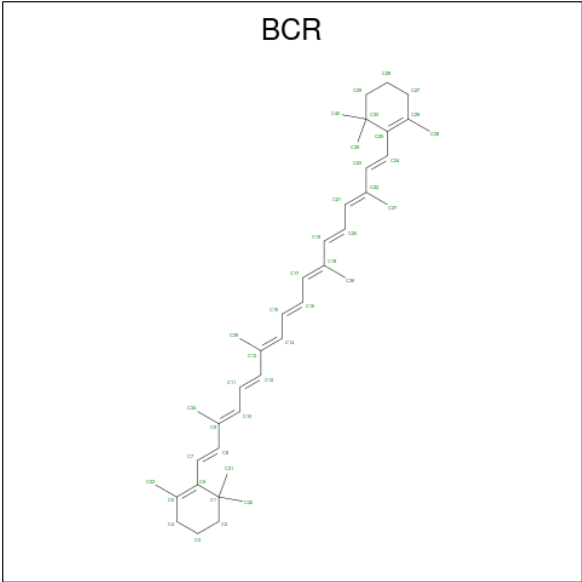
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Cl	0
			1	1	
32	a	1	Total	Cl	0
			1	1	

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



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

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



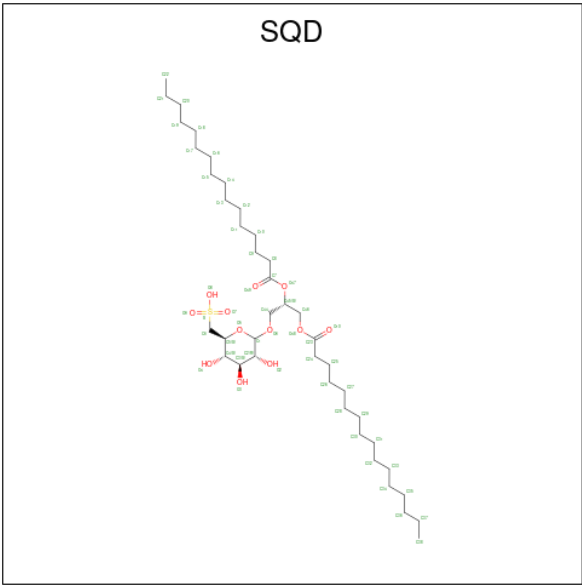
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	C	0
			40	40	
34	B	1	Total	C	0
			40	40	
34	B	1	Total	C	0
			40	40	
34	B	1	Total	C	0
			40	40	
34	C	1	Total	C	0
			40	40	
34	C	1	Total	C	0
			40	40	
34	C	1	Total	C	0
			40	40	
34	C	1	Total	C	0
			40	40	
34	D	1	Total	C	0
			40	40	
34	H	1	Total	C	0
			40	40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

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Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	C	0
			40	40	
34	c	1	Total	C	0
			40	40	
34	c	1	Total	C	0
			40	40	
34	c	1	Total	C	0
			40	40	
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 (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



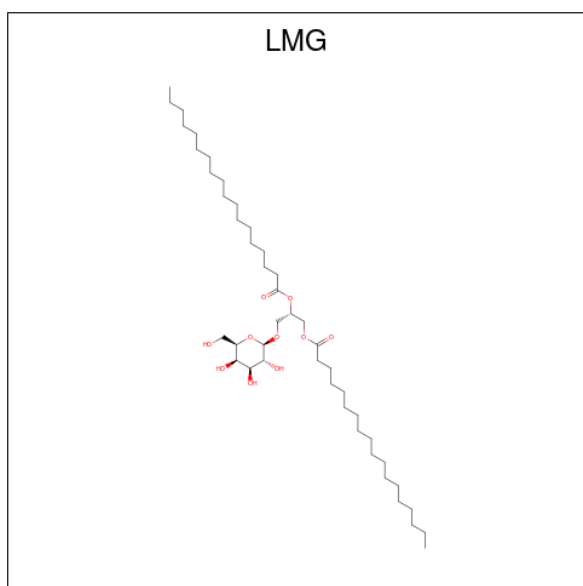
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			54	41	12	1	
35	B	1	Total	C	O	S	0
			50	37	12	1	
35	D	1	Total	C	O	S	0
			52	39	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	

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Mol	Chain	Residues	Atoms				AltConf
35	b	1	Total	C	O	S	0
			54	41	12	1	
35	b	1	Total	C	O	S	0
			50	37	12	1	
35	d	1	Total	C	O	S	0
			52	39	12	1	

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



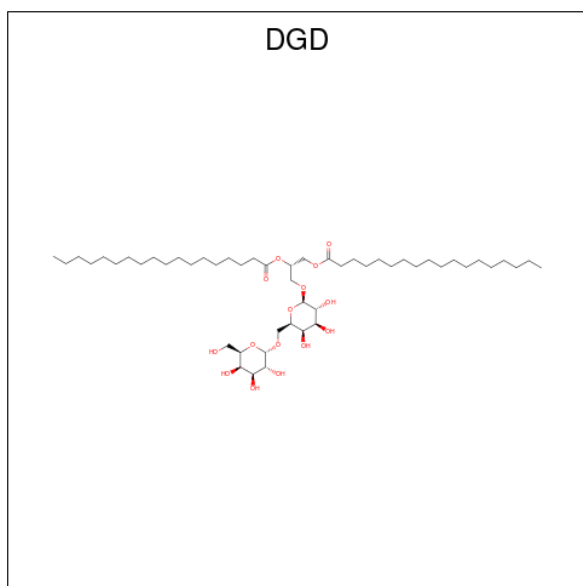
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			48	38	10	
36	B	1	Total	C	O	0
			51	41	10	
36	C	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			46	36	10	
36	D	1	Total	C	O	0
			46	36	10	
36	H	1	Total	C	O	0
			48	38	10	
36	S	1	Total	C	O	0
			52	42	10	
36	a	1	Total	C	O	0
			48	38	10	

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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
			46	36	10	
36	d	1	Total	C	O	0
			46	36	10	
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) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



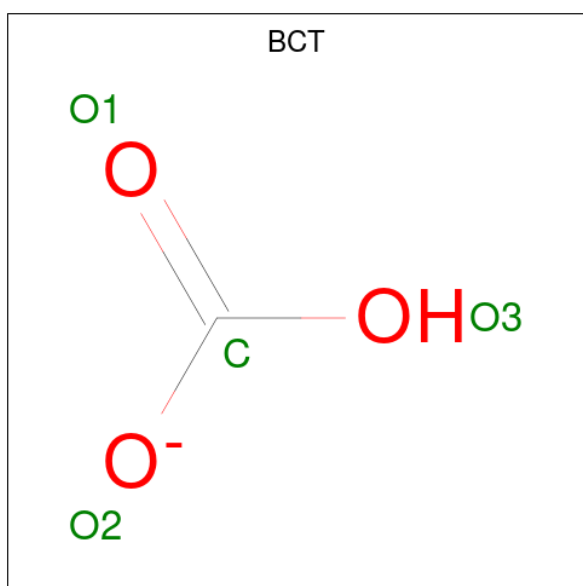
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			55	40	15	
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			66	51	15	
37	C	1	Total	C	O	0
			66	51	15	

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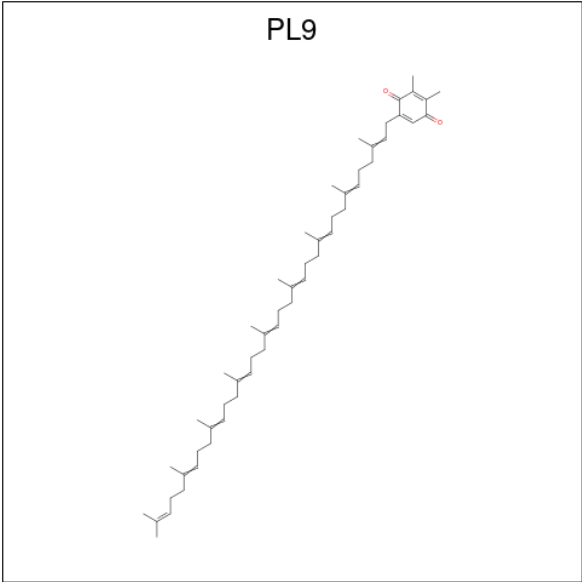
Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			62	47	15	
37	c	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			66	51	15	

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



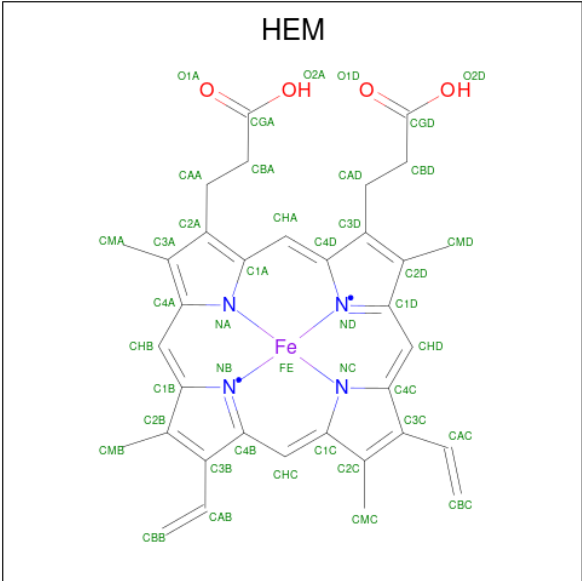
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			4	1	3	
38	d	1	Total	C	O	0
			4	1	3	

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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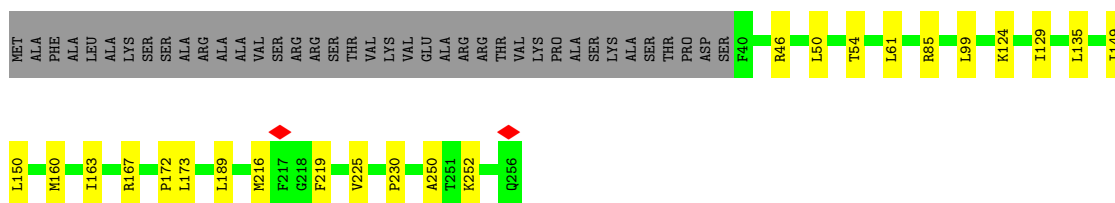
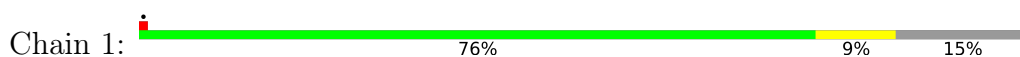
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
40	f	1	43	34	1	4	4	0

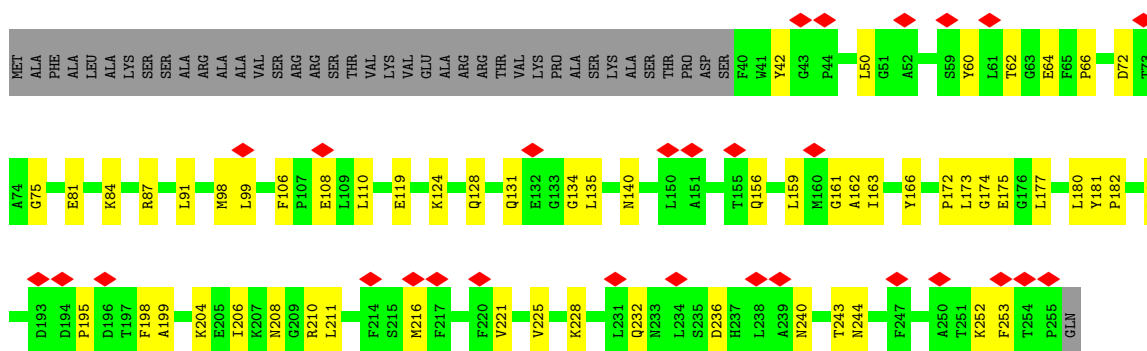
3 Residue-property plots [i](#)

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.

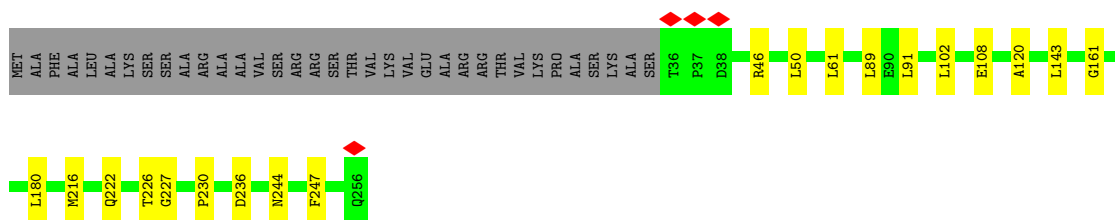
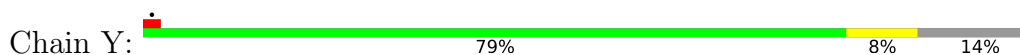
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



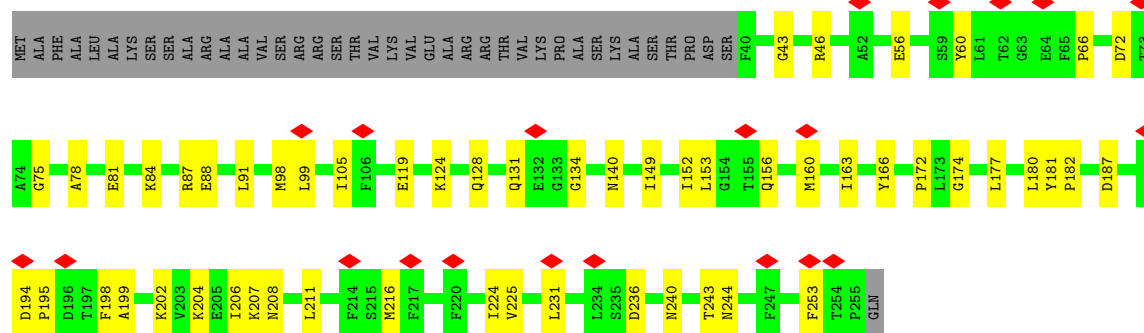
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



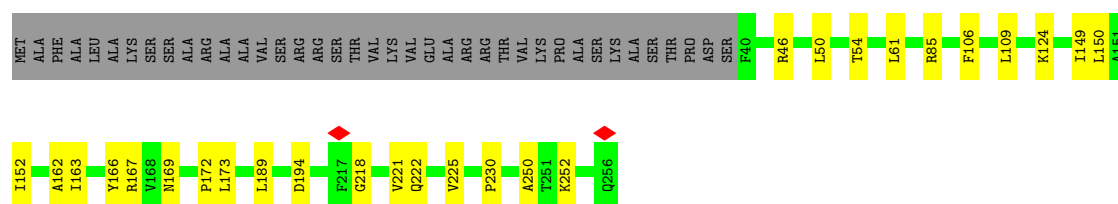
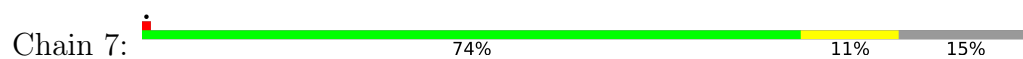
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



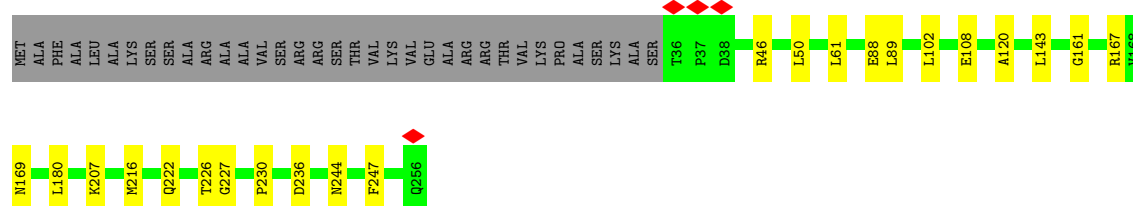
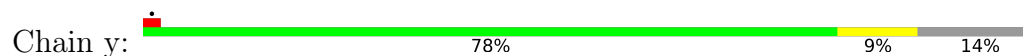
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



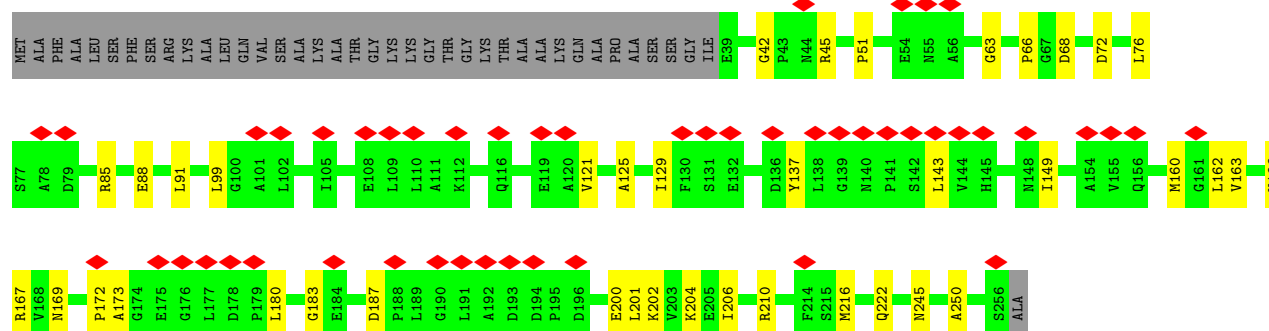
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

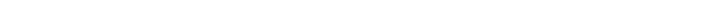


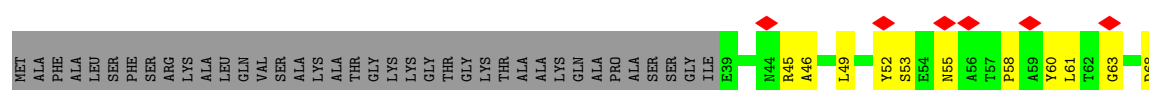
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

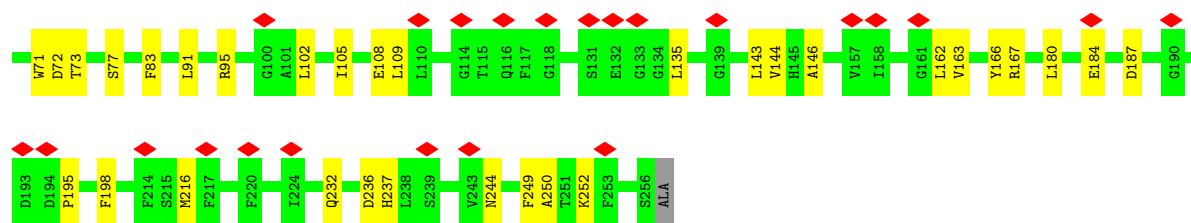


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

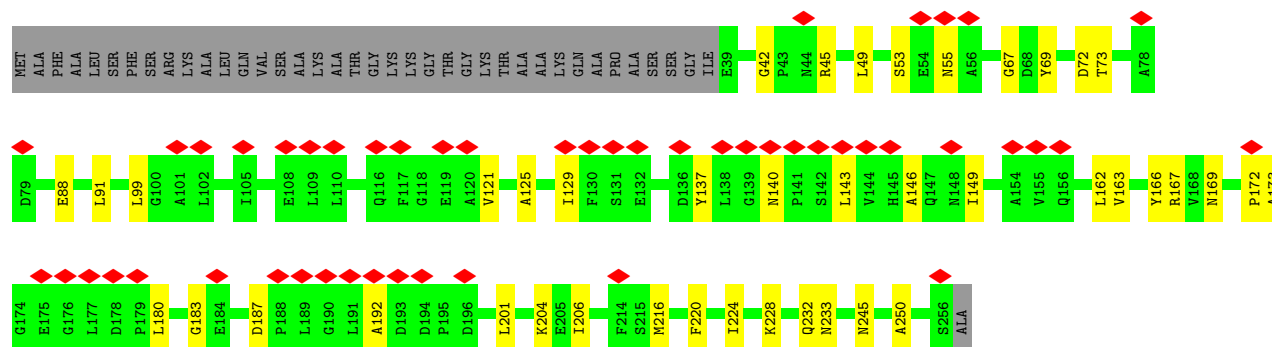


- Chain 3: 

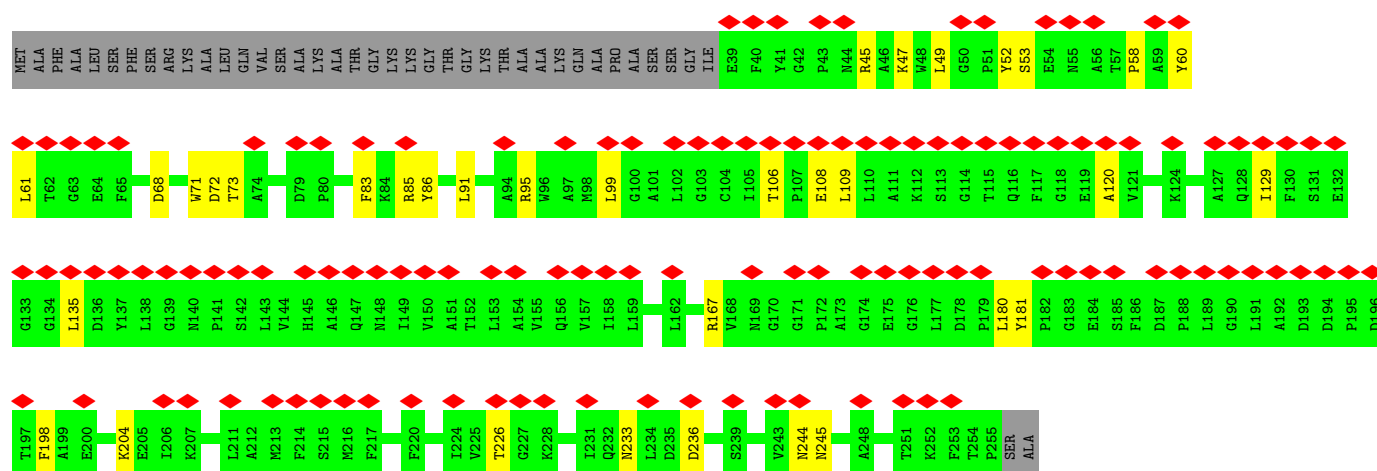




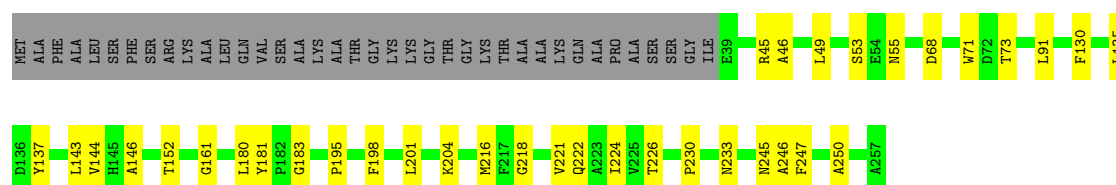
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



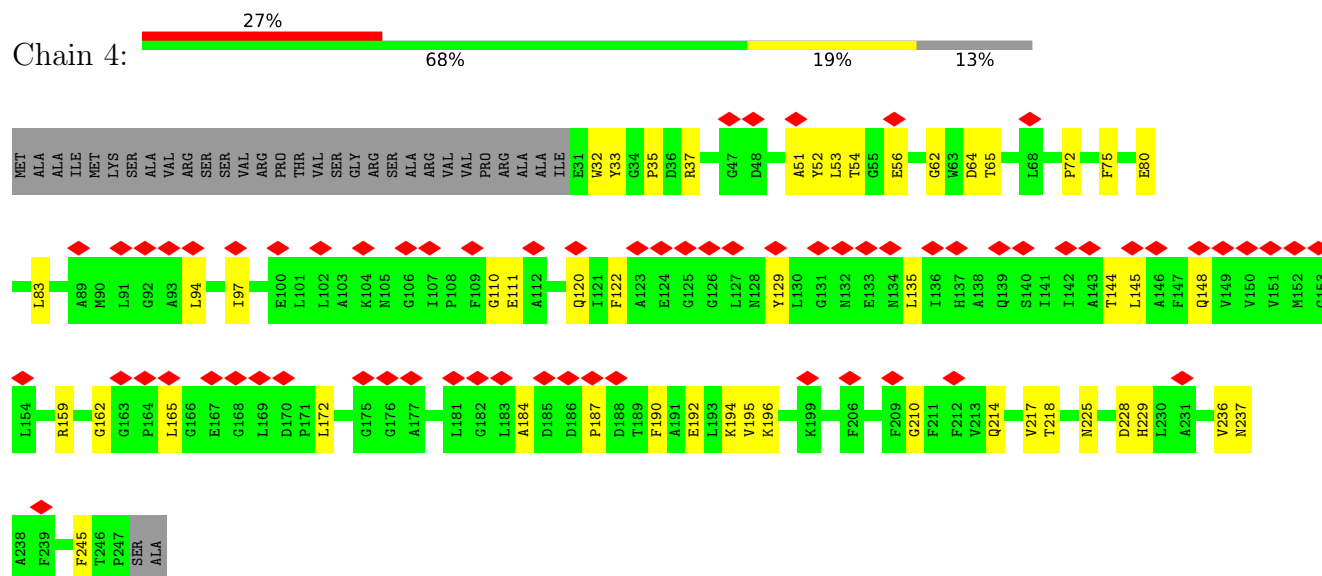
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



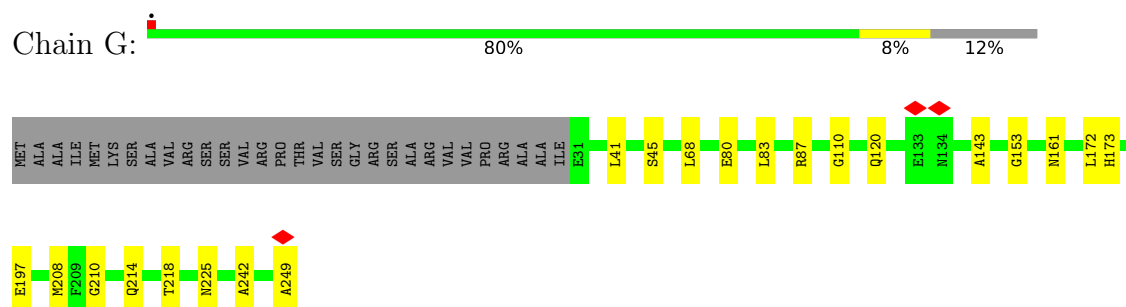
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



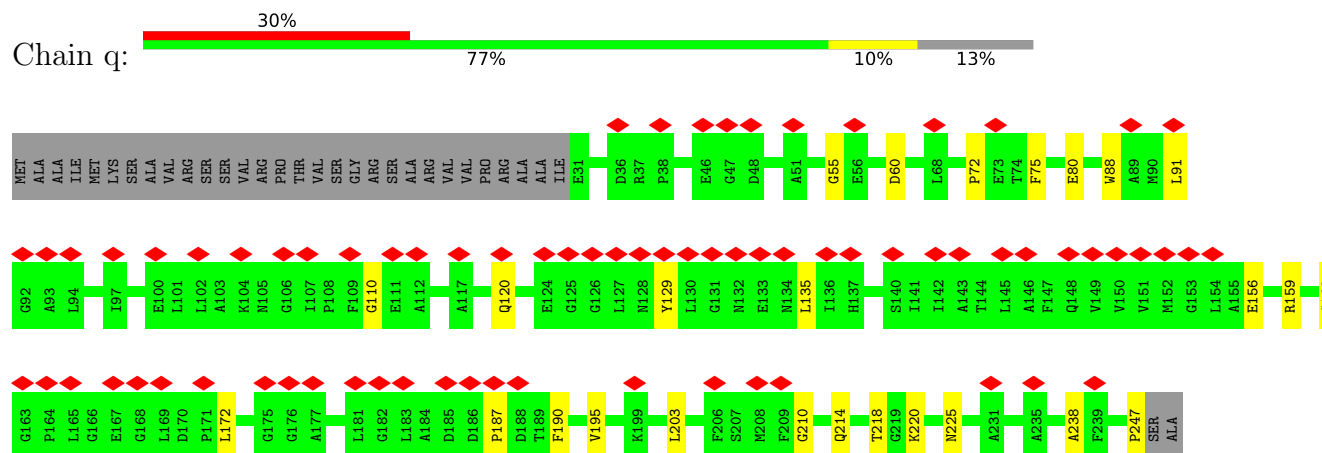
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



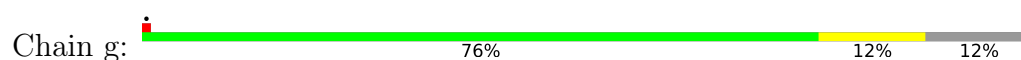
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

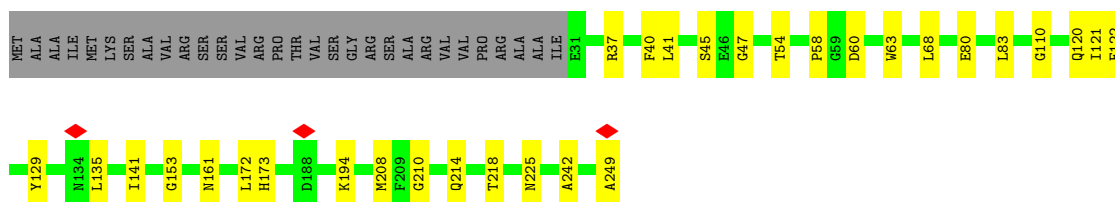


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

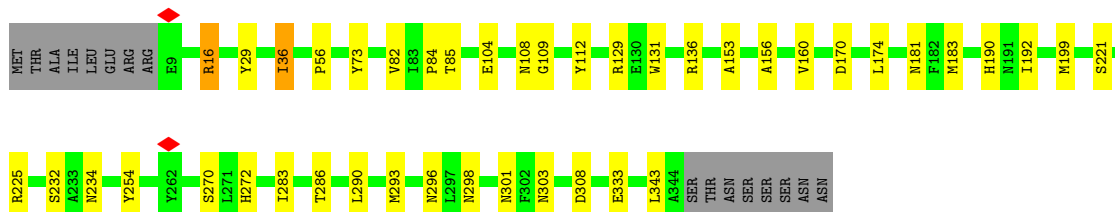
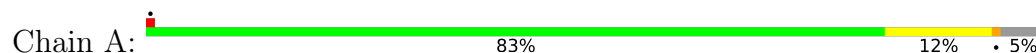


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

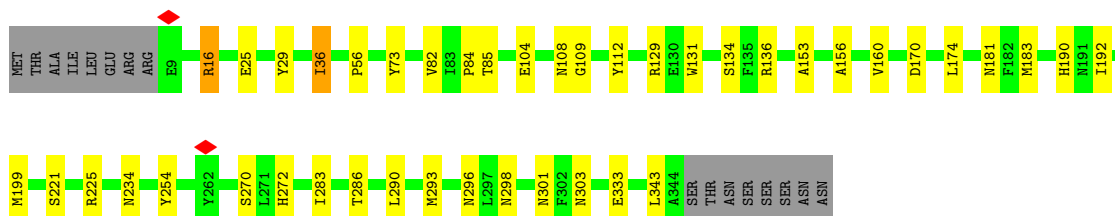
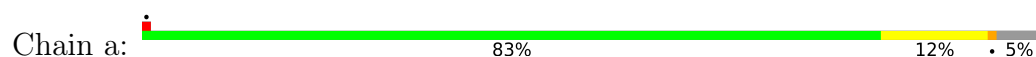




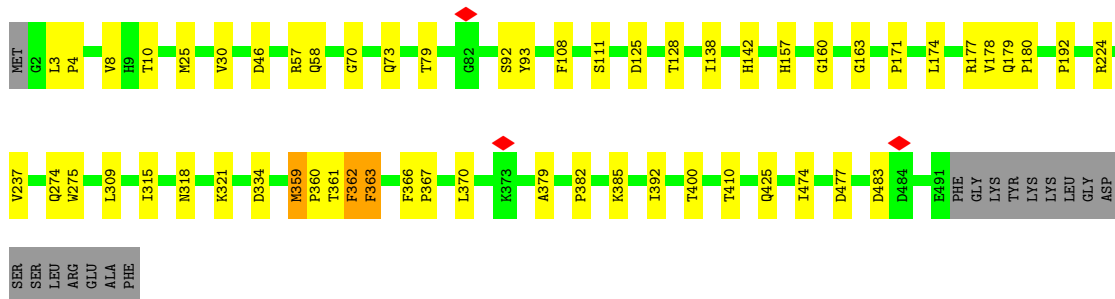
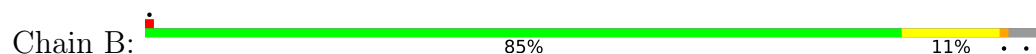
• Molecule 4: Photosystem II protein D1



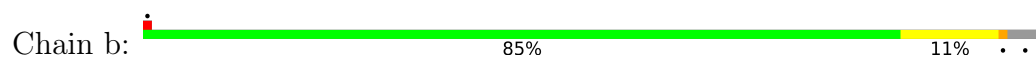
• Molecule 4: Photosystem II protein D1

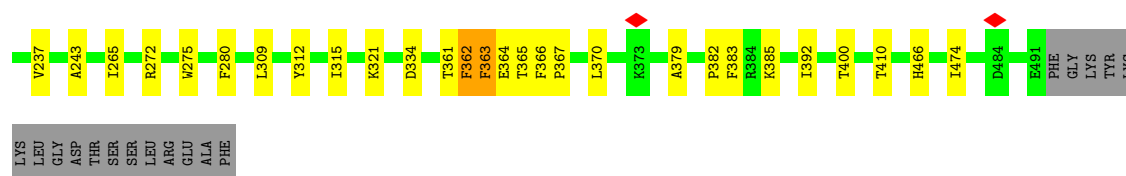


• Molecule 5: Photosystem II CP47 reaction center protein



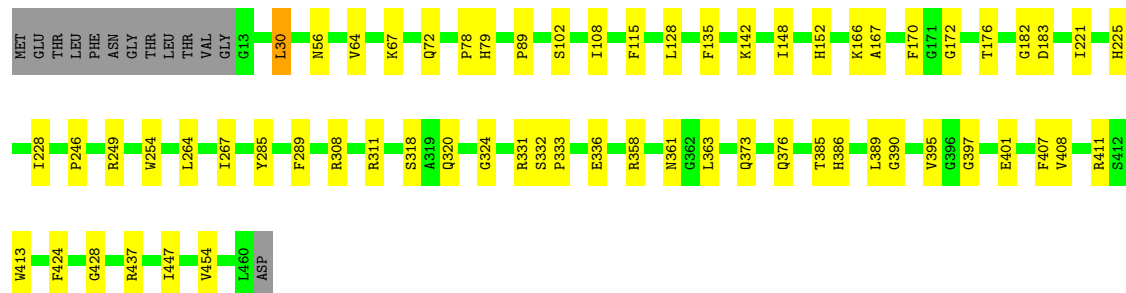
• Molecule 5: Photosystem II CP47 reaction center protein





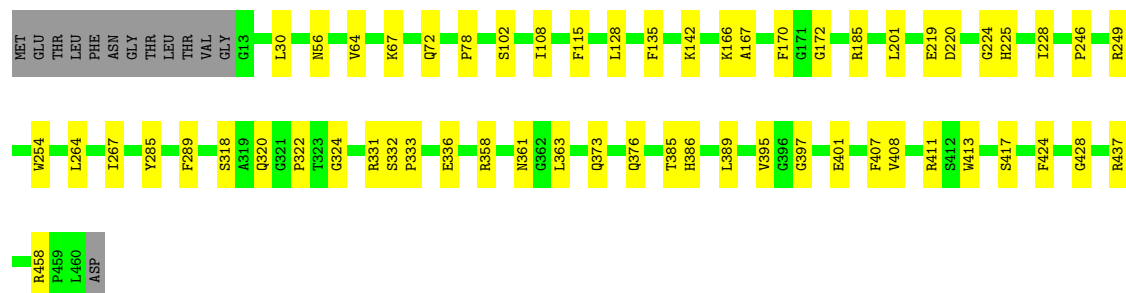
• Molecule 6: Photosystem II CP43 reaction center protein

Chain C: 84% 13%



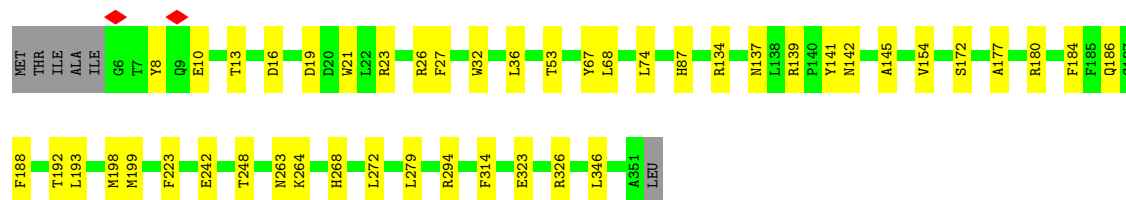
• Molecule 6: Photosystem II CP43 reaction center protein

Chain c: 85% 13%



• Molecule 7: Photosystem II D2 protein

Chain D: 85% 13%



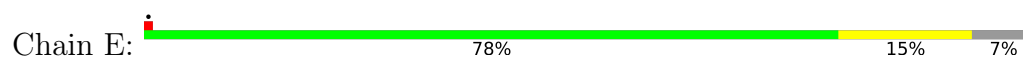
• Molecule 7: Photosystem II D2 protein

Chain d: 85% 13%

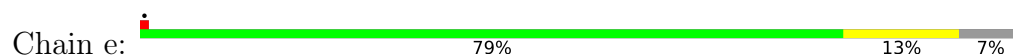




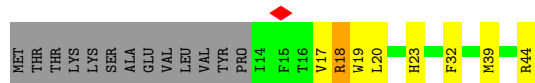
- Molecule 8: Cytochrome b559 subunit alpha



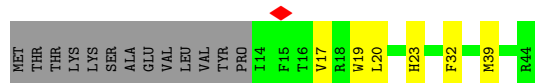
- Molecule 8: Cytochrome b559 subunit alpha



- Molecule 9: Cytochrome b559 subunit beta



- Molecule 9: Cytochrome b559 subunit beta



- Molecule 10: Photosystem II reaction center protein H



- Molecule 10: Photosystem II reaction center protein H



- Molecule 11: Photosystem II reaction center protein I

Chain I:  89% 5% 5%



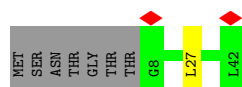
- Molecule 11: Photosystem II reaction center protein I

Chain i:  89% 5% 5%



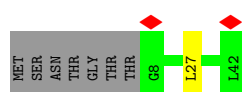
- Molecule 12: Photosystem II reaction center protein J

Chain J:  5% 81% 17%



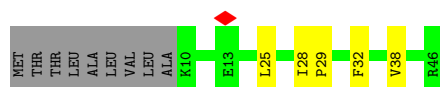
- Molecule 12: Photosystem II reaction center protein J

Chain j:  5% 81% 17%



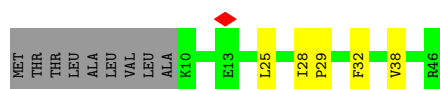
- Molecule 13: Photosystem II reaction center protein K

Chain K:  5% 70% 11% 20%



- Molecule 13: Photosystem II reaction center protein K

Chain k:  5% 70% 11% 20%



- Molecule 14: Photosystem II reaction center protein L

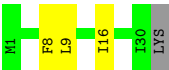
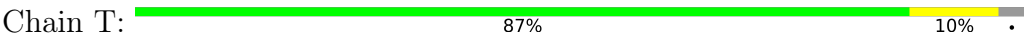
Chain L:  87% 11% 2%



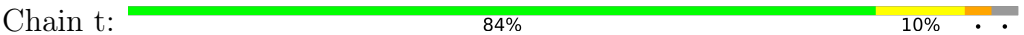
The diagram illustrates a protein structure with various residues highlighted in different colors and shapes. The residues are arranged in a grid-like pattern, with some residues highlighted in red, yellow, and green. The diagram includes labels for specific residues such as MET, ALA, LEU, ARG, ALA, GLN, SER, LYS, GLY, VAL, ARG, ALA, ARG, PRO, ASN, ARG, THR, VAL, VAL, CYS, LYS, GLN, VAL, GLY, GLN, ALA, ALA, ALA, ALA, LEU, ALA, THR, MET, MET, VAL, MET, GLY, SER, ASN, ASN, LYS, L52, T61, T62, N63, L64, K65, E66, L67, K88, A89, L94, T106, S110, Q111, G115, E116, L124, M125, T126, R127, T131, L132, D133, A134, M135, F138, F139, S143, D144, E148, L149, D152, D153, Y157, A158, A159, T160, T161, V162, L173, F174, T175, I176, K182, I198, V194, Y197, S201, and D204. The diagram also includes a legend for the colors and shapes used to highlight the residues.

THR
LEU

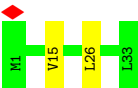
- Molecule 19: Photosystem II reaction center protein T



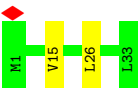
- Molecule 19: Photosystem II reaction center protein T



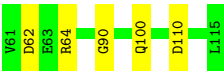
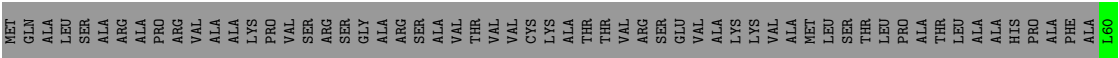
- Molecule 20: Photosystem II reaction center protein Ycf12



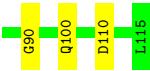
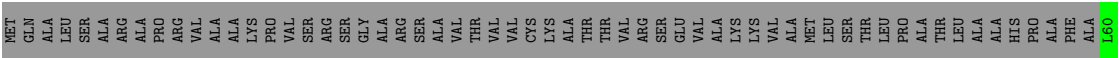
- Molecule 20: Photosystem II reaction center protein Ycf12



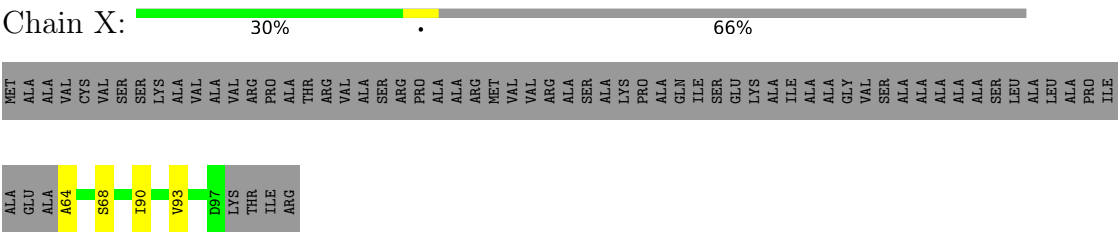
- Molecule 21: Photosystem II reaction center W protein, chloroplastic



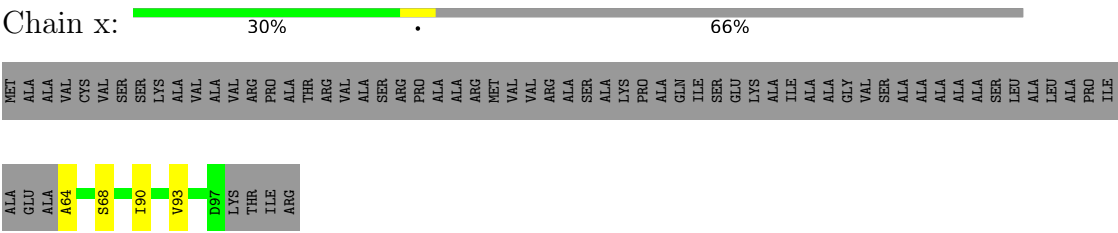
- Molecule 21: Photosystem II reaction center W protein, chloroplastic



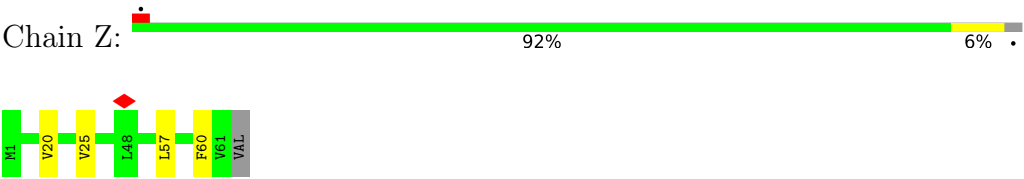
• Molecule 22: 4.1 kDa photosystem II subunit



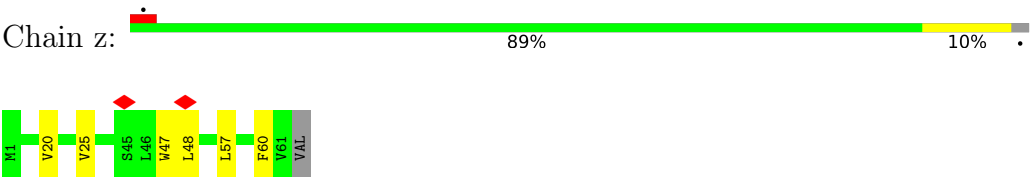
• Molecule 22: 4.1 kDa photosystem II subunit



• 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 (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: LHG, PL9, CHL, PHO, CL, CLA, BCR, BCT, OEX, DGD, NEX, FE2, SQD, LUT, LMG, XAT, HEM

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	0.22	0/1708	0.51	1/2322 (0.0%)
1	1	0.28	0/1717	0.54	0/2334
1	6	0.23	0/1708	0.51	0/2322
1	7	0.27	0/1717	0.53	0/2334
1	Y	0.41	0/1746	0.52	0/2375
1	y	0.40	0/1746	0.52	0/2375
2	2	0.22	0/1715	0.49	0/2334
2	3	0.19	0/1715	0.49	0/2334
2	5	0.19	0/1709	0.50	0/2326
2	8	0.19	0/1715	0.48	0/2334
2	9	0.23	0/1715	0.52	0/2334
2	N	0.32	0/1720	0.53	0/2341
2	n	0.32	0/1720	0.54	0/2341
2	p	0.17	0/1709	0.46	0/2326
3	4	0.20	0/1706	0.49	0/2322
3	G	0.31	0/1717	0.54	0/2337
3	g	0.31	0/1717	0.53	0/2337
3	q	0.20	0/1706	0.50	0/2322
4	A	0.49	2/2718 (0.1%)	0.62	1/3706 (0.0%)
4	a	0.49	2/2718 (0.1%)	0.62	1/3706 (0.0%)
5	B	0.41	0/3964	0.54	0/5397
5	b	0.41	0/3964	0.55	2/5397 (0.0%)
6	C	0.40	0/3611	0.52	0/4920
6	c	0.39	0/3611	0.52	0/4920
7	D	0.47	0/2850	0.62	0/3887
7	d	0.47	0/2850	0.61	0/3887
8	E	0.28	0/637	0.54	0/869
8	e	0.28	0/637	0.54	0/869
9	F	0.44	0/258	0.71	0/349
9	f	0.44	0/258	0.72	0/349
10	H	0.48	0/530	0.64	0/725

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	h	0.47	0/530	0.64	0/725
11	I	0.45	0/291	0.56	0/394
11	i	0.45	0/291	0.56	0/394
12	J	0.29	0/261	0.47	0/356
12	j	0.28	0/261	0.48	0/356
13	K	0.38	0/309	0.74	0/425
13	k	0.38	0/309	0.74	0/425
14	L	0.45	0/314	0.59	0/427
14	l	0.45	0/314	0.59	0/427
15	M	0.43	0/234	0.54	0/321
15	m	0.42	0/234	0.55	0/321
16	O	0.24	0/1771	0.50	0/2386
16	o	0.24	0/1771	0.51	0/2386
17	R	0.33	0/1866	0.59	0/2529
17	r	0.33	0/1866	0.59	0/2529
18	S	0.34	0/1961	0.55	0/2670
18	s	0.35	0/1961	0.56	0/2670
19	T	0.38	0/254	0.58	0/343
19	t	0.39	0/254	0.59	0/343
20	V	0.22	0/232	0.48	0/317
20	v	0.21	0/232	0.47	0/317
21	W	0.35	0/445	0.55	0/603
21	w	0.35	0/445	0.54	0/603
22	X	0.29	0/235	0.48	0/319
22	x	0.29	0/235	0.49	0/319
23	Z	0.24	0/469	0.52	0/644
23	z	0.24	0/469	0.55	0/644
All	All	0.35	4/77326 (0.0%)	0.55	5/105224 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	333	GLU	C-N	-7.66	1.23	1.33
4	a	333	GLU	C-N	-7.36	1.23	1.33
4	a	170	ASP	C-N	6.70	1.42	1.33
4	A	170	ASP	C-N	6.70	1.42	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	333	GLU	O-C-N	7.21	132.18	122.59
4	a	333	GLU	O-C-N	7.12	132.07	122.59
5	b	362	PHE	N-CA-C	5.90	117.80	111.36
5	b	60	MET	CG-SD-CE	-5.11	89.66	100.90
1	0	56	GLU	N-CA-C	5.04	120.96	109.81

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1656	0	1598	41	0
1	1	1665	0	1606	19	0
1	6	1656	0	1598	43	0
1	7	1665	0	1606	19	0
1	Y	1693	0	1629	18	0
1	y	1693	0	1629	19	0
2	2	1667	0	1606	31	0
2	3	1667	0	1606	35	0
2	5	1661	0	1601	28	0
2	8	1667	0	1606	34	0
2	9	1667	0	1606	33	0
2	N	1672	0	1611	26	0
2	n	1672	0	1611	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	p	1661	0	1601	25	0
3	4	1656	0	1596	31	0
3	G	1667	0	1606	17	0
3	g	1667	0	1606	22	0
3	q	1656	0	1596	19	0
4	A	2636	0	2533	33	0
4	a	2636	0	2533	34	0
5	B	3836	0	3709	67	0
5	b	3836	0	3709	49	0
6	C	3490	0	3368	45	0
6	c	3490	0	3368	40	0
7	D	2755	0	2633	41	0
7	d	2755	0	2633	49	0
8	E	619	0	605	6	0
8	e	619	0	605	5	0
9	F	251	0	263	12	0
9	f	251	0	263	10	0
10	H	519	0	549	31	0
10	h	519	0	549	15	0
11	I	283	0	293	2	0
11	i	283	0	293	2	0
12	J	255	0	269	1	0
12	j	255	0	269	1	0
13	K	297	0	308	4	0
13	k	297	0	308	4	0
14	L	306	0	315	5	0
14	l	306	0	315	5	0
15	M	230	0	252	3	0
15	m	230	0	252	3	0
16	O	1742	0	1743	25	0
16	o	1742	0	1743	27	0
17	R	1826	0	1777	27	0
17	r	1826	0	1777	26	0
18	S	1907	0	1847	56	0
18	s	1907	0	1847	63	0
19	T	247	0	260	1	0
19	t	247	0	260	2	0
20	V	232	0	268	3	0
20	v	232	0	268	3	0
21	W	434	0	411	4	0
21	w	434	0	411	3	0
22	X	233	0	253	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	x	233	0	253	3	0
23	Z	458	0	490	3	0
23	z	458	0	490	4	0
24	0	360	0	348	5	0
24	1	360	0	348	13	0
24	2	324	0	278	6	0
24	3	360	0	348	7	0
24	4	324	0	278	4	0
24	5	360	0	348	6	0
24	6	360	0	348	12	0
24	7	360	0	348	10	0
24	8	360	0	348	8	0
24	9	324	0	278	6	0
24	G	324	0	278	10	0
24	N	360	0	348	14	0
24	R	183	0	174	5	0
24	S	182	0	125	10	0
24	Y	360	0	348	15	0
24	g	324	0	278	10	0
24	n	360	0	348	11	0
24	p	360	0	348	5	0
24	q	324	0	278	4	0
24	r	183	0	174	5	0
24	s	182	0	125	8	0
24	y	360	0	348	19	0
25	0	509	0	552	10	0
25	1	509	0	552	7	0
25	2	446	0	432	7	0
25	3	468	0	471	8	0
25	4	446	0	432	6	0
25	5	468	0	471	9	0
25	6	509	0	552	8	0
25	7	509	0	552	5	0
25	8	468	0	471	5	0
25	9	446	0	432	12	0
25	A	239	0	242	5	0
25	B	1040	0	1152	28	0
25	C	845	0	936	21	0
25	D	130	0	144	7	0
25	G	446	0	432	9	0
25	N	468	0	471	8	0
25	R	563	0	529	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	S	471	0	363	19	0
25	Y	509	0	552	19	0
25	a	239	0	242	5	0
25	b	1040	0	1152	27	0
25	c	845	0	936	15	0
25	d	130	0	144	5	0
25	g	446	0	432	10	0
25	n	468	0	471	5	0
25	p	468	0	471	8	0
25	q	446	0	432	9	0
25	r	563	0	529	11	0
25	s	471	0	363	23	0
25	y	509	0	552	20	0
26	0	84	0	112	6	0
26	1	84	0	112	4	0
26	2	84	0	112	5	0
26	3	84	0	112	7	0
26	4	84	0	112	0	0
26	5	84	0	112	1	0
26	6	84	0	112	5	0
26	7	84	0	112	6	0
26	8	84	0	112	9	0
26	9	84	0	112	5	0
26	G	84	0	112	9	0
26	N	84	0	112	5	0
26	R	42	0	56	4	0
26	S	84	0	112	6	0
26	Y	84	0	112	8	0
26	g	84	0	112	5	0
26	n	84	0	112	6	0
26	p	84	0	112	2	0
26	q	84	0	112	1	0
26	r	42	0	56	2	0
26	s	84	0	112	6	0
26	y	84	0	112	8	0
27	0	44	0	56	0	0
27	1	44	0	56	5	0
27	2	44	0	56	1	0
27	3	44	0	56	2	0
27	4	44	0	56	0	0
27	5	44	0	56	0	0
27	6	44	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	7	44	0	56	4	0
27	8	44	0	56	1	0
27	9	44	0	56	2	0
27	G	44	0	56	6	0
27	N	44	0	56	5	0
27	R	44	0	56	4	0
27	Y	44	0	56	5	0
27	g	44	0	56	6	0
27	n	44	0	56	5	0
27	p	44	0	56	0	0
27	q	44	0	56	0	0
27	r	44	0	56	4	0
27	y	44	0	56	3	0
28	0	44	0	56	1	0
28	1	44	0	56	3	0
28	2	44	0	56	0	0
28	3	44	0	56	1	0
28	4	44	0	56	0	0
28	5	44	0	56	0	0
28	6	44	0	56	3	0
28	7	44	0	56	2	0
28	8	44	0	56	1	0
28	9	44	0	56	0	0
28	G	44	0	56	0	0
28	N	44	0	56	4	0
28	R	44	0	56	1	0
28	S	44	0	56	3	0
28	Y	44	0	56	3	0
28	g	44	0	56	0	0
28	n	44	0	56	3	0
28	p	44	0	56	0	0
28	q	44	0	56	0	0
28	r	44	0	56	2	0
28	s	44	0	56	3	0
28	y	44	0	56	2	0
29	0	49	0	74	2	0
29	1	49	0	74	2	0
29	2	49	0	74	0	0
29	3	49	0	74	0	0
29	4	49	0	74	1	0
29	5	49	0	74	0	0
29	6	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	7	49	0	74	2	0
29	8	49	0	74	0	0
29	9	49	0	74	0	0
29	C	47	0	67	5	0
29	D	132	0	183	5	0
29	G	49	0	74	6	0
29	L	49	0	74	5	0
29	N	49	0	74	3	0
29	R	38	0	46	1	0
29	S	45	0	63	5	0
29	Y	49	0	74	3	0
29	c	47	0	67	2	0
29	d	132	0	183	6	0
29	g	49	0	74	6	0
29	l	49	0	74	5	0
29	n	49	0	74	3	0
29	p	49	0	74	0	0
29	q	49	0	74	0	0
29	r	38	0	46	1	0
29	s	45	0	63	10	0
29	y	49	0	74	4	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	128	0	148	4	0
33	a	128	0	148	3	0
34	A	40	0	56	3	0
34	B	120	0	168	10	0
34	C	160	0	224	10	0
34	D	40	0	56	4	0
34	H	40	0	56	1	0
34	a	40	0	56	2	0
34	b	120	0	168	6	0
34	c	160	0	224	12	0
34	d	40	0	56	5	0
34	h	40	0	56	2	0
35	A	51	0	69	4	0
35	B	104	0	142	2	0
35	D	52	0	71	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	a	51	0	69	3	0
35	b	104	0	142	2	0
35	d	52	0	71	2	0
36	A	48	0	66	2	0
36	B	51	0	72	4	0
36	C	51	0	72	0	0
36	D	92	0	124	0	0
36	H	48	0	66	3	0
36	S	52	0	77	2	0
36	a	48	0	66	2	0
36	b	51	0	72	3	0
36	c	51	0	72	0	0
36	d	92	0	124	0	0
36	h	48	0	66	2	0
36	s	52	0	77	1	0
37	C	308	0	418	10	0
37	c	308	0	418	12	0
38	D	4	0	0	2	0
38	d	4	0	0	2	0
39	D	55	0	80	3	0
39	d	55	0	80	3	0
40	F	43	0	30	0	0
40	f	43	0	30	0	0
All	All	105342	0	106006	1526	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1526 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:171:PRO:CD	10:H:85:ALA:HB2	1.58	1.33
5:B:171:PRO:HD3	10:H:85:ALA:CB	1.56	1.32
18:s:58:LYS:HE3	29:s:2630:LHG:O2	1.29	1.23
5:b:366:PHE:HD1	5:b:367:PRO:HD2	1.07	1.19
5:B:171:PRO:CD	10:H:85:ALA:CB	2.19	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	30	59
17	r	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	30	59
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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%)	165 (99%)	1 (1%)	78	80
1	6	165/196 (84%)	165 (100%)	0	100	100
1	7	166/196 (85%)	164 (99%)	2 (1%)	63	72
1	Y	170/196 (87%)	170 (100%)	0	100	100
1	y	170/196 (87%)	169 (99%)	1 (1%)	78	80
2	2	169/194 (87%)	169 (100%)	0	100	100
2	3	169/194 (87%)	167 (99%)	2 (1%)	63	72
2	5	168/194 (87%)	168 (100%)	0	100	100
2	8	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	9	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	N	169/194 (87%)	168 (99%)	1 (1%)	78	80
2	n	169/194 (87%)	169 (100%)	0	100	100
2	p	168/194 (87%)	168 (100%)	0	100	100
3	4	163/187 (87%)	162 (99%)	1 (1%)	78	80
3	G	164/187 (88%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g	164/187 (88%)	164 (100%)	0	100	100
3	q	163/187 (87%)	163 (100%)	0	100	100
4	A	274/289 (95%)	272 (99%)	2 (1%)	76	78
4	a	274/289 (95%)	272 (99%)	2 (1%)	76	78
5	B	392/407 (96%)	388 (99%)	4 (1%)	68	75
5	b	392/407 (96%)	387 (99%)	5 (1%)	61	71
6	C	351/362 (97%)	348 (99%)	3 (1%)	70	76
6	c	351/362 (97%)	348 (99%)	3 (1%)	70	76
7	D	276/281 (98%)	275 (100%)	1 (0%)	84	83
7	d	276/281 (98%)	273 (99%)	3 (1%)	65	74
8	E	67/71 (94%)	66 (98%)	1 (2%)	57	69
8	e	67/71 (94%)	66 (98%)	1 (2%)	57	69
9	F	25/37 (68%)	23 (92%)	2 (8%)	11	36
9	f	25/37 (68%)	24 (96%)	1 (4%)	28	53
10	H	58/75 (77%)	54 (93%)	4 (7%)	14	40
10	h	58/75 (77%)	55 (95%)	3 (5%)	21	48
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%)	34 (100%)	0	100	100
14	l	34/35 (97%)	34 (100%)	0	100	100
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%)	190 (100%)	0	100	100
16	o	190/222 (86%)	190 (100%)	0	100	100
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%)	188 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	s	189/217 (87%)	188 (100%)	1 (0%)	81	81
19	T	27/28 (96%)	26 (96%)	1 (4%)	30	55
19	t	27/28 (96%)	26 (96%)	1 (4%)	30	55
20	V	27/27 (100%)	27 (100%)	0	100	100
20	v	27/27 (100%)	27 (100%)	0	100	100
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%)	23 (96%)	1 (4%)	26	52
22	x	24/67 (36%)	23 (96%)	1 (4%)	26	52
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%)	7617 (99%)	51 (1%)	73	78

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	9	224	ILE
5	b	365	THR
22	x	90	ILE
4	a	16	ARG
5	b	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
2	9	240	ASN
6	c	193	ASN
2	p	169	ASN
4	a	304	GLN
7	d	186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	8	607	-	60,74,74	3.32	20 (33%)	58,114,114	2.33	15 (25%)
25	CLA	G	612	3	47,51,73	1.35	9 (19%)	55,86,113	1.30	5 (9%)
25	CLA	q	602	3	69,73,73	1.15	7 (10%)	82,113,113	1.15	8 (9%)
25	CLA	C	510	-	69,73,73	1.17	10 (14%)	82,113,113	1.29	7 (8%)
34	BCR	B	619	-	41,41,41	0.75	1 (2%)	56,56,56	1.99	19 (33%)
24	CHL	r	607	-	50,64,74	3.39	20 (40%)	46,102,114	2.70	14 (30%)
24	CHL	y	608	-	44,58,74	3.77	19 (43%)	37,94,114	2.86	11 (29%)
25	CLA	7	612	1	69,73,73	1.15	9 (13%)	82,113,113	1.19	10 (12%)
25	CLA	s	604	-	53,57,73	1.29	8 (15%)	61,93,113	1.26	7 (11%)
25	CLA	p	614	-	53,57,73	1.33	7 (13%)	61,93,113	1.22	4 (6%)
29	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.15	4 (7%)
25	CLA	b	611	-	69,73,73	1.22	11 (15%)	82,113,113	1.42	7 (8%)
39	PL9	d	405	-	55,55,55	2.01	14 (25%)	68,69,69	1.51	9 (13%)
26	LUT	S	1620	-	42,43,43	0.76	0	51,60,60	1.66	13 (25%)
27	XAT	y	1622	-	41,47,47	0.99	2 (4%)	54,74,74	4.25	23 (42%)
25	CLA	d	403	-	69,73,73	1.13	9 (13%)	82,113,113	1.16	5 (6%)
24	CHL	6	607	-	60,74,74	3.30	19 (31%)	58,114,114	2.09	16 (27%)
24	CHL	S	601	18	40,54,74	4.10	20 (50%)	34,90,114	2.71	17 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	5	1622	-	41,47,47	0.95	2 (4%)	54,74,74	2.51	18 (33%)
25	CLA	9	602	2	69,73,73	1.13	7 (10%)	82,113,113	1.22	7 (8%)
36	LMG	b	622	-	51,51,55	0.88	2 (3%)	59,59,63	1.12	3 (5%)
25	CLA	3	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
25	CLA	2	611	29	49,53,73	1.36	8 (16%)	58,89,113	1.32	5 (8%)
25	CLA	7	614	-	58,62,73	1.26	8 (13%)	68,99,113	1.20	4 (5%)
25	CLA	s	605	18	54,58,73	1.26	7 (12%)	64,95,113	1.15	4 (6%)
28	NEX	0	1623	-	40,46,46	1.06	3 (7%)	50,70,70	2.21	13 (26%)
37	DGD	C	523	-	67,67,67	0.82	2 (2%)	81,81,81	1.03	5 (6%)
24	CHL	0	606	-	60,74,74	3.42	20 (33%)	58,114,114	2.43	17 (29%)
27	XAT	q	1622	-	41,47,47	0.94	1 (2%)	54,74,74	2.54	17 (31%)
26	LUT	S	1621	-	42,43,43	0.79	0	51,60,60	1.88	16 (31%)
24	CHL	R	607	-	50,64,74	3.41	21 (42%)	46,102,114	2.69	14 (30%)
25	CLA	N	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	4 (4%)
25	CLA	9	610	2	69,73,73	1.13	7 (10%)	82,113,113	1.12	10 (12%)
24	CHL	Y	609	1	60,74,74	3.14	19 (31%)	58,114,114	2.37	15 (25%)
25	CLA	5	610	2	69,73,73	1.15	6 (8%)	82,113,113	1.07	4 (4%)
25	CLA	y	604	-	69,73,73	1.19	9 (13%)	82,113,113	1.23	7 (8%)
25	CLA	1	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	Y	612	1	69,73,73	1.18	9 (13%)	82,113,113	1.28	11 (13%)
25	CLA	S	604	-	53,57,73	1.29	9 (16%)	61,93,113	1.26	7 (11%)
27	XAT	6	1622	-	41,47,47	0.99	2 (4%)	54,74,74	4.21	20 (37%)
27	XAT	9	1622	-	41,47,47	0.94	1 (2%)	54,74,74	2.55	20 (37%)
24	CHL	9	606	-	44,58,74	3.94	19 (43%)	37,94,114	2.52	12 (32%)
24	CHL	S	608	-	43,57,74	3.96	19 (44%)	37,93,114	2.56	13 (35%)
25	CLA	R	611	29	53,57,73	1.27	9 (16%)	61,93,113	1.29	3 (4%)
24	CHL	3	605	2	60,74,74	3.50	19 (31%)	58,114,114	1.84	13 (22%)
25	CLA	4	603	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	8 (9%)
35	SQD	b	623	-	48,50,54	1.14	3 (6%)	58,61,65	1.30	6 (10%)
35	SQD	B	623	-	48,50,54	1.14	3 (6%)	58,61,65	1.29	5 (8%)
25	CLA	R	616	17	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
26	LUT	9	1620	-	42,43,43	0.76	0	51,60,60	1.72	13 (25%)
24	CHL	G	607	-	44,58,74	3.80	19 (43%)	37,94,114	2.81	16 (43%)
29	LHG	N	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	3 (5%)
29	LHG	2	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	y	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.70	15 (29%)
28	NEX	6	1623	-	40,46,46	1.13	3 (7%)	50,70,70	2.21	14 (28%)
24	CHL	7	601	1	60,74,74	3.31	19 (31%)	58,114,114	2.50	19 (32%)
35	SQD	B	621	-	52,54,54	1.09	3 (5%)	62,65,65	1.11	4 (6%)
25	CLA	N	614	-	53,57,73	1.29	8 (15%)	61,93,113	1.27	4 (6%)
24	CHL	q	601	3	60,74,74	3.35	19 (31%)	58,114,114	2.33	19 (32%)
25	CLA	C	513	-	69,73,73	1.14	9 (13%)	82,113,113	1.20	6 (7%)
25	CLA	r	616	17	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
24	CHL	l	606	-	60,74,74	3.29	19 (31%)	58,114,114	2.42	14 (24%)
37	DGD	c	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.01	5 (6%)
25	CLA	b	603	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	9 (10%)
24	CHL	3	608	-	44,58,74	3.92	19 (43%)	37,94,114	2.47	14 (37%)
24	CHL	4	608	-	38,52,74	4.28	18 (47%)	31,87,114	2.61	12 (38%)
25	CLA	A	407	-	53,57,73	1.28	9 (16%)	61,93,113	1.31	5 (8%)
24	CHL	5	607	-	60,74,74	3.37	19 (31%)	58,114,114	2.15	13 (22%)
26	LUT	7	1621	-	42,43,43	0.73	0	51,60,60	1.65	12 (23%)
25	CLA	7	602	1	69,73,73	1.15	9 (13%)	82,113,113	1.15	5 (6%)
26	LUT	8	1620	-	42,43,43	0.67	0	51,60,60	1.74	13 (25%)
25	CLA	c	511	6	69,73,73	1.17	10 (14%)	82,113,113	1.36	7 (8%)
24	CHL	l	605	1	40,54,74	4.08	19 (47%)	34,90,114	2.54	12 (35%)
25	CLA	p	610	2	69,73,73	1.14	6 (8%)	82,113,113	1.13	6 (7%)
25	CLA	B	607	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	11 (13%)
24	CHL	9	601	2	60,74,74	3.35	20 (33%)	58,114,114	1.91	17 (29%)
25	CLA	N	611	29	53,57,73	1.27	9 (16%)	61,93,113	1.28	3 (4%)
36	LMG	d	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.13	4 (7%)
24	CHL	s	601	18	40,54,74	4.09	20 (50%)	34,90,114	2.70	17 (50%)
25	CLA	8	604	-	69,73,73	1.14	8 (11%)	82,113,113	1.19	6 (7%)
25	CLA	n	614	-	53,57,73	1.29	8 (15%)	61,93,113	1.26	4 (6%)
25	CLA	n	611	29	53,57,73	1.28	9 (16%)	61,93,113	1.30	3 (4%)
24	CHL	l	608	-	44,58,74	3.82	19 (43%)	37,94,114	2.64	13 (35%)
25	CLA	0	603	-	69,73,73	1.14	7 (10%)	82,113,113	1.30	5 (6%)
25	CLA	Y	614	-	58,62,73	1.24	7 (12%)	68,99,113	1.23	5 (7%)
26	LUT	3	1621	-	42,43,43	0.75	0	51,60,60	1.60	10 (19%)
34	BCR	h	101	-	41,41,41	0.80	0	56,56,56	2.04	16 (28%)
25	CLA	4	604	-	53,57,73	1.32	7 (13%)	61,93,113	1.22	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	g	610	3	69,73,73	1.12	7 (10%)	82,113,113	1.16	7 (8%)
36	LMG	S	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.11	3 (5%)
36	LMG	D	412	-	46,46,55	0.95	2 (4%)	54,54,63	1.09	4 (7%)
26	LUT	G	1620	-	42,43,43	0.76	0	51,60,60	1.57	7 (13%)
24	CHL	r	608	-	55,69,74	3.35	21 (38%)	52,108,114	2.50	15 (28%)
24	CHL	R	606	-	60,74,74	3.13	20 (33%)	58,114,114	2.47	17 (29%)
37	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.15	6 (7%)
25	CLA	S	614	-	52,56,73	1.29	8 (15%)	61,92,113	1.27	7 (11%)
26	LUT	n	1620	-	42,43,43	0.75	0	51,60,60	1.64	12 (23%)
40	HEM	F	101	8,9	50,50,50	1.32	4 (8%)	67,82,82	1.04	4 (5%)
24	CHL	2	601	2	60,74,74	3.31	21 (35%)	58,114,114	1.97	18 (31%)
34	BCR	a	411	-	41,41,41	0.77	1 (2%)	56,56,56	1.72	11 (19%)
24	CHL	g	608	-	38,52,74	4.11	18 (47%)	31,87,114	2.47	11 (35%)
25	CLA	A	406	-	69,73,73	1.13	8 (11%)	82,113,113	1.18	7 (8%)
29	LHG	c	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.06	3 (6%)
25	CLA	B	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
34	BCR	b	620	-	41,41,41	0.81	1 (2%)	56,56,56	1.89	18 (32%)
25	CLA	N	602	2	69,73,73	1.15	9 (13%)	82,113,113	1.17	9 (10%)
25	CLA	S	603	-	46,50,73	1.38	6 (13%)	53,85,113	1.34	3 (5%)
25	CLA	b	604	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	7 (8%)
24	CHL	G	608	-	38,52,74	4.15	18 (47%)	31,87,114	2.43	10 (32%)
25	CLA	7	610	1	69,73,73	1.12	7 (10%)	82,113,113	1.14	7 (8%)
25	CLA	b	606	-	69,73,73	1.16	9 (13%)	82,113,113	1.11	6 (7%)
24	CHL	p	601	2	60,74,74	3.37	19 (31%)	58,114,114	2.44	15 (25%)
28	NEX	y	1623	-	40,46,46	1.06	4 (10%)	50,70,70	2.37	17 (34%)
25	CLA	R	609	17	62,66,73	1.20	7 (11%)	73,104,113	1.30	4 (5%)
25	CLA	1	604	-	69,73,73	1.15	8 (11%)	82,113,113	1.15	7 (8%)
25	CLA	C	508	-	69,73,73	1.18	9 (13%)	82,113,113	1.30	9 (10%)
25	CLA	G	604	-	53,57,73	1.29	9 (16%)	61,93,113	1.28	8 (13%)
25	CLA	8	603	-	69,73,73	1.14	7 (10%)	82,113,113	1.30	6 (7%)
25	CLA	c	502	-	69,73,73	1.24	10 (14%)	82,113,113	1.60	11 (13%)
24	CHL	G	606	-	44,58,74	3.80	19 (43%)	37,94,114	2.87	16 (43%)
30	OEX	A	401	4,6	0,15,15	-	-	-	-	-
35	SQD	b	621	-	52,54,54	1.08	3 (5%)	62,65,65	1.12	4 (6%)
25	CLA	y	614	-	58,62,73	1.23	7 (12%)	68,99,113	1.23	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	613	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	8 (9%)
36	LMG	c	521	-	51,51,55	0.88	2 (3%)	59,59,63	1.08	4 (6%)
25	CLA	d	402	-	69,73,73	1.21	9 (13%)	82,113,113	1.30	7 (8%)
25	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
25	CLA	1	612	1	69,73,73	1.14	9 (13%)	82,113,113	1.20	10 (12%)
25	CLA	c	504	-	69,73,73	1.14	8 (11%)	82,113,113	1.20	5 (6%)
24	CHL	y	606	-	60,74,74	3.17	20 (33%)	58,114,114	2.27	14 (24%)
25	CLA	8	610	2	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
25	CLA	0	612	1	69,73,73	1.16	8 (11%)	82,113,113	1.18	9 (10%)
27	XAT	3	1622	-	41,47,47	0.93	1 (2%)	54,74,74	2.48	20 (37%)
25	CLA	c	508	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	8 (9%)
25	CLA	Y	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
36	LMG	A	413	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	4 (7%)
26	LUT	7	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.71	10 (19%)
25	CLA	r	612	-	53,57,73	1.29	9 (16%)	61,93,113	1.40	6 (9%)
33	PHO	A	408	-	58,69,69	2.03	12 (20%)	55,99,99	1.70	12 (21%)
29	LHG	d	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	2 (3%)
24	CHL	2	609	2	60,74,74	3.43	20 (33%)	58,114,114	2.27	13 (22%)
25	CLA	b	607	-	69,73,73	1.15	7 (10%)	82,113,113	1.27	12 (14%)
24	CHL	2	608	-	38,52,74	4.17	19 (50%)	31,87,114	2.88	12 (38%)
25	CLA	3	612	2	49,53,73	1.37	6 (12%)	58,89,113	1.45	6 (10%)
25	CLA	4	612	3	47,51,73	1.38	6 (12%)	55,86,113	1.45	9 (16%)
26	LUT	y	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.75	14 (27%)
25	CLA	A	410	-	64,68,73	1.19	9 (14%)	76,107,113	1.34	10 (13%)
24	CHL	8	608	-	44,58,74	3.91	19 (43%)	37,94,114	2.49	14 (37%)
25	CLA	S	602	18	53,57,73	1.31	9 (16%)	61,93,113	1.39	8 (13%)
24	CHL	0	608	-	44,58,74	3.87	19 (43%)	37,94,114	2.79	13 (35%)
29	LHG	d	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.23	2 (4%)
25	CLA	B	614	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	6 (7%)
35	SQD	A	412	-	49,51,54	1.15	3 (6%)	59,62,65	3.31	9 (15%)
25	CLA	b	612	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	9 (10%)
25	CLA	6	611	29	69,73,73	1.15	7 (10%)	82,113,113	1.22	4 (4%)
26	LUT	6	1620	-	42,43,43	0.72	0	51,60,60	1.80	15 (29%)
24	CHL	3	609	2	60,74,74	3.23	19 (31%)	58,114,114	2.33	14 (24%)
25	CLA	q	614	-	53,57,73	1.29	7 (13%)	61,93,113	1.24	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	11 (13%)
25	CLA	R	601	17	53,57,73	1.31	7 (13%)	61,93,113	1.55	8 (13%)
25	CLA	S	613	18	53,57,73	1.30	7 (13%)	61,93,113	1.30	5 (8%)
24	CHL	9	607	-	44,58,74	4.01	19 (43%)	37,94,114	2.43	11 (29%)
25	CLA	a	405	-	69,73,73	1.20	8 (11%)	82,113,113	1.32	9 (10%)
26	LUT	3	1620	-	42,43,43	0.67	0	51,60,60	1.79	13 (25%)
24	CHL	s	607	-	37,51,74	4.23	19 (51%)	30,86,114	2.56	12 (40%)
24	CHL	N	601	2	60,74,74	3.20	19 (31%)	58,114,114	2.64	17 (29%)
29	LHG	1	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	5 (9%)
27	XAT	n	1622	-	41,47,47	1.00	3 (7%)	54,74,74	2.65	21 (38%)
29	LHG	d	408	-	43,43,48	0.99	3 (6%)	46,49,54	1.03	3 (6%)
24	CHL	8	601	2	60,74,74	3.34	20 (33%)	58,114,114	2.35	14 (24%)
26	LUT	N	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.65	11 (21%)
26	LUT	2	1620	-	42,43,43	0.75	0	51,60,60	1.67	11 (21%)
25	CLA	y	603	-	69,73,73	1.16	11 (15%)	82,113,113	1.36	8 (9%)
29	LHG	4	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.11	4 (7%)
25	CLA	5	612	2	49,53,73	1.39	7 (14%)	58,89,113	1.42	6 (10%)
25	CLA	B	605	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	9 (10%)
25	CLA	b	615	-	69,73,73	1.15	9 (13%)	82,113,113	1.13	6 (7%)
29	LHG	C	2630	-	46,46,48	0.94	2 (4%)	49,52,54	1.04	3 (6%)
25	CLA	6	613	1	69,73,73	1.16	6 (8%)	82,113,113	1.21	5 (6%)
28	NEX	9	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.13	12 (24%)
28	NEX	n	1623	-	40,46,46	1.00	3 (7%)	50,70,70	2.24	16 (32%)
25	CLA	Y	613	1	69,73,73	1.17	7 (10%)	82,113,113	1.15	3 (3%)
25	CLA	n	610	2	69,73,73	1.13	8 (11%)	82,113,113	1.11	7 (8%)
26	LUT	1	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.72	17 (33%)
25	CLA	3	604	-	69,73,73	1.14	8 (11%)	82,113,113	1.19	5 (6%)
25	CLA	Y	610	1	69,73,73	1.14	8 (11%)	82,113,113	1.13	7 (8%)
25	CLA	y	613	1	69,73,73	1.17	8 (11%)	82,113,113	1.16	4 (4%)
28	NEX	r	623	-	40,46,46	1.12	4 (10%)	50,70,70	2.26	16 (32%)
24	CHL	4	606	-	44,58,74	4.03	19 (43%)	37,94,114	2.29	15 (40%)
24	CHL	9	609	2	60,74,74	3.48	20 (33%)	58,114,114	2.05	17 (29%)
24	CHL	6	609	1	60,74,74	3.32	19 (31%)	58,114,114	2.03	15 (25%)
26	LUT	0	1621	-	42,43,43	0.78	0	51,60,60	1.66	11 (21%)
25	CLA	0	614	-	58,62,73	1.25	6 (10%)	68,99,113	1.29	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	5	609	2	60,74,74	3.42	20 (33%)	58,114,114	2.19	15 (25%)
25	CLA	G	613	3	69,73,73	1.14	8 (11%)	82,113,113	1.17	3 (3%)
29	LHG	5	2630	25	48,48,48	0.95	2 (4%)	51,54,54	1.07	3 (5%)
24	CHL	9	605	2	42,56,74	4.20	18 (42%)	36,92,114	2.38	15 (41%)
25	CLA	s	602	18	53,57,73	1.30	8 (15%)	61,93,113	1.38	8 (13%)
25	CLA	6	603	-	69,73,73	1.14	7 (10%)	82,113,113	1.28	5 (6%)
24	CHL	5	606	-	40,54,74	4.17	20 (50%)	34,90,114	2.56	12 (35%)
34	BCR	c	514	-	41,41,41	0.72	0	56,56,56	1.58	10 (17%)
24	CHL	4	607	-	44,58,74	4.03	19 (43%)	37,94,114	2.24	14 (37%)
24	CHL	S	606	-	38,52,74	4.08	18 (47%)	31,87,114	3.12	12 (38%)
25	CLA	a	406	-	69,73,73	1.13	8 (11%)	82,113,113	1.18	7 (8%)
27	XAT	8	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.50	20 (37%)
25	CLA	C	504	-	69,73,73	1.14	9 (13%)	82,113,113	1.20	5 (6%)
28	NEX	g	1623	-	40,46,46	1.07	3 (7%)	50,70,70	2.29	18 (36%)
24	CHL	q	605	3	42,56,74	4.21	20 (47%)	36,92,114	2.46	14 (38%)
24	CHL	s	608	-	43,57,74	3.97	19 (44%)	37,93,114	2.55	13 (35%)
25	CLA	G	602	3	69,73,73	1.15	10 (14%)	82,113,113	1.26	7 (8%)
25	CLA	N	610	2	69,73,73	1.13	8 (11%)	82,113,113	1.12	7 (8%)
28	NEX	G	1623	-	40,46,46	1.01	3 (7%)	50,70,70	2.31	20 (40%)
24	CHL	6	605	1	40,54,74	4.22	19 (47%)	34,90,114	2.38	11 (32%)
25	CLA	R	602	17	64,68,73	1.20	8 (12%)	76,107,113	1.31	6 (7%)
25	CLA	y	612	1	69,73,73	1.17	10 (14%)	82,113,113	1.28	11 (13%)
25	CLA	9	613	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	5 (6%)
25	CLA	p	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.24	5 (6%)
25	CLA	r	602	17	64,68,73	1.20	8 (12%)	76,107,113	1.31	6 (7%)
24	CHL	1	607	-	60,74,74	3.25	19 (31%)	58,114,114	2.17	19 (32%)
25	CLA	7	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	5 (6%)
25	CLA	q	603	-	69,73,73	1.15	7 (10%)	82,113,113	1.25	7 (8%)
24	CHL	Y	601	1	60,74,74	3.20	20 (33%)	58,114,114	2.46	18 (31%)
25	CLA	B	617	-	69,73,73	1.14	8 (11%)	82,113,113	1.33	9 (10%)
26	LUT	5	1620	-	42,43,43	0.68	1 (2%)	51,60,60	1.92	13 (25%)
36	LMG	D	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.13	4 (7%)
29	LHG	S	2630	25	44,44,48	0.95	2 (4%)	47,50,54	1.14	3 (6%)
24	CHL	2	607	-	44,58,74	4.03	19 (43%)	37,94,114	2.41	11 (29%)
25	CLA	C	506	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	3	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.00	2 (3%)
26	LUT	g	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.67	12 (23%)
25	CLA	p	613	2	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
26	LUT	Y	1620	-	42,43,43	0.86	1 (2%)	51,60,60	1.70	15 (29%)
24	CHL	n	605	2	60,74,74	3.25	19 (31%)	58,114,114	2.18	19 (32%)
25	CLA	q	613	3	69,73,73	1.14	6 (8%)	82,113,113	1.26	5 (6%)
24	CHL	0	607	-	60,74,74	3.29	19 (31%)	58,114,114	2.39	14 (24%)
26	LUT	5	1621	-	42,43,43	0.72	0	51,60,60	1.66	12 (23%)
25	CLA	3	614	-	53,57,73	1.30	7 (13%)	61,93,113	1.18	5 (8%)
24	CHL	q	608	-	38,52,74	4.34	18 (47%)	31,87,114	2.37	12 (38%)
25	CLA	r	613	17	64,68,73	1.16	6 (9%)	76,107,113	1.27	5 (6%)
24	CHL	g	607	-	44,58,74	3.82	19 (43%)	37,94,114	2.72	16 (43%)
25	CLA	s	603	-	46,50,73	1.37	6 (13%)	53,85,113	1.33	3 (5%)
25	CLA	b	616	-	69,73,73	1.17	9 (13%)	82,113,113	1.40	13 (15%)
27	XAT	p	1622	-	41,47,47	0.97	2 (4%)	54,74,74	2.42	20 (37%)
25	CLA	2	613	2	69,73,73	1.14	7 (10%)	82,113,113	1.19	4 (4%)
24	CHL	3	607	-	60,74,74	3.34	20 (33%)	58,114,114	2.38	16 (27%)
24	CHL	7	606	-	60,74,74	3.29	19 (31%)	58,114,114	2.38	16 (27%)
24	CHL	y	601	1	60,74,74	3.20	20 (33%)	58,114,114	2.52	20 (34%)
25	CLA	9	604	-	53,57,73	1.29	7 (13%)	61,93,113	1.28	4 (6%)
25	CLA	6	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.16	7 (8%)
25	CLA	s	609	18	45,49,73	1.38	7 (15%)	54,84,113	1.31	6 (11%)
28	NEX	R	623	-	40,46,46	1.09	3 (7%)	50,70,70	2.24	15 (30%)
25	CLA	B	610	-	69,73,73	1.15	10 (14%)	82,113,113	1.23	7 (8%)
25	CLA	0	613	1	69,73,73	1.15	6 (8%)	82,113,113	1.18	7 (8%)
24	CHL	1	609	1	60,74,74	3.21	19 (31%)	58,114,114	2.30	16 (27%)
25	CLA	5	604	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	5 (6%)
24	CHL	0	609	1	60,74,74	3.39	19 (31%)	58,114,114	1.86	13 (22%)
25	CLA	8	614	-	53,57,73	1.31	7 (13%)	61,93,113	1.17	5 (8%)
34	BCR	b	619	-	41,41,41	0.75	1 (2%)	56,56,56	1.99	19 (33%)
29	LHG	y	2630	25	48,48,48	0.89	3 (6%)	51,54,54	1.19	5 (9%)
25	CLA	p	604	-	69,73,73	1.17	6 (8%)	82,113,113	1.12	5 (6%)
28	NEX	p	1623	-	40,46,46	0.97	3 (7%)	50,70,70	2.24	15 (30%)
25	CLA	c	506	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
25	CLA	R	610	17	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	7	1623	-	40,46,46	1.16	3 (7%)	50,70,70	2.28	19 (38%)
33	PHO	a	409	-	58,69,69	1.99	11 (18%)	55,99,99	1.85	11 (20%)
25	CLA	q	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.34	6 (9%)
28	NEX	q	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.21	16 (32%)
34	BCR	b	618	-	41,41,41	0.75	0	56,56,56	1.92	15 (26%)
27	XAT	Y	1622	-	41,47,47	0.99	2 (4%)	54,74,74	4.24	23 (42%)
36	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
34	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.92	15 (26%)
24	CHL	p	608	-	44,58,74	3.95	18 (40%)	37,94,114	2.80	12 (32%)
26	LUT	s	1620	-	42,43,43	0.75	0	51,60,60	1.67	13 (25%)
25	CLA	G	610	3	69,73,73	1.12	7 (10%)	82,113,113	1.16	8 (9%)
28	NEX	N	1623	-	40,46,46	1.05	3 (7%)	50,70,70	2.24	14 (28%)
25	CLA	p	612	2	49,53,73	1.38	6 (12%)	58,89,113	1.40	6 (10%)
29	LHG	9	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
25	CLA	S	605	18	54,58,73	1.26	8 (14%)	64,95,113	1.16	5 (7%)
25	CLA	q	612	3	47,51,73	1.37	6 (12%)	55,86,113	1.44	8 (14%)
28	NEX	2	1623	-	40,46,46	1.04	3 (7%)	50,70,70	2.13	13 (26%)
25	CLA	B	603	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	9 (10%)
39	PL9	D	405	-	55,55,55	2.01	14 (25%)	68,69,69	1.51	9 (13%)
25	CLA	R	613	17	64,68,73	1.16	6 (9%)	76,107,113	1.27	5 (6%)
24	CHL	n	606	-	40,54,74	3.95	19 (47%)	34,90,114	3.13	13 (38%)
25	CLA	6	602	1	69,73,73	1.17	8 (11%)	82,113,113	1.11	5 (6%)
25	CLA	r	610	17	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
25	CLA	b	617	-	69,73,73	1.13	8 (11%)	82,113,113	1.33	9 (10%)
25	CLA	a	407	-	53,57,73	1.28	9 (16%)	61,93,113	1.31	4 (6%)
25	CLA	c	505	-	69,73,73	1.16	10 (14%)	82,113,113	1.23	9 (10%)
25	CLA	r	601	17	53,57,73	1.32	8 (15%)	61,93,113	1.56	8 (13%)
26	LUT	G	1621	-	42,43,43	0.76	0	51,60,60	1.71	13 (25%)
25	CLA	3	602	2	69,73,73	1.15	8 (11%)	82,113,113	1.15	7 (8%)
25	CLA	c	513	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	5 (6%)
26	LUT	r	620	-	42,43,43	0.80	1 (2%)	51,60,60	1.80	13 (25%)
25	CLA	9	612	2	47,51,73	1.38	7 (14%)	55,86,113	1.40	5 (9%)
25	CLA	6	612	1	69,73,73	1.16	7 (10%)	82,113,113	1.17	10 (12%)
25	CLA	s	612	18	49,53,73	1.36	8 (16%)	58,89,113	1.47	9 (15%)
25	CLA	c	501	-	69,73,73	1.17	10 (14%)	82,113,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	s	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.11	3 (5%)
26	LUT	4	1621	-	42,43,43	0.74	0	51,60,60	1.58	13 (25%)
35	SQD	a	412	-	49,51,54	1.15	3 (6%)	59,62,65	3.31	9 (15%)
26	LUT	2	1621	-	42,43,43	0.74	0	51,60,60	1.83	12 (23%)
29	LHG	6	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.97	2 (3%)
30	OEX	a	401	4,6	0,15,15	-	-	-		
25	CLA	2	602	2	69,73,73	1.13	8 (11%)	82,113,113	1.20	7 (8%)
34	BCR	C	515	-	41,41,41	0.88	2 (4%)	56,56,56	1.74	12 (21%)
24	CHL	N	608	-	44,58,74	3.75	19 (43%)	37,94,114	2.94	13 (35%)
25	CLA	7	604	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	7 (8%)
26	LUT	1	1620	-	42,43,43	0.76	1 (2%)	51,60,60	1.71	10 (19%)
24	CHL	g	609	3	60,74,74	3.17	21 (35%)	58,114,114	2.24	15 (25%)
24	CHL	p	606	-	40,54,74	4.22	19 (47%)	34,90,114	2.45	14 (41%)
37	DGD	C	518	-	56,56,67	0.89	2 (3%)	70,70,81	1.13	6 (8%)
25	CLA	8	602	2	69,73,73	1.15	9 (13%)	82,113,113	1.16	7 (8%)
26	LUT	0	1620	-	42,43,43	0.72	1 (2%)	51,60,60	1.70	14 (27%)
29	LHG	p	2630	25	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
26	LUT	g	1620	-	42,43,43	0.76	0	51,60,60	1.57	7 (13%)
29	LHG	q	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.14	4 (7%)
24	CHL	N	606	-	40,54,74	3.95	19 (47%)	34,90,114	3.09	13 (38%)
34	BCR	c	517	-	41,41,41	0.81	2 (4%)	56,56,56	1.84	11 (19%)
24	CHL	n	609	2	60,74,74	3.21	20 (33%)	58,114,114	2.19	16 (27%)
24	CHL	g	601	3	60,74,74	3.17	19 (31%)	58,114,114	2.63	20 (34%)
25	CLA	q	610	3	69,73,73	1.14	7 (10%)	82,113,113	1.15	5 (6%)
29	LHG	r	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.21	3 (7%)
24	CHL	8	606	-	40,54,74	4.21	19 (47%)	34,90,114	2.56	14 (41%)
24	CHL	N	605	2	60,74,74	3.29	19 (31%)	58,114,114	2.20	19 (32%)
37	DGD	c	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.15	6 (7%)
26	LUT	R	620	-	42,43,43	0.80	1 (2%)	51,60,60	1.80	13 (25%)
25	CLA	8	613	2	69,73,73	1.14	7 (10%)	82,113,113	1.32	5 (6%)
25	CLA	S	611	29	53,57,73	1.28	9 (16%)	61,93,113	1.29	5 (8%)
29	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	4 (7%)
25	CLA	9	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
38	BCT	d	401	31	3,3,3	1.18	0	2,3,3	4.20	2 (100%)
25	CLA	B	611	-	69,73,73	1.22	11 (15%)	82,113,113	1.43	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	D	409	-	48,48,48	0.91	3 (6%)	51,54,54	0.97	2 (3%)
25	CLA	N	603	-	69,73,73	1.16	11 (15%)	82,113,113	1.32	6 (7%)
38	BCT	D	401	31	3,3,3	1.19	0	2,3,3	4.20	2 (100%)
25	CLA	6	614	-	58,62,73	1.26	6 (10%)	68,99,113	1.28	6 (8%)
24	CHL	4	609	3	60,74,74	3.57	20 (33%)	58,114,114	1.88	15 (25%)
25	CLA	s	614	-	52,56,73	1.29	8 (15%)	61,92,113	1.26	7 (11%)
27	XAT	7	1622	-	41,47,47	0.97	2 (4%)	54,74,74	4.17	22 (40%)
28	NEX	Y	1623	-	40,46,46	1.11	4 (10%)	50,70,70	2.28	14 (28%)
25	CLA	n	603	-	69,73,73	1.16	11 (15%)	82,113,113	1.32	5 (6%)
27	XAT	4	1622	-	41,47,47	0.93	1 (2%)	54,74,74	2.55	18 (33%)
24	CHL	6	601	1	60,74,74	3.33	20 (33%)	58,114,114	2.33	17 (29%)
24	CHL	9	608	-	38,52,74	4.20	19 (50%)	31,87,114	2.65	10 (32%)
24	CHL	n	608	-	44,58,74	3.73	19 (43%)	37,94,114	2.93	11 (29%)
25	CLA	N	613	2	69,73,73	1.14	6 (8%)	82,113,113	1.28	5 (6%)
24	CHL	Y	608	-	44,58,74	3.77	19 (43%)	37,94,114	2.84	11 (29%)
27	XAT	2	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.57	20 (37%)
27	XAT	r	622	-	41,47,47	1.03	2 (4%)	54,74,74	2.39	18 (33%)
25	CLA	C	501	-	69,73,73	1.17	10 (14%)	82,113,113	1.20	5 (6%)
25	CLA	n	613	2	69,73,73	1.13	7 (10%)	82,113,113	1.29	4 (4%)
28	NEX	8	1623	-	40,46,46	0.92	2 (5%)	50,70,70	2.18	12 (24%)
26	LUT	9	1621	-	42,43,43	0.76	0	51,60,60	1.76	15 (29%)
26	LUT	s	1621	-	42,43,43	0.79	0	51,60,60	1.89	16 (31%)
25	CLA	r	603	-	64,68,73	1.20	9 (14%)	76,107,113	1.40	4 (5%)
24	CHL	G	609	3	60,74,74	3.19	21 (35%)	58,114,114	2.23	16 (27%)
25	CLA	y	611	29	69,73,73	1.15	8 (11%)	82,113,113	1.21	5 (6%)
25	CLA	Y	603	-	69,73,73	1.16	11 (15%)	82,113,113	1.36	8 (9%)
25	CLA	8	612	2	49,53,73	1.36	6 (12%)	58,89,113	1.43	6 (10%)
25	CLA	5	602	2	69,73,73	1.16	8 (11%)	82,113,113	1.11	6 (7%)
24	CHL	5	601	2	60,74,74	3.39	19 (31%)	58,114,114	2.41	16 (27%)
25	CLA	1	611	29	69,73,73	1.15	9 (13%)	82,113,113	1.18	3 (3%)
25	CLA	p	602	2	69,73,73	1.17	8 (11%)	82,113,113	1.12	8 (9%)
25	CLA	c	512	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	5 (6%)
25	CLA	8	611	29	53,57,73	1.29	6 (11%)	61,93,113	1.28	5 (8%)
29	LHG	D	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.04	3 (6%)
25	CLA	G	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	505	-	69,73,73	1.17	10 (14%)	82,113,113	1.22	9 (10%)
25	CLA	A	405	-	69,73,73	1.20	8 (11%)	82,113,113	1.31	9 (10%)
25	CLA	4	611	29	49,53,73	1.35	7 (14%)	58,89,113	1.30	3 (5%)
26	LUT	8	1621	-	42,43,43	0.76	0	51,60,60	1.61	12 (23%)
25	CLA	n	604	-	69,73,73	1.18	9 (13%)	82,113,113	1.18	4 (4%)
24	CHL	0	605	1	40,54,74	4.19	19 (47%)	34,90,114	2.44	13 (38%)
25	CLA	N	612	2	49,53,73	1.37	8 (16%)	58,89,113	1.40	6 (10%)
24	CHL	Y	606	-	60,74,74	3.17	20 (33%)	58,114,114	2.26	14 (24%)
25	CLA	c	509	-	69,73,73	1.17	8 (11%)	82,113,113	1.43	5 (6%)
25	CLA	3	611	29	53,57,73	1.30	6 (11%)	61,93,113	1.28	6 (9%)
24	CHL	q	607	-	44,58,74	4.06	18 (40%)	37,94,114	2.19	14 (37%)
25	CLA	c	507	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	11 (13%)
25	CLA	y	602	1	69,73,73	1.16	8 (11%)	82,113,113	1.19	6 (7%)
25	CLA	1	602	1	69,73,73	1.15	8 (11%)	82,113,113	1.16	5 (6%)
29	LHG	7	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.12	4 (7%)
24	CHL	R	608	-	55,69,74	3.35	21 (38%)	52,108,114	2.50	15 (28%)
25	CLA	b	614	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
26	LUT	4	1620	-	42,43,43	0.72	0	51,60,60	1.70	17 (33%)
25	CLA	2	610	2	69,73,73	1.13	6 (8%)	82,113,113	1.14	7 (8%)
25	CLA	6	610	1	69,73,73	1.13	8 (11%)	82,113,113	1.07	5 (6%)
29	LHG	8	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	s	613	18	53,57,73	1.30	7 (13%)	61,93,113	1.30	5 (8%)
34	BCR	d	404	-	41,41,41	0.74	1 (2%)	56,56,56	2.03	15 (26%)
27	XAT	N	1622	-	41,47,47	0.99	3 (7%)	54,74,74	2.68	22 (40%)
25	CLA	1	614	-	58,62,73	1.26	8 (13%)	68,99,113	1.18	4 (5%)
25	CLA	G	614	-	53,57,73	1.30	8 (15%)	61,93,113	1.19	6 (9%)
25	CLA	p	611	29	53,57,73	1.29	6 (11%)	61,93,113	1.28	5 (8%)
25	CLA	0	611	29	69,73,73	1.15	6 (8%)	82,113,113	1.23	5 (6%)
25	CLA	D	403	-	69,73,73	1.13	9 (13%)	82,113,113	1.17	5 (6%)
25	CLA	q	611	29	49,53,73	1.35	7 (14%)	58,89,113	1.33	3 (5%)
24	CHL	r	606	-	60,74,74	3.12	20 (33%)	58,114,114	2.47	17 (29%)
24	CHL	7	605	1	40,54,74	4.08	19 (47%)	34,90,114	2.57	12 (35%)
25	CLA	Y	604	-	69,73,73	1.19	9 (13%)	82,113,113	1.24	7 (8%)
25	CLA	g	611	29	49,53,73	1.36	8 (16%)	58,89,113	1.39	5 (8%)
25	CLA	r	611	29	53,57,73	1.28	9 (16%)	61,93,113	1.30	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	S	607	-	37,51,74	4.22	19 (51%)	30,86,114	2.56	12 (40%)
25	CLA	b	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.09	3 (3%)
25	CLA	n	612	2	49,53,73	1.38	8 (16%)	58,89,113	1.40	6 (10%)
25	CLA	C	511	6	69,73,73	1.17	10 (14%)	82,113,113	1.37	9 (10%)
34	BCR	C	516	-	41,41,41	0.72	0	56,56,56	1.72	11 (19%)
25	CLA	C	512	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	5 (6%)
25	CLA	G	611	29	49,53,73	1.35	7 (14%)	58,89,113	1.40	5 (8%)
25	CLA	g	614	-	53,57,73	1.31	8 (15%)	61,93,113	1.19	6 (9%)
25	CLA	2	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
25	CLA	0	602	1	69,73,73	1.17	9 (13%)	82,113,113	1.13	4 (4%)
37	DGD	C	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.99	4 (5%)
24	CHL	7	607	-	60,74,74	3.26	19 (31%)	58,114,114	2.16	19 (32%)
29	LHG	n	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	3 (5%)
25	CLA	Y	611	29	69,73,73	1.15	8 (11%)	82,113,113	1.22	5 (6%)
36	LMG	a	413	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	3	613	2	69,73,73	1.13	6 (8%)	82,113,113	1.32	5 (6%)
34	BCR	B	620	-	41,41,41	0.81	1 (2%)	56,56,56	1.89	18 (32%)
25	CLA	b	605	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
34	BCR	c	516	-	41,41,41	0.72	0	56,56,56	1.72	11 (19%)
24	CHL	G	605	3	42,56,74	4.12	19 (45%)	36,92,114	2.59	15 (41%)
25	CLA	C	509	-	69,73,73	1.17	8 (11%)	82,113,113	1.43	7 (8%)
24	CHL	p	605	2	60,74,74	3.53	18 (30%)	58,114,114	2.19	13 (22%)
25	CLA	C	502	-	69,73,73	1.23	10 (14%)	82,113,113	1.59	10 (12%)
40	HEM	f	101	8,9	50,50,50	1.38	6 (12%)	67,82,82	1.04	3 (4%)
37	DGD	c	518	-	56,56,67	0.89	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	B	608	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	6 (7%)
28	NEX	s	1623	-	40,46,46	1.16	4 (10%)	50,70,70	2.42	18 (36%)
25	CLA	s	610	18	53,57,73	1.29	9 (16%)	61,93,113	1.20	8 (13%)
25	CLA	g	602	3	69,73,73	1.15	9 (13%)	82,113,113	1.25	7 (8%)
25	CLA	B	604	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	7 (8%)
24	CHL	q	609	3	60,74,74	3.62	20 (33%)	58,114,114	1.93	12 (20%)
25	CLA	1	613	1	69,73,73	1.14	7 (10%)	82,113,113	1.30	6 (7%)
25	CLA	7	611	29	69,73,73	1.15	9 (13%)	82,113,113	1.20	3 (3%)
25	CLA	B	606	-	69,73,73	1.17	9 (13%)	82,113,113	1.10	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	R	603	-	64,68,73	1.19	8 (12%)	76,107,113	1.40	4 (5%)
24	CHL	6	608	-	44,58,74	3.88	19 (43%)	37,94,114	2.78	14 (37%)
24	CHL	0	601	1	60,74,74	3.33	19 (31%)	58,114,114	2.12	15 (25%)
29	LHG	0	2630	25	48,48,48	0.94	2 (4%)	51,54,54	0.97	2 (3%)
27	XAT	1	1622	-	41,47,47	0.98	2 (4%)	54,74,74	4.20	23 (42%)
25	CLA	5	611	29	53,57,73	1.29	7 (13%)	61,93,113	1.23	4 (6%)
25	CLA	2	614	-	53,57,73	1.29	7 (13%)	61,93,113	1.20	4 (6%)
29	LHG	Y	2630	25	48,48,48	0.89	3 (6%)	51,54,54	1.22	5 (9%)
25	CLA	4	613	3	69,73,73	1.14	6 (8%)	82,113,113	1.19	5 (6%)
27	XAT	0	1622	-	41,47,47	1.00	2 (4%)	54,74,74	4.15	23 (42%)
25	CLA	r	604	-	52,56,73	1.33	9 (17%)	61,92,113	1.34	4 (6%)
25	CLA	2	612	2	47,51,73	1.38	8 (17%)	55,86,113	1.40	5 (9%)
35	SQD	d	413	-	50,52,54	1.10	3 (6%)	60,63,65	1.17	6 (10%)
25	CLA	b	613	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	8 (9%)
25	CLA	4	614	-	53,57,73	1.30	8 (15%)	61,93,113	1.24	4 (6%)
28	NEX	1	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.34	18 (36%)
24	CHL	g	605	3	42,56,74	4.12	19 (45%)	36,92,114	2.64	15 (41%)
25	CLA	g	603	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
29	LHG	s	2630	25	44,44,48	0.96	2 (4%)	47,50,54	1.13	3 (6%)
36	LMG	H	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.26	7 (12%)
37	DGD	C	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.99	4 (5%)
26	LUT	n	1621	-	42,43,43	0.83	1 (2%)	51,60,60	1.67	10 (19%)
25	CLA	0	610	1	69,73,73	1.14	8 (11%)	82,113,113	1.08	6 (7%)
25	CLA	n	602	2	69,73,73	1.15	9 (13%)	82,113,113	1.17	9 (10%)
29	LHG	R	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.21	3 (7%)
24	CHL	N	609	2	60,74,74	3.18	20 (33%)	58,114,114	2.22	15 (25%)
25	CLA	7	613	1	69,73,73	1.15	7 (10%)	82,113,113	1.31	6 (7%)
33	PHO	a	408	-	58,69,69	2.02	12 (20%)	55,99,99	1.71	12 (21%)
24	CHL	q	606	-	44,58,74	4.07	19 (43%)	37,94,114	2.17	15 (40%)
36	LMG	d	412	-	46,46,55	0.95	2 (4%)	54,54,63	1.10	4 (7%)
25	CLA	B	612	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	9 (10%)
36	LMG	C	521	-	51,51,55	0.88	2 (3%)	59,59,63	1.08	4 (6%)
25	CLA	g	613	3	69,73,73	1.15	8 (11%)	82,113,113	1.17	3 (3%)
28	NEX	3	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.20	15 (30%)
28	NEX	4	1623	-	40,46,46	1.04	3 (7%)	50,70,70	2.24	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	7	609	1	60,74,74	3.22	19 (31%)	58,114,114	2.31	14 (24%)
25	CLA	R	604	-	52,56,73	1.33	9 (17%)	61,92,113	1.33	4 (6%)
25	CLA	4	610	3	69,73,73	1.15	8 (11%)	82,113,113	1.17	4 (4%)
25	CLA	5	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	5 (6%)
24	CHL	N	607	-	60,74,74	3.19	19 (31%)	58,114,114	2.50	19 (32%)
25	CLA	B	616	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	13 (15%)
24	CHL	1	601	1	60,74,74	3.31	19 (31%)	58,114,114	2.47	18 (31%)
24	CHL	2	606	-	44,58,74	3.95	19 (43%)	37,94,114	2.63	13 (35%)
34	BCR	c	515	-	41,41,41	0.87	2 (4%)	56,56,56	1.75	11 (19%)
36	LMG	h	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.22	5 (8%)
25	CLA	R	612	-	53,57,73	1.29	9 (16%)	61,93,113	1.39	6 (9%)
25	CLA	b	610	-	69,73,73	1.14	9 (13%)	82,113,113	1.22	7 (8%)
25	CLA	5	613	2	69,73,73	1.14	6 (8%)	82,113,113	1.30	3 (3%)
24	CHL	5	608	-	44,58,74	3.92	19 (43%)	37,94,114	2.81	11 (29%)
24	CHL	p	609	2	60,74,74	3.40	20 (33%)	58,114,114	2.23	15 (25%)
25	CLA	4	602	3	69,73,73	1.15	6 (8%)	82,113,113	1.13	6 (7%)
24	CHL	4	605	3	42,56,74	4.20	19 (45%)	36,92,114	2.39	13 (36%)
24	CHL	3	601	2	60,74,74	3.32	19 (31%)	58,114,114	2.35	15 (25%)
24	CHL	4	601	3	60,74,74	3.40	20 (33%)	58,114,114	2.26	16 (27%)
25	CLA	S	609	18	45,49,73	1.38	7 (15%)	54,84,113	1.32	6 (11%)
25	CLA	B	615	-	69,73,73	1.15	9 (13%)	82,113,113	1.13	6 (7%)
27	XAT	g	1622	-	41,47,47	0.96	2 (4%)	54,74,74	2.48	20 (37%)
25	CLA	a	410	-	64,68,73	1.20	9 (14%)	76,107,113	1.34	10 (13%)
25	CLA	1	610	1	69,73,73	1.11	7 (10%)	82,113,113	1.14	7 (8%)
24	CHL	g	606	-	44,58,74	3.81	19 (43%)	37,94,114	2.86	16 (43%)
24	CHL	G	601	3	60,74,74	3.17	19 (31%)	58,114,114	2.58	18 (31%)
24	CHL	n	601	2	60,74,74	3.19	19 (31%)	58,114,114	2.68	18 (31%)
25	CLA	2	604	-	53,57,73	1.29	8 (15%)	61,93,113	1.28	6 (9%)
24	CHL	7	608	-	44,58,74	3.76	19 (43%)	37,94,114	2.77	12 (32%)
25	CLA	5	614	-	53,57,73	1.33	6 (11%)	61,93,113	1.25	5 (8%)
25	CLA	0	604	-	69,73,73	1.14	7 (10%)	82,113,113	1.11	4 (4%)
24	CHL	5	605	2	60,74,74	3.51	18 (30%)	58,114,114	2.29	15 (25%)
34	BCR	H	101	-	41,41,41	0.80	0	56,56,56	2.04	16 (28%)
25	CLA	r	609	17	62,66,73	1.20	8 (12%)	73,104,113	1.29	4 (5%)
25	CLA	g	604	-	53,57,73	1.30	8 (15%)	61,93,113	1.28	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	8	605	2	60,74,74	3.50	19 (31%)	58,114,114	1.85	13 (22%)
28	NEX	S	1623	-	40,46,46	1.07	3 (7%)	50,70,70	2.29	16 (32%)
28	NEX	5	1623	-	40,46,46	0.97	3 (7%)	50,70,70	2.38	16 (32%)
24	CHL	n	607	-	60,74,74	3.18	19 (31%)	58,114,114	2.51	19 (32%)
24	CHL	y	607	-	60,74,74	3.29	20 (33%)	58,114,114	2.53	20 (34%)
25	CLA	3	610	2	69,73,73	1.15	7 (10%)	82,113,113	1.09	4 (4%)
24	CHL	Y	607	-	60,74,74	3.29	20 (33%)	58,114,114	2.53	19 (32%)
34	BCR	A	411	-	41,41,41	0.77	1 (2%)	56,56,56	1.72	11 (19%)
25	CLA	g	612	3	47,51,73	1.34	9 (19%)	55,86,113	1.30	5 (9%)
35	SQD	D	413	-	50,52,54	1.10	3 (6%)	60,63,65	1.17	6 (10%)
24	CHL	6	606	-	60,74,74	3.39	20 (33%)	58,114,114	2.50	15 (25%)
24	CHL	s	606	-	38,52,74	4.09	18 (47%)	31,87,114	3.12	12 (38%)
25	CLA	c	503	-	69,73,73	1.15	10 (14%)	82,113,113	1.25	8 (9%)
29	LHG	D	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.24	2 (4%)
24	CHL	3	606	-	40,54,74	4.20	19 (47%)	34,90,114	2.52	13 (38%)
29	LHG	G	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.13	4 (7%)
25	CLA	B	602	-	69,73,73	1.16	9 (13%)	82,113,113	1.09	3 (3%)
27	XAT	R	622	-	41,47,47	1.02	2 (4%)	54,74,74	2.39	17 (31%)
25	CLA	S	612	18	49,53,73	1.36	8 (16%)	58,89,113	1.47	9 (15%)
25	CLA	C	503	-	69,73,73	1.16	10 (14%)	82,113,113	1.24	7 (8%)
34	BCR	C	517	-	41,41,41	0.81	2 (4%)	56,56,56	1.84	11 (19%)
37	DGD	c	523	-	67,67,67	0.82	2 (2%)	81,81,81	1.03	5 (6%)
24	CHL	Y	605	1	40,54,74	4.02	19 (47%)	34,90,114	2.67	11 (32%)
25	CLA	9	614	-	53,57,73	1.30	8 (15%)	61,93,113	1.20	4 (6%)
34	BCR	C	514	-	41,41,41	0.73	0	56,56,56	1.59	10 (17%)
27	XAT	G	1622	-	41,47,47	0.95	2 (4%)	54,74,74	2.48	21 (38%)
26	LUT	6	1621	-	42,43,43	0.79	0	51,60,60	1.64	10 (19%)
26	LUT	p	1621	-	42,43,43	0.71	0	51,60,60	1.62	10 (19%)
24	CHL	y	609	1	60,74,74	3.13	19 (31%)	58,114,114	2.37	17 (29%)
26	LUT	N	1620	-	42,43,43	0.74	0	51,60,60	1.59	10 (19%)
29	LHG	g	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.13	4 (7%)
26	LUT	q	1621	-	42,43,43	0.72	0	51,60,60	1.67	12 (23%)
24	CHL	2	605	2	42,56,74	4.19	18 (42%)	36,92,114	2.37	15 (41%)
26	LUT	p	1620	-	42,43,43	0.70	0	51,60,60	1.87	10 (19%)
26	LUT	q	1620	-	42,43,43	0.69	0	51,60,60	1.65	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	D	402	-	69,73,73	1.21	9 (13%)	82,113,113	1.30	7 (8%)
25	CLA	9	611	29	49,53,73	1.36	9 (18%)	58,89,113	1.31	5 (8%)
24	CHL	8	609	2	60,74,74	3.25	19 (31%)	58,114,114	2.35	13 (22%)
34	BCR	D	404	-	41,41,41	0.74	1 (2%)	56,56,56	2.03	15 (26%)
25	CLA	s	611	29	53,57,73	1.29	9 (16%)	61,93,113	1.30	4 (6%)
24	CHL	y	605	1	40,54,74	4.03	19 (47%)	34,90,114	2.66	11 (32%)
25	CLA	c	510	-	69,73,73	1.18	10 (14%)	82,113,113	1.30	7 (8%)
25	CLA	y	610	1	69,73,73	1.12	8 (11%)	82,113,113	1.13	7 (8%)
25	CLA	b	608	-	69,73,73	1.16	9 (13%)	82,113,113	1.21	6 (7%)
25	CLA	S	610	18	53,57,73	1.30	8 (15%)	61,93,113	1.19	8 (13%)
24	CHL	p	607	-	60,74,74	3.43	19 (31%)	58,114,114	2.05	13 (22%)
33	PHO	A	409	-	58,69,69	1.99	11 (18%)	55,99,99	1.85	11 (20%)
26	LUT	Y	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.75	14 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	8	607	-	3/3/20/26	24/39/137/137	-
25	CLA	G	612	3	1/1/10/20	7/13/89/115	-
25	CLA	q	602	3	1/1/15/20	16/39/115/115	-
25	CLA	C	510	-	1/1/15/20	9/39/115/115	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CHL	r	607	-	3/3/18/26	16/27/125/137	-
24	CHL	y	608	-	3/3/16/26	4/20/118/137	-
25	CLA	7	612	1	1/1/15/20	14/39/115/115	-
25	CLA	s	604	-	1/1/11/20	8/20/96/115	-
25	CLA	p	614	-	-	9/20/96/115	-
29	LHG	l	101	-	-	18/53/53/53	-
25	CLA	b	611	-	1/1/15/20	11/39/115/115	-
39	PL9	d	405	-	-	14/53/73/73	0/1/1/1
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
27	XAT	y	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	d	403	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	6	607	-	3/3/20/26	24/39/137/137	-
24	CHL	S	601	18	3/3/16/26	8/15/113/137	-
27	XAT	5	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	9	602	2	1/1/15/20	15/39/115/115	-
36	LMG	b	622	-	-	8/46/66/70	0/1/1/1
25	CLA	3	603	-	1/1/15/20	15/39/115/115	-
25	CLA	2	611	29	1/1/11/20	9/15/91/115	-
25	CLA	7	614	-	1/1/12/20	13/26/102/115	-
25	CLA	s	605	18	1/1/12/20	8/21/97/115	-
28	NEX	0	1623	-	-	5/27/83/83	0/3/3/3
37	DGD	C	523	-	-	13/55/95/95	0/2/2/2
24	CHL	0	606	-	3/3/20/26	21/39/137/137	-
27	XAT	q	1622	-	-	3/31/93/93	0/4/4/4
26	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	R	607	-	3/3/18/26	16/27/125/137	-
25	CLA	N	604	-	1/1/15/20	12/39/115/115	-
25	CLA	9	610	2	1/1/15/20	5/39/115/115	-
24	CHL	Y	609	1	3/3/20/26	16/39/137/137	-
25	CLA	5	610	2	1/1/15/20	8/39/115/115	-
25	CLA	y	604	-	-	20/39/115/115	-
25	CLA	1	603	-	1/1/15/20	17/39/115/115	-
25	CLA	Y	612	1	1/1/15/20	17/39/115/115	-
25	CLA	S	604	-	1/1/11/20	7/20/96/115	-
27	XAT	6	1622	-	-	2/31/93/93	0/4/4/4
27	XAT	9	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	9	606	-	3/3/16/26	10/20/118/137	-
24	CHL	S	608	-	3/3/16/26	9/19/117/137	-
25	CLA	R	611	29	1/1/11/20	10/20/96/115	-
24	CHL	3	605	2	3/3/20/26	17/39/137/137	-
25	CLA	4	603	-	1/1/15/20	17/39/115/115	-
35	SQD	b	623	-	-	14/45/65/69	0/1/1/1
35	SQD	B	623	-	-	12/45/65/69	0/1/1/1
25	CLA	R	616	17	-	22/39/115/115	-
26	LUT	9	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	G	607	-	3/3/16/26	7/20/118/137	-
29	LHG	N	2630	25	-	15/53/53/53	-
29	LHG	2	2630	25	-	22/53/53/53	-
26	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
28	NEX	6	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	7	601	1	3/3/20/26	14/39/137/137	-
35	SQD	B	621	-	-	17/49/69/69	0/1/1/1
25	CLA	N	614	-	1/1/11/20	7/20/96/115	-
24	CHL	q	601	3	3/3/20/26	19/39/137/137	-
25	CLA	C	513	-	1/1/15/20	15/39/115/115	-
25	CLA	r	616	17	-	22/39/115/115	-
24	CHL	1	606	-	3/3/20/26	18/39/137/137	-
37	DGD	c	524	-	-	9/55/95/95	0/2/2/2
25	CLA	b	603	-	1/1/15/20	10/39/115/115	-
24	CHL	3	608	-	3/3/16/26	11/20/118/137	-
24	CHL	4	608	-	3/3/15/26	6/13/111/137	-
25	CLA	A	407	-	1/1/11/20	4/20/96/115	-
24	CHL	5	607	-	3/3/20/26	20/39/137/137	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	7	602	1	1/1/15/20	14/39/115/115	-
26	LUT	8	1620	-	-	4/29/67/67	0/2/2/2
25	CLA	c	511	6	-	12/39/115/115	-
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
25	CLA	p	610	2	1/1/15/20	11/39/115/115	-
25	CLA	B	607	-	-	17/39/115/115	-
24	CHL	9	601	2	3/3/20/26	20/39/137/137	-
25	CLA	N	611	29	1/1/11/20	10/20/96/115	-
36	LMG	d	411	-	-	8/41/61/70	0/1/1/1
24	CHL	s	601	18	3/3/16/26	7/15/113/137	-
25	CLA	8	604	-	1/1/15/20	10/39/115/115	-
25	CLA	n	614	-	1/1/11/20	8/20/96/115	-
25	CLA	n	611	29	1/1/11/20	10/20/96/115	-
24	CHL	1	608	-	3/3/16/26	8/20/118/137	-
25	CLA	0	603	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Y	614	-	1/1/12/20	11/26/102/115	-
26	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	4	604	-	1/1/11/20	12/20/96/115	-
25	CLA	g	610	3	1/1/15/20	12/39/115/115	-
36	LMG	S	2631	-	-	12/47/67/70	0/1/1/1
36	LMG	D	412	-	-	5/41/61/70	0/1/1/1
26	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	r	608	-	3/3/19/26	12/33/131/137	-
24	CHL	R	606	-	3/3/20/26	21/39/137/137	-
37	DGD	C	519	-	-	19/51/91/95	0/2/2/2
25	CLA	S	614	-	1/1/11/20	6/19/95/115	-
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
40	HEM	F	101	8,9	-	5/14/54/54	-
24	CHL	2	601	2	3/3/20/26	22/39/137/137	-
34	BCR	a	411	-	-	2/29/63/63	0/2/2/2
24	CHL	g	608	-	3/3/15/26	3/13/111/137	-
25	CLA	A	406	-	1/1/15/20	1/39/115/115	-
29	LHG	c	2630	-	-	15/51/51/53	-
25	CLA	B	609	-	1/1/15/20	11/39/115/115	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
25	CLA	N	602	2	1/1/15/20	7/39/115/115	-
25	CLA	S	603	-	1/1/10/20	6/12/88/115	-
25	CLA	b	604	-	1/1/15/20	10/39/115/115	-
24	CHL	G	608	-	3/3/15/26	6/13/111/137	-
25	CLA	7	610	1	1/1/15/20	14/39/115/115	-
25	CLA	b	606	-	1/1/15/20	13/39/115/115	-
24	CHL	p	601	2	3/3/20/26	19/39/137/137	-
28	NEX	y	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	R	609	17	1/1/13/20	5/31/107/115	-
25	CLA	c	502	-	1/1/15/20	17/39/115/115	-
25	CLA	1	604	-	1/1/15/20	15/39/115/115	-
25	CLA	C	508	-	1/1/15/20	13/39/115/115	-
25	CLA	G	604	-	1/1/11/20	7/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	603	-	1/1/15/20	14/39/115/115	-
24	CHL	G	606	-	3/3/16/26	4/20/118/137	-
35	SQD	b	621	-	-	17/49/69/69	0/1/1/1
25	CLA	y	614	-	1/1/12/20	11/26/102/115	-
25	CLA	B	613	-	1/1/15/20	11/39/115/115	-
36	LMG	c	521	-	-	10/46/66/70	0/1/1/1
25	CLA	d	402	-	1/1/15/20	15/39/115/115	-
25	CLA	b	609	-	1/1/15/20	11/39/115/115	-
25	CLA	1	612	1	1/1/15/20	18/39/115/115	-
25	CLA	c	504	-	1/1/15/20	15/39/115/115	-
24	CHL	y	606	-	3/3/20/26	18/39/137/137	-
25	CLA	8	610	2	1/1/15/20	10/39/115/115	-
25	CLA	0	612	1	1/1/15/20	14/39/115/115	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	c	508	-	1/1/15/20	11/39/115/115	-
25	CLA	Y	602	1	1/1/15/20	11/39/115/115	-
36	LMG	A	413	-	-	12/43/63/70	0/1/1/1
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	r	612	-	1/1/11/20	10/20/96/115	-
33	PHO	A	408	-	-	10/37/103/103	0/5/6/6
29	LHG	d	409	-	-	10/53/53/53	-
24	CHL	2	609	2	3/3/20/26	22/39/137/137	-
25	CLA	b	607	-	-	17/39/115/115	-
24	CHL	2	608	-	3/3/15/26	4/13/111/137	-
25	CLA	3	612	2	1/1/11/20	8/15/91/115	-
25	CLA	4	612	3	1/1/10/20	9/13/89/115	-
26	LUT	y	1621	-	-	4/29/67/67	0/2/2/2
25	CLA	A	410	-	1/1/14/20	4/33/109/115	-
24	CHL	8	608	-	3/3/16/26	11/20/118/137	-
25	CLA	S	602	18	-	9/20/96/115	-
24	CHL	0	608	-	3/3/16/26	7/20/118/137	-
29	LHG	d	410	-	-	12/43/43/53	-
25	CLA	B	614	-	1/1/15/20	8/39/115/115	-
35	SQD	A	412	-	-	18/46/66/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	612	-	1/1/15/20	9/39/115/115	-
25	CLA	6	611	29	1/1/15/20	14/39/115/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	3	609	2	3/3/20/26	19/39/137/137	-
25	CLA	q	614	-	1/1/11/20	9/20/96/115	-
25	CLA	C	507	-	1/1/15/20	11/39/115/115	-
25	CLA	R	601	17	1/1/11/20	10/20/96/115	-
25	CLA	S	613	18	-	10/20/96/115	-
24	CHL	9	607	-	3/3/16/26	10/20/118/137	-
25	CLA	a	405	-	1/1/15/20	13/39/115/115	-
26	LUT	3	1620	-	-	5/29/67/67	0/2/2/2
24	CHL	s	607	-	3/3/15/26	4/12/110/137	-
24	CHL	N	601	2	3/3/20/26	9/39/137/137	-
29	LHG	1	2630	25	-	15/53/53/53	-
27	XAT	n	1622	-	-	2/31/93/93	0/4/4/4
29	LHG	d	408	-	-	10/48/48/53	-
24	CHL	8	601	2	3/3/20/26	19/39/137/137	-
26	LUT	N	1621	-	-	5/29/67/67	0/2/2/2
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	y	603	-	1/1/15/20	15/39/115/115	-
29	LHG	4	2630	25	-	17/53/53/53	-
25	CLA	5	612	2	1/1/11/20	8/15/91/115	-
25	CLA	B	605	-	1/1/15/20	13/39/115/115	-
25	CLA	b	615	-	1/1/15/20	15/39/115/115	-
29	LHG	C	2630	-	-	19/51/51/53	-
25	CLA	6	613	1	-	19/39/115/115	-
28	NEX	9	1623	-	-	4/27/83/83	0/3/3/3
28	NEX	n	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	Y	613	1	-	11/39/115/115	-
25	CLA	n	610	2	1/1/15/20	7/39/115/115	-
26	LUT	1	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	3	604	-	1/1/15/20	7/39/115/115	-
25	CLA	Y	610	1	1/1/15/20	10/39/115/115	-
25	CLA	y	613	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	r	623	-	-	2/27/83/83	0/3/3/3
24	CHL	4	606	-	3/3/16/26	6/20/118/137	-
24	CHL	9	609	2	3/3/20/26	20/39/137/137	-
24	CHL	6	609	1	3/3/20/26	21/39/137/137	-
26	LUT	0	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	0	614	-	1/1/12/20	9/26/102/115	-
24	CHL	5	609	2	3/3/20/26	21/39/137/137	-
25	CLA	G	613	3	1/1/15/20	12/39/115/115	-
29	LHG	5	2630	25	-	12/53/53/53	-
24	CHL	9	605	2	3/3/16/26	6/18/116/137	-
25	CLA	s	602	18	-	9/20/96/115	-
25	CLA	6	603	-	1/1/15/20	12/39/115/115	-
24	CHL	5	606	-	3/3/16/26	4/15/113/137	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
24	CHL	4	607	-	3/3/16/26	13/20/118/137	-
24	CHL	S	606	-	3/3/15/26	8/13/111/137	-
25	CLA	a	406	-	1/1/15/20	1/39/115/115	-
27	XAT	8	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	C	504	-	1/1/15/20	15/39/115/115	-
28	NEX	g	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	q	605	3	3/3/16/26	7/18/116/137	-
24	CHL	s	608	-	3/3/16/26	9/19/117/137	-
25	CLA	G	602	3	1/1/15/20	11/39/115/115	-
25	CLA	N	610	2	1/1/15/20	7/39/115/115	-
28	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	6	605	1	3/3/16/26	5/15/113/137	-
25	CLA	R	602	17	1/1/14/20	8/33/109/115	-
25	CLA	y	612	1	1/1/15/20	17/39/115/115	-
25	CLA	9	613	2	1/1/15/20	8/39/115/115	-
25	CLA	p	603	-	1/1/15/20	16/39/115/115	-
25	CLA	r	602	17	1/1/14/20	8/33/109/115	-
24	CHL	1	607	-	3/3/20/26	19/39/137/137	-
25	CLA	7	603	-	1/1/15/20	17/39/115/115	-
25	CLA	q	603	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	Y	601	1	3/3/20/26	12/39/137/137	-
25	CLA	B	617	-	1/1/15/20	11/39/115/115	-
26	LUT	5	1620	-	-	3/29/67/67	0/2/2/2
36	LMG	D	411	-	-	8/41/61/70	0/1/1/1
29	LHG	S	2630	25	-	14/49/49/53	-
24	CHL	2	607	-	3/3/16/26	11/20/118/137	-
25	CLA	C	506	-	1/1/15/20	20/39/115/115	-
29	LHG	3	2630	25	-	11/53/53/53	-
26	LUT	g	1621	-	-	1/29/67/67	0/2/2/2
25	CLA	p	613	2	1/1/15/20	11/39/115/115	-
26	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
24	CHL	n	605	2	3/3/20/26	22/39/137/137	-
25	CLA	q	613	3	1/1/15/20	14/39/115/115	-
24	CHL	0	607	-	3/3/20/26	22/39/137/137	-
26	LUT	5	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	3	614	-	1/1/11/20	10/20/96/115	-
24	CHL	q	608	-	3/3/15/26	5/13/111/137	-
25	CLA	r	613	17	-	15/33/109/115	-
24	CHL	g	607	-	3/3/16/26	9/20/118/137	-
25	CLA	s	603	-	1/1/10/20	6/12/88/115	-
25	CLA	b	616	-	1/1/15/20	8/39/115/115	-
27	XAT	p	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	2	613	2	1/1/15/20	8/39/115/115	-
24	CHL	3	607	-	3/3/20/26	24/39/137/137	-
24	CHL	7	606	-	3/3/20/26	18/39/137/137	-
24	CHL	y	601	1	3/3/20/26	12/39/137/137	-
25	CLA	9	604	-	1/1/11/20	8/20/96/115	-
25	CLA	s	609	18	1/1/10/20	6/10/86/115	-
25	CLA	6	604	-	-	19/39/115/115	-
28	NEX	R	623	-	-	2/27/83/83	0/3/3/3
25	CLA	B	610	-	1/1/15/20	6/39/115/115	-
25	CLA	0	613	1	-	12/39/115/115	-
24	CHL	1	609	1	3/3/20/26	17/39/137/137	-
25	CLA	5	604	-	1/1/15/20	16/39/115/115	-
24	CHL	0	609	1	3/3/20/26	21/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	614	-	1/1/11/20	10/20/96/115	-
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
29	LHG	y	2630	25	-	25/53/53/53	-
25	CLA	p	604	-	1/1/15/20	15/39/115/115	-
28	NEX	p	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	c	506	-	1/1/15/20	20/39/115/115	-
25	CLA	R	610	17	1/1/15/20	15/39/115/115	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
33	PHO	a	409	-	-	9/37/103/103	0/5/6/6
25	CLA	q	604	-	-	14/20/96/115	-
28	NEX	q	1623	-	-	3/27/83/83	0/3/3/3
34	BCR	b	618	-	-	4/29/63/63	0/2/2/2
27	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
36	LMG	B	622	-	-	8/46/66/70	0/1/1/1
34	BCR	B	618	-	-	4/29/63/63	0/2/2/2
24	CHL	p	608	-	3/3/16/26	11/20/118/137	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	G	610	3	1/1/15/20	12/39/115/115	-
28	NEX	N	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	p	612	2	1/1/11/20	6/15/91/115	-
29	LHG	9	2630	25	-	20/53/53/53	-
25	CLA	S	605	18	1/1/12/20	9/21/97/115	-
25	CLA	q	612	3	1/1/10/20	8/13/89/115	-
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	B	603	-	1/1/15/20	10/39/115/115	-
39	PL9	D	405	-	-	14/53/73/73	0/1/1/1
25	CLA	R	613	17	-	15/33/109/115	-
24	CHL	n	606	-	3/3/16/26	8/15/113/137	-
25	CLA	6	602	1	1/1/15/20	13/39/115/115	-
25	CLA	r	610	17	1/1/15/20	15/39/115/115	-
25	CLA	b	617	-	1/1/15/20	11/39/115/115	-
25	CLA	c	505	-	1/1/15/20	16/39/115/115	-
25	CLA	a	407	-	1/1/11/20	4/20/96/115	-
25	CLA	r	601	17	1/1/11/20	10/20/96/115	-
26	LUT	G	1621	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	3	602	2	1/1/15/20	11/39/115/115	-
25	CLA	c	513	-	1/1/15/20	17/39/115/115	-
26	LUT	r	620	-	-	0/29/67/67	0/2/2/2
25	CLA	9	612	2	1/1/10/20	5/13/89/115	-
25	CLA	6	612	1	1/1/15/20	14/39/115/115	-
25	CLA	s	612	18	1/1/11/20	5/15/91/115	-
25	CLA	c	501	-	1/1/15/20	12/39/115/115	-
36	LMG	s	2631	-	-	10/47/67/70	0/1/1/1
26	LUT	4	1621	-	-	7/29/67/67	0/2/2/2
35	SQD	a	412	-	-	18/46/66/69	0/1/1/1
26	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
29	LHG	6	2630	25	-	19/53/53/53	-
25	CLA	2	602	2	-	13/39/115/115	-
34	BCR	C	515	-	-	4/29/63/63	0/2/2/2
24	CHL	N	608	-	3/3/16/26	6/20/118/137	-
25	CLA	7	604	-	1/1/15/20	19/39/115/115	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	g	609	3	3/3/20/26	16/39/137/137	-
24	CHL	p	606	-	3/3/16/26	7/15/113/137	-
37	DGD	C	518	-	-	7/44/84/95	0/2/2/2
25	CLA	8	602	2	1/1/15/20	10/39/115/115	-
26	LUT	0	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	p	2630	25	-	11/53/53/53	-
26	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	q	2630	25	-	17/53/53/53	-
24	CHL	N	606	-	3/3/16/26	8/15/113/137	-
34	BCR	c	517	-	-	0/29/63/63	0/2/2/2
24	CHL	n	609	2	3/3/20/26	21/39/137/137	-
24	CHL	g	601	3	3/3/20/26	18/39/137/137	-
25	CLA	q	610	3	1/1/15/20	10/39/115/115	-
29	LHG	r	2630	25	-	16/42/42/53	-
24	CHL	8	606	-	3/3/16/26	6/15/113/137	-
24	CHL	N	605	2	3/3/20/26	25/39/137/137	-
37	DGD	c	519	-	-	19/51/91/95	0/2/2/2
26	LUT	R	620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	613	2	-	14/39/115/115	-
25	CLA	S	611	29	1/1/11/20	7/20/96/115	-
29	LHG	L	101	-	-	16/53/53/53	-
25	CLA	9	603	-	1/1/15/20	23/39/115/115	-
25	CLA	B	611	-	1/1/15/20	11/39/115/115	-
29	LHG	D	409	-	-	10/53/53/53	-
25	CLA	N	603	-	1/1/15/20	9/39/115/115	-
25	CLA	6	614	-	1/1/12/20	7/26/102/115	-
24	CHL	4	609	3	3/3/20/26	20/39/137/137	-
25	CLA	s	614	-	1/1/11/20	6/19/95/115	-
27	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
28	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	n	603	-	1/1/15/20	9/39/115/115	-
27	XAT	4	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	6	601	1	3/3/20/26	9/39/137/137	-
24	CHL	9	608	-	3/3/15/26	6/13/111/137	-
24	CHL	n	608	-	3/3/16/26	11/20/118/137	-
25	CLA	N	613	2	1/1/15/20	15/39/115/115	-
24	CHL	Y	608	-	3/3/16/26	4/20/118/137	-
27	XAT	2	1622	-	-	2/31/93/93	0/4/4/4
27	XAT	r	622	-	-	0/31/93/93	0/4/4/4
25	CLA	C	501	-	1/1/15/20	12/39/115/115	-
25	CLA	n	613	2	1/1/15/20	15/39/115/115	-
28	NEX	8	1623	-	-	3/27/83/83	0/3/3/3
26	LUT	9	1621	-	-	2/29/67/67	0/2/2/2
26	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	r	603	-	1/1/14/20	10/33/109/115	-
24	CHL	G	609	3	3/3/20/26	16/39/137/137	-
25	CLA	y	611	29	1/1/15/20	8/39/115/115	-
25	CLA	Y	603	-	1/1/15/20	14/39/115/115	-
25	CLA	8	612	2	1/1/11/20	7/15/91/115	-
25	CLA	5	602	2	1/1/15/20	16/39/115/115	-
24	CHL	5	601	2	3/3/20/26	19/39/137/137	-
25	CLA	1	611	29	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	p	602	2	1/1/15/20	13/39/115/115	-
25	CLA	c	512	-	1/1/15/20	16/39/115/115	-
25	CLA	8	611	29	1/1/11/20	8/20/96/115	-
29	LHG	D	408	-	-	10/48/48/53	-
25	CLA	G	603	-	1/1/15/20	11/39/115/115	-
25	CLA	C	505	-	1/1/15/20	16/39/115/115	-
25	CLA	A	405	-	1/1/15/20	13/39/115/115	-
25	CLA	4	611	29	1/1/11/20	8/15/91/115	-
26	LUT	8	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	n	604	-	1/1/15/20	12/39/115/115	-
24	CHL	0	605	1	3/3/16/26	7/15/113/137	-
25	CLA	N	612	2	1/1/11/20	8/15/91/115	-
24	CHL	Y	606	-	3/3/20/26	18/39/137/137	-
25	CLA	c	509	-	1/1/15/20	4/39/115/115	-
25	CLA	3	611	29	1/1/11/20	8/20/96/115	-
24	CHL	q	607	-	3/3/16/26	13/20/118/137	-
25	CLA	c	507	-	1/1/15/20	10/39/115/115	-
25	CLA	y	602	1	1/1/15/20	11/39/115/115	-
25	CLA	1	602	1	1/1/15/20	13/39/115/115	-
29	LHG	7	2630	25	-	17/53/53/53	-
24	CHL	R	608	-	3/3/19/26	12/33/131/137	-
25	CLA	b	614	-	1/1/15/20	8/39/115/115	-
26	LUT	4	1620	-	-	6/29/67/67	0/2/2/2
25	CLA	2	610	2	1/1/15/20	5/39/115/115	-
25	CLA	6	610	1	1/1/15/20	5/39/115/115	-
29	LHG	8	2630	25	-	9/53/53/53	-
25	CLA	s	613	18	-	10/20/96/115	-
34	BCR	d	404	-	-	4/29/63/63	0/2/2/2
27	XAT	N	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	1	614	-	1/1/12/20	13/26/102/115	-
25	CLA	G	614	-	1/1/11/20	11/20/96/115	-
25	CLA	p	611	29	1/1/11/20	7/20/96/115	-
25	CLA	0	611	29	1/1/15/20	9/39/115/115	-
25	CLA	D	403	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	q	611	29	1/1/11/20	8/15/91/115	-
24	CHL	r	606	-	3/3/20/26	21/39/137/137	-
24	CHL	7	605	1	3/3/16/26	8/15/113/137	-
25	CLA	Y	604	-	-	18/39/115/115	-
25	CLA	g	611	29	1/1/11/20	7/15/91/115	-
25	CLA	r	611	29	1/1/11/20	11/20/96/115	-
24	CHL	S	607	-	3/3/15/26	4/12/110/137	-
25	CLA	b	602	-	1/1/15/20	19/39/115/115	-
25	CLA	n	612	2	1/1/11/20	8/15/91/115	-
25	CLA	C	511	6	-	12/39/115/115	-
34	BCR	C	516	-	-	7/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	17/39/115/115	-
25	CLA	G	611	29	1/1/11/20	7/15/91/115	-
25	CLA	g	614	-	1/1/11/20	11/20/96/115	-
25	CLA	2	603	-	1/1/15/20	22/39/115/115	-
25	CLA	0	602	1	1/1/15/20	13/39/115/115	-
37	DGD	C	524	-	-	9/55/95/95	0/2/2/2
37	DGD	c	520	-	-	10/48/88/95	0/2/2/2
24	CHL	7	607	-	3/3/20/26	19/39/137/137	-
29	LHG	n	2630	25	-	15/53/53/53	-
25	CLA	Y	611	29	1/1/15/20	8/39/115/115	-
36	LMG	a	413	-	-	12/43/63/70	0/1/1/1
25	CLA	3	613	2	-	12/39/115/115	-
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
25	CLA	b	605	-	1/1/15/20	13/39/115/115	-
34	BCR	c	516	-	-	7/29/63/63	0/2/2/2
24	CHL	G	605	3	3/3/16/26	9/18/116/137	-
25	CLA	C	509	-	1/1/15/20	4/39/115/115	-
24	CHL	p	605	2	3/3/20/26	15/39/137/137	-
25	CLA	C	502	-	1/1/15/20	17/39/115/115	-
40	HEM	f	101	8,9	-	3/14/54/54	-
37	DGD	c	518	-	-	7/44/84/95	0/2/2/2
25	CLA	B	608	-	1/1/15/20	16/39/115/115	-
28	NEX	s	1623	-	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	610	18	1/1/11/20	9/20/96/115	-
25	CLA	g	602	3	1/1/15/20	11/39/115/115	-
25	CLA	B	604	-	1/1/15/20	10/39/115/115	-
24	CHL	q	609	3	3/3/20/26	22/39/137/137	-
25	CLA	1	613	1	-	12/39/115/115	-
25	CLA	7	611	29	1/1/15/20	10/39/115/115	-
25	CLA	B	606	-	1/1/15/20	13/39/115/115	-
25	CLA	R	603	-	1/1/14/20	10/33/109/115	-
24	CHL	6	608	-	3/3/16/26	8/20/118/137	-
24	CHL	0	601	1	3/3/20/26	10/39/137/137	-
29	LHG	0	2630	25	-	17/53/53/53	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	5	611	29	1/1/11/20	12/20/96/115	-
25	CLA	2	614	-	-	9/20/96/115	-
29	LHG	Y	2630	25	-	23/53/53/53	-
25	CLA	4	613	3	1/1/15/20	16/39/115/115	-
27	XAT	0	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	r	604	-	1/1/11/20	10/19/95/115	-
25	CLA	2	612	2	1/1/10/20	5/13/89/115	-
35	SQD	d	413	-	-	8/47/67/69	0/1/1/1
25	CLA	b	613	-	1/1/15/20	11/39/115/115	-
25	CLA	4	614	-	1/1/11/20	10/20/96/115	-
28	NEX	1	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	g	605	3	3/3/16/26	9/18/116/137	-
25	CLA	g	603	-	1/1/15/20	11/39/115/115	-
29	LHG	s	2630	25	-	15/49/49/53	-
36	LMG	H	102	-	-	15/43/63/70	0/1/1/1
37	DGD	C	520	-	-	10/48/88/95	0/2/2/2
26	LUT	n	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	0	610	1	1/1/15/20	5/39/115/115	-
25	CLA	n	602	2	1/1/15/20	5/39/115/115	-
29	LHG	R	2630	25	-	16/42/42/53	-
24	CHL	N	609	2	3/3/20/26	19/39/137/137	-
25	CLA	7	613	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PHO	a	408	-	-	10/37/103/103	0/5/6/6
24	CHL	q	606	-	3/3/16/26	5/20/118/137	-
36	LMG	d	412	-	-	6/41/61/70	0/1/1/1
25	CLA	B	612	-	1/1/15/20	9/39/115/115	-
36	LMG	C	521	-	-	10/46/66/70	0/1/1/1
25	CLA	g	613	3	1/1/15/20	10/39/115/115	-
28	NEX	3	1623	-	-	5/27/83/83	0/3/3/3
28	NEX	4	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	7	609	1	3/3/20/26	17/39/137/137	-
25	CLA	R	604	-	1/1/11/20	10/19/95/115	-
25	CLA	4	610	3	1/1/15/20	13/39/115/115	-
25	CLA	5	603	-	1/1/15/20	15/39/115/115	-
24	CHL	N	607	-	3/3/20/26	15/39/137/137	-
25	CLA	B	616	-	1/1/15/20	8/39/115/115	-
24	CHL	1	601	1	3/3/20/26	13/39/137/137	-
24	CHL	2	606	-	3/3/16/26	8/20/118/137	-
34	BCR	c	515	-	-	4/29/63/63	0/2/2/2
36	LMG	h	102	-	-	14/43/63/70	0/1/1/1
25	CLA	R	612	-	1/1/11/20	10/20/96/115	-
25	CLA	b	610	-	1/1/15/20	6/39/115/115	-
25	CLA	5	613	2	1/1/15/20	14/39/115/115	-
24	CHL	5	608	-	3/3/16/26	10/20/118/137	-
24	CHL	p	609	2	3/3/20/26	21/39/137/137	-
25	CLA	4	602	3	1/1/15/20	12/39/115/115	-
24	CHL	4	605	3	3/3/16/26	12/18/116/137	-
24	CHL	3	601	2	3/3/20/26	19/39/137/137	-
24	CHL	4	601	3	3/3/20/26	18/39/137/137	-
25	CLA	S	609	18	1/1/10/20	6/10/86/115	-
25	CLA	B	615	-	1/1/15/20	15/39/115/115	-
27	XAT	g	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	a	410	-	1/1/14/20	4/33/109/115	-
25	CLA	1	610	1	1/1/15/20	13/39/115/115	-
24	CHL	g	606	-	3/3/16/26	4/20/118/137	-
24	CHL	G	601	3	3/3/20/26	17/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	n	601	2	3/3/20/26	10/39/137/137	-
25	CLA	2	604	-	1/1/11/20	10/20/96/115	-
24	CHL	7	608	-	3/3/16/26	11/20/118/137	-
25	CLA	5	614	-	-	9/20/96/115	-
25	CLA	0	604	-	1/1/15/20	18/39/115/115	-
24	CHL	5	605	2	3/3/20/26	19/39/137/137	-
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	r	609	17	1/1/13/20	5/31/107/115	-
25	CLA	g	604	-	1/1/11/20	9/20/96/115	-
24	CHL	8	605	2	3/3/20/26	15/39/137/137	-
28	NEX	S	1623	-	-	4/27/83/83	0/3/3/3
28	NEX	5	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	n	607	-	3/3/20/26	15/39/137/137	-
24	CHL	y	607	-	3/3/20/26	16/39/137/137	-
25	CLA	3	610	2	1/1/15/20	7/39/115/115	-
24	CHL	Y	607	-	3/3/20/26	19/39/137/137	-
34	BCR	A	411	-	-	2/29/63/63	0/2/2/2
25	CLA	g	612	3	1/1/10/20	7/13/89/115	-
35	SQD	D	413	-	-	8/47/67/69	0/1/1/1
24	CHL	6	606	-	3/3/20/26	21/39/137/137	-
24	CHL	s	606	-	3/3/15/26	8/13/111/137	-
25	CLA	c	503	-	1/1/15/20	14/39/115/115	-
29	LHG	D	410	-	-	10/43/43/53	-
24	CHL	3	606	-	3/3/16/26	8/15/113/137	-
29	LHG	G	2630	25	-	10/53/53/53	-
25	CLA	B	602	-	1/1/15/20	19/39/115/115	-
27	XAT	R	622	-	-	0/31/93/93	0/4/4/4
25	CLA	S	612	18	1/1/11/20	5/15/91/115	-
25	CLA	C	503	-	1/1/15/20	10/39/115/115	-
34	BCR	C	517	-	-	0/29/63/63	0/2/2/2
37	DGD	c	523	-	-	13/55/95/95	0/2/2/2
24	CHL	Y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	9	614	-	-	9/20/96/115	-
34	BCR	C	514	-	-	4/29/63/63	0/2/2/2
27	XAT	G	1622	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	6	1621	-	-	2/29/67/67	0/2/2/2
26	LUT	p	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	y	609	1	3/3/20/26	15/39/137/137	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	g	2630	25	-	10/53/53/53	-
26	LUT	q	1621	-	-	5/29/67/67	0/2/2/2
24	CHL	2	605	2	3/3/16/26	6/18/116/137	-
26	LUT	p	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	q	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	D	402	-	1/1/15/20	15/39/115/115	-
25	CLA	9	611	29	1/1/11/20	9/15/91/115	-
24	CHL	8	609	2	3/3/20/26	20/39/137/137	-
34	BCR	D	404	-	-	4/29/63/63	0/2/2/2
25	CLA	s	611	29	1/1/11/20	8/20/96/115	-
24	CHL	y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	c	510	-	1/1/15/20	9/39/115/115	-
25	CLA	y	610	1	1/1/15/20	10/39/115/115	-
25	CLA	b	608	-	1/1/15/20	15/39/115/115	-
25	CLA	S	610	18	1/1/11/20	9/20/96/115	-
24	CHL	p	607	-	3/3/20/26	24/39/137/137	-
33	PHO	A	409	-	-	9/37/103/103	0/5/6/6
26	LUT	Y	1621	-	-	4/29/67/67	0/2/2/2

The worst 5 of 4746 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	609	CHL	C2C-C3C	11.54	1.47	1.36
24	9	609	CHL	C2C-C3C	11.47	1.47	1.36
24	4	609	CHL	C2C-C3C	11.24	1.47	1.36
24	2	609	CHL	C2C-C3C	11.16	1.47	1.36
24	q	608	CHL	C2C-C3C	11.15	1.47	1.36

The worst 5 of 5235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	1622	XAT	C37-C21-C36	-17.98	81.26	107.37
27	y	1622	XAT	C37-C21-C36	-17.97	81.26	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	1622	XAT	C37-C21-C36	-17.83	81.47	107.37
27	0	1622	XAT	C37-C21-C36	-17.75	81.58	107.37
27	1	1622	XAT	C37-C21-C36	-17.27	82.29	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 5626 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	C1C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	607	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

398 monomers are involved in 799 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	q	602	CLA	1	0
25	C	510	CLA	1	0
34	B	619	BCR	3	0
24	r	607	CHL	2	0
24	y	608	CHL	1	0
25	s	604	CLA	11	0
25	p	614	CLA	1	0
29	l	101	LHG	5	0
39	d	405	PL9	3	0
26	S	1620	LUT	1	0
27	y	1622	XAT	3	0
25	d	403	CLA	1	0
24	6	607	CHL	3	0
24	S	601	CHL	5	0
25	9	602	CLA	4	0
36	b	622	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	3	603	CLA	2	0
25	7	614	CLA	1	0
25	s	605	CLA	10	0
28	0	1623	NEX	1	0
37	C	523	DGD	3	0
24	0	606	CHL	1	0
26	S	1621	LUT	5	0
24	R	607	CHL	2	0
25	9	610	CLA	1	0
24	Y	609	CHL	8	0
25	y	604	CLA	1	0
25	1	603	CLA	1	0
25	Y	612	CLA	2	0
25	S	604	CLA	9	0
27	9	1622	XAT	2	0
24	9	606	CHL	1	0
24	S	608	CHL	2	0
25	R	611	CLA	1	0
24	3	605	CHL	1	0
25	4	603	CLA	1	0
25	R	616	CLA	3	0
26	9	1620	LUT	1	0
24	G	607	CHL	1	0
29	N	2630	LHG	3	0
26	y	1620	LUT	3	0
28	6	1623	NEX	3	0
24	7	601	CHL	3	0
35	B	621	SQD	2	0
25	N	614	CLA	1	0
24	q	601	CHL	1	0
25	C	513	CLA	6	0
25	r	616	CLA	4	0
24	1	606	CHL	2	0
37	c	524	DGD	5	0
25	b	603	CLA	3	0
24	3	608	CHL	2	0
24	4	608	CHL	1	0
25	A	407	CLA	1	0
24	5	607	CHL	1	0
26	7	1621	LUT	1	0
25	7	602	CLA	3	0
26	8	1620	LUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	511	CLA	2	0
25	p	610	CLA	2	0
25	B	607	CLA	2	0
24	9	601	CHL	2	0
24	s	601	CHL	3	0
25	n	614	CLA	1	0
24	l	608	CHL	4	0
26	3	1621	LUT	5	0
34	h	101	BCR	2	0
25	g	610	CLA	2	0
36	S	2631	LMG	2	0
26	G	1620	LUT	4	0
24	r	608	CHL	3	0
24	R	606	CHL	1	0
37	C	519	DGD	1	0
26	n	1620	LUT	4	0
24	2	601	CHL	1	0
34	a	411	BCR	2	0
24	g	608	CHL	1	0
25	A	406	CLA	1	0
29	c	2630	LHG	2	0
25	B	609	CLA	2	0
34	b	620	BCR	1	0
25	N	602	CLA	1	0
24	G	608	CHL	2	0
25	b	606	CLA	2	0
28	y	1623	NEX	2	0
25	R	609	CLA	1	0
25	1	604	CLA	3	0
25	C	508	CLA	2	0
25	8	603	CLA	1	0
35	b	621	SQD	2	0
25	B	613	CLA	5	0
25	d	402	CLA	4	0
25	b	609	CLA	1	0
25	c	504	CLA	3	0
25	0	612	CLA	2	0
27	3	1622	XAT	2	0
25	c	508	CLA	1	0
25	Y	602	CLA	2	0
36	A	413	LMG	2	0
26	7	1620	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	408	PHO	2	0
29	d	409	LHG	2	0
25	b	607	CLA	2	0
24	2	608	CHL	2	0
25	4	612	CLA	1	0
26	y	1621	LUT	5	0
24	8	608	CHL	2	0
25	S	602	CLA	2	0
24	0	608	CHL	1	0
25	B	614	CLA	2	0
35	A	412	SQD	4	0
25	b	612	CLA	3	0
26	6	1620	LUT	1	0
24	3	609	CHL	3	0
25	C	507	CLA	1	0
25	R	601	CLA	1	0
24	9	607	CHL	1	0
25	a	405	CLA	3	0
26	3	1620	LUT	2	0
24	s	607	CHL	1	0
24	N	601	CHL	2	0
29	1	2630	LHG	2	0
27	n	1622	XAT	5	0
29	d	408	LHG	4	0
24	8	601	CHL	2	0
26	N	1621	LUT	3	0
26	2	1620	LUT	2	0
25	y	603	CLA	4	0
29	4	2630	LHG	1	0
25	5	612	CLA	2	0
25	B	605	CLA	3	0
25	b	615	CLA	2	0
29	C	2630	LHG	5	0
25	6	613	CLA	1	0
28	n	1623	NEX	3	0
25	Y	613	CLA	3	0
25	n	610	CLA	1	0
26	1	1621	LUT	2	0
25	Y	610	CLA	1	0
25	y	613	CLA	2	0
28	r	623	NEX	2	0
24	6	609	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	0	1621	LUT	4	0
24	5	609	CHL	3	0
25	G	613	CLA	2	0
25	s	602	CLA	2	0
24	S	606	CHL	2	0
25	a	406	CLA	1	0
27	8	1622	XAT	1	0
25	C	504	CLA	1	0
24	s	608	CHL	2	0
25	G	602	CLA	3	0
25	N	610	CLA	2	0
25	R	602	CLA	1	0
25	y	612	CLA	2	0
25	9	613	CLA	2	0
25	p	603	CLA	2	0
25	r	602	CLA	1	0
24	1	607	CHL	3	0
25	7	603	CLA	1	0
25	q	603	CLA	2	0
24	Y	601	CHL	4	0
25	B	617	CLA	1	0
29	S	2630	LHG	5	0
24	2	607	CHL	1	0
25	C	506	CLA	1	0
26	g	1621	LUT	3	0
26	Y	1620	LUT	6	0
24	n	605	CHL	2	0
25	q	613	CLA	3	0
24	0	607	CHL	2	0
26	5	1621	LUT	1	0
24	q	608	CHL	1	0
25	r	613	CLA	1	0
24	g	607	CHL	1	0
25	b	616	CLA	1	0
25	2	613	CLA	1	0
24	3	607	CHL	1	0
24	7	606	CHL	1	0
24	y	601	CHL	6	0
25	9	604	CLA	1	0
25	6	604	CLA	1	0
28	R	623	NEX	1	0
25	B	610	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	0	613	CLA	1	0
24	1	609	CHL	3	0
25	5	604	CLA	2	0
34	b	619	BCR	2	0
29	y	2630	LHG	4	0
25	p	604	CLA	1	0
28	7	1623	NEX	2	0
33	a	409	PHO	1	0
25	q	604	CLA	1	0
34	b	618	BCR	3	0
27	Y	1622	XAT	5	0
36	B	622	LMG	4	0
34	B	618	BCR	3	0
24	p	608	CHL	1	0
26	s	1620	LUT	1	0
25	G	610	CLA	2	0
28	N	1623	NEX	4	0
25	p	612	CLA	1	0
25	S	605	CLA	8	0
25	B	603	CLA	3	0
39	D	405	PL9	3	0
25	R	613	CLA	2	0
24	n	606	CHL	2	0
25	6	602	CLA	2	0
25	b	617	CLA	1	0
25	a	407	CLA	1	0
25	c	505	CLA	3	0
25	r	601	CLA	2	0
26	G	1621	LUT	5	0
25	3	602	CLA	3	0
25	c	513	CLA	3	0
26	r	620	LUT	2	0
25	6	612	CLA	2	0
25	c	501	CLA	1	0
36	s	2631	LMG	1	0
35	a	412	SQD	3	0
26	2	1621	LUT	3	0
29	6	2630	LHG	1	0
25	2	602	CLA	2	0
34	C	515	BCR	1	0
24	N	608	CHL	1	0
26	1	1620	LUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	609	CHL	2	0
24	p	606	CHL	1	0
37	C	518	DGD	2	0
25	8	602	CLA	3	0
26	0	1620	LUT	2	0
26	g	1620	LUT	2	0
24	N	606	CHL	2	0
34	c	517	BCR	4	0
24	n	609	CHL	2	0
24	g	601	CHL	6	0
29	r	2630	LHG	1	0
24	8	606	CHL	1	0
24	N	605	CHL	1	0
37	c	519	DGD	3	0
26	R	620	LUT	4	0
25	8	613	CLA	1	0
29	L	101	LHG	5	0
25	9	603	CLA	3	0
38	d	401	BCT	2	0
29	D	409	LHG	2	0
25	N	603	CLA	3	0
38	D	401	BCT	2	0
24	4	609	CHL	2	0
27	7	1622	XAT	4	0
28	Y	1623	NEX	3	0
25	n	603	CLA	1	0
24	6	601	CHL	1	0
24	9	608	CHL	2	0
25	N	613	CLA	1	0
24	Y	608	CHL	1	0
27	2	1622	XAT	1	0
27	r	622	XAT	4	0
25	C	501	CLA	2	0
25	n	613	CLA	1	0
28	8	1623	NEX	1	0
26	9	1621	LUT	4	0
26	s	1621	LUT	5	0
25	r	603	CLA	2	0
24	G	609	CHL	2	0
25	y	611	CLA	7	0
25	Y	603	CLA	6	0
25	5	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	5	601	CHL	1	0
25	p	602	CLA	1	0
25	c	512	CLA	1	0
29	D	408	LHG	3	0
25	G	603	CLA	2	0
25	C	505	CLA	3	0
25	A	405	CLA	3	0
25	4	611	CLA	1	0
26	8	1621	LUT	7	0
24	0	605	CHL	1	0
25	3	611	CLA	1	0
25	c	507	CLA	2	0
25	y	602	CLA	3	0
25	1	602	CLA	2	0
29	7	2630	LHG	2	0
24	R	608	CHL	3	0
25	b	614	CLA	2	0
25	6	610	CLA	3	0
34	d	404	BCR	5	0
27	N	1622	XAT	5	0
25	1	614	CLA	1	0
25	0	611	CLA	1	0
25	D	403	CLA	3	0
25	q	611	CLA	2	0
24	r	606	CHL	1	0
25	Y	604	CLA	1	0
24	S	607	CHL	1	0
25	b	602	CLA	1	0
25	C	511	CLA	3	0
34	C	516	BCR	4	0
25	C	512	CLA	1	0
25	2	603	CLA	2	0
25	0	602	CLA	2	0
37	C	524	DGD	5	0
24	7	607	CHL	4	0
29	n	2630	LHG	3	0
25	Y	611	CLA	5	0
36	a	413	LMG	2	0
25	3	613	CLA	2	0
34	B	620	BCR	4	0
25	b	605	CLA	3	0
34	c	516	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	605	CHL	1	0
25	C	509	CLA	1	0
25	C	502	CLA	1	0
37	c	518	DGD	2	0
25	B	608	CLA	2	0
28	s	1623	NEX	3	0
25	g	602	CLA	3	0
25	B	604	CLA	1	0
24	q	609	CHL	2	0
25	R	603	CLA	2	0
24	6	608	CHL	3	0
29	0	2630	LHG	2	0
27	1	1622	XAT	5	0
29	Y	2630	LHG	3	0
25	4	613	CLA	2	0
35	d	413	SQD	2	0
25	b	613	CLA	5	0
28	1	1623	NEX	3	0
25	g	603	CLA	2	0
29	s	2630	LHG	10	0
36	H	102	LMG	3	0
26	n	1621	LUT	2	0
25	0	610	CLA	3	0
25	n	602	CLA	1	0
29	R	2630	LHG	1	0
24	N	609	CHL	4	0
25	7	613	CLA	1	0
33	a	408	PHO	2	0
25	B	612	CLA	3	0
25	g	613	CLA	3	0
28	3	1623	NEX	1	0
24	7	609	CHL	2	0
25	4	610	CLA	1	0
25	5	603	CLA	2	0
24	N	607	CHL	4	0
25	B	616	CLA	1	0
24	1	601	CHL	3	0
24	2	606	CHL	2	0
34	c	515	BCR	3	0
36	h	102	LMG	2	0
25	b	610	CLA	2	0
25	5	613	CLA	2	0

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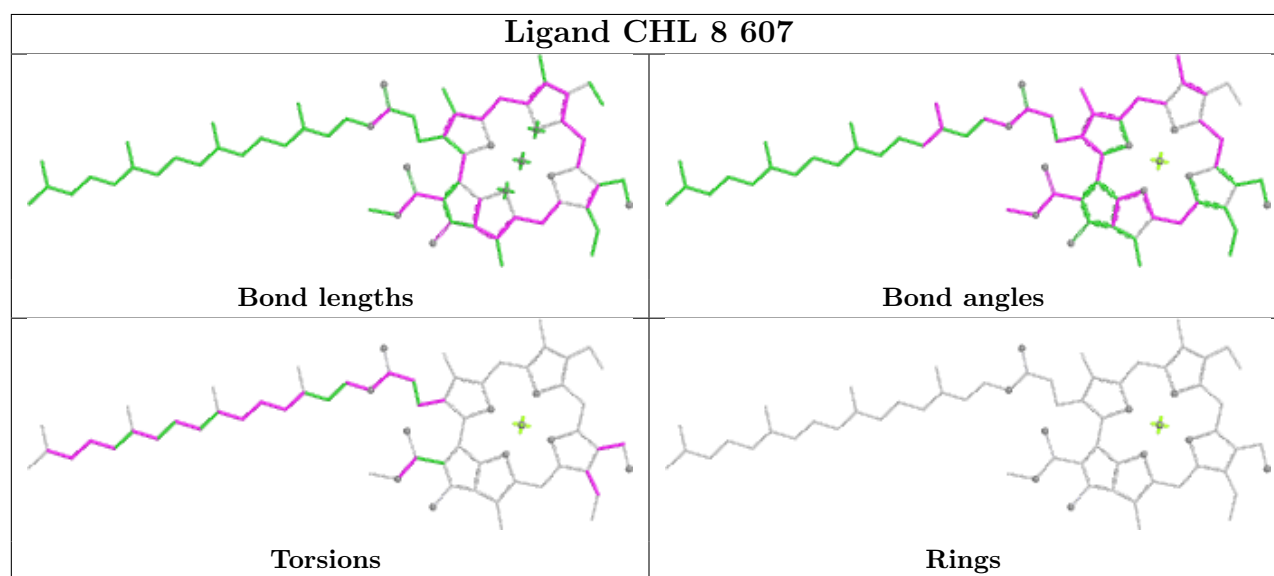
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24	p	609	CHL	3	0
24	4	601	CHL	1	0
25	B	615	CLA	2	0
27	g	1622	XAT	6	0
24	G	601	CHL	4	0
24	n	601	CHL	3	0
25	2	604	CLA	2	0
24	7	608	CHL	1	0
25	0	604	CLA	1	0
34	H	101	BCR	1	0
25	r	609	CLA	2	0
24	8	605	CHL	1	0
28	S	1623	NEX	3	0
24	n	607	CHL	2	0
24	y	607	CHL	2	0
24	Y	607	CHL	1	0
34	A	411	BCR	3	0
35	D	413	SQD	2	0
24	6	606	CHL	3	0
24	s	606	CHL	2	0
24	3	606	CHL	1	0
29	G	2630	LHG	6	0
25	B	602	CLA	2	0
27	R	622	XAT	4	0
34	C	517	BCR	4	0
37	c	523	DGD	3	0
24	Y	605	CHL	1	0
34	C	514	BCR	1	0
27	G	1622	XAT	6	0
26	6	1621	LUT	4	0
26	p	1621	LUT	2	0
24	y	609	CHL	9	0
26	N	1620	LUT	2	0
29	g	2630	LHG	6	0
26	q	1621	LUT	1	0
25	D	402	CLA	4	0
25	9	611	CLA	1	0
24	8	609	CHL	3	0
34	D	404	BCR	4	0
24	y	605	CHL	1	0
25	c	510	CLA	1	0

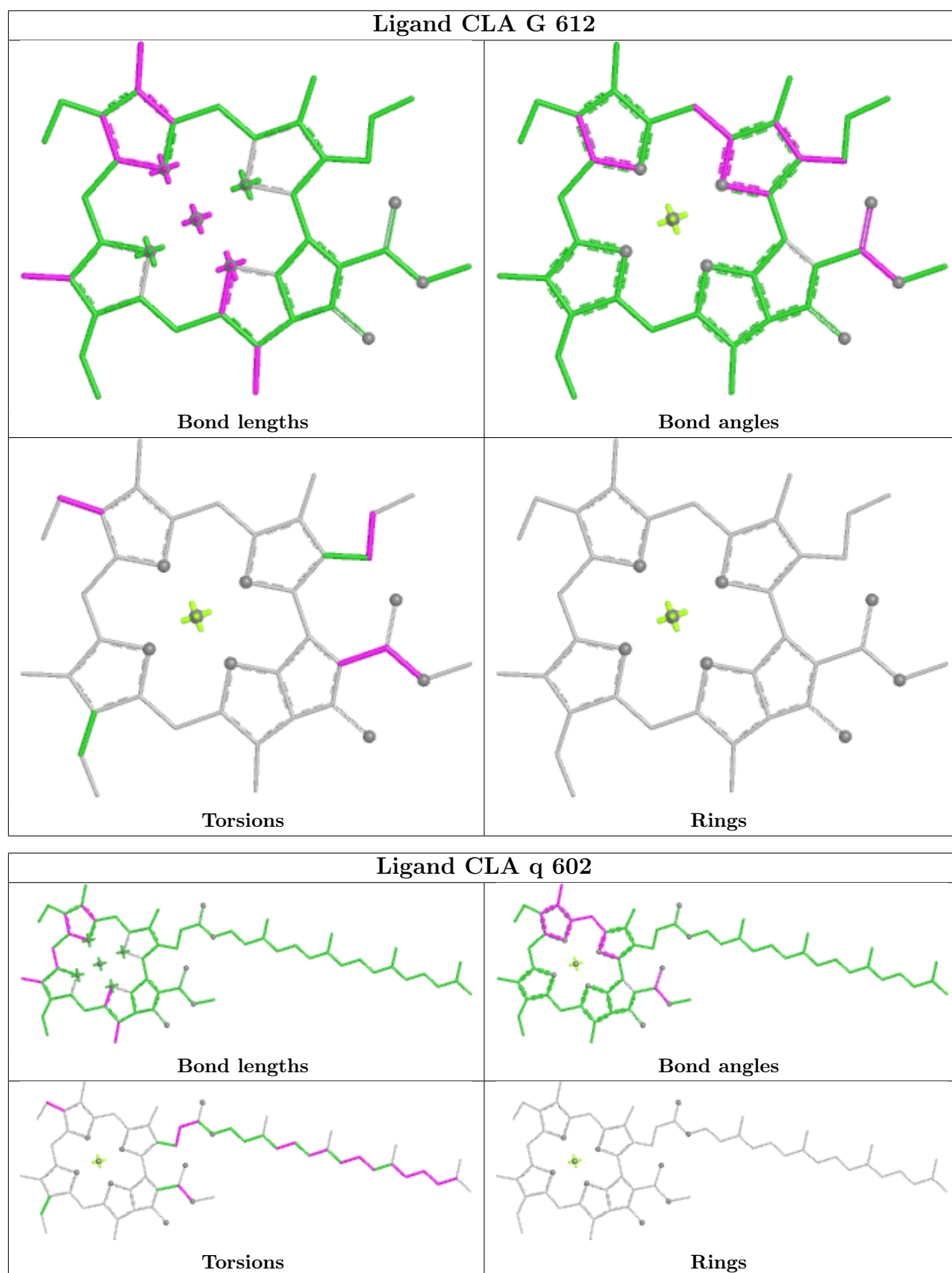
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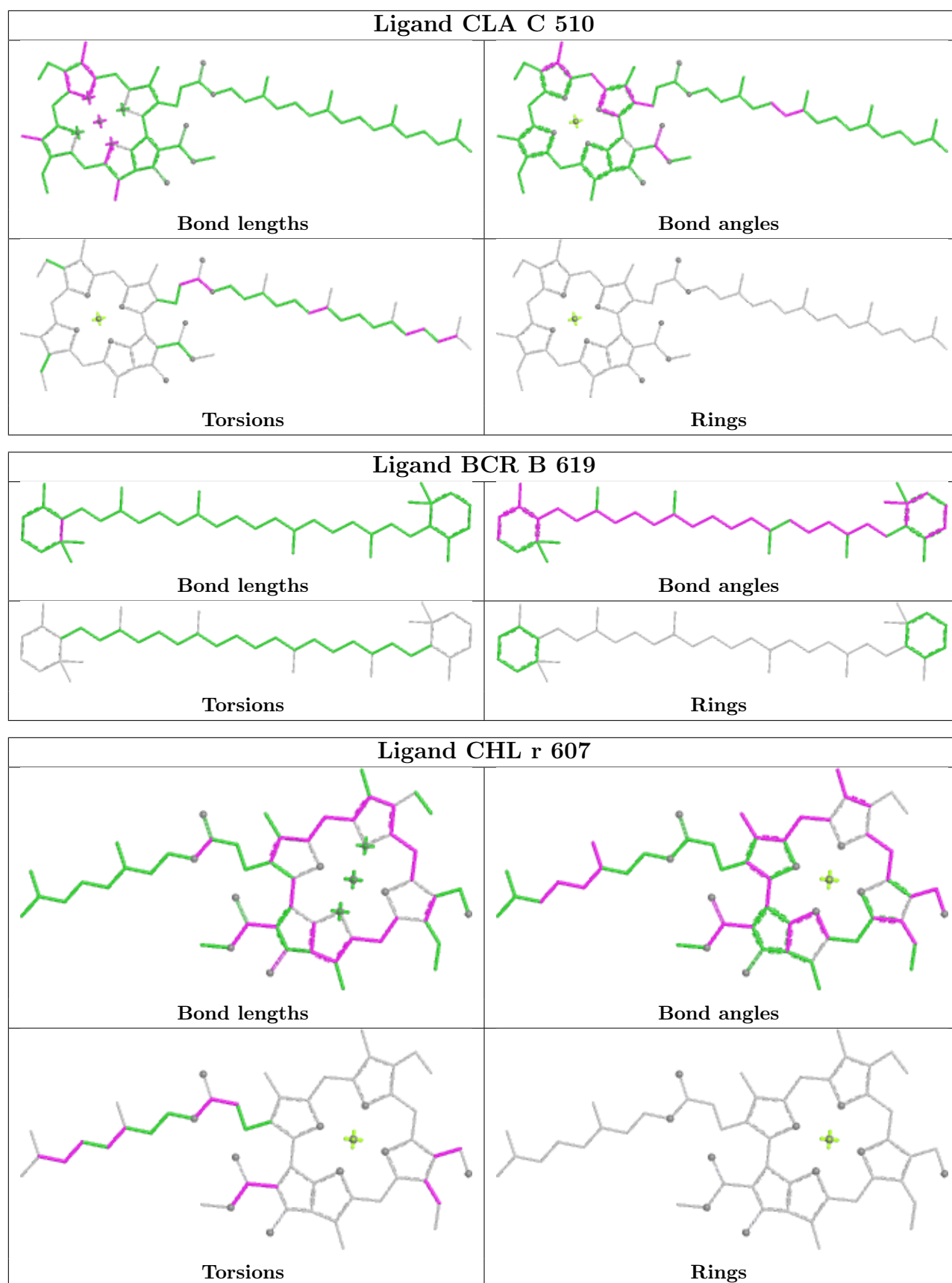
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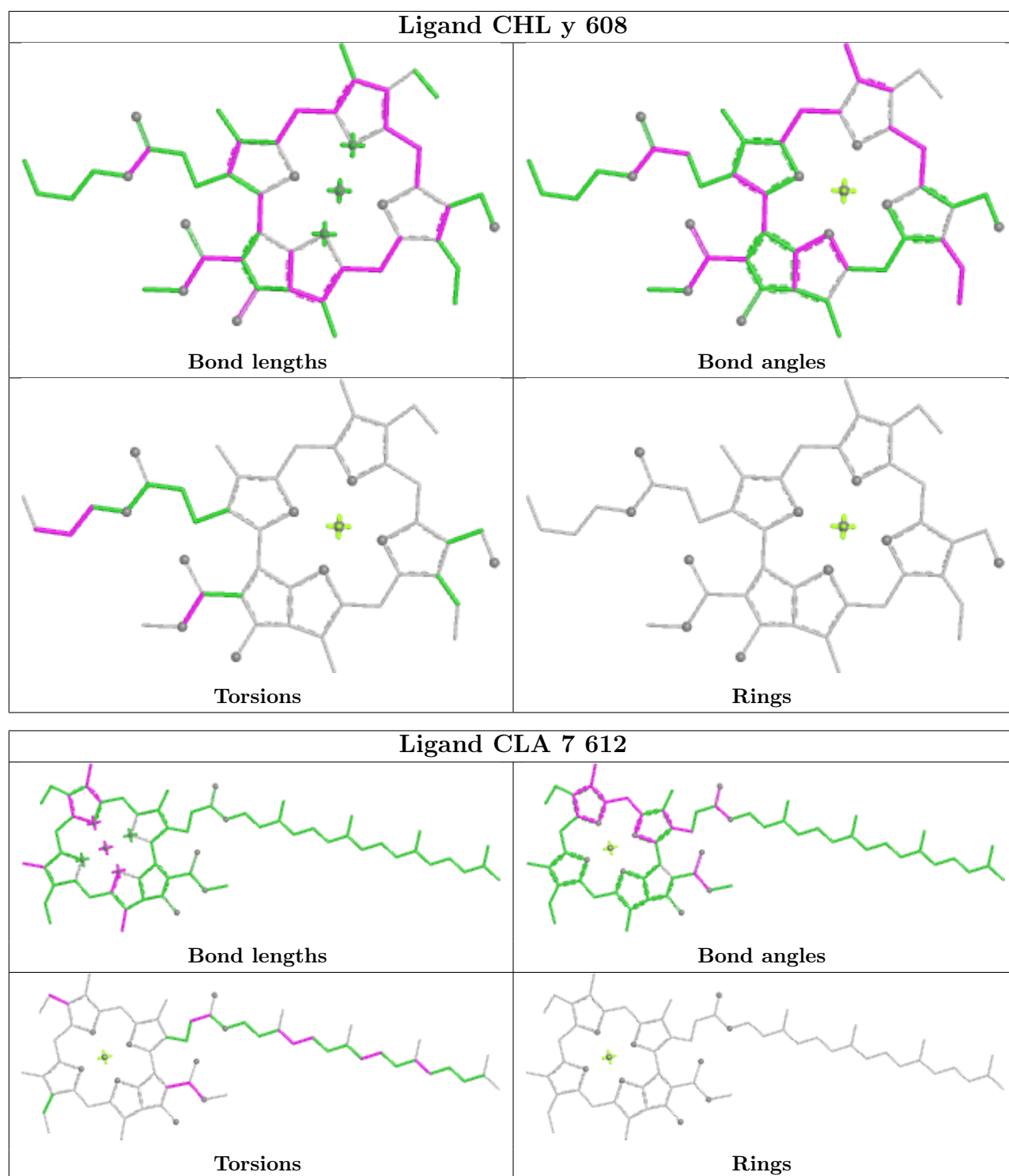
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	y	610	CLA	2	0
25	b	608	CLA	2	0
33	A	409	PHO	2	0
26	Y	1621	LUT	2	0

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

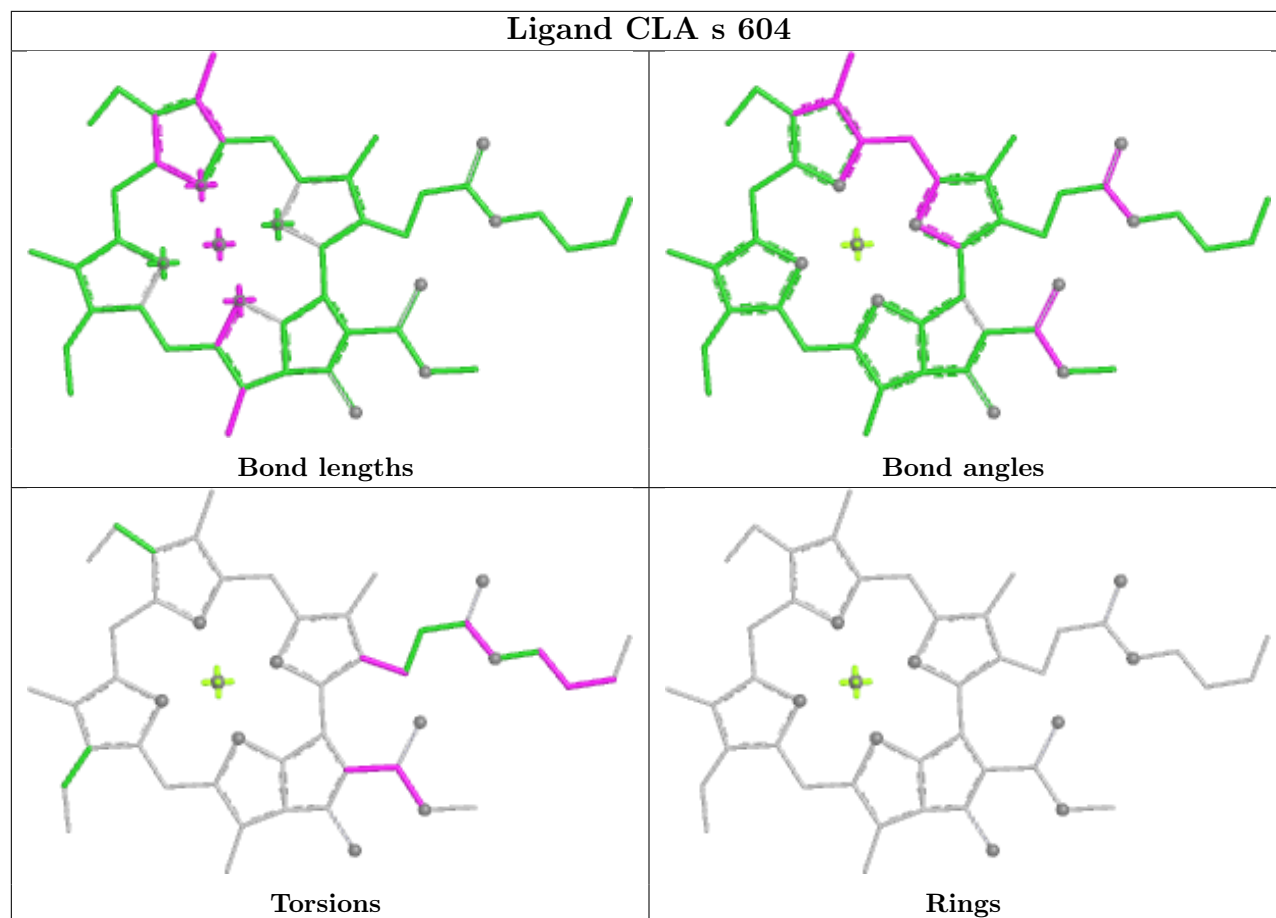




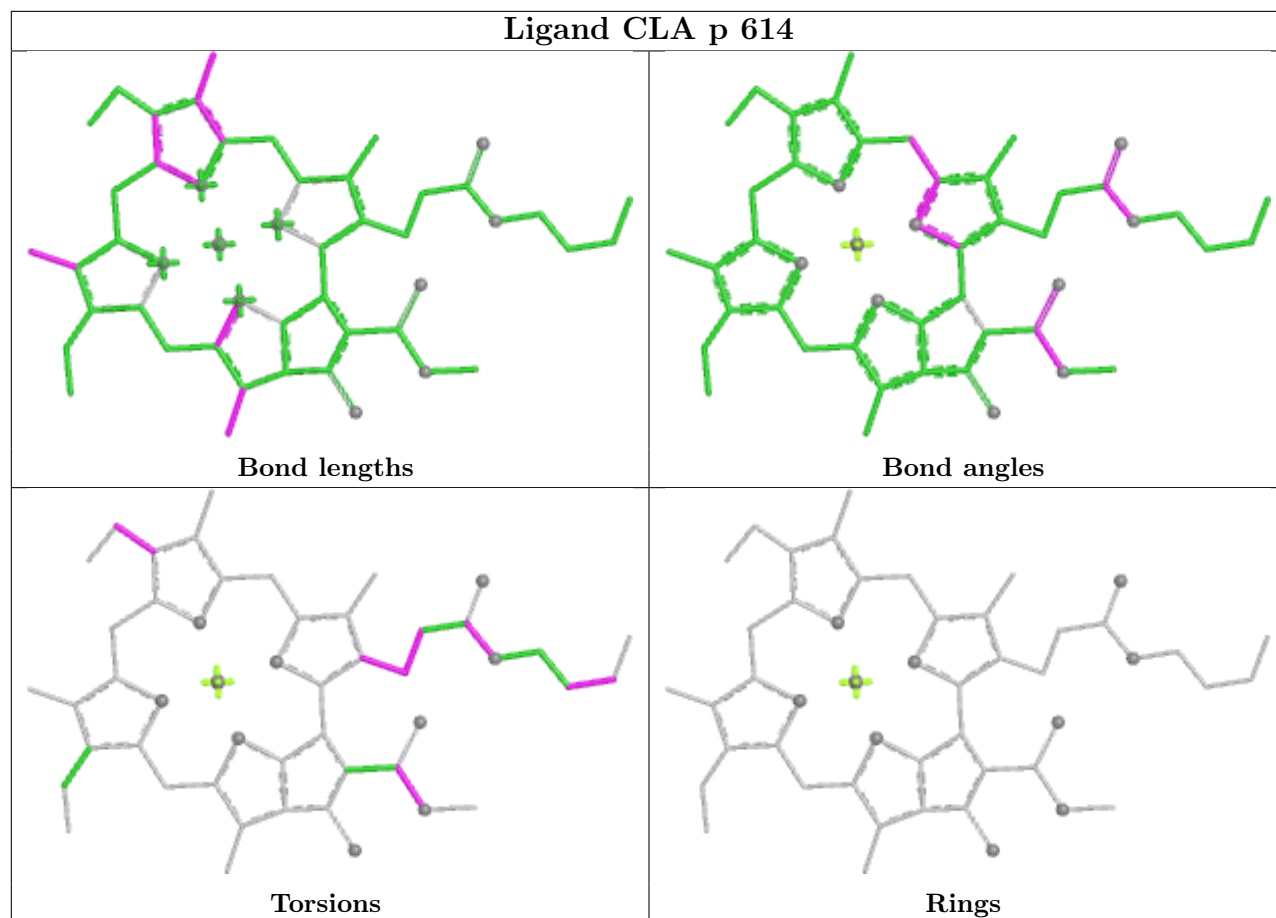


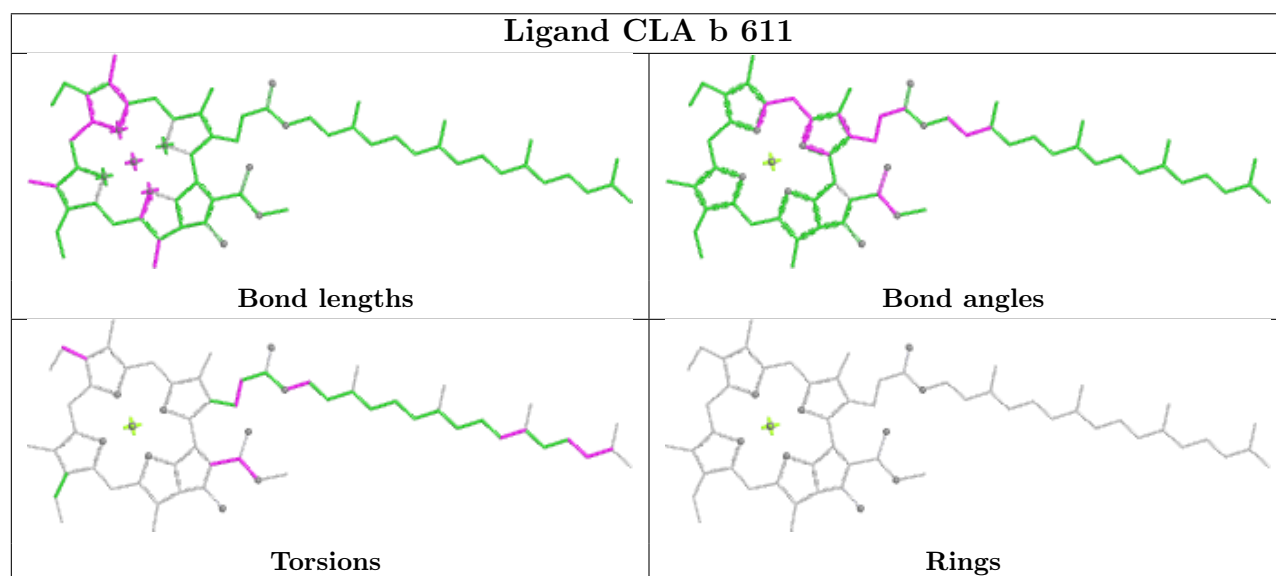
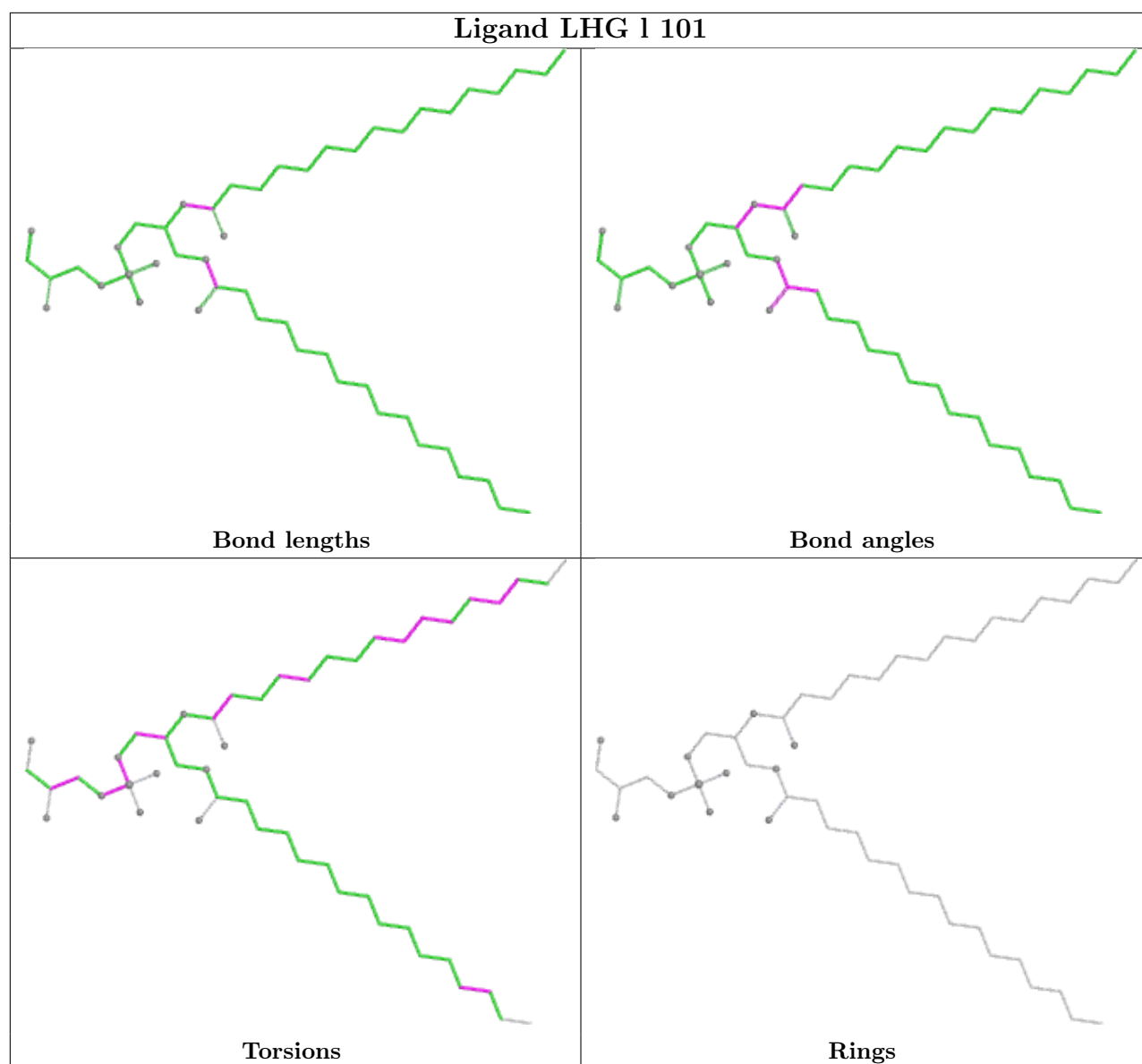


