



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2025 – 05:18 pm GMT

PDB ID : 9HD7 / pdb_00009hd7
EMDB ID : EMD-52056
Title : Cryo-EM structure of photosystem II C2S2M2L2 supercomplex from the green alga *Chlorella ohadii*
Authors : Kopecny, D.; Kouril, R.; Ardhad, R.; Skolidis, I.; Kastitis, P.
Deposited on : 2024-11-11
Resolution : 2.95 Å (reported)
Based on initial models : 8C29, 7OUI

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:

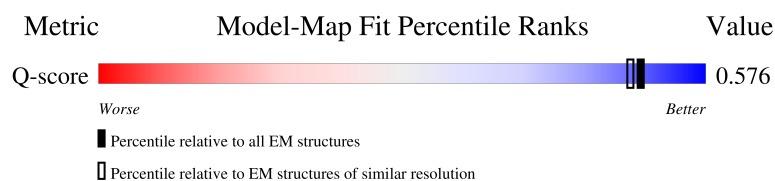
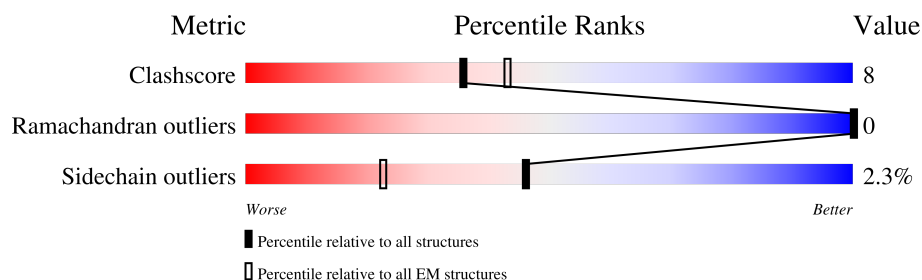
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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) : 2.46

1 Overall quality at a glance

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

The reported resolution of this entry is 2.95 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13114 (2.45 - 3.45)

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

Mol	Chain	Length	Quality of chain
1	1	249	<div> <div>42%</div> <div>71% 16% • 12%</div> </div>
1	11	249	<div> <div>49%</div> <div>67% 21% • 10%</div> </div>
1	14	249	<div> <div>48%</div> <div>69% 19% • 10%</div> </div>
1	4	249	<div> <div>43%</div> <div>71% 15% • 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	249	
1	g	249	
2	12	247	
2	15	247	
2	2	247	
2	5	247	
2	N	247	
2	n	247	
3	3	259	
3	6	259	
4	7	140	
4	8	140	
5	13	243	
5	16	243	
6	A	353	
6	a	353	
7	B	508	
7	b	508	
8	C	473	
8	c	473	
9	D	352	
9	d	352	
10	E	83	
10	e	83	
11	F	41	

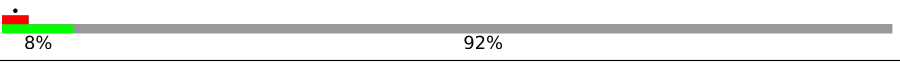
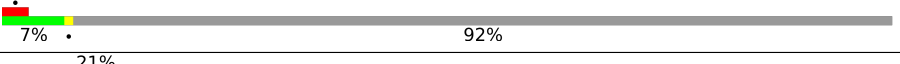
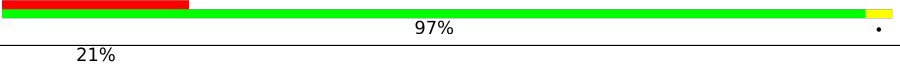
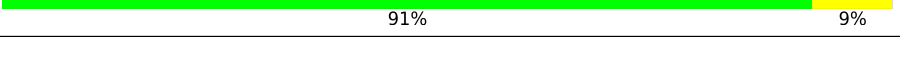


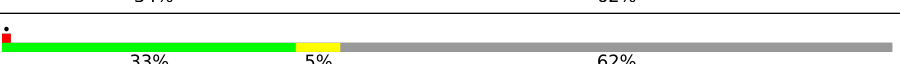
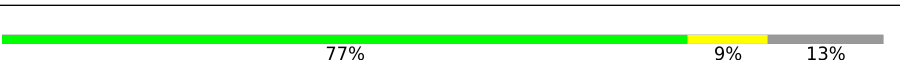

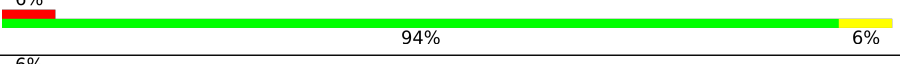
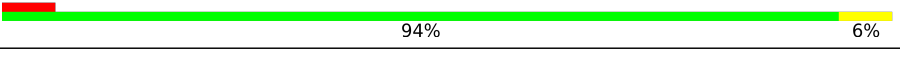
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Mol	Chain	Length	Quality of chain
11	f	41	
12	H	80	
12	h	80	
13	I	38	
13	i	38	
14	J	42	
14	j	42	
15	K	42	
15	k	42	
16	L	38	
16	l	38	
17	M	34	
17	m	34	
18	O	305	
18	o	305	
19	P	915	
19	p	915	
20	Q	203	
20	q	203	
21	R	297	
21	r	297	
22	S	293	
22	s	293	
23	T	31	
23	t	31	

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Mol	Chain	Length	Quality of chain
24	U	367	
24	u	367	
25	V	33	
25	v	33	
26	W	447	
26	w	447	
27	X	100	
27	x	100	
28	Y	256	
28	y	256	
29	Z	62	
29	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
30	CHL	1	601	X	-	-	-
30	CHL	1	605	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	1	608	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	11	601	X	-	-	-
30	CHL	11	605	X	-	-	-
30	CHL	11	606	X	-	-	-
30	CHL	11	607	X	-	-	-
30	CHL	11	608	X	-	-	-
30	CHL	11	609	X	-	-	-
30	CHL	12	601	X	-	-	-
30	CHL	12	605	X	-	-	-
30	CHL	12	606	X	-	-	-
30	CHL	12	607	X	-	-	-
30	CHL	12	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	13	601	X	-	-	-
30	CHL	13	605	X	-	-	-
30	CHL	13	606	X	-	-	-
30	CHL	13	607	X	-	-	-
30	CHL	13	608	X	-	-	-
30	CHL	13	609	X	-	-	-
30	CHL	14	601	X	-	-	-
30	CHL	14	605	X	-	-	-
30	CHL	14	606	X	-	-	-
30	CHL	14	607	X	-	-	-
30	CHL	14	608	X	-	-	-
30	CHL	14	609	X	-	-	-
30	CHL	15	601	X	-	-	-
30	CHL	15	605	X	-	-	-
30	CHL	15	606	X	-	-	-
30	CHL	15	607	X	-	-	-
30	CHL	15	608	X	-	-	-
30	CHL	16	601	X	-	-	-
30	CHL	16	605	X	-	-	-
30	CHL	16	606	X	-	-	-
30	CHL	16	607	X	-	-	-
30	CHL	16	608	X	-	-	-
30	CHL	16	609	X	-	-	-
30	CHL	2	601	X	-	-	-
30	CHL	2	605	X	-	-	-
30	CHL	2	606	X	-	-	-
30	CHL	2	607	X	-	-	-
30	CHL	2	608	X	-	-	-
30	CHL	2	609	X	-	-	-
30	CHL	3	601	X	-	-	-
30	CHL	3	605	X	-	-	-
30	CHL	3	606	X	-	-	-
30	CHL	3	607	X	-	-	-
30	CHL	3	608	X	-	-	-
30	CHL	3	609	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	605	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	609	X	-	-	-
30	CHL	5	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	5	605	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	609	X	-	-	-
30	CHL	6	601	X	-	-	-
30	CHL	6	605	X	-	-	-
30	CHL	6	606	X	-	-	-
30	CHL	6	607	X	-	-	-
30	CHL	6	608	X	-	-	-
30	CHL	6	609	X	-	-	-
30	CHL	G	601	X	-	-	-
30	CHL	G	605	X	-	-	-
30	CHL	G	606	X	-	-	-
30	CHL	G	607	X	-	-	-
30	CHL	G	608	X	-	-	-
30	CHL	G	609	X	-	-	-
30	CHL	N	601	X	-	-	-
30	CHL	N	605	X	-	-	-
30	CHL	N	606	X	-	-	-
30	CHL	N	607	X	-	-	-
30	CHL	N	608	X	-	-	-
30	CHL	N	609	X	-	-	-
30	CHL	R	605	X	-	-	-
30	CHL	R	606	X	-	-	-
30	CHL	R	607	X	-	-	-
30	CHL	S	601	X	-	-	-
30	CHL	S	606	X	-	-	-
30	CHL	S	607	X	-	-	-
30	CHL	S	608	X	-	-	-
30	CHL	Y	601	X	-	-	-
30	CHL	Y	605	X	-	-	-
30	CHL	Y	606	X	-	-	-
30	CHL	Y	607	X	-	-	-
30	CHL	Y	608	X	-	-	-
30	CHL	Y	609	X	-	-	-
30	CHL	g	601	X	-	-	-
30	CHL	g	605	X	-	-	-
30	CHL	g	606	X	-	-	-
30	CHL	g	607	X	-	-	-
30	CHL	g	608	X	-	-	-
30	CHL	g	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	n	601	X	-	-	-
30	CHL	n	605	X	-	-	-
30	CHL	n	606	X	-	-	-
30	CHL	n	607	X	-	-	-
30	CHL	n	608	X	-	-	-
30	CHL	n	609	X	-	-	-
30	CHL	r	605	X	-	-	-
30	CHL	r	606	X	-	-	-
30	CHL	r	607	X	-	-	-
30	CHL	s	601	X	-	-	-
30	CHL	s	606	X	-	-	-
30	CHL	s	607	X	-	-	-
30	CHL	s	608	X	-	-	-
30	CHL	y	601	X	-	-	-
30	CHL	y	605	X	-	-	-
30	CHL	y	606	X	-	-	-
30	CHL	y	607	X	-	-	-
30	CHL	y	608	X	-	-	-
30	CHL	y	609	X	-	-	-
31	CLA	1	602	X	-	-	-
31	CLA	1	603	X	-	-	-
31	CLA	1	604	X	-	-	-
31	CLA	1	610	X	-	-	-
31	CLA	1	611	X	-	-	-
31	CLA	1	612	X	-	-	-
31	CLA	1	613	X	-	-	-
31	CLA	1	614	X	-	-	-
31	CLA	11	602	X	-	-	-
31	CLA	11	603	X	-	-	-
31	CLA	11	604	X	-	-	-
31	CLA	11	610	X	-	-	-
31	CLA	11	611	X	-	-	-
31	CLA	11	612	X	-	-	-
31	CLA	11	613	X	-	-	-
31	CLA	11	614	X	-	-	-
31	CLA	12	602	X	-	-	-
31	CLA	12	603	X	-	-	-
31	CLA	12	604	X	-	-	-
31	CLA	12	609	X	-	-	-
31	CLA	12	610	X	-	-	-
31	CLA	12	611	X	-	-	-
31	CLA	12	612	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	12	613	X	-	-	-
31	CLA	13	602	X	-	-	-
31	CLA	13	603	X	-	-	-
31	CLA	13	604	X	-	-	-
31	CLA	13	610	X	-	-	-
31	CLA	13	611	X	-	-	-
31	CLA	13	612	X	-	-	-
31	CLA	13	613	X	-	-	-
31	CLA	13	614	X	-	-	-
31	CLA	13	615	X	-	-	-
31	CLA	14	602	X	-	-	-
31	CLA	14	603	X	-	-	-
31	CLA	14	604	X	-	-	-
31	CLA	14	610	X	-	-	-
31	CLA	14	611	X	-	-	-
31	CLA	14	612	X	-	-	-
31	CLA	14	613	X	-	-	-
31	CLA	14	614	X	-	-	-
31	CLA	15	602	X	-	-	-
31	CLA	15	603	X	-	-	-
31	CLA	15	604	X	-	-	-
31	CLA	15	609	X	-	-	-
31	CLA	15	610	X	-	-	-
31	CLA	15	611	X	-	-	-
31	CLA	15	612	X	-	-	-
31	CLA	15	613	X	-	-	-
31	CLA	16	602	X	-	-	-
31	CLA	16	603	X	-	-	-
31	CLA	16	604	X	-	-	-
31	CLA	16	610	X	-	-	-
31	CLA	16	611	X	-	-	-
31	CLA	16	612	X	-	-	-
31	CLA	16	613	X	-	-	-
31	CLA	16	614	X	-	-	-
31	CLA	16	615	X	-	-	-
31	CLA	2	602	X	-	-	-
31	CLA	2	603	X	-	-	-
31	CLA	2	604	X	-	-	-
31	CLA	2	610	X	-	-	-
31	CLA	2	611	X	-	-	-
31	CLA	2	612	X	-	-	-
31	CLA	2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	3	602	X	-	-	-
31	CLA	3	603	X	-	-	-
31	CLA	3	604	X	-	-	-
31	CLA	3	610	X	-	-	-
31	CLA	3	611	X	-	-	-
31	CLA	3	612	X	-	-	-
31	CLA	3	613	X	-	-	-
31	CLA	3	614	X	-	-	-
31	CLA	3	615	X	-	-	-
31	CLA	4	602	X	-	-	-
31	CLA	4	603	X	-	-	-
31	CLA	4	604	X	-	-	-
31	CLA	4	610	X	-	-	-
31	CLA	4	611	X	-	-	-
31	CLA	4	612	X	-	-	-
31	CLA	4	613	X	-	-	-
31	CLA	4	614	X	-	-	-
31	CLA	5	602	X	-	-	-
31	CLA	5	603	X	-	-	-
31	CLA	5	604	X	-	-	-
31	CLA	5	610	X	-	-	-
31	CLA	5	611	X	-	-	-
31	CLA	5	612	X	-	-	-
31	CLA	5	613	X	-	-	-
31	CLA	6	602	X	-	-	-
31	CLA	6	603	X	-	-	-
31	CLA	6	604	X	-	-	-
31	CLA	6	610	X	-	-	-
31	CLA	6	611	X	-	-	-
31	CLA	6	612	X	-	-	-
31	CLA	6	613	X	-	-	-
31	CLA	6	614	X	-	-	-
31	CLA	6	615	X	-	-	-
31	CLA	A	402	X	-	-	-
31	CLA	A	403	X	-	-	-
31	CLA	A	404	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C	514	X	-	-	-
31	CLA	D	404	X	-	-	-
31	CLA	D	405	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	N	602	X	-	-	-
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N	615	X	-	-	-
31	CLA	R	601	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R	614	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	615	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	610	X	-	-	-
31	CLA	Y	611	X	-	-	-
31	CLA	Y	612	X	-	-	-
31	CLA	Y	613	X	-	-	-
31	CLA	Y	614	X	-	-	-
31	CLA	Y	615	X	-	-	-
31	CLA	a	403	X	-	-	-
31	CLA	a	404	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	b	601	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c	514	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	r	601	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r	614	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	615	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-
31	CLA	y	614	X	-	-	-
31	CLA	y	615	X	-	-	-
33	LUT	12	614	-	-	X	-

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 112944 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 Lhcbm-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1673	1084	267	317	5		
1	4	220	Total	C	N	O	S	0	0
			1673	1084	267	317	5		
1	11	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	14	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	G	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		
1	g	223	Total	C	N	O	S	0	0
			1693	1094	272	322	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	196	Total	C	N	O	S	0	0
			1496	966	249	276	5		
2	5	196	Total	C	N	O	S	0	0
			1496	966	249	276	5		
2	12	170	Total	C	N	O	S	0	0
			1330	863	220	242	5		
2	15	170	Total	C	N	O	S	0	0
			1330	863	220	242	5		
2	N	220	Total	C	N	O	S	0	0
			1679	1085	278	311	5		
2	n	220	Total	C	N	O	S	0	0
			1679	1085	278	311	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

- Molecule 4 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	107	Total	C	N	O	S	0	0
			816	522	136	156	2		
4	8	107	Total	C	N	O	S	0	0
			816	522	136	156	2		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	13	215	Total	C	N	O	S	0	0
			1645	1064	268	308	5		
5	16	215	Total	C	N	O	S	0	0
			1645	1064	268	308	5		

- Molecule 6 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		
6	a	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		

- Molecule 7 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	505	Total	C	N	O	S	0	0
			3963	2588	669	694	12		
7	b	505	Total	C	N	O	S	0	0
			3963	2588	669	694	12		

- Molecule 8 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	449	Total	C	N	O	S	0	0
			3491	2284	585	607	15		
8	c	449	Total	C	N	O	S	0	0
			3491	2284	585	607	15		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		
9	d	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	80	Total	C	N	O	0	0
			646	420	105	121		
10	e	80	Total	C	N	O	0	0
			646	420	105	121		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	37	Total	C	N	O	S	0	0
			303	206	49	47	1		
11	f	37	Total	C	N	O	S	0	0
			303	206	49	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	67	Total	C	N	O	S	0	0
			507	336	73	95	3		
12	h	67	Total	C	N	O	S	0	0
			507	336	73	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	34	Total	C	N	O	S	0	0
			274	187	41	45	1		
13	i	34	Total	C	N	O	S	0	0
			274	187	41	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	38	Total	C	N	O	0	0
			270	182	42	46		
14	j	38	Total	C	N	O	0	0
			270	182	42	46		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	37	Total	C	N	O	0	0
			295	204	43	48		
15	k	37	Total	C	N	O	0	0
			295	204	43	48		

- Molecule 16 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	37	Total	C	N	O	0	0
			303	203	48	52		
16	l	37	Total	C	N	O	0	0
			303	203	48	52		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	30	Total	C	N	O	0	0
			228	157	33	38		
17	m	30	Total	C	N	O	0	0
			228	157	33	38		

- Molecule 18 is a protein called Chloroplast oxygen-evolving enhancer protein 1b (PsbO).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	238	Total	C	N	O	S	0	0
			1759	1106	288	357	8		
18	o	238	Total	C	N	O	S	0	0
			1759	1106	288	357	8		

- Molecule 19 is a protein called PWWP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	p	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

- Molecule 20 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	144	Total	C	N	O		0	0
			1122	701	207	214			
20	q	144	Total	C	N	O		0	0
			1122	701	207	214			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	231	Total	C	N	O	S	0	0
			1783	1132	303	342	6		
21	r	231	Total	C	N	O	S	0	0
			1783	1132	303	342	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		
22	s	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	30	Total	C	N	O	S	0	0
			246	172	36	37	1		
23	t	30	Total	C	N	O	S	0	0
			246	172	36	37	1		

- Molecule 24 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	30	Total	C	N	O		0	0
			233	156	40	37			
24	u	30	Total	C	N	O		0	0
			233	156	40	37			

- Molecule 25 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	33	Total	C	N	O	S	0	0
			241	160	39	41	1		
25	v	33	Total	C	N	O	S	0	0
			241	160	39	41	1		

- Molecule 26 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	60	Total	C	N	O	0	0
			468	301	74	93		
26	w	60	Total	C	N	O	0	0
			468	301	74	93		

- Molecule 27 is a protein called Photosystem II reaction center protein X (PsbX).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	38	Total	C	N	O	0	0
			258	162	47	49		
27	x	38	Total	C	N	O	0	0
			258	162	47	49		

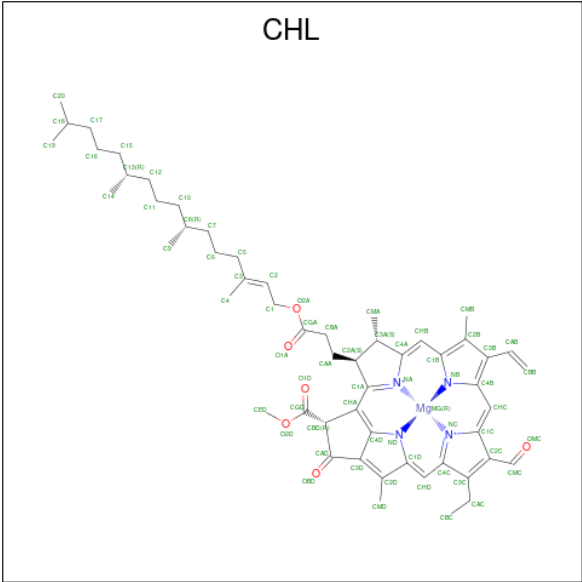
- Molecule 28 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	222	Total	C	N	O	S	0	0
			1694	1102	271	316	5		
28	y	222	Total	C	N	O	S	0	0
			1694	1102	271	316	5		

- Molecule 29 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		
29	z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	6	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
30	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	11	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	11	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	11	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	11	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	11	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	11	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	12	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	12	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	12	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	12	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	12	1	Total 53	C 42	Mg 1	N 4	O 6	0
30	13	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	13	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	13	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	13	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	14	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	14	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	14	1	Total 47	C 36	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	14	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	14	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	15	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	15	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	15	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	15	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	15	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	16	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	16	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	16	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	16	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	16	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	16	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	G	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	G	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	N	1	Total 53	C 42	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
30	N	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	N	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	R	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	Y	1	Total 44	C 35	Mg 1	N 4	O 4	0
30	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	g	1	Total 50	C 39	Mg 1	N 4	O 6	0

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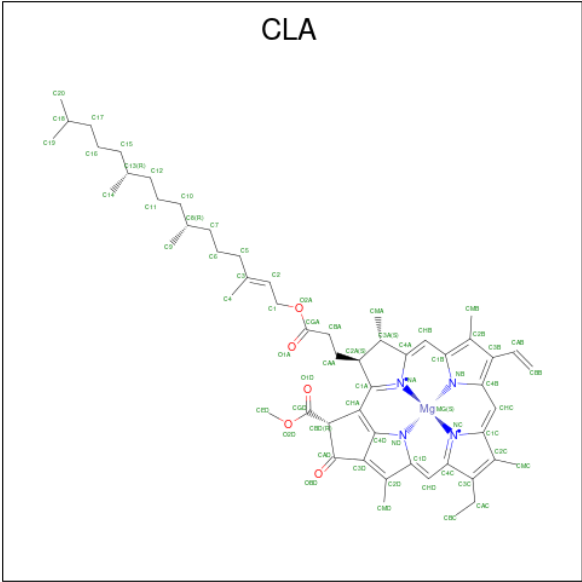
Mol	Chain	Residues	Atoms					AltConf
30	g	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	n	1	Total 52	C 41	Mg 1	N 4	O 6	0
30	n	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	n	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
30	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	r	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	r	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
30	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
30	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	y	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	y	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	y	1	66	55	1	4	6	0

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	1	1	Total 60	50	1	4	5	0
31	1	1	Total 47	37	1	4	5	0
31	1	1	Total 50	40	1	4	5	0
31	1	1	Total 55	45	1	4	5	0
31	1	1	Total 50	40	1	4	5	0
31	1	1	Total 46	36	1	4	5	0
31	1	1	Total 55	45	1	4	5	0
31	1	1	Total 46	36	1	4	5	0
31	2	1	Total 55	45	1	4	5	0
31	2	1	Total 55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
31	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	11	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	11	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	11	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	11	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	11	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	14	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	14	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	14	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	14	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	14	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	15	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	15	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	16	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	16	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	16	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	Y	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
31	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	n	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	r	1	Total 49	C 39	Mg 1	N 4	O 5	0

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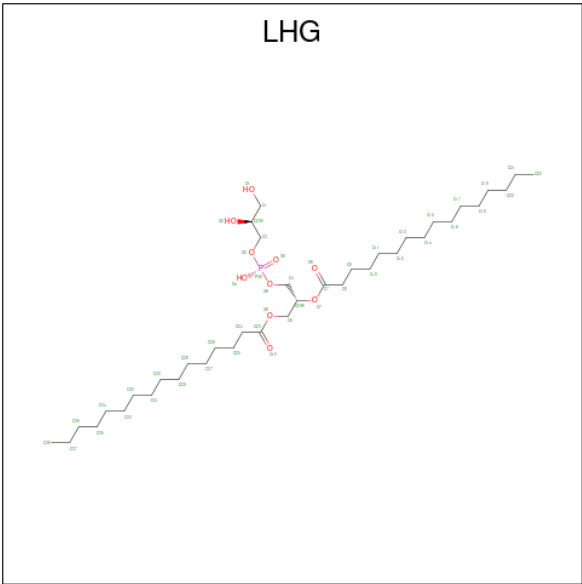
Mol	Chain	Residues	Atoms					AltConf
31	r	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	r	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
31	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	s	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
32	1	1	Total	C	O	P	0
			43	32	10	1	
32	3	1	Total	C	O	P	0
			44	33	10	1	
32	3	1	Total	C	O	P	0
			47	36	10	1	
32	4	1	Total	C	O	P	0
			47	36	10	1	
32	6	1	Total	C	O	P	0
			44	33	10	1	
32	6	1	Total	C	O	P	0
			47	36	10	1	
32	11	1	Total	C	O	P	0
			49	38	10	1	
32	13	1	Total	C	O	P	0
			40	29	10	1	
32	14	1	Total	C	O	P	0
			49	38	10	1	

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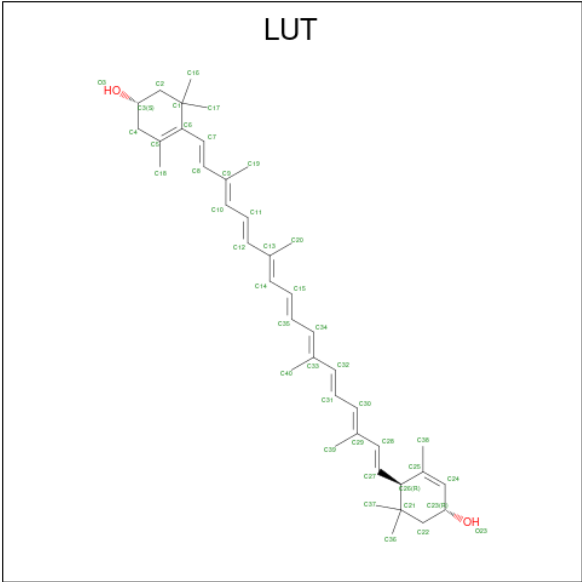
Mol	Chain	Residues	Atoms				AltConf
32	16	1	Total 40	C 29	O 10	P 1	0
32	A	1	Total 49	C 38	O 10	P 1	0
32	A	1	Total 44	C 33	O 10	P 1	0
32	A	1	Total 43	C 32	O 10	P 1	0
32	A	1	Total 49	C 38	O 10	P 1	0
32	C	1	Total 42	C 31	O 10	P 1	0
32	D	1	Total 49	C 38	O 10	P 1	0
32	D	1	Total 39	C 28	O 10	P 1	0
32	D	1	Total 49	C 38	O 10	P 1	0
32	G	1	Total 49	C 38	O 10	P 1	0
32	L	1	Total 47	C 36	O 10	P 1	0
32	N	1	Total 49	C 38	O 10	P 1	0
32	R	1	Total 44	C 33	O 10	P 1	0
32	R	1	Total 38	C 27	O 10	P 1	0
32	R	1	Total 47	C 36	O 10	P 1	0
32	S	1	Total 49	C 38	O 10	P 1	0
32	S	1	Total 45	C 34	O 10	P 1	0
32	Y	1	Total 47	C 36	O 10	P 1	0
32	Y	1	Total 49	C 38	O 10	P 1	0
32	Y	1	Total 47	C 36	O 10	P 1	0
32	a	1	Total 49	C 38	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	O	P	0
			49	38	10	1	
32	a	1	Total	C	O	P	0
			44	33	10	1	
32	a	1	Total	C	O	P	0
			43	32	10	1	
32	c	1	Total	C	O	P	0
			42	31	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			39	28	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	g	1	Total	C	O	P	0
			49	38	10	1	
32	l	1	Total	C	O	P	0
			47	36	10	1	
32	n	1	Total	C	O	P	0
			49	38	10	1	
32	r	1	Total	C	O	P	0
			44	33	10	1	
32	r	1	Total	C	O	P	0
			38	27	10	1	
32	r	1	Total	C	O	P	0
			47	36	10	1	
32	s	1	Total	C	O	P	0
			49	38	10	1	
32	s	1	Total	C	O	P	0
			45	34	10	1	
32	y	1	Total	C	O	P	0
			47	36	10	1	
32	y	1	Total	C	O	P	0
			49	38	10	1	
32	y	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 33 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			42	40	2	
33	1	1	Total	C	O	0
			42	40	2	
33	2	1	Total	C	O	0
			42	40	2	
33	2	1	Total	C	O	0
			42	40	2	
33	3	1	Total	C	O	0
			42	40	2	
33	3	1	Total	C	O	0
			42	40	2	
33	4	1	Total	C	O	0
			42	40	2	
33	4	1	Total	C	O	0
			42	40	2	
33	5	1	Total	C	O	0
			42	40	2	
33	5	1	Total	C	O	0
			42	40	2	
33	6	1	Total	C	O	0
			42	40	2	
33	6	1	Total	C	O	0
			42	40	2	
33	11	1	Total	C	O	0
			42	40	2	
33	11	1	Total	C	O	0
			42	40	2	

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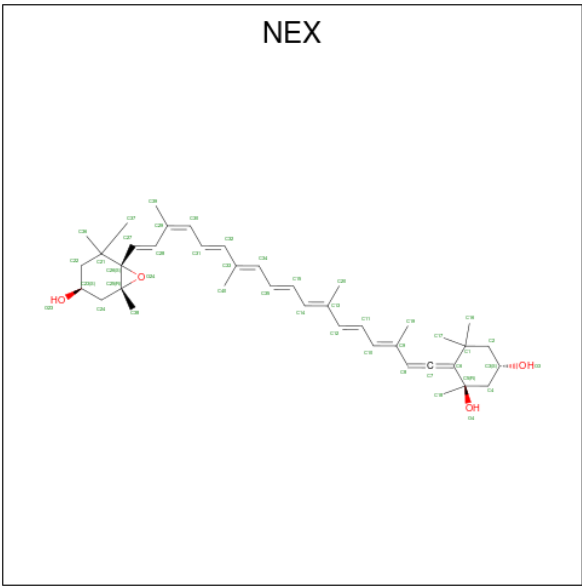
Mol	Chain	Residues	Atoms			AltConf
33	12	1	Total 42	C 40	O 2	0
33	12	1	Total 42	C 40	O 2	0
33	13	1	Total 42	C 40	O 2	0
33	13	1	Total 42	C 40	O 2	0
33	14	1	Total 42	C 40	O 2	0
33	14	1	Total 42	C 40	O 2	0
33	15	1	Total 42	C 40	O 2	0
33	15	1	Total 42	C 40	O 2	0
33	16	1	Total 42	C 40	O 2	0
33	16	1	Total 42	C 40	O 2	0
33	G	1	Total 42	C 40	O 2	0
33	G	1	Total 42	C 40	O 2	0
33	N	1	Total 42	C 40	O 2	0
33	N	1	Total 42	C 40	O 2	0
33	R	1	Total 42	C 40	O 2	0
33	S	1	Total 42	C 40	O 2	0
33	S	1	Total 42	C 40	O 2	0
33	Y	1	Total 42	C 40	O 2	0
33	Y	1	Total 42	C 40	O 2	0
33	g	1	Total 42	C 40	O 2	0
33	g	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
33	n	1	Total	C	O	0
			42	40	2	
33	n	1	Total	C	O	0
			42	40	2	
33	r	1	Total	C	O	0
			42	40	2	
33	s	1	Total	C	O	0
			42	40	2	
33	s	1	Total	C	O	0
			42	40	2	
33	y	1	Total	C	O	0
			42	40	2	
33	y	1	Total	C	O	0
			42	40	2	

- Molecule 34 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).



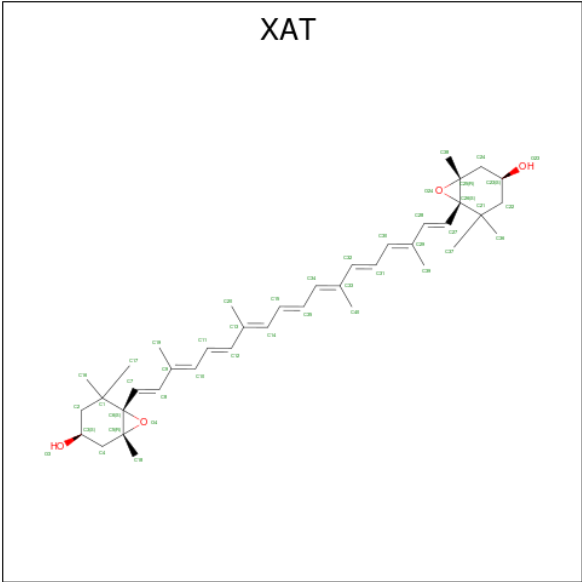
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			16	14	2	
34	2	1	Total	C	O	0
			32	30	2	
34	3	1	Total	C	O	0
			44	40	4	

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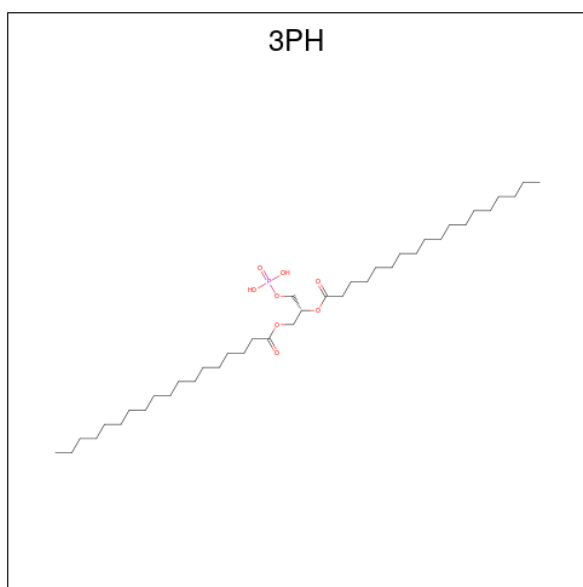
Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total	C	O	0
			16	14	2	
34	5	1	Total	C	O	0
			32	30	2	
34	6	1	Total	C	O	0
			44	40	4	
34	11	1	Total	C	O	0
			16	14	2	
34	12	1	Total	C	O	0
			27	25	2	
34	13	1	Total	C	O	0
			44	40	4	
34	14	1	Total	C	O	0
			16	14	2	
34	15	1	Total	C	O	0
			27	25	2	
34	16	1	Total	C	O	0
			44	40	4	
34	G	1	Total	C	O	0
			43	39	4	
34	N	1	Total	C	O	0
			44	40	4	
34	R	1	Total	C	O	0
			44	40	4	
34	S	1	Total	C	O	0
			44	40	4	
34	Y	1	Total	C	O	0
			44	40	4	
34	g	1	Total	C	O	0
			44	40	4	
34	n	1	Total	C	O	0
			44	40	4	
34	r	1	Total	C	O	0
			44	40	4	
34	s	1	Total	C	O	0
			44	40	4	
34	y	1	Total	C	O	0
			44	40	4	

- Molecule 35 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) (labeled as "Ligand of Interest" by depositor).



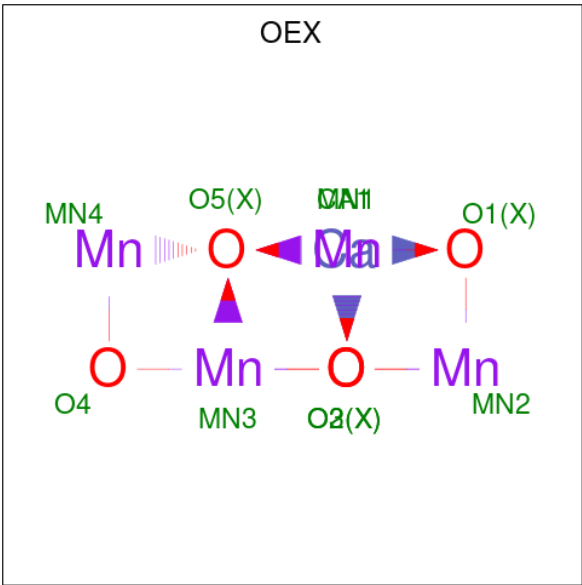
Mol	Chain	Residues	Atoms			AltConf
35	3	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	11	1	Total	C	O	0
			44	40	4	
35	14	1	Total	C	O	0
			44	40	4	
35	G	1	Total	C	O	0
			44	40	4	
35	R	1	Total	C	O	0
			44	40	4	
35	g	1	Total	C	O	0
			44	40	4	
35	r	1	Total	C	O	0
			44	40	4	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



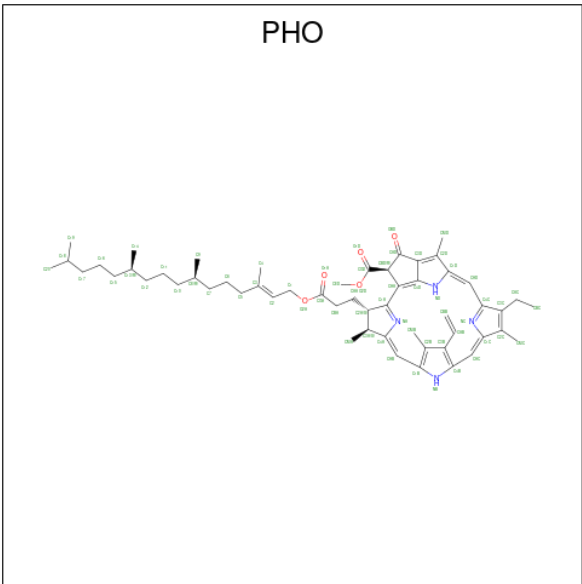
Mol	Chain	Residues	Atoms				AltConf
36	7	1	Total	C	O	P	0
			48	39	8	1	
36	8	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			38	29	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	b	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 37 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



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

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



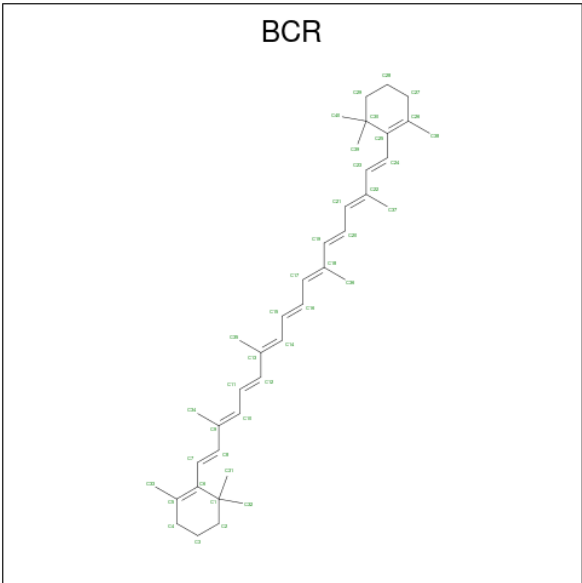
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	N	O	0
			64	55	4	5	

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

- Molecule 39 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



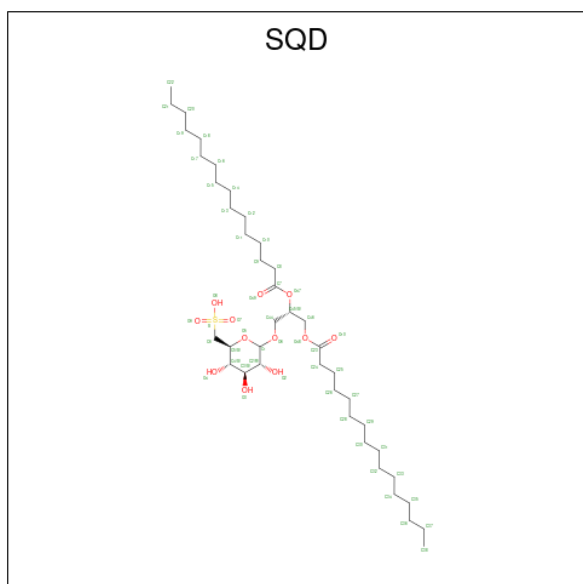
Mol	Chain	Residues	Atoms		AltConf
39	A	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	B	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	C	1	Total	C	0
			40	40	
39	D	1	Total	C	0
			40	40	

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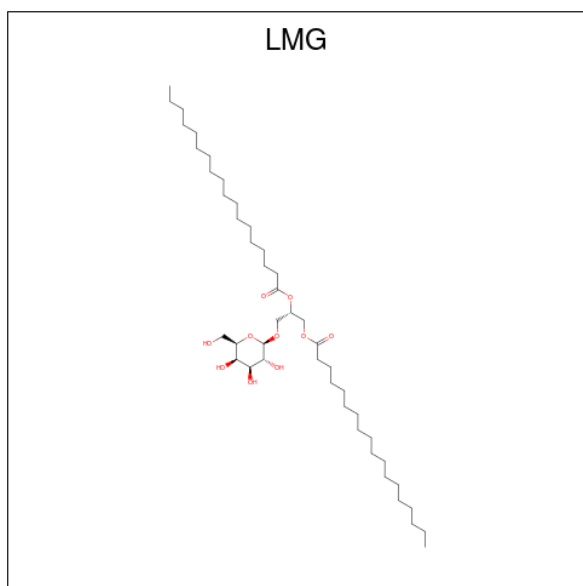
Mol	Chain	Residues	Atoms	AltConf
39	H	1	Total C 40 40	0
39	J	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	d	1	Total C 40 40	0
39	h	1	Total C 40 40	0
39	j	1	Total C 40 40	0

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	C	O	S	0
			51	38	12	1	
40	D	1	Total	C	O	S	0
			54	41	12	1	
40	D	1	Total	C	O	S	0
			46	33	12	1	
40	L	1	Total	C	O	S	0
			50	37	12	1	
40	a	1	Total	C	O	S	0
			51	38	12	1	
40	d	1	Total	C	O	S	0
			54	41	12	1	
40	d	1	Total	C	O	S	0
			46	33	12	1	
40	l	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



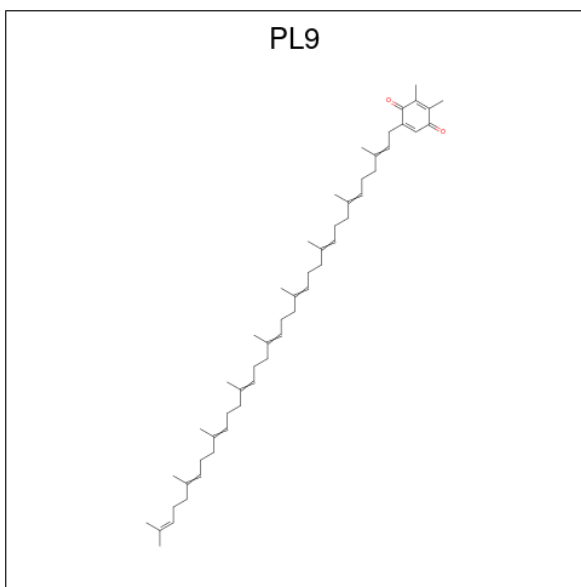
Mol	Chain	Residues	Atoms			AltConf
41	A	1	Total	C	O	0
			55	45	10	
41	B	1	Total	C	O	0
			49	39	10	
41	B	1	Total	C	O	0
			48	38	10	

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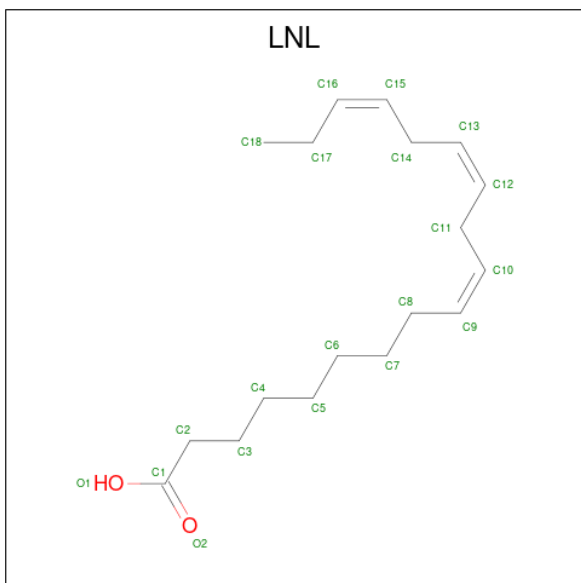
Mol	Chain	Residues	Atoms			AltConf
41	C	1	Total	C	O	0
			47	37	10	
41	C	1	Total	C	O	0
			55	45	10	
41	D	1	Total	C	O	0
			44	34	10	
41	D	1	Total	C	O	0
			48	38	10	
41	H	1	Total	C	O	0
			35	30	5	
41	J	1	Total	C	O	0
			51	41	10	
41	K	1	Total	C	O	0
			51	41	10	
41	S	1	Total	C	O	0
			42	32	10	
41	b	1	Total	C	O	0
			49	39	10	
41	b	1	Total	C	O	0
			46	36	10	
41	c	1	Total	C	O	0
			47	37	10	
41	c	1	Total	C	O	0
			55	45	10	
41	d	1	Total	C	O	0
			44	34	10	
41	d	1	Total	C	O	0
			35	30	5	
41	d	1	Total	C	O	0
			48	38	10	
41	j	1	Total	C	O	0
			51	41	10	
41	s	1	Total	C	O	0
			42	32	10	
41	v	1	Total	C	O	0
			51	41	10	
41	w	1	Total	C	O	0
			55	45	10	

- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



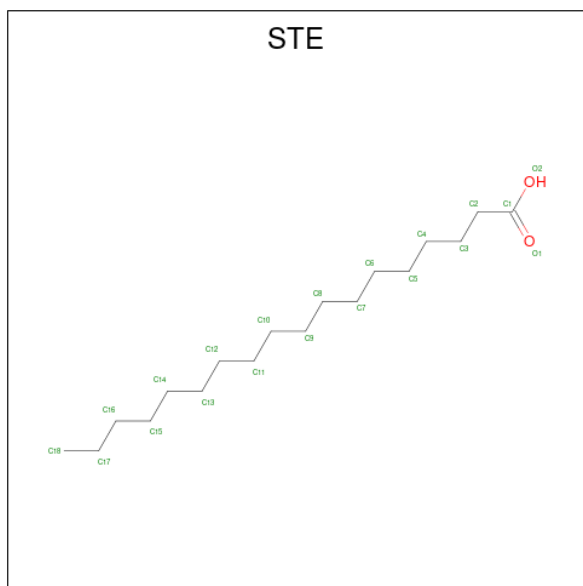
Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	C	O	0
			55	53	2	
42	D	1	Total	C	O	0
			55	53	2	
42	a	1	Total	C	O	0
			55	53	2	
42	d	1	Total	C	O	0
			55	53	2	

- Molecule 43 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$).



Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			20	18	2	
43	C	1	Total	C	O	0
			20	18	2	
43	C	1	Total	C	O	0
			20	18	2	
43	H	1	Total	C	O	0
			20	18	2	
43	I	1	Total	C	O	0
			20	18	2	
43	R	1	Total	C	O	0
			20	18	2	
43	W	1	Total	C	O	0
			20	18	2	
43	W	1	Total	C	O	0
			20	18	2	
43	X	1	Total	C	O	0
			20	18	2	
43	Y	1	Total	C	O	0
			20	18	2	
43	Y	1	Total	C	O	0
			20	18	2	
43	a	1	Total	C	O	0
			20	18	2	
43	c	1	Total	C	O	0
			20	18	2	
43	c	1	Total	C	O	0
			20	18	2	
43	h	1	Total	C	O	0
			20	18	2	
43	i	1	Total	C	O	0
			20	18	2	
43	r	1	Total	C	O	0
			20	18	2	
43	w	1	Total	C	O	0
			20	18	2	
43	x	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	
43	y	1	Total	C	O	0
			20	18	2	

- Molecule 44 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).

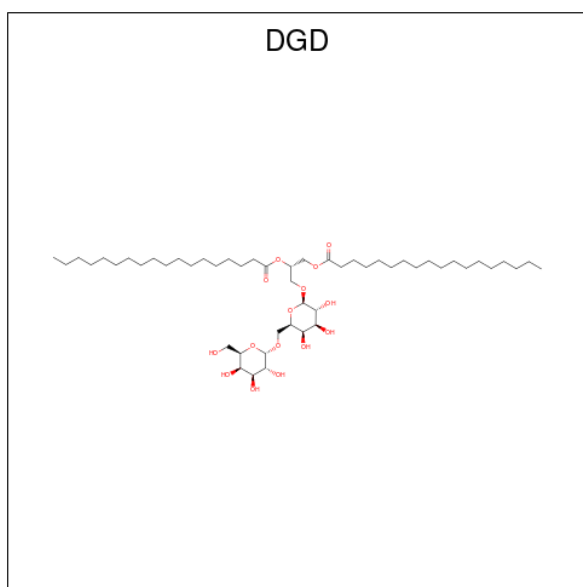


Mol	Chain	Residues	Atoms			AltConf
44	B	1	Total	C	O	0
			20	18	2	
44	b	1	Total	C	O	0
			20	18	2	

- Molecule 45 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
45	C	1	Total	Cl	0
			1	1	
45	c	1	Total	Cl	0
			1	1	

- Molecule 46 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

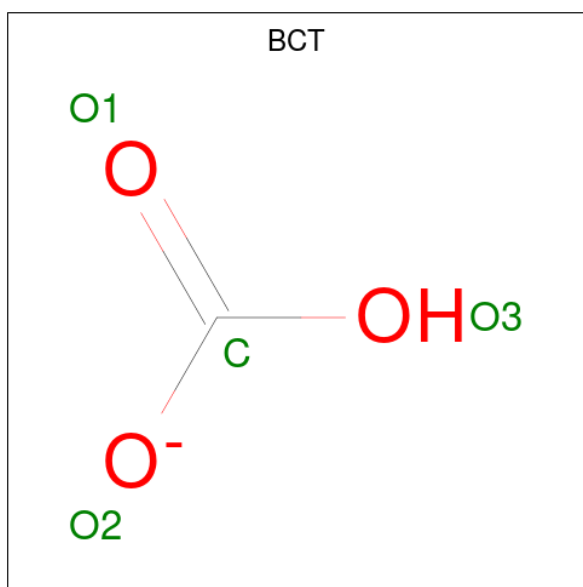


Mol	Chain	Residues	Atoms			AltConf
46	C	1	Total	C	O	0
			66	51	15	
46	C	1	Total	C	O	0
			58	43	15	
46	C	1	Total	C	O	0
			59	44	15	
46	W	1	Total	C	O	0
			46	36	10	
46	c	1	Total	C	O	0
			66	51	15	
46	c	1	Total	C	O	0
			58	43	15	
46	c	1	Total	C	O	0
			59	44	15	
46	w	1	Total	C	O	0
			40	30	10	

- Molecule 47 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

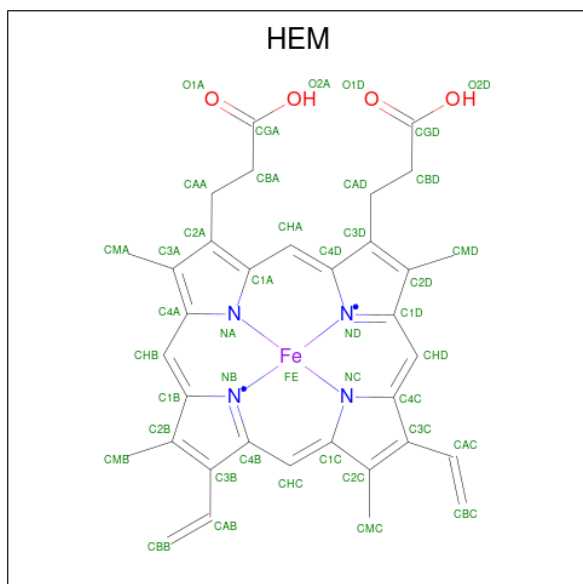
Mol	Chain	Residues	Atoms		AltConf
47	D	1	Total	Fe	0
			1	1	
47	d	1	Total	Fe	0
			1	1	

- Molecule 48 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 49 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



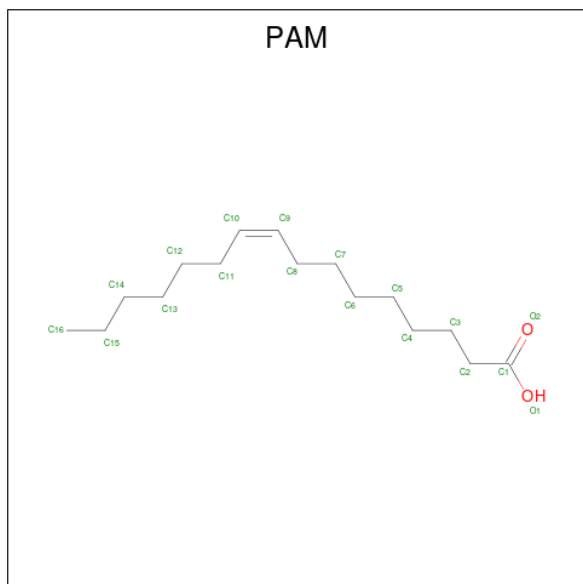
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Continued from previous page...

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

- Molecule 50 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).

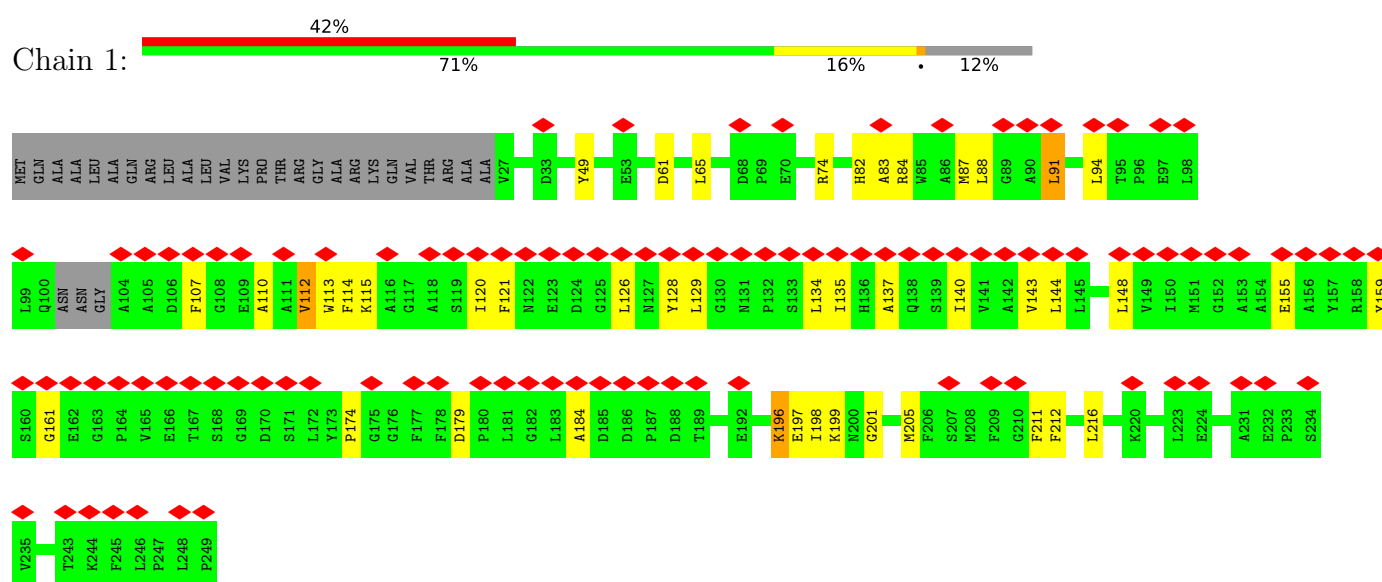


Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			18	16	2	
50	n	1	Total	C	O	0
			18	16	2	

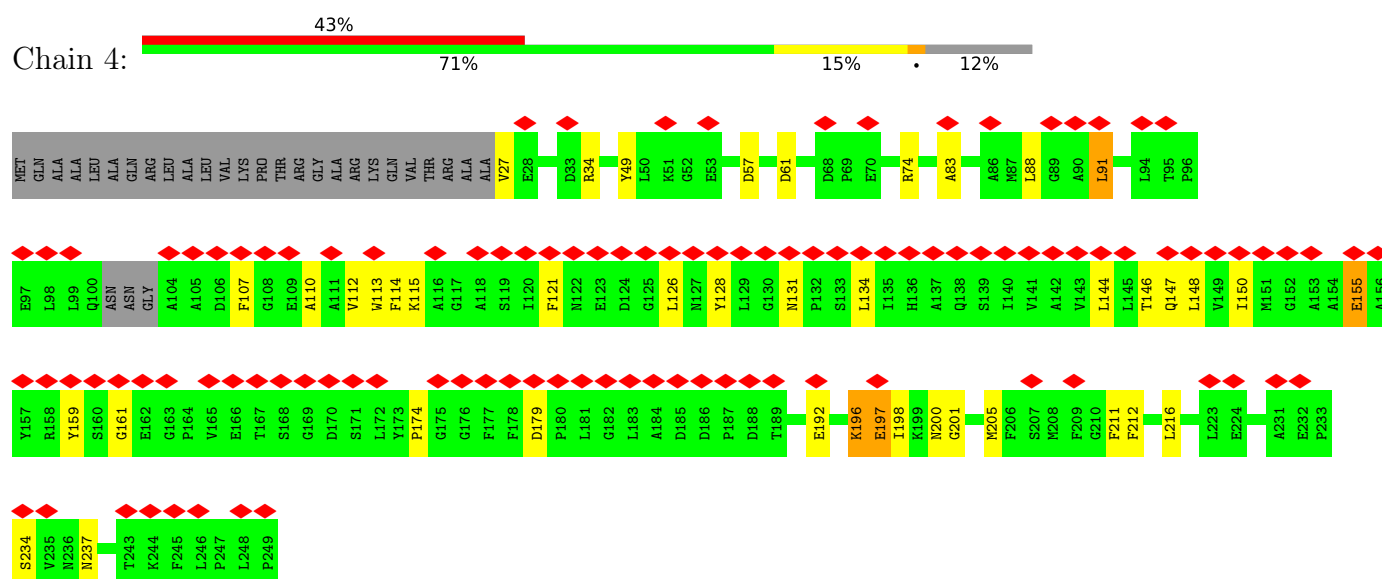
3 Residue-property plots

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

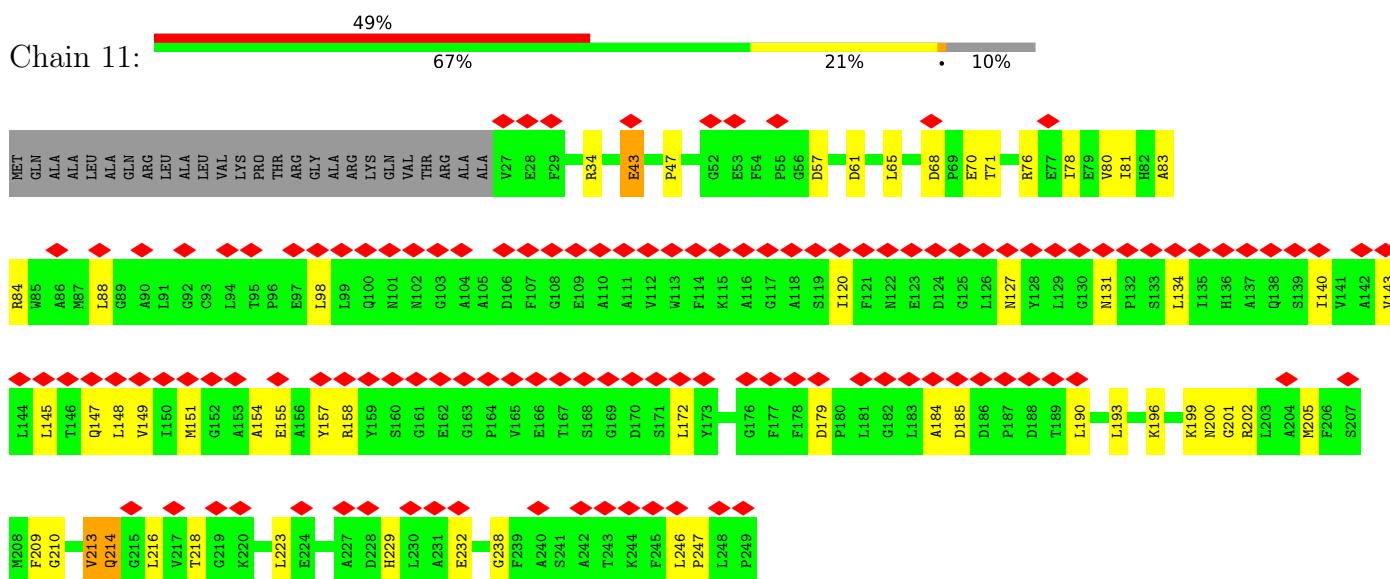
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



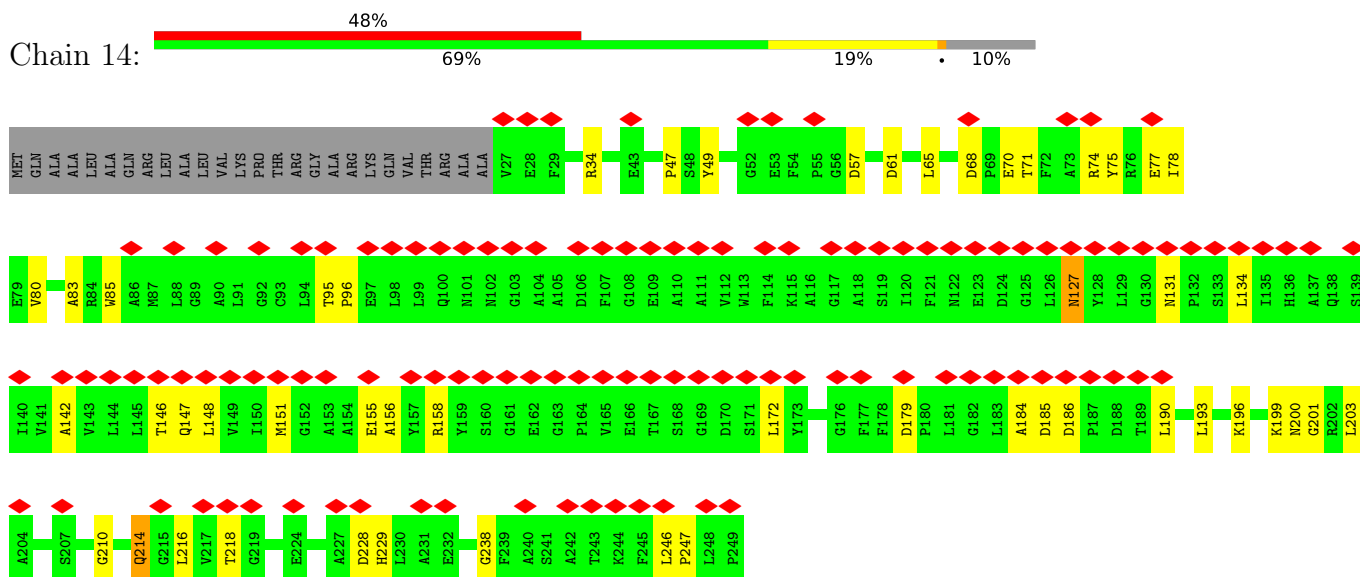
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



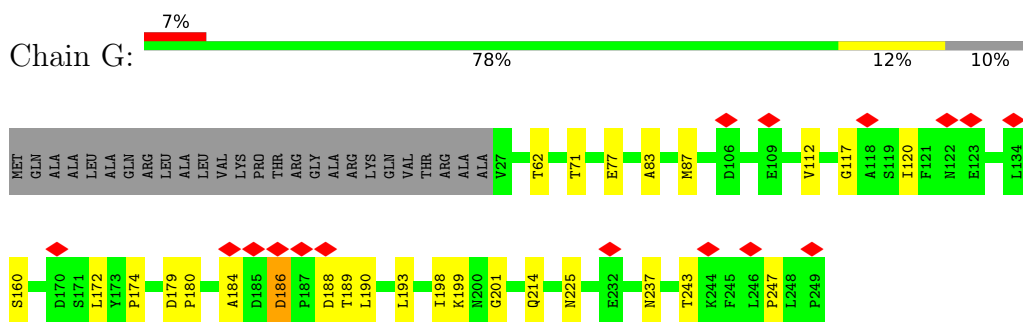
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I



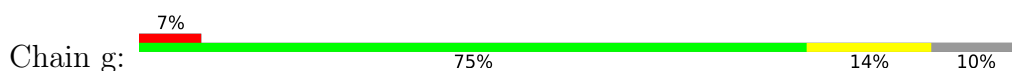
- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

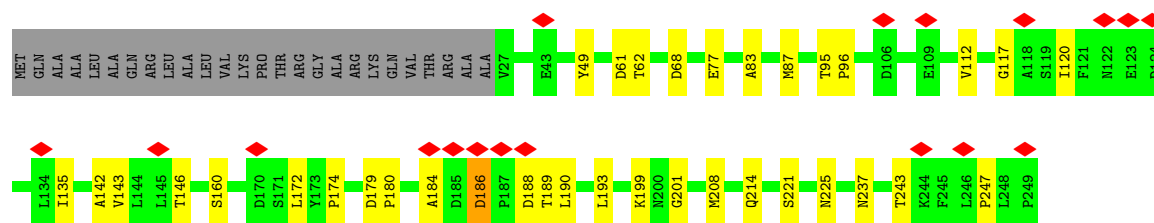


- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

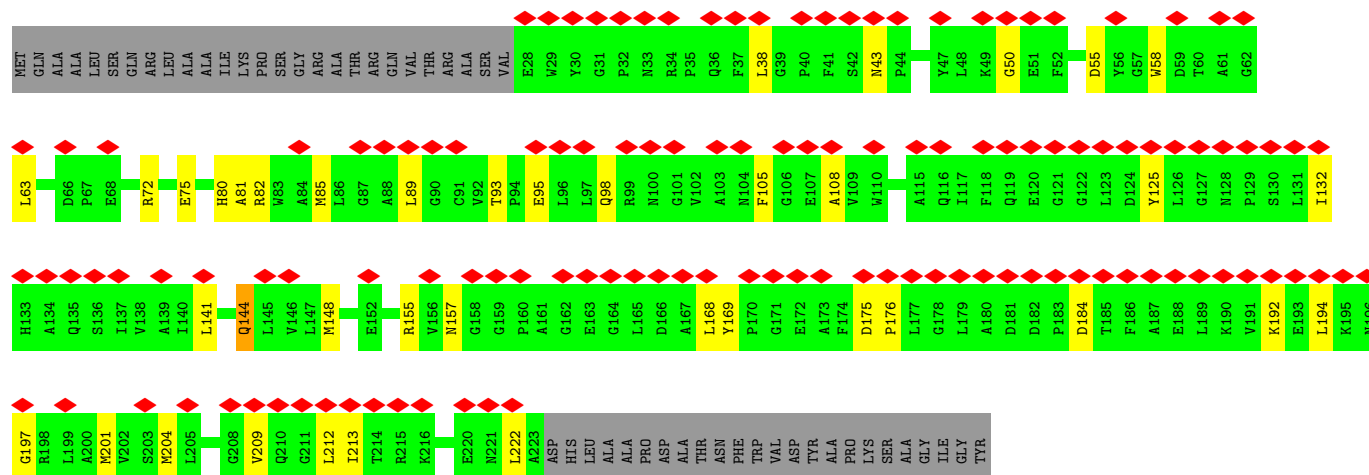


- Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

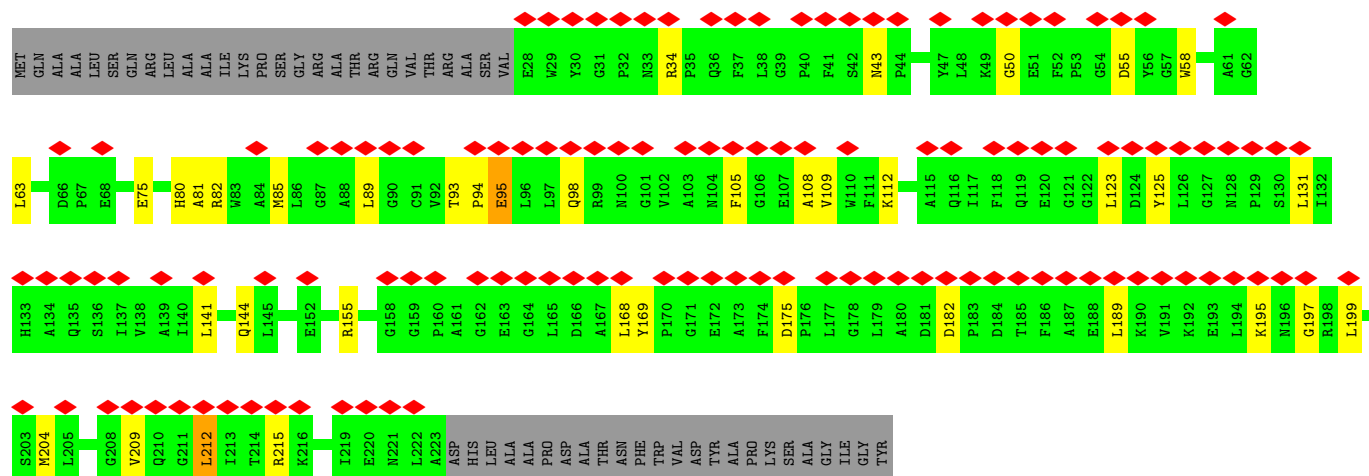




- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

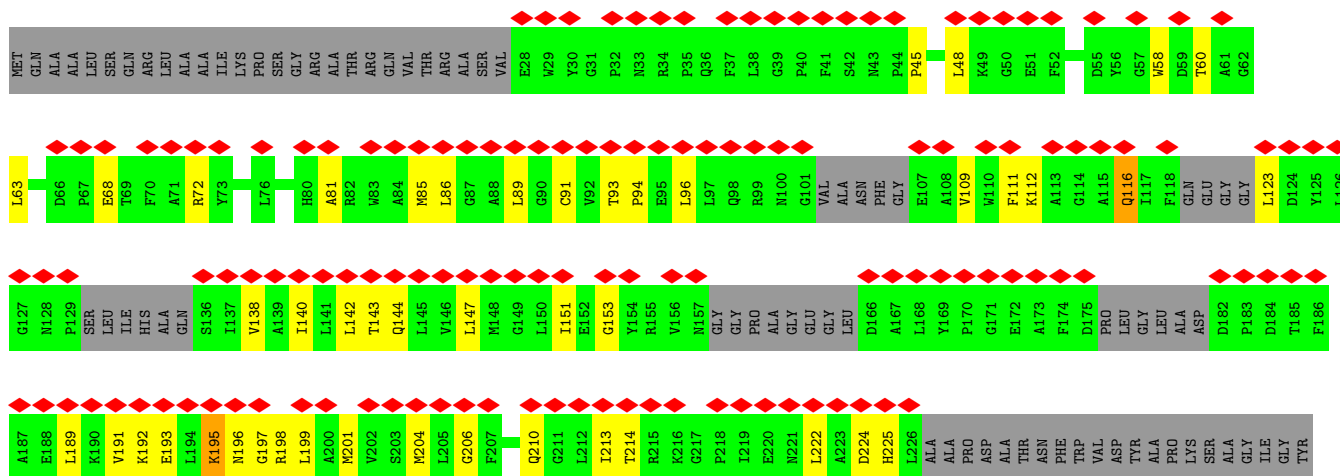


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

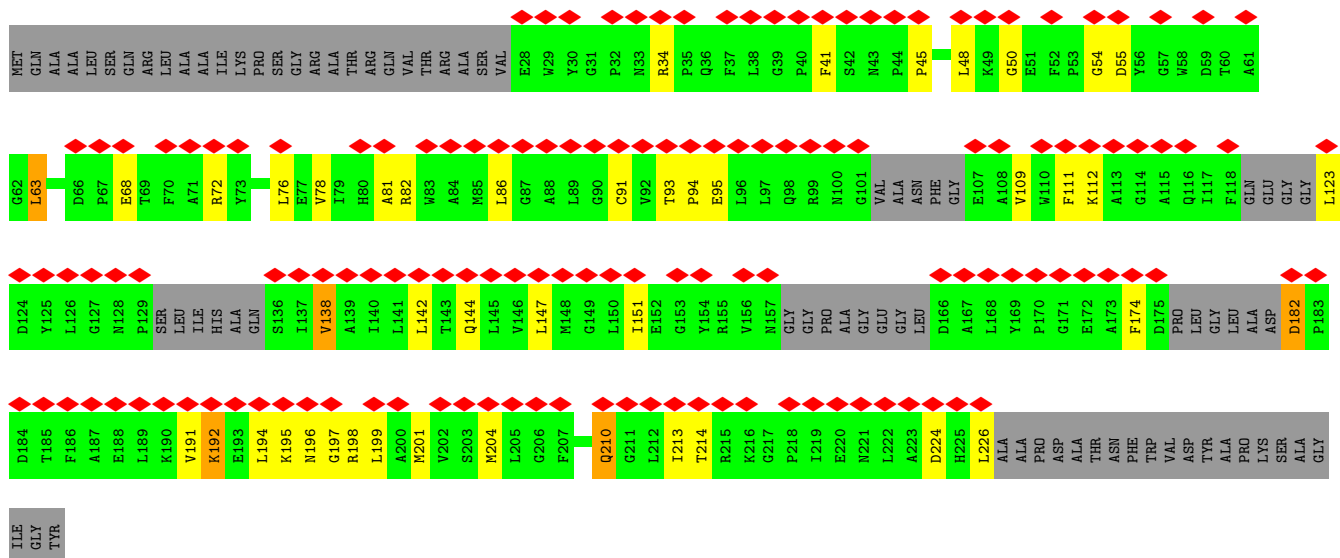


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

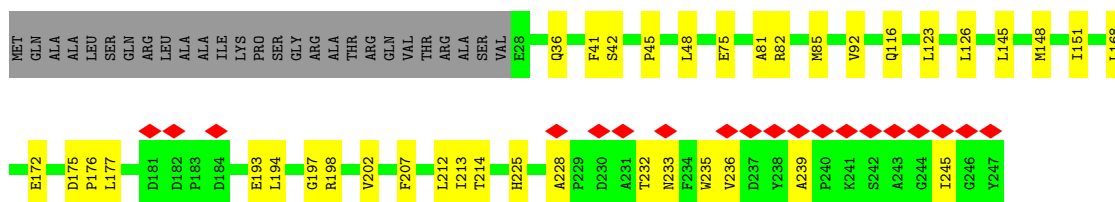
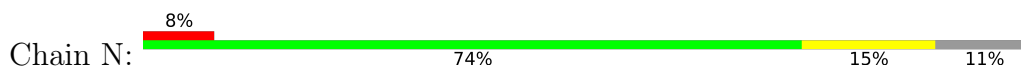




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

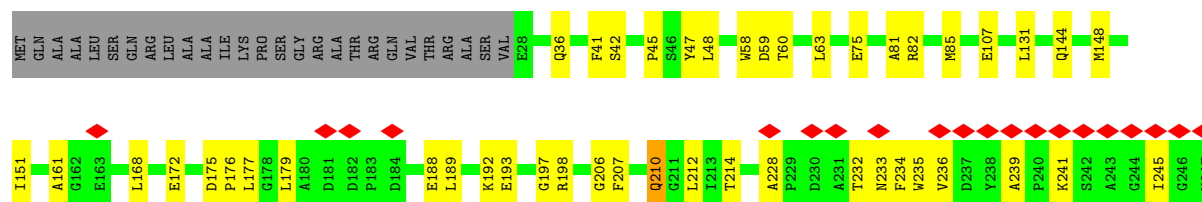


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

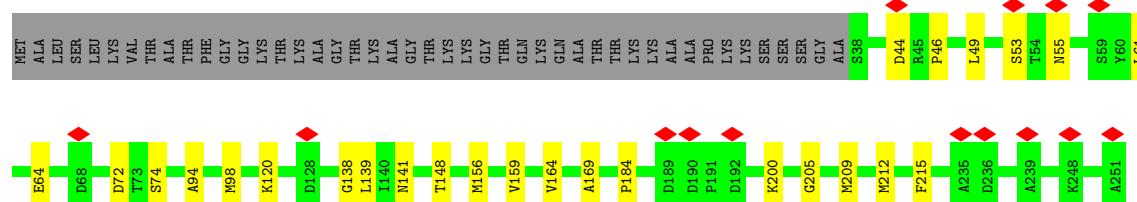


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

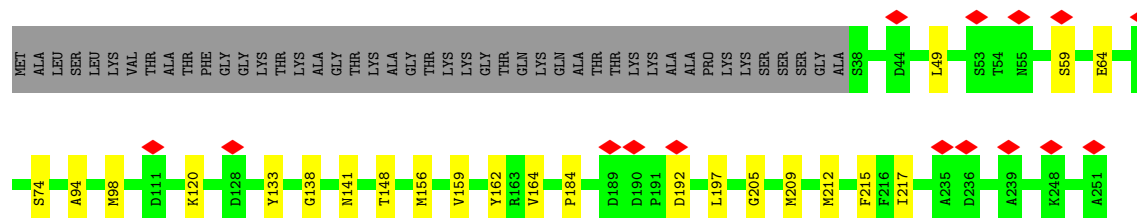
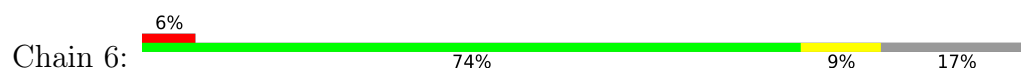




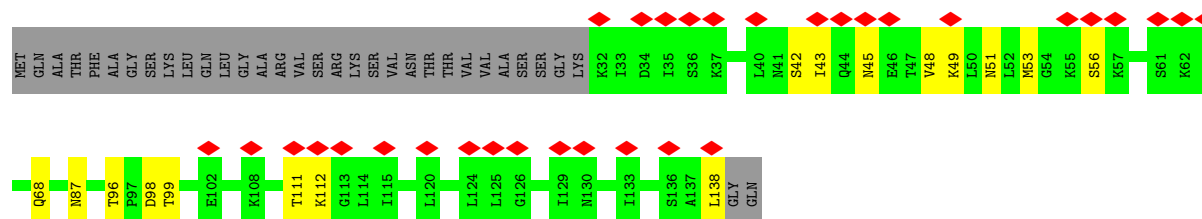
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



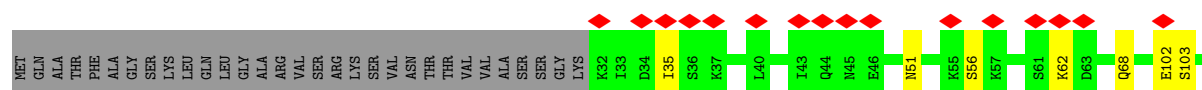
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



- Molecule 4: Chloroplast photosystem II 10 kDa protein

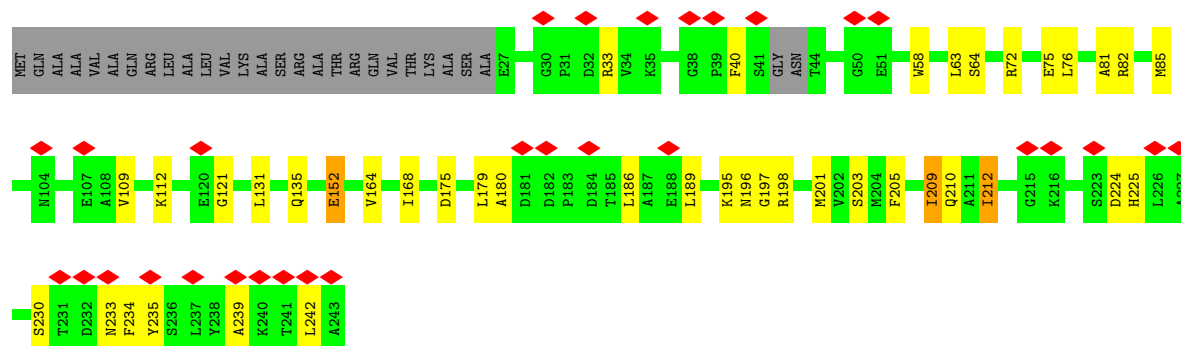
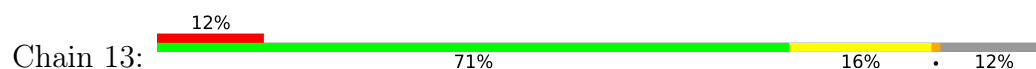


- Molecule 4: Chloroplast photosystem II 10 kDa protein

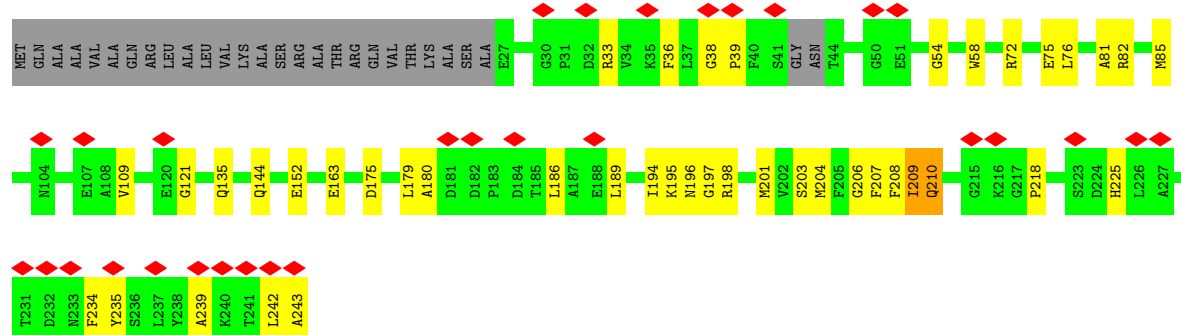




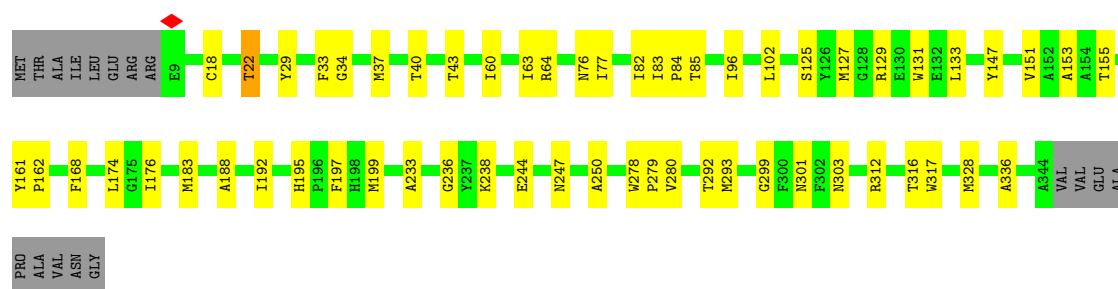
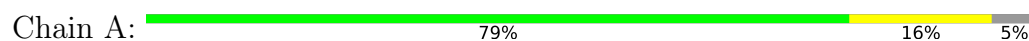
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic



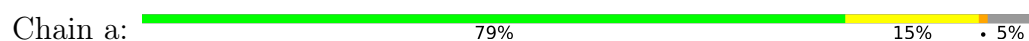
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

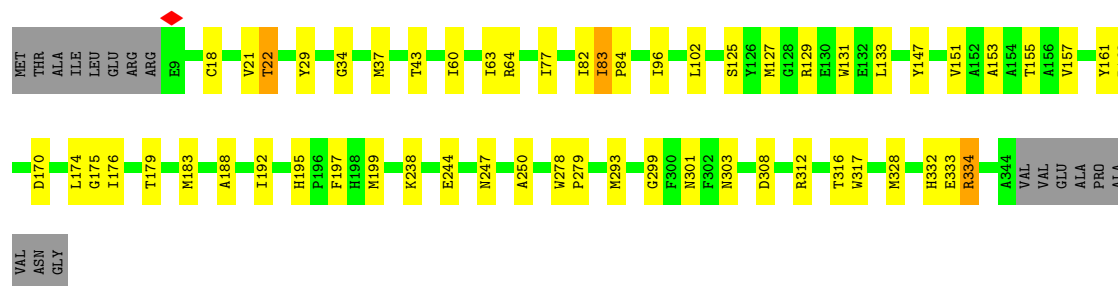


- Molecule 6: Photosystem II protein D1



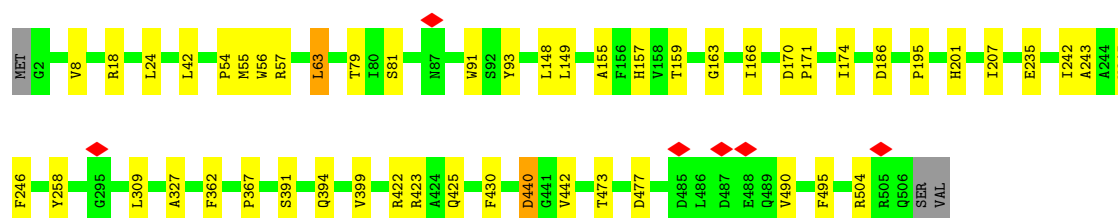
- Molecule 6: Photosystem II protein D1





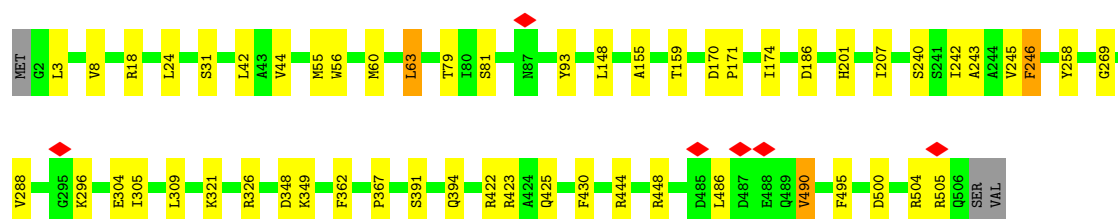
- Molecule 7: Photosystem II CP47 reaction center protein

Chain B: 89% 10%



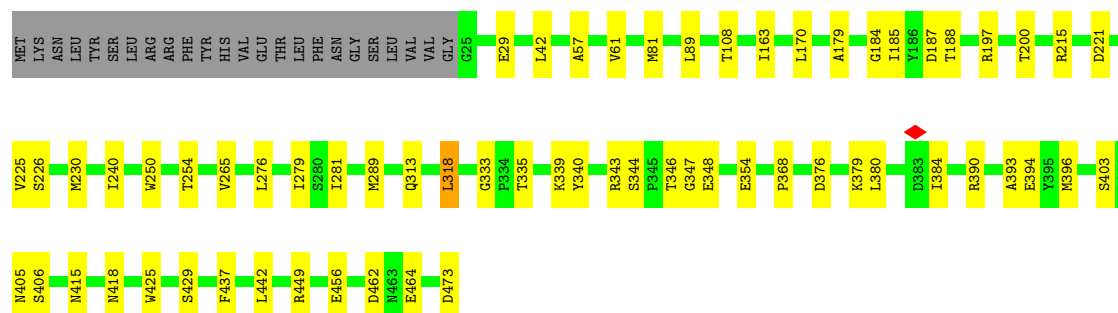
- Molecule 7: Photosystem II CP47 reaction center protein

Chain b: 89% 10%



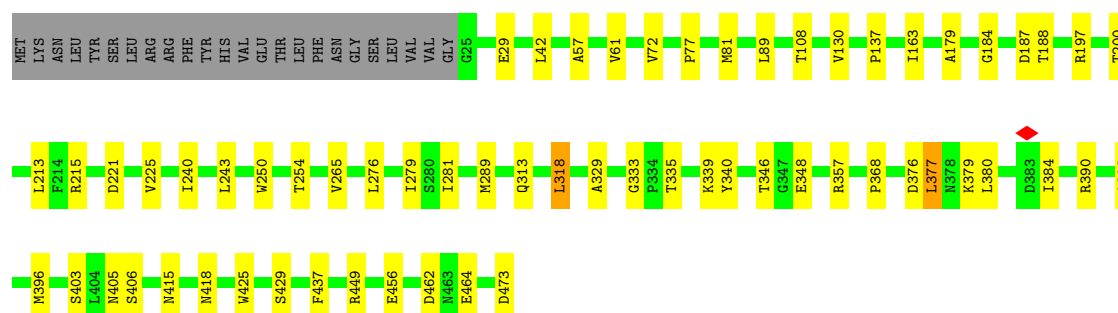
- Molecule 8: Photosystem II CP43 reaction center protein

Chain C: 81% 13% 5%



- Molecule 8: Photosystem II CP43 reaction center protein

Chain c: 82% 13% 5%



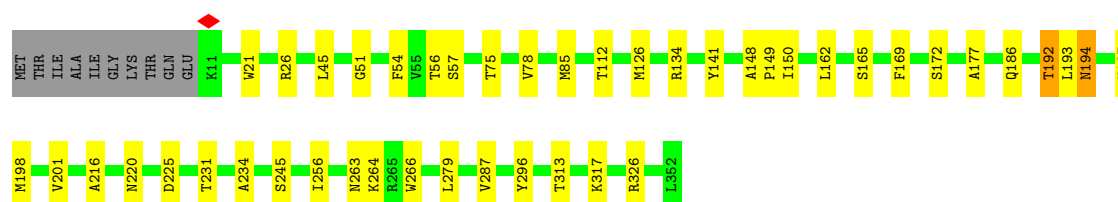
• Molecule 9: Photosystem II D2 protein

Chain D: 86% 11% ..



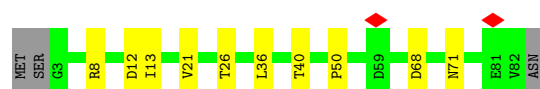
• Molecule 9: Photosystem II D2 protein

Chain d: 84% 12% ..



• Molecule 10: Cytochrome b559 subunit alpha

Chain E: 84% 12% .



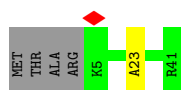
• Molecule 10: Cytochrome b559 subunit alpha

Chain e: 83% 13% .

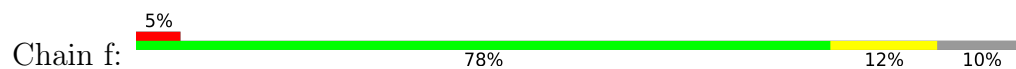


• Molecule 11: Cytochrome b559 subunit beta

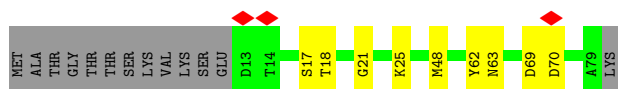
Chain F: 88% 10%



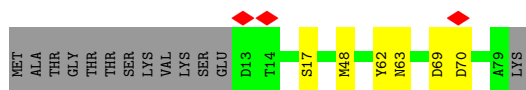
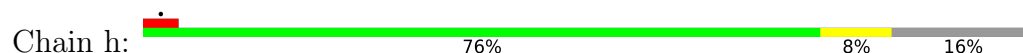
- Molecule 11: Cytochrome b559 subunit beta



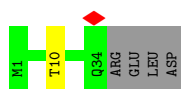
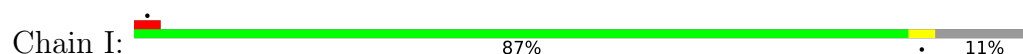
- Molecule 12: Photosystem II reaction center protein H



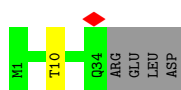
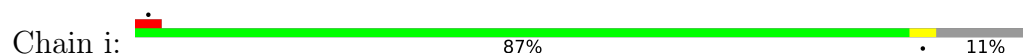
- Molecule 12: Photosystem II reaction center protein H



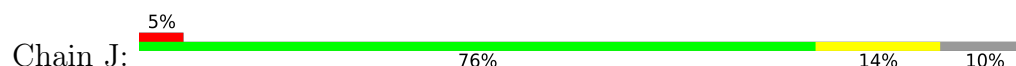
- Molecule 13: Photosystem II reaction center protein I



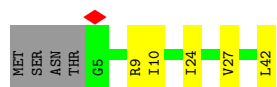
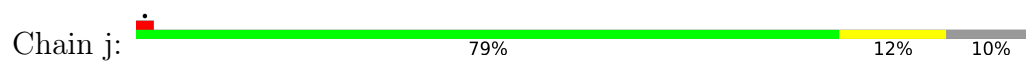
- Molecule 13: Photosystem II reaction center protein I



- Molecule 14: Photosystem II reaction center protein J



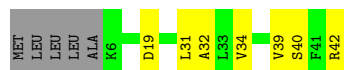
- Molecule 14: Photosystem II reaction center protein J



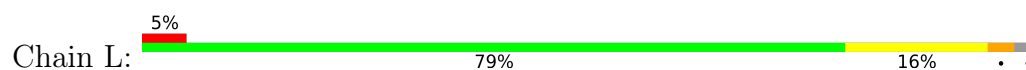
- Molecule 15: Photosystem II reaction center protein K



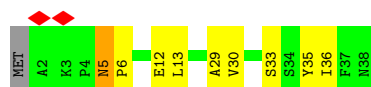
- Molecule 15: Photosystem II reaction center protein K



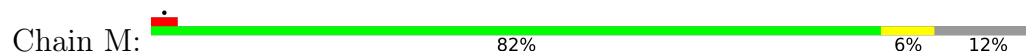
- Molecule 16: Photosystem II reaction center protein L



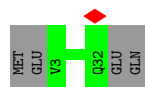
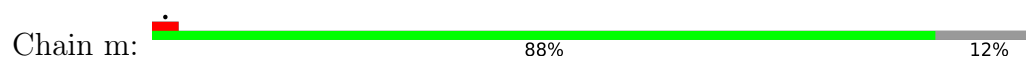
- Molecule 16: Photosystem II reaction center protein L



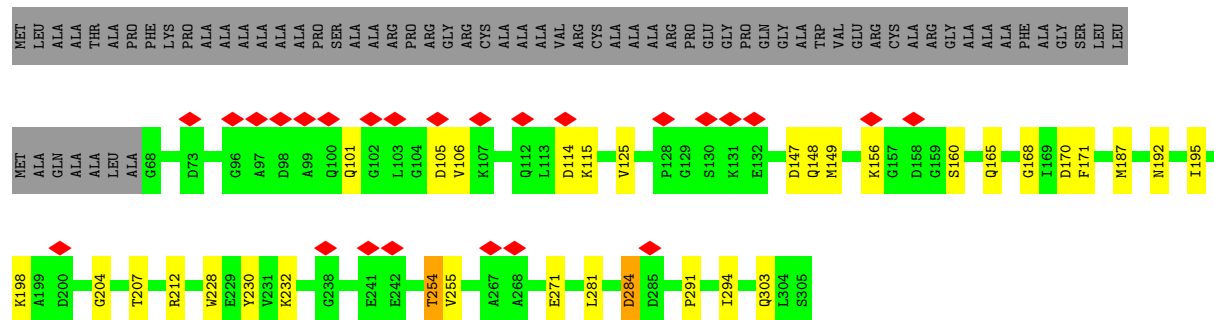
- Molecule 17: Photosystem II reaction center protein M



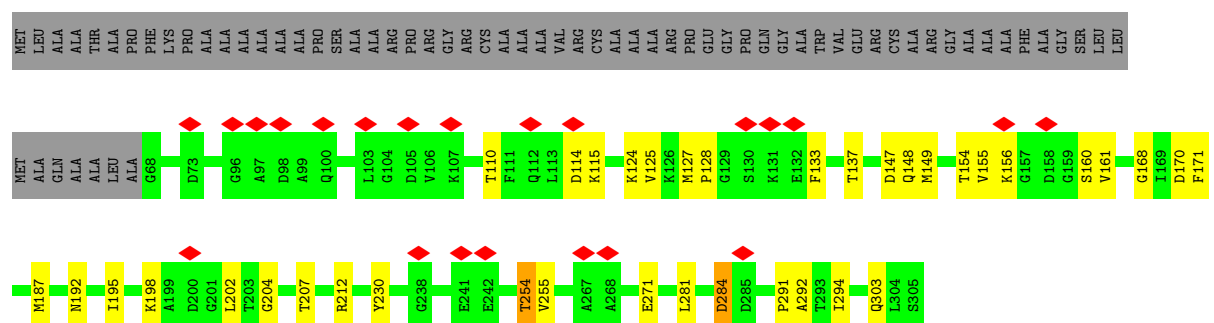
- Molecule 17: Photosystem II reaction center protein M



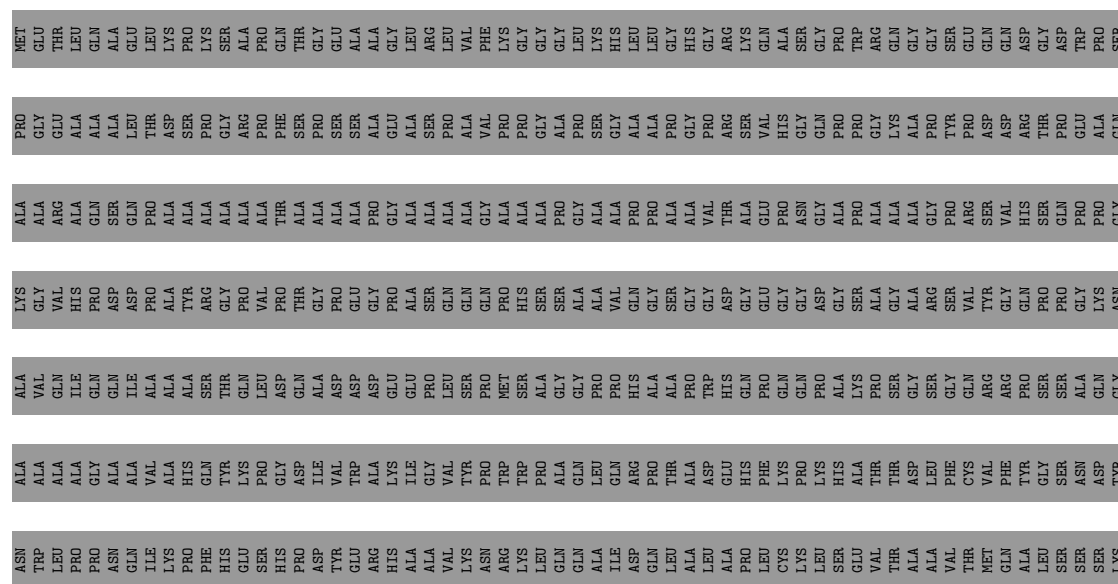
• Molecule 18: Chloroplast oxygen-evolving enhancer protein 1b (PsbO)

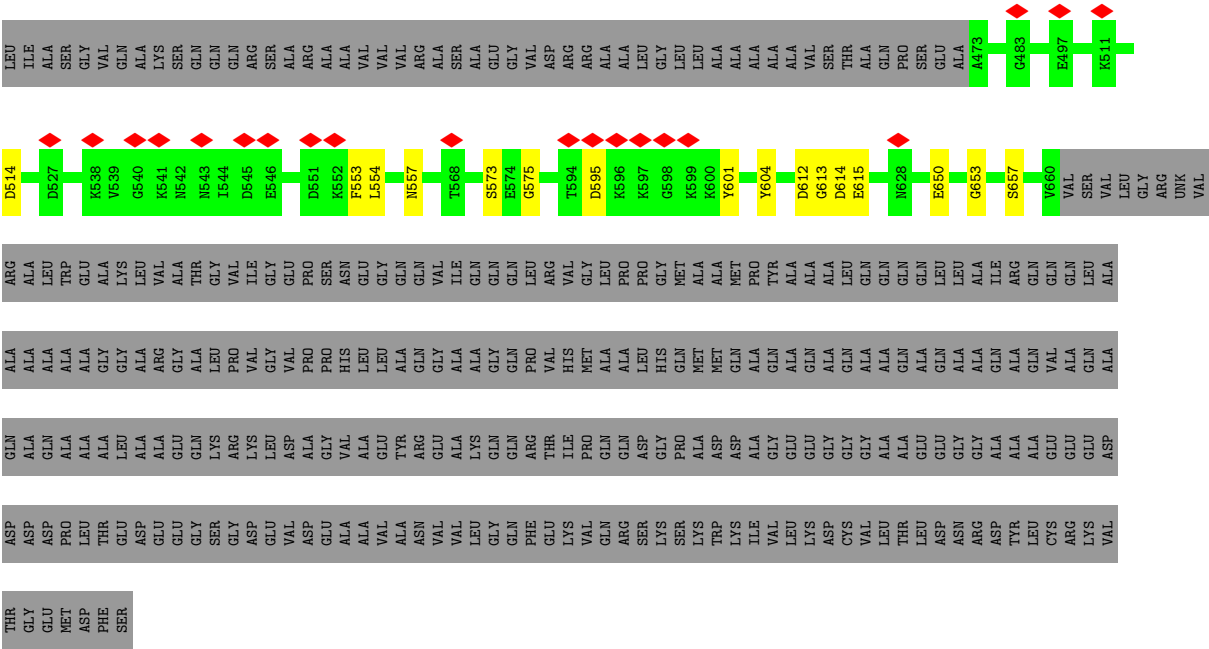


• Molecule 18: Chloroplast oxygen-evolving enhancer protein 1b (PsbO)

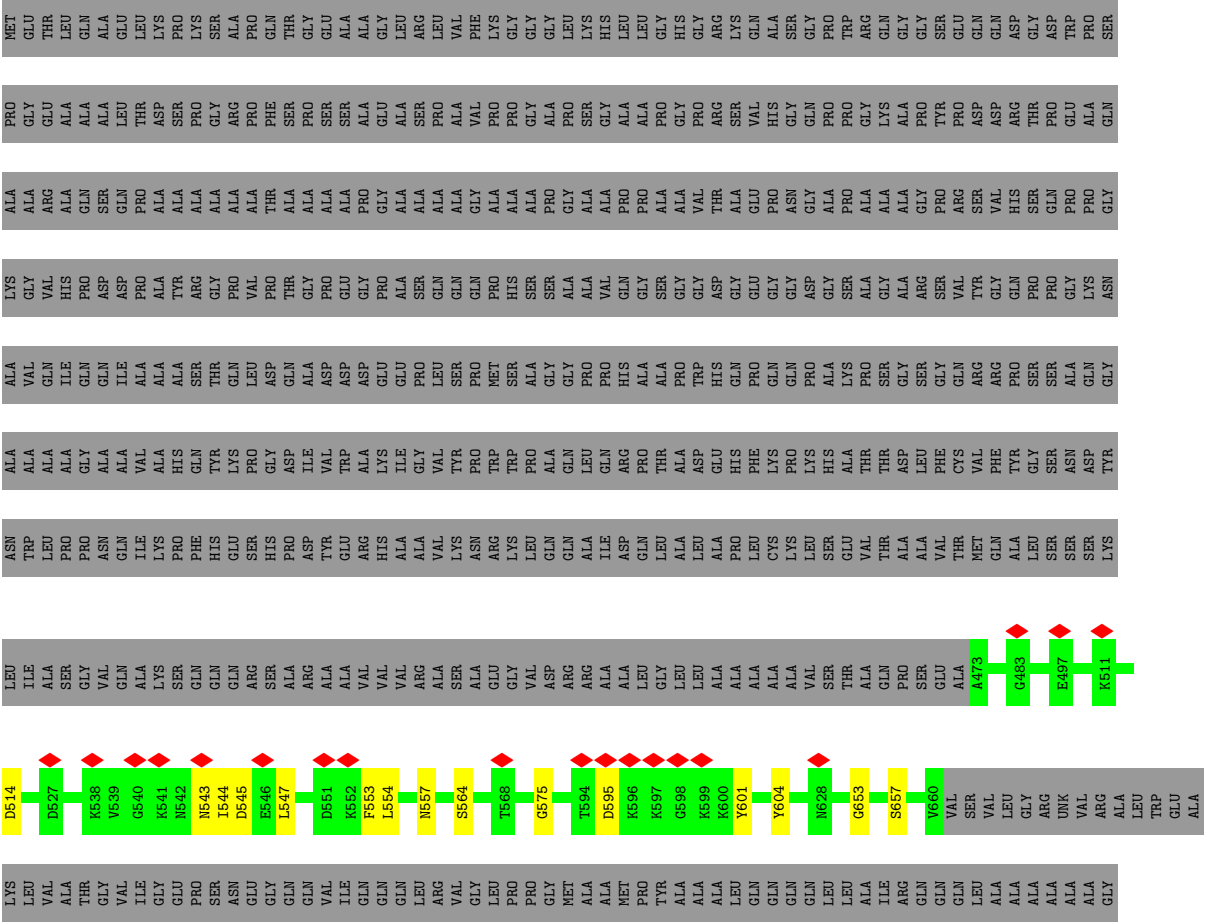


• Molecule 19: PWWP domain-containing protein

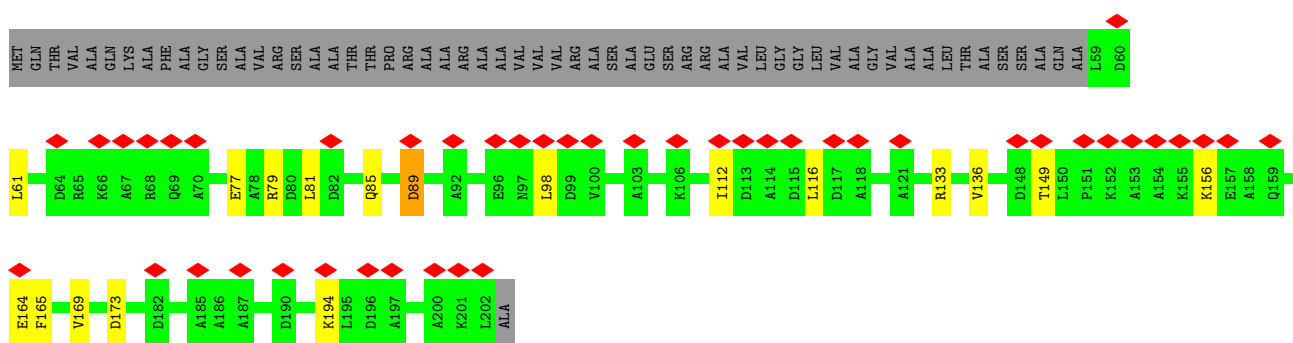




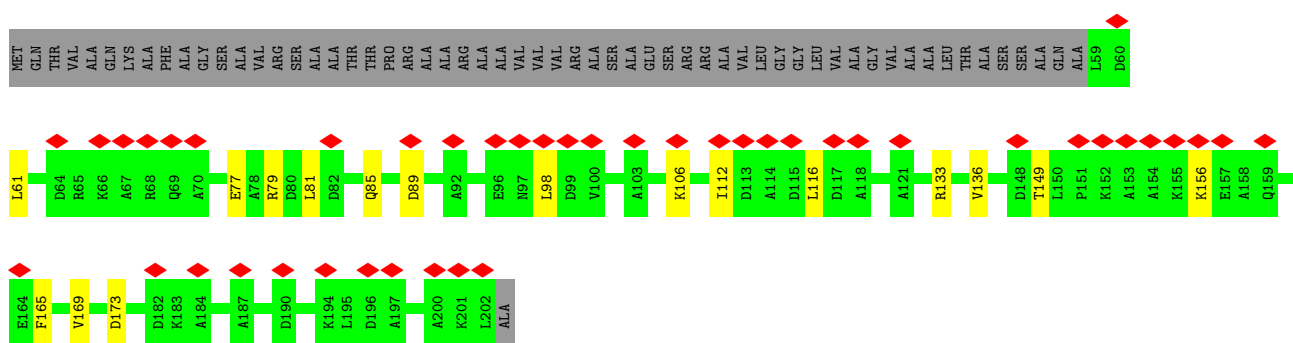
● Molecule 19: PWWP domain-containing protein



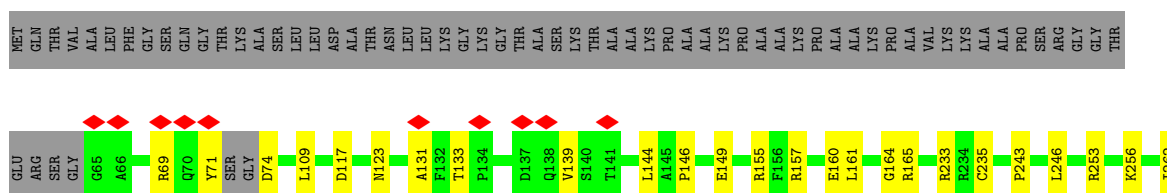
- Molecule 20: Chloroplast oxygen-evolving enhancer protein 3

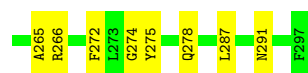


- Molecule 20: Chloroplast oxygen-evolving enhancer protein 3



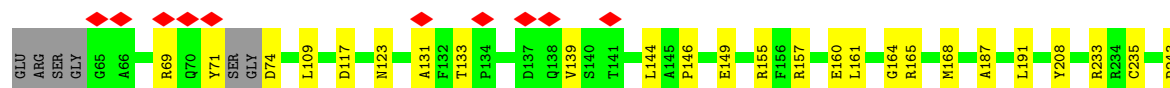
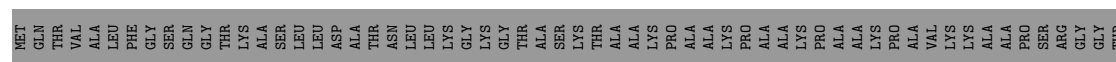
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic





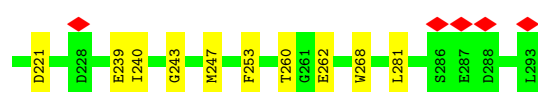
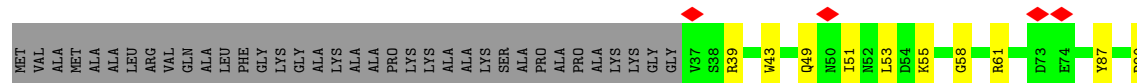
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain r: 66% 12% 22%



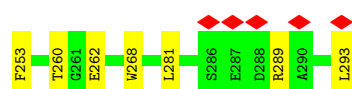
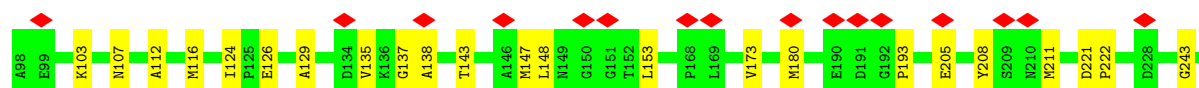
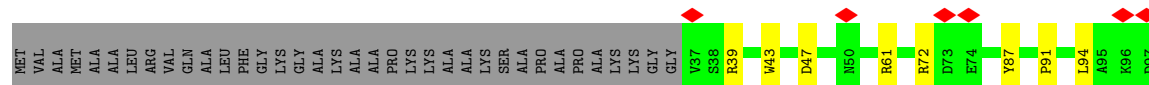
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain S: 8% 73% 15% 12%



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

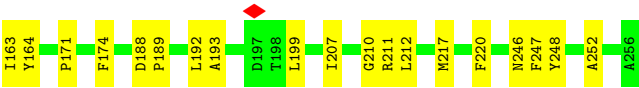
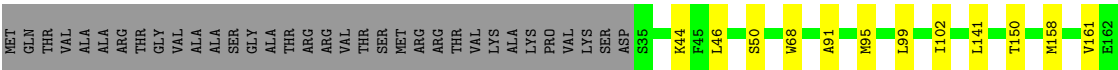
Chain s: 9% 75% 13% 12%



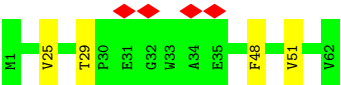
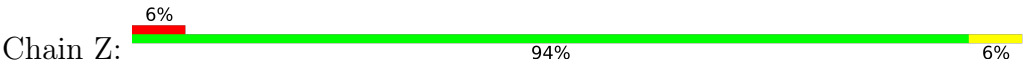
- Molecule 23: Photosystem II reaction center protein T

Chain T: 94%

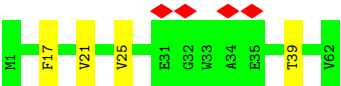
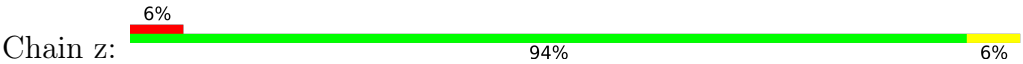
Chain y: 75% 12% 13%



• Molecule 29: Photosystem II reaction center protein Z



• Molecule 29: 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	225372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.292	Depositor
Minimum map value	-0.740	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	454.56, 454.56, 454.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94699997, 0.94699997, 0.94699997	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PAM, CL, LNL, CLA, BCR, DGD, PL9, LHG, LUT, PHO, CHL, BCT, LMG, OEX, 3PH, NEX, STE, SQD, XAT, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.35	2/1720 (0.1%)	0.31	0/2339
1	11	0.54	5/1741 (0.3%)	0.30	0/2369
1	14	0.69	5/1741 (0.3%)	0.38	2/2369 (0.1%)
1	4	0.37	3/1720 (0.2%)	0.33	1/2339 (0.0%)
1	G	0.13	0/1741	0.25	0/2369
1	g	0.12	0/1741	0.24	0/2369
2	12	0.61	3/1362 (0.2%)	0.44	2/1844 (0.1%)
2	15	0.36	3/1362 (0.2%)	0.34	0/1844
2	2	0.15	0/1536	0.33	0/2088
2	5	0.15	0/1536	0.29	0/2088
2	N	0.14	0/1727	0.26	0/2352
2	n	0.14	0/1727	0.33	1/2352 (0.0%)
3	3	0.12	0/1675	0.24	0/2283
3	6	0.14	0/1675	0.27	0/2283
4	7	0.10	0/831	0.24	0/1122
4	8	0.10	0/831	0.24	0/1122
5	13	0.54	6/1688 (0.4%)	0.32	0/2296
5	16	0.53	5/1688 (0.3%)	0.31	0/2296
6	A	0.18	0/2714	0.34	0/3701
6	a	0.21	0/2714	0.39	1/3701 (0.0%)
7	B	0.15	0/4094	0.26	0/5576
7	b	0.15	0/4094	0.26	0/5576
8	C	0.15	0/3611	0.26	0/4921
8	c	0.15	0/3611	0.26	0/4921
9	D	0.16	0/2825	0.29	0/3849
9	d	0.17	0/2825	0.29	0/3849
10	E	0.12	0/664	0.24	0/905
10	e	0.12	0/664	0.24	0/905
11	F	0.13	0/313	0.23	0/426
11	f	0.14	0/313	0.25	0/426
12	H	0.14	0/518	0.24	0/708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	h	0.14	0/518	0.24	0/708
13	I	0.17	0/282	0.28	0/382
13	i	0.17	0/282	0.28	0/382
14	J	0.12	0/276	0.25	0/377
14	j	0.12	0/276	0.24	0/377
15	K	0.18	0/305	0.37	0/420
15	k	0.18	0/305	0.38	0/420
16	L	0.18	0/311	0.29	0/422
16	l	0.18	0/311	0.28	0/422
17	M	0.16	0/231	0.27	0/316
17	m	0.15	0/231	0.28	0/316
18	O	0.11	0/1790	0.26	0/2420
18	o	0.10	0/1790	0.24	0/2420
19	P	0.09	0/1473	0.21	0/1991
19	p	0.09	0/1473	0.20	0/1991
20	Q	0.11	0/1132	0.23	0/1521
20	q	0.11	0/1132	0.24	0/1521
21	R	0.15	0/1820	0.27	0/2475
21	r	0.14	0/1820	0.24	0/2475
22	S	0.16	0/1985	0.32	0/2711
22	s	0.12	0/1985	0.28	0/2711
23	T	0.14	0/253	0.20	0/343
23	t	0.14	0/253	0.20	0/343
24	U	0.12	0/238	0.24	0/326
24	u	0.15	0/238	0.30	0/326
25	V	0.08	0/242	0.19	0/329
25	v	0.08	0/242	0.19	0/329
26	W	0.14	0/477	0.23	0/650
26	w	0.15	0/477	0.25	0/650
27	X	0.11	0/259	0.18	0/353
27	x	0.11	0/259	0.19	0/353
28	Y	0.15	0/1741	0.25	0/2367
28	y	0.15	0/1741	0.24	0/2367
29	Z	0.11	0/491	0.24	0/672
29	z	0.10	0/491	0.24	0/672
All	All	0.24	32/84132 (0.0%)	0.28	7/114446 (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
6	a	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14	229	HIS	C-N	19.06	1.59	1.33
1	14	214	GLN	C-N	16.36	1.53	1.33
1	11	214	GLN	C-N	14.82	1.53	1.33
2	12	224	ASP	C-N	14.44	1.51	1.33
2	12	196	ASN	C-N	12.55	1.50	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12	225	HIS	O-C-N	6.57	128.93	122.09
6	a	332	HIS	CA-CB-CG	6.53	120.33	113.80
2	n	210	GLN	CA-CB-CG	5.64	125.37	114.10
2	12	224	ASP	O-C-N	-5.61	116.17	122.12
1	14	228	ASP	CA-C-N	-5.42	113.22	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	a	334	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1673	0	1609	34	0
1	11	1693	0	1625	34	0
1	14	1693	0	1625	33	0
1	4	1673	0	1609	26	0
1	G	1693	0	1625	19	0
1	g	1693	0	1625	25	0
2	12	1330	0	1299	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	15	1330	0	1299	40	0
2	2	1496	0	1463	33	0
2	5	1496	0	1463	27	0
2	N	1679	0	1626	24	0
2	n	1679	0	1626	36	0
3	3	1630	0	1583	18	0
3	6	1630	0	1583	18	0
4	7	816	0	831	11	0
4	8	816	0	831	5	0
5	13	1645	0	1602	29	0
5	16	1645	0	1602	31	0
6	A	2632	0	2532	43	0
6	a	2632	0	2532	37	0
7	B	3963	0	3831	34	0
7	b	3963	0	3831	35	0
8	C	3491	0	3379	42	0
8	c	3491	0	3379	43	0
9	D	2730	0	2630	33	0
9	d	2730	0	2630	30	0
10	E	646	0	631	6	0
10	e	646	0	631	8	0
11	F	303	0	311	1	0
11	f	303	0	311	5	0
12	H	507	0	520	7	0
12	h	507	0	520	5	0
13	I	274	0	280	1	0
13	i	274	0	280	1	0
14	J	270	0	282	5	0
14	j	270	0	282	5	0
15	K	295	0	311	6	0
15	k	295	0	311	6	0
16	L	303	0	311	5	0
16	l	303	0	311	7	0
17	M	228	0	257	1	0
17	m	228	0	257	0	0
18	O	1759	0	1714	20	0
18	o	1759	0	1714	21	0
19	P	1443	0	1408	10	0
19	p	1443	0	1408	9	0
20	Q	1122	0	1151	12	0
20	q	1122	0	1151	11	0
21	R	1783	0	1705	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	r	1783	0	1705	24	0
22	S	1934	0	1878	33	0
22	s	1934	0	1878	31	0
23	T	246	0	262	2	0
23	t	246	0	262	3	0
24	U	233	0	246	0	0
24	u	233	0	246	5	0
25	V	241	0	275	1	0
25	v	241	0	275	2	0
26	W	468	0	450	7	0
26	w	468	0	450	5	0
27	X	258	0	273	2	0
27	x	258	0	273	5	0
28	Y	1694	0	1641	18	0
28	y	1694	0	1641	26	0
29	Z	478	0	513	2	0
29	z	478	0	513	2	0
30	1	311	0	240	14	0
30	11	314	0	249	9	0
30	12	250	0	183	8	0
30	13	345	0	302	14	0
30	14	318	0	255	7	0
30	15	258	0	199	16	0
30	16	345	0	302	11	0
30	2	311	0	247	13	0
30	3	365	0	351	11	0
30	4	321	0	263	19	0
30	5	315	0	253	8	0
30	6	365	0	351	15	0
30	G	329	0	280	11	0
30	N	357	0	332	19	0
30	R	173	0	154	12	0
30	S	204	0	164	8	0
30	Y	364	0	358	10	0
30	g	332	0	286	13	0
30	n	356	0	330	18	0
30	r	173	0	154	6	0
30	s	204	0	164	11	0
30	y	364	0	358	9	0
31	1	409	0	336	18	0
31	11	413	0	350	20	0
31	12	410	0	344	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	13	495	0	462	25	0
31	14	442	0	409	27	0
31	15	410	0	344	41	0
31	16	495	0	462	23	0
31	2	349	0	277	17	0
31	3	521	0	504	12	0
31	4	427	0	373	10	0
31	5	352	0	281	14	0
31	6	515	0	487	14	0
31	A	250	0	265	8	0
31	B	1025	0	1116	31	0
31	C	820	0	877	24	0
31	D	130	0	144	6	0
31	G	457	0	448	10	0
31	N	492	0	448	12	0
31	R	631	0	608	21	0
31	S	613	0	586	19	0
31	Y	545	0	558	23	0
31	a	185	0	193	5	0
31	b	1025	0	1116	39	0
31	c	820	0	877	26	0
31	d	195	0	216	10	0
31	g	457	0	448	10	0
31	n	492	0	448	22	0
31	r	636	0	621	25	0
31	s	613	0	586	24	0
31	y	540	0	545	23	0
32	1	43	0	59	1	0
32	11	49	0	74	3	0
32	13	40	0	53	3	0
32	14	49	0	74	3	0
32	16	40	0	53	3	0
32	3	91	0	125	3	0
32	4	47	0	67	2	0
32	6	91	0	125	5	0
32	A	185	0	268	11	0
32	C	42	0	57	4	0
32	D	137	0	196	5	0
32	G	49	0	74	2	0
32	L	47	0	67	4	0
32	N	49	0	74	2	0
32	R	129	0	174	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	S	94	0	137	7	0
32	Y	143	0	208	9	0
32	a	185	0	268	8	0
32	c	42	0	57	3	0
32	d	137	0	196	5	0
32	g	49	0	74	5	0
32	l	47	0	67	4	0
32	n	49	0	74	5	0
32	r	129	0	174	11	0
32	s	94	0	137	7	0
32	y	143	0	208	7	0
33	1	84	0	112	6	0
33	11	84	0	112	7	0
33	12	84	0	112	35	0
33	13	84	0	112	3	0
33	14	84	0	112	5	0
33	15	84	0	112	13	0
33	16	84	0	112	6	0
33	2	84	0	112	9	0
33	3	84	0	112	3	0
33	4	84	0	112	7	0
33	5	84	0	112	3	0
33	6	84	0	112	4	0
33	G	84	0	112	3	0
33	N	84	0	112	6	0
33	R	42	0	56	1	0
33	S	84	0	112	8	0
33	Y	84	0	112	4	0
33	g	84	0	112	4	0
33	n	84	0	112	8	0
33	r	42	0	56	4	0
33	s	84	0	112	10	0
33	y	84	0	112	6	0
34	1	16	0	20	0	0
34	11	16	0	20	0	0
34	12	27	0	33	2	0
34	13	44	0	56	0	0
34	14	16	0	20	0	0
34	15	27	0	33	3	0
34	16	44	0	56	0	0
34	2	32	0	39	0	0
34	3	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	4	16	0	20	0	0
34	5	32	0	39	0	0
34	6	44	0	56	4	0
34	G	43	0	53	1	0
34	N	44	0	56	1	0
34	R	44	0	56	1	0
34	S	44	0	56	1	0
34	Y	44	0	56	1	0
34	g	44	0	56	0	0
34	n	44	0	56	1	0
34	r	44	0	56	1	0
34	s	44	0	56	1	0
34	y	44	0	56	0	0
35	11	44	0	56	1	0
35	14	44	0	56	1	0
35	3	44	0	56	3	0
35	6	44	0	56	4	0
35	G	44	0	56	1	0
35	R	44	0	56	2	0
35	g	44	0	56	2	0
35	r	44	0	56	1	0
36	7	48	0	75	1	0
36	8	48	0	75	2	0
36	B	86	0	127	7	0
36	T	48	0	75	4	0
36	b	39	0	54	1	0
37	A	10	0	0	0	0
37	a	10	0	0	0	0
38	A	64	0	74	0	0
38	D	64	0	74	4	0
38	a	128	0	148	1	0
39	A	40	0	56	2	0
39	B	120	0	168	7	0
39	C	120	0	168	5	0
39	D	40	0	56	2	0
39	H	40	0	56	3	0
39	J	40	0	56	3	0
39	a	40	0	56	1	0
39	b	120	0	168	5	0
39	c	120	0	168	4	0
39	d	40	0	56	1	0
39	h	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	j	40	0	56	3	0
40	A	51	0	68	0	0
40	D	100	0	136	2	0
40	L	50	0	64	3	0
40	a	51	0	68	0	0
40	d	100	0	136	7	0
40	l	50	0	64	2	0
41	A	55	0	86	1	0
41	B	97	0	137	3	0
41	C	102	0	153	2	0
41	D	92	0	124	2	0
41	H	35	0	51	0	0
41	J	51	0	75	5	0
41	K	51	0	72	3	0
41	S	42	0	54	3	0
41	b	95	0	130	2	0
41	c	102	0	153	2	0
41	d	127	0	175	4	0
41	j	51	0	75	5	0
41	s	42	0	54	2	0
41	v	51	0	72	1	0
41	w	55	0	86	3	0
42	A	55	0	80	2	0
42	D	55	0	80	2	0
42	a	55	0	80	4	0
42	d	55	0	80	2	0
43	A	20	0	29	0	0
43	C	40	0	58	1	0
43	H	20	0	29	4	0
43	I	20	0	29	0	0
43	R	20	0	29	0	0
43	W	40	0	58	2	0
43	X	20	0	29	1	0
43	Y	40	0	58	2	0
43	a	20	0	29	0	0
43	c	40	0	58	1	0
43	h	20	0	29	2	0
43	i	20	0	29	0	0
43	r	20	0	29	0	0
43	w	20	0	29	1	0
43	x	20	0	29	1	0
43	y	60	0	87	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	B	20	0	35	1	0
44	b	20	0	35	0	0
45	C	1	0	0	0	0
45	c	1	0	0	0	0
46	C	183	0	246	9	0
46	W	46	0	64	4	0
46	c	183	0	246	8	0
46	w	40	0	52	2	0
47	D	1	0	0	0	0
47	d	1	0	0	0	0
48	D	4	0	1	0	0
48	d	4	0	0	0	0
49	F	43	0	30	2	0
49	f	43	0	30	2	0
50	N	18	0	29	1	0
50	n	18	0	29	1	0
All	All	112944	0	113167	1728	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 1728 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)
31:12:612:CLA:C3B	33:12:614:LUT:H183	1.22	1.54
31:12:612:CLA:CAB	33:12:614:LUT:H183	1.53	1.36
31:12:612:CLA:C3B	33:12:614:LUT:C18	2.18	1.21
31:12:612:CLA:CAB	33:12:614:LUT:C18	2.22	1.17
1:11:210:GLY:O	1:11:214:GLN:HG3	1.44	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
1	11	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
1	14	221/249 (89%)	213 (96%)	8 (4%)	0	100	100
1	4	216/249 (87%)	208 (96%)	8 (4%)	0	100	100
1	G	221/249 (89%)	217 (98%)	4 (2%)	0	100	100
1	g	221/249 (89%)	215 (97%)	6 (3%)	0	100	100
2	12	158/247 (64%)	154 (98%)	4 (2%)	0	100	100
2	15	158/247 (64%)	150 (95%)	8 (5%)	0	100	100
2	2	194/247 (78%)	187 (96%)	7 (4%)	0	100	100
2	5	194/247 (78%)	190 (98%)	4 (2%)	0	100	100
2	N	218/247 (88%)	209 (96%)	9 (4%)	0	100	100
2	n	218/247 (88%)	210 (96%)	8 (4%)	0	100	100
3	3	212/259 (82%)	204 (96%)	8 (4%)	0	100	100
3	6	212/259 (82%)	206 (97%)	6 (3%)	0	100	100
4	7	105/140 (75%)	104 (99%)	1 (1%)	0	100	100
4	8	105/140 (75%)	102 (97%)	3 (3%)	0	100	100
5	13	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
5	16	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
6	A	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
6	a	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
7	B	503/508 (99%)	488 (97%)	15 (3%)	0	100	100
7	b	503/508 (99%)	486 (97%)	17 (3%)	0	100	100
8	C	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
8	c	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
9	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
9	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
10	E	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
10	e	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
11	F	35/41 (85%)	35 (100%)	0	0	100	100
11	f	35/41 (85%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	H	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
12	h	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
13	I	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
13	i	32/38 (84%)	28 (88%)	4 (12%)	0	100	100
14	J	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
14	j	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
15	K	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
15	k	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
16	L	35/38 (92%)	35 (100%)	0	0	100	100
16	l	35/38 (92%)	35 (100%)	0	0	100	100
17	M	28/34 (82%)	28 (100%)	0	0	100	100
17	m	28/34 (82%)	28 (100%)	0	0	100	100
18	O	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
18	o	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
19	P	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
19	p	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
20	Q	142/203 (70%)	139 (98%)	3 (2%)	0	100	100
20	q	142/203 (70%)	137 (96%)	5 (4%)	0	100	100
21	R	226/297 (76%)	219 (97%)	7 (3%)	0	100	100
21	r	226/297 (76%)	220 (97%)	6 (3%)	0	100	100
22	S	255/293 (87%)	248 (97%)	7 (3%)	0	100	100
22	s	255/293 (87%)	244 (96%)	11 (4%)	0	100	100
23	T	28/31 (90%)	28 (100%)	0	0	100	100
23	t	28/31 (90%)	28 (100%)	0	0	100	100
24	U	28/367 (8%)	28 (100%)	0	0	100	100
24	u	28/367 (8%)	28 (100%)	0	0	100	100
25	V	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
25	v	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
26	W	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
26	w	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
27	X	36/100 (36%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	x	36/100 (36%)	36 (100%)	0	0	100	100
28	Y	220/256 (86%)	217 (99%)	3 (1%)	0	100	100
28	y	220/256 (86%)	215 (98%)	5 (2%)	0	100	100
29	Z	60/62 (97%)	60 (100%)	0	0	100	100
29	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	10460/15046 (70%)	10166 (97%)	294 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	170/190 (90%)	165 (97%)	5 (3%)	37	61
1	11	172/190 (90%)	166 (96%)	6 (4%)	31	56
1	14	172/190 (90%)	167 (97%)	5 (3%)	37	61
1	4	170/190 (90%)	164 (96%)	6 (4%)	31	56
1	G	172/190 (90%)	166 (96%)	6 (4%)	31	56
1	g	172/190 (90%)	167 (97%)	5 (3%)	37	61
2	12	136/187 (73%)	132 (97%)	4 (3%)	37	61
2	15	136/187 (73%)	129 (95%)	7 (5%)	20	43
2	2	150/187 (80%)	147 (98%)	3 (2%)	50	72
2	5	150/187 (80%)	143 (95%)	7 (5%)	22	46
2	N	167/187 (89%)	161 (96%)	6 (4%)	30	55
2	n	167/187 (89%)	162 (97%)	5 (3%)	36	60
3	3	165/196 (84%)	162 (98%)	3 (2%)	54	75
3	6	165/196 (84%)	162 (98%)	3 (2%)	54	75
4	7	88/113 (78%)	86 (98%)	2 (2%)	45	69
4	8	88/113 (78%)	83 (94%)	5 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	13	168/187 (90%)	161 (96%)	7 (4%)	25	50
5	16	168/187 (90%)	162 (96%)	6 (4%)	30	55
6	A	274/287 (96%)	269 (98%)	5 (2%)	54	75
6	a	274/287 (96%)	268 (98%)	6 (2%)	47	69
7	B	403/406 (99%)	396 (98%)	7 (2%)	56	76
7	b	403/406 (99%)	395 (98%)	8 (2%)	50	72
8	C	351/373 (94%)	345 (98%)	6 (2%)	56	76
8	c	351/373 (94%)	344 (98%)	7 (2%)	50	72
9	D	277/285 (97%)	274 (99%)	3 (1%)	70	83
9	d	277/285 (97%)	272 (98%)	5 (2%)	54	75
10	E	71/74 (96%)	70 (99%)	1 (1%)	62	79
10	e	71/74 (96%)	71 (100%)	0	100	100
11	F	31/34 (91%)	31 (100%)	0	100	100
11	f	31/34 (91%)	31 (100%)	0	100	100
12	H	57/68 (84%)	55 (96%)	2 (4%)	31	56
12	h	57/68 (84%)	55 (96%)	2 (4%)	31	56
13	I	31/35 (89%)	31 (100%)	0	100	100
13	i	31/35 (89%)	31 (100%)	0	100	100
14	J	27/31 (87%)	27 (100%)	0	100	100
14	j	27/31 (87%)	27 (100%)	0	100	100
15	K	33/37 (89%)	32 (97%)	1 (3%)	36	60
15	k	33/37 (89%)	32 (97%)	1 (3%)	36	60
16	L	34/35 (97%)	32 (94%)	2 (6%)	16	37
16	l	34/35 (97%)	31 (91%)	3 (9%)	8	22
17	M	26/30 (87%)	26 (100%)	0	100	100
17	m	26/30 (87%)	26 (100%)	0	100	100
18	O	182/217 (84%)	178 (98%)	4 (2%)	47	69
18	o	182/217 (84%)	178 (98%)	4 (2%)	47	69
19	P	147/651 (23%)	145 (99%)	2 (1%)	62	79
19	p	147/651 (23%)	146 (99%)	1 (1%)	81	90
20	Q	108/143 (76%)	105 (97%)	3 (3%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	q	108/143 (76%)	106 (98%)	2 (2%)	52	73
21	R	182/225 (81%)	177 (97%)	5 (3%)	40	64
21	r	182/225 (81%)	178 (98%)	4 (2%)	47	69
22	S	192/212 (91%)	190 (99%)	2 (1%)	73	85
22	s	192/212 (91%)	190 (99%)	2 (1%)	73	85
23	T	26/27 (96%)	26 (100%)	0	100	100
23	t	26/27 (96%)	26 (100%)	0	100	100
24	U	25/241 (10%)	25 (100%)	0	100	100
24	u	25/241 (10%)	25 (100%)	0	100	100
25	V	27/27 (100%)	27 (100%)	0	100	100
25	v	27/27 (100%)	26 (96%)	1 (4%)	29	54
26	W	50/362 (14%)	47 (94%)	3 (6%)	16	37
26	w	50/362 (14%)	46 (92%)	4 (8%)	10	25
27	X	26/66 (39%)	25 (96%)	1 (4%)	28	53
27	x	26/66 (39%)	26 (100%)	0	100	100
28	Y	171/197 (87%)	169 (99%)	2 (1%)	67	82
28	y	171/197 (87%)	170 (99%)	1 (1%)	84	91
29	Z	52/52 (100%)	52 (100%)	0	100	100
29	z	52/52 (100%)	51 (98%)	1 (2%)	52	73
All	All	8382/11484 (73%)	8190 (98%)	192 (2%)	46	69

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	Q	89	ASP
7	b	505	ARG
21	R	144	LEU
6	a	21	VAL
8	c	462	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	80	ASN

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Mol	Chain	Res	Type
28	y	234	ASN
6	a	267	ASN
28	y	209	ASN
21	r	80	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 612 ligands modelled in this entry, 4 are monoatomic - leaving 608 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	$\# Z > 2$
30	CHL	n	607	-	66,74,74	1.46	10 (15%)	73,114,114	1.81	11 (15%)
31	CLA	c	505	-	55,63,73	1.44	7 (12%)	64,101,113	1.81	10 (15%)
31	CLA	B	612	7	65,73,73	1.34	7 (10%)	76,113,113	1.83	10 (13%)
32	LHG	y	618	-	46,46,48	1.41	8 (17%)	49,52,54	0.74	2 (4%)
31	CLA	b	609	7	65,73,73	1.35	7 (10%)	76,113,113	1.71	10 (13%)
31	CLA	C	503	8	65,73,73	1.33	7 (10%)	76,113,113	1.77	10 (13%)
40	SQD	d	412	-	53,54,54	0.17	0	62,65,65	0.21	0
32	LHG	N	616	31	48,48,48	1.30	7 (14%)	51,54,54	0.78	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LUT	Y	622	-	42,43,43	0.43	1 (2%)	51,60,60	0.40	0
30	CHL	y	601	28	66,74,74	1.45	10 (15%)	73,114,114	1.90	11 (15%)
31	CLA	12	612	2	50,58,73	1.51	7 (14%)	58,95,113	1.83	9 (15%)
30	CHL	R	605	21	56,64,74	1.58	10 (17%)	61,102,114	2.02	12 (19%)
31	CLA	C	502	8	65,73,73	1.32	7 (10%)	76,113,113	1.67	10 (13%)
31	CLA	3	604	-	65,73,73	1.37	7 (10%)	76,113,113	1.68	12 (15%)
43	LNL	y	621	-	19,19,19	0.43	0	18,19,19	0.50	0
30	CHL	5	601	2	51,59,74	1.68	11 (21%)	55,96,114	2.01	12 (21%)
31	CLA	C	505	-	55,63,73	1.44	7 (12%)	64,101,113	1.81	10 (15%)
31	CLA	b	607	-	65,73,73	1.33	7 (10%)	76,113,113	1.73	9 (11%)
30	CHL	3	609	3	66,74,74	1.49	11 (16%)	73,114,114	1.85	10 (13%)
30	CHL	s	606	22	66,74,74	1.48	9 (13%)	73,114,114	1.85	10 (13%)
31	CLA	15	603	-	55,63,73	1.45	7 (12%)	64,101,113	1.90	10 (15%)
31	CLA	S	604	-	65,73,73	1.35	7 (10%)	76,113,113	1.62	9 (11%)
30	CHL	12	601	2	50,58,74	1.66	10 (20%)	52,94,114	2.13	11 (21%)
30	CHL	n	608	-	50,58,74	1.62	9 (18%)	52,94,114	2.17	11 (21%)
31	CLA	N	604	-	55,63,73	1.48	7 (12%)	64,101,113	1.83	9 (14%)
38	PHO	a	406	-	51,69,69	0.43	0	47,99,99	0.68	1 (2%)
31	CLA	C	508	-	65,73,73	1.33	7 (10%)	76,113,113	1.55	13 (17%)
35	XAT	3	620	-	39,47,47	0.13	0	54,74,74	0.73	1 (1%)
31	CLA	d	405	9	65,73,73	1.34	7 (10%)	76,113,113	1.64	11 (14%)
31	CLA	r	602	21	65,73,73	1.34	7 (10%)	76,113,113	1.76	12 (15%)
35	XAT	r	616	-	39,47,47	0.11	0	54,74,74	0.83	3 (5%)
31	CLA	4	604	-	50,58,73	1.54	7 (14%)	58,95,113	1.97	7 (12%)
30	CHL	4	605	1	46,54,74	1.74	10 (21%)	49,90,114	2.13	11 (22%)
31	CLA	b	614	7	65,73,73	1.35	7 (10%)	76,113,113	1.73	12 (15%)
32	LHG	G	615	31	48,48,48	1.33	8 (16%)	51,54,54	0.73	2 (3%)
30	CHL	N	608	-	50,58,74	1.63	9 (18%)	52,94,114	2.14	13 (25%)
30	CHL	y	605	28	56,64,74	1.58	10 (17%)	61,102,114	1.83	12 (19%)
31	CLA	3	613	3	55,63,73	1.45	7 (12%)	64,101,113	1.80	8 (12%)
43	LNL	a	412	-	19,19,19	0.44	0	18,19,19	0.48	0
30	CHL	14	609	-	56,64,74	1.63	11 (19%)	61,102,114	2.03	14 (22%)
39	BCR	A	407	-	41,41,41	0.11	0	56,56,56	0.23	0
30	CHL	16	609	-	61,69,74	1.56	10 (16%)	67,108,114	1.91	12 (17%)
38	PHO	D	402	-	51,69,69	0.45	0	47,99,99	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	13	611	32	65,73,73	1.36	7 (10%)	76,113,113	1.71	10 (13%)
31	CLA	d	402	-	65,73,73	1.33	7 (10%)	76,113,113	1.62	14 (18%)
31	CLA	13	615	5	45,53,73	1.56	7 (15%)	52,89,113	1.94	7 (13%)
33	LUT	g	616	-	42,43,43	0.38	0	51,60,60	0.39	0
30	CHL	12	606	-	51,59,74	1.68	10 (19%)	55,96,114	2.12	11 (20%)
30	CHL	2	605	2	46,54,74	1.73	10 (21%)	49,90,114	1.99	9 (18%)
33	LUT	5	614	-	42,43,43	0.35	0	51,60,60	0.42	0
34	NEX	16	619	-	38,46,46	0.44	1 (2%)	50,70,70	0.39	0
31	CLA	13	612	5	45,53,73	1.60	7 (15%)	52,89,113	1.92	7 (13%)
42	PL9	a	410	-	55,55,55	0.09	0	68,69,69	0.18	0
33	LUT	G	617	-	42,43,43	0.45	1 (2%)	51,60,60	0.44	1 (1%)
31	CLA	2	611	-	46,54,73	1.55	7 (15%)	53,90,113	1.89	9 (16%)
32	LHG	s	621	-	48,48,48	1.35	8 (16%)	51,54,54	0.78	2 (3%)
31	CLA	11	610	-	55,63,73	1.46	6 (10%)	64,101,113	1.90	13 (20%)
30	CHL	6	601	3	61,69,74	1.54	11 (18%)	67,108,114	1.87	12 (17%)
33	LUT	n	617	-	42,43,43	0.37	0	51,60,60	0.35	0
34	NEX	13	619	-	38,46,46	0.42	1 (2%)	50,70,70	0.40	0
31	CLA	r	603	21	65,73,73	1.36	7 (10%)	76,113,113	1.77	11 (14%)
30	CHL	3	601	3	61,69,74	1.54	9 (14%)	67,108,114	1.83	12 (17%)
31	CLA	14	612	1	43,51,73	1.60	7 (16%)	49,86,113	1.88	6 (12%)
31	CLA	c	508	-	65,73,73	1.34	7 (10%)	76,113,113	1.88	11 (14%)
34	NEX	R	617	-	38,46,46	0.41	1 (2%)	50,70,70	0.46	0
31	CLA	3	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.62	11 (14%)
34	NEX	S	620	-	38,46,46	0.46	1 (2%)	50,70,70	0.49	0
31	CLA	y	610	28	65,73,73	1.35	7 (10%)	76,113,113	1.72	11 (14%)
31	CLA	12	613	-	45,53,73	1.58	7 (15%)	52,89,113	1.89	8 (15%)
30	CHL	y	606	-	66,74,74	1.46	10 (15%)	73,114,114	1.86	11 (15%)
39	BCR	H	103	-	41,41,41	0.13	0	56,56,56	0.33	0
30	CHL	6	606	-	56,64,74	1.60	9 (16%)	61,102,114	1.94	9 (14%)
30	CHL	y	609	28	66,74,74	1.48	10 (15%)	73,114,114	1.88	13 (17%)
31	CLA	b	611	7	65,73,73	1.36	7 (10%)	76,113,113	1.68	10 (13%)
34	NEX	2	616	-	29,33,46	0.48	1 (3%)	38,48,70	0.50	0
33	LUT	y	622	-	42,43,43	0.39	0	51,60,60	0.49	0
31	CLA	B	604	7	65,73,73	1.35	7 (10%)	76,113,113	1.74	12 (15%)
31	CLA	S	615	22	47,55,73	1.54	7 (14%)	54,91,113	1.97	6 (11%)
30	CHL	6	608	-	50,58,74	1.65	9 (18%)	52,94,114	2.11	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PH	b	623	-	38,38,47	0.29	0	42,43,52	0.33	0
32	LHG	D	412	-	48,48,48	1.43	8 (16%)	51,54,54	0.74	2 (3%)
30	CHL	r	605	21	56,64,74	1.59	10 (17%)	61,102,114	2.01	12 (19%)
31	CLA	r	601	21	49,57,73	1.51	7 (14%)	55,93,113	1.78	7 (12%)
31	CLA	s	612	22	45,53,73	1.59	7 (15%)	52,89,113	1.94	9 (17%)
32	LHG	4	615	31	46,46,48	1.40	8 (17%)	49,52,54	0.71	2 (4%)
31	CLA	B	613	7	65,73,73	1.32	7 (10%)	76,113,113	1.85	10 (13%)
32	LHG	A	413	-	43,43,48	1.39	8 (18%)	46,49,54	0.83	2 (4%)
31	CLA	G	612	1	43,51,73	1.58	7 (16%)	49,86,113	1.97	7 (14%)
31	CLA	3	615	3	46,54,73	1.54	7 (15%)	53,90,113	1.98	10 (18%)
30	CHL	11	609	-	56,64,74	1.63	11 (19%)	61,102,114	2.02	11 (18%)
31	CLA	15	612	-	50,58,73	1.53	8 (16%)	58,95,113	1.82	8 (13%)
33	LUT	s	619	-	42,43,43	0.33	0	51,60,60	0.42	1 (1%)
31	CLA	B	603	7	65,73,73	1.35	7 (10%)	76,113,113	1.73	11 (14%)
30	CHL	g	605	1	48,56,74	1.67	9 (18%)	51,92,114	2.10	10 (19%)
31	CLA	n	612	2	45,53,73	1.57	7 (15%)	52,89,113	1.99	8 (15%)
31	CLA	n	613	2	55,63,73	1.55	7 (12%)	64,101,113	1.64	7 (10%)
31	CLA	c	514	8	65,73,73	1.34	7 (10%)	76,113,113	1.62	11 (14%)
31	CLA	1	602	1	60,68,73	1.40	7 (11%)	70,107,113	1.77	13 (18%)
31	CLA	14	610	-	65,73,73	1.35	6 (9%)	76,113,113	1.77	12 (15%)
31	CLA	G	603	1	55,63,73	1.46	7 (12%)	64,101,113	1.88	8 (12%)
30	CHL	15	601	2	50,58,74	1.66	10 (20%)	52,94,114	2.13	11 (21%)
31	CLA	2	612	-	46,54,73	1.56	7 (15%)	53,90,113	1.92	8 (15%)
30	CHL	13	607	-	61,69,74	1.53	10 (16%)	67,108,114	1.97	12 (17%)
30	CHL	S	601	22	46,54,74	1.71	9 (19%)	49,90,114	2.16	11 (22%)
32	LHG	S	621	-	48,48,48	1.36	8 (16%)	51,54,54	0.77	2 (3%)
31	CLA	b	612	7	65,73,73	1.35	7 (10%)	76,113,113	1.81	8 (10%)
41	LMG	b	620	-	49,49,55	0.19	0	57,57,63	0.16	0
46	DGD	C	518	-	59,59,67	0.18	0	73,73,81	0.17	0
31	CLA	5	611	-	46,54,73	1.55	7 (15%)	53,90,113	1.84	8 (15%)
31	CLA	b	613	7	65,73,73	1.33	7 (10%)	76,113,113	1.84	10 (13%)
31	CLA	4	602	1	60,68,73	1.39	7 (11%)	70,107,113	1.76	11 (15%)
43	LNL	Y	620	-	19,19,19	0.43	0	18,19,19	0.48	0
31	CLA	A	406	6	55,63,73	1.46	7 (12%)	64,101,113	1.79	8 (12%)
31	CLA	B	608	7	65,73,73	1.35	7 (10%)	76,113,113	1.63	11 (14%)
40	SQD	D	413	-	45,46,54	0.19	0	54,57,65	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	6	609	3	66,74,74	1.49	10 (15%)	73,114,114	1.84	12 (16%)
33	LUT	3	618	-	42,43,43	0.42	1 (2%)	51,60,60	0.44	0
30	CHL	Y	606	-	66,74,74	1.46	10 (15%)	73,114,114	1.86	12 (16%)
30	CHL	15	606	-	51,59,74	1.68	10 (19%)	55,96,114	2.09	12 (21%)
31	CLA	N	603	2	60,68,73	1.40	7 (11%)	70,107,113	1.81	10 (14%)
31	CLA	14	602	1	60,68,73	1.42	7 (11%)	70,107,113	1.79	12 (17%)
30	CHL	4	607	-	51,59,74	1.68	10 (19%)	55,96,114	2.01	9 (16%)
41	LMG	H	102	-	34,34,55	0.21	0	36,36,63	0.18	0
50	PAM	n	620	-	17,17,17	0.45	0	17,17,17	0.49	0
31	CLA	c	510	8	65,73,73	1.33	7 (10%)	76,113,113	1.84	9 (11%)
31	CLA	g	602	1	65,73,73	1.35	7 (10%)	76,113,113	1.72	10 (13%)
32	LHG	y	617	-	46,46,48	1.44	8 (17%)	49,52,54	0.73	2 (4%)
30	CHL	N	605	2	61,69,74	1.52	10 (16%)	67,108,114	1.83	11 (16%)
31	CLA	1	613	1	55,63,73	1.46	7 (12%)	64,101,113	1.80	9 (14%)
30	CHL	n	605	2	61,69,74	1.53	10 (16%)	67,108,114	1.88	13 (19%)
31	CLA	1	603	1	47,55,73	1.53	7 (14%)	54,91,113	1.97	7 (12%)
31	CLA	n	604	-	55,63,73	1.47	7 (12%)	64,101,113	1.82	10 (15%)
31	CLA	12	611	-	45,53,73	1.59	7 (15%)	52,89,113	1.91	9 (17%)
30	CHL	G	608	-	52,60,74	1.66	10 (19%)	56,97,114	2.02	9 (16%)
31	CLA	B	615	7	65,73,73	1.36	7 (10%)	76,113,113	1.78	12 (15%)
33	LUT	13	617	-	42,43,43	0.37	0	51,60,60	0.54	1 (1%)
32	LHG	D	409	-	38,38,48	1.39	8 (21%)	41,44,54	0.79	2 (4%)
31	CLA	n	611	32	60,68,73	1.43	7 (11%)	70,107,113	1.78	8 (11%)
31	CLA	13	614	5	45,53,73	1.56	7 (15%)	52,89,113	1.92	9 (17%)
31	CLA	g	614	1	49,57,73	1.52	7 (14%)	55,93,113	1.85	6 (10%)
31	CLA	2	604	-	50,58,73	1.56	8 (16%)	58,95,113	1.83	10 (17%)
31	CLA	r	604	-	48,56,73	1.54	7 (14%)	55,92,113	1.86	10 (18%)
31	CLA	S	603	22	42,50,73	1.57	7 (16%)	48,85,113	2.06	8 (16%)
31	CLA	b	604	7	65,73,73	1.35	7 (10%)	76,113,113	1.73	10 (13%)
31	CLA	a	404	-	65,73,73	1.33	7 (10%)	76,113,113	1.63	11 (14%)
31	CLA	b	601	-	55,63,73	1.44	7 (12%)	64,101,113	1.82	10 (15%)
31	CLA	s	602	22	65,73,73	1.36	7 (10%)	76,113,113	1.69	8 (10%)
32	LHG	13	616	31	39,39,48	1.50	8 (20%)	42,45,54	0.81	2 (4%)
43	LNL	x	201	-	19,19,19	0.42	0	18,19,19	0.47	0
32	LHG	R	619	-	46,46,48	1.39	8 (17%)	49,52,54	0.78	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	Y	601	28	66,74,74	1.45	10 (15%)	73,114,114	1.91	11 (15%)
31	CLA	C	512	8	65,73,73	1.33	7 (10%)	76,113,113	1.73	11 (14%)
33	LUT	4	617	-	42,43,43	0.37	0	51,60,60	0.31	0
33	LUT	s	618	-	42,43,43	0.35	0	51,60,60	0.51	0
31	CLA	15	602	2	60,68,73	1.41	7 (11%)	70,107,113	1.70	11 (15%)
31	CLA	Y	604	-	55,63,73	1.48	7 (12%)	64,101,113	1.82	8 (12%)
31	CLA	16	603	-	60,68,73	1.39	7 (11%)	70,107,113	1.74	10 (14%)
32	LHG	3	617	-	46,46,48	1.39	8 (17%)	49,52,54	0.75	2 (4%)
30	CHL	R	607	-	51,59,74	1.66	10 (19%)	55,96,114	2.09	13 (23%)
31	CLA	4	614	1	46,54,73	1.56	7 (15%)	53,90,113	1.94	9 (16%)
31	CLA	g	603	1	55,63,73	1.46	7 (12%)	64,101,113	1.89	8 (12%)
41	LMG	C	520	-	47,47,55	0.19	0	55,55,63	0.16	0
30	CHL	1	601	1	61,69,74	1.53	10 (16%)	67,108,114	1.94	14 (20%)
30	CHL	1	608	-	50,58,74	1.66	9 (18%)	52,94,114	2.04	11 (21%)
41	LMG	D	414	-	48,48,55	0.19	0	56,56,63	0.15	0
31	CLA	16	602	5	65,73,73	1.37	8 (12%)	76,113,113	1.76	11 (14%)
31	CLA	B	616	7	60,68,73	1.38	7 (11%)	70,107,113	1.88	12 (17%)
30	CHL	r	607	-	51,59,74	1.65	10 (19%)	55,96,114	2.10	13 (23%)
34	NEX	y	624	-	38,46,46	0.45	1 (2%)	50,70,70	0.65	1 (2%)
39	BCR	B	617	-	41,41,41	0.14	0	56,56,56	0.25	0
34	NEX	14	618	-	13,17,46	0.38	0	19,29,70	0.48	0
33	LUT	16	618	-	42,43,43	0.41	1 (2%)	51,60,60	0.37	0
41	LMG	J	102	-	51,51,55	0.18	0	59,59,63	0.17	0
31	CLA	Y	613	28	65,73,73	1.34	7 (10%)	76,113,113	1.64	9 (11%)
31	CLA	3	603	3	55,63,73	1.45	7 (12%)	64,101,113	1.87	7 (10%)
40	SQD	a	409	-	50,51,54	0.19	0	59,62,65	0.26	0
31	CLA	5	612	-	46,54,73	1.57	7 (15%)	53,90,113	1.91	7 (13%)
31	CLA	r	608	21	65,73,73	1.32	7 (10%)	76,113,113	1.70	11 (14%)
46	DGD	c	519	-	60,60,67	0.18	0	74,74,81	0.19	0
31	CLA	11	602	1	60,68,73	1.41	7 (11%)	70,107,113	1.79	13 (18%)
31	CLA	13	610	-	65,73,73	1.35	6 (9%)	76,113,113	1.73	11 (14%)
30	CHL	13	606	-	61,69,74	1.52	9 (14%)	67,108,114	1.85	11 (16%)
39	BCR	B	619	-	41,41,41	0.12	0	56,56,56	0.24	0
31	CLA	1	610	1	55,63,73	1.49	7 (12%)	64,101,113	1.70	11 (17%)
31	CLA	R	609	21	65,73,73	1.34	7 (10%)	76,113,113	1.65	8 (10%)
31	CLA	a	403	6	65,73,73	1.34	7 (10%)	76,113,113	1.75	12 (15%)
32	LHG	r	619	-	46,46,48	1.40	8 (17%)	49,52,54	0.76	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	g	601	1	66,74,74	1.47	9 (13%)	73,114,114	1.82	13 (17%)
31	CLA	6	602	3	60,68,73	1.40	7 (11%)	70,107,113	1.72	11 (15%)
39	BCR	c	516	-	41,41,41	0.12	0	56,56,56	0.32	0
31	CLA	A	404	-	65,73,73	1.33	7 (10%)	76,113,113	1.63	11 (14%)
30	CHL	12	608	2	53,61,74	1.66	10 (18%)	57,98,114	1.97	13 (22%)
30	CHL	N	609	2	66,74,74	1.47	10 (15%)	73,114,114	1.87	13 (17%)
39	BCR	D	406	-	41,41,41	0.13	0	56,56,56	0.21	0
41	LMG	c	520	-	47,47,55	0.19	0	55,55,63	0.17	0
31	CLA	c	513	8	55,63,73	1.44	7 (12%)	64,101,113	1.86	10 (15%)
32	LHG	6	617	-	46,46,48	1.36	8 (17%)	49,52,54	0.75	2 (4%)
31	CLA	c	511	8	65,73,73	1.32	7 (10%)	76,113,113	1.79	12 (15%)
30	CHL	4	606	-	47,55,74	1.67	9 (19%)	50,91,114	2.17	9 (18%)
31	CLA	N	610	2	60,68,73	1.40	7 (11%)	70,107,113	1.75	9 (12%)
39	BCR	C	516	-	41,41,41	0.12	0	56,56,56	0.31	0
43	LNL	C	524	-	19,19,19	0.44	0	18,19,19	0.50	0
43	LNL	W	502	-	19,19,19	0.44	0	18,19,19	0.52	0
30	CHL	1	607	-	51,59,74	1.68	11 (21%)	55,96,114	2.09	12 (21%)
30	CHL	3	608	-	50,58,74	1.64	9 (18%)	52,94,114	2.10	12 (23%)
46	DGD	c	517	-	67,67,67	0.18	0	81,81,81	0.18	0
34	NEX	N	619	-	38,46,46	0.42	1 (2%)	50,70,70	0.40	0
31	CLA	r	611	21	49,57,73	1.51	7 (14%)	55,93,113	1.92	6 (10%)
32	LHG	l	102	-	46,46,48	1.30	8 (17%)	49,52,54	0.77	2 (4%)
31	CLA	C	504	8	65,73,73	1.34	7 (10%)	76,113,113	1.77	13 (17%)
31	CLA	5	604	-	50,58,73	1.56	7 (14%)	58,95,113	1.81	10 (17%)
43	LNL	W	503	-	19,19,19	0.42	0	18,19,19	0.49	0
31	CLA	S	614	22	65,73,73	1.35	7 (10%)	76,113,113	1.67	10 (13%)
33	LUT	S	618	-	42,43,43	0.36	0	51,60,60	0.43	0
49	HEM	F	101	11,10	41,50,50	0.81	1 (2%)	45,82,82	0.70	1 (2%)
31	CLA	Y	615	-	56,64,73	1.45	7 (12%)	65,102,113	1.81	11 (16%)
31	CLA	S	612	22	45,53,73	1.73	8 (17%)	52,89,113	1.66	7 (13%)
30	CHL	5	608	-	50,58,74	1.65	9 (18%)	52,94,114	2.07	9 (17%)
31	CLA	11	604	-	46,54,73	1.57	7 (15%)	53,90,113	1.92	7 (13%)
34	NEX	11	618	-	13,17,46	0.36	0	19,29,70	0.48	0
30	CHL	5	605	2	46,54,74	1.73	10 (21%)	49,90,114	1.99	9 (18%)
32	LHG	11	615	31	48,48,48	1.38	8 (16%)	51,54,54	0.74	2 (3%)
33	LUT	S	619	-	42,43,43	0.35	0	51,60,60	0.37	0
46	DGD	C	519	-	60,60,67	0.18	0	74,74,81	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	STE	b	622	-	19,19,19	0.60	0	19,19,19	0.99	2 (10%)
48	BCT	D	403	47	2,3,3	0.88	0	2,3,3	3.15	2 (100%)
31	CLA	R	601	21	49,57,73	1.51	7 (14%)	55,93,113	1.76	9 (16%)
33	LUT	n	618	-	42,43,43	0.40	1 (2%)	51,60,60	0.33	0
33	LUT	3	619	-	42,43,43	0.40	1 (2%)	51,60,60	0.42	0
30	CHL	15	605	-	46,54,74	1.73	10 (21%)	49,90,114	2.29	8 (16%)
34	NEX	5	616	-	29,33,46	0.48	1 (3%)	38,48,70	0.50	0
31	CLA	N	611	32	60,68,73	1.43	8 (13%)	70,107,113	1.78	8 (11%)
30	CHL	11	601	1	66,74,74	1.48	10 (15%)	73,114,114	1.83	13 (17%)
31	CLA	b	616	7	60,68,73	1.37	7 (11%)	70,107,113	1.86	11 (15%)
35	XAT	6	620	-	39,47,47	0.13	0	54,74,74	0.75	1 (1%)
41	LMG	K	102	-	51,51,55	0.20	0	59,59,63	0.15	0
32	LHG	r	621	-	43,43,48	1.48	8 (18%)	46,49,54	0.81	2 (4%)
41	LMG	D	410	-	44,44,55	0.19	0	52,52,63	0.17	0
39	BCR	b	618	-	41,41,41	0.14	0	56,56,56	0.24	0
31	CLA	13	613	5	50,58,73	1.53	7 (14%)	58,95,113	1.91	8 (13%)
34	NEX	12	616	-	24,28,46	0.36	0	32,42,70	0.56	0
30	CHL	11	608	-	51,59,74	1.67	11 (21%)	55,96,114	2.05	13 (23%)
31	CLA	r	609	21	65,73,73	1.35	7 (10%)	76,113,113	1.70	9 (11%)
31	CLA	g	610	1	65,73,73	1.35	7 (10%)	76,113,113	1.71	11 (14%)
33	LUT	R	615	-	42,43,43	0.38	0	51,60,60	0.38	0
30	CHL	g	606	-	50,58,74	1.63	8 (16%)	52,94,114	2.03	9 (17%)
41	LMG	d	415	-	48,48,55	0.19	0	56,56,63	0.15	0
30	CHL	16	601	5	56,64,74	1.62	11 (19%)	61,102,114	2.02	12 (19%)
31	CLA	R	608	21	65,73,73	1.32	7 (10%)	76,113,113	1.69	12 (15%)
36	3PH	B	624	-	37,37,47	0.30	0	41,42,52	0.33	0
39	BCR	b	619	-	41,41,41	0.12	0	56,56,56	0.25	0
31	CLA	S	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.77	13 (17%)
39	BCR	h	102	-	41,41,41	0.13	0	56,56,56	0.33	0
37	OEX	a	402	8,6	0,15,15	-	-	-	-	-
31	CLA	r	614	-	55,63,73	1.43	7 (12%)	64,101,113	1.80	10 (15%)
33	LUT	15	615	-	42,43,43	0.34	0	51,60,60	0.31	0
31	CLA	Y	603	28	60,68,73	1.39	7 (11%)	70,107,113	1.84	11 (15%)
31	CLA	16	613	5	50,58,73	1.53	7 (14%)	58,95,113	1.94	8 (13%)
49	HEM	f	101	11,10	41,50,50	0.81	1 (2%)	45,82,82	0.70	1 (2%)
30	CHL	6	605	3	66,74,74	1.48	10 (15%)	73,114,114	1.95	13 (17%)
31	CLA	G	610	1	65,73,73	1.35	6 (9%)	76,113,113	1.74	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	13	601	5	56,64,74	1.62	10 (17%)	61,102,114	2.01	13 (21%)
31	CLA	D	405	9	65,73,73	1.34	7 (10%)	76,113,113	1.63	10 (13%)
31	CLA	R	614	-	55,63,73	1.44	7 (12%)	64,101,113	1.86	11 (17%)
31	CLA	g	612	1	43,51,73	1.58	7 (16%)	49,86,113	1.97	7 (14%)
34	NEX	s	620	-	38,46,46	0.45	1 (2%)	50,70,70	0.46	0
43	LNL	c	523	-	19,19,19	0.43	0	18,19,19	0.49	0
31	CLA	S	602	22	65,73,73	1.35	7 (10%)	76,113,113	1.73	11 (14%)
33	LUT	2	615	-	42,43,43	0.37	0	51,60,60	0.31	0
39	BCR	B	618	-	41,41,41	0.14	0	56,56,56	0.24	0
33	LUT	G	616	-	42,43,43	0.38	0	51,60,60	0.40	0
33	LUT	5	615	-	42,43,43	0.37	0	51,60,60	0.32	0
31	CLA	5	610	2	50,58,73	1.52	7 (14%)	58,95,113	1.78	12 (20%)
43	LNL	c	524	-	19,19,19	0.44	0	18,19,19	0.50	0
32	LHG	s	617	31	44,44,48	1.36	7 (15%)	47,50,54	0.72	2 (4%)
30	CHL	G	607	-	50,58,74	1.65	9 (18%)	52,94,114	2.13	10 (19%)
31	CLA	b	610	-	65,73,73	1.32	7 (10%)	76,113,113	1.75	12 (15%)
43	LNL	h	101	-	19,19,19	0.44	0	18,19,19	0.49	0
31	CLA	s	610	22	65,73,73	1.34	7 (10%)	76,113,113	1.71	10 (13%)
31	CLA	12	609	2	55,63,73	1.46	7 (12%)	64,101,113	1.75	8 (12%)
34	NEX	1	618	-	13,17,46	0.37	0	19,29,70	0.49	0
39	BCR	J	101	-	41,41,41	0.21	0	56,56,56	0.47	0
30	CHL	Y	608	-	44,52,74	1.63	7 (15%)	46,87,114	2.15	7 (15%)
43	LNL	A	412	-	19,19,19	0.44	0	18,19,19	0.49	0
32	LHG	r	618	31	37,37,48	1.42	7 (18%)	40,43,54	0.87	2 (5%)
30	CHL	G	605	1	48,56,74	1.67	8 (16%)	51,92,114	2.12	10 (19%)
33	LUT	N	618	-	42,43,43	0.39	1 (2%)	51,60,60	0.36	0
41	LMG	s	616	-	42,42,55	0.19	0	50,50,63	0.18	0
30	CHL	n	609	2	66,74,74	1.47	10 (15%)	73,114,114	1.88	12 (16%)
30	CHL	5	607	-	56,64,74	1.61	10 (17%)	61,102,114	2.00	11 (18%)
30	CHL	11	607	-	46,54,74	1.73	10 (21%)	49,90,114	2.05	12 (24%)
31	CLA	c	512	8	65,73,73	1.33	7 (10%)	76,113,113	1.74	11 (14%)
31	CLA	14	611	32	60,68,73	1.43	7 (11%)	70,107,113	1.75	10 (14%)
41	LMG	d	411	-	34,34,55	0.21	0	36,36,63	0.15	0
33	LUT	14	616	-	42,43,43	0.30	0	51,60,60	0.41	1 (1%)
35	XAT	R	616	-	39,47,47	0.12	0	54,74,74	0.82	3 (5%)
31	CLA	4	612	1	46,54,73	1.60	7 (15%)	53,90,113	1.75	7 (13%)
30	CHL	s	607	-	43,51,74	1.67	9 (20%)	45,86,114	2.32	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	r	610	32	60,68,73	1.42	7 (11%)	70,107,113	1.79	9 (12%)
31	CLA	g	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.68	8 (10%)
31	CLA	r	612	21	50,58,73	1.51	7 (14%)	58,95,113	1.85	10 (17%)
41	LMG	A	409	-	55,55,55	0.17	0	63,63,63	0.16	0
31	CLA	R	603	21	65,73,73	1.33	7 (10%)	76,113,113	1.81	11 (14%)
33	LUT	11	616	-	42,43,43	0.33	0	51,60,60	0.47	1 (1%)
33	LUT	12	614	-	42,43,43	0.38	0	51,60,60	0.46	0
36	3PH	8	201	-	47,47,47	0.30	0	51,52,52	0.41	0
34	NEX	g	618	-	38,46,46	0.39	1 (2%)	50,70,70	0.48	0
33	LUT	1	617	-	42,43,43	0.37	0	51,60,60	0.30	0
33	LUT	r	615	-	42,43,43	0.39	0	51,60,60	0.36	0
34	NEX	n	619	-	38,46,46	0.43	1 (2%)	50,70,70	0.39	0
31	CLA	R	611	21	49,57,73	1.51	7 (14%)	55,93,113	1.90	7 (12%)
31	CLA	N	602	2	65,73,73	1.33	7 (10%)	76,113,113	1.75	10 (13%)
39	BCR	c	515	-	41,41,41	0.11	0	56,56,56	0.23	0
32	LHG	A	411	-	48,48,48	1.37	8 (16%)	51,54,54	0.74	2 (3%)
41	LMG	d	410	-	44,44,55	0.19	0	52,52,63	0.19	0
34	NEX	Y	623	-	38,46,46	0.47	1 (2%)	50,70,70	0.40	0
31	CLA	3	602	3	60,68,73	1.40	7 (11%)	70,107,113	1.72	12 (17%)
31	CLA	n	614	2	45,53,73	1.57	8 (17%)	52,89,113	1.90	7 (13%)
30	CHL	14	608	-	51,59,74	1.68	10 (19%)	55,96,114	2.00	12 (21%)
43	LNL	C	523	-	19,19,19	0.43	0	18,19,19	0.50	0
32	LHG	1	615	31	42,42,48	1.44	8 (19%)	45,48,54	0.76	2 (4%)
33	LUT	2	614	-	42,43,43	0.32	0	51,60,60	0.29	0
41	LMG	B	621	-	49,49,55	0.19	0	57,57,63	0.19	0
39	BCR	j	101	-	41,41,41	0.20	0	56,56,56	0.47	0
30	CHL	16	607	-	61,69,74	1.52	11 (18%)	67,108,114	2.00	11 (16%)
31	CLA	c	509	8	60,68,73	1.42	7 (11%)	70,107,113	1.78	12 (17%)
31	CLA	3	614	3	50,58,73	1.54	7 (14%)	58,95,113	1.84	8 (13%)
42	PL9	D	407	-	55,55,55	0.09	0	68,69,69	0.18	0
32	LHG	d	413	-	48,48,48	1.43	8 (16%)	51,54,54	0.75	2 (3%)
31	CLA	12	603	-	55,63,73	1.45	7 (12%)	64,101,113	1.85	8 (12%)
31	CLA	B	601	-	55,63,73	1.44	7 (12%)	64,101,113	1.82	10 (15%)
32	LHG	6	616	31	43,43,48	1.43	8 (18%)	46,49,54	0.79	2 (4%)
43	LNL	r	620	-	19,19,19	0.44	0	18,19,19	0.51	0
31	CLA	15	610	-	45,53,73	1.57	7 (15%)	52,89,113	1.93	8 (15%)
30	CHL	4	609	-	66,74,74	1.49	11 (16%)	73,114,114	1.79	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	606	7	65,73,73	1.34	7 (10%)	76,113,113	1.61	11 (14%)
31	CLA	6	610	3	60,68,73	1.42	7 (11%)	70,107,113	1.71	12 (17%)
30	CHL	r	606	21	66,74,74	1.45	10 (15%)	73,114,114	1.86	14 (19%)
34	NEX	G	618	-	38,45,46	0.75	2 (5%)	48,67,70	0.51	0
31	CLA	C	509	8	60,68,73	1.42	7 (11%)	70,107,113	1.78	12 (17%)
31	CLA	16	610	-	65,73,73	1.35	7 (10%)	76,113,113	1.75	11 (14%)
32	LHG	L	102	-	46,46,48	1.31	8 (17%)	49,52,54	0.77	2 (4%)
31	CLA	C	511	8	65,73,73	1.32	7 (10%)	76,113,113	1.79	12 (15%)
30	CHL	14	607	-	50,58,74	1.66	10 (20%)	52,94,114	1.97	11 (21%)
31	CLA	16	615	-	45,53,73	1.58	7 (15%)	52,89,113	1.78	10 (19%)
34	NEX	3	621	-	38,46,46	0.45	1 (2%)	50,70,70	0.34	0
31	CLA	1	614	1	46,54,73	1.56	7 (15%)	53,90,113	1.96	9 (16%)
30	CHL	G	606	-	47,55,74	1.67	8 (17%)	50,91,114	2.06	9 (18%)
31	CLA	11	611	32	50,58,73	1.55	7 (14%)	58,95,113	1.84	7 (12%)
30	CHL	g	607	-	50,58,74	1.65	9 (18%)	52,94,114	2.11	9 (17%)
30	CHL	2	609	2	66,74,74	1.50	10 (15%)	73,114,114	1.80	11 (15%)
44	STE	B	623	-	19,19,19	0.58	0	19,19,19	1.01	2 (10%)
31	CLA	s	609	22	55,63,73	1.47	7 (12%)	64,101,113	1.74	7 (10%)
43	LNL	X	201	-	19,19,19	0.43	0	18,19,19	0.49	0
30	CHL	3	605	3	66,74,74	1.47	10 (15%)	73,114,114	1.93	14 (19%)
41	LMG	b	621	-	46,46,55	0.18	0	54,54,63	0.16	0
31	CLA	r	613	21	65,73,73	1.35	7 (10%)	76,113,113	1.80	10 (13%)
43	LNL	y	619	-	19,19,19	0.43	0	18,19,19	0.50	0
36	3PH	B	620	-	47,47,47	0.27	0	51,52,52	0.29	0
40	SQD	l	101	-	49,50,54	0.18	0	58,61,65	0.20	0
41	LMG	c	522	-	55,55,55	0.18	0	63,63,63	0.16	0
30	CHL	Y	609	28	66,74,74	1.47	10 (15%)	73,114,114	1.87	11 (15%)
30	CHL	N	601	2	53,61,74	1.65	10 (18%)	57,98,114	1.99	10 (17%)
30	CHL	N	606	-	61,69,74	1.54	10 (16%)	67,108,114	1.94	11 (16%)
31	CLA	B	602	7	65,73,73	1.35	7 (10%)	76,113,113	1.70	12 (15%)
42	PL9	d	407	-	55,55,55	0.09	0	68,69,69	0.18	0
30	CHL	5	609	2	66,74,74	1.50	10 (15%)	73,114,114	1.81	11 (15%)
32	LHG	a	414	-	42,42,48	1.45	8 (19%)	45,48,54	0.78	2 (4%)
31	CLA	4	603	1	55,63,73	1.46	7 (12%)	64,101,113	1.86	10 (15%)
39	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.26	0
31	CLA	s	614	22	65,73,73	1.35	7 (10%)	76,113,113	1.66	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LNL	H	101	-	19,19,19	0.43	0	18,19,19	0.49	0
32	LHG	c	521	-	41,41,48	1.46	8 (19%)	44,47,54	0.78	2 (4%)
30	CHL	4	601	1	61,69,74	1.54	9 (14%)	67,108,114	1.94	14 (20%)
31	CLA	G	614	1	49,57,73	1.53	7 (14%)	55,93,113	1.85	6 (10%)
31	CLA	R	610	32	60,68,73	1.40	7 (11%)	70,107,113	1.70	10 (14%)
41	LMG	C	522	-	55,55,55	0.18	0	63,63,63	0.16	0
31	CLA	2	610	2	50,58,73	1.52	7 (14%)	58,95,113	1.85	11 (18%)
40	SQD	A	408	-	50,51,54	0.19	0	59,62,65	0.26	0
31	CLA	12	604	-	55,63,73	1.46	7 (12%)	64,101,113	1.69	11 (17%)
31	CLA	b	608	7	65,73,73	1.35	7 (10%)	76,113,113	1.65	12 (15%)
32	LHG	C	521	-	41,41,48	1.45	8 (19%)	44,47,54	0.78	2 (4%)
32	LHG	D	408	-	48,48,48	1.30	7 (14%)	51,54,54	0.72	2 (3%)
33	LUT	15	614	-	42,43,43	0.38	0	51,60,60	0.49	0
31	CLA	S	610	22	65,73,73	1.33	7 (10%)	76,113,113	1.70	12 (15%)
30	CHL	S	606	22	66,74,74	1.49	10 (15%)	73,114,114	1.85	12 (16%)
30	CHL	1	606	-	47,55,74	1.67	9 (19%)	50,91,114	2.14	9 (18%)
31	CLA	12	602	2	60,68,73	1.41	7 (11%)	70,107,113	1.72	12 (17%)
31	CLA	c	507	8	65,73,73	1.35	7 (10%)	76,113,113	1.67	10 (13%)
31	CLA	Y	612	28	65,73,73	1.35	7 (10%)	76,113,113	1.70	13 (17%)
41	LMG	j	102	-	51,51,55	0.18	0	59,59,63	0.17	0
31	CLA	R	602	21	65,73,73	1.37	7 (10%)	76,113,113	1.71	11 (14%)
30	CHL	2	607	-	56,64,74	1.60	11 (19%)	61,102,114	2.01	10 (16%)
31	CLA	2	602	2	55,63,73	1.46	7 (12%)	64,101,113	1.82	12 (18%)
40	SQD	D	411	-	53,54,54	0.18	0	62,65,65	0.21	0
31	CLA	15	609	2	55,63,73	1.47	7 (12%)	64,101,113	1.84	12 (18%)
31	CLA	14	614	1	49,57,73	1.53	7 (14%)	55,93,113	1.92	7 (12%)
31	CLA	C	507	8	65,73,73	1.35	7 (10%)	76,113,113	1.69	10 (13%)
32	LHG	d	408	-	48,48,48	1.28	7 (14%)	51,54,54	0.73	2 (3%)
31	CLA	b	602	7	65,73,73	1.34	7 (10%)	76,113,113	1.69	11 (14%)
31	CLA	b	606	7	65,73,73	1.35	7 (10%)	76,113,113	1.63	11 (14%)
30	CHL	g	608	-	52,60,74	1.66	11 (21%)	56,97,114	2.02	10 (17%)
33	LUT	11	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.41	0
31	CLA	N	613	2	55,63,73	1.46	7 (12%)	64,101,113	1.84	7 (10%)
31	CLA	n	603	2	60,68,73	1.40	7 (11%)	70,107,113	1.85	9 (12%)
30	CHL	3	606	-	56,64,74	1.59	9 (16%)	61,102,114	1.94	8 (13%)
31	CLA	G	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.68	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	13	609	-	61,69,74	1.57	9 (14%)	67,108,114	1.83	10 (14%)
31	CLA	n	602	2	65,73,73	1.35	7 (10%)	76,113,113	1.73	9 (11%)
31	CLA	3	610	3	60,68,73	1.38	7 (11%)	70,107,113	1.75	11 (15%)
46	DGD	C	517	-	67,67,67	0.17	0	81,81,81	0.18	0
31	CLA	16	611	32	65,73,73	1.36	7 (10%)	76,113,113	1.68	10 (13%)
39	BCR	d	406	-	41,41,41	0.13	0	56,56,56	0.21	0
31	CLA	b	603	7	65,73,73	1.35	7 (10%)	76,113,113	1.73	11 (14%)
31	CLA	c	502	8	65,73,73	1.32	7 (10%)	76,113,113	1.67	10 (13%)
30	CHL	12	605	-	46,54,74	1.74	10 (21%)	49,90,114	2.24	8 (16%)
31	CLA	A	403	-	65,73,73	1.33	7 (10%)	76,113,113	1.65	13 (17%)
30	CHL	5	606	-	46,54,74	1.71	10 (21%)	49,90,114	2.17	10 (20%)
30	CHL	14	601	1	66,74,74	1.48	10 (15%)	73,114,114	1.82	13 (17%)
46	DGD	W	501	-	46,46,67	0.20	0	54,54,81	0.31	0
42	PL9	A	410	-	55,55,55	0.08	0	68,69,69	0.18	0
43	LNL	w	503	-	19,19,19	0.44	0	18,19,19	0.52	0
33	LUT	y	623	-	42,43,43	0.43	1 (2%)	51,60,60	0.40	0
31	CLA	C	510	8	65,73,73	1.34	7 (10%)	76,113,113	1.84	9 (11%)
32	LHG	a	413	-	43,43,48	1.39	7 (16%)	46,49,54	0.83	2 (4%)
31	CLA	4	610	1	65,73,73	1.40	8 (12%)	76,113,113	1.46	10 (13%)
33	LUT	1	616	-	42,43,43	0.36	0	51,60,60	0.35	0
32	LHG	a	401	-	48,48,48	1.40	8 (16%)	51,54,54	0.72	2 (3%)
30	CHL	3	607	-	66,74,74	1.47	10 (15%)	73,114,114	1.90	13 (17%)
31	CLA	c	506	8	65,73,73	1.35	7 (10%)	76,113,113	1.74	10 (13%)
30	CHL	6	607	-	66,74,74	1.47	10 (15%)	73,114,114	1.89	13 (17%)
31	CLA	b	605	7	65,73,73	1.35	7 (10%)	76,113,113	1.75	9 (11%)
31	CLA	c	504	8	65,73,73	1.34	7 (10%)	76,113,113	1.78	12 (15%)
34	NEX	6	621	-	38,46,46	0.46	1 (2%)	50,70,70	0.35	0
31	CLA	1	604	-	50,58,73	1.54	7 (14%)	58,95,113	1.91	12 (20%)
31	CLA	11	614	-	49,57,73	1.53	7 (14%)	55,93,113	1.91	7 (12%)
30	CHL	y	608	-	44,52,74	1.62	8 (18%)	46,87,114	2.15	8 (17%)
33	LUT	6	618	-	42,43,43	0.43	1 (2%)	51,60,60	0.43	0
31	CLA	11	612	1	43,51,73	1.60	7 (16%)	49,86,113	1.87	7 (14%)
31	CLA	N	615	2	47,55,73	1.53	7 (14%)	54,91,113	2.00	9 (16%)
31	CLA	G	604	-	50,58,73	1.54	7 (14%)	58,95,113	1.86	9 (15%)
31	CLA	C	506	8	65,73,73	1.35	7 (10%)	76,113,113	1.74	9 (11%)
31	CLA	Y	602	28	65,73,73	1.35	7 (10%)	76,113,113	1.71	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	13	604	-	55,63,73	1.47	7 (12%)	64,101,113	1.75	9 (14%)
32	LHG	Y	618	-	46,46,48	1.42	8 (17%)	49,52,54	0.75	2 (4%)
32	LHG	A	415	-	48,48,48	1.40	8 (16%)	51,54,54	0.75	2 (3%)
33	LUT	12	615	-	42,43,43	0.36	0	51,60,60	0.33	0
33	LUT	Y	621	-	42,43,43	0.39	0	51,60,60	0.49	0
43	LNL	I	101	-	19,19,19	0.43	0	18,19,19	0.50	0
46	DGD	c	518	-	59,59,67	0.18	0	73,73,81	0.17	0
33	LUT	4	616	-	42,43,43	0.39	1 (2%)	51,60,60	0.39	0
31	CLA	1	612	1	46,54,73	1.57	7 (15%)	53,90,113	1.85	6 (11%)
31	CLA	Y	614	28	49,57,73	1.51	7 (14%)	55,93,113	1.94	9 (16%)
31	CLA	y	603	28	60,68,73	1.40	7 (11%)	70,107,113	1.82	11 (15%)
31	CLA	d	404	9	65,73,73	1.33	7 (10%)	76,113,113	1.72	12 (15%)
31	CLA	6	603	3	55,63,73	1.45	7 (12%)	64,101,113	1.91	8 (12%)
32	LHG	14	615	31	48,48,48	1.39	8 (16%)	51,54,54	0.73	2 (3%)
31	CLA	B	610	-	65,73,73	1.32	7 (10%)	76,113,113	1.76	13 (17%)
33	LUT	16	617	-	42,43,43	0.38	0	51,60,60	0.54	1 (1%)
32	LHG	g	615	31	48,48,48	1.30	6 (12%)	51,54,54	0.70	2 (3%)
31	CLA	4	611	32	50,58,73	1.54	7 (14%)	58,95,113	1.87	9 (15%)
32	LHG	3	616	31	43,43,48	1.42	8 (18%)	46,49,54	0.78	2 (4%)
50	PAM	N	621	-	17,17,17	0.46	0	17,17,17	0.46	0
31	CLA	16	614	5	45,53,73	1.56	7 (15%)	52,89,113	1.91	9 (17%)
31	CLA	G	613	1	65,73,73	1.34	7 (10%)	76,113,113	1.69	10 (13%)
31	CLA	16	612	5	45,53,73	1.59	7 (15%)	52,89,113	1.93	7 (13%)
31	CLA	14	613	1	55,63,73	1.46	7 (12%)	64,101,113	1.78	9 (14%)
30	CHL	s	601	22	46,54,74	1.71	9 (19%)	49,90,114	2.16	11 (22%)
46	DGD	w	502	-	40,40,67	0.21	0	48,48,81	0.22	0
31	CLA	g	613	1	65,73,73	1.34	7 (10%)	76,113,113	1.68	10 (13%)
31	CLA	S	609	22	55,63,73	1.47	7 (12%)	64,101,113	1.85	9 (14%)
39	BCR	c	526	-	41,41,41	0.12	0	56,56,56	0.22	0
32	LHG	R	621	-	43,43,48	1.46	8 (18%)	46,49,54	0.79	2 (4%)
30	CHL	11	606	-	47,55,74	1.70	9 (19%)	50,91,114	2.04	12 (24%)
31	CLA	12	610	-	45,53,73	1.56	7 (15%)	52,89,113	1.92	8 (15%)
30	CHL	1	605	1	46,54,74	1.73	10 (21%)	49,90,114	2.13	11 (22%)
31	CLA	15	604	-	55,63,73	1.47	7 (12%)	64,101,113	1.70	9 (14%)
33	LUT	14	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.39	0
31	CLA	R	613	21	60,68,73	1.40	7 (11%)	70,107,113	1.86	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	n	610	2	60,68,73	1.39	7 (11%)	70,107,113	1.80	11 (15%)
34	NEX	r	617	-	38,46,46	0.40	1 (2%)	50,70,70	0.45	0
30	CHL	n	606	-	61,69,74	1.53	10 (16%)	67,108,114	1.95	13 (19%)
39	BCR	C	526	-	41,41,41	0.12	0	56,56,56	0.22	0
31	CLA	l	611	32	50,58,73	1.54	8 (16%)	58,95,113	1.84	9 (15%)
31	CLA	s	613	22	49,57,73	1.52	7 (14%)	55,93,113	1.85	8 (14%)
31	CLA	C	513	8	55,63,73	1.45	7 (12%)	64,101,113	1.85	10 (15%)
40	SQD	L	101	-	49,50,54	0.18	0	58,61,65	0.22	0
31	CLA	13	602	5	65,73,73	1.36	7 (10%)	76,113,113	1.71	10 (13%)
31	CLA	15	613	-	45,53,73	1.59	8 (17%)	52,89,113	1.85	8 (15%)
30	CHL	12	607	-	50,58,74	1.65	8 (16%)	52,94,114	2.14	10 (19%)
31	CLA	14	604	-	55,63,73	1.47	7 (12%)	64,101,113	1.79	8 (12%)
33	LUT	6	619	-	42,43,43	0.41	1 (2%)	51,60,60	0.41	0
36	3PH	T	101	-	47,47,47	0.28	0	51,52,52	0.29	0
31	CLA	s	603	22	42,50,73	1.58	7 (16%)	48,85,113	2.04	8 (16%)
31	CLA	g	604	-	50,58,73	1.54	7 (14%)	58,95,113	1.88	10 (17%)
30	CHL	16	606	-	61,69,74	1.53	9 (14%)	67,108,114	1.86	11 (16%)
31	CLA	y	613	28	65,73,73	1.34	7 (10%)	76,113,113	1.65	9 (11%)
31	CLA	s	605	22	50,58,73	1.52	7 (14%)	58,95,113	1.80	8 (13%)
48	BCT	d	403	47	2,3,3	0.88	0	2,3,3	3.17	2 (100%)
31	CLA	c	503	8	65,73,73	1.33	7 (10%)	76,113,113	1.77	10 (13%)
31	CLA	s	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.78	13 (17%)
30	CHL	16	608	-	50,58,74	1.63	9 (18%)	52,94,114	2.12	13 (25%)
41	LMG	B	622	-	48,48,55	0.18	0	56,56,63	0.20	0
39	BCR	C	515	-	41,41,41	0.11	0	56,56,56	0.23	0
33	LUT	13	618	-	42,43,43	0.40	1 (2%)	51,60,60	0.36	0
30	CHL	Y	605	28	56,64,74	1.59	10 (17%)	61,102,114	2.02	11 (18%)
30	CHL	1	609	-	56,64,74	1.62	11 (19%)	61,102,114	1.94	12 (19%)
30	CHL	Y	607	-	66,74,74	1.45	10 (15%)	73,114,114	1.89	13 (17%)
31	CLA	2	613	2	47,55,73	1.53	7 (14%)	54,91,113	1.75	9 (16%)
31	CLA	y	614	28	49,57,73	1.52	7 (14%)	55,93,113	1.95	9 (16%)
31	CLA	5	613	2	50,58,73	1.52	7 (14%)	58,95,113	1.74	9 (15%)
31	CLA	11	613	1	55,63,73	1.46	7 (12%)	64,101,113	1.78	9 (14%)
32	LHG	y	616	31	48,48,48	1.27	6 (12%)	51,54,54	0.79	2 (3%)
36	3PH	7	201	-	47,47,47	0.28	0	51,52,52	0.31	0
31	CLA	6	614	3	50,58,73	1.53	7 (14%)	58,95,113	1.89	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	14	606	-	47,55,74	1.71	10 (21%)	50,91,114	2.03	10 (20%)
31	CLA	B	605	7	65,73,73	1.35	7 (10%)	76,113,113	1.74	9 (11%)
31	CLA	C	514	8	65,73,73	1.33	7 (10%)	76,113,113	1.59	9 (11%)
31	CLA	G	602	1	65,73,73	1.33	7 (10%)	76,113,113	1.61	11 (14%)
32	LHG	S	617	31	44,44,48	1.38	8 (18%)	47,50,54	0.77	2 (4%)
31	CLA	S	605	22	50,58,73	1.53	7 (14%)	58,95,113	1.79	8 (13%)
31	CLA	B	611	7	65,73,73	1.36	7 (10%)	76,113,113	1.69	10 (13%)
31	CLA	b	615	7	65,73,73	1.36	7 (10%)	76,113,113	1.77	11 (14%)
30	CHL	s	608	-	49,57,74	1.66	9 (18%)	52,93,114	2.16	11 (21%)
31	CLA	5	603	2	55,63,73	1.47	7 (12%)	64,101,113	1.92	8 (12%)
31	CLA	11	603	-	55,63,73	1.46	7 (12%)	64,101,113	1.76	9 (14%)
31	CLA	s	615	22	47,55,73	1.54	7 (14%)	54,91,113	1.96	7 (12%)
43	LNL	R	620	-	19,19,19	0.44	0	18,19,19	0.51	0
31	CLA	6	613	3	55,63,73	1.46	7 (12%)	64,101,113	1.75	8 (12%)
32	LHG	Y	617	-	46,46,48	1.44	8 (17%)	49,52,54	0.76	2 (4%)
41	LMG	v	101	-	51,51,55	0.19	0	59,59,63	0.16	0
31	CLA	Y	610	28	65,73,73	1.35	7 (10%)	76,113,113	1.72	11 (14%)
31	CLA	y	604	-	55,63,73	1.48	7 (12%)	64,101,113	1.83	9 (14%)
30	CHL	R	606	21	66,74,74	1.44	10 (15%)	73,114,114	1.88	15 (20%)
31	CLA	N	614	2	45,53,73	1.56	8 (17%)	52,89,113	1.83	8 (15%)
30	CHL	15	608	2	61,69,74	1.56	10 (16%)	67,108,114	1.76	11 (16%)
31	CLA	5	602	2	55,63,73	1.46	7 (12%)	64,101,113	1.76	10 (15%)
40	SQD	d	414	-	45,46,54	0.19	0	54,57,65	0.23	0
31	CLA	y	615	-	56,64,73	1.44	7 (12%)	65,102,113	1.81	11 (16%)
30	CHL	2	601	2	47,55,74	1.67	10 (21%)	50,91,114	1.82	10 (20%)
35	XAT	G	619	-	39,47,47	0.10	0	54,74,74	0.43	0
30	CHL	g	609	1	66,74,74	1.49	10 (15%)	73,114,114	1.86	12 (16%)
30	CHL	13	605	5	56,64,74	1.60	10 (17%)	61,102,114	2.06	14 (22%)
31	CLA	n	615	2	47,55,73	1.53	8 (17%)	54,91,113	1.98	10 (18%)
34	NEX	15	616	-	24,28,46	0.36	0	32,42,70	0.58	0
30	CHL	S	608	-	49,57,74	1.66	9 (18%)	52,93,114	2.14	10 (19%)
32	LHG	Y	616	31	48,48,48	1.28	6 (12%)	51,54,54	0.79	2 (3%)
41	LMG	S	616	-	42,42,55	0.19	0	50,50,63	0.18	0
31	CLA	6	604	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	12 (15%)
31	CLA	y	612	28	65,73,73	1.36	7 (10%)	76,113,113	1.70	13 (17%)
31	CLA	6	615	3	50,58,73	1.52	6 (12%)	58,95,113	1.97	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	y	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.70	11 (14%)
31	CLA	16	604	-	55,63,73	1.48	7 (12%)	64,101,113	1.74	10 (15%)
32	LHG	a	411	-	48,48,48	1.35	8 (16%)	51,54,54	0.73	2 (3%)
43	LNL	i	101	-	19,19,19	0.44	0	18,19,19	0.50	0
31	CLA	6	611	32	65,73,73	1.34	7 (10%)	76,113,113	1.61	12 (15%)
31	CLA	13	603	-	60,68,73	1.39	7 (11%)	70,107,113	1.82	11 (15%)
31	CLA	B	609	7	65,73,73	1.35	7 (10%)	76,113,113	1.70	9 (11%)
32	LHG	n	616	31	48,48,48	1.32	7 (14%)	51,54,54	0.77	2 (3%)
35	XAT	14	619	-	39,47,47	0.10	0	54,74,74	0.44	0
31	CLA	3	612	3	65,73,73	1.36	7 (10%)	76,113,113	1.74	11 (14%)
30	CHL	2	606	-	46,54,74	1.72	10 (21%)	49,90,114	2.16	11 (22%)
31	CLA	6	612	3	55,63,73	1.47	7 (12%)	64,101,113	1.85	10 (15%)
35	XAT	g	619	-	39,47,47	0.10	0	54,74,74	0.44	0
34	NEX	4	618	-	13,17,46	0.35	0	19,29,70	0.49	0
38	PHO	a	405	-	51,69,69	0.37	0	47,99,99	0.66	1 (2%)
30	CHL	15	607	-	50,58,74	1.65	9 (18%)	52,94,114	2.17	12 (23%)
37	OEX	A	401	8,6	0,15,15	-	-	-	-	-
33	LUT	g	617	-	42,43,43	0.45	1 (2%)	51,60,60	0.44	1 (1%)
31	CLA	2	603	2	55,63,73	1.47	7 (12%)	64,101,113	1.94	8 (12%)
38	PHO	A	405	-	51,69,69	0.38	0	47,99,99	0.66	1 (2%)
30	CHL	2	608	-	50,58,74	1.65	9 (18%)	52,94,114	2.11	10 (19%)
31	CLA	14	603	-	55,63,73	1.46	7 (12%)	64,101,113	1.77	10 (15%)
30	CHL	G	609	1	66,74,74	1.49	10 (15%)	73,114,114	1.85	13 (17%)
41	LMG	w	501	-	55,55,55	0.17	0	63,63,63	0.17	0
31	CLA	s	604	-	65,73,73	1.35	7 (10%)	76,113,113	1.62	8 (10%)
30	CHL	y	607	-	66,74,74	1.45	10 (15%)	73,114,114	1.89	13 (17%)
43	LNL	y	620	-	19,19,19	0.42	0	18,19,19	0.48	0
30	CHL	13	608	-	50,58,74	1.64	9 (18%)	52,94,114	2.11	13 (25%)
31	CLA	R	604	-	48,56,73	1.54	7 (14%)	55,92,113	1.86	10 (18%)
32	LHG	16	616	31	39,39,48	1.51	8 (20%)	42,45,54	0.81	2 (4%)
43	LNL	Y	619	-	19,19,19	0.43	0	18,19,19	0.50	0
31	CLA	D	404	9	65,73,73	1.31	7 (10%)	76,113,113	1.76	11 (14%)
31	CLA	4	613	1	55,63,73	1.46	7 (12%)	64,101,113	1.73	10 (15%)
30	CHL	N	607	-	66,74,74	1.47	10 (15%)	73,114,114	1.84	11 (15%)
31	CLA	A	402	6	65,73,73	1.35	7 (10%)	76,113,113	1.74	11 (14%)
30	CHL	4	608	-	50,58,74	1.66	9 (18%)	52,94,114	2.06	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	607	-	65,73,73	1.33	7 (10%)	76,113,113	1.74	8 (10%)
32	LHG	R	618	31	37,37,48	1.44	7 (18%)	40,43,54	0.86	2 (5%)
30	CHL	16	605	5	56,64,74	1.60	10 (17%)	61,102,114	2.03	13 (21%)
31	CLA	R	612	21	50,58,73	1.57	7 (14%)	58,95,113	1.67	8 (13%)
32	LHG	A	414	-	42,42,48	1.46	8 (19%)	45,48,54	0.79	2 (4%)
33	LUT	N	617	-	42,43,43	0.37	0	51,60,60	0.34	0
30	CHL	S	607	-	43,51,74	1.67	9 (20%)	45,86,114	2.31	10 (22%)
31	CLA	Y	611	32	65,73,73	1.35	7 (10%)	76,113,113	1.72	11 (14%)
31	CLA	15	611	-	45,53,73	1.59	7 (15%)	52,89,113	1.91	9 (17%)
39	BCR	a	408	-	41,41,41	0.11	0	56,56,56	0.24	0
31	CLA	a	407	6	55,63,73	1.45	7 (12%)	64,101,113	1.78	8 (12%)
35	XAT	11	619	-	39,47,47	0.09	0	54,74,74	0.46	0
31	CLA	N	612	2	45,53,73	1.57	7 (15%)	52,89,113	2.00	8 (15%)
31	CLA	S	613	22	49,57,73	1.52	7 (14%)	55,93,113	1.86	9 (16%)
32	LHG	d	409	-	38,38,48	1.40	8 (21%)	41,44,54	0.79	2 (4%)
31	CLA	y	602	28	60,68,73	1.40	7 (11%)	70,107,113	1.75	9 (12%)
30	CHL	11	605	-	48,56,74	1.66	8 (16%)	51,92,114	1.88	12 (23%)
30	CHL	G	601	1	66,74,74	1.47	9 (13%)	73,114,114	1.81	11 (15%)
31	CLA	B	614	7	65,73,73	1.34	7 (10%)	76,113,113	1.73	11 (14%)
30	CHL	14	605	1	48,56,74	1.69	8 (16%)	51,92,114	2.08	11 (21%)
30	CHL	n	601	2	52,60,74	1.66	10 (19%)	56,97,114	2.13	13 (23%)

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
30	CHL	n	607	-	3/3/20/26	18/39/137/137	-
31	CLA	c	505	-	1/1/13/20	12/25/103/115	-
31	CLA	B	612	7	1/1/15/20	16/37/115/115	-
32	LHG	y	618	-	-	28/51/51/53	-
31	CLA	b	609	7	1/1/15/20	21/37/115/115	-
31	CLA	C	503	8	1/1/15/20	8/37/115/115	-
40	SQD	d	412	-	-	12/49/69/69	0/1/1/1
32	LHG	N	616	31	-	23/53/53/53	-
33	LUT	Y	622	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	y	601	28	3/3/20/26	14/39/137/137	-
31	CLA	12	612	2	1/1/12/20	12/19/97/115	-
30	CHL	R	605	21	3/3/18/26	9/27/125/137	-
31	CLA	C	502	8	1/1/15/20	14/37/115/115	-
31	CLA	3	604	-	1/1/15/20	20/37/115/115	-
43	LNL	y	621	-	-	3/17/17/17	-
30	CHL	5	601	2	3/3/17/26	9/21/119/137	-
31	CLA	C	505	-	1/1/13/20	8/25/103/115	-
31	CLA	b	607	-	1/1/15/20	17/37/115/115	-
30	CHL	3	609	3	3/3/20/26	14/39/137/137	-
30	CHL	s	606	22	3/3/20/26	21/39/137/137	-
31	CLA	15	603	-	1/1/13/20	8/25/103/115	-
31	CLA	S	604	-	1/1/15/20	18/37/115/115	-
30	CHL	12	601	2	3/3/16/26	7/20/118/137	-
30	CHL	n	608	-	3/3/16/26	13/20/118/137	-
31	CLA	N	604	-	1/1/13/20	13/25/103/115	-
38	PHO	a	406	-	-	5/37/103/103	0/5/6/6
31	CLA	C	508	-	1/1/15/20	18/37/115/115	-
35	XAT	3	620	-	-	0/31/93/93	0/4/4/4
31	CLA	d	405	9	1/1/15/20	16/37/115/115	-
31	CLA	r	602	21	1/1/15/20	10/37/115/115	-
35	XAT	r	616	-	-	0/31/93/93	0/4/4/4
31	CLA	4	604	-	1/1/12/20	9/19/97/115	-
30	CHL	4	605	1	3/3/16/26	6/15/113/137	-
31	CLA	b	614	7	1/1/15/20	17/37/115/115	-
32	LHG	G	615	31	-	21/53/53/53	-
30	CHL	N	608	-	3/3/16/26	10/20/118/137	-
30	CHL	y	605	28	3/3/18/26	8/27/125/137	-
31	CLA	3	613	3	1/1/13/20	13/25/103/115	-
43	LNL	a	412	-	-	5/17/17/17	-
30	CHL	14	609	-	3/3/18/26	16/27/125/137	-
39	BCR	A	407	-	-	1/29/63/63	0/2/2/2
30	CHL	16	609	-	3/3/19/26	13/33/131/137	-
38	PHO	D	402	-	-	9/37/103/103	0/5/6/6
31	CLA	13	611	32	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	d	402	-	1/1/15/20	17/37/115/115	-
31	CLA	13	615	5	1/1/11/20	4/13/91/115	-
33	LUT	g	616	-	-	2/29/67/67	0/2/2/2
30	CHL	12	606	-	3/3/17/26	6/21/119/137	-
30	CHL	2	605	2	3/3/16/26	11/15/113/137	-
33	LUT	5	614	-	-	4/29/67/67	0/2/2/2
34	NEX	16	619	-	-	2/27/83/83	0/3/3/3
31	CLA	13	612	5	1/1/11/20	2/13/91/115	-
42	PL9	a	410	-	-	9/53/73/73	0/1/1/1
33	LUT	G	617	-	-	0/29/67/67	0/2/2/2
31	CLA	2	611	-	1/1/11/20	8/15/93/115	-
32	LHG	s	621	-	-	18/53/53/53	-
31	CLA	11	610	-	1/1/13/20	8/25/103/115	-
30	CHL	6	601	3	3/3/19/26	15/33/131/137	-
33	LUT	n	617	-	-	0/29/67/67	0/2/2/2
34	NEX	13	619	-	-	2/27/83/83	0/3/3/3
31	CLA	r	603	21	1/1/15/20	15/37/115/115	-
30	CHL	3	601	3	3/3/19/26	14/33/131/137	-
31	CLA	14	612	1	1/1/10/20	6/11/89/115	-
31	CLA	c	508	-	1/1/15/20	18/37/115/115	-
34	NEX	R	617	-	-	3/27/83/83	0/3/3/3
31	CLA	3	611	32	1/1/15/20	12/37/115/115	-
34	NEX	S	620	-	-	2/27/83/83	0/3/3/3
31	CLA	y	610	28	1/1/15/20	7/37/115/115	-
31	CLA	12	613	-	1/1/11/20	5/13/91/115	-
30	CHL	y	606	-	3/3/20/26	15/39/137/137	-
39	BCR	H	103	-	-	2/29/63/63	0/2/2/2
30	CHL	6	606	-	3/3/18/26	10/27/125/137	-
30	CHL	y	609	28	3/3/20/26	18/39/137/137	-
31	CLA	b	611	7	1/1/15/20	13/37/115/115	-
34	NEX	2	616	-	-	2/25/56/83	0/2/2/3
33	LUT	y	622	-	-	2/29/67/67	0/2/2/2
31	CLA	B	604	7	1/1/15/20	11/37/115/115	-
31	CLA	S	615	22	1/1/11/20	7/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	6	608	-	3/3/16/26	8/20/118/137	-
36	3PH	b	623	-	-	5/40/40/49	-
32	LHG	D	412	-	-	21/53/53/53	-
30	CHL	r	605	21	3/3/18/26	13/27/125/137	-
31	CLA	r	601	21	1/1/11/20	10/18/96/115	-
31	CLA	s	612	22	1/1/11/20	3/13/91/115	-
32	LHG	4	615	31	-	13/51/51/53	-
31	CLA	B	613	7	1/1/15/20	21/37/115/115	-
32	LHG	A	413	-	-	12/48/48/53	-
31	CLA	G	612	1	1/1/10/20	3/11/89/115	-
31	CLA	3	615	3	1/1/11/20	5/15/93/115	-
30	CHL	11	609	-	3/3/18/26	20/27/125/137	-
31	CLA	15	612	-	1/1/12/20	10/19/97/115	-
33	LUT	s	619	-	-	0/29/67/67	0/2/2/2
31	CLA	B	603	7	1/1/15/20	11/37/115/115	-
30	CHL	g	605	1	3/3/16/26	9/18/116/137	-
31	CLA	n	612	2	1/1/11/20	6/13/91/115	-
31	CLA	n	613	2	1/1/13/20	10/25/103/115	-
31	CLA	c	514	8	1/1/15/20	16/37/115/115	-
31	CLA	1	602	1	1/1/14/20	12/31/109/115	-
31	CLA	14	610	-	1/1/15/20	18/37/115/115	-
31	CLA	G	603	1	1/1/13/20	14/25/103/115	-
30	CHL	15	601	2	3/3/16/26	7/20/118/137	-
31	CLA	2	612	-	1/1/11/20	6/15/93/115	-
30	CHL	13	607	-	3/3/19/26	14/33/131/137	-
30	CHL	S	601	22	3/3/16/26	7/15/113/137	-
32	LHG	S	621	-	-	22/53/53/53	-
31	CLA	b	612	7	1/1/15/20	18/37/115/115	-
41	LMG	b	620	-	-	4/44/64/70	0/1/1/1
46	DGD	C	518	-	-	5/47/87/95	0/2/2/2
31	CLA	5	611	-	1/1/11/20	6/15/93/115	-
31	CLA	b	613	7	1/1/15/20	18/37/115/115	-
31	CLA	4	602	1	1/1/14/20	13/31/109/115	-
43	LNL	Y	620	-	-	5/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	406	6	1/1/13/20	7/25/103/115	-
31	CLA	B	608	7	1/1/15/20	16/37/115/115	-
40	SQD	D	413	-	-	8/41/61/69	0/1/1/1
30	CHL	6	609	3	3/3/20/26	15/39/137/137	-
33	LUT	3	618	-	-	0/29/67/67	0/2/2/2
30	CHL	Y	606	-	3/3/20/26	16/39/137/137	-
30	CHL	15	606	-	3/3/17/26	8/21/119/137	-
31	CLA	N	603	2	1/1/14/20	11/31/109/115	-
31	CLA	14	602	1	1/1/14/20	12/31/109/115	-
30	CHL	4	607	-	3/3/17/26	8/21/119/137	-
41	LMG	H	102	-	-	2/36/36/70	-
50	PAM	n	620	-	-	2/15/15/15	-
31	CLA	c	510	8	1/1/15/20	11/37/115/115	-
31	CLA	g	602	1	1/1/15/20	15/37/115/115	-
32	LHG	y	617	-	-	26/51/51/53	-
30	CHL	N	605	2	3/3/19/26	14/33/131/137	-
31	CLA	1	613	1	1/1/13/20	9/25/103/115	-
30	CHL	n	605	2	3/3/19/26	16/33/131/137	-
31	CLA	1	603	1	1/1/11/20	3/16/94/115	-
31	CLA	n	604	-	1/1/13/20	13/25/103/115	-
31	CLA	12	611	-	1/1/11/20	6/13/91/115	-
30	CHL	G	608	-	3/3/17/26	10/23/121/137	-
31	CLA	B	615	7	1/1/15/20	11/37/115/115	-
33	LUT	13	617	-	-	2/29/67/67	0/2/2/2
32	LHG	D	409	-	-	11/43/43/53	-
31	CLA	n	611	32	1/1/14/20	10/31/109/115	-
31	CLA	13	614	5	1/1/11/20	8/13/91/115	-
31	CLA	g	614	1	1/1/11/20	5/18/96/115	-
31	CLA	2	604	-	1/1/12/20	8/19/97/115	-
31	CLA	r	604	-	1/1/11/20	4/17/95/115	-
31	CLA	S	603	22	1/1/10/20	6/10/88/115	-
31	CLA	b	604	7	1/1/15/20	14/37/115/115	-
31	CLA	a	404	-	1/1/15/20	16/37/115/115	-
31	CLA	b	601	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	602	22	1/1/15/20	14/37/115/115	-
32	LHG	13	616	31	-	25/44/44/53	-
43	LNL	x	201	-	-	6/17/17/17	-
32	LHG	R	619	-	-	13/51/51/53	-
30	CHL	Y	601	28	3/3/20/26	14/39/137/137	-
31	CLA	C	512	8	1/1/15/20	17/37/115/115	-
33	LUT	4	617	-	-	0/29/67/67	0/2/2/2
33	LUT	s	618	-	-	2/29/67/67	0/2/2/2
31	CLA	15	602	2	1/1/14/20	17/31/109/115	-
31	CLA	Y	604	-	1/1/13/20	10/25/103/115	-
31	CLA	16	603	-	1/1/14/20	12/31/109/115	-
32	LHG	3	617	-	-	31/51/51/53	-
30	CHL	R	607	-	3/3/17/26	9/21/119/137	-
31	CLA	4	614	1	1/1/11/20	7/15/93/115	-
31	CLA	g	603	1	1/1/13/20	15/25/103/115	-
41	LMG	C	520	-	-	9/42/62/70	0/1/1/1
30	CHL	1	601	1	3/3/19/26	15/33/131/137	-
30	CHL	1	608	-	3/3/16/26	12/20/118/137	-
41	LMG	D	414	-	-	12/43/63/70	0/1/1/1
31	CLA	16	602	5	1/1/15/20	13/37/115/115	-
31	CLA	B	616	7	1/1/14/20	14/31/109/115	-
30	CHL	r	607	-	3/3/17/26	5/21/119/137	-
34	NEX	y	624	-	-	4/27/83/83	0/3/3/3
39	BCR	B	617	-	-	2/29/63/63	0/2/2/2
34	NEX	14	618	-	-	0/6/37/83	0/2/2/3
33	LUT	16	618	-	-	0/29/67/67	0/2/2/2
41	LMG	J	102	-	-	10/46/66/70	0/1/1/1
31	CLA	Y	613	28	1/1/15/20	11/37/115/115	-
31	CLA	3	603	3	1/1/13/20	10/25/103/115	-
40	SQD	a	409	-	-	7/46/66/69	0/1/1/1
31	CLA	5	612	-	1/1/11/20	9/15/93/115	-
31	CLA	r	608	21	1/1/15/20	5/37/115/115	-
46	DGD	c	519	-	-	8/48/88/95	0/2/2/2
31	CLA	11	602	1	1/1/14/20	14/31/109/115	-
31	CLA	13	610	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	13	606	-	3/3/19/26	13/33/131/137	-
39	BCR	B	619	-	-	1/29/63/63	0/2/2/2
31	CLA	1	610	1	1/1/13/20	7/25/103/115	-
31	CLA	R	609	21	1/1/15/20	18/37/115/115	-
31	CLA	a	403	6	1/1/15/20	12/37/115/115	-
32	LHG	r	619	-	-	19/51/51/53	-
30	CHL	g	601	1	3/3/20/26	17/39/137/137	-
31	CLA	6	602	3	1/1/14/20	11/31/109/115	-
39	BCR	c	516	-	-	4/29/63/63	0/2/2/2
31	CLA	A	404	-	1/1/15/20	16/37/115/115	-
30	CHL	12	608	2	3/3/17/26	14/24/122/137	-
30	CHL	N	609	2	3/3/20/26	22/39/137/137	-
39	BCR	D	406	-	-	3/29/63/63	0/2/2/2
41	LMG	c	520	-	-	9/42/62/70	0/1/1/1
31	CLA	c	513	8	1/1/13/20	6/25/103/115	-
32	LHG	6	617	-	-	27/51/51/53	-
31	CLA	c	511	8	1/1/15/20	13/37/115/115	-
30	CHL	4	606	-	2/2/16/26	6/17/115/137	-
31	CLA	N	610	2	1/1/14/20	5/31/109/115	-
39	BCR	C	516	-	-	4/29/63/63	0/2/2/2
43	LNL	C	524	-	-	4/17/17/17	-
43	LNL	W	502	-	-	4/17/17/17	-
30	CHL	1	607	-	3/3/17/26	7/21/119/137	-
30	CHL	3	608	-	3/3/16/26	7/20/118/137	-
46	DGD	c	517	-	-	17/55/95/95	0/2/2/2
34	NEX	N	619	-	-	2/27/83/83	0/3/3/3
31	CLA	r	611	21	1/1/11/20	6/18/96/115	-
32	LHG	l	102	-	-	21/51/51/53	-
31	CLA	C	504	8	1/1/15/20	11/37/115/115	-
31	CLA	5	604	-	1/1/12/20	9/19/97/115	-
43	LNL	W	503	-	-	3/17/17/17	-
31	CLA	S	614	22	1/1/15/20	13/37/115/115	-
33	LUT	S	618	-	-	1/29/67/67	0/2/2/2
49	HEM	F	101	11,10	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	Y	615	-	1/1/13/20	15/27/105/115	-
31	CLA	S	612	22	1/1/11/20	6/13/91/115	-
30	CHL	5	608	-	3/3/16/26	9/20/118/137	-
31	CLA	11	604	-	1/1/11/20	10/15/93/115	-
34	NEX	11	618	-	-	0/6/37/83	0/2/2/3
30	CHL	5	605	2	3/3/16/26	10/15/113/137	-
32	LHG	11	615	31	-	18/53/53/53	-
33	LUT	S	619	-	-	0/29/67/67	0/2/2/2
46	DGD	C	519	-	-	8/48/88/95	0/2/2/2
44	STE	b	622	-	-	9/17/17/17	-
31	CLA	R	601	21	1/1/11/20	8/18/96/115	-
33	LUT	n	618	-	-	0/29/67/67	0/2/2/2
33	LUT	3	619	-	-	0/29/67/67	0/2/2/2
30	CHL	15	605	-	3/3/16/26	8/15/113/137	-
34	NEX	5	616	-	-	2/25/56/83	0/2/2/3
31	CLA	N	611	32	1/1/14/20	10/31/109/115	-
30	CHL	11	601	1	3/3/20/26	15/39/137/137	-
31	CLA	b	616	7	1/1/14/20	14/31/109/115	-
35	XAT	6	620	-	-	0/31/93/93	0/4/4/4
41	LMG	K	102	-	-	12/46/66/70	0/1/1/1
32	LHG	r	621	-	-	20/48/48/53	-
41	LMG	D	410	-	-	6/39/59/70	0/1/1/1
39	BCR	b	618	-	-	0/29/63/63	0/2/2/2
31	CLA	13	613	5	1/1/12/20	8/19/97/115	-
34	NEX	12	616	-	-	2/19/50/83	0/2/2/3
30	CHL	11	608	-	3/3/17/26	11/21/119/137	-
31	CLA	r	609	21	1/1/15/20	17/37/115/115	-
31	CLA	g	610	1	1/1/15/20	9/37/115/115	-
33	LUT	R	615	-	-	0/29/67/67	0/2/2/2
30	CHL	g	606	-	3/3/16/26	4/20/118/137	-
41	LMG	d	415	-	-	12/43/63/70	0/1/1/1
30	CHL	16	601	5	3/3/18/26	14/27/125/137	-
31	CLA	R	608	21	1/1/15/20	7/37/115/115	-
36	3PH	B	624	-	-	6/39/39/49	-
39	BCR	b	619	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	S	611	32	1/1/15/20	15/37/115/115	-
39	BCR	h	102	-	-	2/29/63/63	0/2/2/2
31	CLA	r	614	-	1/1/13/20	13/25/103/115	-
33	LUT	15	615	-	-	1/29/67/67	0/2/2/2
31	CLA	Y	603	28	1/1/14/20	11/31/109/115	-
31	CLA	16	613	5	1/1/12/20	9/19/97/115	-
49	HEM	f	101	11,10	-	4/12/54/54	-
30	CHL	6	605	3	3/3/20/26	14/39/137/137	-
31	CLA	G	610	1	1/1/15/20	7/37/115/115	-
30	CHL	13	601	5	3/3/18/26	15/27/125/137	-
31	CLA	D	405	9	1/1/15/20	16/37/115/115	-
31	CLA	R	614	-	1/1/13/20	10/25/103/115	-
31	CLA	g	612	1	1/1/10/20	3/11/89/115	-
34	NEX	s	620	-	-	2/27/83/83	0/3/3/3
43	LNL	c	523	-	-	4/17/17/17	-
31	CLA	S	602	22	1/1/15/20	12/37/115/115	-
33	LUT	2	615	-	-	1/29/67/67	0/2/2/2
39	BCR	B	618	-	-	0/29/63/63	0/2/2/2
33	LUT	G	616	-	-	2/29/67/67	0/2/2/2
33	LUT	5	615	-	-	2/29/67/67	0/2/2/2
31	CLA	5	610	2	1/1/12/20	10/19/97/115	-
43	LNL	c	524	-	-	4/17/17/17	-
32	LHG	s	617	31	-	21/49/49/53	-
30	CHL	G	607	-	3/3/16/26	7/20/118/137	-
31	CLA	b	610	-	1/1/15/20	17/37/115/115	-
43	LNL	h	101	-	-	3/17/17/17	-
31	CLA	s	610	22	1/1/15/20	15/37/115/115	-
31	CLA	12	609	2	1/1/13/20	14/25/103/115	-
34	NEX	1	618	-	-	0/6/37/83	0/2/2/3
39	BCR	J	101	-	-	6/29/63/63	0/2/2/2
30	CHL	Y	608	-	3/3/15/26	4/13/111/137	-
43	LNL	A	412	-	-	0/17/17/17	-
32	LHG	r	618	31	-	17/42/42/53	-
30	CHL	G	605	1	3/3/16/26	9/18/116/137	-
33	LUT	N	618	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	s	616	-	-	10/37/57/70	0/1/1/1
30	CHL	n	609	2	3/3/20/26	16/39/137/137	-
30	CHL	5	607	-	3/3/18/26	8/27/125/137	-
30	CHL	11	607	-	3/3/16/26	10/15/113/137	-
31	CLA	c	512	8	1/1/15/20	16/37/115/115	-
31	CLA	14	611	32	1/1/14/20	13/31/109/115	-
41	LMG	d	411	-	-	4/36/36/70	-
33	LUT	14	616	-	-	0/29/67/67	0/2/2/2
35	XAT	R	616	-	-	0/31/93/93	0/4/4/4
31	CLA	4	612	1	1/1/11/20	7/15/93/115	-
30	CHL	s	607	-	3/3/15/26	7/12/110/137	-
31	CLA	r	610	32	1/1/14/20	9/31/109/115	-
31	CLA	g	611	32	1/1/15/20	13/37/115/115	-
31	CLA	r	612	21	1/1/12/20	7/19/97/115	-
41	LMG	A	409	-	-	6/50/70/70	0/1/1/1
31	CLA	R	603	21	1/1/15/20	18/37/115/115	-
33	LUT	11	616	-	-	1/29/67/67	0/2/2/2
33	LUT	12	614	-	-	5/29/67/67	0/2/2/2
36	3PH	8	201	-	-	6/49/49/49	-
34	NEX	g	618	-	-	2/27/83/83	0/3/3/3
33	LUT	1	617	-	-	0/29/67/67	0/2/2/2
33	LUT	r	615	-	-	0/29/67/67	0/2/2/2
34	NEX	n	619	-	-	2/27/83/83	0/3/3/3
31	CLA	R	611	21	1/1/11/20	7/18/96/115	-
31	CLA	N	602	2	1/1/15/20	16/37/115/115	-
39	BCR	c	515	-	-	2/29/63/63	0/2/2/2
32	LHG	A	411	-	-	20/53/53/53	-
41	LMG	d	410	-	-	8/39/59/70	0/1/1/1
34	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
31	CLA	3	602	3	1/1/14/20	13/31/109/115	-
31	CLA	n	614	2	1/1/11/20	9/13/91/115	-
30	CHL	14	608	-	3/3/17/26	14/21/119/137	-
43	LNL	C	523	-	-	4/17/17/17	-
32	LHG	1	615	31	-	14/47/47/53	-
33	LUT	2	614	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	B	621	-	-	7/44/64/70	0/1/1/1
39	BCR	j	101	-	-	6/29/63/63	0/2/2/2
30	CHL	16	607	-	3/3/19/26	17/33/131/137	-
31	CLA	c	509	8	1/1/14/20	12/31/109/115	-
31	CLA	3	614	3	1/1/12/20	9/19/97/115	-
42	PL9	D	407	-	-	12/53/73/73	0/1/1/1
32	LHG	d	413	-	-	17/53/53/53	-
31	CLA	12	603	-	1/1/13/20	11/25/103/115	-
31	CLA	B	601	-	1/1/13/20	12/25/103/115	-
32	LHG	6	616	31	-	16/48/48/53	-
43	LNL	r	620	-	-	8/17/17/17	-
31	CLA	15	610	-	1/1/11/20	4/13/91/115	-
30	CHL	4	609	-	3/3/20/26	25/39/137/137	-
31	CLA	B	606	7	1/1/15/20	18/37/115/115	-
31	CLA	6	610	3	1/1/14/20	15/31/109/115	-
30	CHL	r	606	21	3/3/20/26	20/39/137/137	-
34	NEX	G	618	-	-	2/27/79/83	0/3/3/3
31	CLA	C	509	8	1/1/14/20	12/31/109/115	-
31	CLA	16	610	-	1/1/15/20	9/37/115/115	-
32	LHG	L	102	-	-	22/51/51/53	-
31	CLA	C	511	8	1/1/15/20	12/37/115/115	-
30	CHL	14	607	-	3/3/16/26	8/20/118/137	-
31	CLA	16	615	-	1/1/11/20	4/13/91/115	-
34	NEX	3	621	-	-	2/27/83/83	0/3/3/3
31	CLA	1	614	1	1/1/11/20	7/15/93/115	-
30	CHL	G	606	-	3/3/16/26	2/17/115/137	-
31	CLA	11	611	32	1/1/12/20	8/19/97/115	-
30	CHL	g	607	-	3/3/16/26	8/20/118/137	-
30	CHL	2	609	2	3/3/20/26	24/39/137/137	-
44	STE	B	623	-	-	6/17/17/17	-
31	CLA	s	609	22	1/1/13/20	10/25/103/115	-
43	LNL	X	201	-	-	5/17/17/17	-
30	CHL	3	605	3	3/3/20/26	16/39/137/137	-
41	LMG	b	621	-	-	7/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	r	613	21	1/1/15/20	12/37/115/115	-
43	LNL	y	619	-	-	5/17/17/17	-
36	3PH	B	620	-	-	10/49/49/49	-
40	SQD	l	101	-	-	9/45/65/69	0/1/1/1
41	LMG	c	522	-	-	4/50/70/70	0/1/1/1
30	CHL	Y	609	28	3/3/20/26	18/39/137/137	-
30	CHL	N	601	2	3/3/17/26	11/24/122/137	-
30	CHL	N	606	-	3/3/19/26	14/33/131/137	-
31	CLA	B	602	7	1/1/15/20	10/37/115/115	-
42	PL9	d	407	-	-	12/53/73/73	0/1/1/1
30	CHL	5	609	2	3/3/20/26	14/39/137/137	-
32	LHG	a	414	-	-	21/47/47/53	-
31	CLA	4	603	1	1/1/13/20	5/25/103/115	-
39	BCR	b	617	-	-	2/29/63/63	0/2/2/2
31	CLA	s	614	22	1/1/15/20	17/37/115/115	-
43	LNL	H	101	-	-	3/17/17/17	-
32	LHG	c	521	-	-	19/46/46/53	-
30	CHL	4	601	1	3/3/19/26	15/33/131/137	-
31	CLA	G	614	1	1/1/11/20	5/18/96/115	-
31	CLA	R	610	32	1/1/14/20	18/31/109/115	-
41	LMG	C	522	-	-	4/50/70/70	0/1/1/1
31	CLA	2	610	2	1/1/12/20	6/19/97/115	-
40	SQD	A	408	-	-	7/46/66/69	0/1/1/1
31	CLA	12	604	-	1/1/13/20	7/25/103/115	-
31	CLA	b	608	7	1/1/15/20	16/37/115/115	-
32	LHG	C	521	-	-	18/46/46/53	-
32	LHG	D	408	-	-	16/53/53/53	-
33	LUT	15	614	-	-	5/29/67/67	0/2/2/2
31	CLA	S	610	22	1/1/15/20	15/37/115/115	-
30	CHL	S	606	22	3/3/20/26	19/39/137/137	-
30	CHL	1	606	-	3/3/16/26	8/17/115/137	-
31	CLA	12	602	2	1/1/14/20	14/31/109/115	-
31	CLA	c	507	8	1/1/15/20	20/37/115/115	-
31	CLA	Y	612	28	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	j	102	-	-	10/46/66/70	0/1/1/1
31	CLA	R	602	21	1/1/15/20	13/37/115/115	-
30	CHL	2	607	-	3/3/18/26	8/27/125/137	-
31	CLA	2	602	2	1/1/13/20	14/25/103/115	-
40	SQD	D	411	-	-	11/49/69/69	0/1/1/1
31	CLA	15	609	2	1/1/13/20	11/25/103/115	-
31	CLA	14	614	1	1/1/11/20	9/18/96/115	-
31	CLA	C	507	8	1/1/15/20	19/37/115/115	-
32	LHG	d	408	-	-	19/53/53/53	-
31	CLA	b	602	7	1/1/15/20	10/37/115/115	-
31	CLA	b	606	7	1/1/15/20	16/37/115/115	-
30	CHL	g	608	-	3/3/17/26	8/23/121/137	-
33	LUT	11	617	-	-	0/29/67/67	0/2/2/2
31	CLA	N	613	2	1/1/13/20	15/25/103/115	-
31	CLA	n	603	2	1/1/14/20	14/31/109/115	-
30	CHL	3	606	-	3/3/18/26	8/27/125/137	-
31	CLA	G	611	32	1/1/15/20	11/37/115/115	-
30	CHL	13	609	-	3/3/19/26	16/33/131/137	-
31	CLA	n	602	2	1/1/15/20	20/37/115/115	-
31	CLA	3	610	3	1/1/14/20	18/31/109/115	-
46	DGD	C	517	-	-	17/55/95/95	0/2/2/2
31	CLA	16	611	32	1/1/15/20	13/37/115/115	-
39	BCR	d	406	-	-	3/29/63/63	0/2/2/2
31	CLA	b	603	7	1/1/15/20	12/37/115/115	-
31	CLA	c	502	8	1/1/15/20	16/37/115/115	-
30	CHL	12	605	-	3/3/16/26	8/15/113/137	-
31	CLA	A	403	-	1/1/15/20	17/37/115/115	-
30	CHL	5	606	-	3/3/16/26	9/15/113/137	-
30	CHL	14	601	1	3/3/20/26	20/39/137/137	-
46	DGD	W	501	-	-	9/41/61/95	0/1/1/2
42	PL9	A	410	-	-	9/53/73/73	0/1/1/1
43	LNL	w	503	-	-	4/17/17/17	-
33	LUT	y	623	-	-	1/29/67/67	0/2/2/2
31	CLA	C	510	8	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	a	413	-	-	13/48/48/53	-
31	CLA	4	610	1	1/1/15/20	16/37/115/115	-
33	LUT	1	616	-	-	0/29/67/67	0/2/2/2
32	LHG	a	401	-	-	12/53/53/53	-
30	CHL	3	607	-	3/3/20/26	20/39/137/137	-
31	CLA	c	506	8	1/1/15/20	11/37/115/115	-
30	CHL	6	607	-	3/3/20/26	20/39/137/137	-
31	CLA	b	605	7	1/1/15/20	13/37/115/115	-
31	CLA	c	504	8	1/1/15/20	11/37/115/115	-
34	NEX	6	621	-	-	2/27/83/83	0/3/3/3
31	CLA	1	604	-	1/1/12/20	5/19/97/115	-
31	CLA	11	614	-	1/1/11/20	9/18/96/115	-
30	CHL	y	608	-	3/3/15/26	5/13/111/137	-
33	LUT	6	618	-	-	0/29/67/67	0/2/2/2
31	CLA	11	612	1	1/1/10/20	5/11/89/115	-
31	CLA	N	615	2	1/1/11/20	5/16/94/115	-
31	CLA	G	604	-	1/1/12/20	7/19/97/115	-
31	CLA	C	506	8	1/1/15/20	11/37/115/115	-
31	CLA	Y	602	28	1/1/15/20	14/37/115/115	-
31	CLA	13	604	-	1/1/13/20	10/25/103/115	-
32	LHG	Y	618	-	-	30/51/51/53	-
32	LHG	A	415	-	-	13/53/53/53	-
33	LUT	12	615	-	-	1/29/67/67	0/2/2/2
33	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
43	LNL	I	101	-	-	4/17/17/17	-
46	DGD	c	518	-	-	5/47/87/95	0/2/2/2
33	LUT	4	616	-	-	0/29/67/67	0/2/2/2
31	CLA	1	612	1	1/1/11/20	7/15/93/115	-
31	CLA	Y	614	28	1/1/11/20	5/18/96/115	-
31	CLA	y	603	28	1/1/14/20	13/31/109/115	-
31	CLA	d	404	9	1/1/15/20	16/37/115/115	-
31	CLA	6	603	3	1/1/13/20	9/25/103/115	-
32	LHG	14	615	31	-	25/53/53/53	-
31	CLA	B	610	-	1/1/15/20	17/37/115/115	-
33	LUT	16	617	-	-	1/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	g	615	31	-	23/53/53/53	-
31	CLA	4	611	32	1/1/12/20	6/19/97/115	-
32	LHG	3	616	31	-	12/48/48/53	-
50	PAM	N	621	-	-	3/15/15/15	-
31	CLA	16	614	5	1/1/11/20	8/13/91/115	-
31	CLA	G	613	1	1/1/15/20	16/37/115/115	-
31	CLA	16	612	5	1/1/11/20	3/13/91/115	-
31	CLA	14	613	1	1/1/13/20	13/25/103/115	-
30	CHL	s	601	22	3/3/16/26	7/15/113/137	-
46	DGD	w	502	-	-	8/35/55/95	0/1/1/2
31	CLA	g	613	1	1/1/15/20	12/37/115/115	-
31	CLA	S	609	22	1/1/13/20	6/25/103/115	-
39	BCR	c	526	-	-	2/29/63/63	0/2/2/2
32	LHG	R	621	-	-	16/48/48/53	-
30	CHL	11	606	-	3/3/16/26	6/17/115/137	-
31	CLA	12	610	-	1/1/11/20	5/13/91/115	-
30	CHL	1	605	1	3/3/16/26	7/15/113/137	-
31	CLA	15	604	-	1/1/13/20	5/25/103/115	-
33	LUT	14	617	-	-	0/29/67/67	0/2/2/2
31	CLA	R	613	21	1/1/14/20	12/31/109/115	-
31	CLA	n	610	2	1/1/14/20	11/31/109/115	-
34	NEX	r	617	-	-	3/27/83/83	0/3/3/3
30	CHL	n	606	-	3/3/19/26	15/33/131/137	-
39	BCR	C	526	-	-	1/29/63/63	0/2/2/2
31	CLA	1	611	32	1/1/12/20	8/19/97/115	-
31	CLA	s	613	22	1/1/11/20	6/18/96/115	-
31	CLA	C	513	8	1/1/13/20	6/25/103/115	-
40	SQD	L	101	-	-	13/45/65/69	0/1/1/1
31	CLA	13	602	5	1/1/15/20	19/37/115/115	-
31	CLA	15	613	-	1/1/11/20	5/13/91/115	-
30	CHL	12	607	-	3/3/16/26	11/20/118/137	-
31	CLA	14	604	-	1/1/13/20	14/25/103/115	-
33	LUT	6	619	-	-	0/29/67/67	0/2/2/2
36	3PH	T	101	-	-	10/49/49/49	-
31	CLA	s	603	22	1/1/10/20	5/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	g	604	-	1/1/12/20	8/19/97/115	-
30	CHL	16	606	-	3/3/19/26	15/33/131/137	-
31	CLA	y	613	28	1/1/15/20	13/37/115/115	-
31	CLA	s	605	22	1/1/12/20	7/19/97/115	-
31	CLA	c	503	8	1/1/15/20	11/37/115/115	-
31	CLA	s	611	32	1/1/15/20	17/37/115/115	-
30	CHL	16	608	-	3/3/16/26	7/20/118/137	-
41	LMG	B	622	-	-	6/43/63/70	0/1/1/1
39	BCR	C	515	-	-	2/29/63/63	0/2/2/2
33	LUT	13	618	-	-	0/29/67/67	0/2/2/2
30	CHL	Y	605	28	3/3/18/26	13/27/125/137	-
30	CHL	1	609	-	3/3/18/26	15/27/125/137	-
30	CHL	Y	607	-	3/3/20/26	16/39/137/137	-
31	CLA	2	613	2	1/1/11/20	7/16/94/115	-
31	CLA	y	614	28	1/1/11/20	6/18/96/115	-
31	CLA	5	613	2	1/1/12/20	8/19/97/115	-
31	CLA	11	613	1	1/1/13/20	13/25/103/115	-
32	LHG	y	616	31	-	18/53/53/53	-
36	3PH	7	201	-	-	5/49/49/49	-
31	CLA	6	614	3	1/1/12/20	11/19/97/115	-
30	CHL	14	606	-	3/3/16/26	5/17/115/137	-
31	CLA	B	605	7	1/1/15/20	13/37/115/115	-
31	CLA	C	514	8	1/1/15/20	16/37/115/115	-
31	CLA	G	602	1	1/1/15/20	15/37/115/115	-
32	LHG	S	617	31	-	24/49/49/53	-
31	CLA	S	605	22	1/1/12/20	9/19/97/115	-
31	CLA	B	611	7	1/1/15/20	13/37/115/115	-
31	CLA	b	615	7	1/1/15/20	12/37/115/115	-
30	CHL	s	608	-	3/3/16/26	7/19/117/137	-
31	CLA	5	603	2	1/1/13/20	9/25/103/115	-
31	CLA	11	603	-	1/1/13/20	9/25/103/115	-
31	CLA	s	615	22	1/1/11/20	8/16/94/115	-
43	LNL	R	620	-	-	6/17/17/17	-
31	CLA	6	613	3	1/1/13/20	11/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	Y	617	-	-	25/51/51/53	-
41	LMG	v	101	-	-	11/46/66/70	0/1/1/1
31	CLA	Y	610	28	1/1/15/20	7/37/115/115	-
31	CLA	y	604	-	1/1/13/20	8/25/103/115	-
30	CHL	R	606	21	3/3/20/26	19/39/137/137	-
31	CLA	N	614	2	1/1/11/20	5/13/91/115	-
30	CHL	15	608	2	3/3/19/26	12/33/131/137	-
31	CLA	5	602	2	1/1/13/20	14/25/103/115	-
40	SQD	d	414	-	-	7/41/61/69	0/1/1/1
31	CLA	y	615	-	1/1/13/20	16/27/105/115	-
30	CHL	2	601	2	2/2/16/26	4/17/115/137	-
35	XAT	G	619	-	-	0/31/93/93	0/4/4/4
30	CHL	g	609	1	3/3/20/26	14/39/137/137	-
30	CHL	13	605	5	3/3/18/26	10/27/125/137	-
31	CLA	n	615	2	1/1/11/20	5/16/94/115	-
34	NEX	15	616	-	-	2/19/50/83	0/2/2/3
30	CHL	S	608	-	3/3/16/26	10/19/117/137	-
32	LHG	Y	616	31	-	14/53/53/53	-
41	LMG	S	616	-	-	4/37/57/70	0/1/1/1
31	CLA	6	604	-	1/1/15/20	21/37/115/115	-
31	CLA	y	612	28	1/1/15/20	16/37/115/115	-
31	CLA	6	615	3	1/1/12/20	11/19/97/115	-
31	CLA	y	611	32	1/1/15/20	10/37/115/115	-
31	CLA	16	604	-	1/1/13/20	6/25/103/115	-
32	LHG	a	411	-	-	15/53/53/53	-
43	LNL	i	101	-	-	4/17/17/17	-
31	CLA	6	611	32	1/1/15/20	13/37/115/115	-
31	CLA	13	603	-	1/1/14/20	13/31/109/115	-
31	CLA	B	609	7	1/1/15/20	20/37/115/115	-
32	LHG	n	616	31	-	29/53/53/53	-
35	XAT	14	619	-	-	0/31/93/93	0/4/4/4
31	CLA	3	612	3	1/1/15/20	17/37/115/115	-
30	CHL	2	606	-	3/3/16/26	8/15/113/137	-
31	CLA	6	612	3	1/1/13/20	12/25/103/115	-
35	XAT	g	619	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	NEX	4	618	-	-	0/6/37/83	0/2/2/3
38	PHO	a	405	-	-	7/37/103/103	0/5/6/6
30	CHL	15	607	-	3/3/16/26	10/20/118/137	-
33	LUT	g	617	-	-	0/29/67/67	0/2/2/2
31	CLA	2	603	2	1/1/13/20	10/25/103/115	-
38	PHO	A	405	-	-	8/37/103/103	0/5/6/6
30	CHL	2	608	-	3/3/16/26	7/20/118/137	-
31	CLA	14	603	-	1/1/13/20	11/25/103/115	-
30	CHL	G	609	1	3/3/20/26	12/39/137/137	-
41	LMG	w	501	-	-	6/50/70/70	0/1/1/1
31	CLA	s	604	-	1/1/15/20	16/37/115/115	-
30	CHL	y	607	-	3/3/20/26	15/39/137/137	-
43	LNL	y	620	-	-	5/17/17/17	-
30	CHL	13	608	-	3/3/16/26	7/20/118/137	-
31	CLA	R	604	-	1/1/11/20	4/17/95/115	-
32	LHG	16	616	31	-	26/44/44/53	-
43	LNL	Y	619	-	-	3/17/17/17	-
31	CLA	D	404	9	1/1/15/20	14/37/115/115	-
31	CLA	4	613	1	1/1/13/20	8/25/103/115	-
30	CHL	N	607	-	3/3/20/26	15/39/137/137	-
31	CLA	A	402	6	1/1/15/20	12/37/115/115	-
30	CHL	4	608	-	3/3/16/26	12/20/118/137	-
31	CLA	B	607	-	1/1/15/20	10/37/115/115	-
32	LHG	R	618	31	-	14/42/42/53	-
30	CHL	16	605	5	3/3/18/26	9/27/125/137	-
31	CLA	R	612	21	1/1/12/20	8/19/97/115	-
32	LHG	A	414	-	-	22/47/47/53	-
33	LUT	N	617	-	-	0/29/67/67	0/2/2/2
30	CHL	S	607	-	3/3/15/26	4/12/110/137	-
31	CLA	Y	611	32	1/1/15/20	10/37/115/115	-
31	CLA	15	611	-	1/1/11/20	6/13/91/115	-
39	BCR	a	408	-	-	1/29/63/63	0/2/2/2
31	CLA	a	407	6	1/1/13/20	8/25/103/115	-
35	XAT	11	619	-	-	0/31/93/93	0/4/4/4
31	CLA	N	612	2	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	S	613	22	1/1/11/20	6/18/96/115	-
32	LHG	d	409	-	-	16/43/43/53	-
31	CLA	y	602	28	1/1/14/20	12/31/109/115	-
30	CHL	11	605	-	2/2/16/26	9/18/116/137	-
30	CHL	G	601	1	3/3/20/26	14/39/137/137	-
31	CLA	B	614	7	1/1/15/20	18/37/115/115	-
30	CHL	14	605	1	3/3/16/26	11/18/116/137	-
30	CHL	n	601	2	3/3/17/26	11/23/121/137	-

The worst 5 of 3421 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	610	CLA	MG-NA	5.50	2.19	2.06
30	13	601	CHL	CMC-C2C	5.50	1.56	1.45
30	4	608	CHL	CMC-C2C	5.48	1.56	1.45
30	16	601	CHL	CMC-C2C	5.48	1.56	1.45
30	3	609	CHL	CMC-C2C	5.48	1.56	1.45

The worst 5 of 4054 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	15	605	CHL	C4A-NA-C1A	11.53	111.89	106.71
31	c	510	CLA	C4A-NA-C1A	11.50	111.88	106.71
31	C	510	CLA	C4A-NA-C1A	11.47	111.86	106.71
31	B	613	CLA	C4A-NA-C1A	11.42	111.84	106.71
31	b	613	CLA	C4A-NA-C1A	11.38	111.82	106.71

5 of 621 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	1	601	CHL	NC
30	1	601	CHL	ND
30	1	601	CHL	NA
30	1	605	CHL	NC
30	1	605	CHL	ND

5 of 5945 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
30	1	605	CHL	CHA-CBD-CGD-O1D
30	1	606	CHL	C1C-C2C-CMC-OMC
30	1	606	CHL	C3C-C2C-CMC-OMC
30	1	608	CHL	O1A-CGA-O2A-C1

There are no ring outliers.