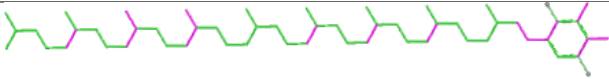
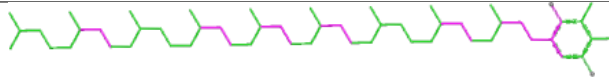
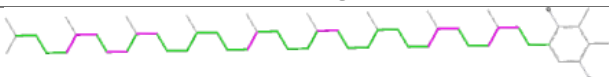
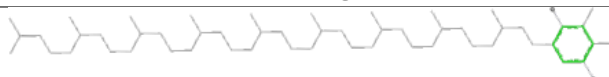
Ligand CLA s 604

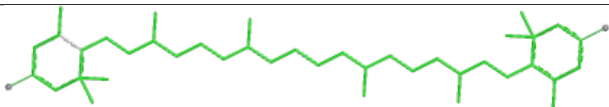
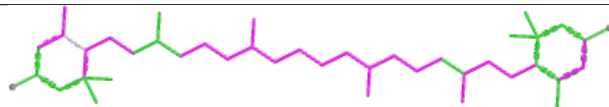
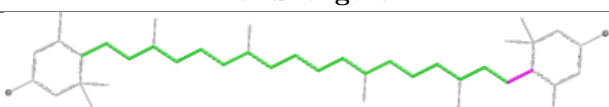
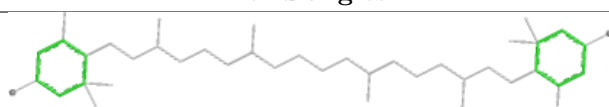


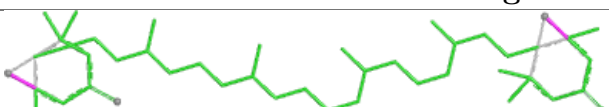
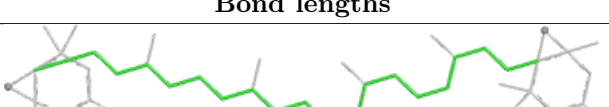
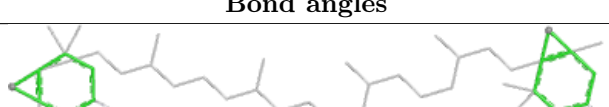
Ligand CLA p 614

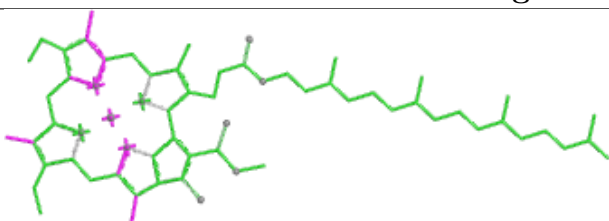
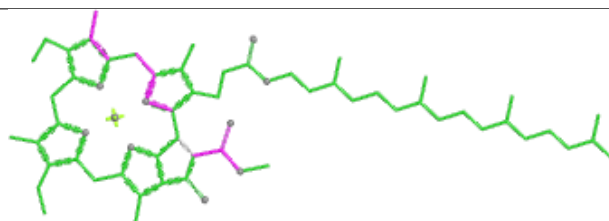
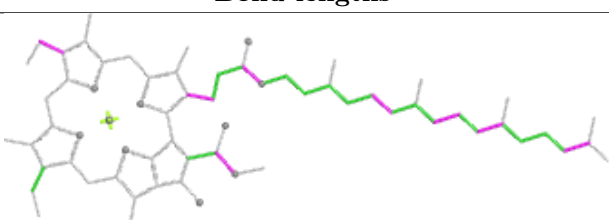
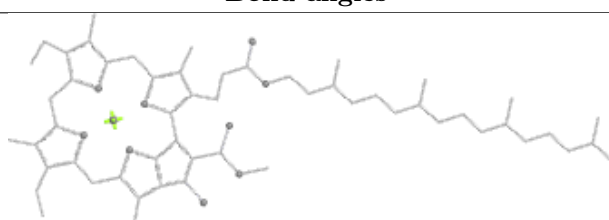


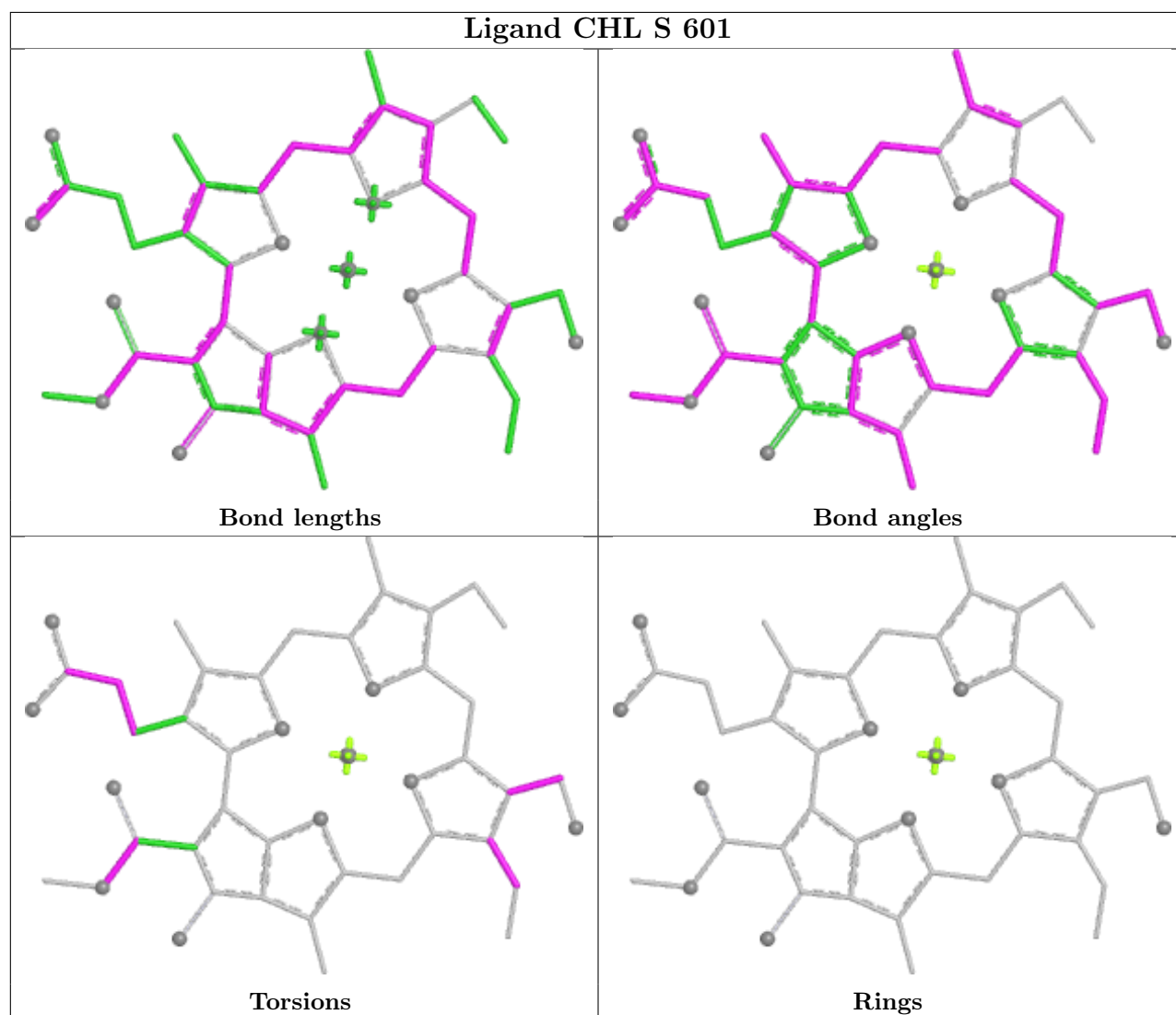
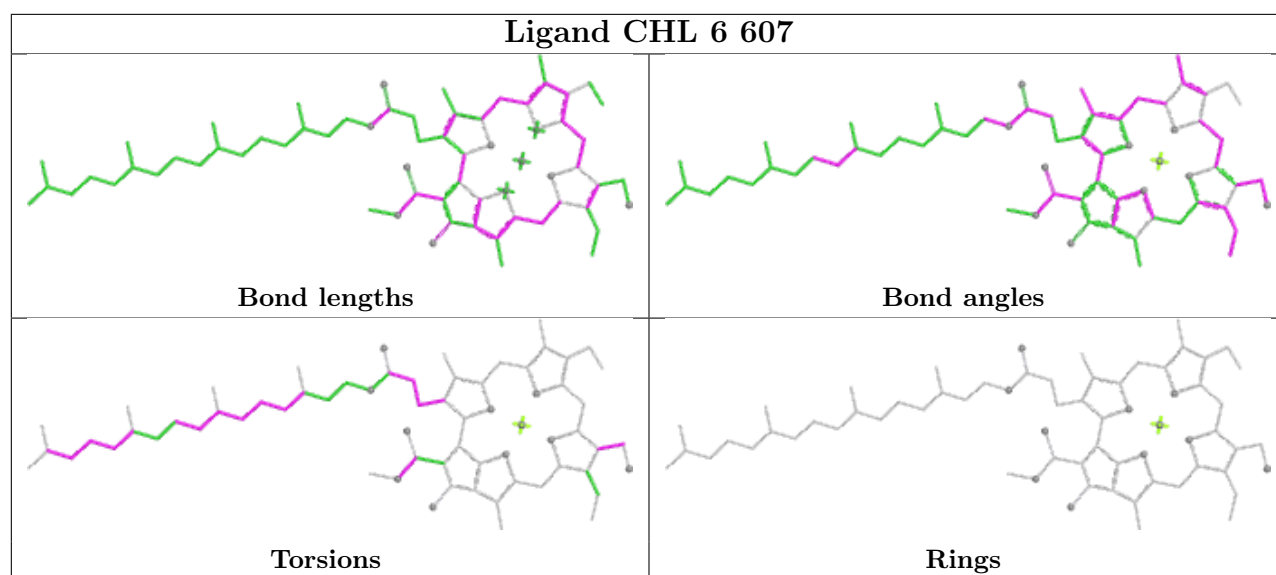


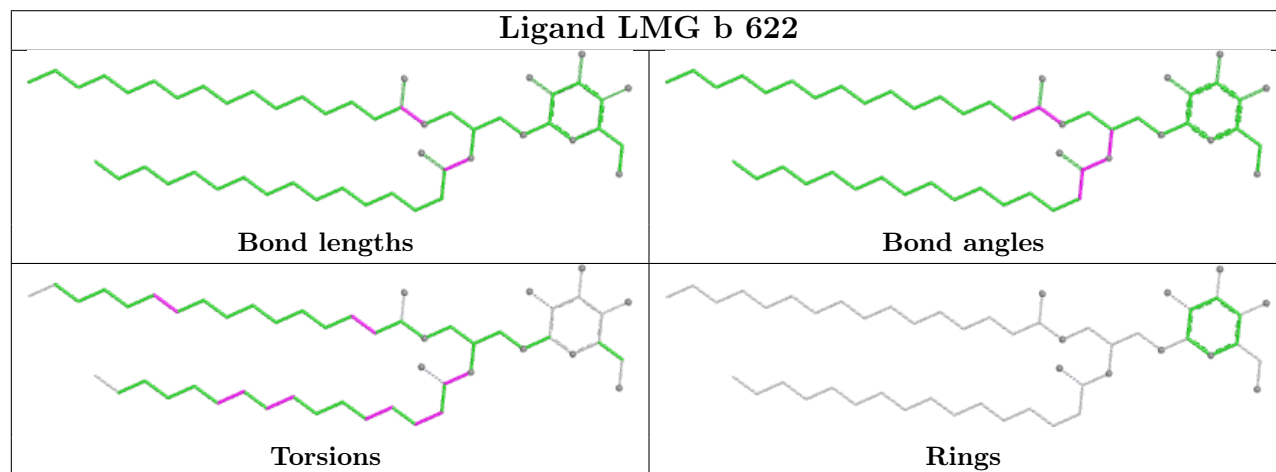
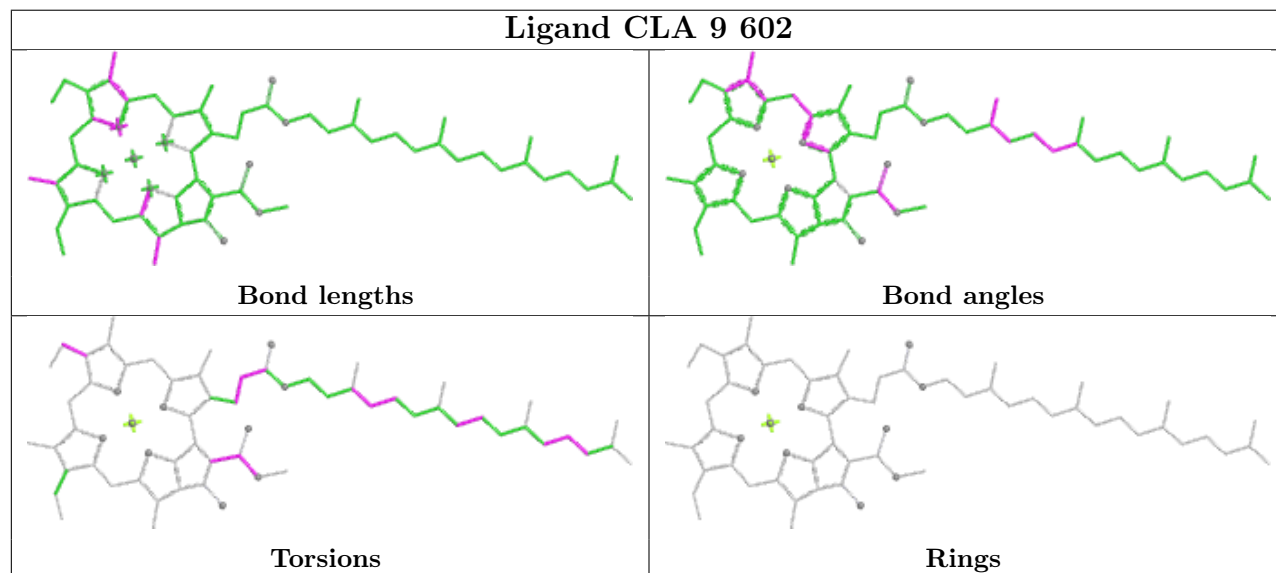
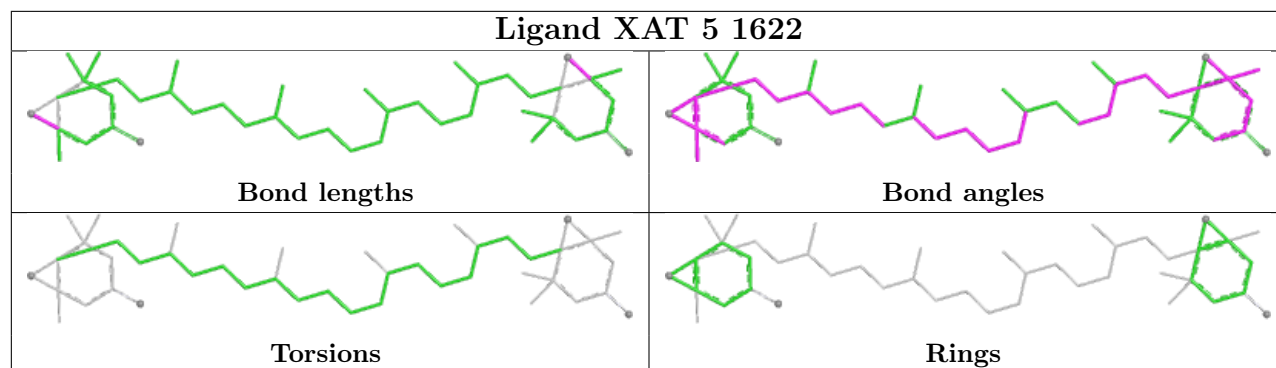
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT S 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

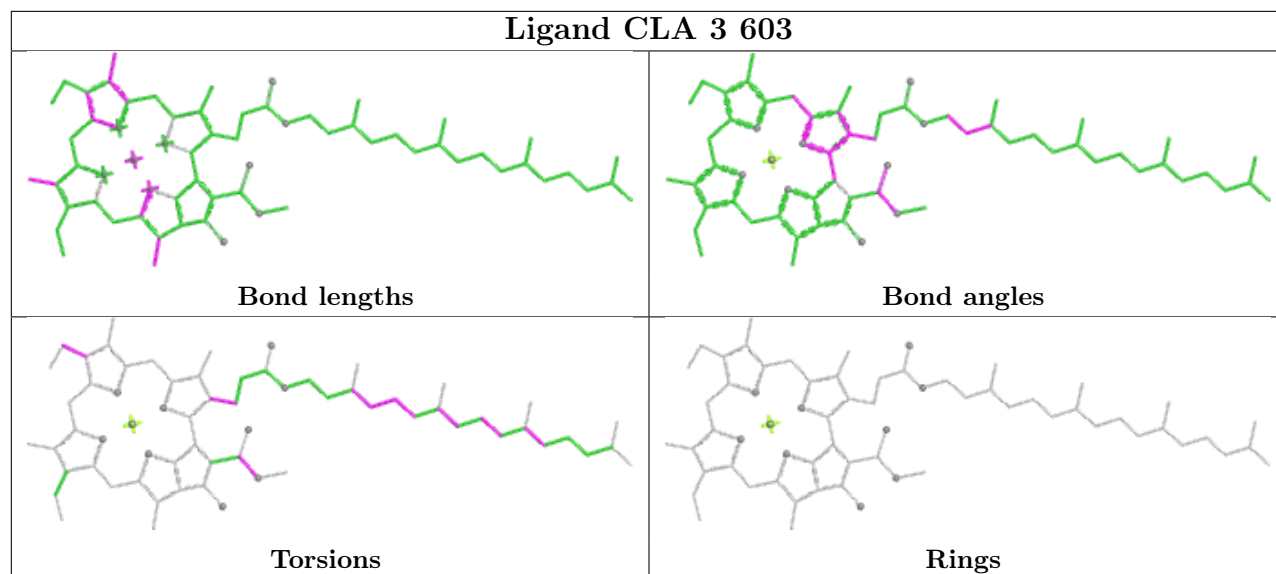
Ligand XAT y 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

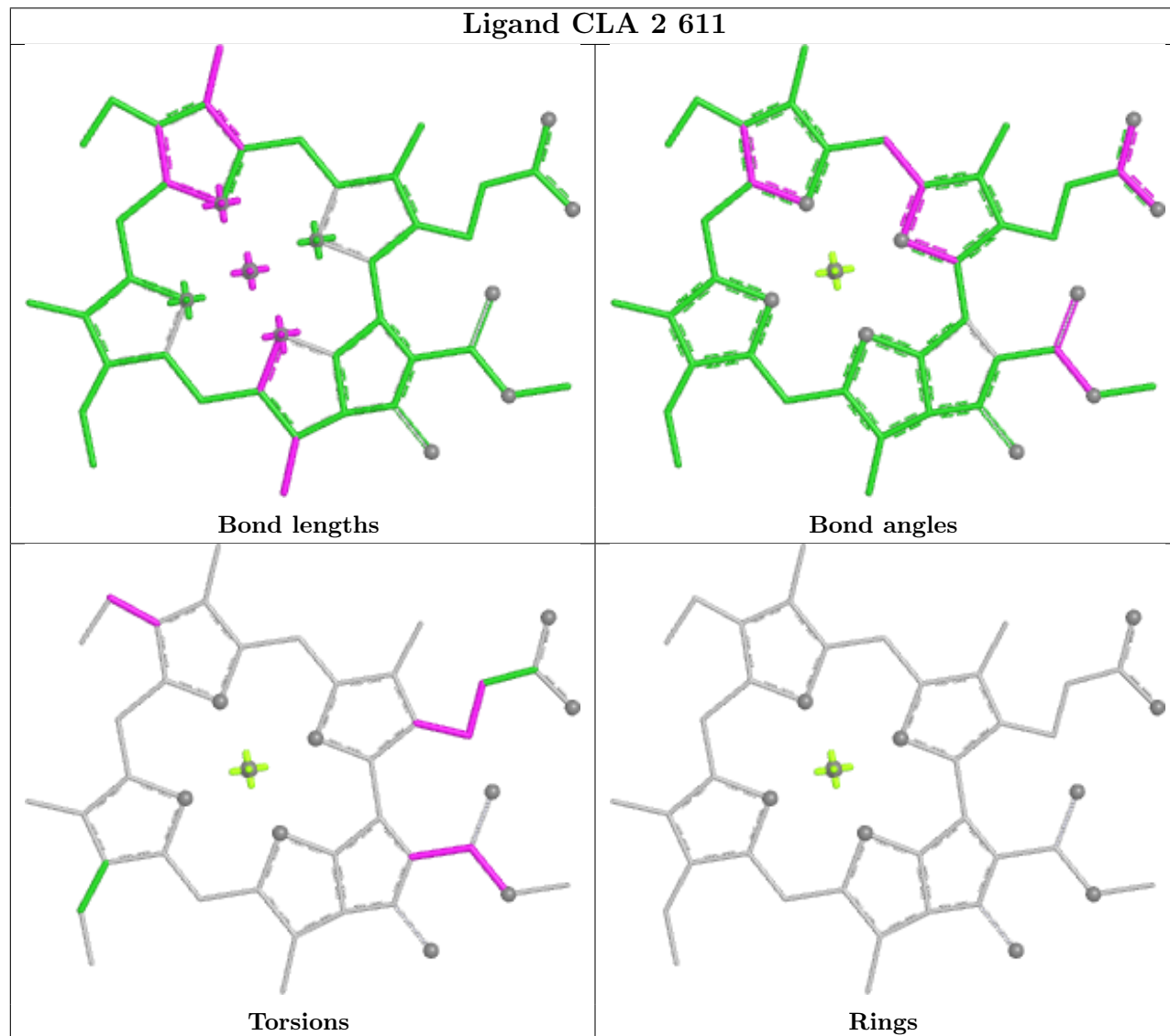




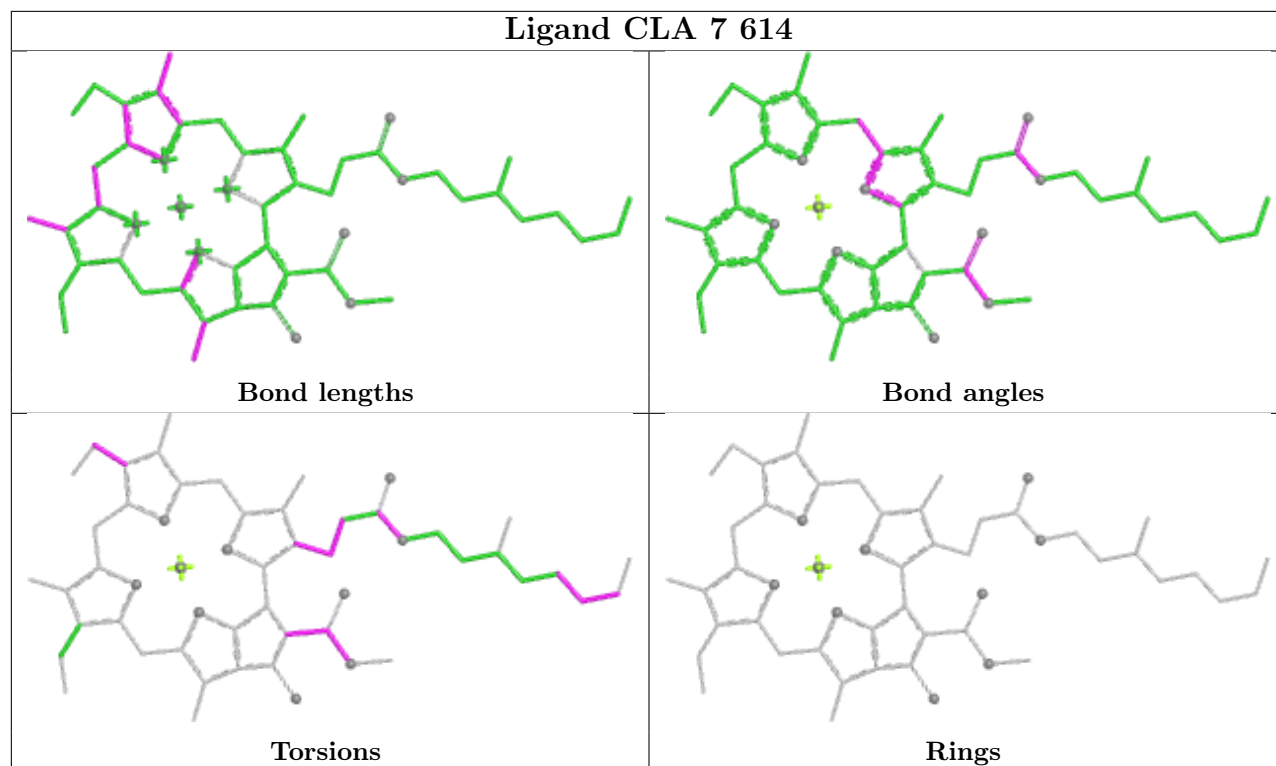
Ligand CLA 3 603



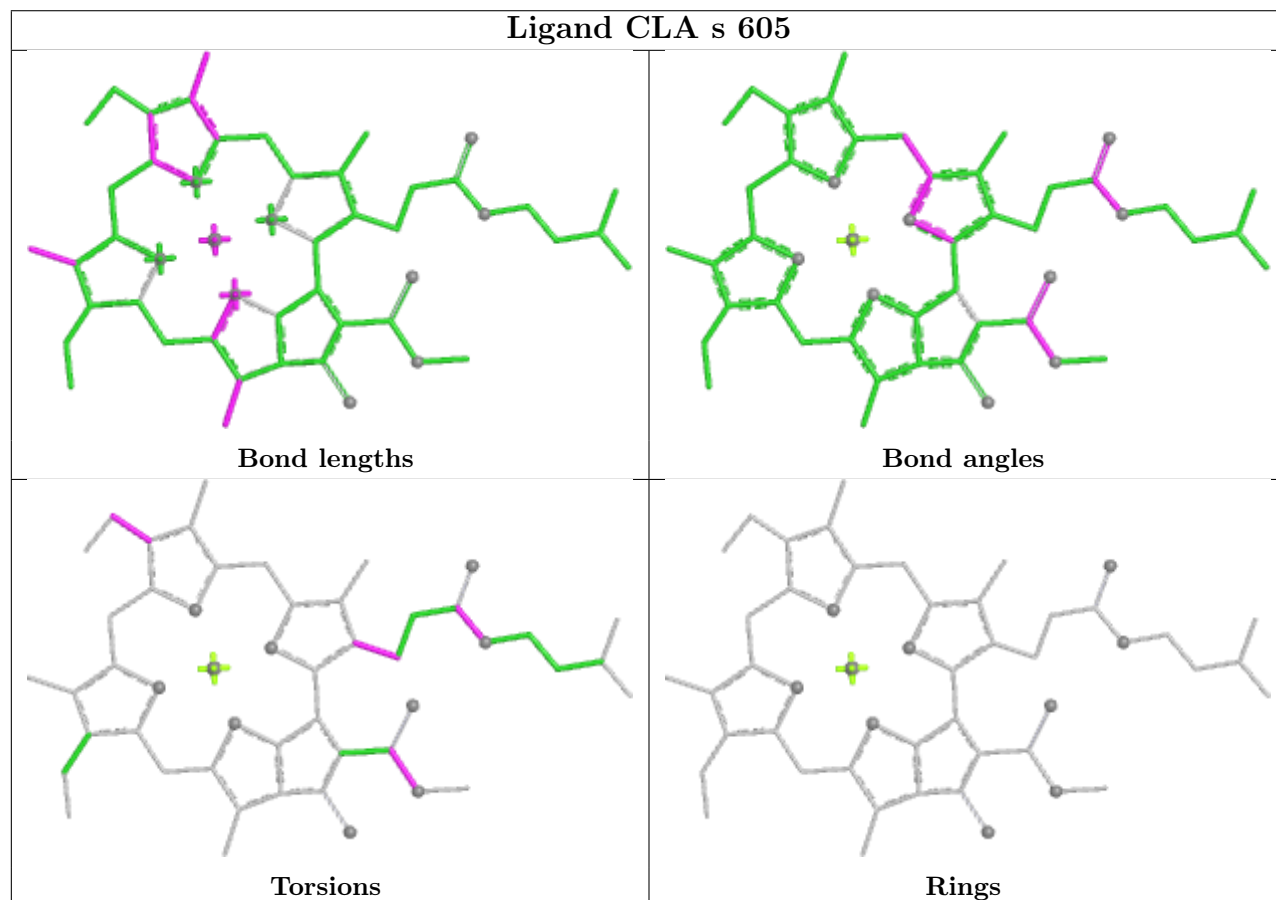
Ligand CLA 2 611

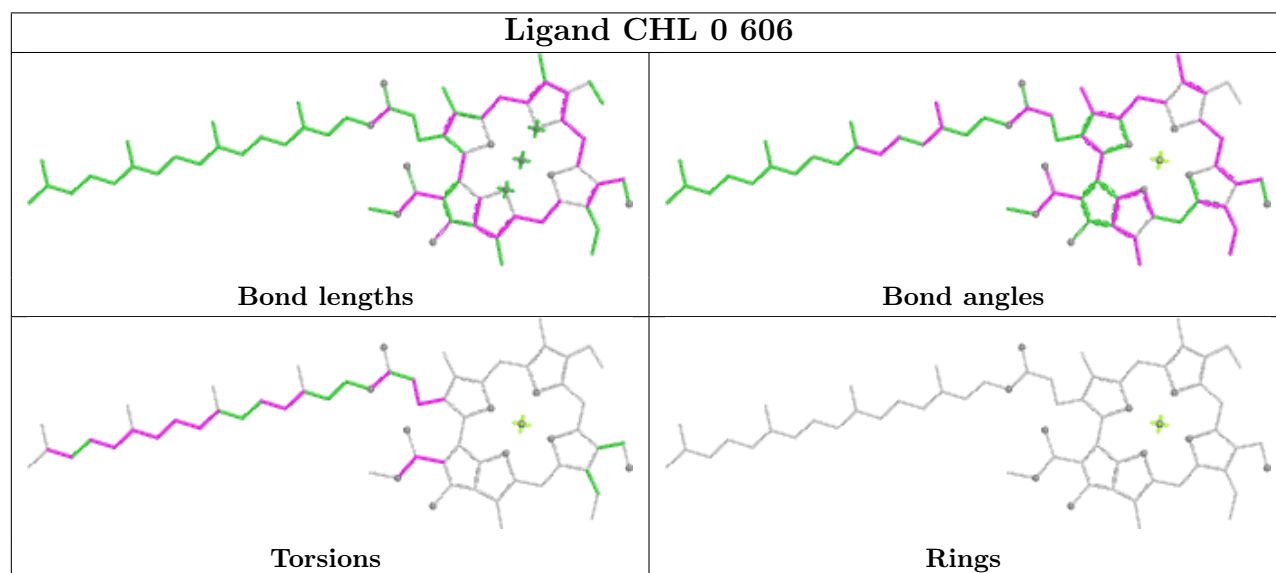
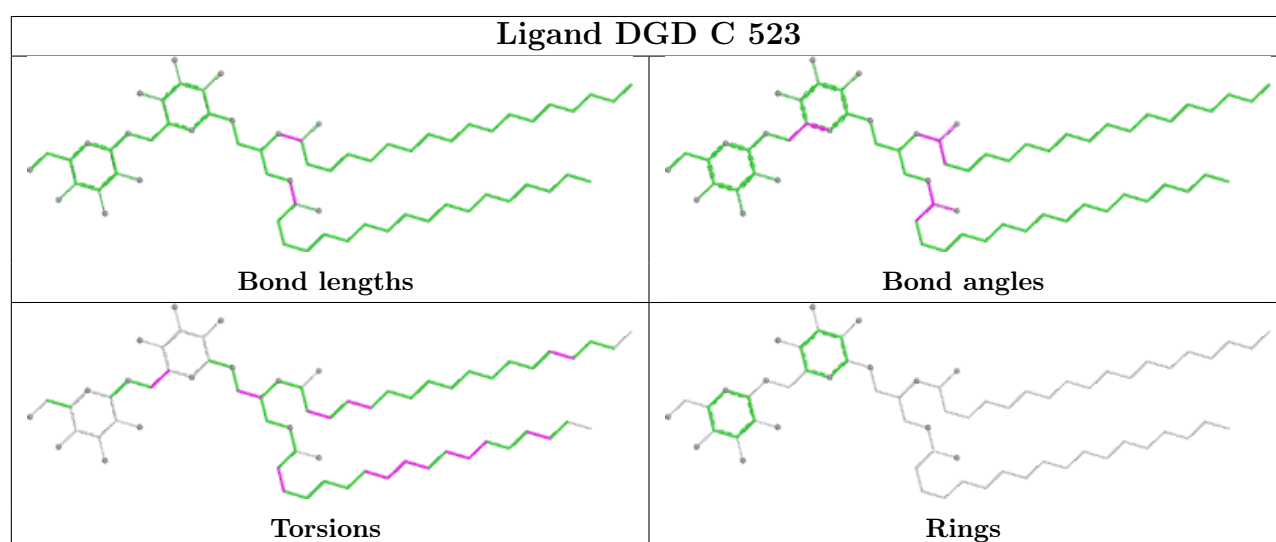
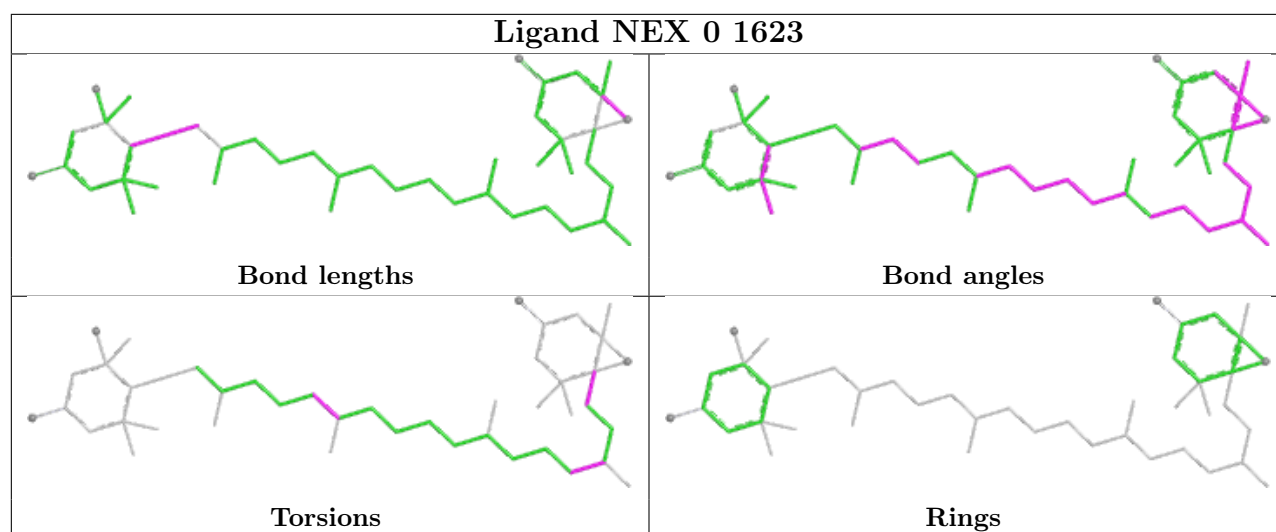


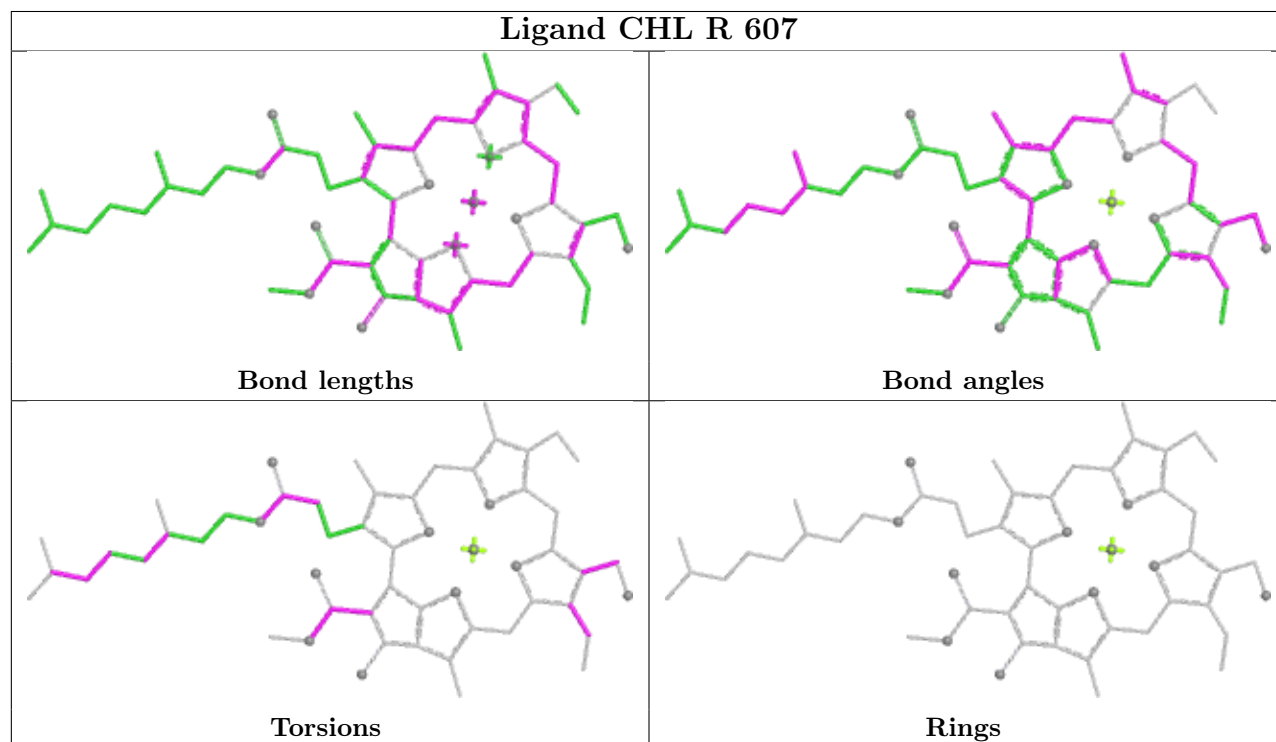
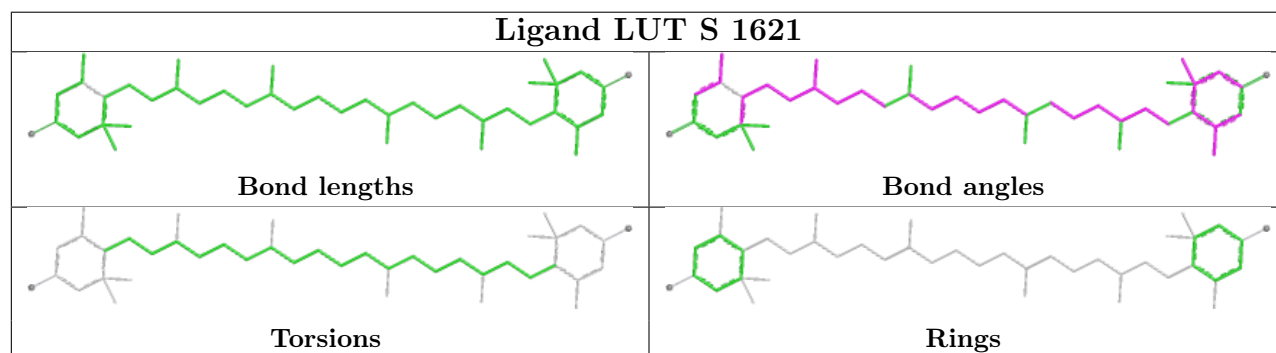
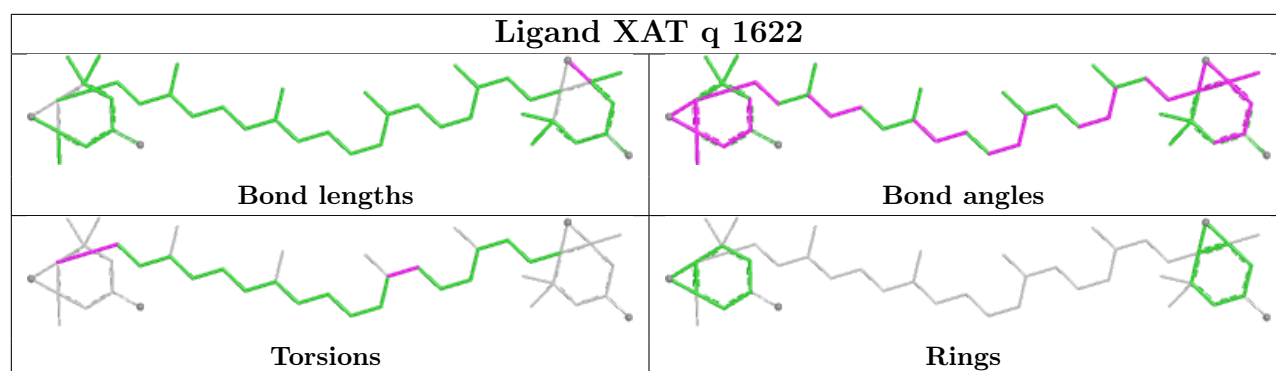
Ligand CLA 7 614

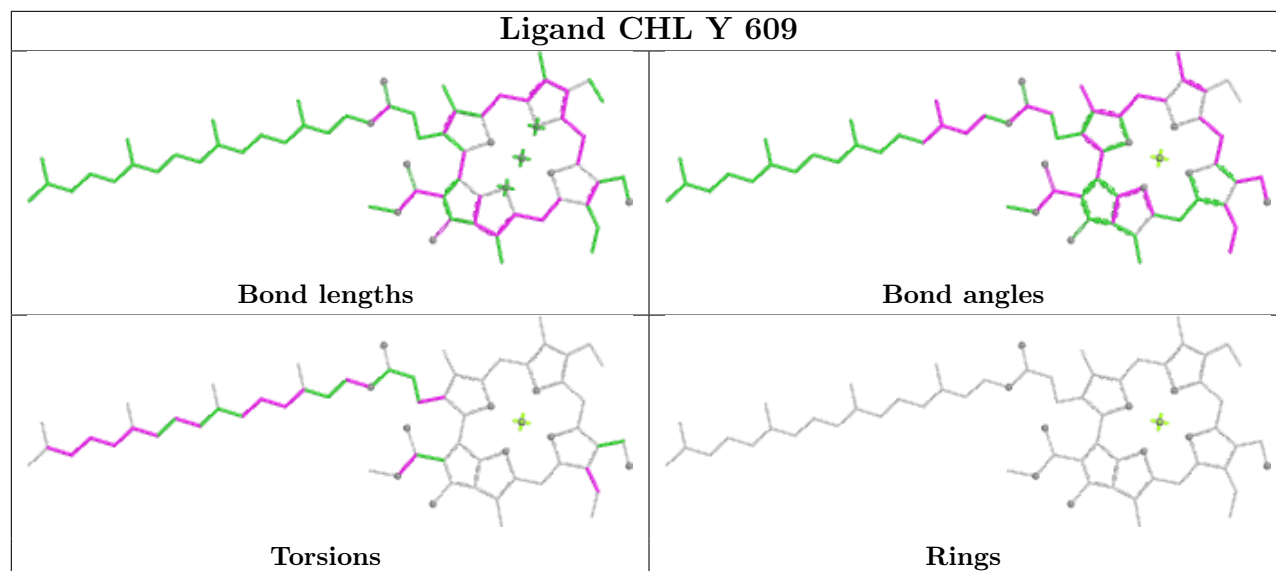
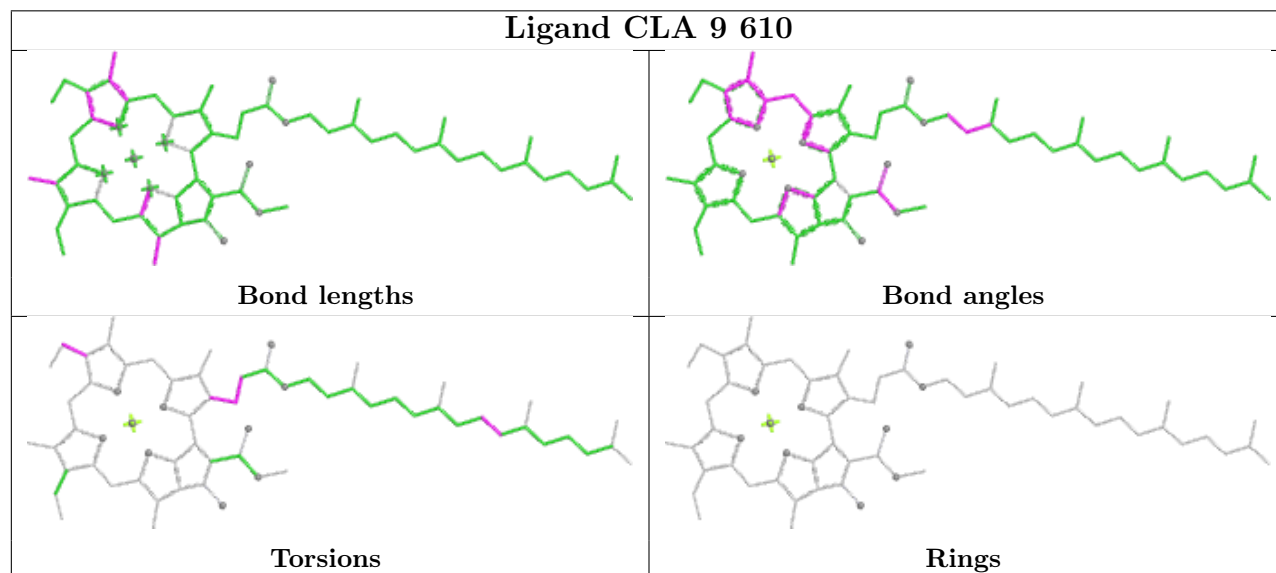
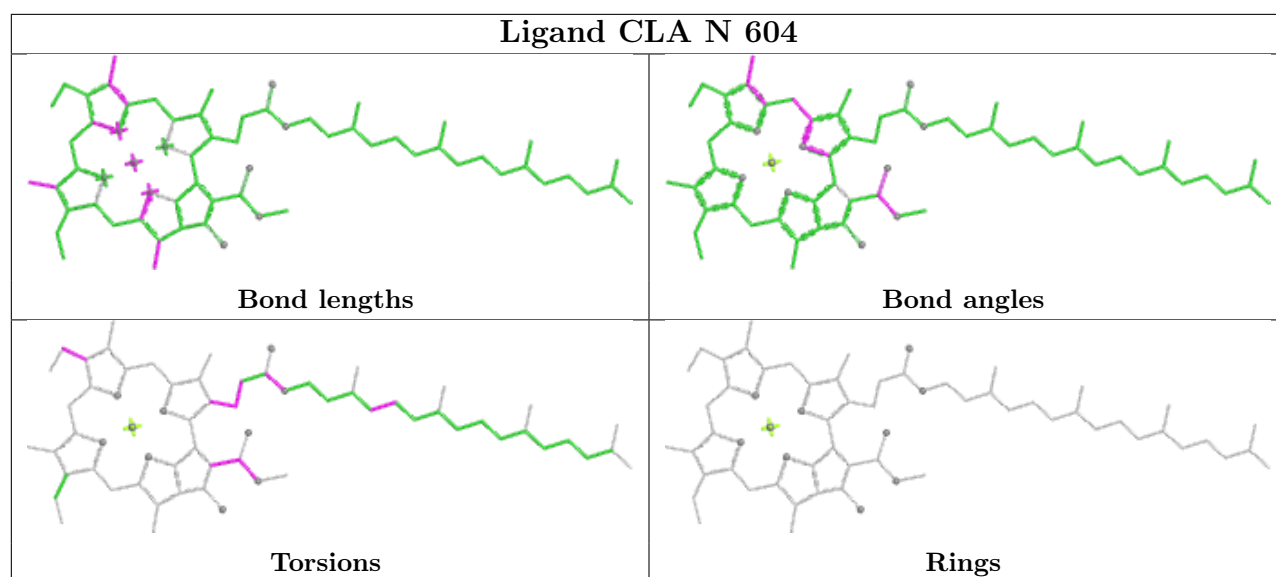


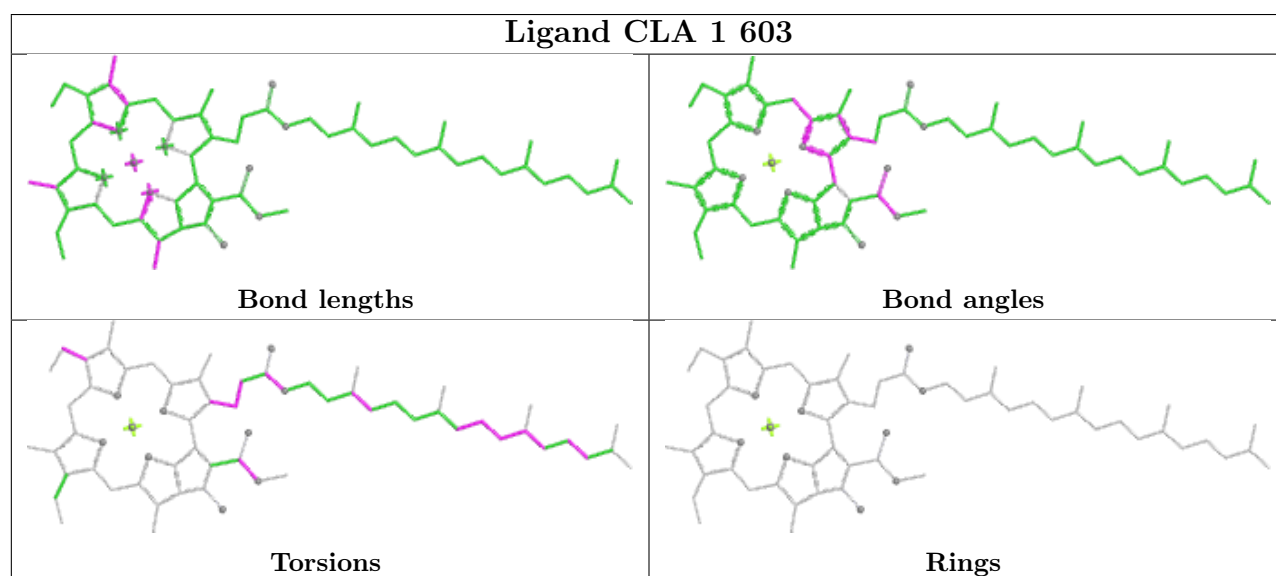
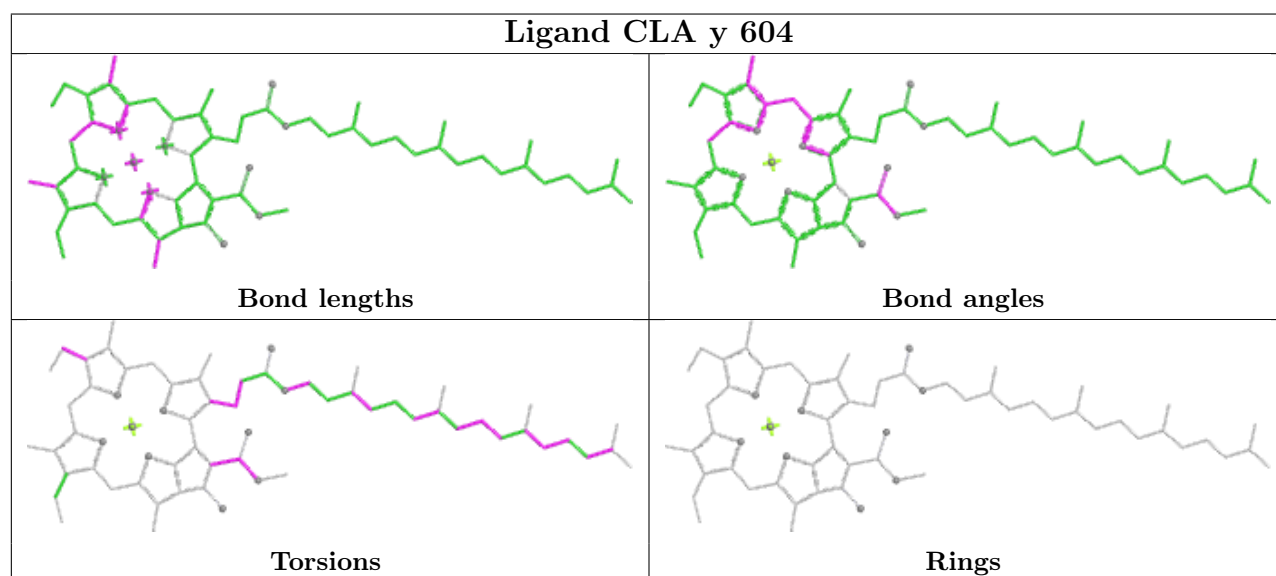
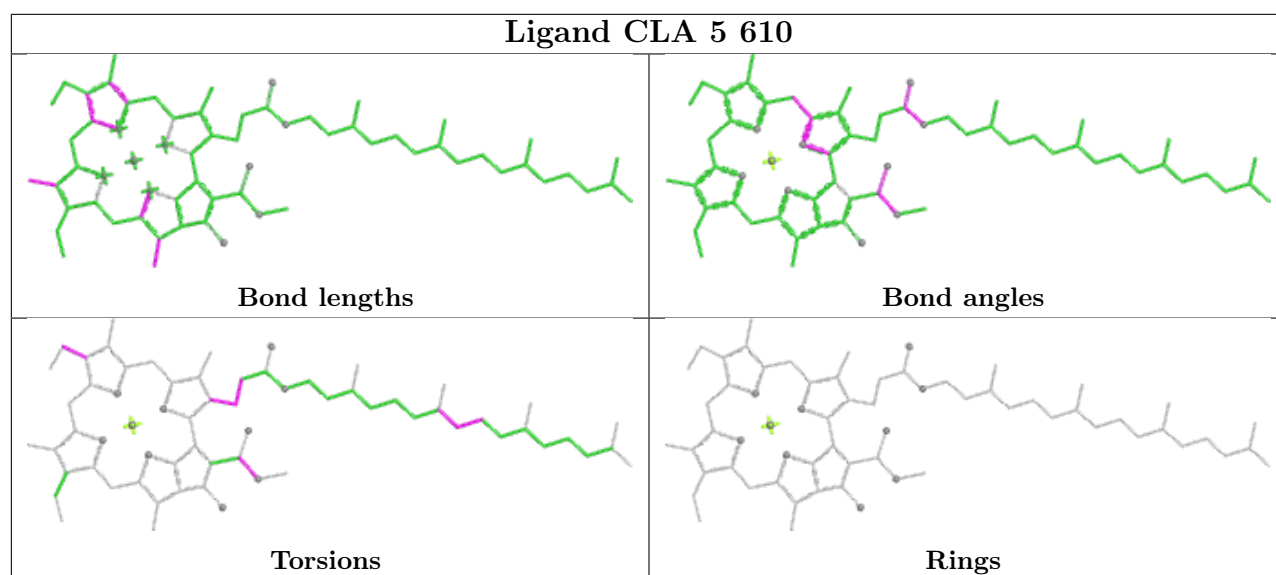
Ligand CLA s 605



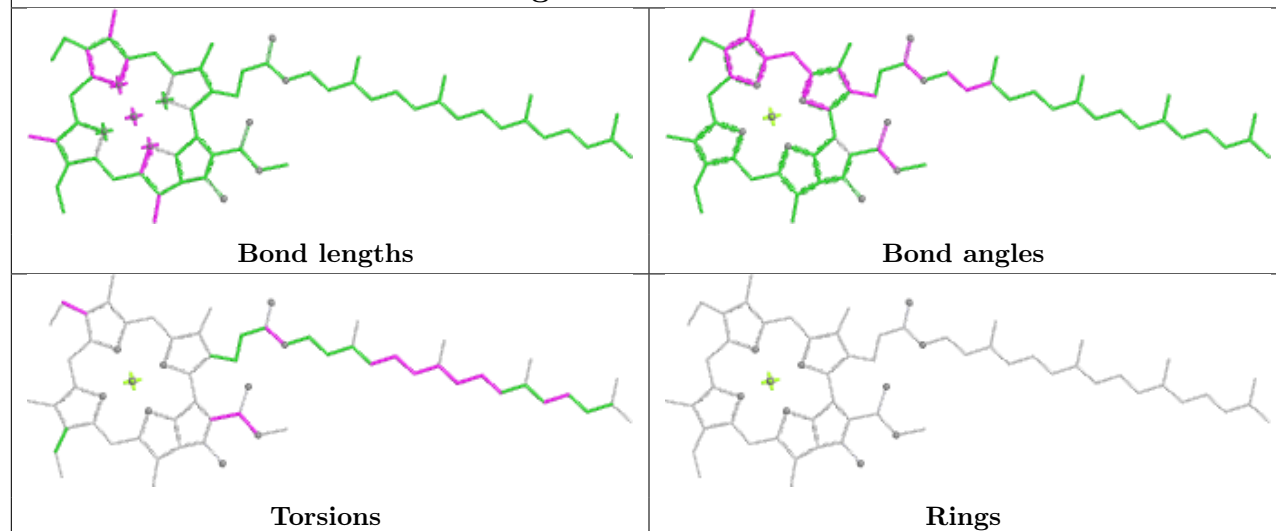




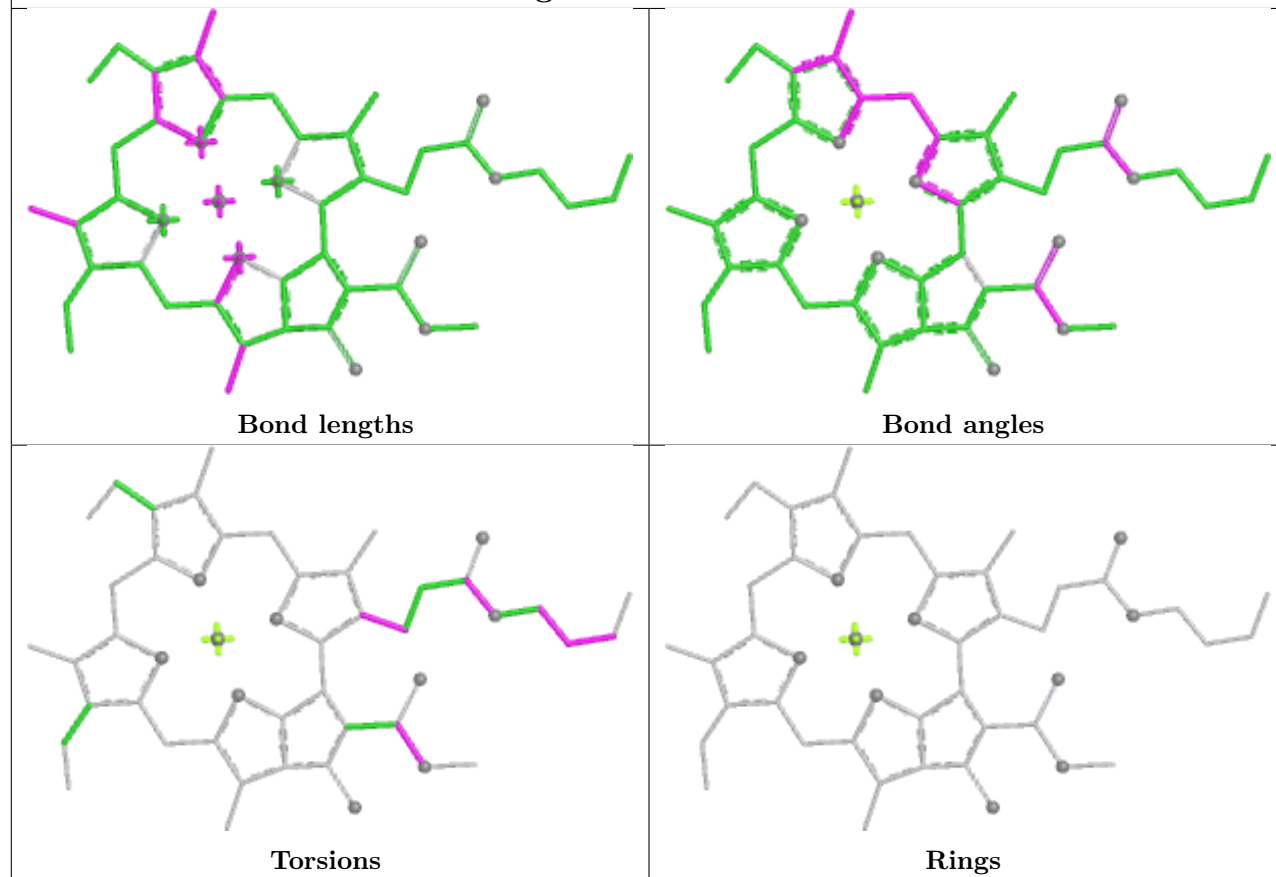


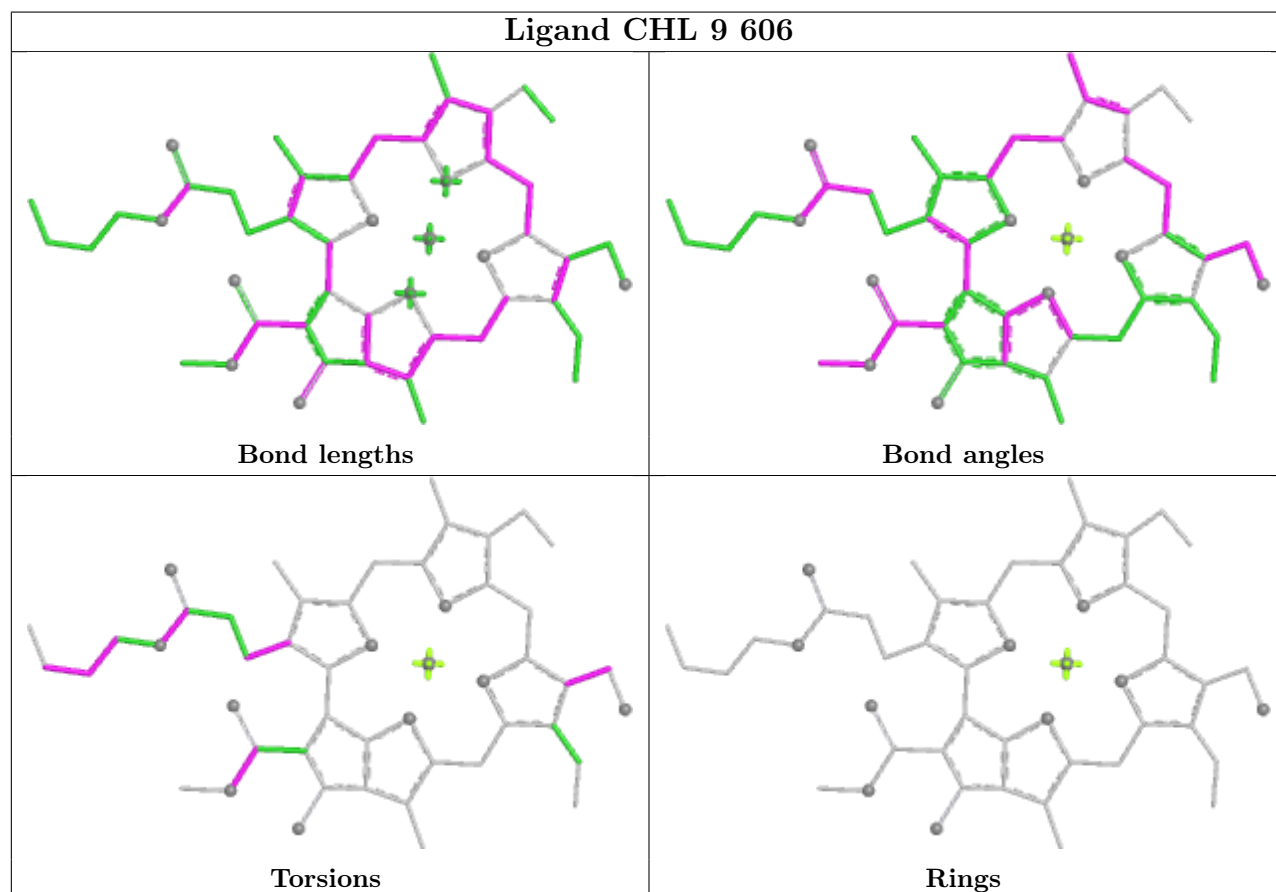
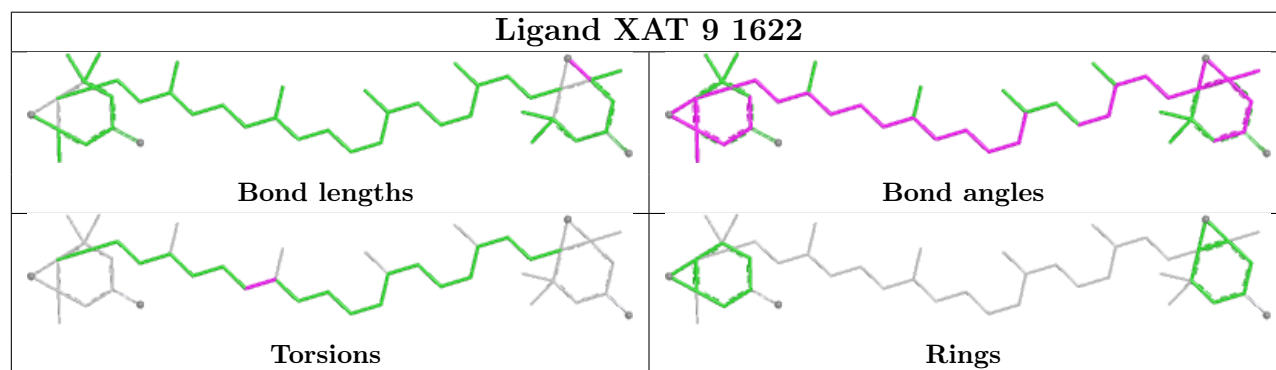
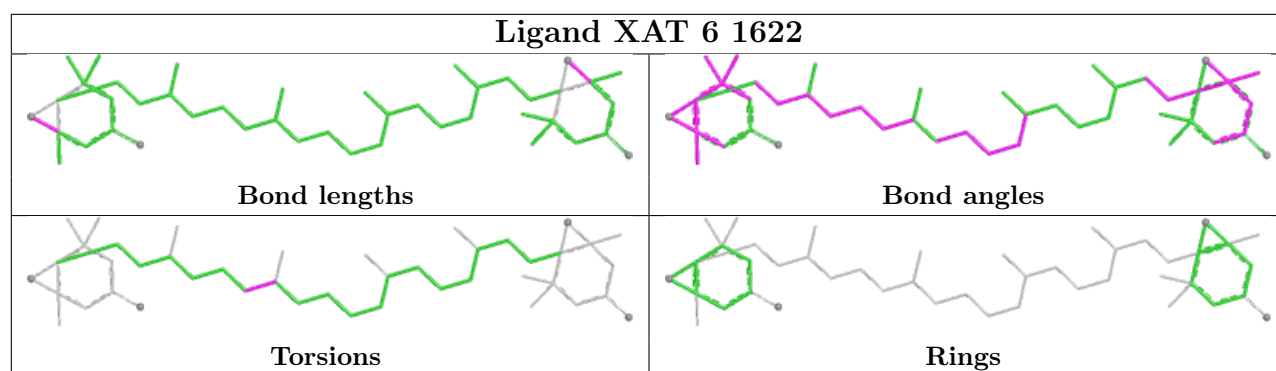


Ligand CLA Y 612

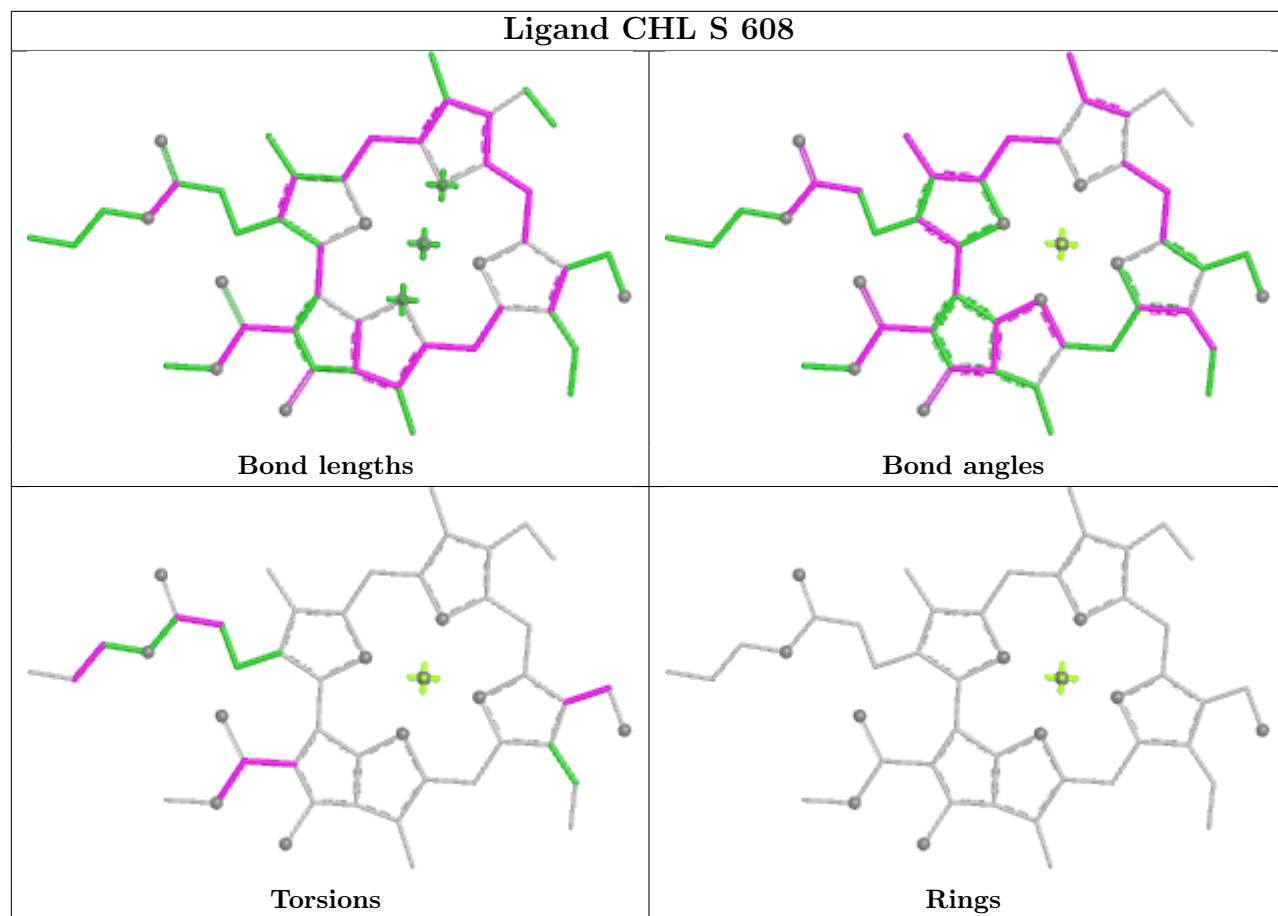


Ligand CLA S 604

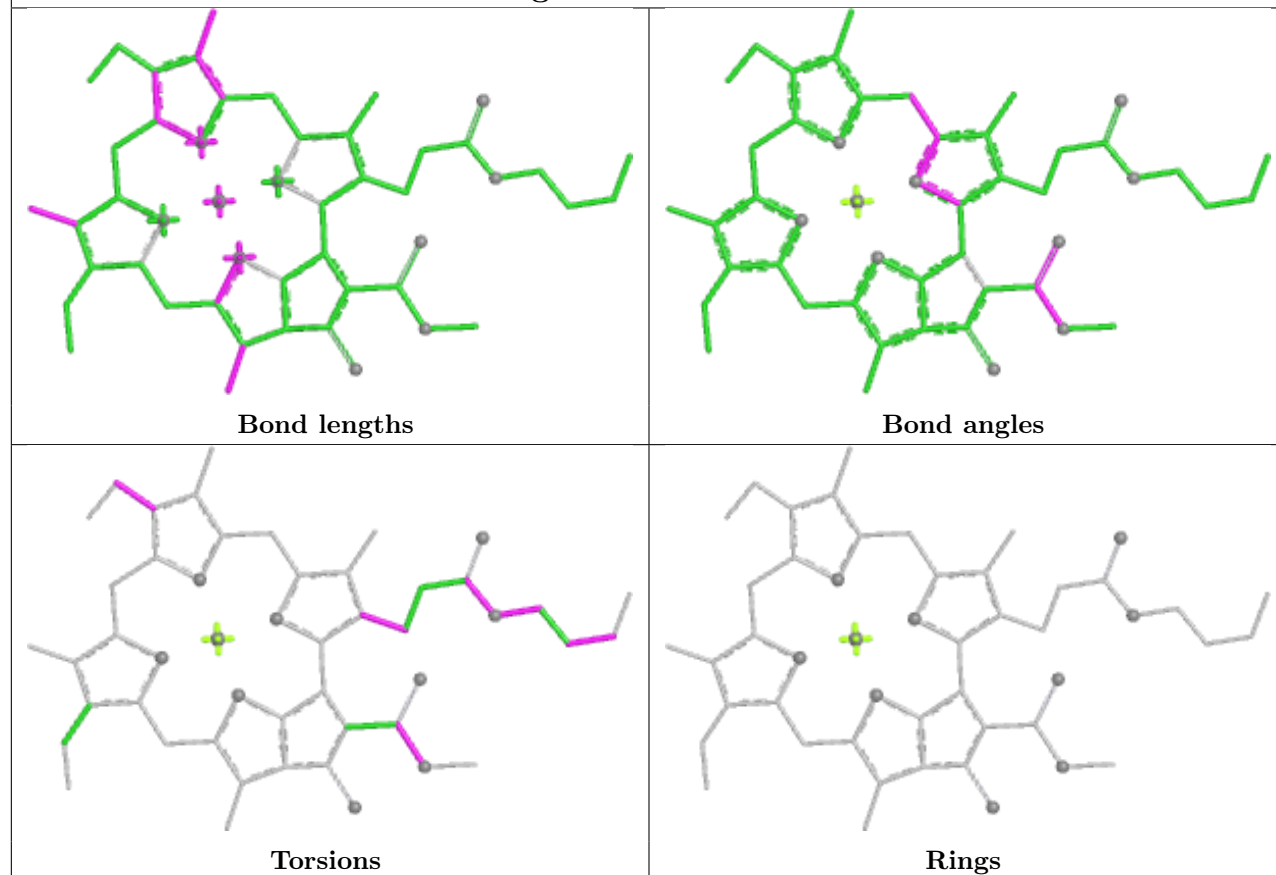




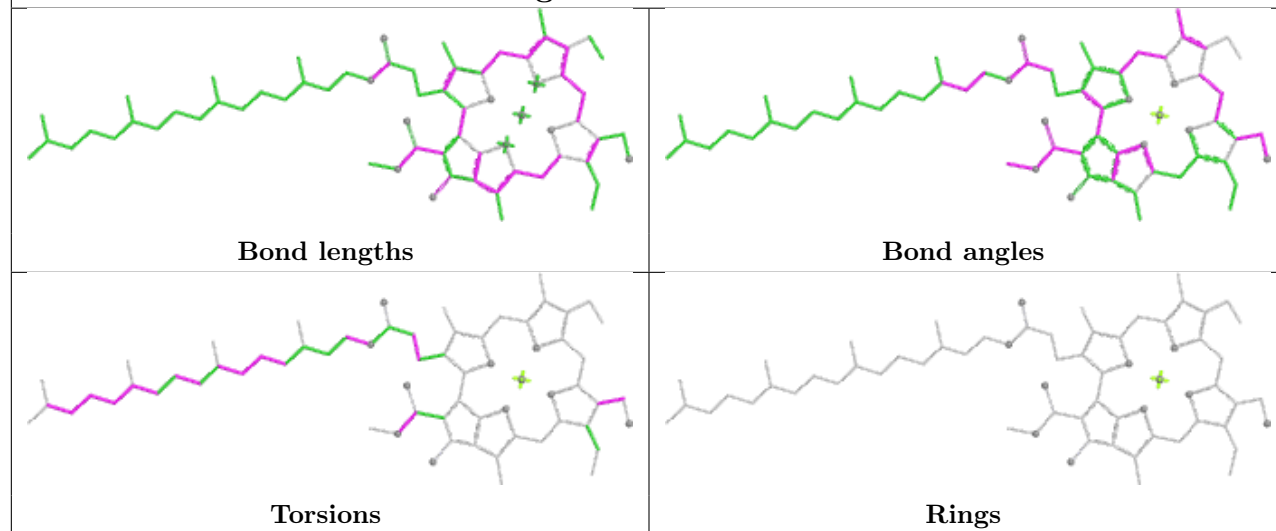
Ligand CHL S 608

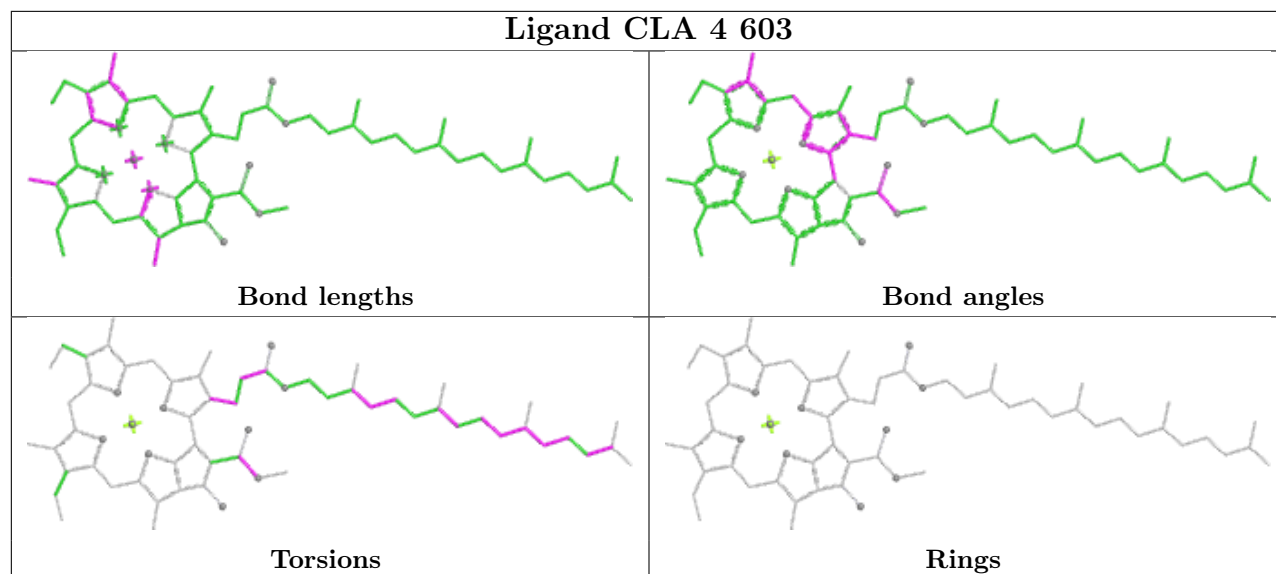
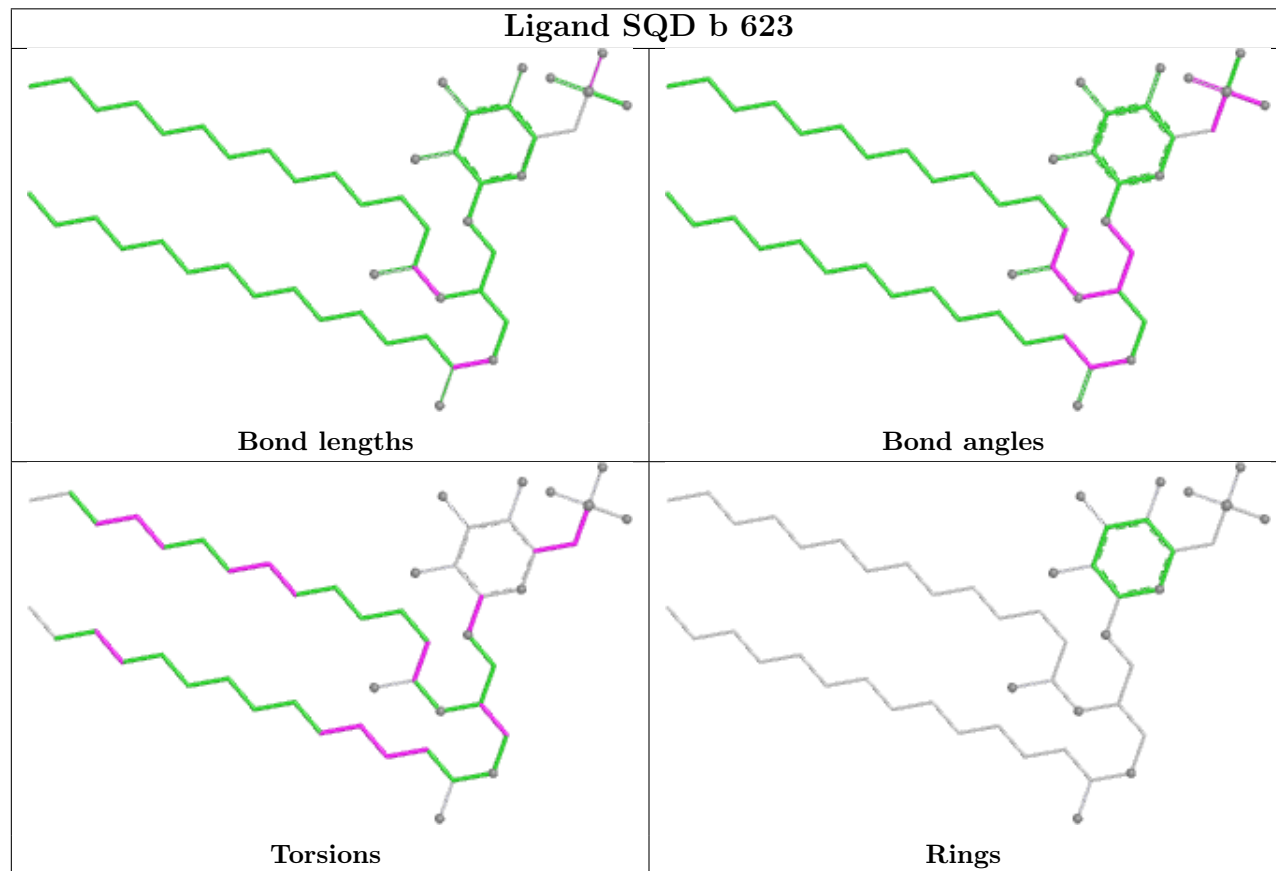


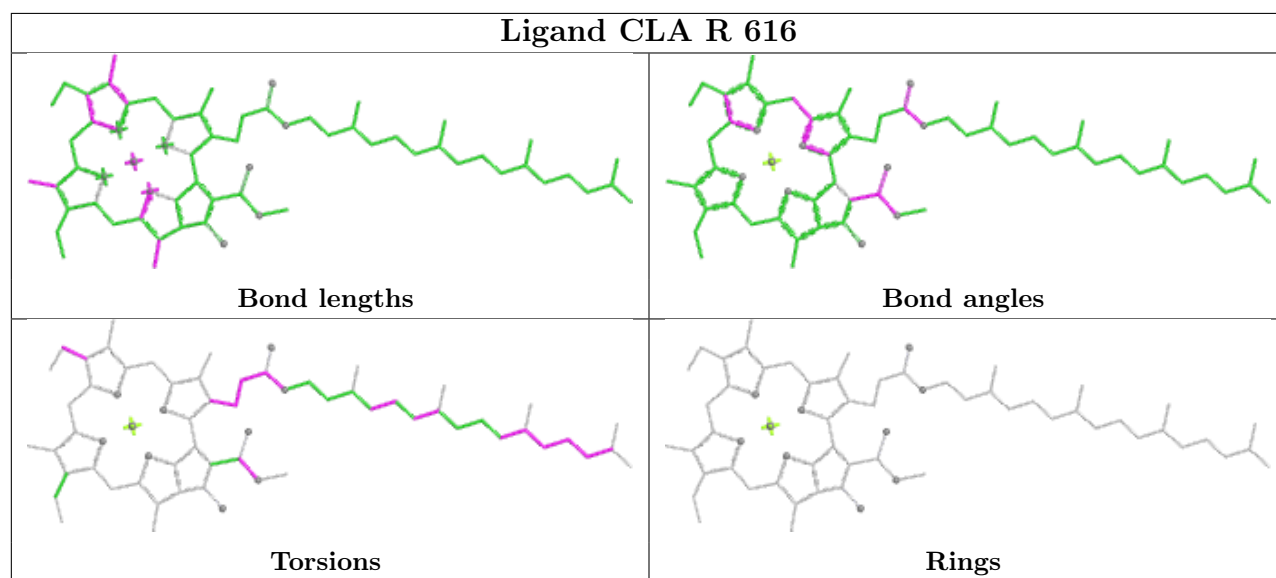
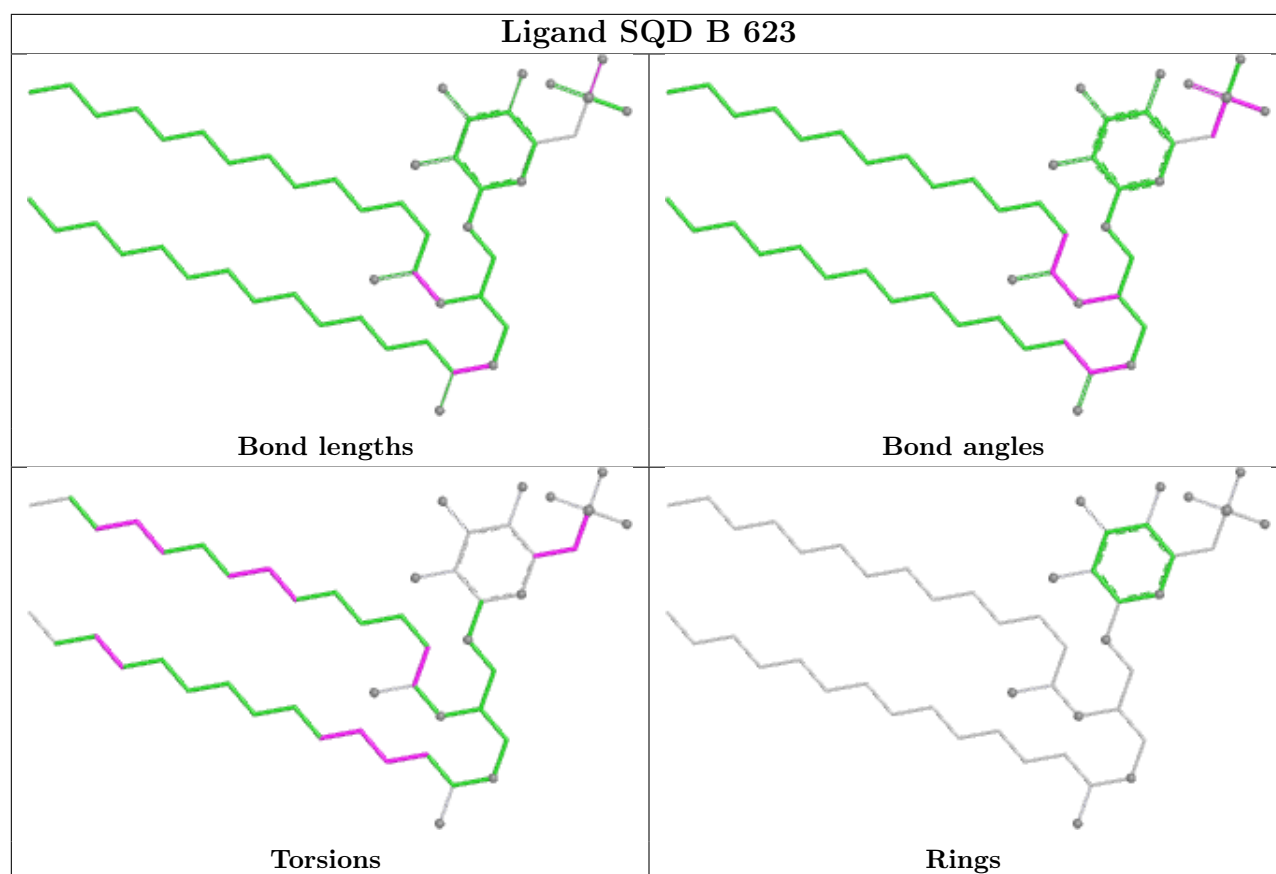
Ligand CLA R 611

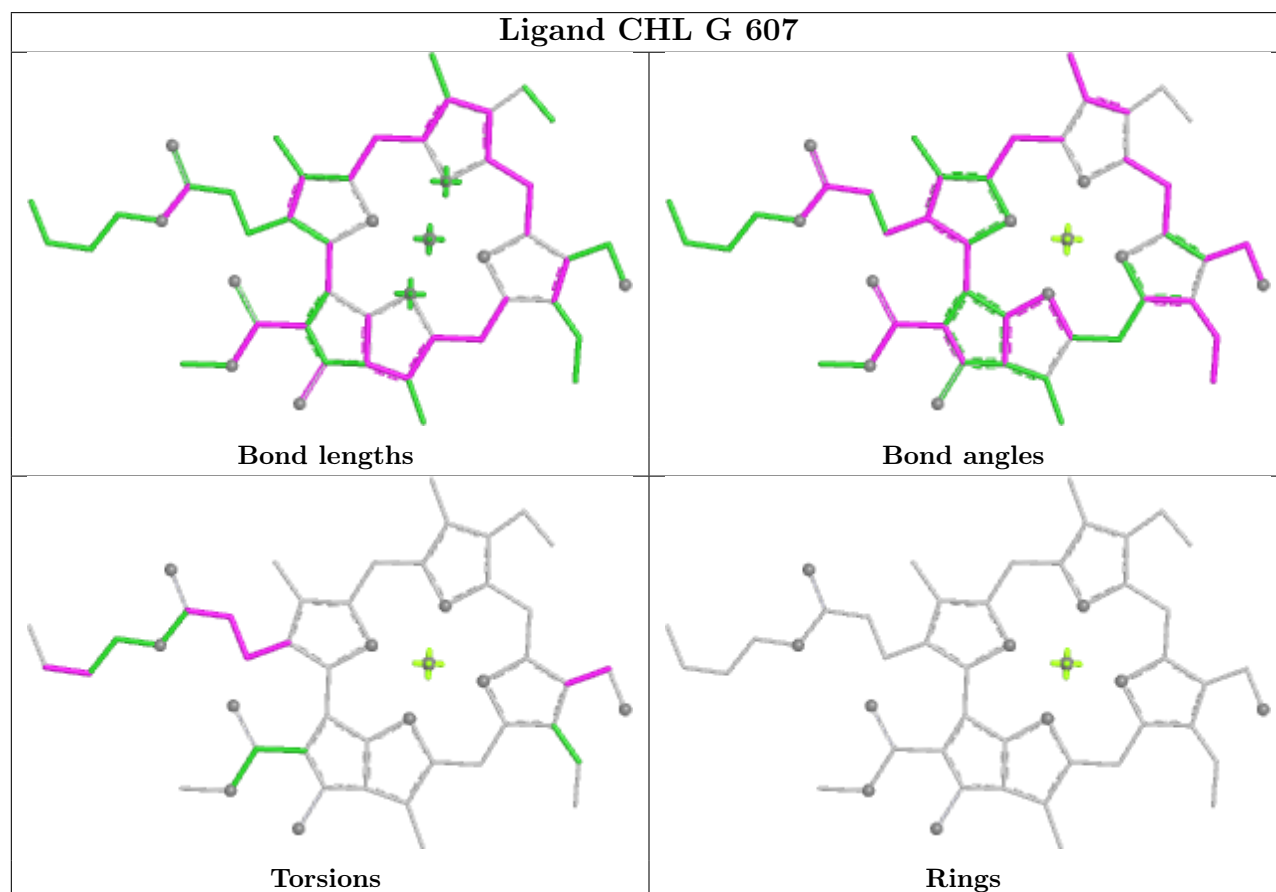
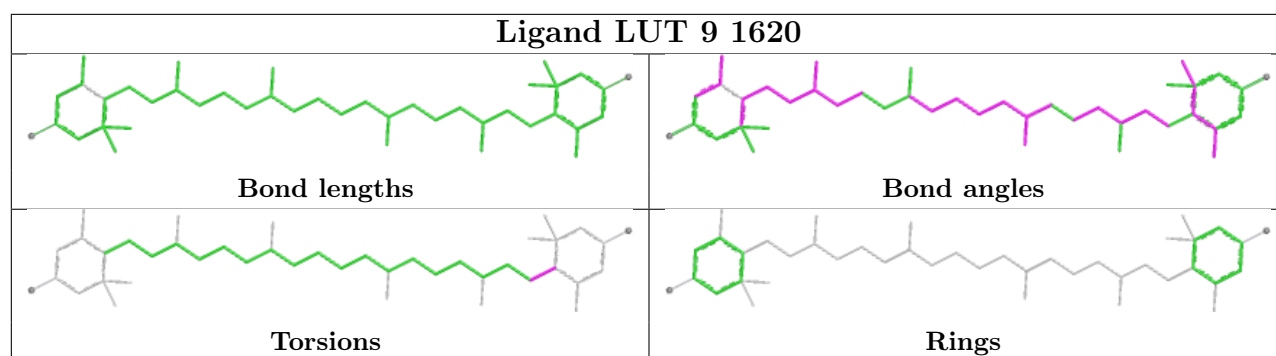


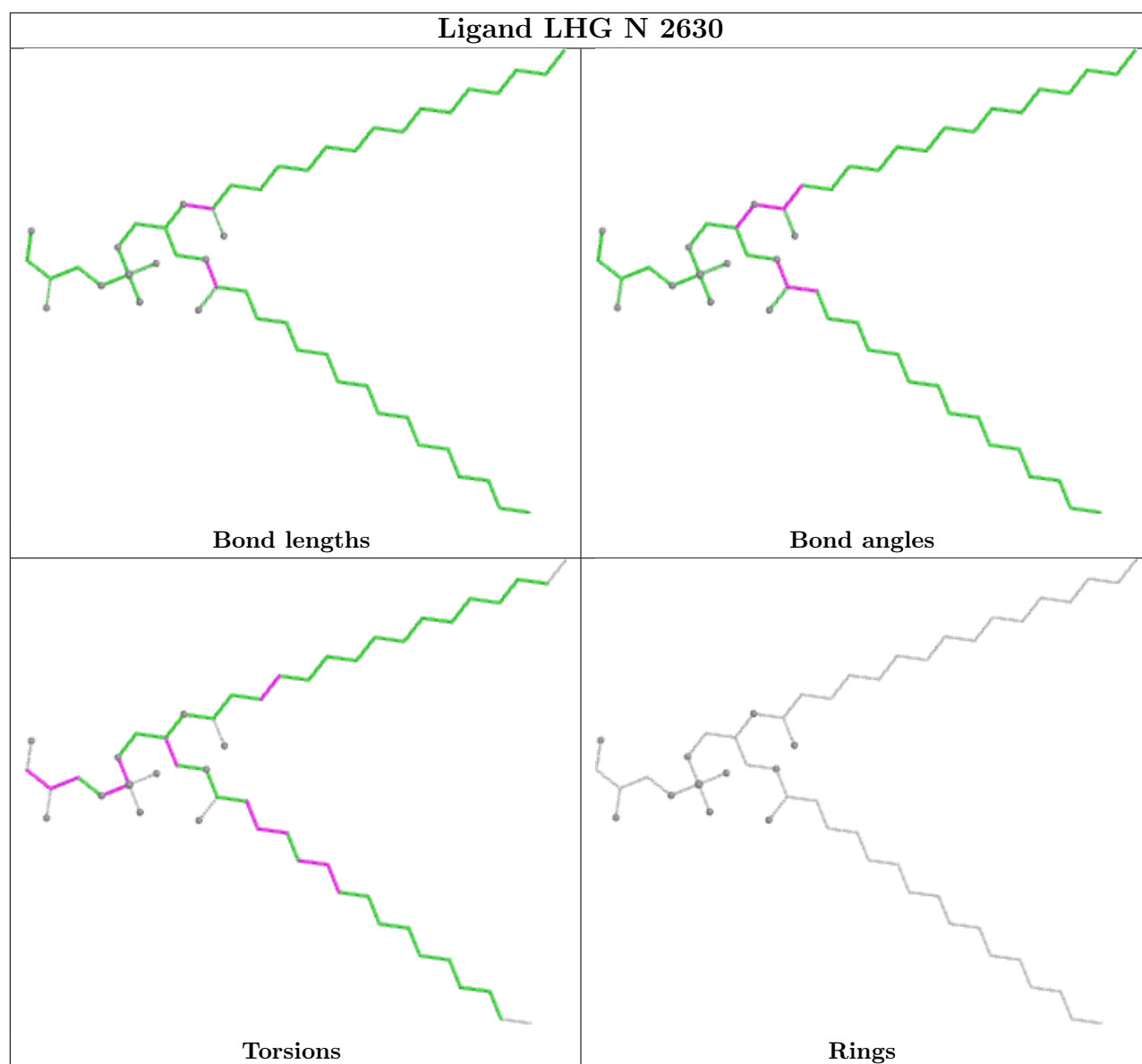
Ligand CHL 3 605

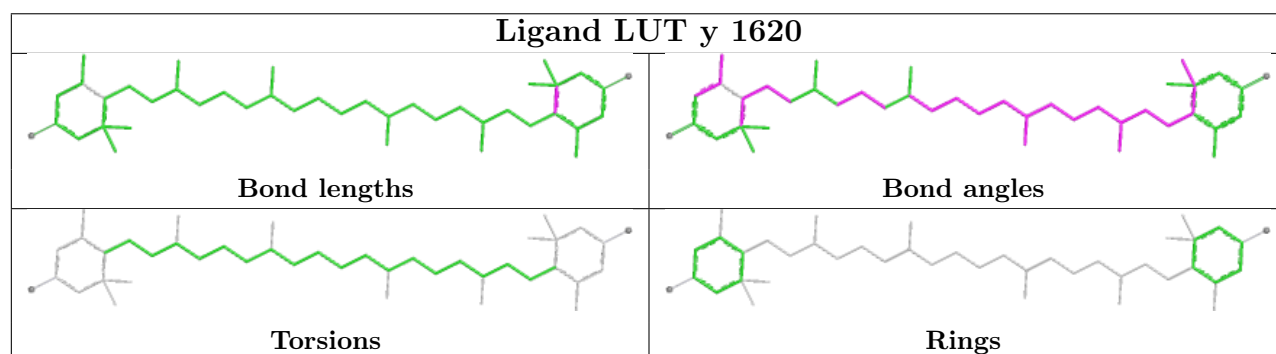
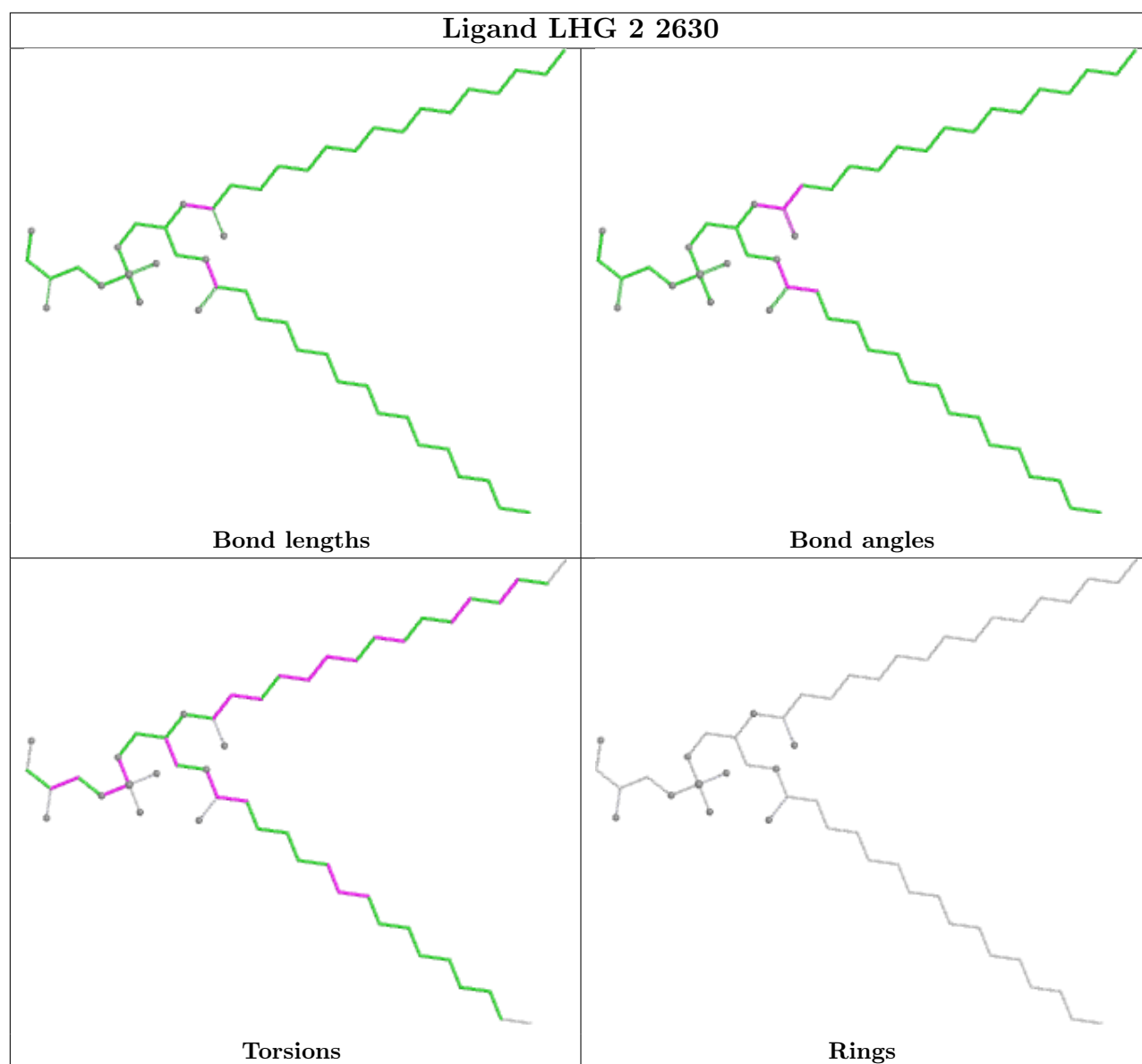


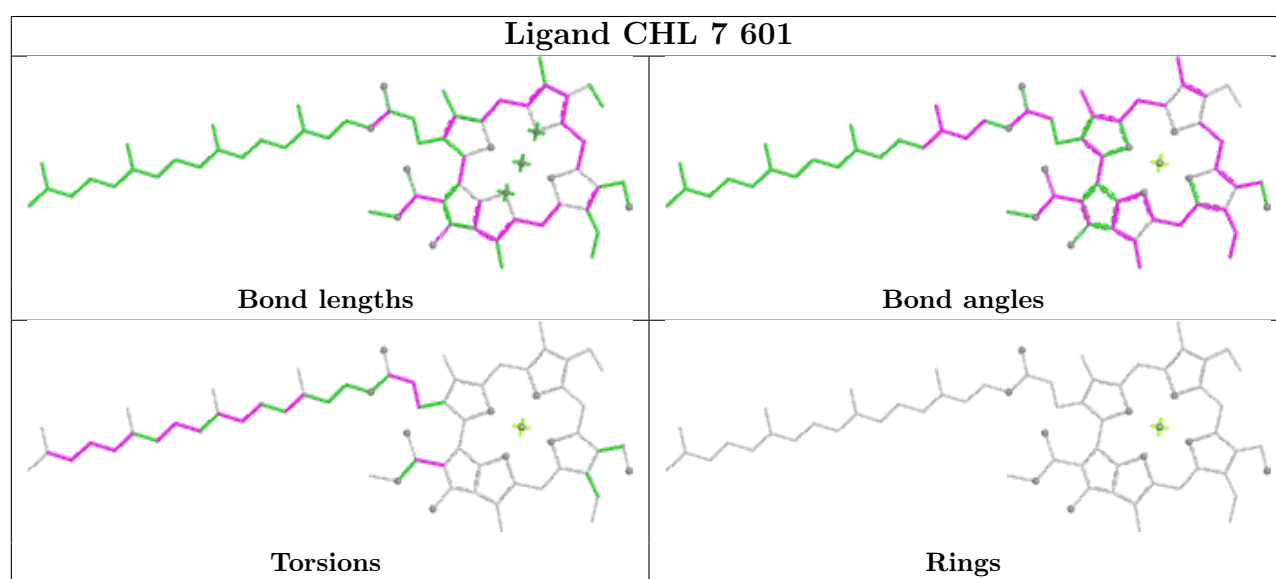
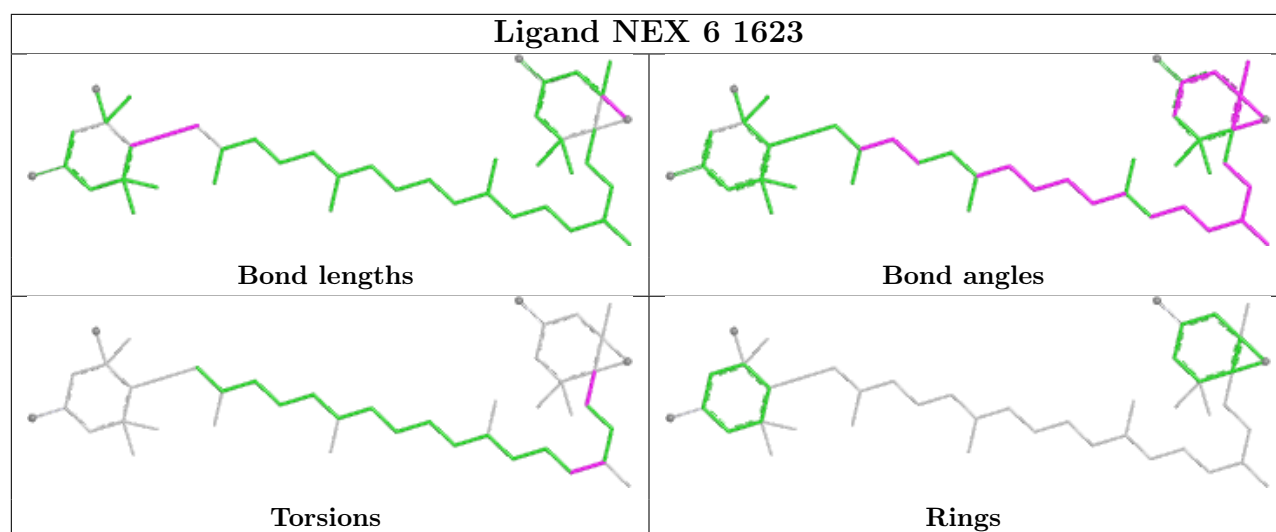
Ligand CLA 4 603**Ligand SQD b 623**

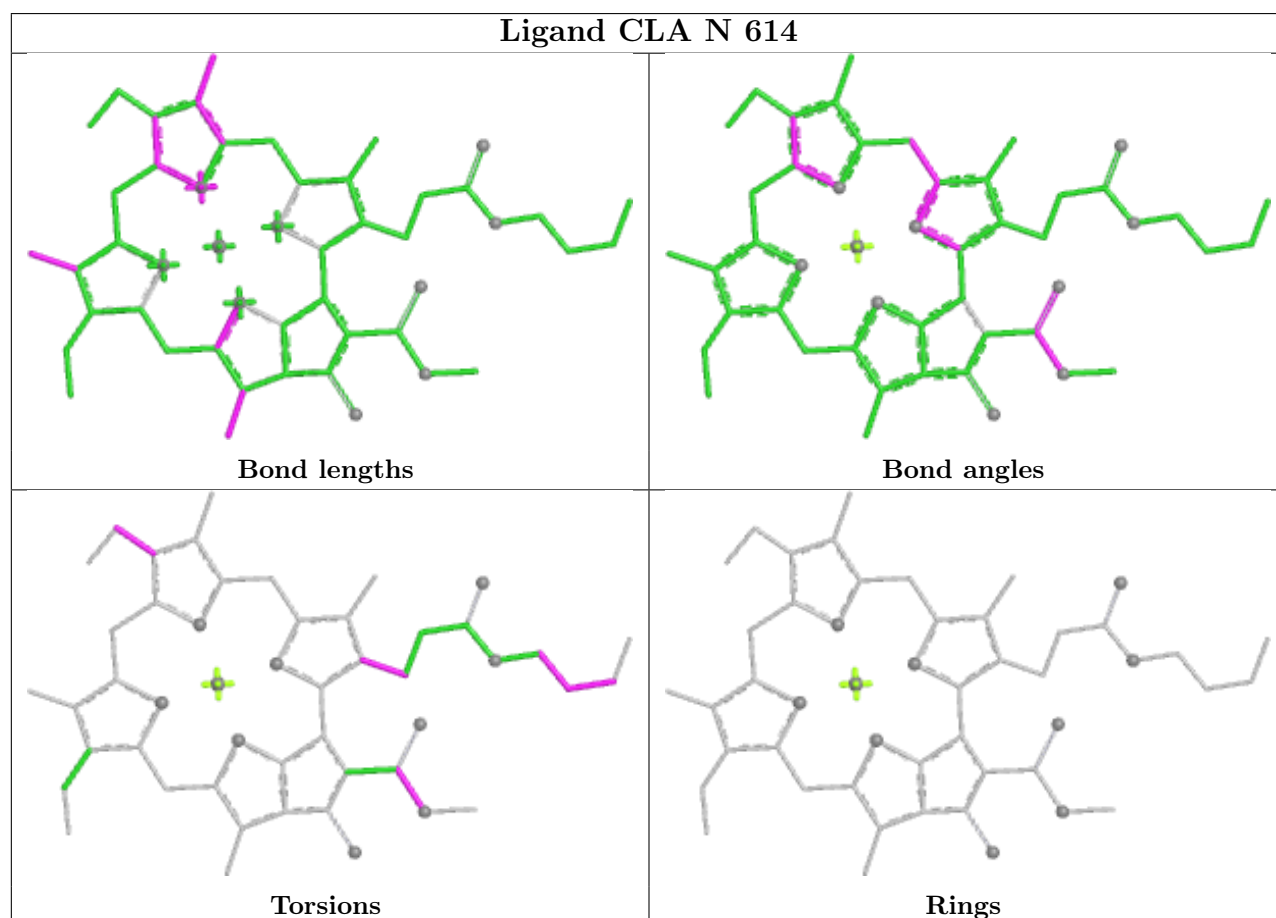
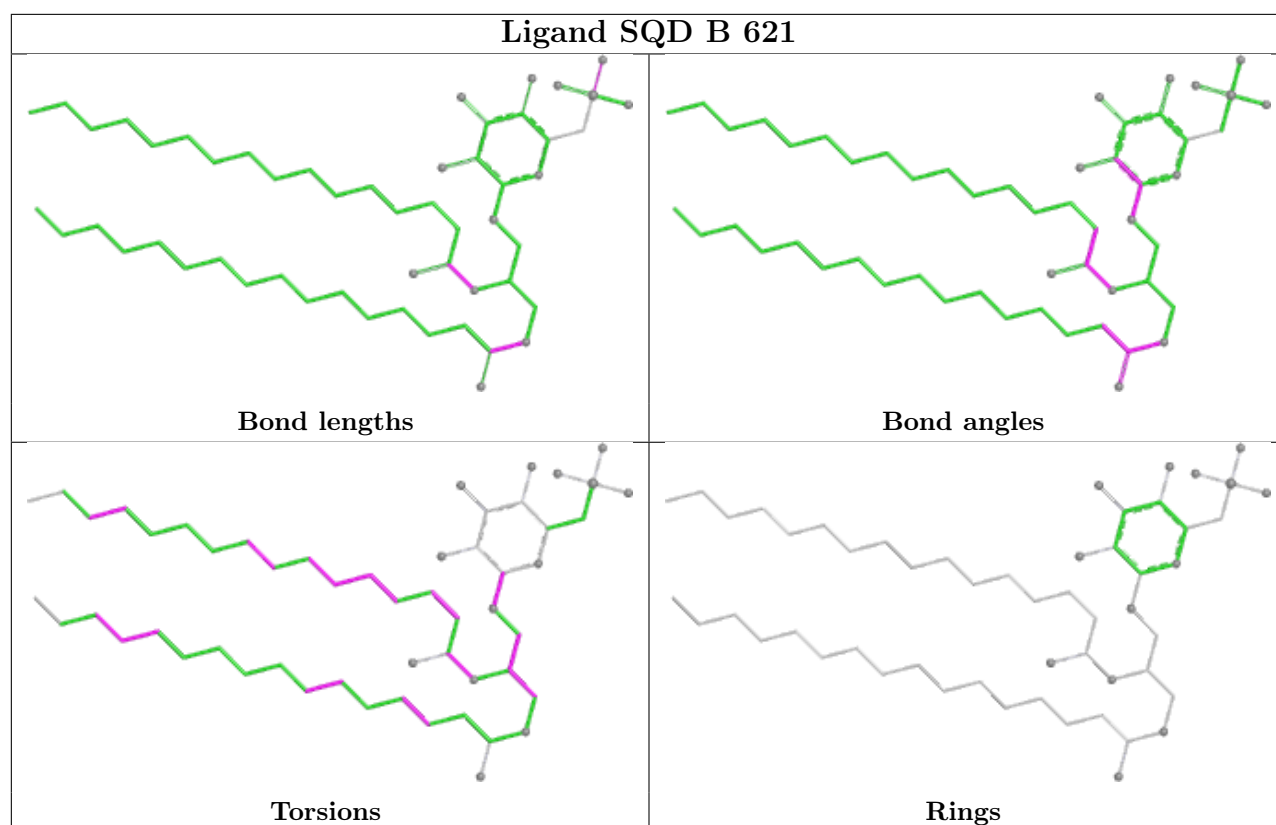


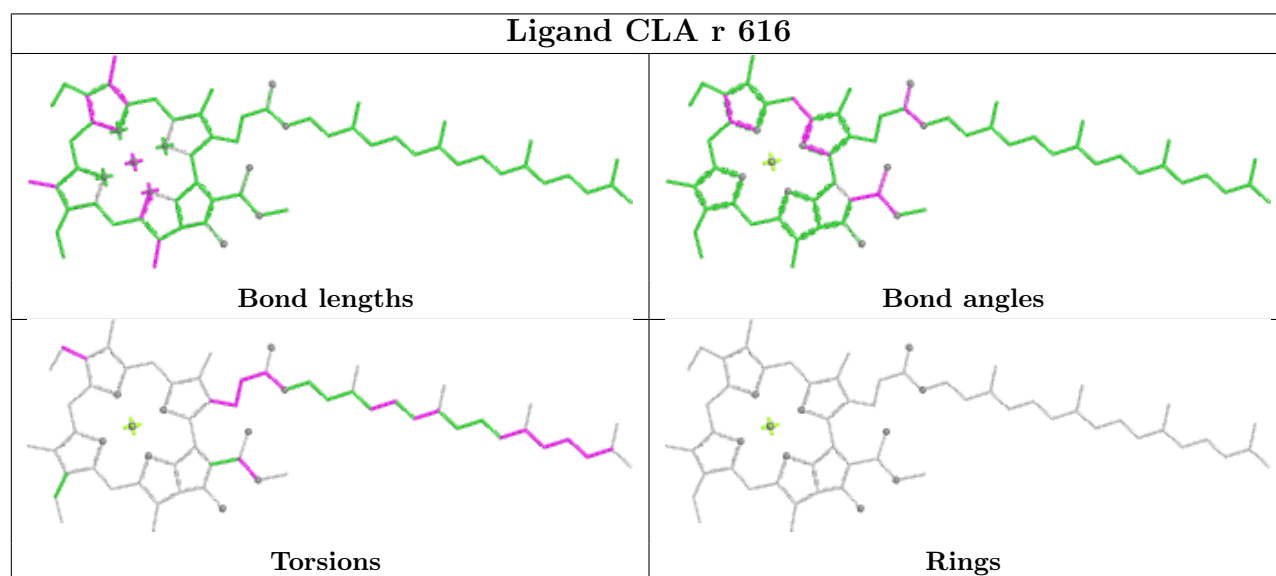
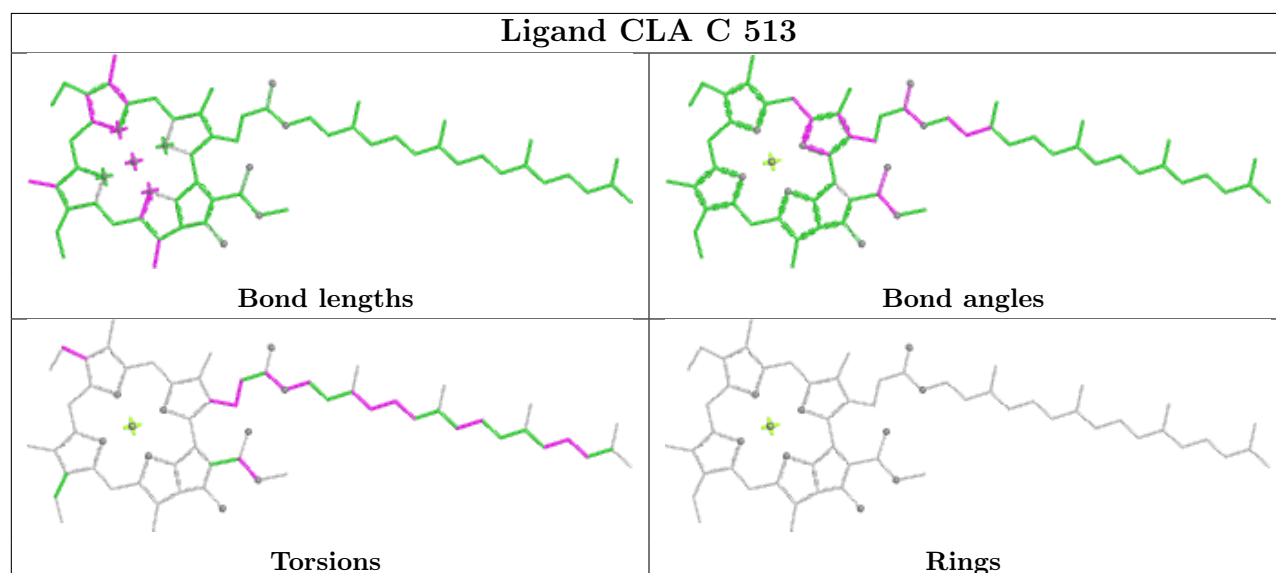
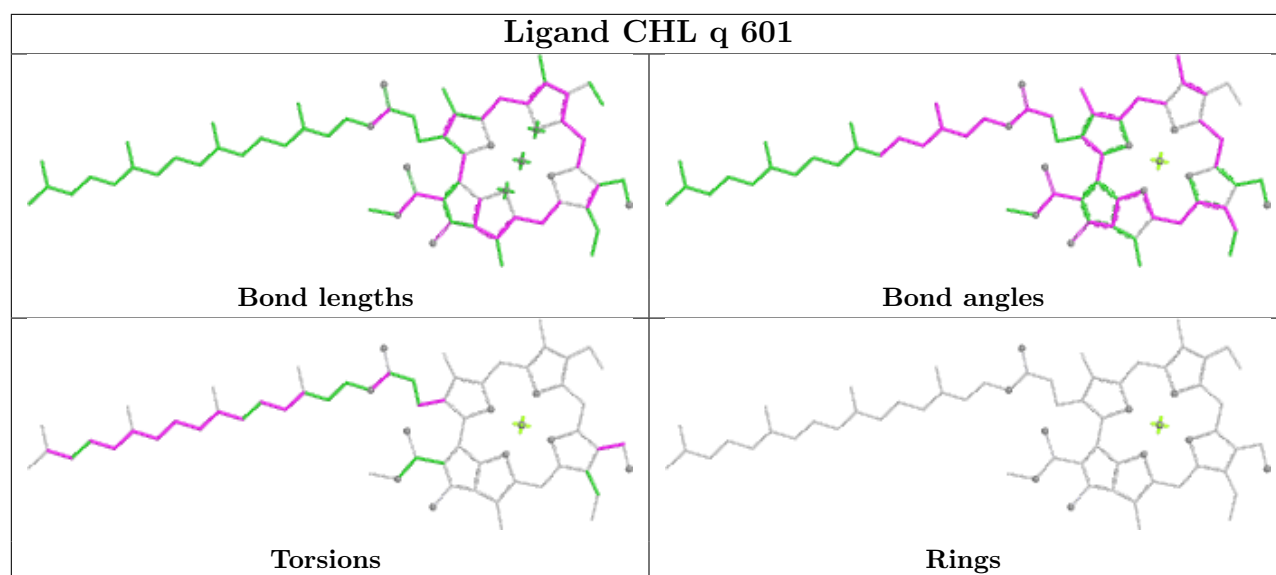


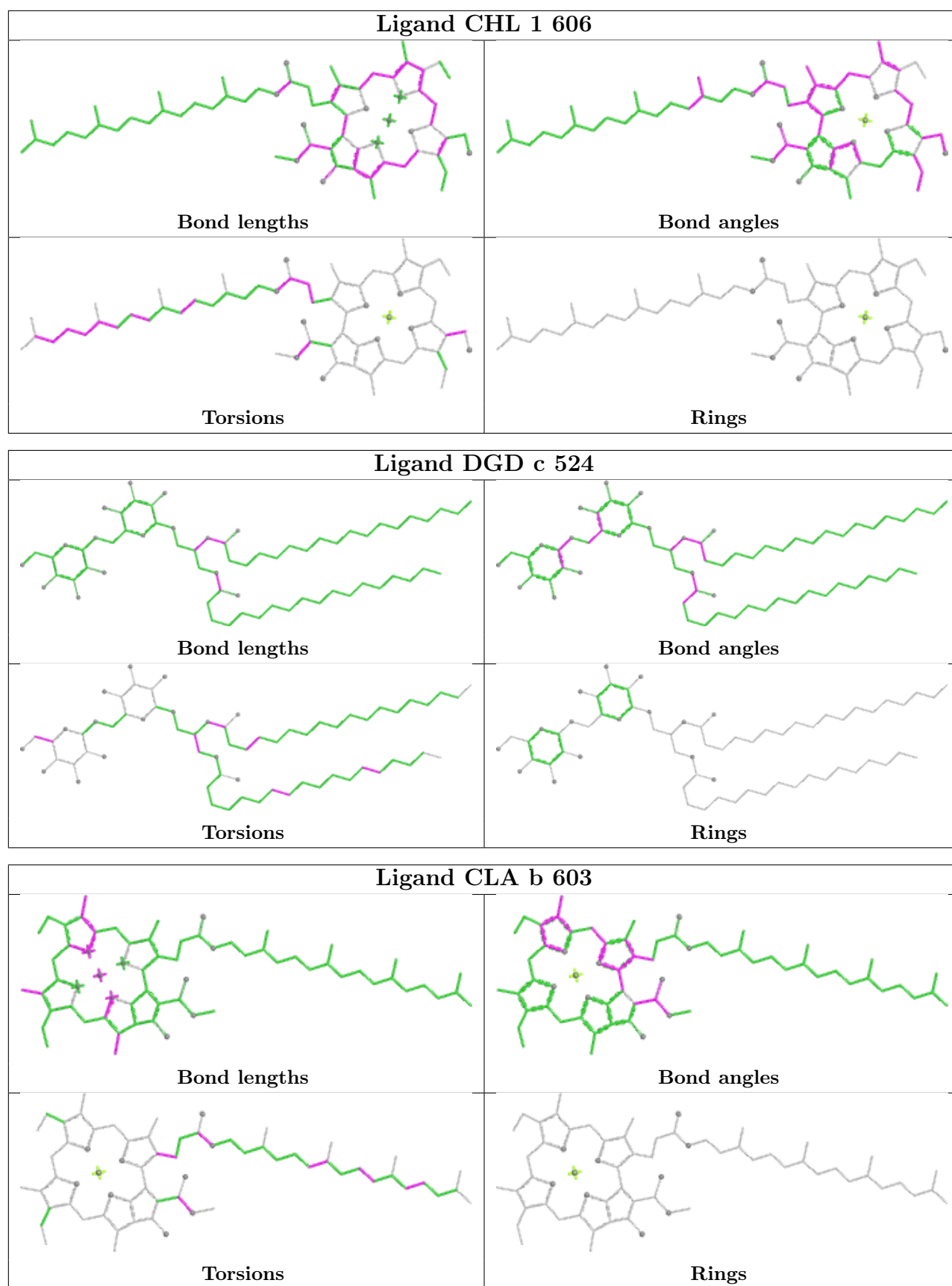


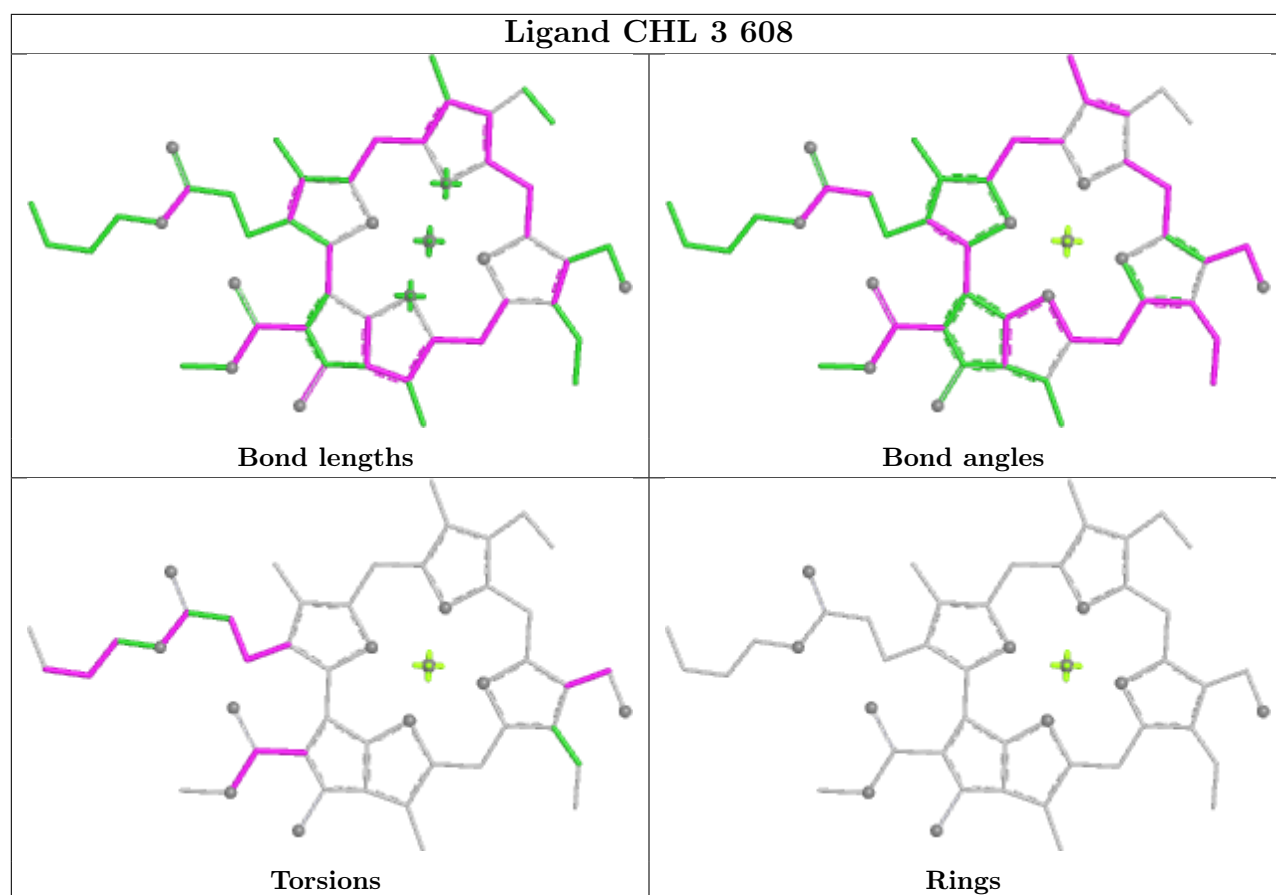




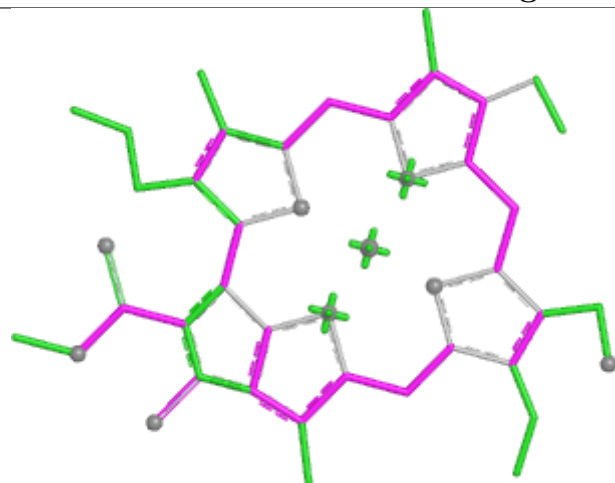




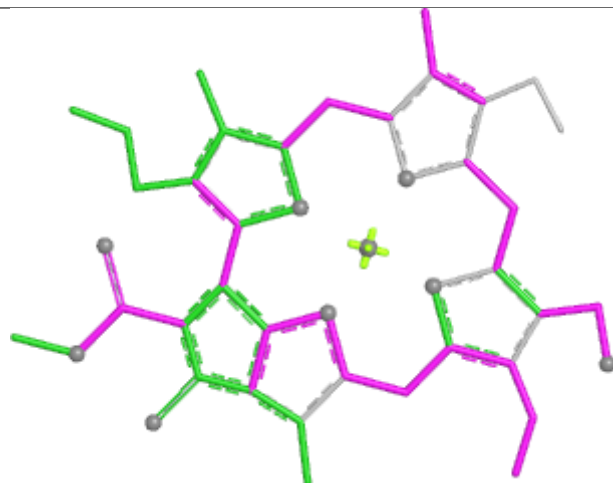




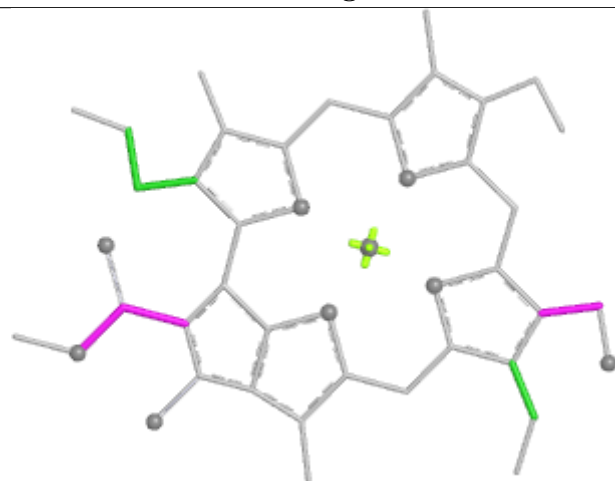
Ligand CHL 4 608



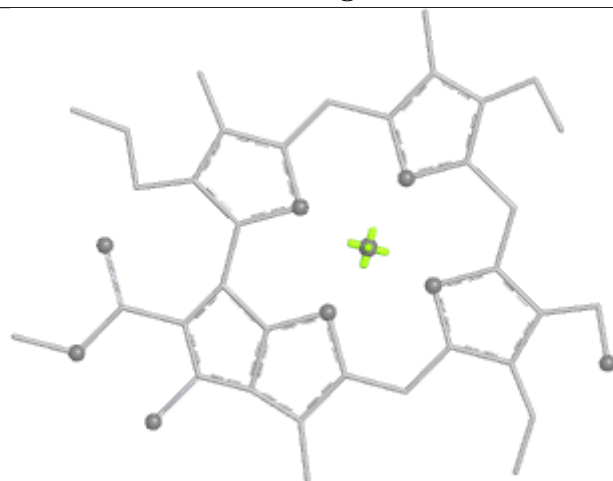
Bond lengths



Bond angles

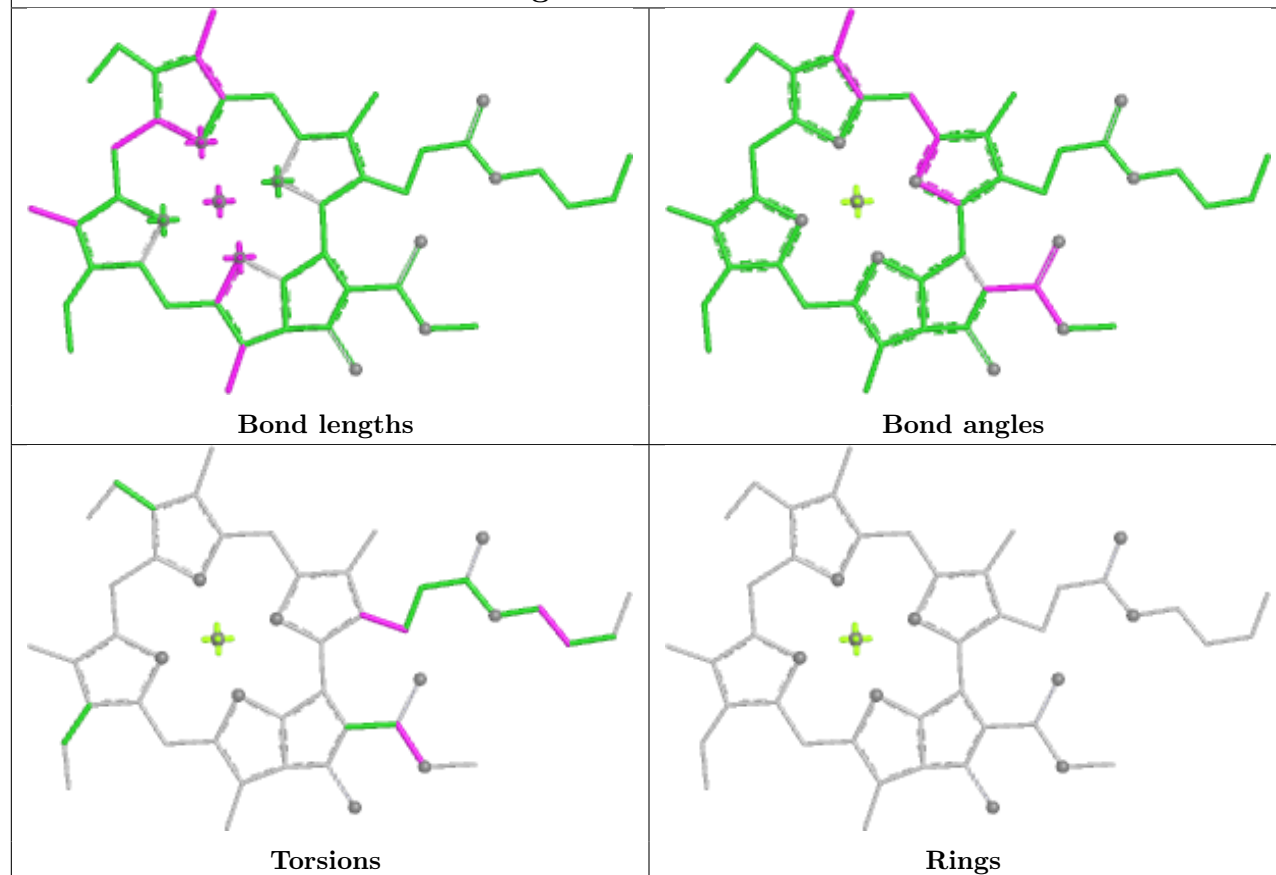


Torsions

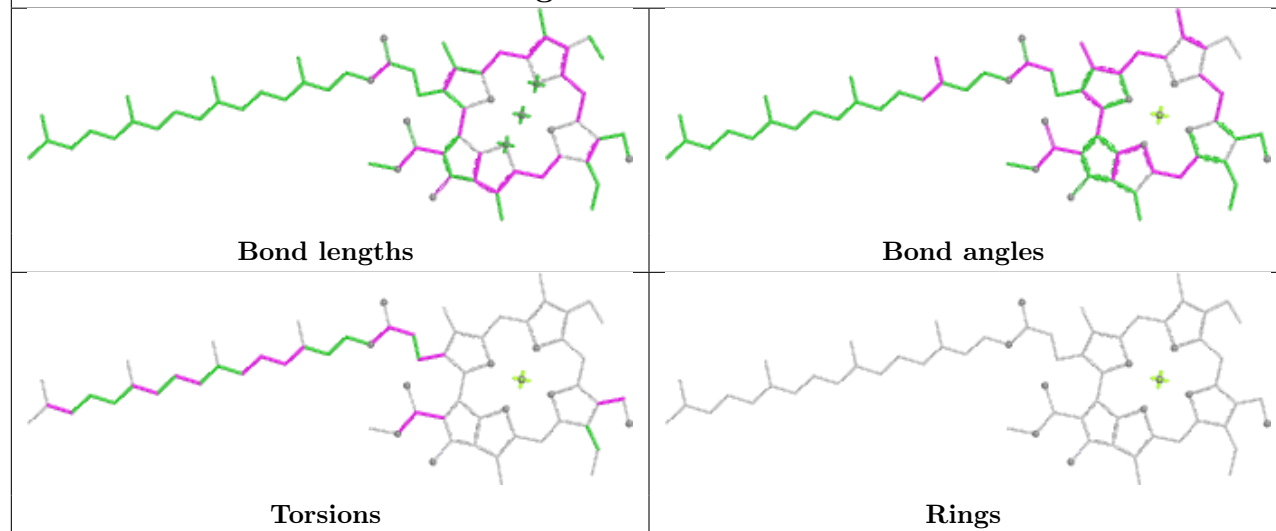


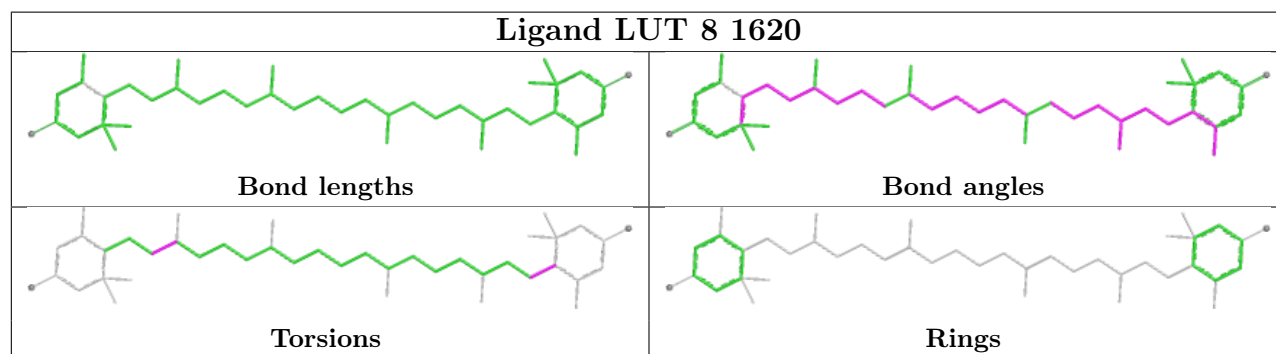
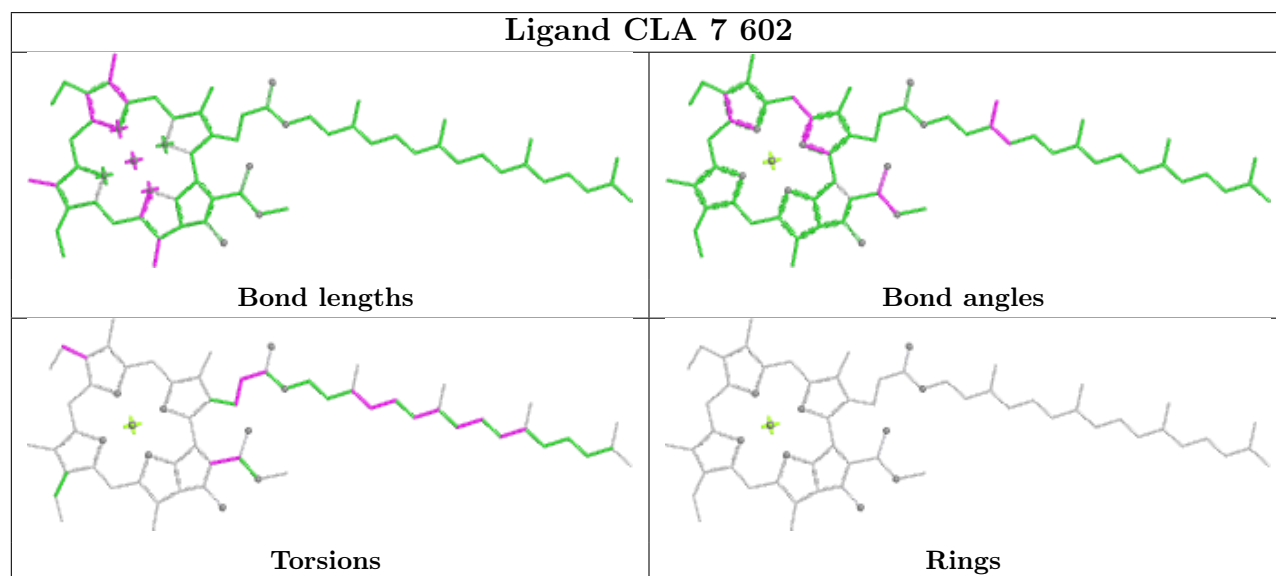
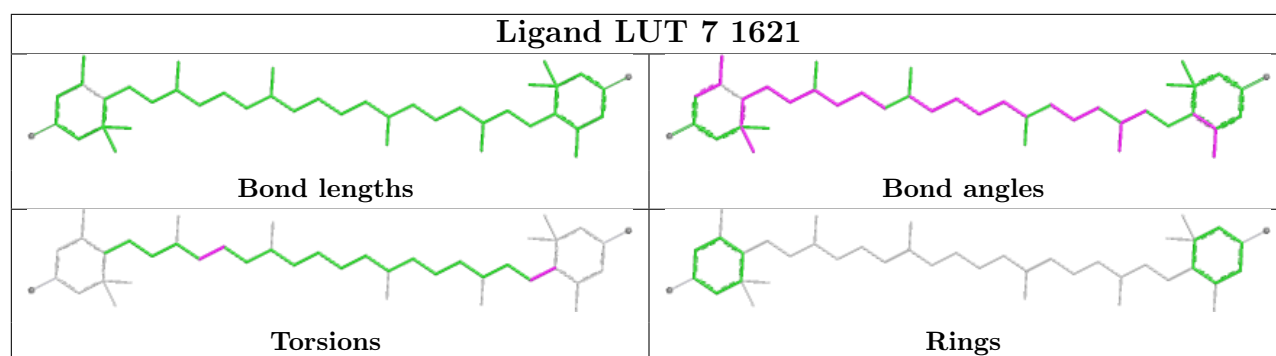
Rings

Ligand CLA A 407

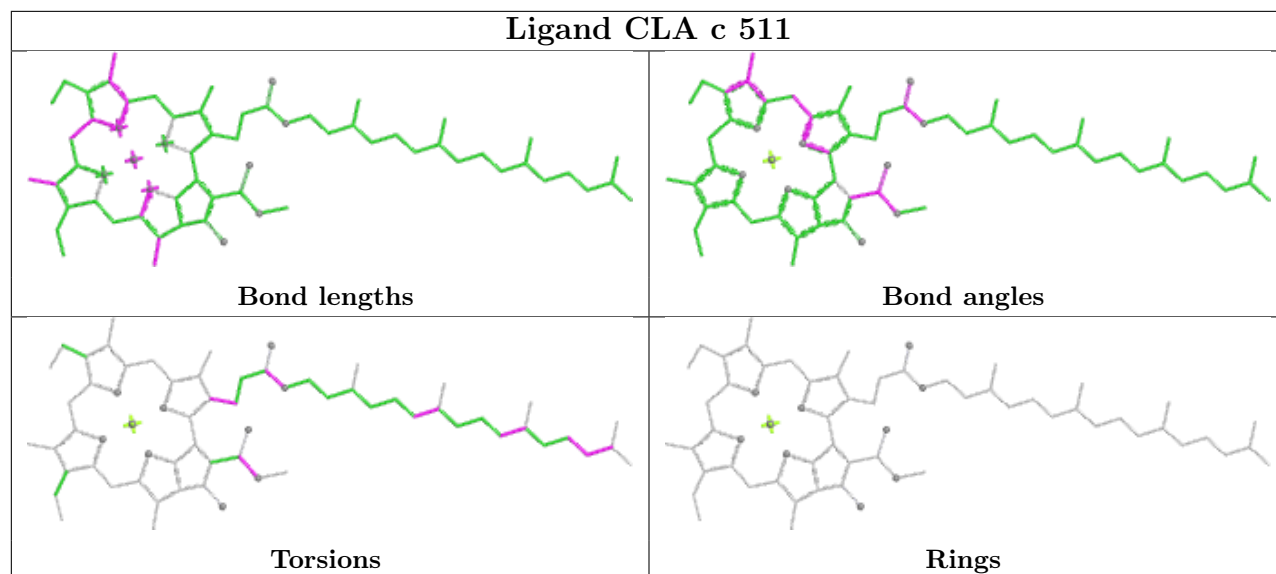


Ligand CHL 5 607

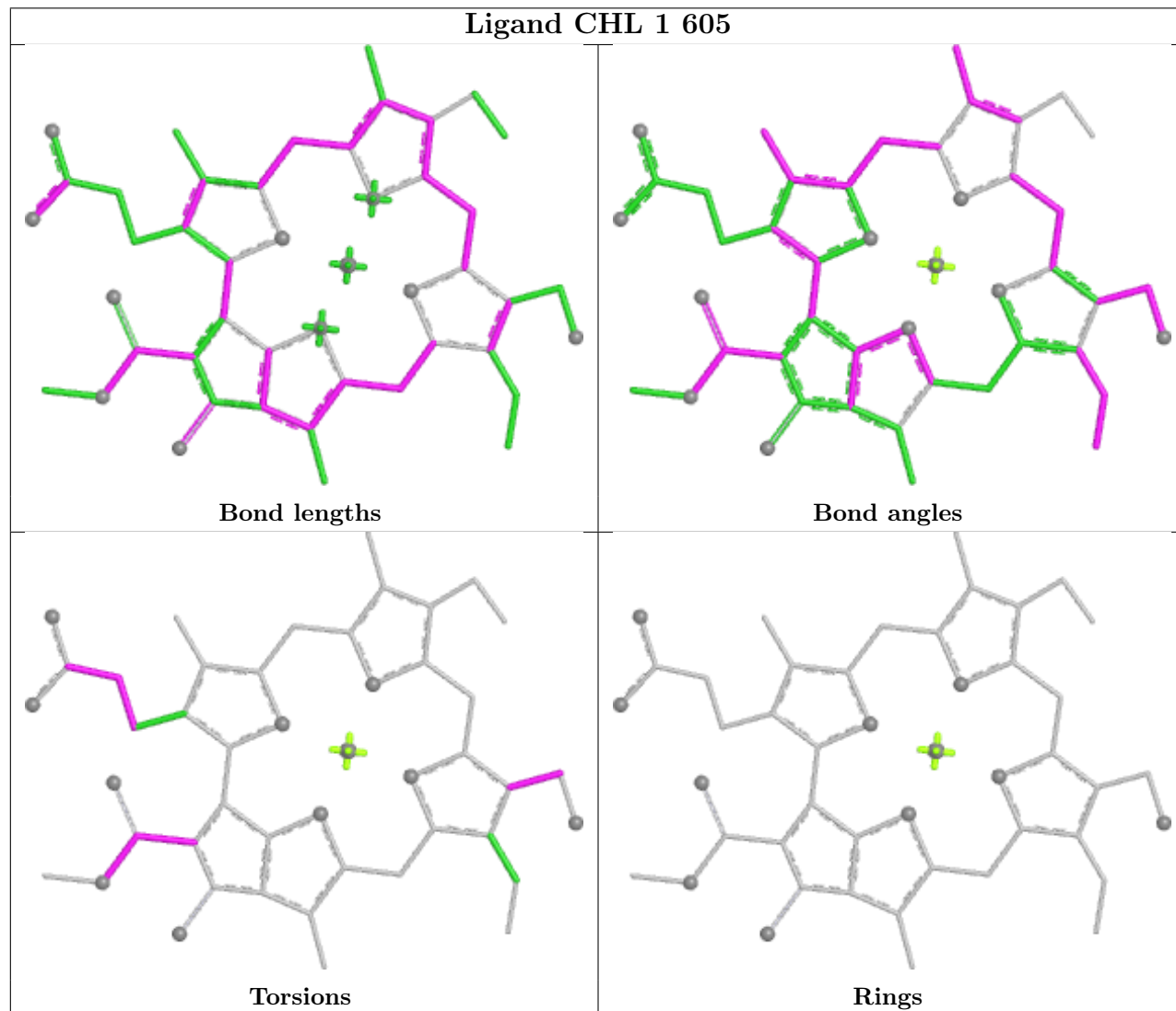


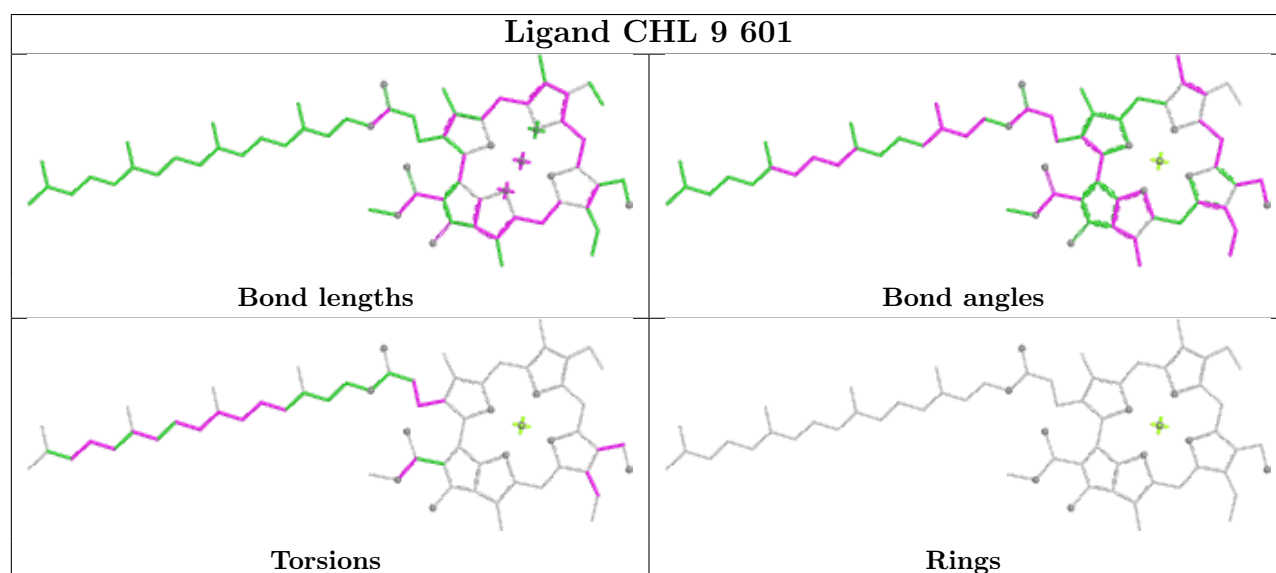
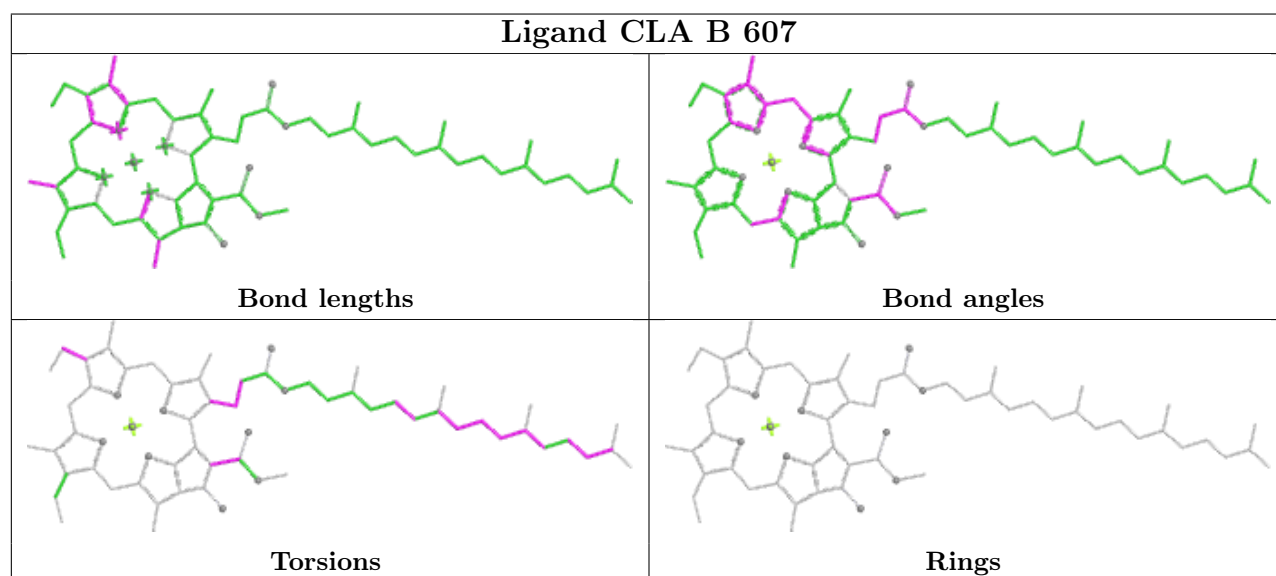
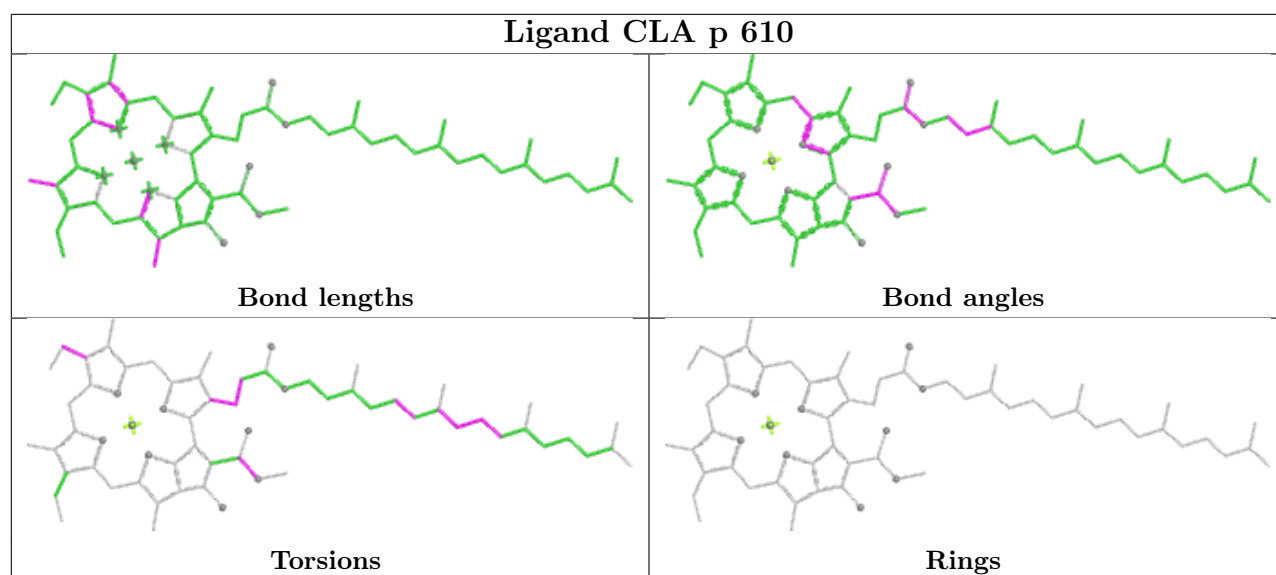


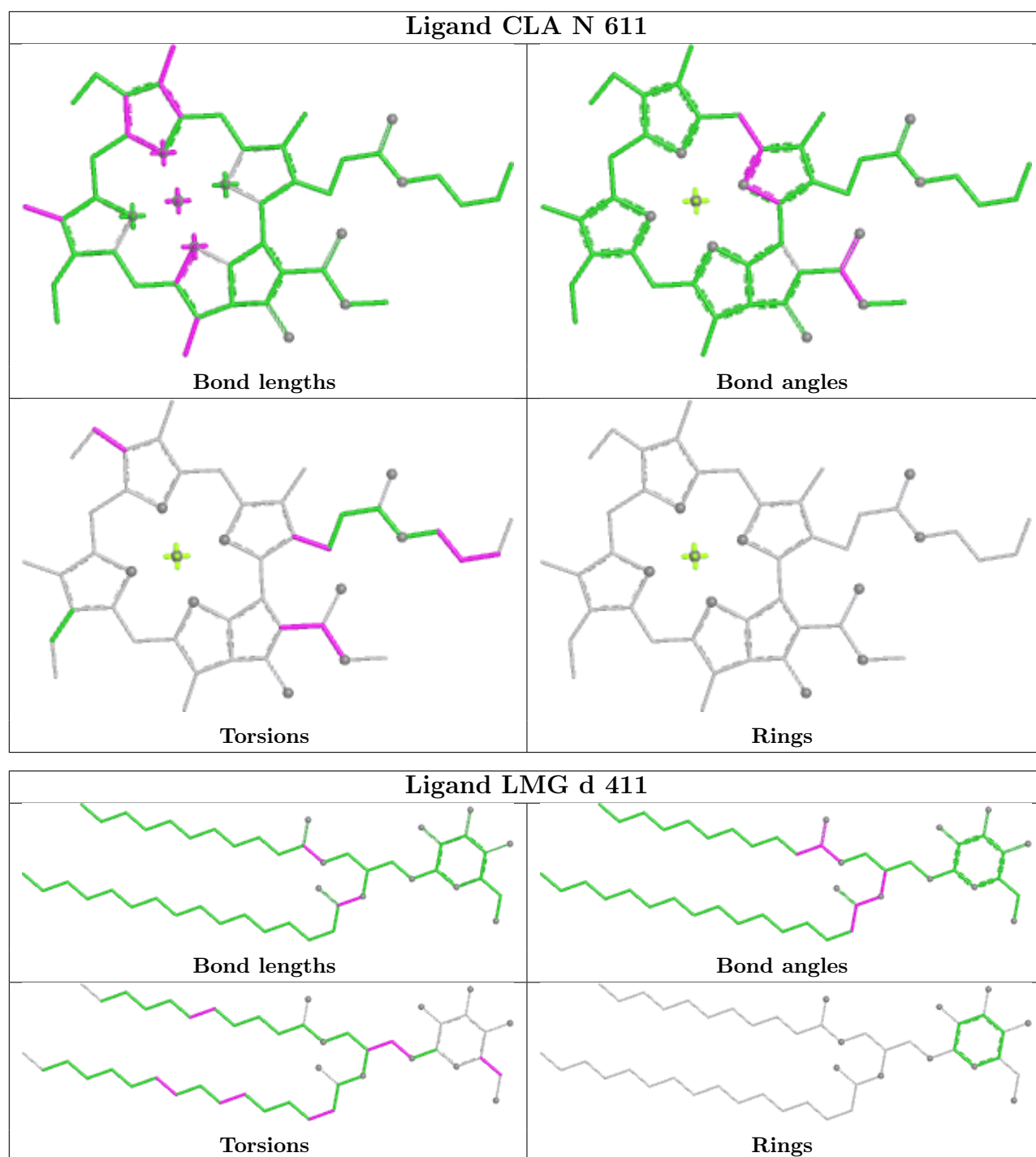
Ligand CLA c 511



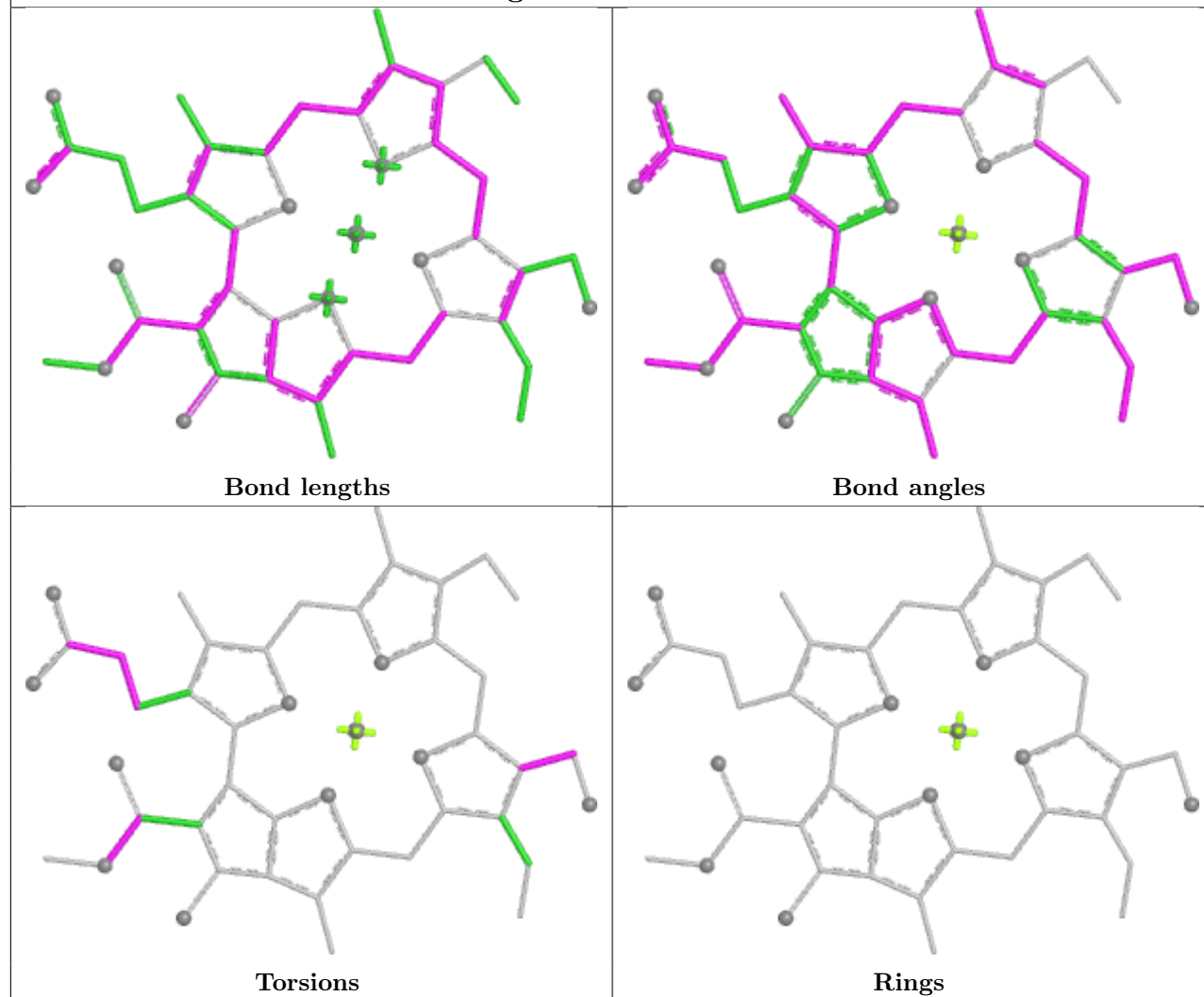
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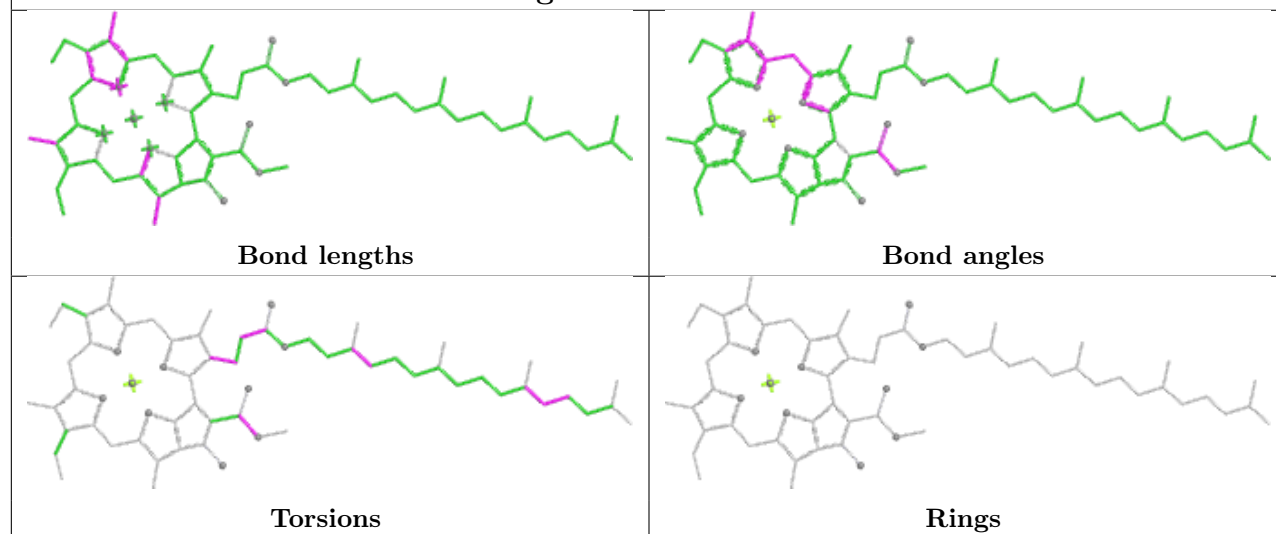




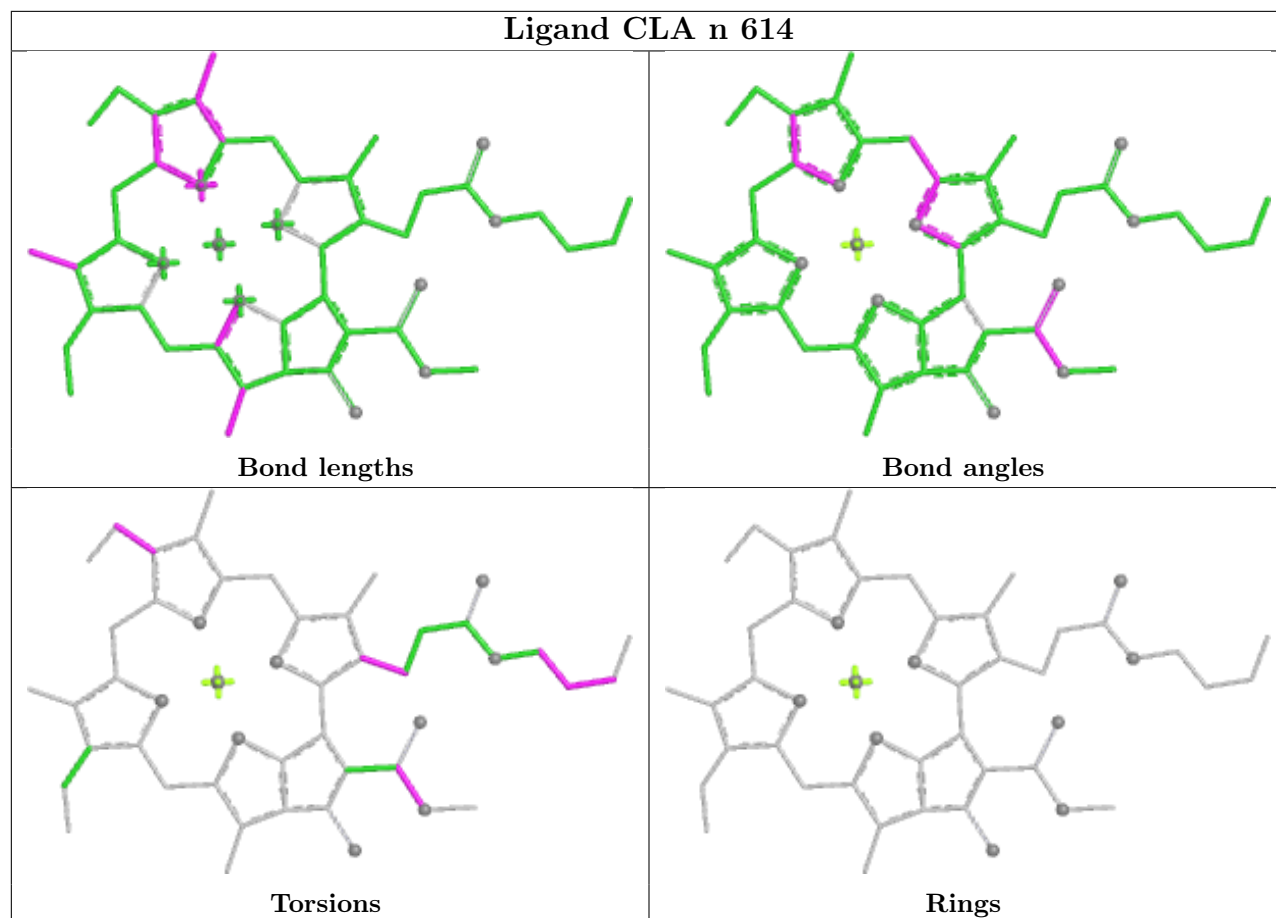
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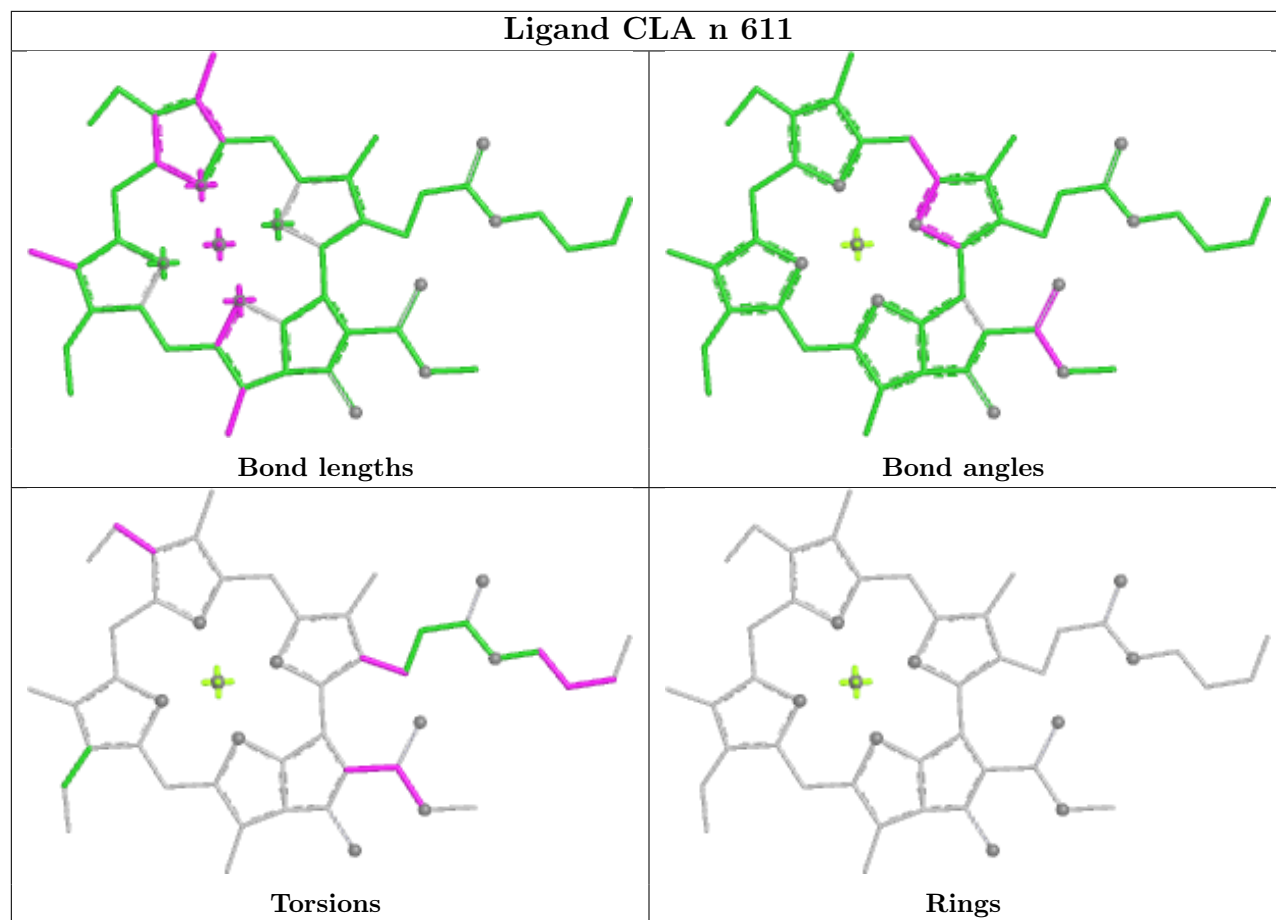
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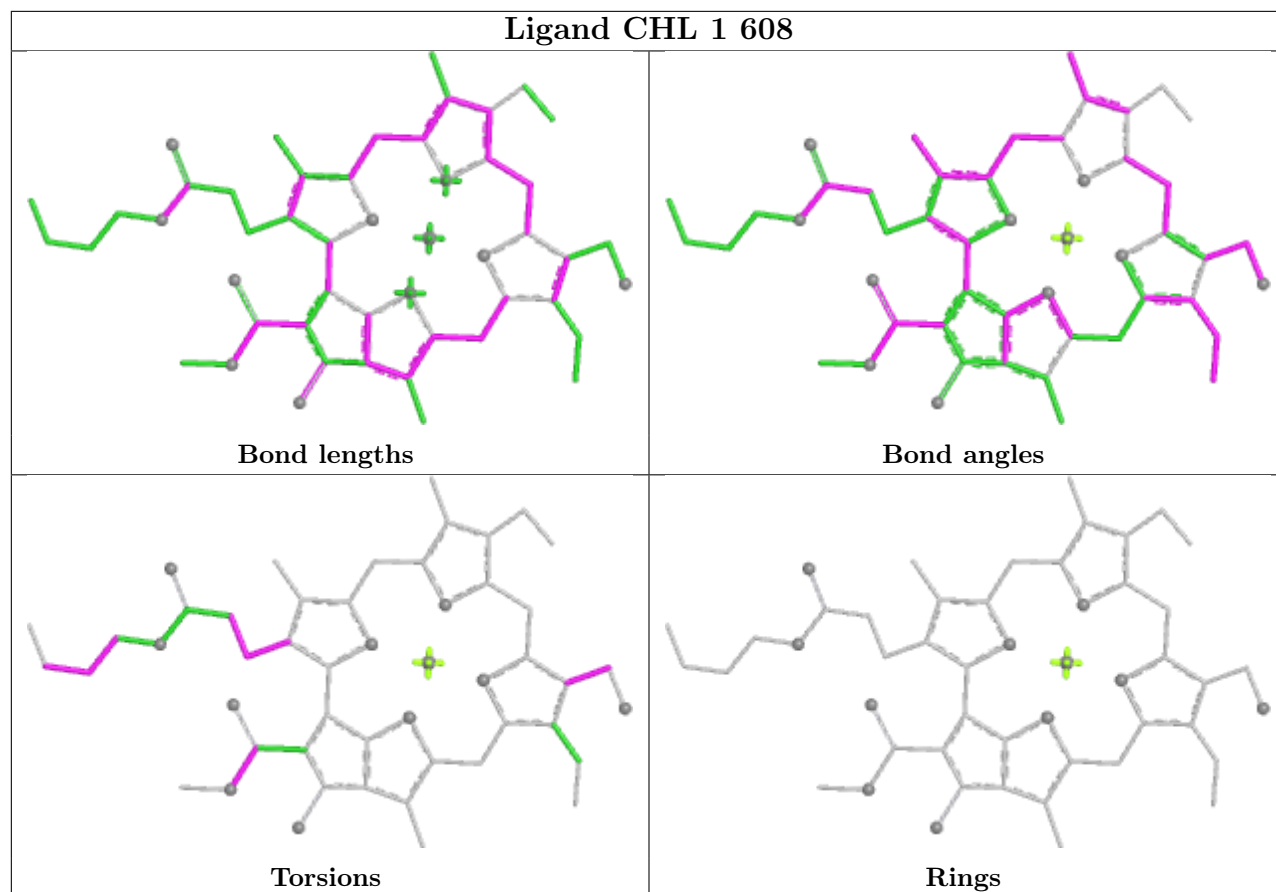
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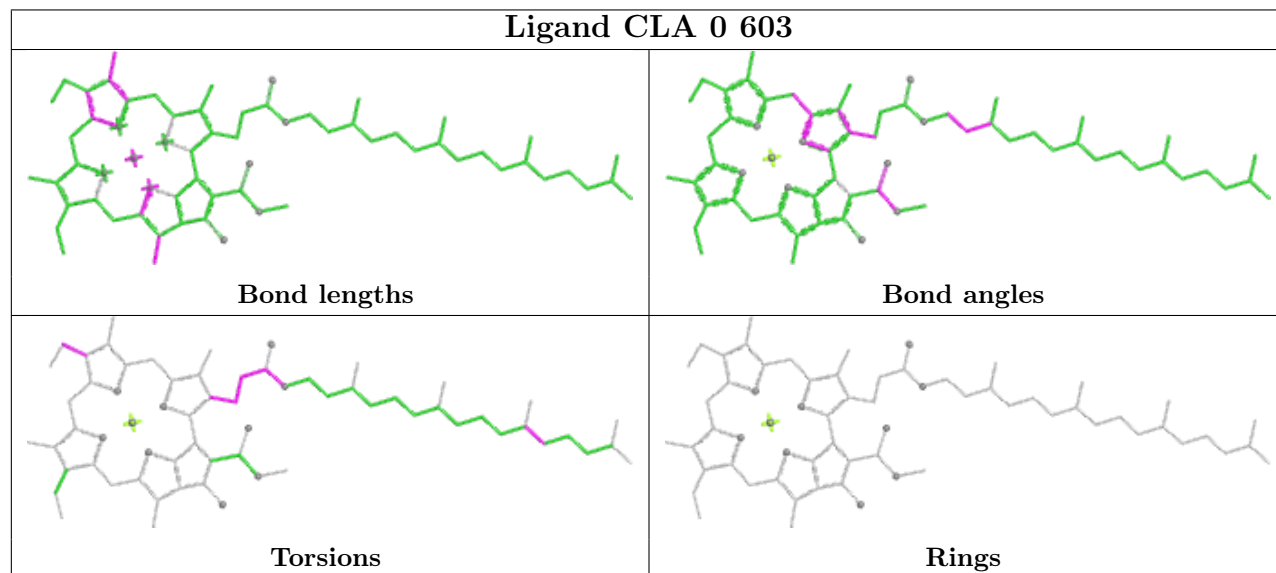
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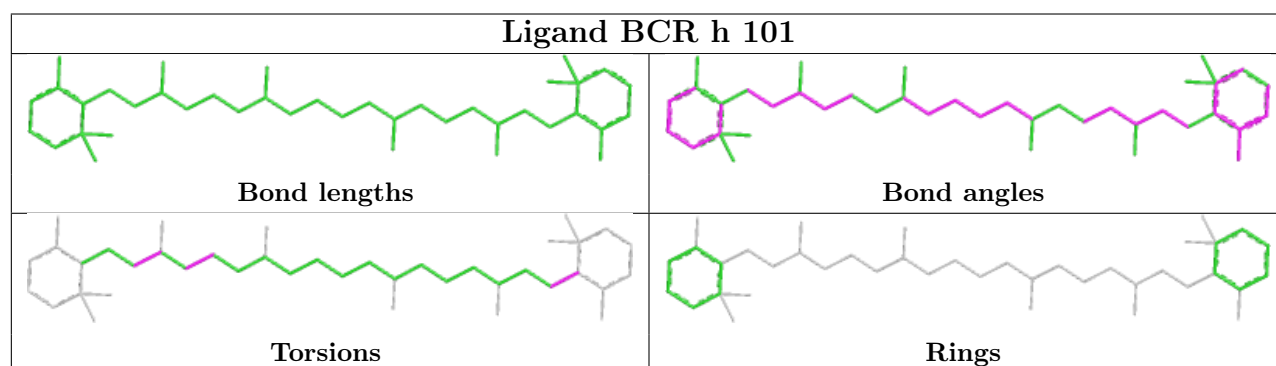
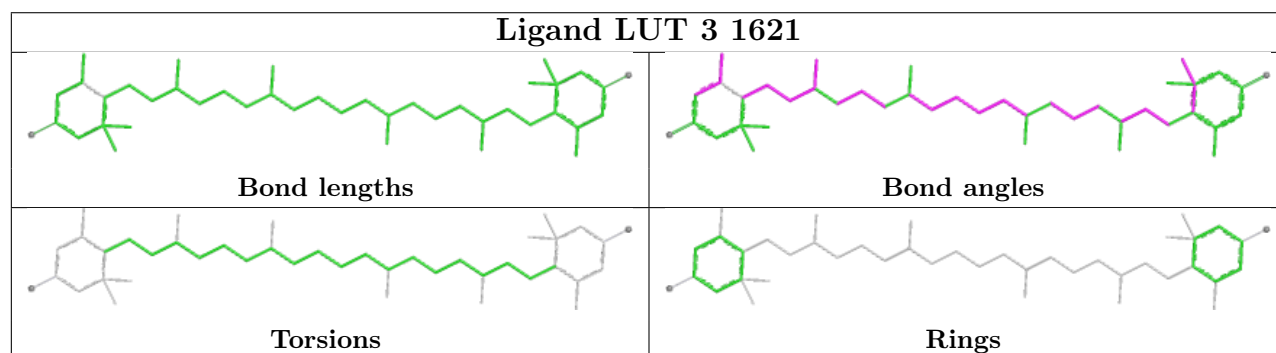
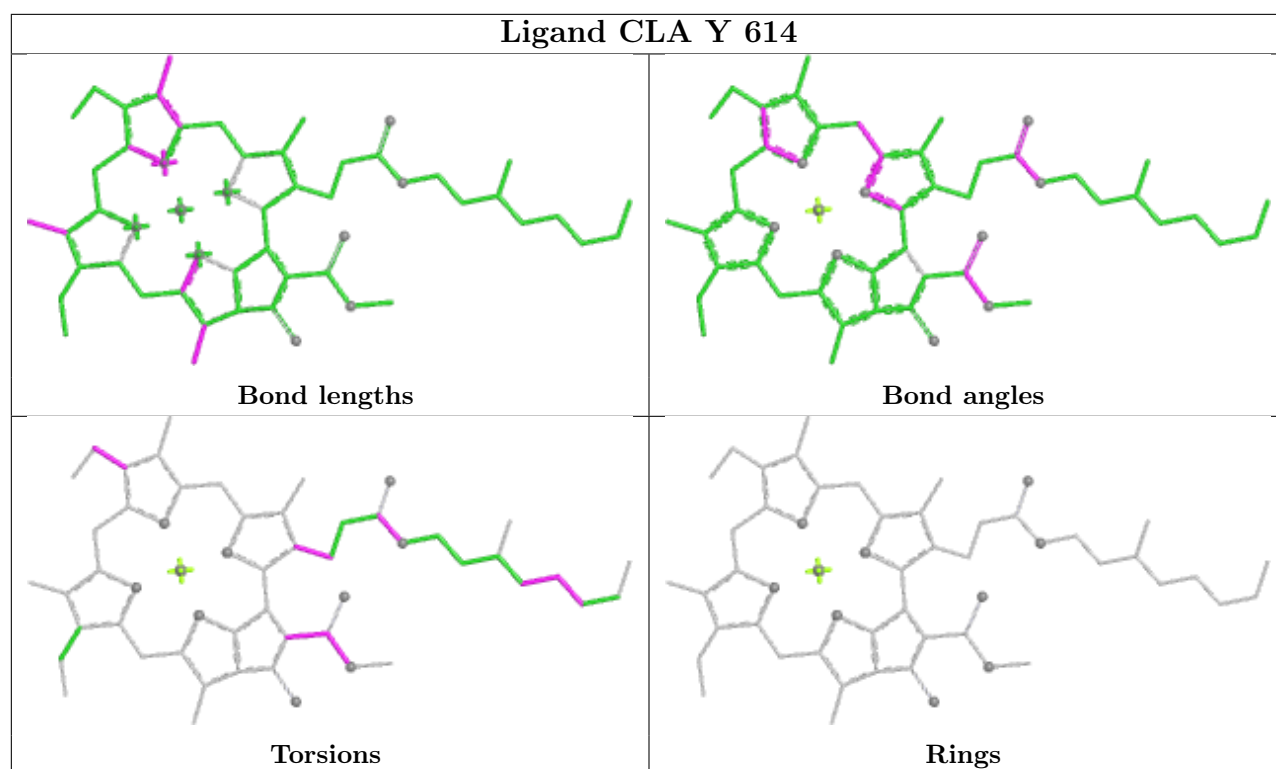