521 monomers are involved in 1093 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	n	607	CHL	8	0
31	c	505	CLA	2	0
31	B	612	CLA	4	0
32	y	618	LHG	2	0
31	b	609	CLA	2	0
31	C	503	CLA	1	0
40	d	412	SQD	3	0
32	N	616	LHG	2	0
33	Y	622	LUT	1	0
30	y	601	CHL	3	0
31	12	612	CLA	27	0
30	R	605	CHL	3	0
31	C	502	CLA	3	0
31	3	604	CLA	1	0
43	y	621	LNL	1	0
31	C	505	CLA	3	0
31	b	607	CLA	3	0
30	3	609	CHL	1	0
30	s	606	CHL	7	0
31	15	603	CLA	12	0
31	S	604	CLA	4	0
30	n	608	CHL	2	0
31	N	604	CLA	3	0
38	a	406	PHO	1	0
35	3	620	XAT	3	0
31	d	405	CLA	2	0
31	r	602	CLA	5	0
35	r	616	XAT	1	0
31	4	604	CLA	2	0
30	4	605	CHL	1	0
31	b	614	CLA	2	0
32	G	615	LHG	2	0
30	N	608	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	y	605	CHL	2	0
31	3	613	CLA	1	0
30	14	609	CHL	2	0
39	A	407	BCR	2	0
30	16	609	CHL	1	0
38	D	402	PHO	4	0
31	13	611	CLA	1	0
31	d	402	CLA	5	0
31	13	615	CLA	1	0
33	g	616	LUT	3	0
30	12	606	CHL	1	0
30	2	605	CHL	1	0
33	5	614	LUT	2	0
42	a	410	PL9	4	0
32	s	621	LHG	4	0
31	11	610	CLA	3	0
33	n	617	LUT	7	0
31	r	603	CLA	3	0
30	3	601	CHL	1	0
31	14	612	CLA	3	0
31	c	508	CLA	1	0
34	R	617	NEX	1	0
34	S	620	NEX	1	0
31	y	610	CLA	2	0
39	H	103	BCR	3	0
30	6	606	CHL	1	0
30	y	609	CHL	1	0
31	b	611	CLA	3	0
33	y	622	LUT	4	0
31	B	604	CLA	3	0
31	S	615	CLA	1	0
30	6	608	CHL	4	0
36	b	623	3PH	1	0
30	r	605	CHL	2	0
31	r	601	CLA	2	0
31	s	612	CLA	2	0
32	4	615	LHG	2	0
31	B	613	CLA	3	0
32	A	413	LHG	2	0
30	11	609	CHL	2	0
31	15	612	CLA	8	0
33	s	619	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	603	CLA	1	0
30	g	605	CHL	1	0
31	n	612	CLA	2	0
31	n	613	CLA	4	0
31	c	514	CLA	3	0
31	1	602	CLA	2	0
31	14	610	CLA	5	0
31	2	612	CLA	1	0
30	13	607	CHL	3	0
32	S	621	LHG	3	0
31	b	612	CLA	4	0
41	b	620	LMG	1	0
46	C	518	DGD	6	0
31	5	611	CLA	2	0
31	b	613	CLA	3	0
31	4	602	CLA	1	0
43	Y	620	LNL	1	0
31	A	406	CLA	1	0
31	B	608	CLA	1	0
30	6	609	CHL	1	0
33	3	618	LUT	2	0
30	Y	606	CHL	4	0
30	15	606	CHL	1	0
31	14	602	CLA	7	0
30	4	607	CHL	2	0
50	n	620	PAM	1	0
31	c	510	CLA	1	0
31	g	602	CLA	1	0
30	N	605	CHL	2	0
31	1	613	CLA	1	0
30	n	605	CHL	3	0
31	1	603	CLA	2	0
31	n	604	CLA	2	0
31	12	611	CLA	5	0
30	G	608	CHL	4	0
31	B	615	CLA	3	0
33	13	617	LUT	2	0
32	D	409	LHG	2	0
31	n	611	CLA	3	0
31	13	614	CLA	4	0
31	2	604	CLA	3	0
31	S	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	604	CLA	4	0
31	b	601	CLA	2	0
31	s	602	CLA	2	0
32	13	616	LHG	3	0
43	x	201	LNL	1	0
32	R	619	LHG	4	0
30	Y	601	CHL	1	0
31	C	512	CLA	4	0
33	4	617	LUT	2	0
33	s	618	LUT	7	0
31	15	602	CLA	6	0
31	16	603	CLA	5	0
32	3	617	LHG	2	0
30	R	607	CHL	2	0
31	g	603	CLA	2	0
41	C	520	LMG	1	0
30	1	601	CHL	3	0
30	1	608	CHL	4	0
41	D	414	LMG	1	0
31	16	602	CLA	3	0
31	B	616	CLA	2	0
30	r	607	CHL	1	0
39	B	617	BCR	3	0
33	16	618	LUT	4	0
41	J	102	LMG	5	0
31	Y	613	CLA	3	0
31	r	608	CLA	3	0
46	c	519	DGD	3	0
31	11	602	CLA	5	0
31	13	610	CLA	3	0
30	13	606	CHL	2	0
39	B	619	BCR	1	0
31	1	610	CLA	8	0
31	R	609	CLA	1	0
31	a	403	CLA	5	0
32	r	619	LHG	4	0
30	g	601	CHL	1	0
31	A	404	CLA	1	0
30	12	608	CHL	1	0
30	N	609	CHL	1	0
39	D	406	BCR	2	0
41	c	520	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	513	CLA	2	0
32	6	617	LHG	3	0
31	c	511	CLA	1	0
30	4	606	CHL	4	0
31	N	610	CLA	3	0
43	W	502	LNL	1	0
30	1	607	CHL	3	0
30	3	608	CHL	1	0
46	c	517	DGD	2	0
34	N	619	NEX	1	0
31	r	611	CLA	2	0
32	l	102	LHG	4	0
31	C	504	CLA	4	0
31	5	604	CLA	2	0
43	W	503	LNL	1	0
31	S	614	CLA	2	0
33	S	618	LUT	4	0
49	F	101	HEM	2	0
31	Y	615	CLA	2	0
31	S	612	CLA	2	0
30	5	608	CHL	3	0
31	11	604	CLA	2	0
30	5	605	CHL	2	0
32	11	615	LHG	3	0
33	S	619	LUT	4	0
46	C	519	DGD	3	0
31	R	601	CLA	1	0
33	n	618	LUT	1	0
33	3	619	LUT	1	0
30	15	605	CHL	3	0
31	N	611	CLA	1	0
30	11	601	CHL	1	0
31	b	616	CLA	3	0
35	6	620	XAT	4	0
41	K	102	LMG	3	0
32	r	621	LHG	4	0
41	D	410	LMG	1	0
39	b	618	BCR	1	0
31	13	613	CLA	2	0
34	12	616	NEX	2	0
30	11	608	CHL	3	0
31	r	609	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g	610	CLA	2	0
33	R	615	LUT	1	0
30	g	606	CHL	2	0
41	d	415	LMG	1	0
30	16	601	CHL	2	0
31	R	608	CLA	2	0
36	B	624	3PH	2	0
39	b	619	BCR	1	0
31	S	611	CLA	3	0
39	h	102	BCR	4	0
31	r	614	CLA	3	0
33	15	615	LUT	4	0
31	Y	603	CLA	1	0
31	16	613	CLA	3	0
49	f	101	HEM	2	0
30	6	605	CHL	5	0
31	G	610	CLA	4	0
30	13	601	CHL	2	0
31	D	405	CLA	2	0
31	R	614	CLA	2	0
34	s	620	NEX	1	0
43	c	523	LNL	1	0
31	S	602	CLA	1	0
33	2	615	LUT	4	0
39	B	618	BCR	3	0
33	G	616	LUT	3	0
33	5	615	LUT	1	0
31	5	610	CLA	3	0
32	s	617	LHG	3	0
30	G	607	CHL	2	0
31	b	610	CLA	6	0
43	h	101	LNL	2	0
31	s	610	CLA	3	0
31	12	609	CLA	13	0
39	J	101	BCR	3	0
32	r	618	LHG	3	0
30	G	605	CHL	1	0
33	N	618	LUT	1	0
41	s	616	LMG	2	0
30	n	609	CHL	1	0
30	5	607	CHL	1	0
30	11	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c	512	CLA	3	0
31	14	611	CLA	3	0
41	d	411	LMG	2	0
33	14	616	LUT	4	0
35	R	616	XAT	2	0
31	4	612	CLA	1	0
30	s	607	CHL	1	0
31	r	610	CLA	4	0
31	r	612	CLA	1	0
41	A	409	LMG	1	0
31	R	603	CLA	6	0
33	11	616	LUT	5	0
33	12	614	LUT	33	0
36	8	201	3PH	2	0
33	1	617	LUT	2	0
33	r	615	LUT	4	0
34	n	619	NEX	1	0
31	N	602	CLA	2	0
39	c	515	BCR	1	0
32	A	411	LHG	2	0
41	d	410	LMG	1	0
34	Y	623	NEX	1	0
31	3	602	CLA	2	0
31	n	614	CLA	1	0
30	14	608	CHL	1	0
43	C	523	LNL	1	0
32	1	615	LHG	1	0
33	2	614	LUT	5	0
41	B	621	LMG	2	0
39	j	101	BCR	3	0
30	16	607	CHL	2	0
31	c	509	CLA	2	0
31	3	614	CLA	3	0
42	D	407	PL9	2	0
32	d	413	LHG	1	0
31	12	603	CLA	3	0
31	B	601	CLA	2	0
32	6	616	LHG	2	0
30	4	609	CHL	4	0
31	B	606	CLA	3	0
31	6	610	CLA	4	0
30	r	606	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	G	618	NEX	1	0
31	C	509	CLA	2	0
31	16	610	CLA	3	0
32	L	102	LHG	4	0
31	C	511	CLA	2	0
30	14	607	CHL	1	0
31	16	615	CLA	4	0
34	3	621	NEX	3	0
30	G	606	CHL	1	0
31	11	611	CLA	1	0
30	g	607	CHL	2	0
30	2	609	CHL	7	0
44	B	623	STE	1	0
31	s	609	CLA	2	0
43	X	201	LNL	1	0
30	3	605	CHL	4	0
41	b	621	LMG	1	0
31	r	613	CLA	2	0
43	y	619	LNL	3	0
36	B	620	3PH	5	0
40	l	101	SQD	2	0
41	c	522	LMG	1	0
30	Y	609	CHL	1	0
30	N	601	CHL	1	0
30	N	606	CHL	3	0
31	B	602	CLA	3	0
42	d	407	PL9	2	0
30	5	609	CHL	2	0
32	a	414	LHG	3	0
31	4	603	CLA	1	0
39	b	617	BCR	3	0
31	s	614	CLA	1	0
43	H	101	LNL	4	0
32	c	521	LHG	3	0
30	4	601	CHL	4	0
31	R	610	CLA	2	0
41	C	522	LMG	1	0
31	2	610	CLA	2	0
31	12	604	CLA	5	0
31	b	608	CLA	1	0
32	C	521	LHG	4	0
32	D	408	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	15	614	LUT	9	0
31	S	610	CLA	4	0
30	S	606	CHL	4	0
30	1	606	CHL	2	0
31	12	602	CLA	7	0
31	c	507	CLA	3	0
31	Y	612	CLA	4	0
41	j	102	LMG	5	0
31	R	602	CLA	5	0
31	2	602	CLA	2	0
40	D	411	SQD	2	0
31	C	507	CLA	1	0
32	d	408	LHG	3	0
31	b	602	CLA	4	0
31	b	606	CLA	1	0
30	g	608	CHL	4	0
33	11	617	LUT	2	0
31	N	613	CLA	2	0
31	n	603	CLA	1	0
30	3	606	CHL	2	0
31	G	611	CLA	1	0
30	13	609	CHL	4	0
31	n	602	CLA	4	0
31	3	610	CLA	2	0
46	C	517	DGD	2	0
31	16	611	CLA	2	0
39	d	406	BCR	1	0
31	c	502	CLA	4	0
30	12	605	CHL	4	0
31	A	403	CLA	3	0
30	14	601	CHL	3	0
46	W	501	DGD	4	0
42	A	410	PL9	2	0
43	w	503	LNL	1	0
33	y	623	LUT	2	0
31	C	510	CLA	1	0
32	a	413	LHG	2	0
31	4	610	CLA	3	0
33	1	616	LUT	4	0
32	a	401	LHG	2	0
30	3	607	CHL	3	0
31	c	506	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	6	607	CHL	5	0
31	b	605	CLA	4	0
31	c	504	CLA	3	0
34	6	621	NEX	4	0
31	1	604	CLA	3	0
33	6	618	LUT	3	0
31	11	612	CLA	3	0
31	N	615	CLA	1	0
31	G	604	CLA	2	0
31	C	506	CLA	3	0
31	Y	602	CLA	5	0
31	13	604	CLA	1	0
32	Y	618	LHG	4	0
32	A	415	LHG	2	0
33	12	615	LUT	2	0
33	Y	621	LUT	3	0
46	c	518	DGD	5	0
33	4	616	LUT	5	0
31	1	612	CLA	1	0
31	Y	614	CLA	2	0
31	y	603	CLA	1	0
31	d	404	CLA	3	0
31	6	603	CLA	1	0
32	14	615	LHG	3	0
31	B	610	CLA	4	0
33	16	617	LUT	2	0
32	g	615	LHG	5	0
32	3	616	LHG	1	0
50	N	621	PAM	1	0
31	16	614	CLA	2	0
31	G	613	CLA	1	0
31	14	613	CLA	3	0
46	w	502	DGD	2	0
31	g	613	CLA	3	0
31	S	609	CLA	1	0
39	c	526	BCR	3	0
32	R	621	LHG	3	0
30	11	606	CHL	1	0
30	1	605	CHL	1	0
31	15	604	CLA	7	0
33	14	617	LUT	1	0
31	R	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	n	610	CLA	4	0
34	r	617	NEX	1	0
30	n	606	CHL	2	0
39	C	526	BCR	3	0
31	l	611	CLA	1	0
31	s	613	CLA	1	0
31	C	513	CLA	1	0
40	L	101	SQD	3	0
31	13	602	CLA	5	0
31	15	613	CLA	4	0
30	12	607	CHL	2	0
31	14	604	CLA	1	0
33	6	619	LUT	1	0
36	T	101	3PH	4	0
31	s	603	CLA	1	0
31	g	604	CLA	2	0
30	16	606	CHL	1	0
31	y	613	CLA	5	0
31	c	503	CLA	2	0
31	s	611	CLA	4	0
30	16	608	CHL	2	0
41	B	622	LMG	1	0
39	C	515	BCR	2	0
33	13	618	LUT	1	0
30	Y	605	CHL	1	0
30	1	609	CHL	2	0
30	Y	607	CHL	4	0
31	2	613	CLA	4	0
31	y	614	CLA	2	0
31	5	613	CLA	3	0
31	11	613	CLA	3	0
32	y	616	LHG	5	0
36	7	201	3PH	1	0
31	6	614	CLA	1	0
30	14	606	CHL	1	0
31	B	605	CLA	2	0
31	C	514	CLA	2	0
31	G	602	CLA	2	0
32	S	617	LHG	4	0
31	B	611	CLA	1	0
31	b	615	CLA	4	0
30	s	608	CHL	5	0

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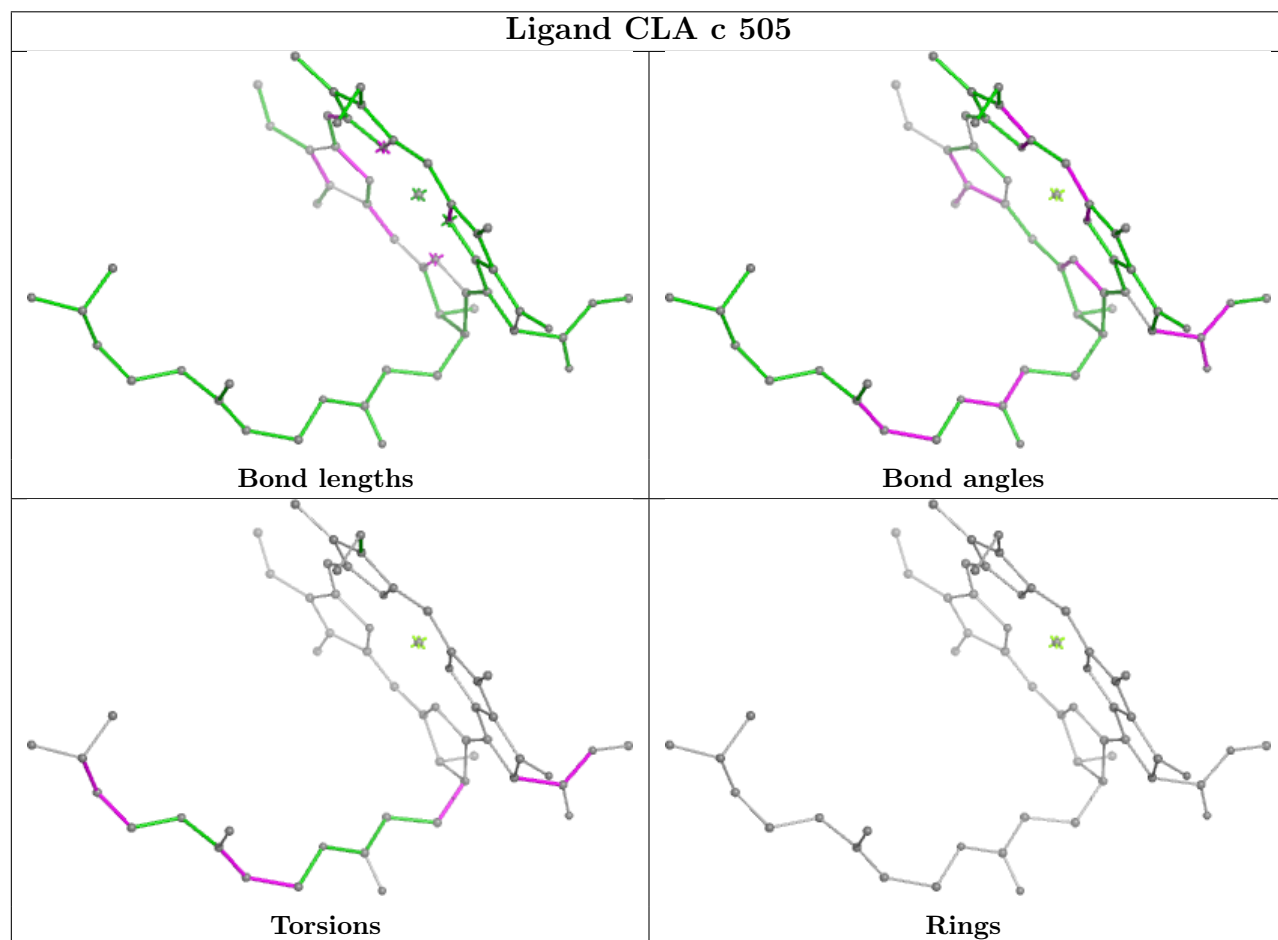
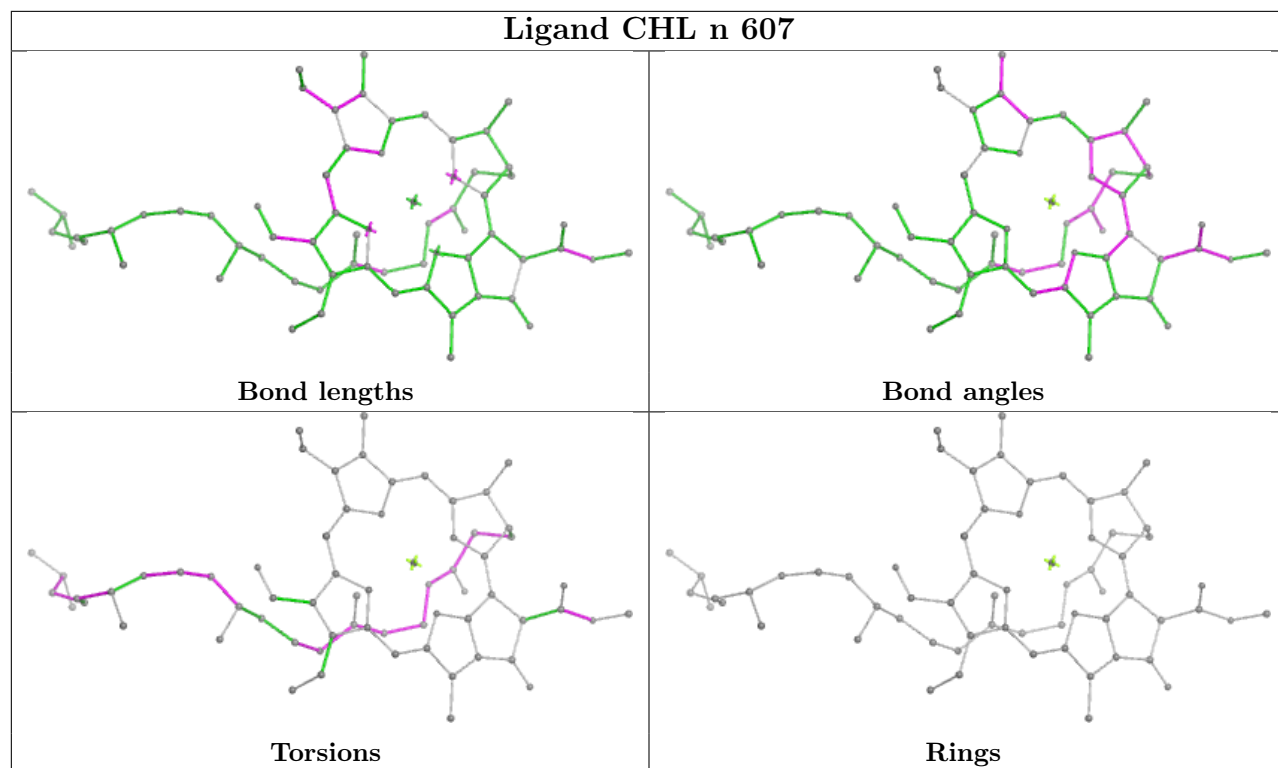
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	603	CLA	2	0
31	11	603	CLA	4	0
31	s	615	CLA	2	0
31	6	613	CLA	3	0
41	v	101	LMG	1	0
31	Y	610	CLA	2	0
30	R	606	CHL	7	0
30	15	608	CHL	10	0
31	5	602	CLA	2	0
40	d	414	SQD	4	0
31	y	615	CLA	2	0
35	G	619	XAT	1	0
30	g	609	CHL	3	0
30	13	605	CHL	2	0
31	n	615	CLA	2	0
34	15	616	NEX	3	0
30	S	608	CHL	4	0
32	Y	616	LHG	5	0
41	S	616	LMG	3	0
31	6	604	CLA	1	0
31	y	612	CLA	5	0
31	6	615	CLA	3	0
31	y	611	CLA	4	0
31	16	604	CLA	1	0
32	a	411	LHG	1	0
31	6	611	CLA	1	0
31	13	603	CLA	8	0
31	B	609	CLA	2	0
32	n	616	LHG	5	0
35	14	619	XAT	1	0
31	3	612	CLA	3	0
35	g	619	XAT	2	0
30	15	607	CHL	2	0
33	g	617	LUT	1	0
31	2	603	CLA	5	0
30	2	608	CHL	5	0
31	14	603	CLA	6	0
30	G	609	CHL	2	0
41	w	501	LMG	3	0
31	s	604	CLA	9	0
30	y	607	CHL	4	0
30	13	608	CHL	2	0

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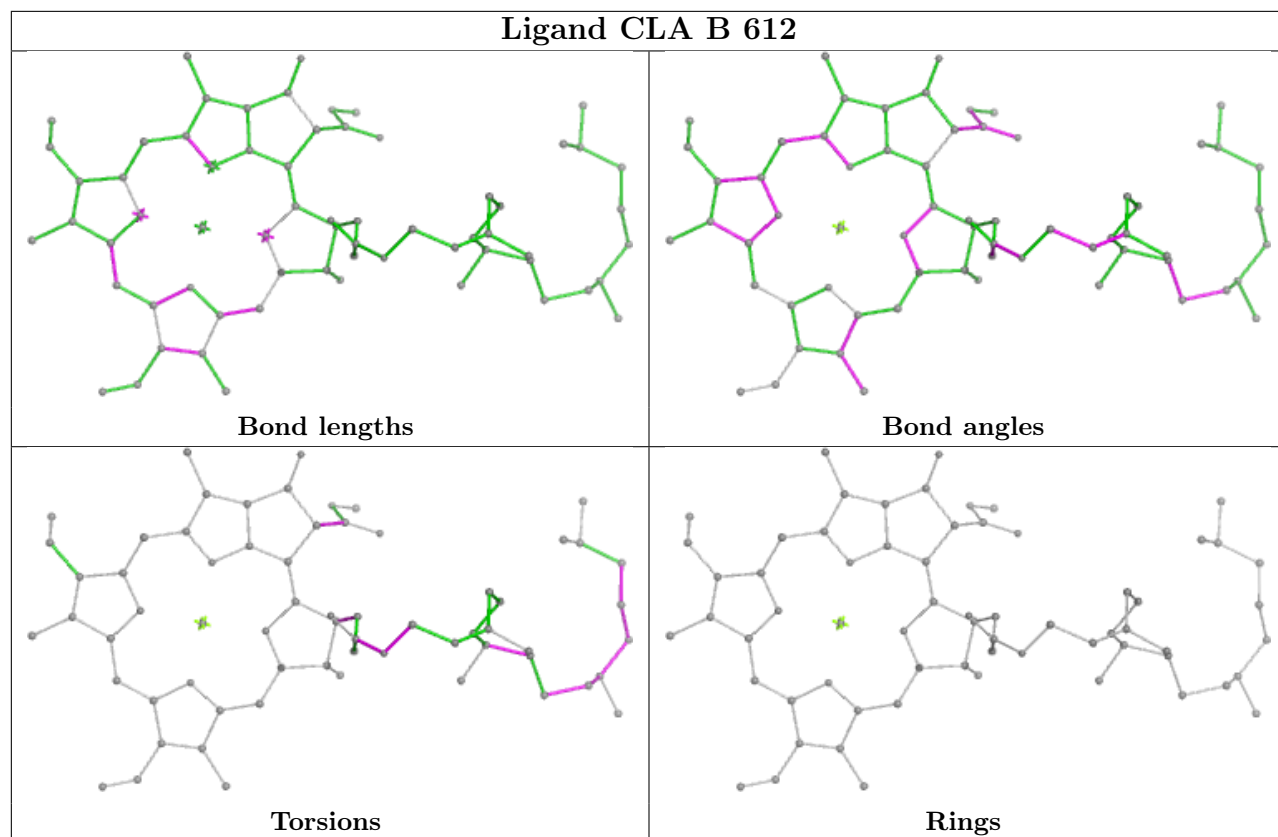
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	R	604	CLA	1	0
32	16	616	LHG	3	0
43	Y	619	LNL	1	0
31	D	404	CLA	4	0
31	4	613	CLA	2	0
30	N	607	CHL	8	0
31	A	402	CLA	4	0
30	4	608	CHL	5	0
31	B	607	CLA	1	0
32	R	618	LHG	2	0
30	16	605	CHL	3	0
31	R	612	CLA	1	0
32	A	414	LHG	5	0
33	N	617	LUT	5	0
30	S	607	CHL	1	0
31	Y	611	CLA	4	0
31	15	611	CLA	4	0
39	a	408	BCR	1	0
35	11	619	XAT	1	0
31	S	613	CLA	1	0
32	d	409	LHG	1	0
31	y	602	CLA	2	0
30	11	605	CHL	1	0
30	G	601	CHL	1	0
31	B	614	CLA	2	0
30	n	601	CHL	2	0

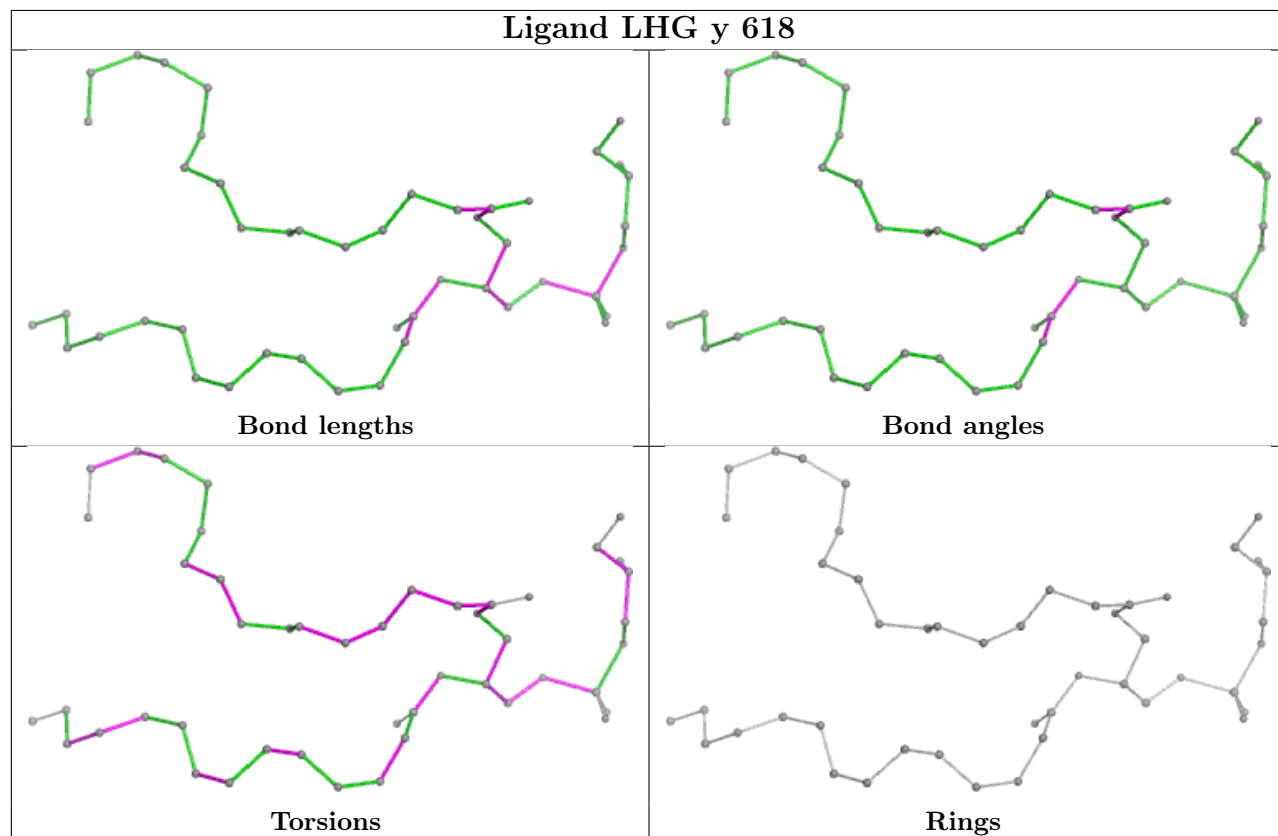
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

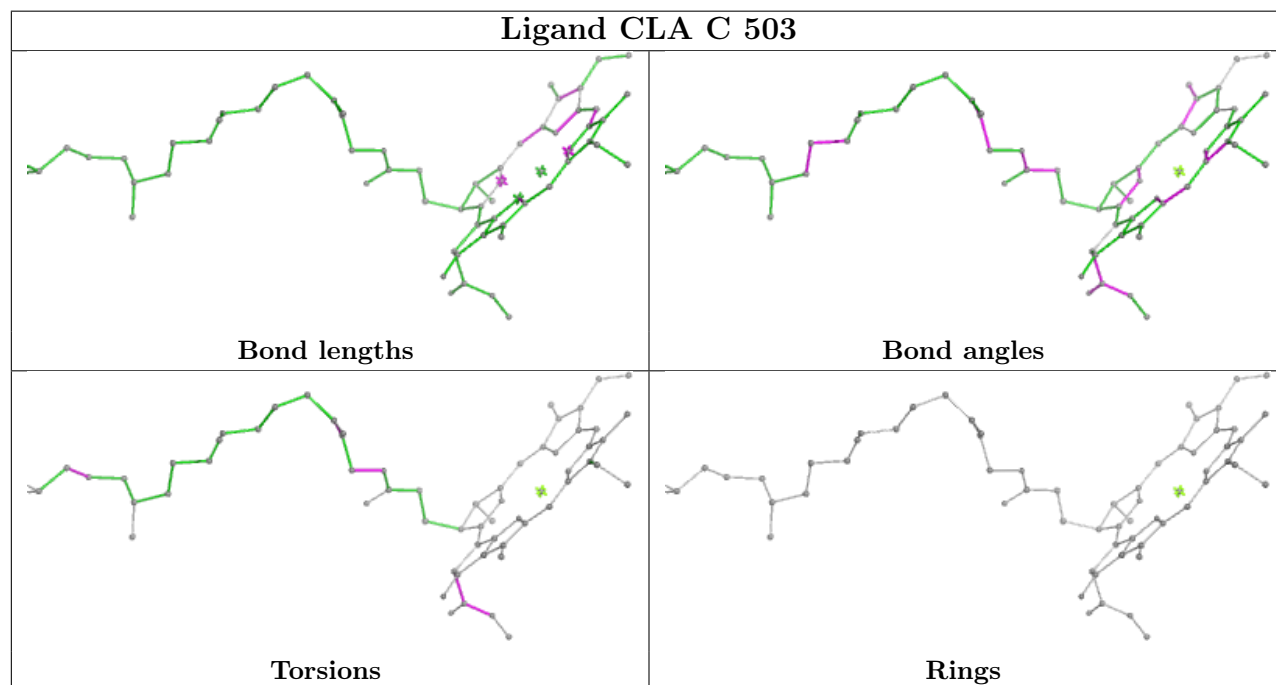
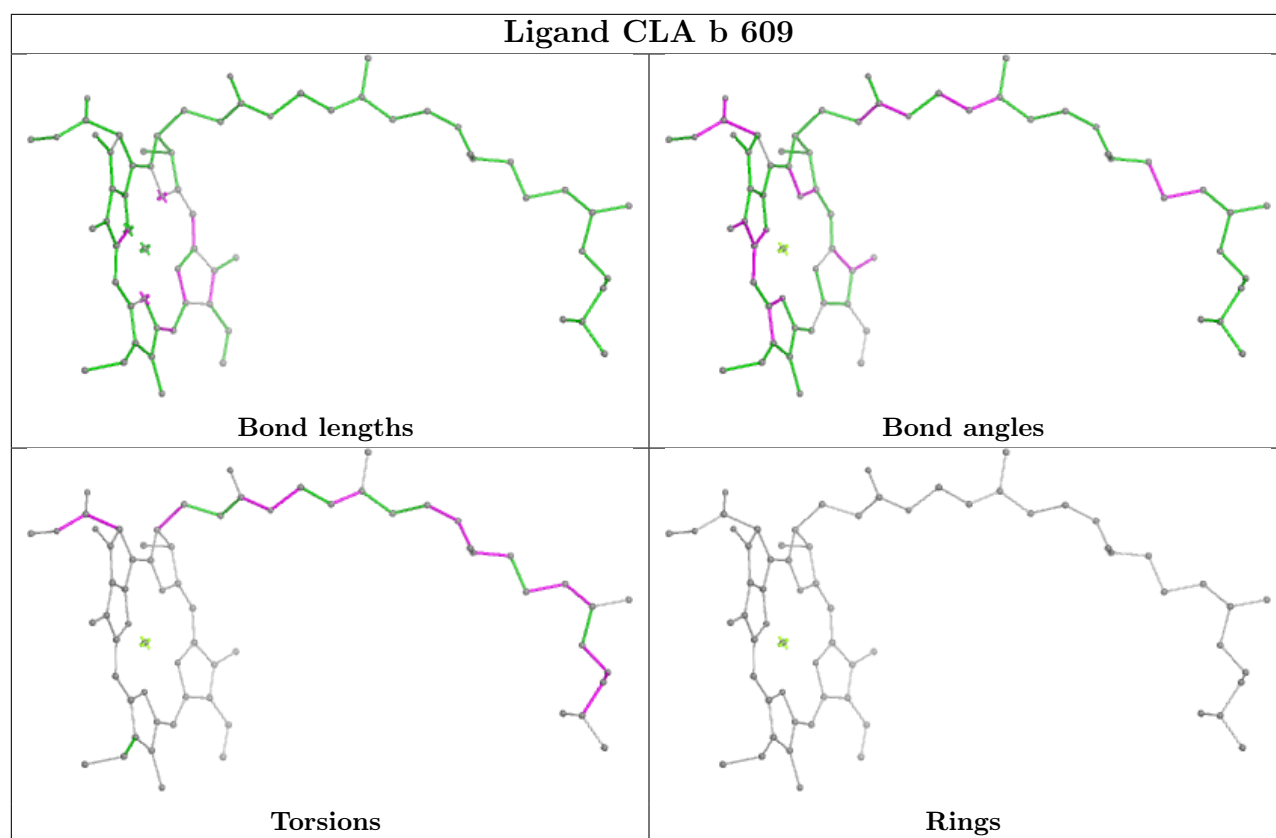


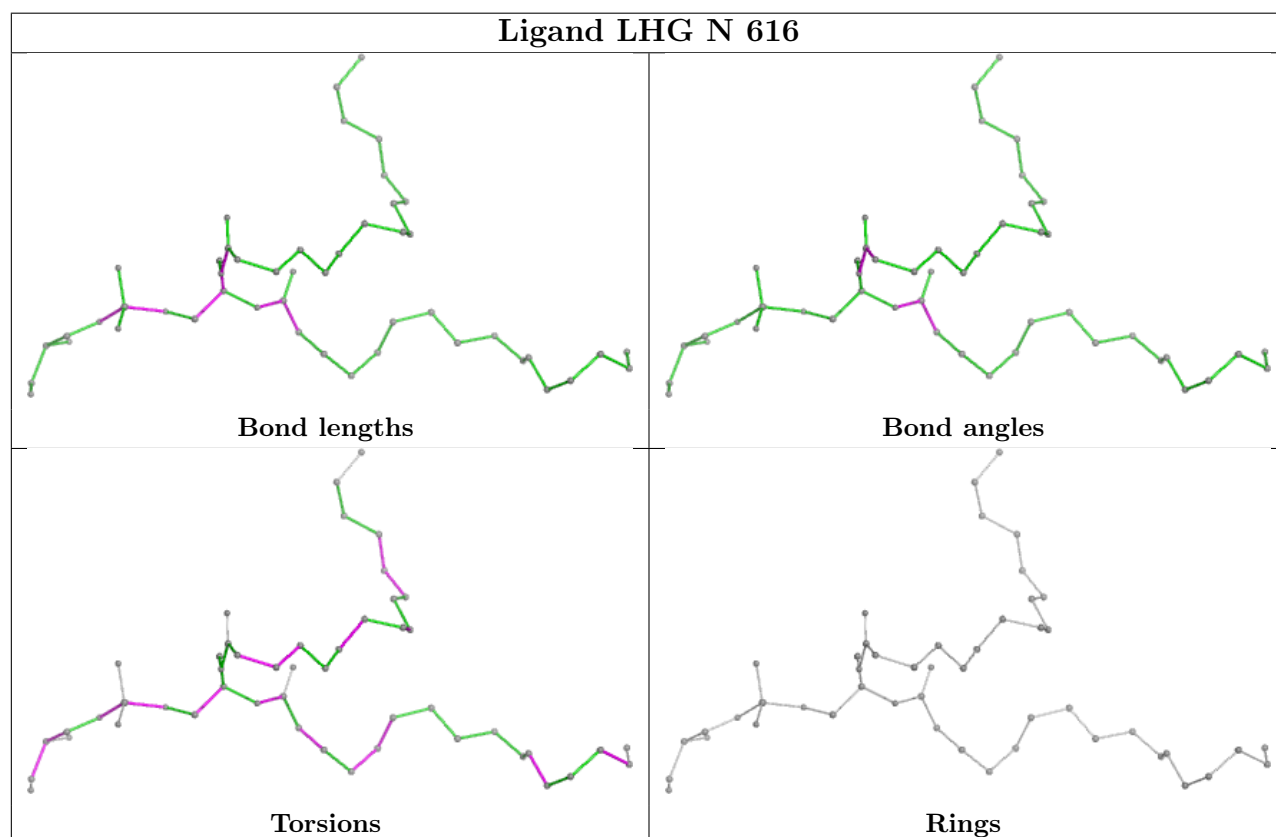
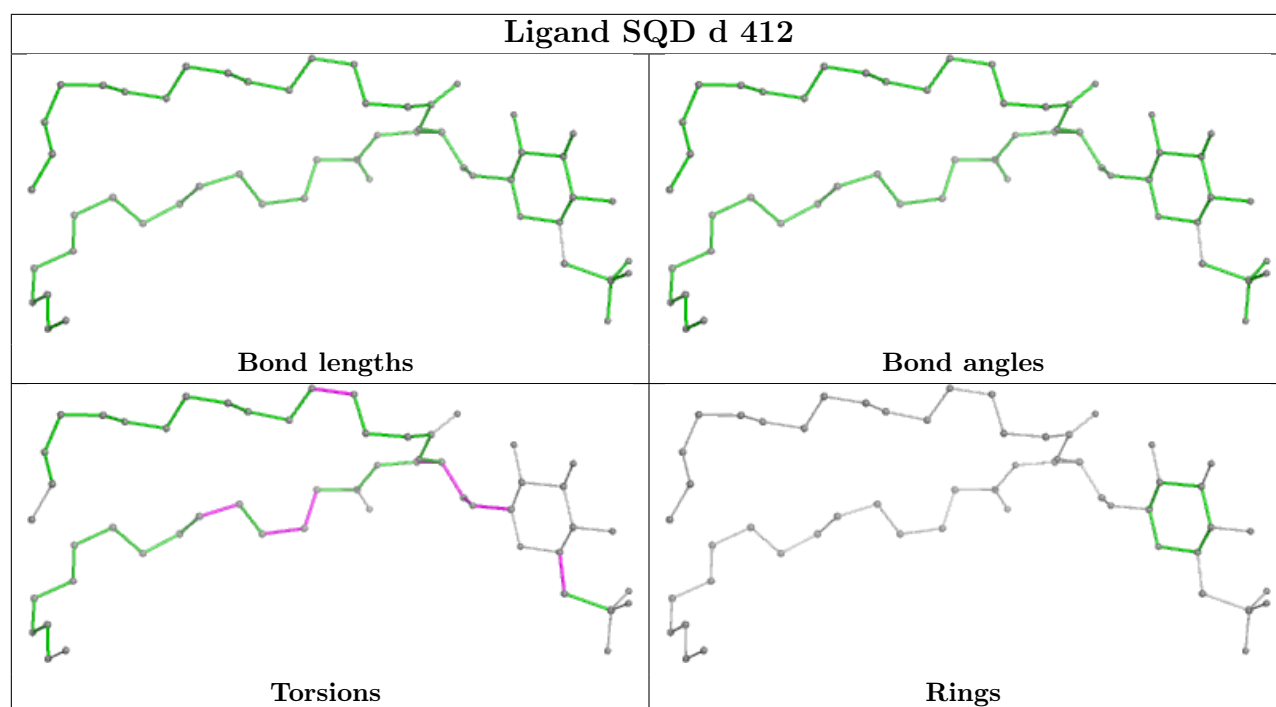
Ligand CLA B 612

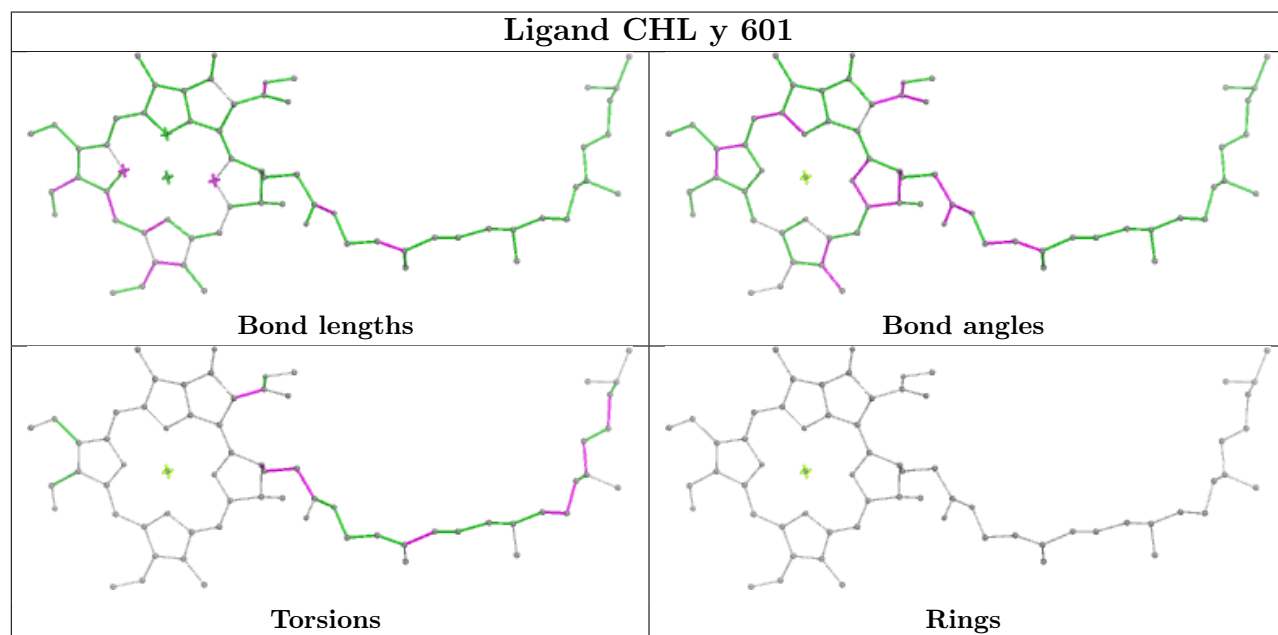
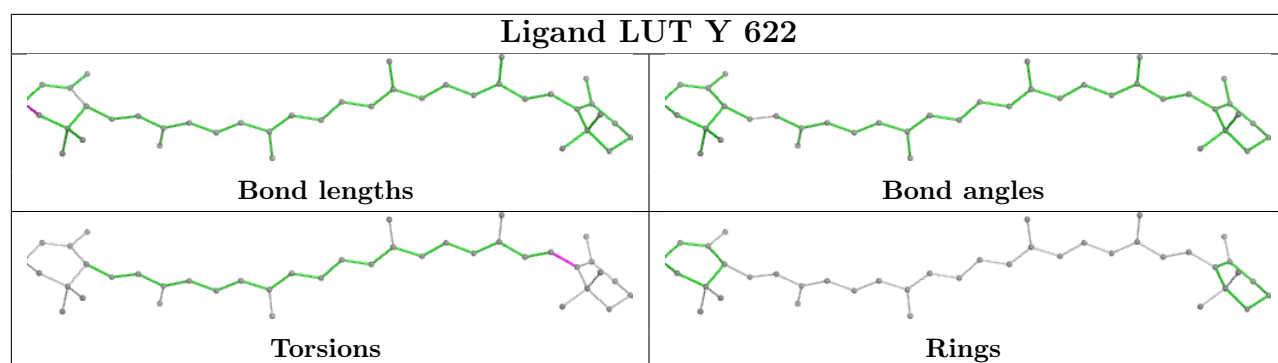


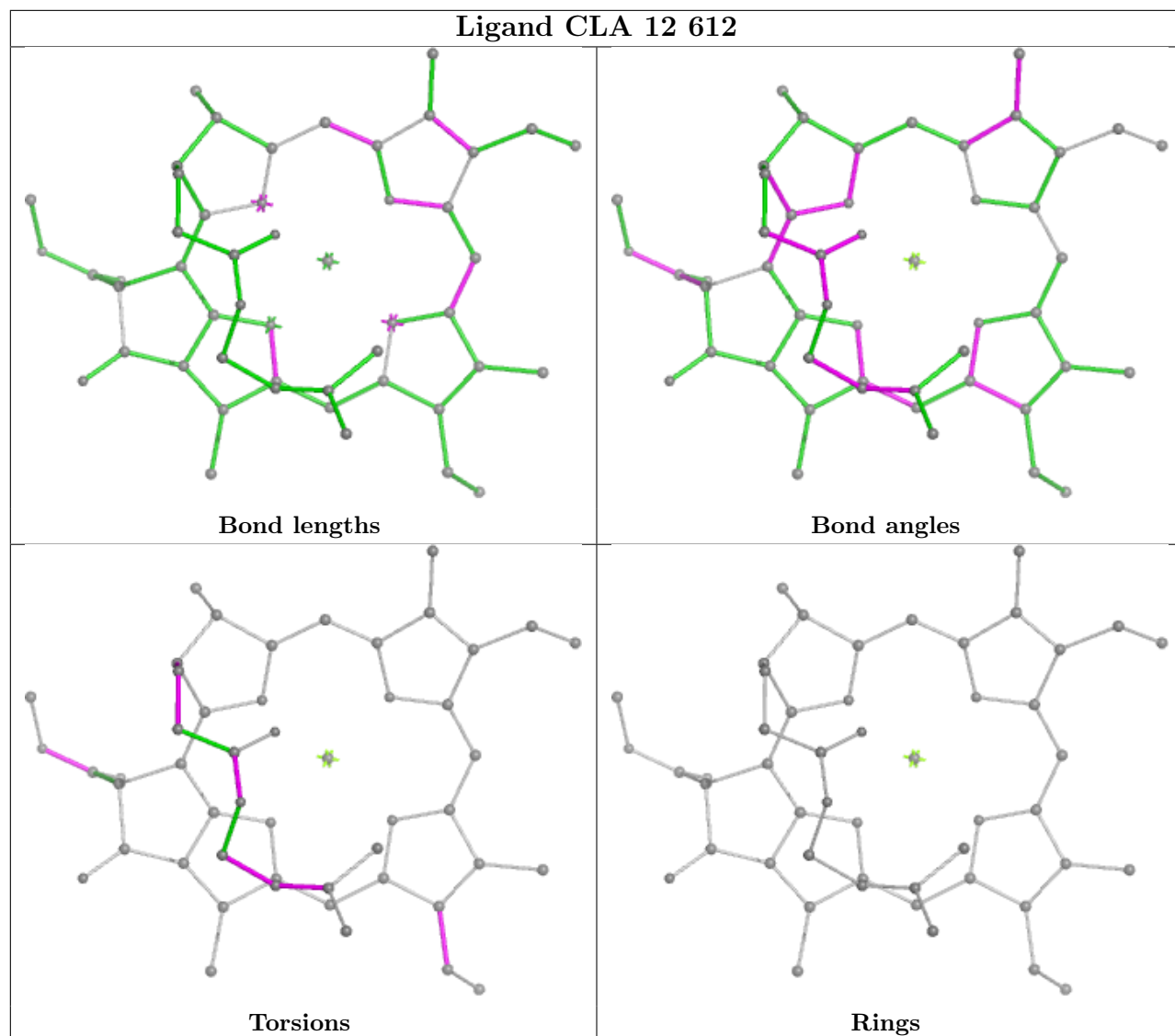
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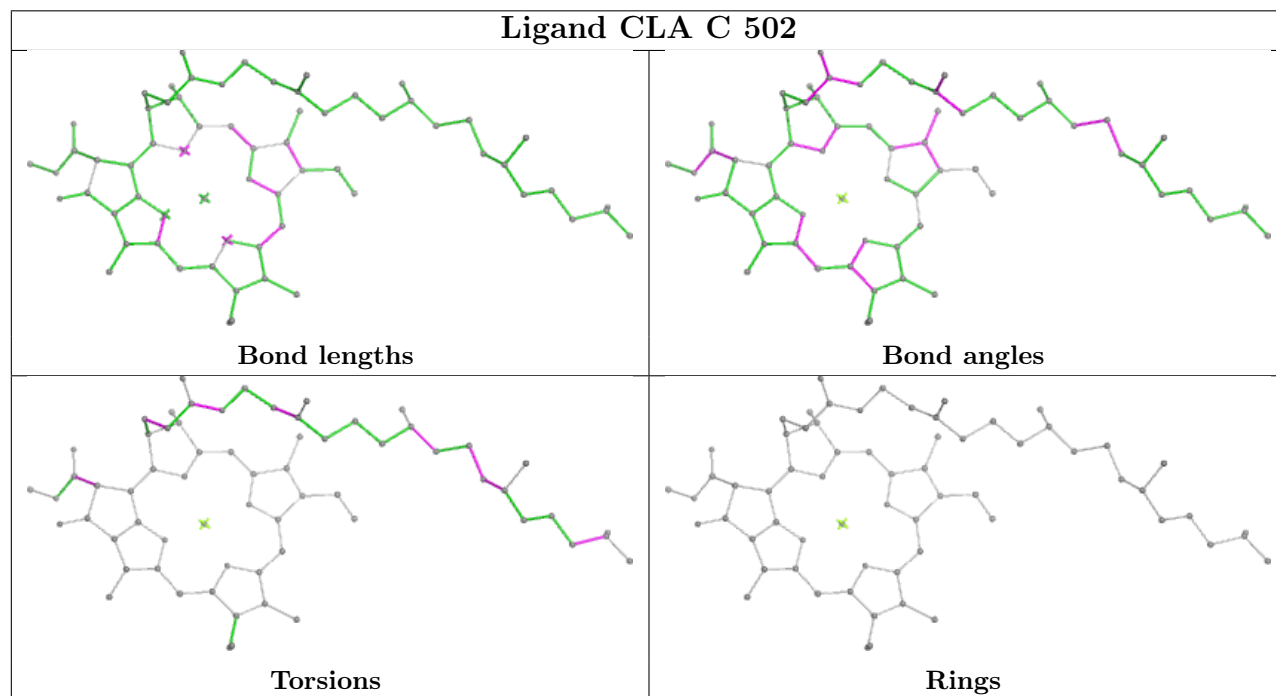
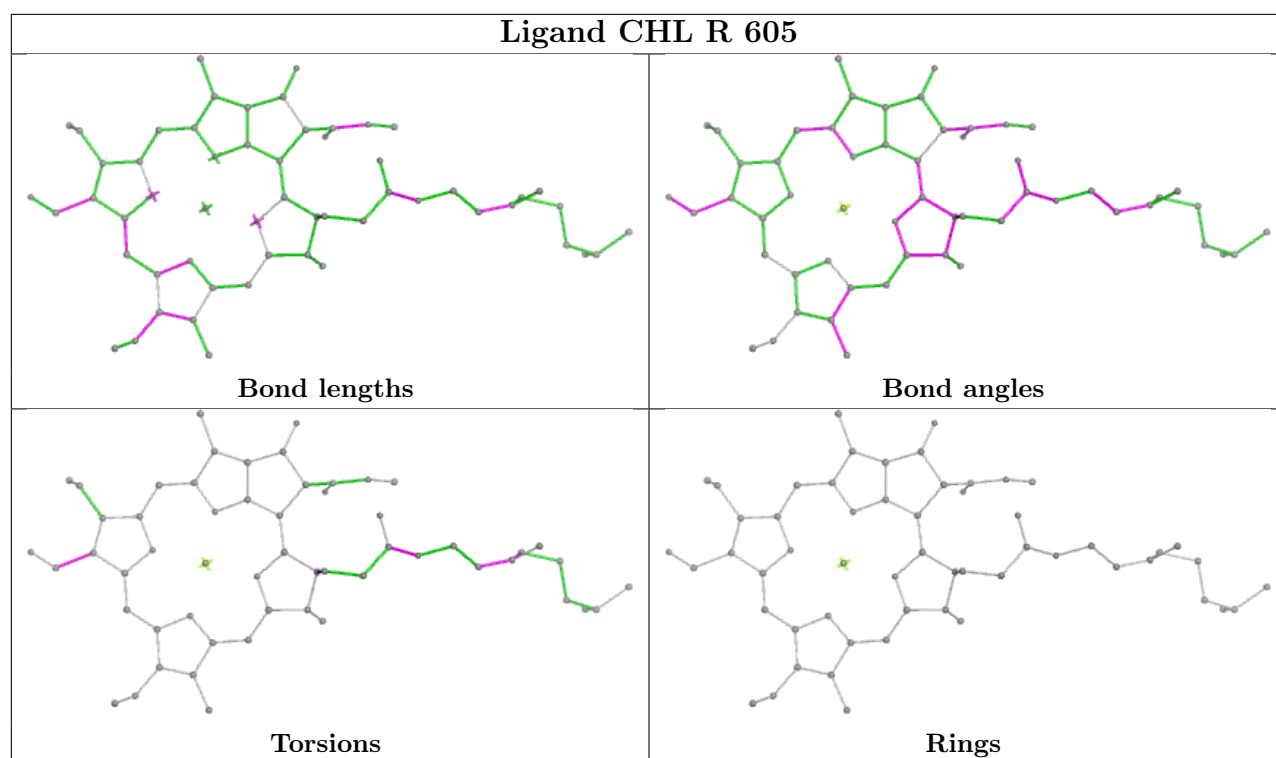


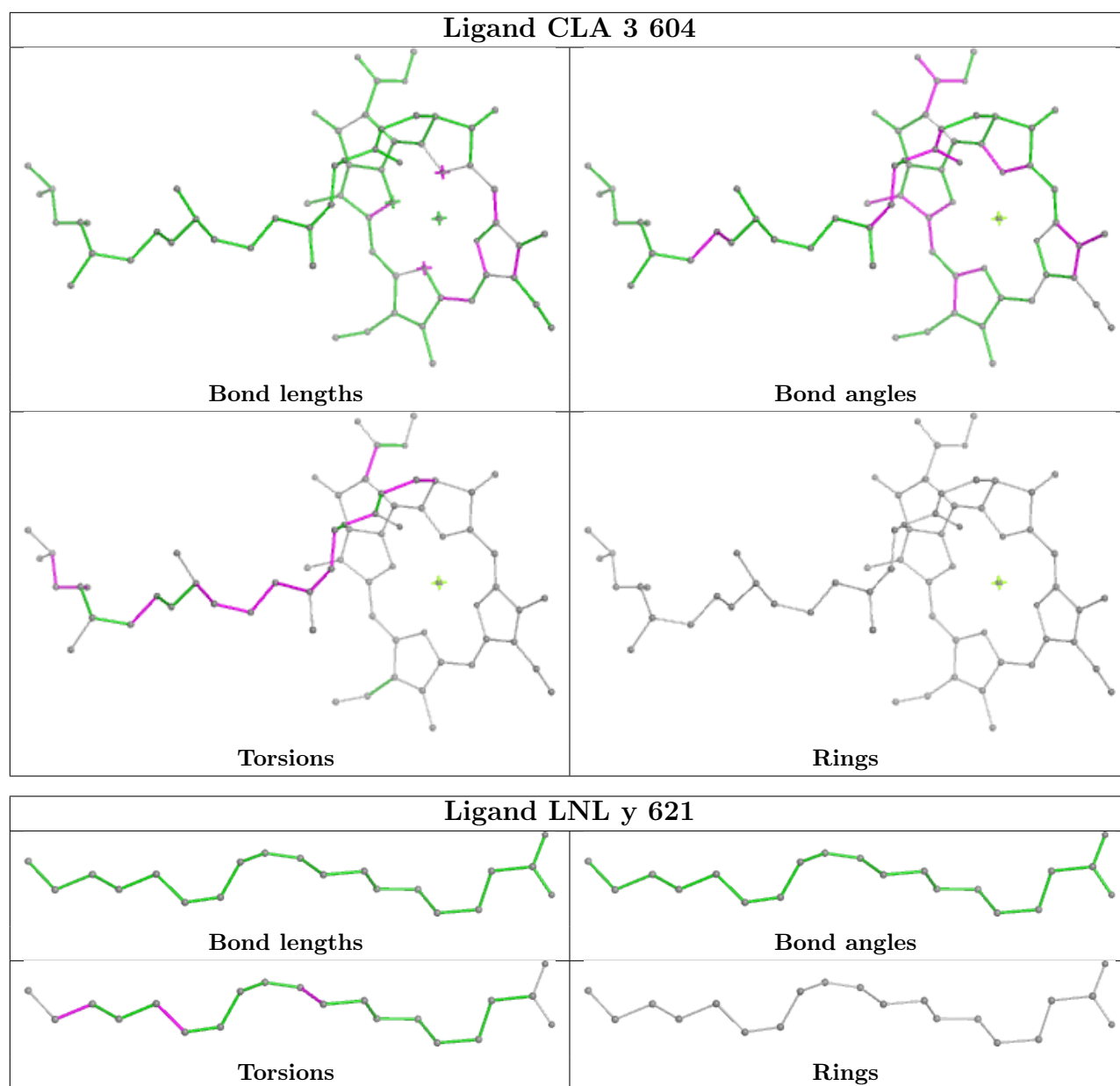




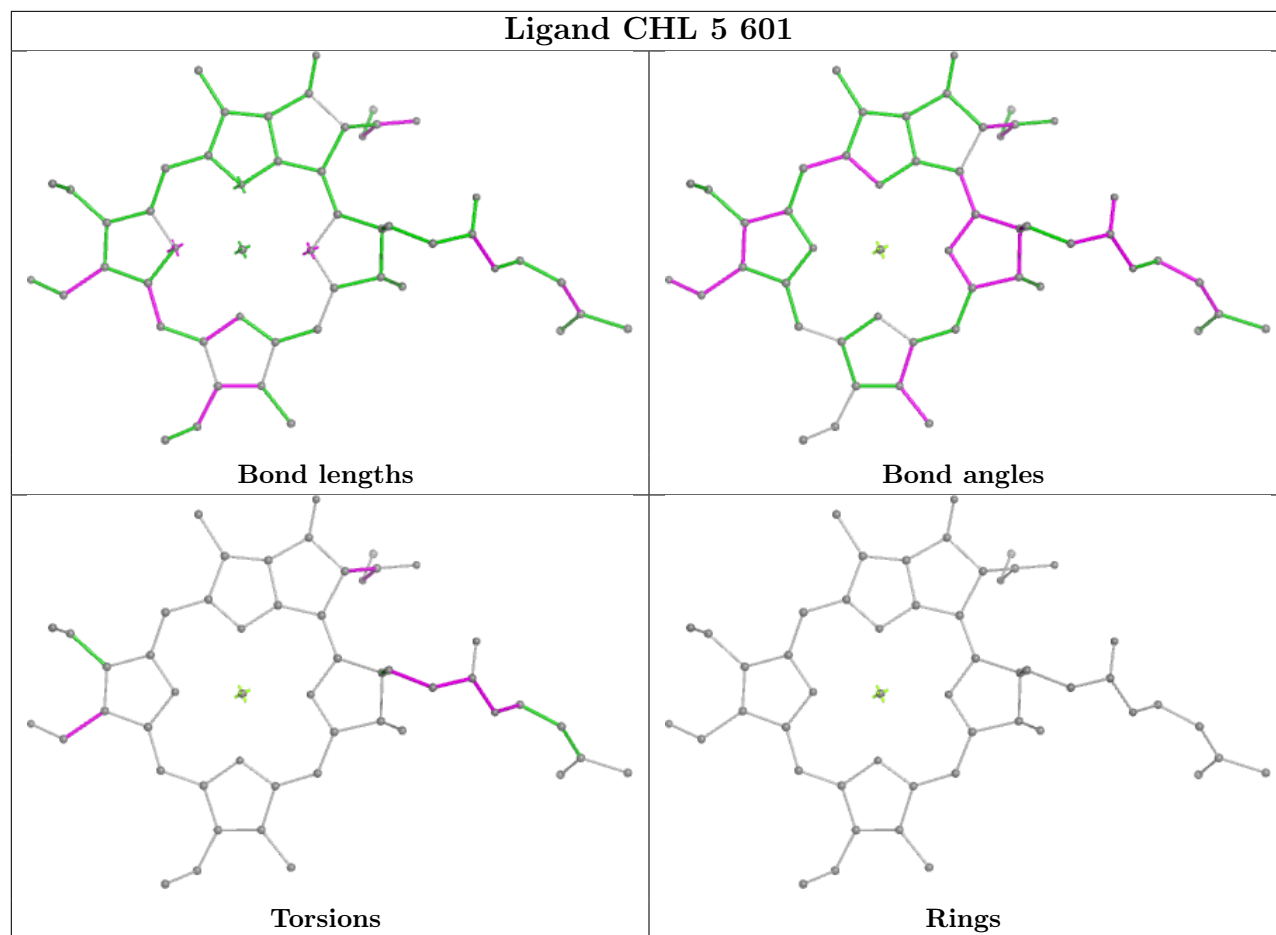


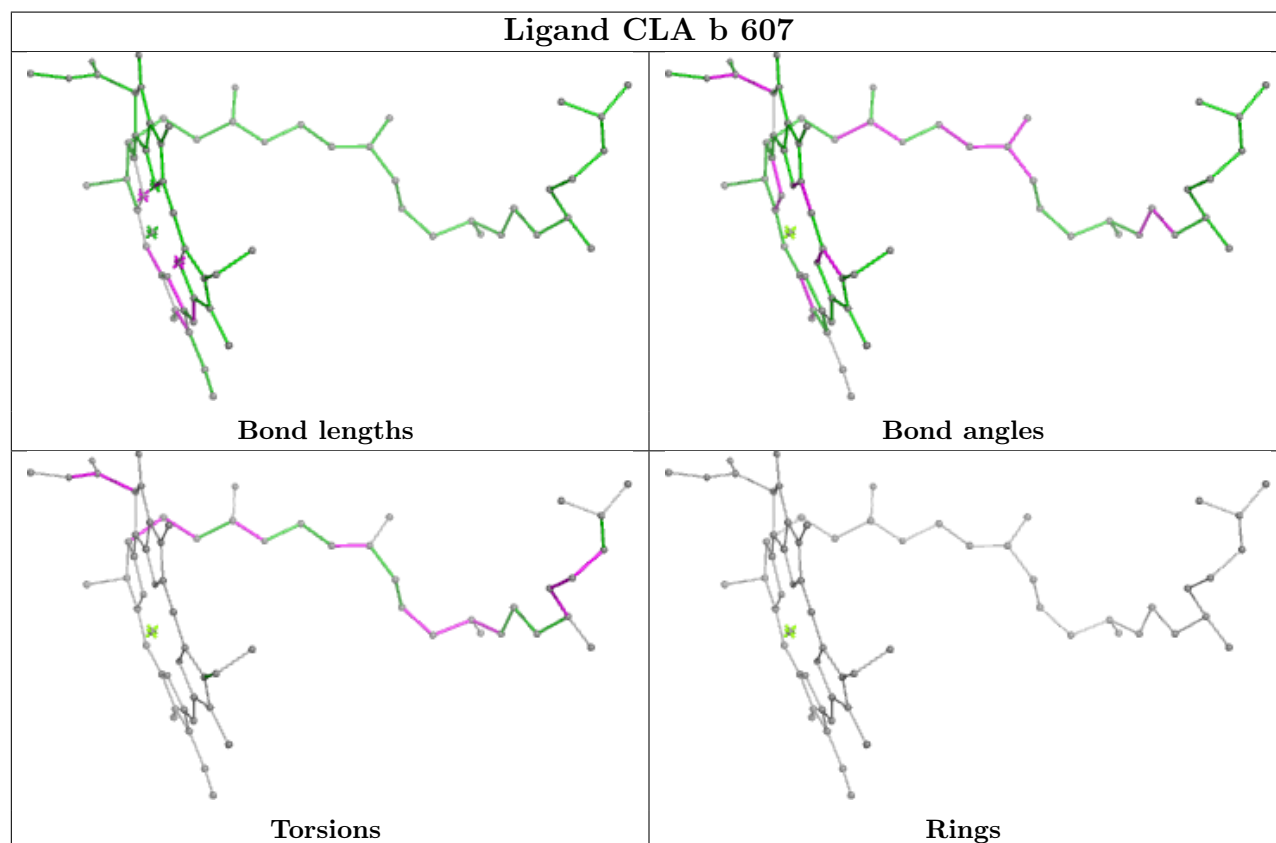
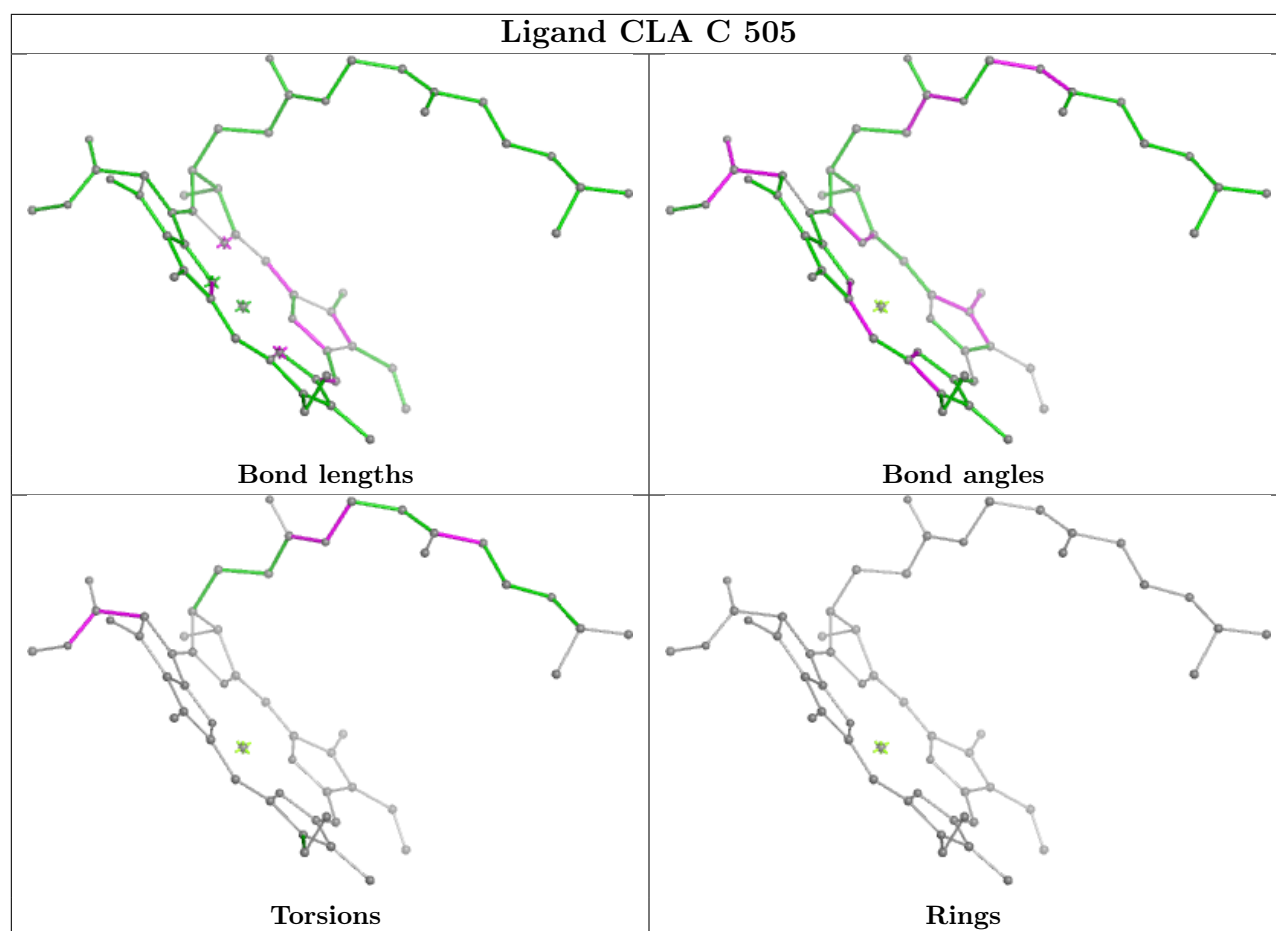


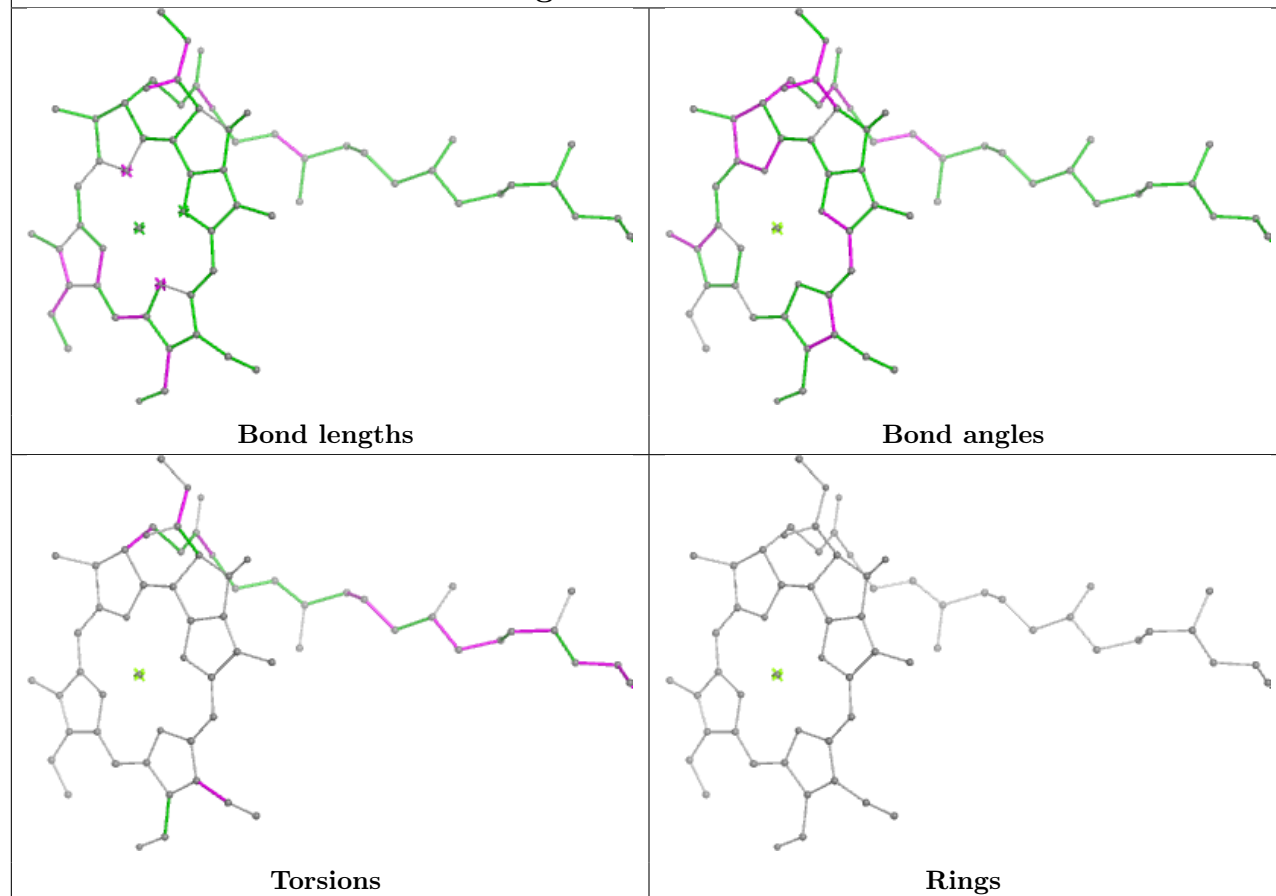
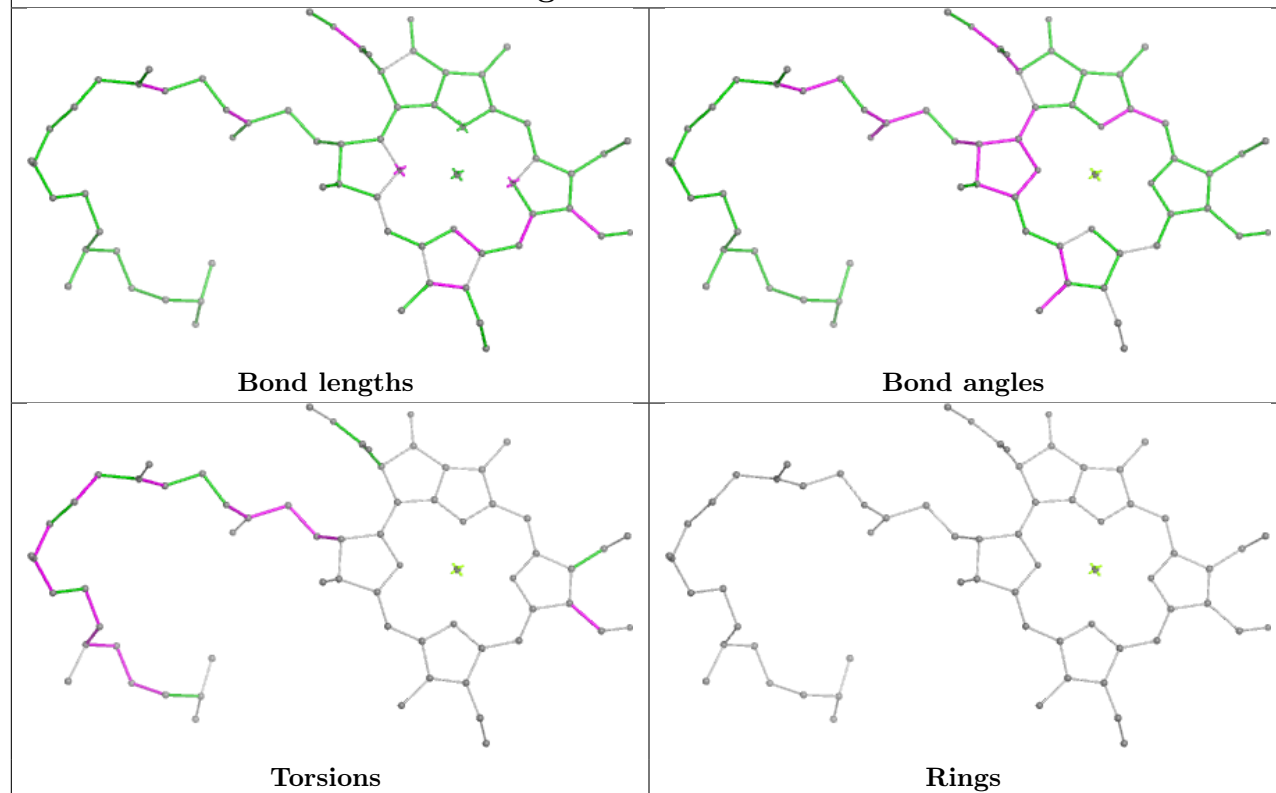


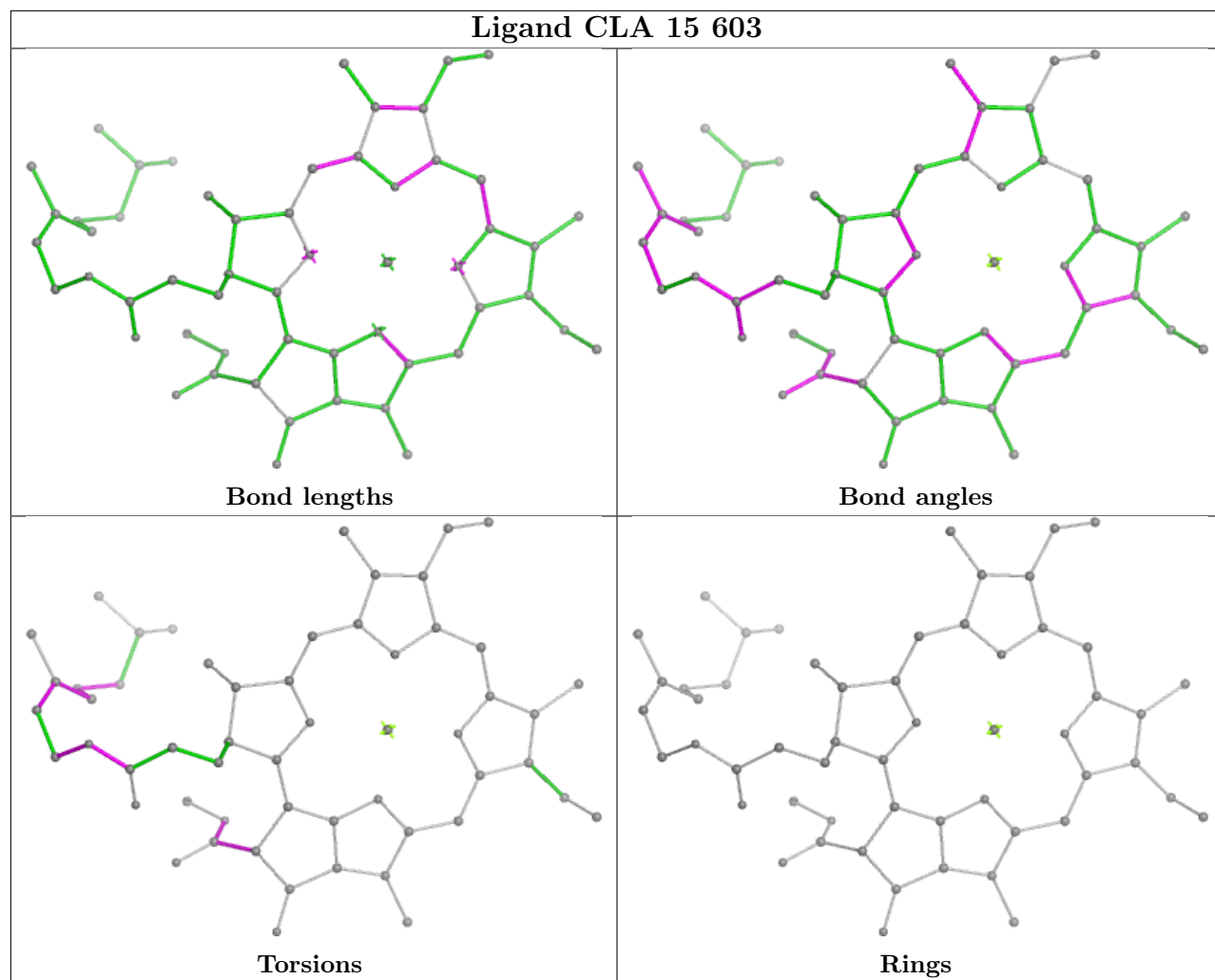


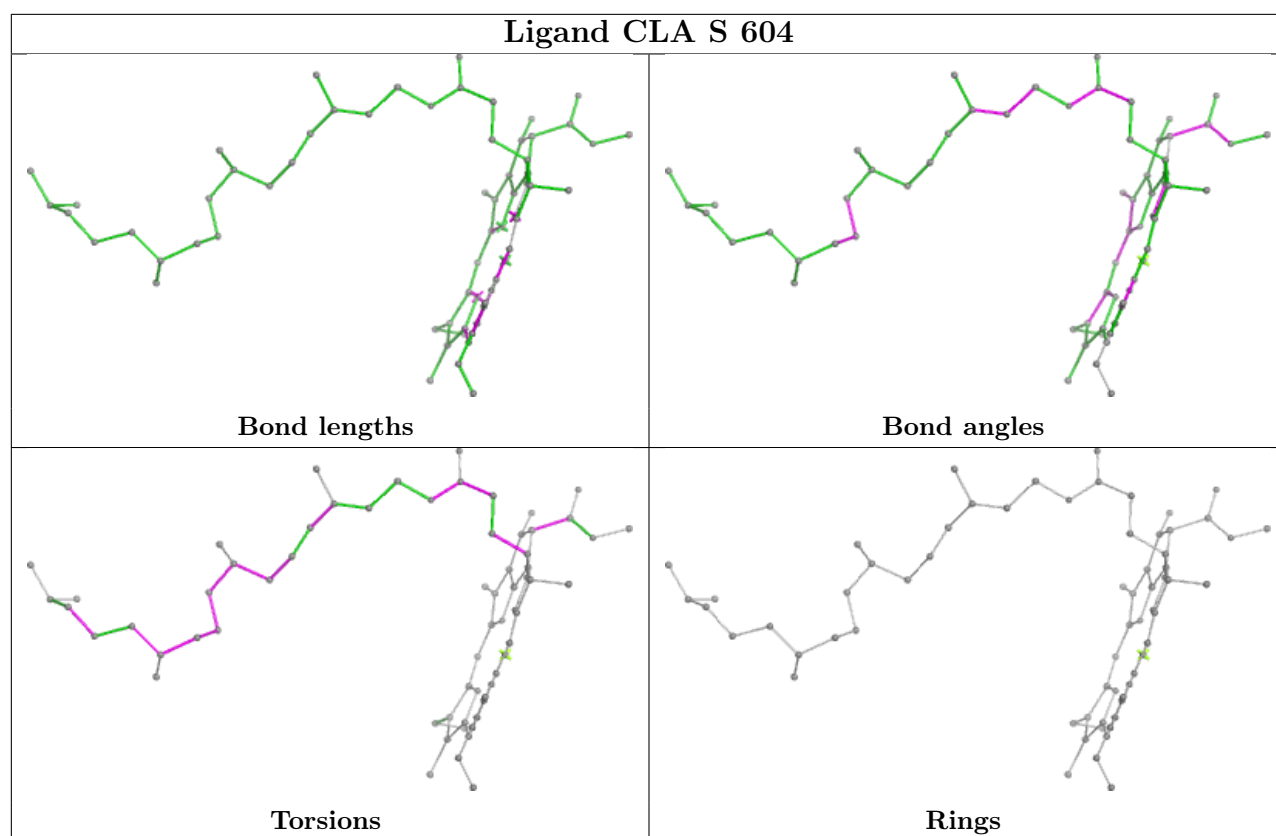
Ligand CHL 5 601

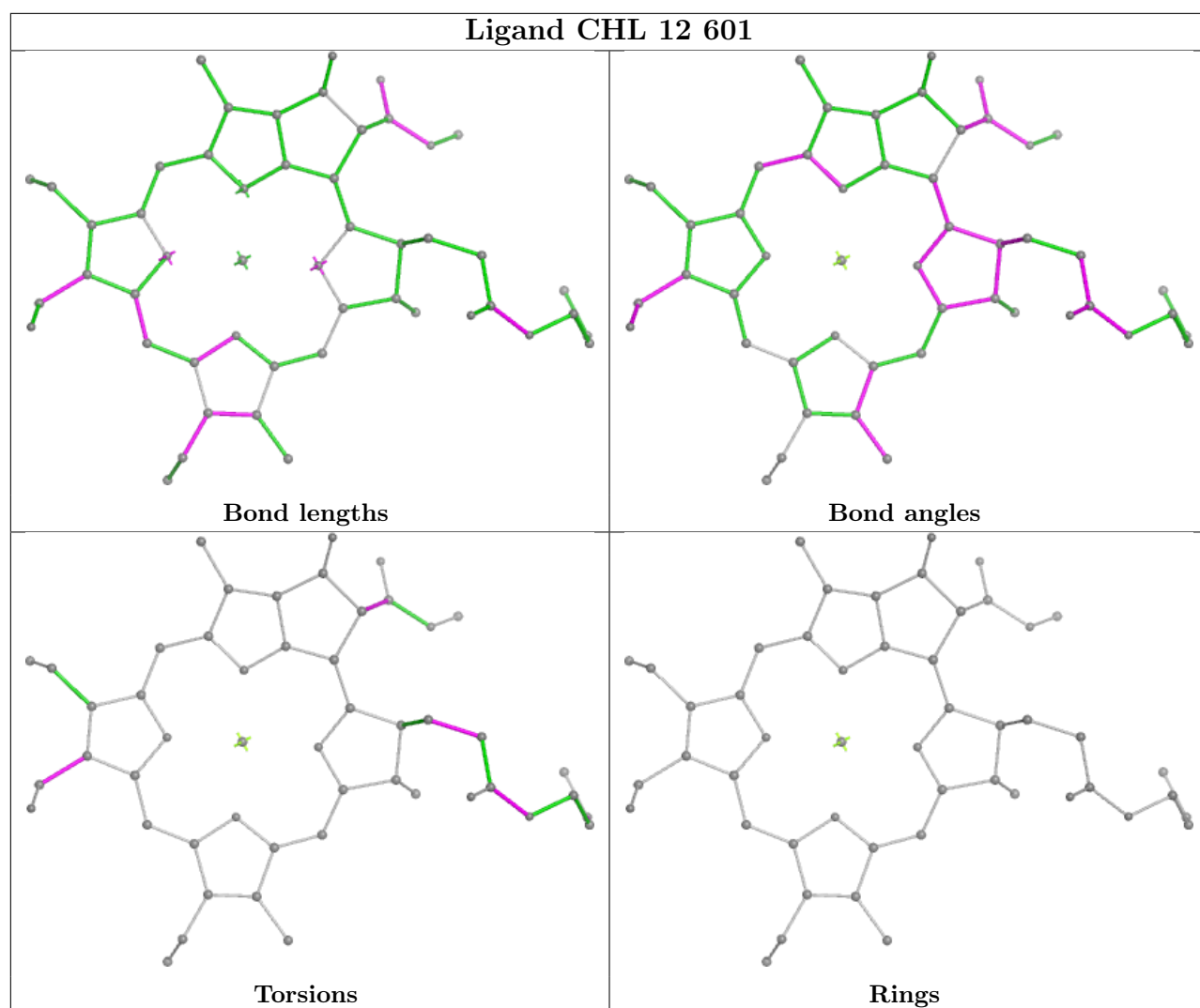




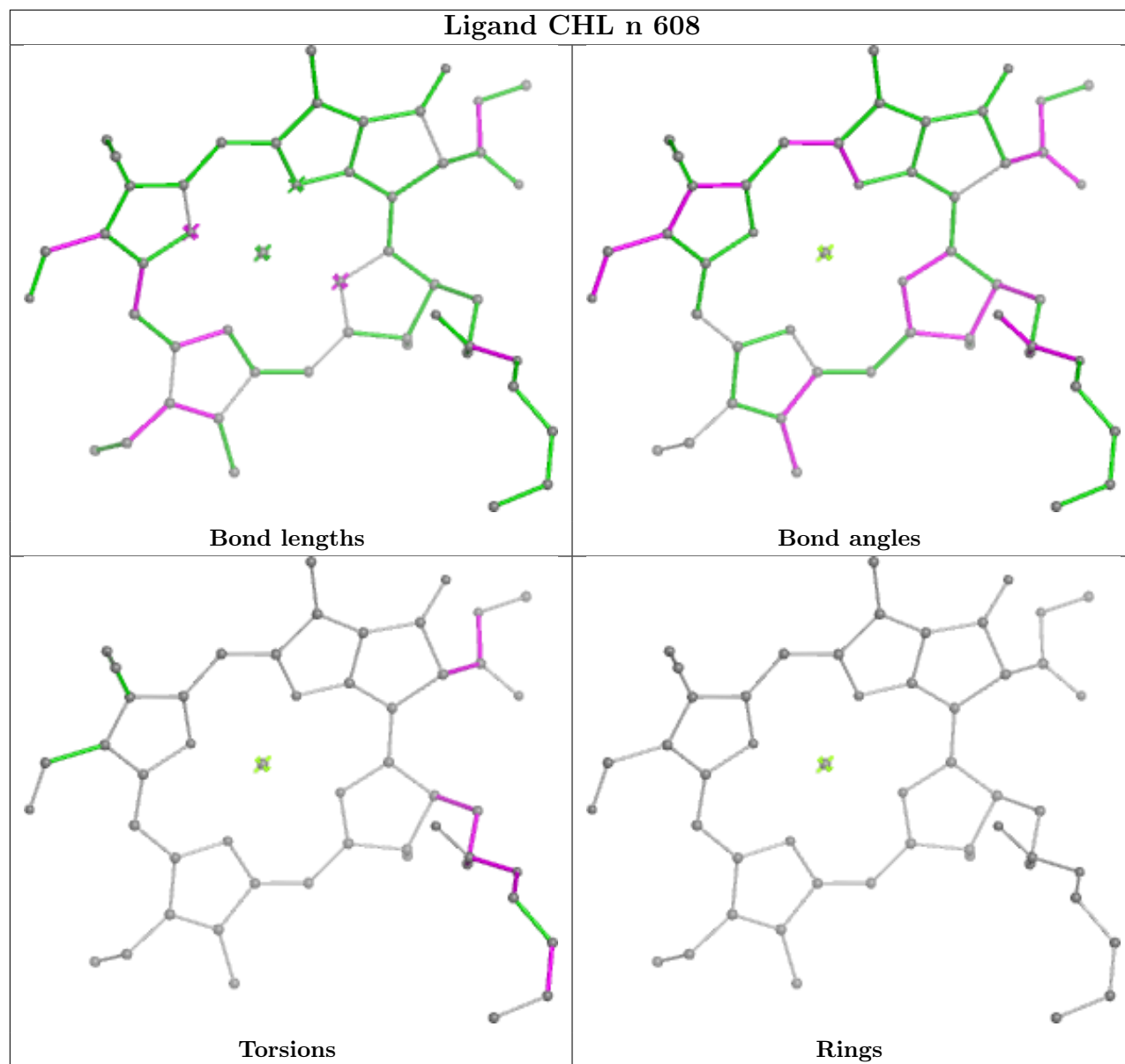
Ligand CHL 3 609**Ligand CHL s 606**

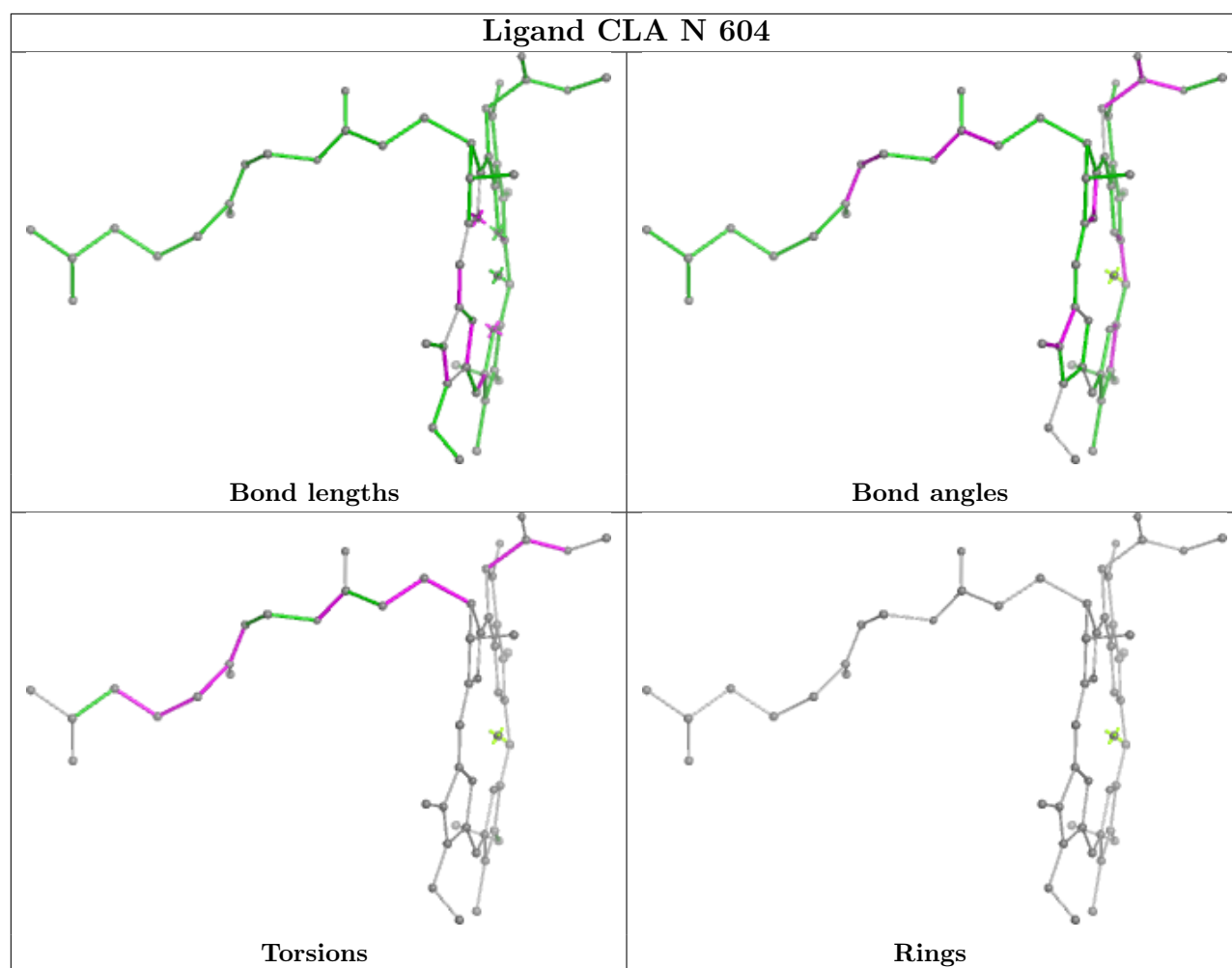


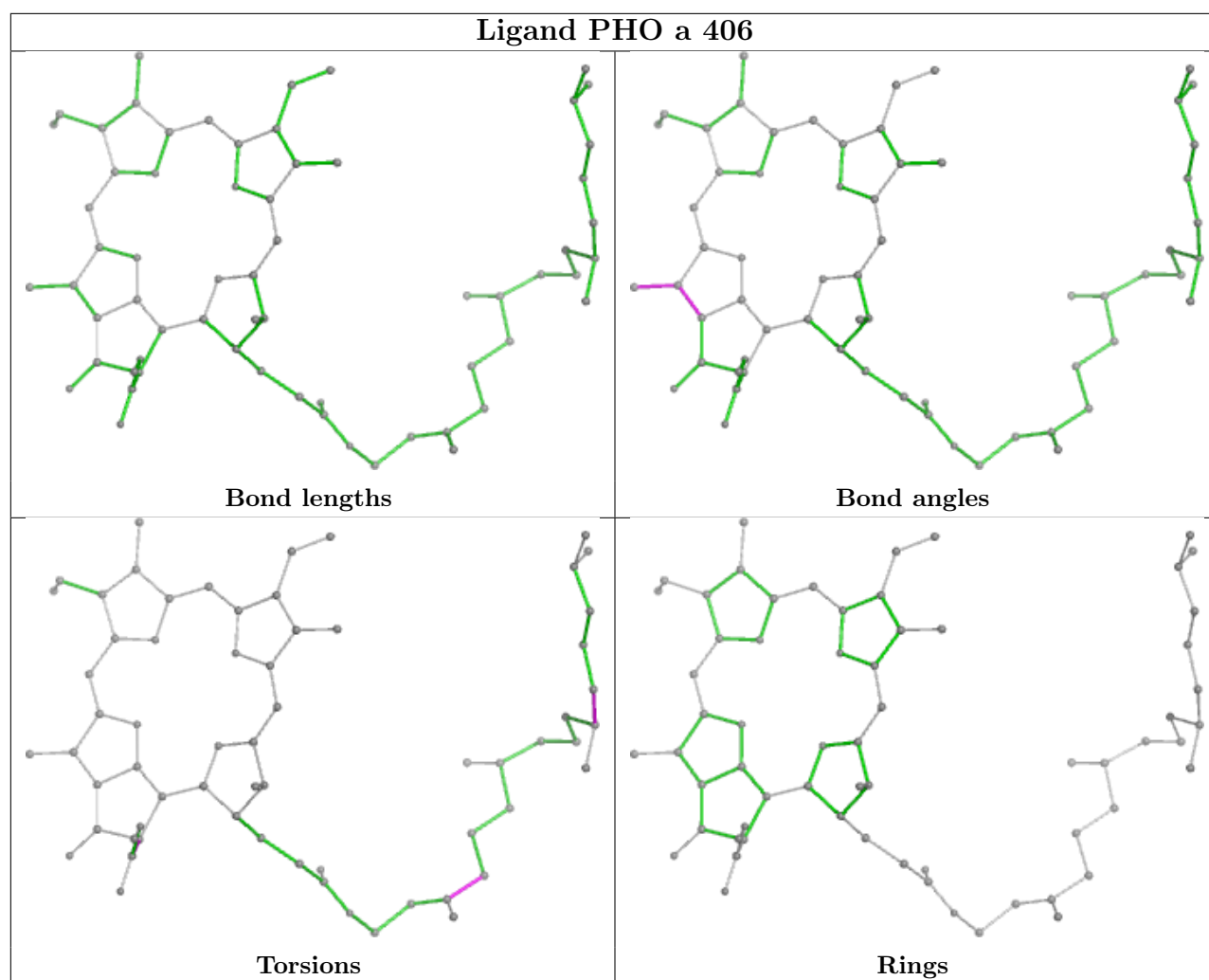


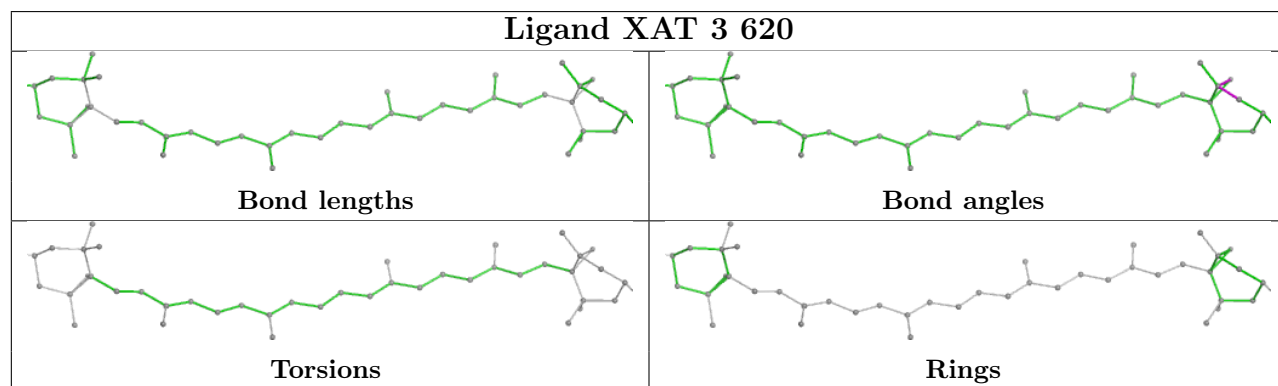
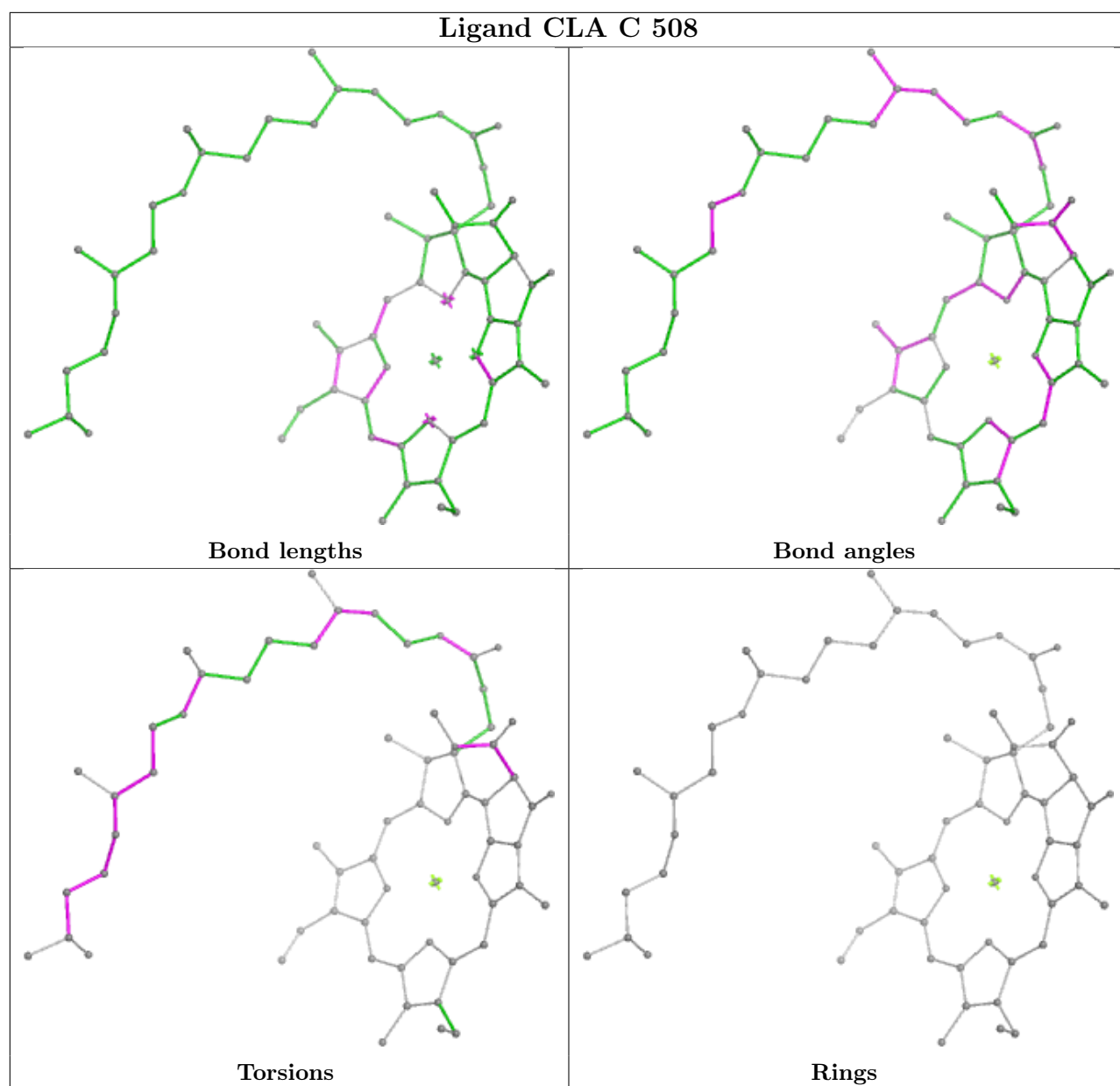


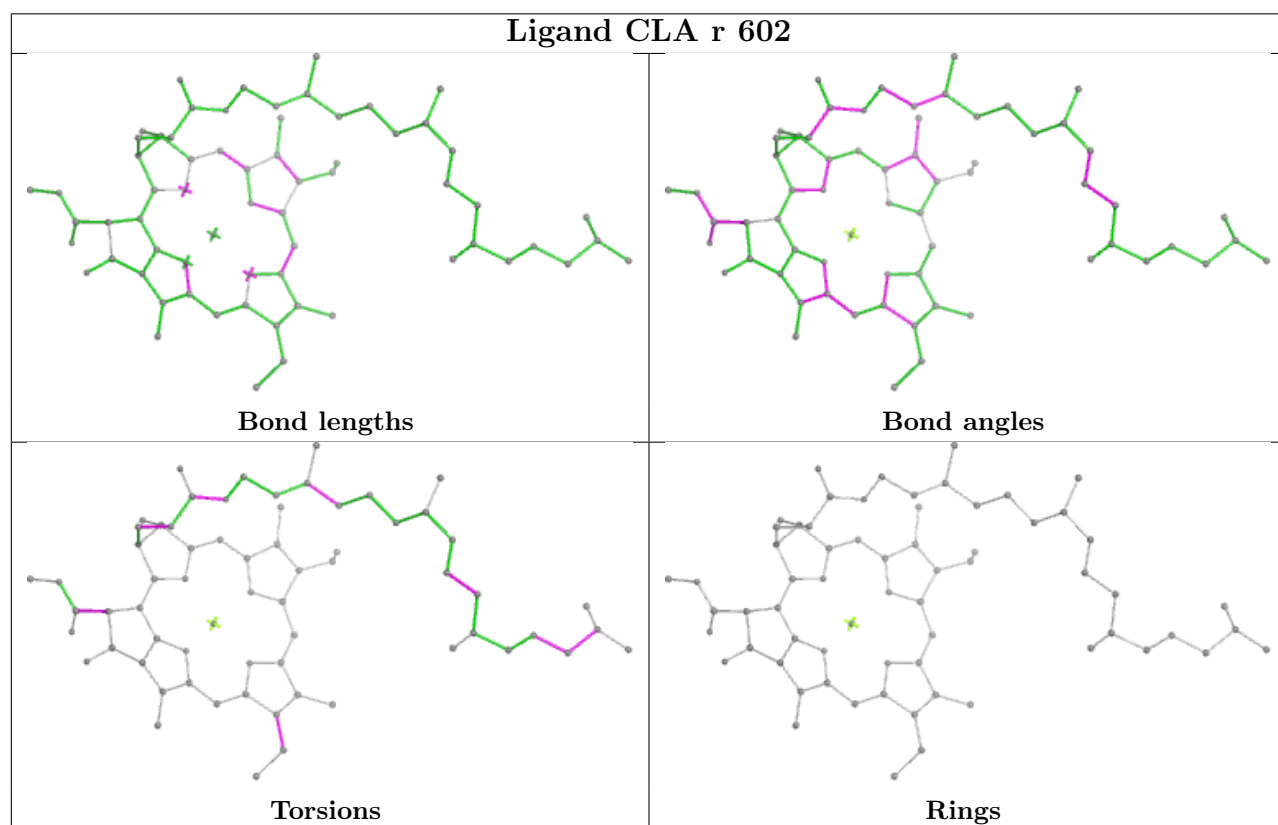
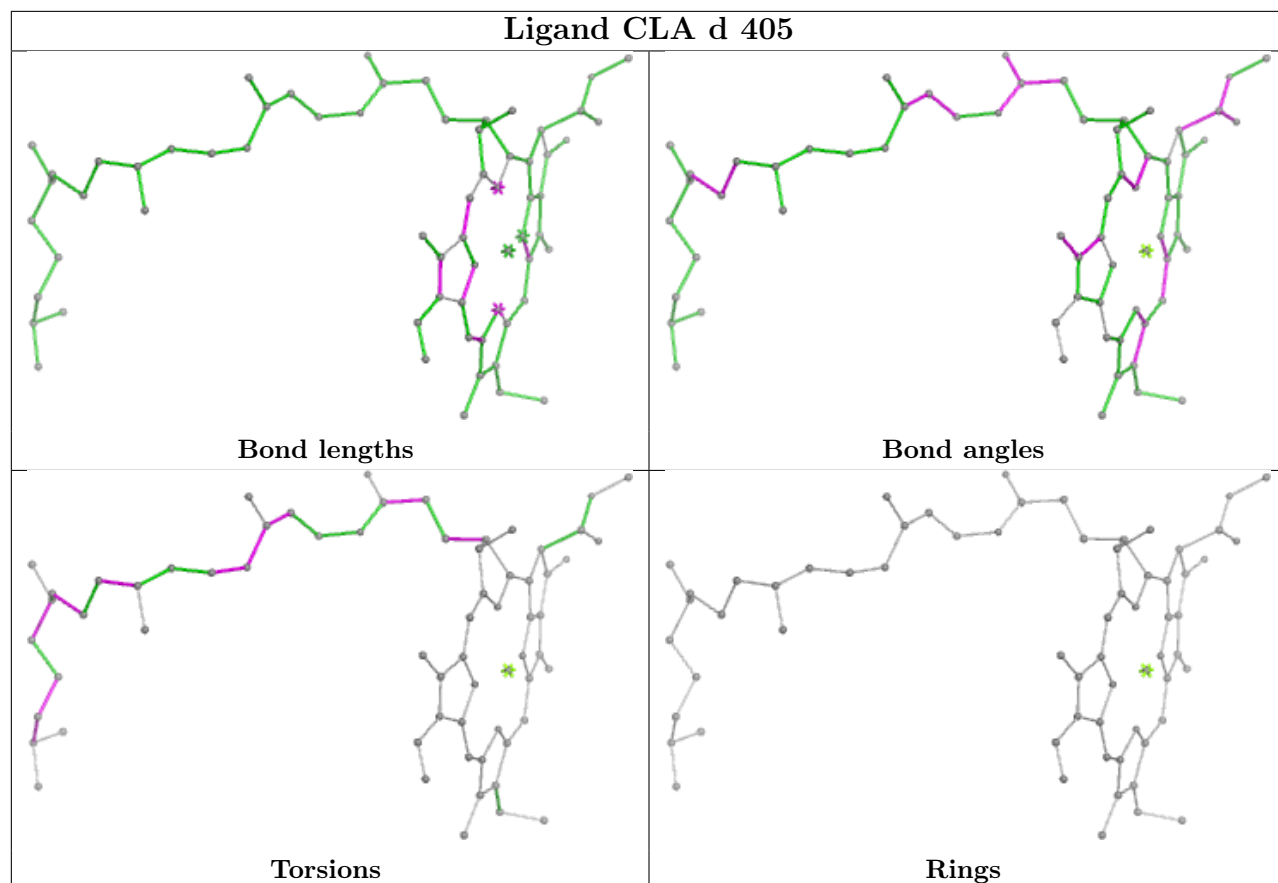
Ligand CHL n 608

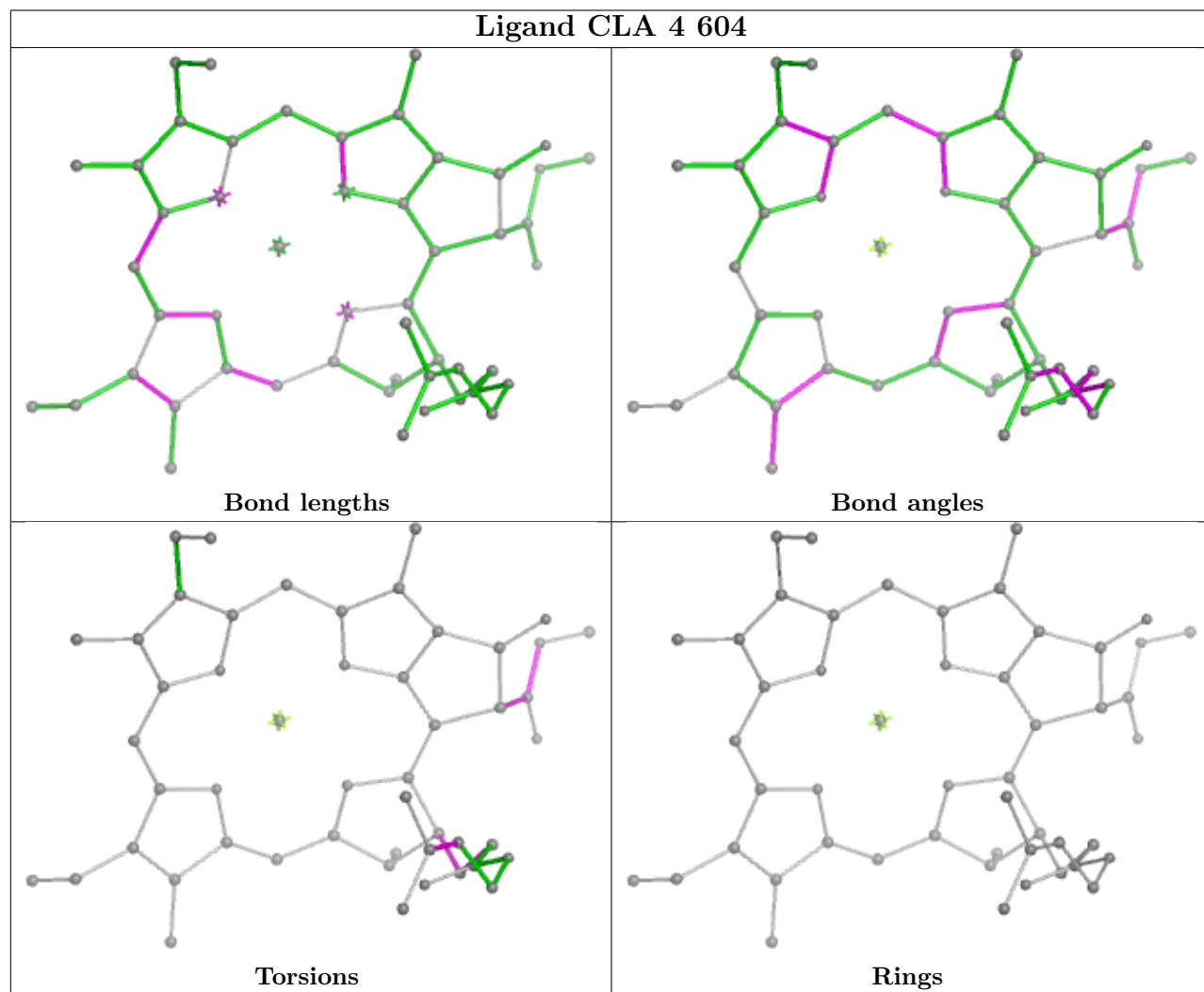
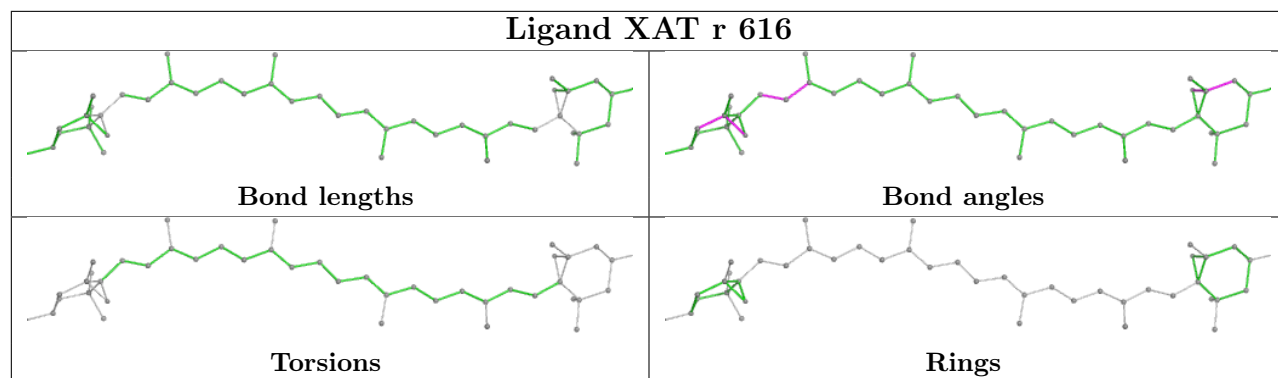




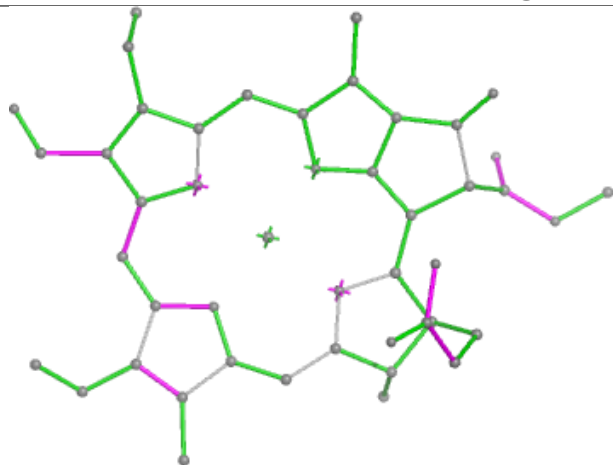




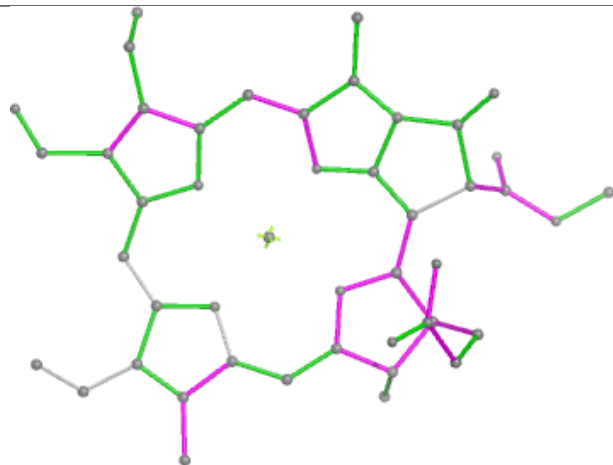




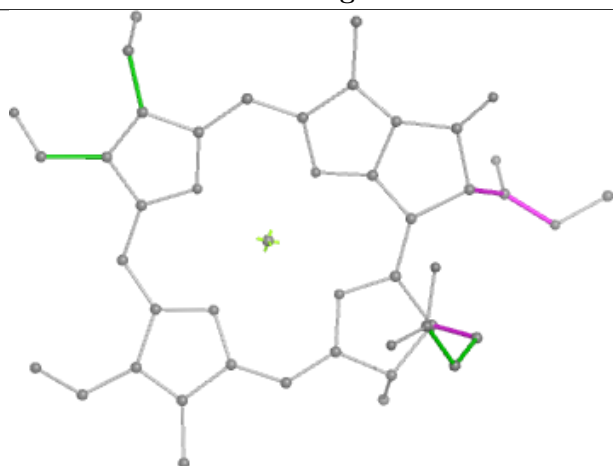
Ligand CHL 4 605



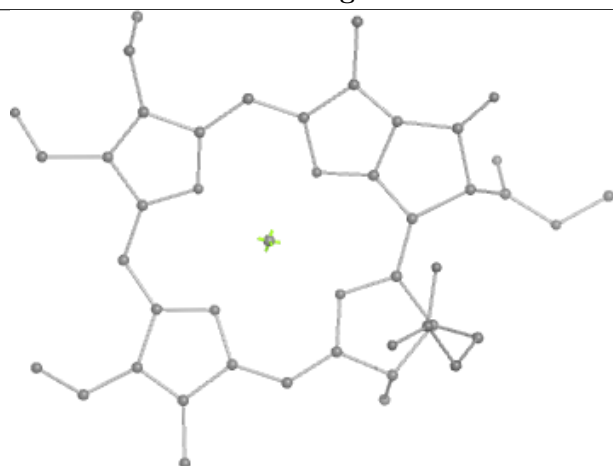
Bond lengths



Bond angles

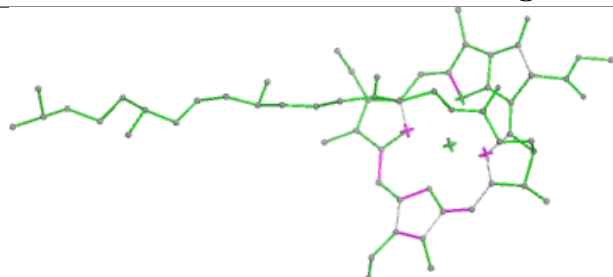


Torsions

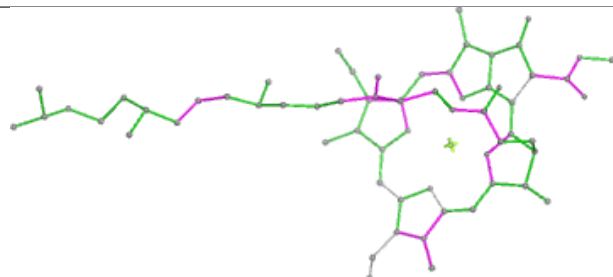


Rings

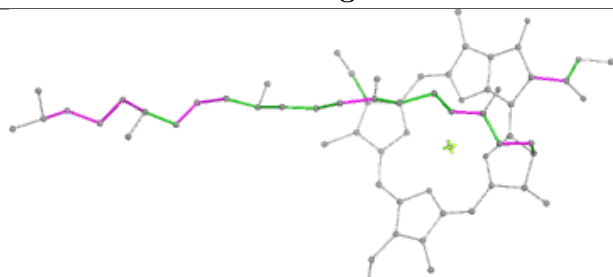
Ligand CLA b 614



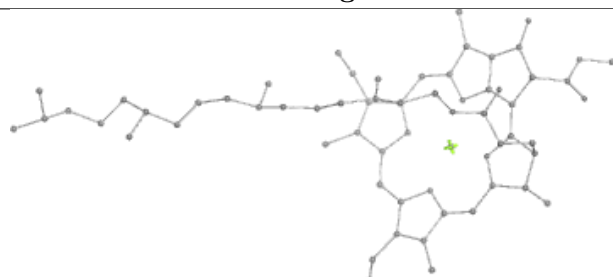
Bond lengths



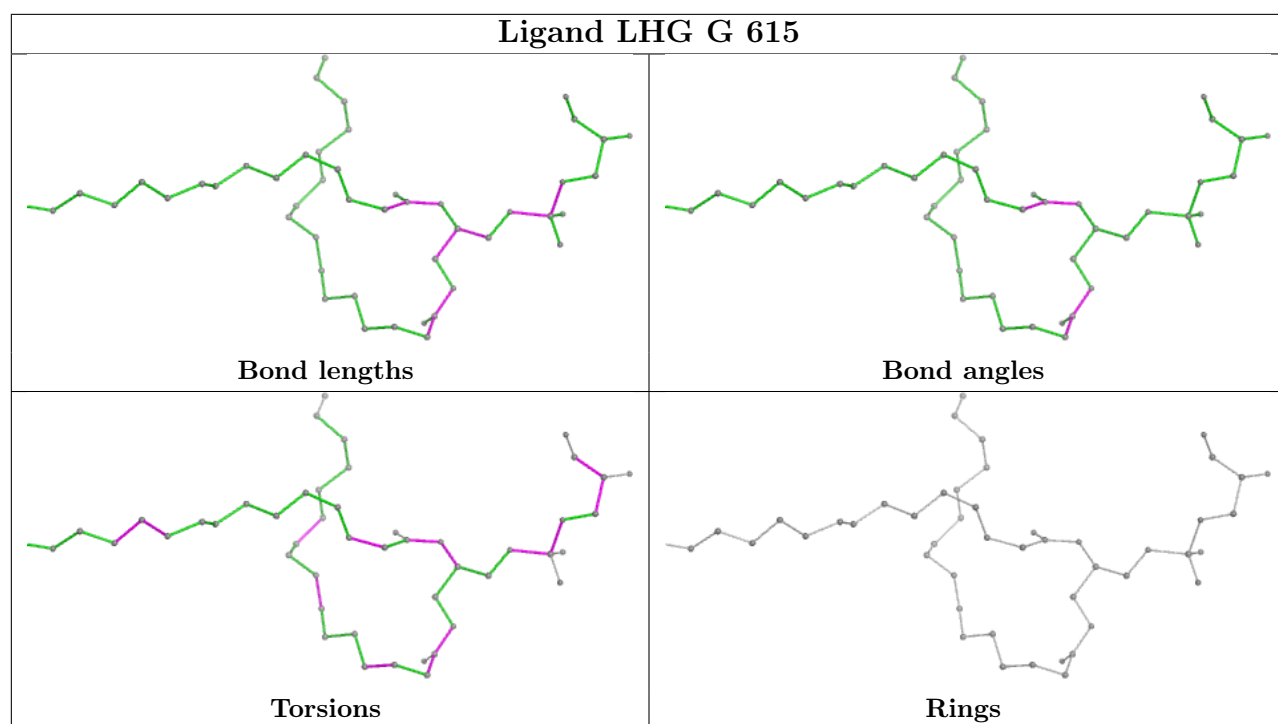
Bond angles

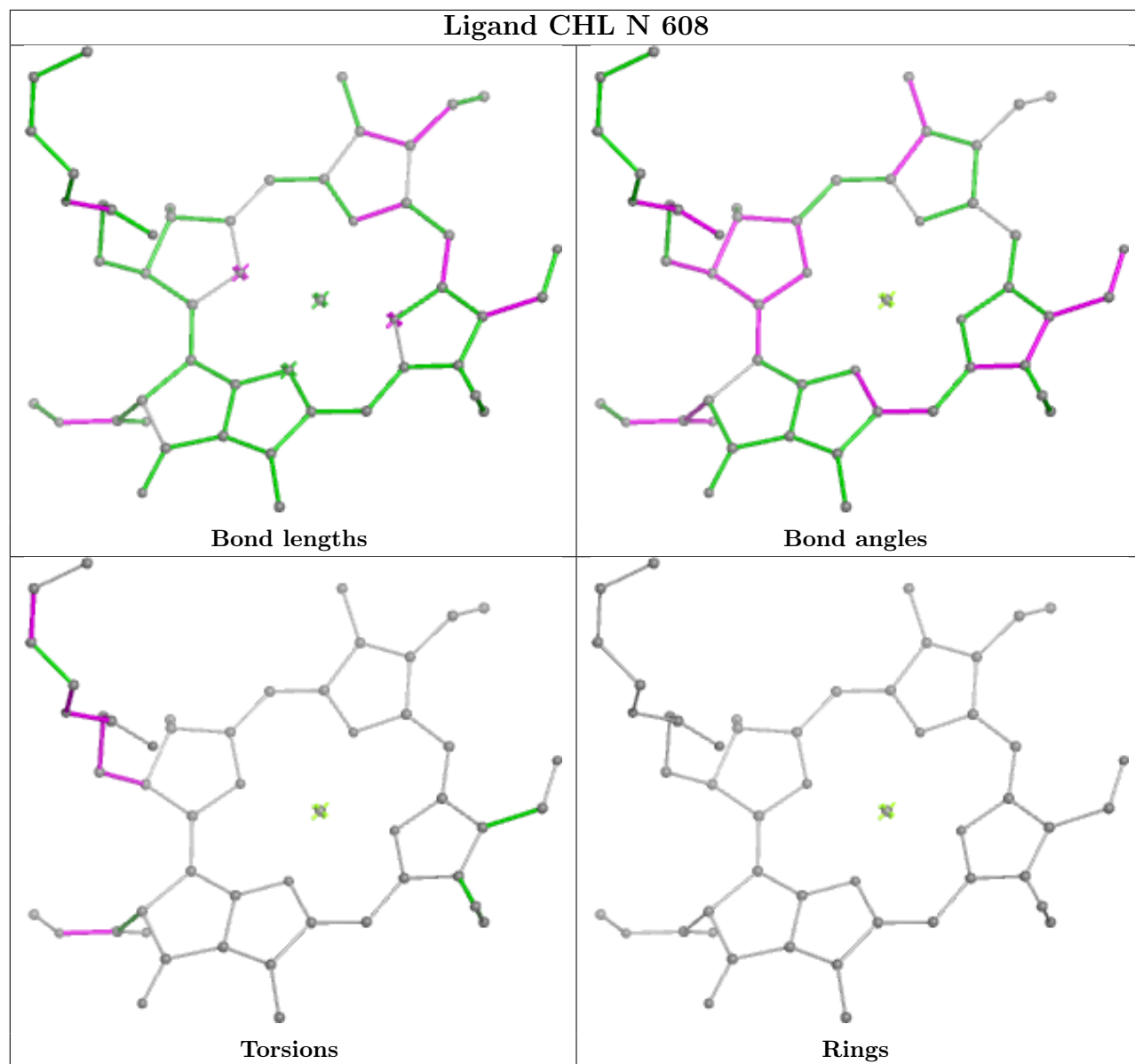


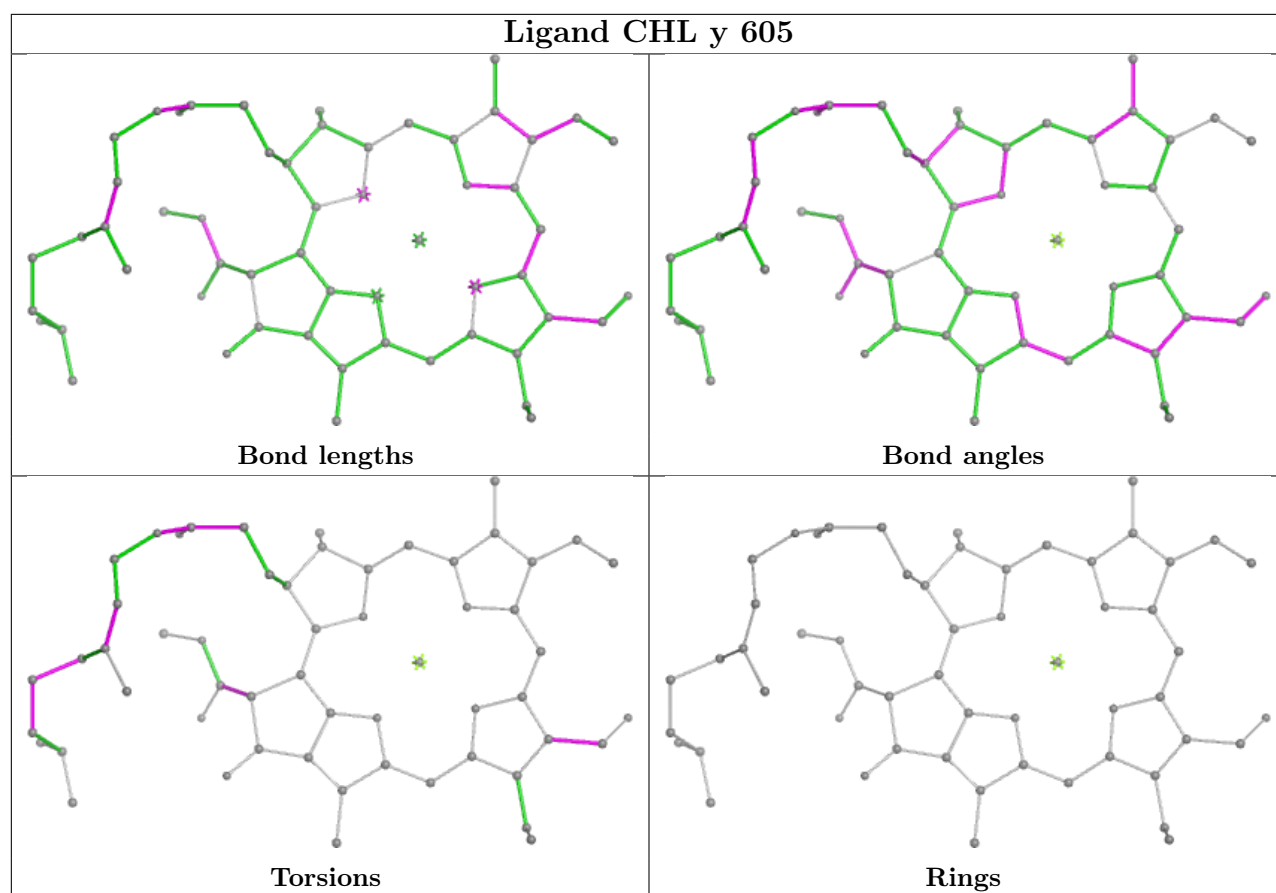
Torsions

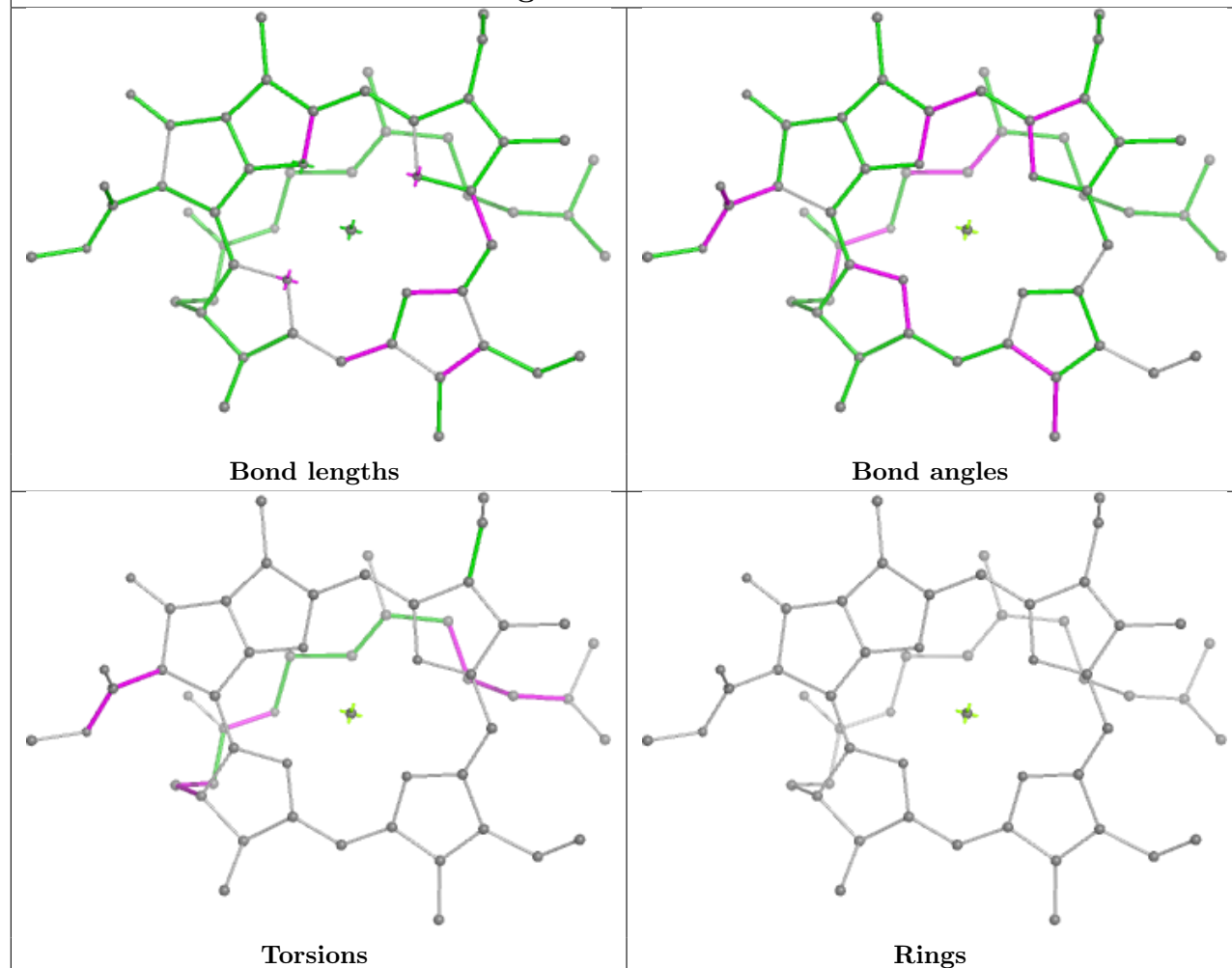
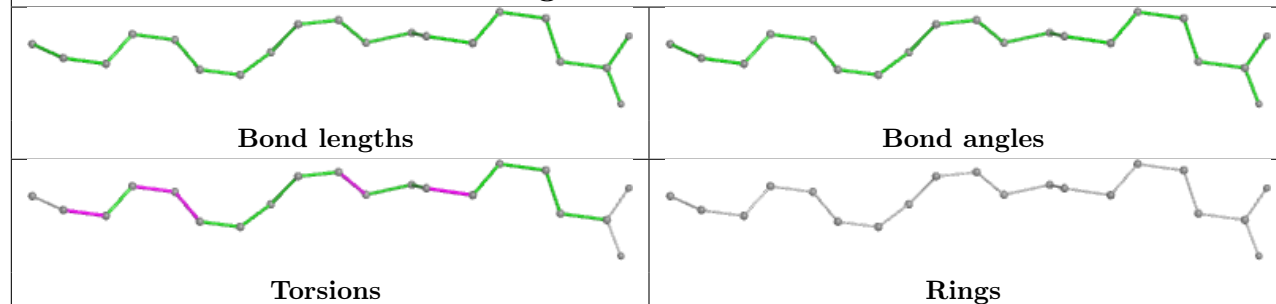


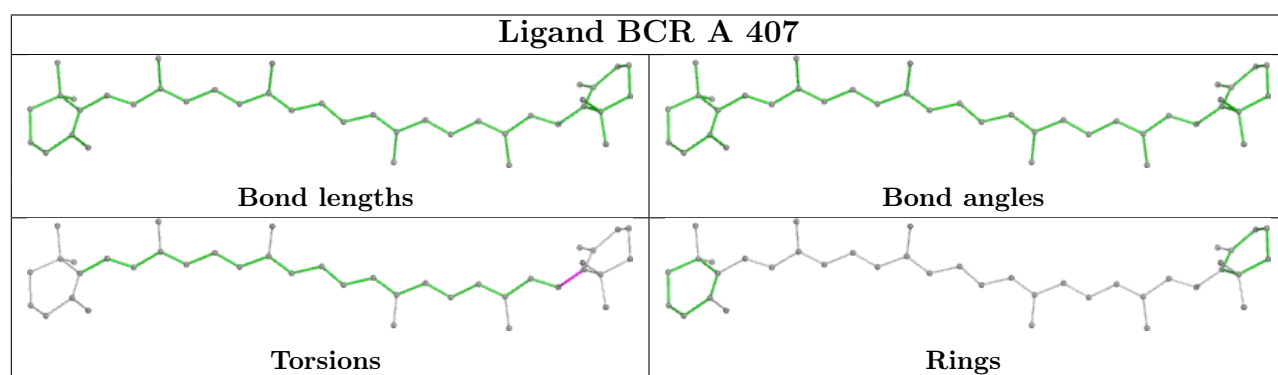
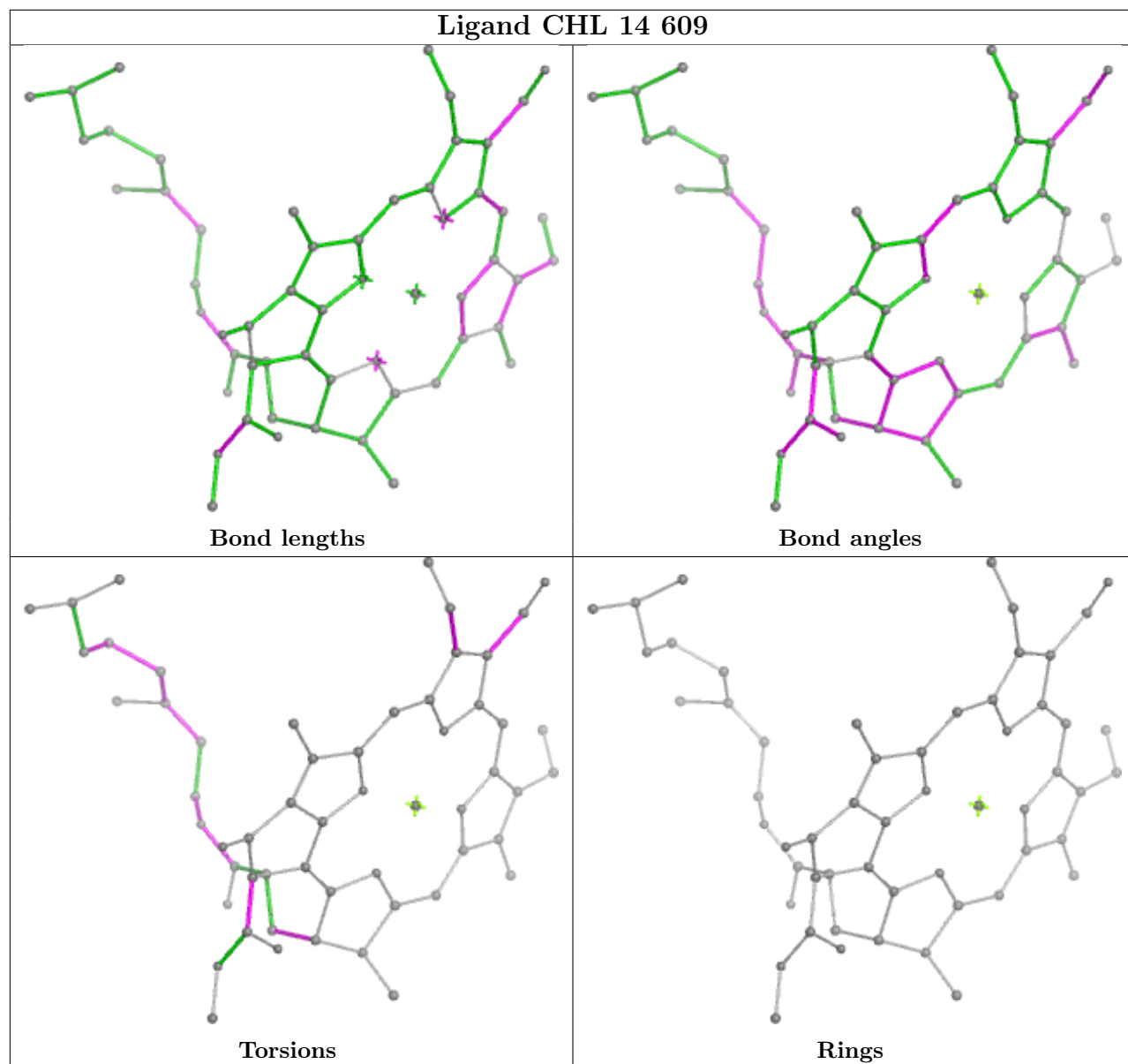
Rings

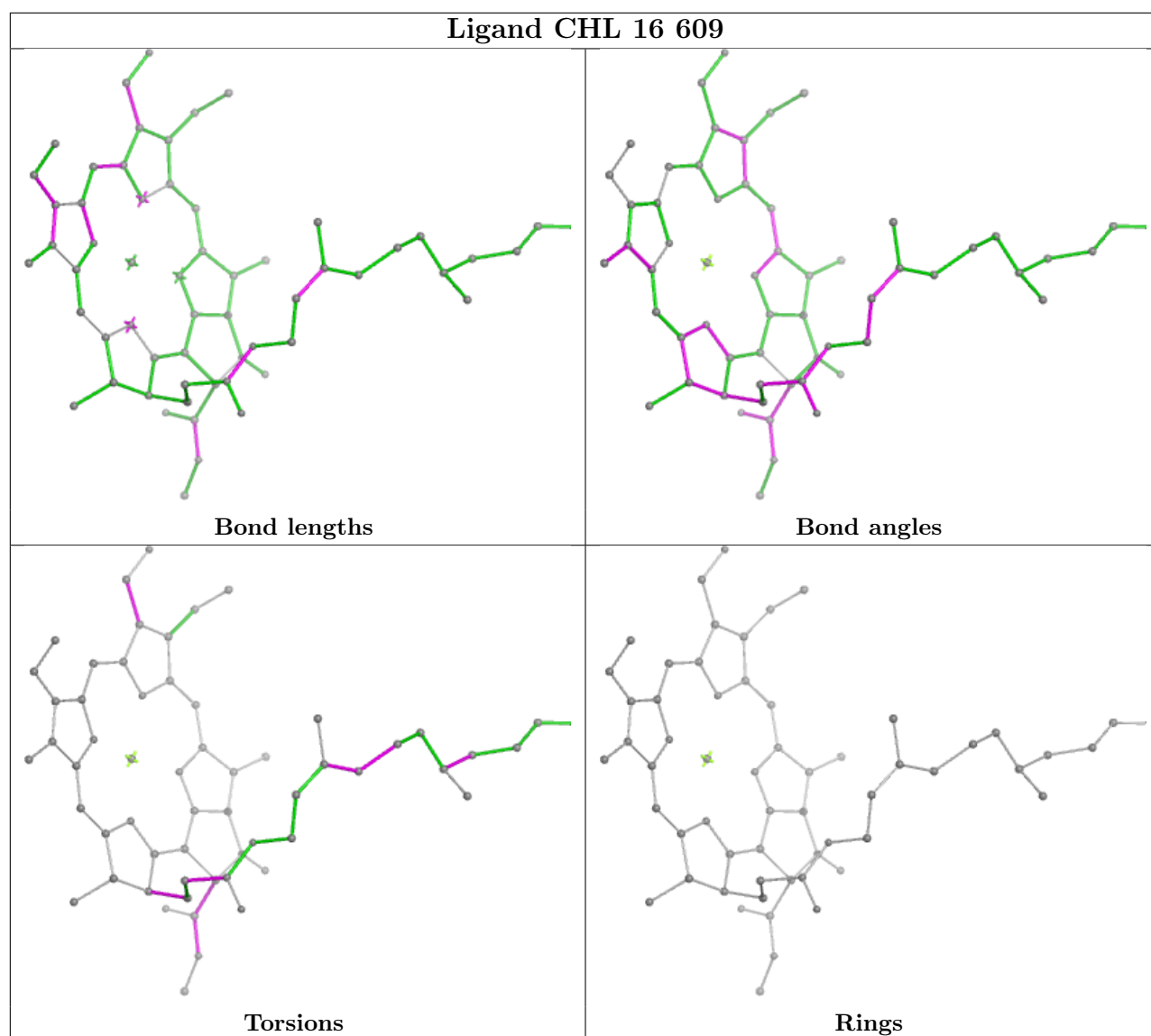


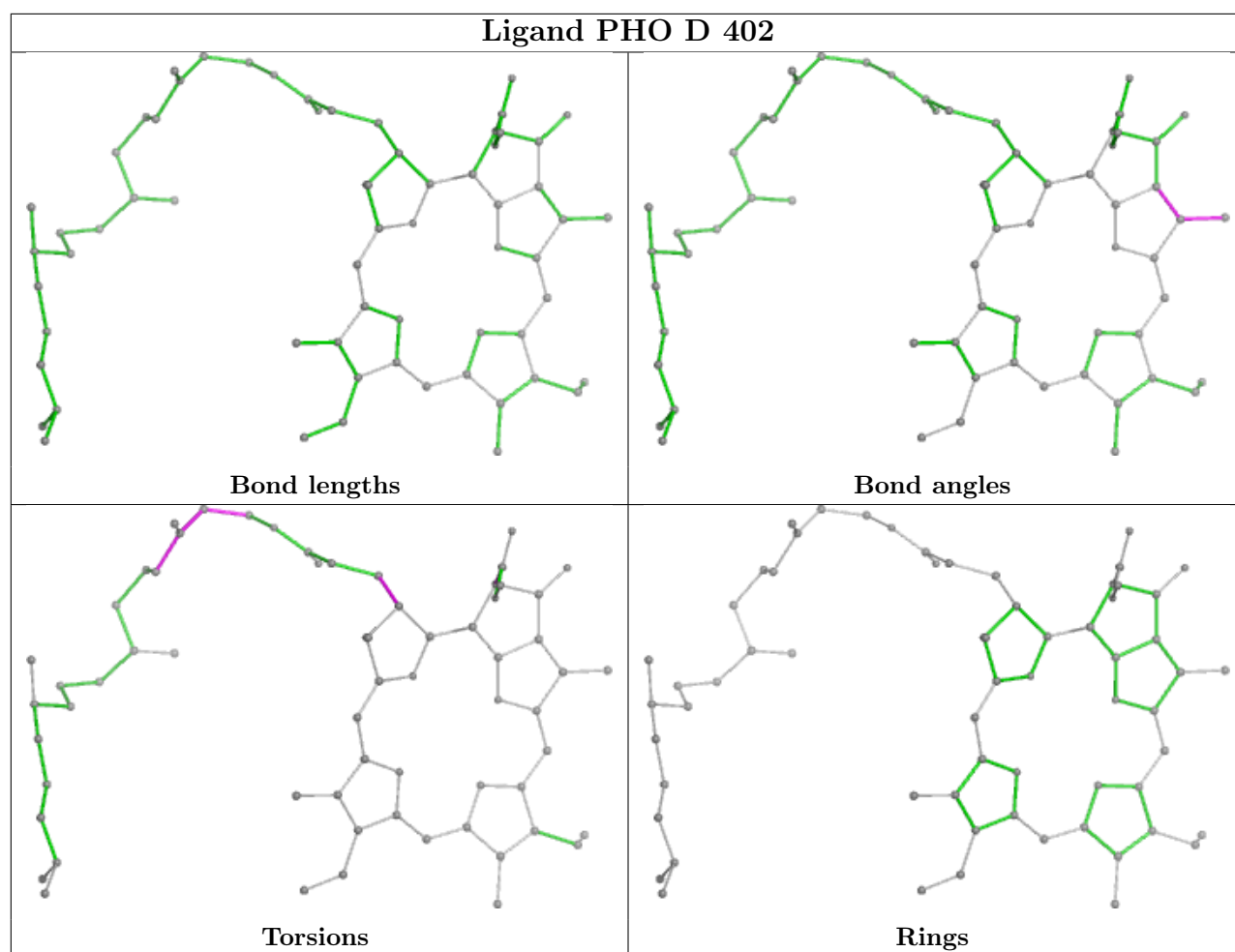


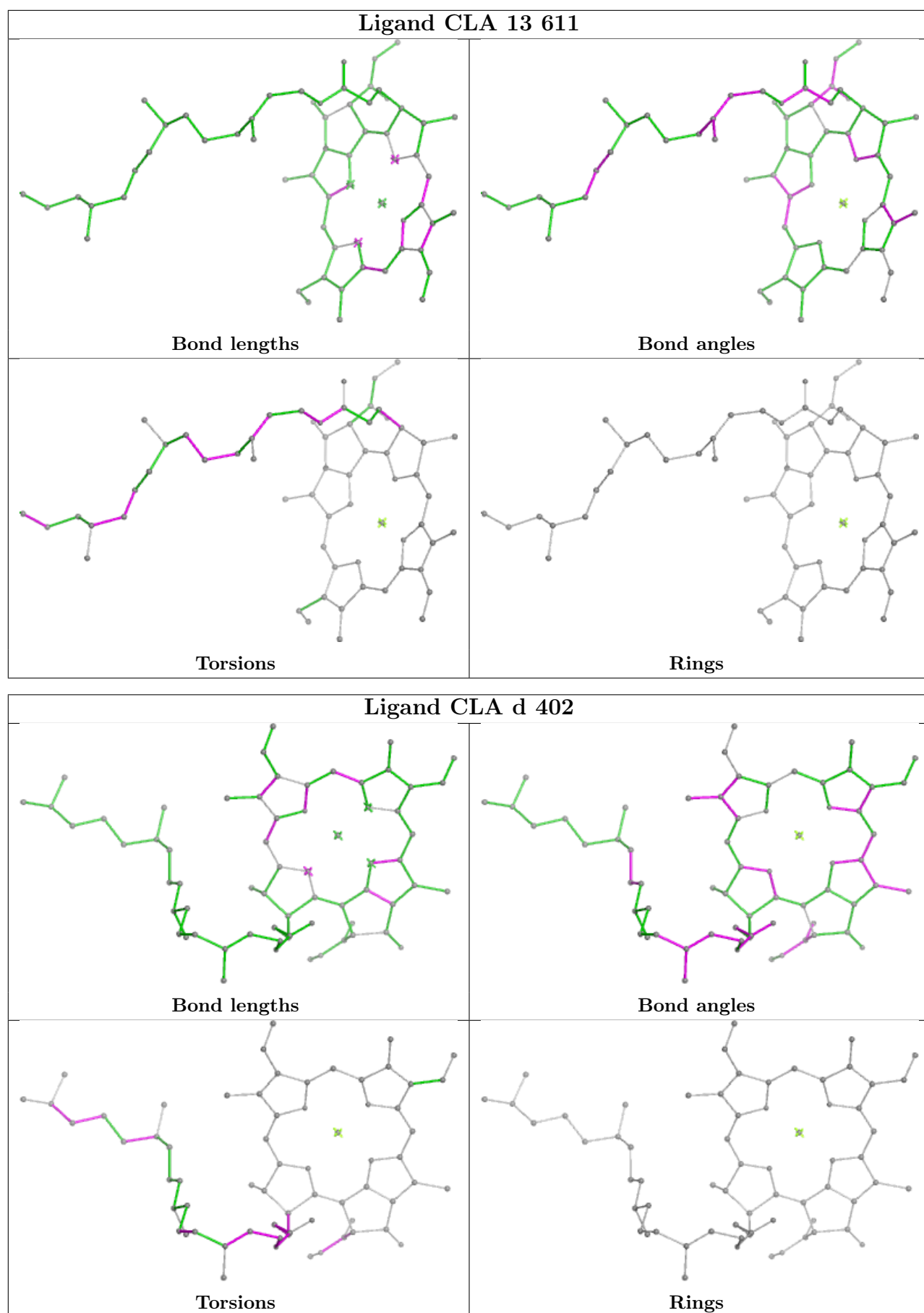


Ligand CLA 3 613**Ligand LNL a 412**

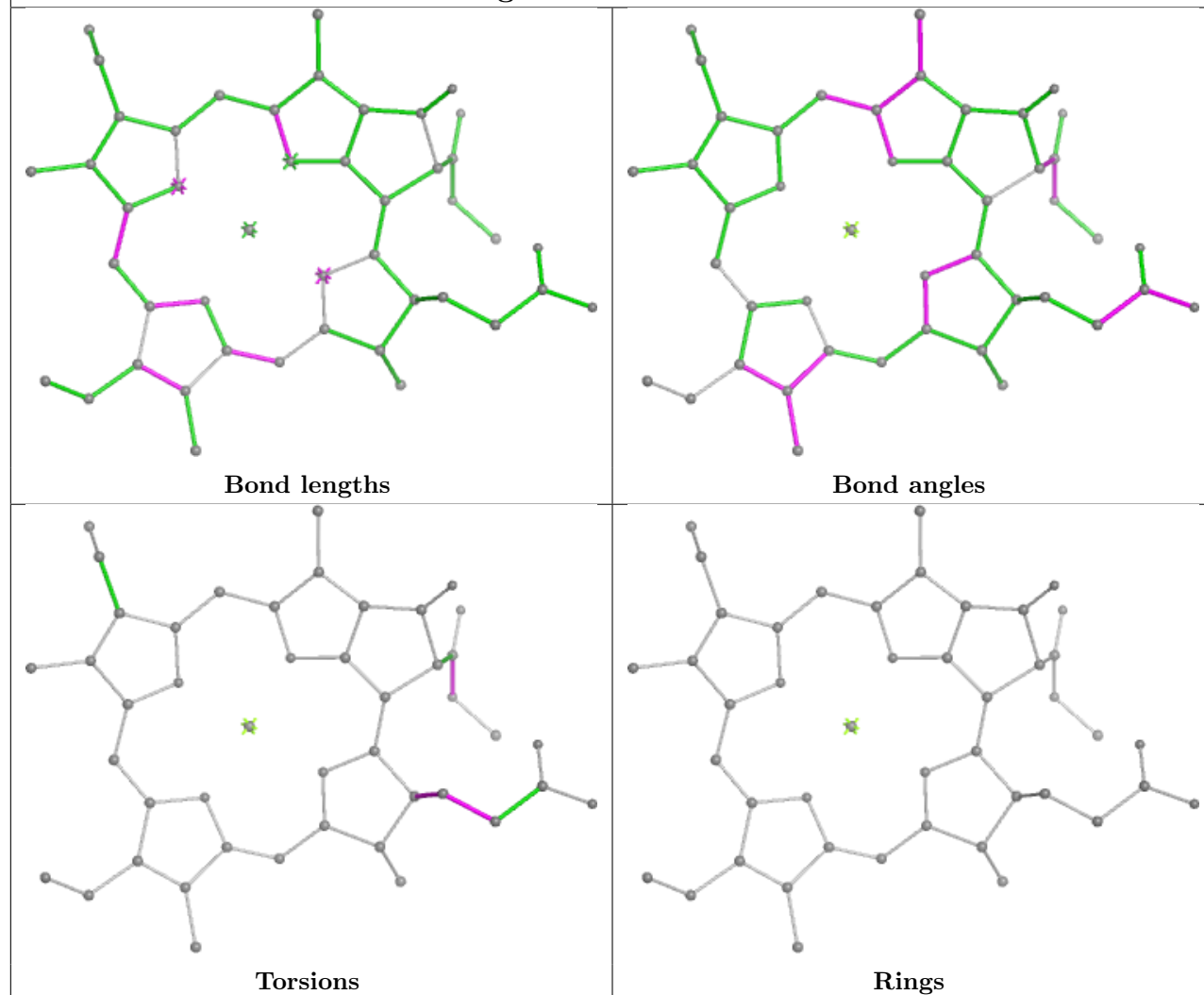




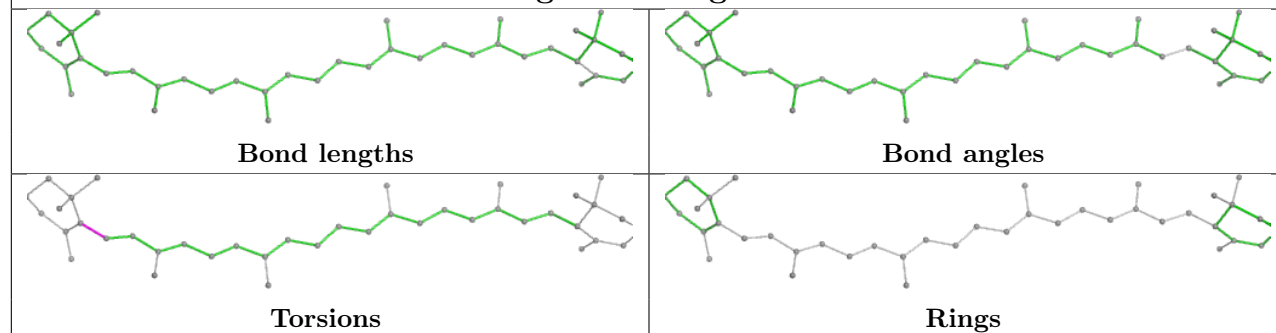


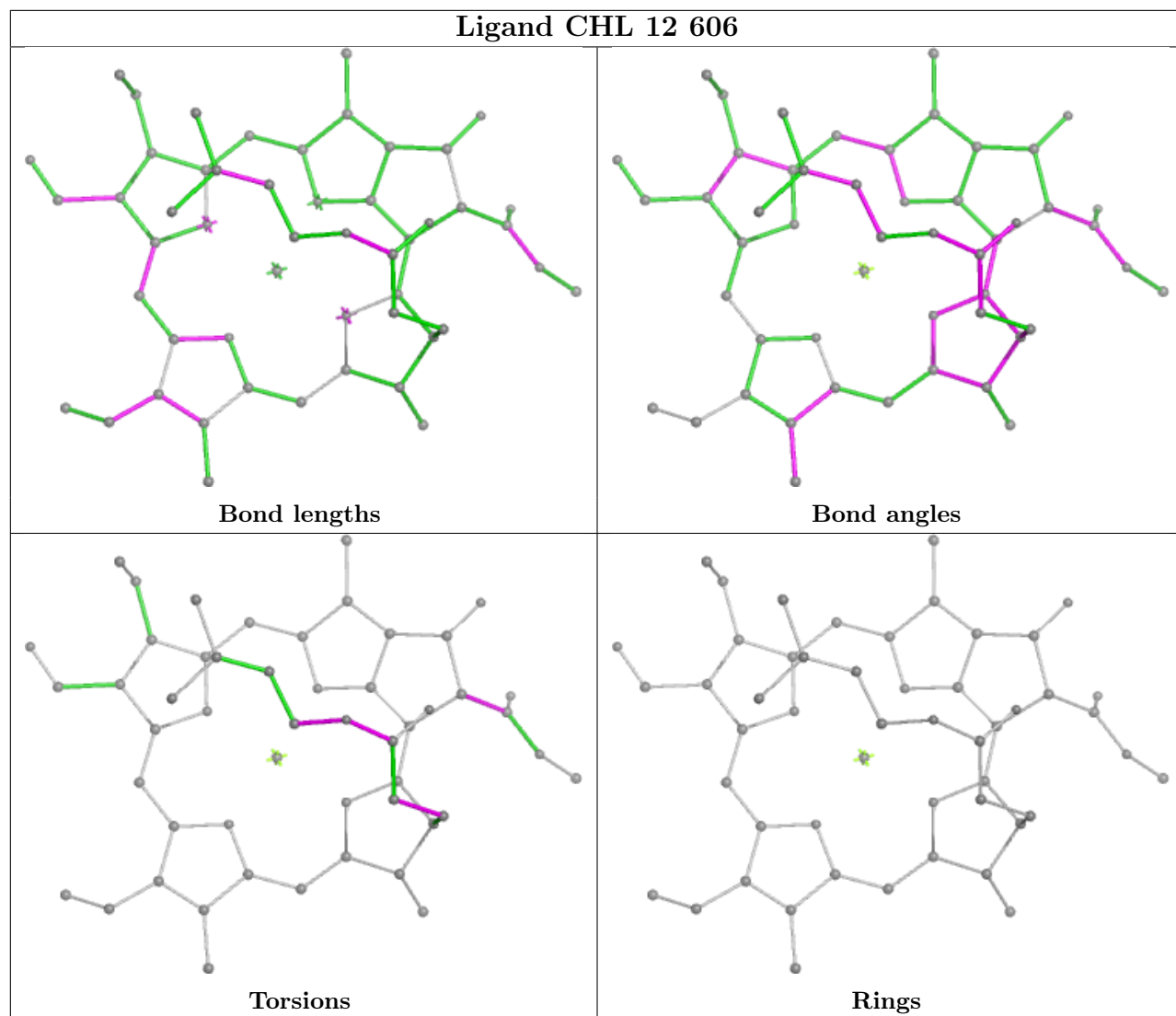


Ligand CLA 13 615

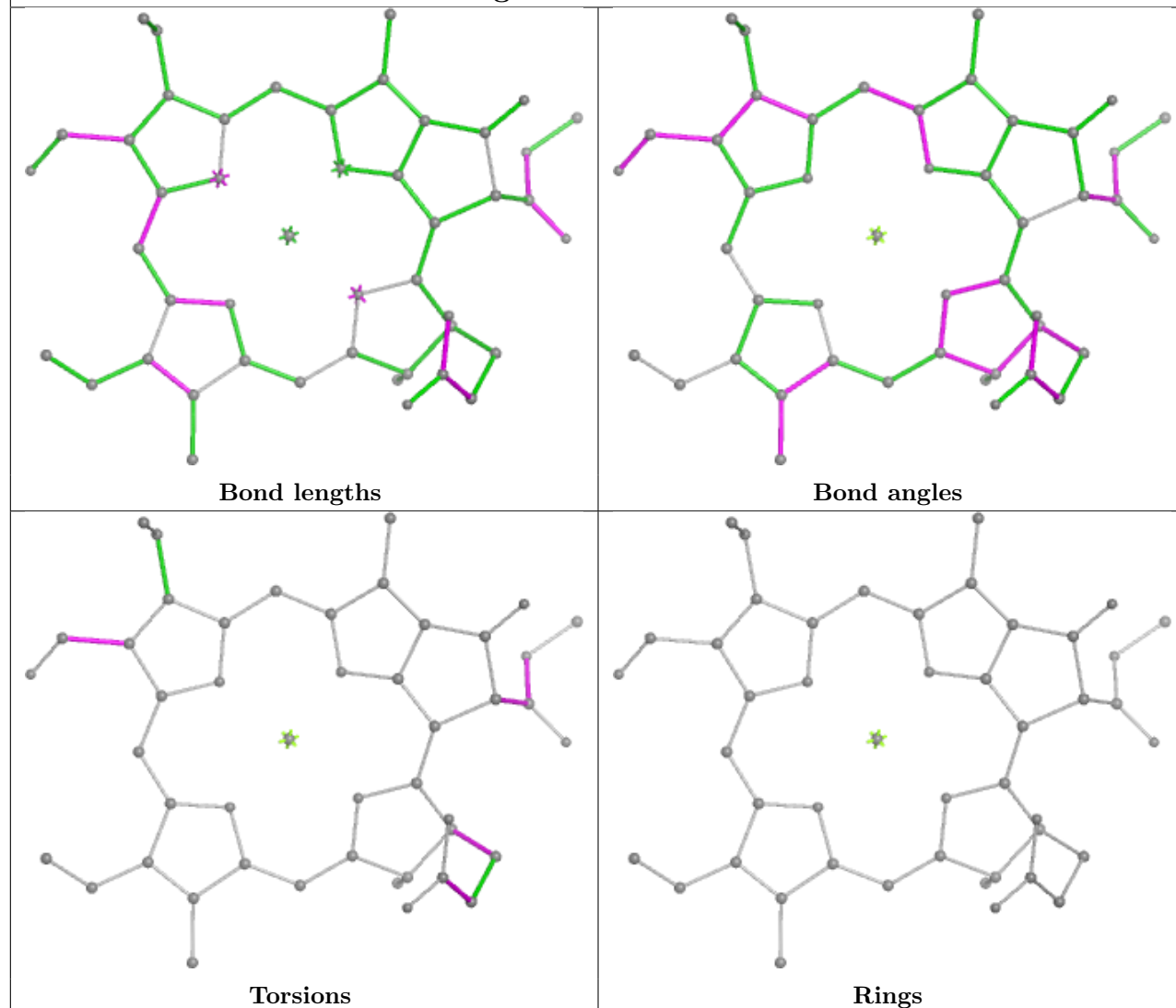


Ligand LUT g 616

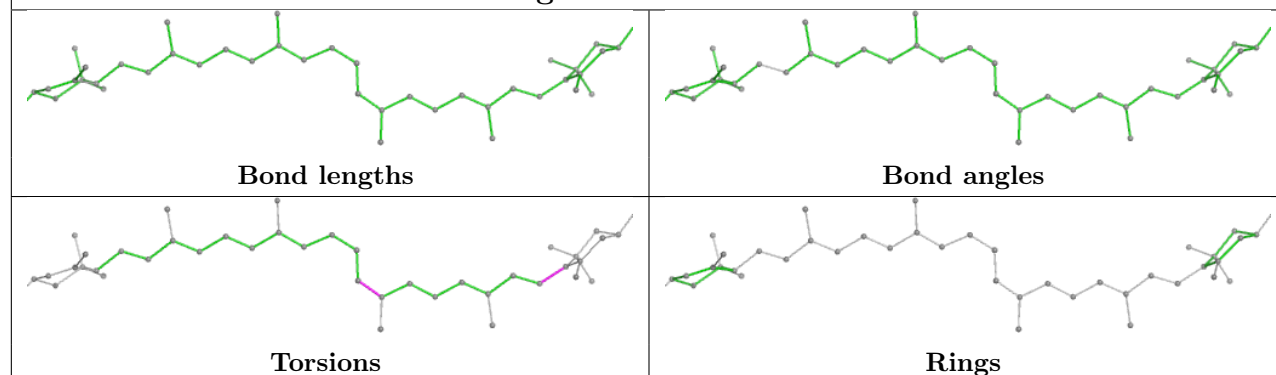


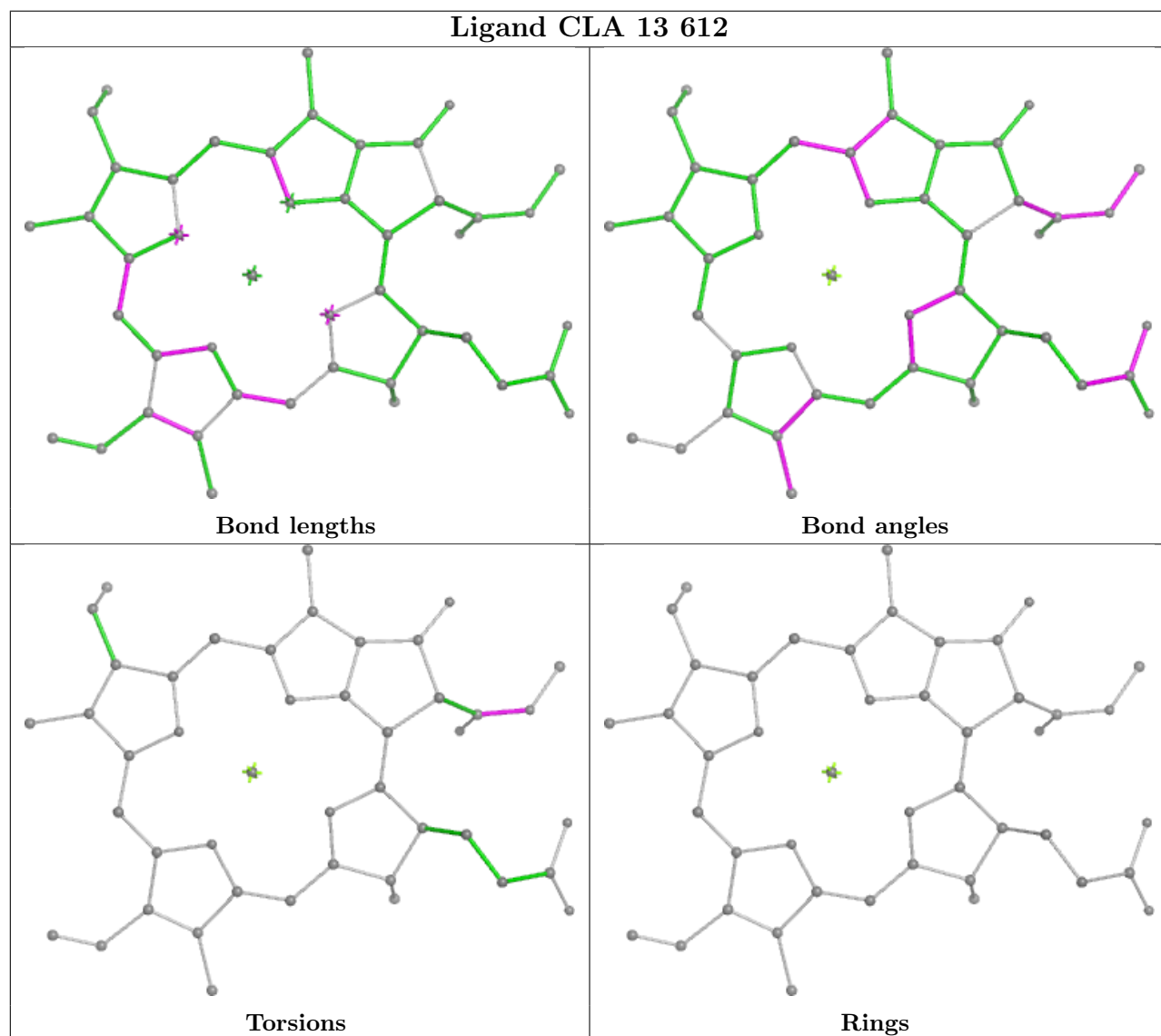
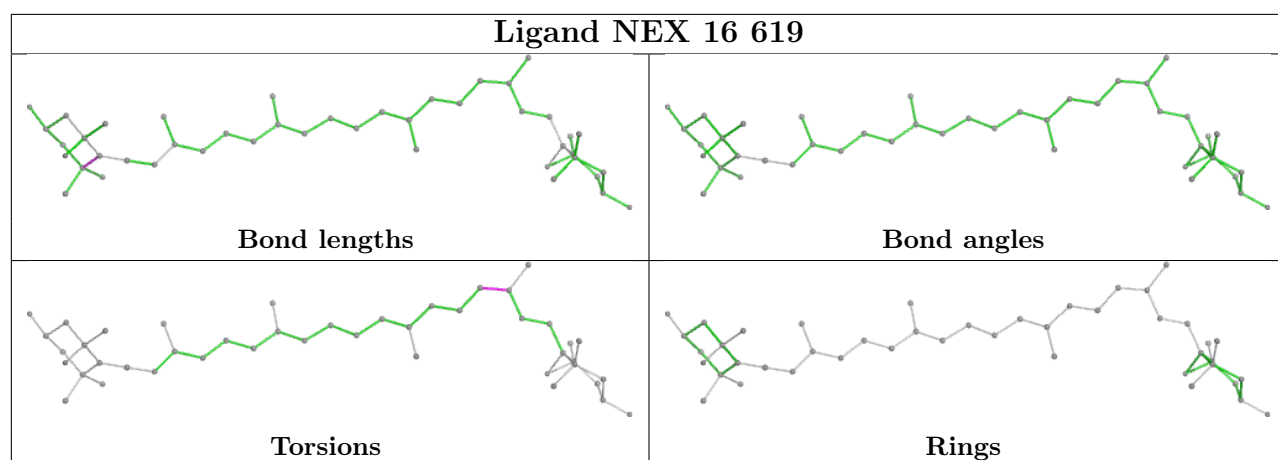


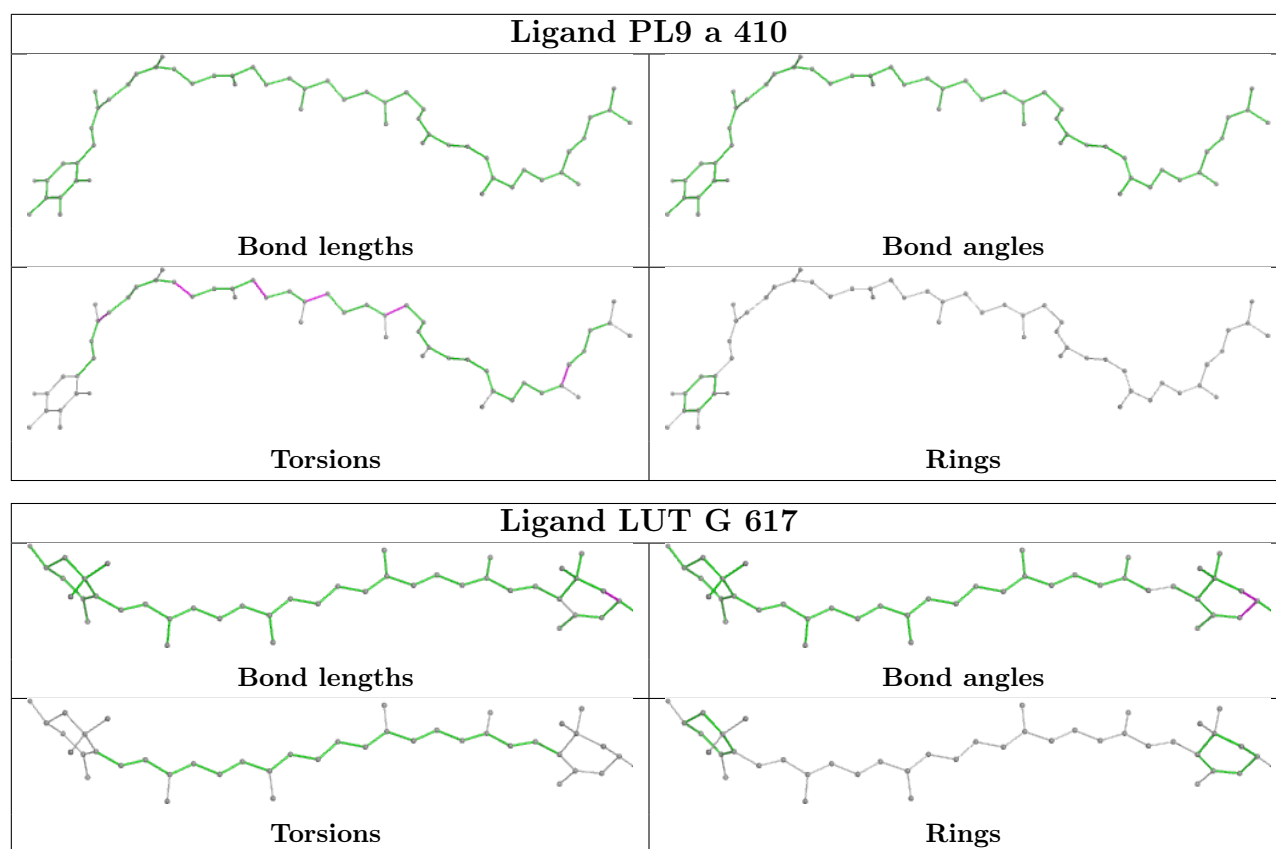
Ligand CHL 2 605



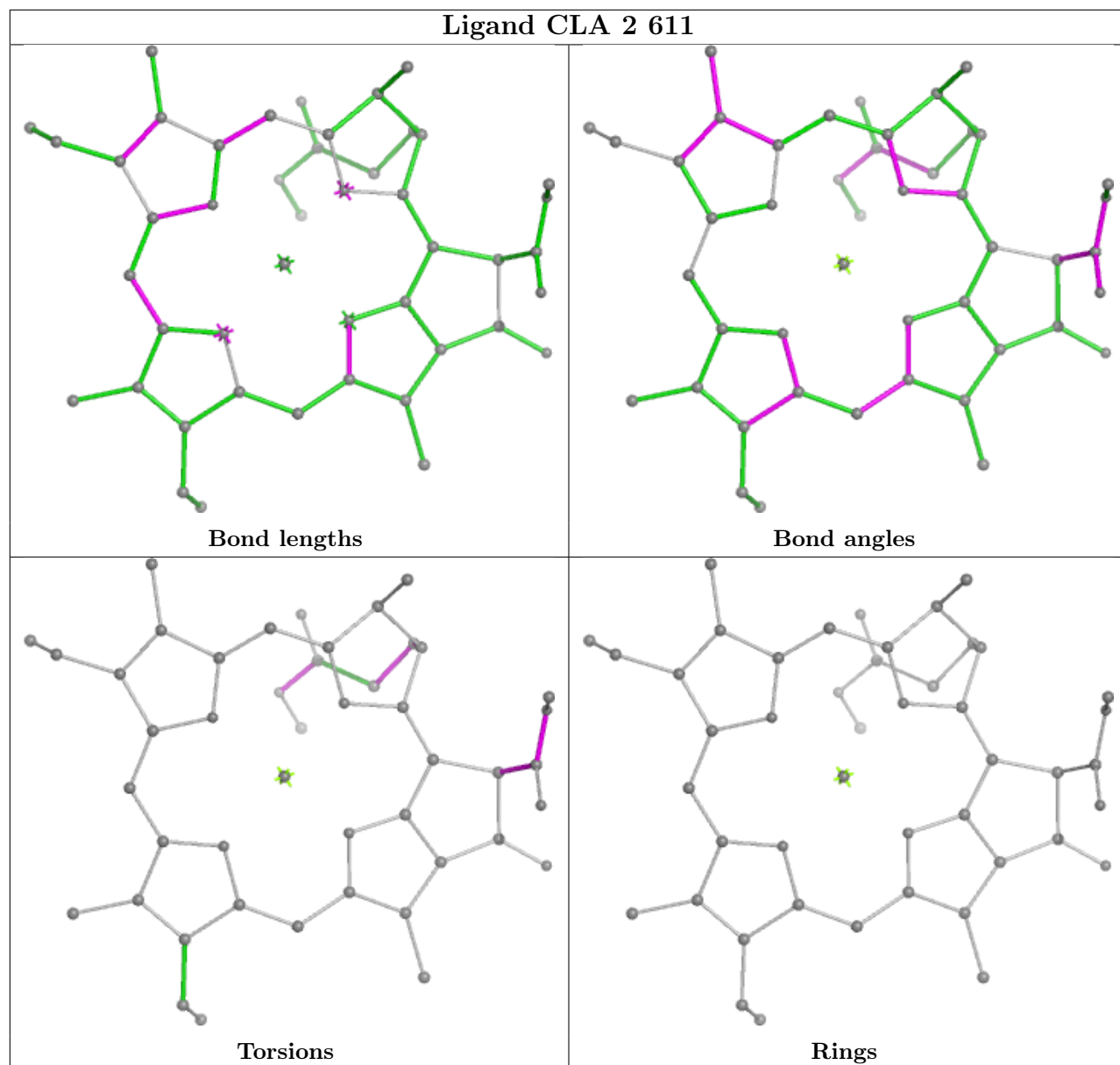
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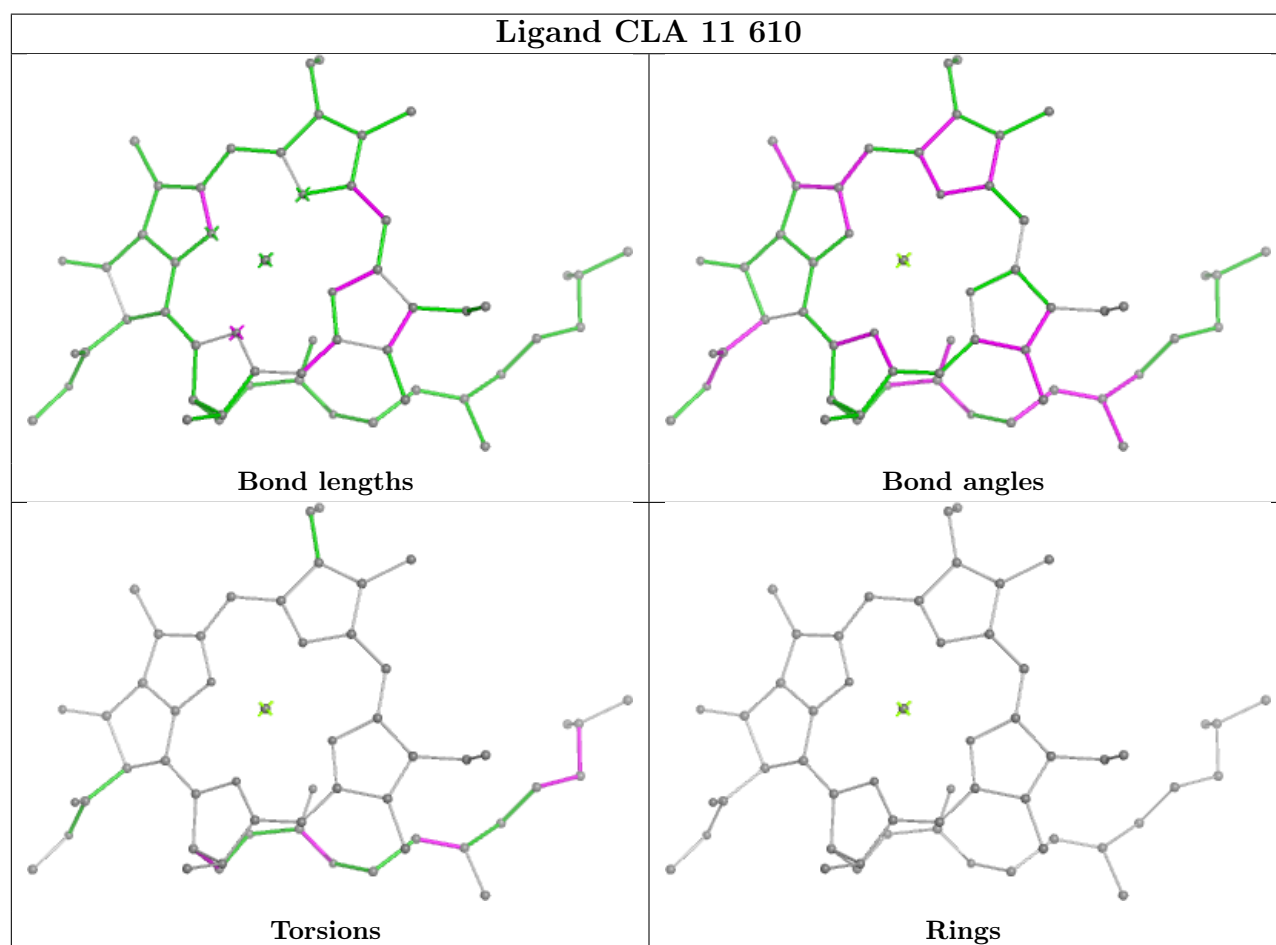
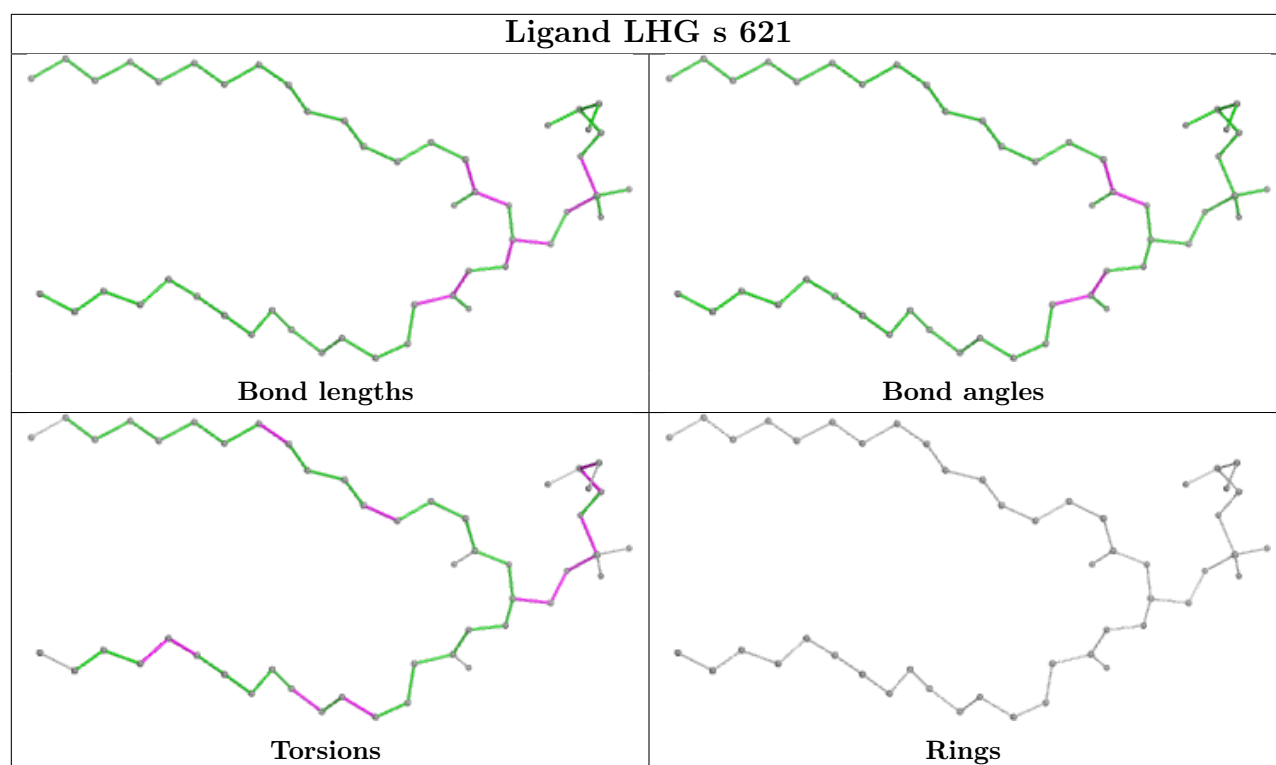


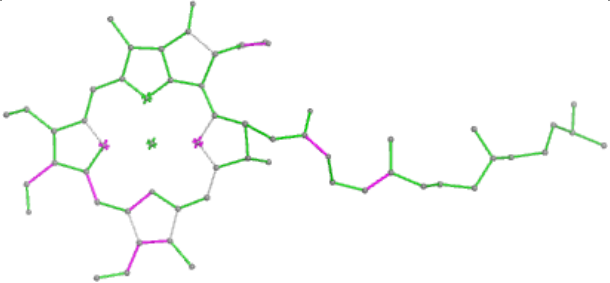
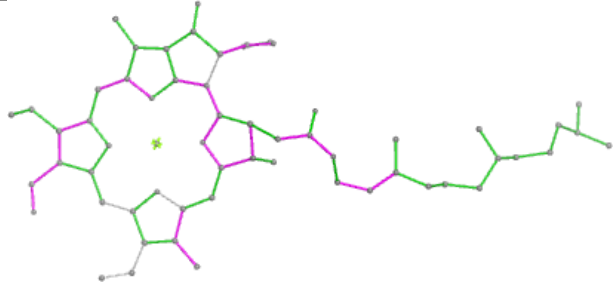
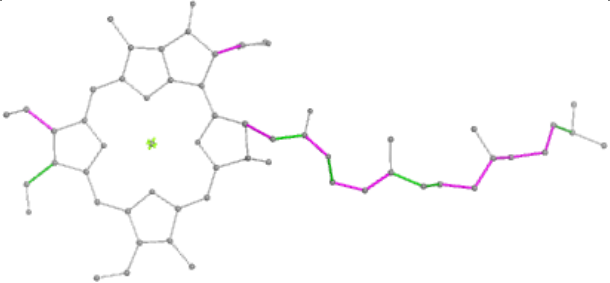
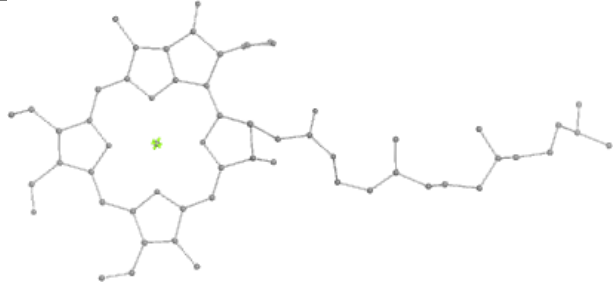
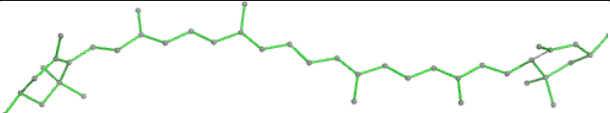
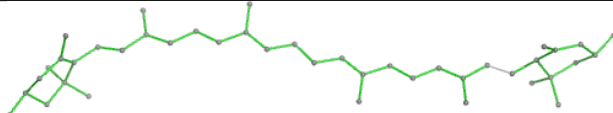
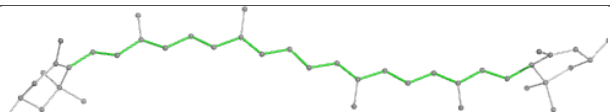
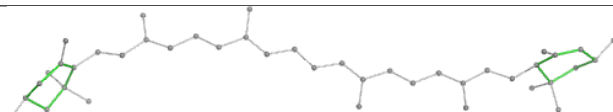
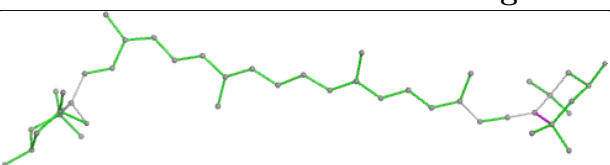
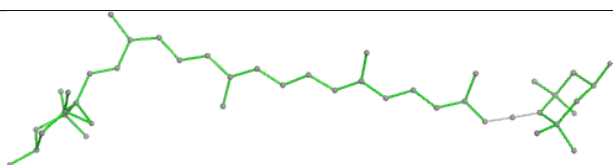
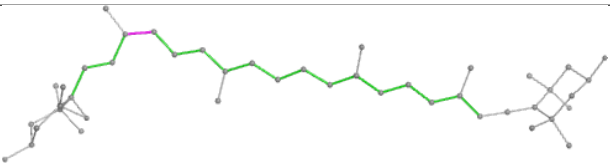
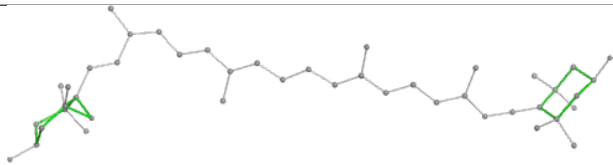




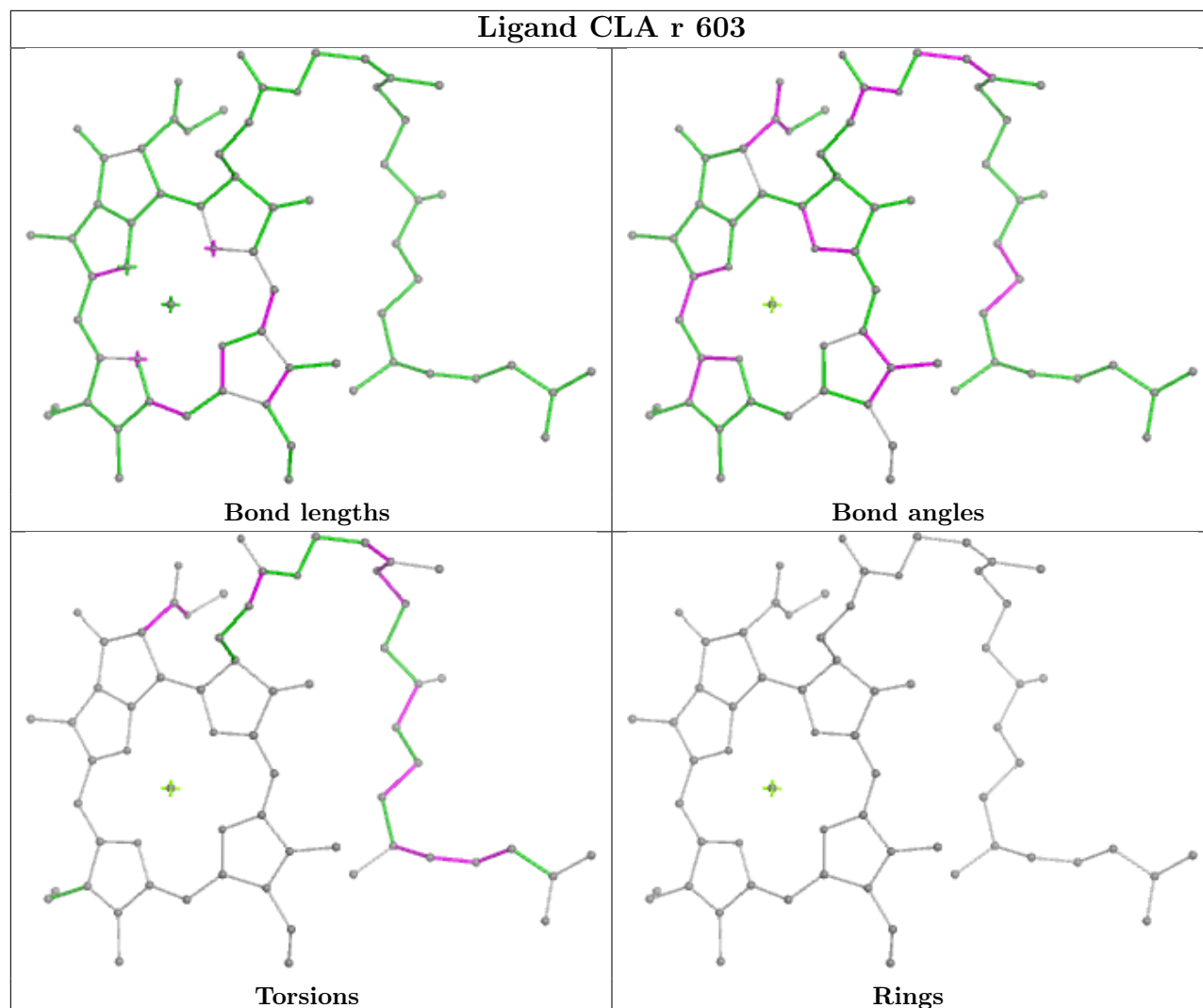
Ligand CLA 2 611



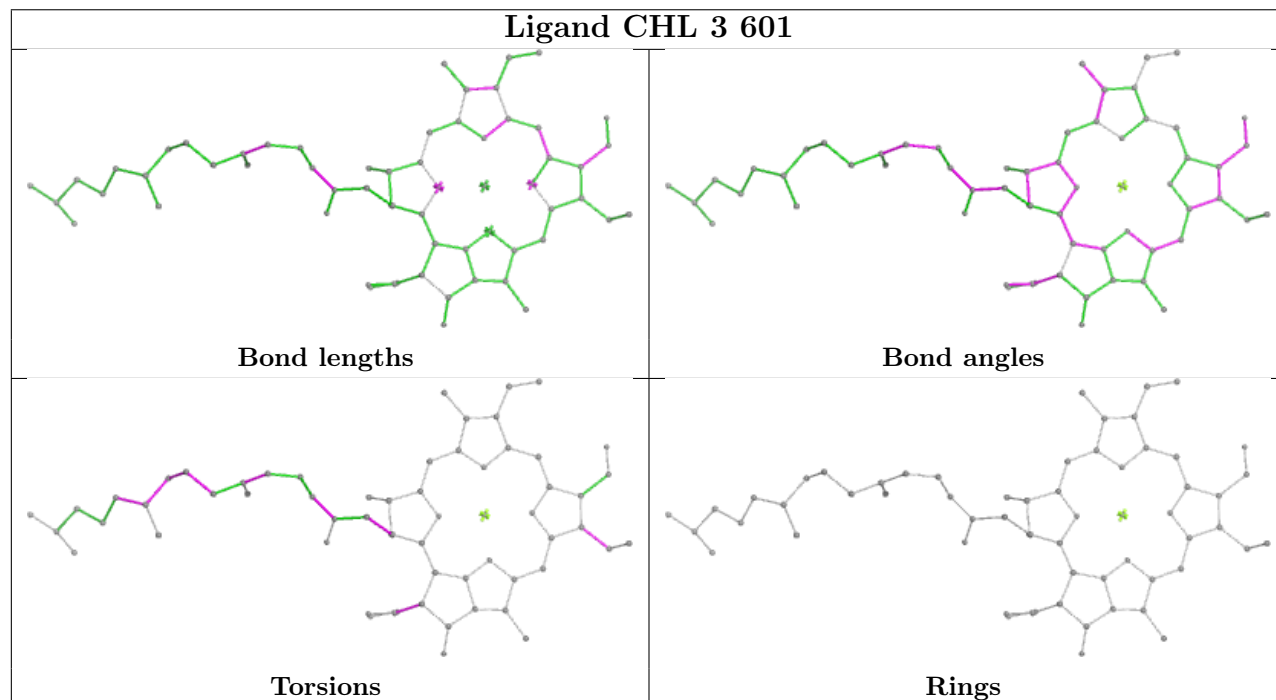


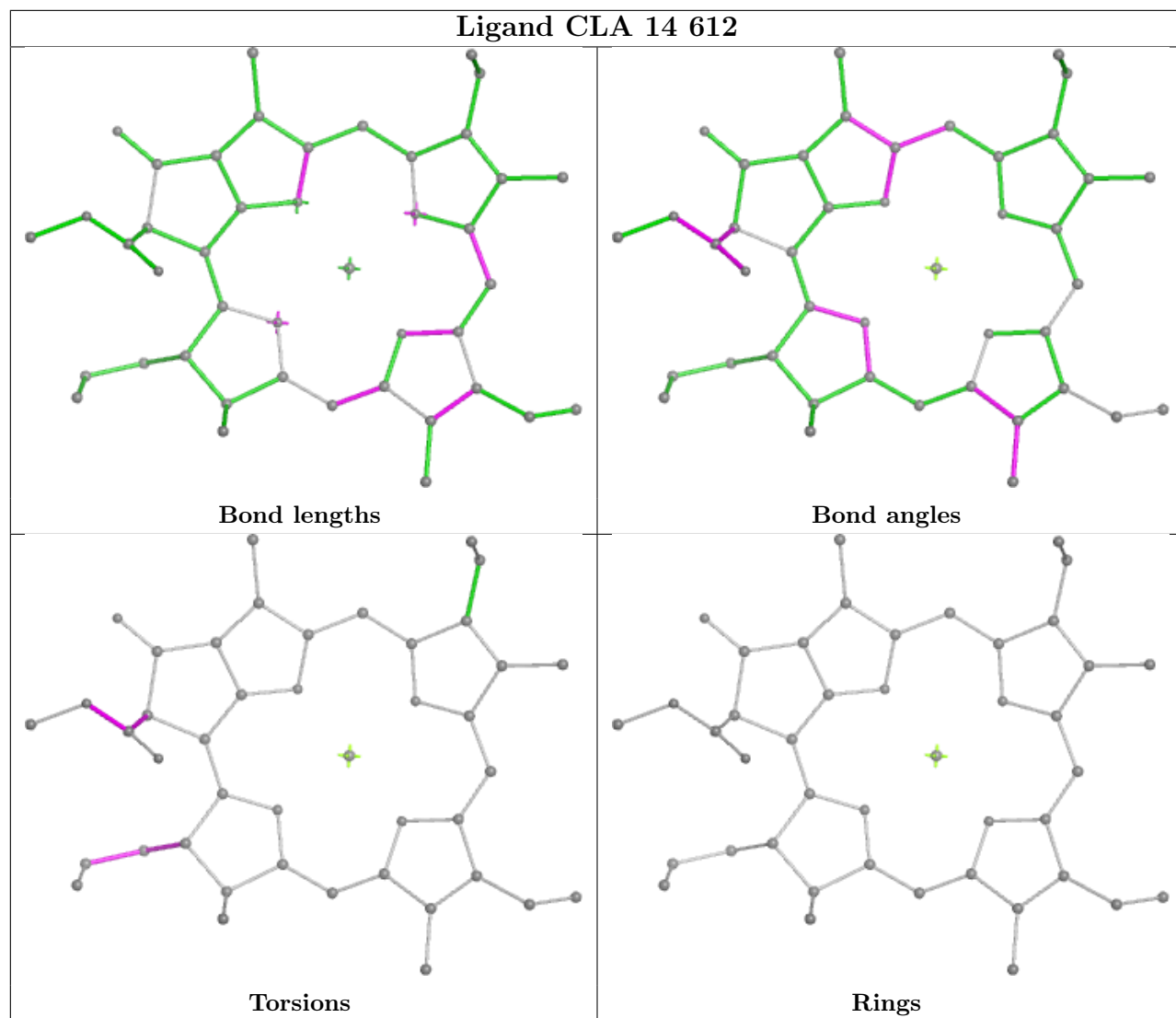
Ligand CHL 6 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT n 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand NEX 13 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA r 603

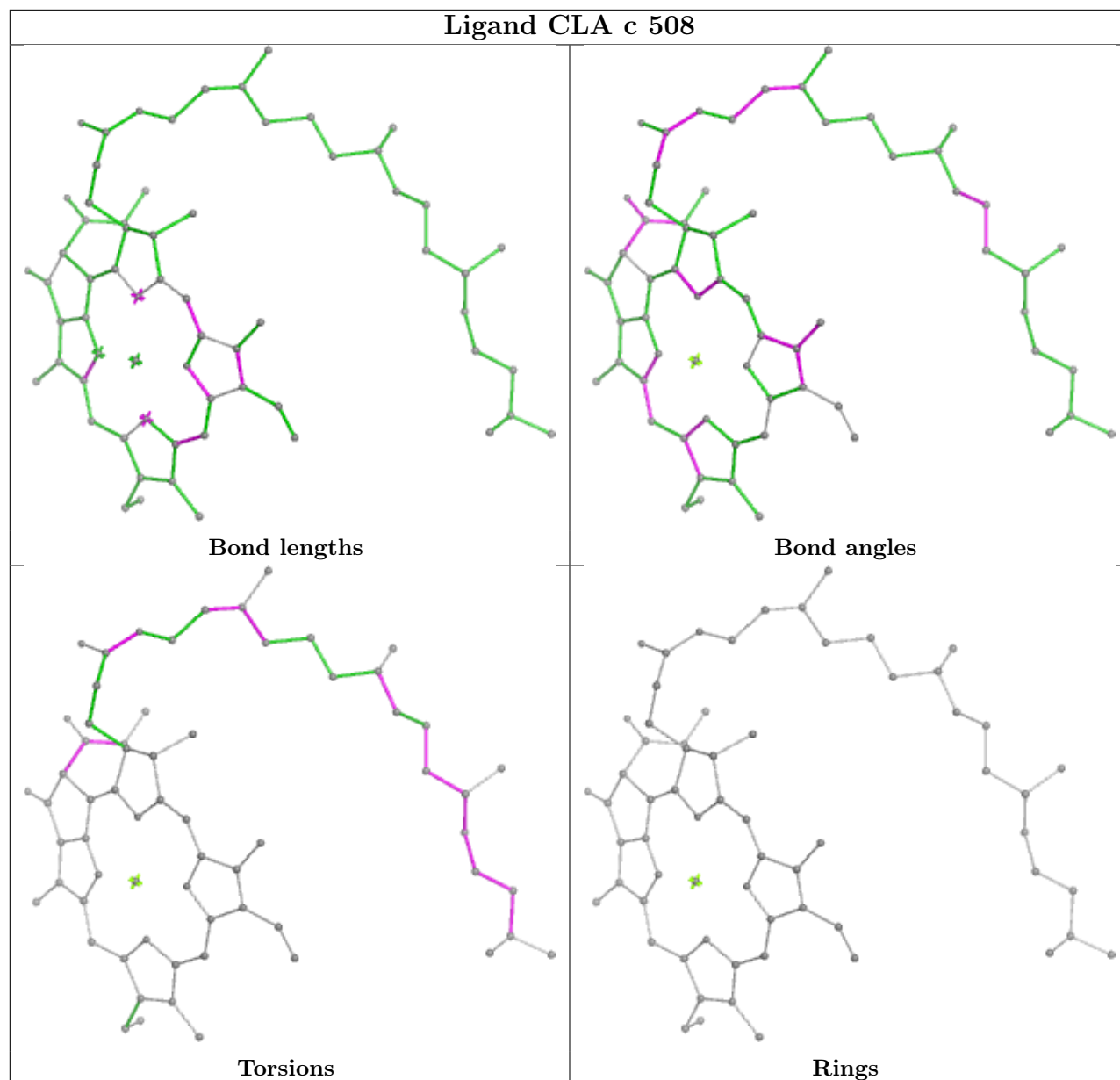


Ligand CHL 3 601

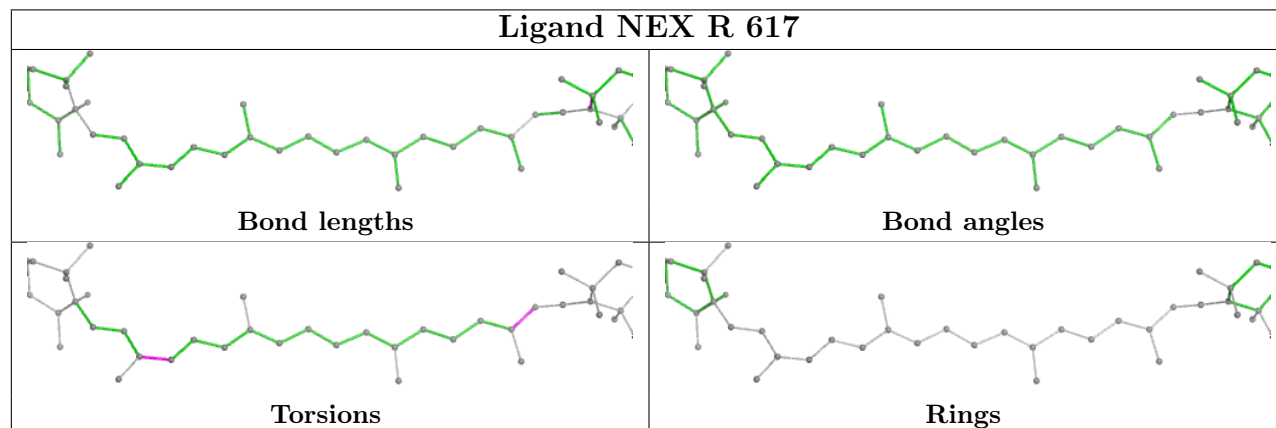




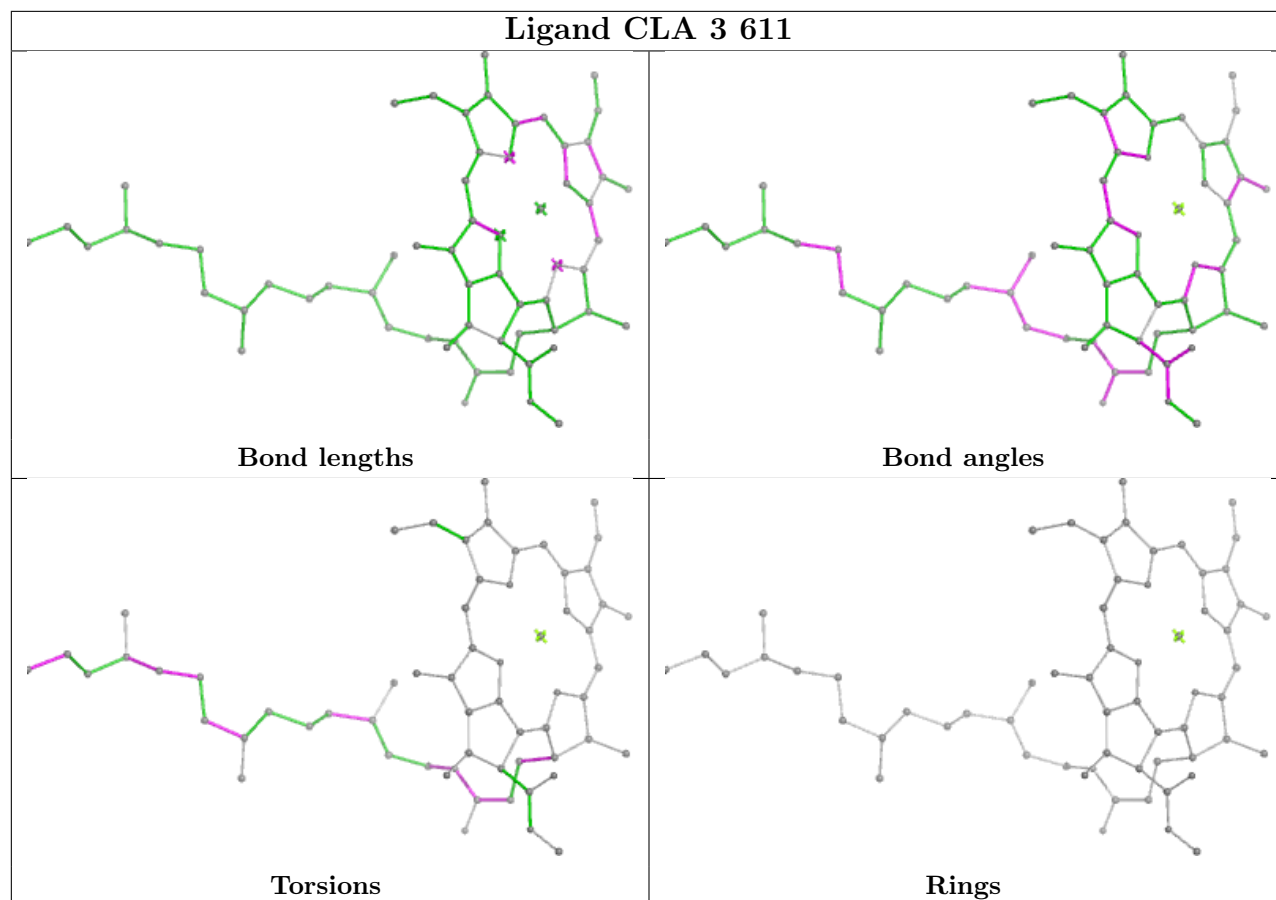
Ligand CLA c 508



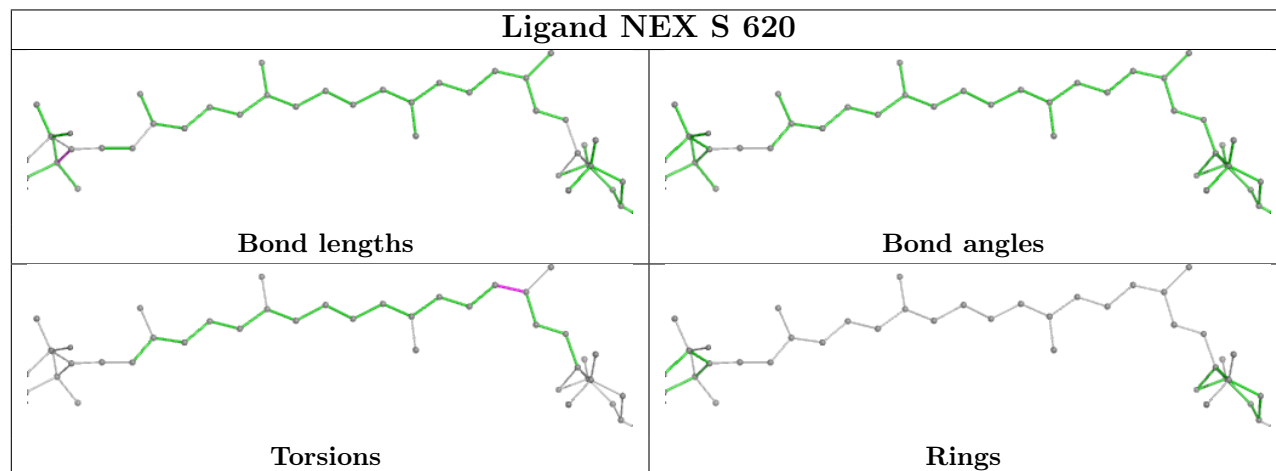
Ligand NEX R 617

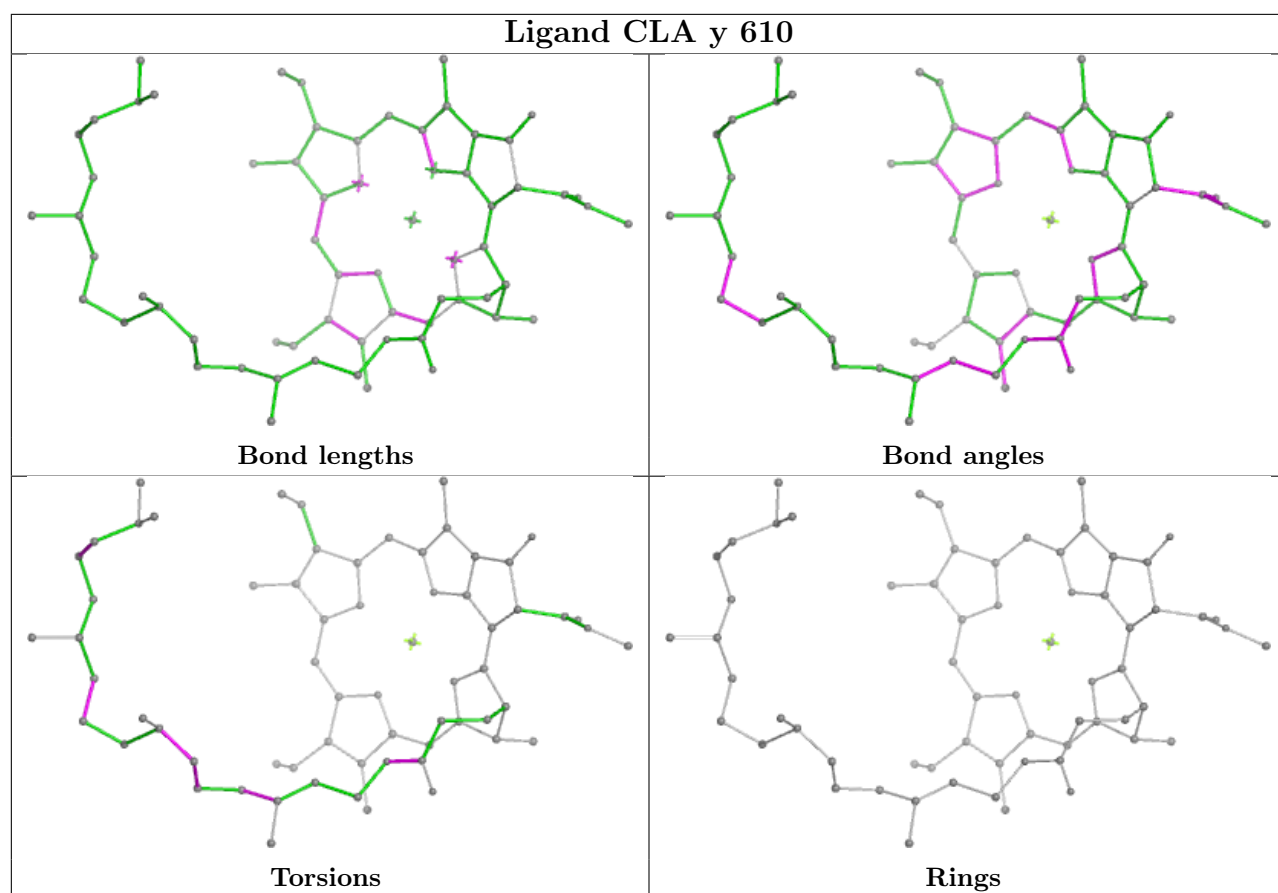


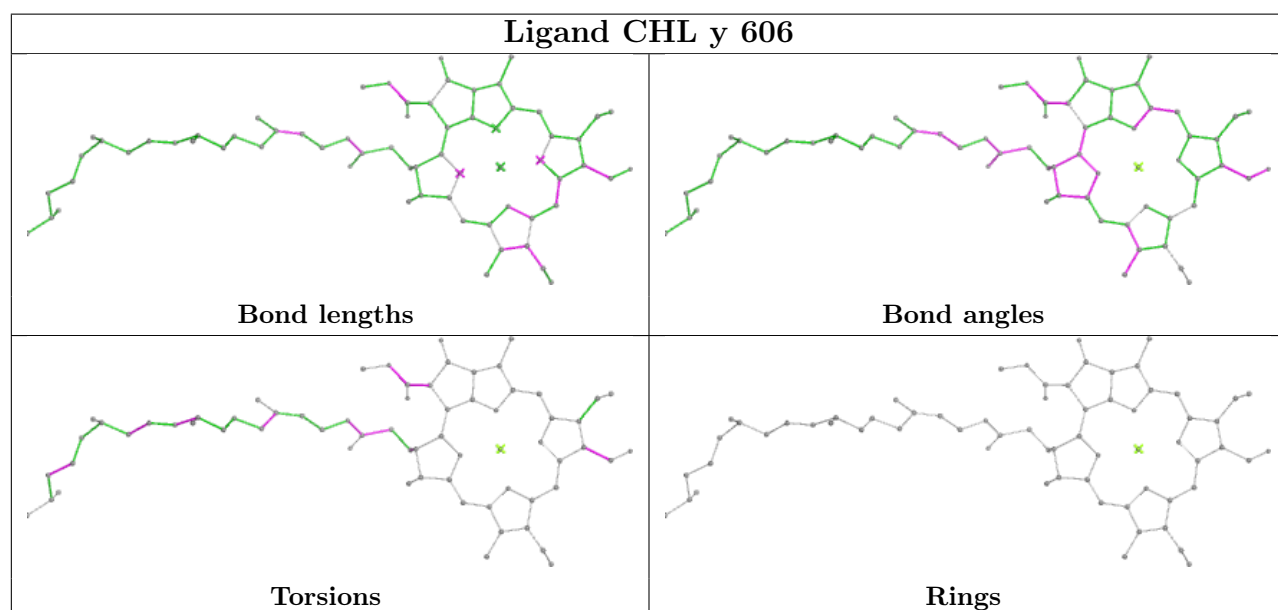
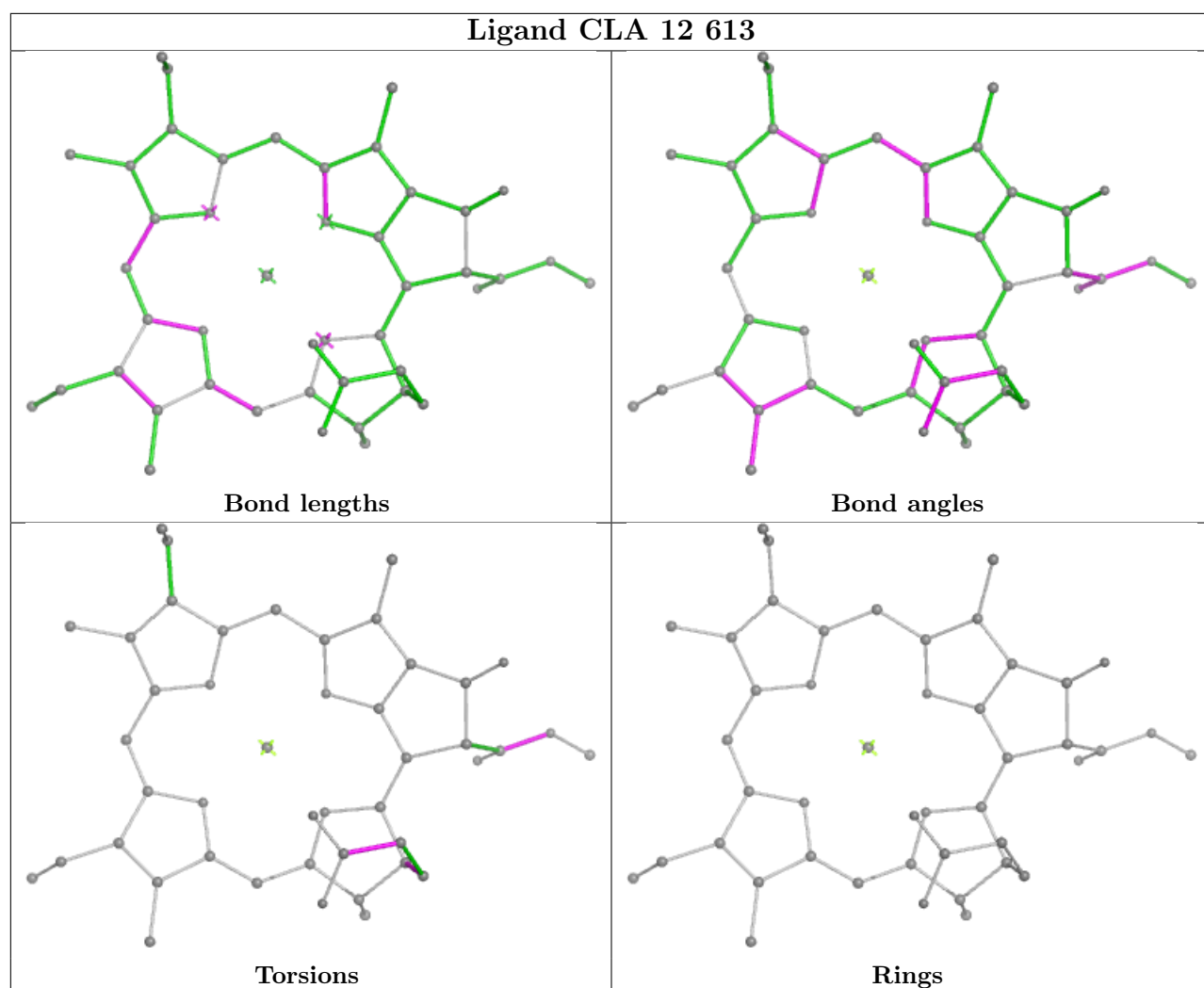
Ligand CLA 3 611

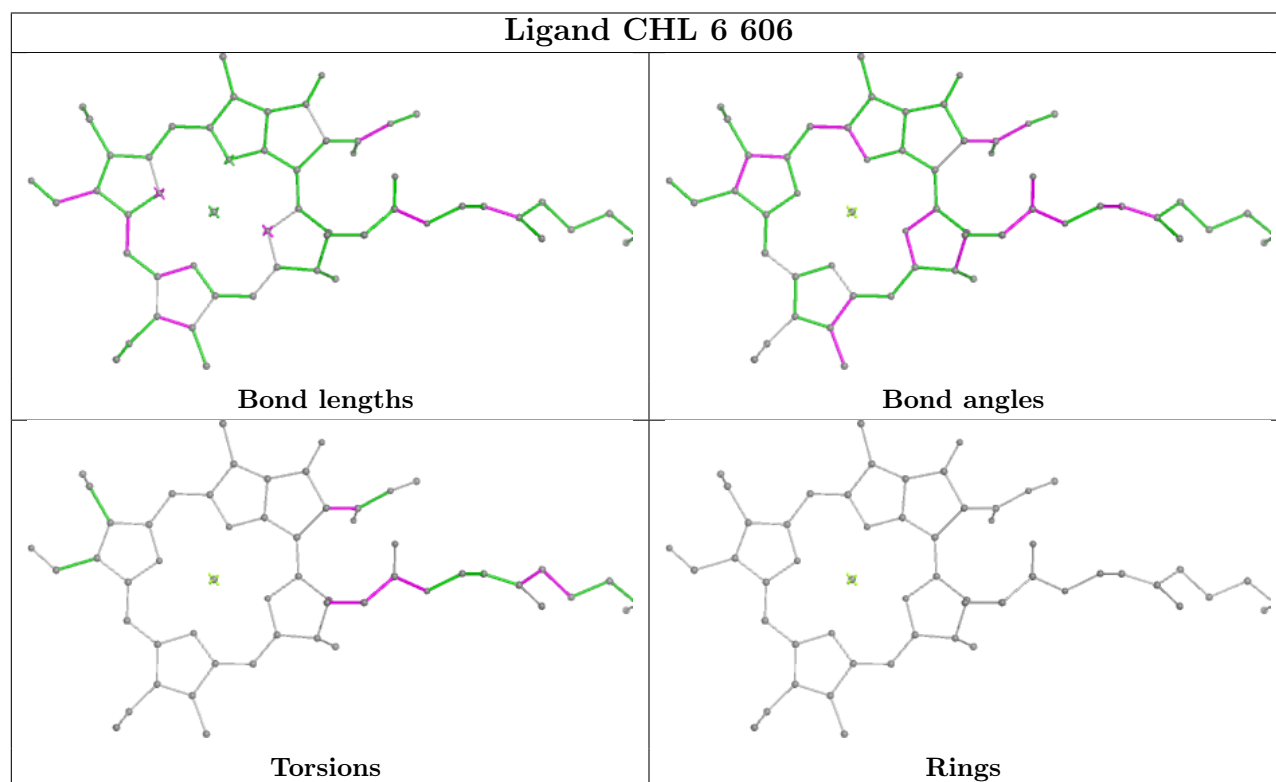
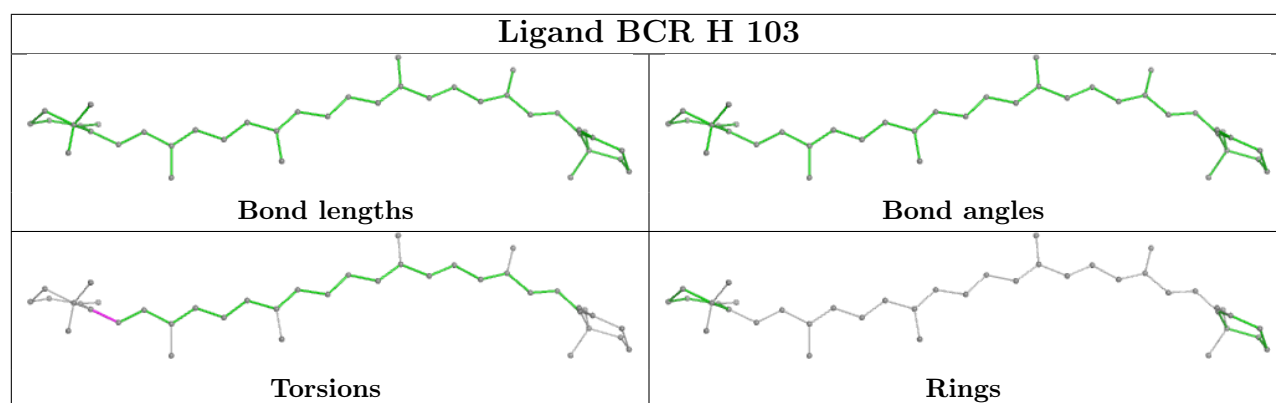


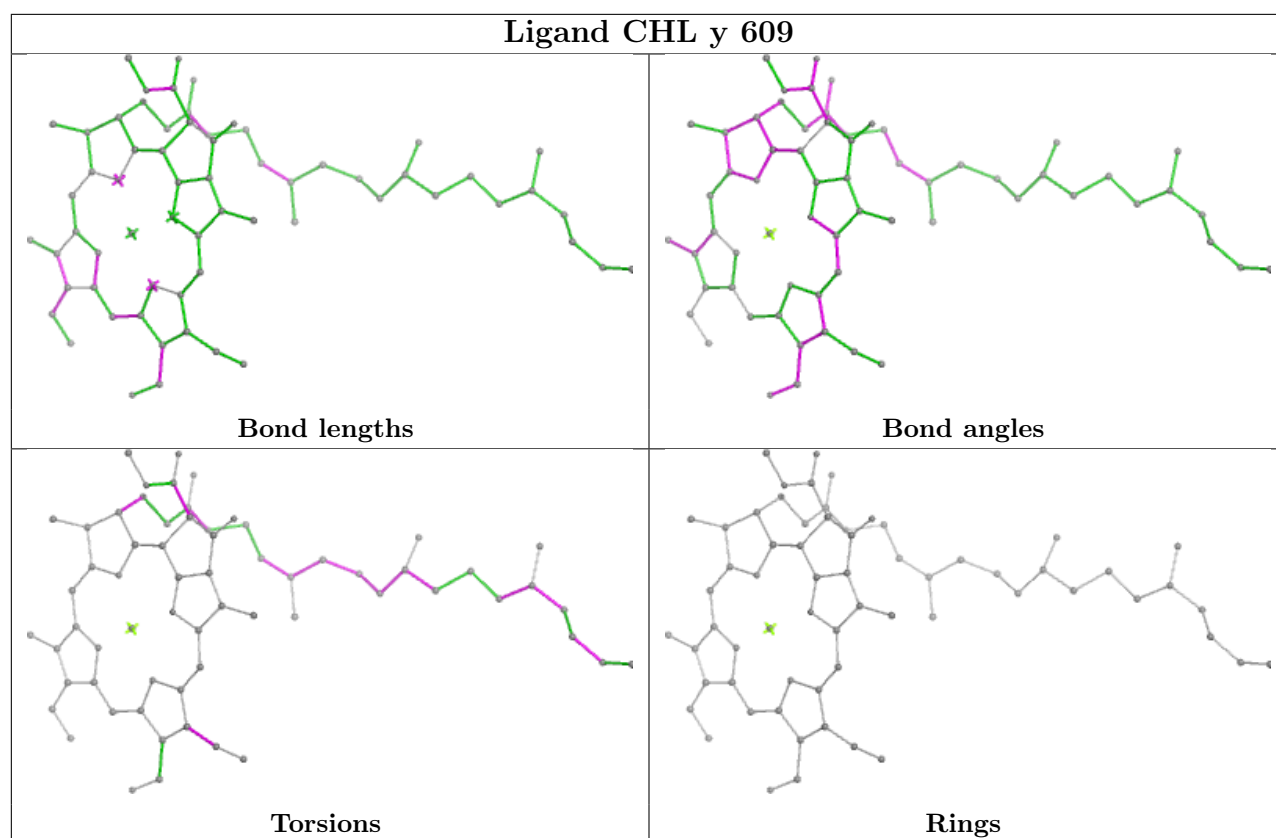
Ligand NEX S 620



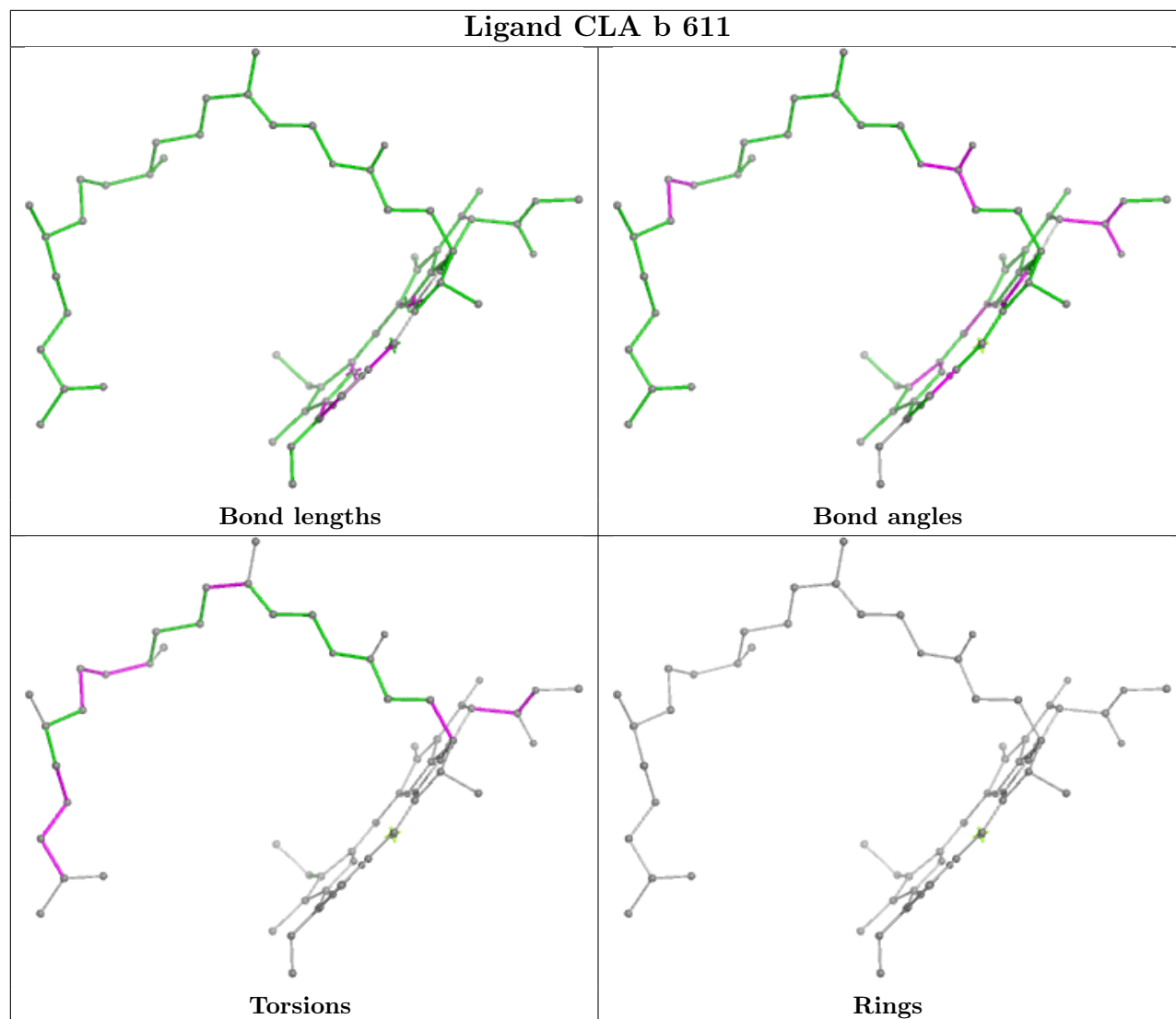




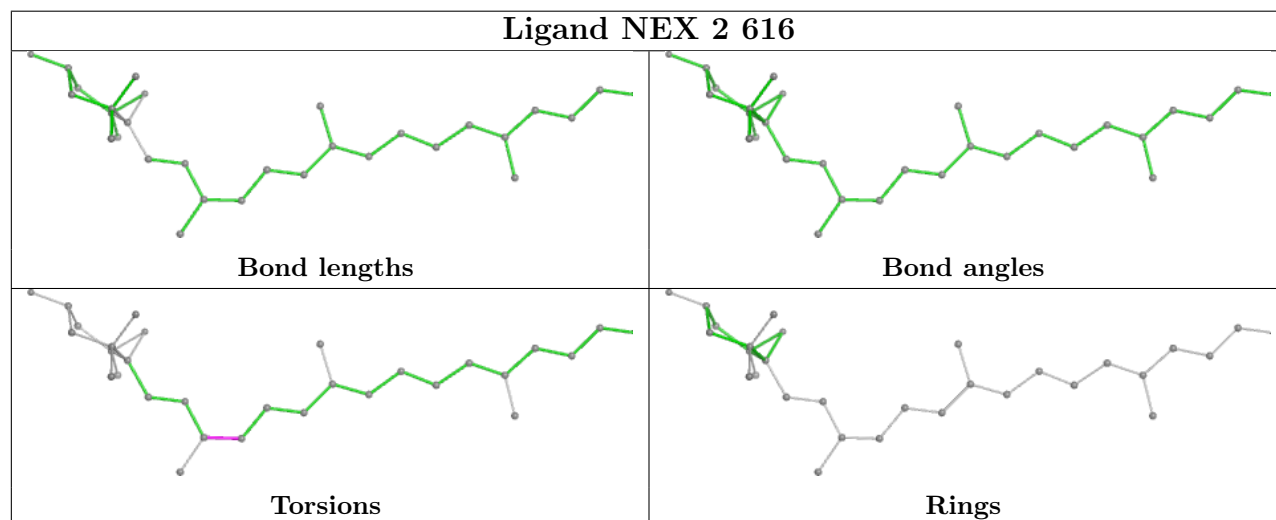


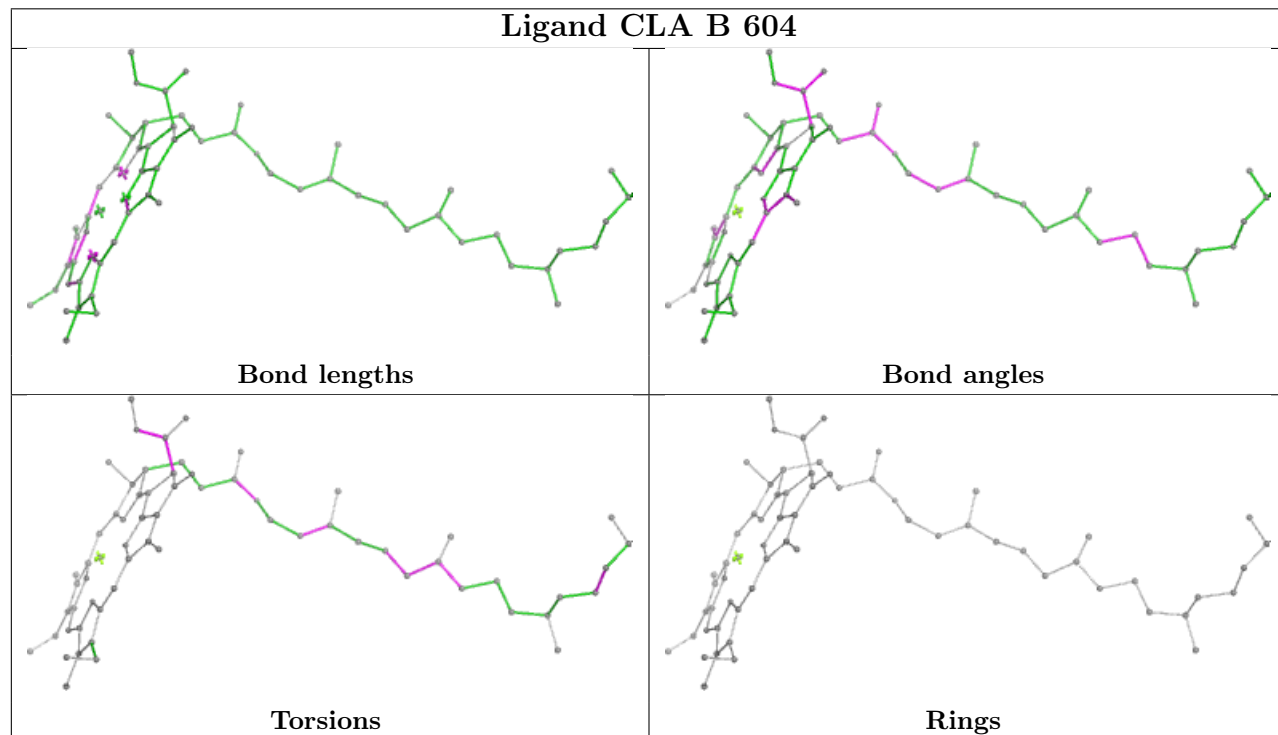
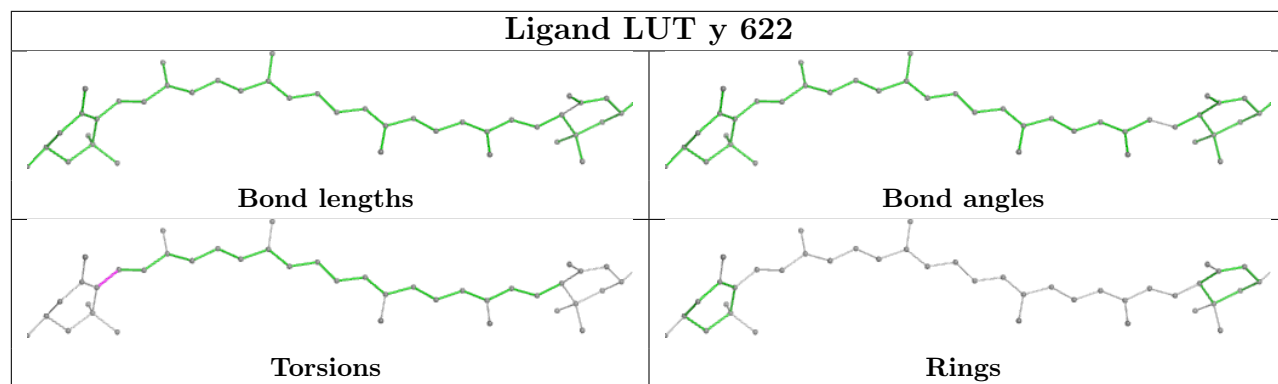


Ligand CLA b 611

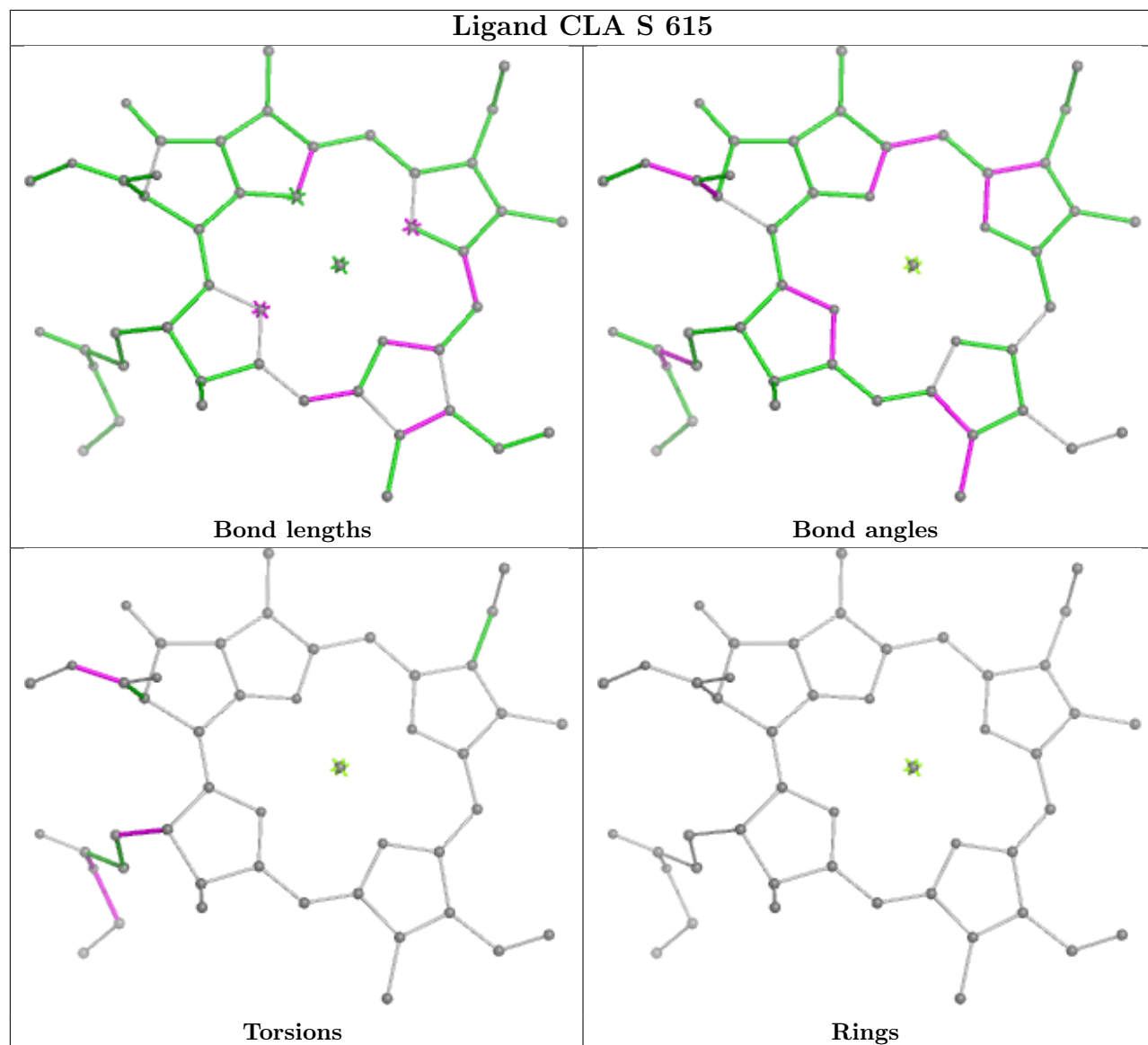


Ligand NEX 2 616

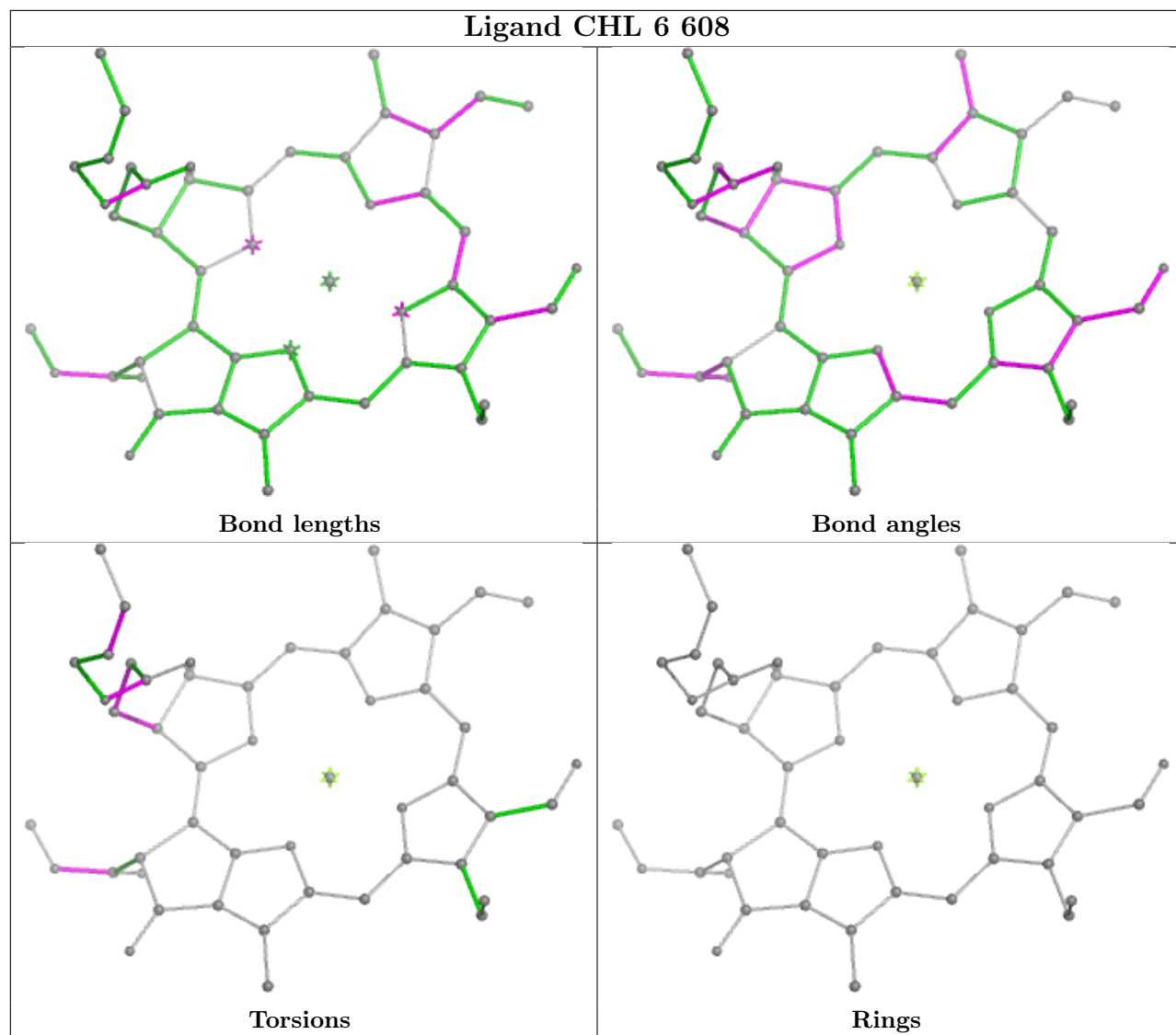


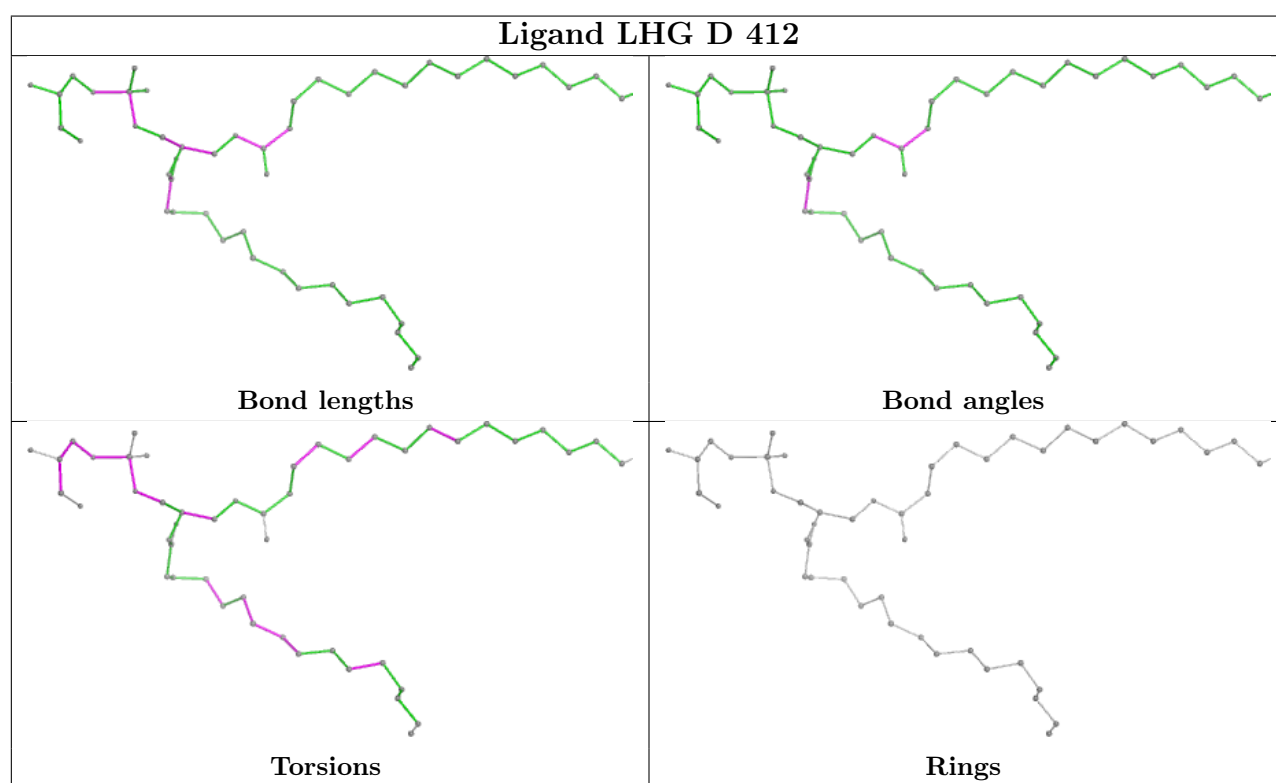
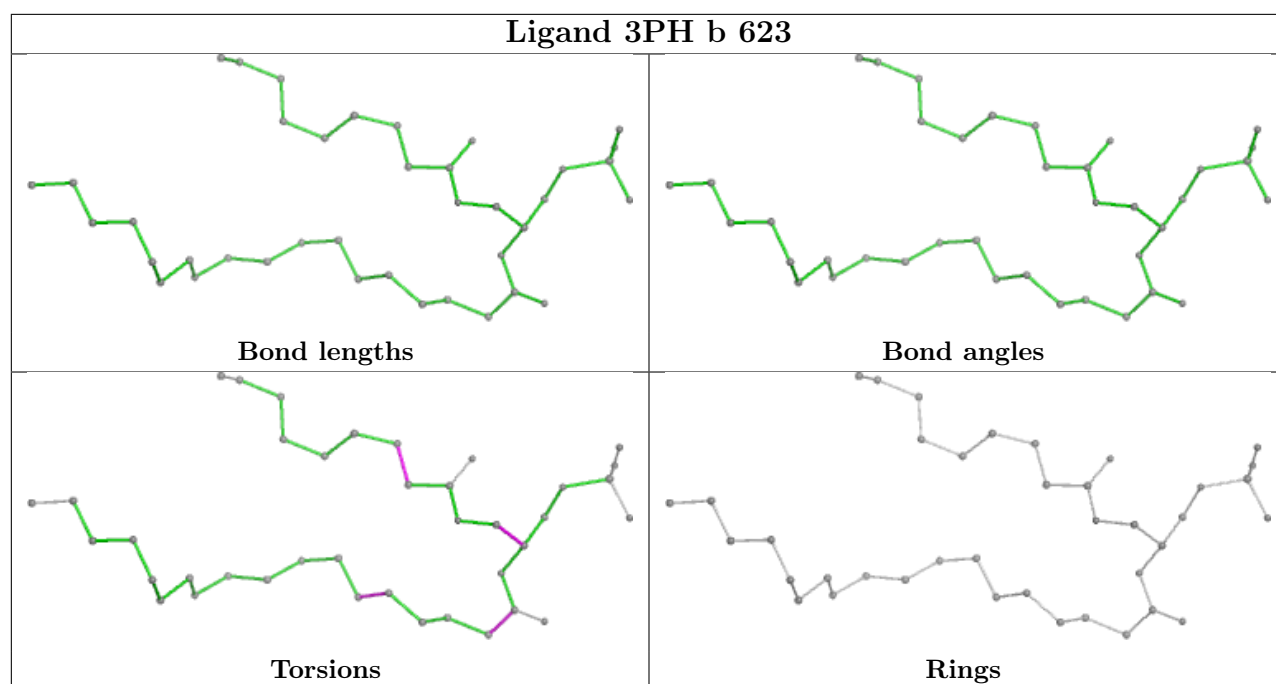