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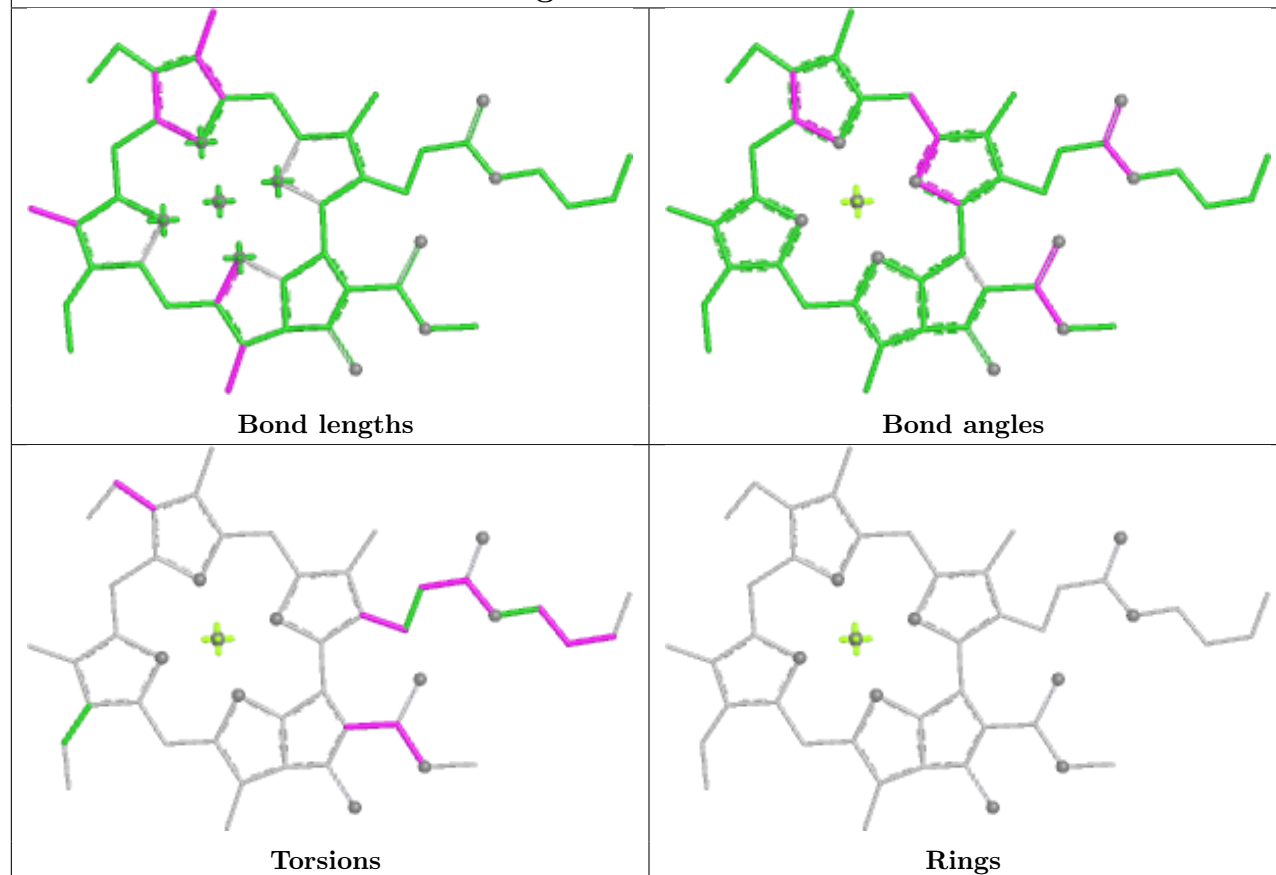


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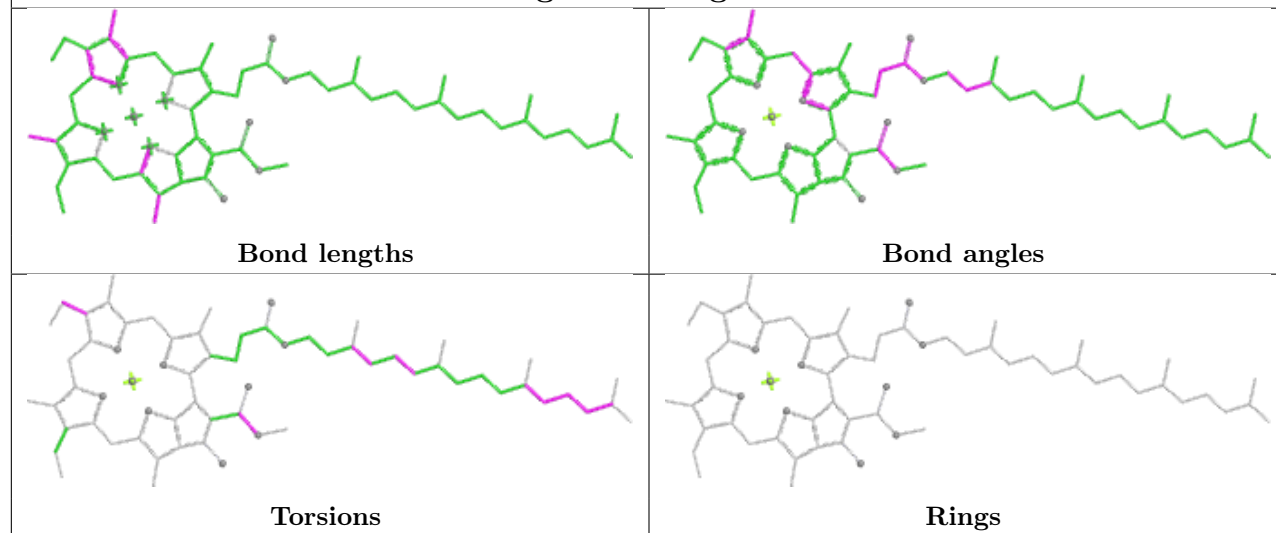


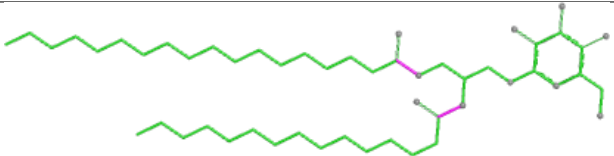
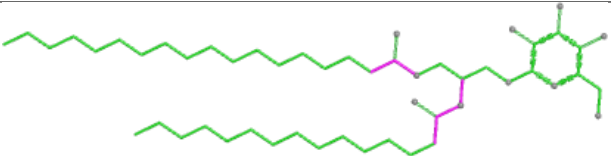
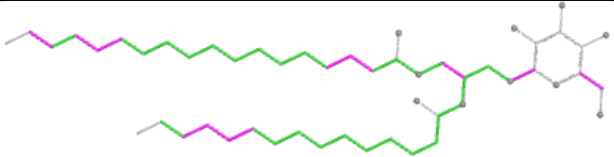
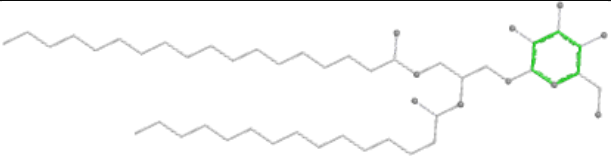


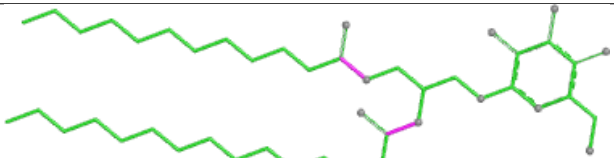
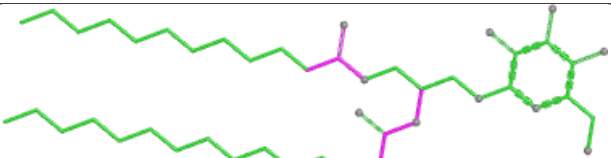
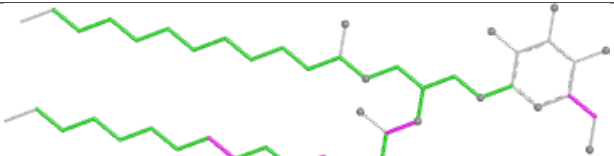
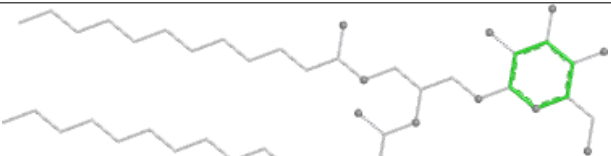
Ligand CLA 4 604

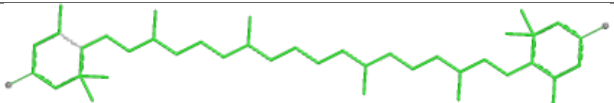
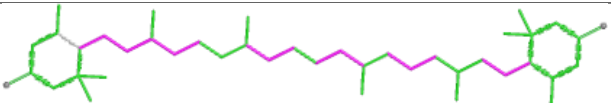
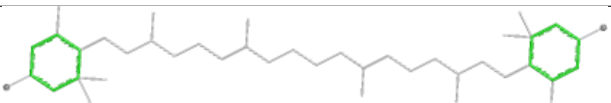


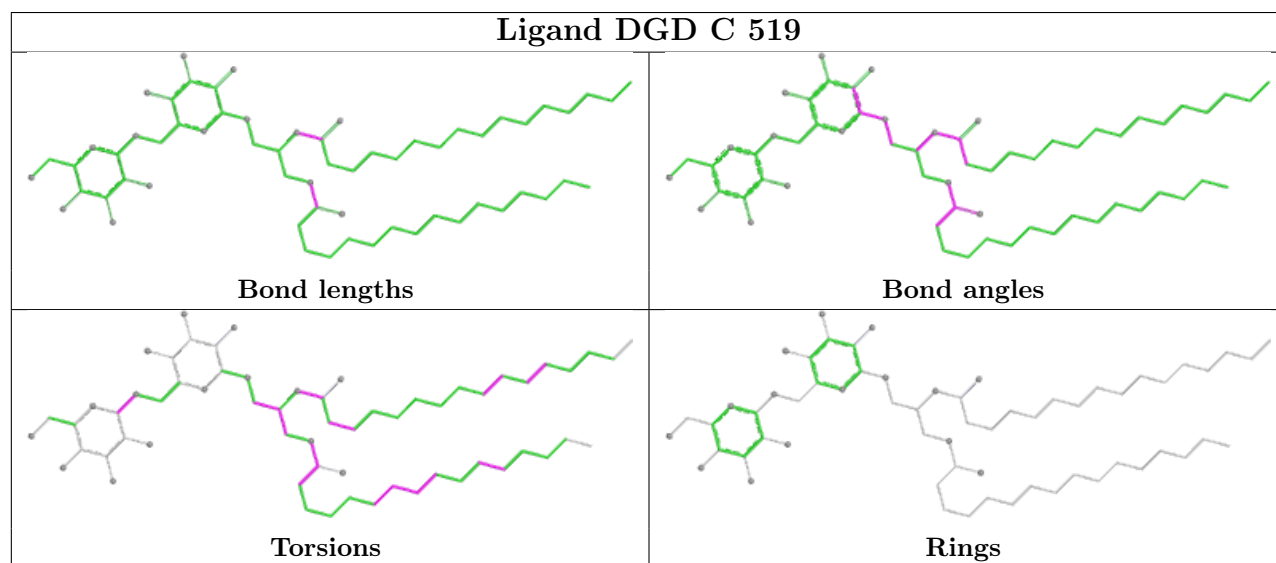
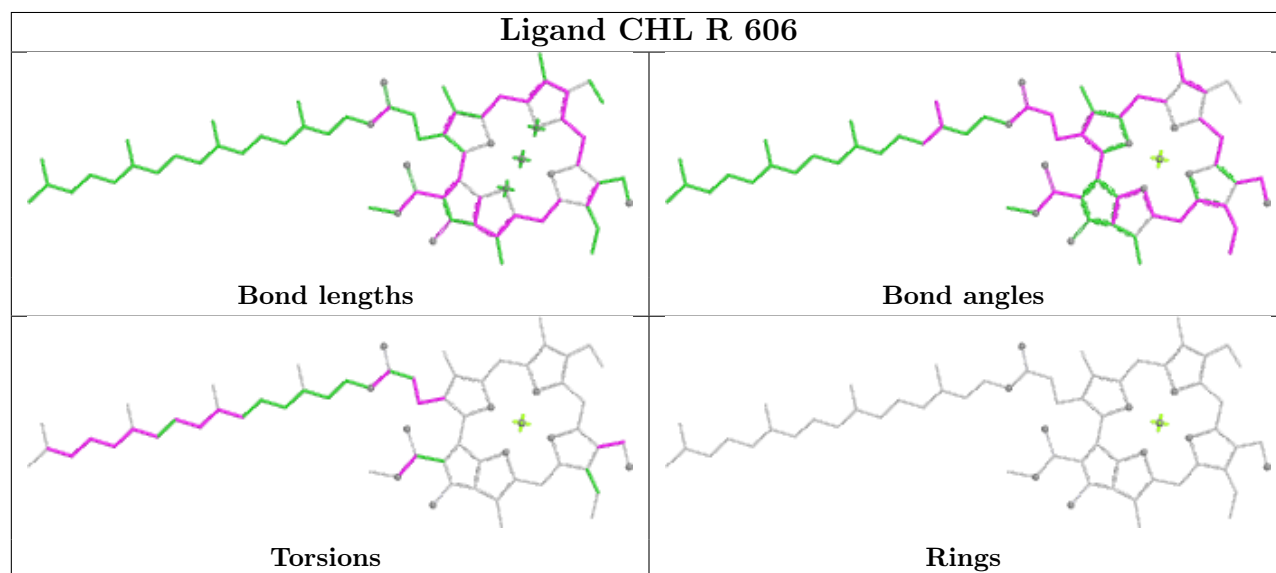
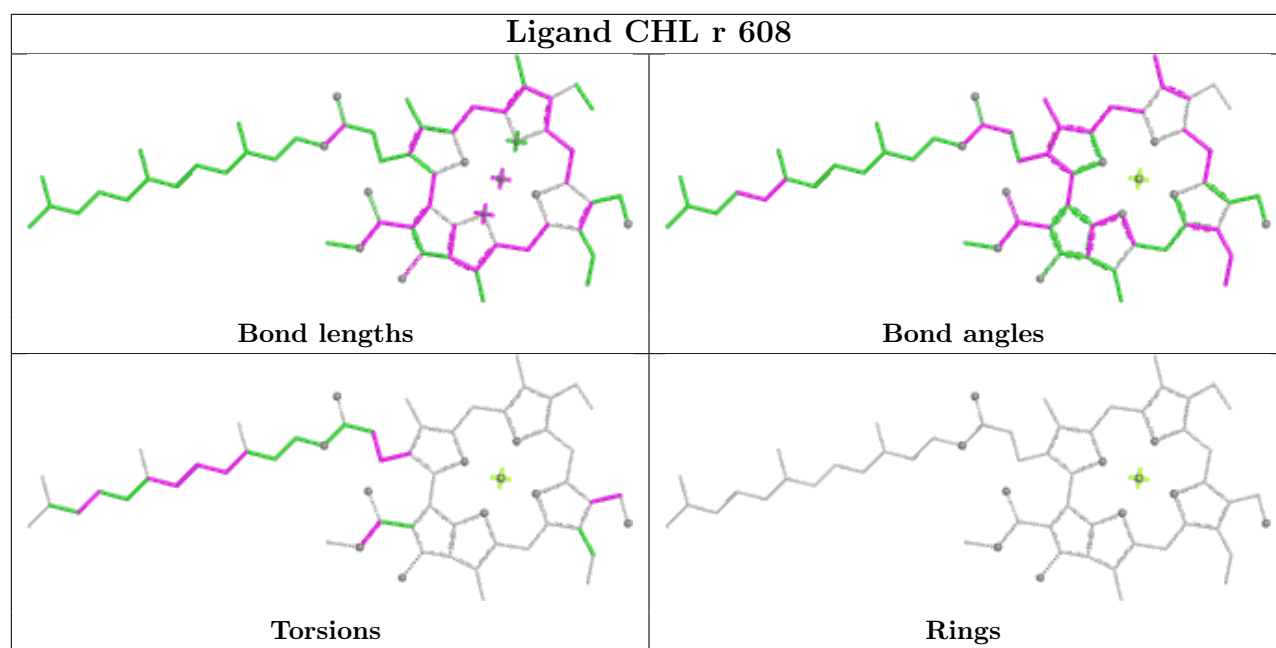
Ligand CLA g 610

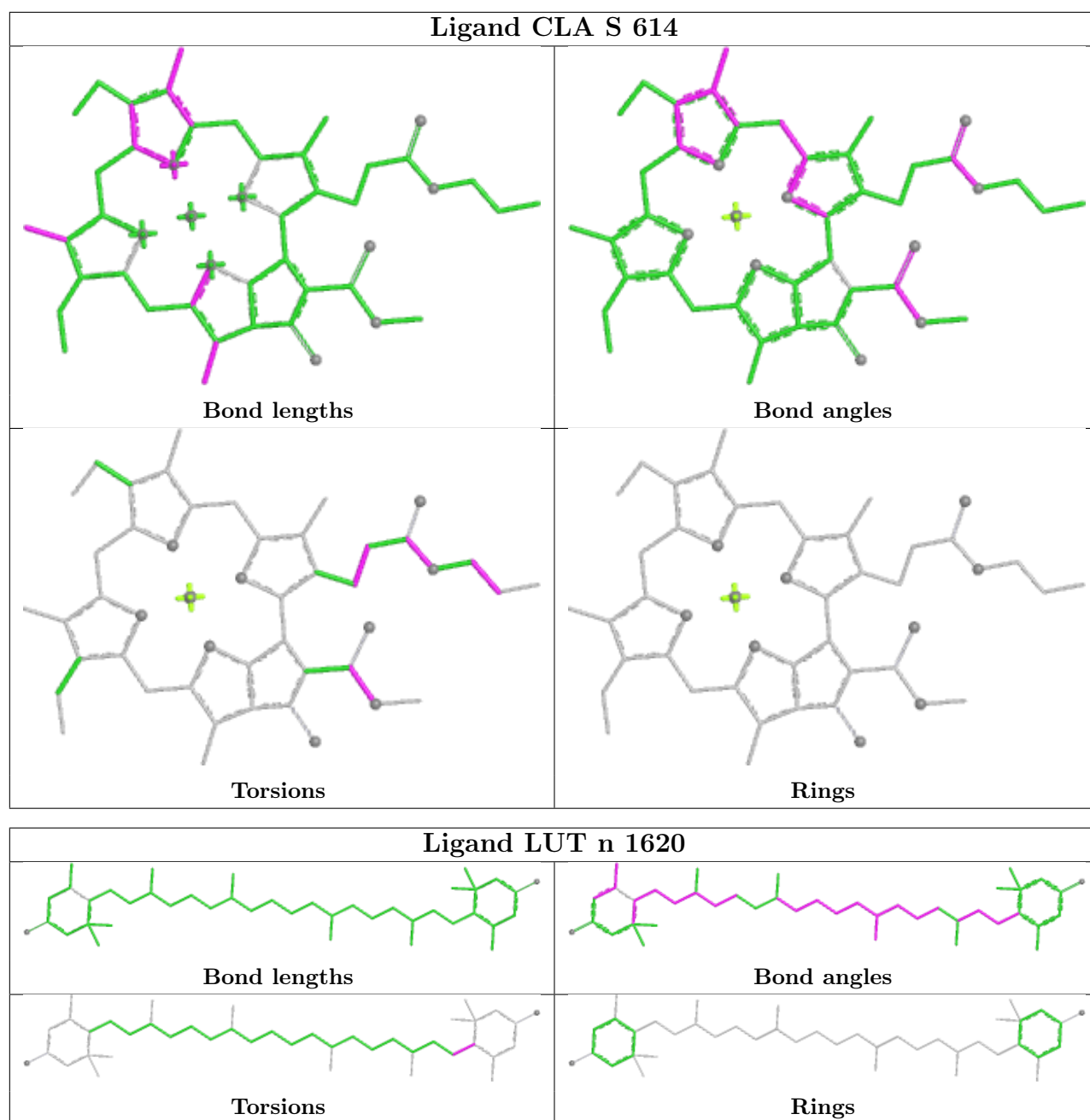


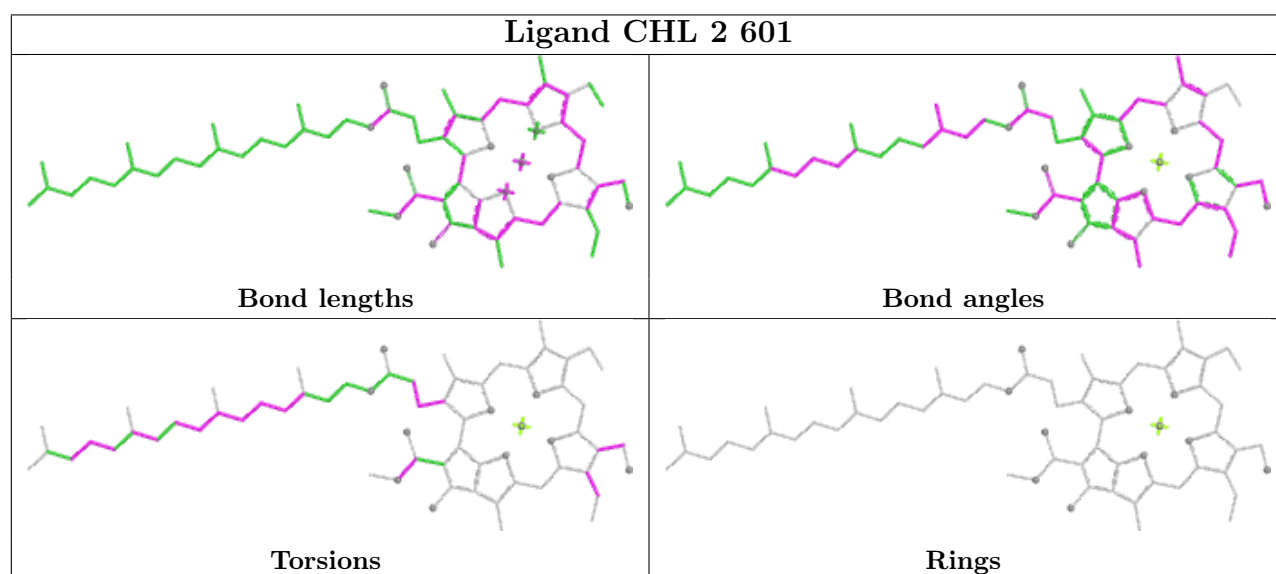
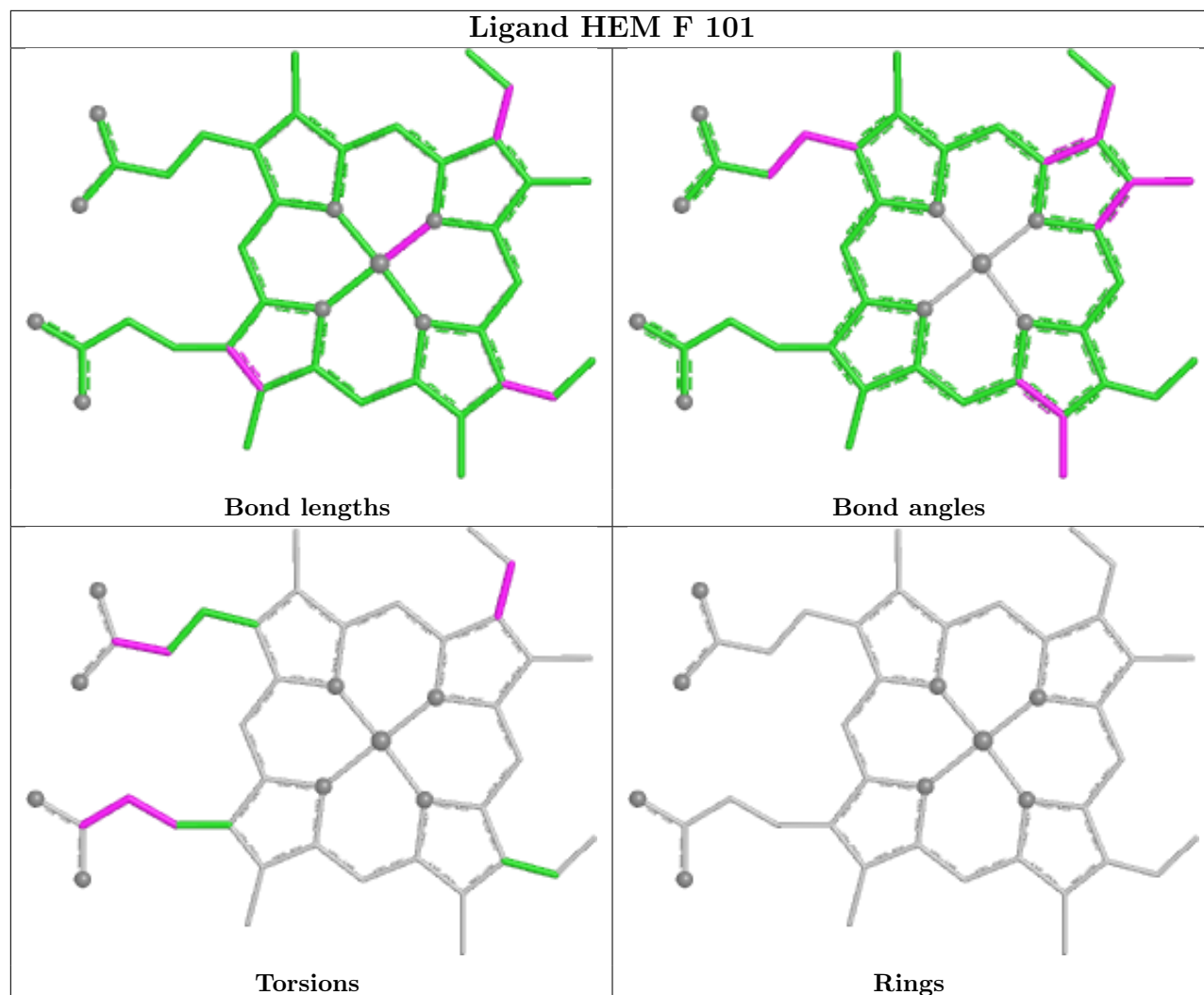
Ligand LMG S 2631	
 Bond lengths	 Bond angles
 Torsions	 Rings

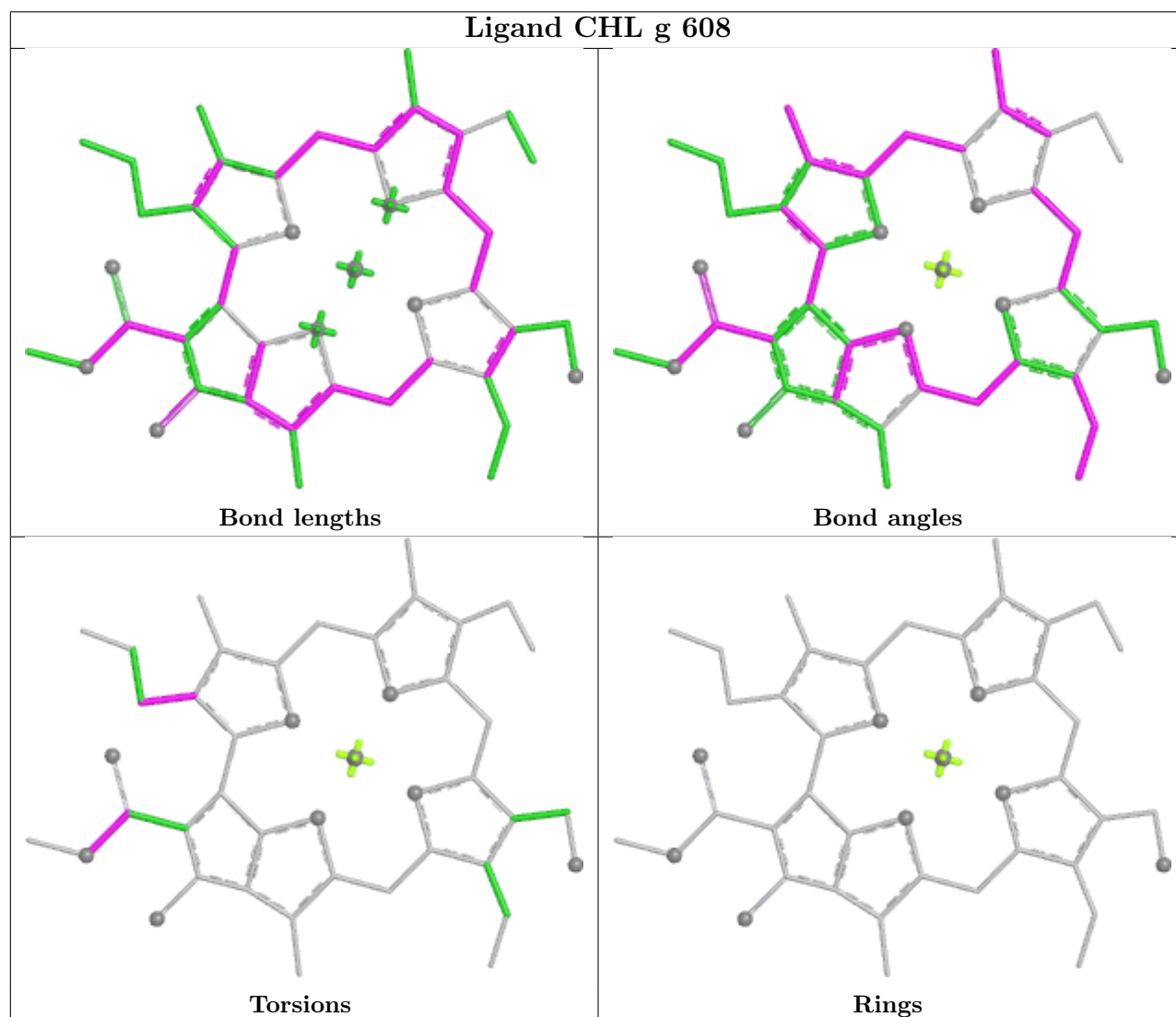
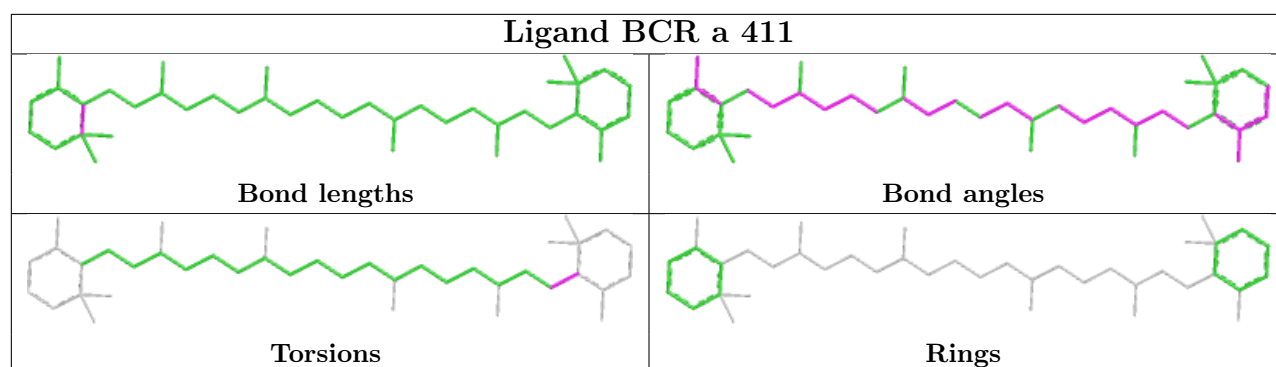
Ligand LMG D 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

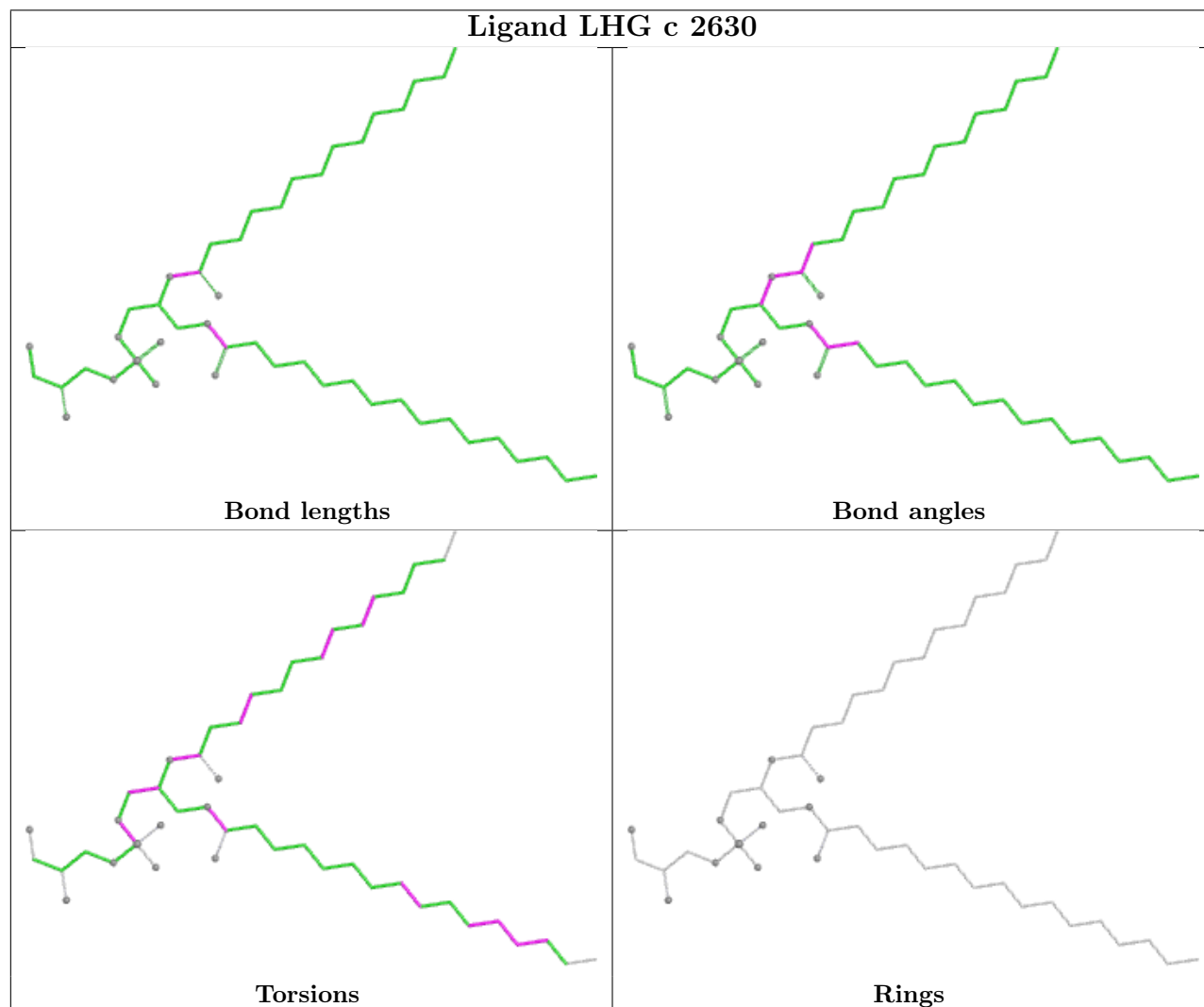
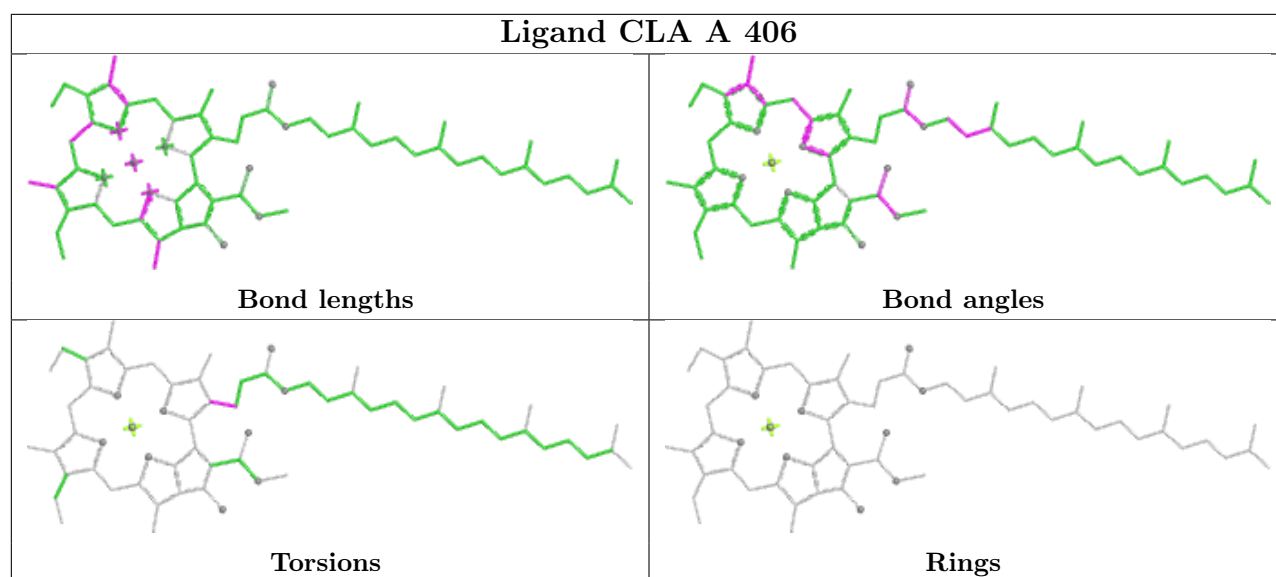
Ligand LUT G 1620	
 Bond lengths	 Bond angles
 Torsions	 Rings

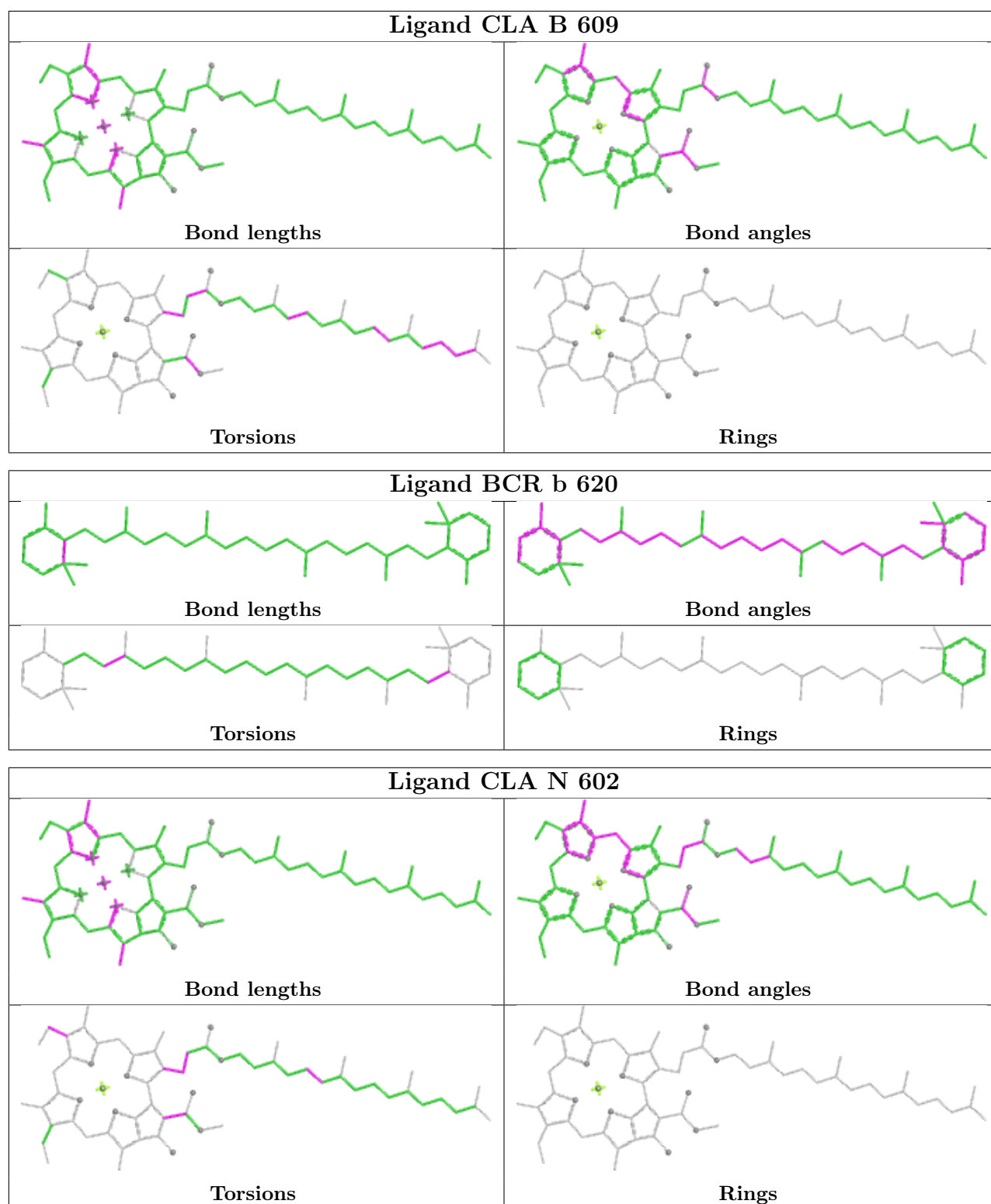




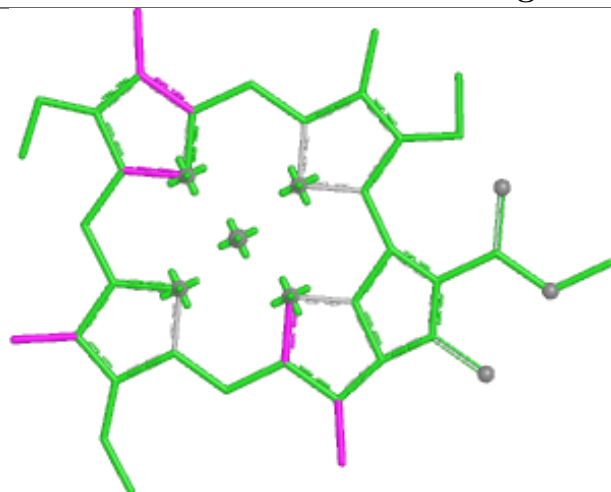




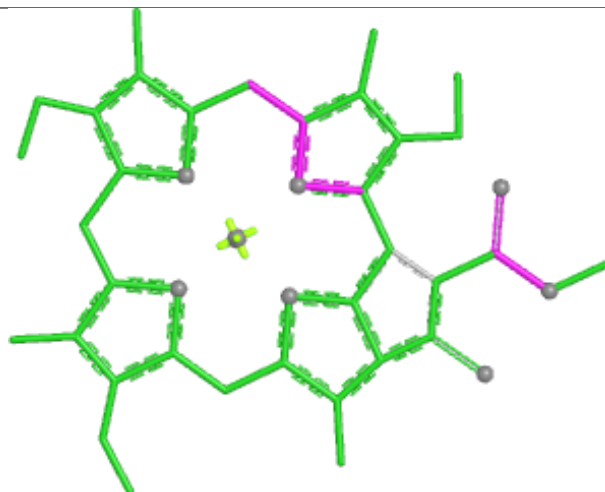




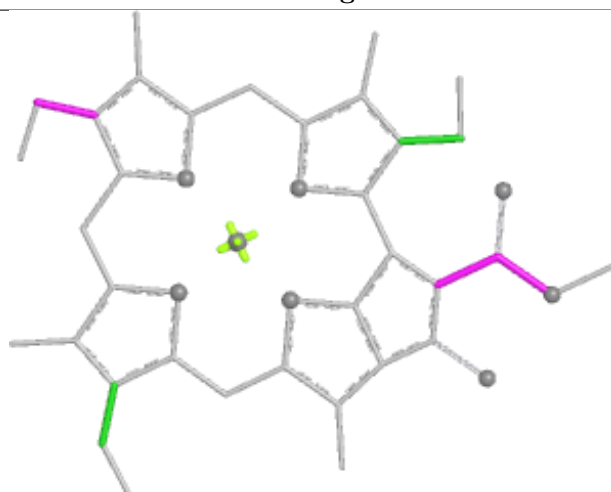
Ligand CLA S 603



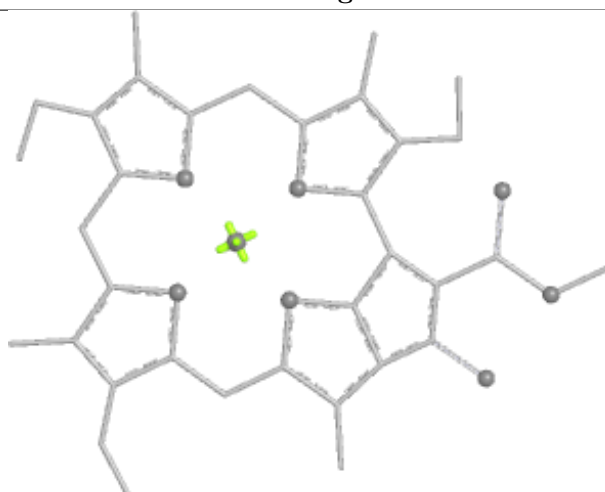
Bond lengths



Bond angles

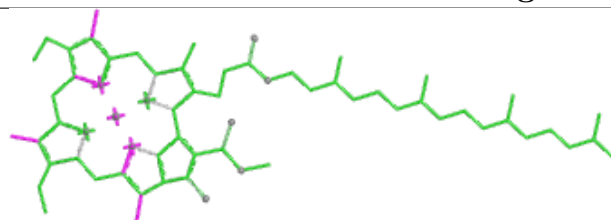


Torsions

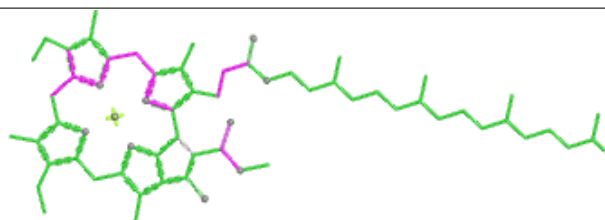


Rings

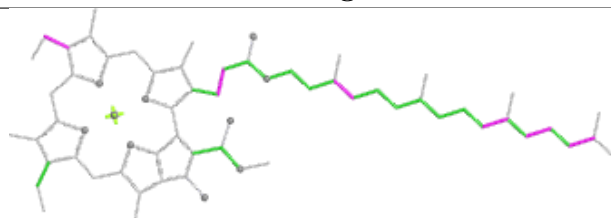
Ligand CLA b 604



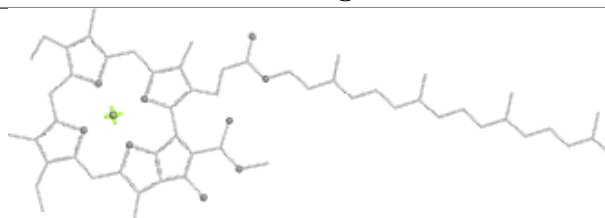
Bond lengths



Bond angles

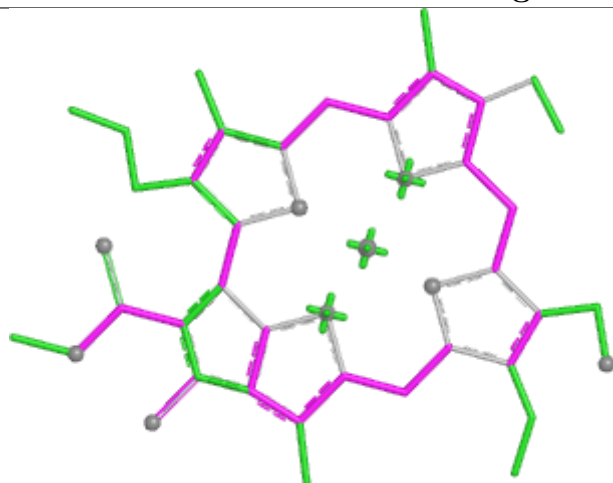


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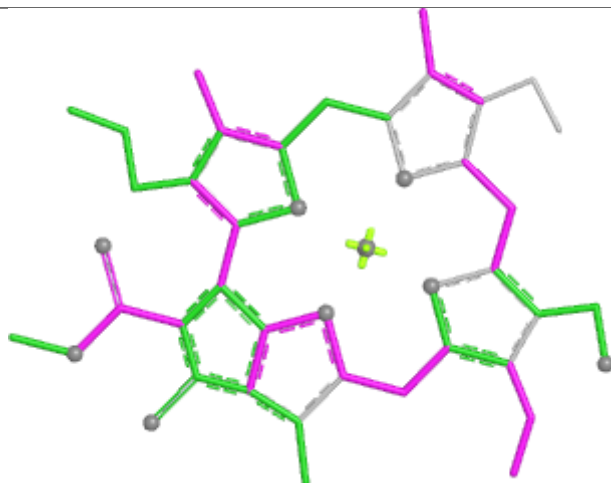


Rings

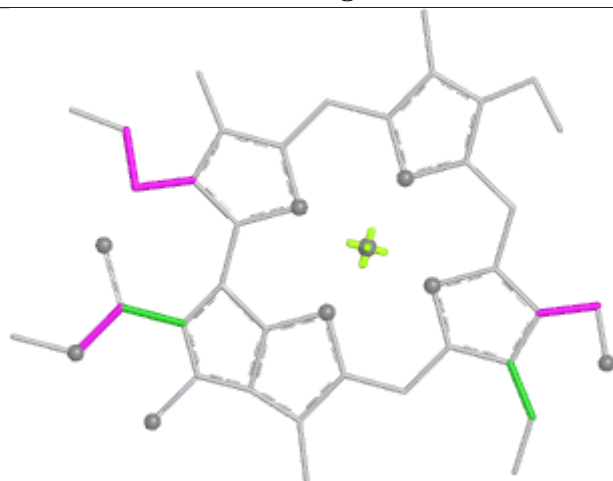
Ligand CHL G 608



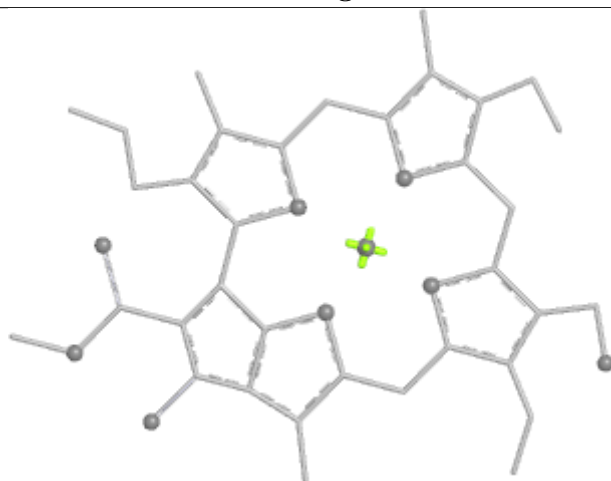
Bond lengths



Bond angles

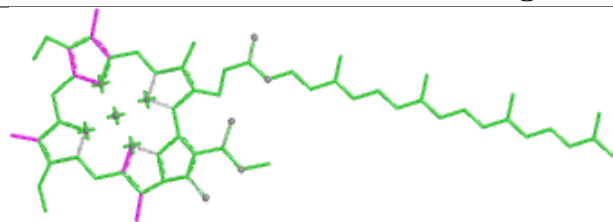


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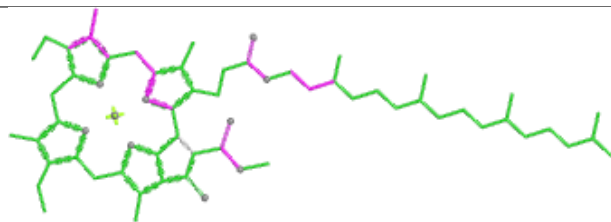


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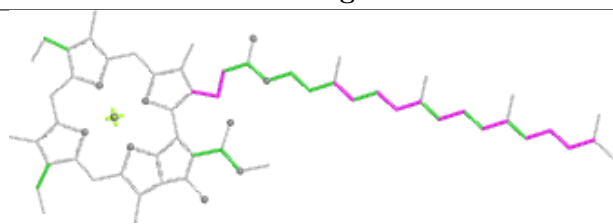
Ligand CLA 7 610



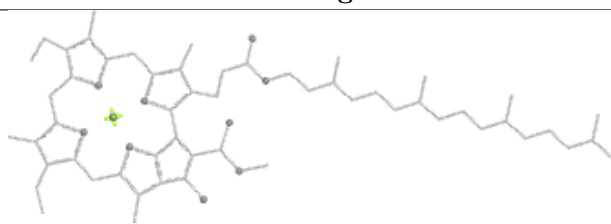
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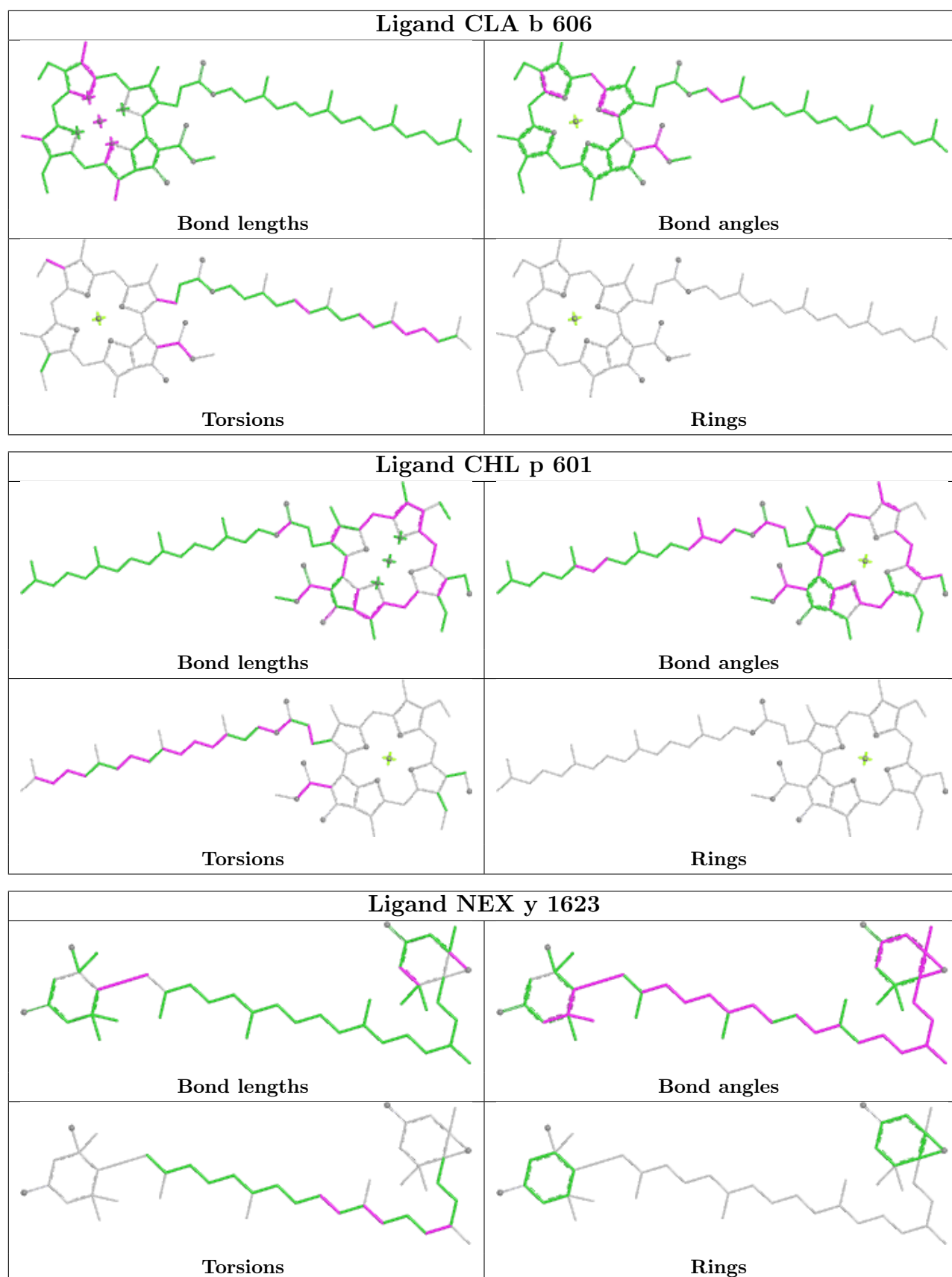
Bond angles



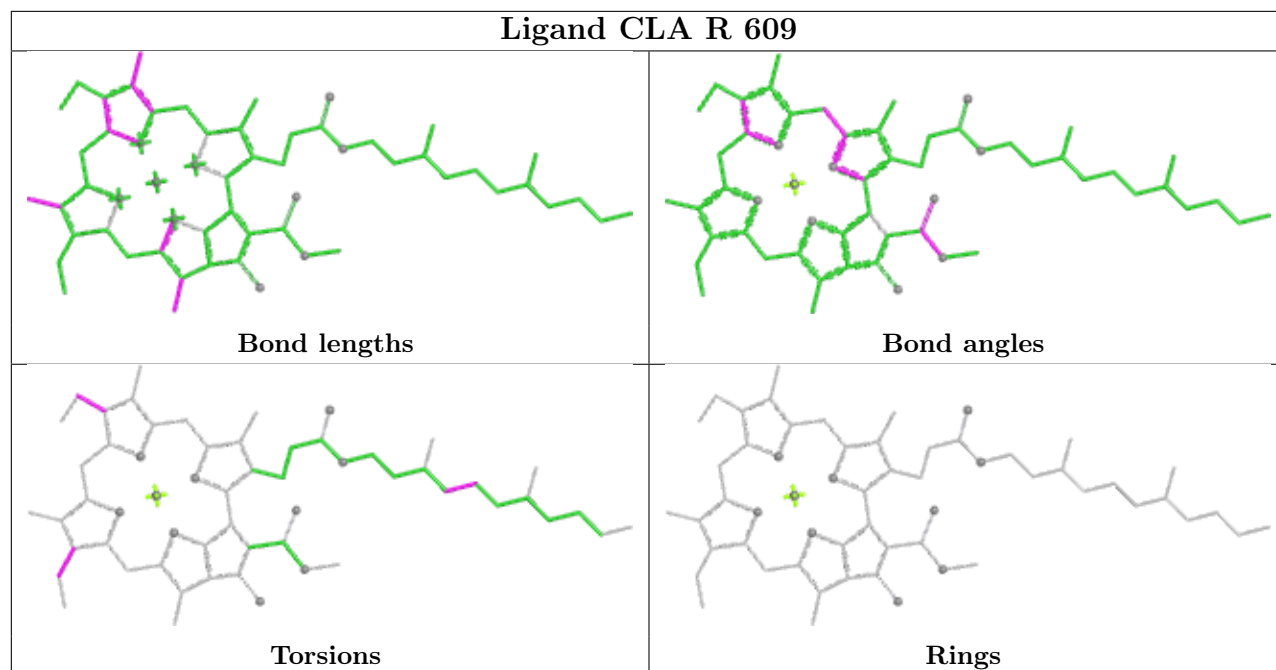
Torsions



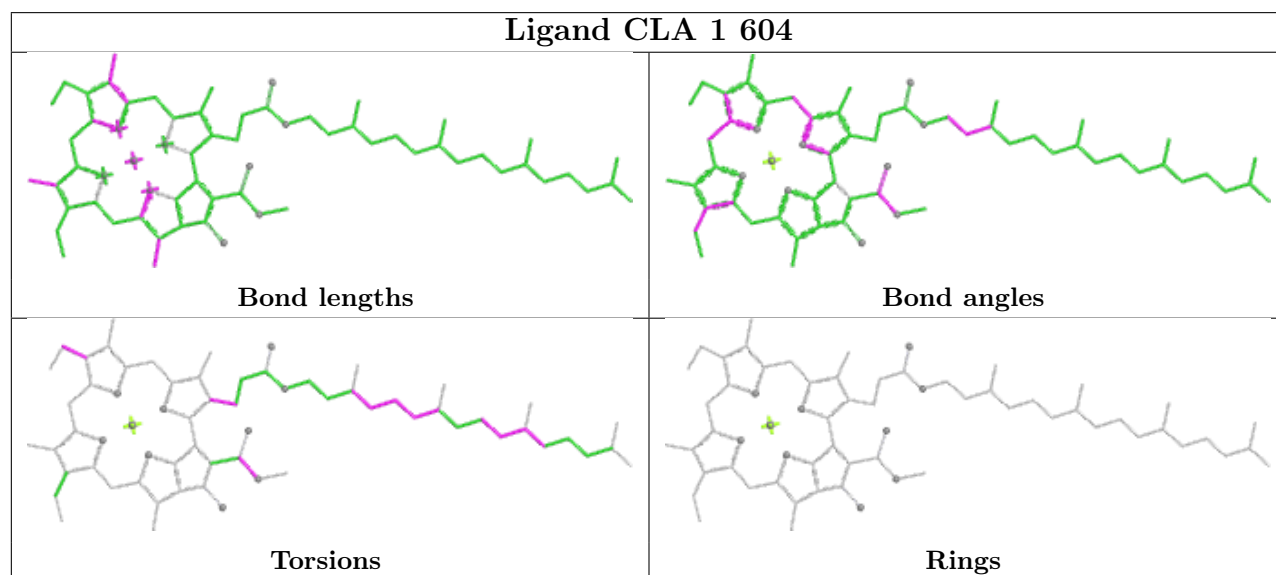
Rings



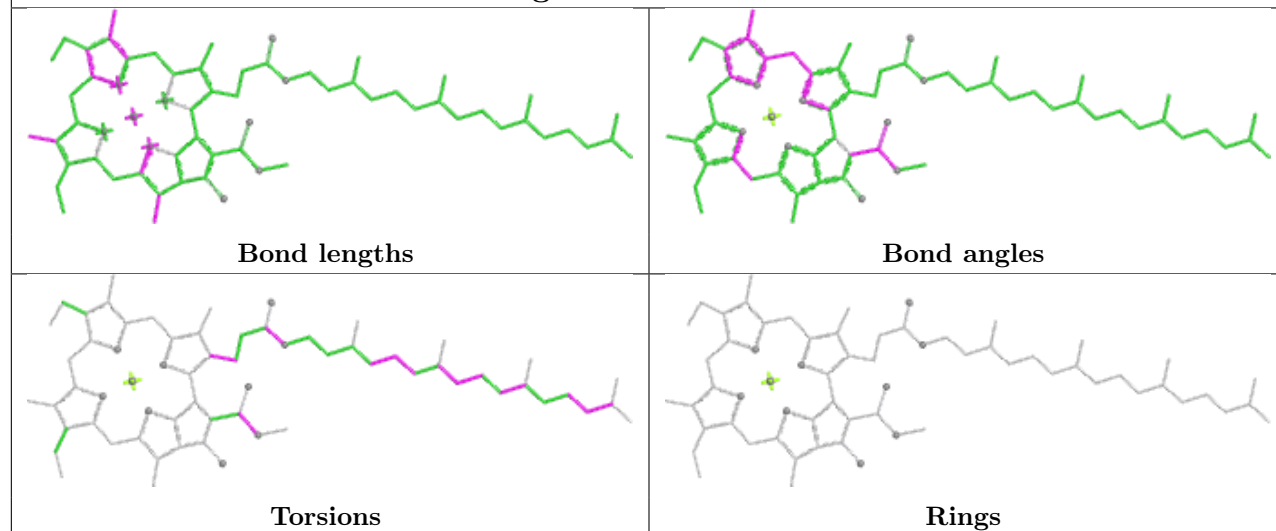
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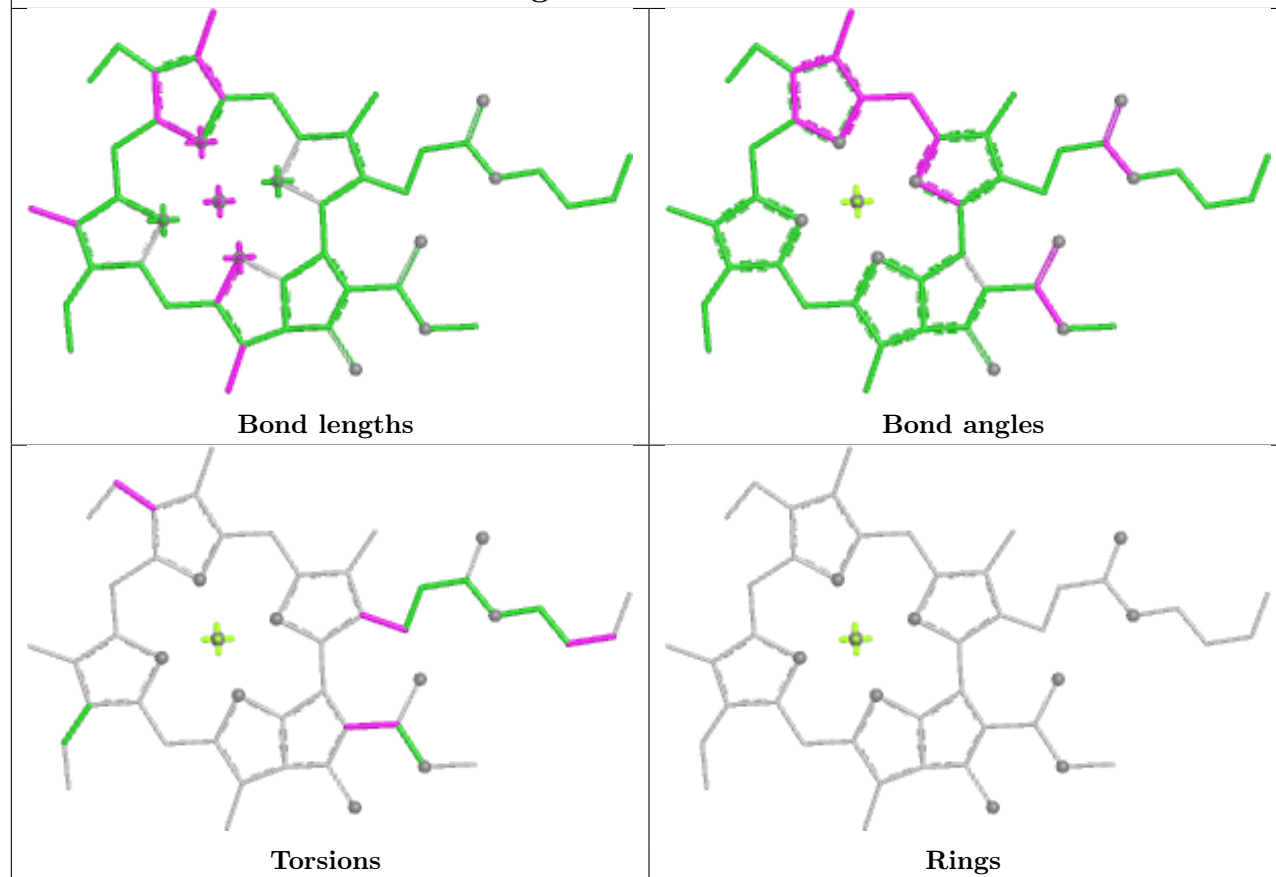
Ligand CLA 1 604

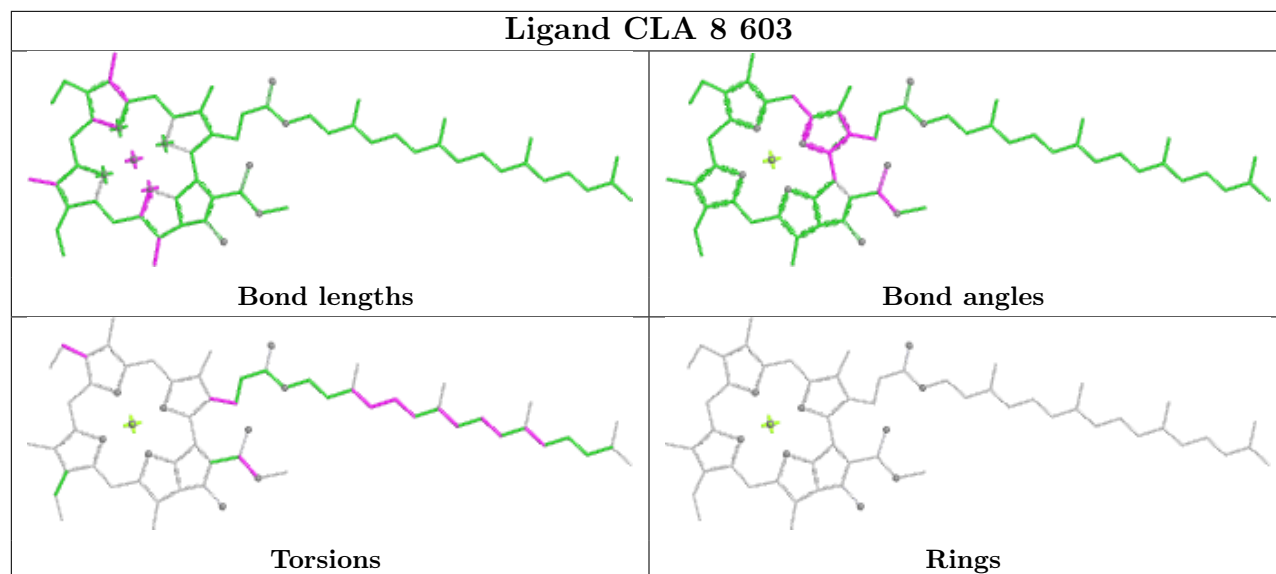
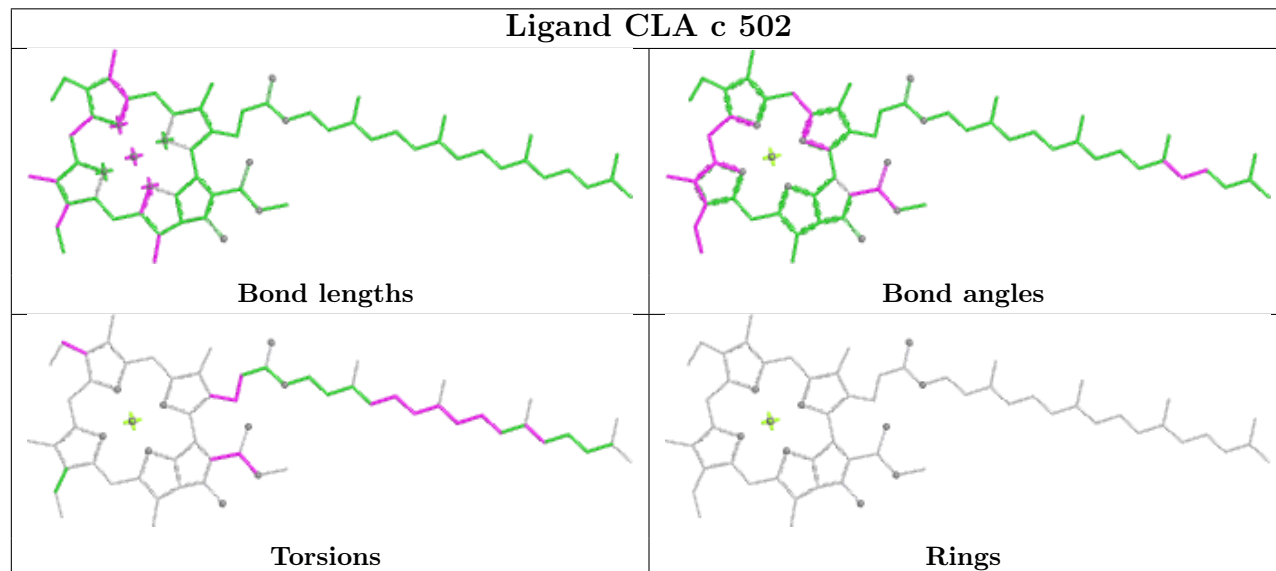


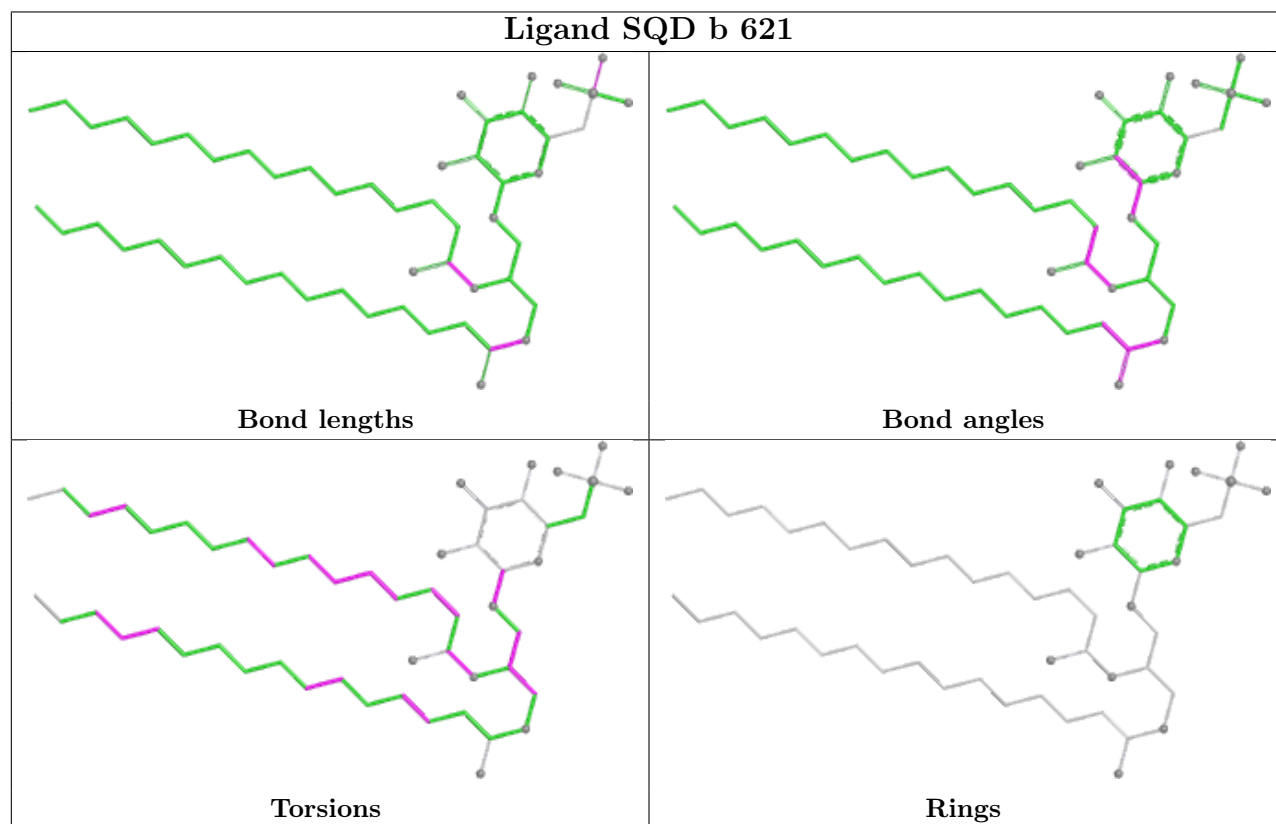
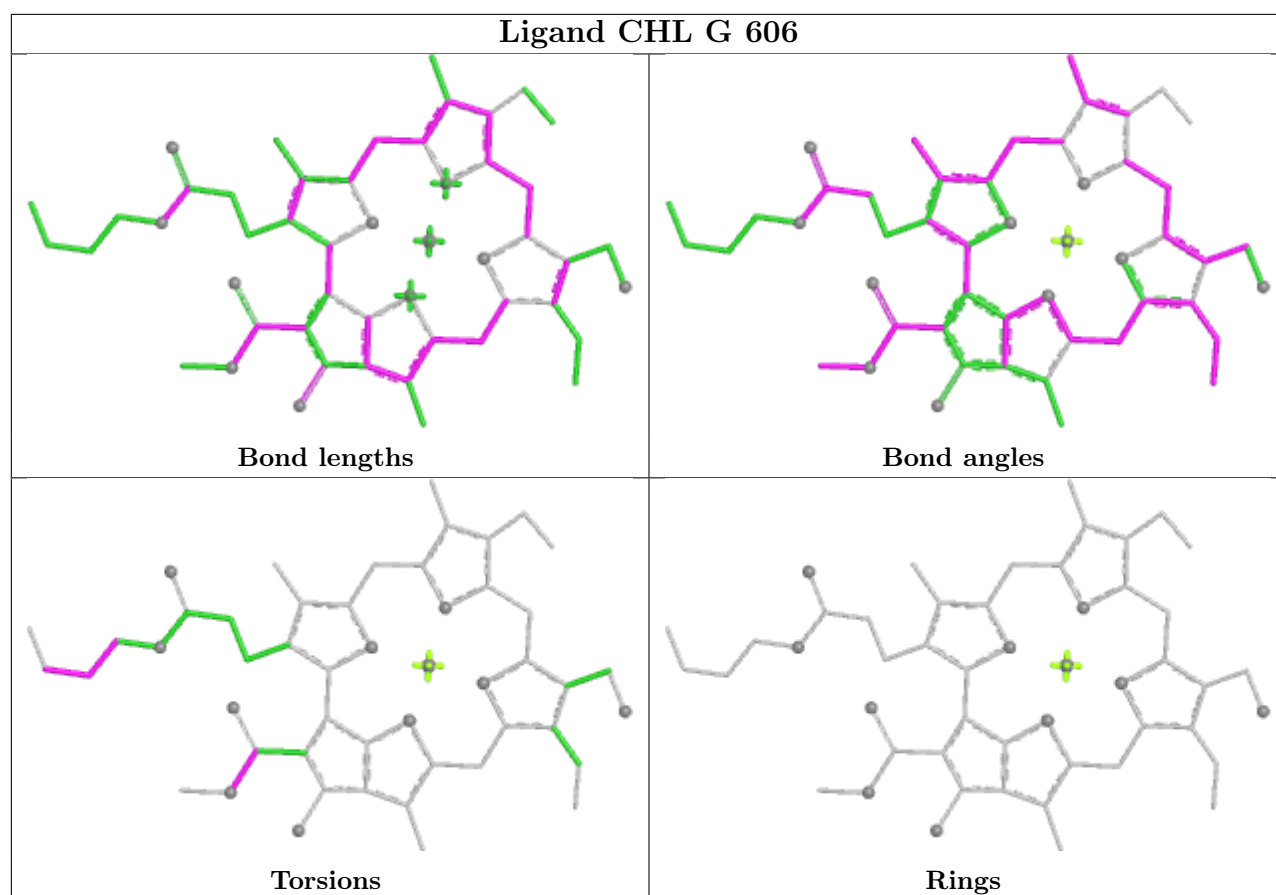
Ligand CLA C 508



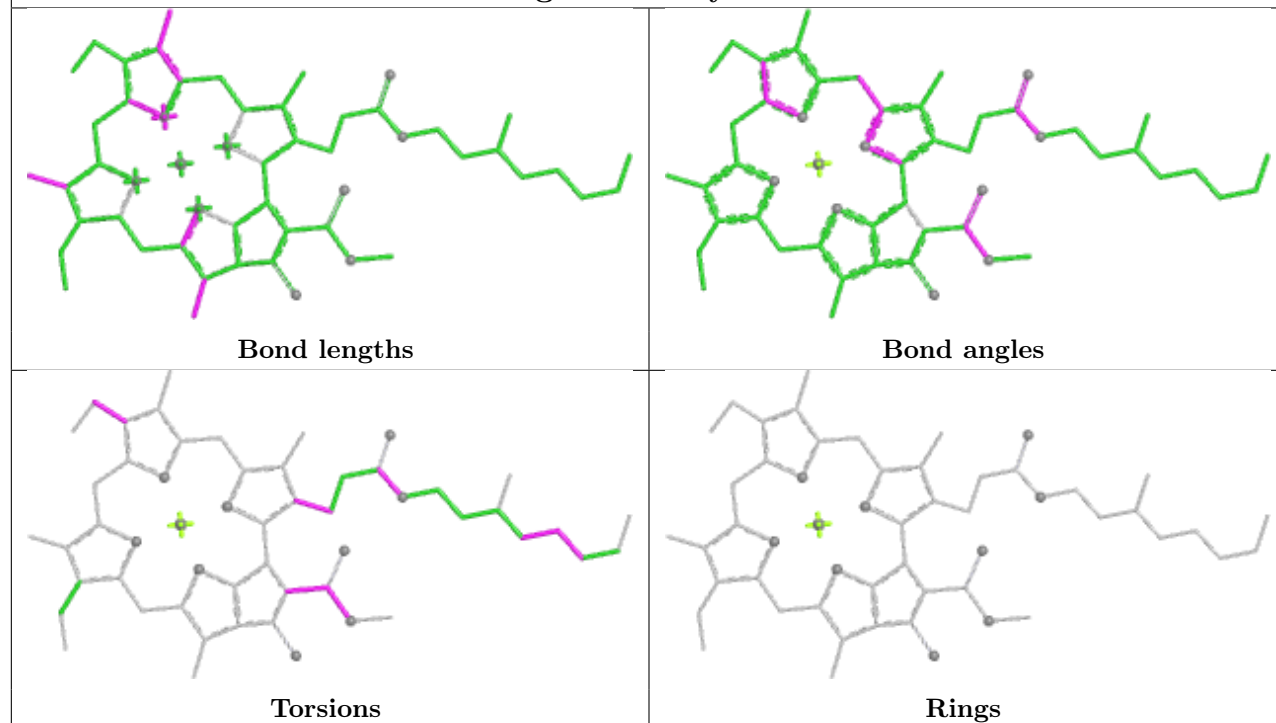
Ligand CLA G 604



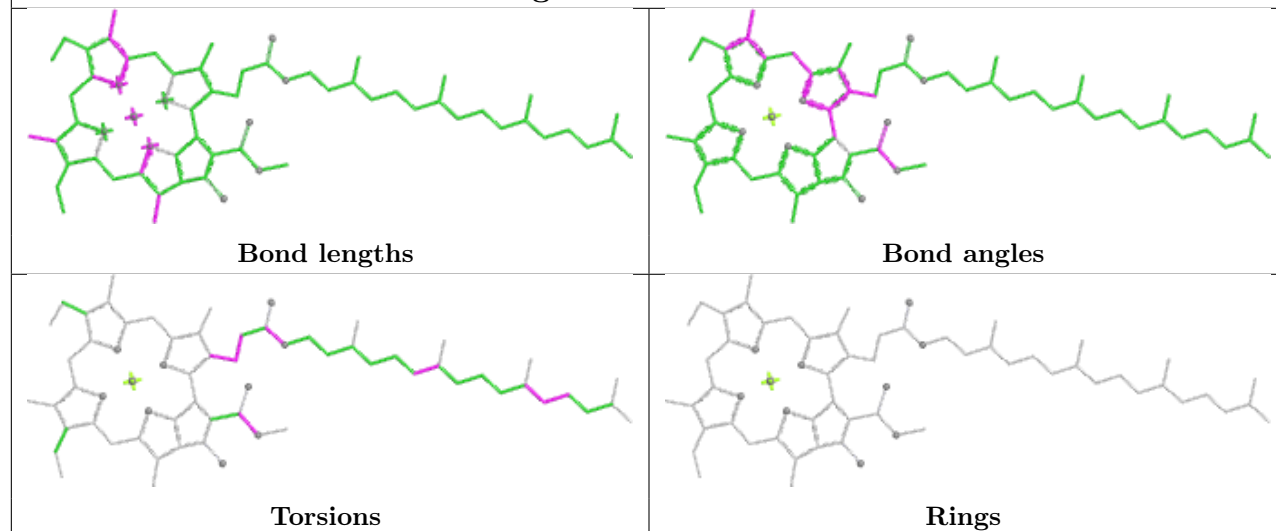
Ligand CLA 8 603**Ligand CLA c 502**

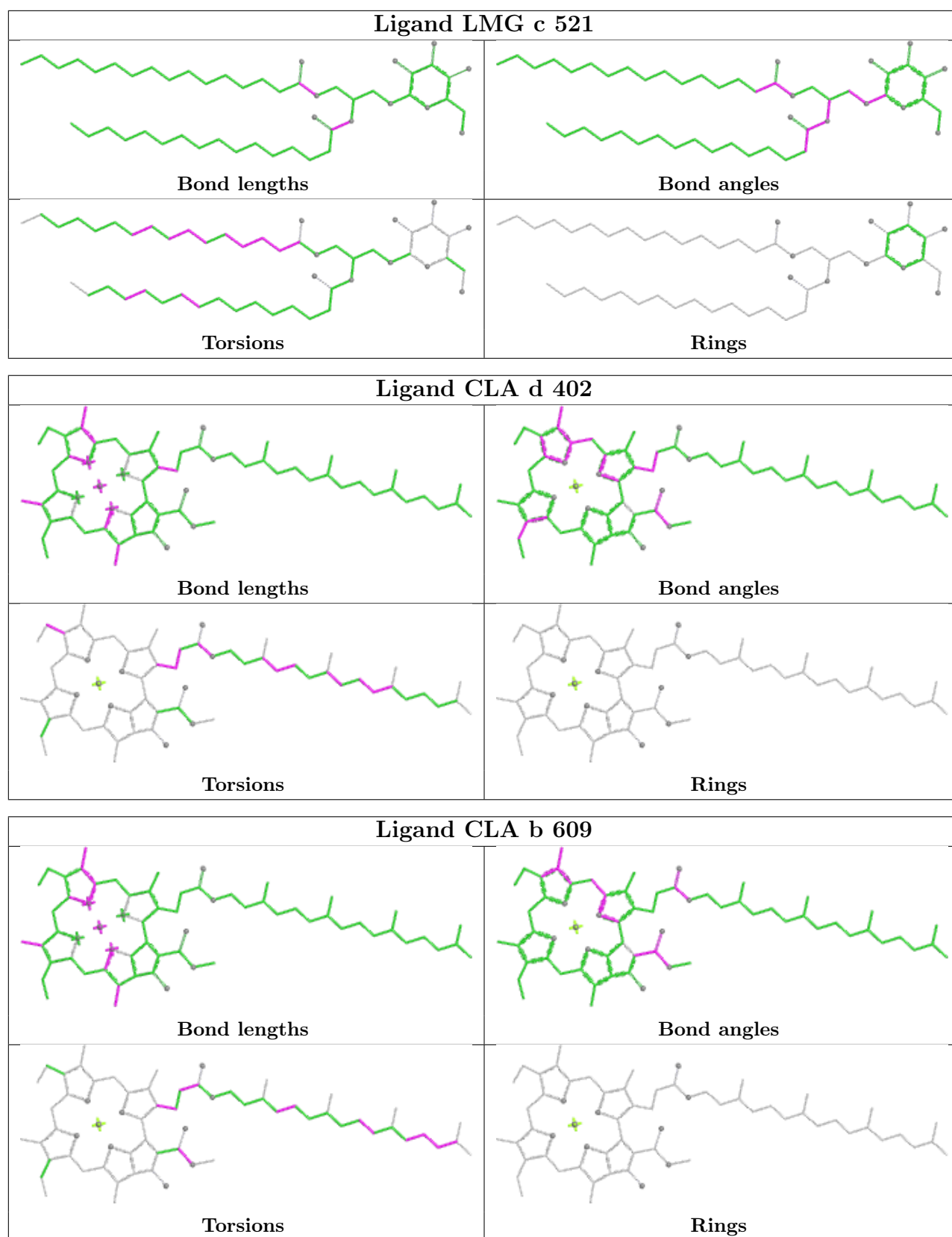


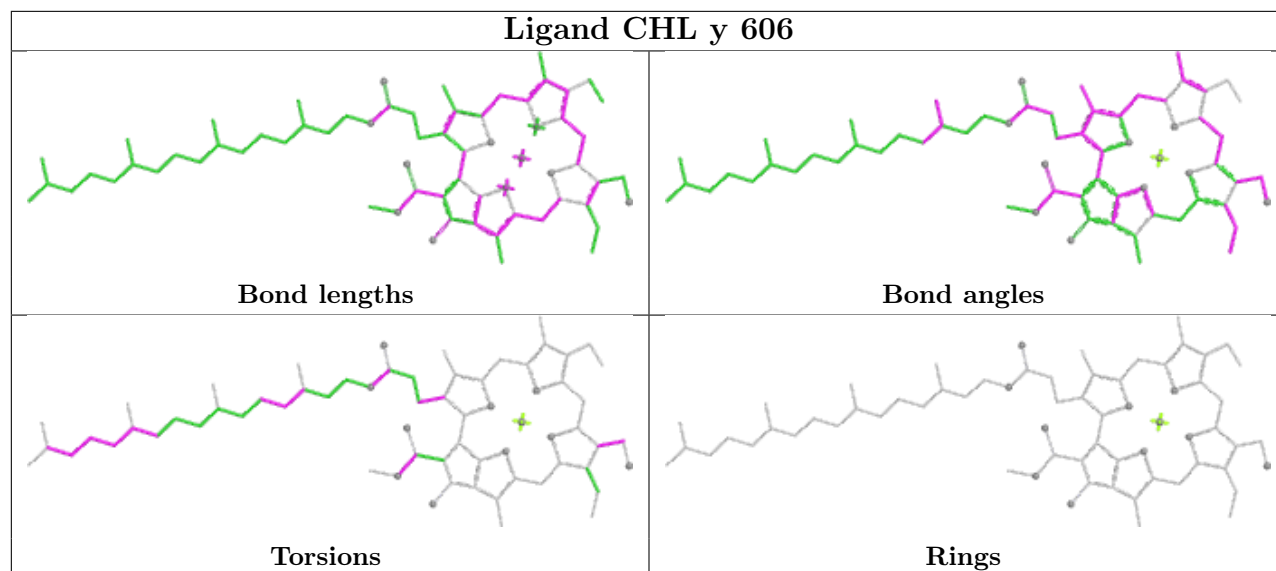
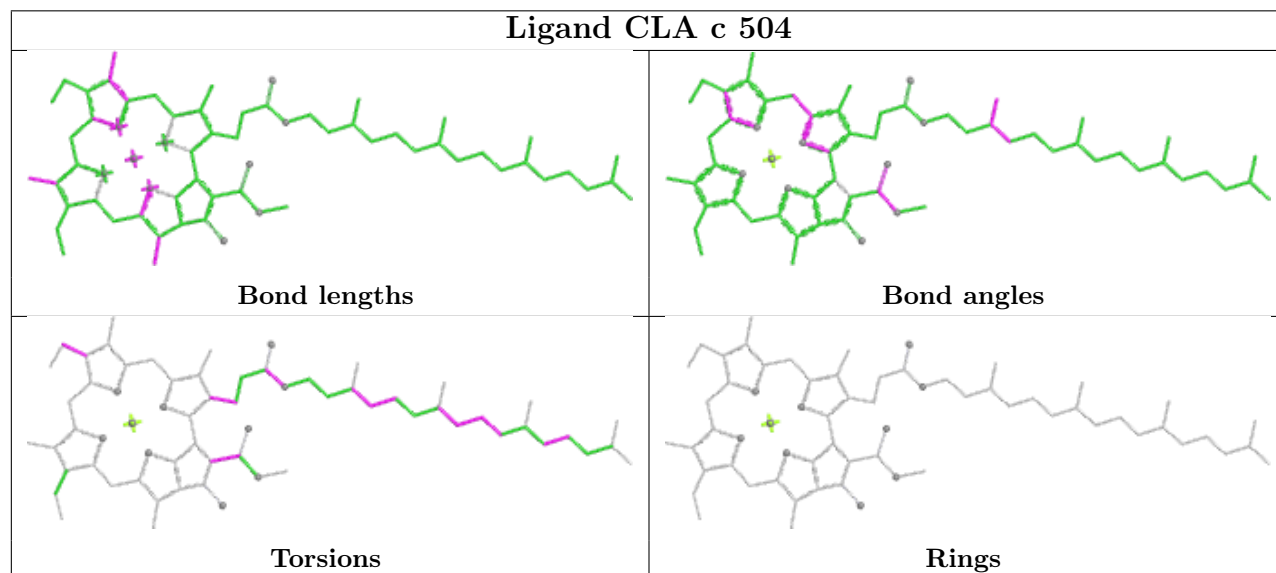
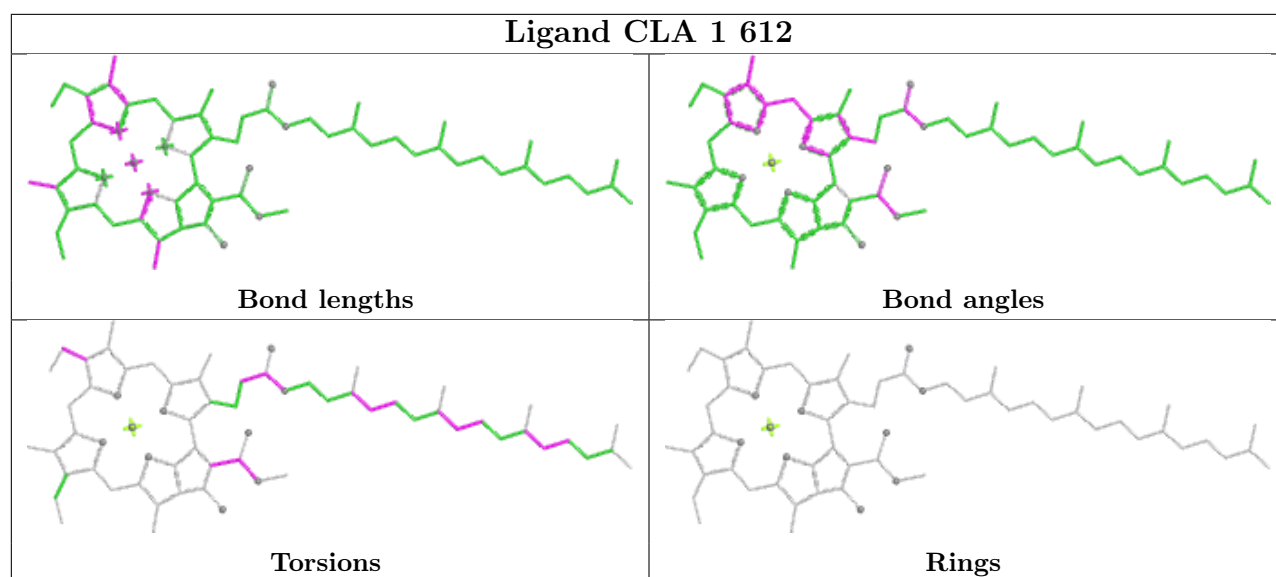
Ligand CLA y 614

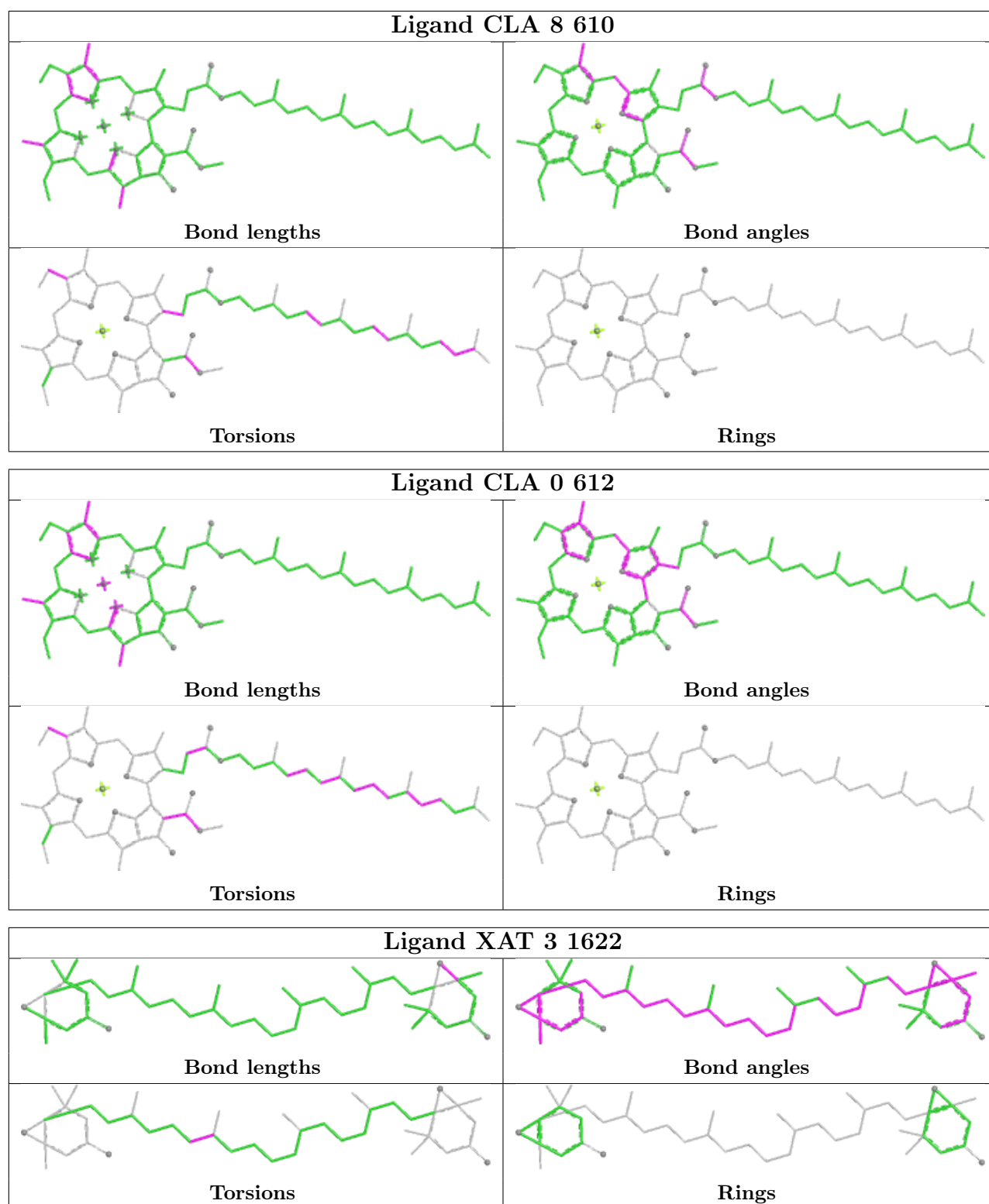


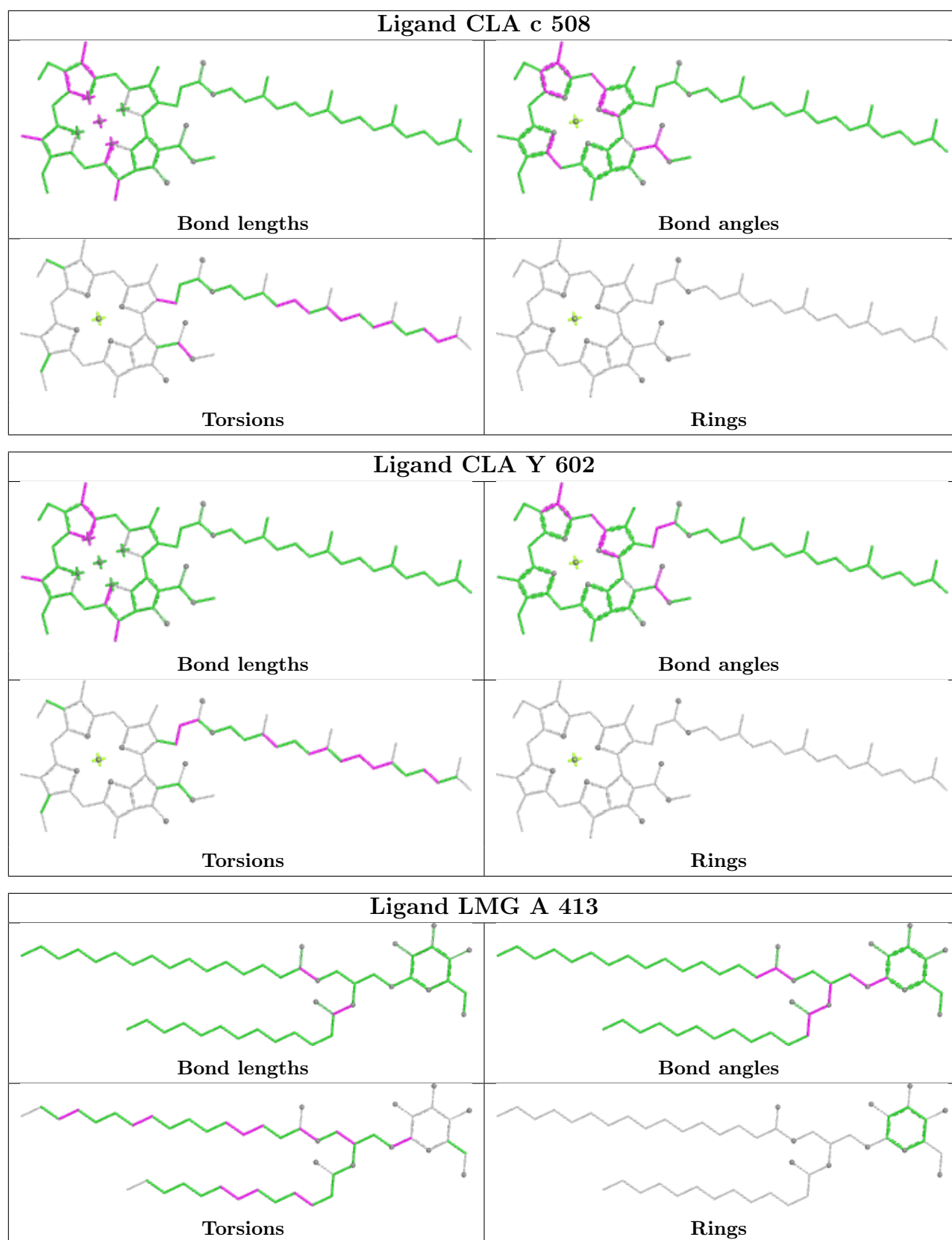
Ligand CLA B 613

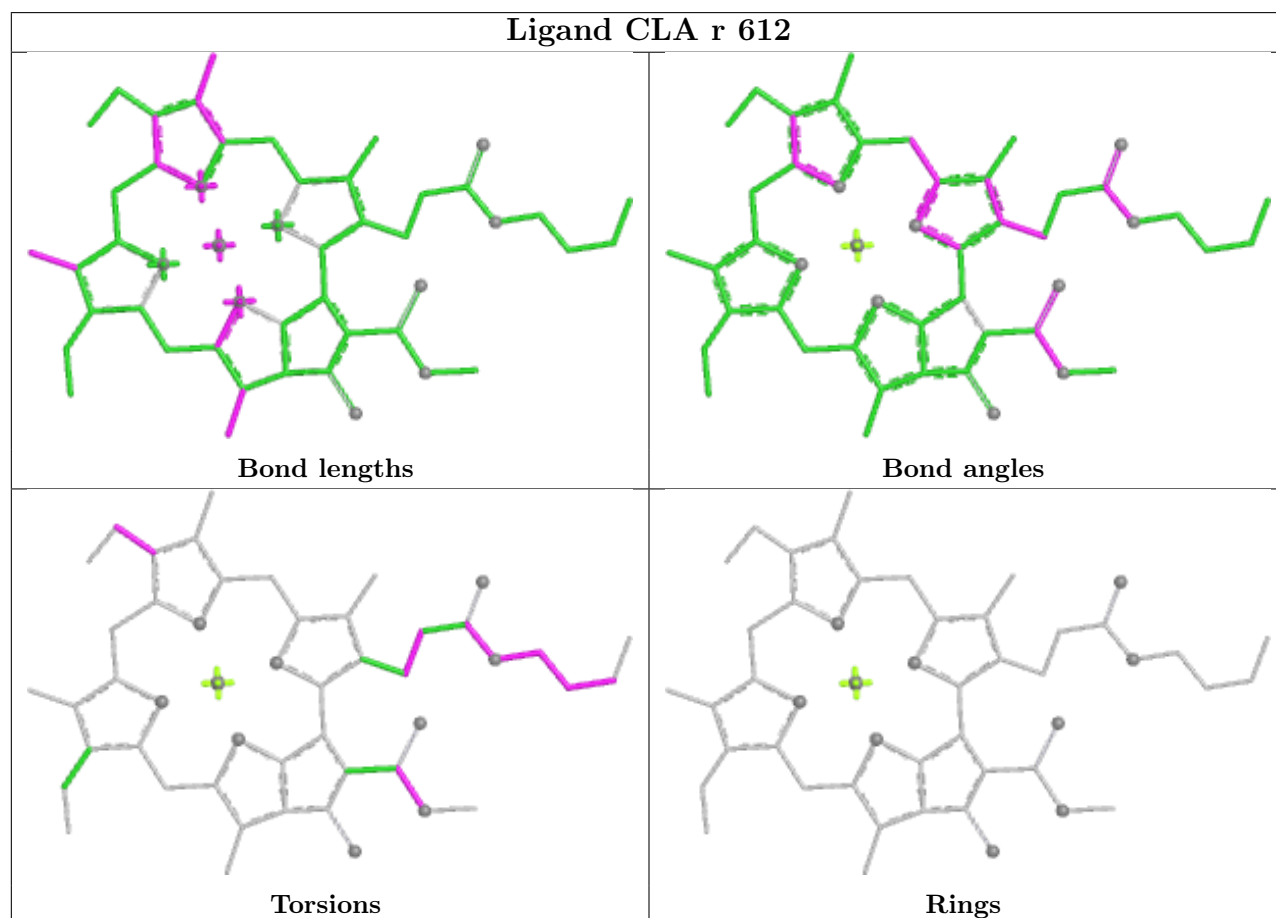
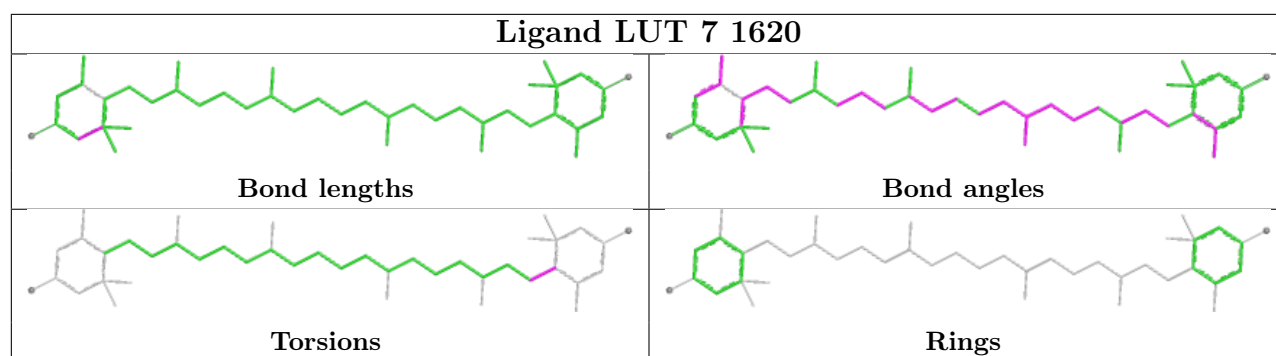


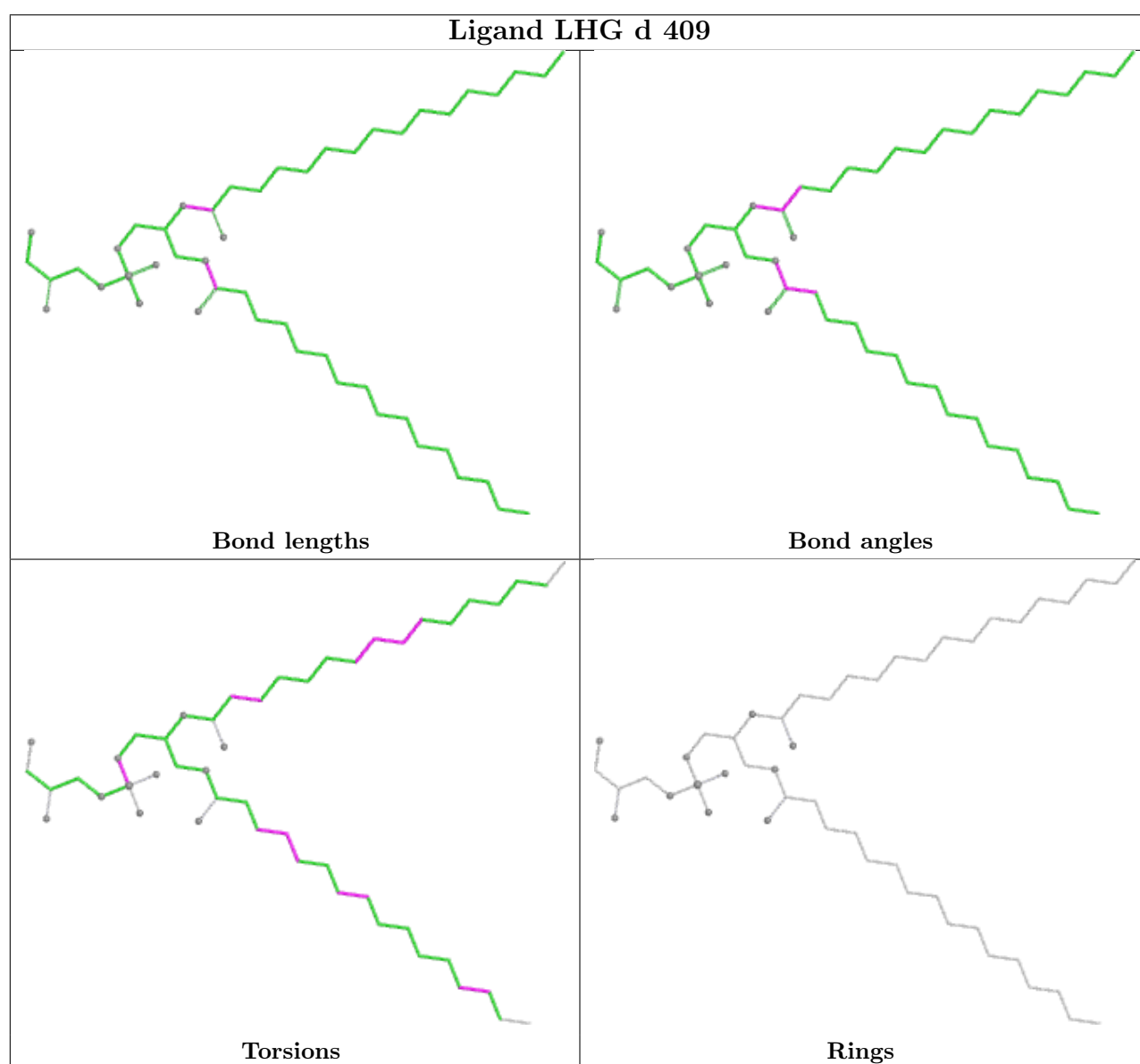
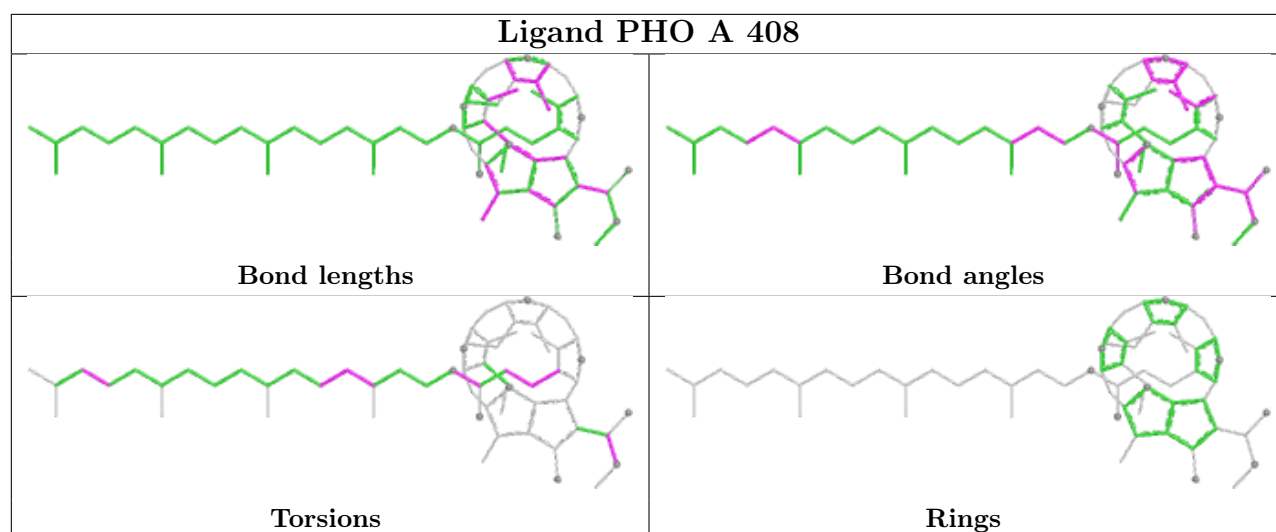


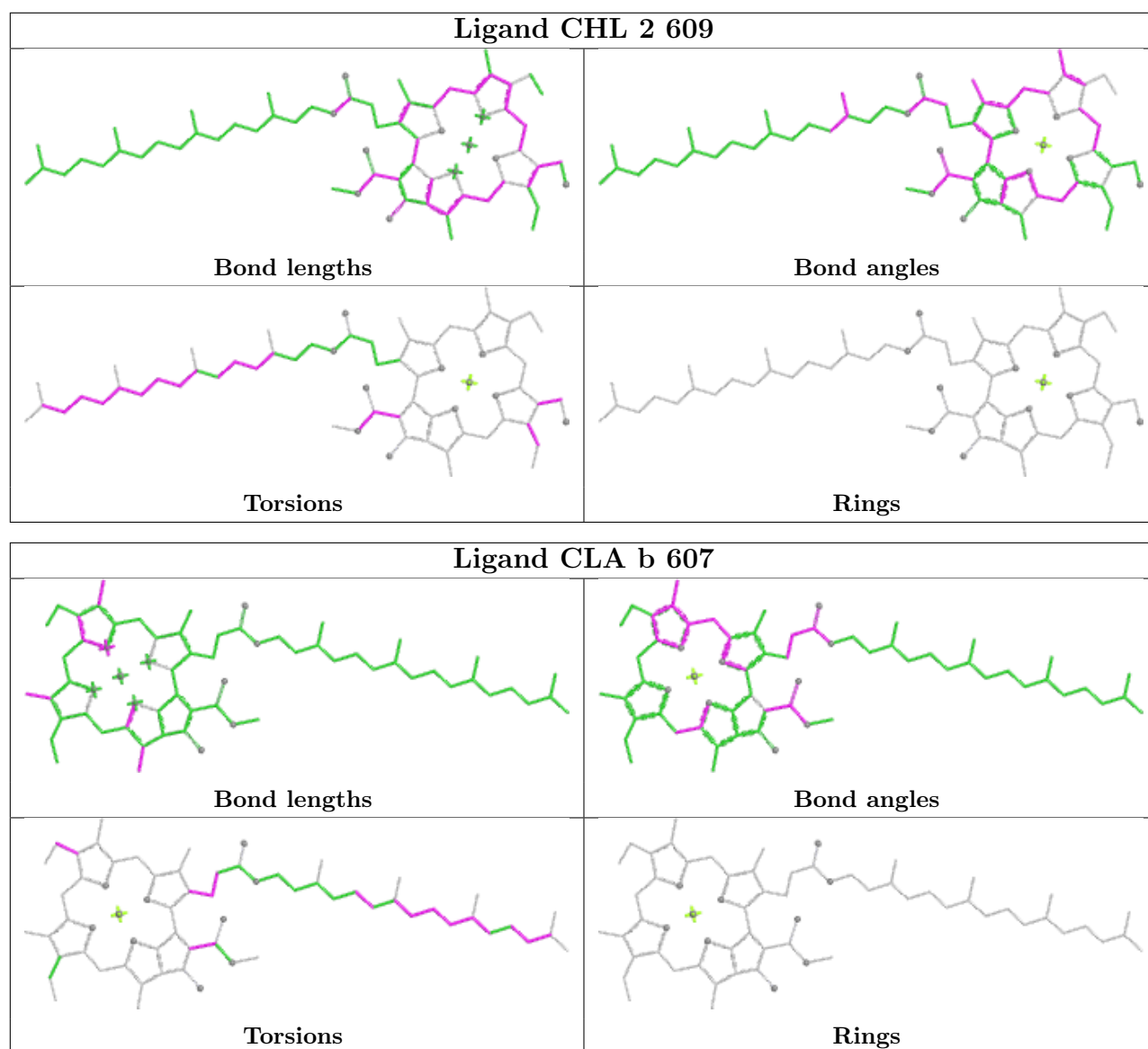




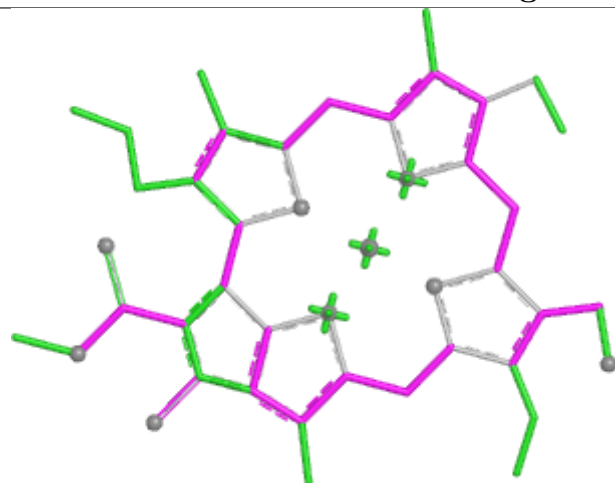




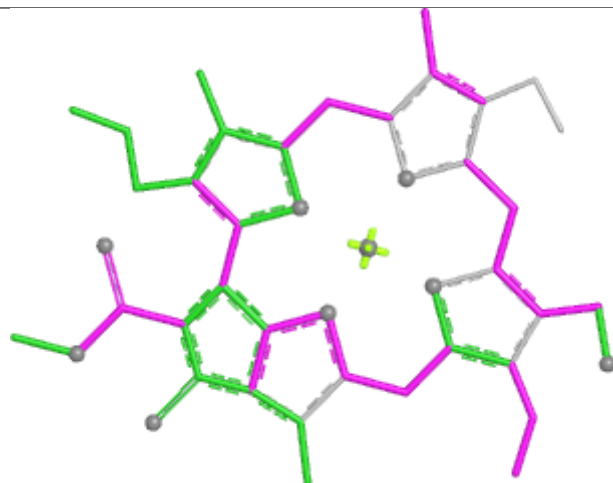




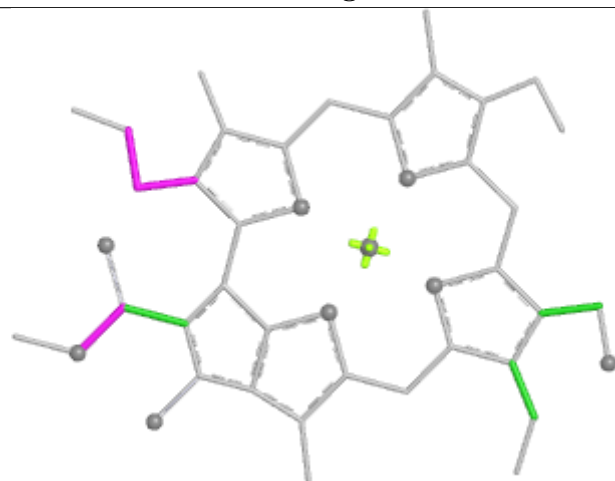
Ligand CHL 2 608



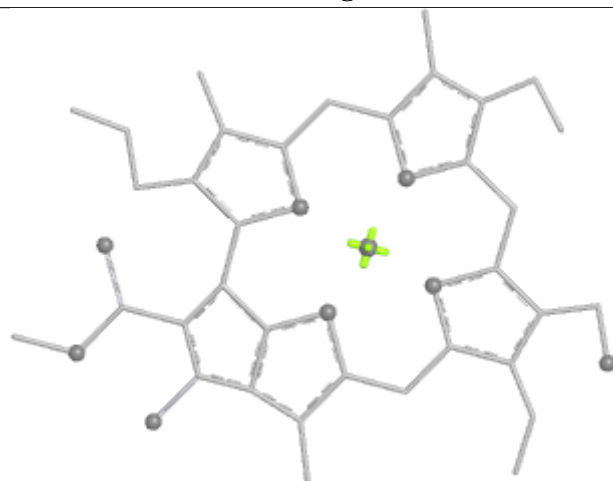
Bond lengths



Bond angles

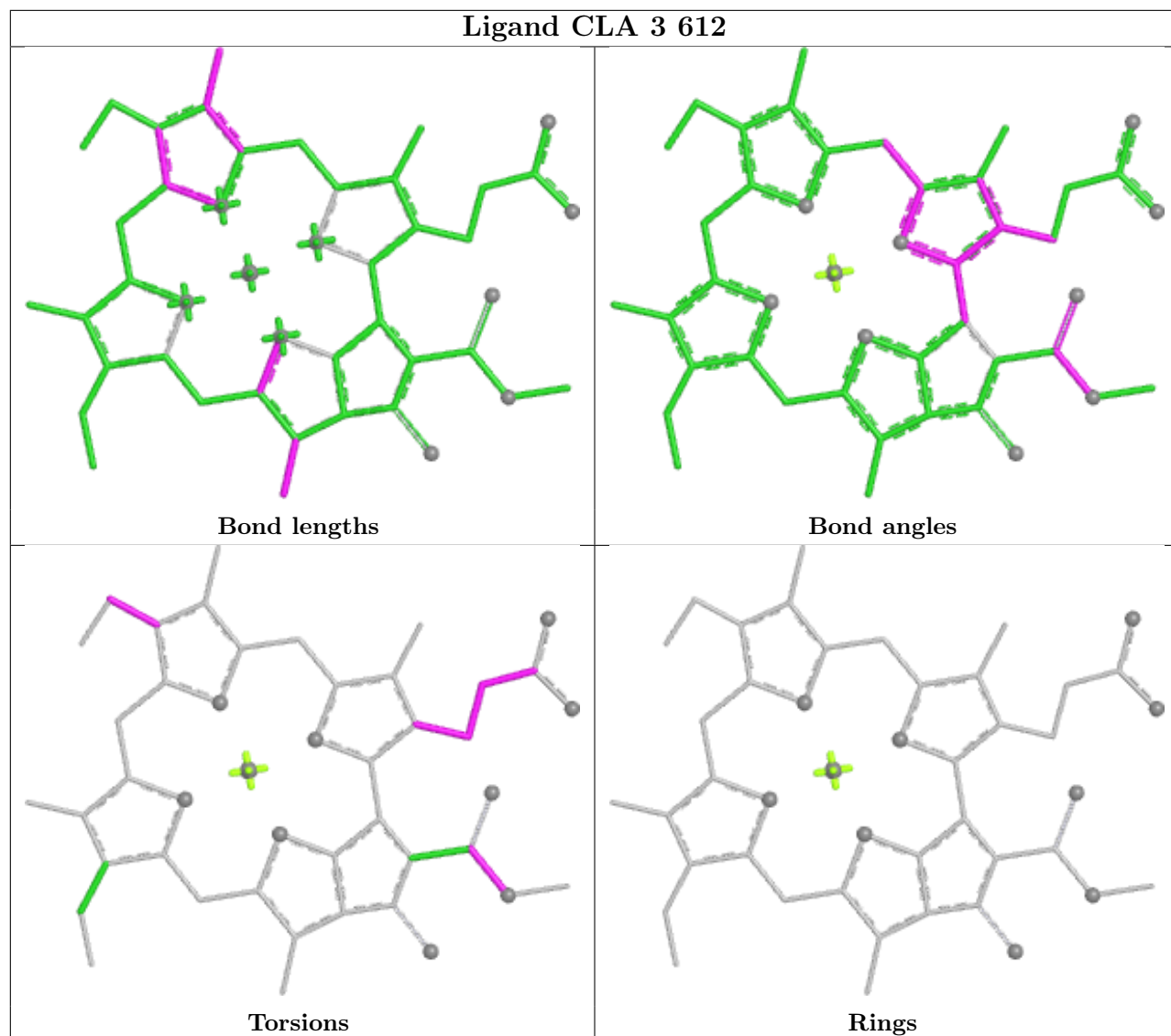


Torsions

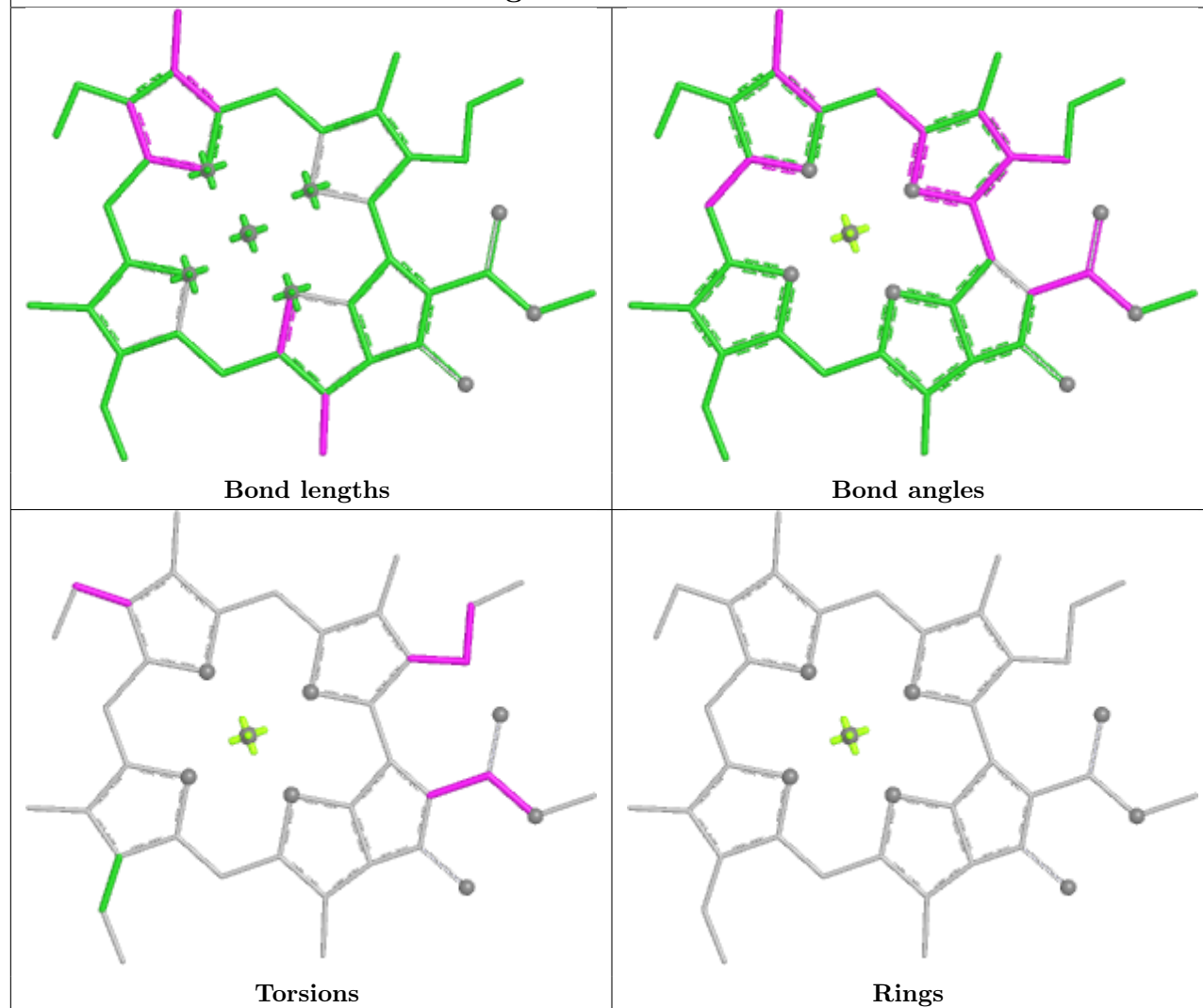


Rings

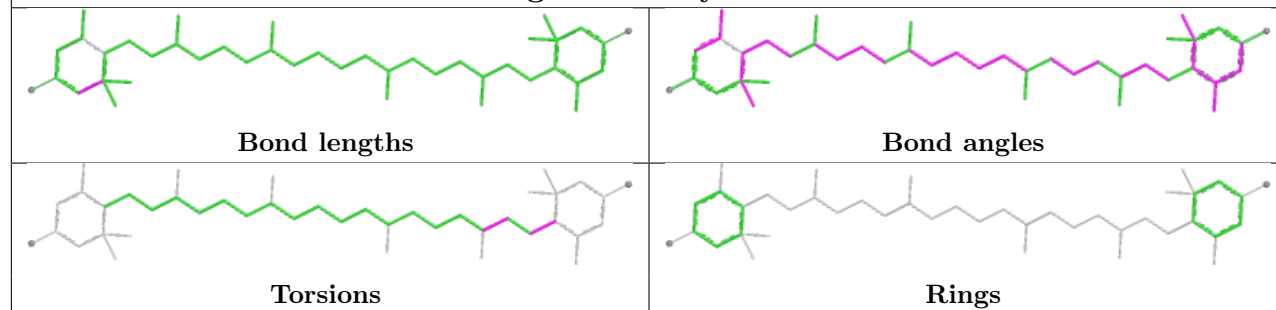
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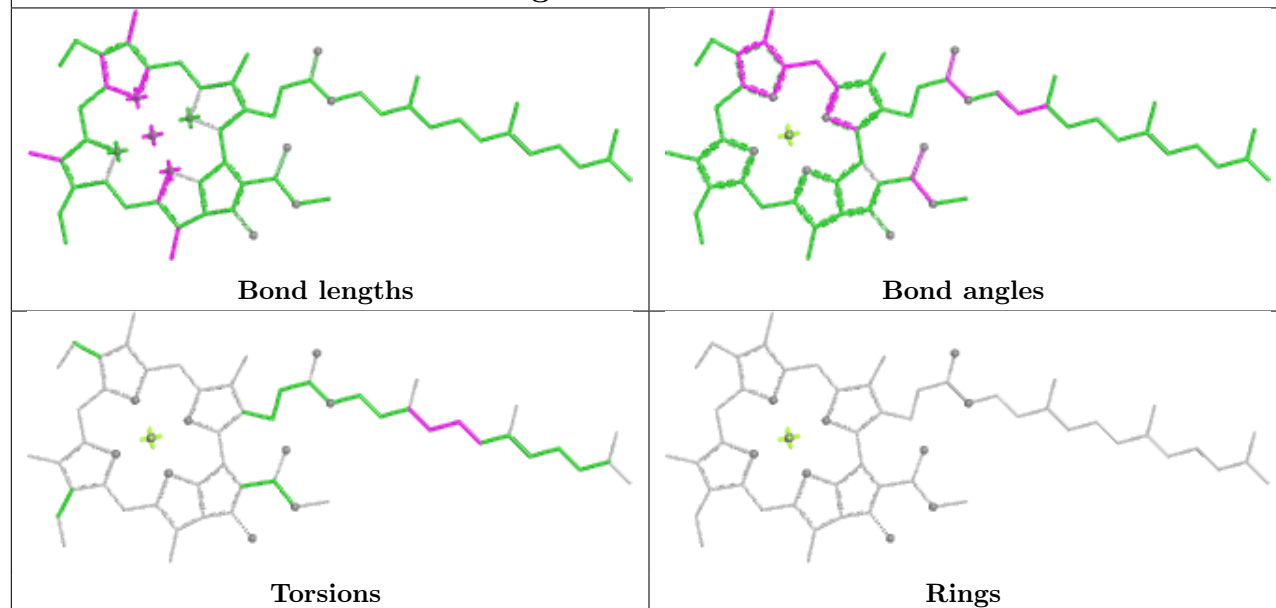
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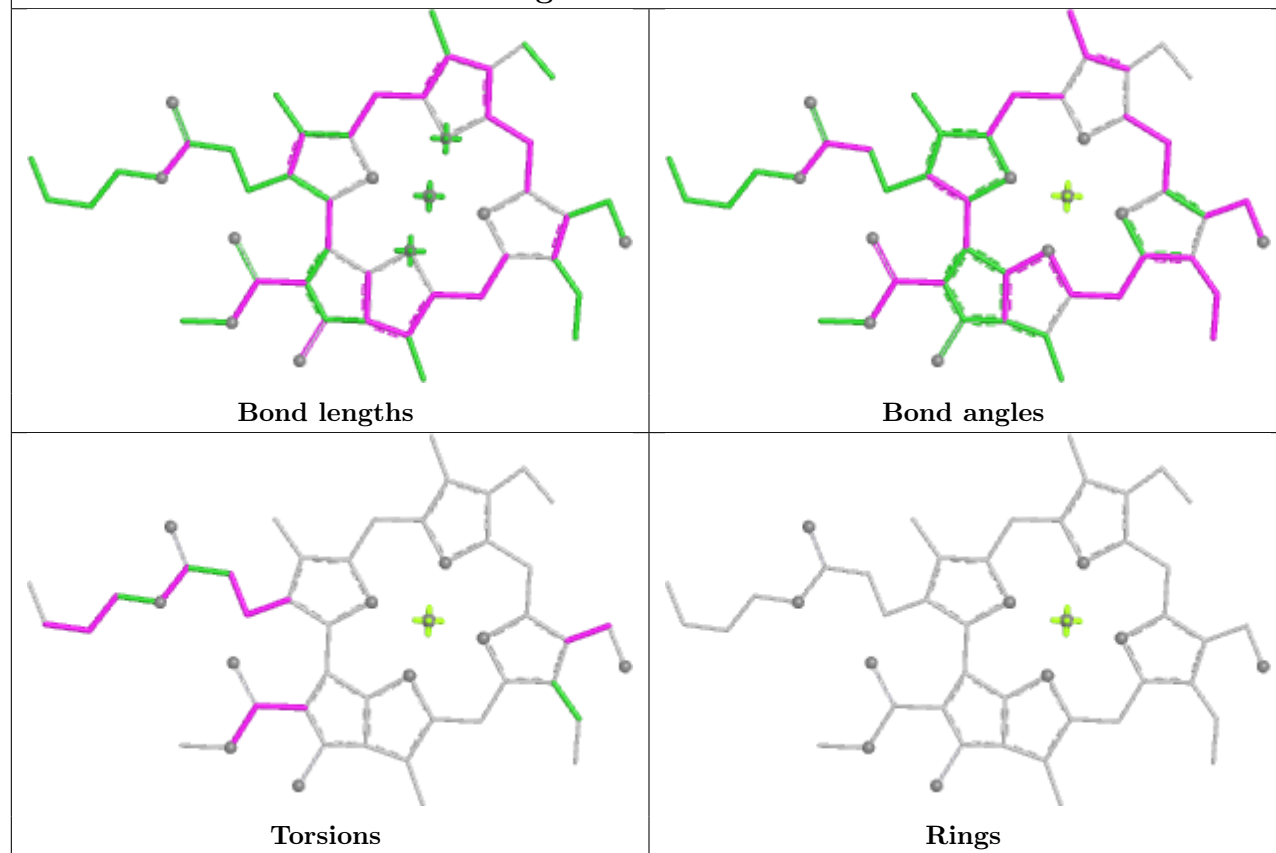
Ligand LUT y 1621



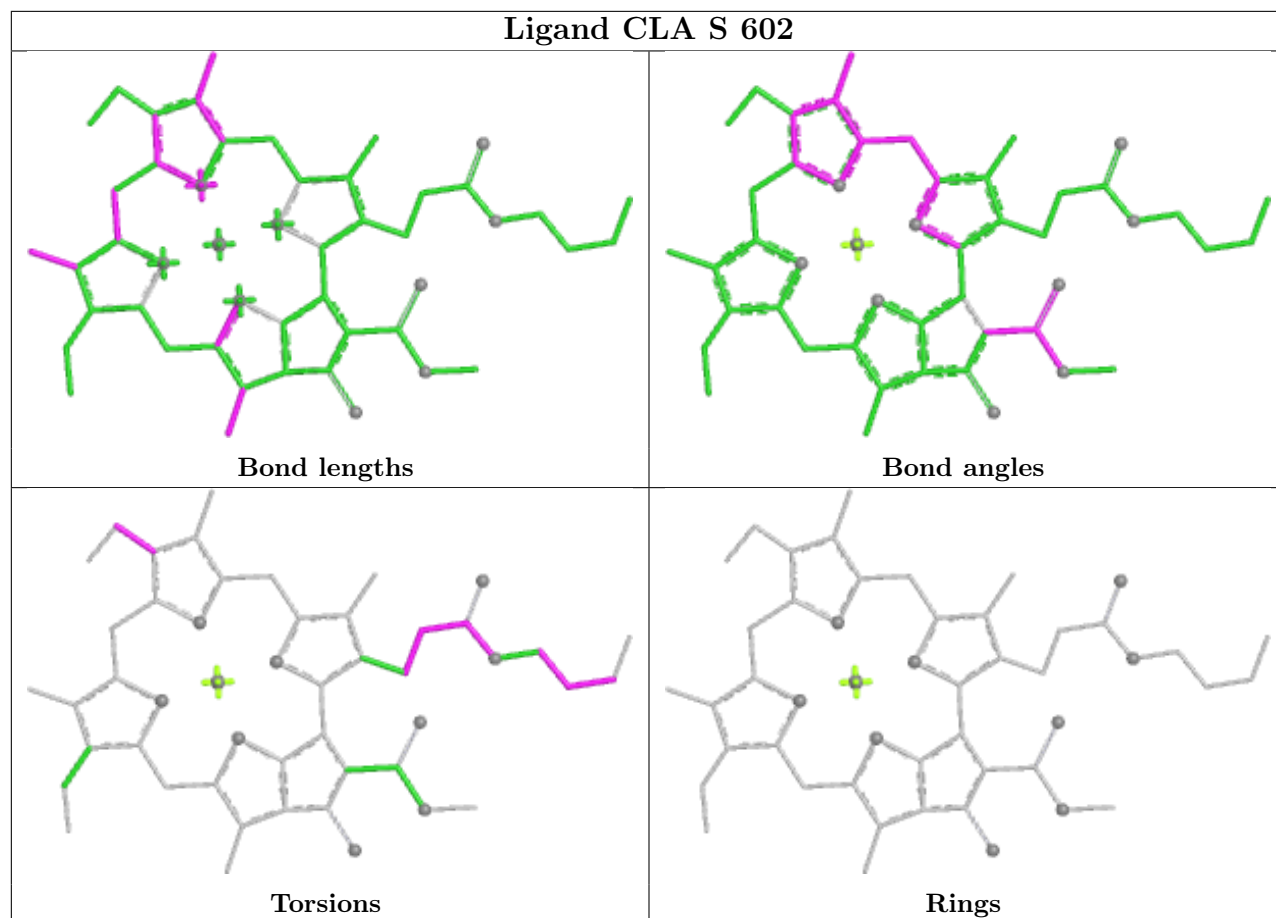
Ligand CLA A 410

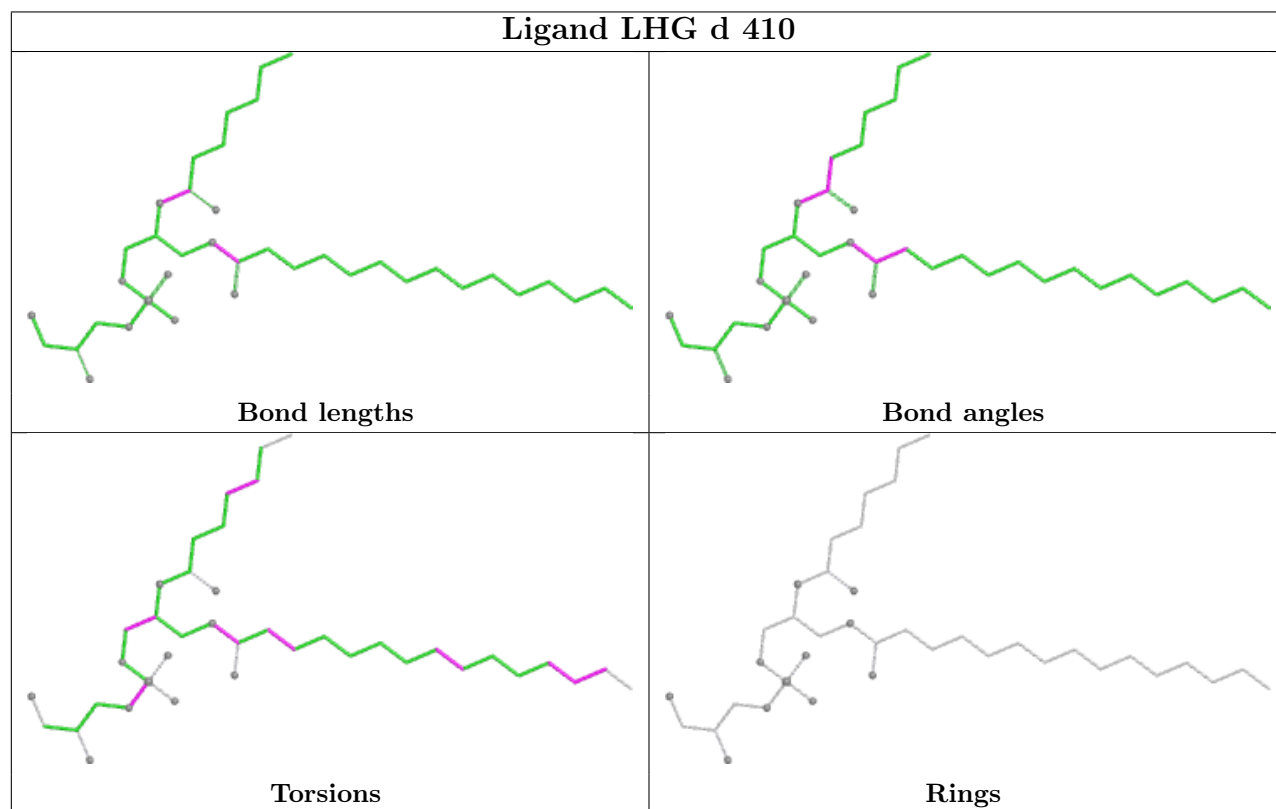
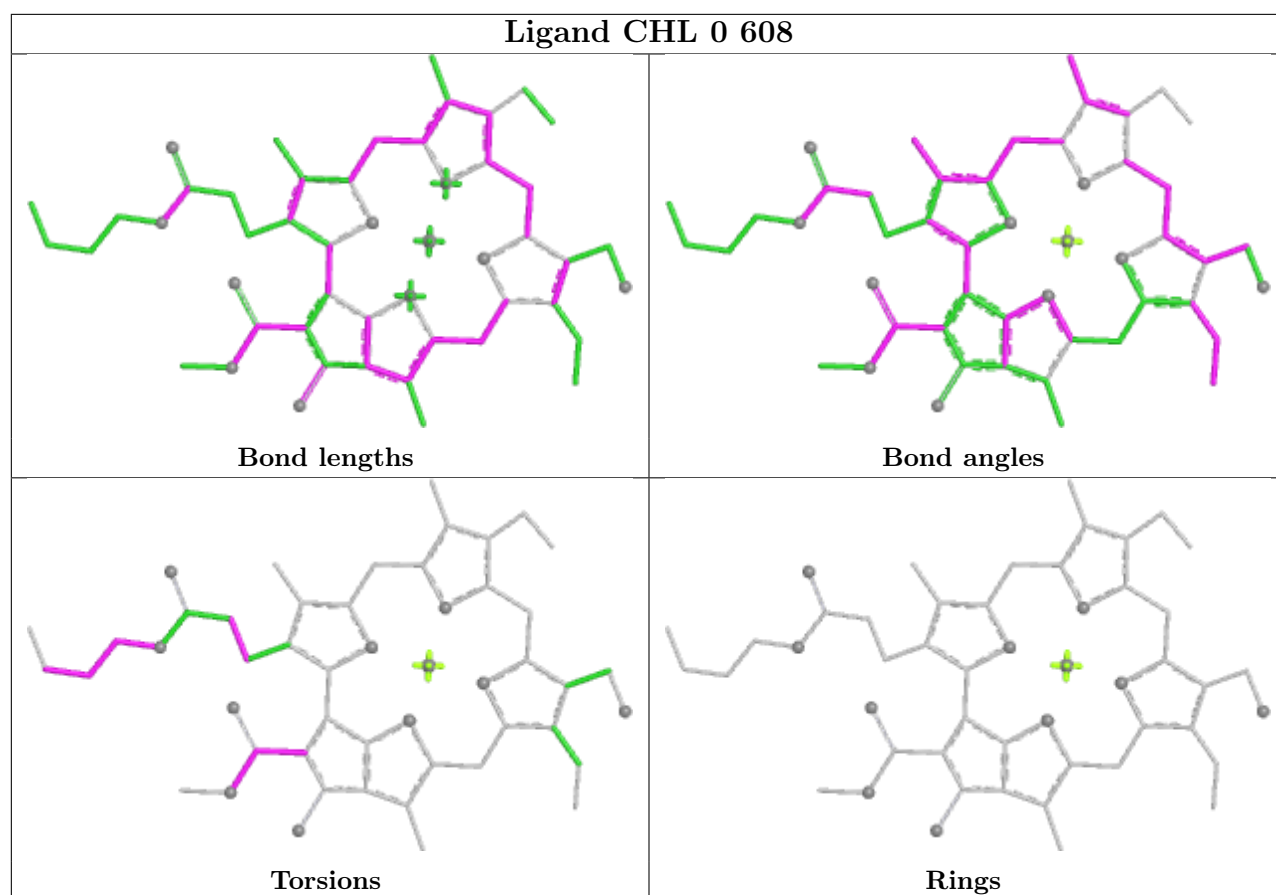


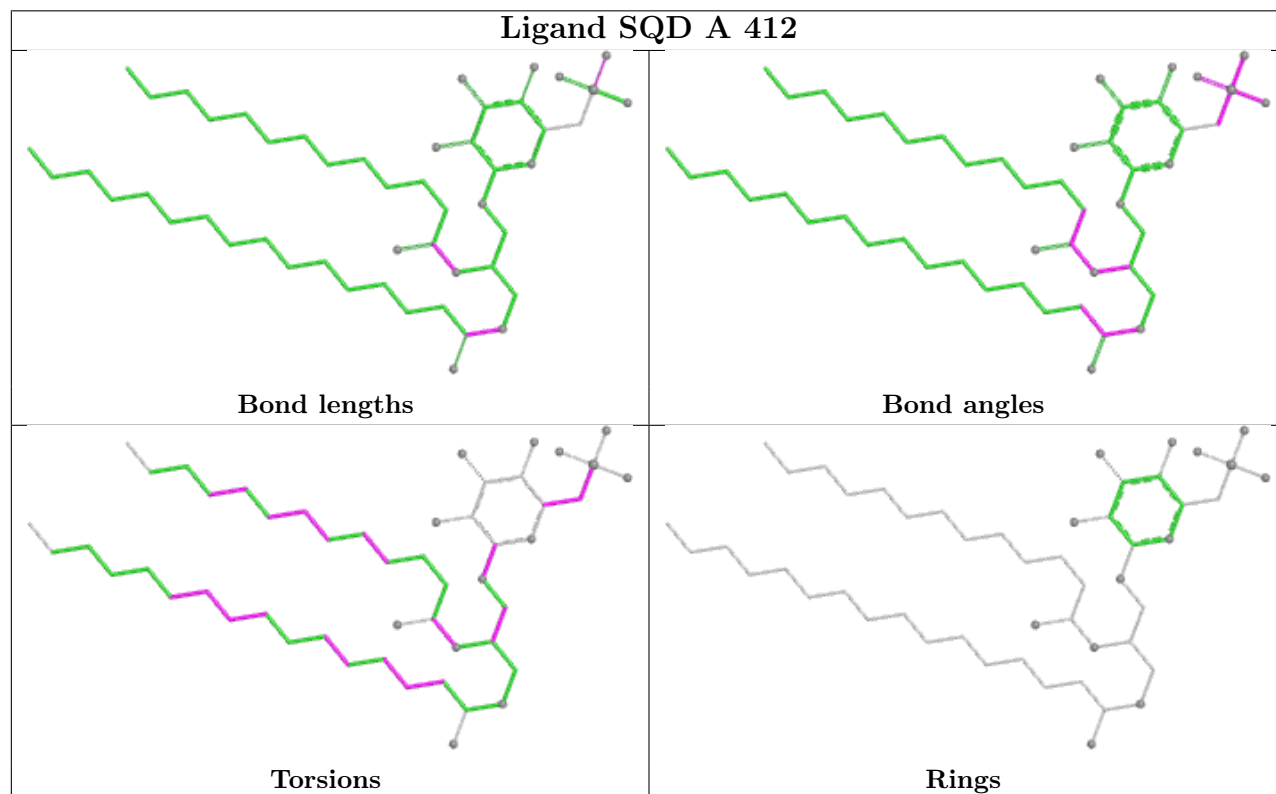
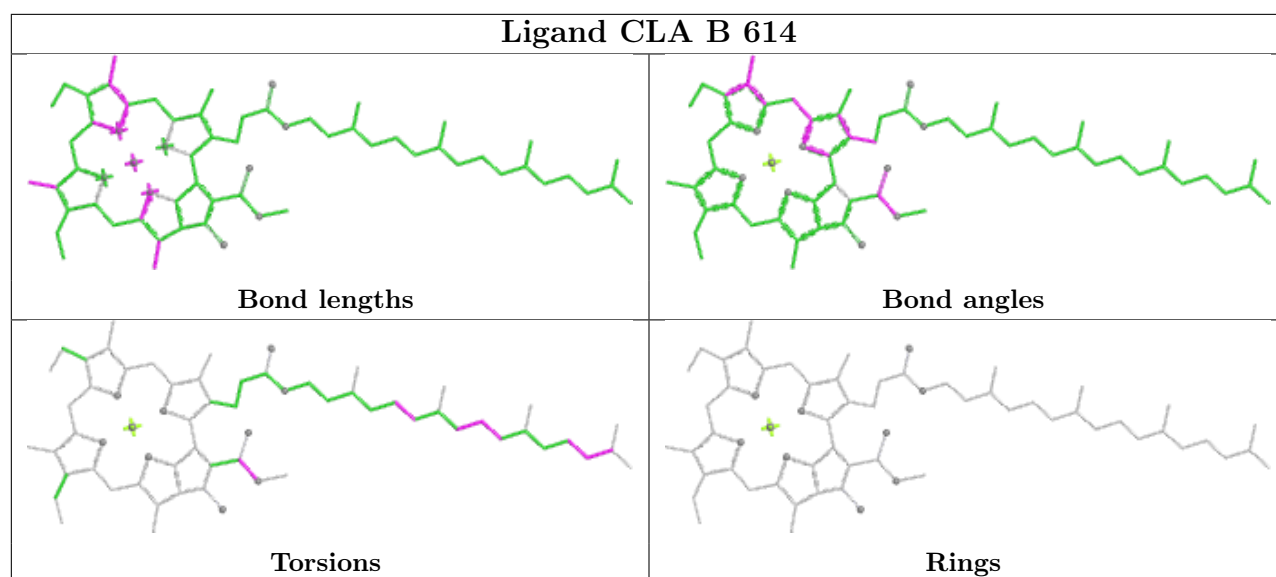
Ligand CHL 8 608

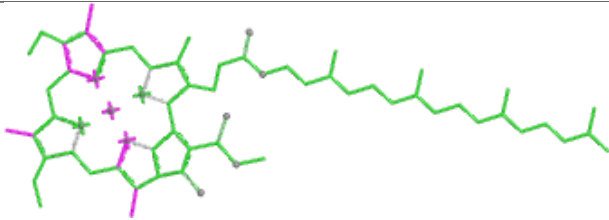
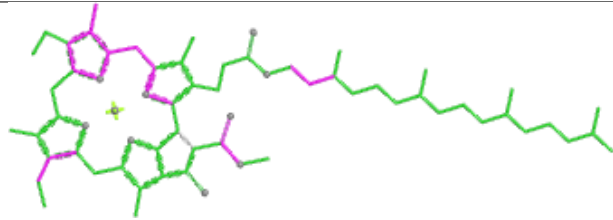
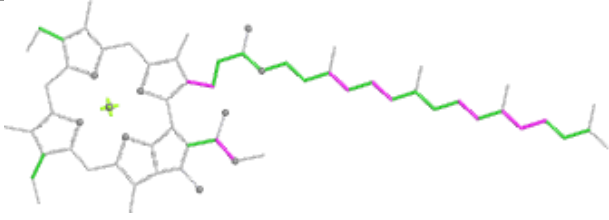
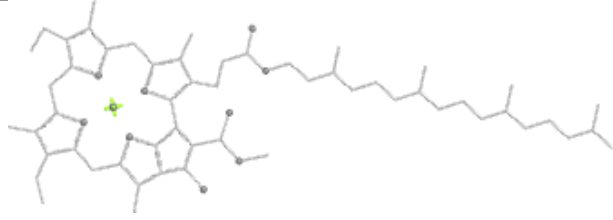


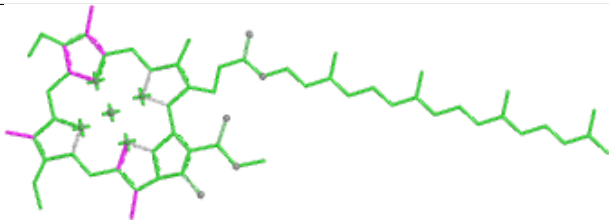
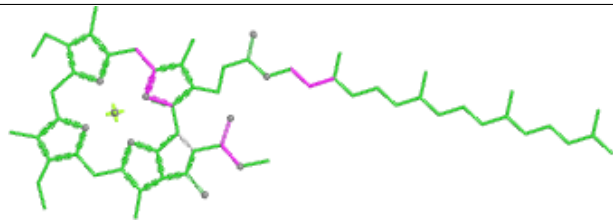
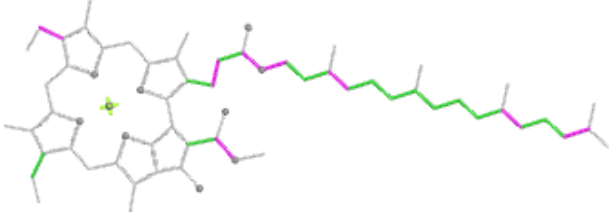
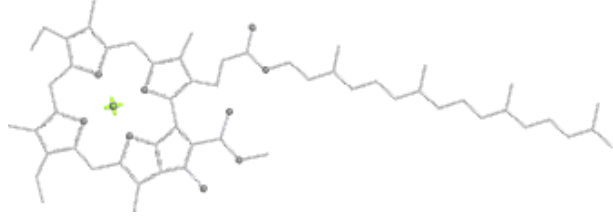
Ligand CLA S 602

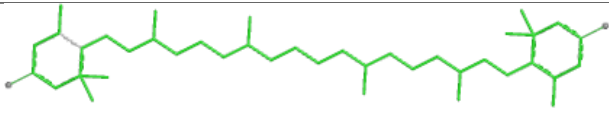
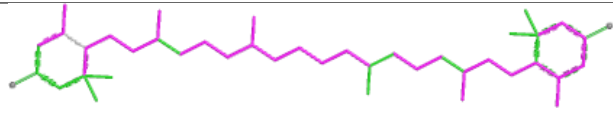
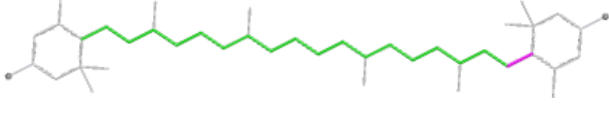
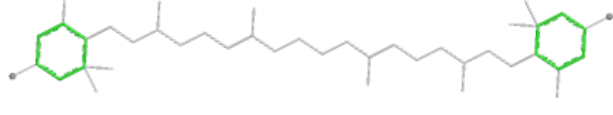


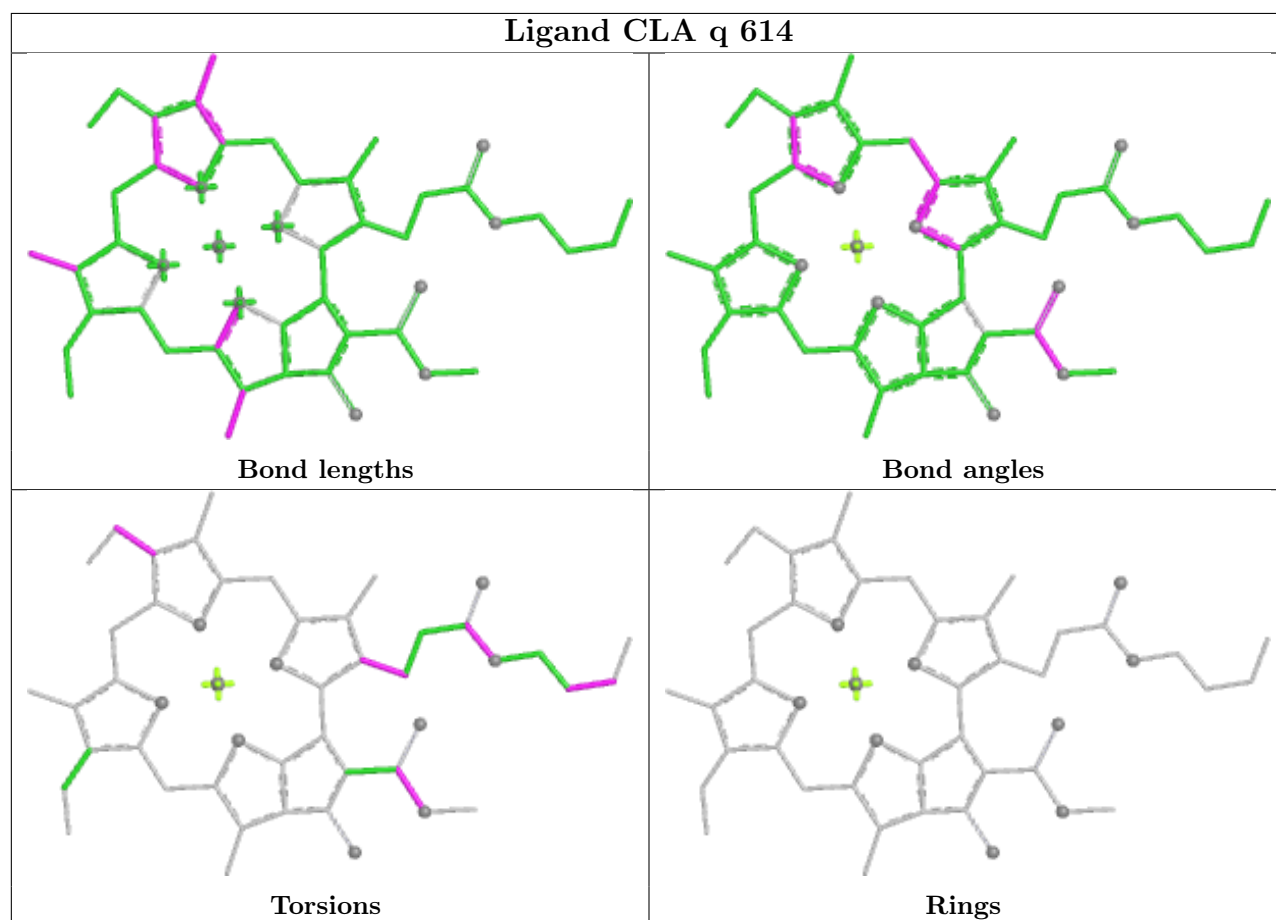
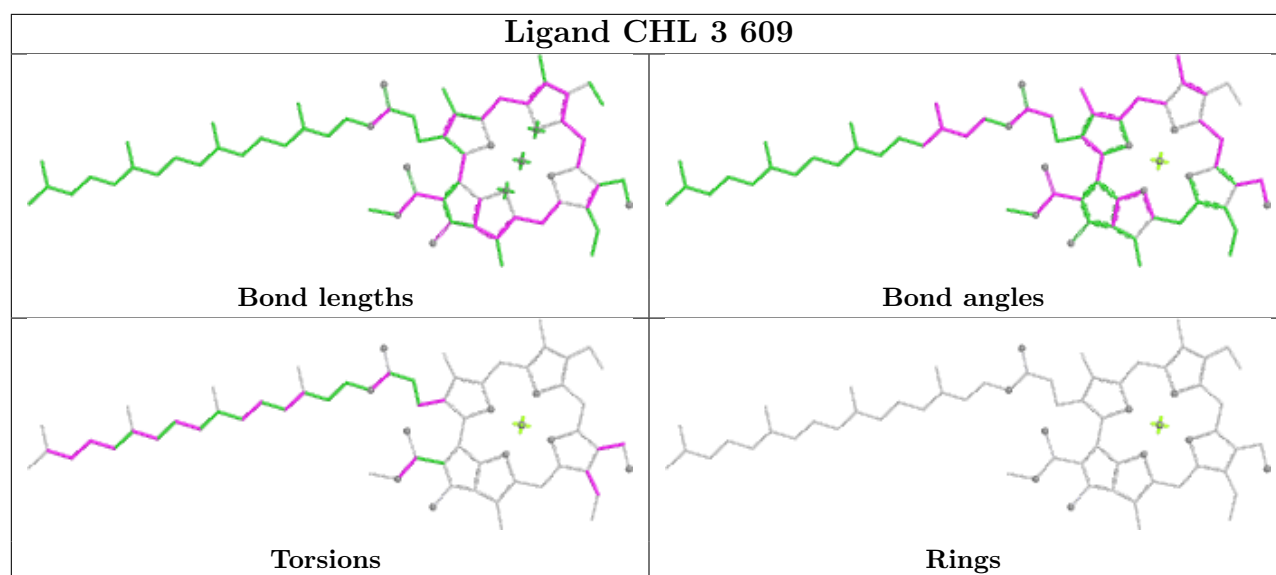


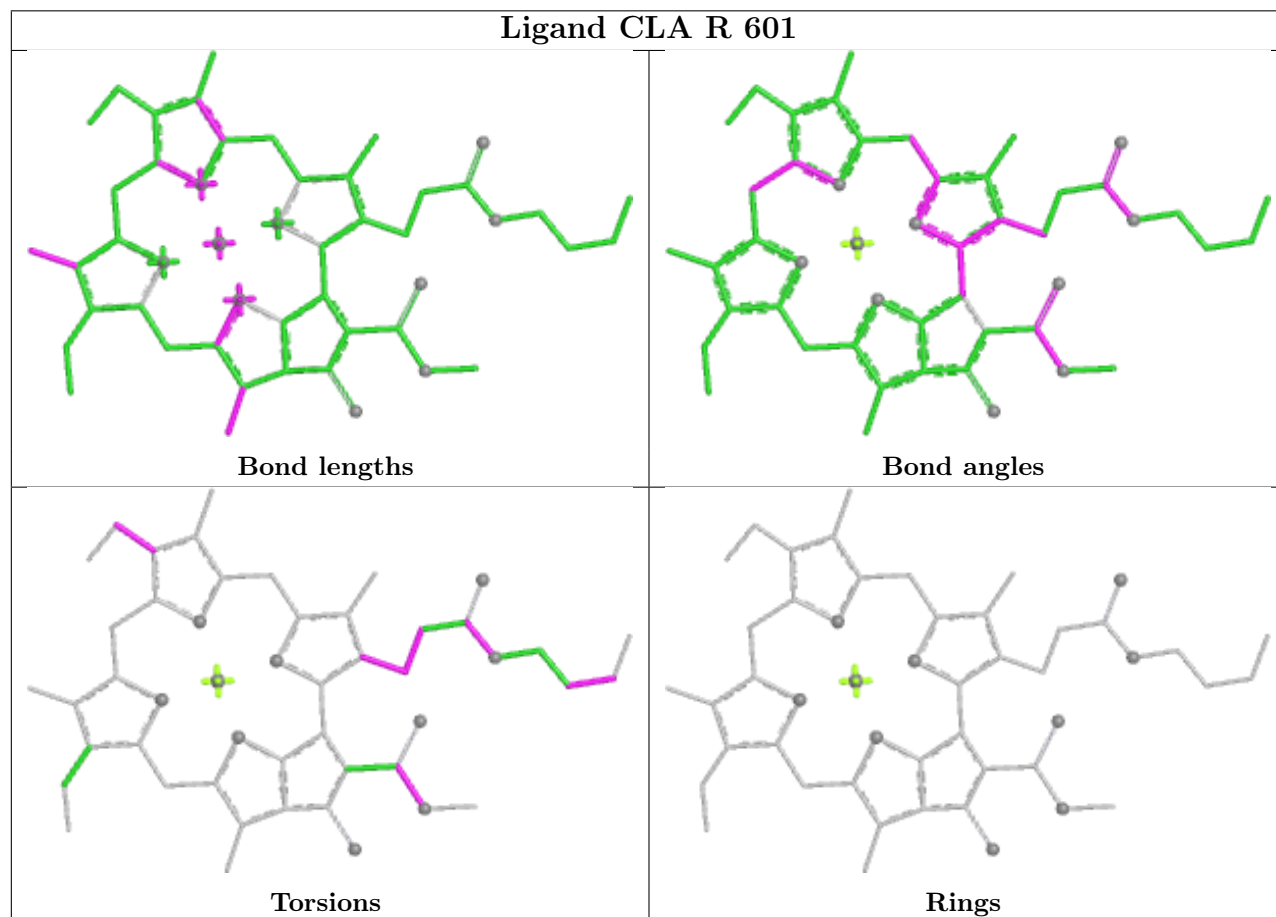
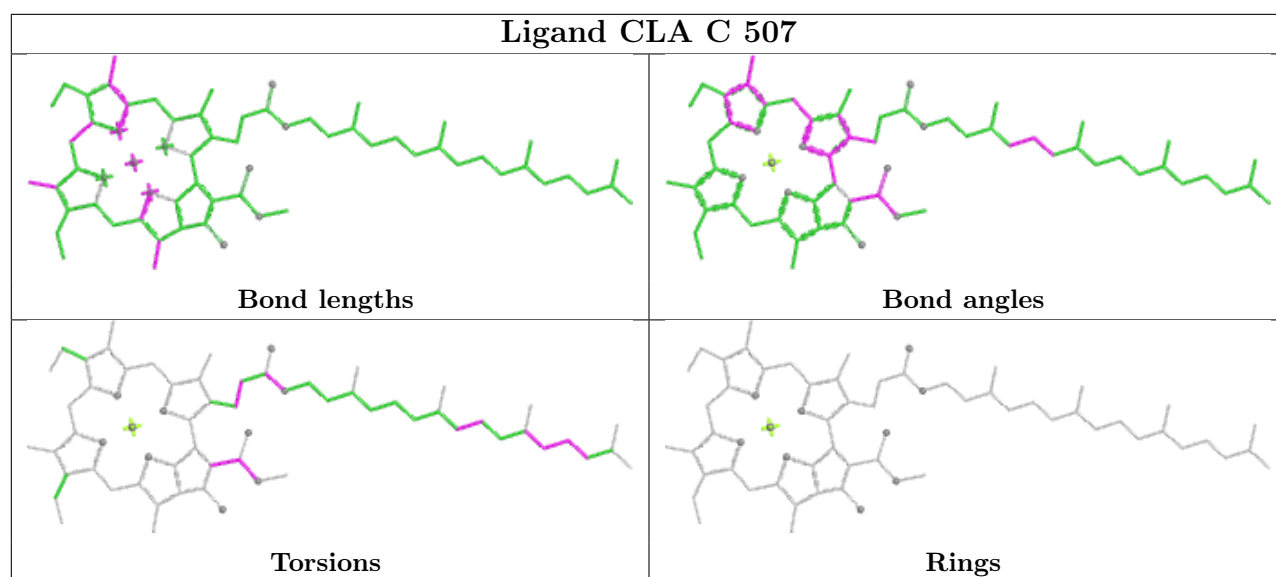


Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

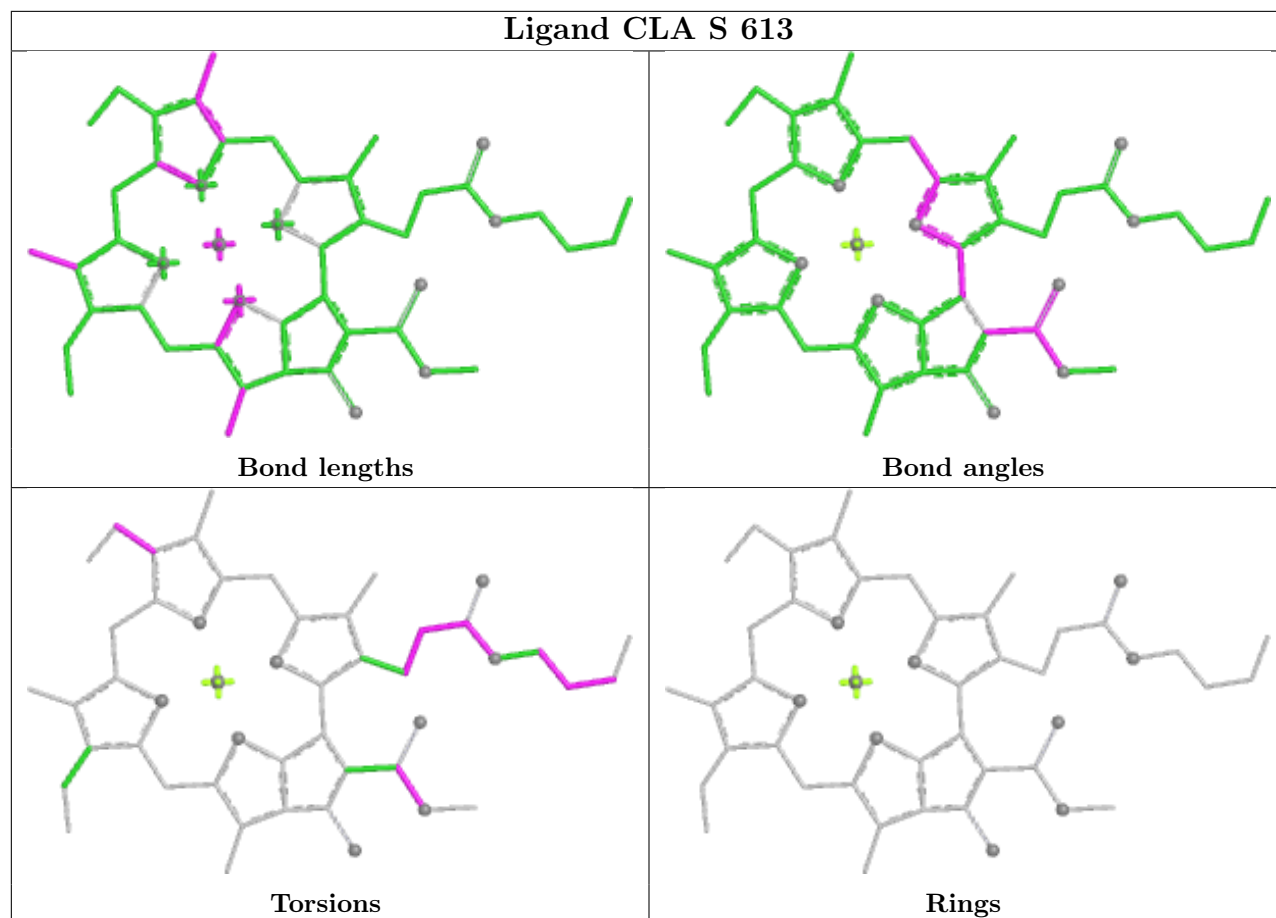
Ligand CLA 6 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 6 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

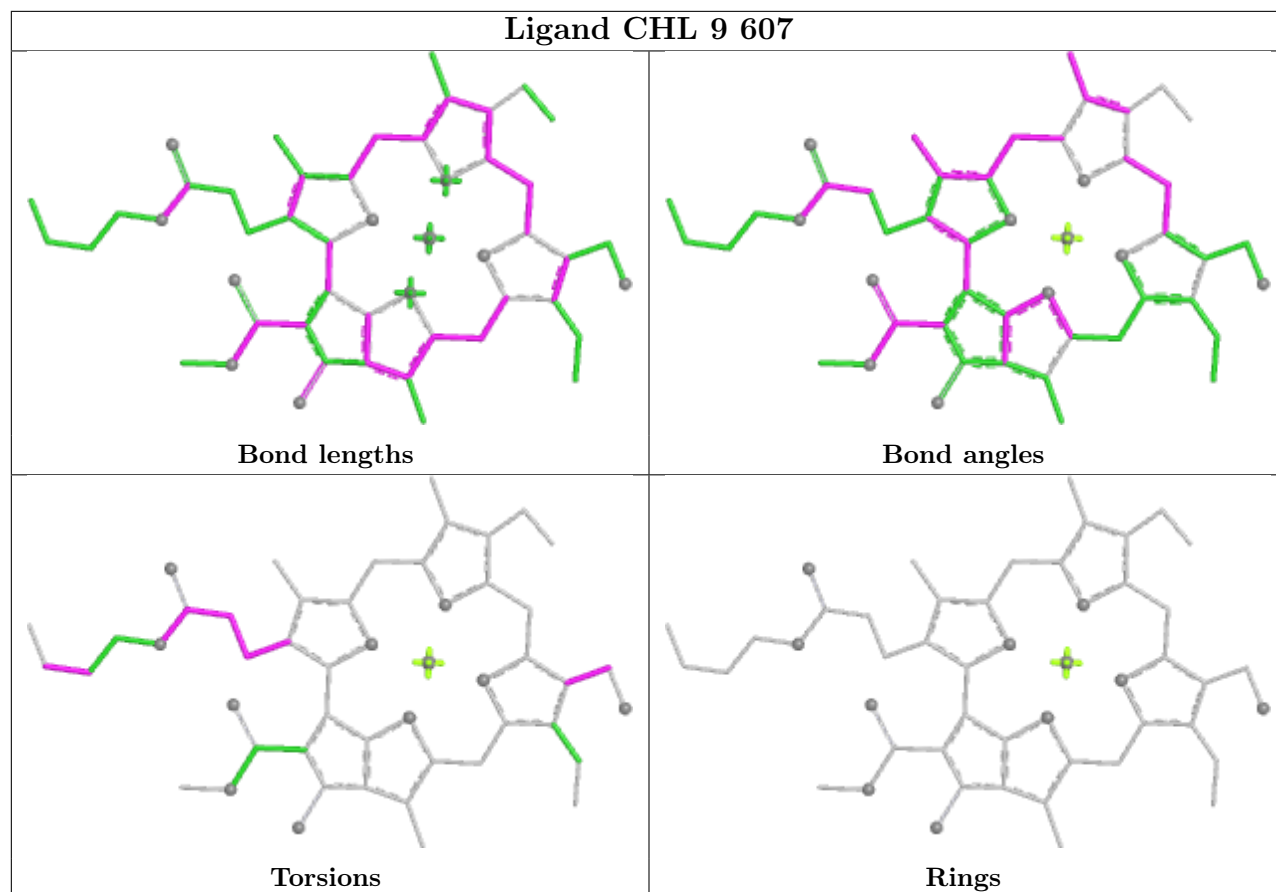




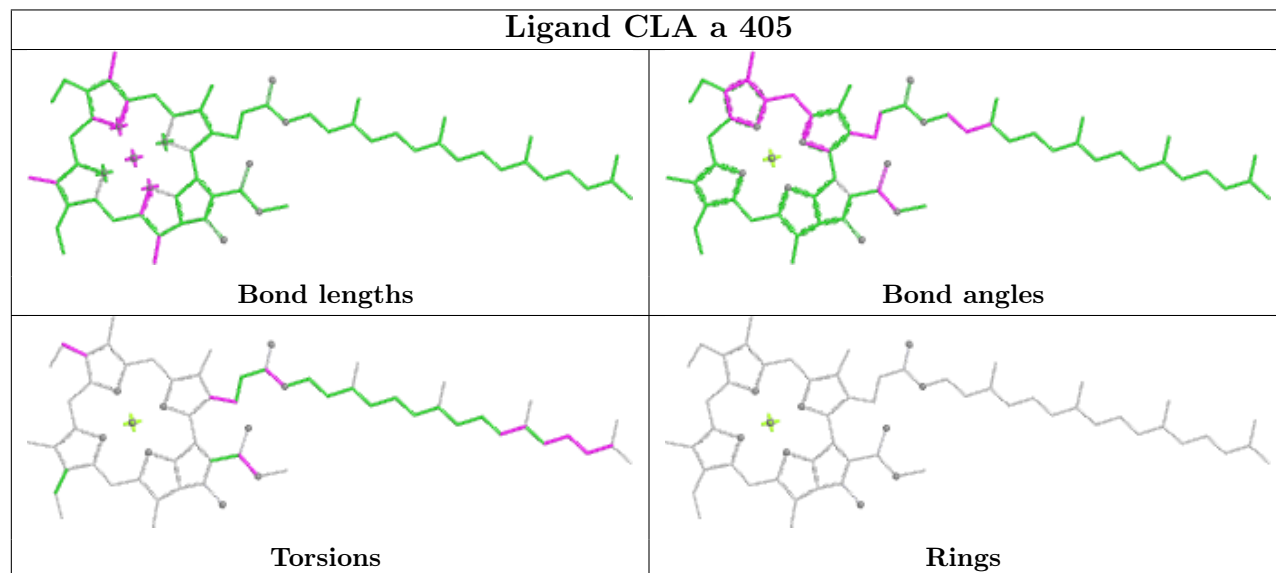
Ligand CLA S 613

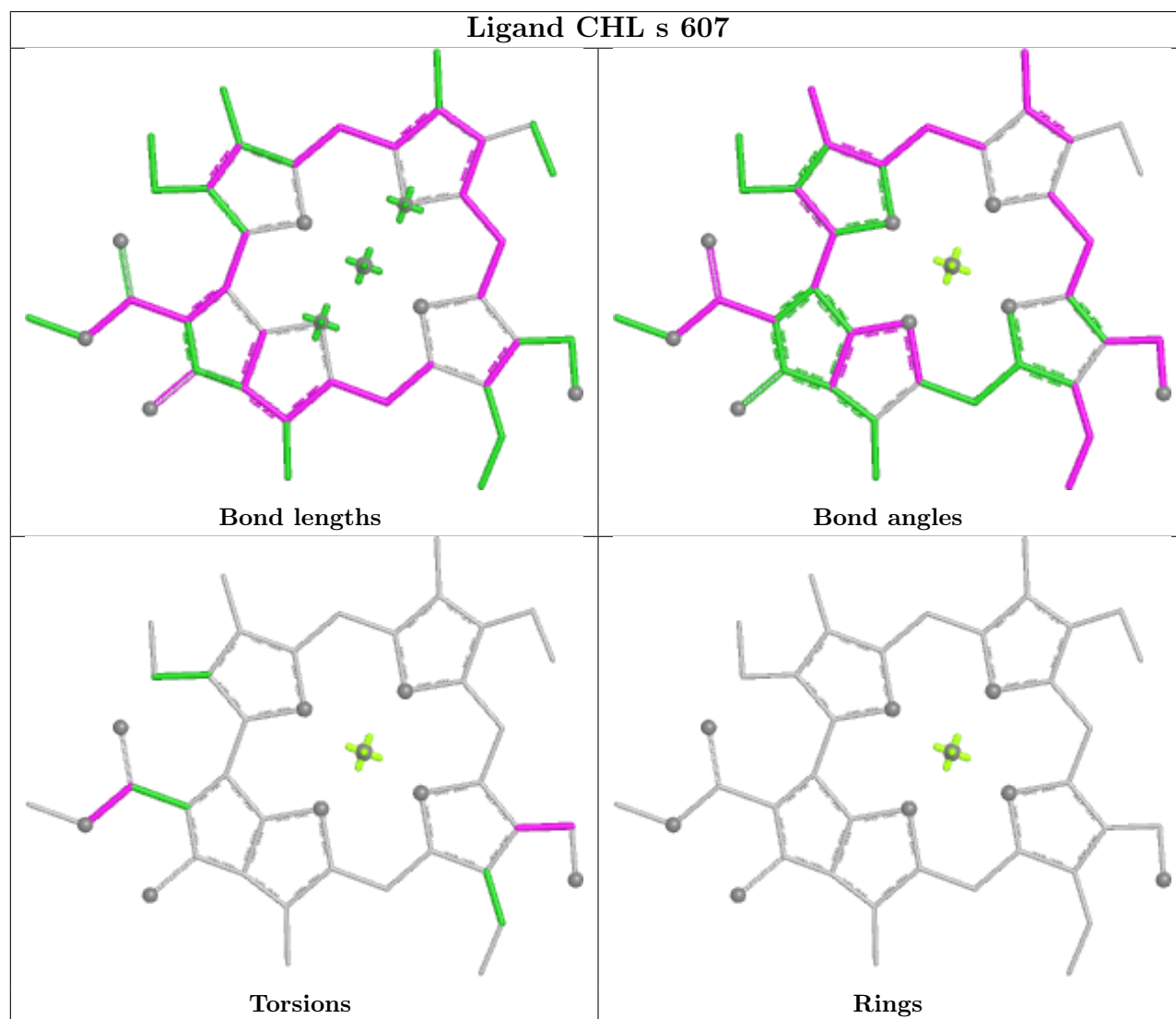
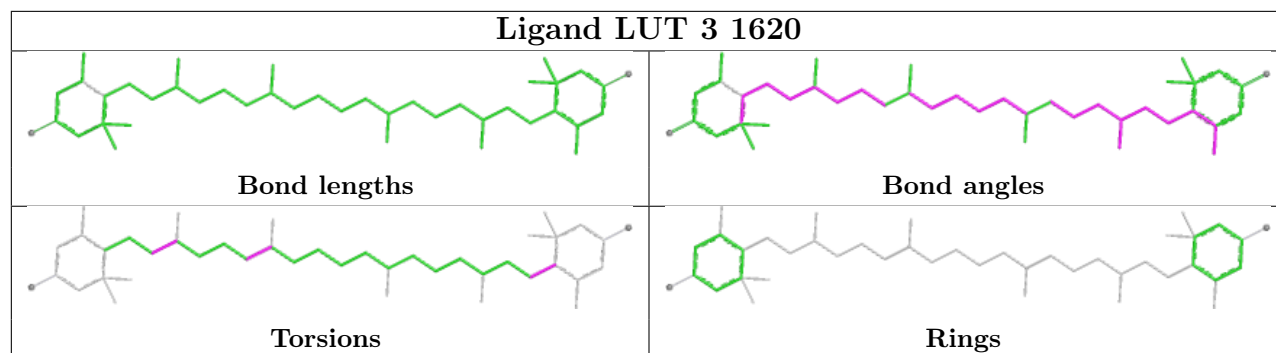


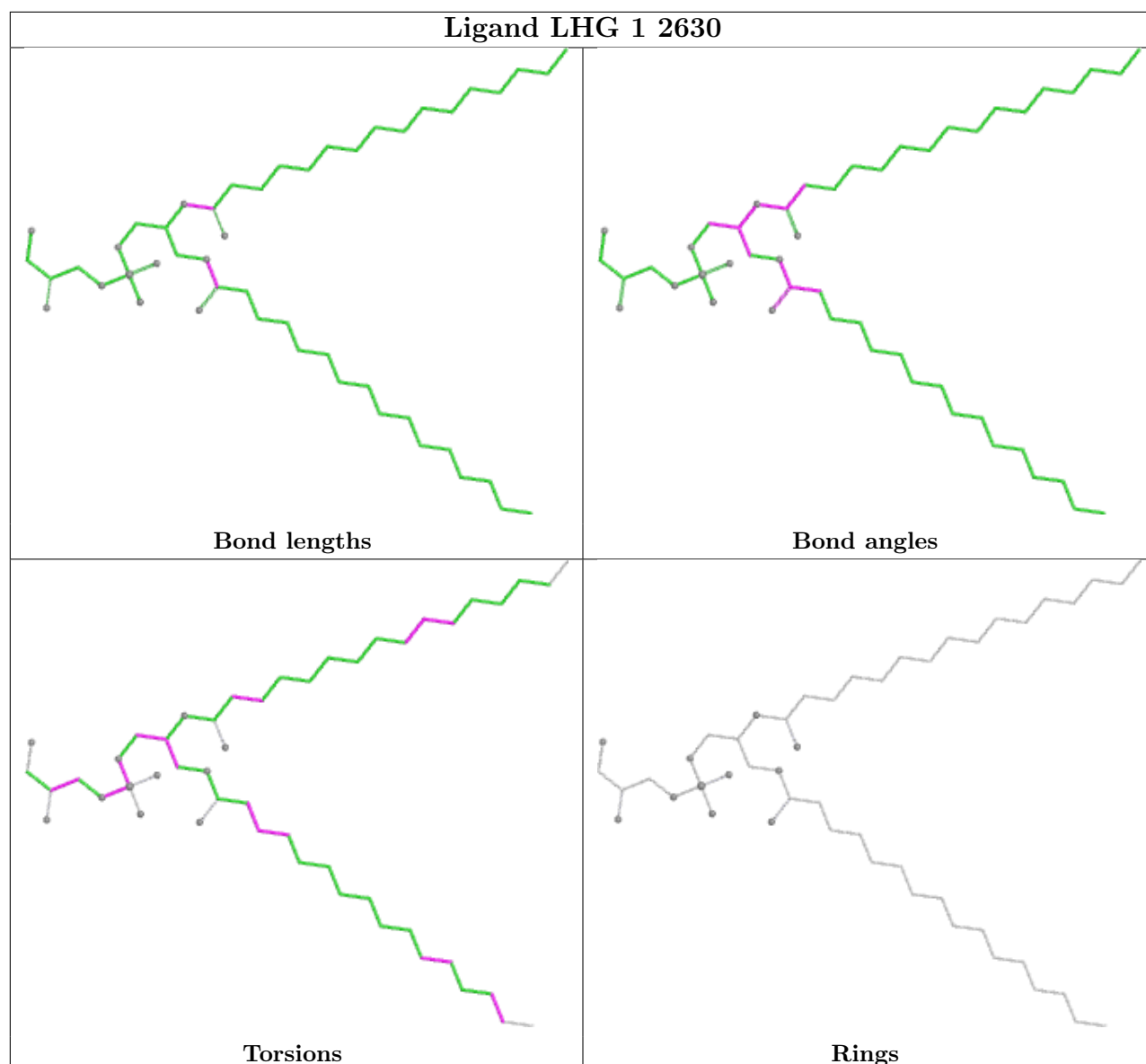
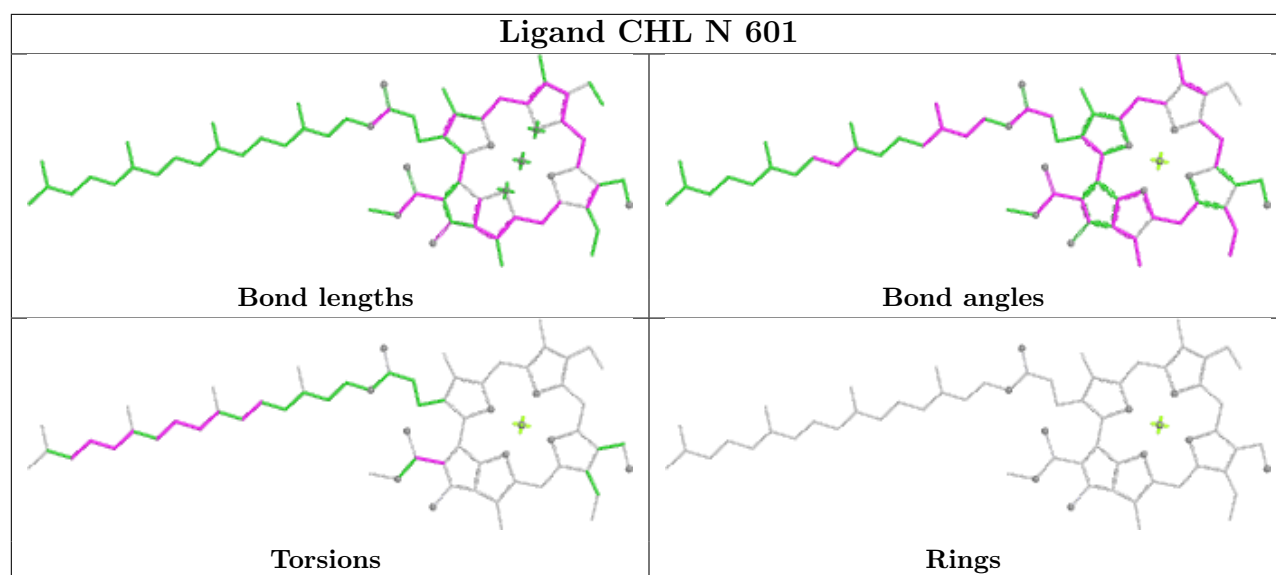
Ligand CHL 9 607