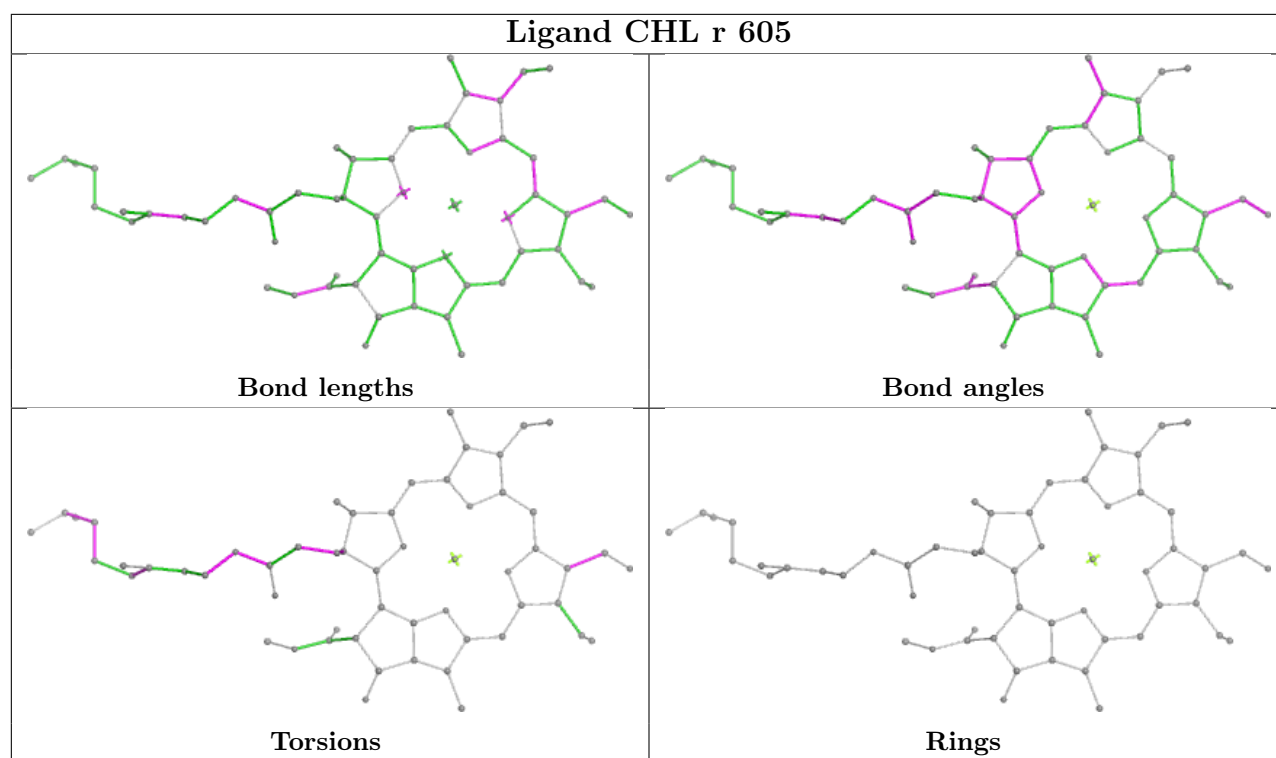
Ligand CLA S 615



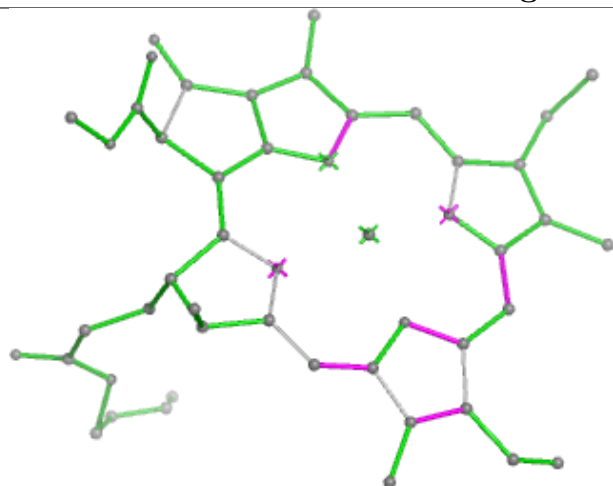
Ligand CHL 6 608



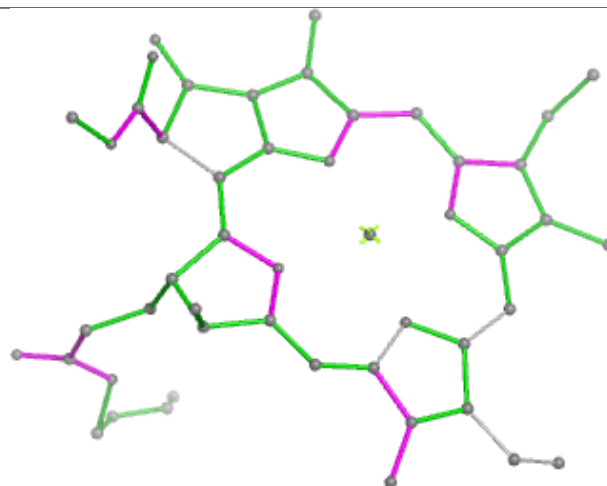




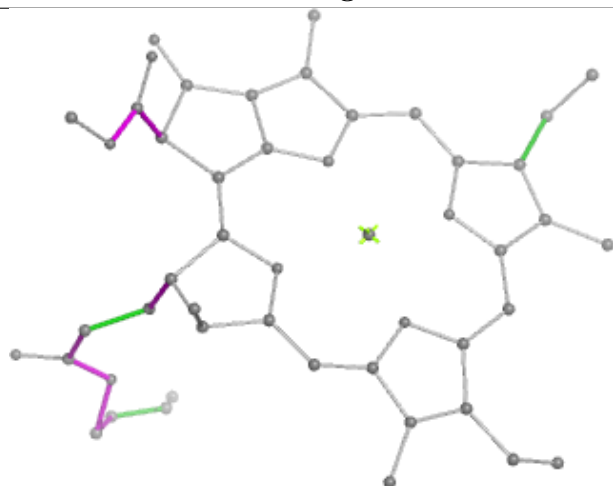
Ligand CLA r 601



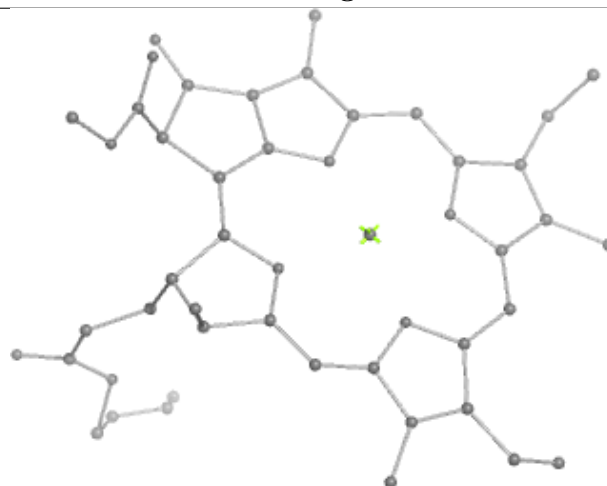
Bond lengths



Bond angles

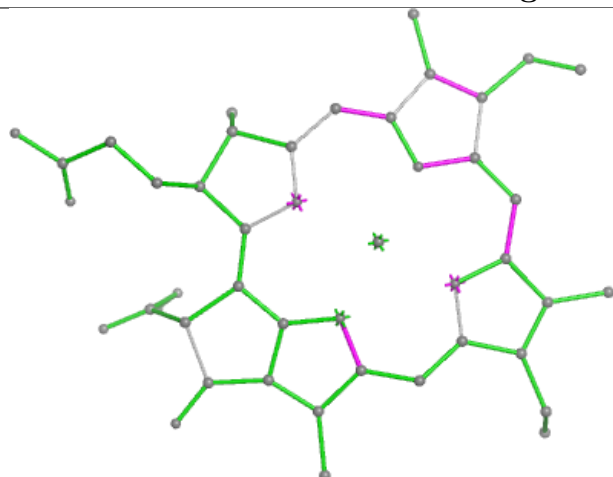


Torsions

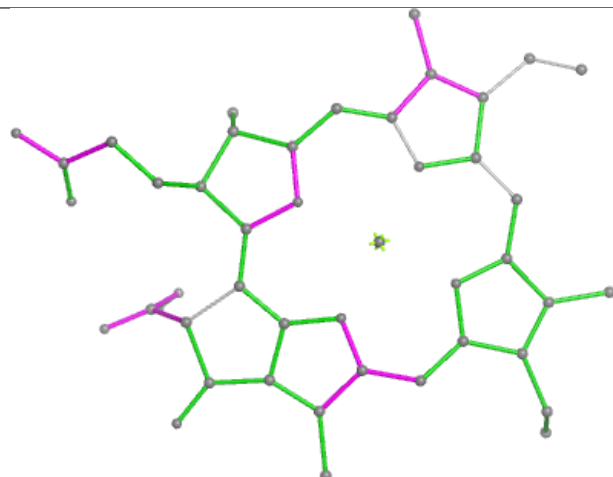


Rings

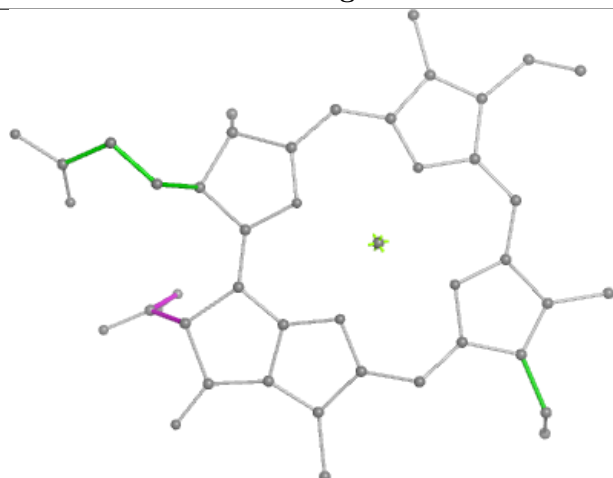
Ligand CLA s 612



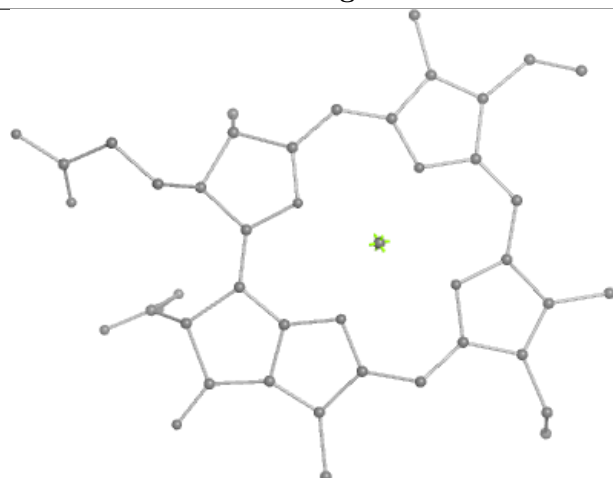
Bond lengths



Bond angles

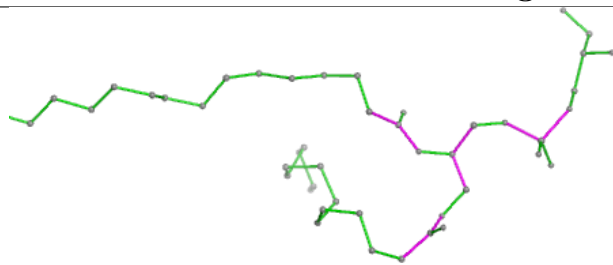


Torsions

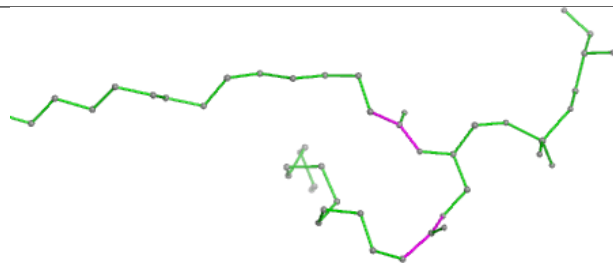


Rings

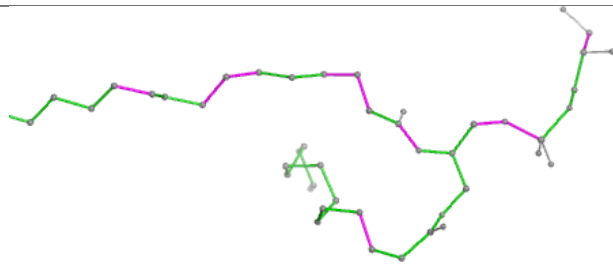
Ligand LHG 4 615



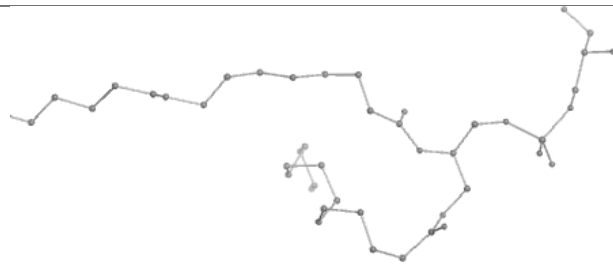
Bond lengths



Bond angles

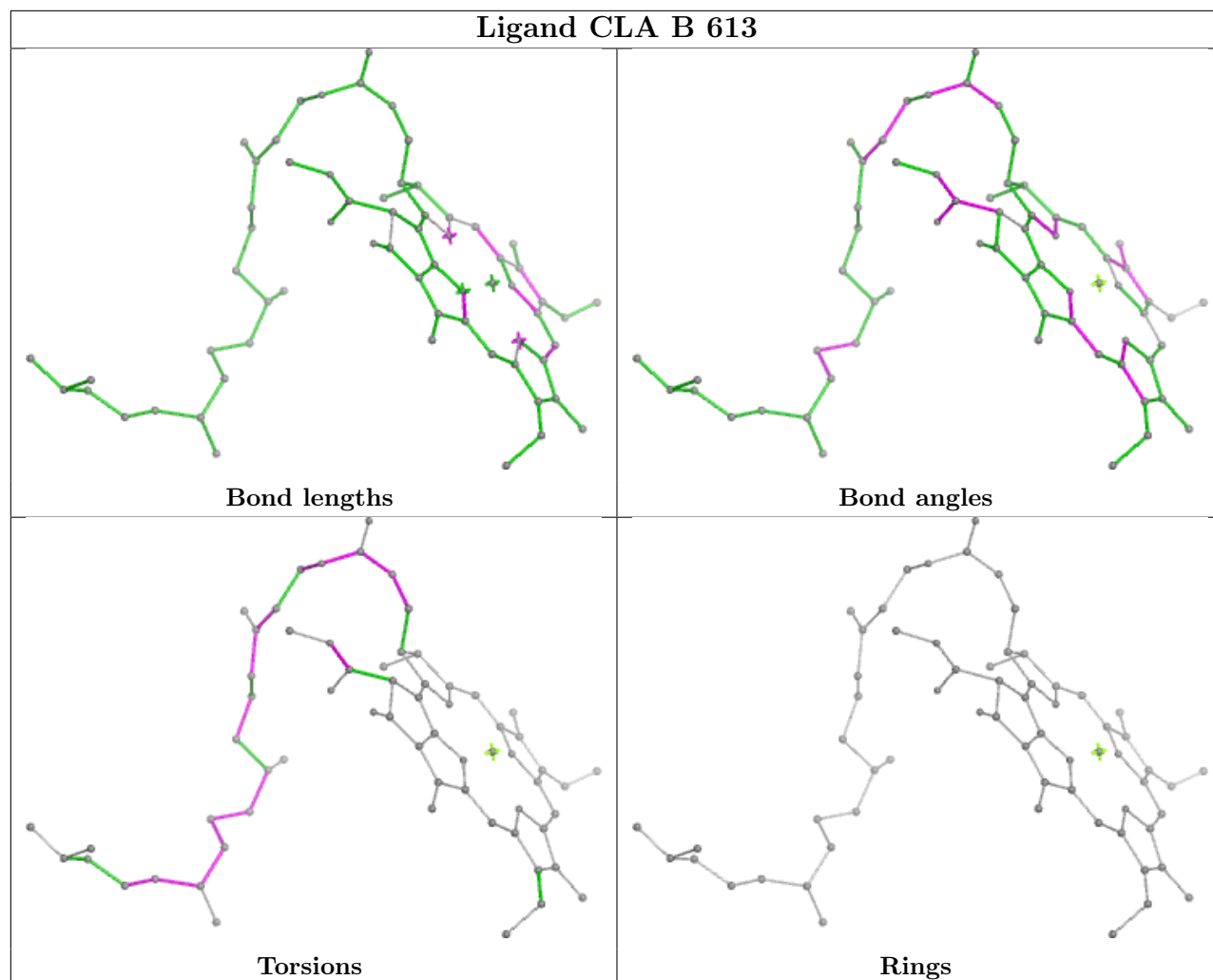


Torsions

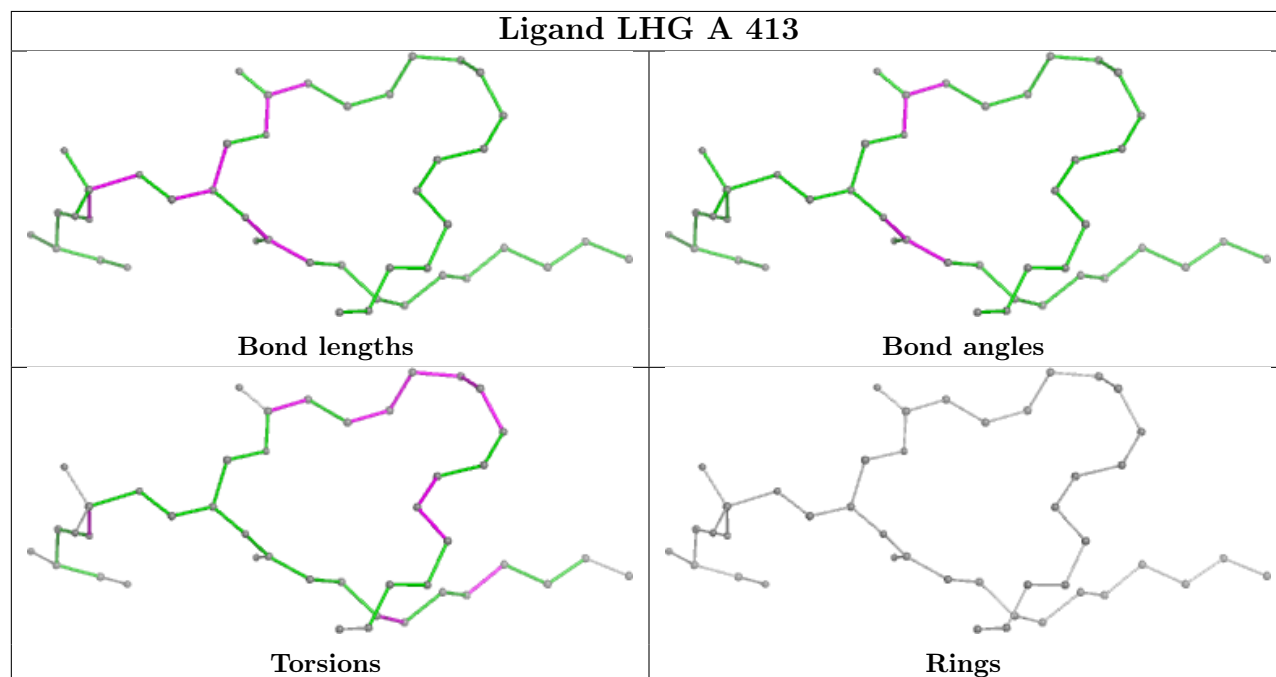


Rings

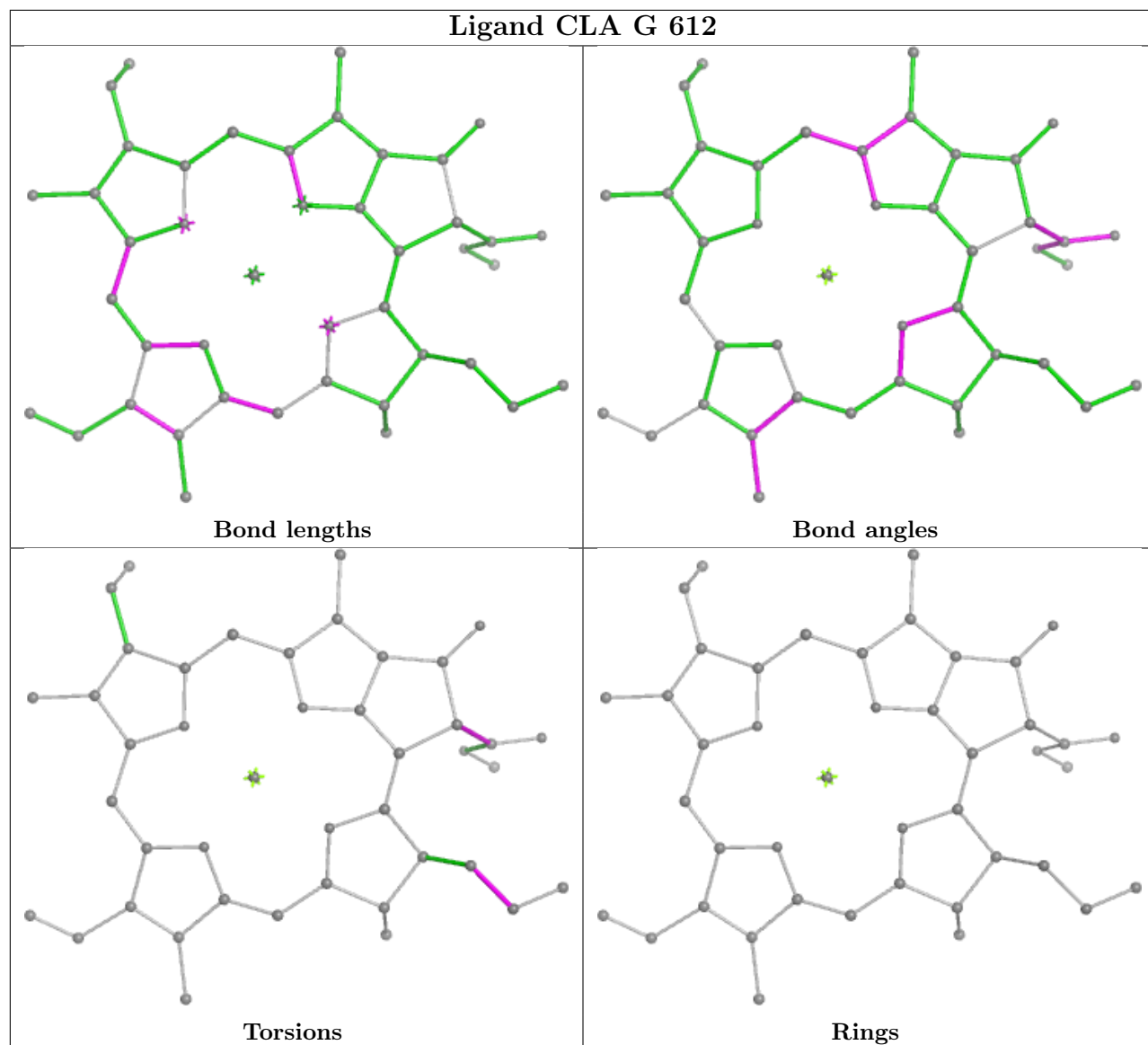
Ligand CLA B 613



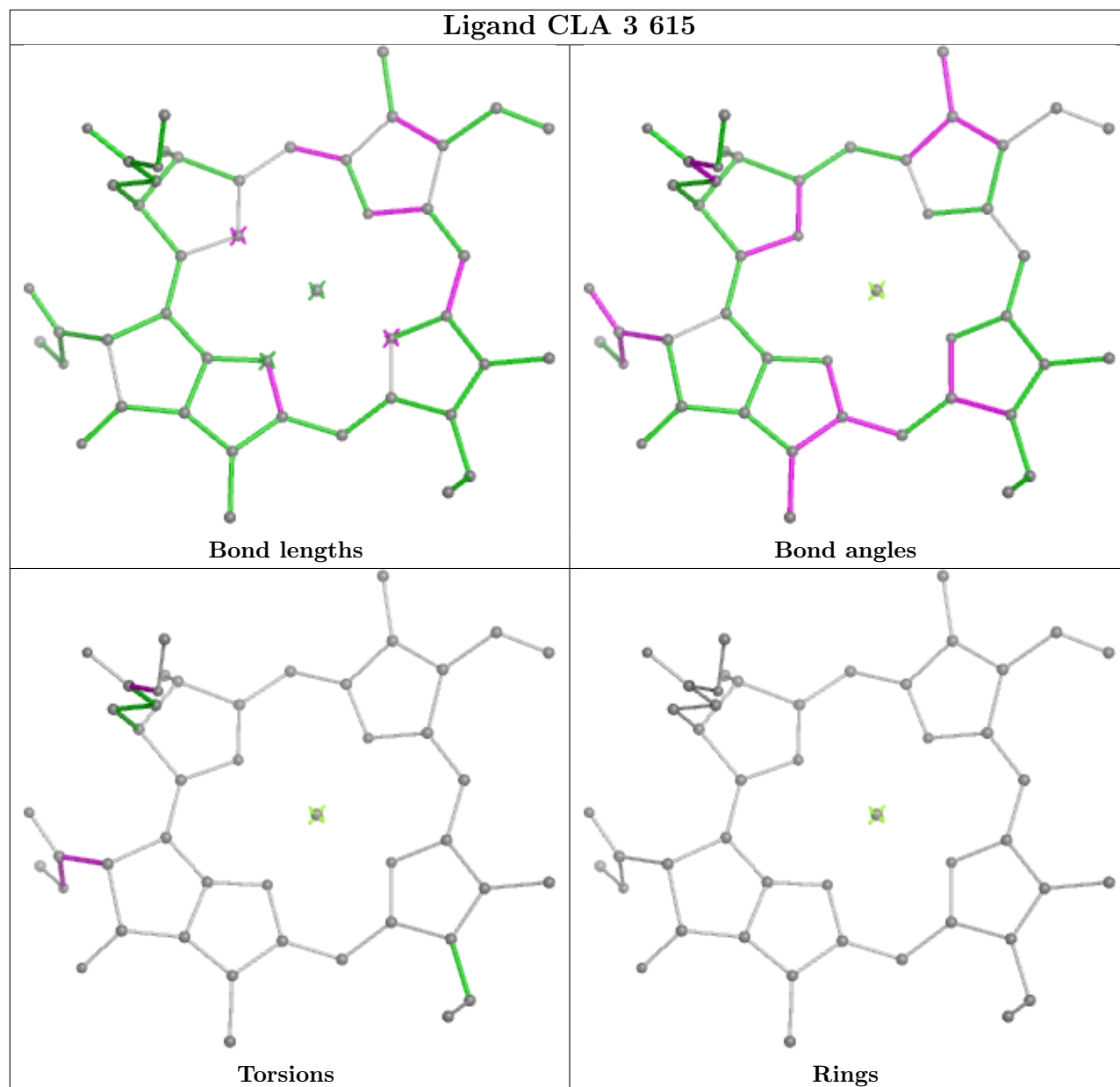
Ligand LHG A 413

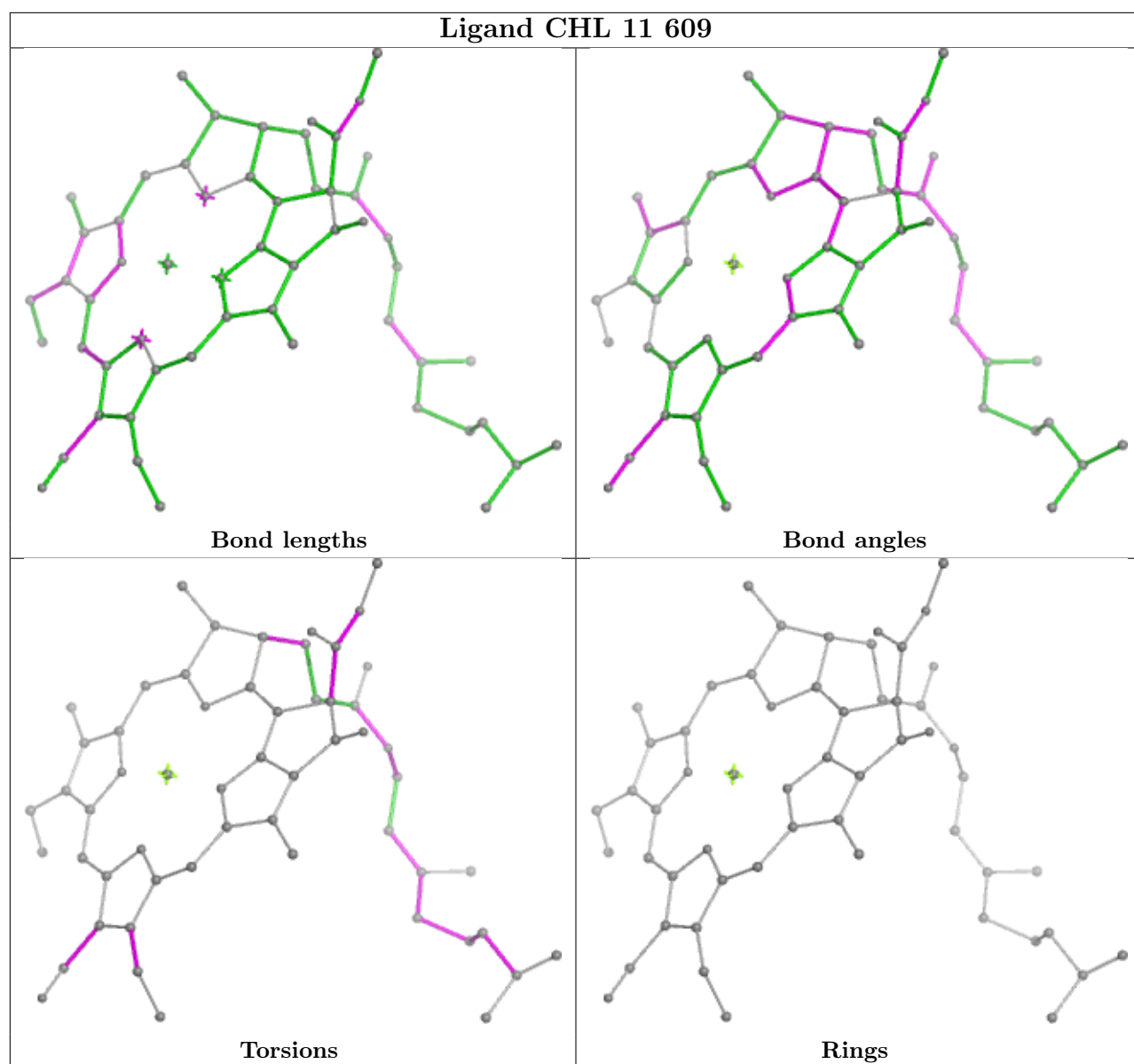


Ligand CLA G 612

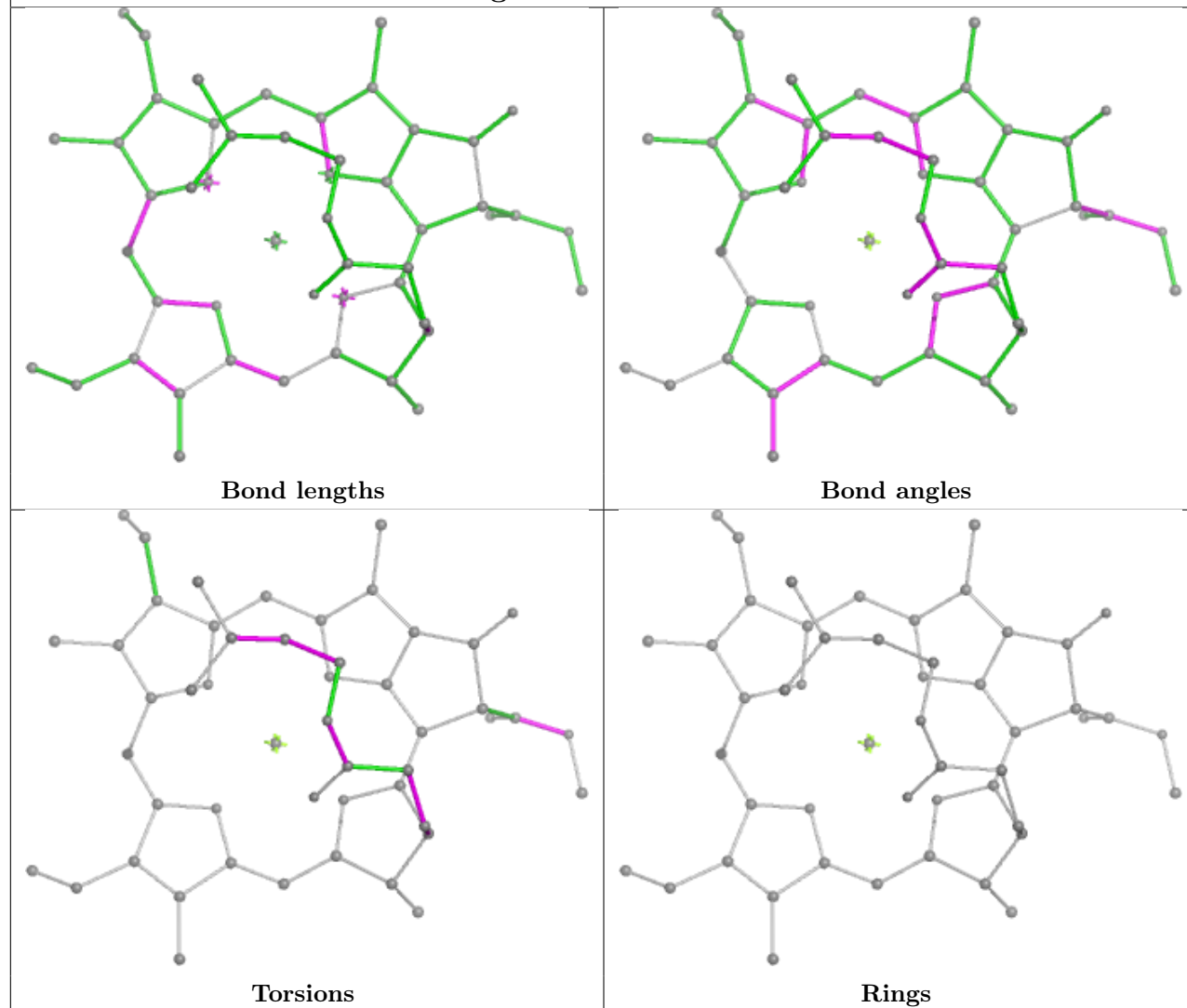


Ligand CLA 3 615

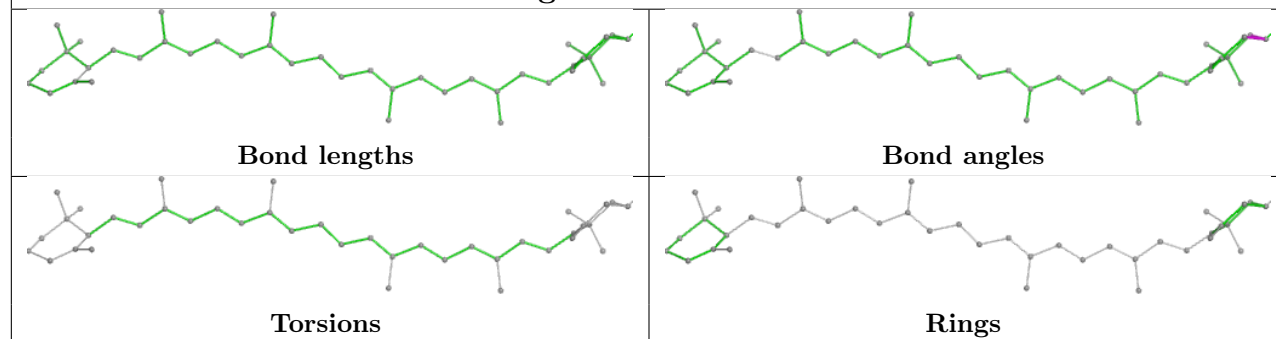


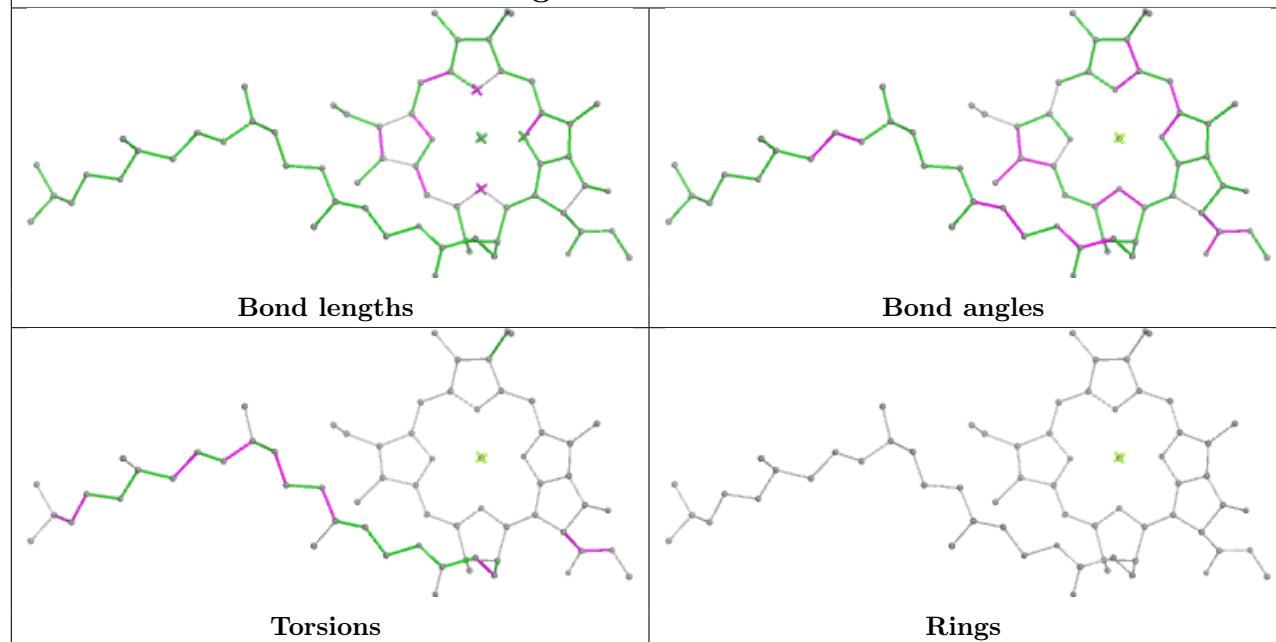
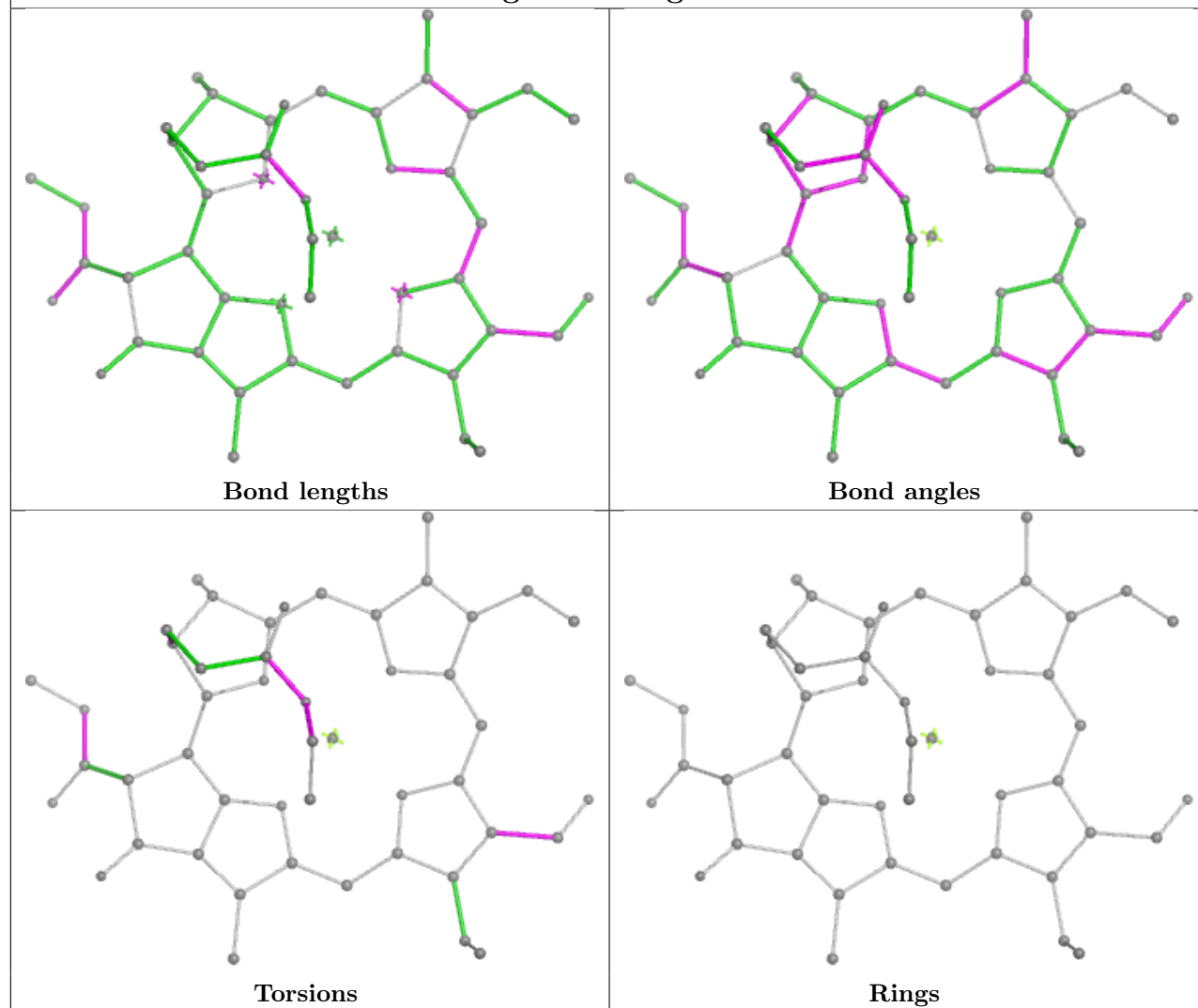


Ligand CLA 15 612

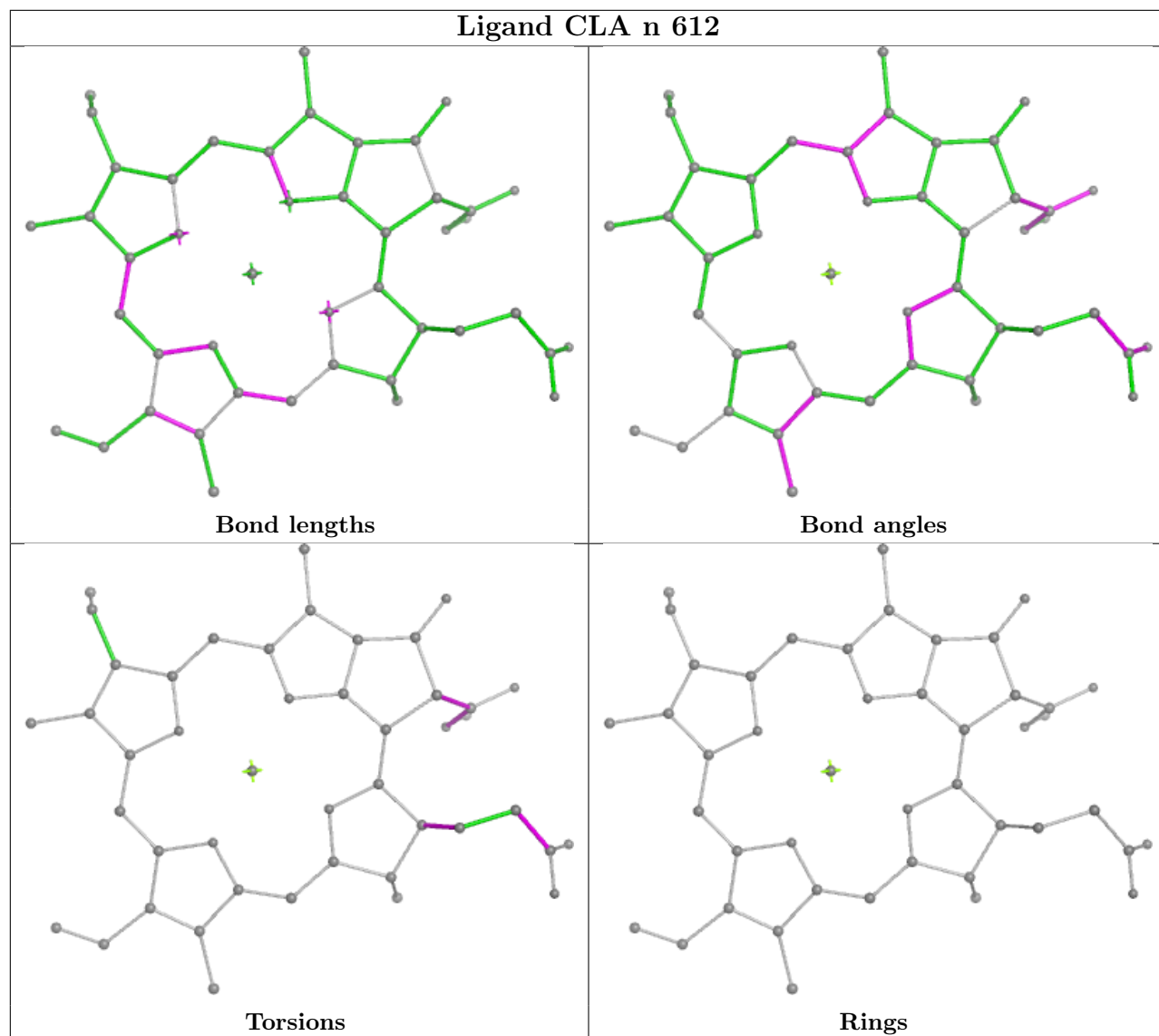


Ligand LUT s 619

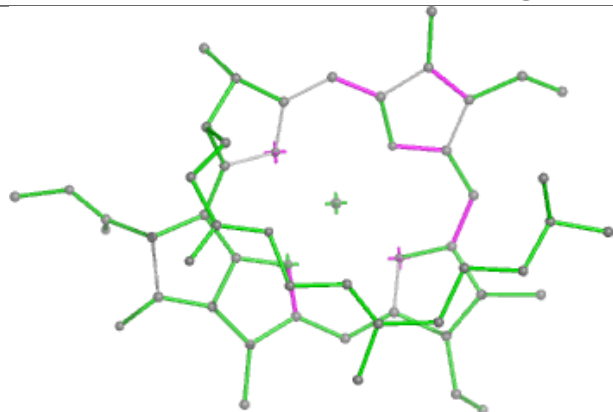


Ligand CLA B 603**Ligand CHL g 605**

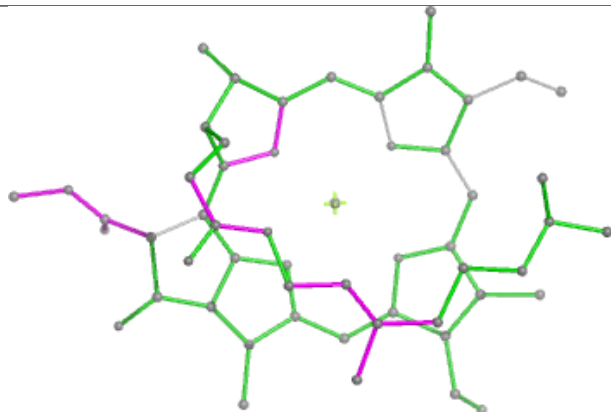
Ligand CLA n 612



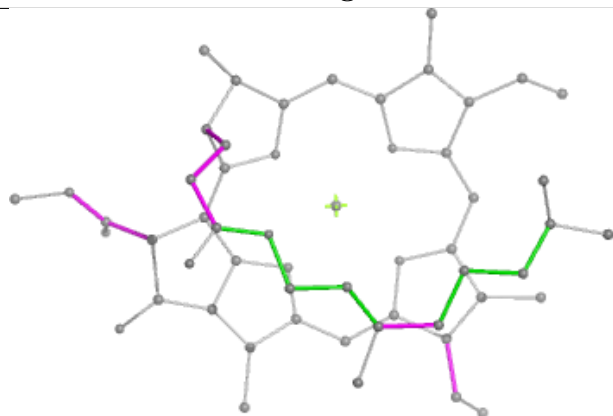
Ligand CLA n 613



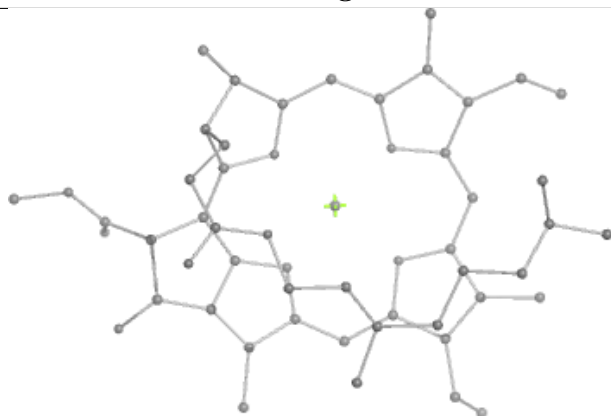
Bond lengths



Bond angles



Torsions



Rings

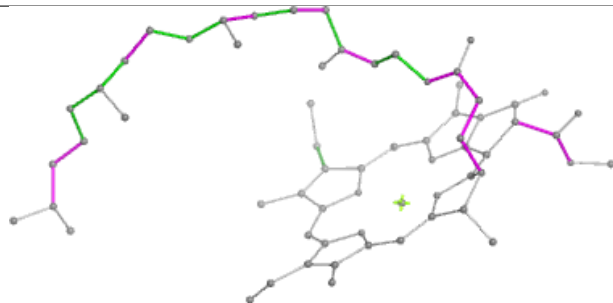
Ligand CLA c 514



Bond lengths



Bond angles

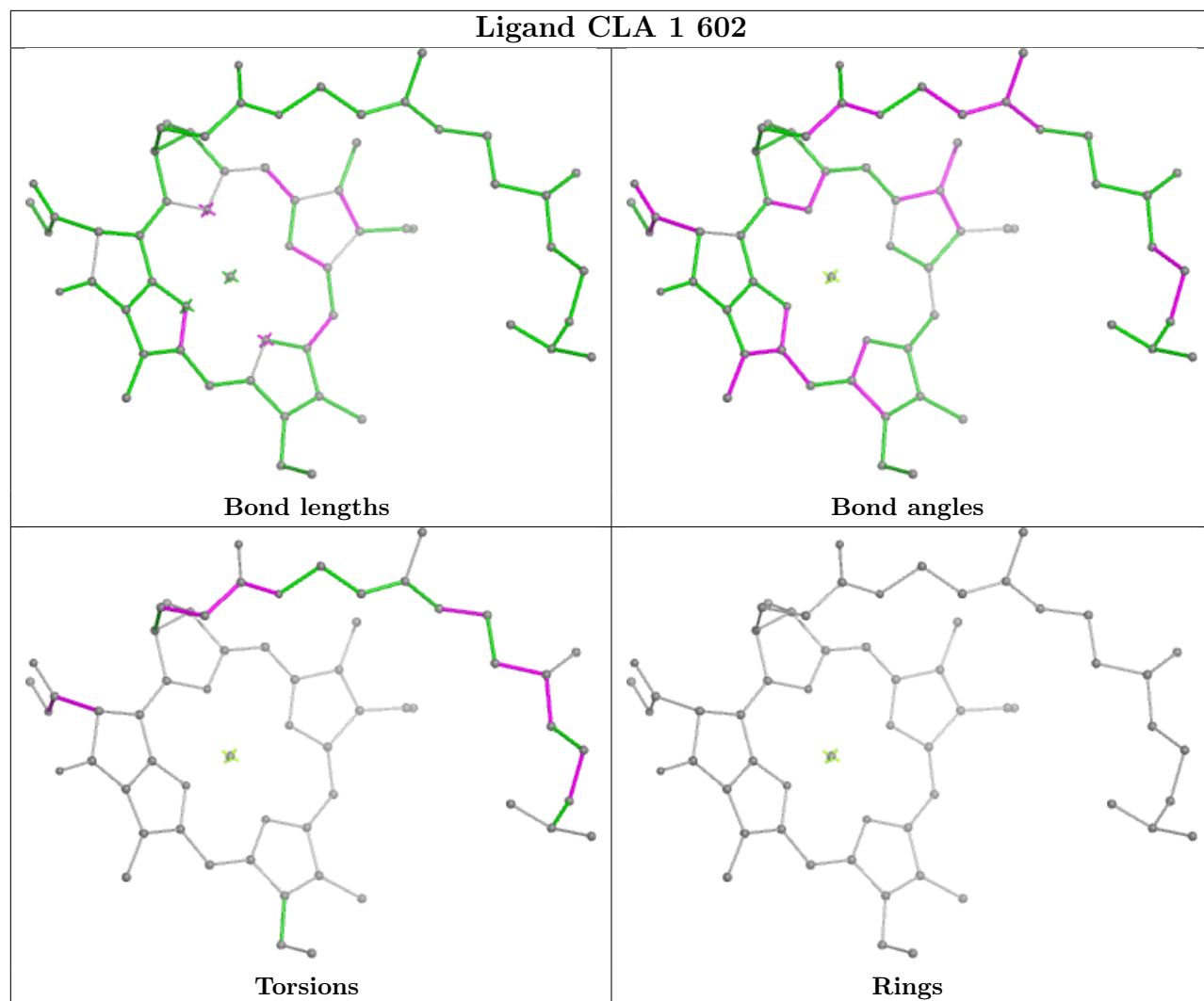


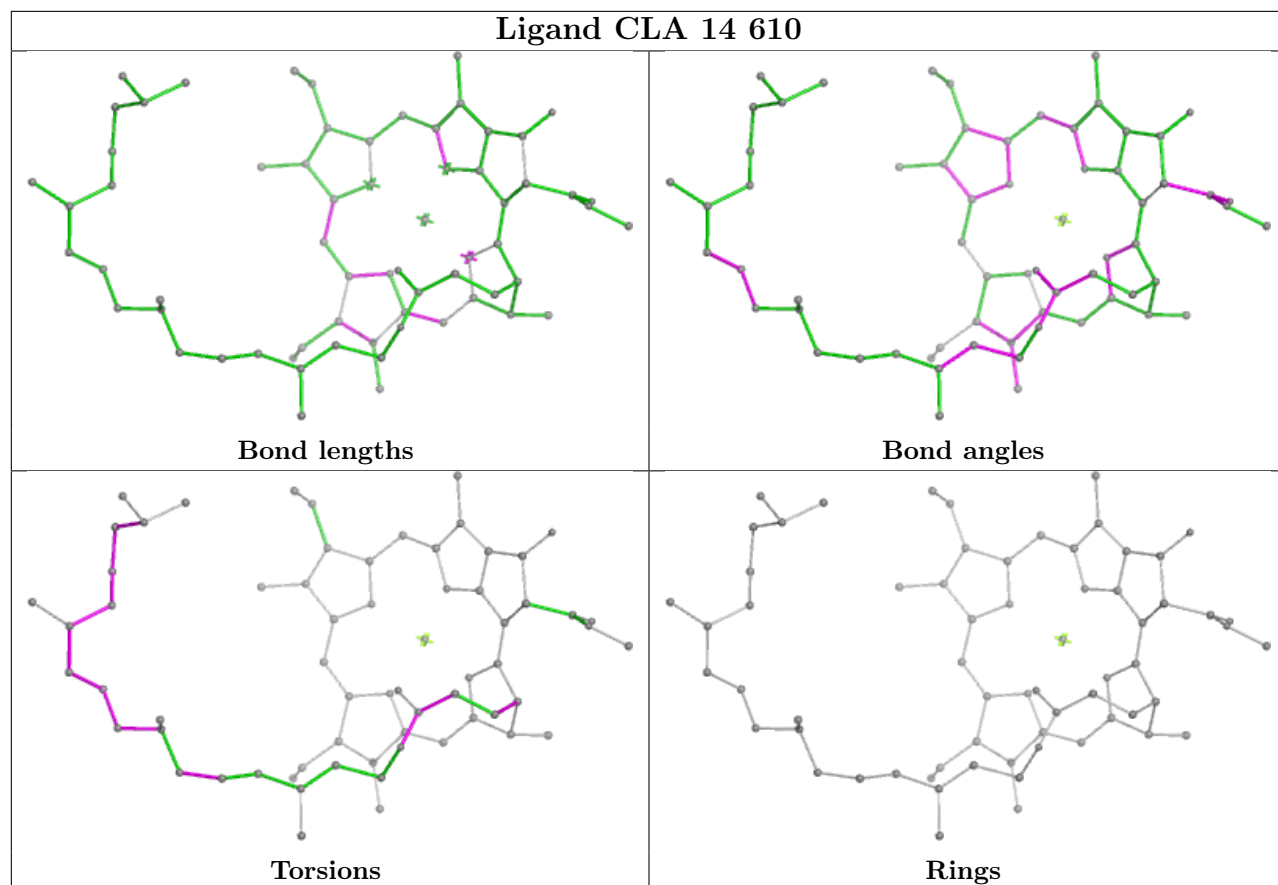
Torsions

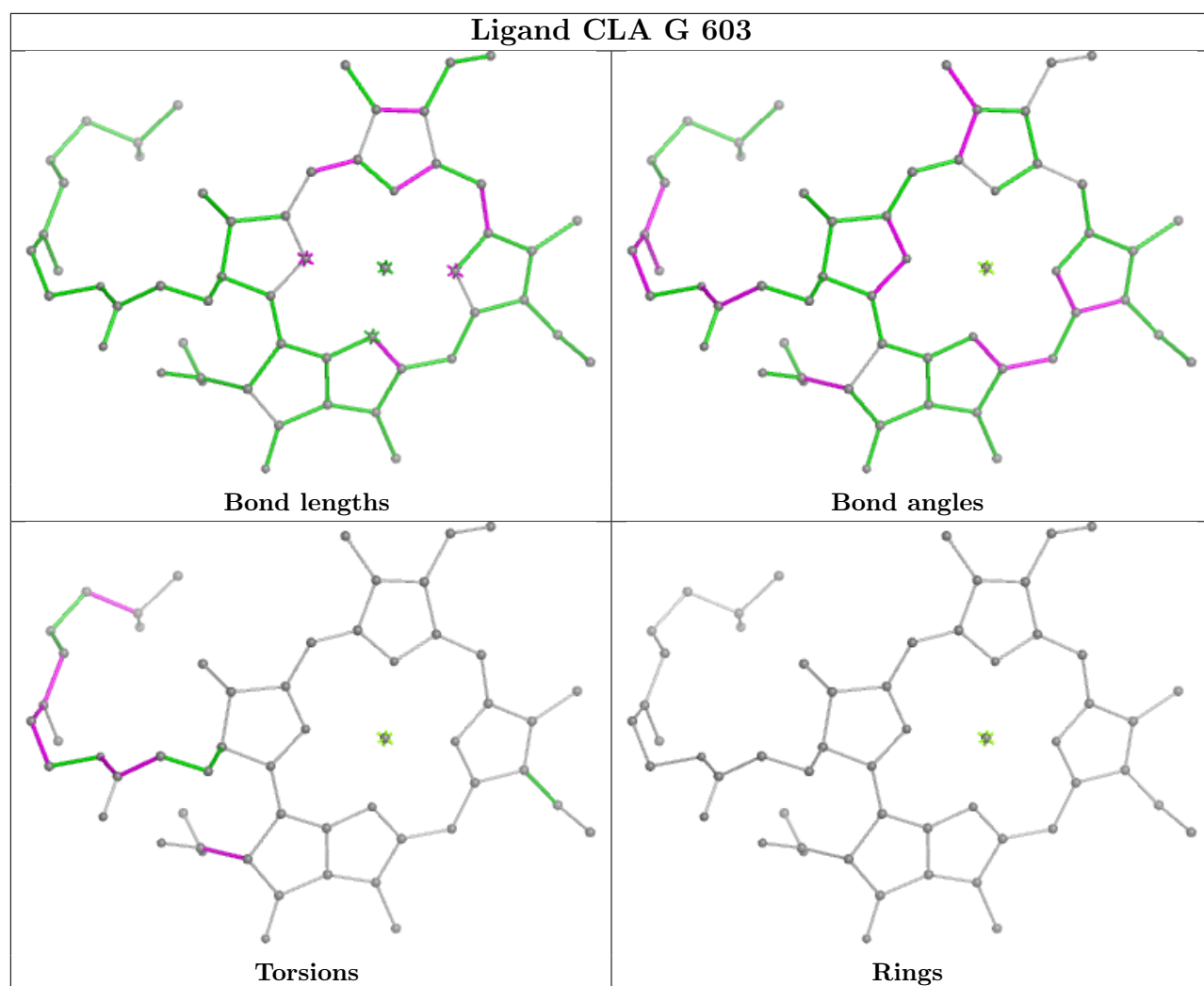


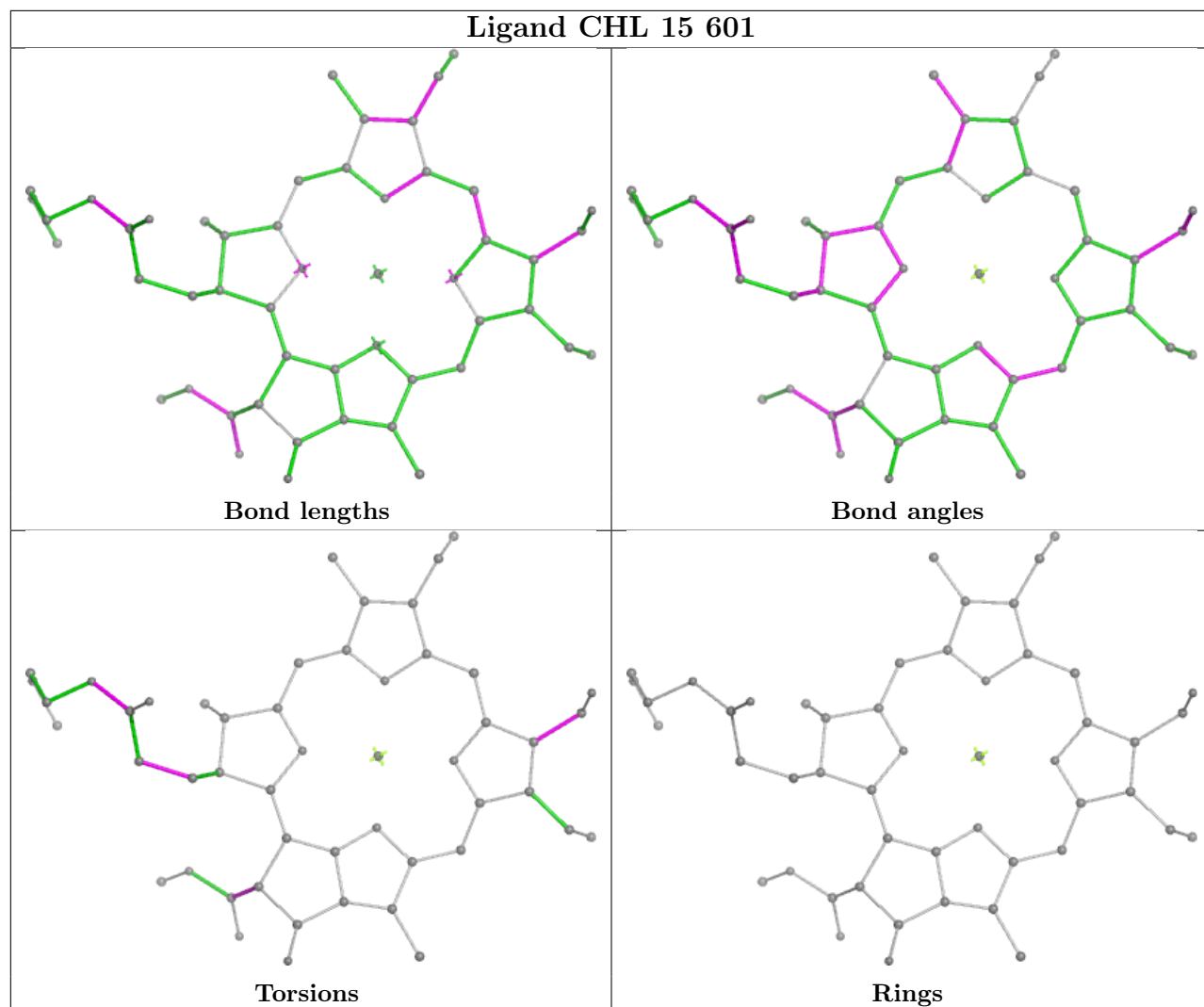
Rings

Ligand CLA 1 602

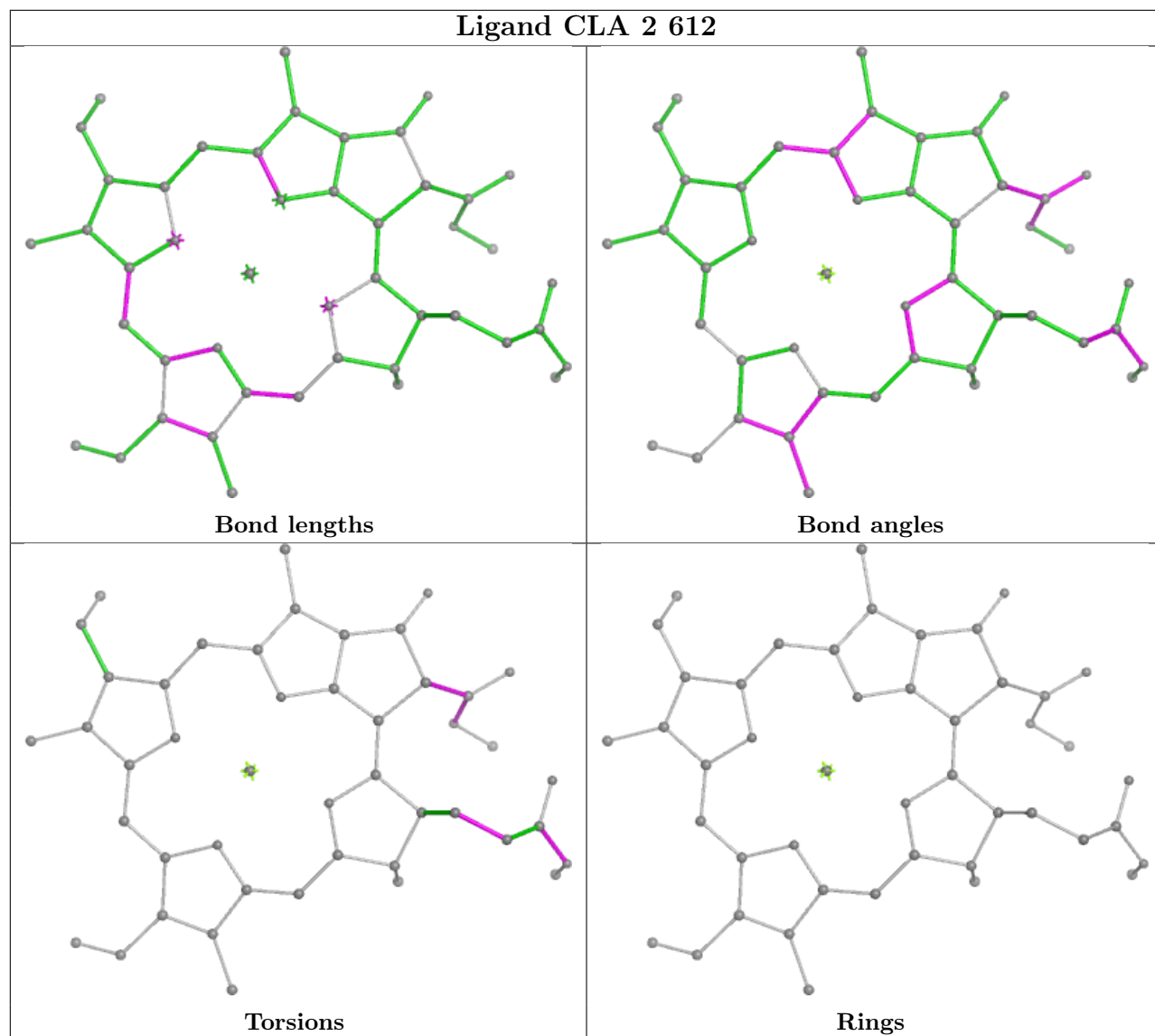


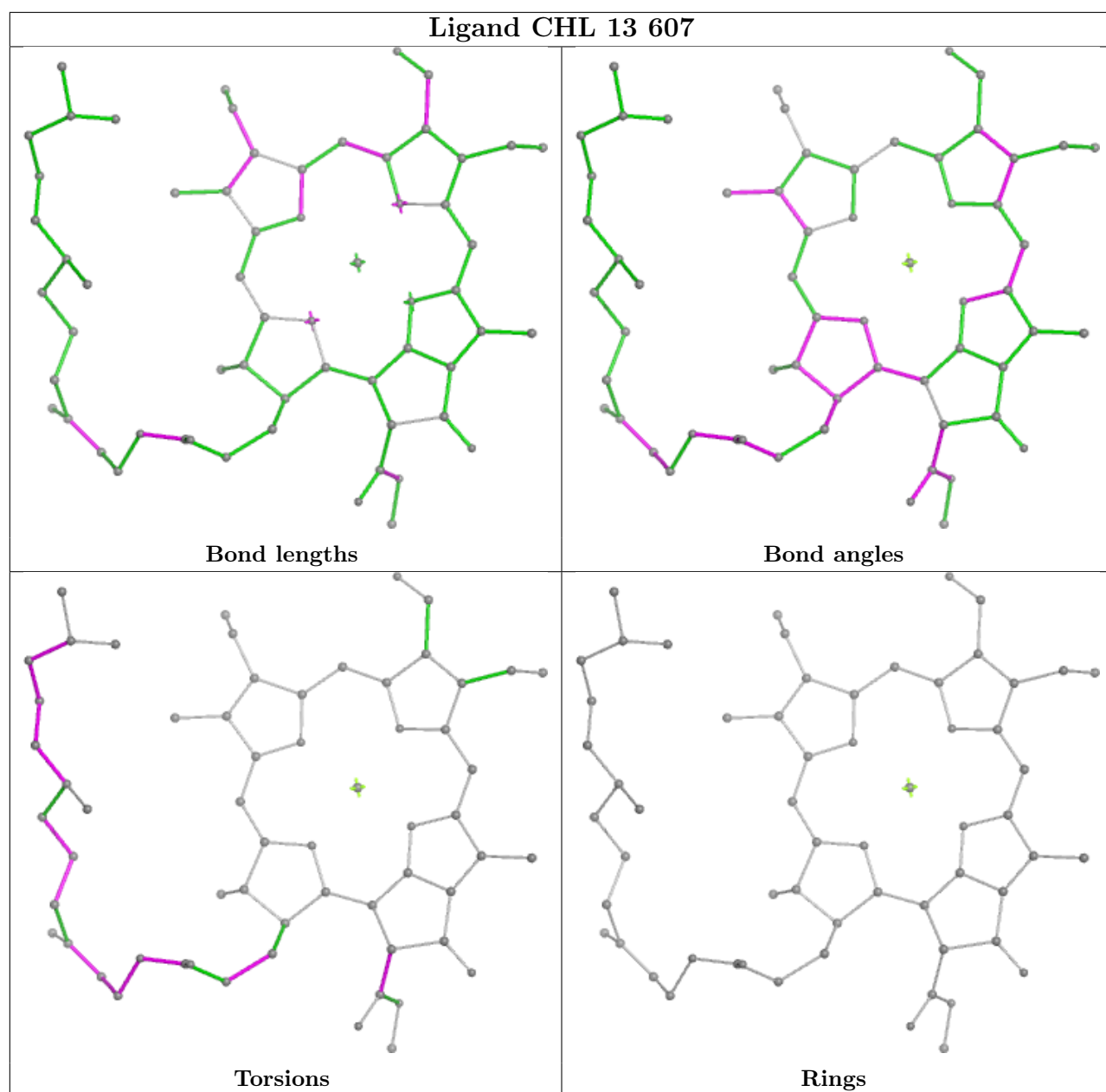




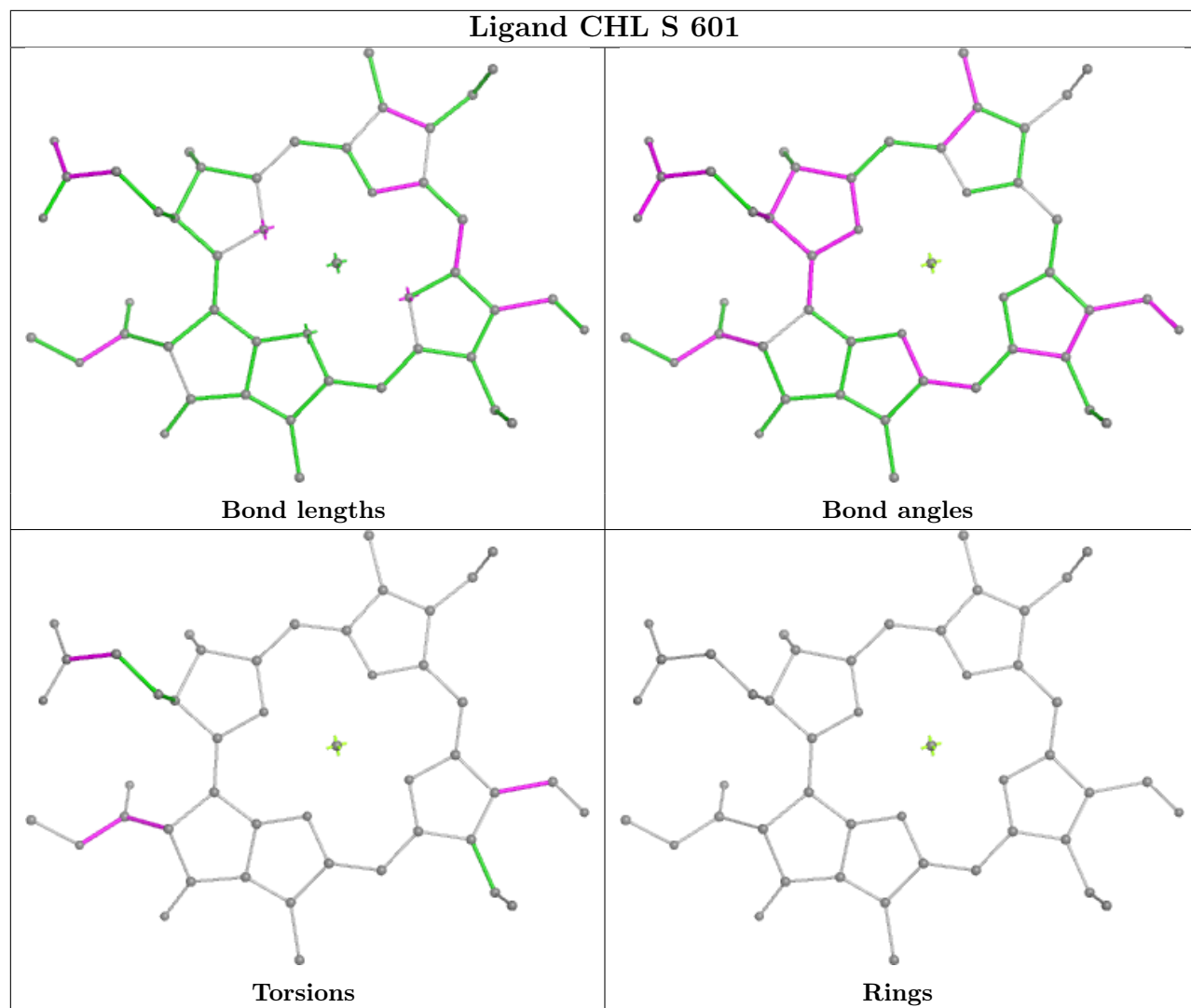


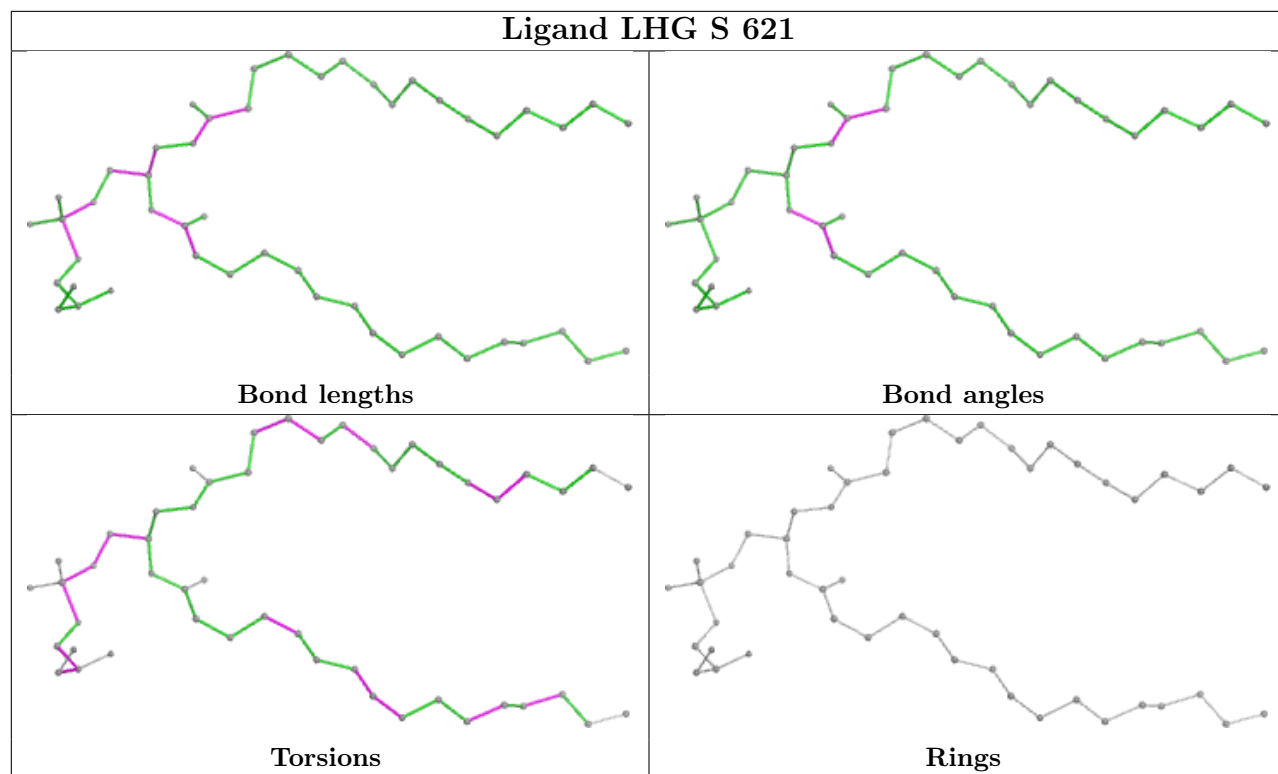
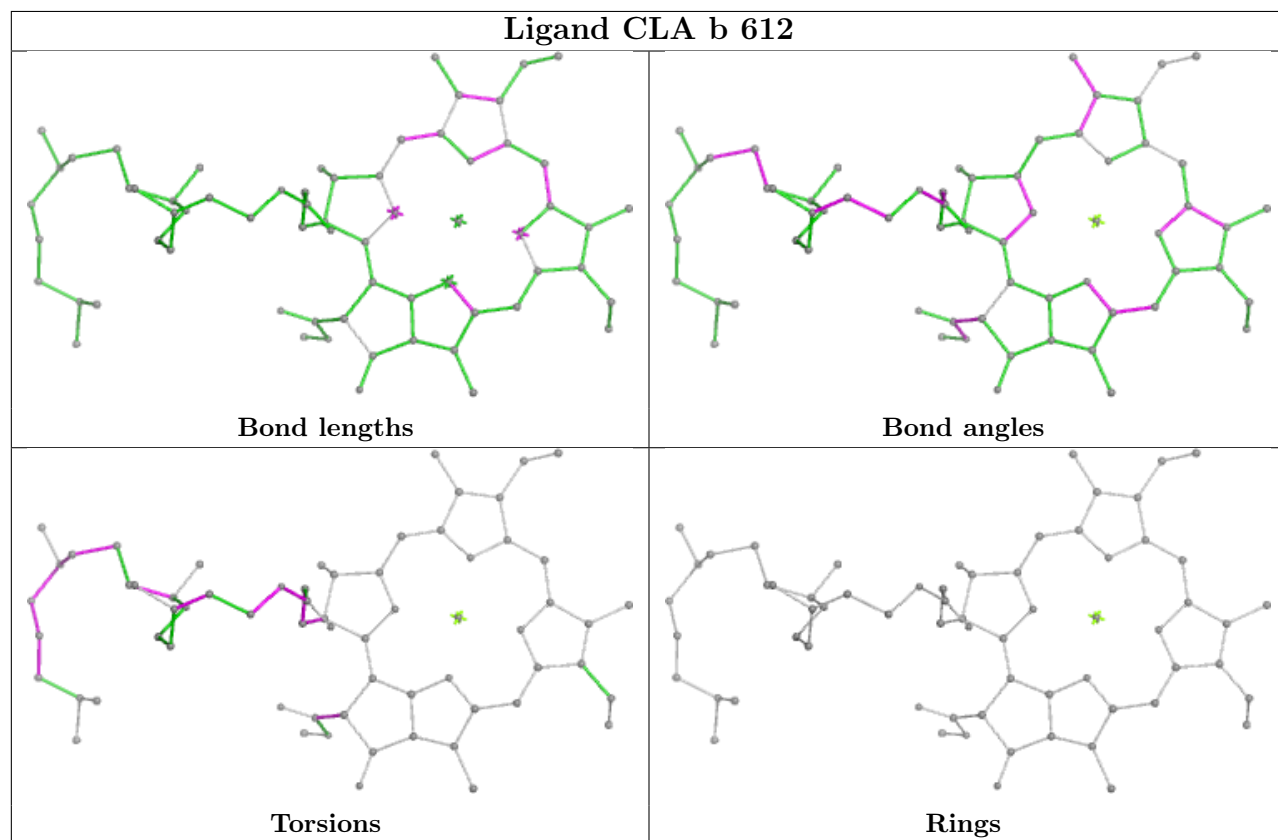
Ligand CLA 2 612

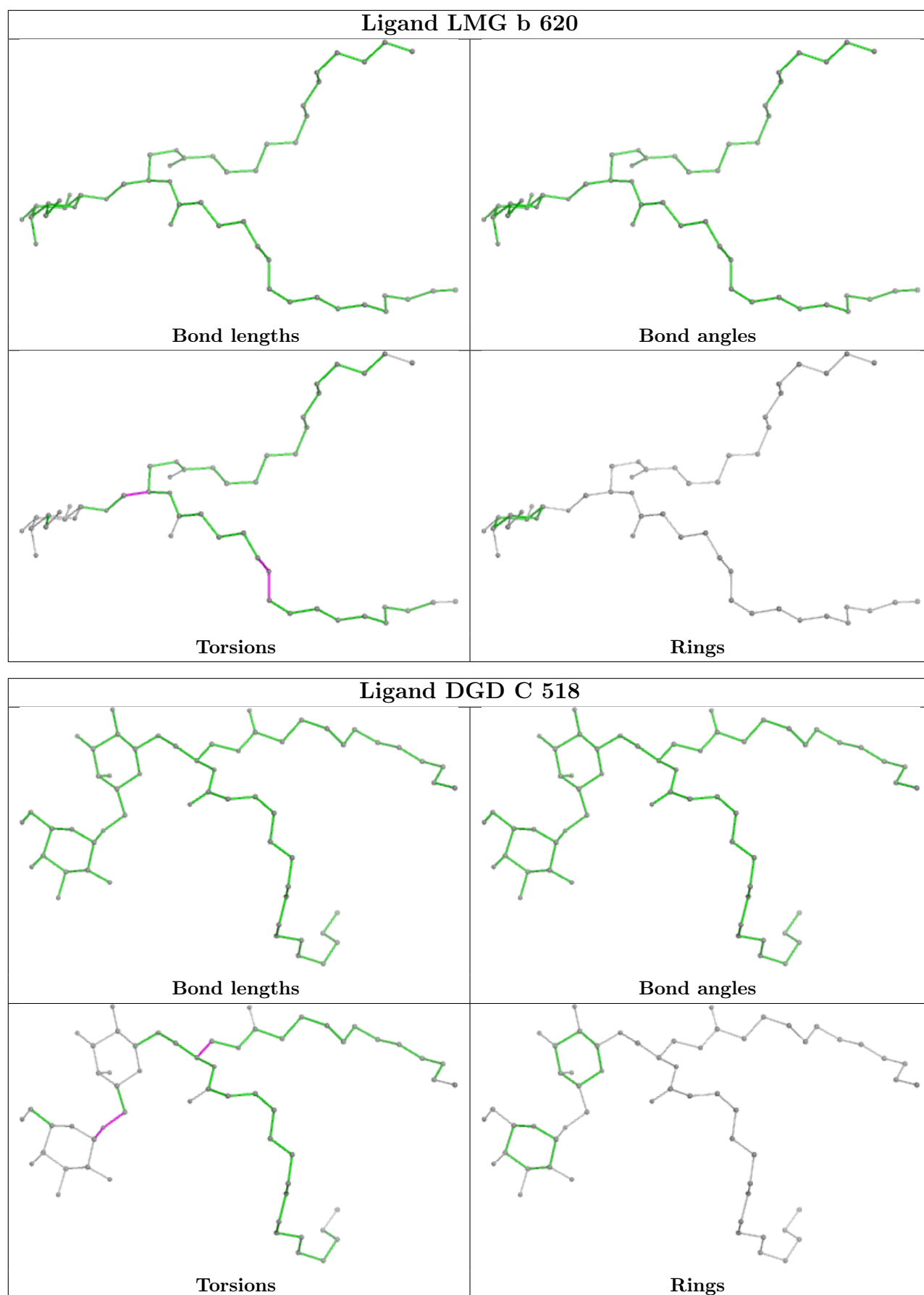




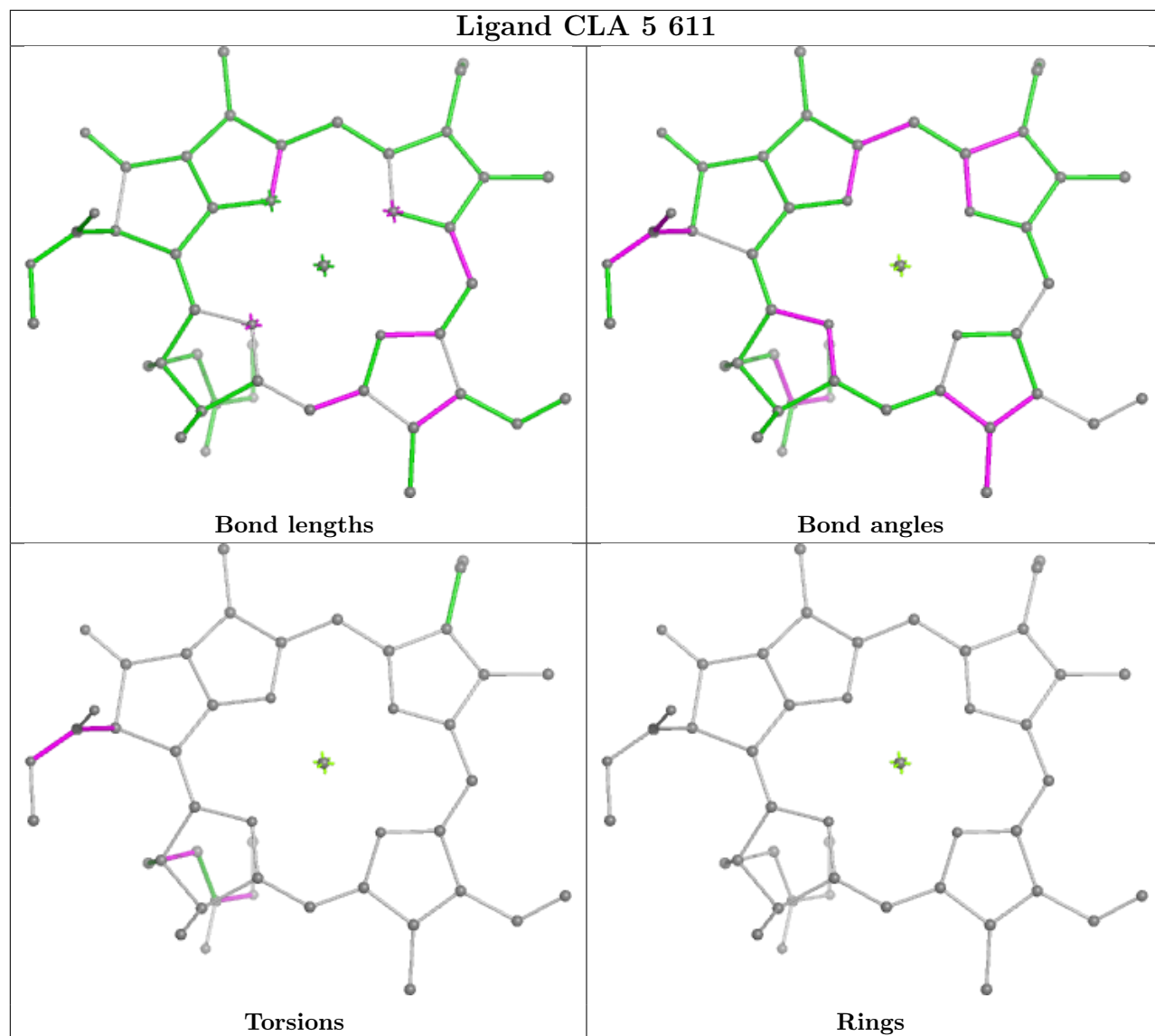
Ligand CHL S 601

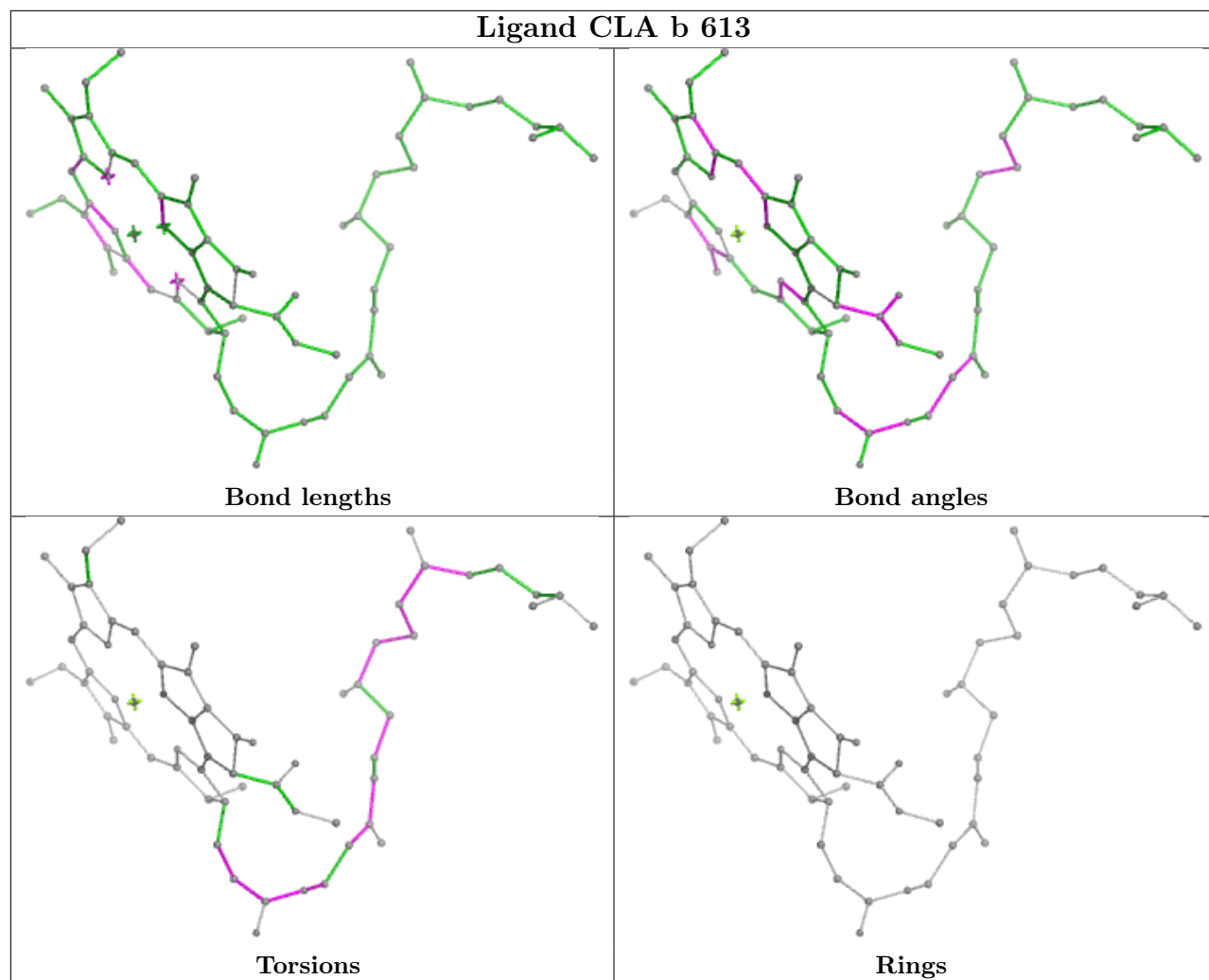


Ligand LHG S 621**Ligand CLA b 612**

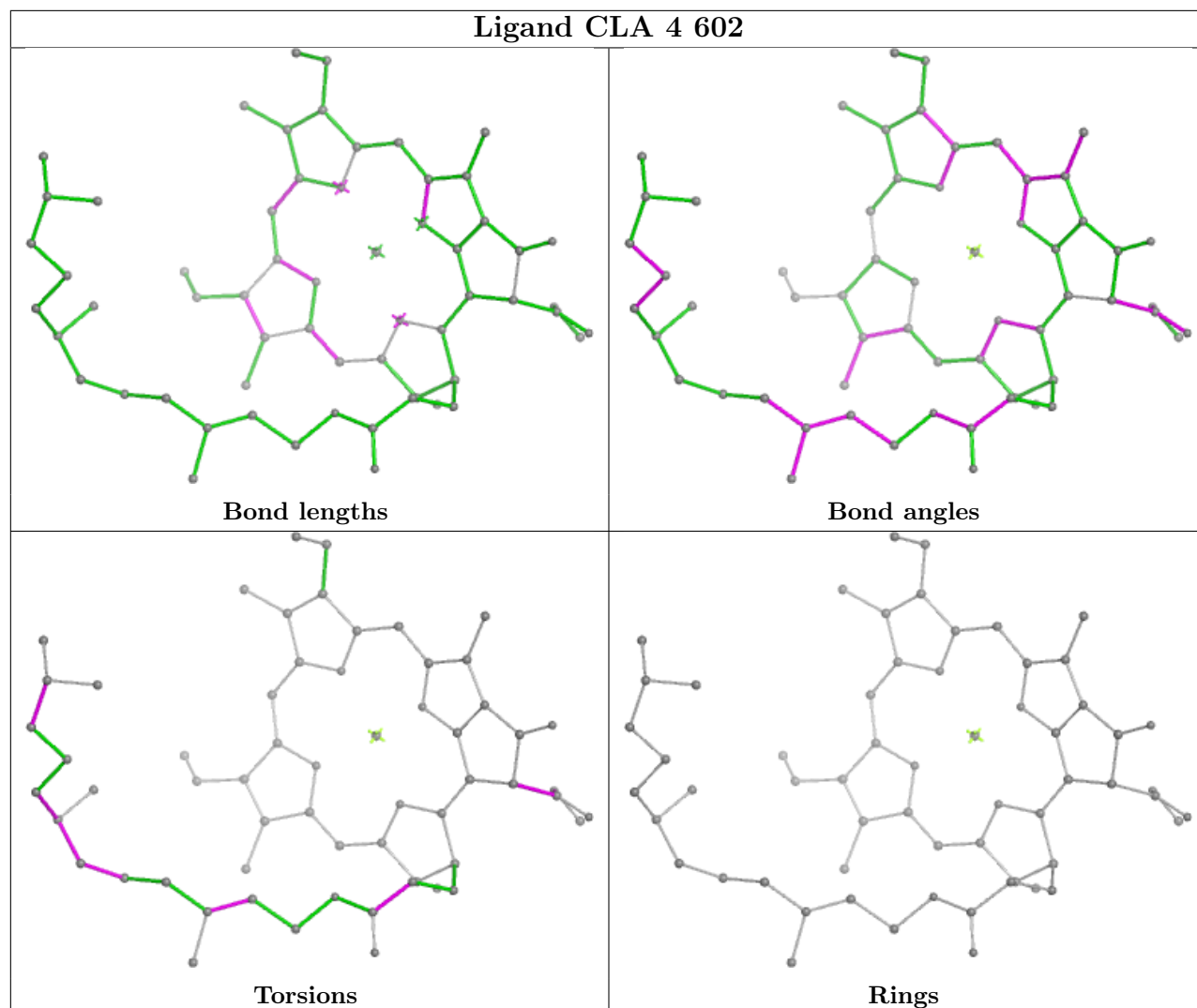


Ligand CLA 5 611

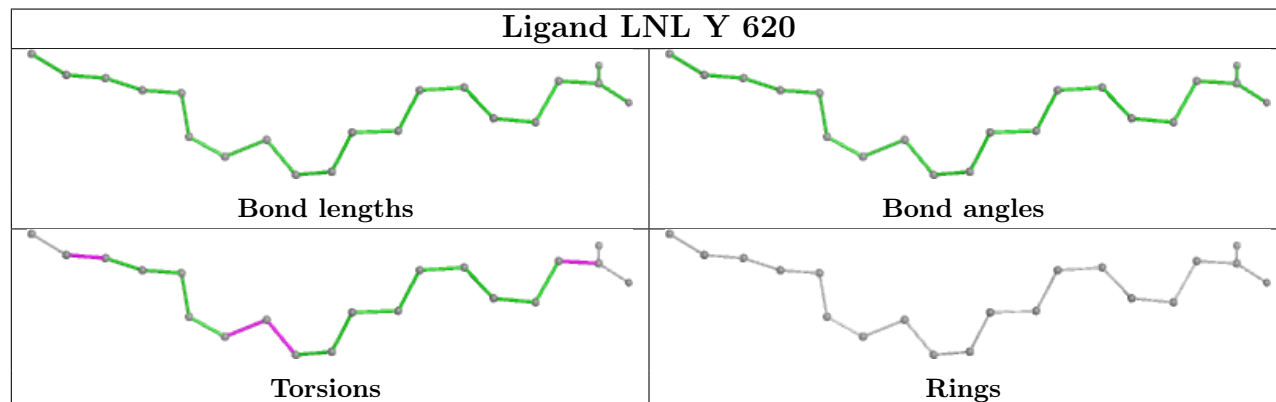


Ligand CLA b 613

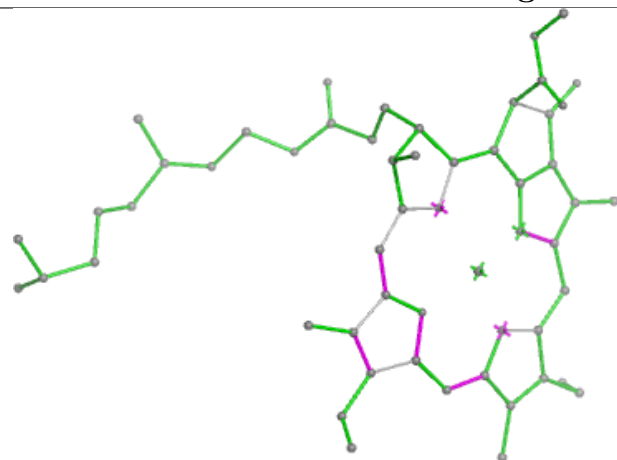
Ligand CLA 4 602



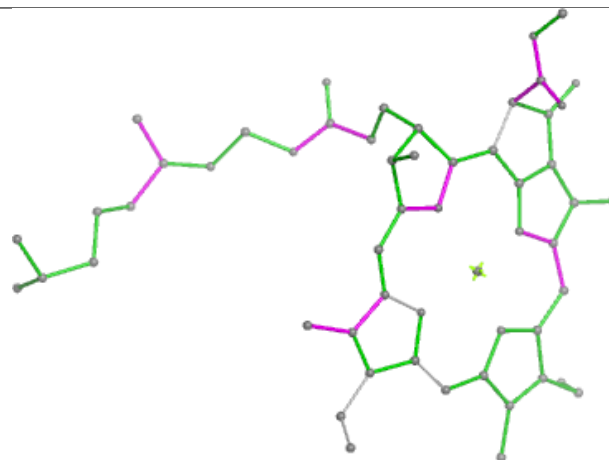
Ligand LNL Y 620



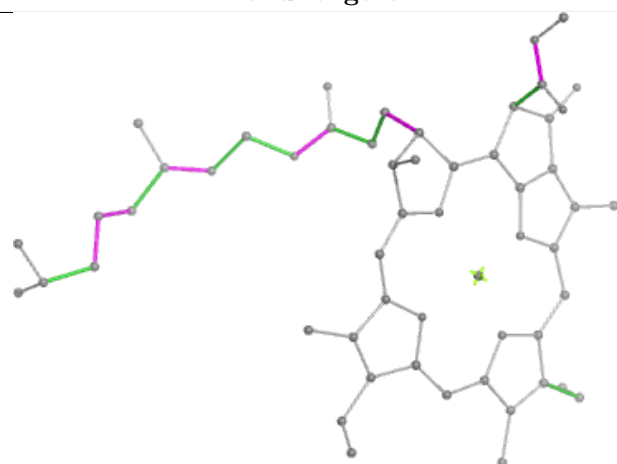
Ligand CLA A 406



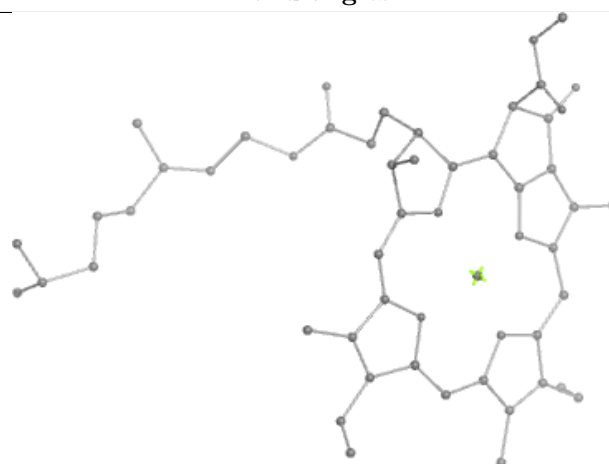
Bond lengths



Bond angles

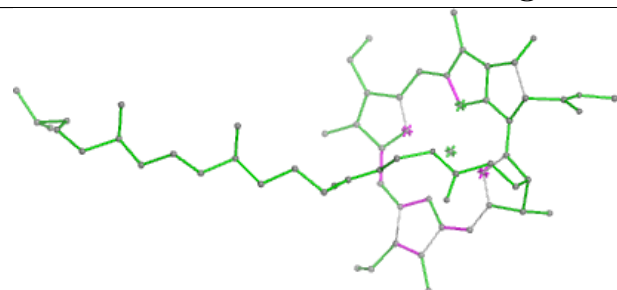


Torsions

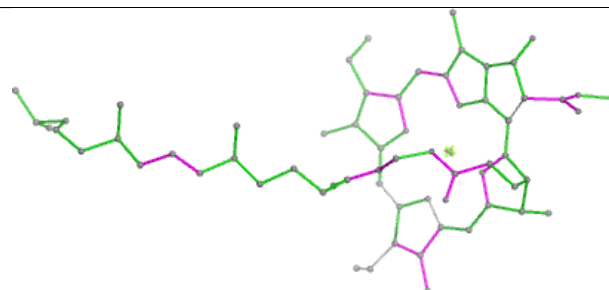


Rings

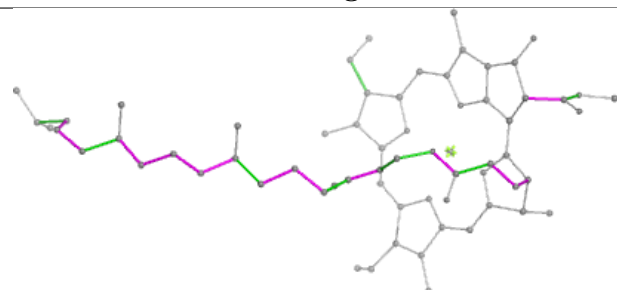
Ligand CLA B 608



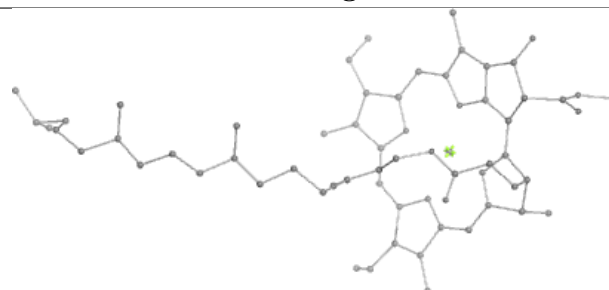
Bond lengths



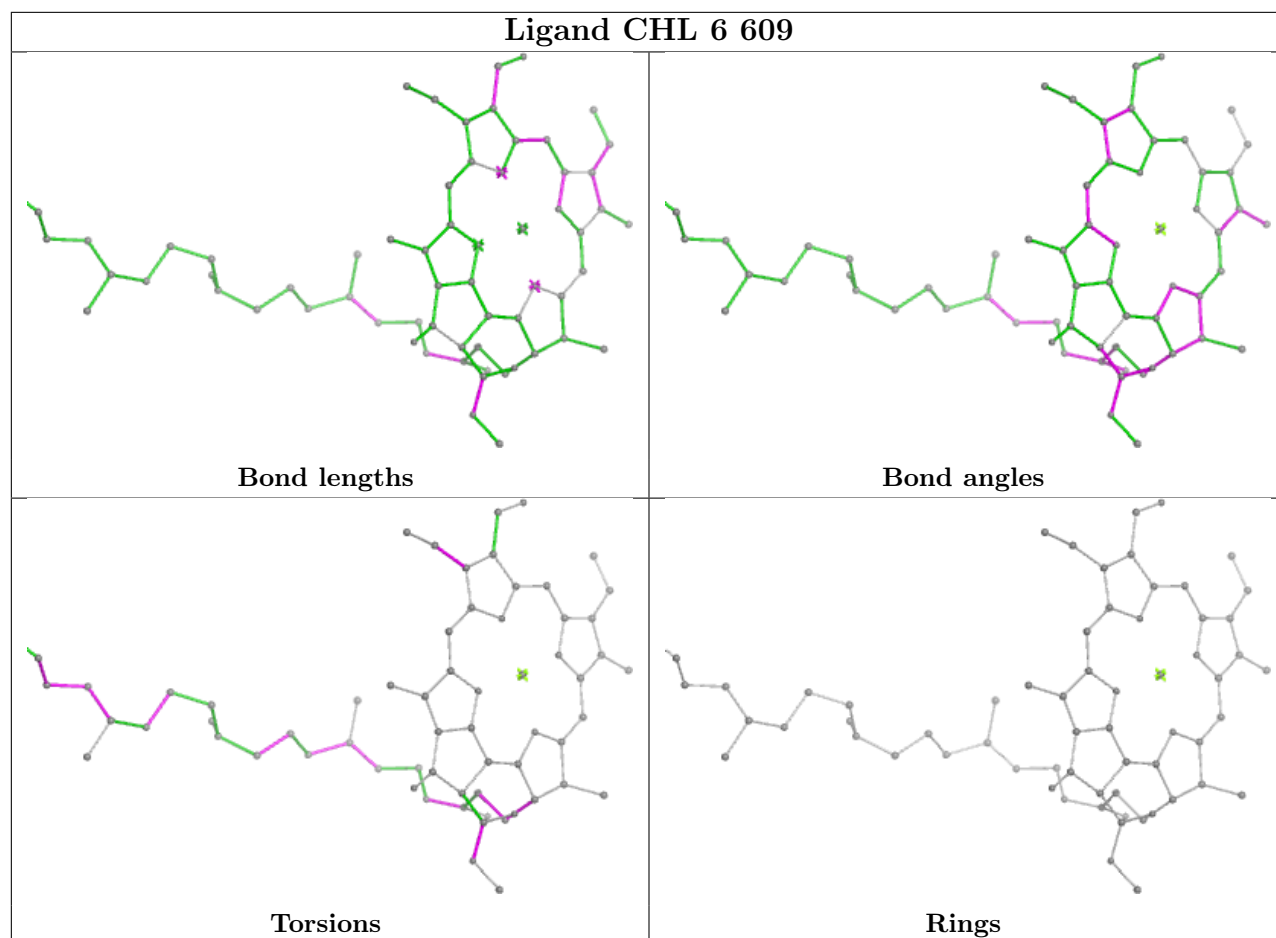
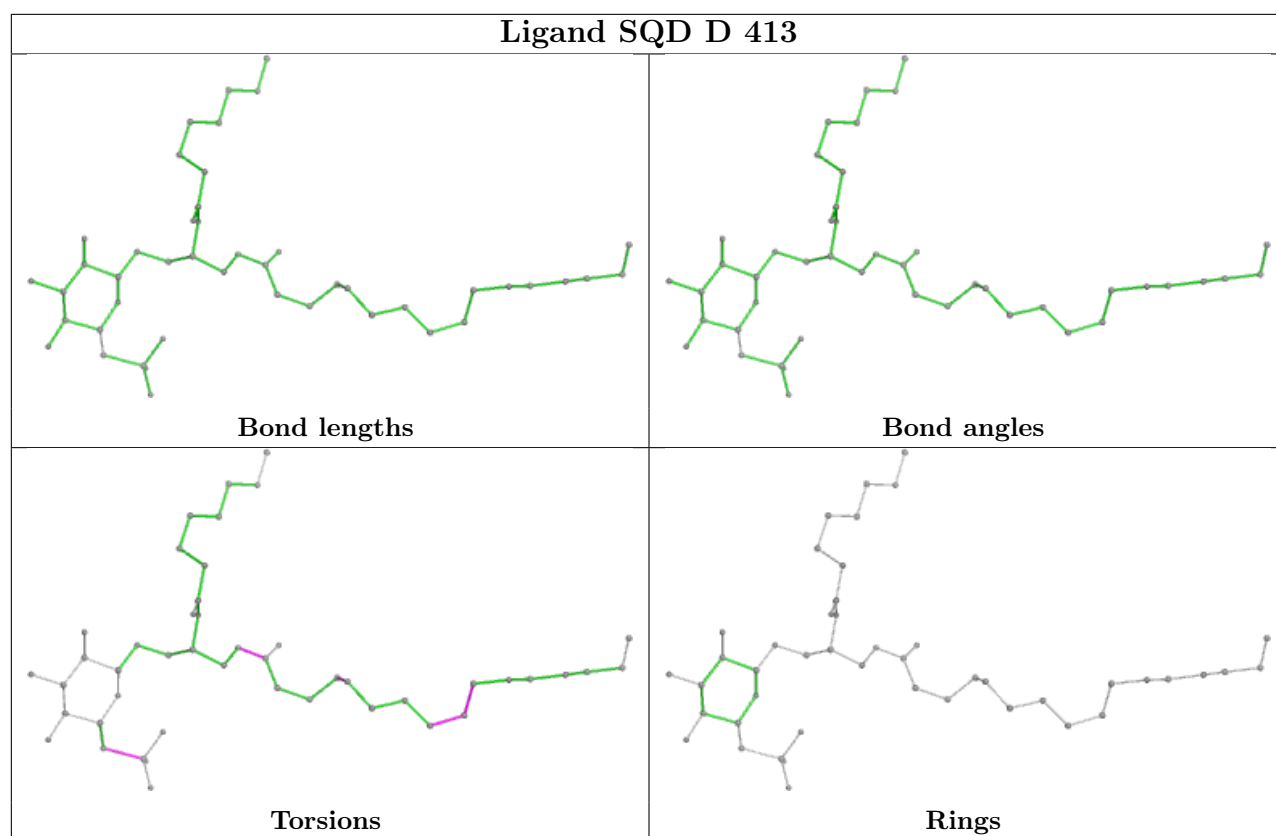
Bond angles

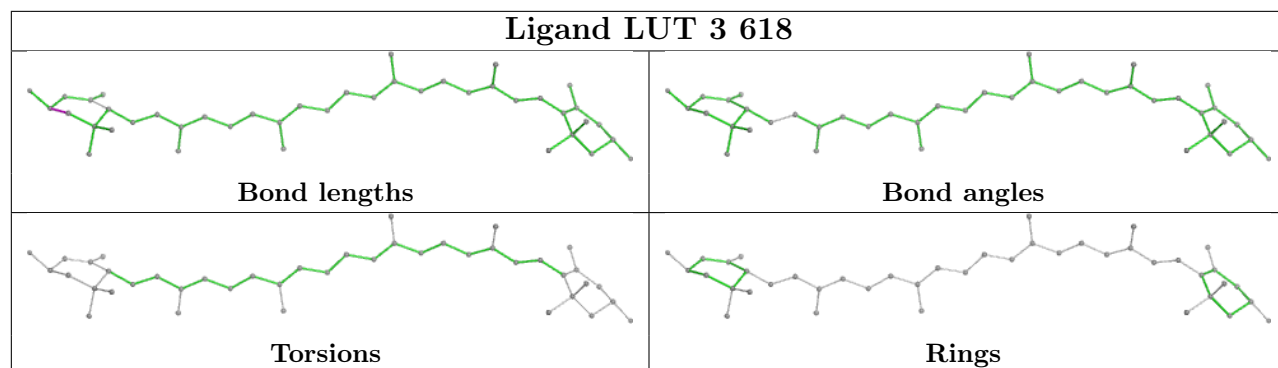
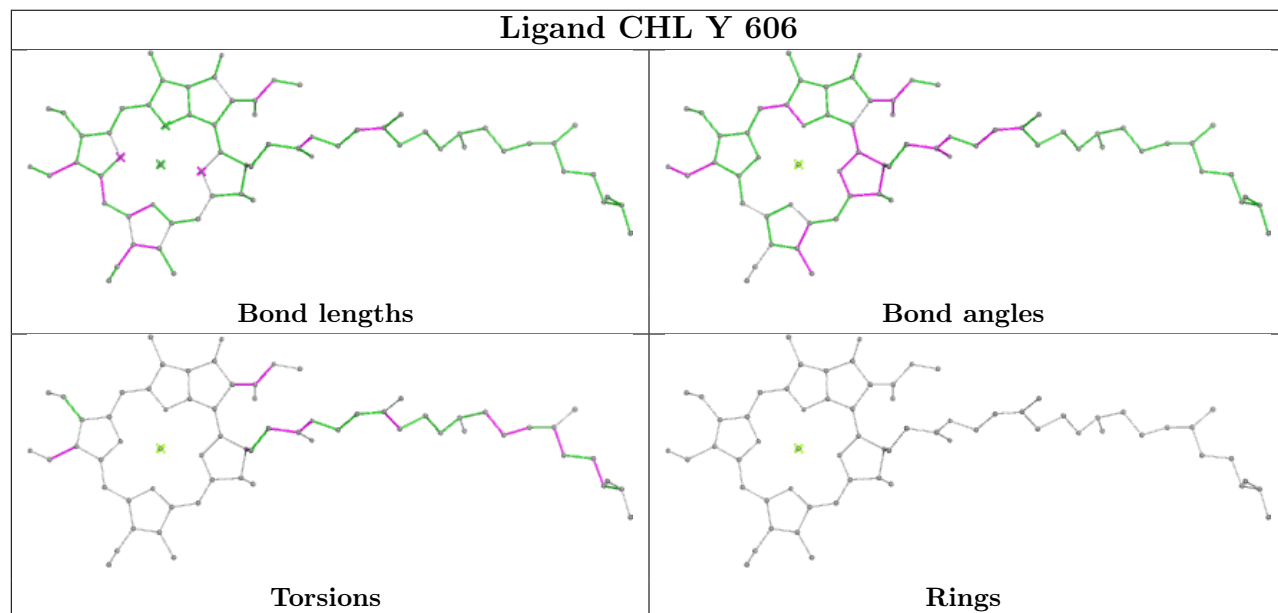


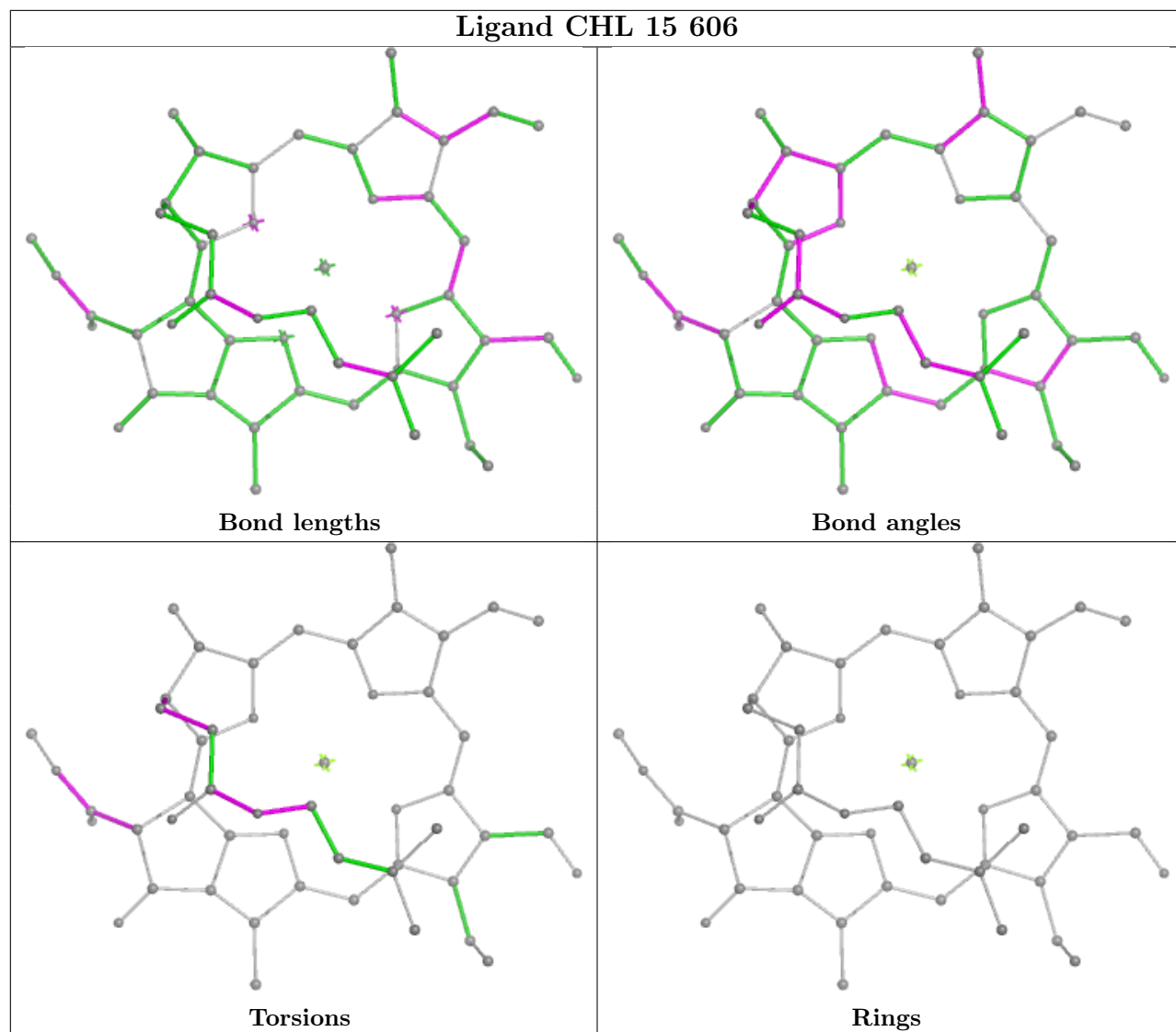
Torsions



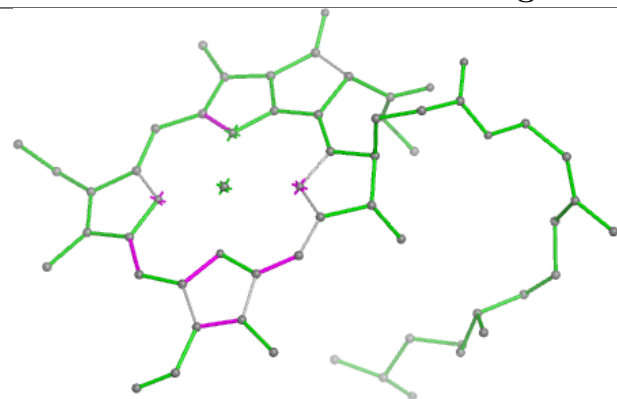
Rings



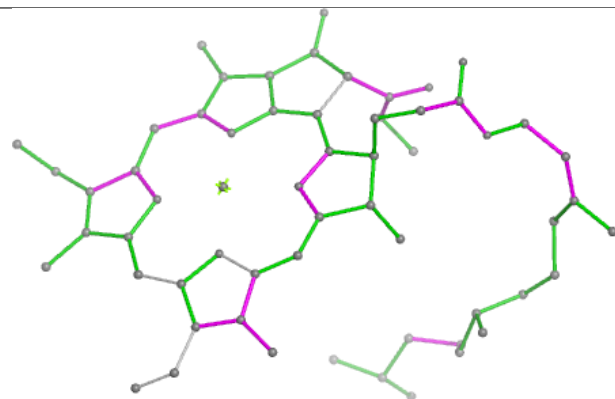
Ligand LUT 3 618**Ligand CHL Y 606**



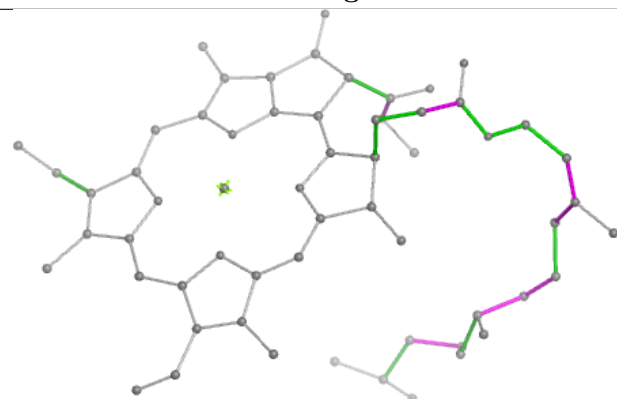
Ligand CLA N 603



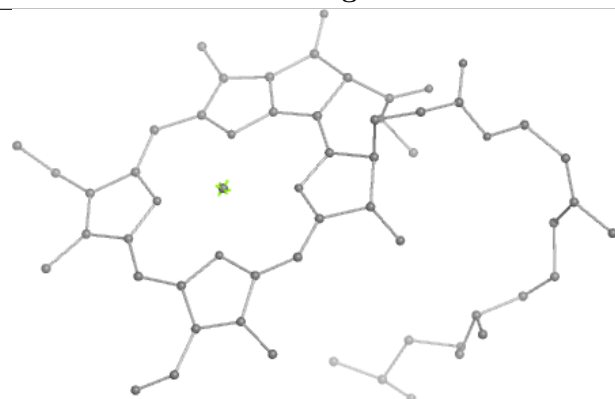
Bond lengths



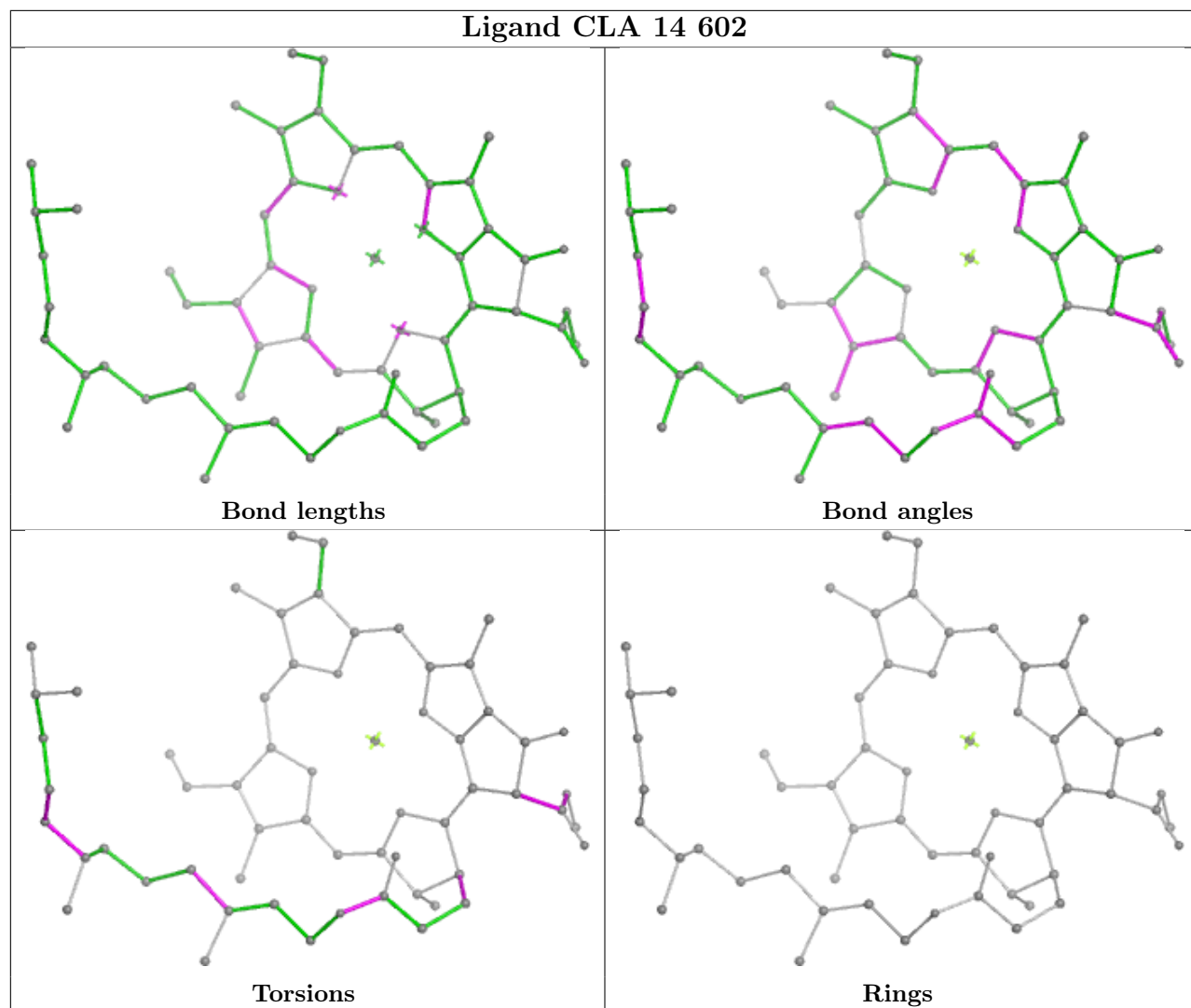
Bond angles



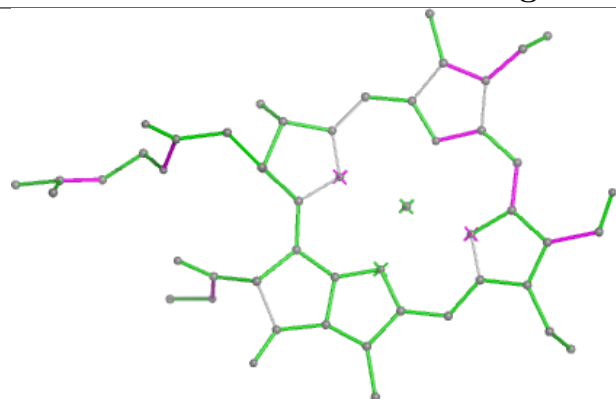
Torsions



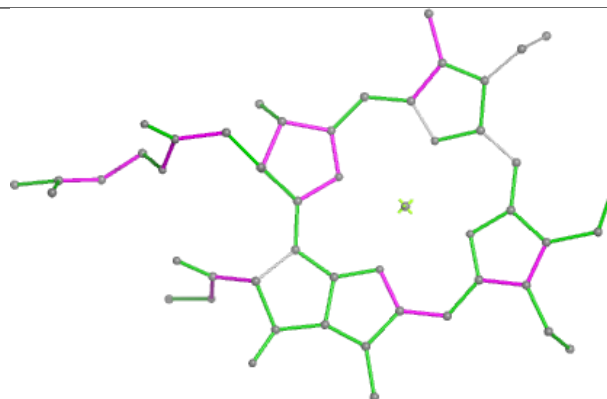
Rings



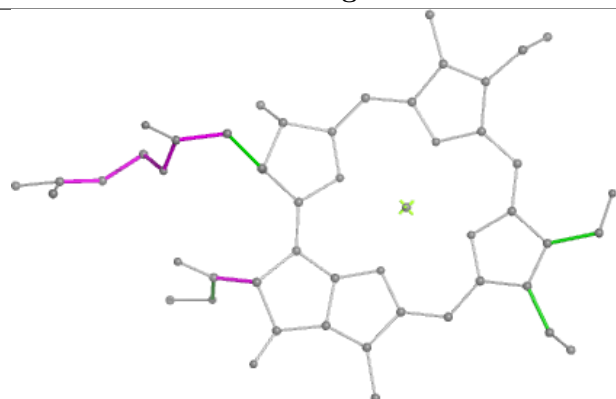
Ligand CHL 4 607



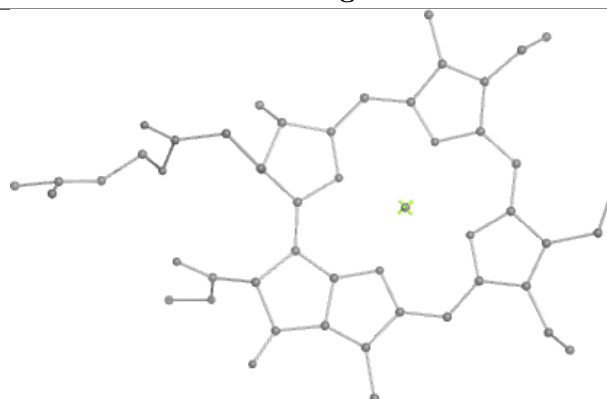
Bond lengths



Bond angles

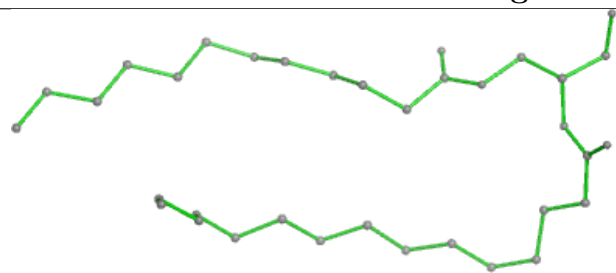


Torsions

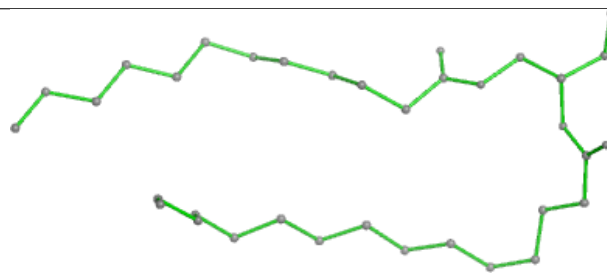


Rings

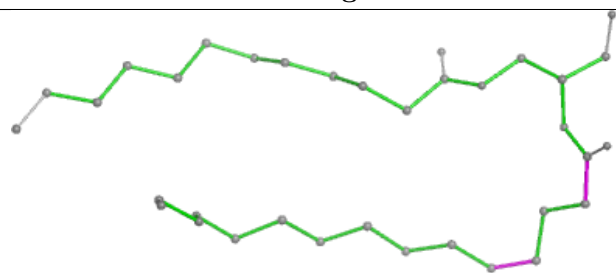
Ligand LMG H 102



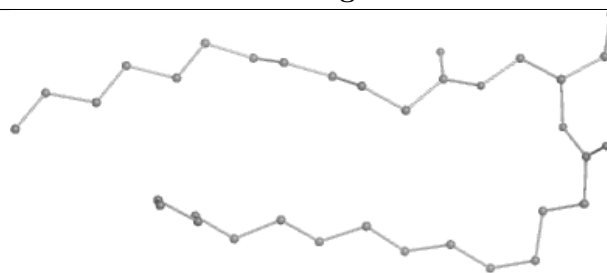
Bond lengths



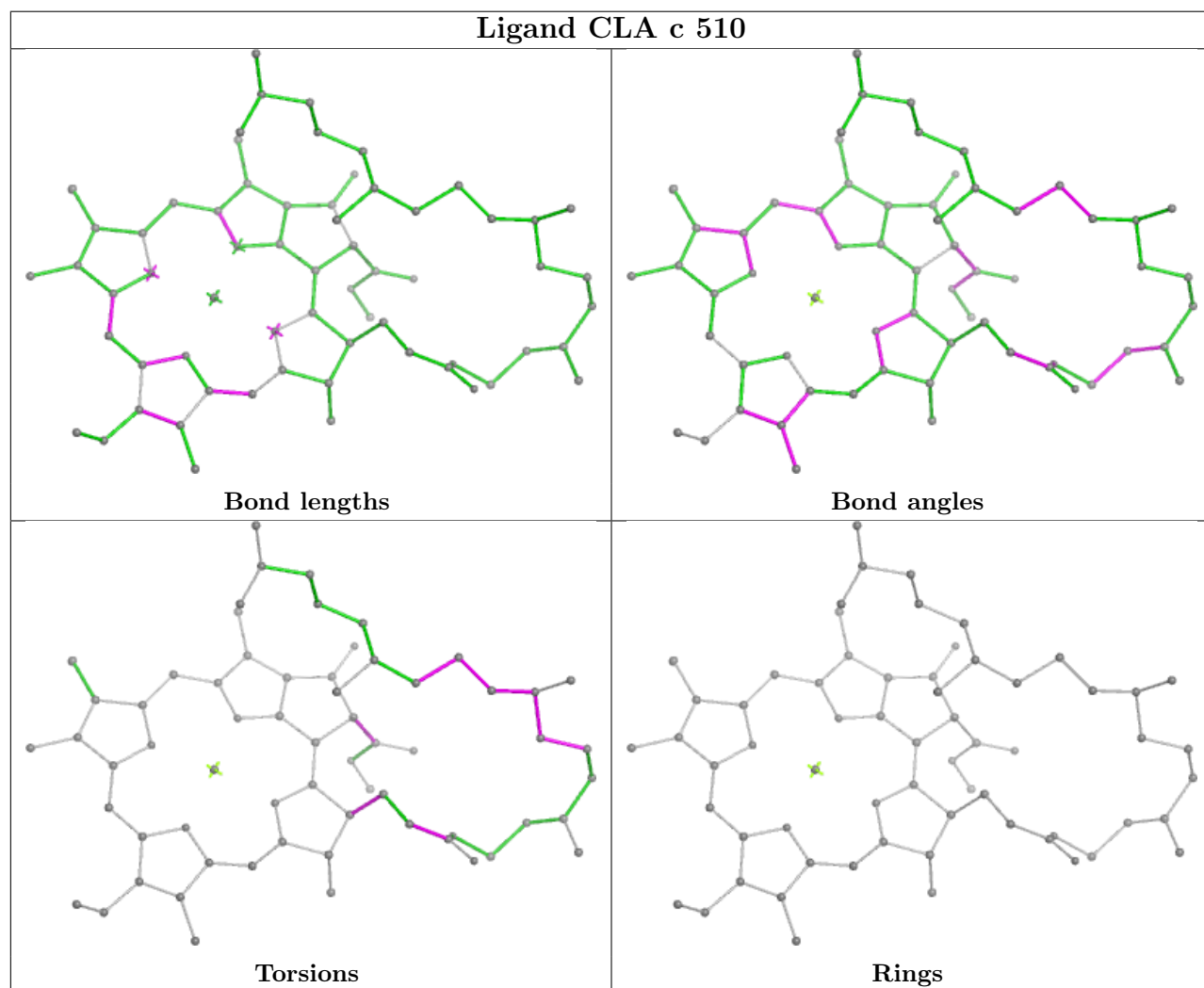
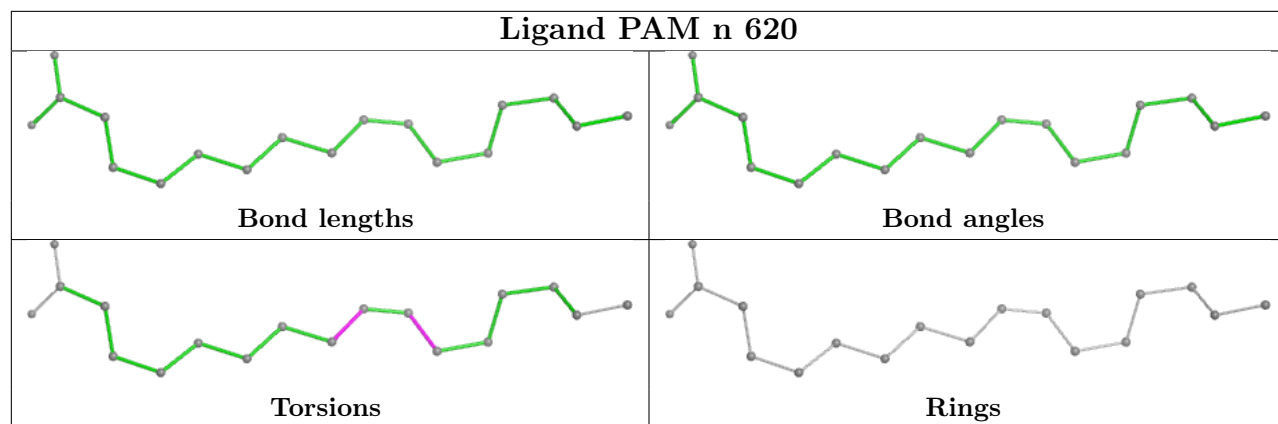
Bond angles



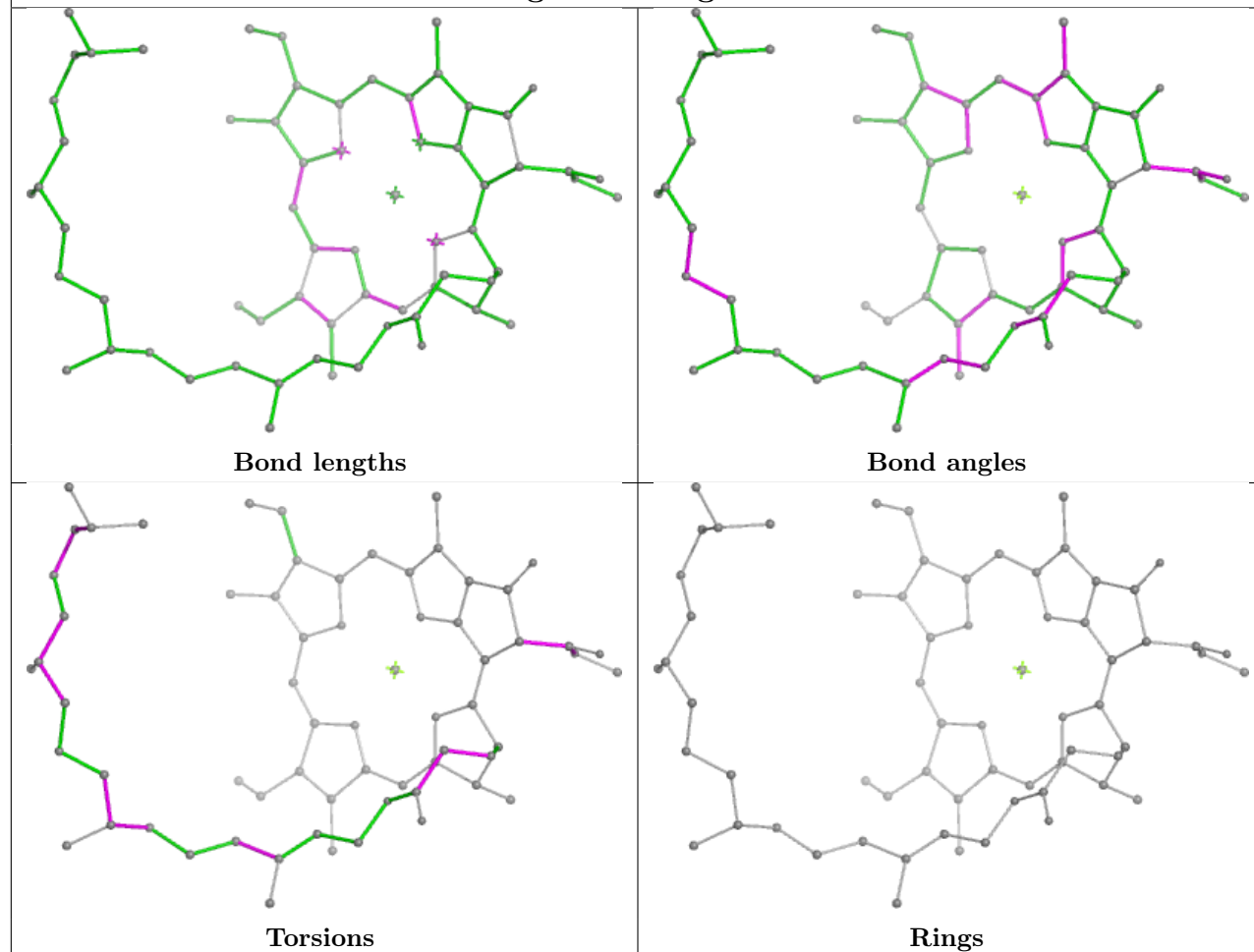
Torsions



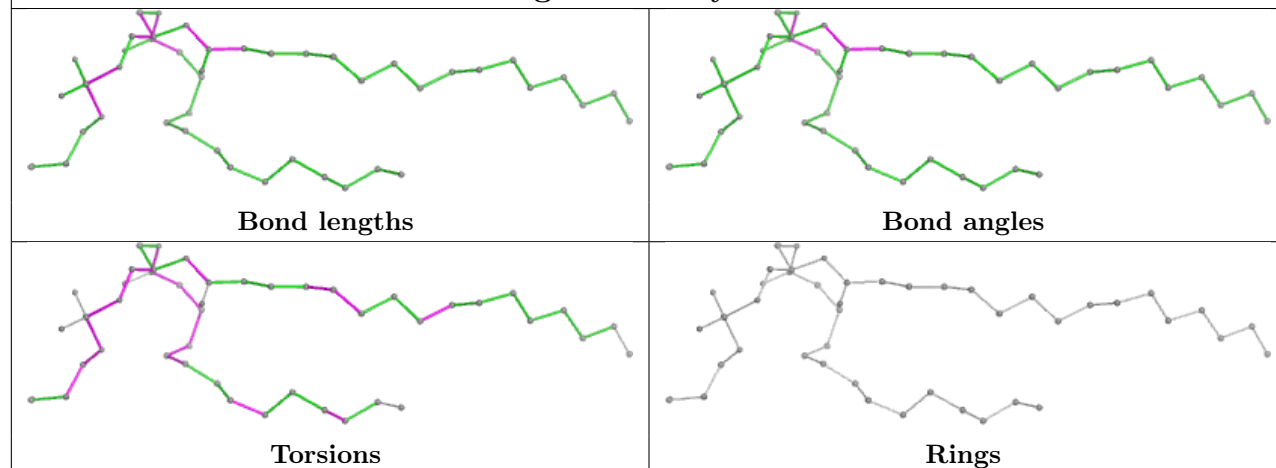
Rings

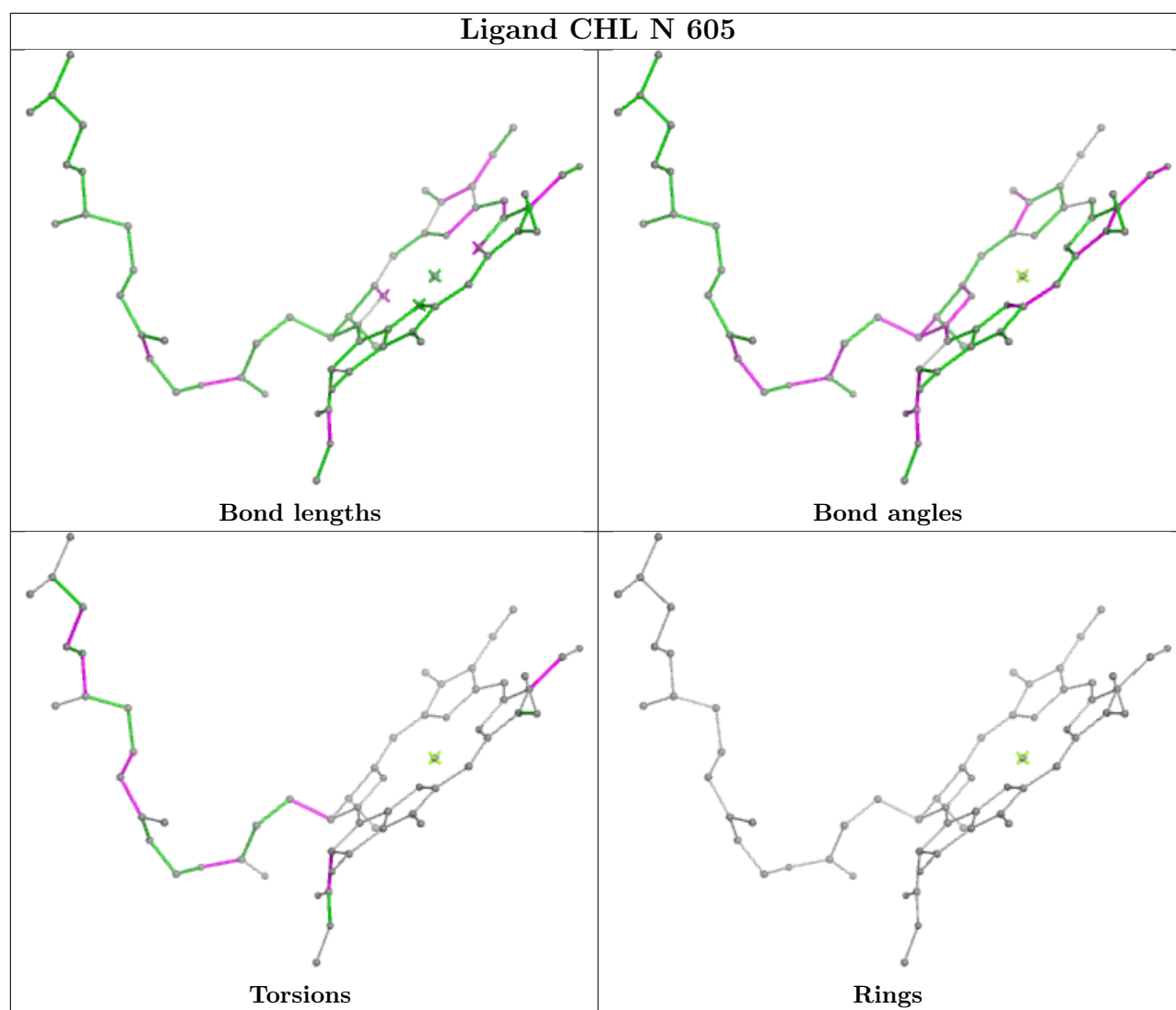


Ligand CLA g 602

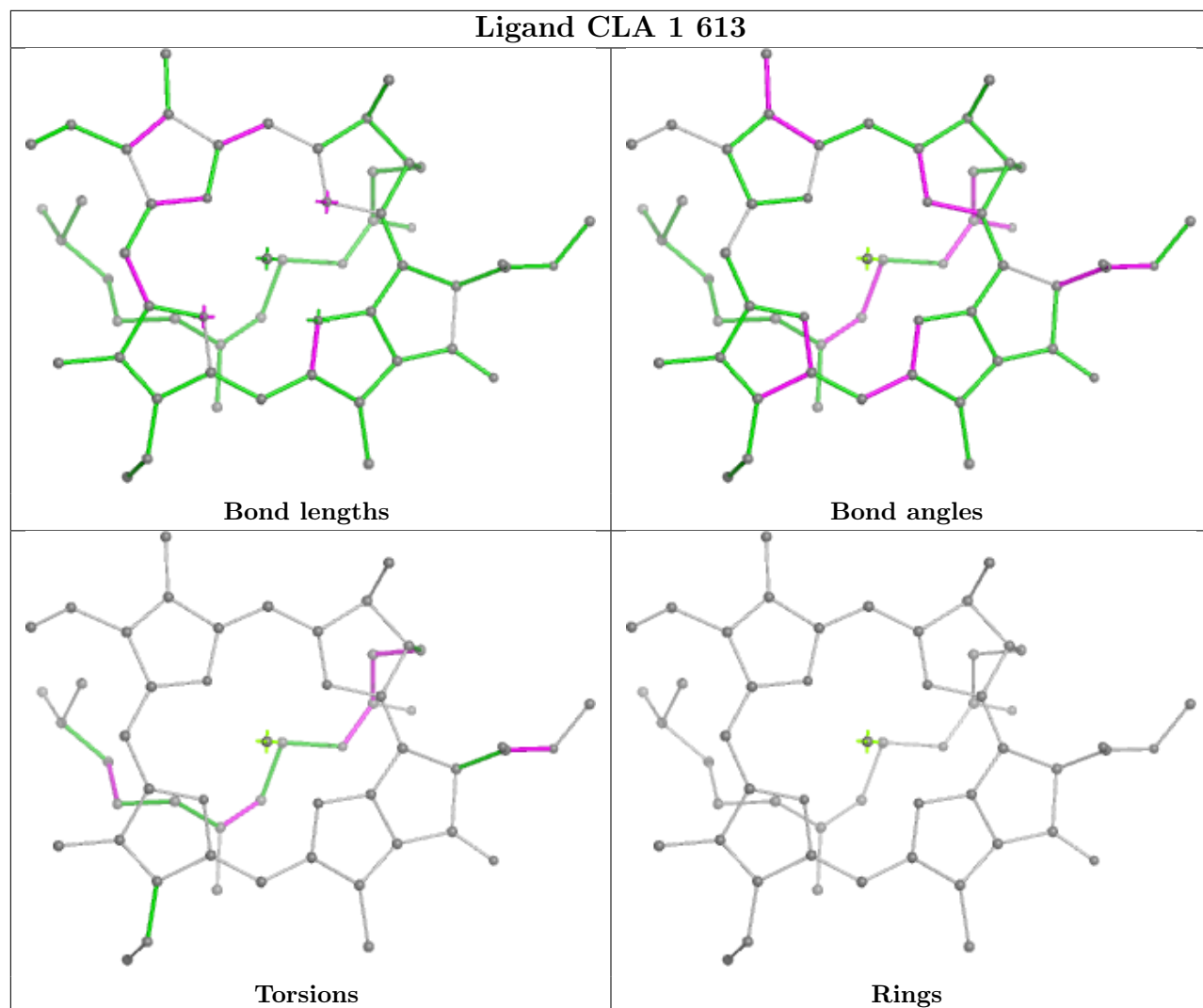


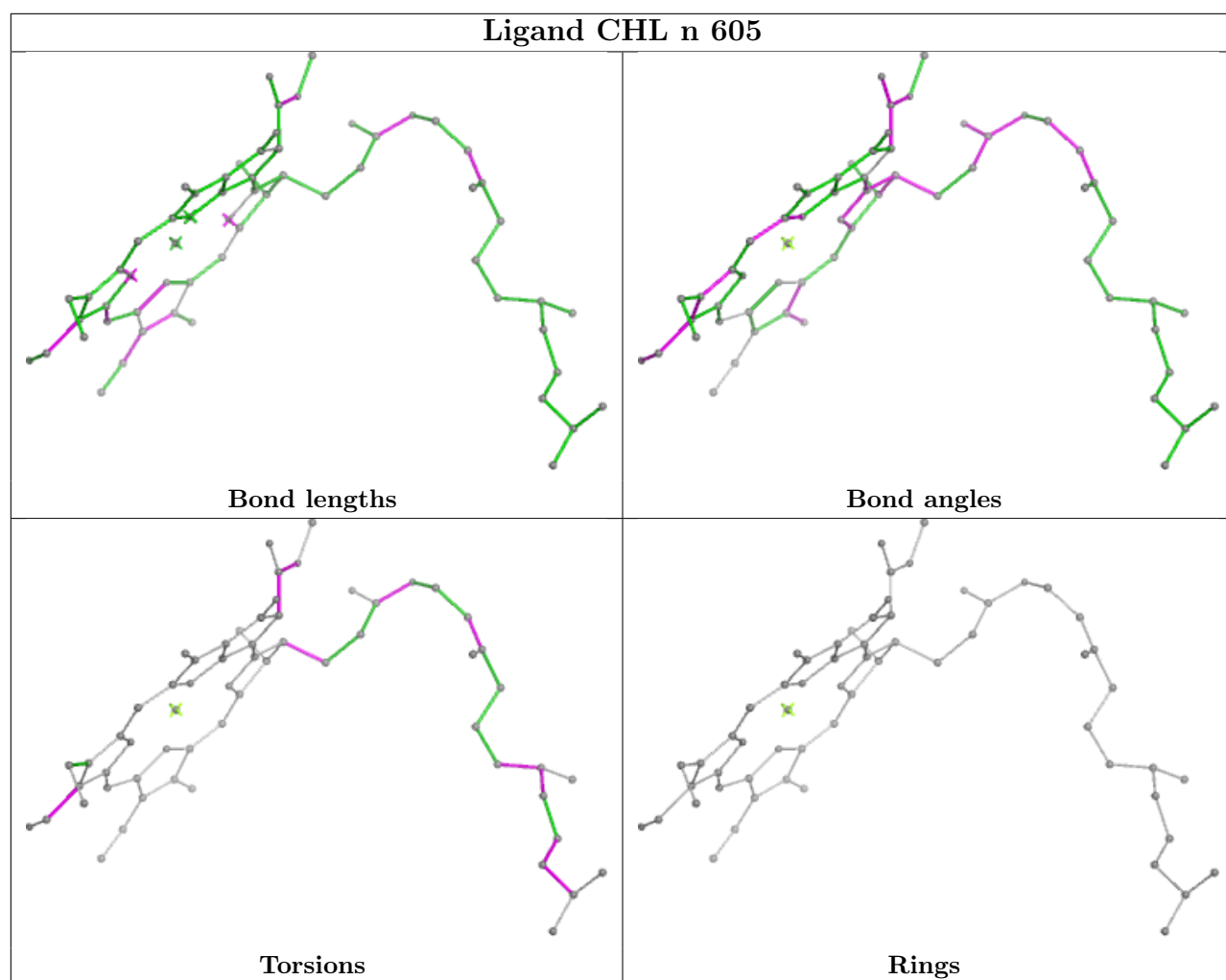
Ligand LHG y 617



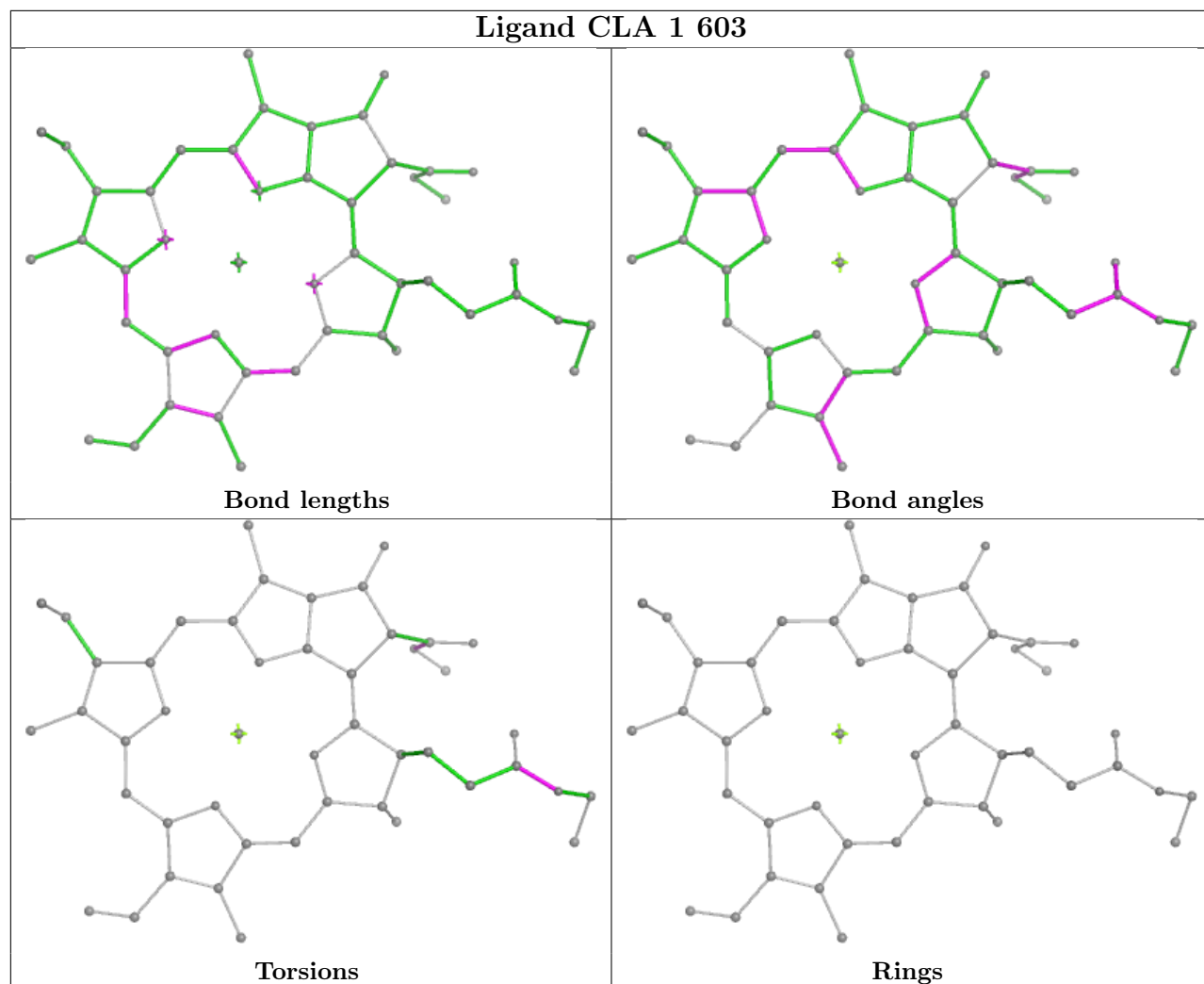


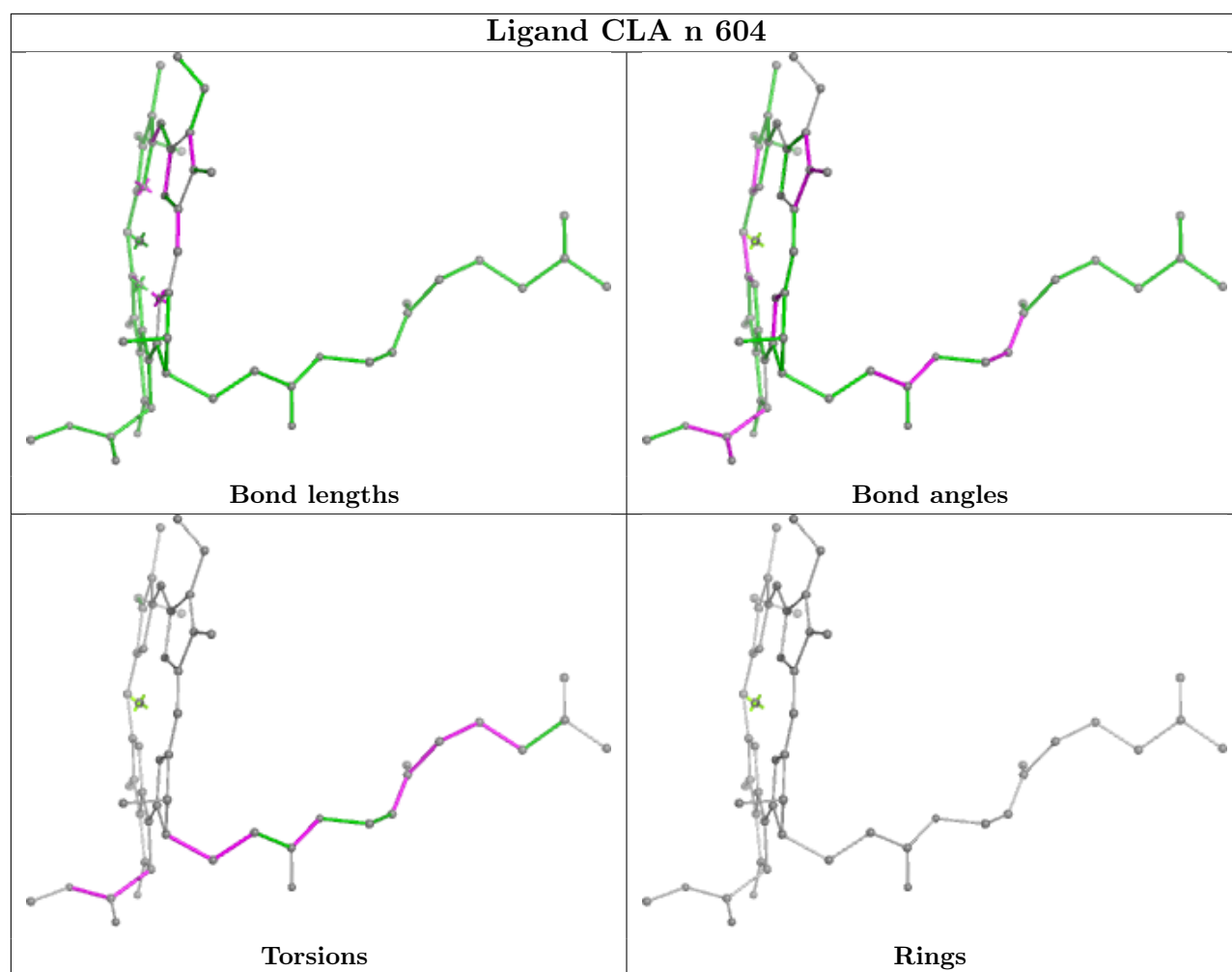
Ligand CLA 1 613

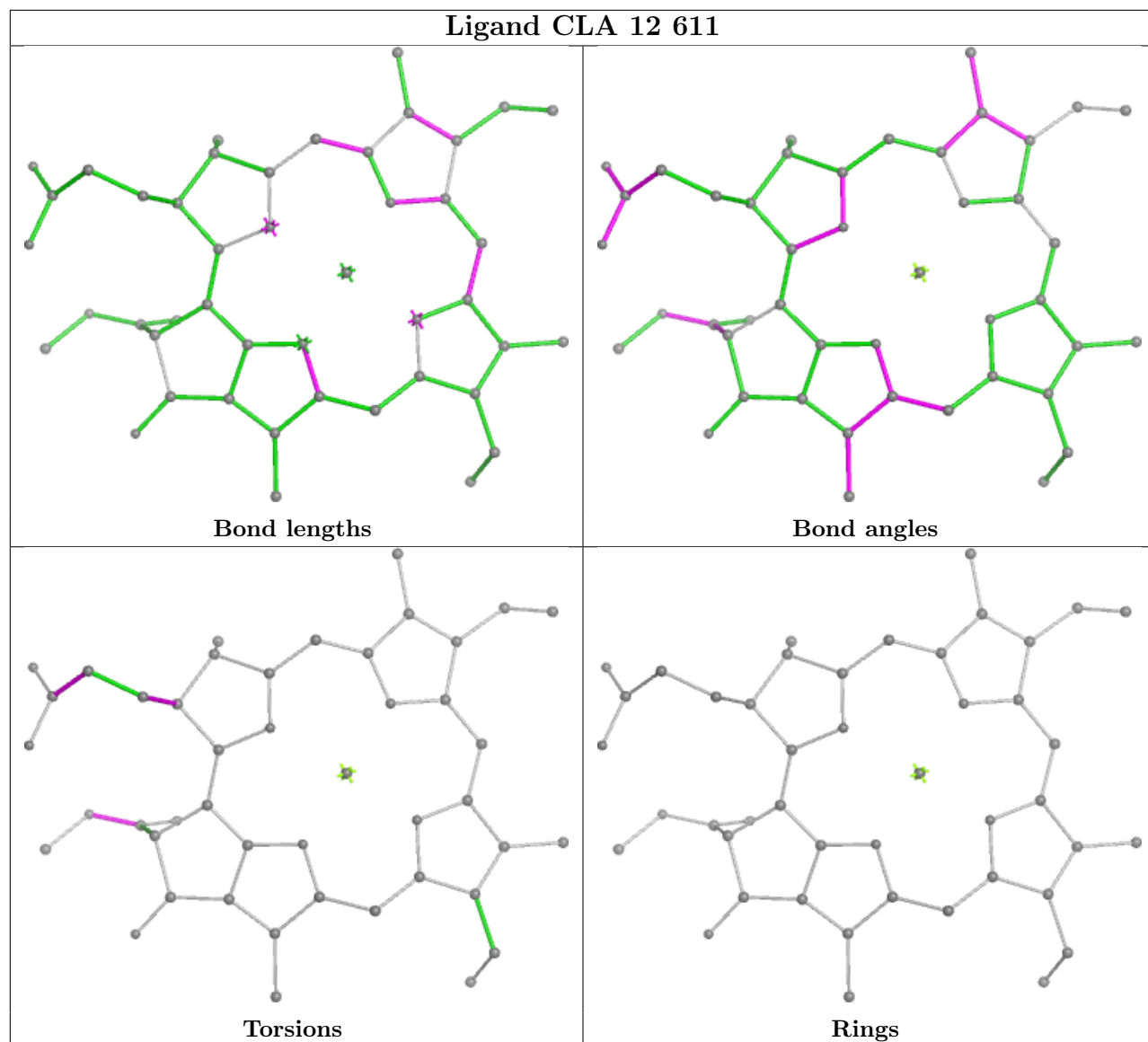


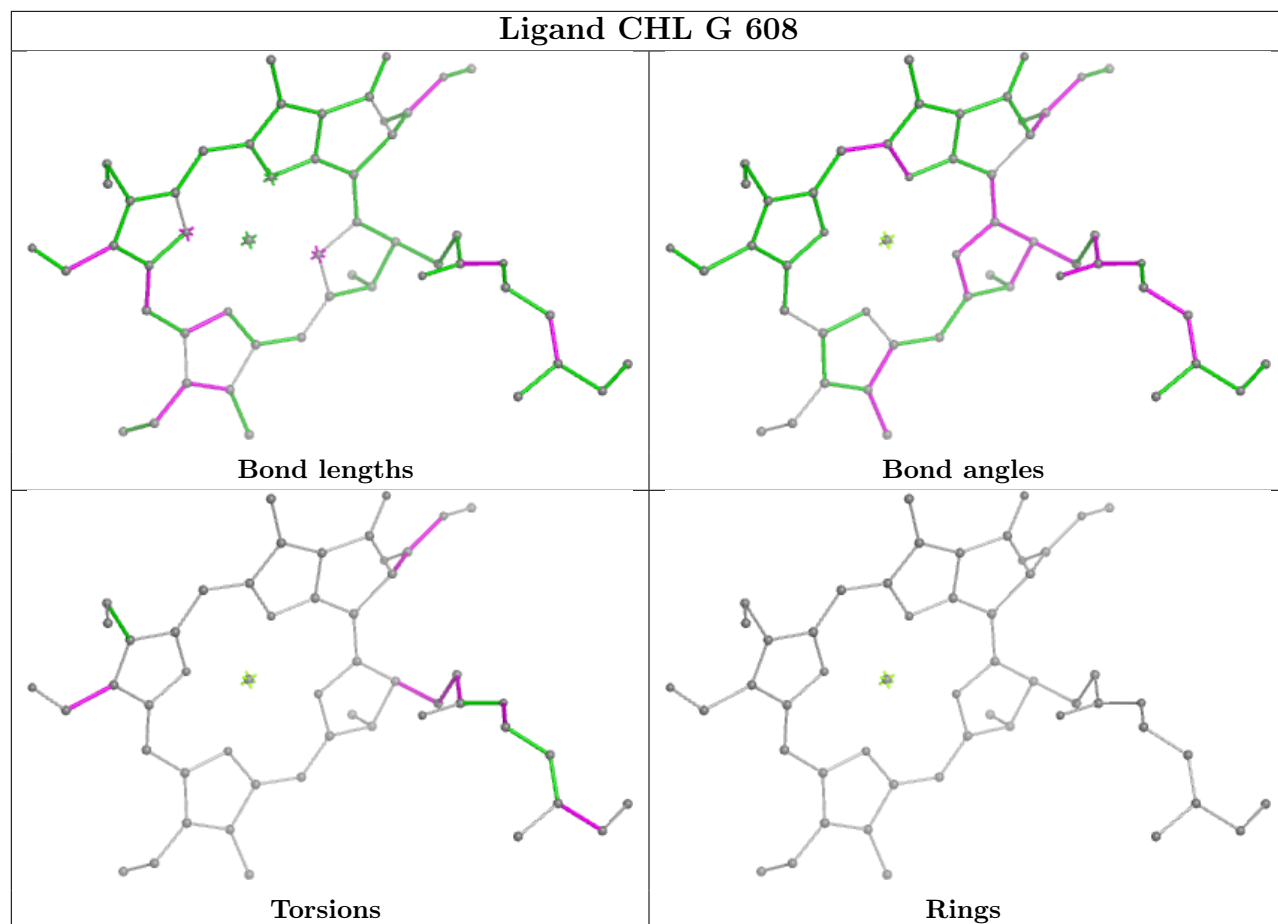


Ligand CLA 1 603

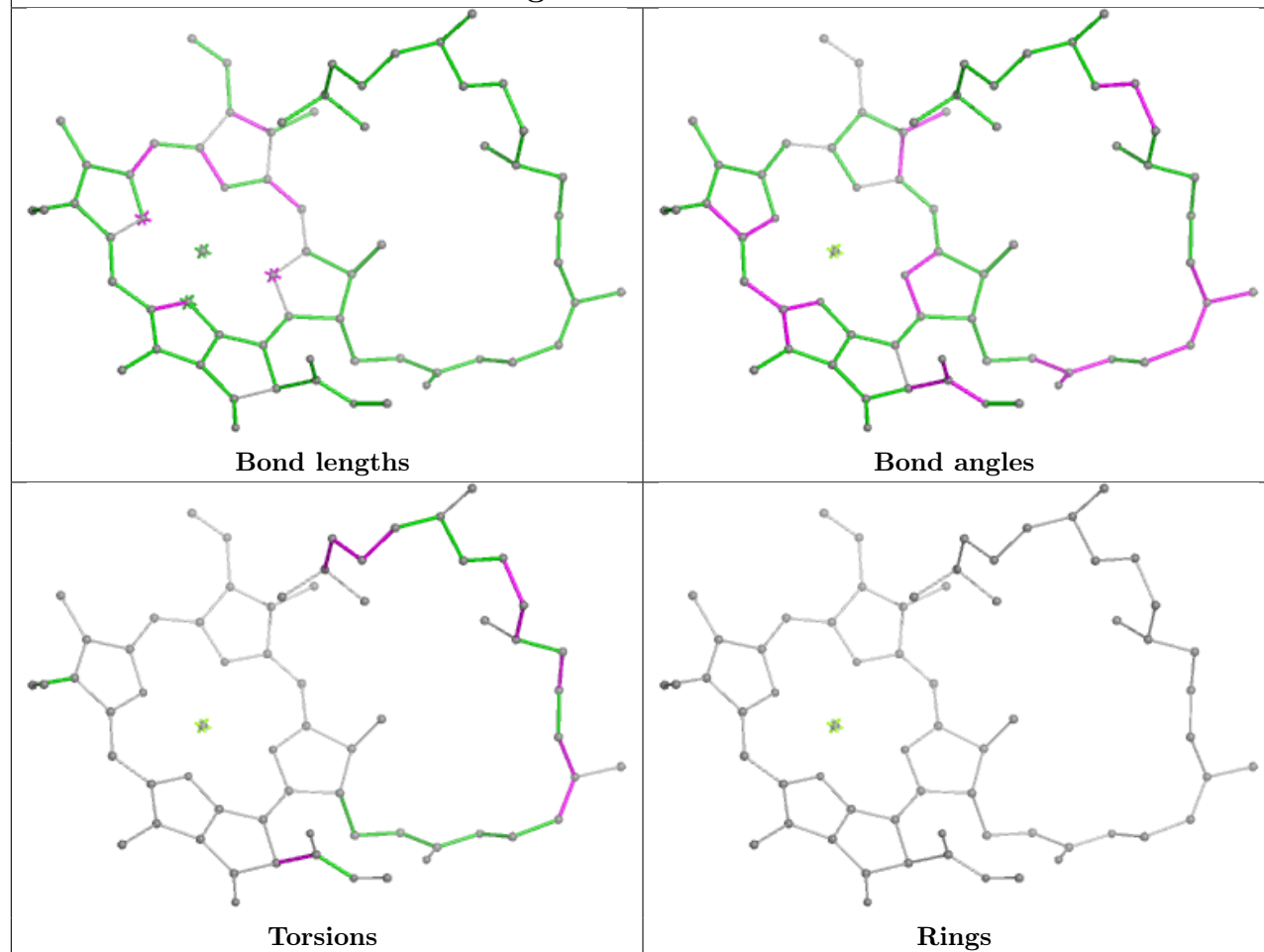




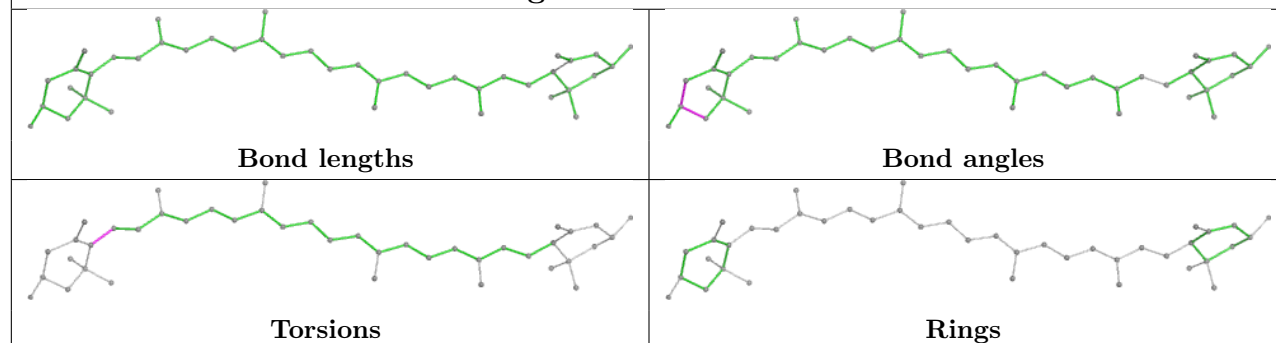


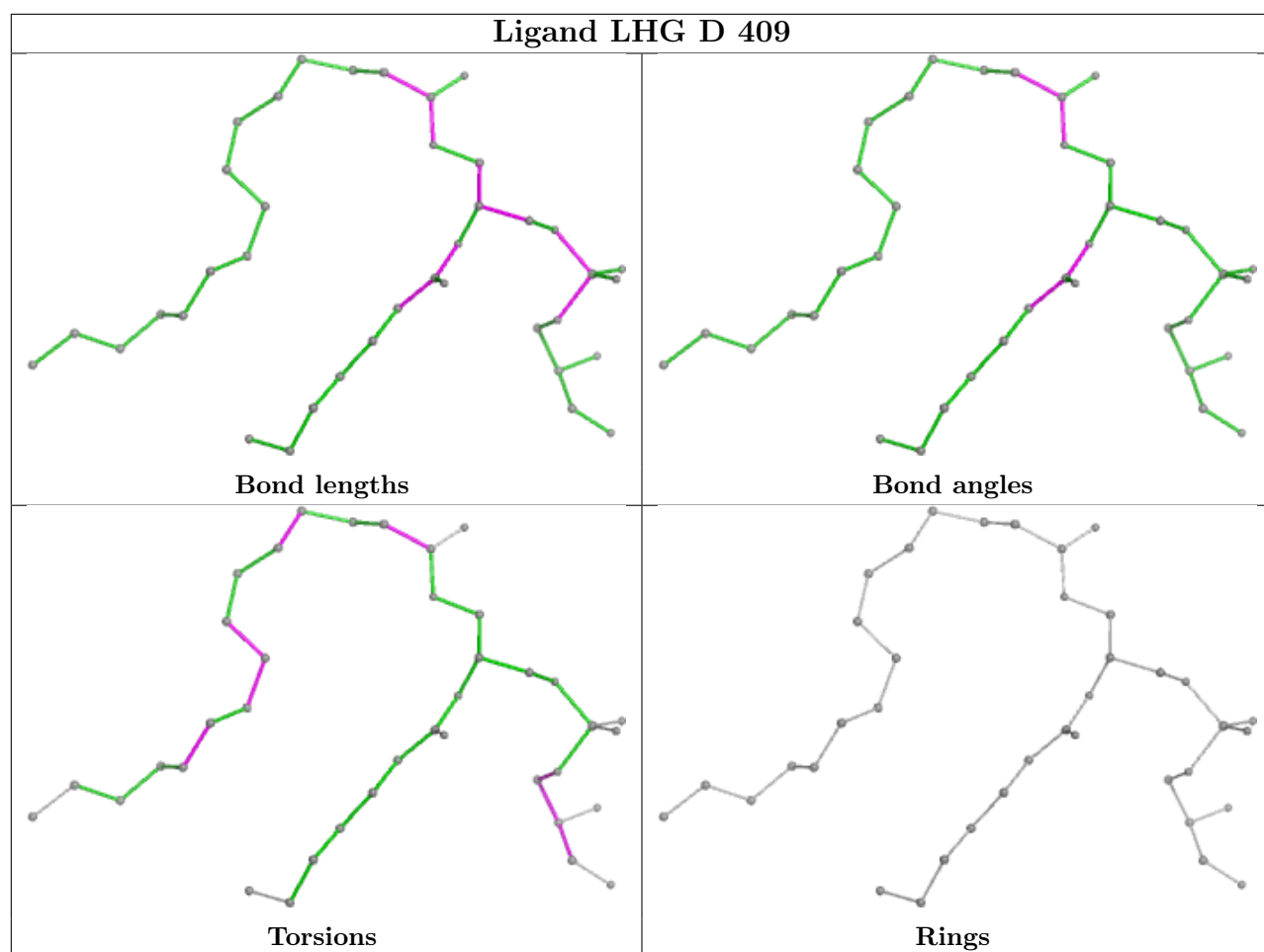


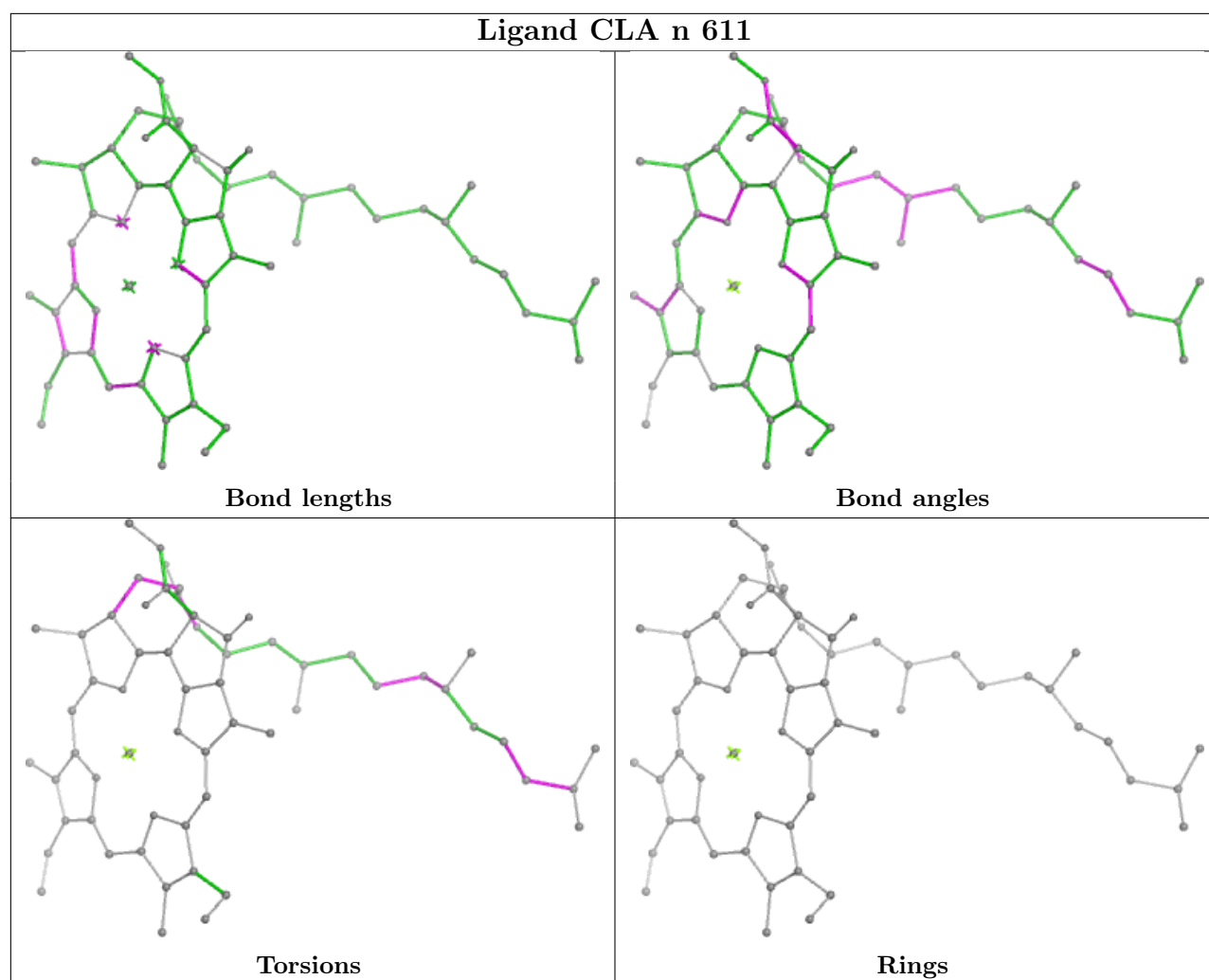
Ligand CLA B 615

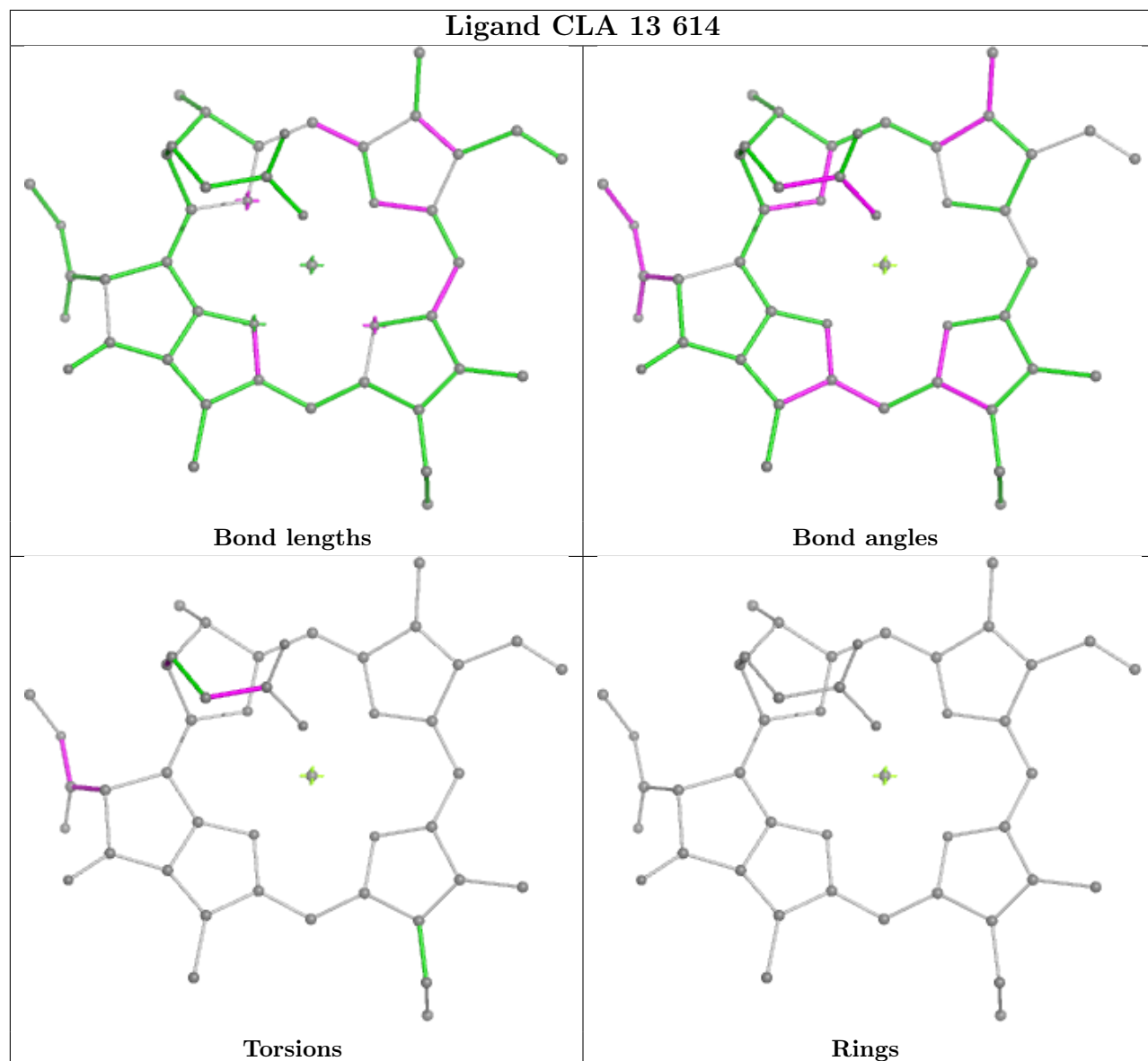


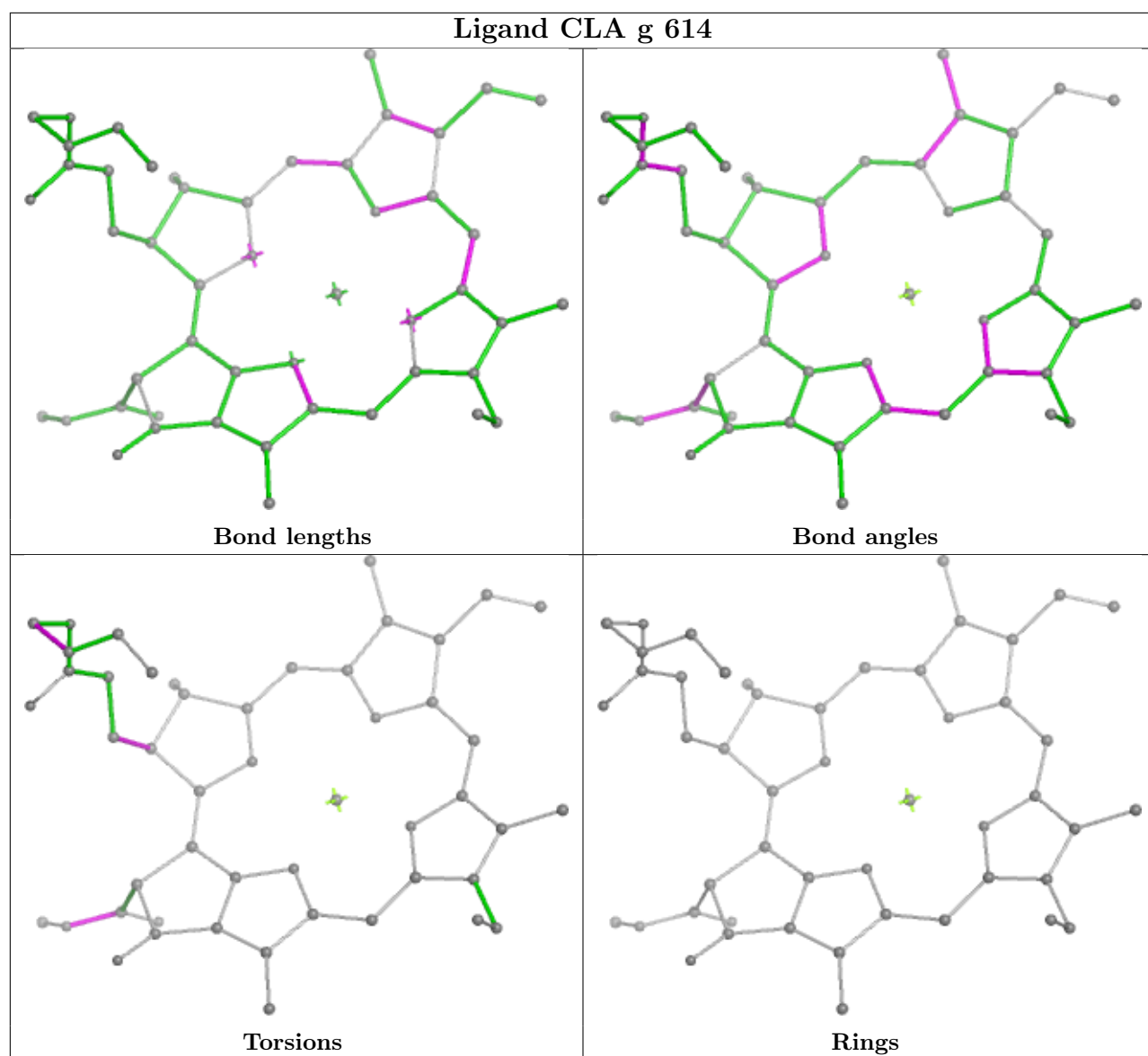
Ligand LUT 13 617



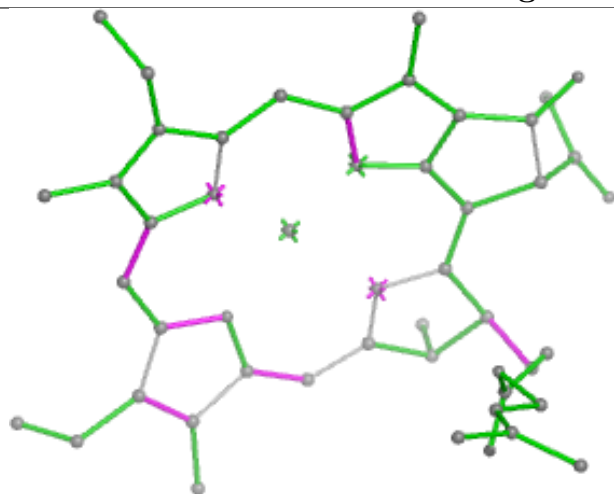




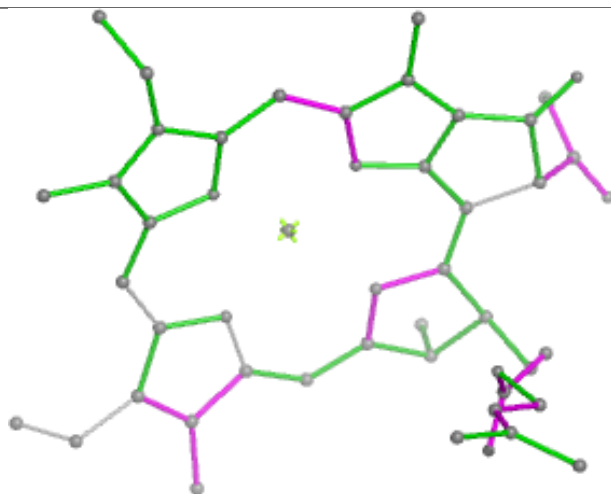




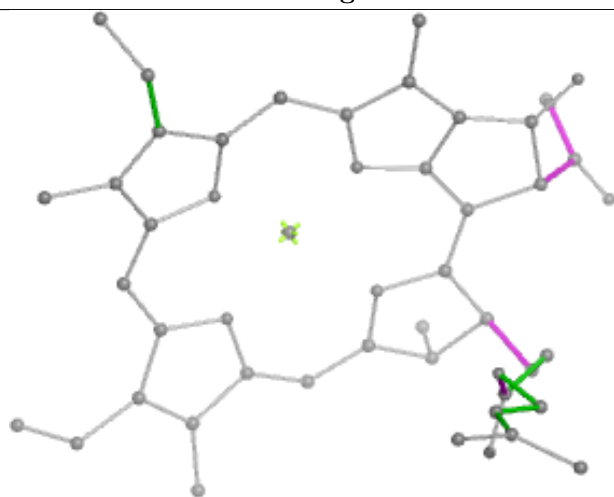
Ligand CLA 2 604



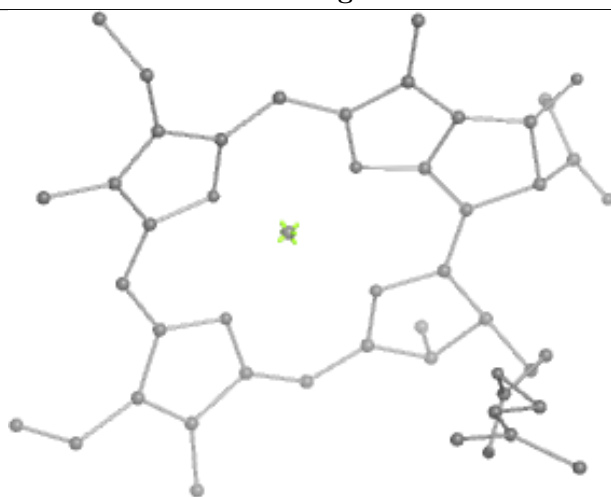
Bond lengths



Bond angles

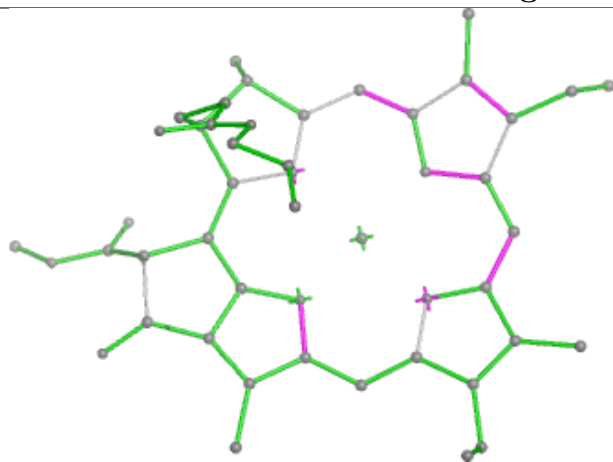


Torsions

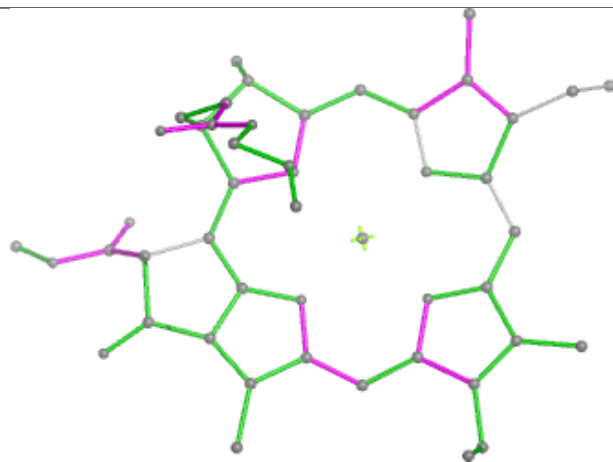


Rings

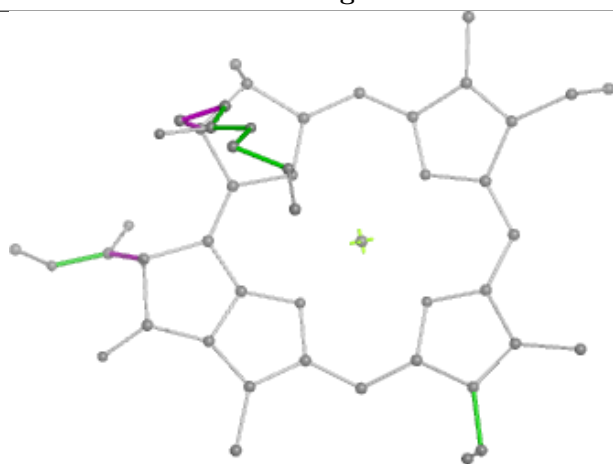
Ligand CLA r 604



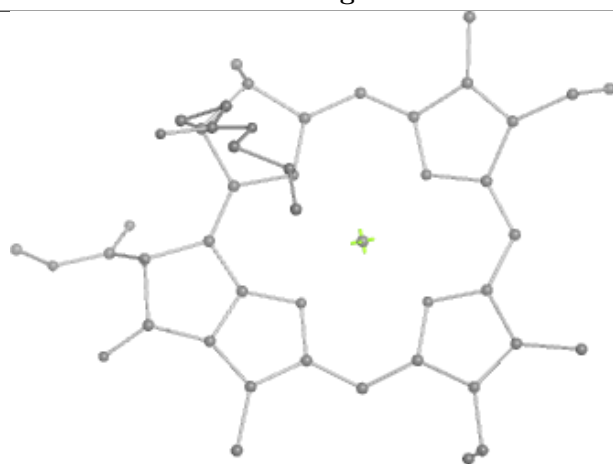
Bond lengths



Bond angles

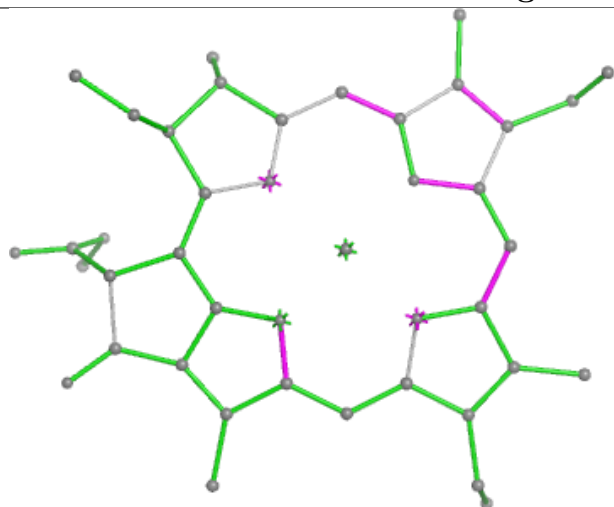


Torsions

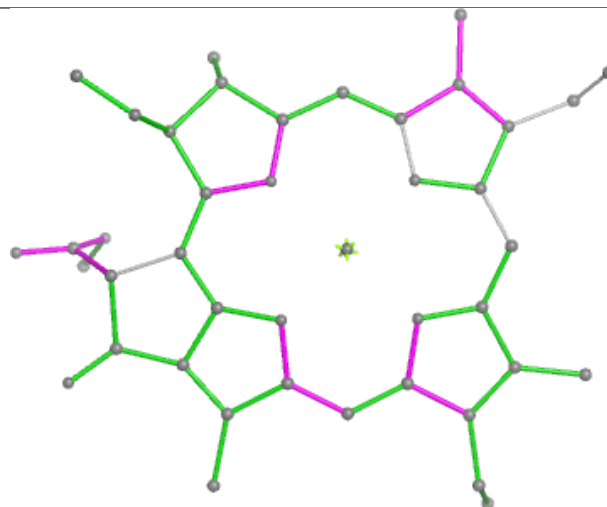


Rings

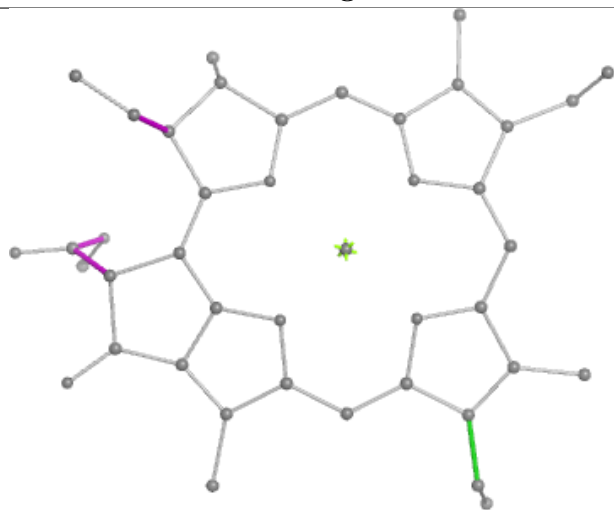
Ligand CLA S 603



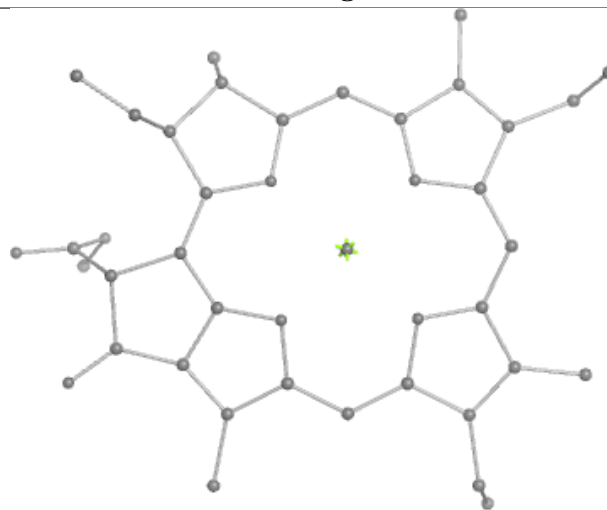
Bond lengths



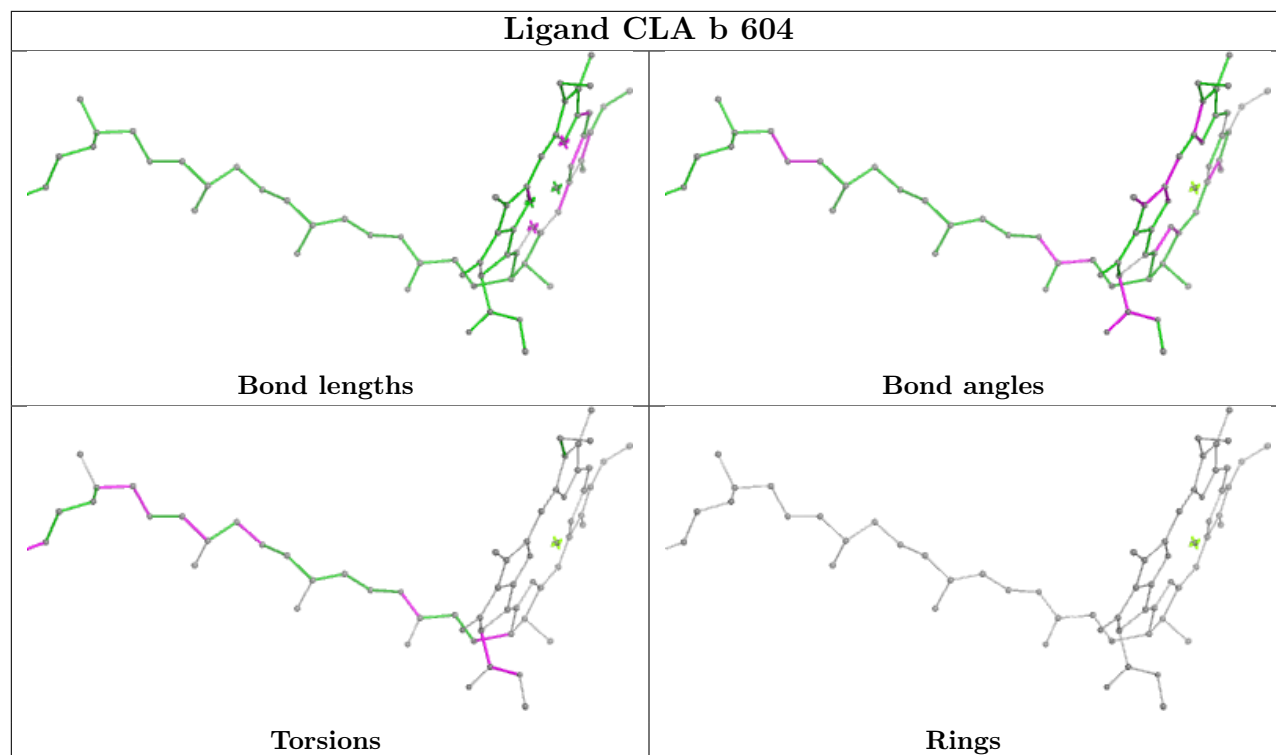
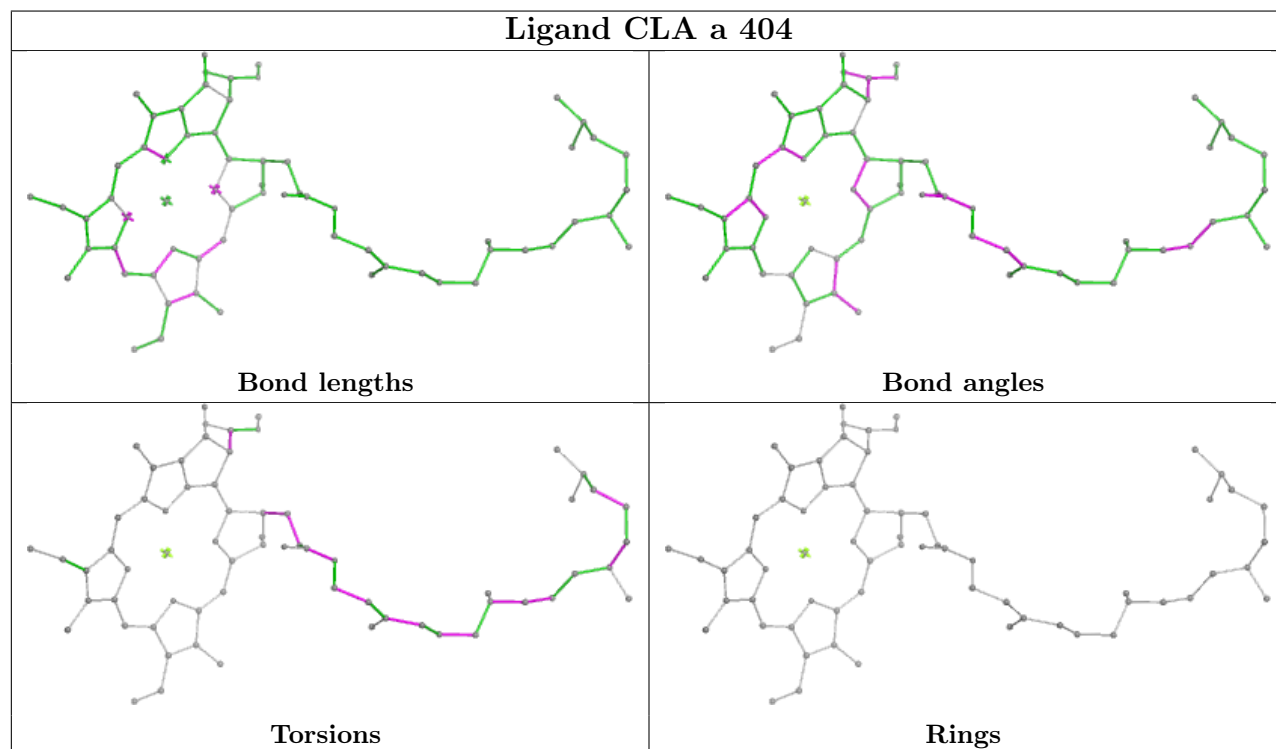
Bond angles

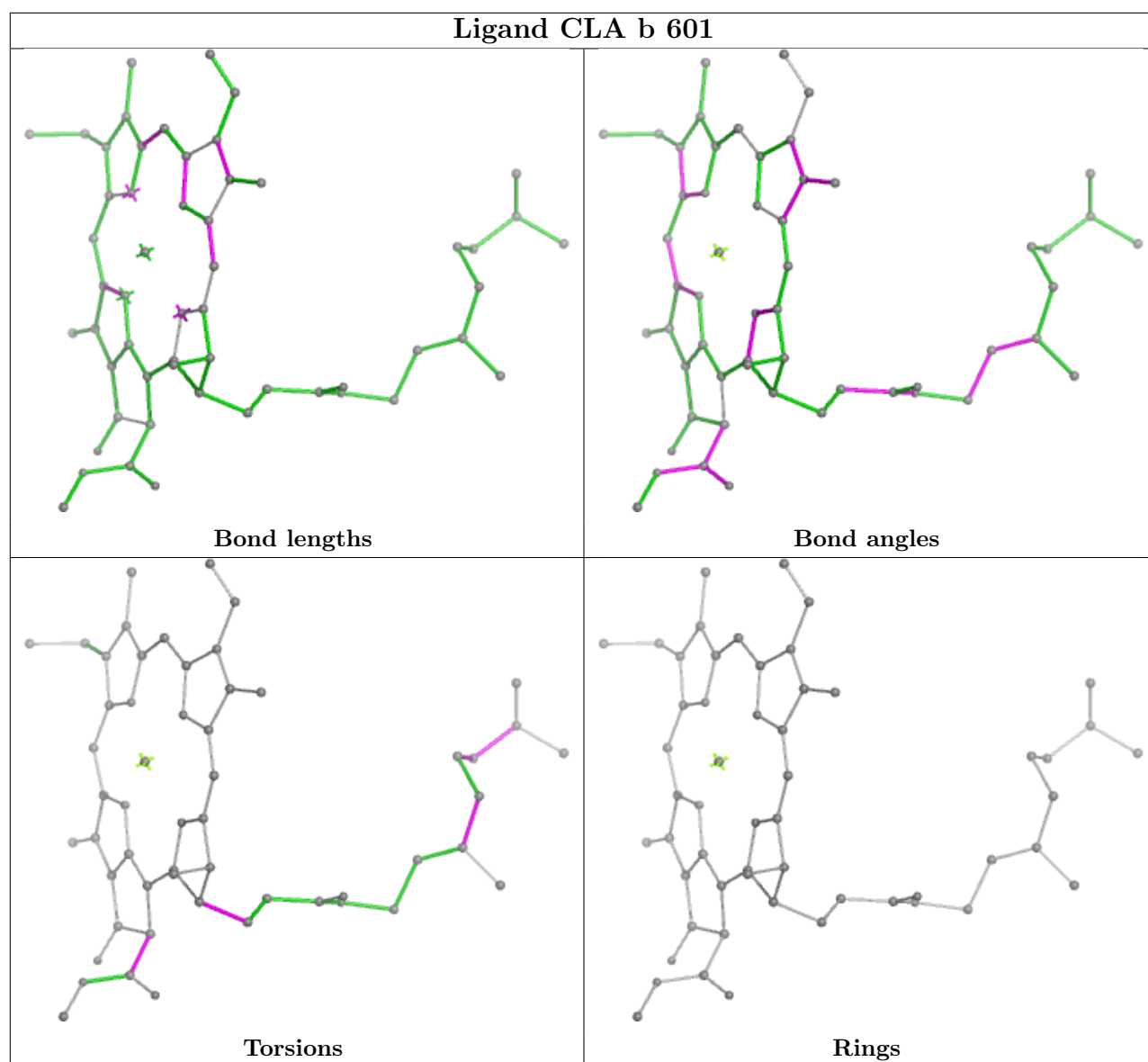


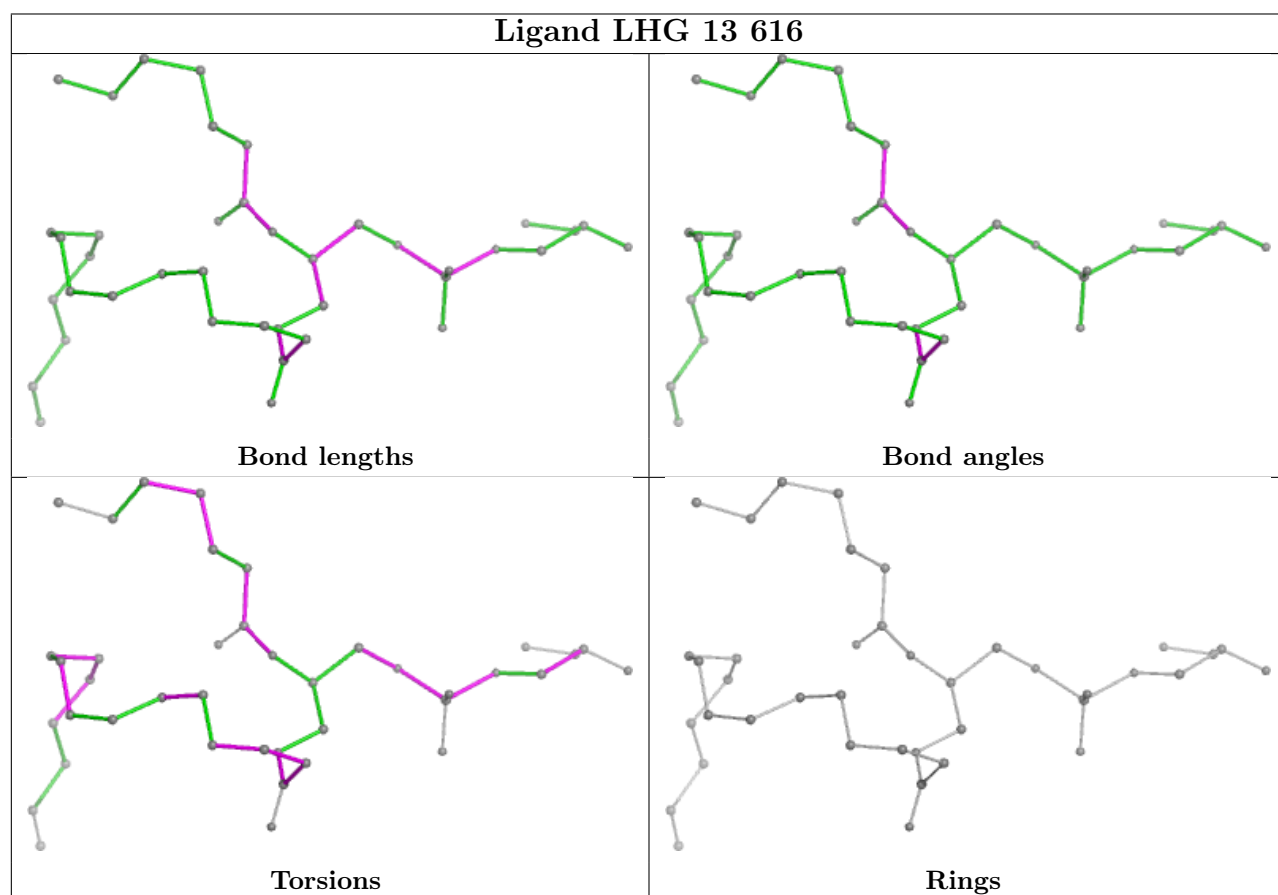
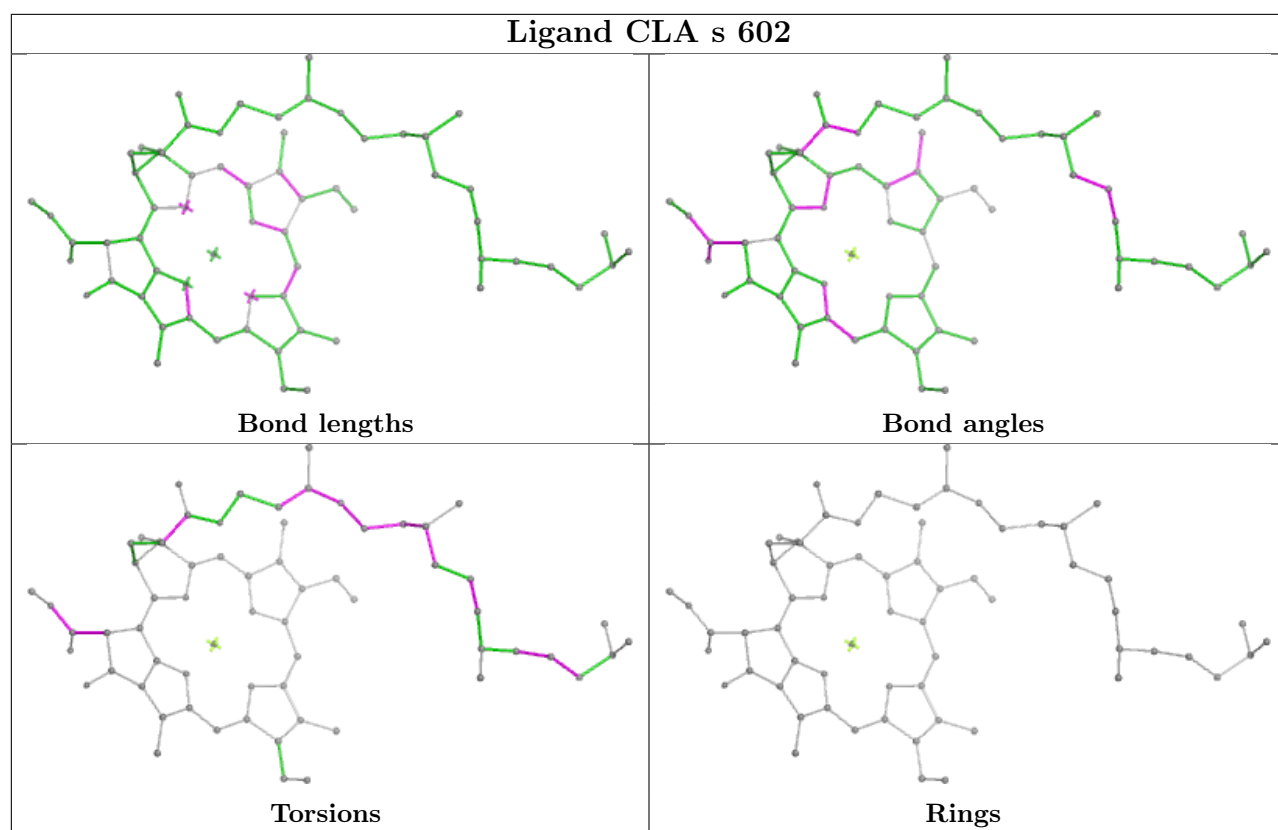
Torsions

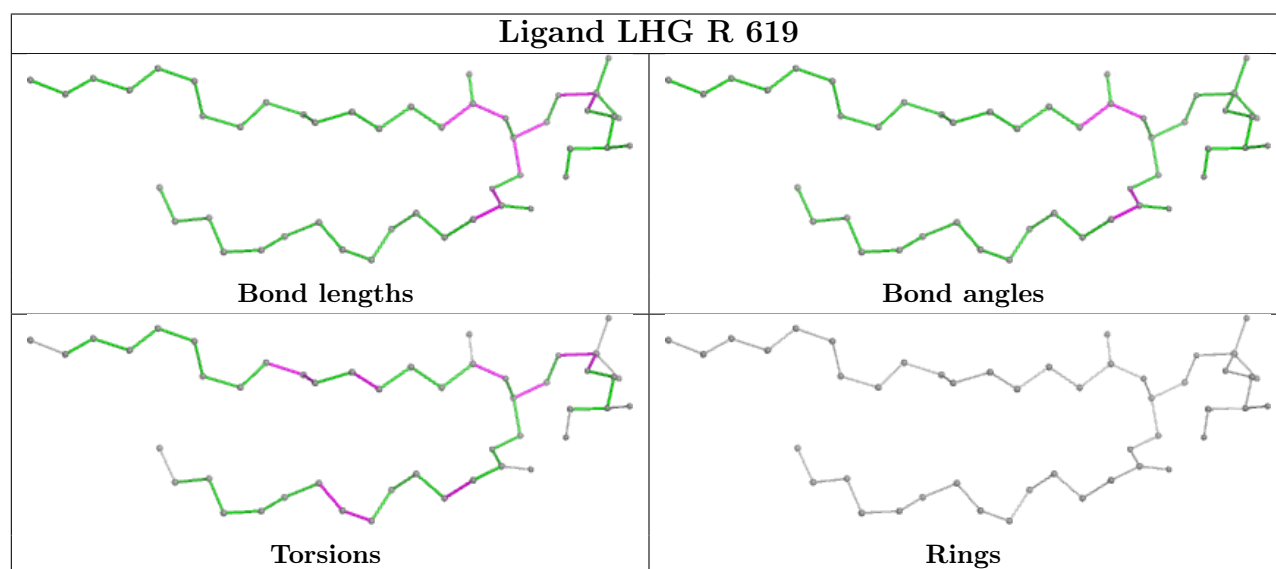
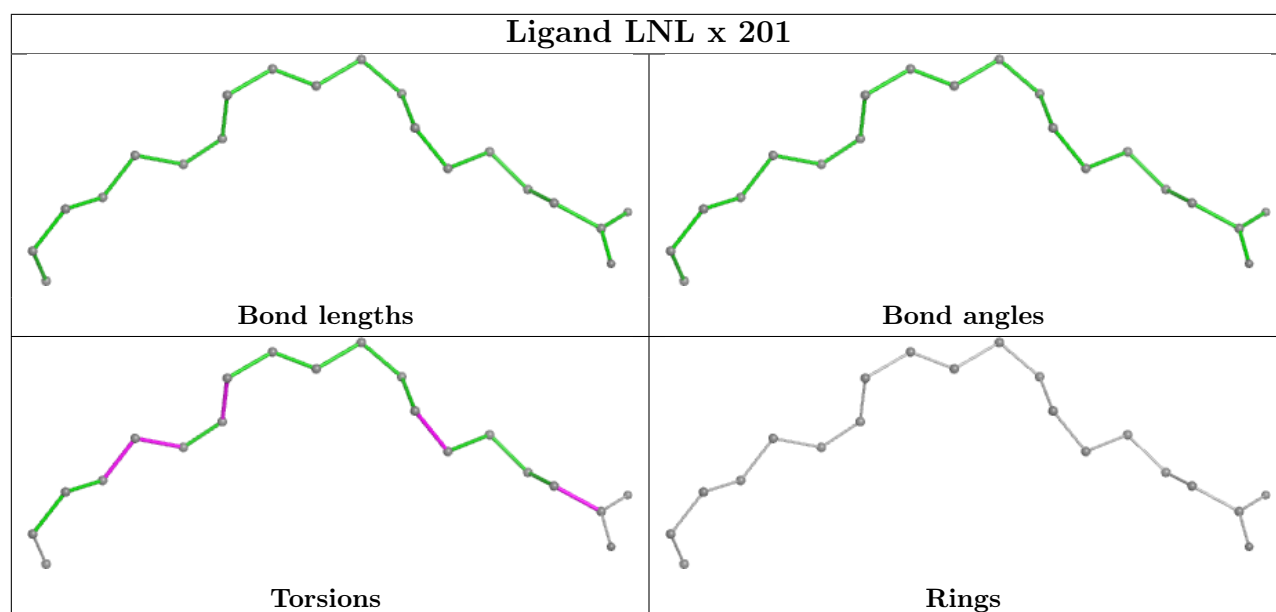


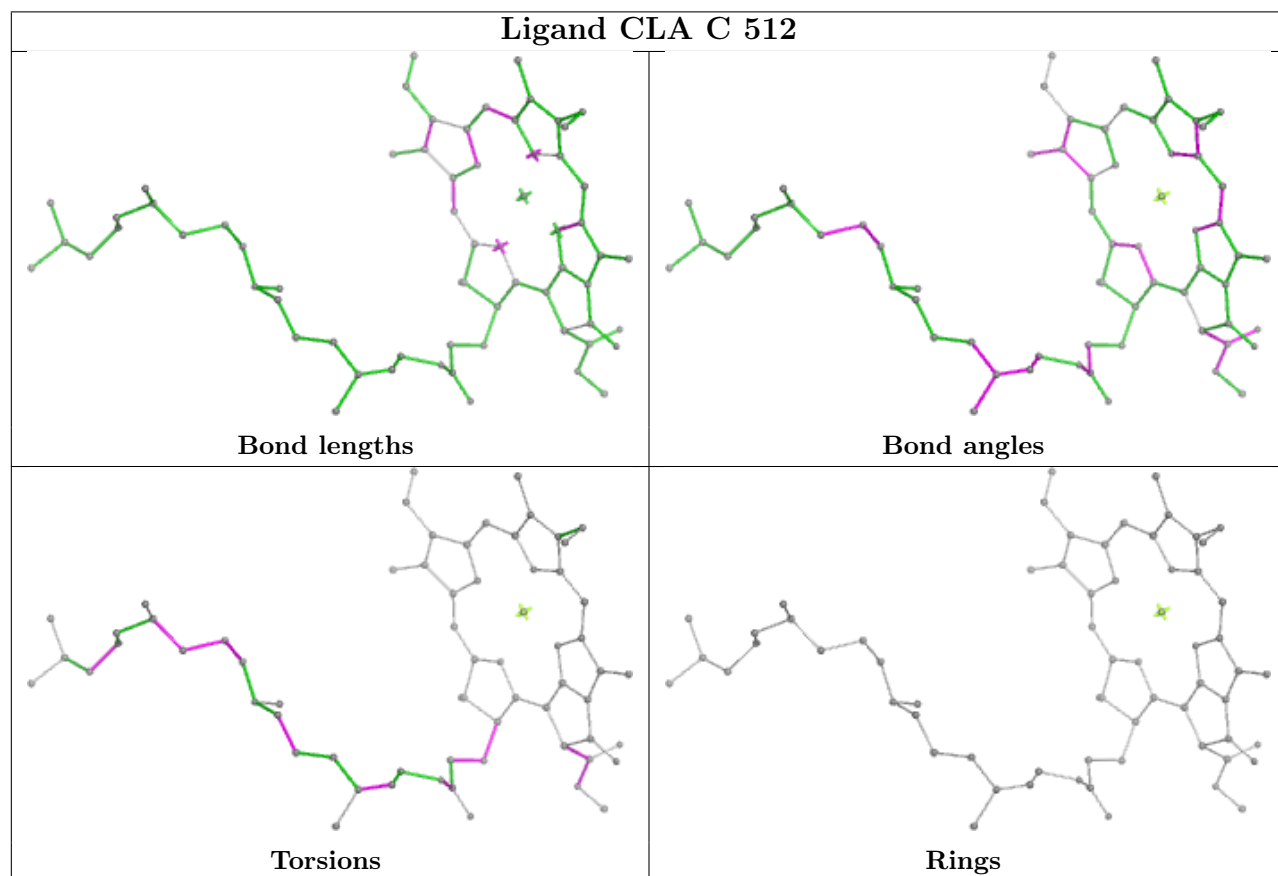
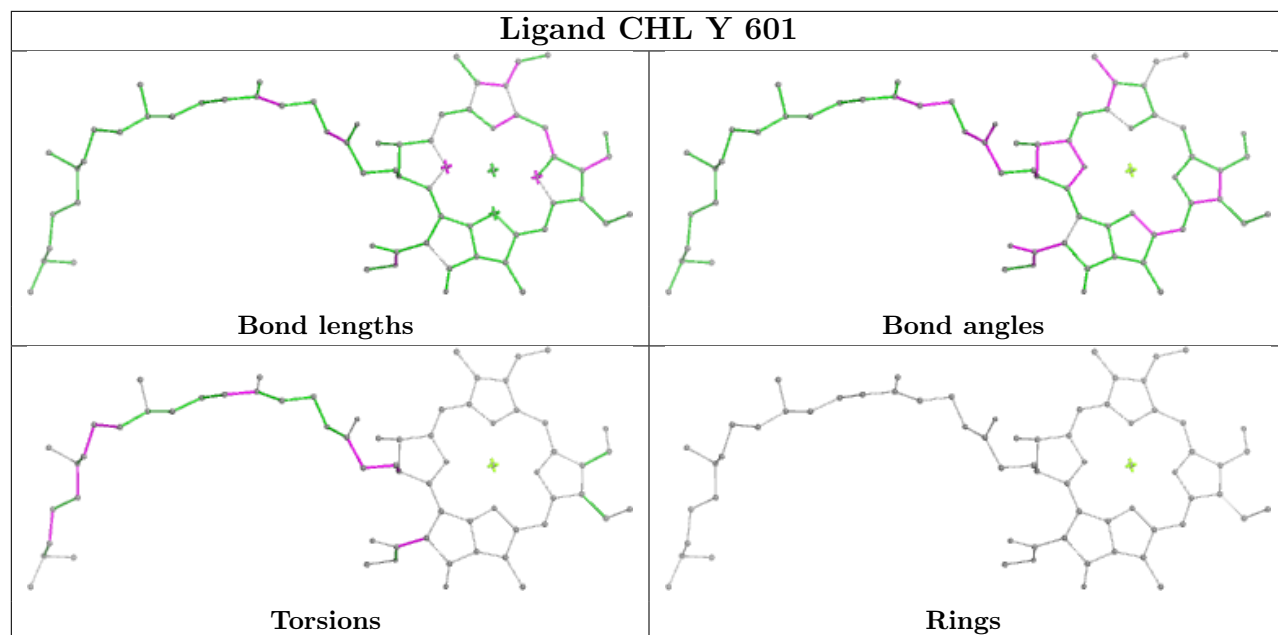
Rings

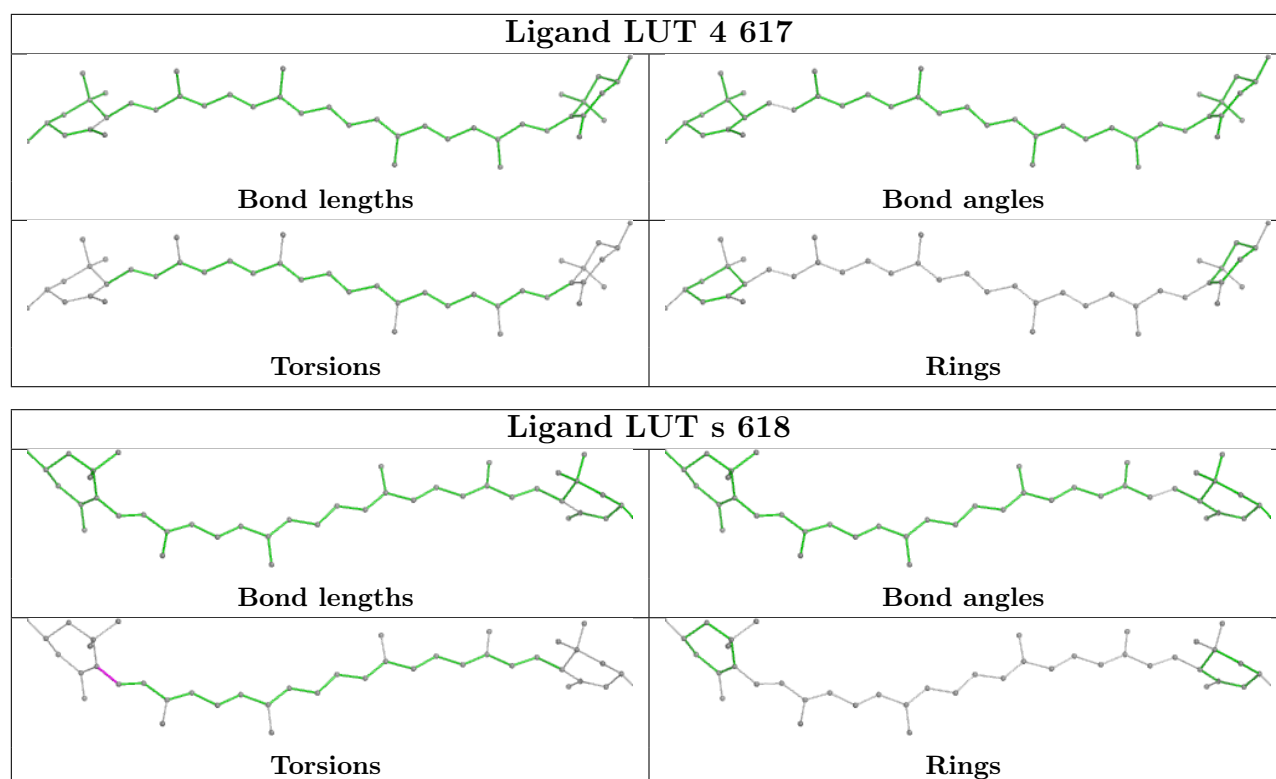
Ligand CLA b 604**Ligand CLA a 404**

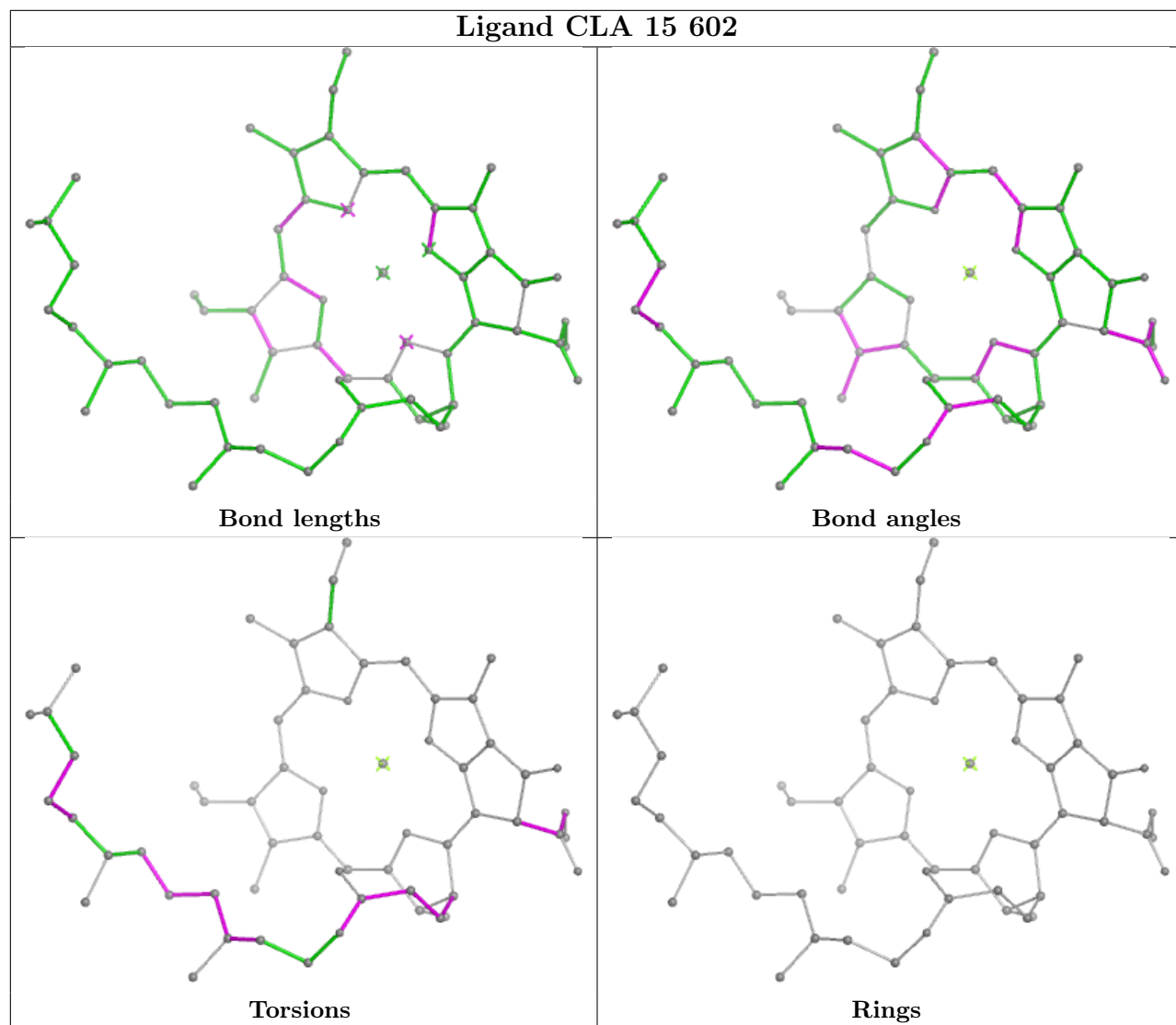


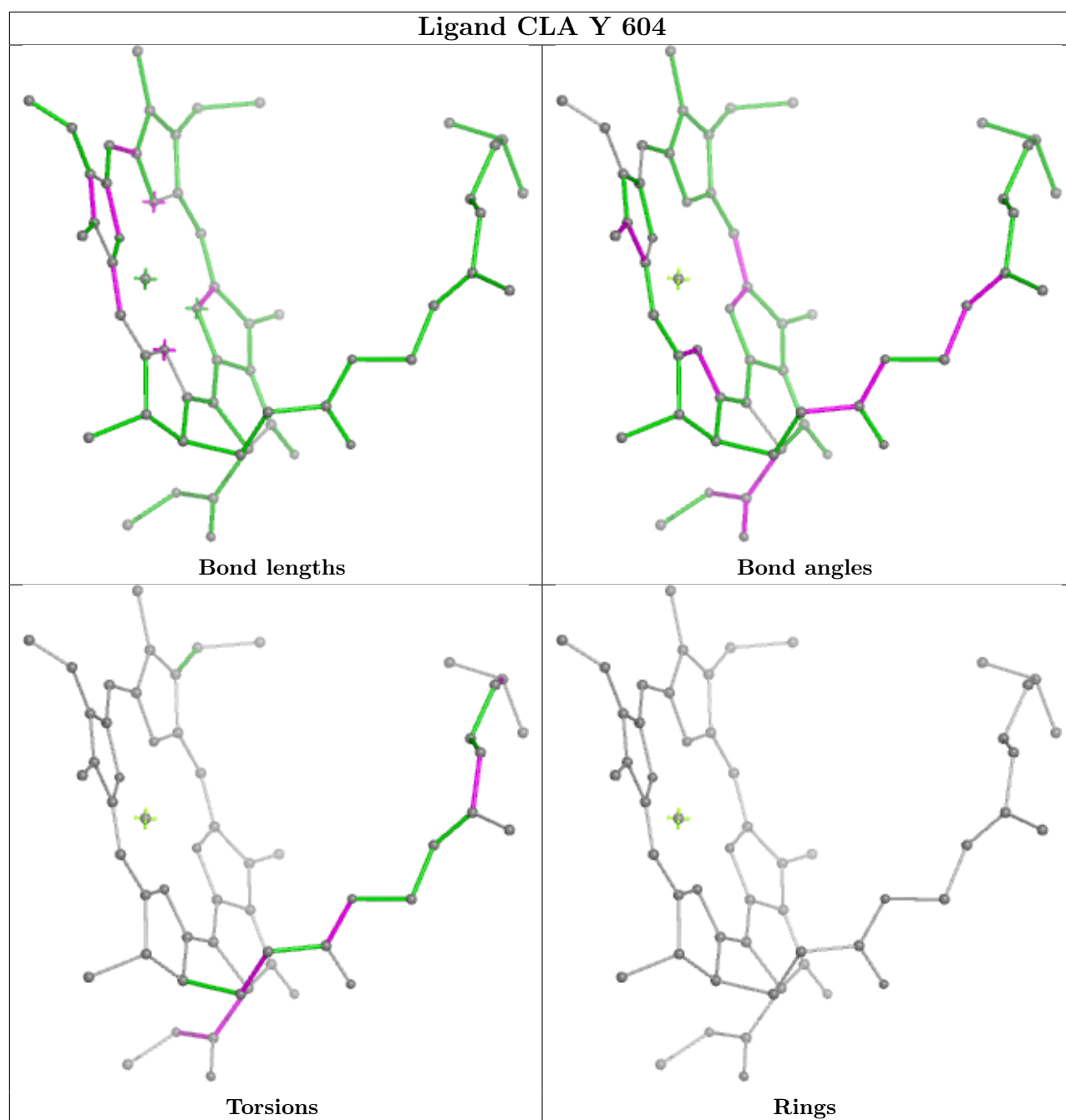


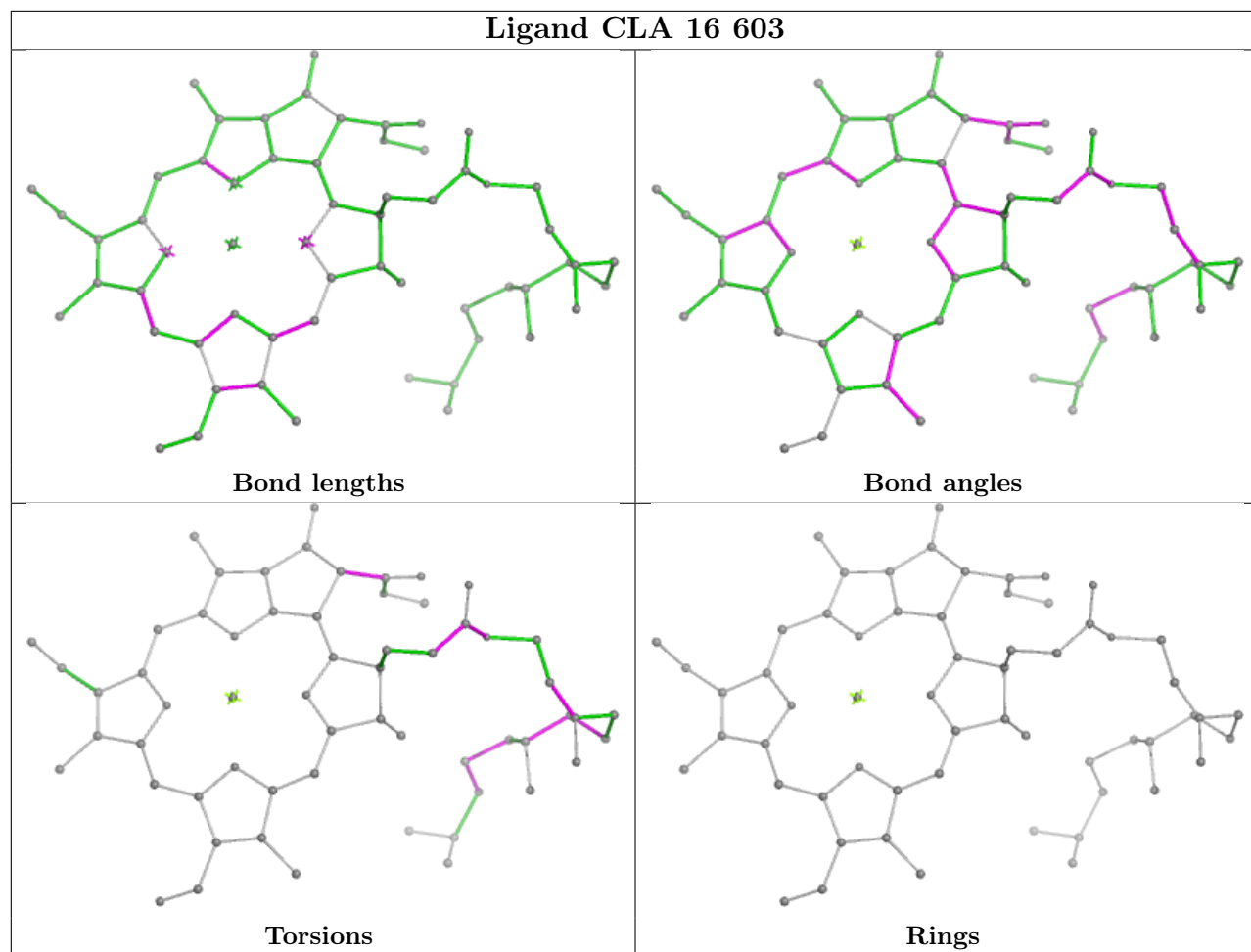


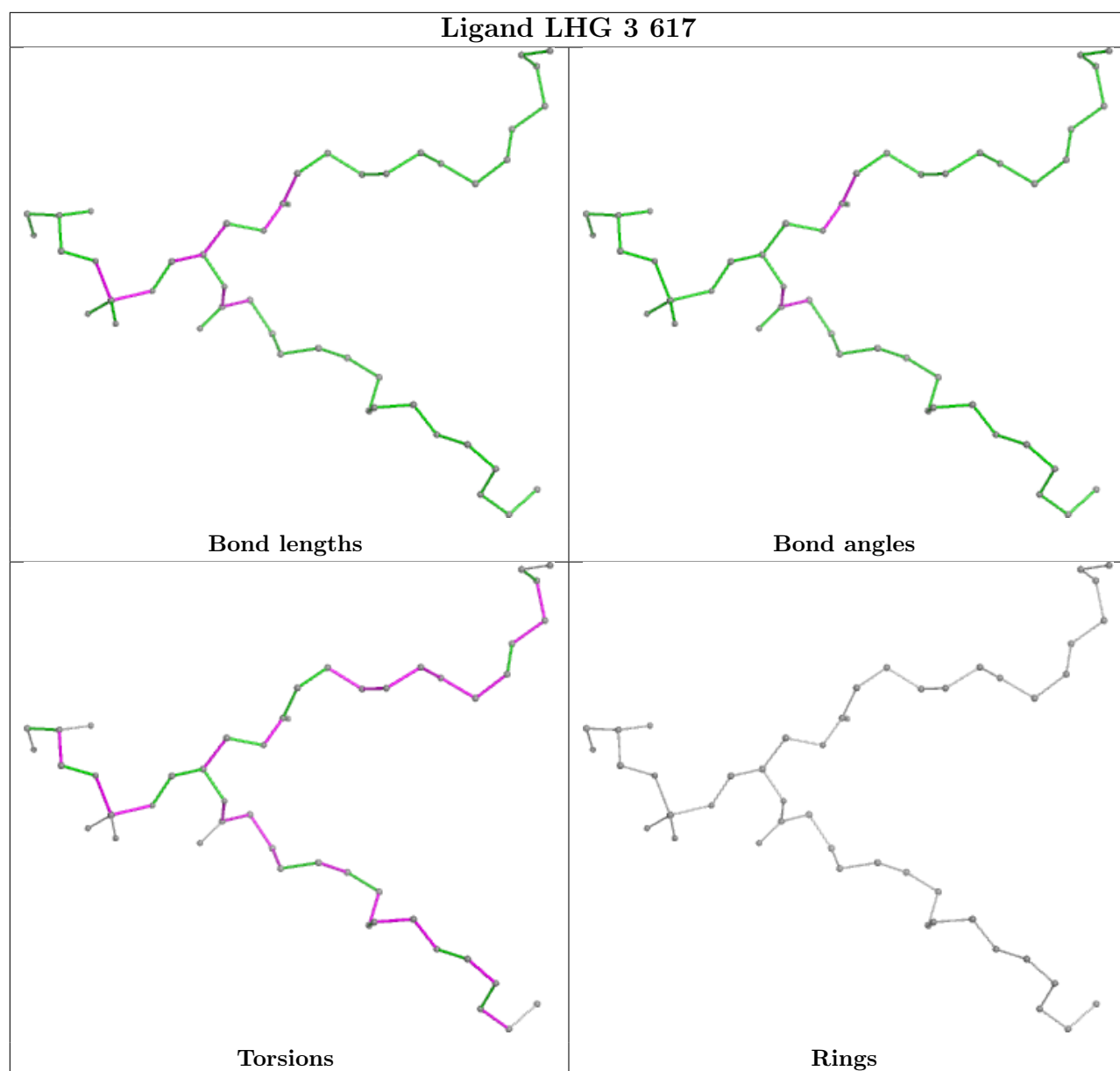




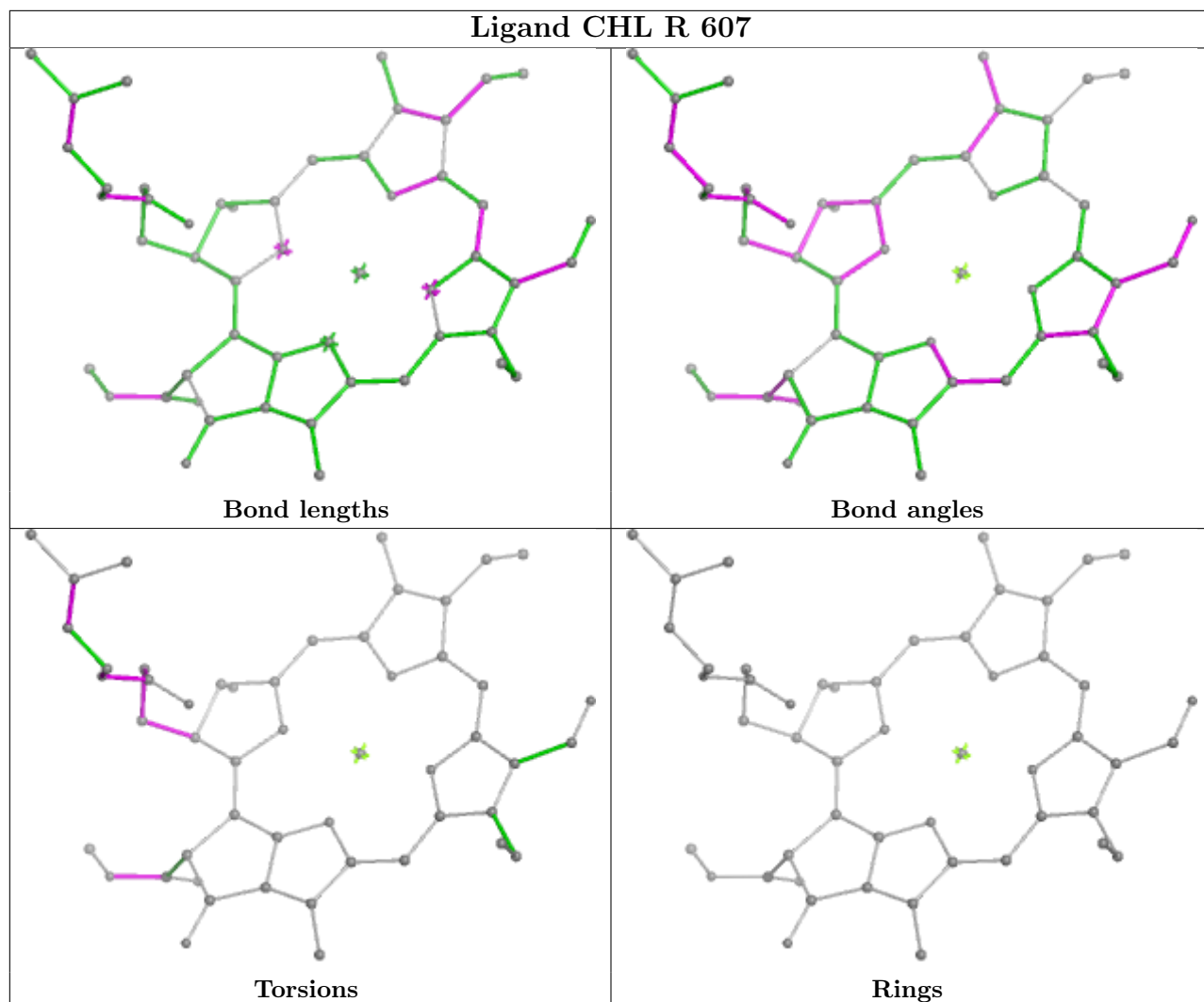




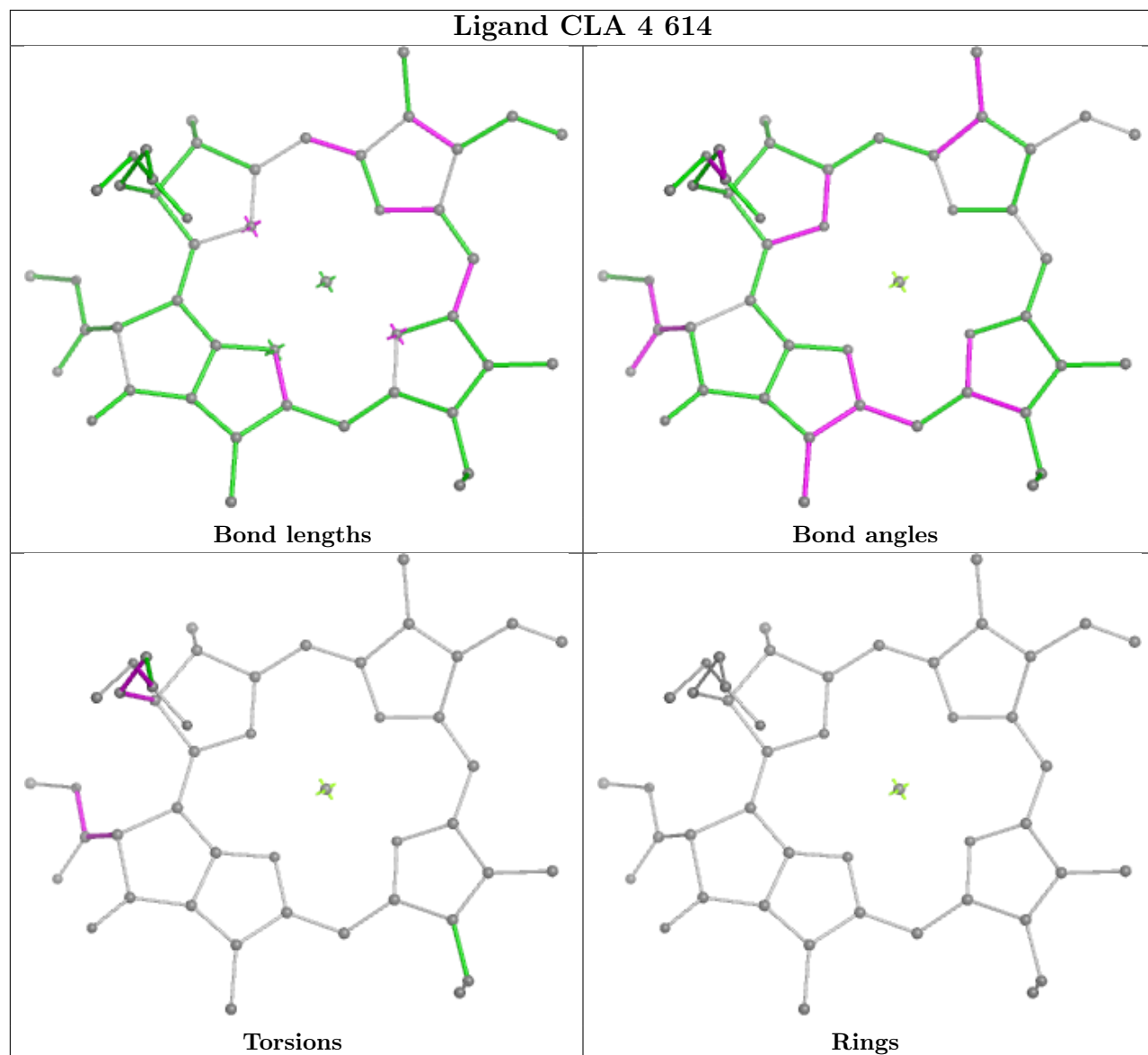




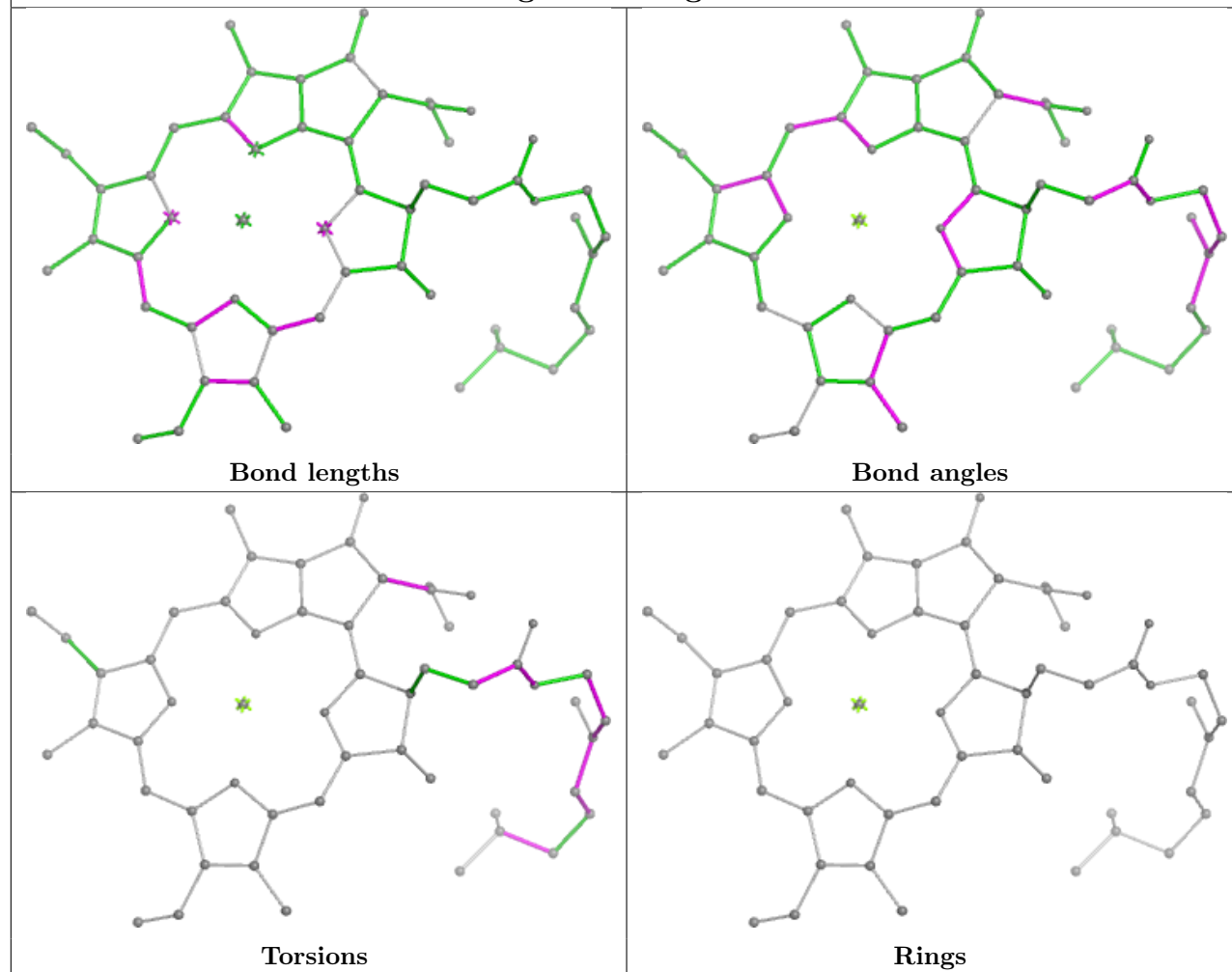
Ligand CHL R 607

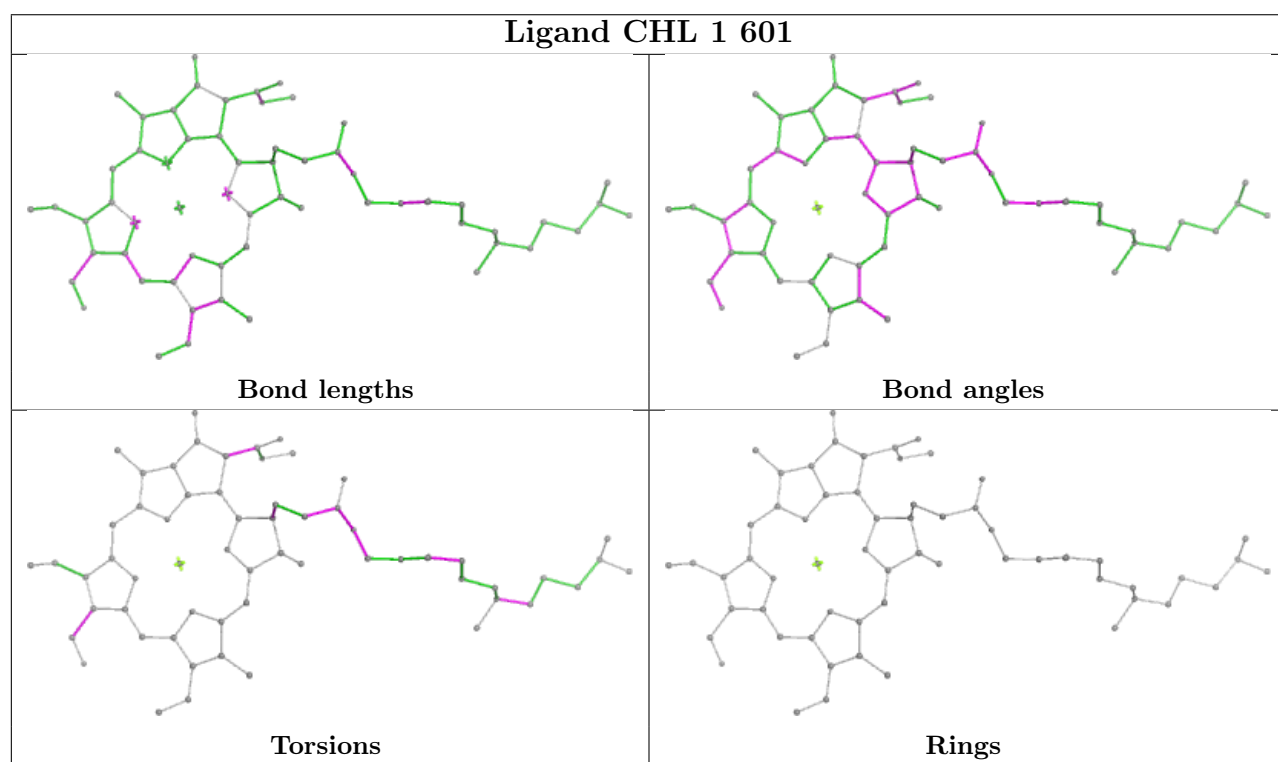
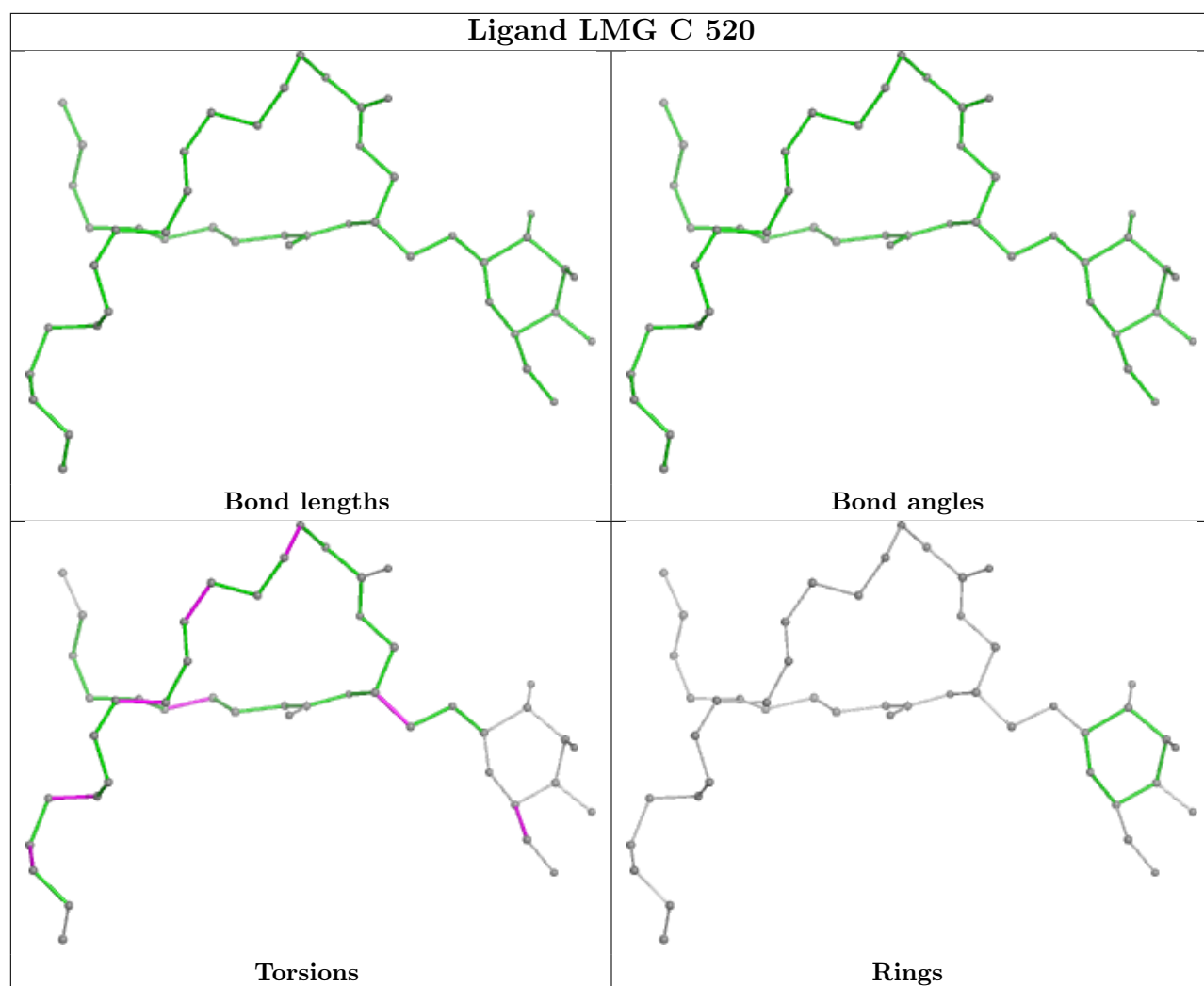


Ligand CLA 4 614

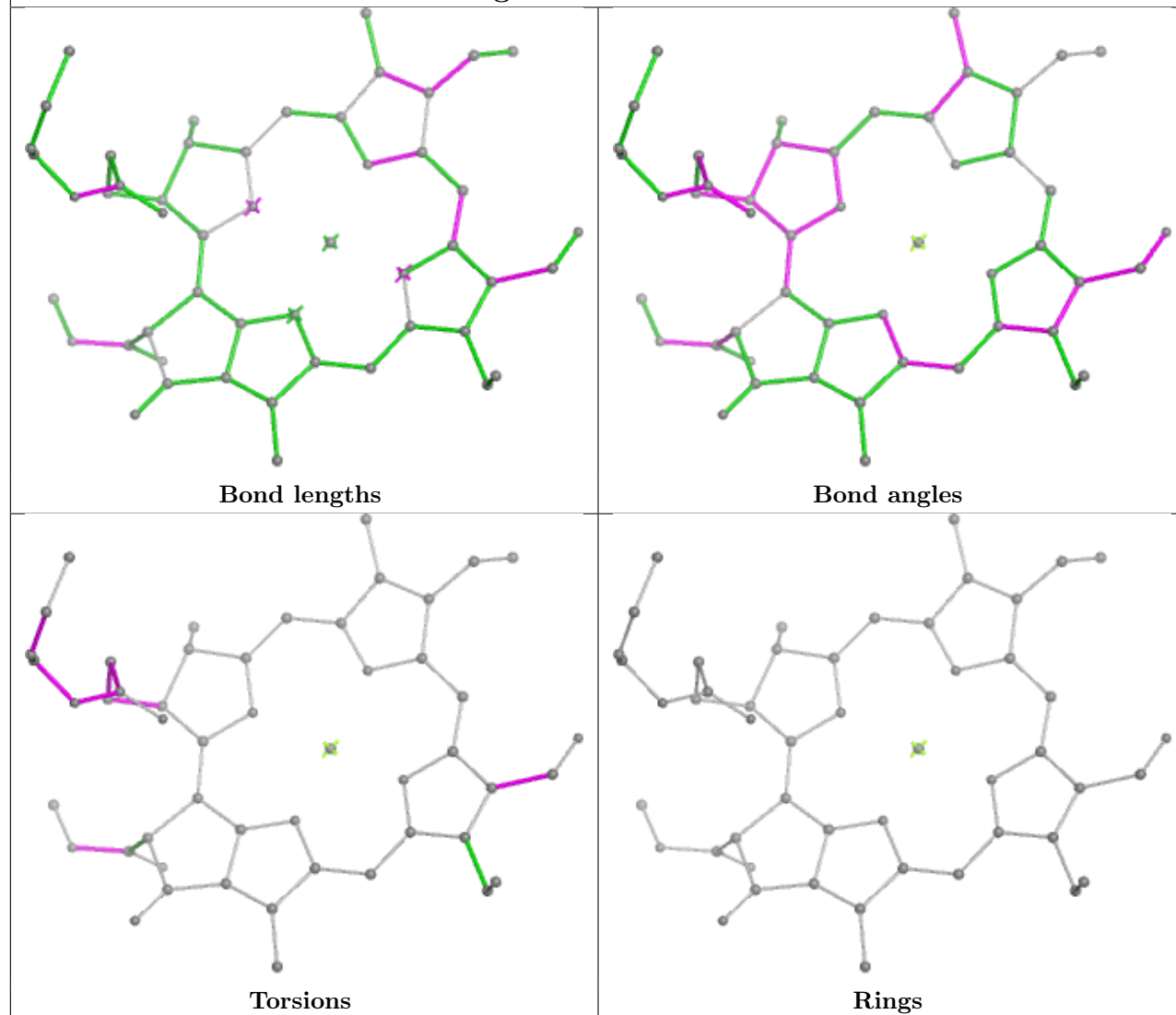


Ligand CLA g 603

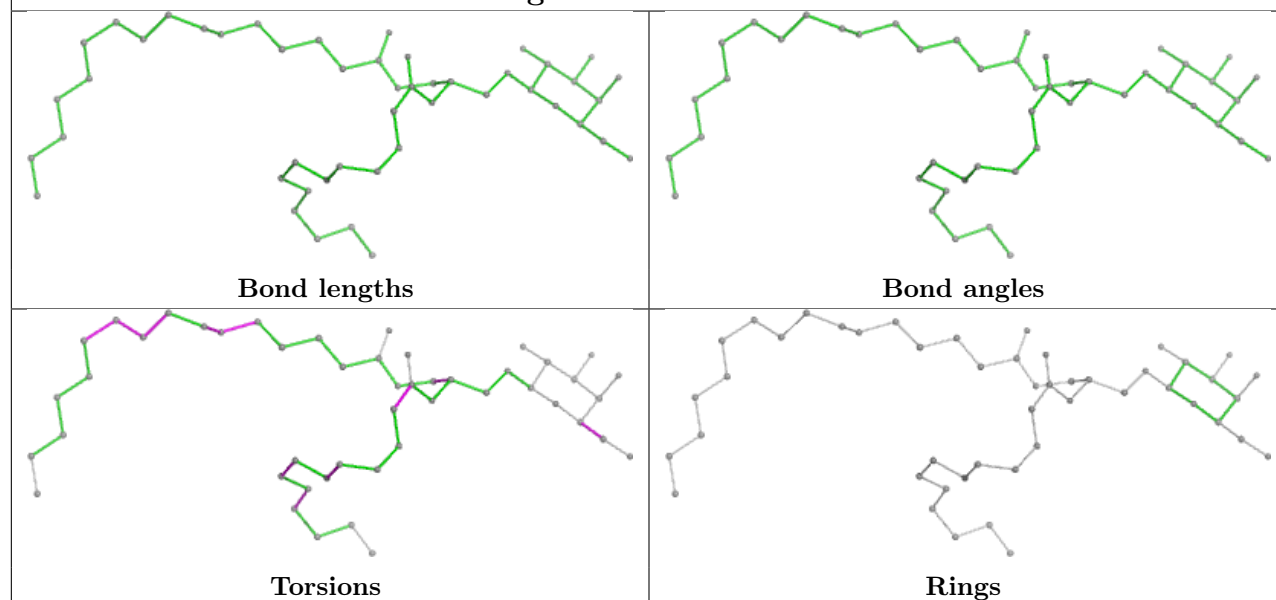


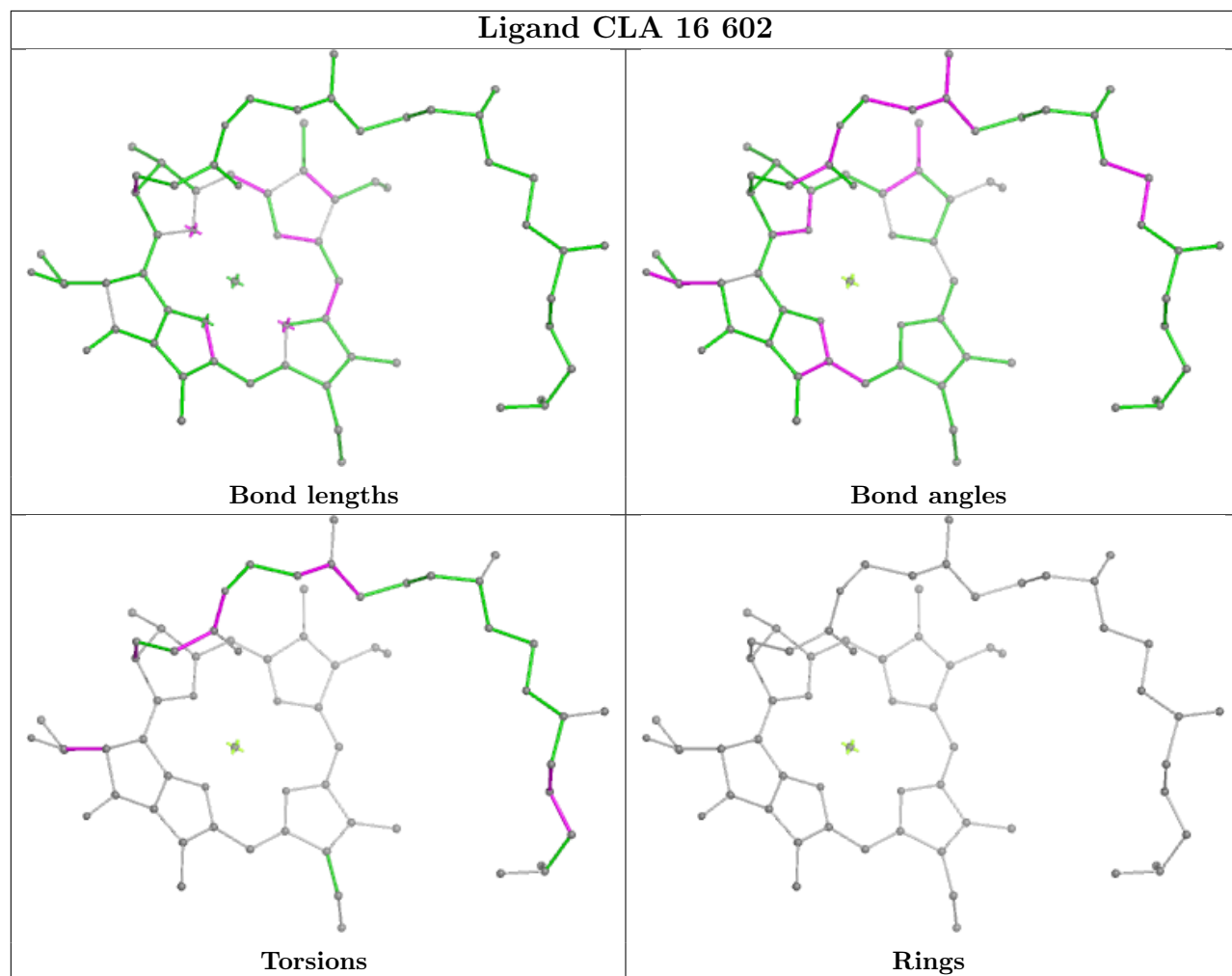


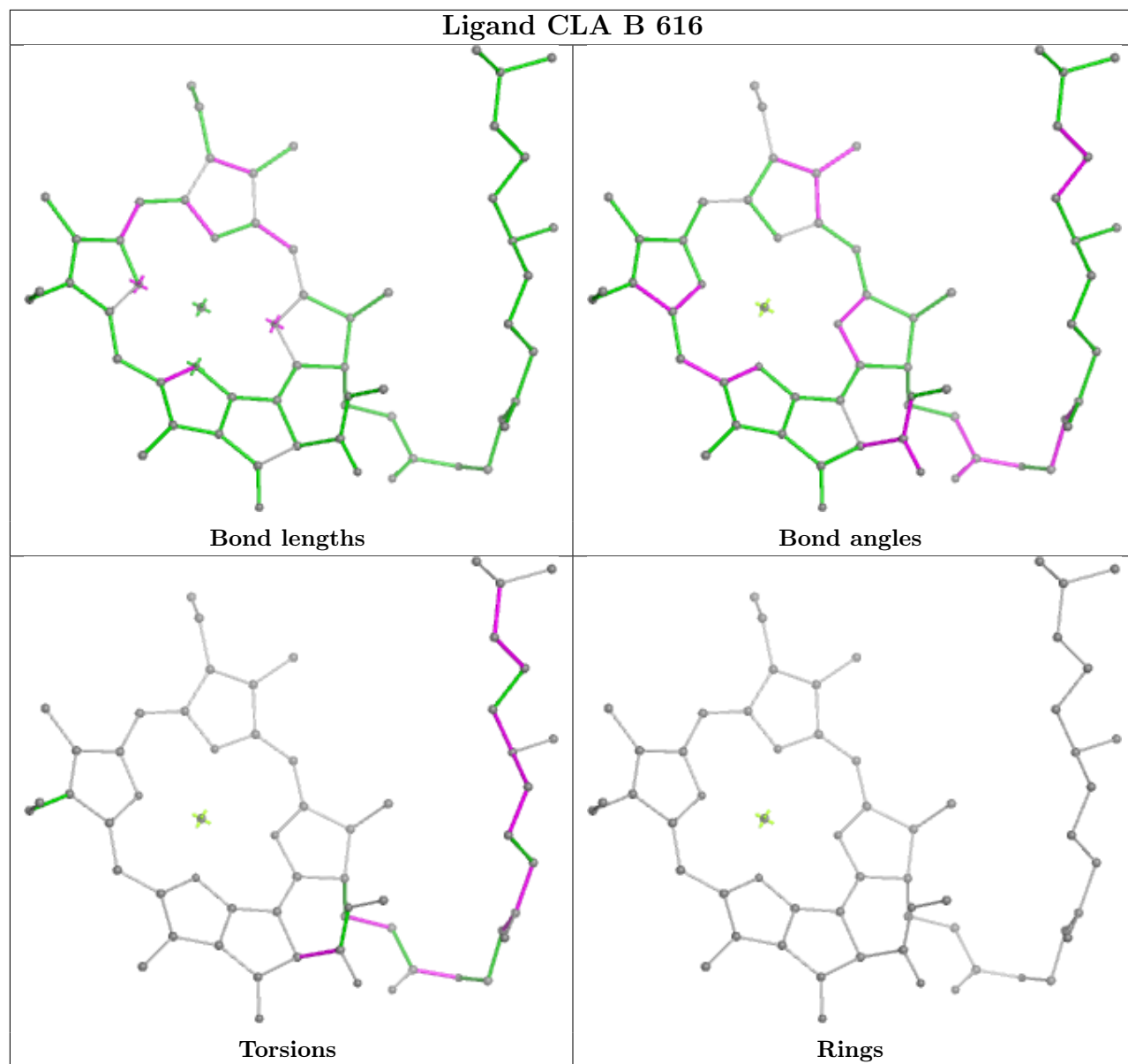
Ligand CHL 1 608



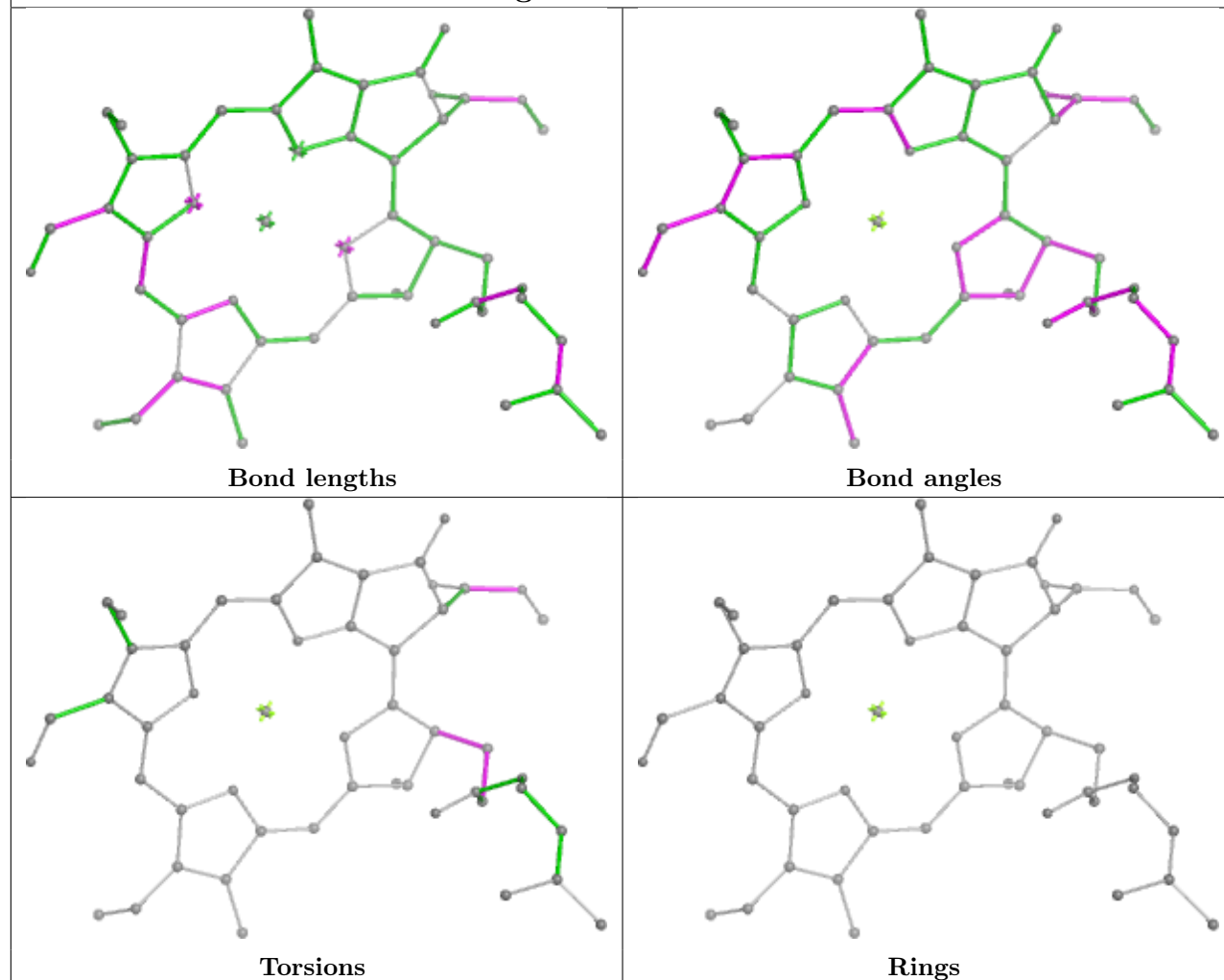
Ligand LMG D 414



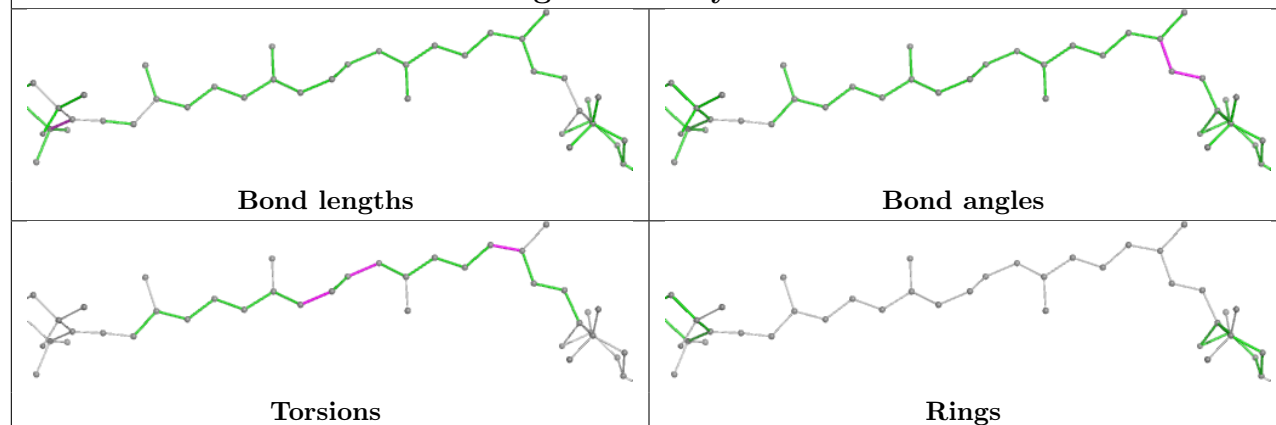


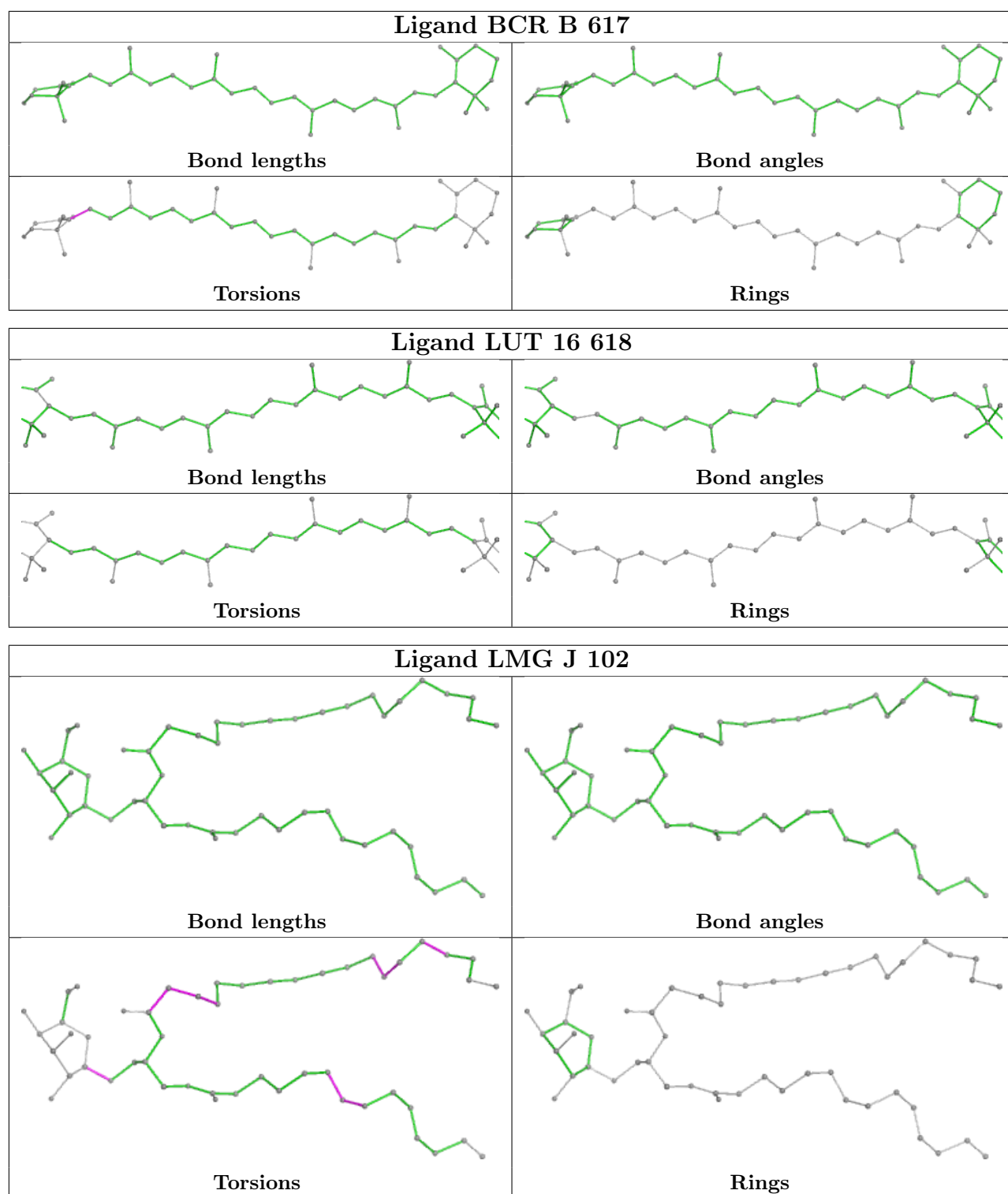


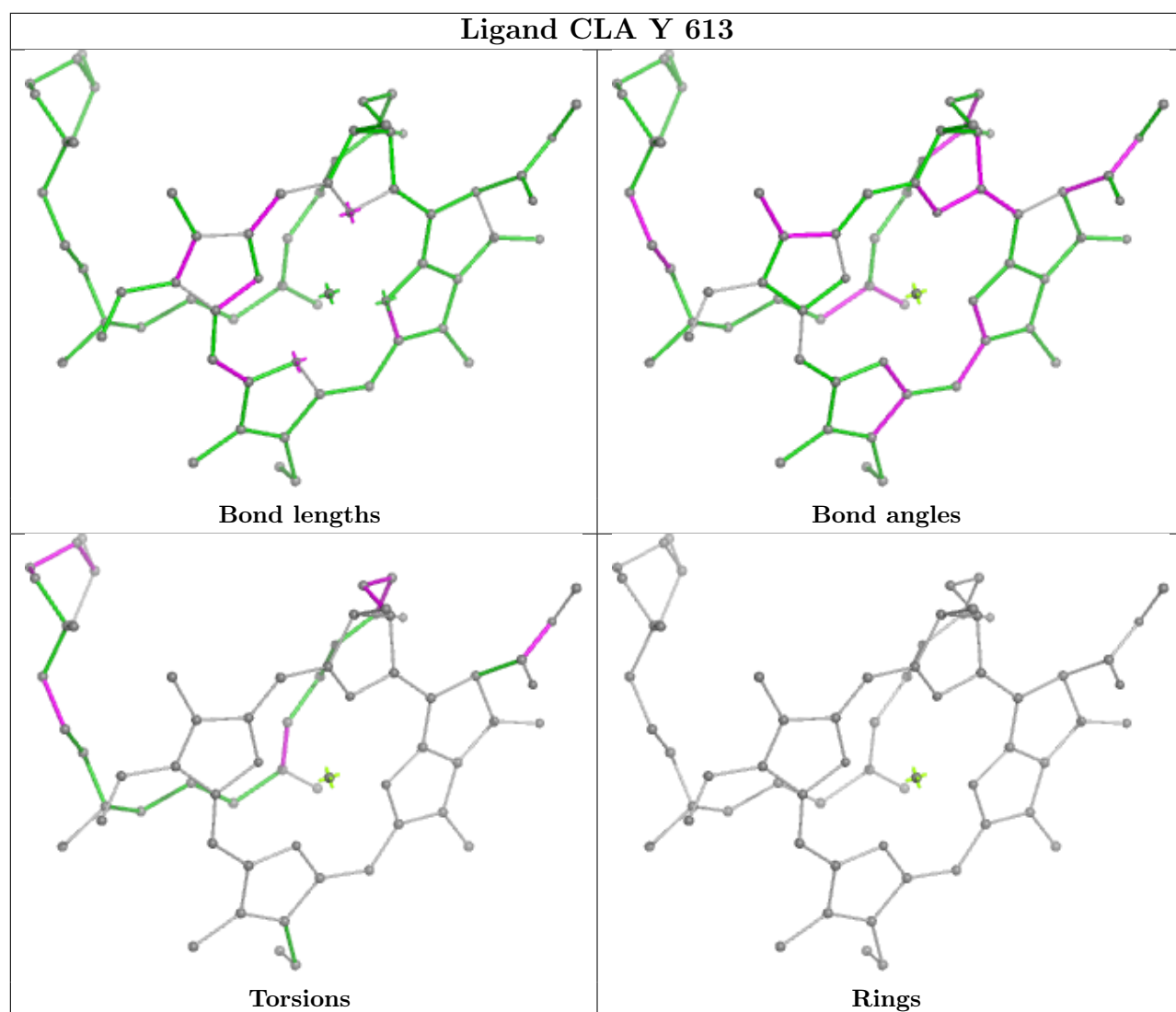
Ligand CHL r 607



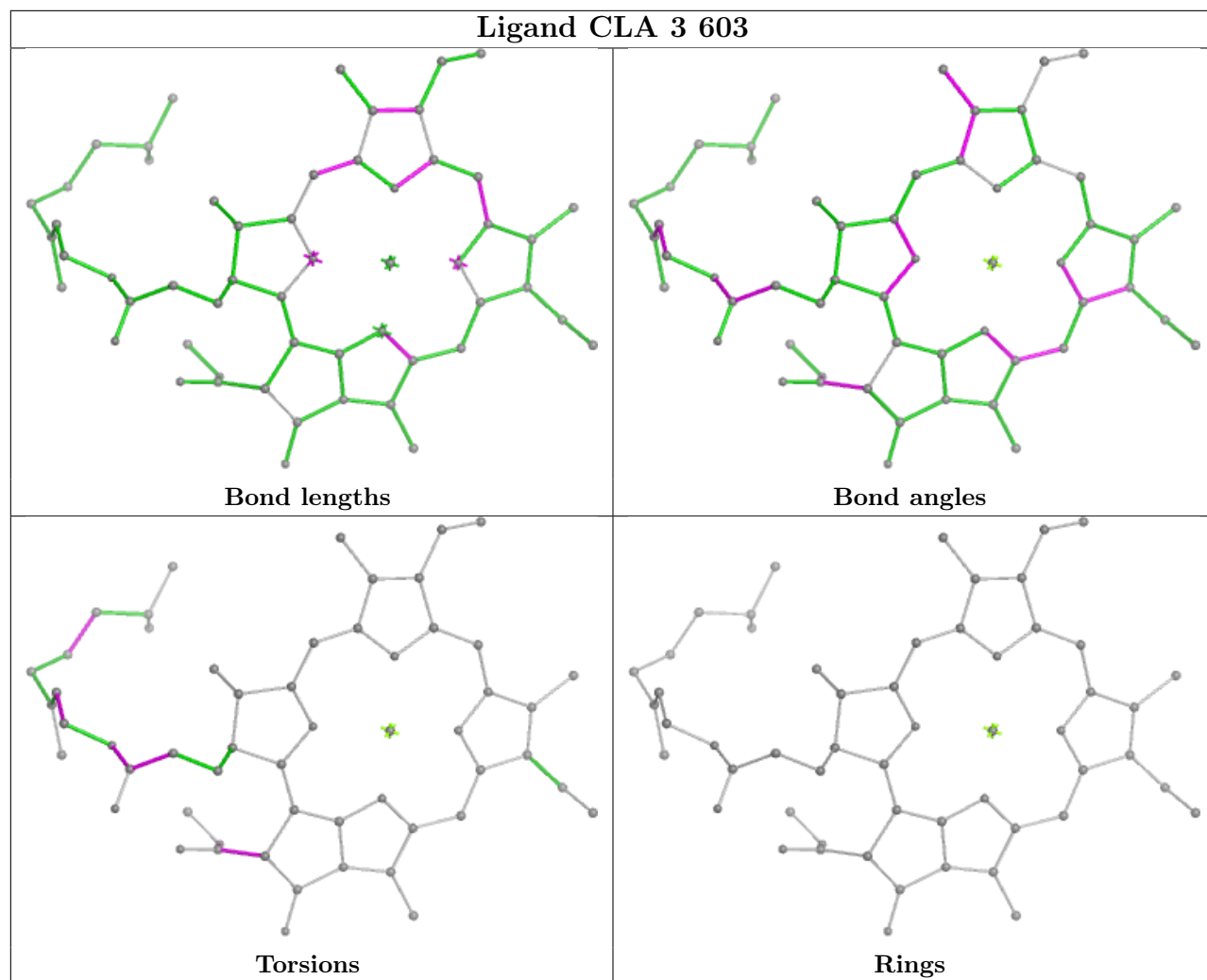
Ligand NEX y 624

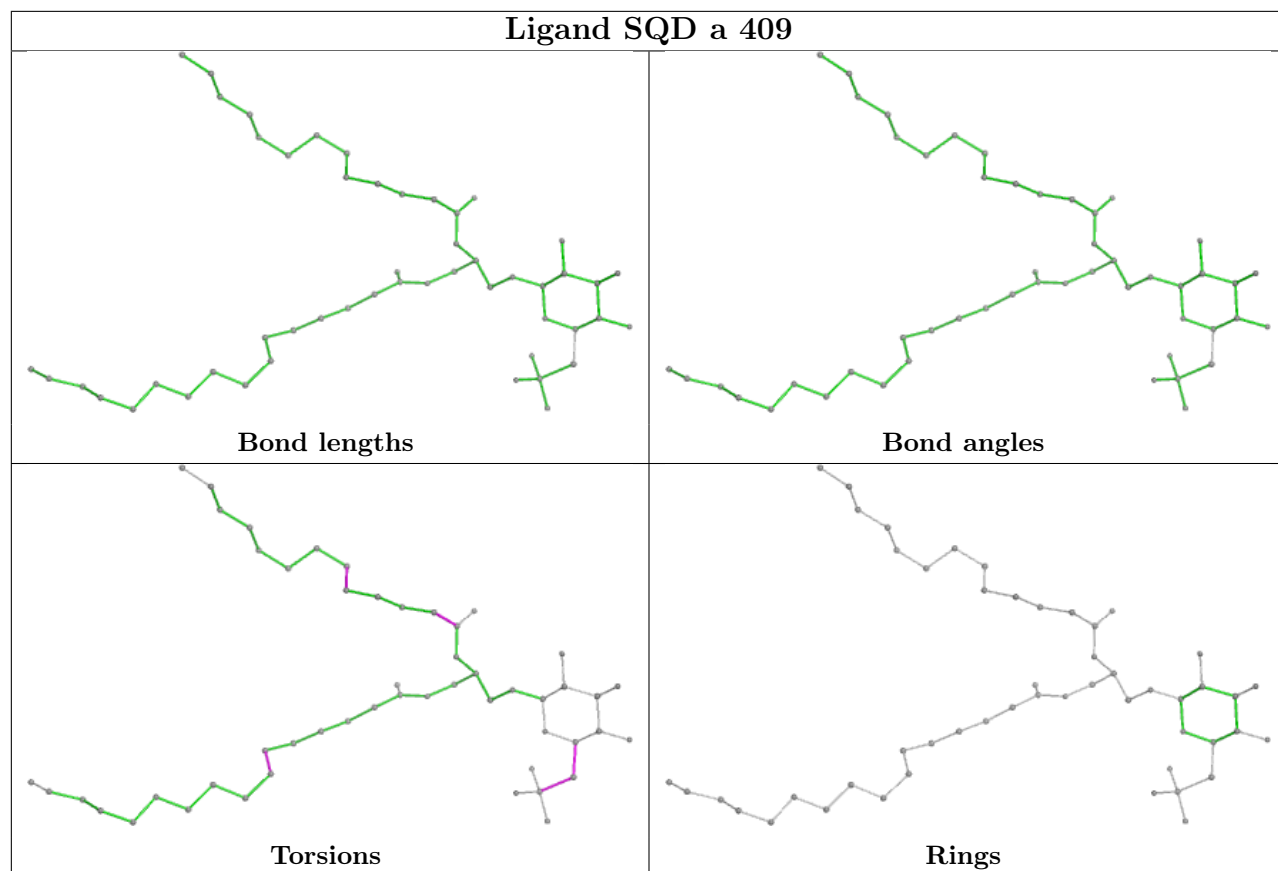




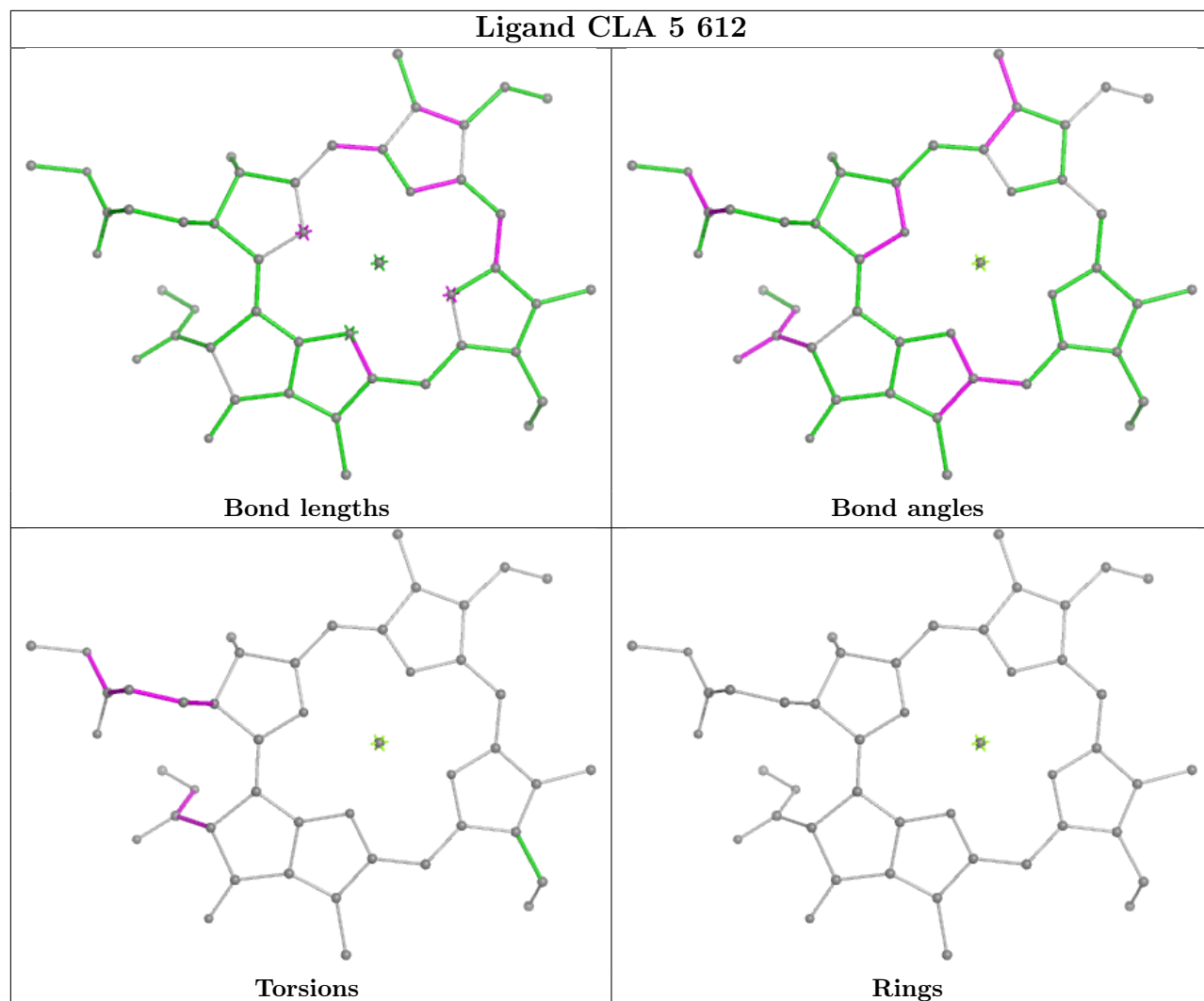


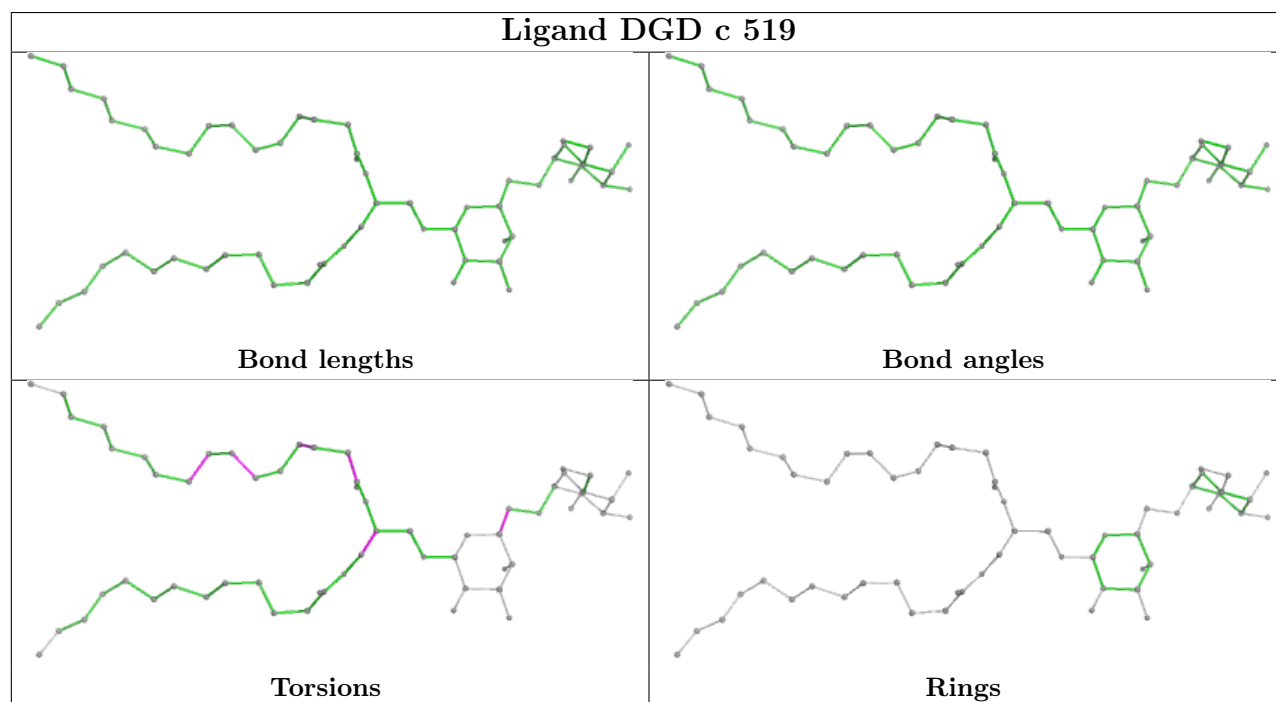
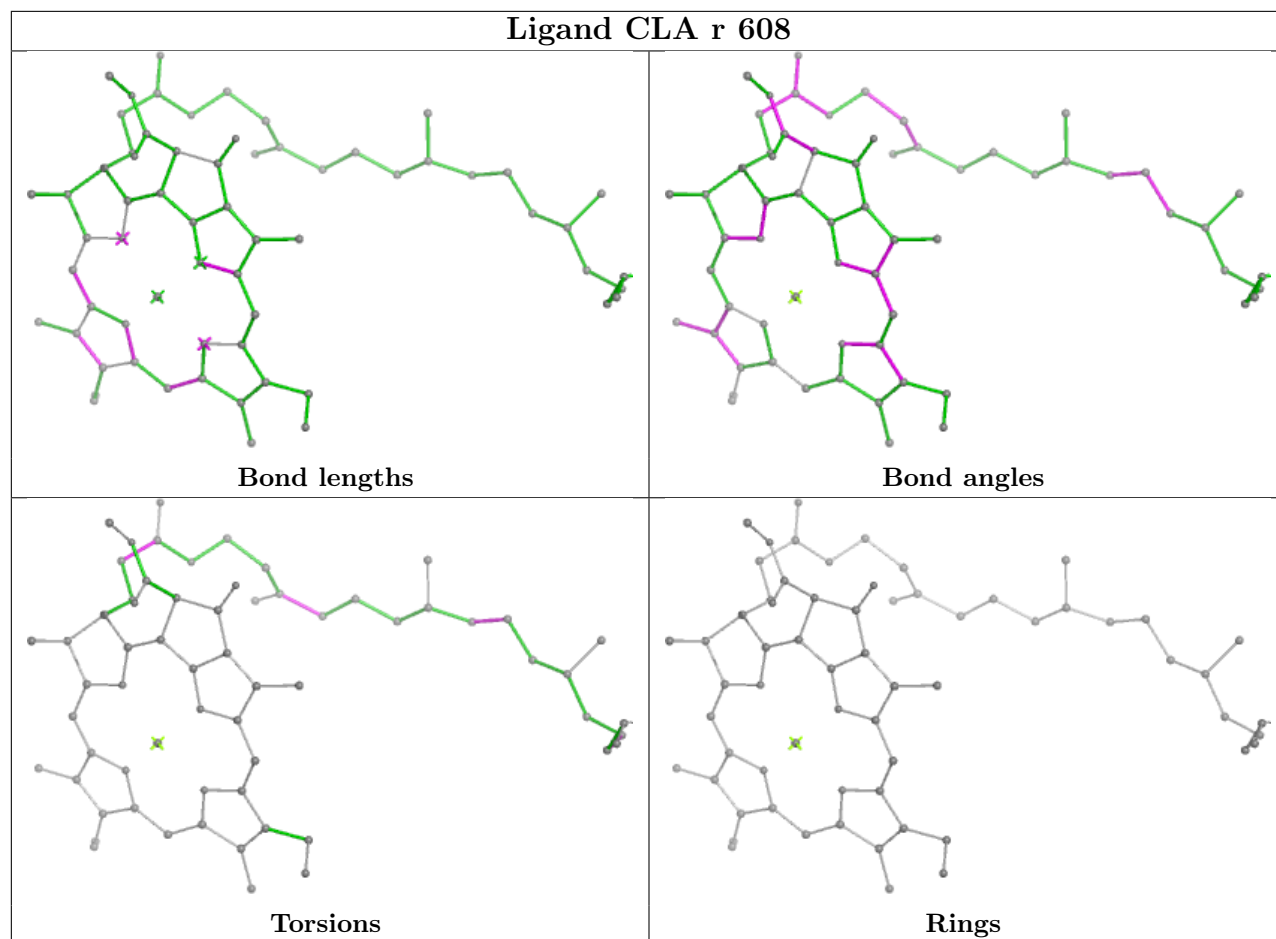
Ligand CLA 3 603

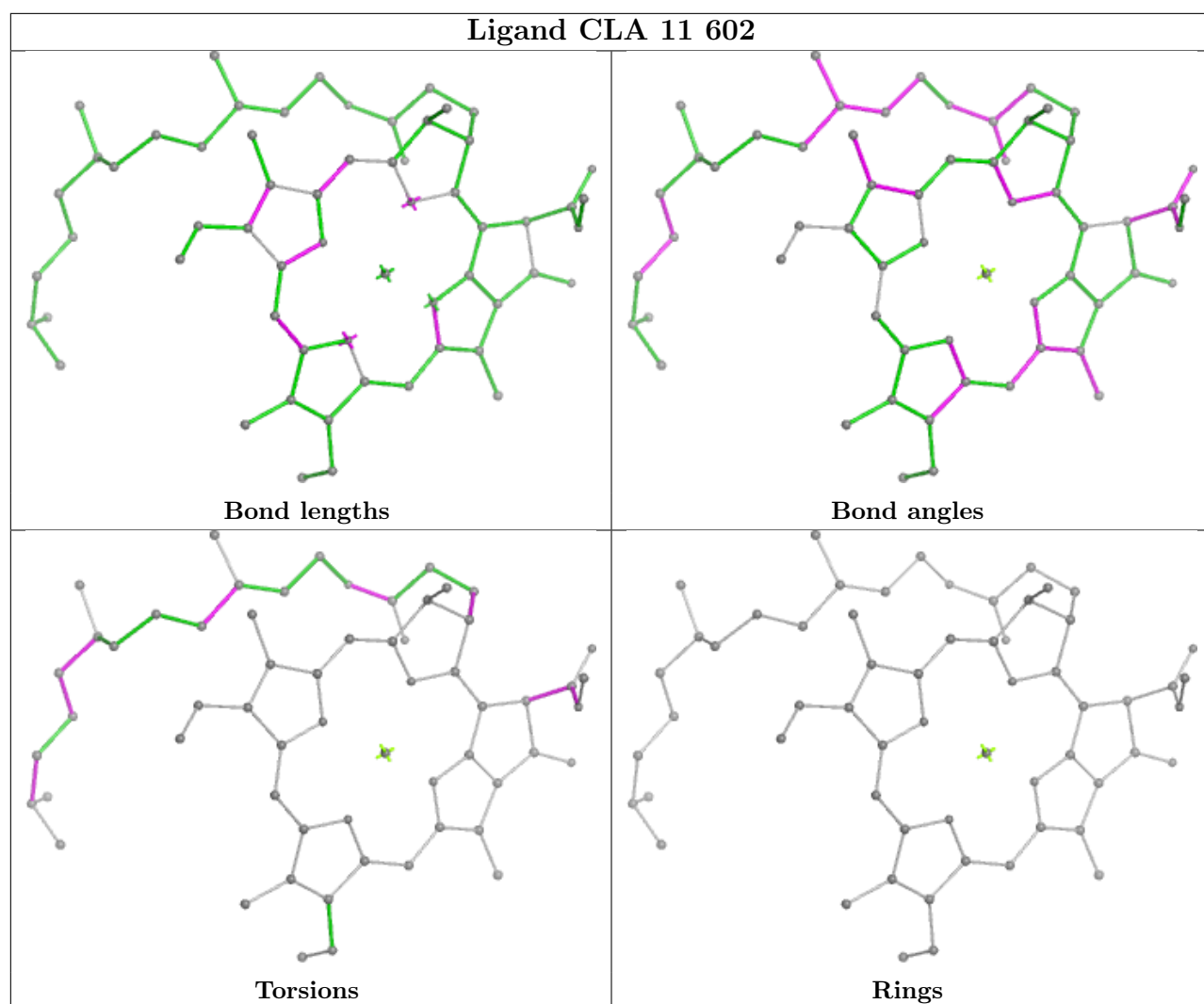


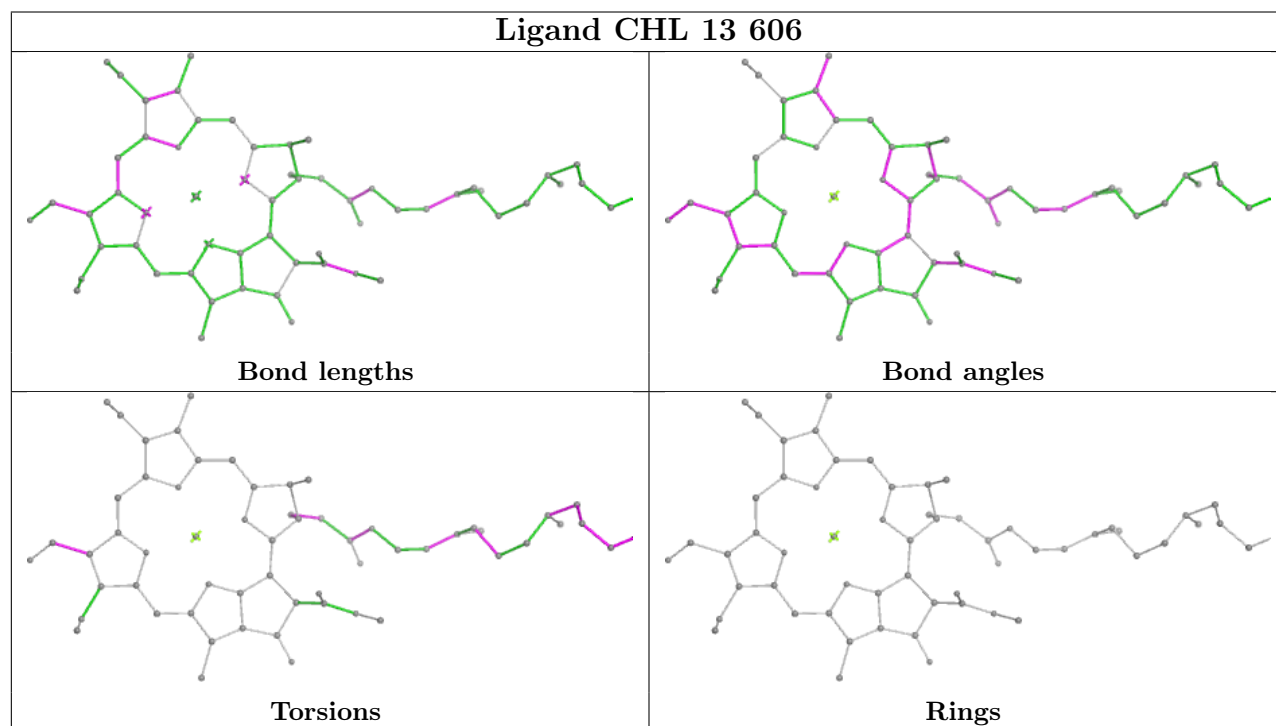
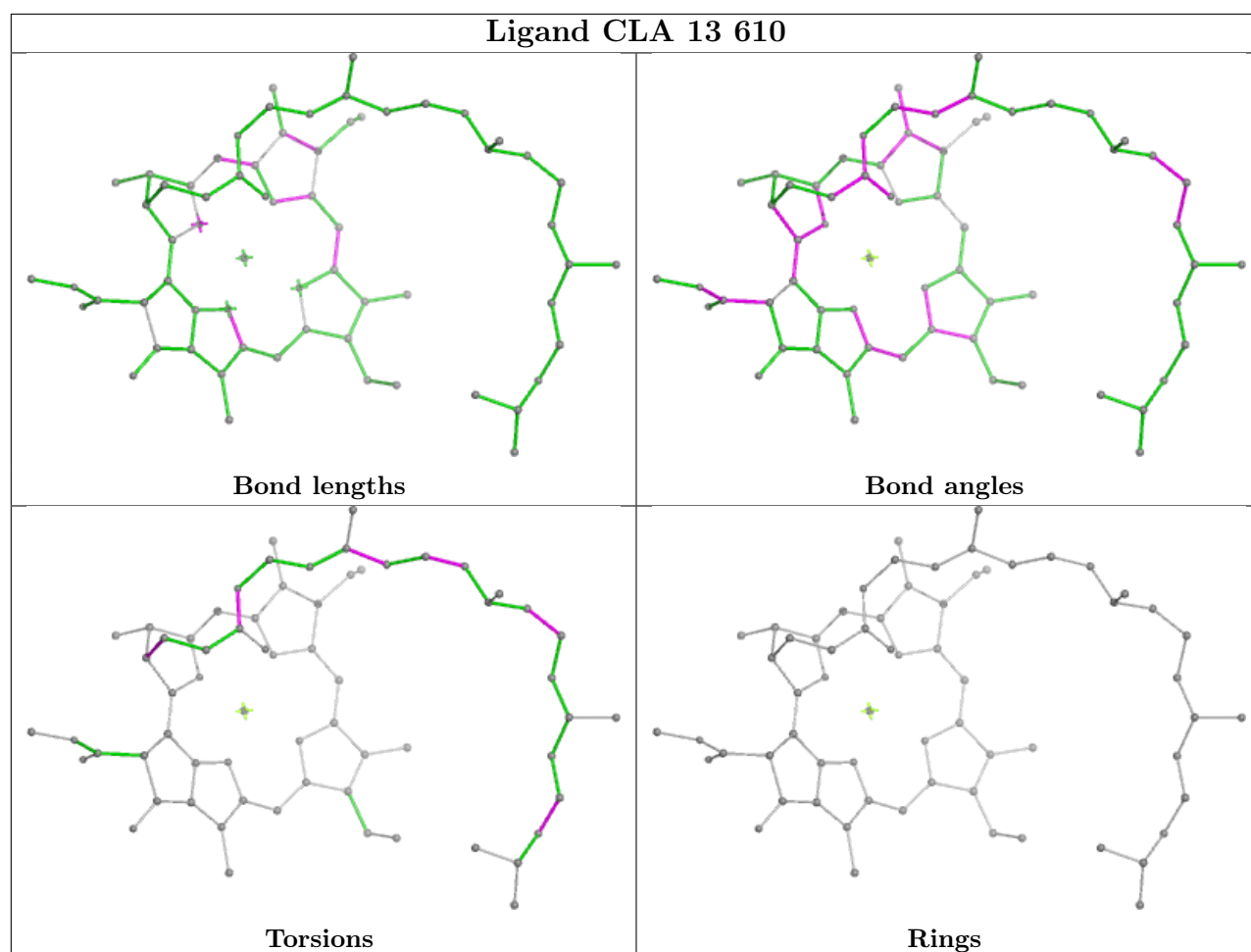


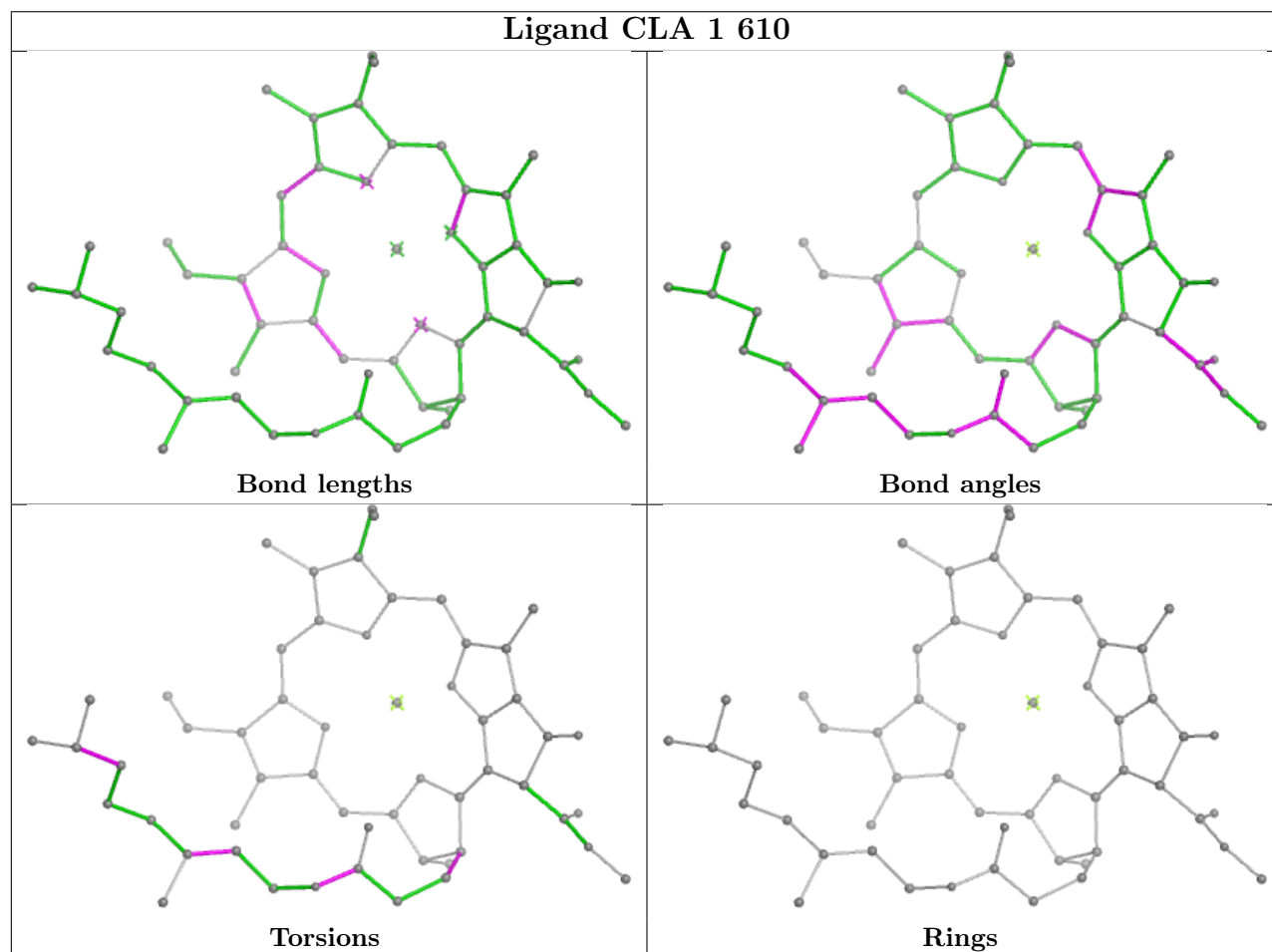
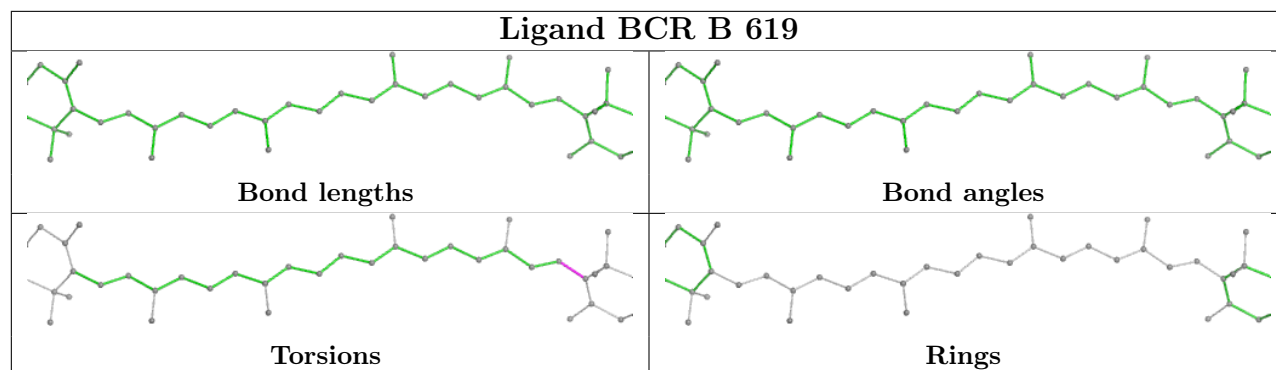
Ligand CLA 5 612



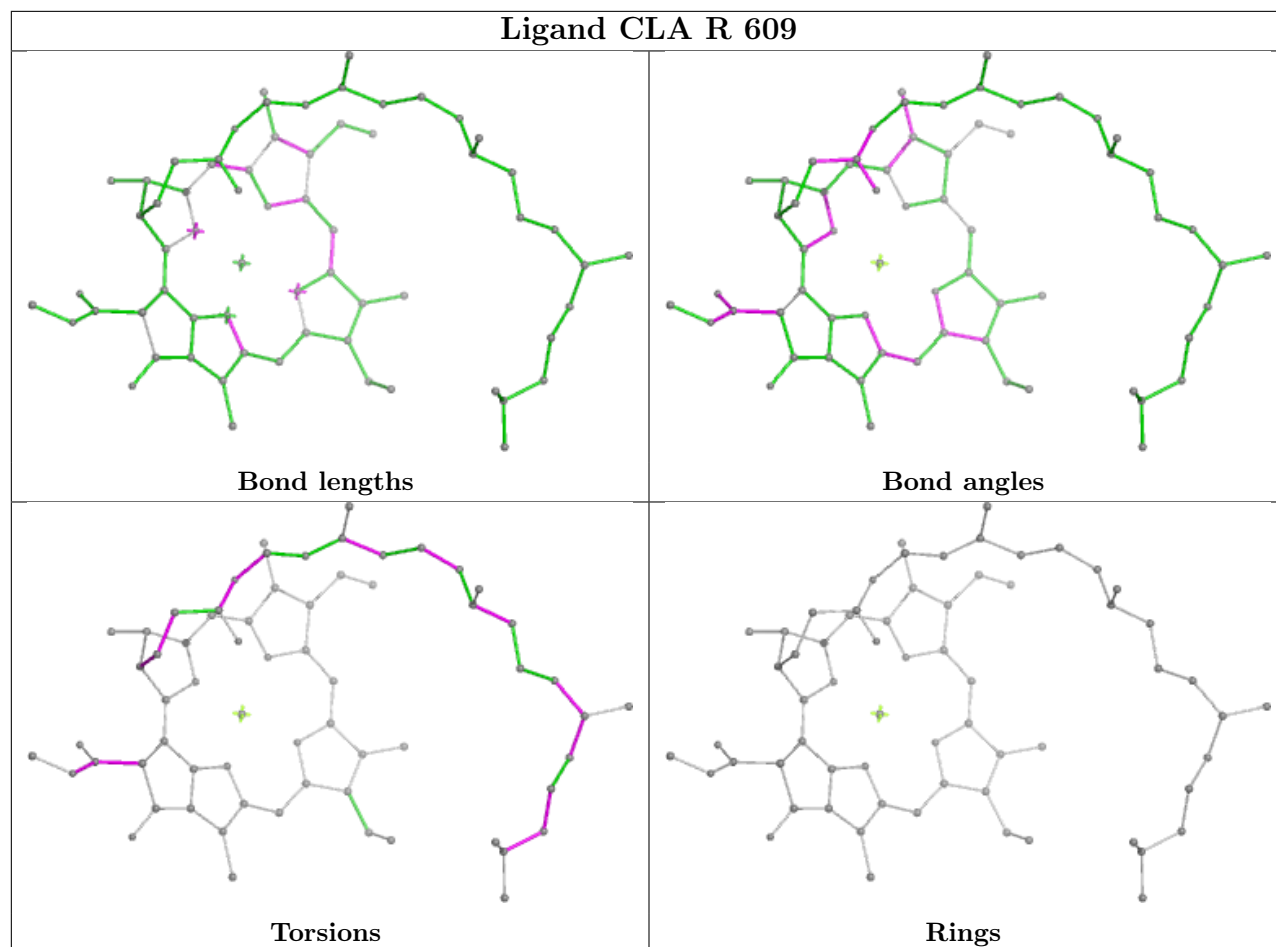




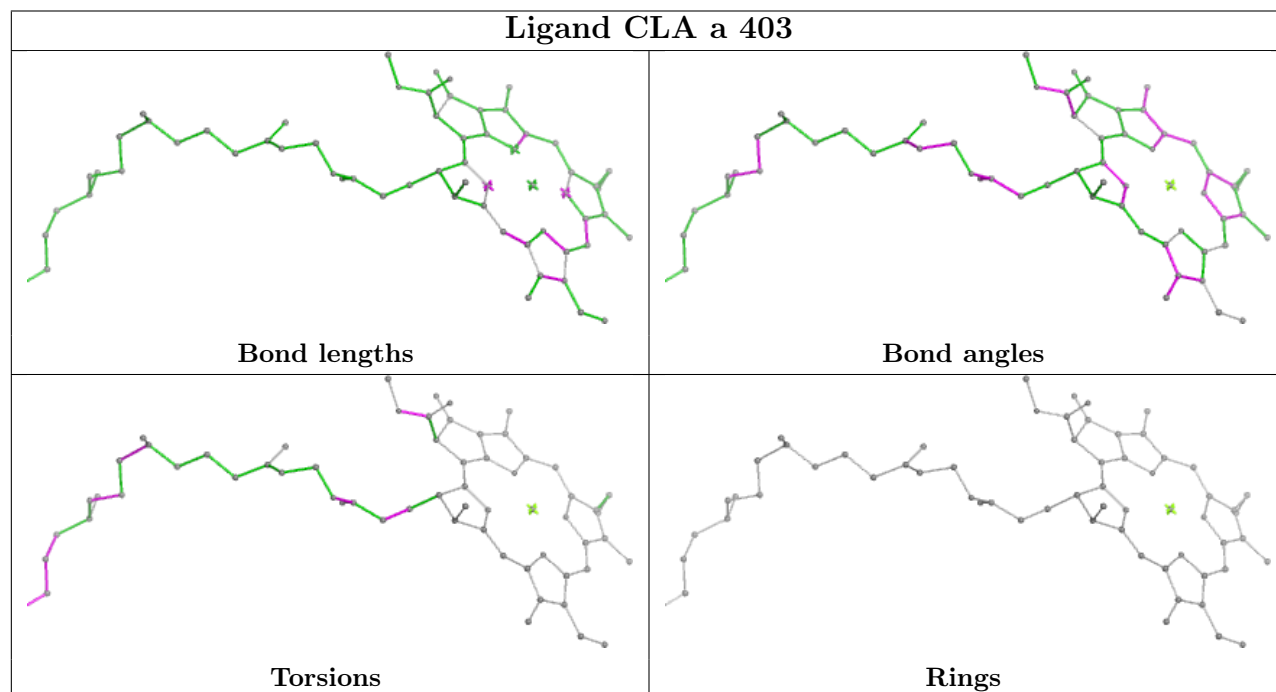


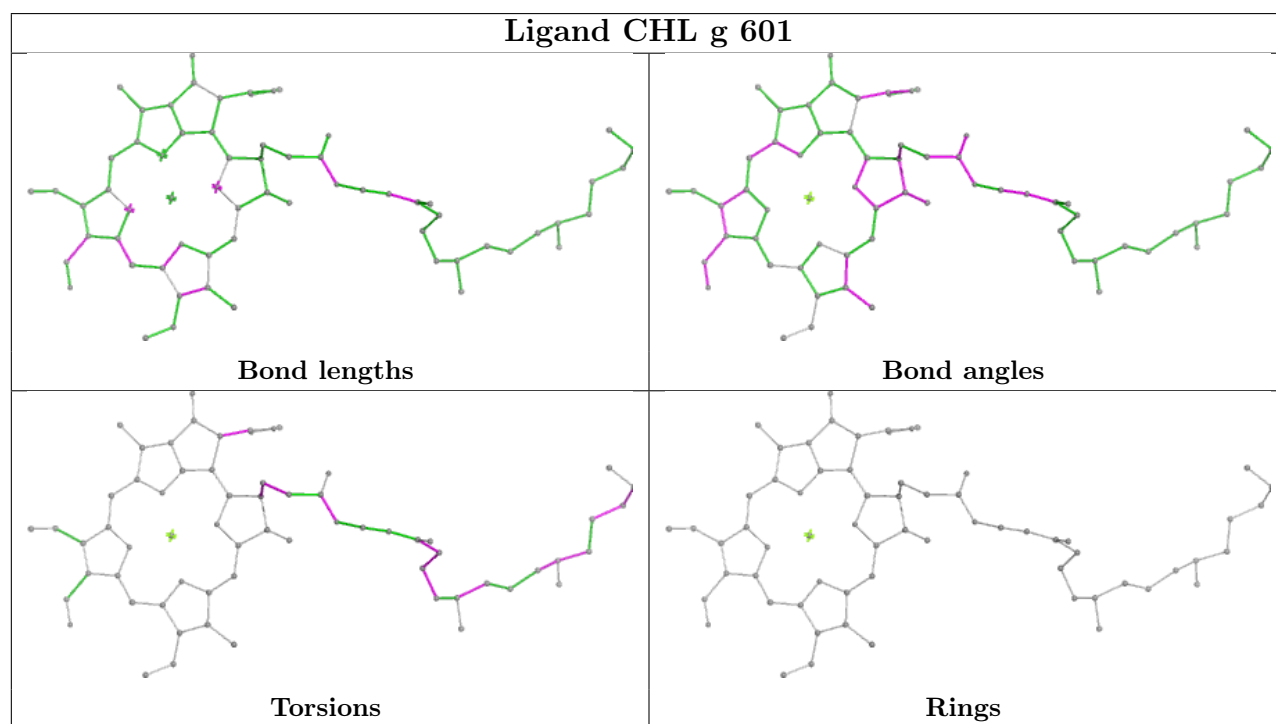
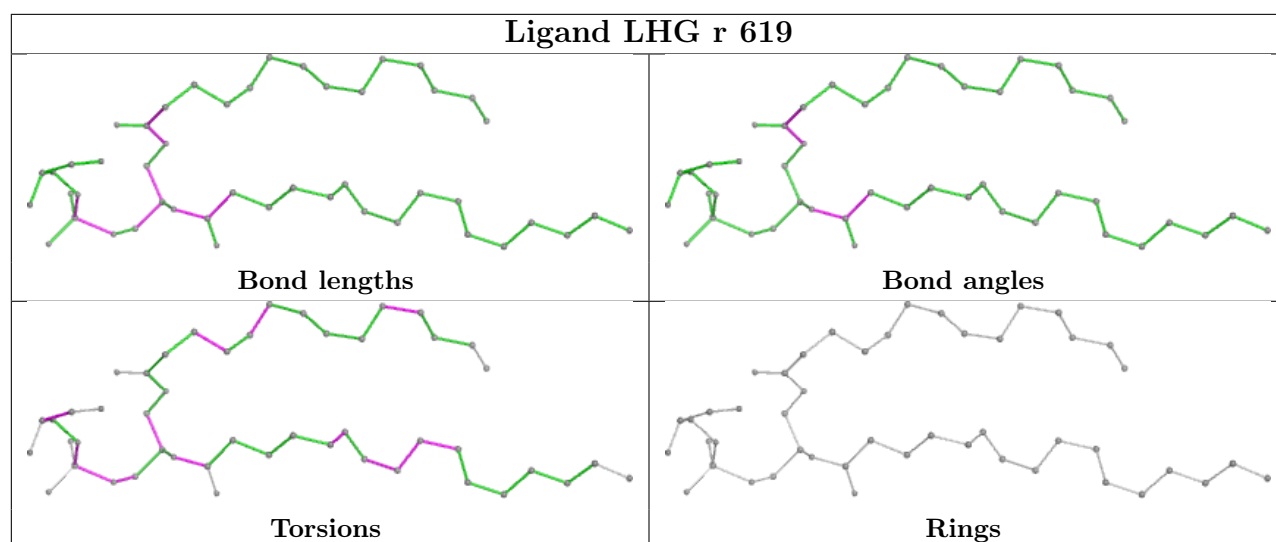


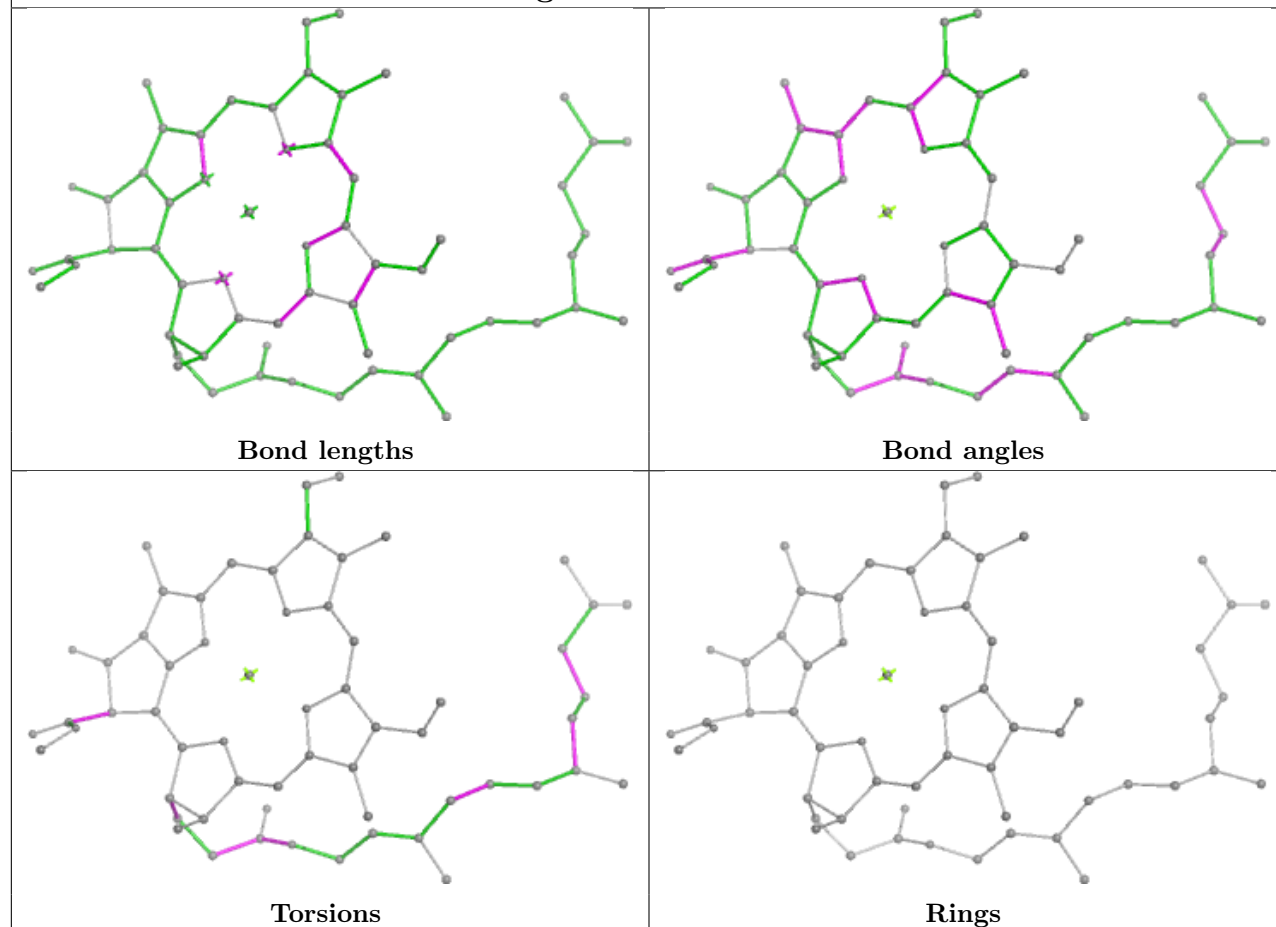
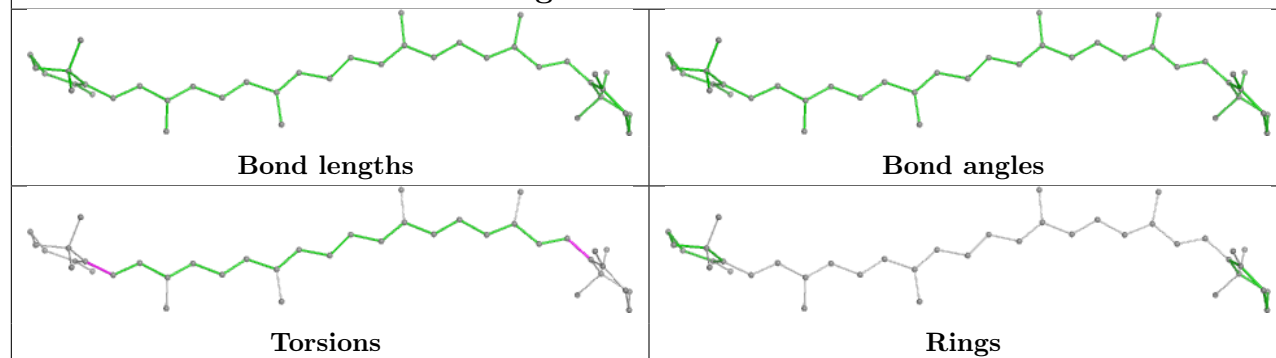
Ligand CLA R 609

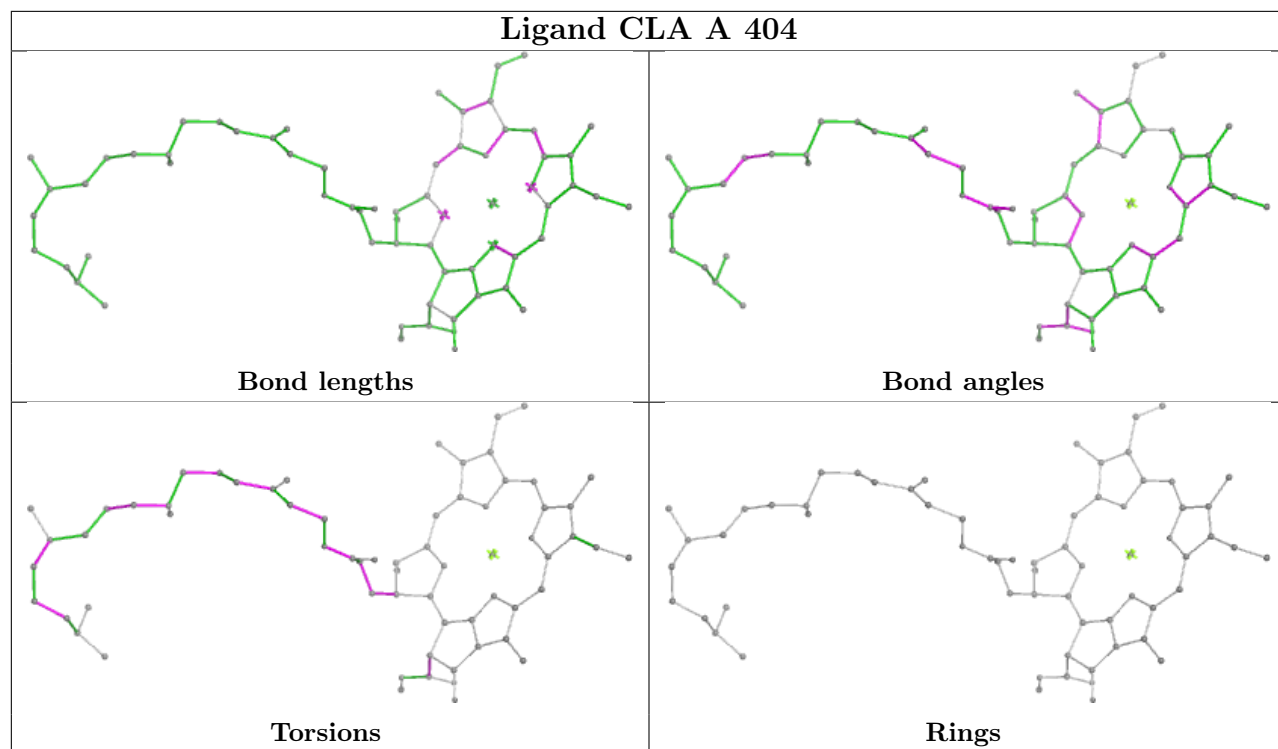


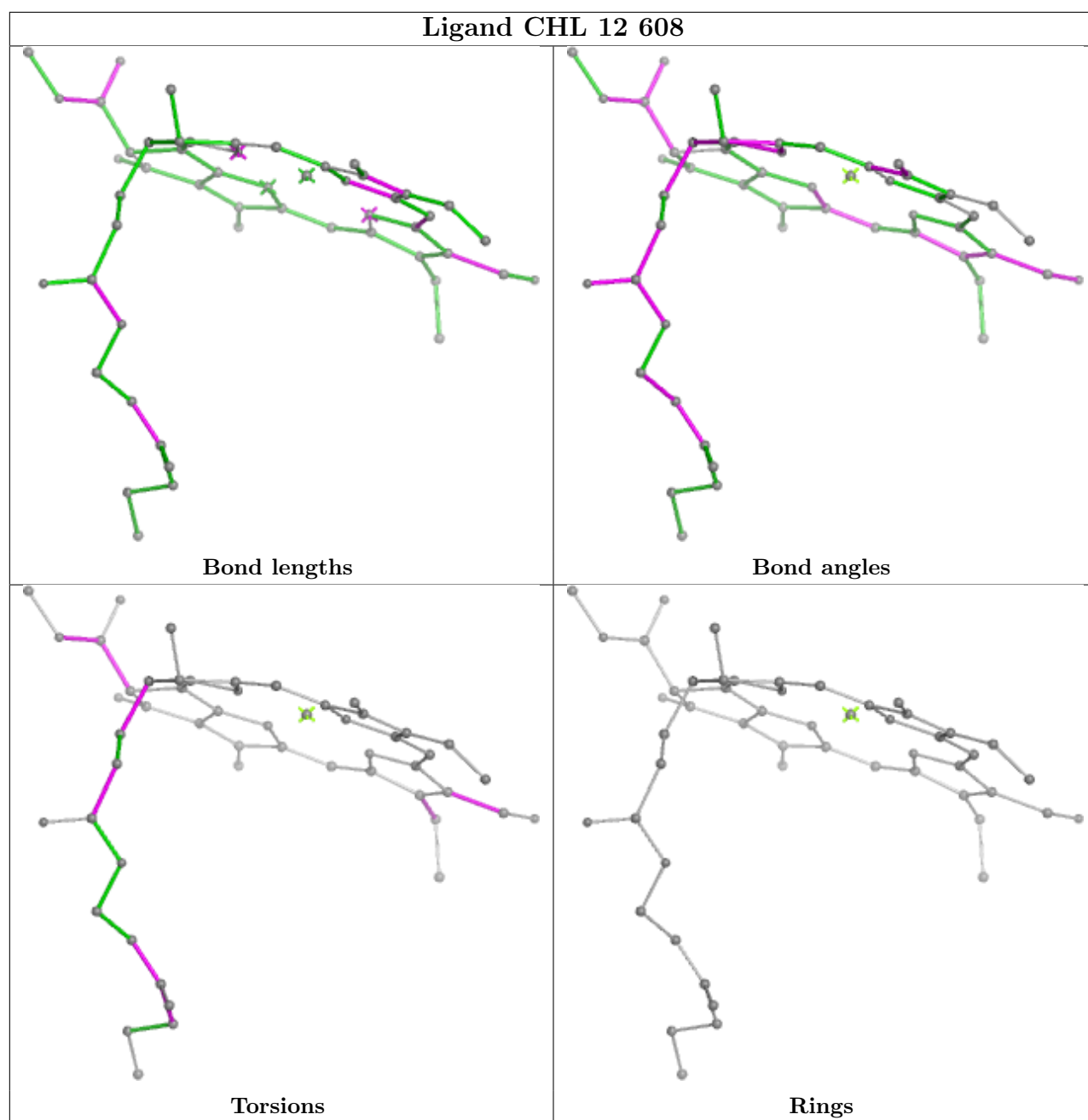
Ligand CLA a 403

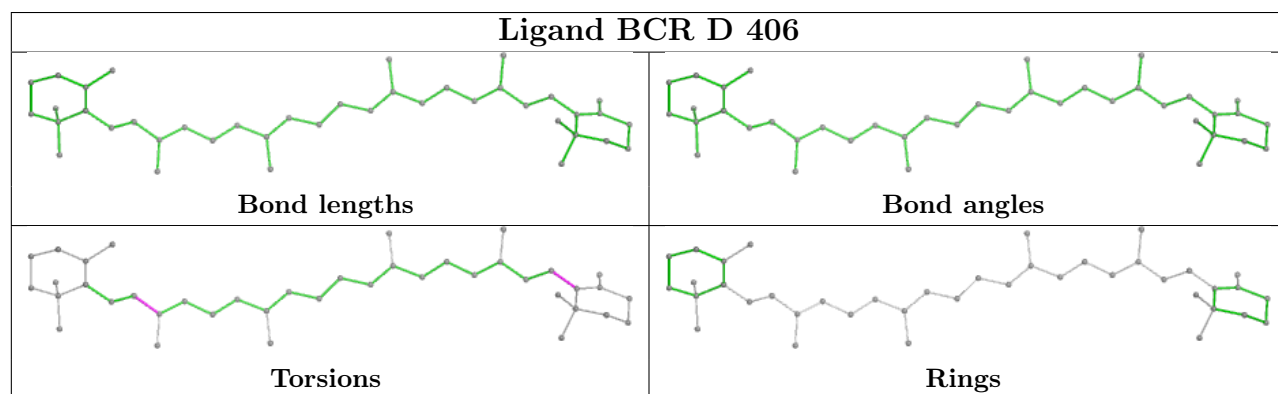
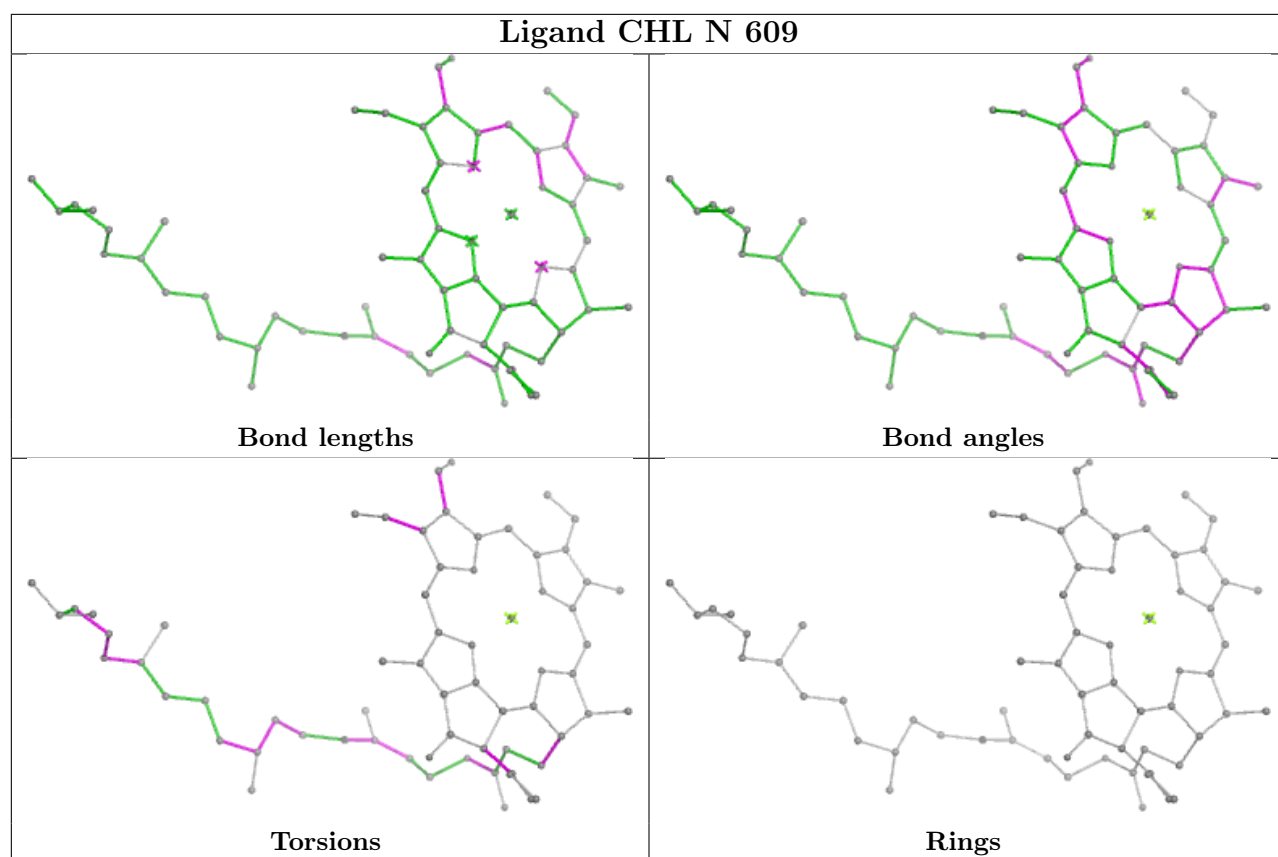


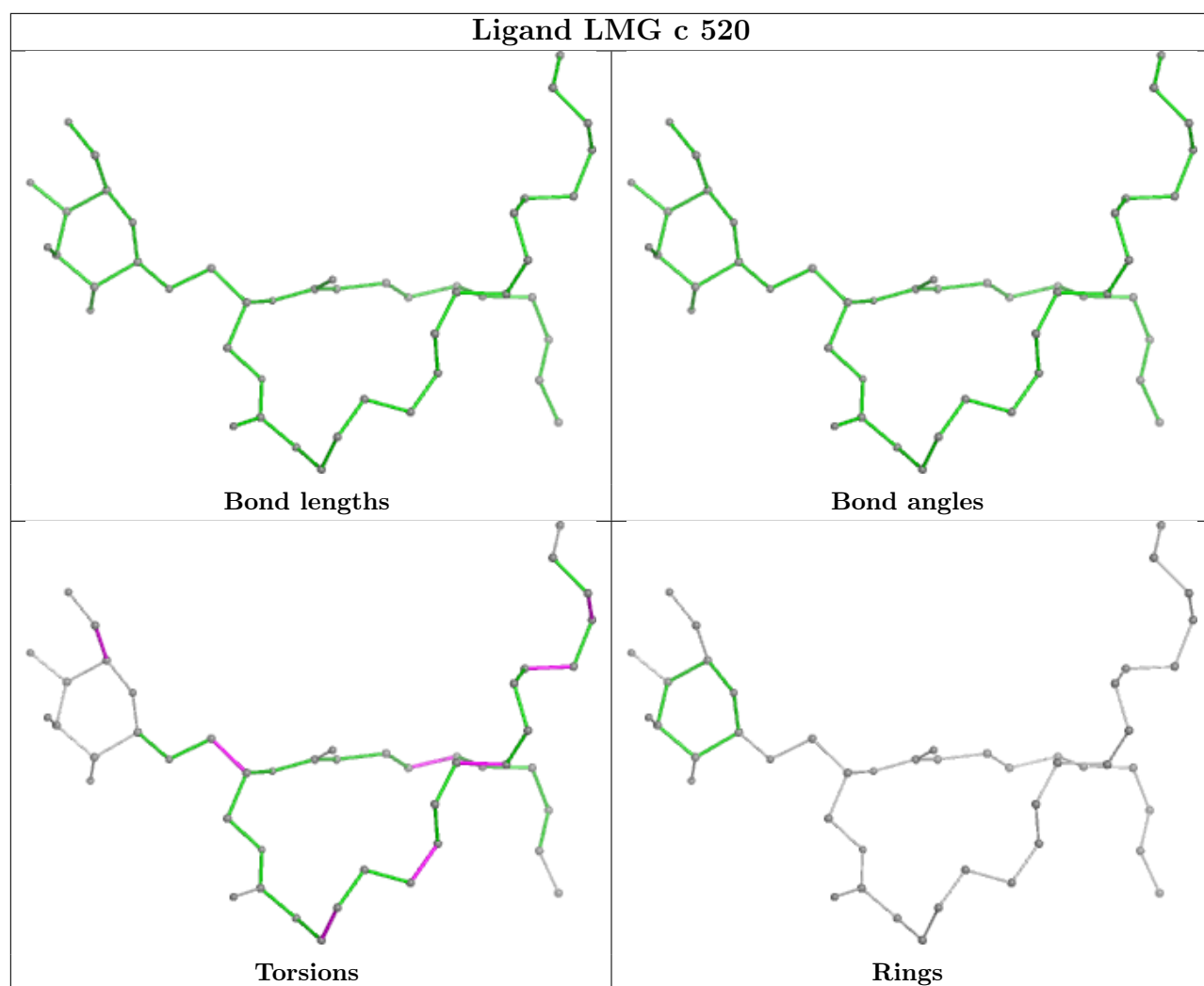


Ligand CLA 6 602**Ligand BCR c 516**

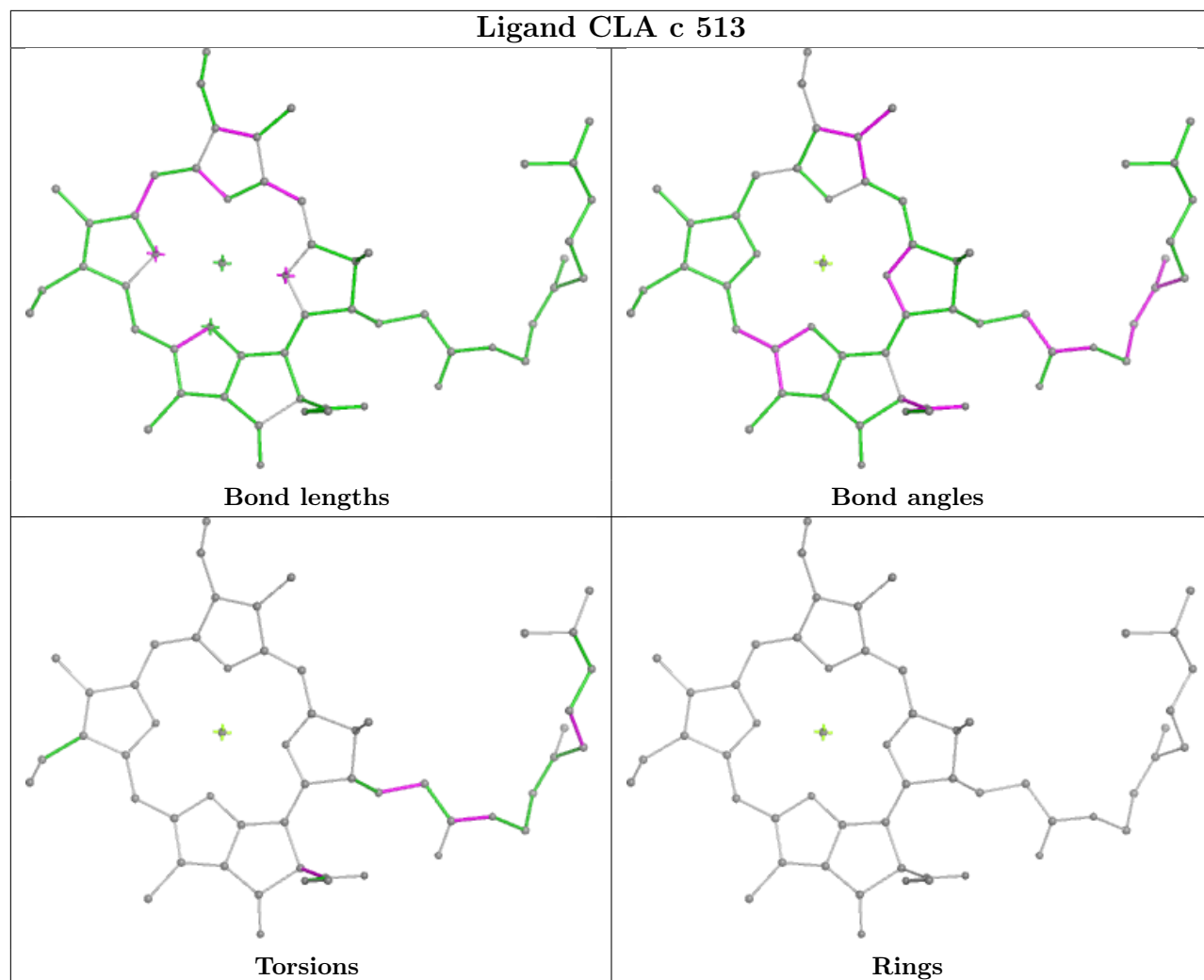


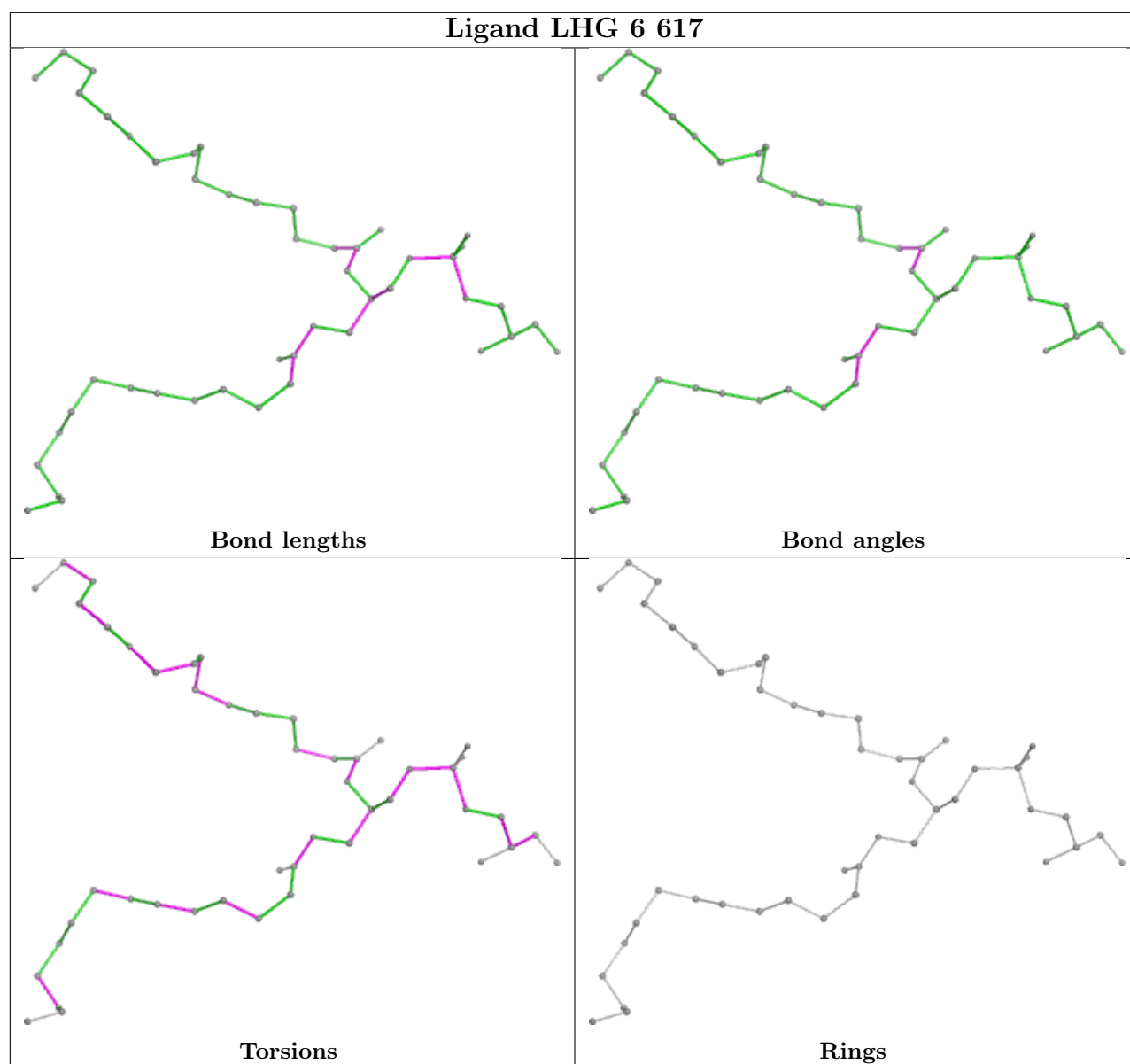




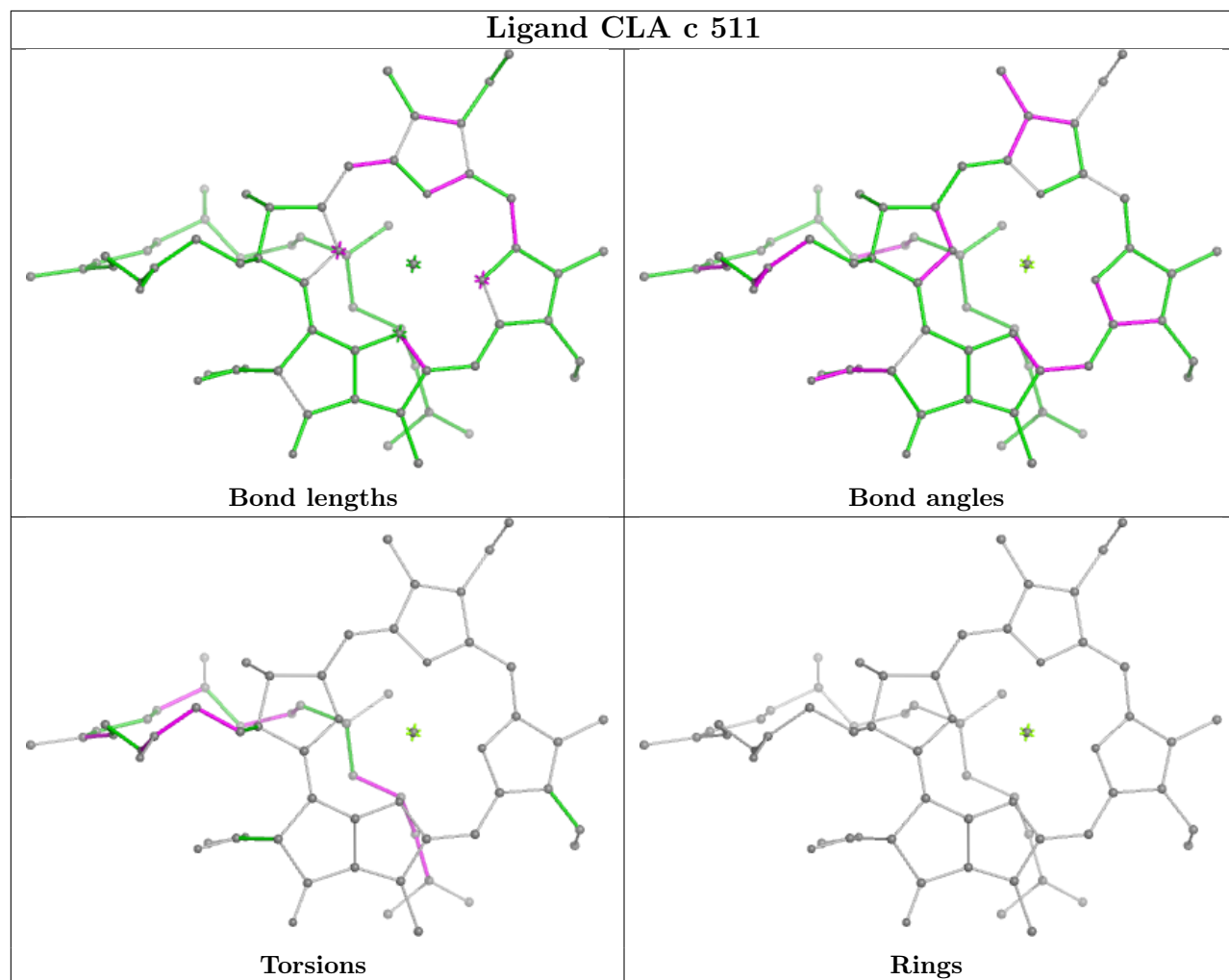


Ligand CLA c 513

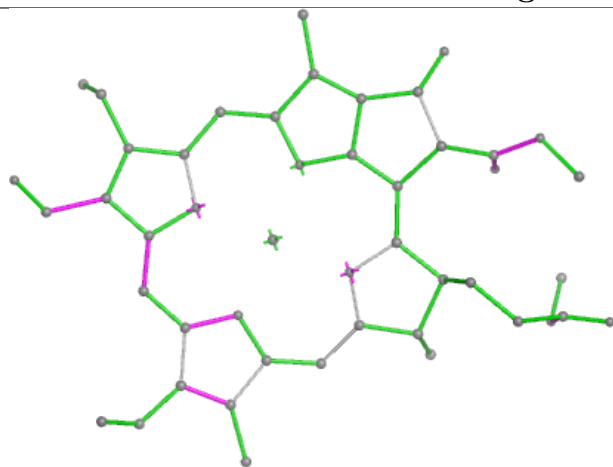




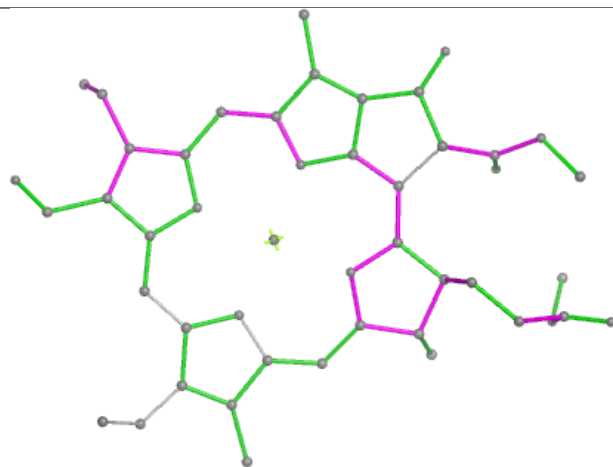
Ligand CLA c 511



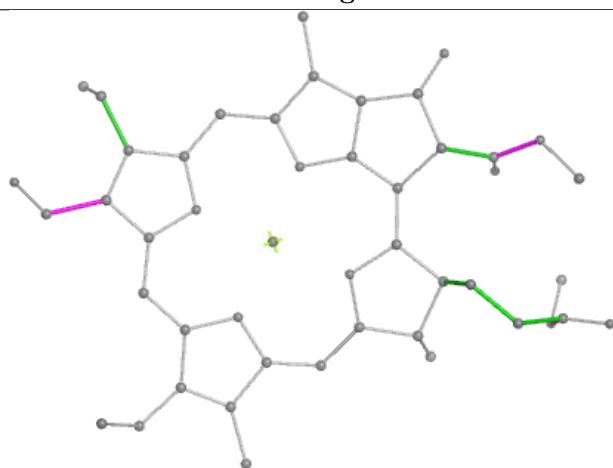
Ligand CHL 4 606



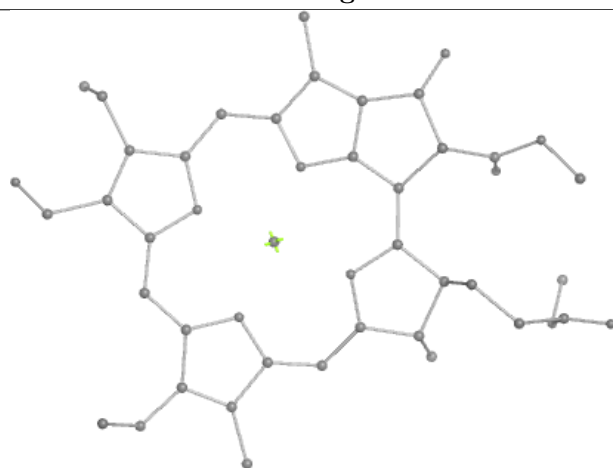
Bond lengths



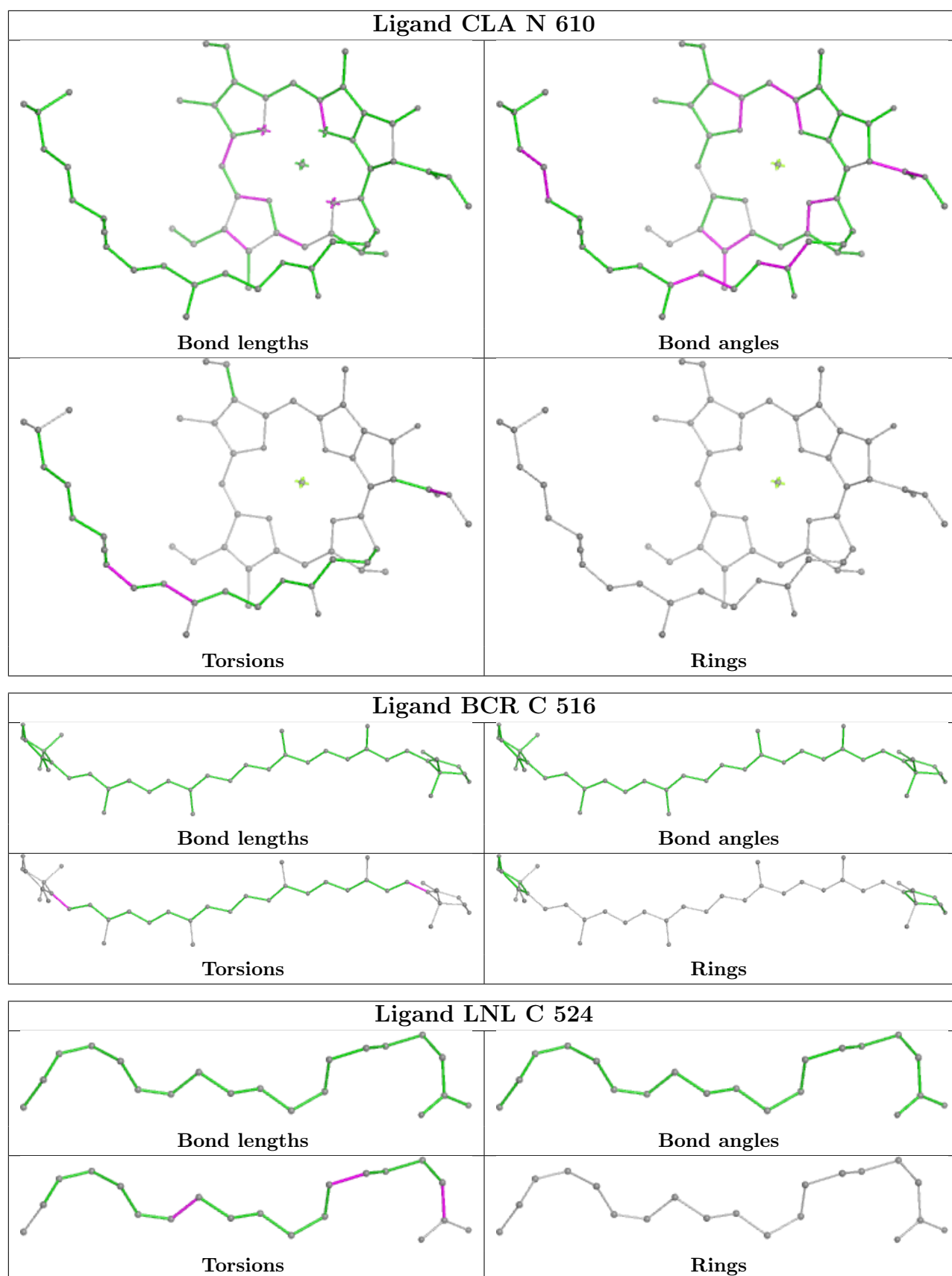
Bond angles

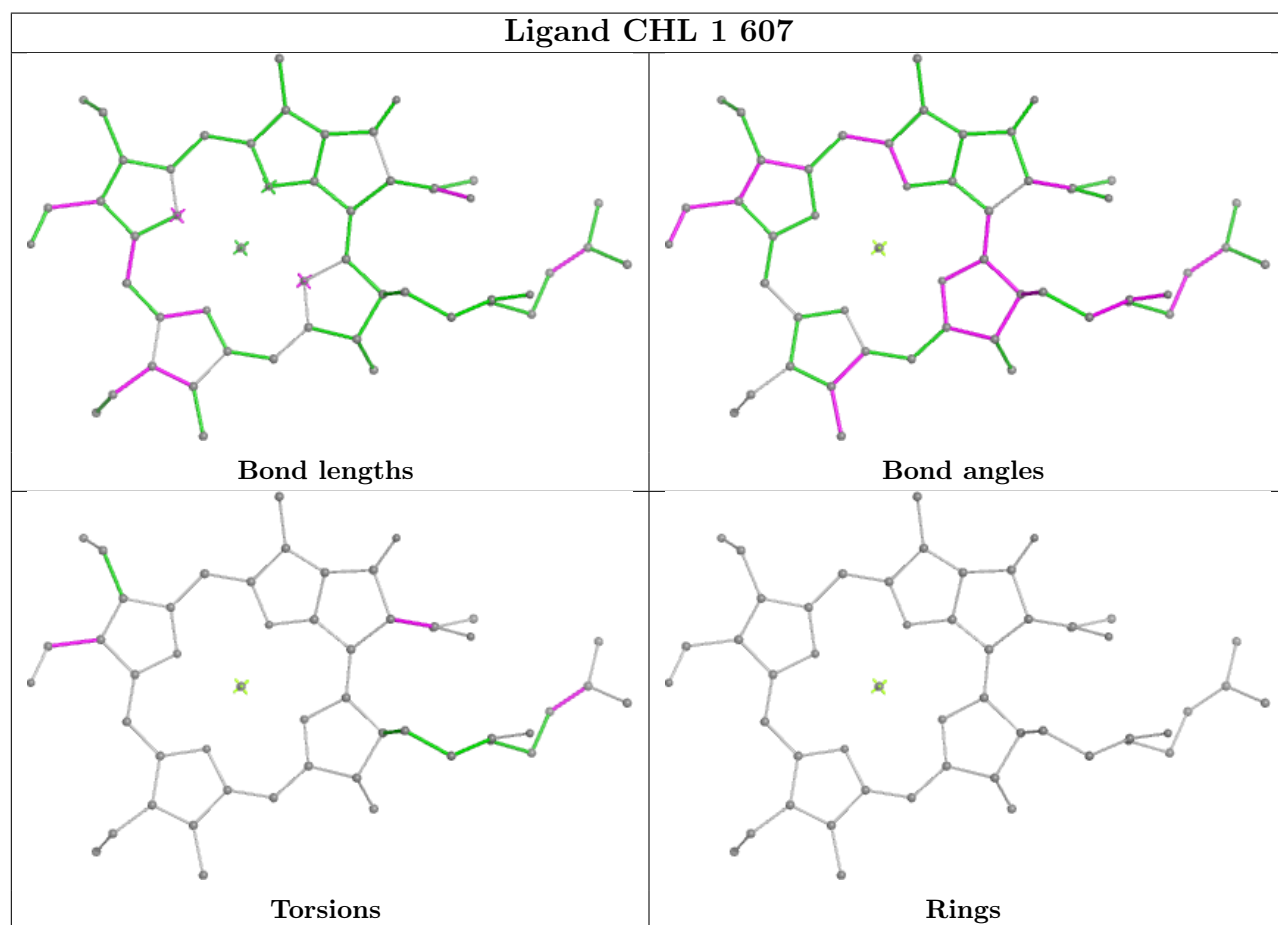
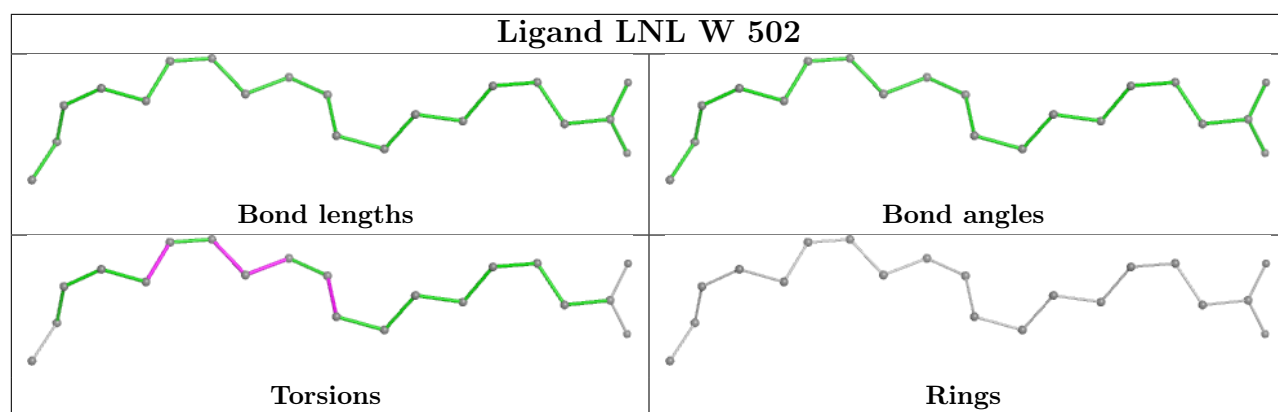


Torsions

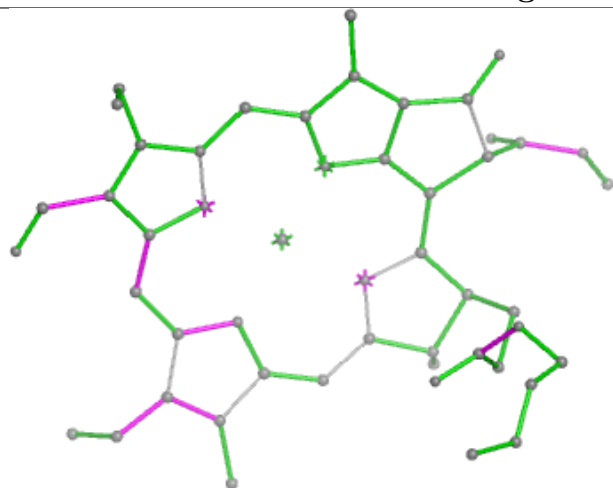


Rings

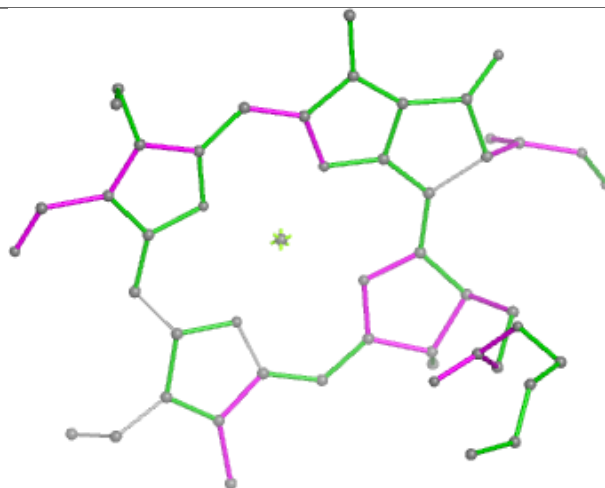




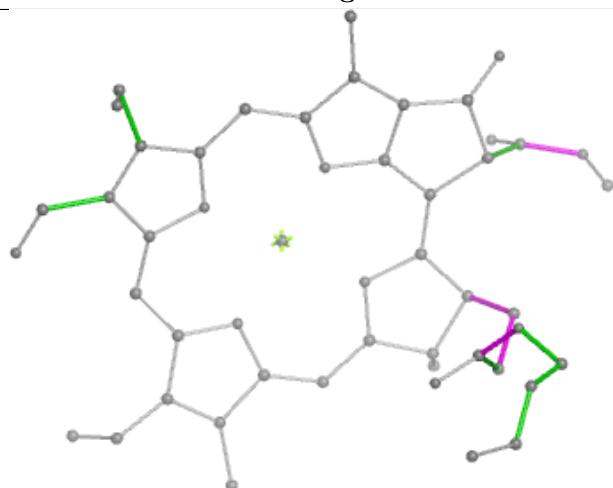
Ligand CHL 3 608



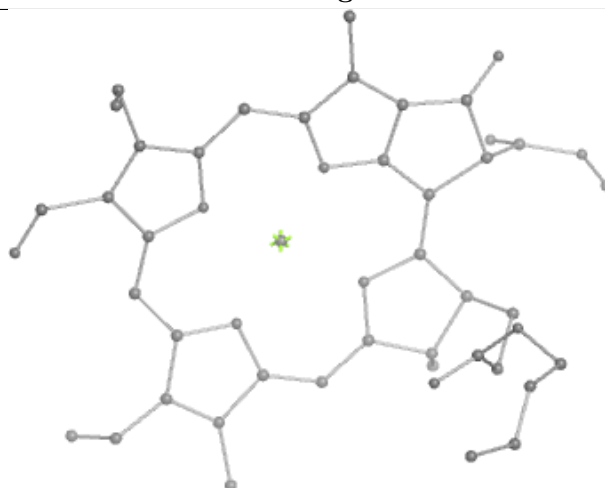
Bond lengths



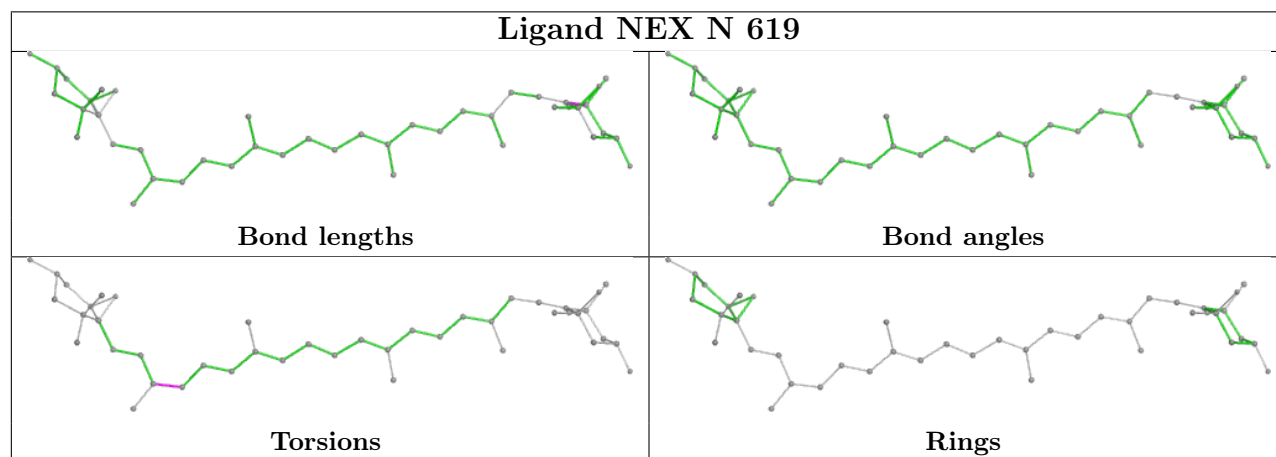
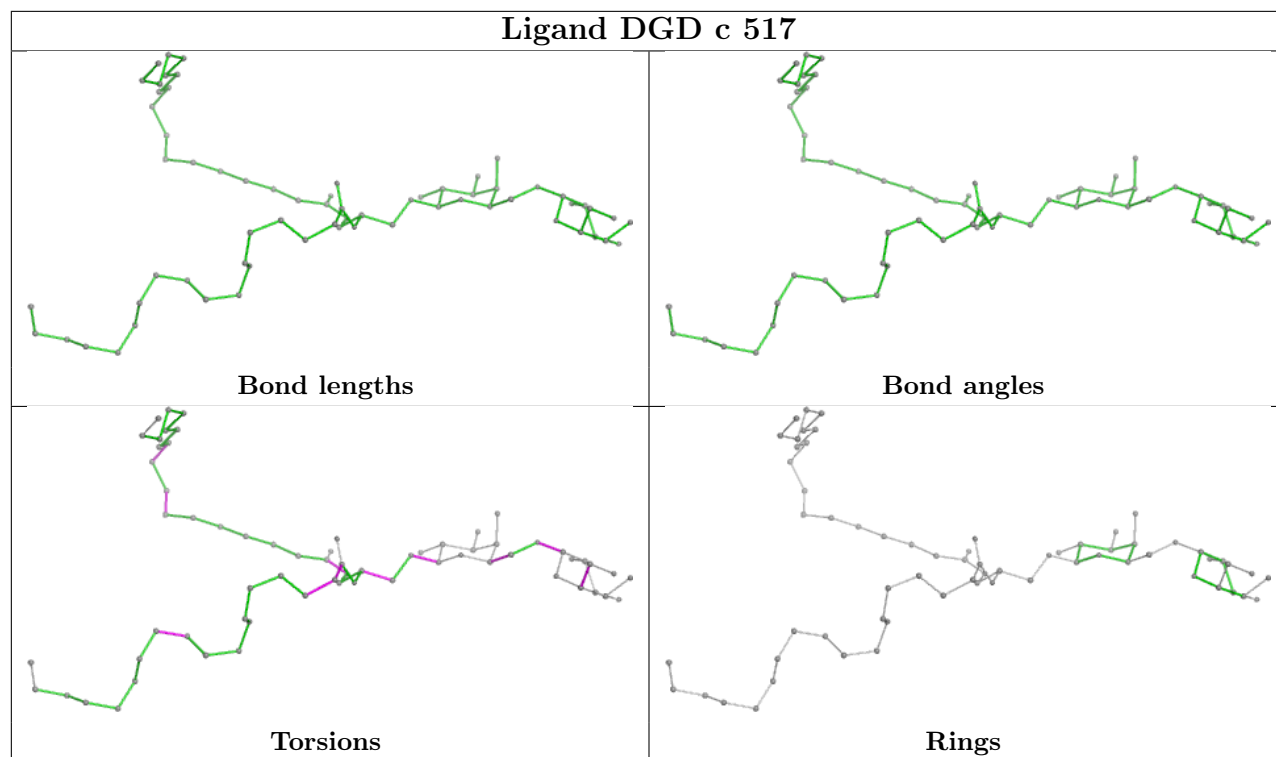
Bond angles



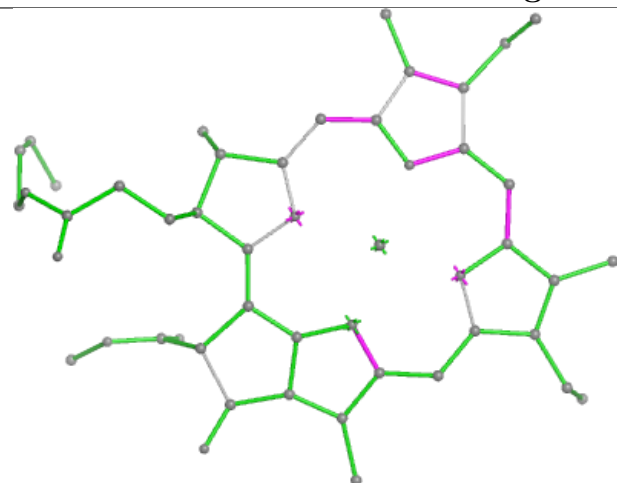
Torsions



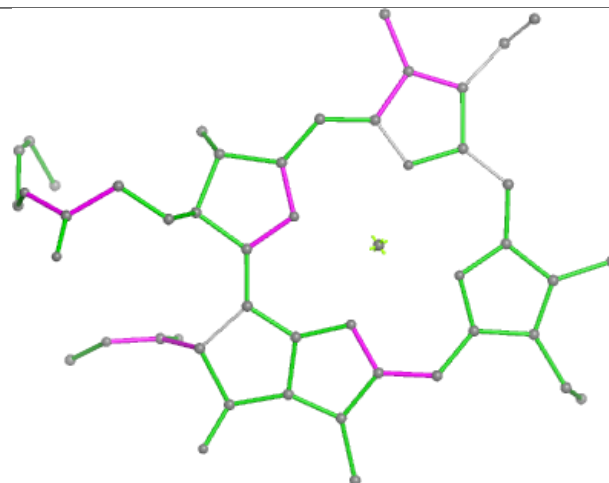
Rings



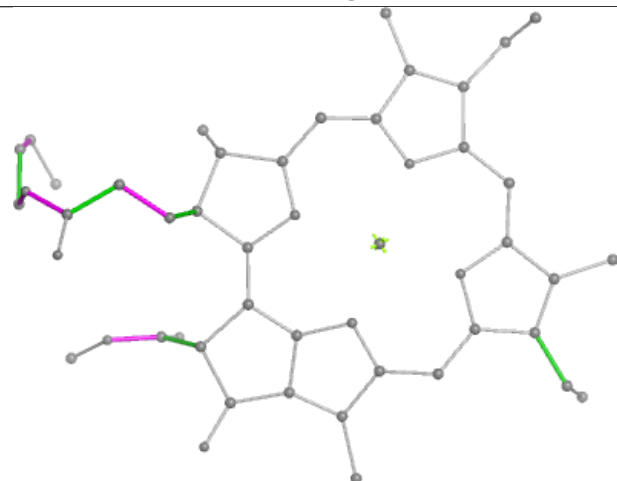
Ligand CLA r 611



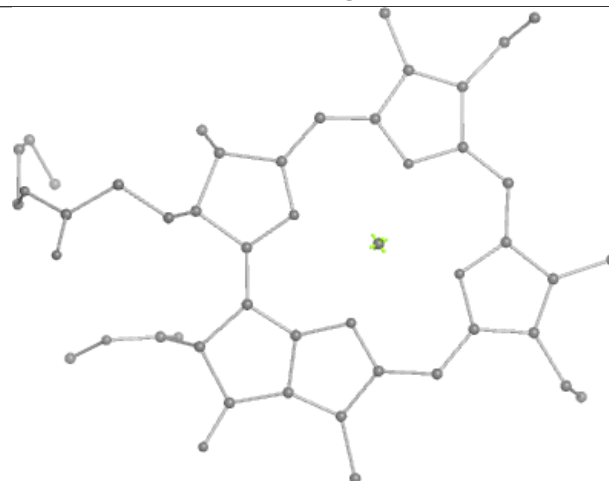
Bond lengths



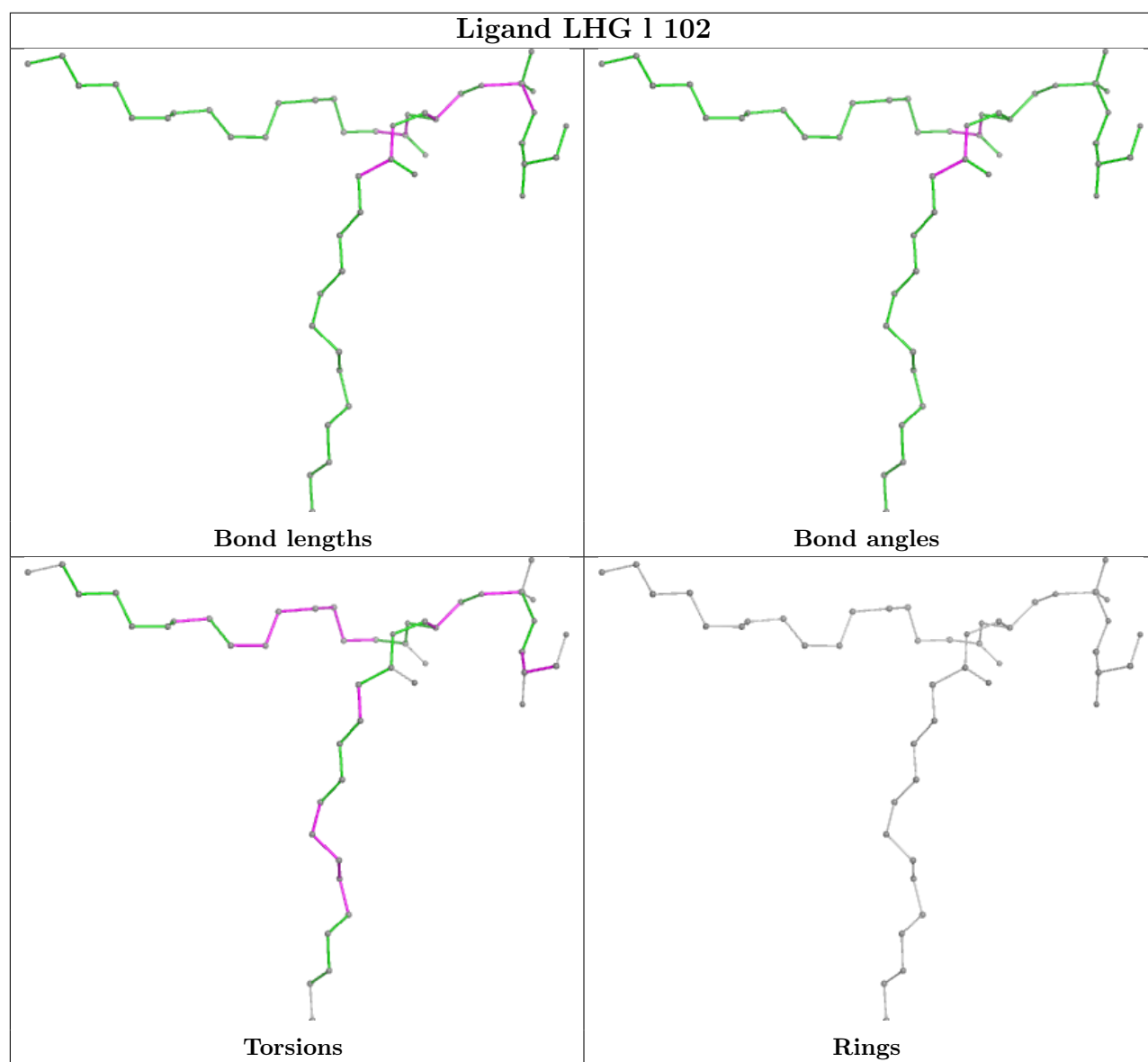
Bond angles



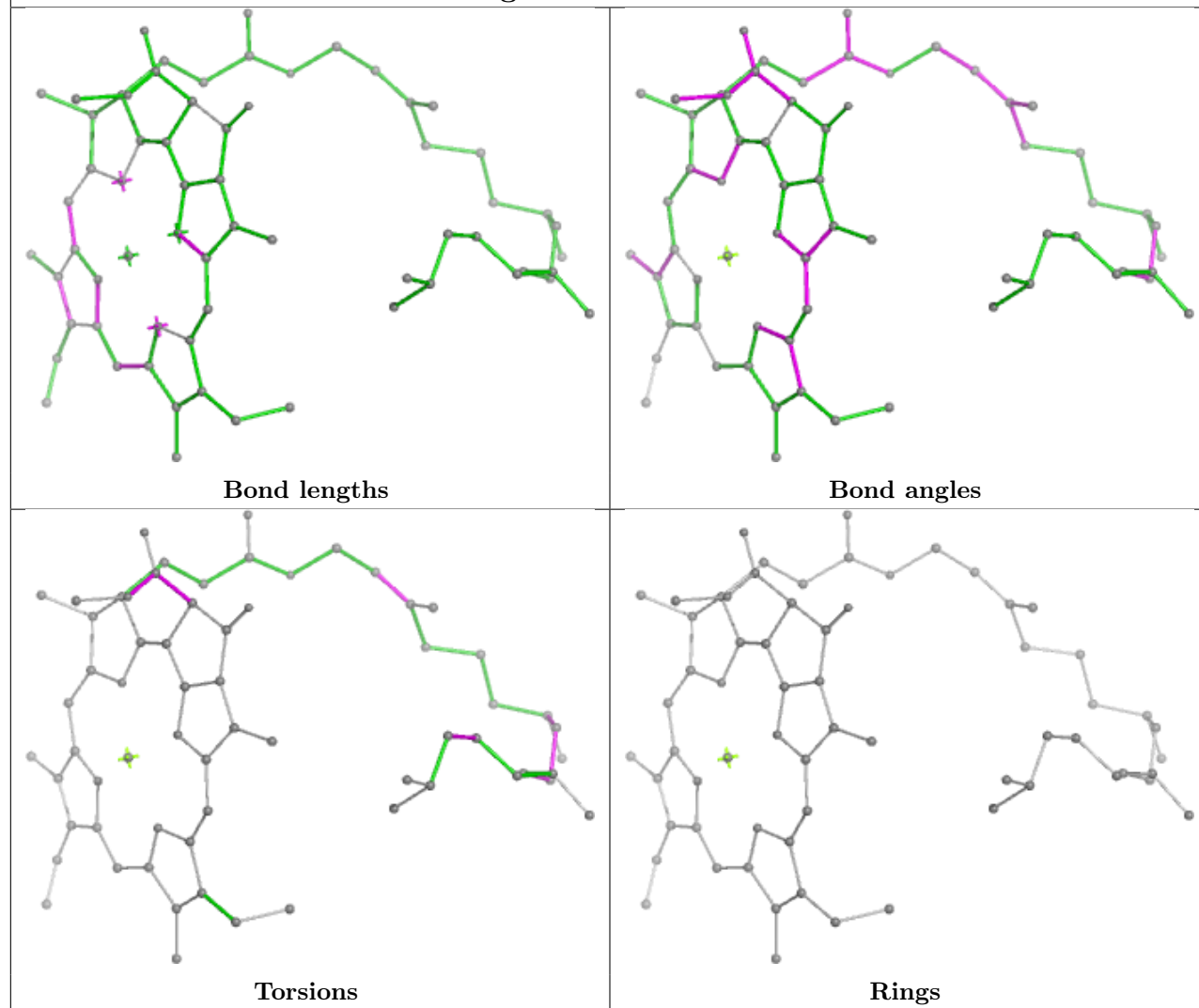
Torsions



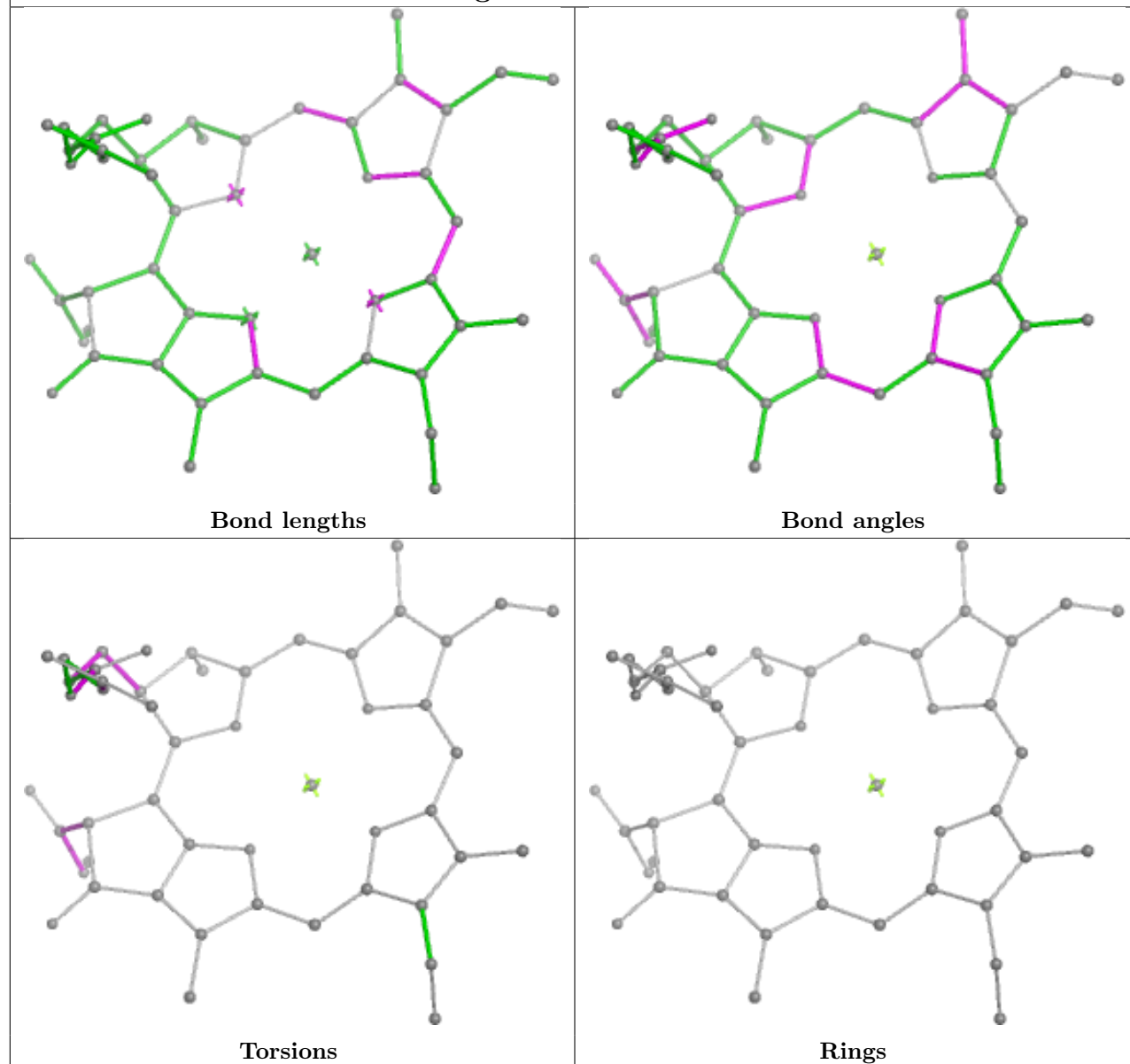
Rings



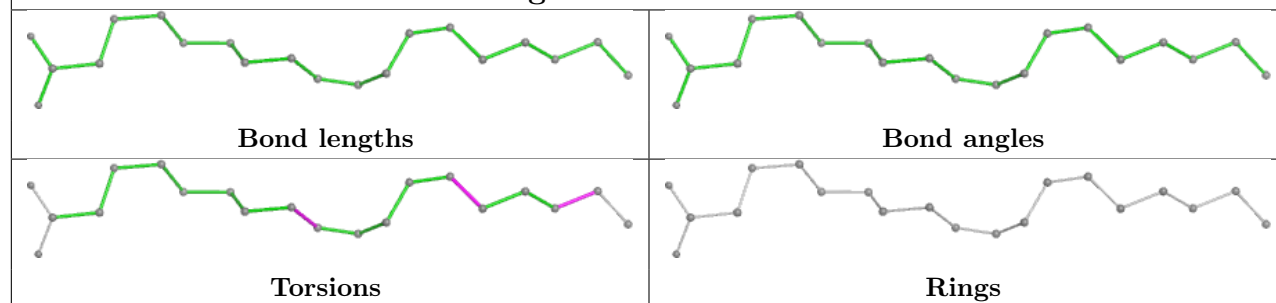
Ligand CLA C 504



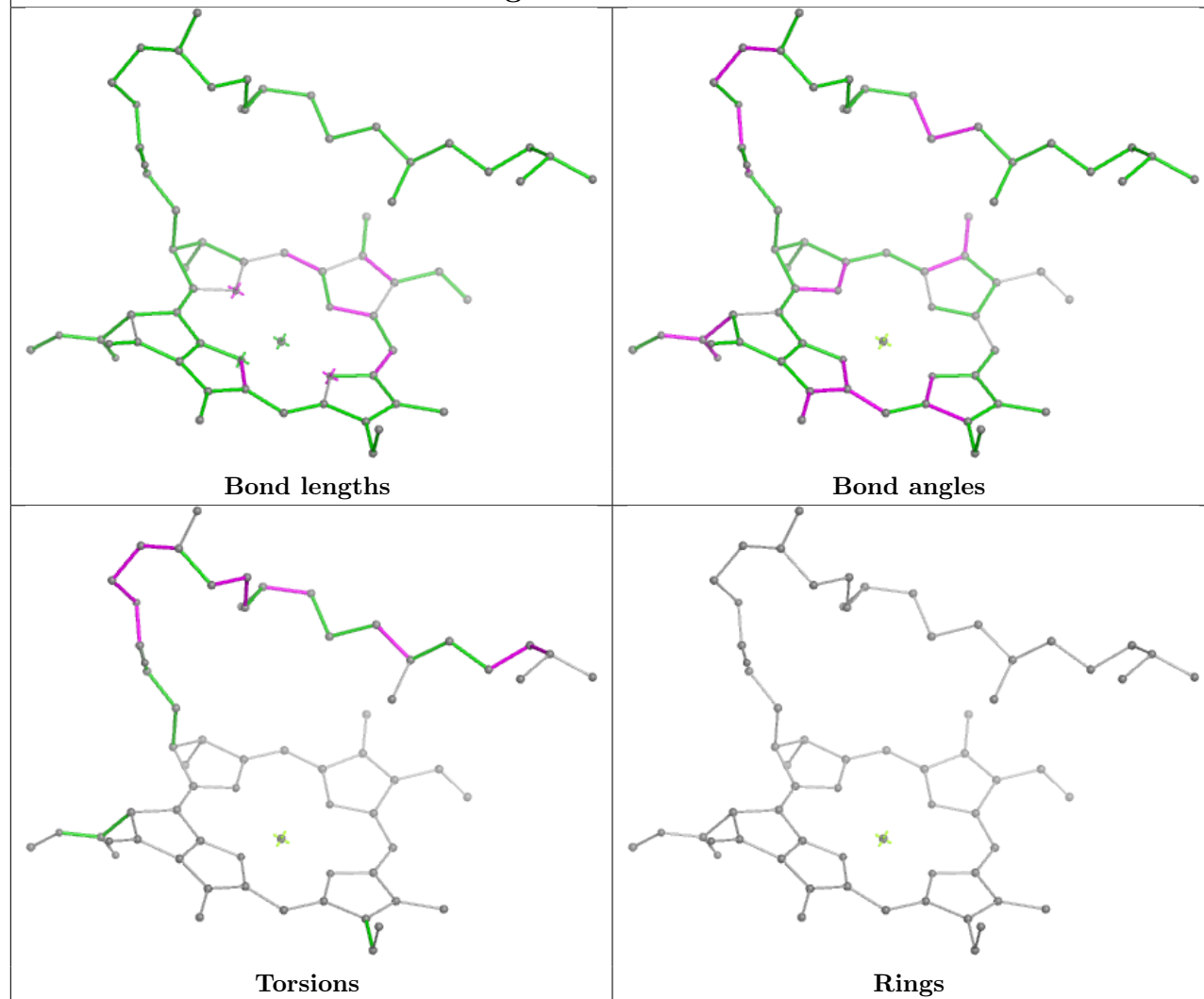
Ligand CLA 5 604



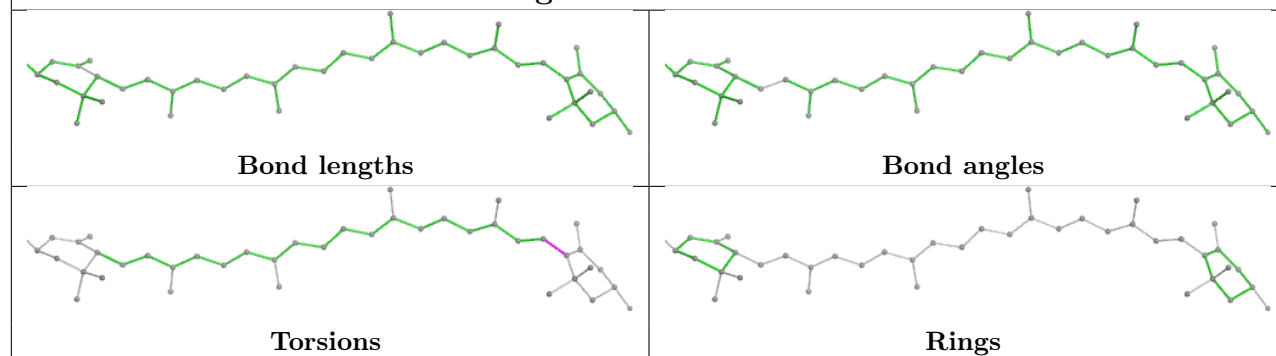
Ligand LNL W 503

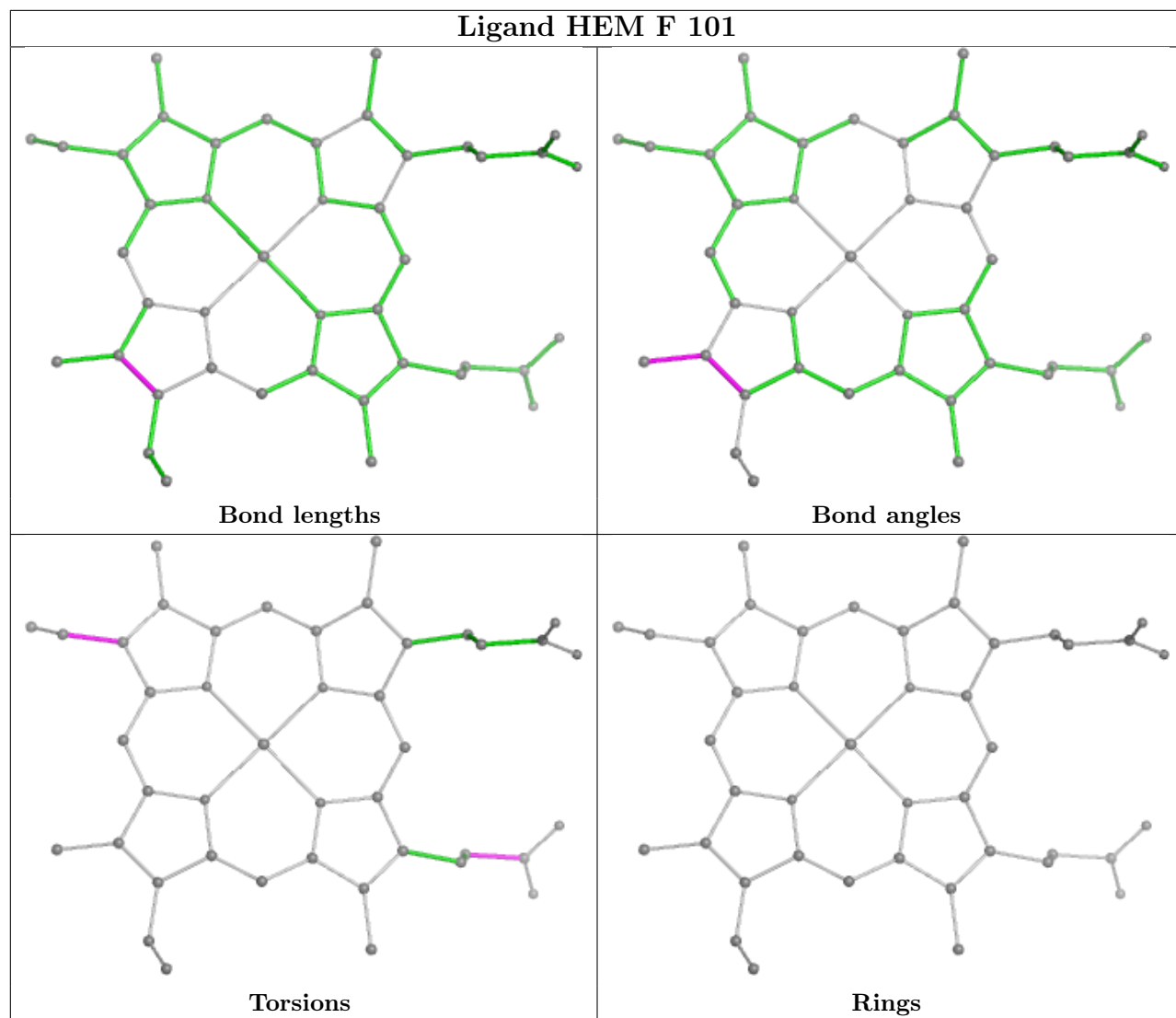


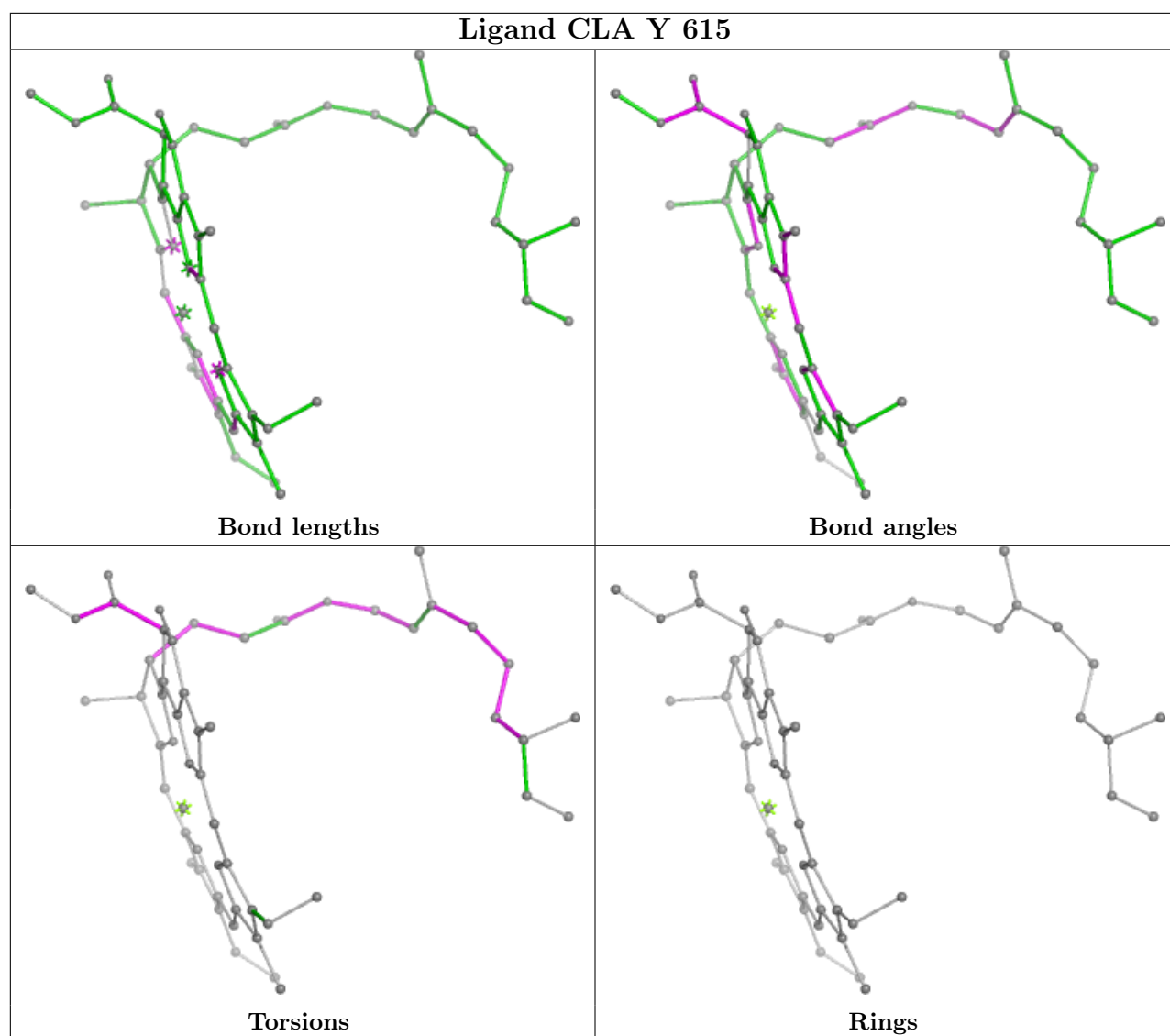
Ligand CLA S 614



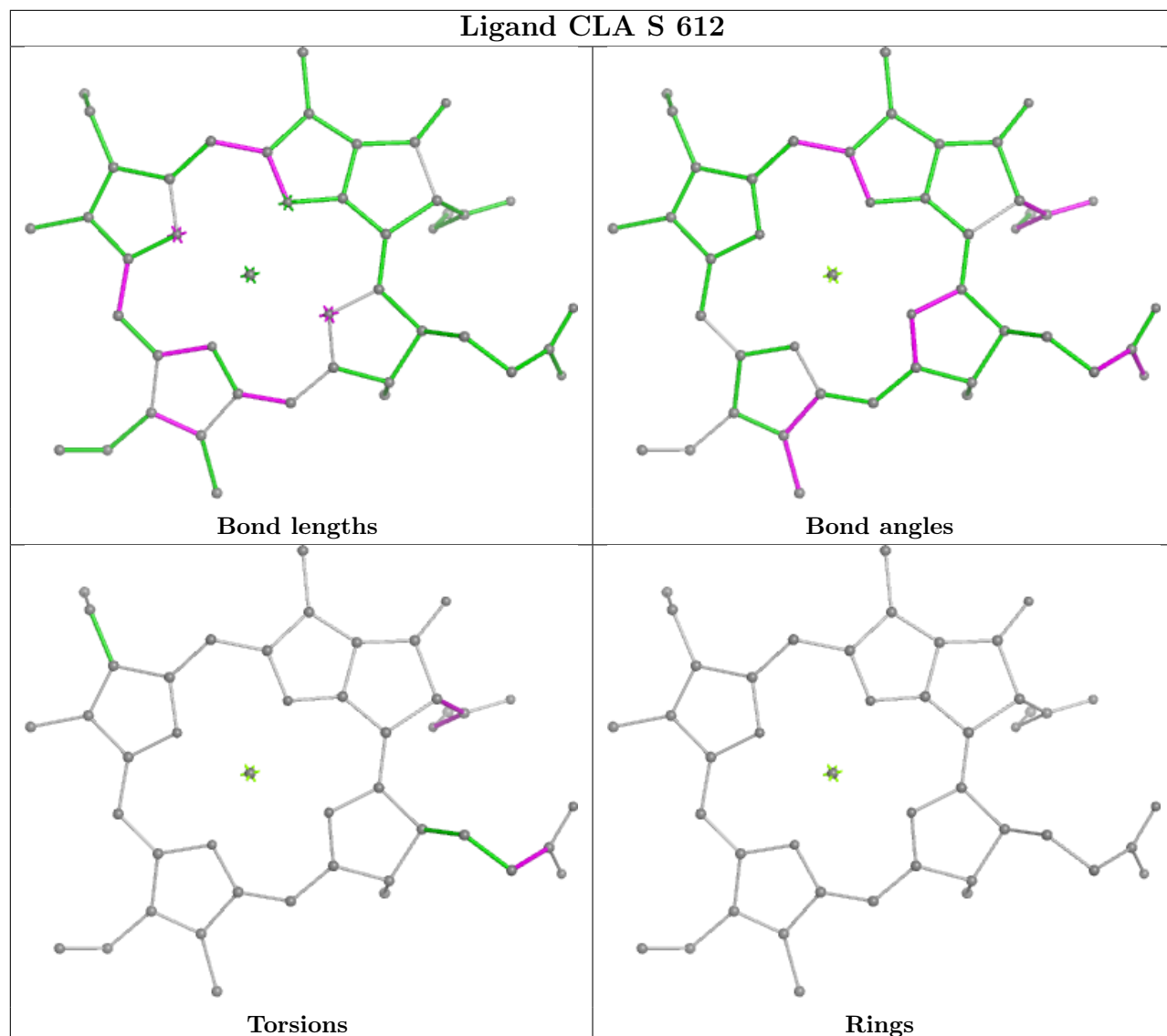
Ligand LUT S 618



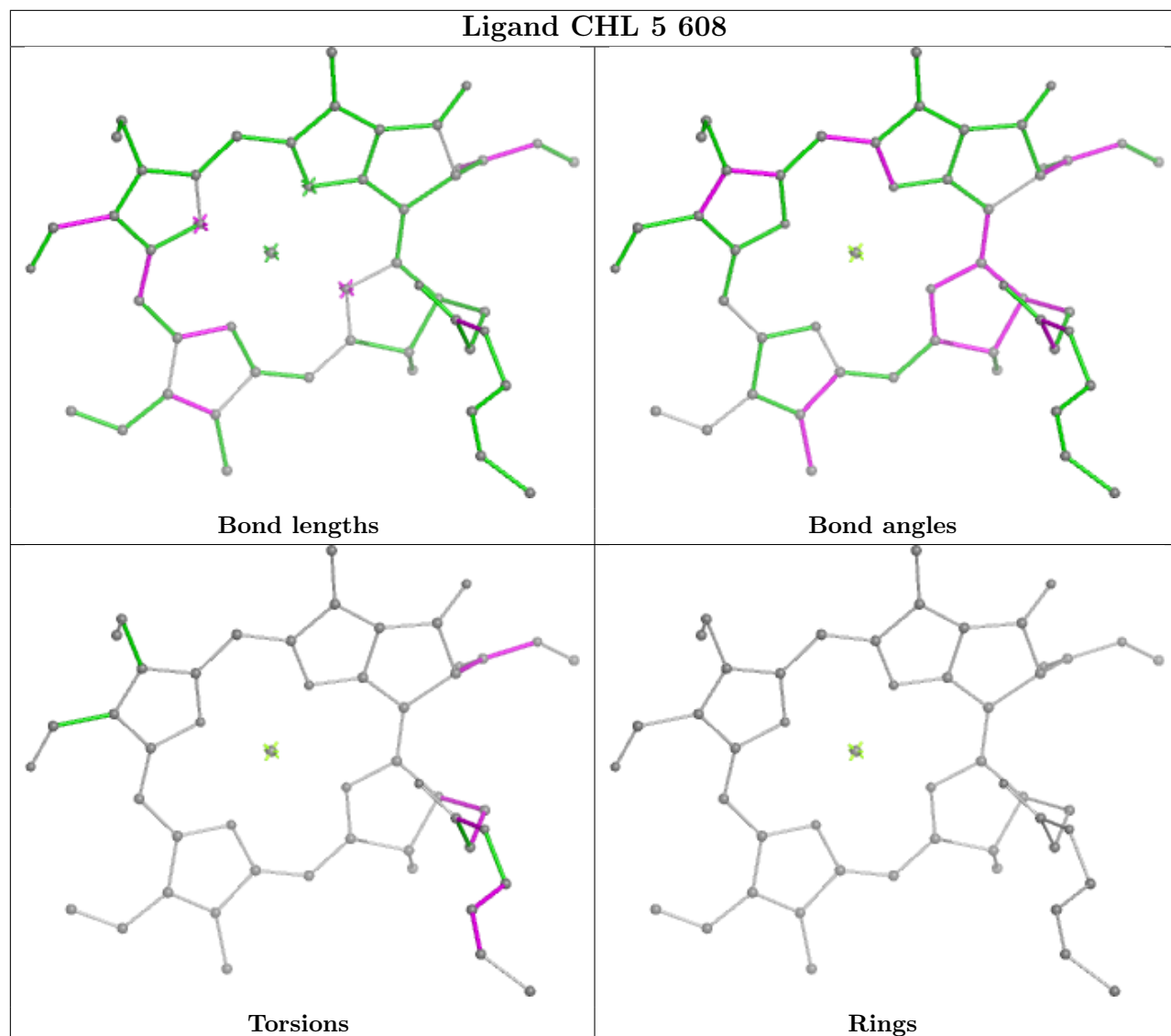


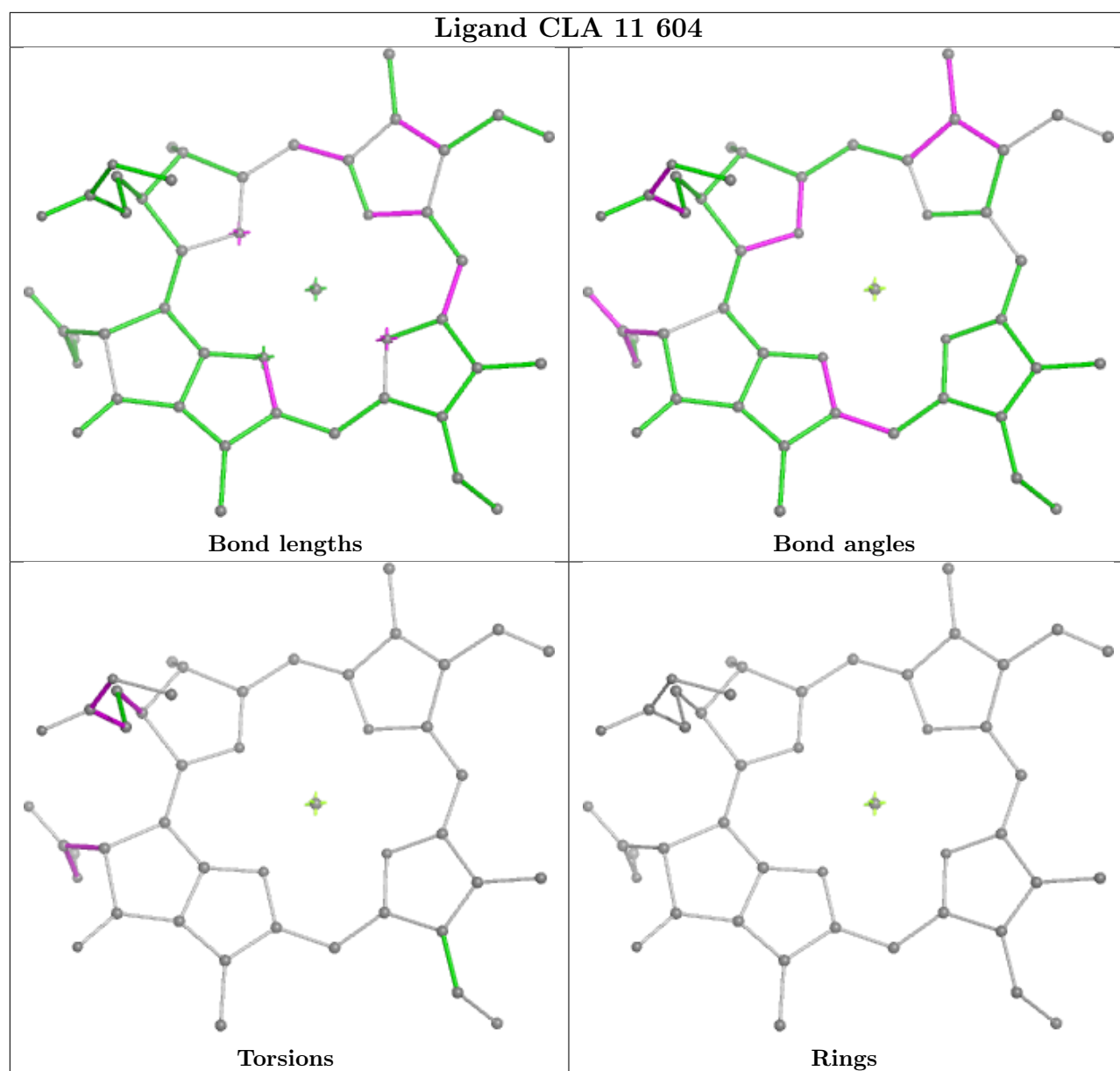


Ligand CLA S 612

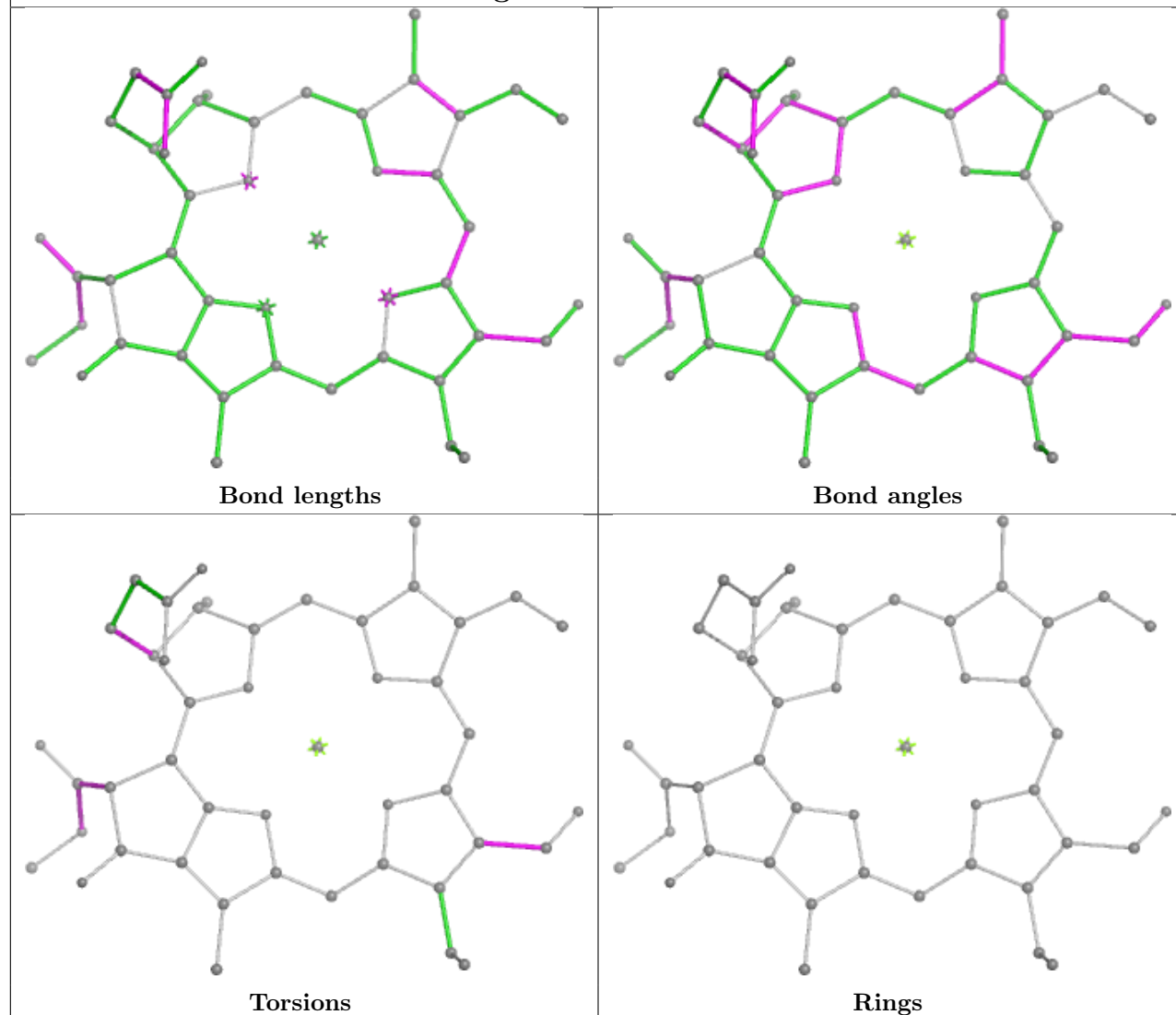


Ligand CHL 5 608

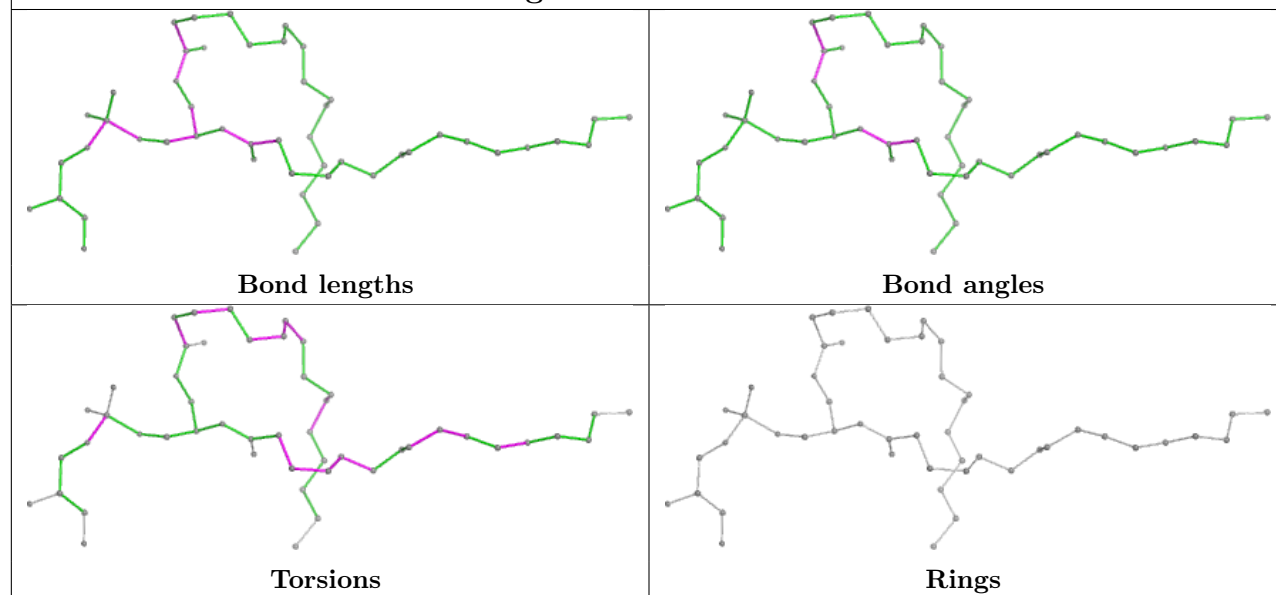


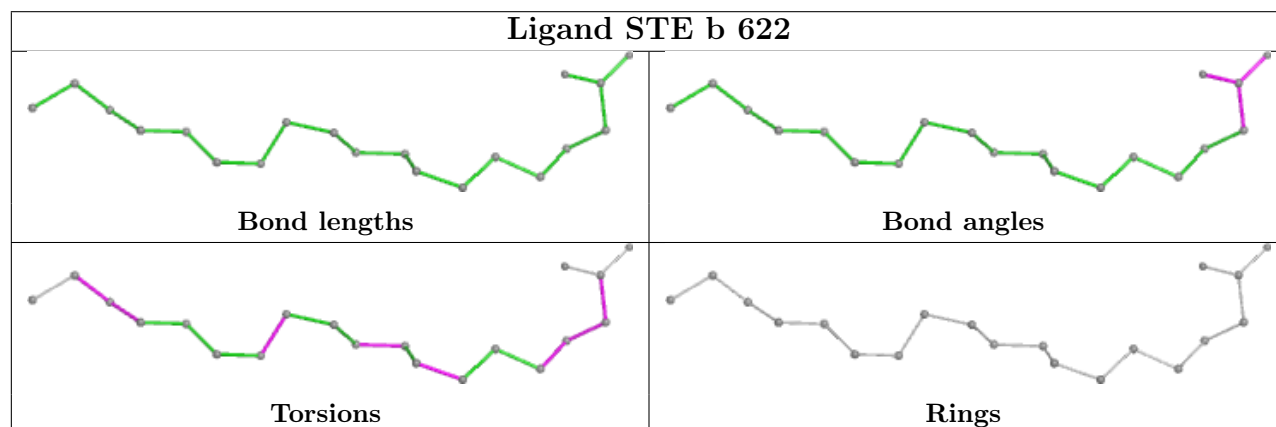
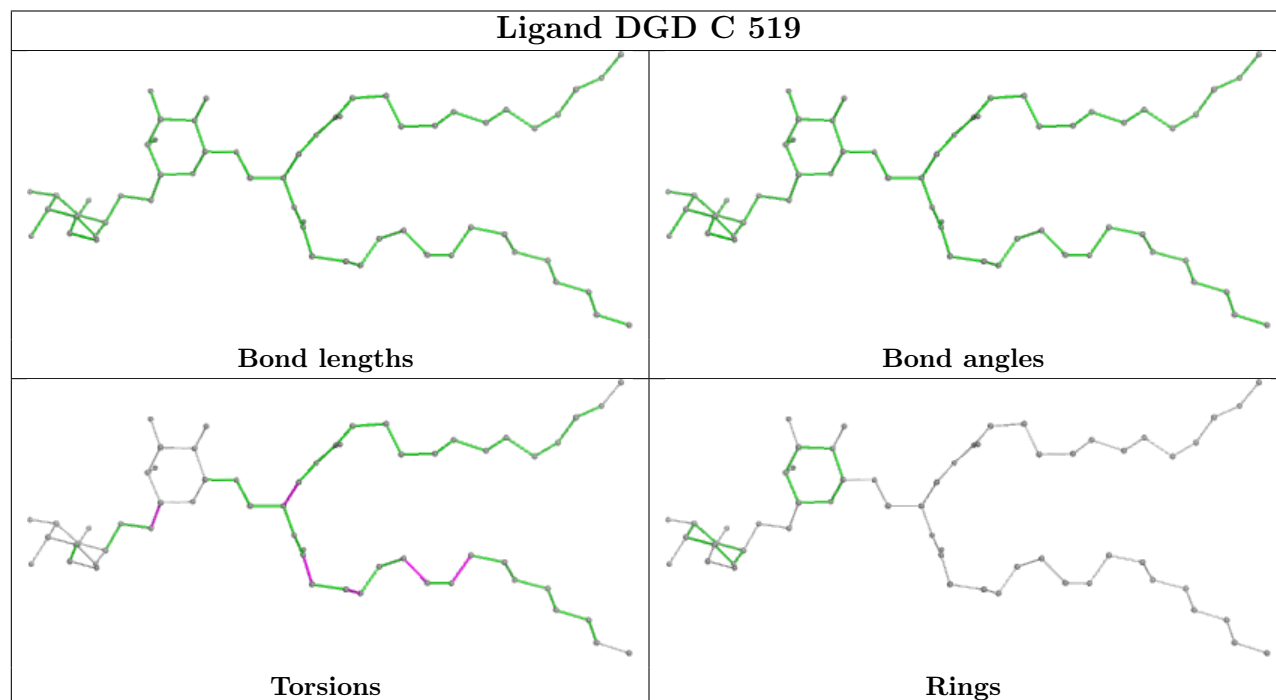
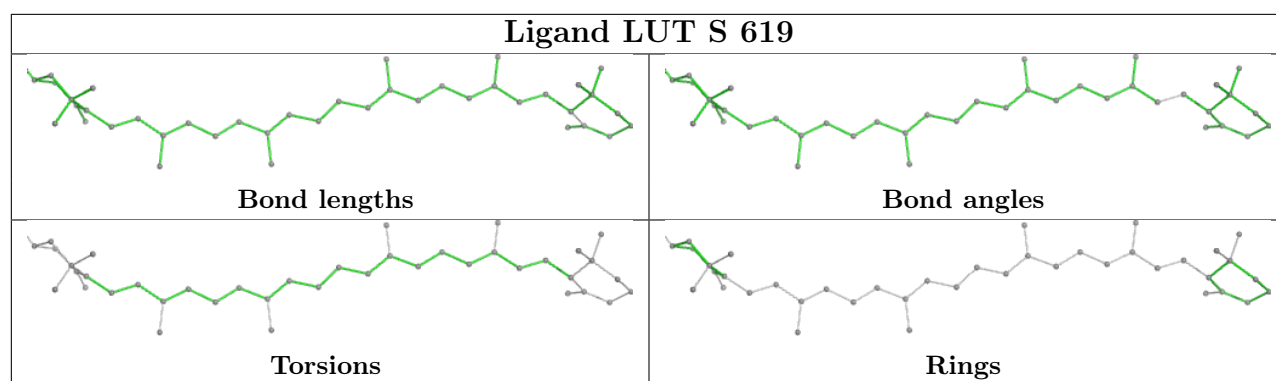


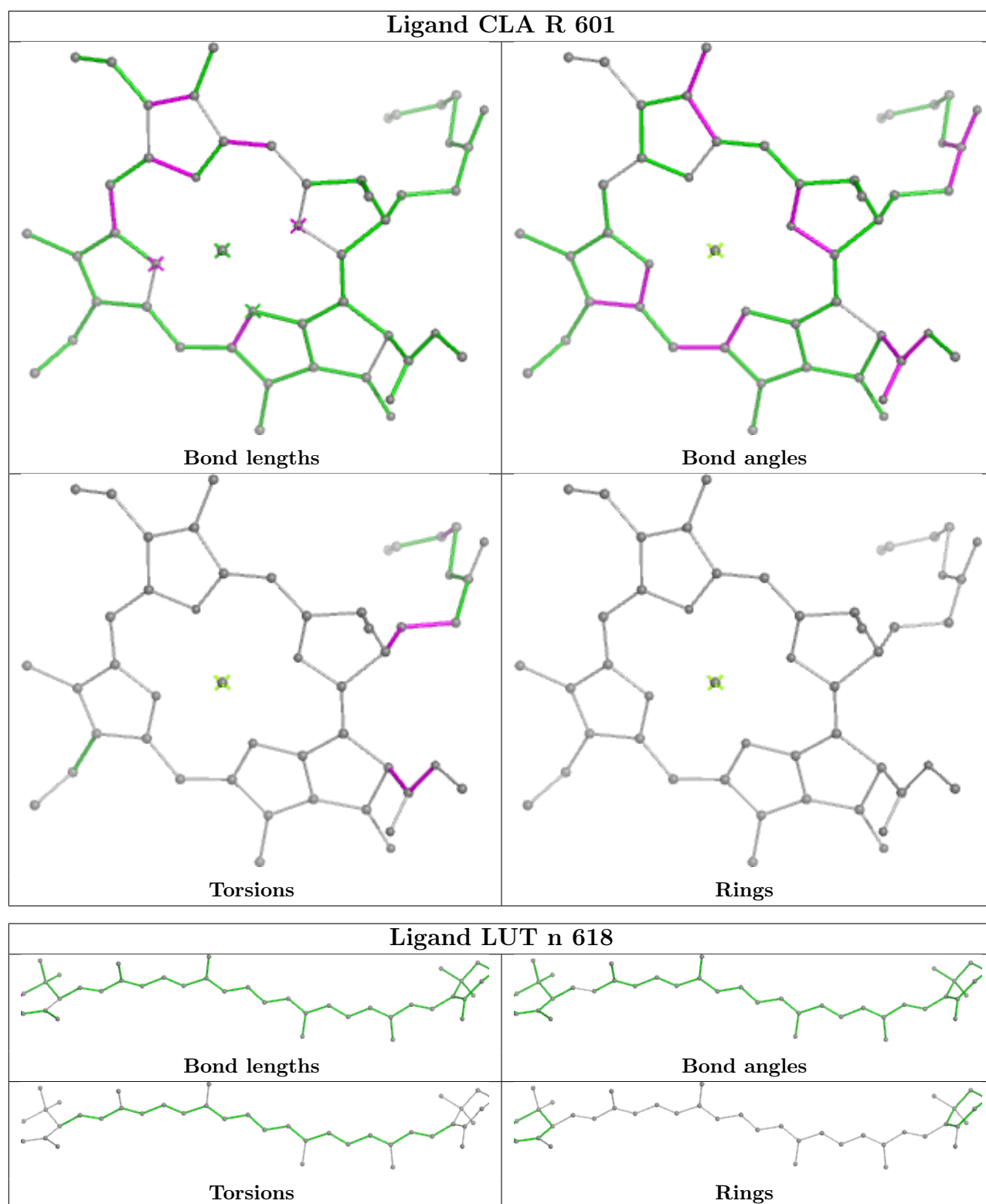
Ligand CHL 5 605

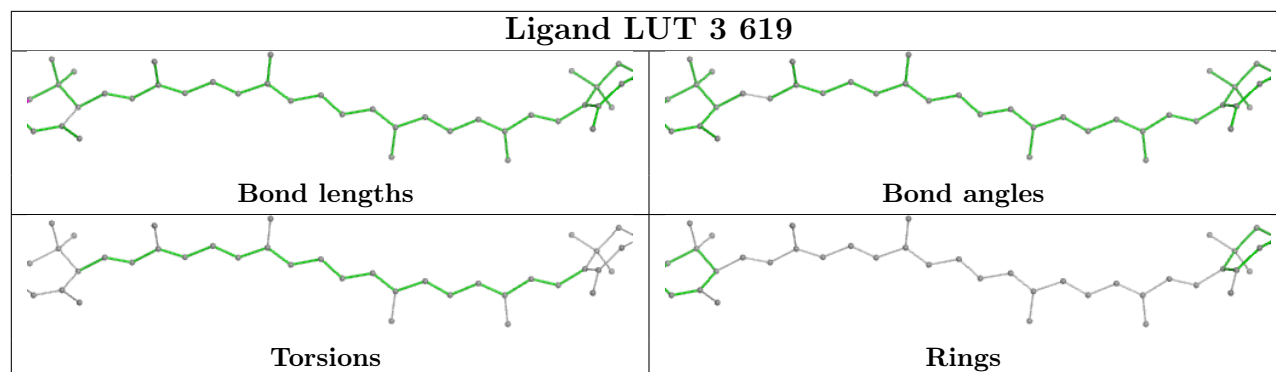
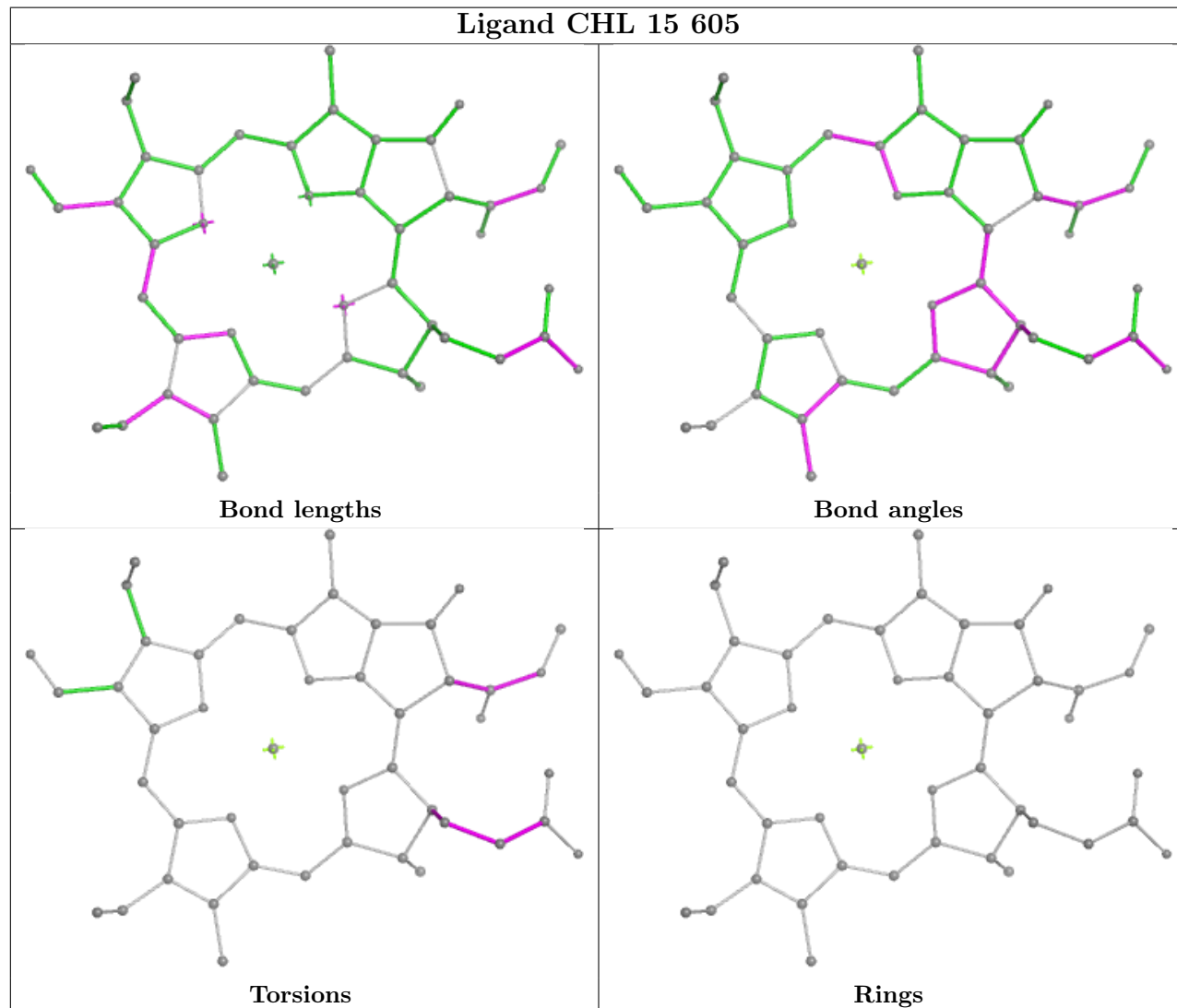


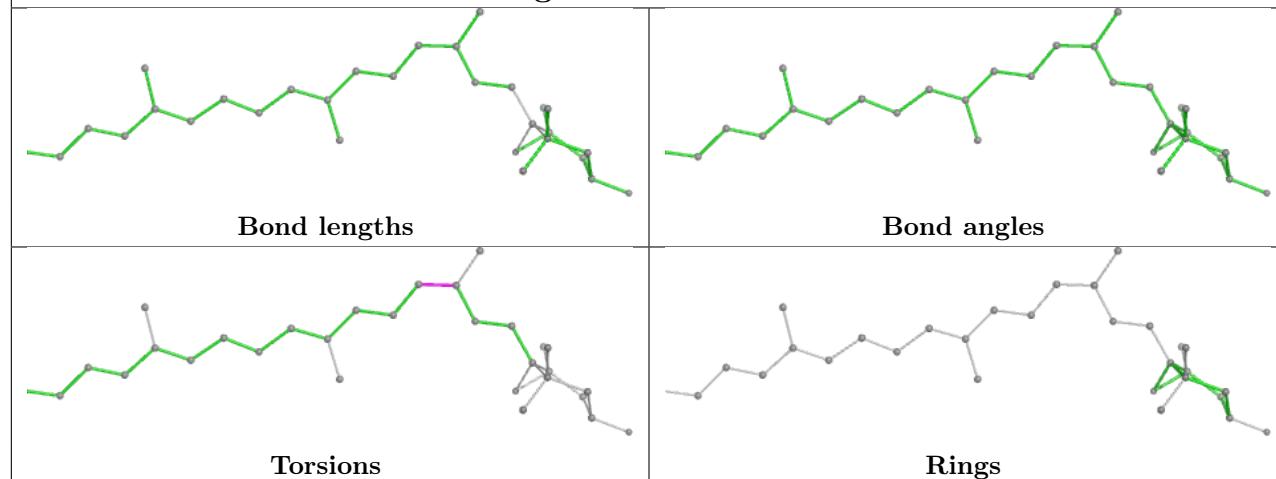
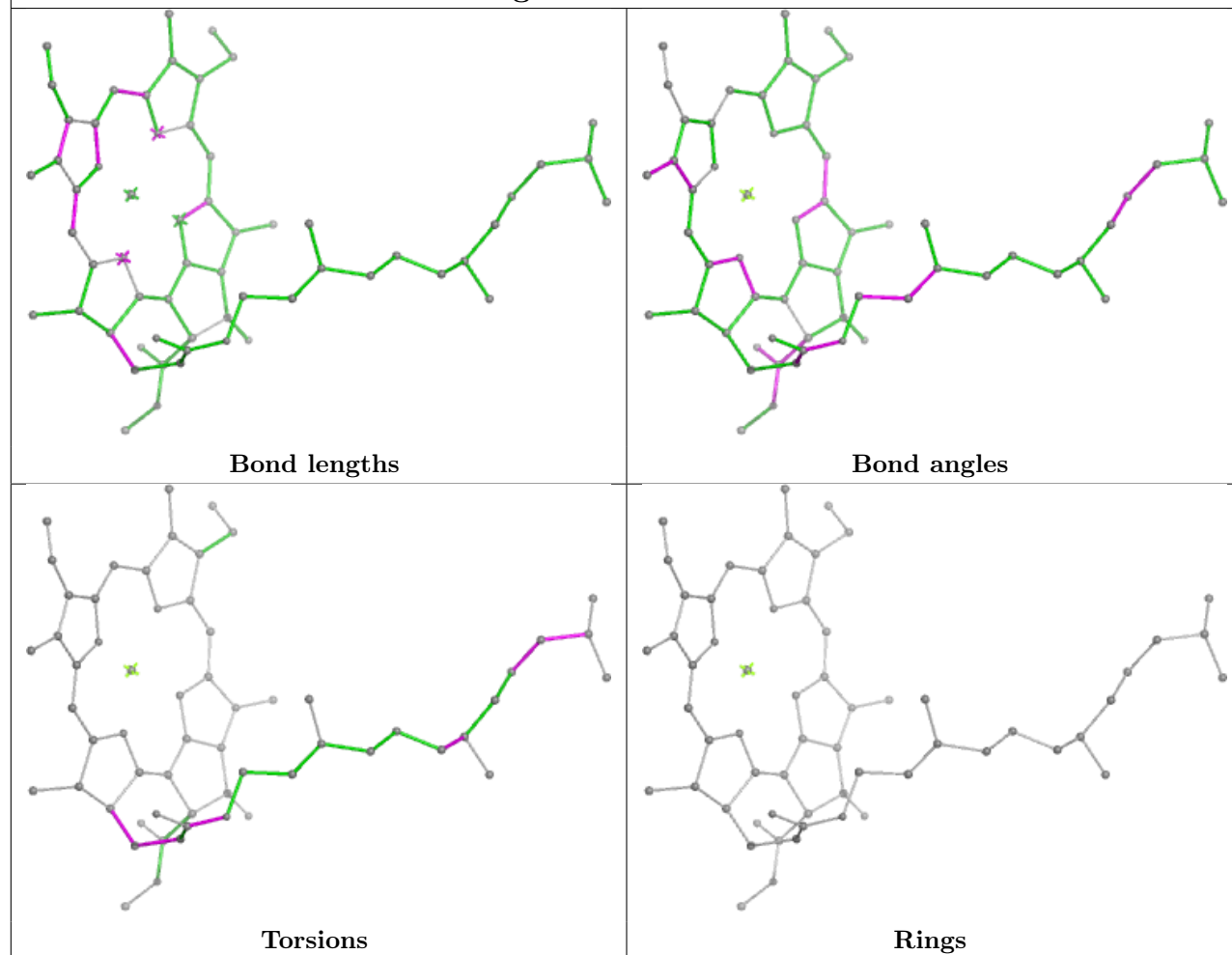
Ligand LHG 11 615

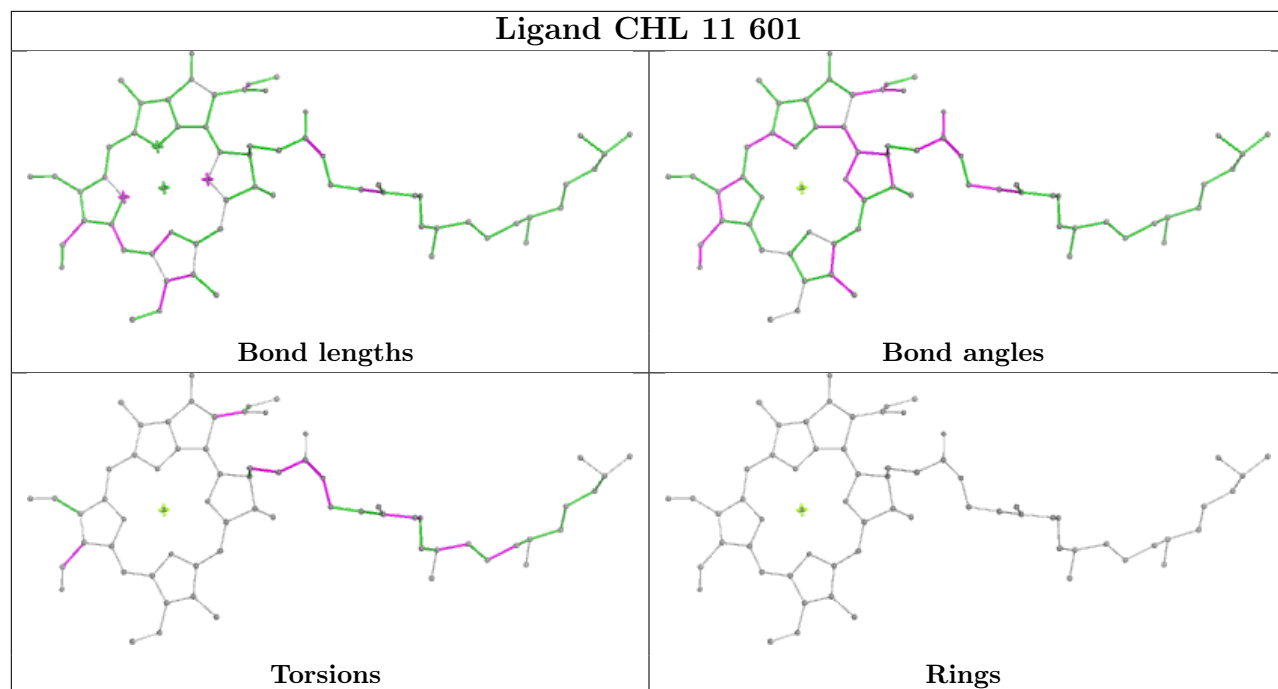




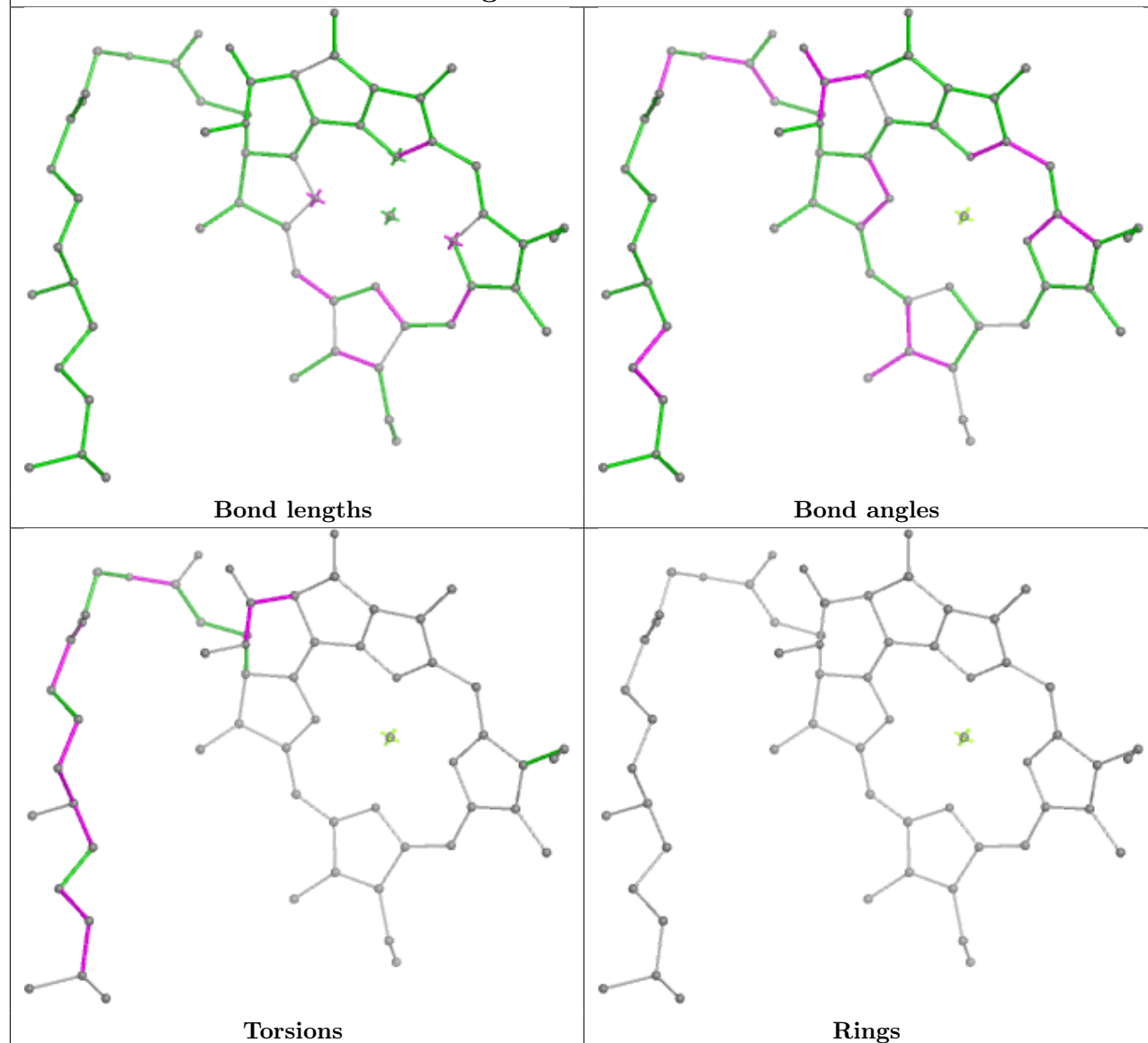


Ligand LUT 3 619**Ligand CHL 15 605**

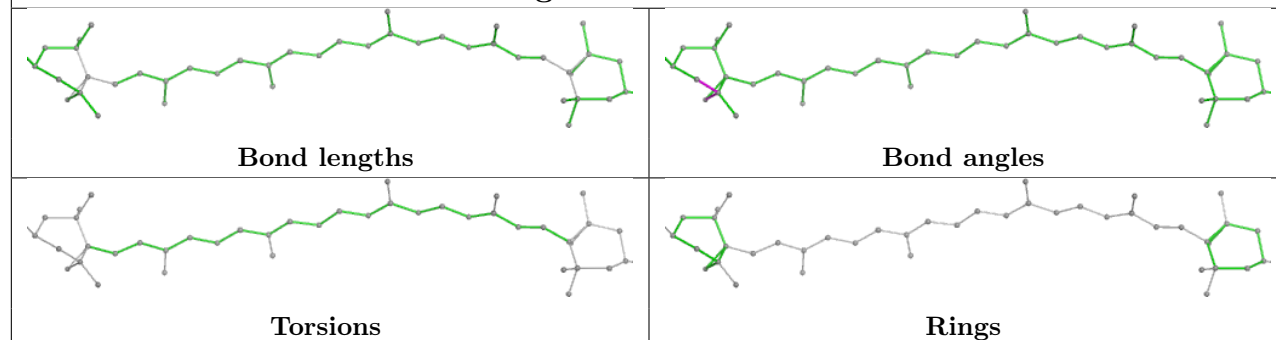
Ligand NEX 5 616**Ligand CLA N 611**

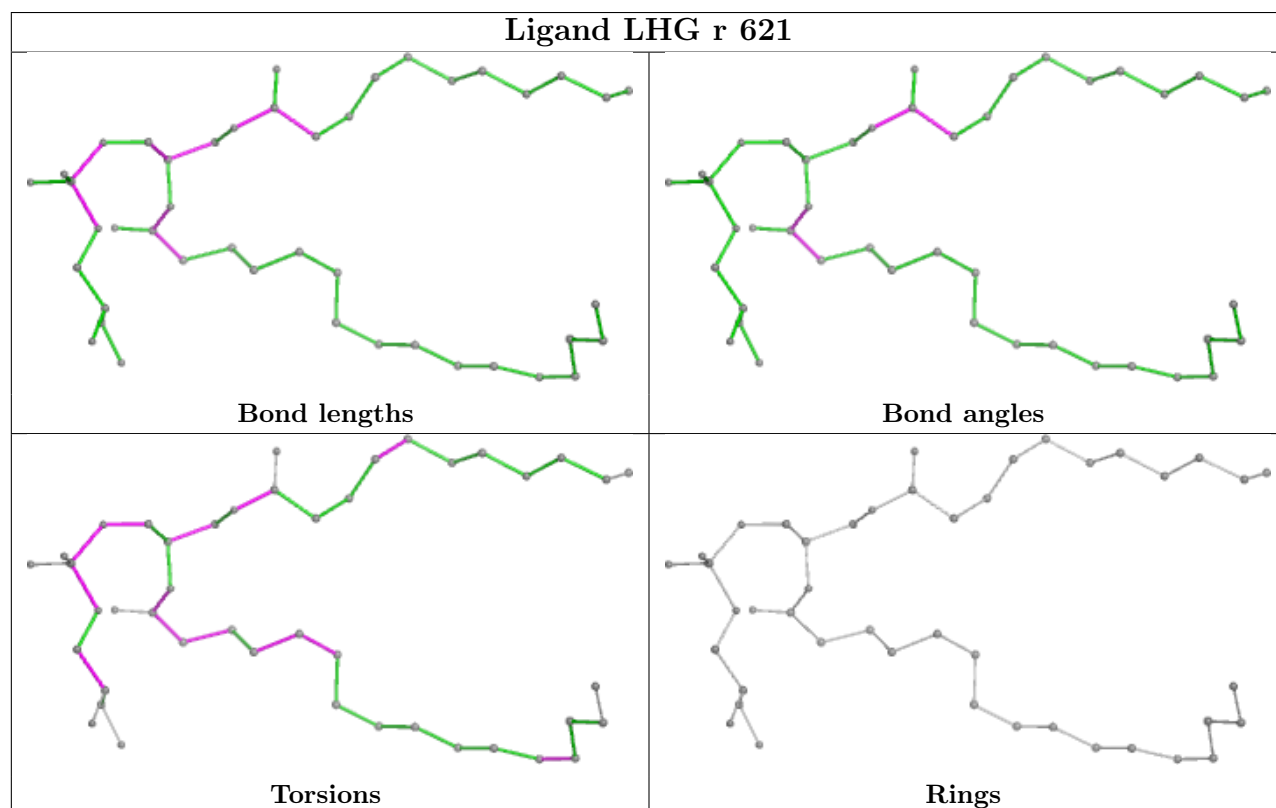
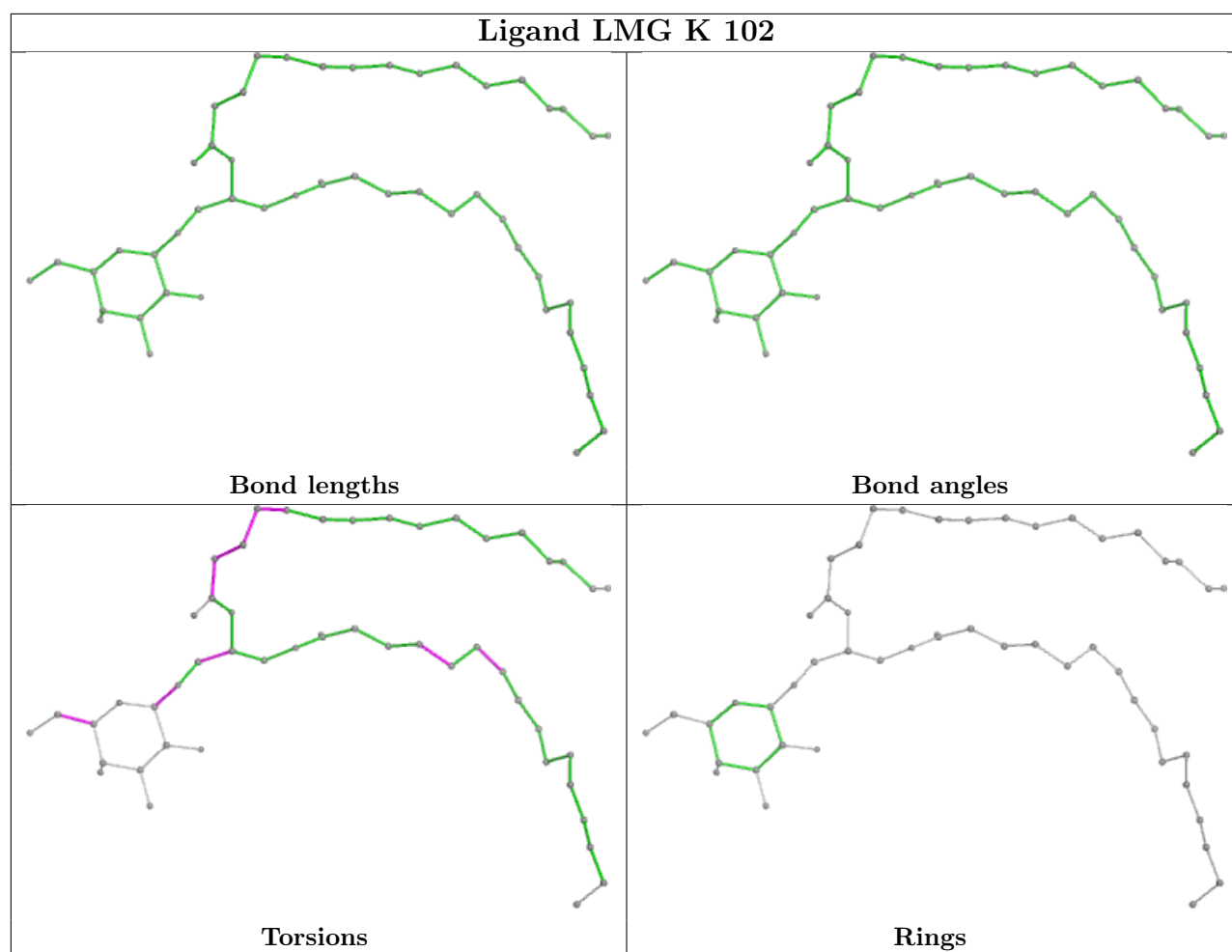


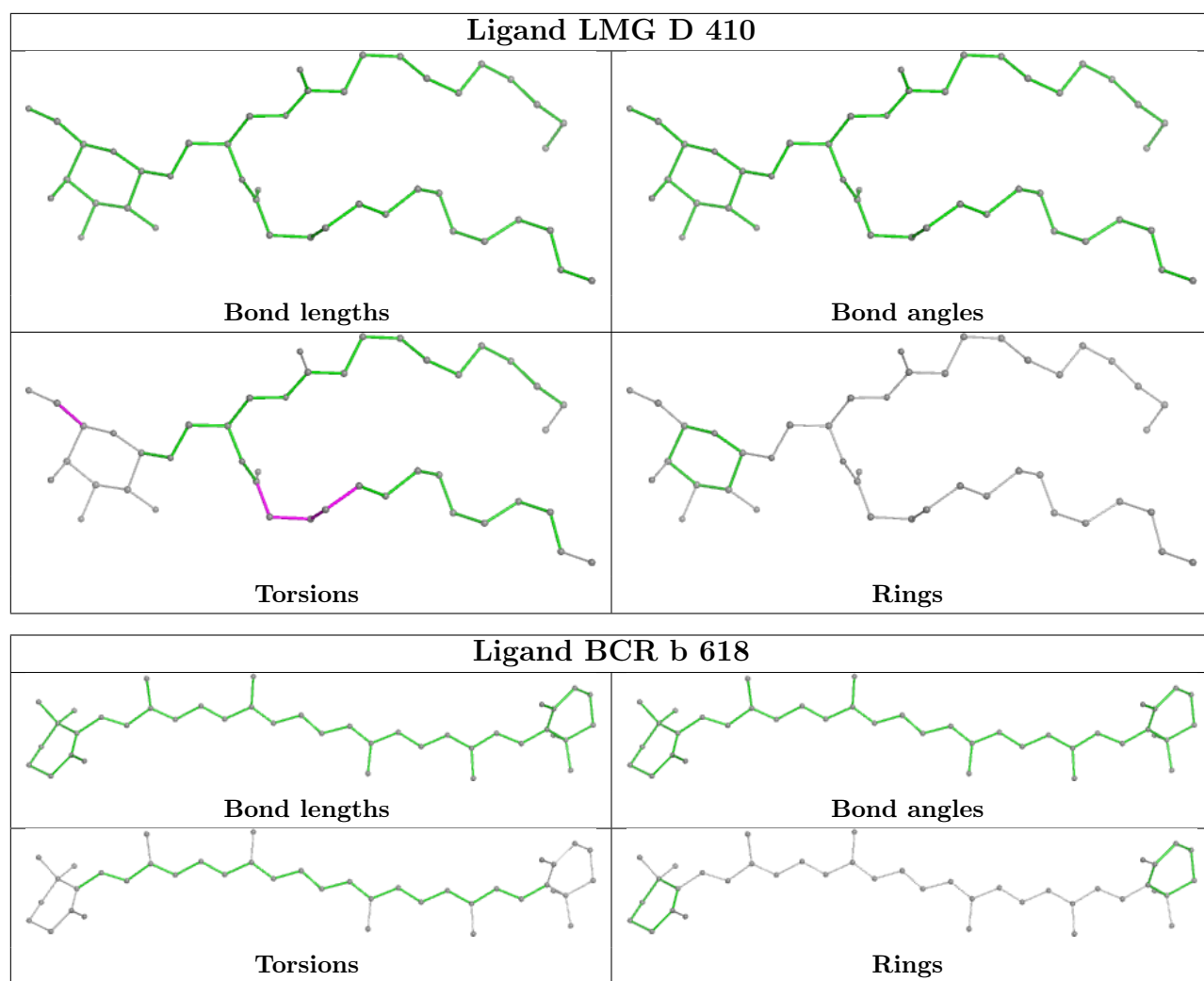
Ligand CLA b 616

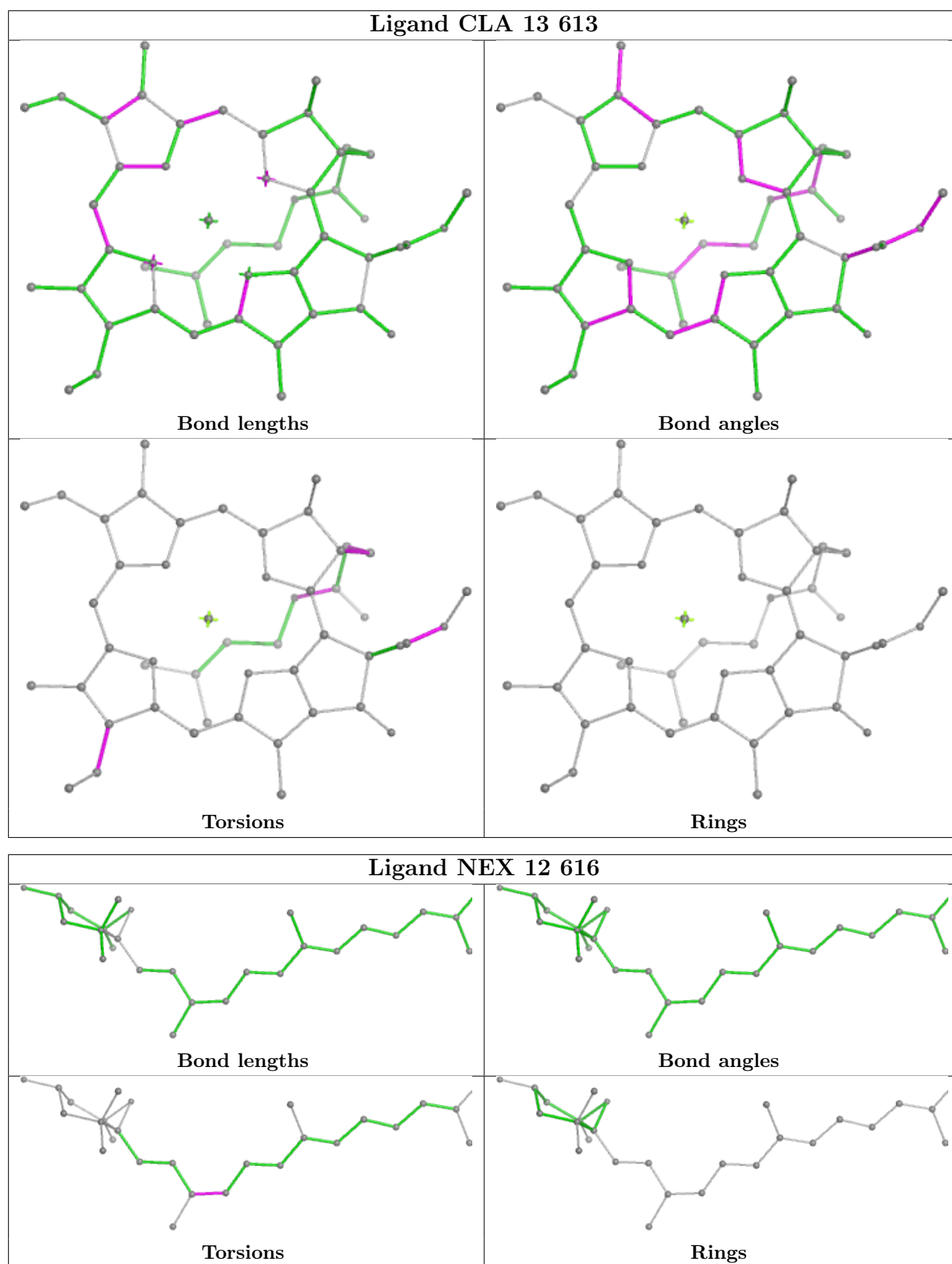


Ligand XAT 6 620

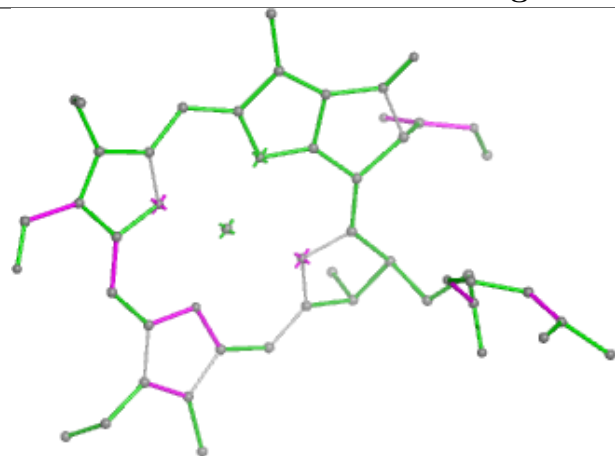




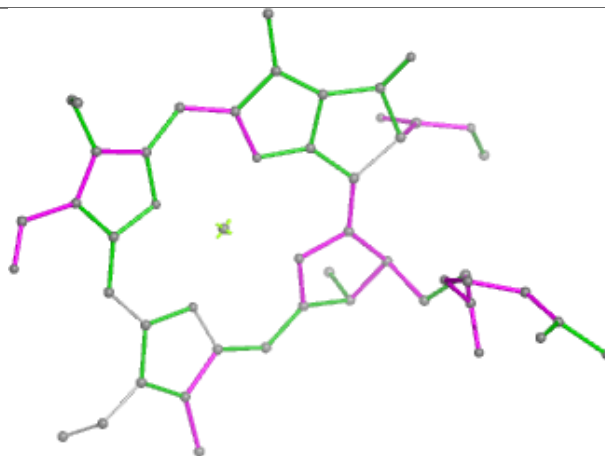




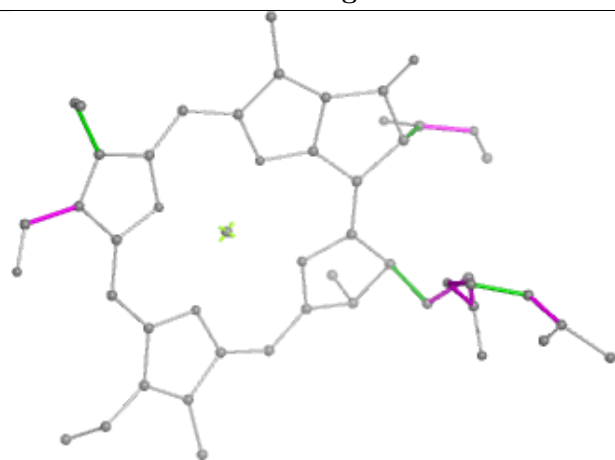
Ligand CHL 11 608



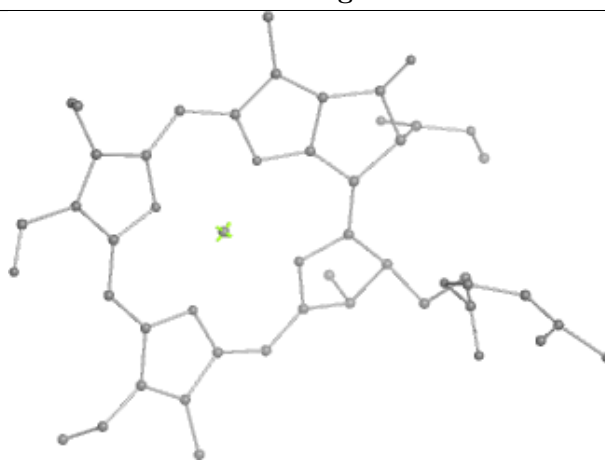
Bond lengths



Bond angles

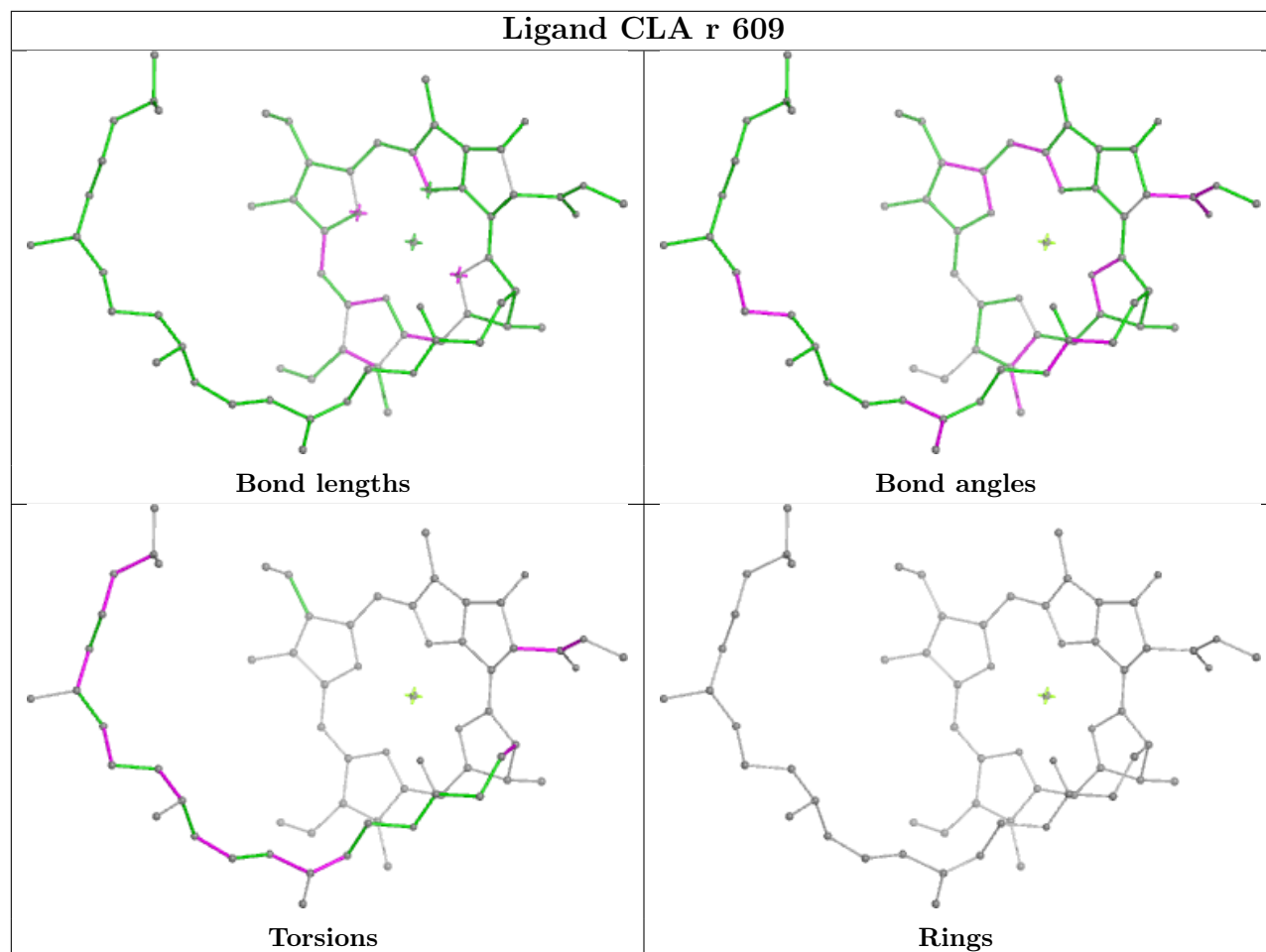


Torsions

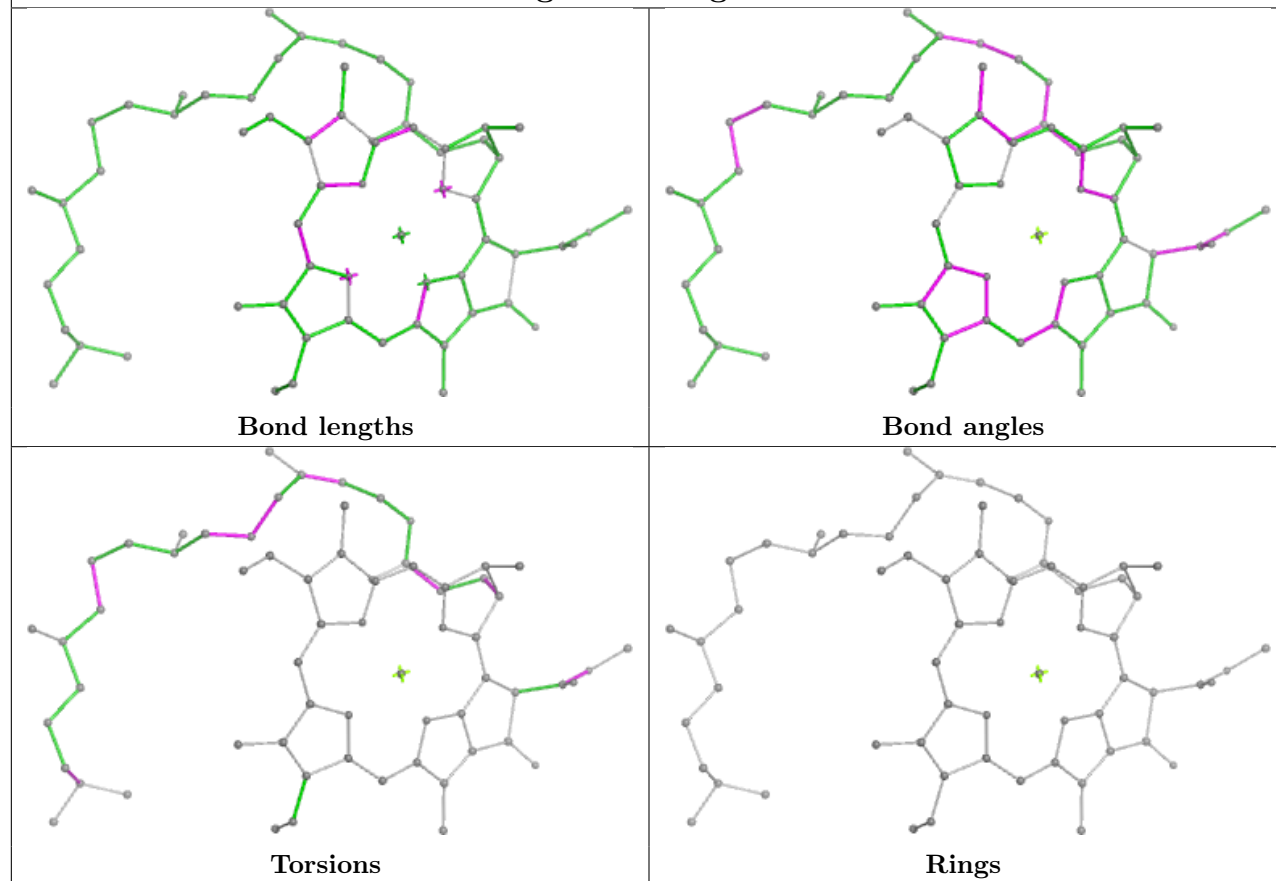


Rings

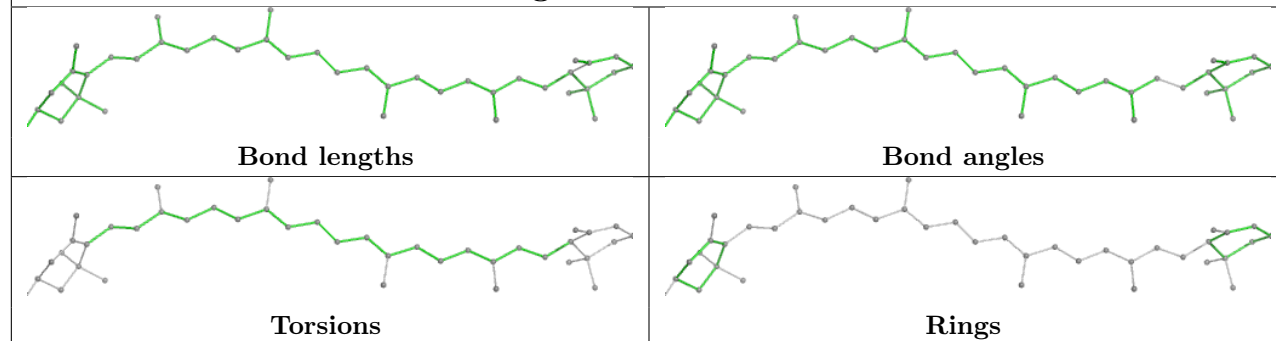
Ligand CLA r 609



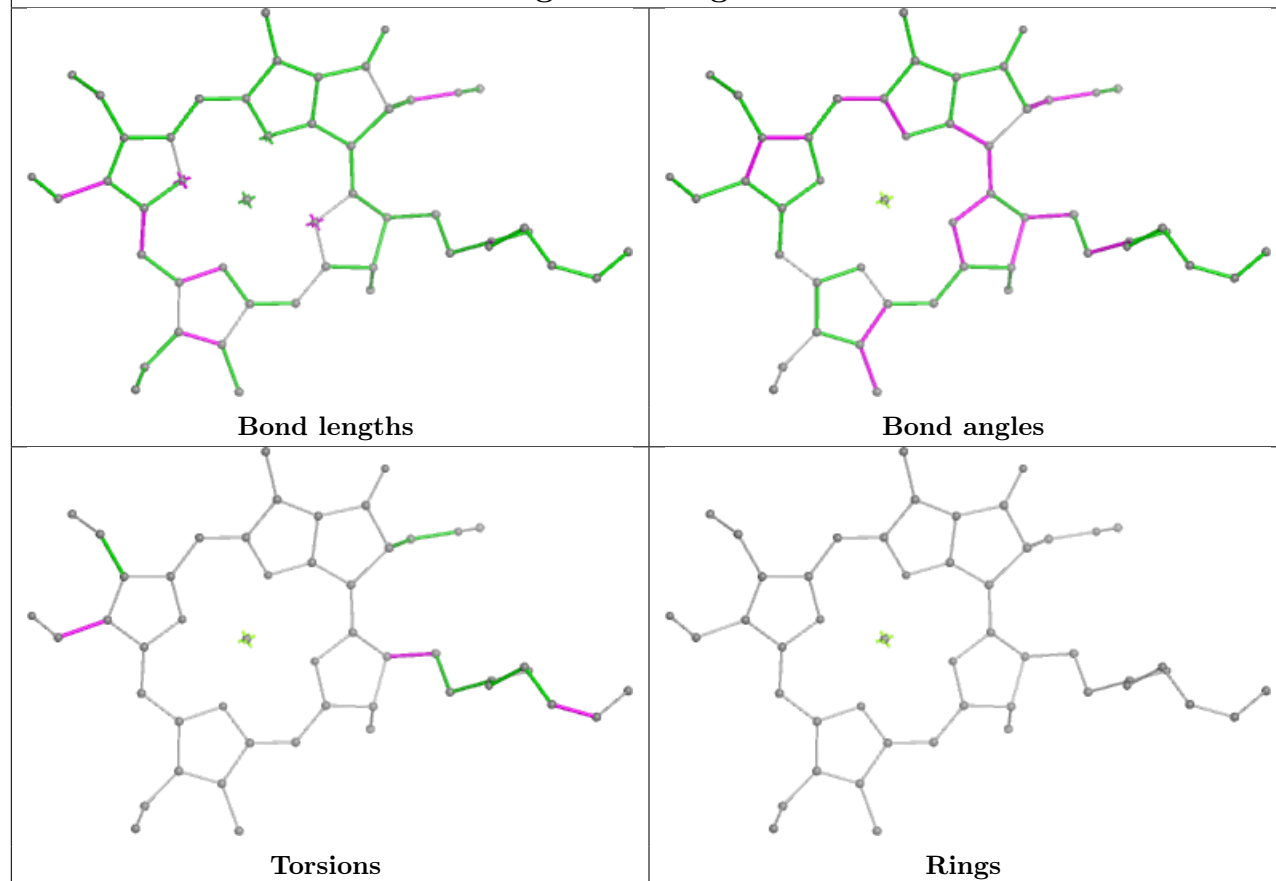
Ligand CLA g 610



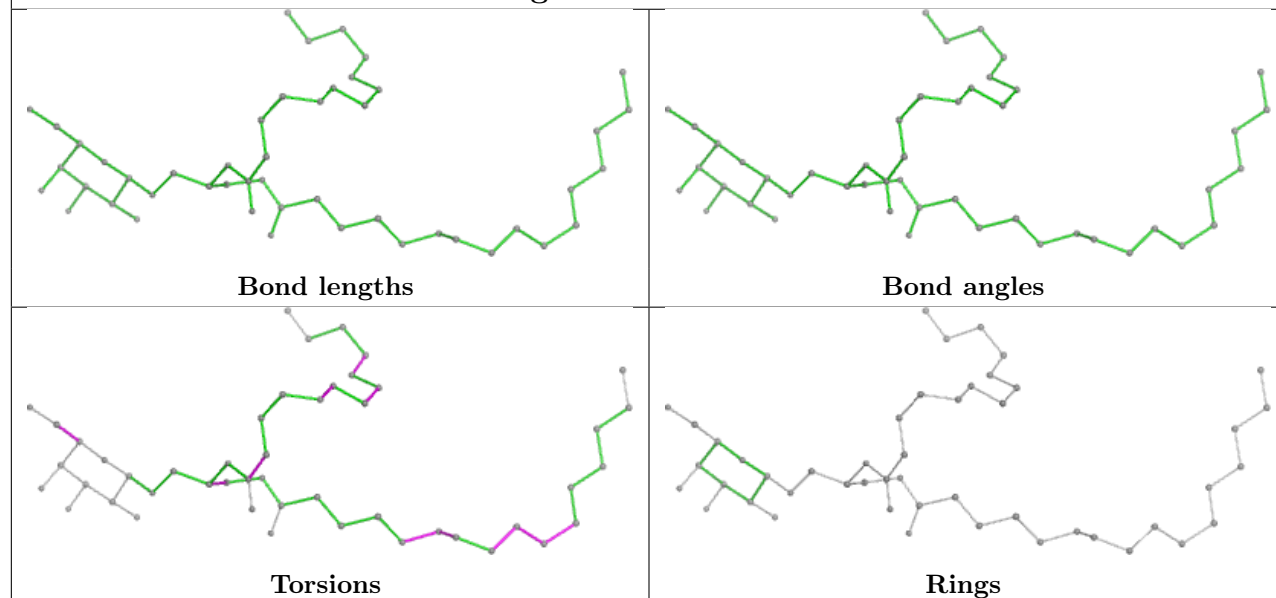
Ligand LUT R 615

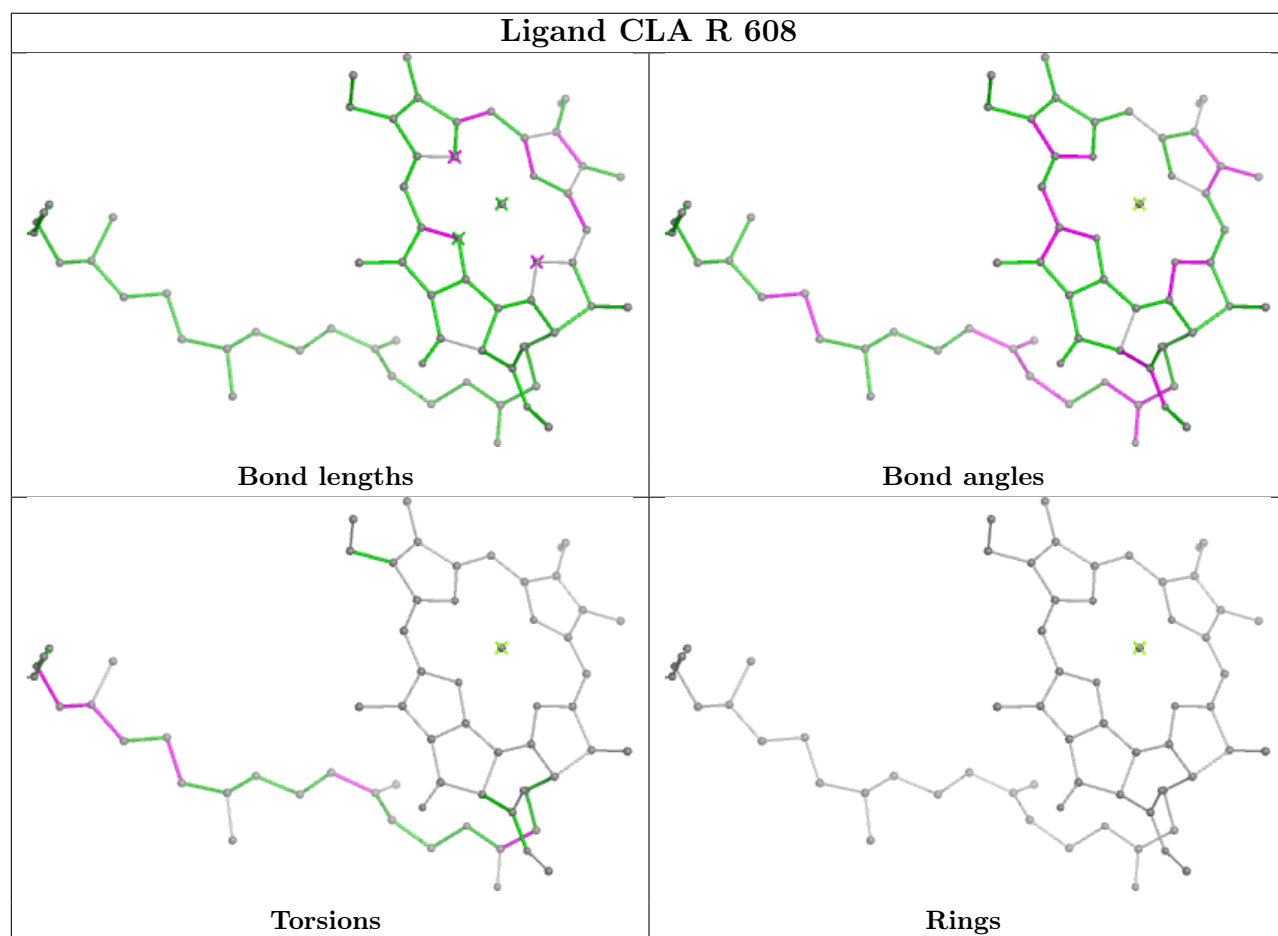
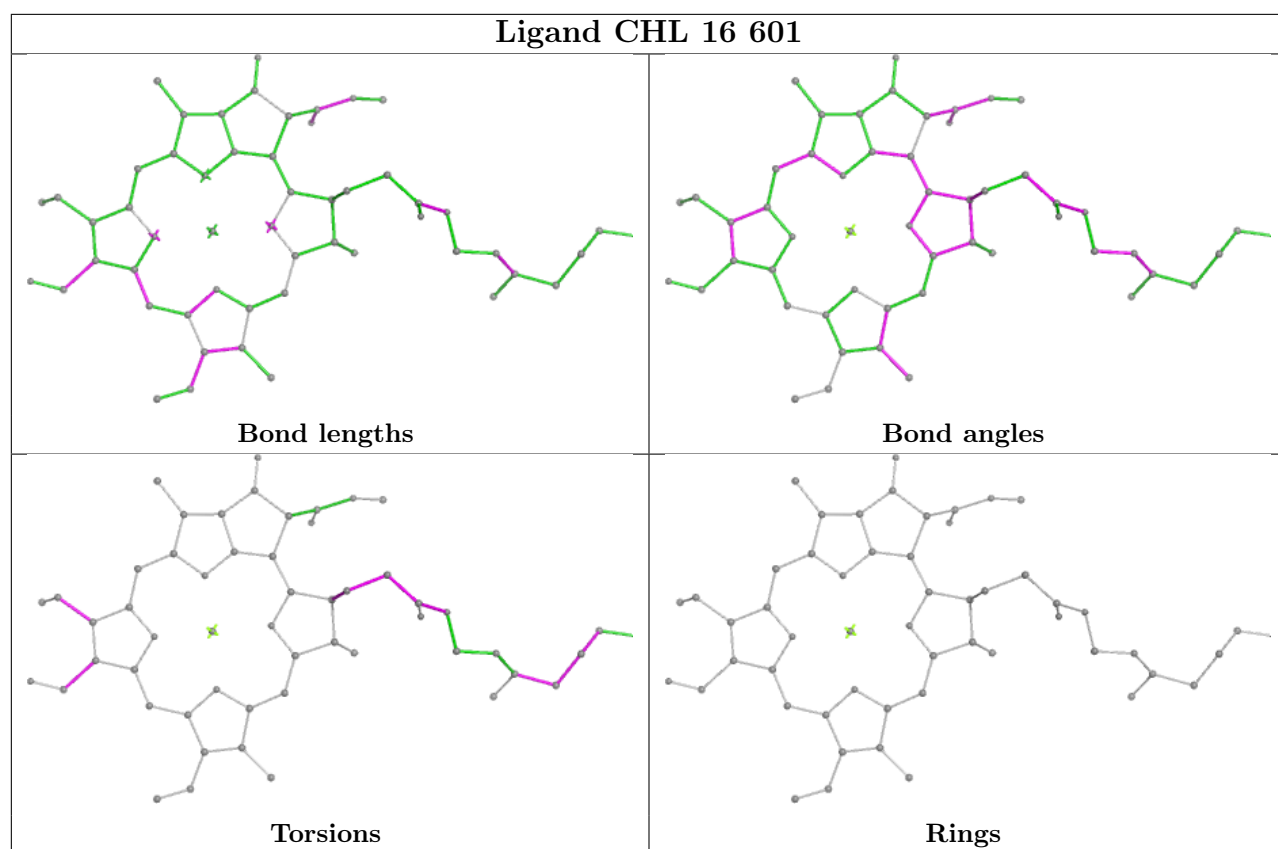


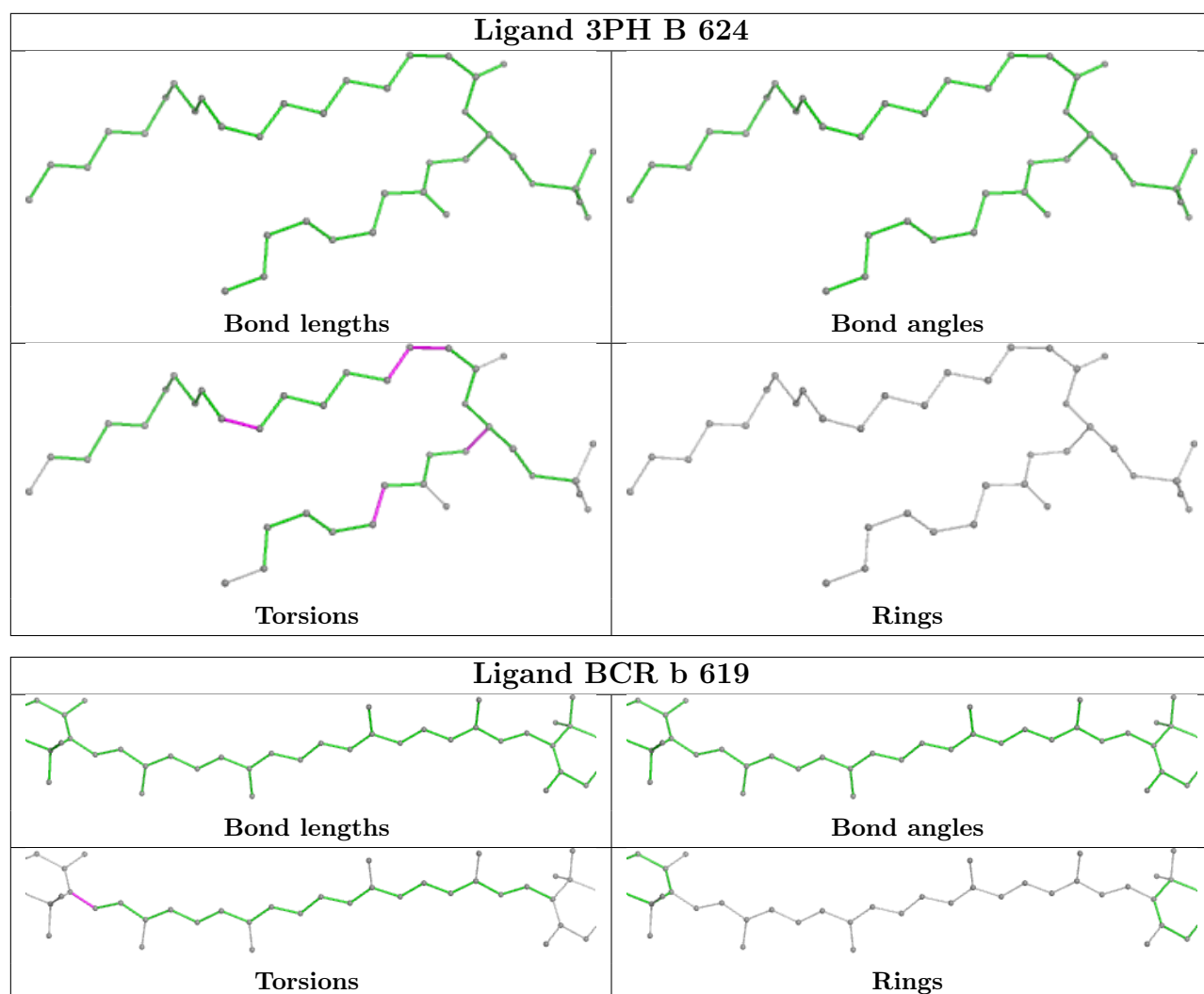
Ligand CHL g 606

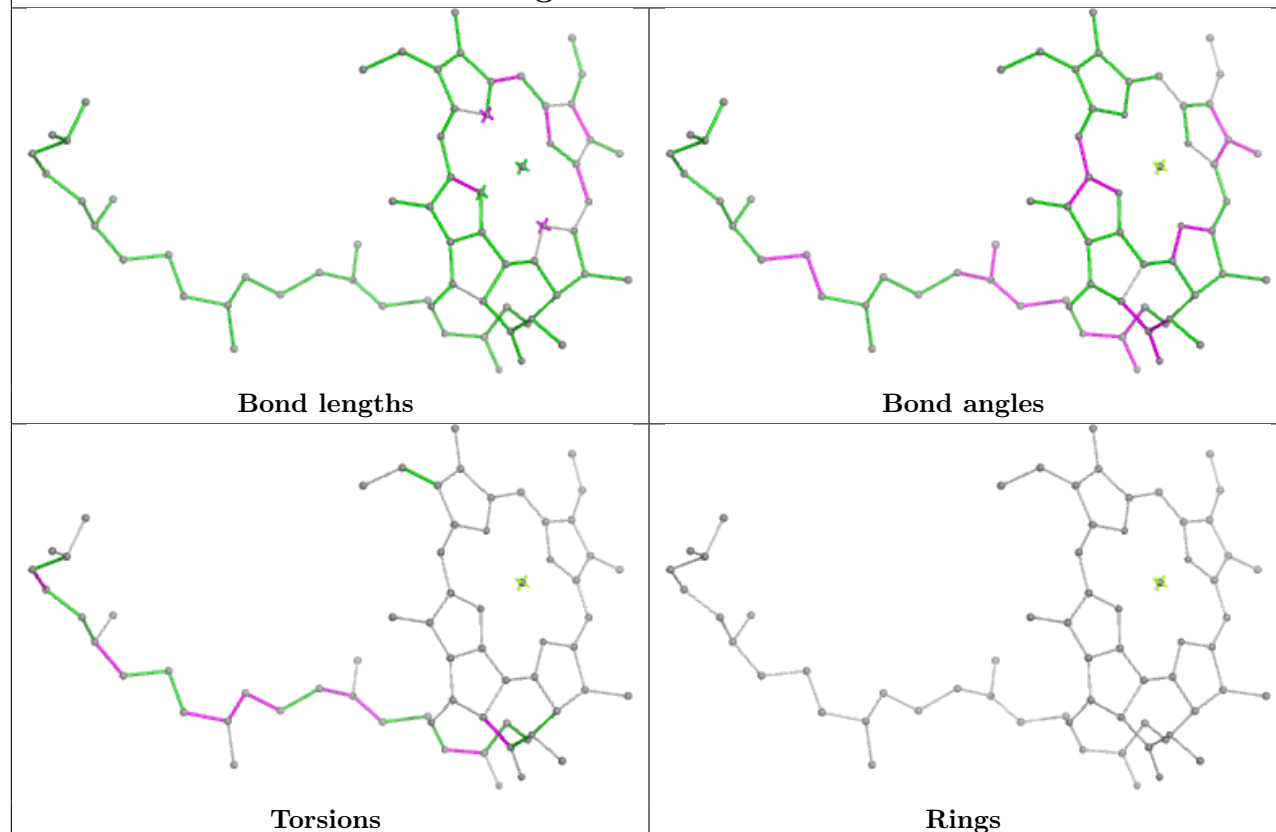
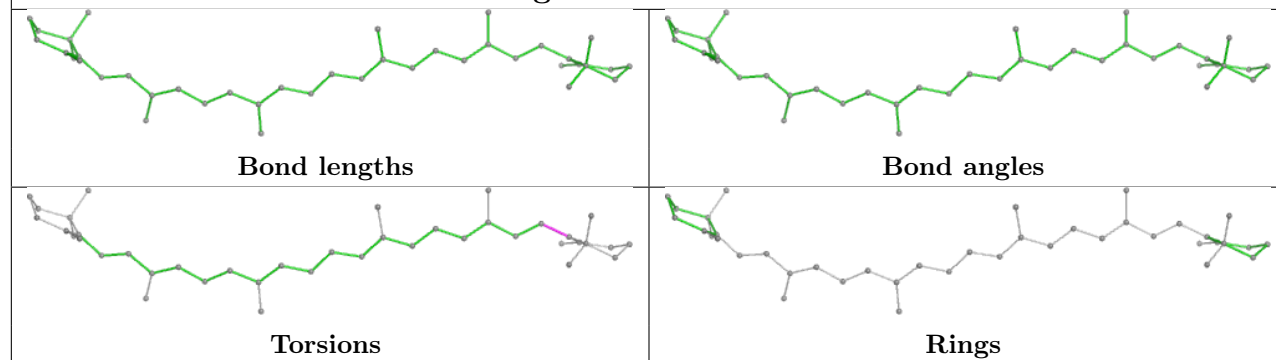