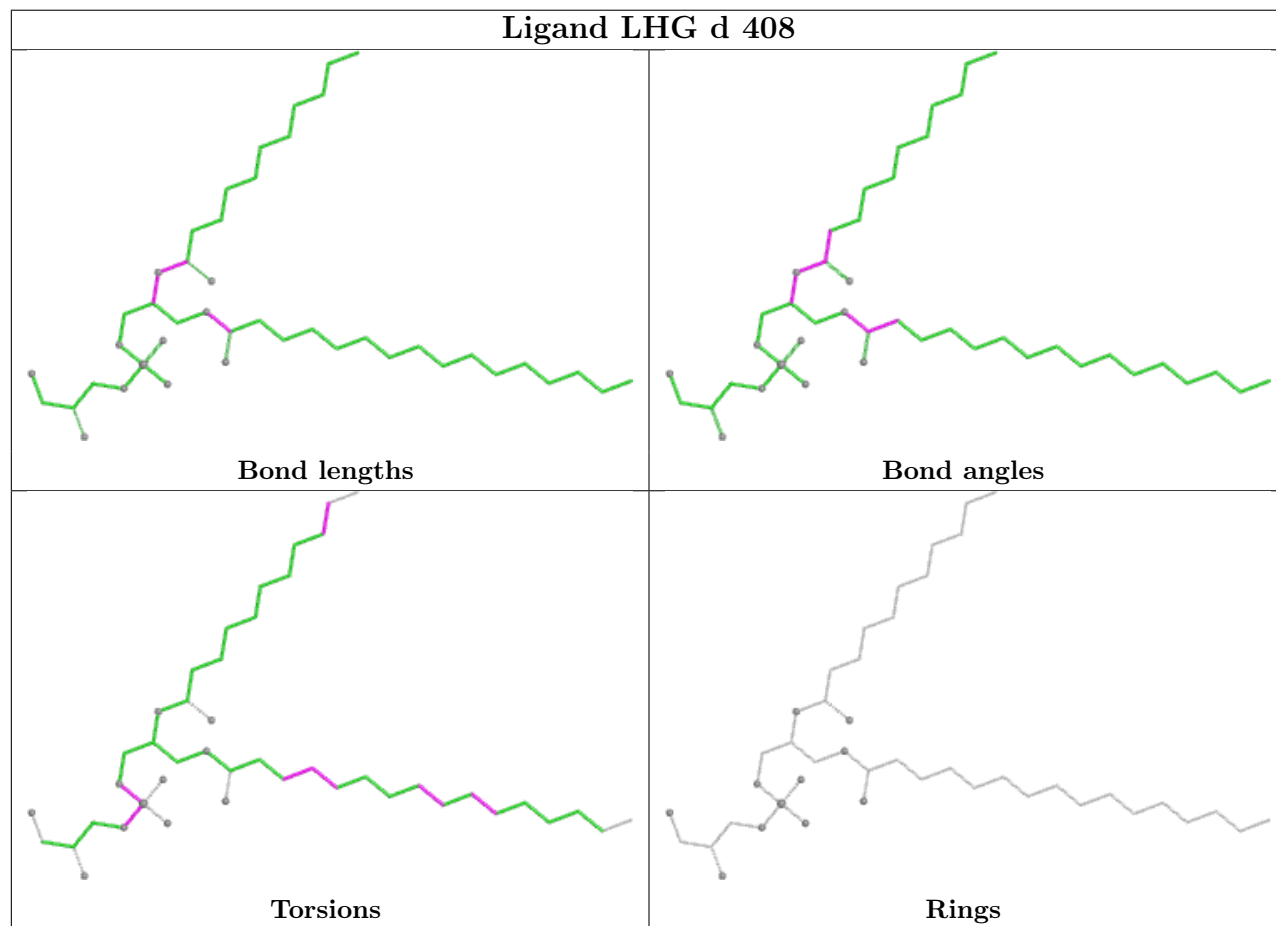
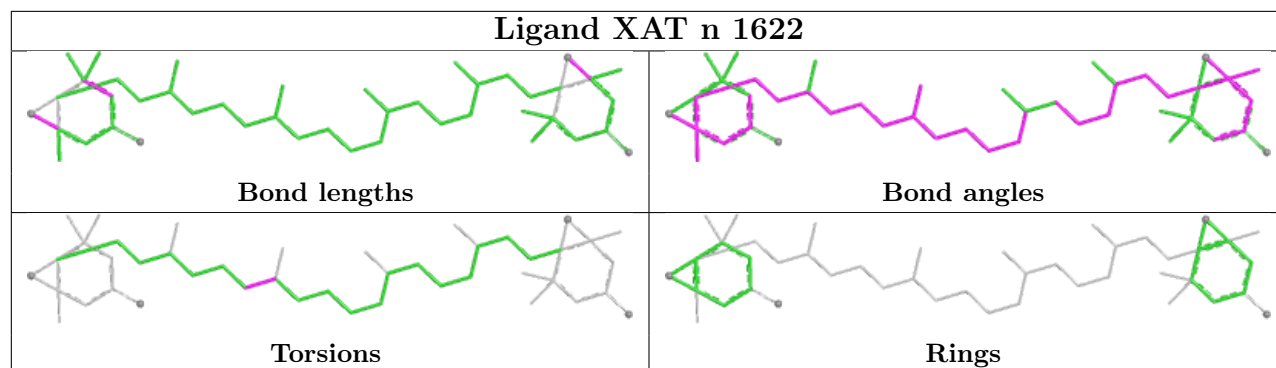


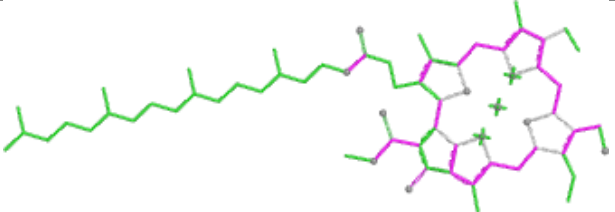
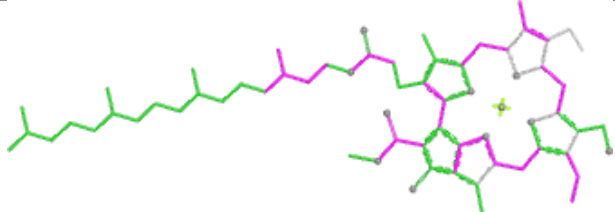
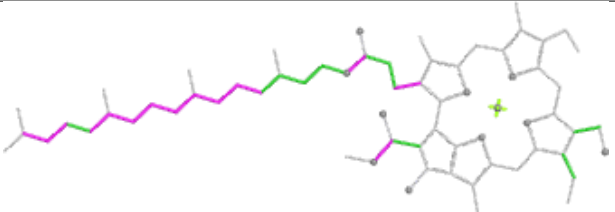
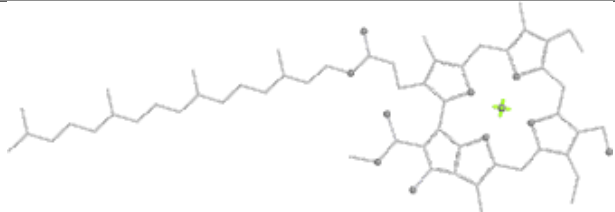
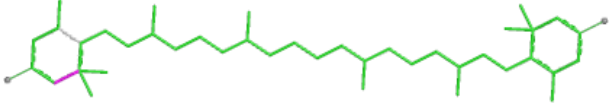
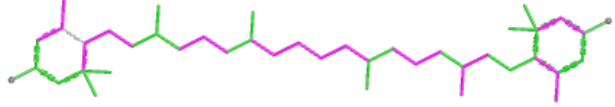
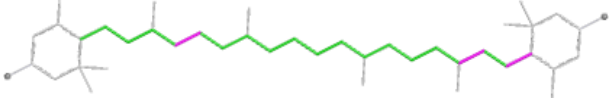
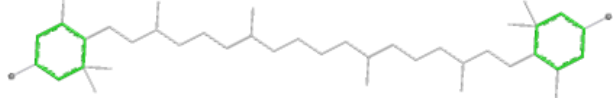
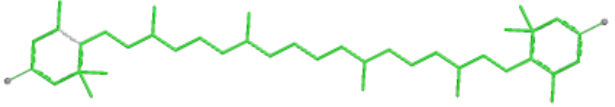
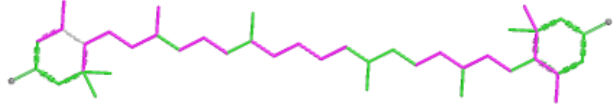
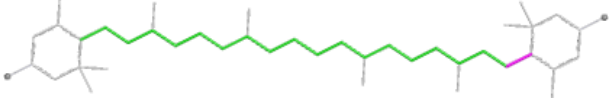
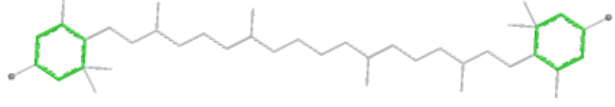
Ligand CLA a 405

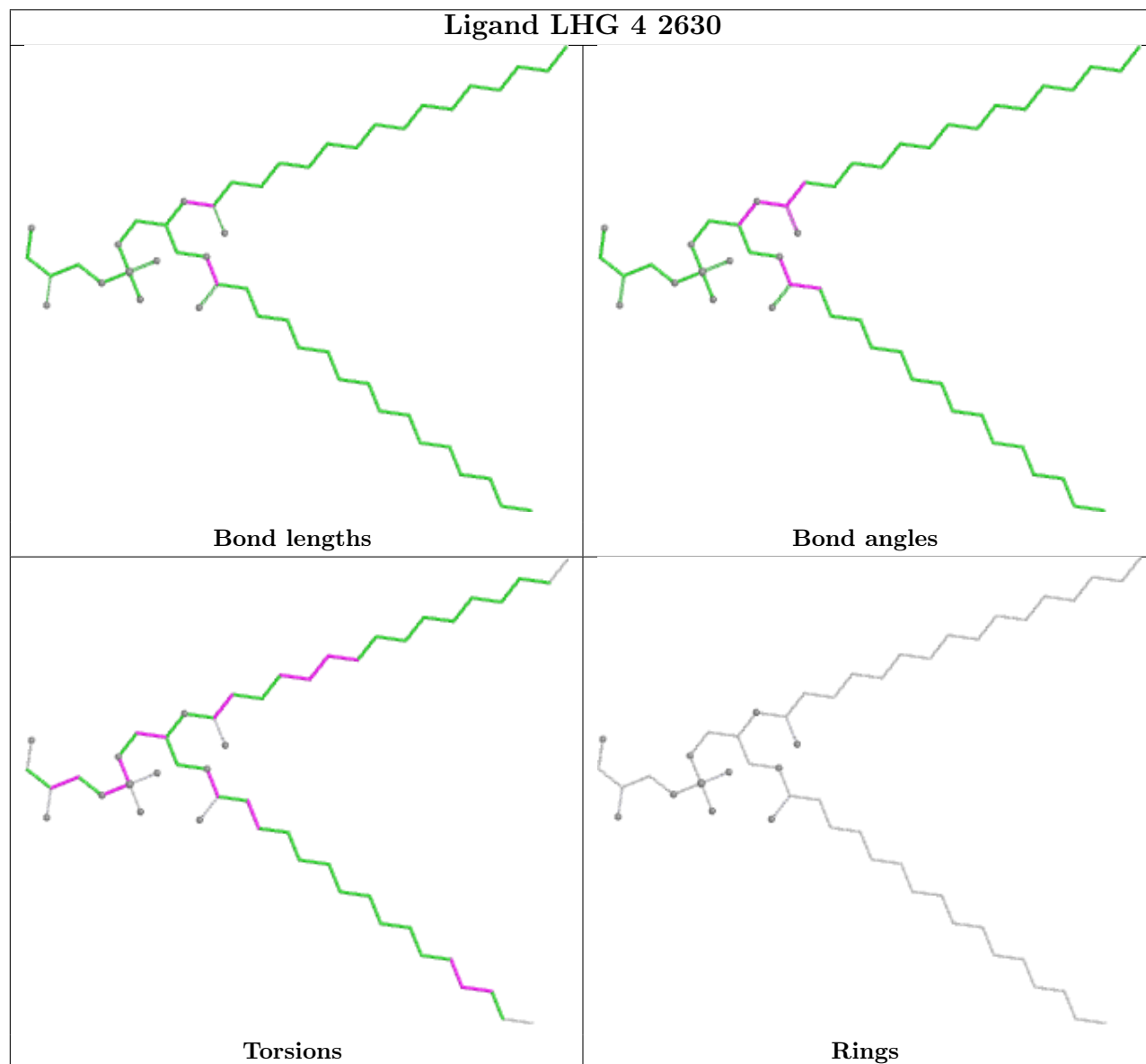
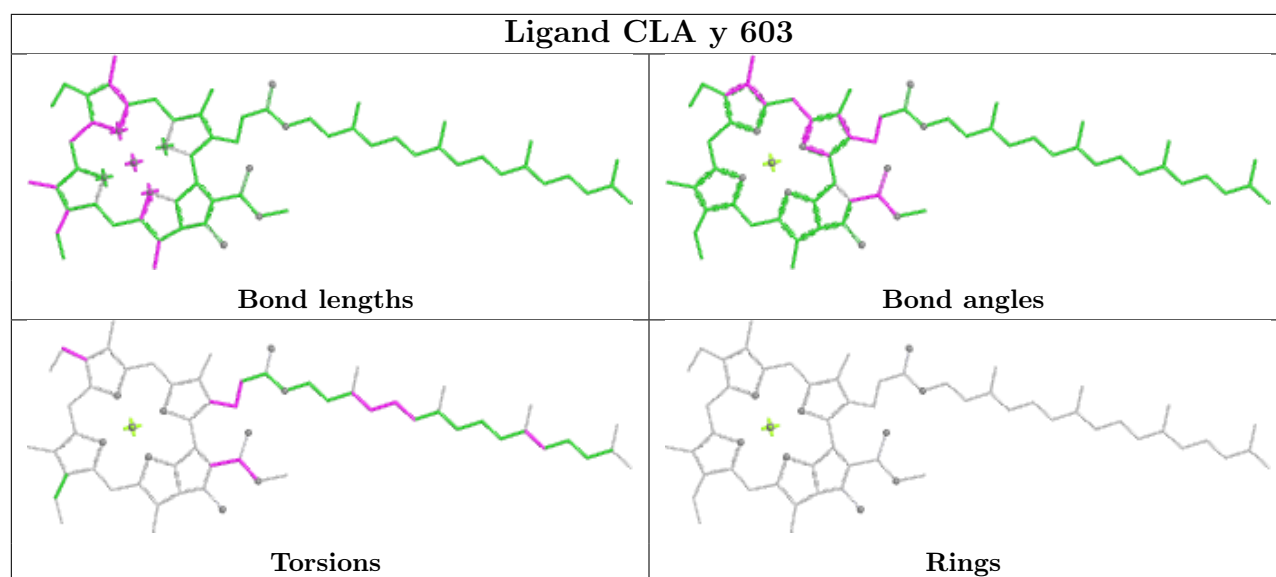




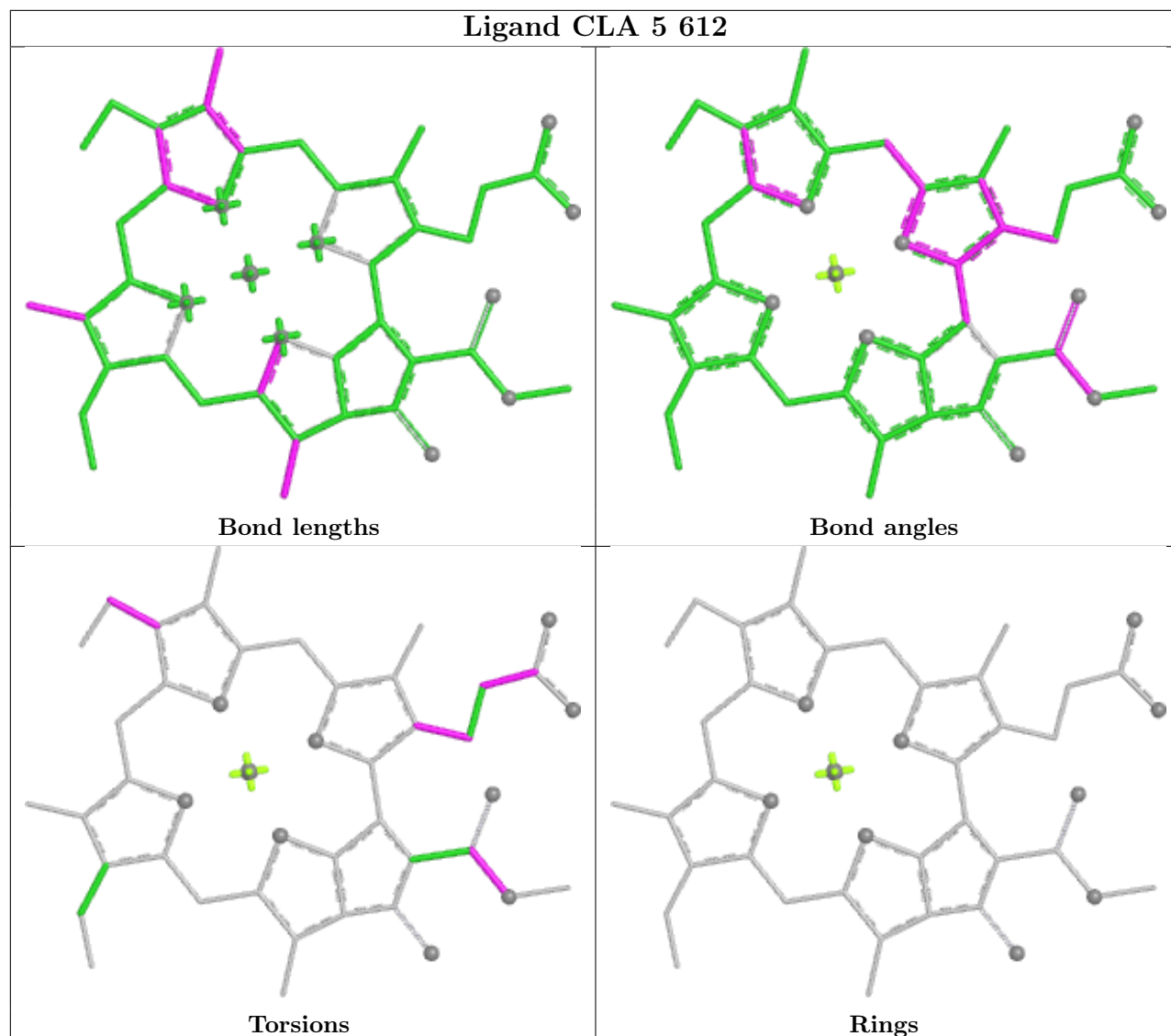




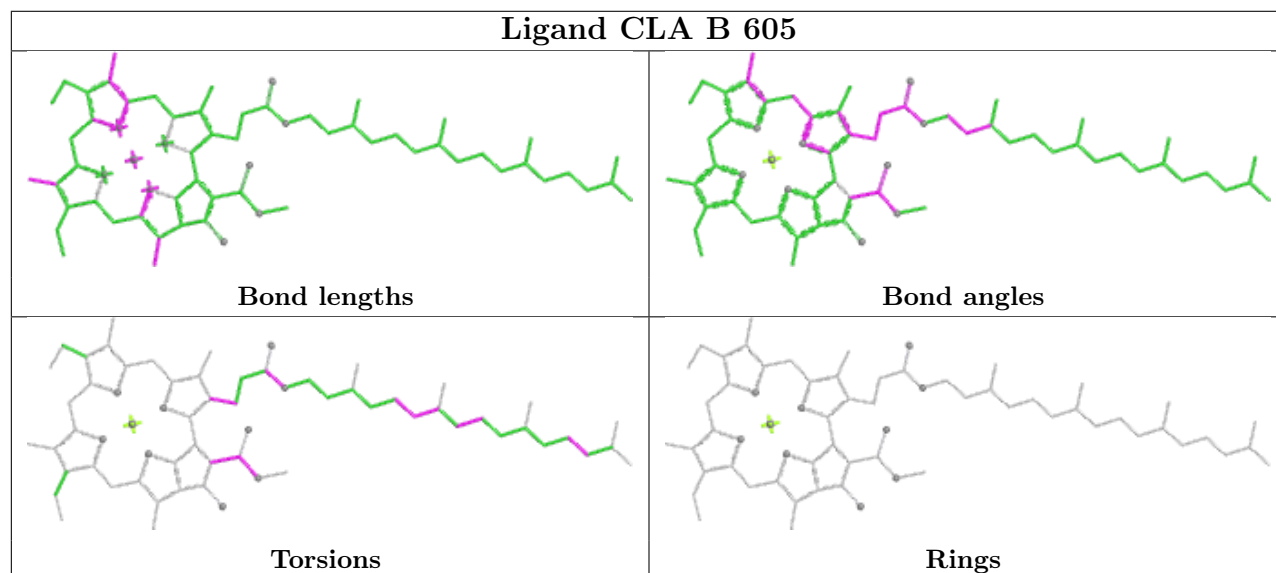
Ligand CHL 8 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT N 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 2 1620	
 Bond lengths	 Bond angles
 Torsions	 Rings

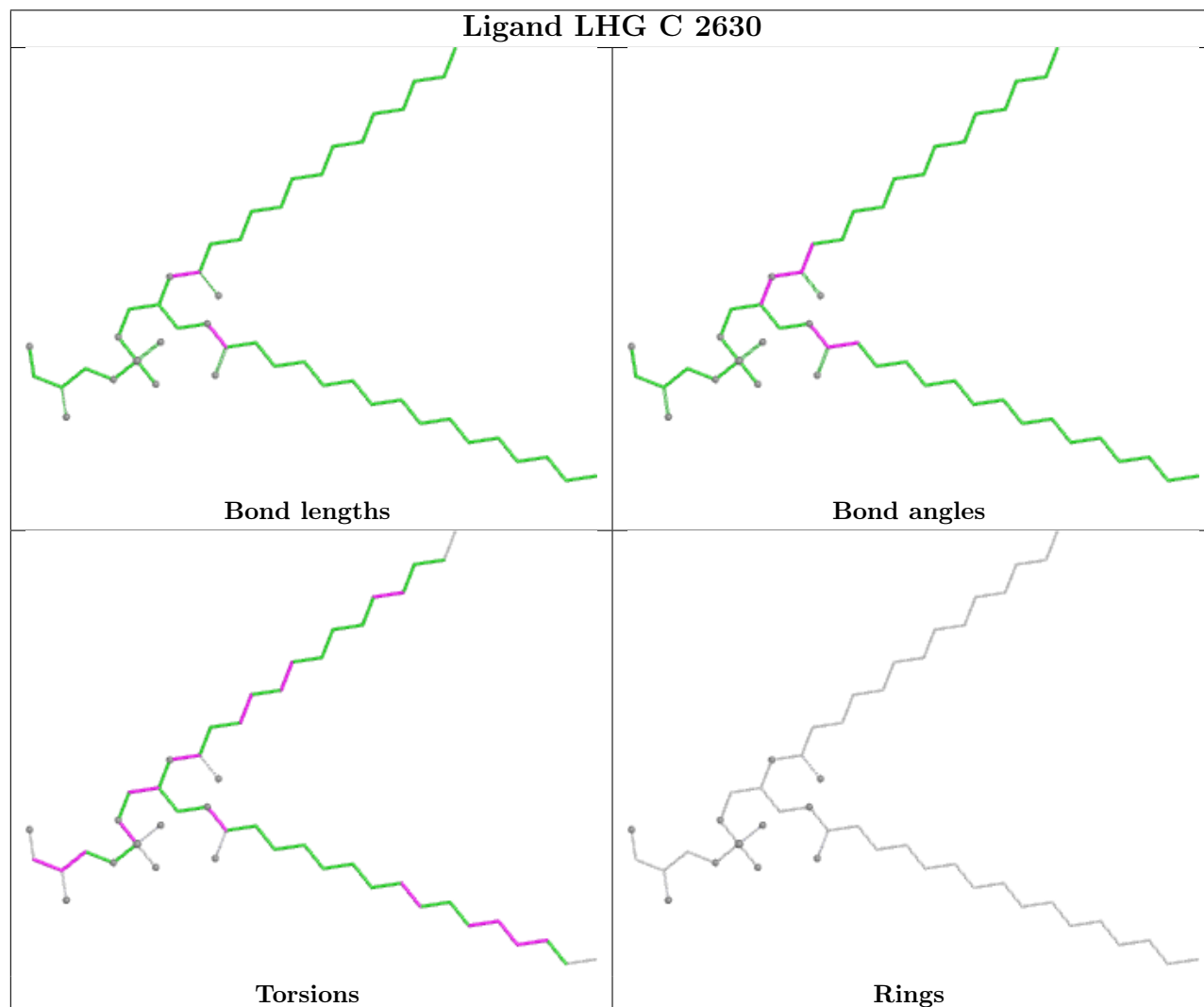
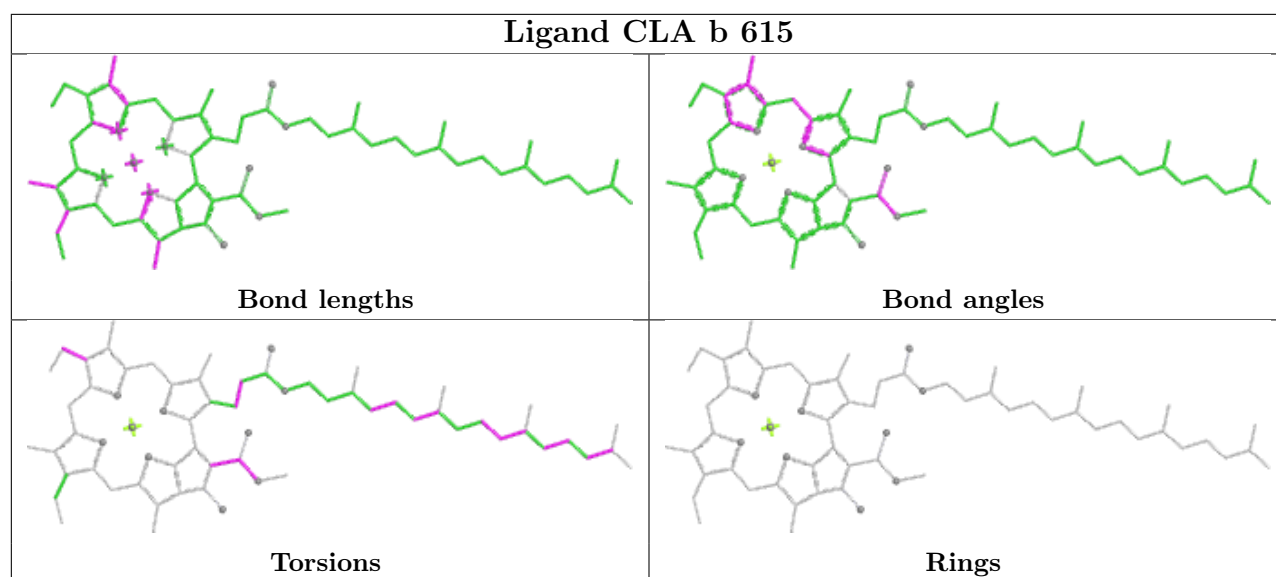


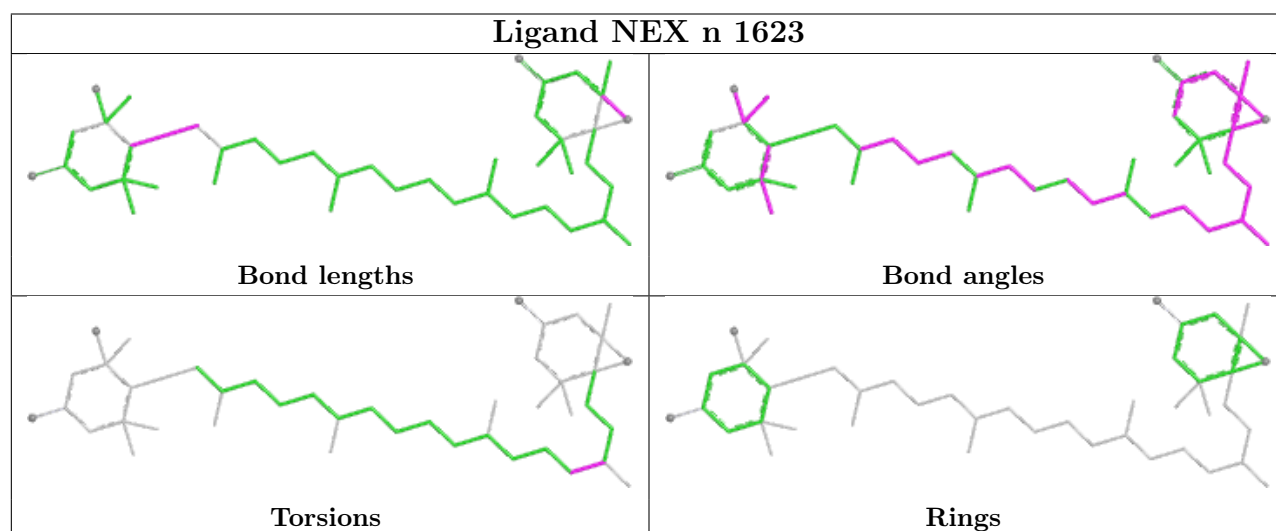
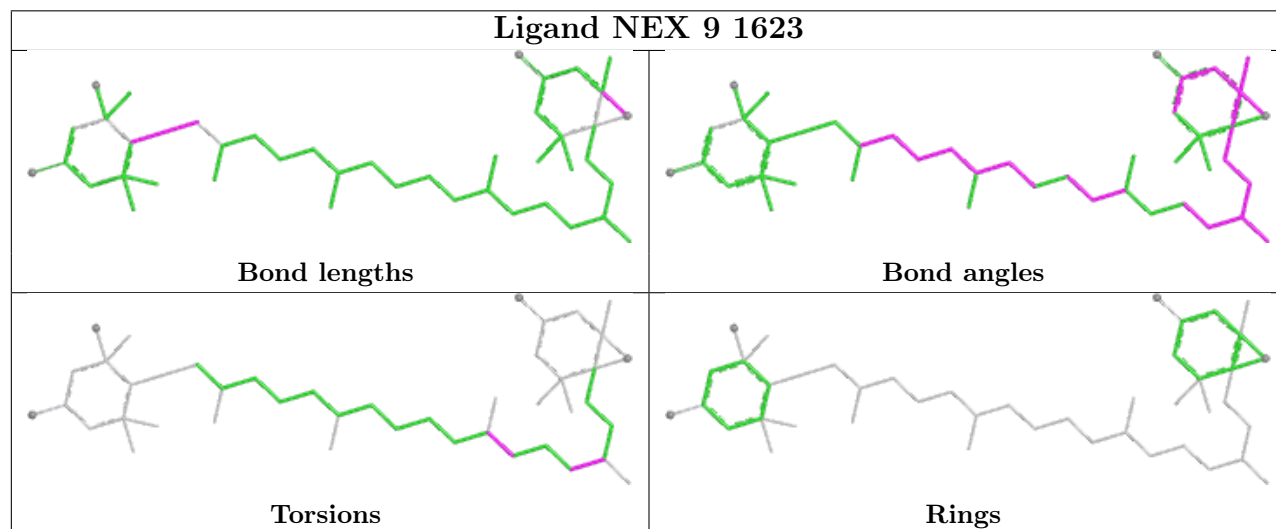
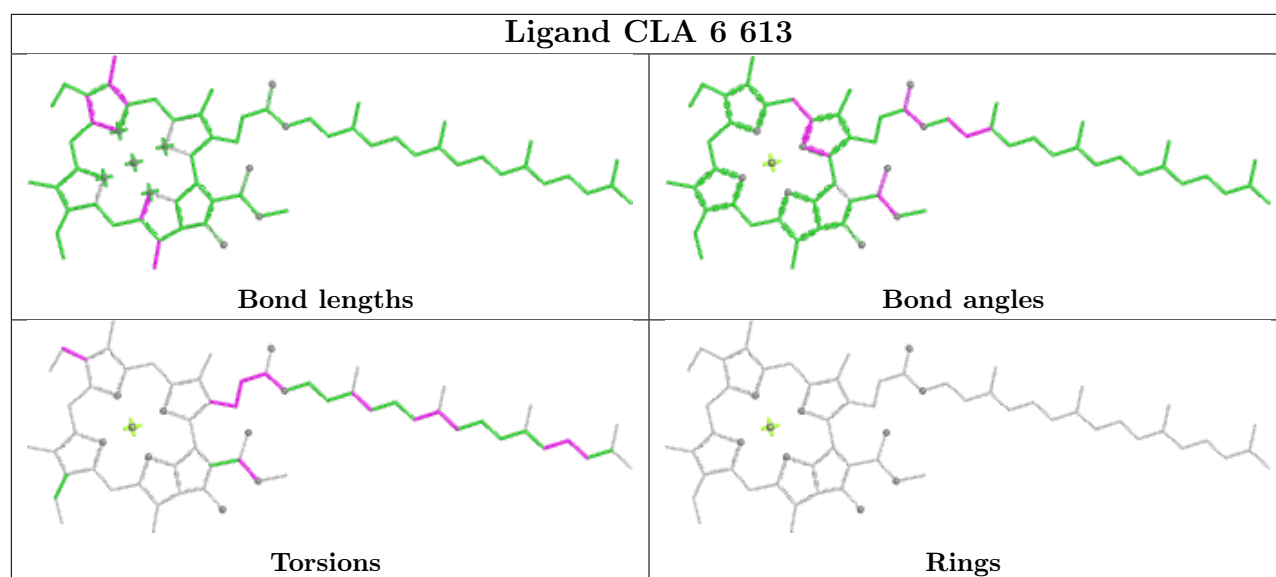
Ligand CLA 5 612

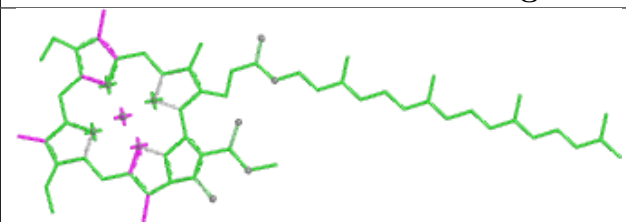
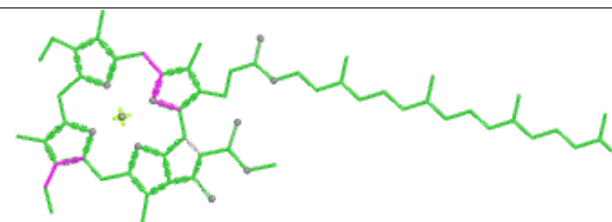
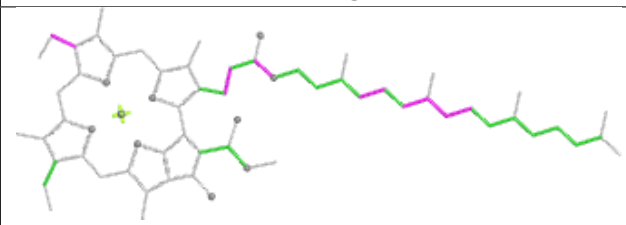
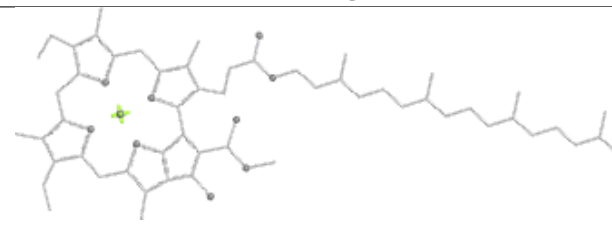
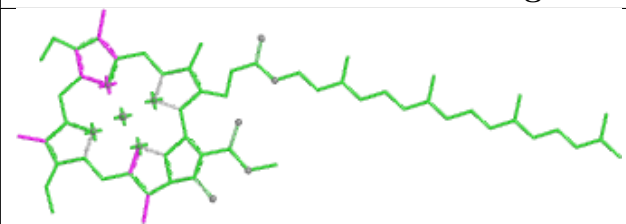
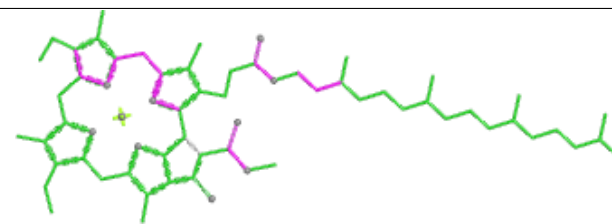
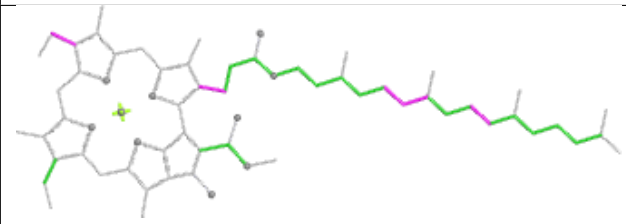
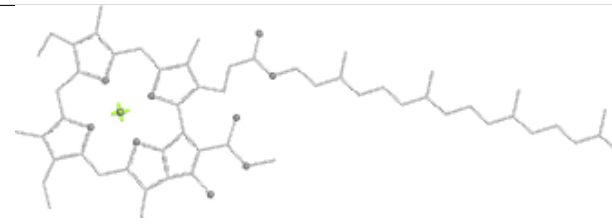
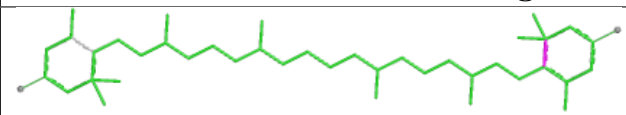
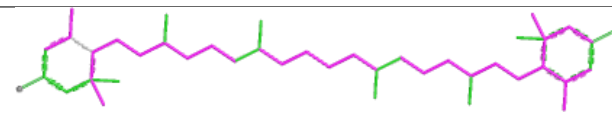
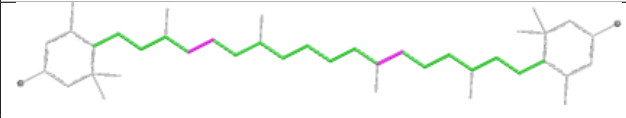
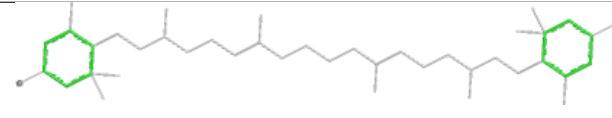


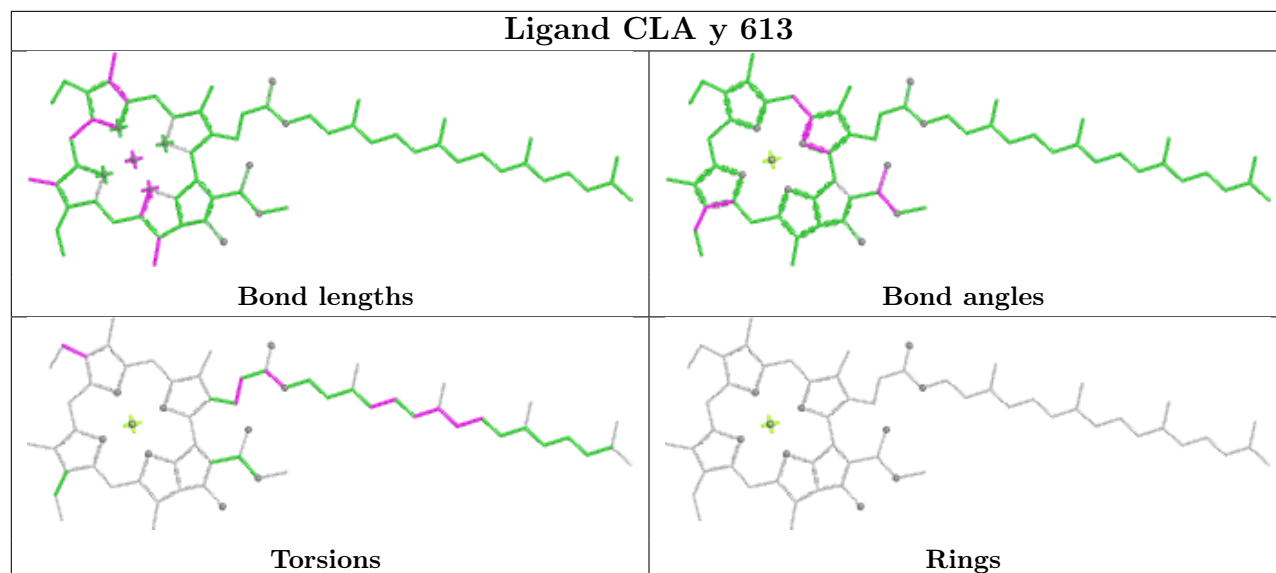
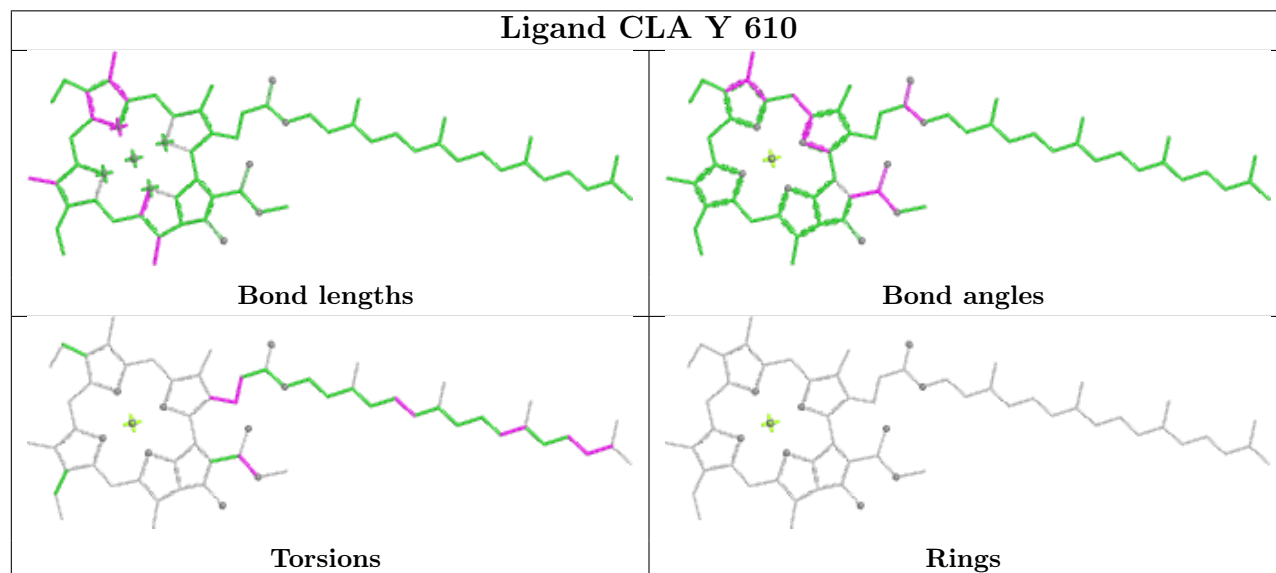
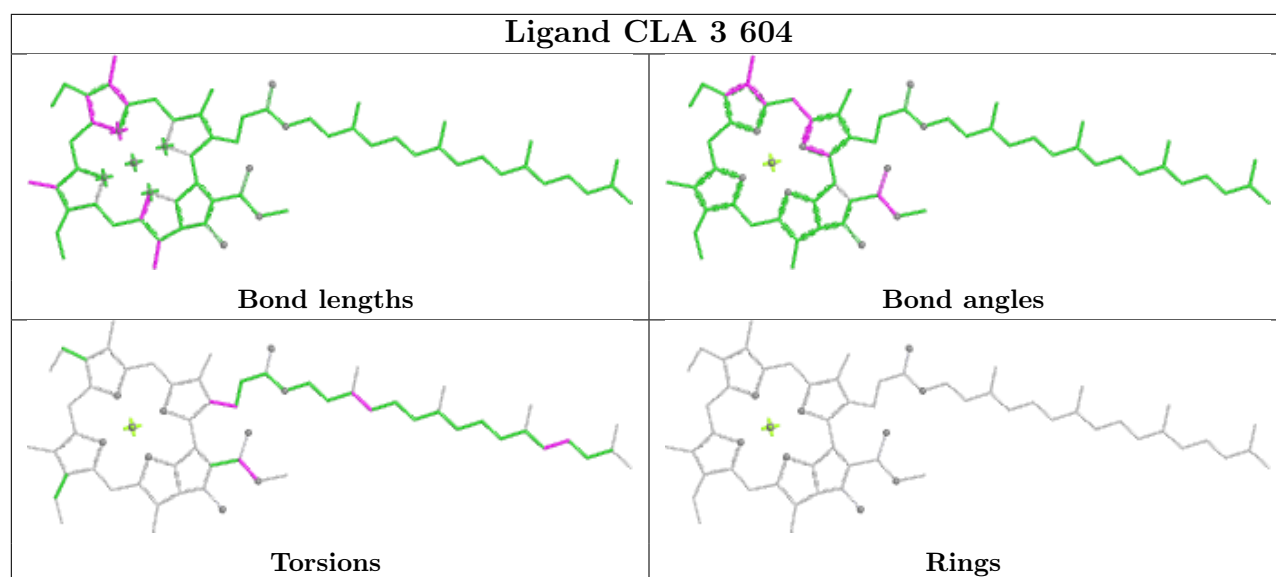
Ligand CLA B 605

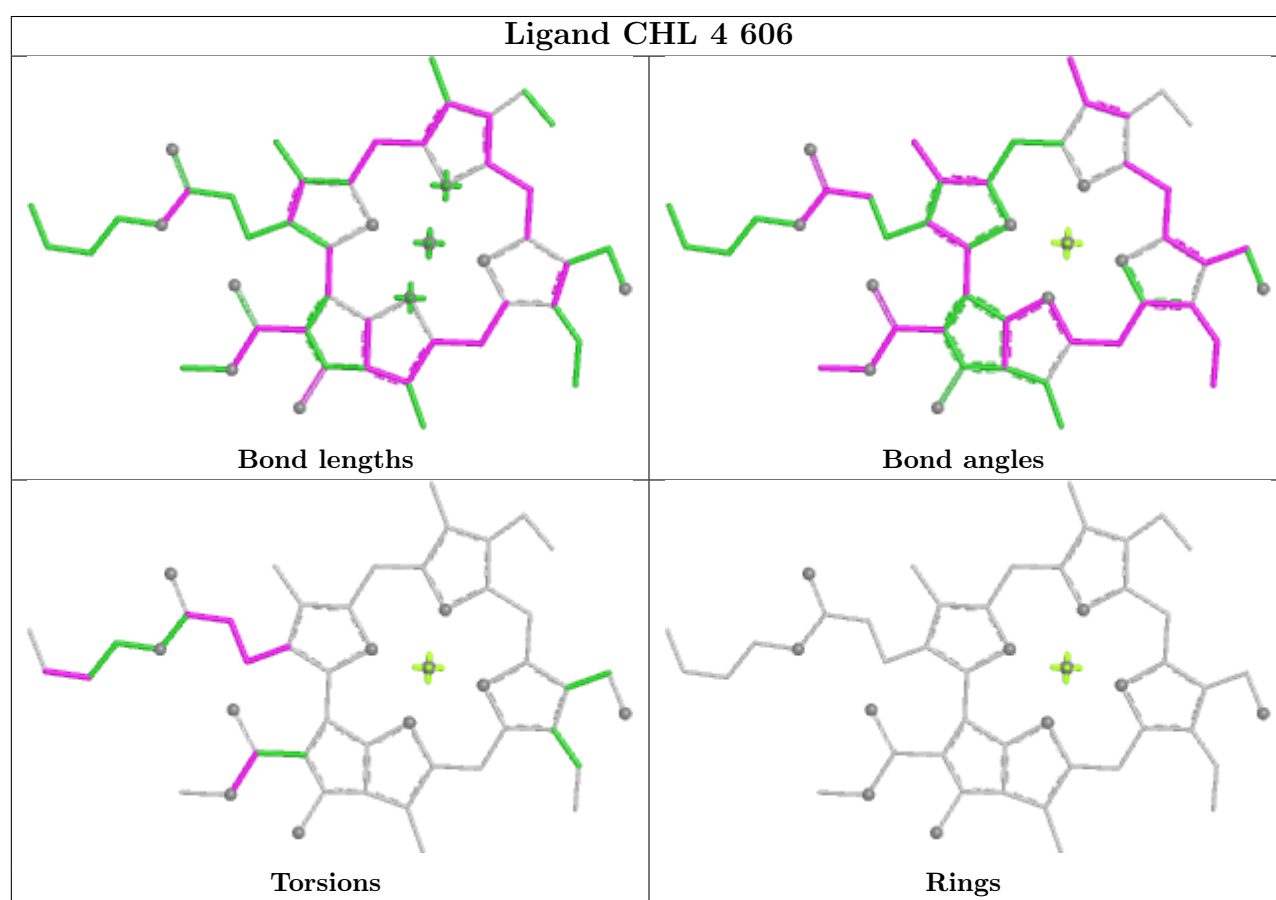
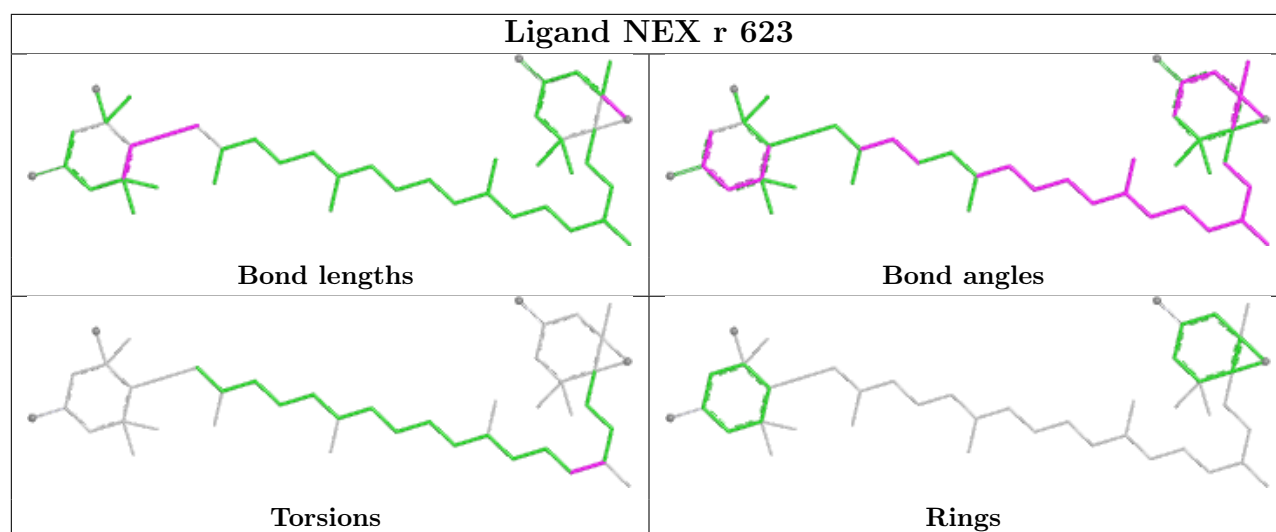


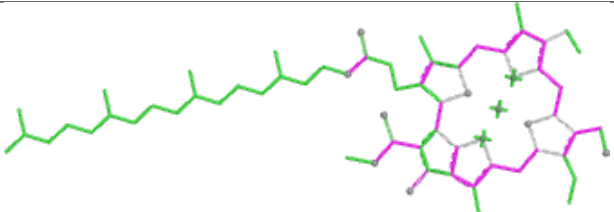
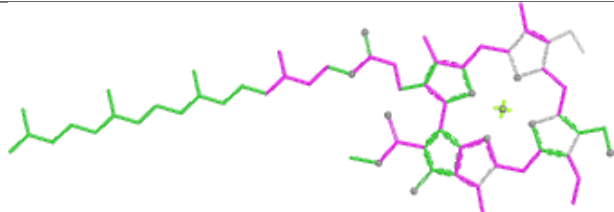
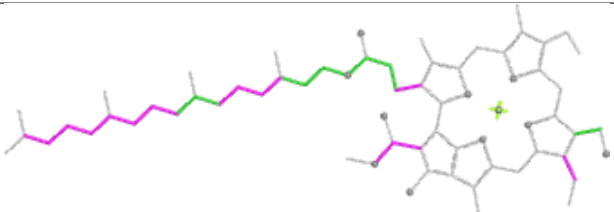
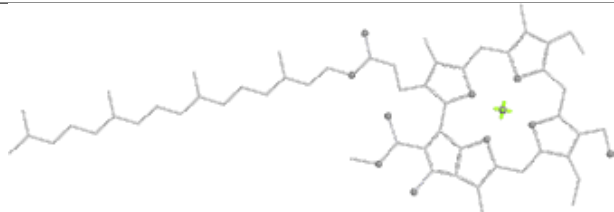


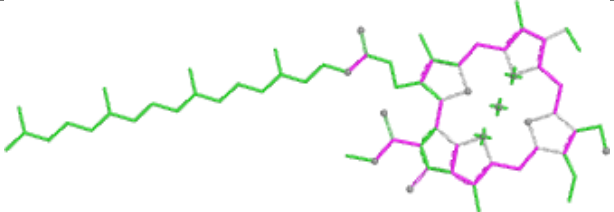
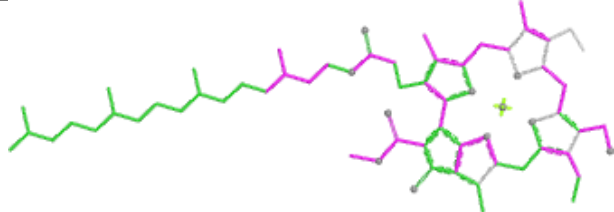
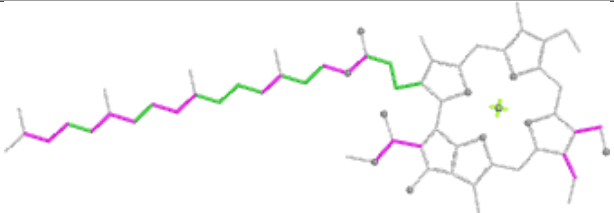
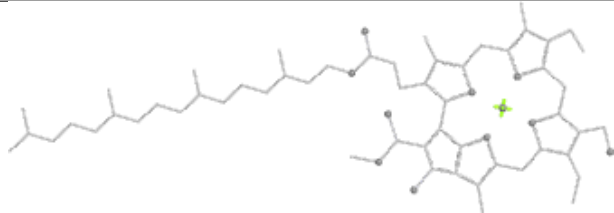


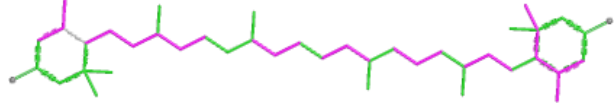
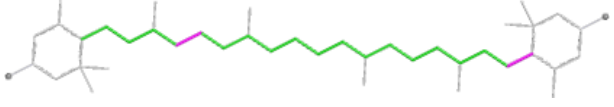
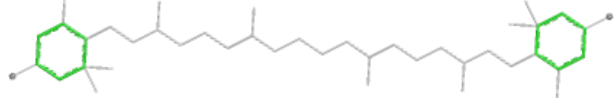
Ligand CLA Y 613	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA n 610	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT 1 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

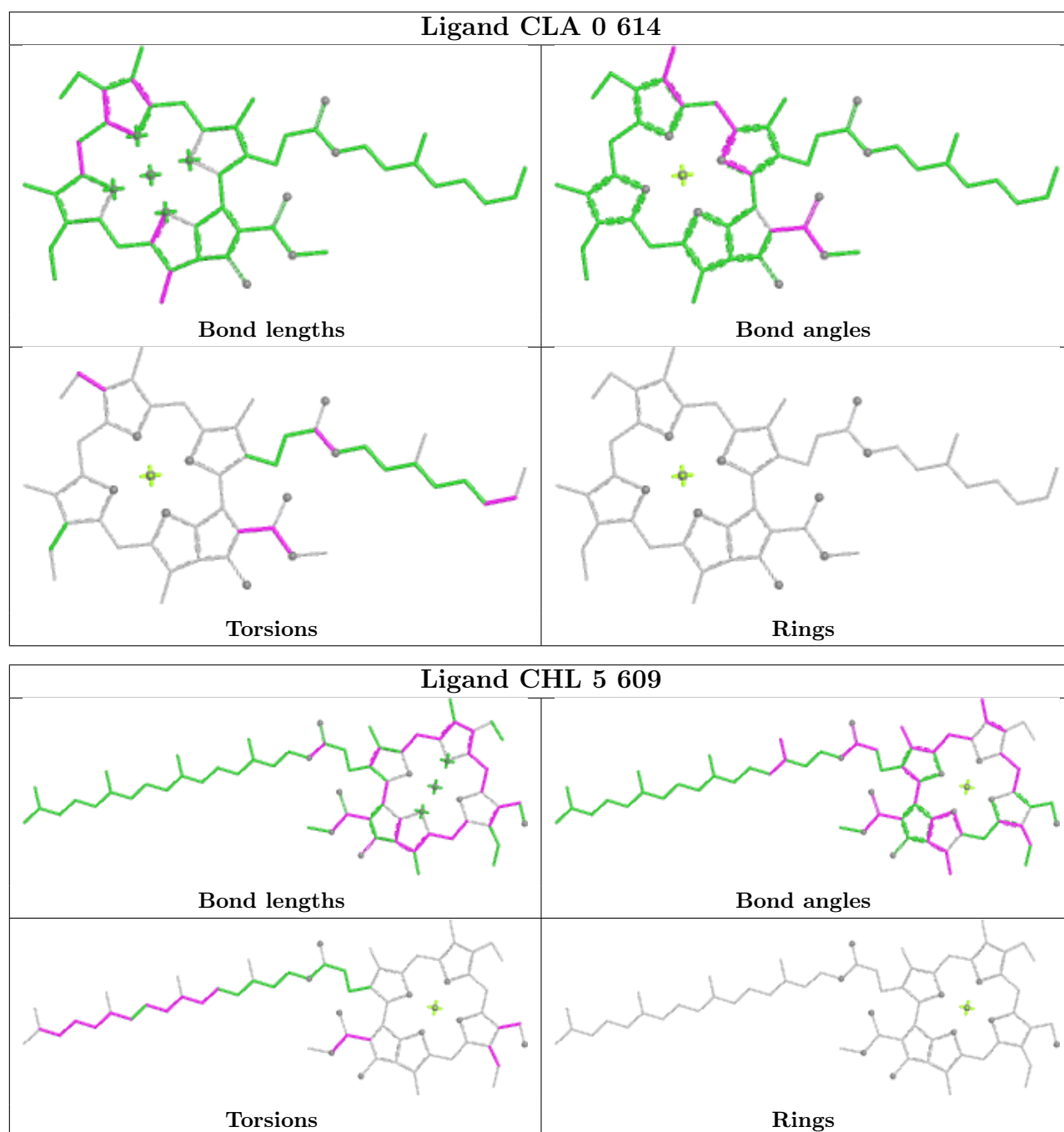


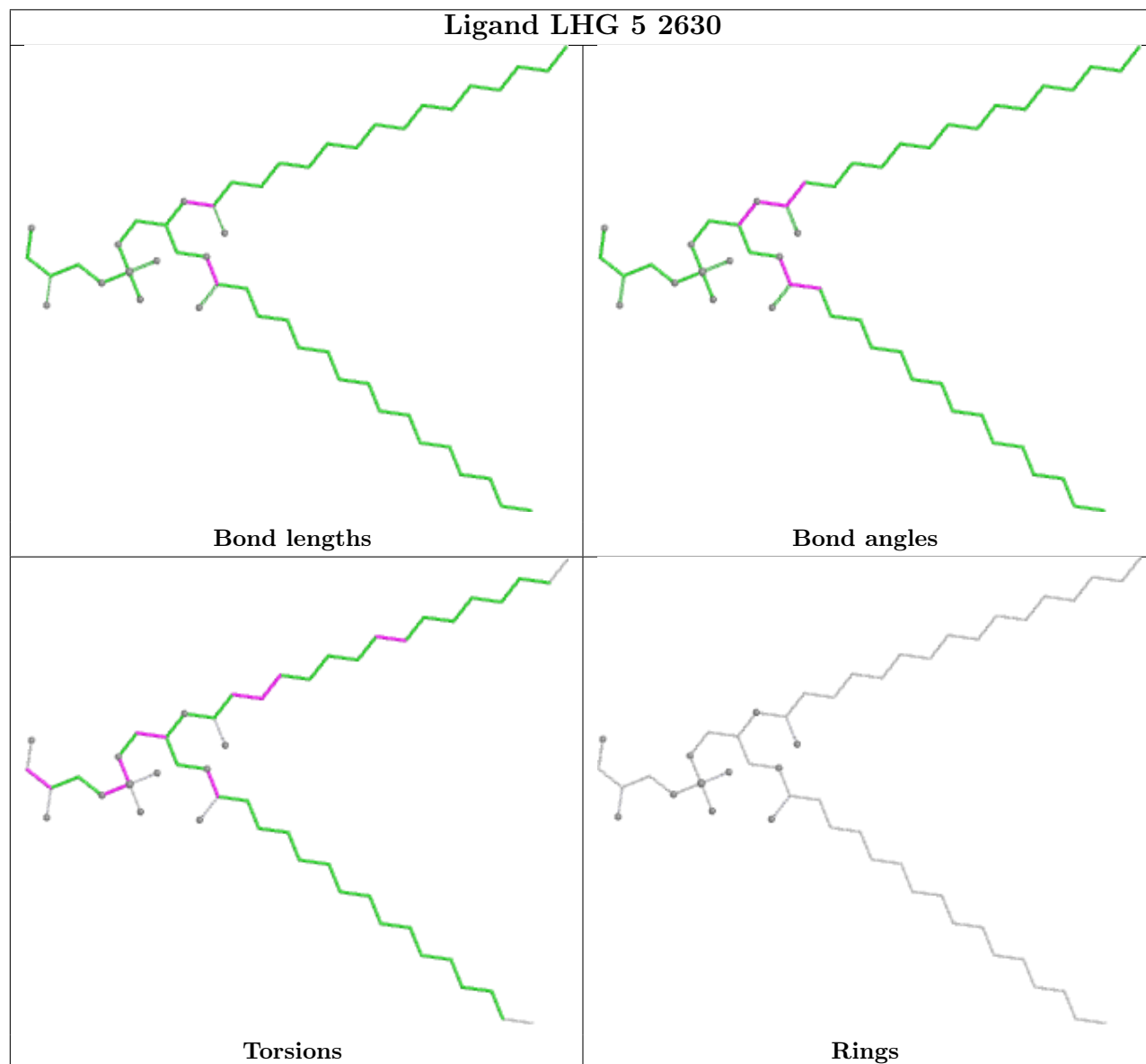
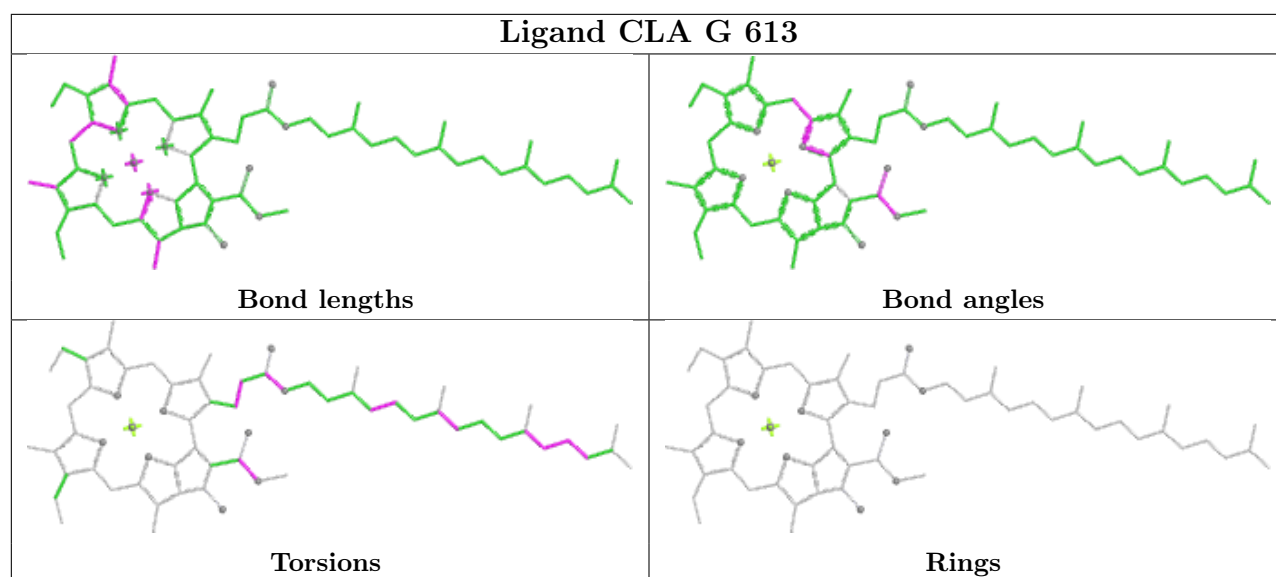


Ligand CHL 9 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

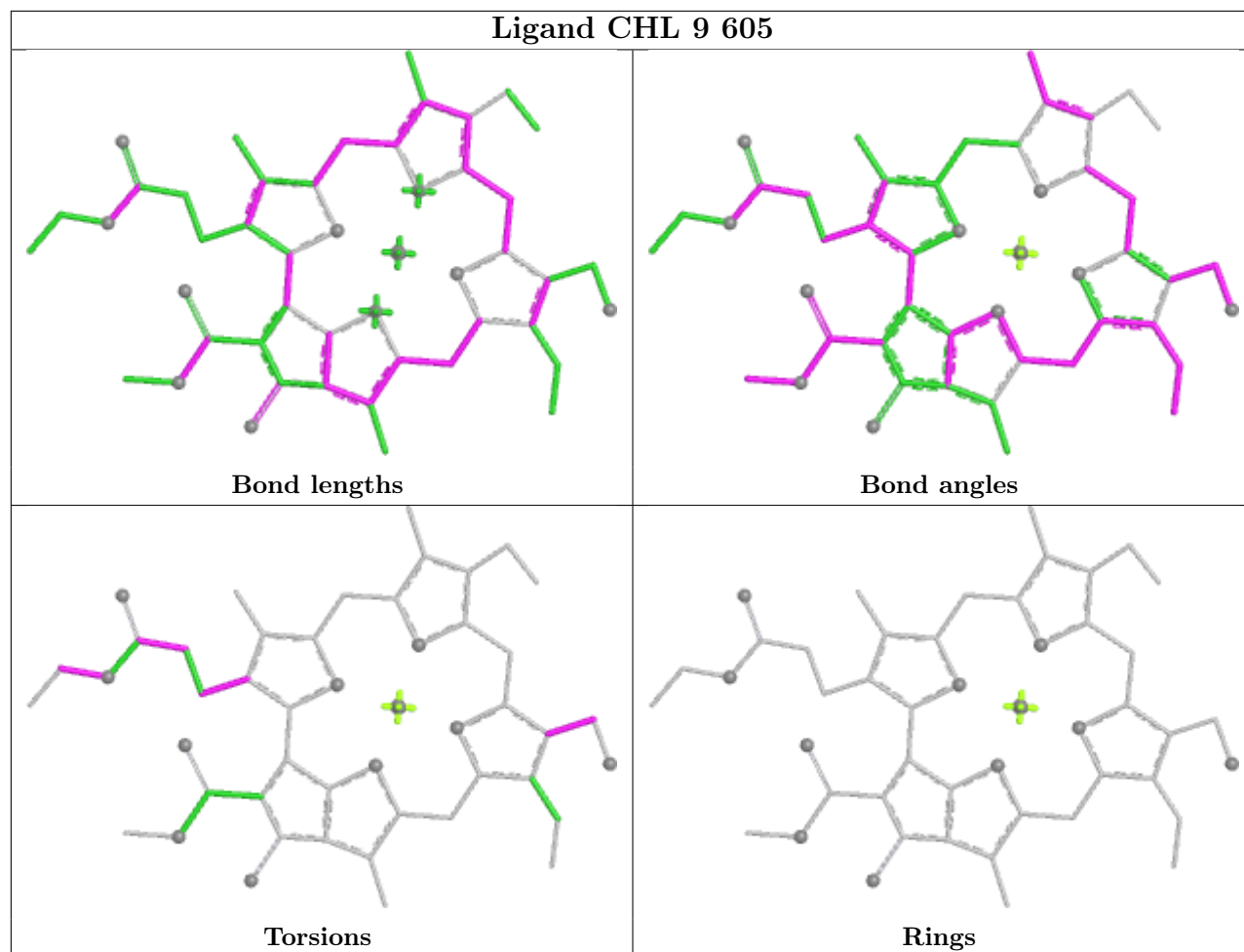
Ligand CHL 6 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 0 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

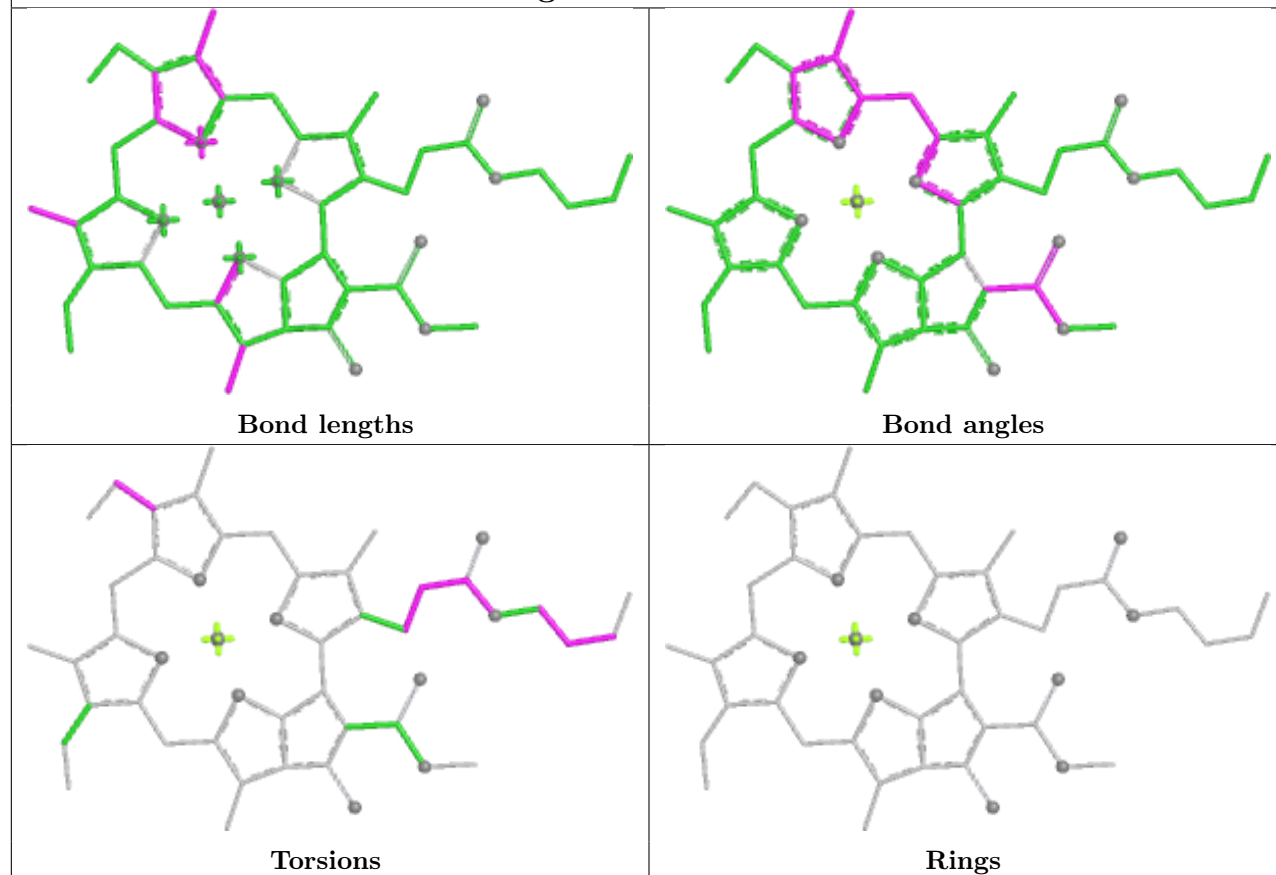




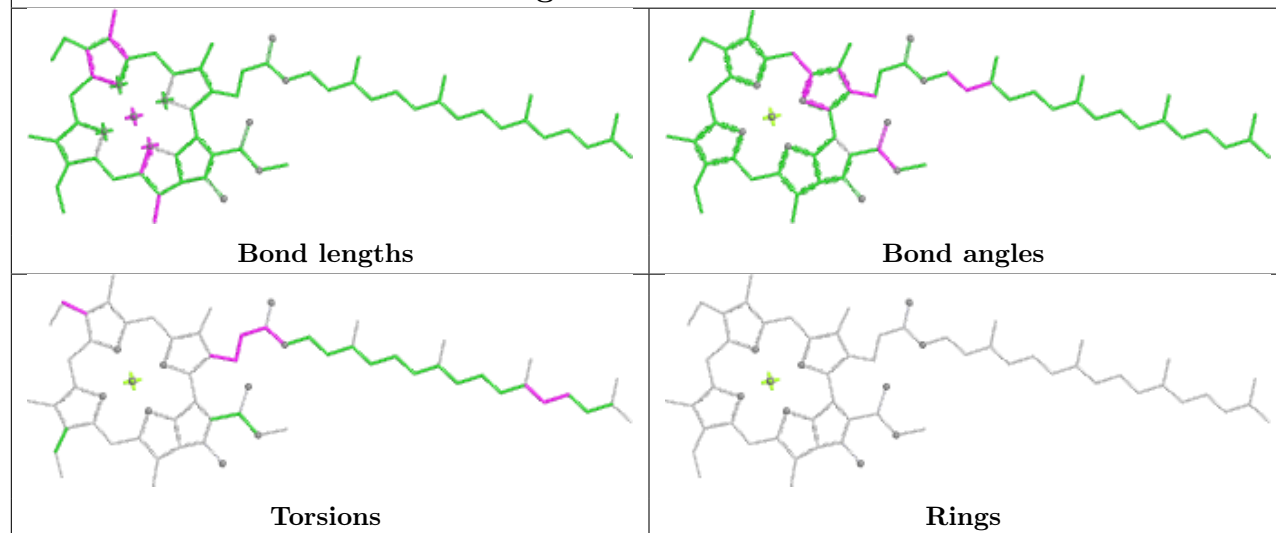
Ligand CHL 9 605



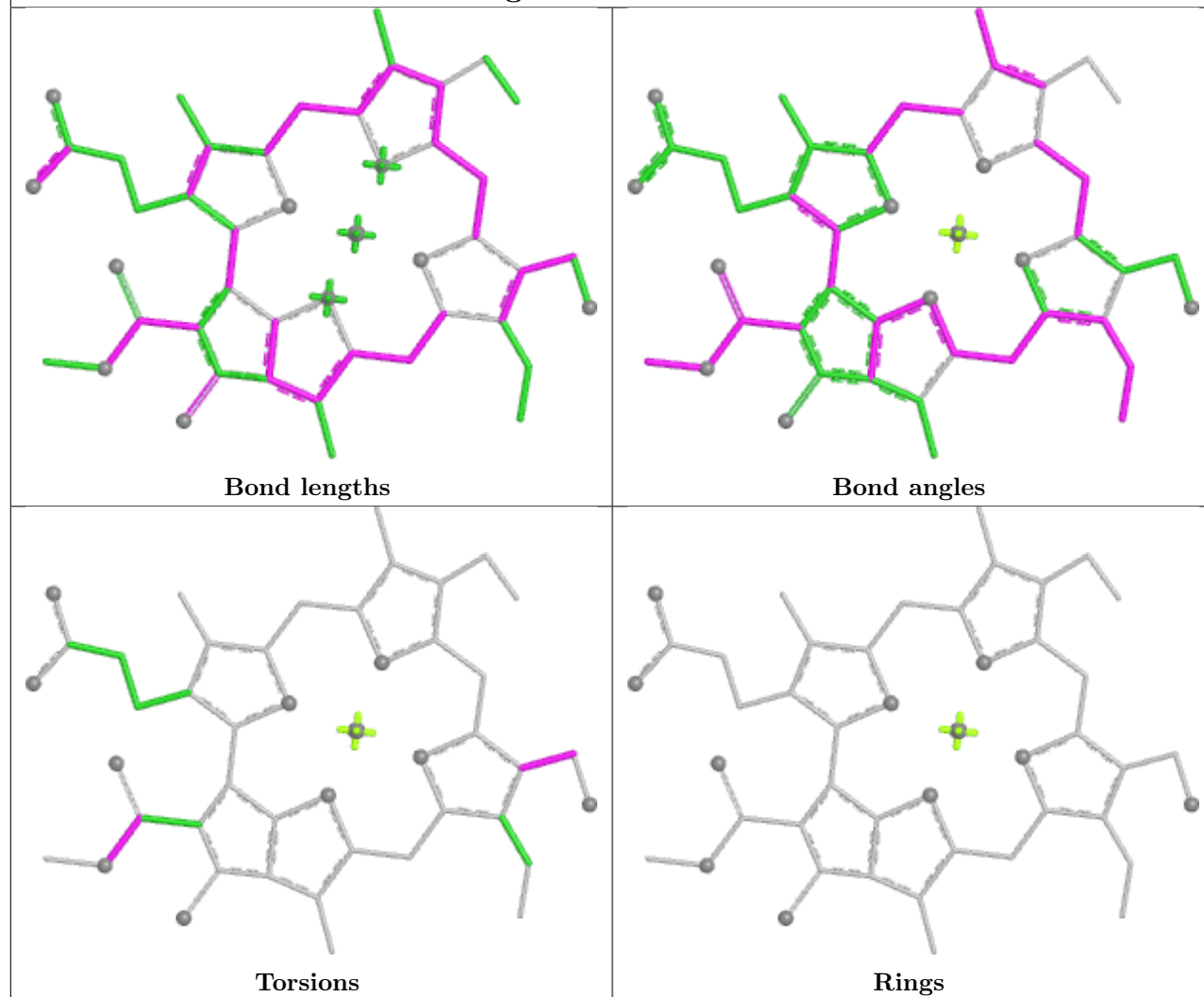
Ligand CLA s 602



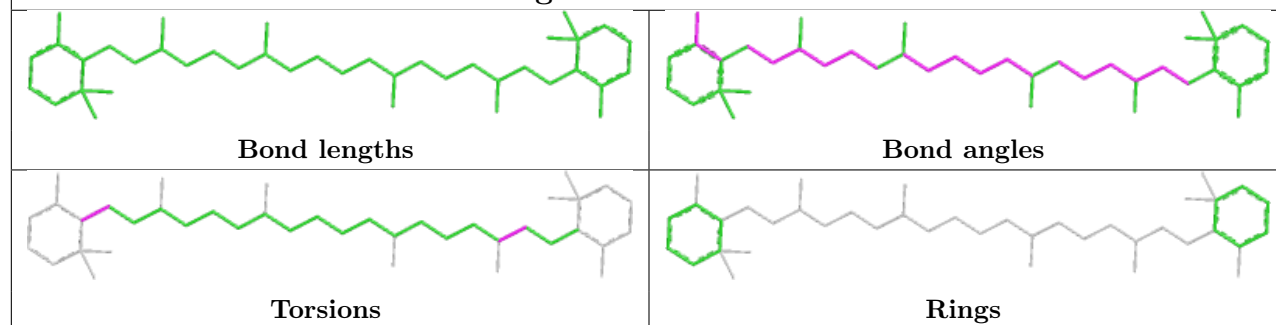
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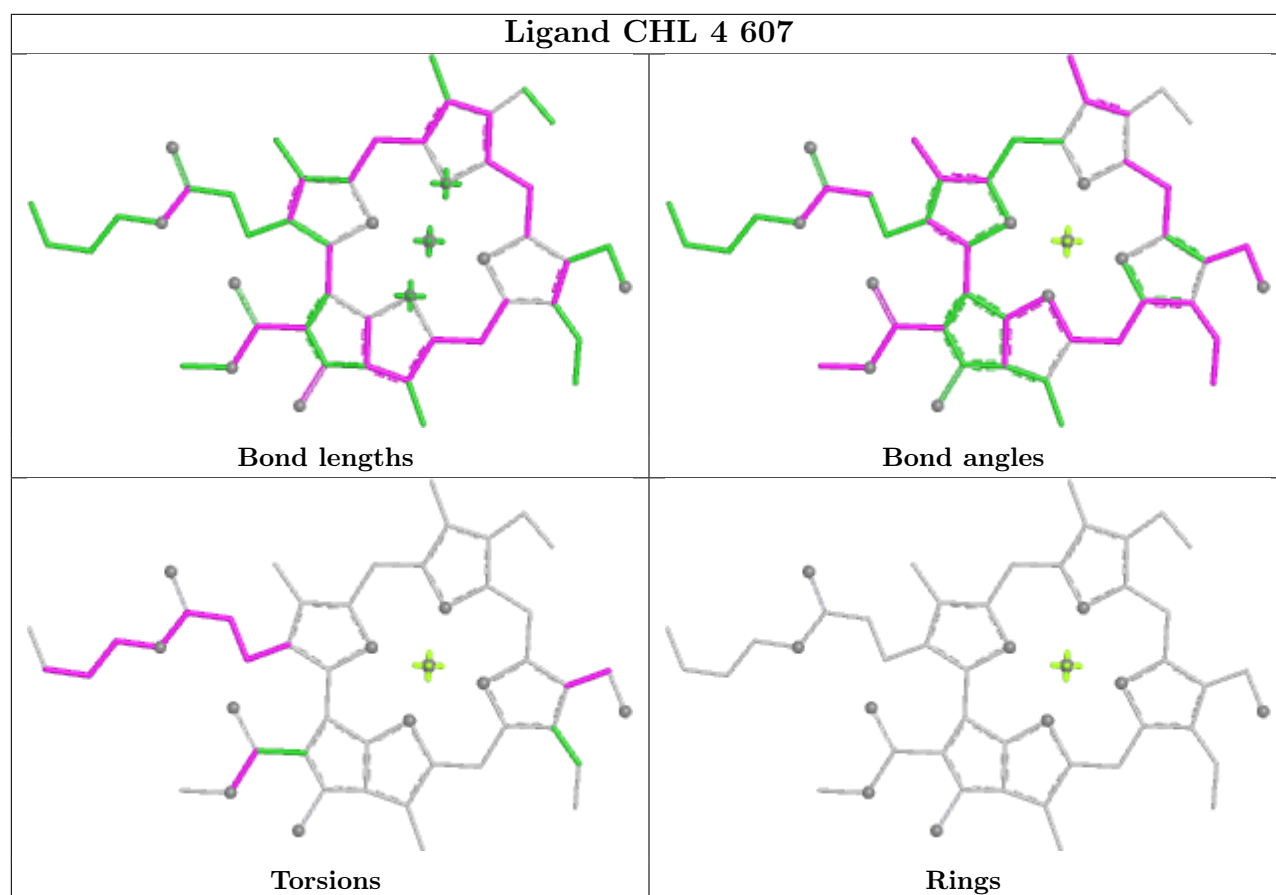


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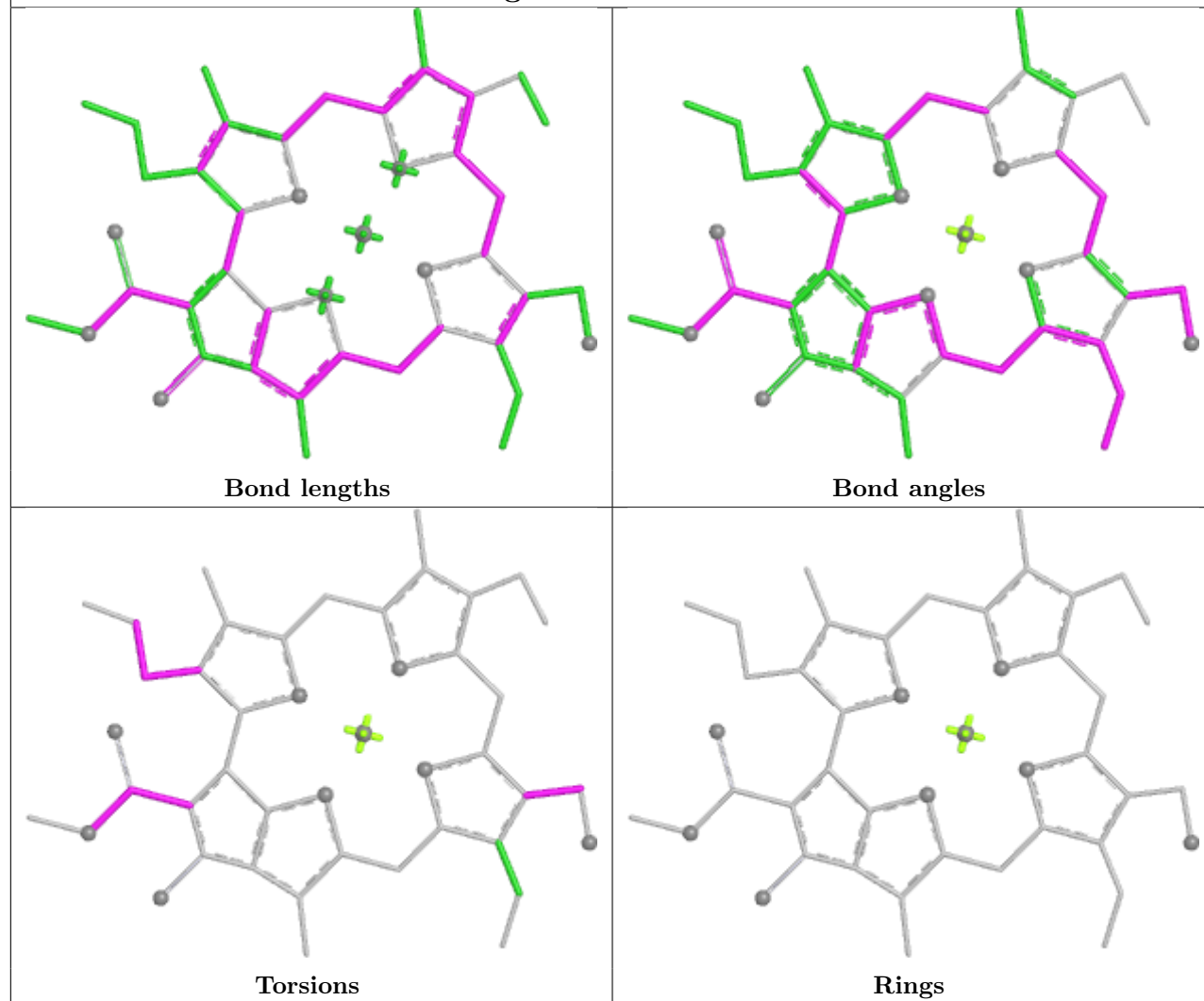


Ligand BCR c 514

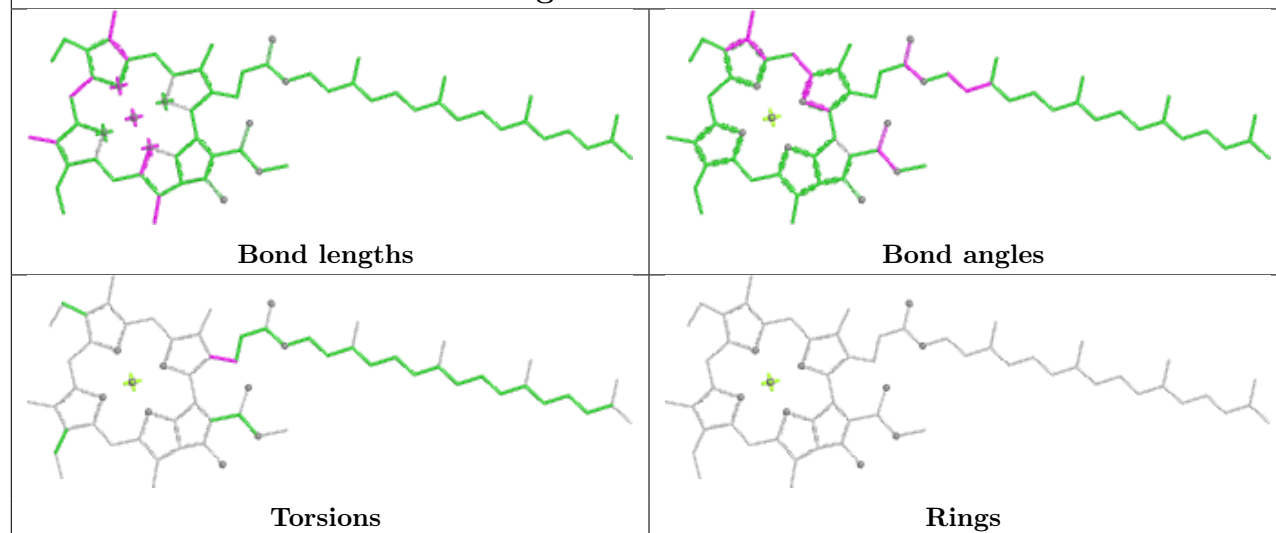


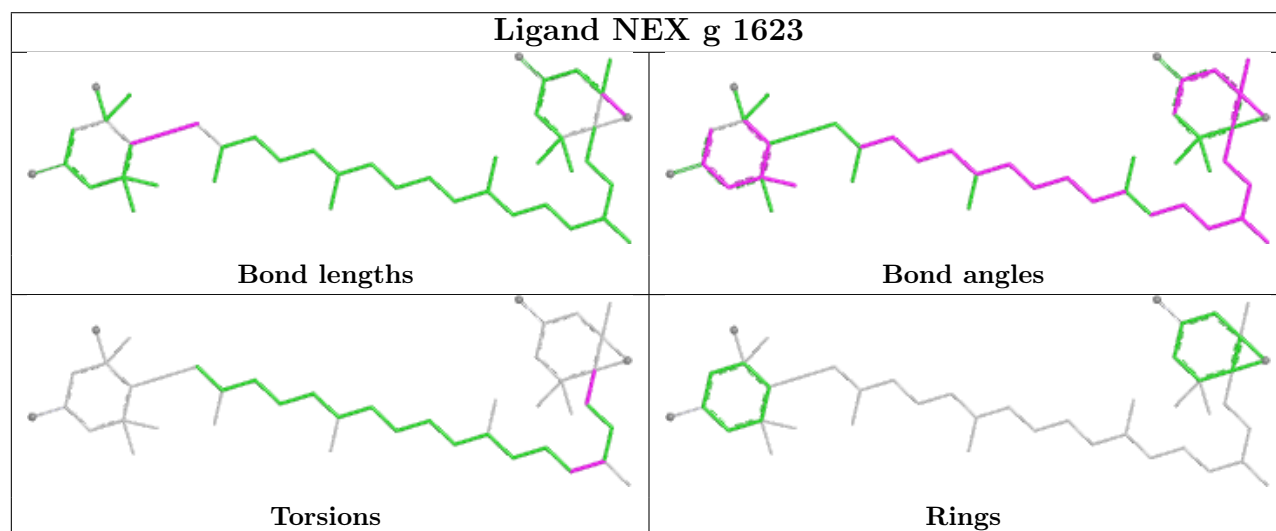
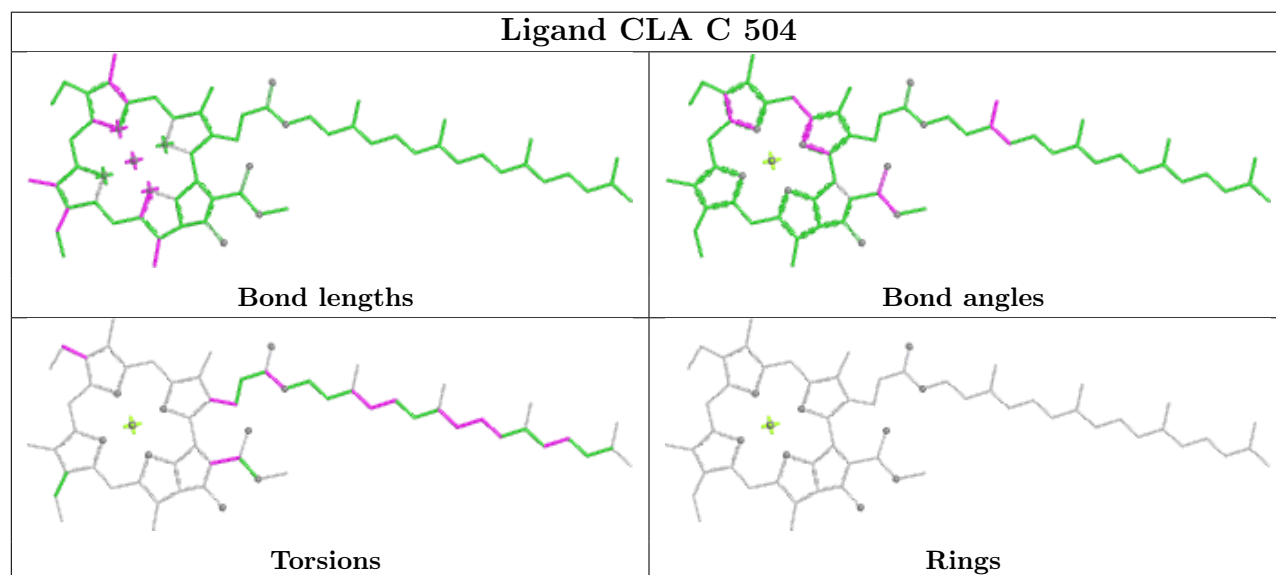
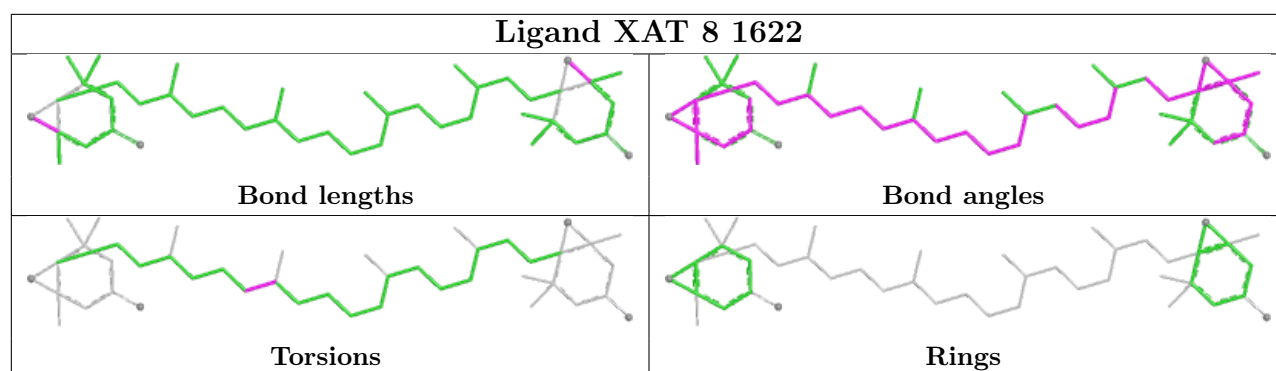


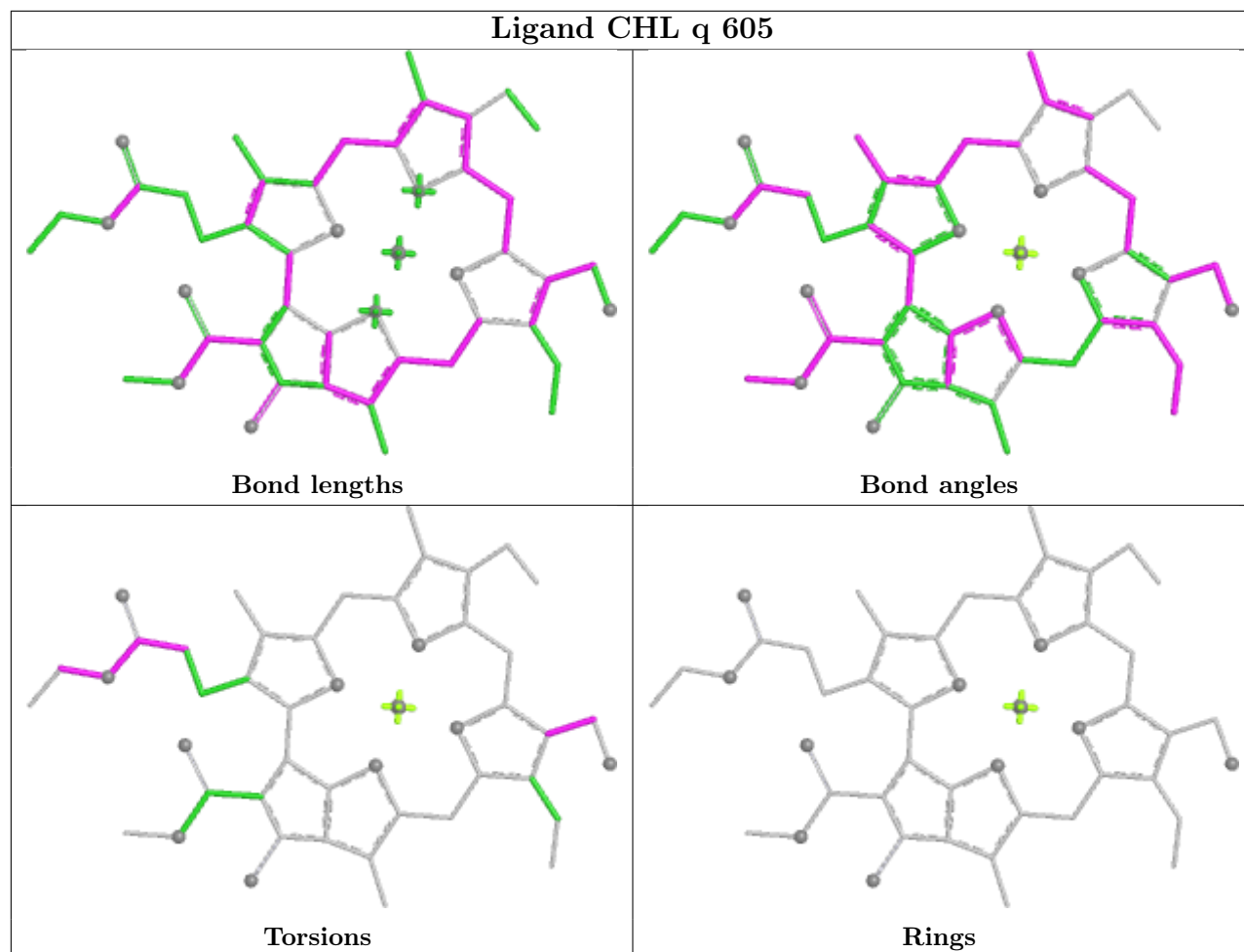
Ligand CHL S 606



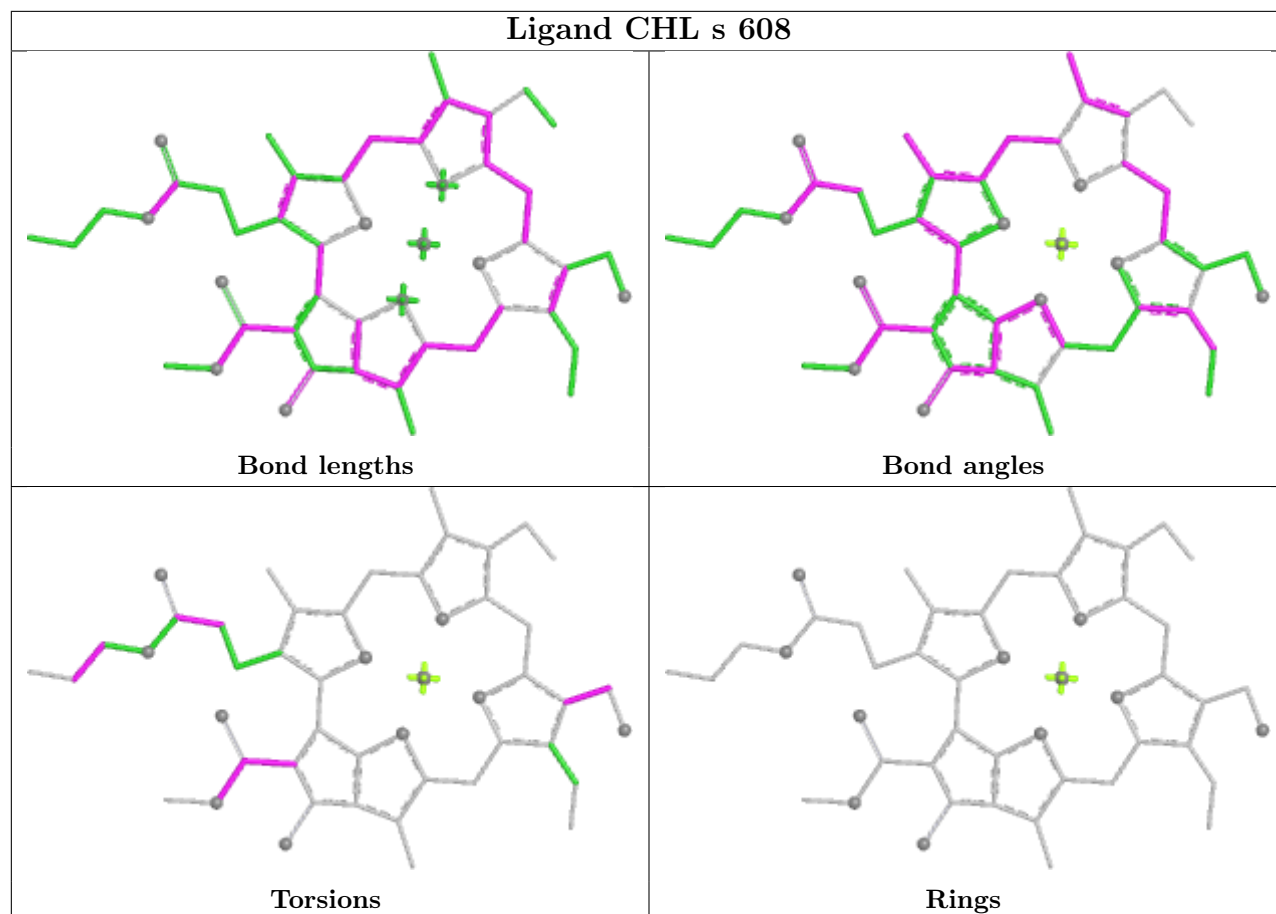
Ligand CLA a 406



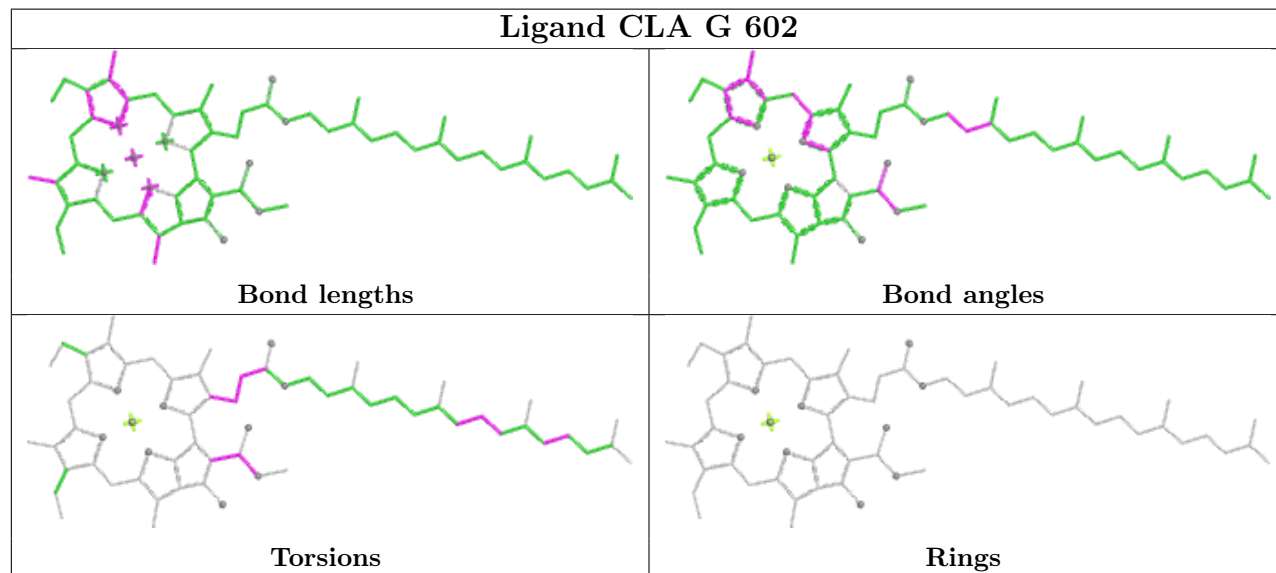


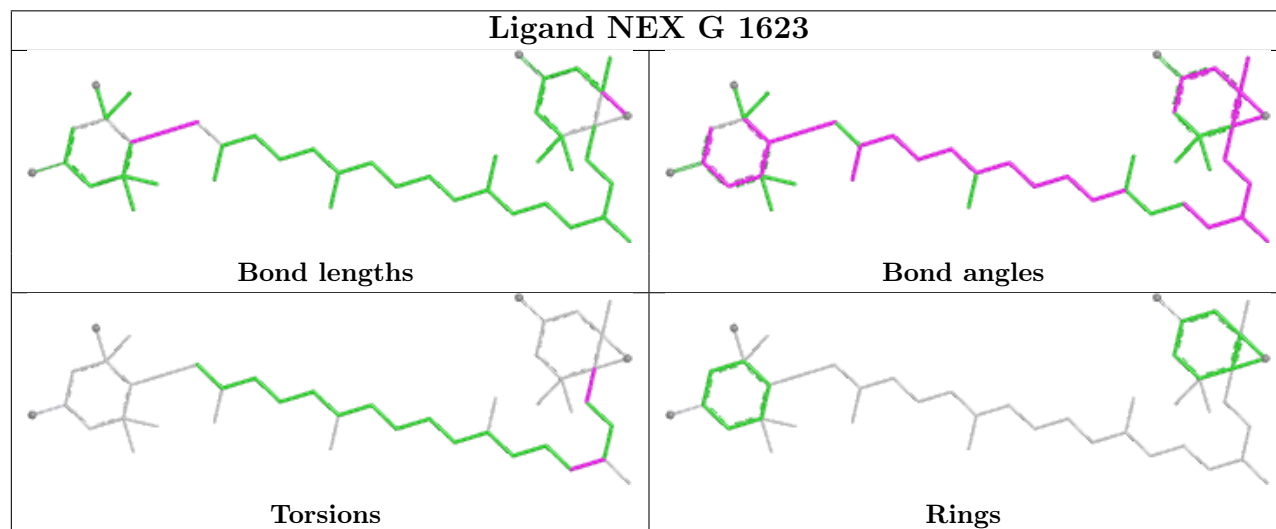
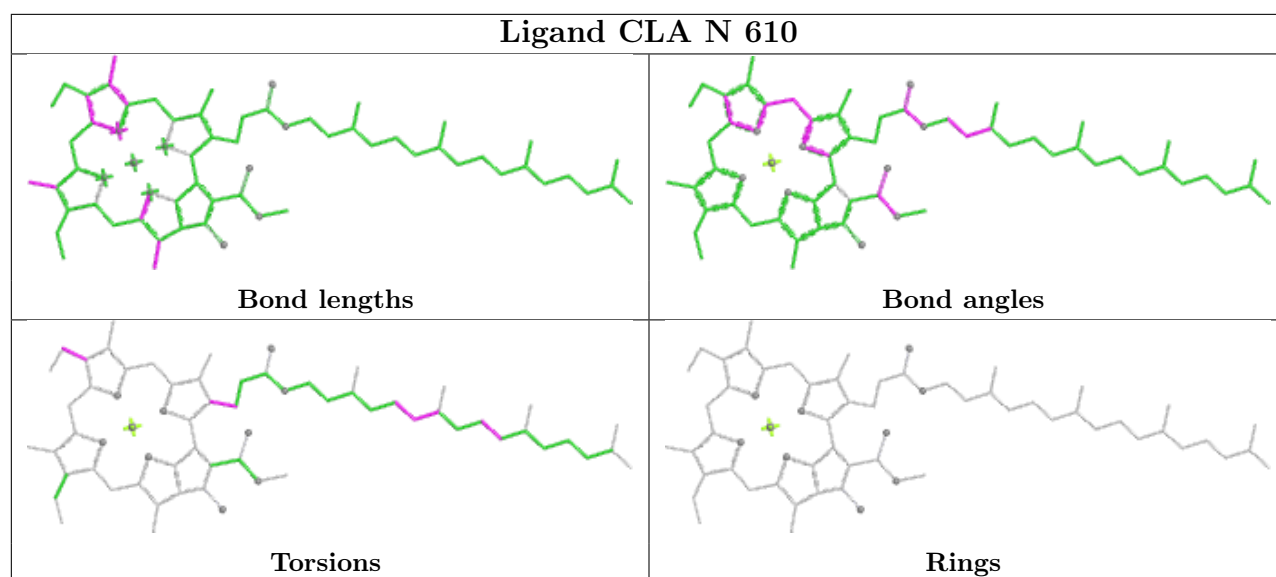


Ligand CHL s 608

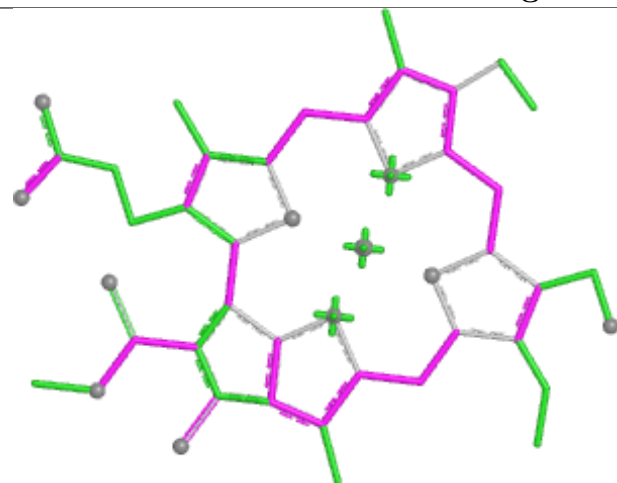


Ligand CLA G 602

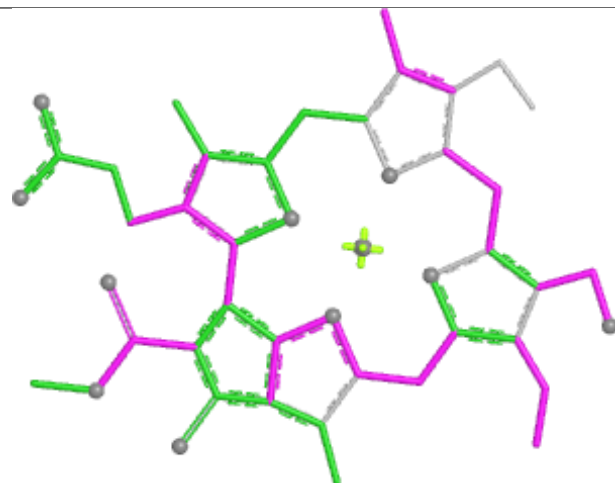




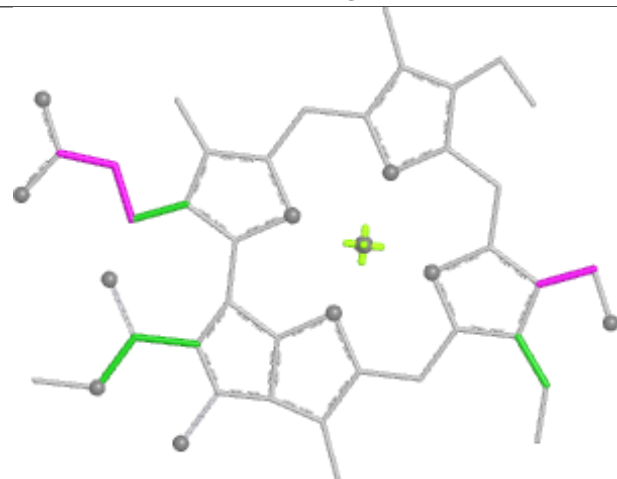
Ligand CHL 6 605



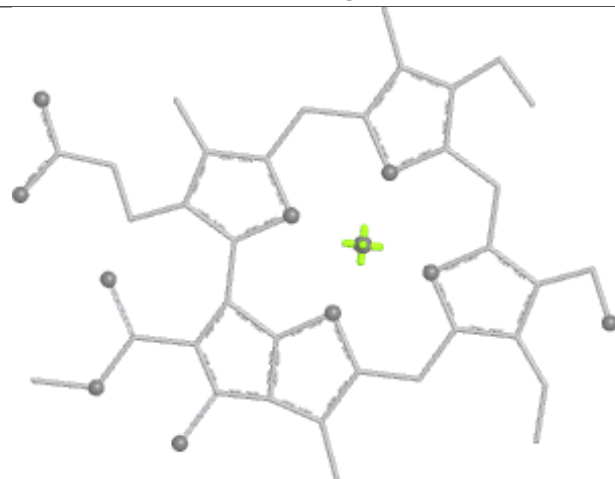
Bond lengths



Bond angles

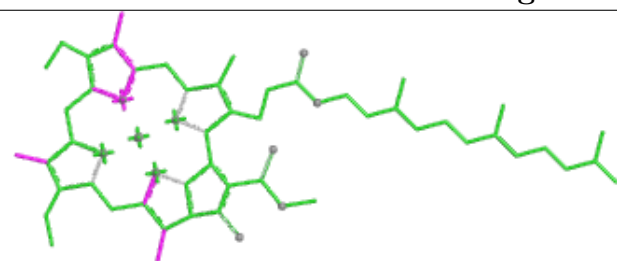


Torsions

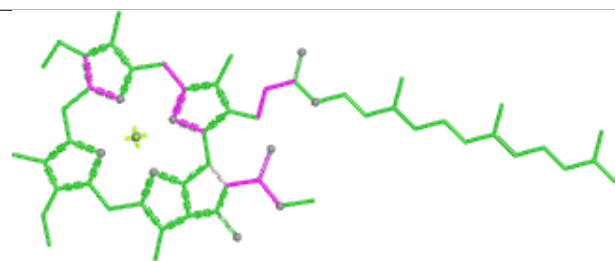


Rings

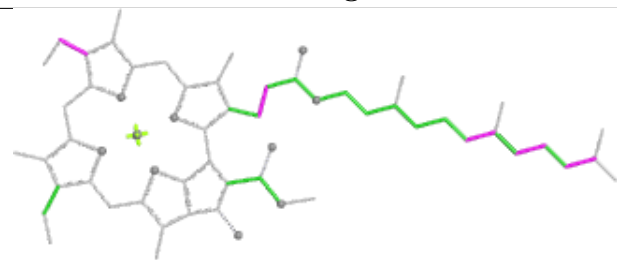
Ligand CLA R 602



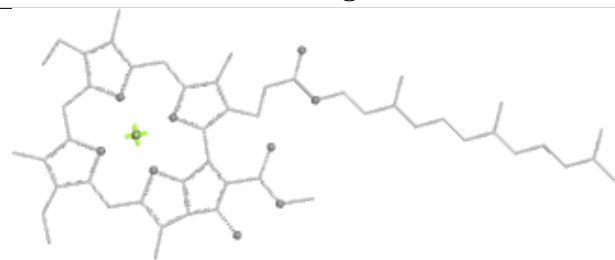
Bond lengths



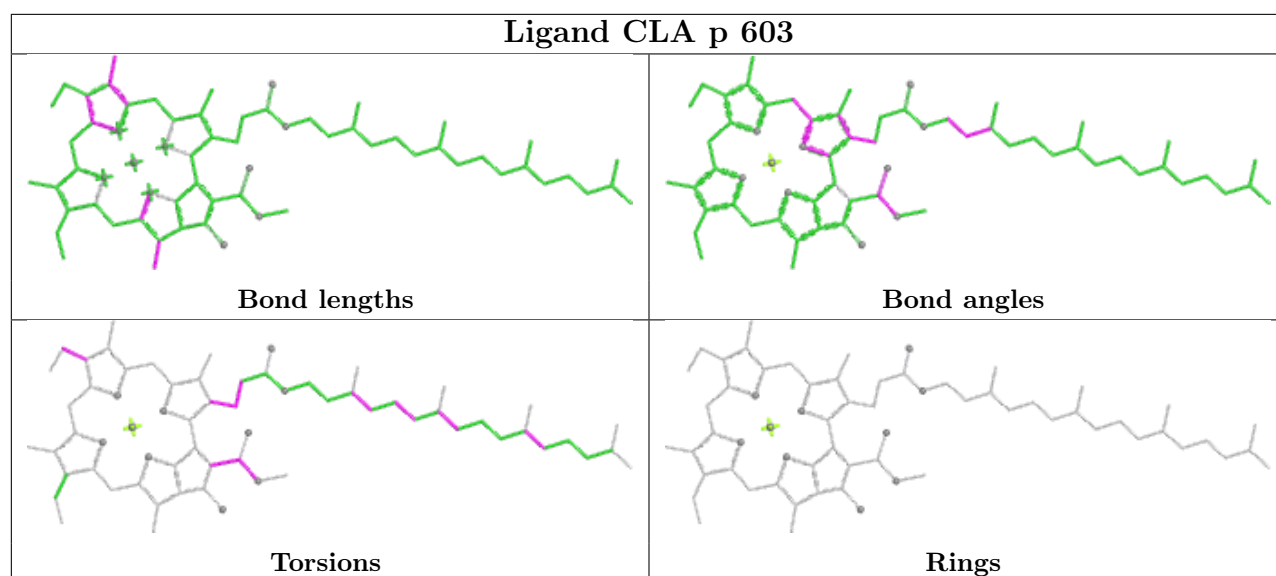
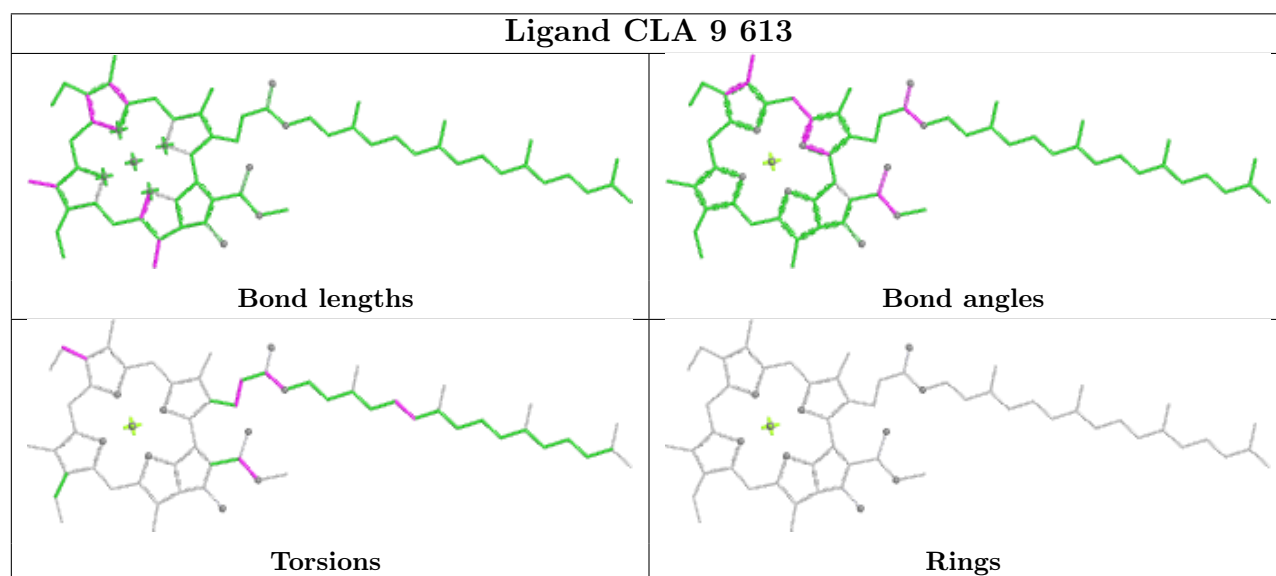
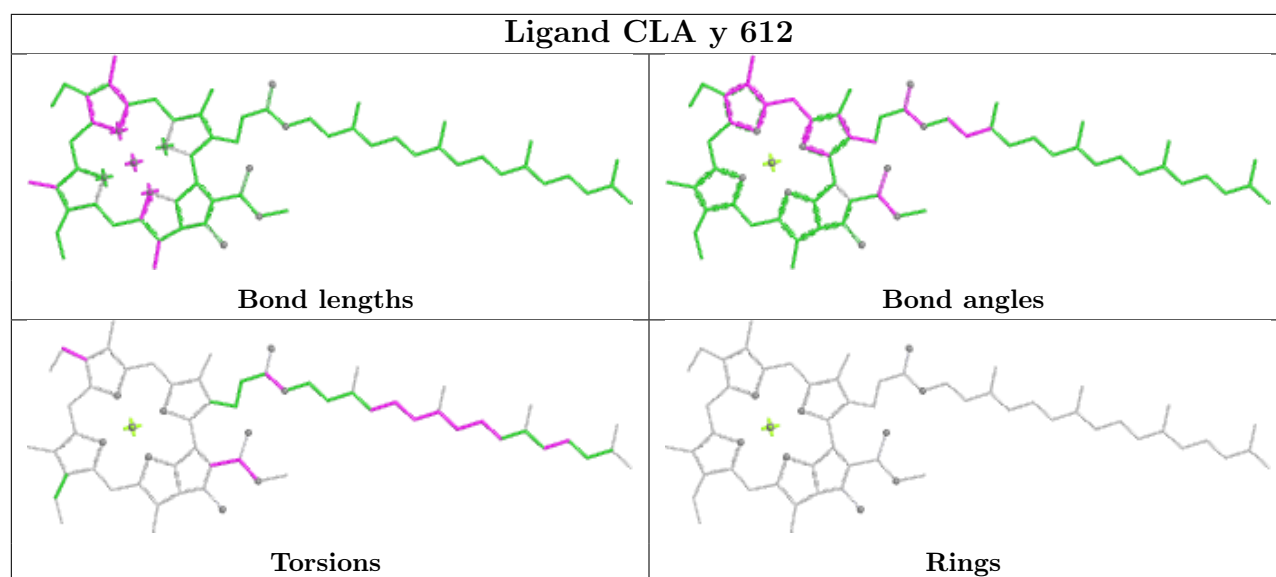
Bond angles

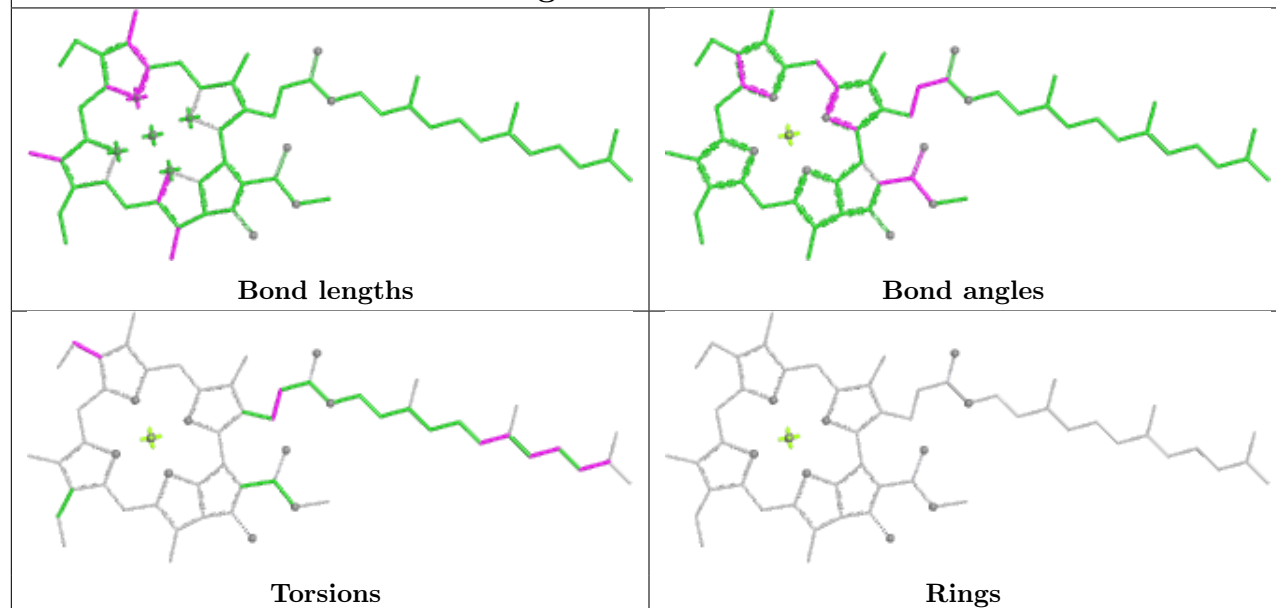
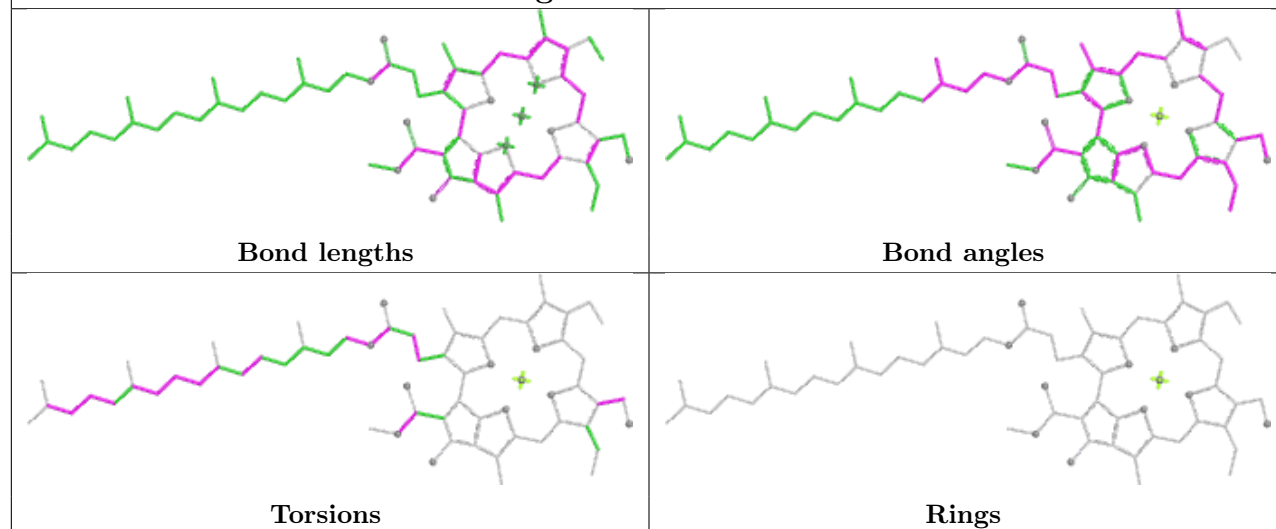


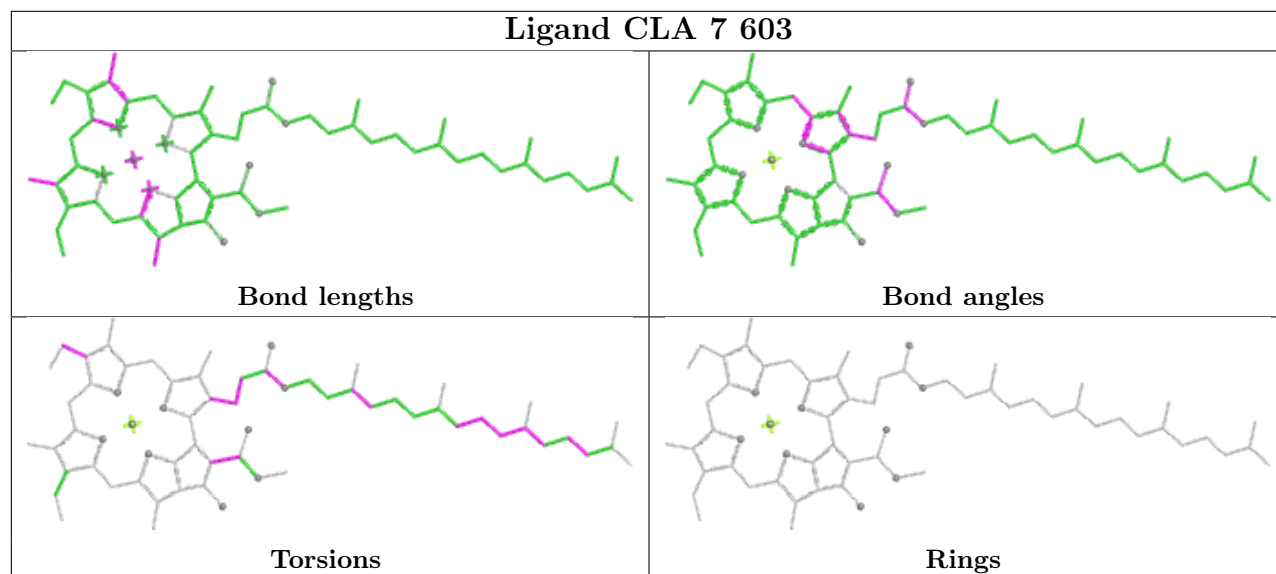
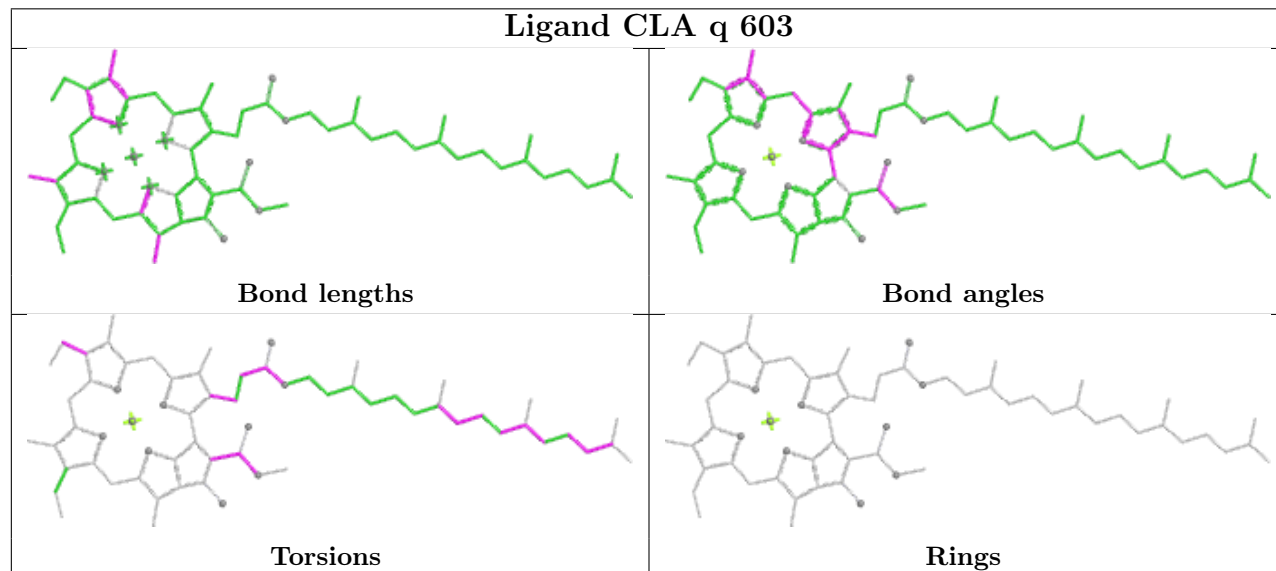
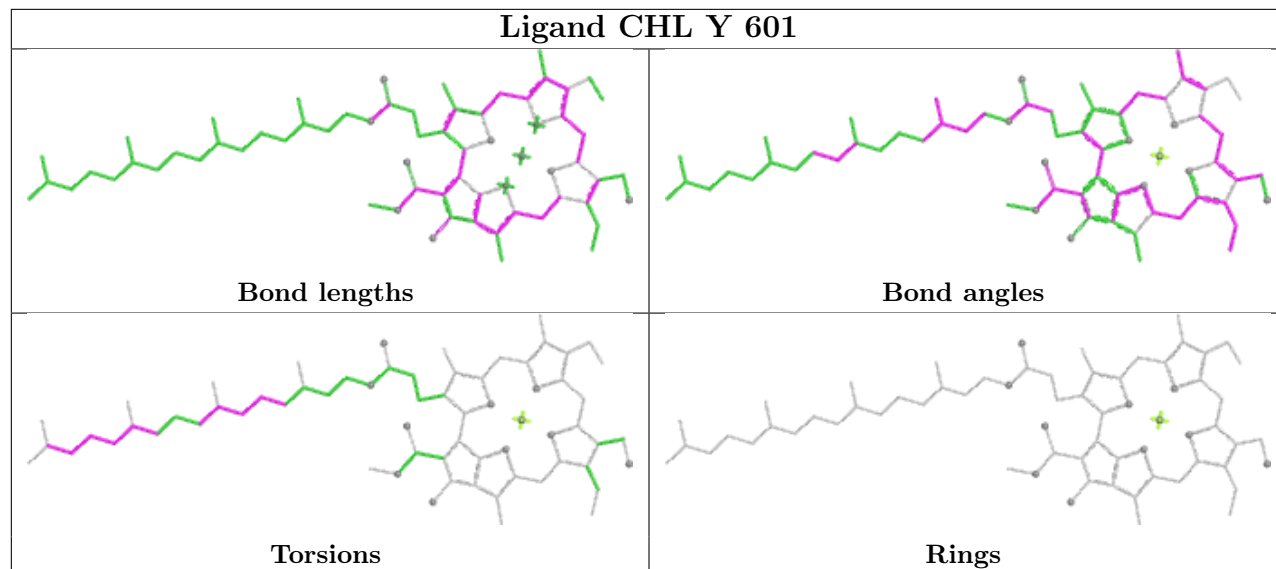
Torsions

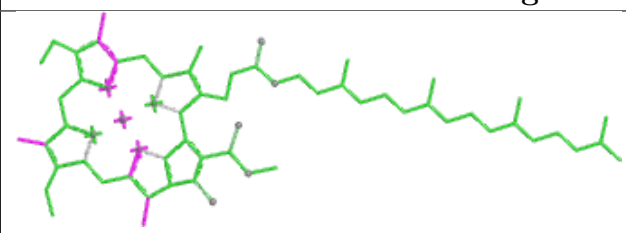
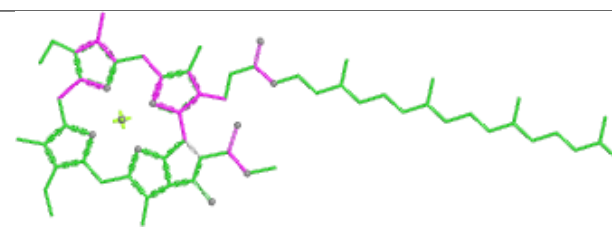
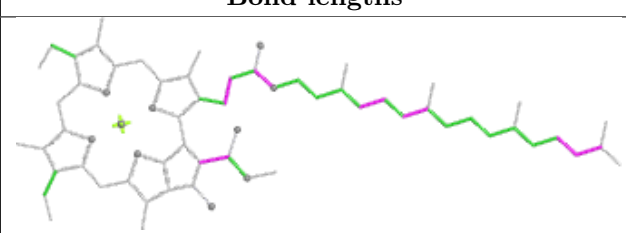
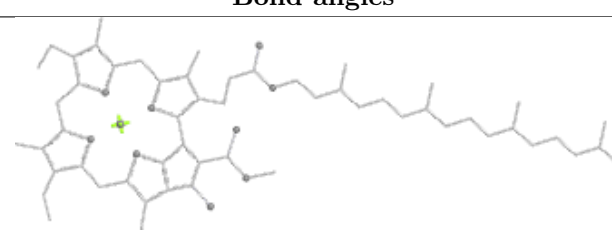


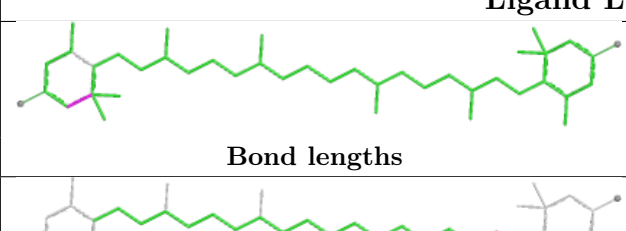
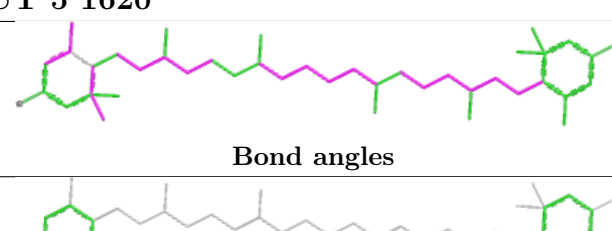
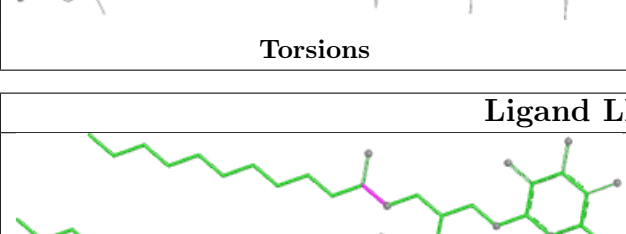
Rings

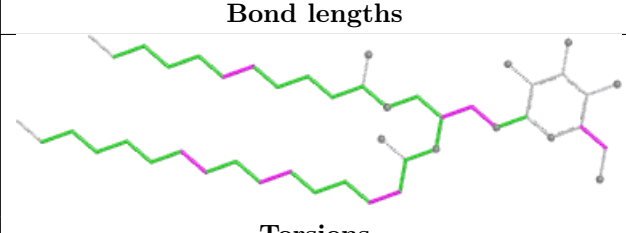
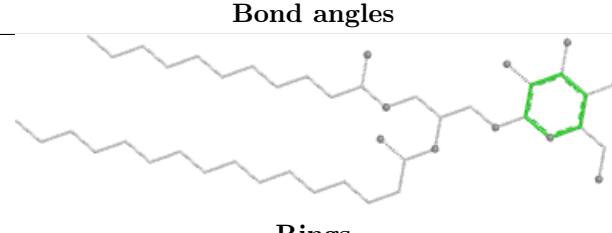


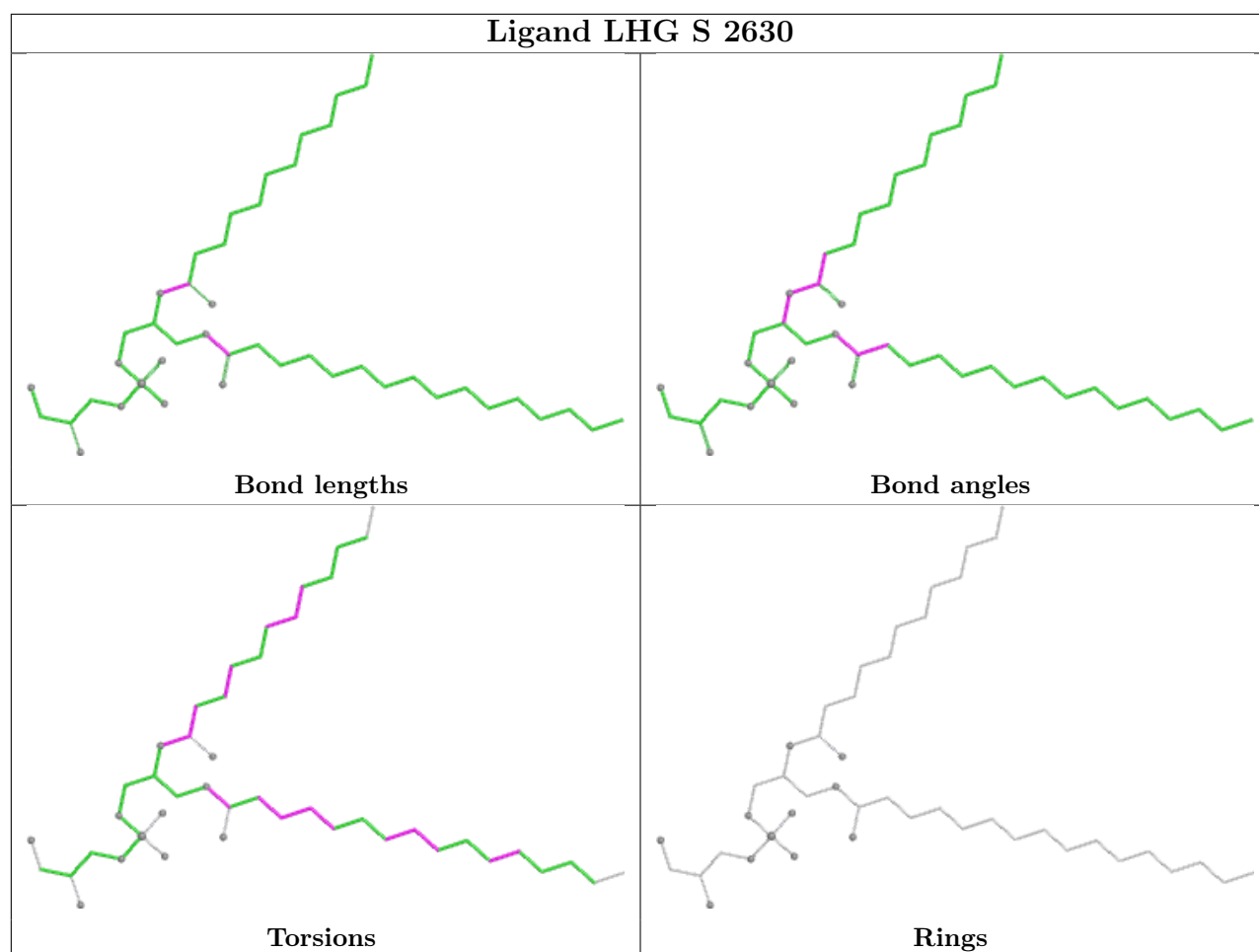
Ligand CLA r 602**Ligand CHL 1 607**

Ligand CLA 7 603**Ligand CLA q 603****Ligand CHL Y 601**

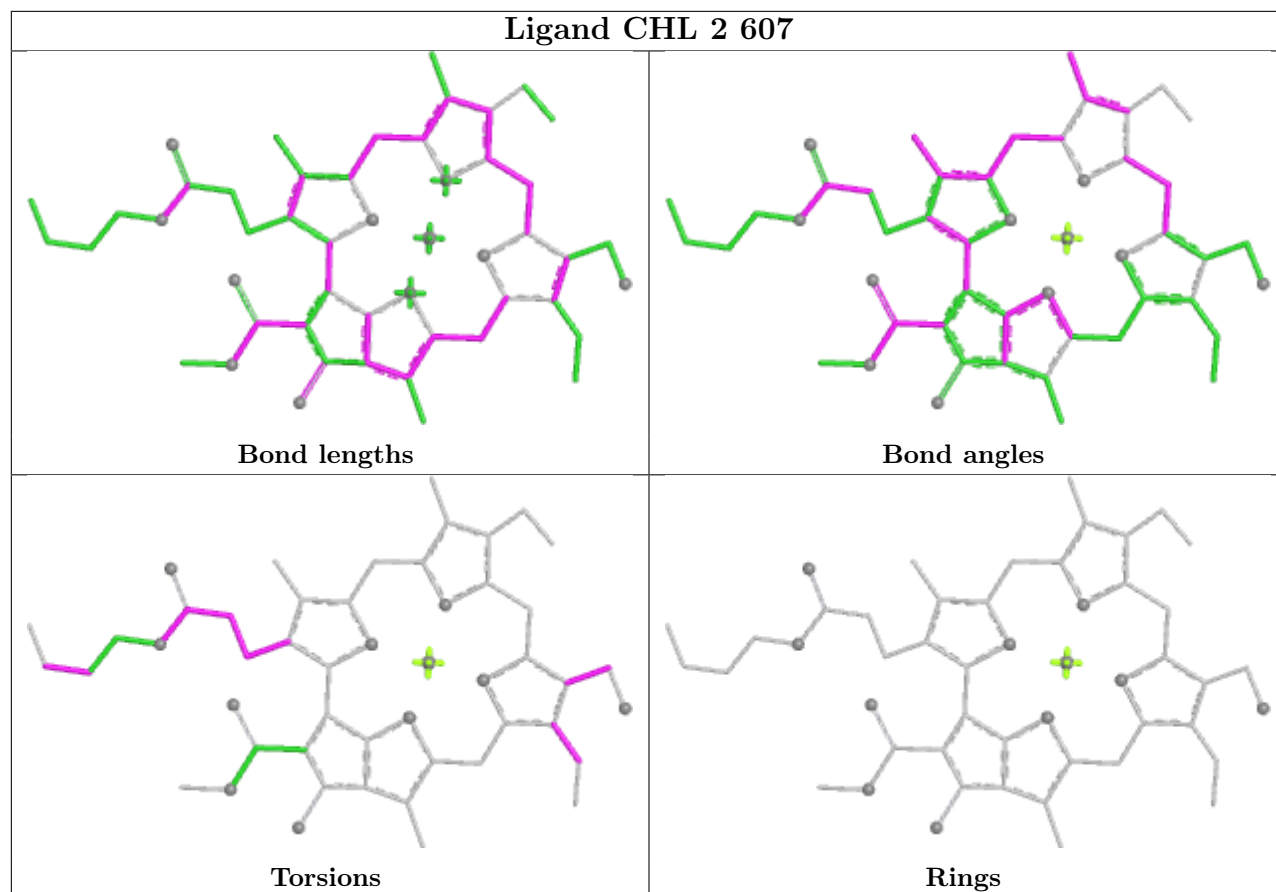
Ligand CLA B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 5 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

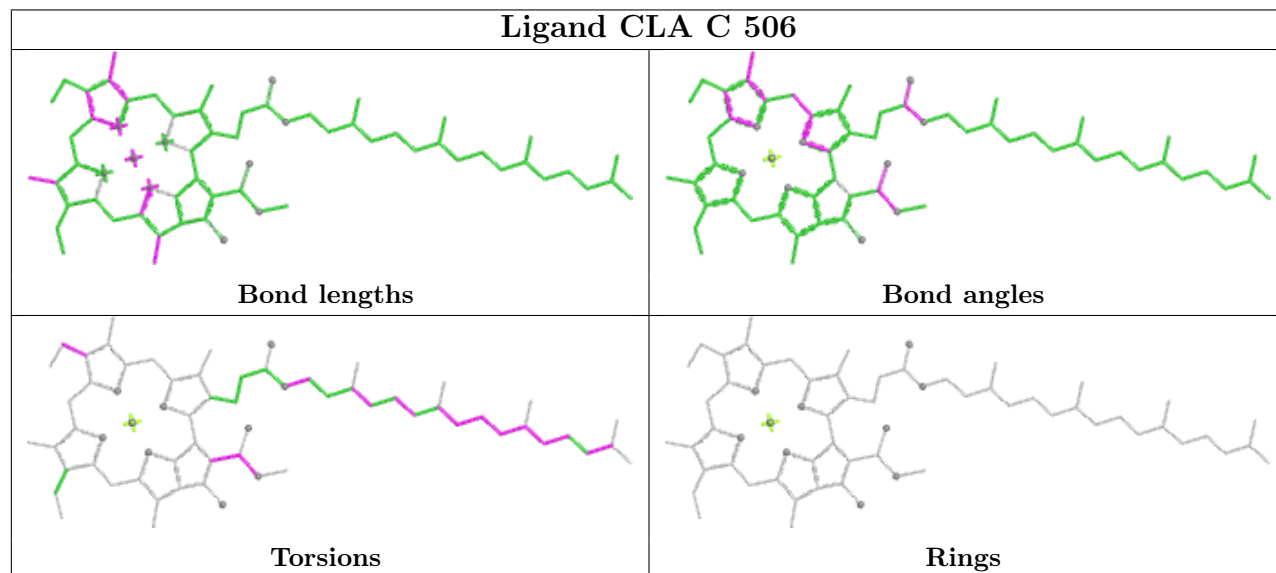
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

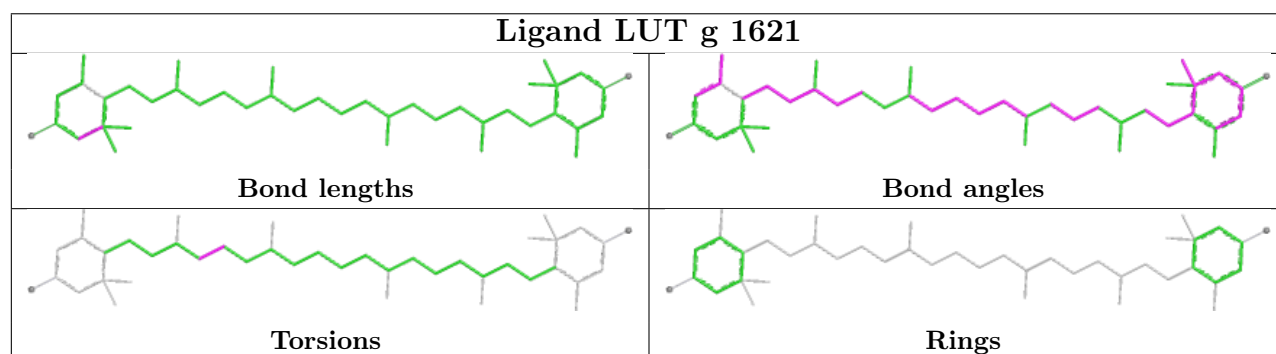
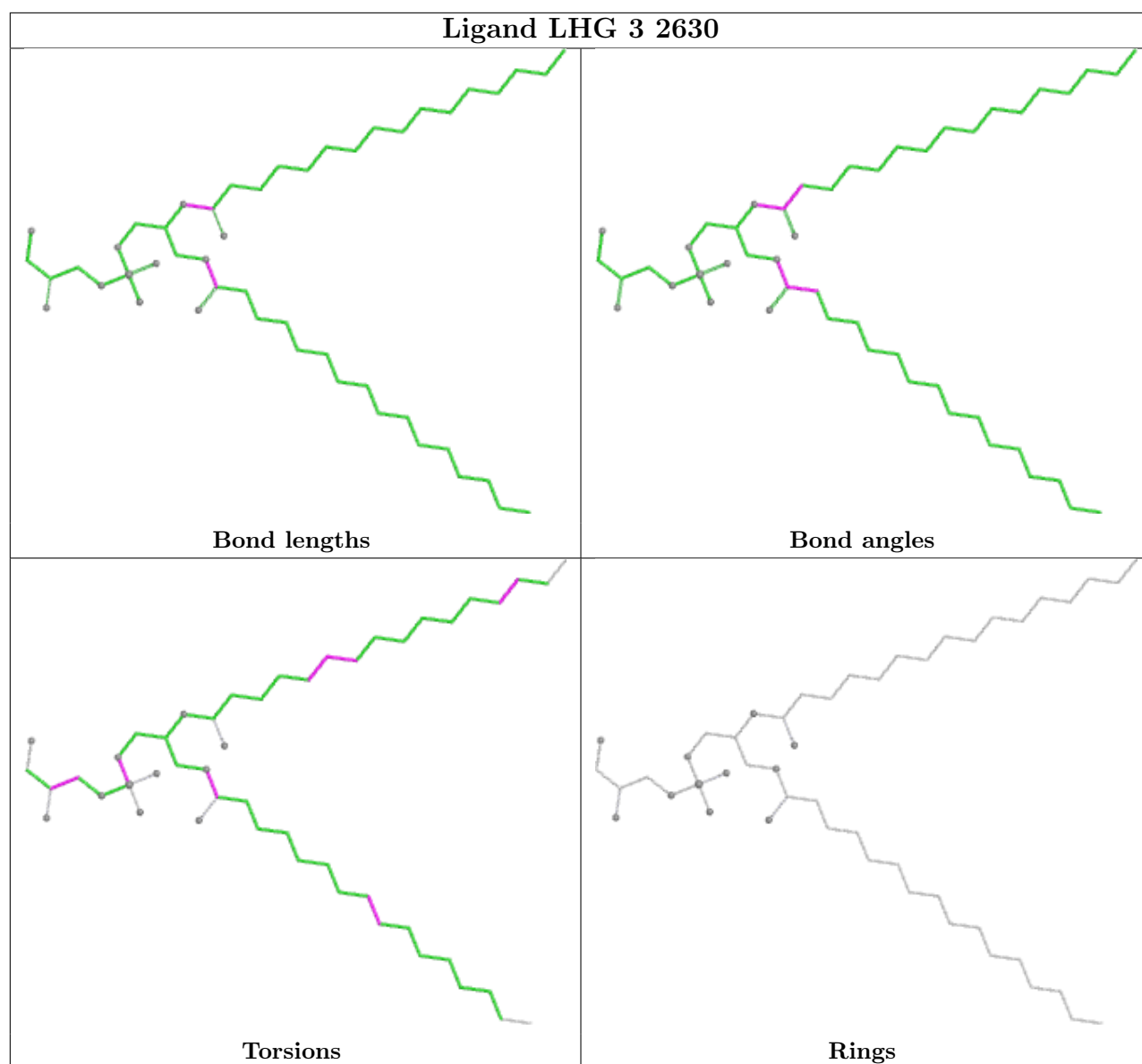


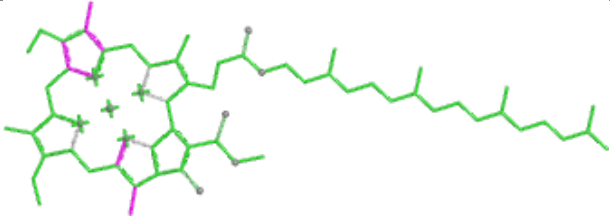
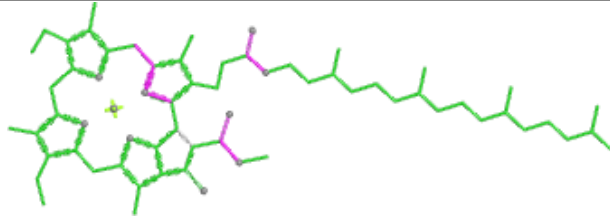
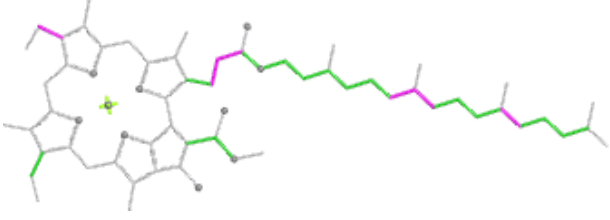
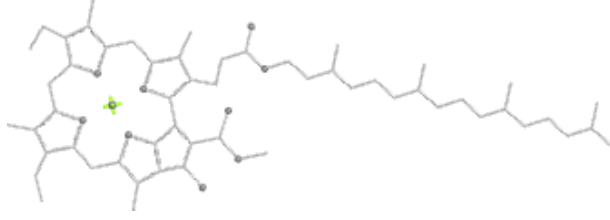
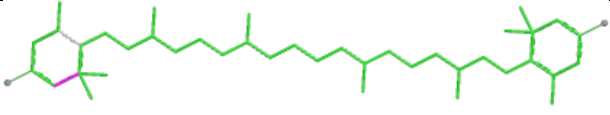
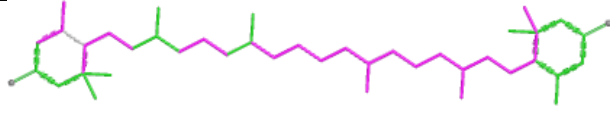
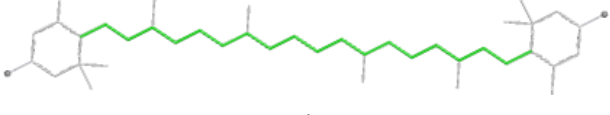
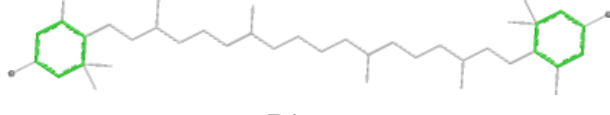
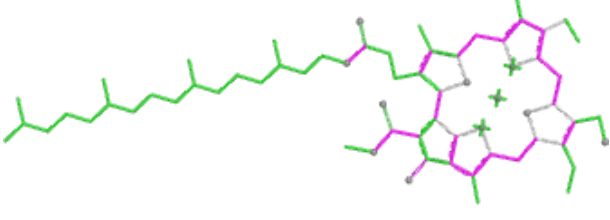
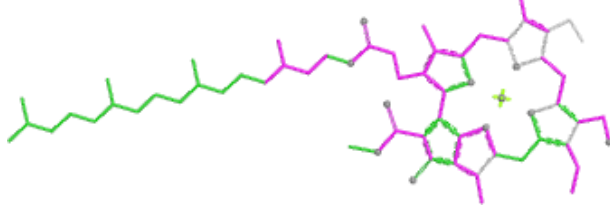
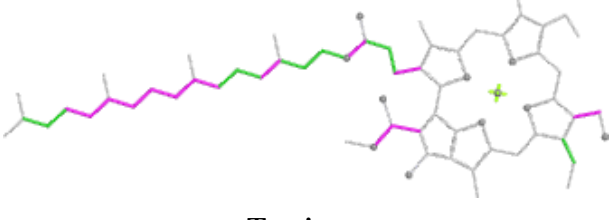
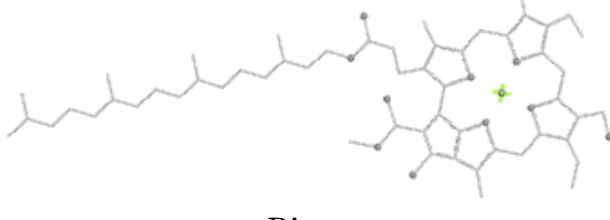
Ligand CHL 2 607

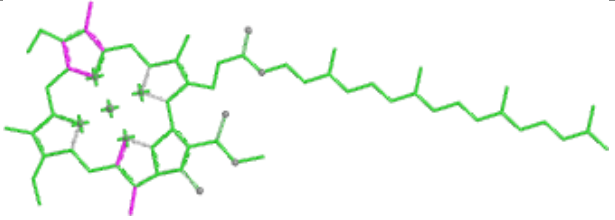
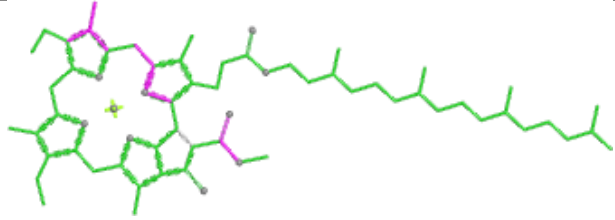
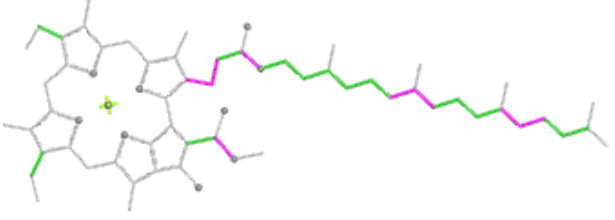
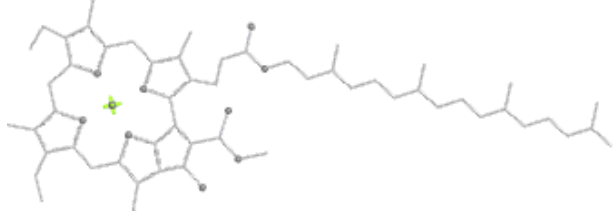
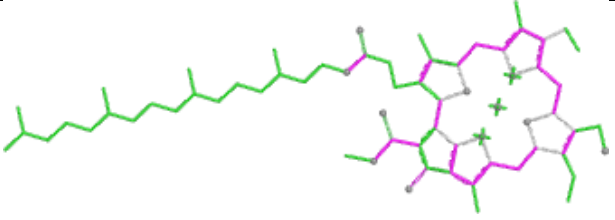
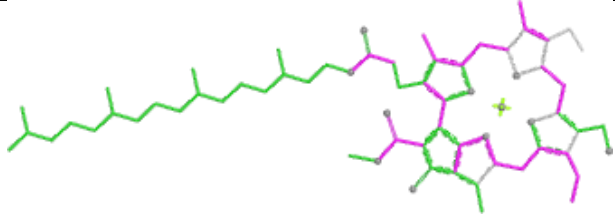
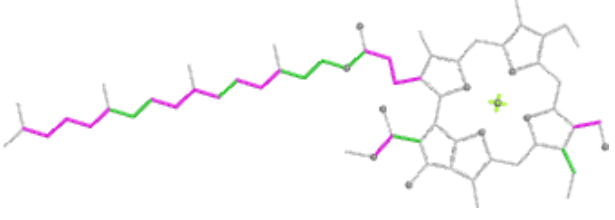
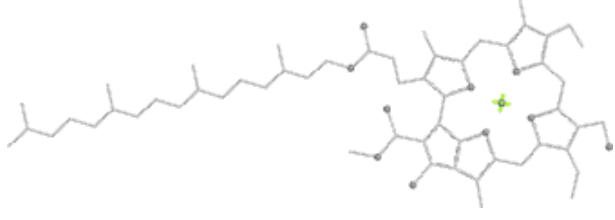
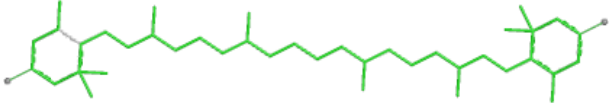
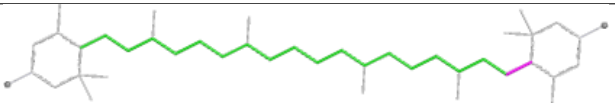
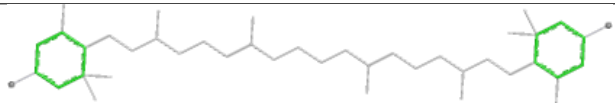


Ligand CLA C 506

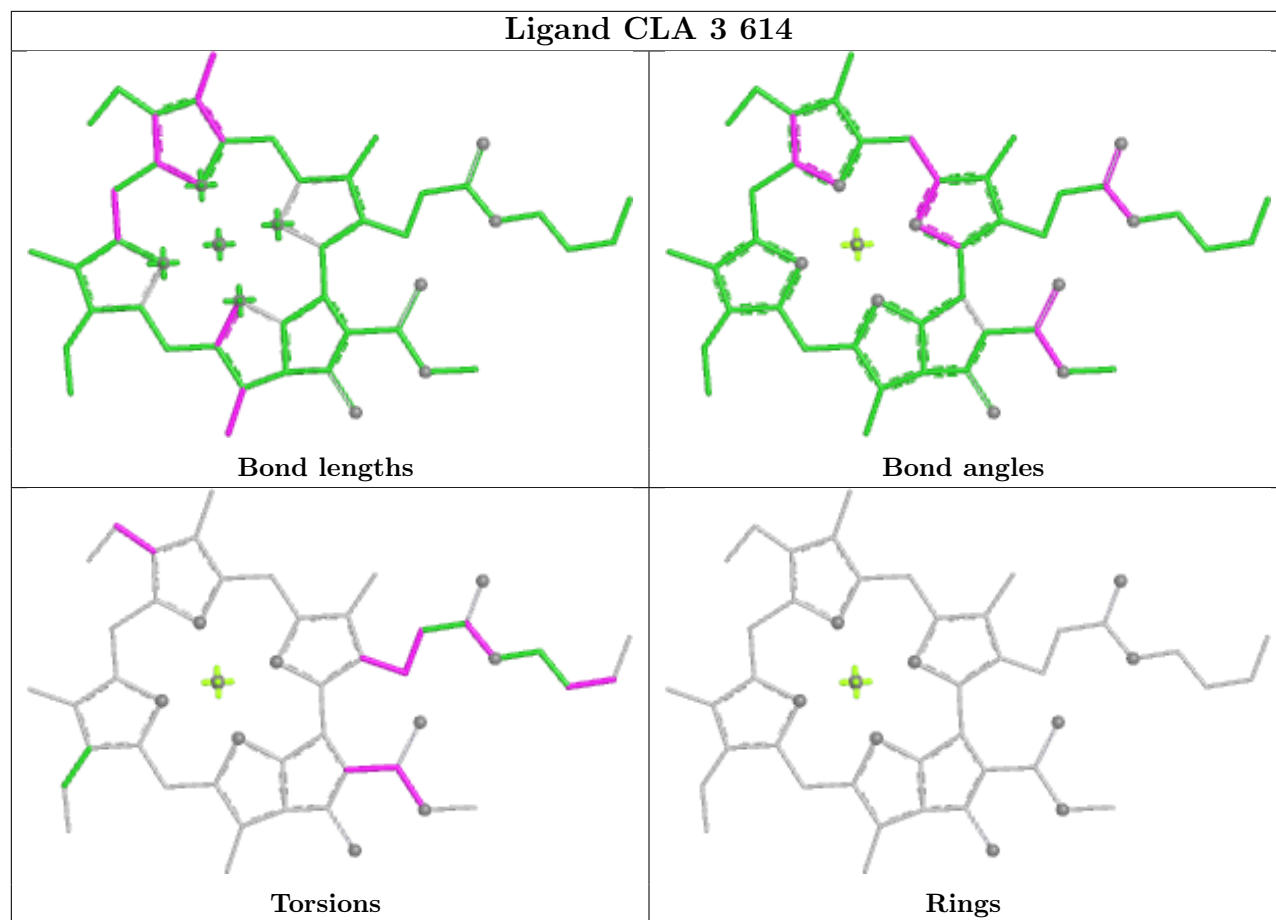




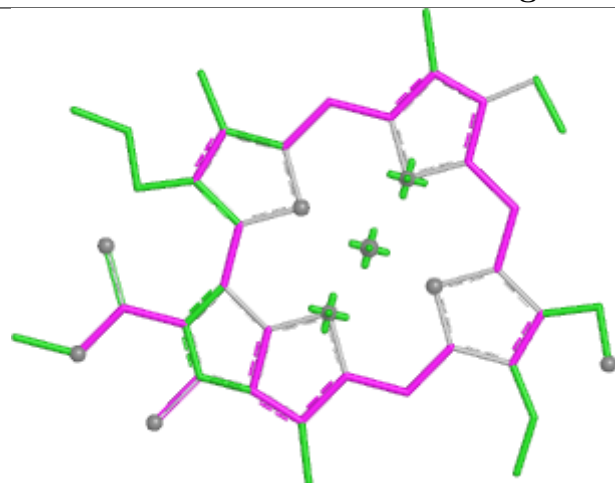
Ligand CLA p 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT Y 1620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL n 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 0 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 5 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

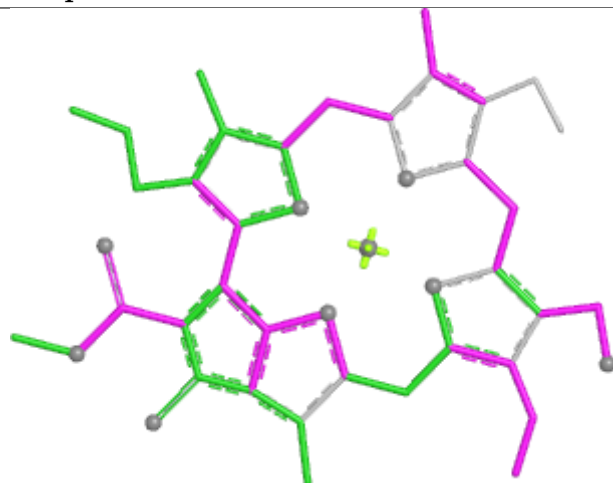
Ligand CLA 3 614



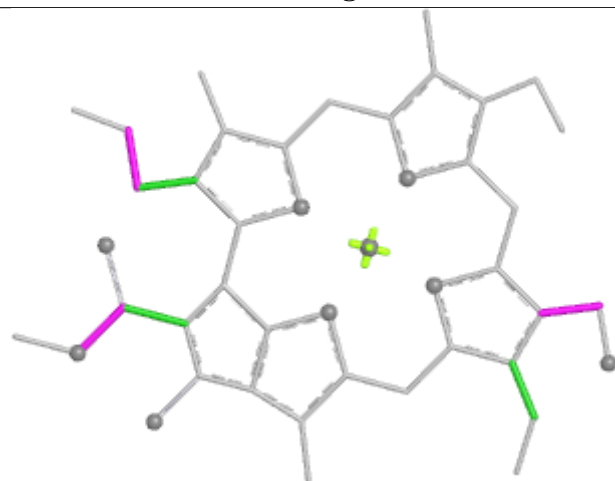
Ligand CHL q 608



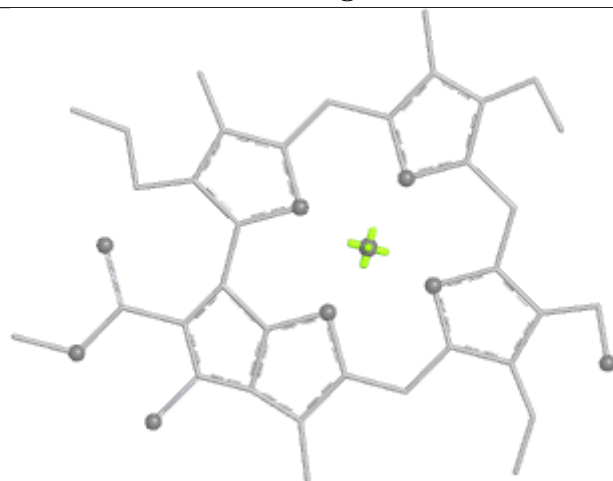
Bond lengths



Bond angles

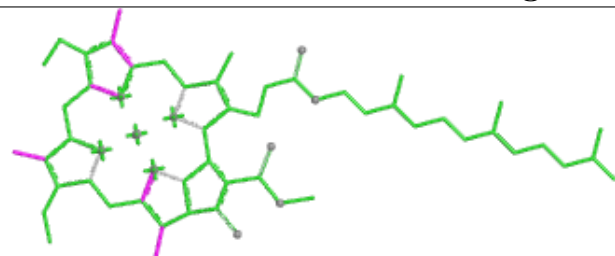


Torsions

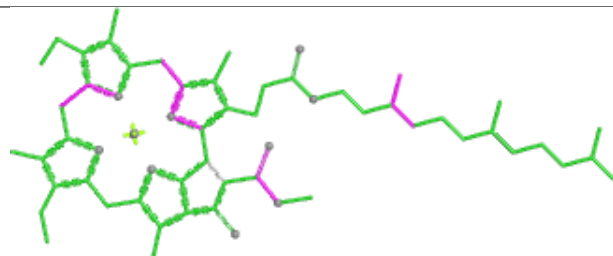


Rings

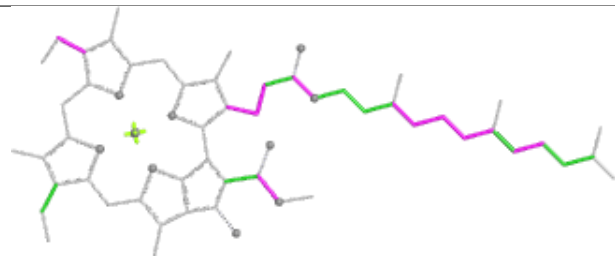
Ligand CLA r 613



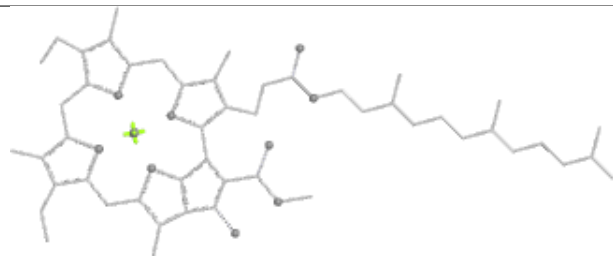
Bond lengths



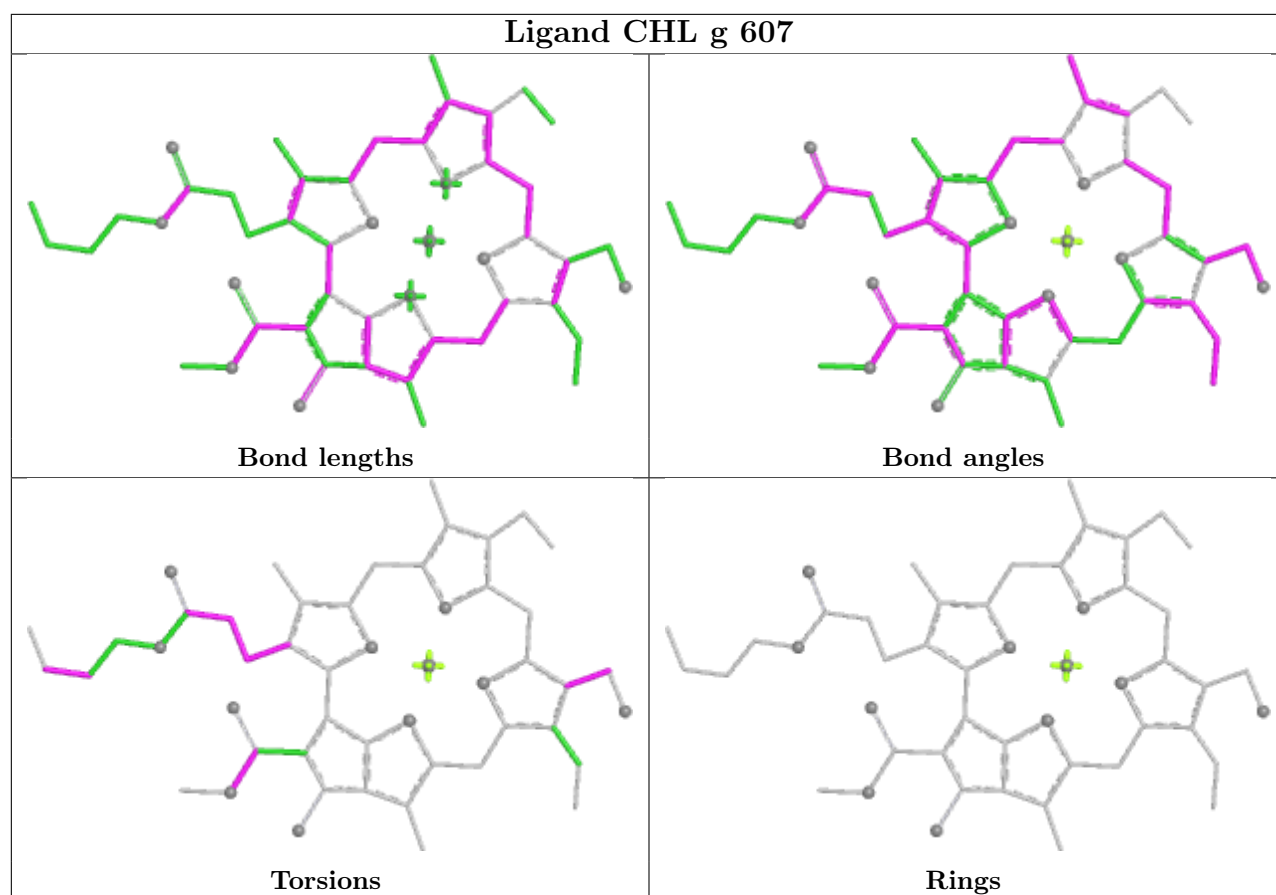
Bond angles



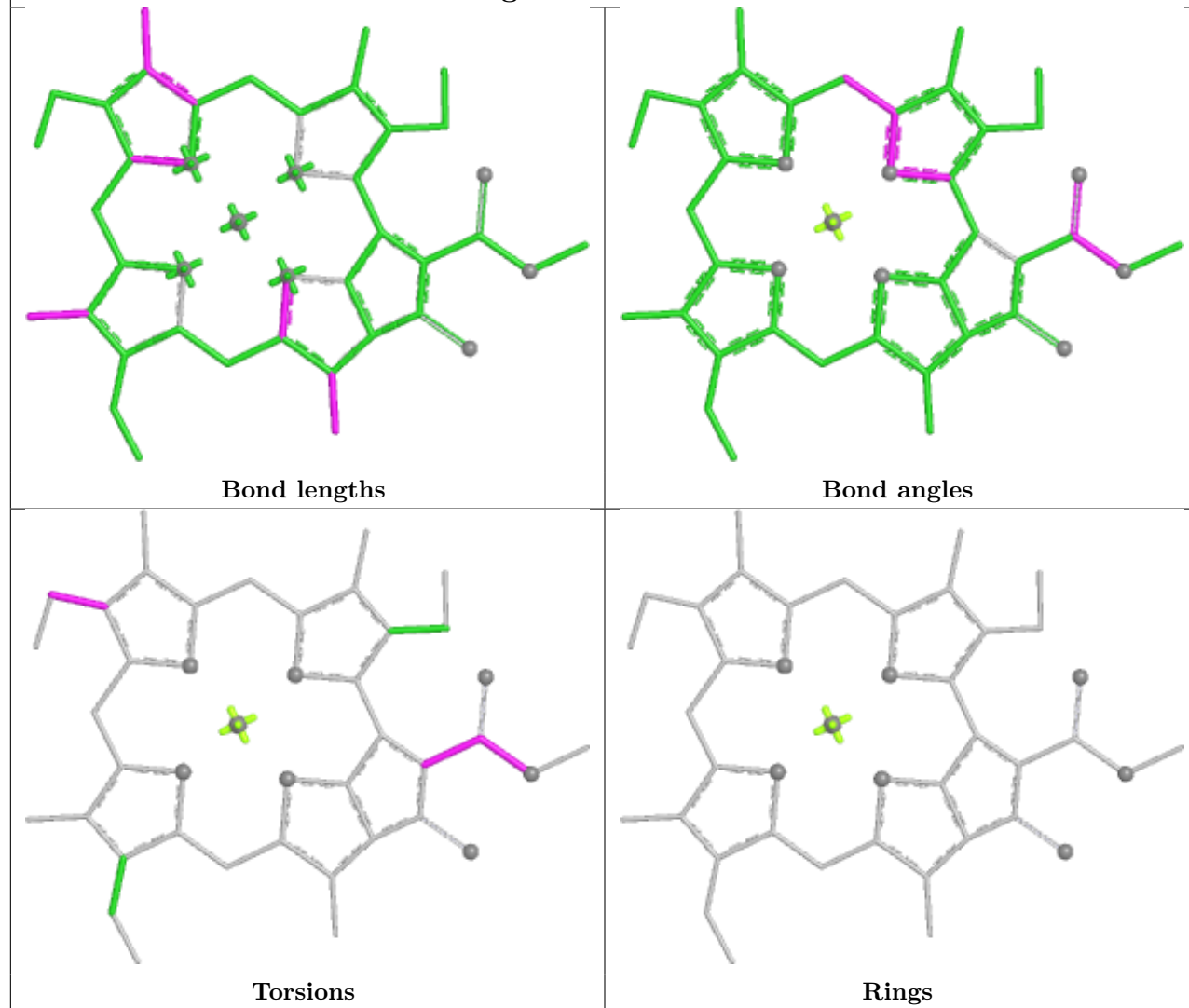
Torsions



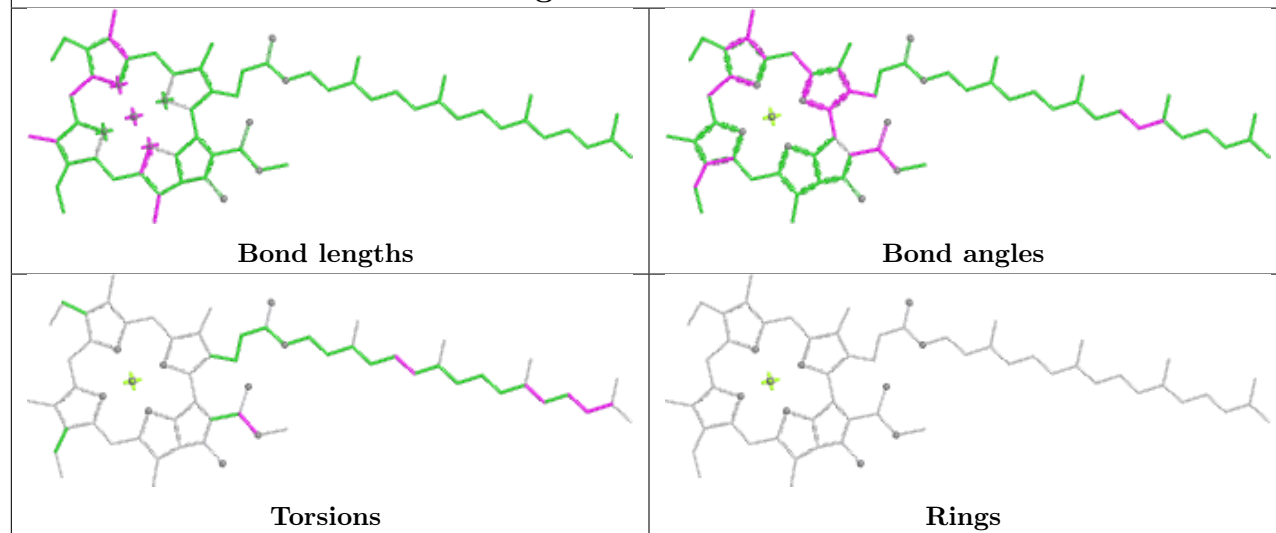
Rings

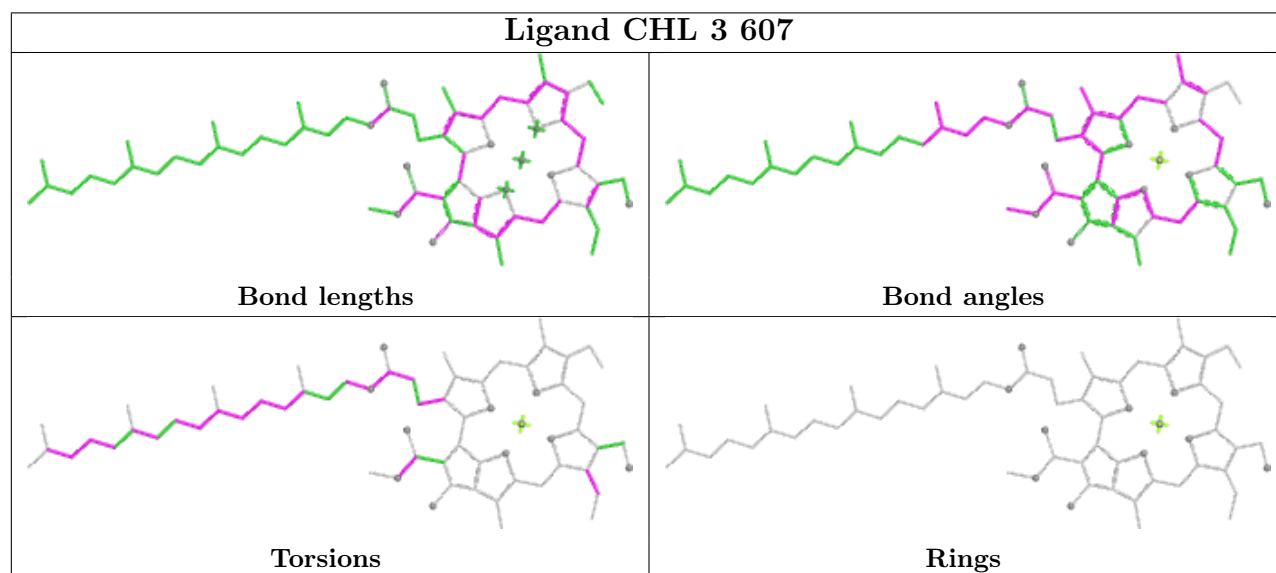
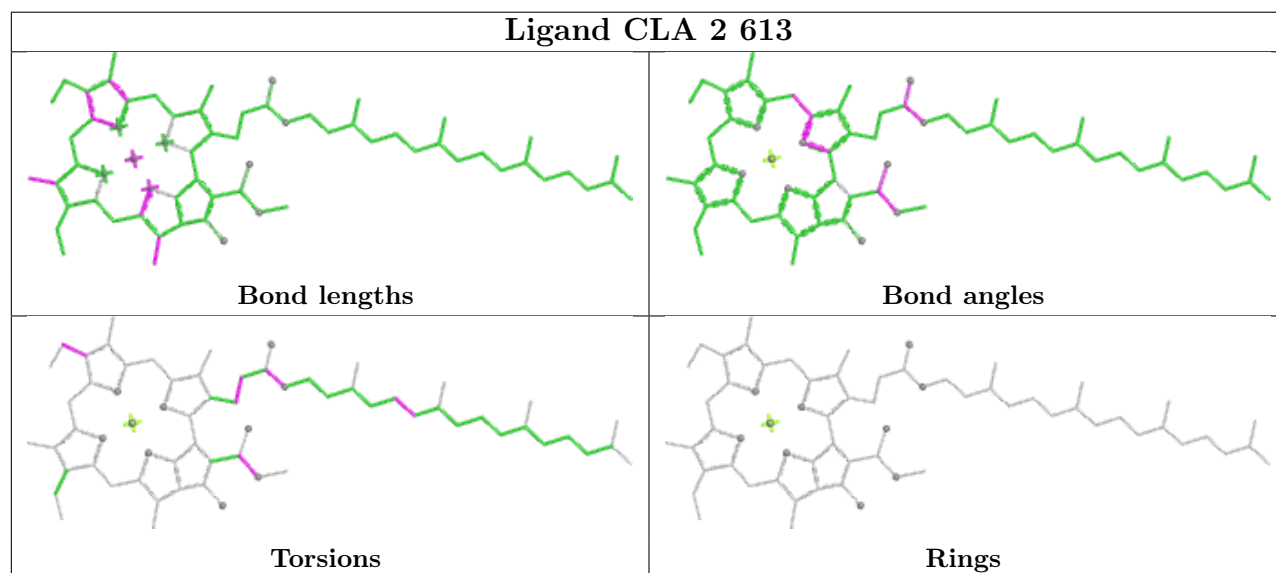
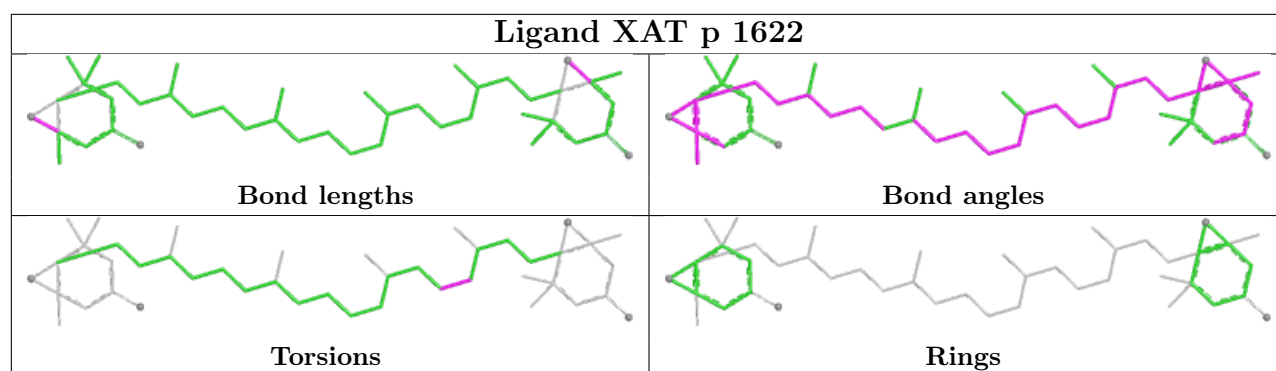