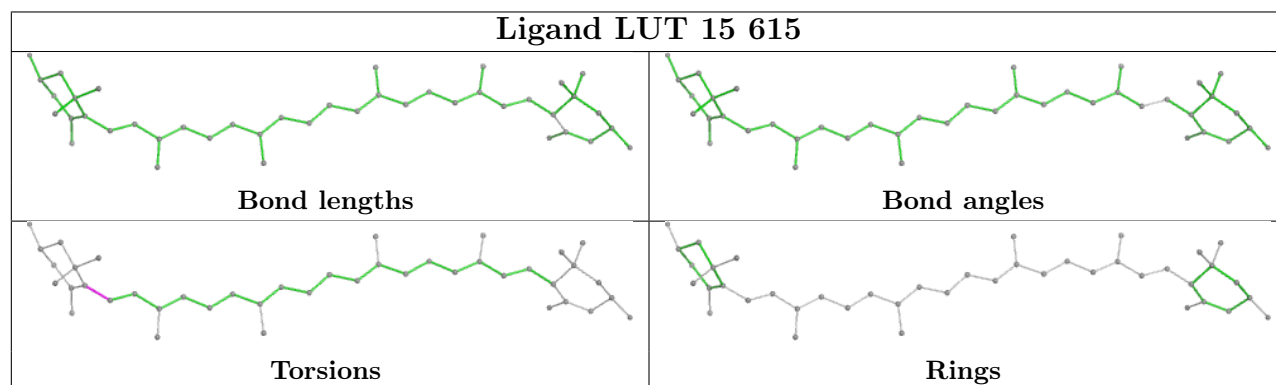
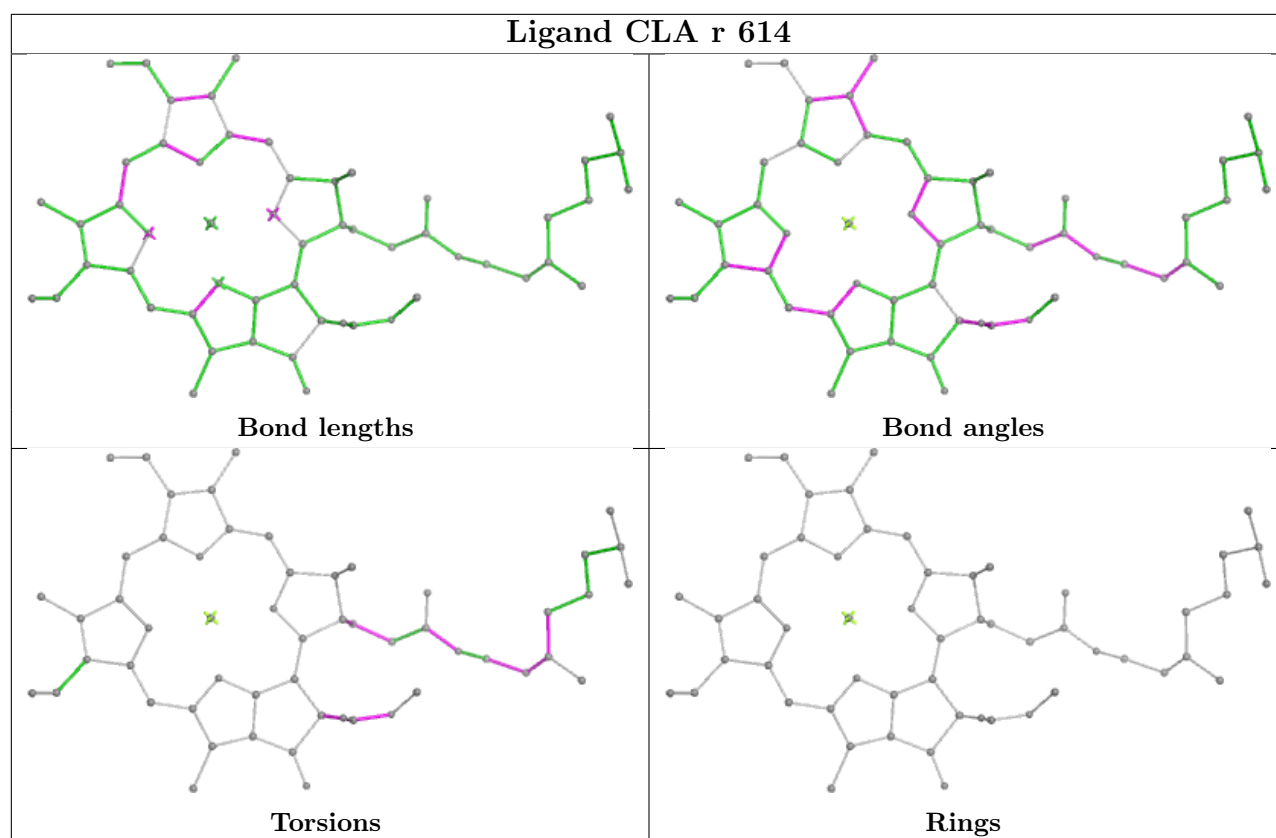
Ligand LMG d 415



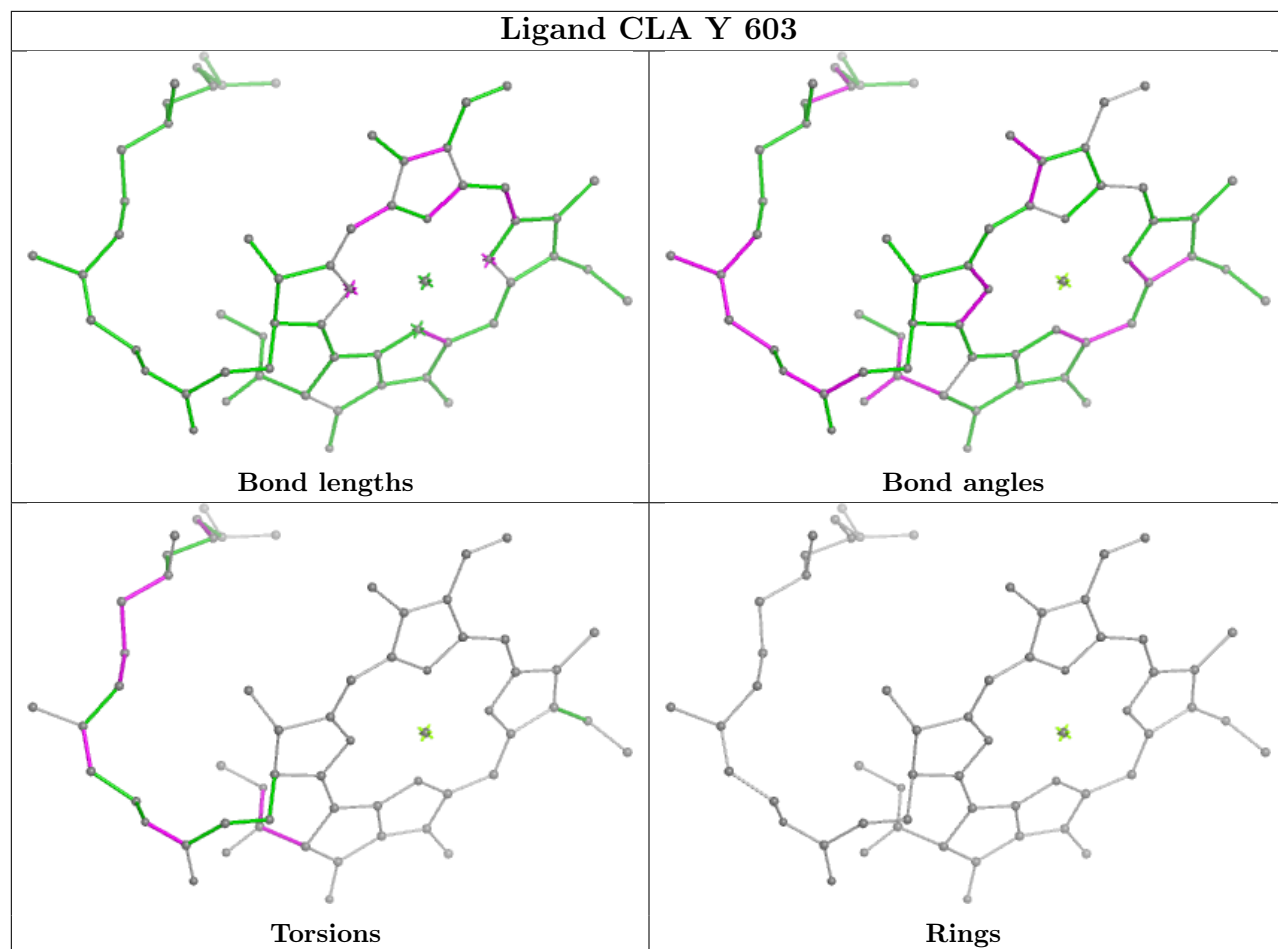


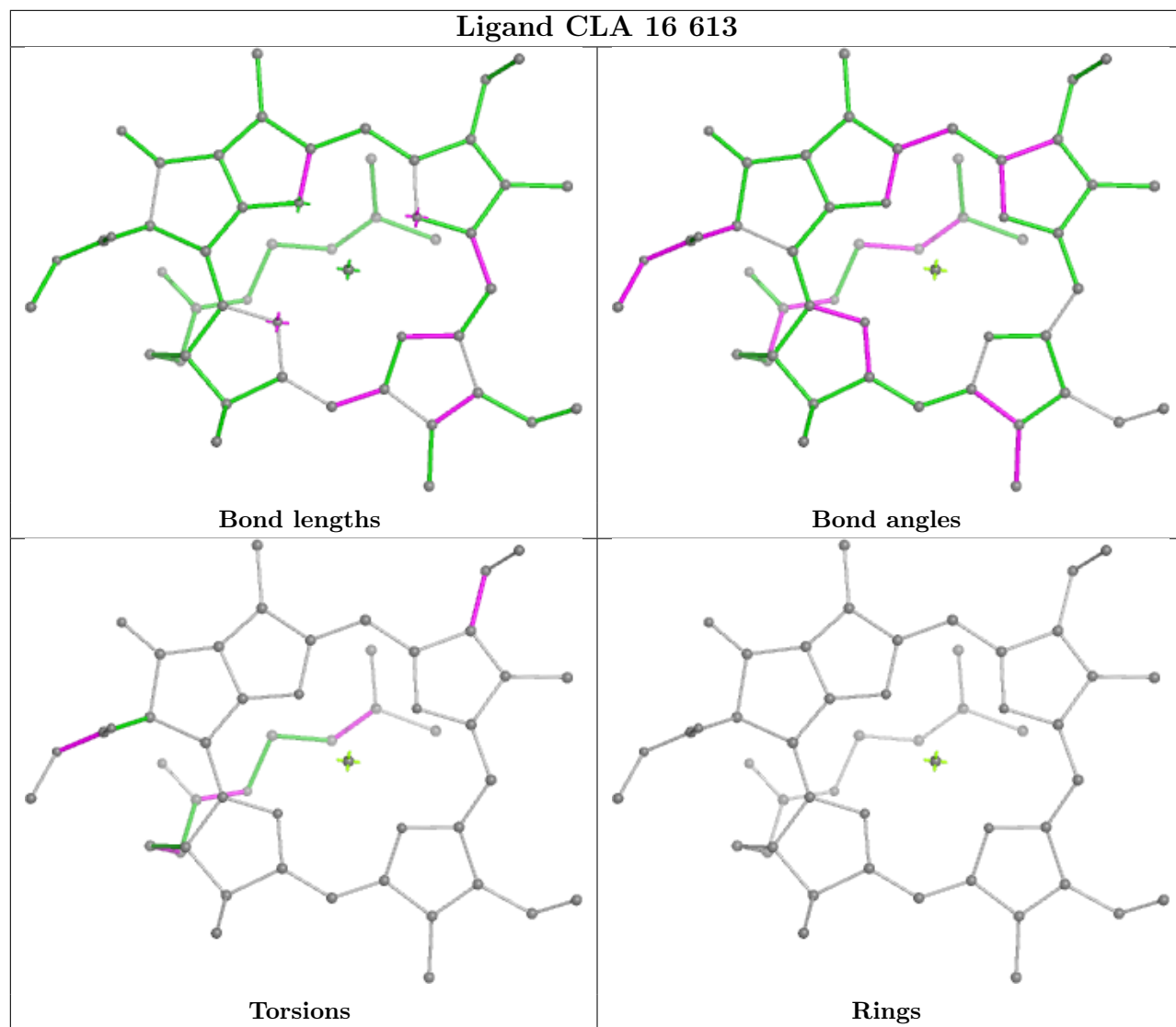


Ligand CLA S 611**Ligand BCR h 102**

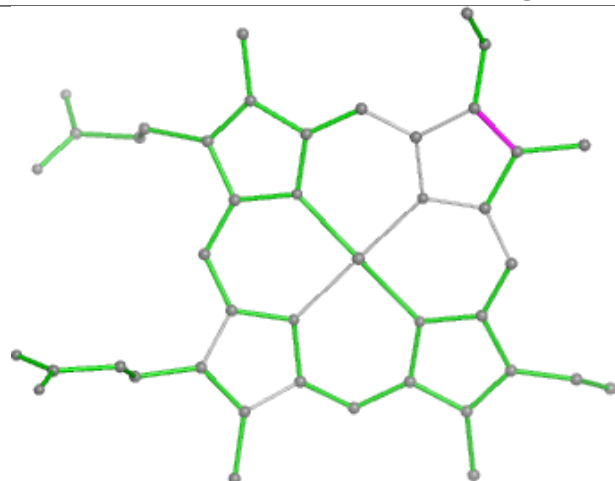


Ligand CLA Y 603

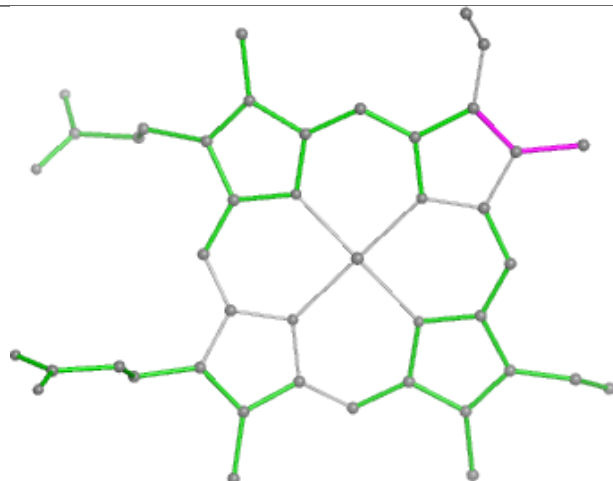




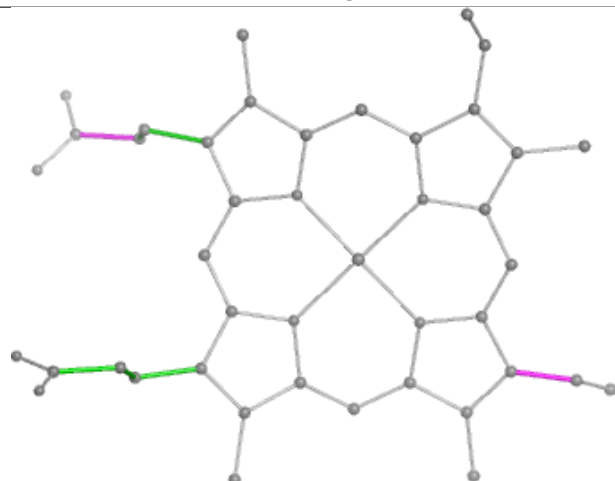
Ligand HEM f 101



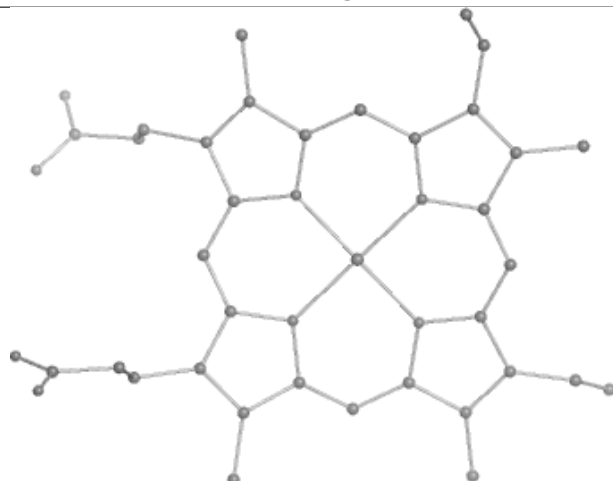
Bond lengths



Bond angles

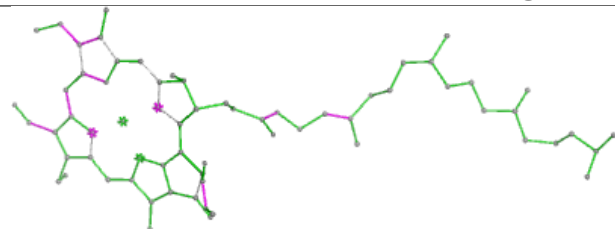


Torsions

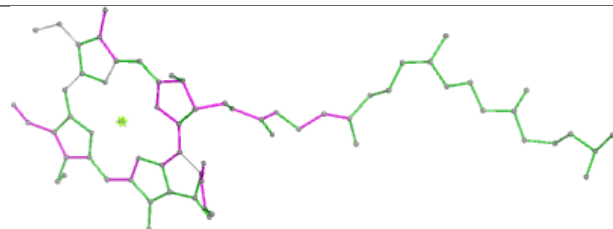


Rings

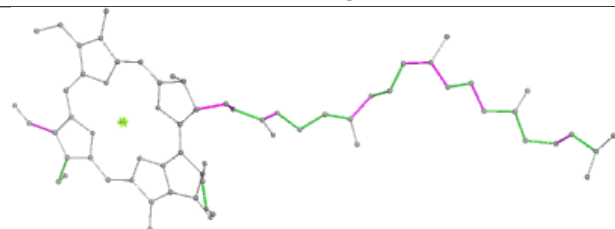
Ligand CHL 6 605



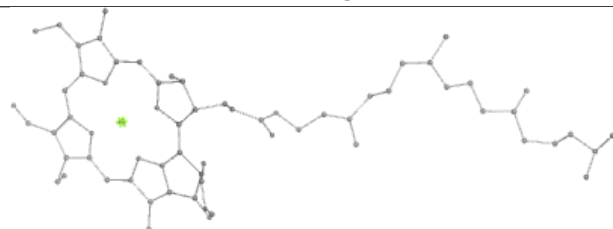
Bond lengths



Bond angles

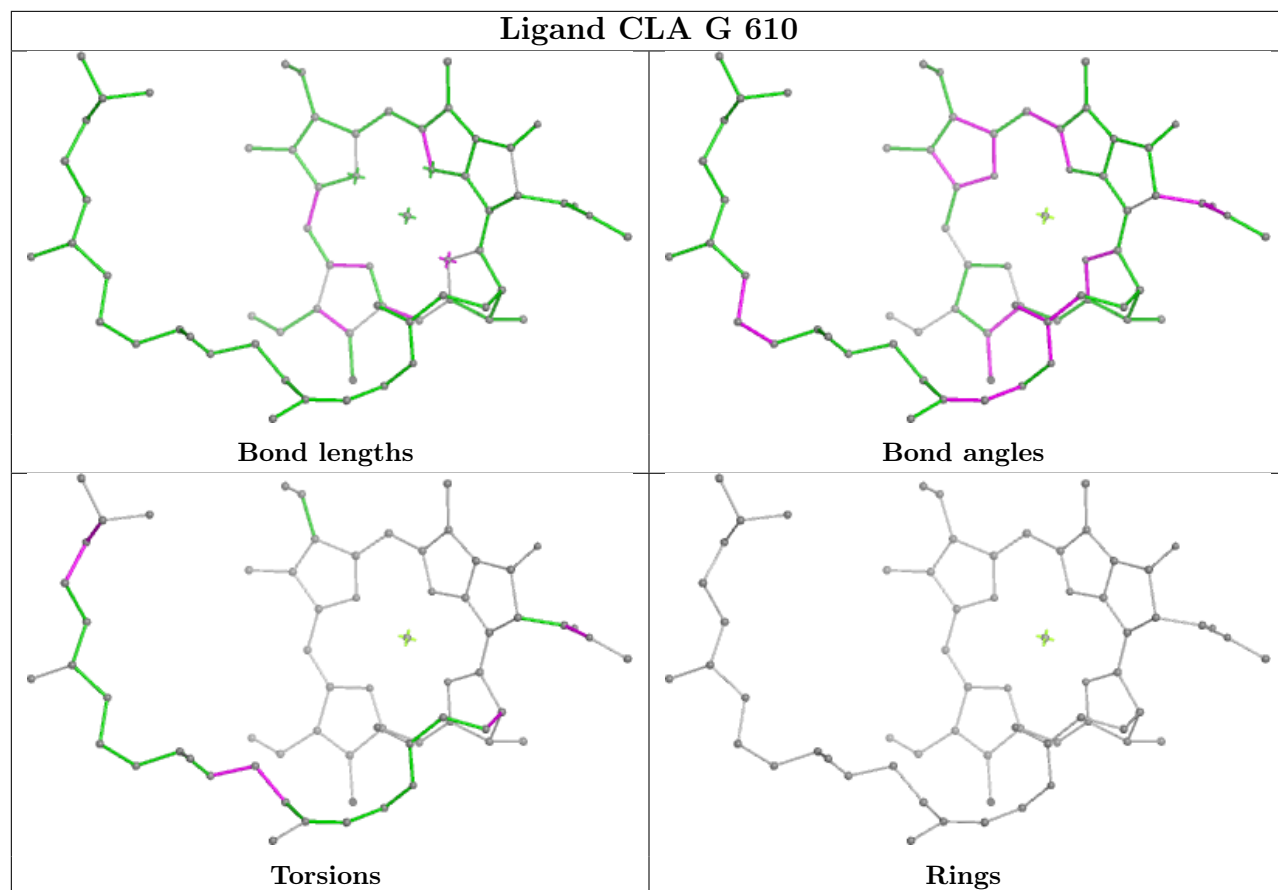


Torsions

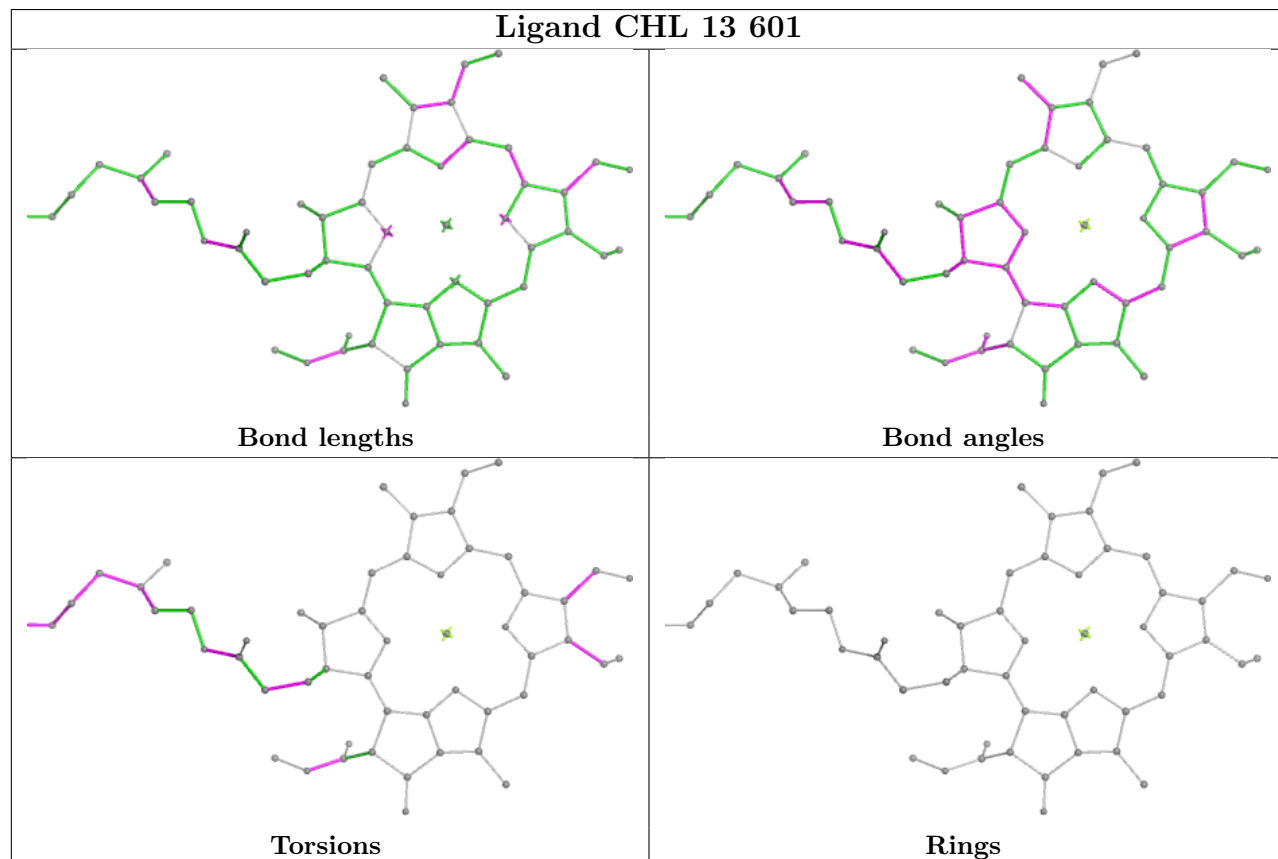


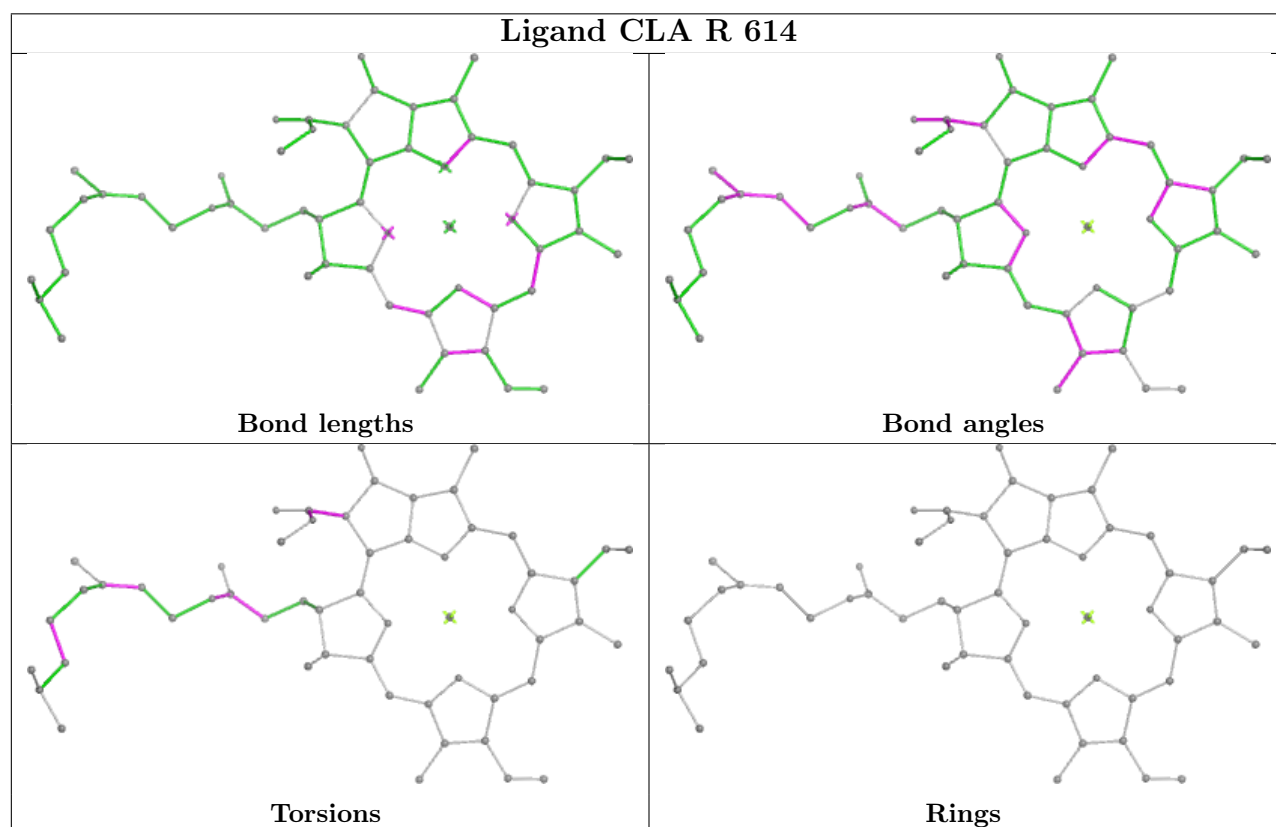
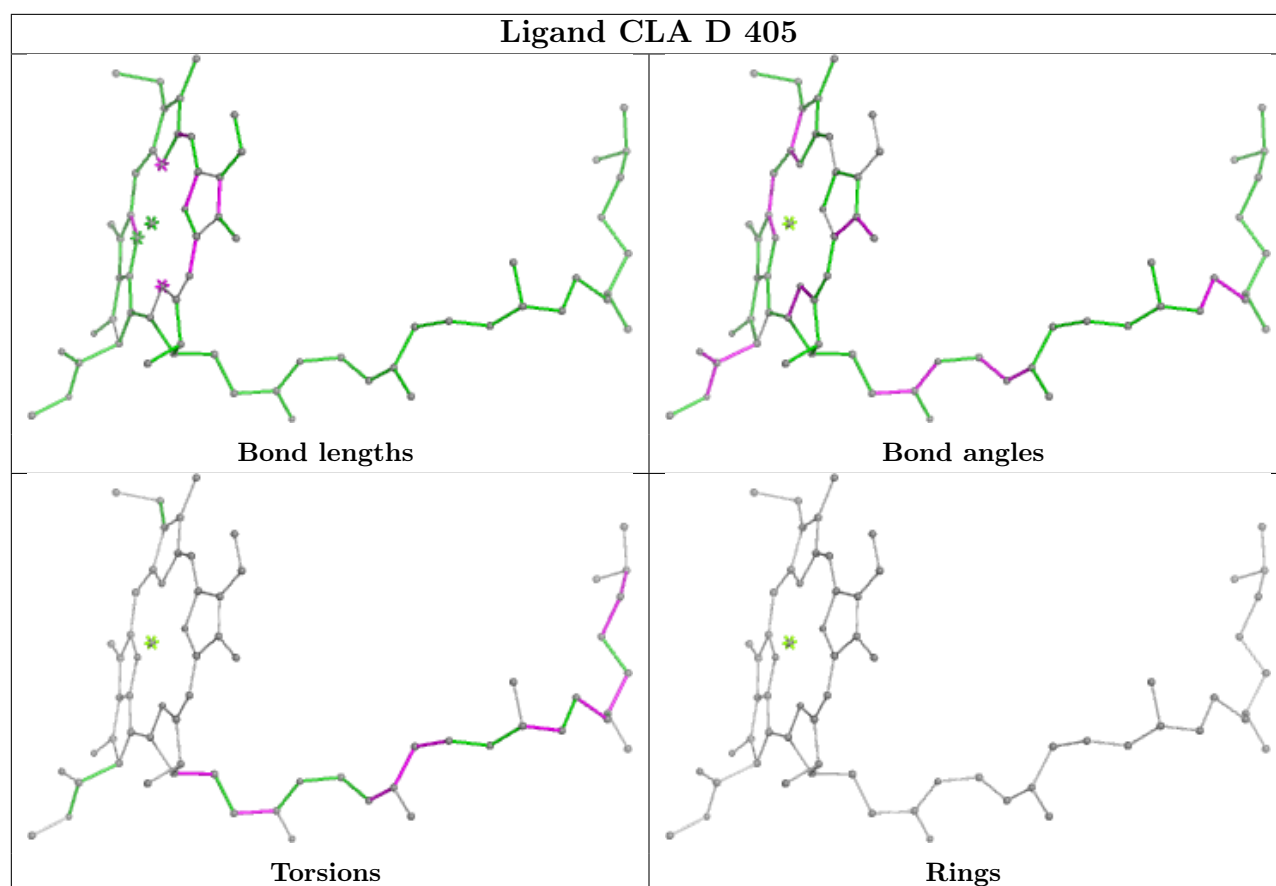
Rings

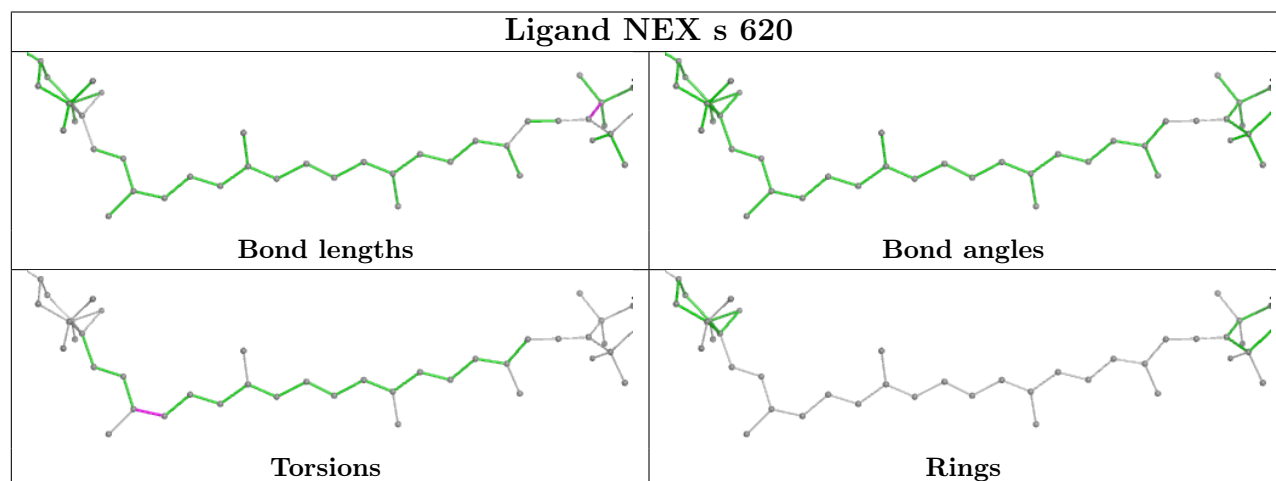
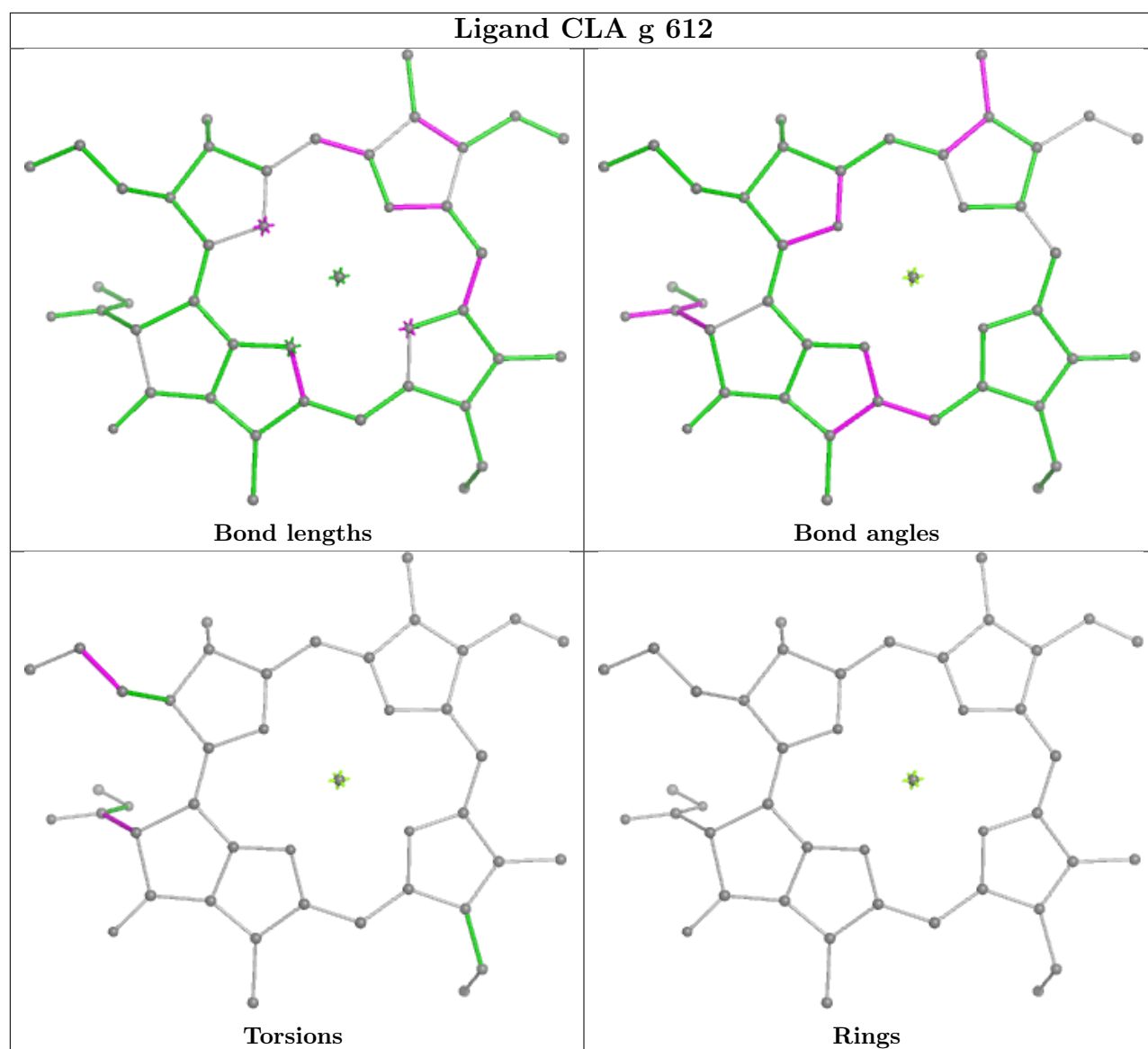
Ligand CLA G 610

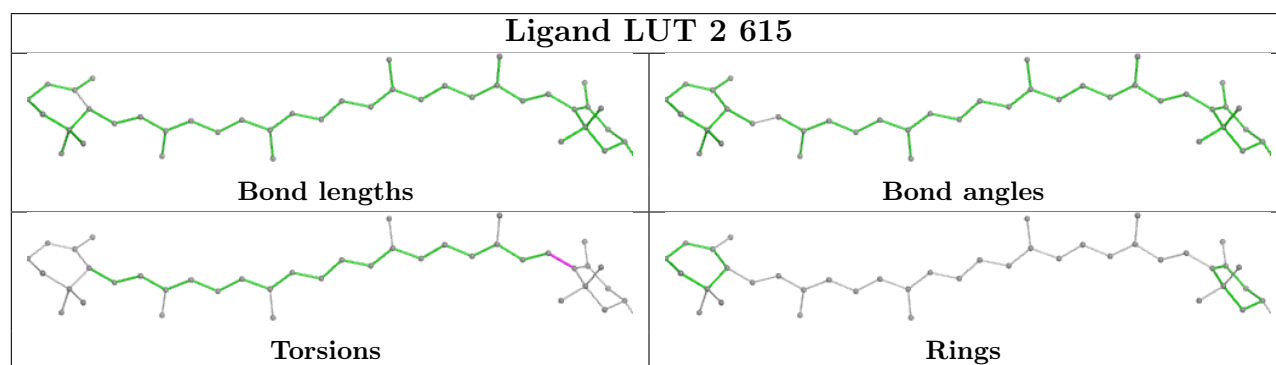
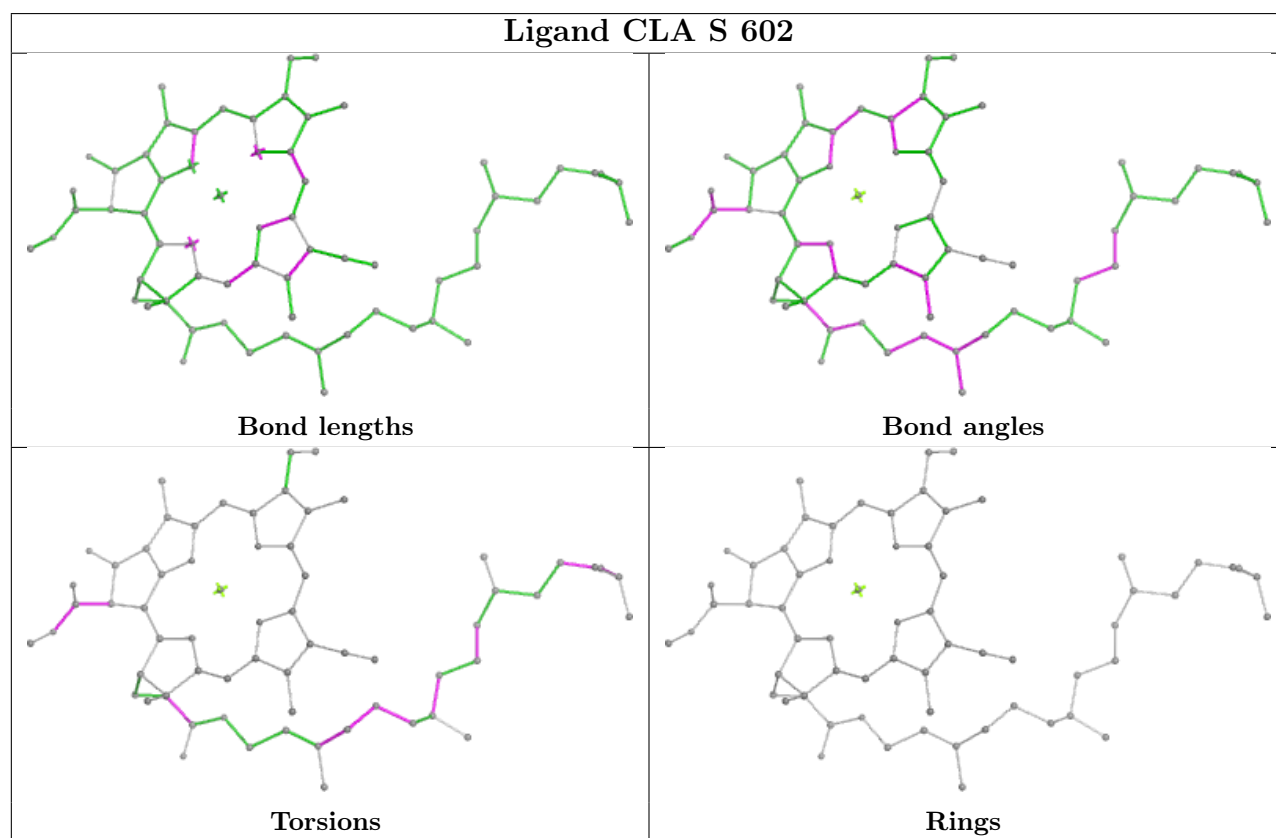
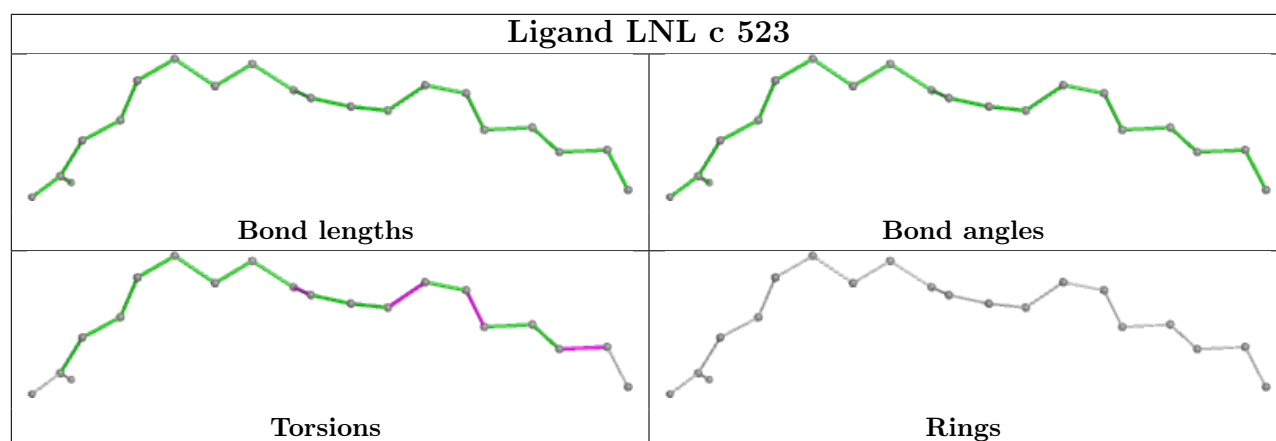


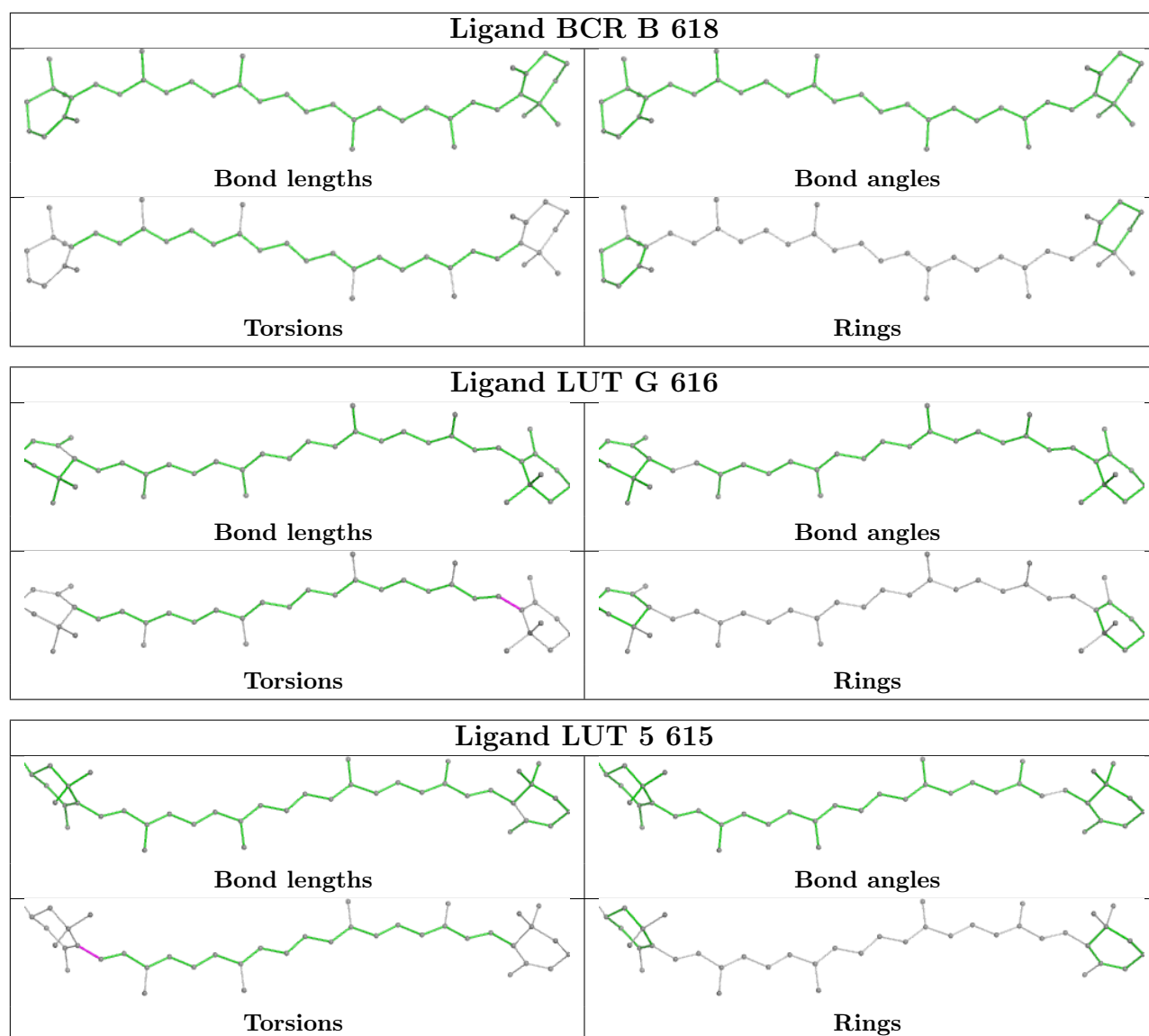
Ligand CHL 13 601



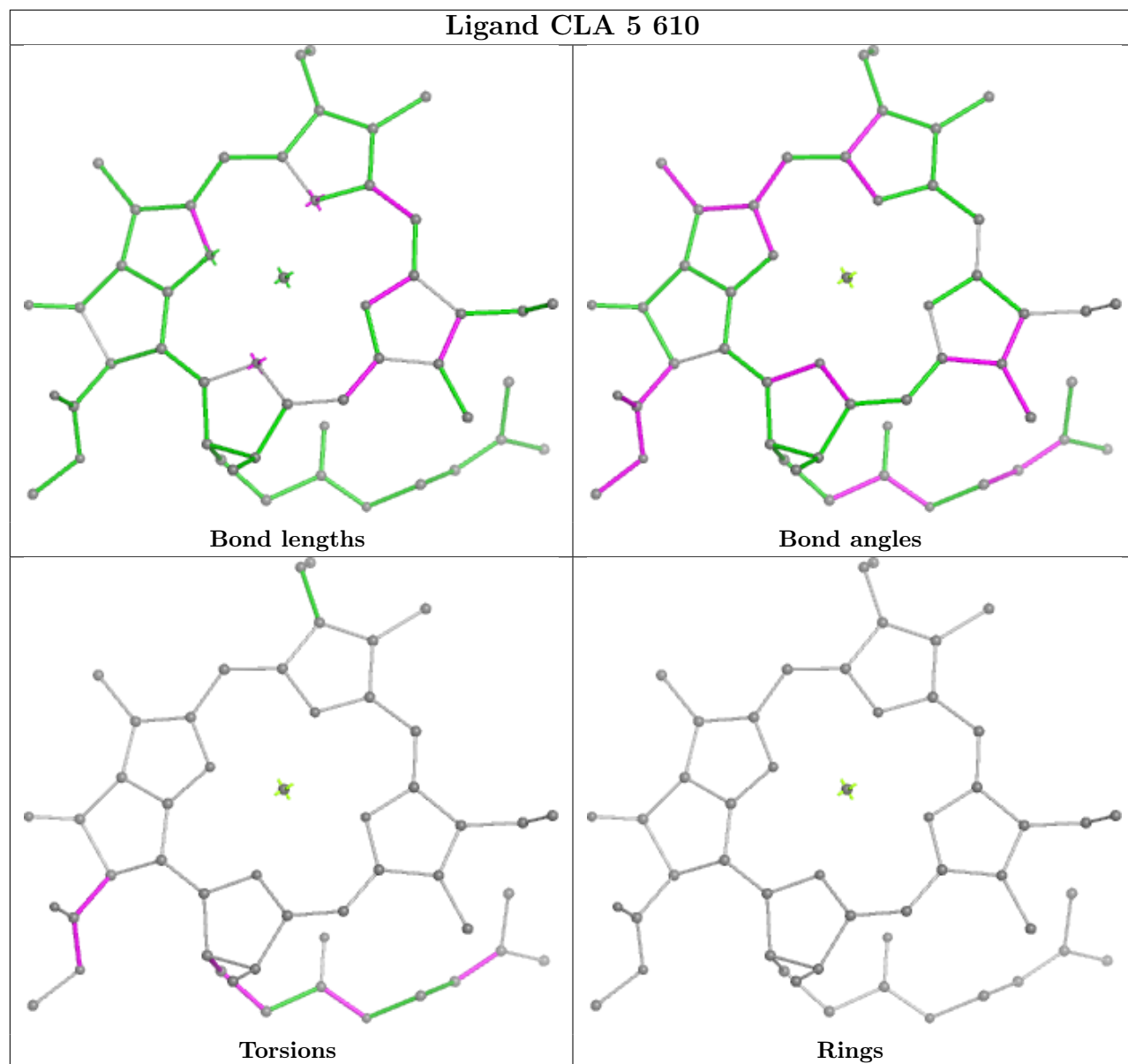




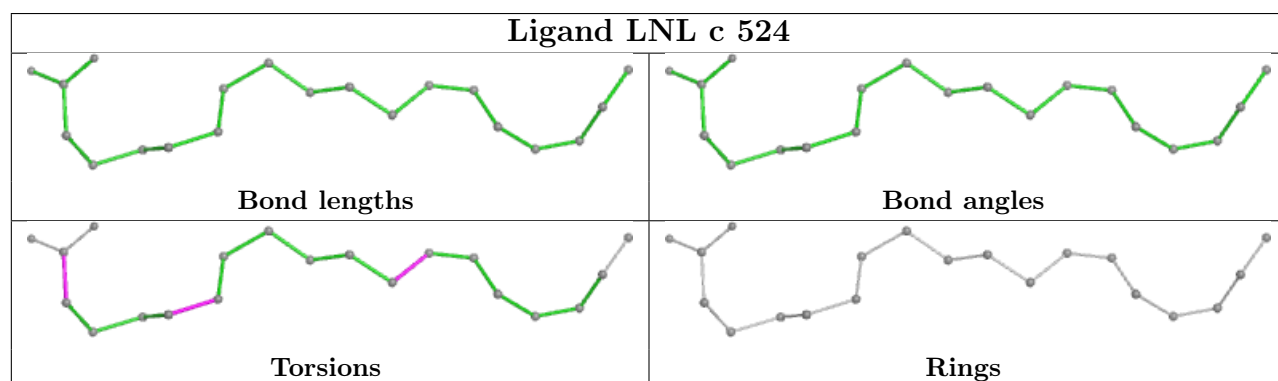


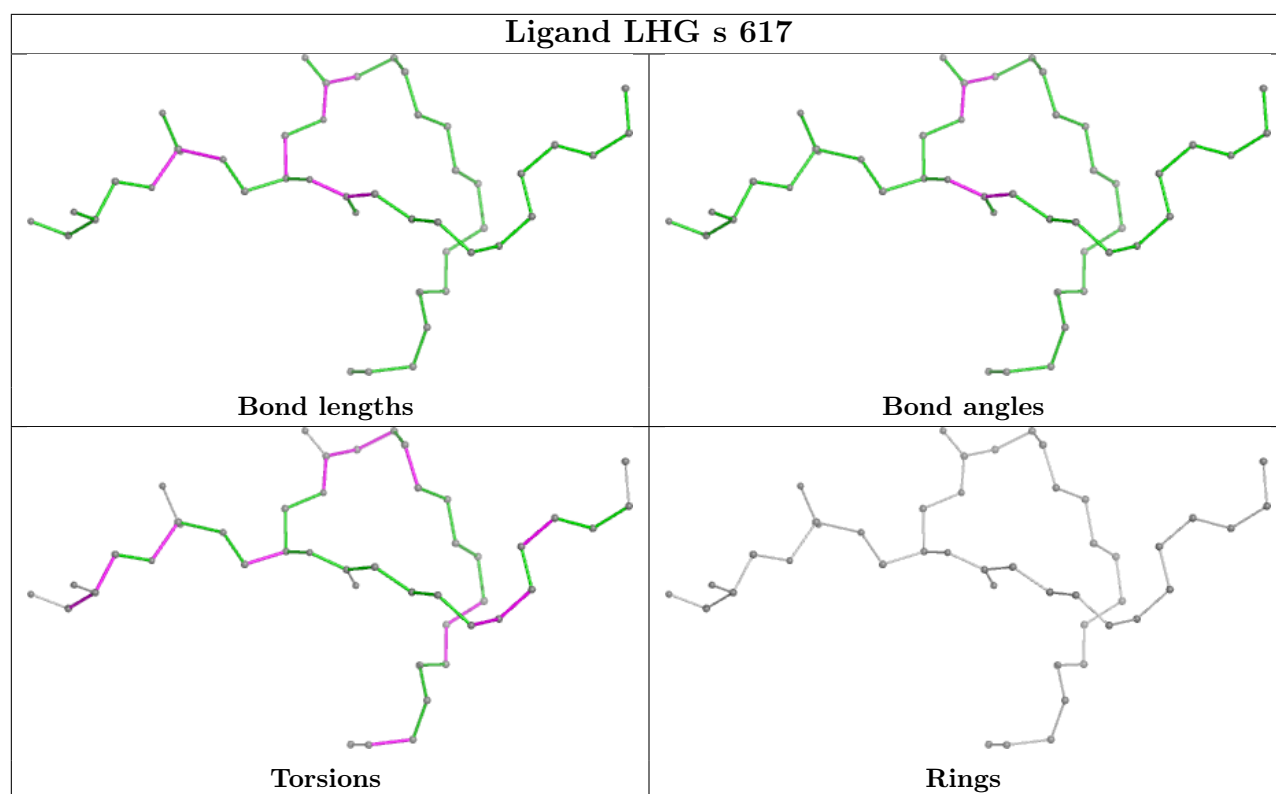


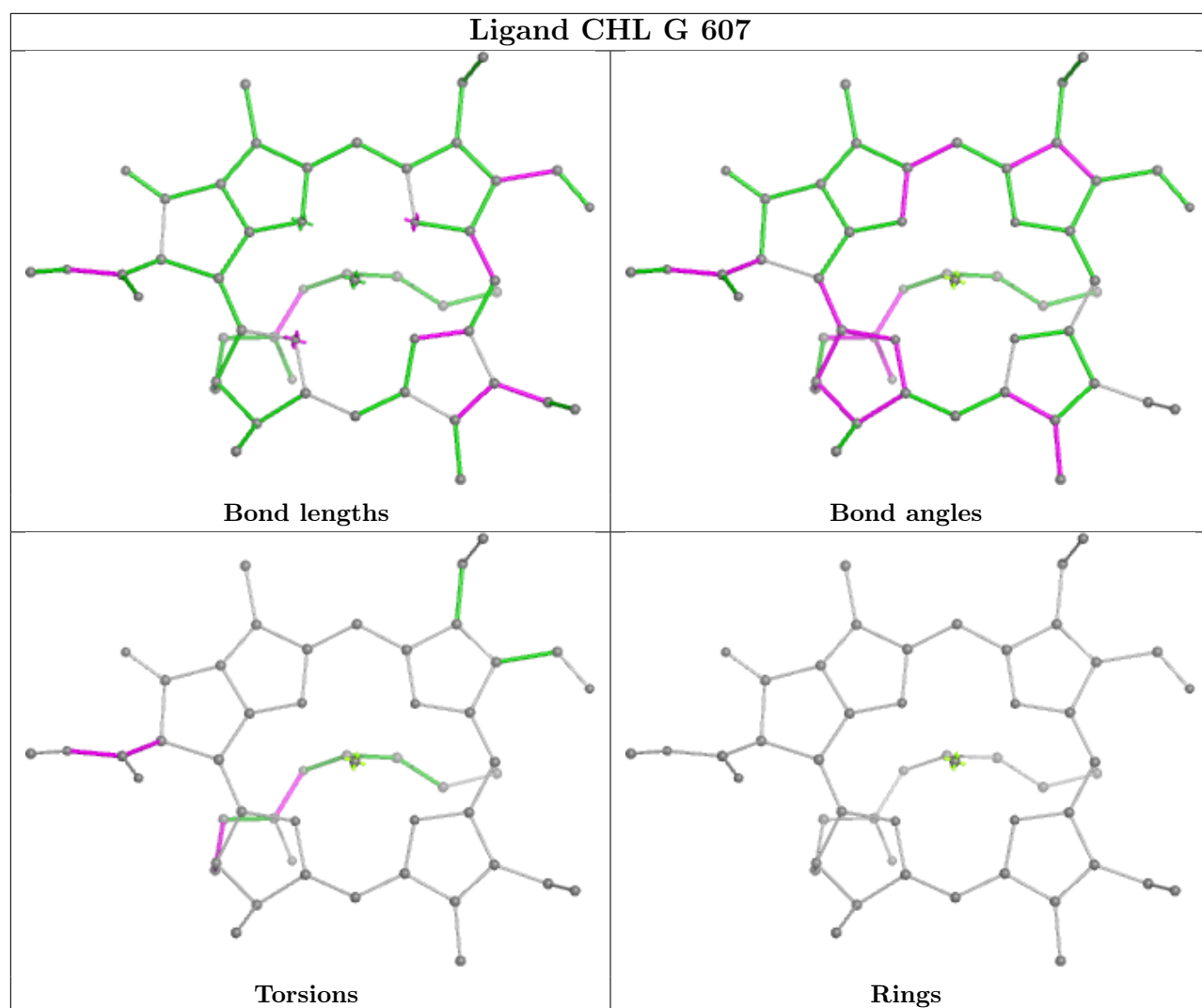
Ligand CLA 5 610



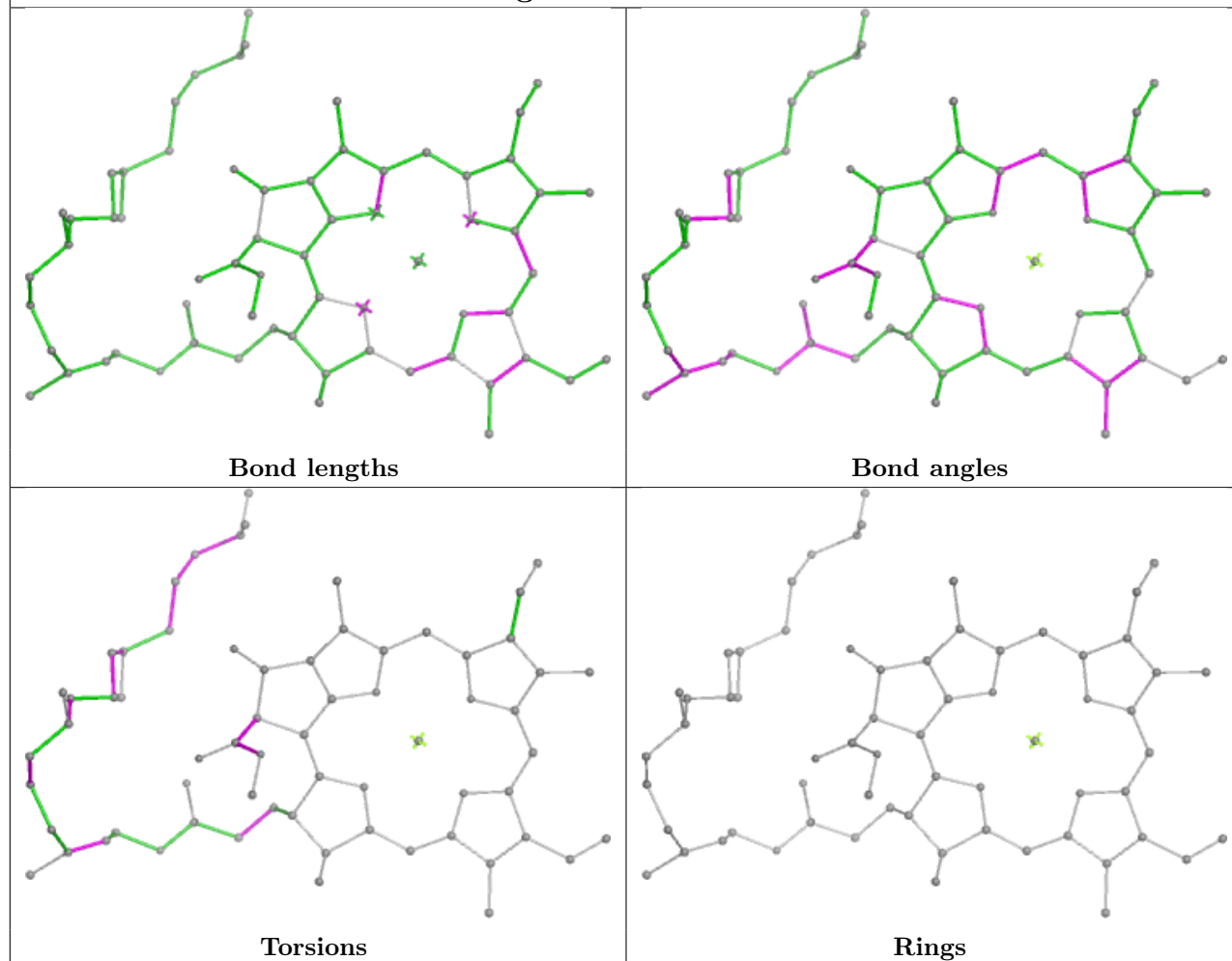
Ligand LNL c 524



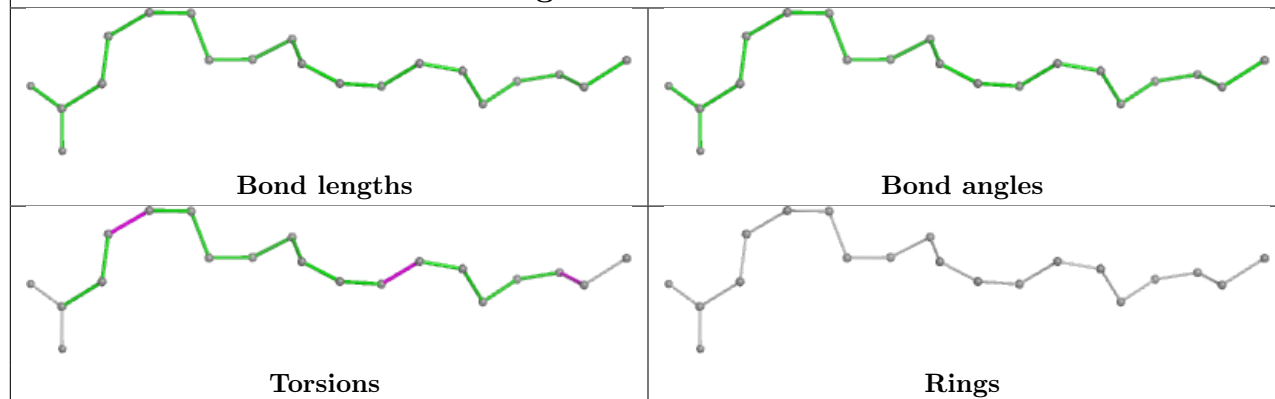


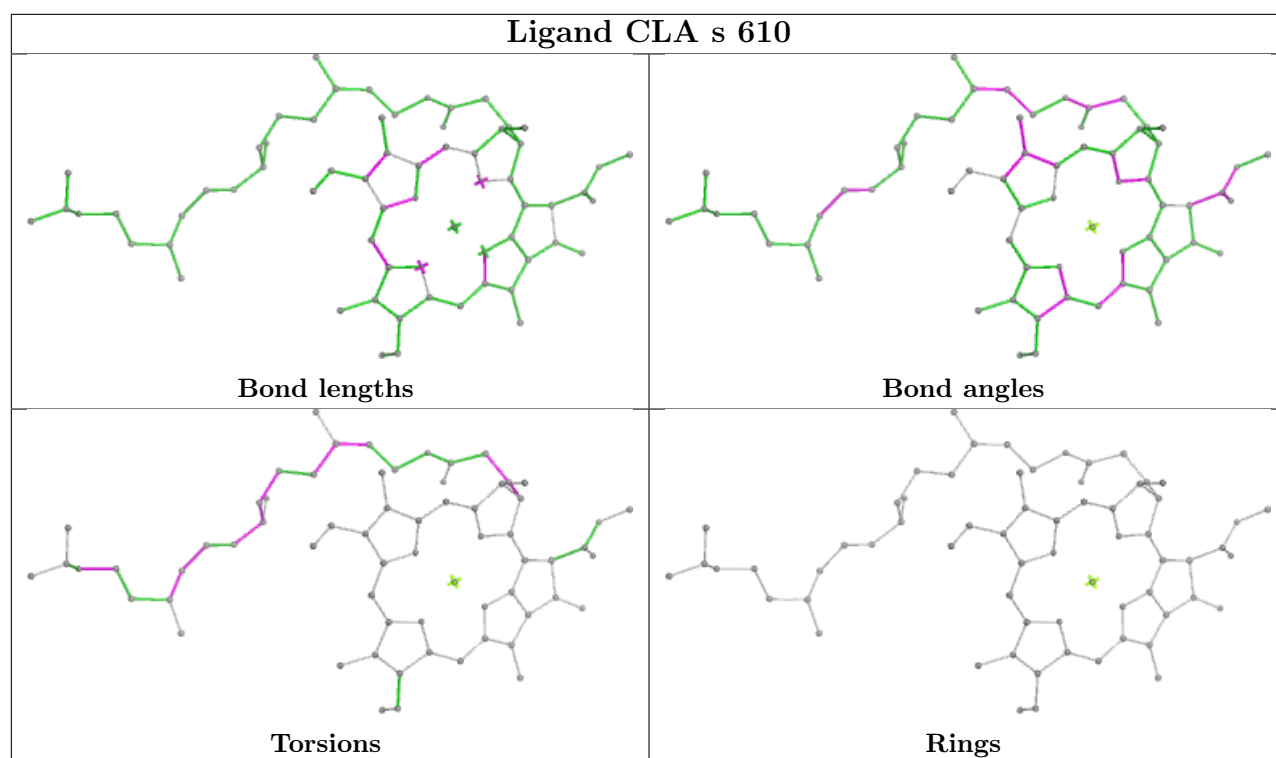


Ligand CLA b 610

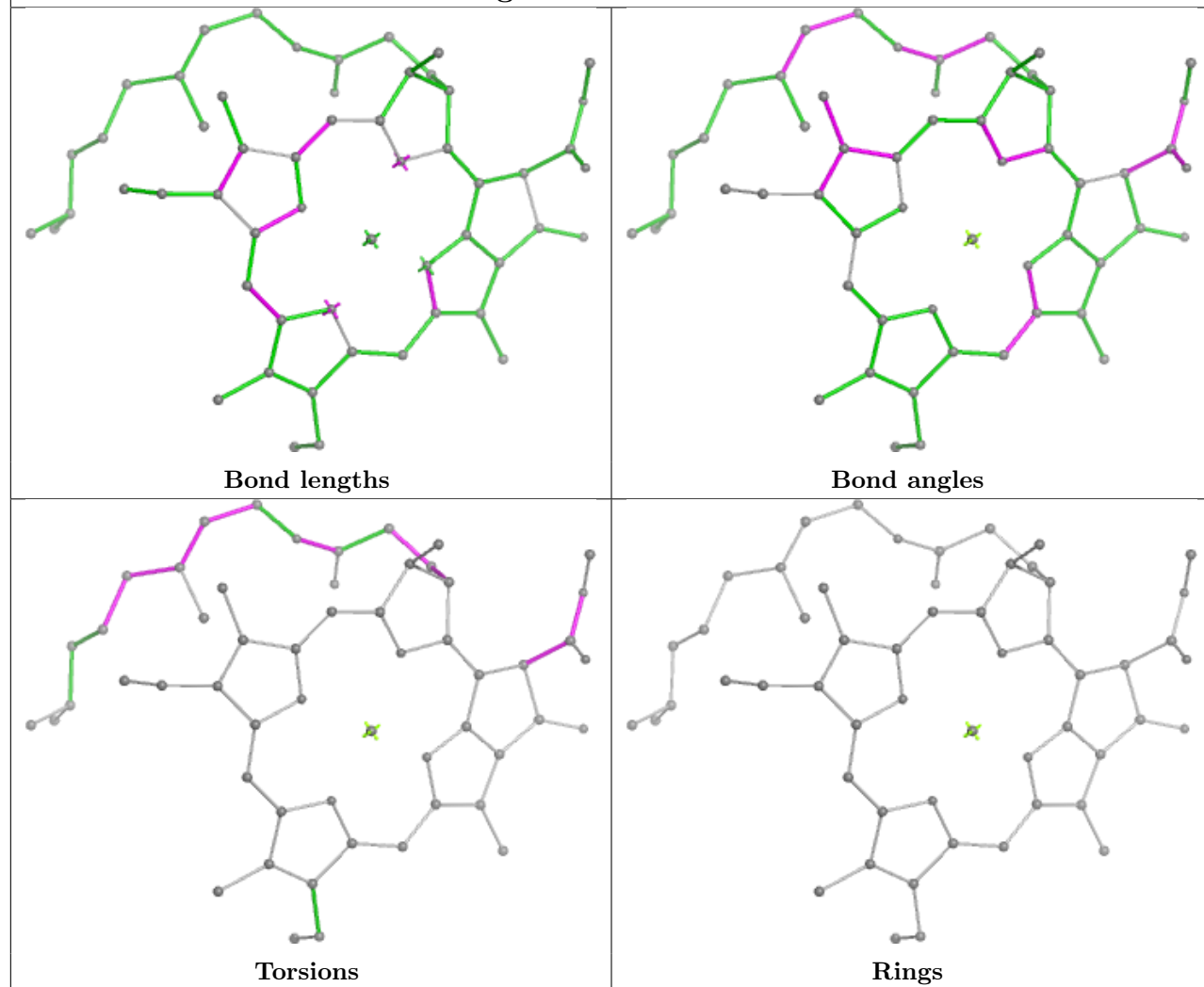


Ligand LNL h 101

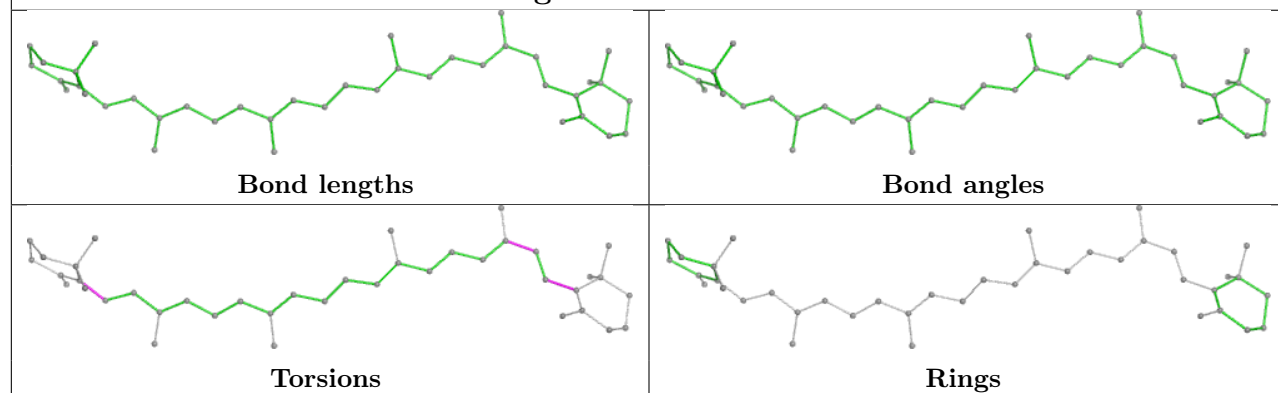


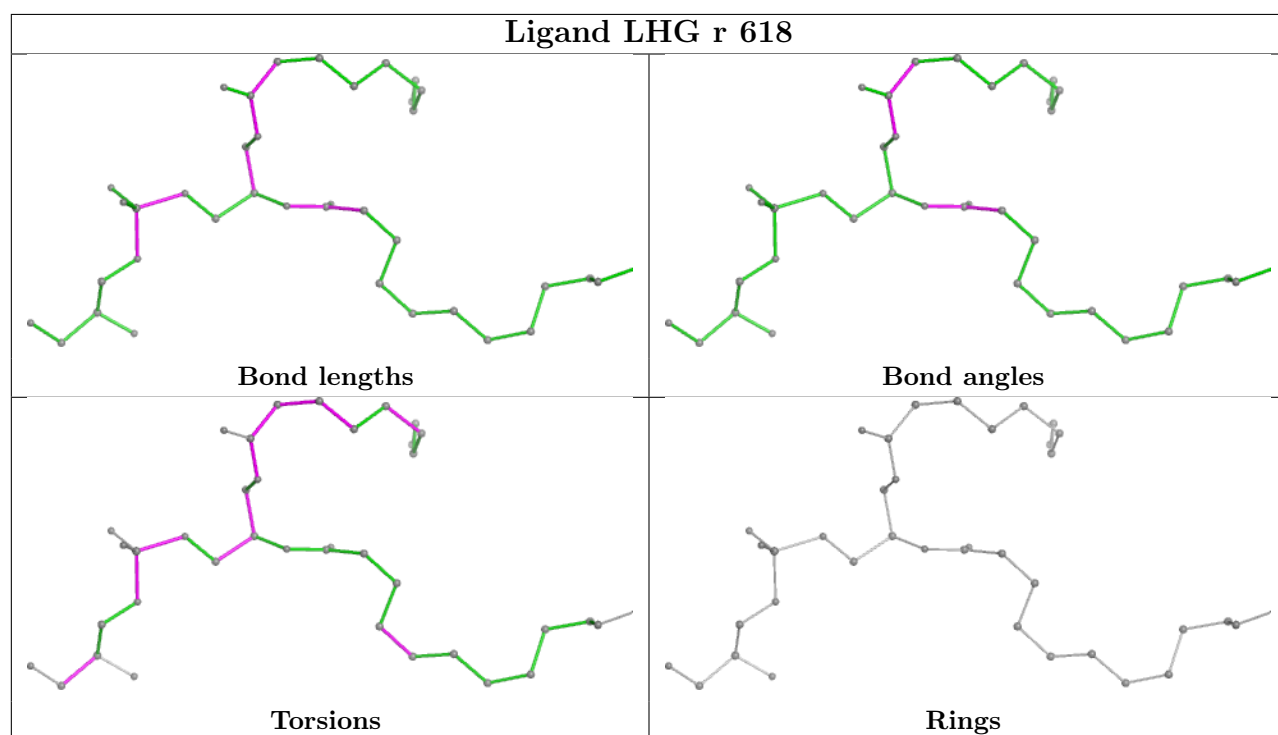
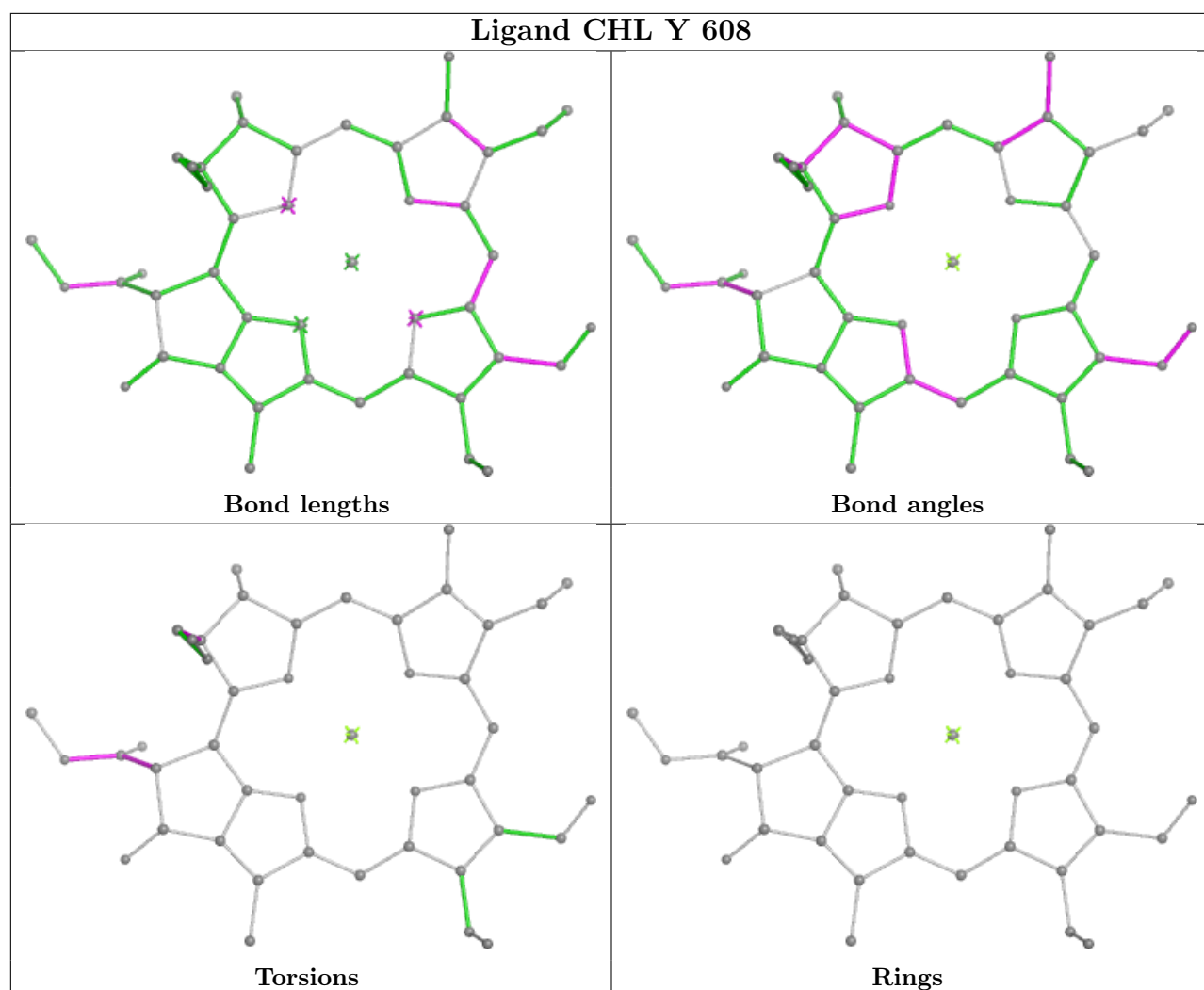


Ligand CLA 12 609

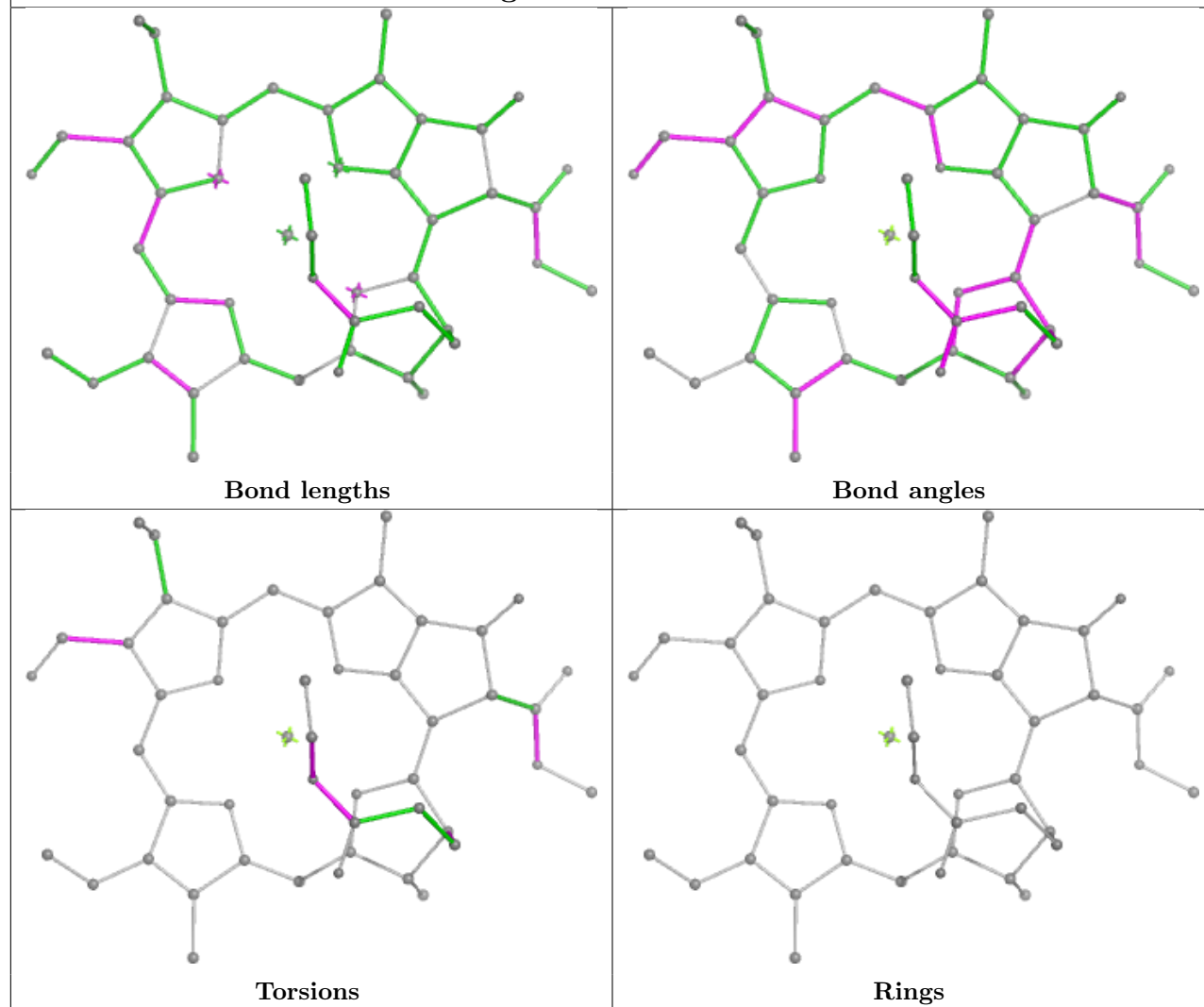


Ligand BCR J 101

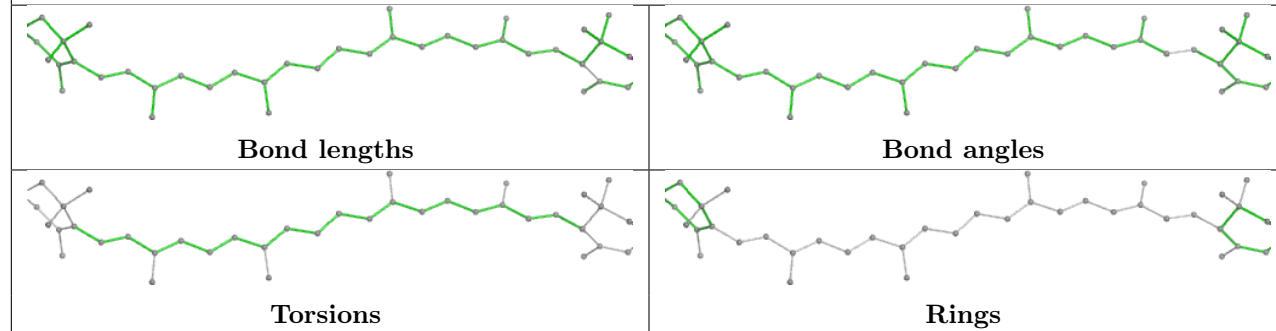


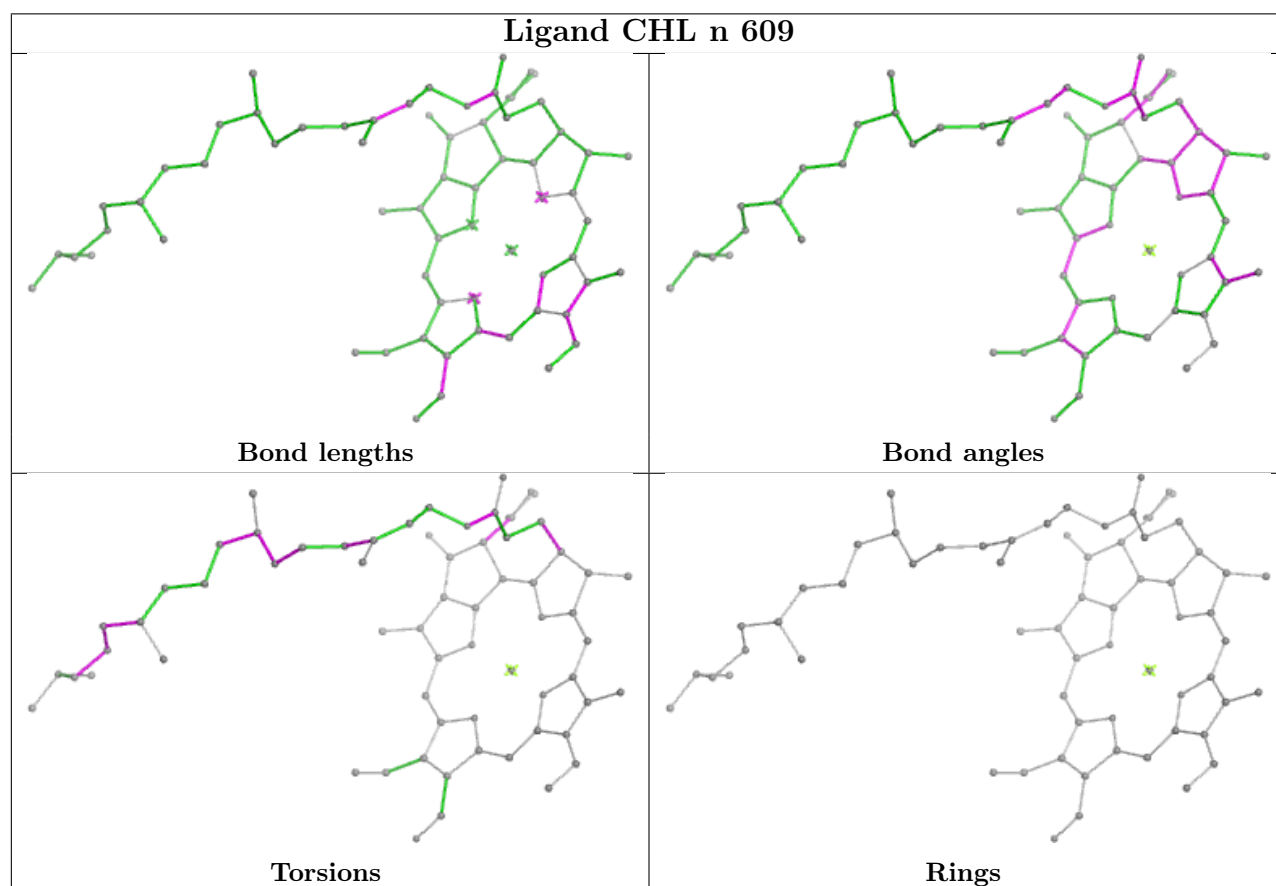
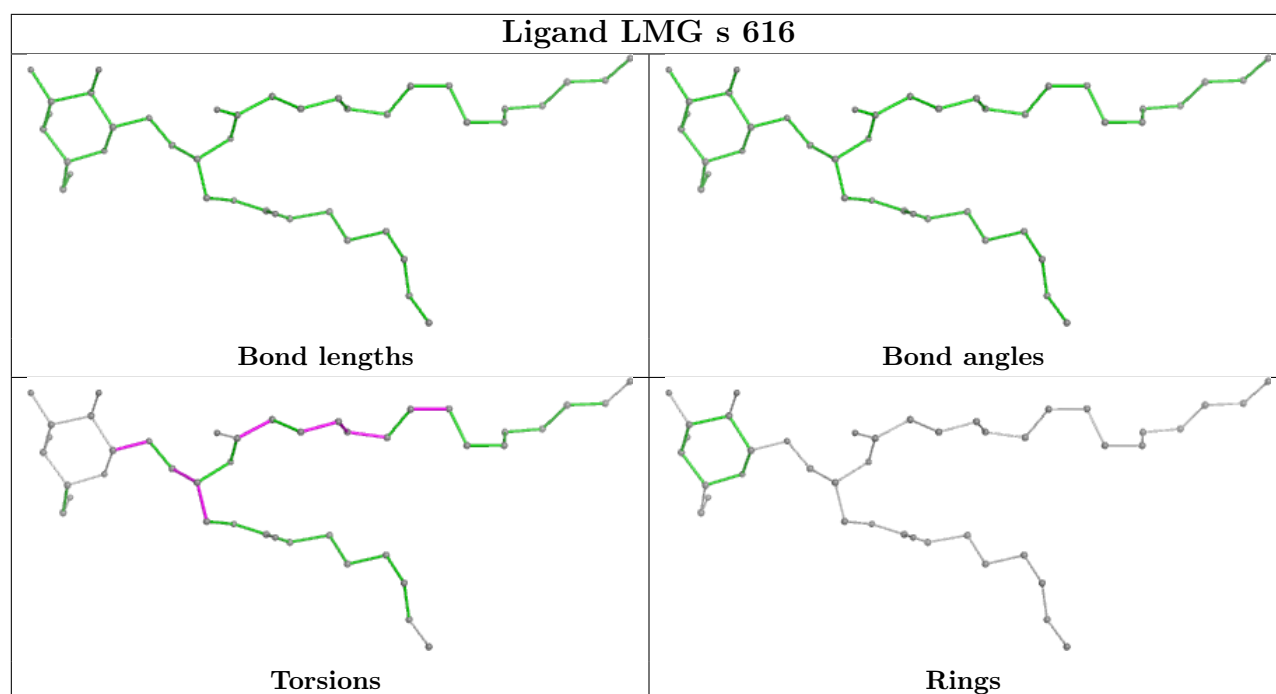


Ligand CHL G 605

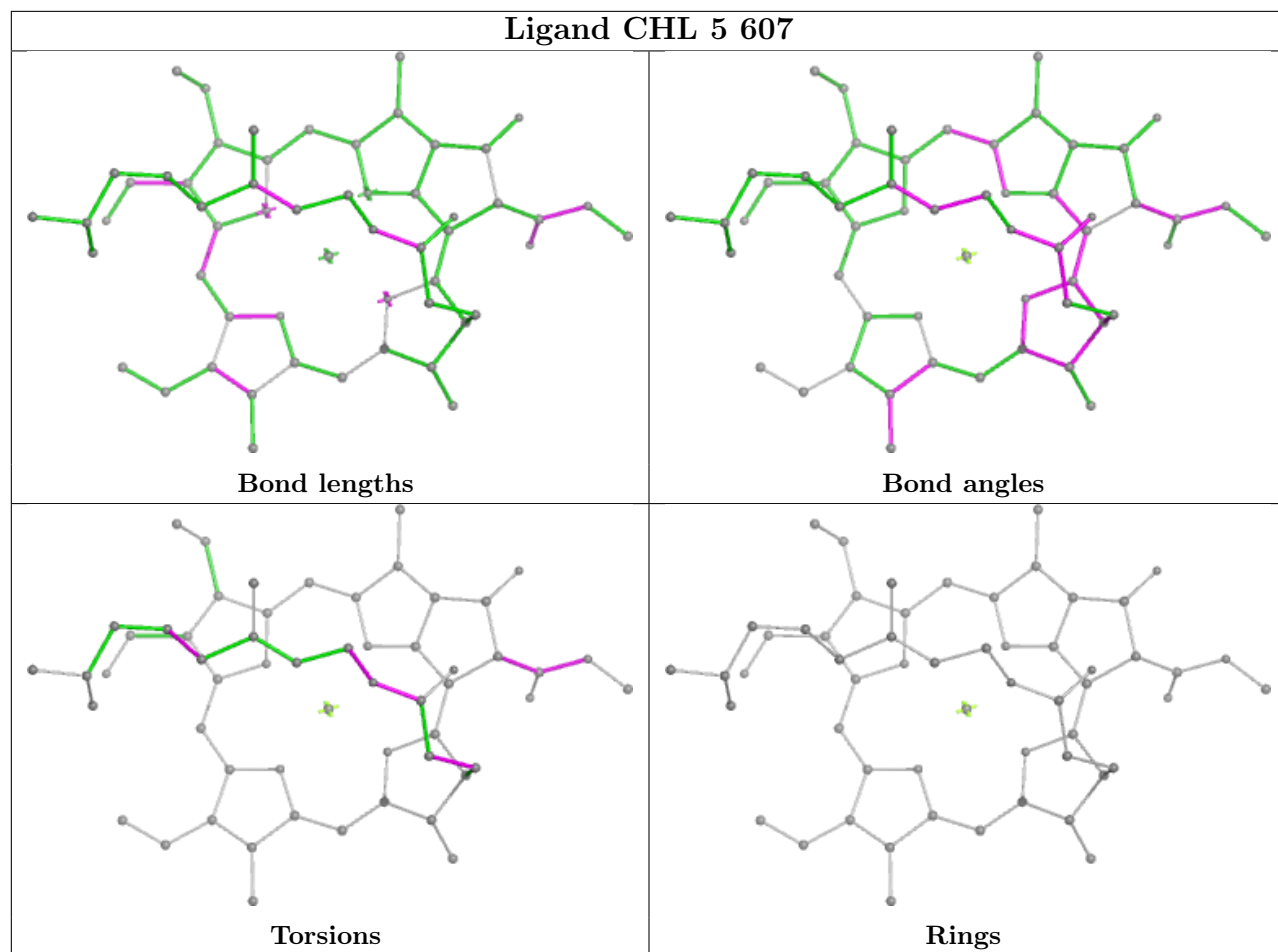


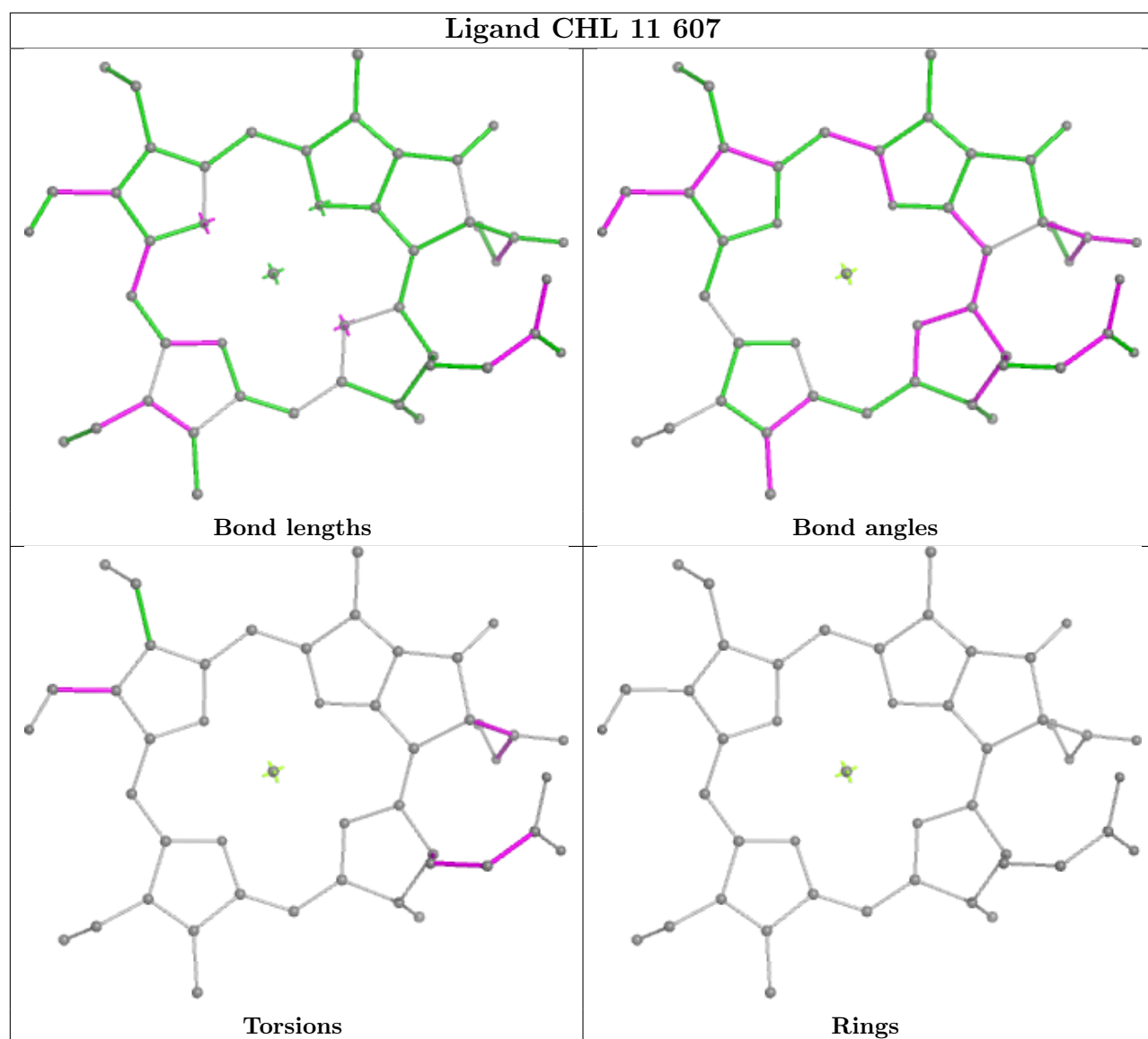
Ligand LUT N 618

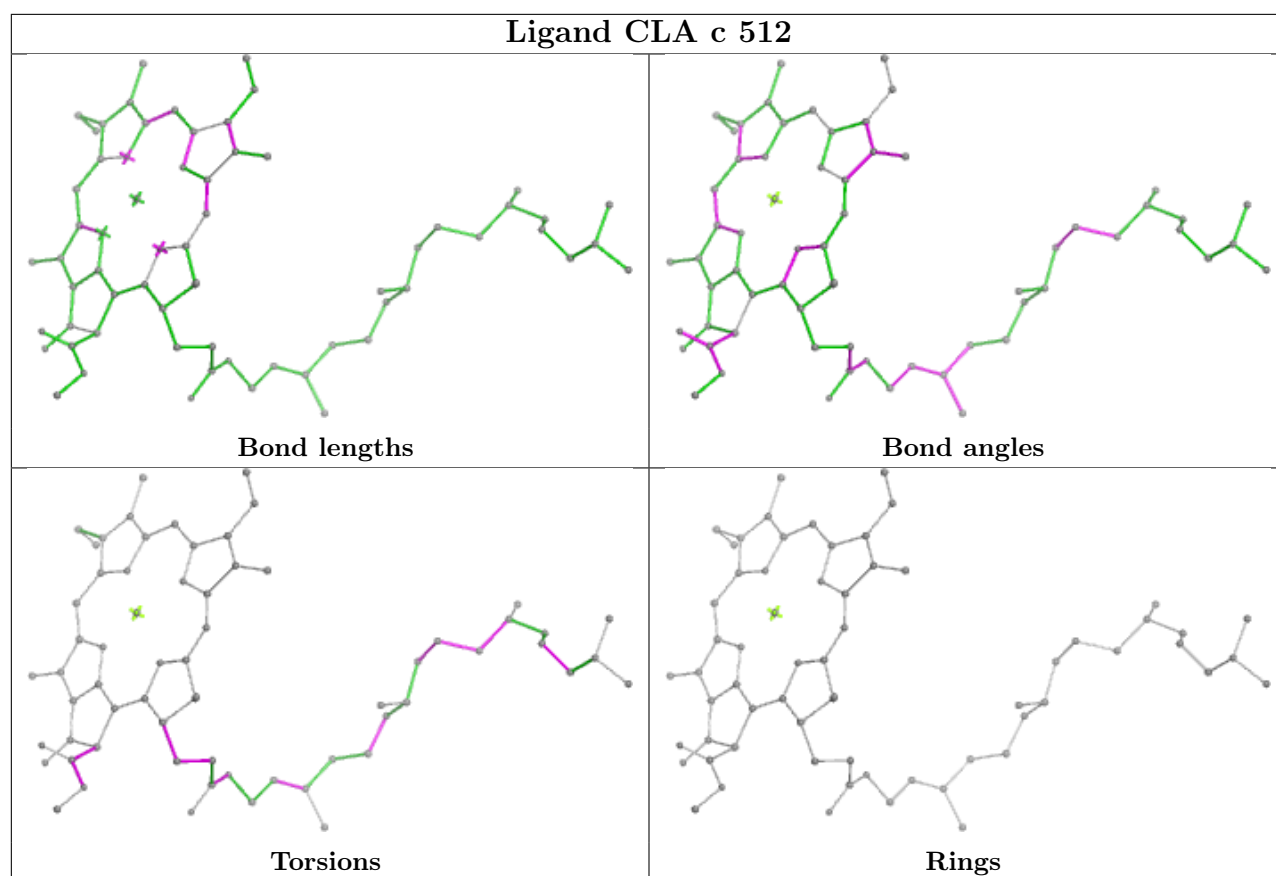


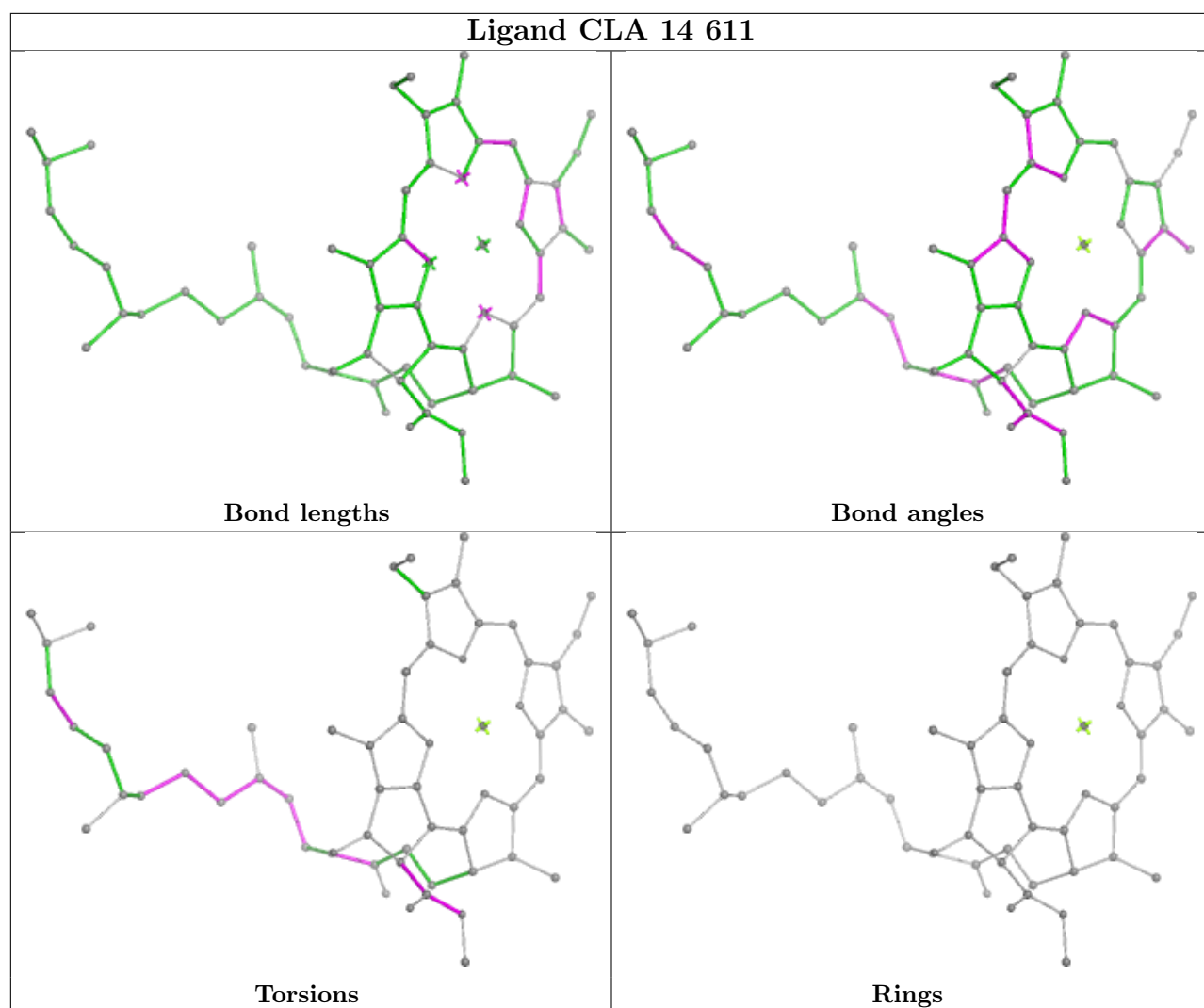


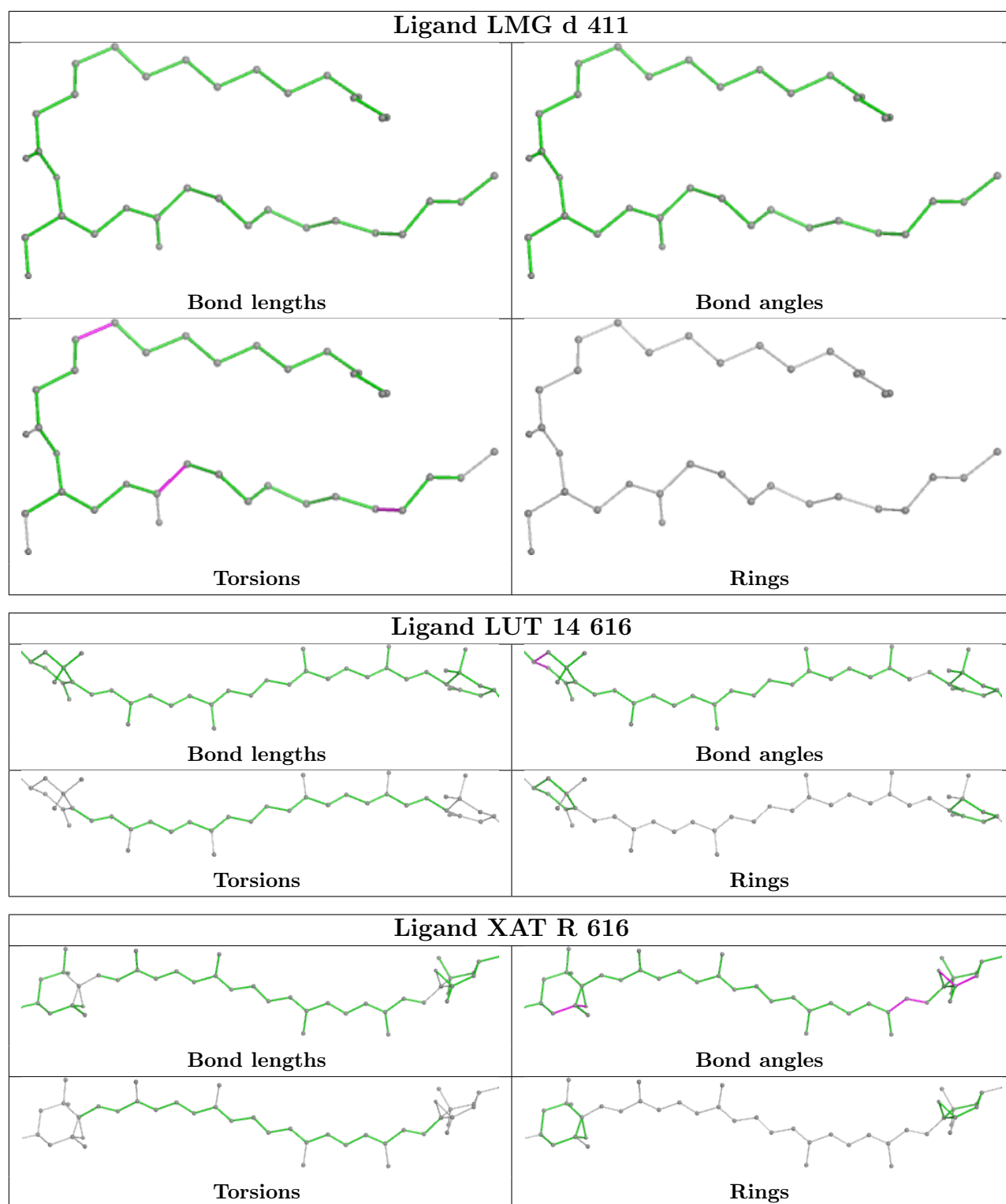
Ligand CHL 5 607



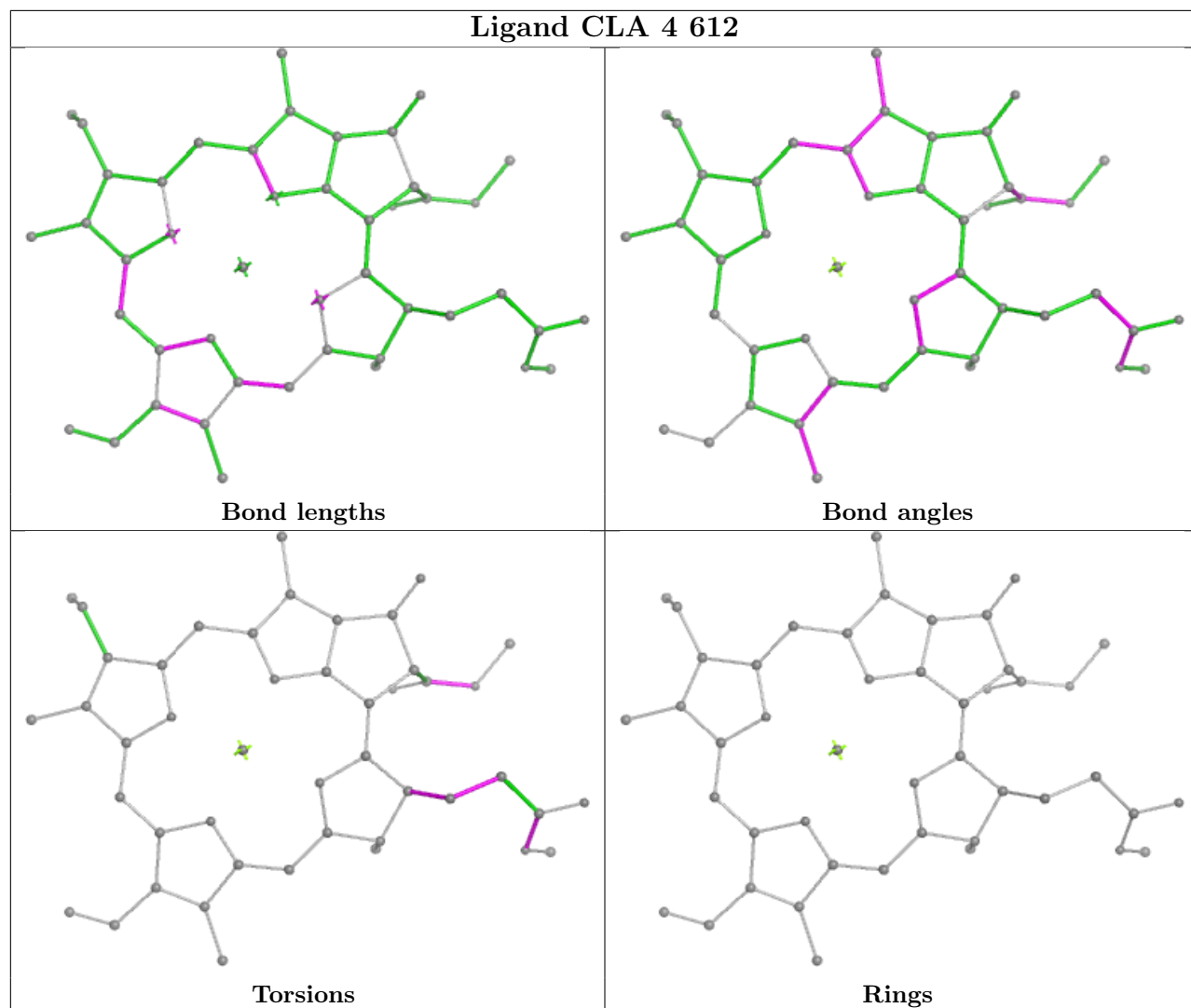




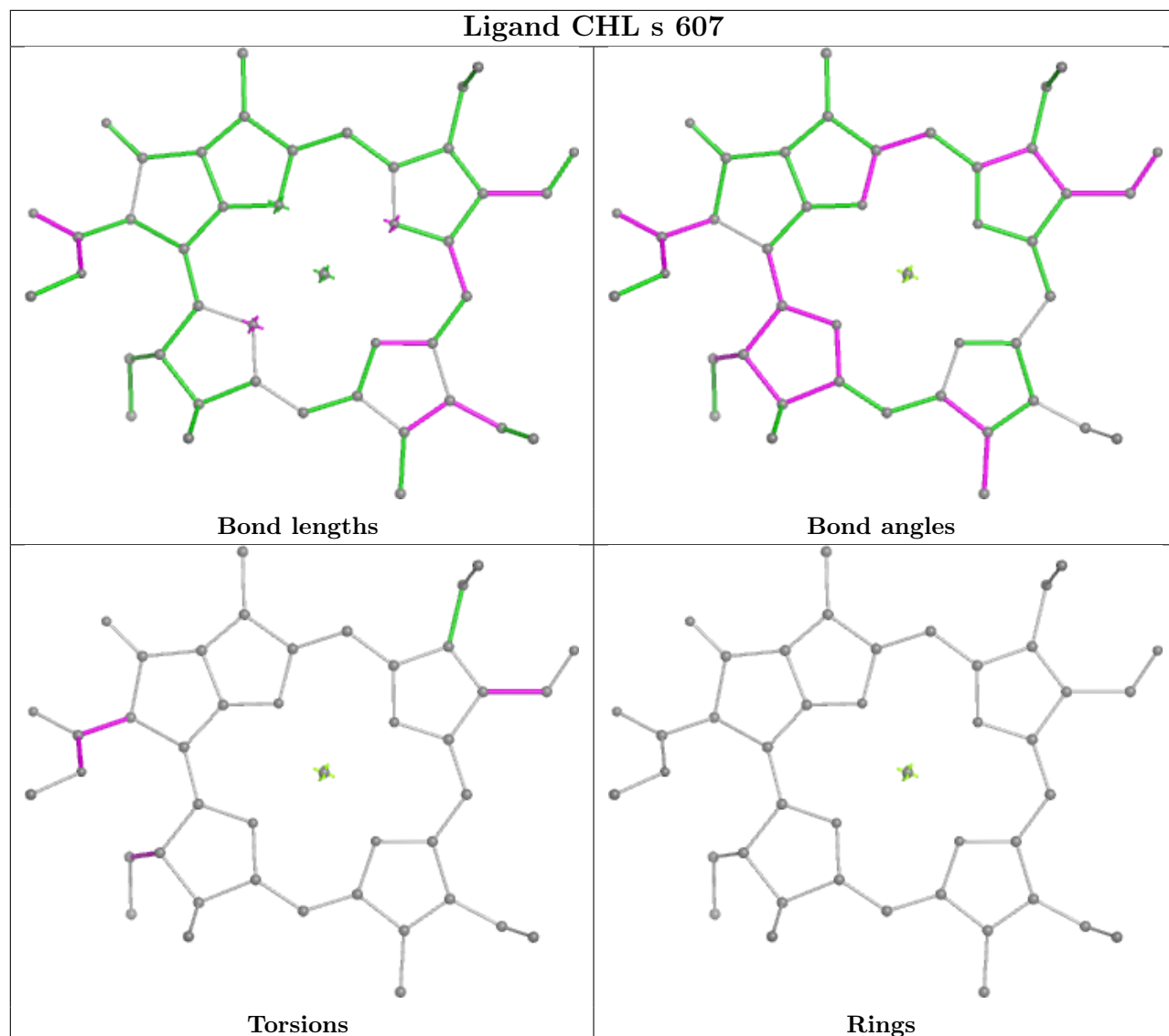




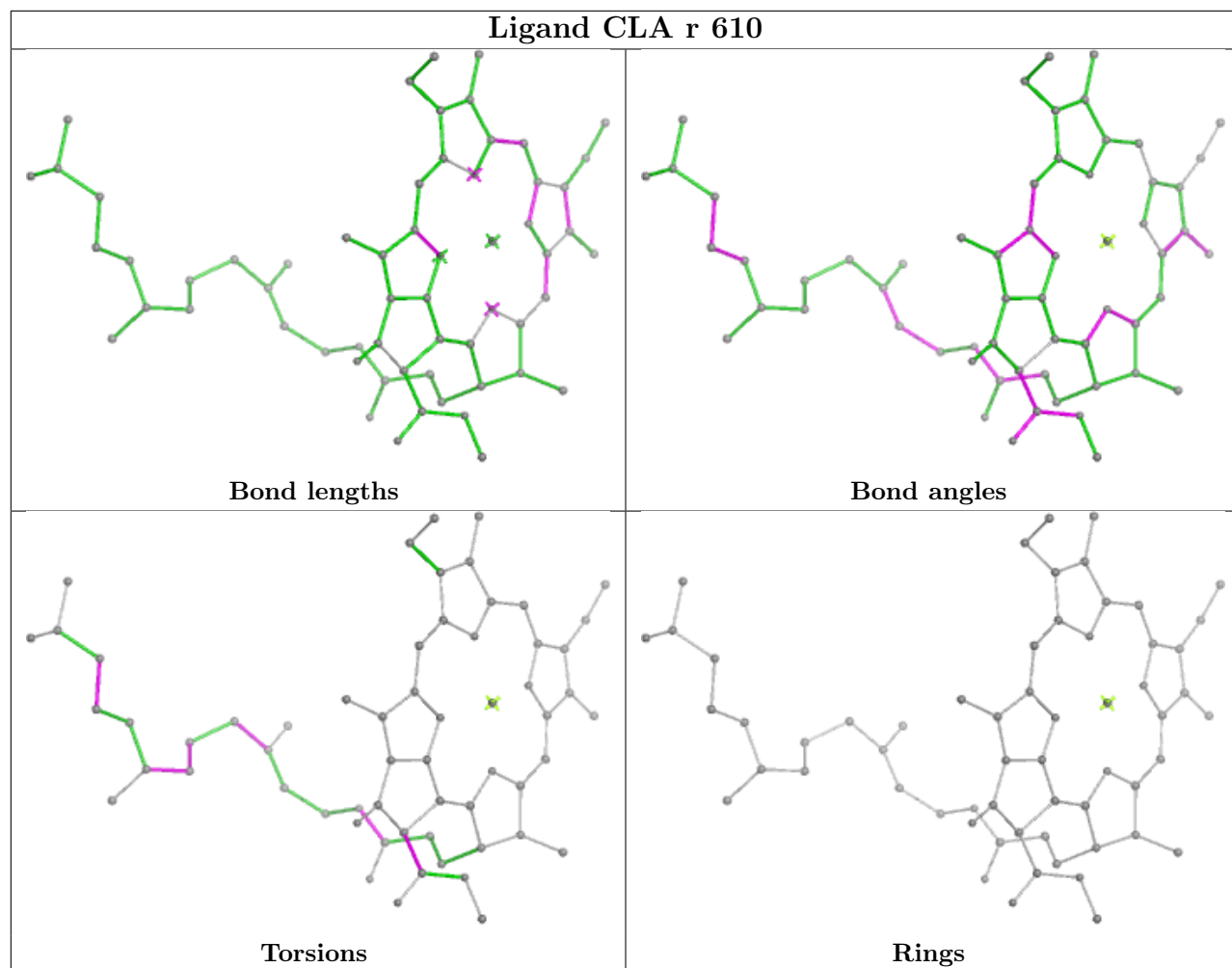
Ligand CLA 4 612

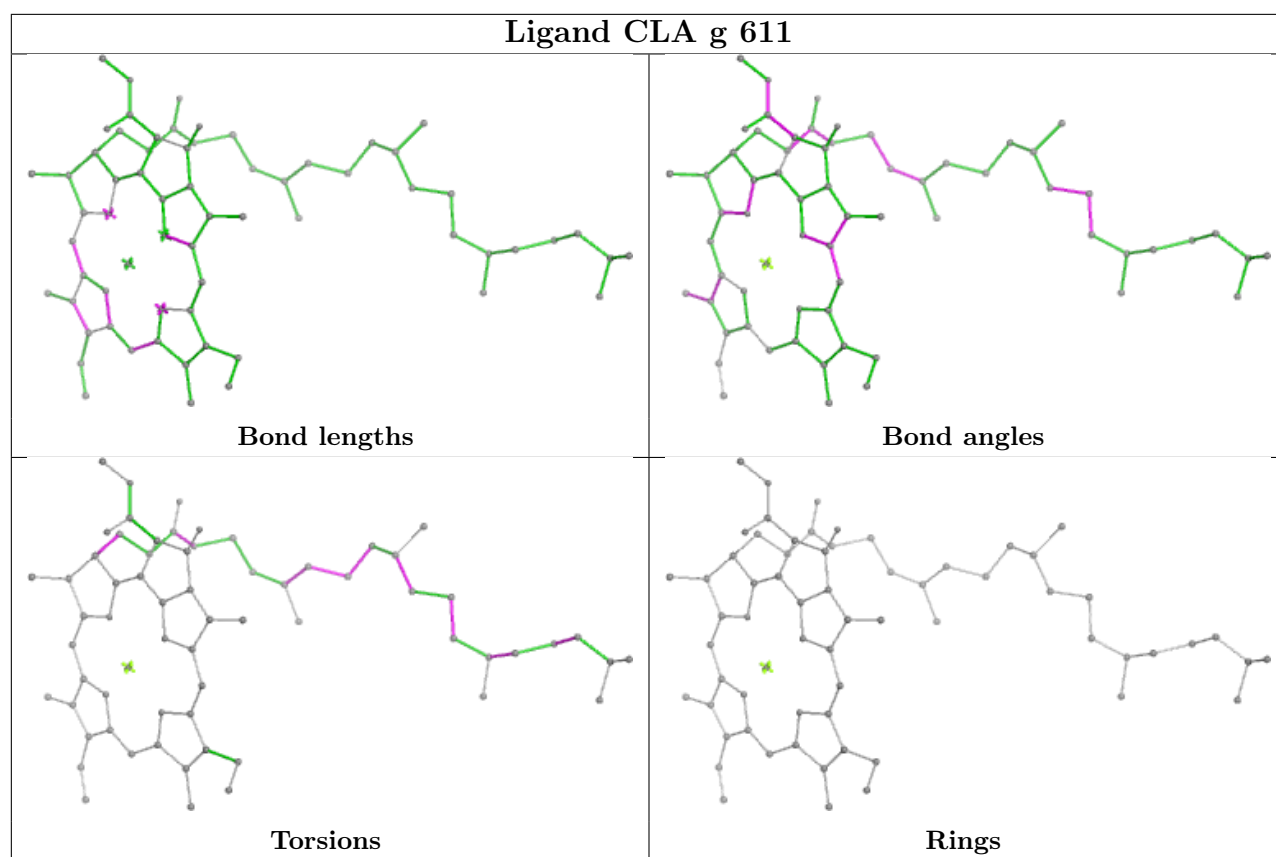


Ligand CHL s 607

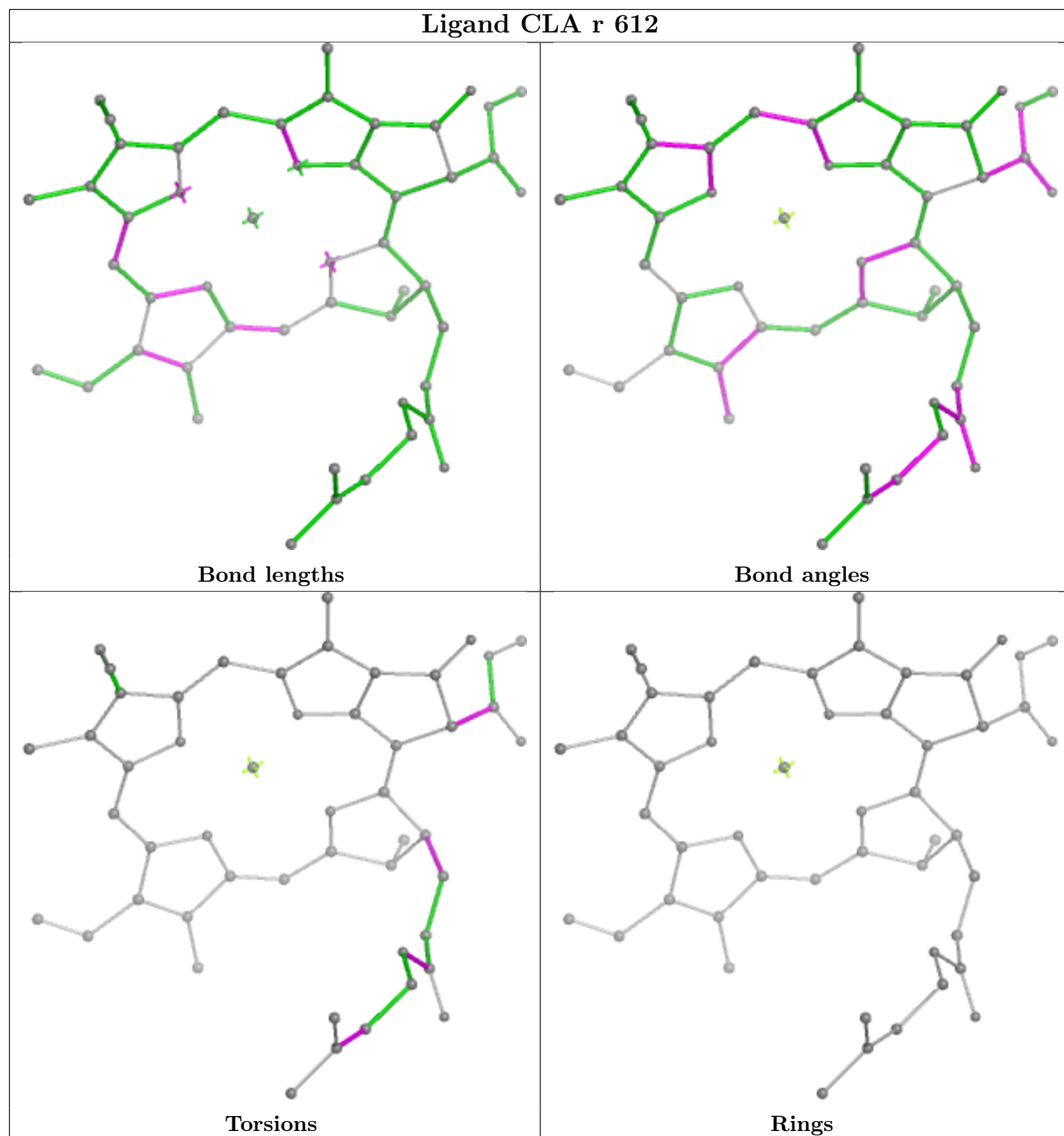


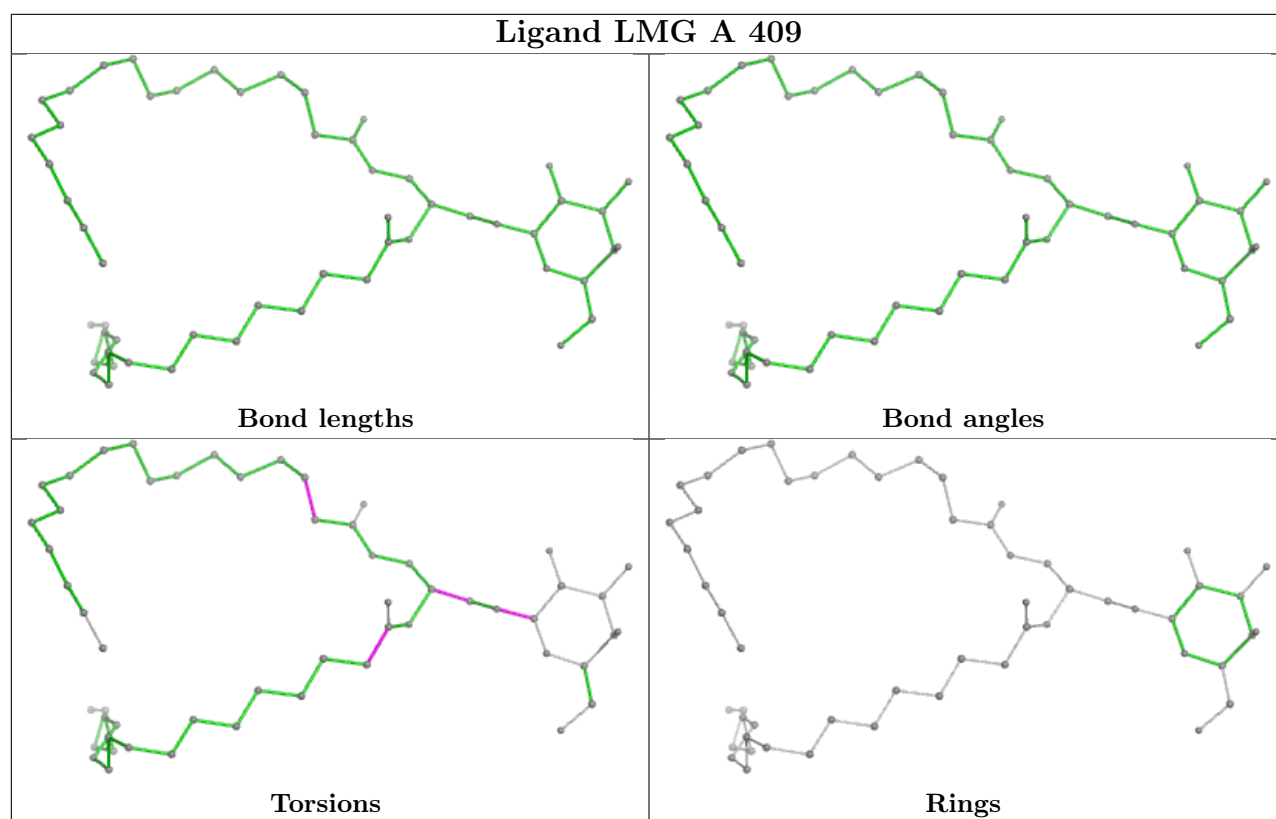
Ligand CLA r 610

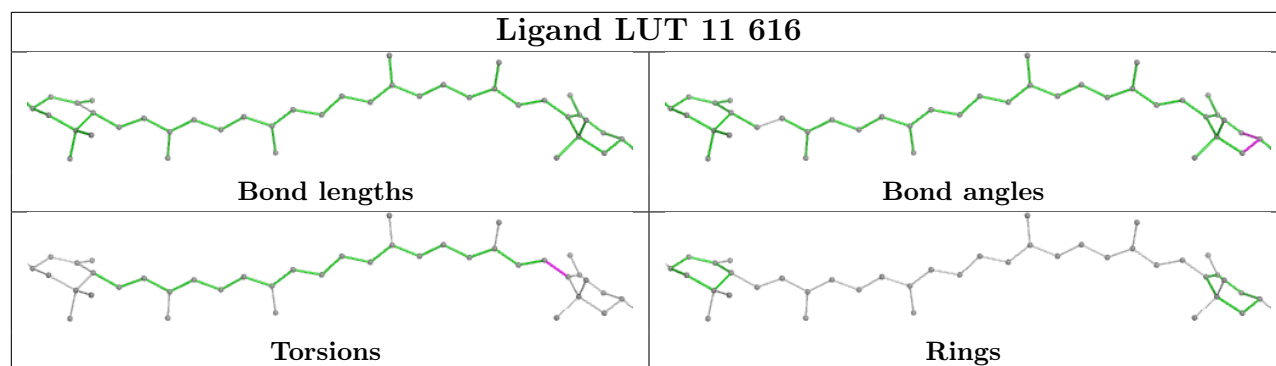
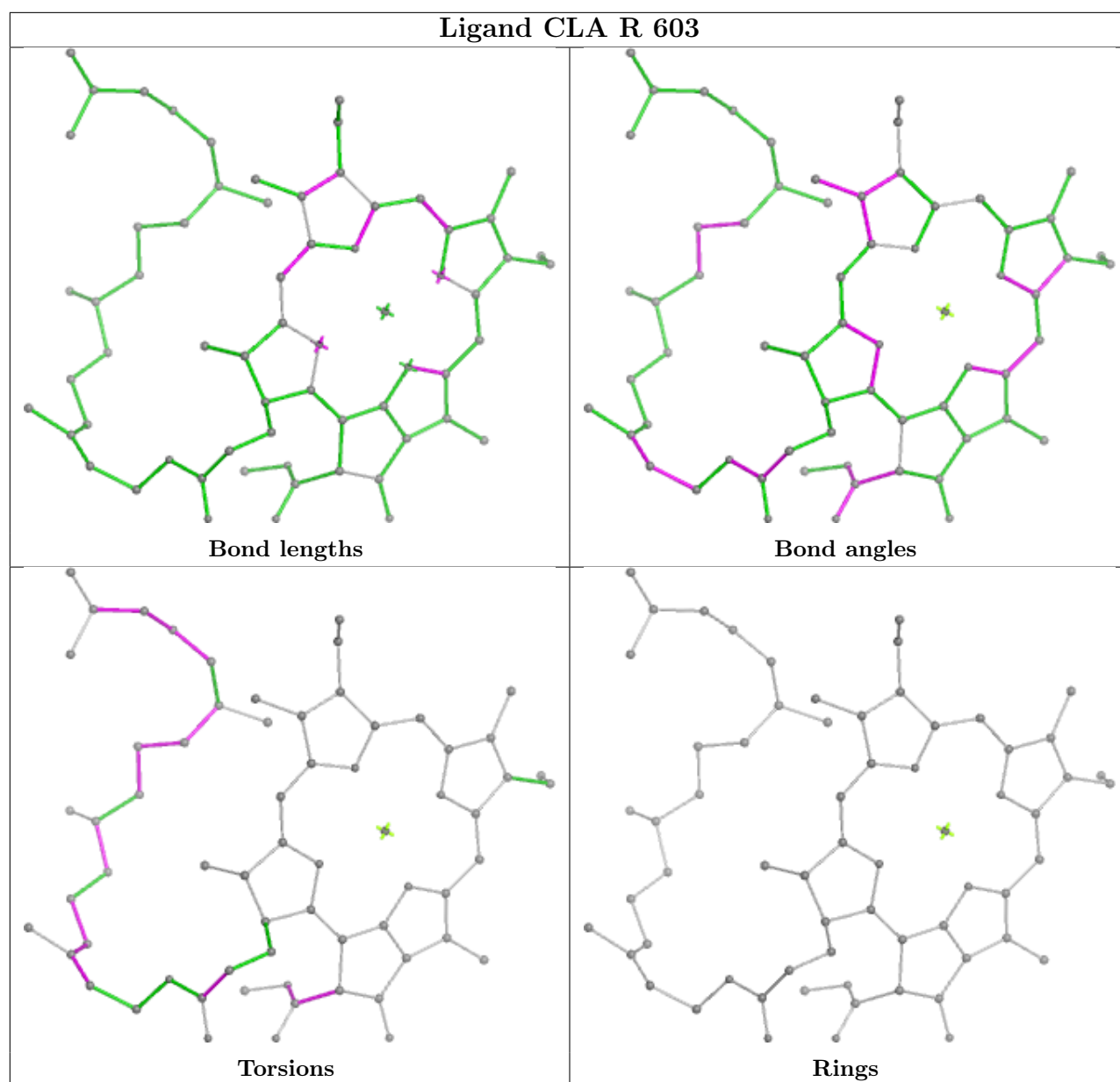


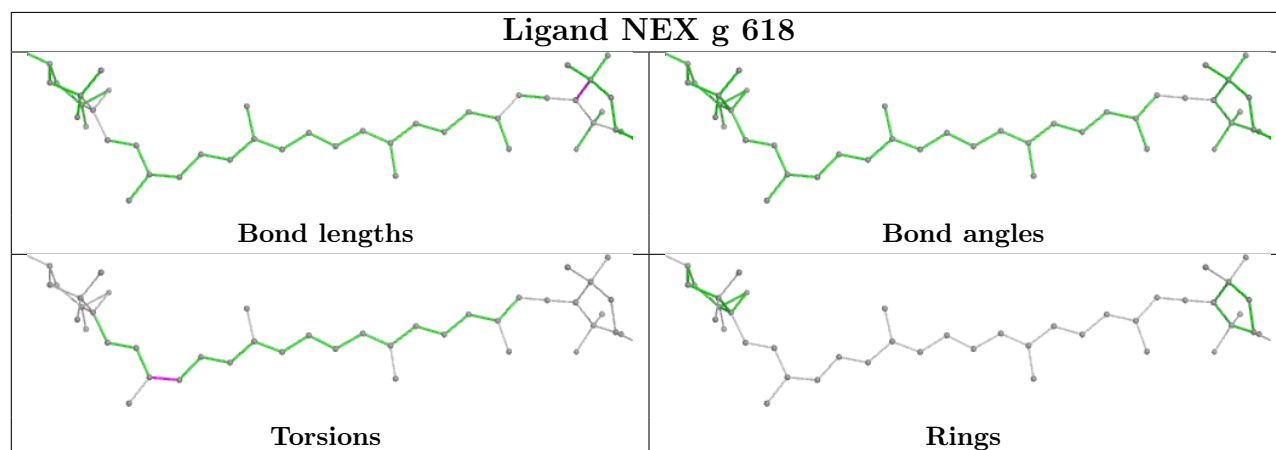
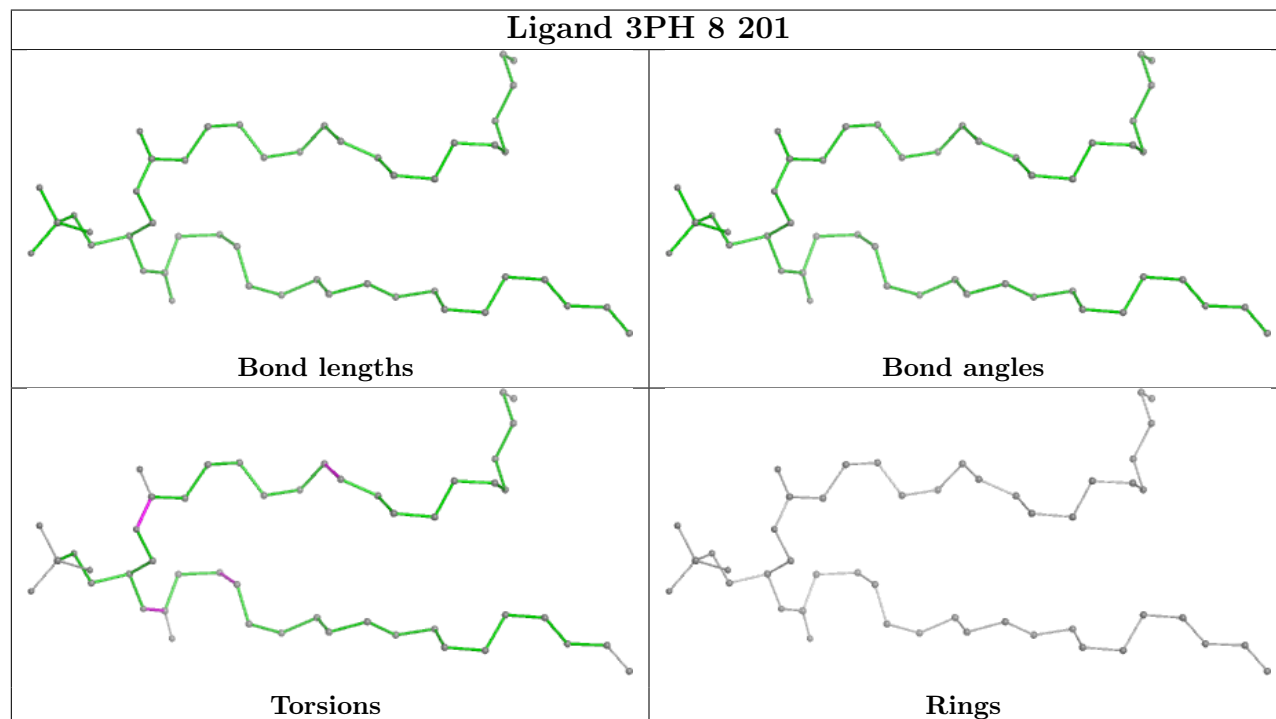
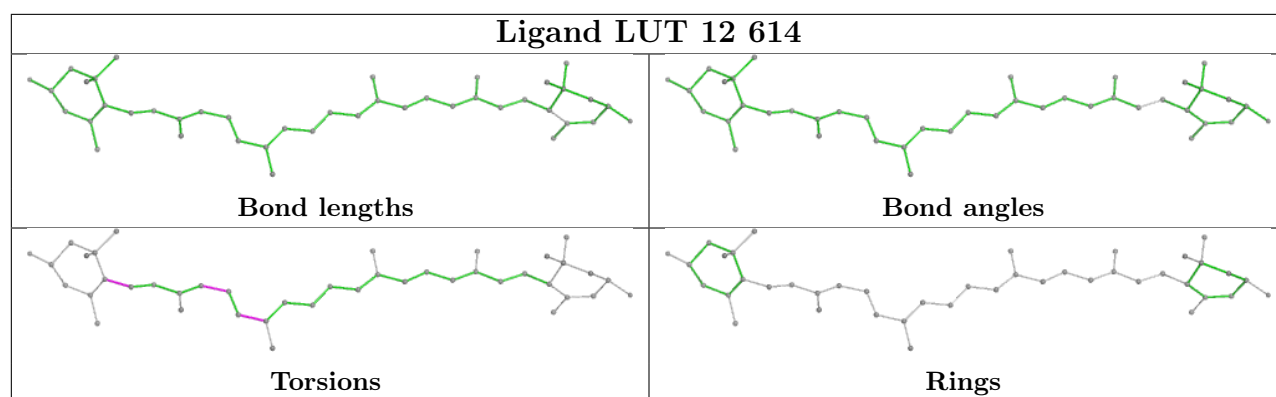


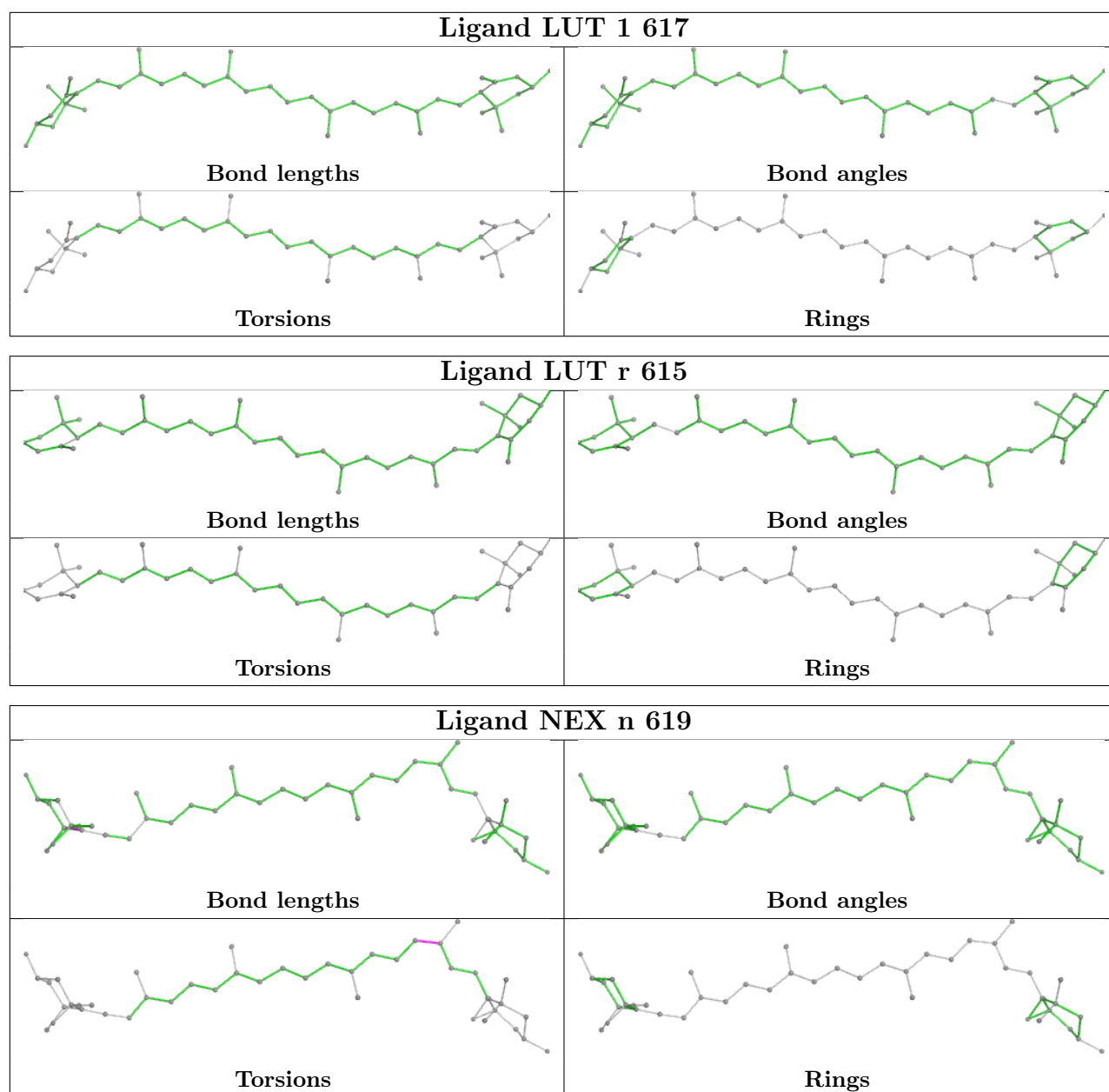
Ligand CLA r 612



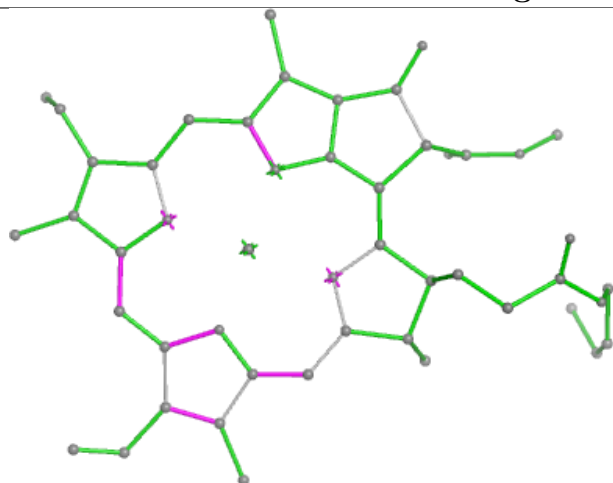




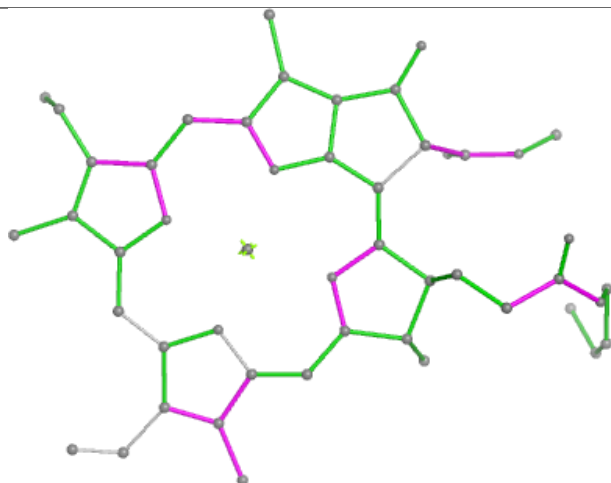




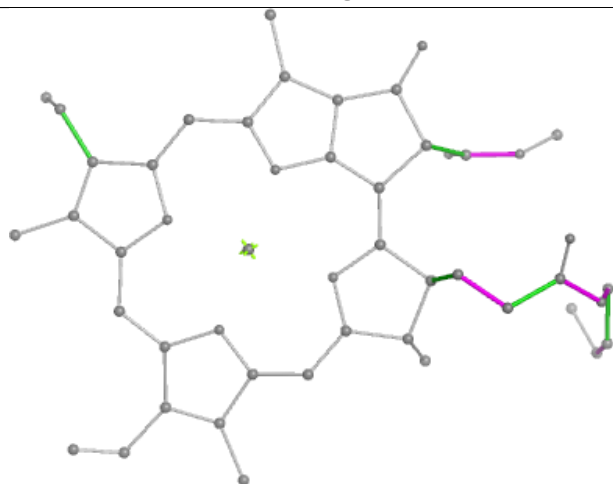
Ligand CLA R 611



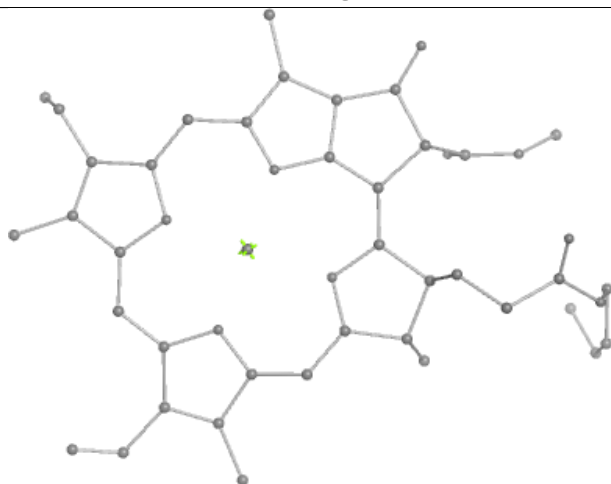
Bond lengths



Bond angles

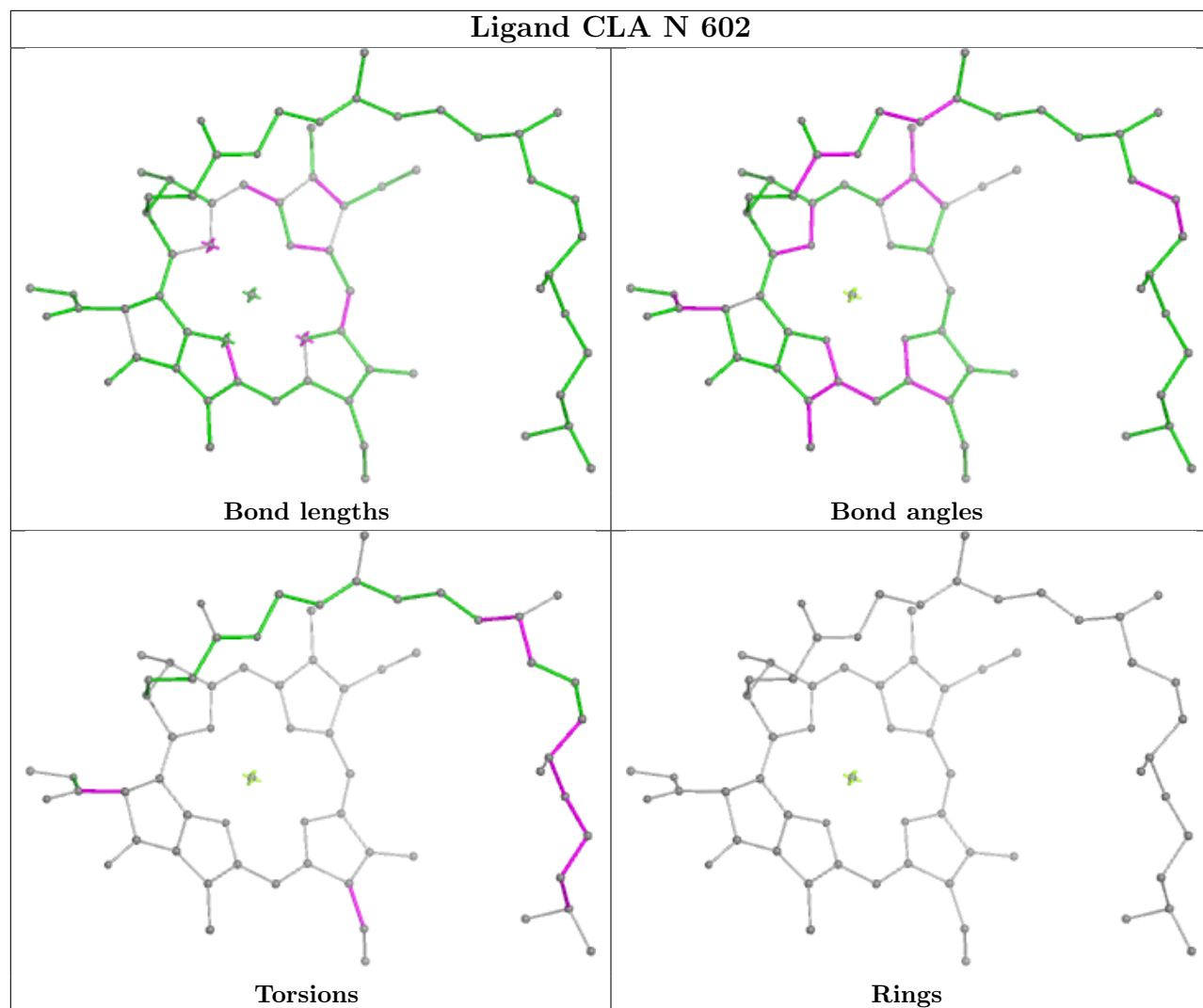


Torsions

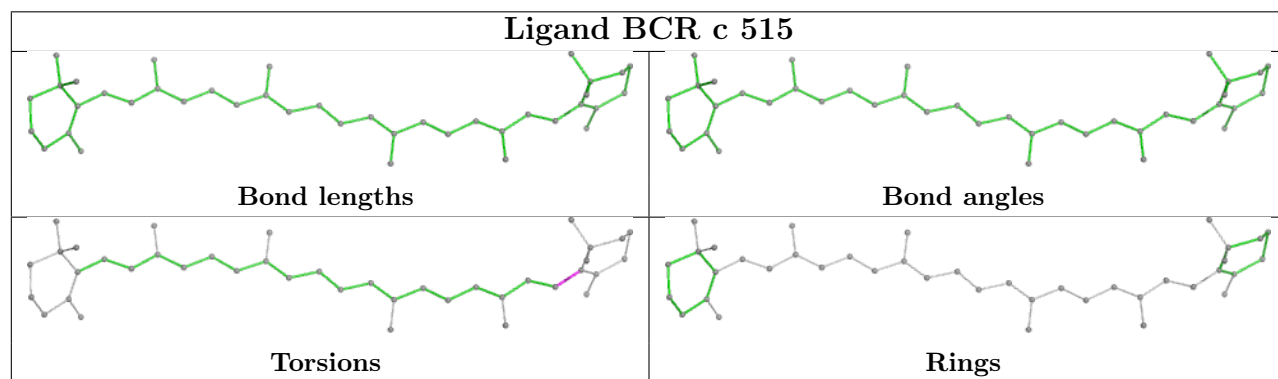


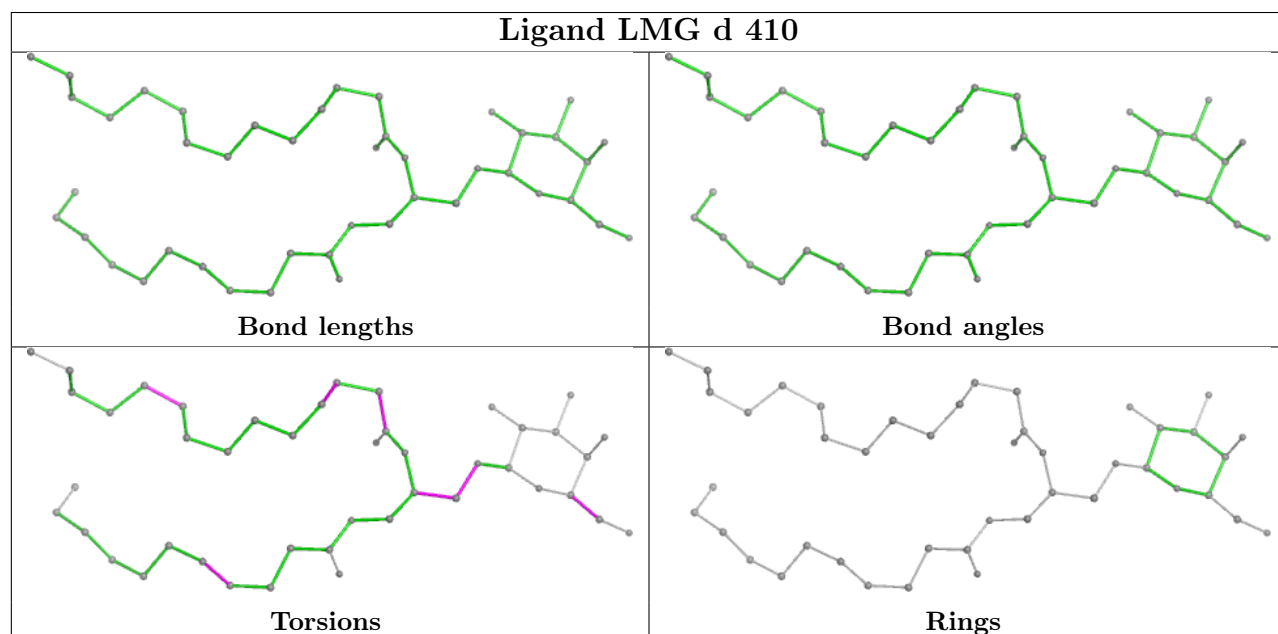
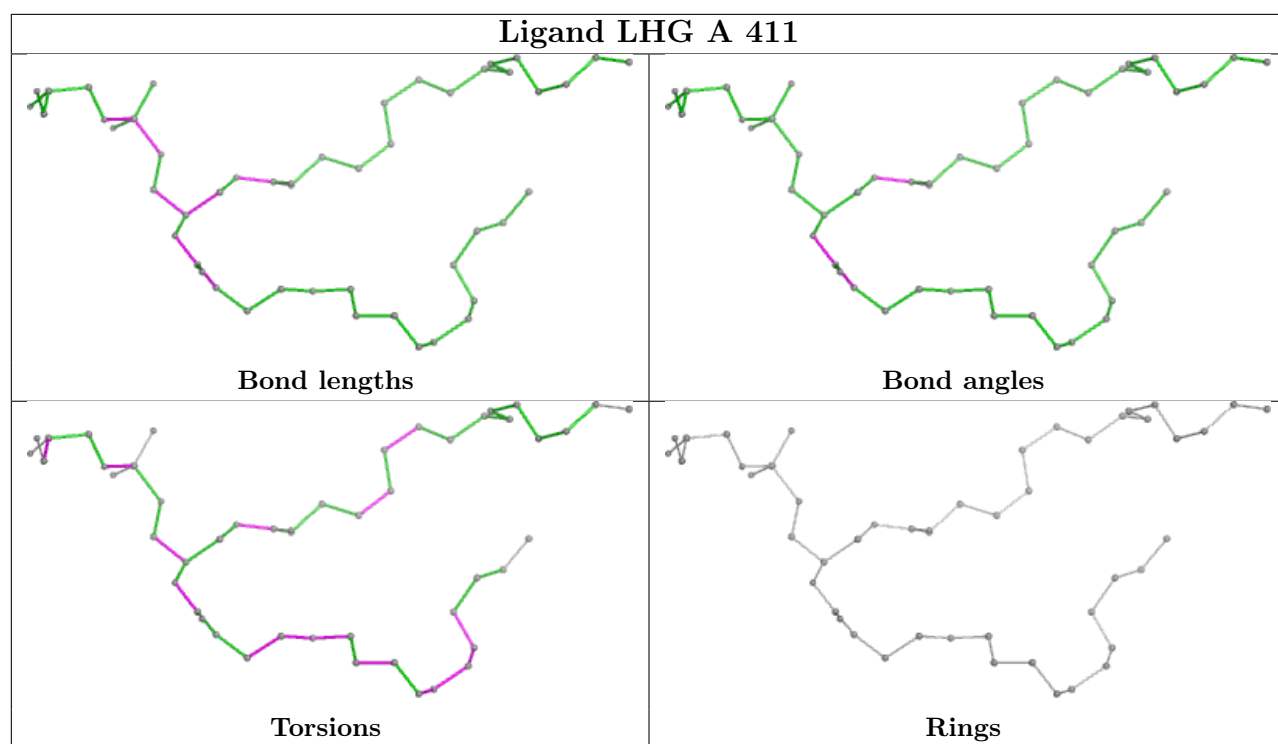
Rings

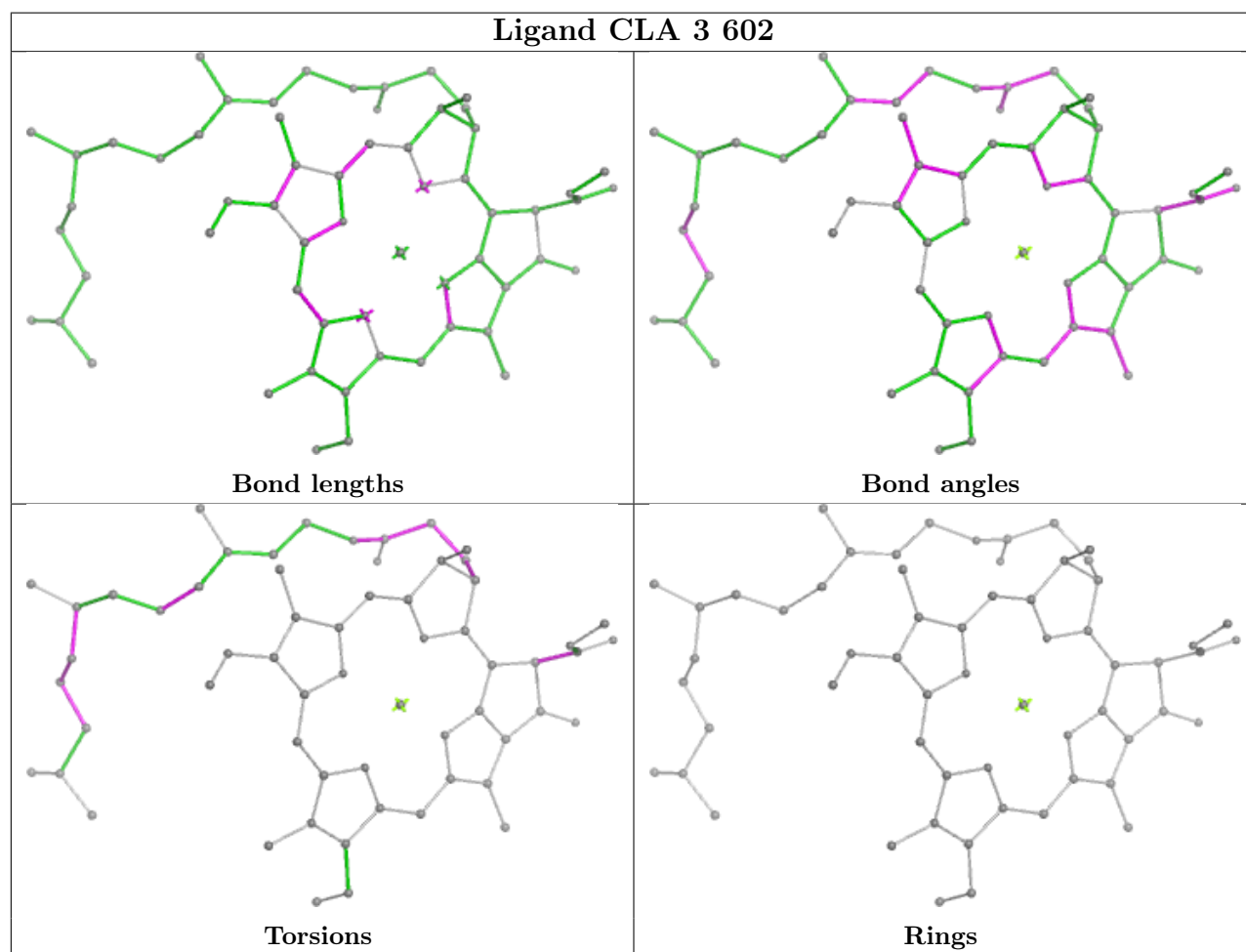
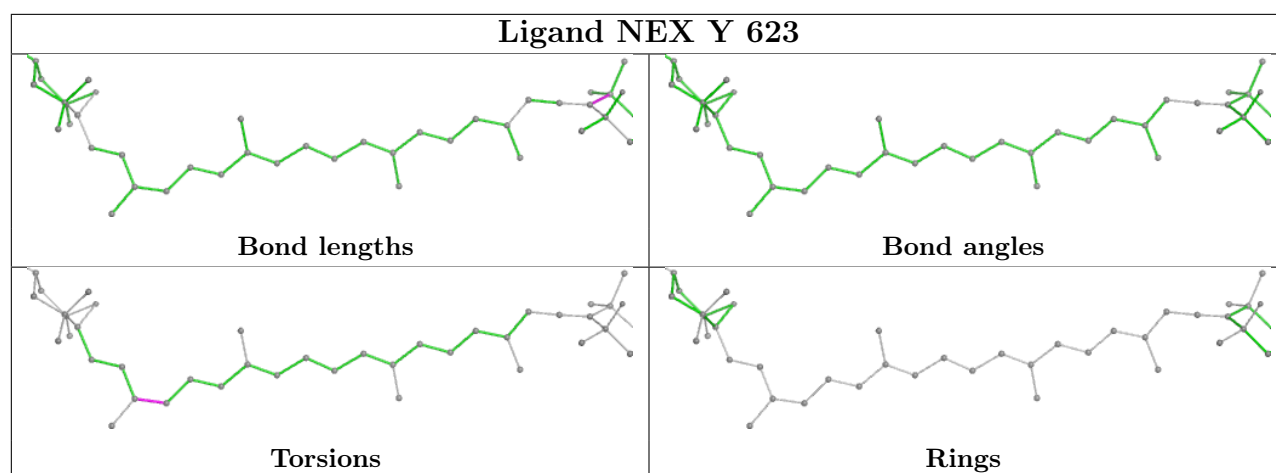
Ligand CLA N 602



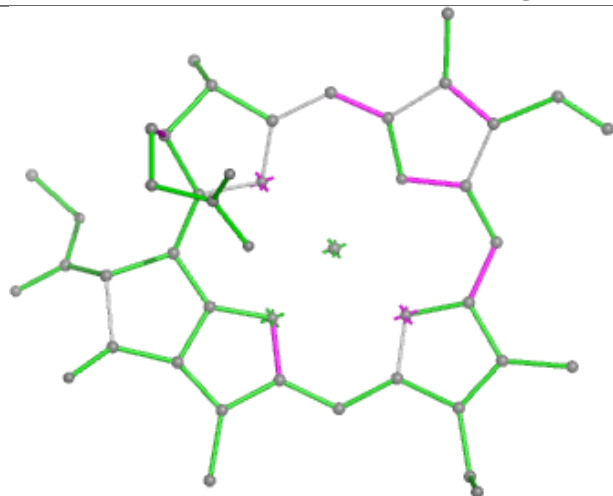
Ligand BCR c 515



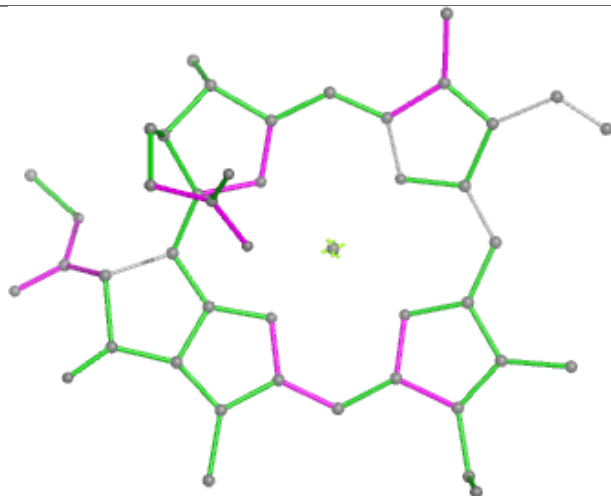




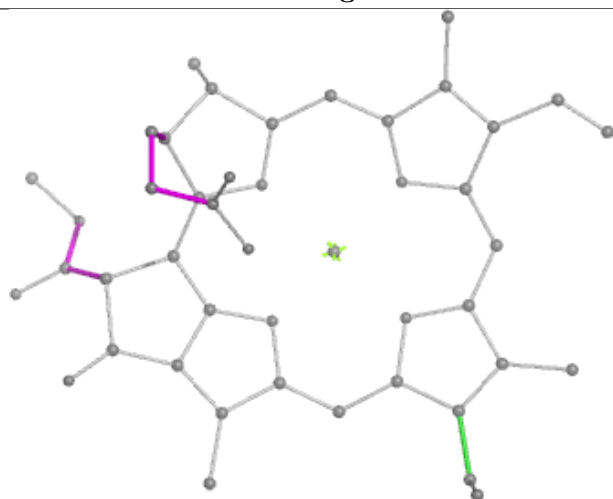
Ligand CLA n 614



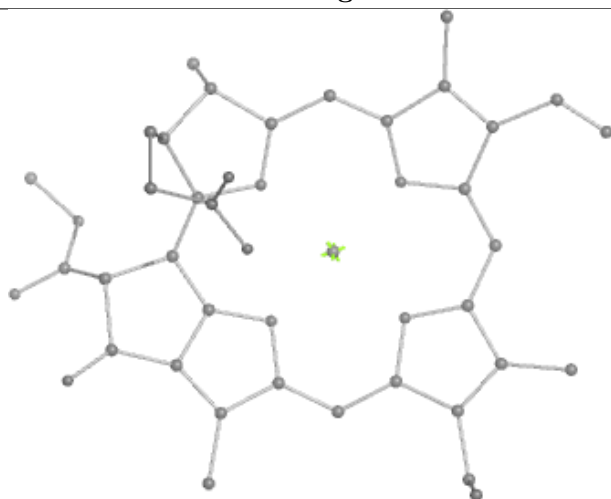
Bond lengths



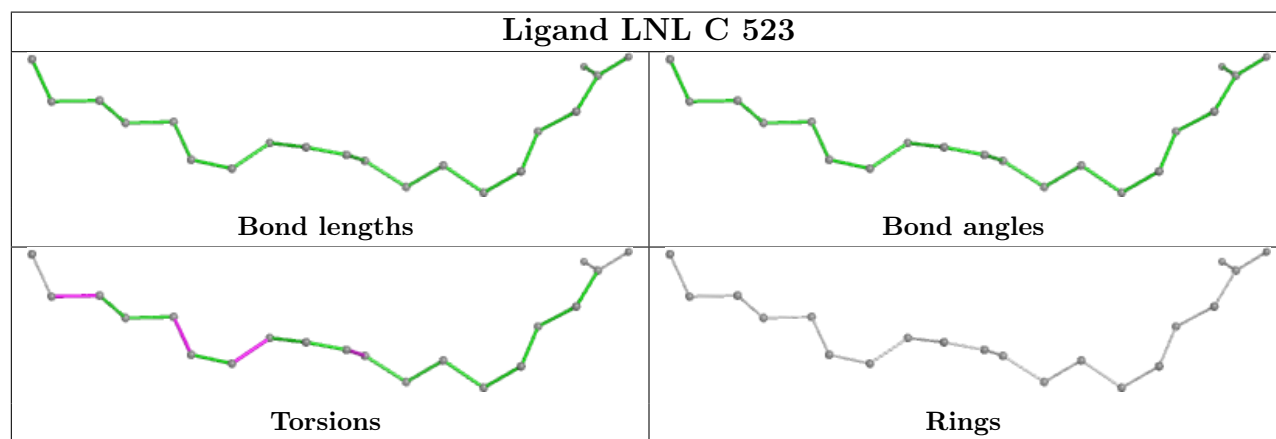
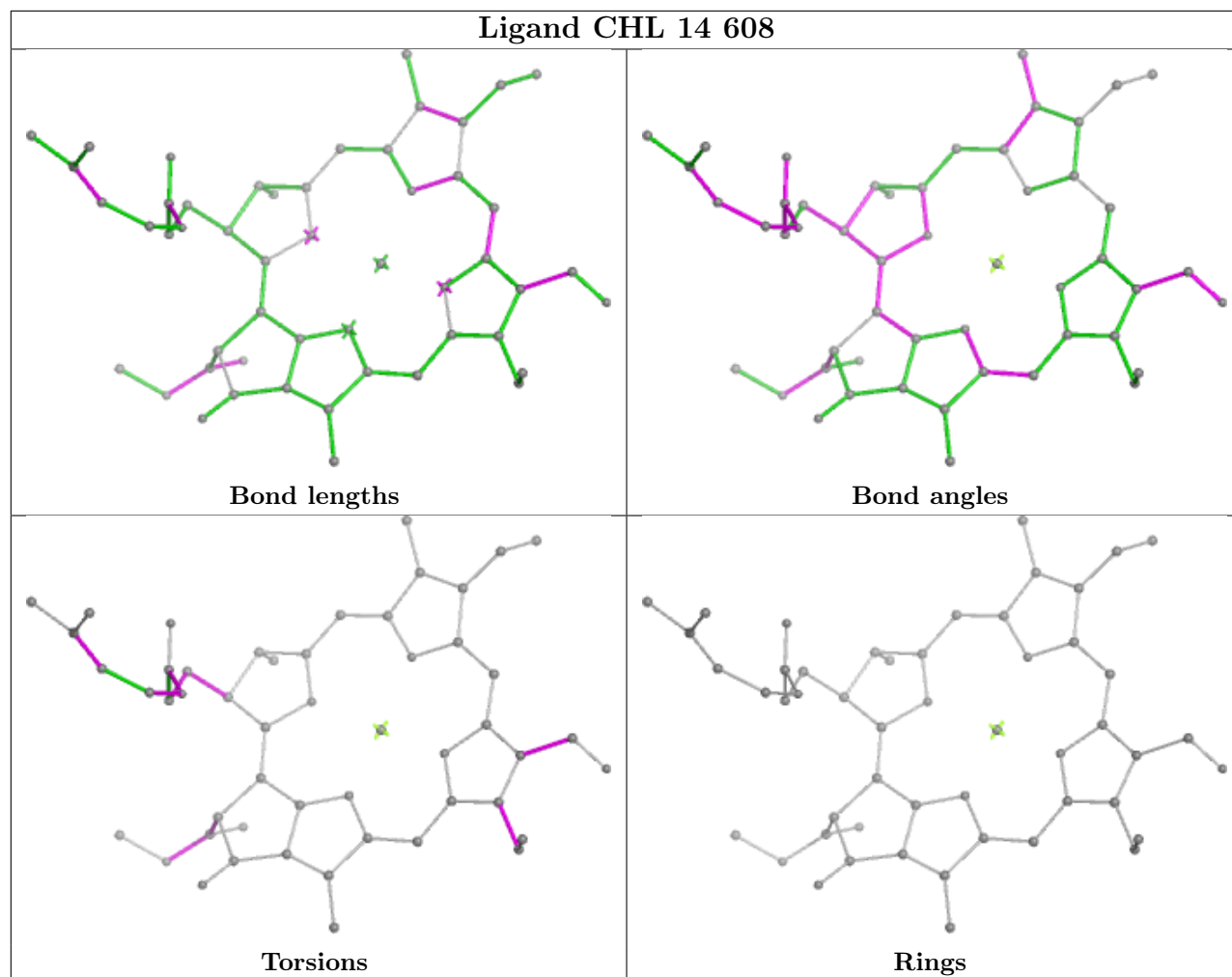
Bond angles

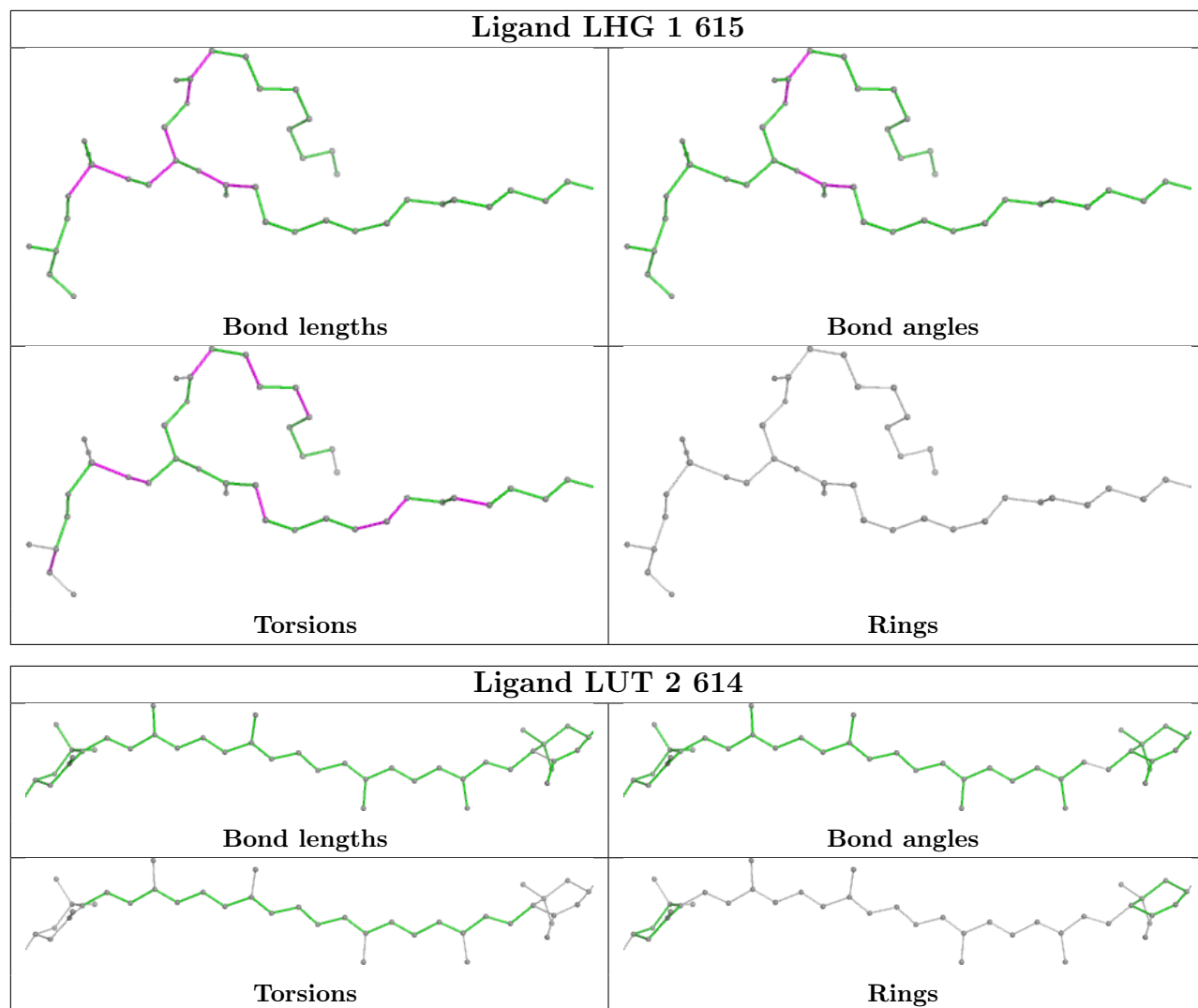


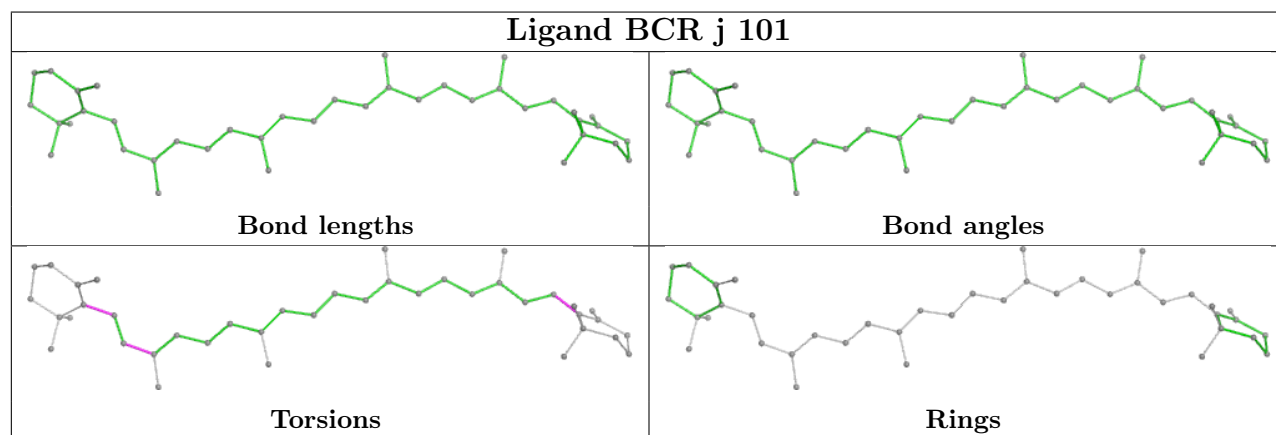
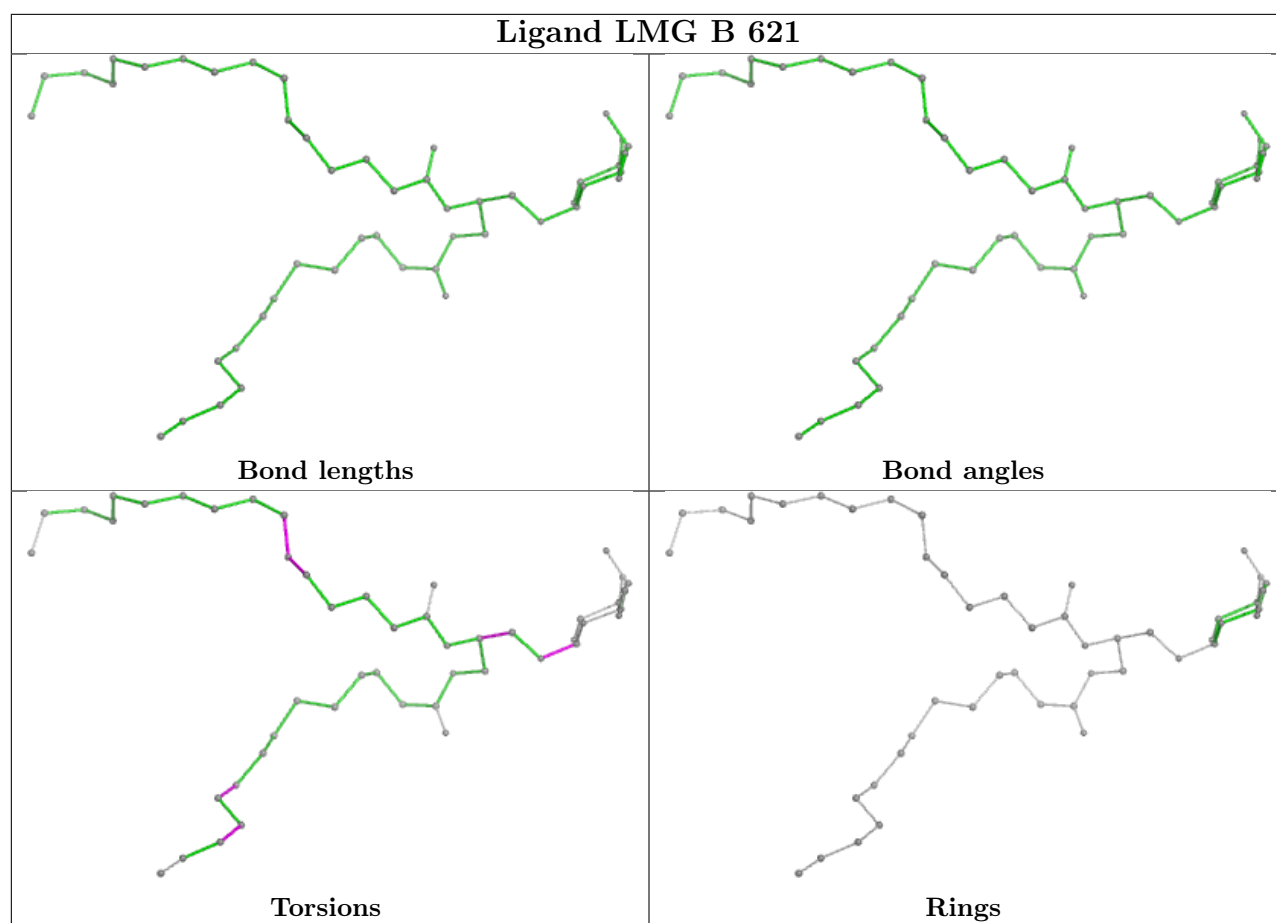
Torsions

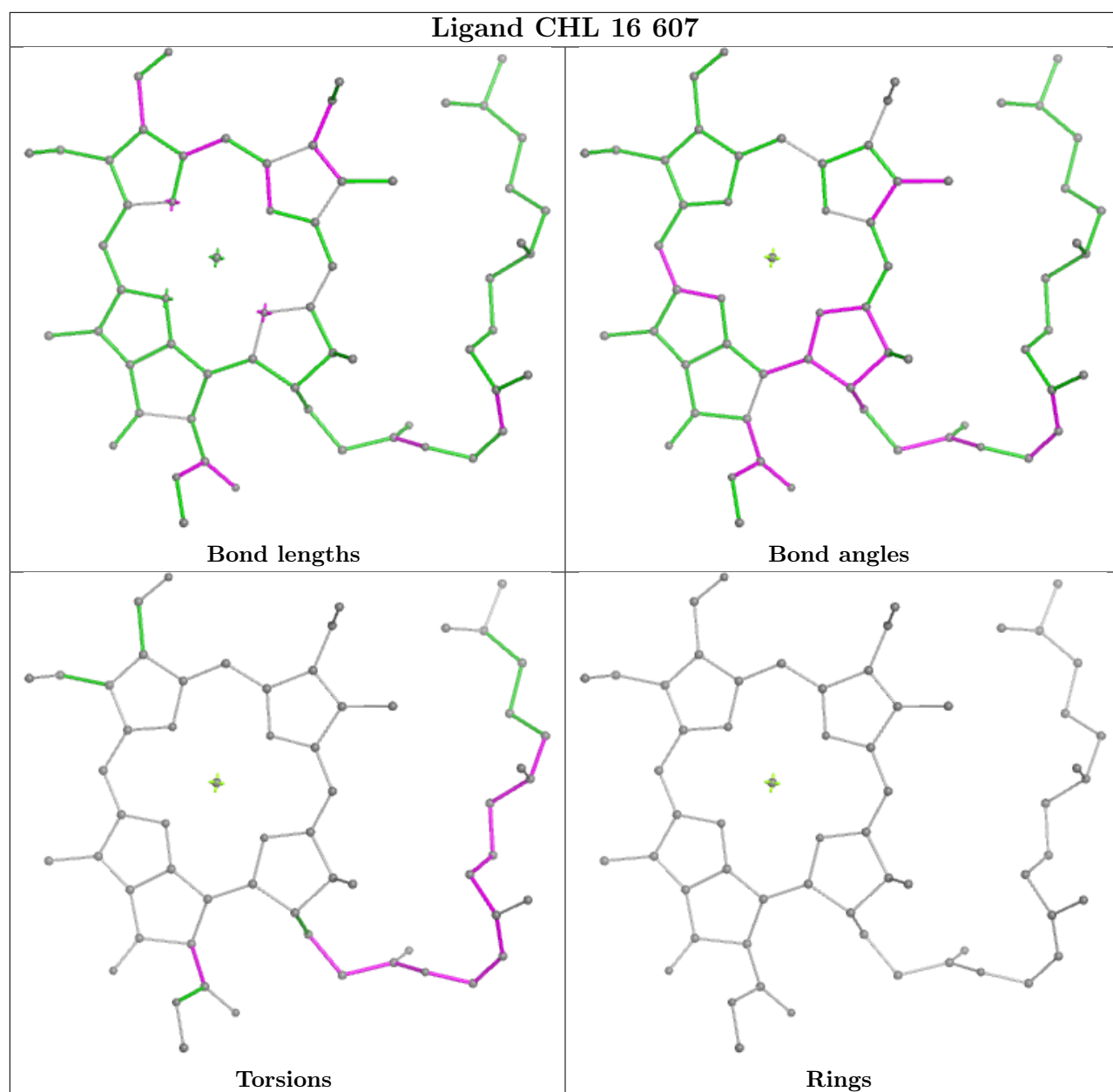


Rings

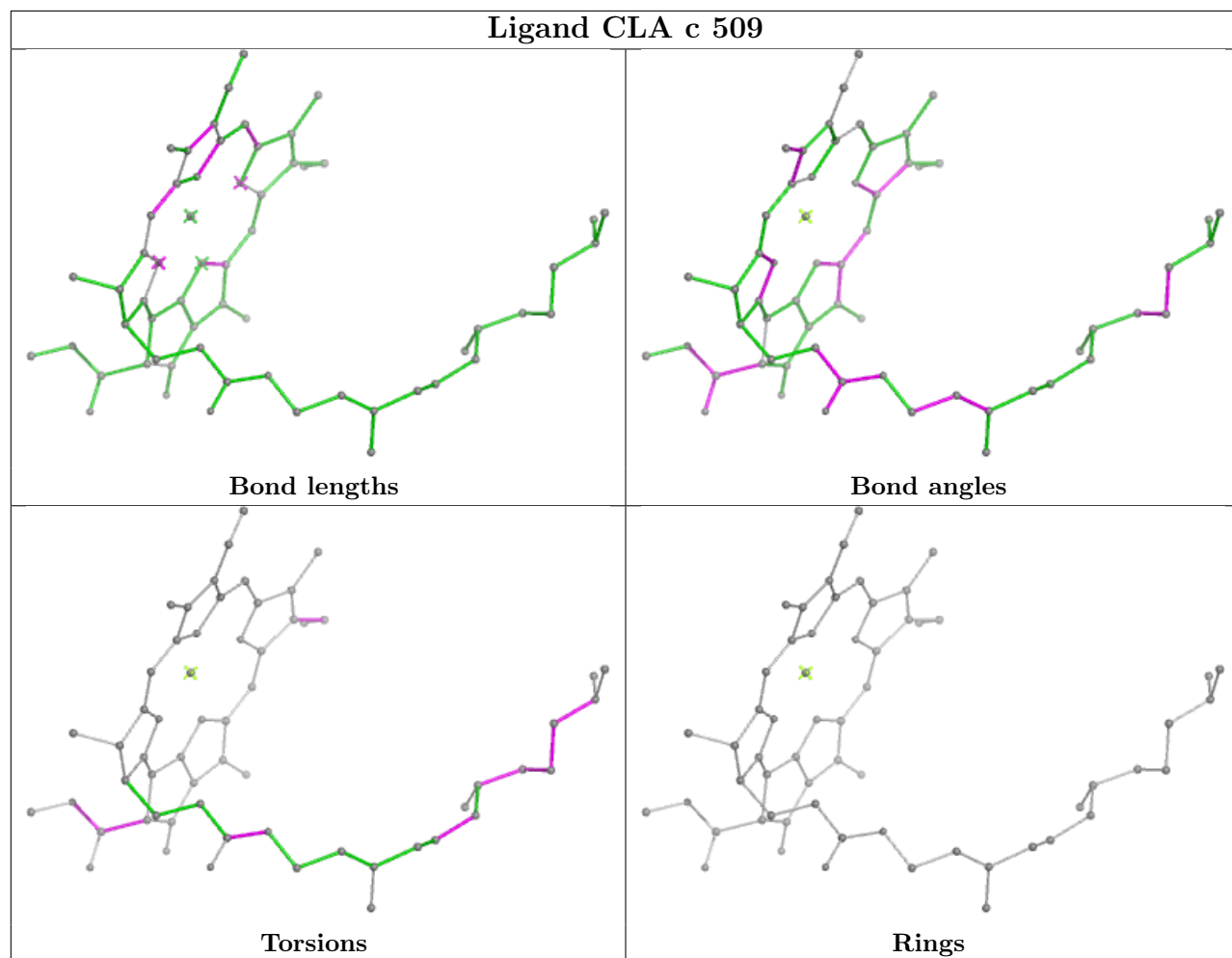




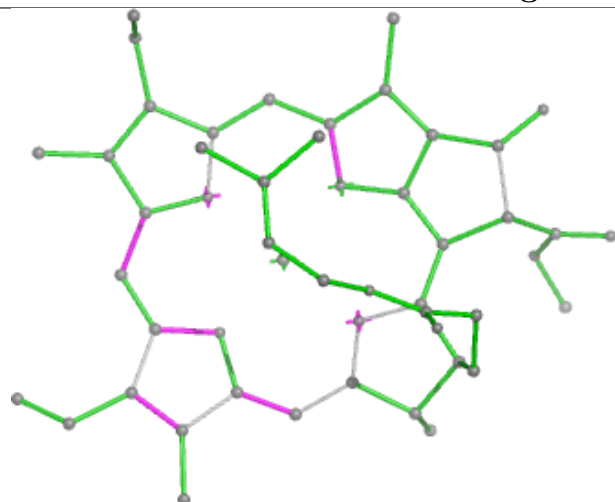




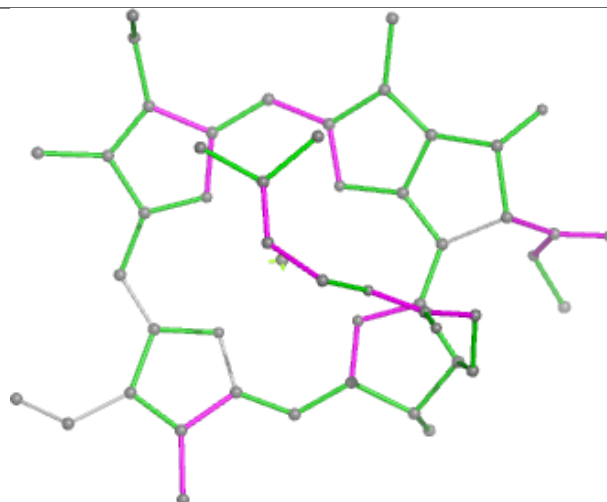
Ligand CLA c 509



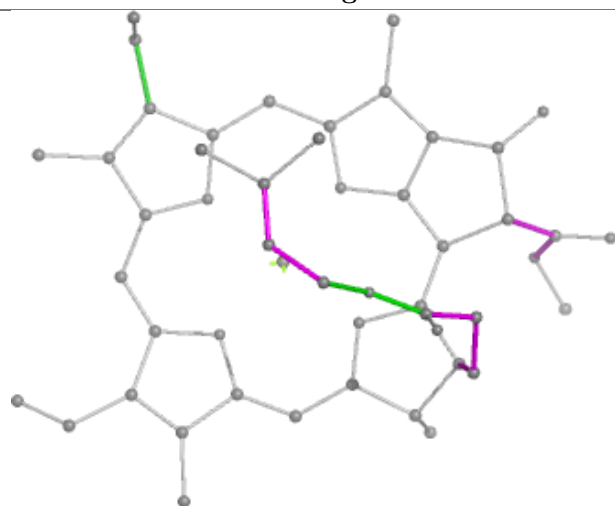
Ligand CLA 3 614



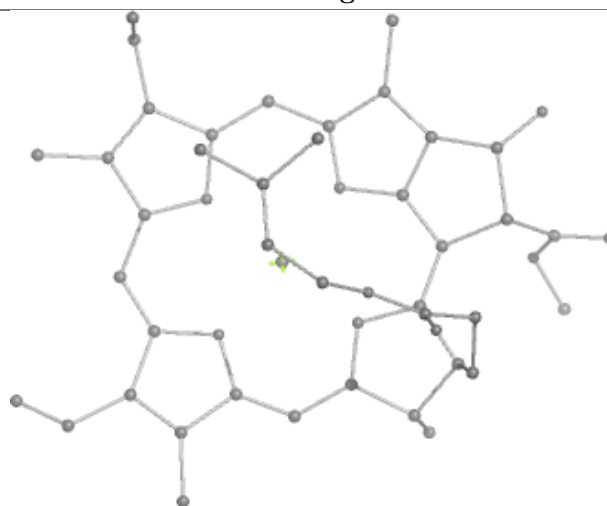
Bond lengths



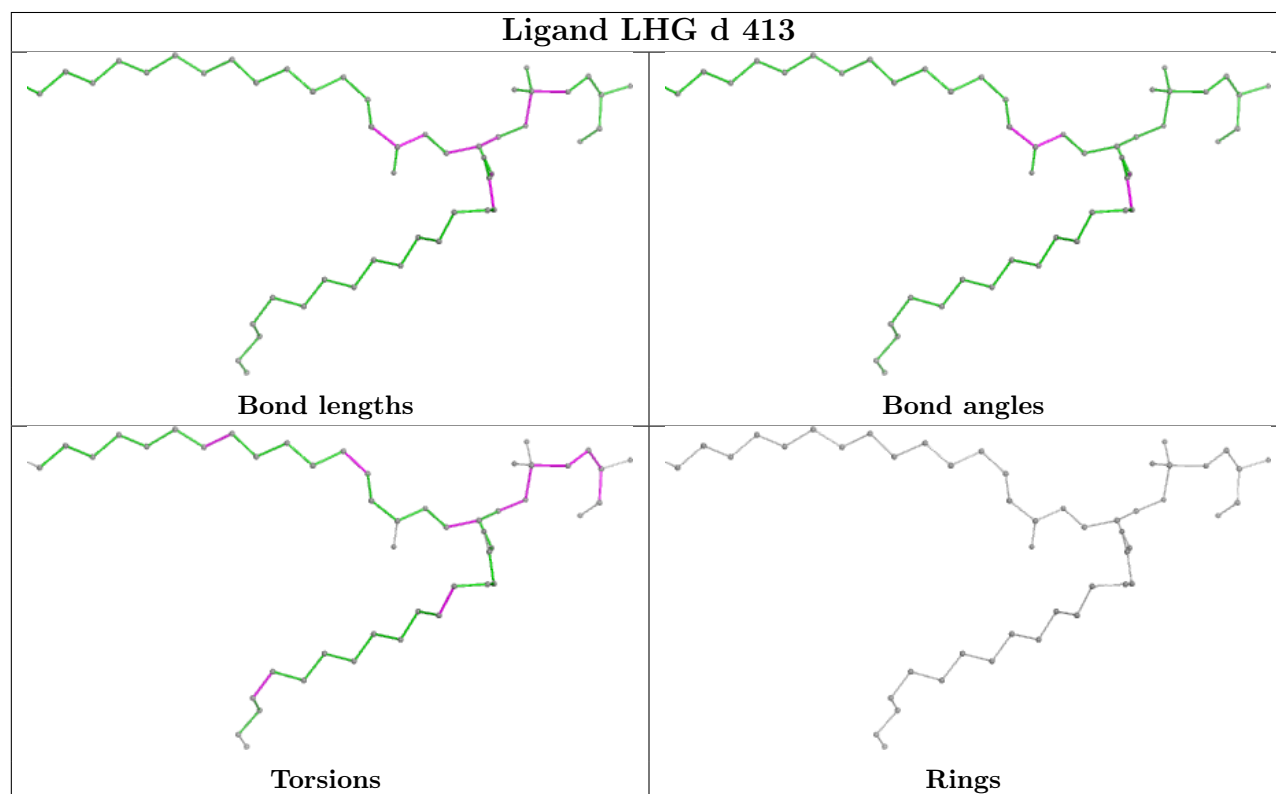
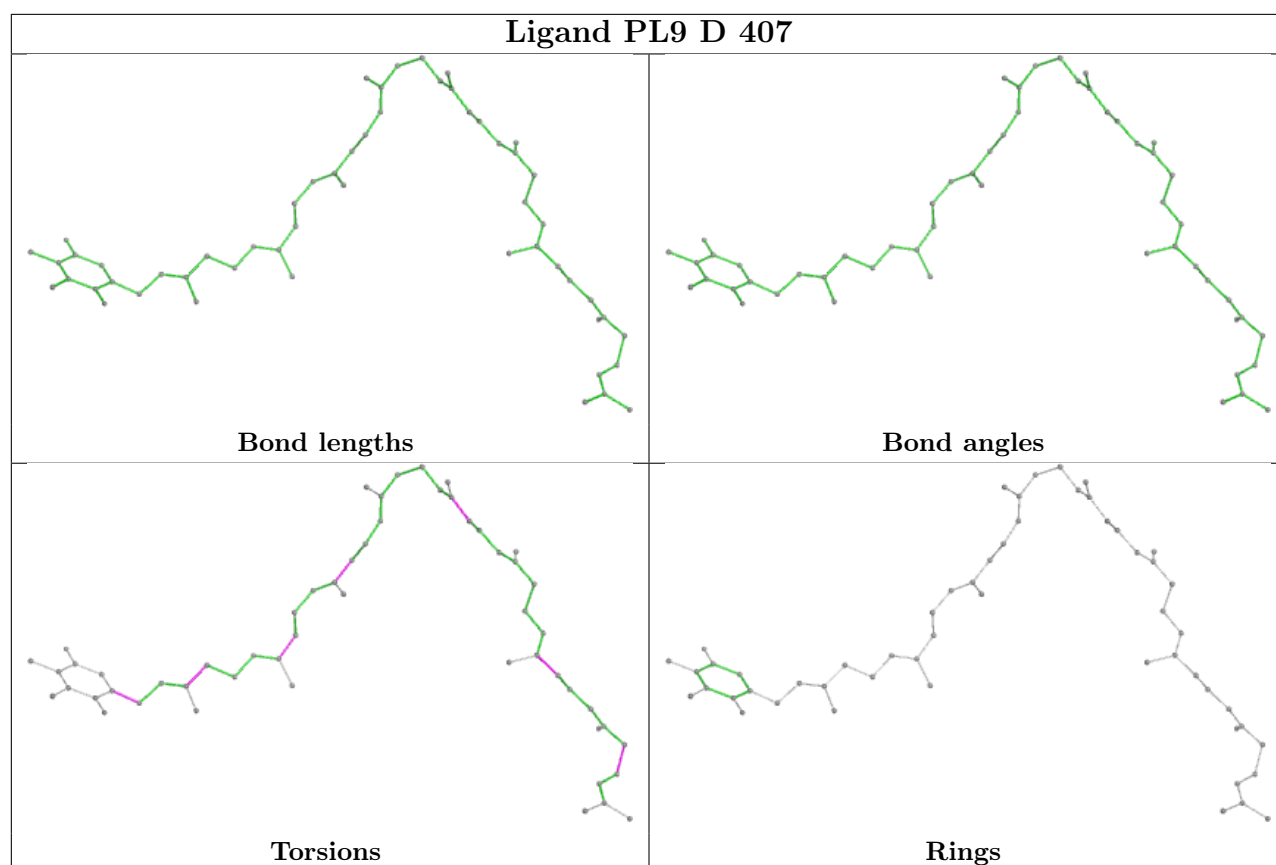
Bond angles

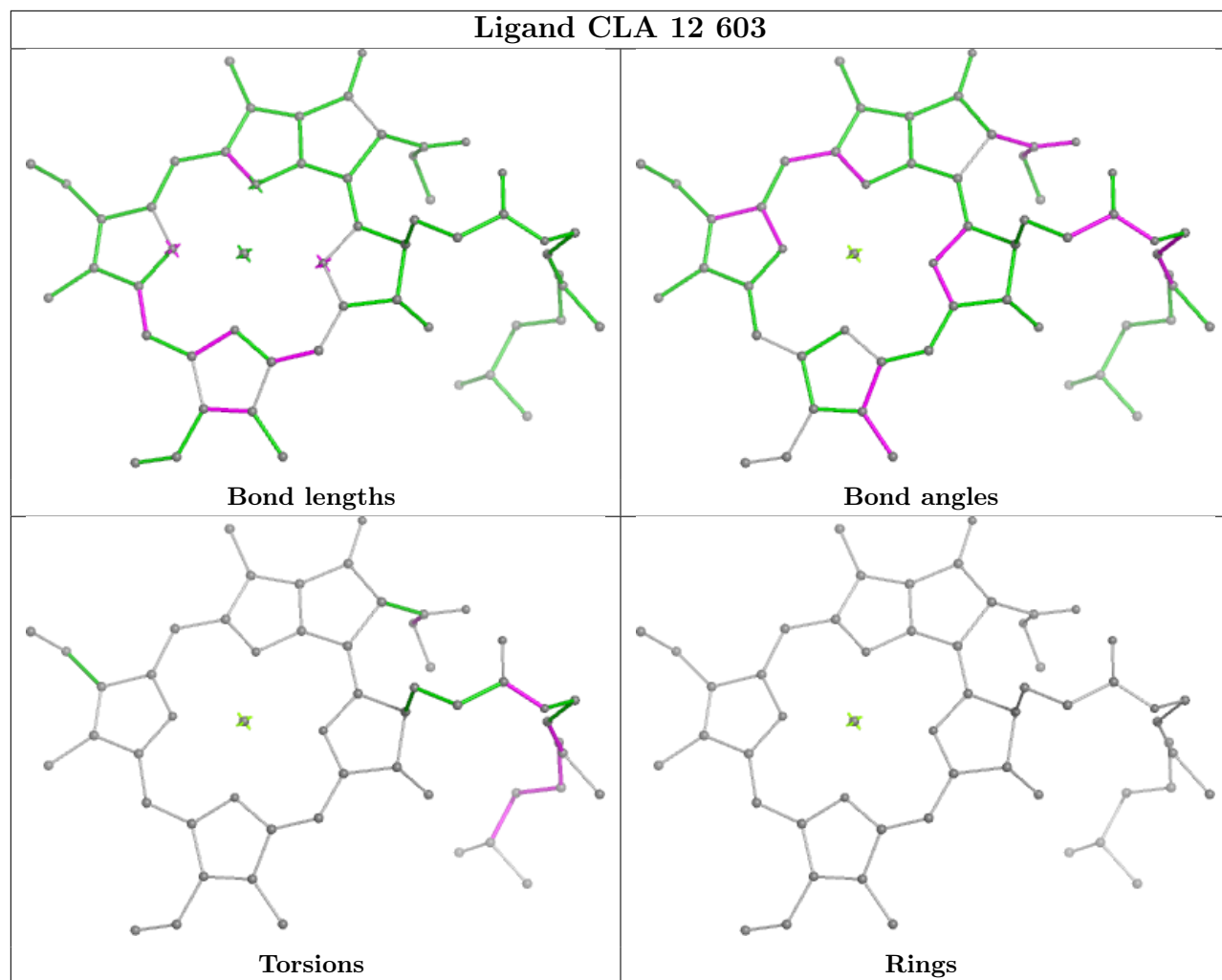


Torsions

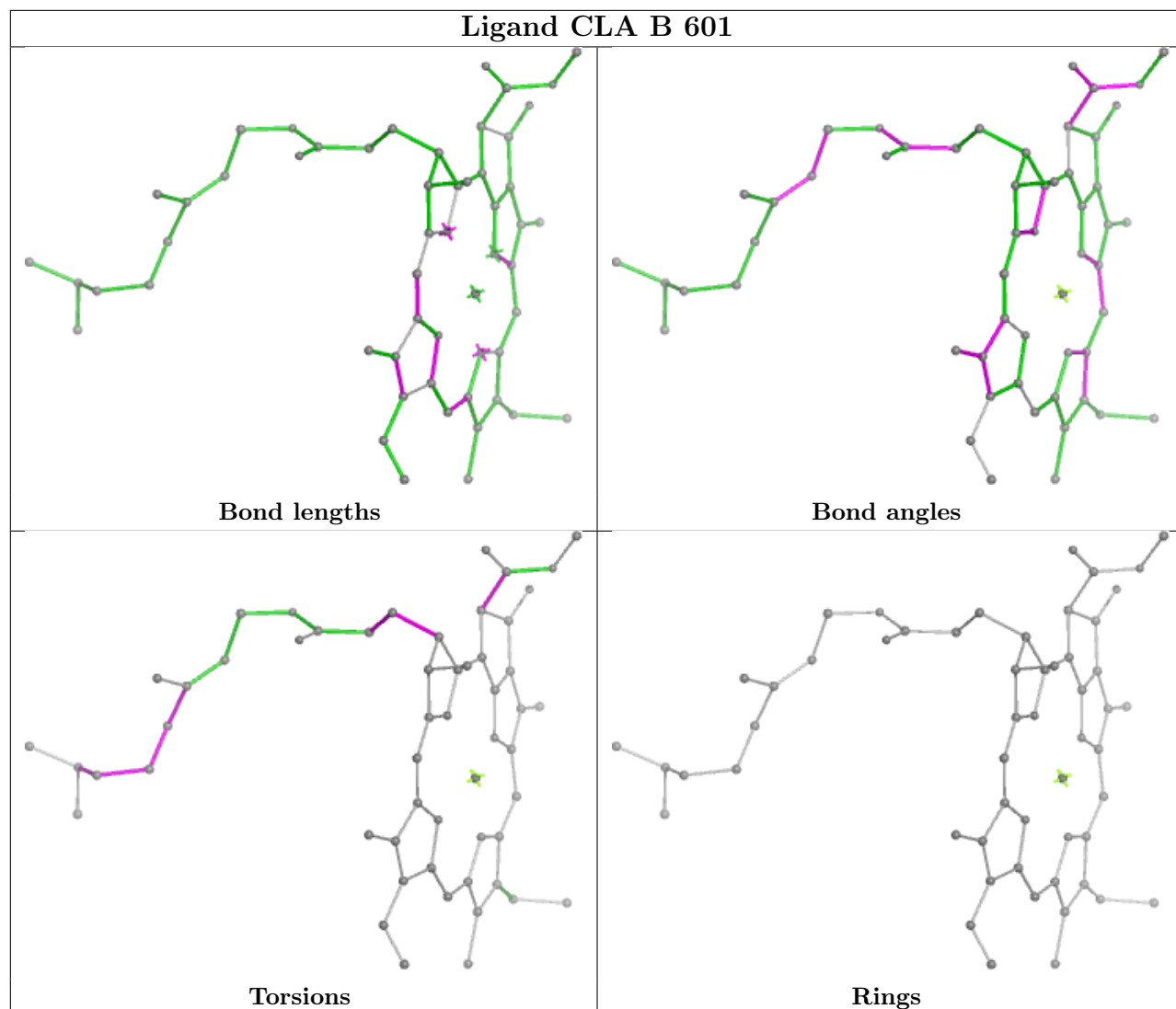


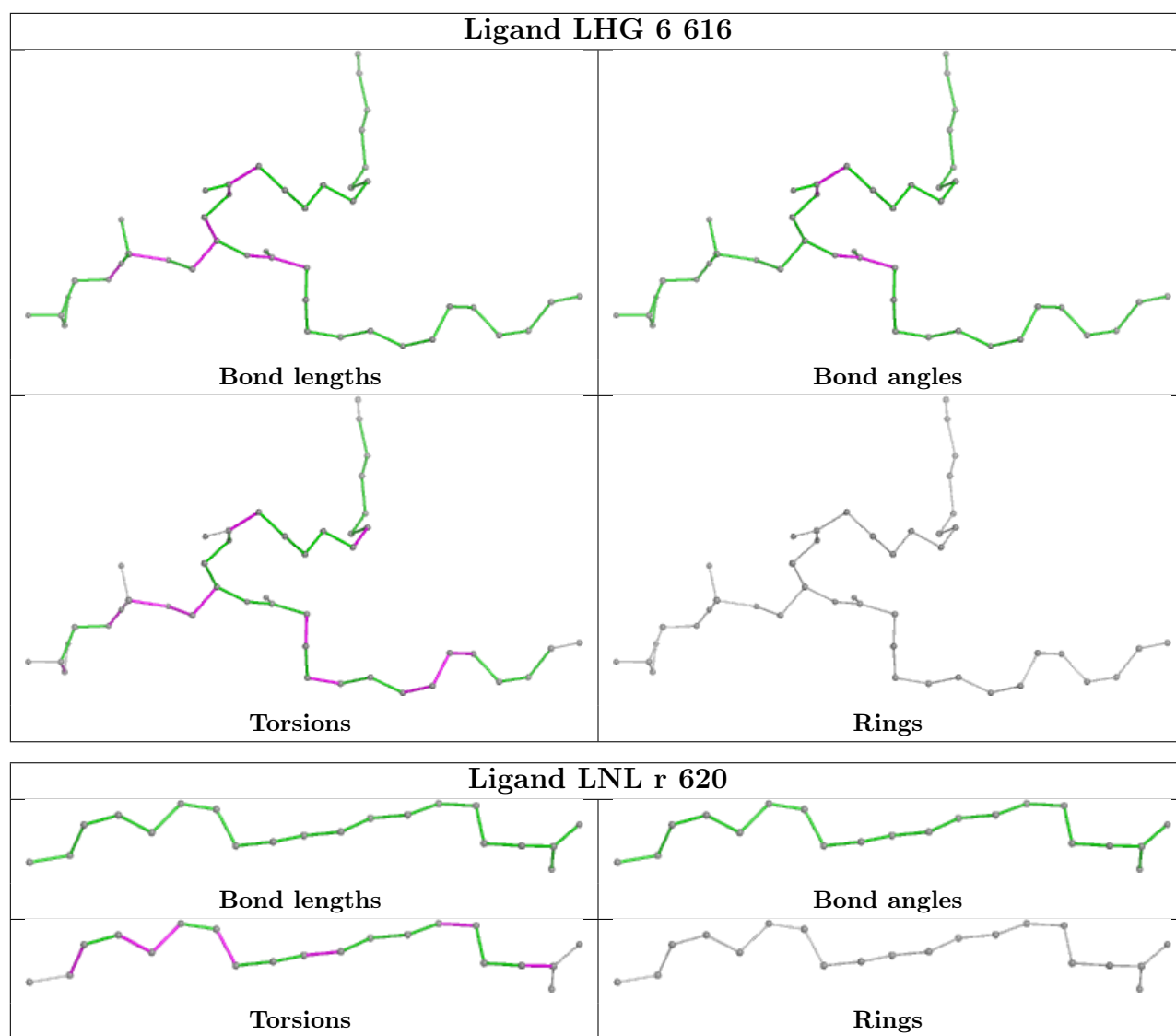
Rings

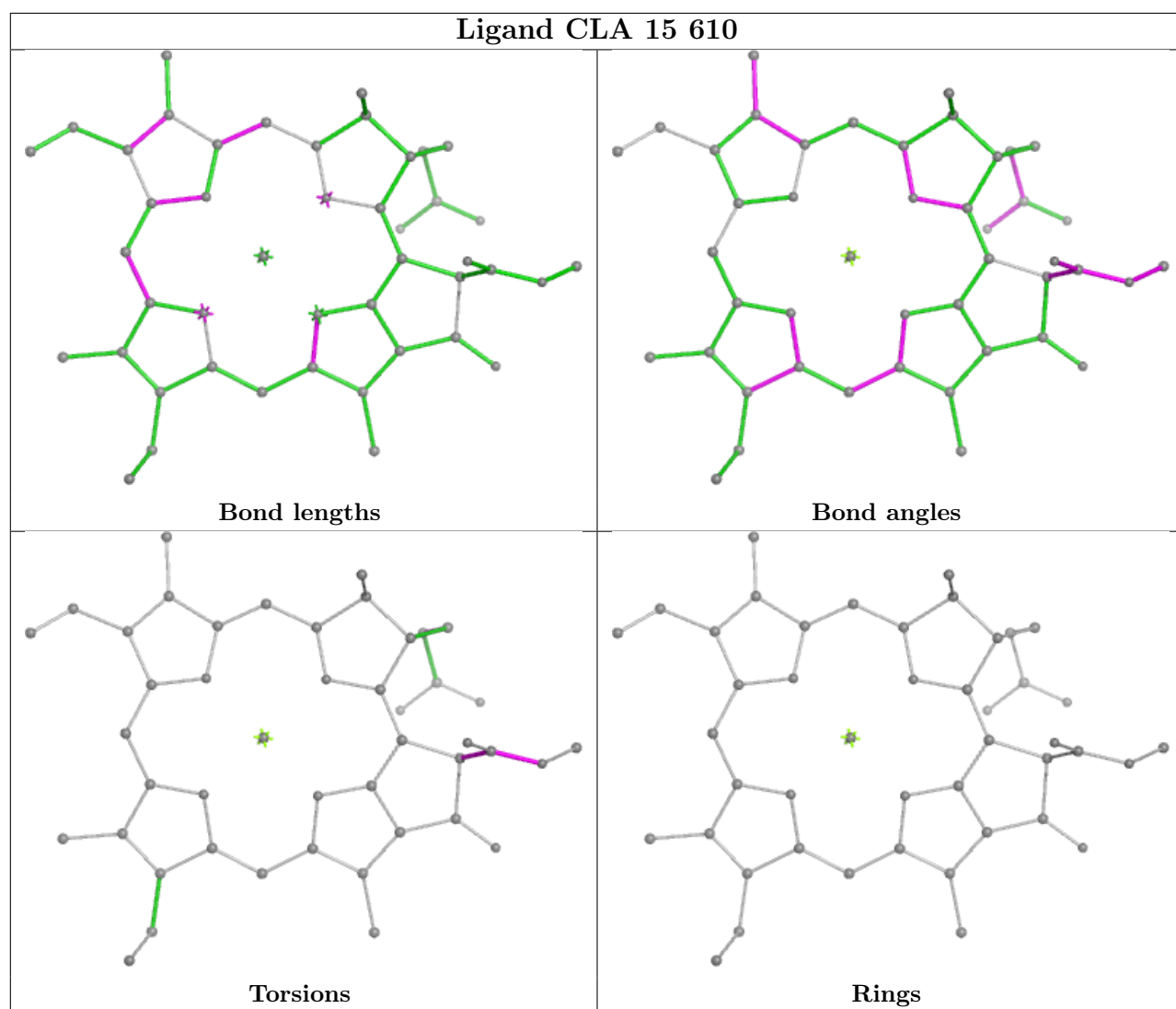


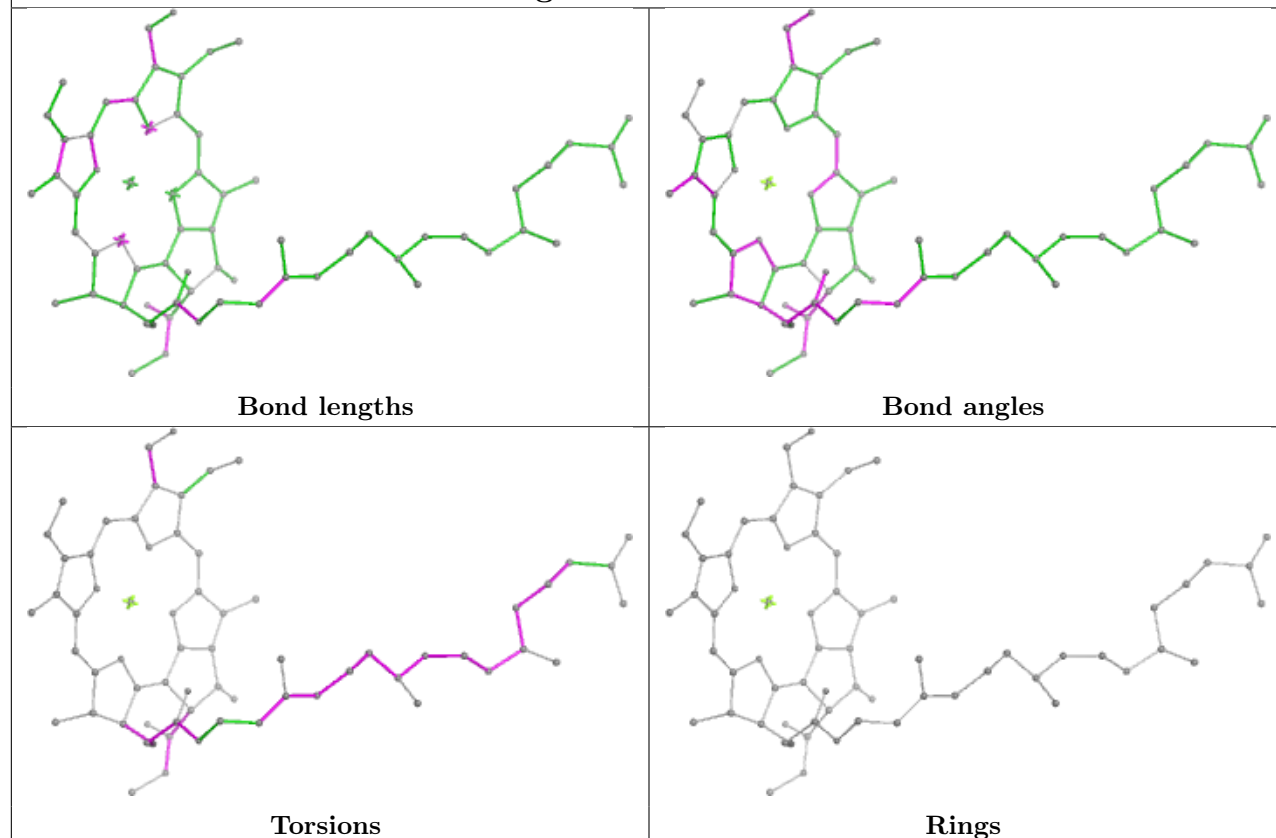
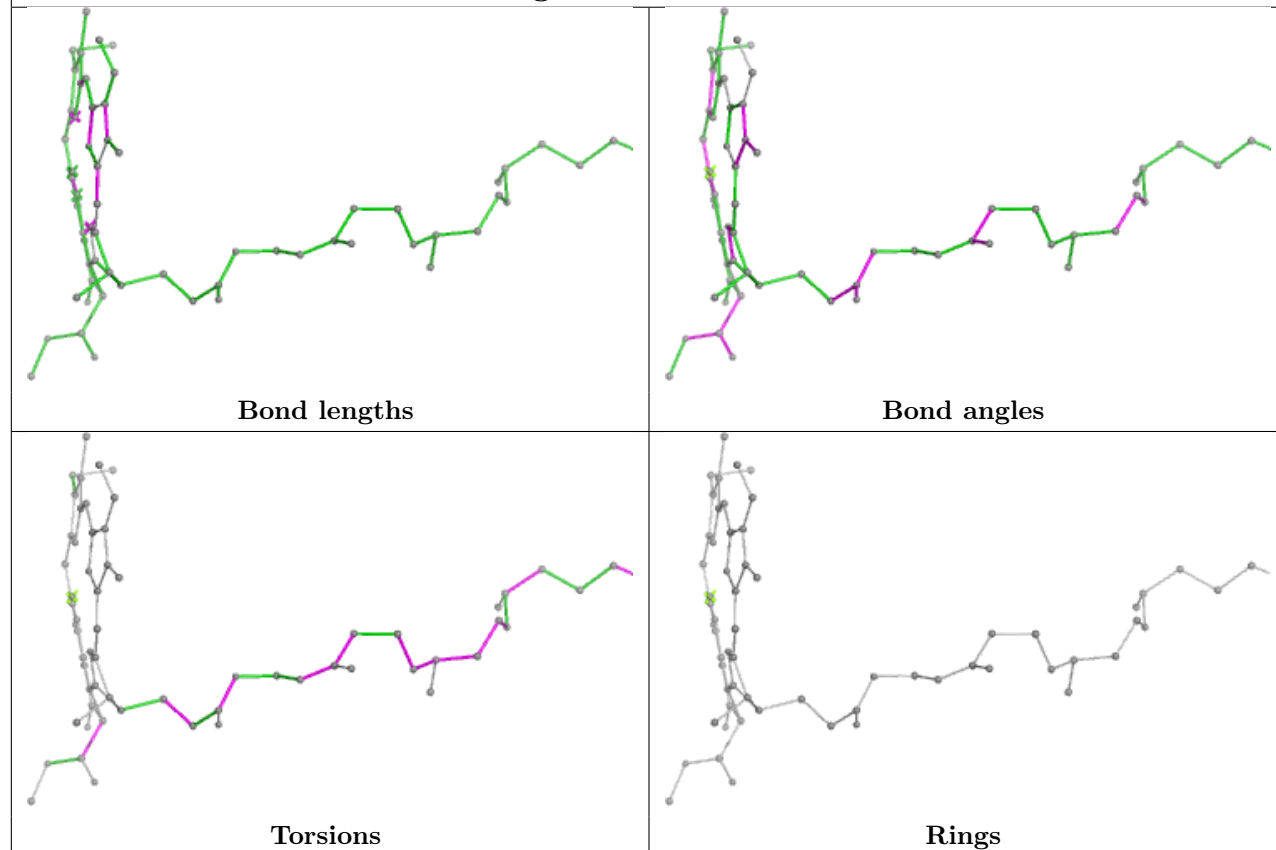


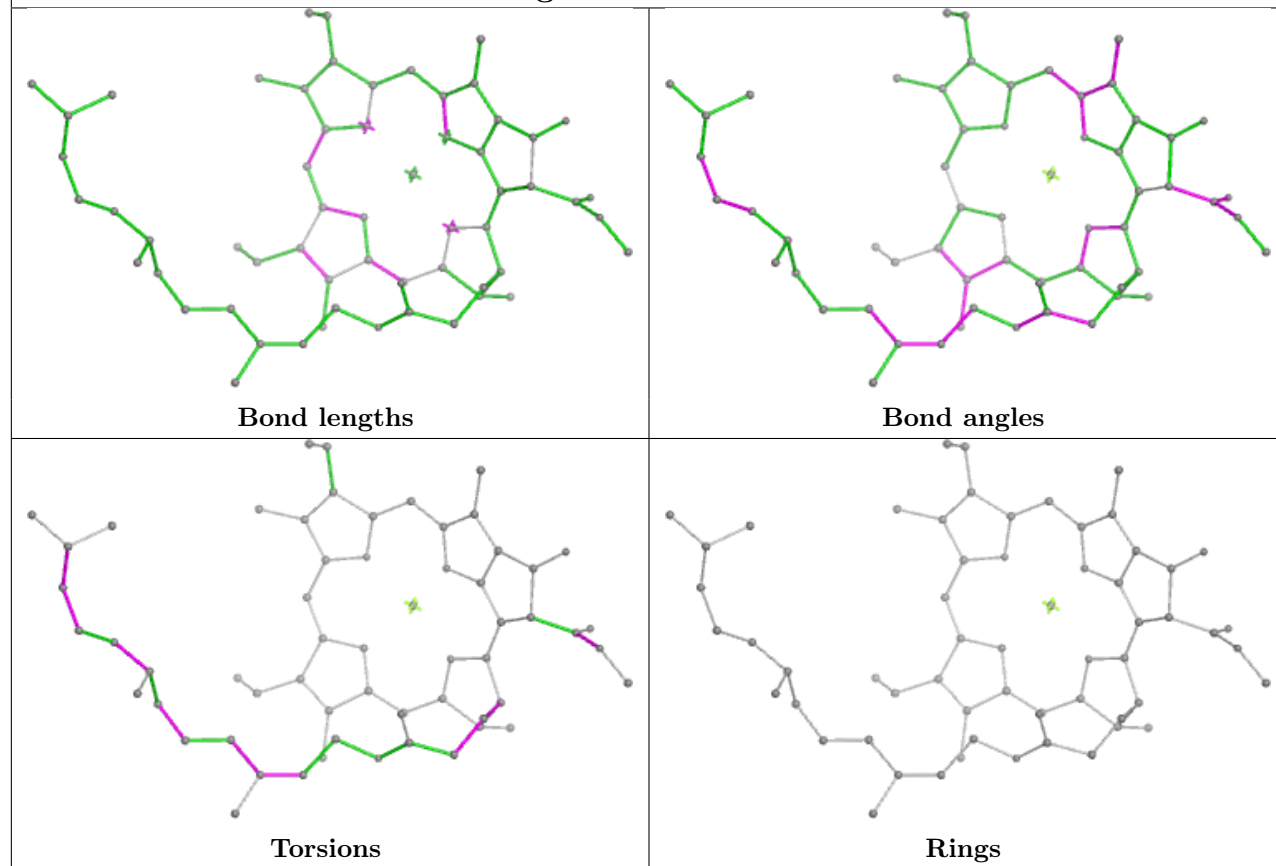
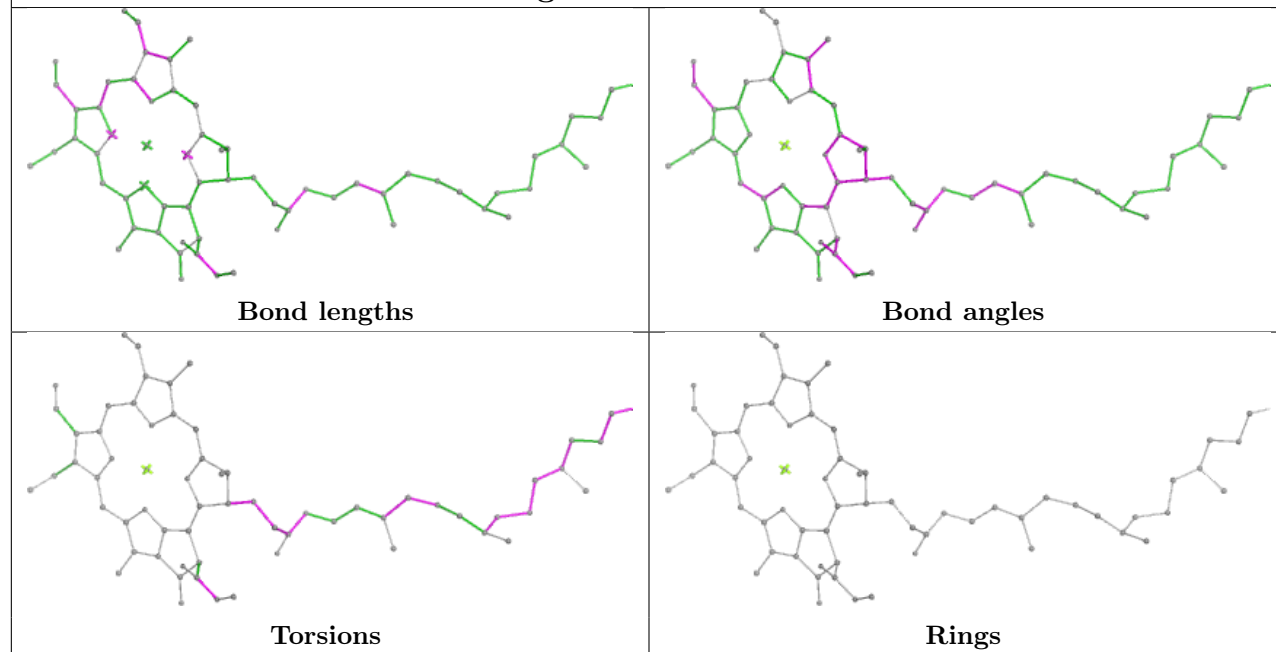
Ligand CLA B 601

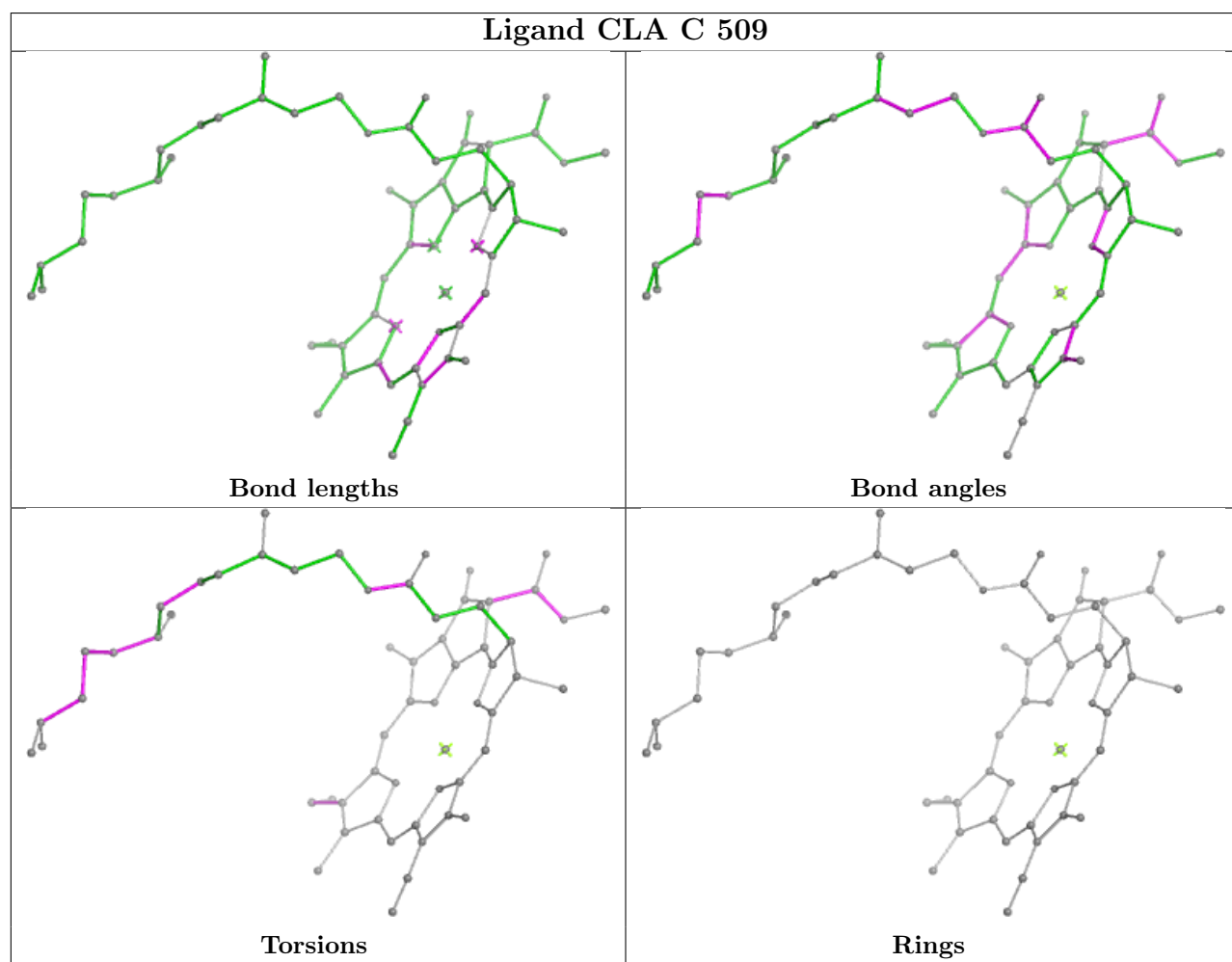
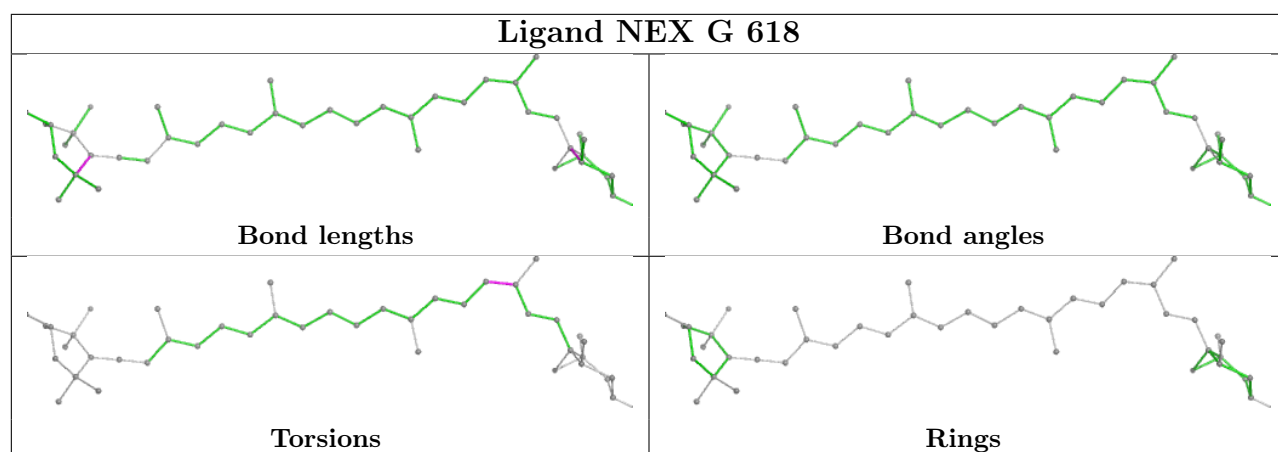


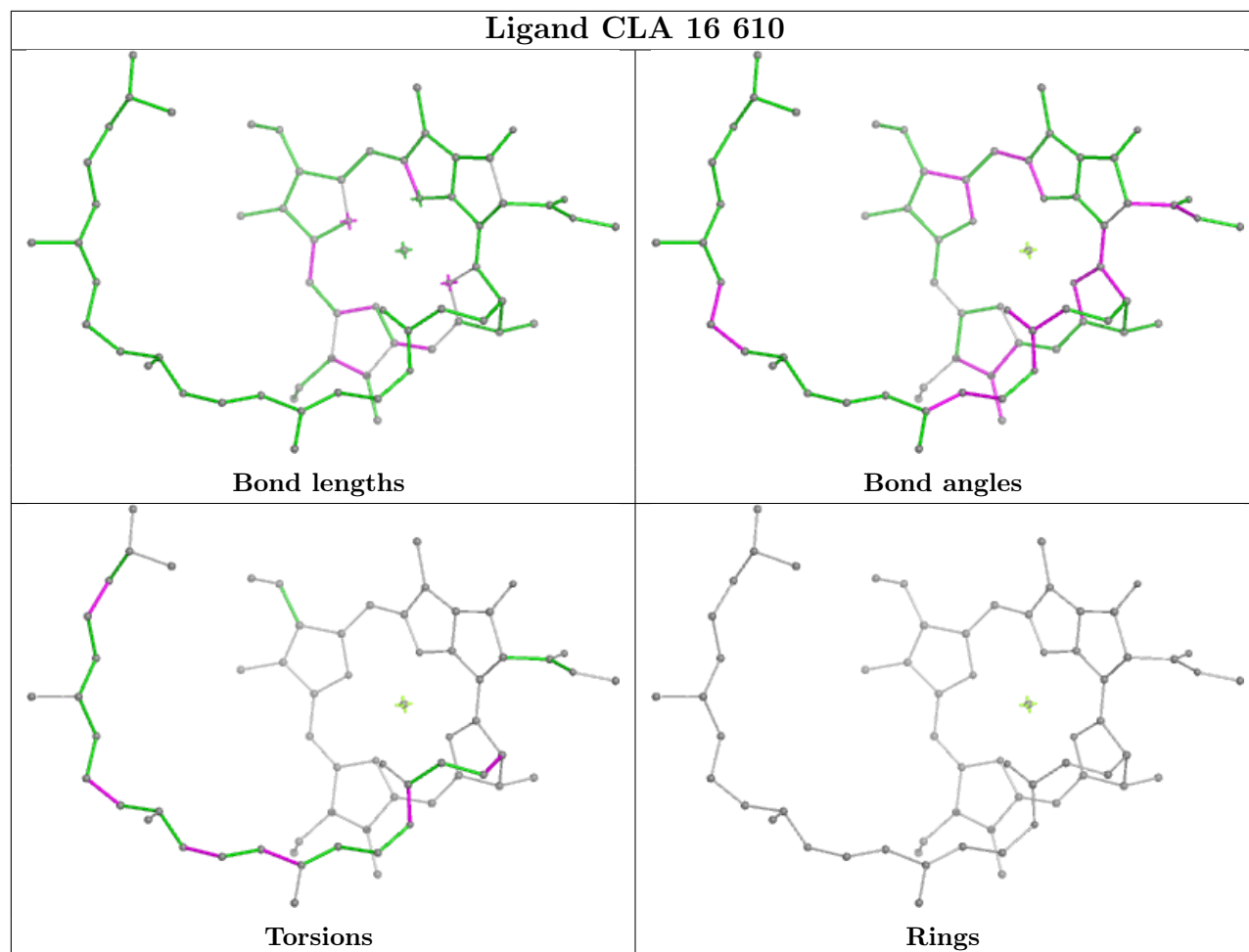


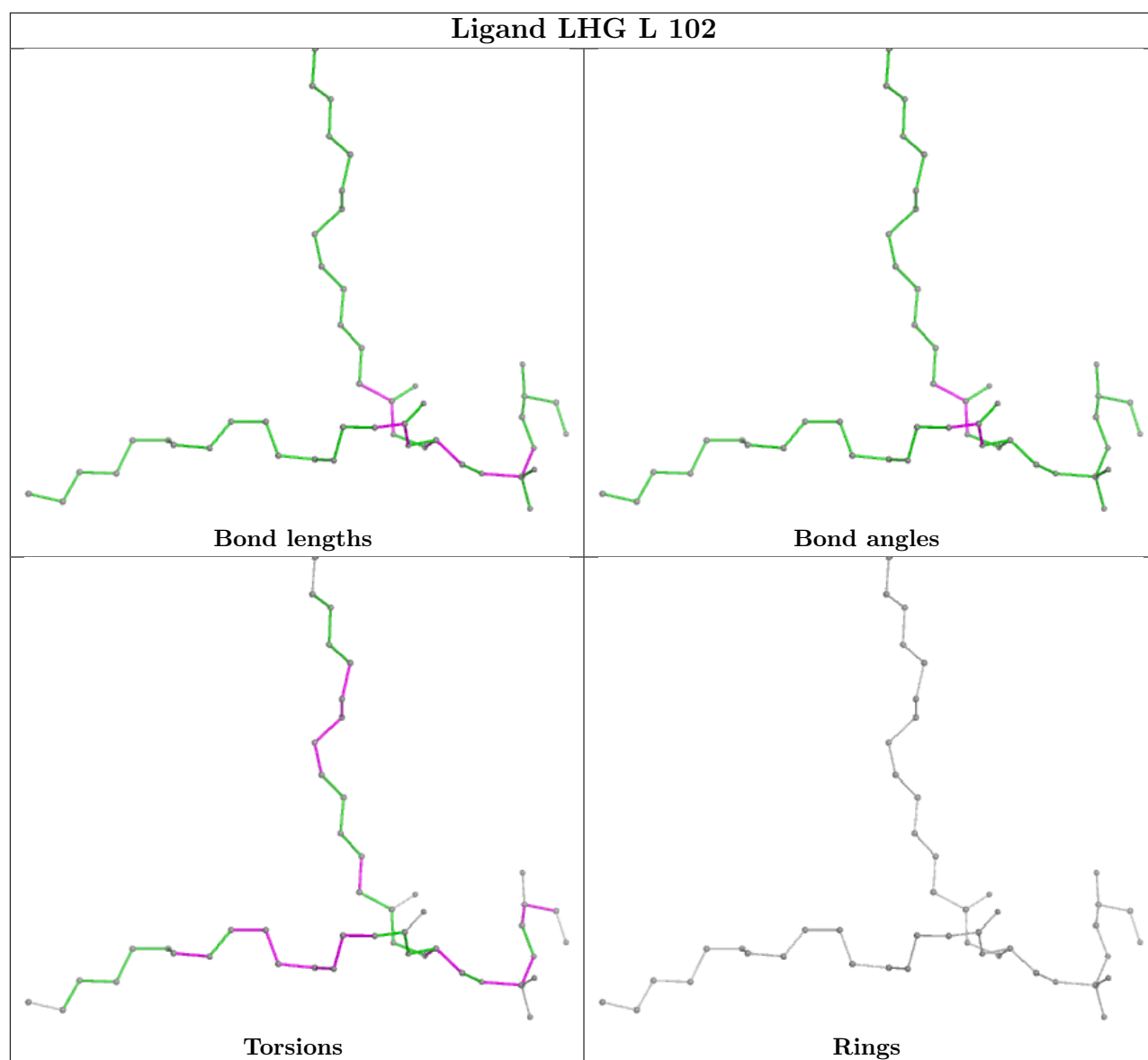


Ligand CHL 4 609**Ligand CLA B 606**

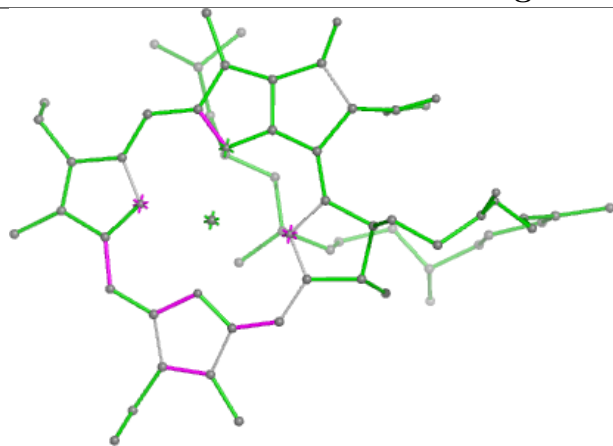
Ligand CLA 6 610**Ligand CHL r 606**



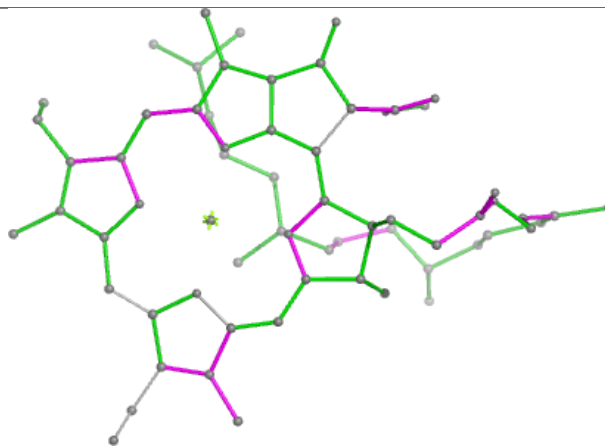




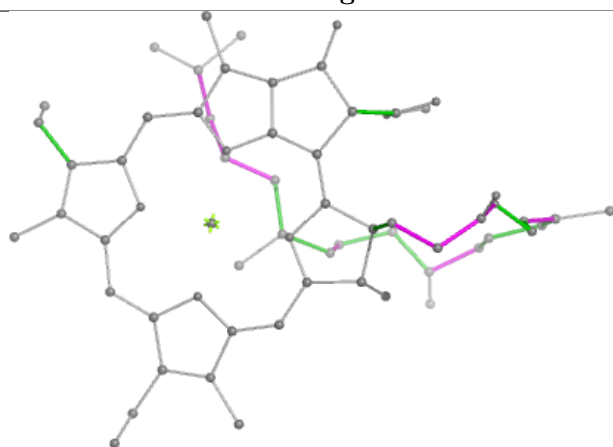
Ligand CLA C 511



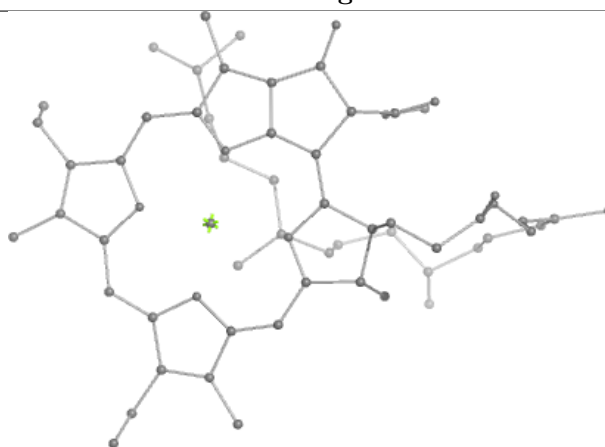
Bond lengths



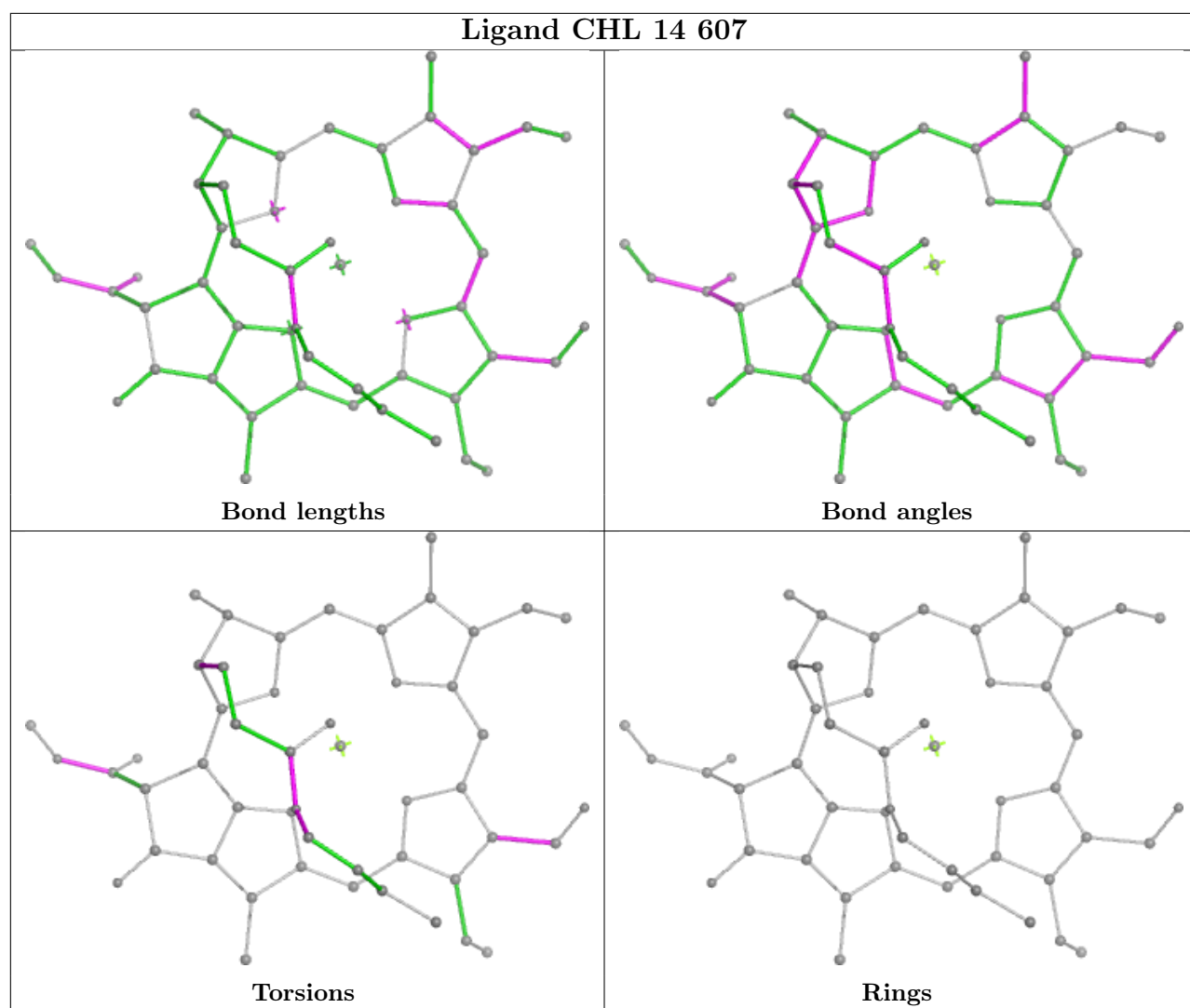
Bond angles



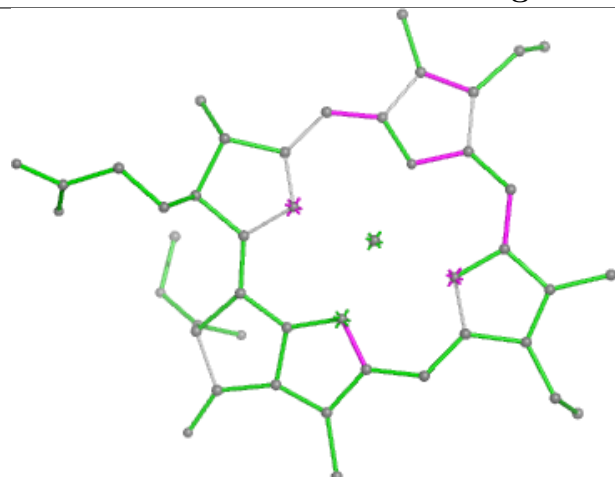
Torsions



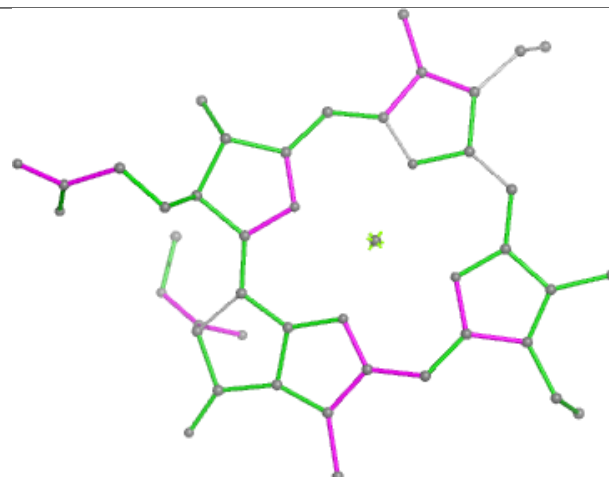
Rings



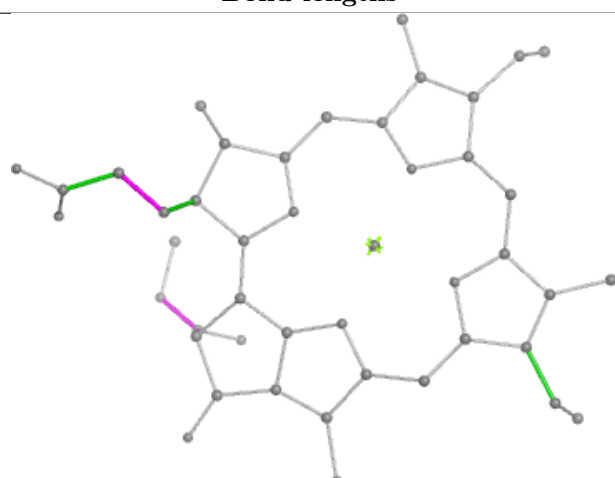
Ligand CLA 16 615



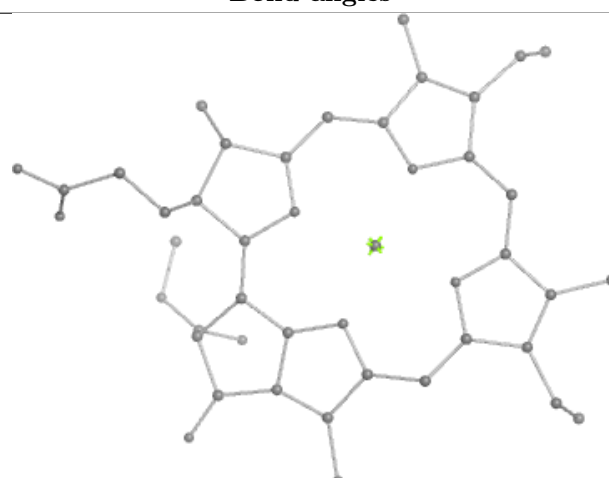
Bond lengths



Bond angles

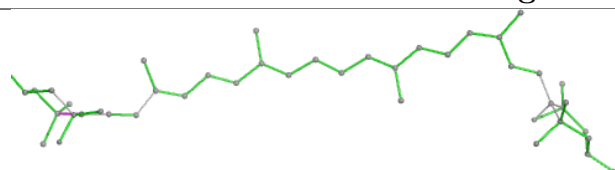


Torsions

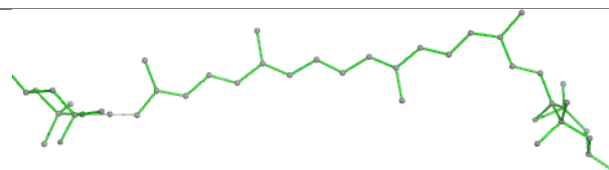


Rings

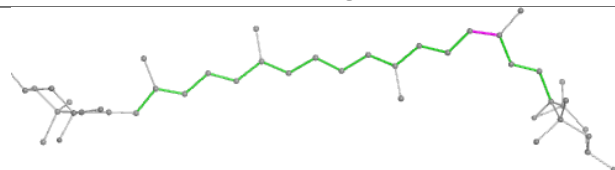
Ligand NEX 3 621



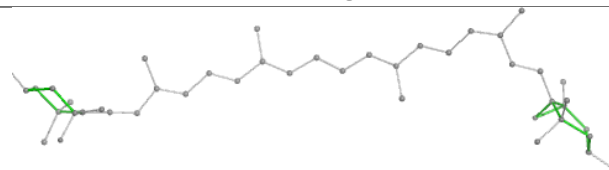
Bond lengths



Bond angles

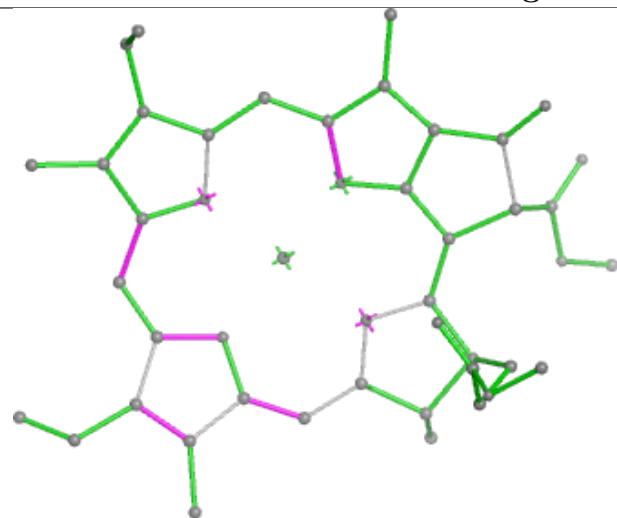


Torsions

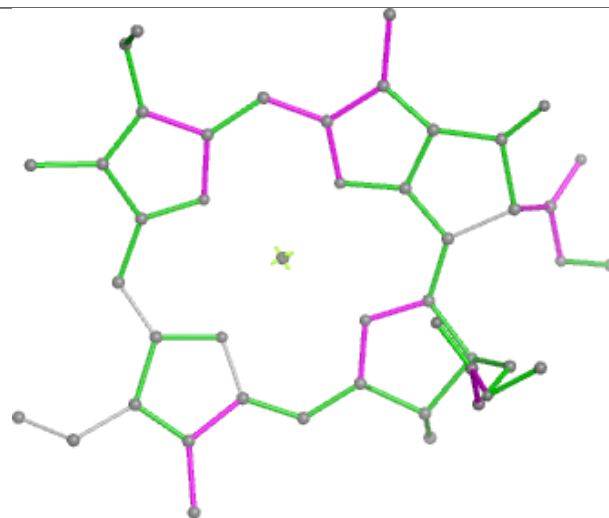


Rings

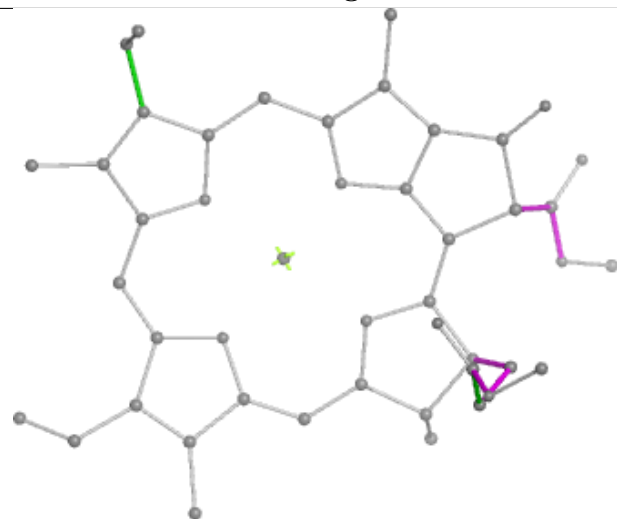
Ligand CLA 1 614



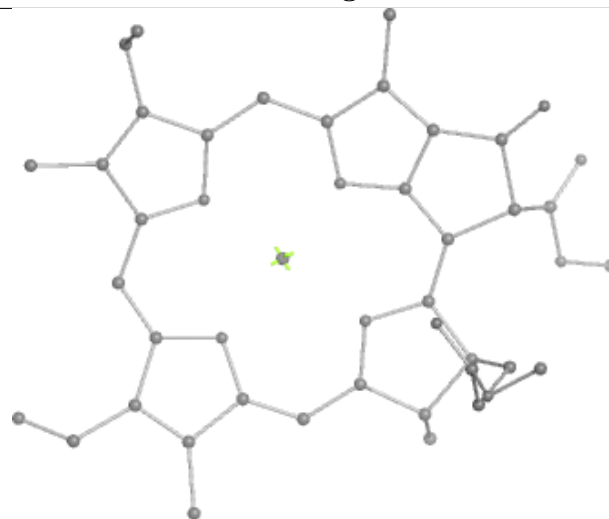
Bond lengths



Bond angles

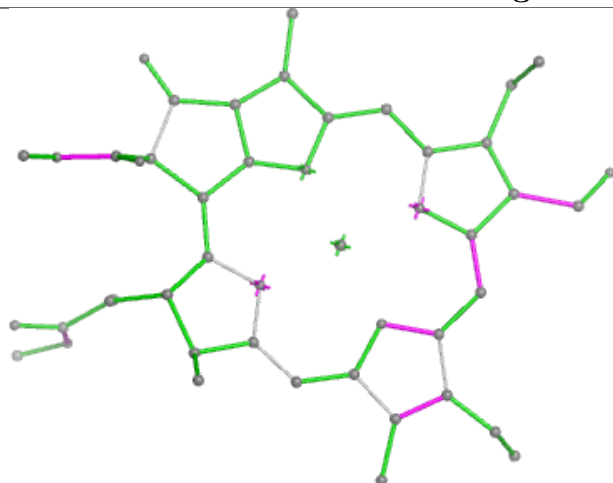


Torsions

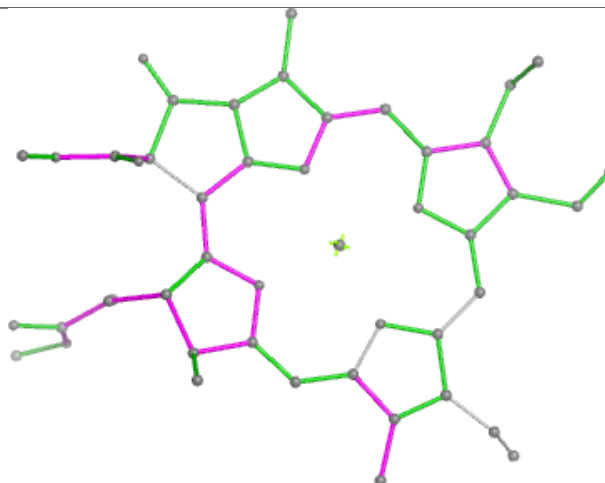


Rings

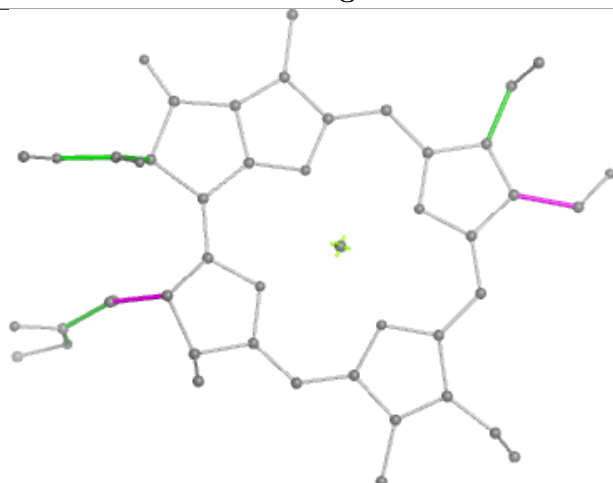
Ligand CHL G 606



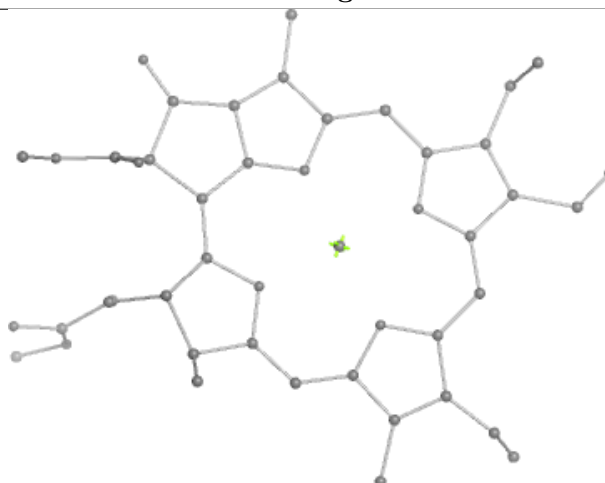
Bond lengths



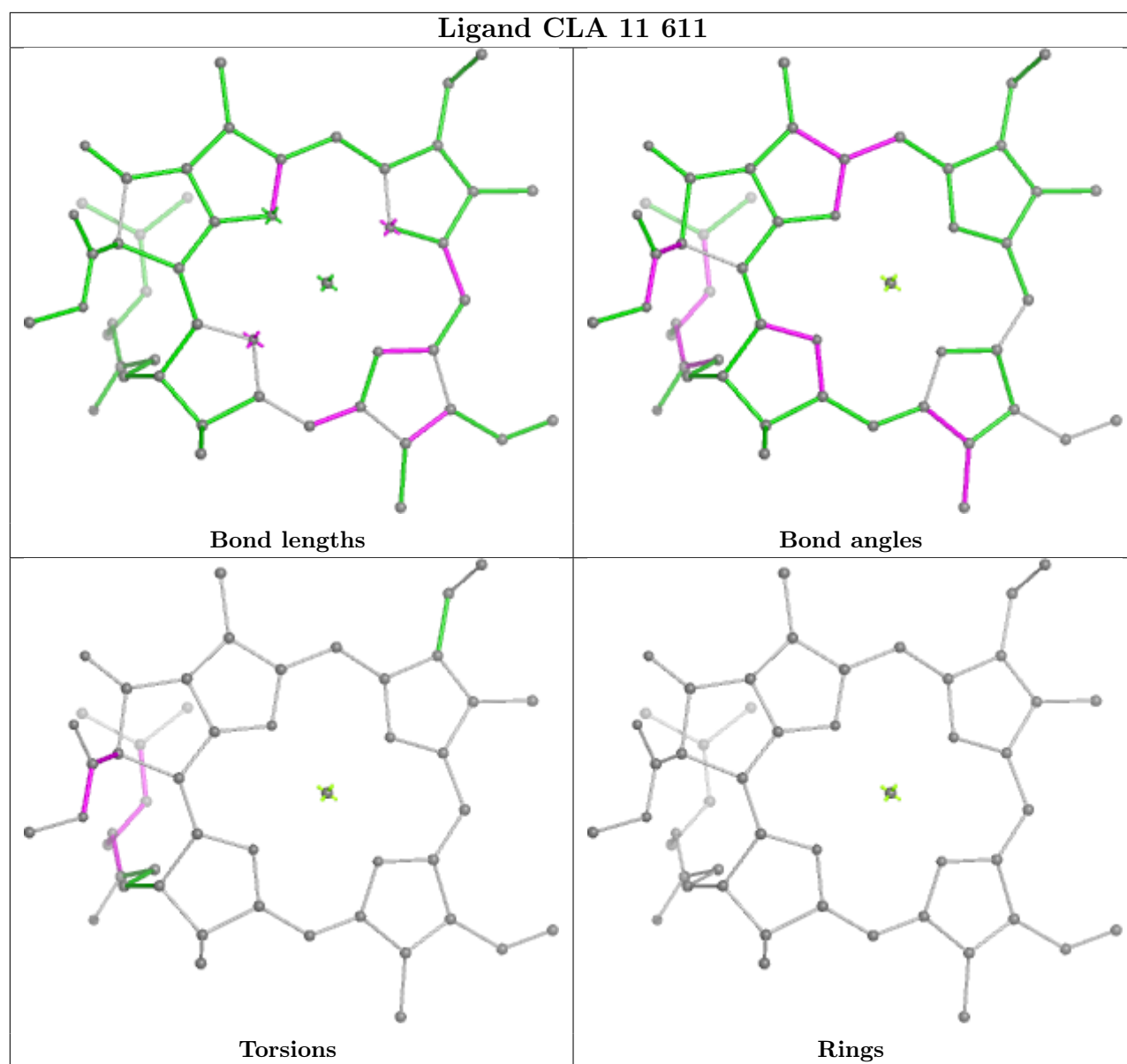
Bond angles



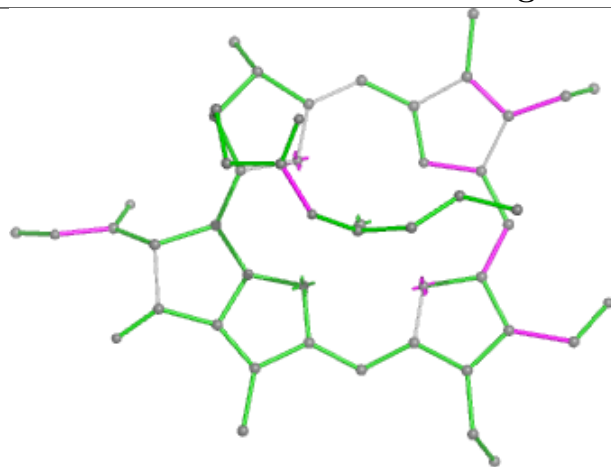
Torsions



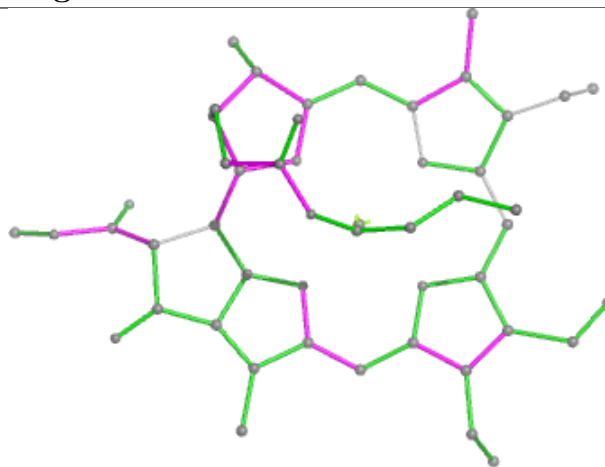
Rings



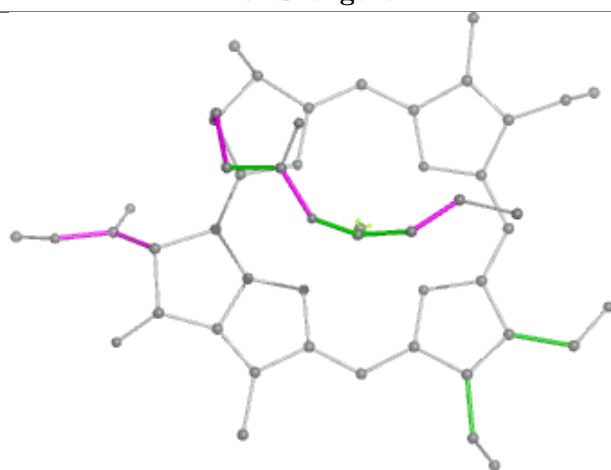
Ligand CHL g 607



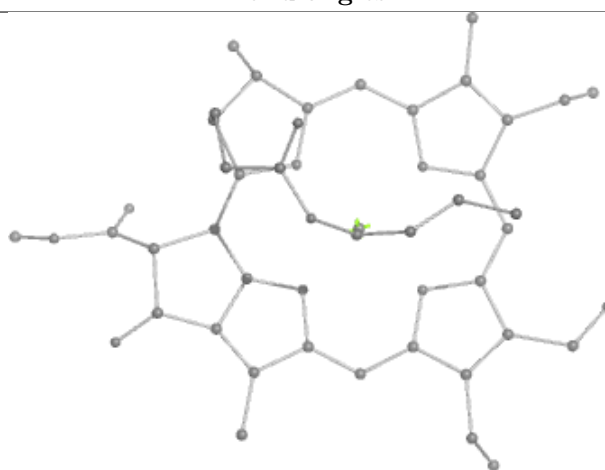
Bond lengths



Bond angles

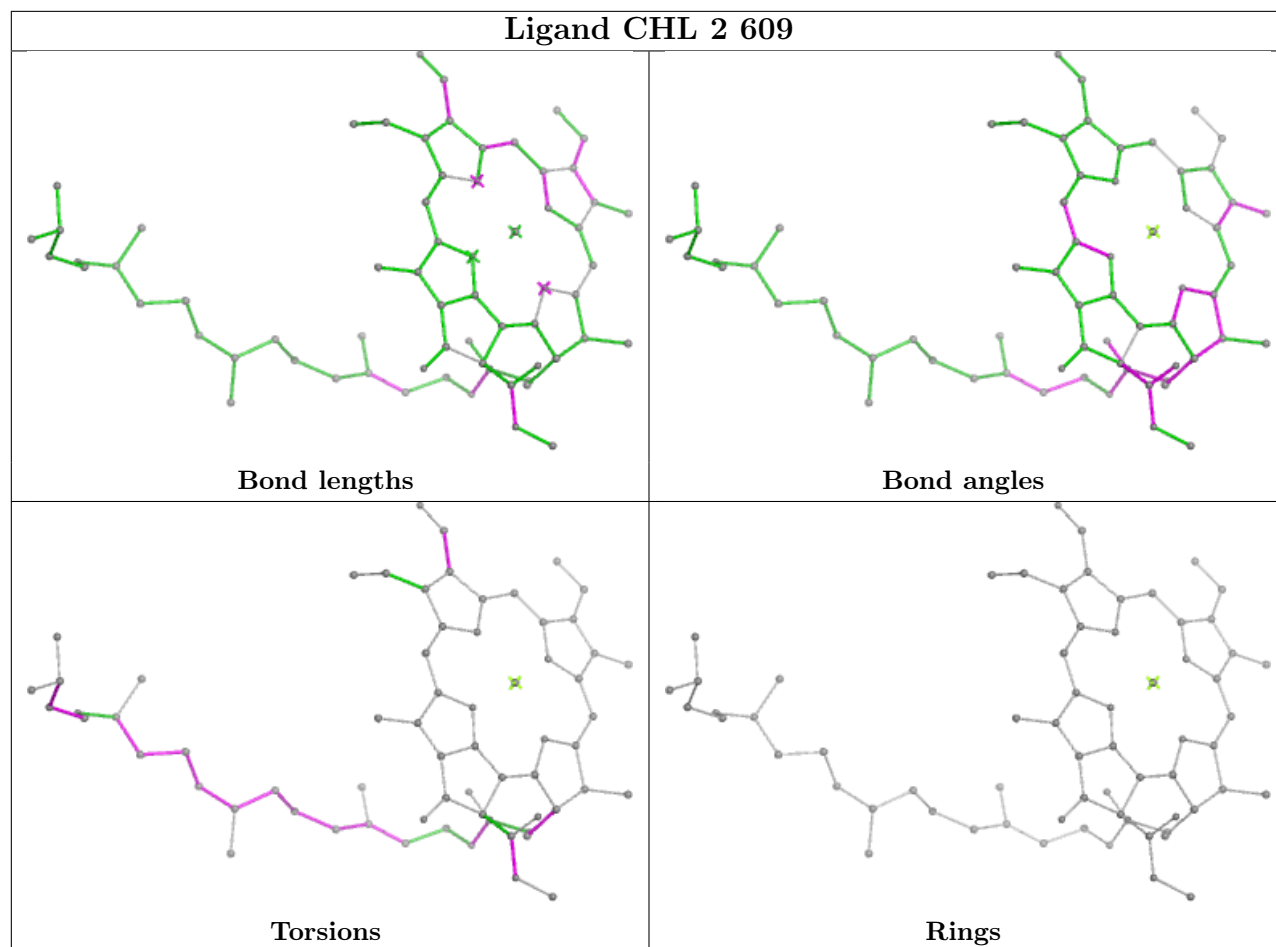


Torsions

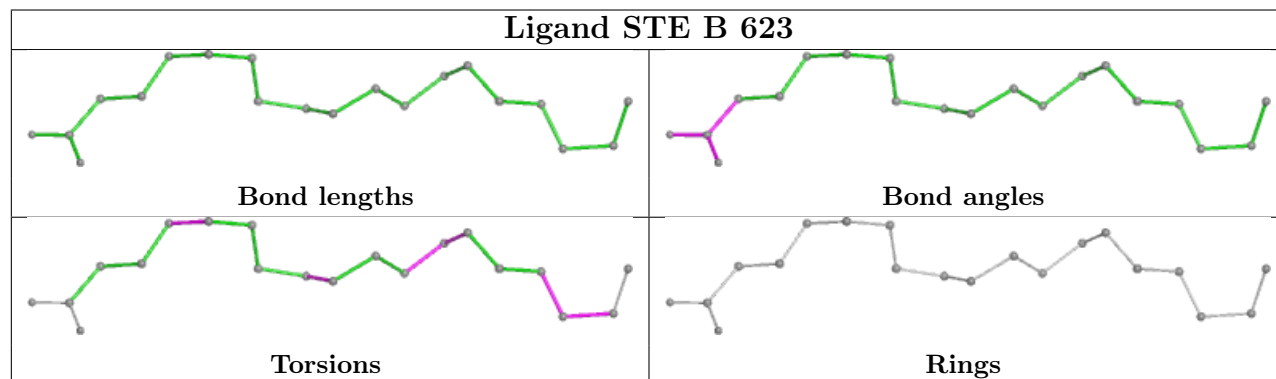


Rings

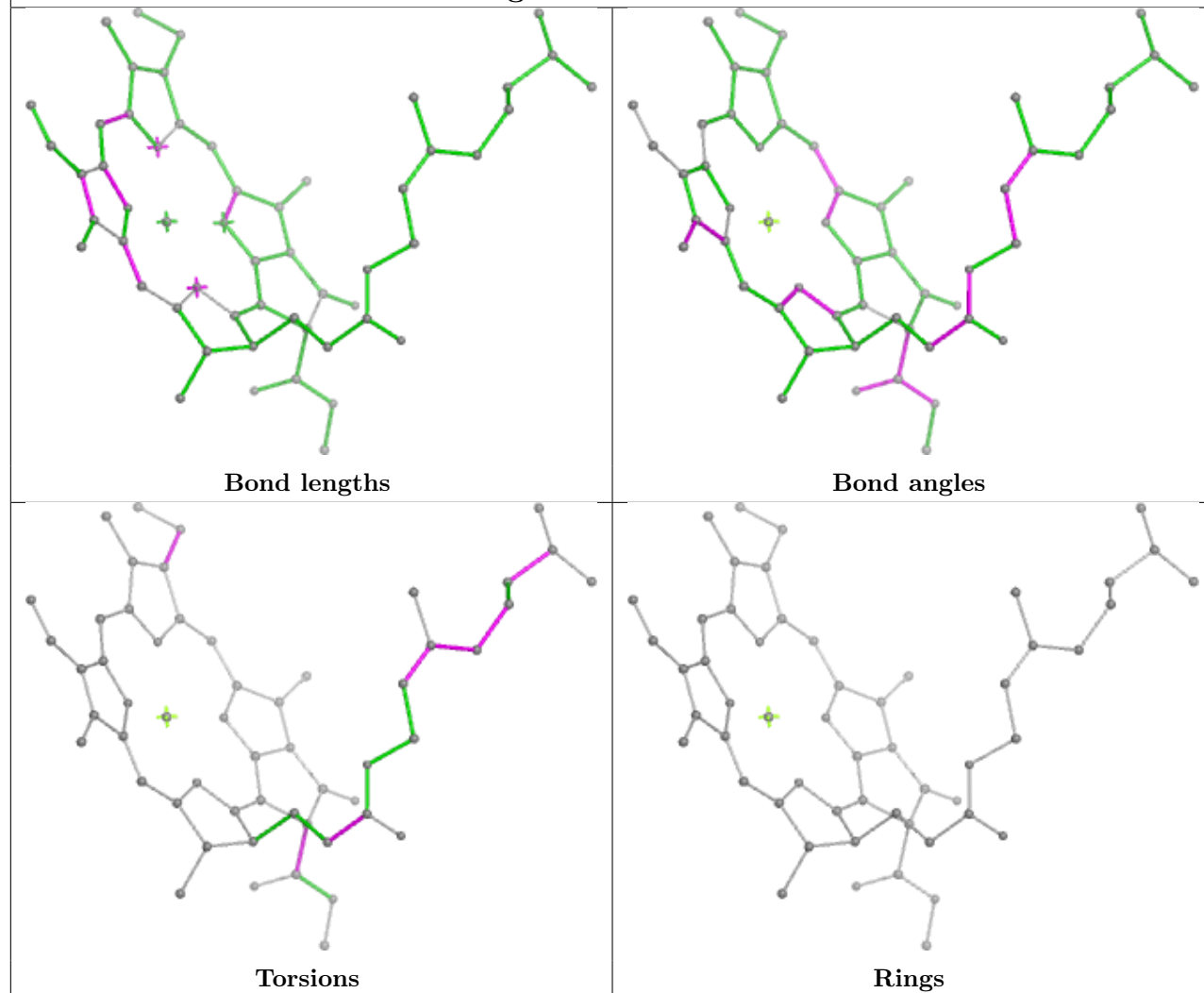
Ligand CHL 2 609



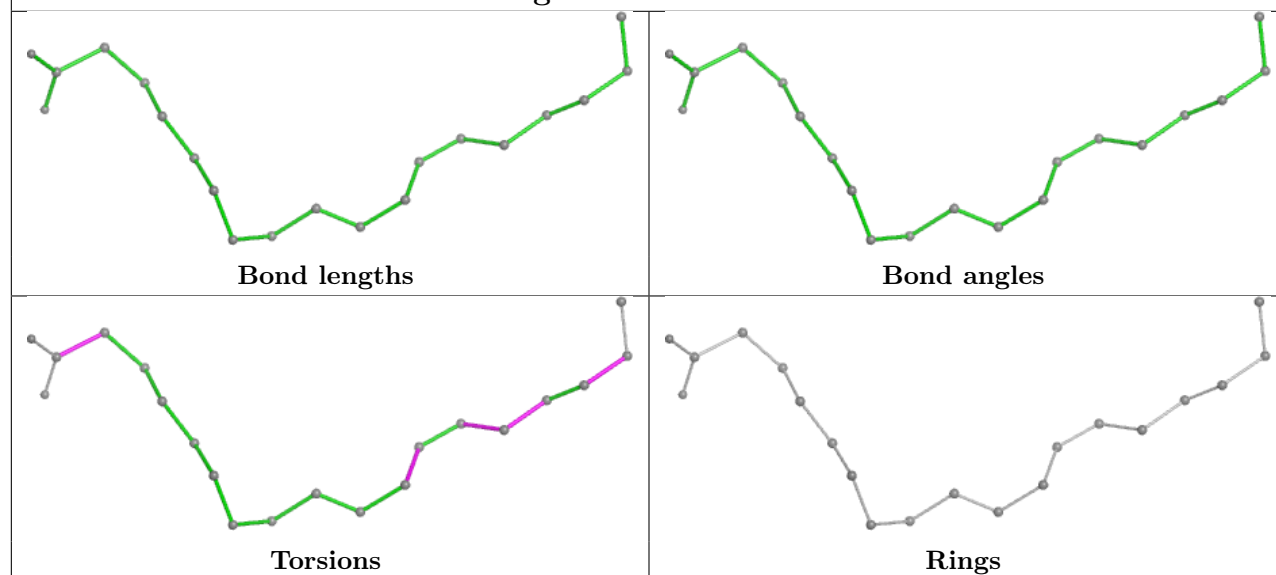
Ligand STE B 623

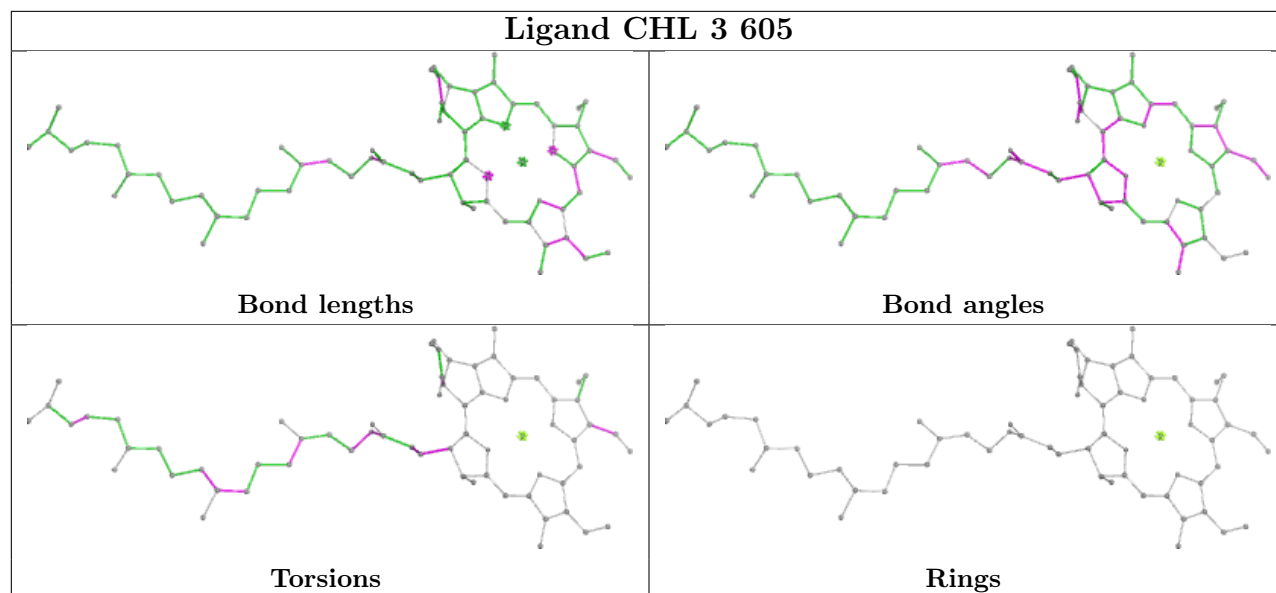
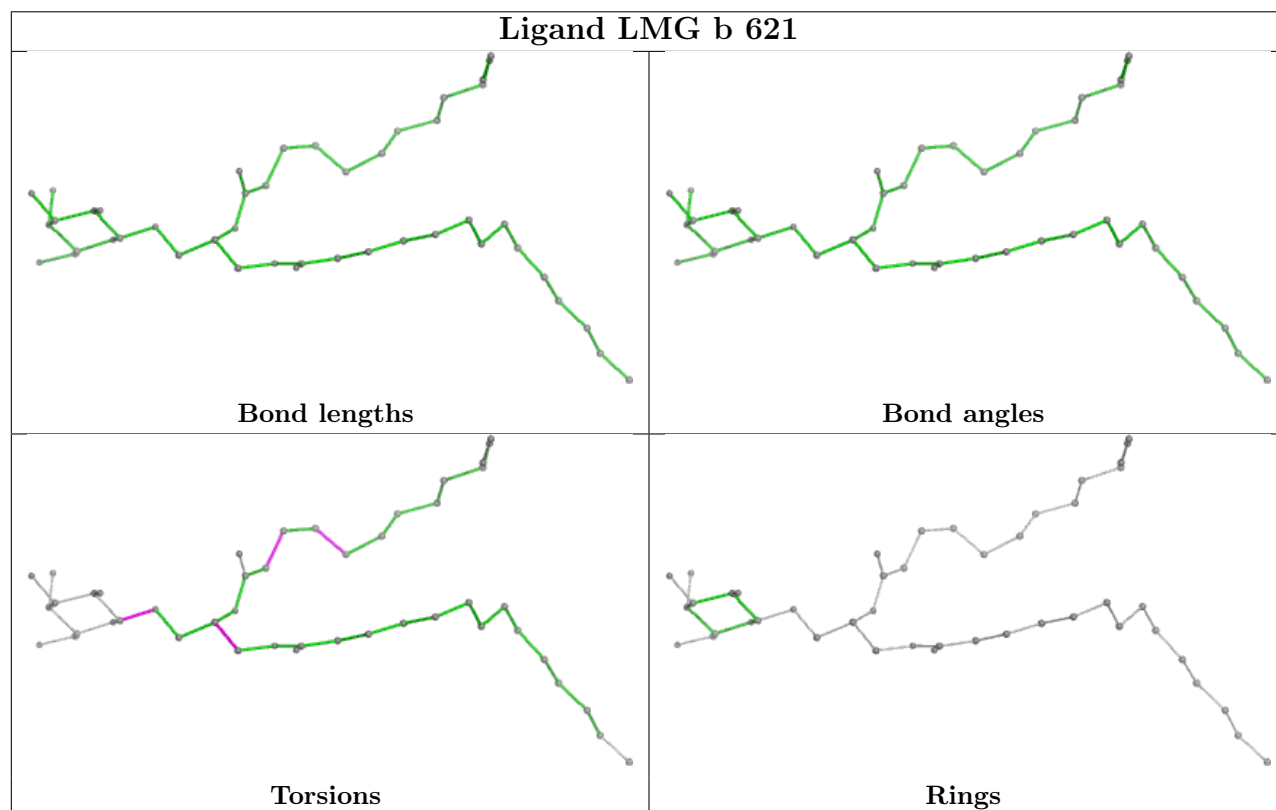


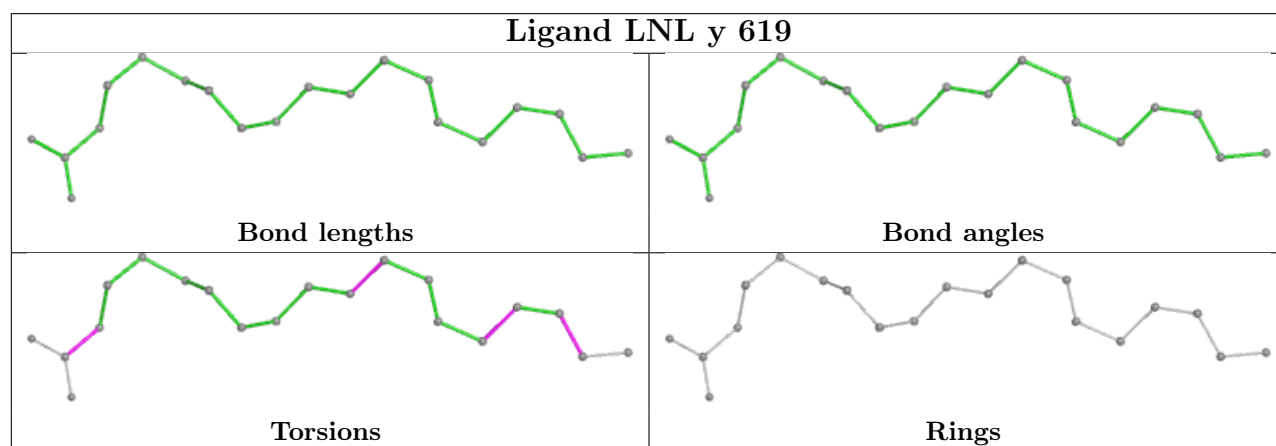
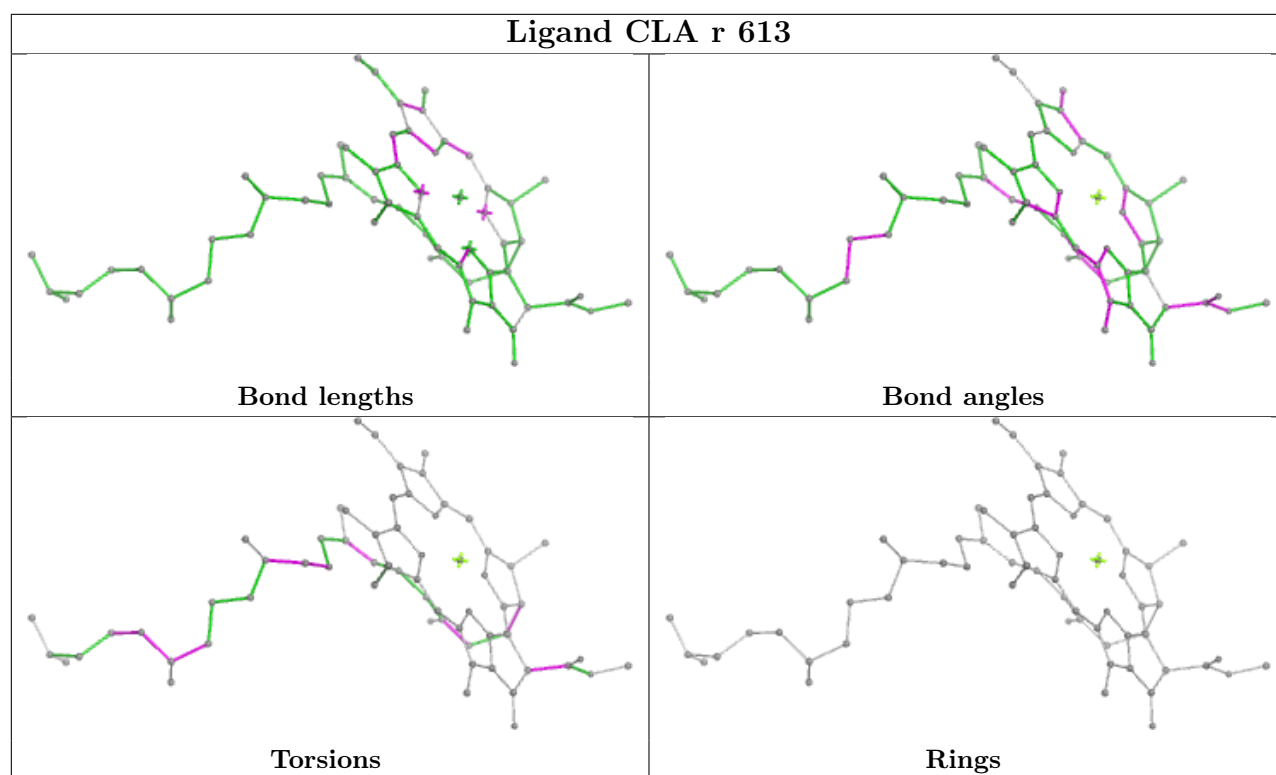
Ligand CLA s 609

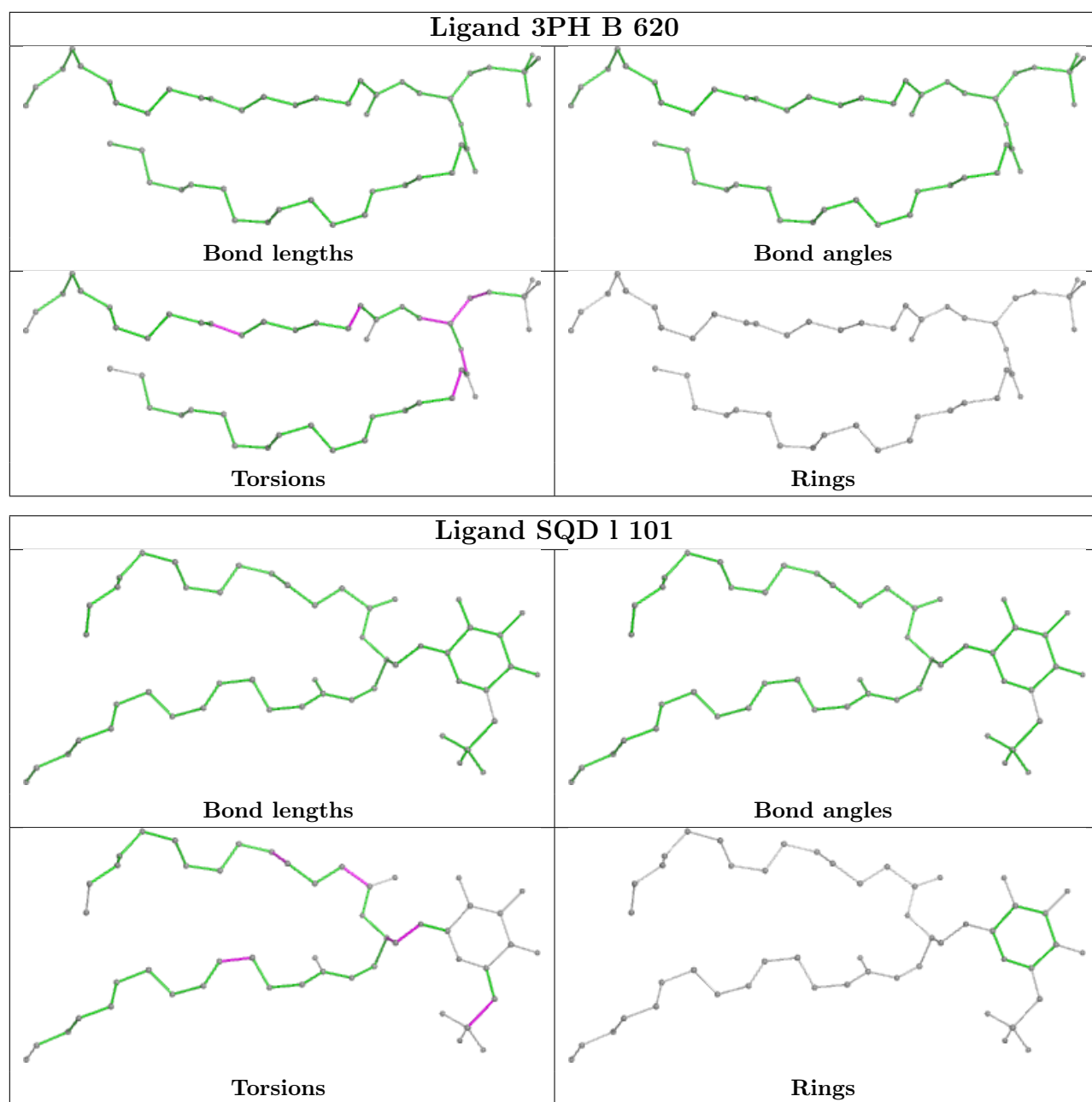


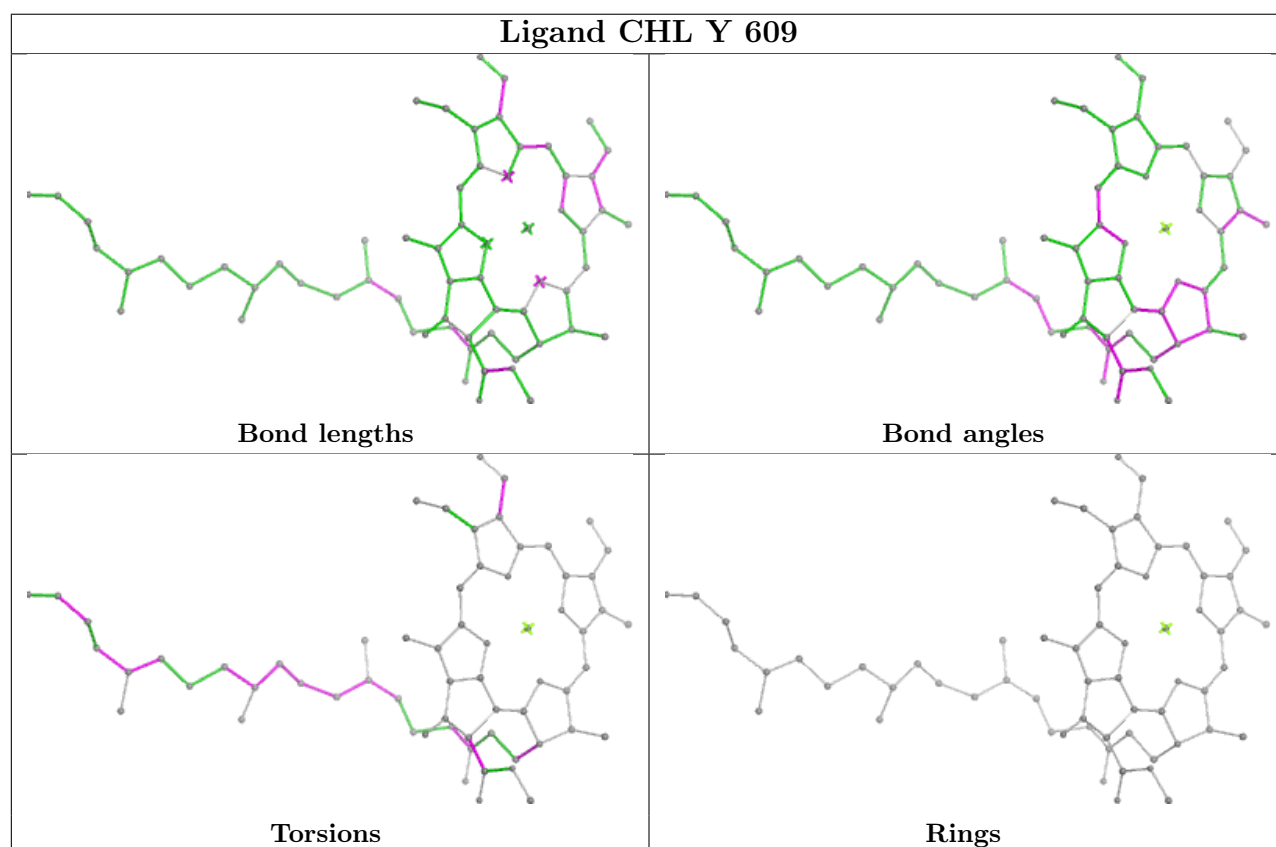
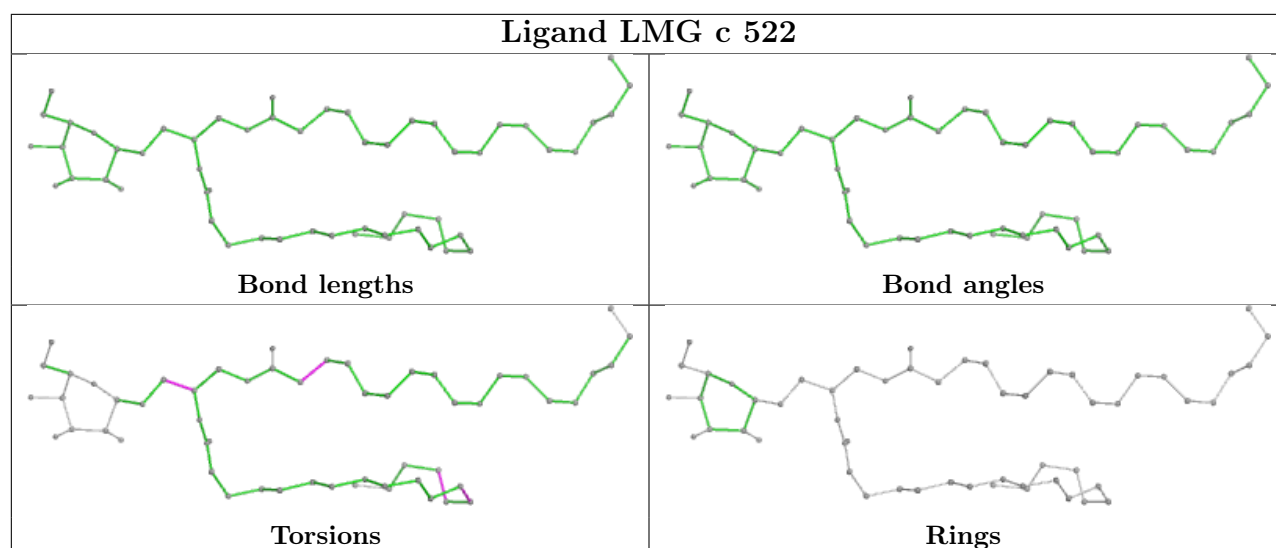
Ligand LNL X 201



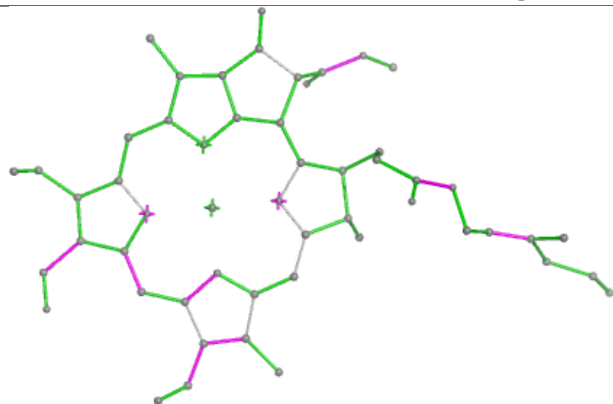
Ligand CHL 3 605**Ligand LMG b 621**



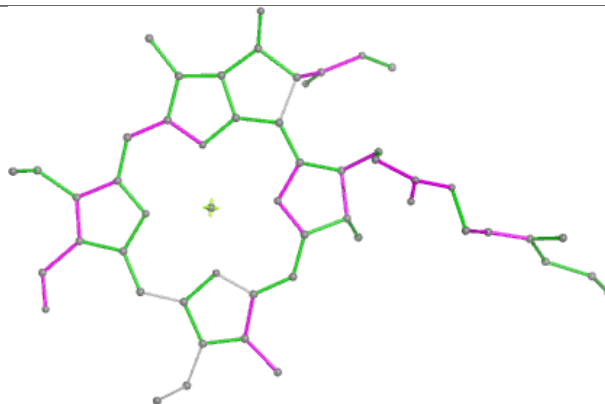




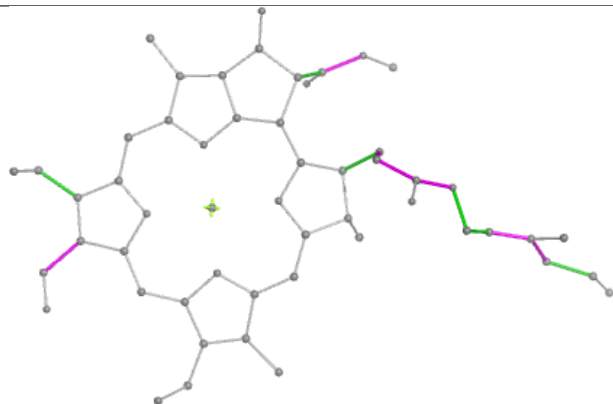
Ligand CHL N 601



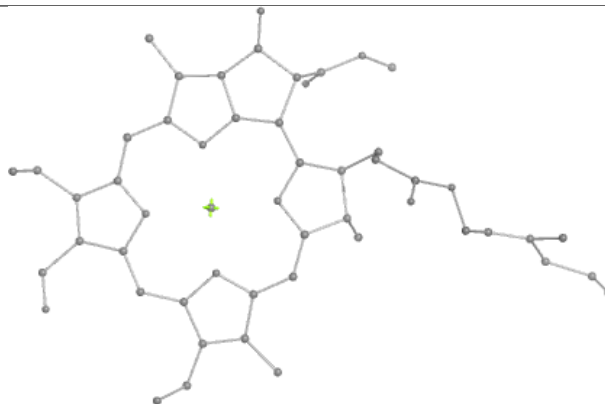
Bond lengths



Bond angles

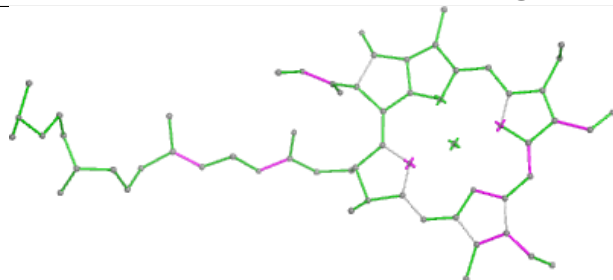


Torsions

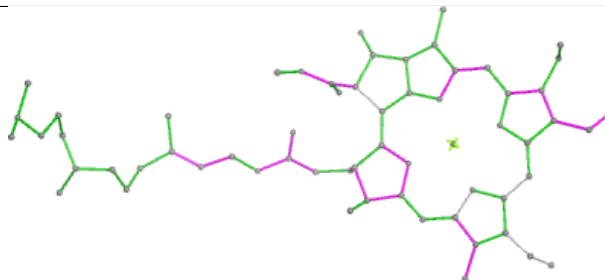


Rings

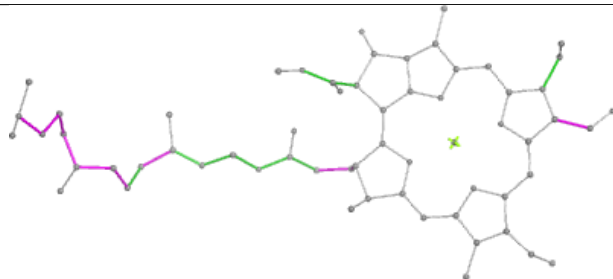
Ligand CHL N 606



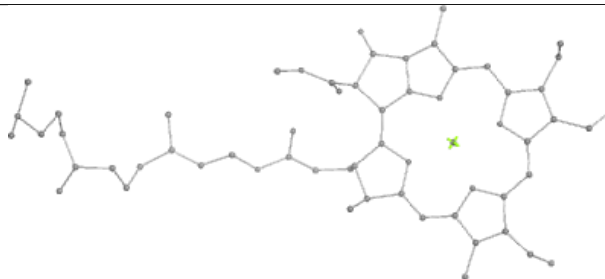
Bond lengths



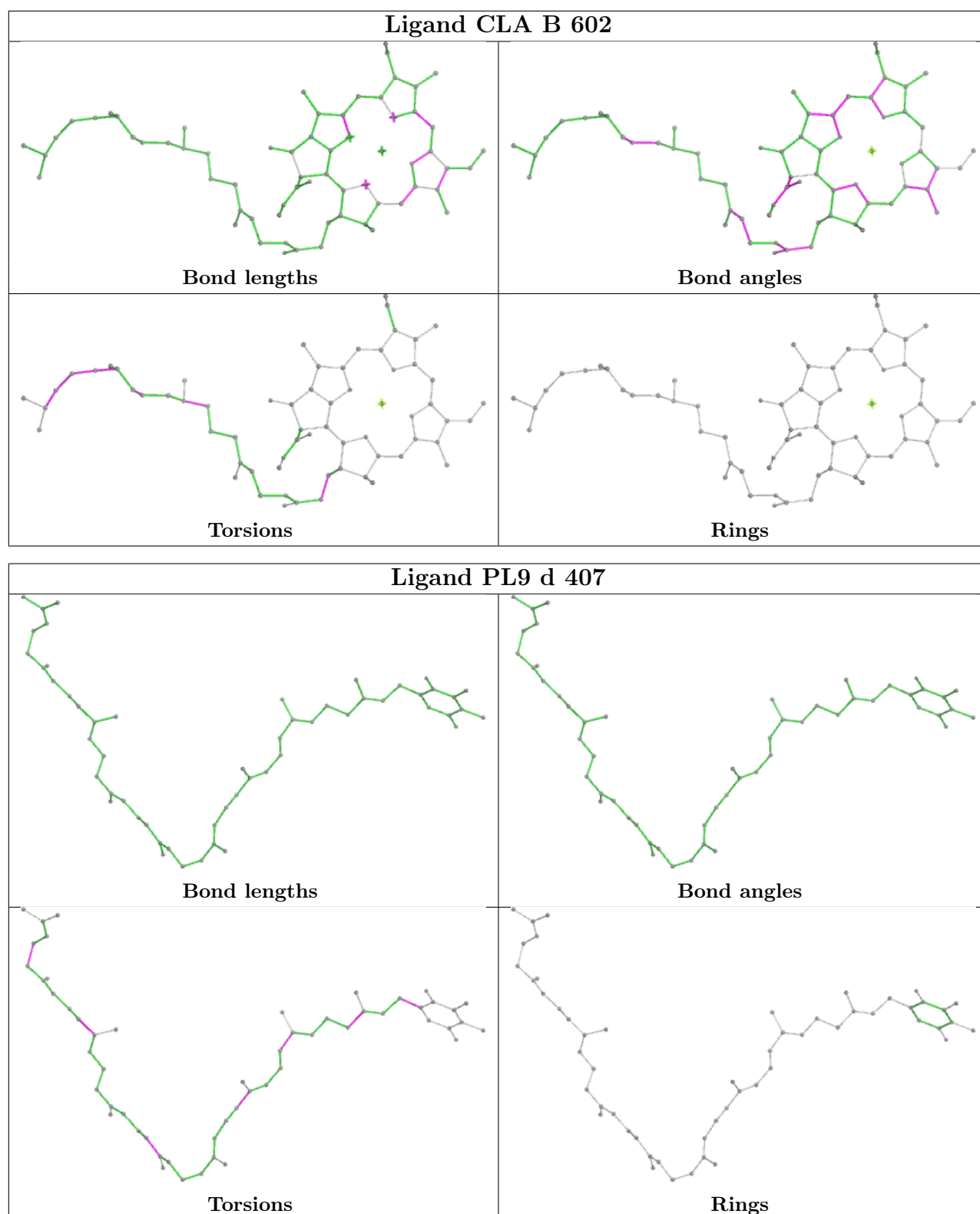
Bond angles



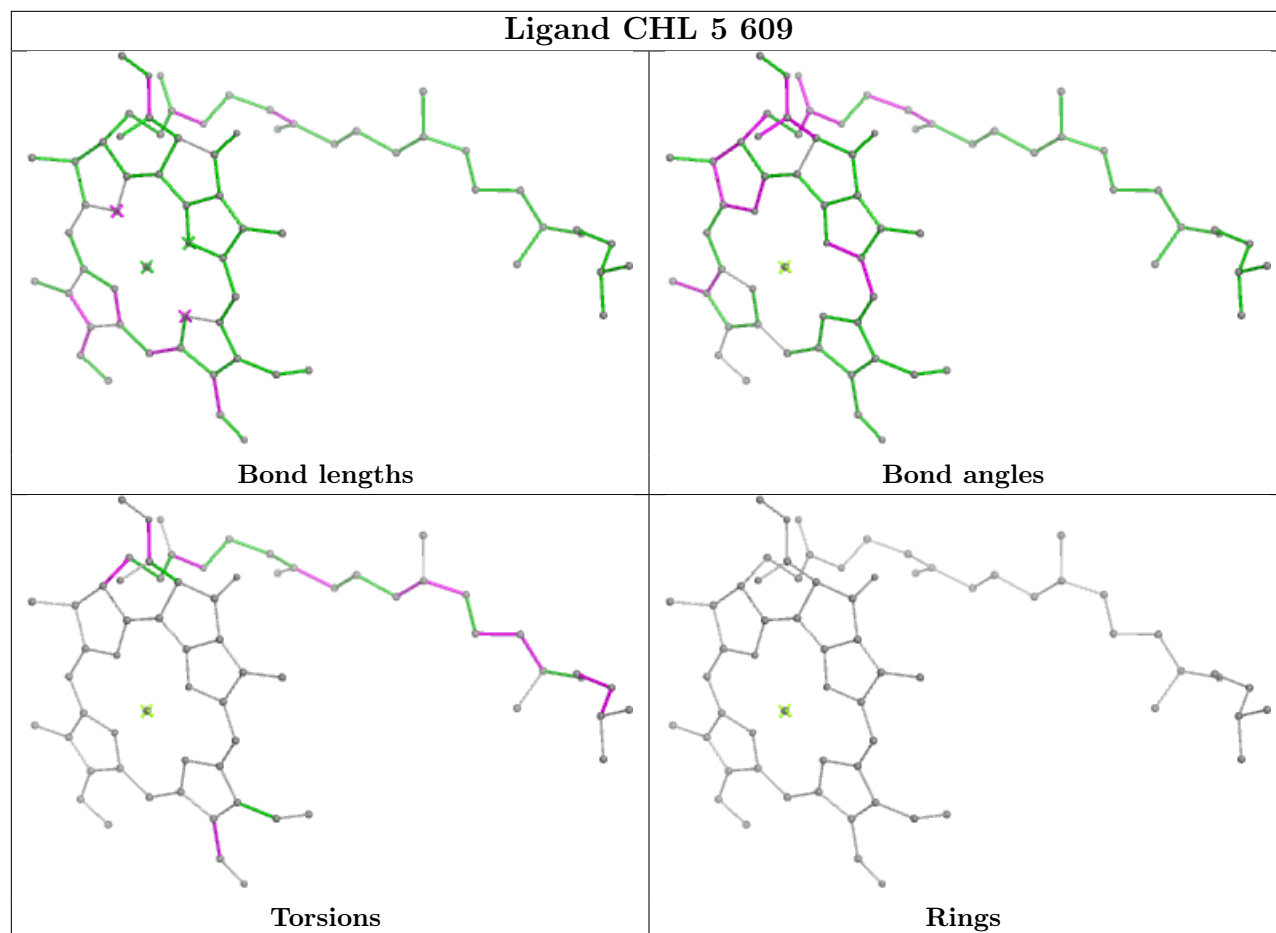
Torsions



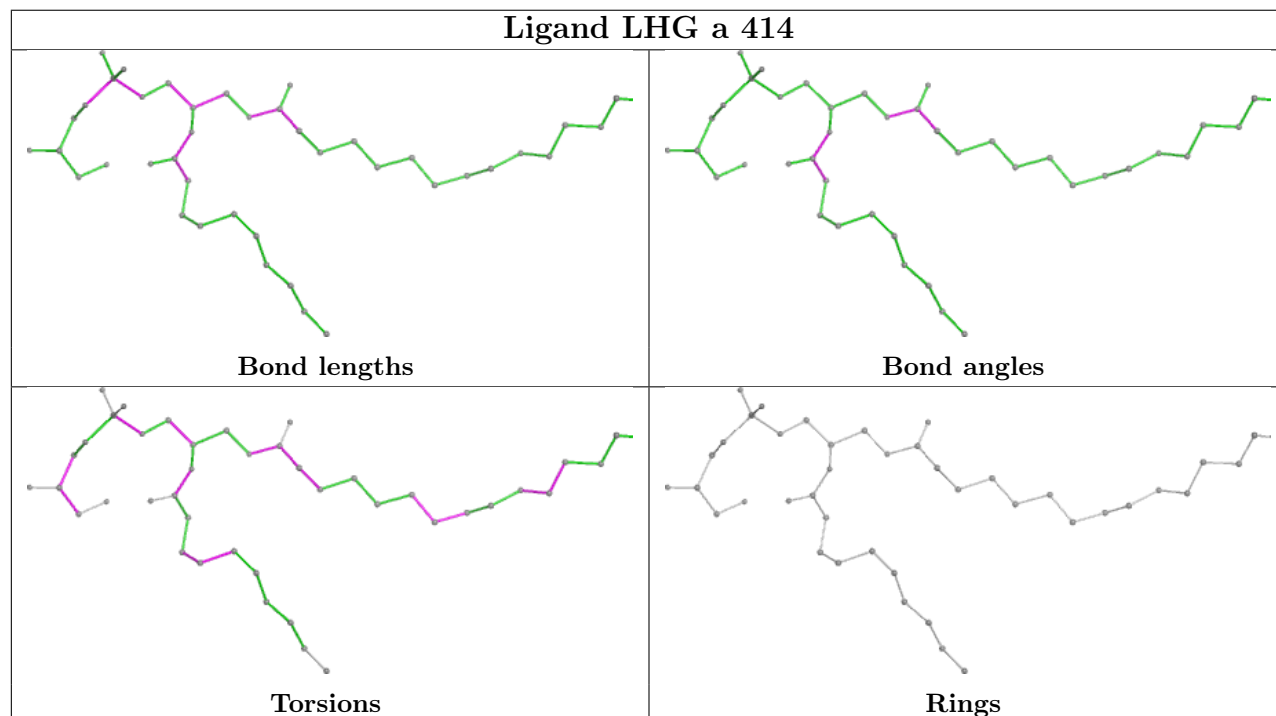
Rings

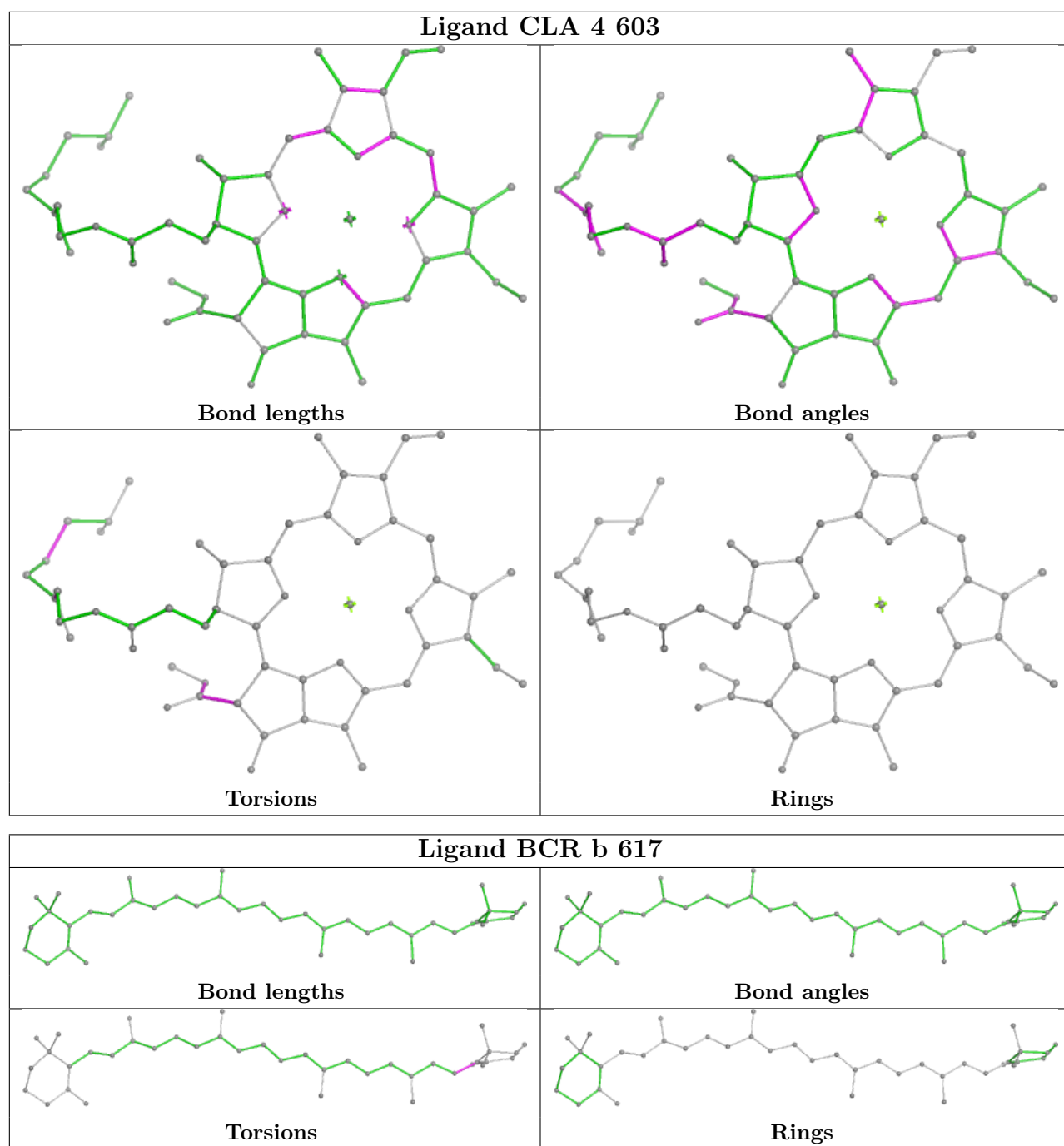


Ligand CHL 5 609

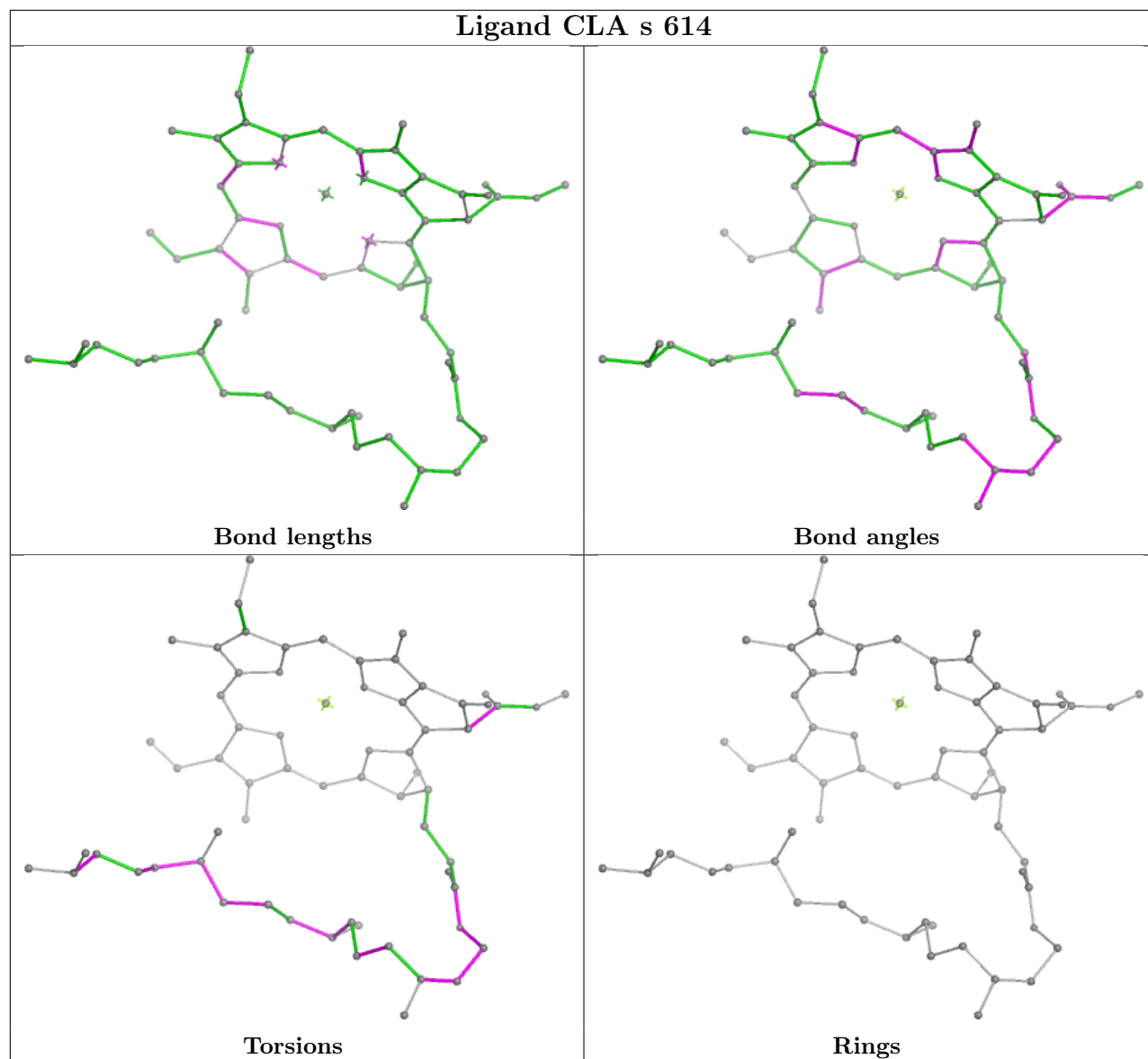


Ligand LHG a 414

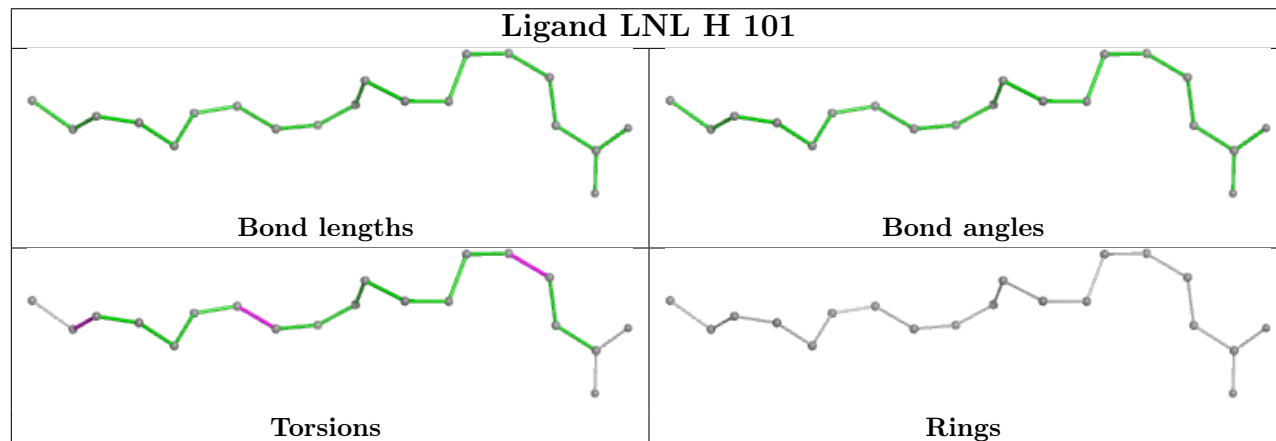


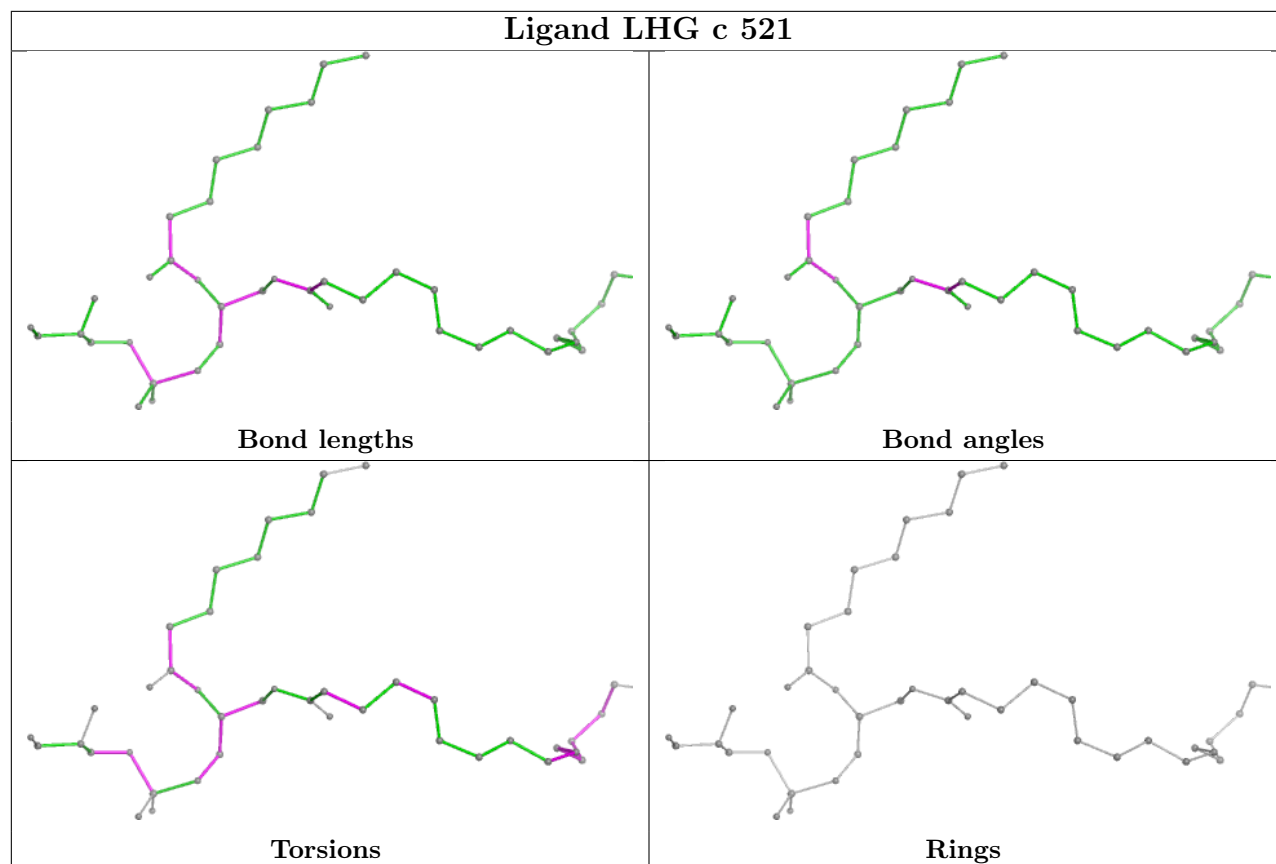
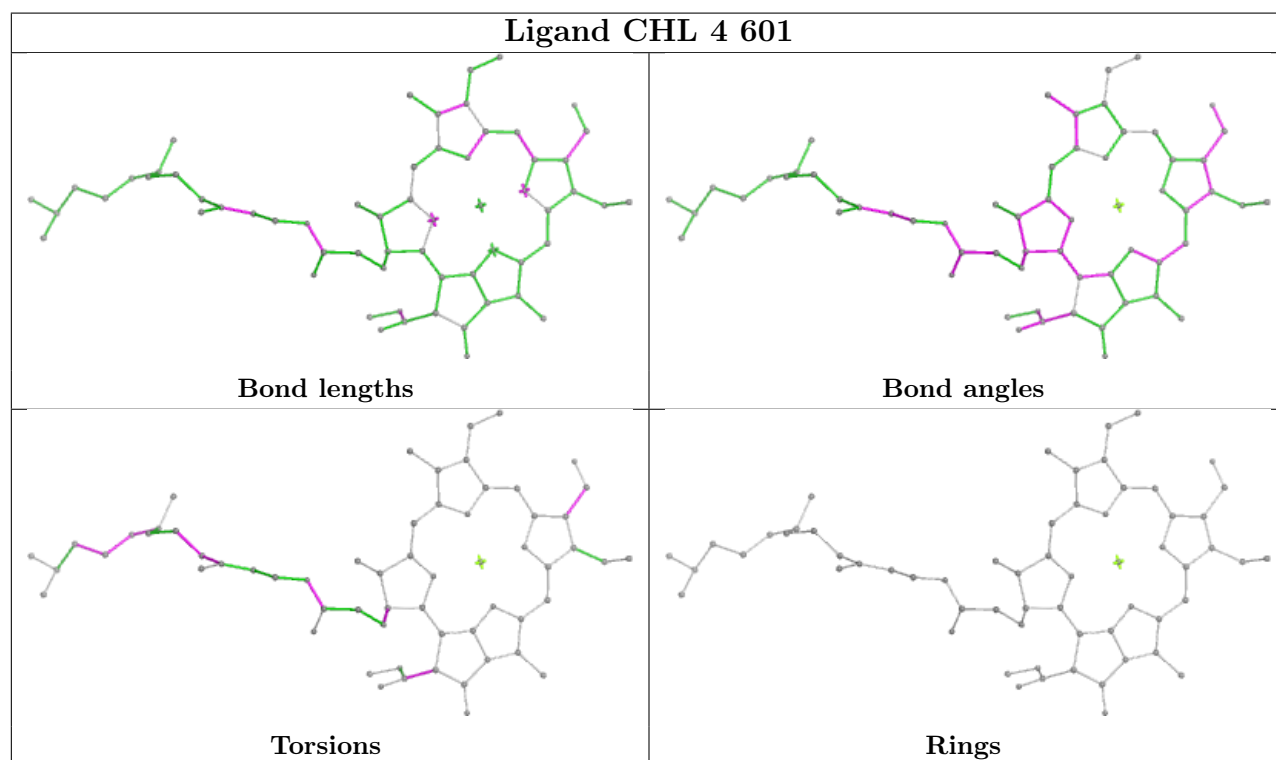


Ligand CLA s 614

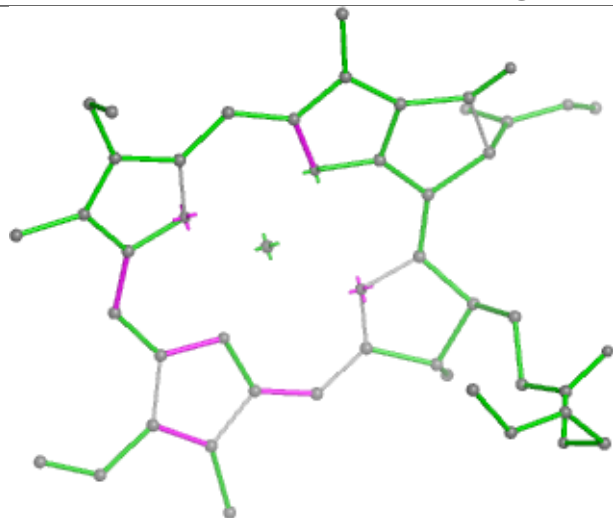


Ligand LNL H 101

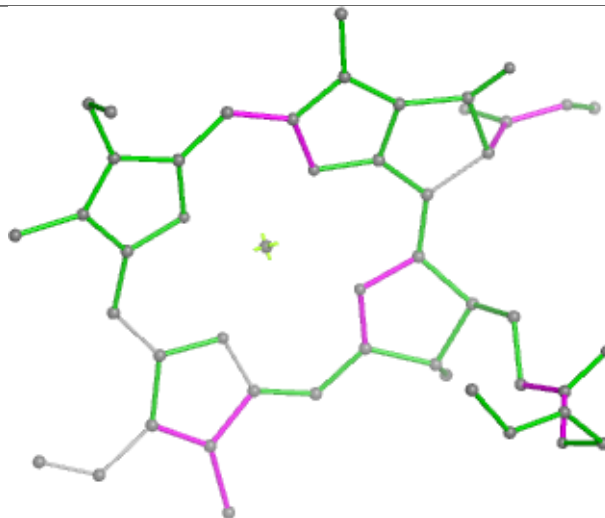


Ligand LHG c 521**Ligand CHL 4 601**

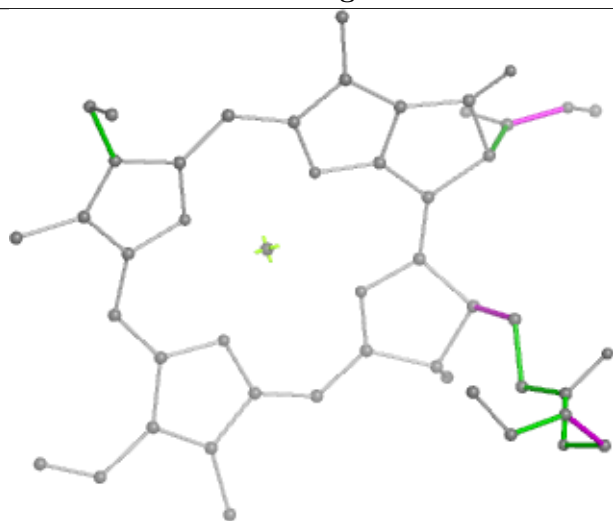
Ligand CLA G 614



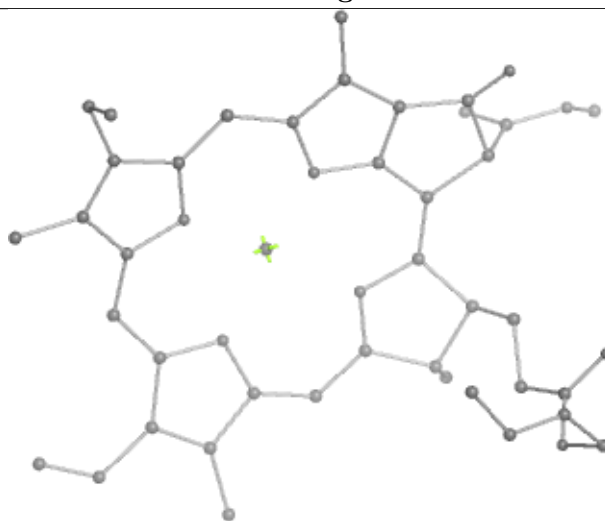
Bond lengths



Bond angles

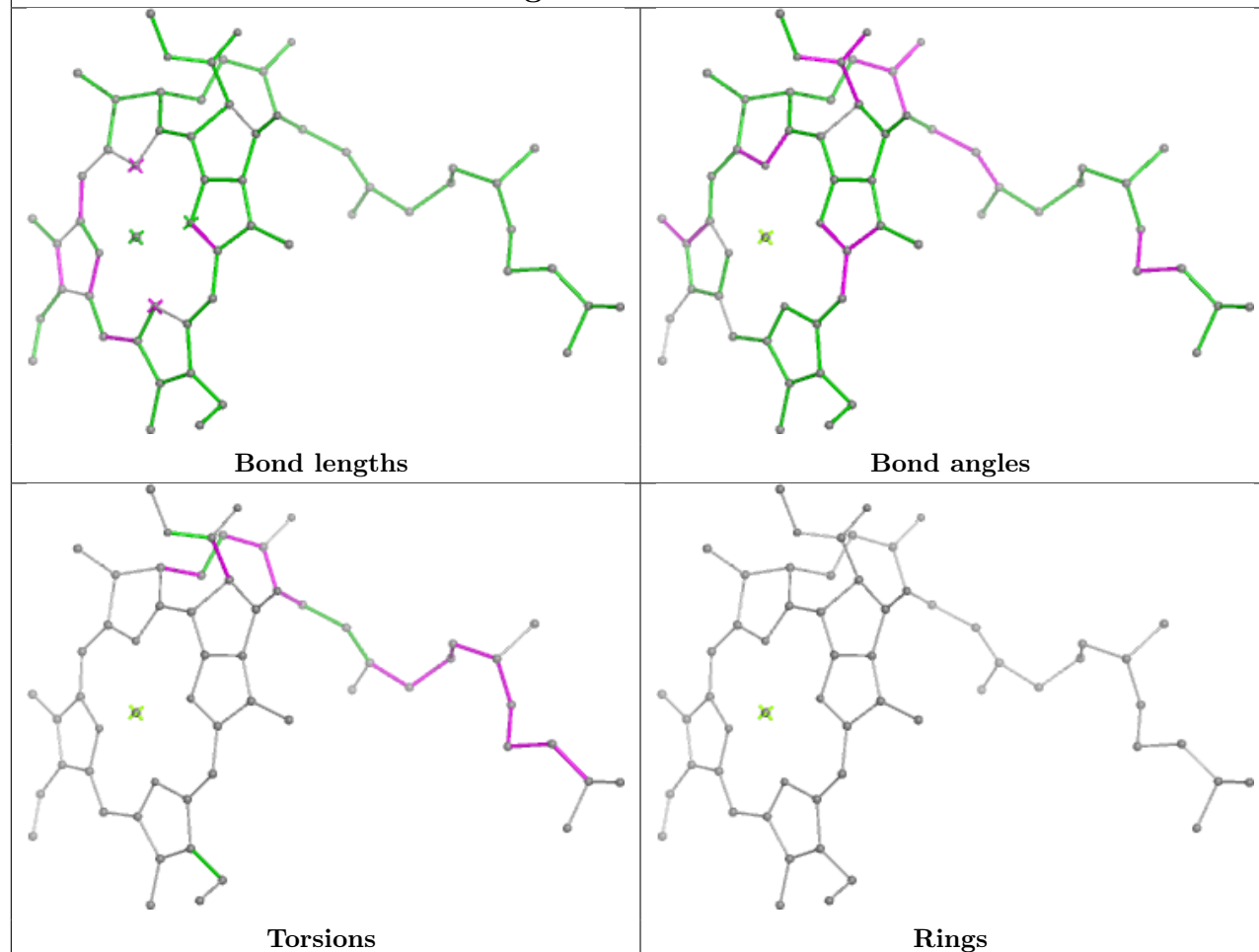


Torsions

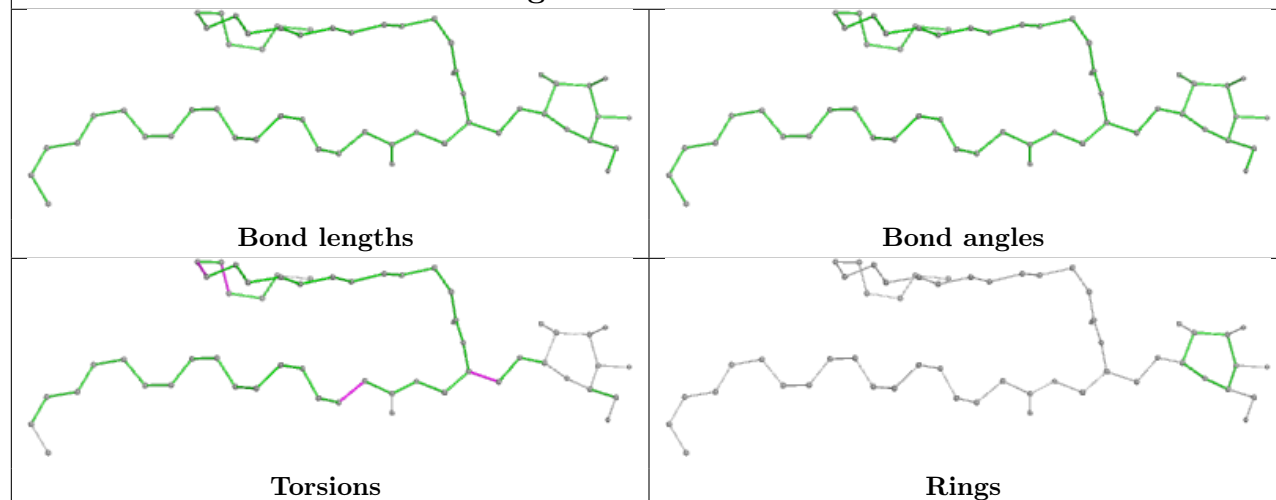


Rings

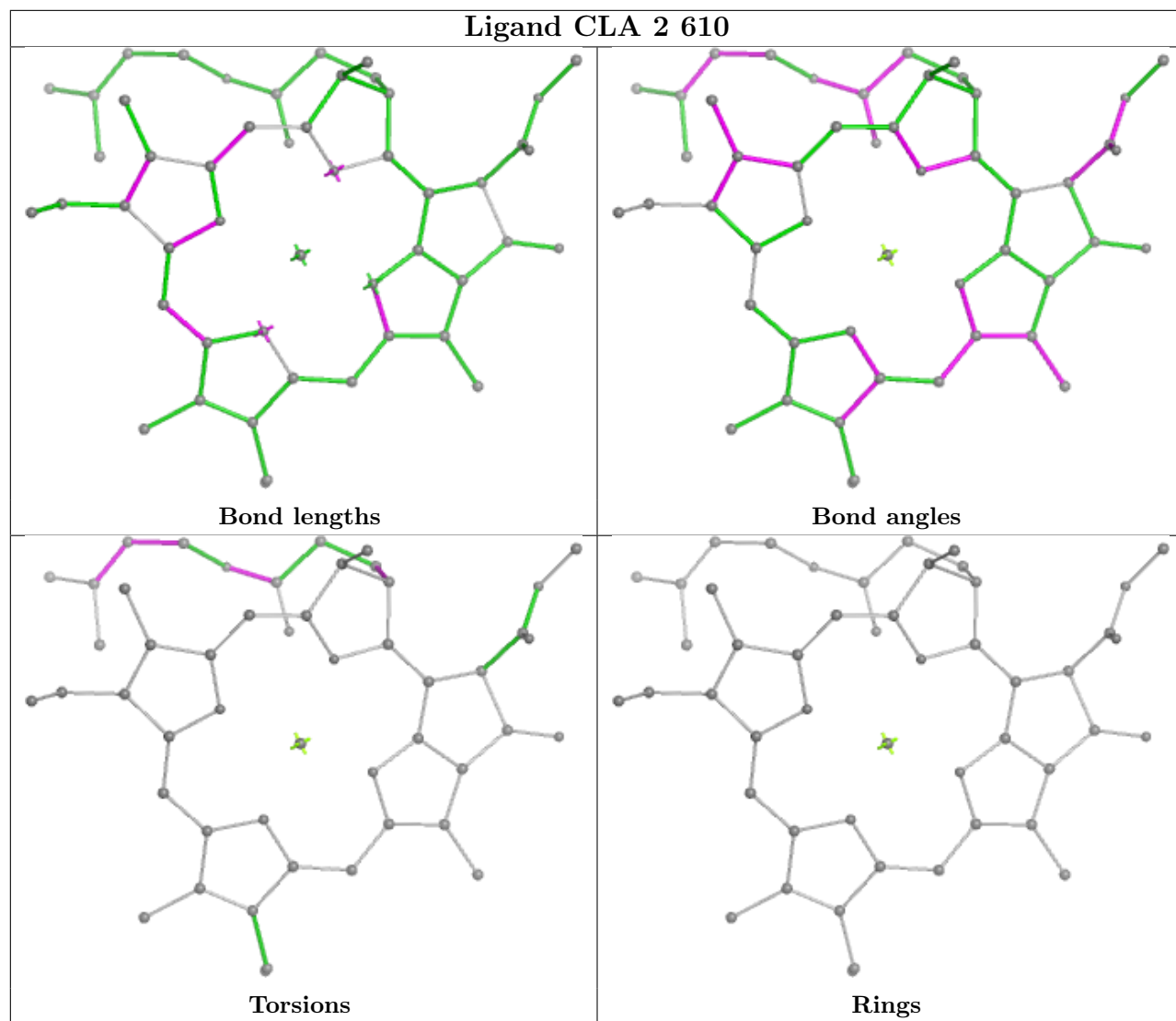
Ligand CLA R 610

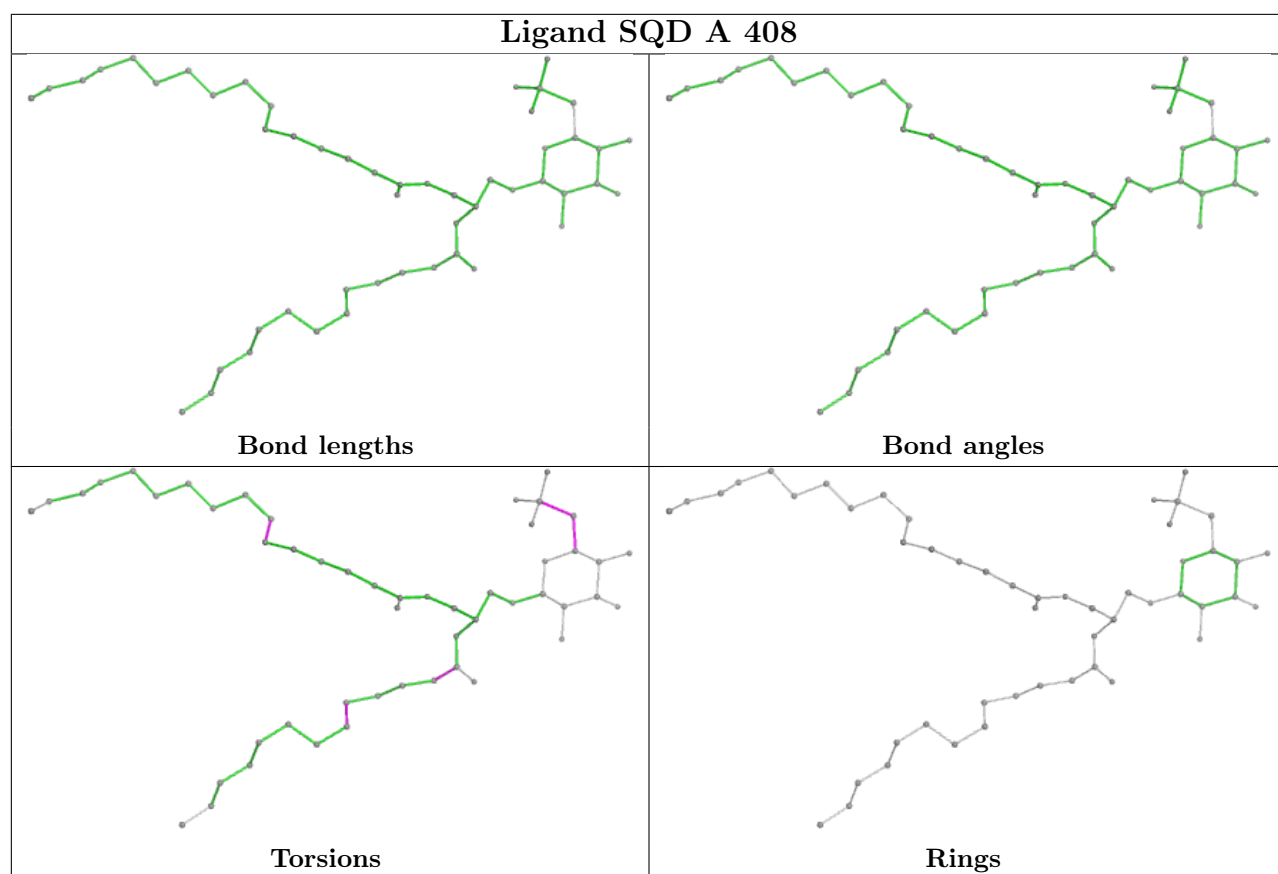


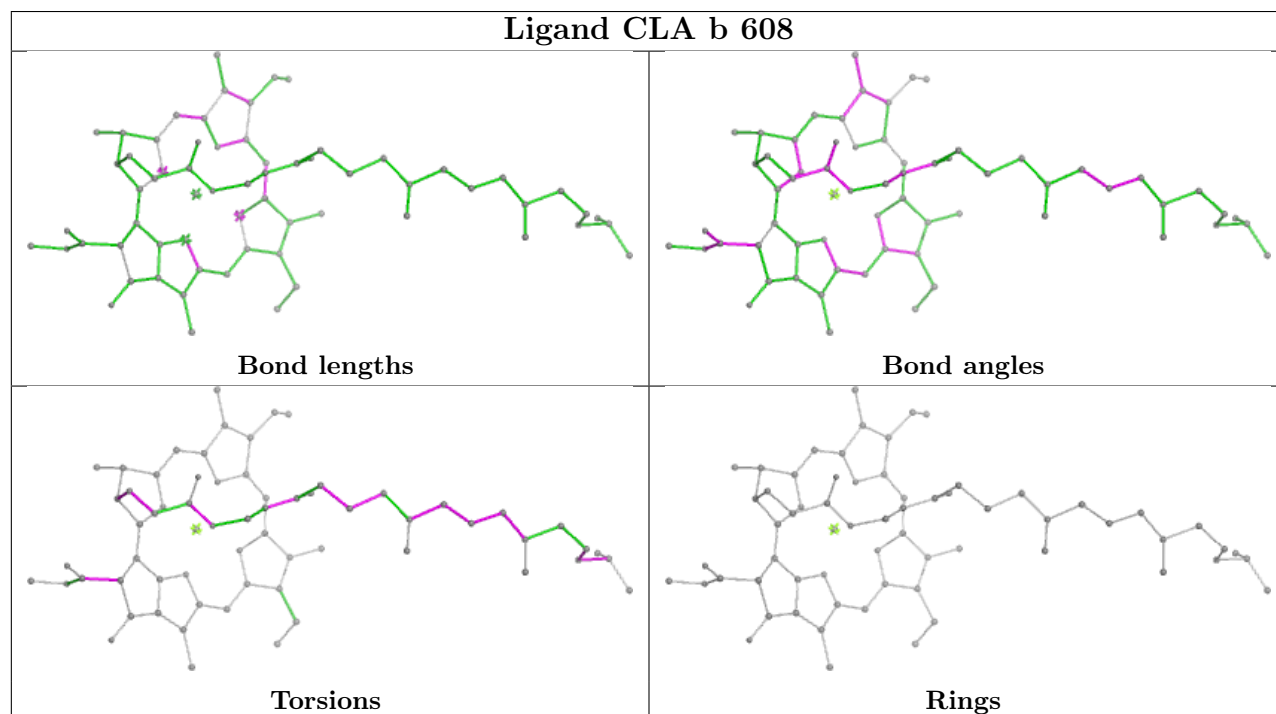
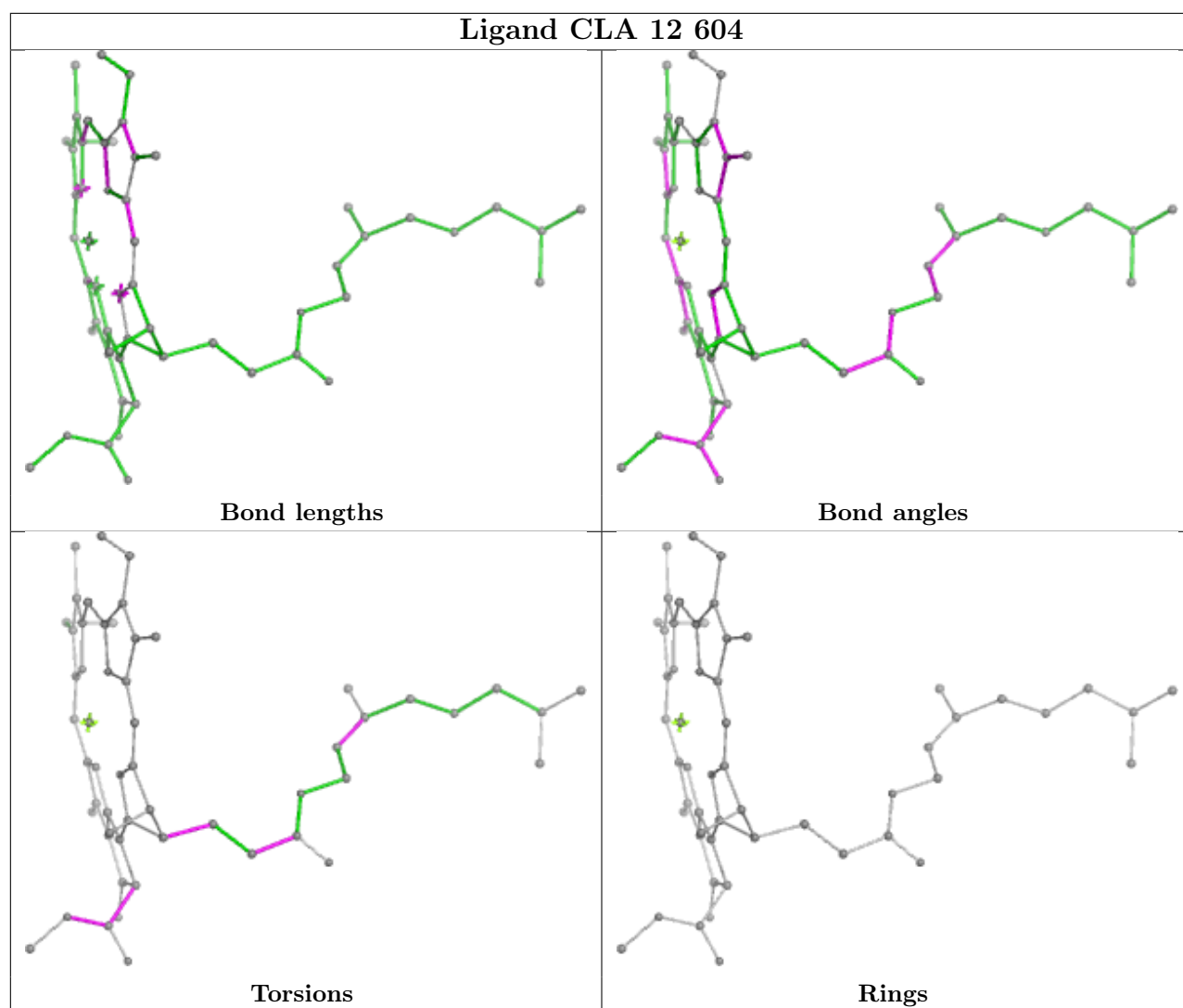
Ligand LMG C 522

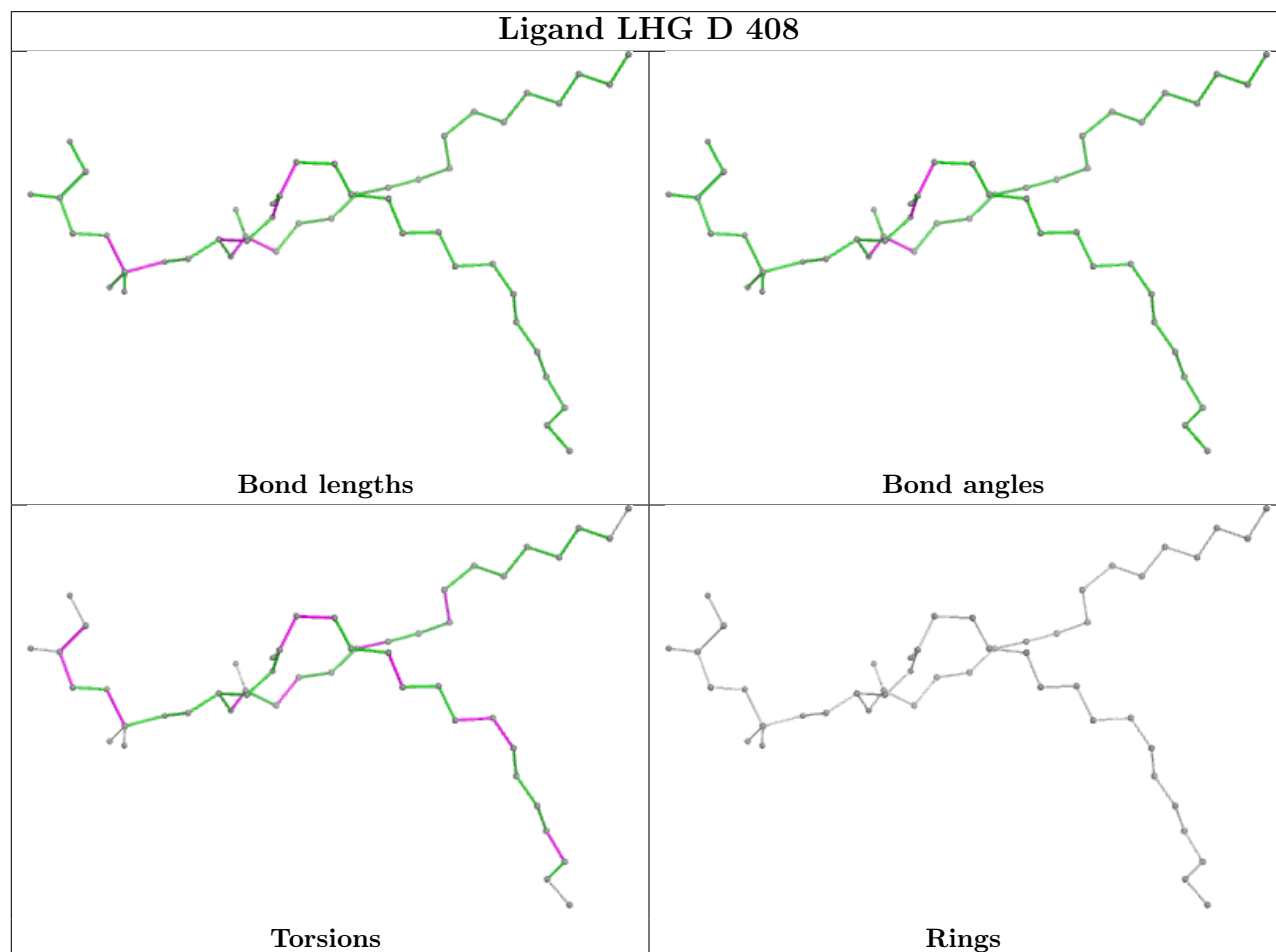
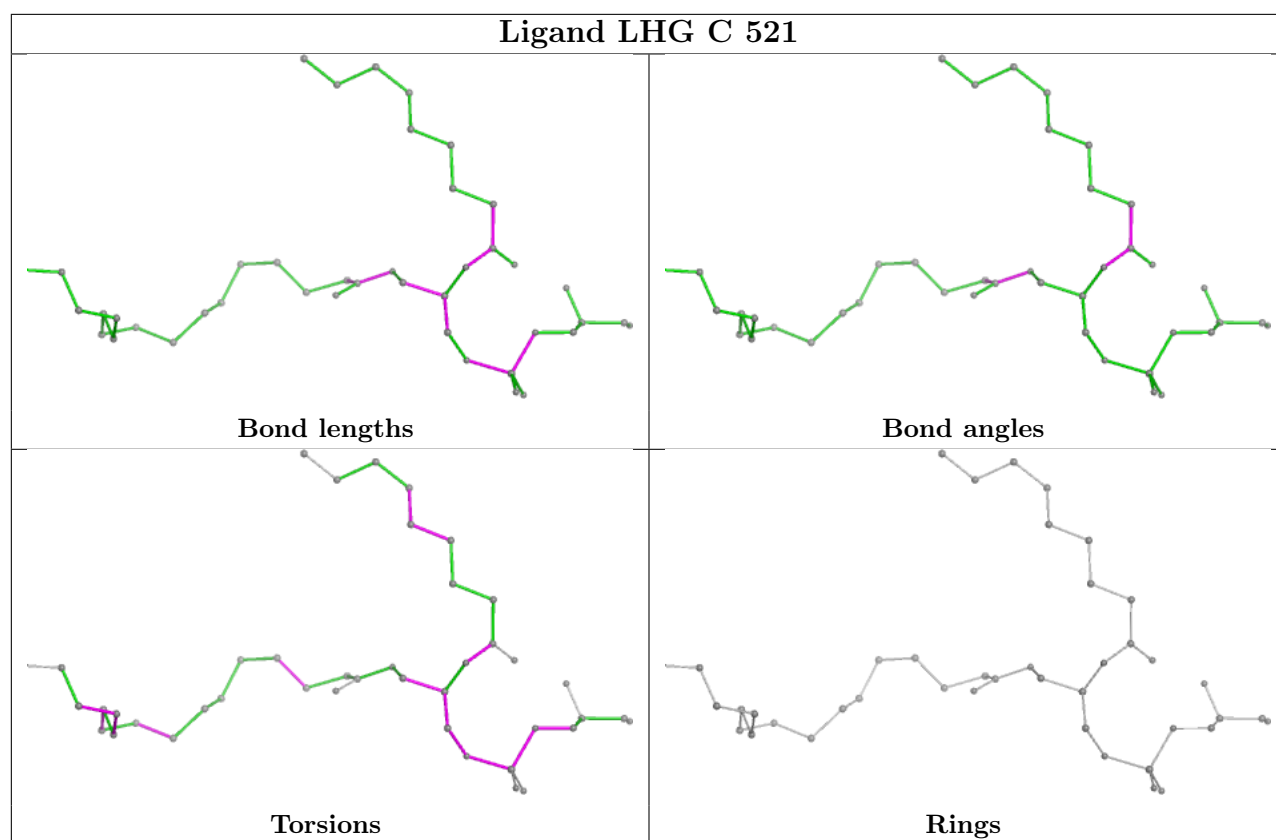


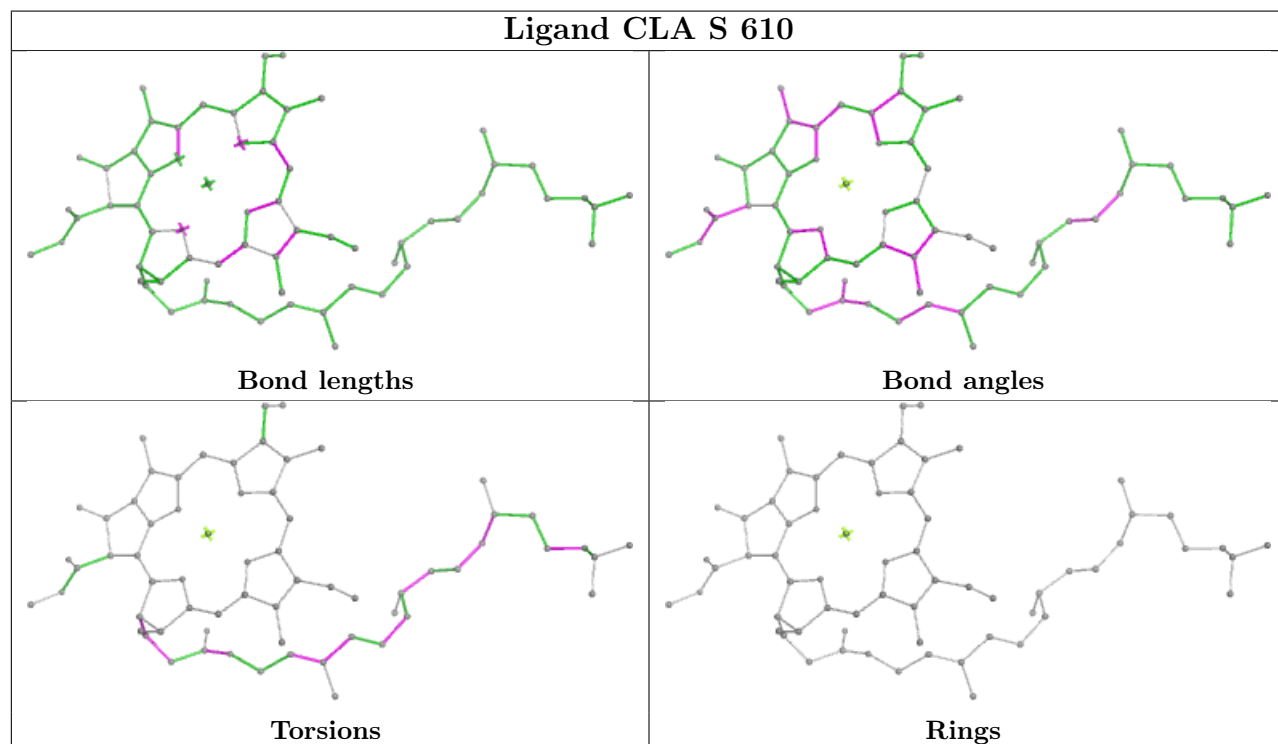
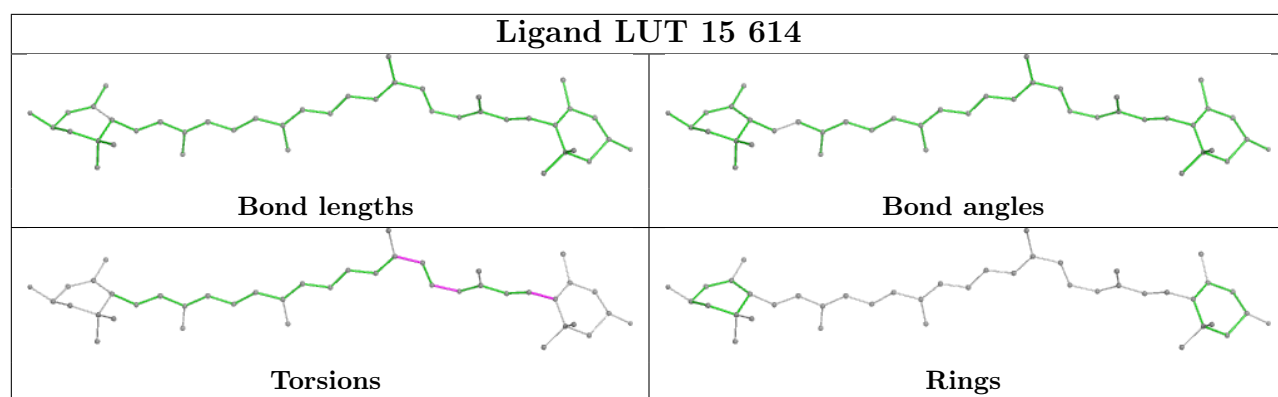
Ligand CLA 2 610

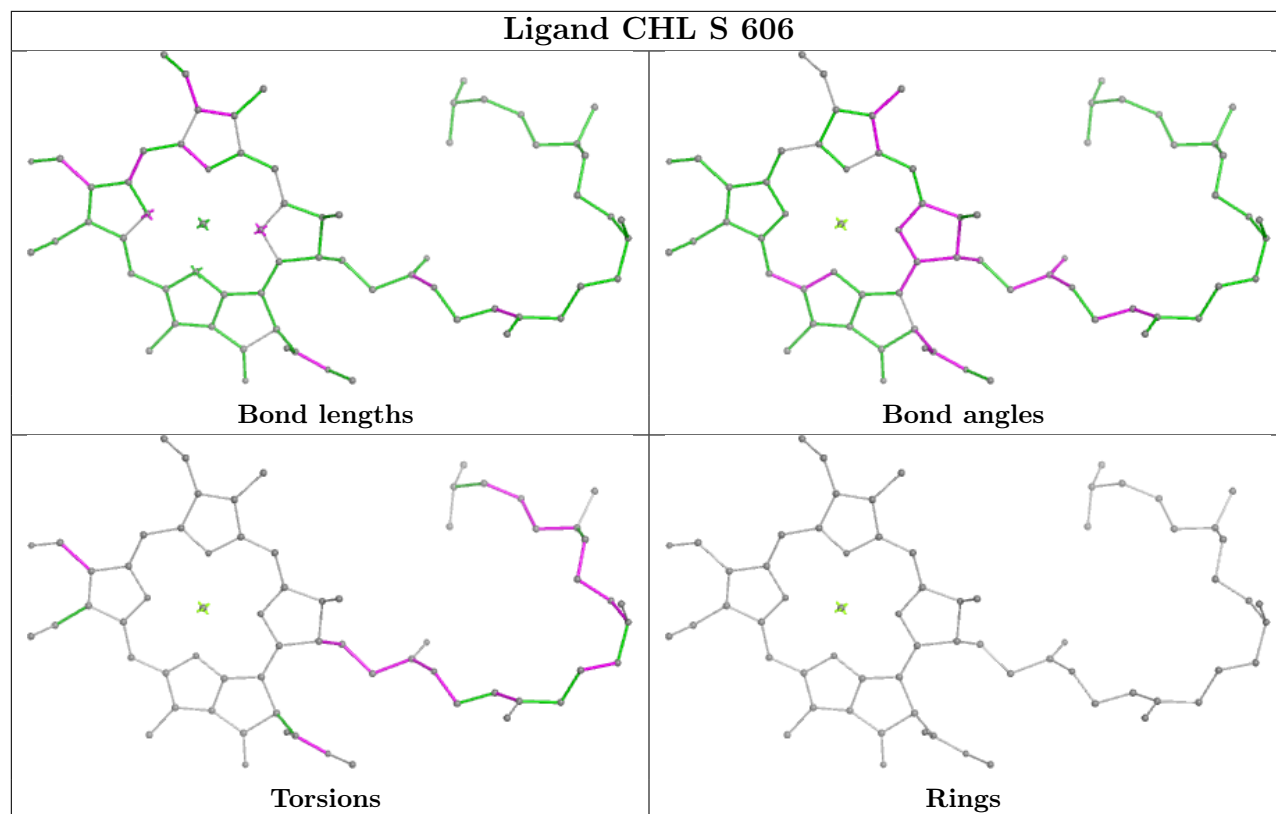




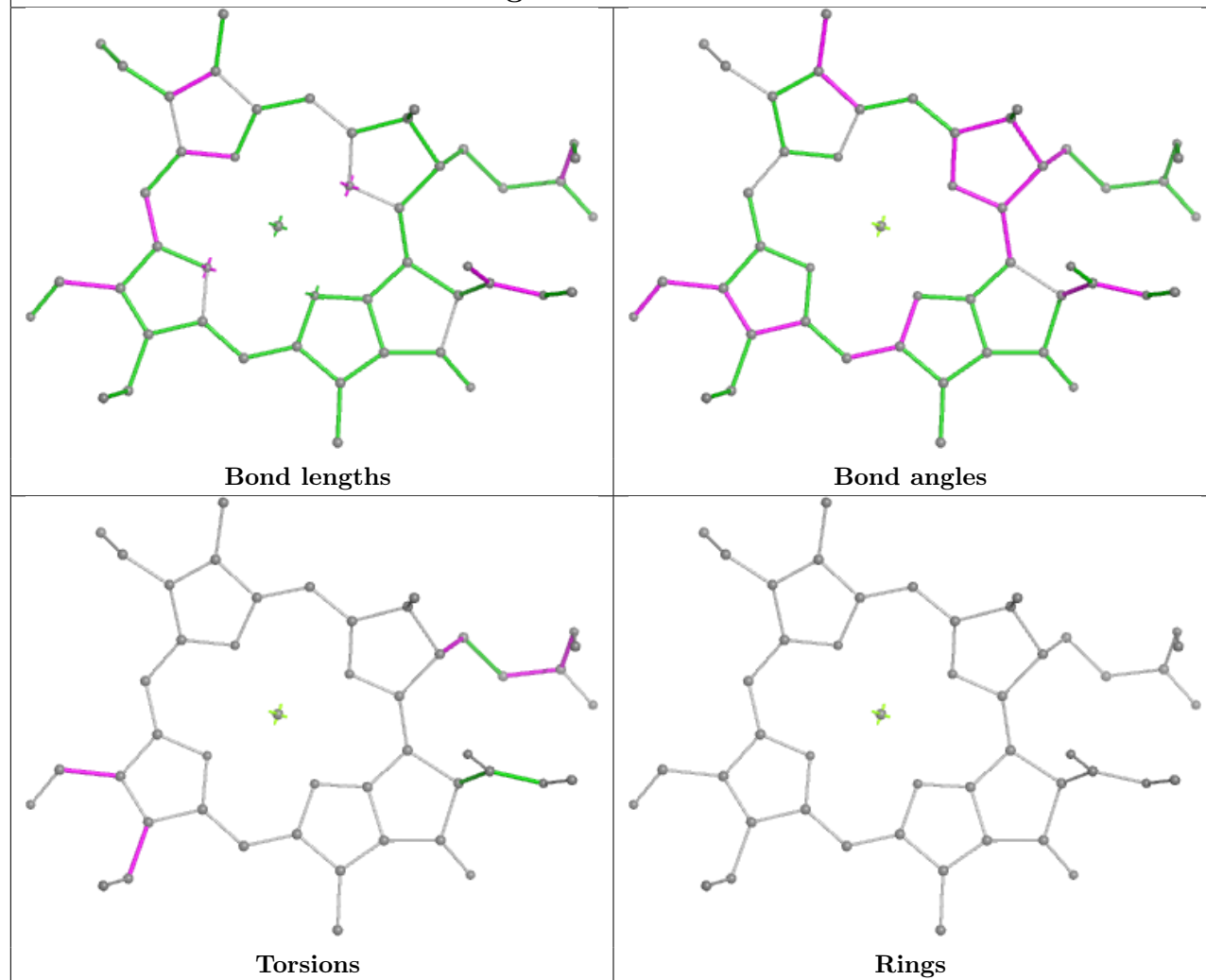


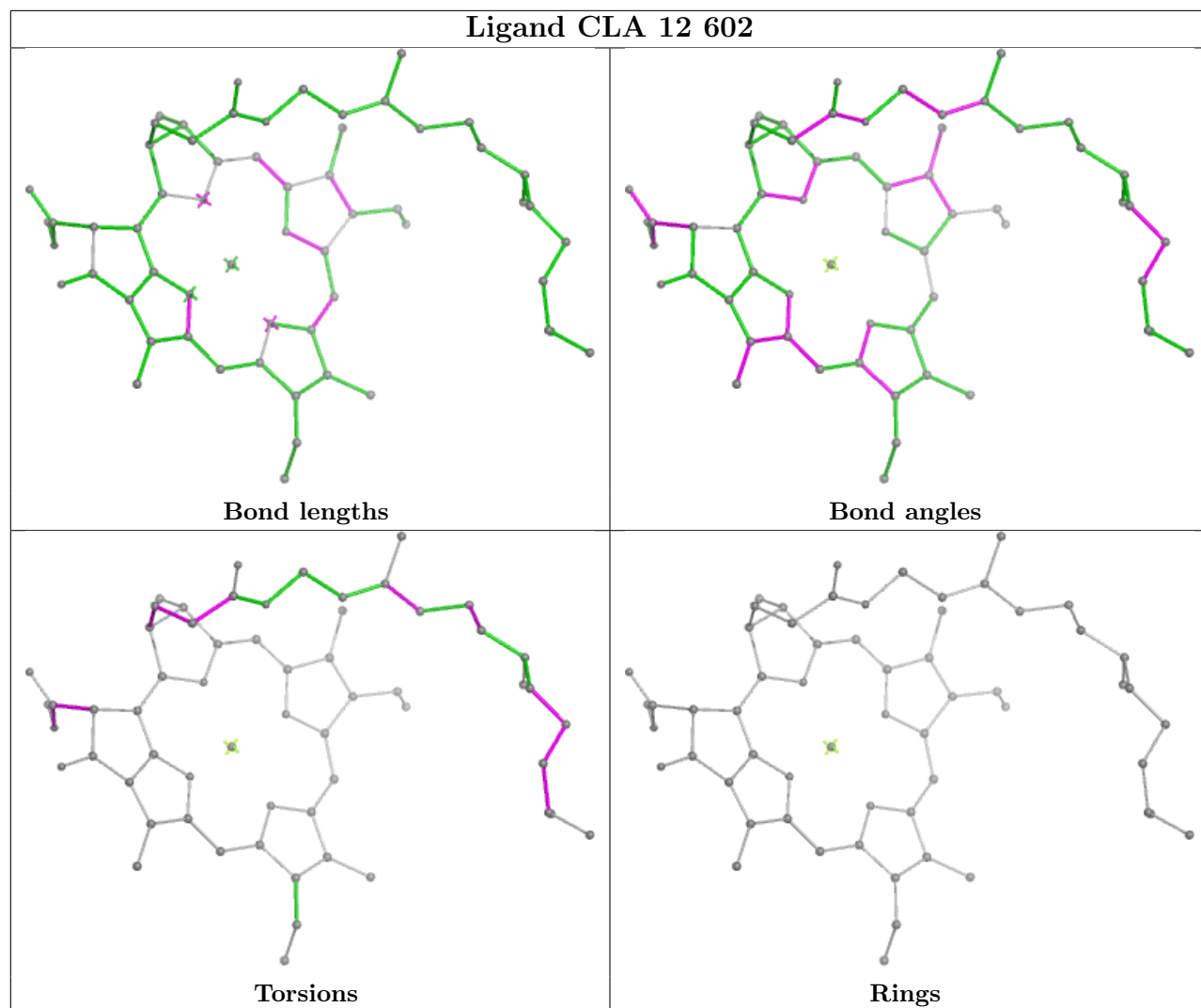




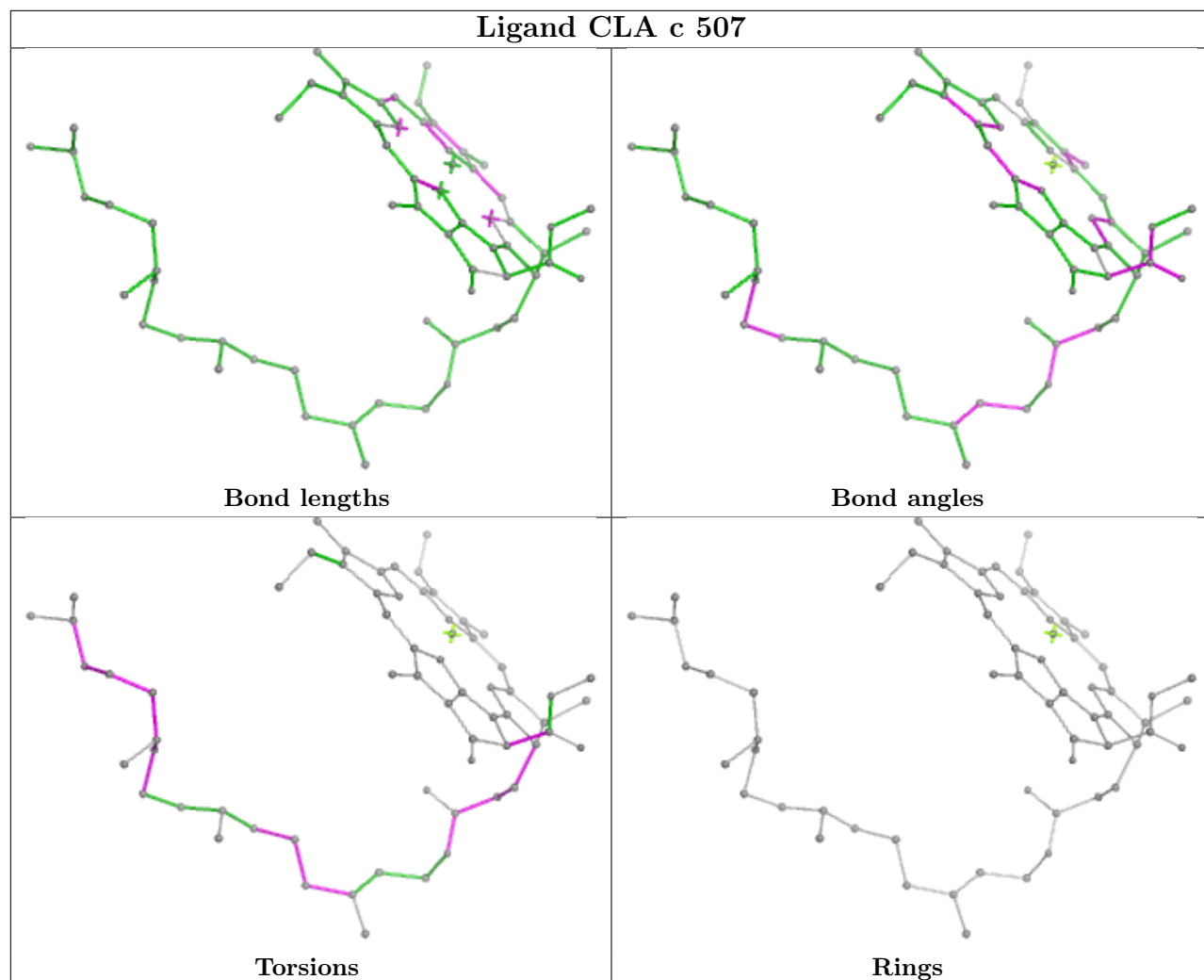


Ligand CHL 1 606

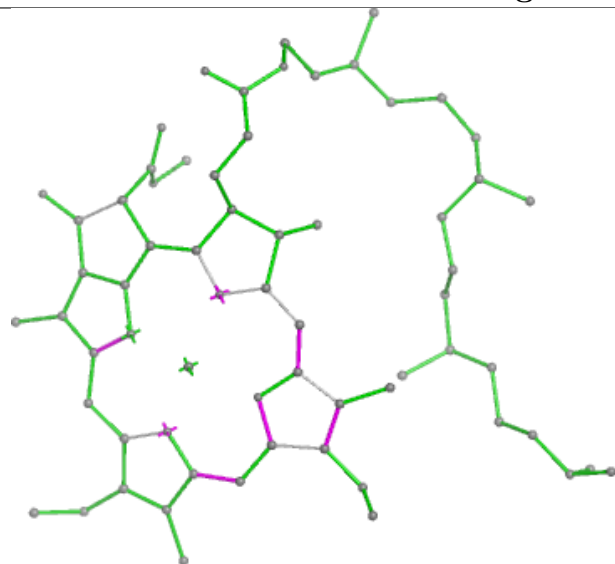




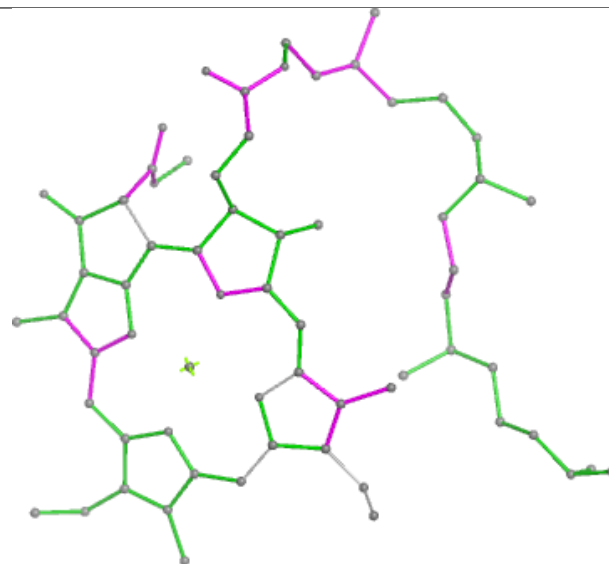
Ligand CLA c 507



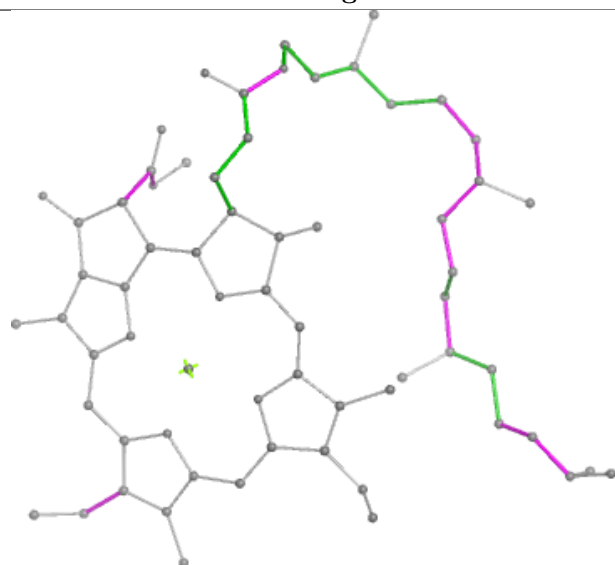
Ligand CLA Y 612



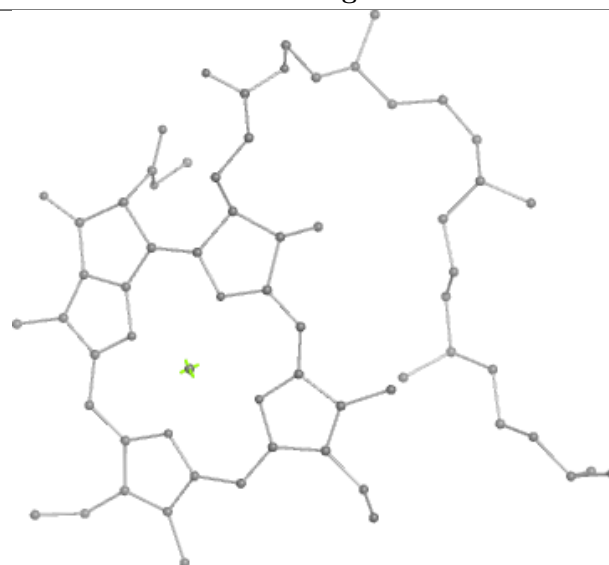
Bond lengths



Bond angles

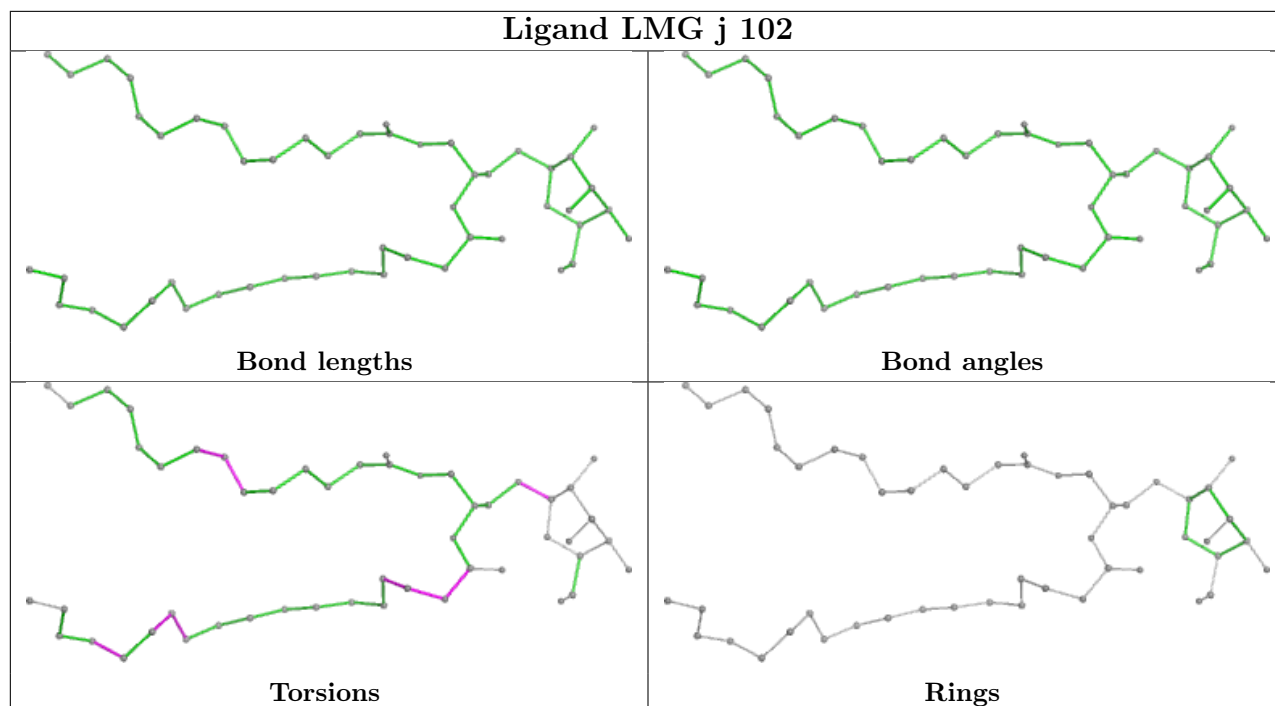


Torsions

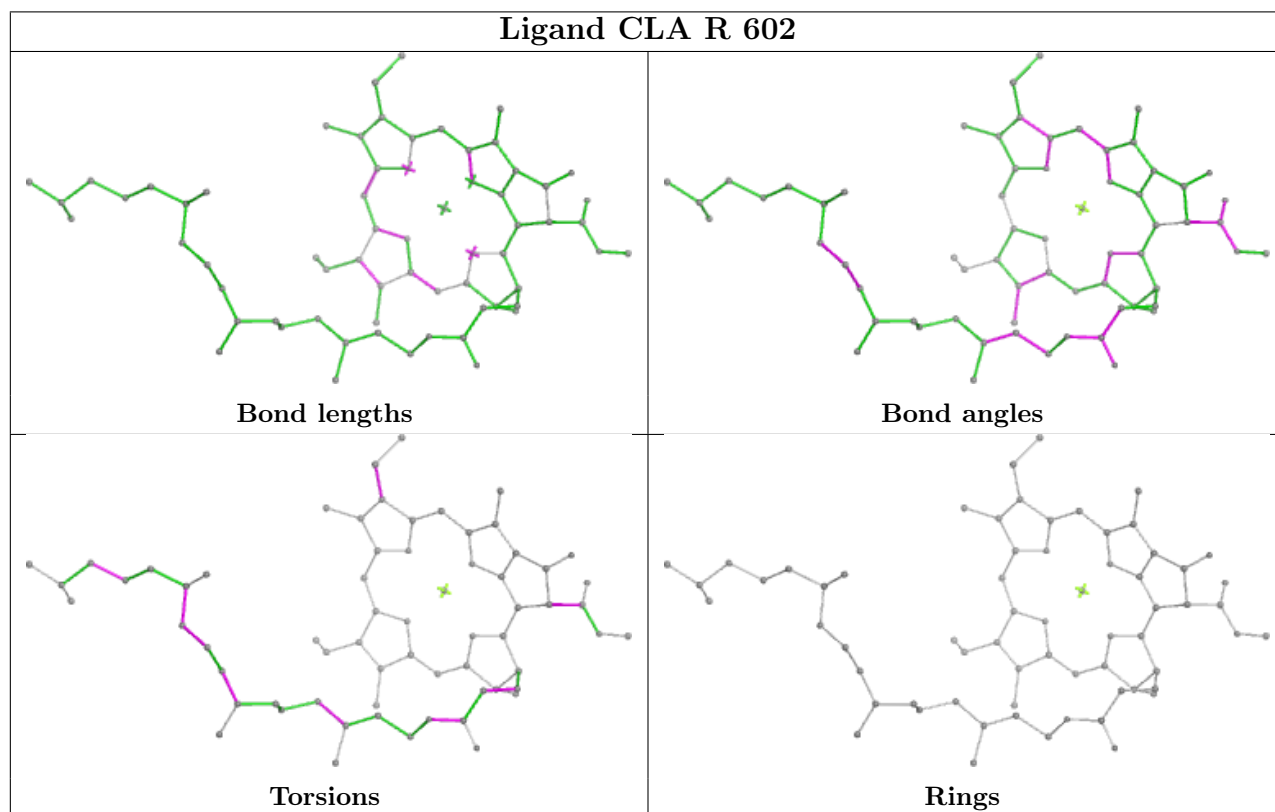


Rings

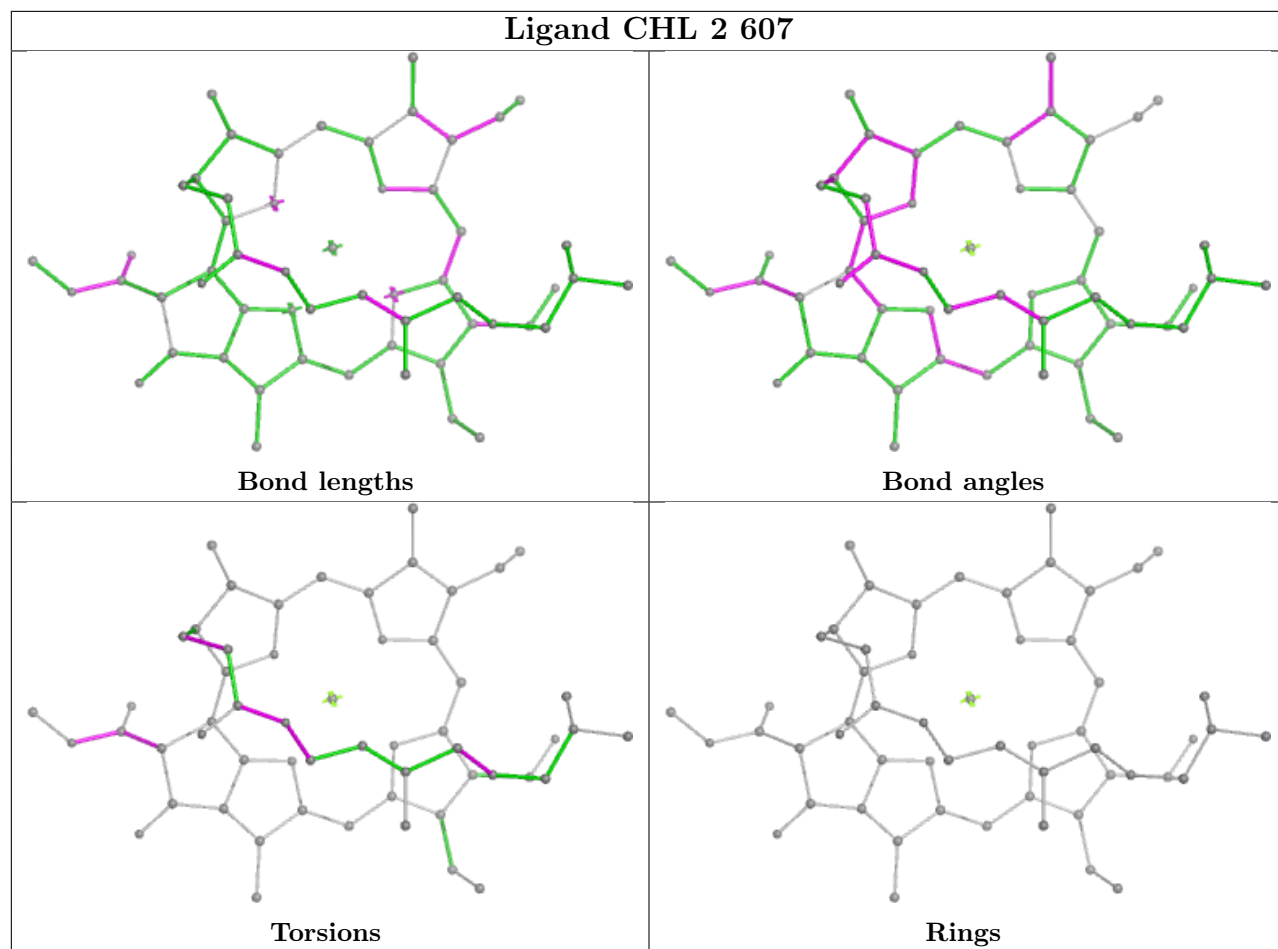
Ligand LMG j 102



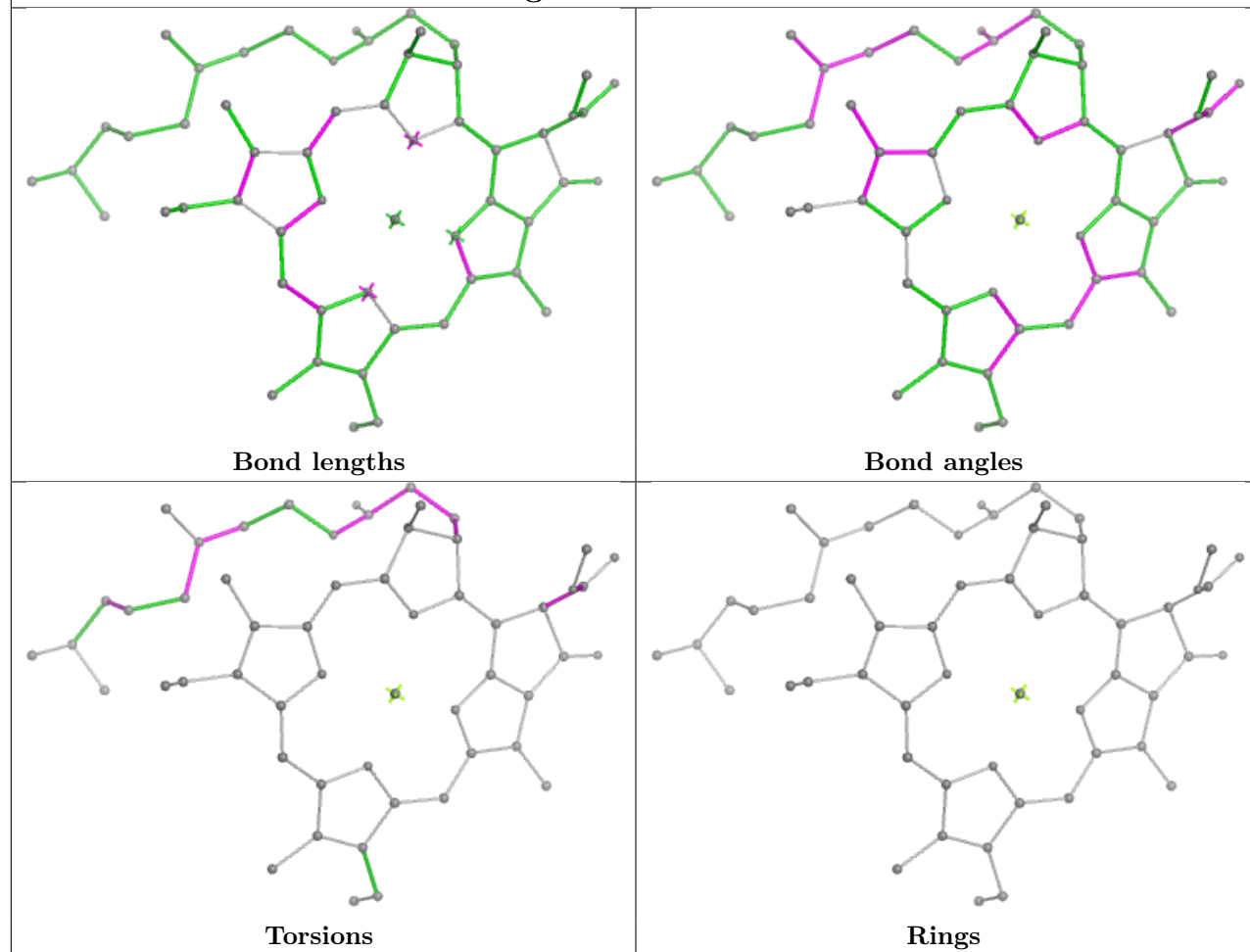
Ligand CLA R 602



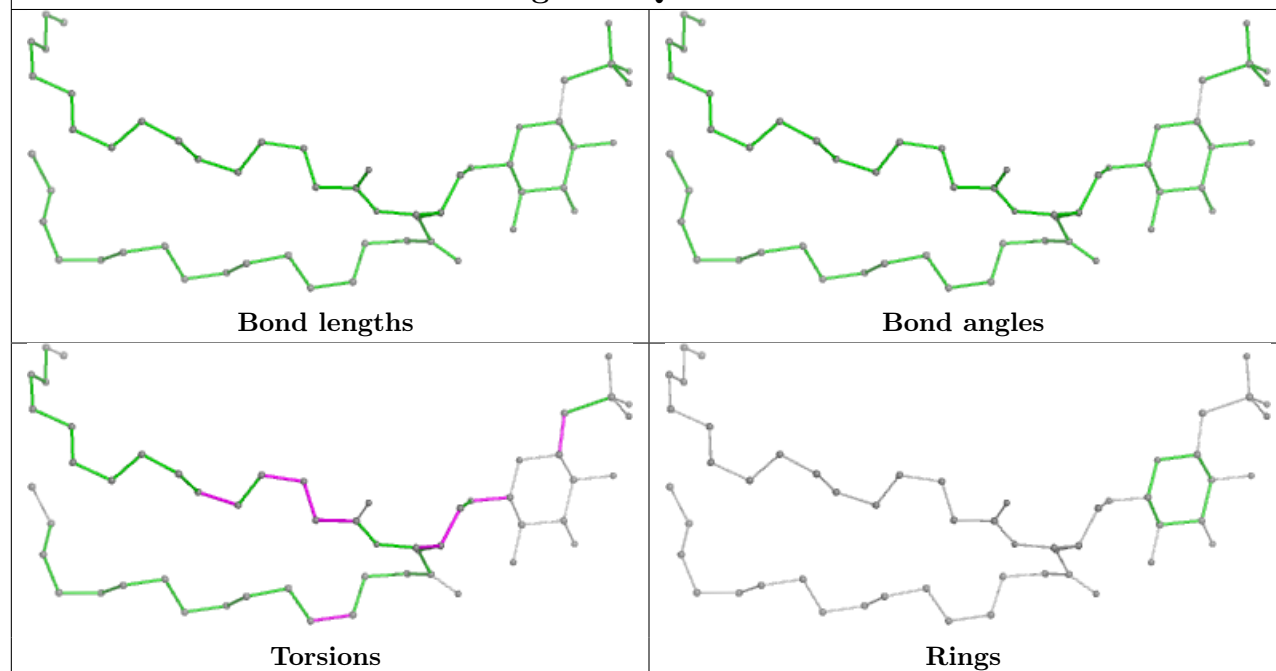
Ligand CHL 2 607



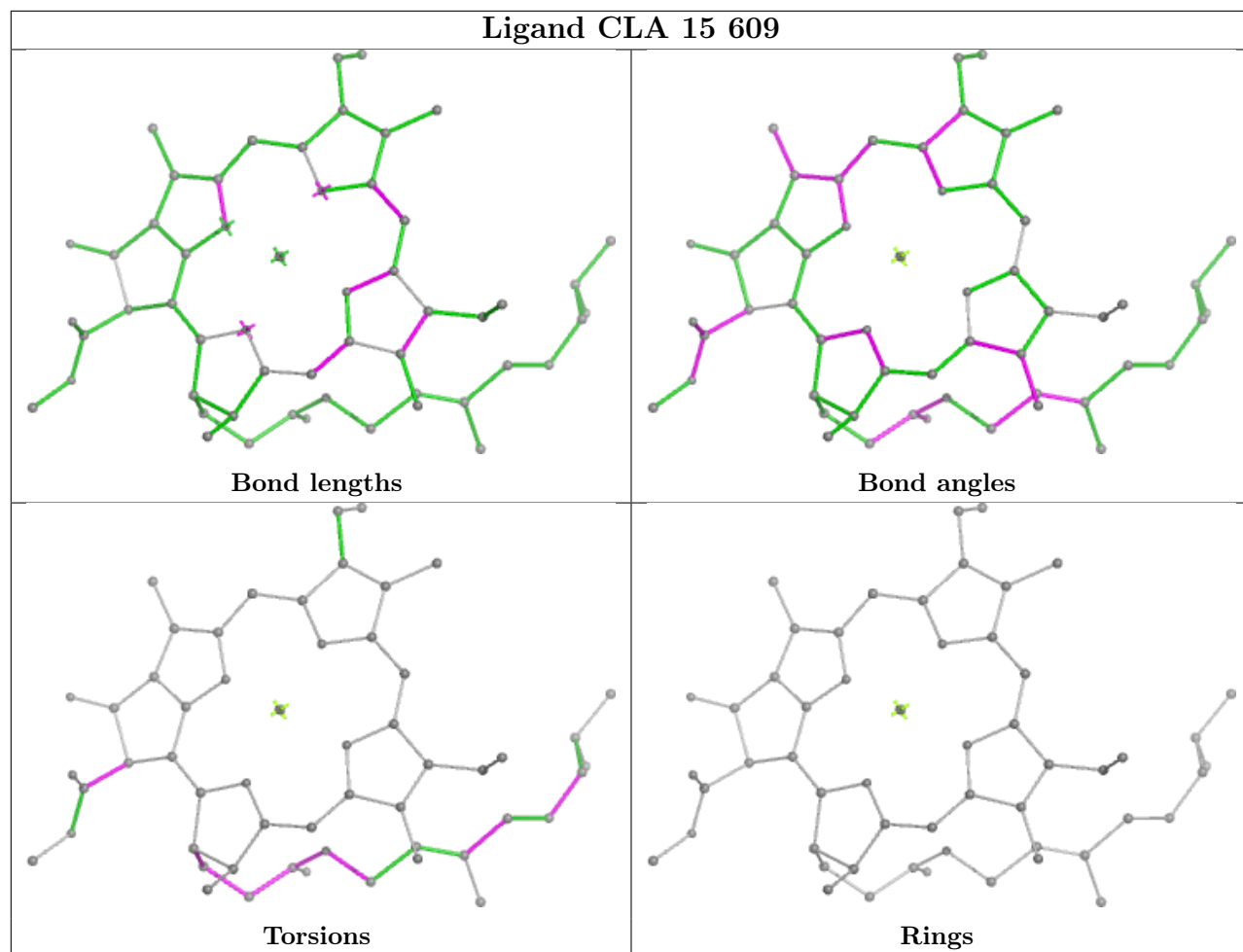
Ligand CLA 2 602

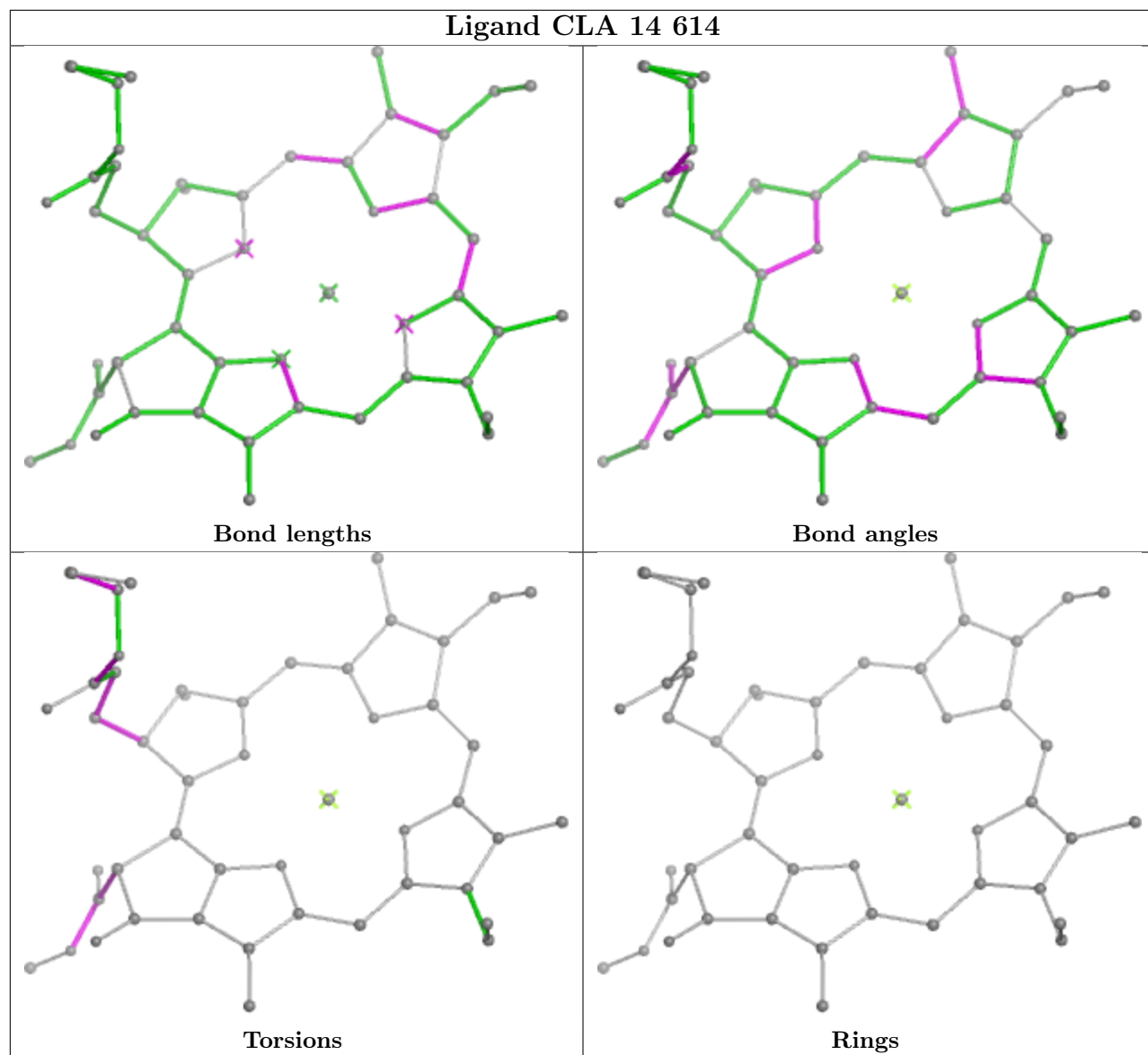


Ligand SQD D 411

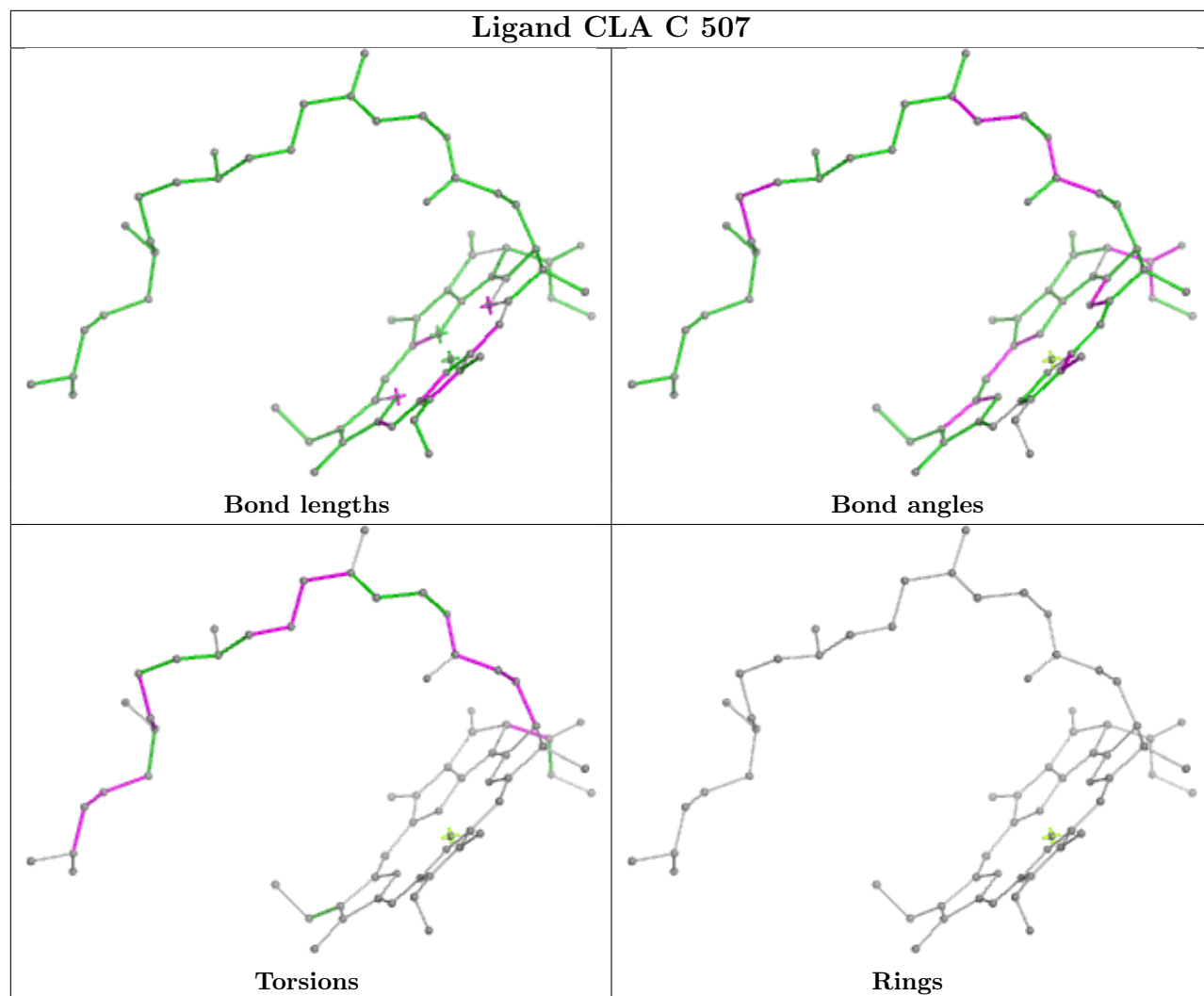


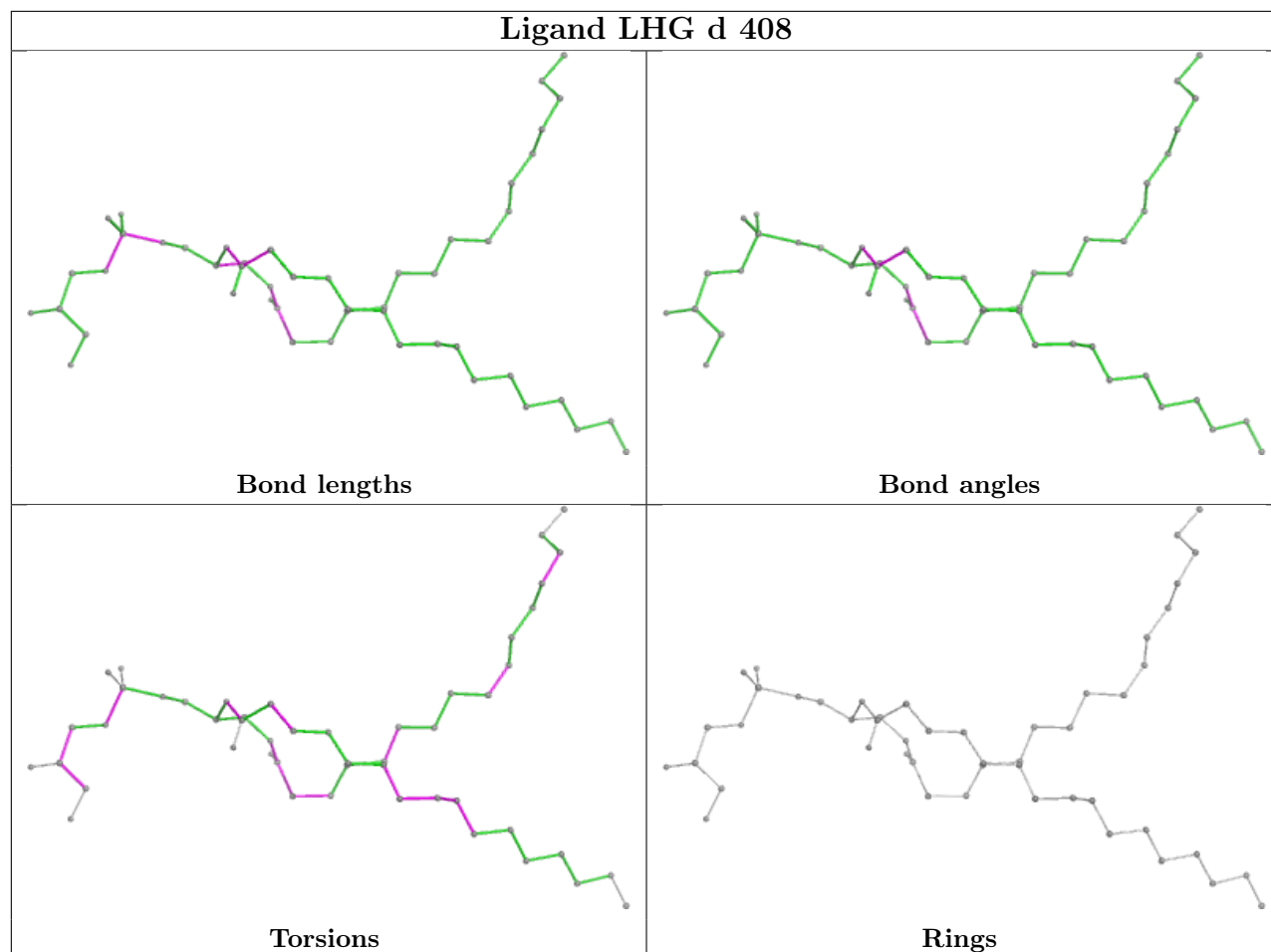
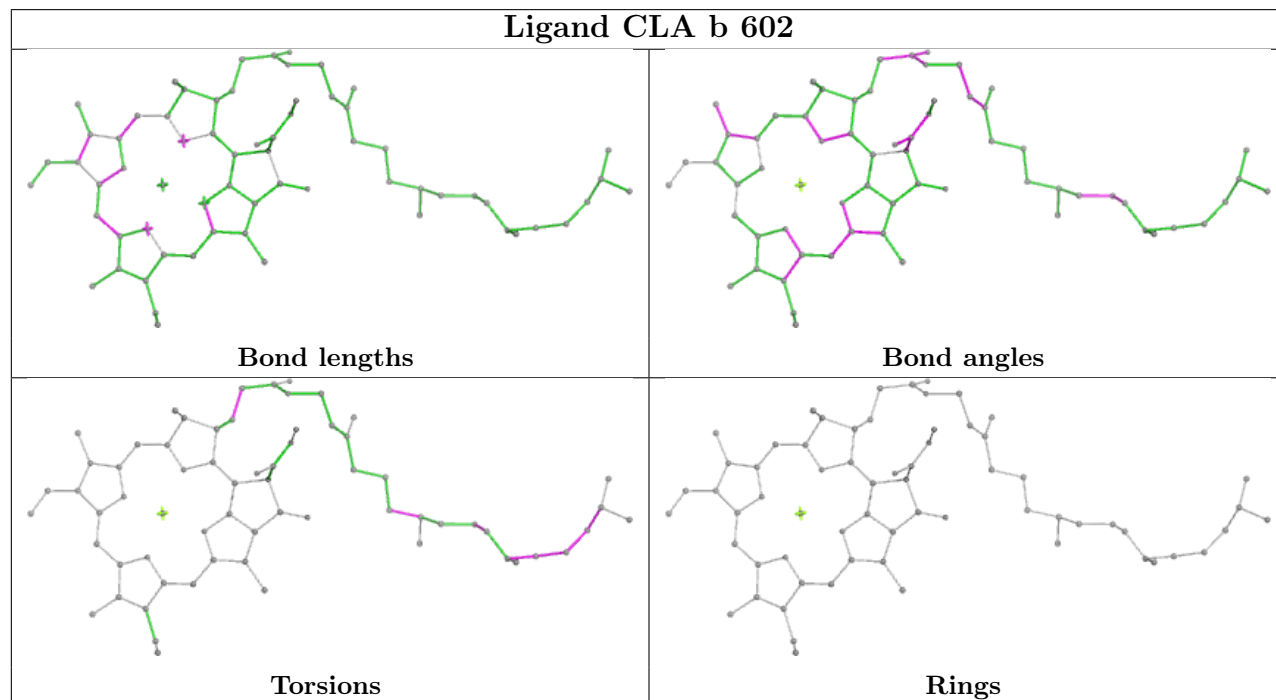
Ligand CLA 15 609

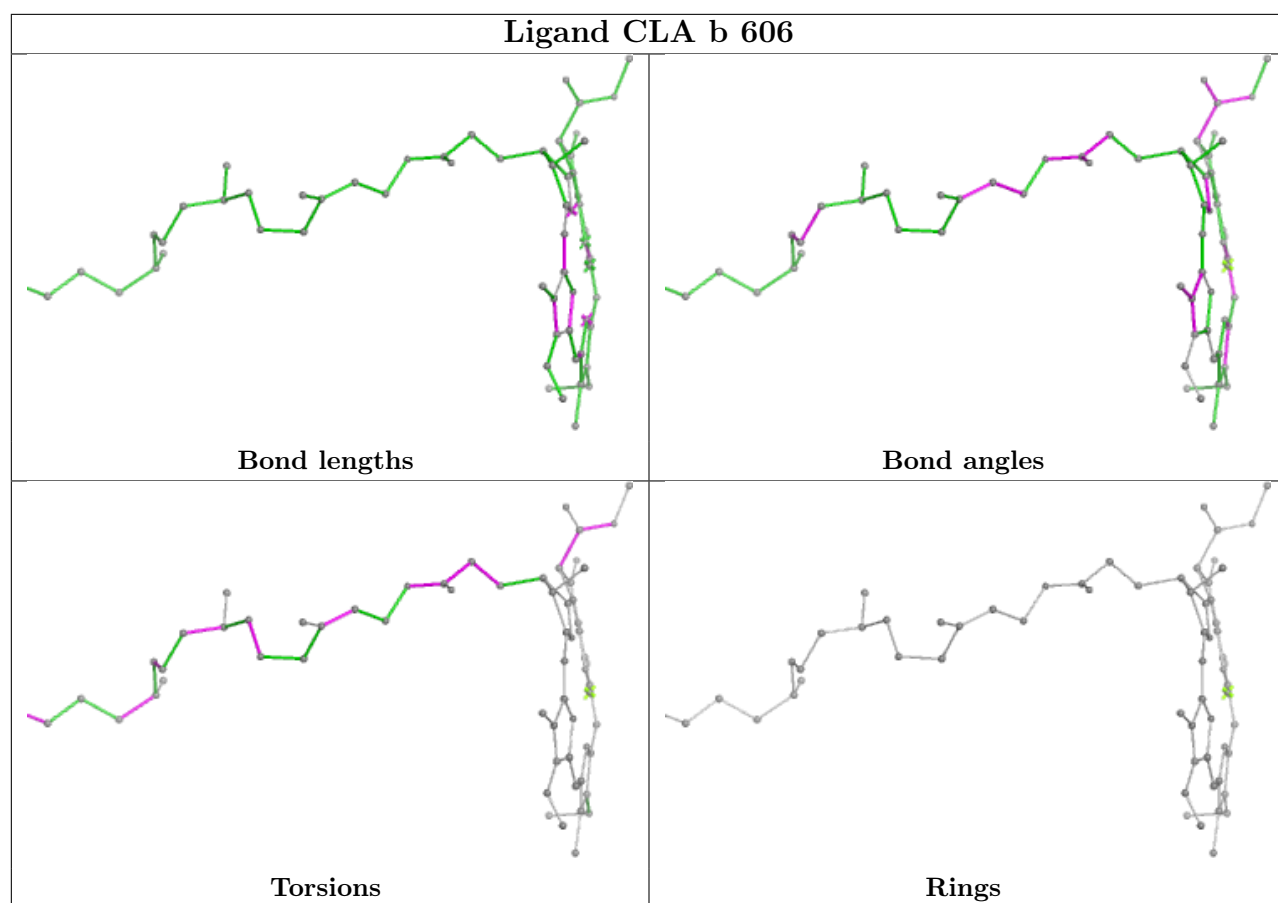


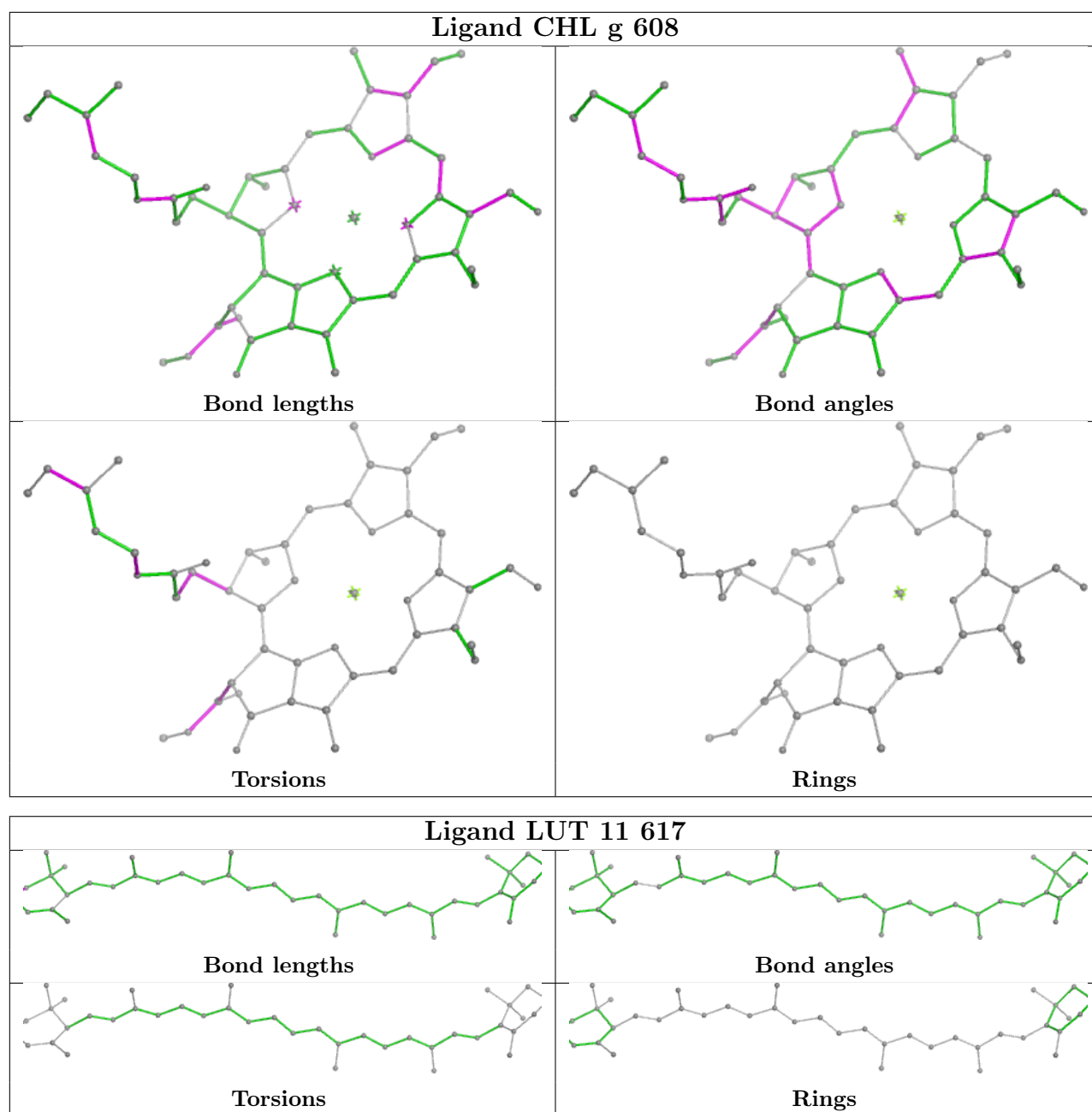


Ligand CLA C 507

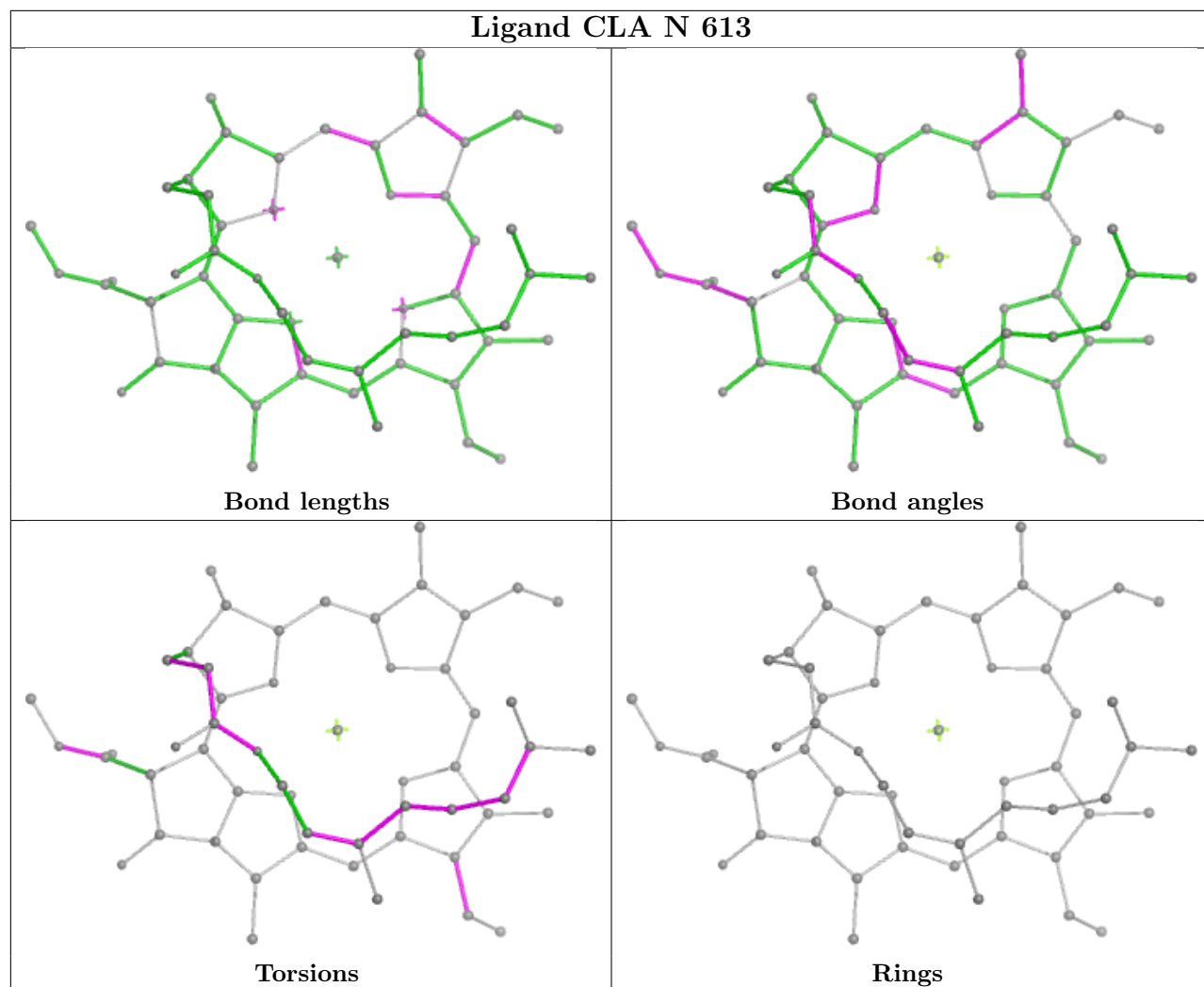


Ligand LHG d 408**Ligand CLA b 602**

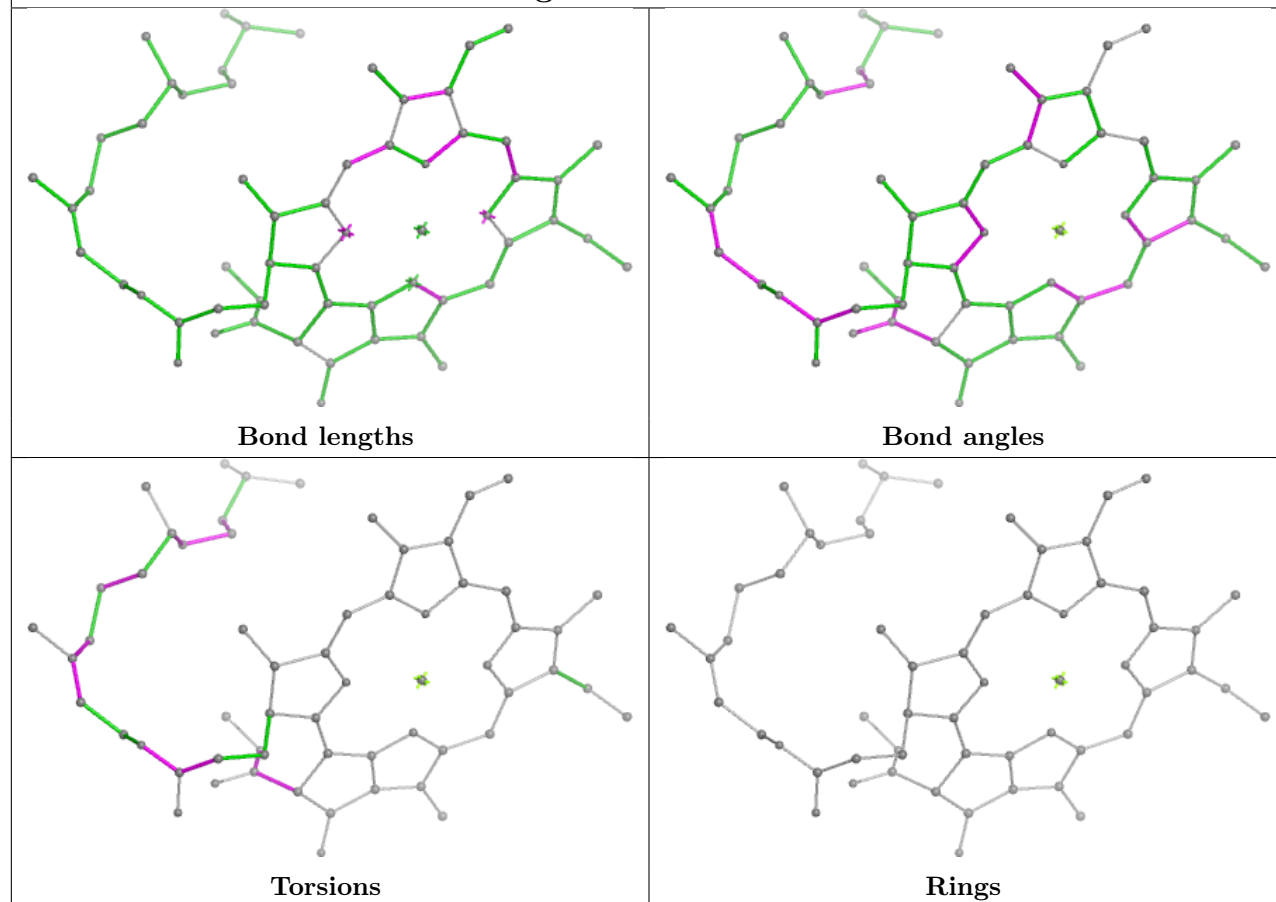




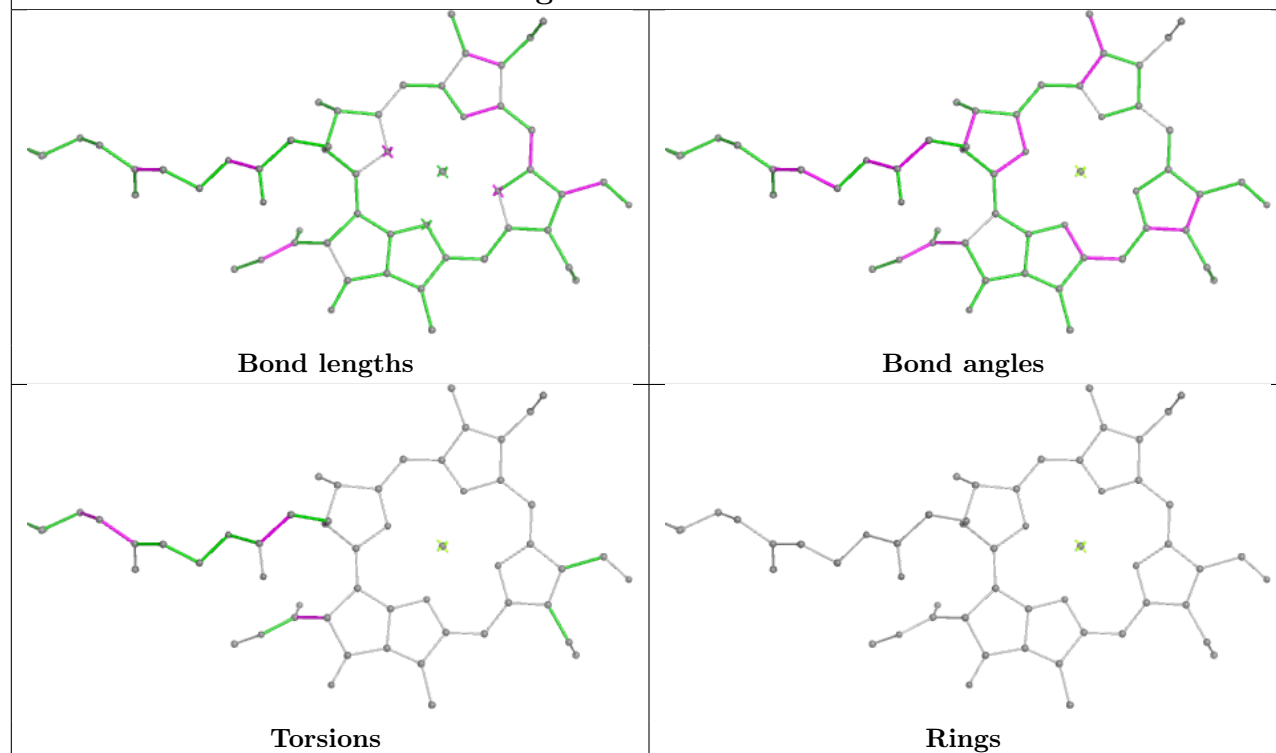
Ligand CLA N 613

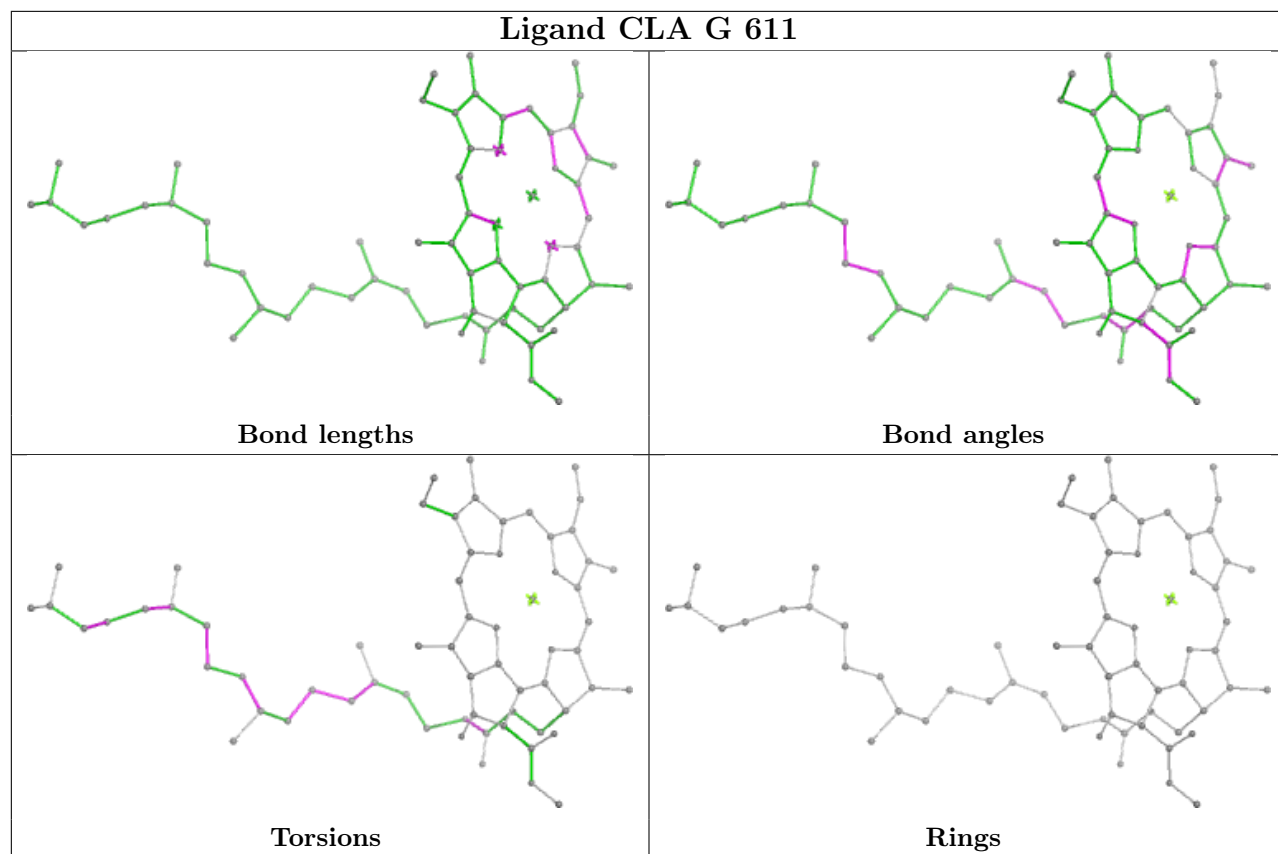


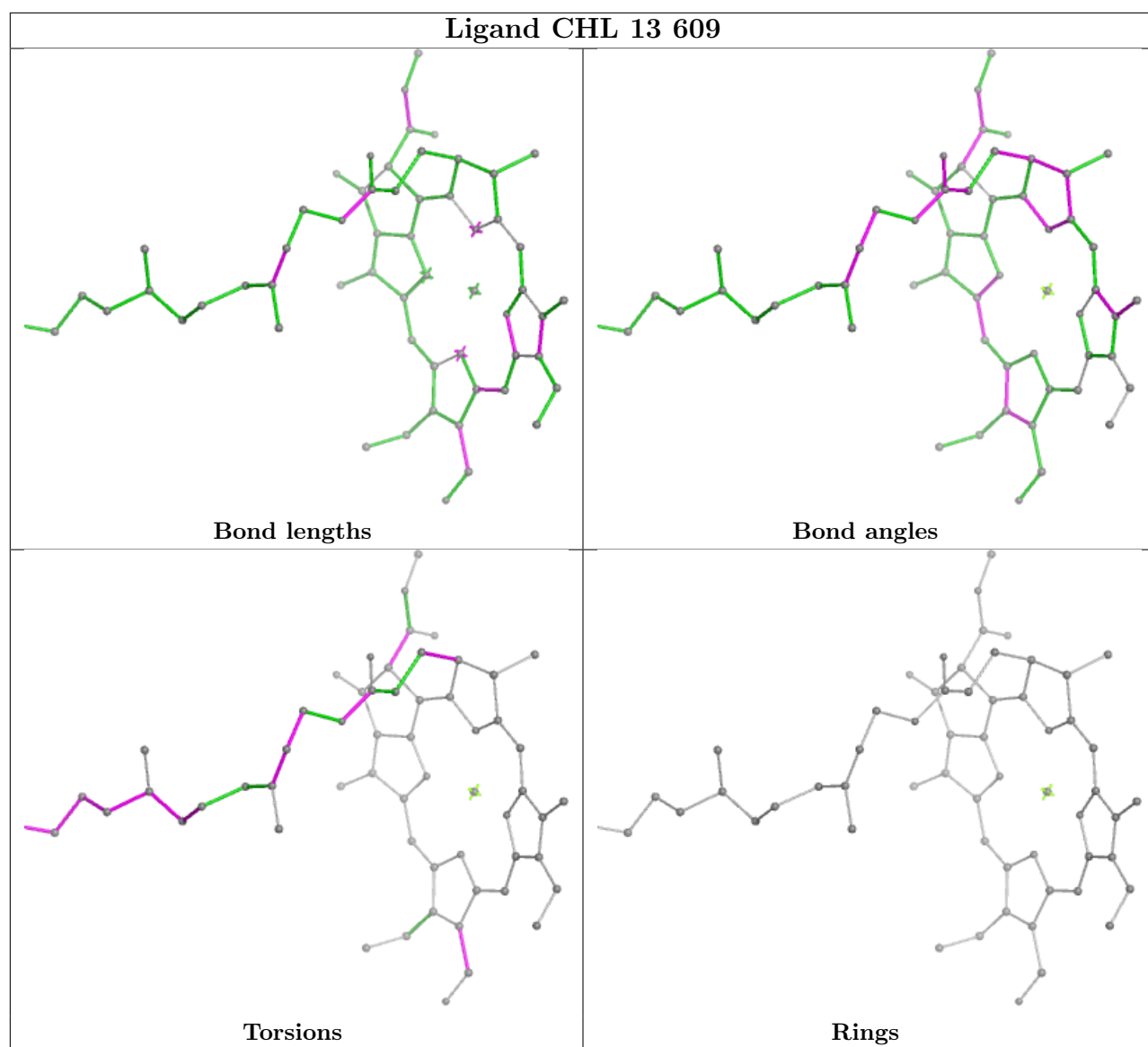
Ligand CLA n 603



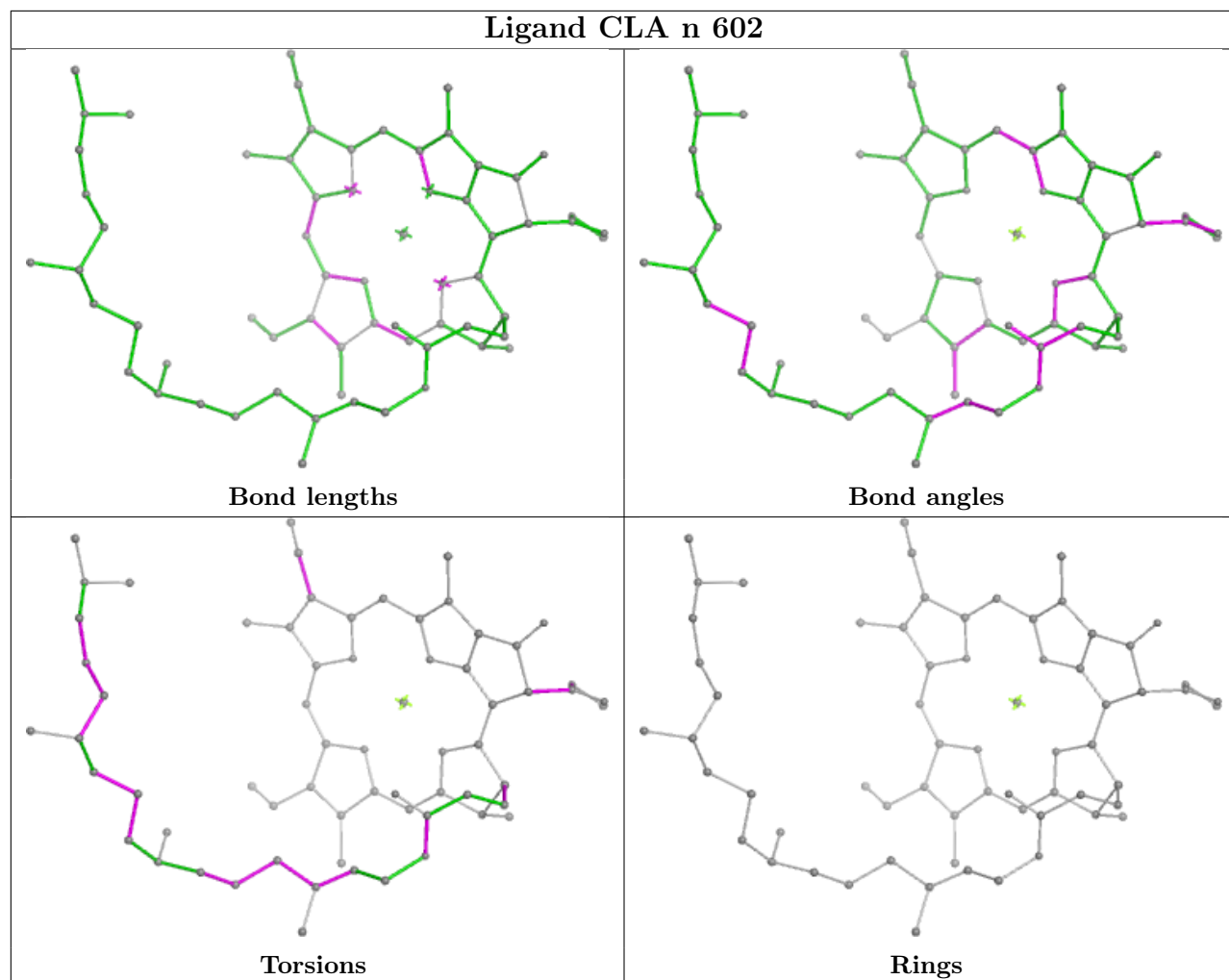
Ligand CHL 3 606

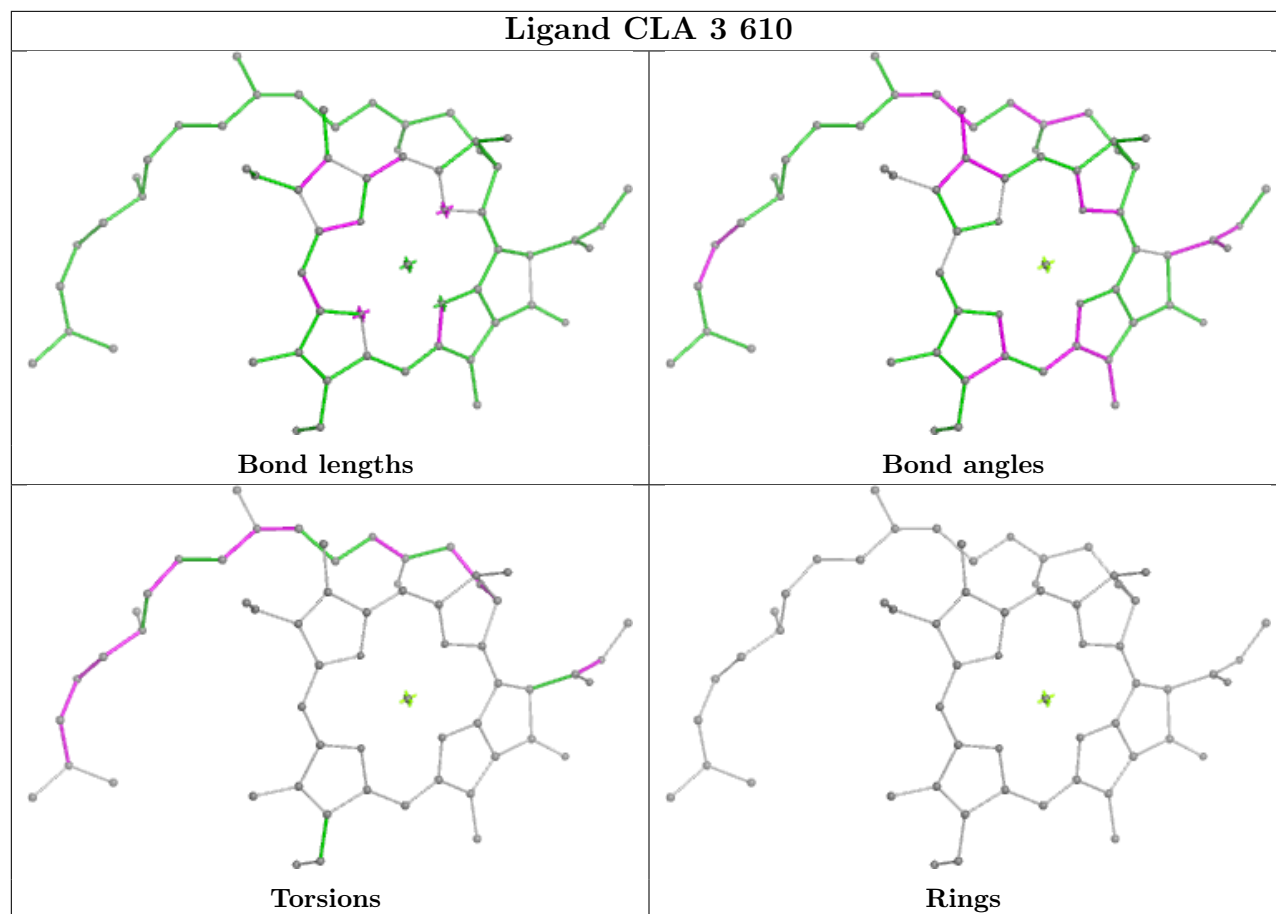
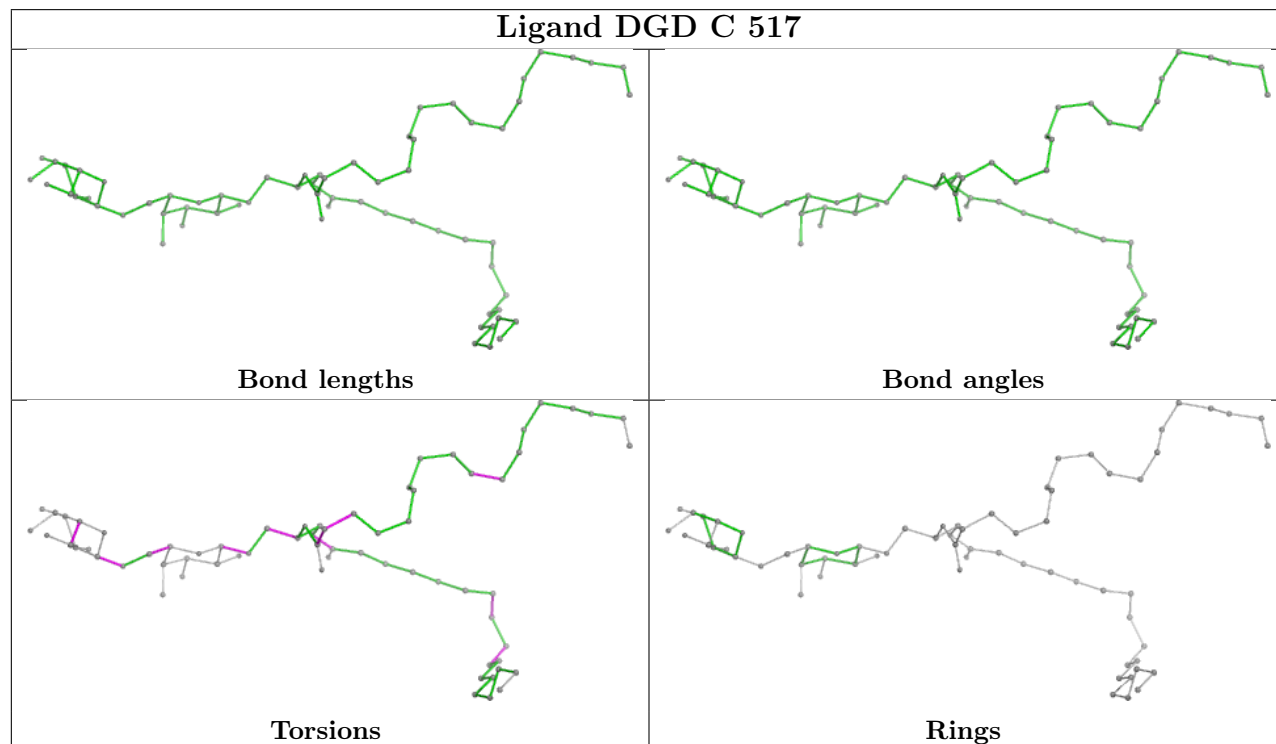


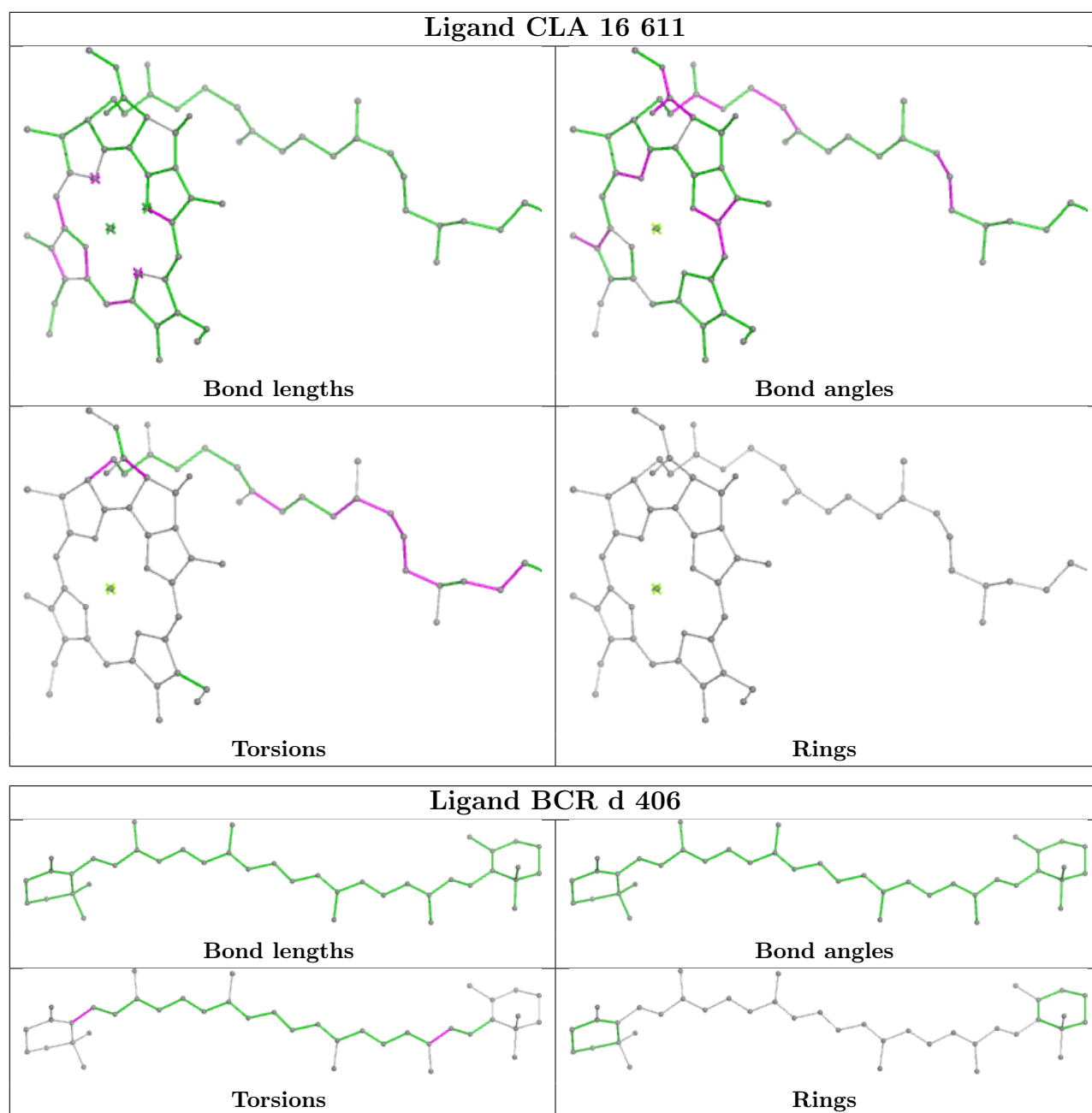


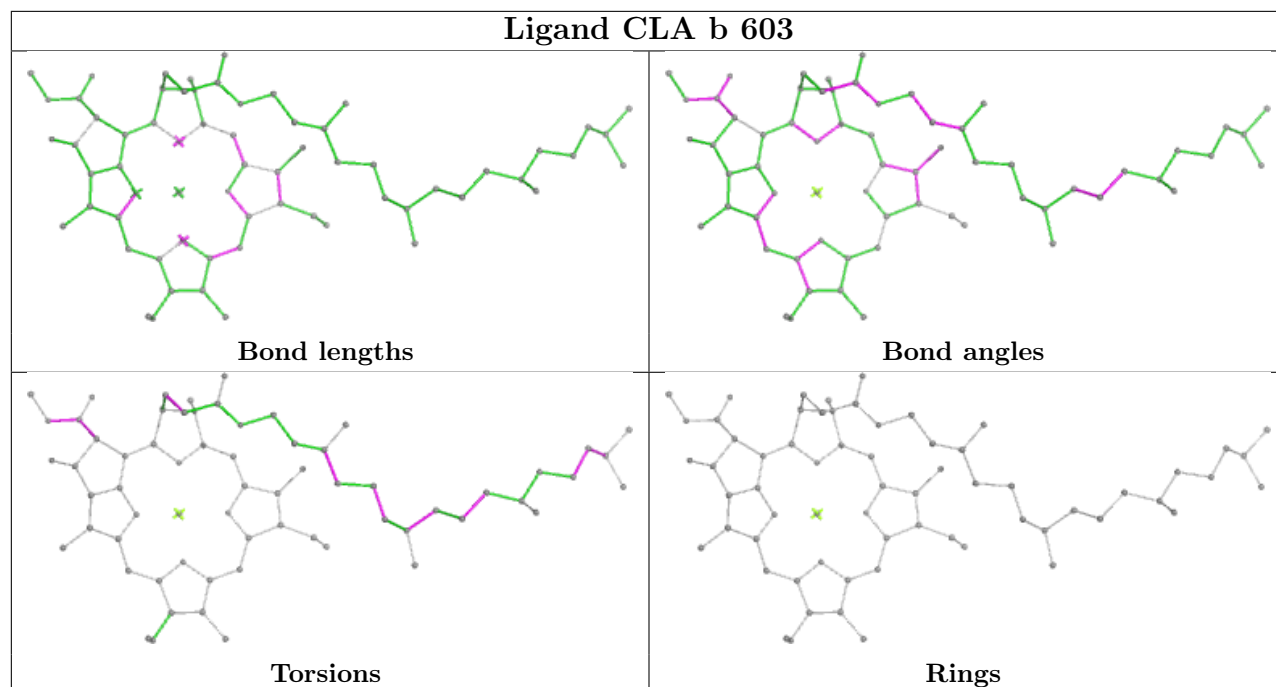
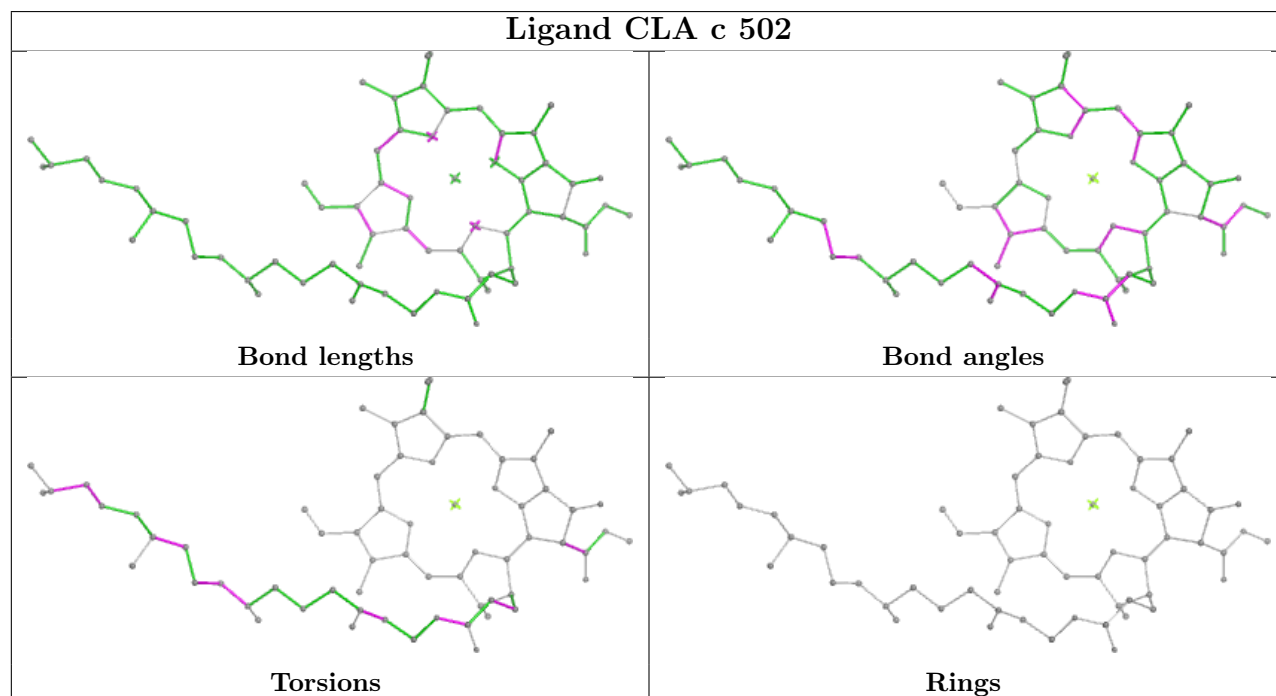


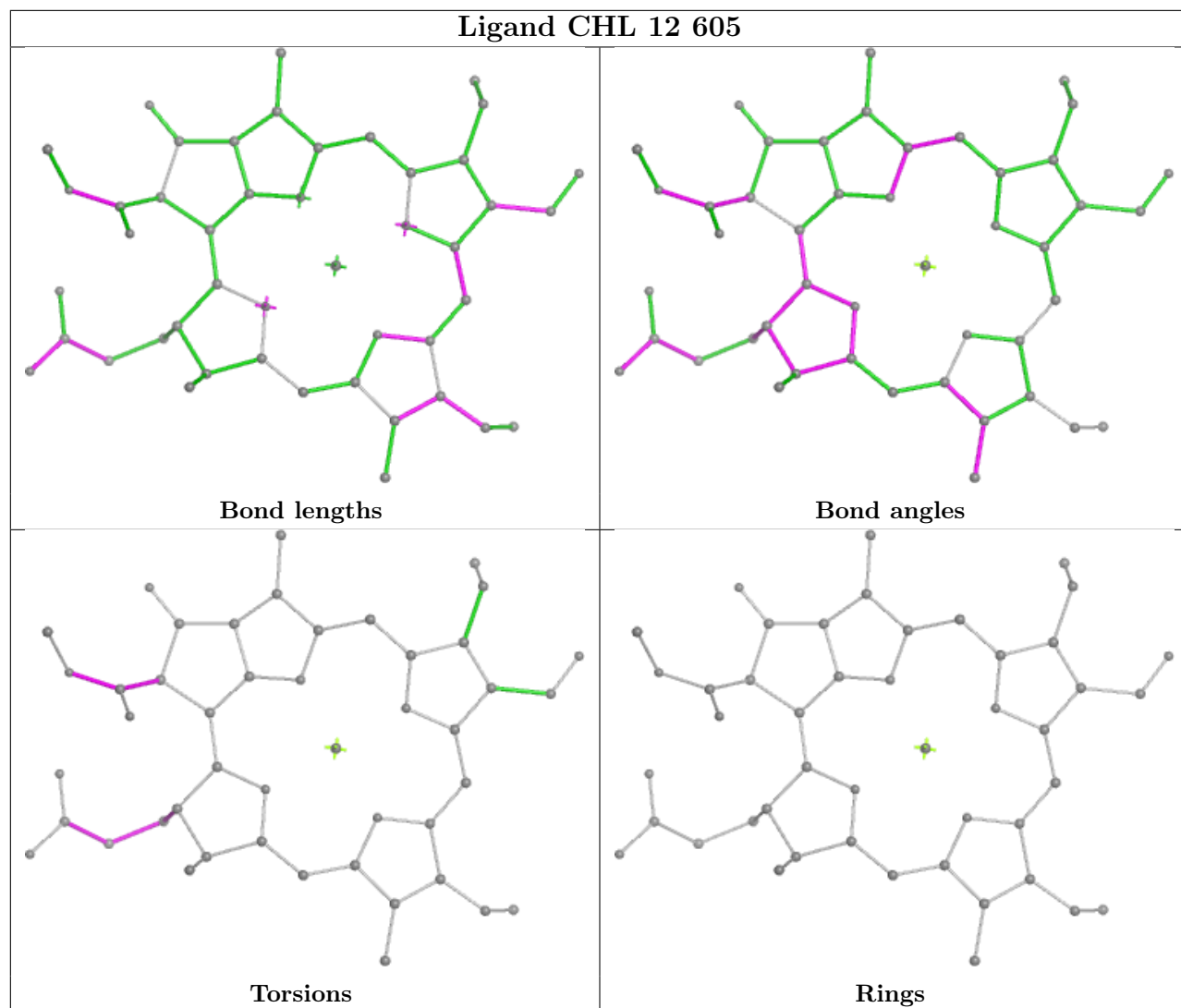
Ligand CLA n 602

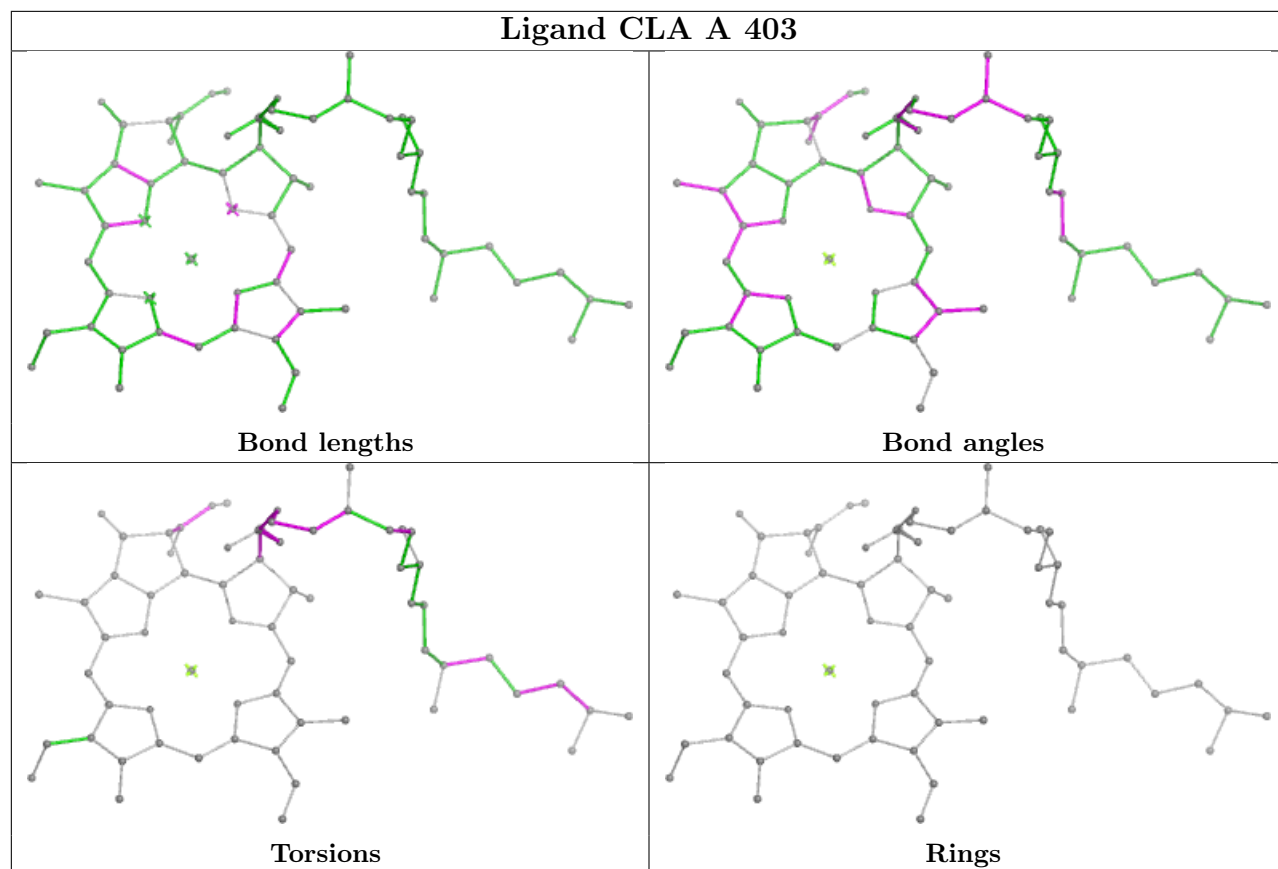


Ligand CLA 3 610**Ligand DGD C 517**

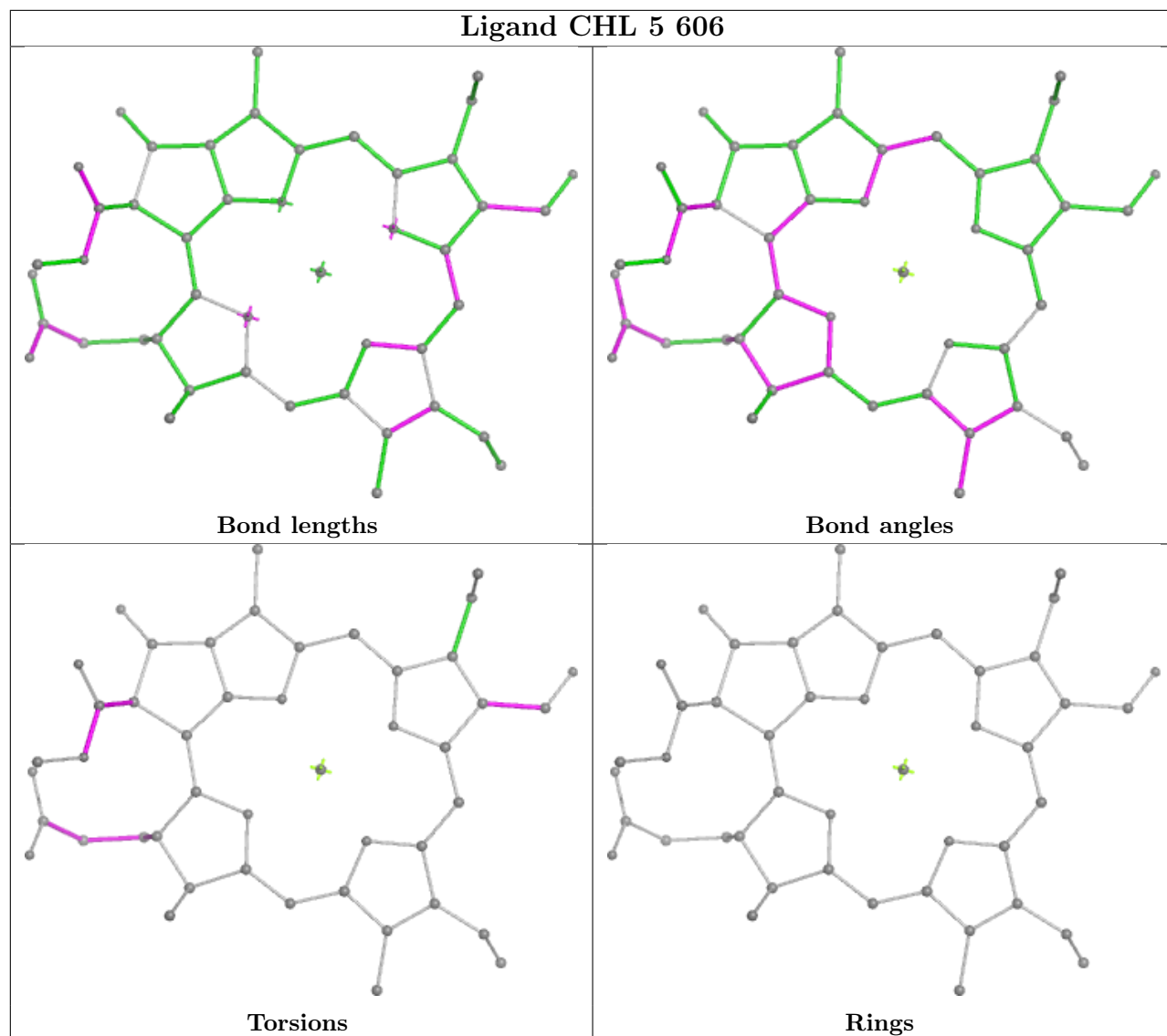


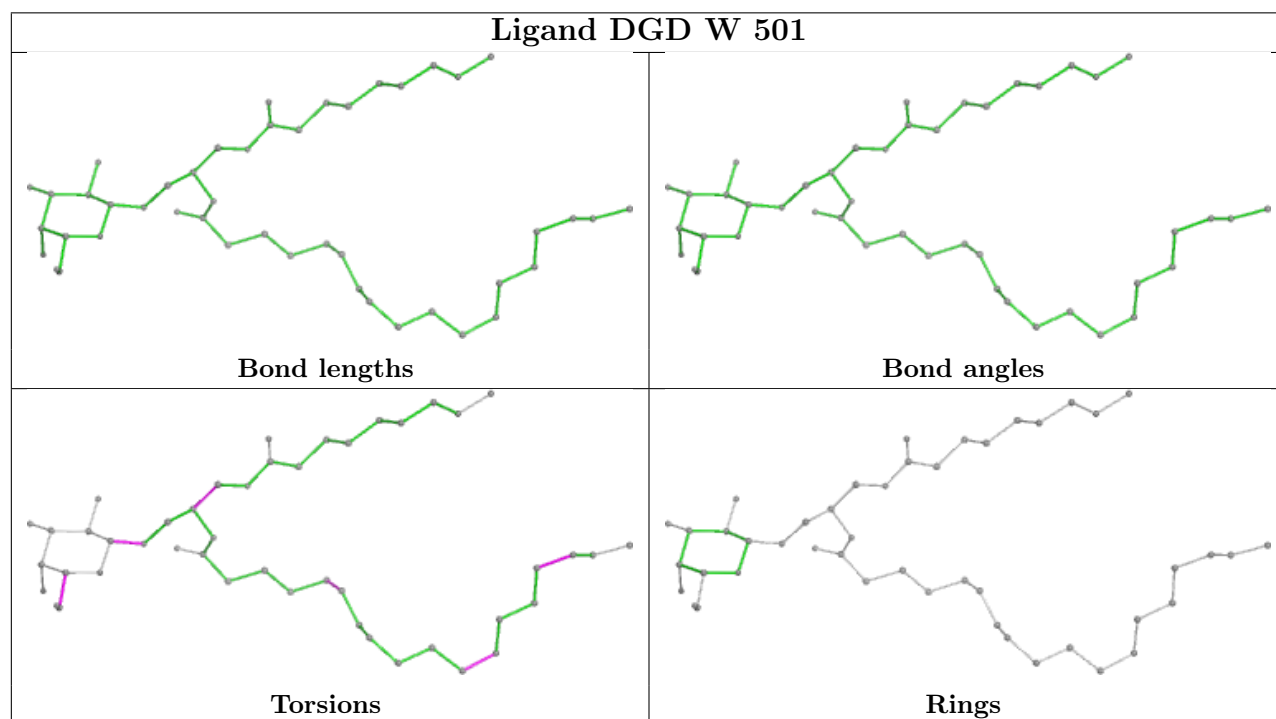
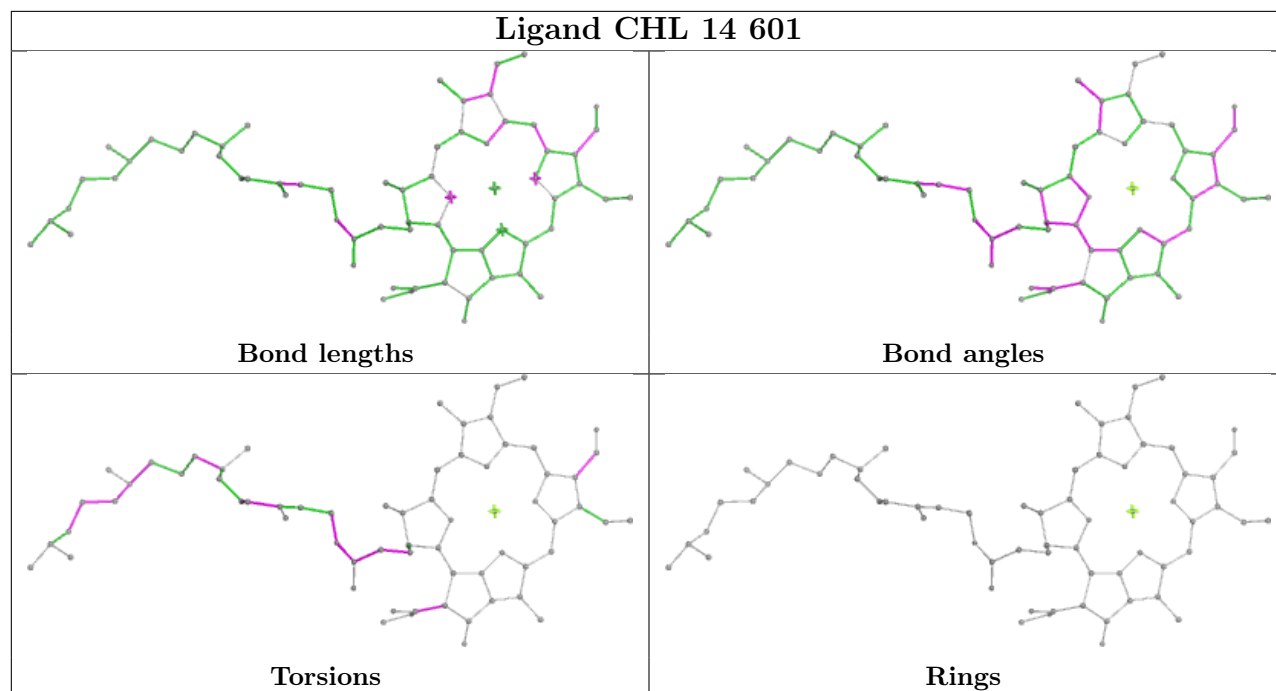
Ligand CLA b 603**Ligand CLA c 502**

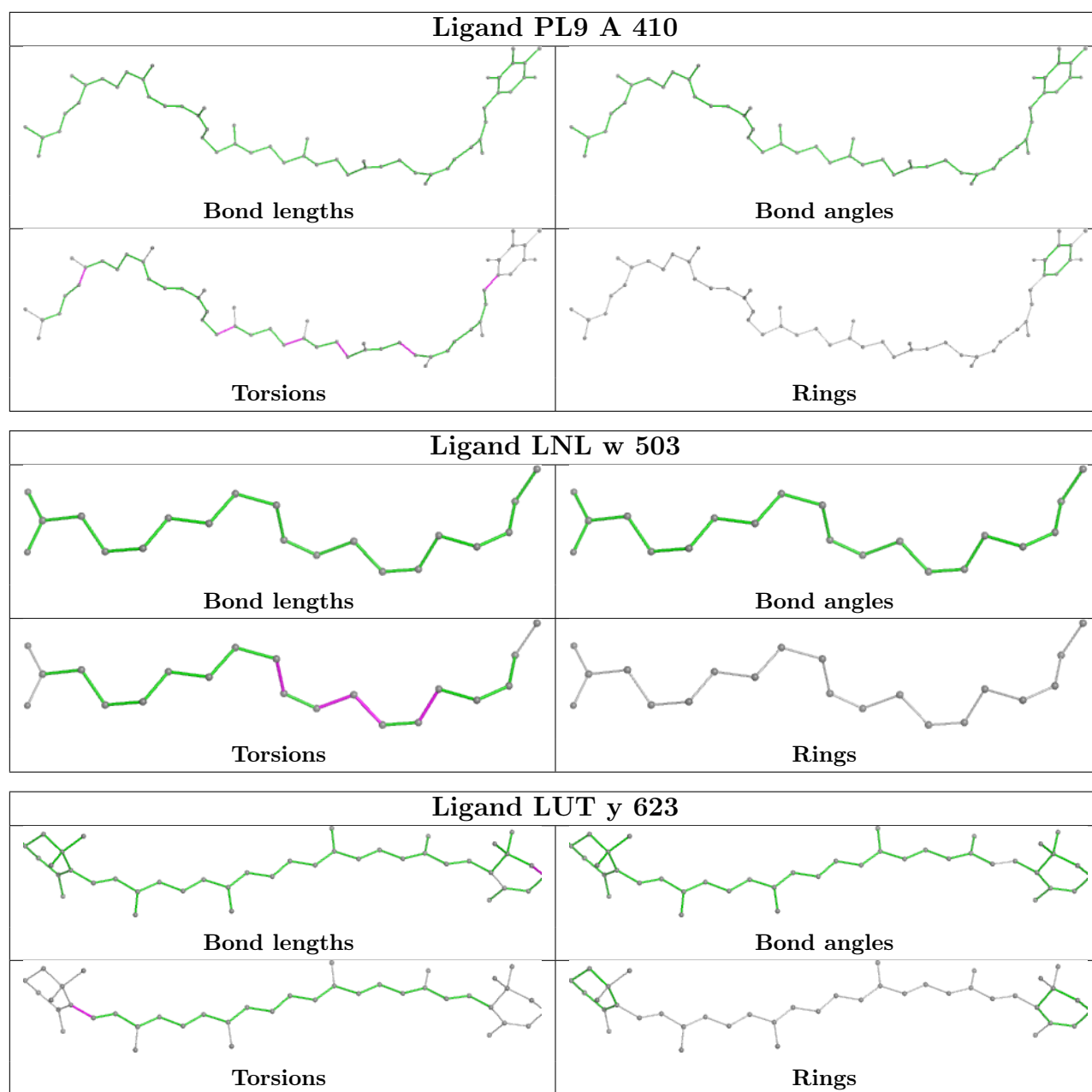


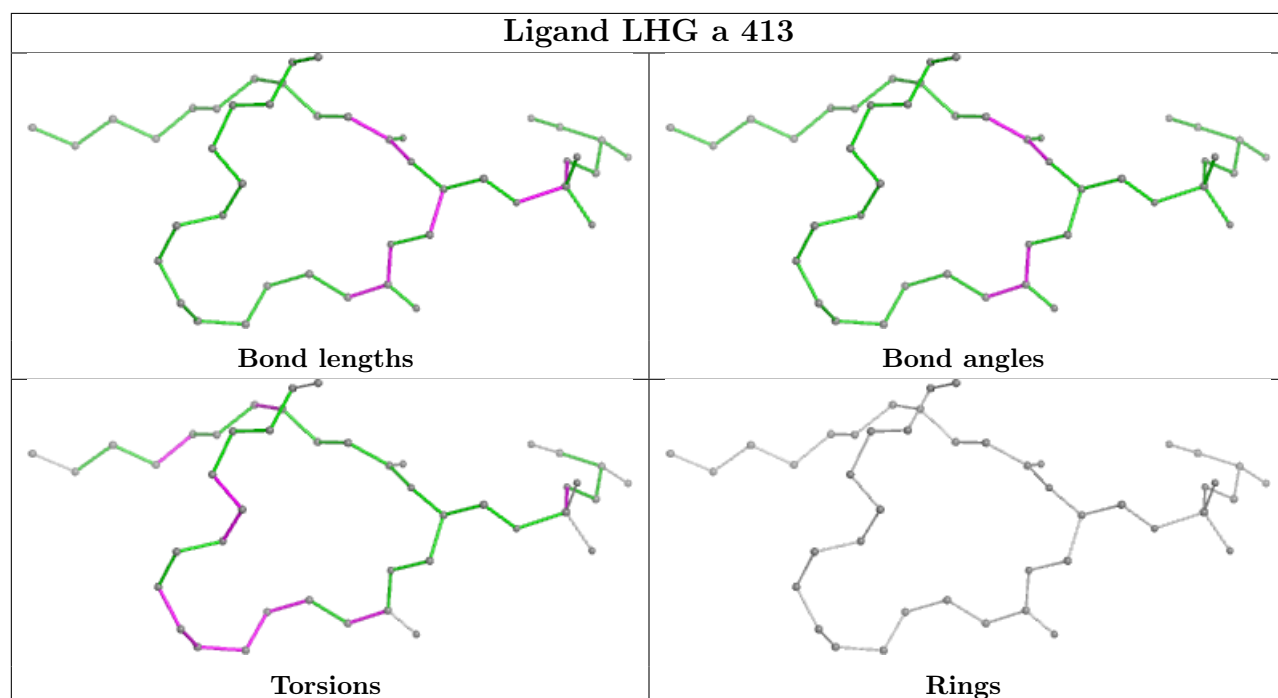
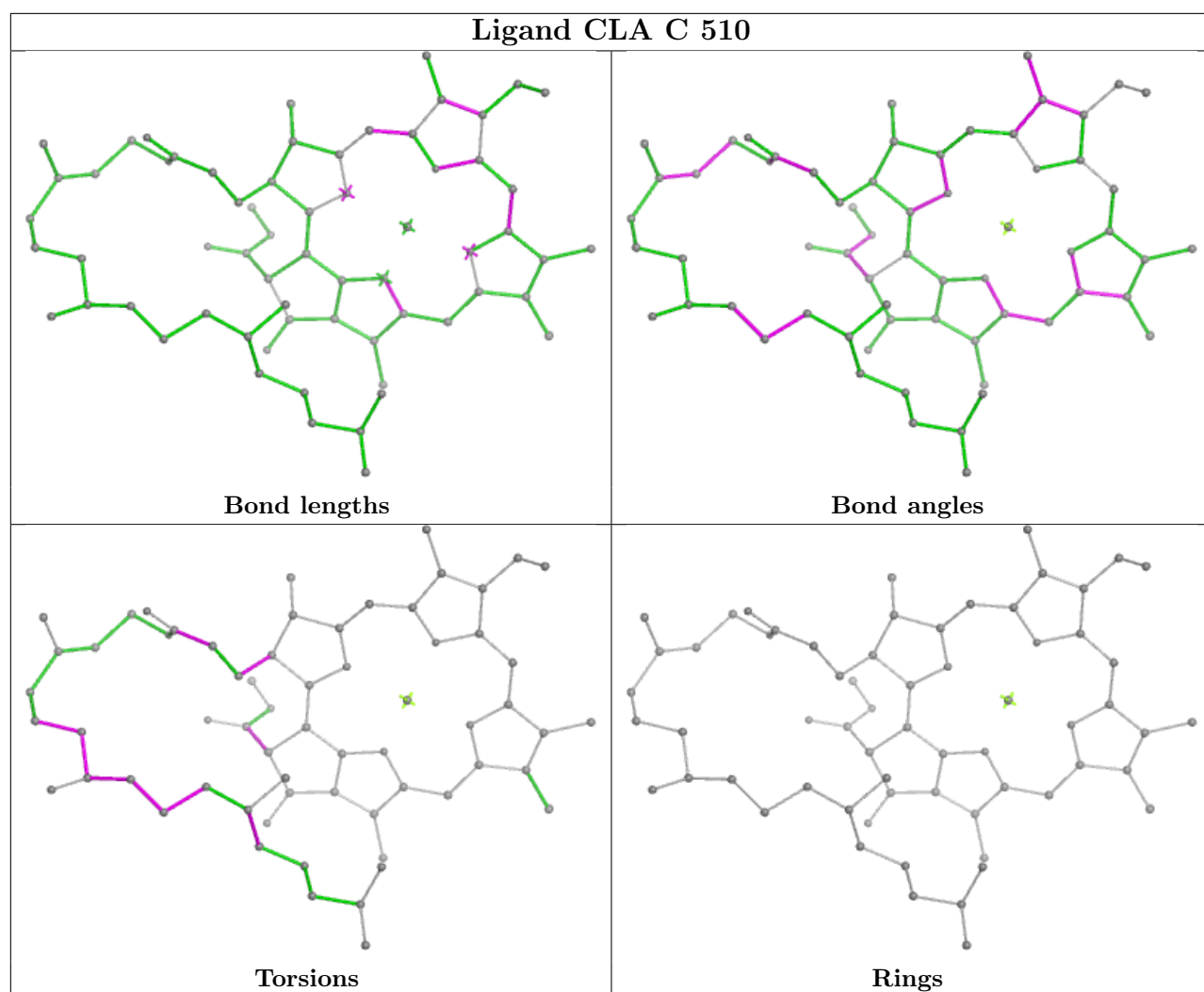


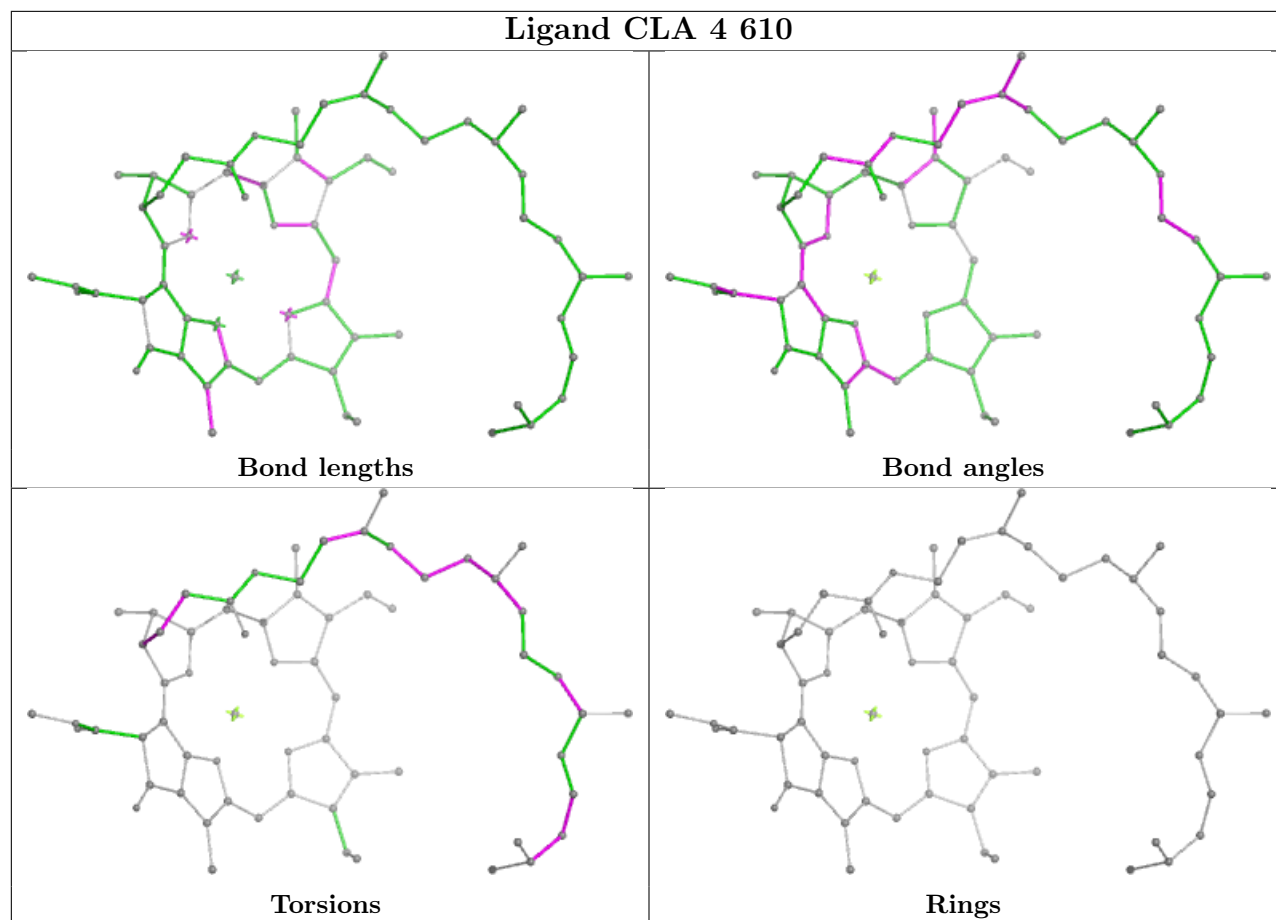
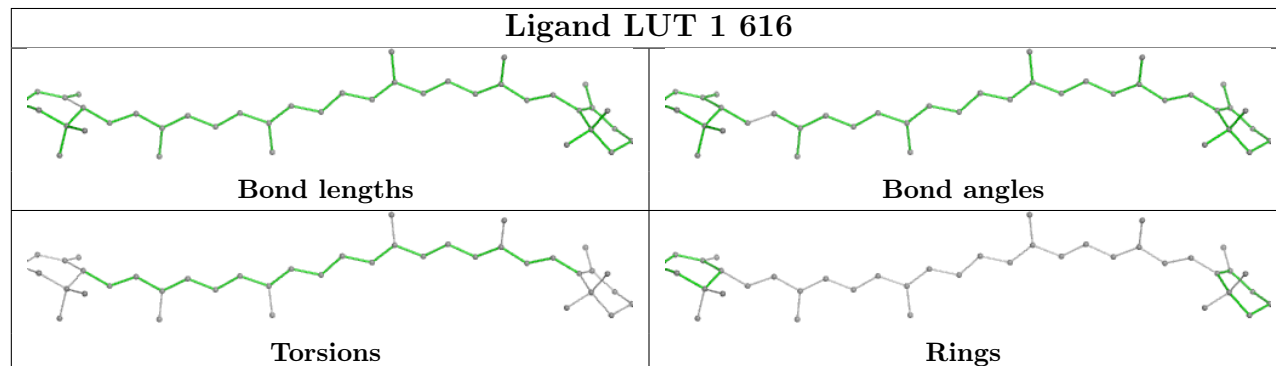
Ligand CHL 5 606