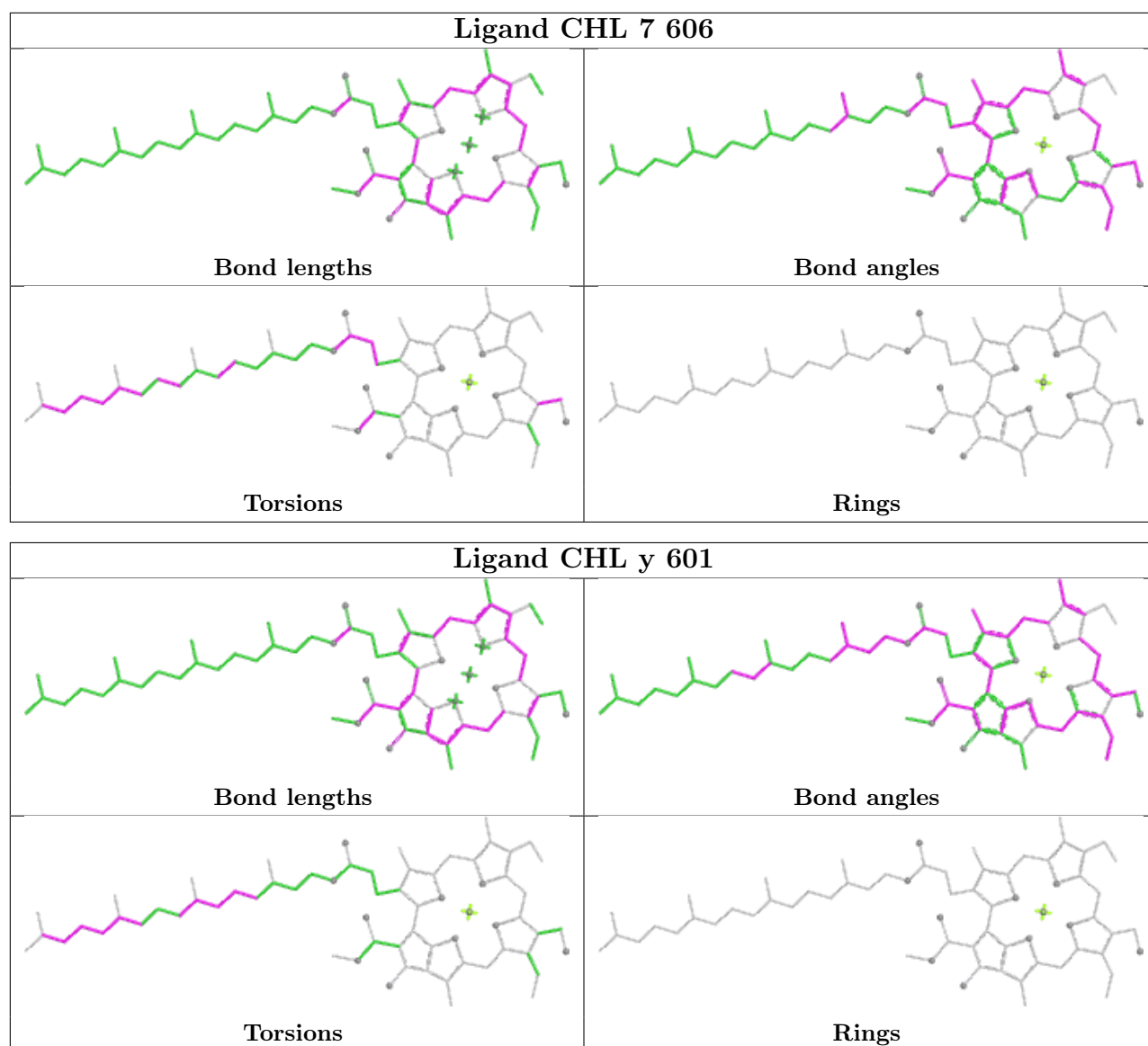
Ligand CLA s 603



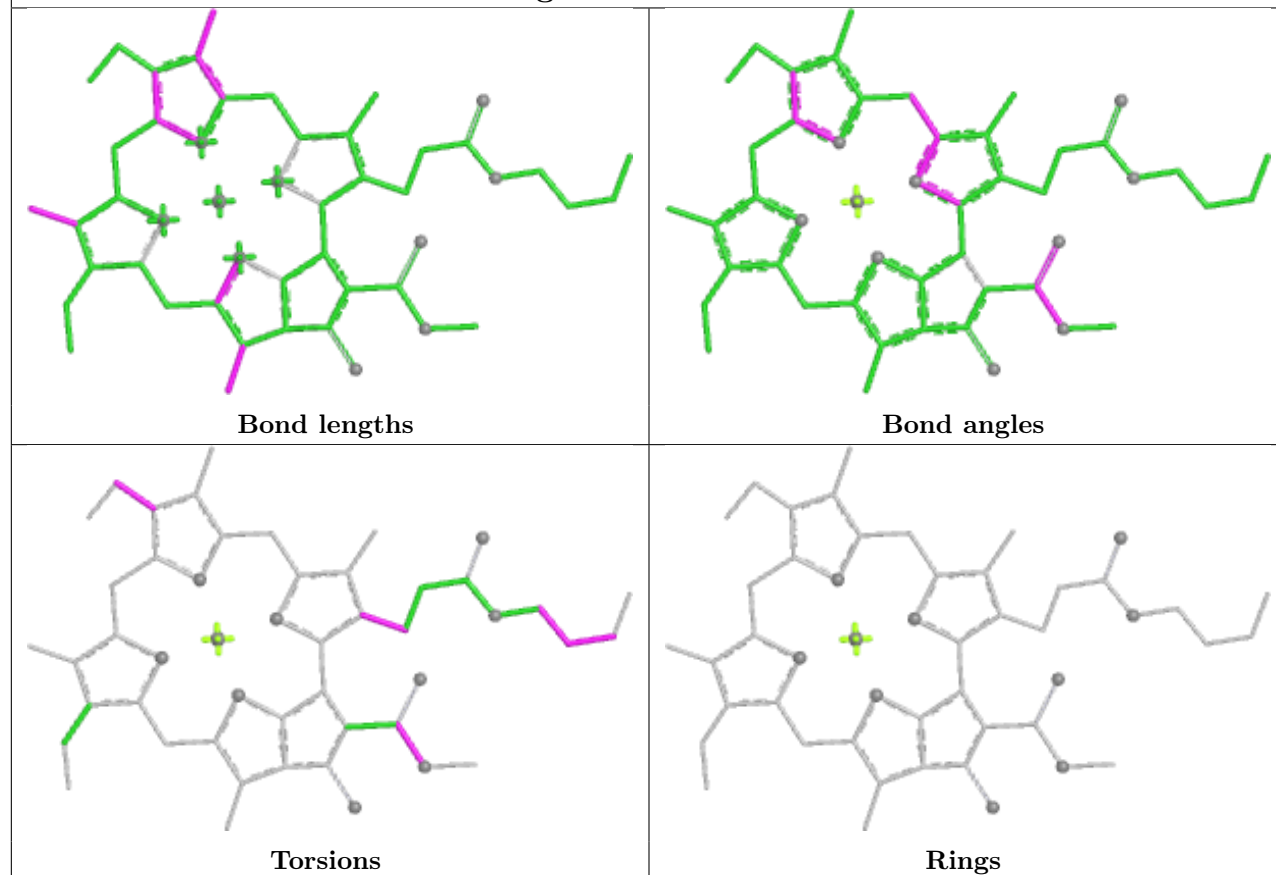
Ligand CLA b 616



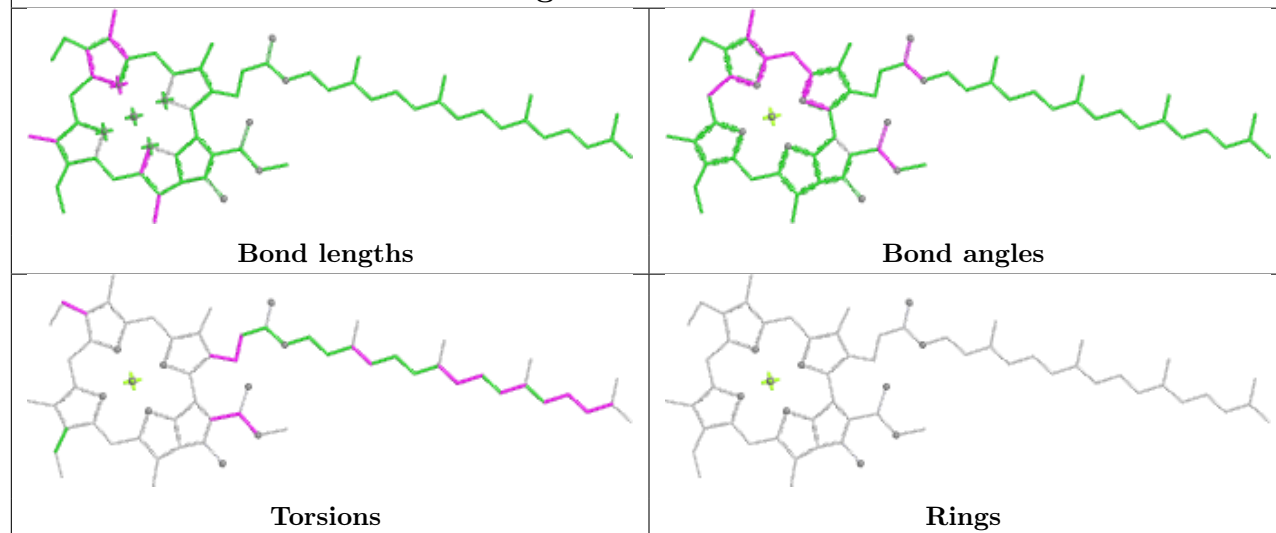




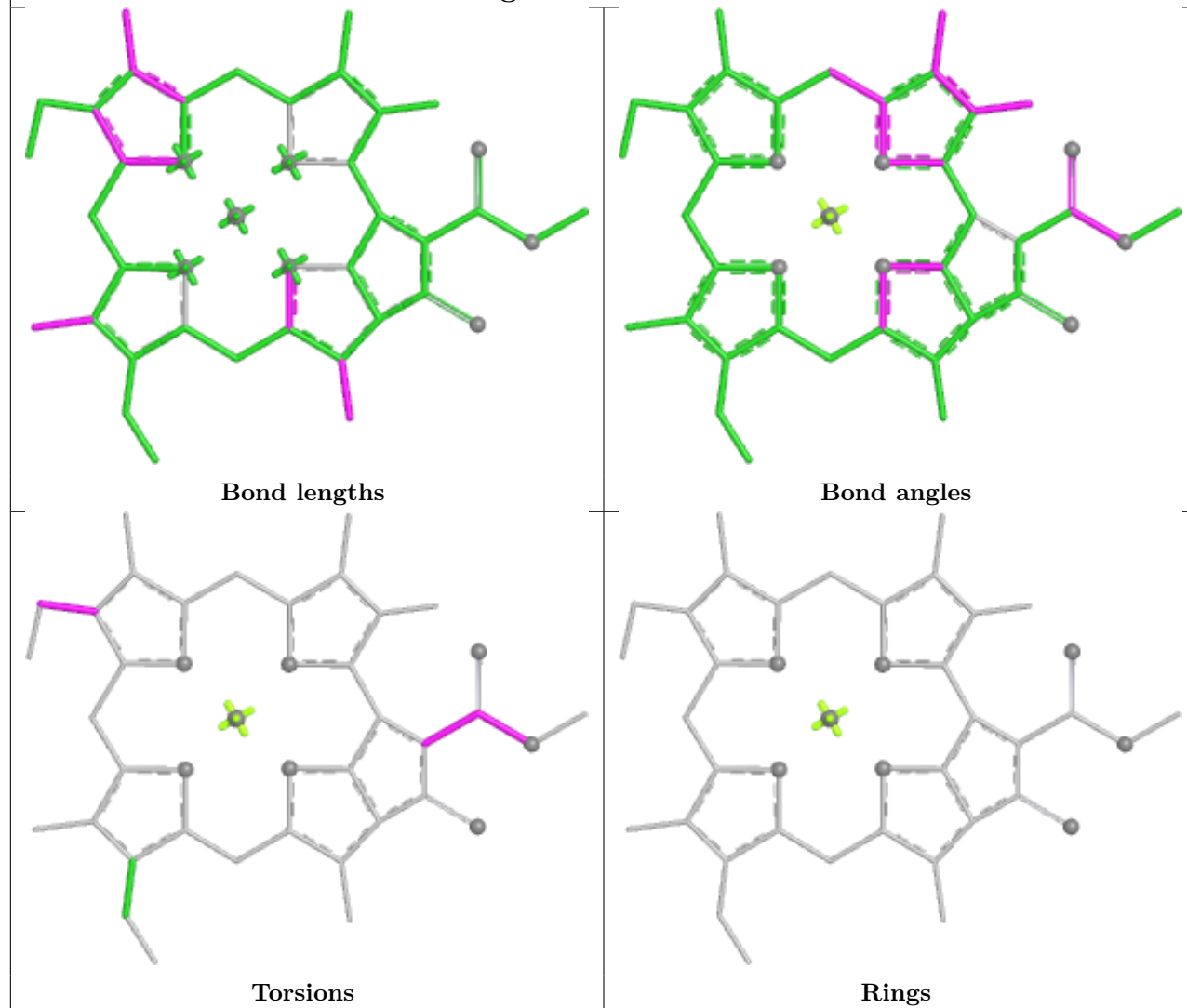
Ligand CLA 9 604



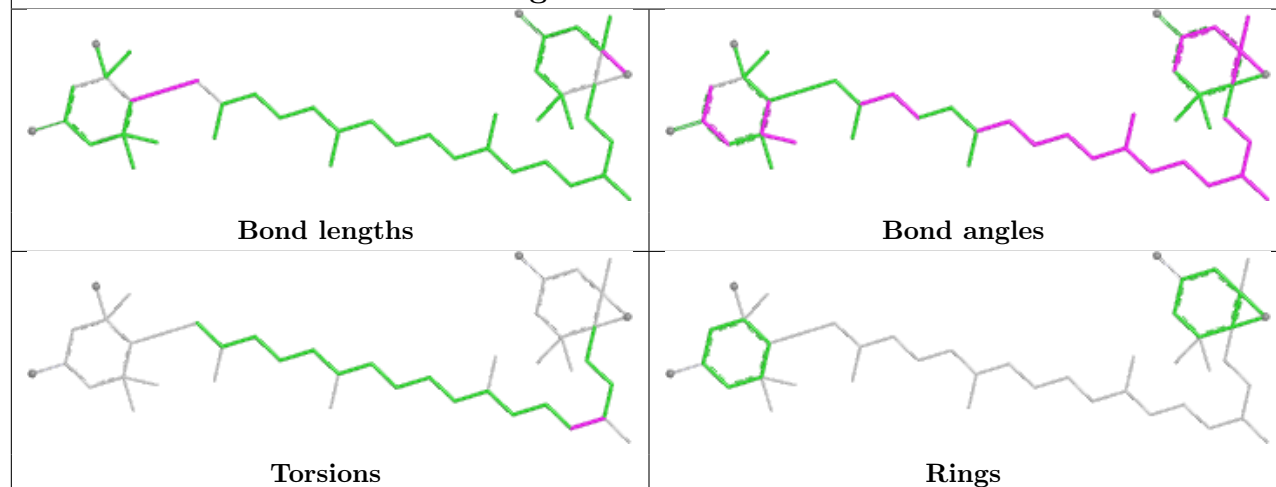
Ligand CLA 6 604

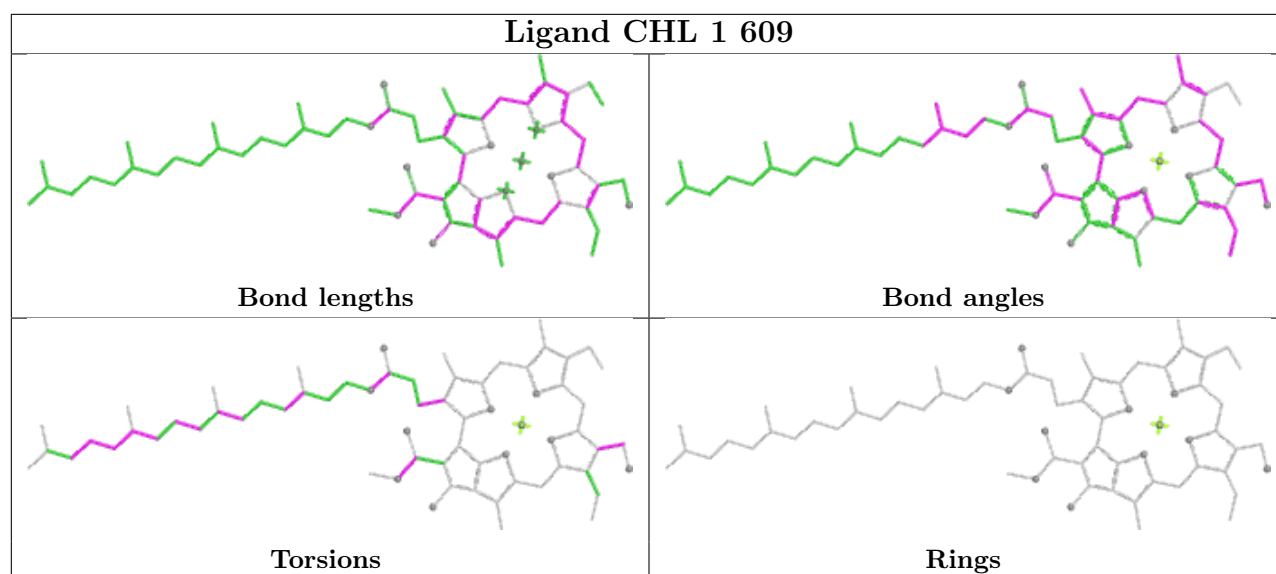
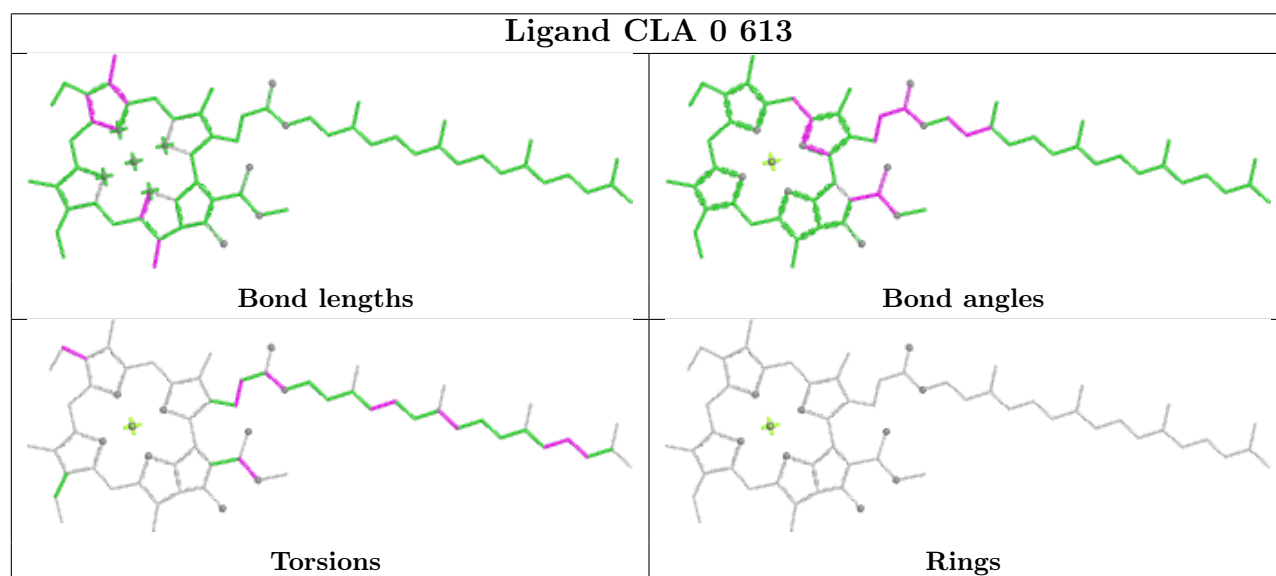
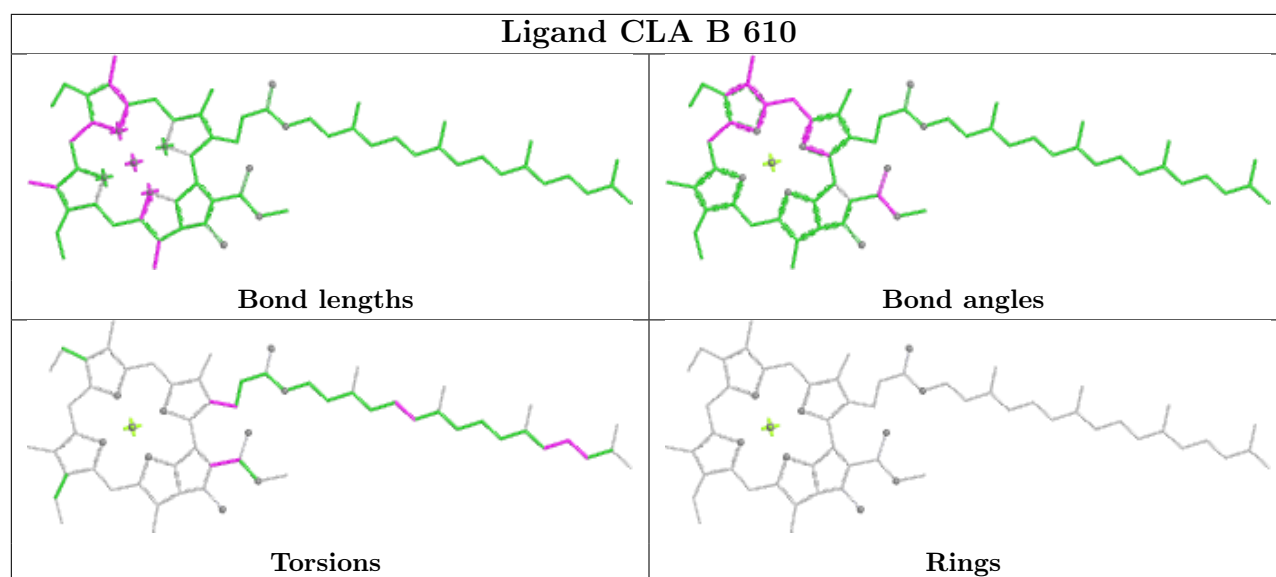


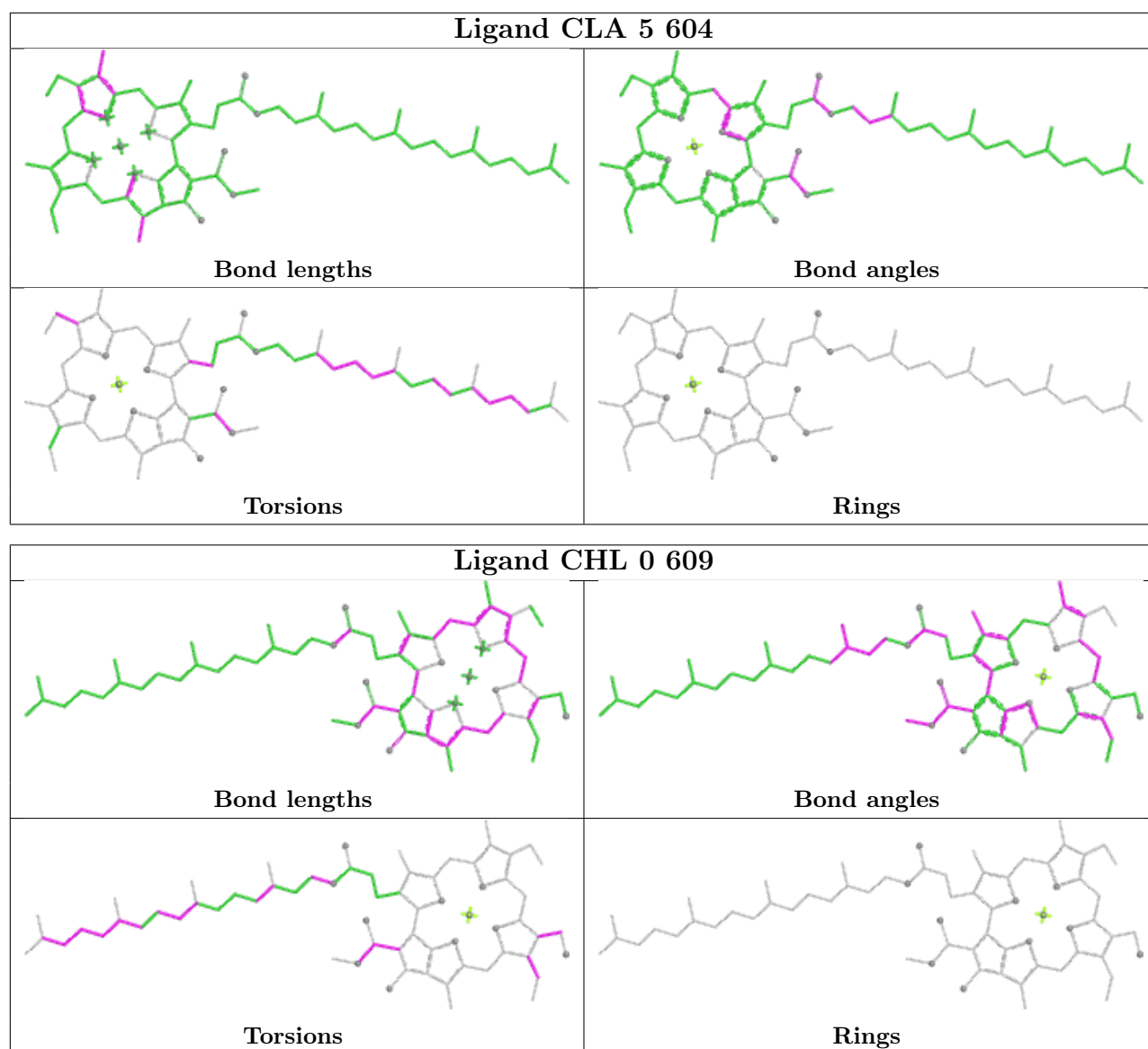
Ligand CLA s 609

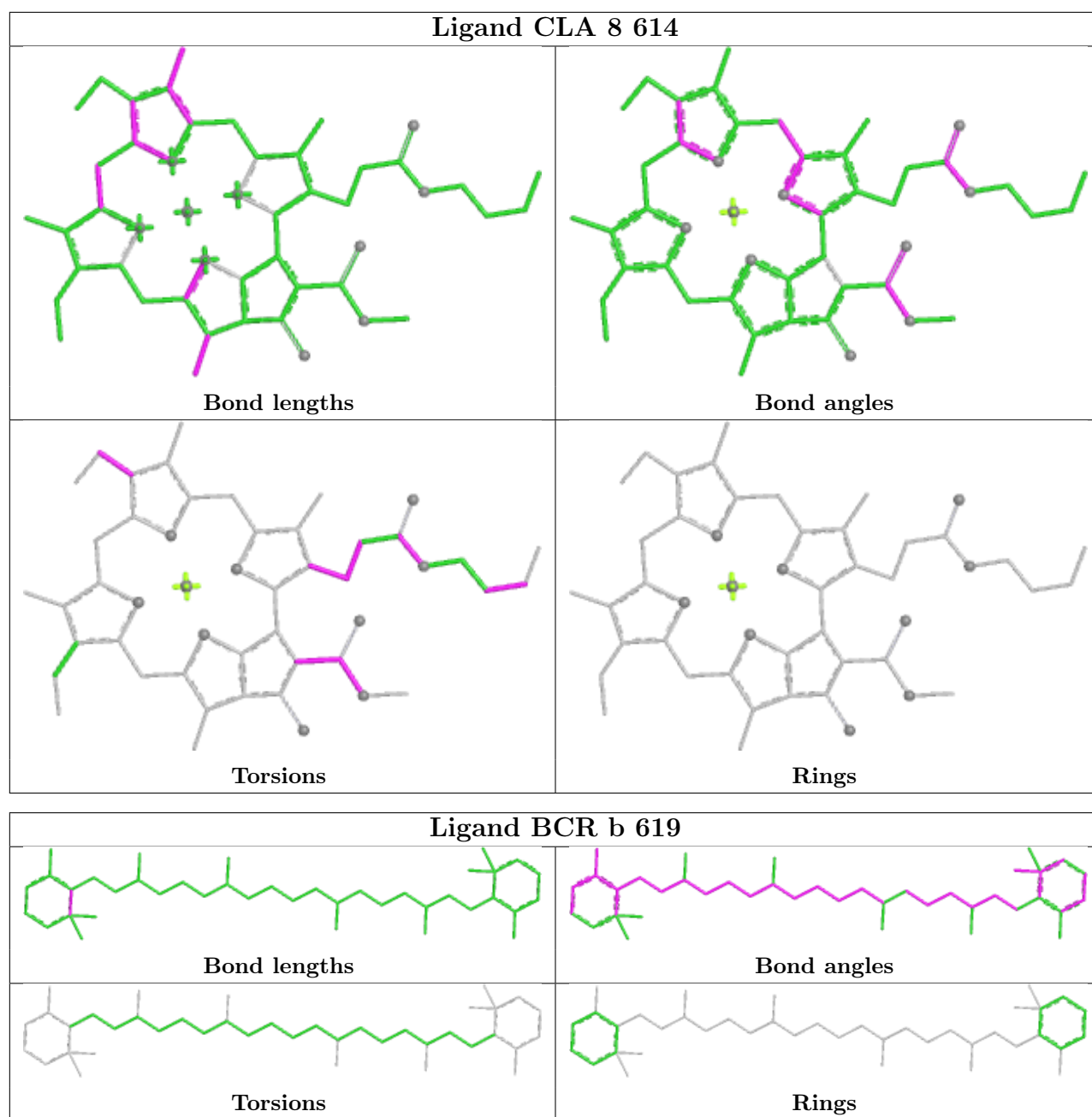


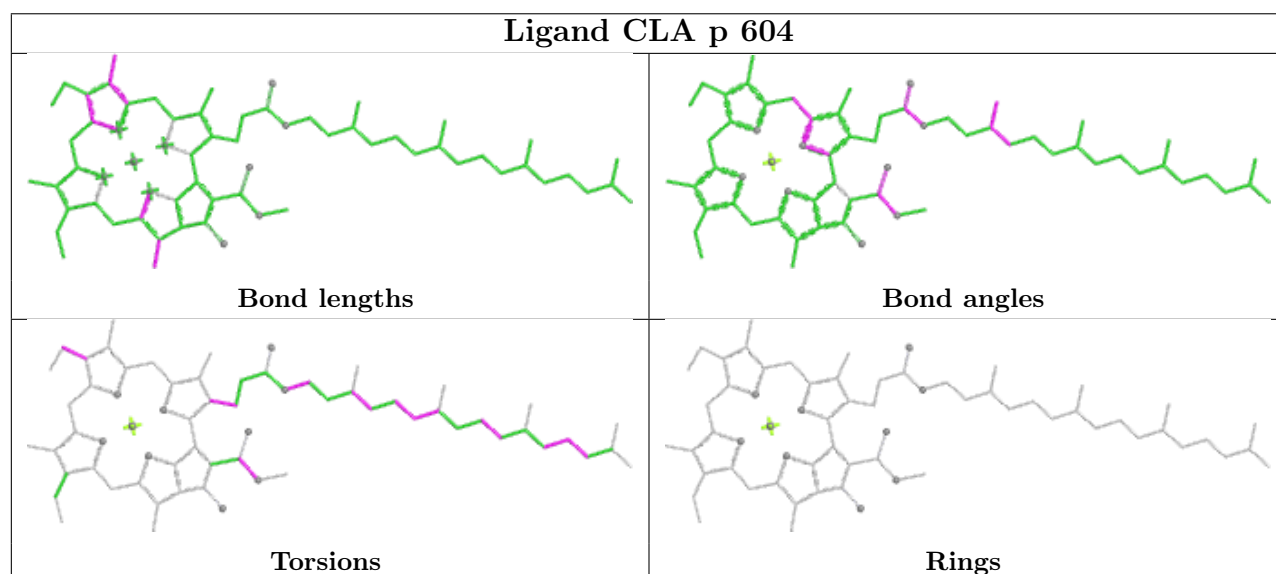
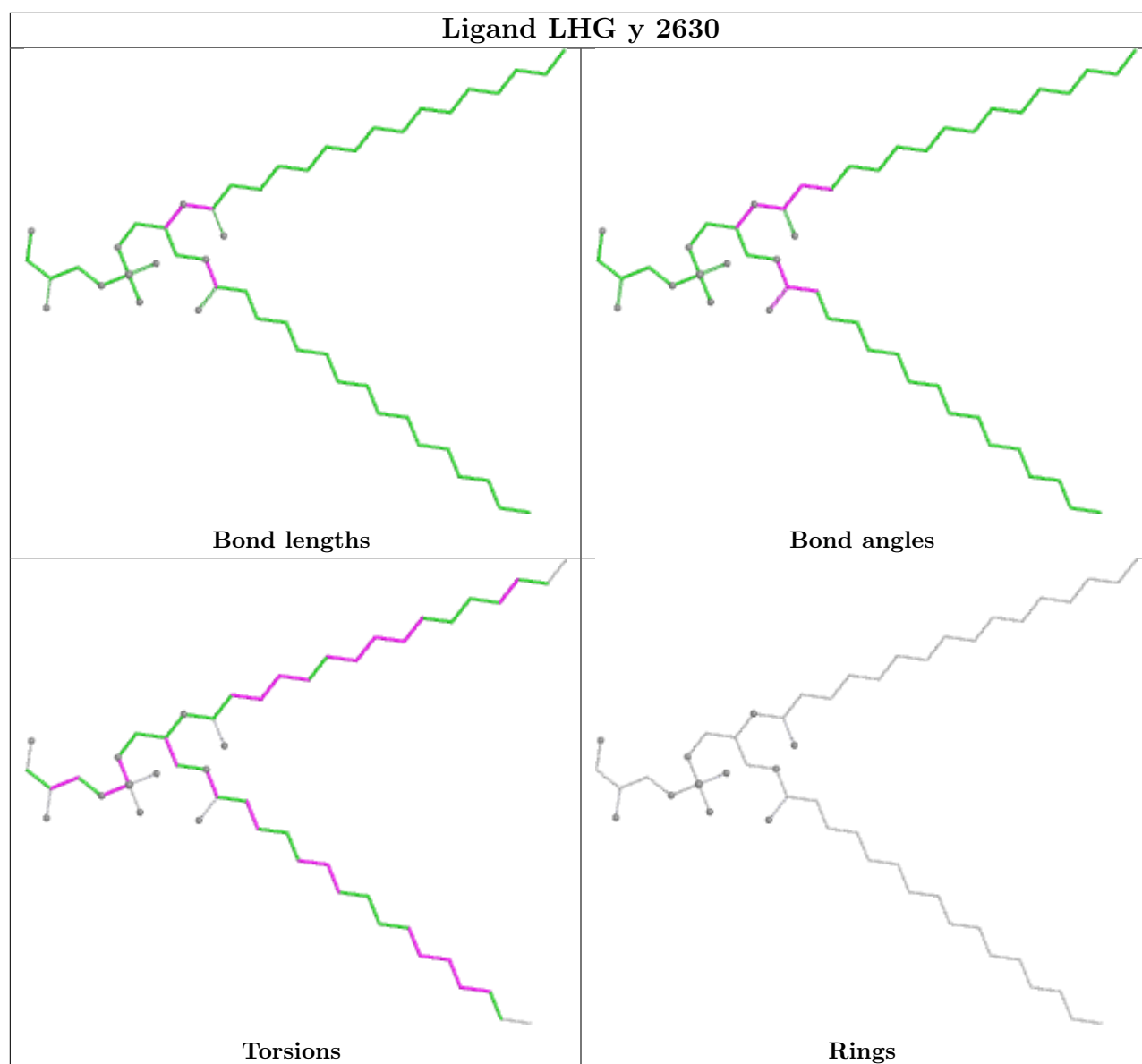
Ligand NEX R 623

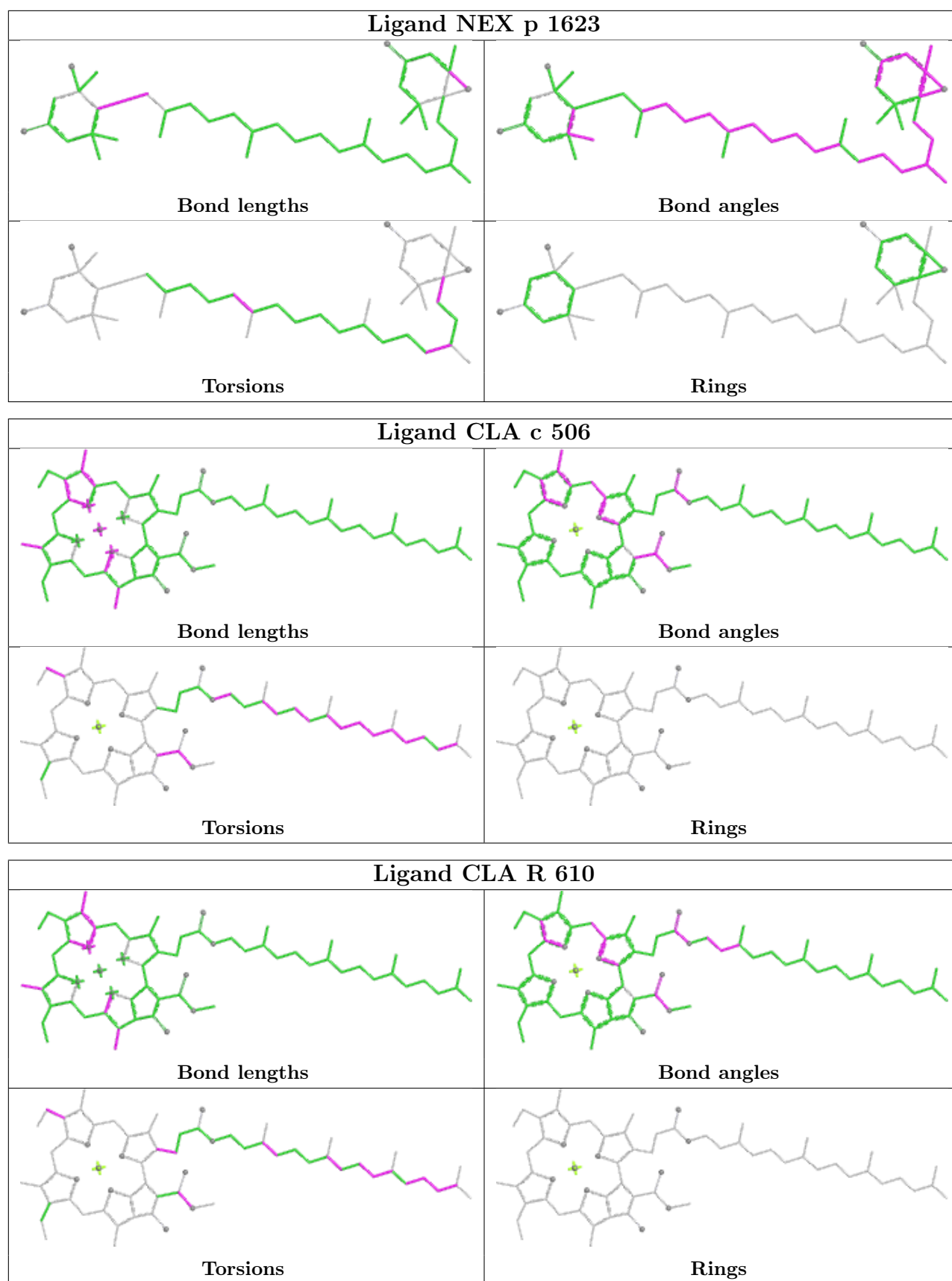


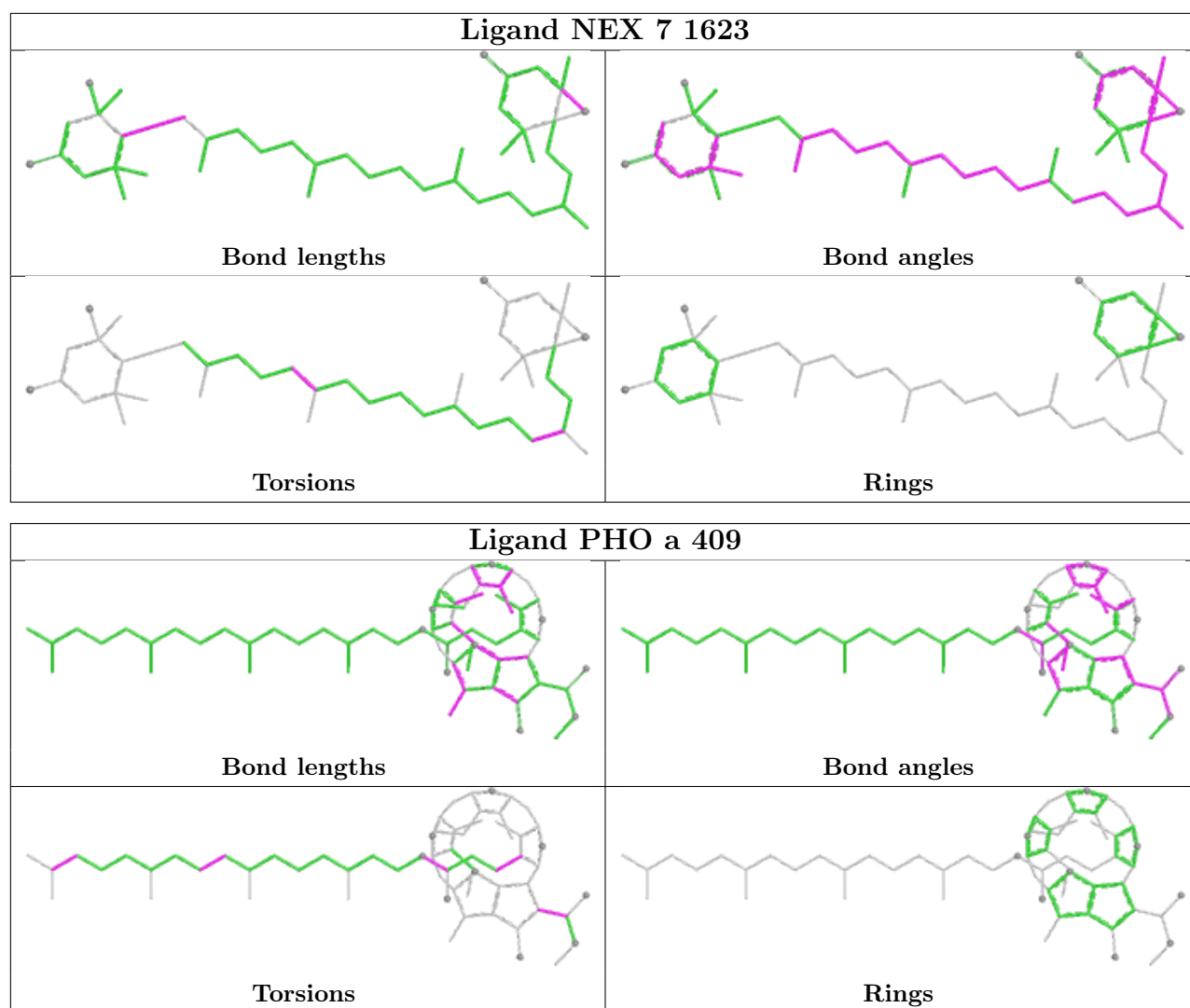




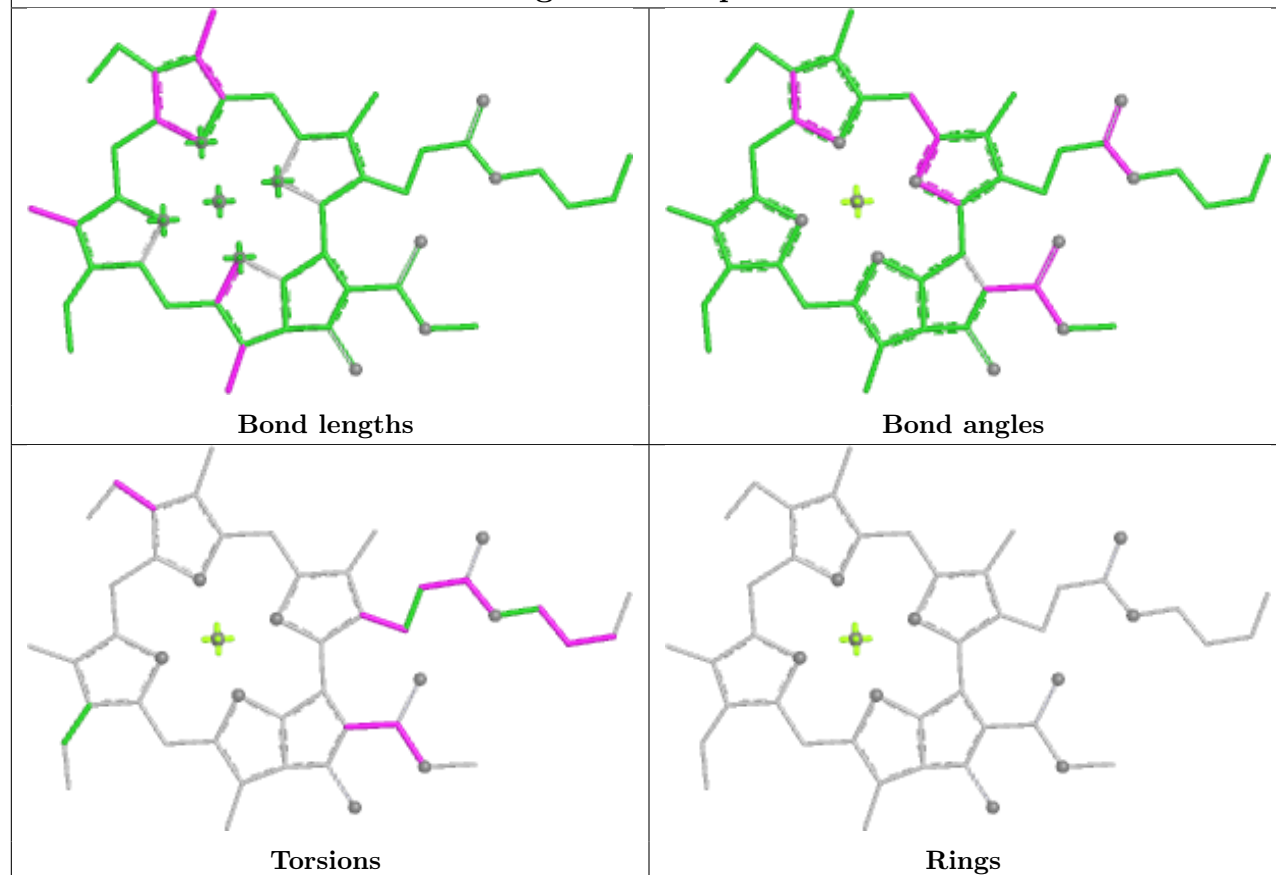




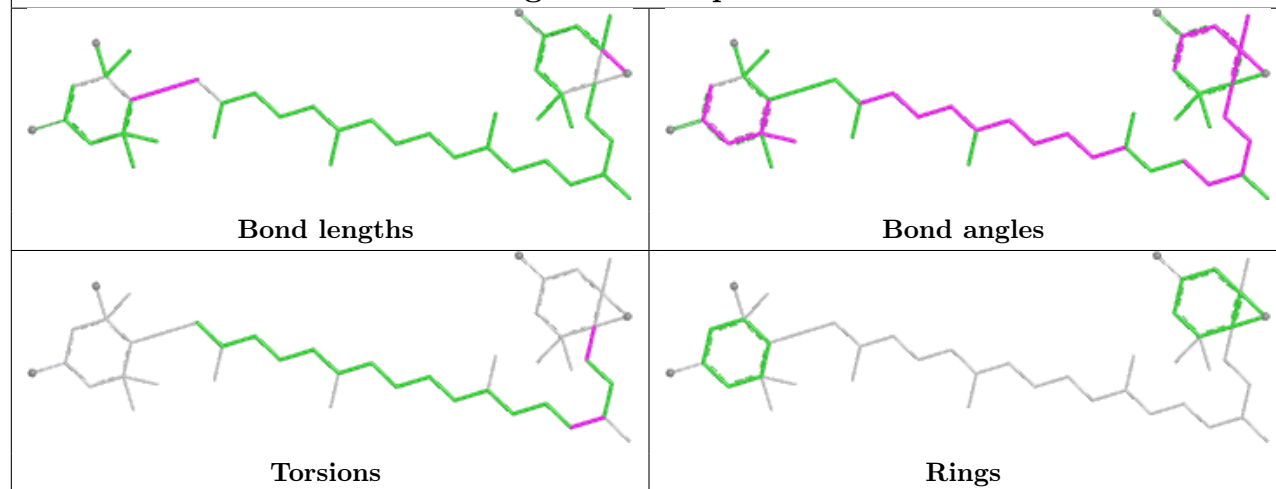


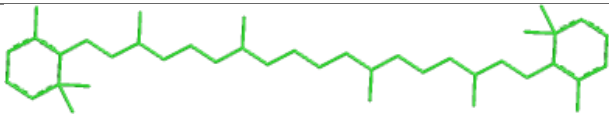
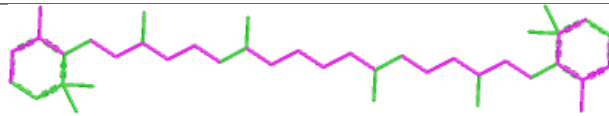
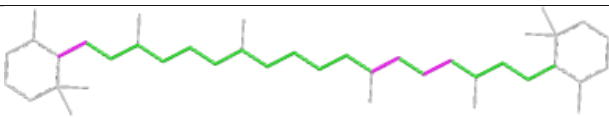
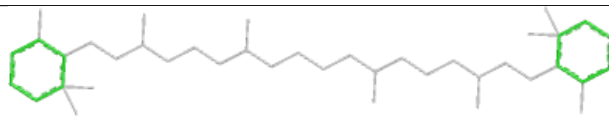


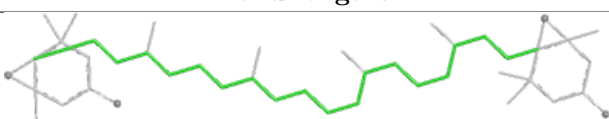
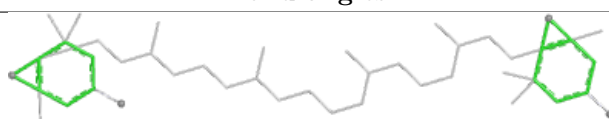
Ligand CLA q 604

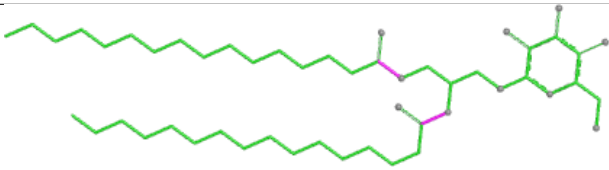
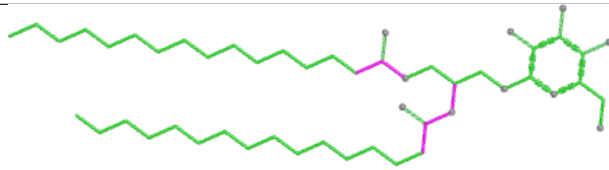
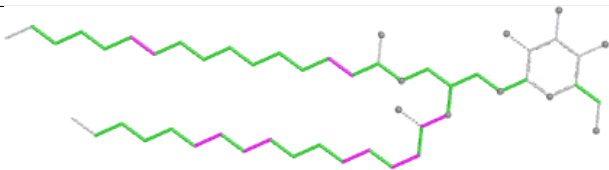
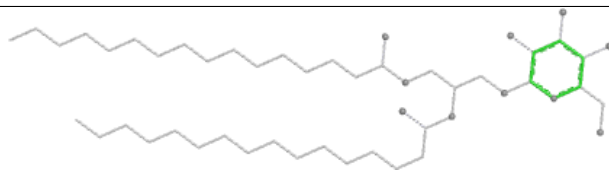


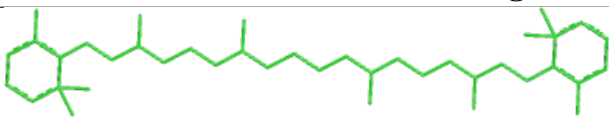
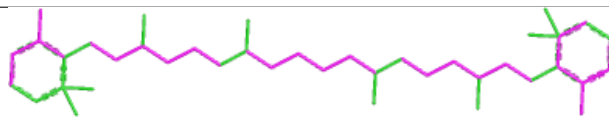
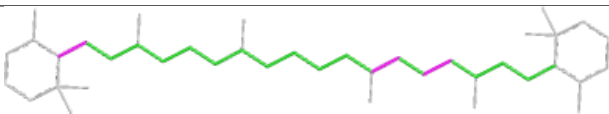
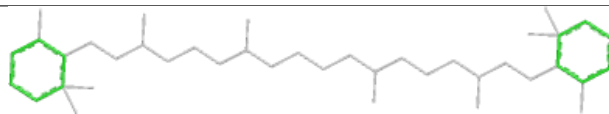
Ligand NEX q 1623

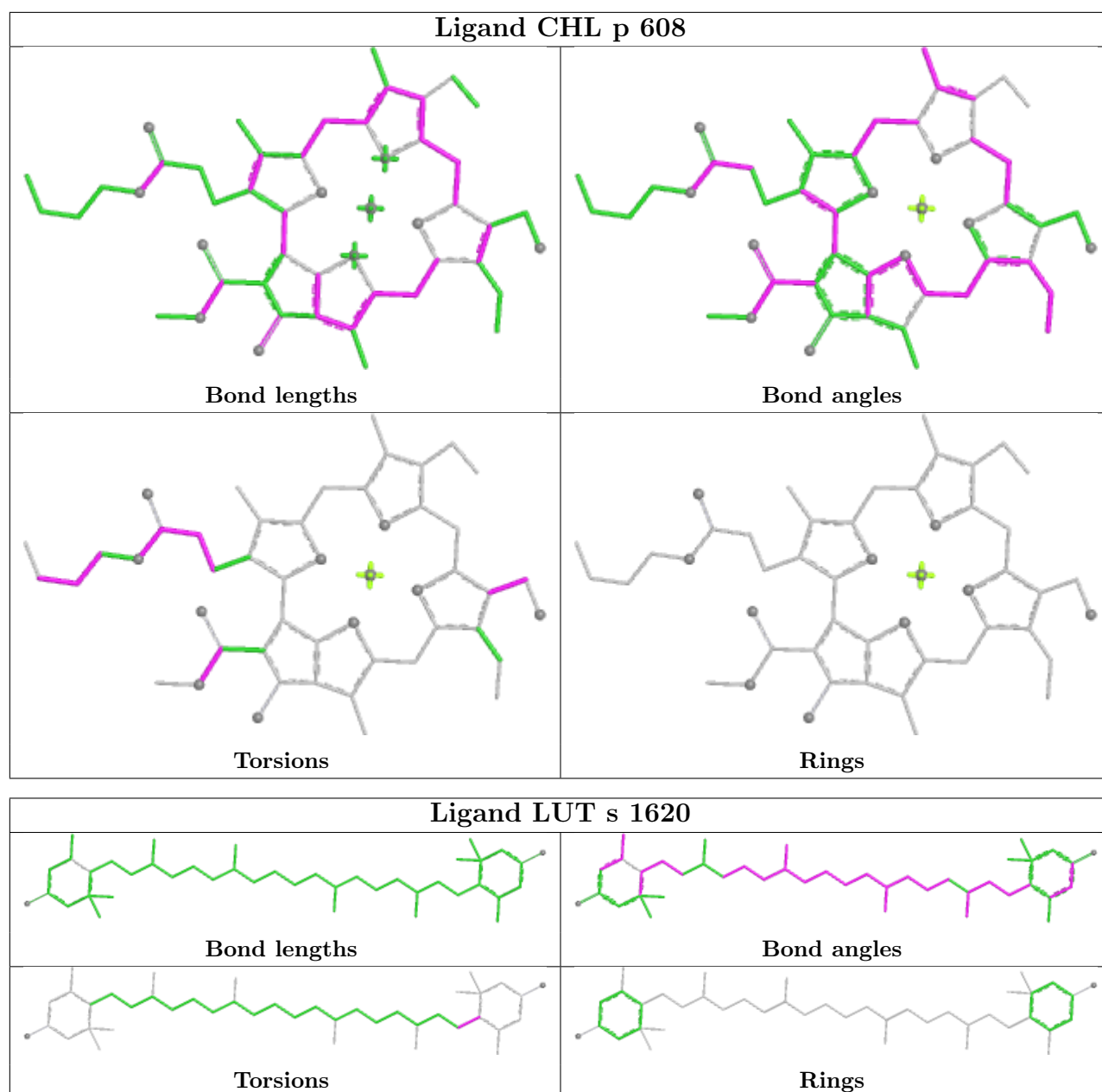


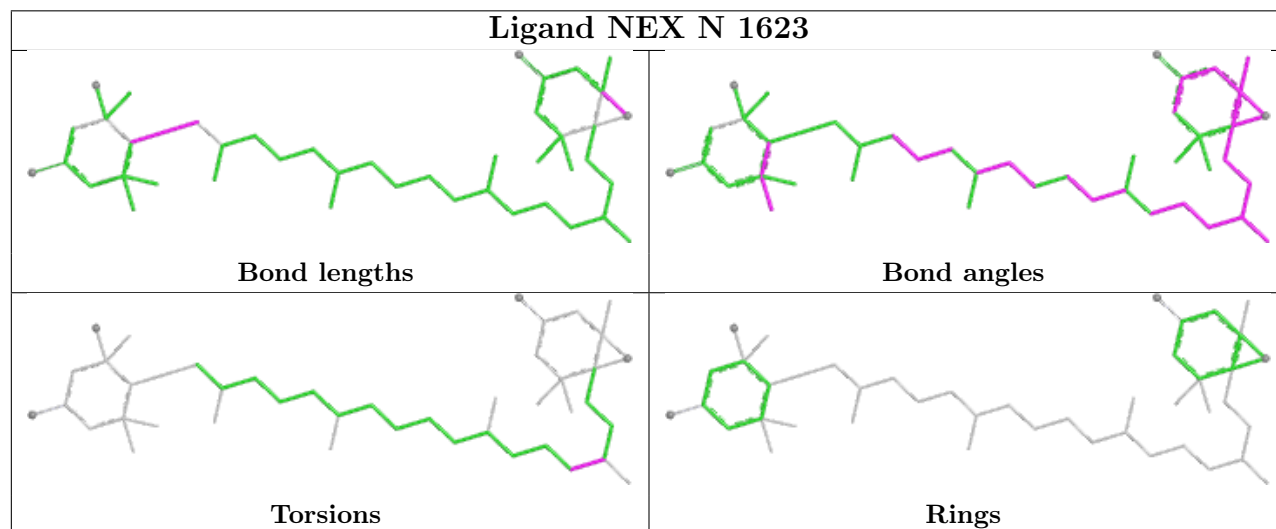
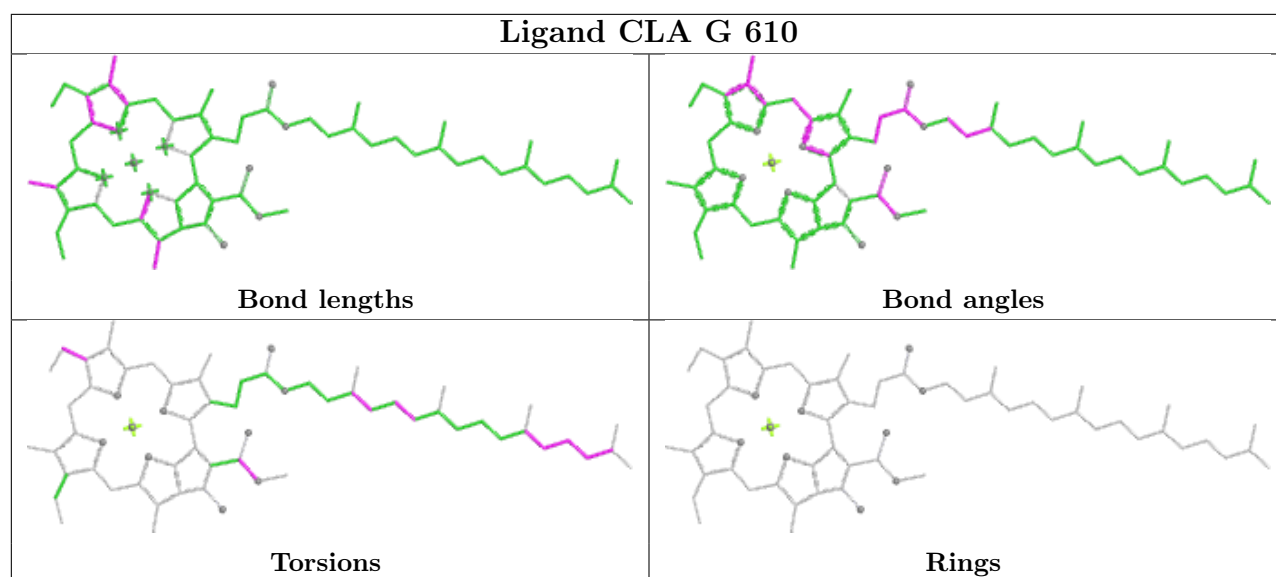
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT Y 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

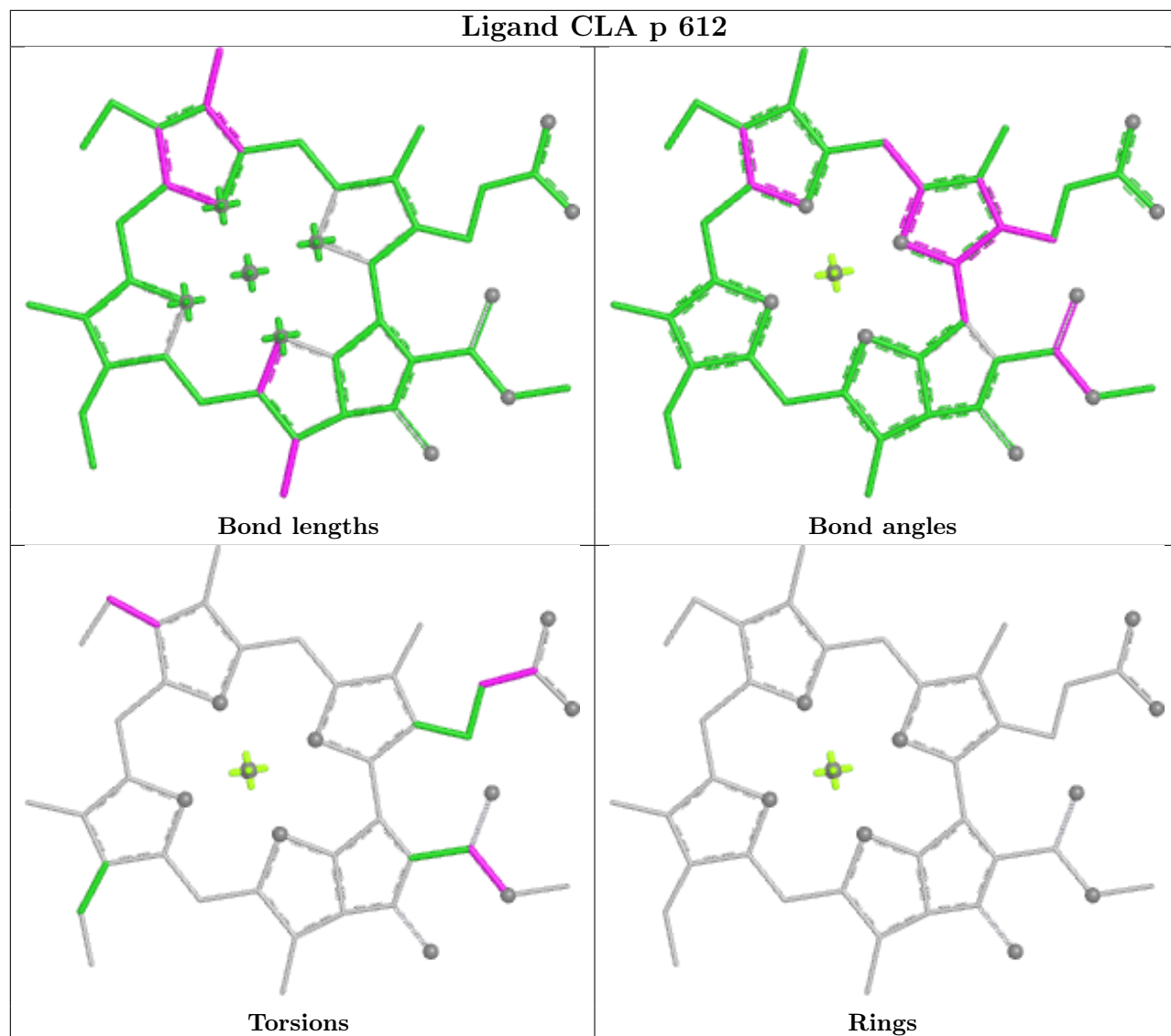
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

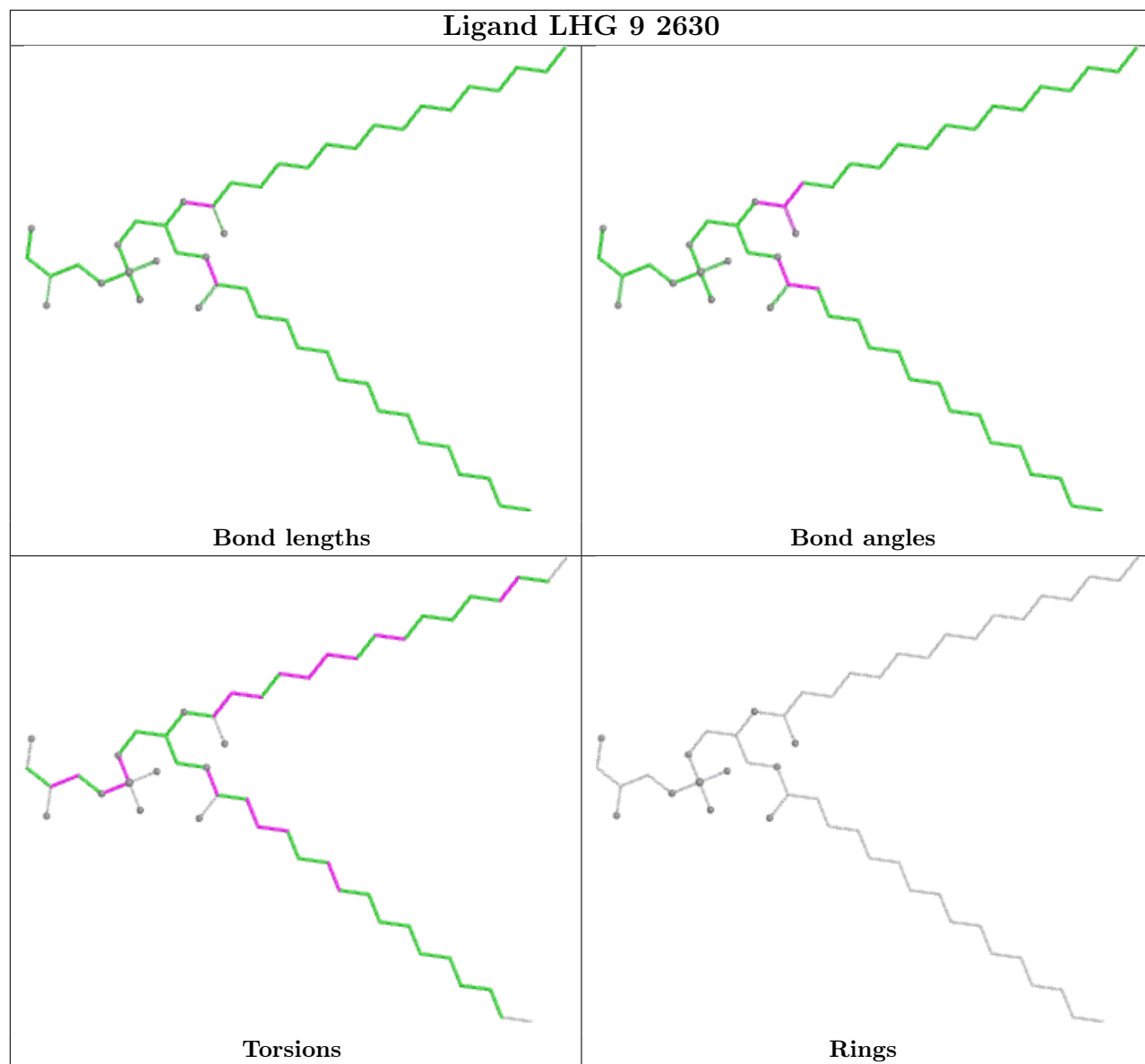
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



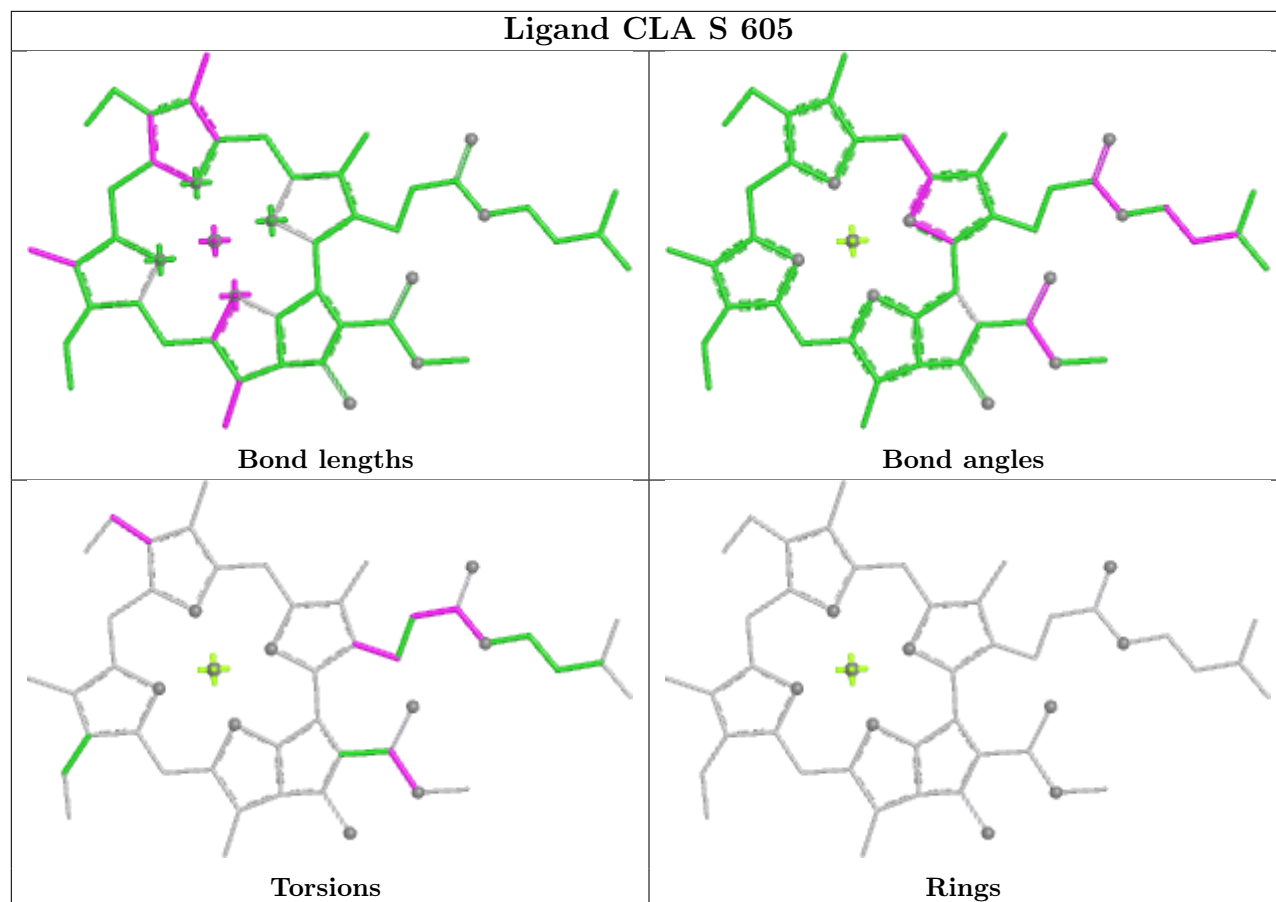


Ligand CLA p 612

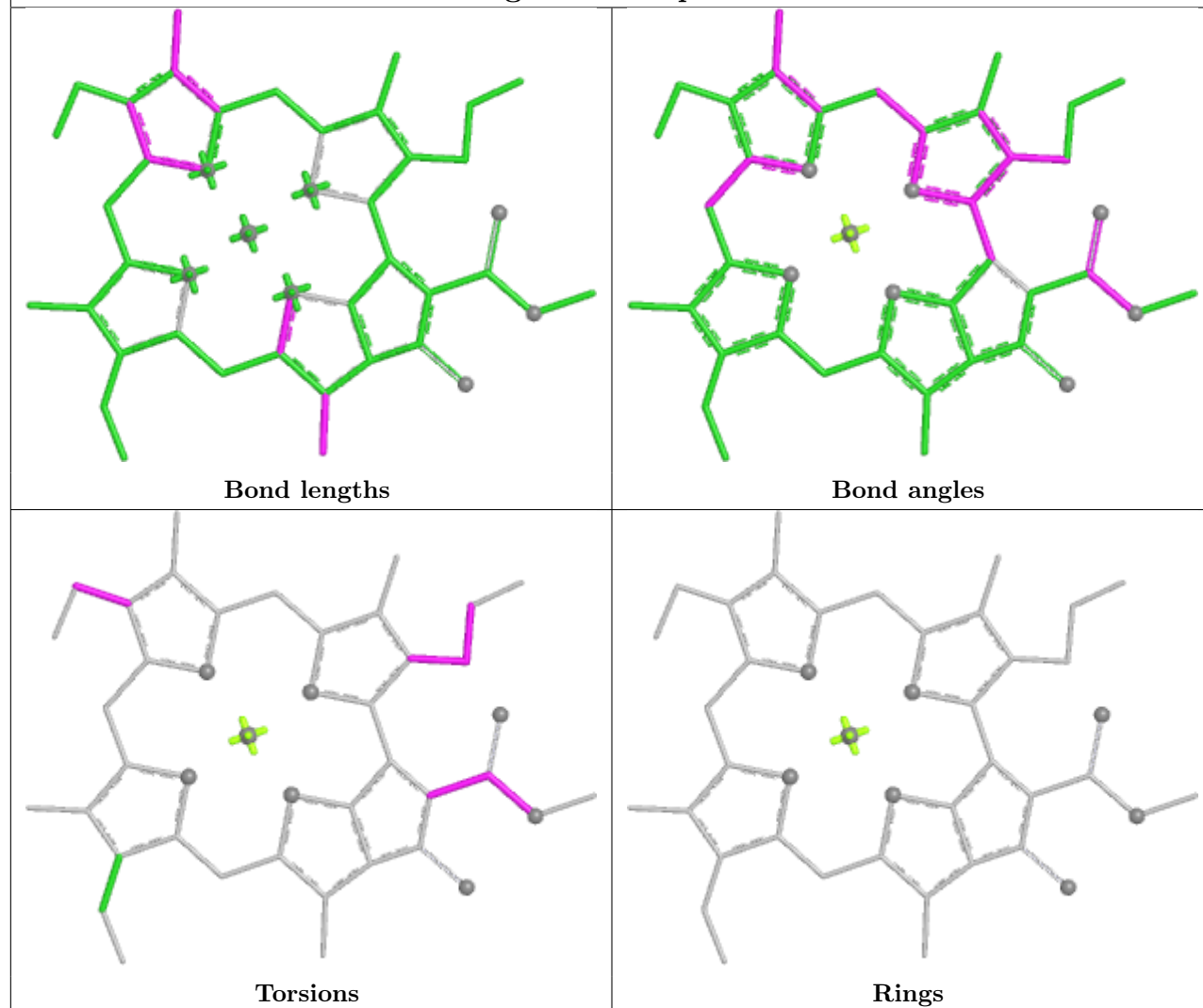




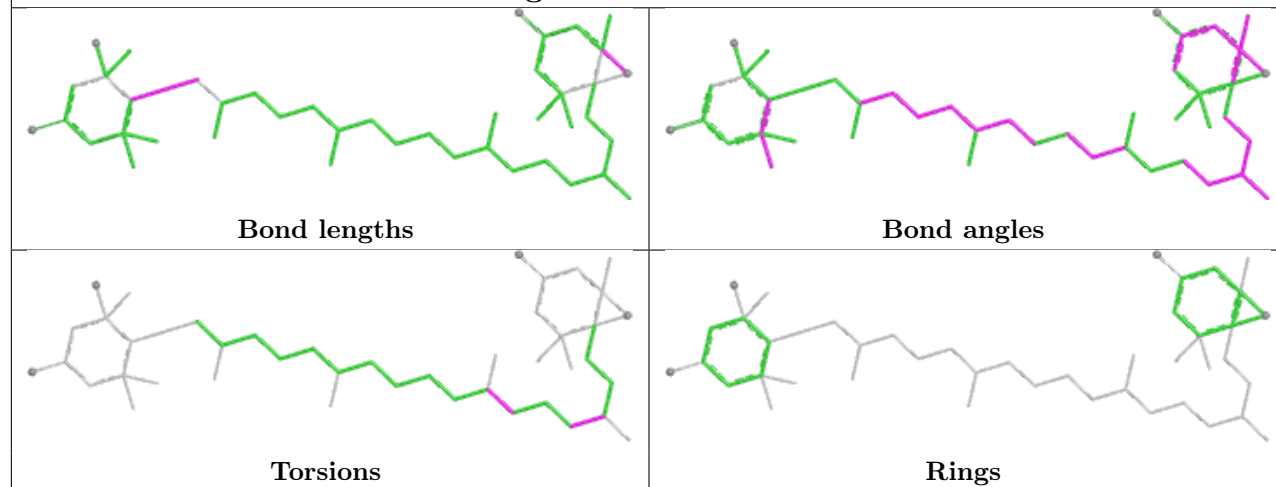
Ligand CLA S 605

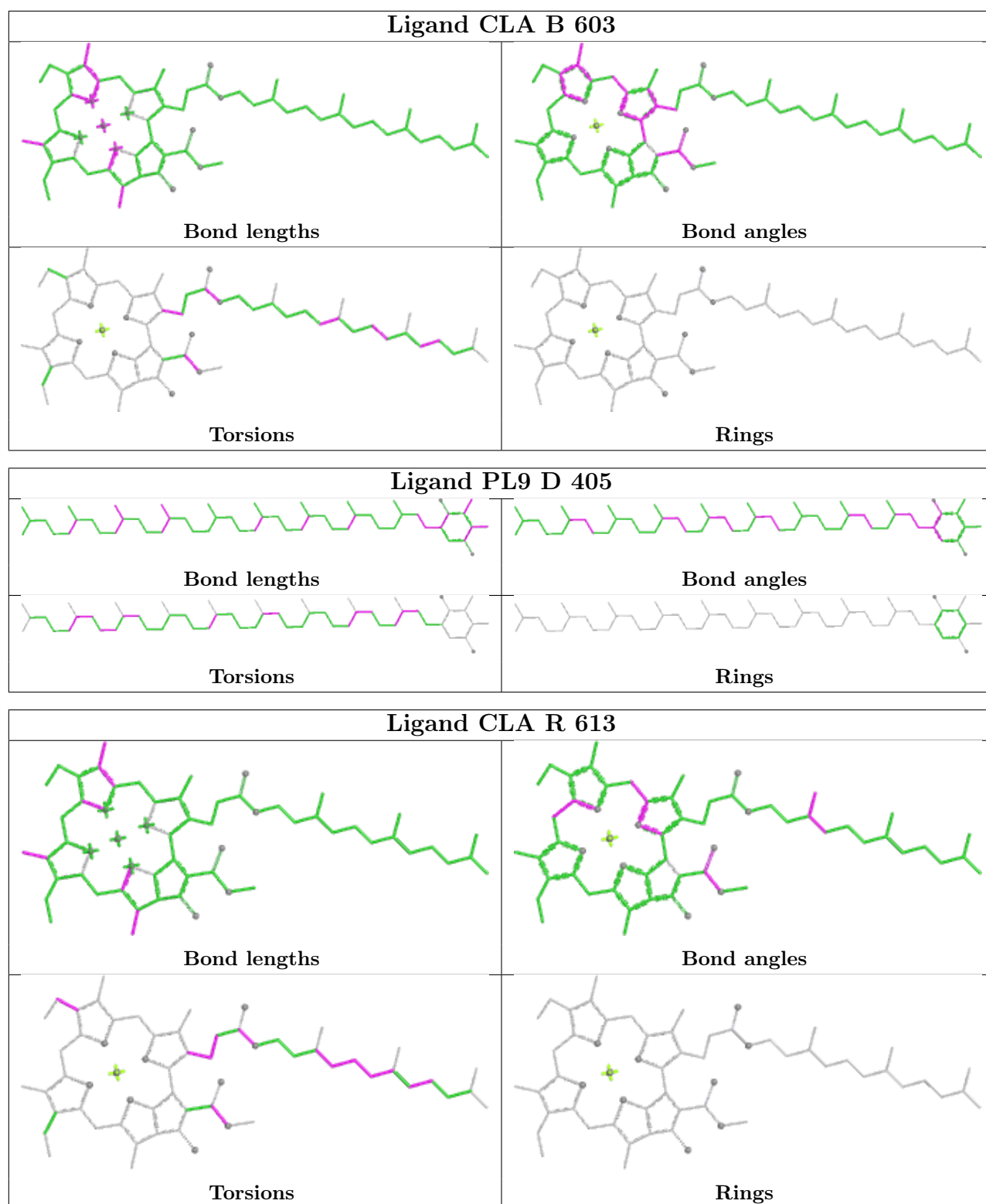


Ligand CLA q 612

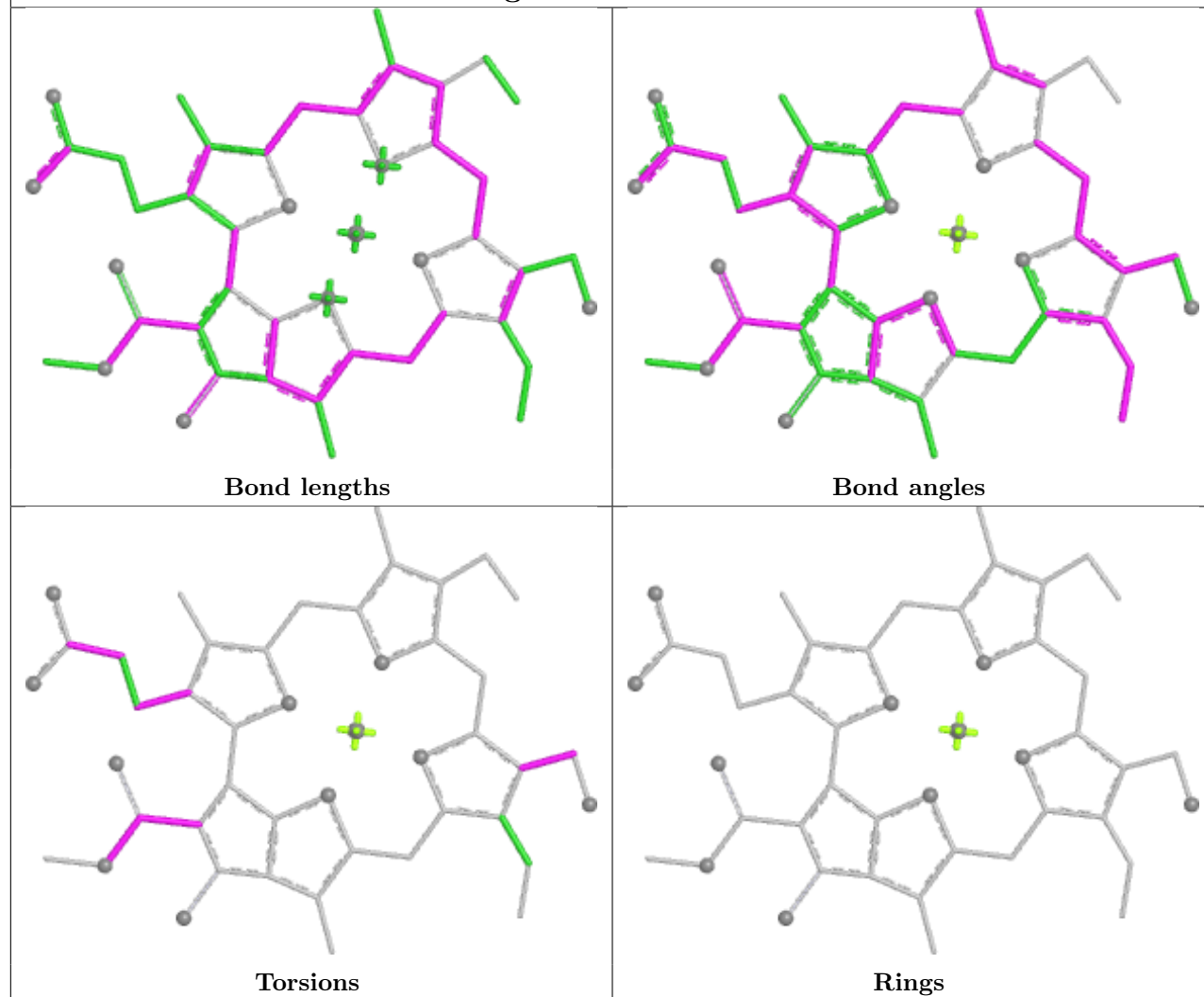


Ligand NEX 2 1623

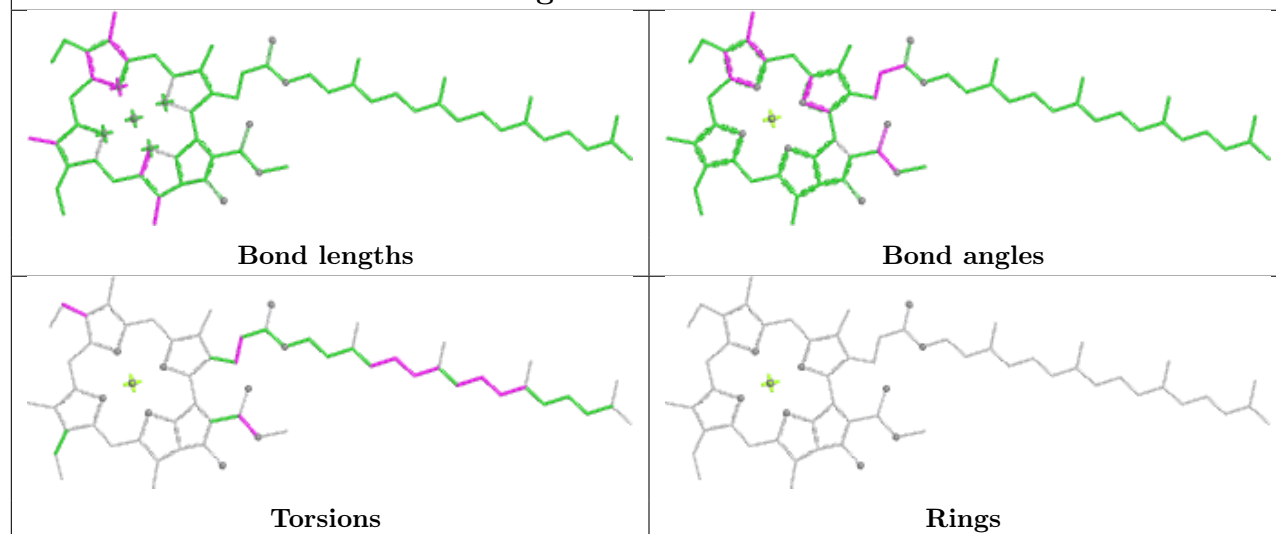


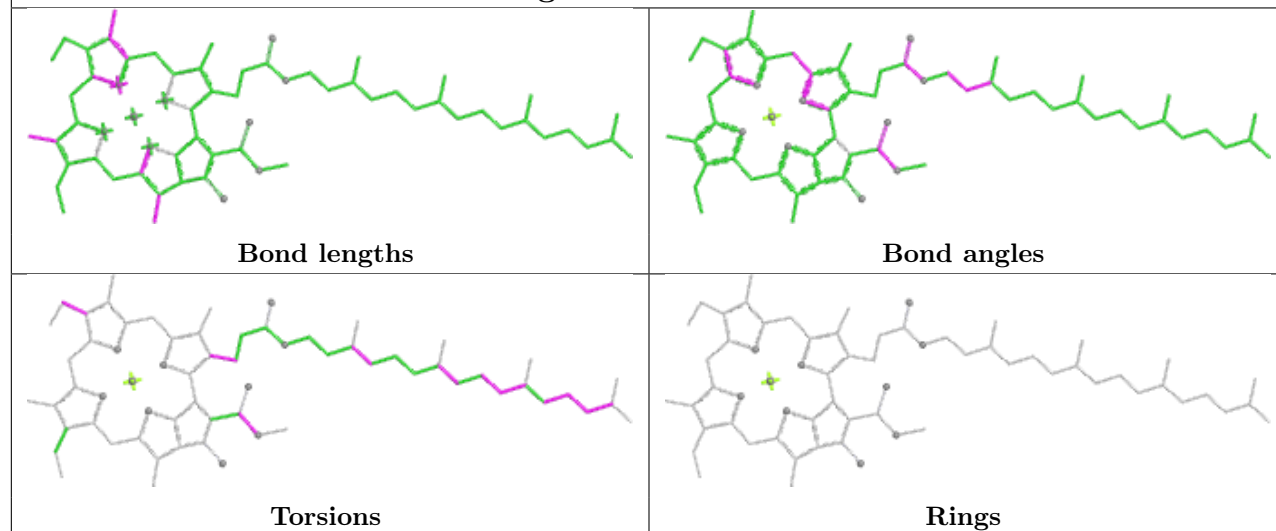
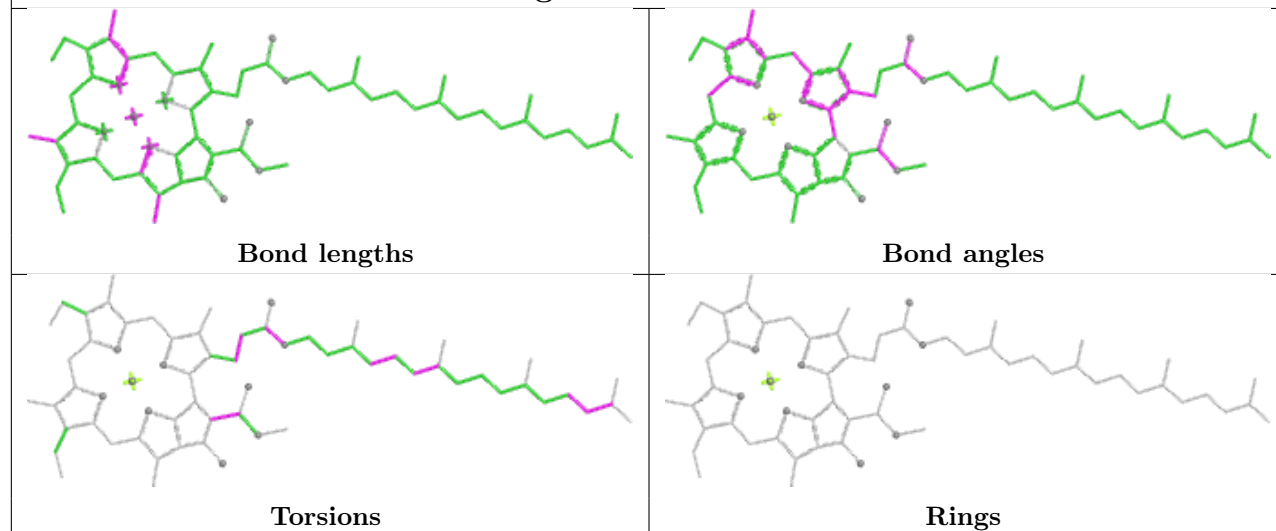


Ligand CHL n 606

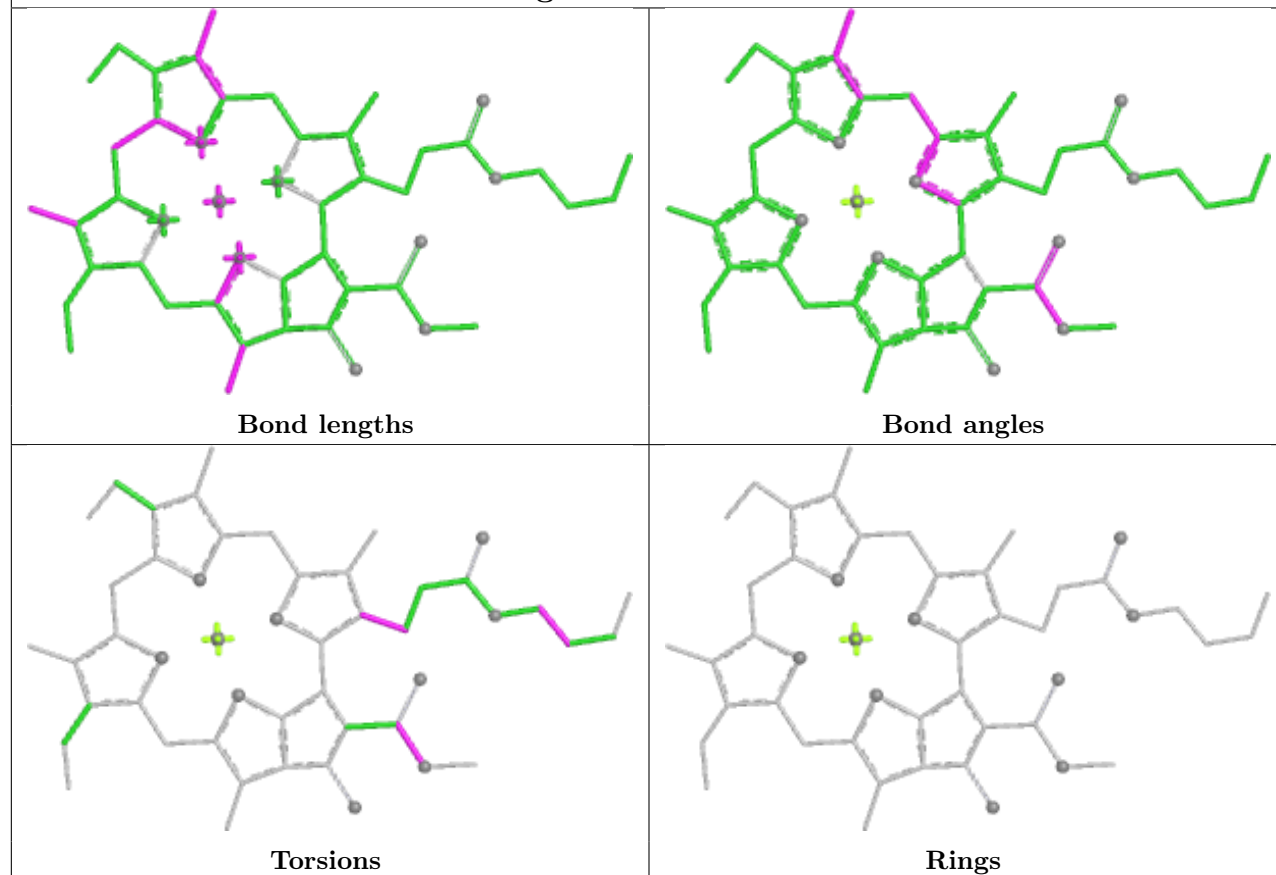


Ligand CLA 6 602

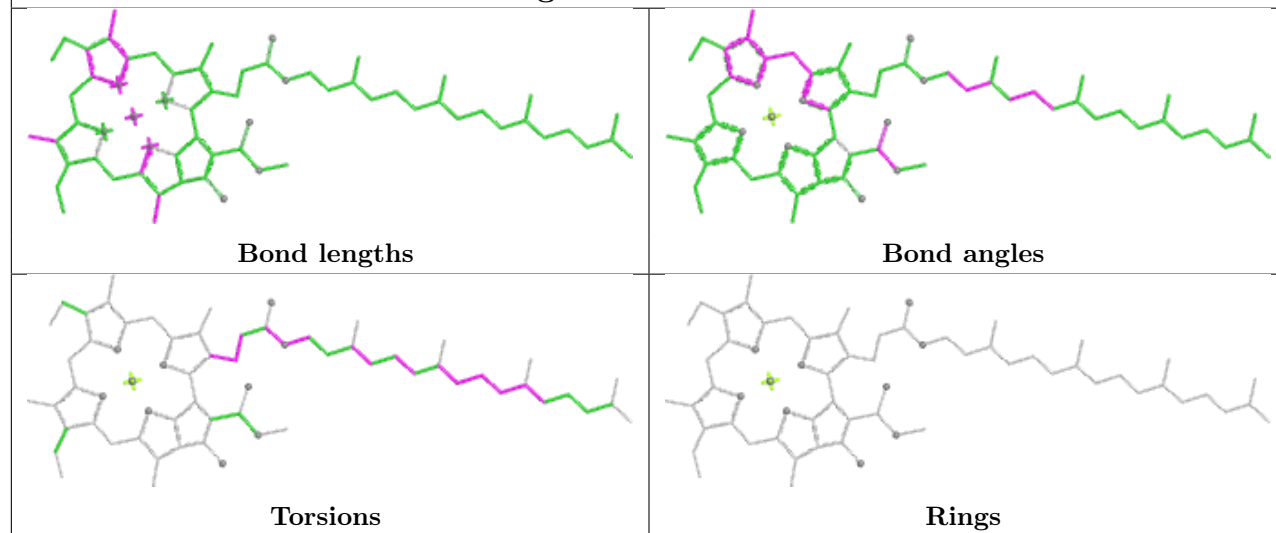


Ligand CLA r 610**Ligand CLA b 617**

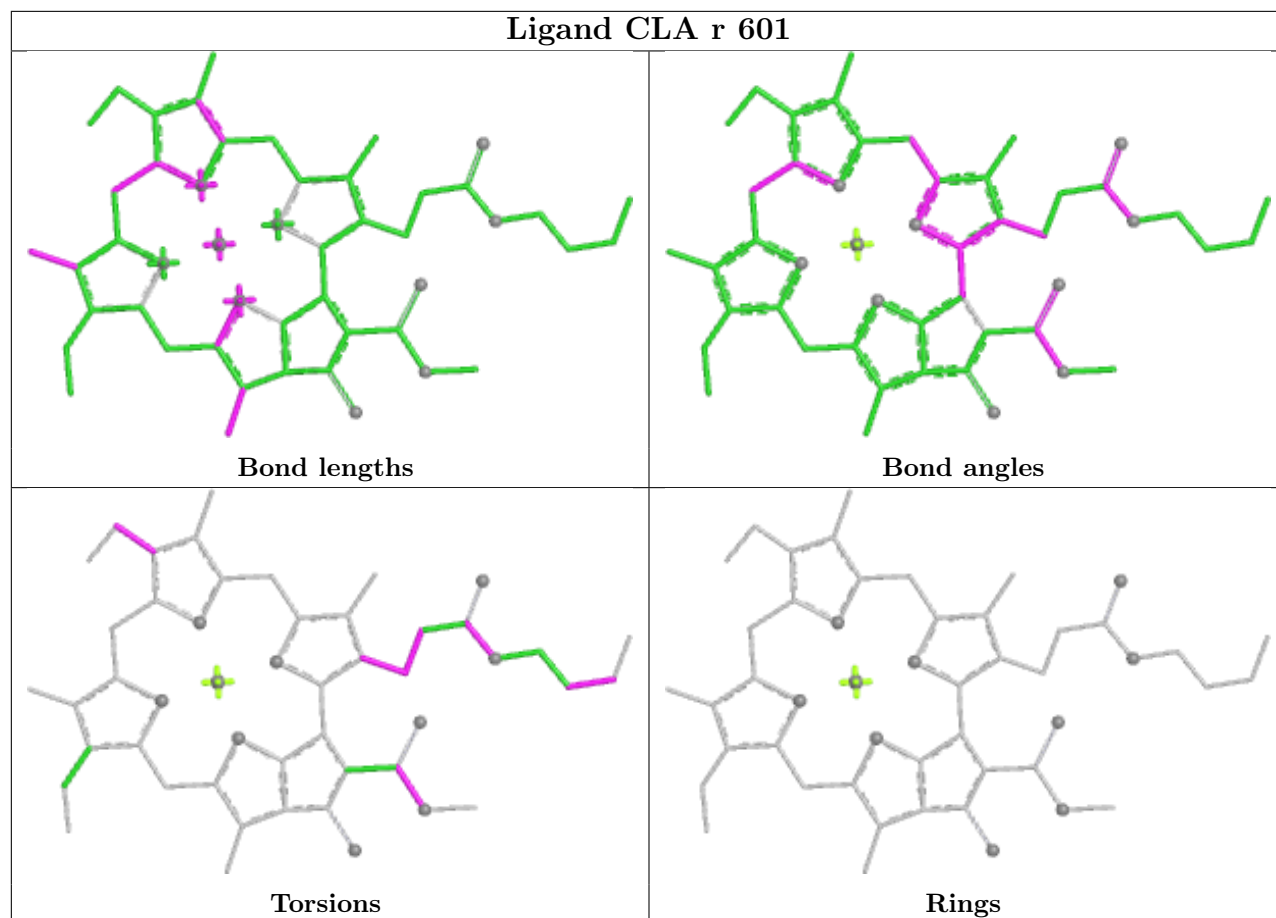
Ligand CLA a 407



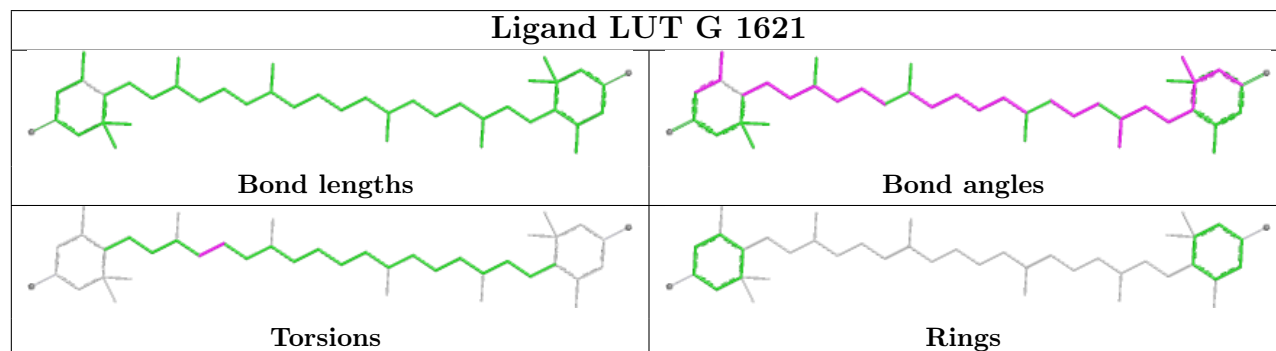
Ligand CLA c 505

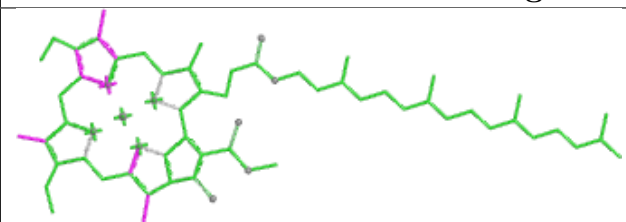
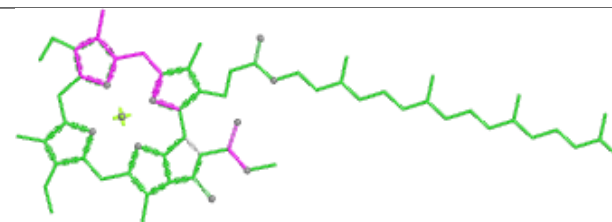
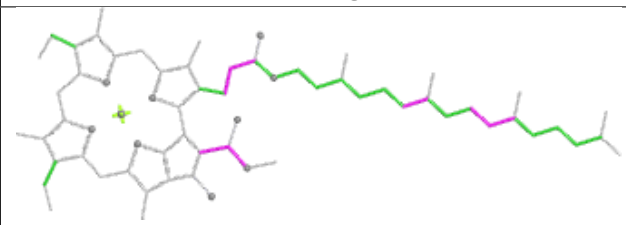
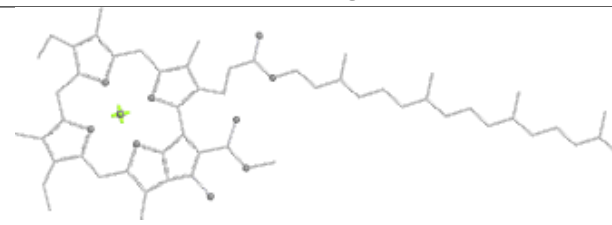


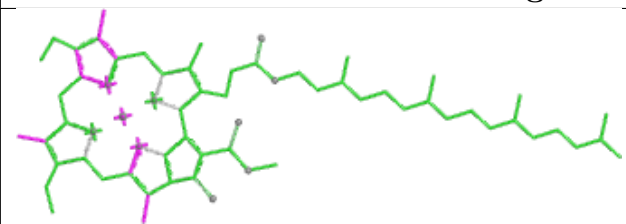
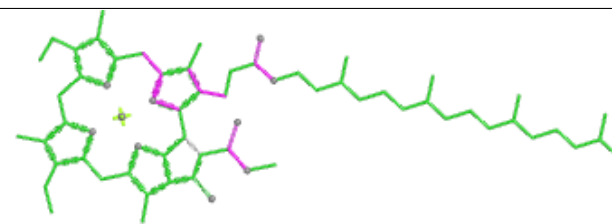
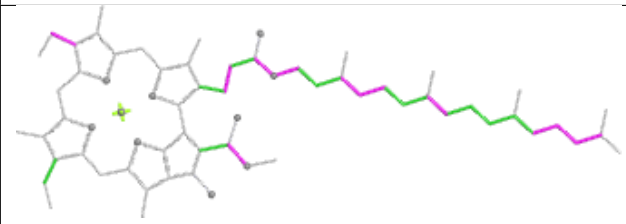
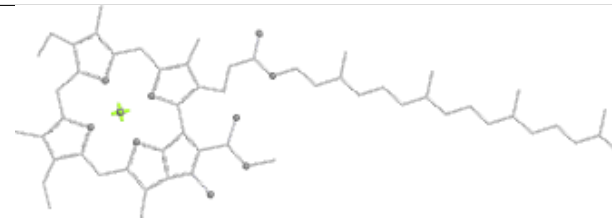
Ligand CLA r 601

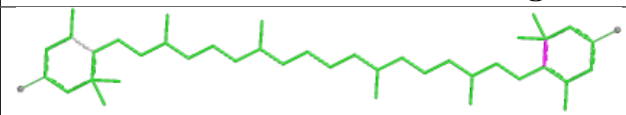
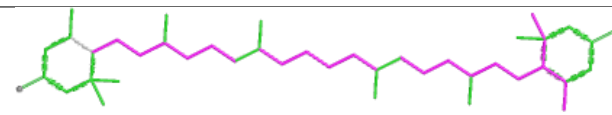
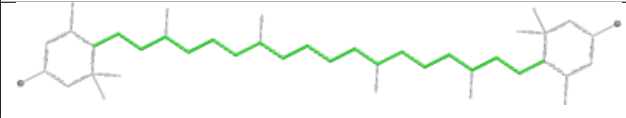
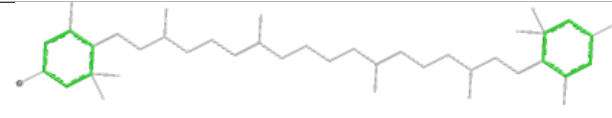


Ligand LUT G 1621

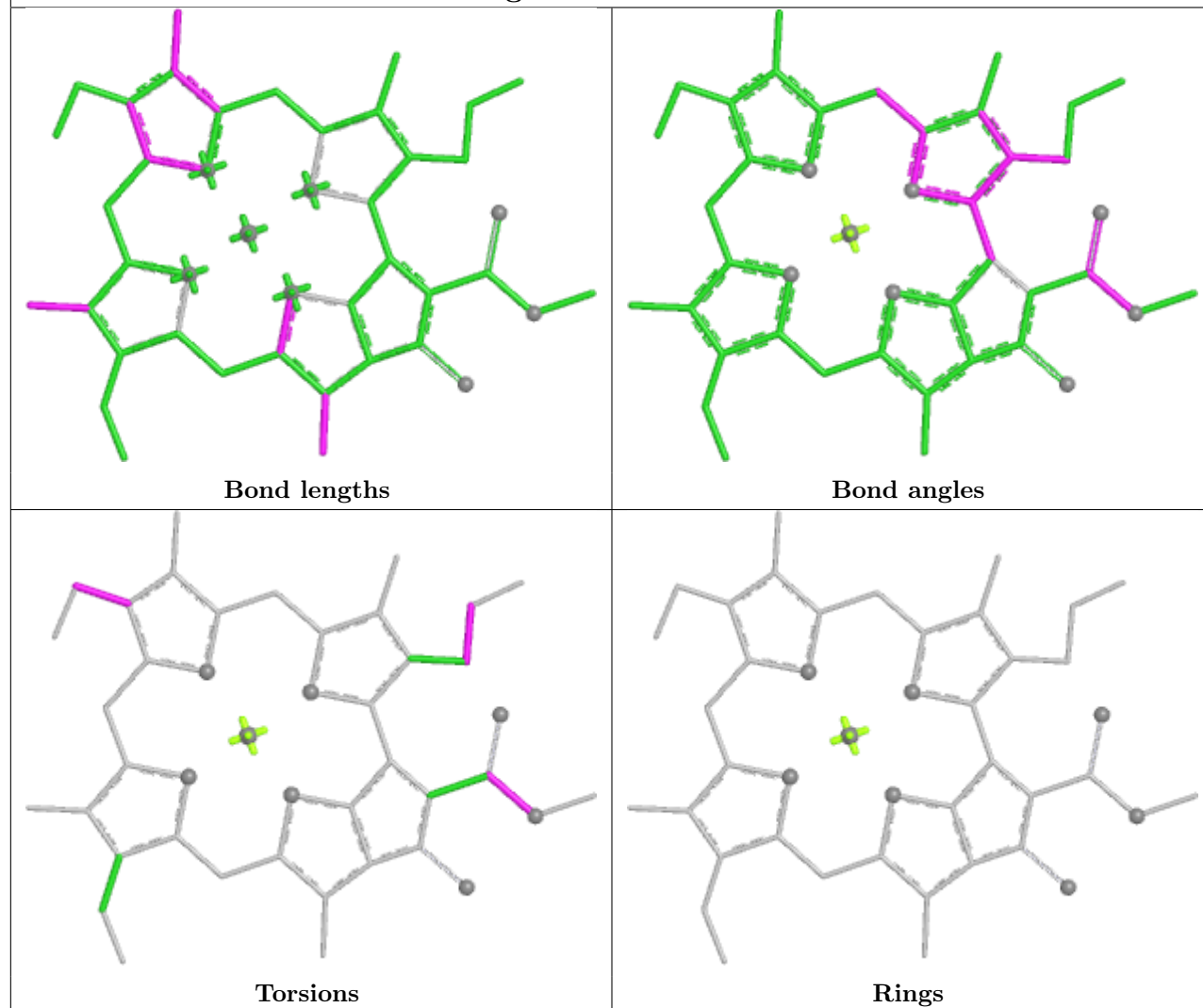


Ligand CLA 3 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

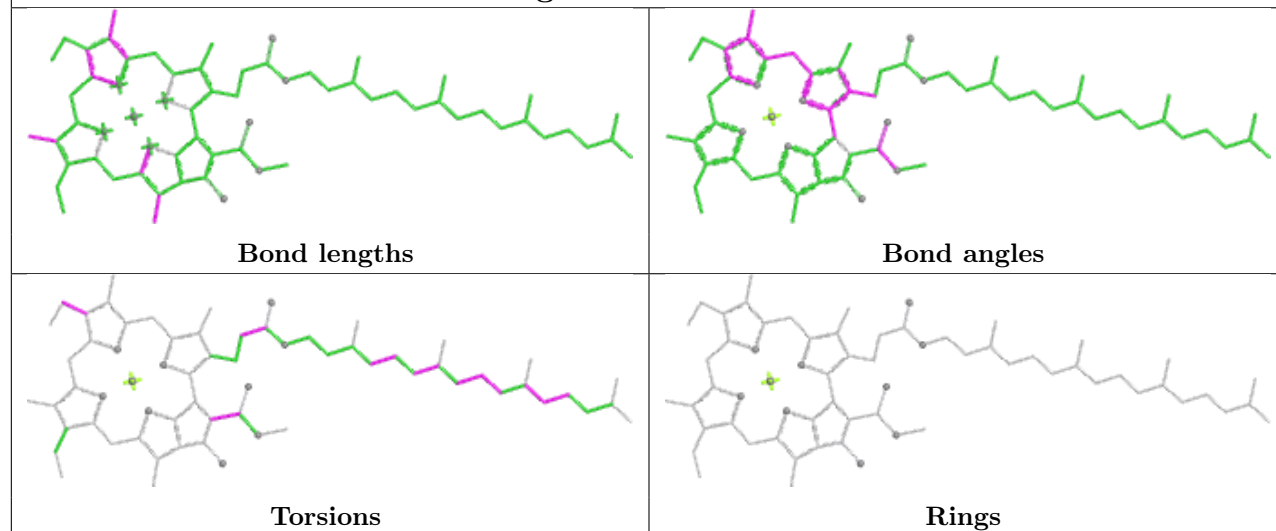
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT r 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

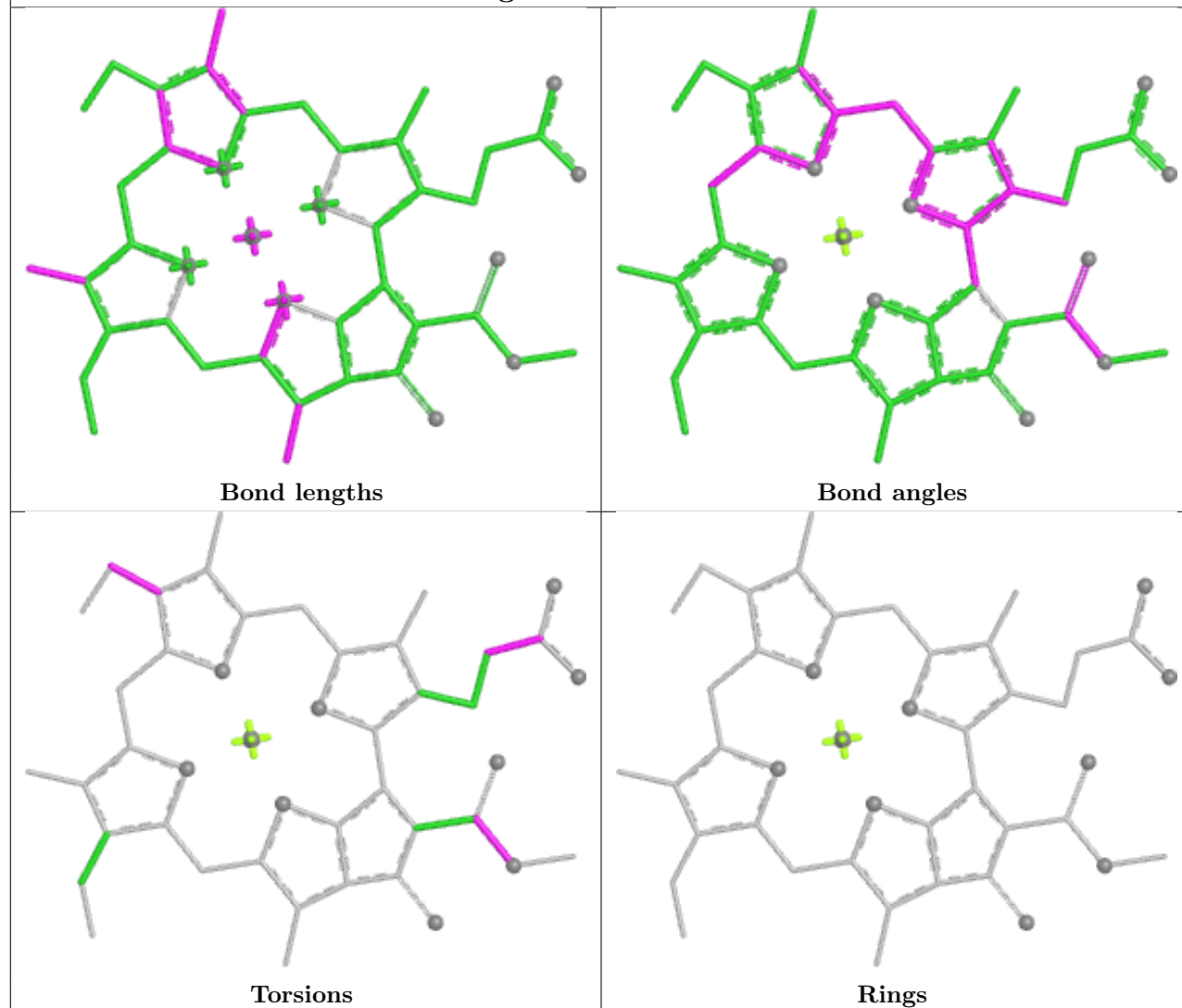
Ligand CLA 9 612



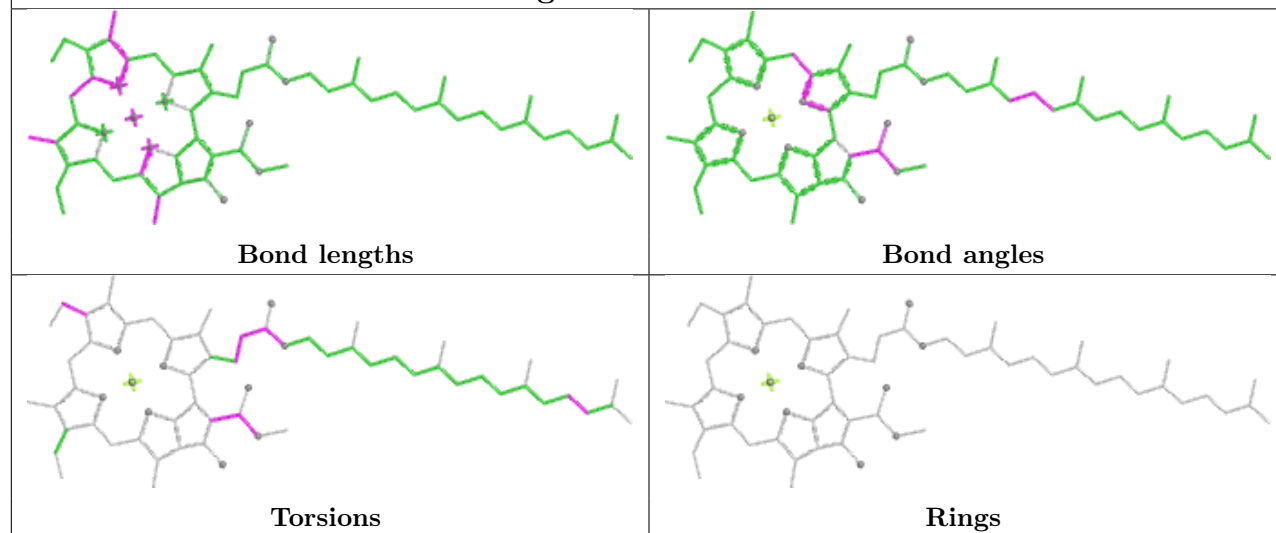
Ligand CLA 6 612

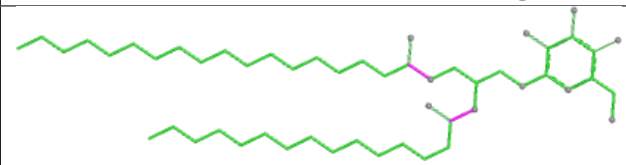
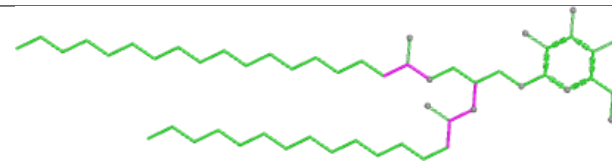
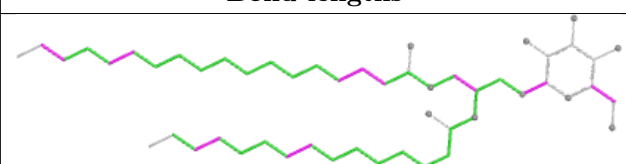
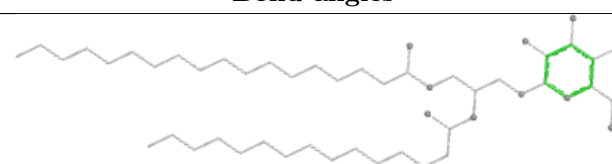


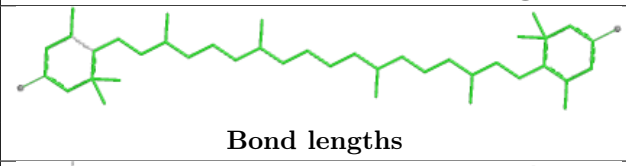
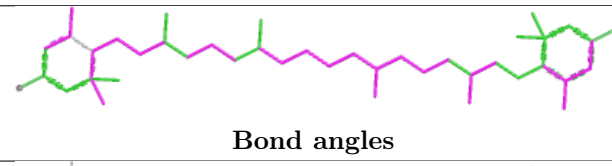
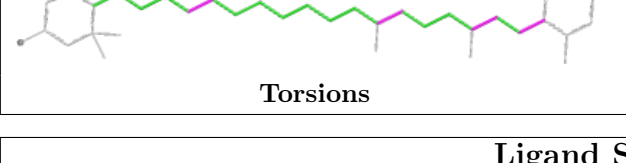
Ligand CLA s 612

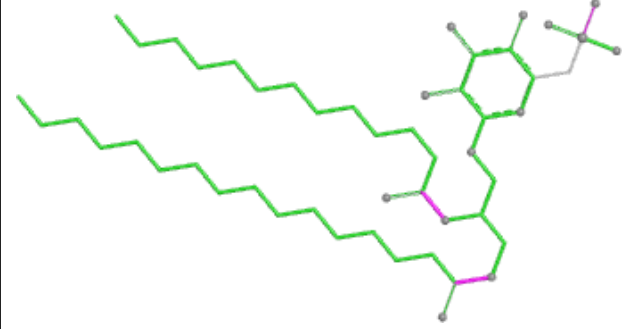
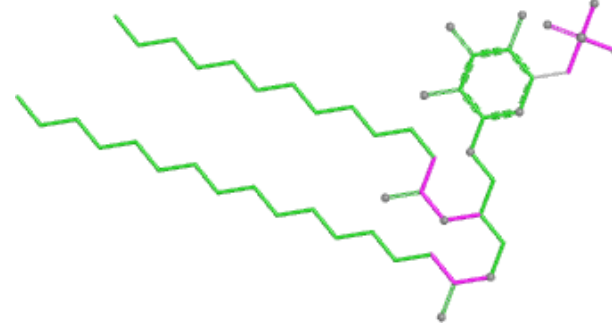
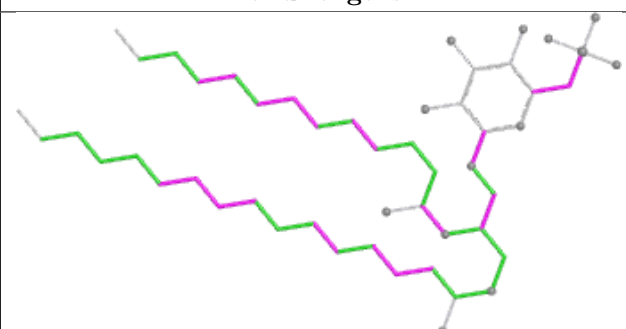
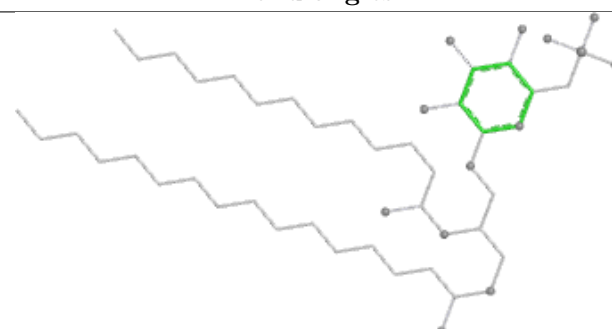


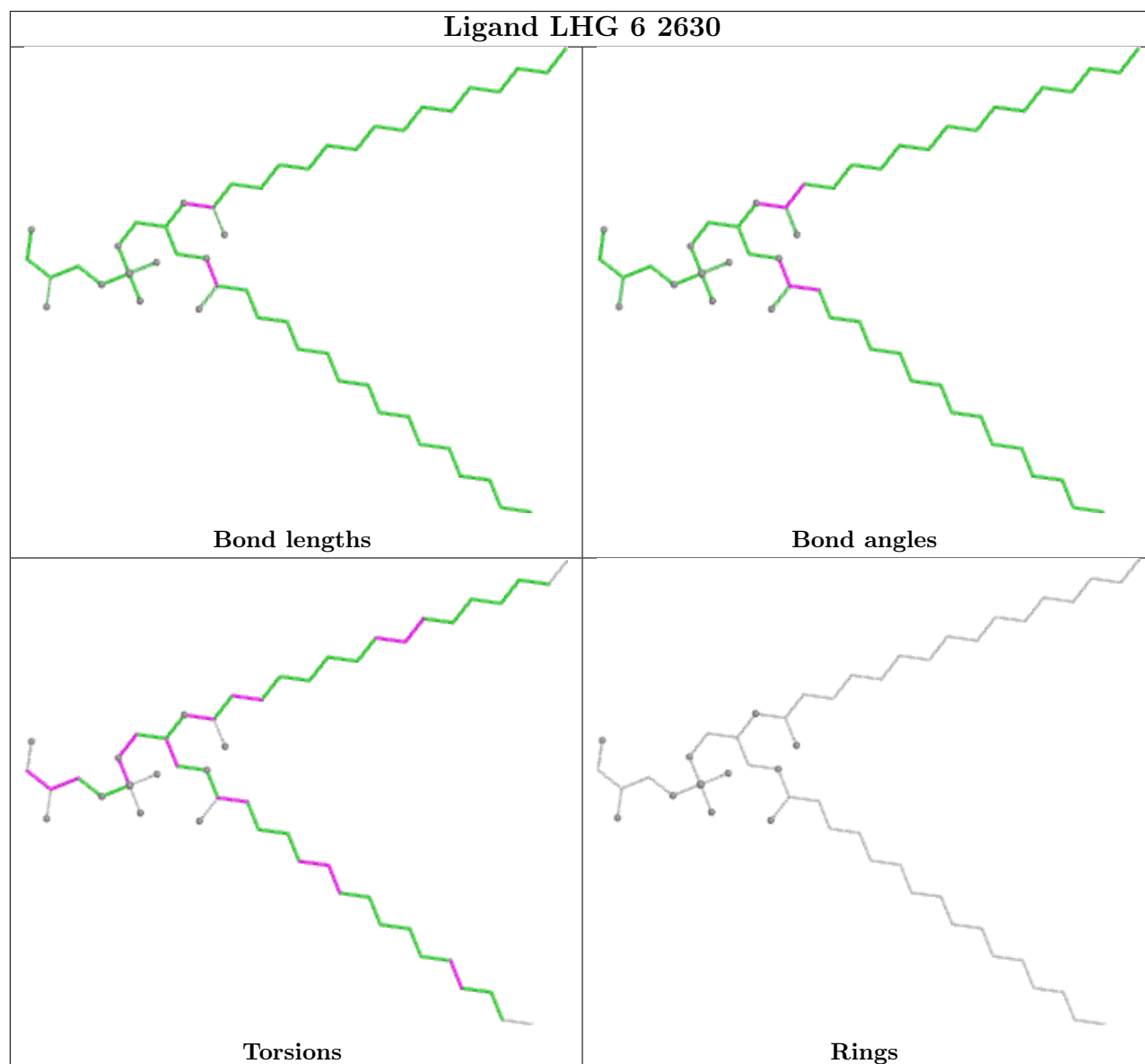
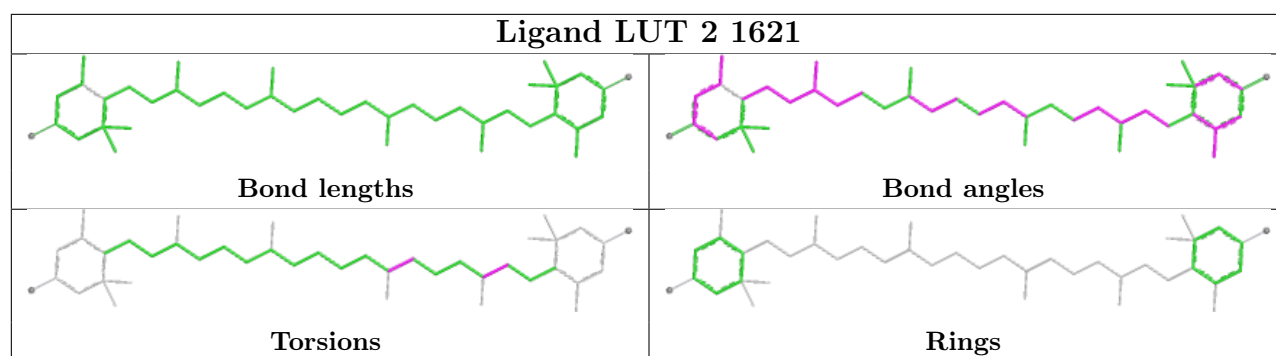
Ligand CLA c 501

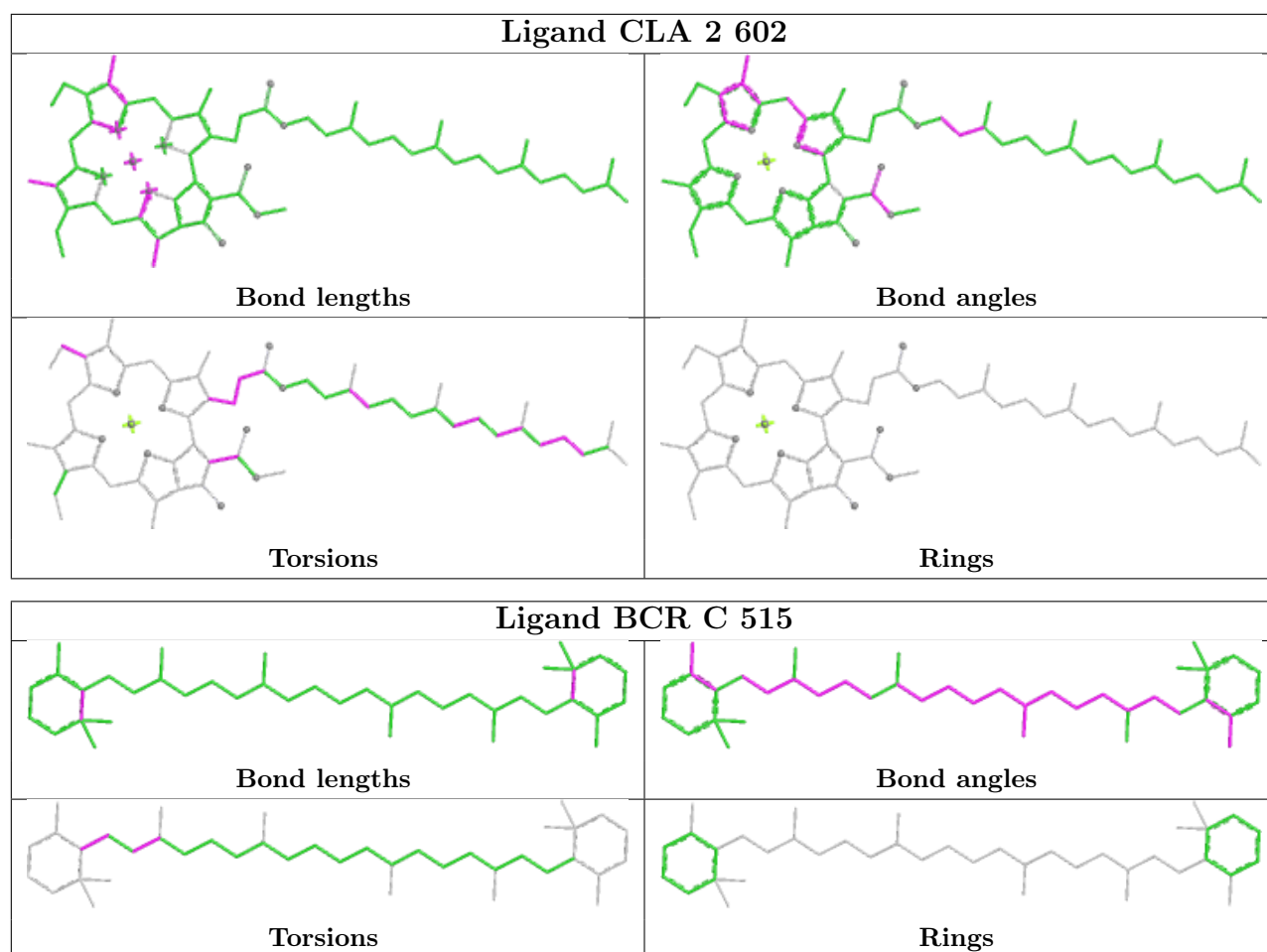


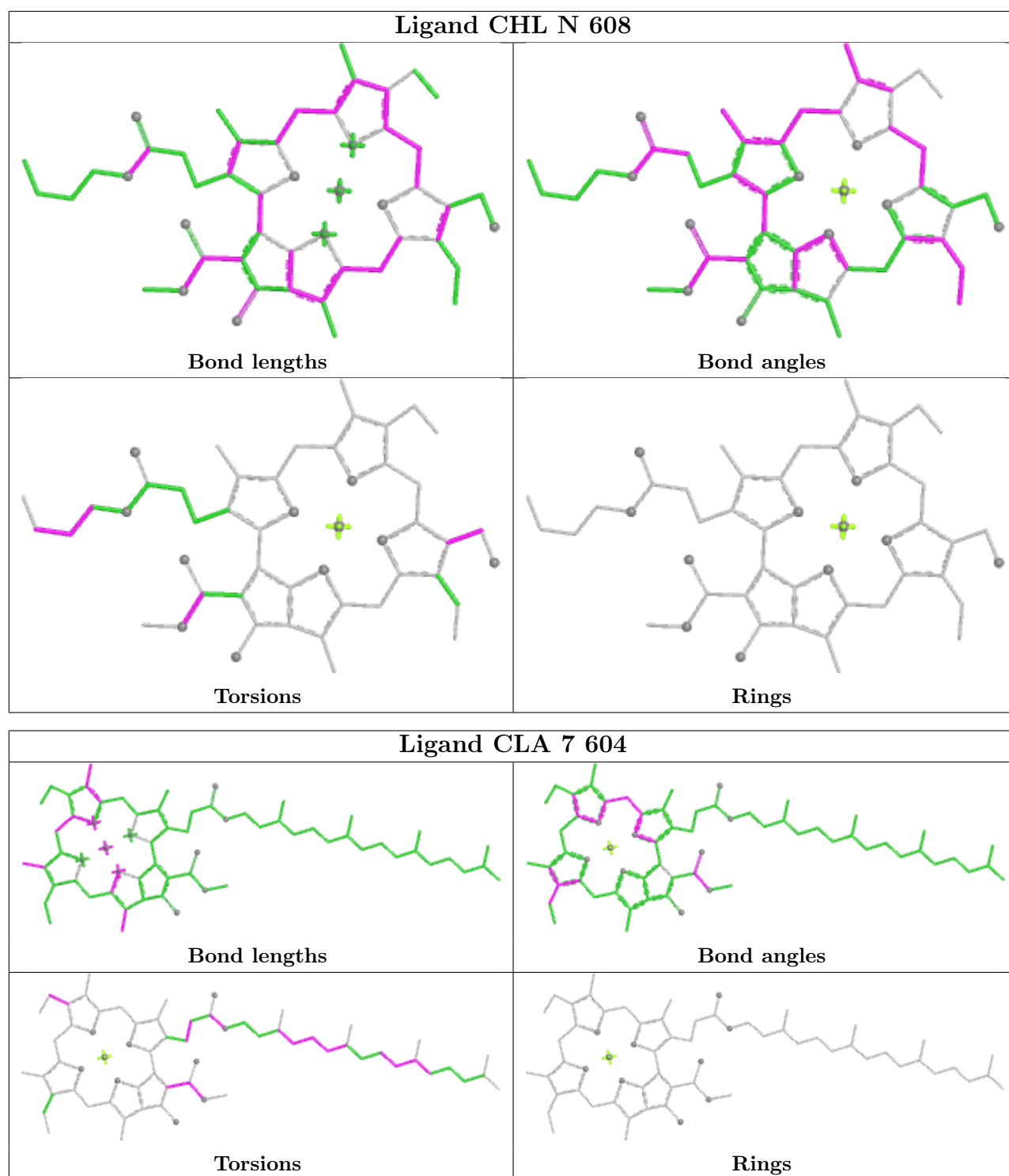
Ligand LMG s 2631	
 Bond lengths	 Bond angles
 Torsions	 Rings

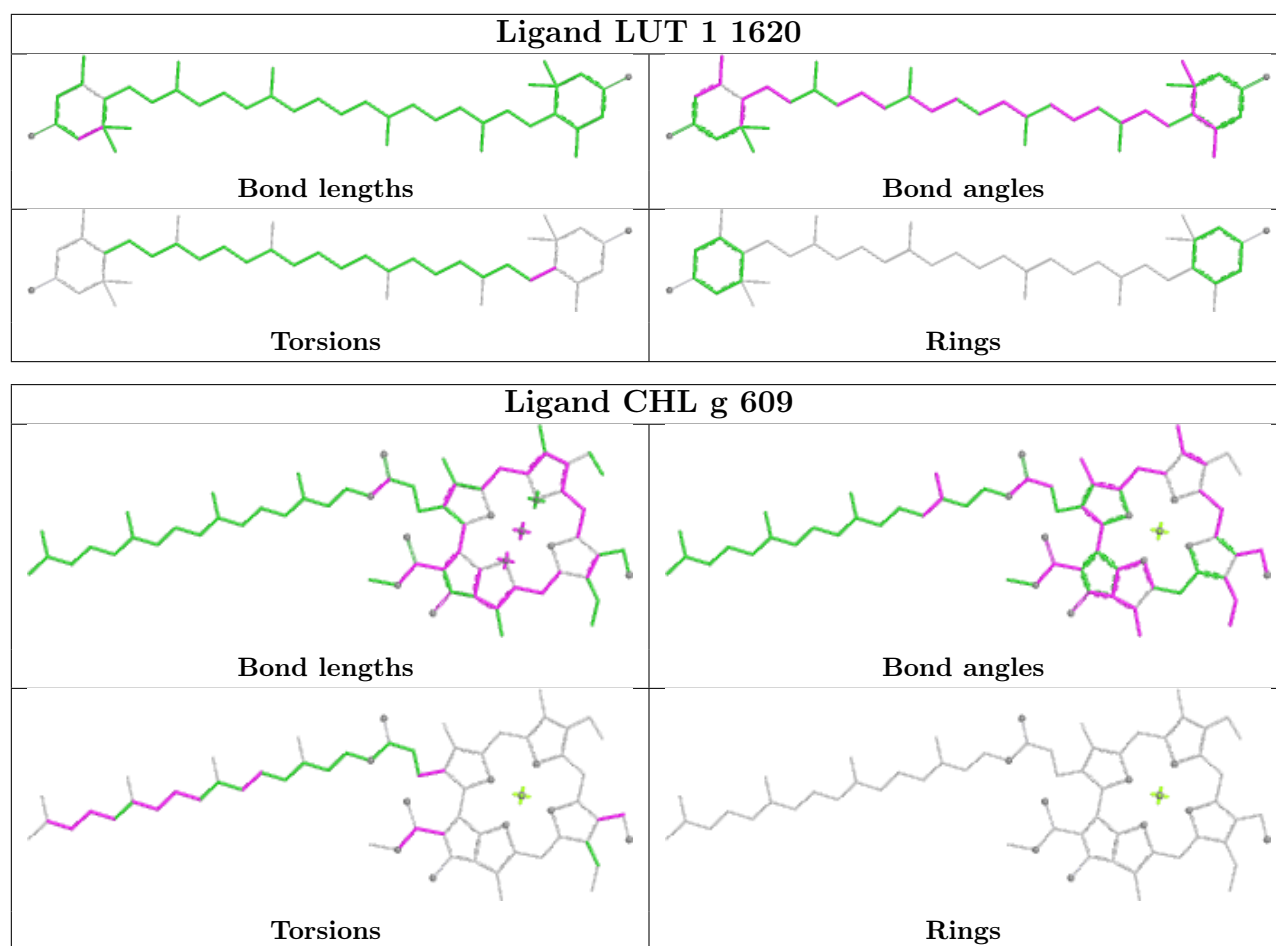
Ligand LUT 4 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD a 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

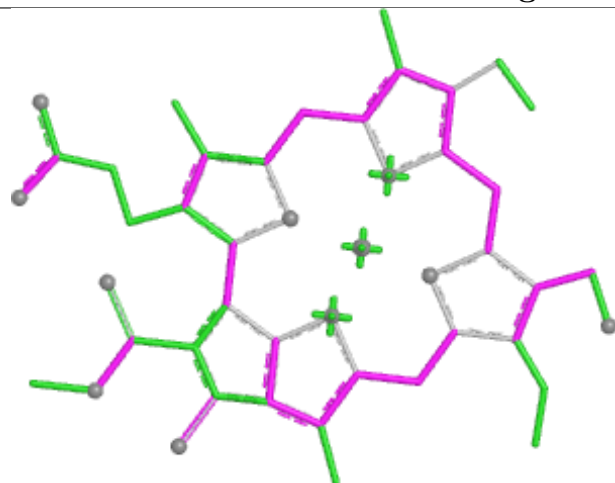




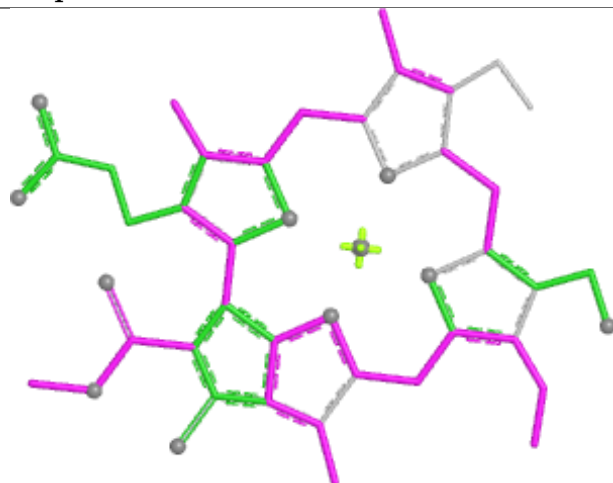




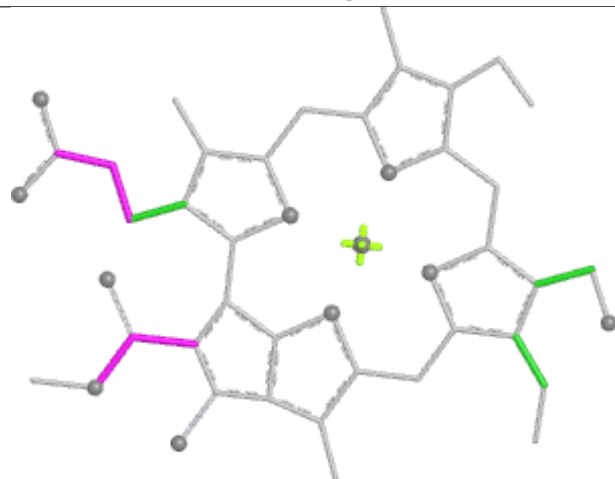
Ligand CHL p 606



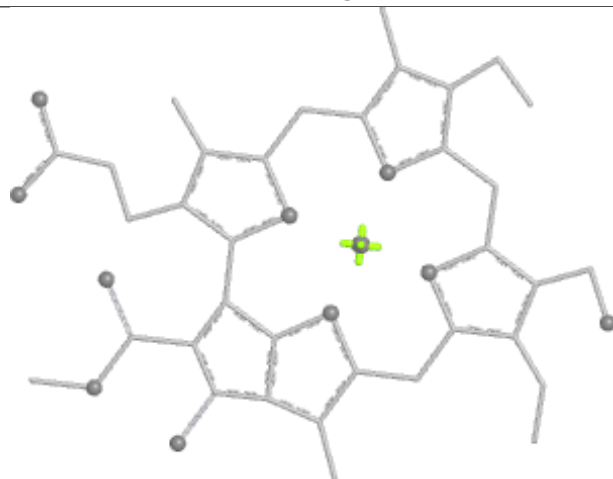
Bond lengths



Bond angles

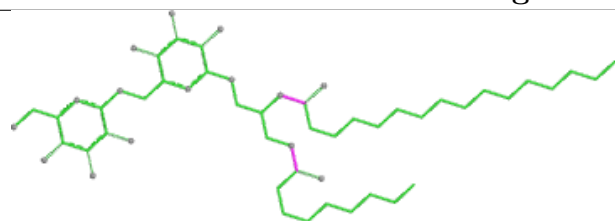


Torsions

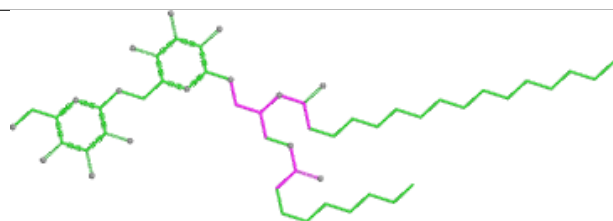


Rings

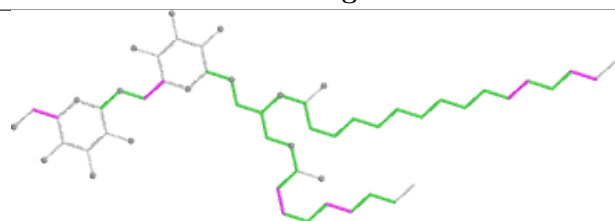
Ligand DGD C 518



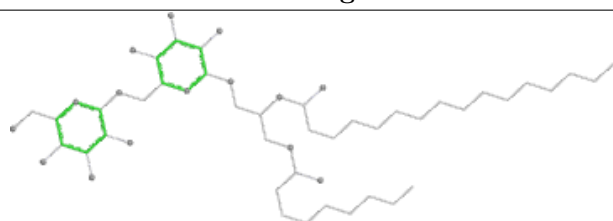
Bond lengths



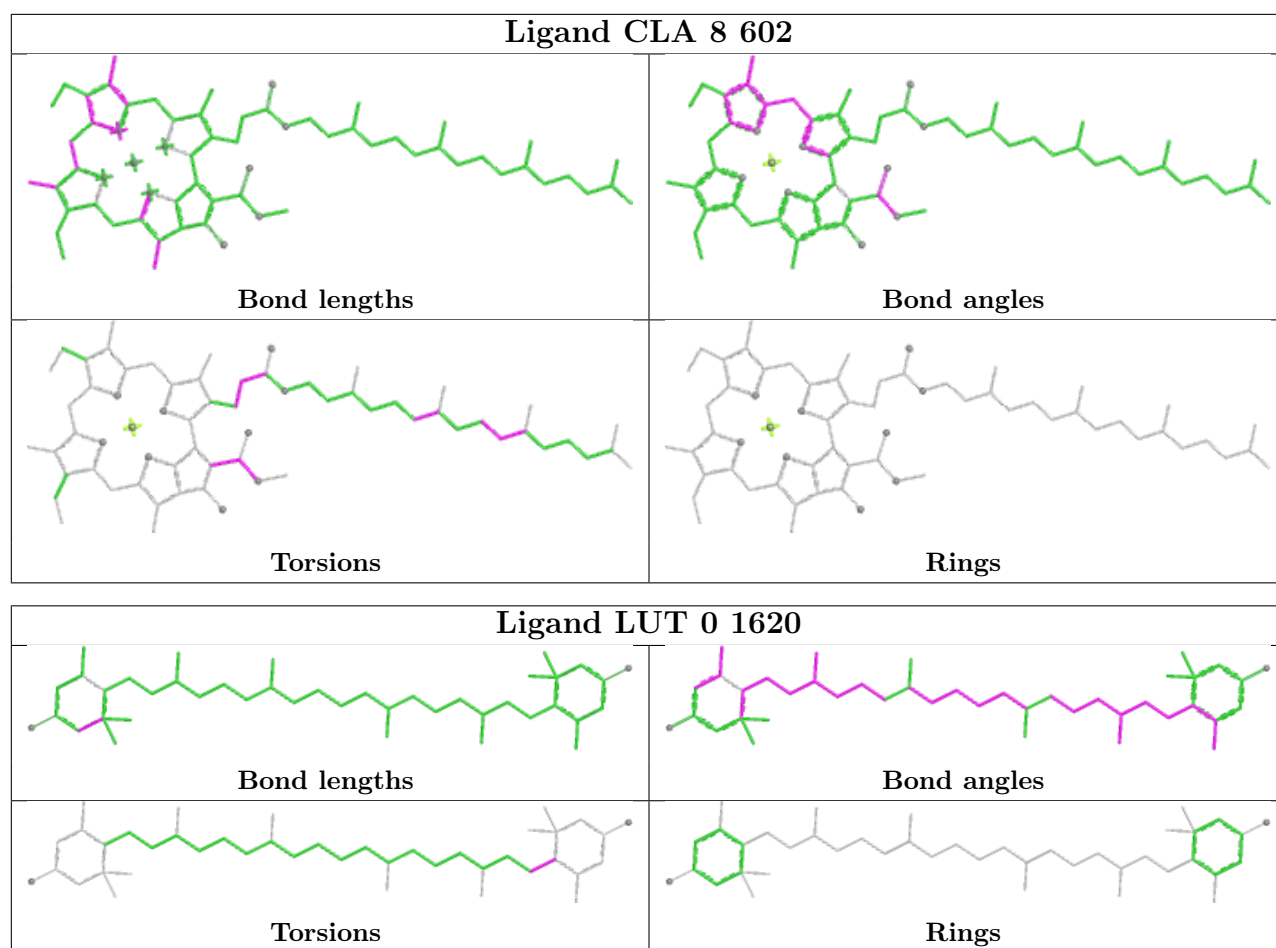
Bond angles

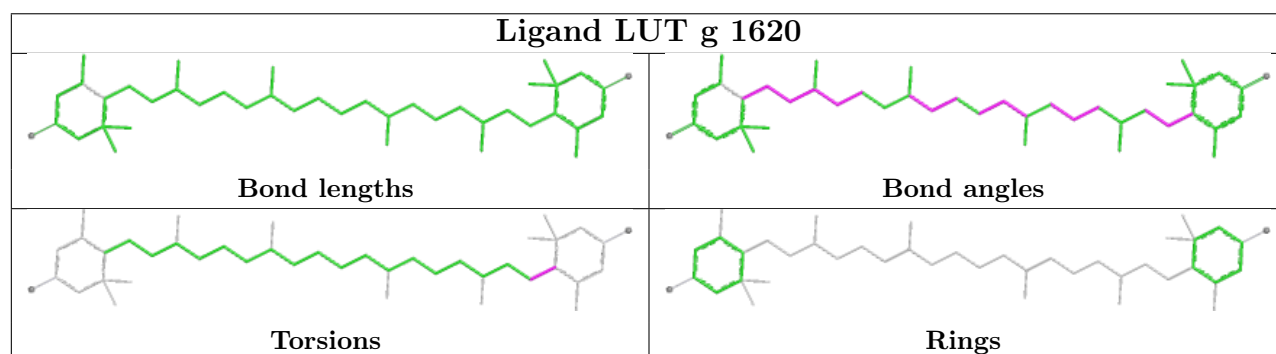
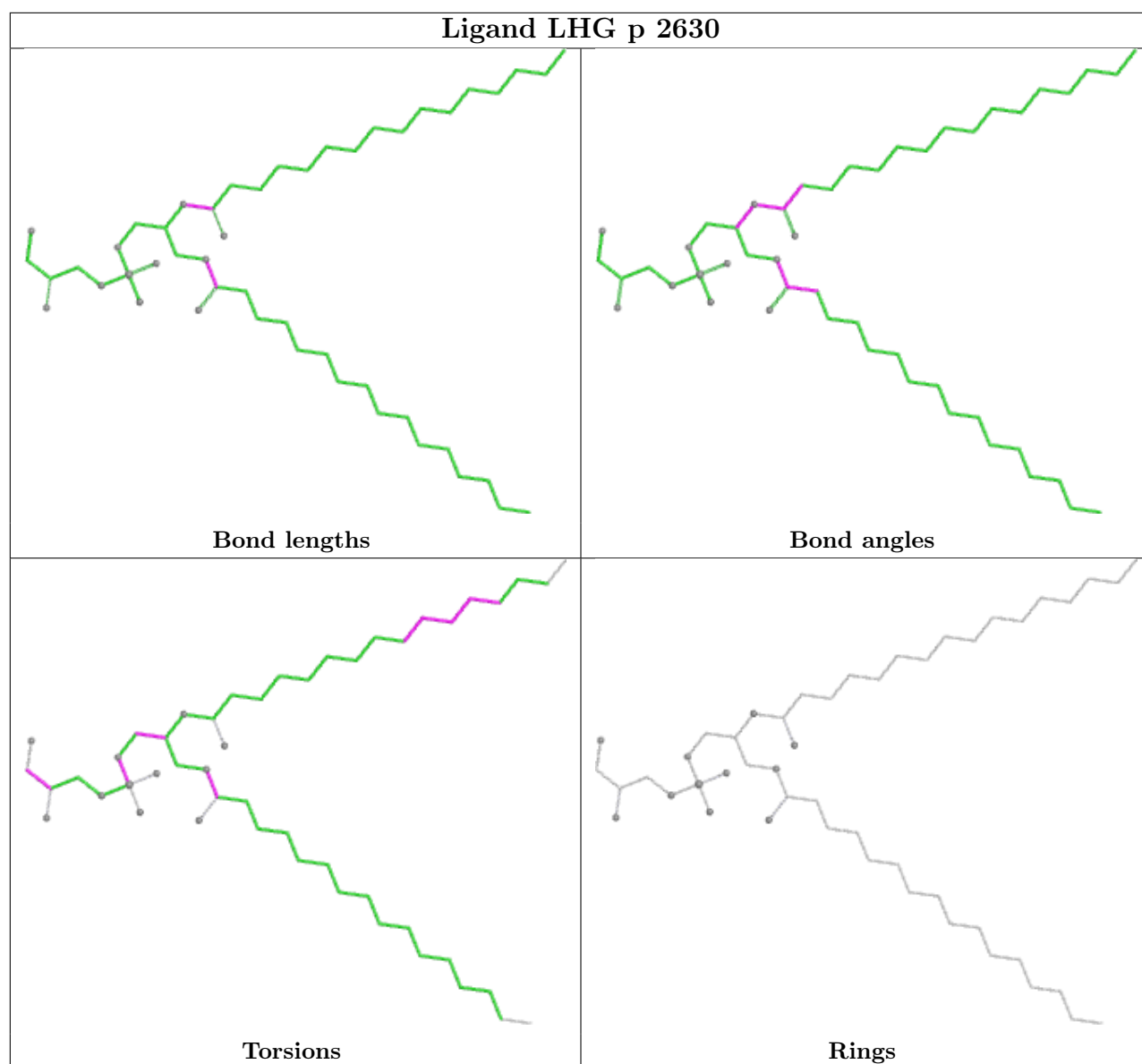


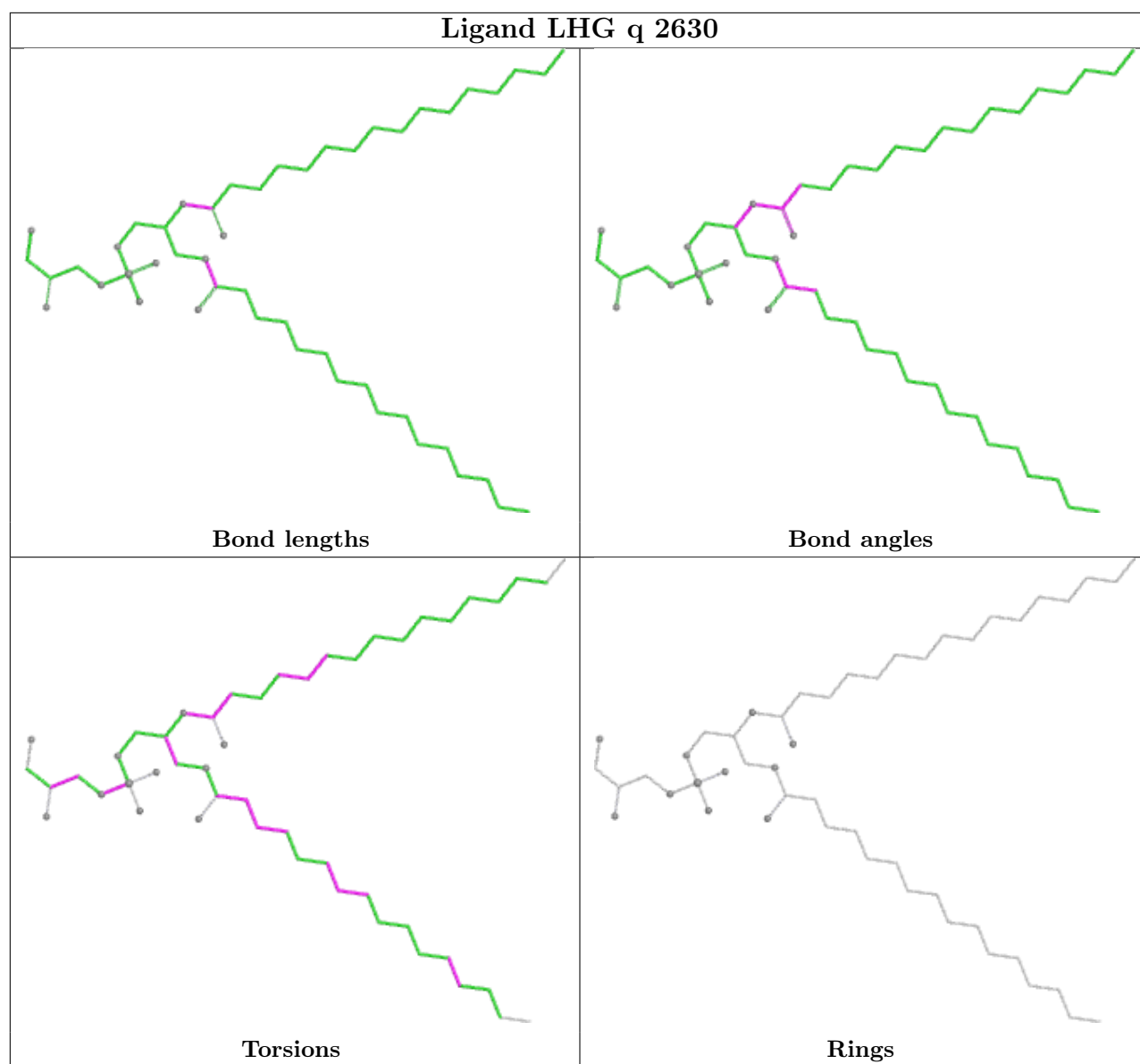
Torsions

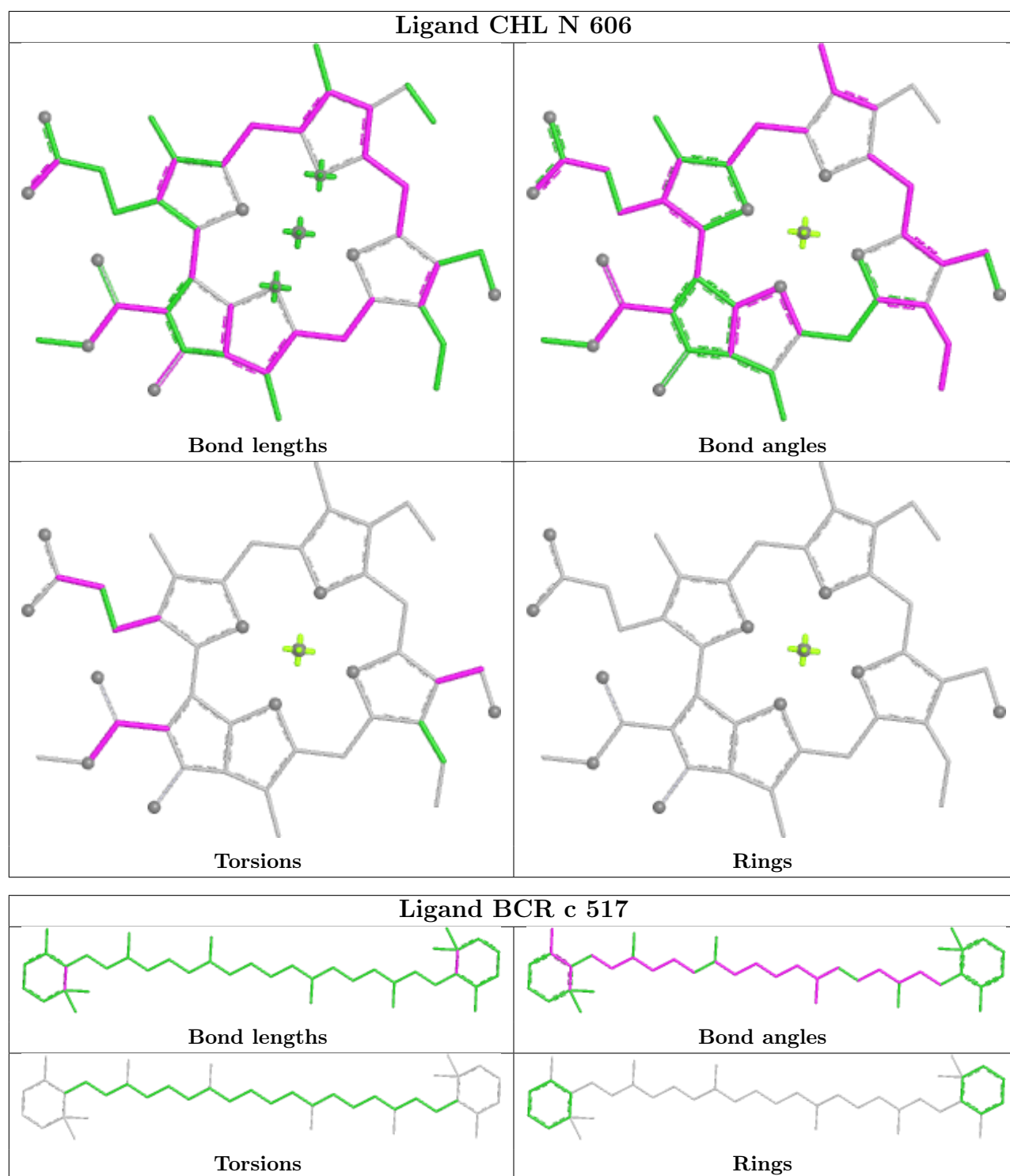


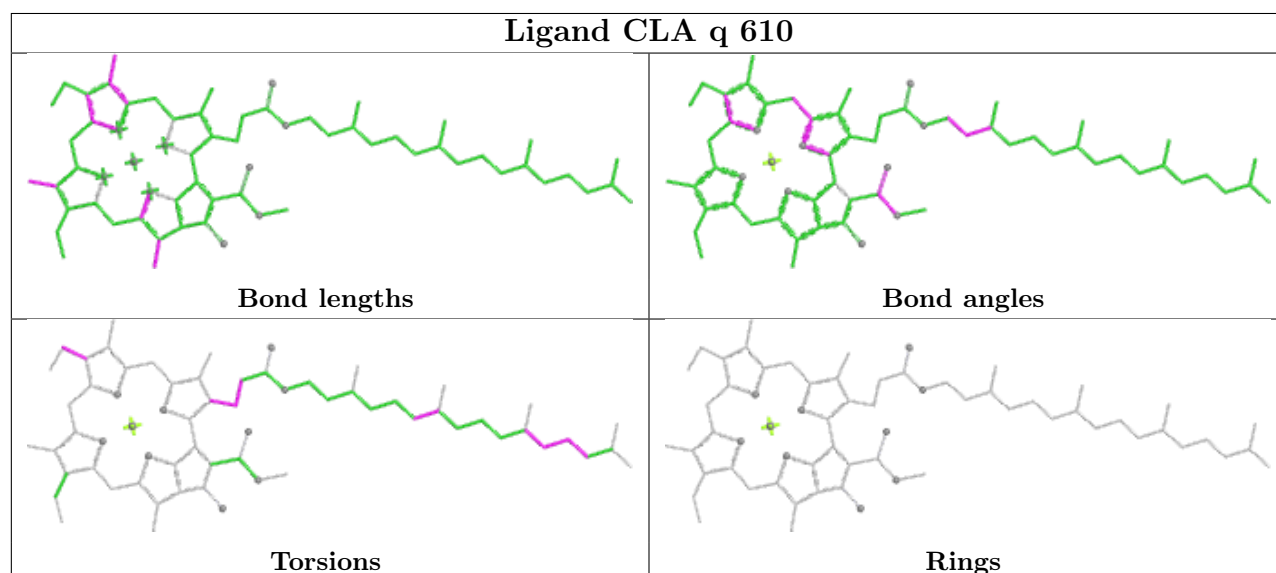
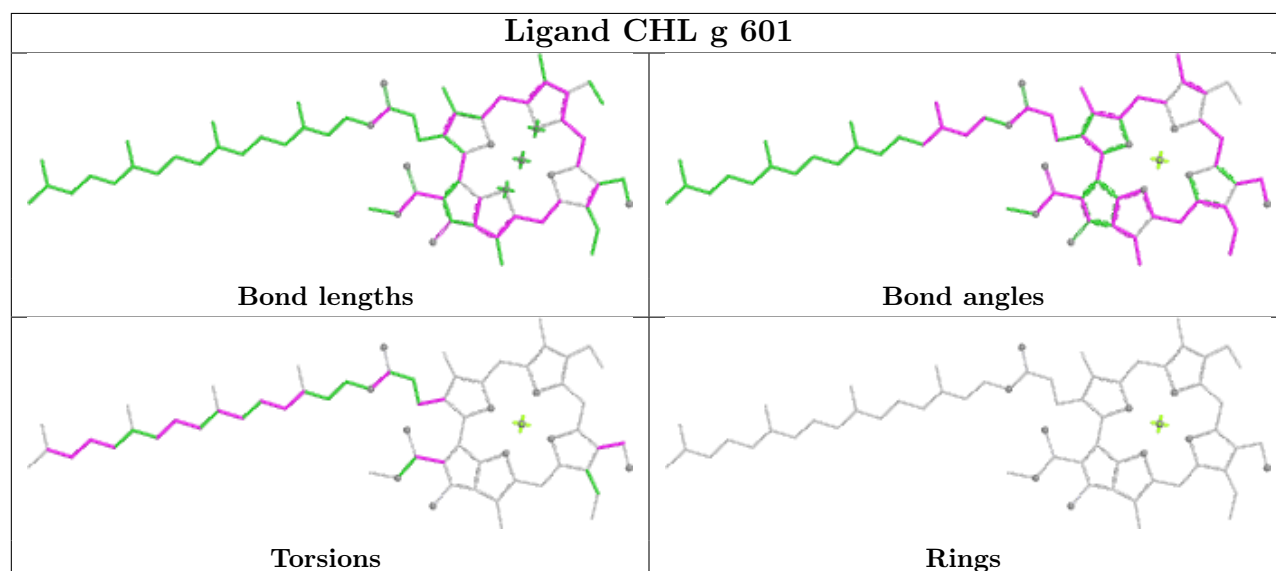
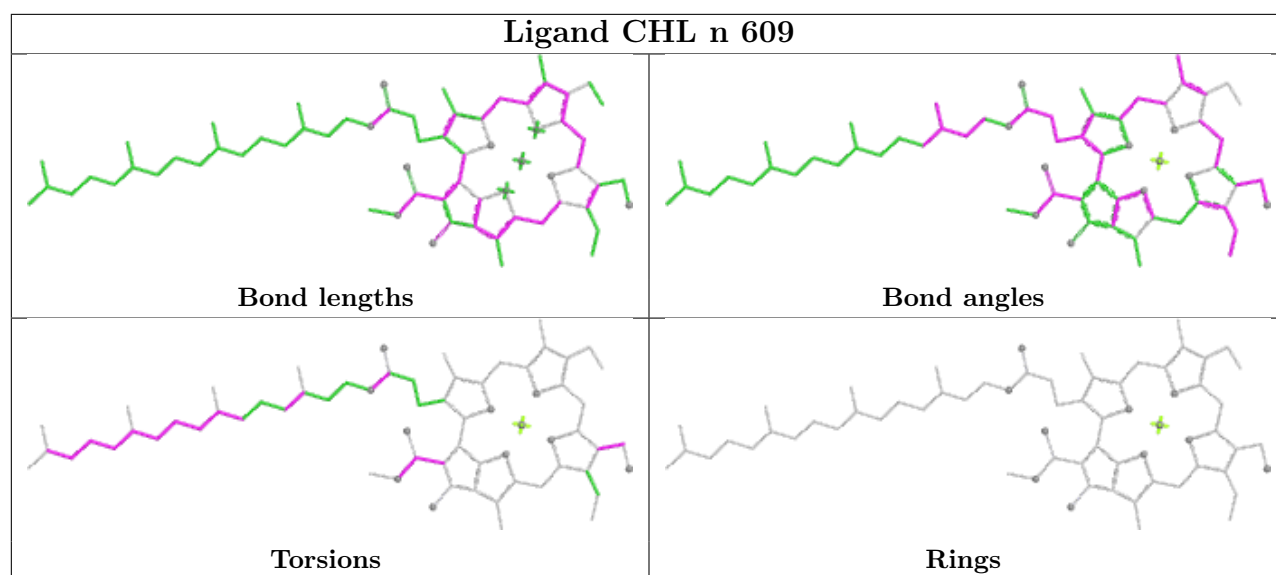
Rings

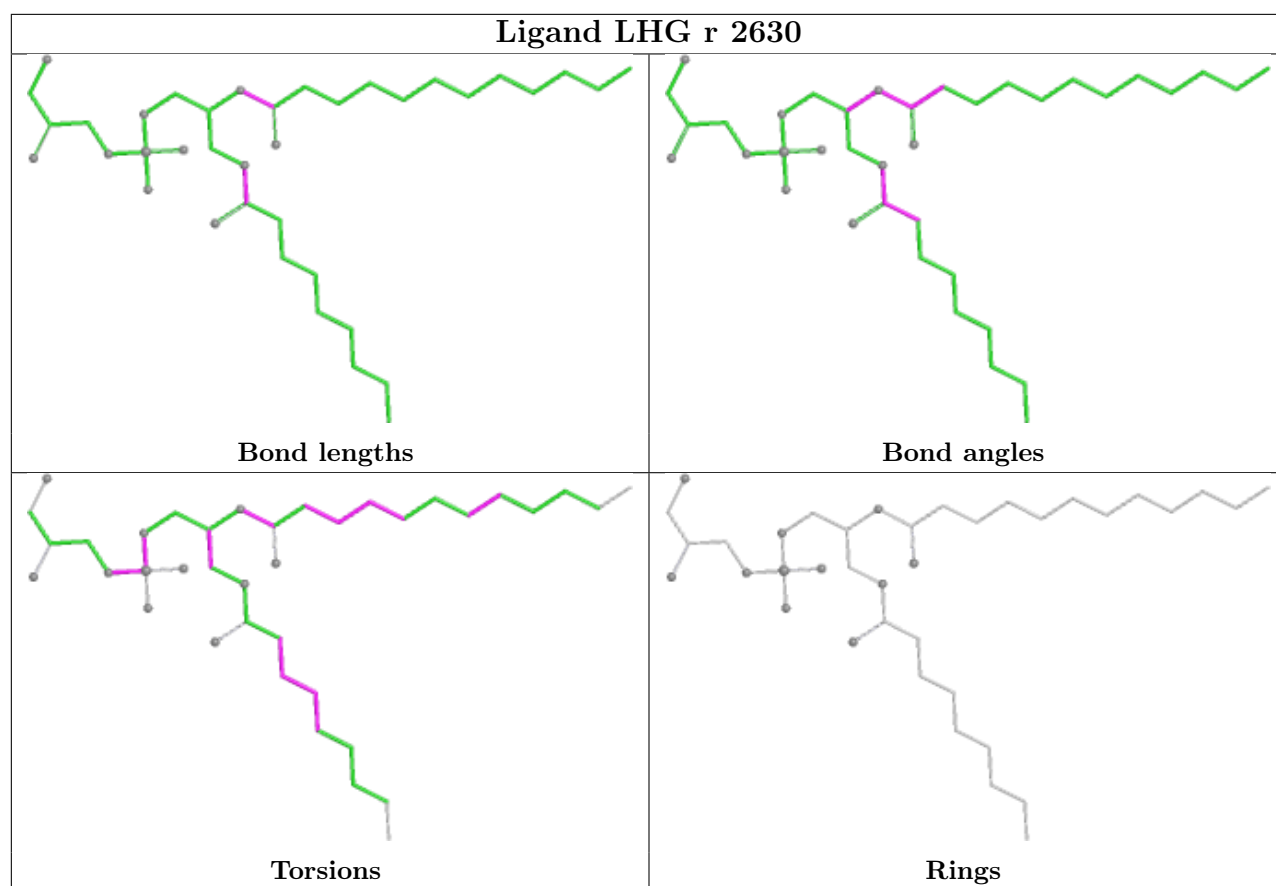




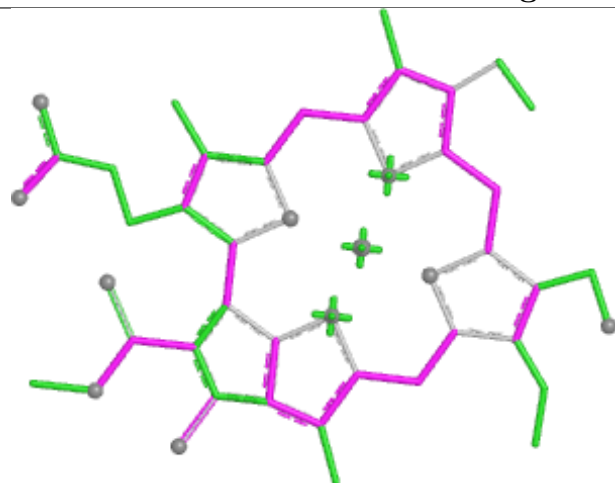




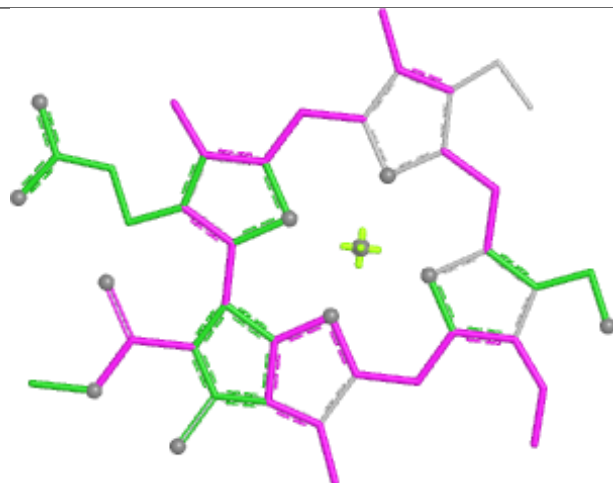




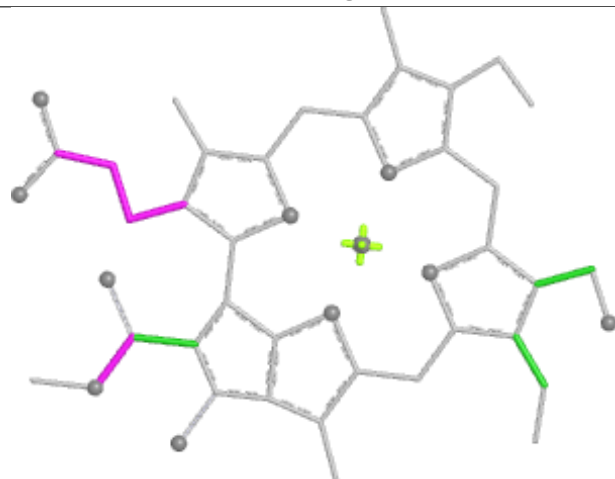
Ligand CHL 8 606



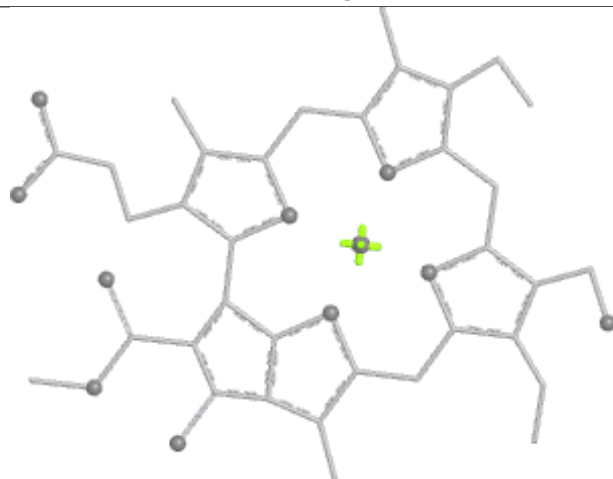
Bond lengths



Bond angles

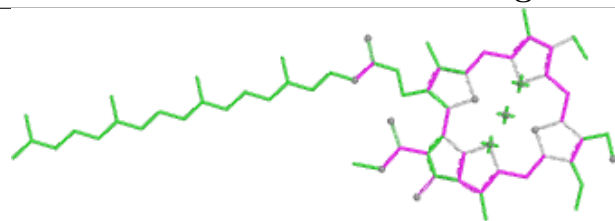


Torsions

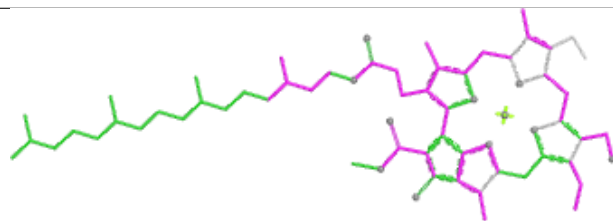


Rings

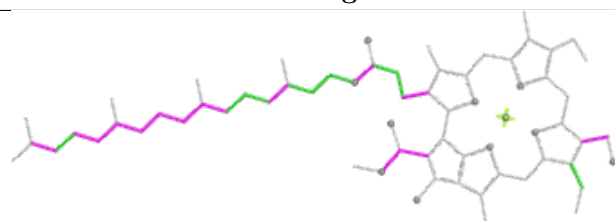
Ligand CHL N 605



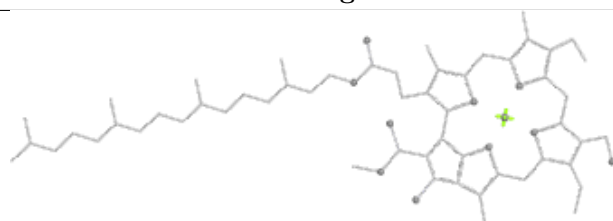
Bond lengths



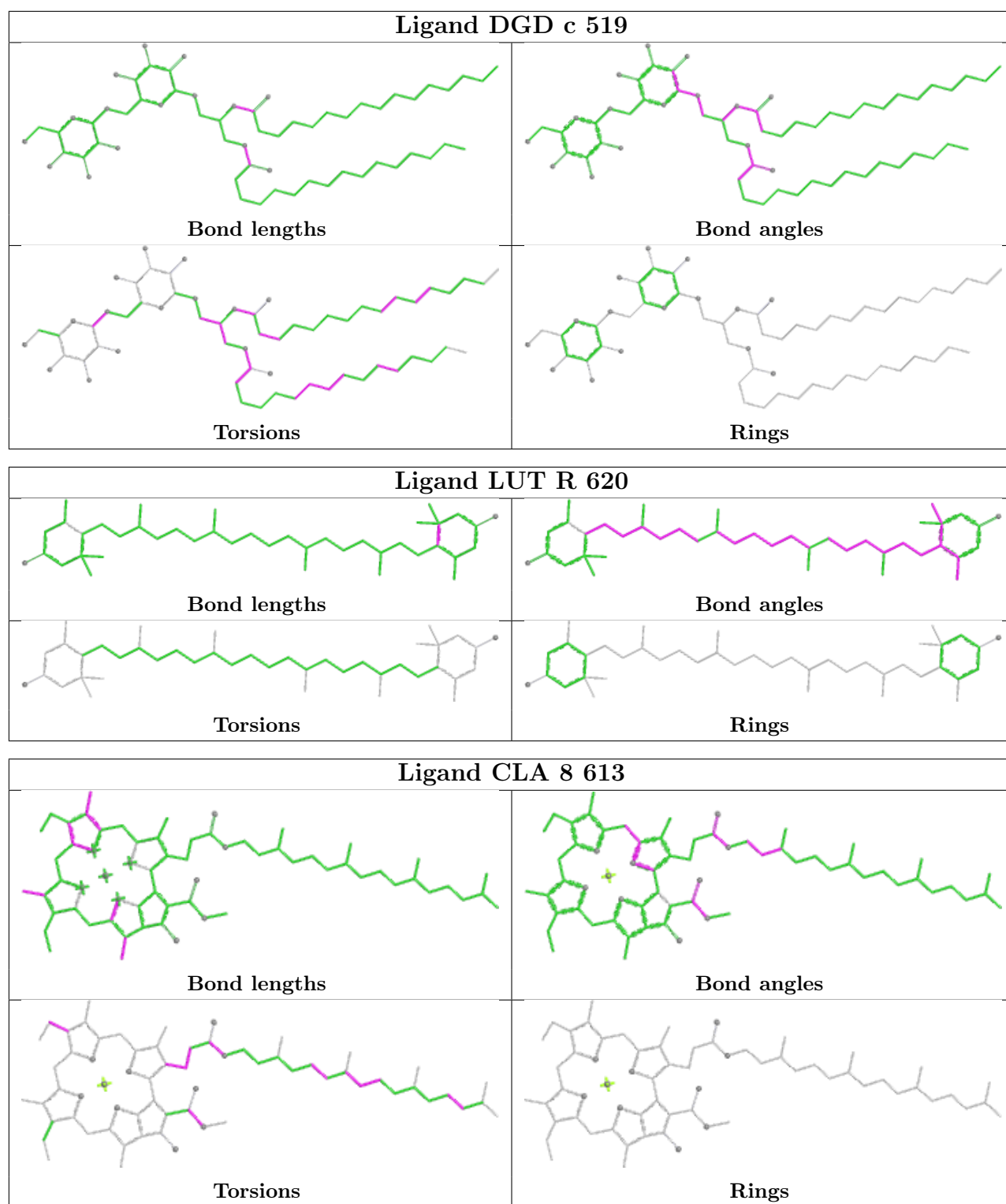
Bond angles



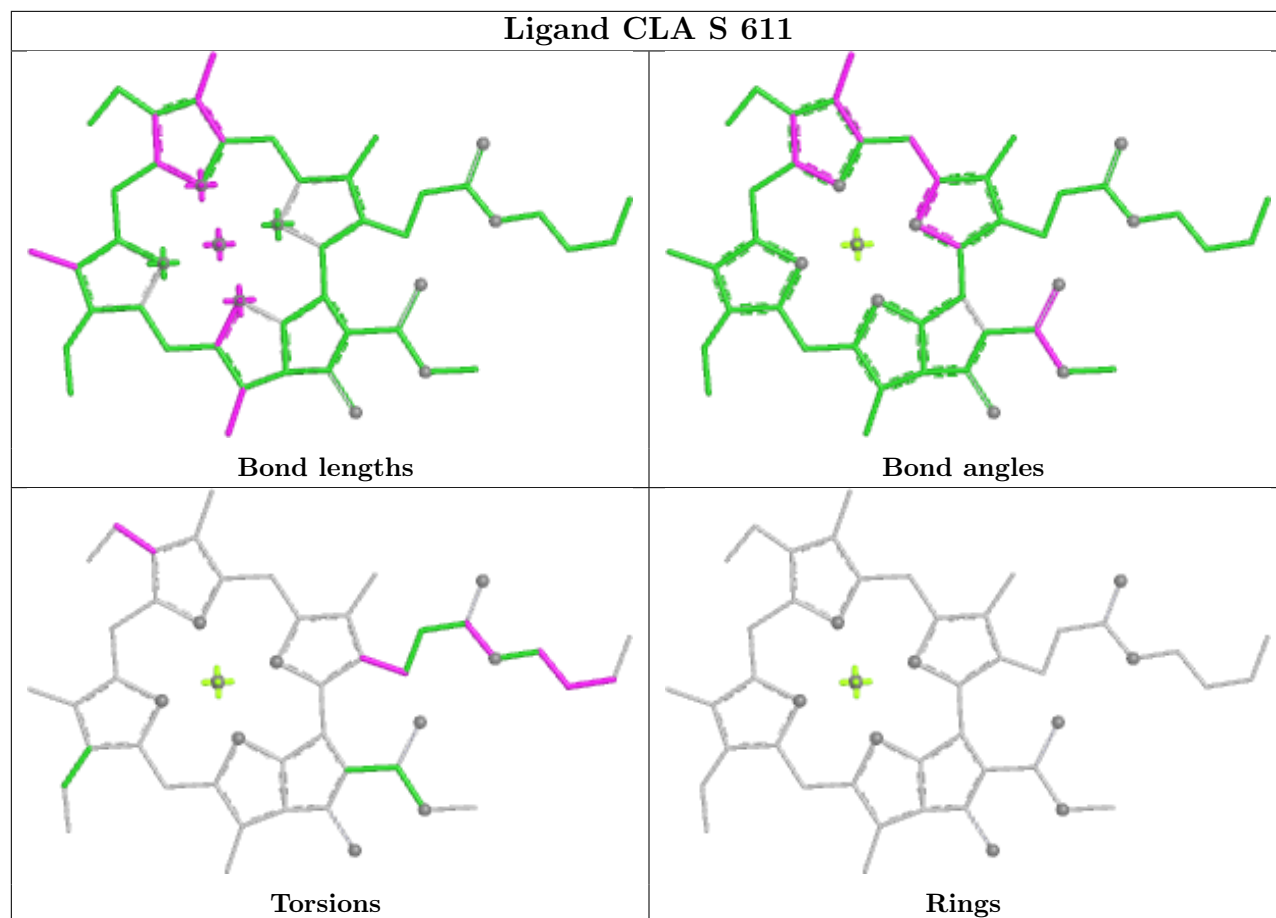
Torsions

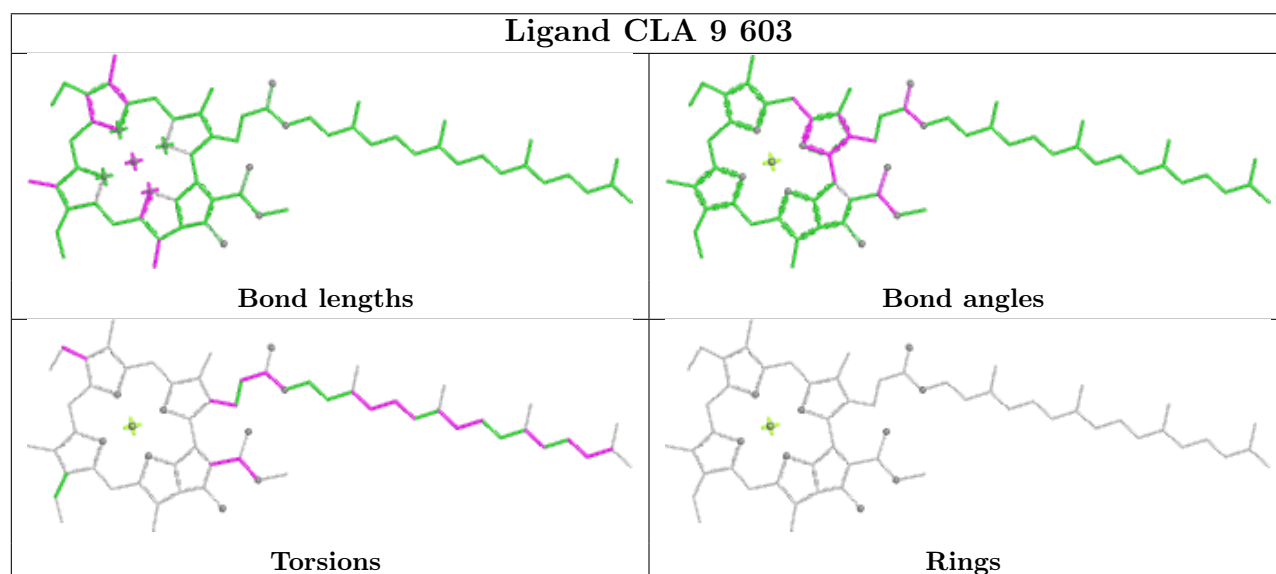
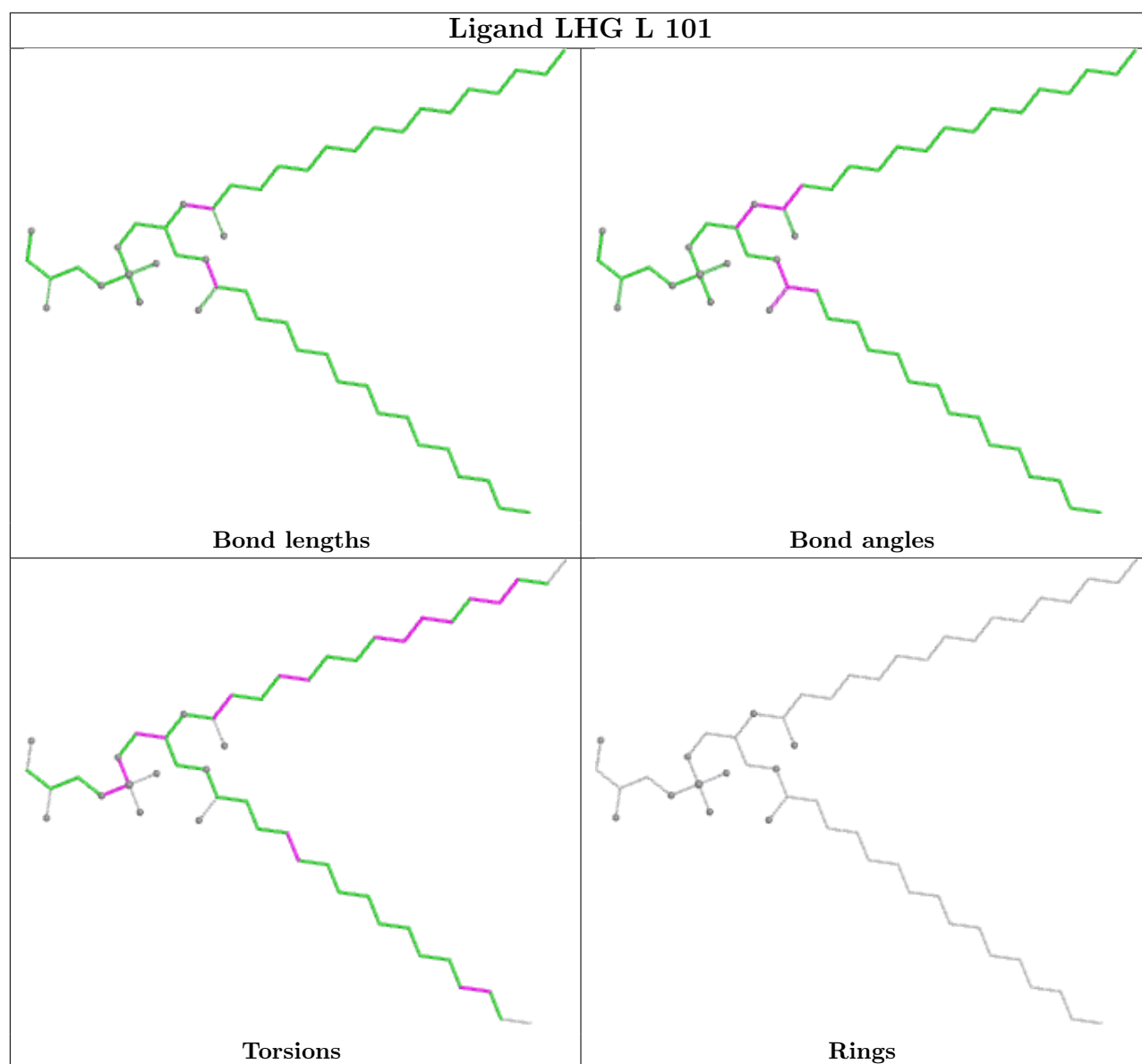