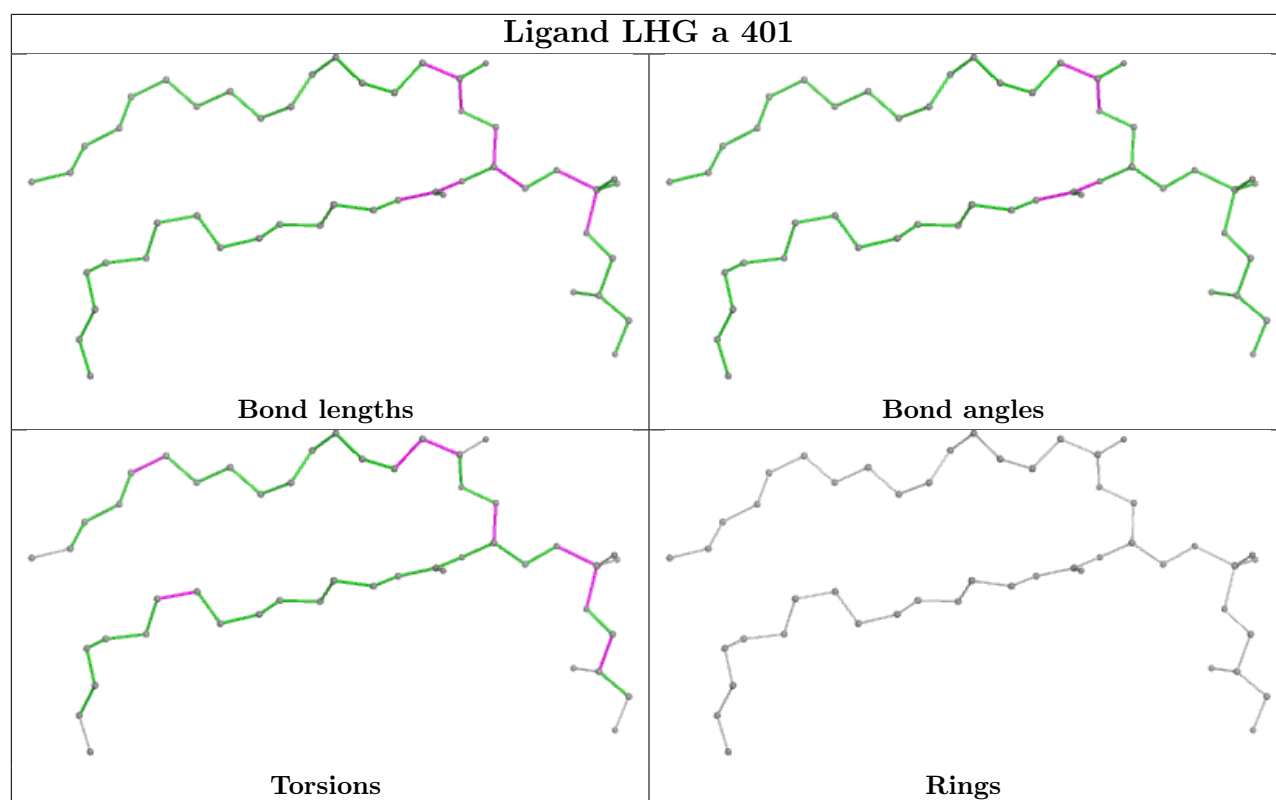




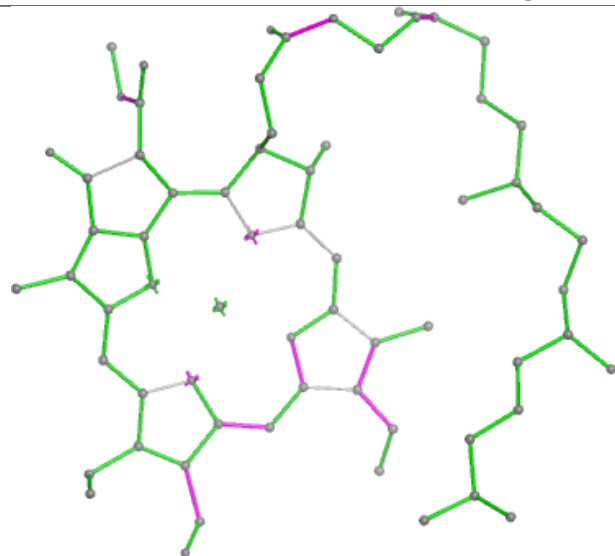




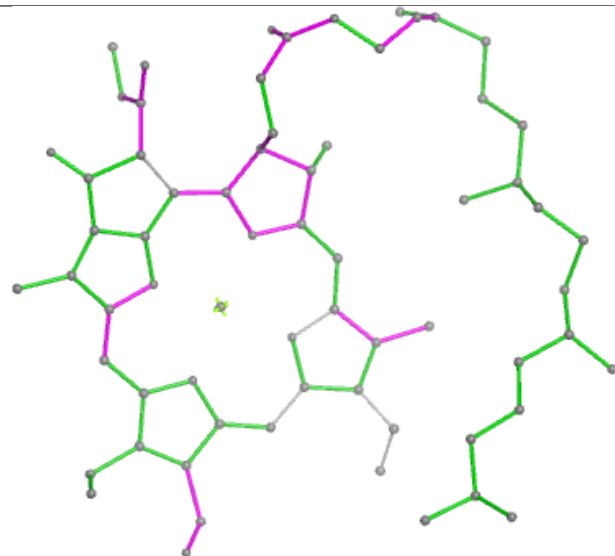
Ligand CLA 4 610**Ligand LUT 1 616**



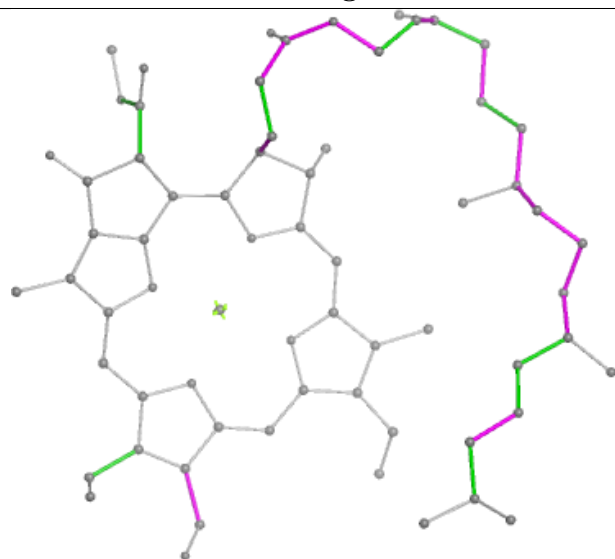
Ligand CHL 3 607



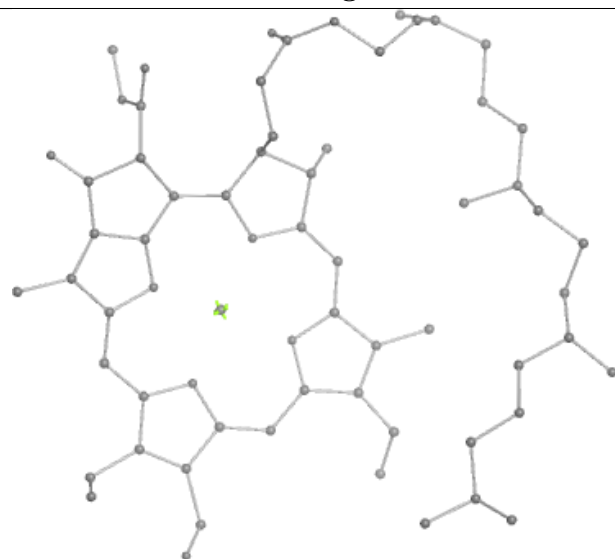
Bond lengths



Bond angles

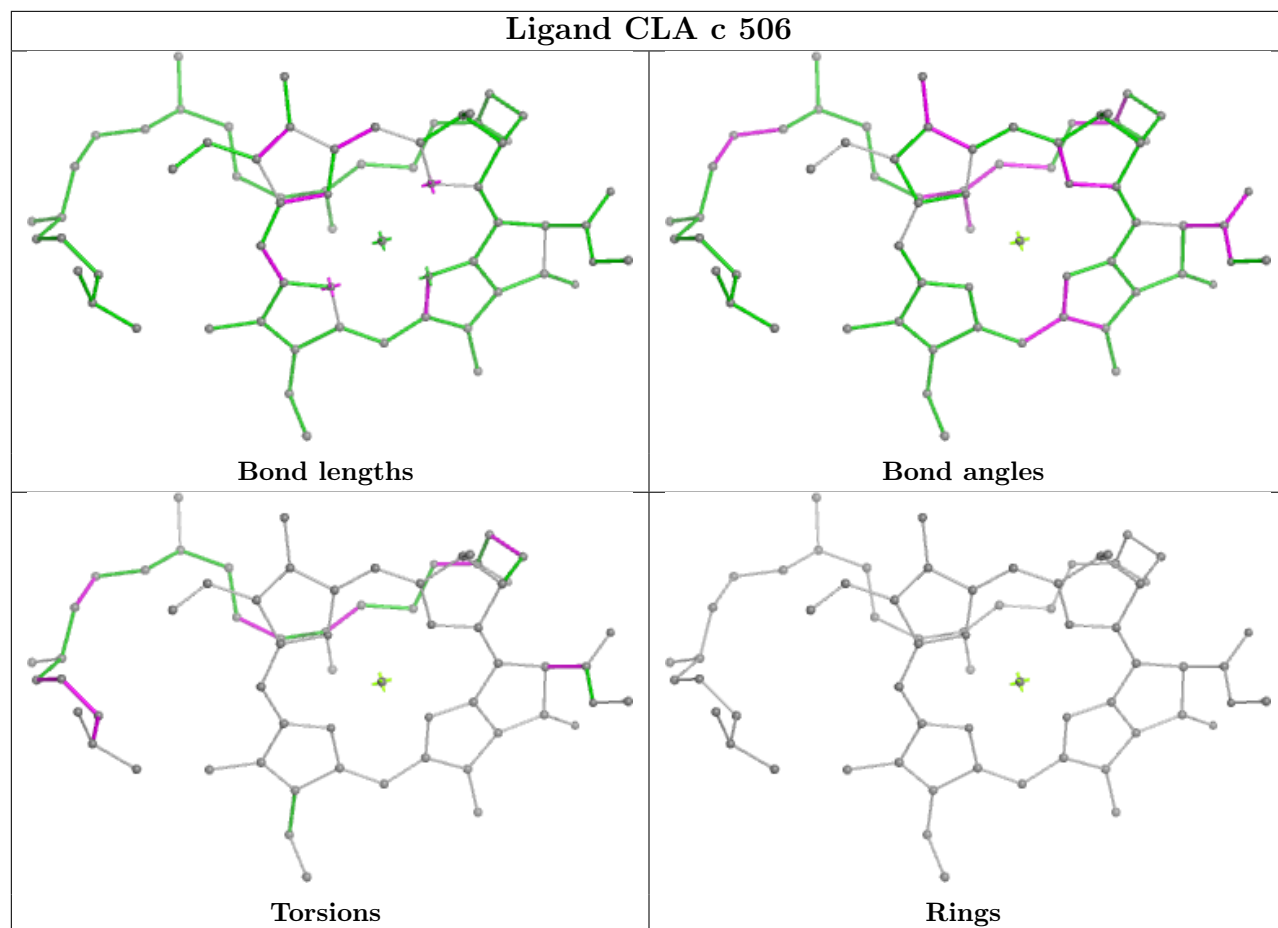


Torsions

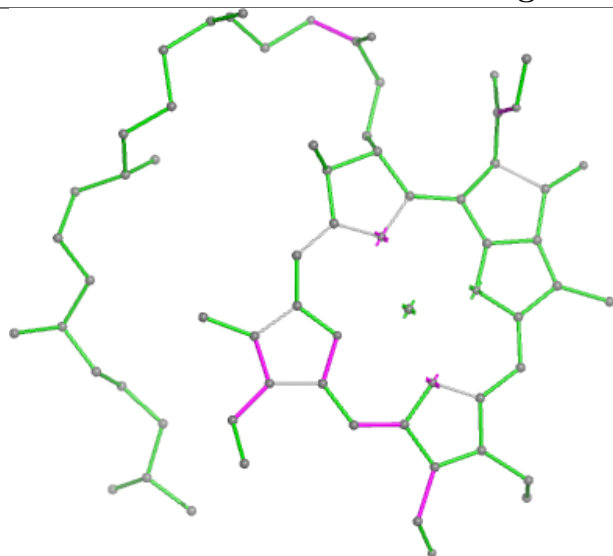


Rings

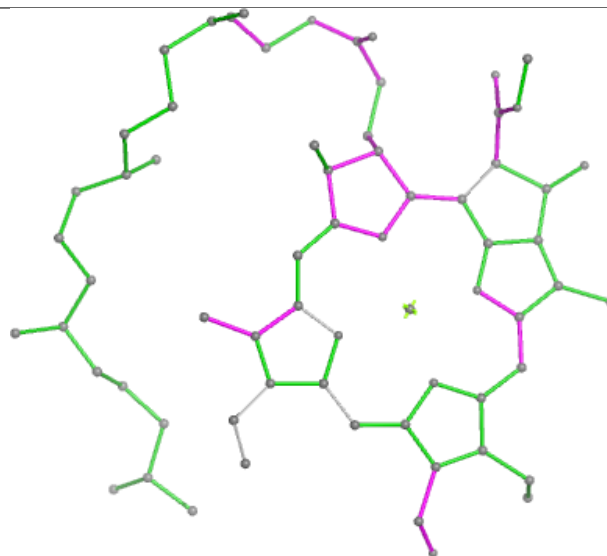
Ligand CLA c 506



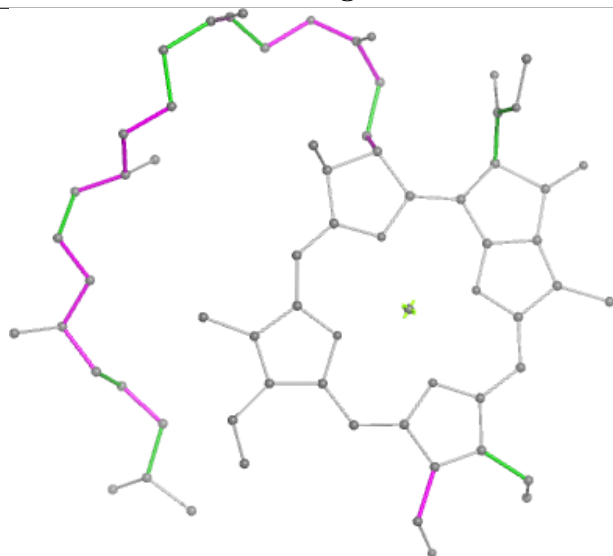
Ligand CHL 6 607



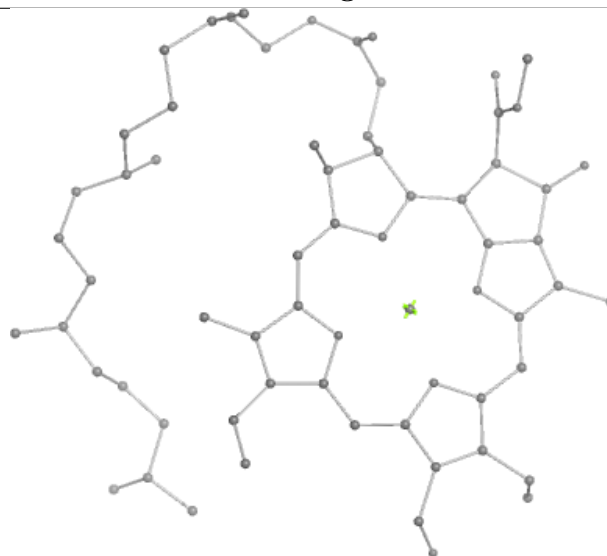
Bond lengths



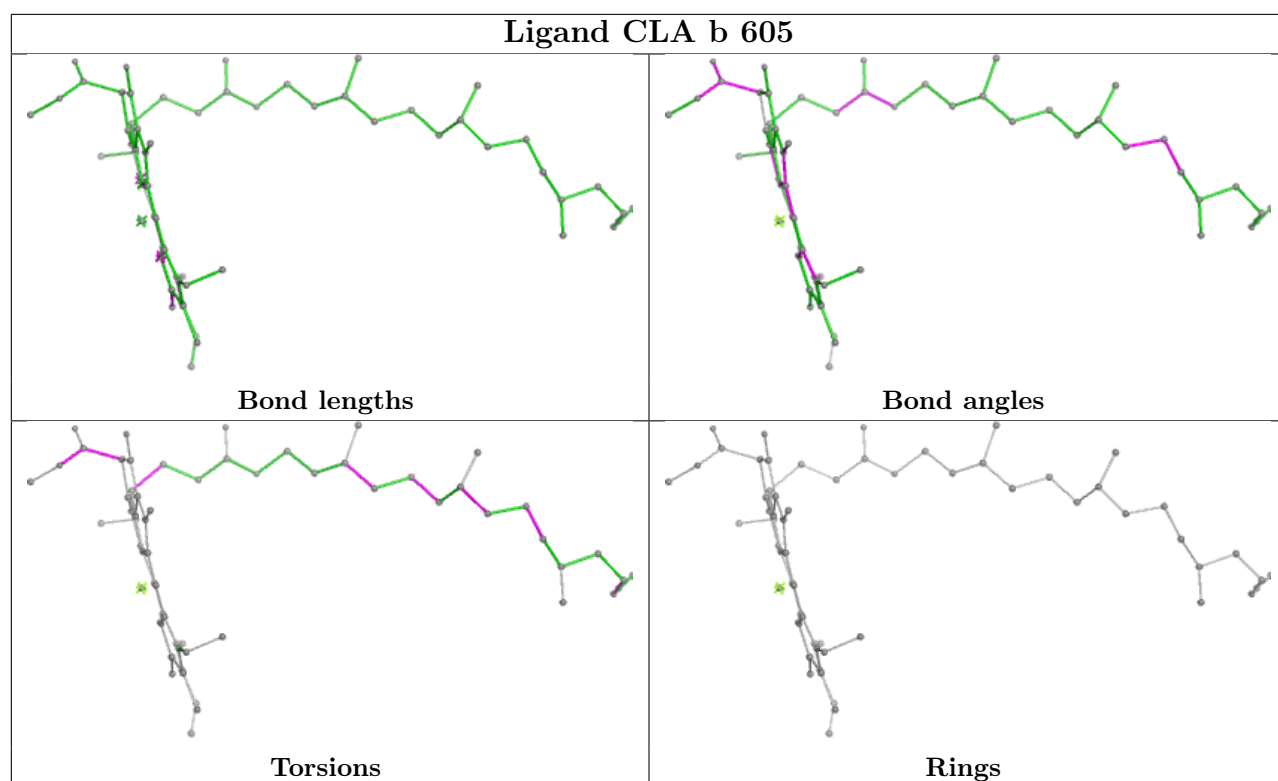
Bond angles



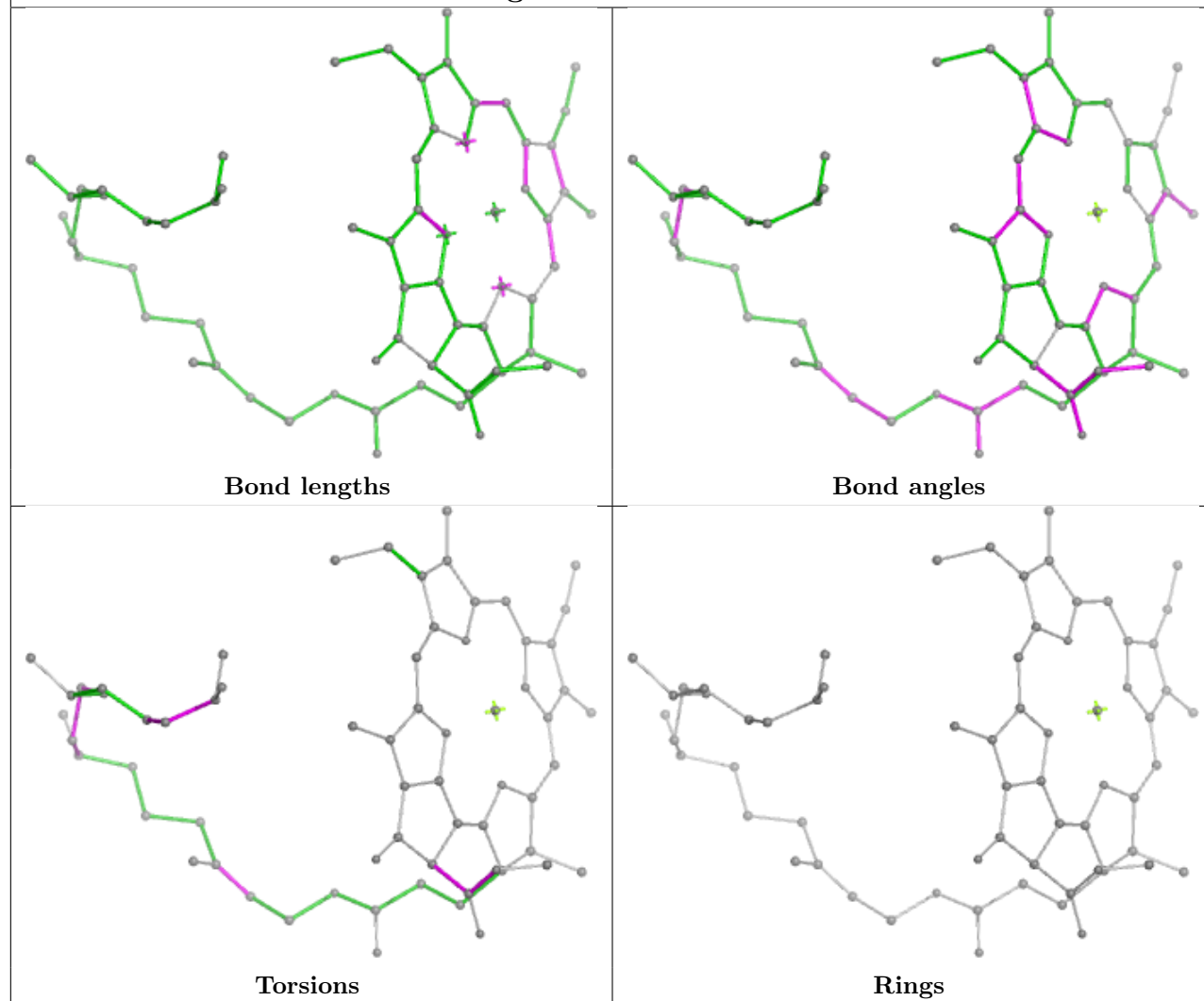
Torsions



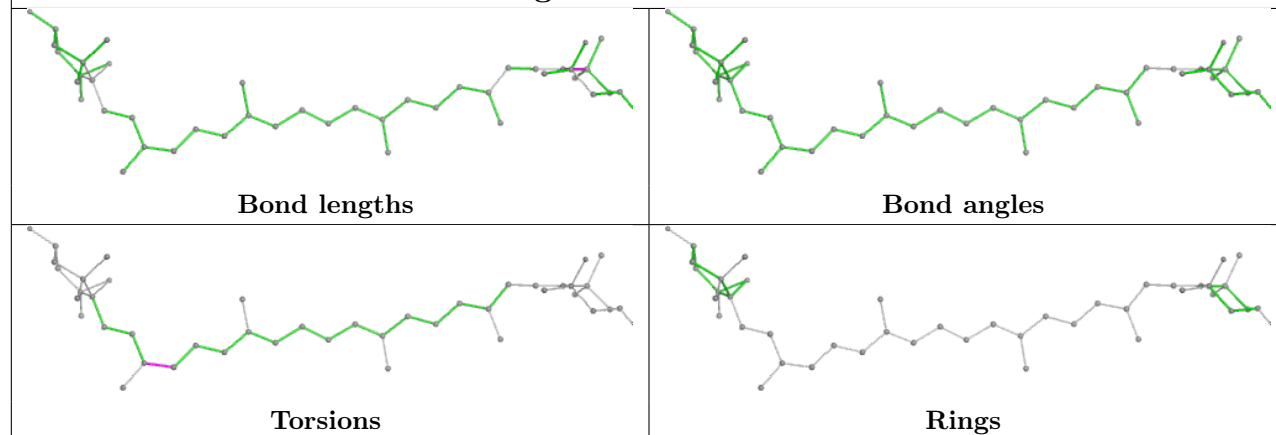
Rings



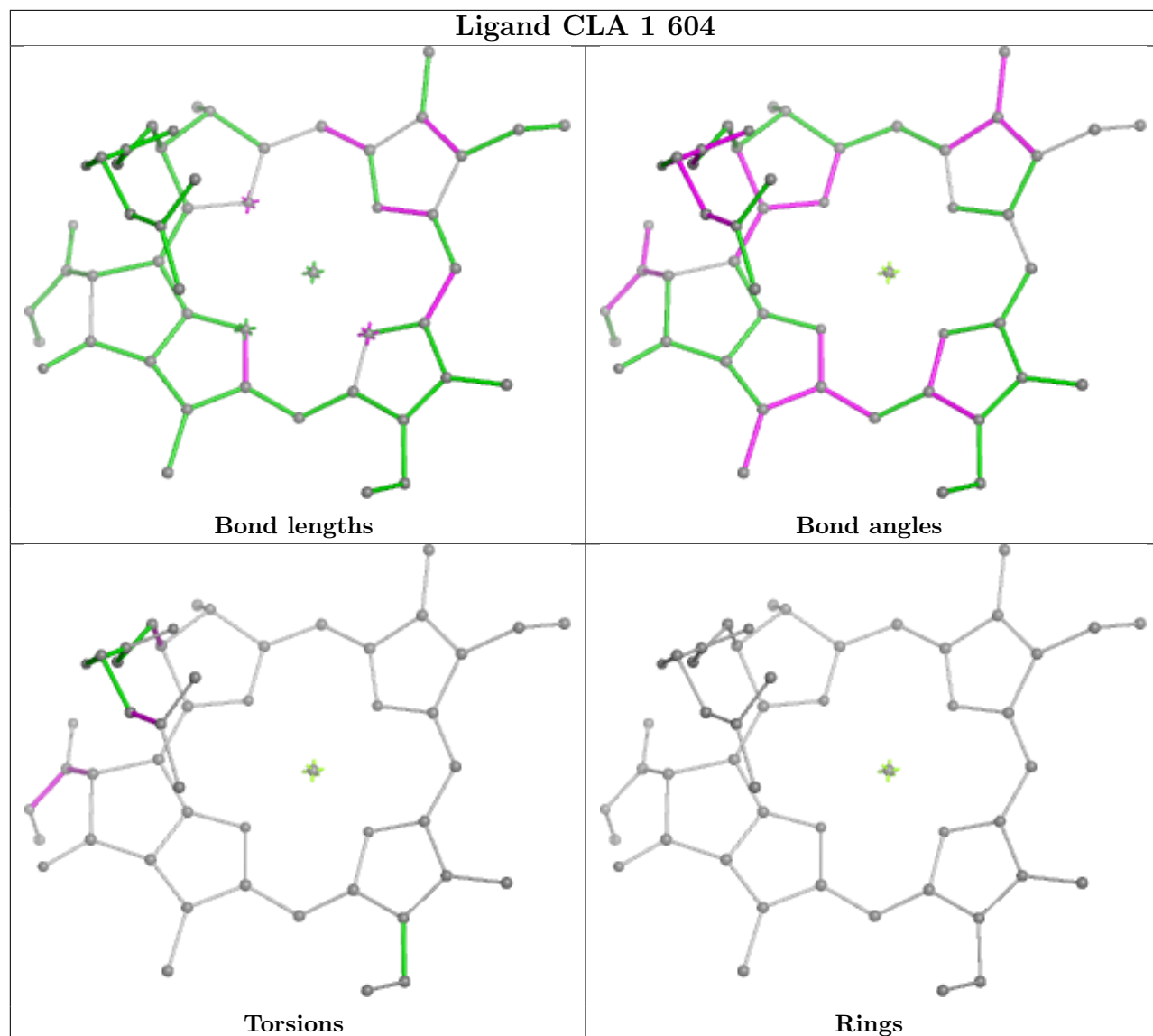
Ligand CLA c 504

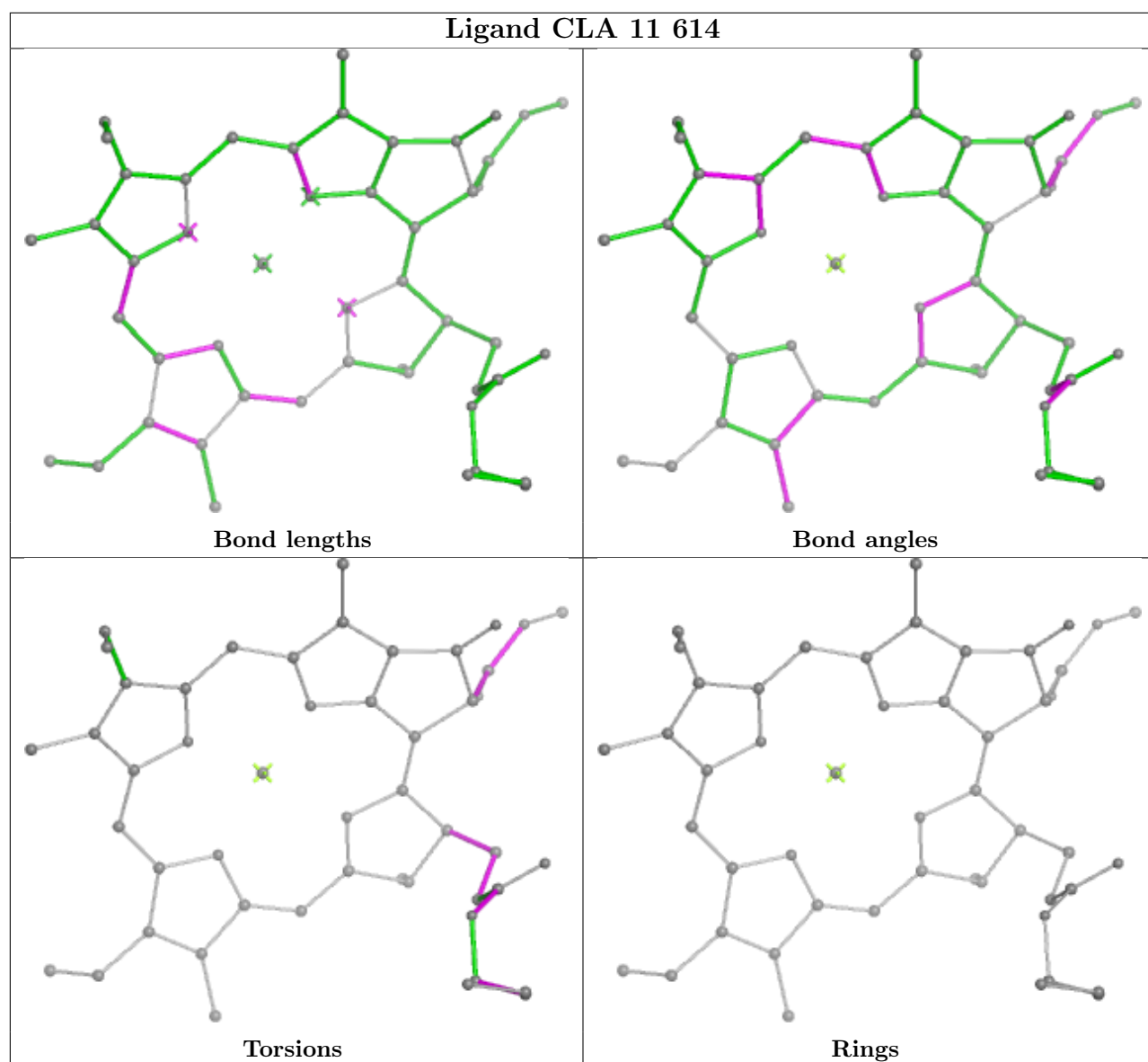


Ligand NEX 6 621

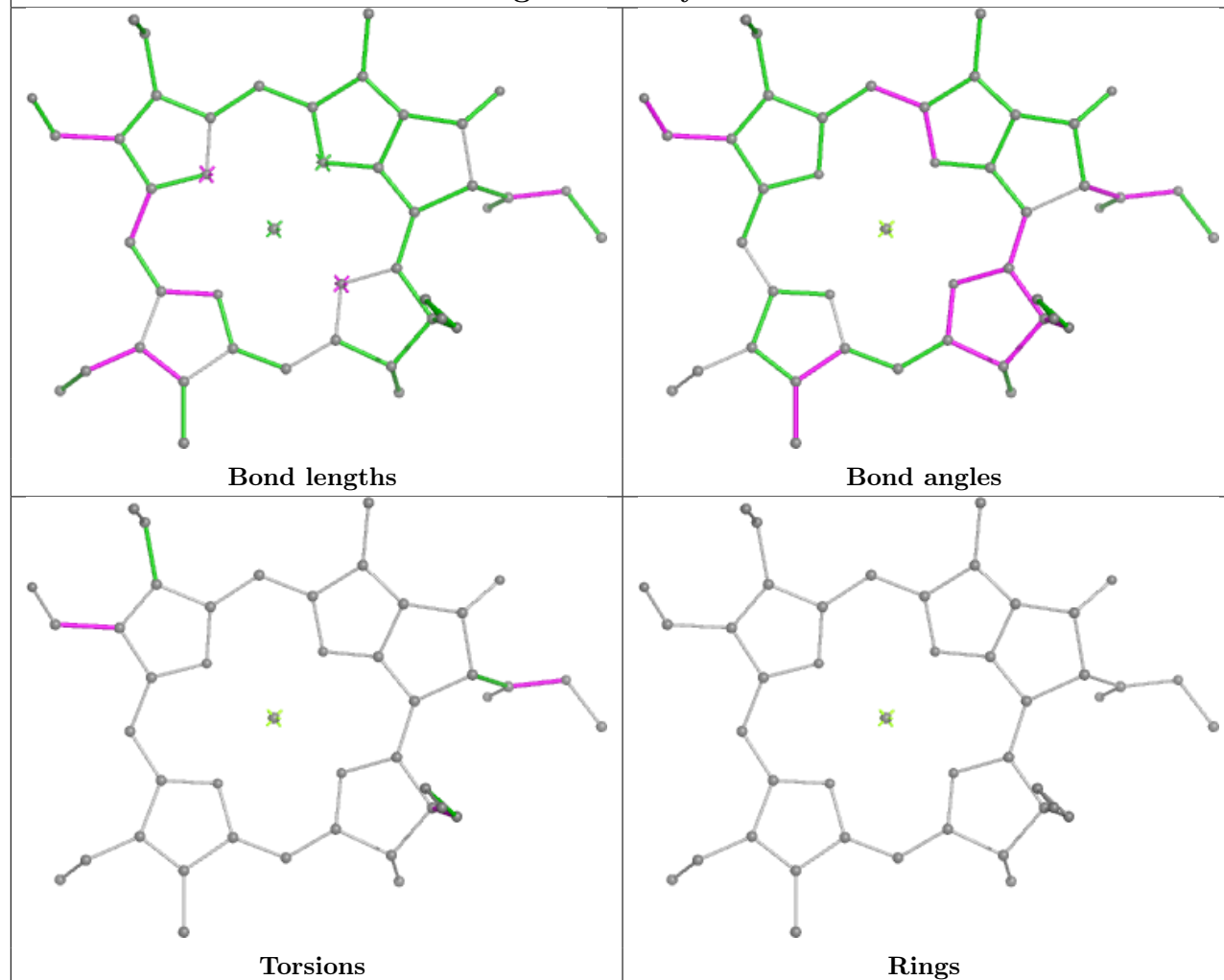


Ligand CLA 1 604

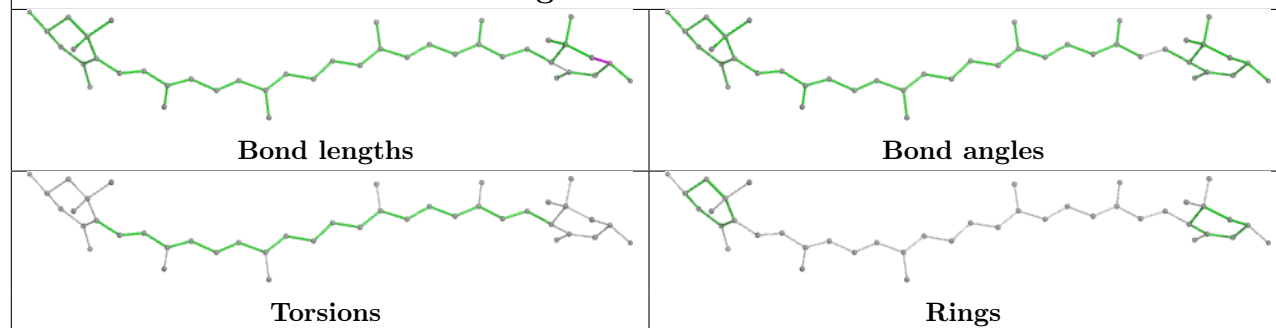


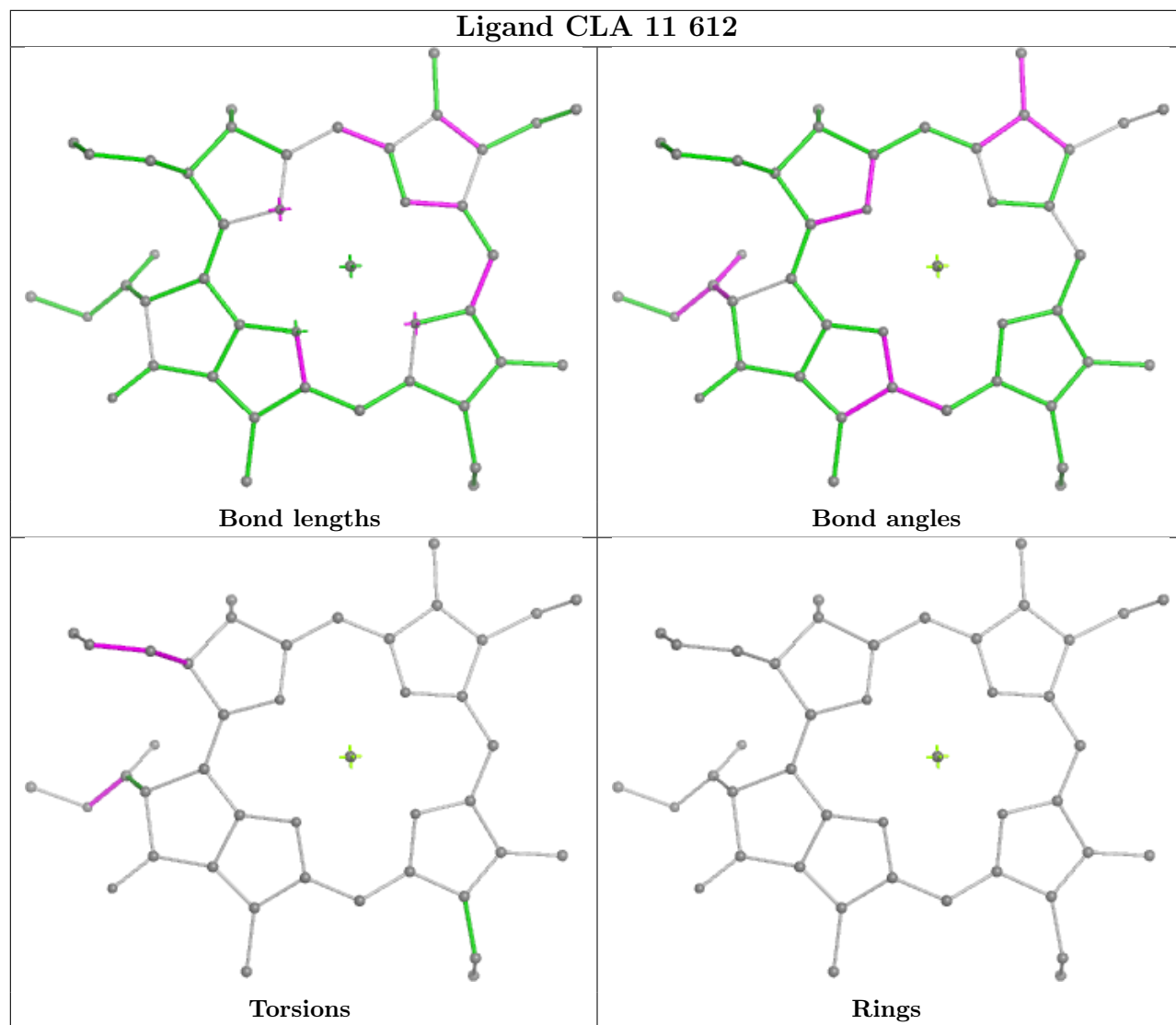


Ligand CHL y 608

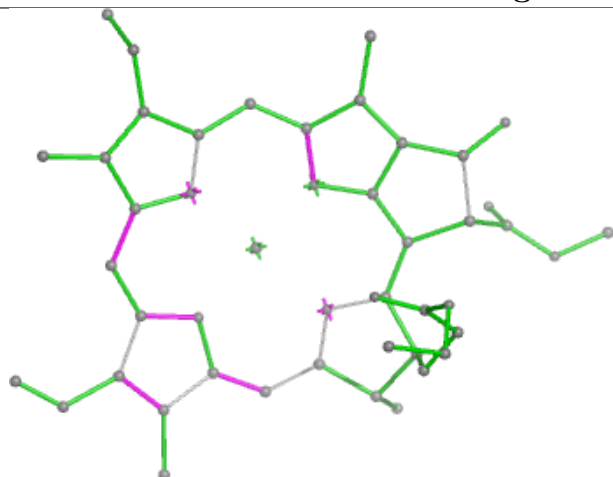


Ligand LUT 6 618

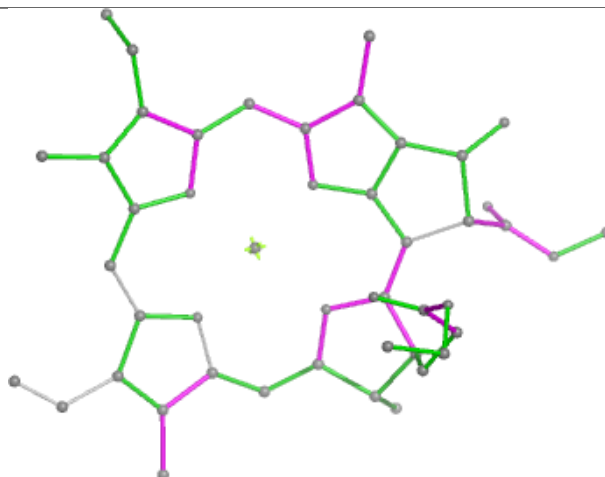




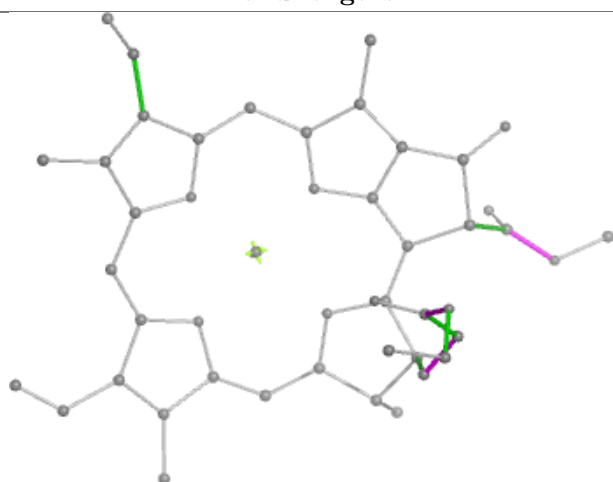
Ligand CLA N 615



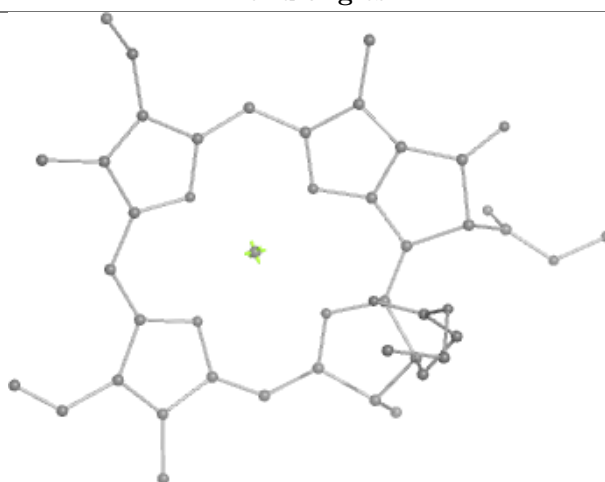
Bond lengths



Bond angles

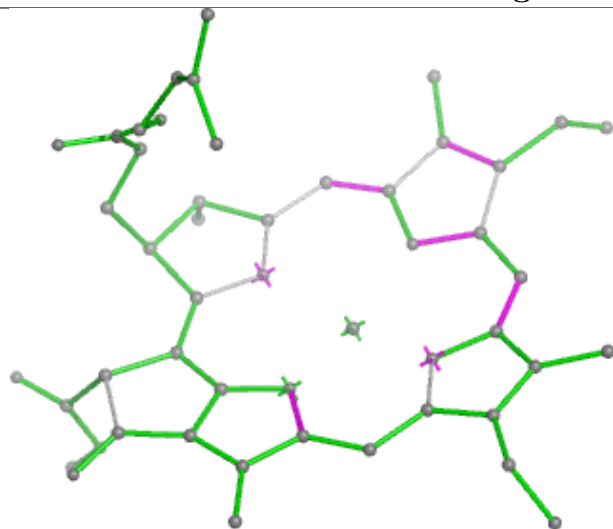


Torsions

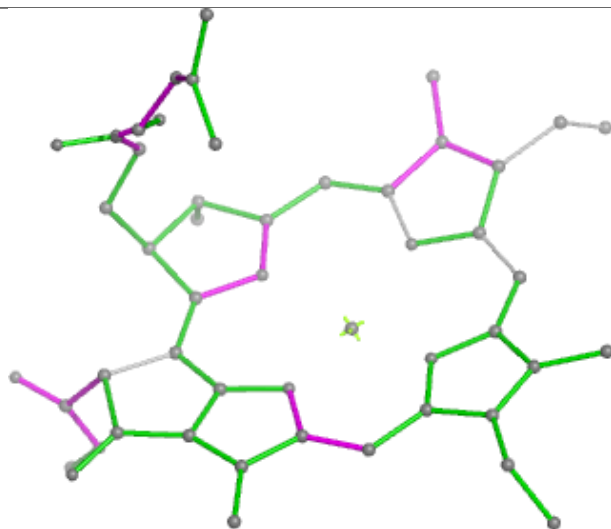


Rings

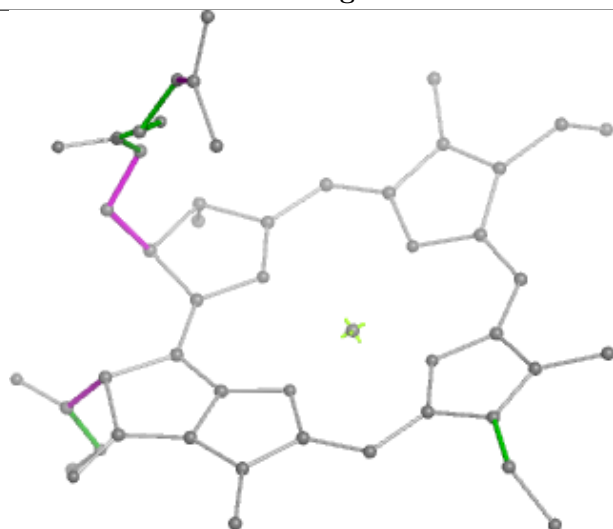
Ligand CLA G 604



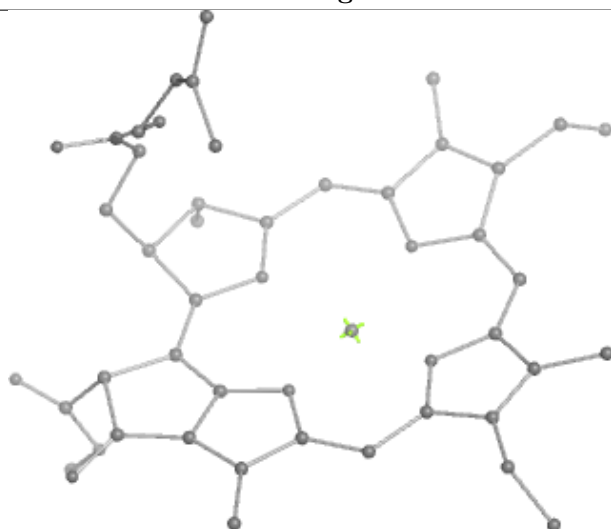
Bond lengths



Bond angles

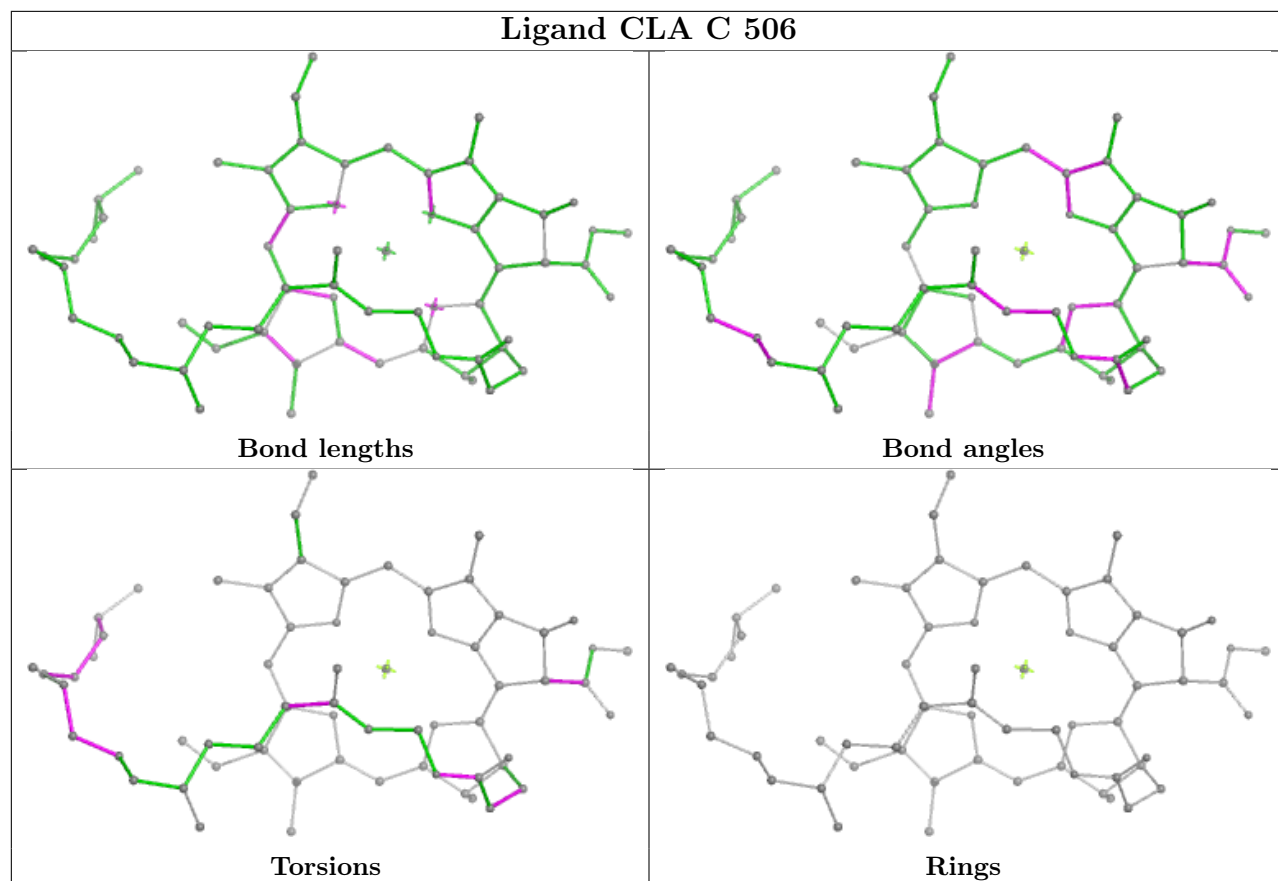


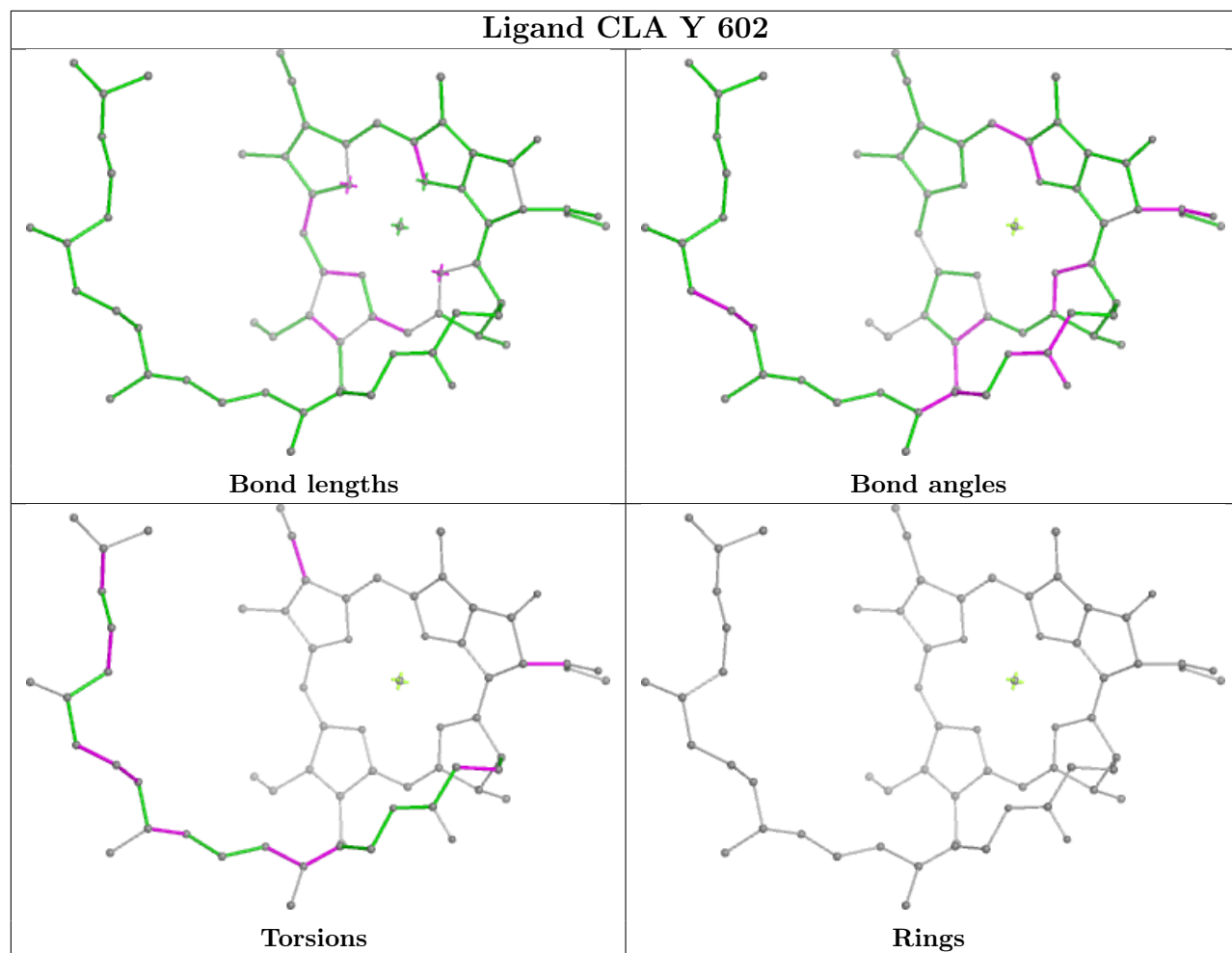
Torsions

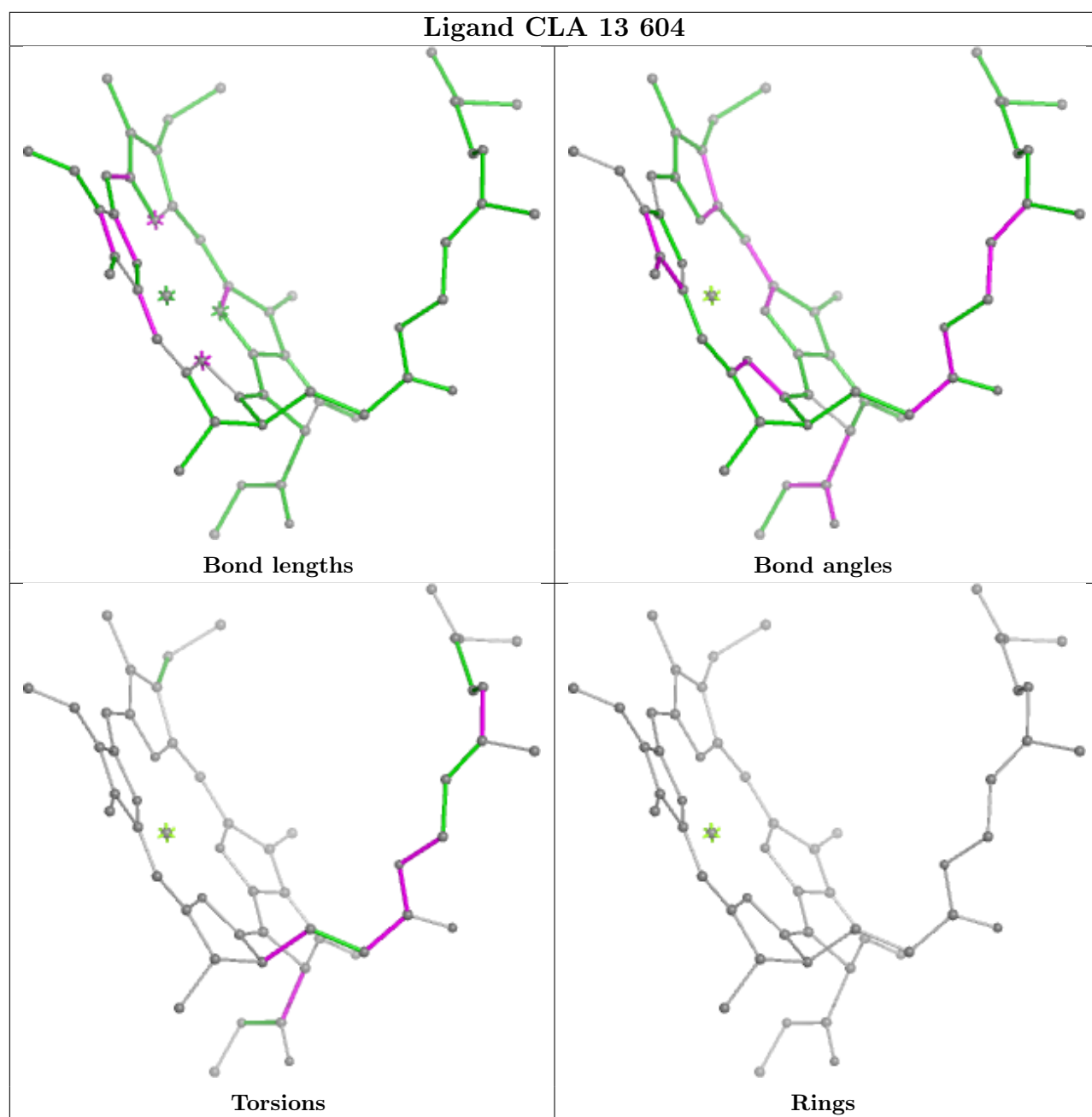


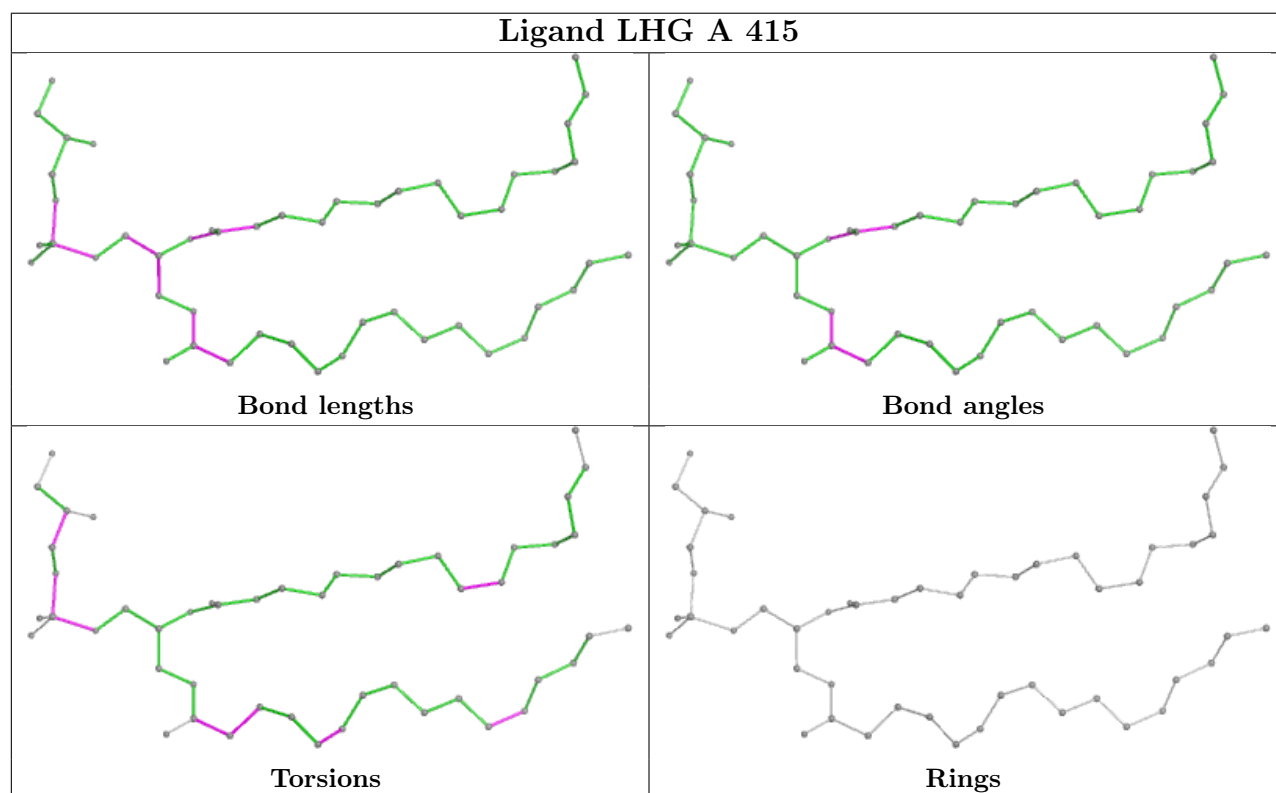
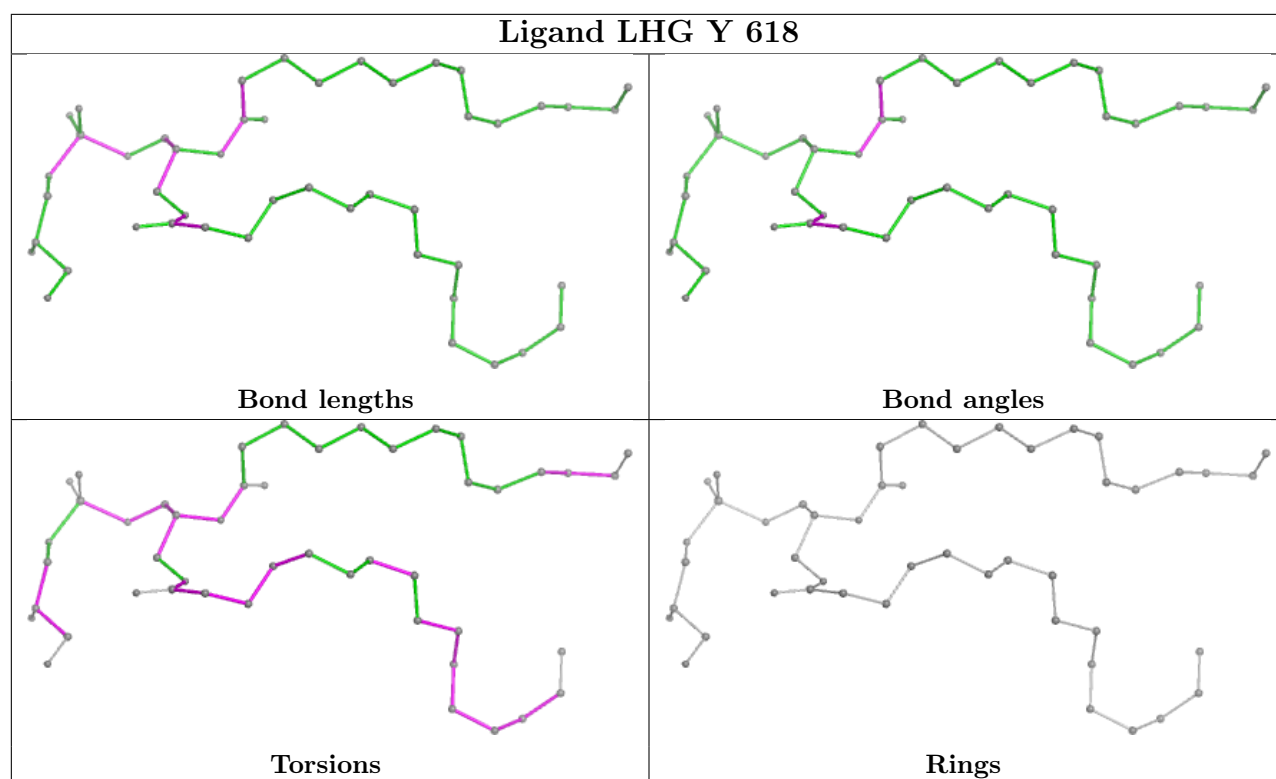
Rings

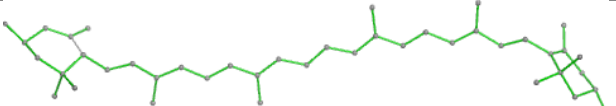

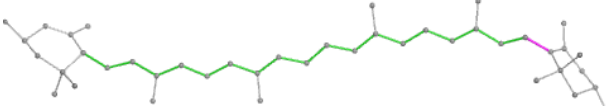
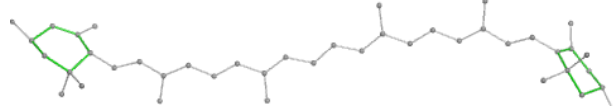
Ligand CLA C 506


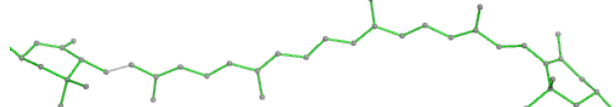






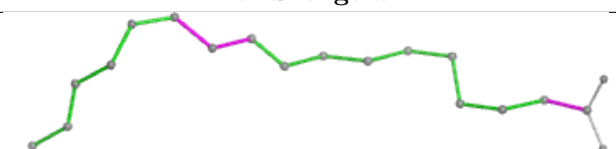



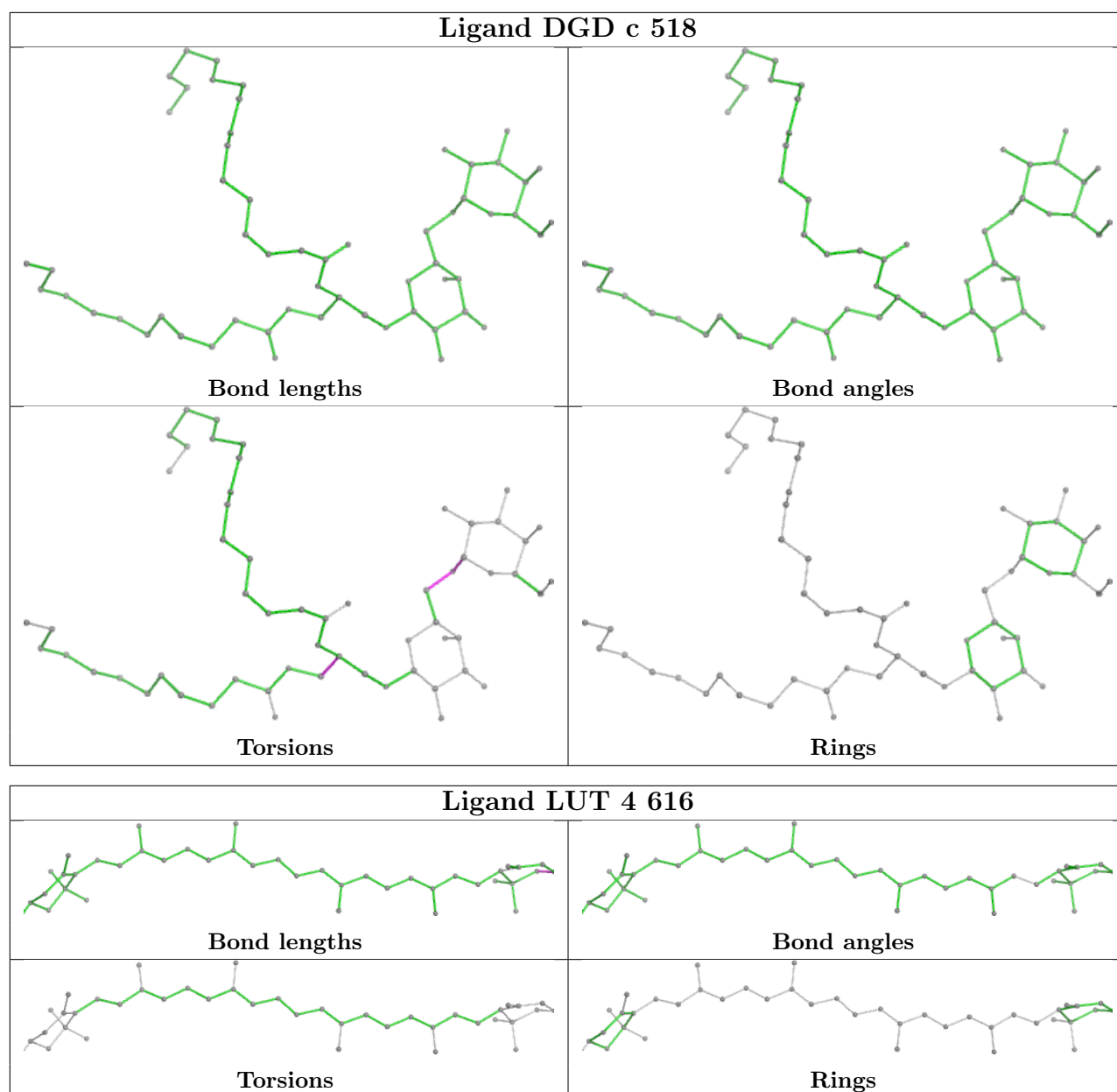




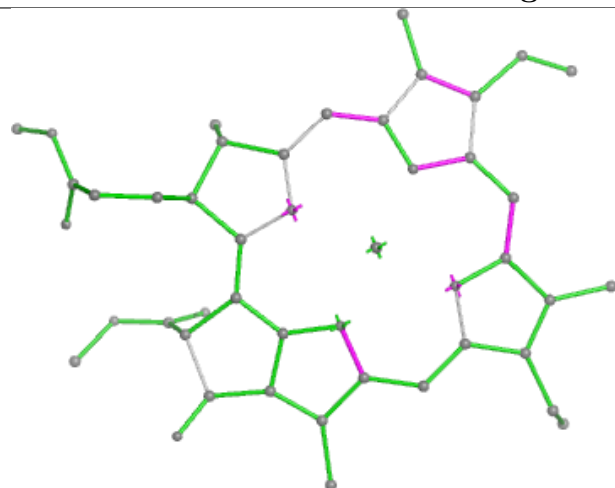
Ligand LUT 12 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT Y 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

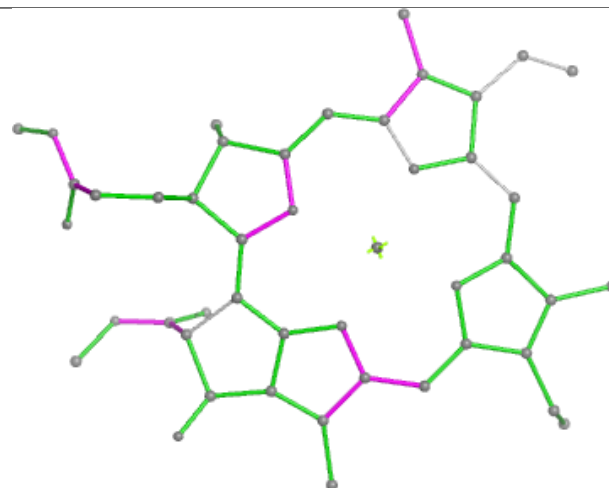
Ligand LNL I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



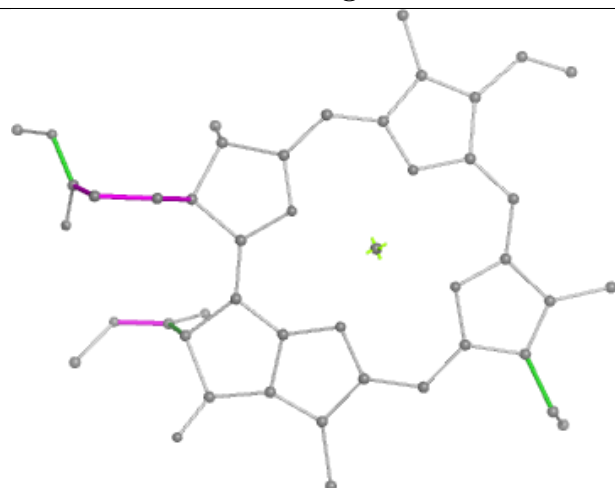
Ligand CLA 1 612



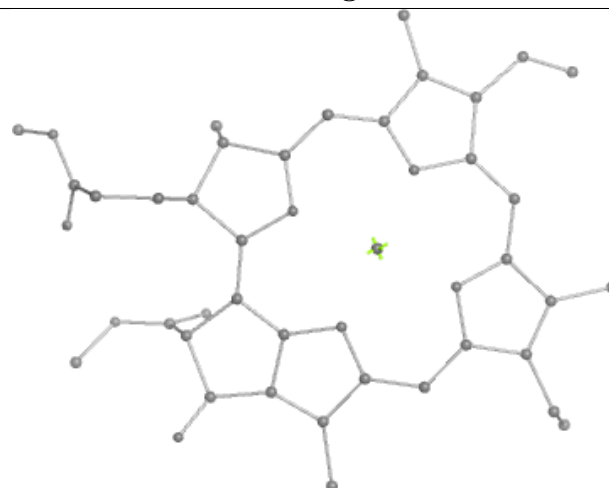
Bond lengths



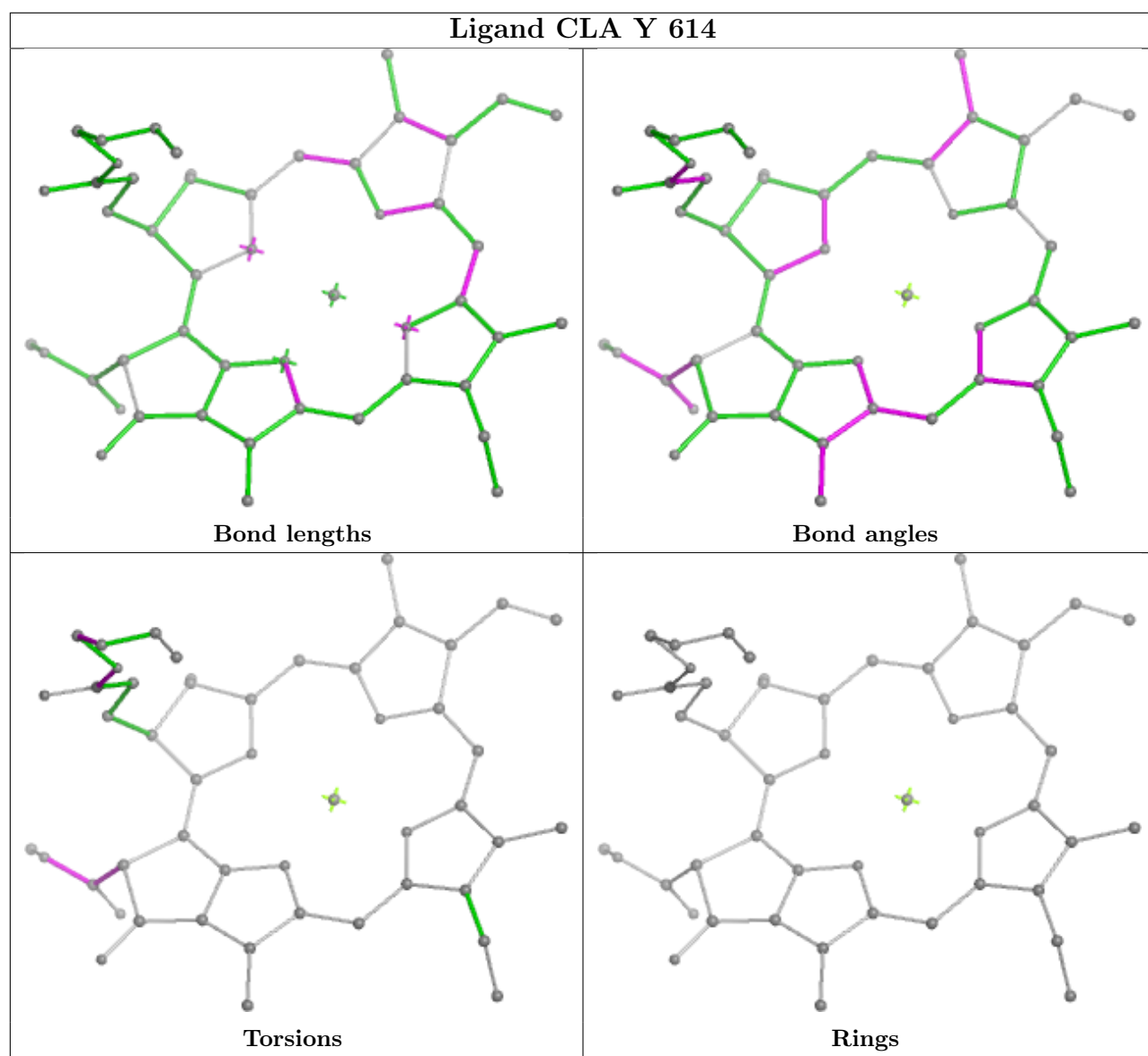
Bond angles



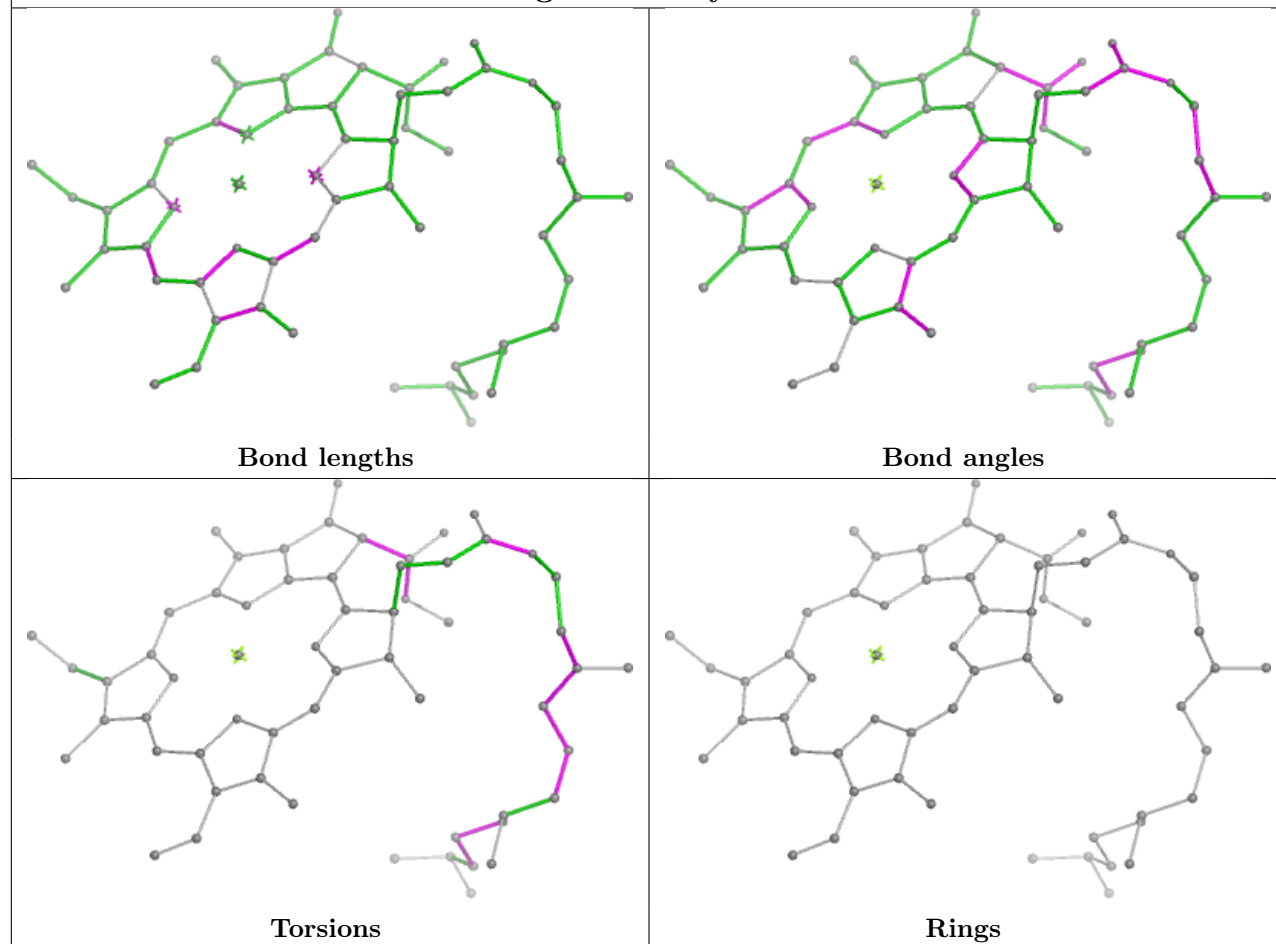
Torsions



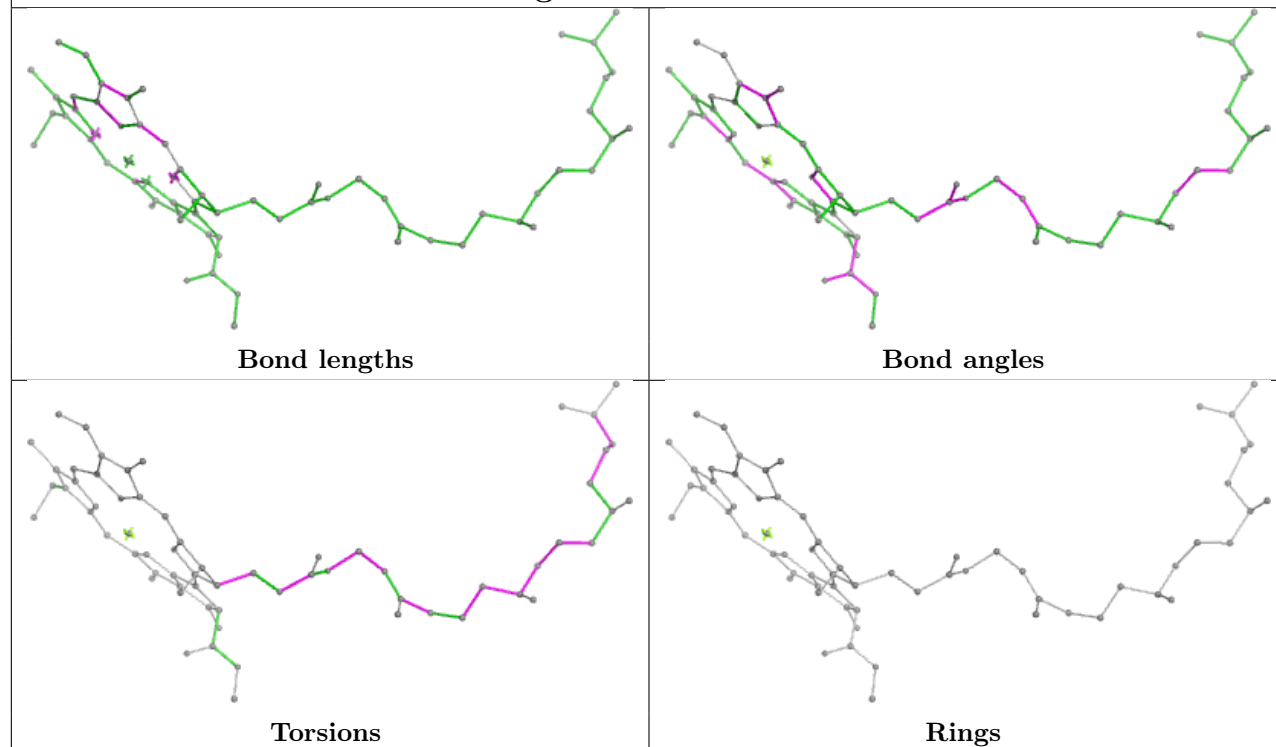
Rings

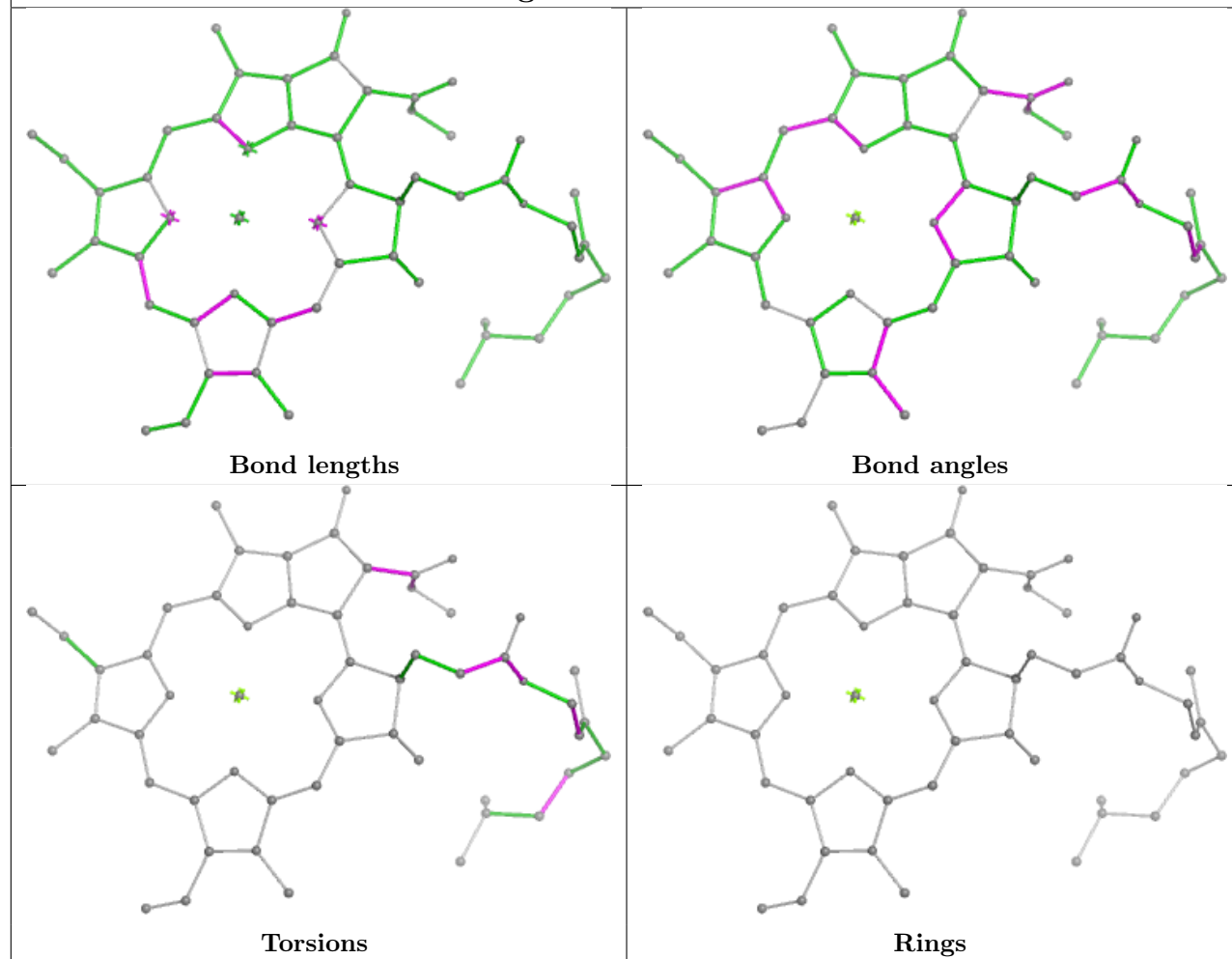
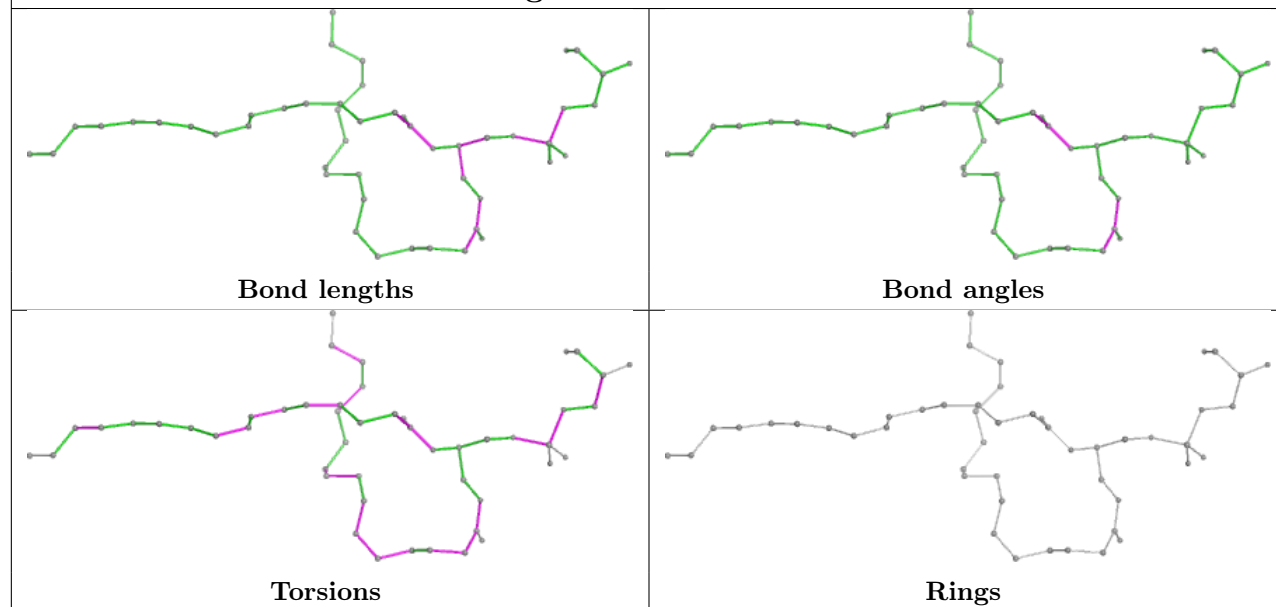


Ligand CLA y 603

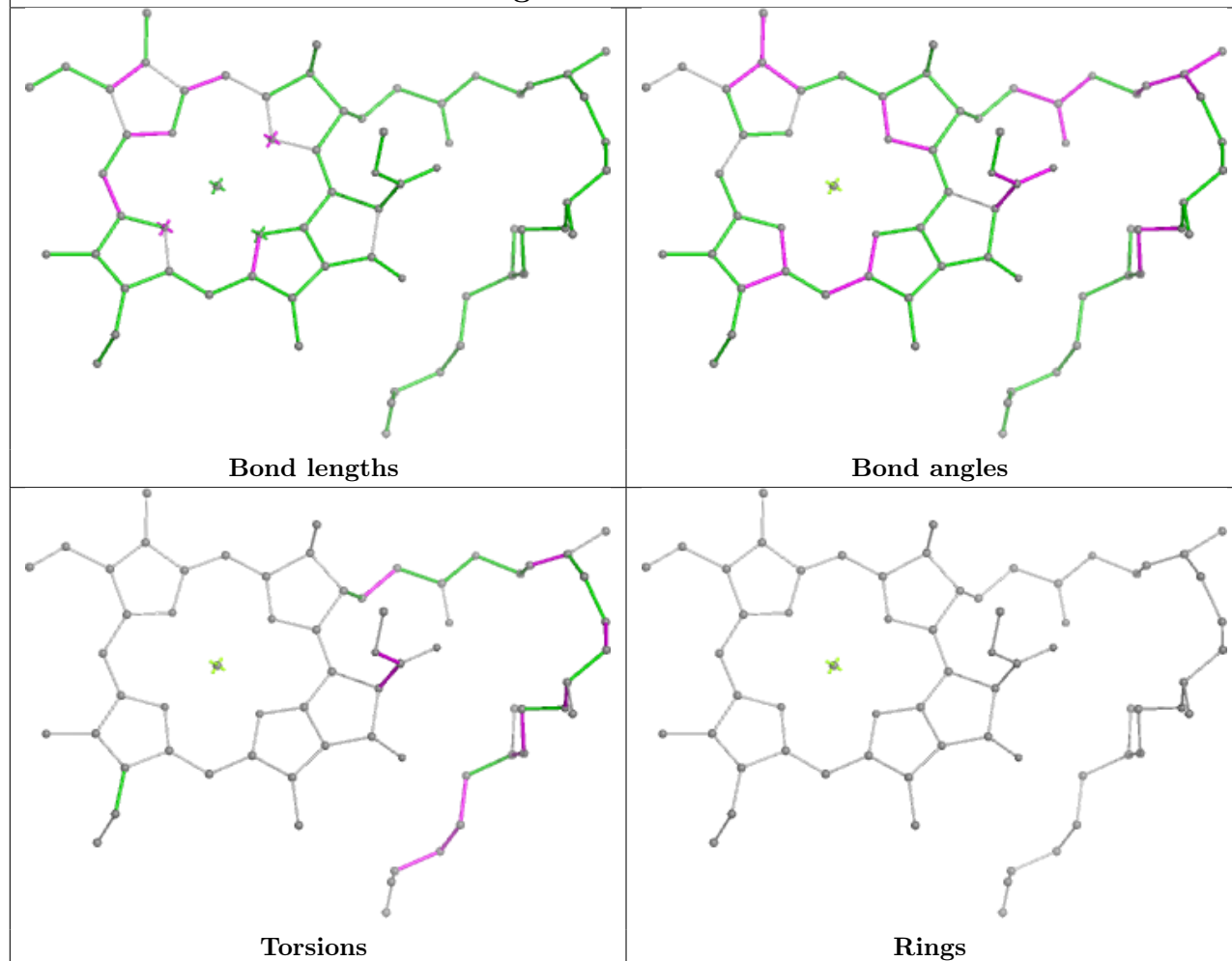


Ligand CLA d 404

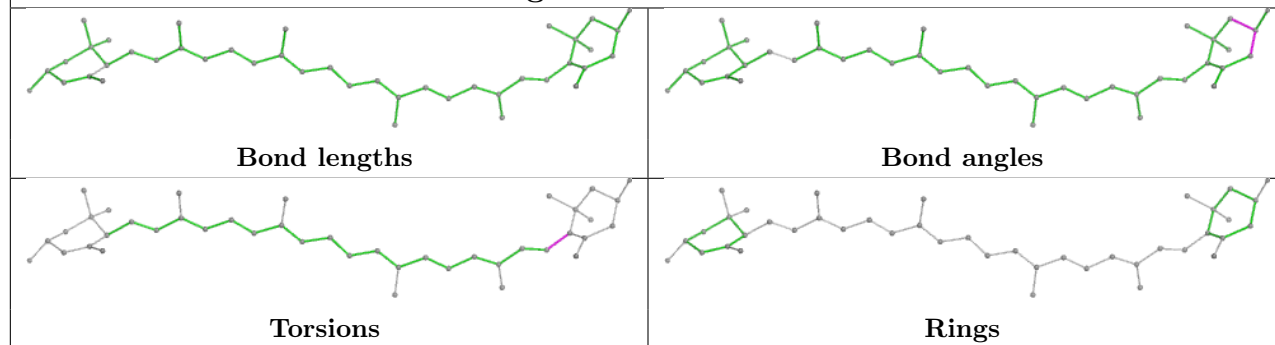


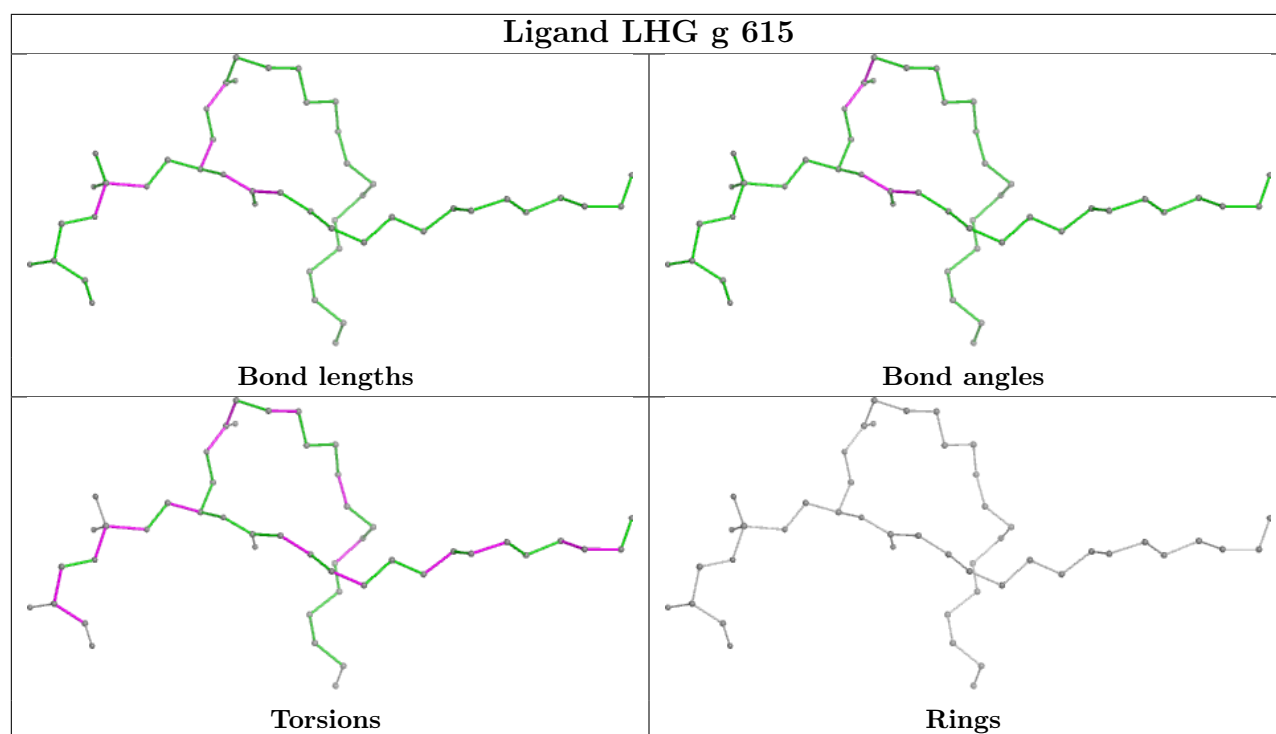
Ligand CLA 6 603**Ligand LHG 14 615**

Ligand CLA B 610

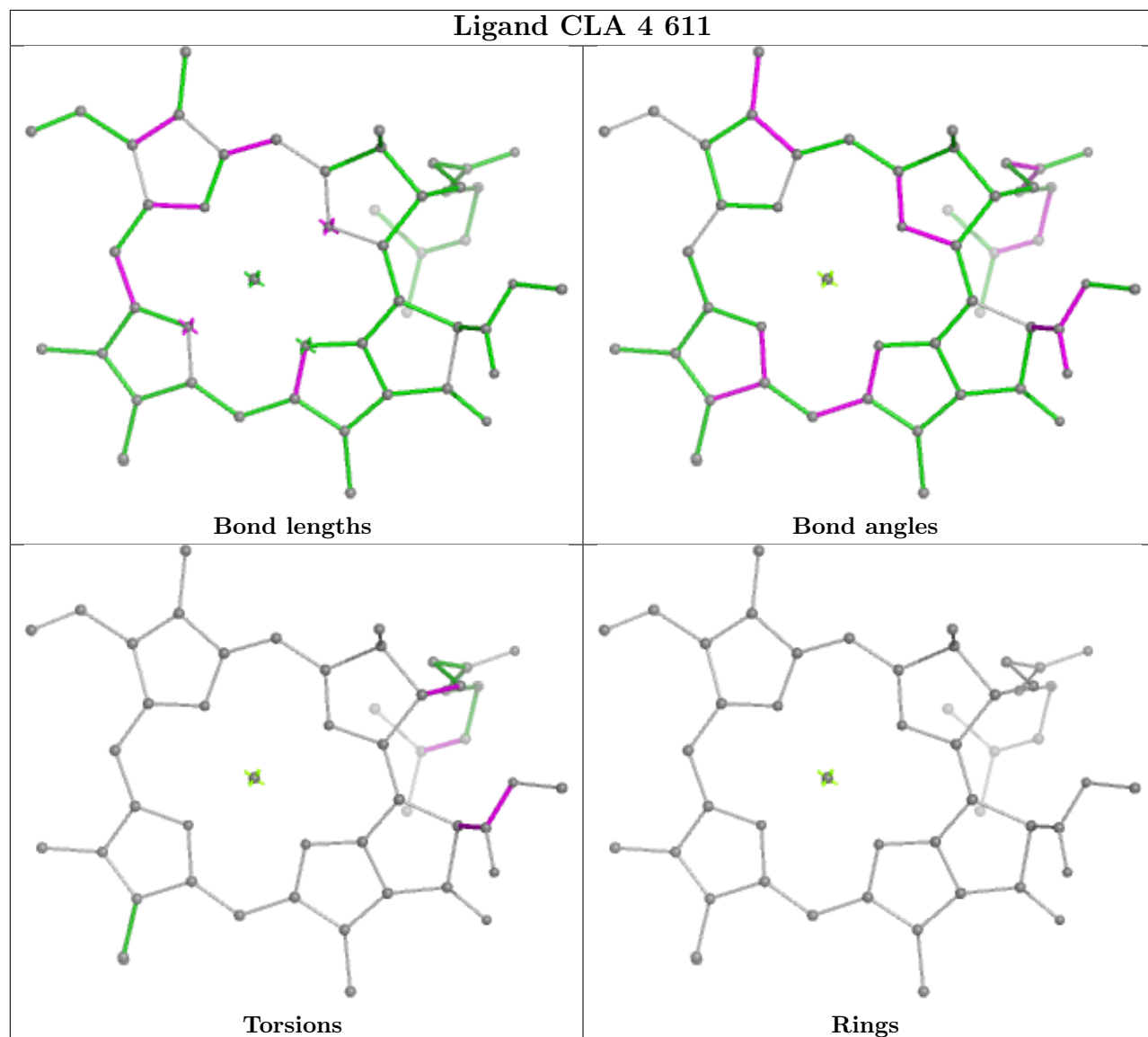


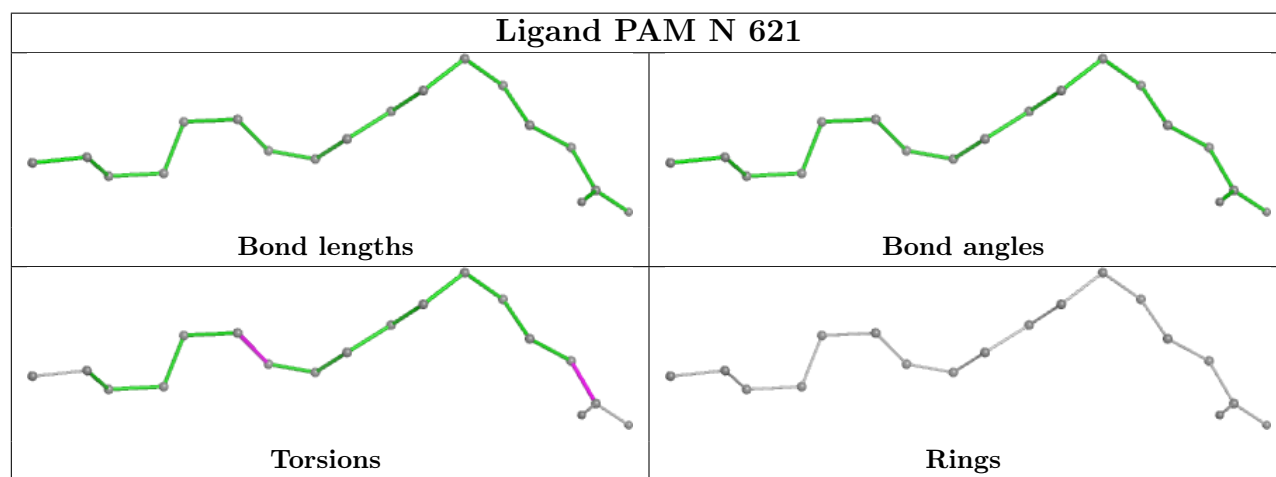
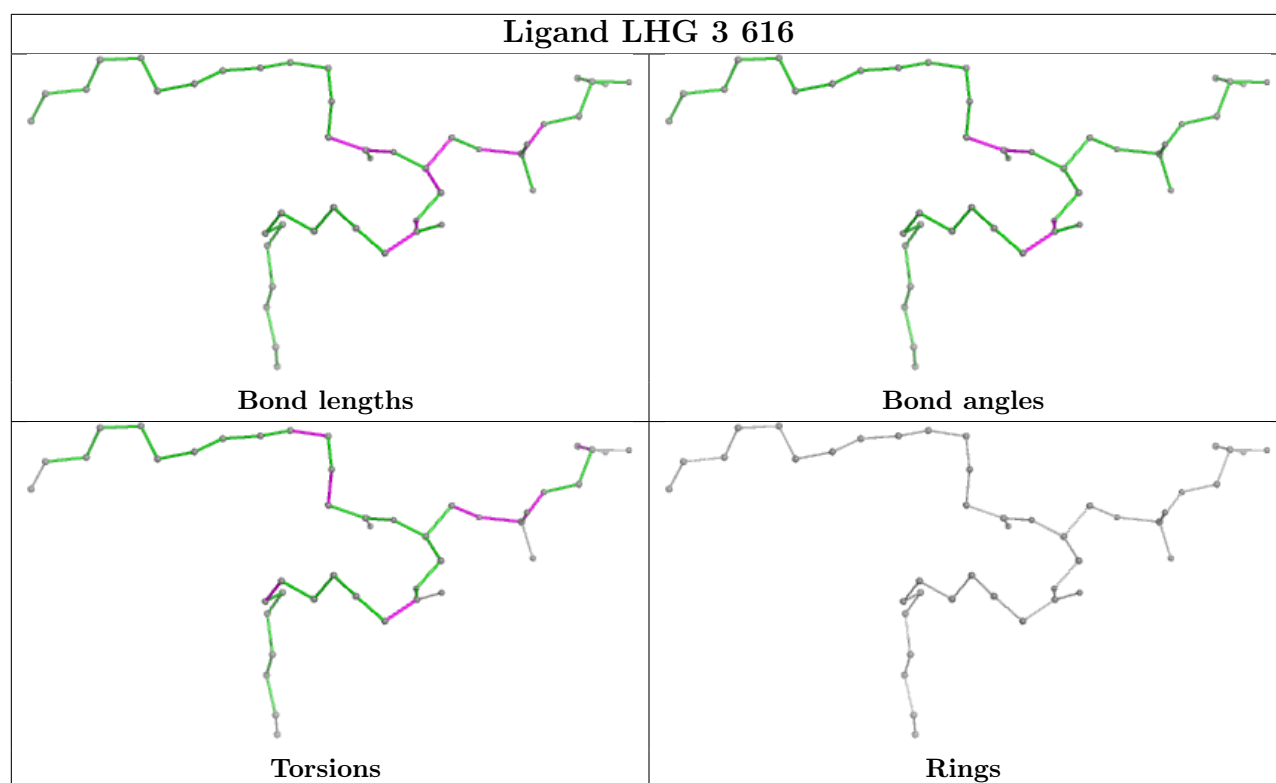
Ligand LUT 16 617

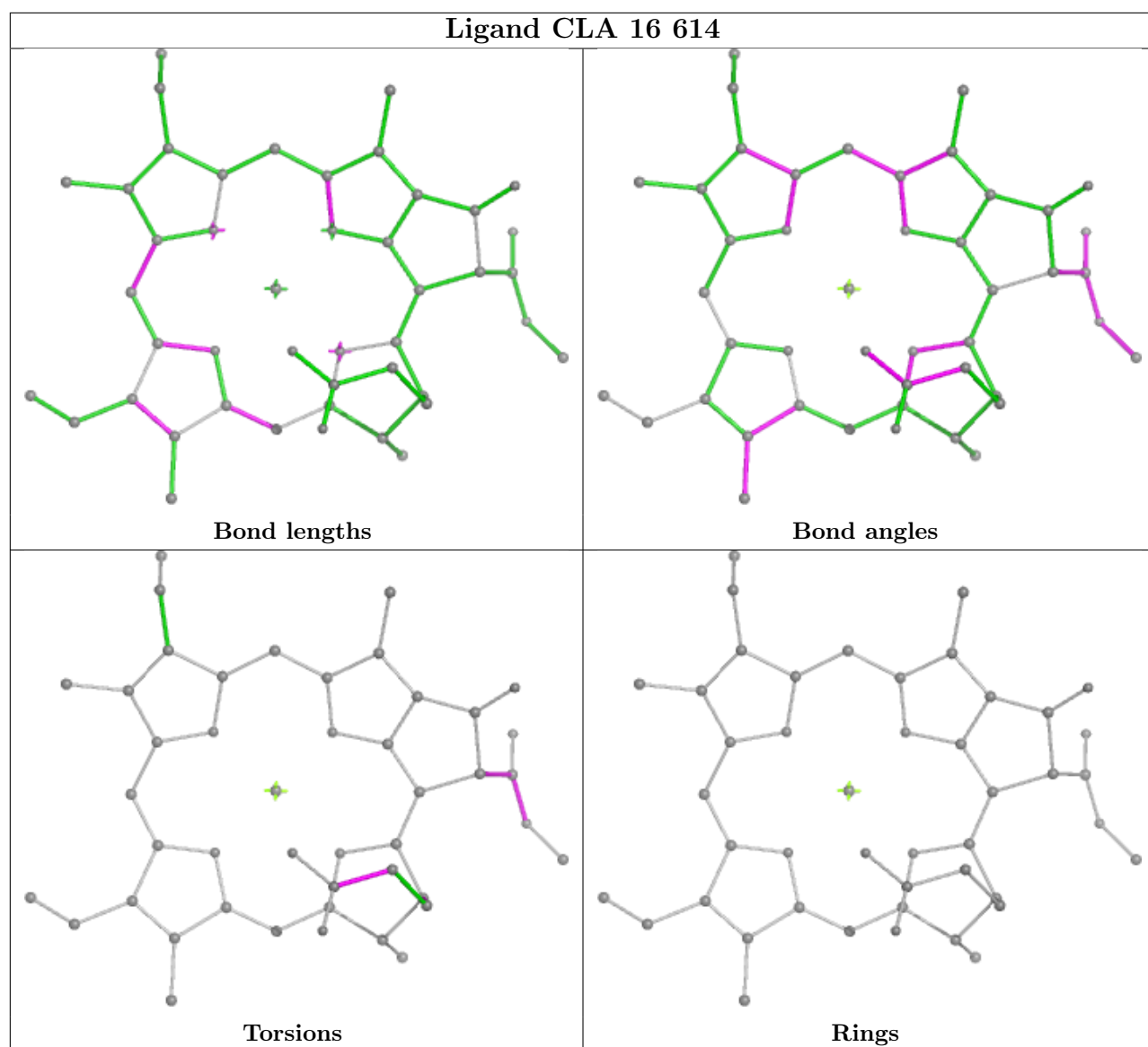




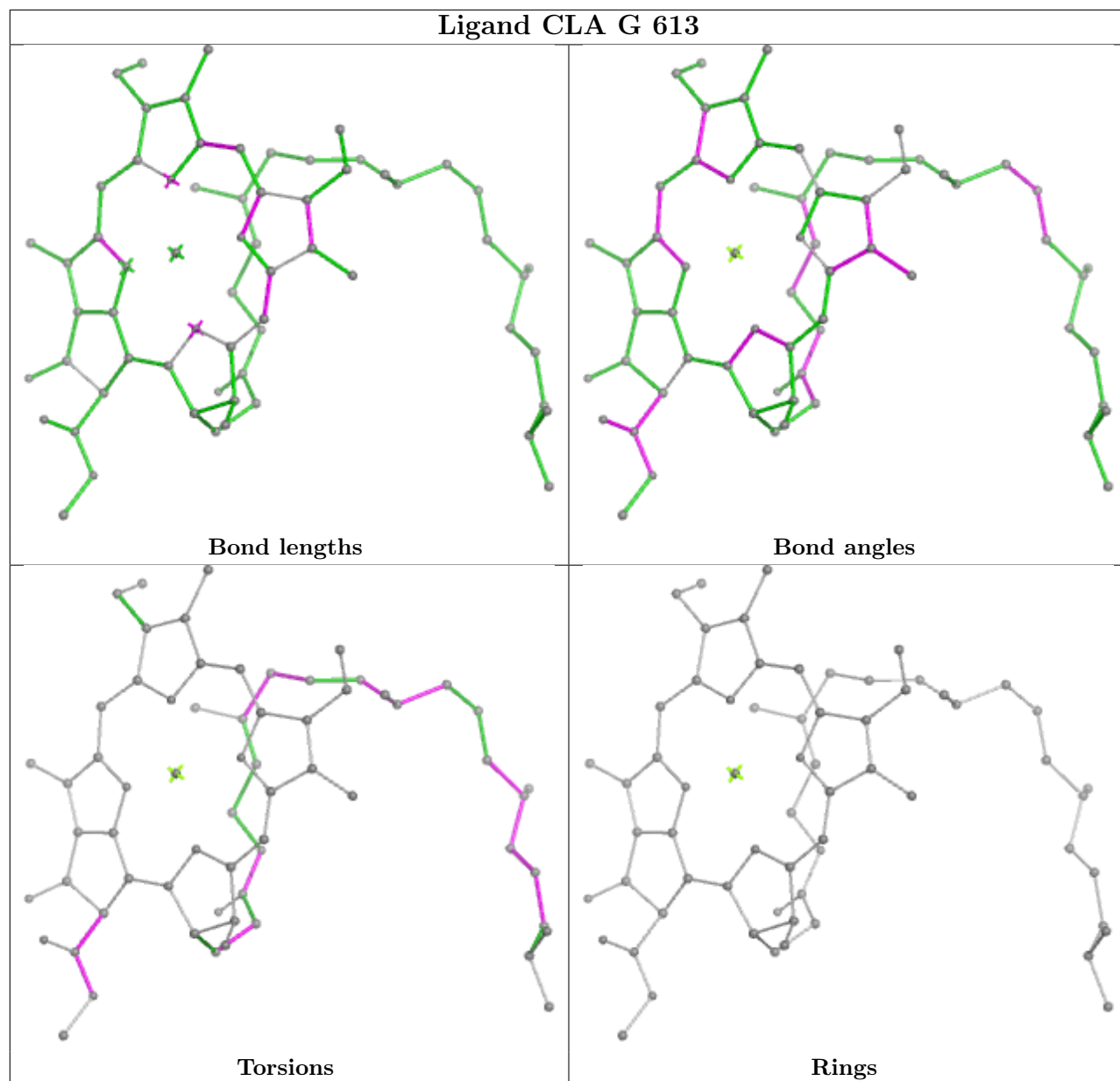
Ligand CLA 4 611

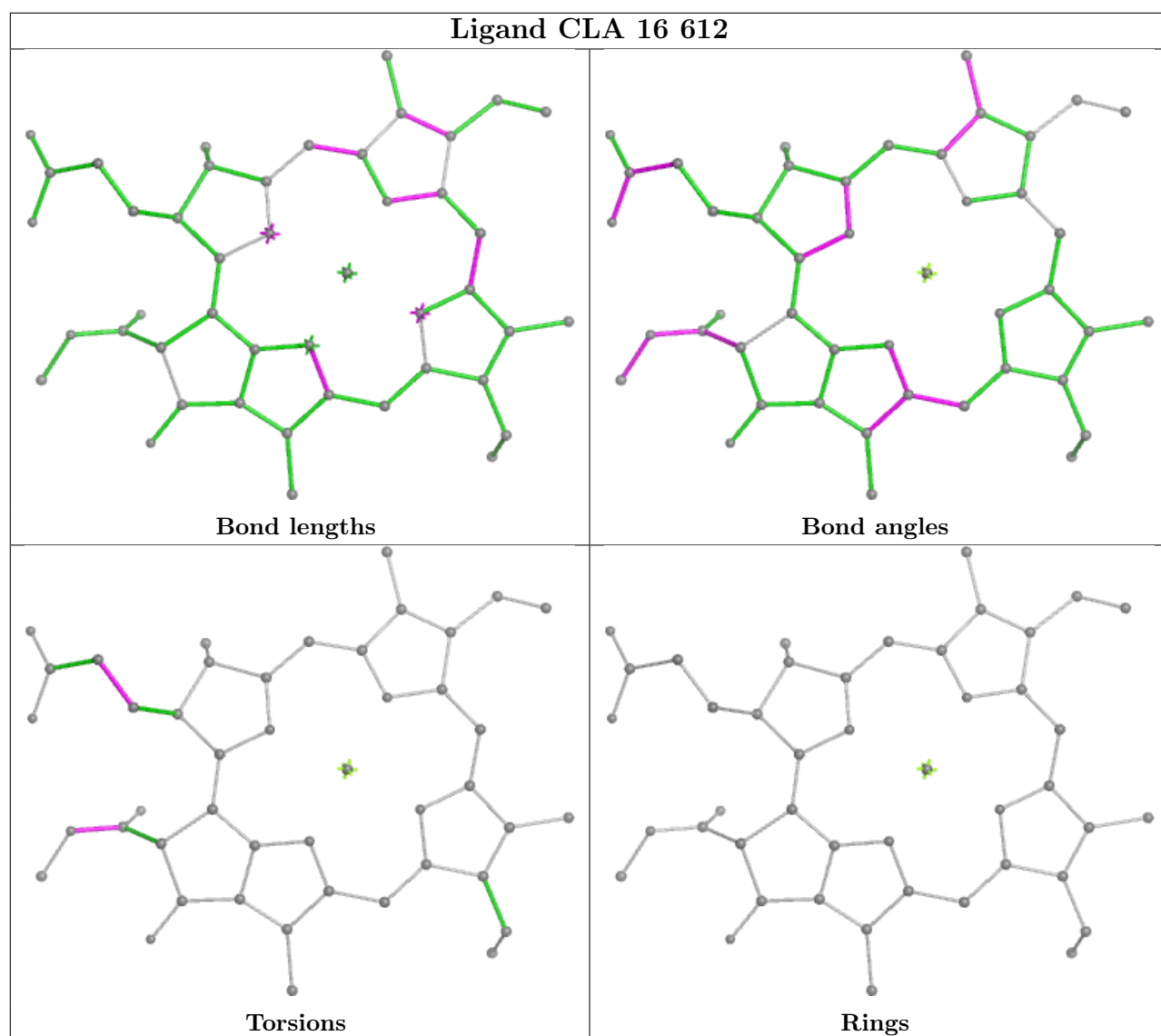


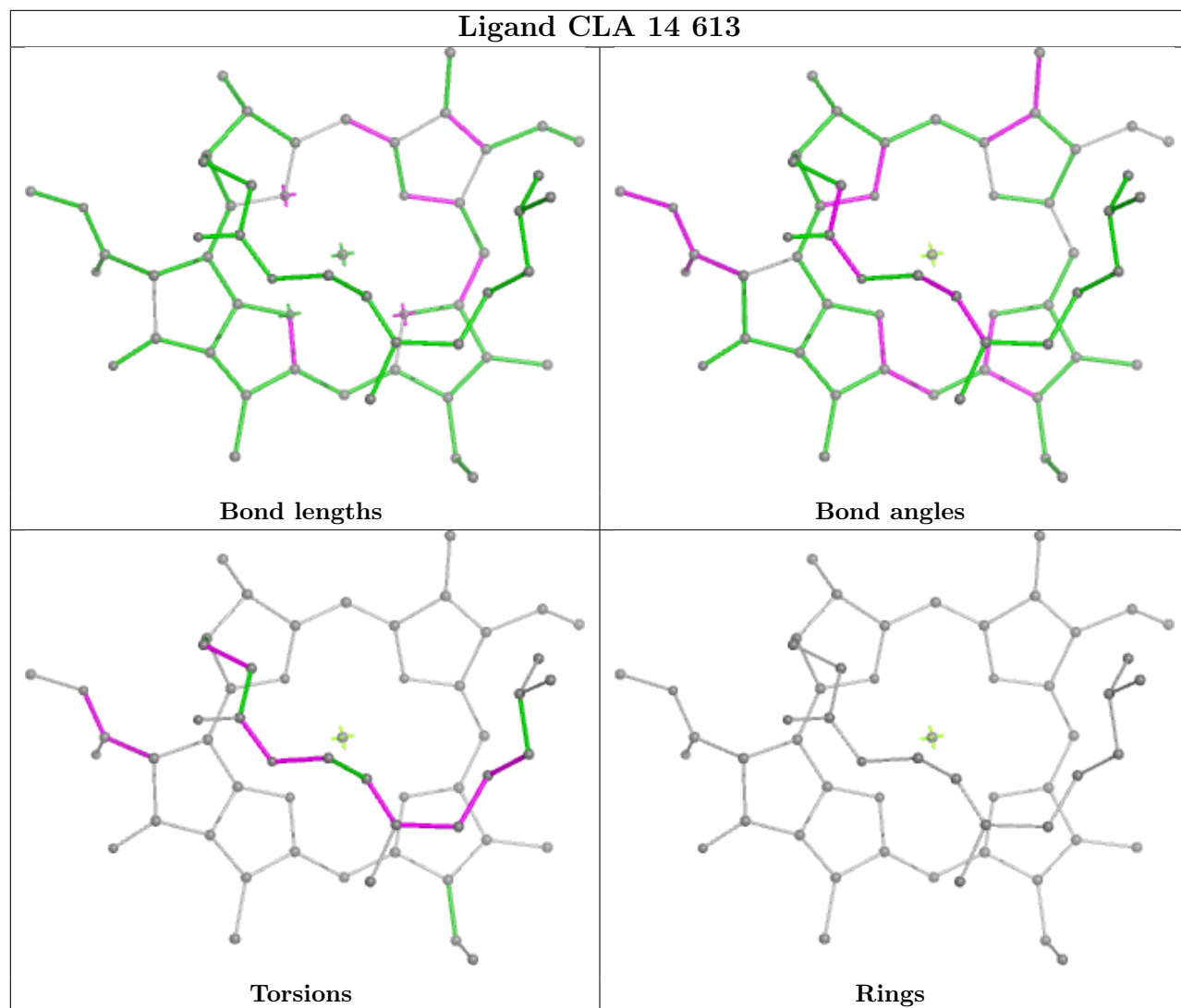




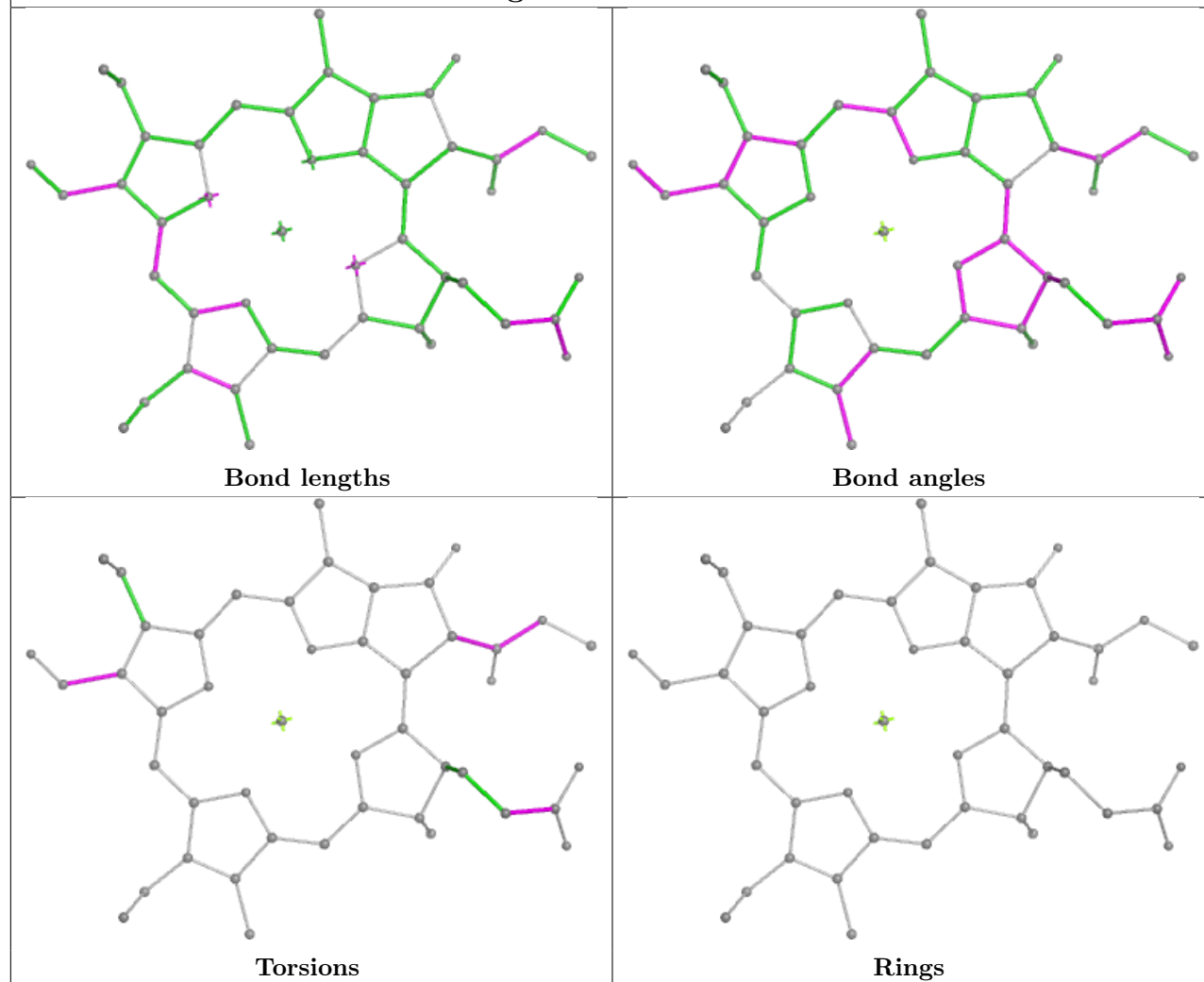
Ligand CLA G 613



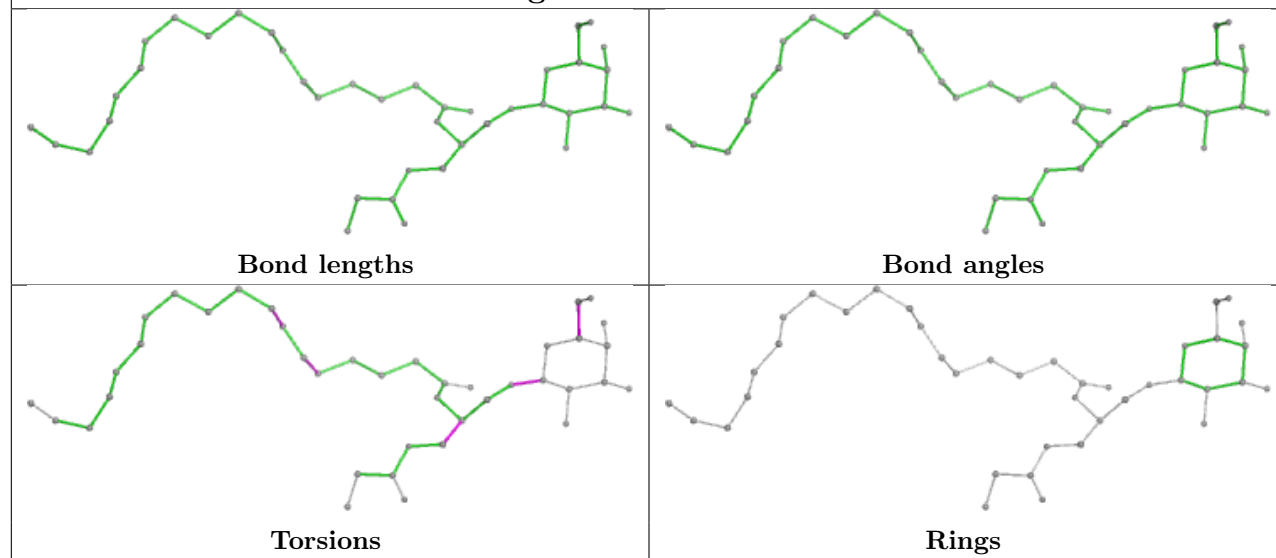




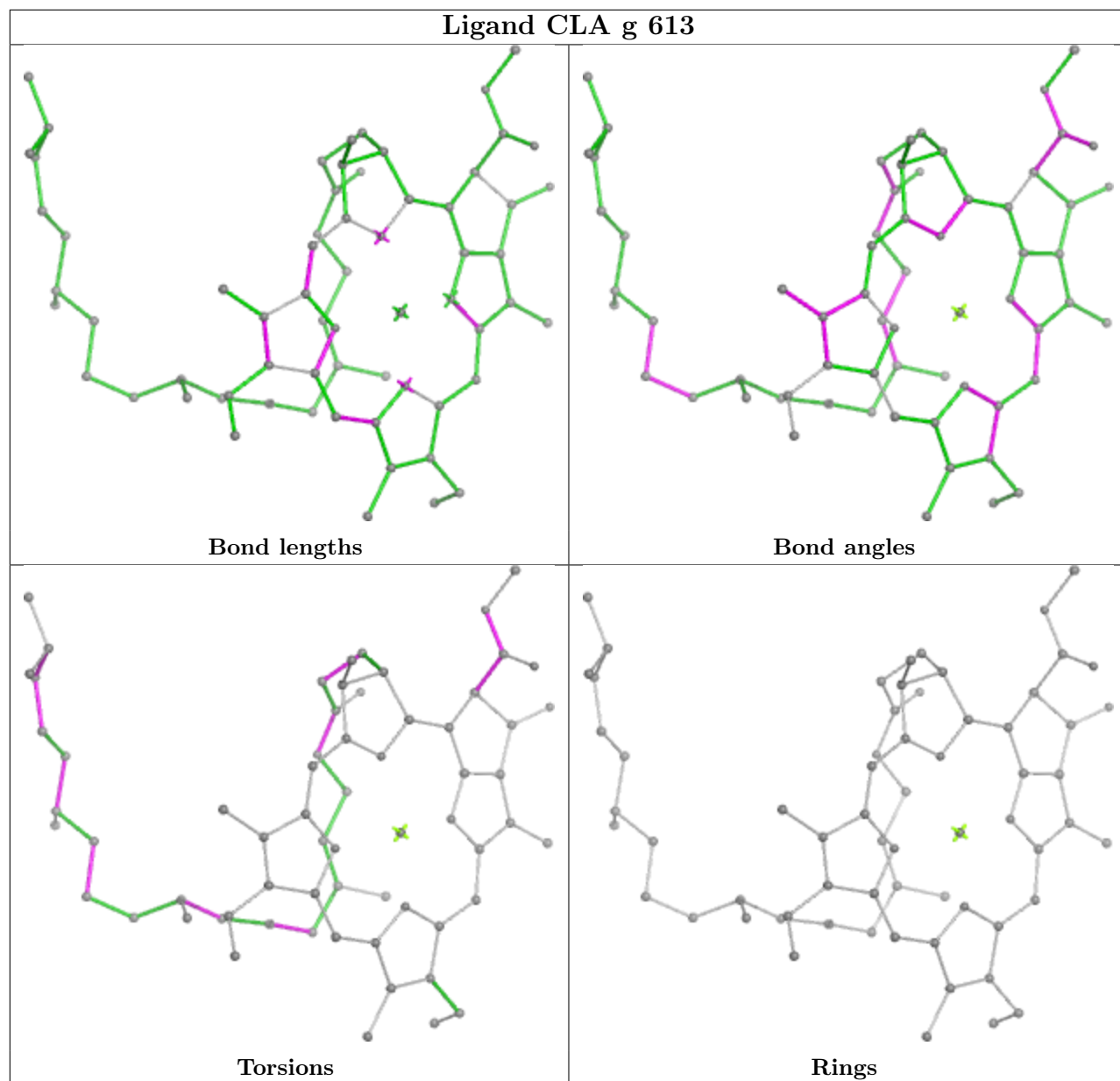
Ligand CHL s 601



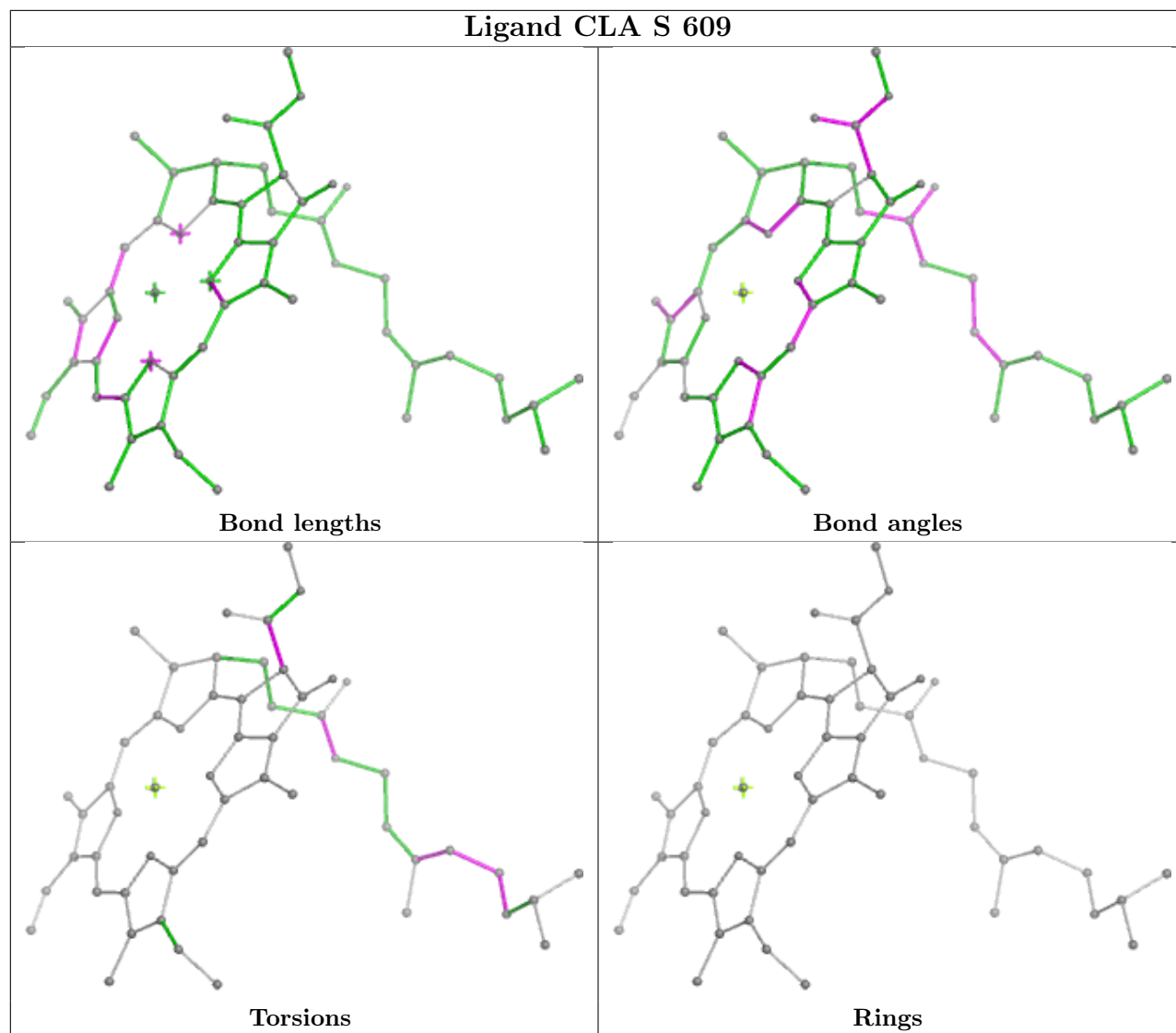
Ligand DGD w 502



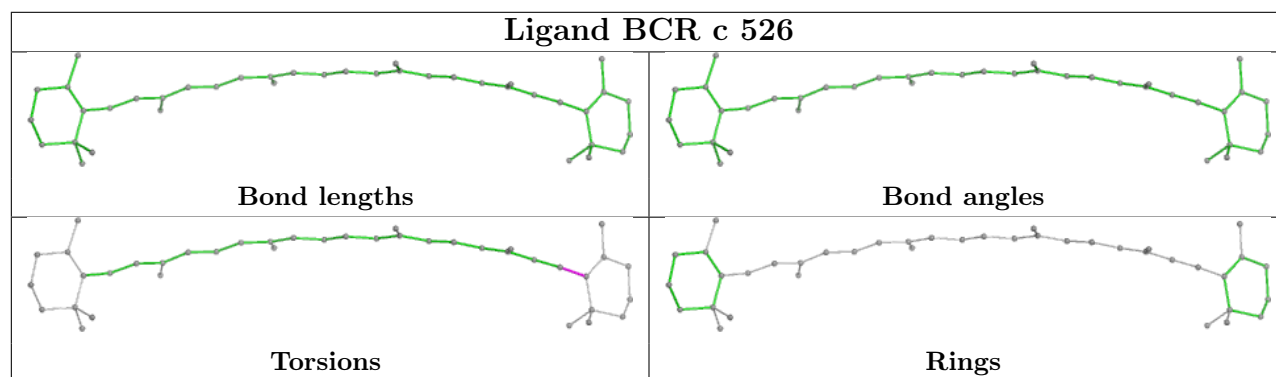
Ligand CLA g 613

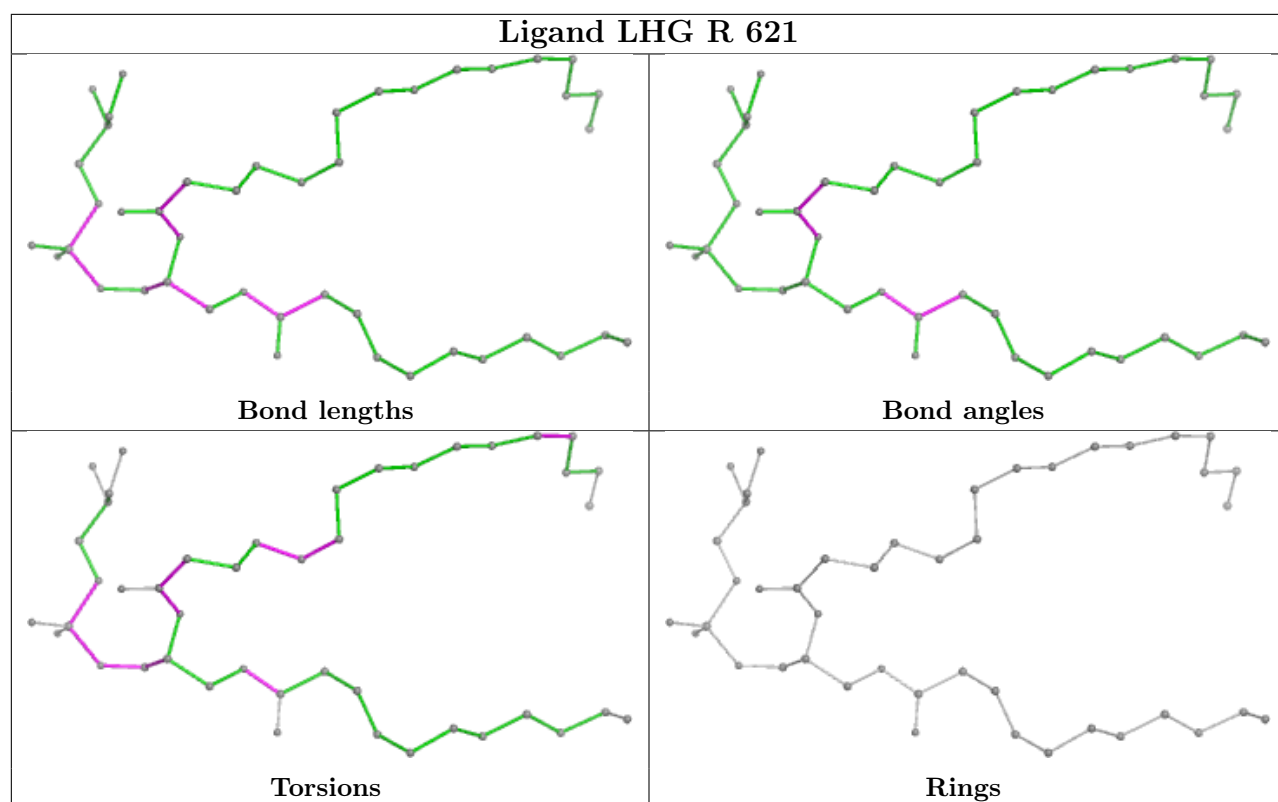


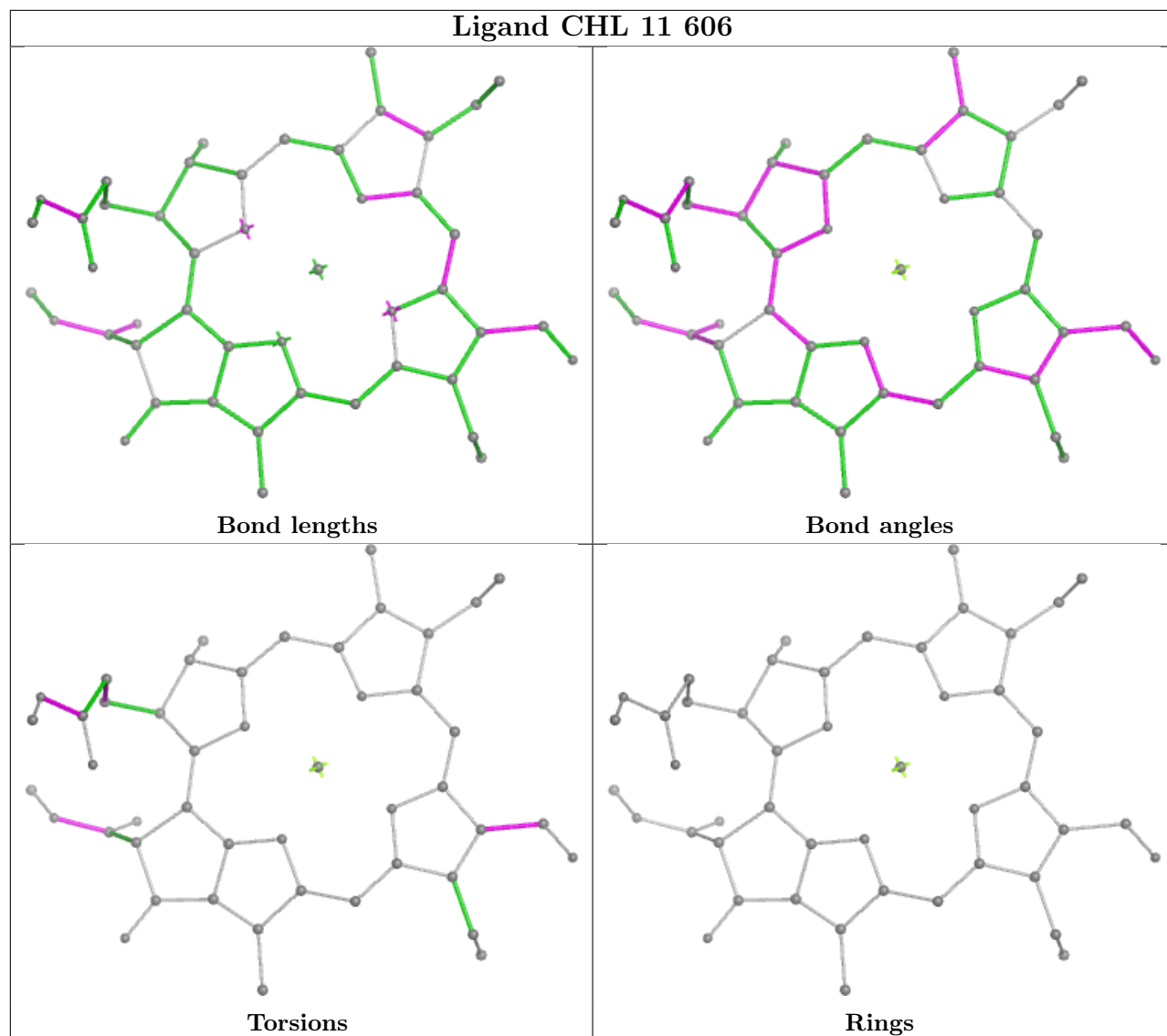
Ligand CLA S 609



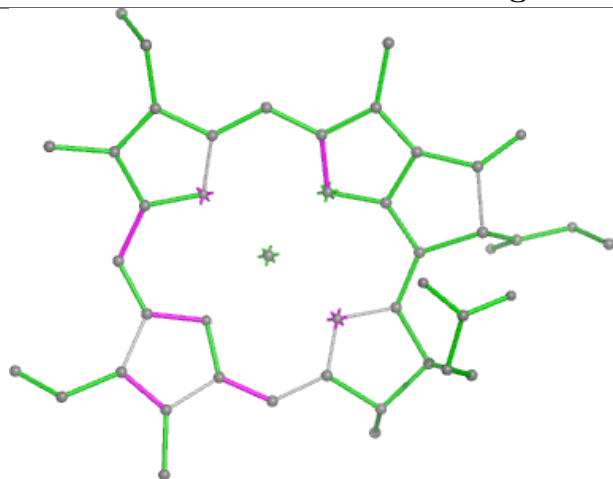
Ligand BCR c 526



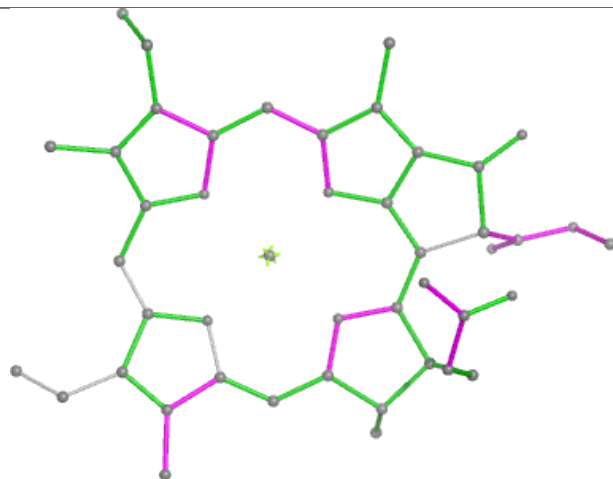




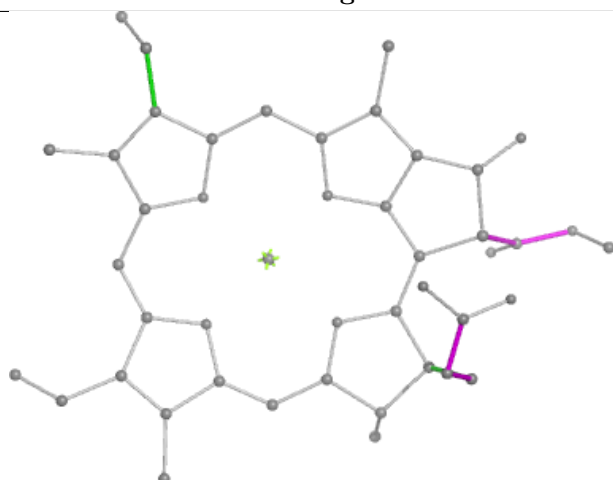
Ligand CLA 12 610



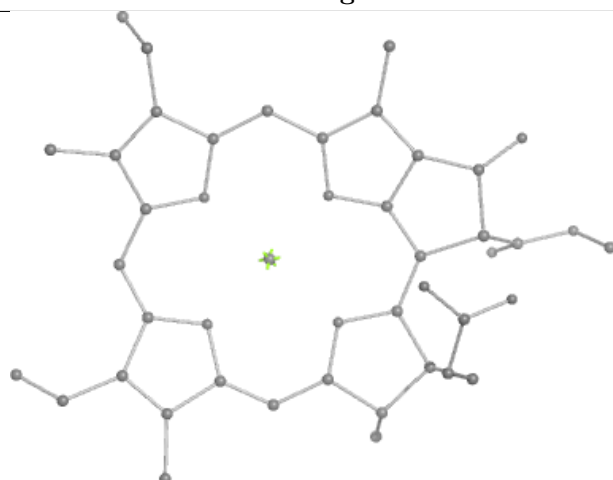
Bond lengths



Bond angles

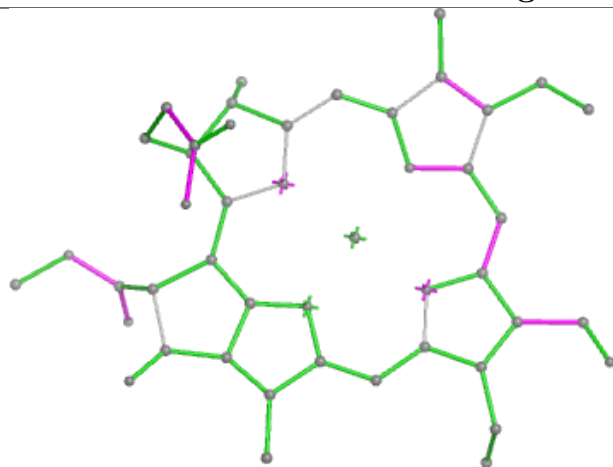


Torsions

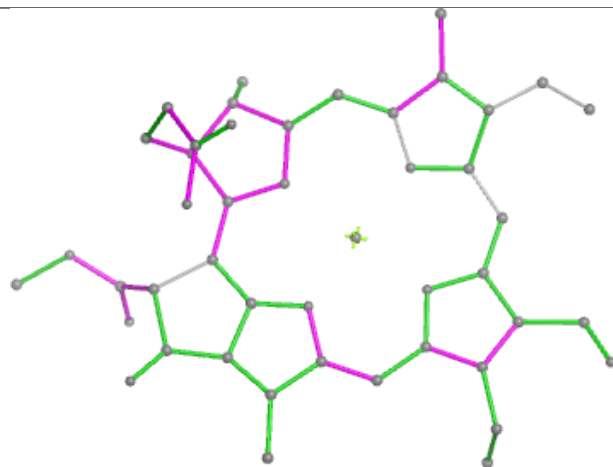


Rings

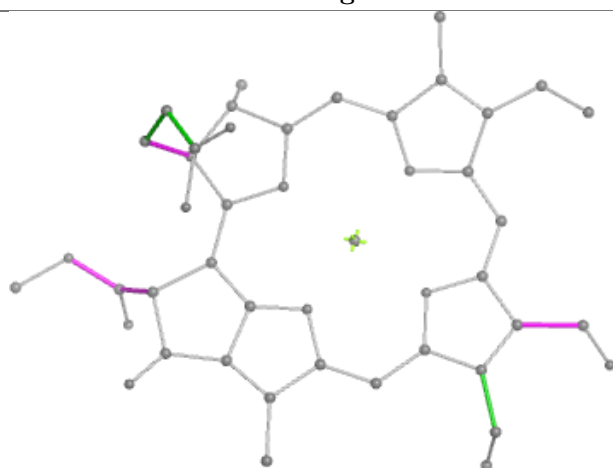
Ligand CHL 1 605



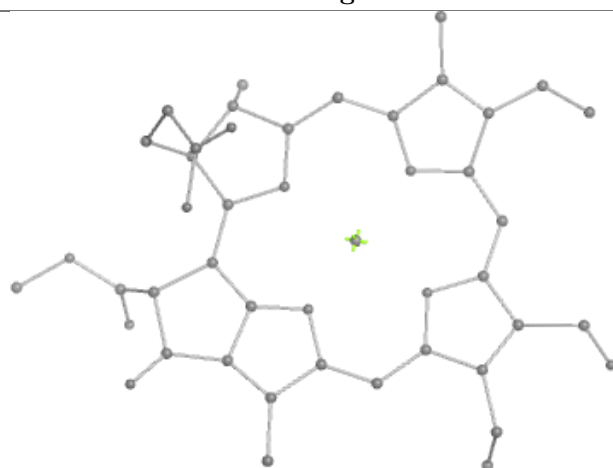
Bond lengths



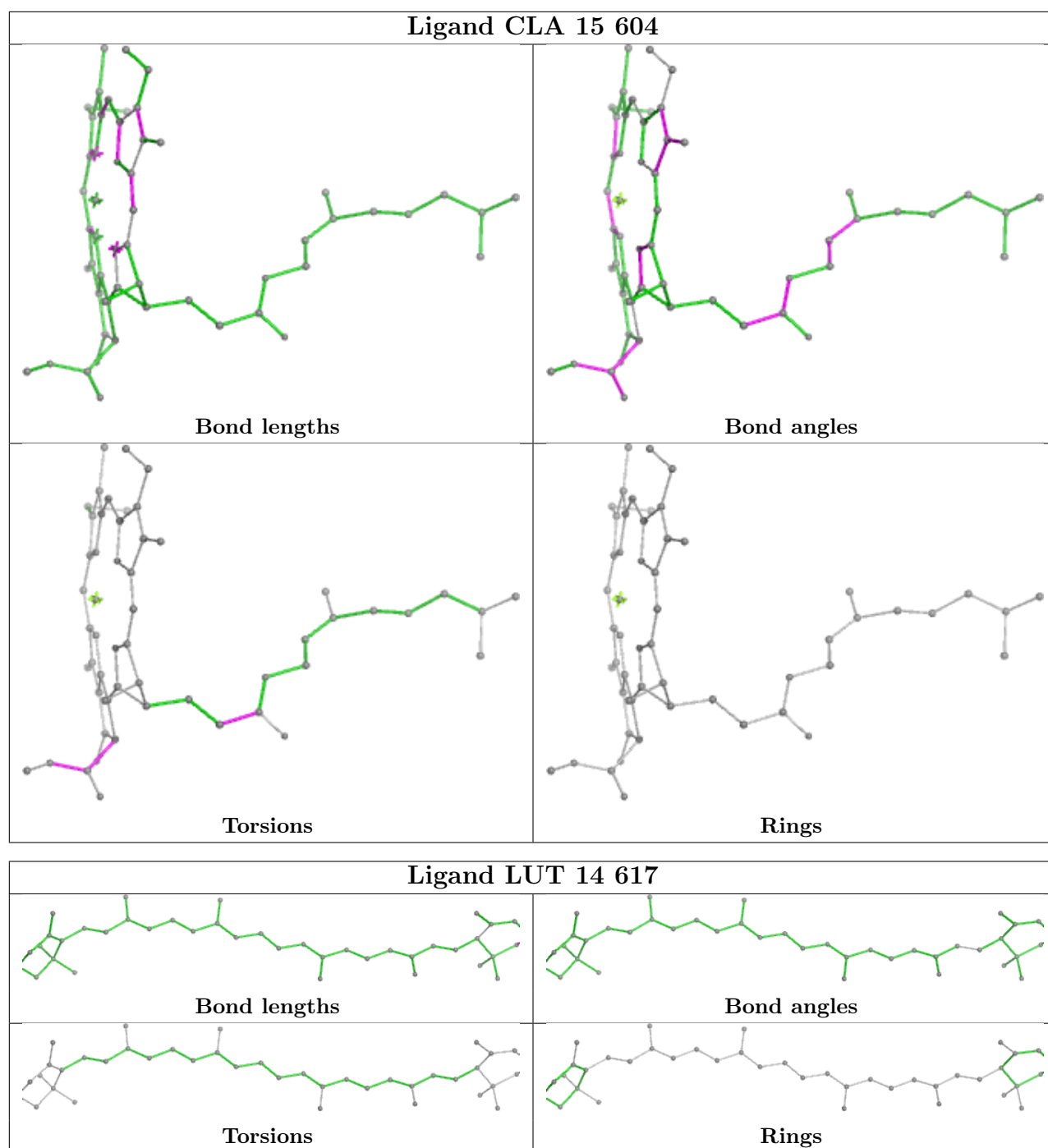
Bond angles



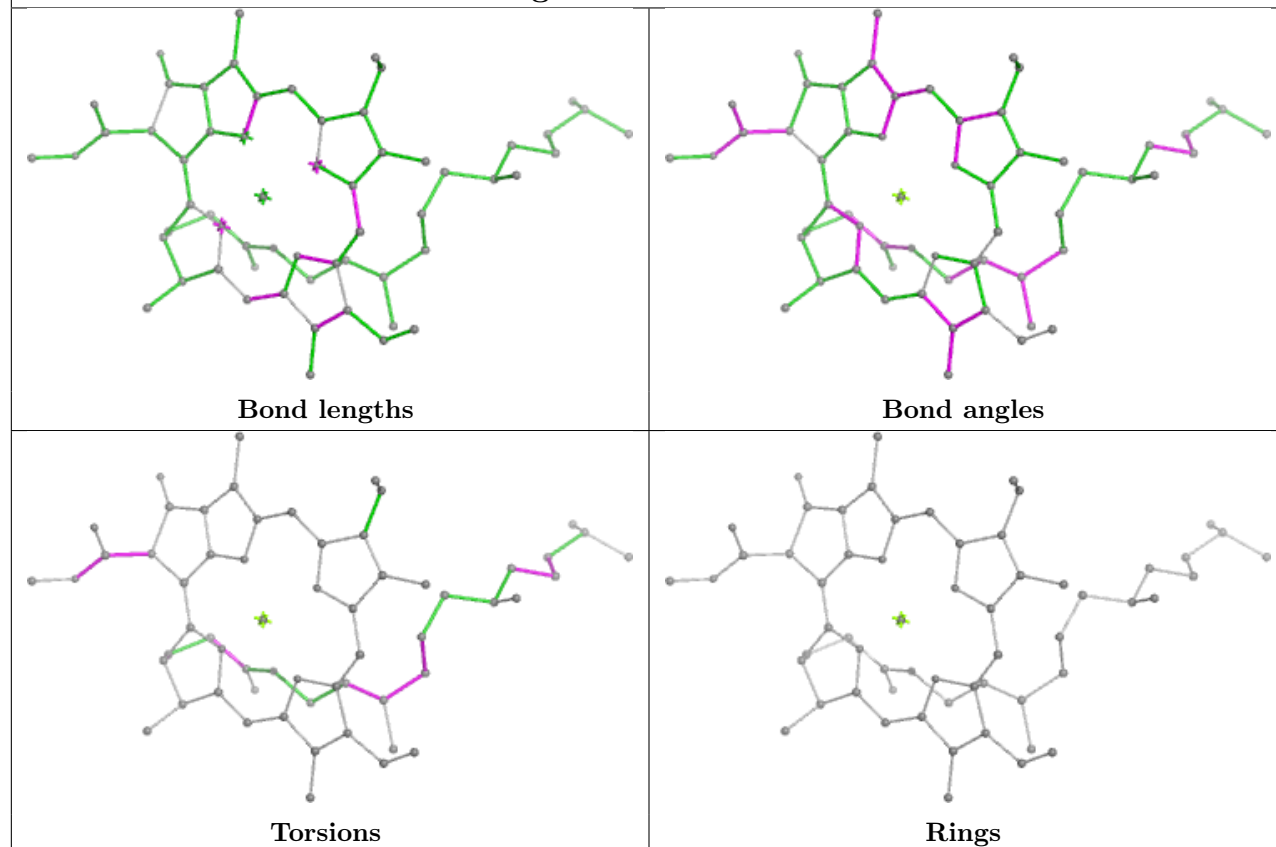
Torsions



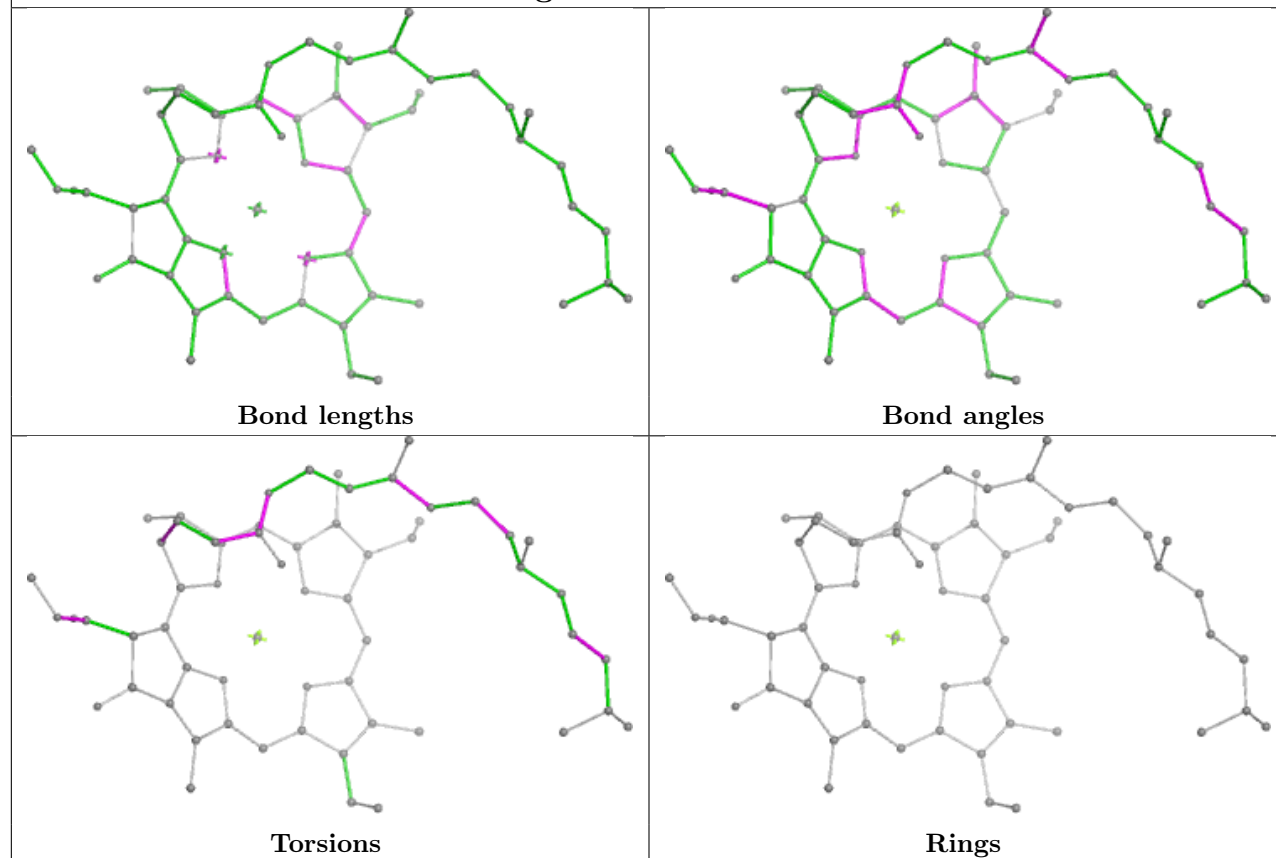
Rings

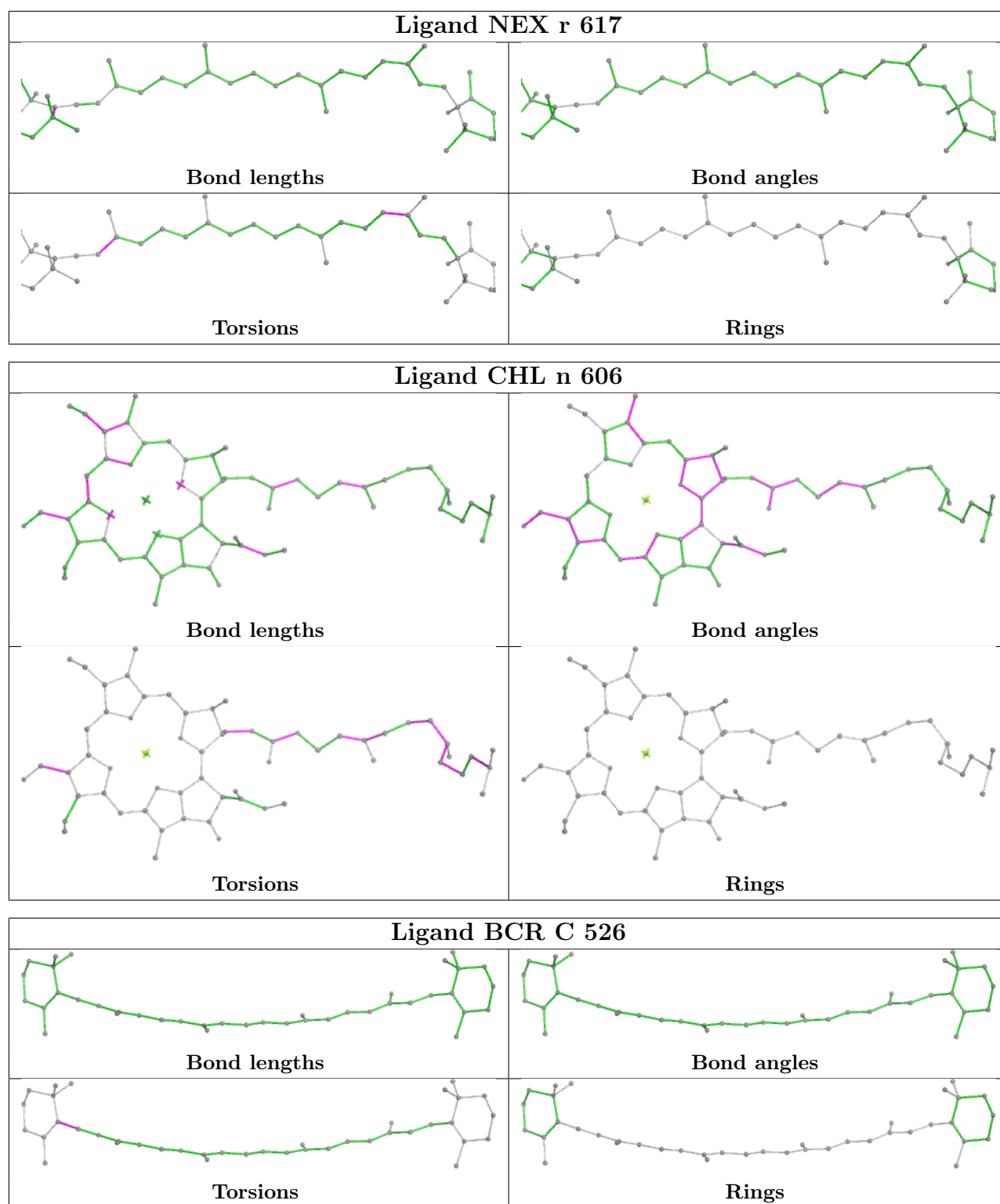


Ligand CLA R 613

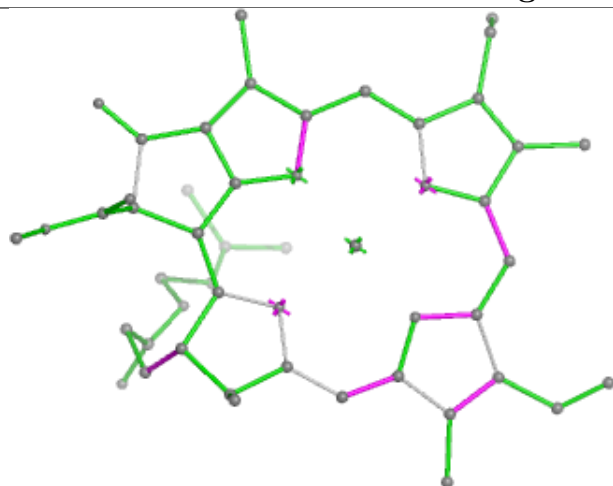


Ligand CLA n 610

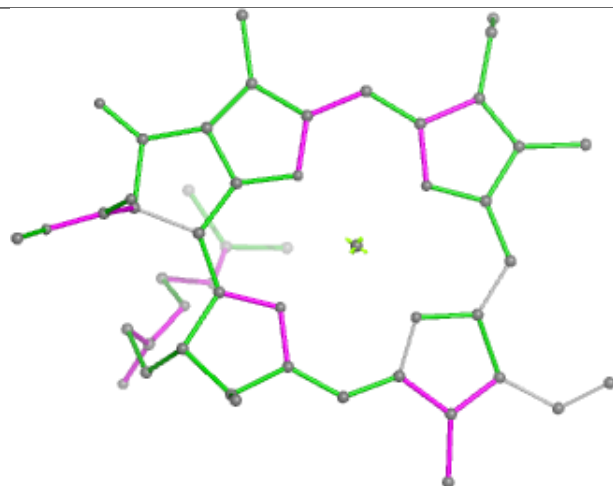




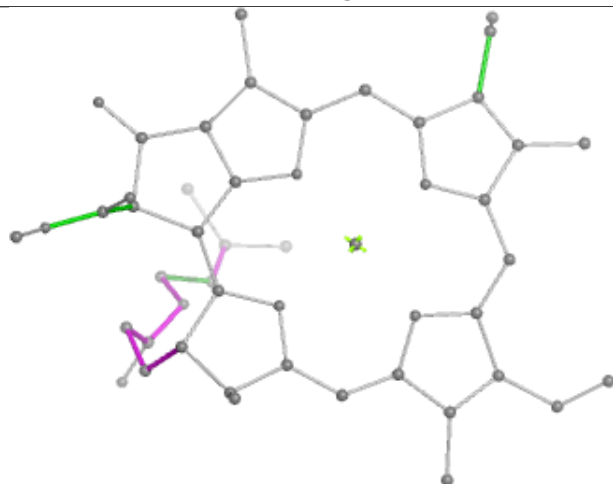
Ligand CLA 1 611



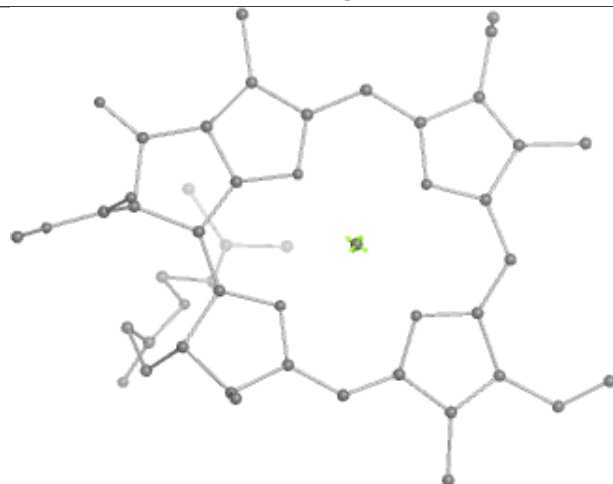
Bond lengths



Bond angles

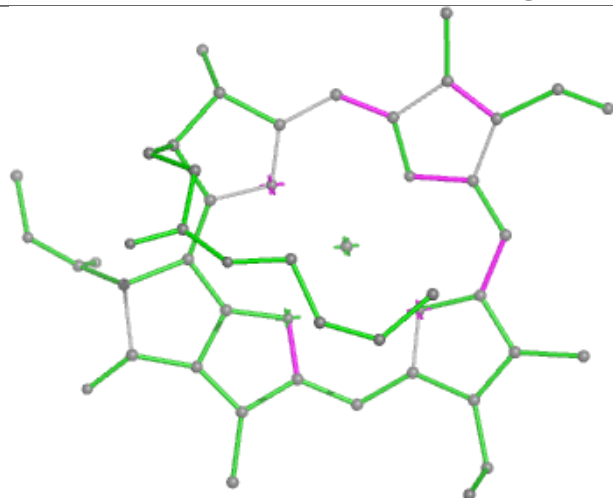


Torsions

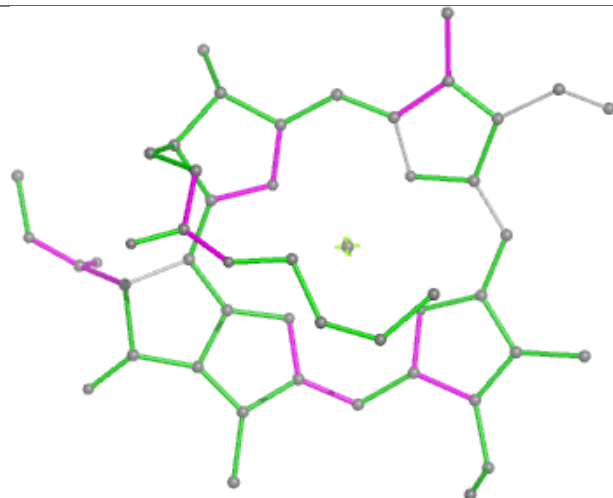


Rings

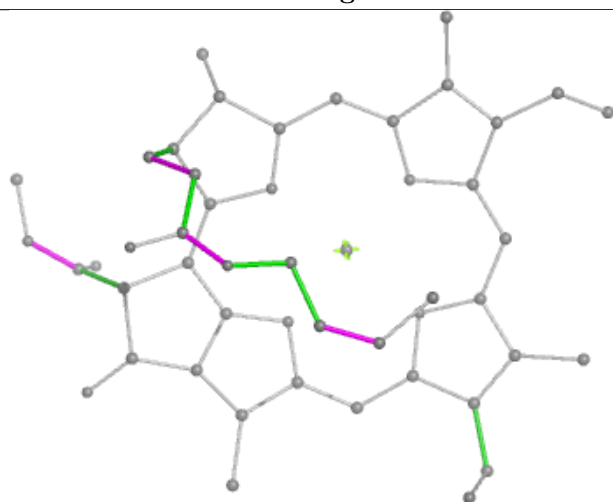
Ligand CLA s 613



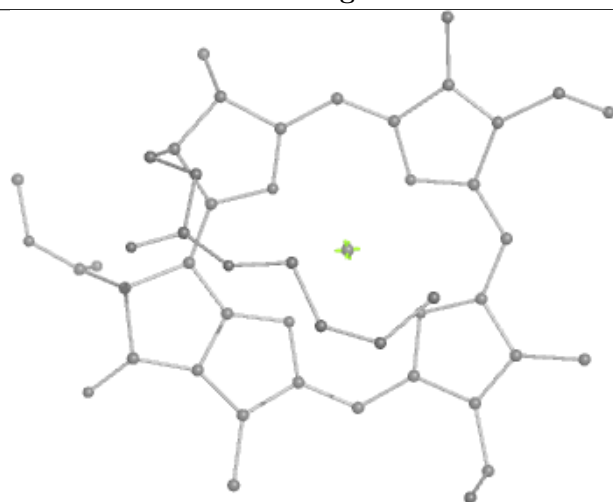
Bond lengths



Bond angles

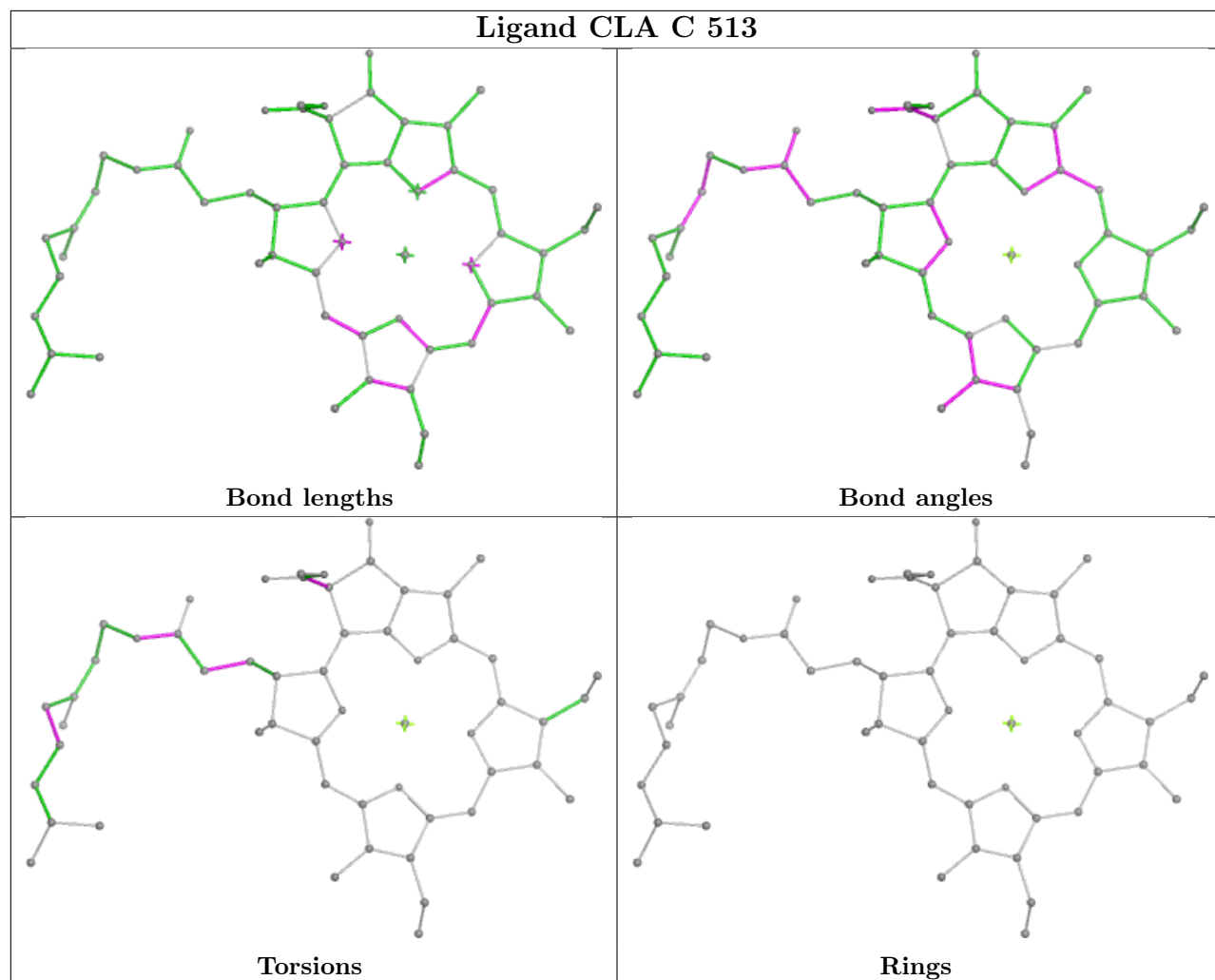


Torsions

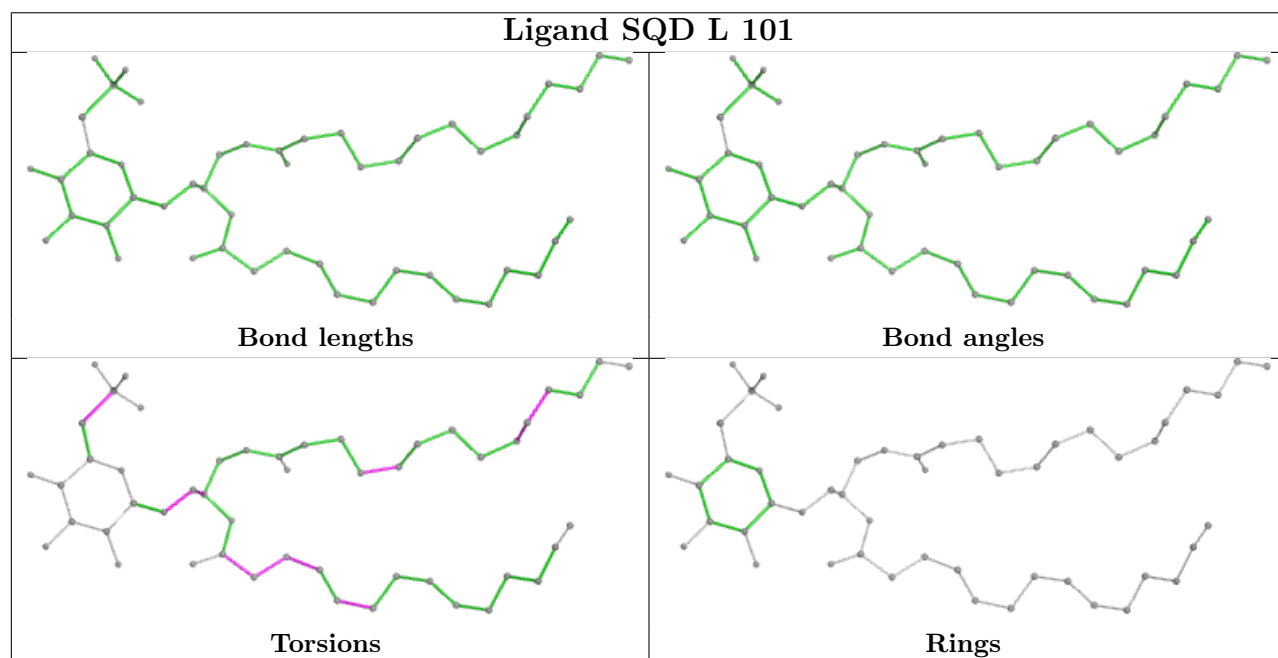


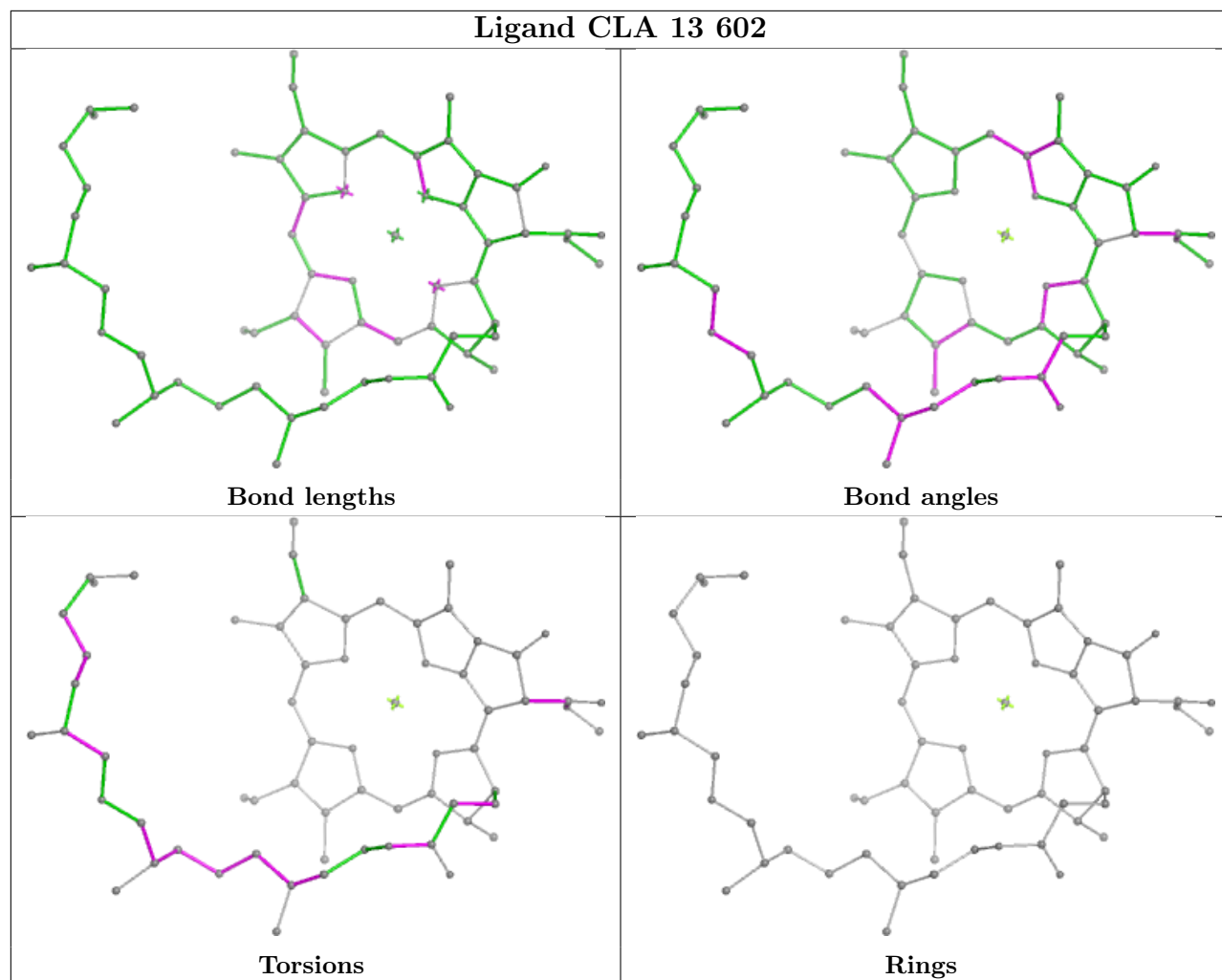
Rings

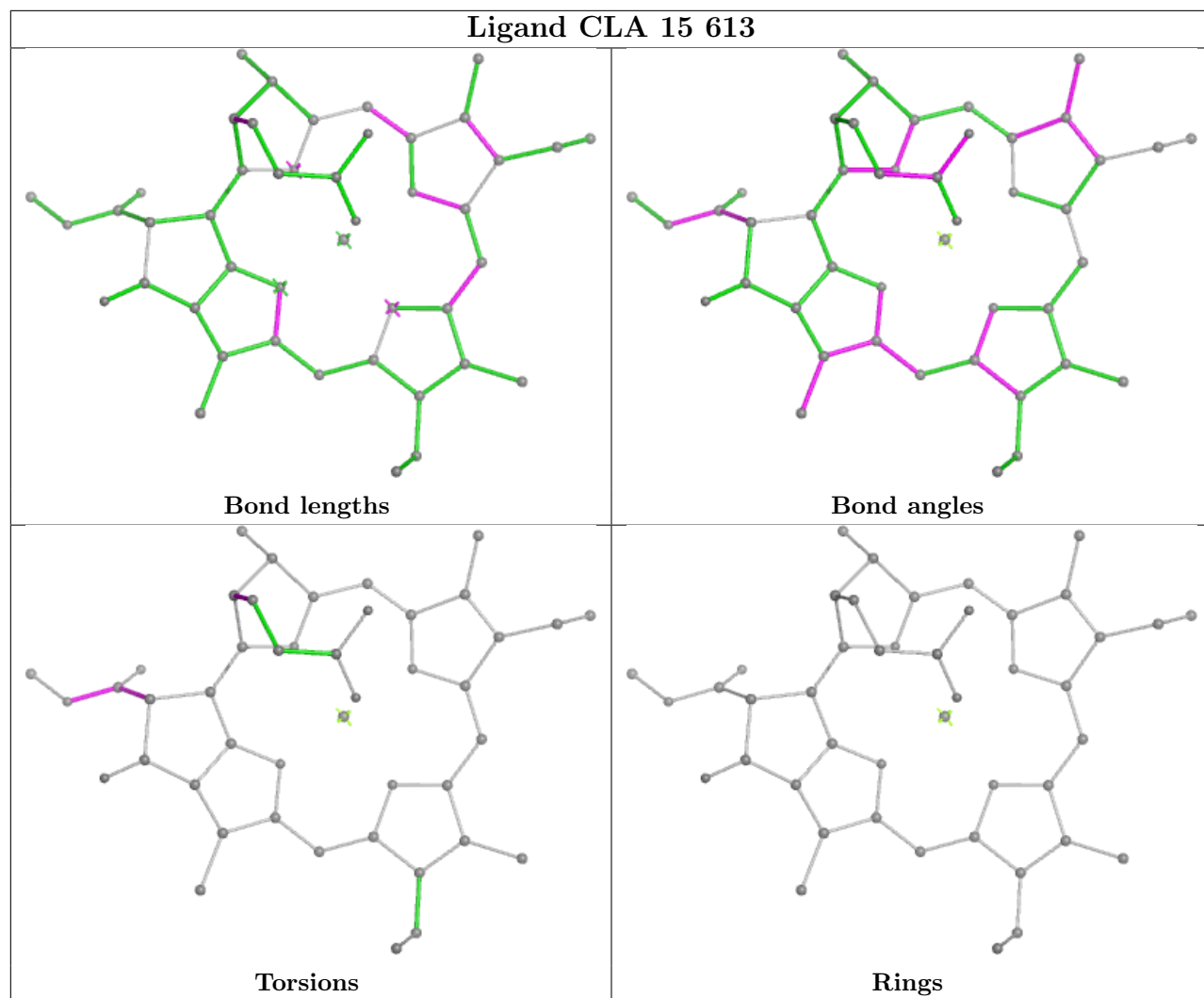
Ligand CLA C 513

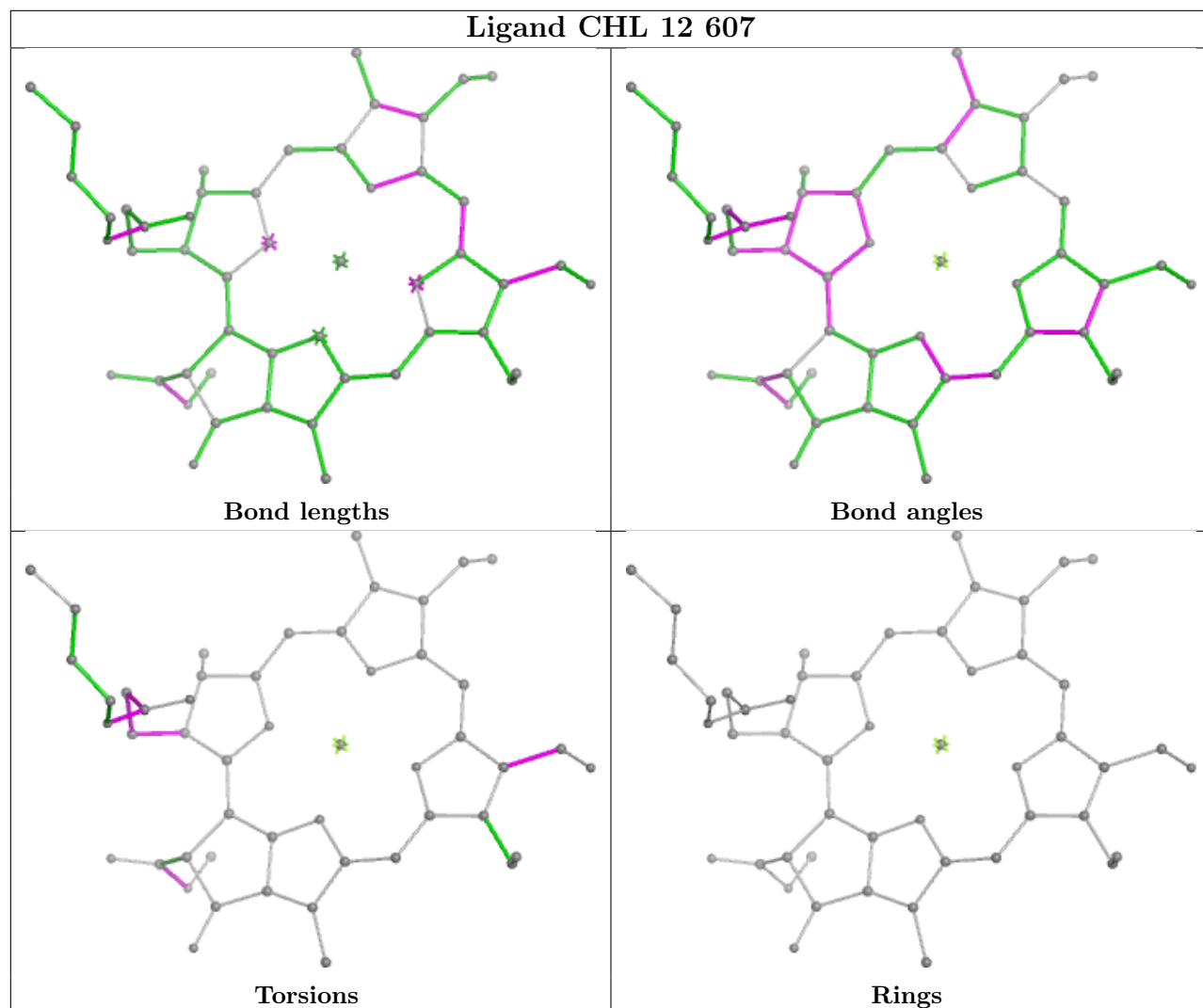


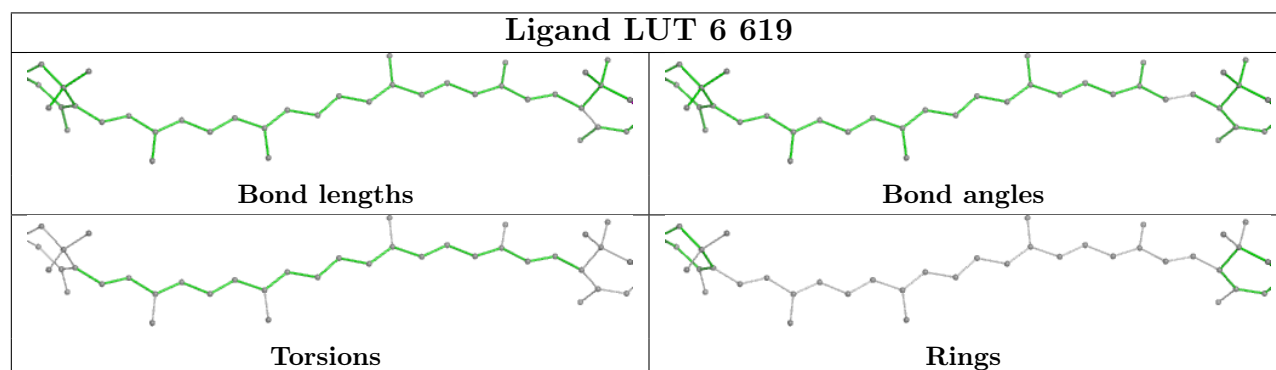
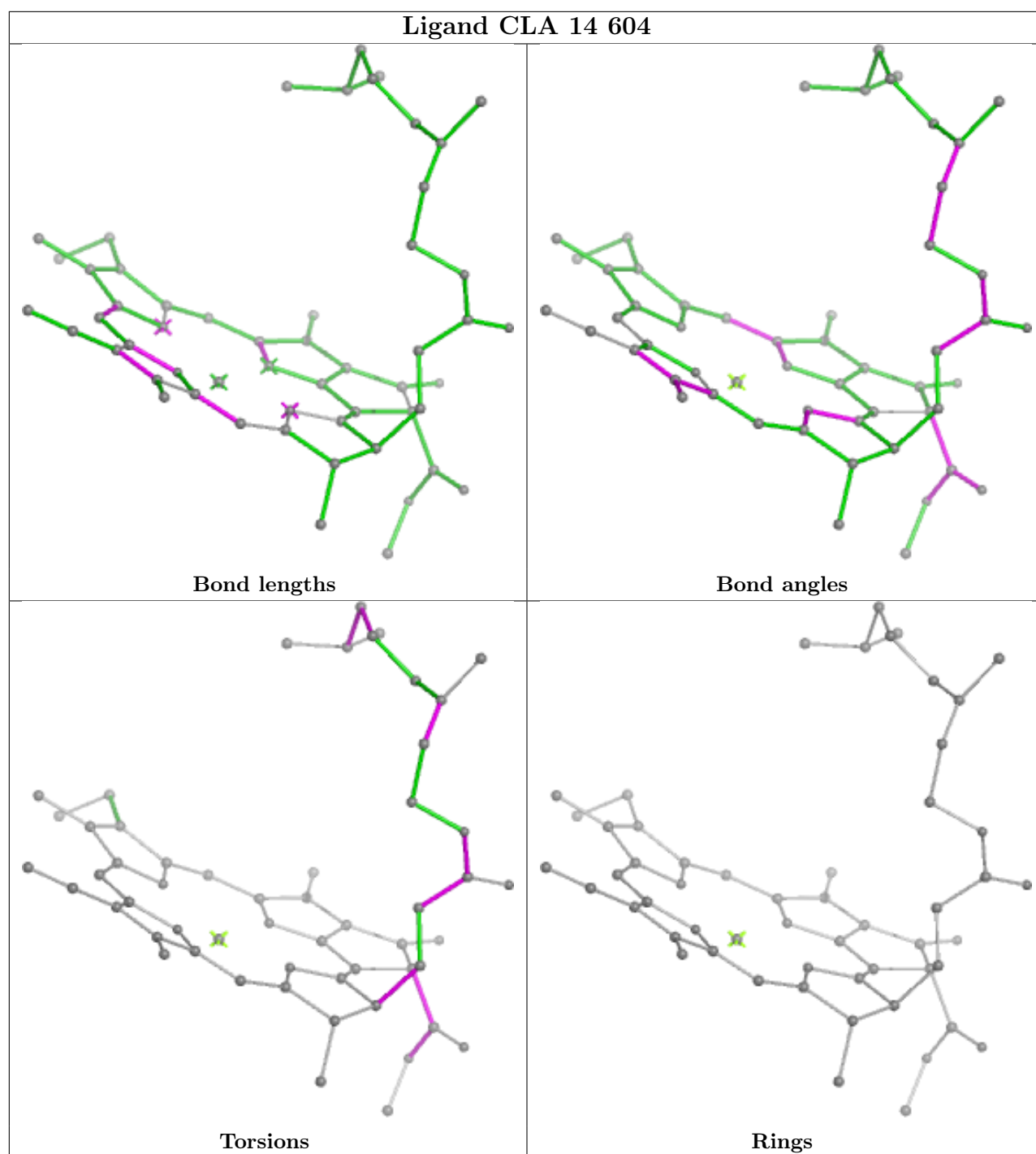
Ligand SQD L 101

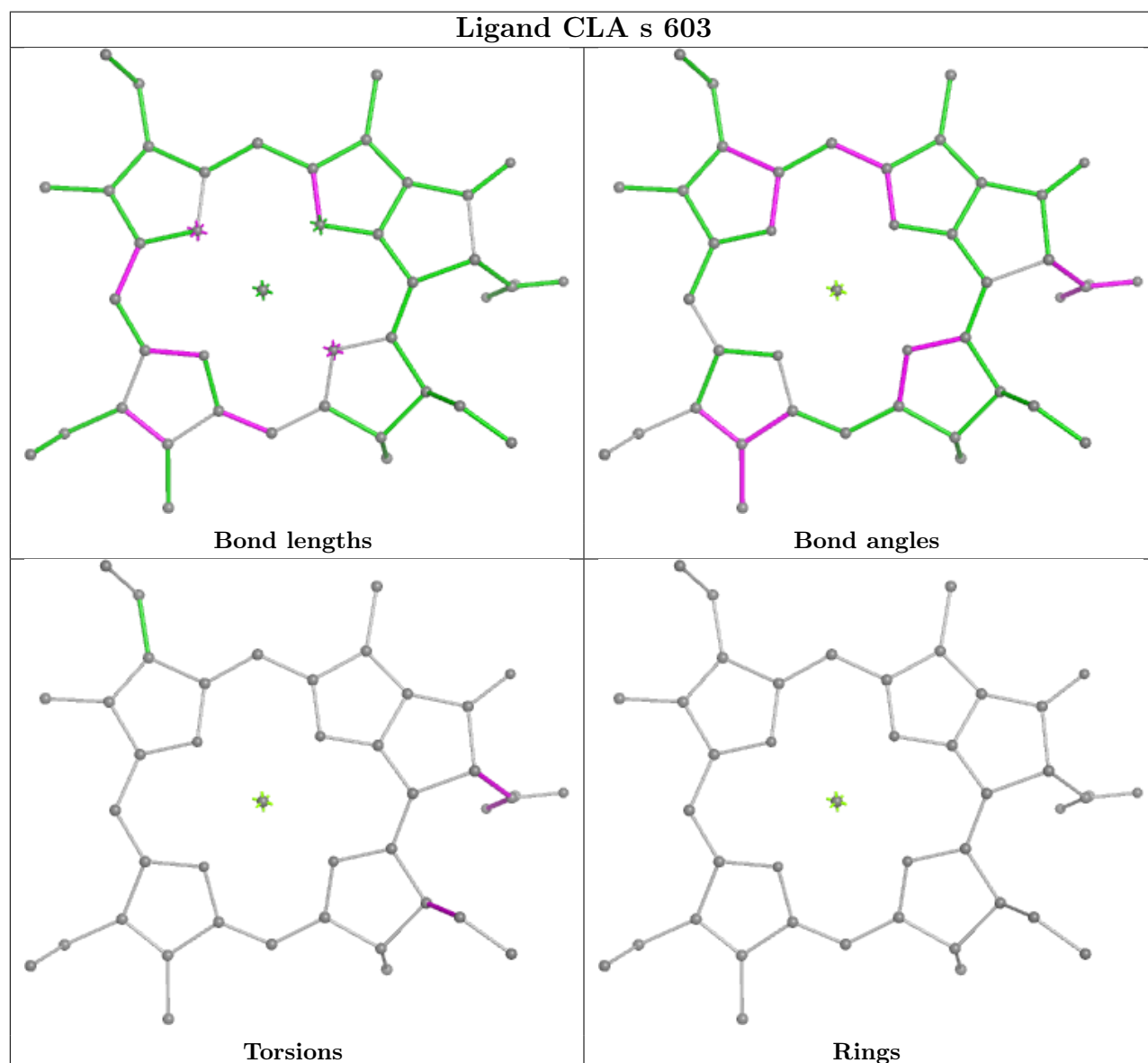
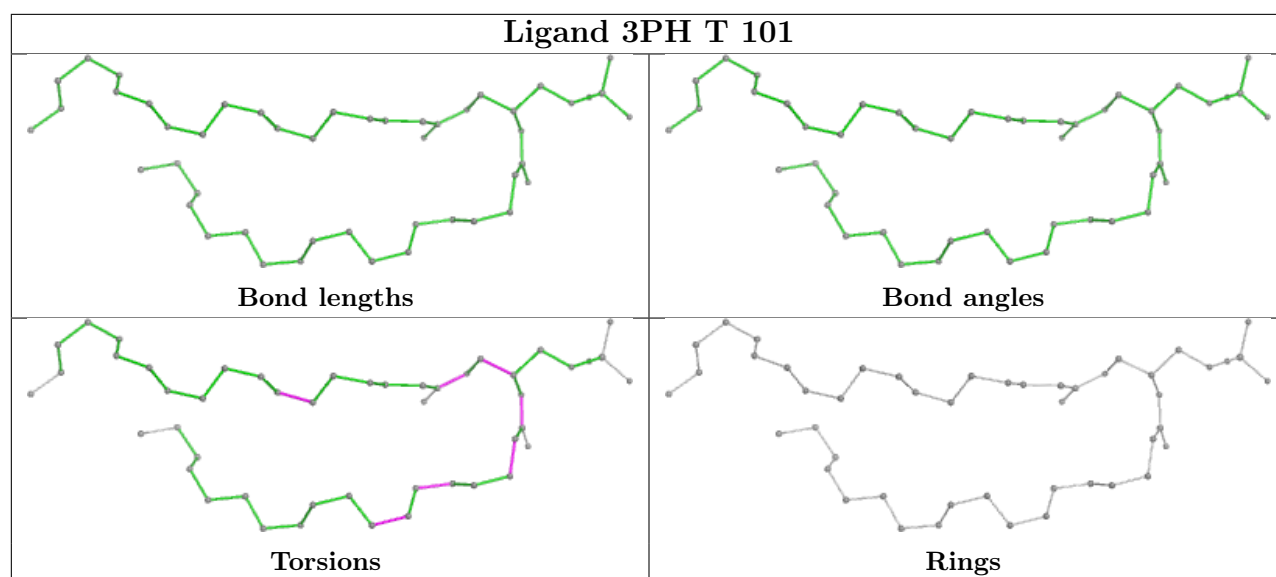




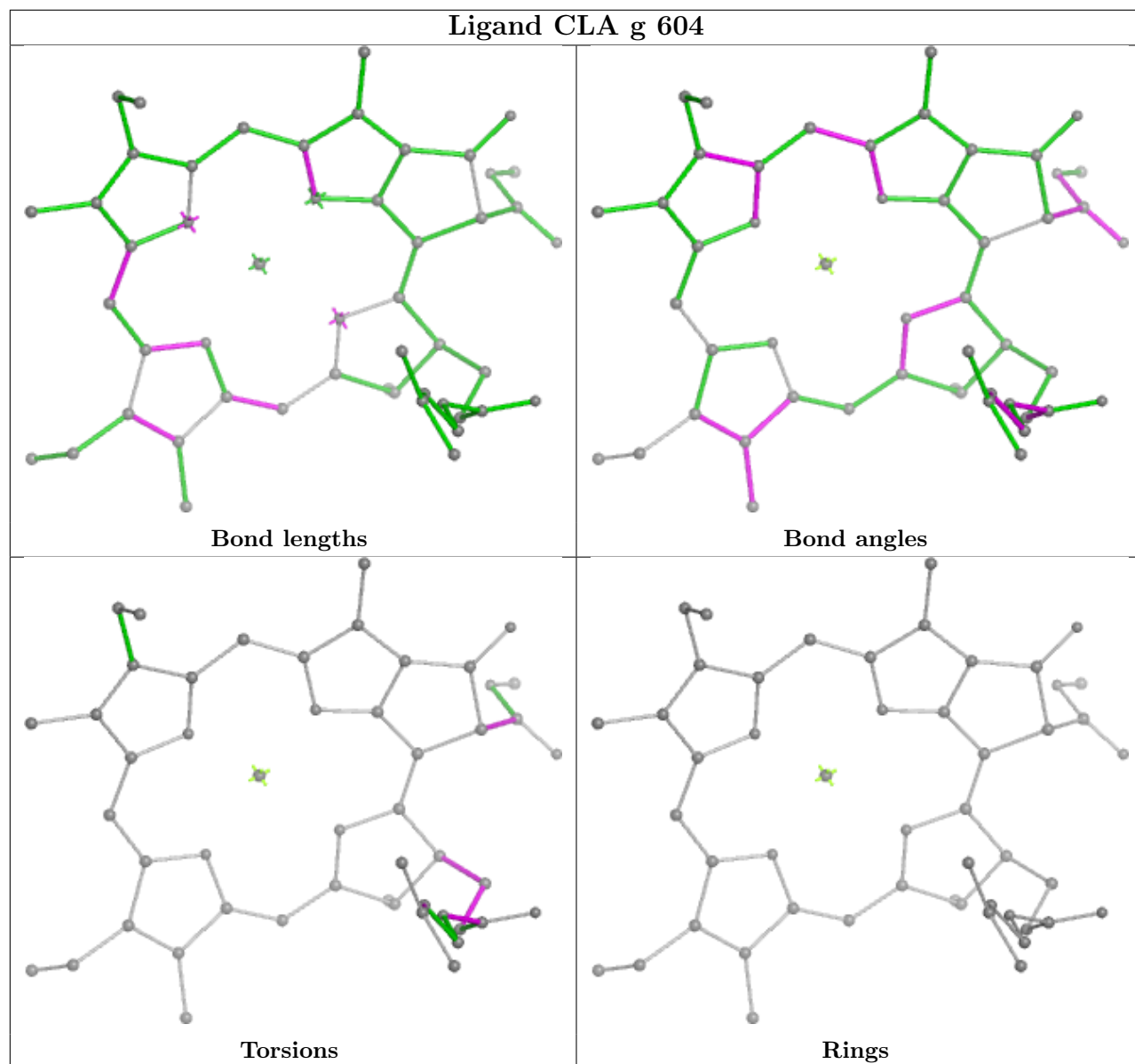


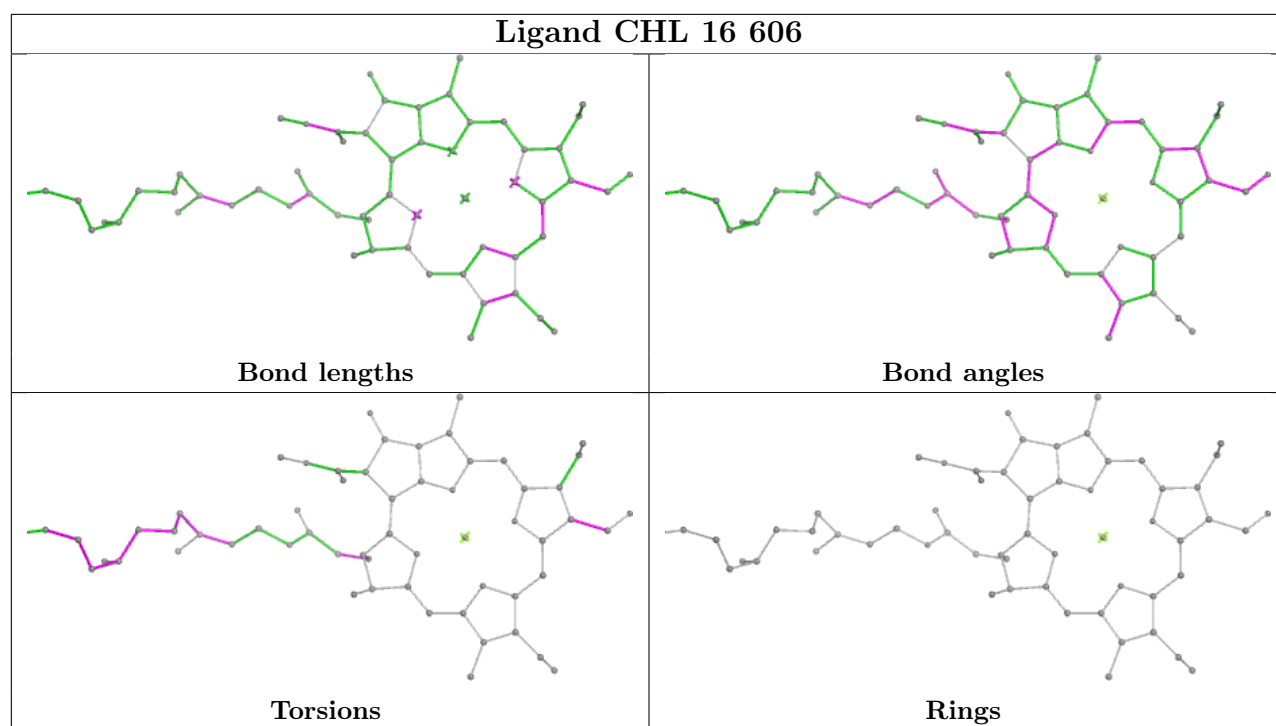




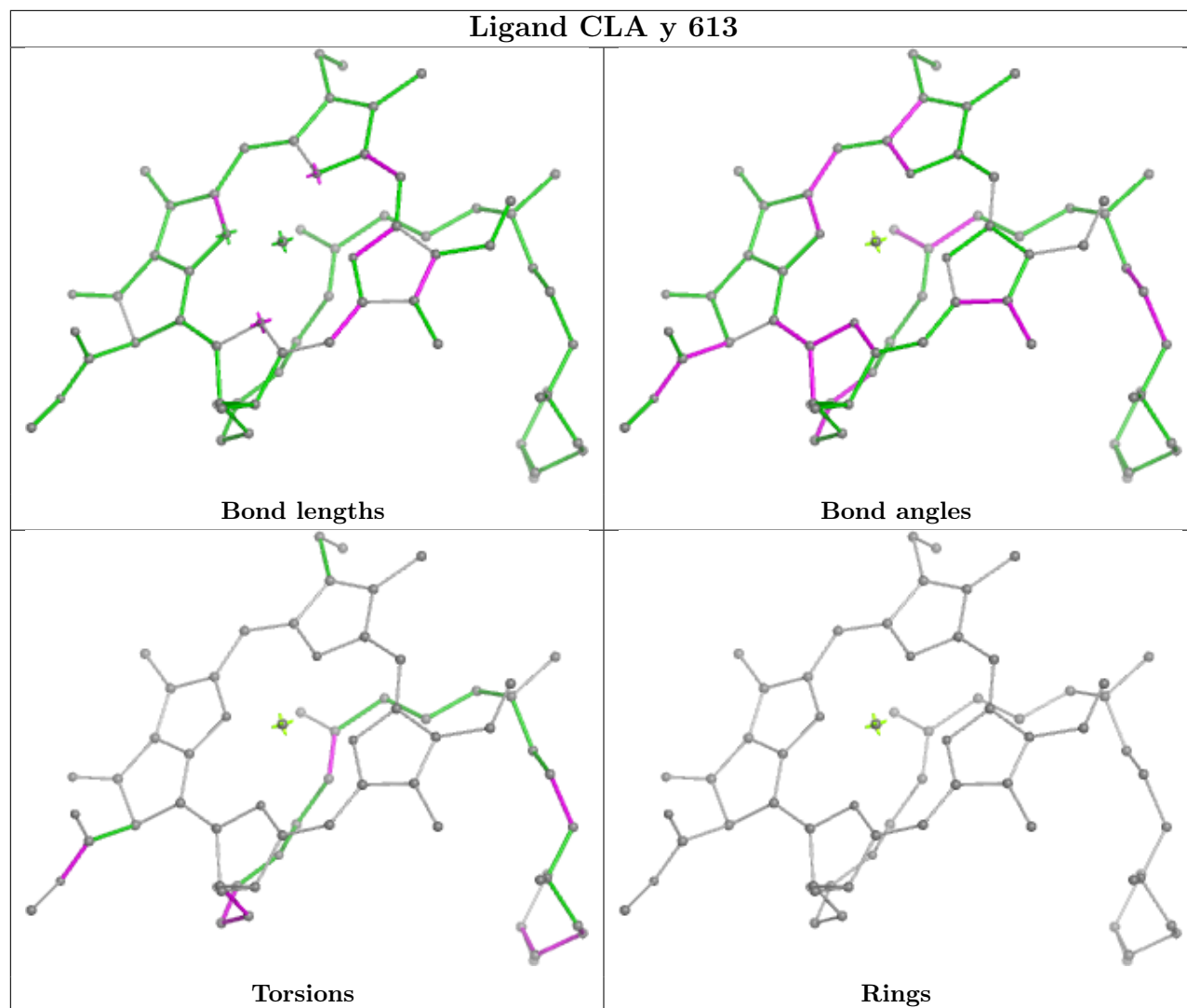


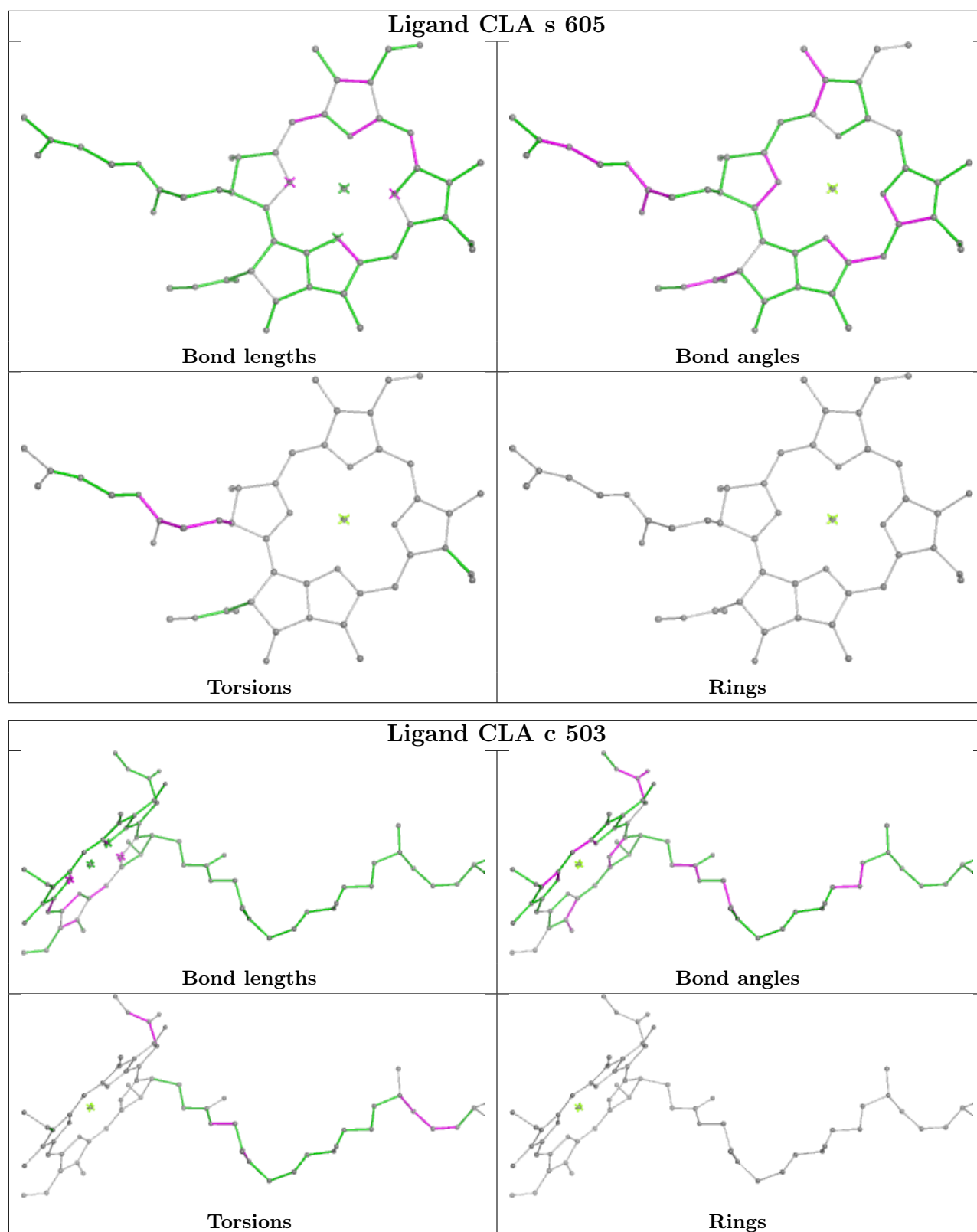
Ligand CLA g 604



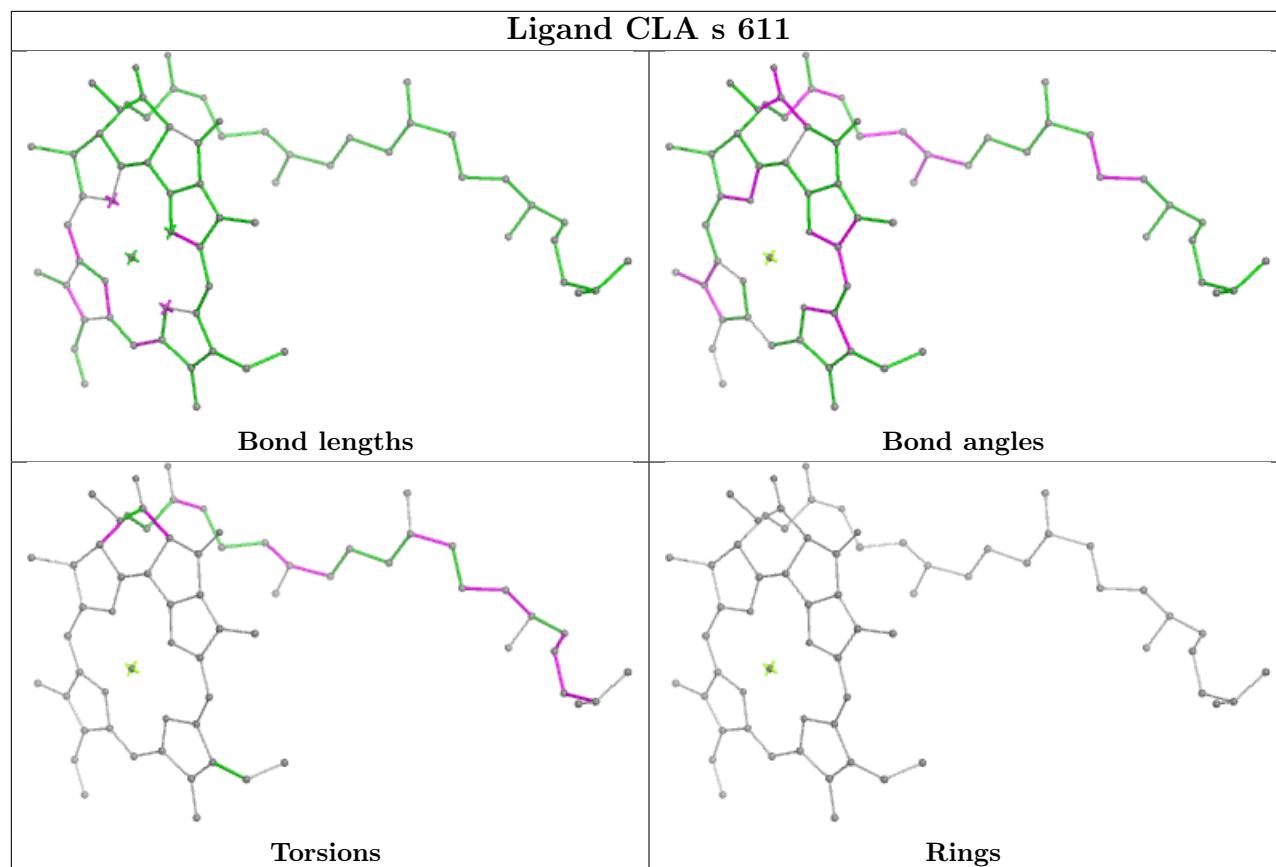


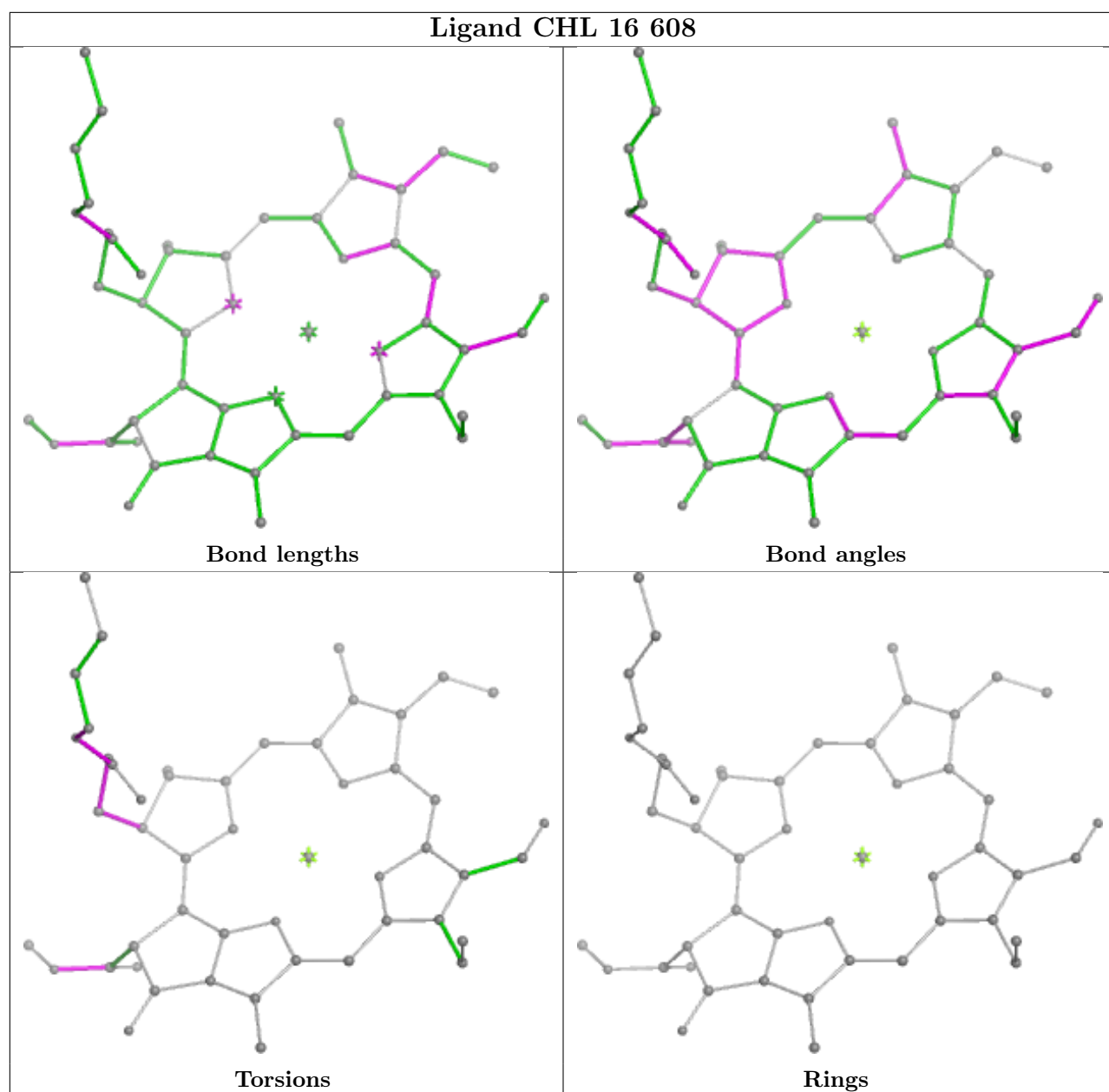
Ligand CLA y 613

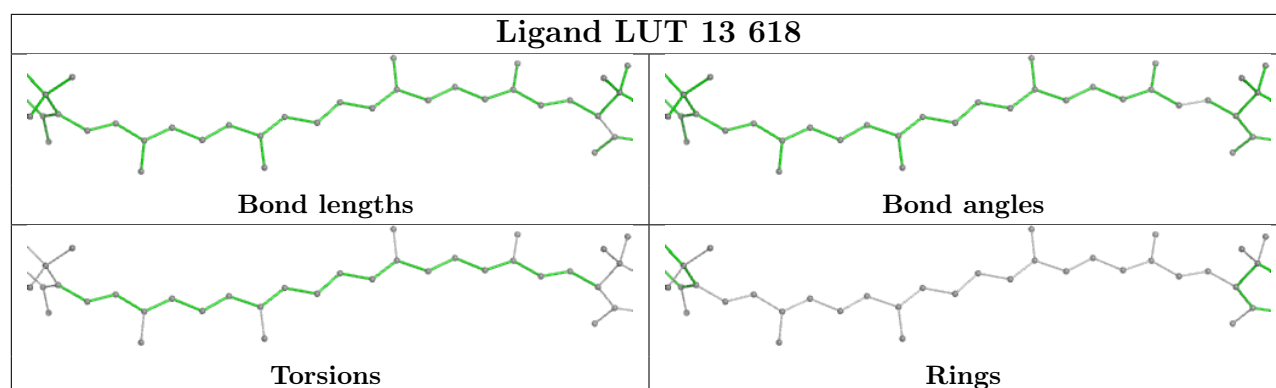
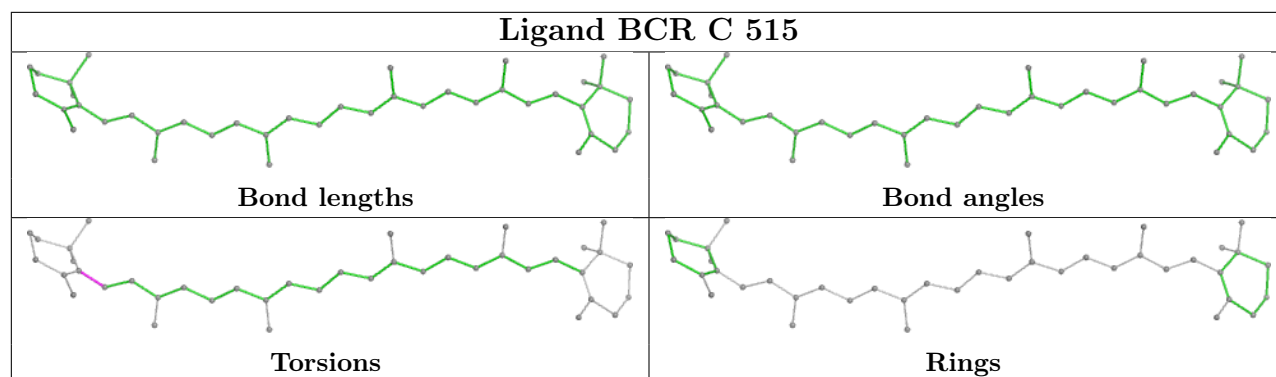
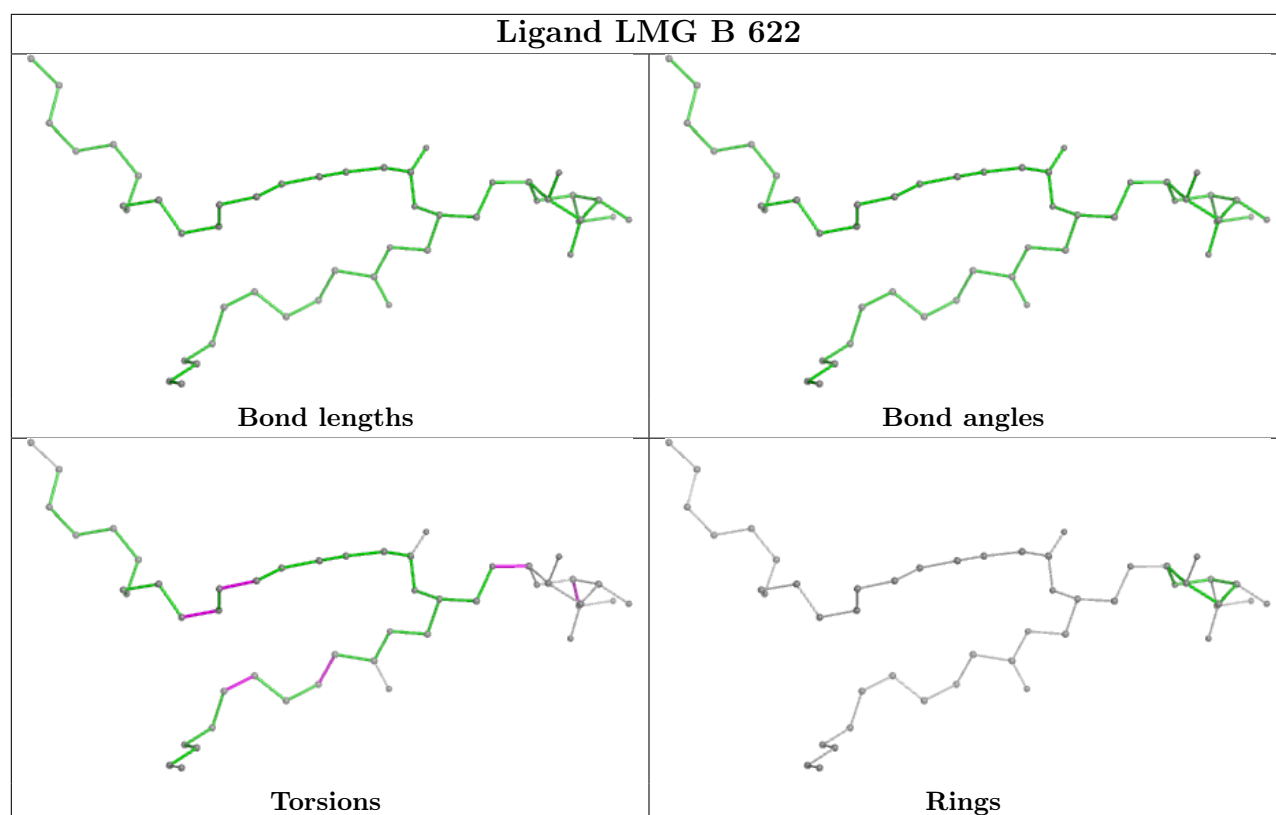


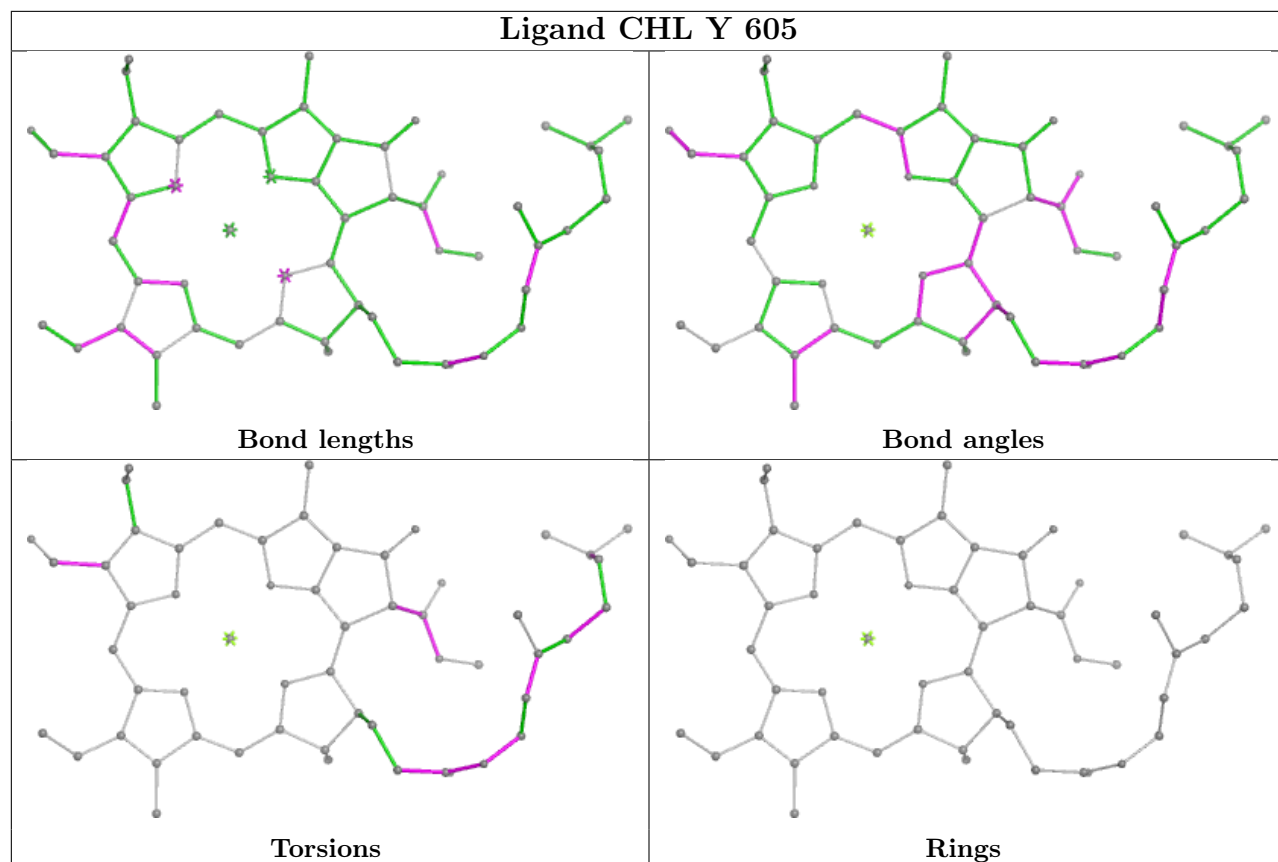


Ligand CLA s 611

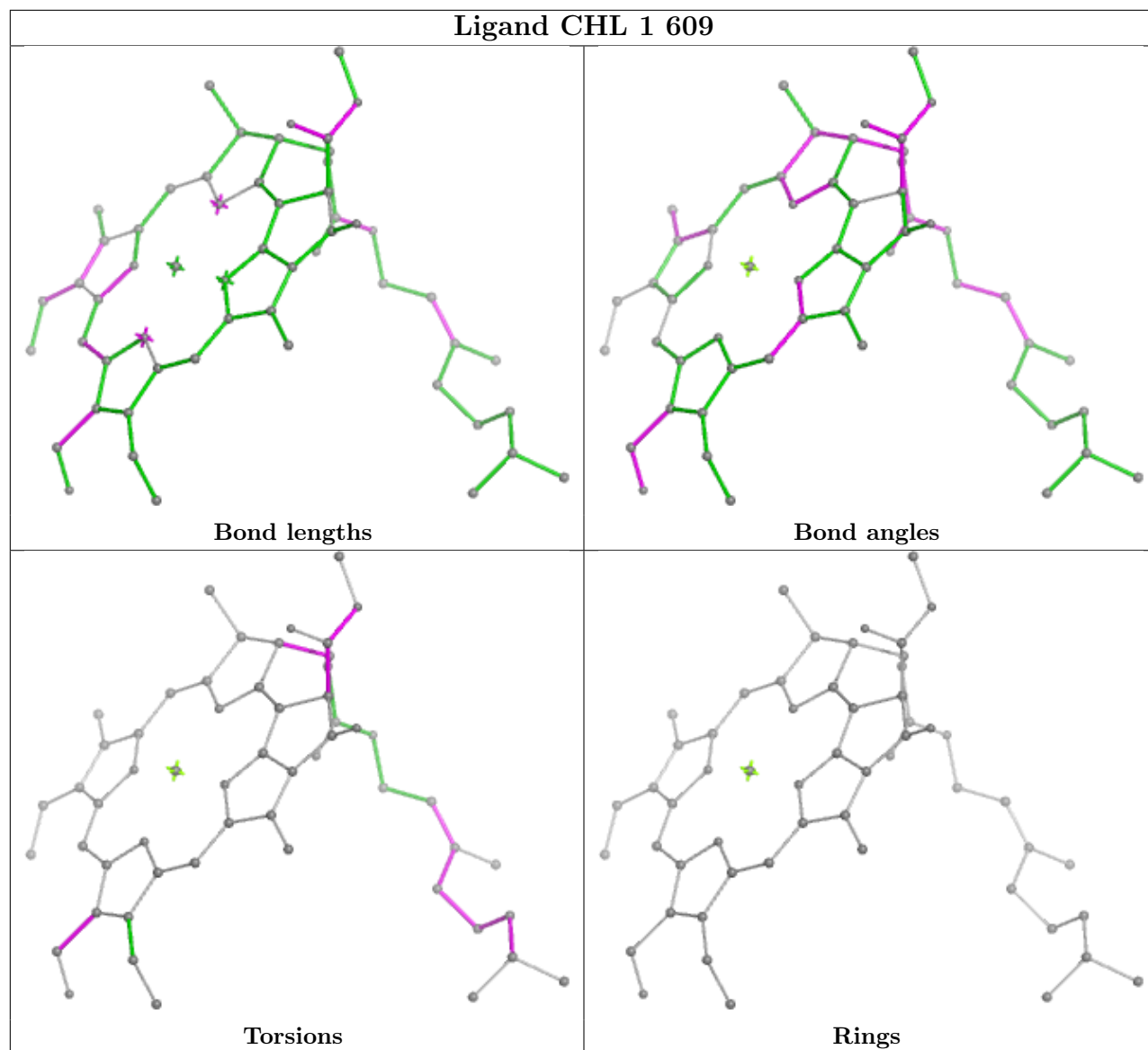


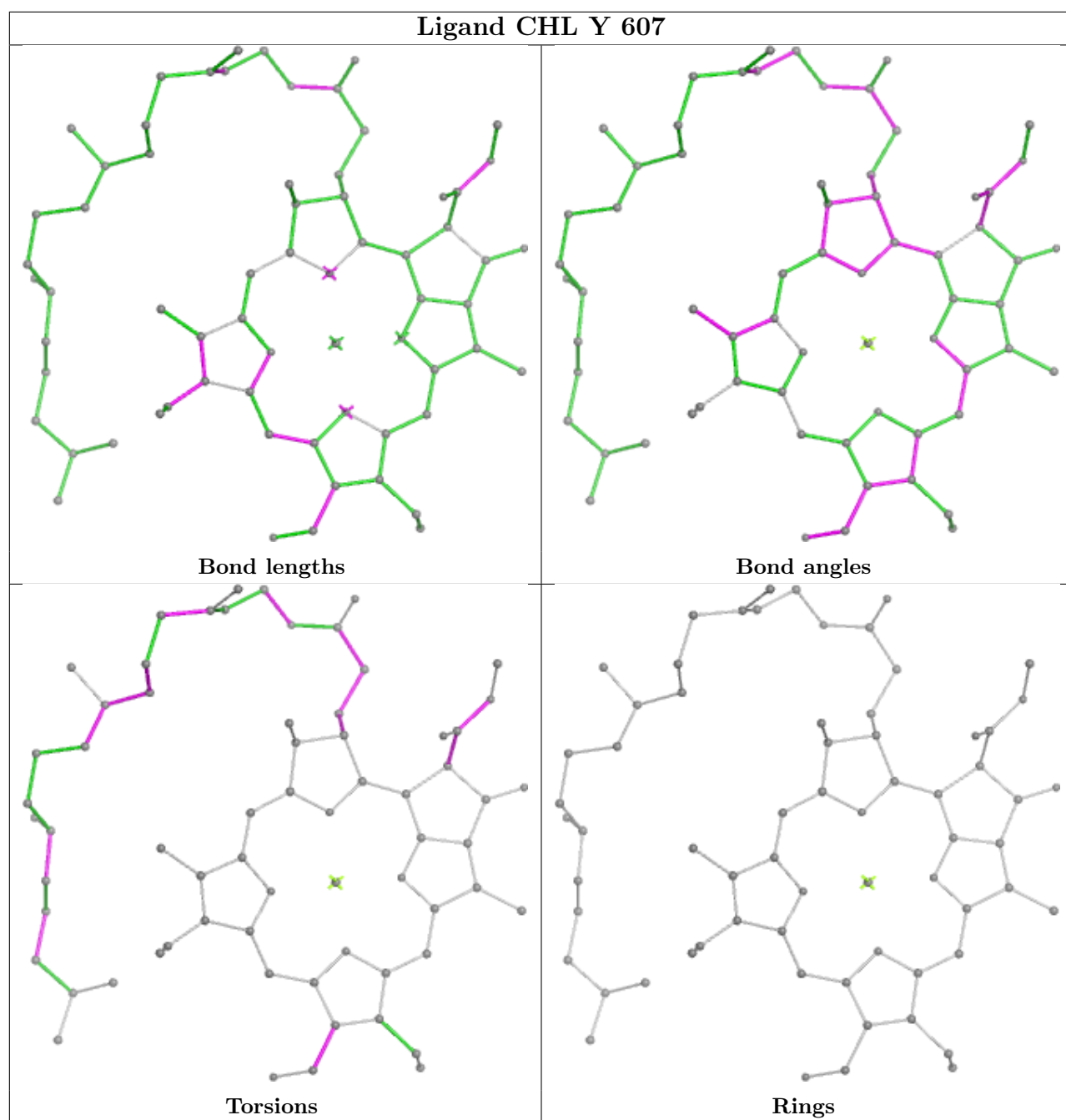




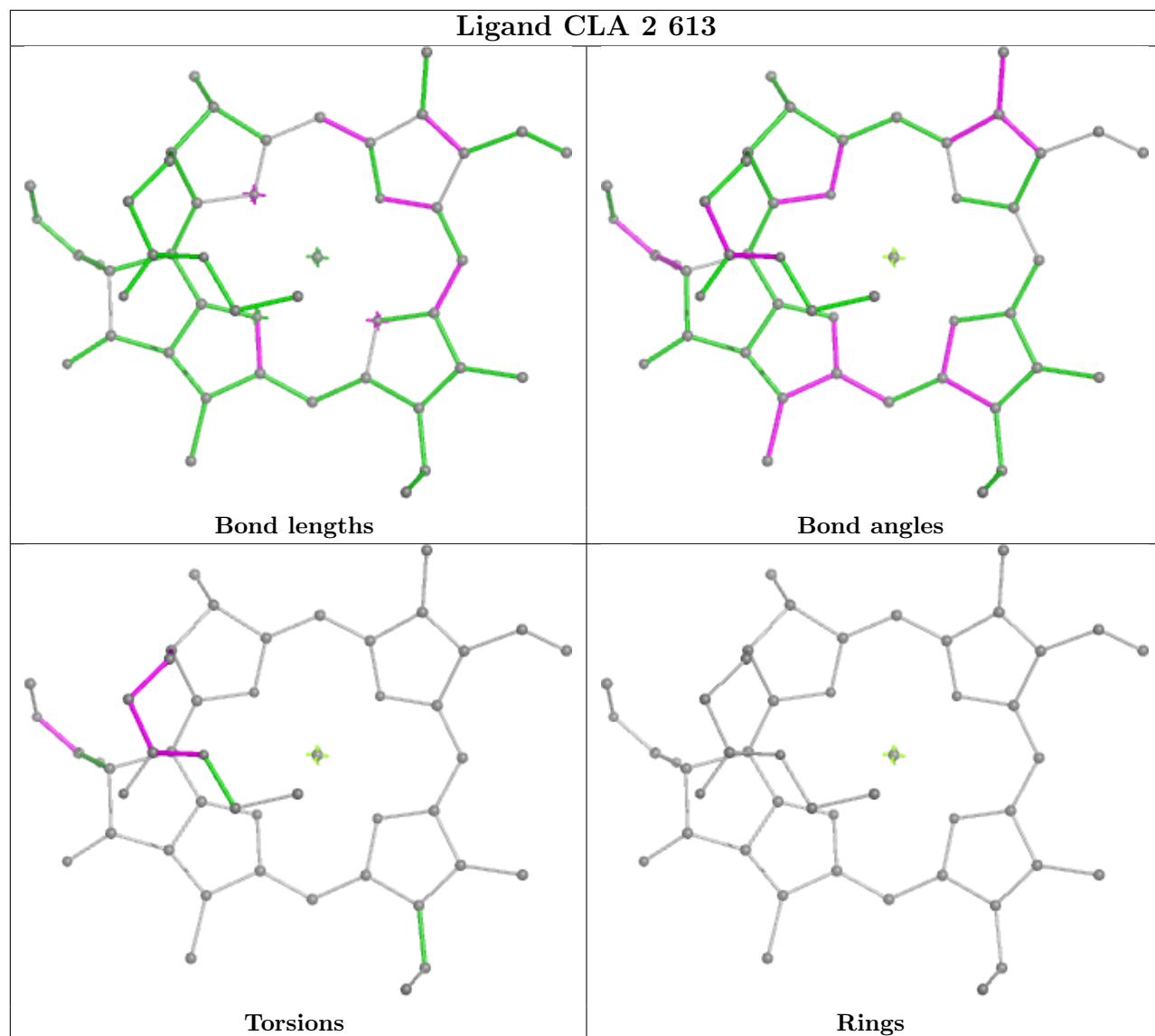


Ligand CHL 1 609

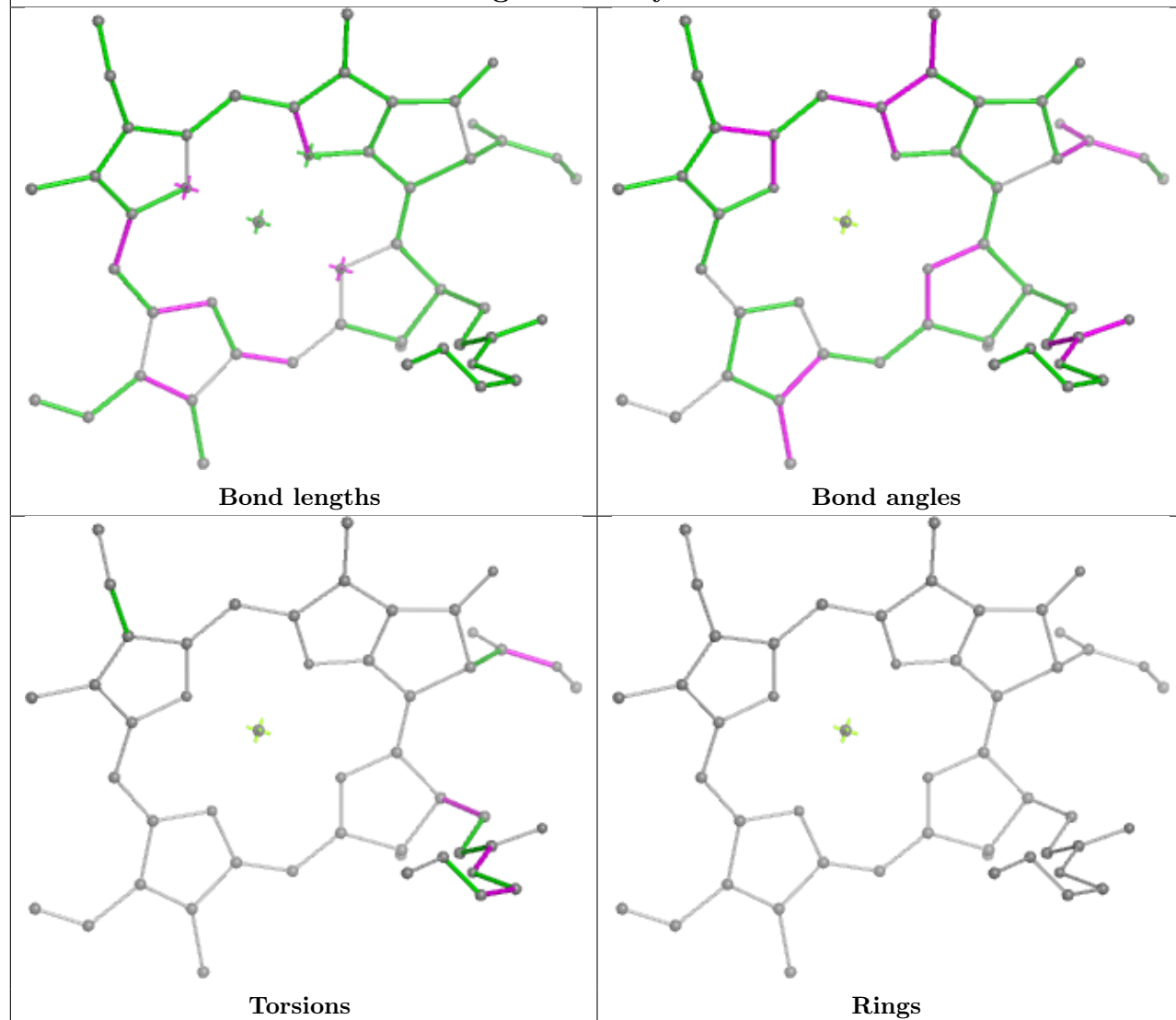




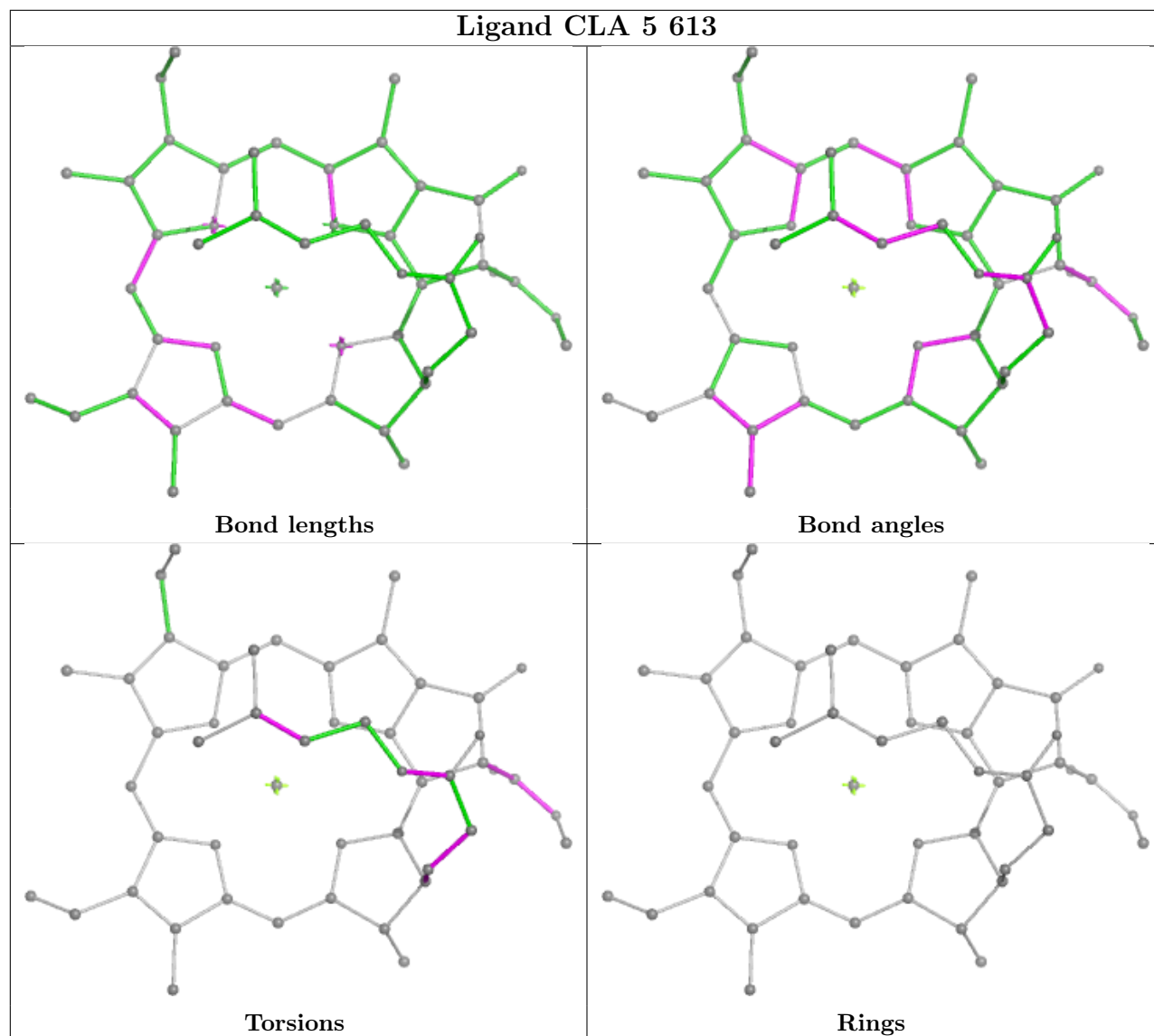
Ligand CLA 2 613

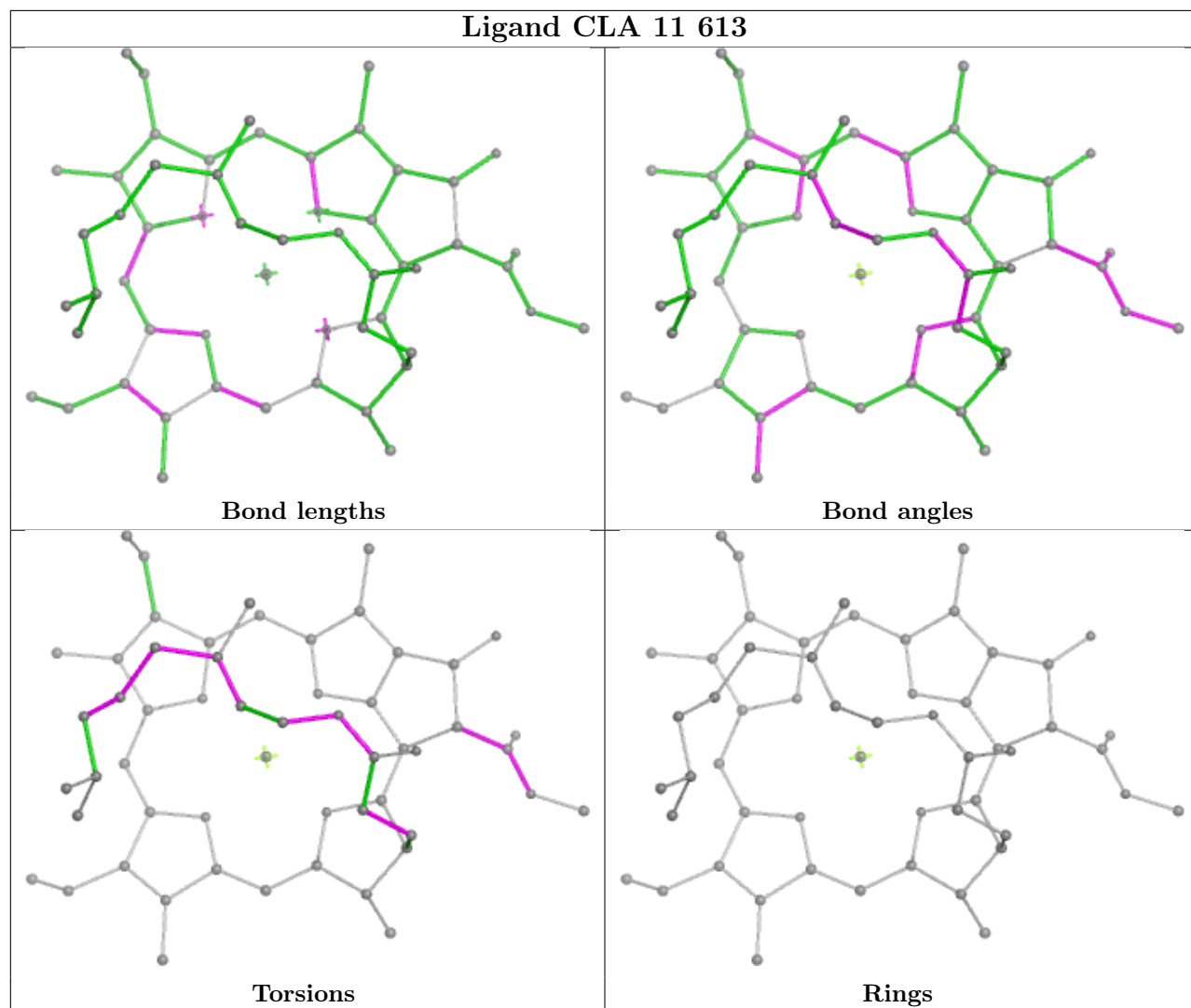


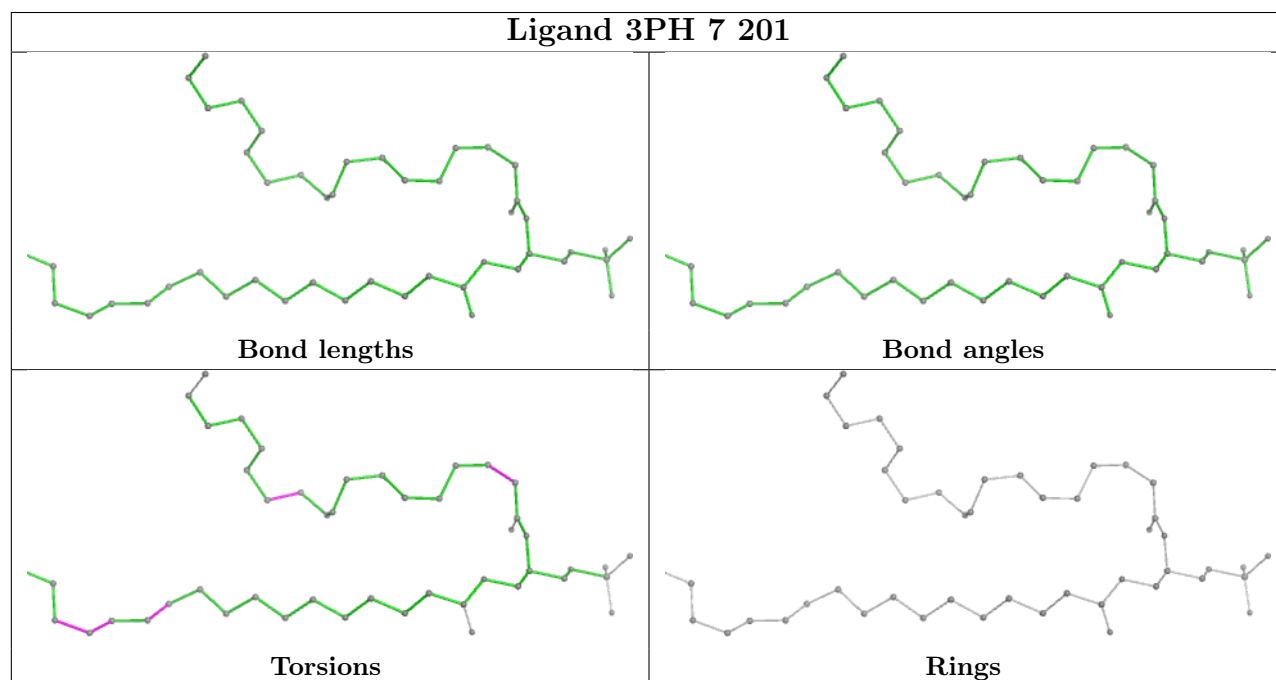
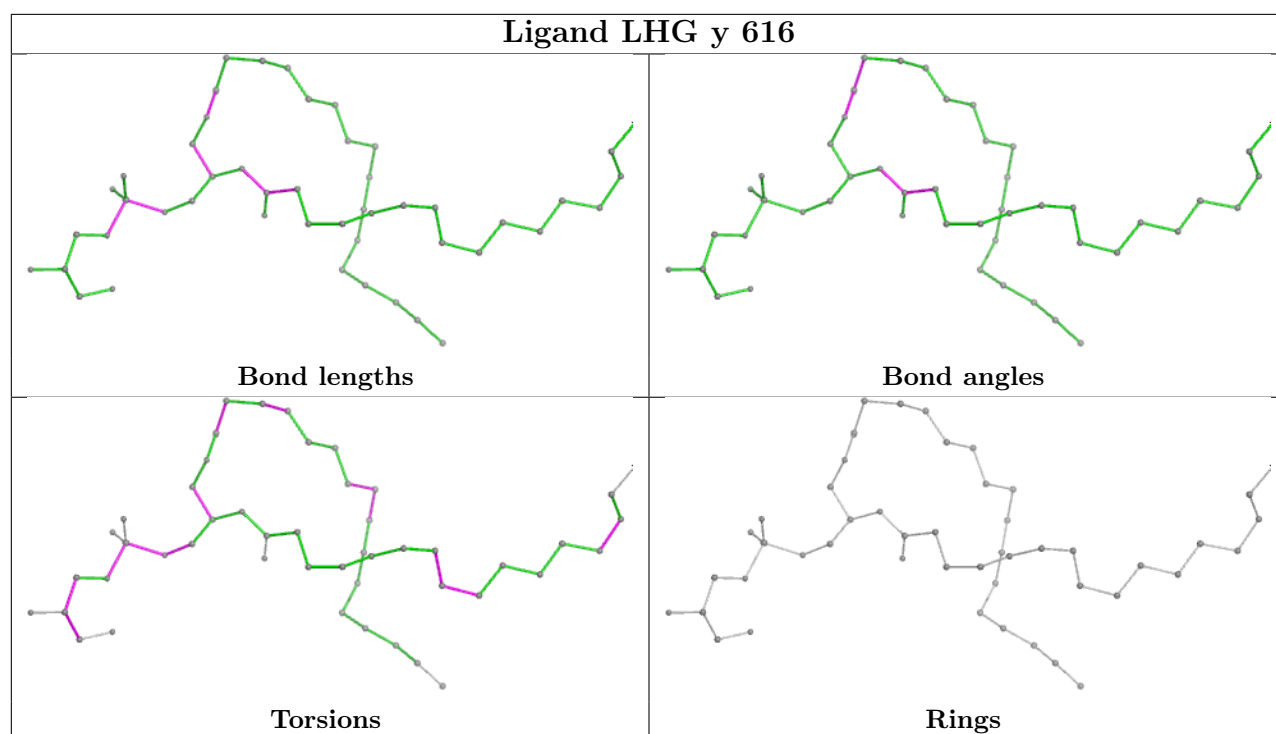
Ligand CLA y 614