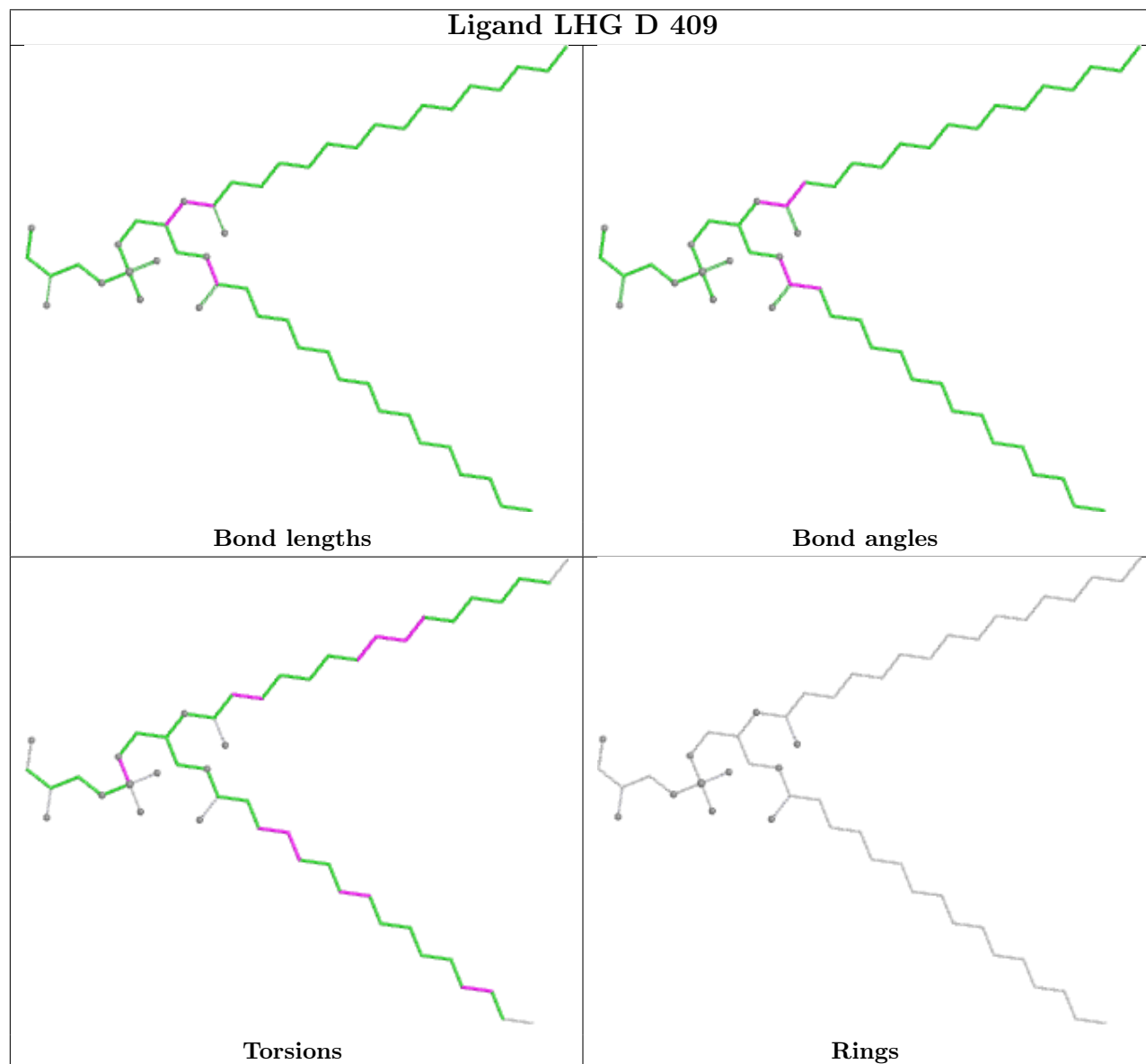
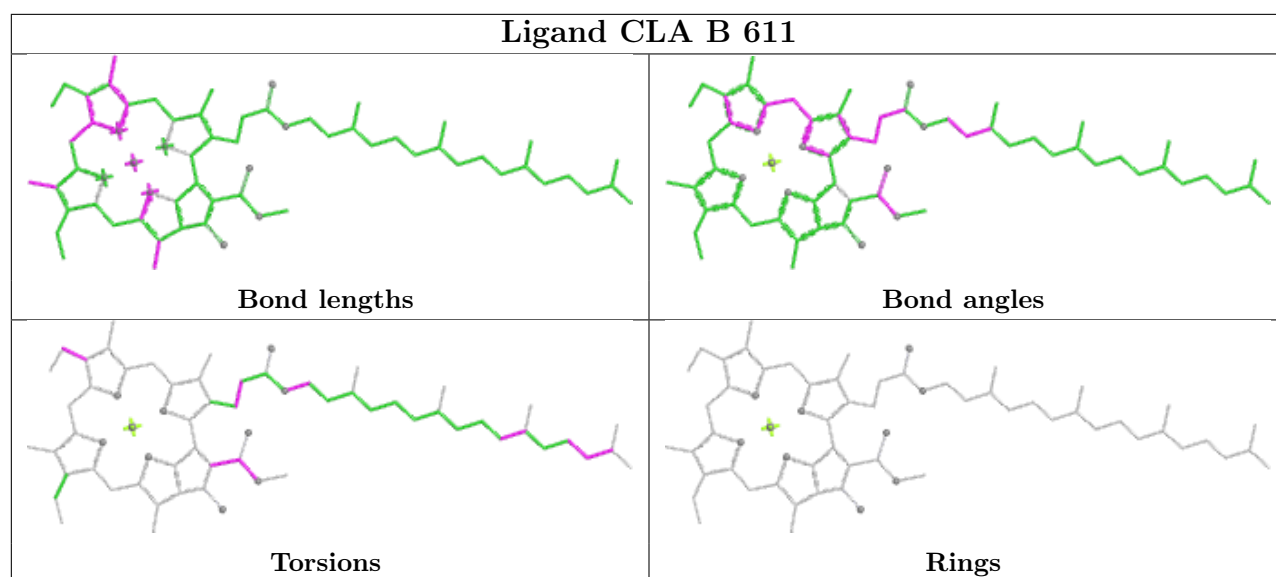
Rings

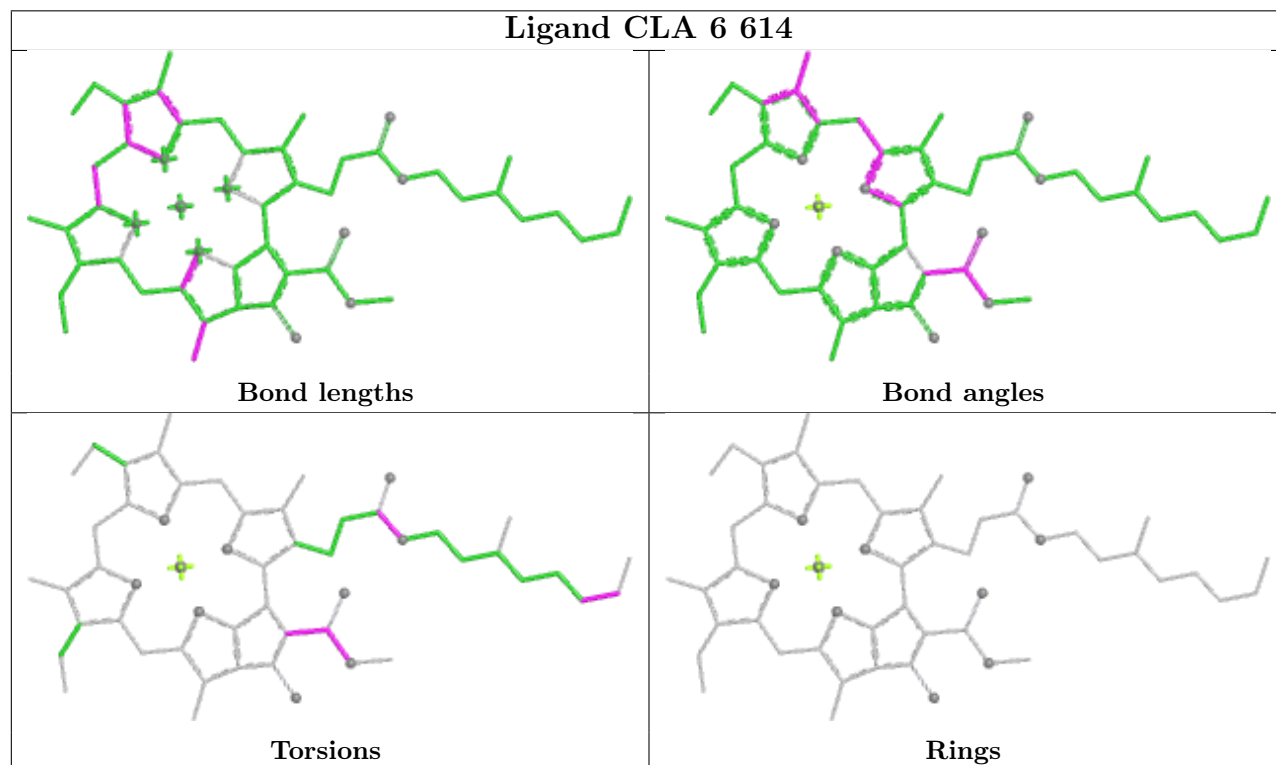
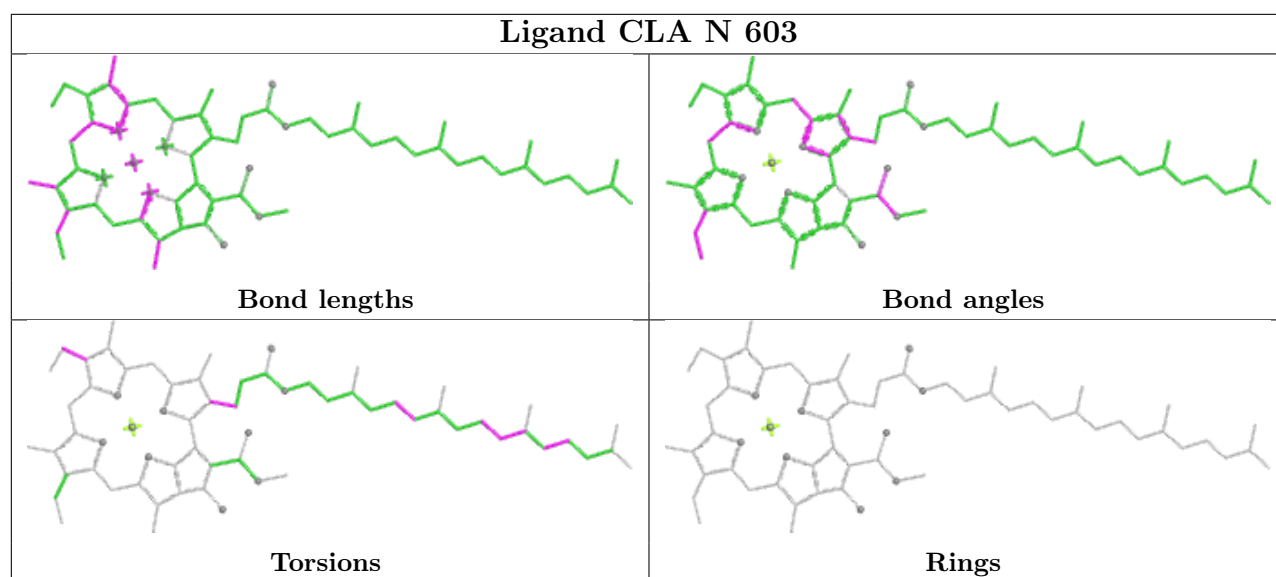


Ligand CLA S 611

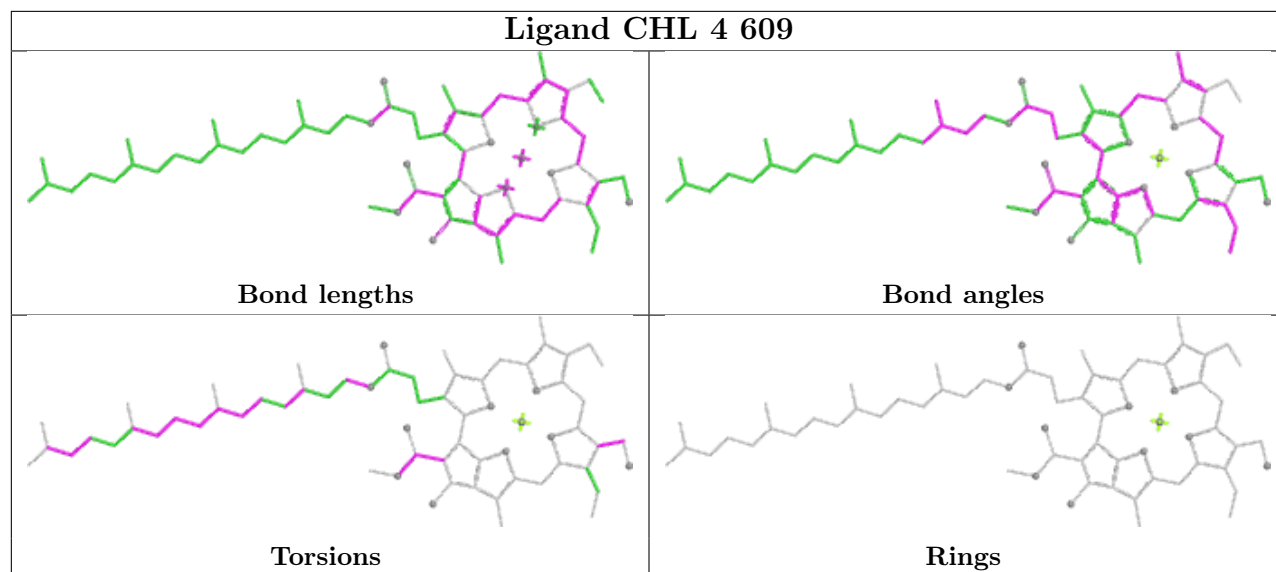




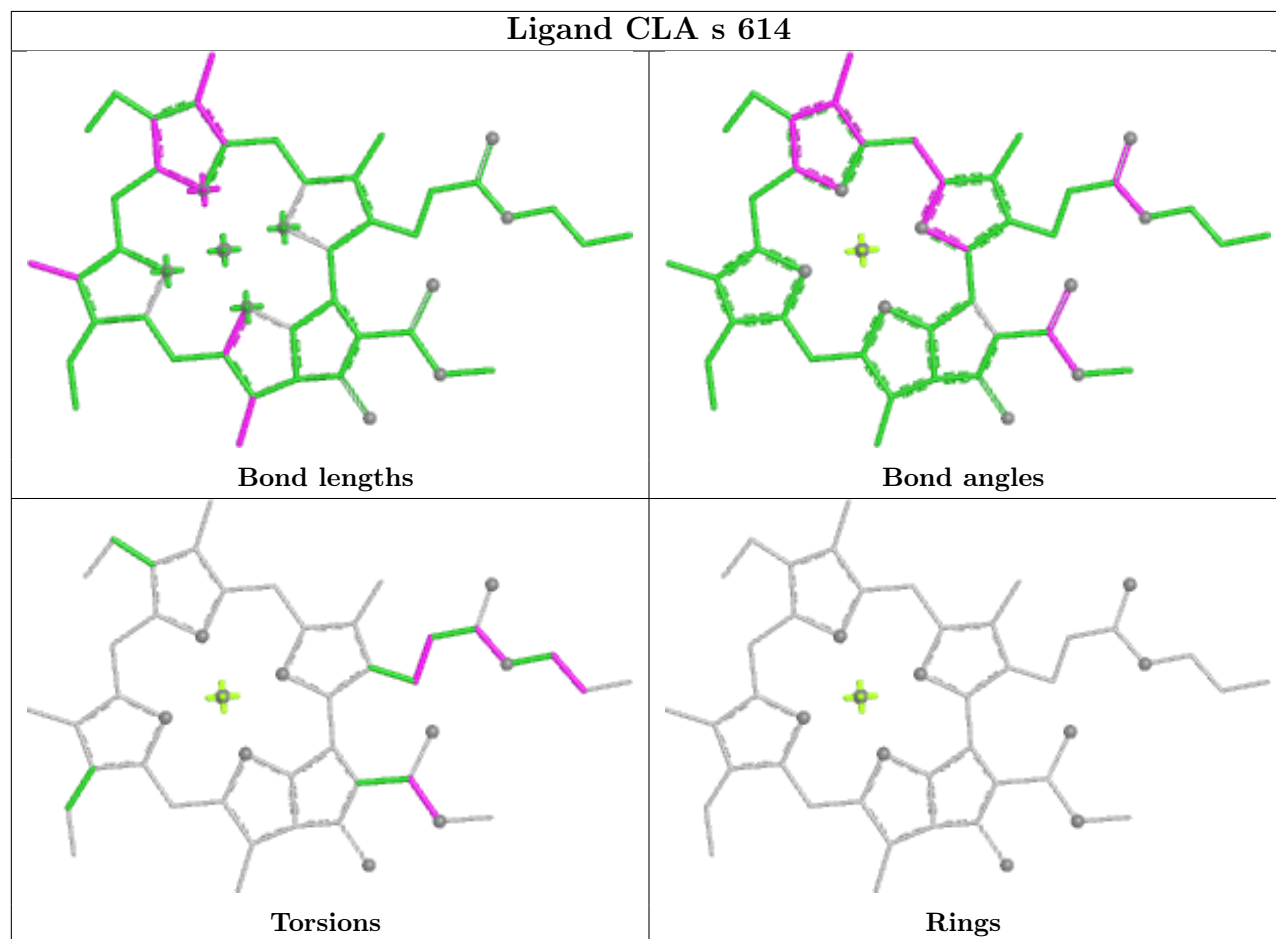


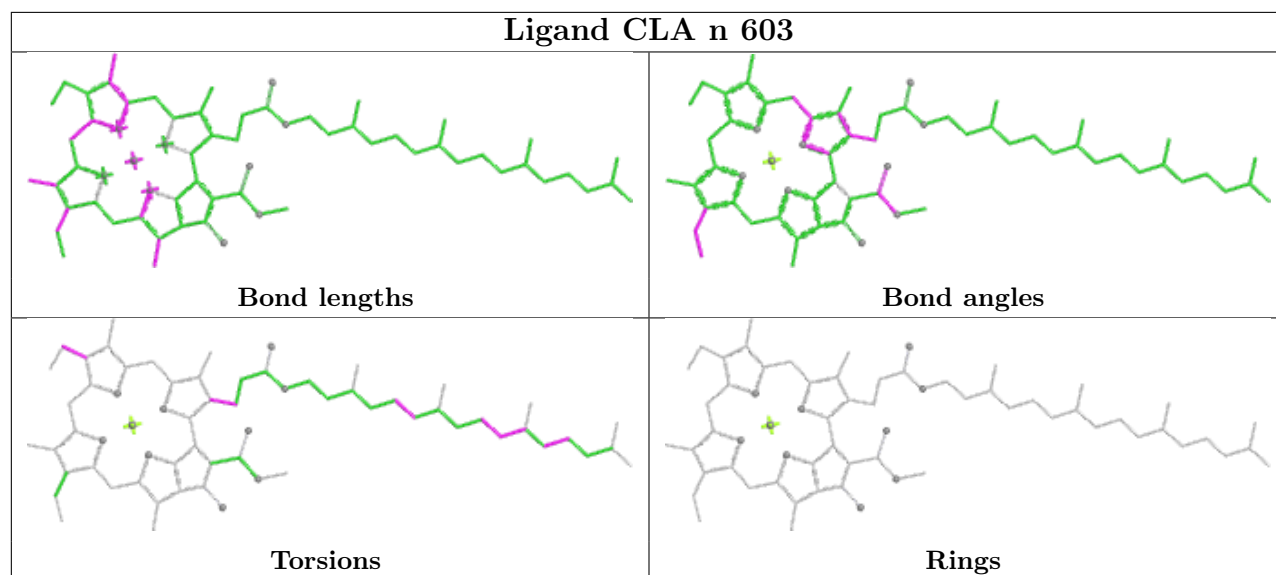
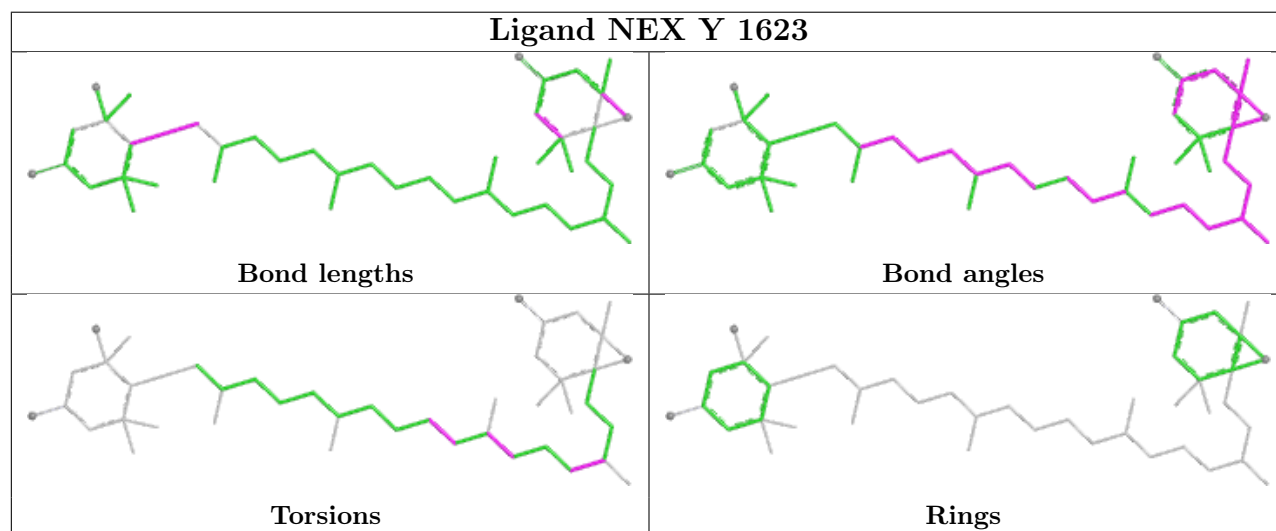
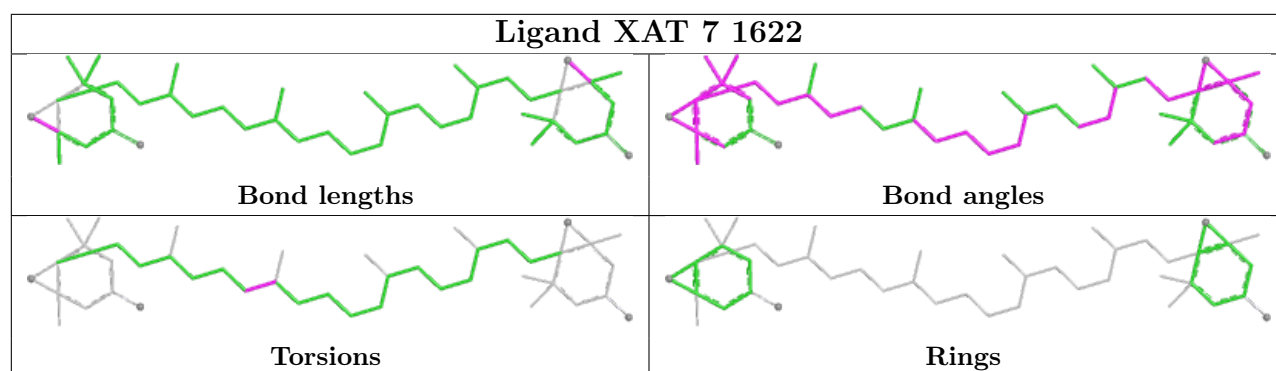


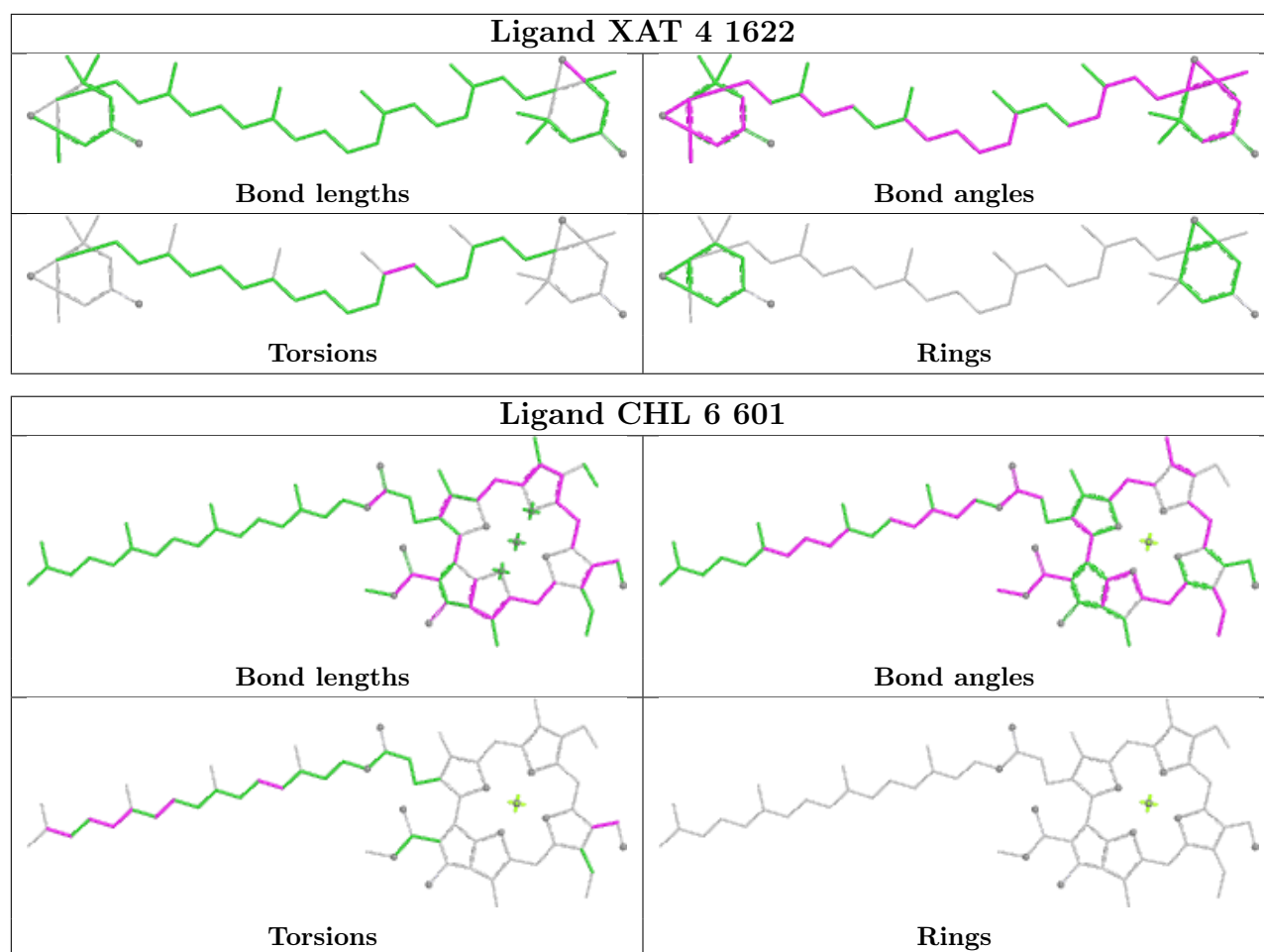
Ligand CHL 4 609



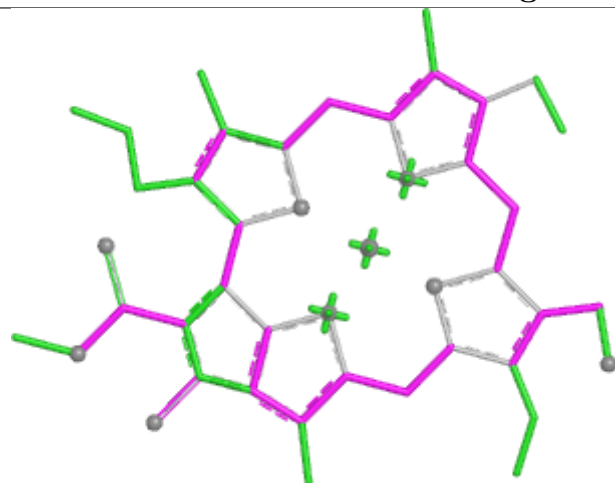
Ligand CLA s 614



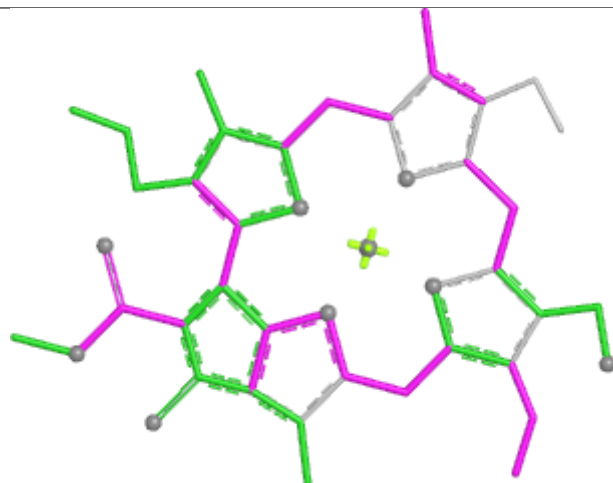




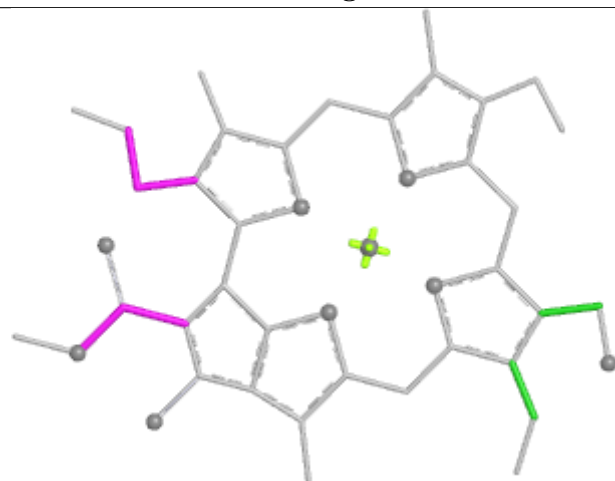
Ligand CHL 9 608



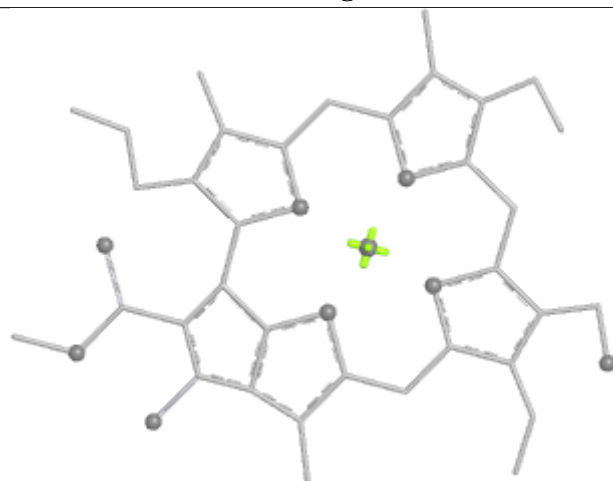
Bond lengths



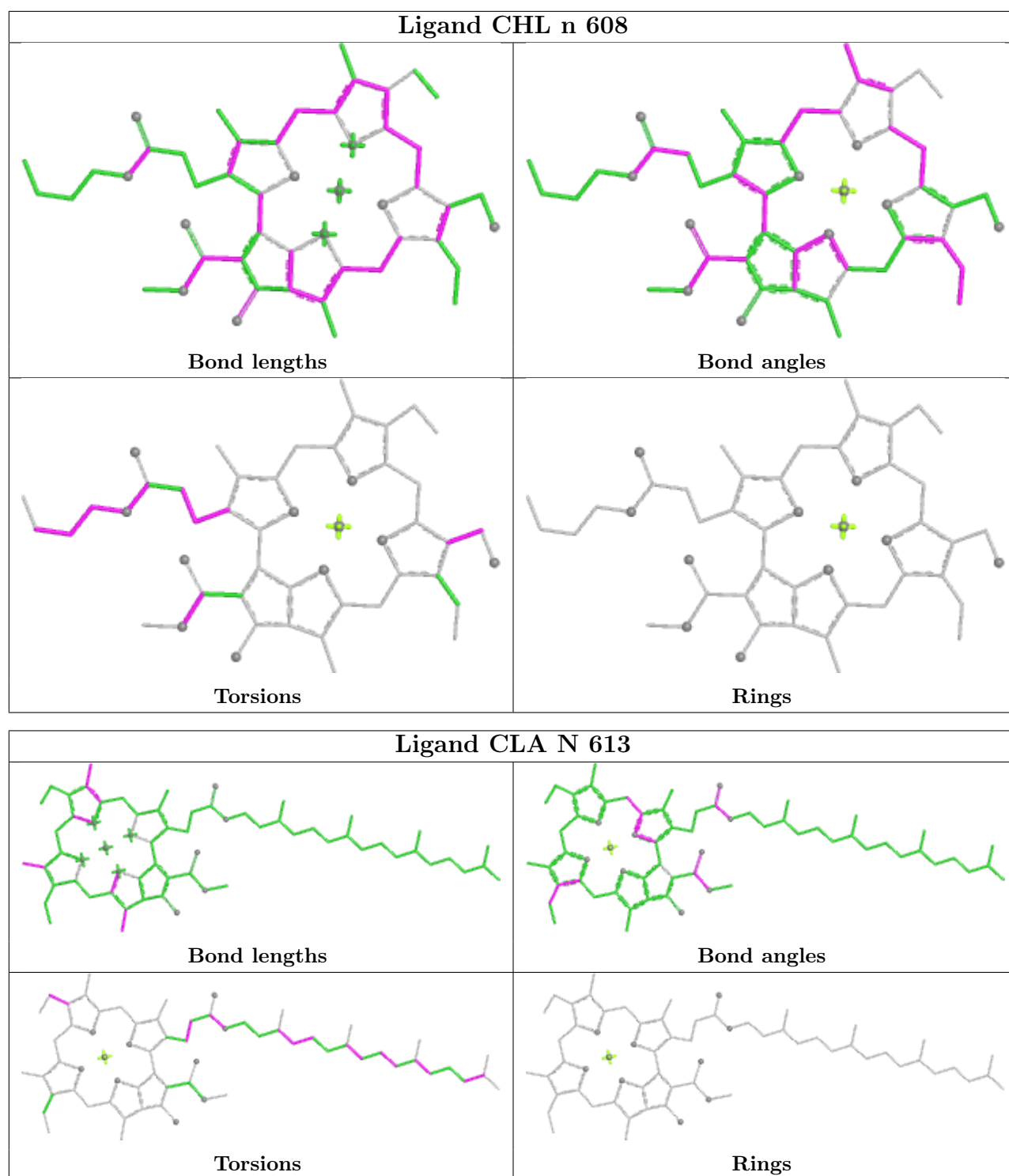
Bond angles

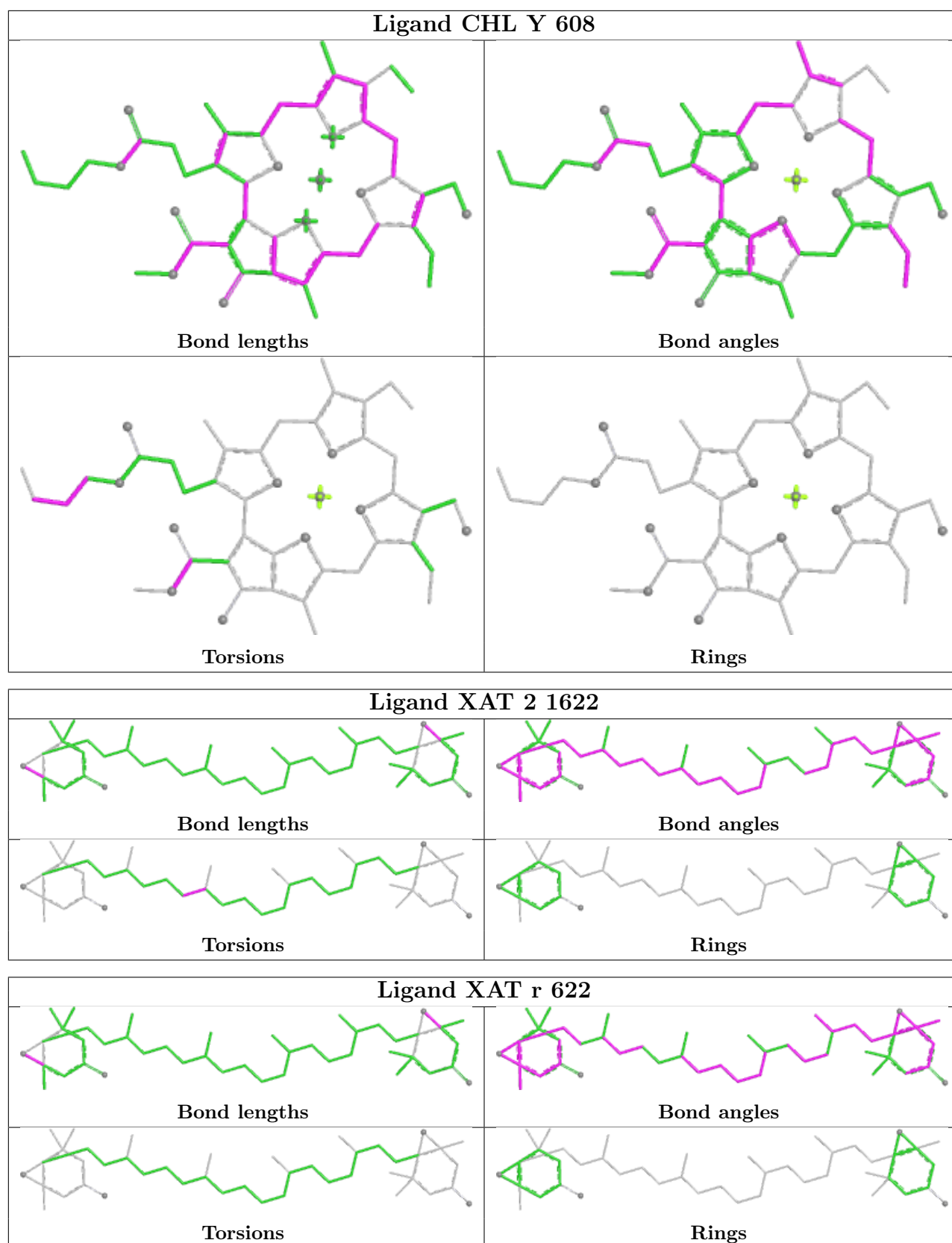


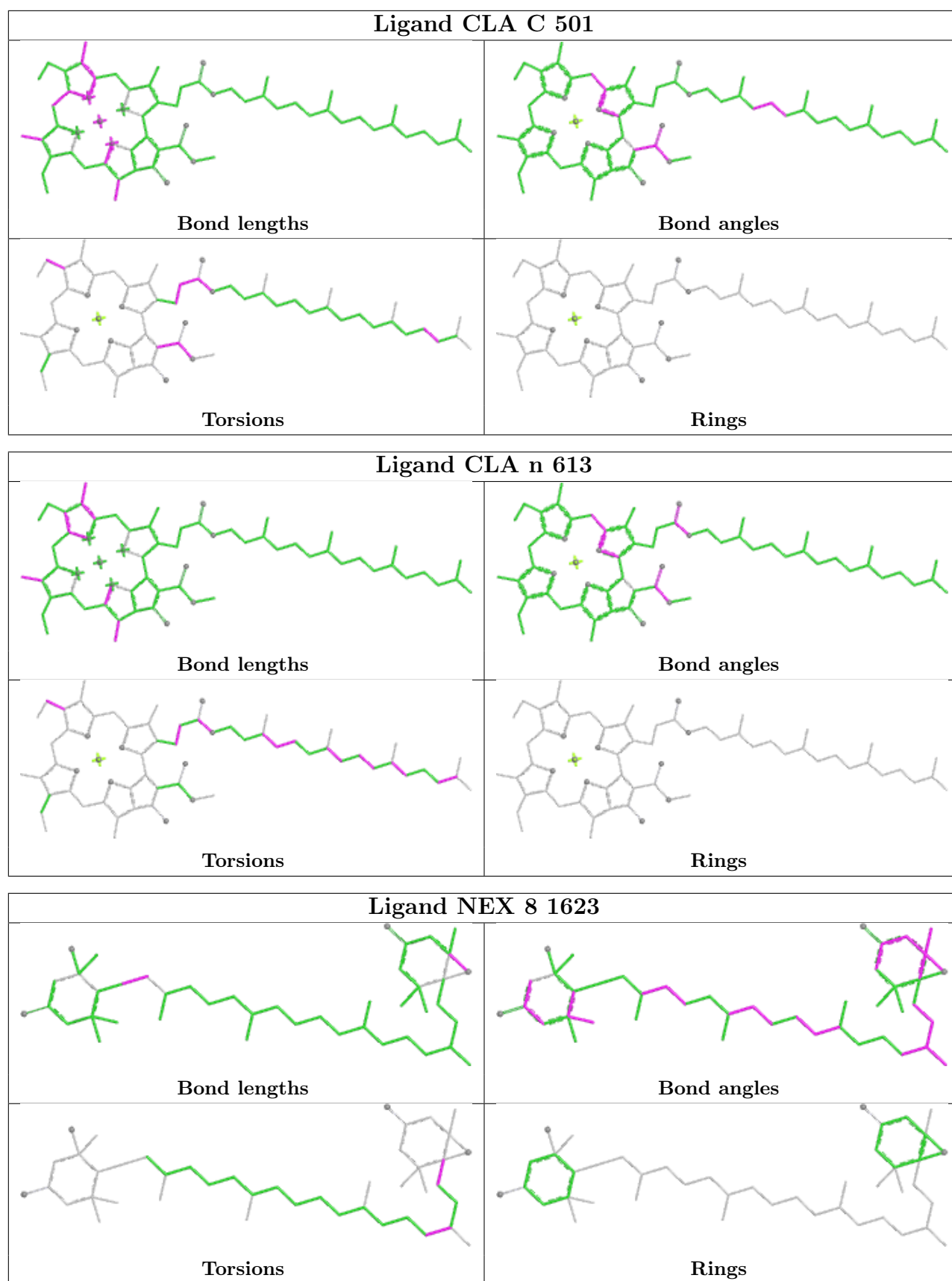
Torsions

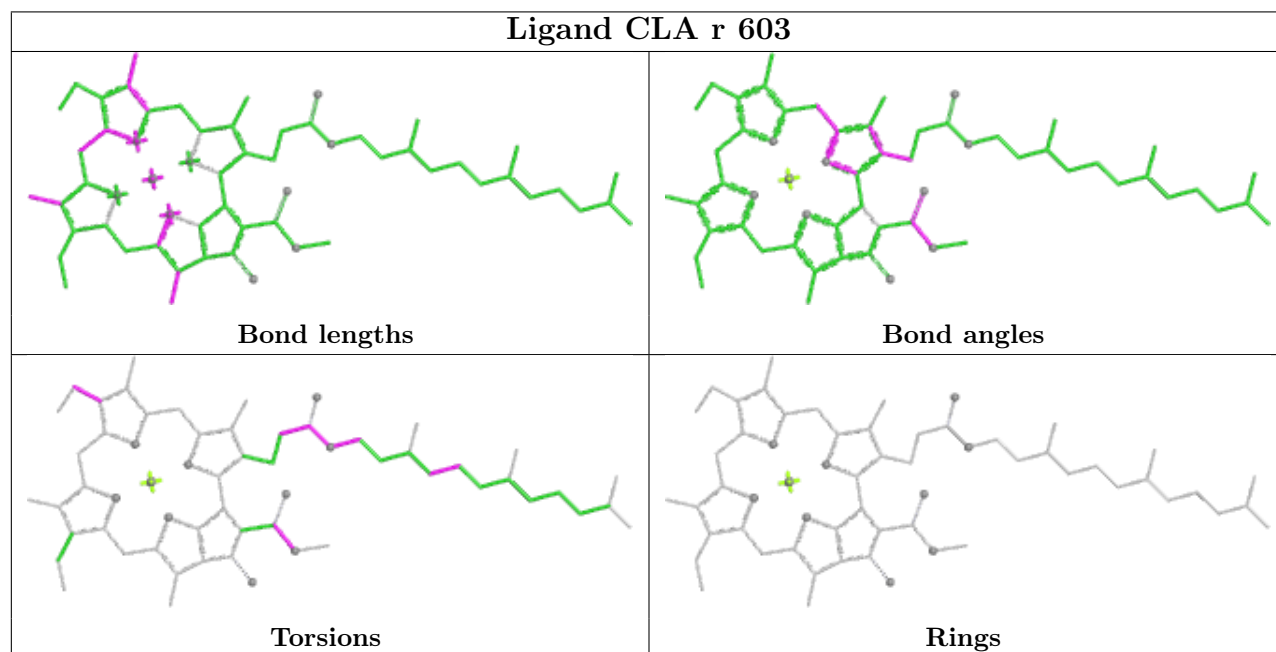
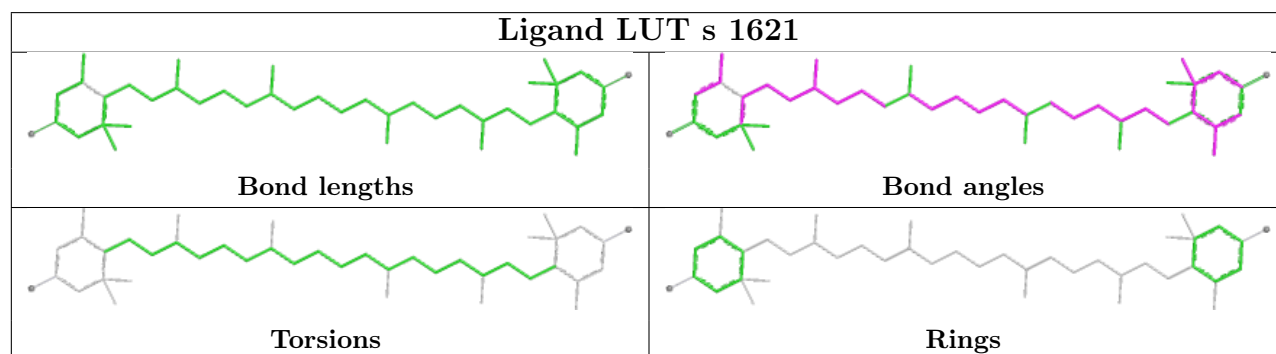
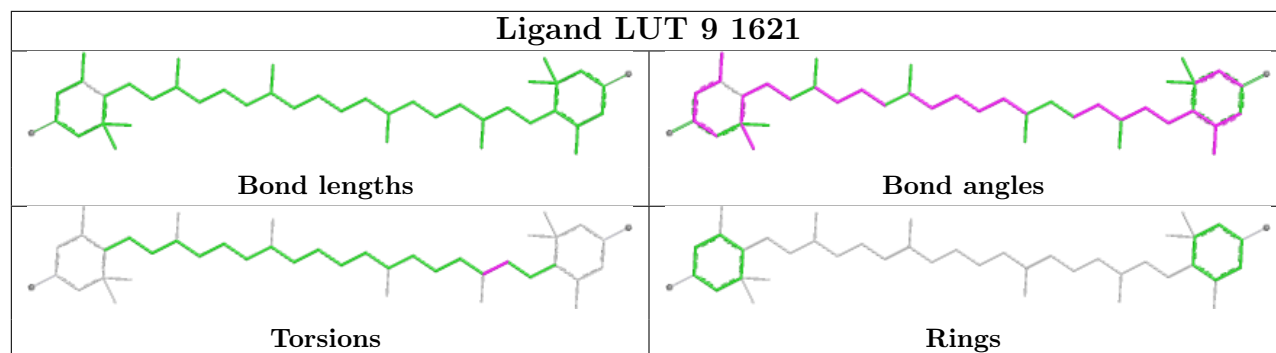


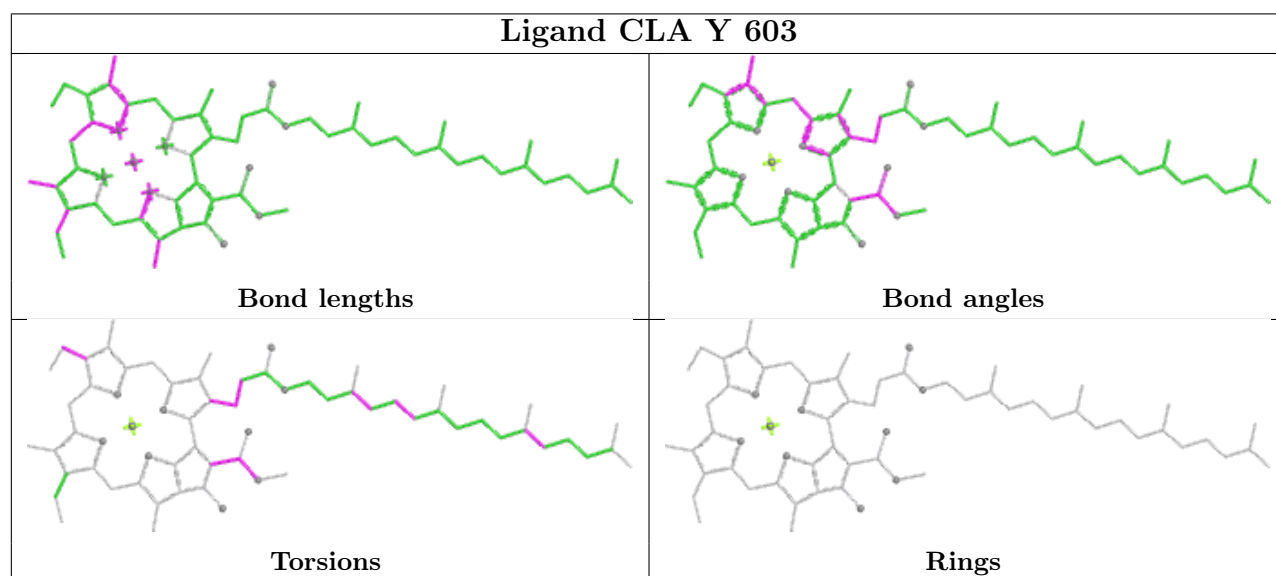
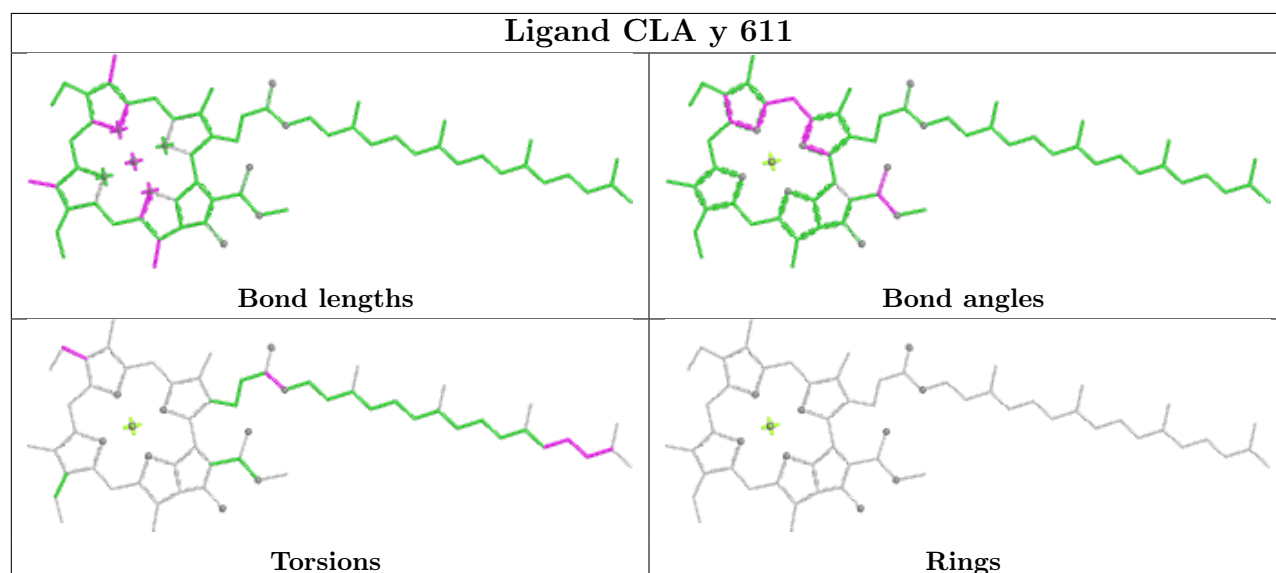
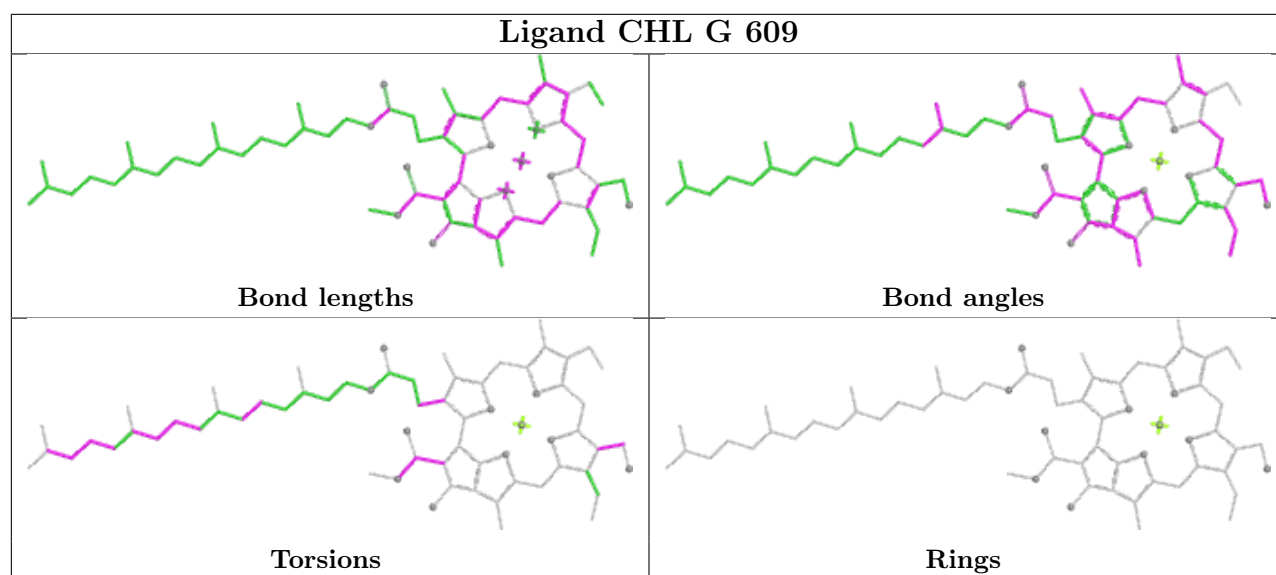
Rings



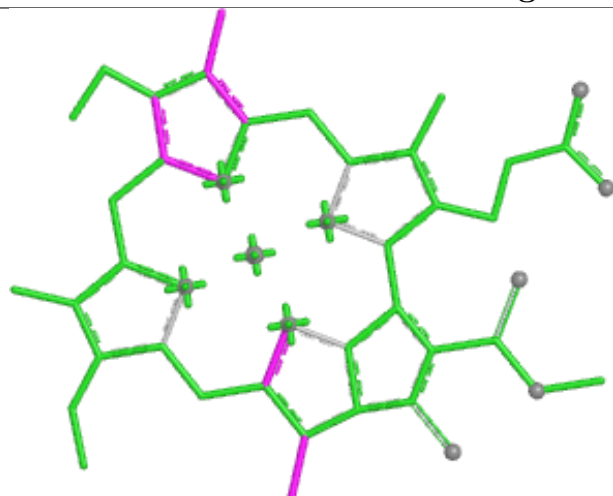




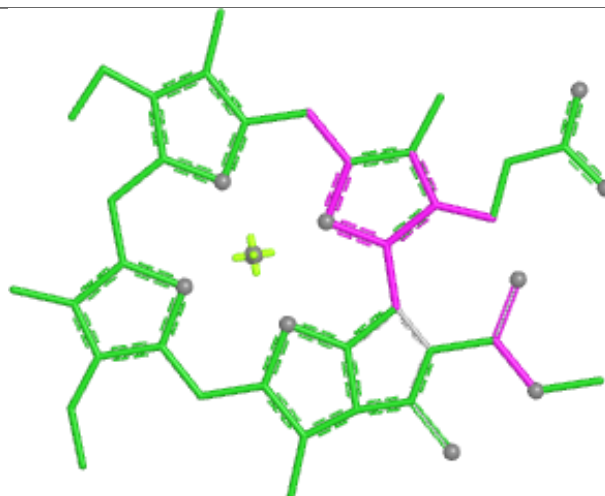




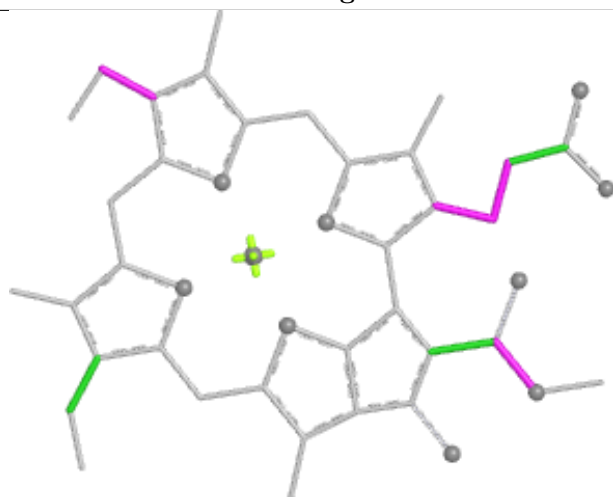
Ligand CLA 8 612



Bond lengths



Bond angles

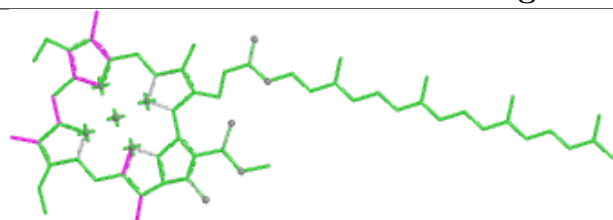


Torsions

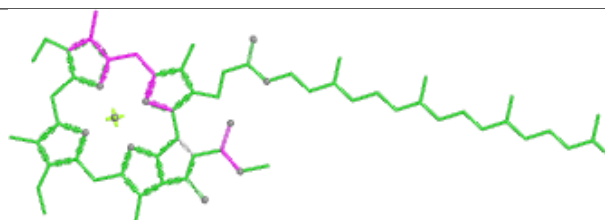


Rings

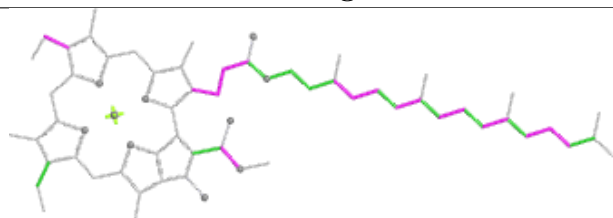
Ligand CLA 5 602



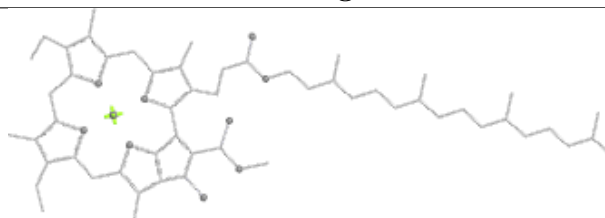
Bond lengths



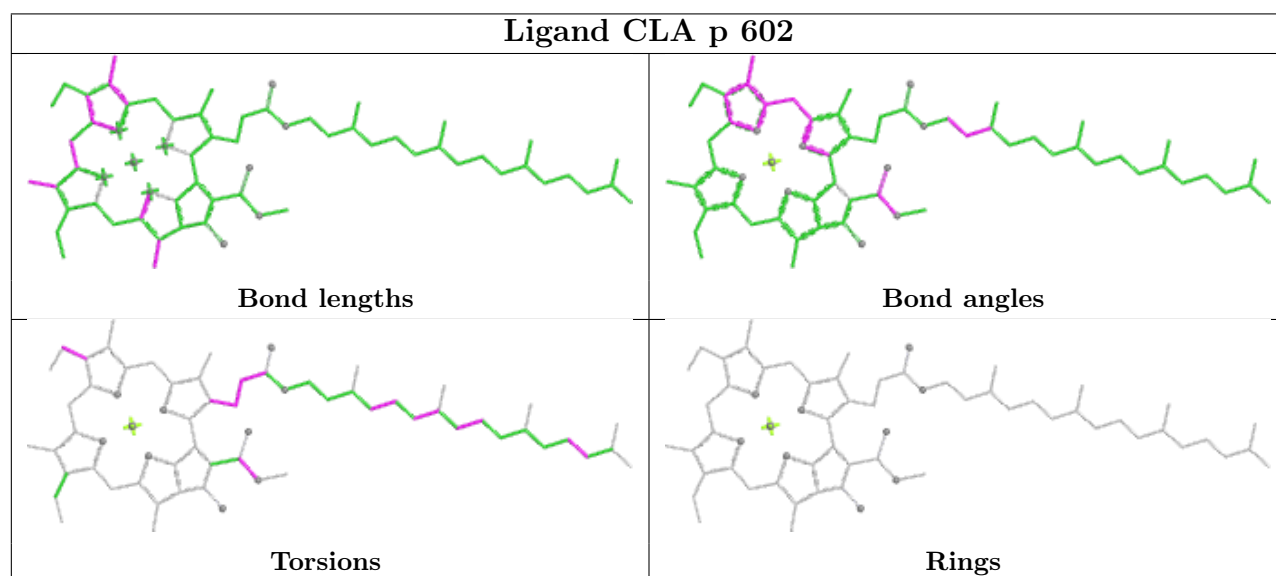
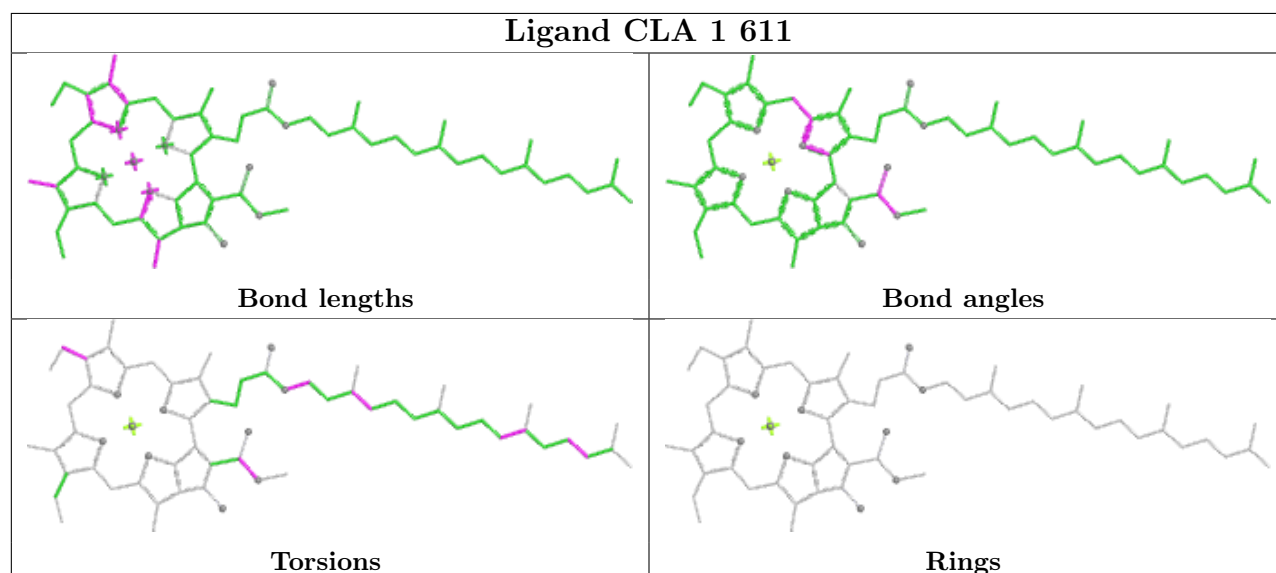
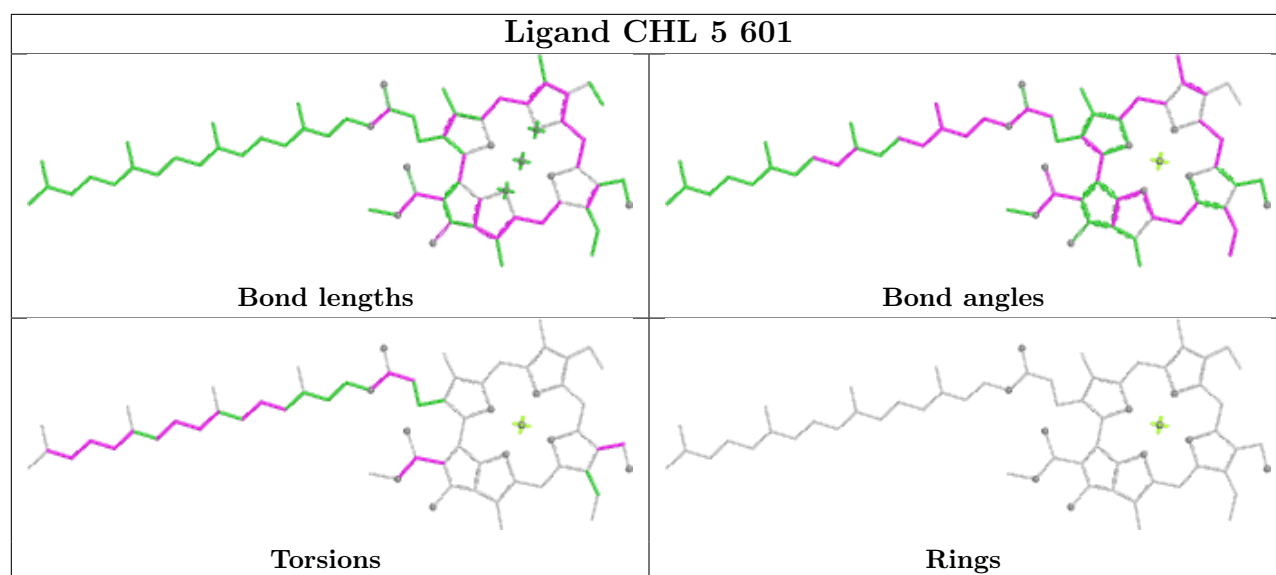
Bond angles



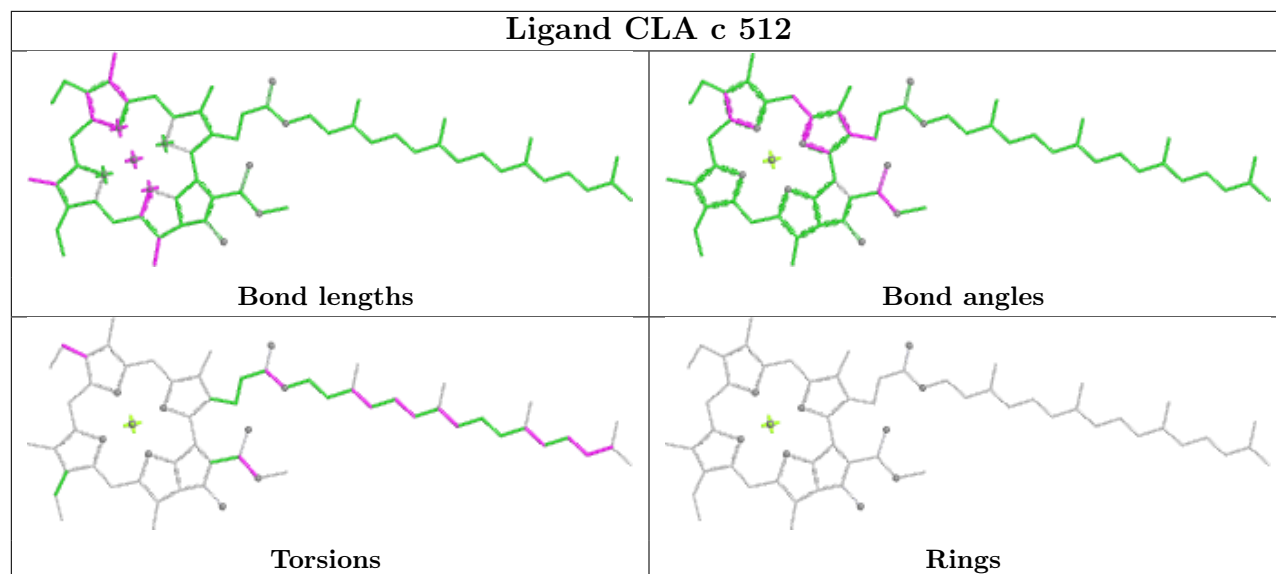
Torsions



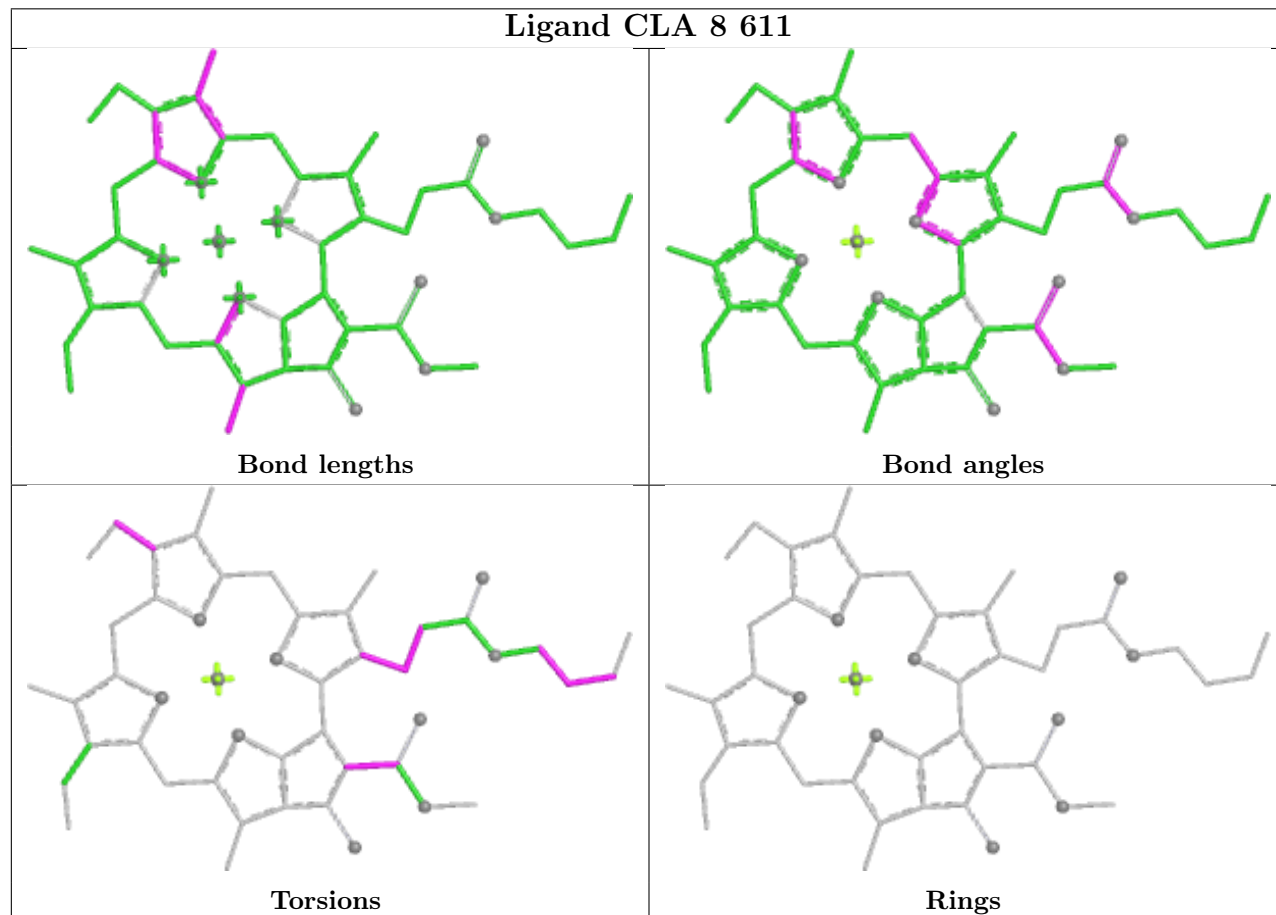
Rings

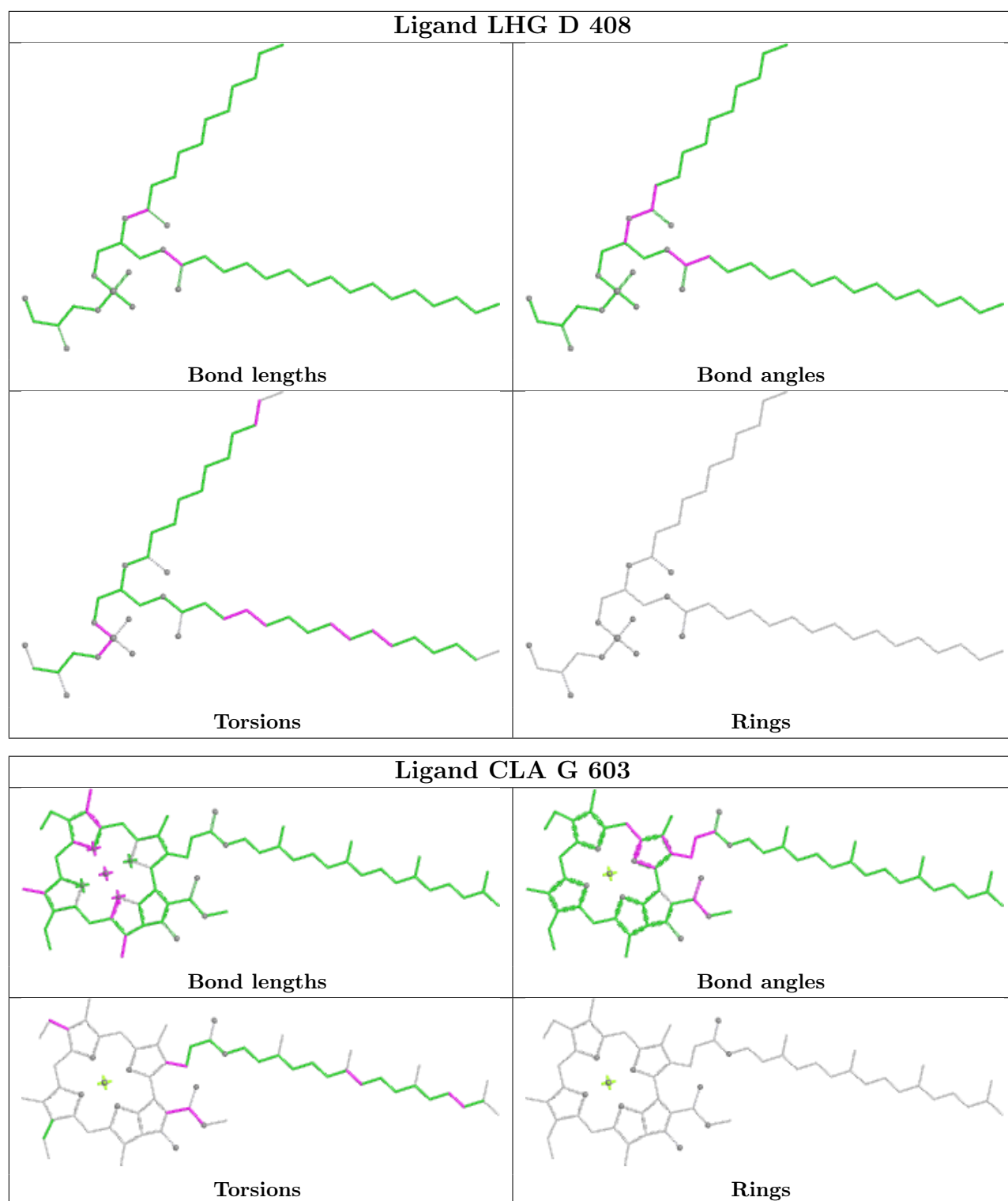


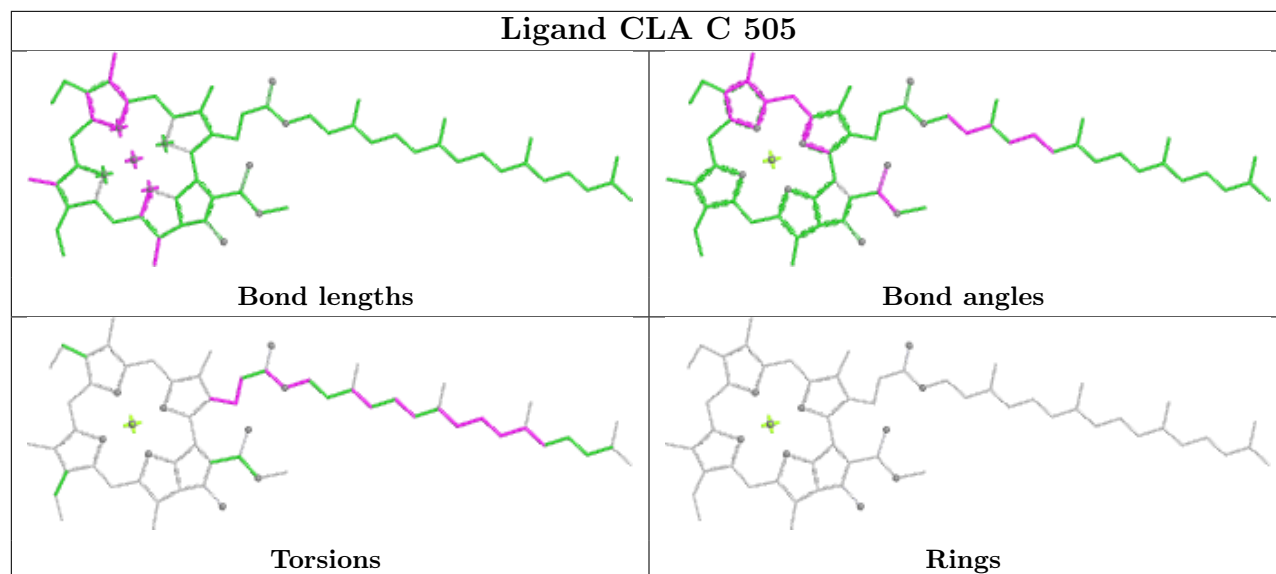
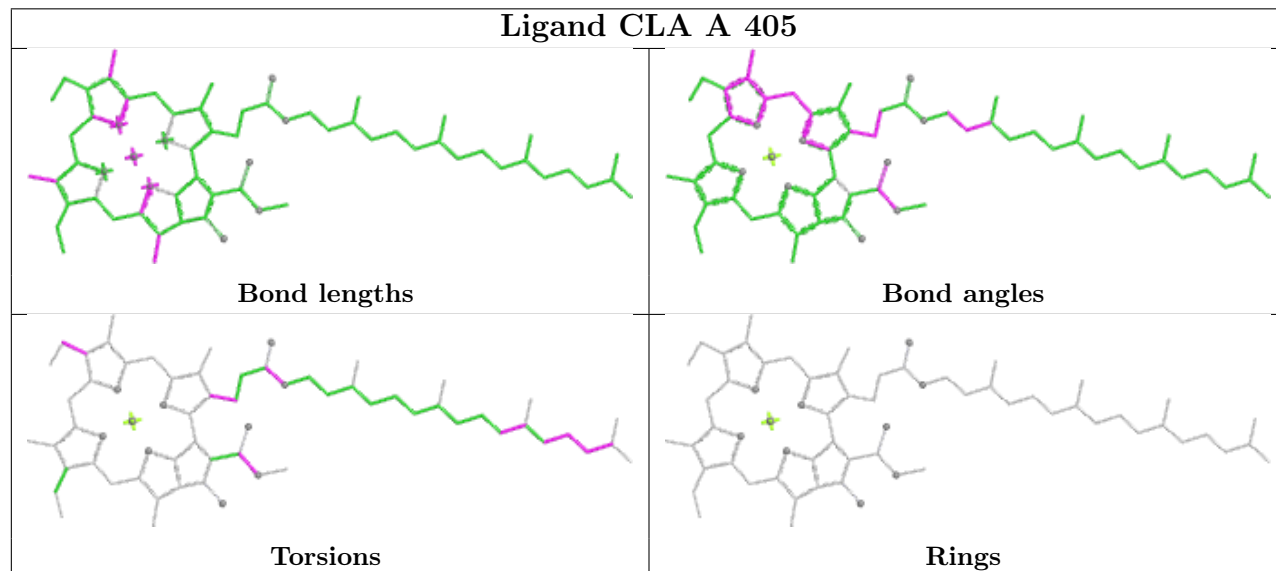
Ligand CLA c 512



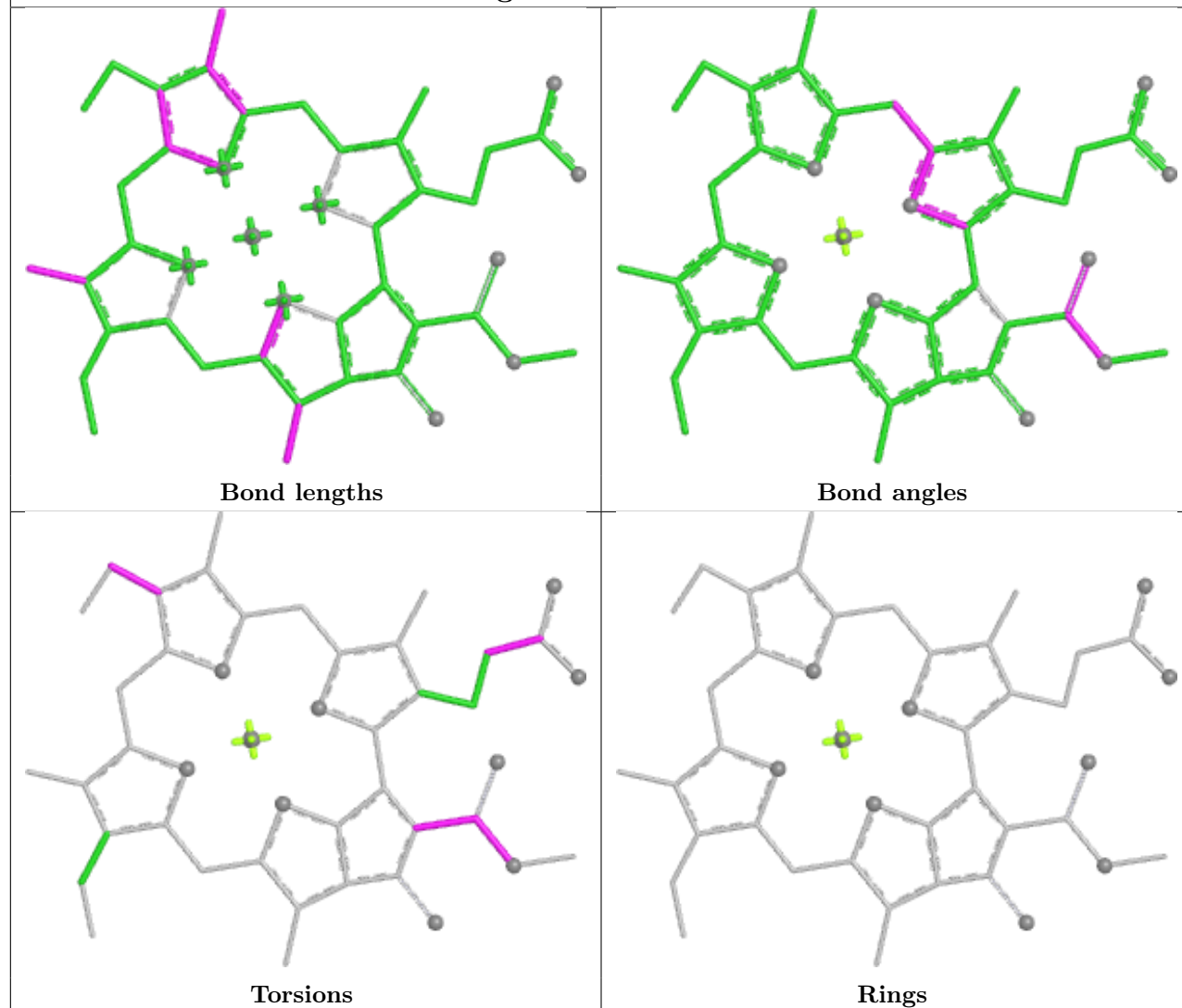
Ligand CLA 8 611



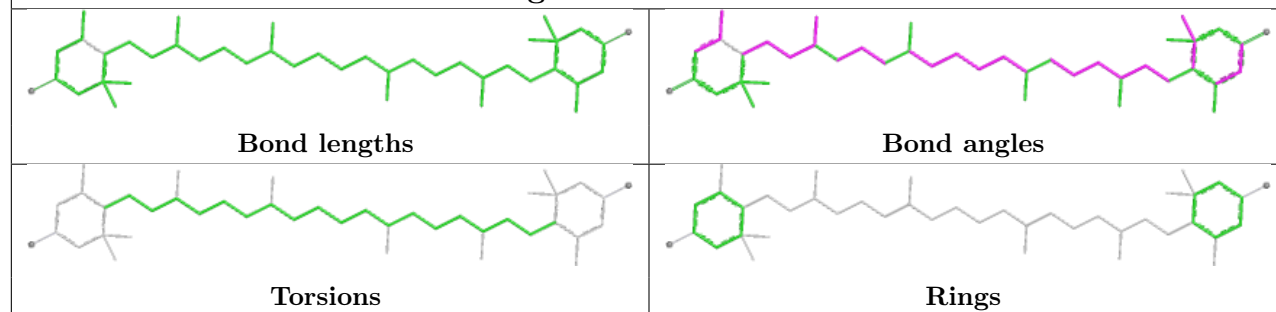


Ligand CLA C 505**Ligand CLA A 405**

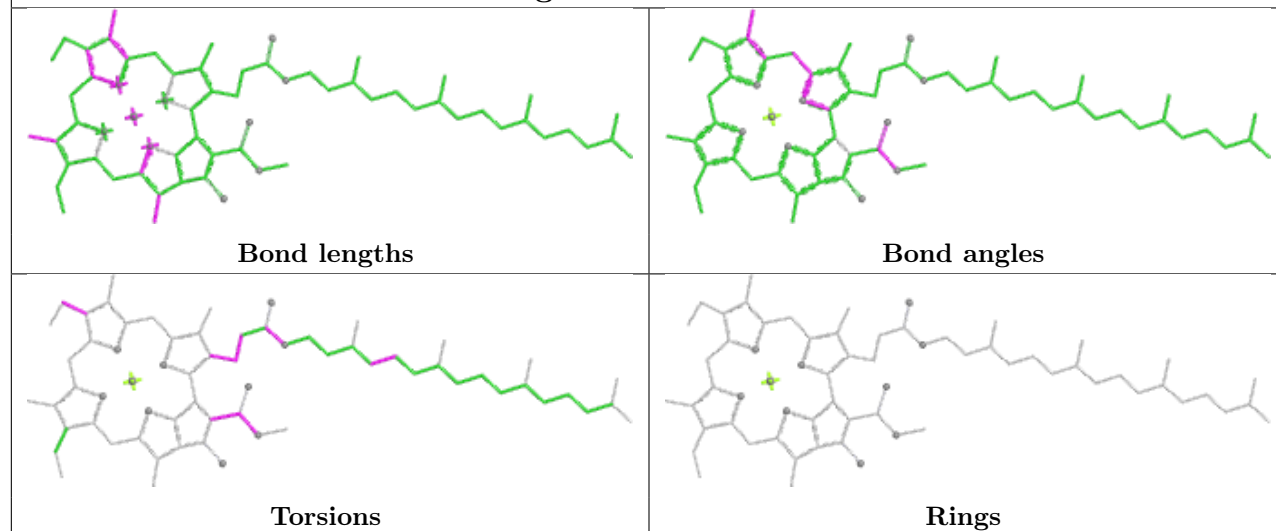
Ligand CLA 4 611



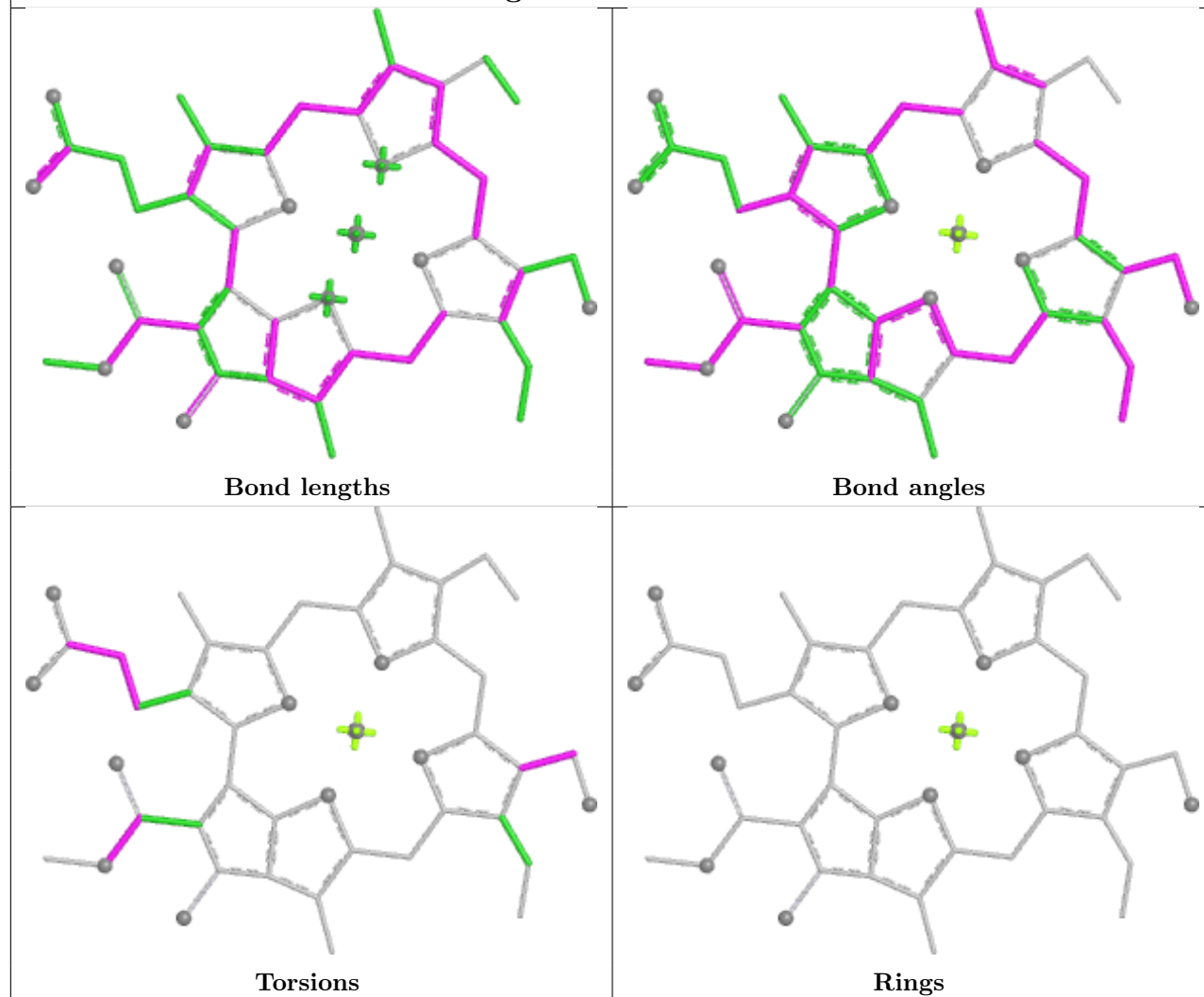
Ligand LUT 8 1621



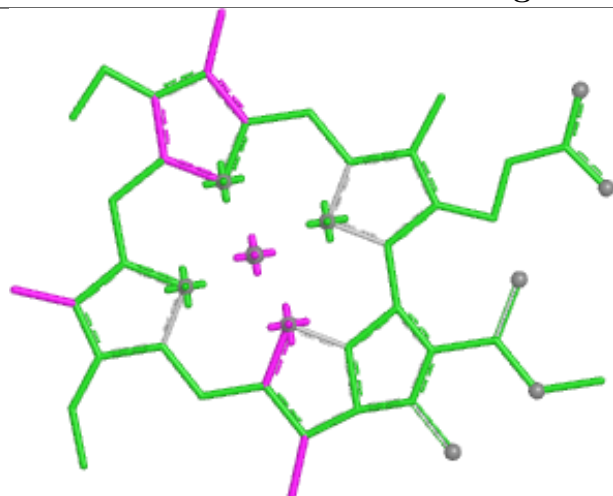
Ligand CLA n 604



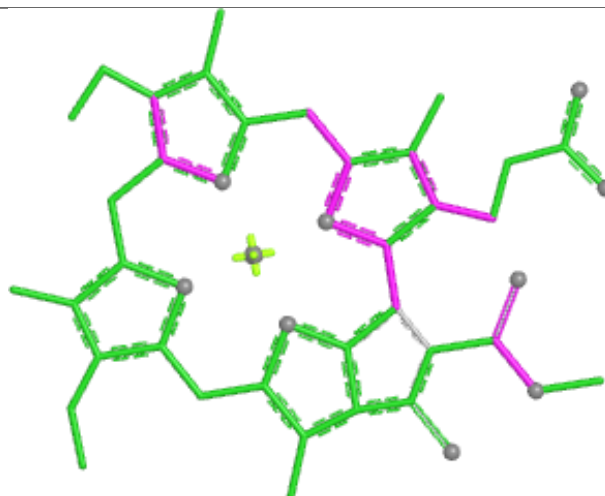
Ligand CHL 0 605



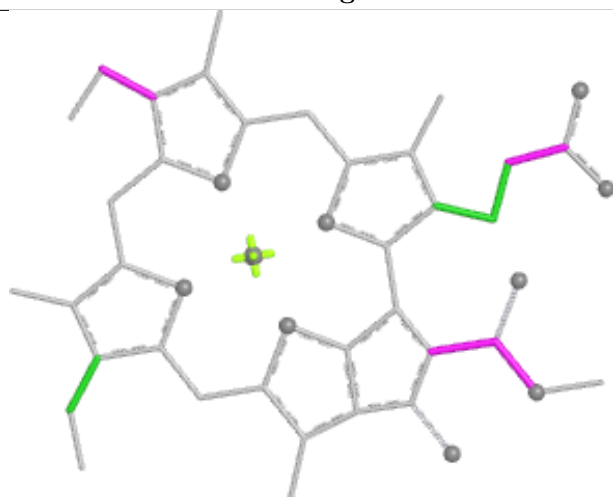
Ligand CLA N 612



Bond lengths



Bond angles

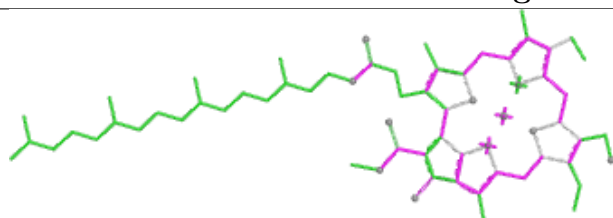


Torsions

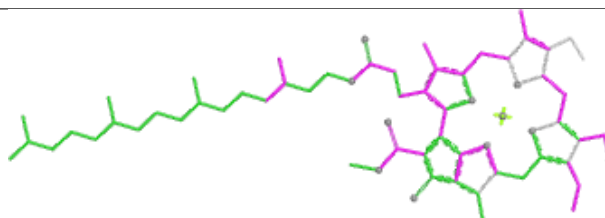


Rings

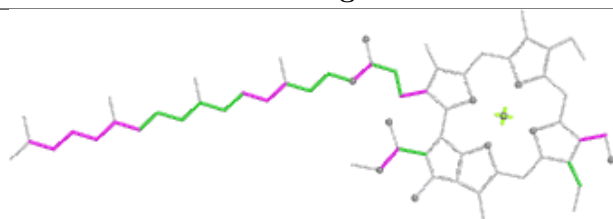
Ligand CHL Y 606



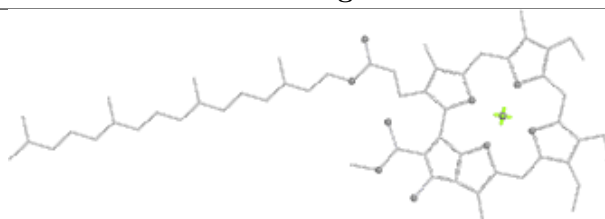
Bond lengths



Bond angles

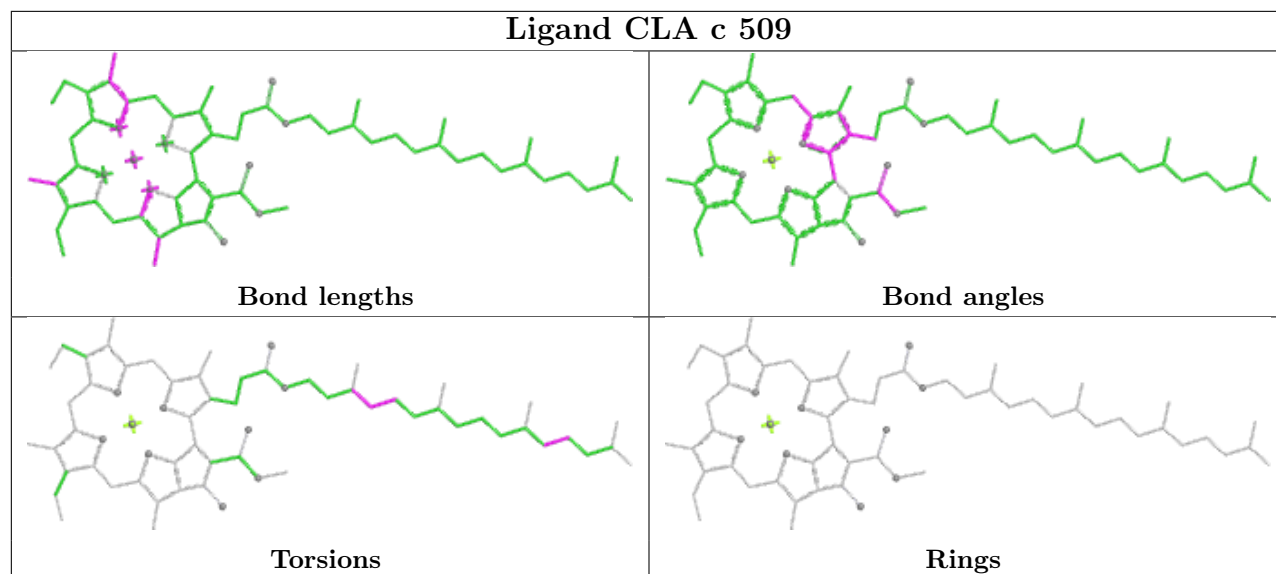


Torsions

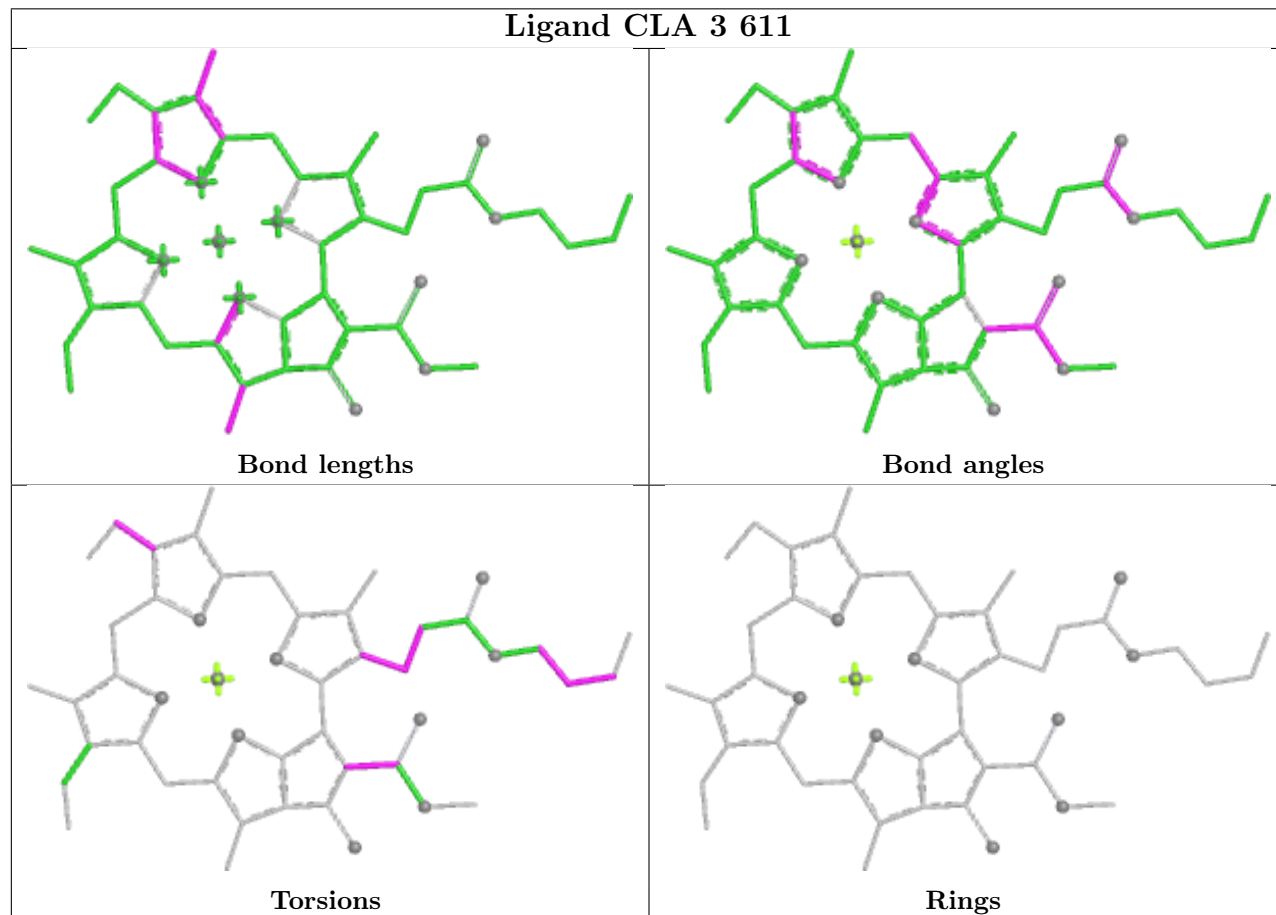


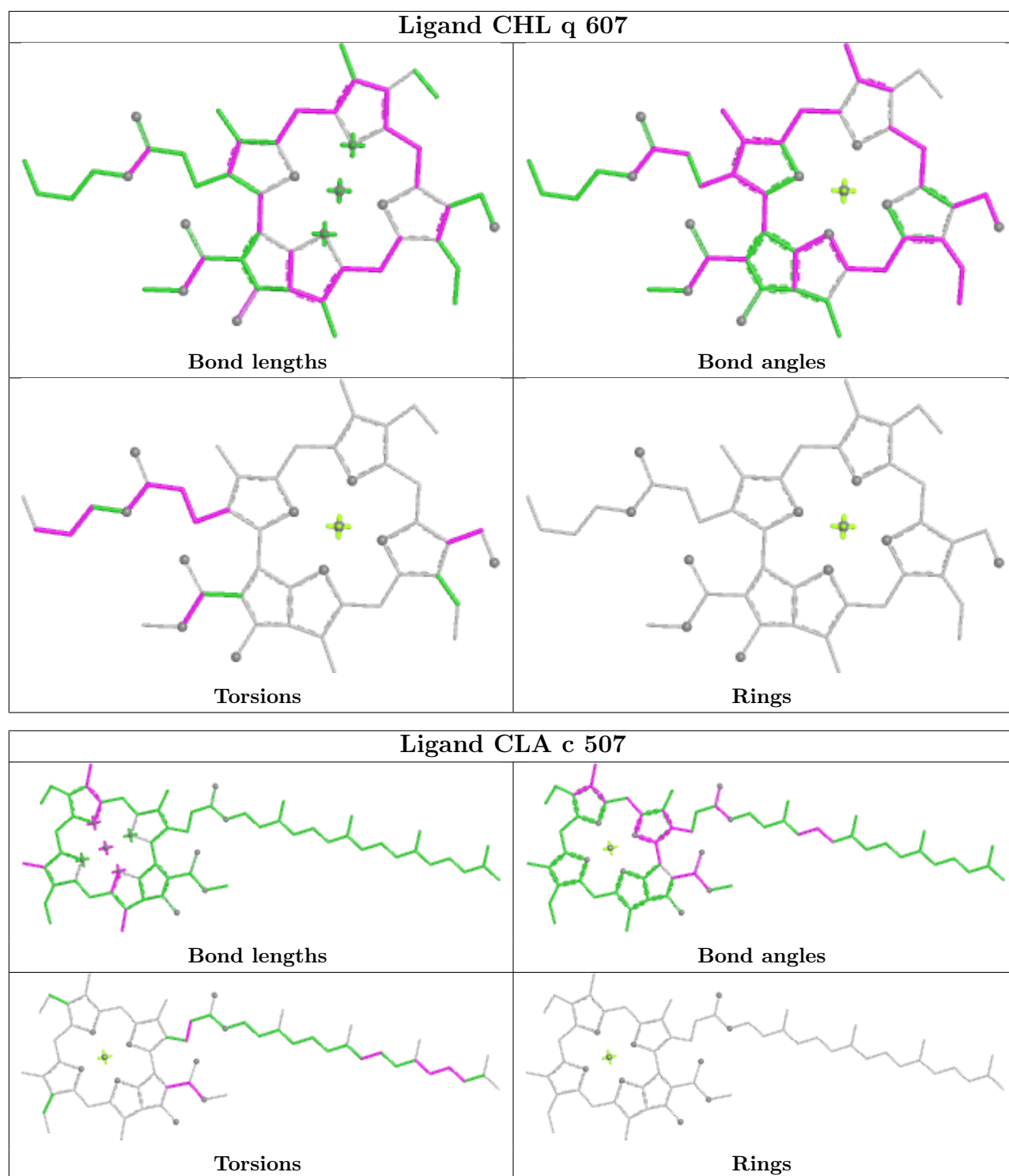
Rings

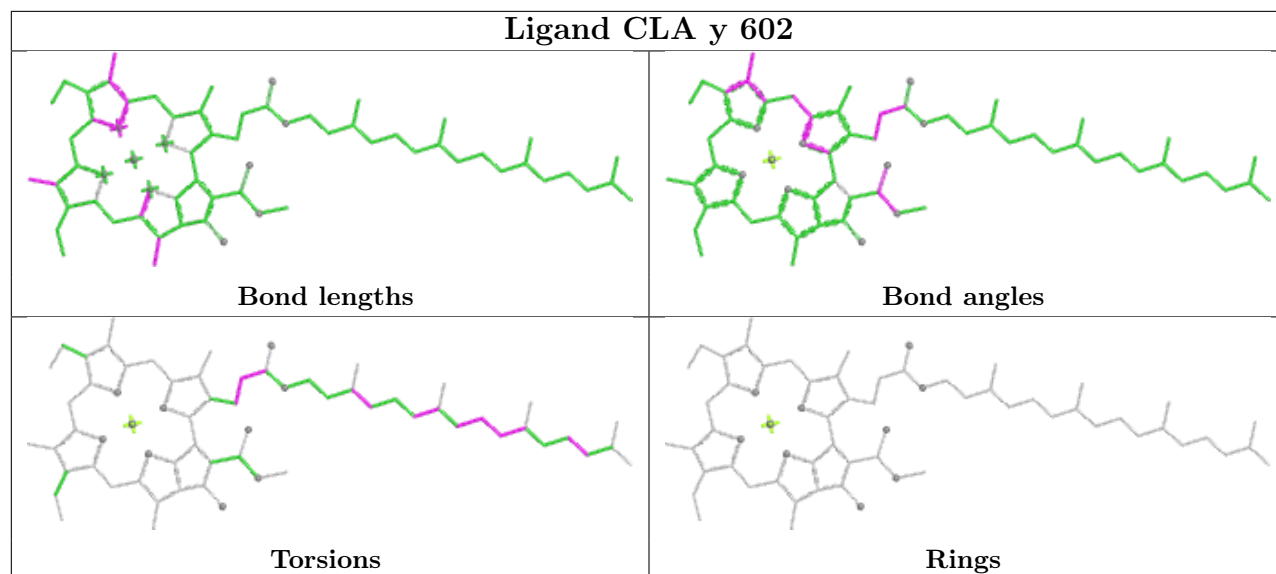
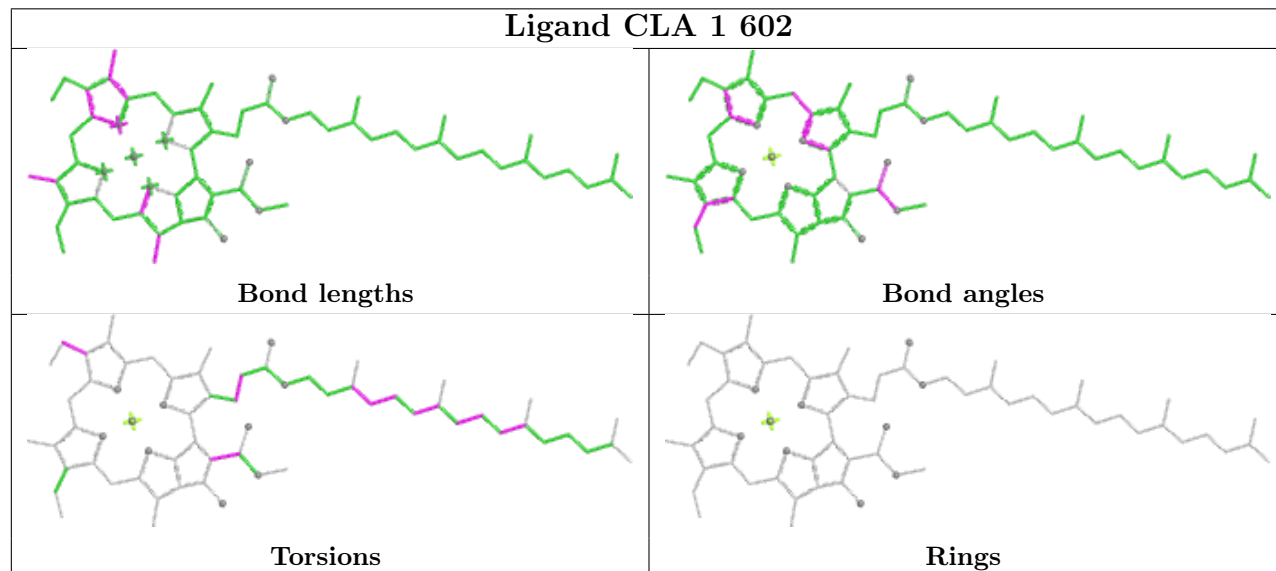
Ligand CLA c 509

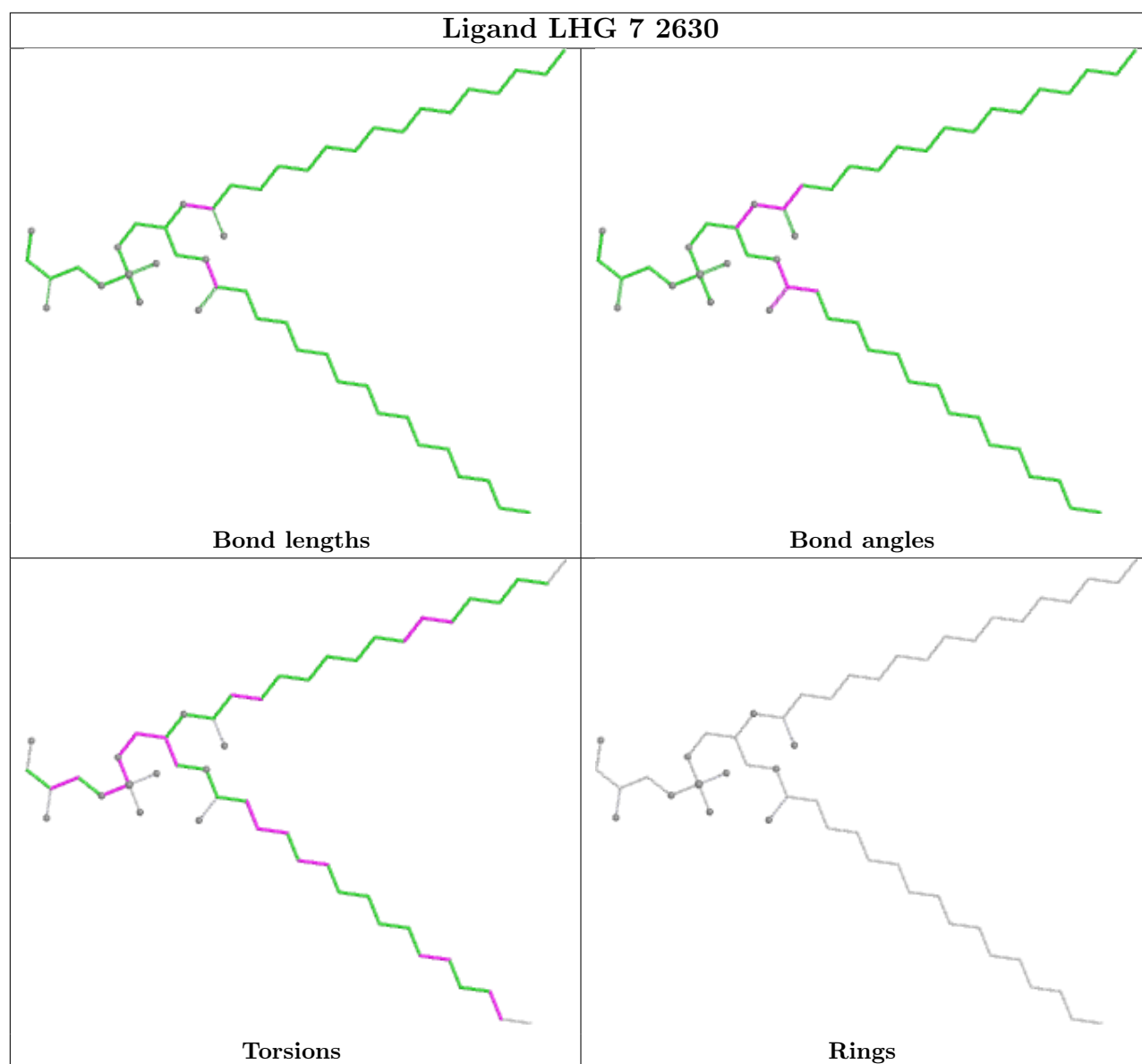


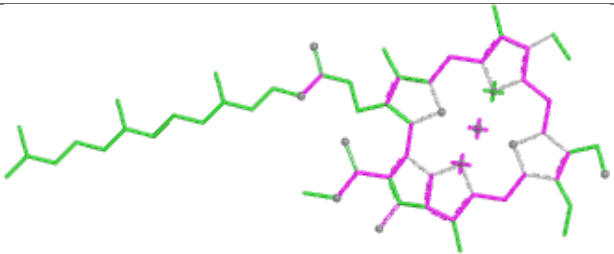
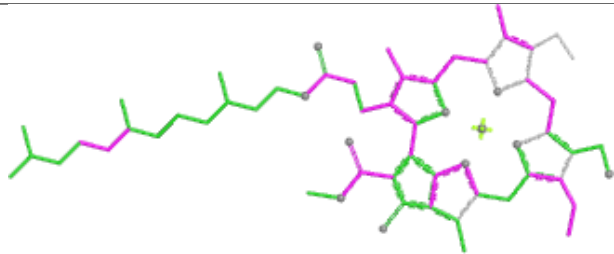
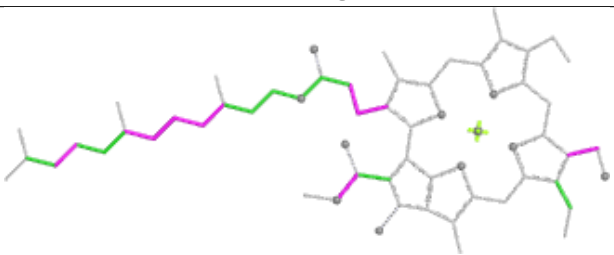
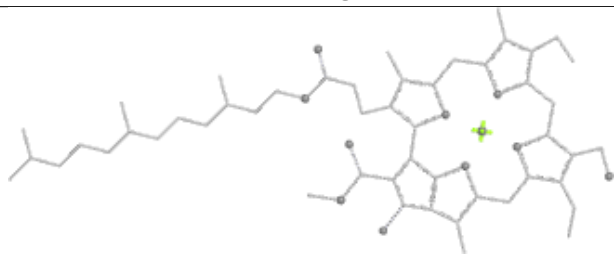
Ligand CLA 3 611

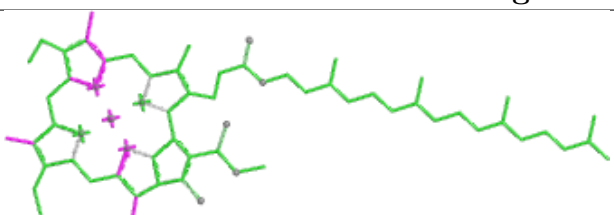
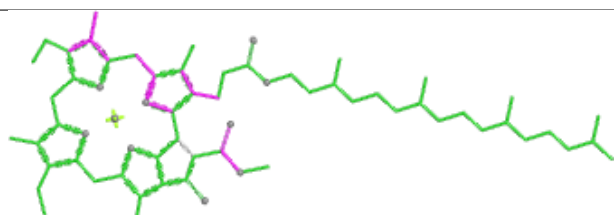
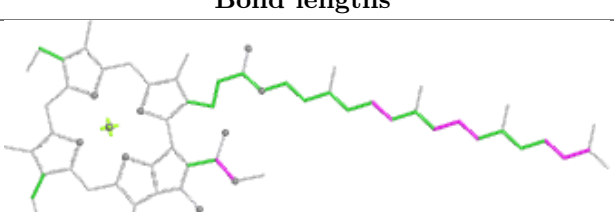
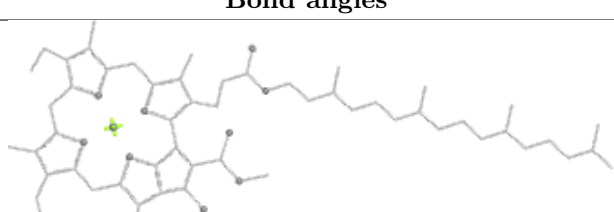


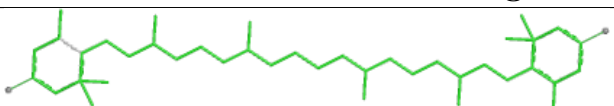
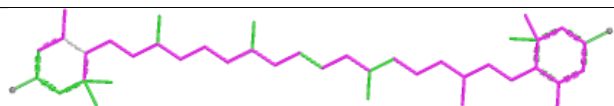
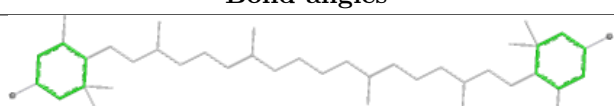


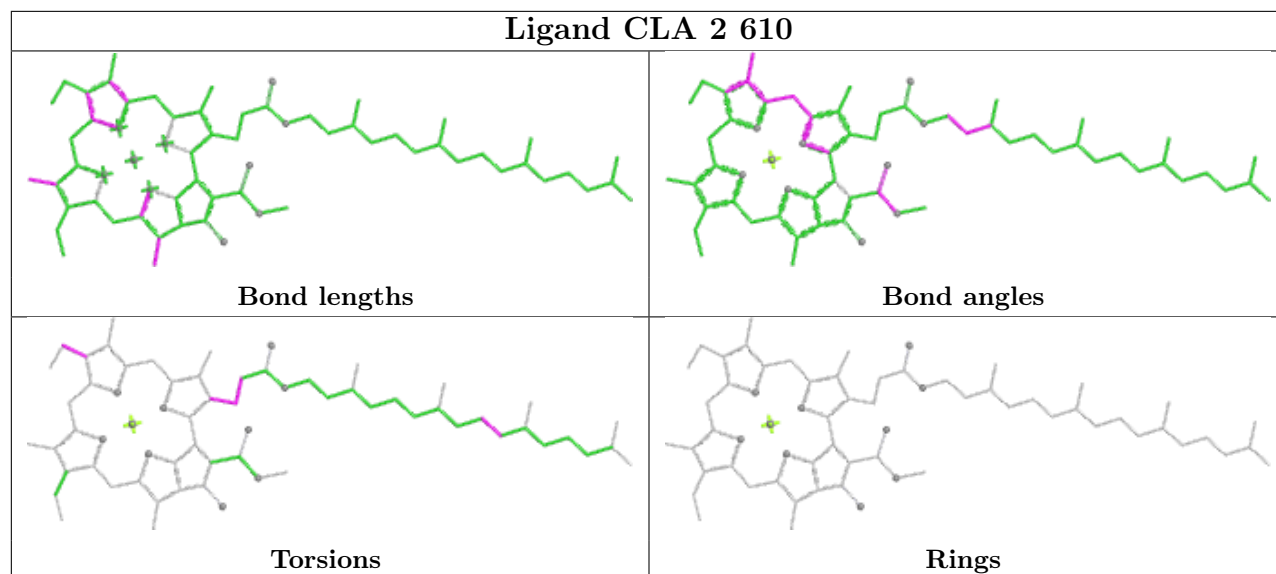
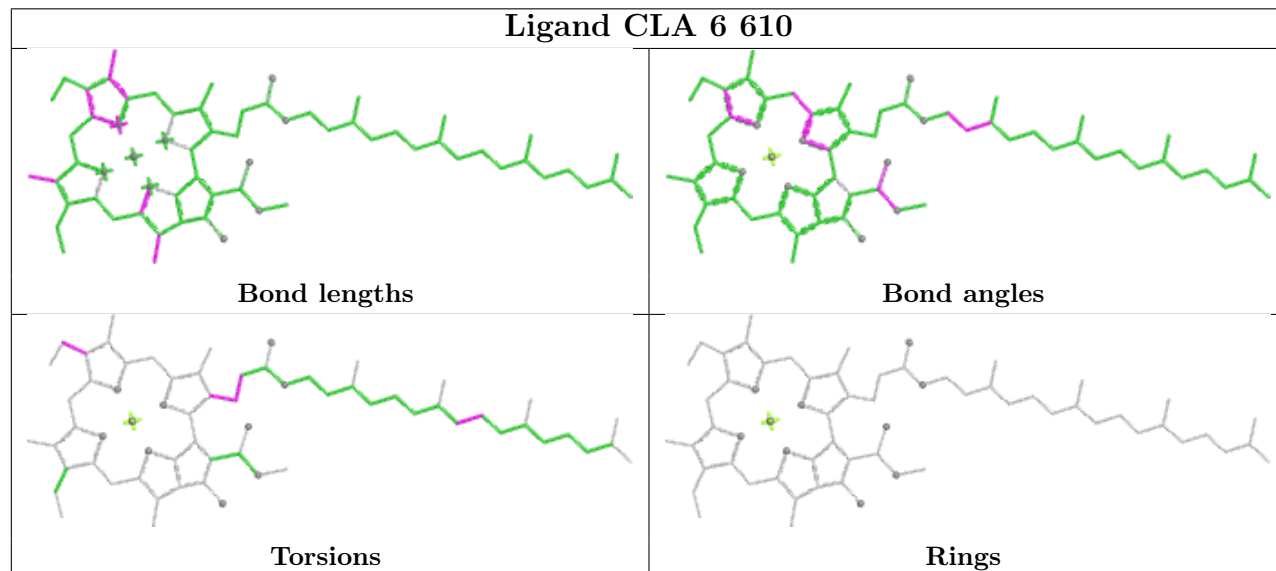
Ligand CLA y 602**Ligand CLA 1 602**

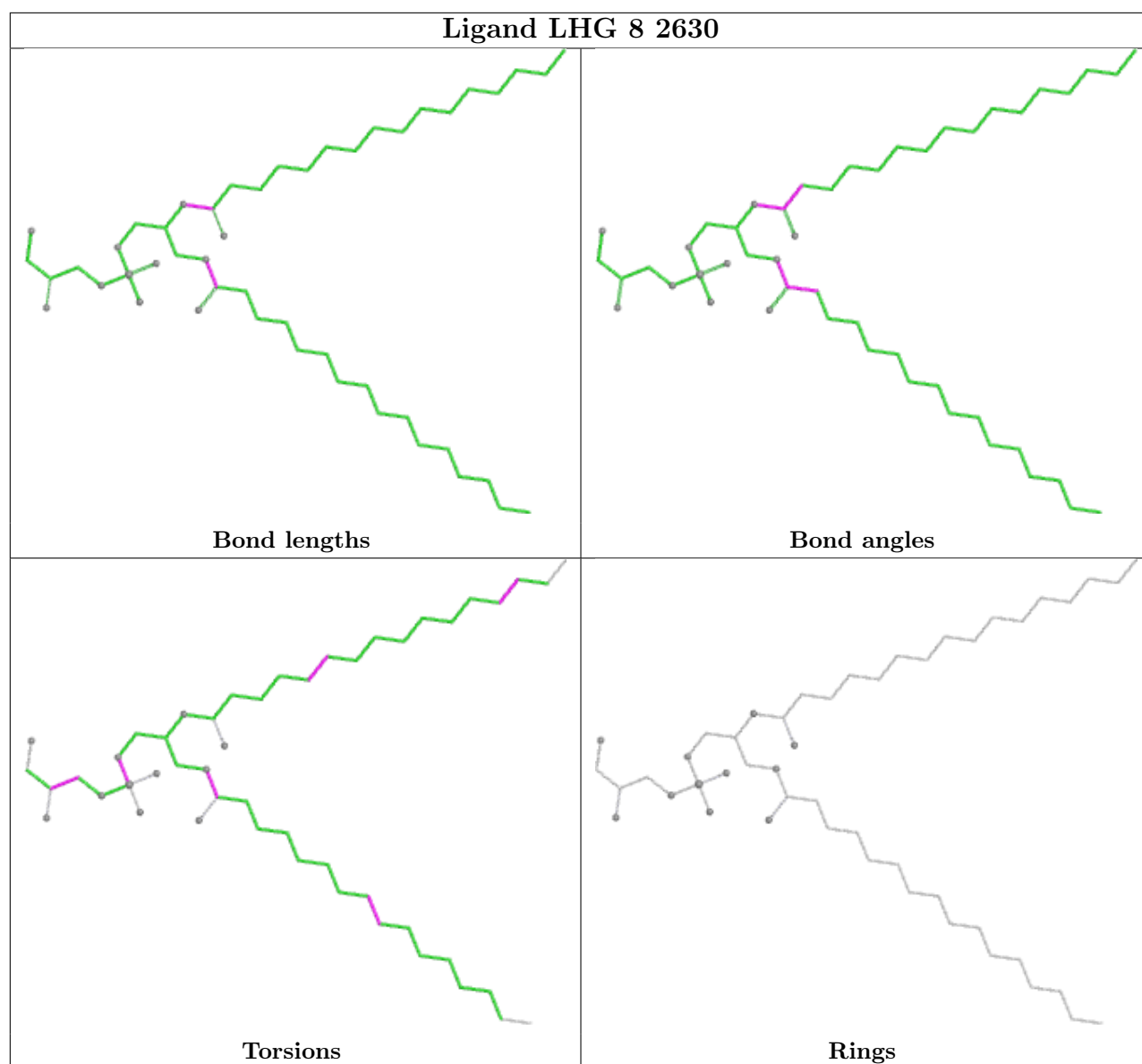


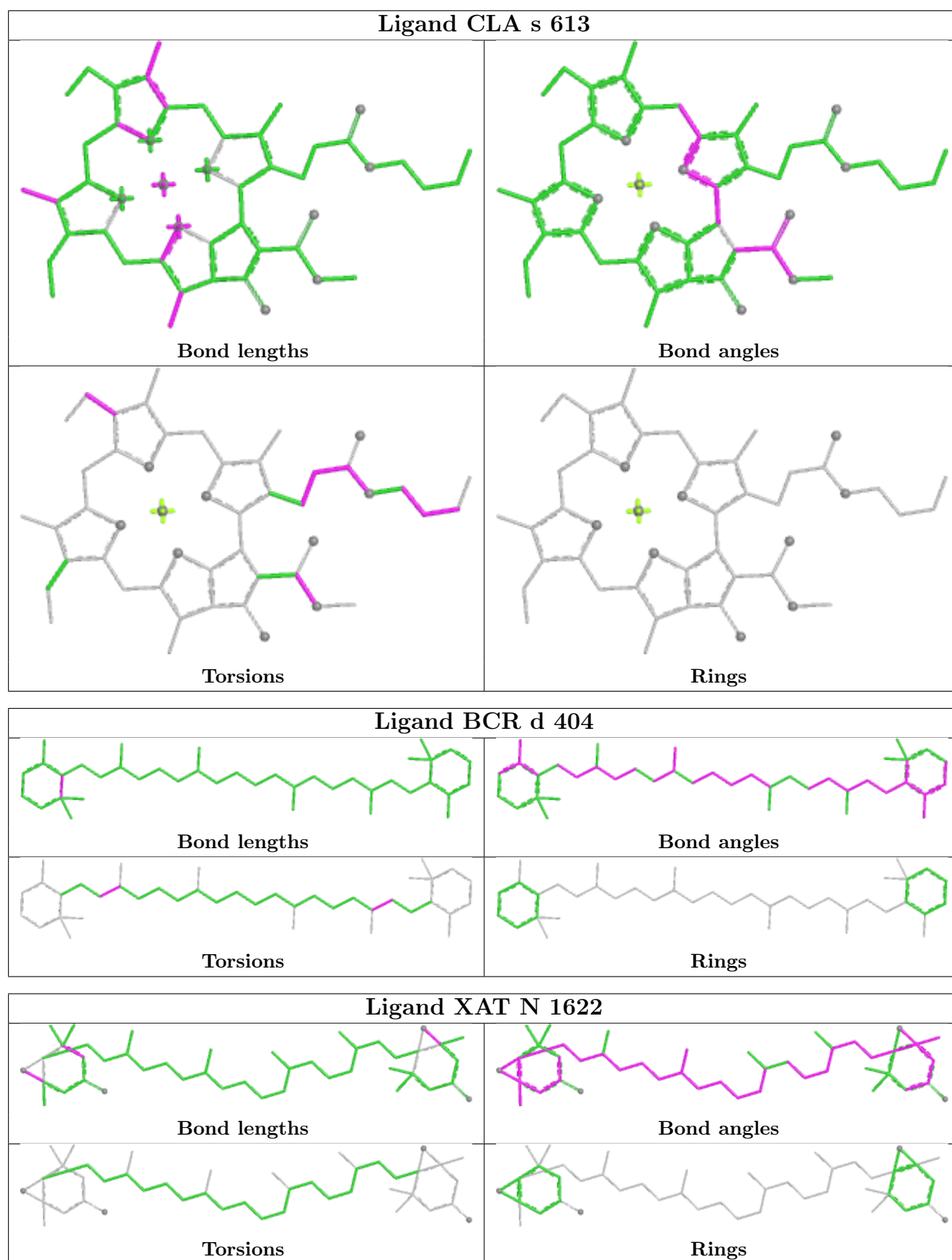
Ligand CHL R 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

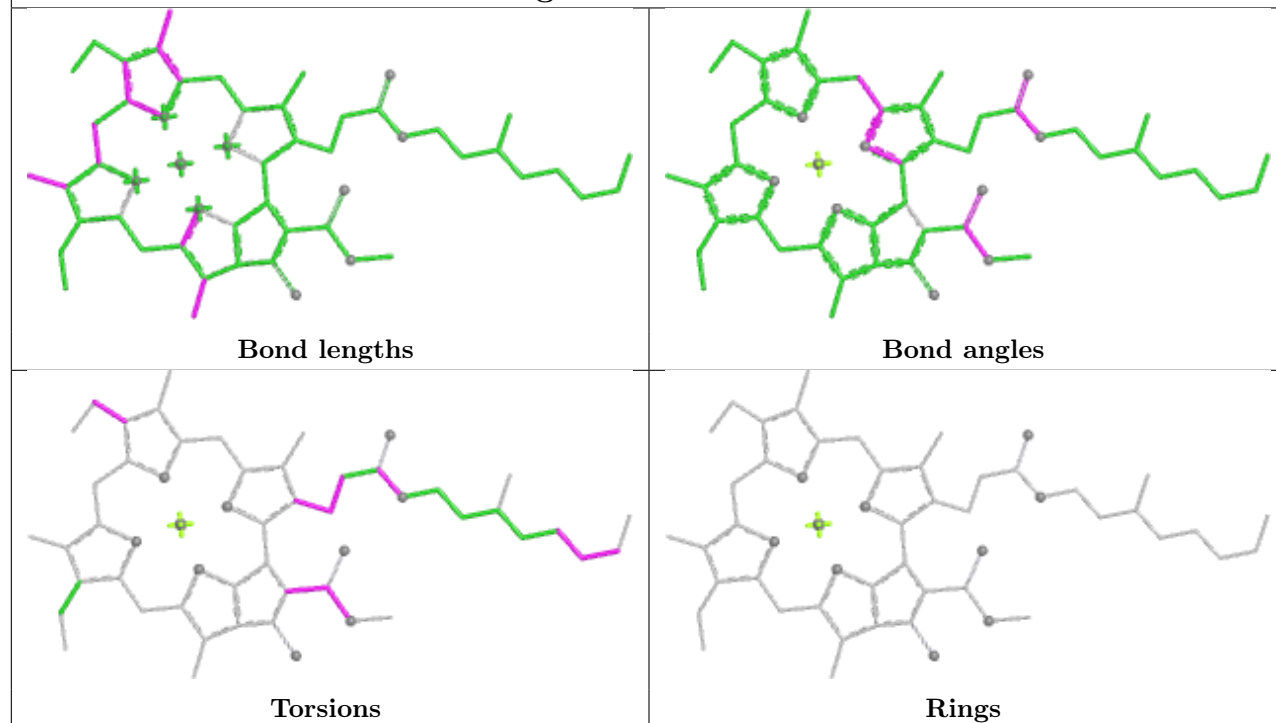
Ligand LUT 4 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 610**Ligand CLA 6 610**

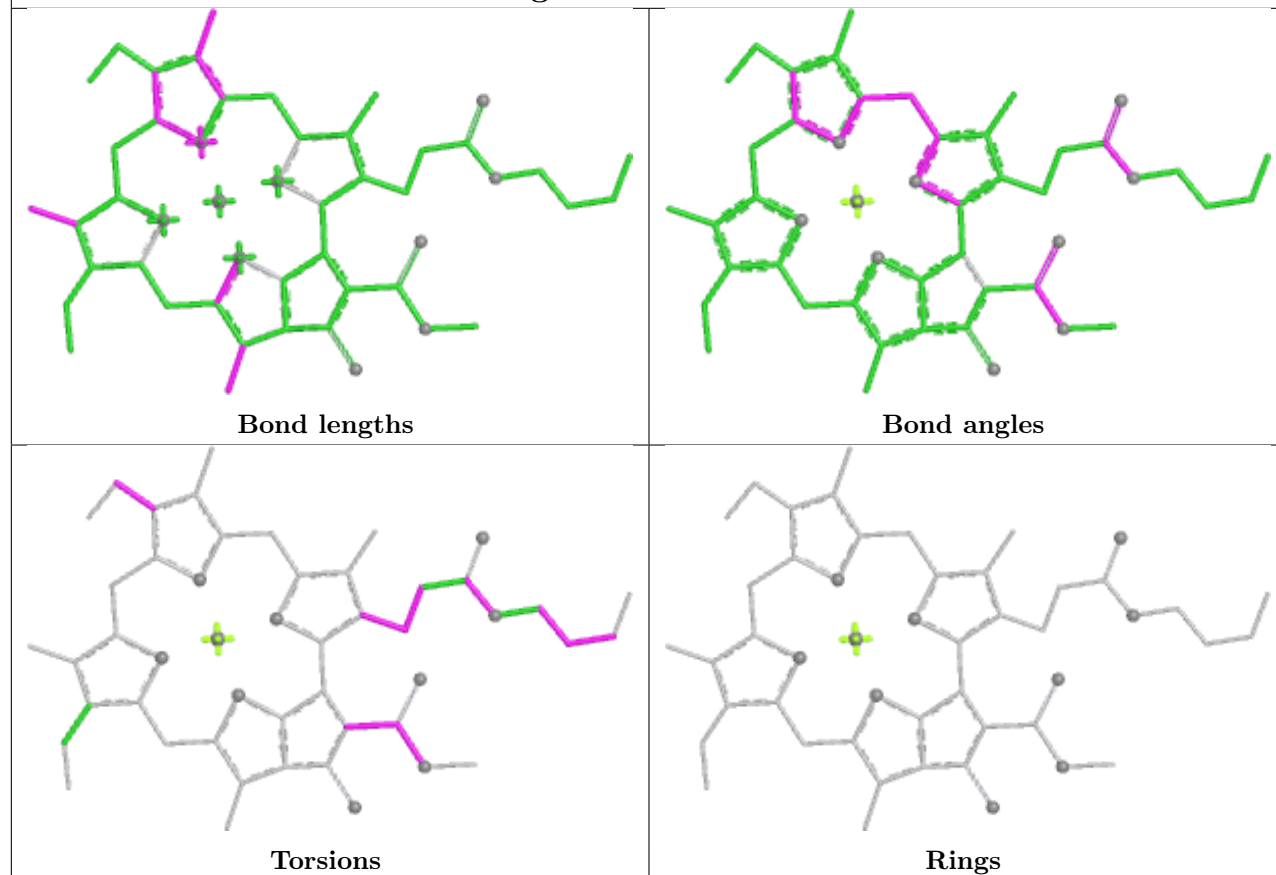




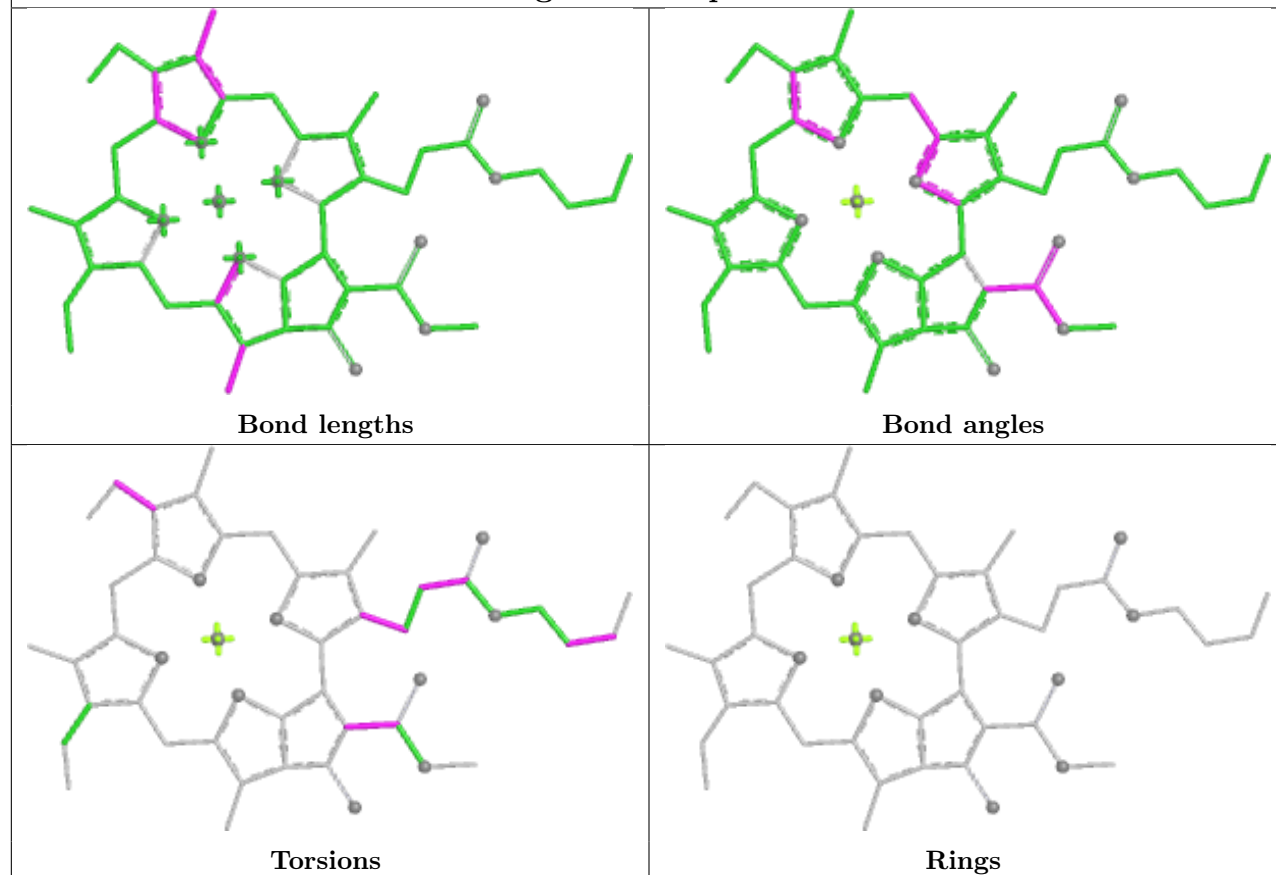
Ligand CLA 1 614



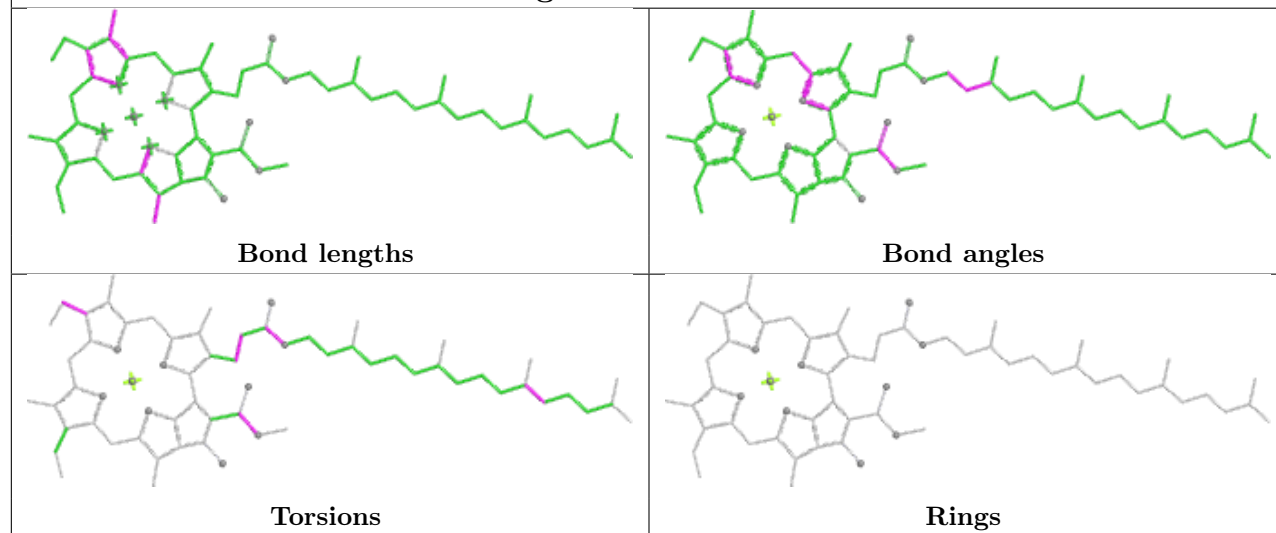
Ligand CLA G 614



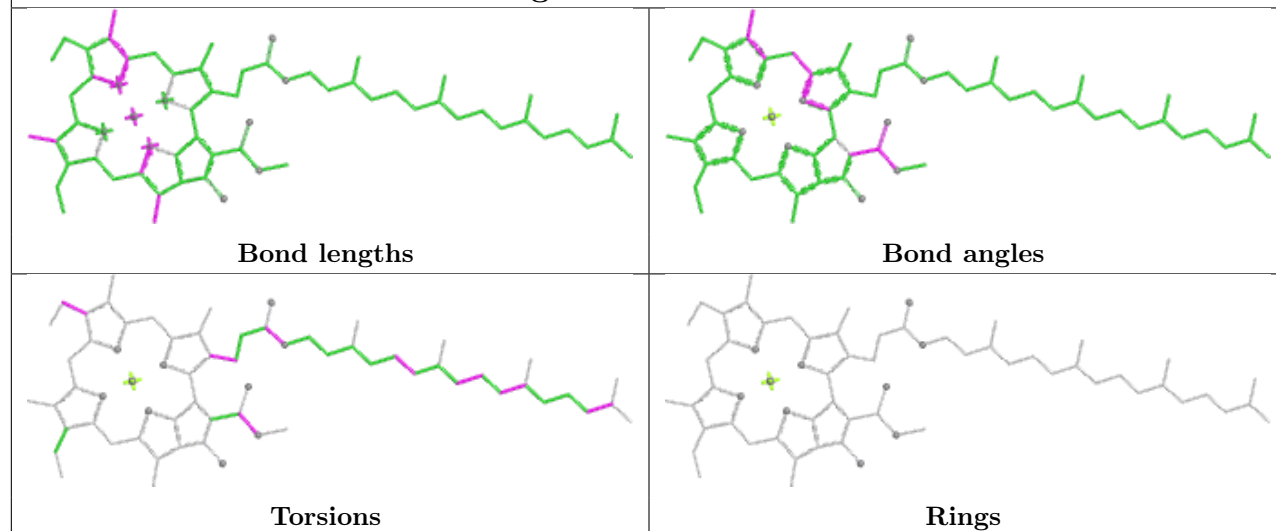
Ligand CLA p 611



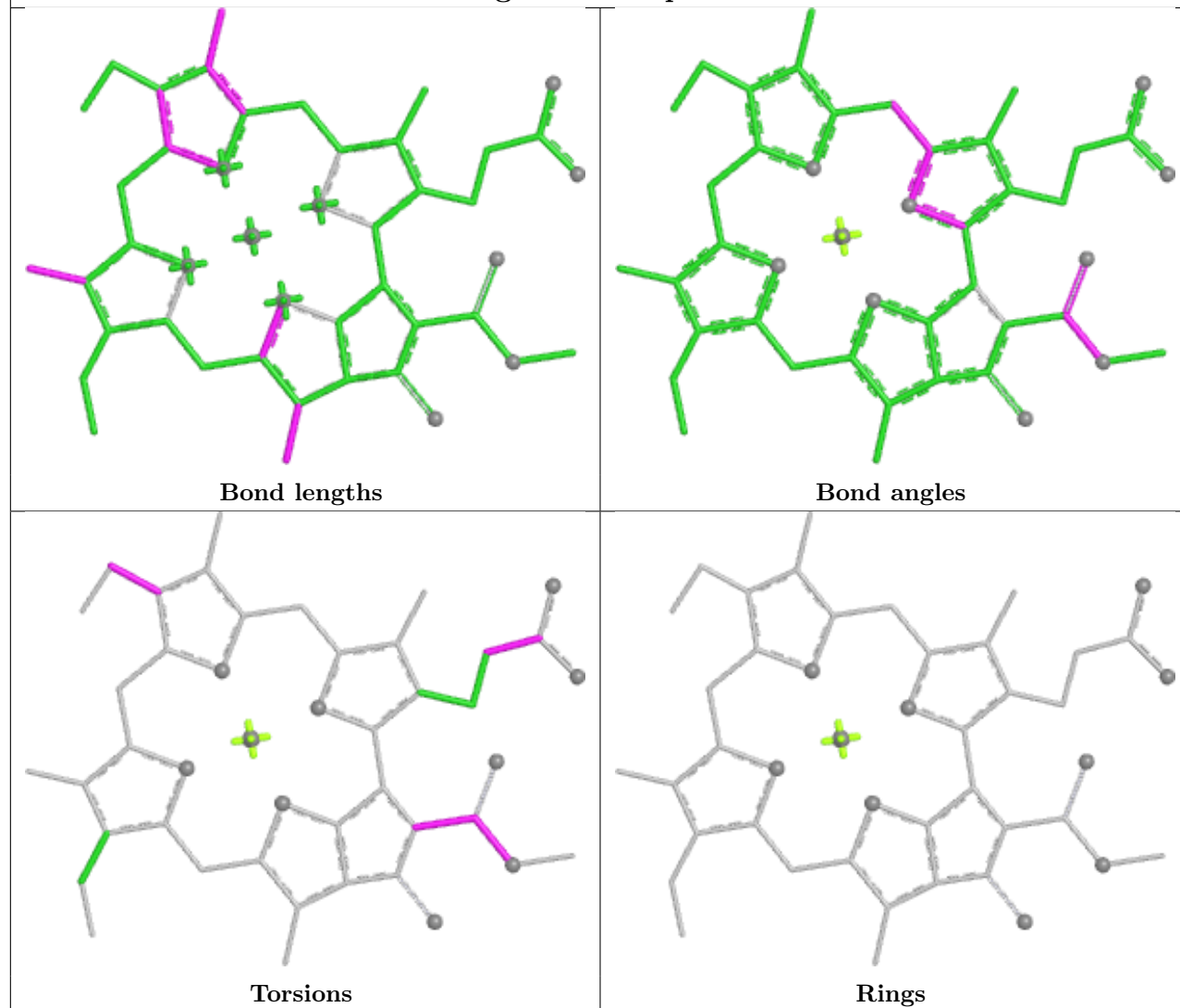
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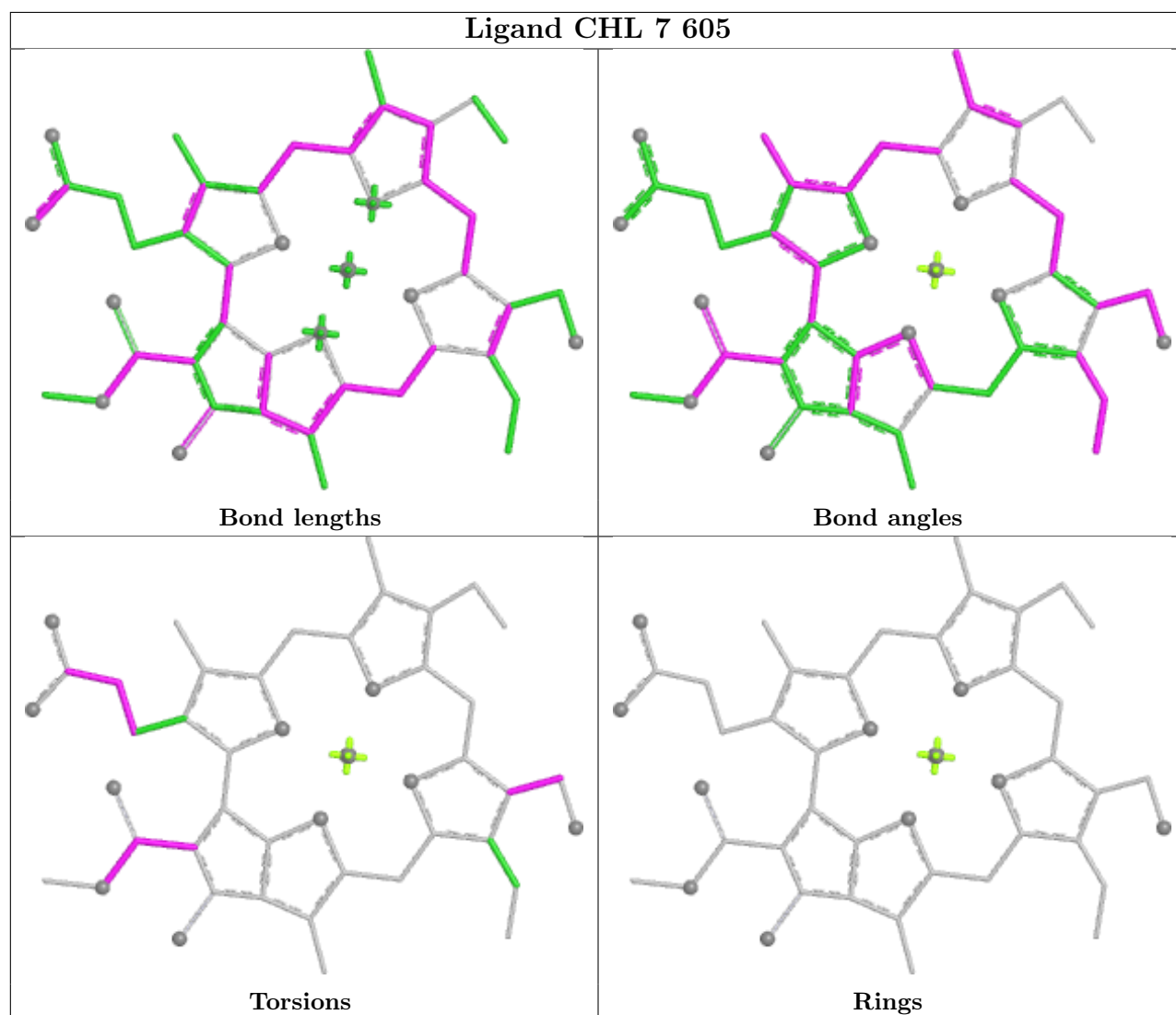
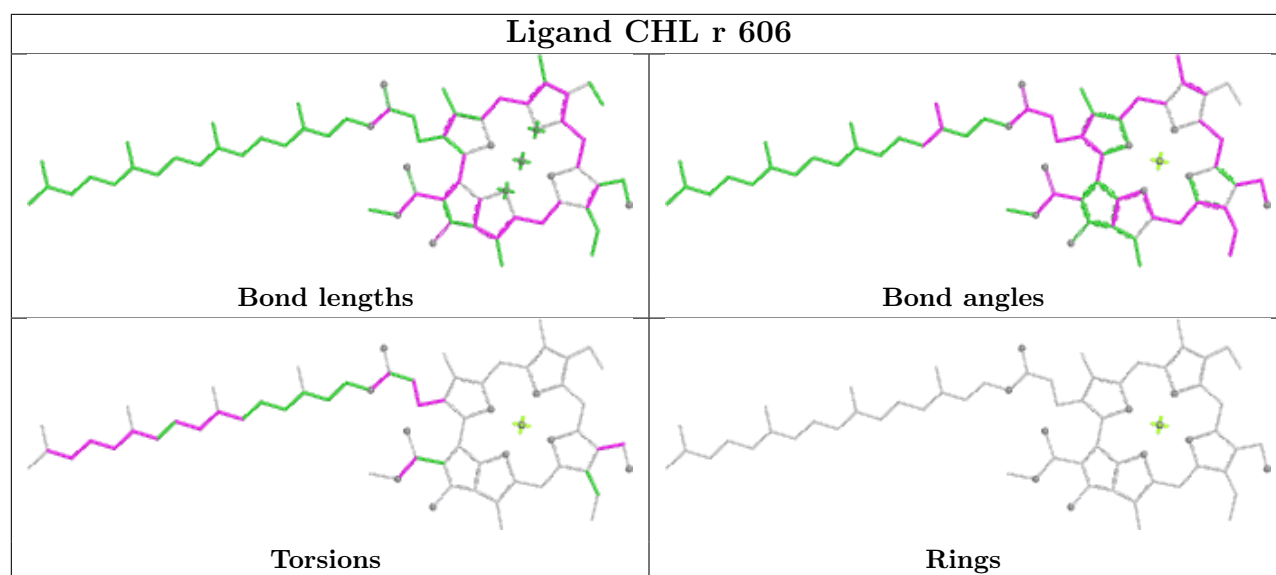


Ligand CLA D 403

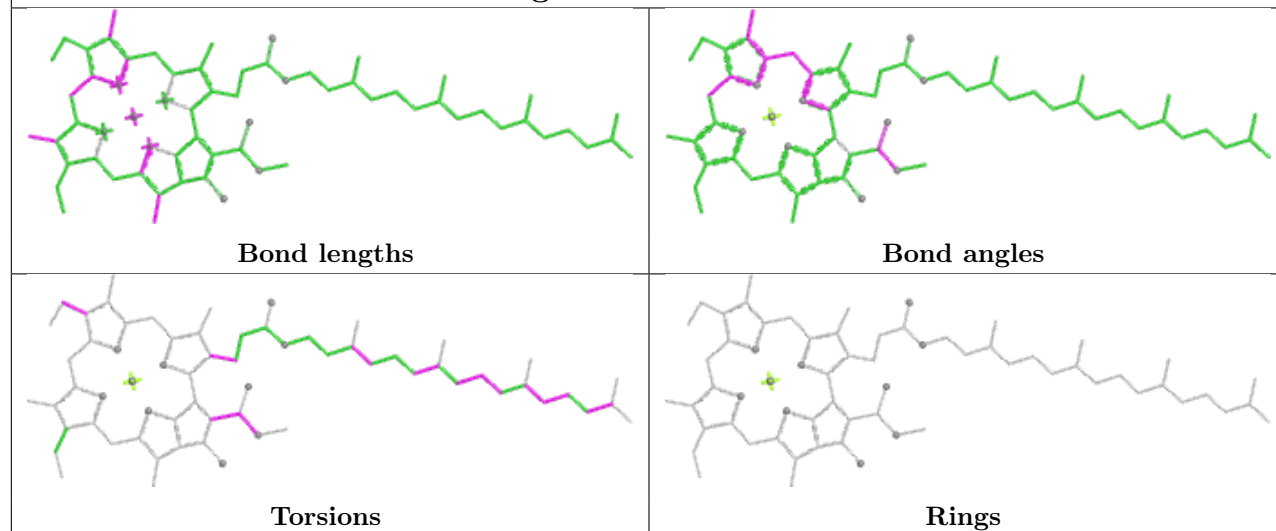


Ligand CLA q 611

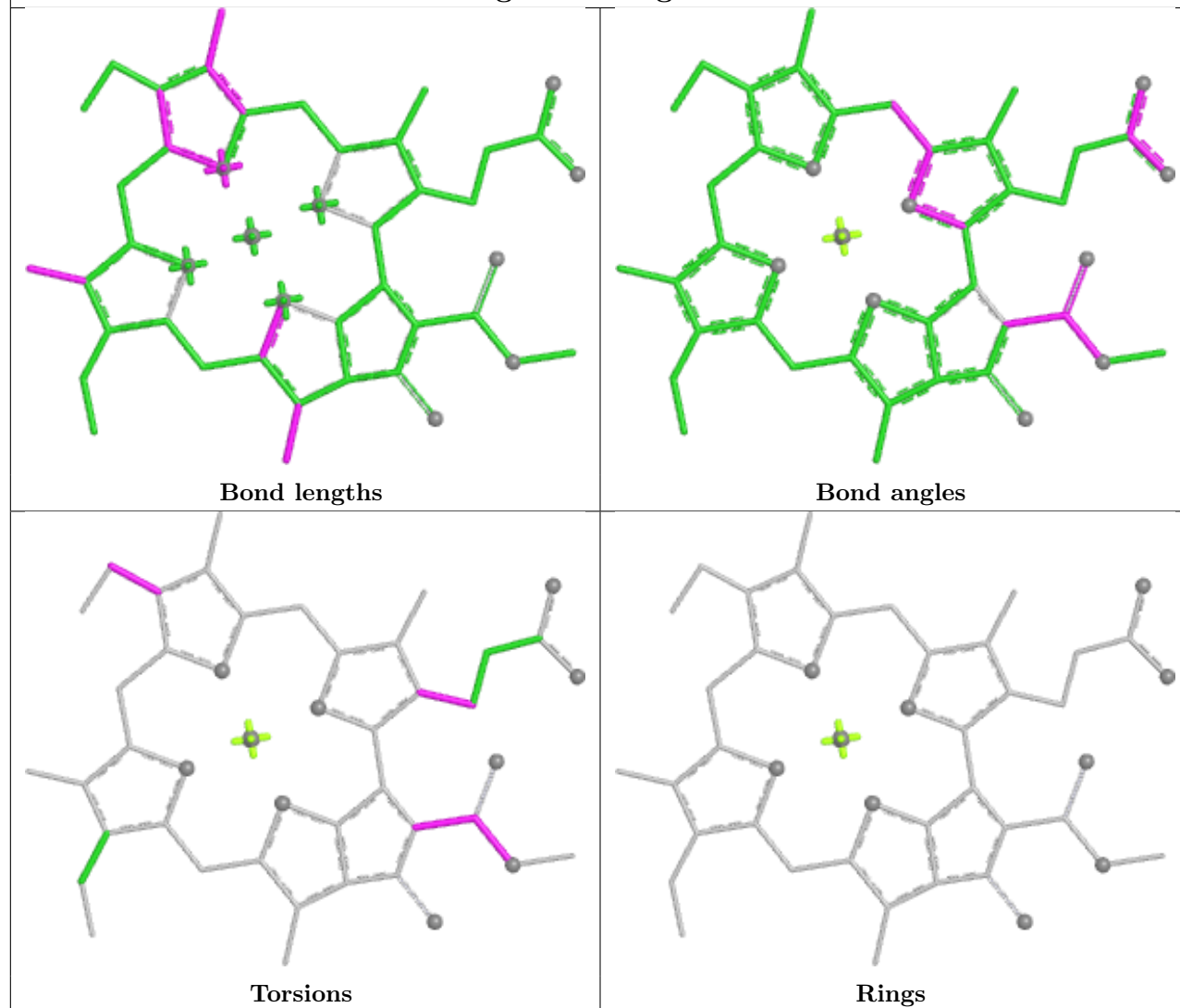




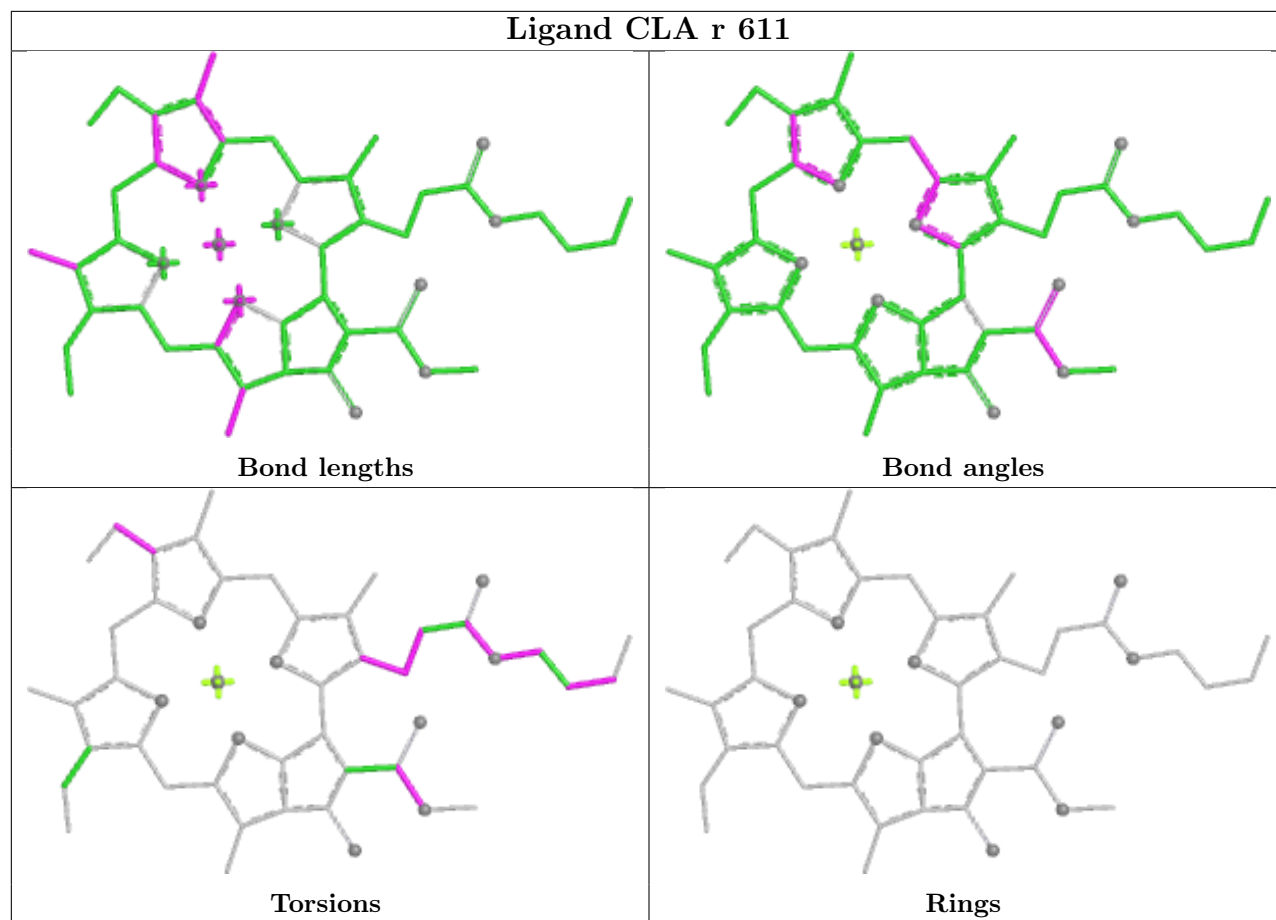
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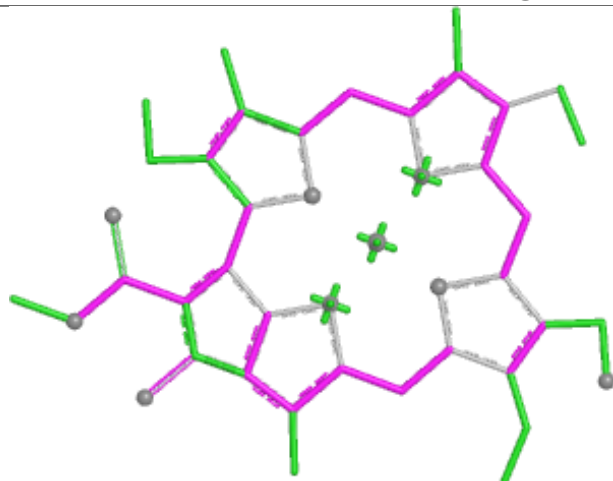
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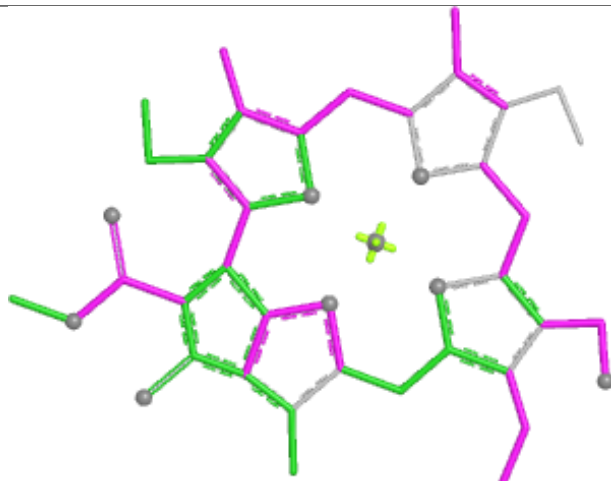
Ligand CLA r 611



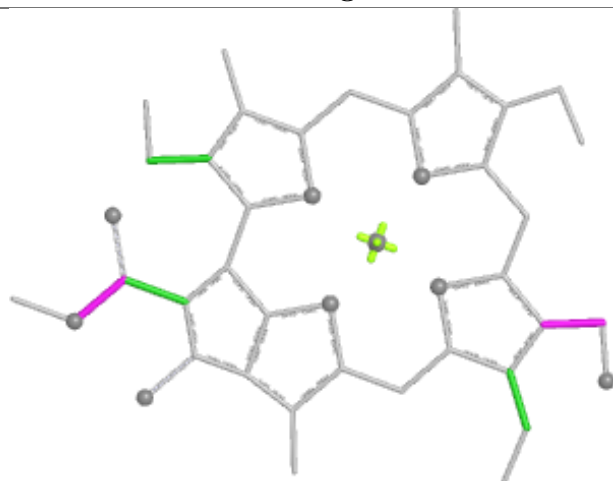
Ligand CHL S 607



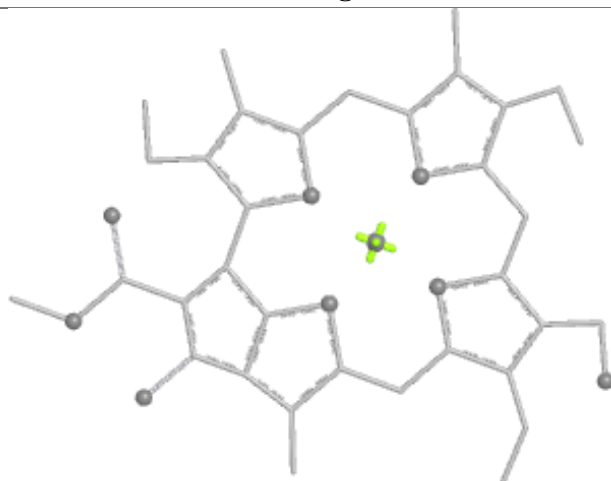
Bond lengths



Bond angles

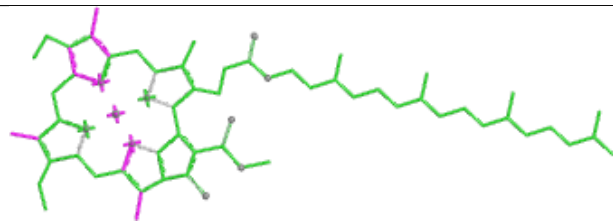


Torsions

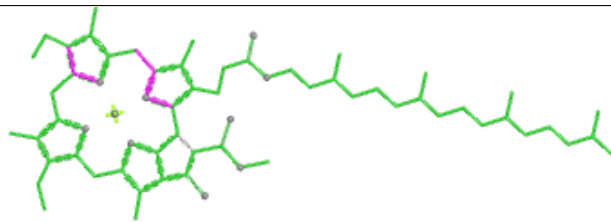


Rings

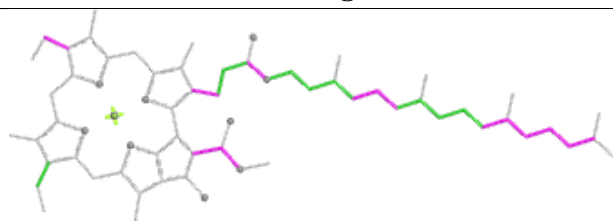
Ligand CLA b 602



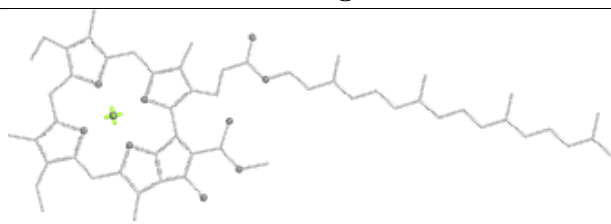
Bond lengths



Bond angles

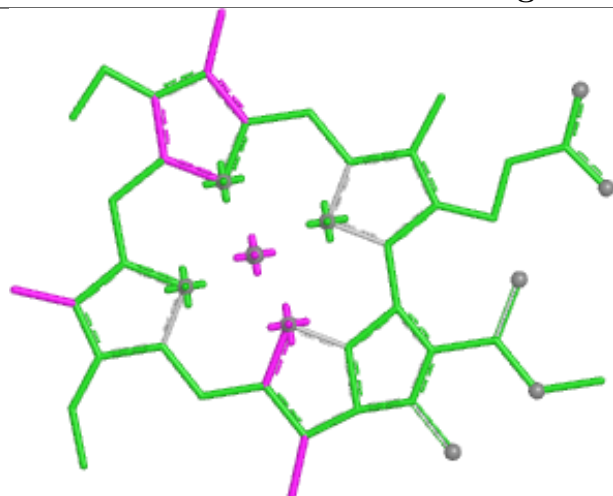


Torsions

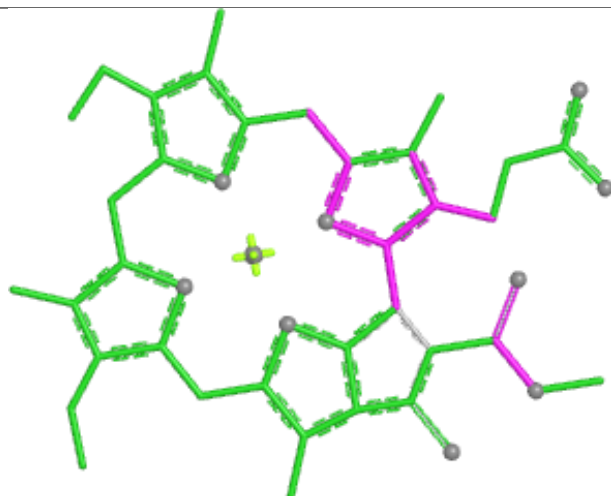


Rings

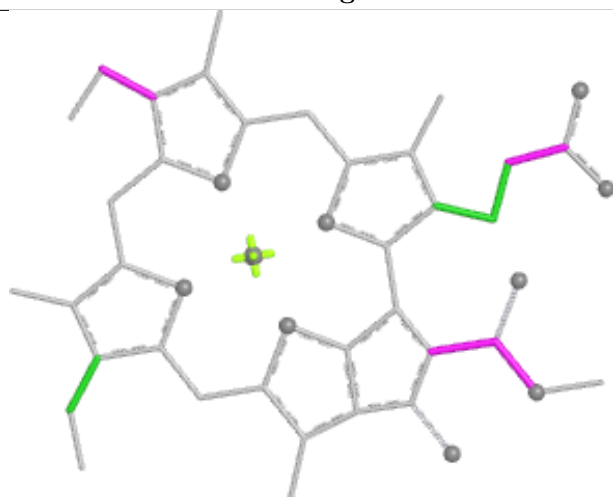
Ligand CLA n 612



Bond lengths



Bond angles

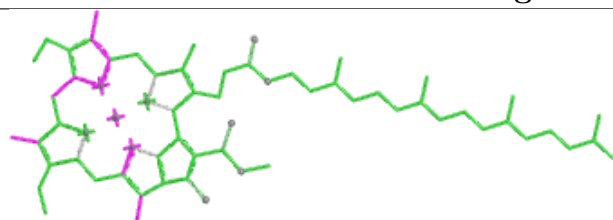


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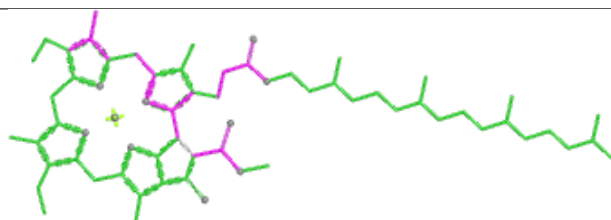


Rings

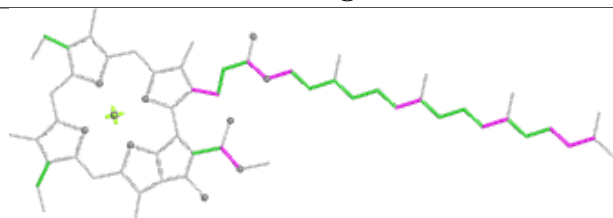
Ligand CLA C 511



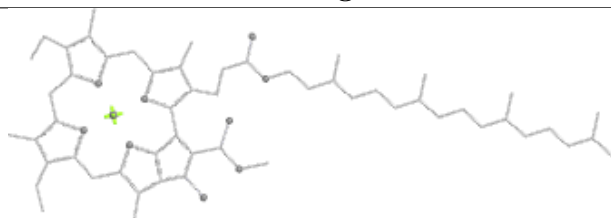
Bond lengths



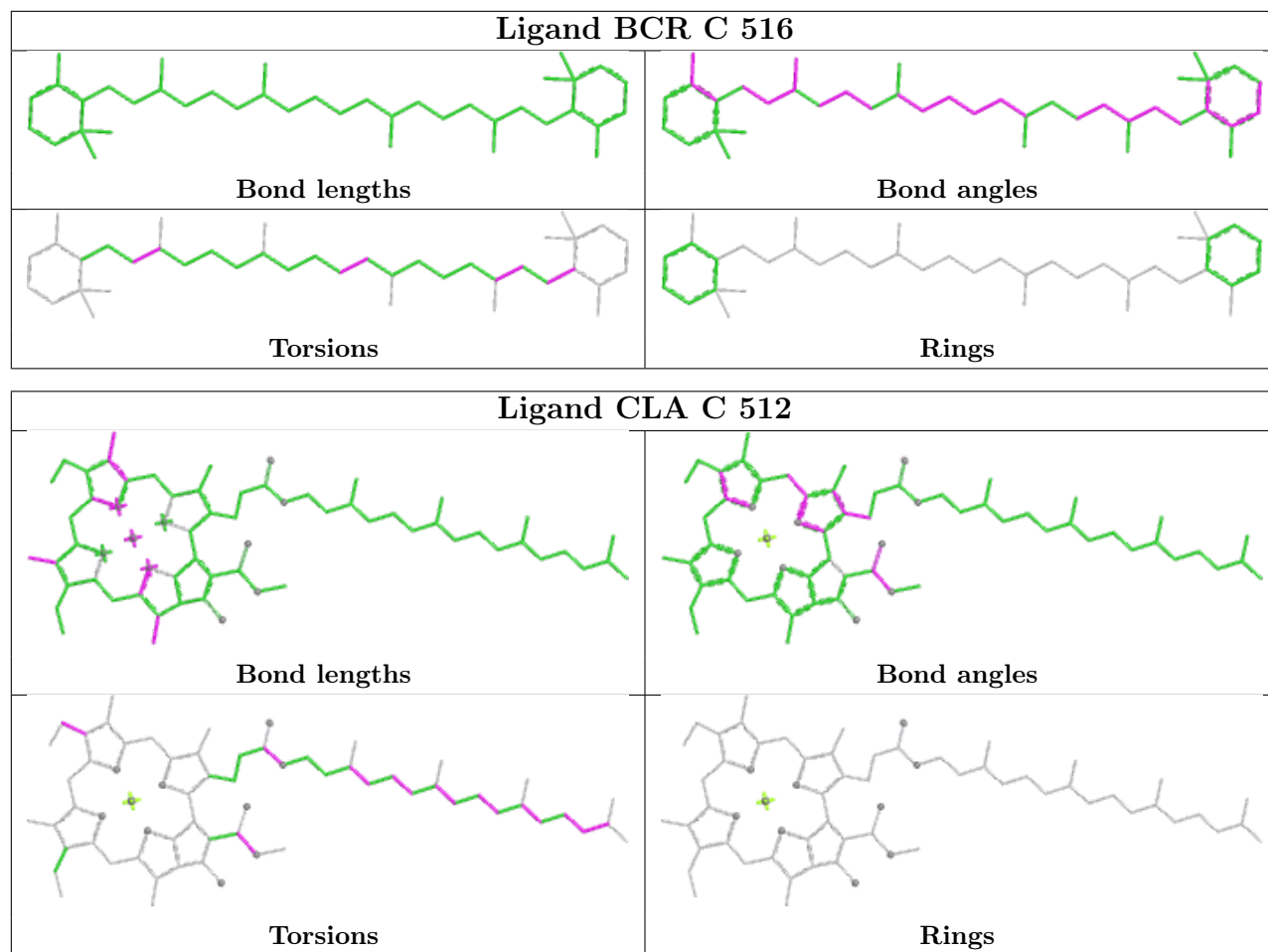
Bond angles

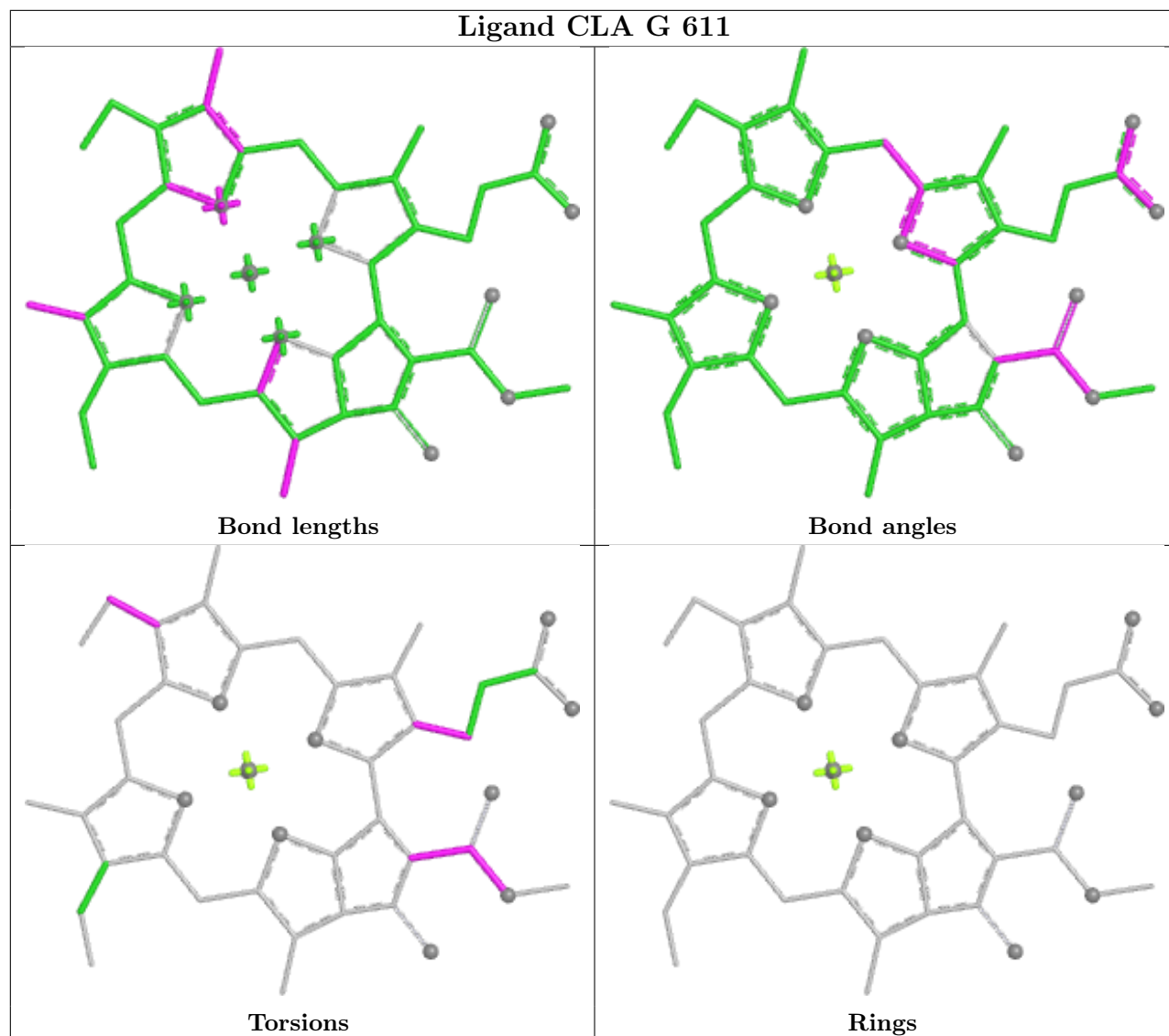


Torsions

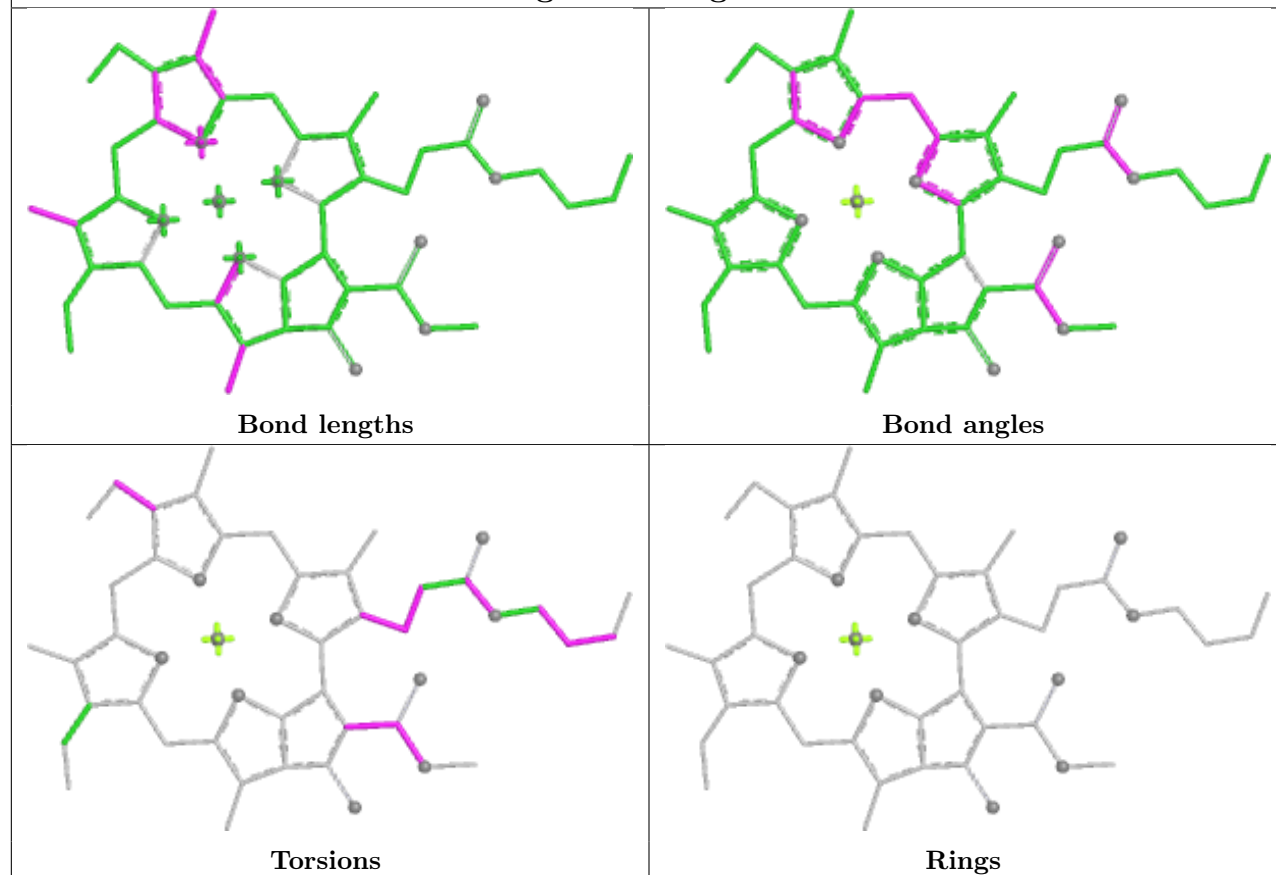


Rings

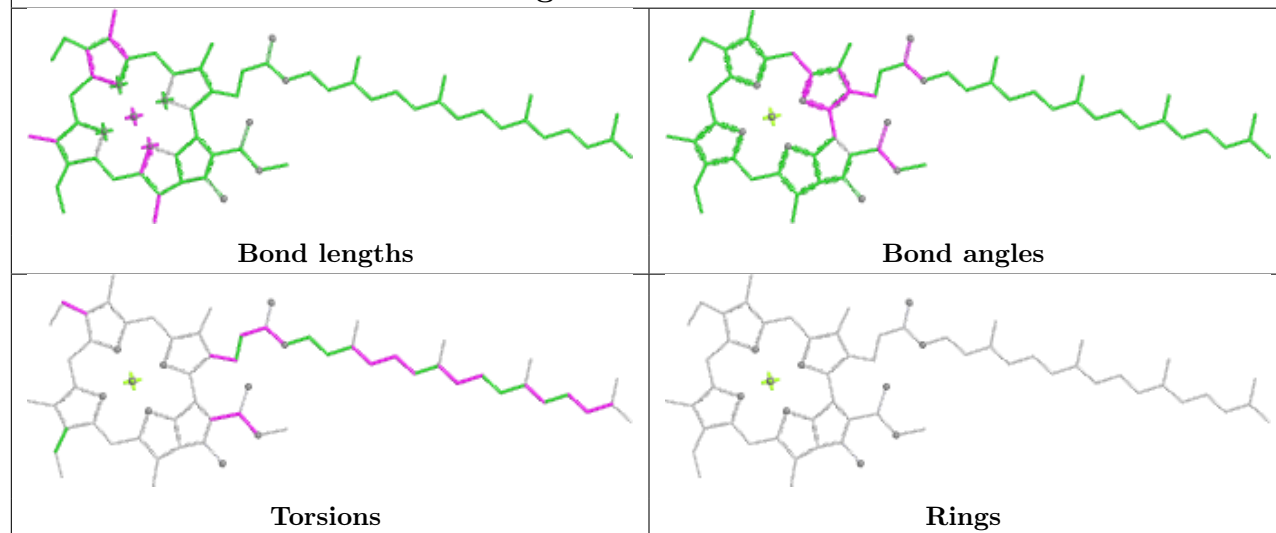


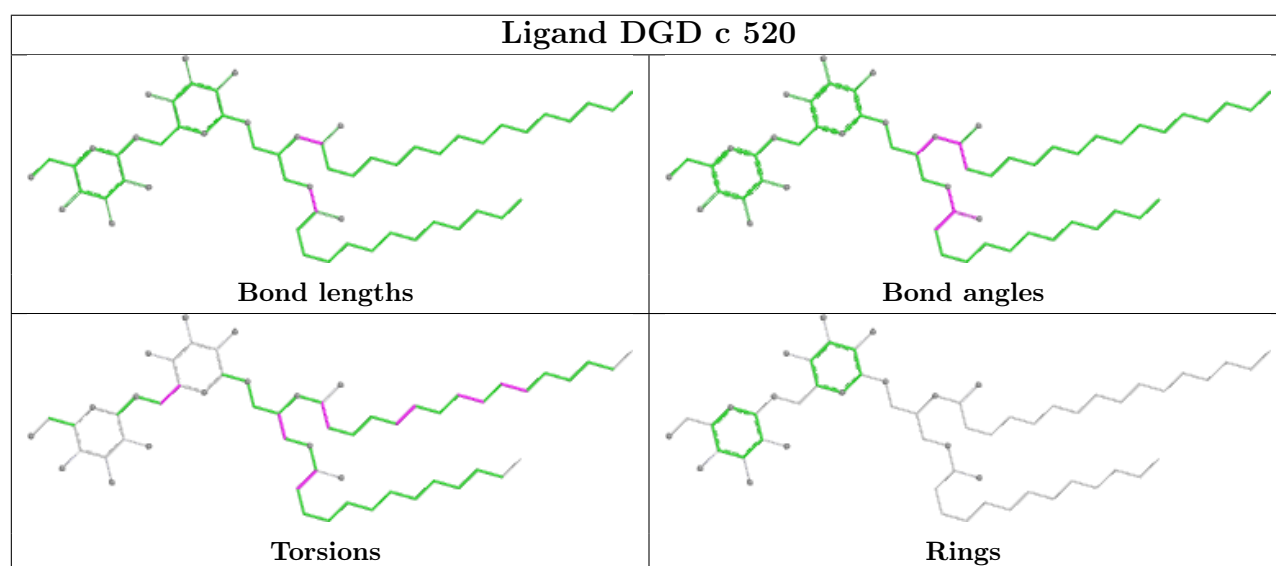
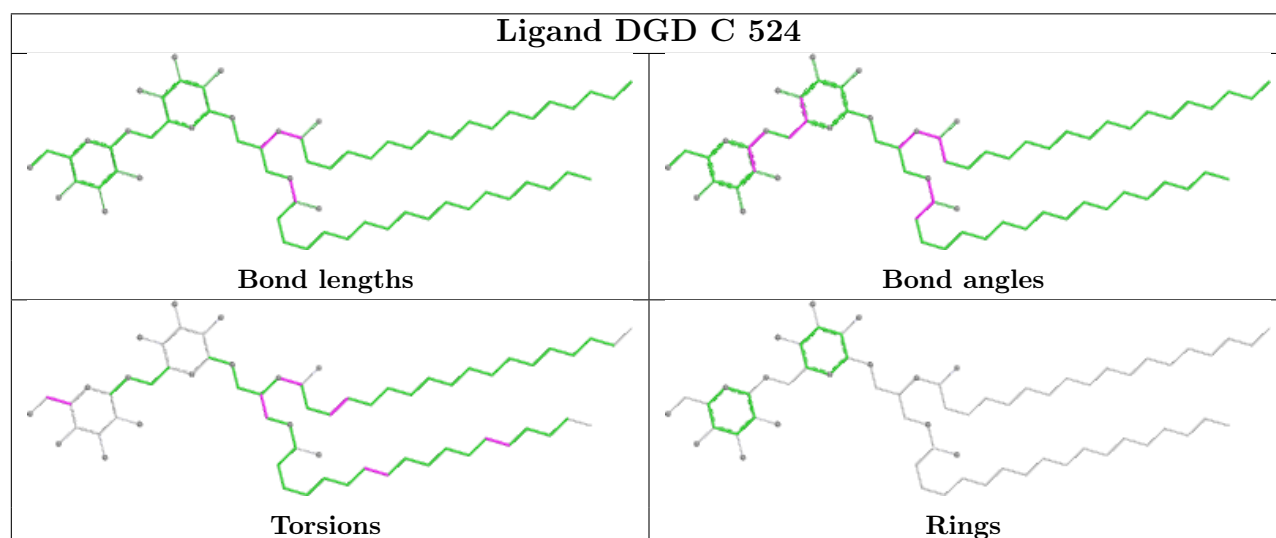
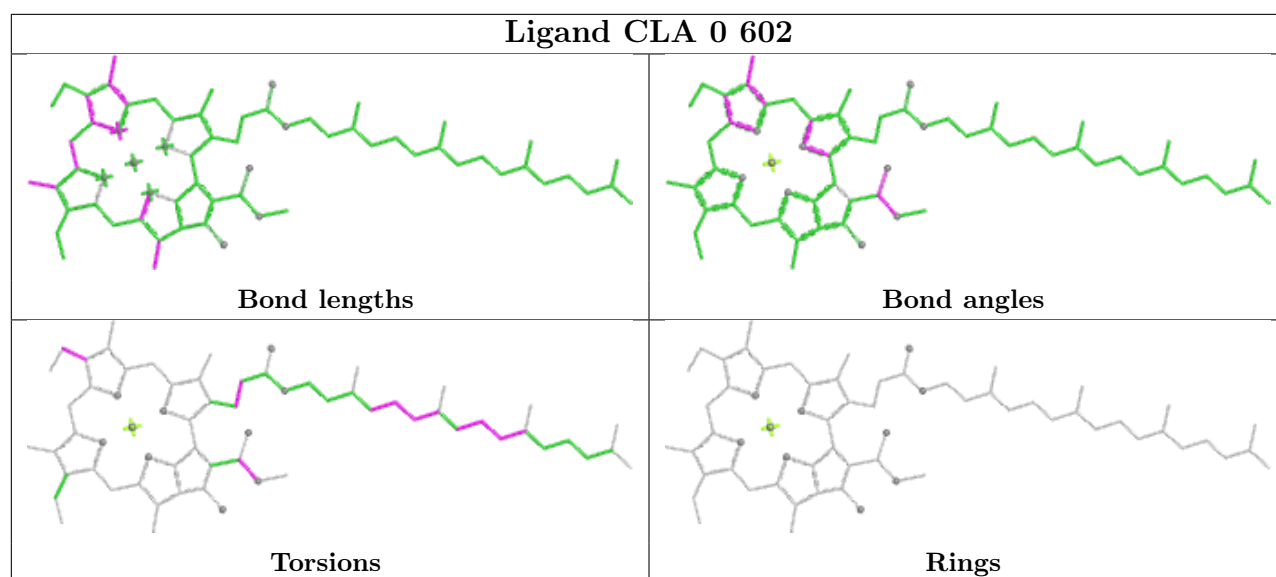


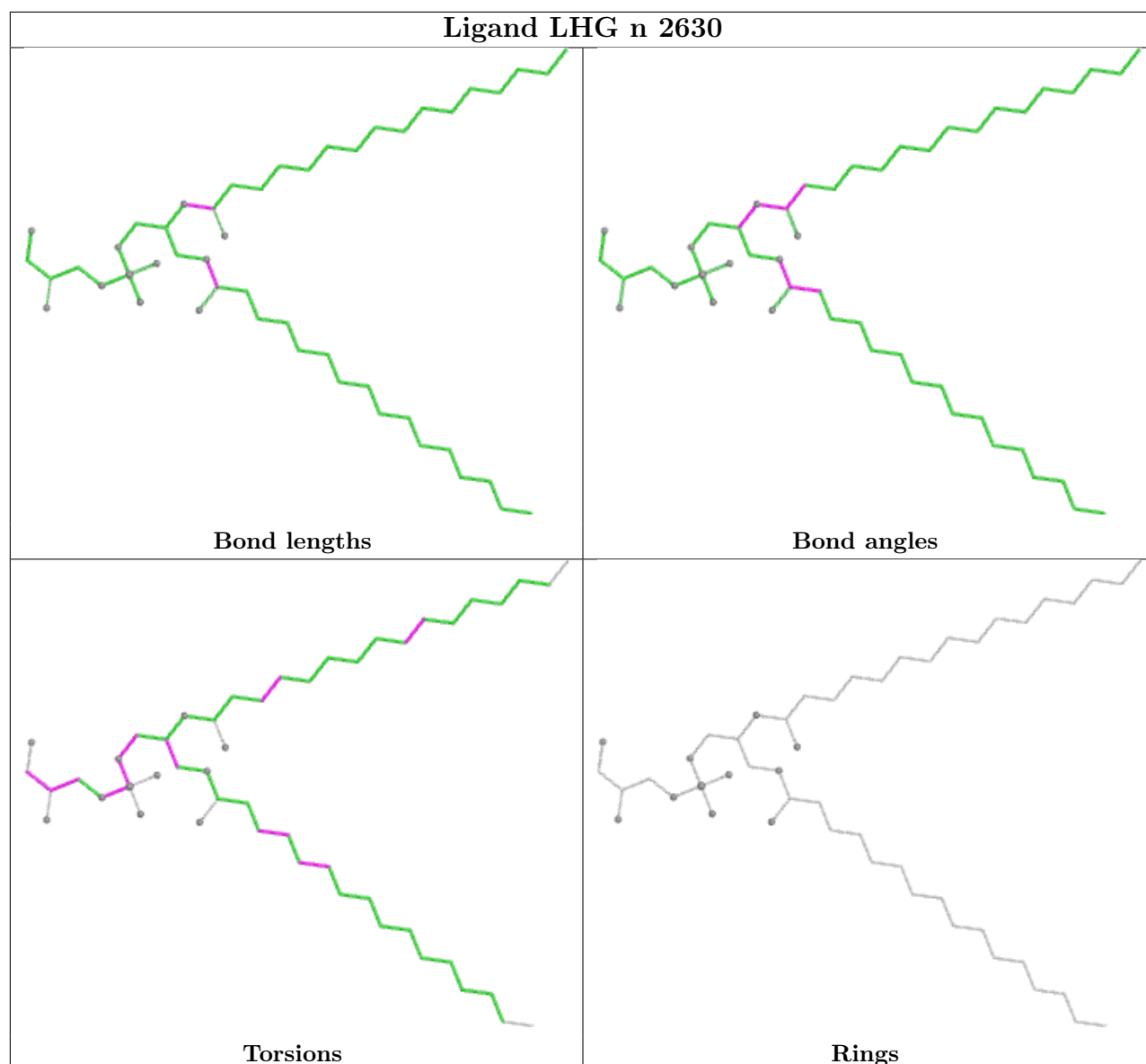
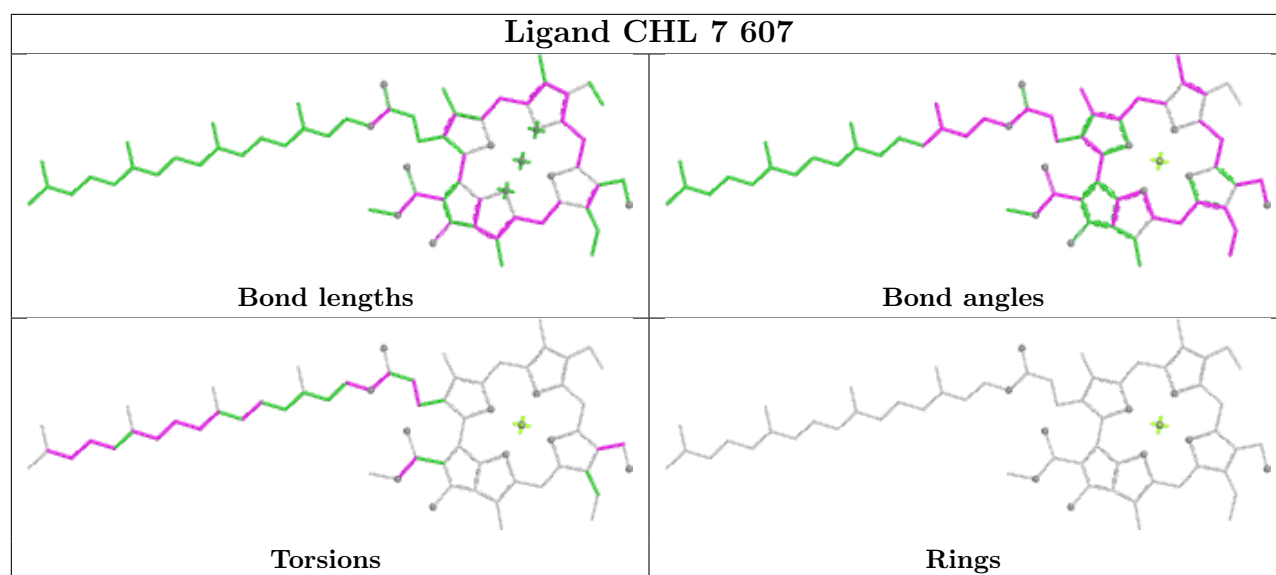
Ligand CLA g 614

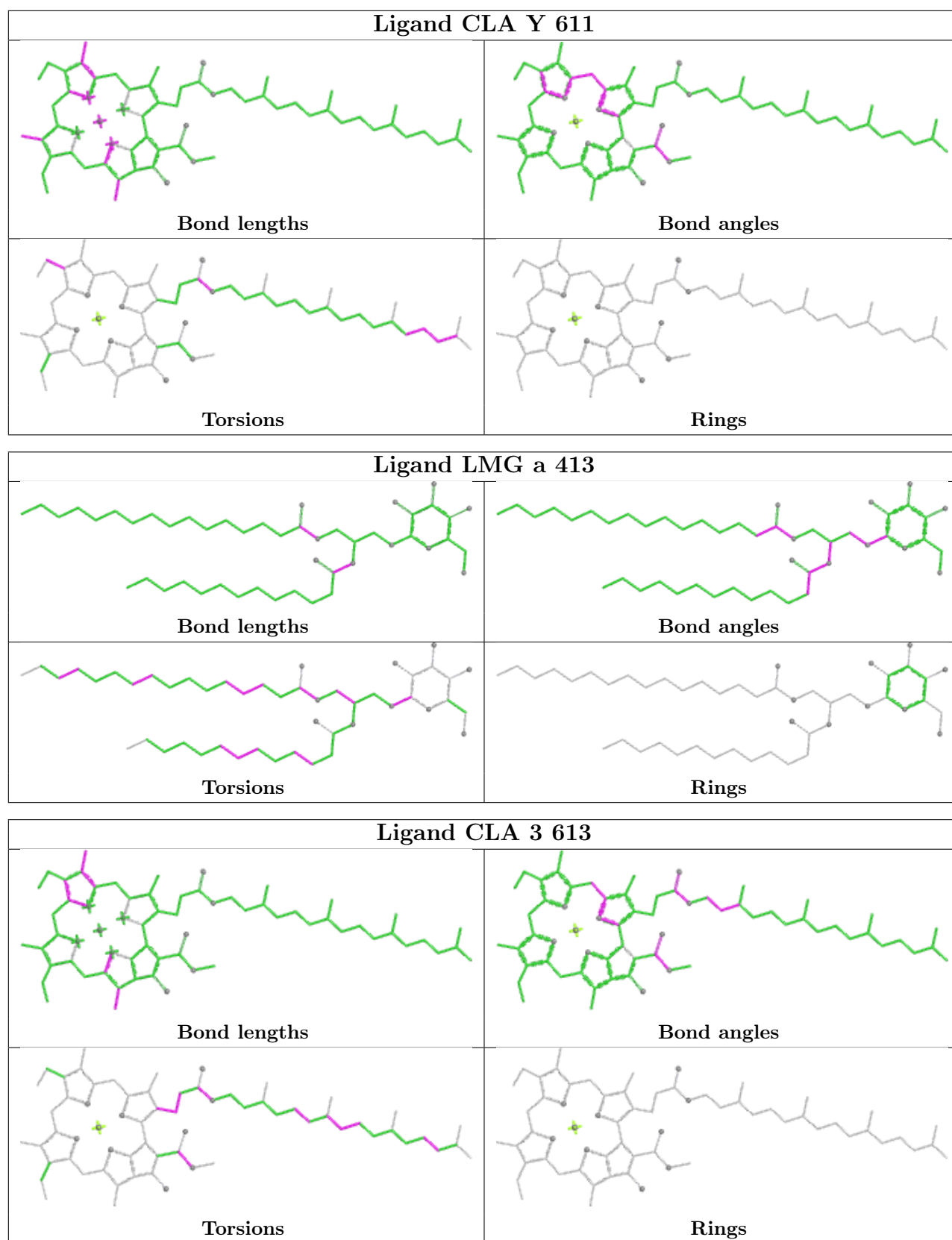


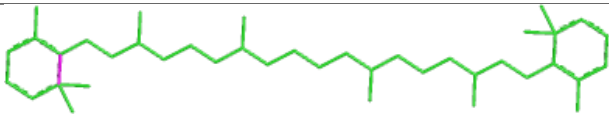
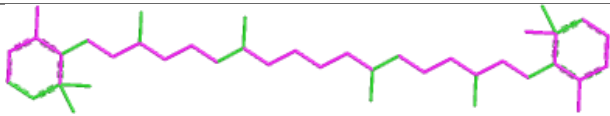
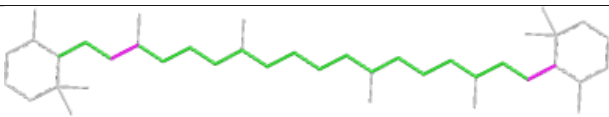
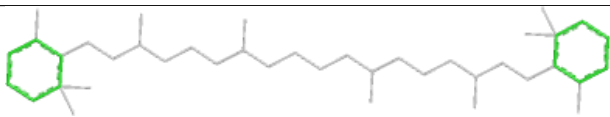
Ligand CLA 2 603

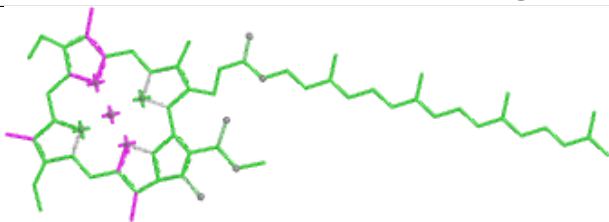
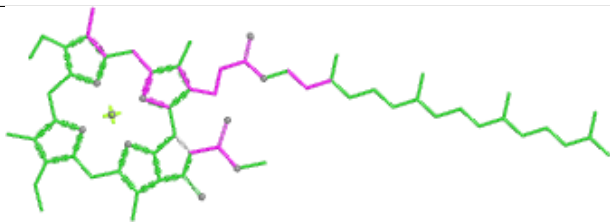
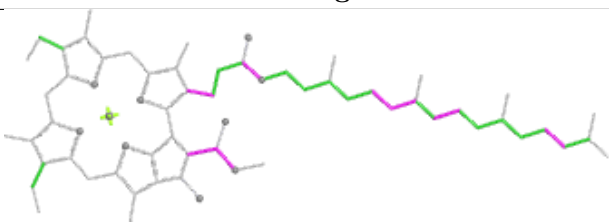
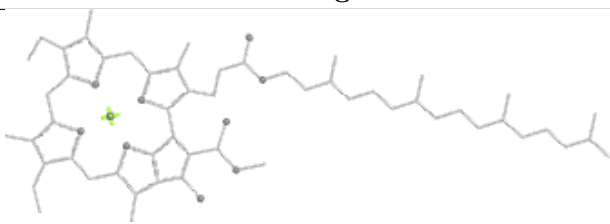


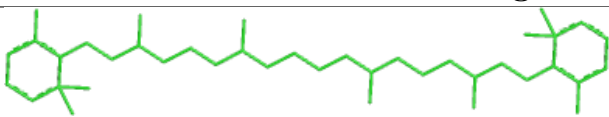
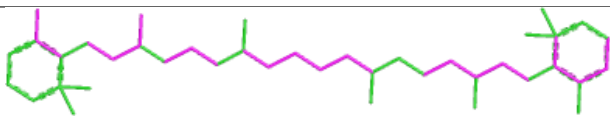
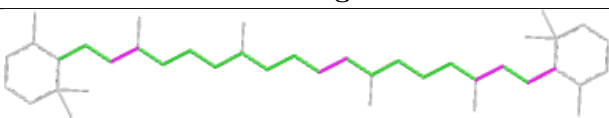
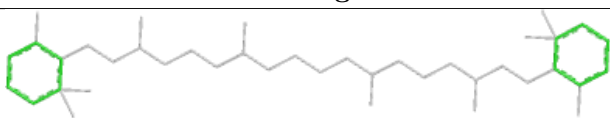


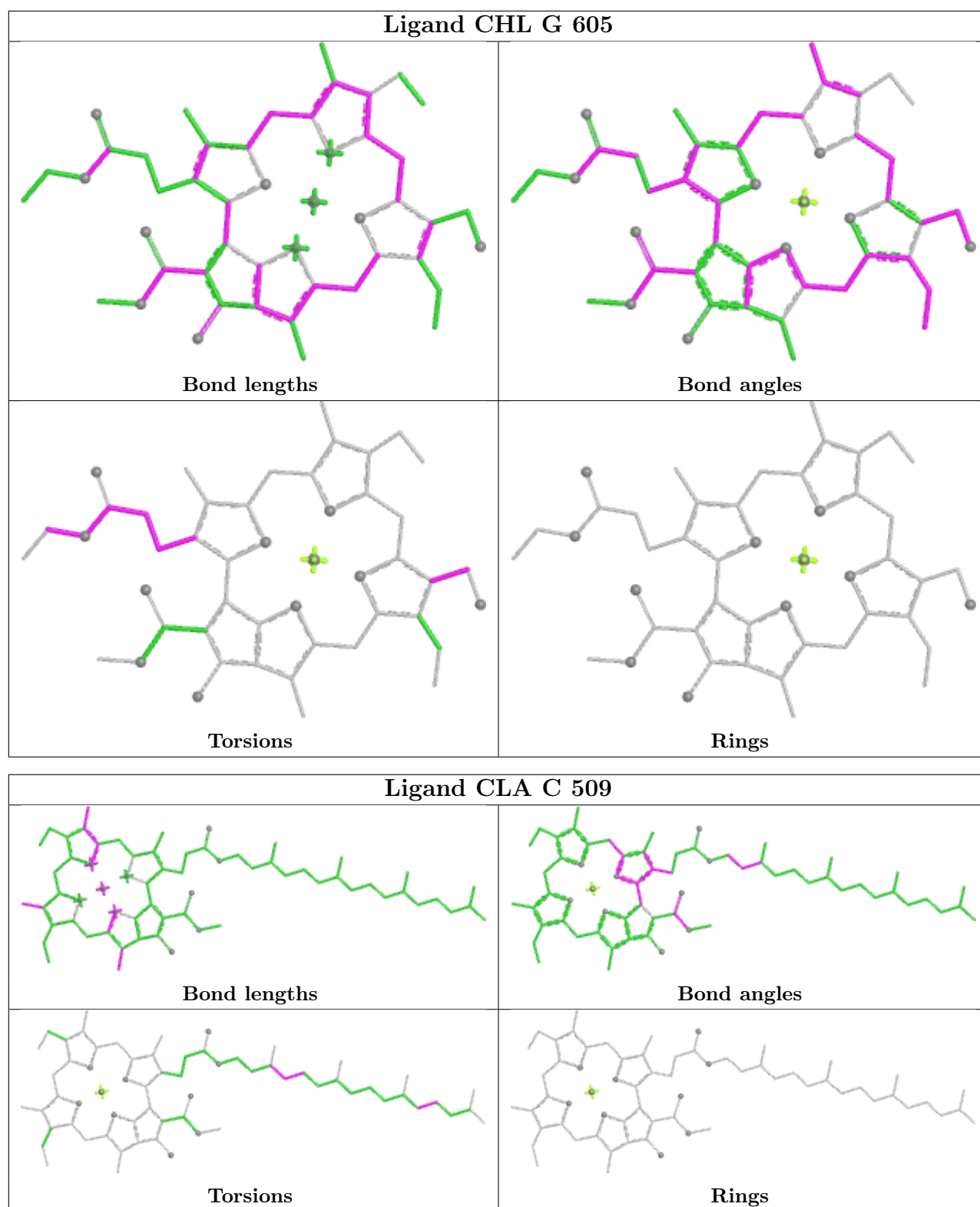


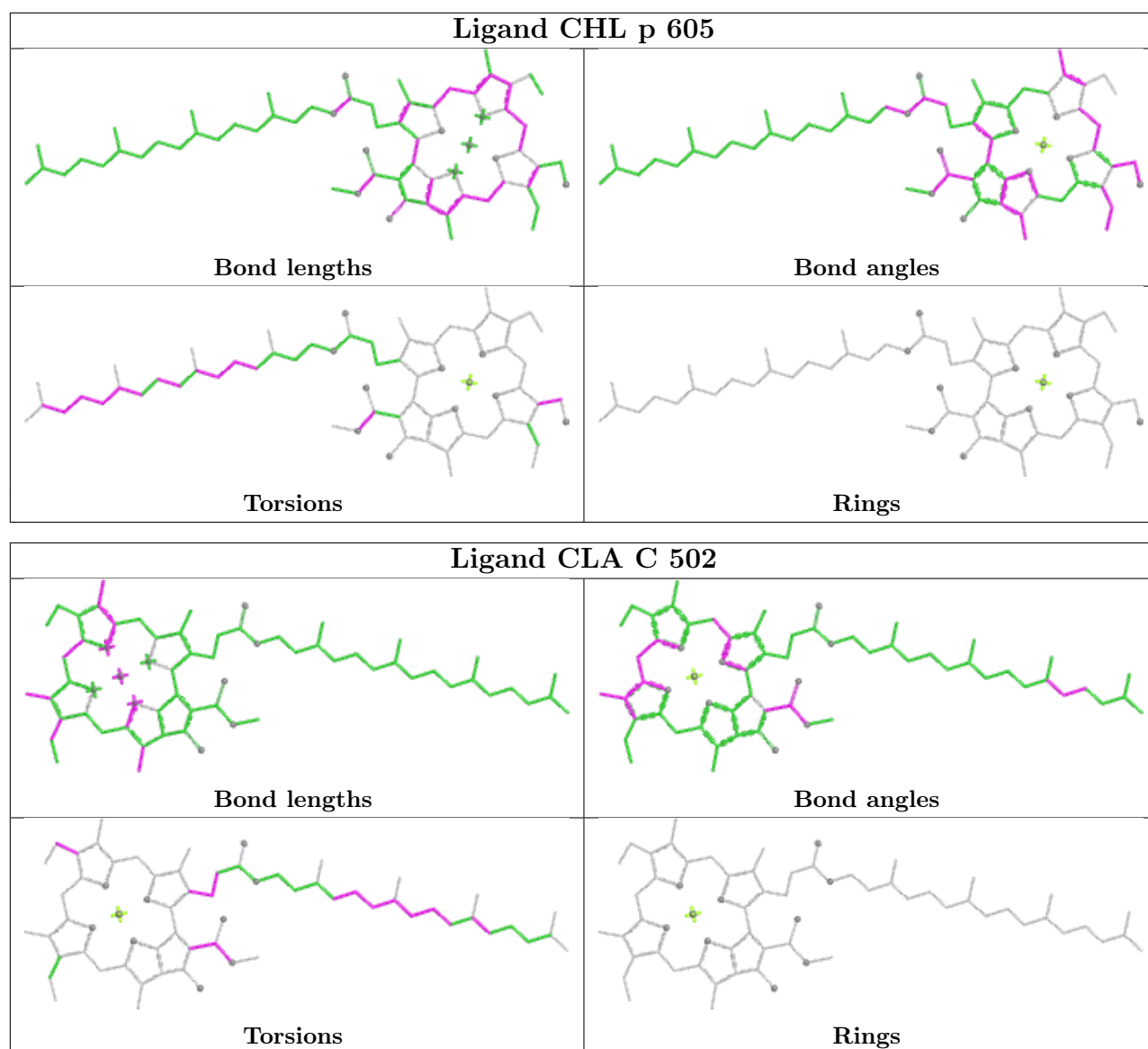


Ligand BCR B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

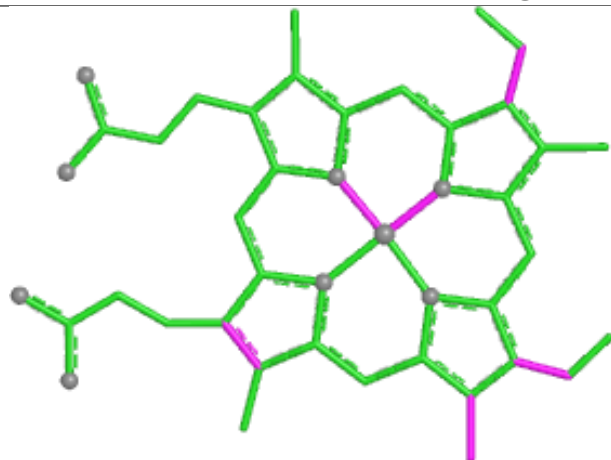
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

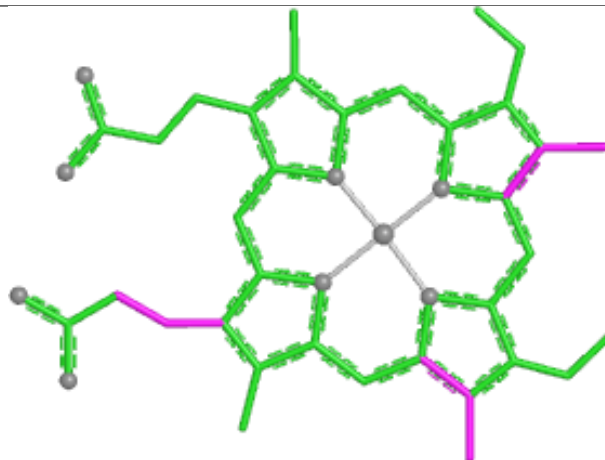




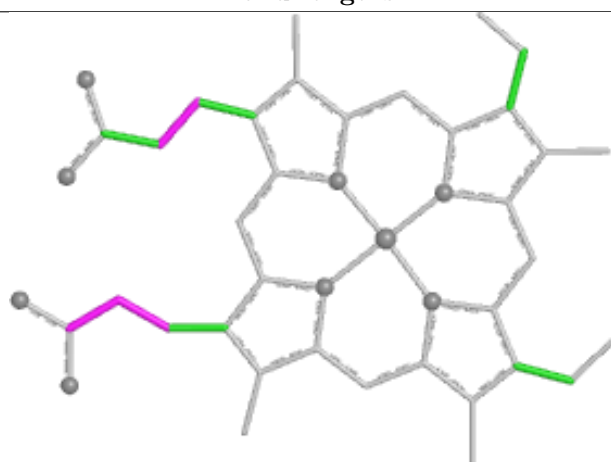
Ligand HEM f 101



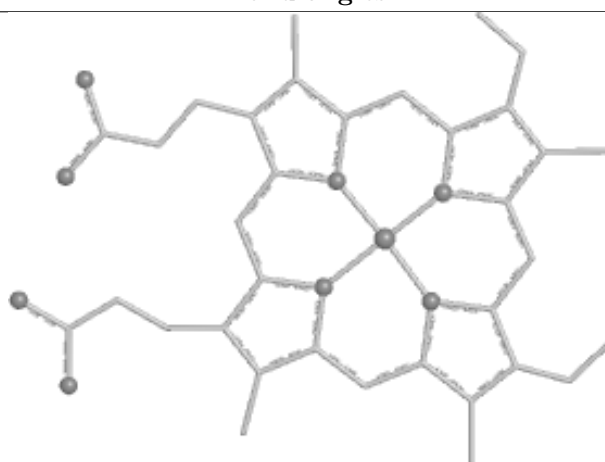
Bond lengths



Bond angles

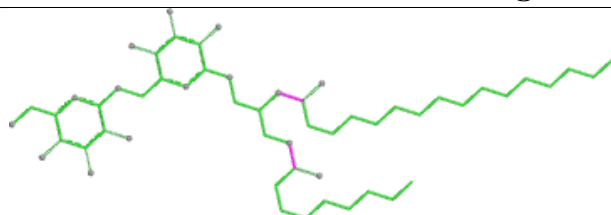


Torsions

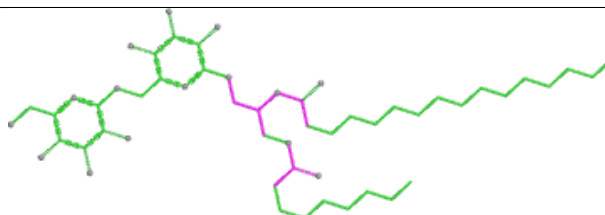


Rings

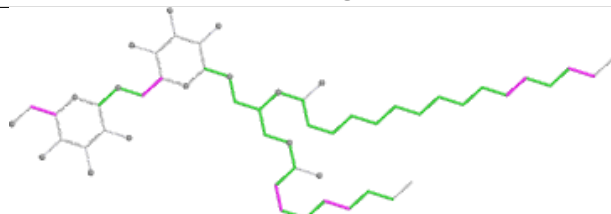
Ligand DGD c 518



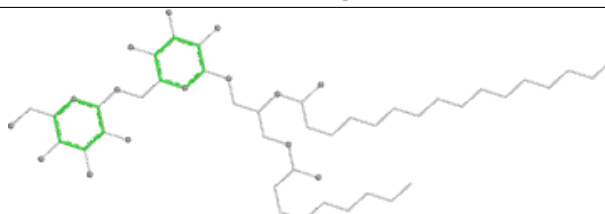
Bond lengths



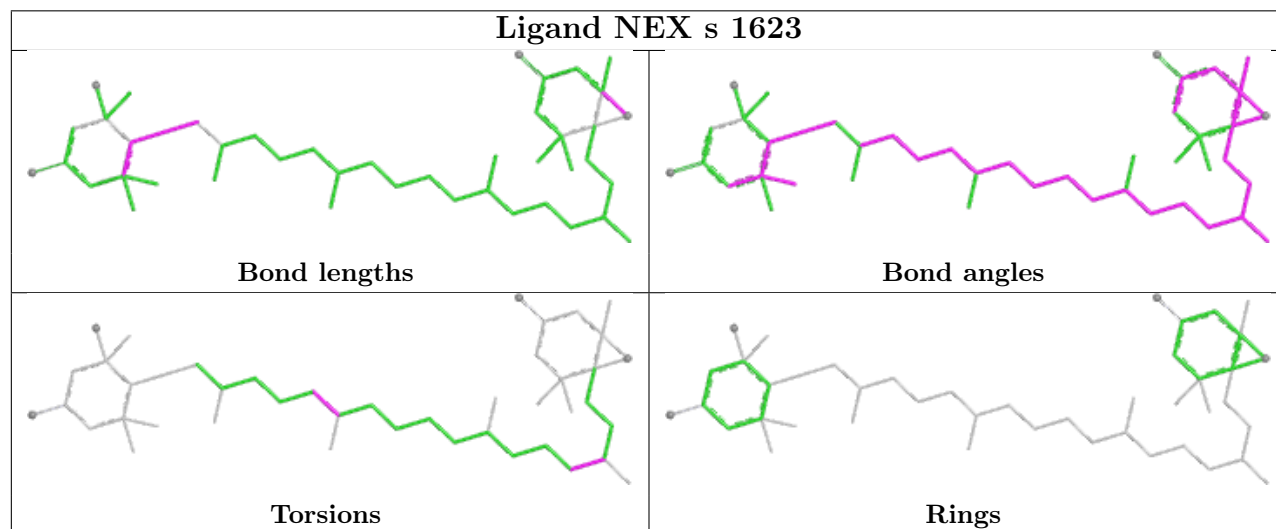
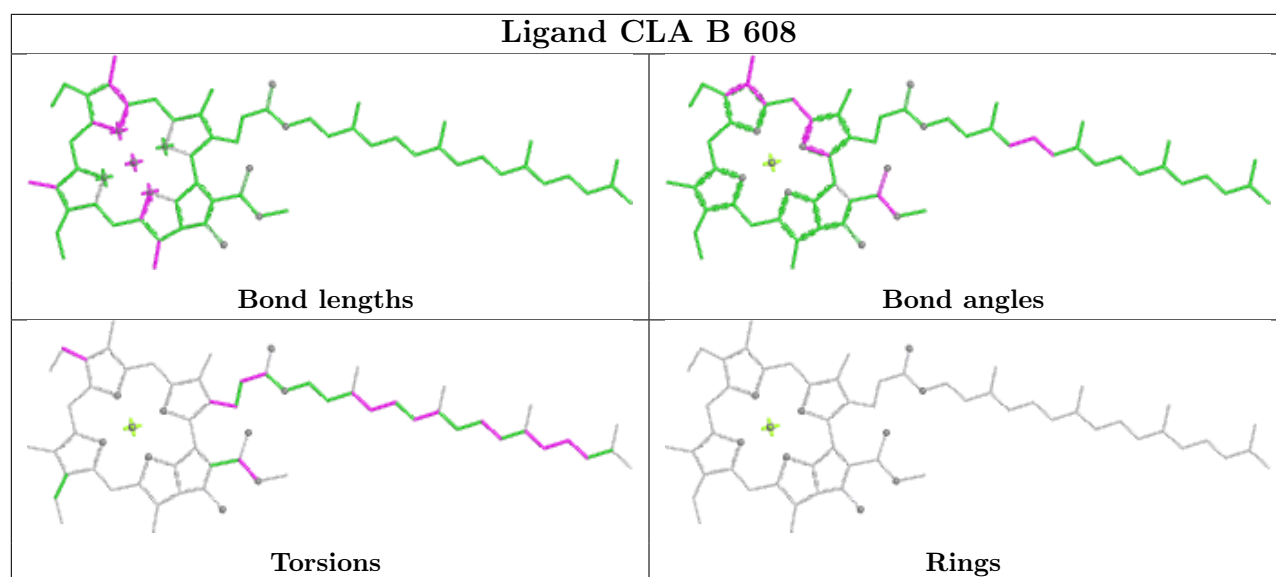
Bond angles



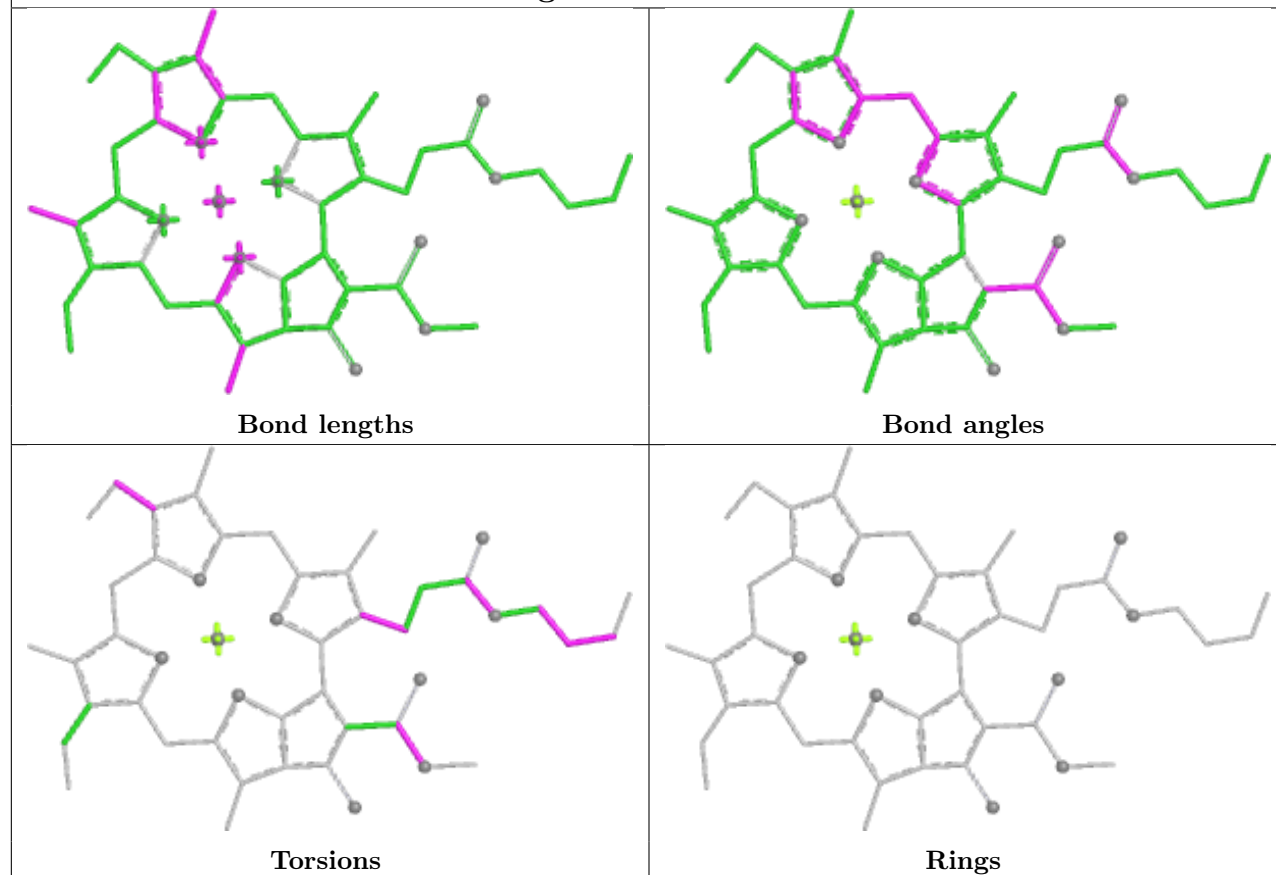
Torsions



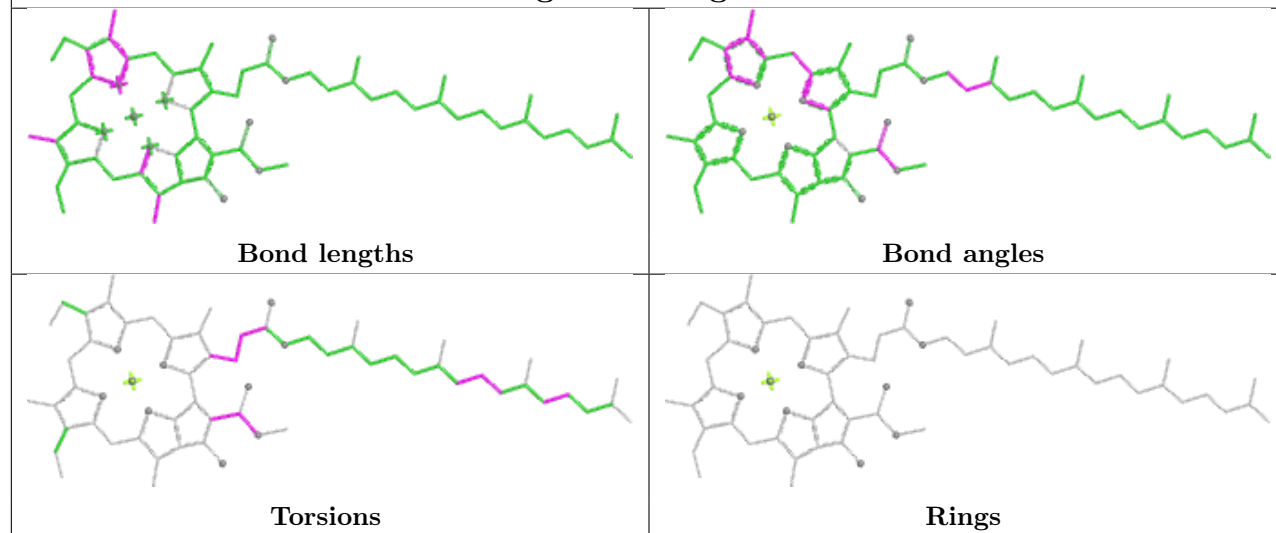
Rings

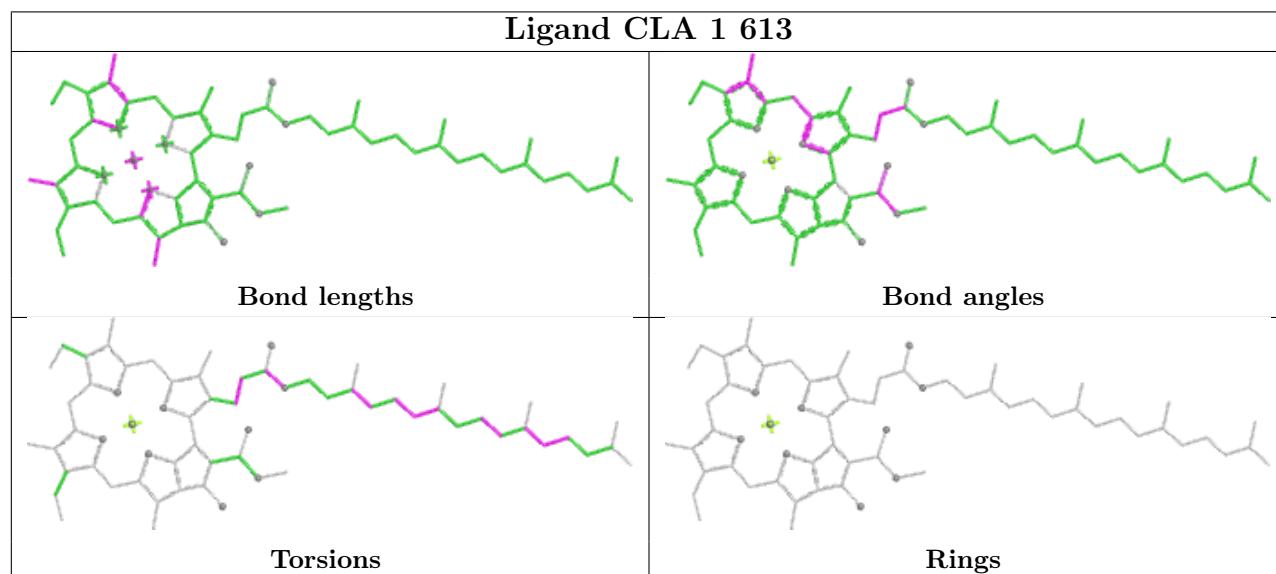
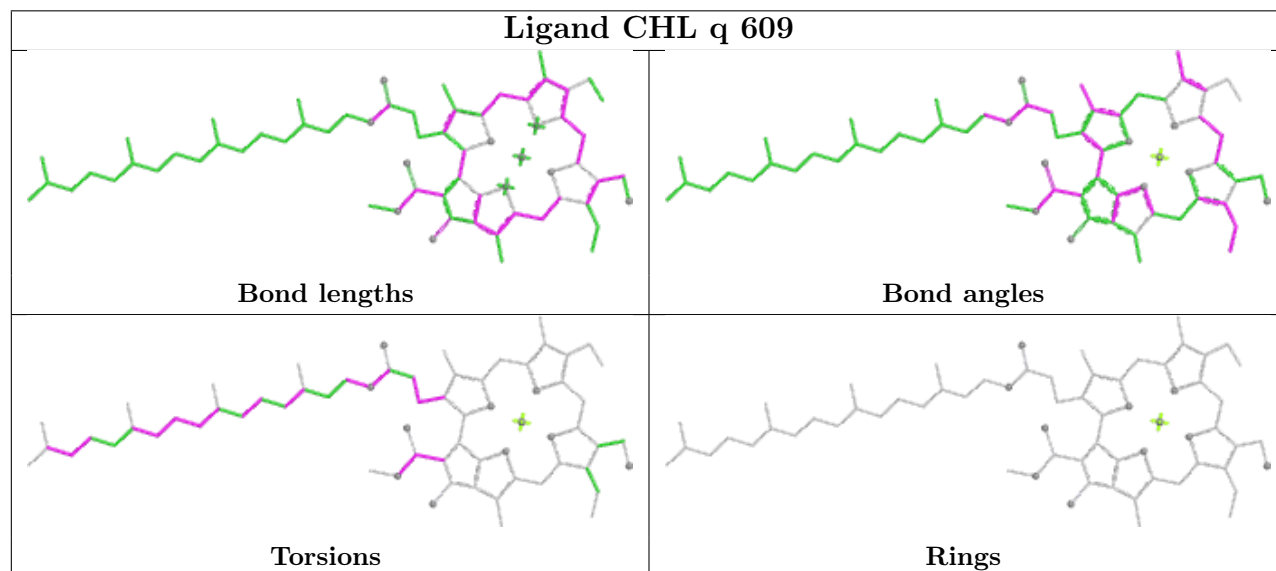
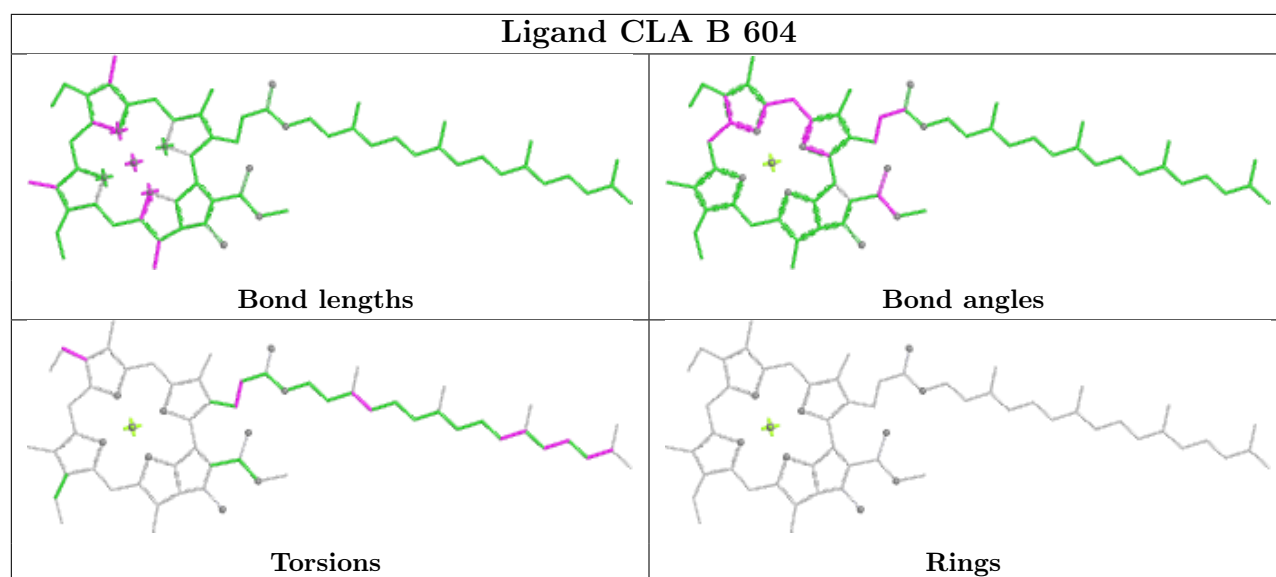


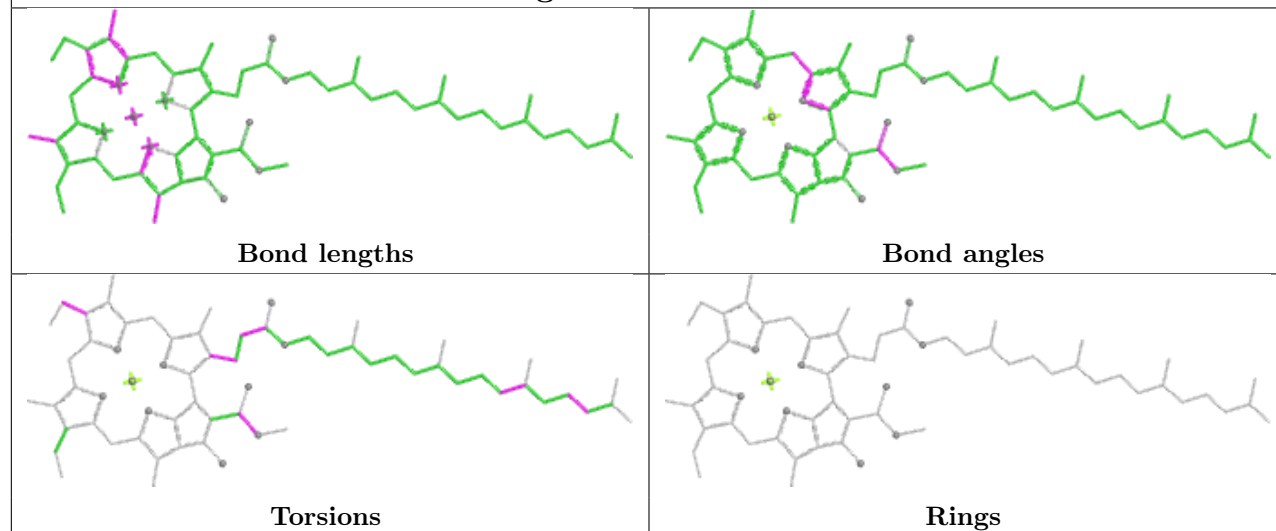
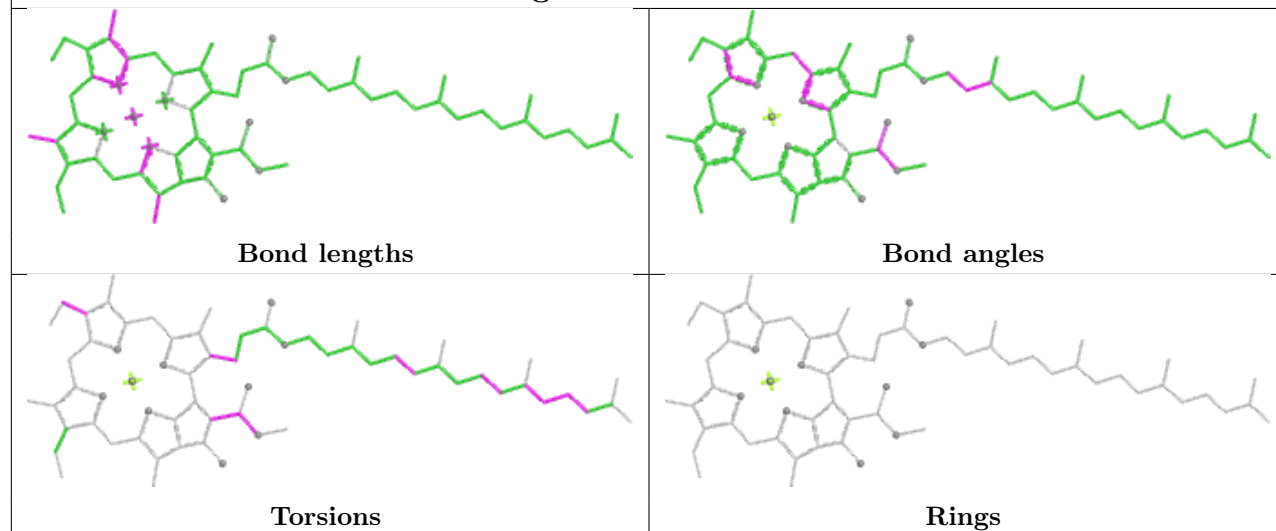
Ligand CLA s 610

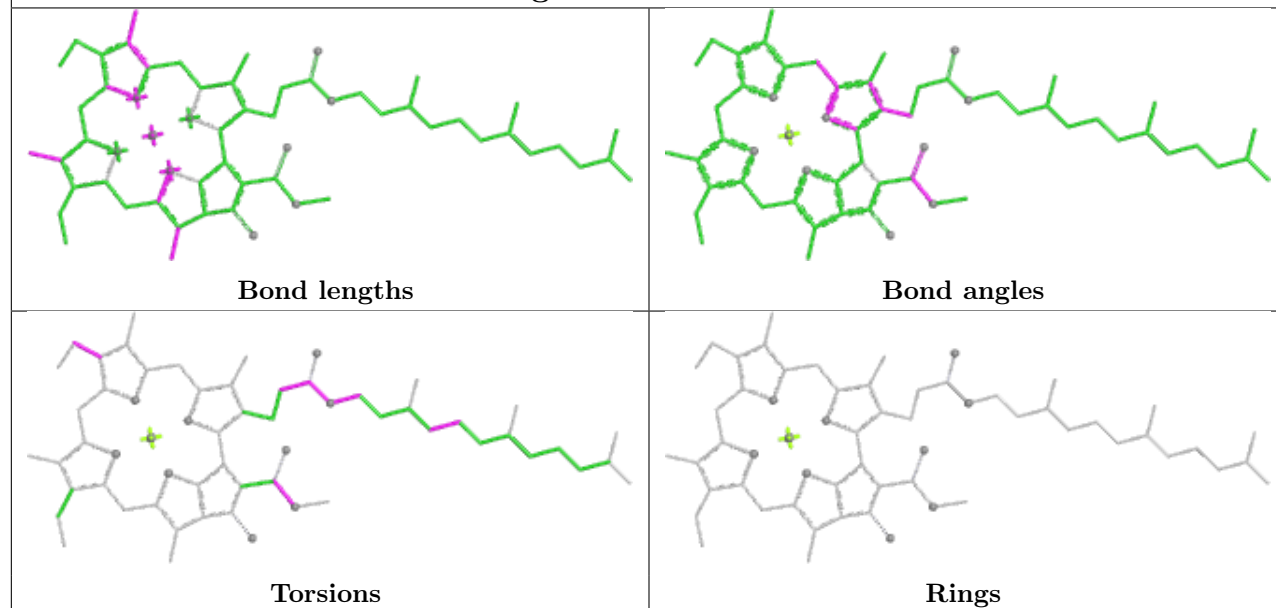
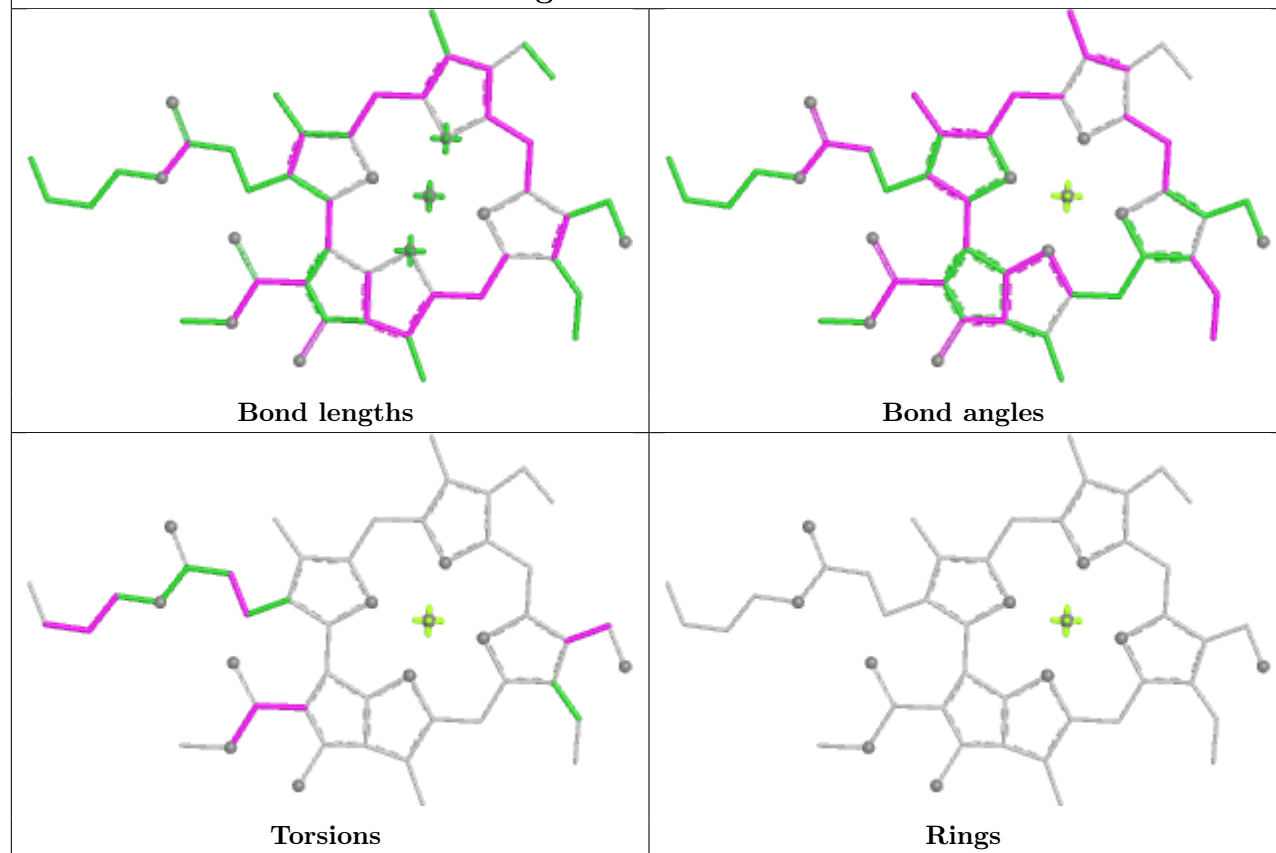


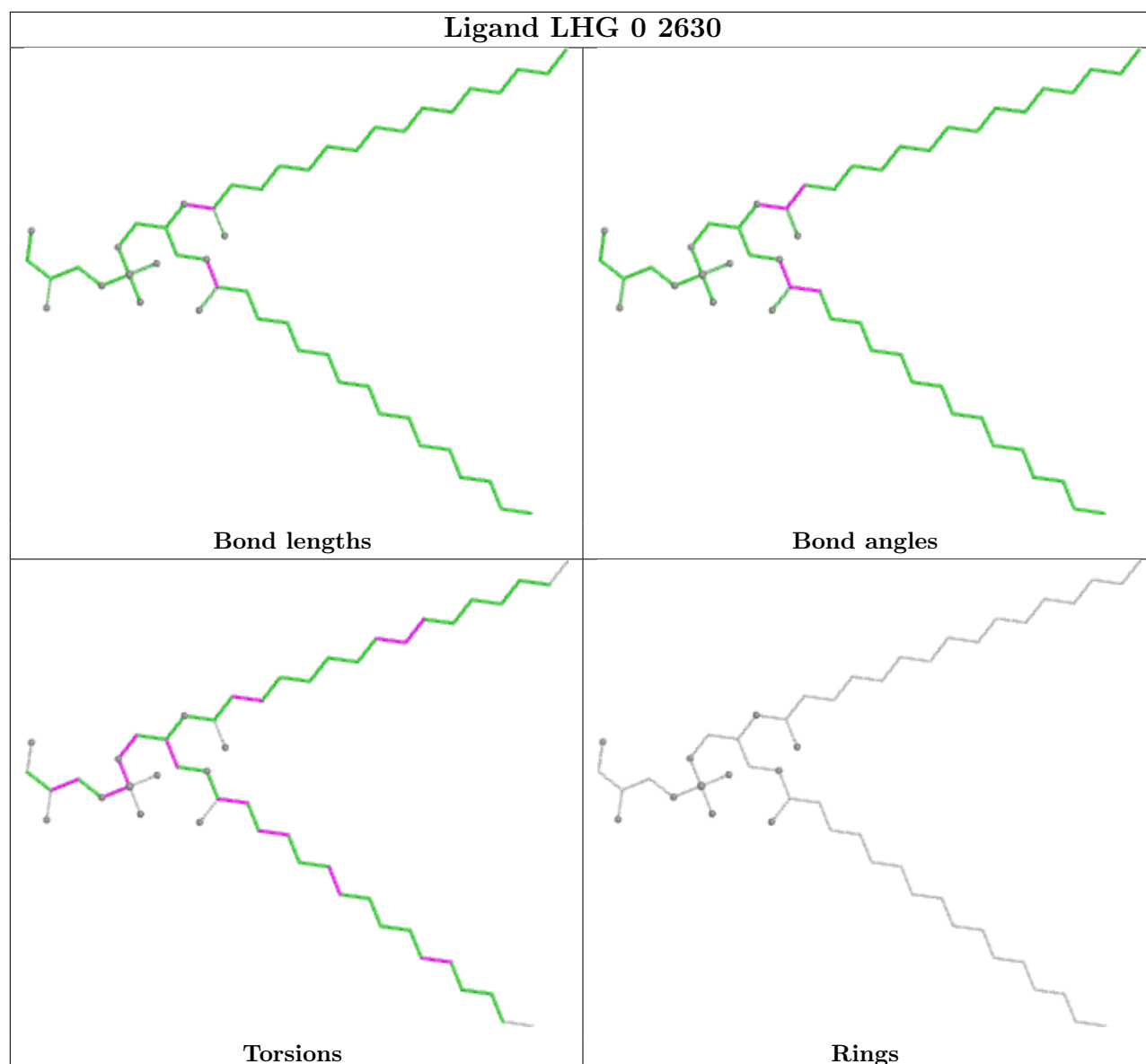
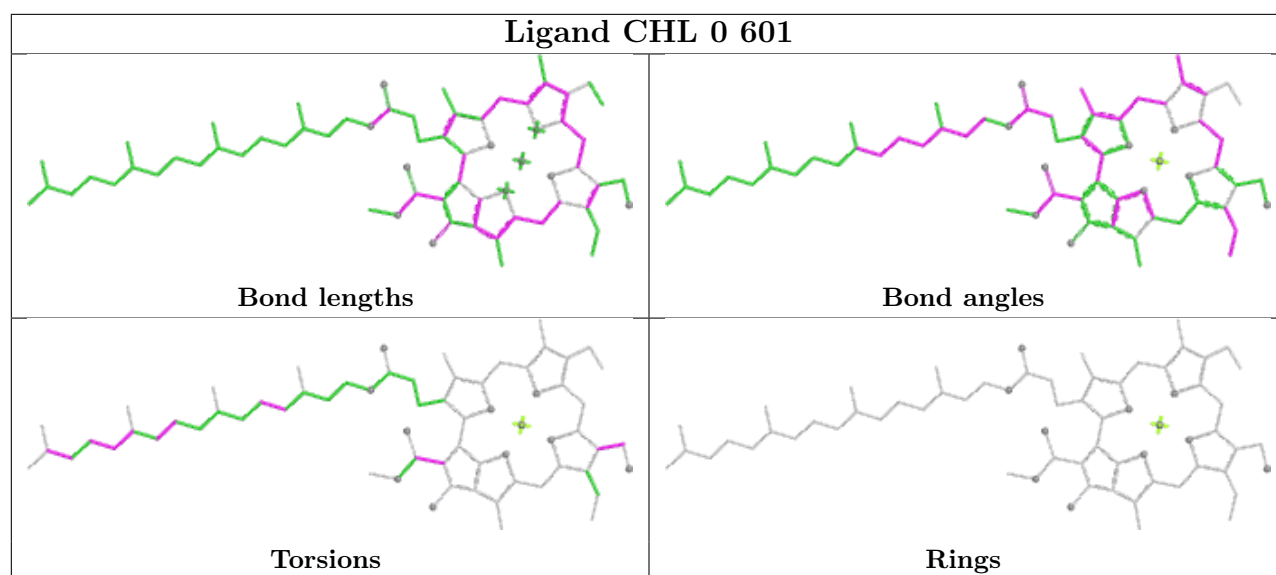
Ligand CLA g 602

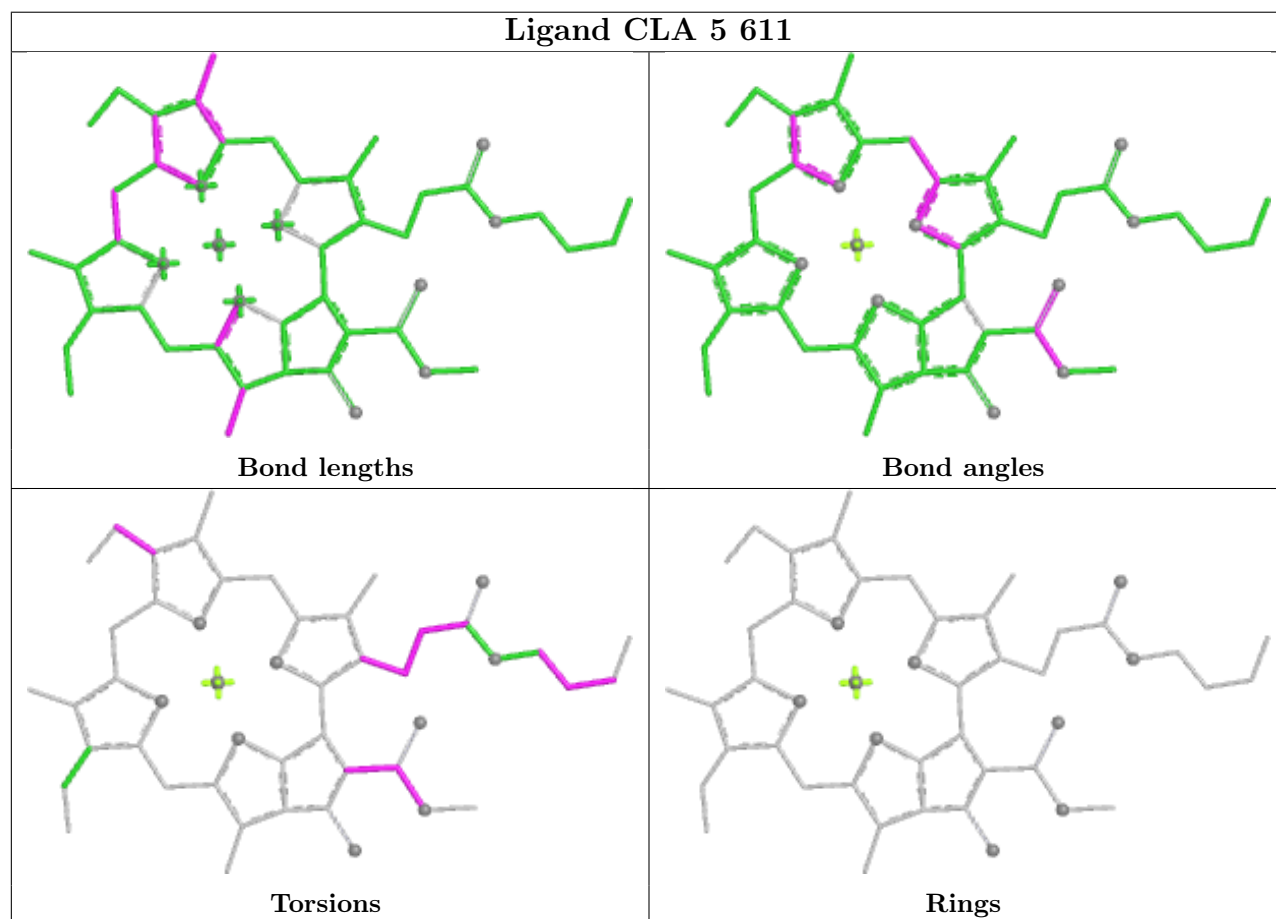
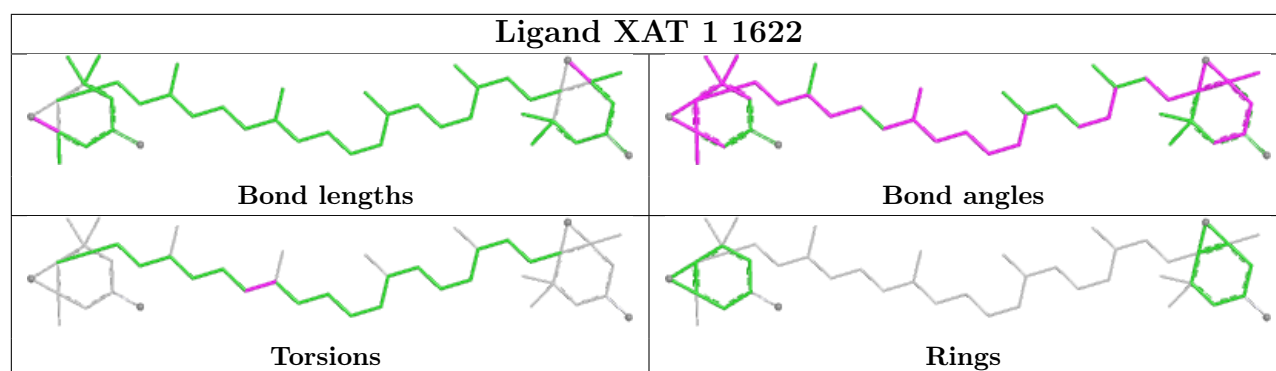




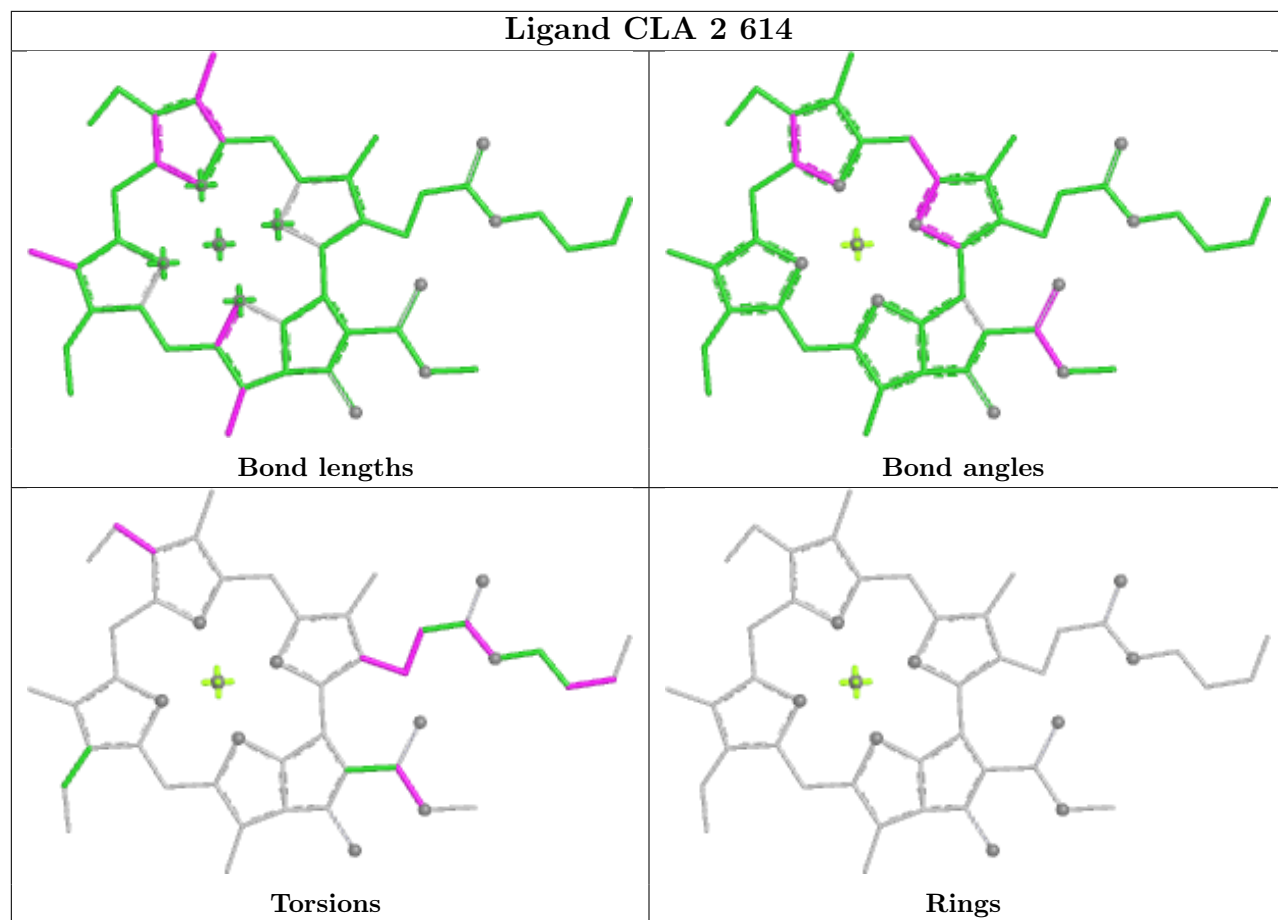
Ligand CLA 7 611**Ligand CLA B 606**

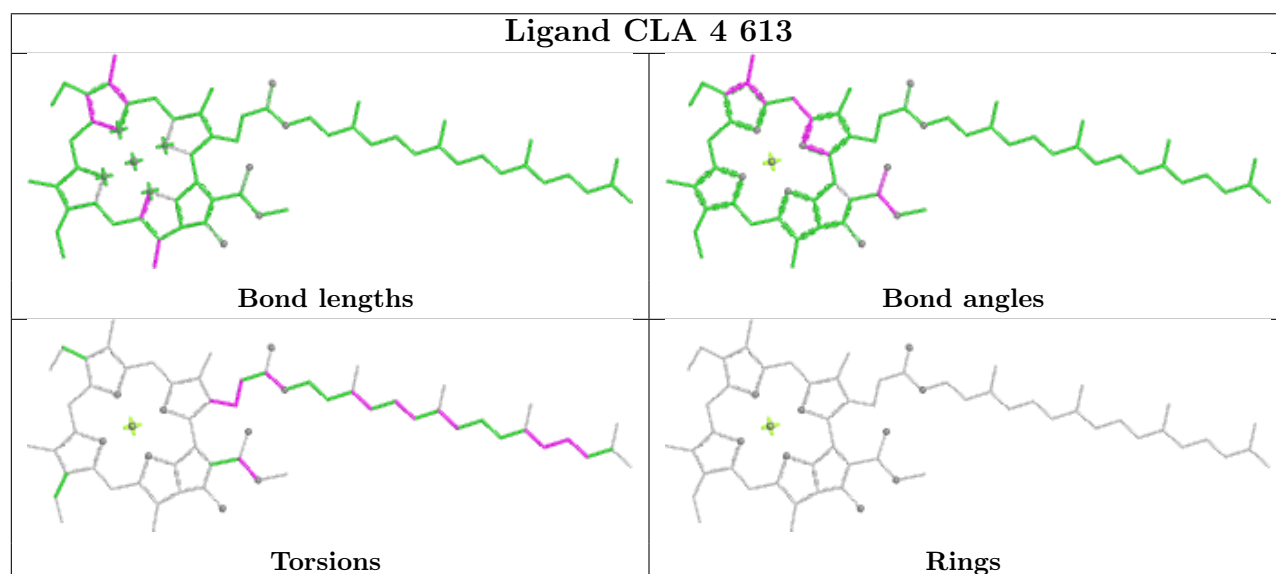
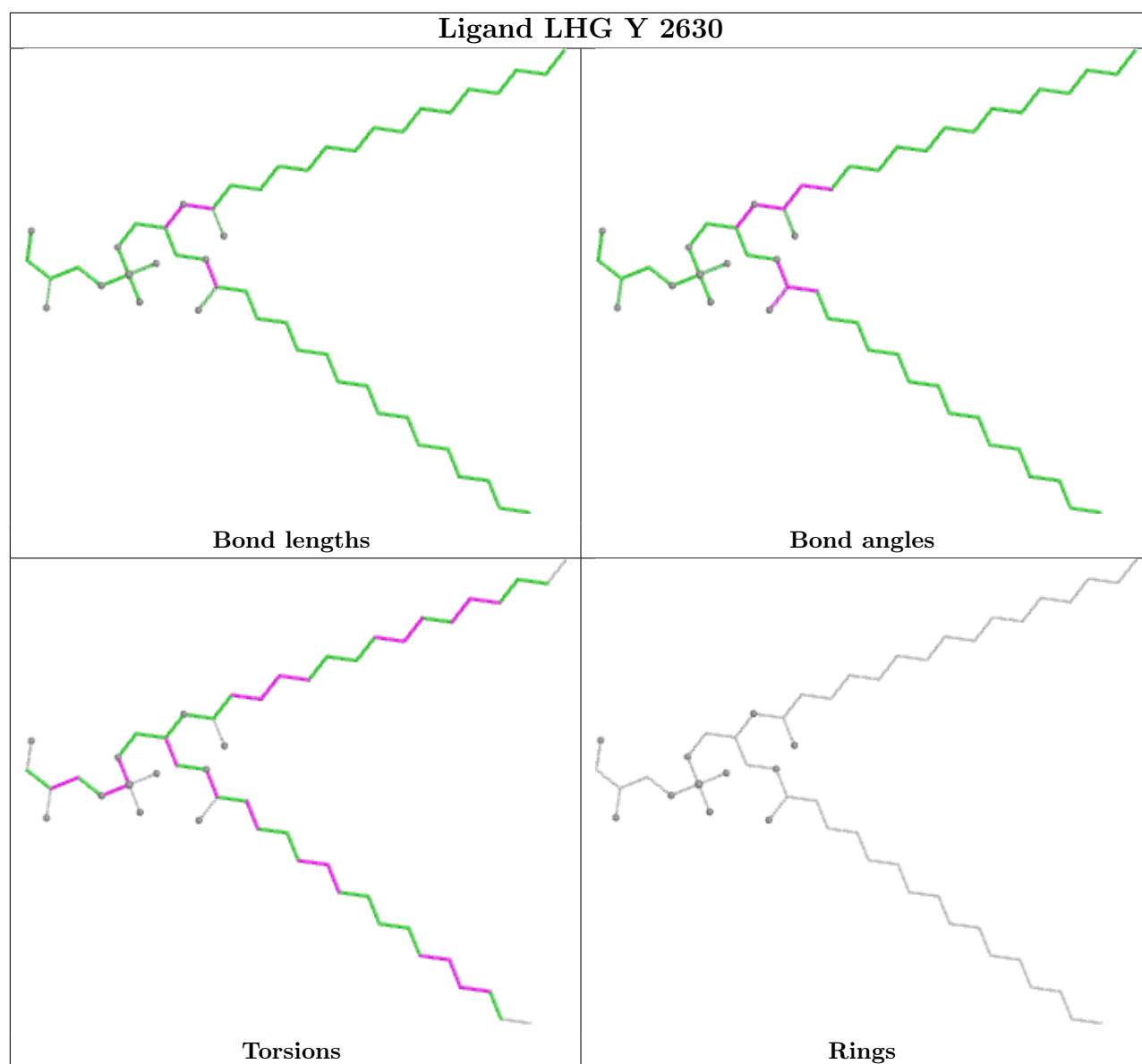
Ligand CLA R 603**Ligand CHL 6 608**

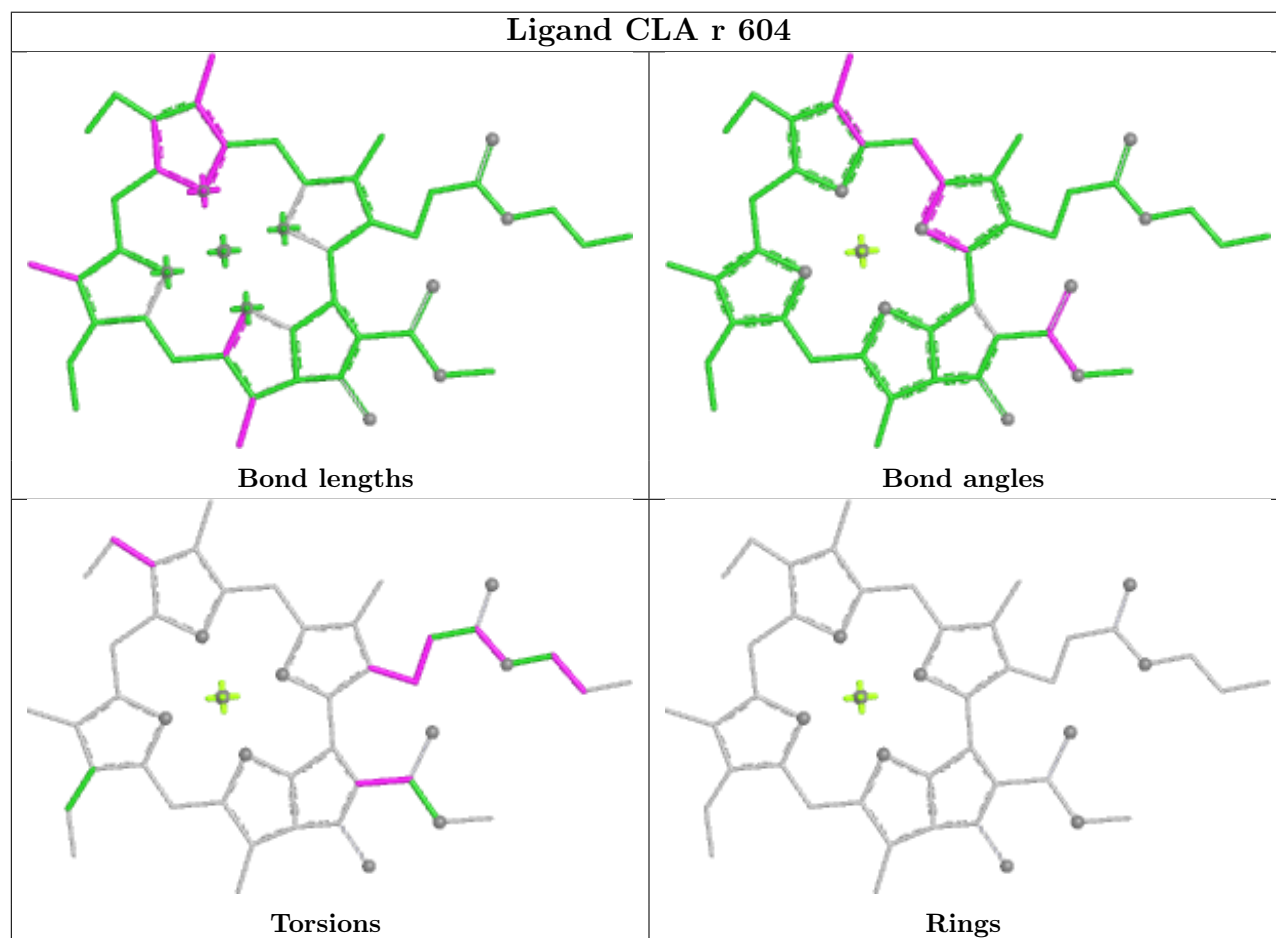
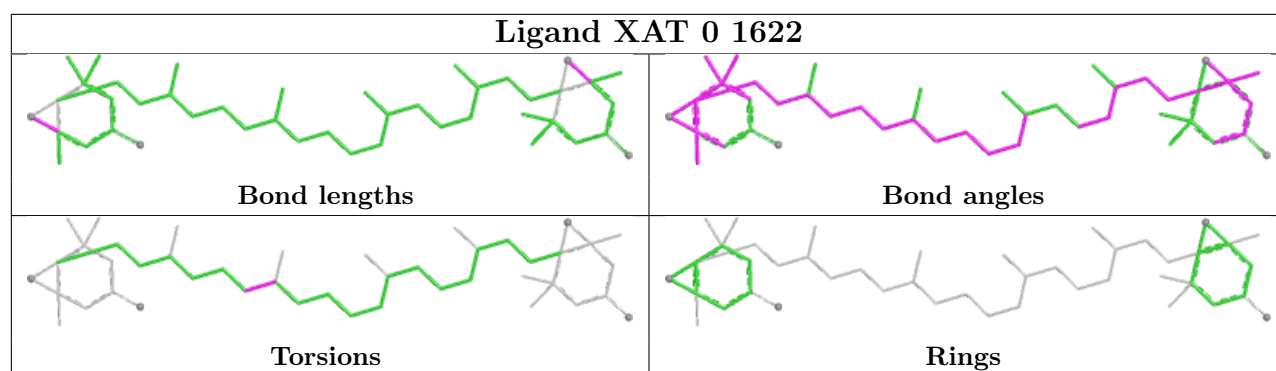




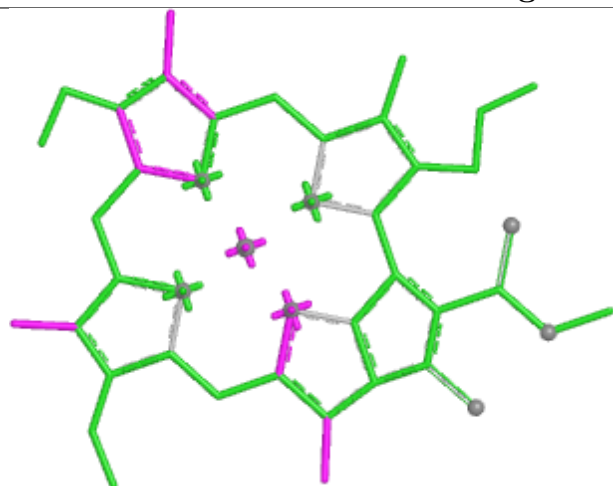
Ligand CLA 2 614



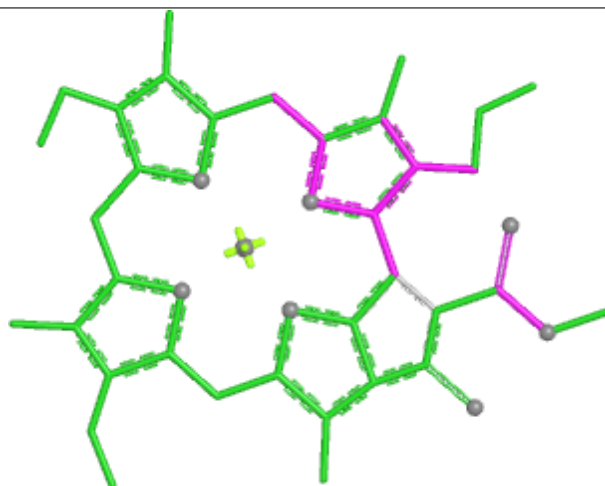




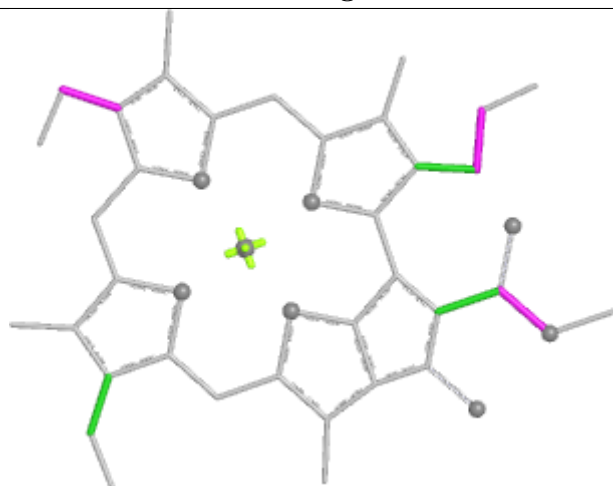
Ligand CLA 2 612



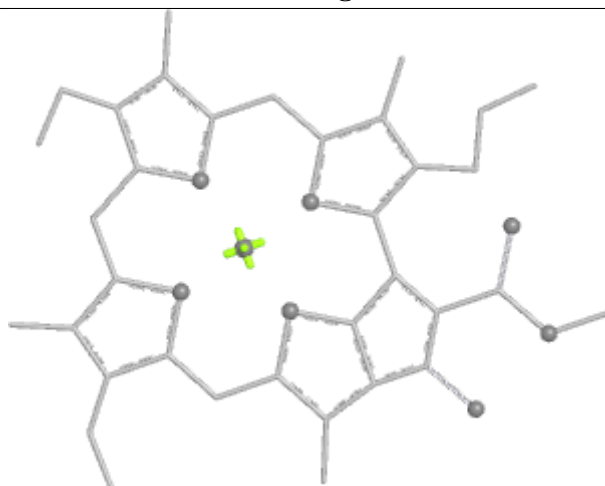
Bond lengths



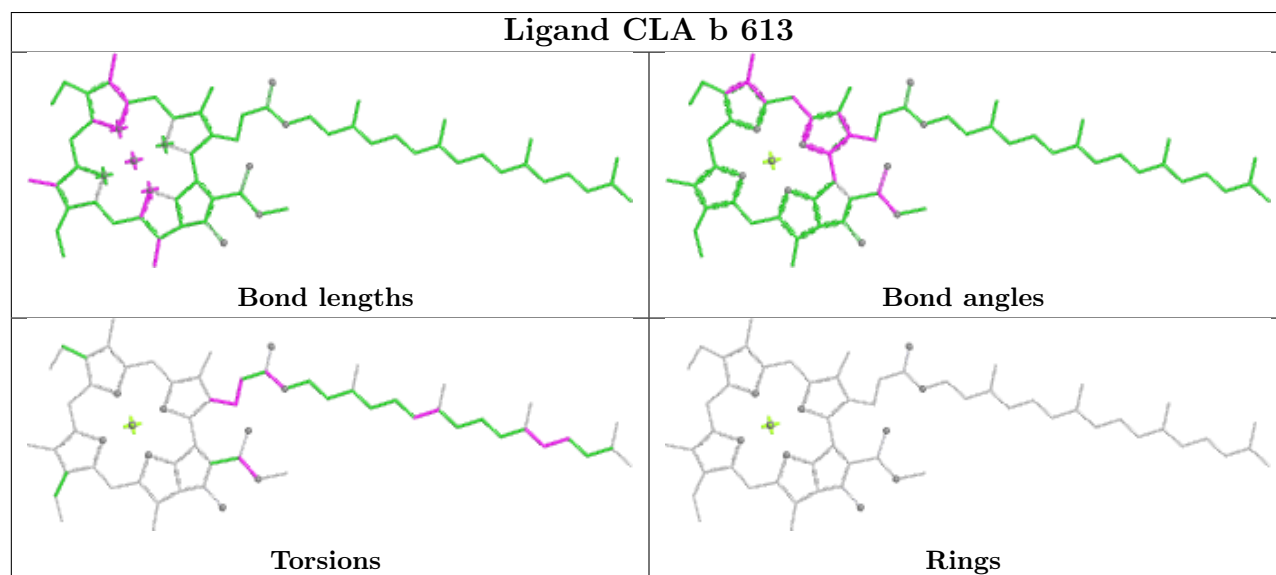
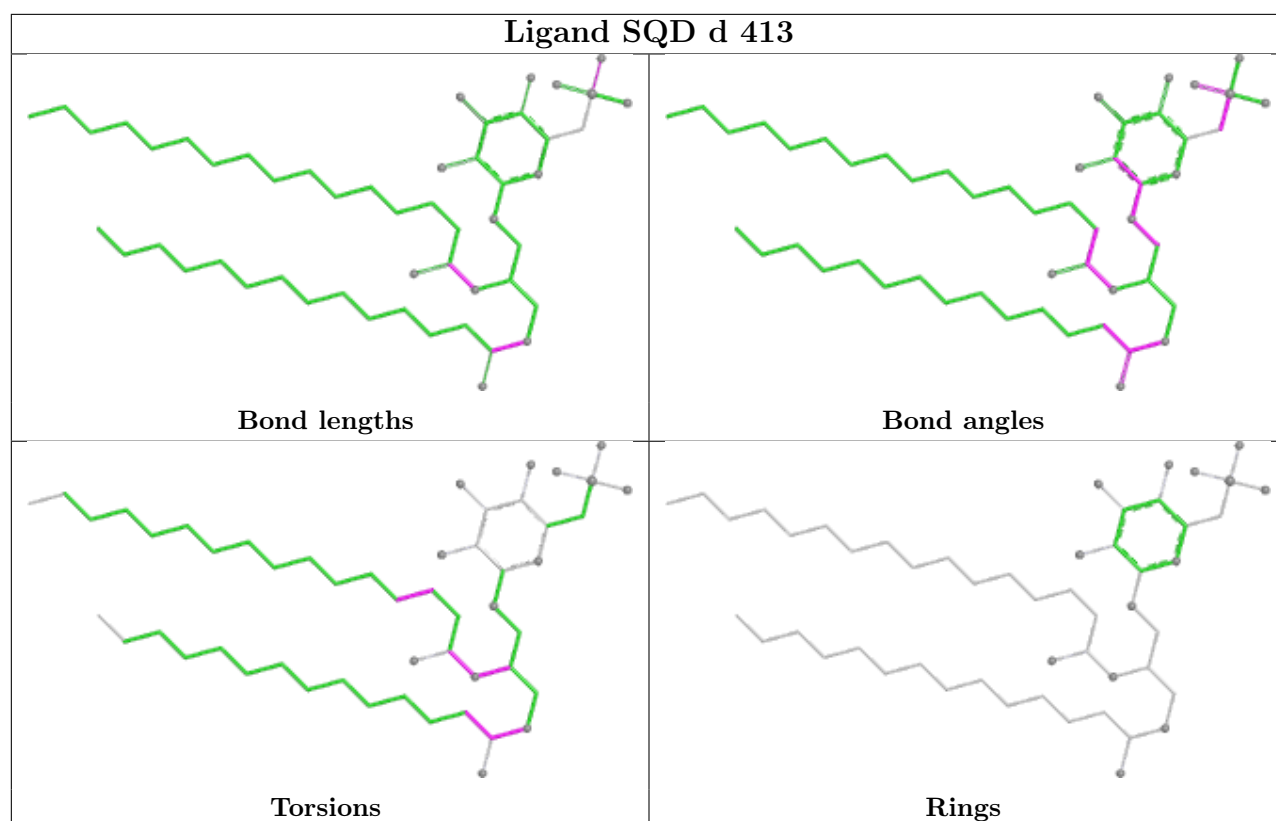
Bond angles



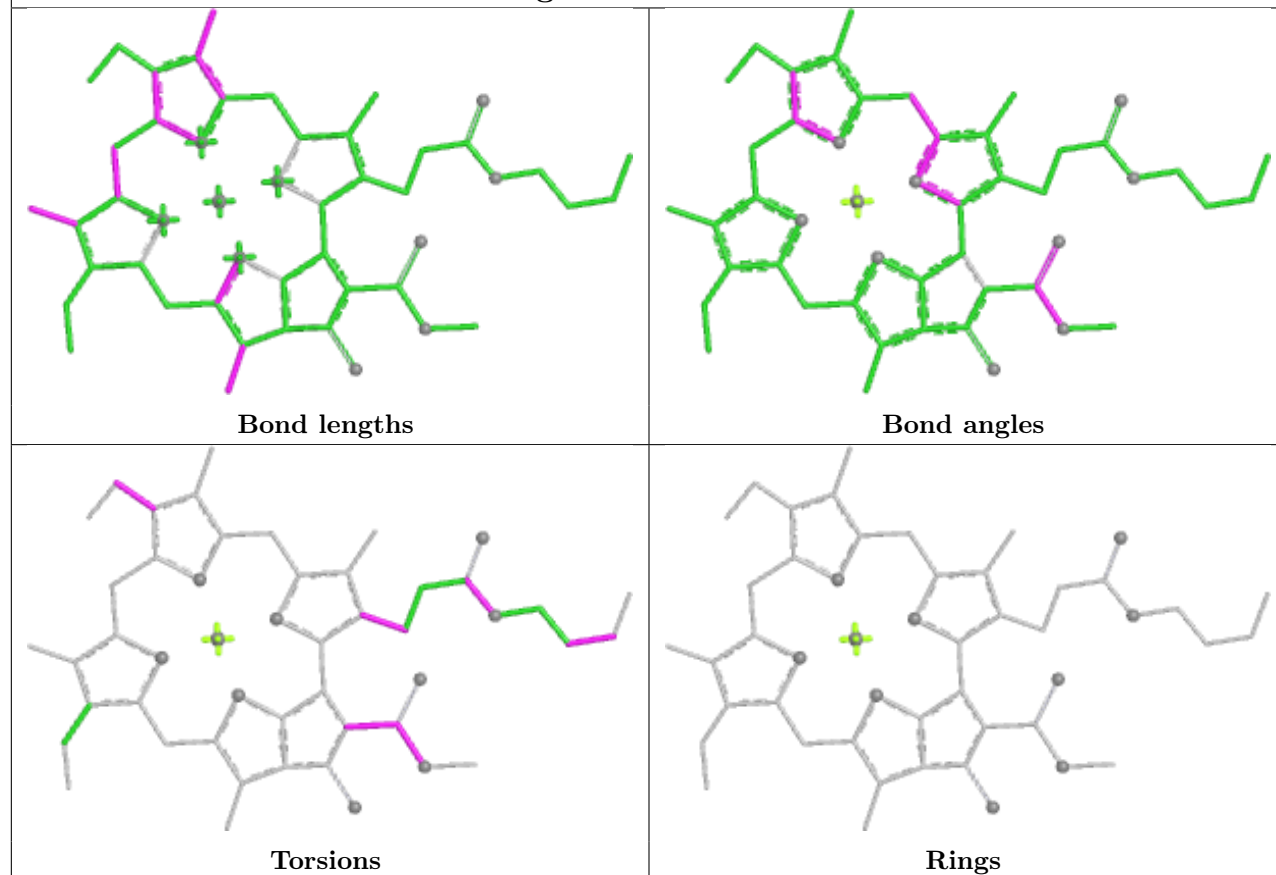
Torsions



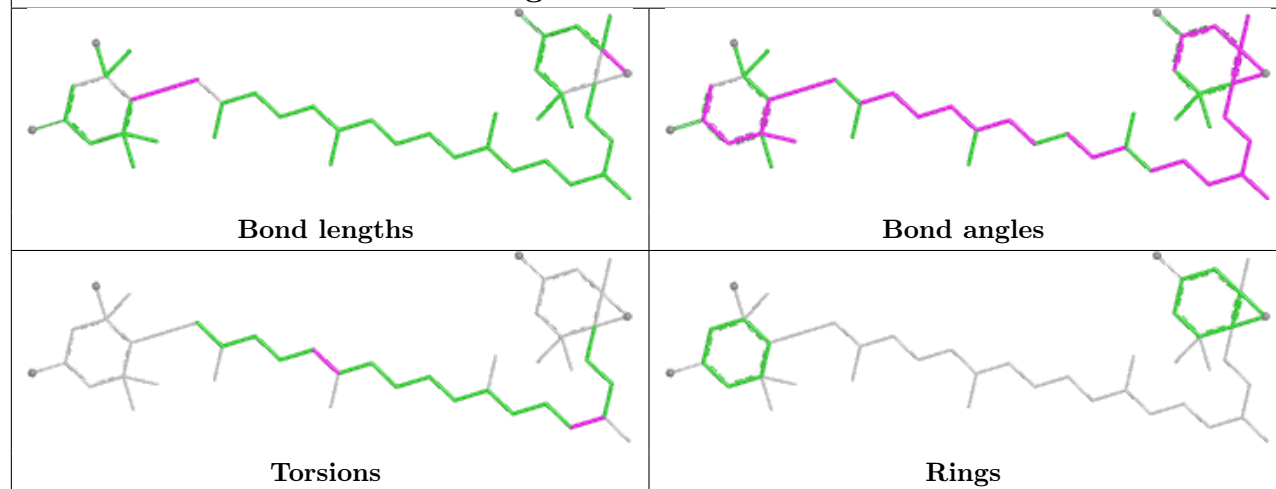
Rings

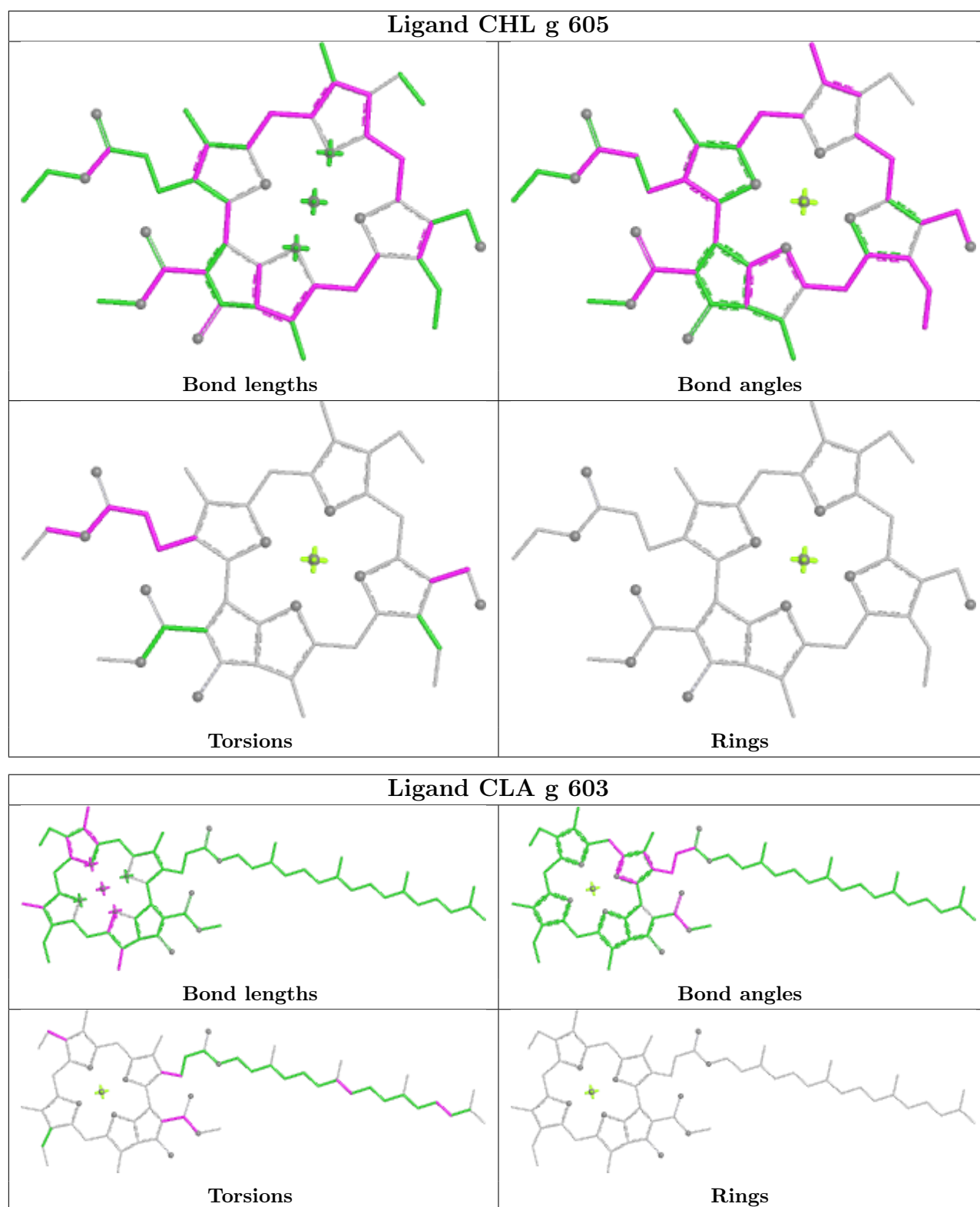


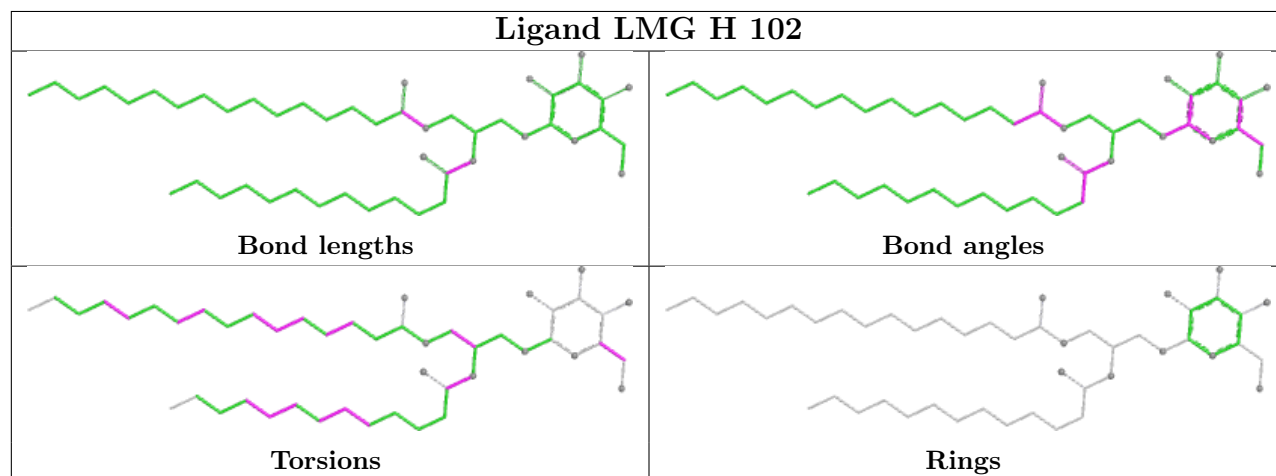
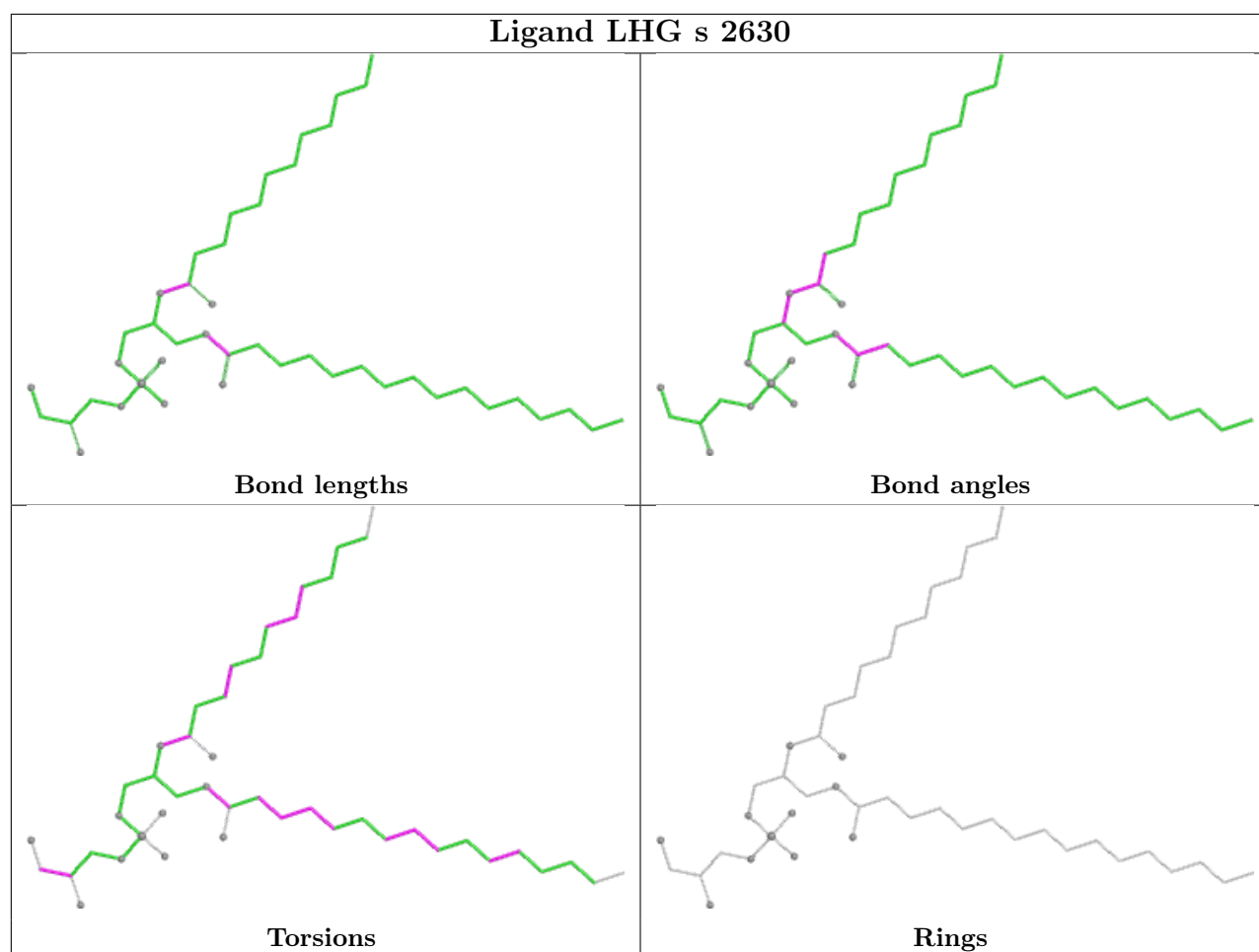
Ligand CLA 4 614

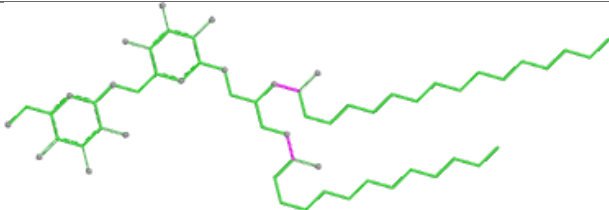
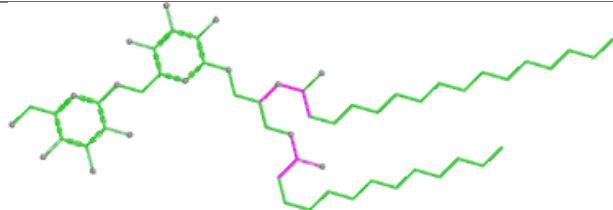
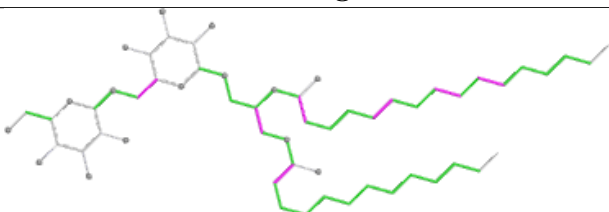
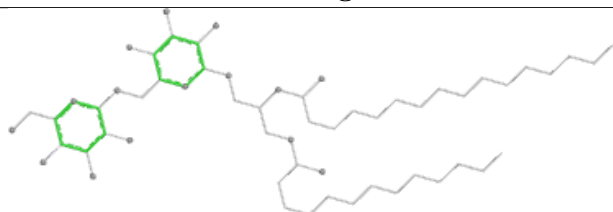


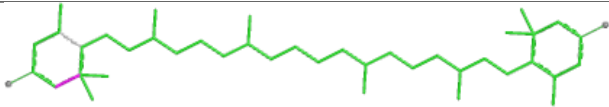
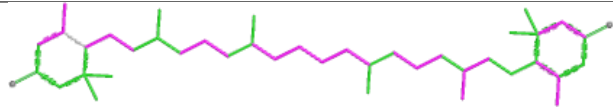
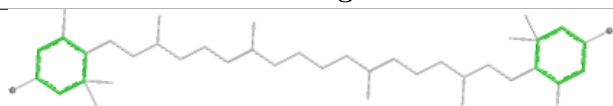
Ligand NEX 1 1623

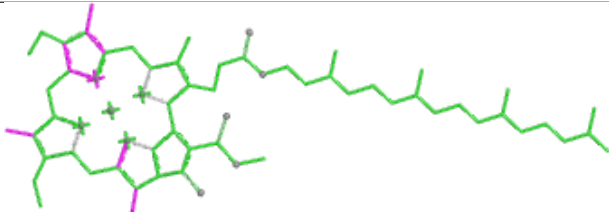
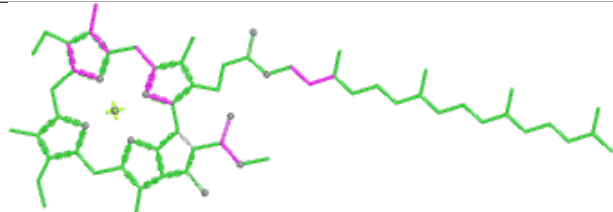
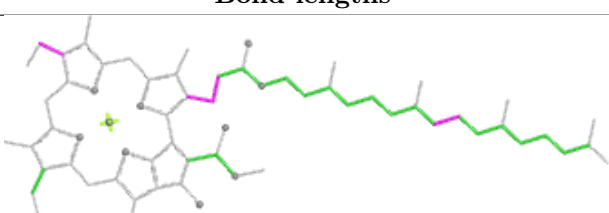
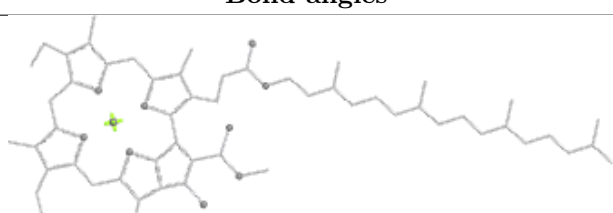




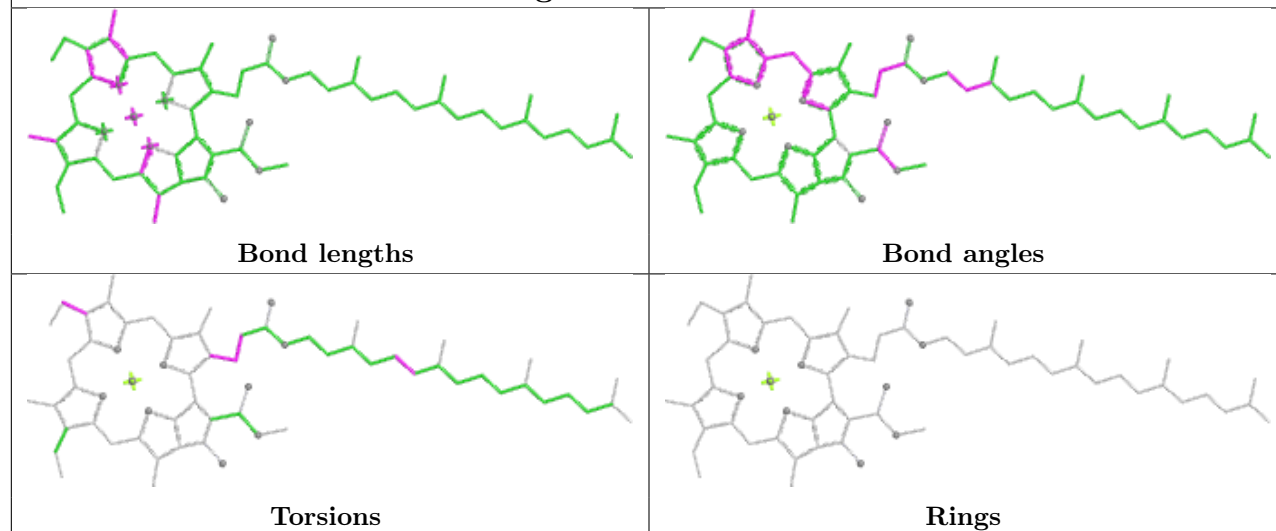


Ligand DGD C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

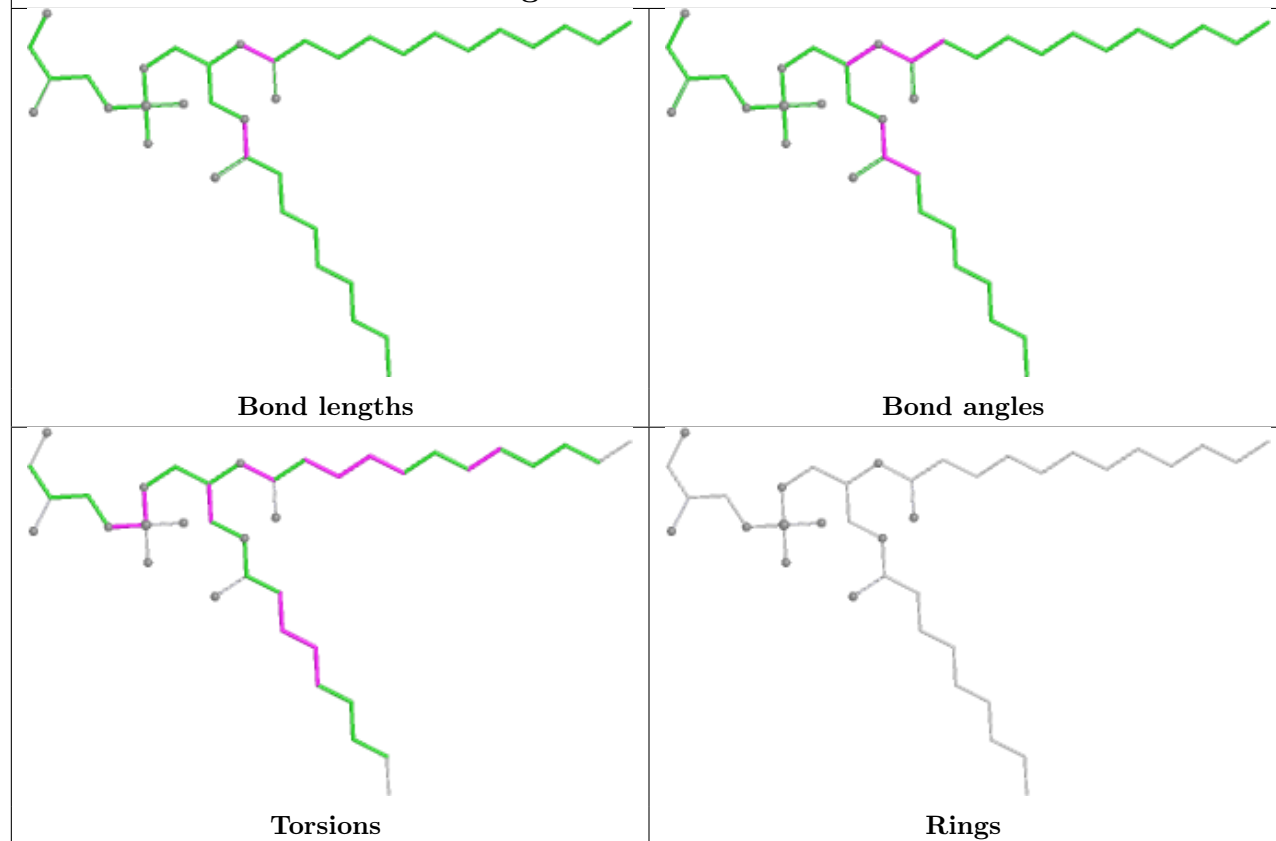
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Bond lengths	Bond angles
	
Torsions	Rings

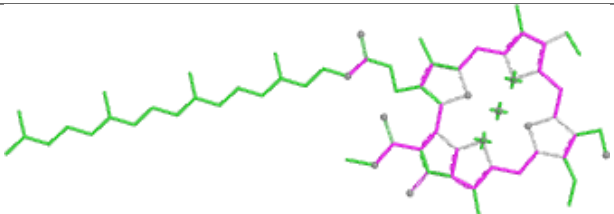
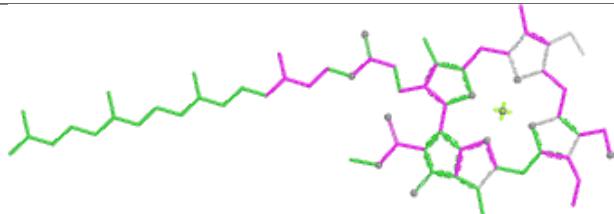
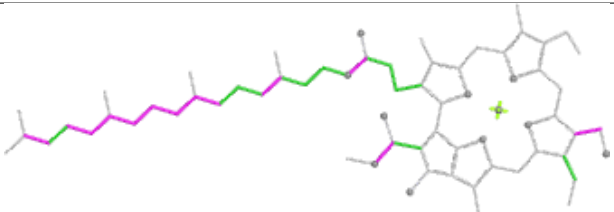
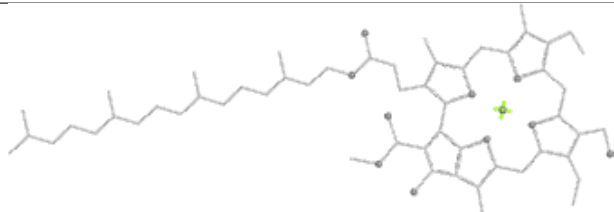
Ligand CLA 0 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

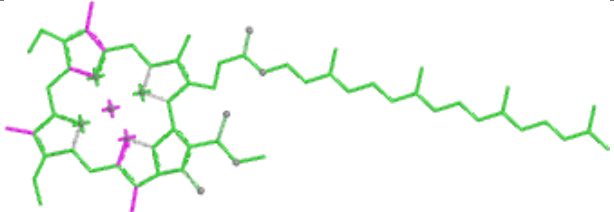
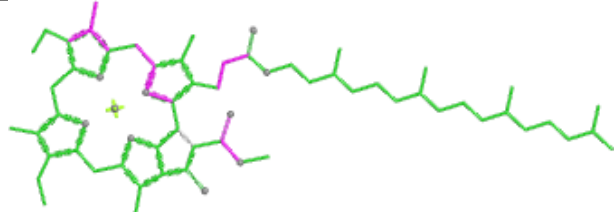
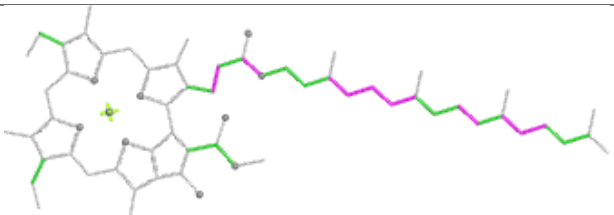
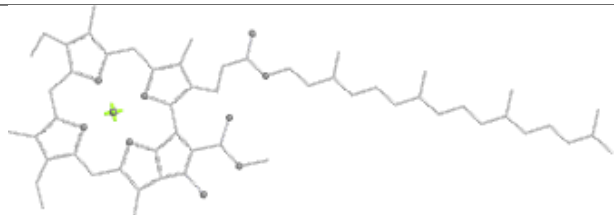
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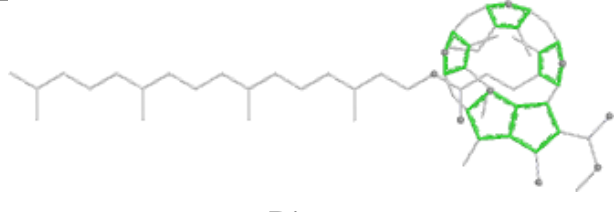


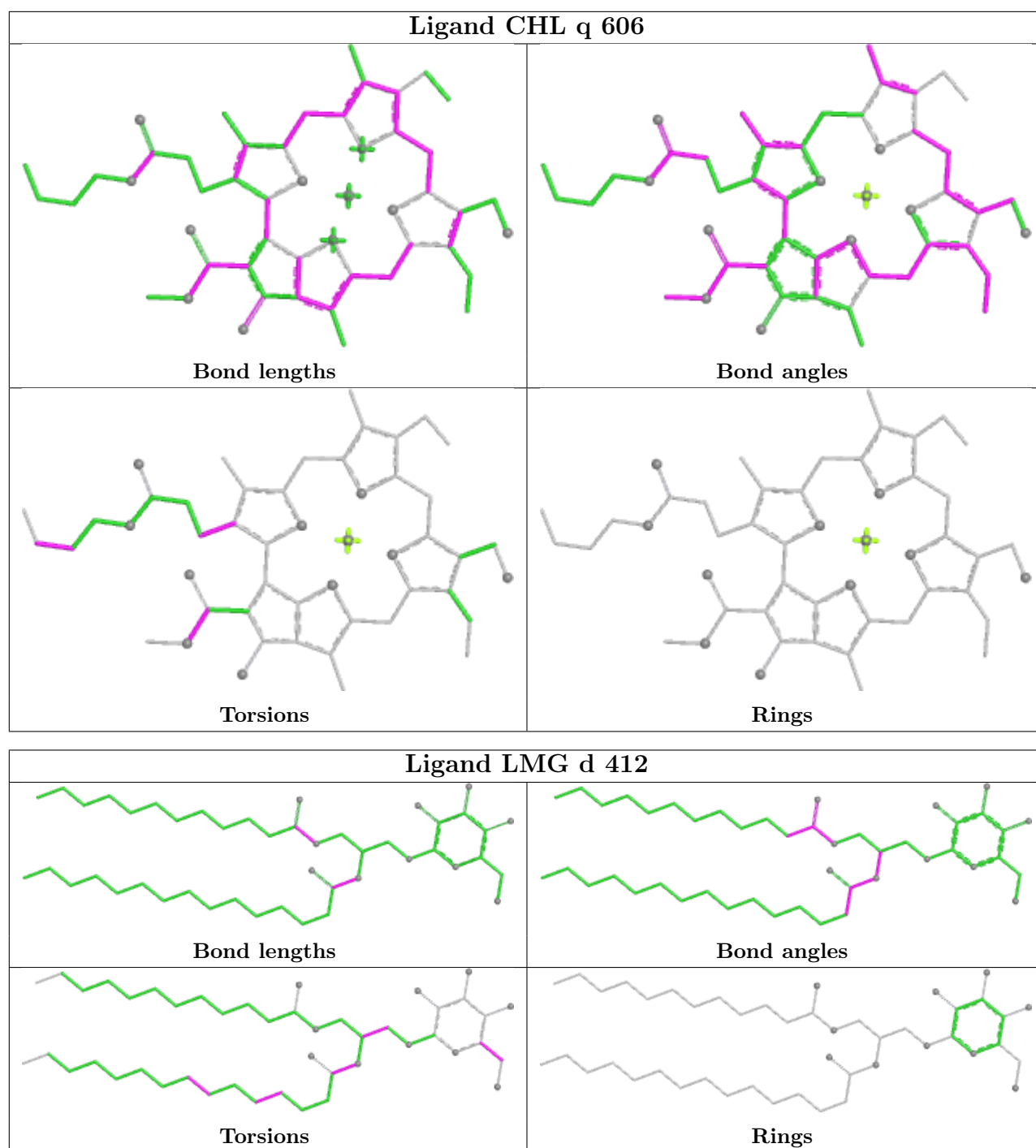
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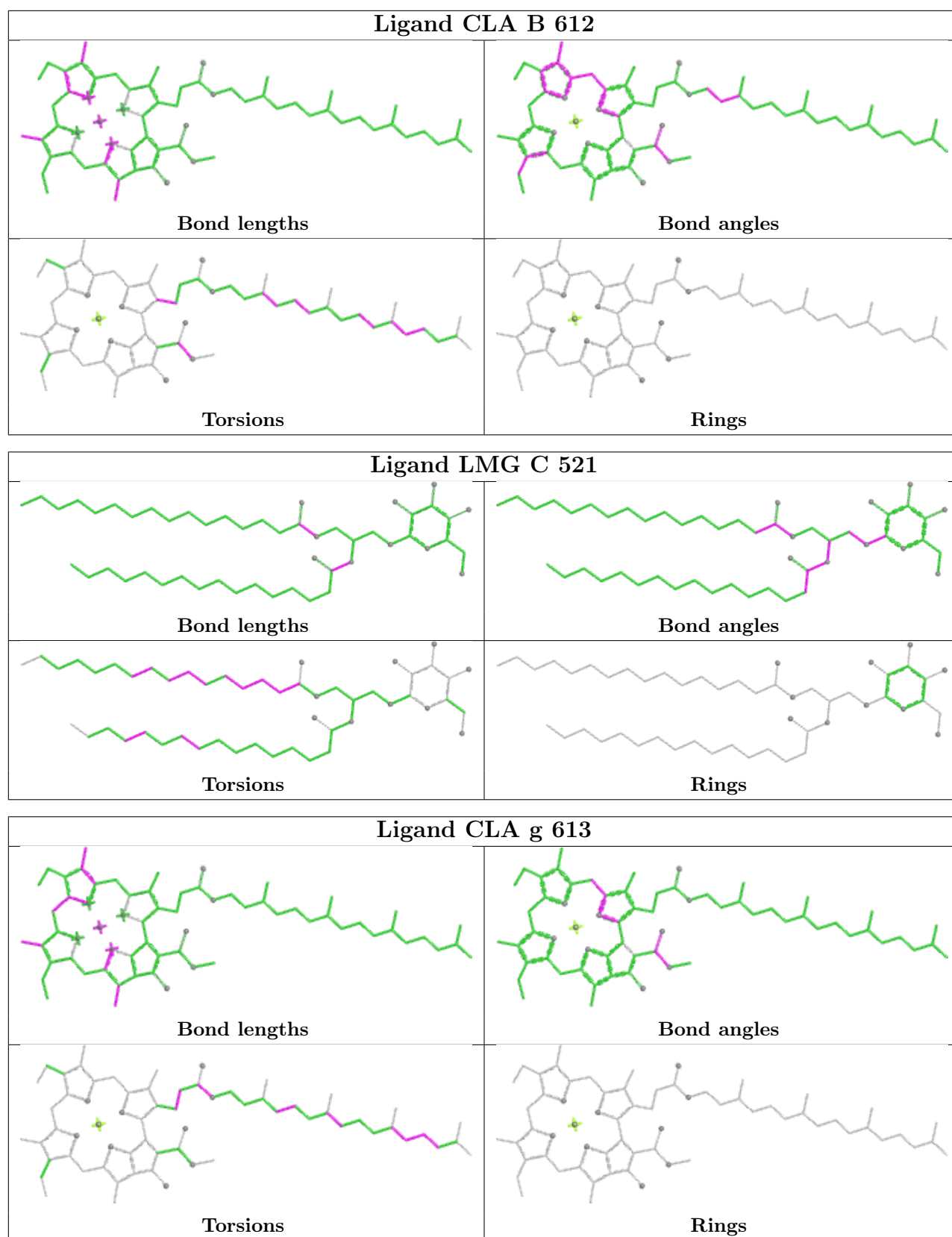


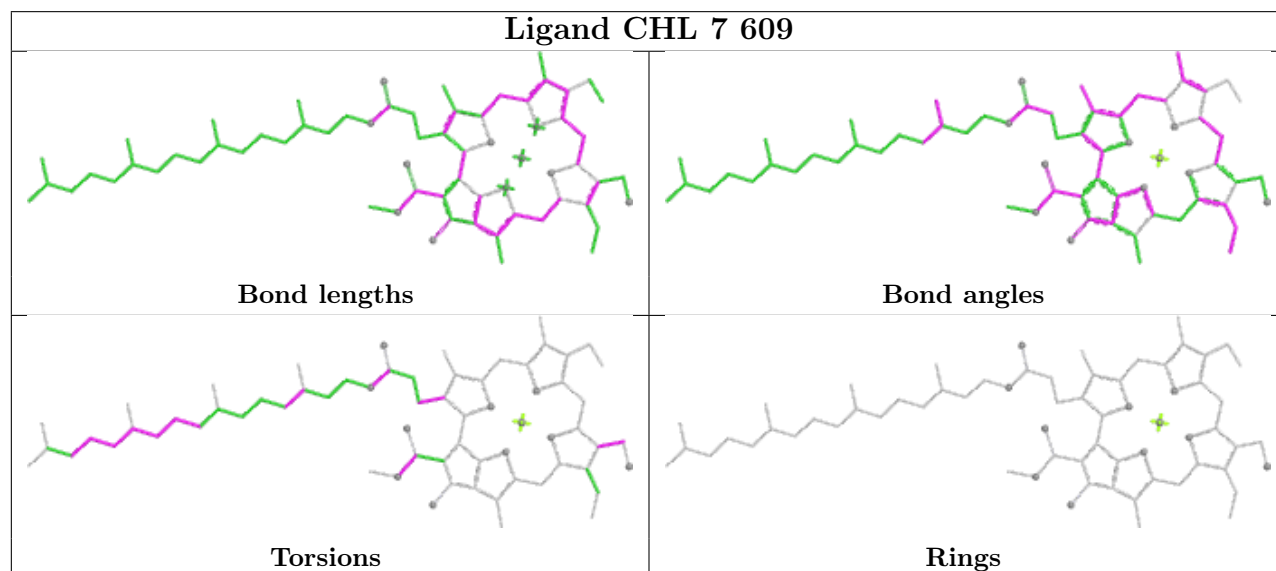
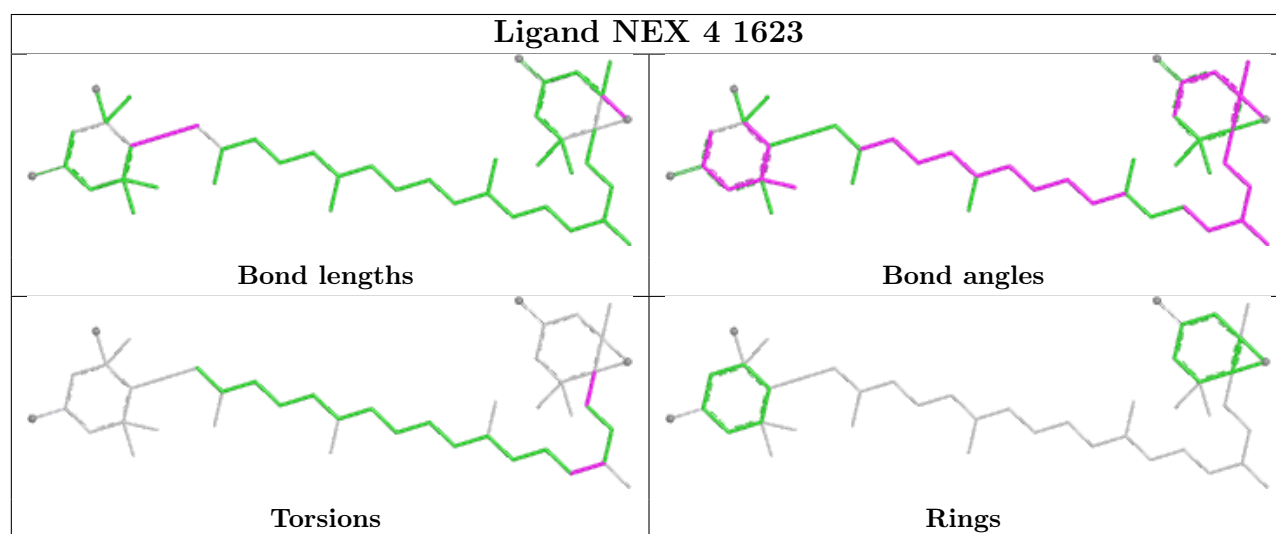
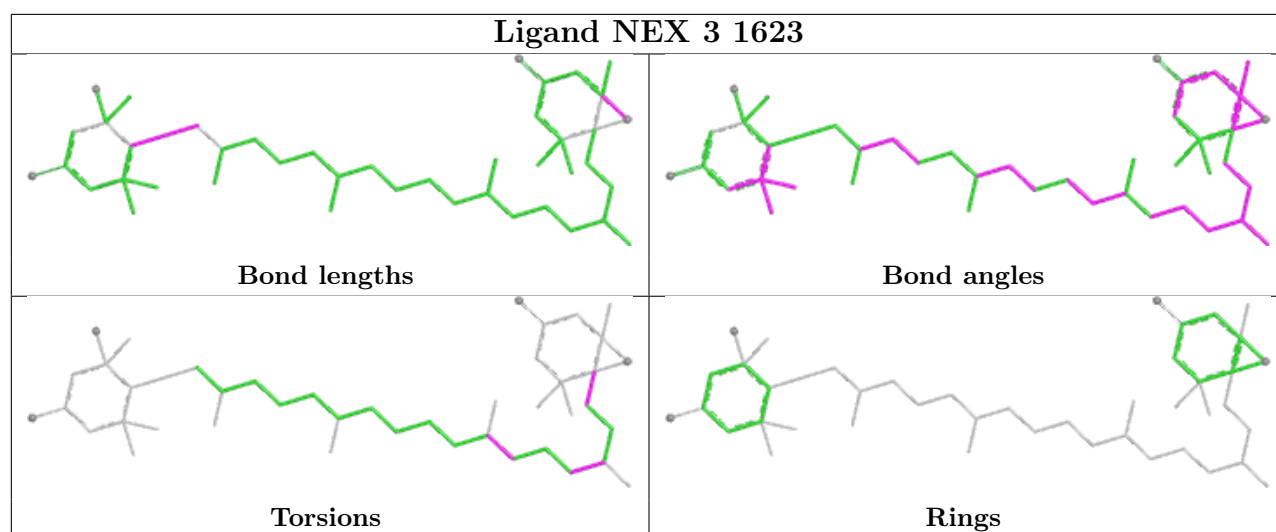
Ligand CHL N 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 7 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

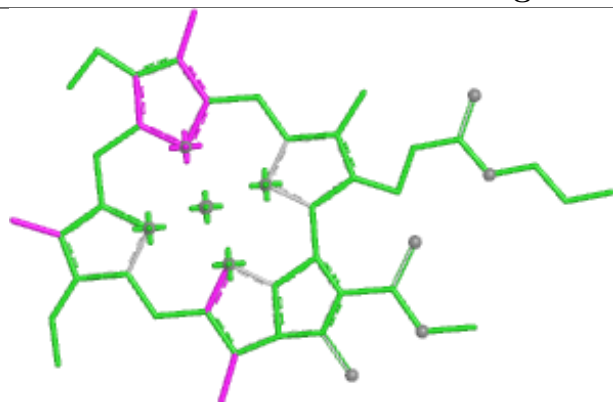
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Bond lengths	Bond angles
	
Torsions	Rings



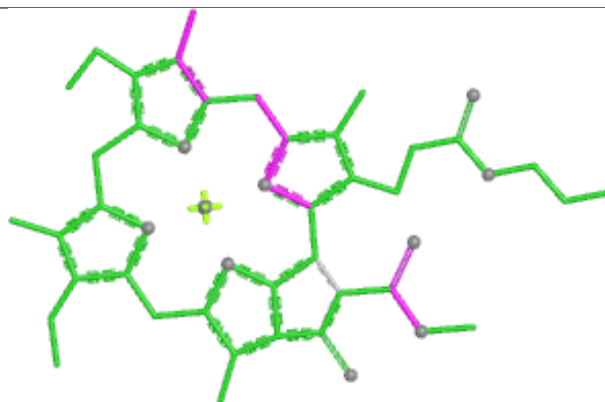




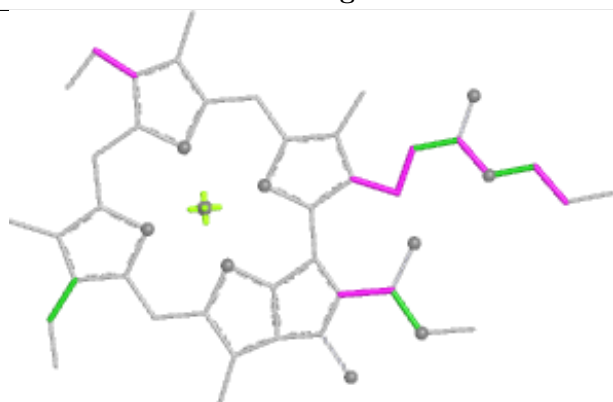
Ligand CLA R 604



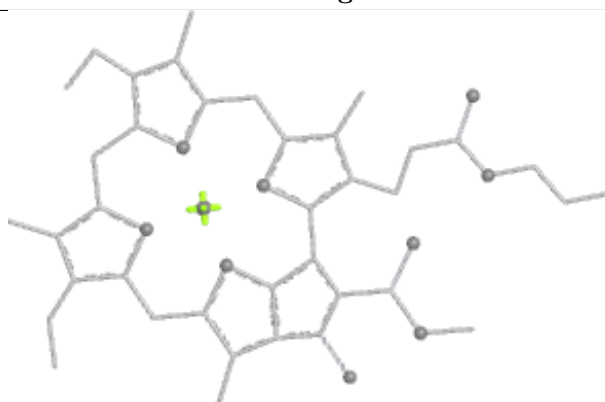
Bond lengths



Bond angles

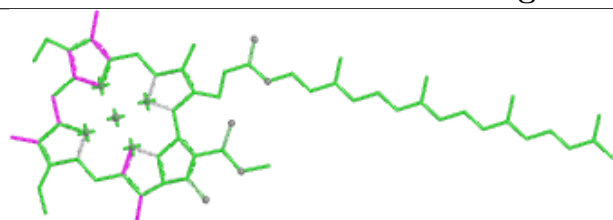


Torsions

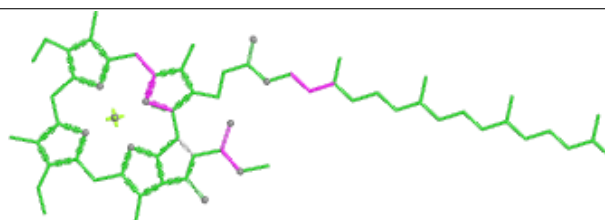


Rings

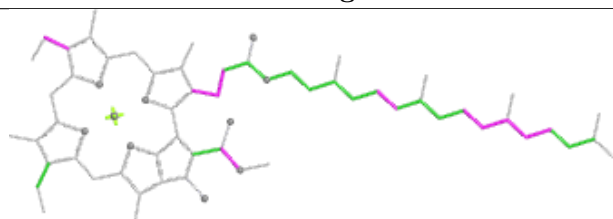
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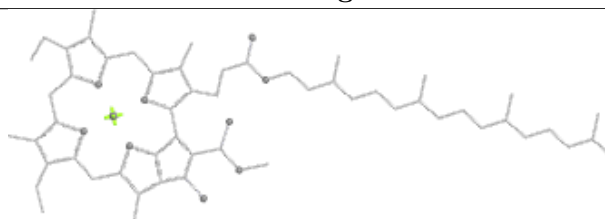
Bond lengths



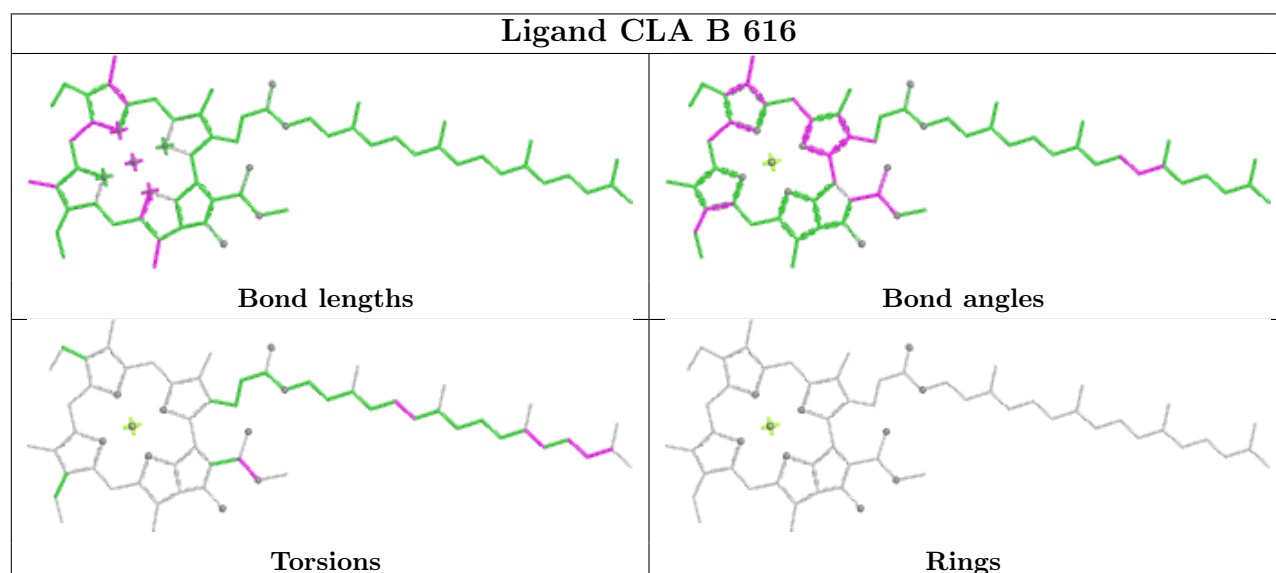
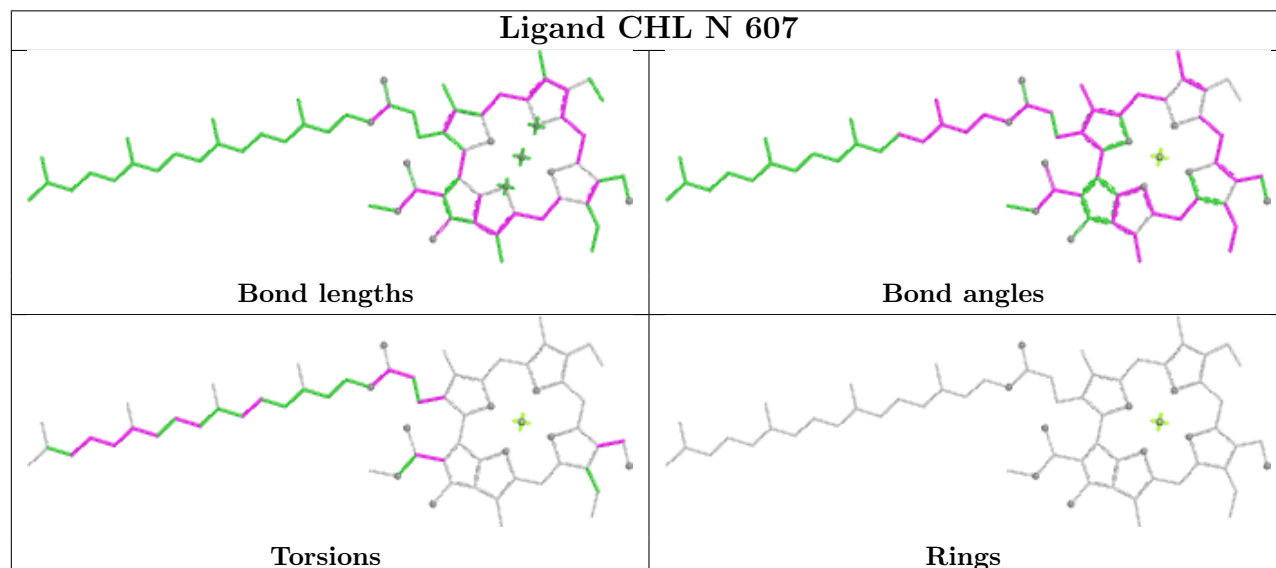
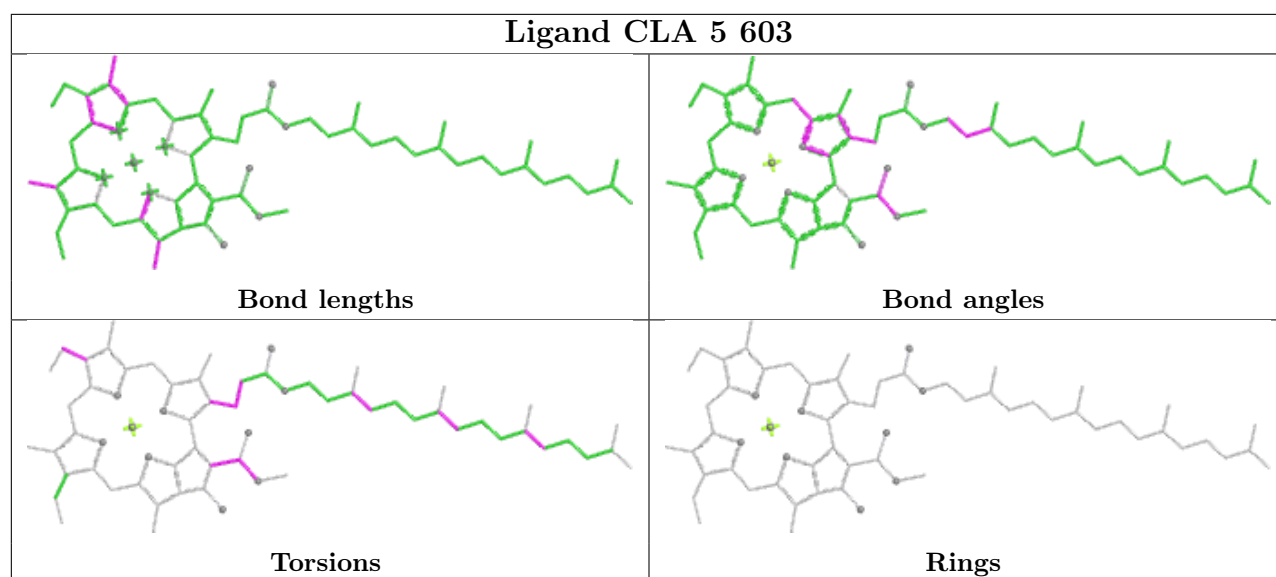
Bond angles

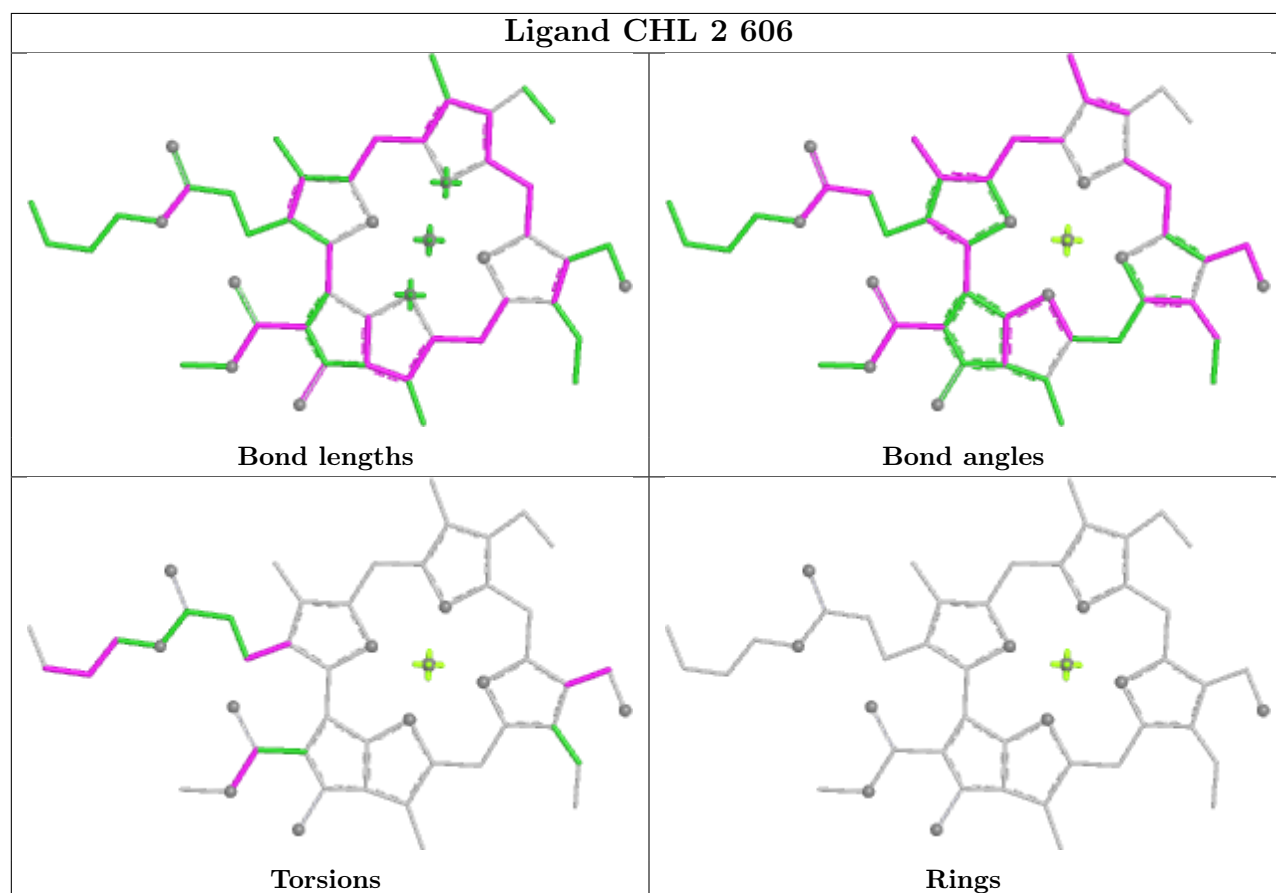
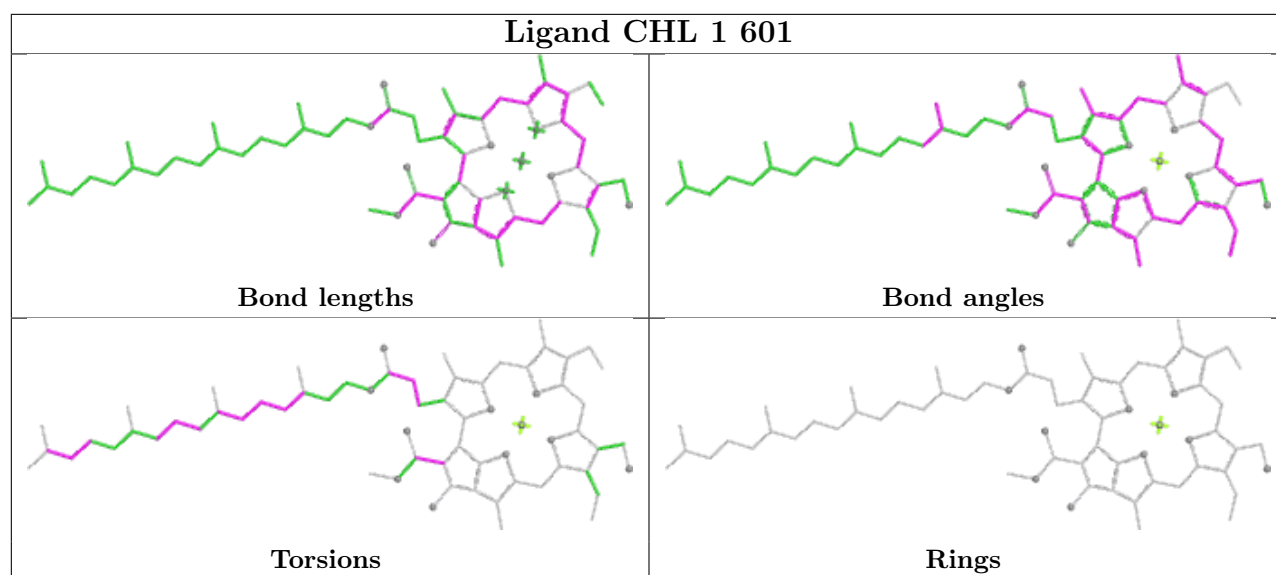


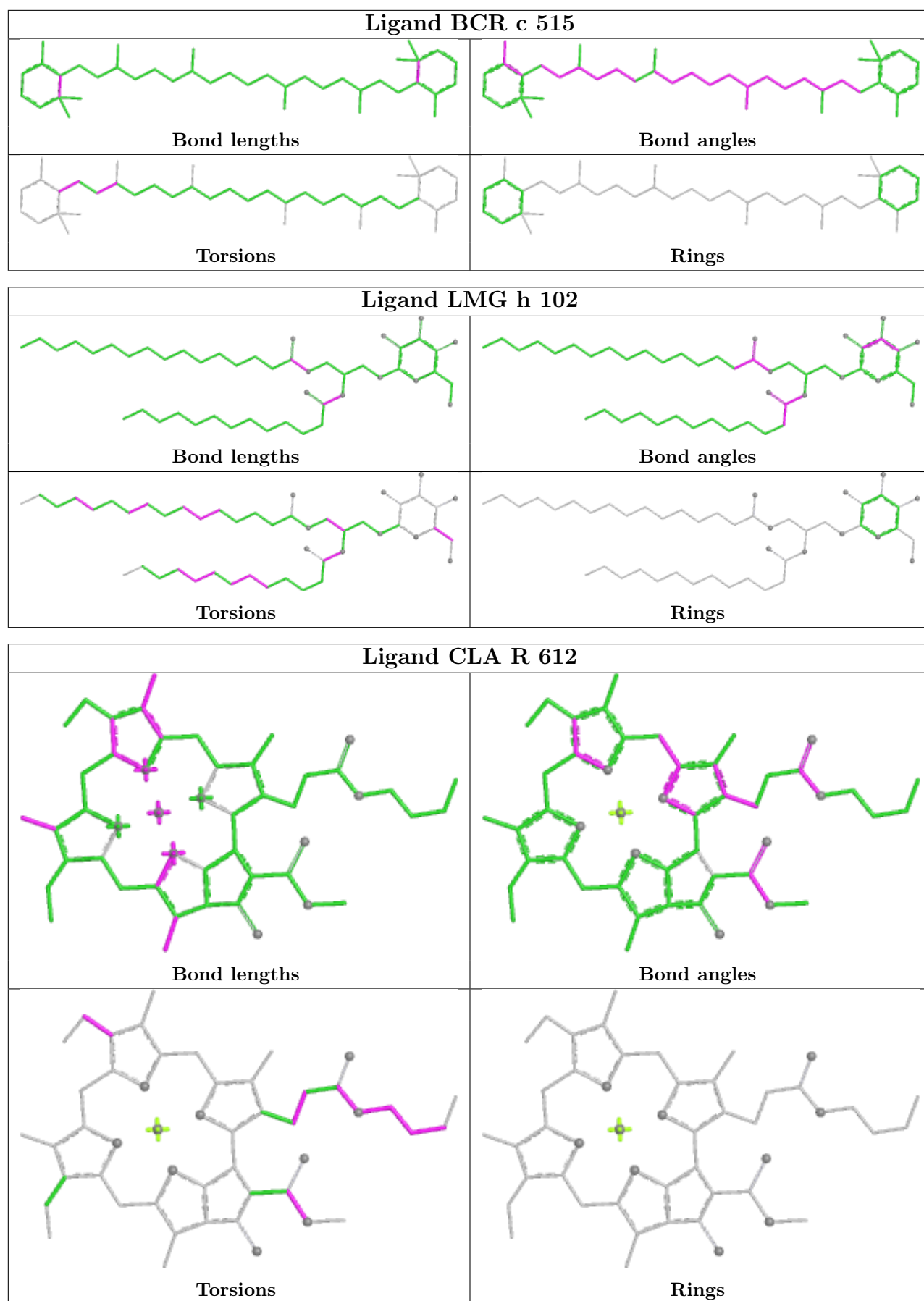
Torsions

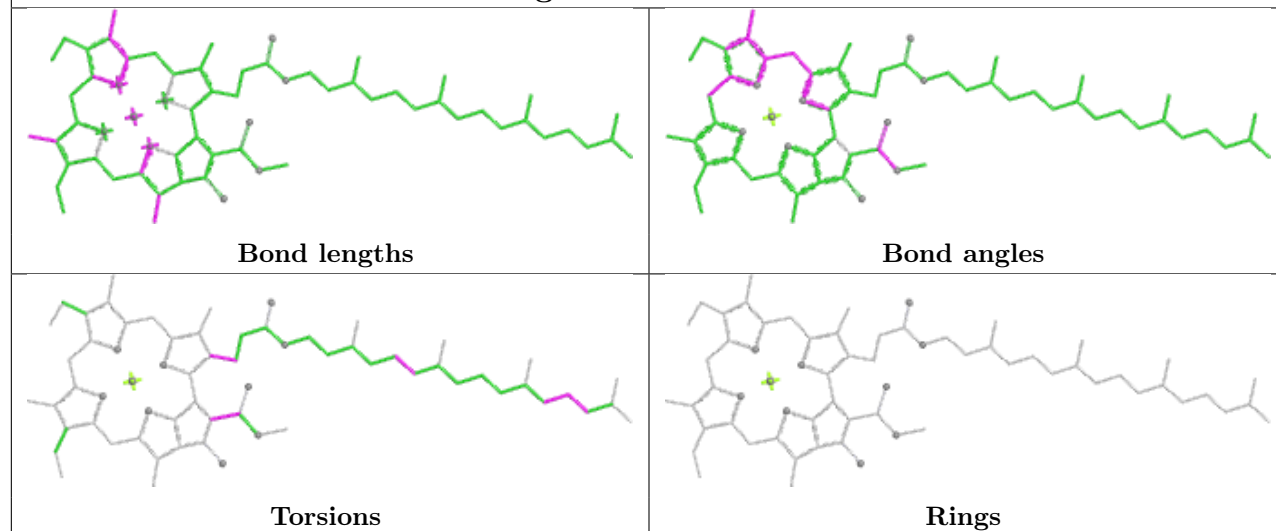
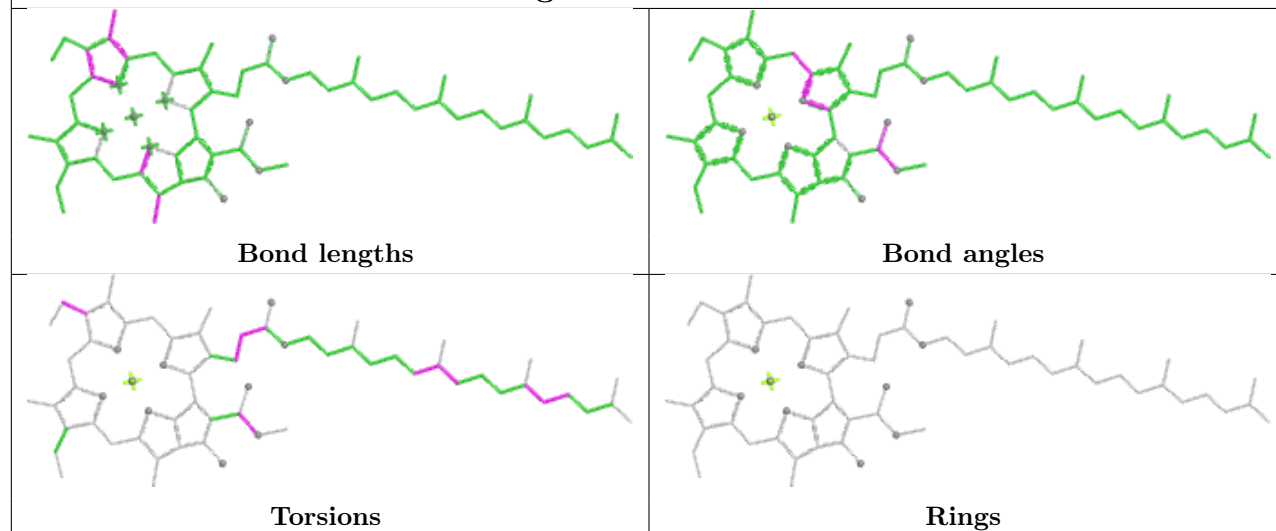


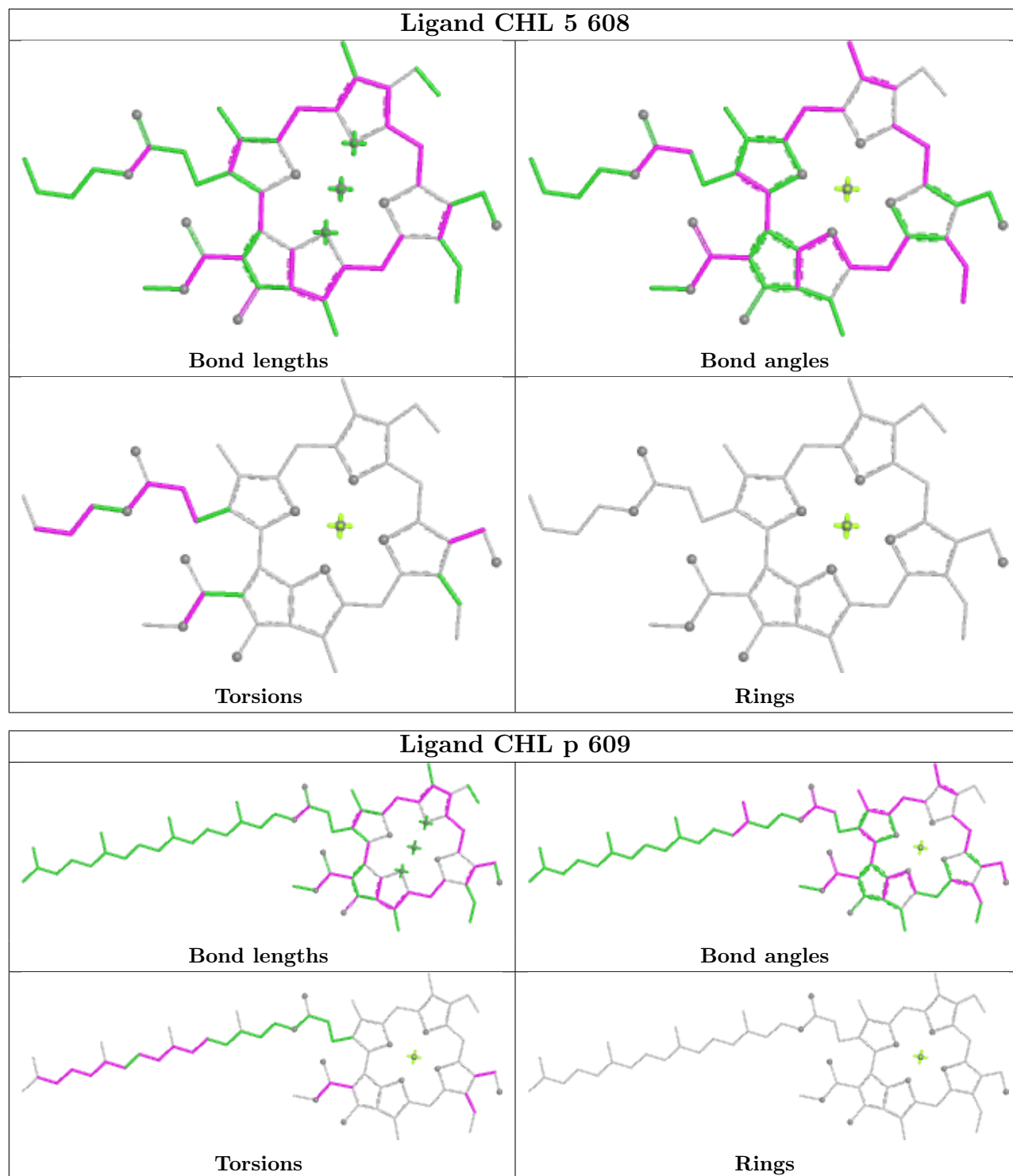
Rings



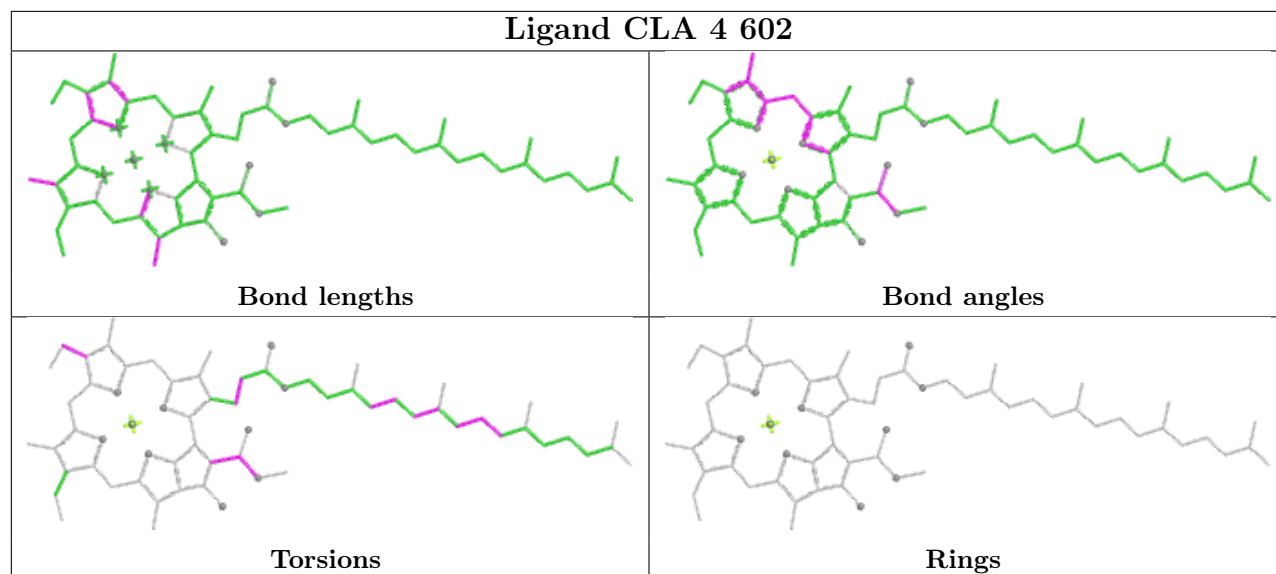




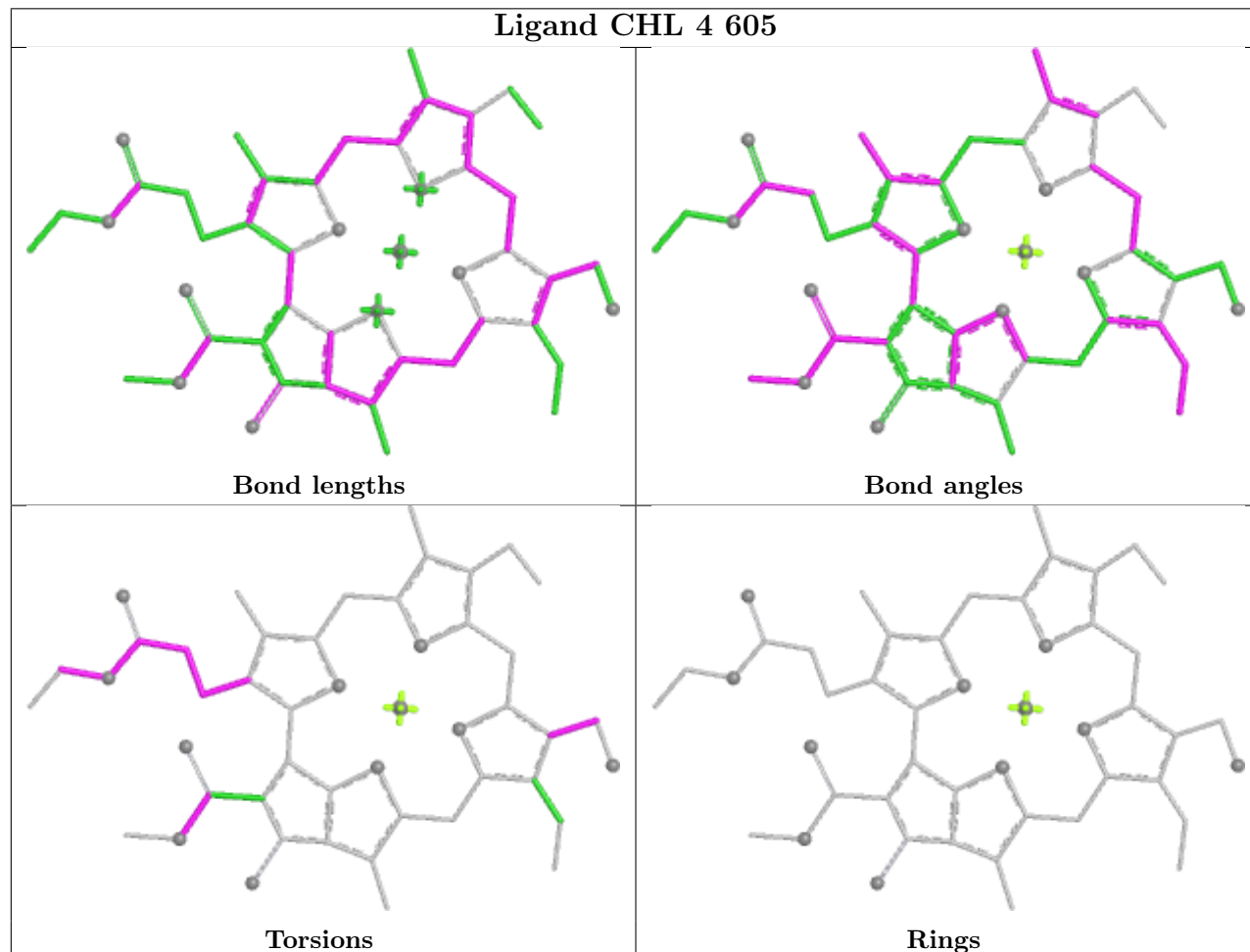
Ligand CLA b 610**Ligand CLA 5 613**

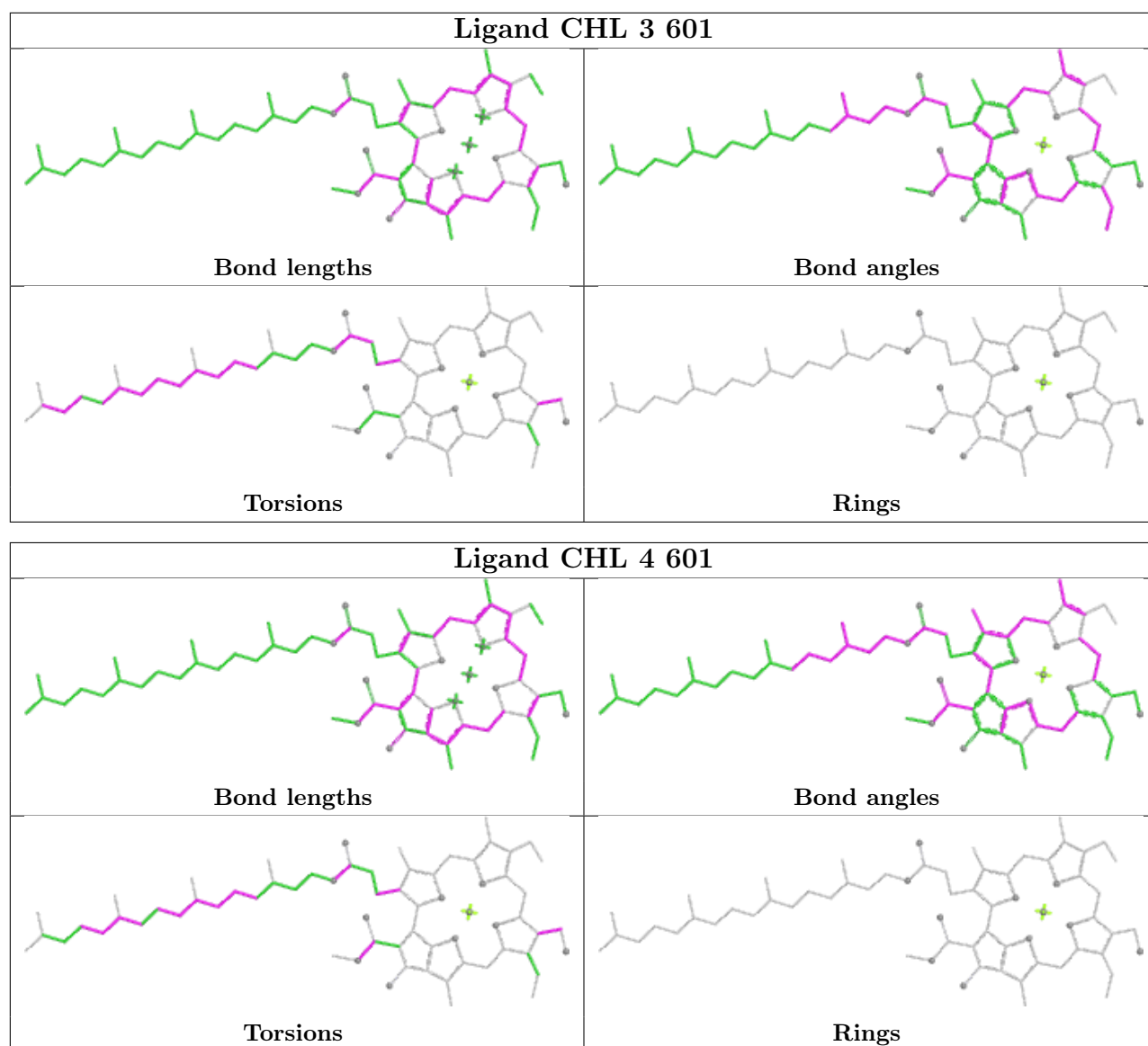


Ligand CLA 4 602

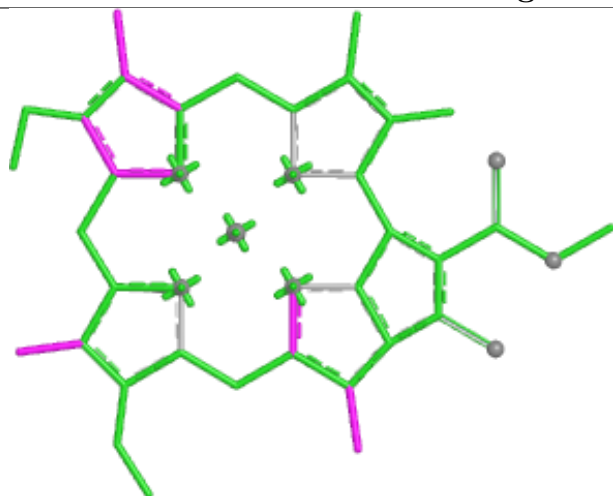


Ligand CHL 4 605

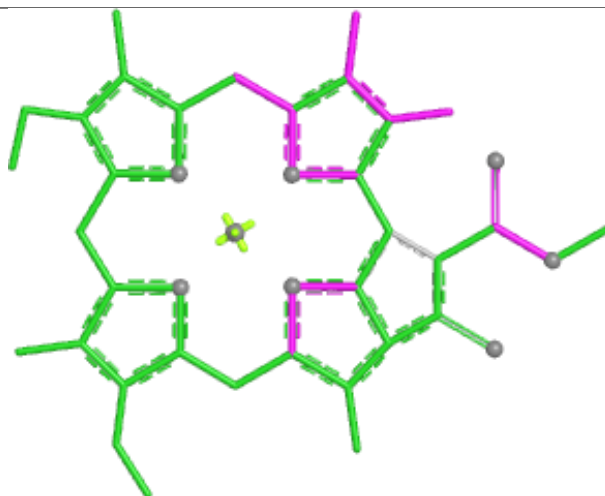




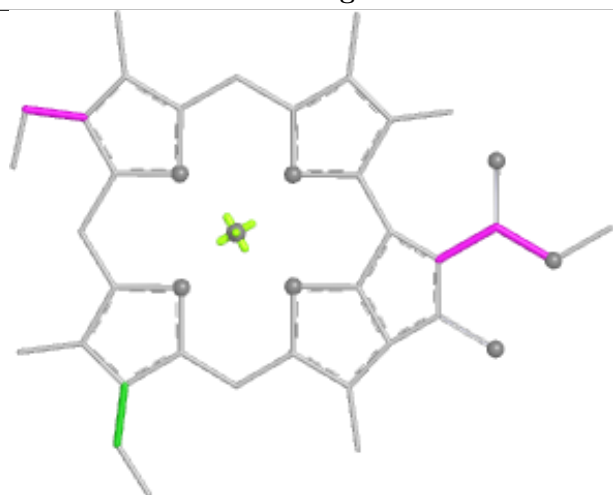
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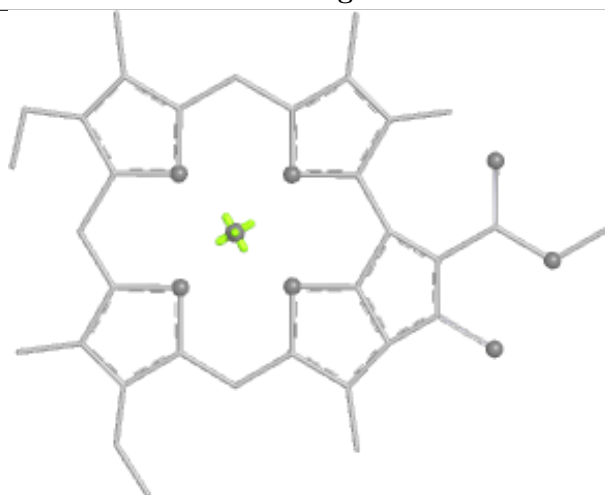
Bond lengths



Bond angles

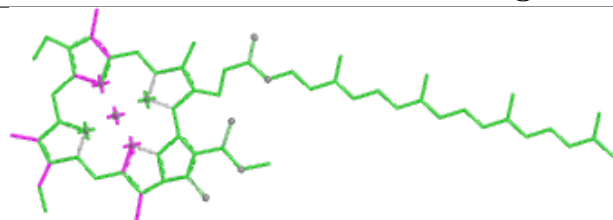


Torsions

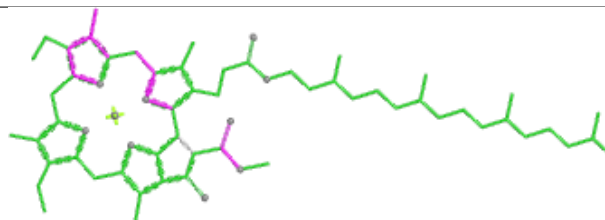


Rings

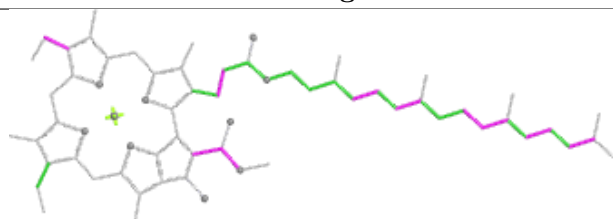
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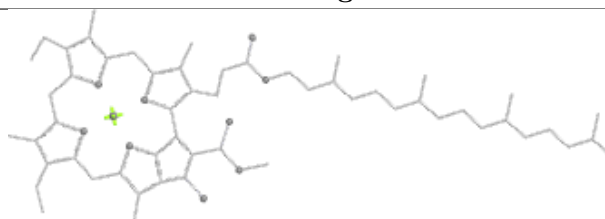
Bond lengths



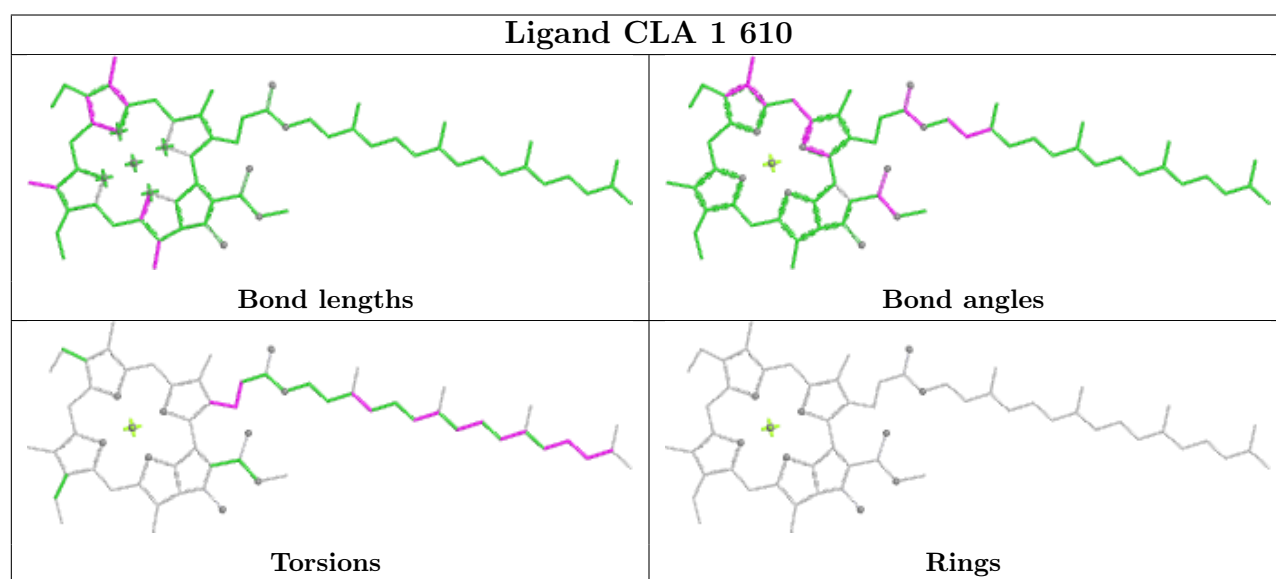
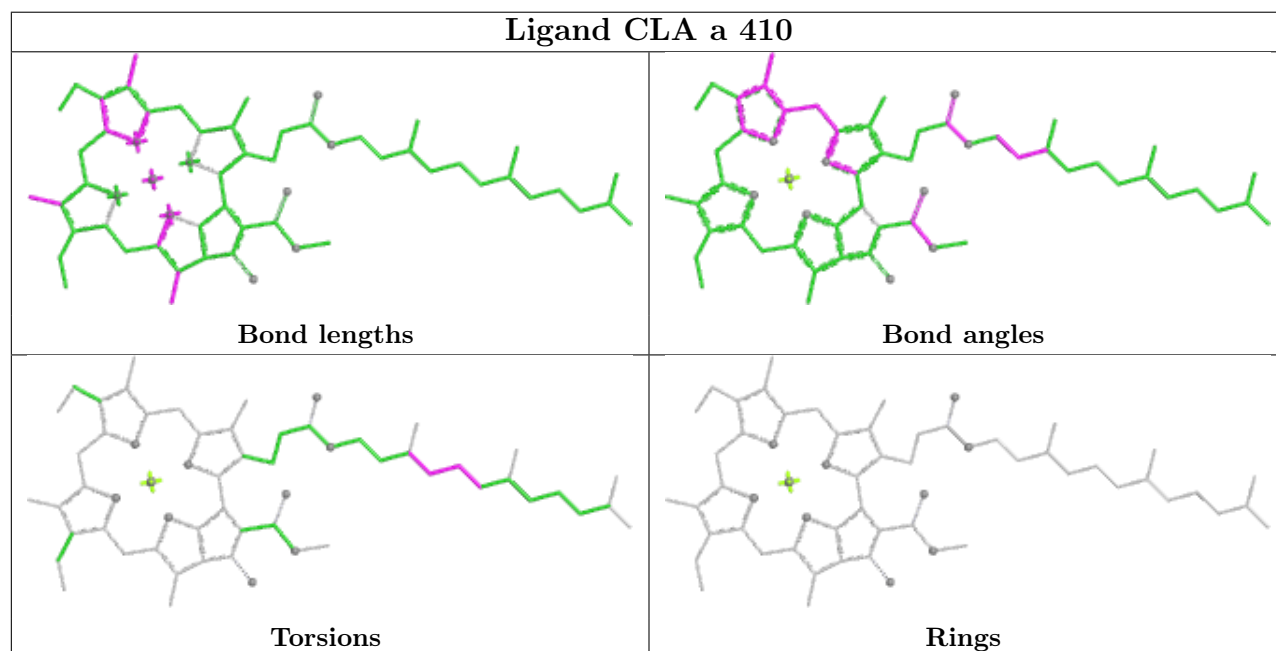
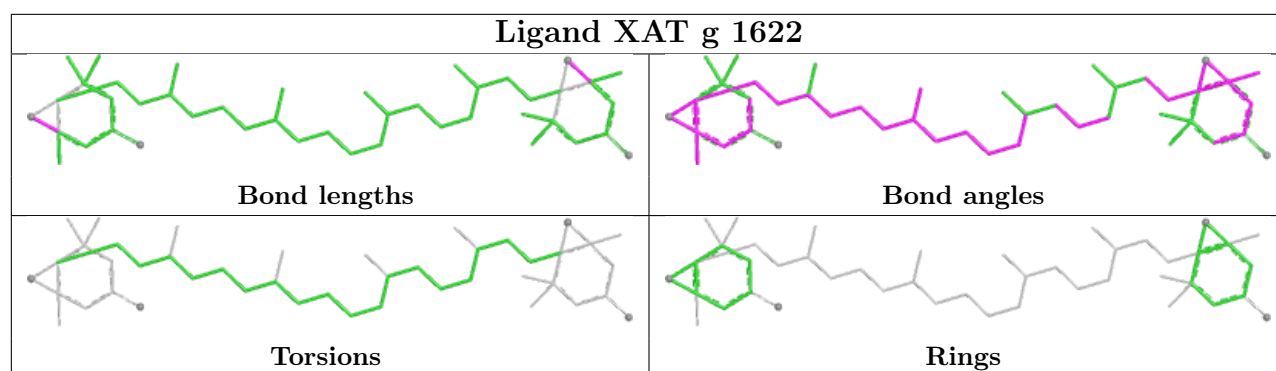
Bond angles

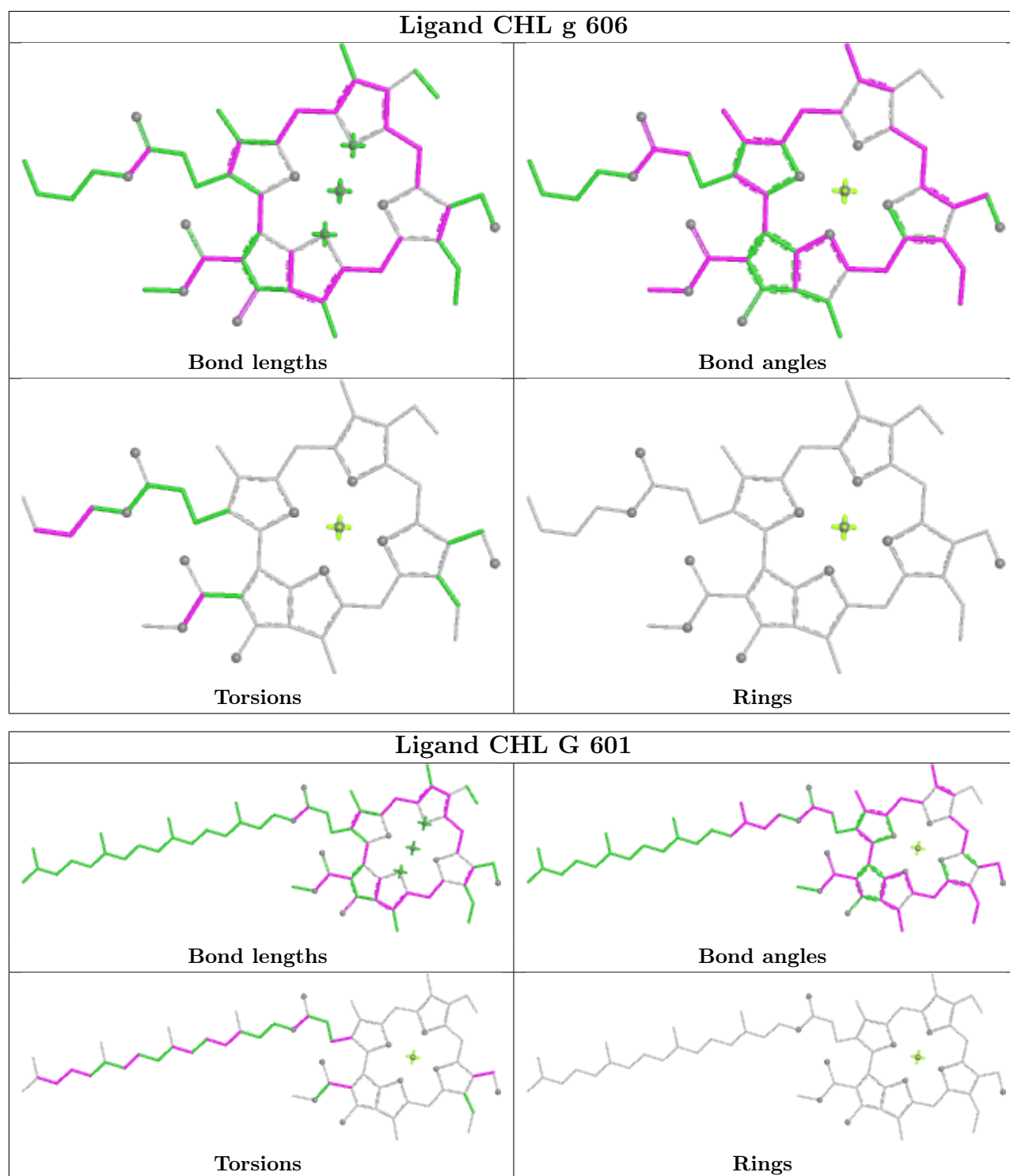


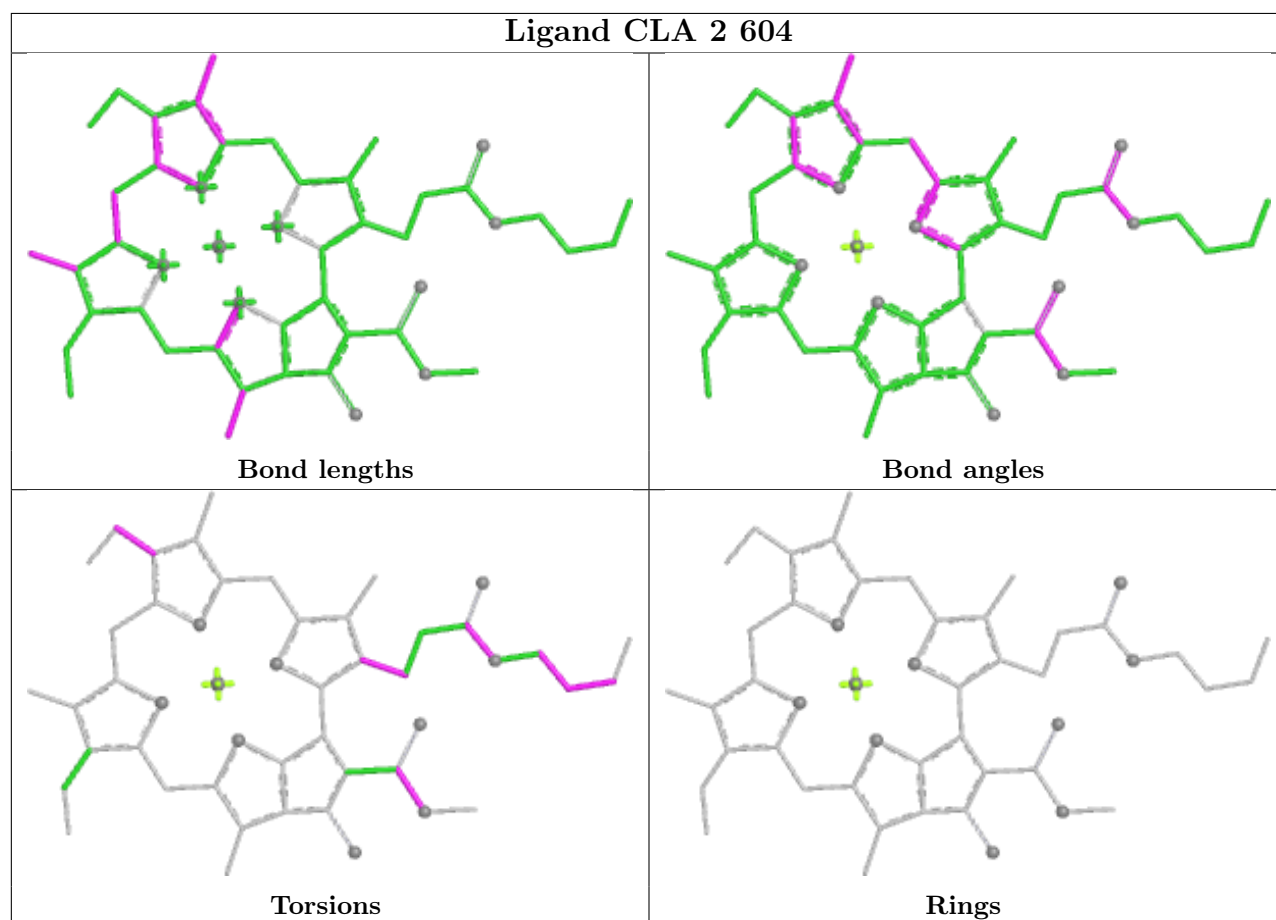
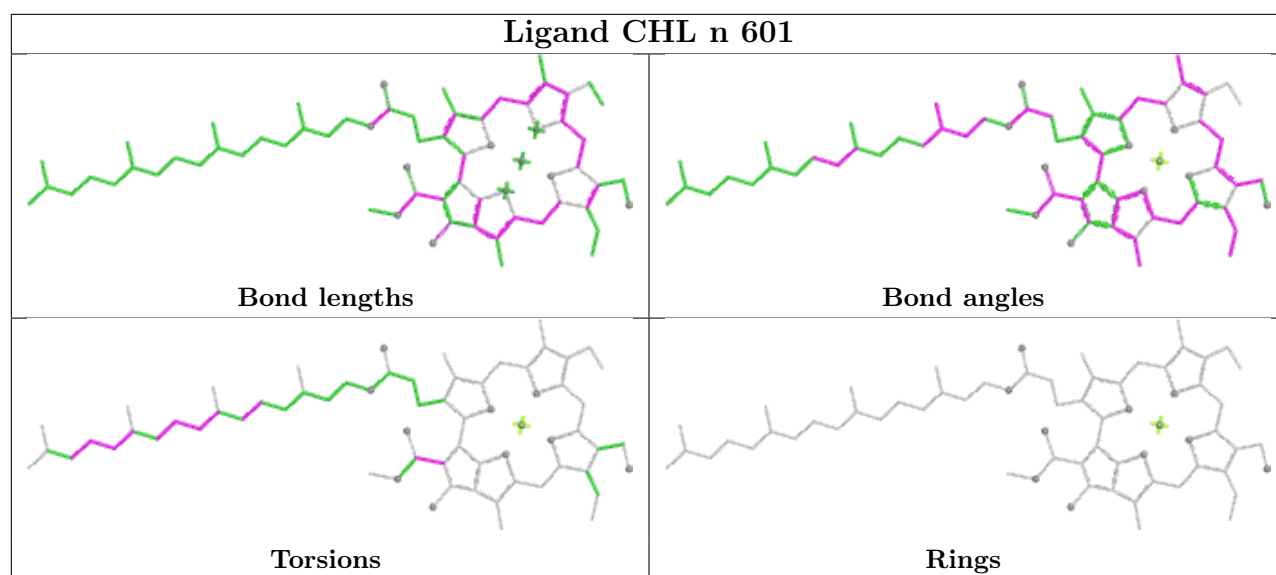
Torsions

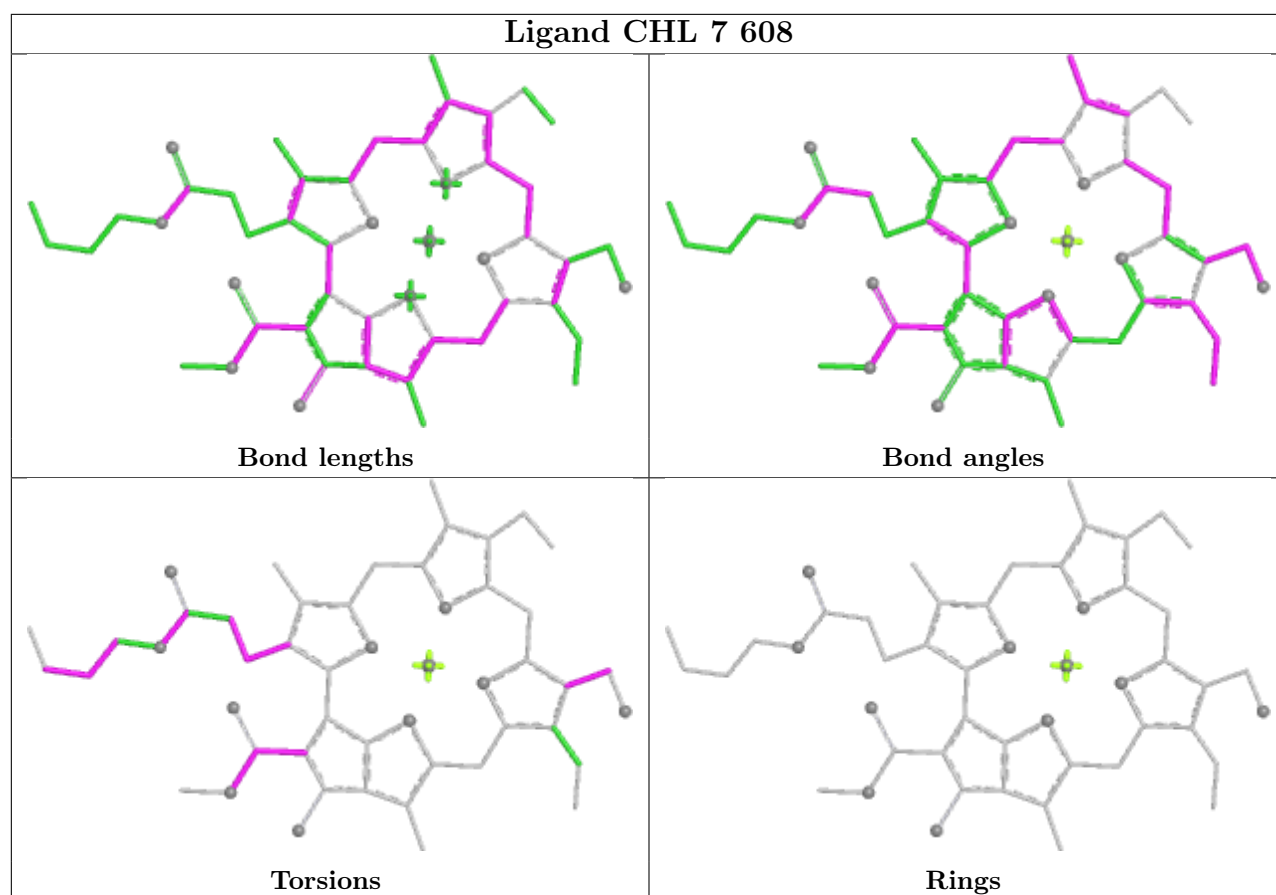


Rings

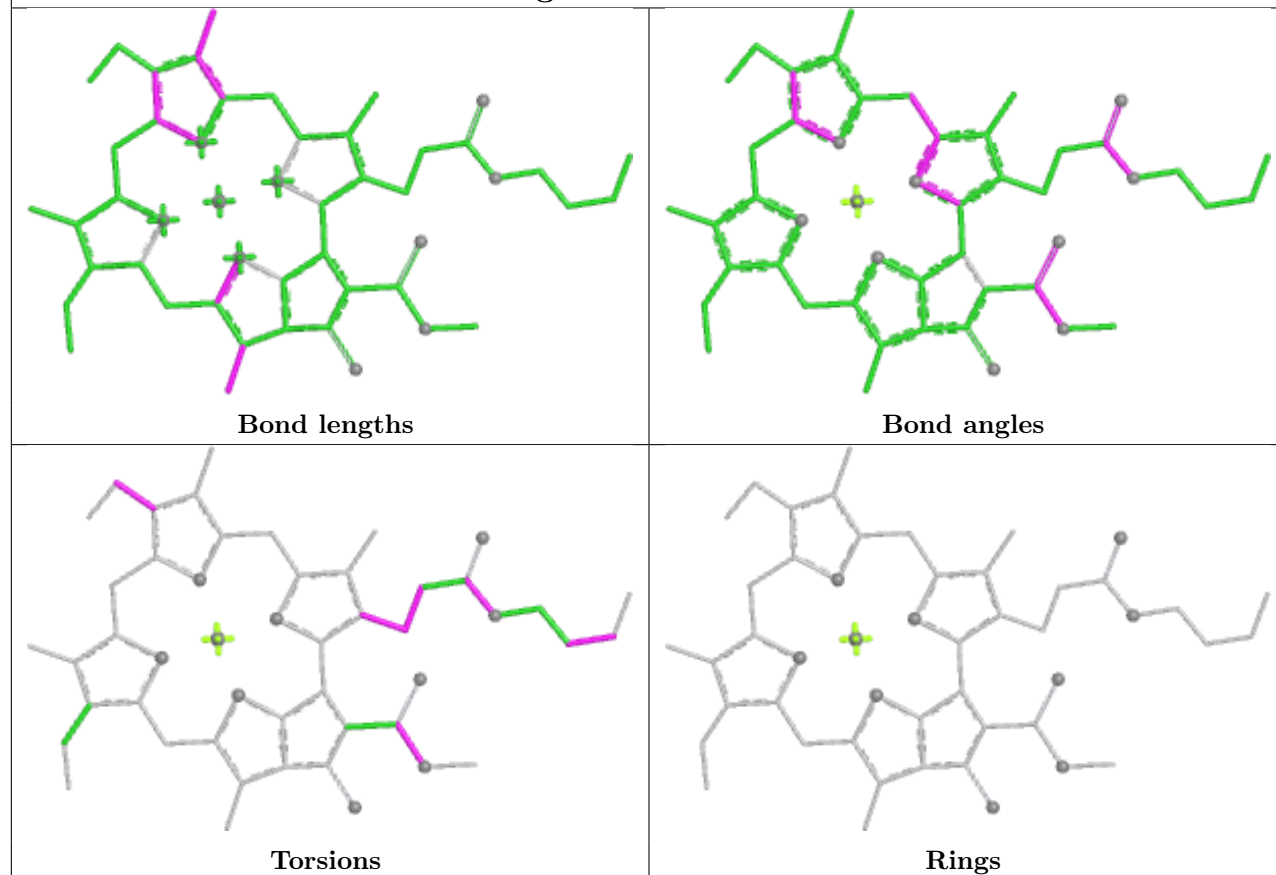




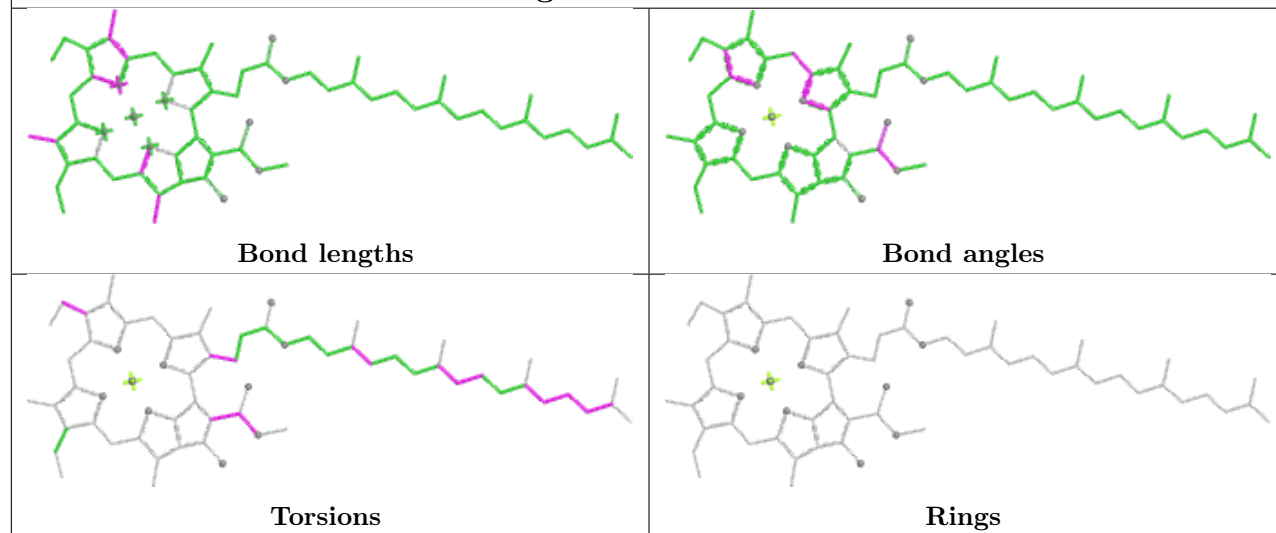


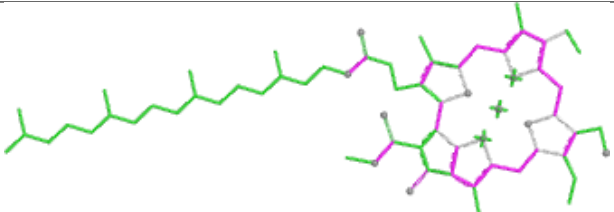
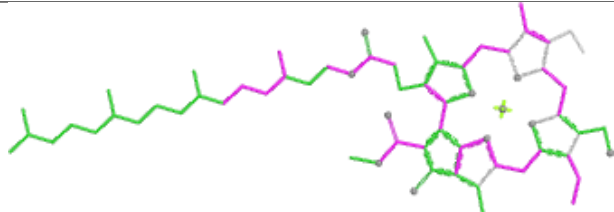
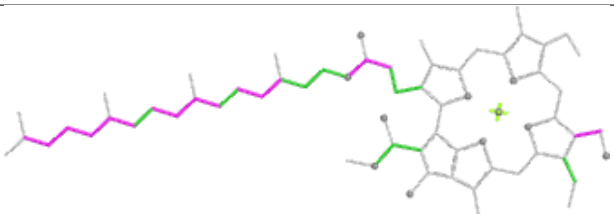
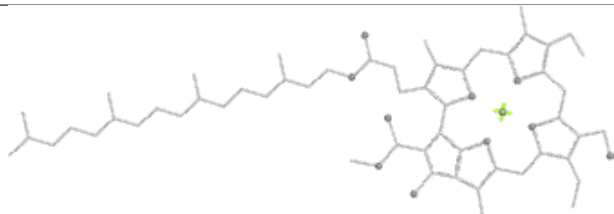


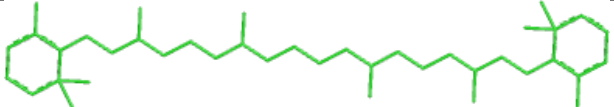
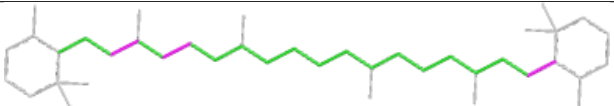
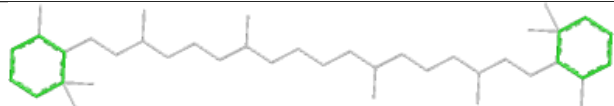
Ligand CLA 5 614

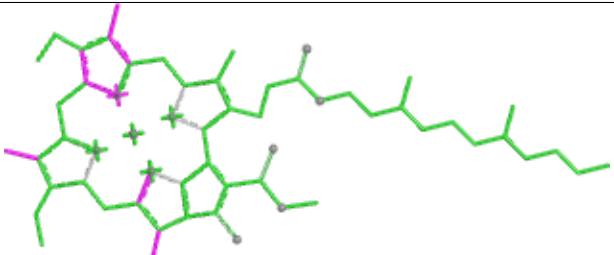
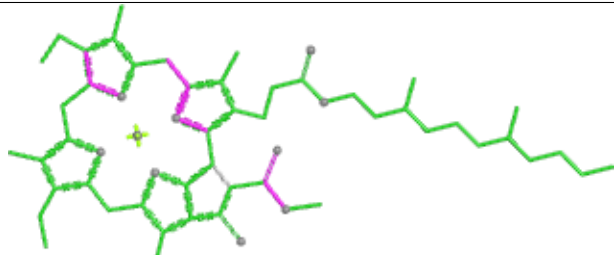
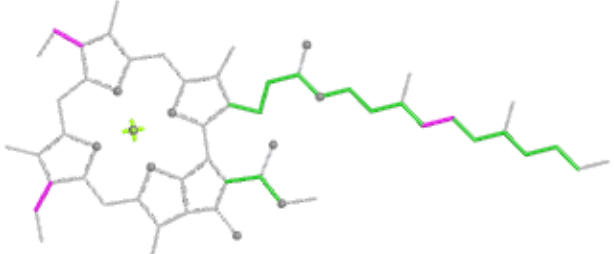
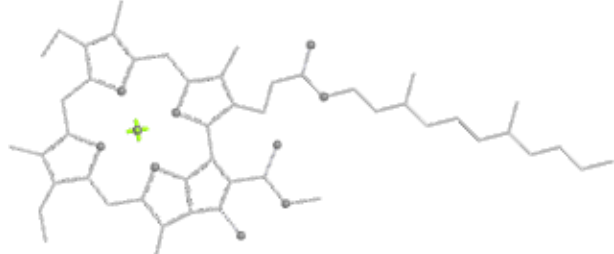


Ligand CLA 0 604

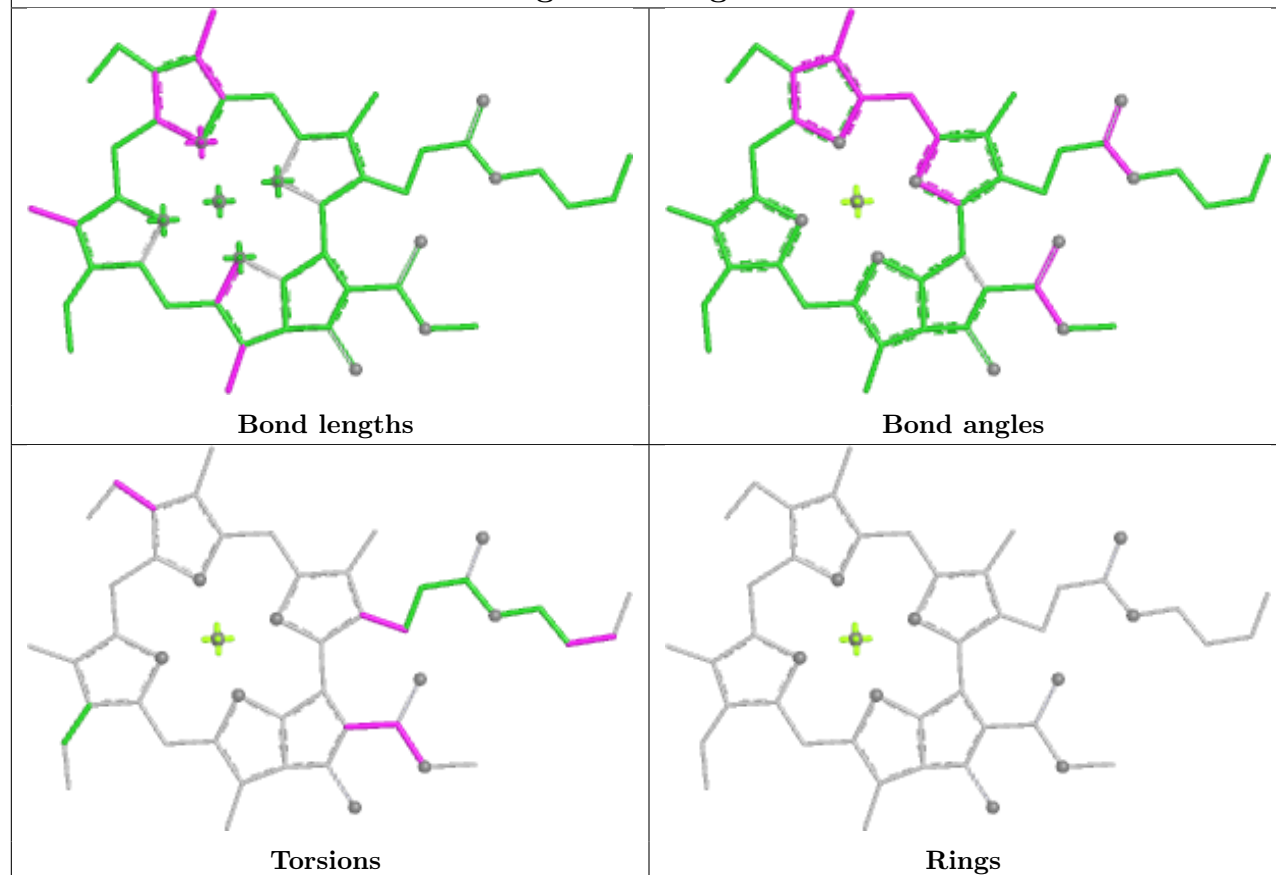


Ligand CHL 5 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

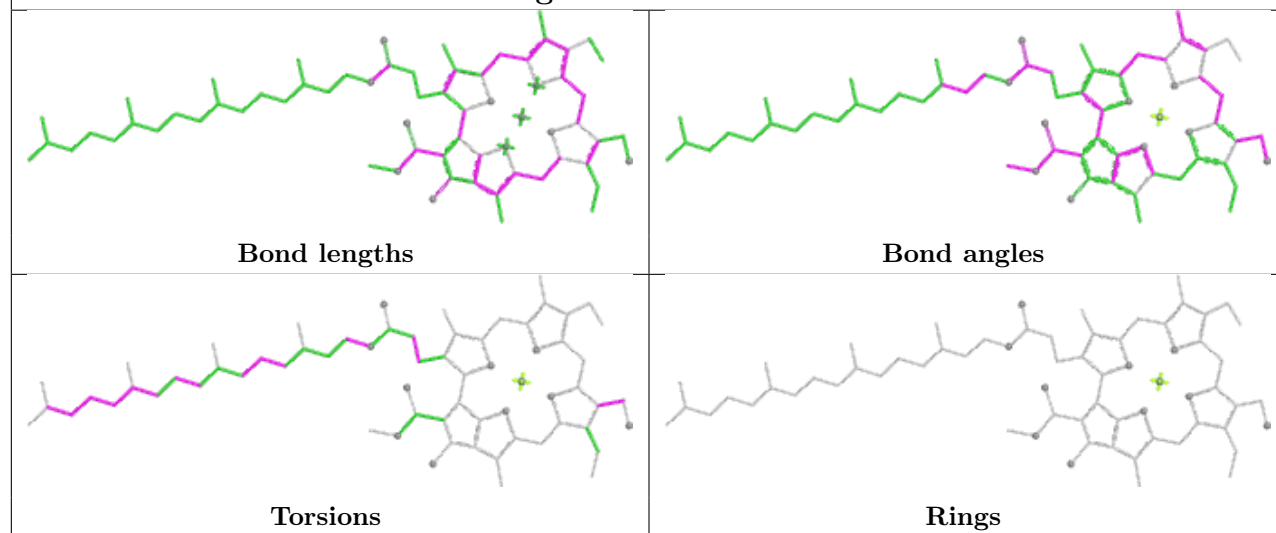
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

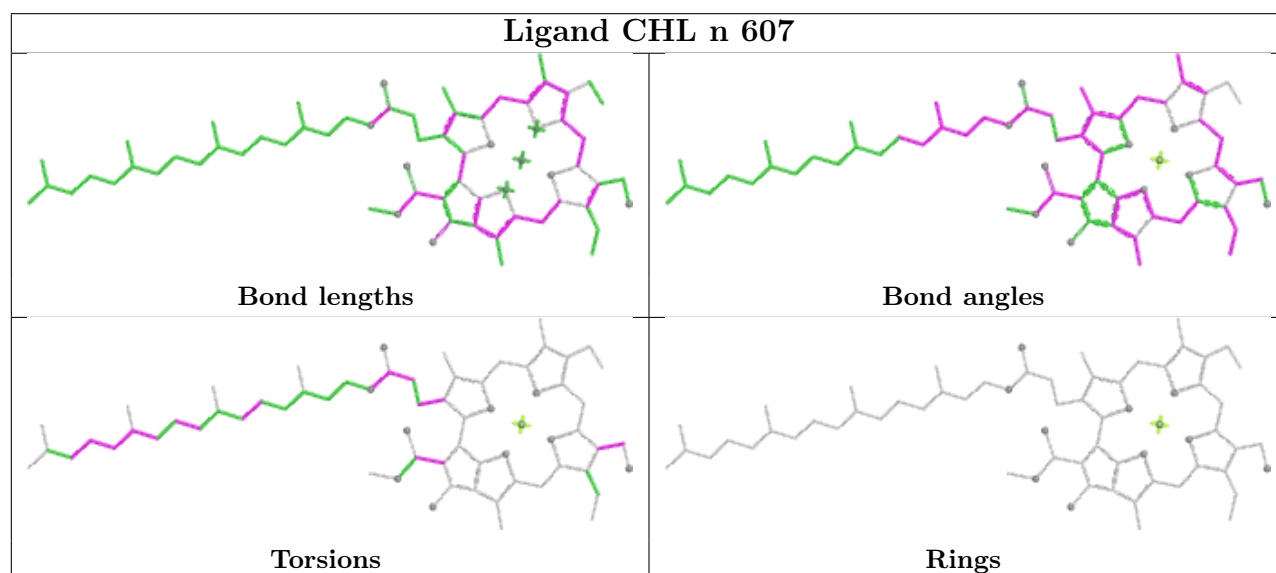
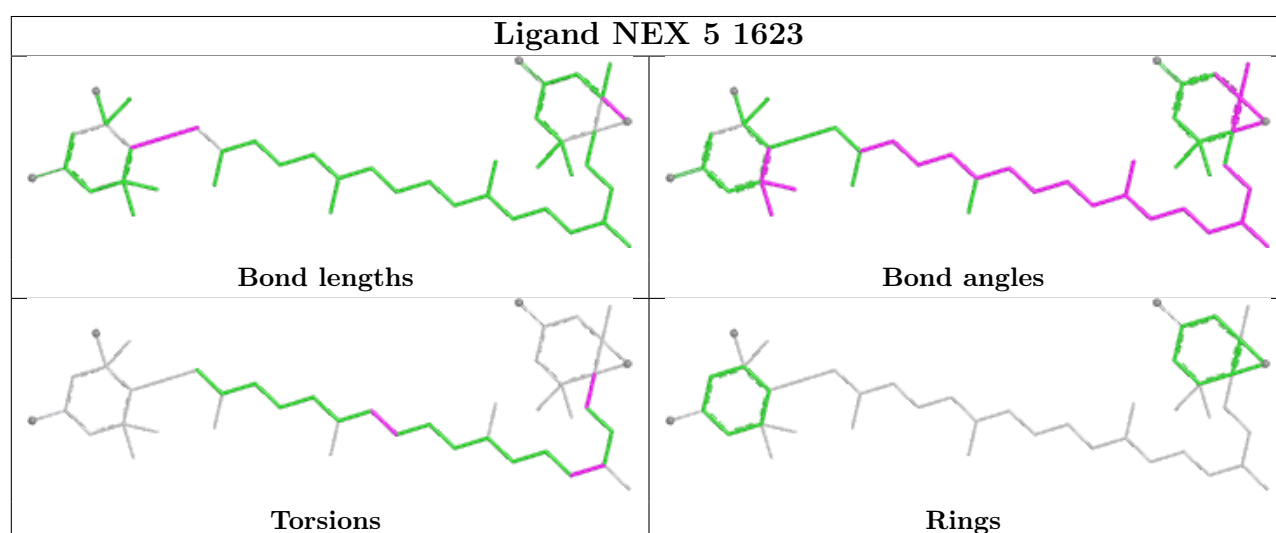
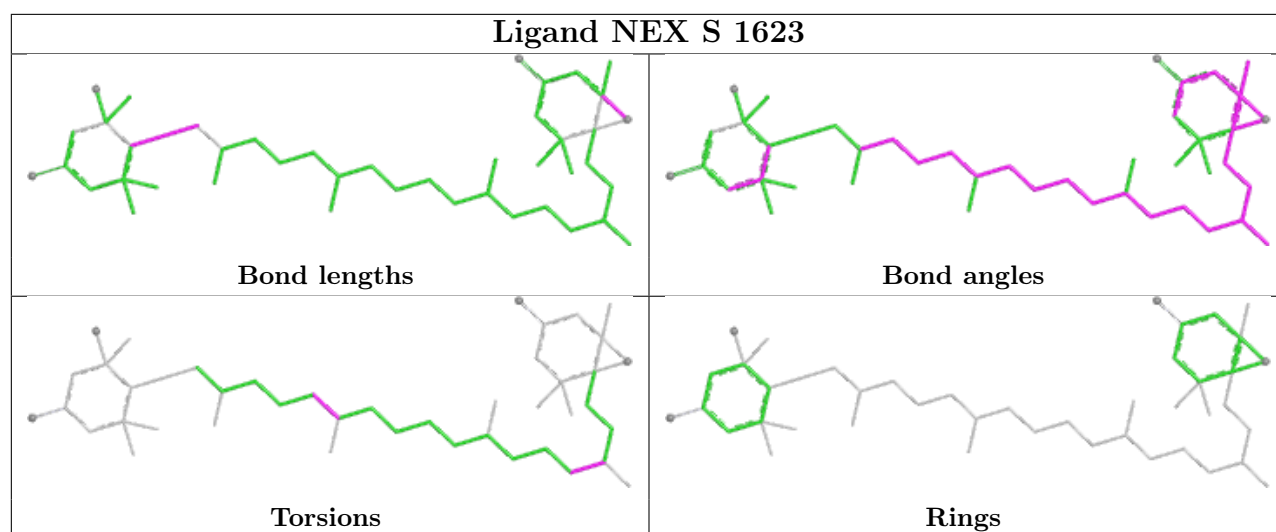
Ligand CLA r 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

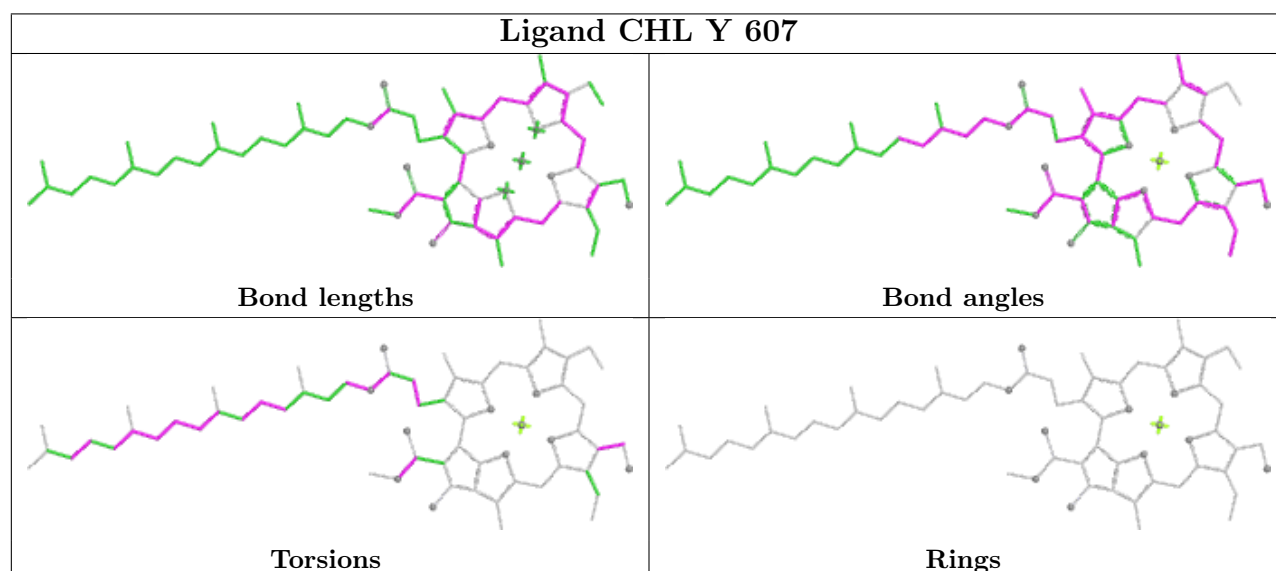
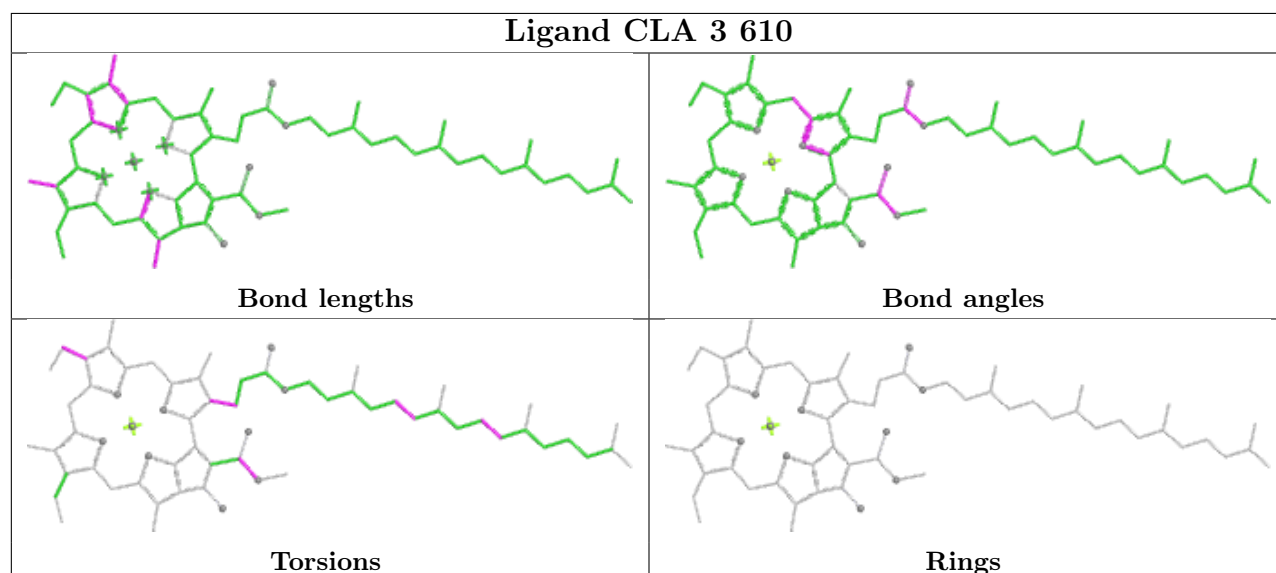
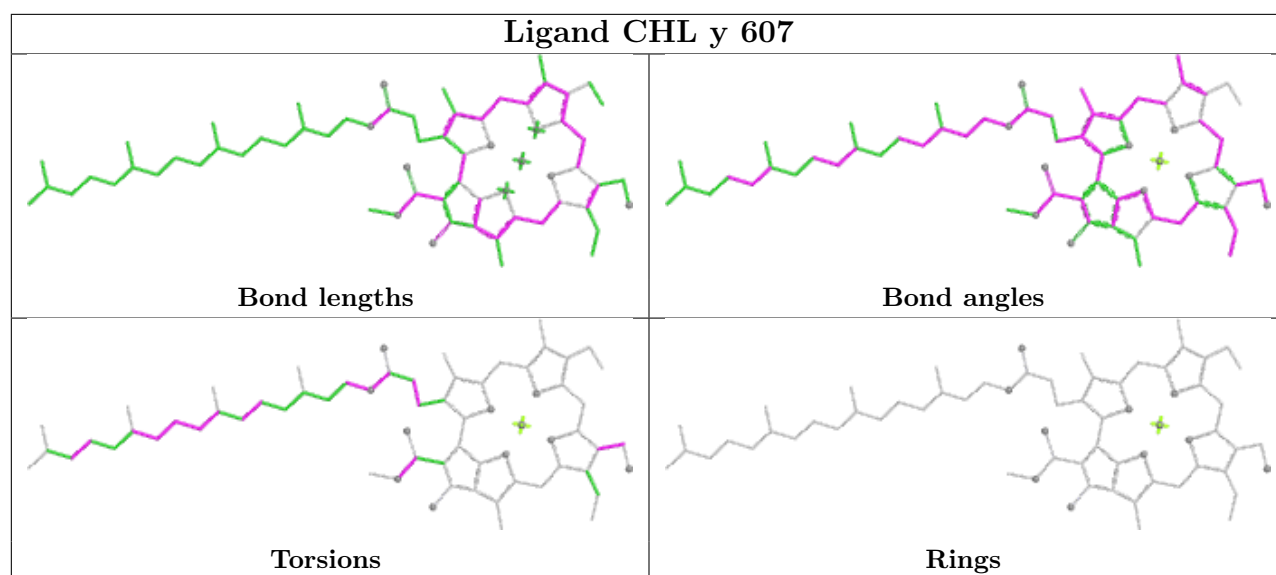
Ligand CLA g 604

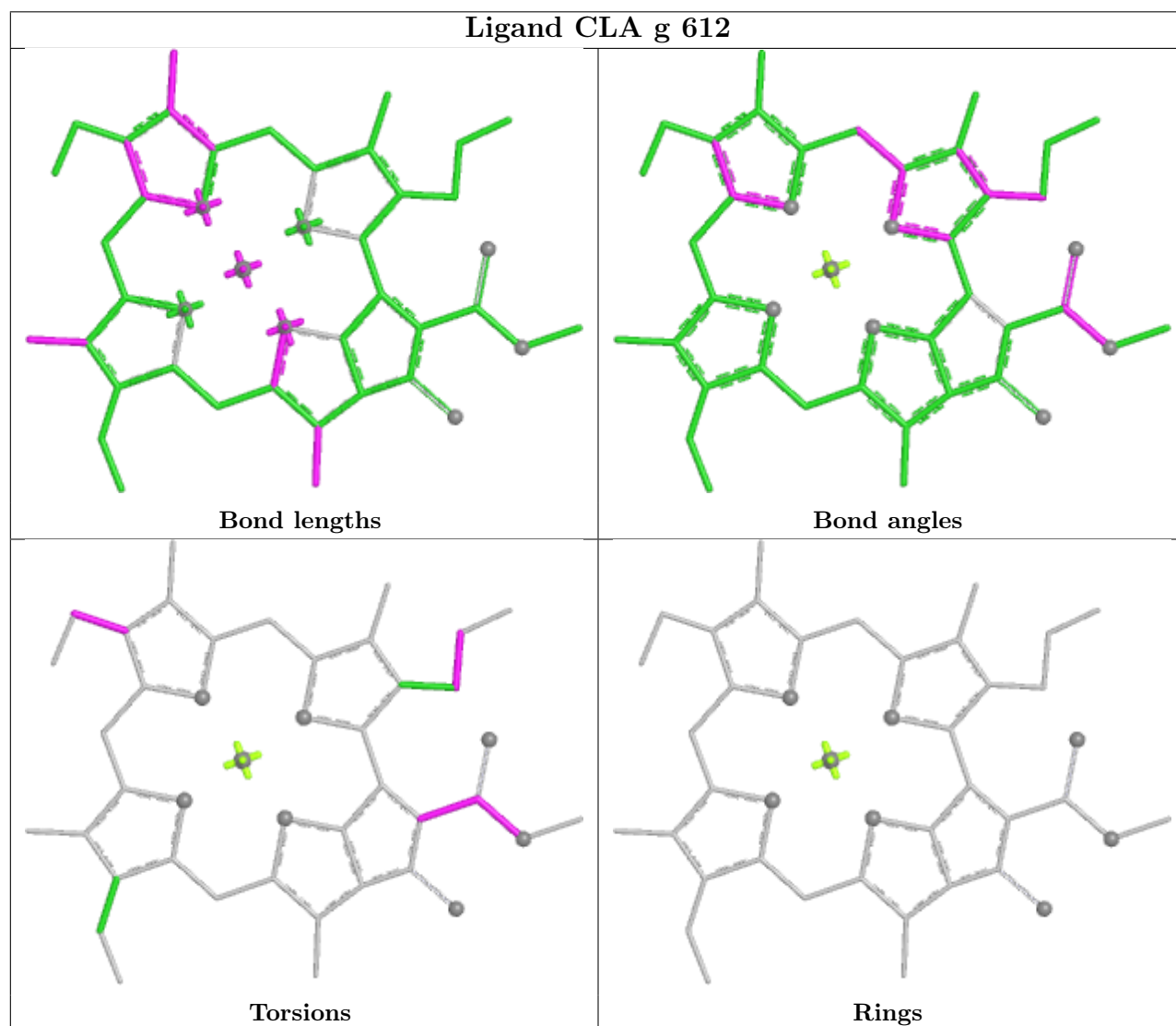
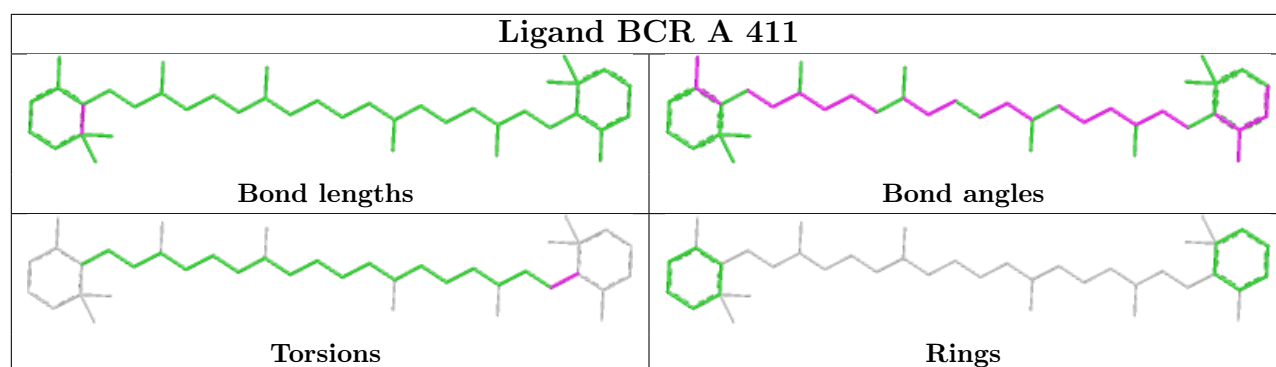


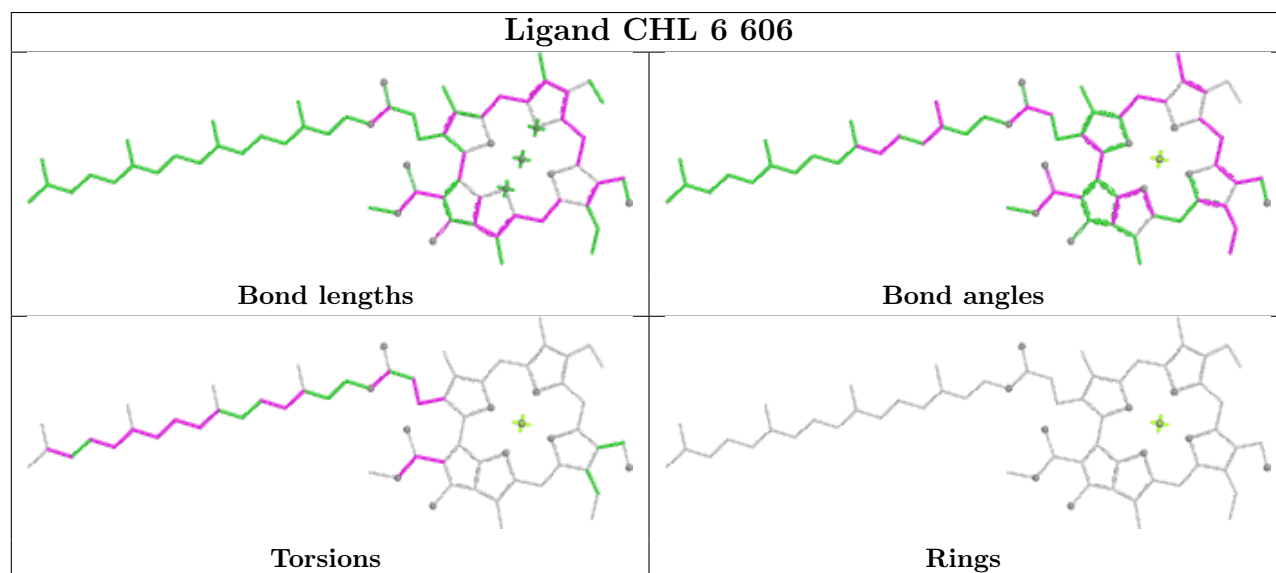
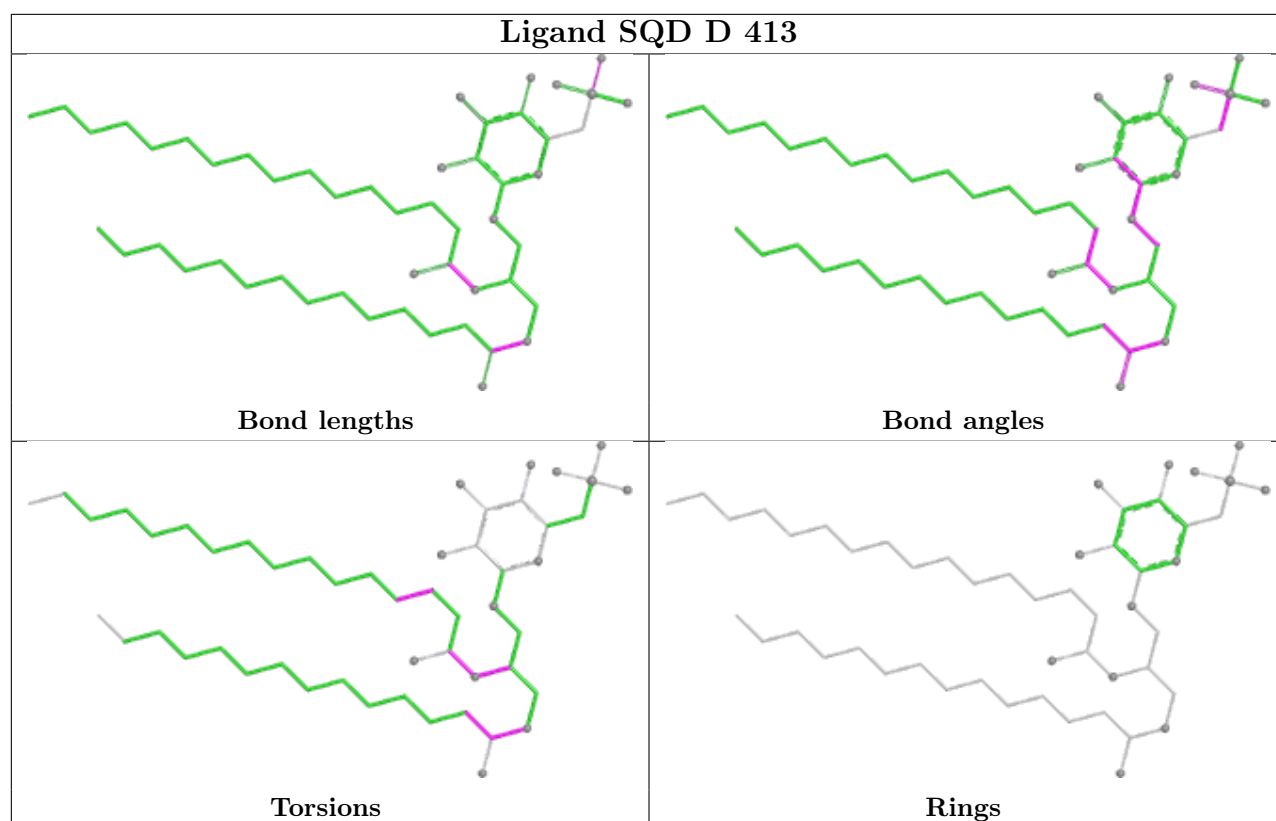
Ligand CHL 8 605



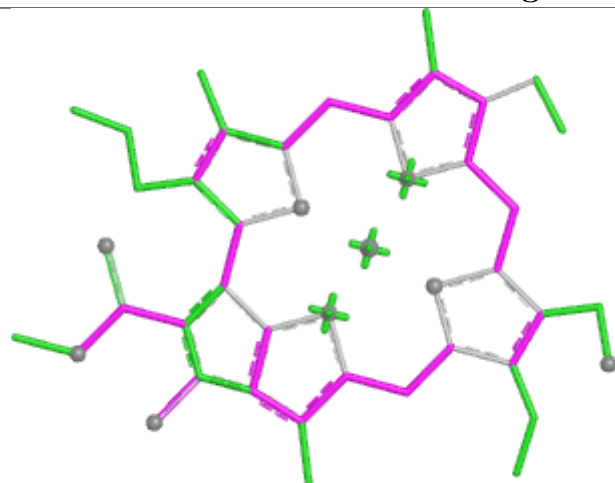




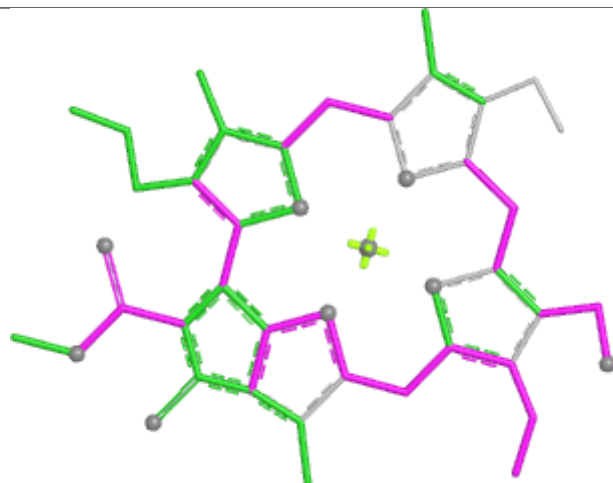




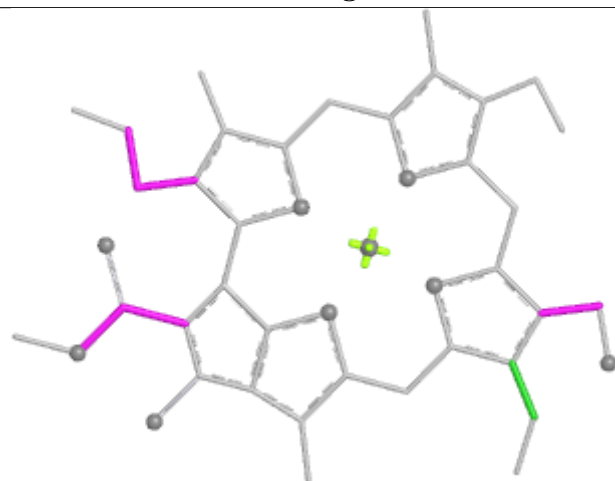
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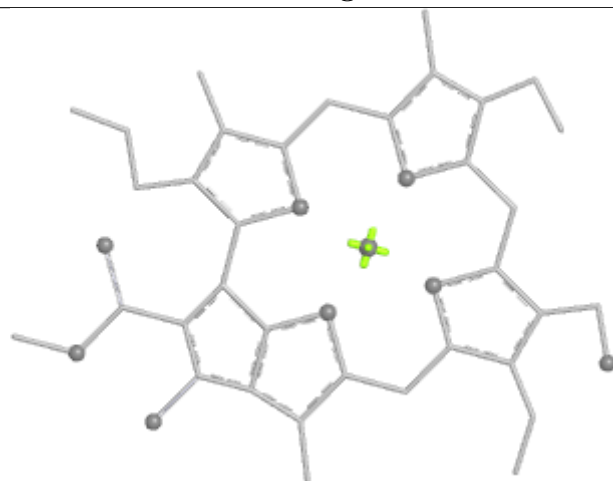
Bond lengths



Bond angles

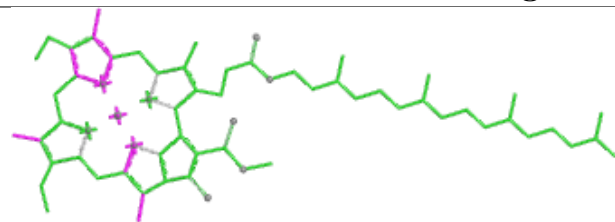


Torsions

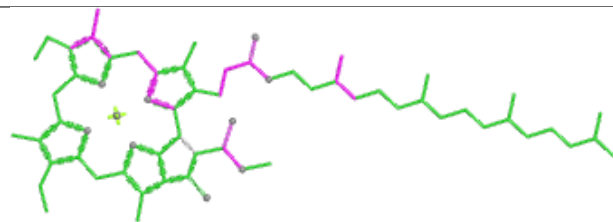


Rings

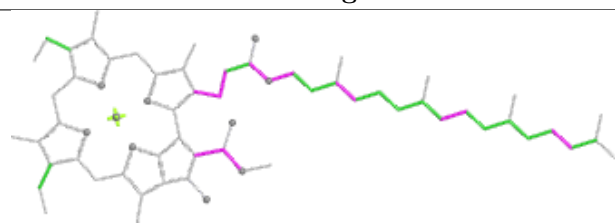
Ligand CLA c 503



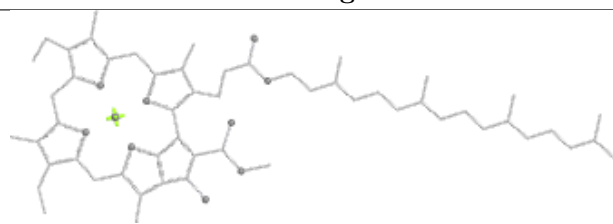
Bond lengths



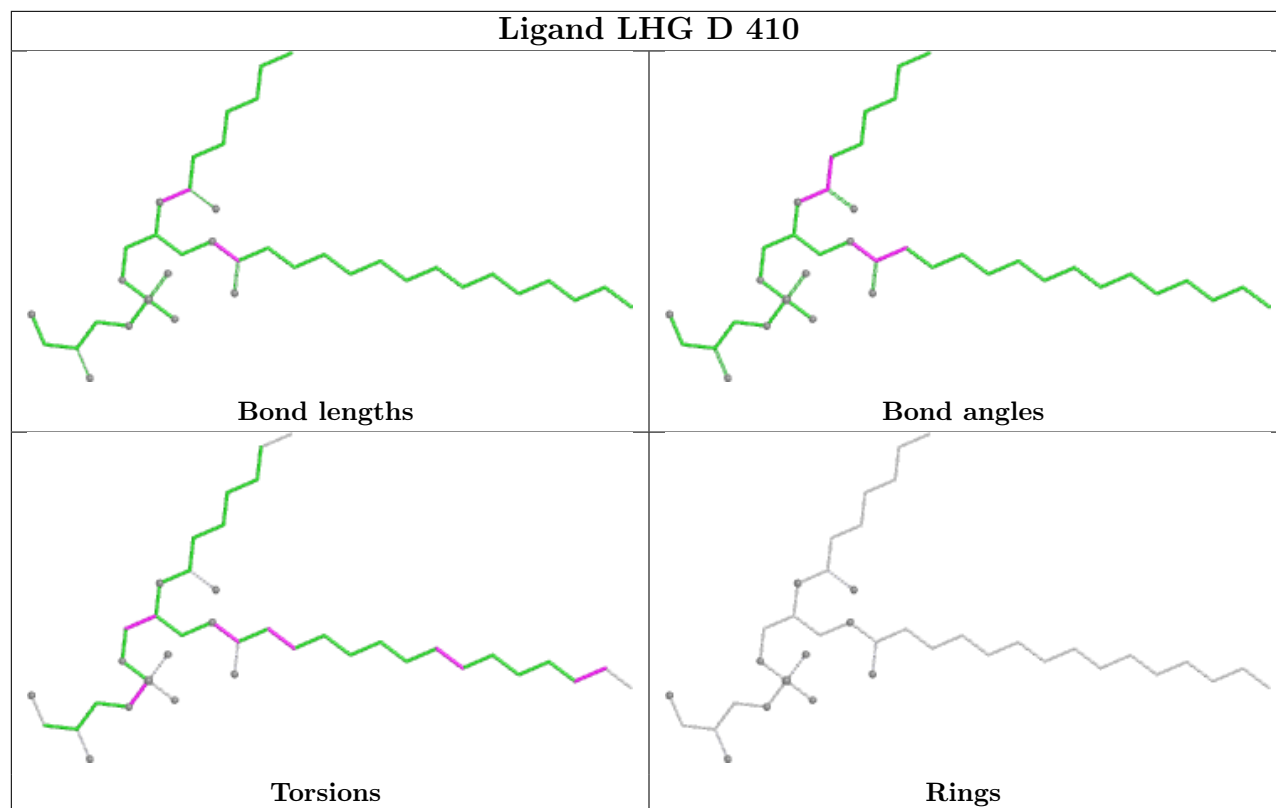
Bond angles



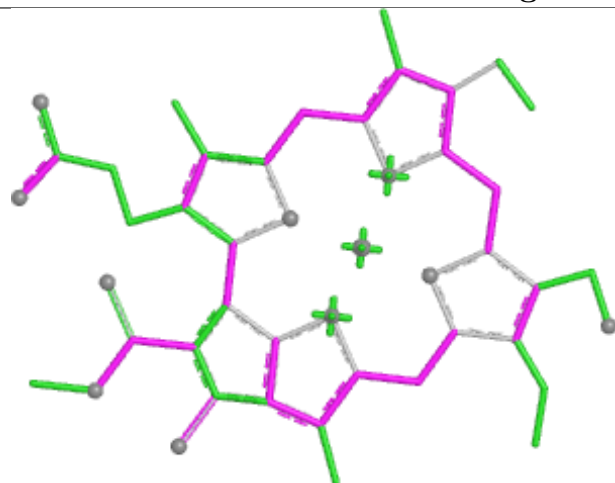
Torsions



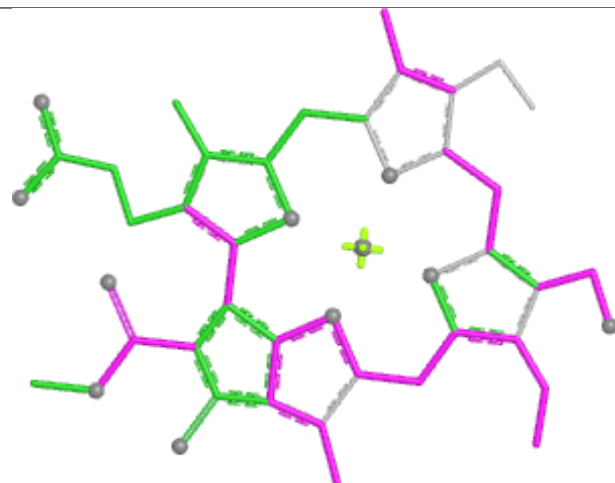
Rings



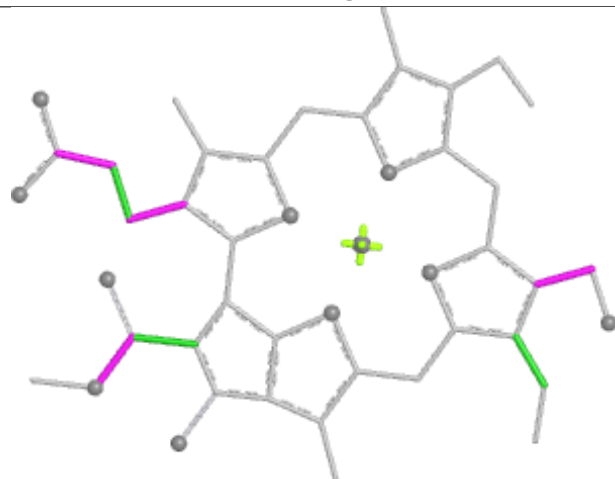
Ligand CHL 3 606



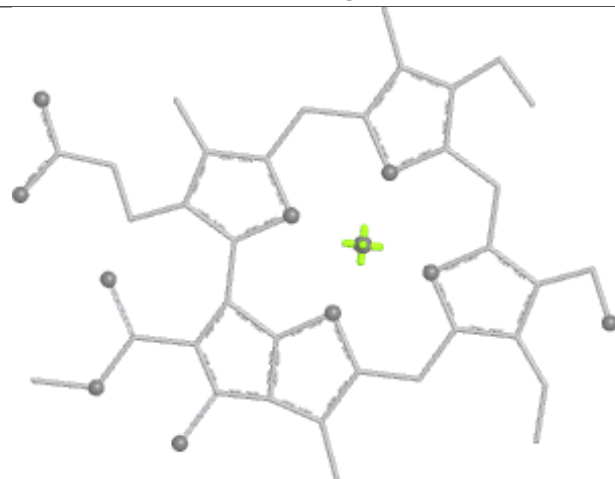
Bond lengths



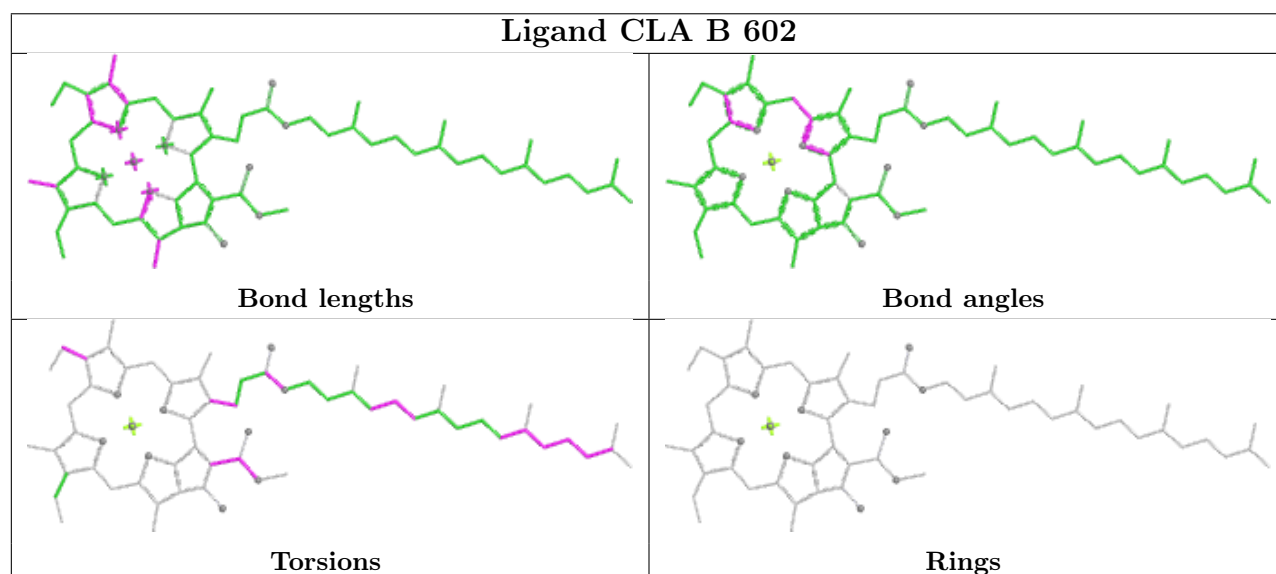
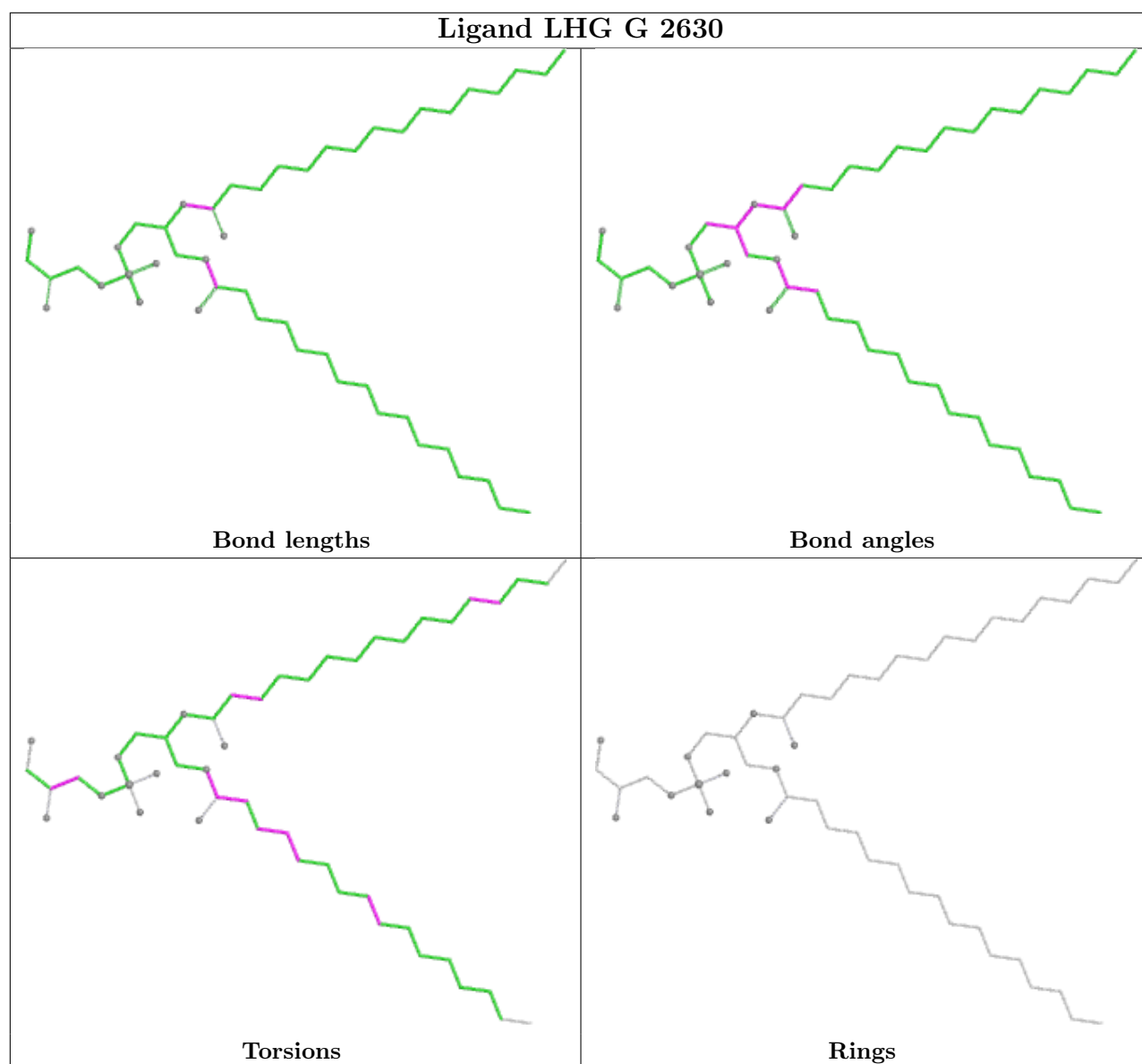
Bond angles

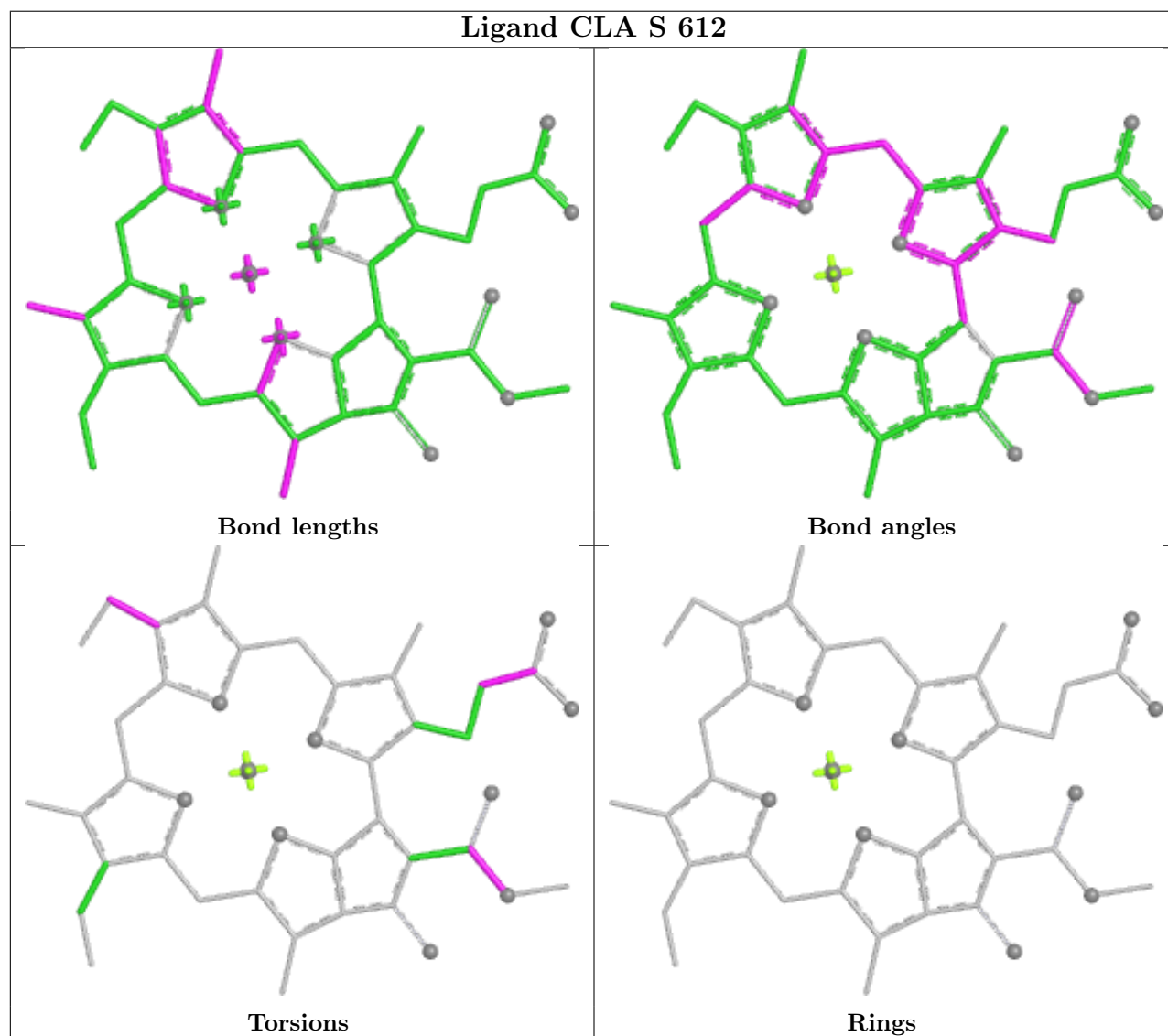
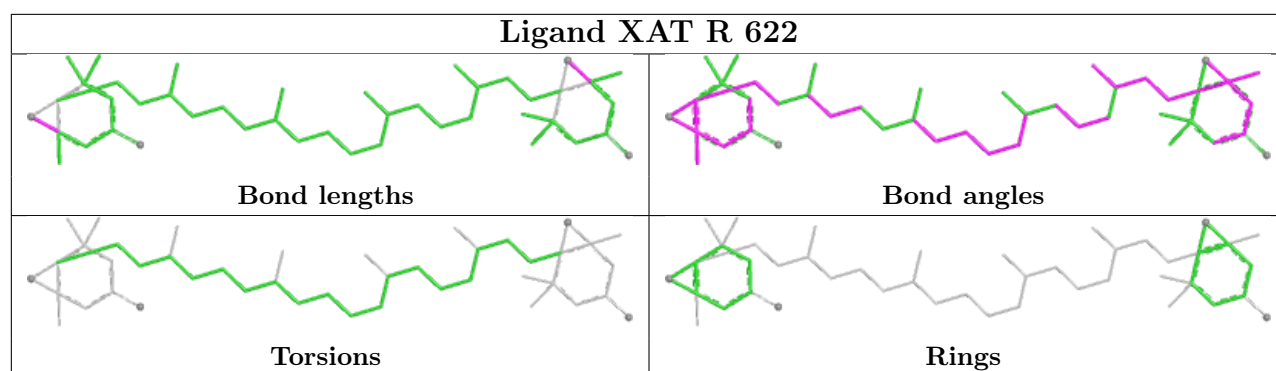


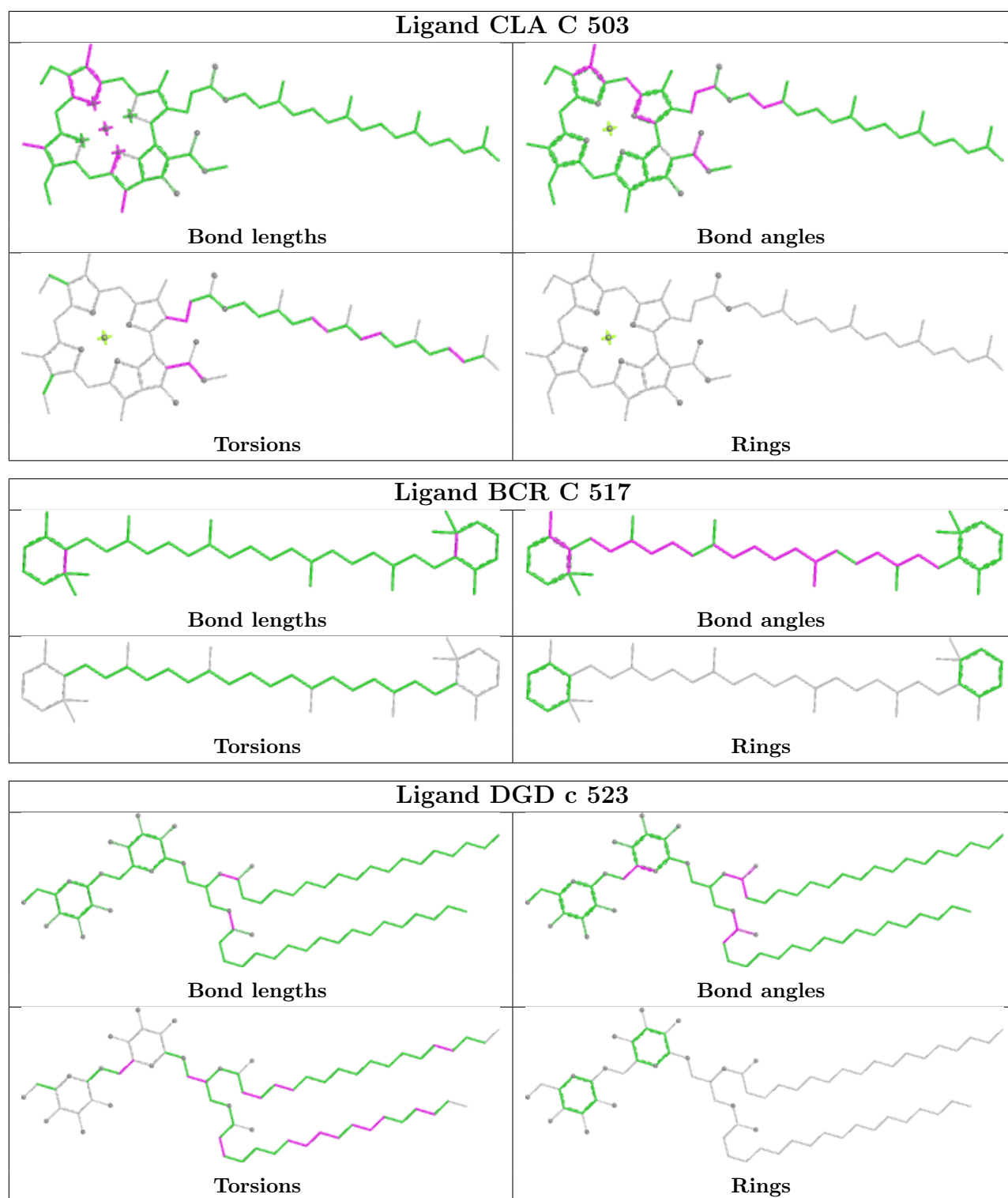
Torsions



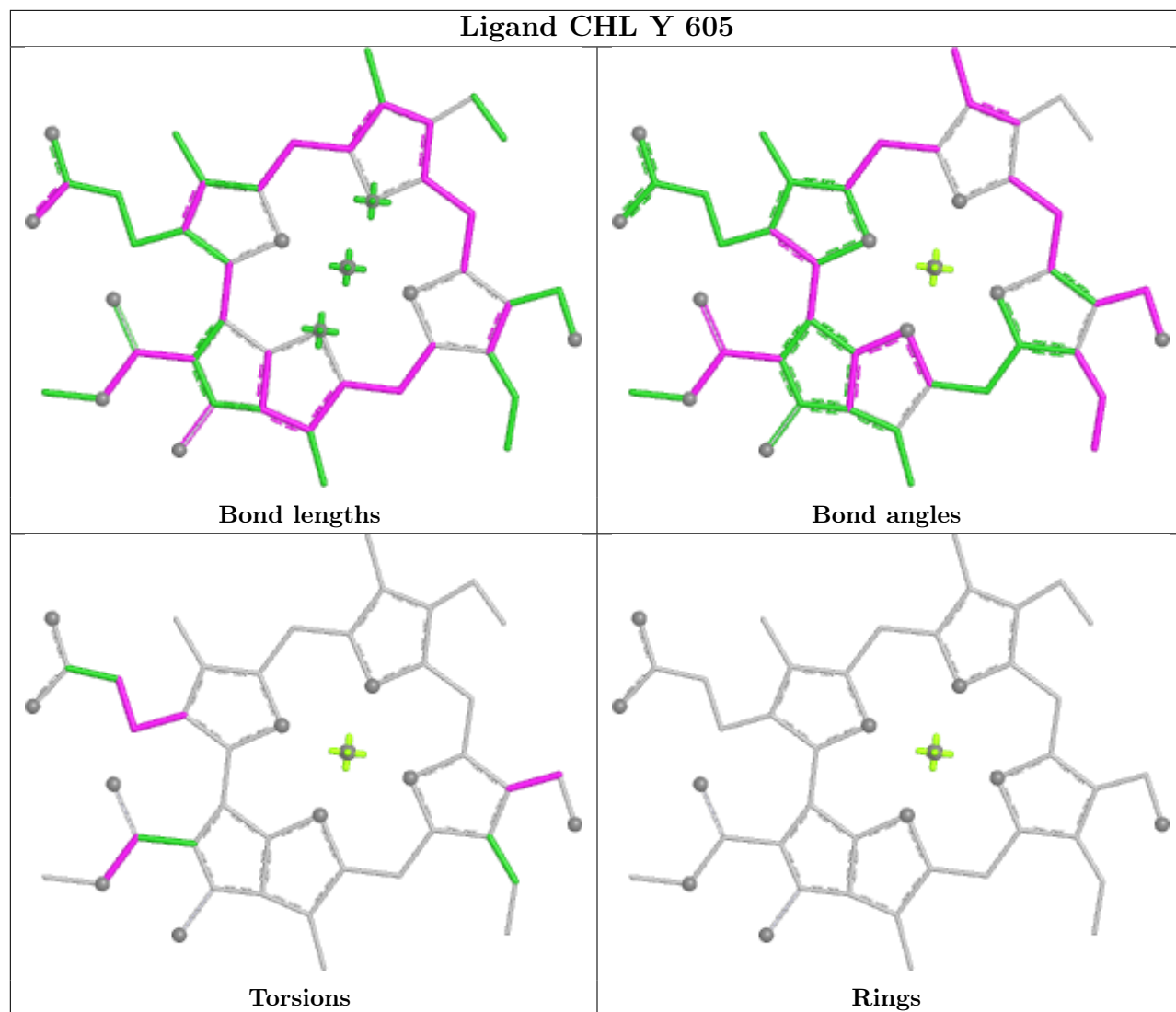
Rings

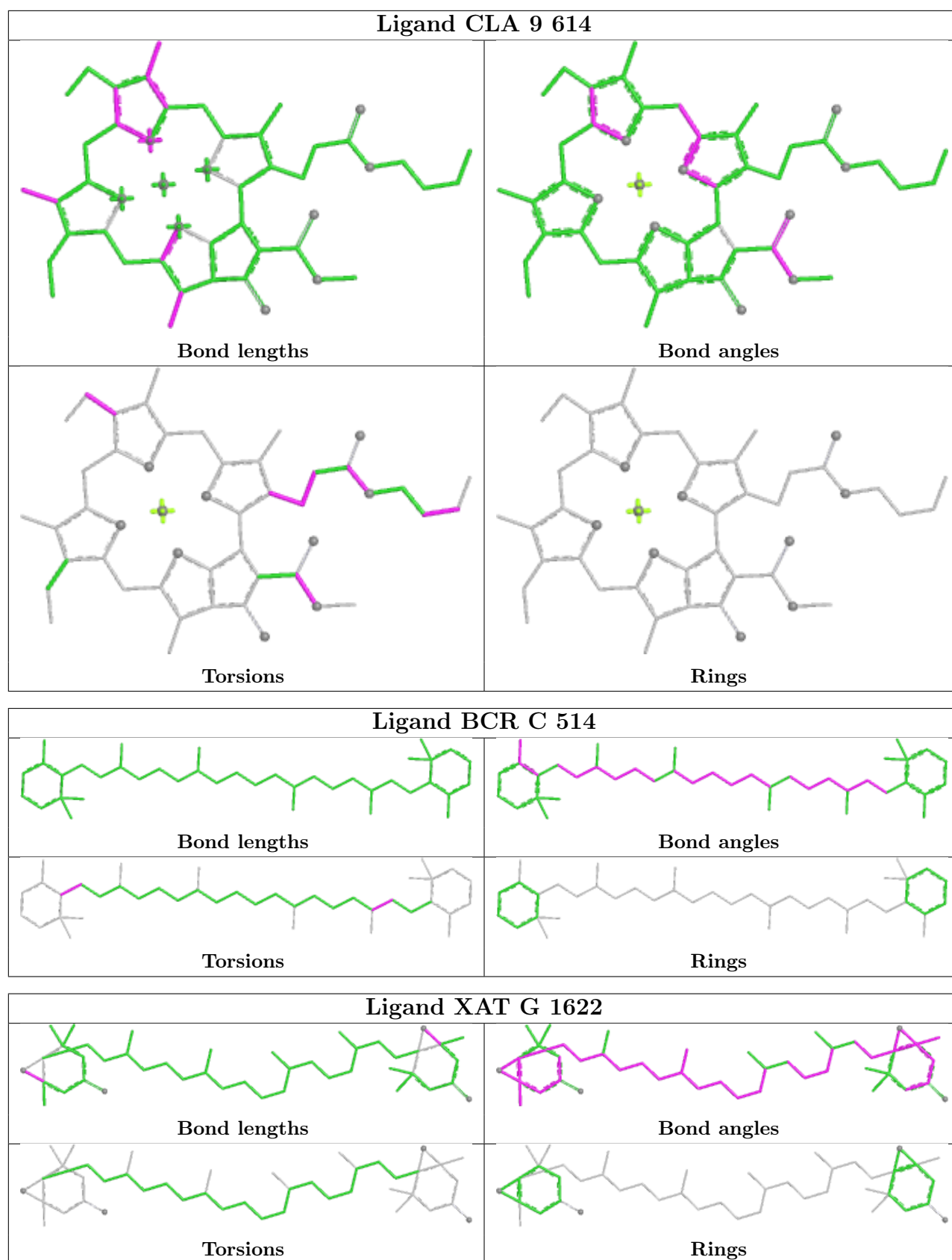


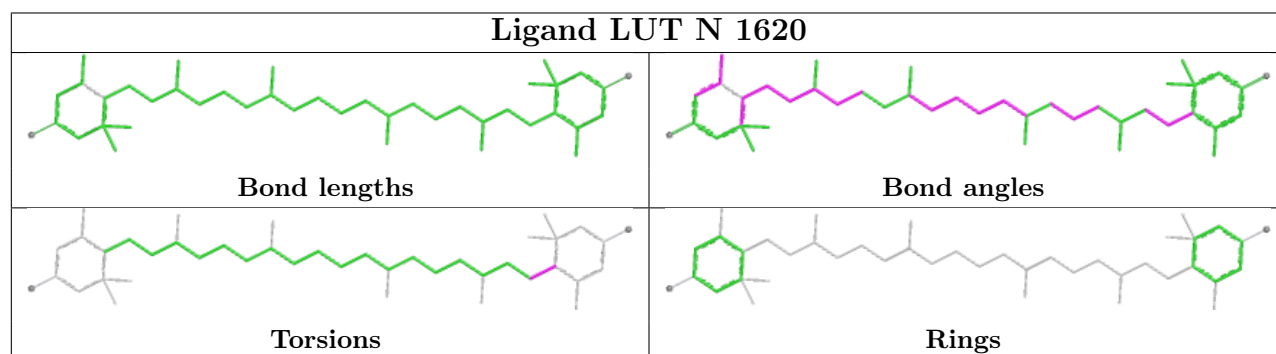
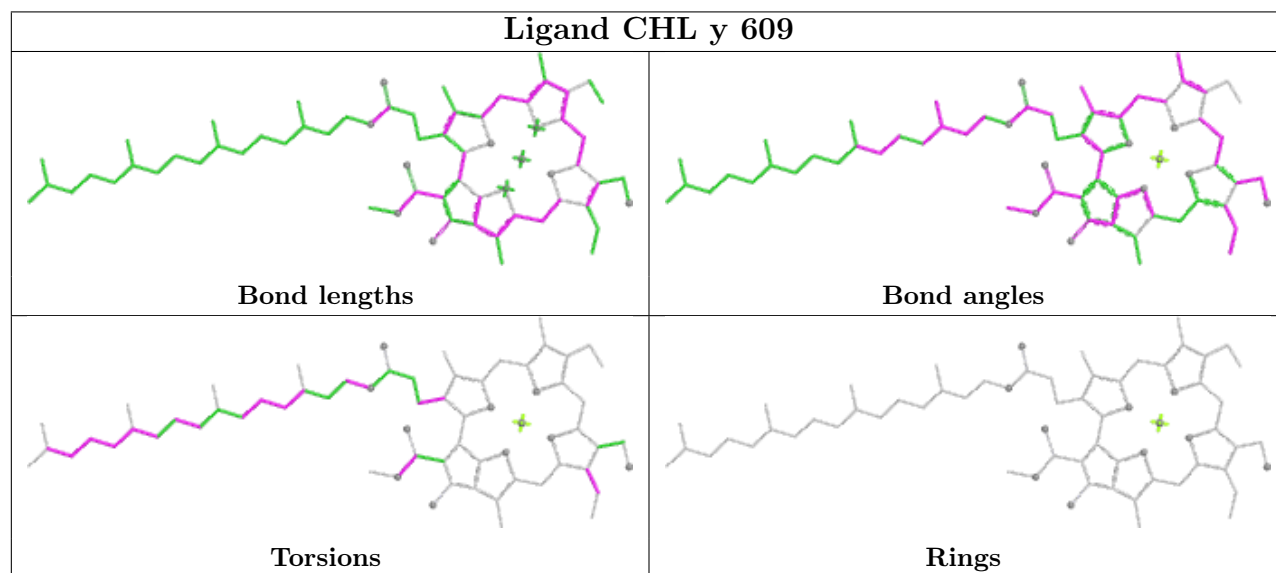
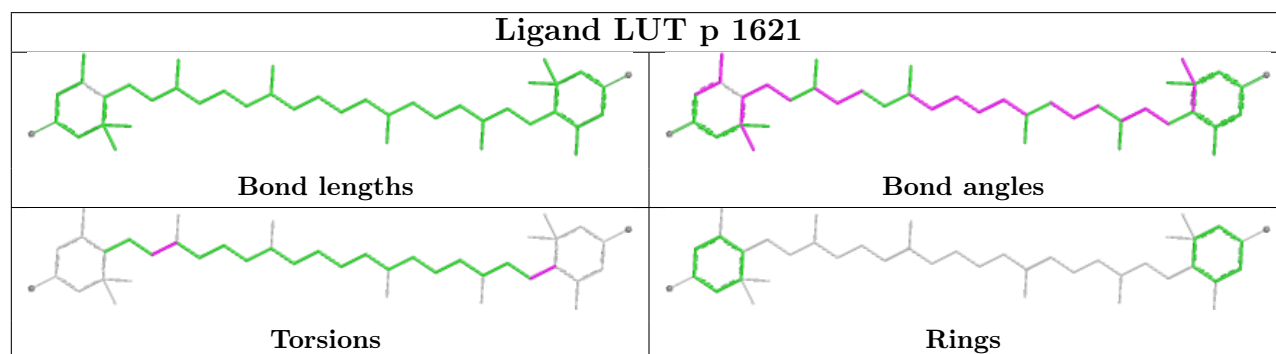
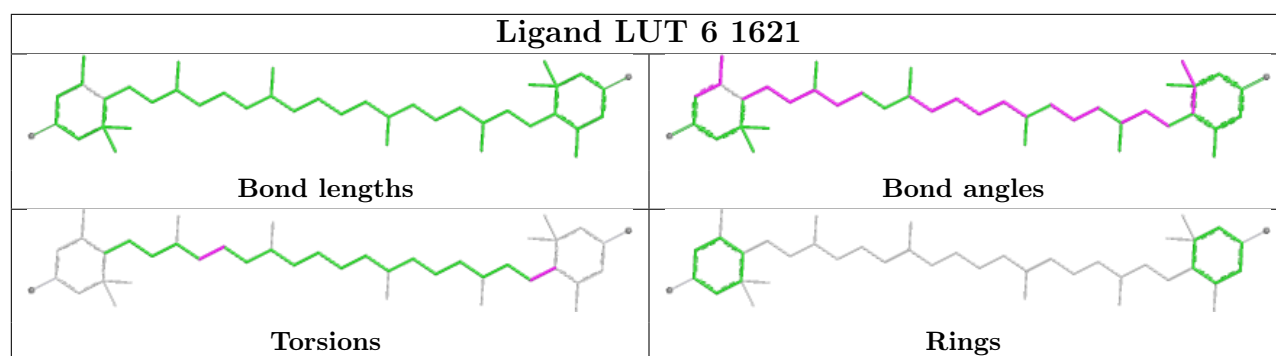


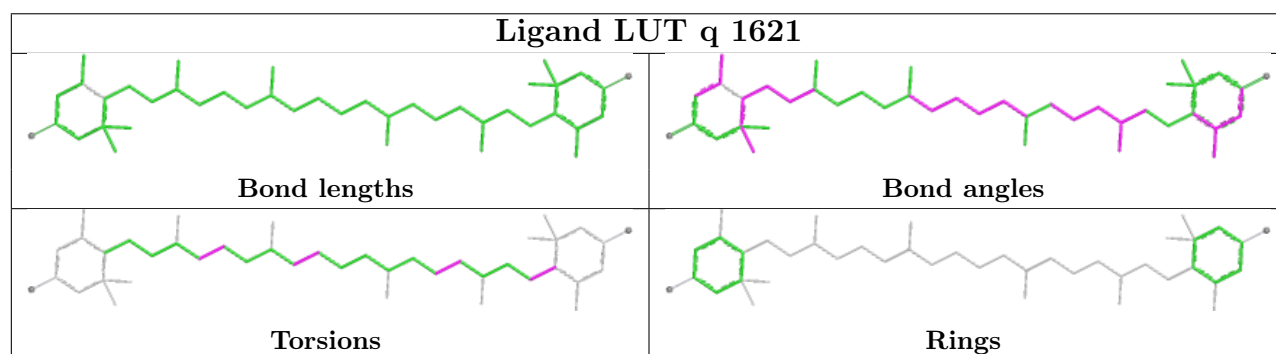
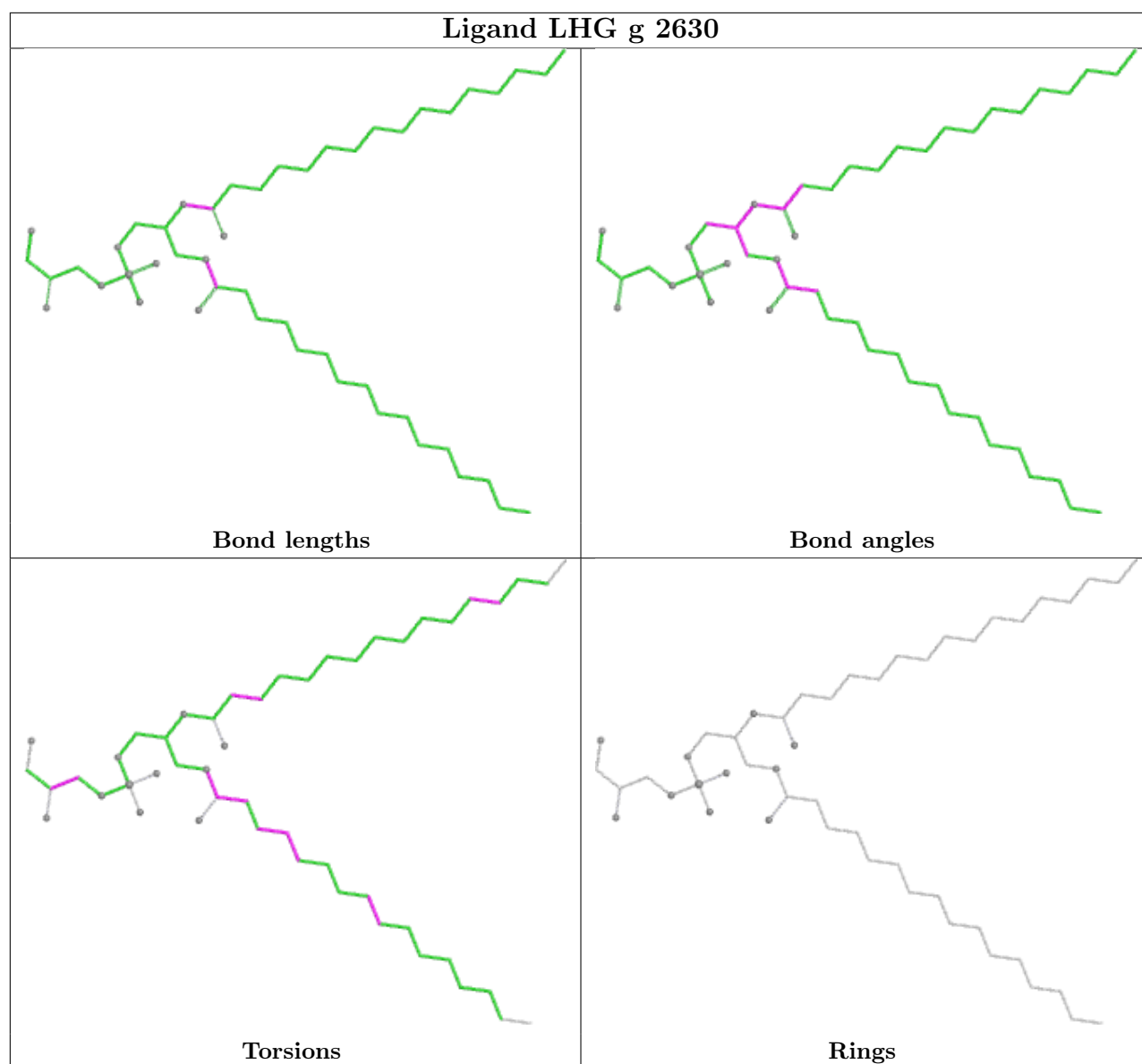


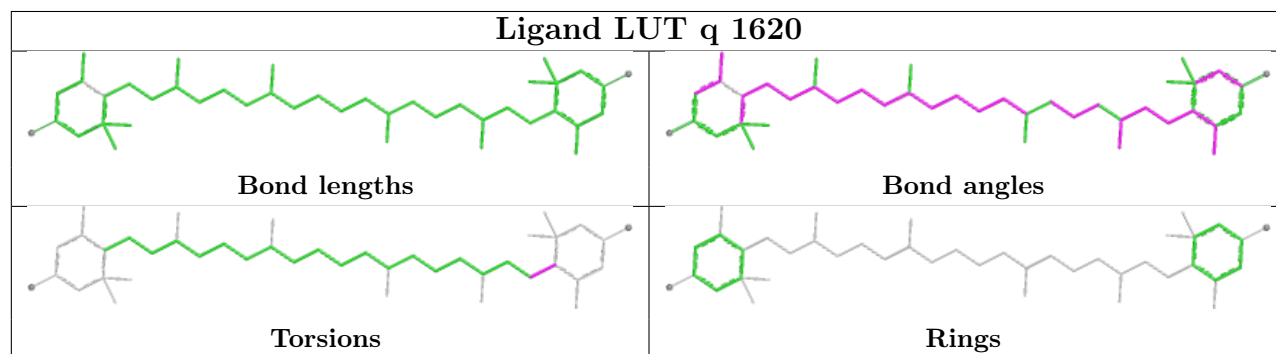
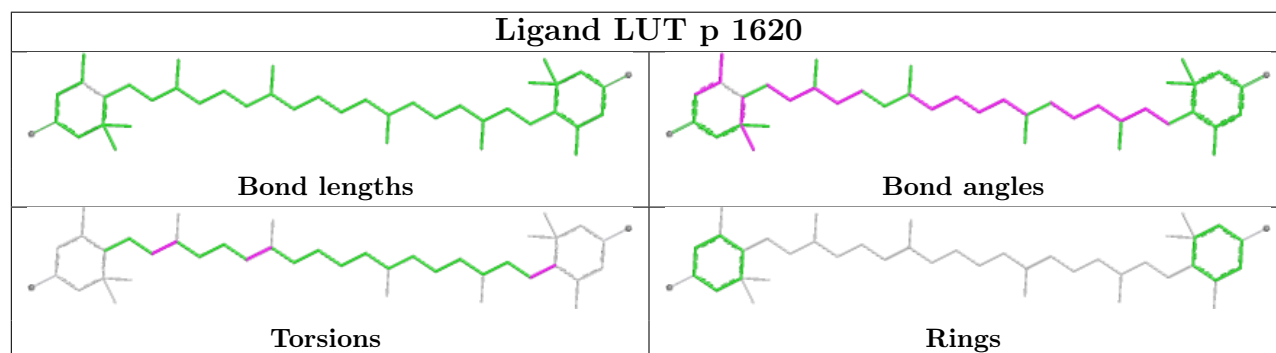
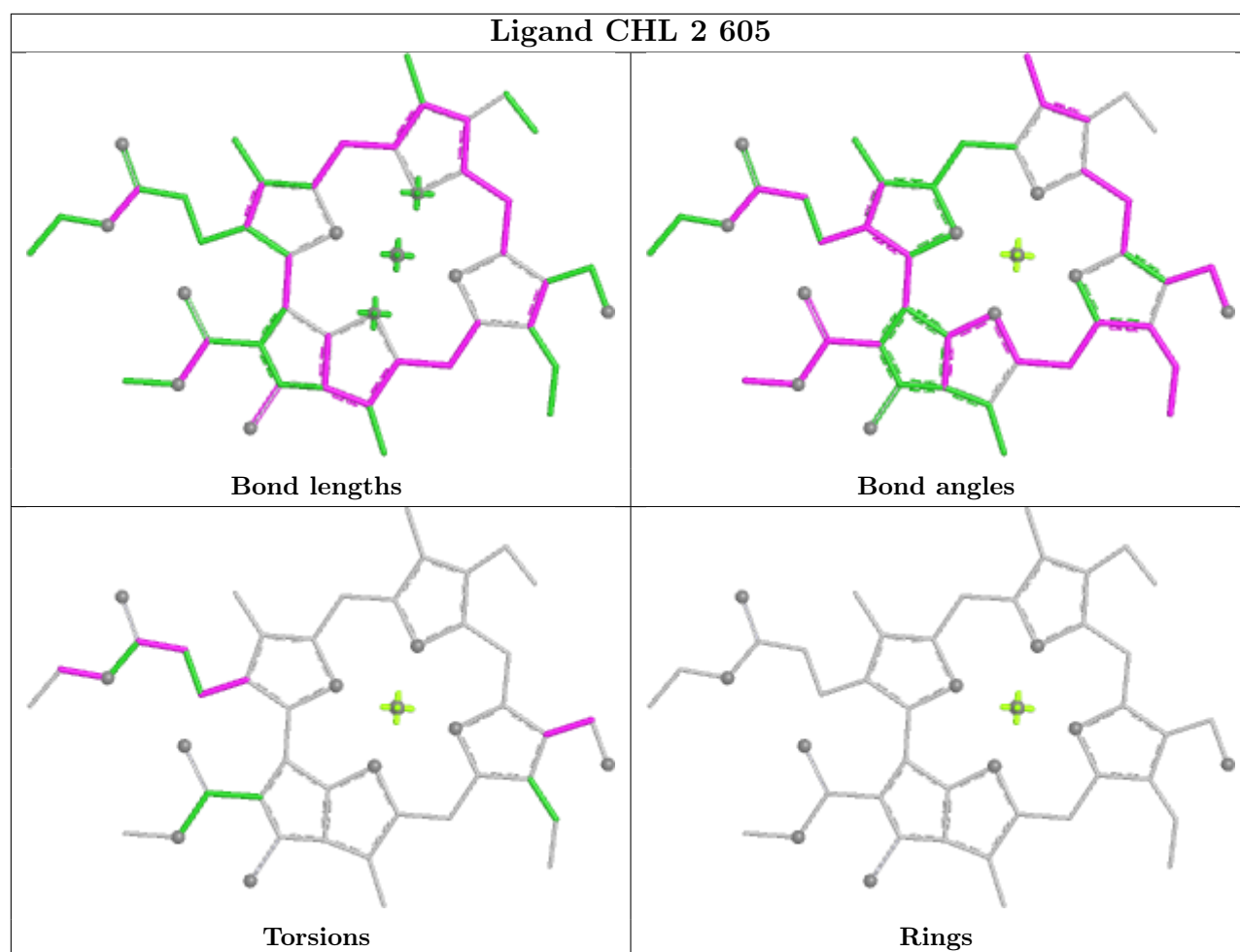
Ligand CHL Y 605



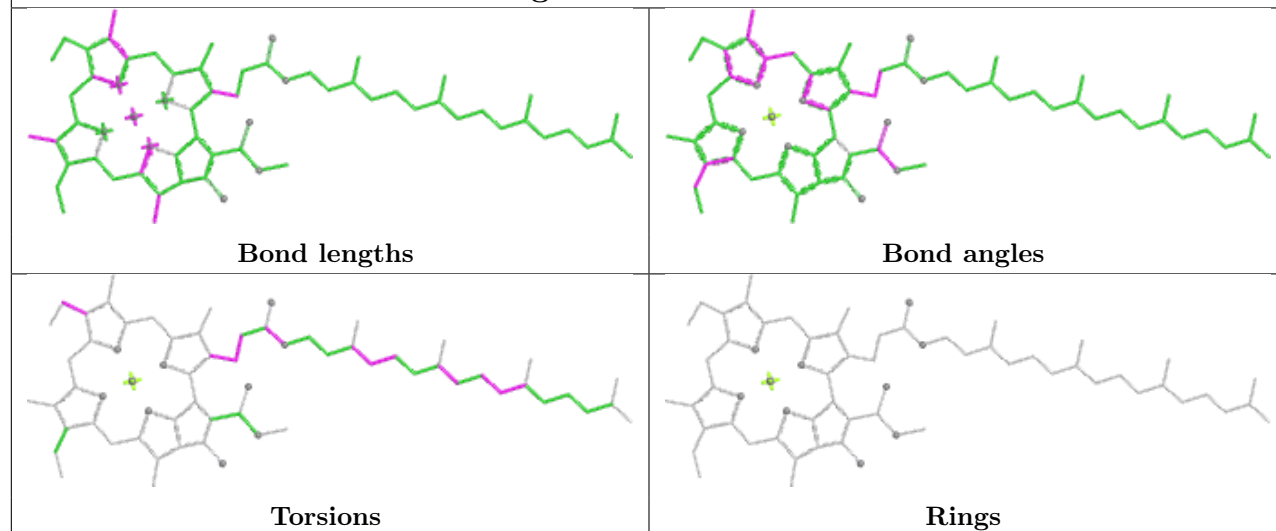




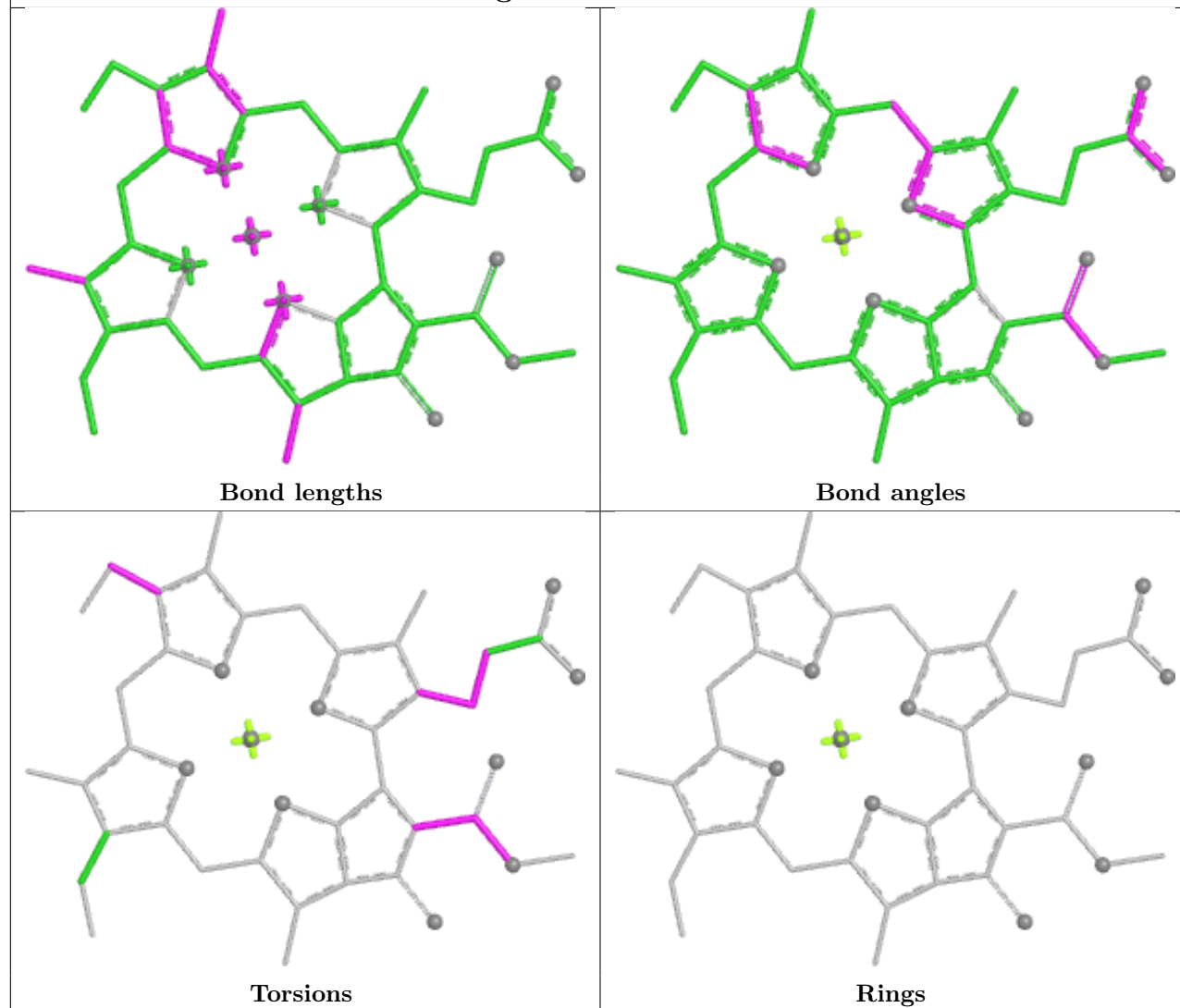


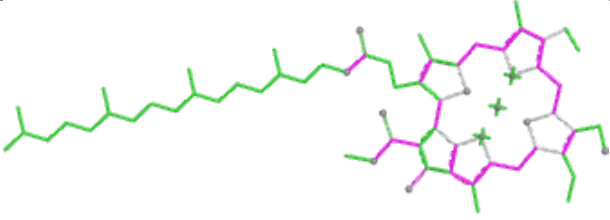
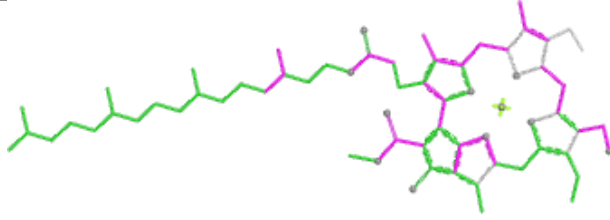
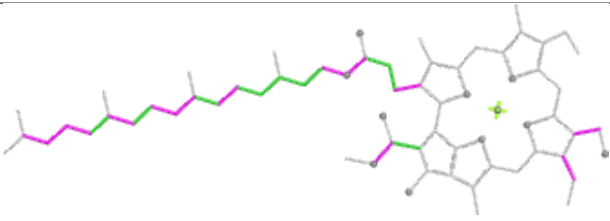
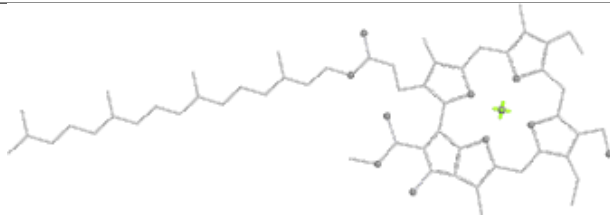
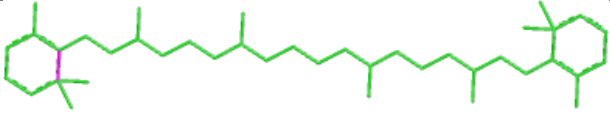
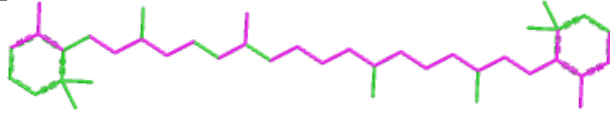
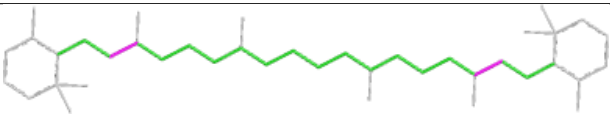
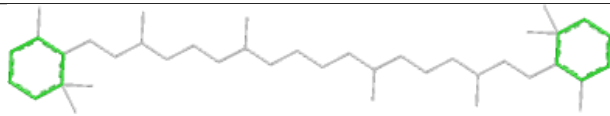


Ligand CLA D 402

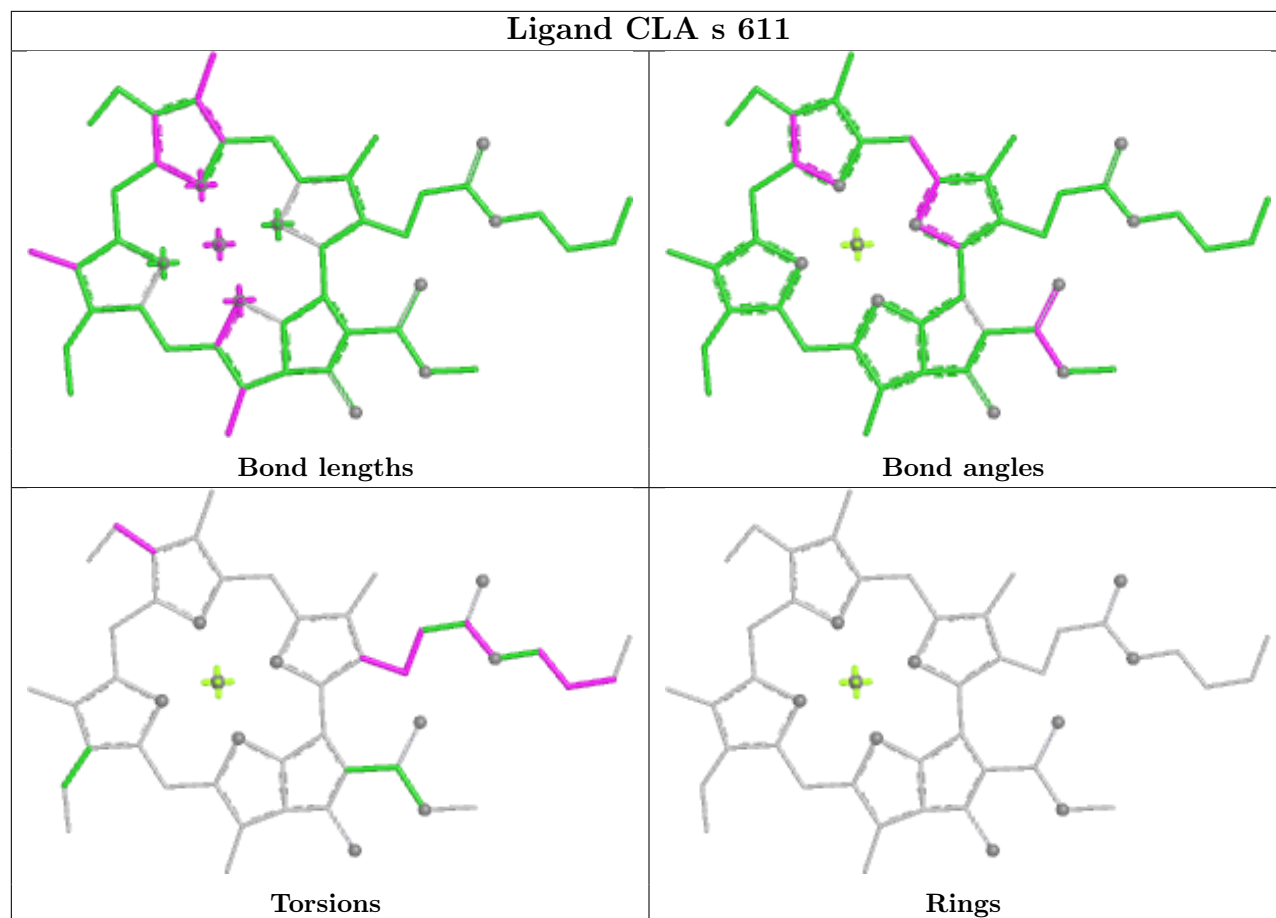


Ligand CLA 9 611

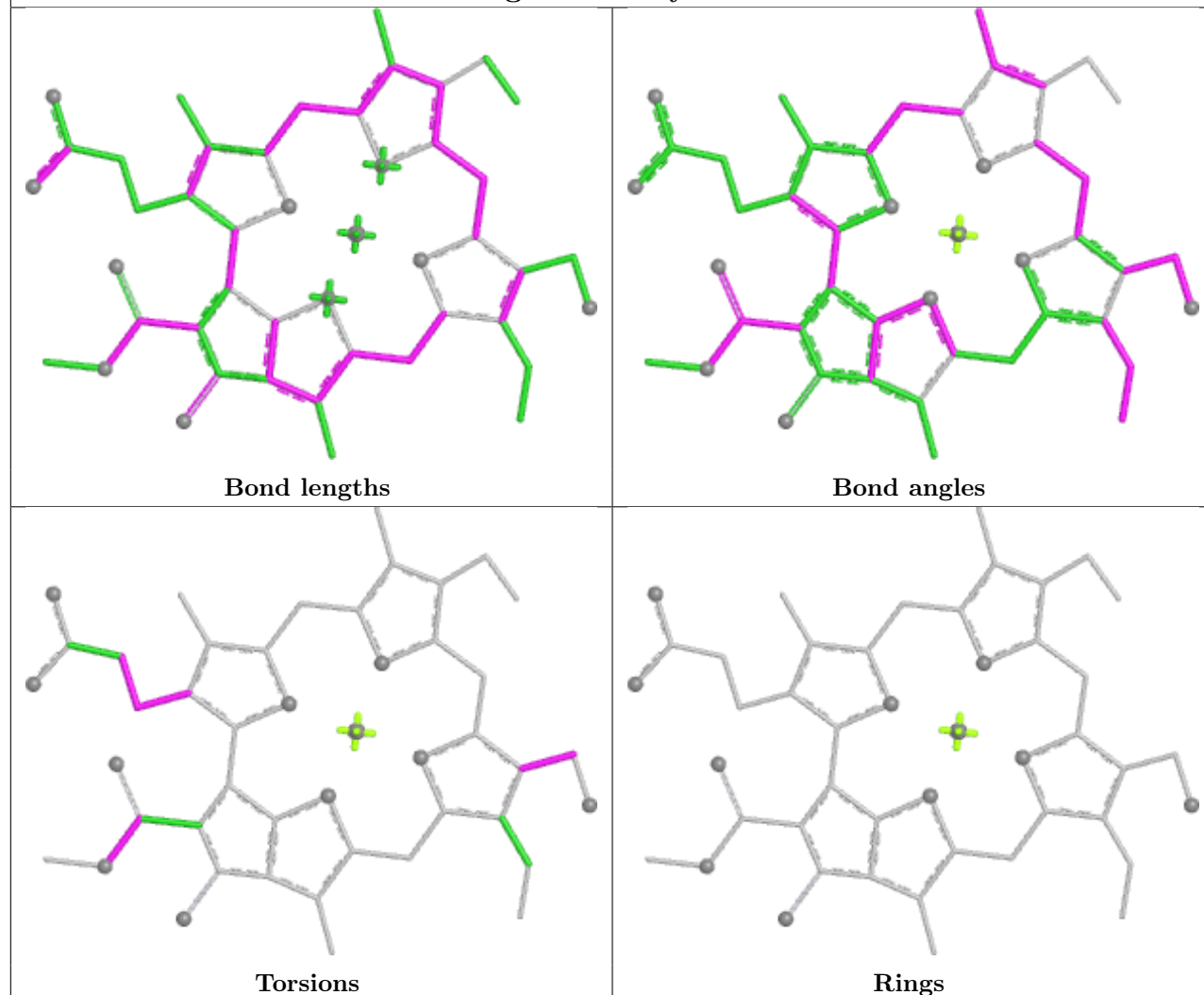


Ligand CHL 8 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

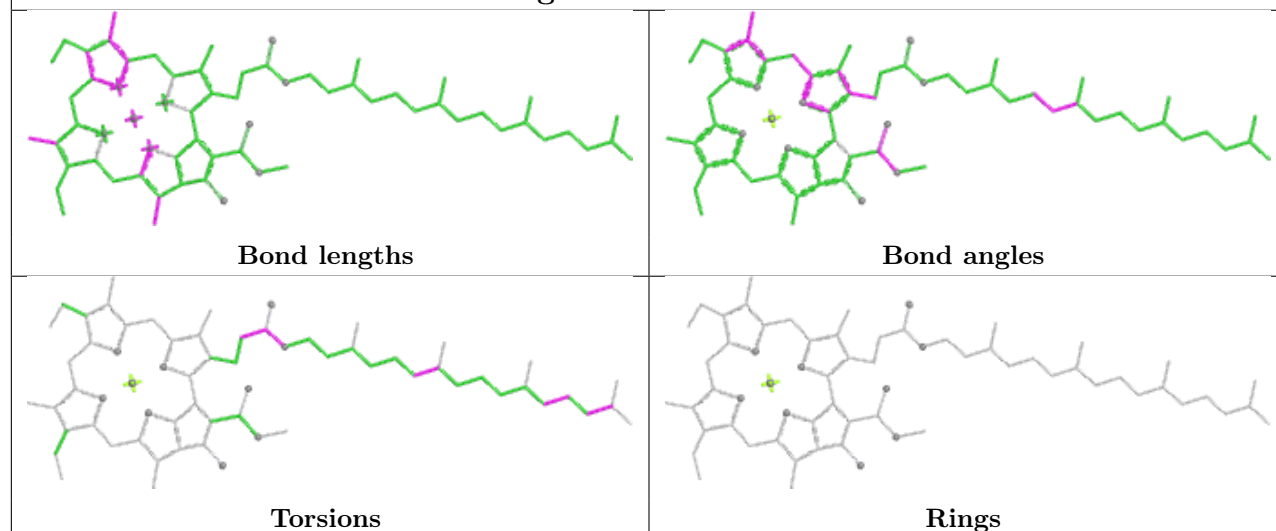
Ligand CLA s 611

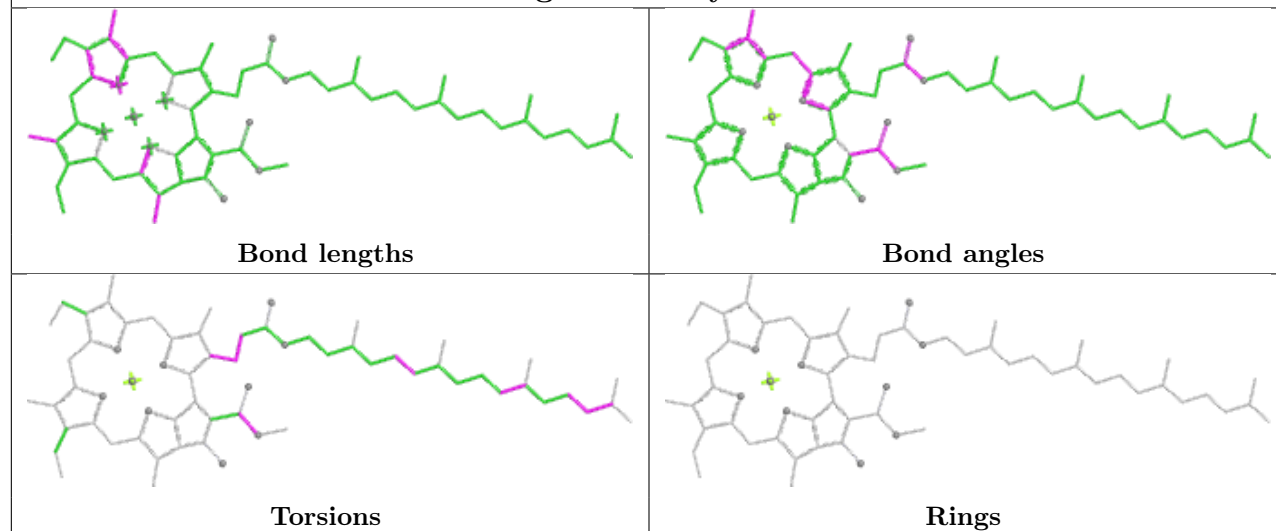
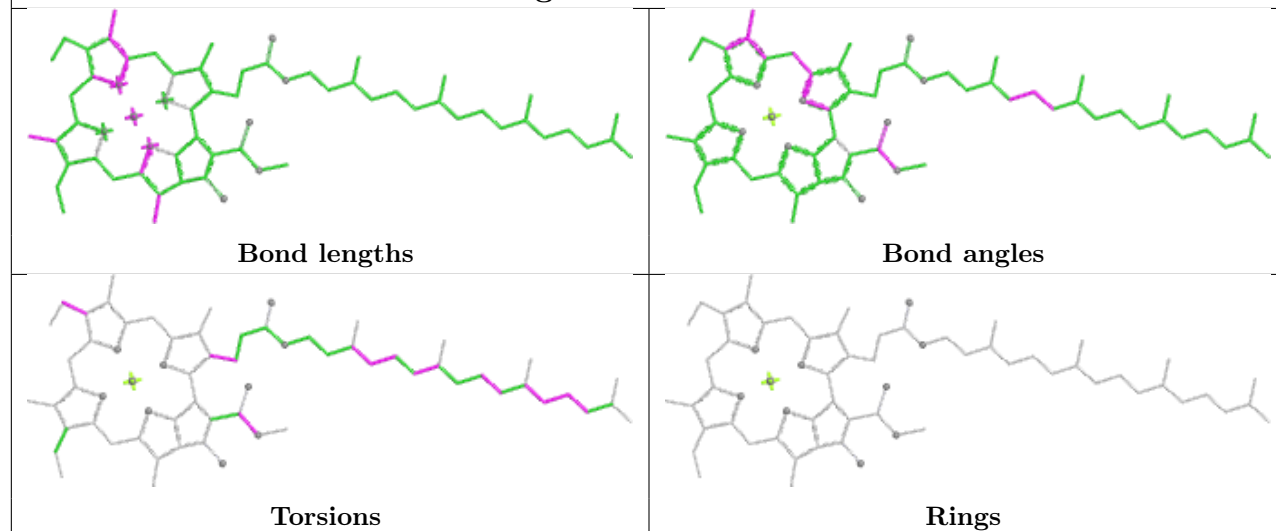


Ligand CHL y 605

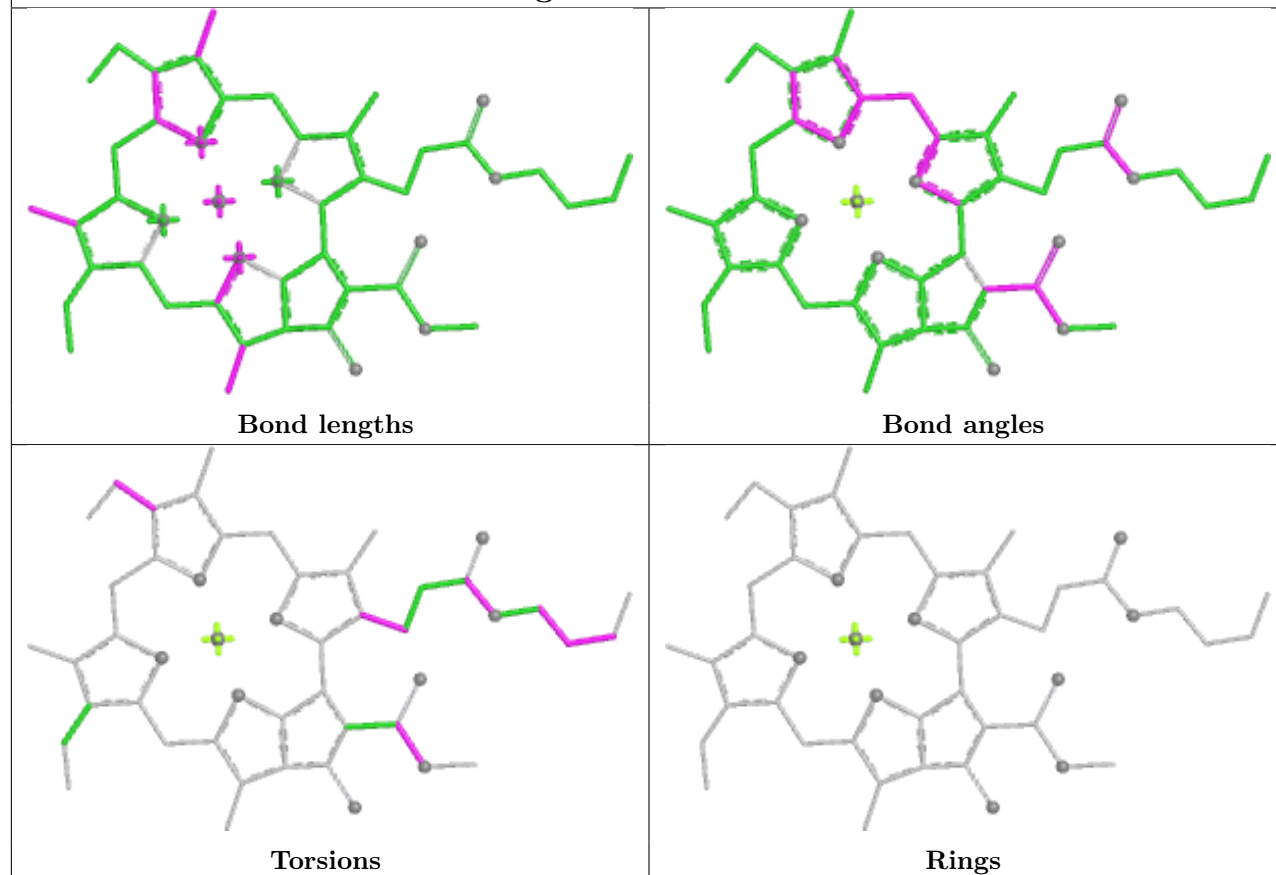


Ligand CLA c 510

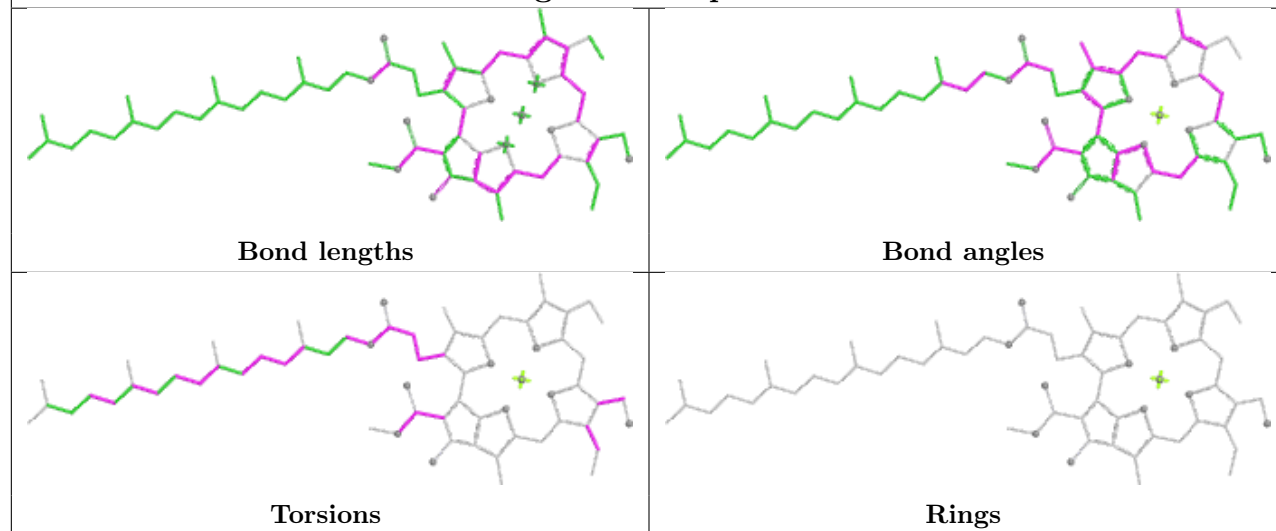


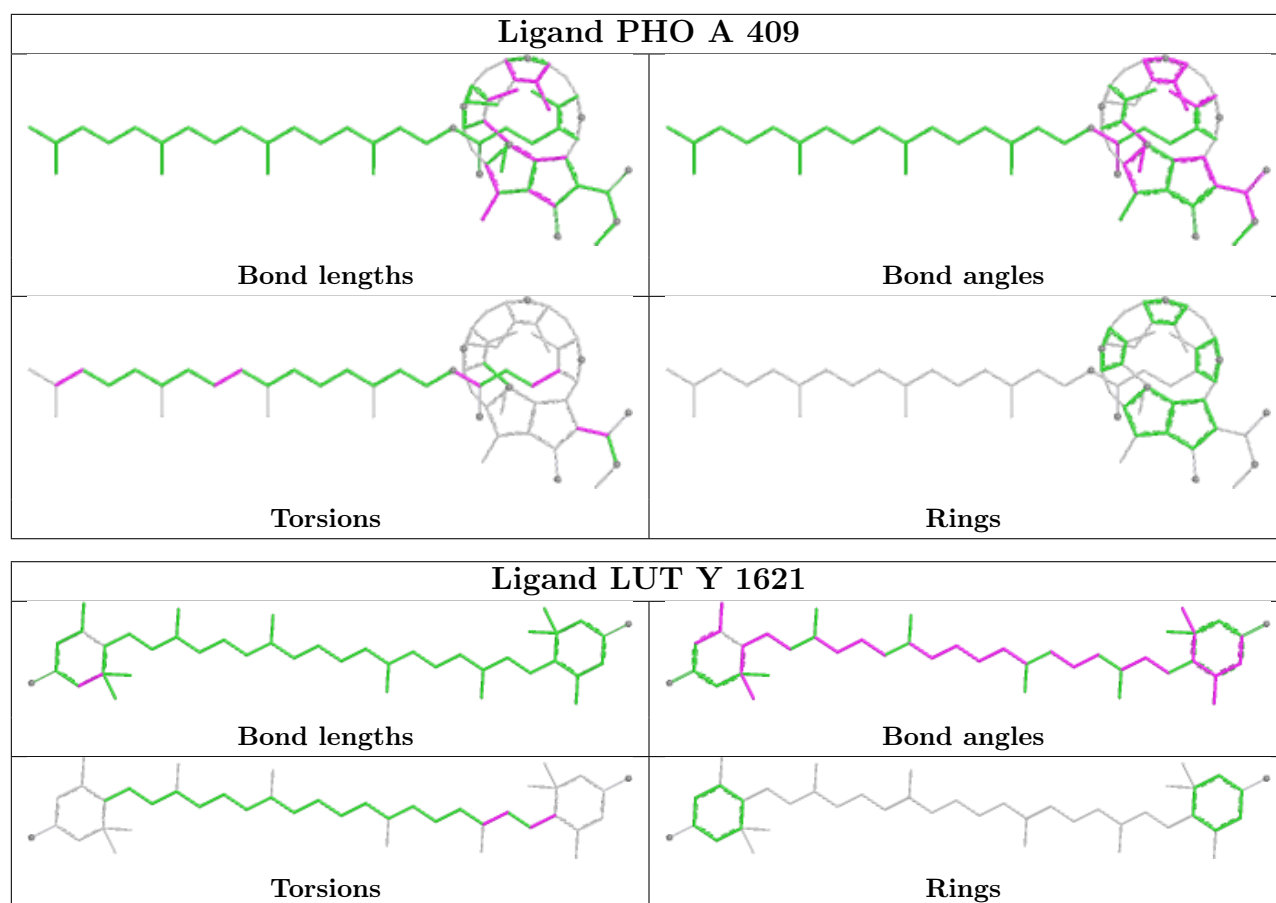
Ligand CLA y 610**Ligand CLA b 608**

Ligand CLA S 610



Ligand CHL p 607





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.

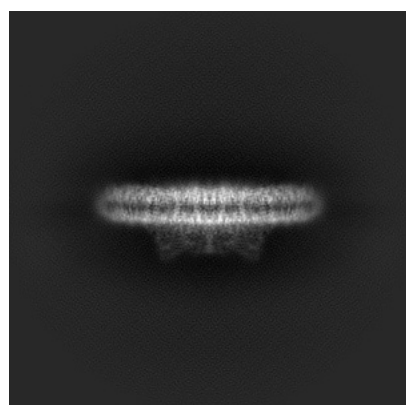
6 Map visualisation [i](#)

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.

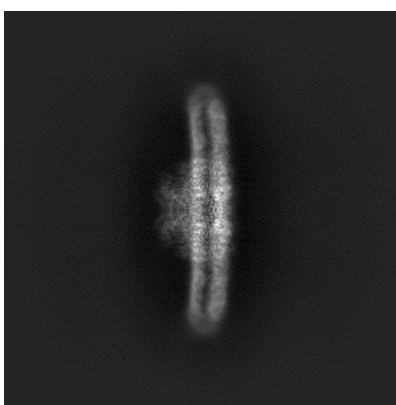
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

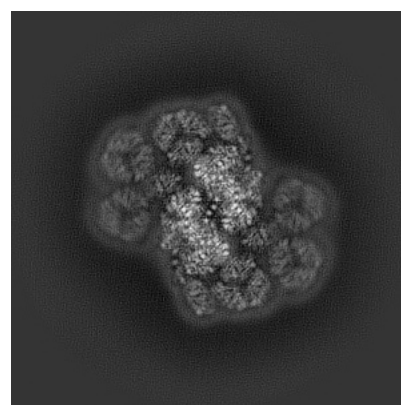
6.1.1 Primary map



X



Y

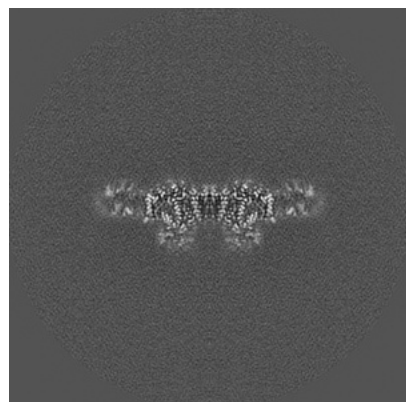


Z

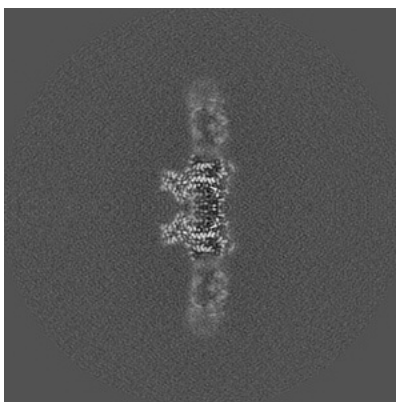
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

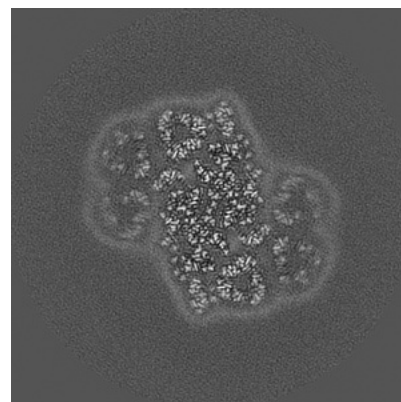
6.2.1 Primary map



X Index: 192



Y Index: 192

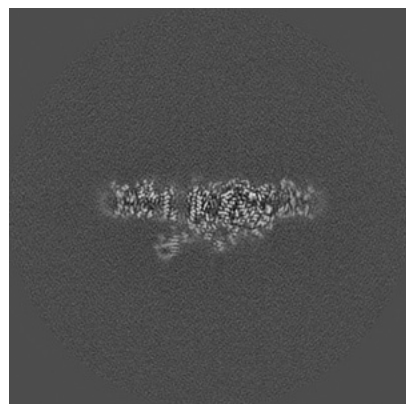


Z Index: 192

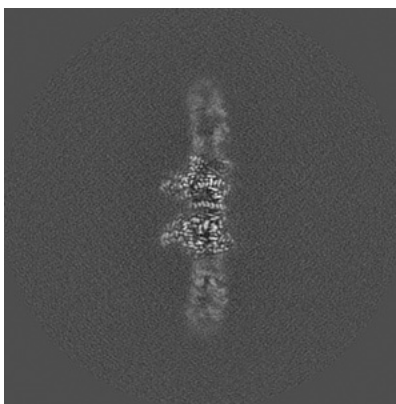
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

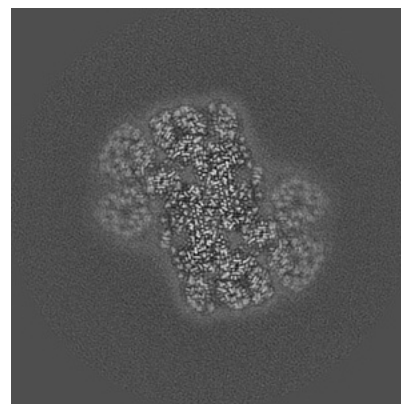
6.3.1 Primary map



X Index: 207



Y Index: 196

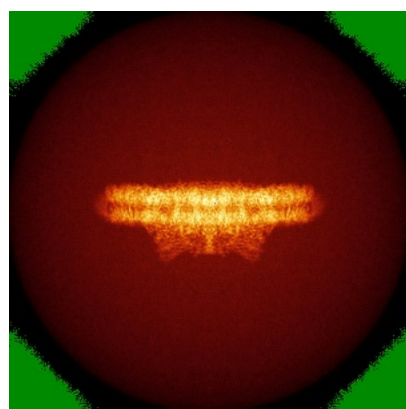


Z Index: 204

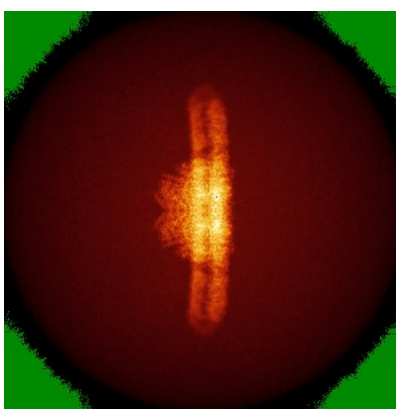
The images above show the largest variance slices of the map in three orthogonal directions.

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

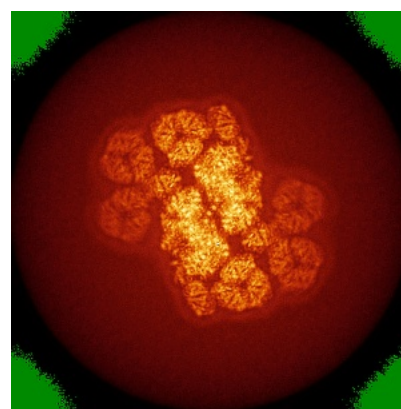
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

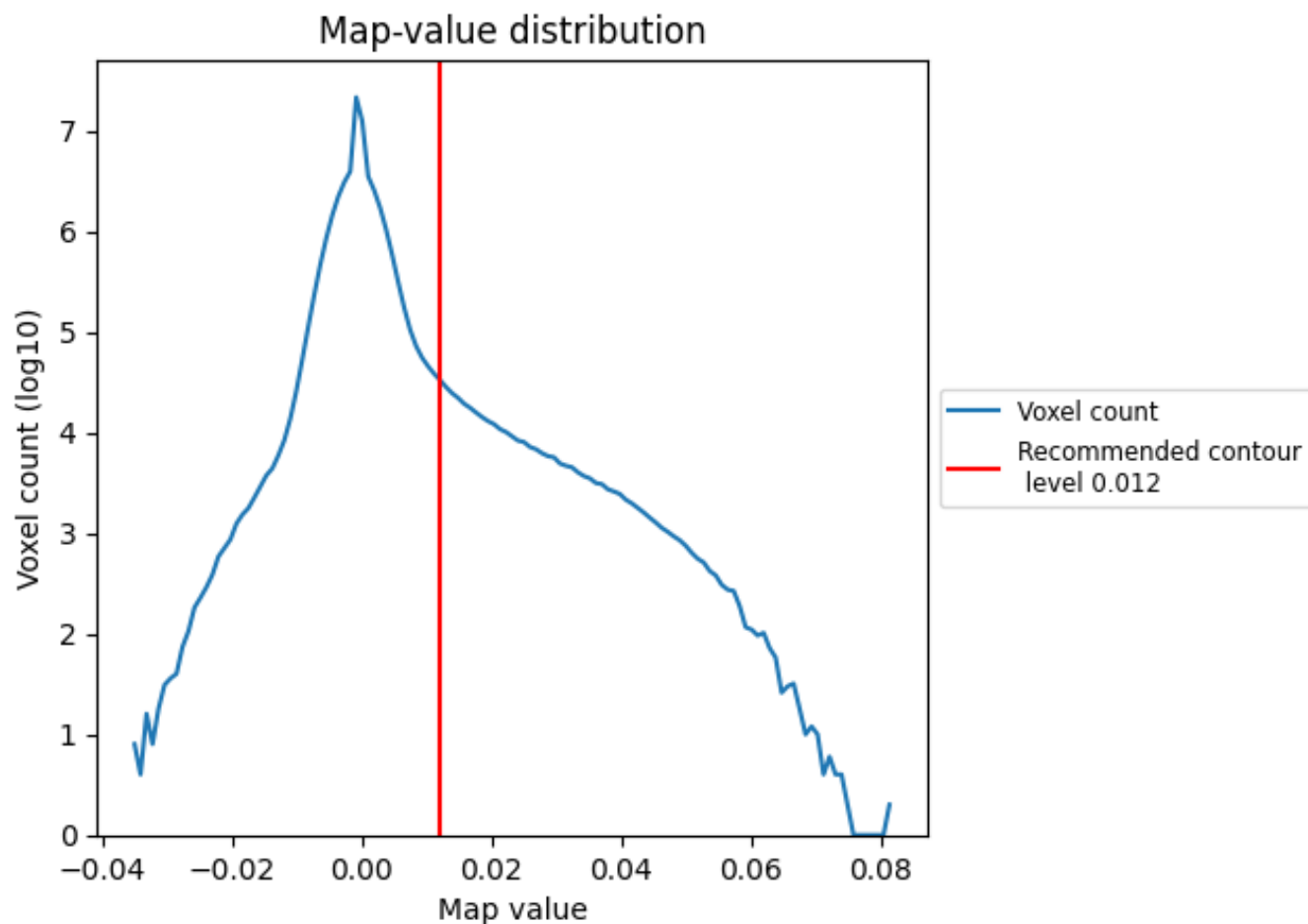
6.6 Mask visualisation

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

7 Map analysis [i](#)

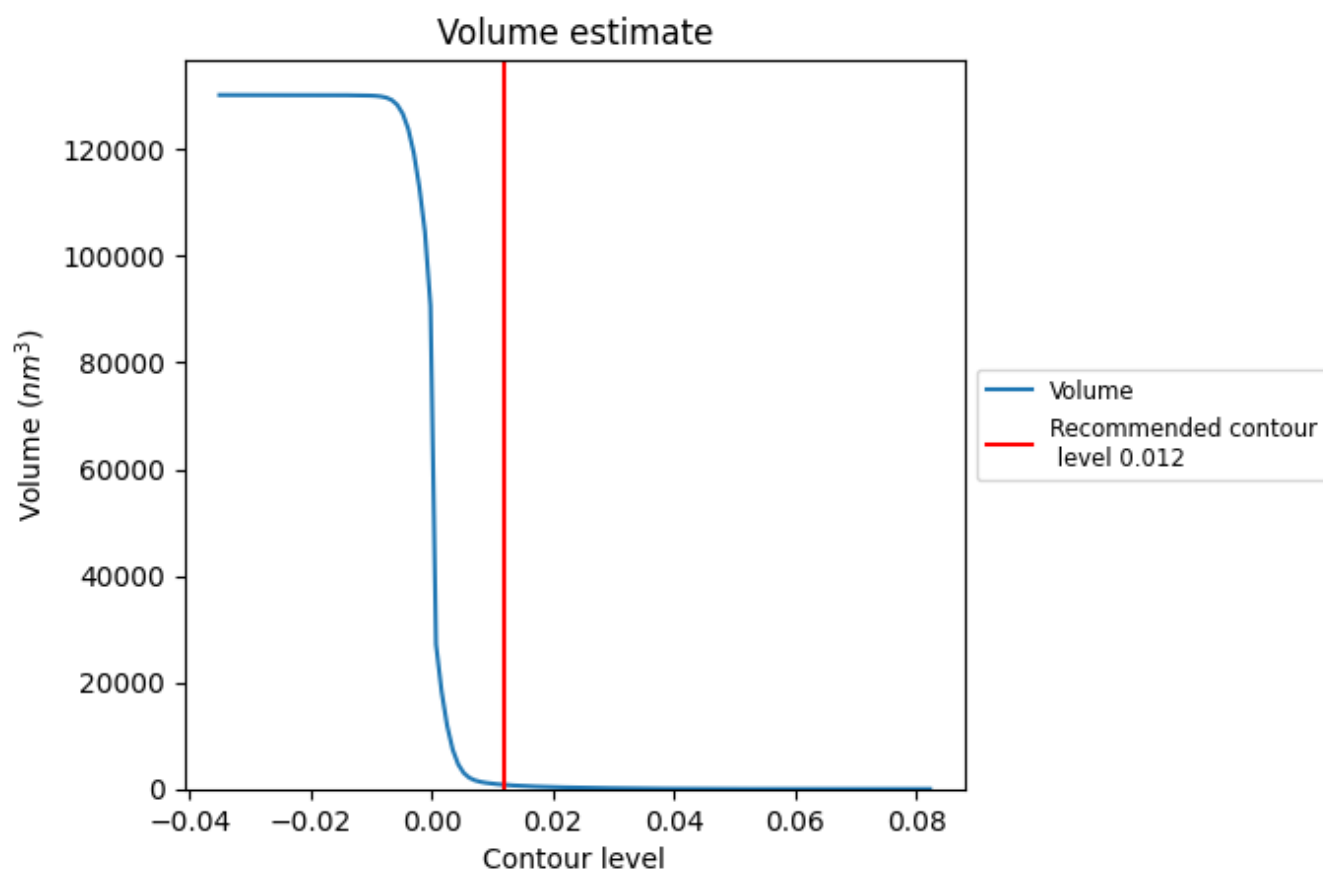
This section contains the results of statistical analysis of the map.

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.

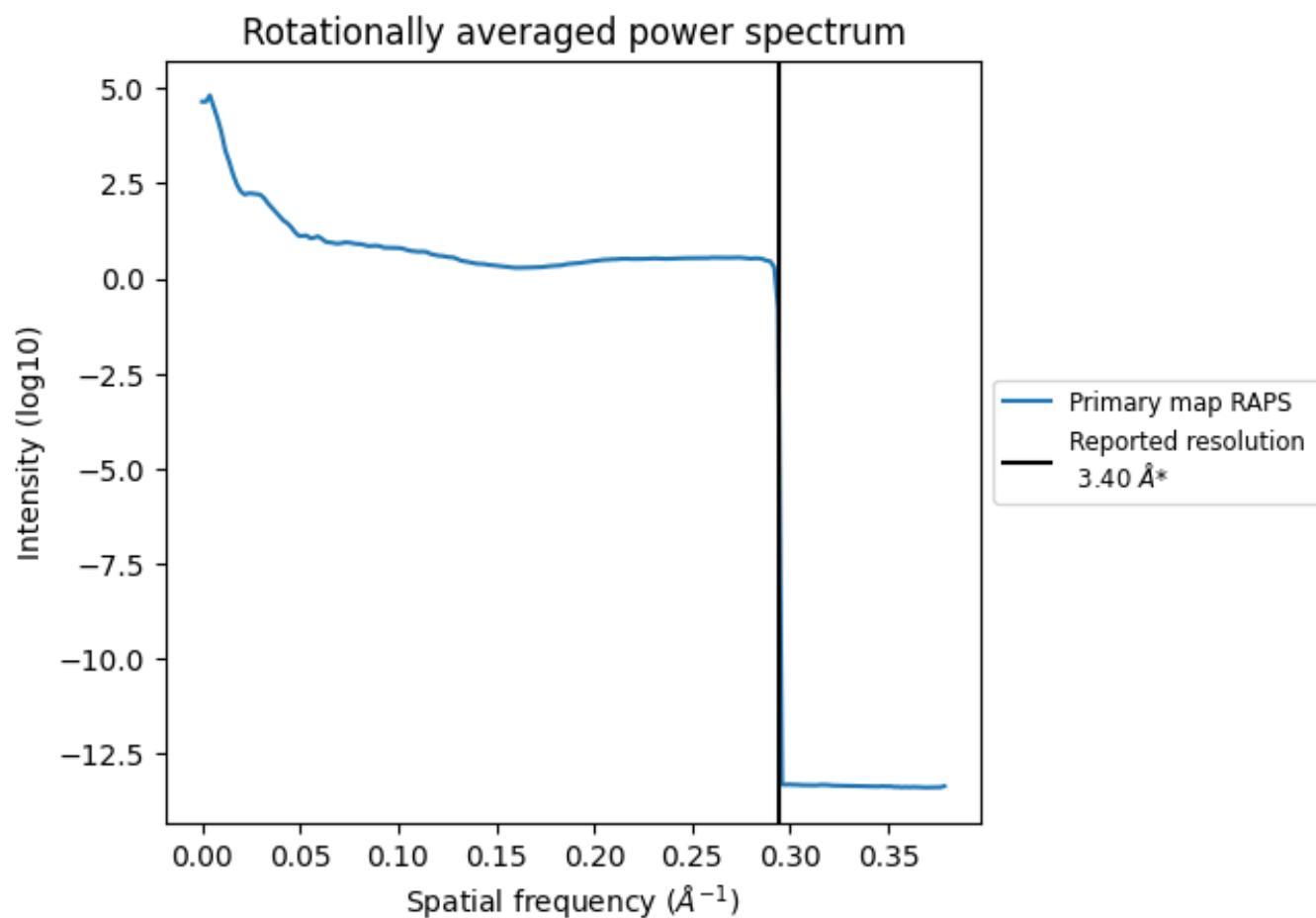
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm^3 ; 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 ⓘ

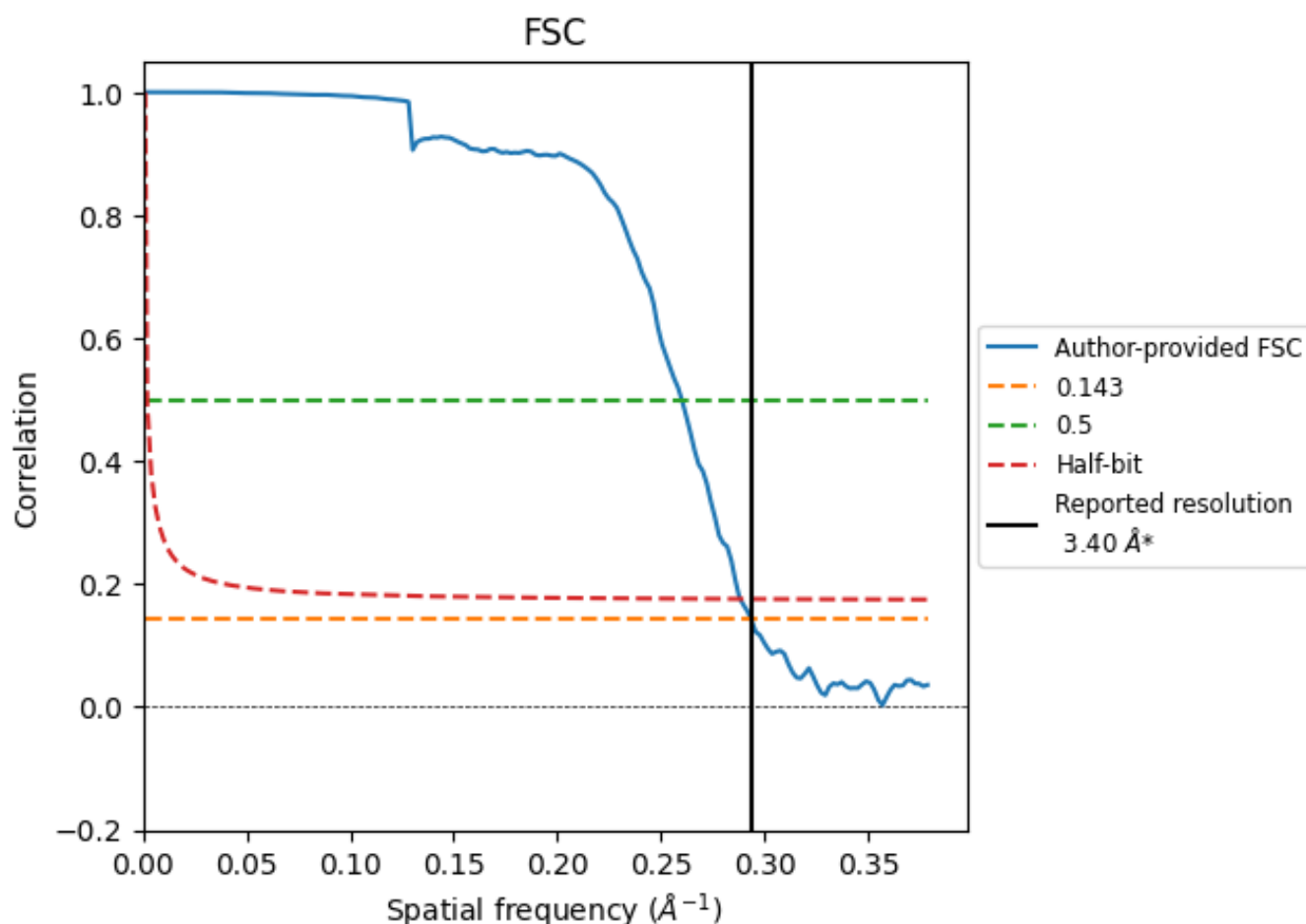


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

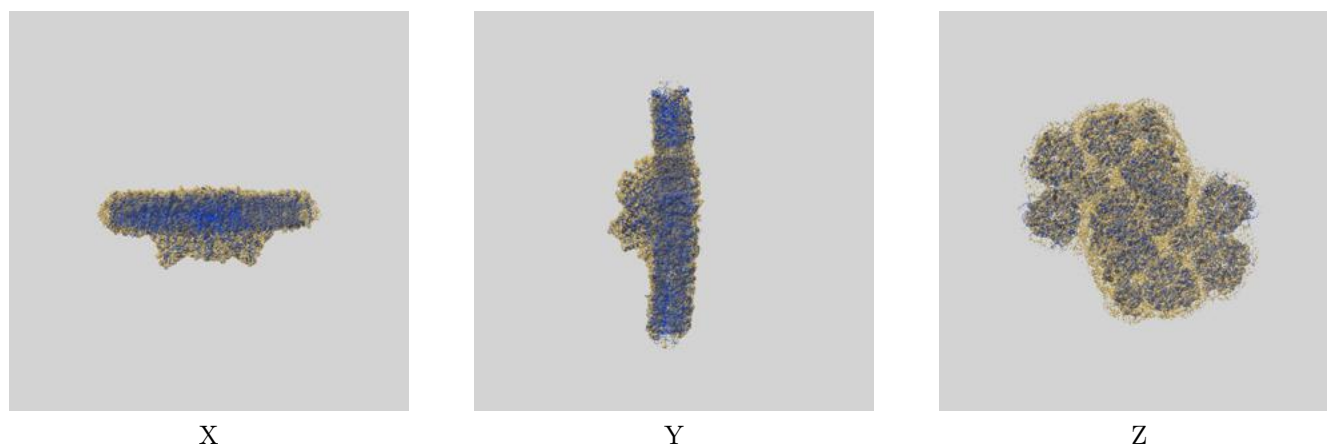
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.84	3.47
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

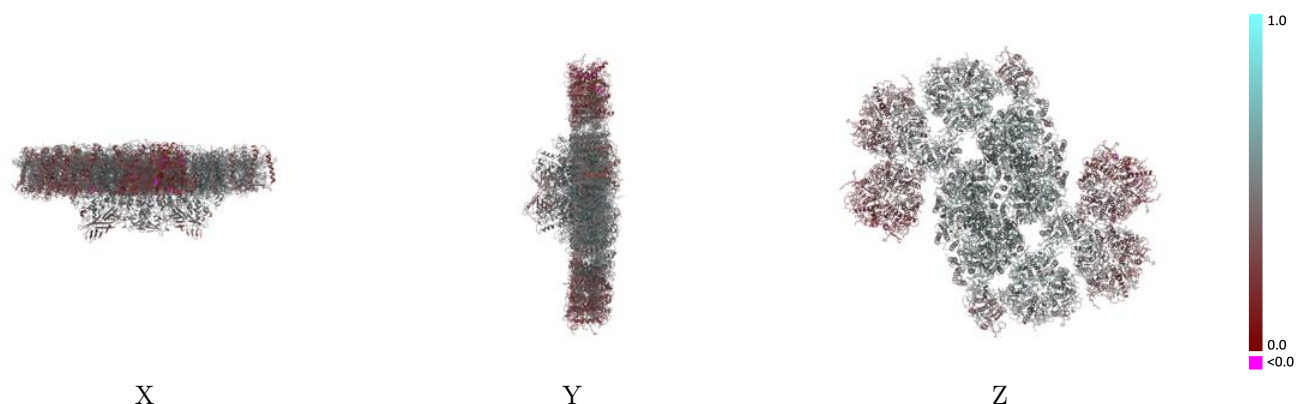
This section contains information regarding the fit between EMDB map EMD-9956 and PDB model 6KAD. Per-residue inclusion information can be found in section [3](#) on page [54](#).

9.1 Map-model overlay [i](#)



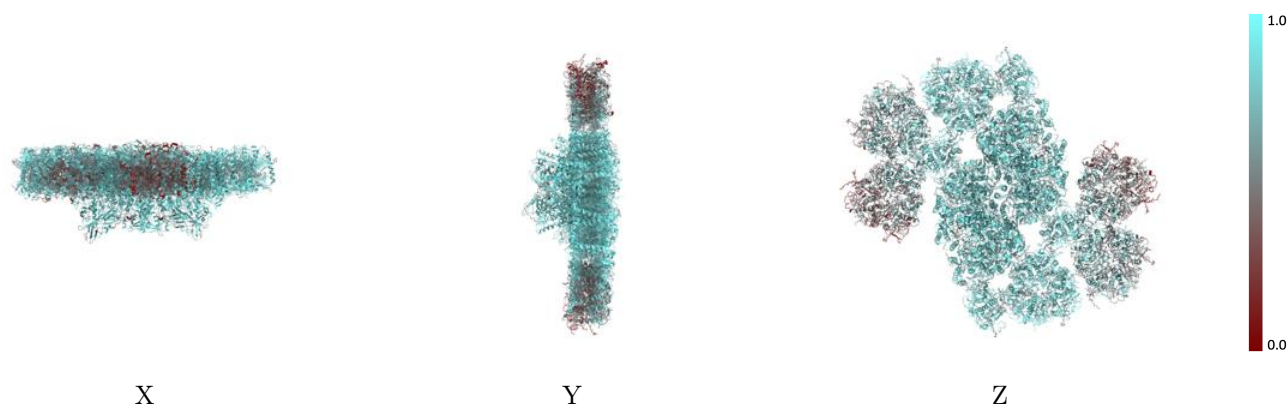
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



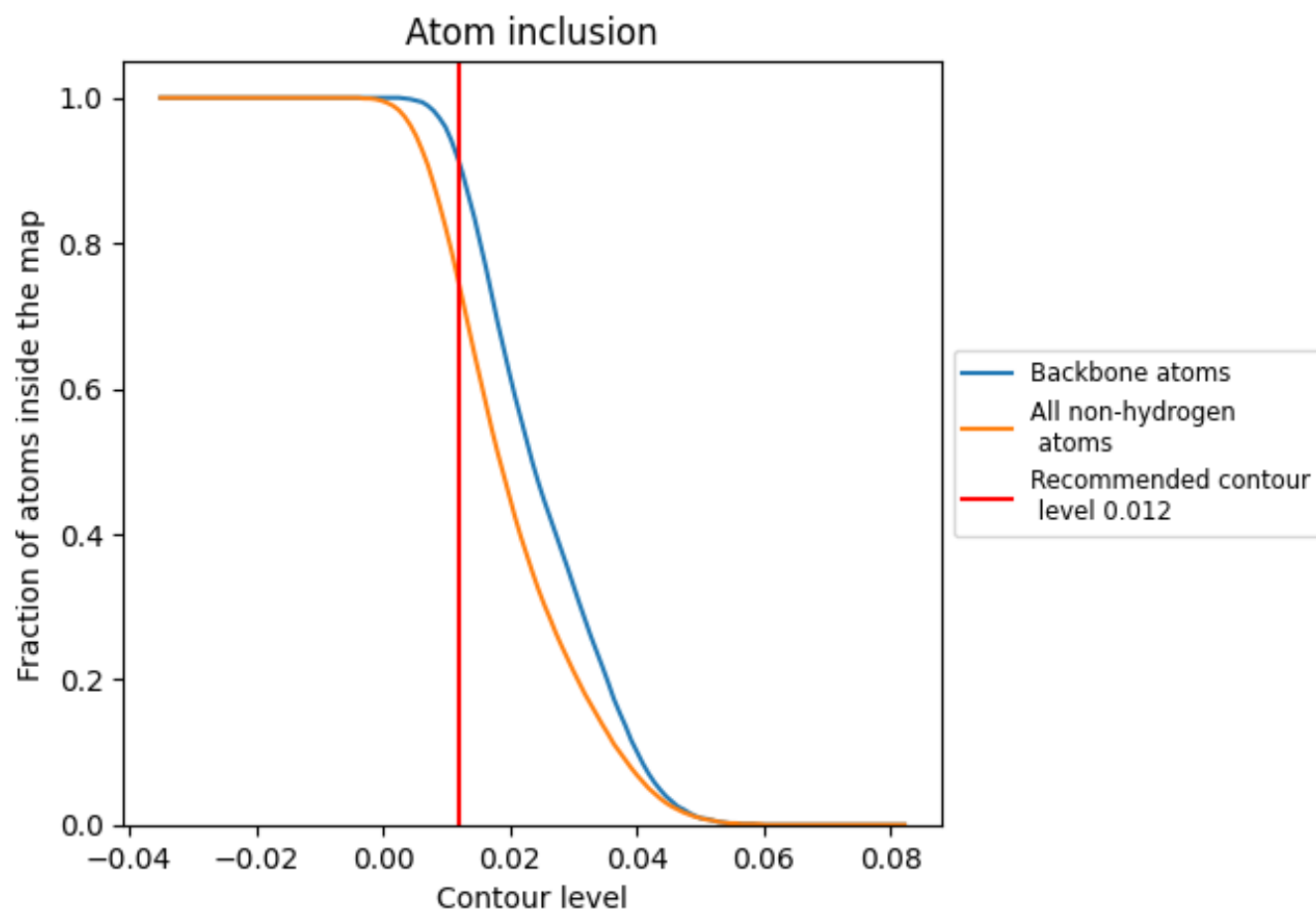
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

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	 0.7440	 0.4470
0	 0.5850	 0.3510
1	 0.7050	 0.4440
2	 0.5550	 0.3430
3	 0.5780	 0.3480
4	 0.4720	 0.2850
5	 0.3430	 0.2540
6	 0.5790	 0.3470
7	 0.7090	 0.4440
8	 0.5770	 0.3480
9	 0.5530	 0.3450
A	 0.8910	 0.5300
B	 0.8700	 0.5130
C	 0.8510	 0.5210
D	 0.8760	 0.5310
E	 0.8360	 0.4570
F	 0.8250	 0.4730
G	 0.8140	 0.4810
H	 0.8670	 0.5040
I	 0.9180	 0.5410
J	 0.8200	 0.4730
K	 0.8190	 0.4820
L	 0.8620	 0.5240
M	 0.8250	 0.4920
N	 0.8130	 0.4780
O	 0.7010	 0.4070
R	 0.8070	 0.4930
S	 0.7660	 0.4230
T	 0.8260	 0.5120
V	 0.7170	 0.4120
W	 0.8640	 0.5140
X	 0.8460	 0.4760
Y	 0.8580	 0.5270
Z	 0.7480	 0.4270
a	 0.8920	 0.5310



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Chain	Atom inclusion	Q-score
b	 0.8710	 0.5120
c	 0.8510	 0.5200
d	 0.8730	 0.5330
e	 0.8330	 0.4510
f	 0.8210	 0.4720
g	 0.8150	 0.4810
h	 0.8460	 0.5020
i	 0.9110	 0.5400
j	 0.8160	 0.4750
k	 0.8230	 0.4810
l	 0.8620	 0.5230
m	 0.8250	 0.4950
n	 0.8150	 0.4800
o	 0.7020	 0.4060
p	 0.3400	 0.2440
q	 0.4670	 0.2820
r	 0.8080	 0.4940
s	 0.7690	 0.4240
t	 0.8260	 0.5120
v	 0.7170	 0.4140
w	 0.8670	 0.5090
x	 0.8410	 0.4710
y	 0.8590	 0.5250
z	 0.7330	 0.4220