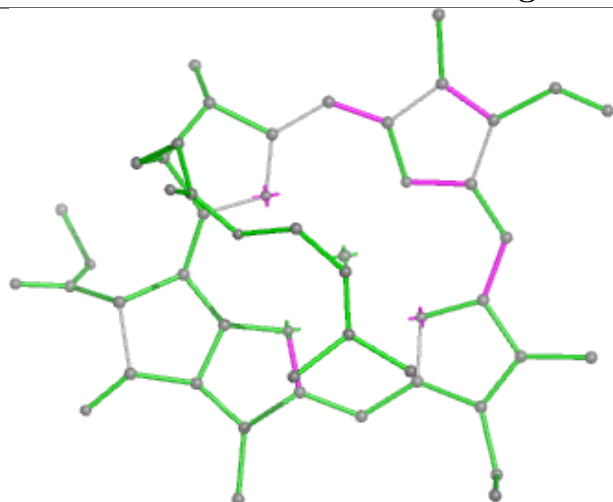
Ligand CLA 5 613



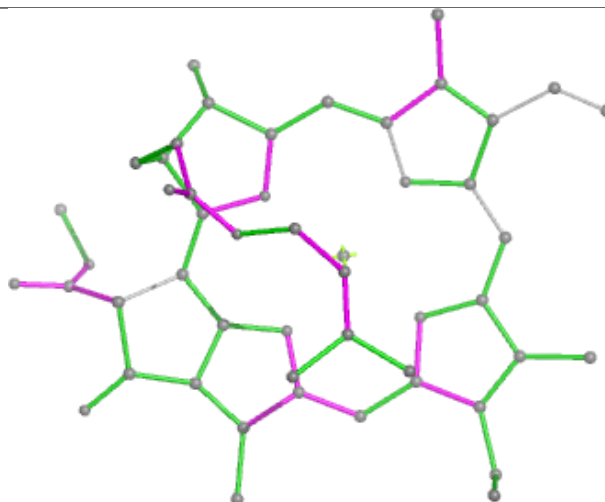




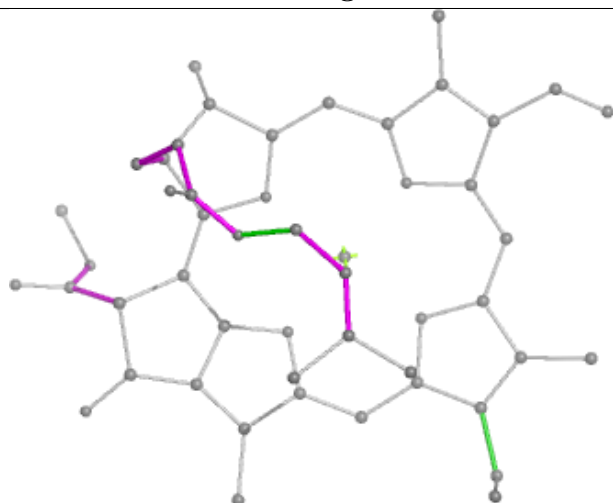
Ligand CLA 6 614



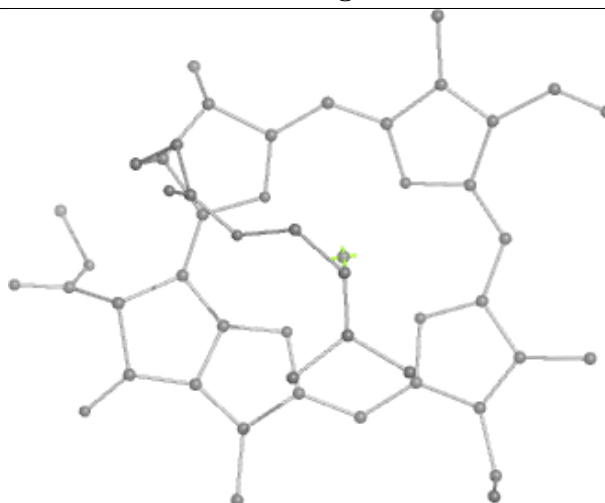
Bond lengths



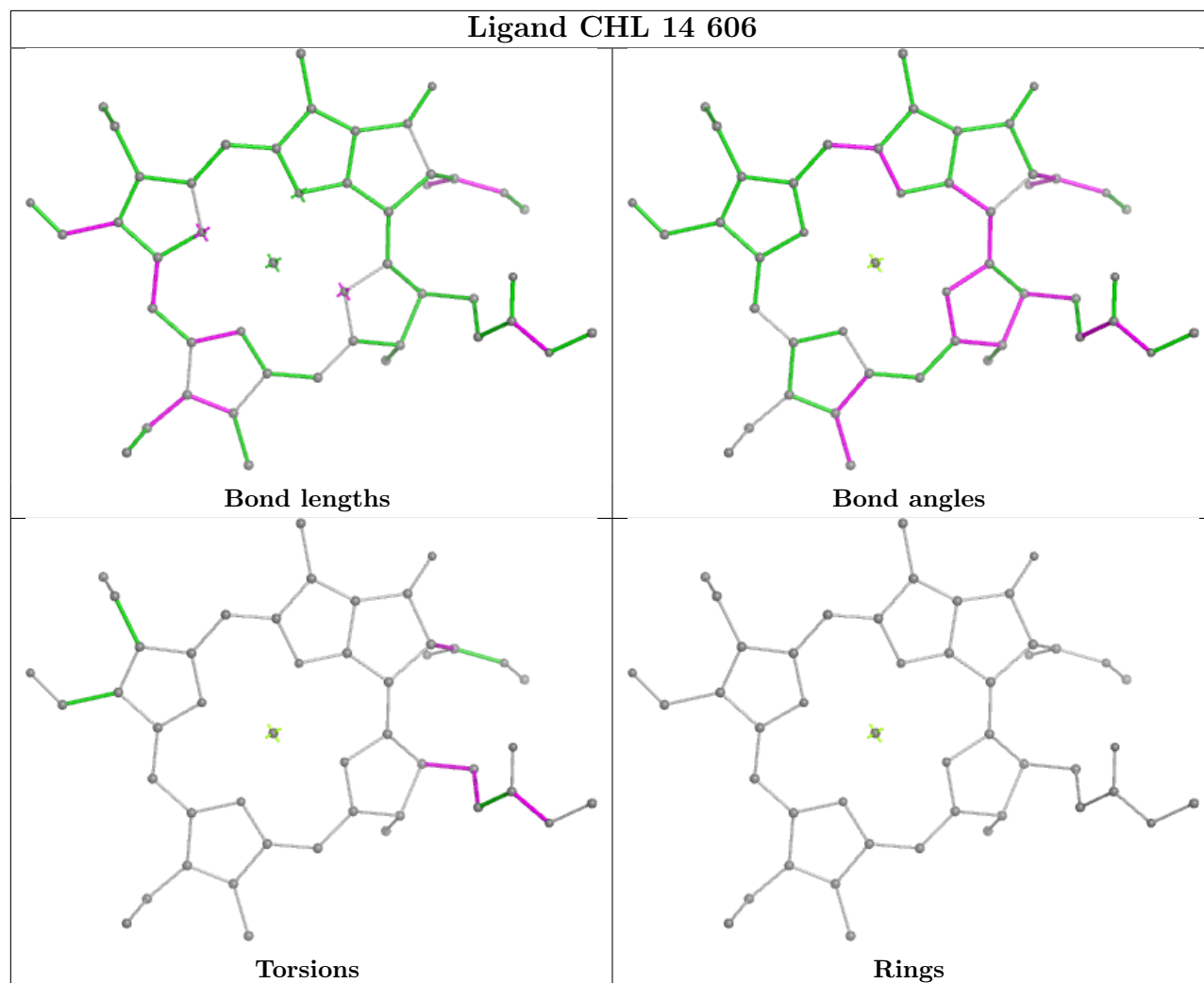
Bond angles

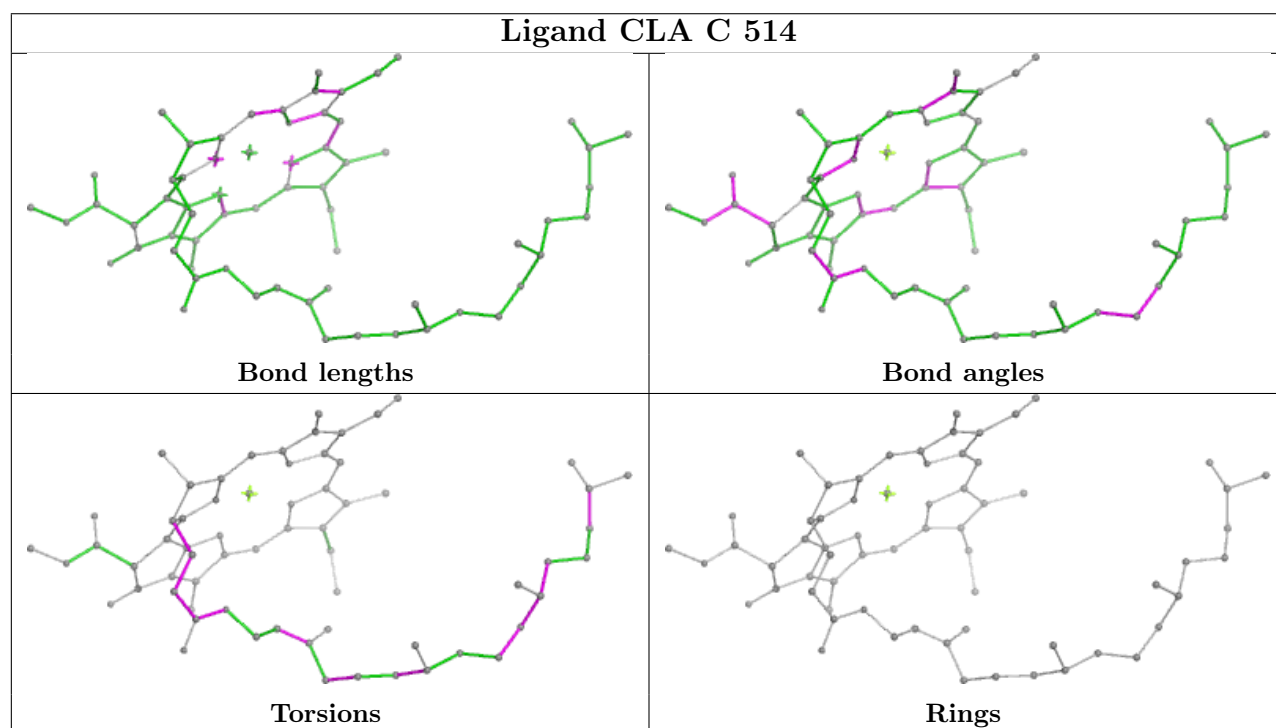
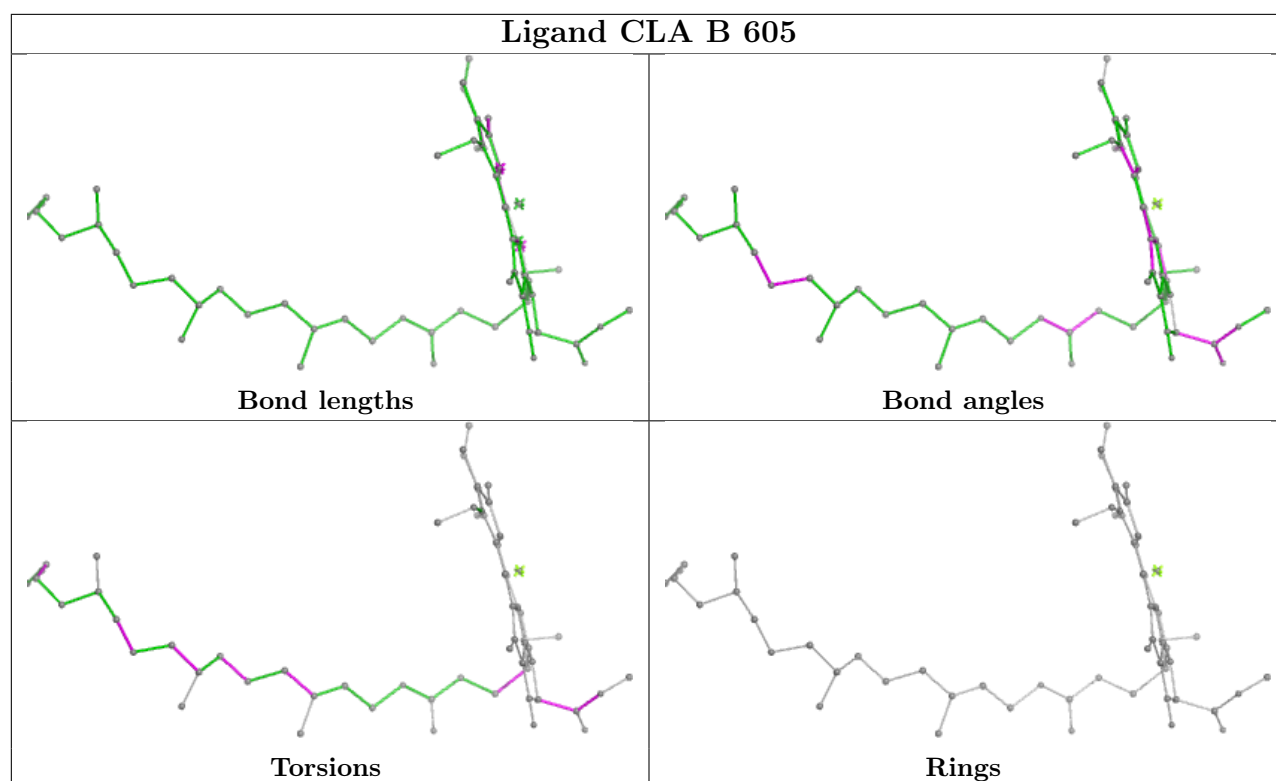


Torsions

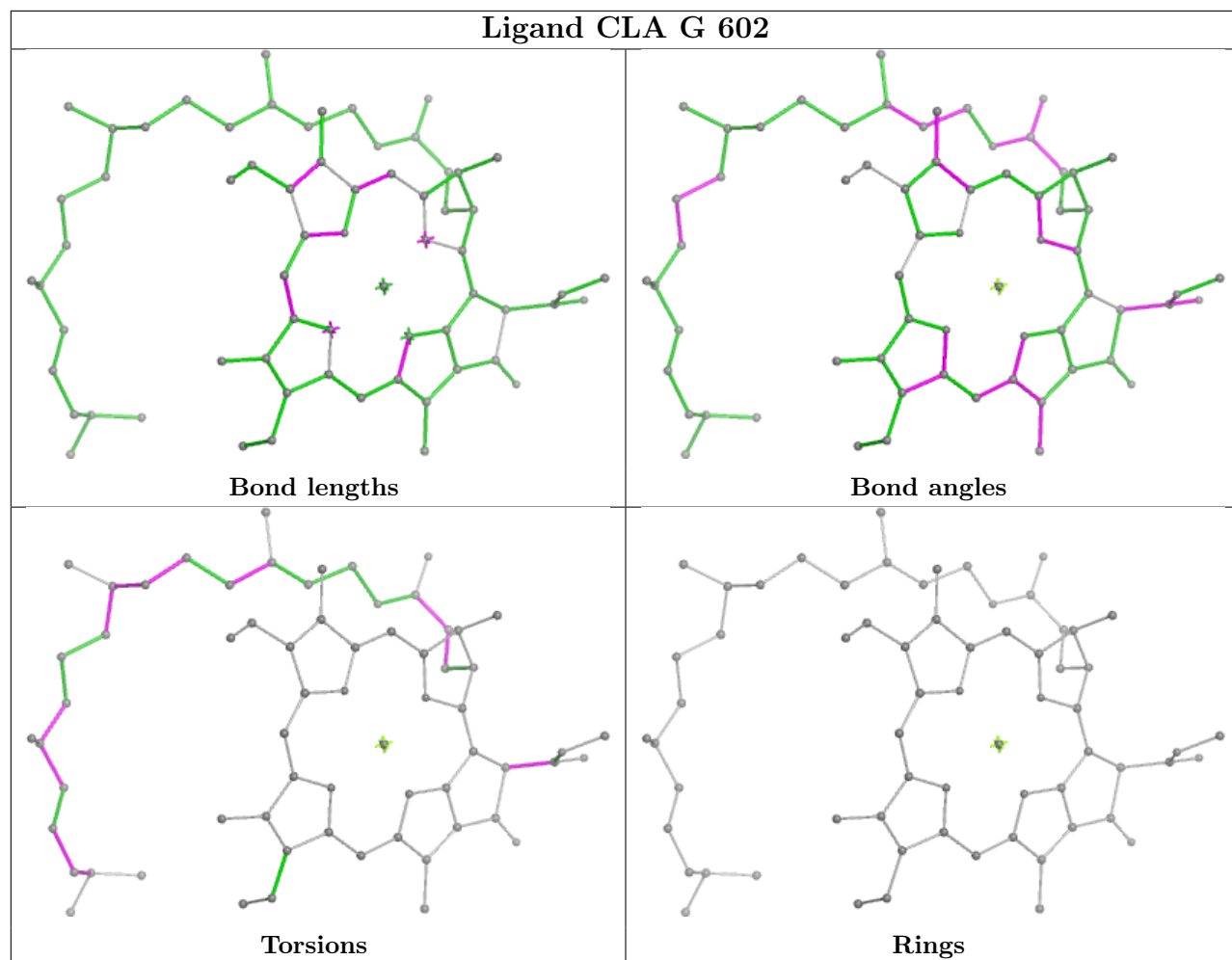


Rings

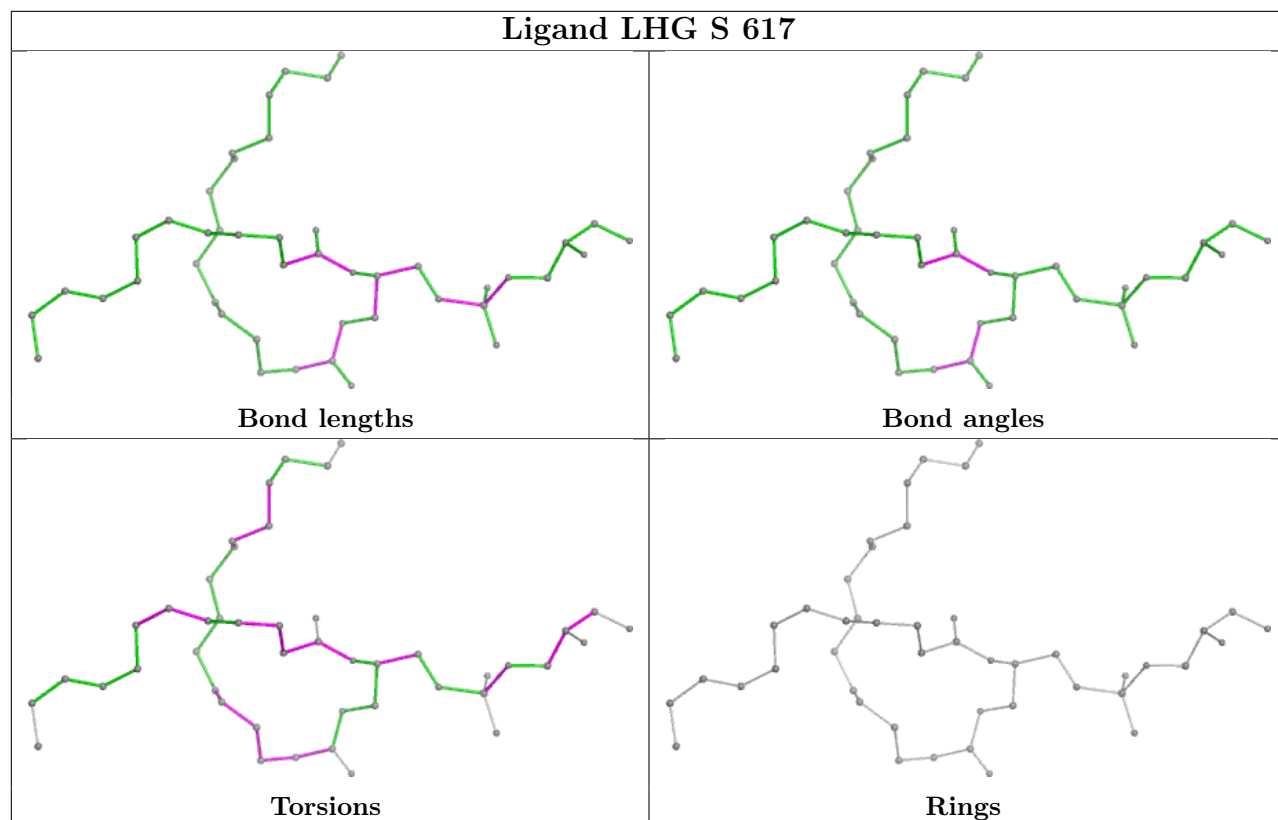




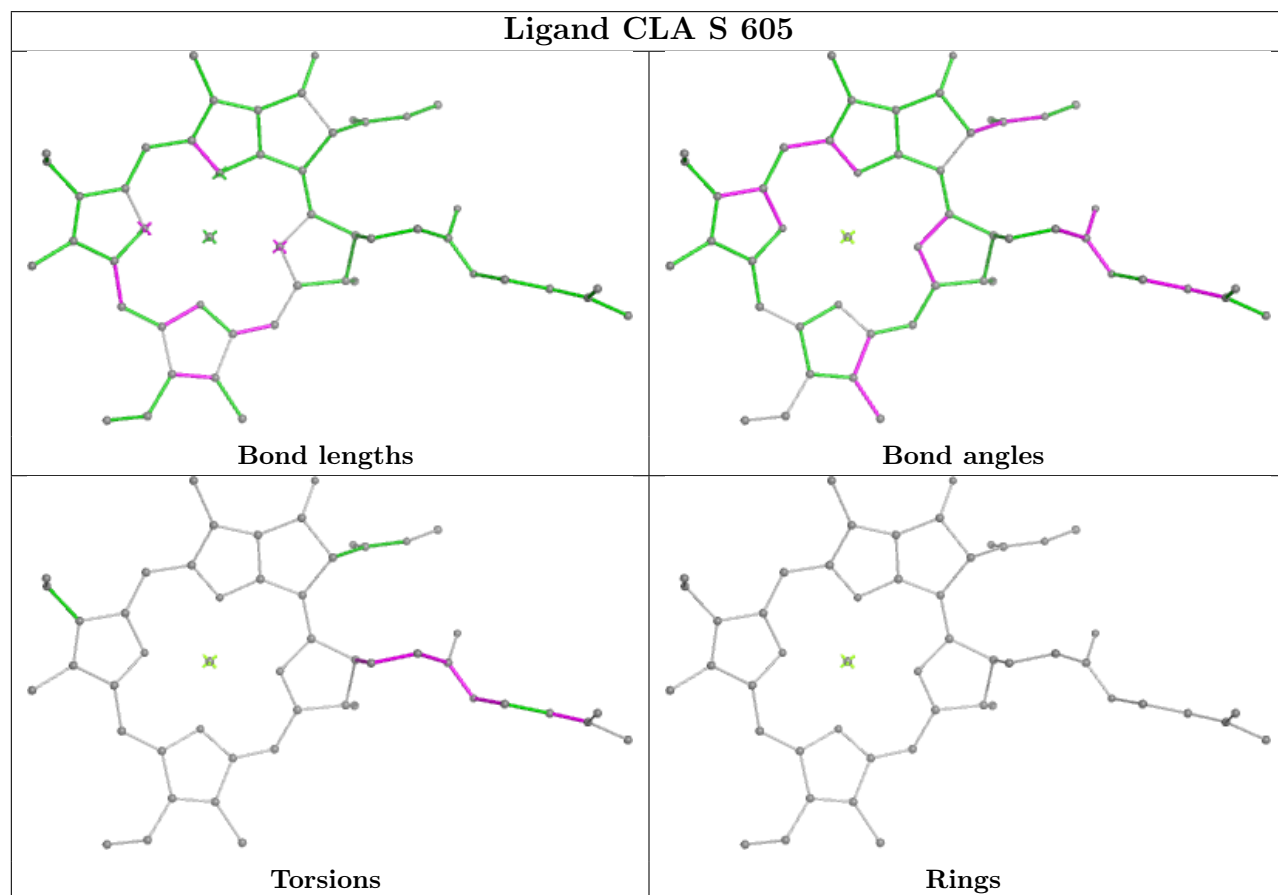
Ligand CLA G 602

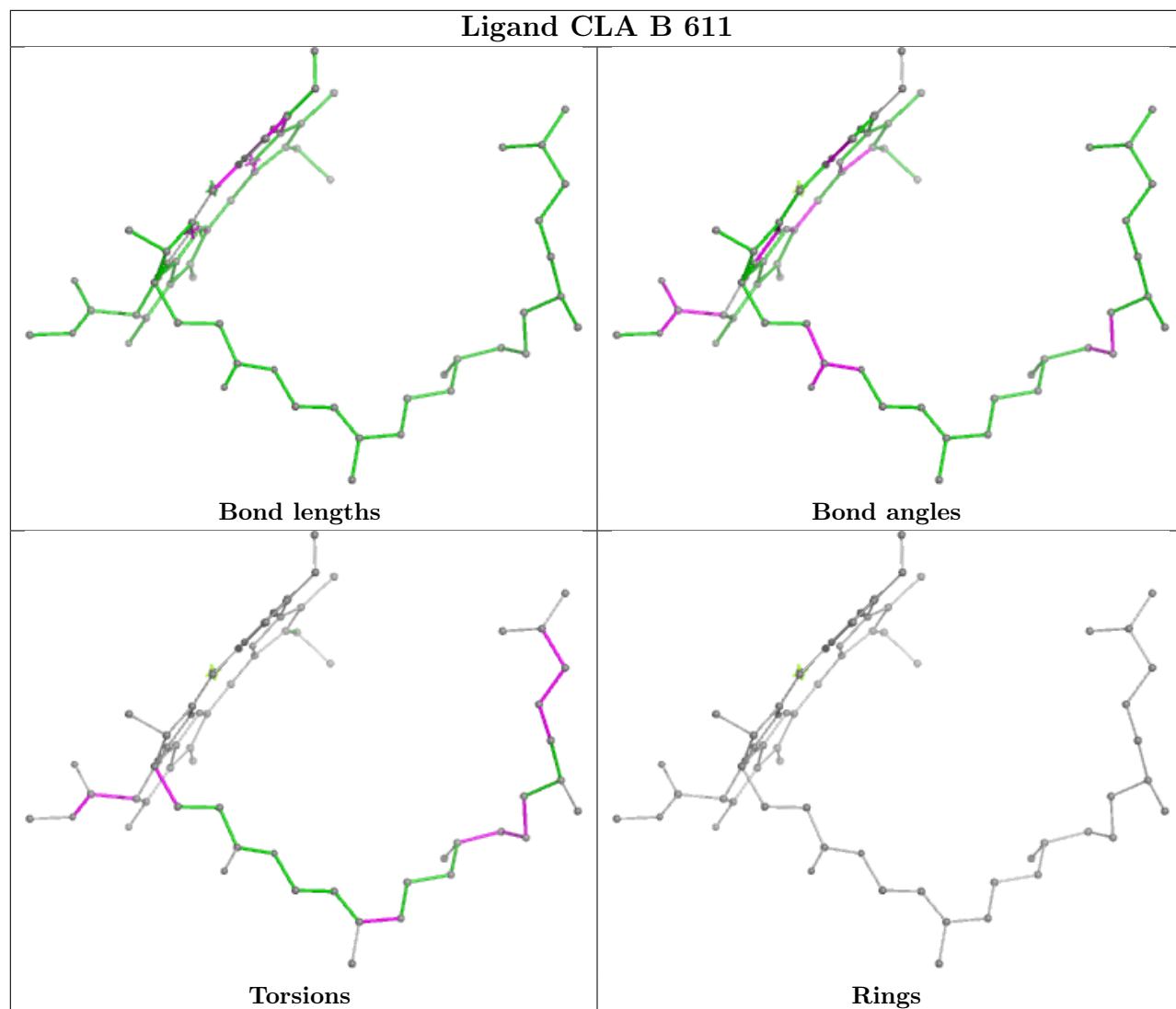


Ligand LHG S 617

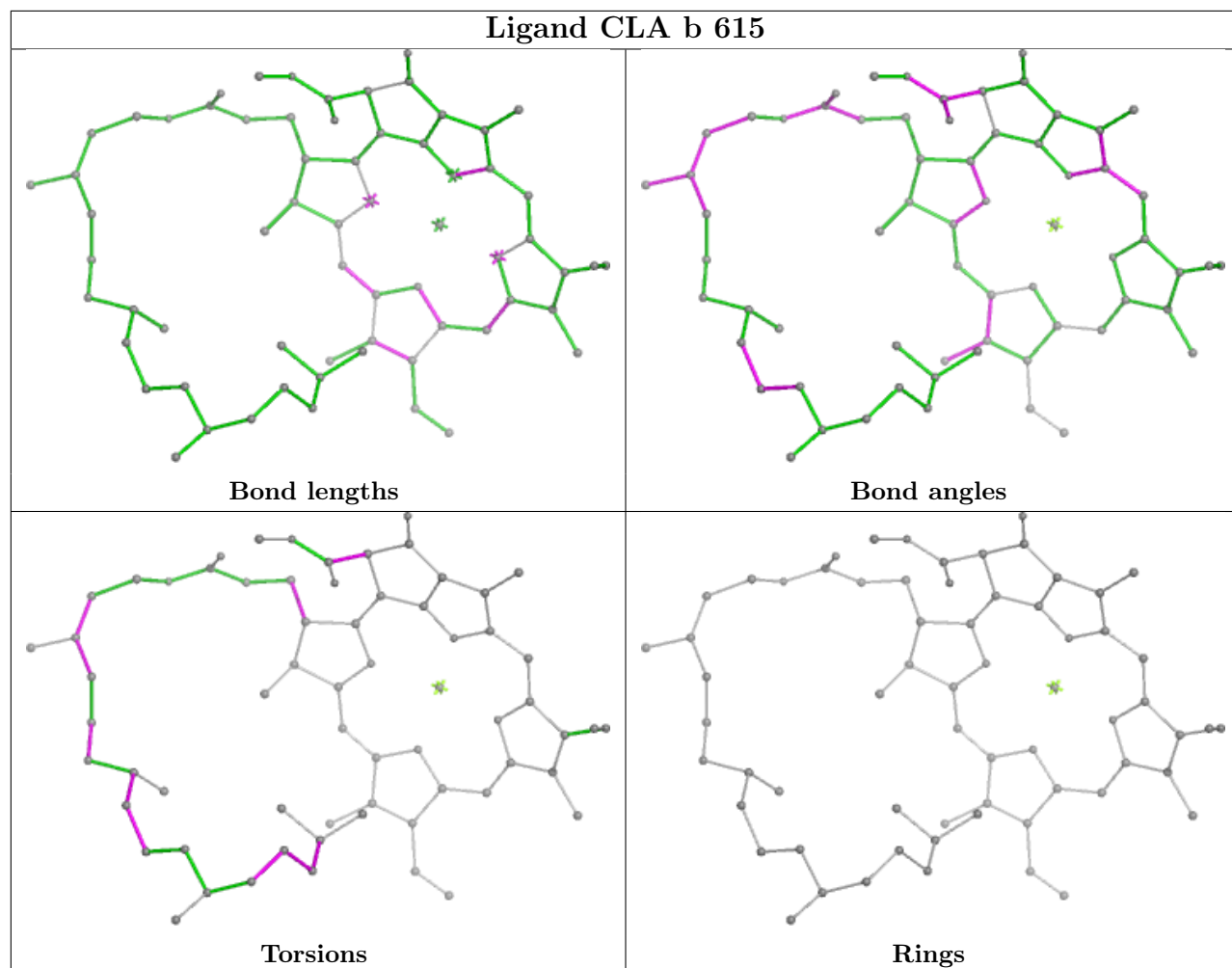


Ligand CLA S 605

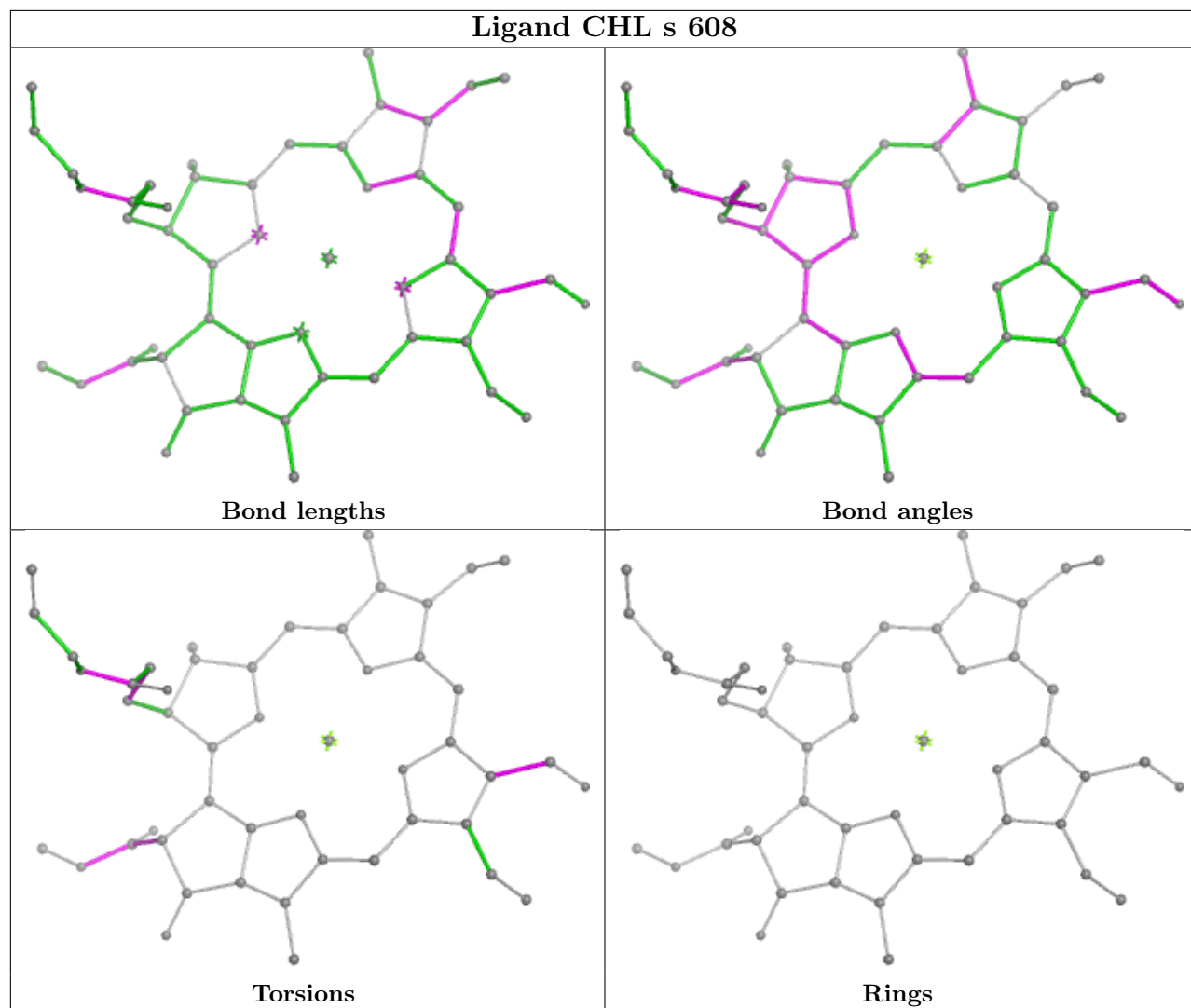




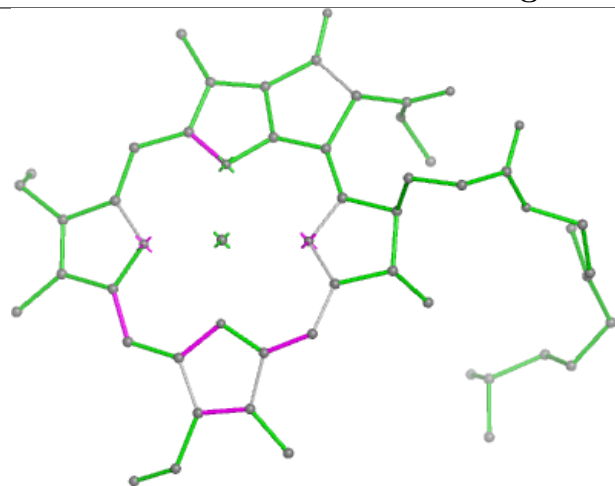
Ligand CLA b 615



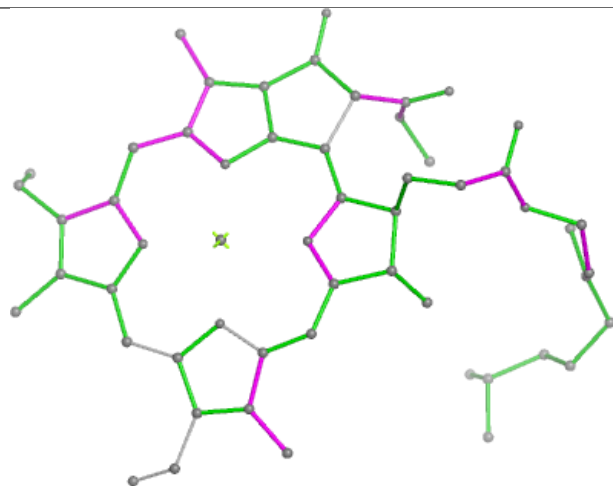
Ligand CHL s 608



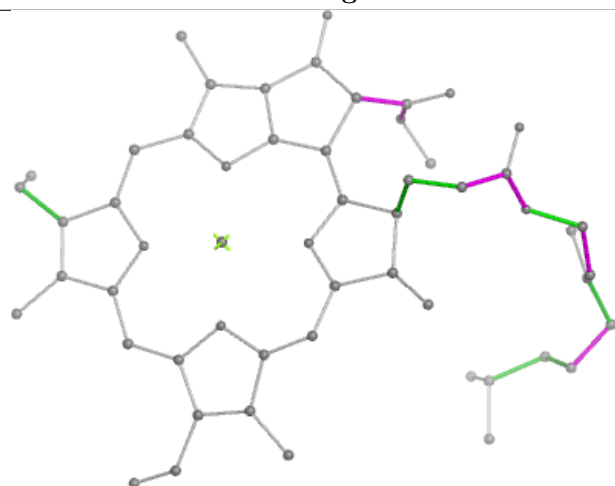
Ligand CLA 5 603



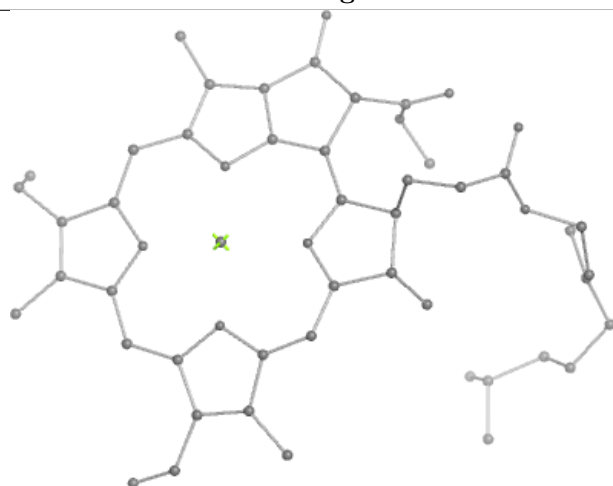
Bond lengths



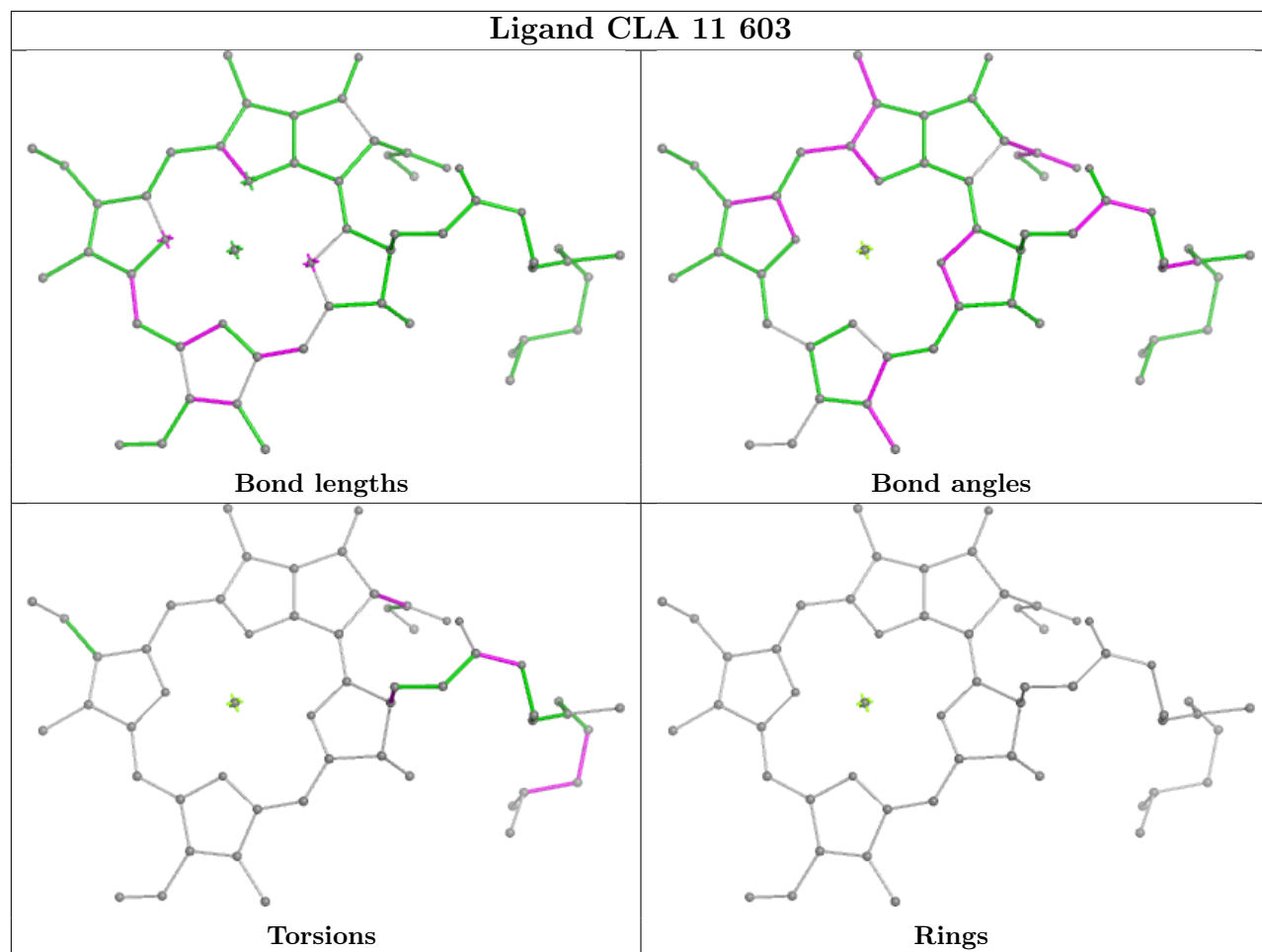
Bond angles

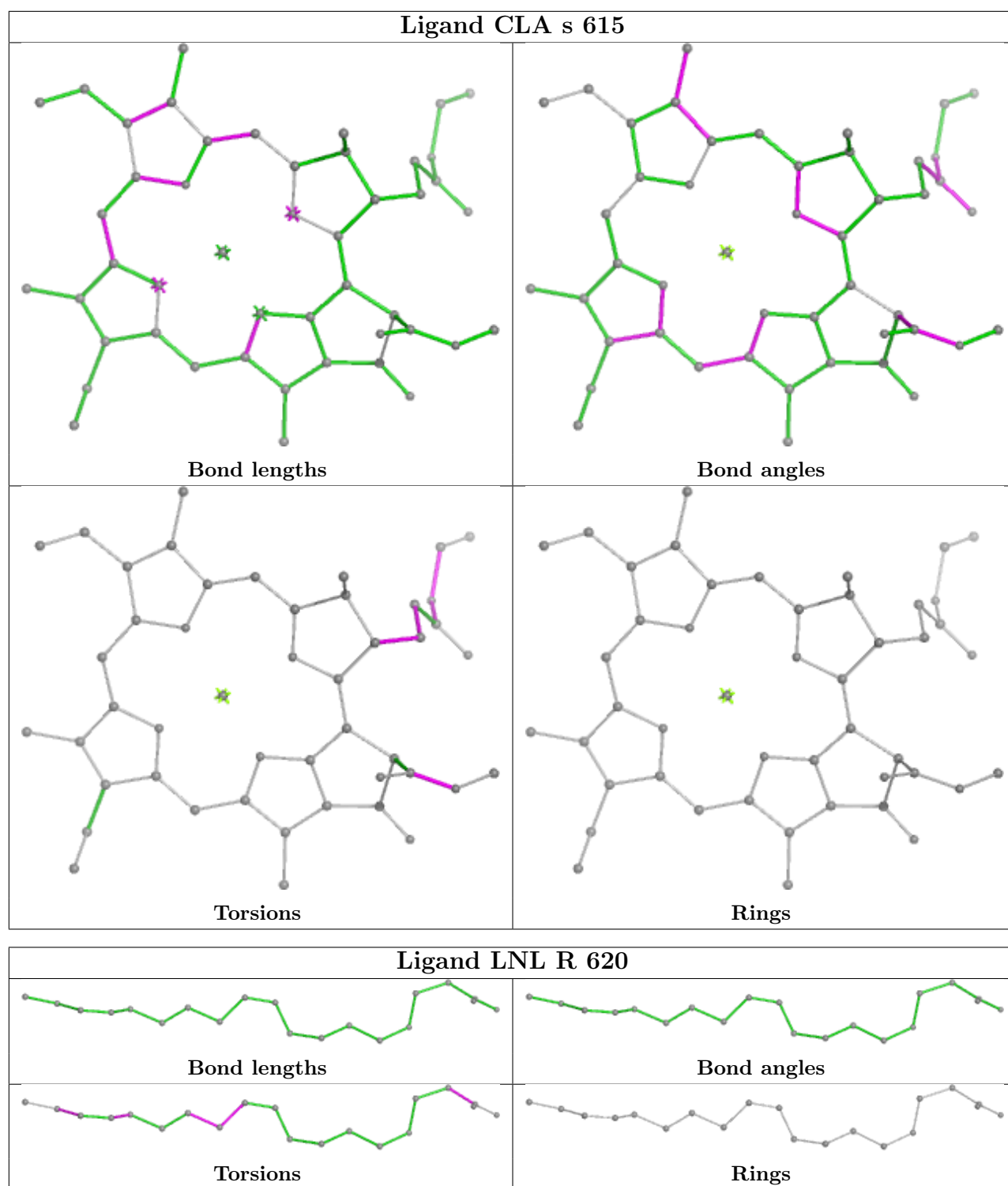


Torsions

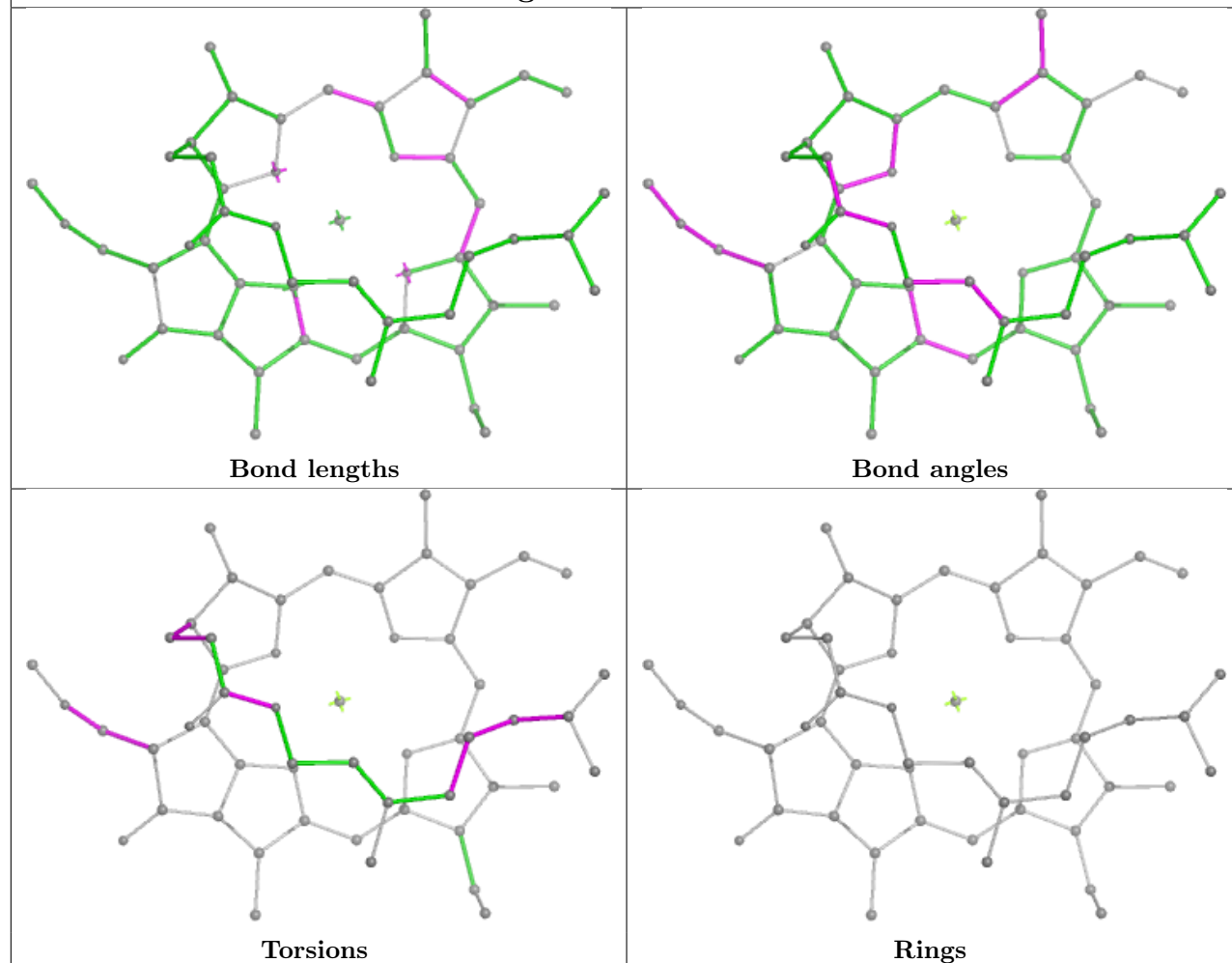


Rings

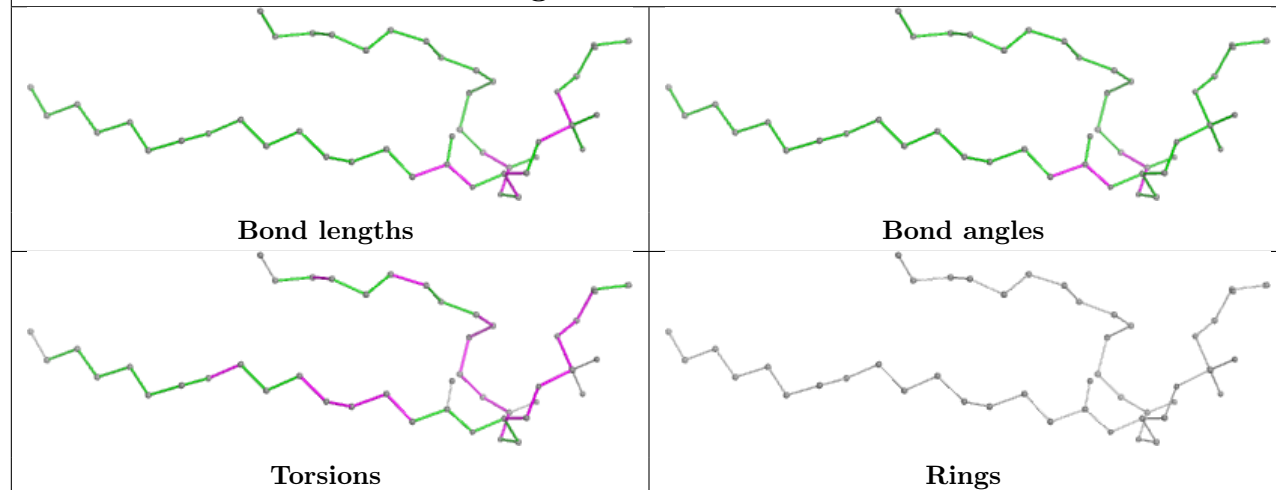


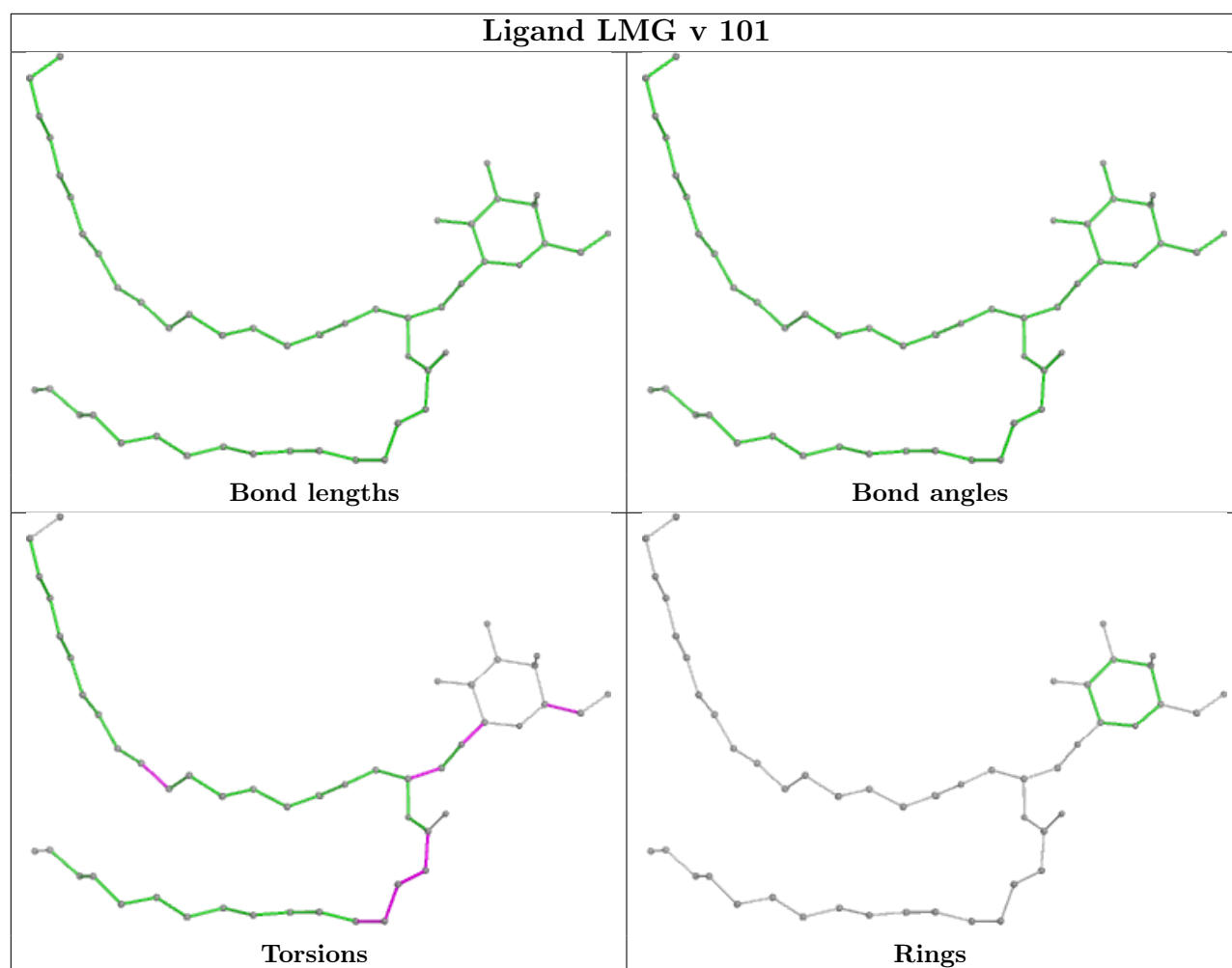


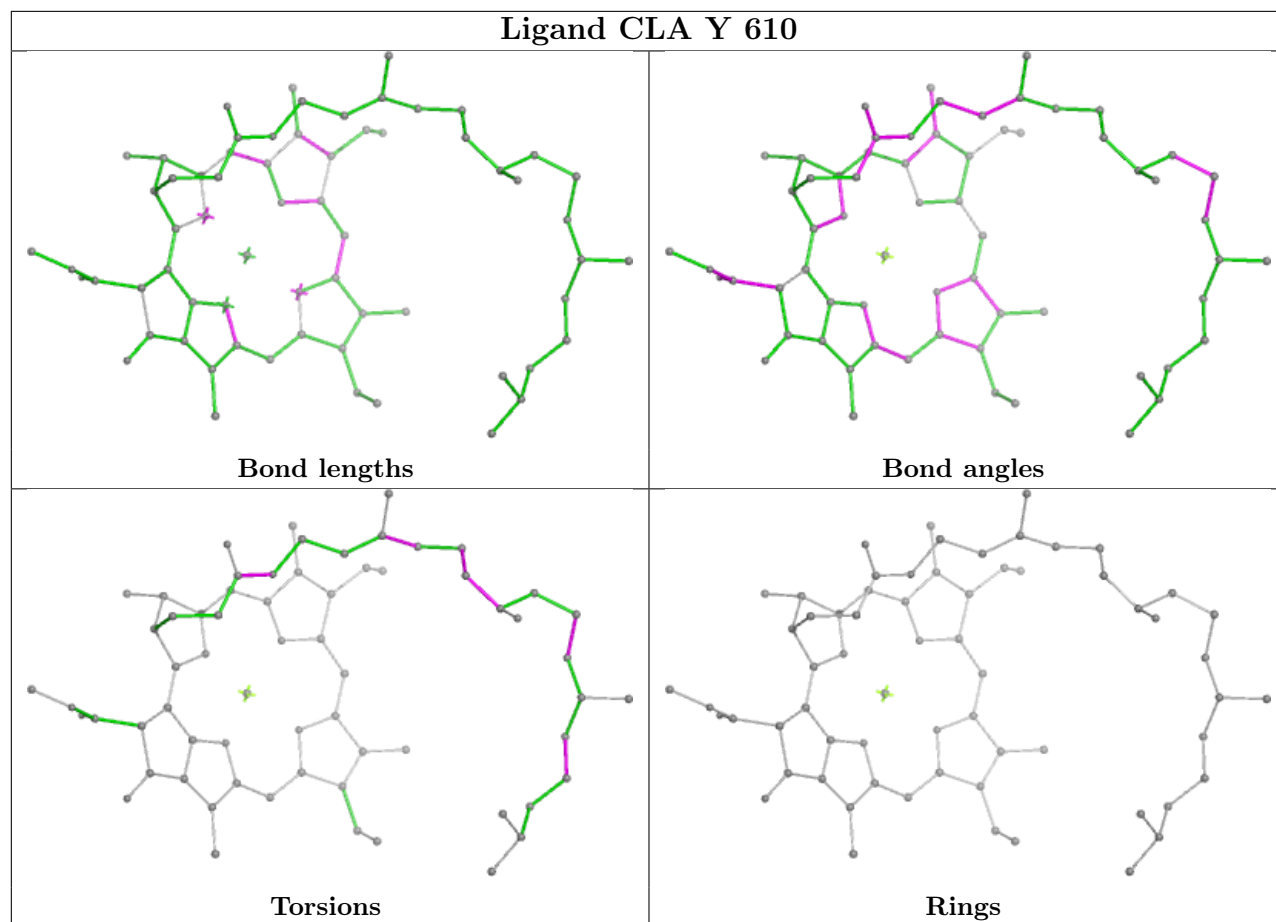
Ligand CLA 6 613



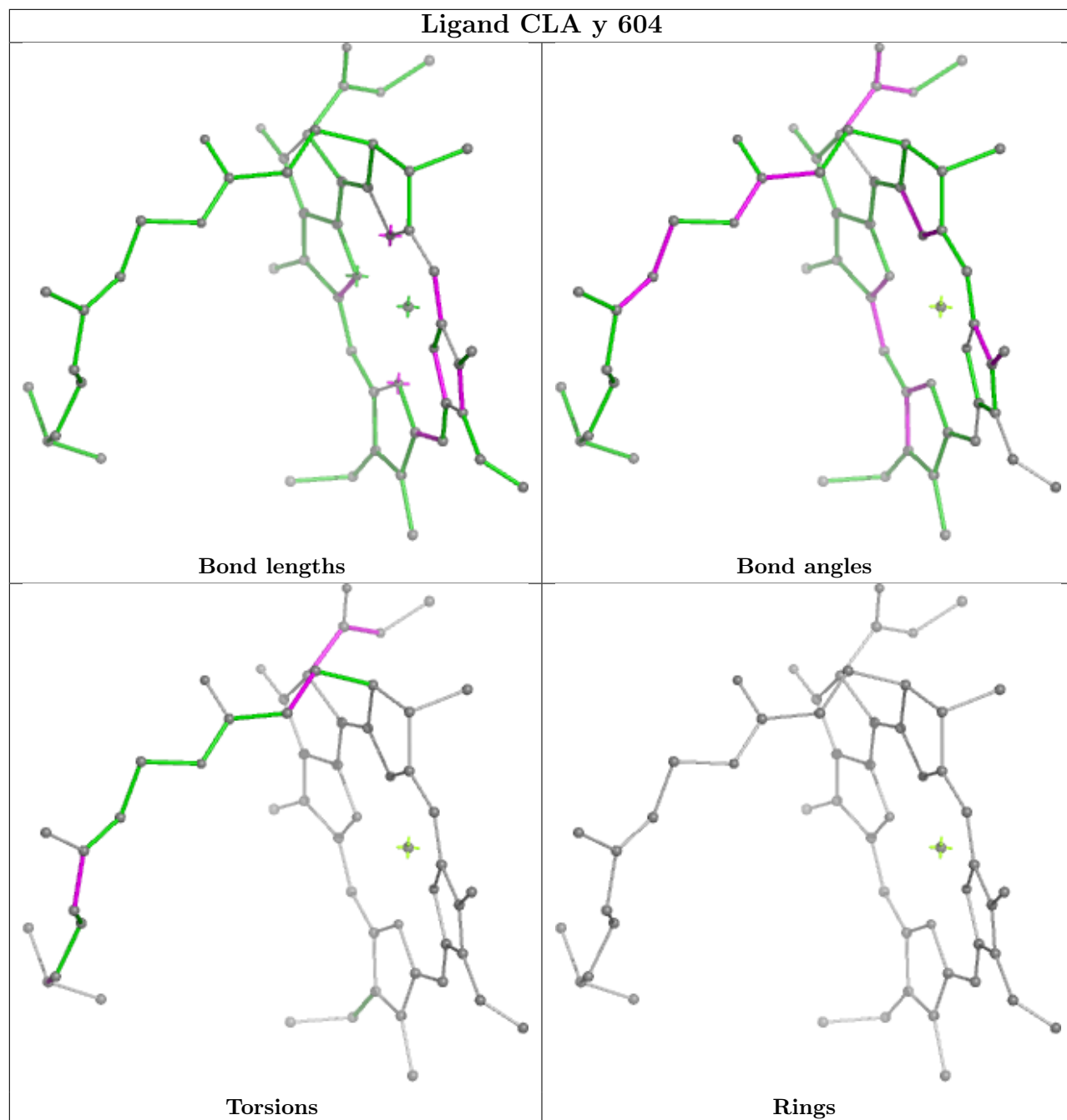
Ligand LHG Y 617

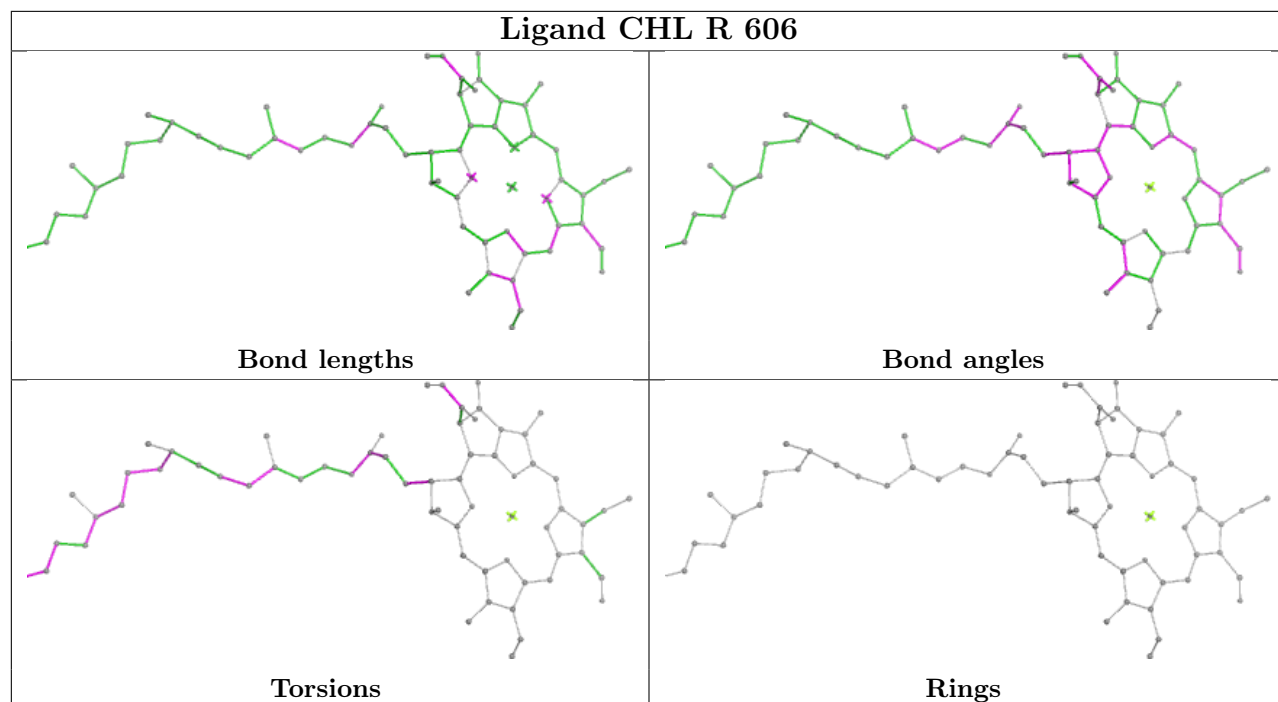




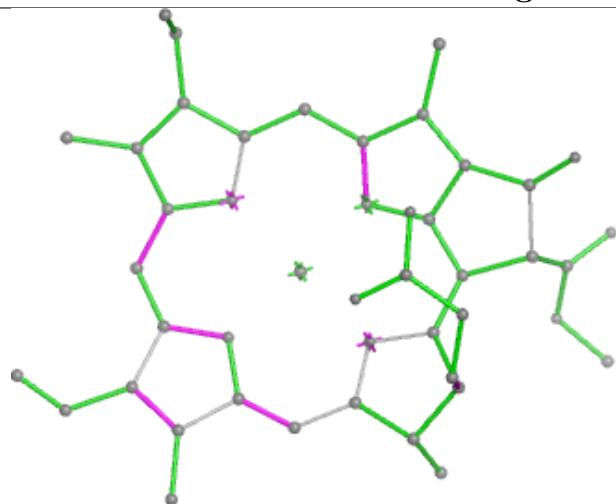


Ligand CLA y 604

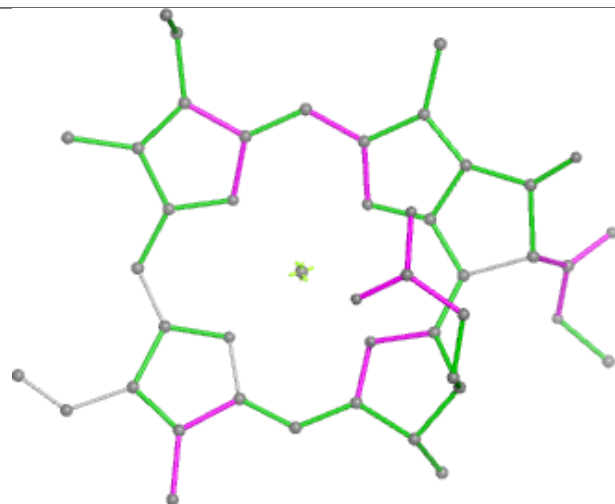




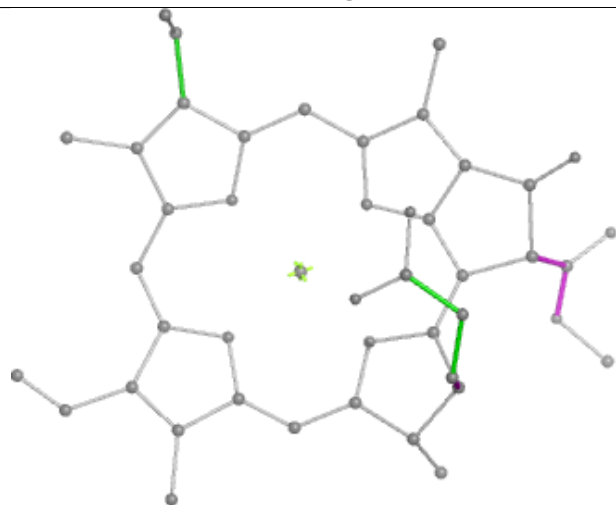
Ligand CLA N 614



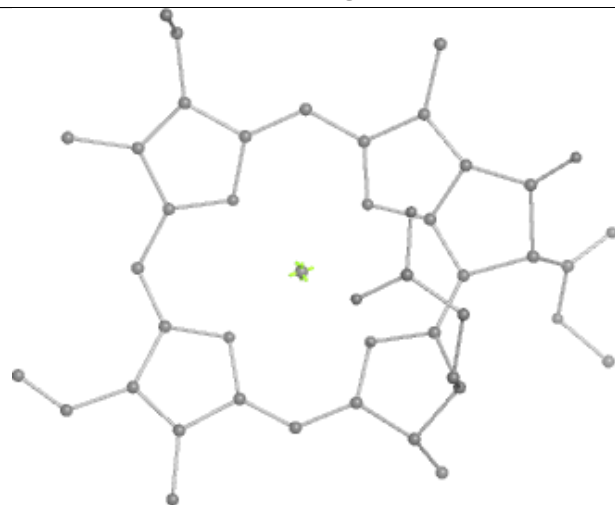
Bond lengths



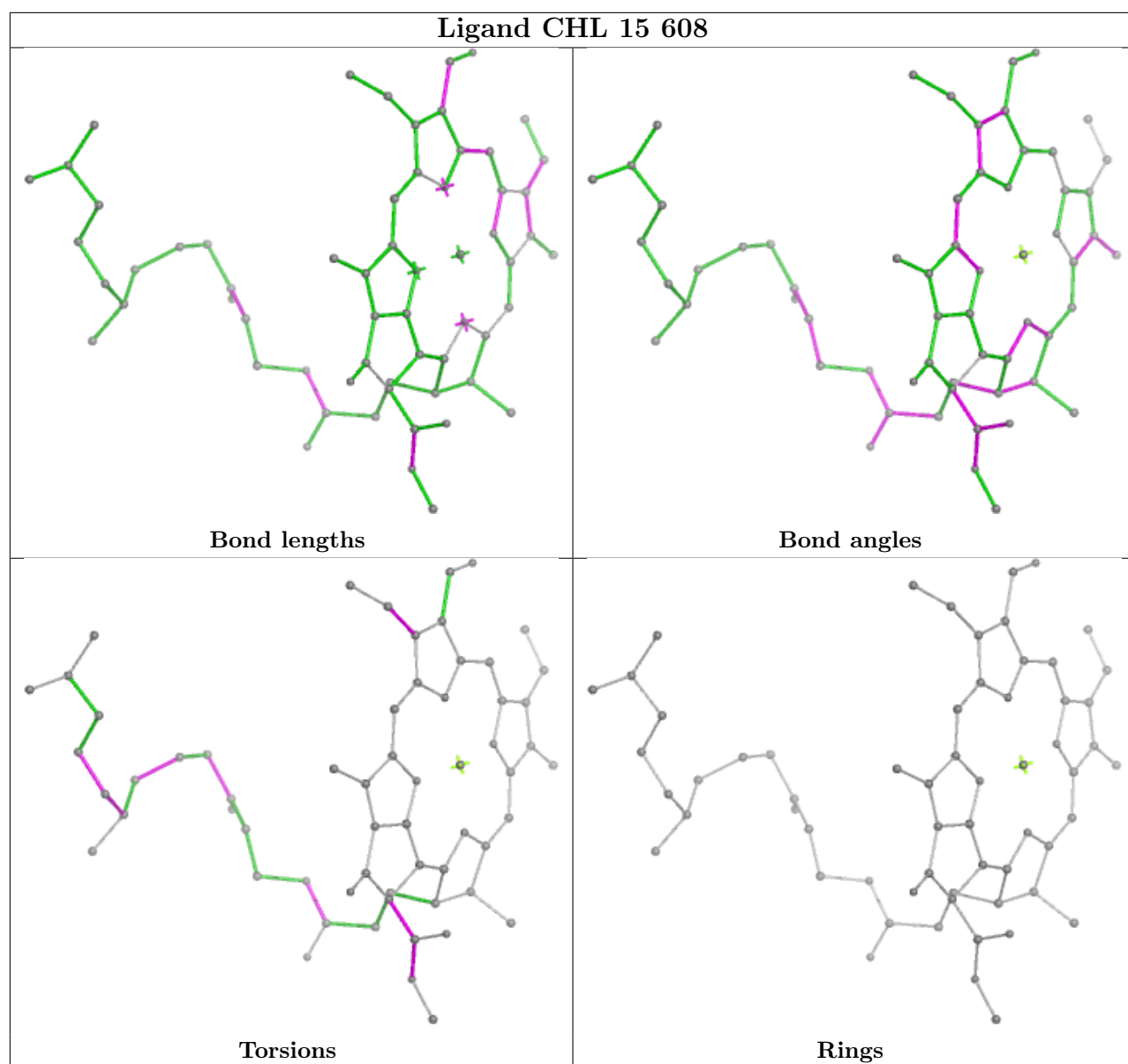
Bond angles



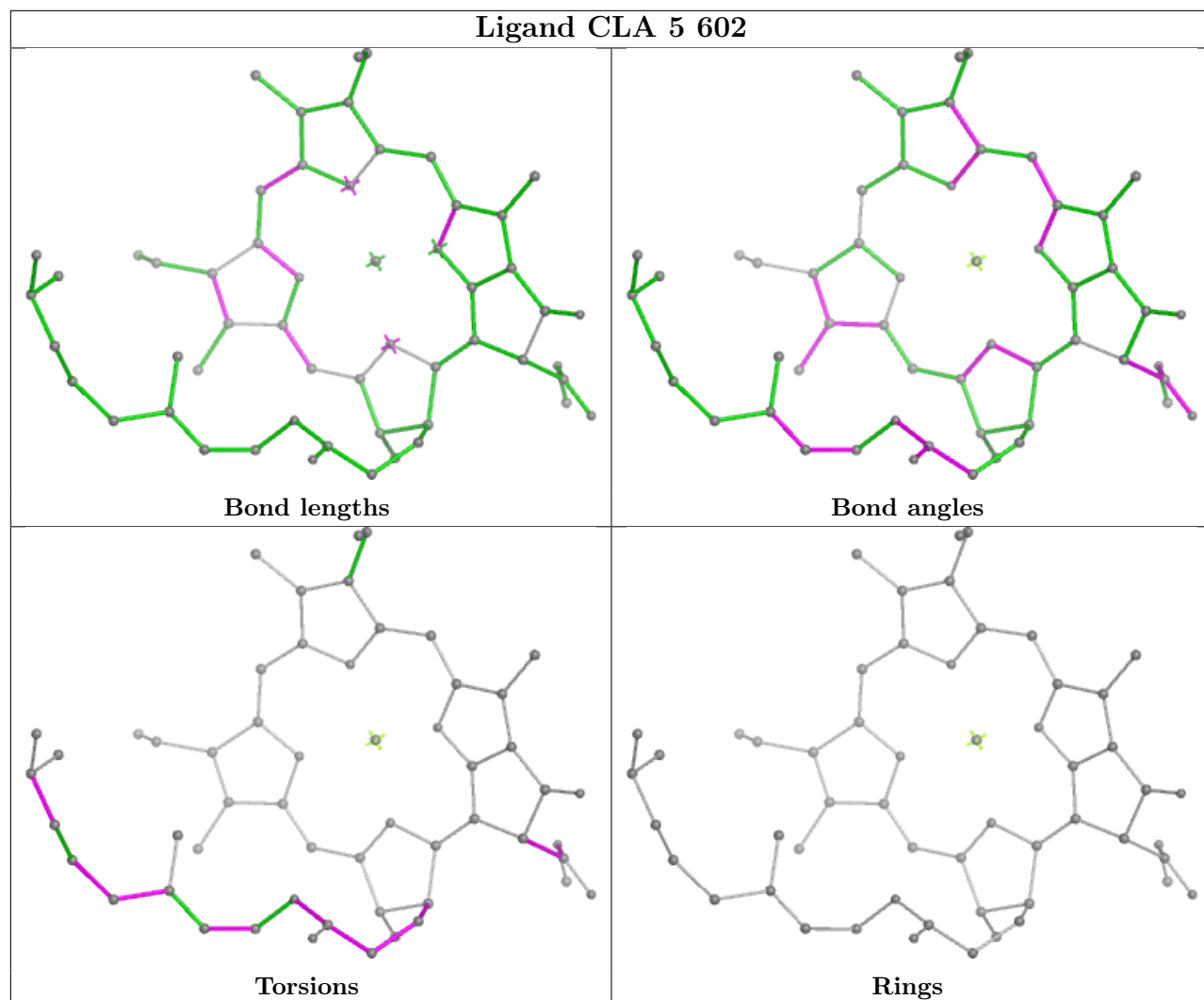
Torsions

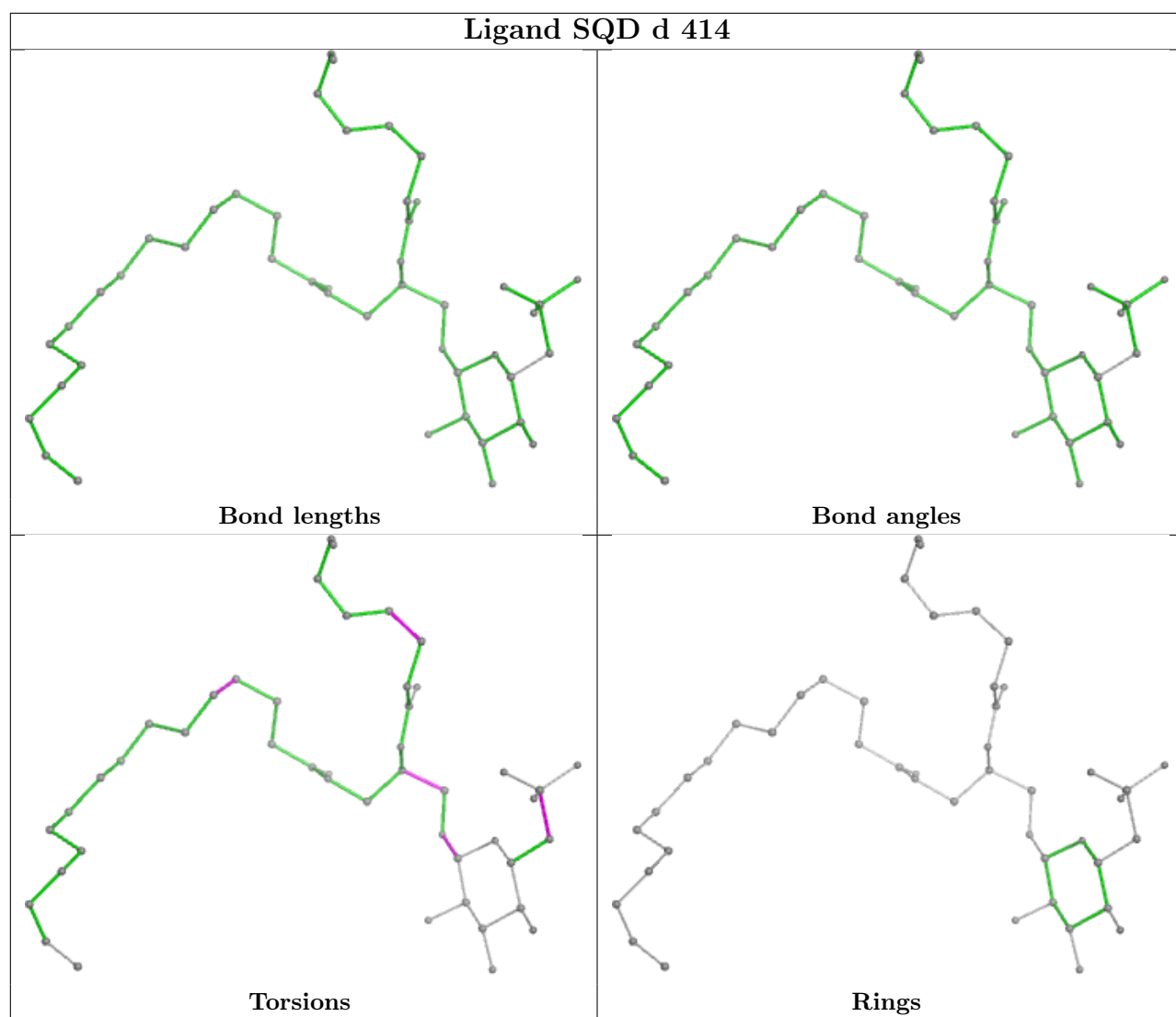


Rings

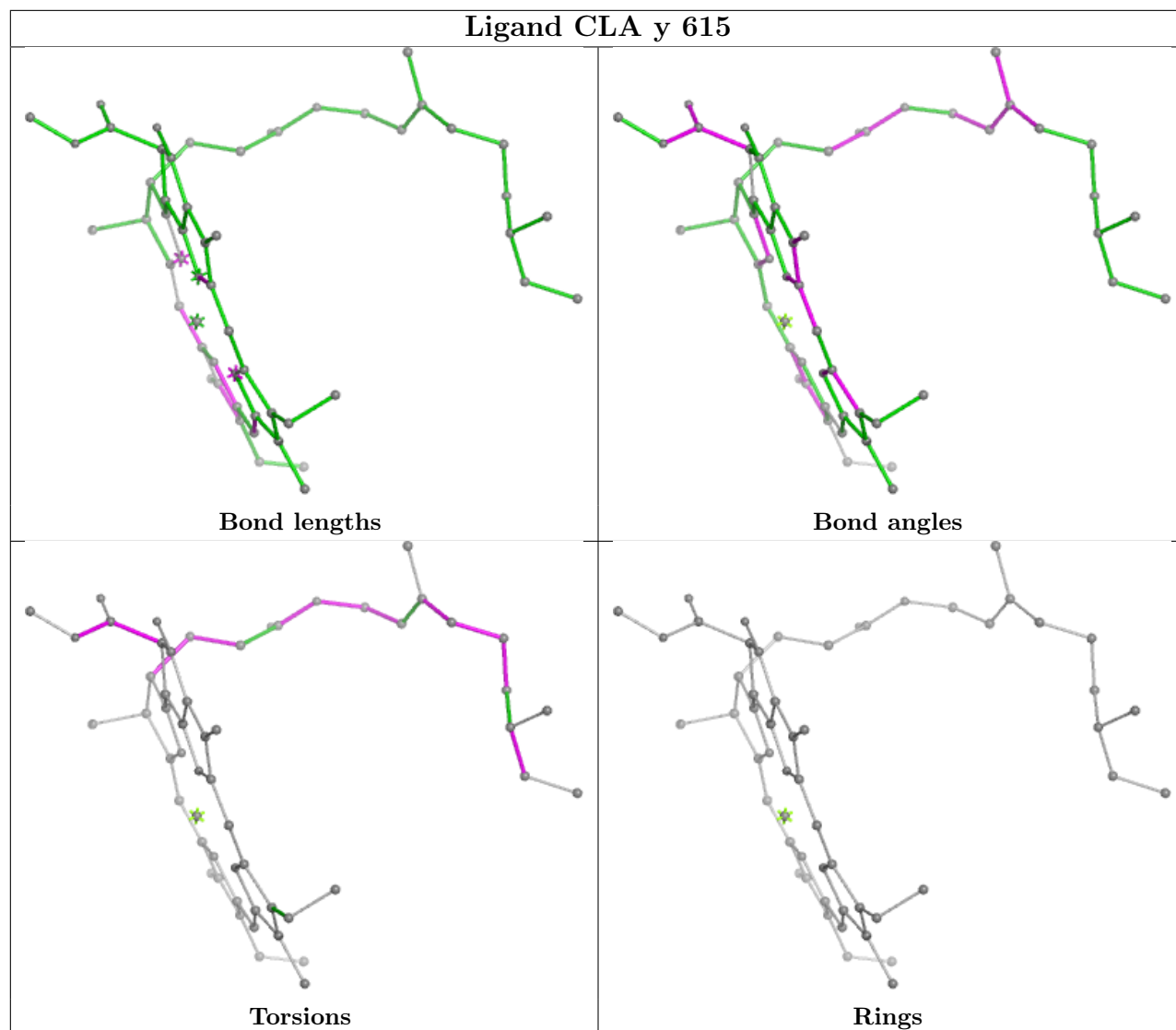


Ligand CLA 5 602

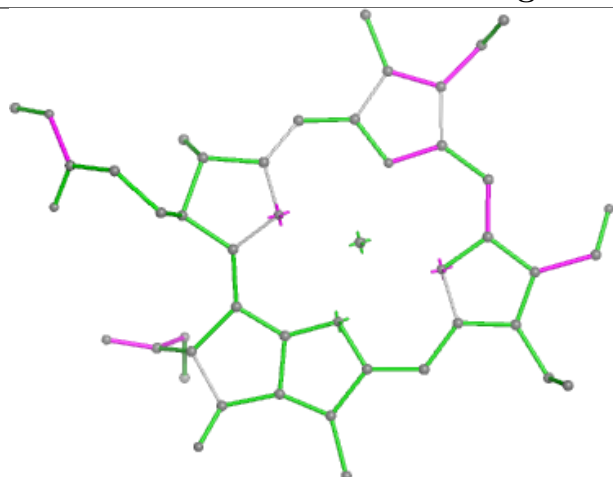




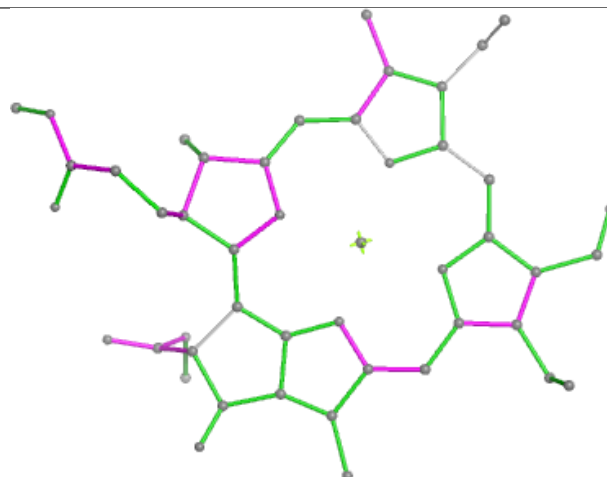
Ligand CLA y 615



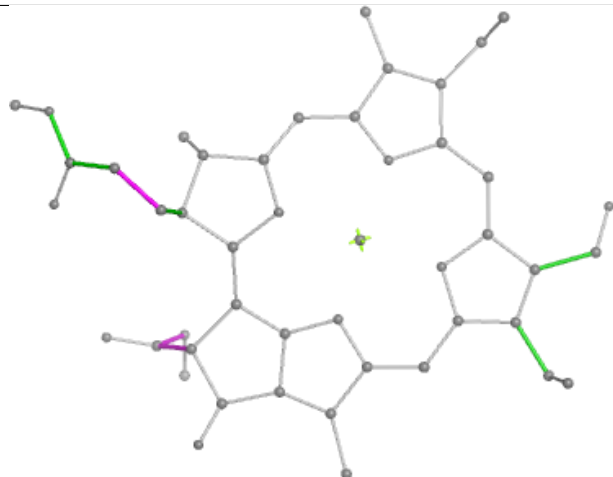
Ligand CHL 2 601



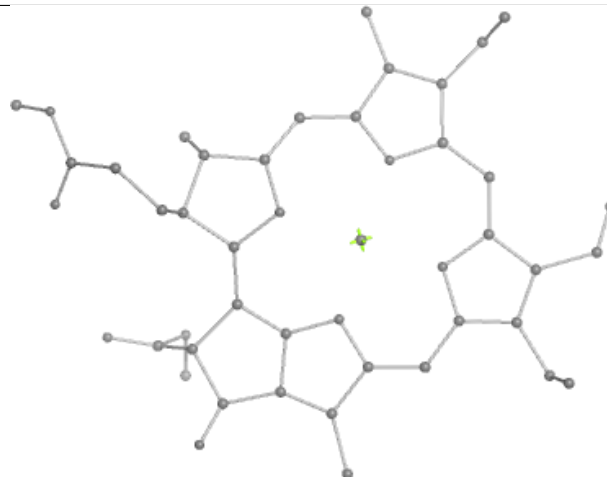
Bond lengths



Bond angles

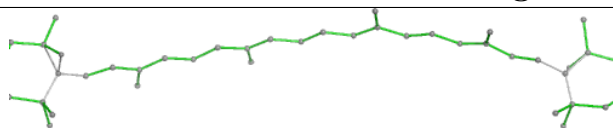


Torsions

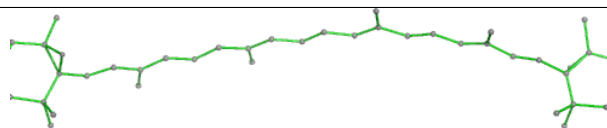


Rings

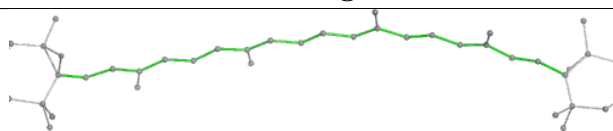
Ligand XAT G 619



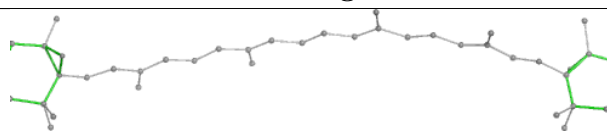
Bond lengths



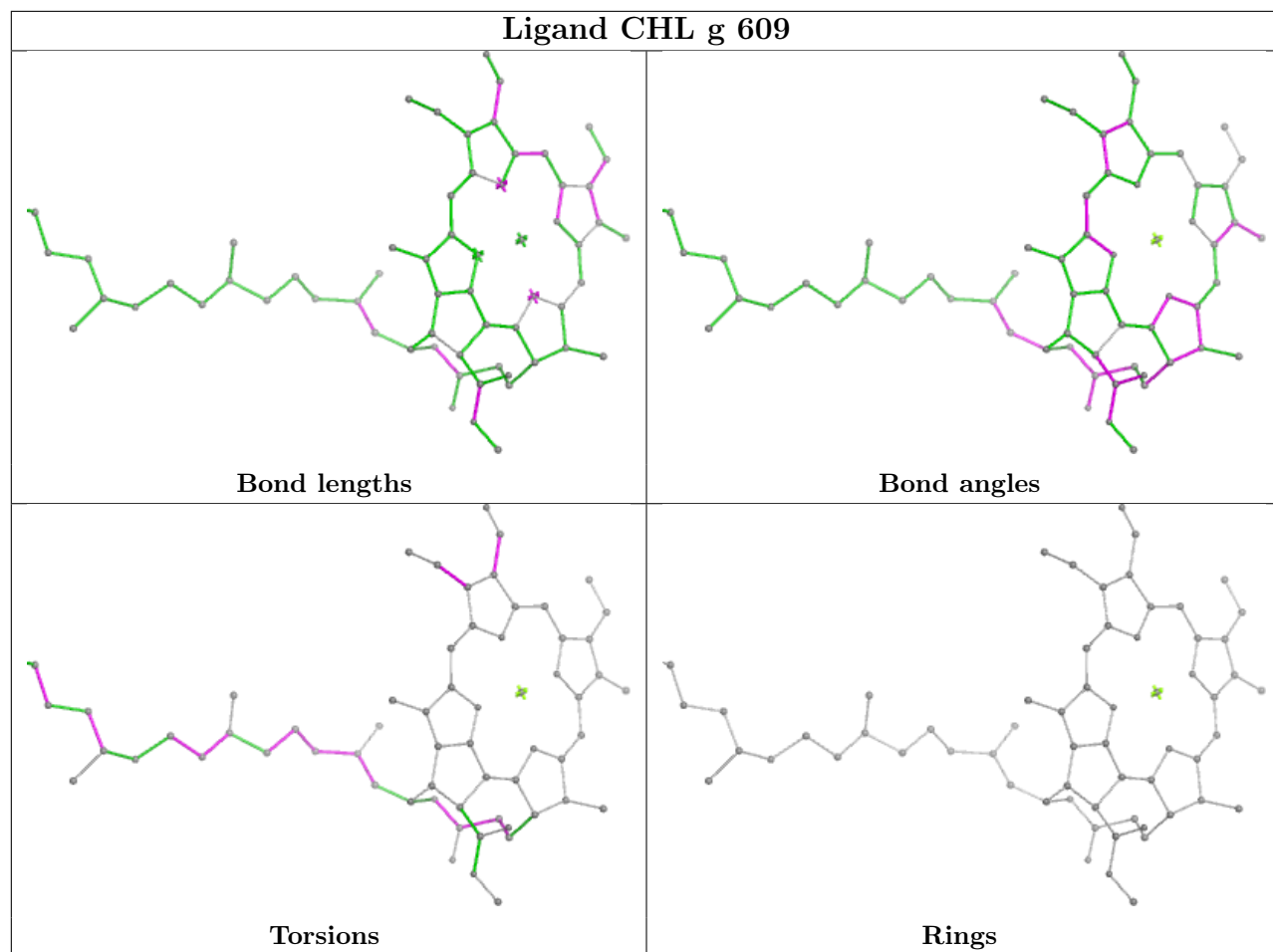
Bond angles

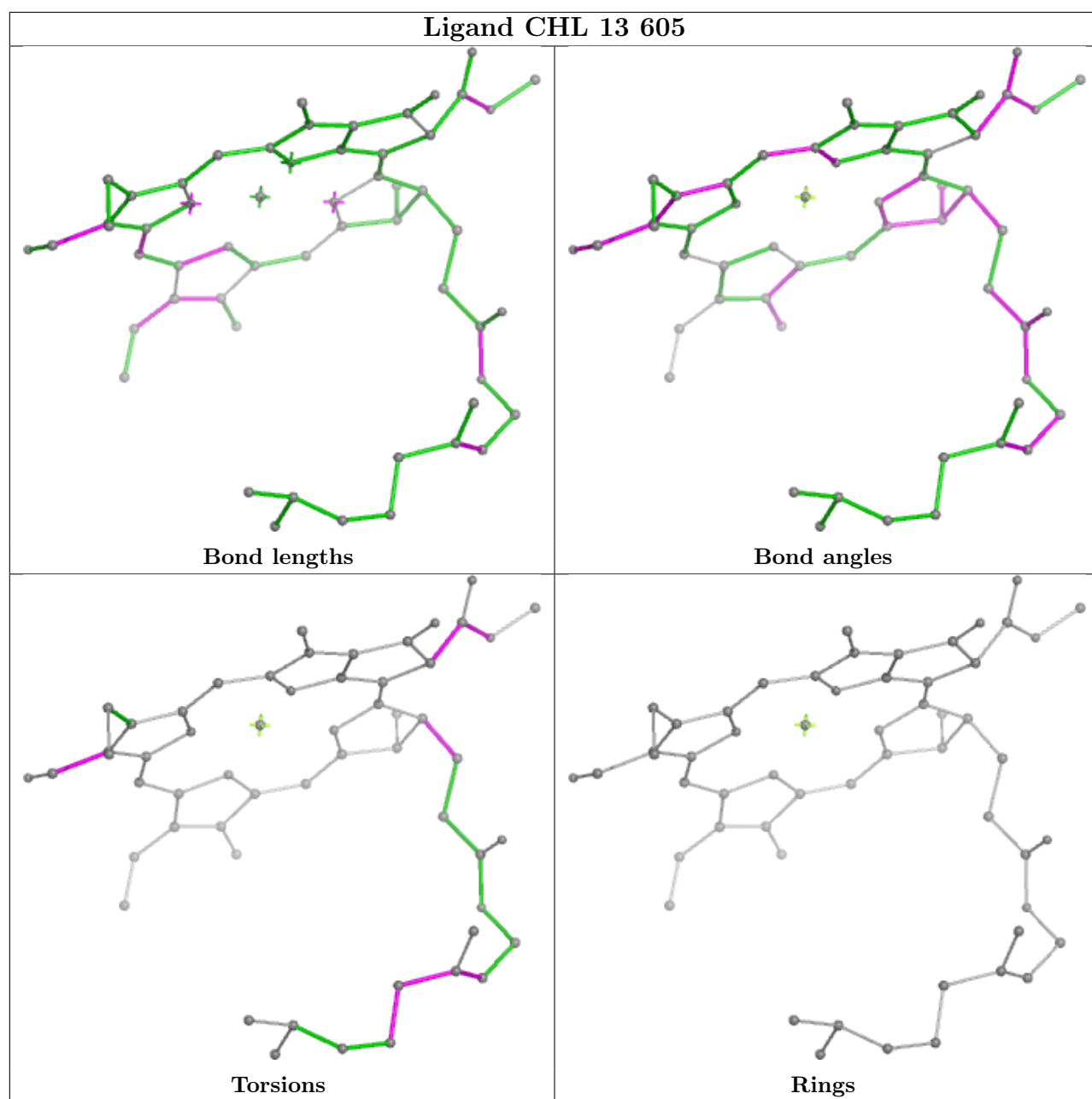


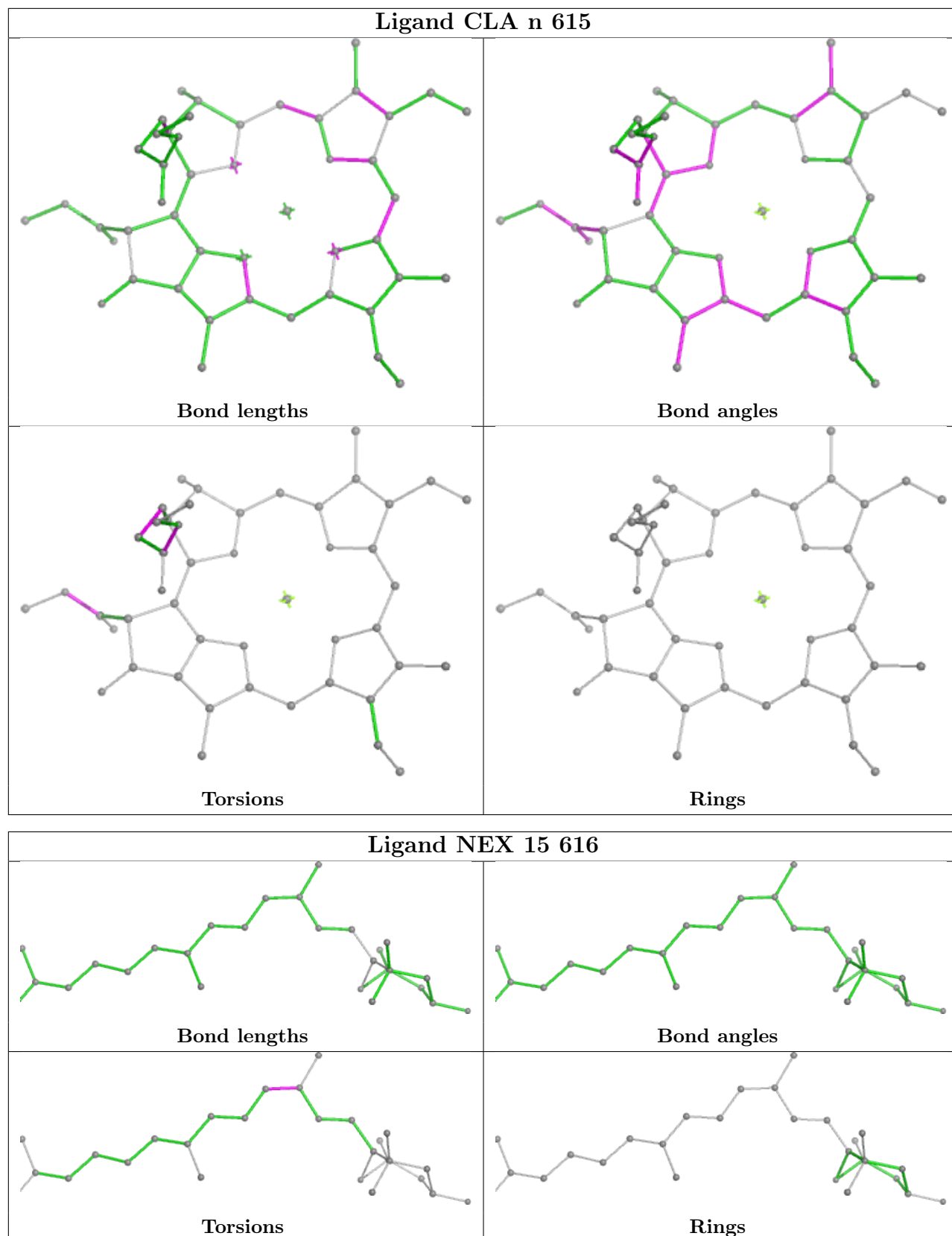
Torsions



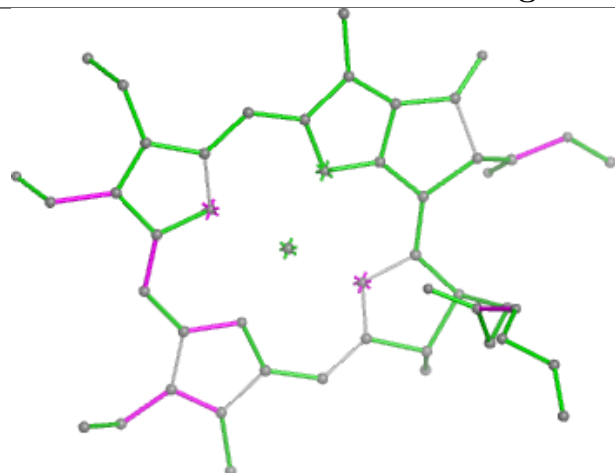
Rings



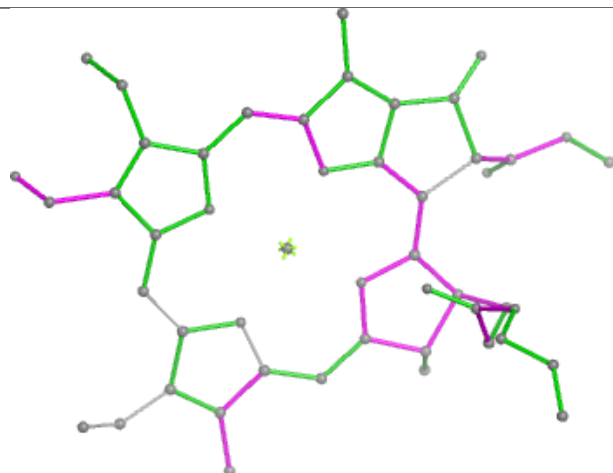




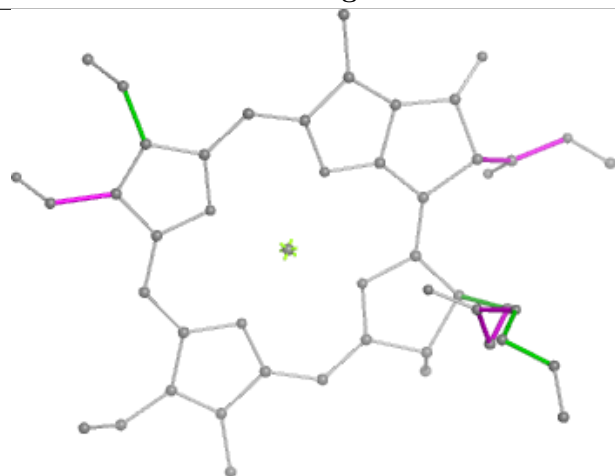
Ligand CHL S 608



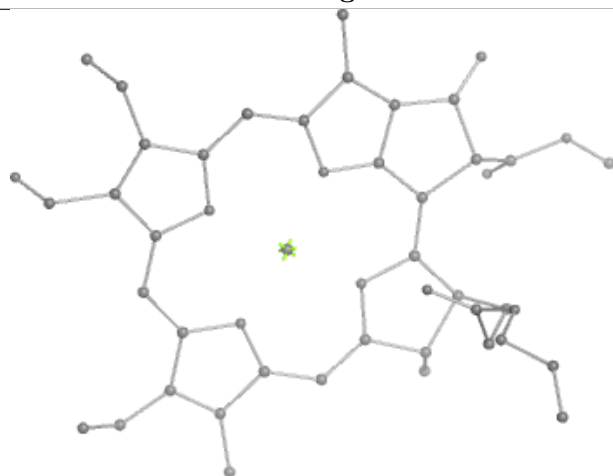
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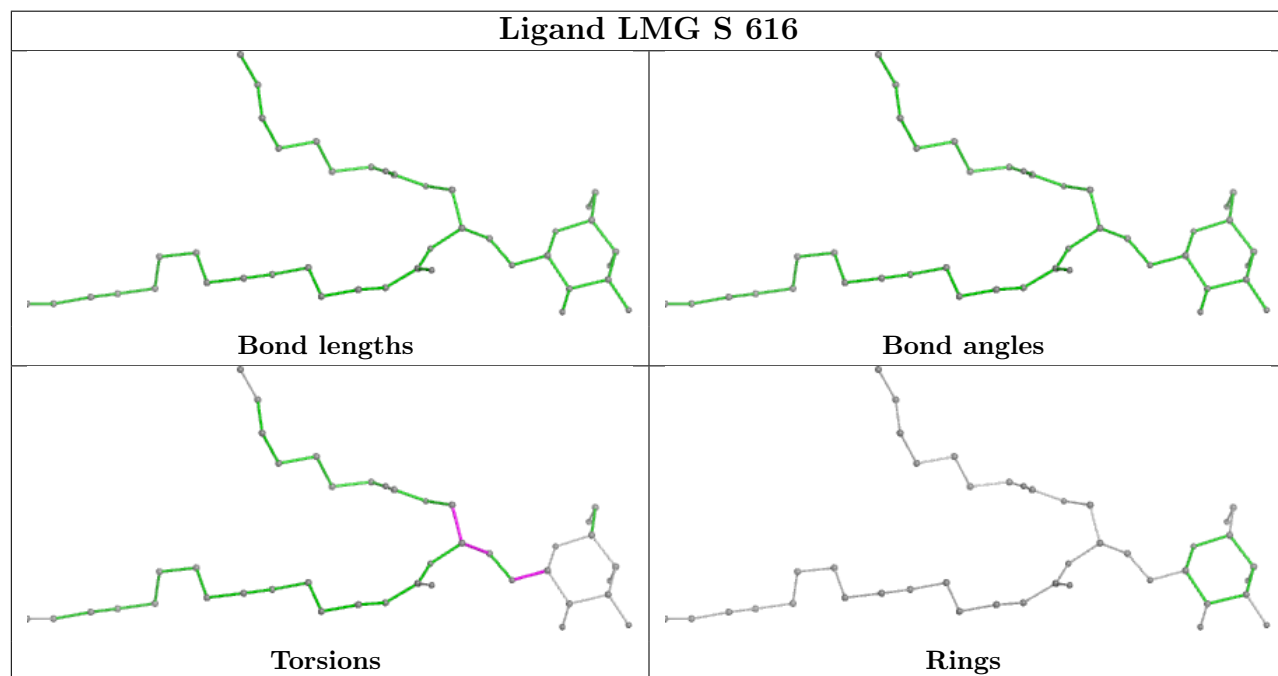
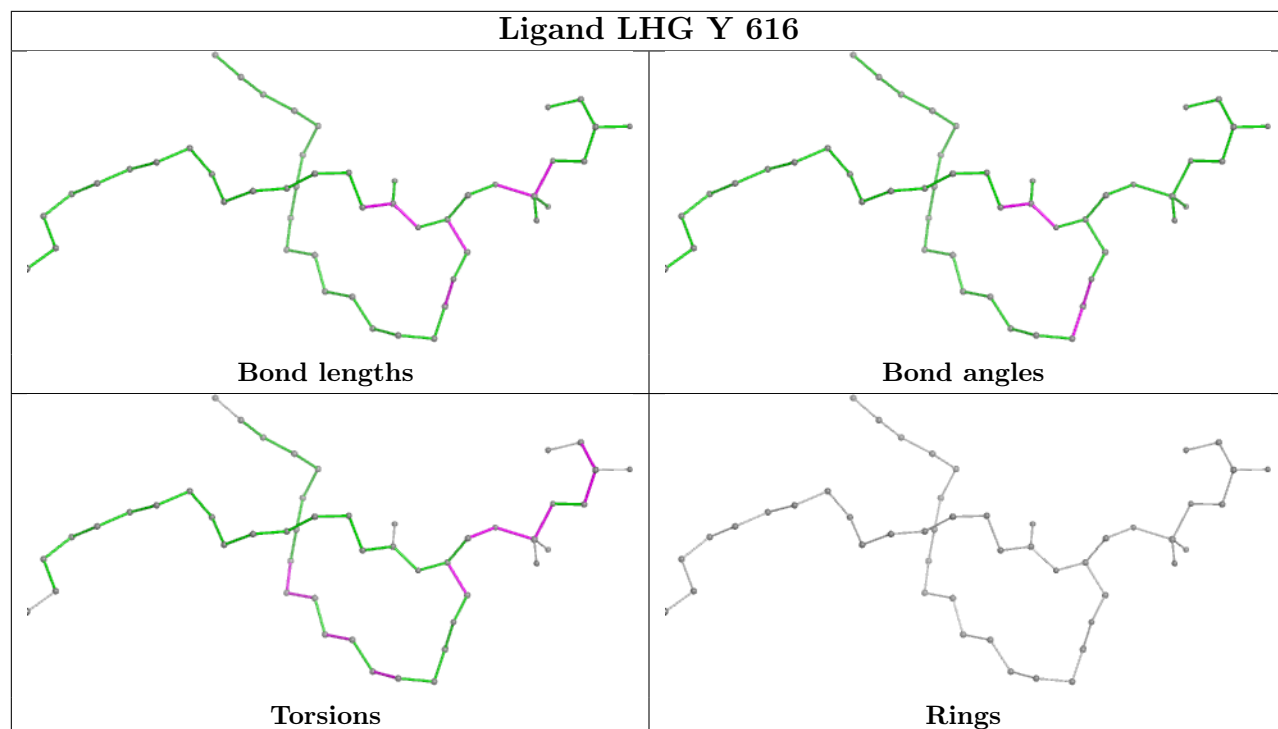
Bond angles

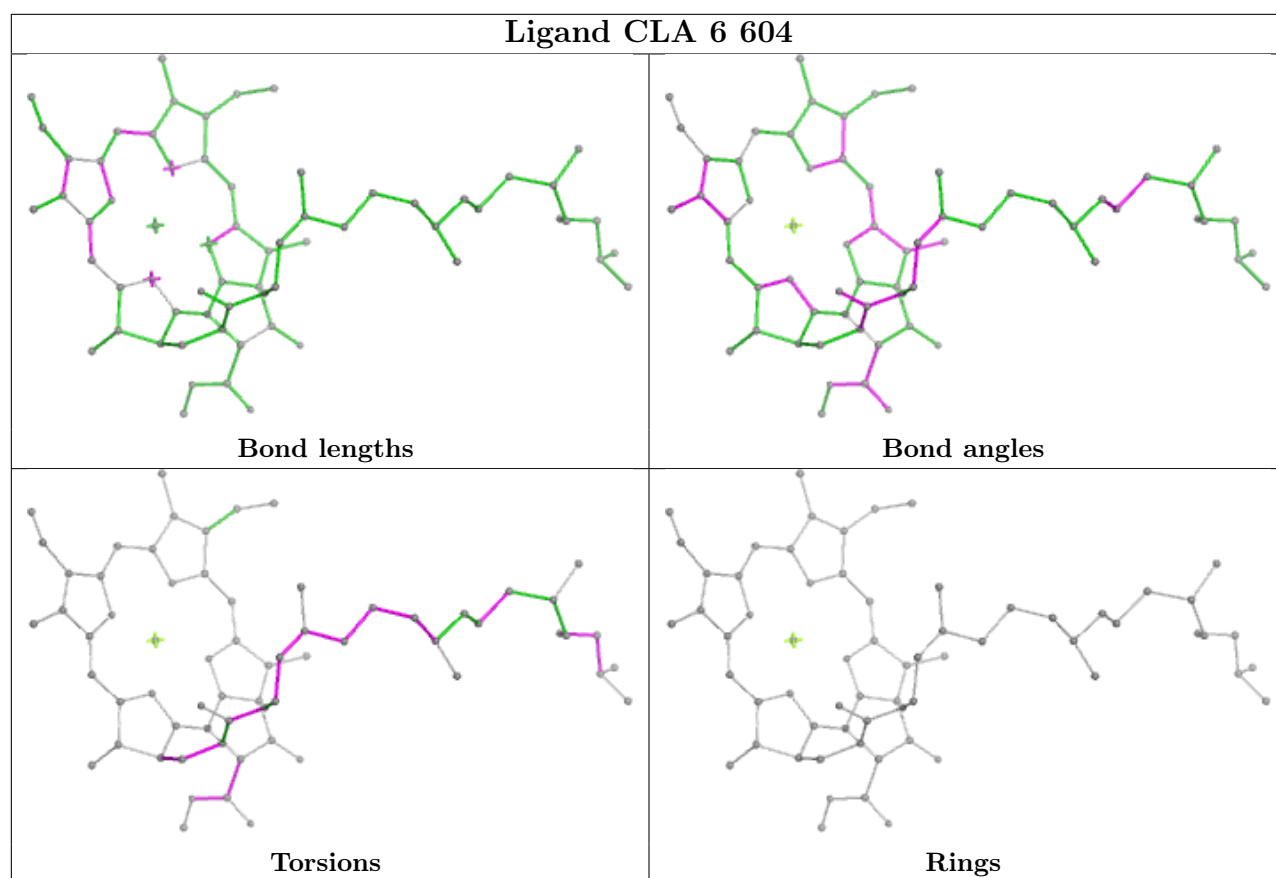


Torsions

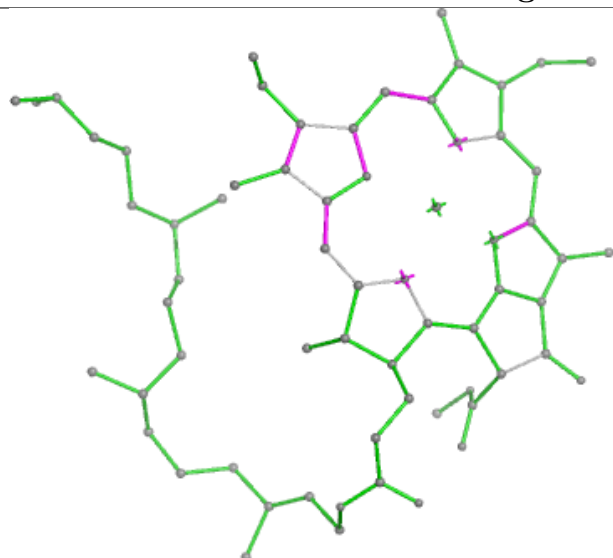


Rings

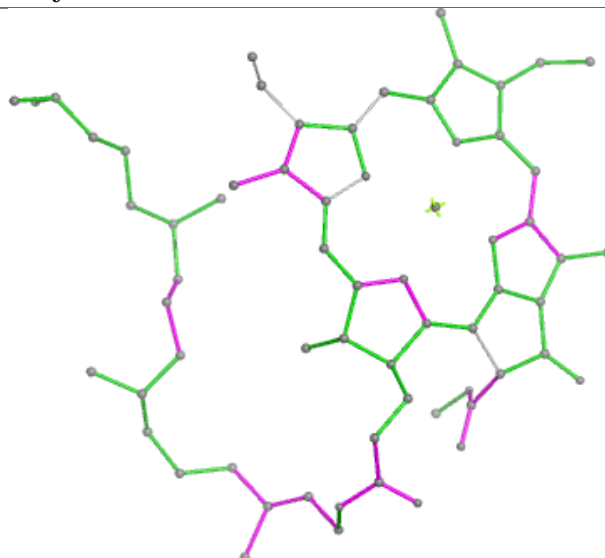




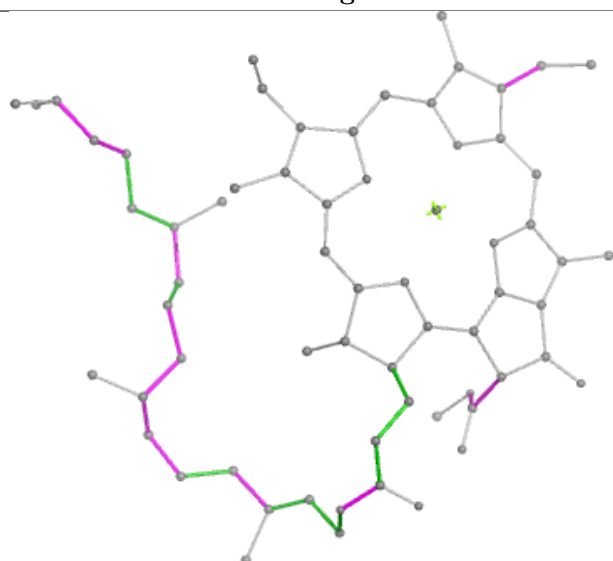
Ligand CLA y 612



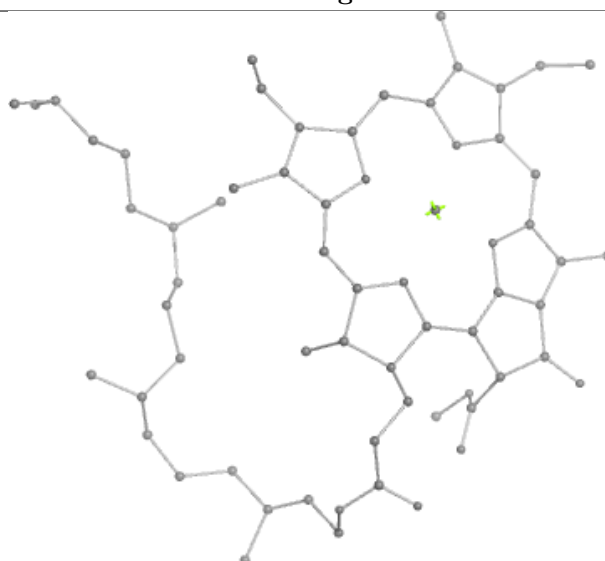
Bond lengths



Bond angles

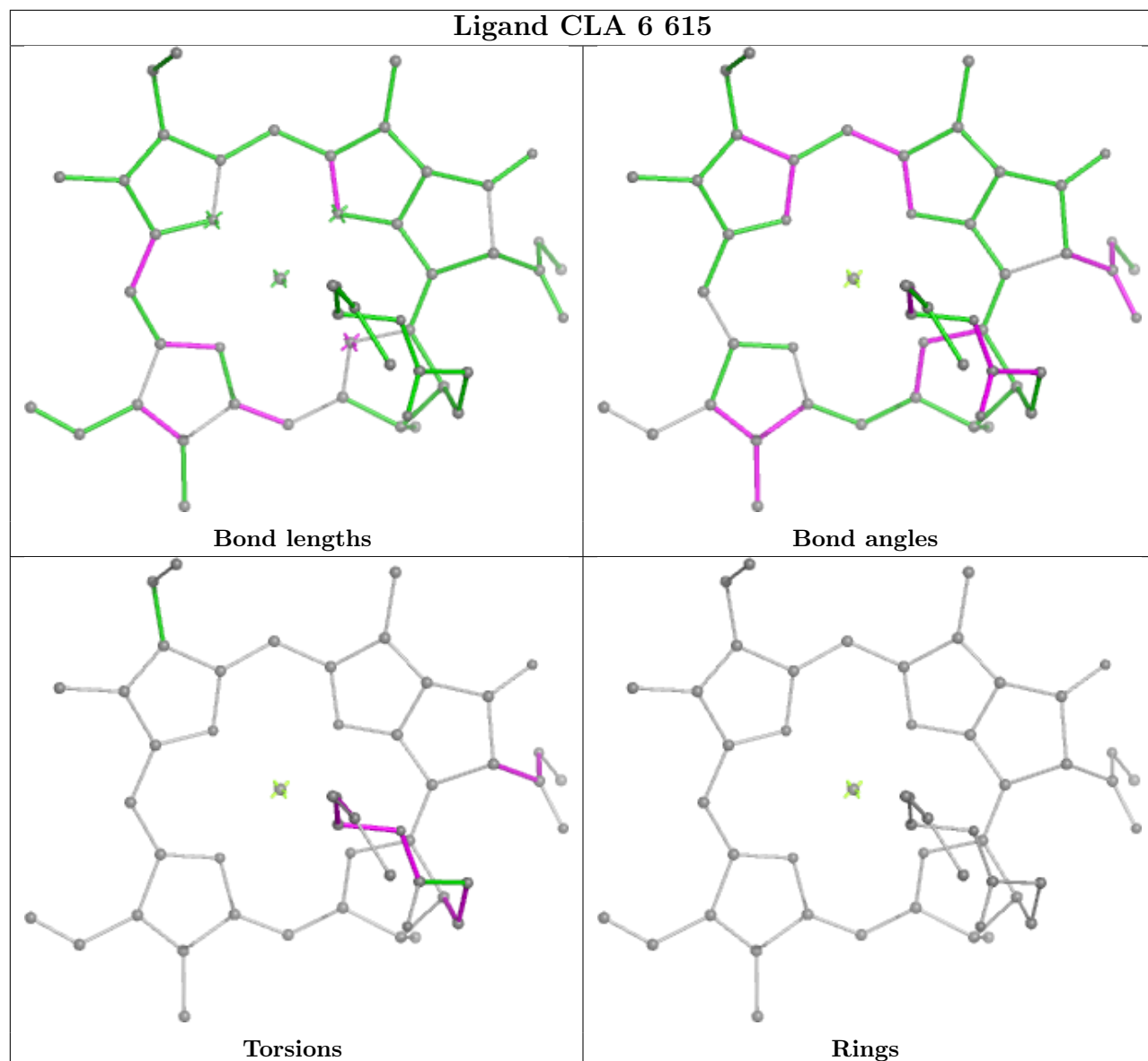


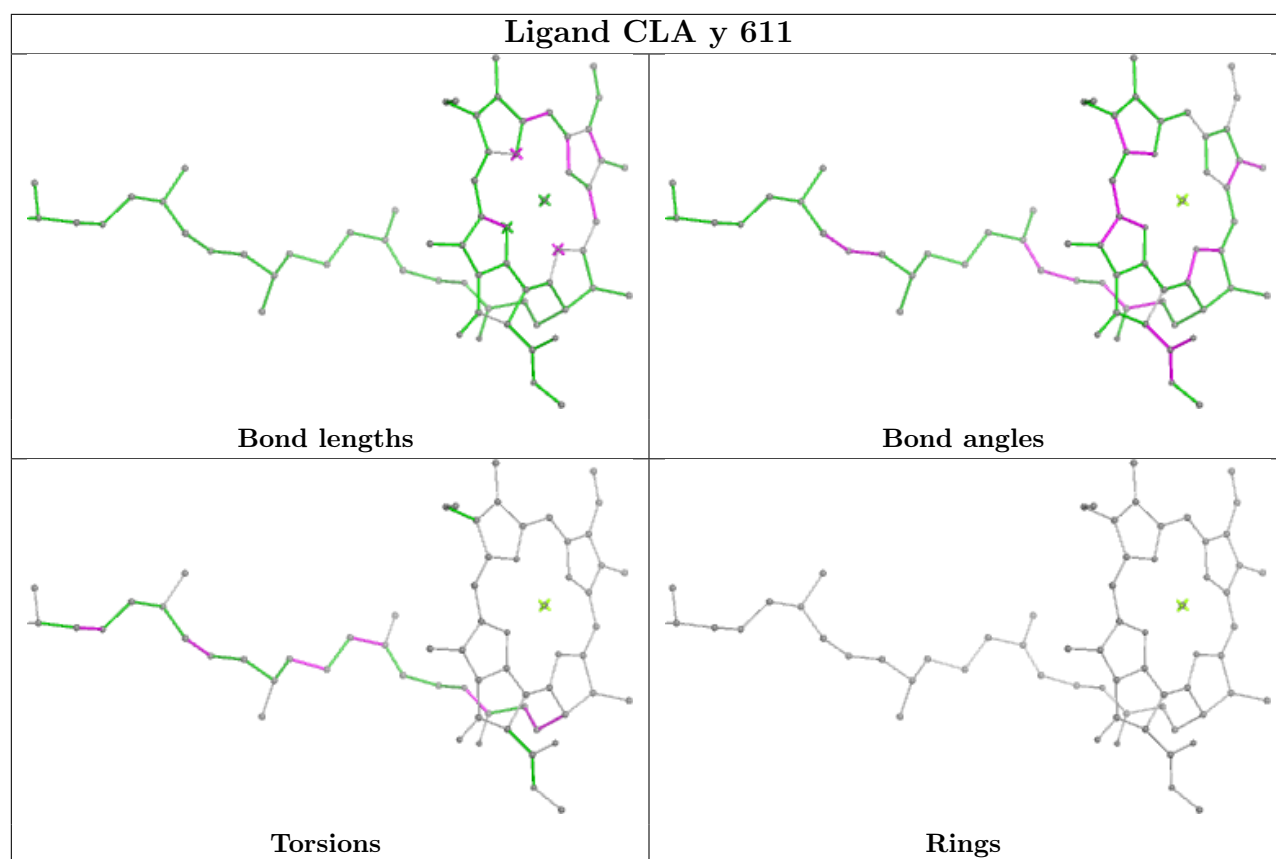
Torsions

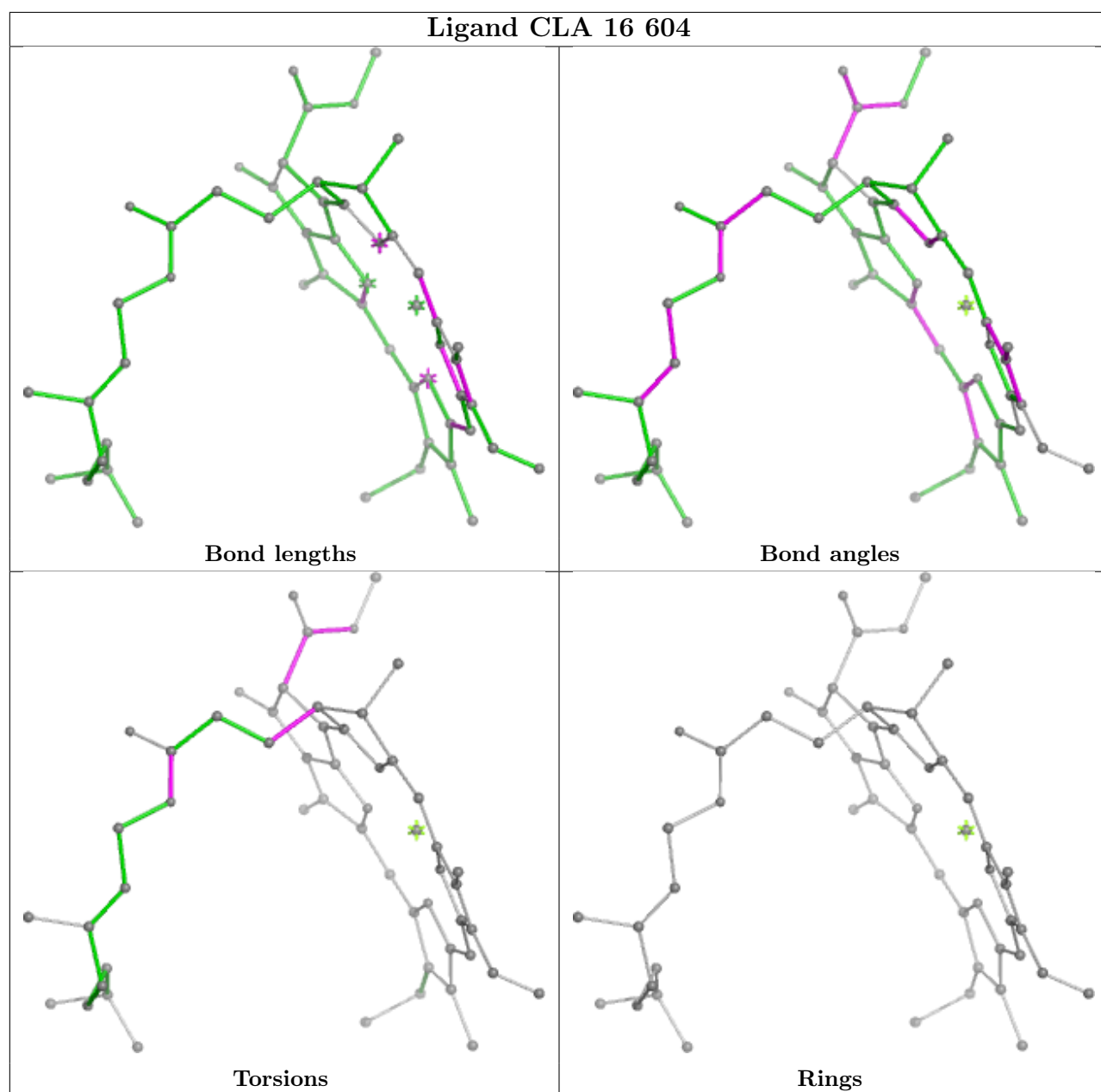


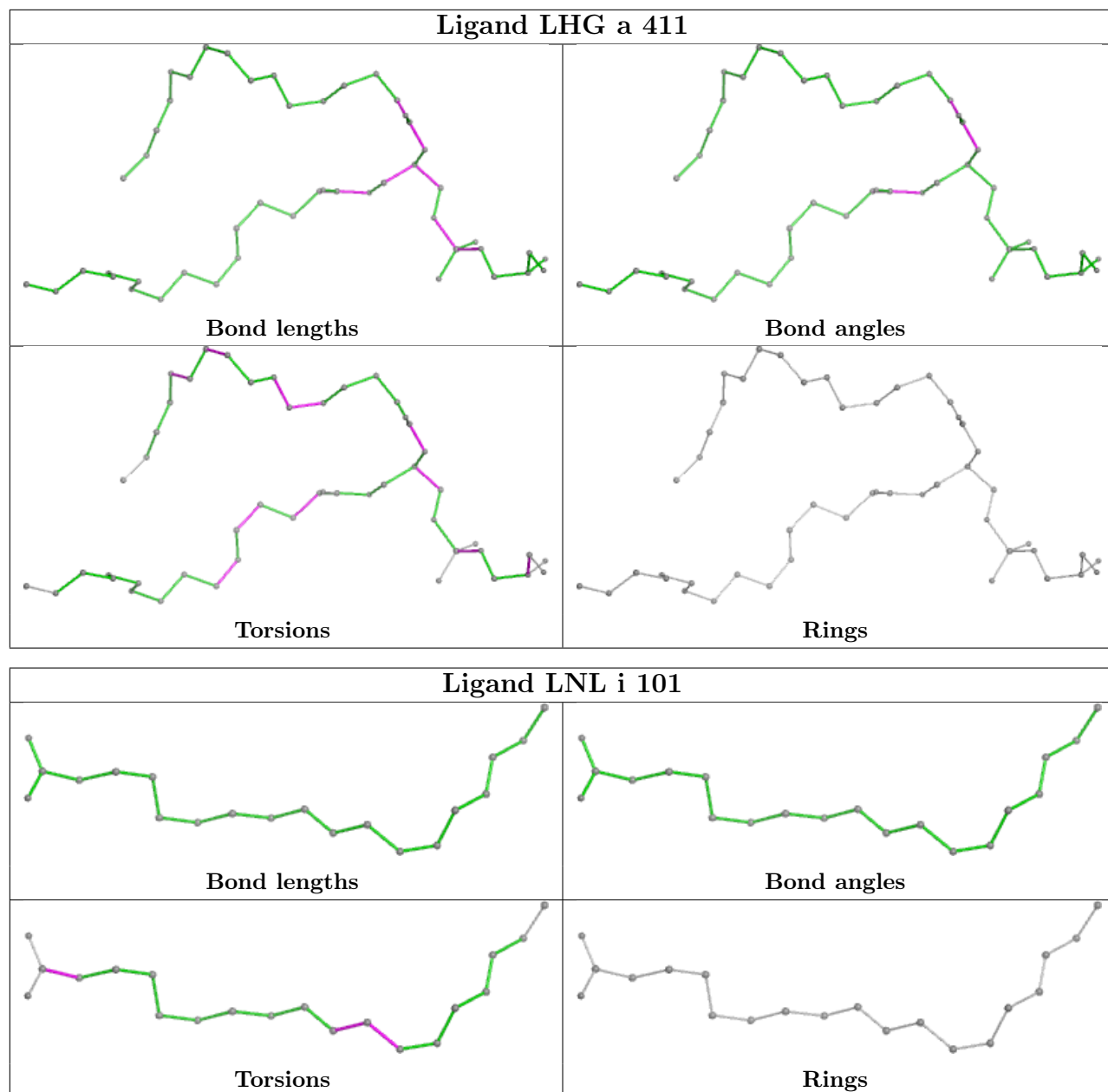
Rings

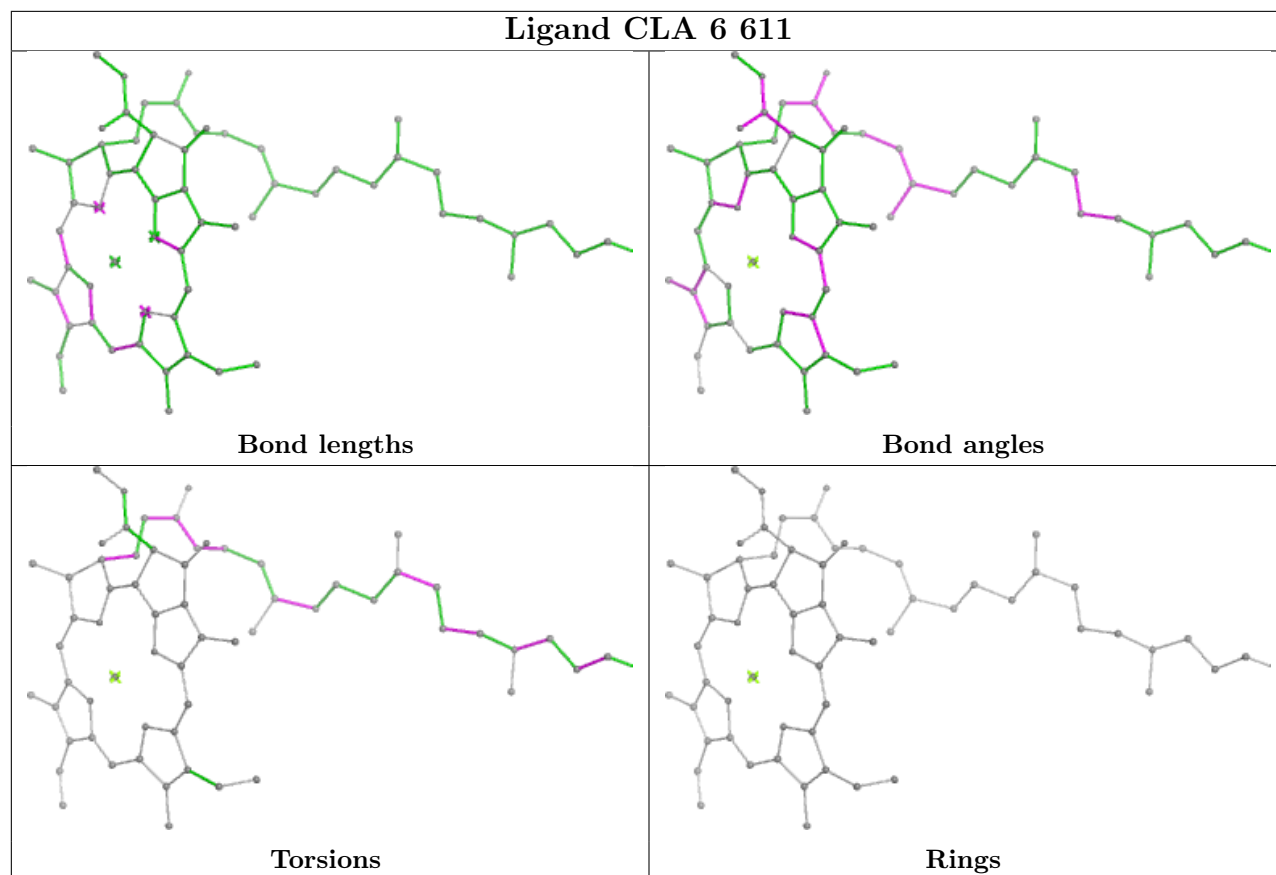
Ligand CLA 6 615

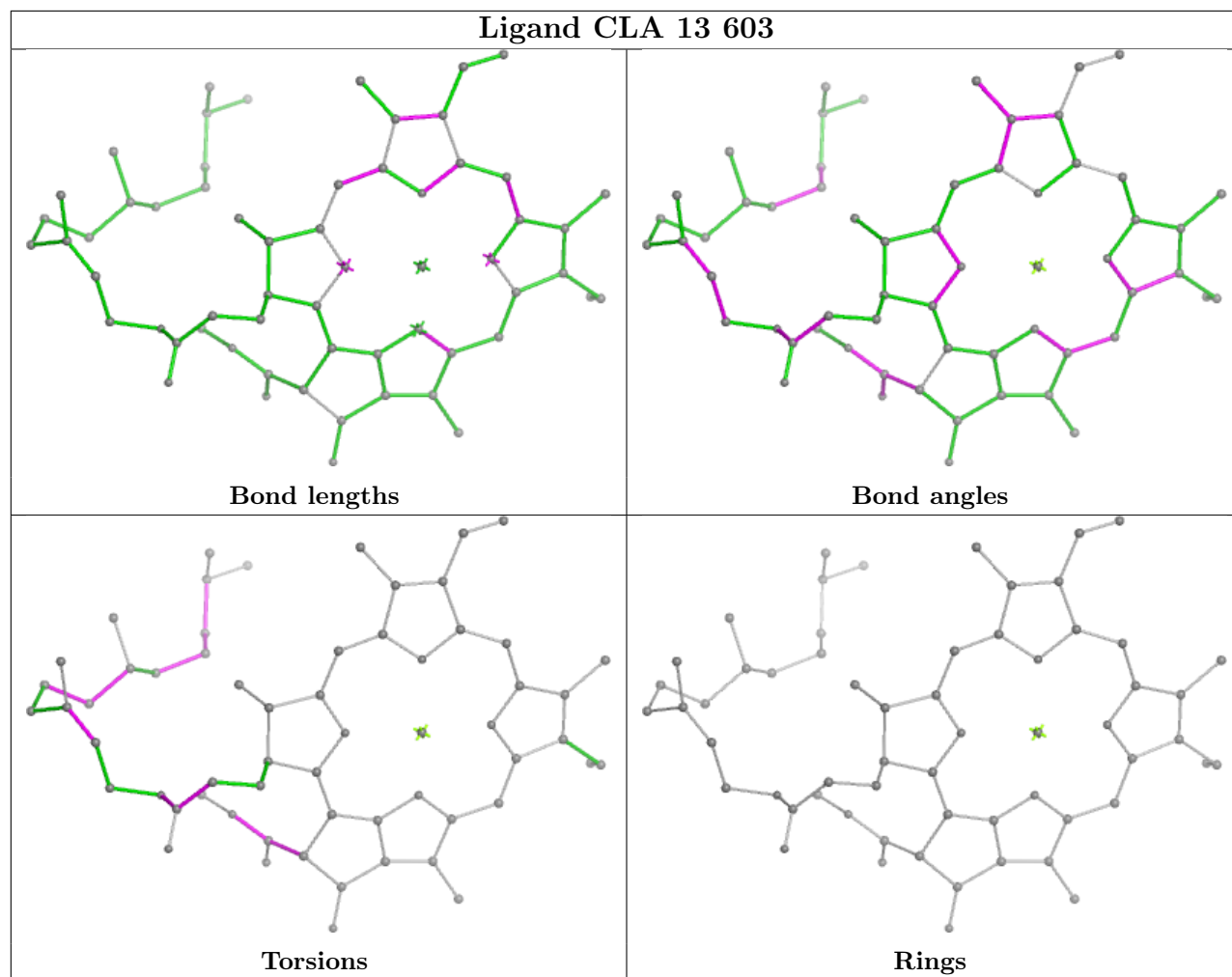


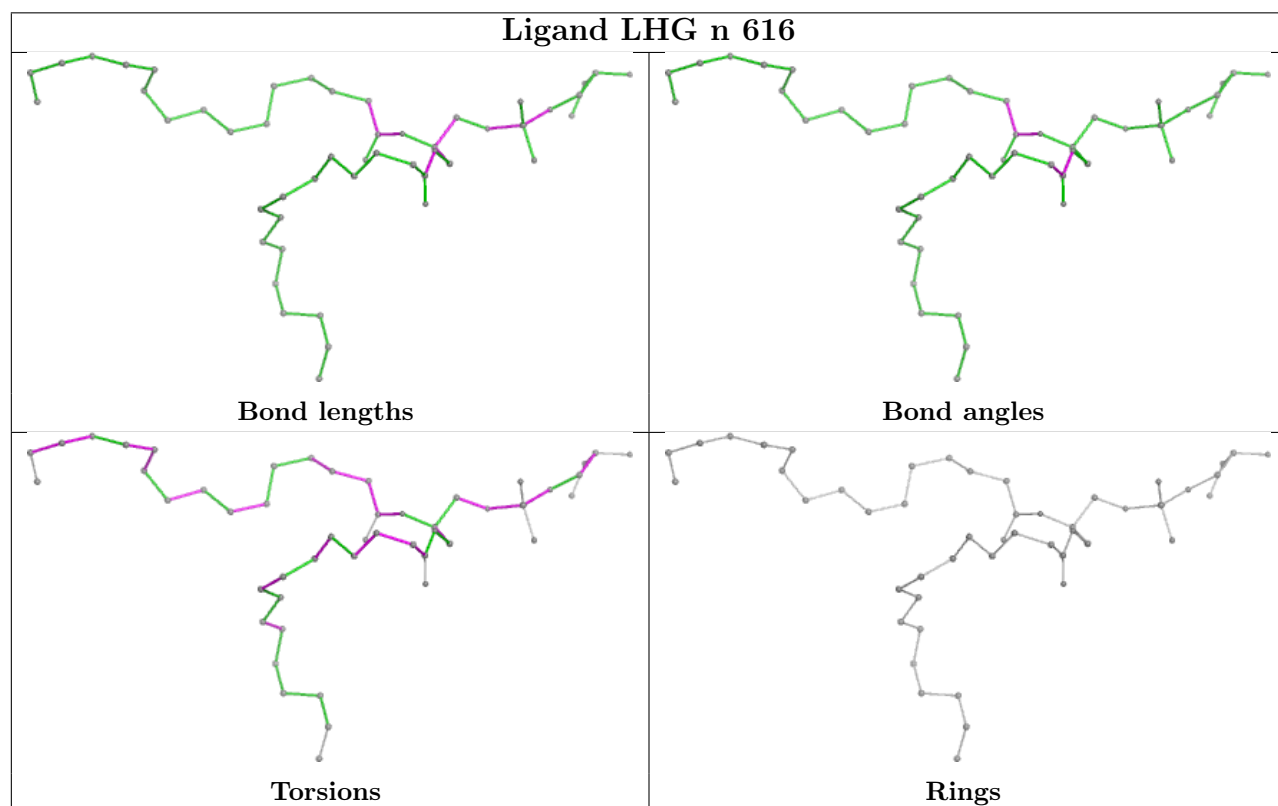
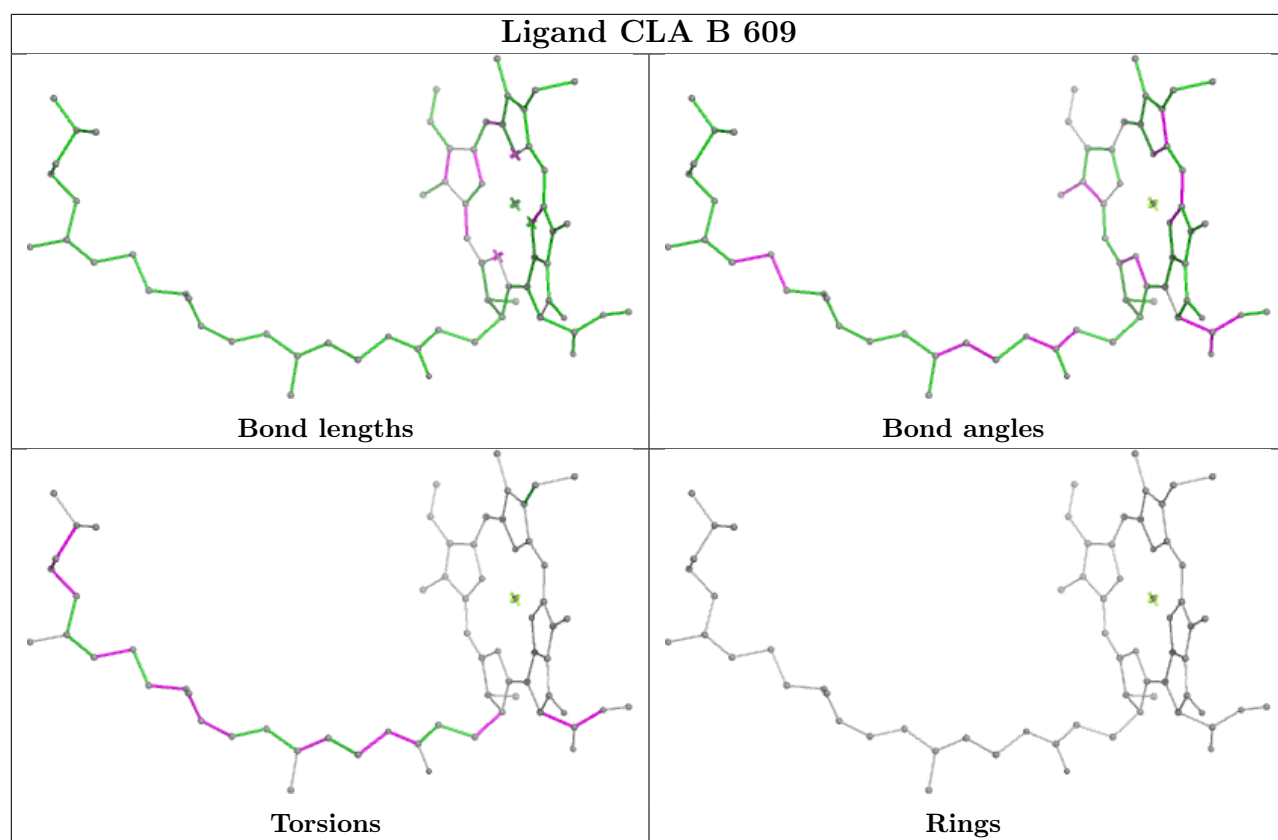


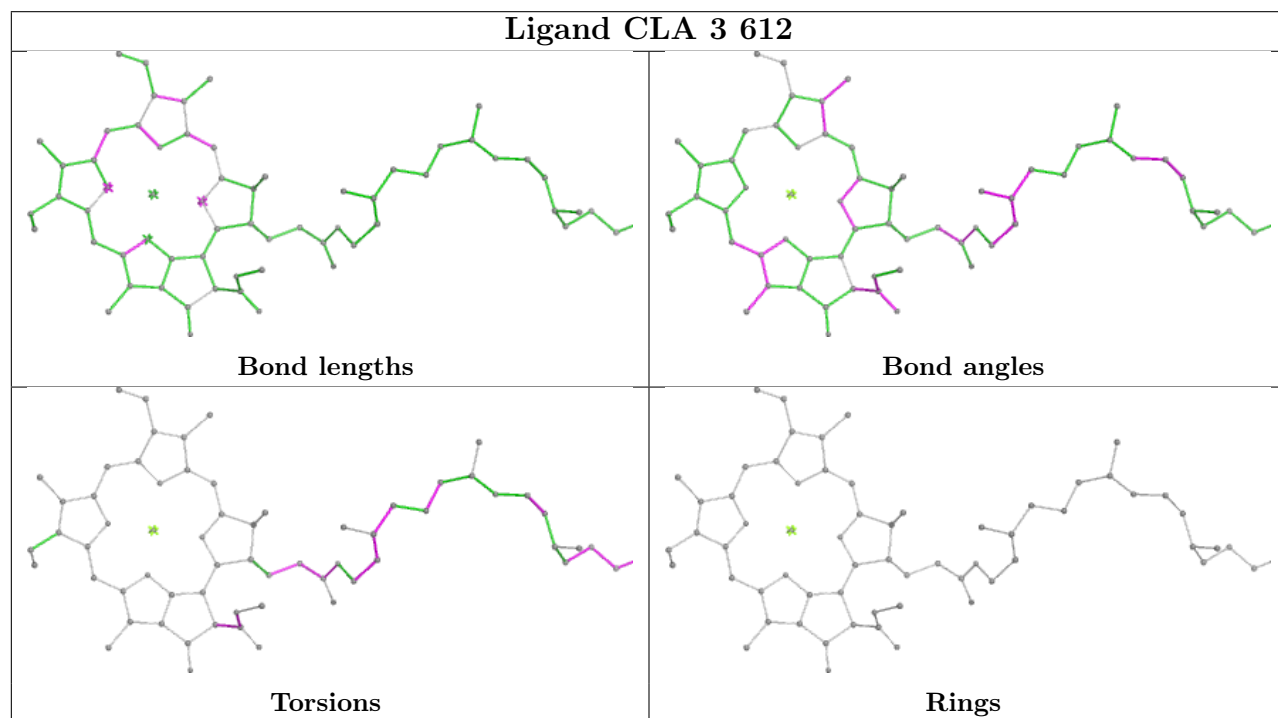
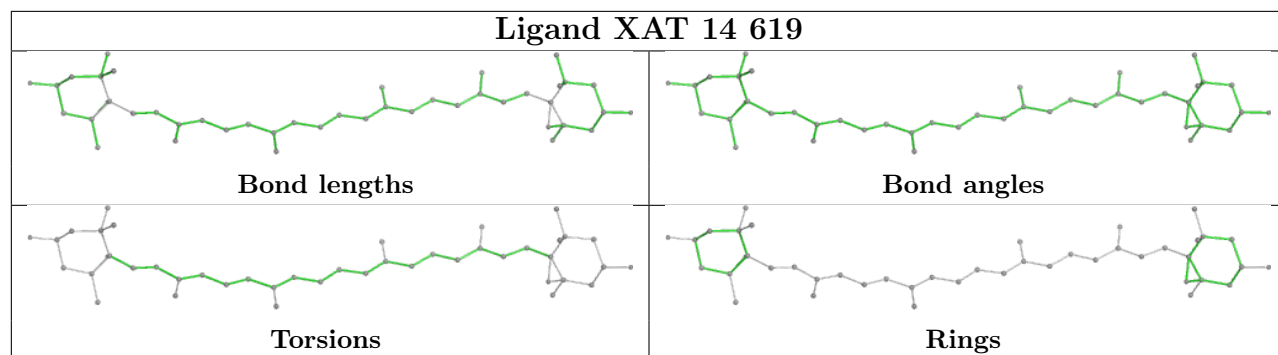




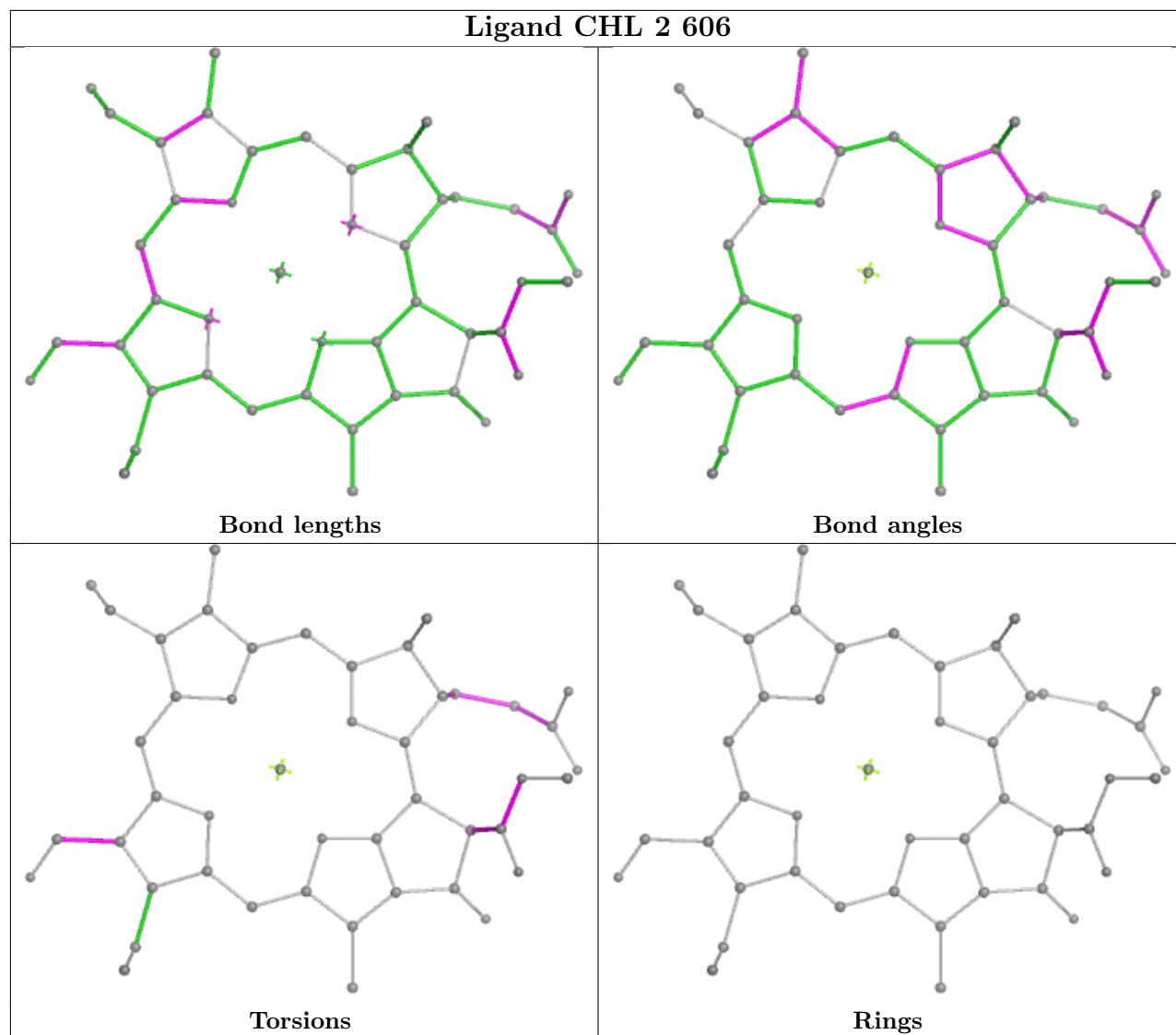


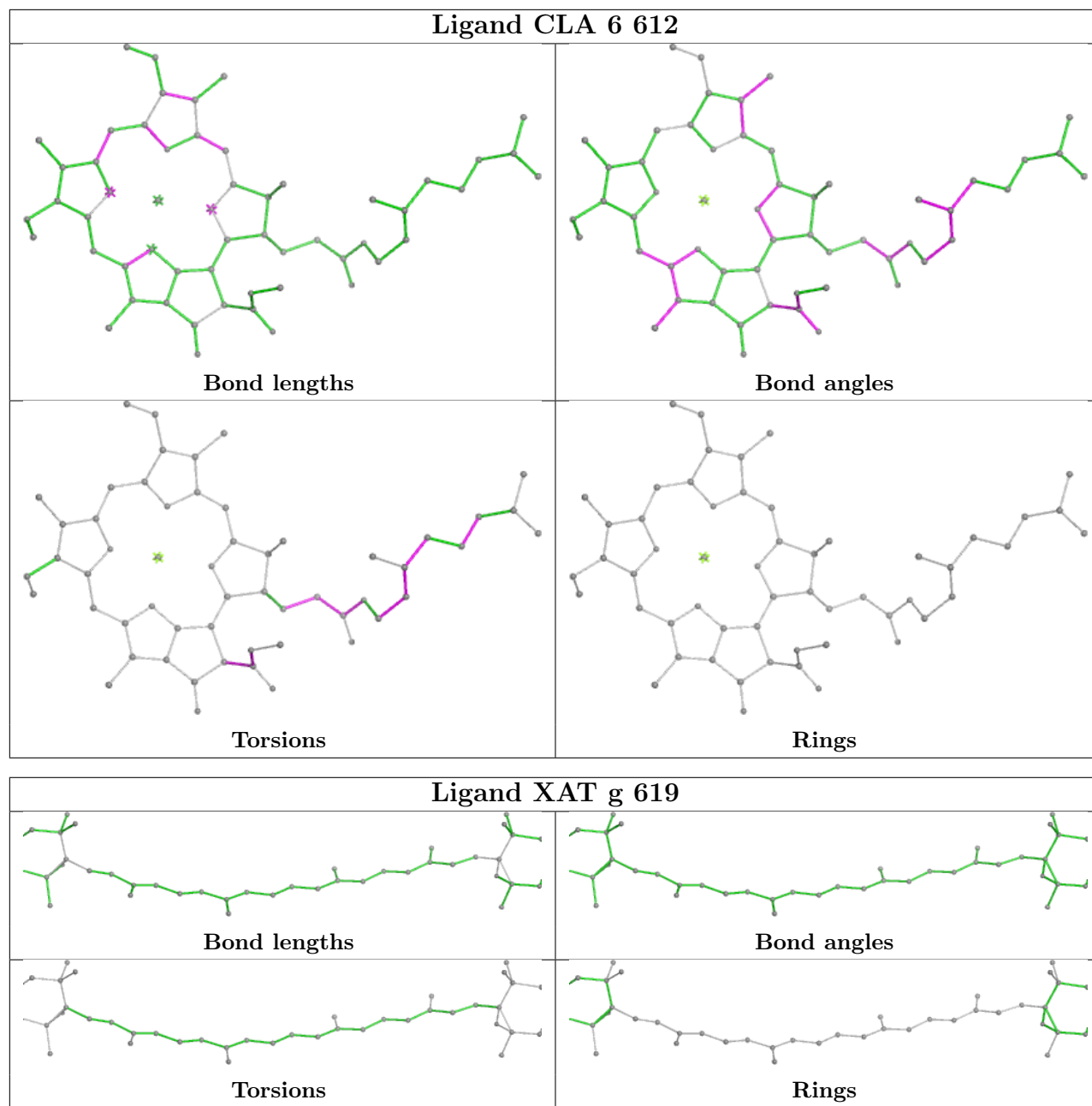


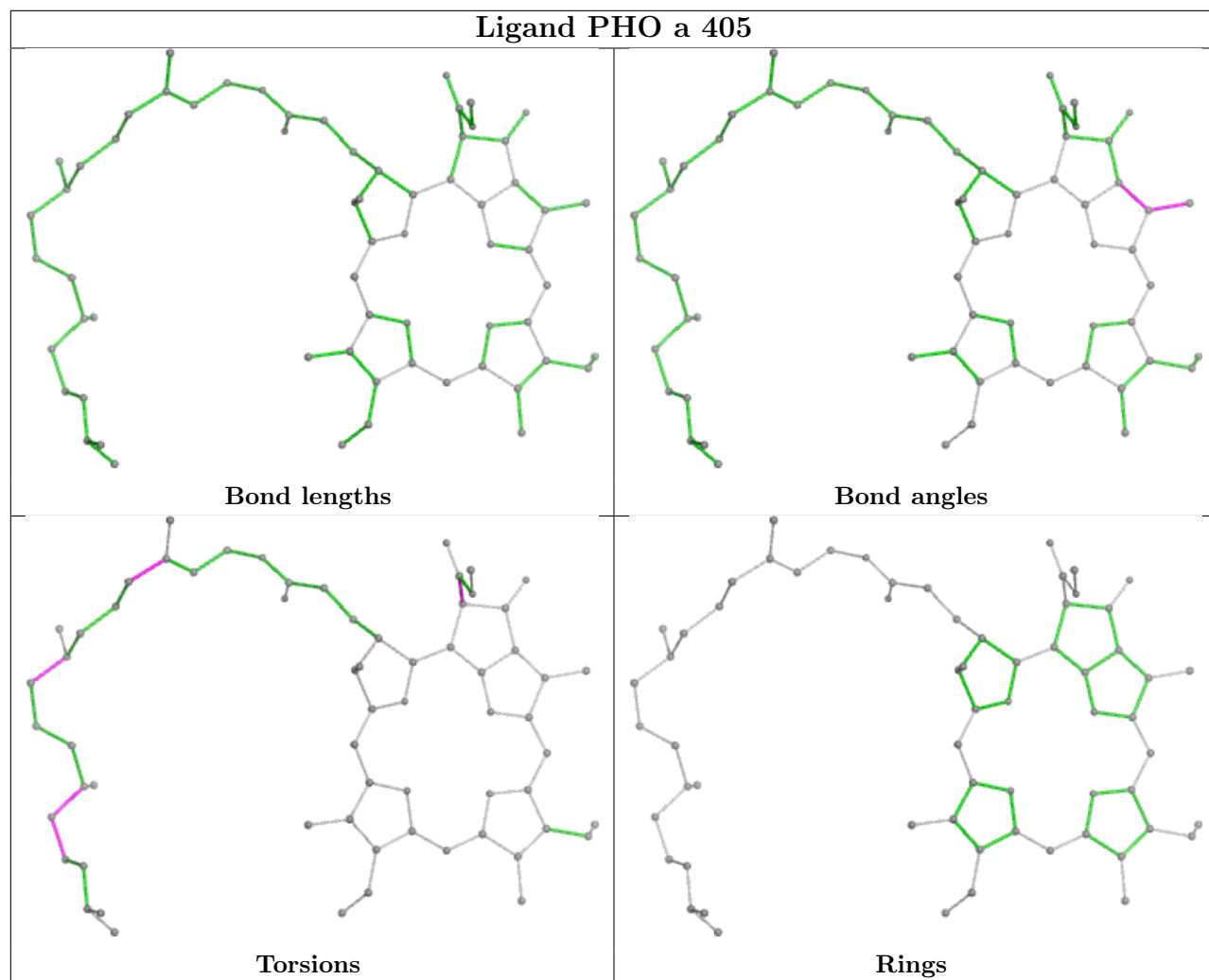


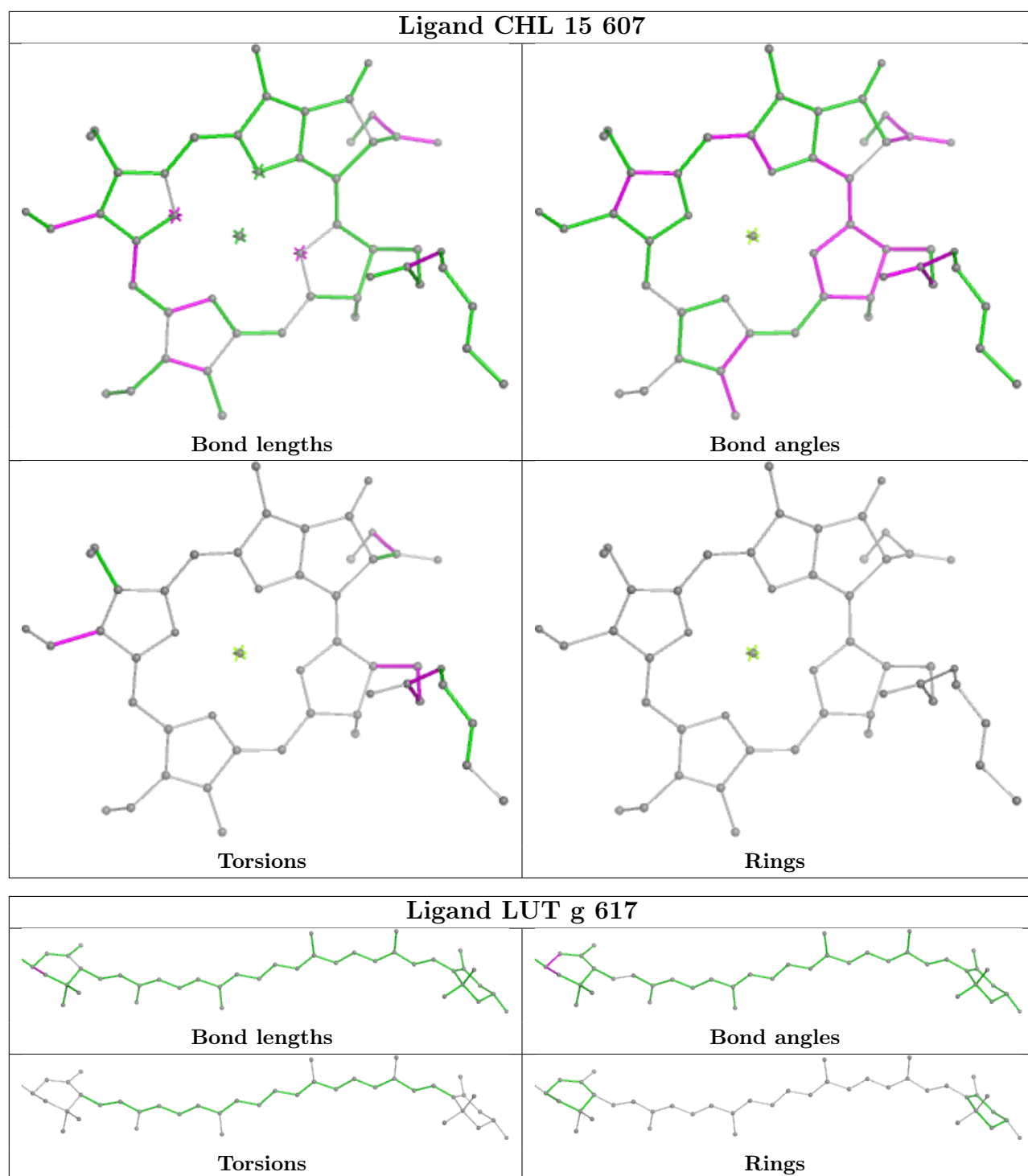


Ligand CHL 2 606

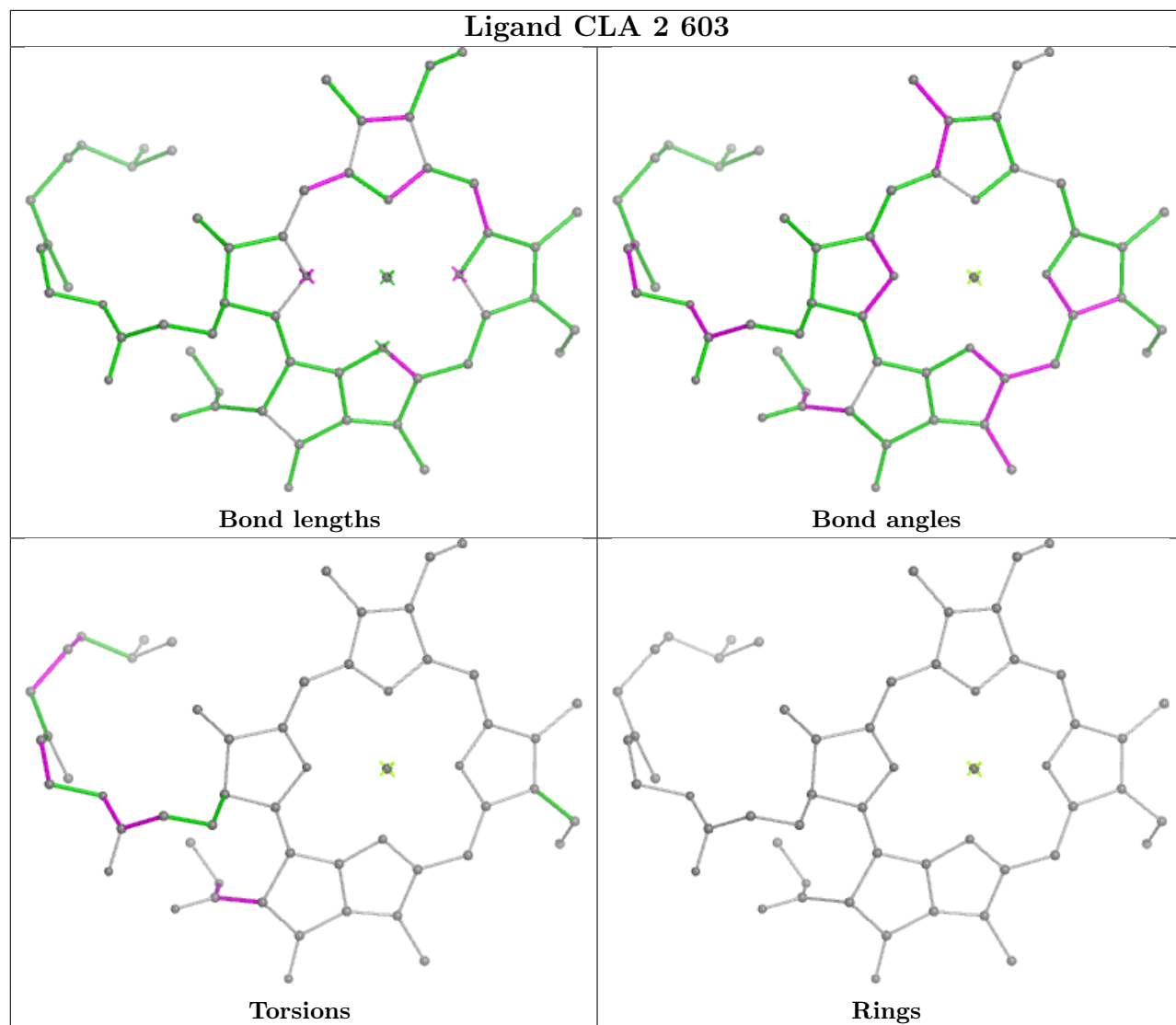


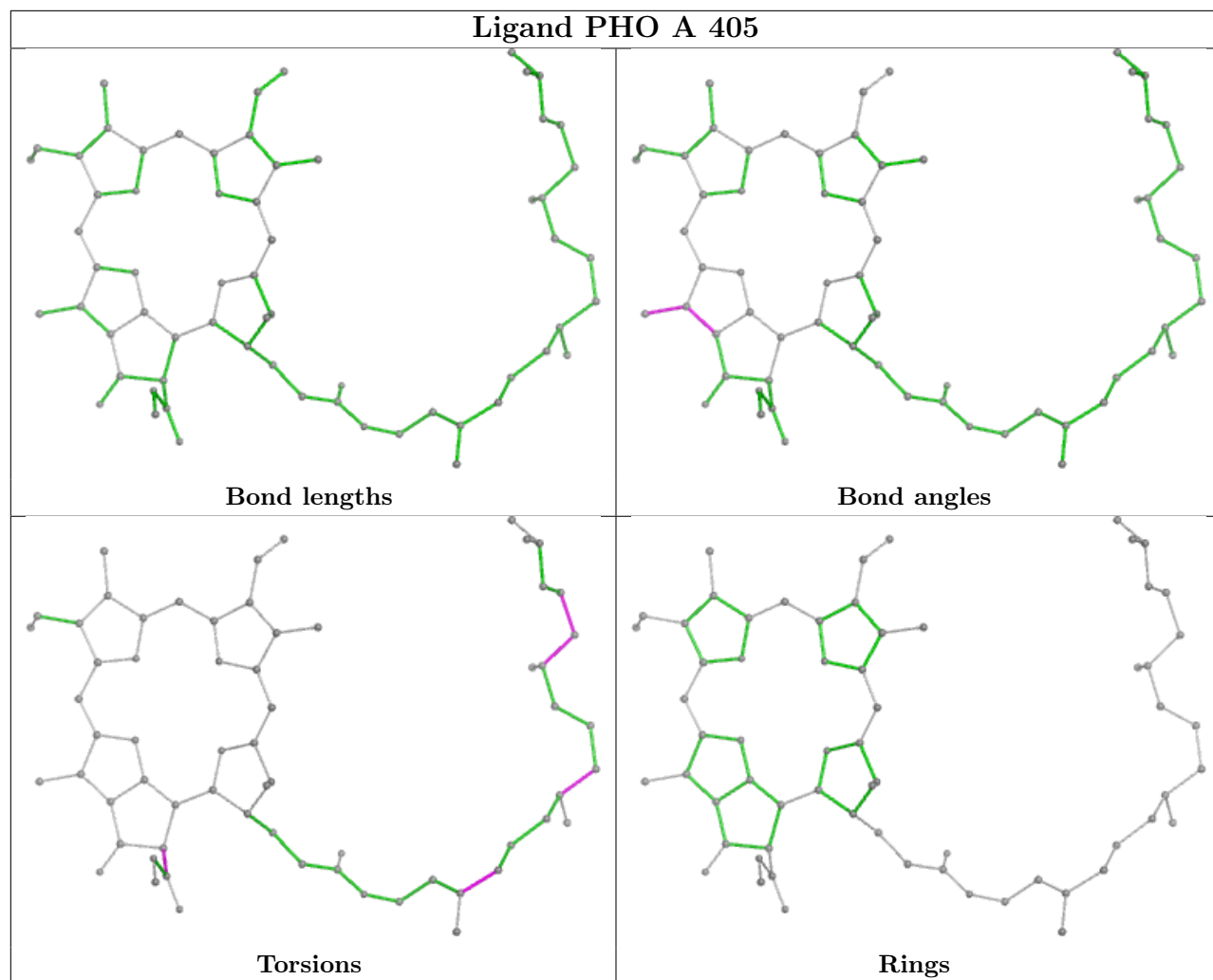




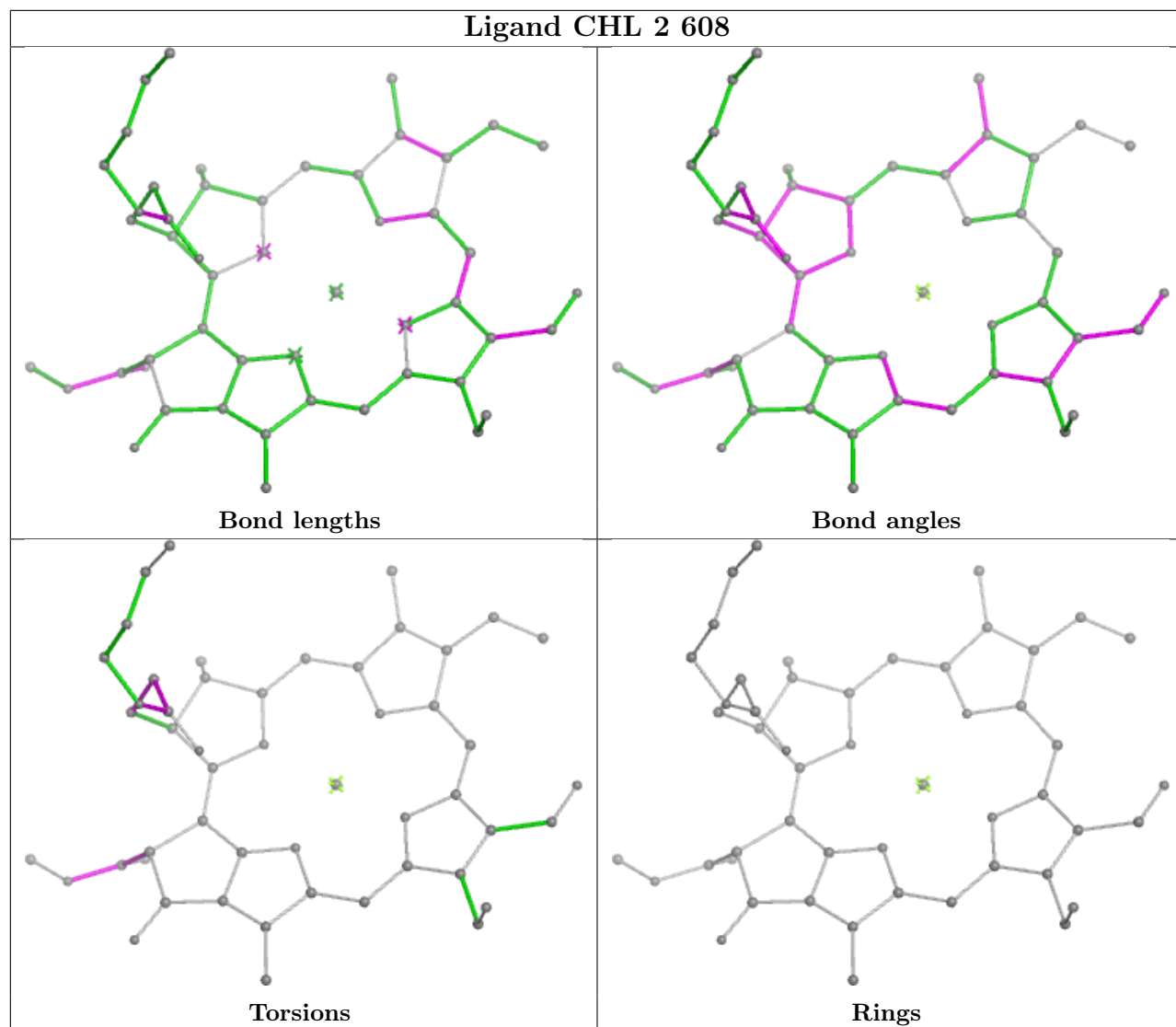


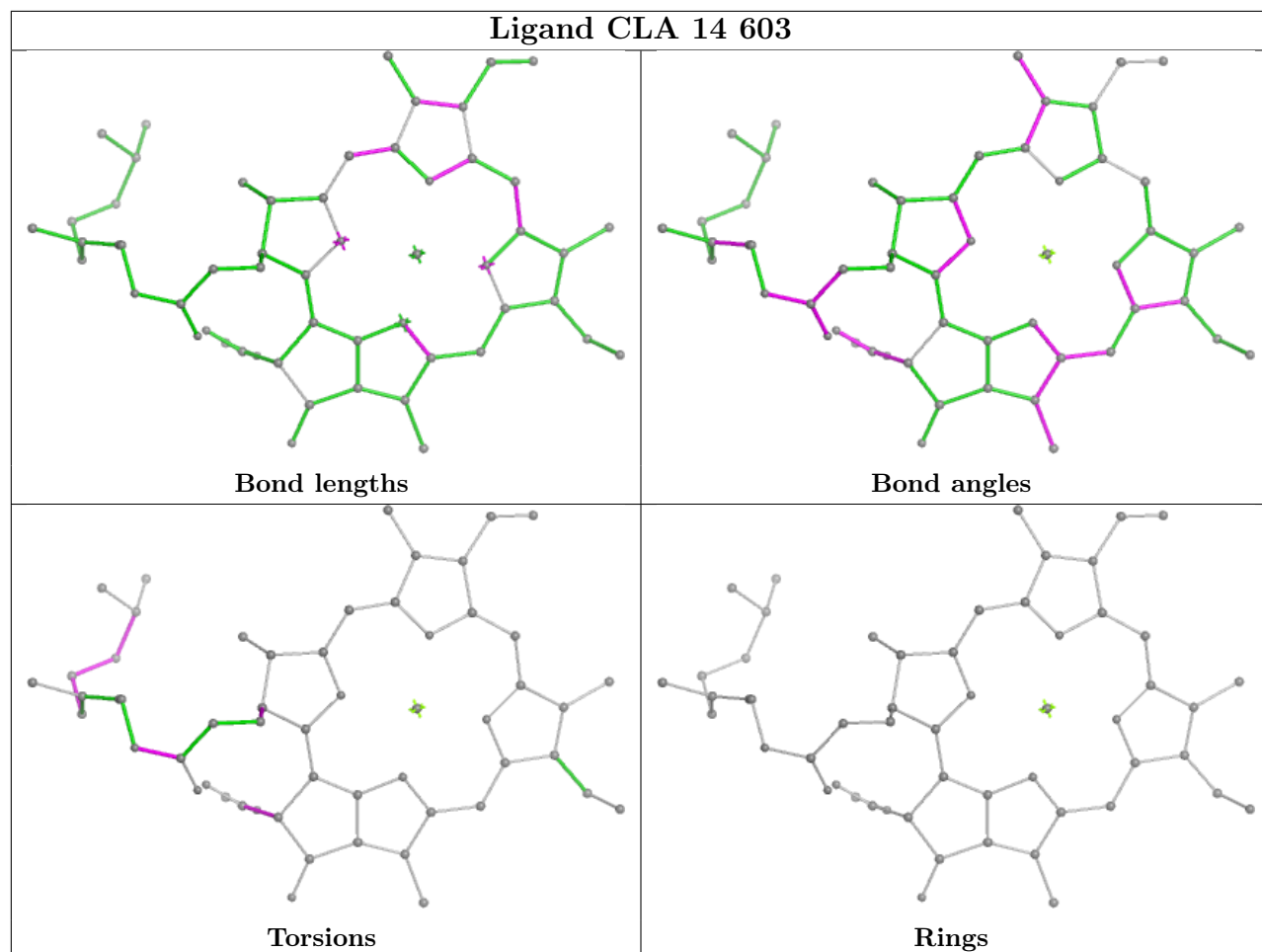
Ligand CLA 2 603

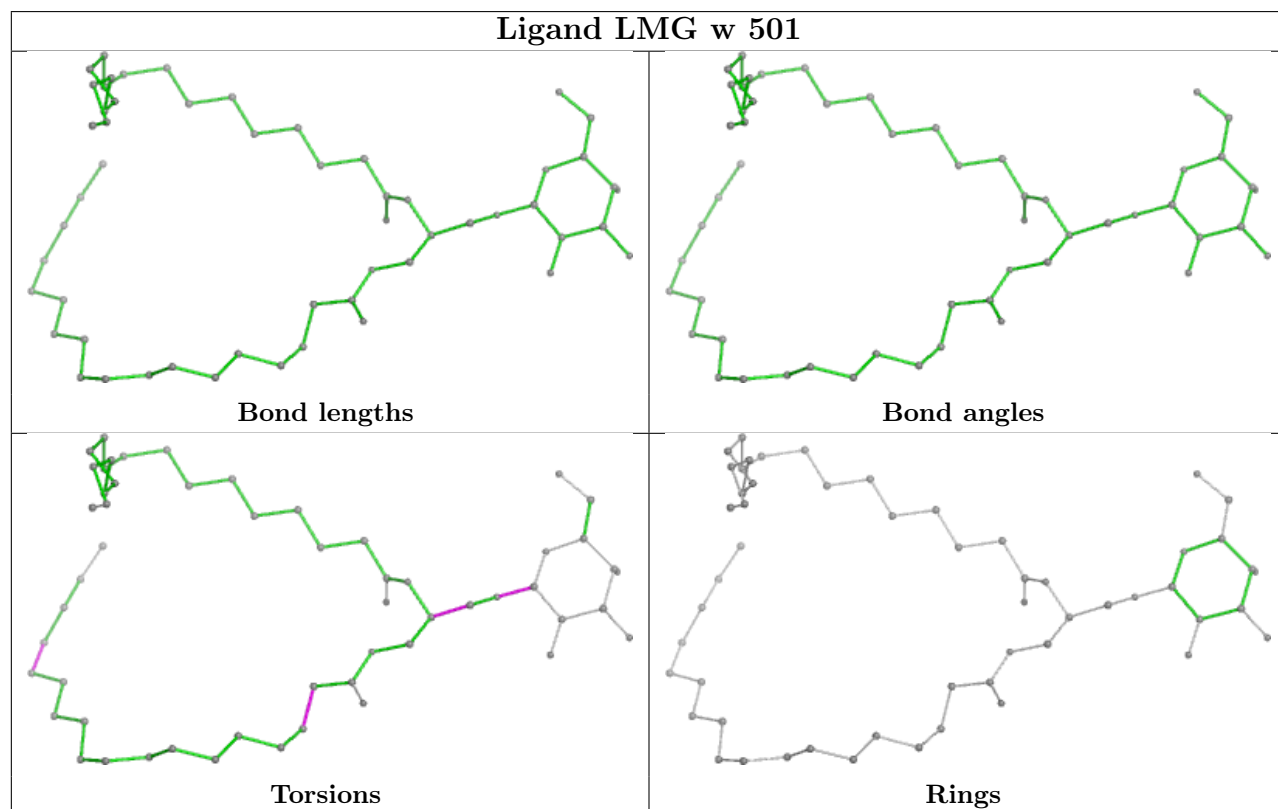
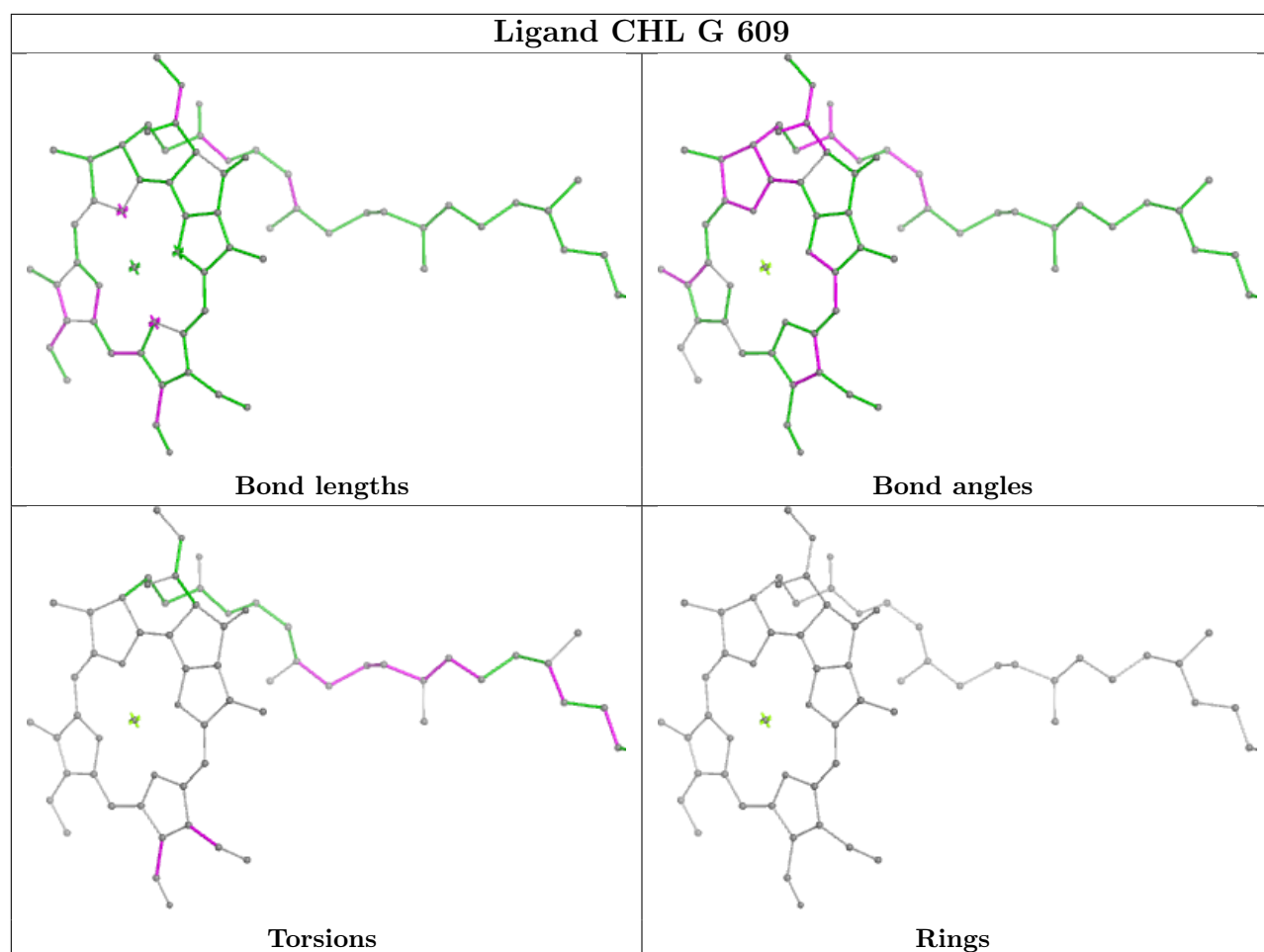


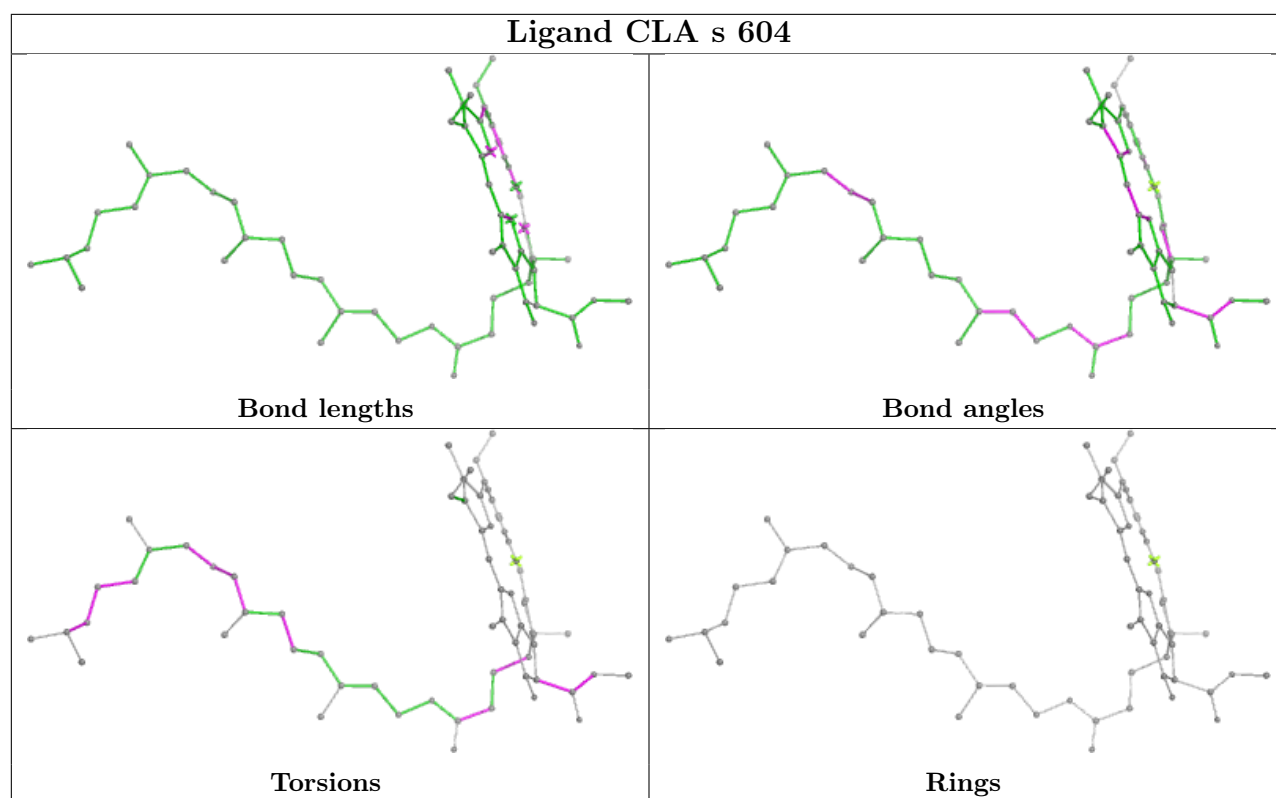


Ligand CHL 2 608

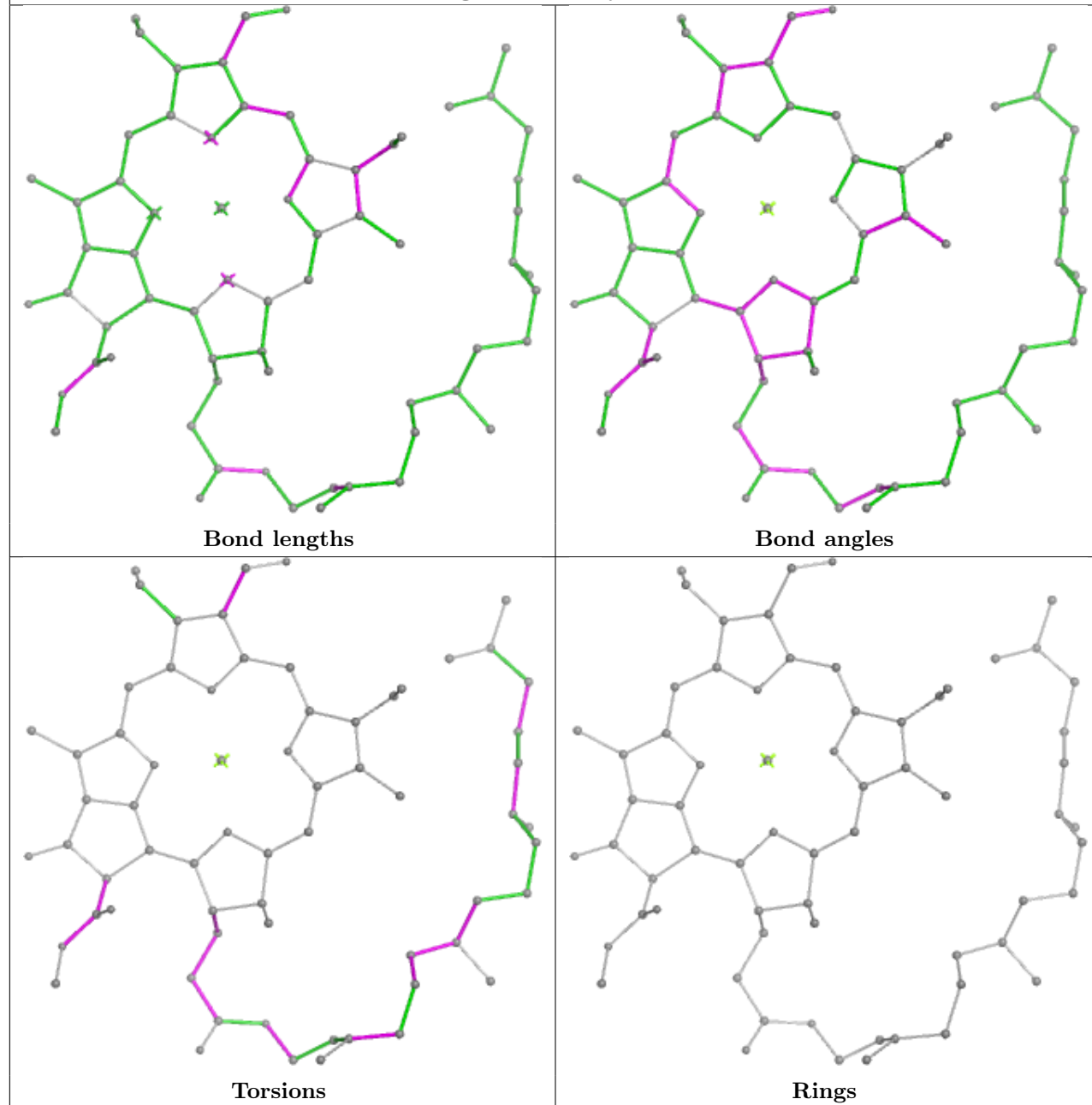




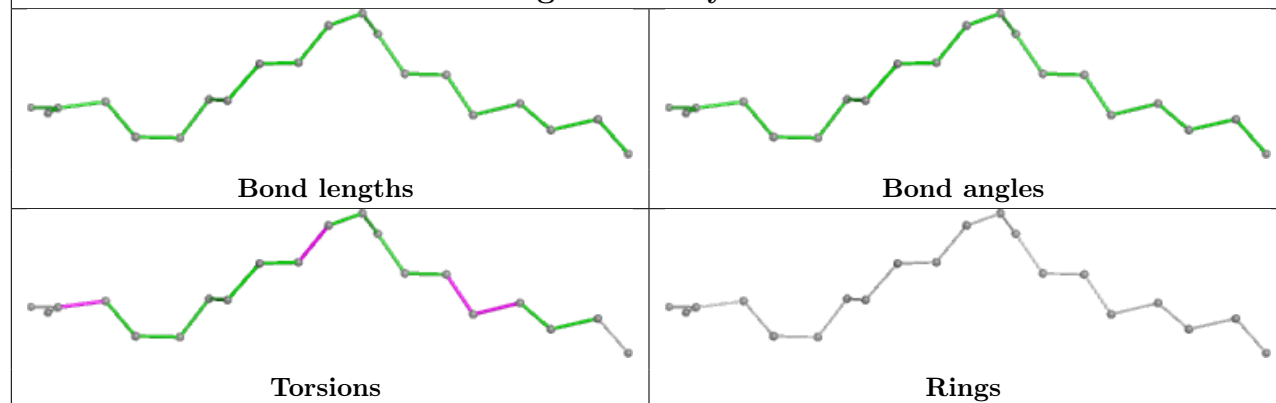


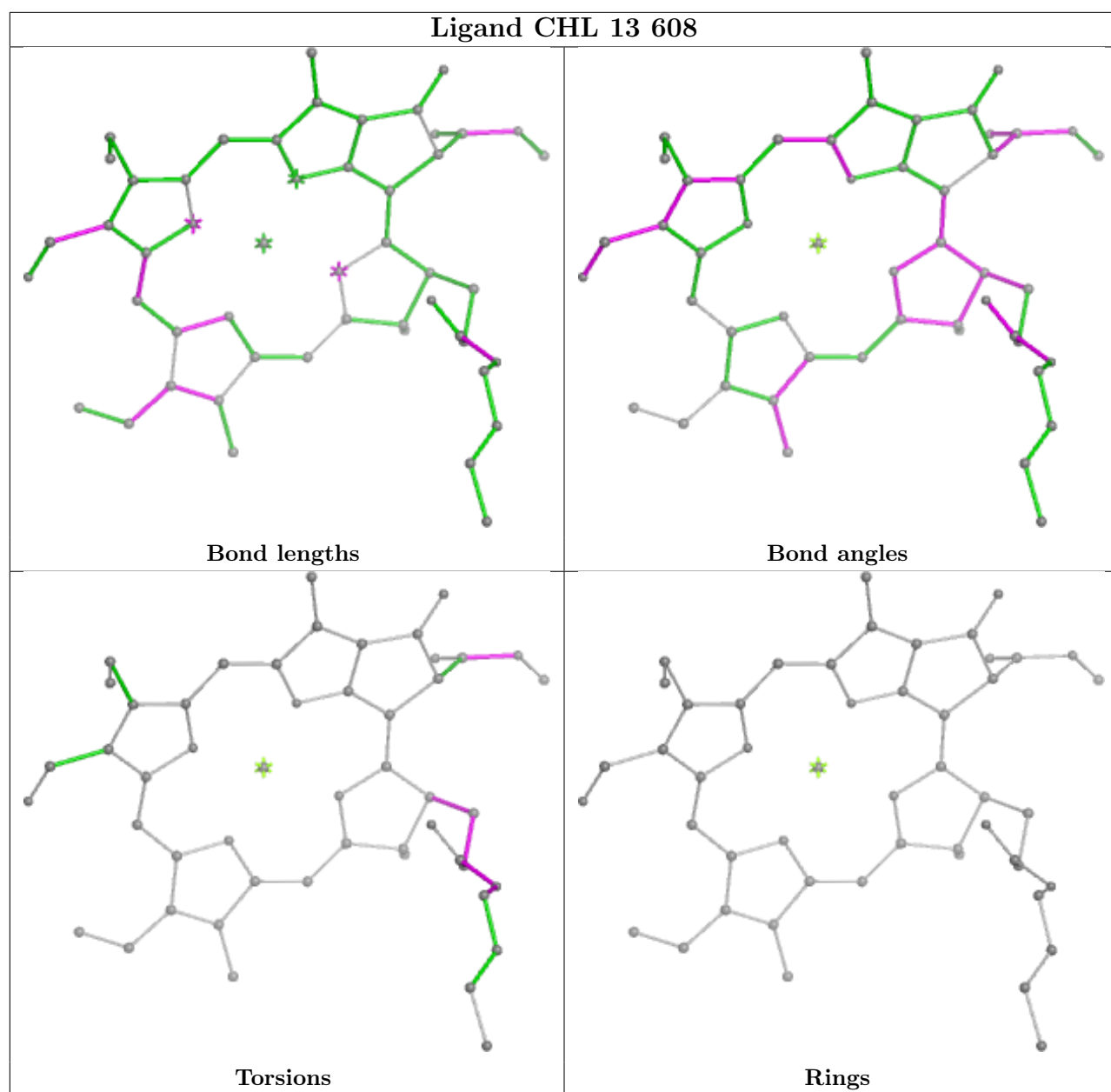


Ligand CHL y 607

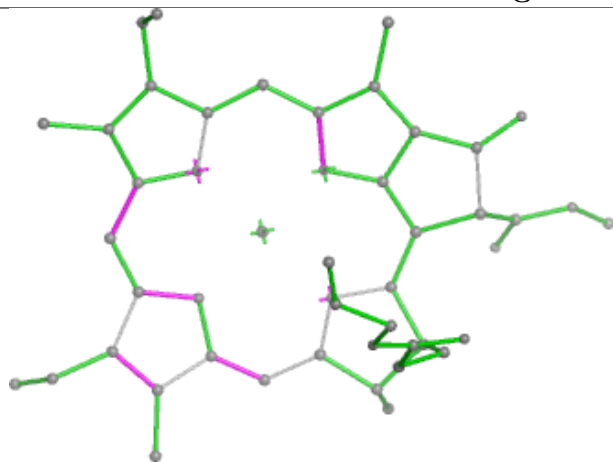


Ligand LNL y 620

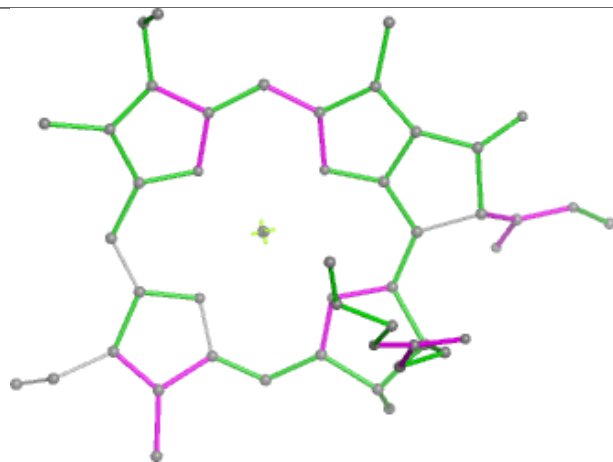




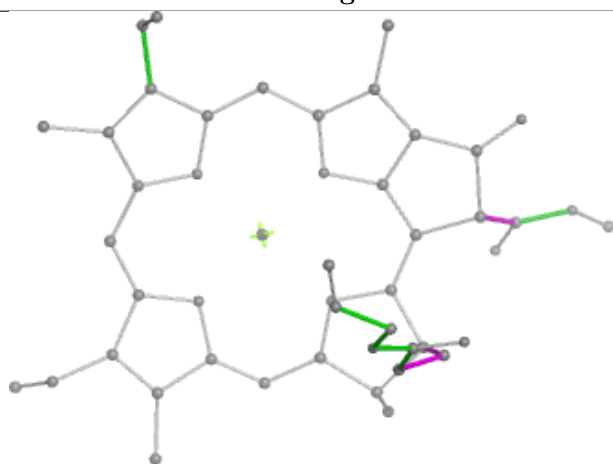
Ligand CLA R 604



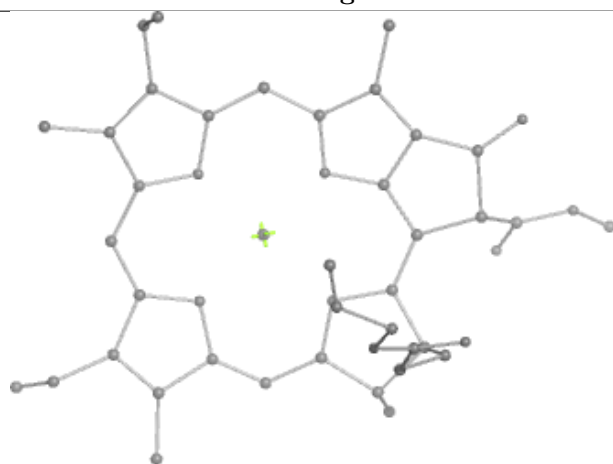
Bond lengths



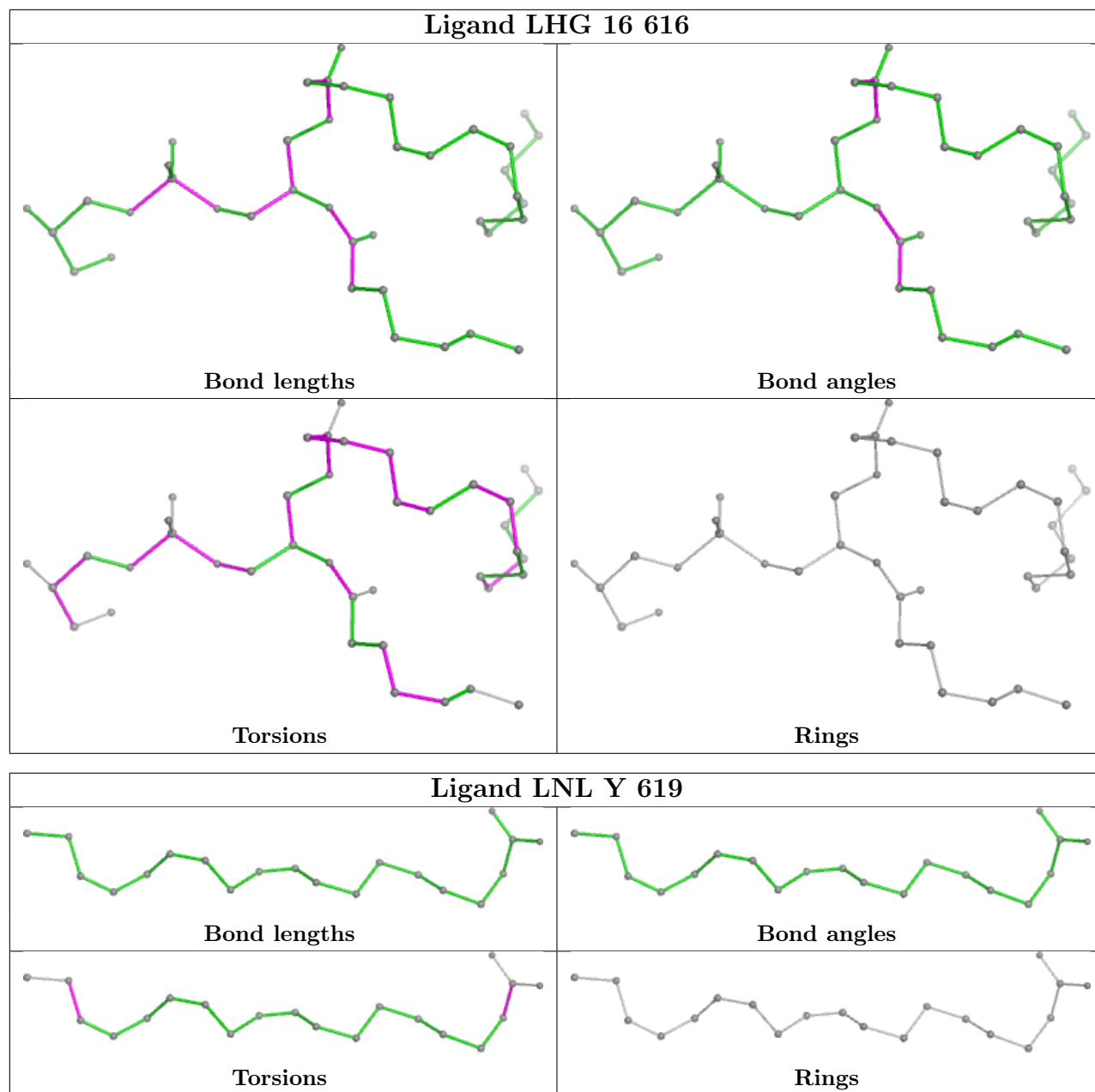
Bond angles

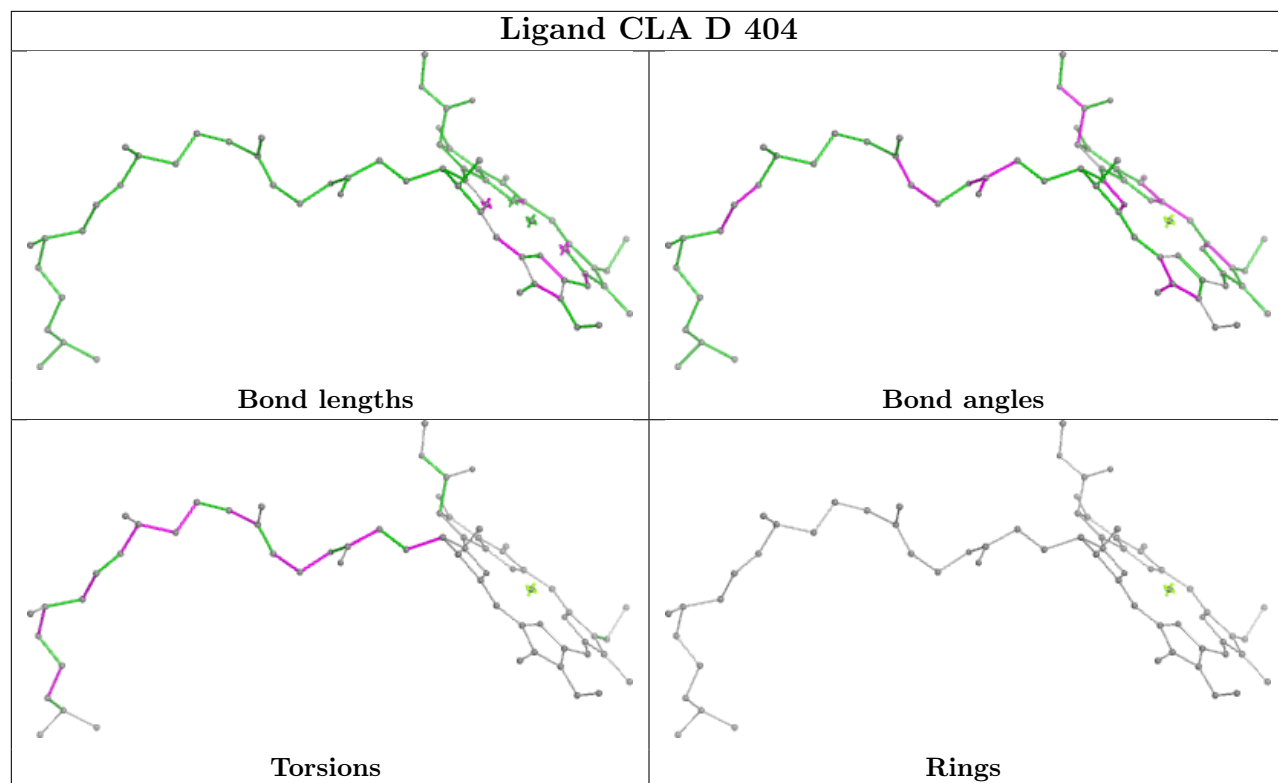


Torsions

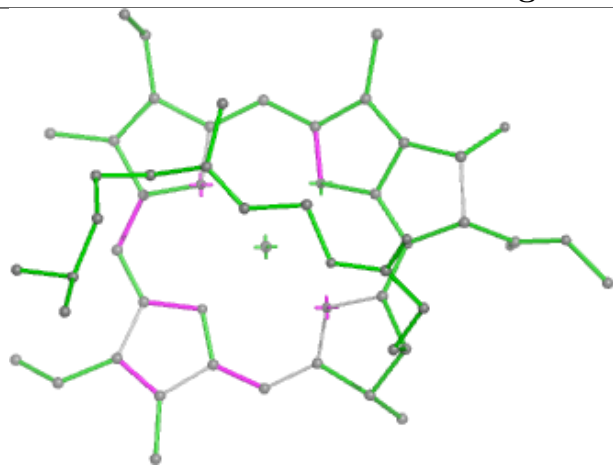


Rings

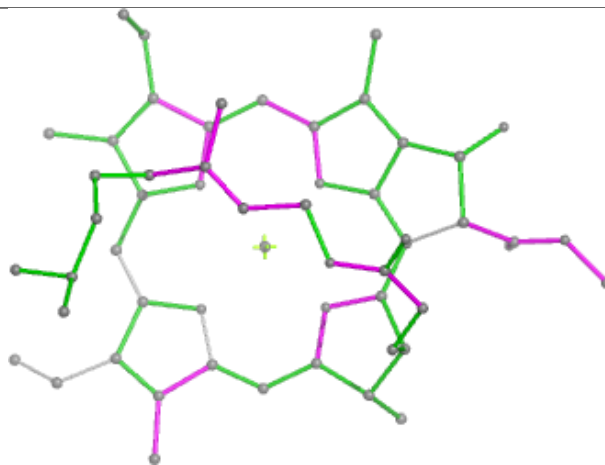




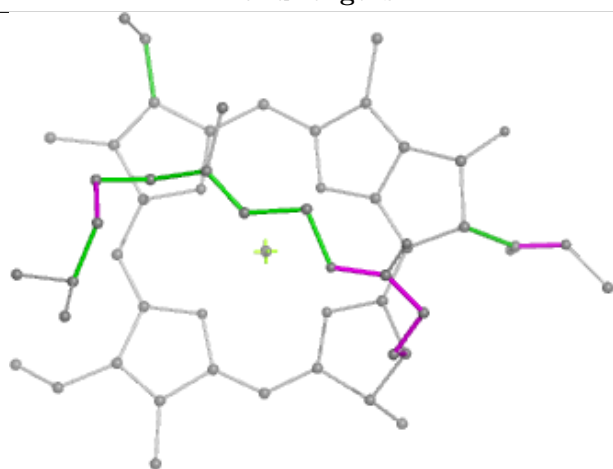
Ligand CLA 4 613



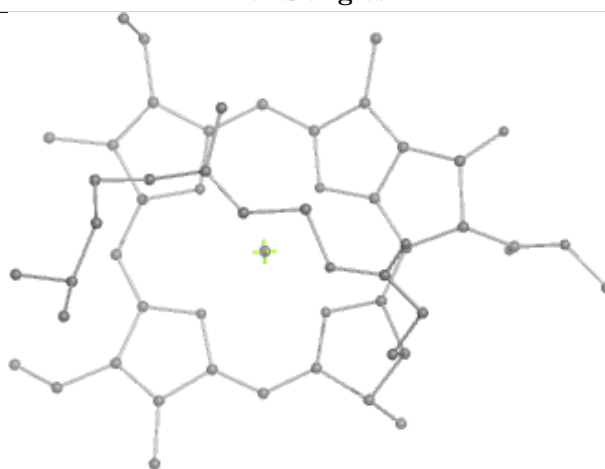
Bond lengths



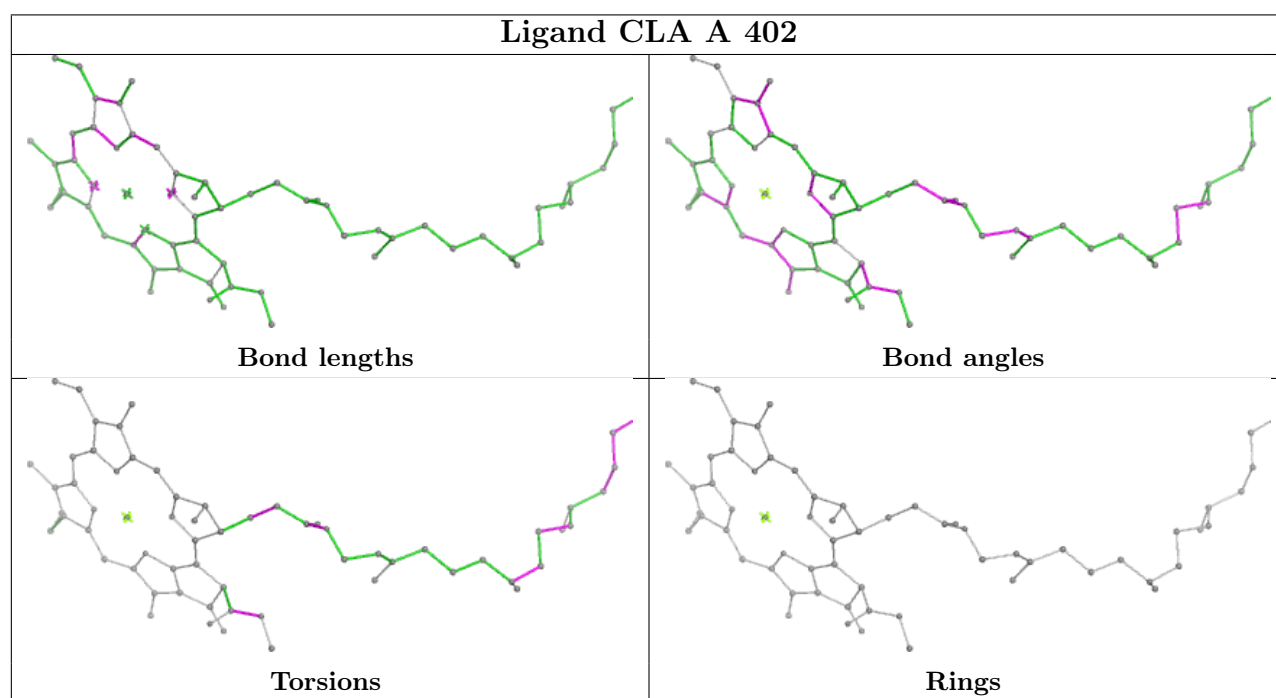
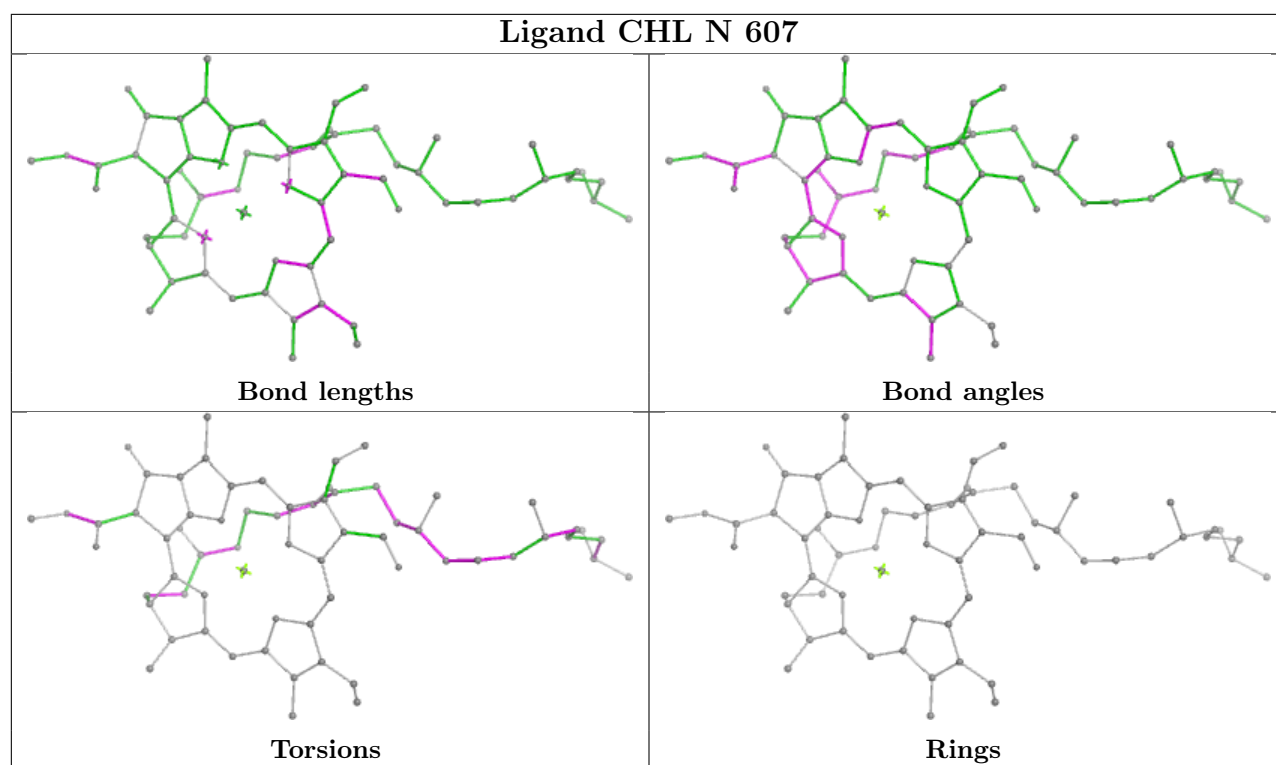
Bond angles



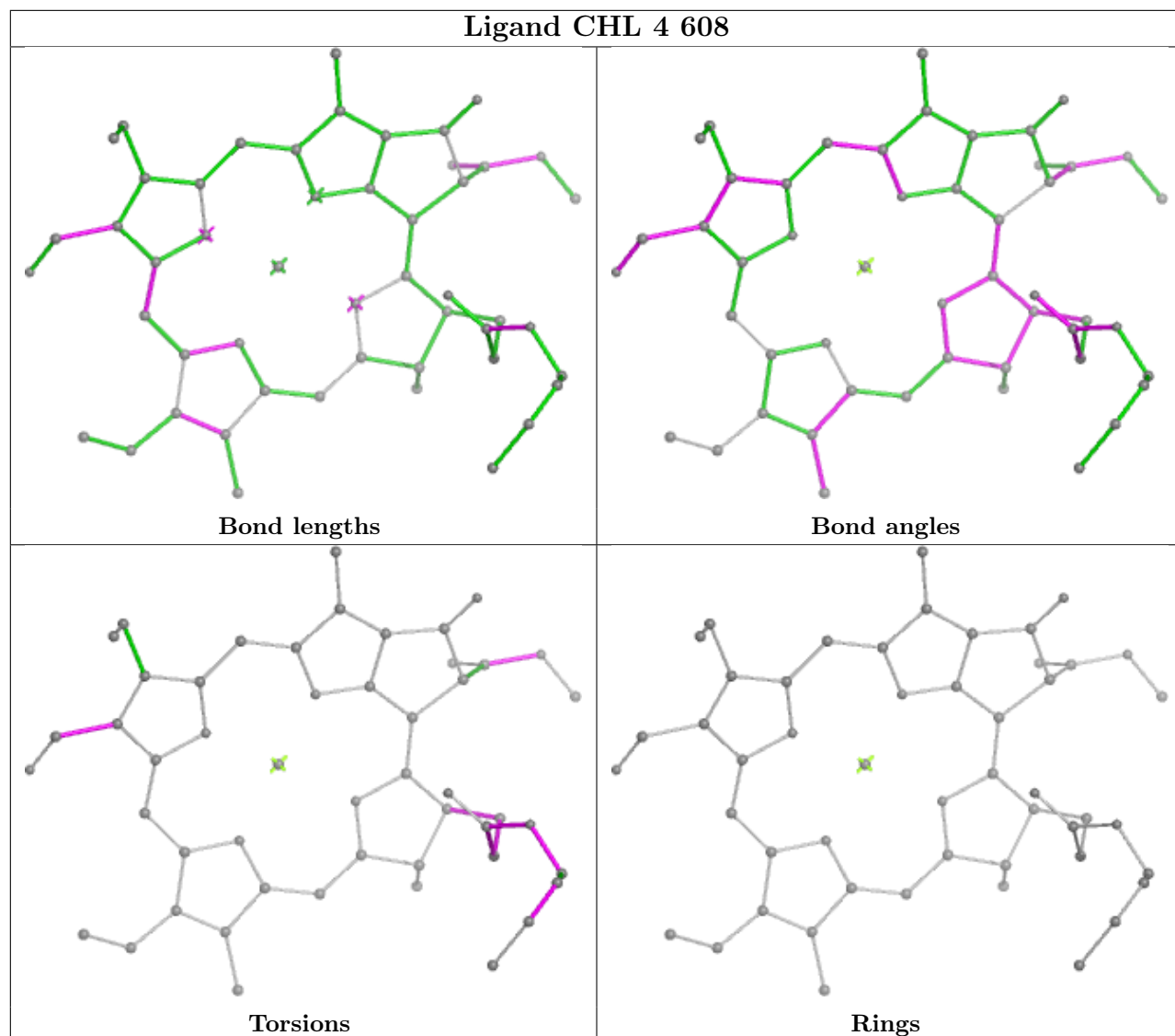
Torsions



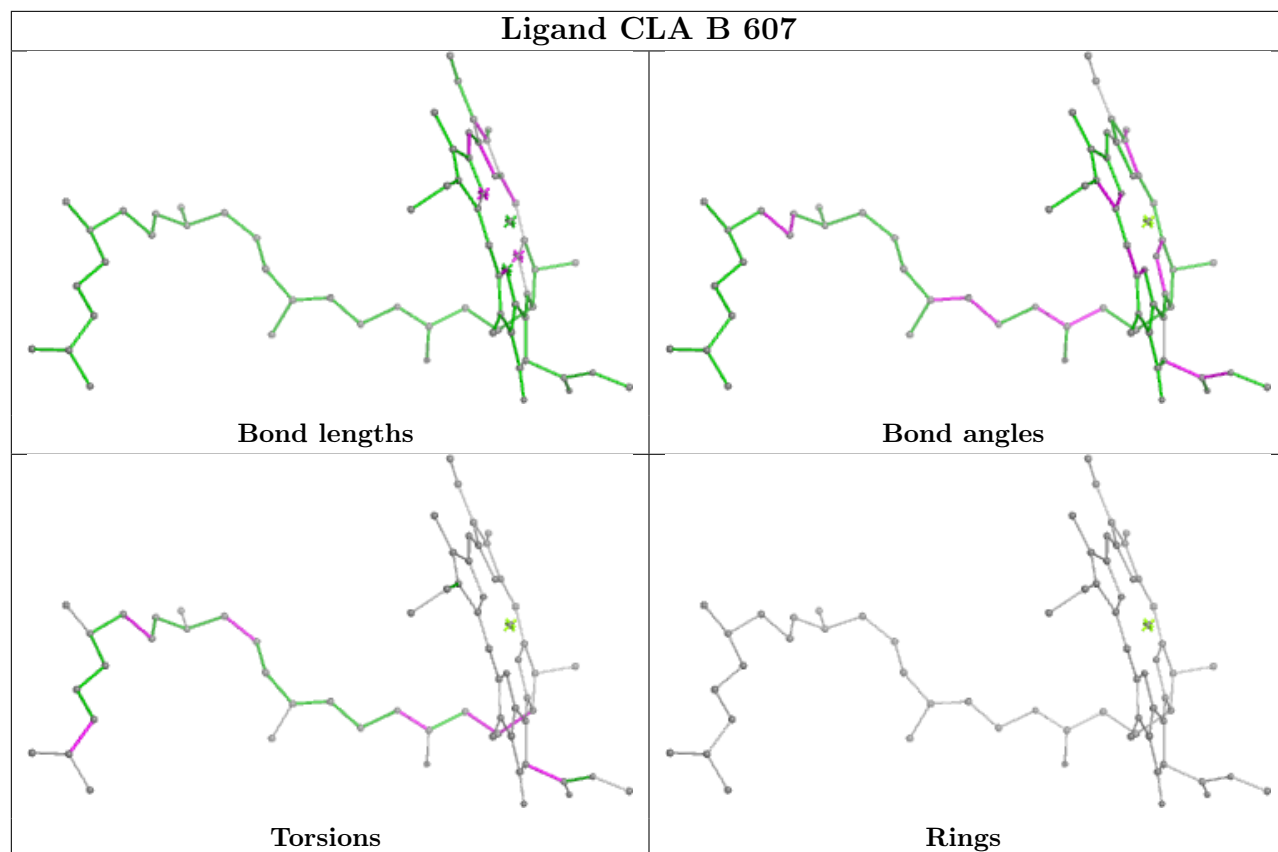
Rings



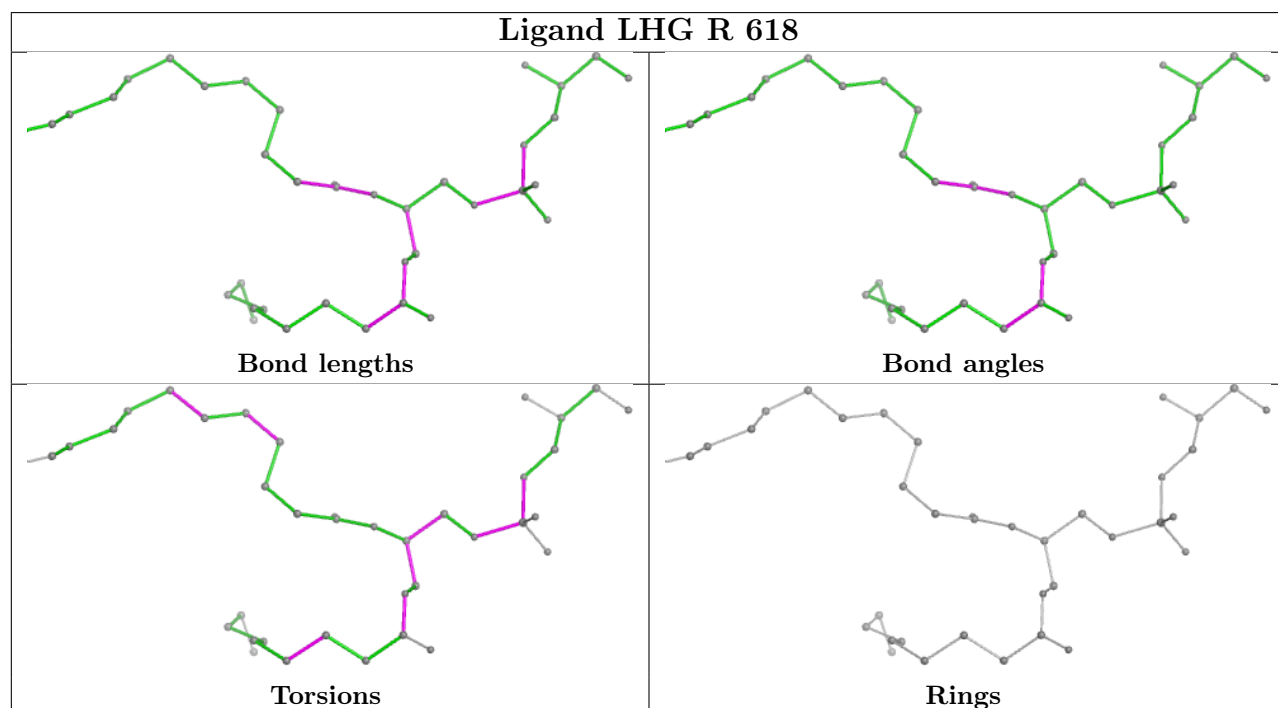
Ligand CHL 4 608

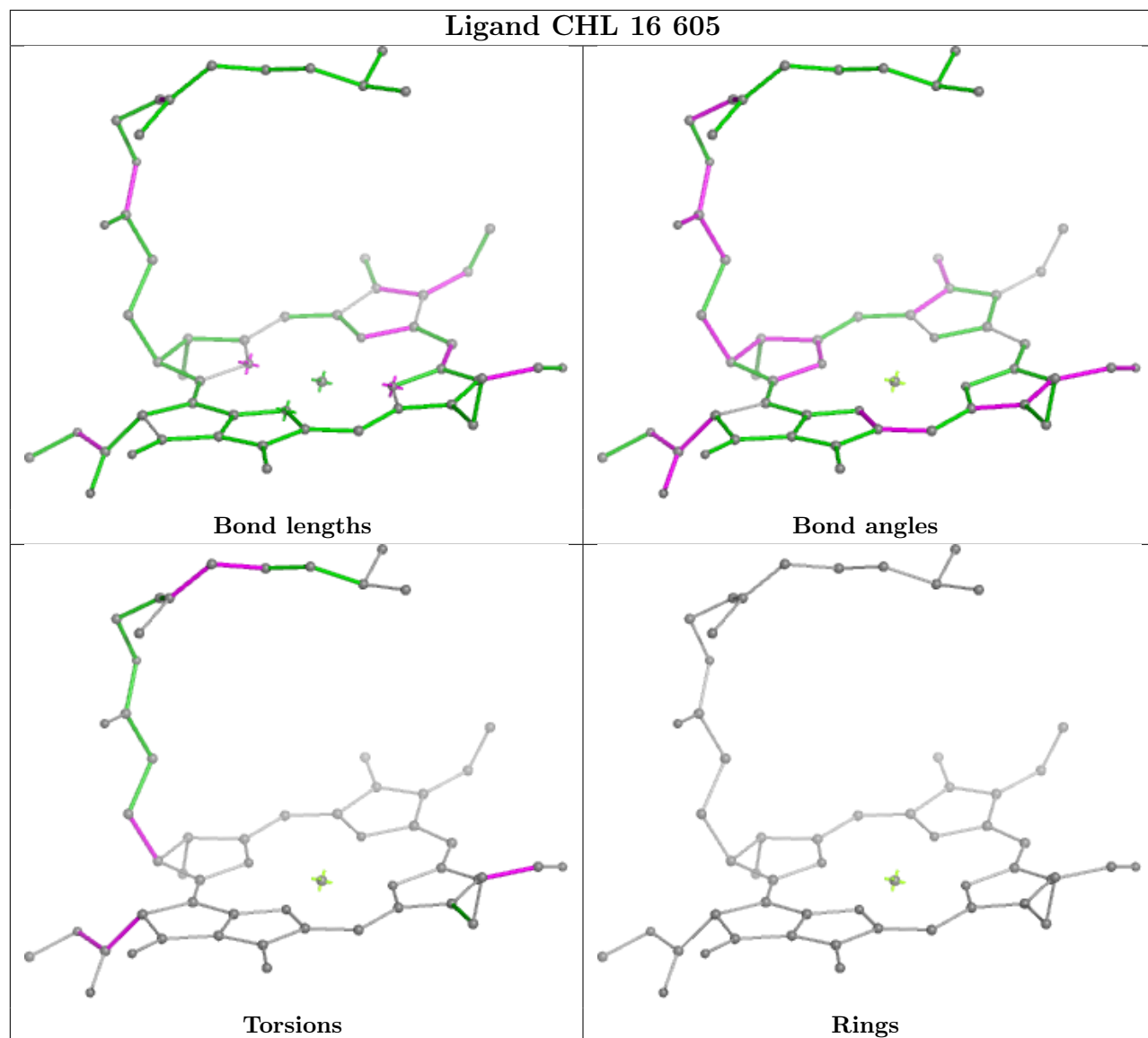


Ligand CLA B 607

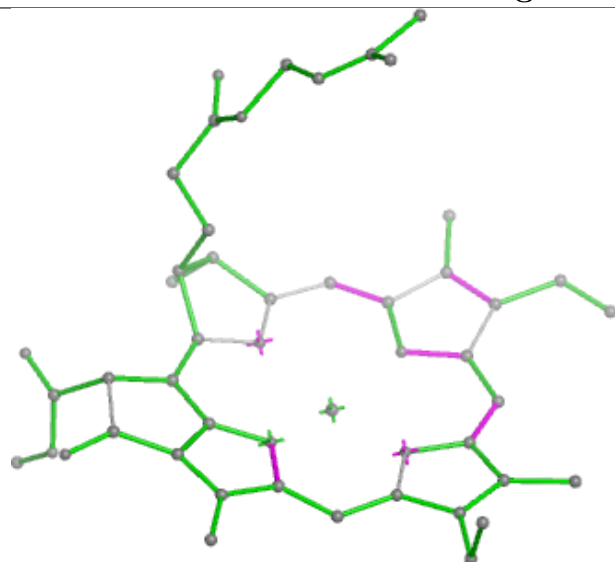


Ligand LHG R 618

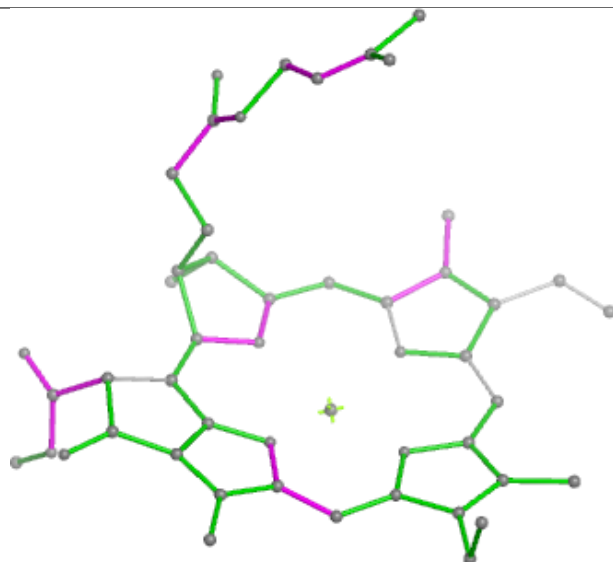




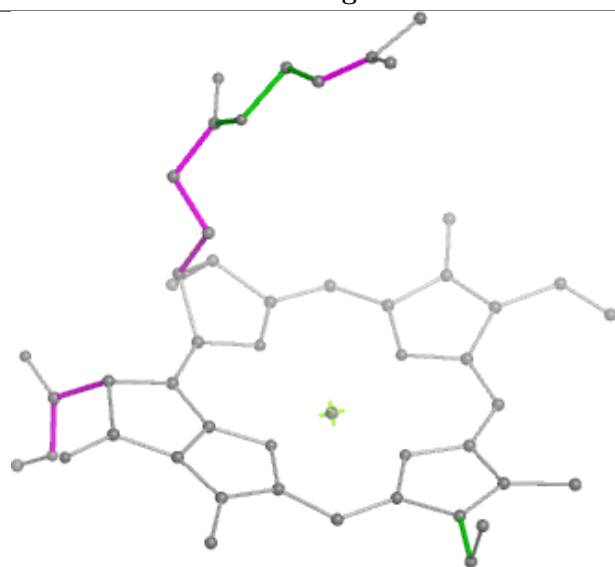
Ligand CLA R 612



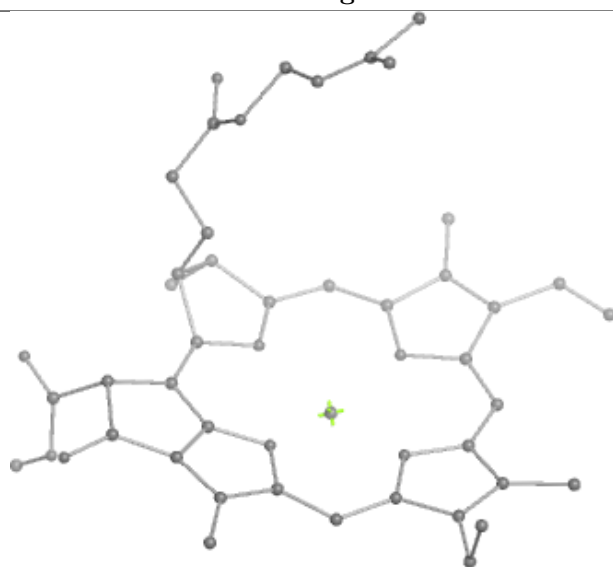
Bond lengths



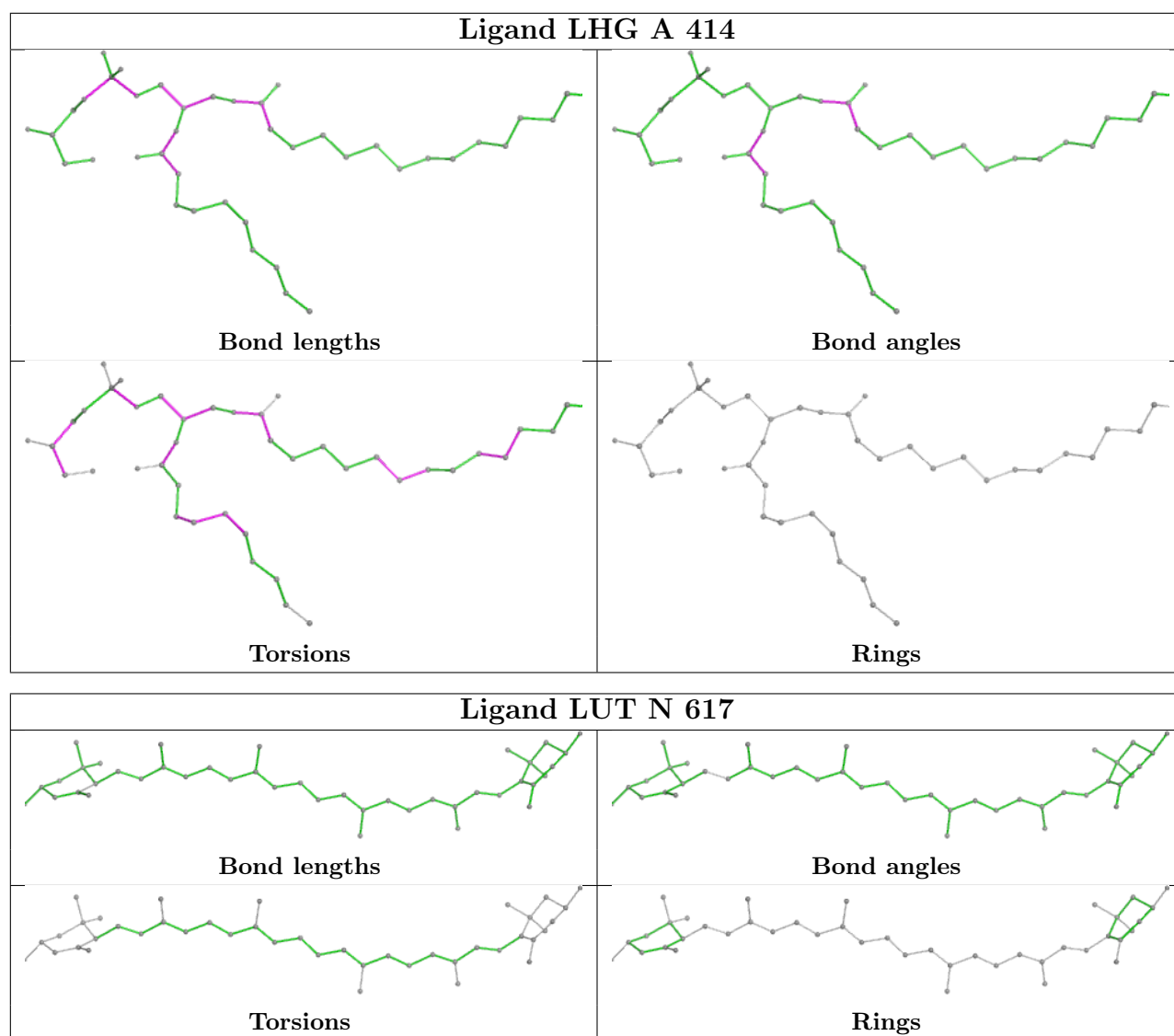
Bond angles



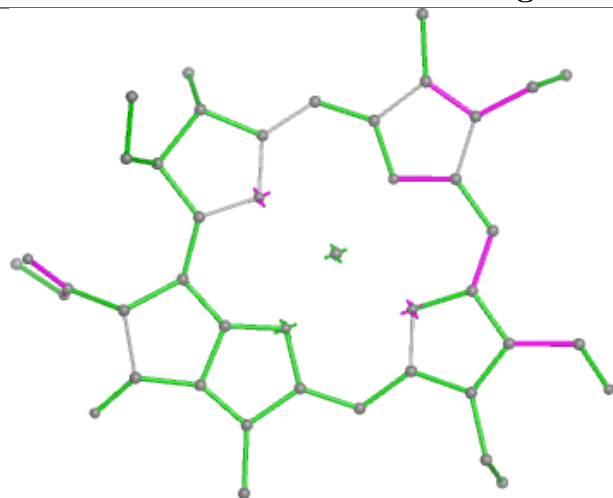
Torsions



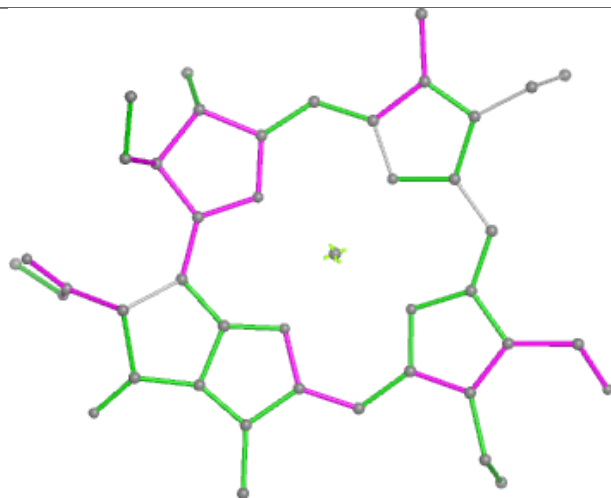
Rings



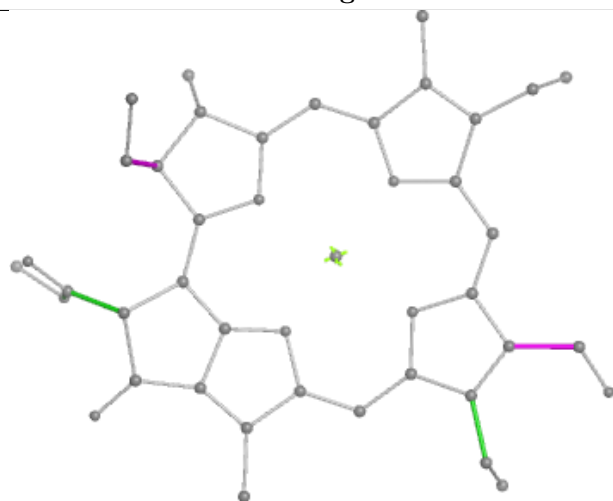
Ligand CHL S 607



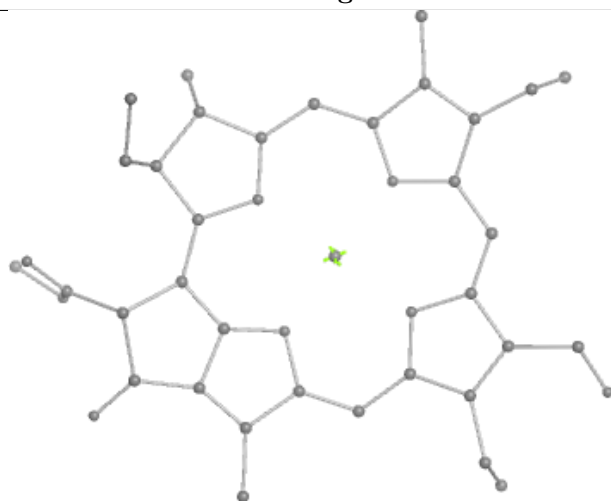
Bond lengths



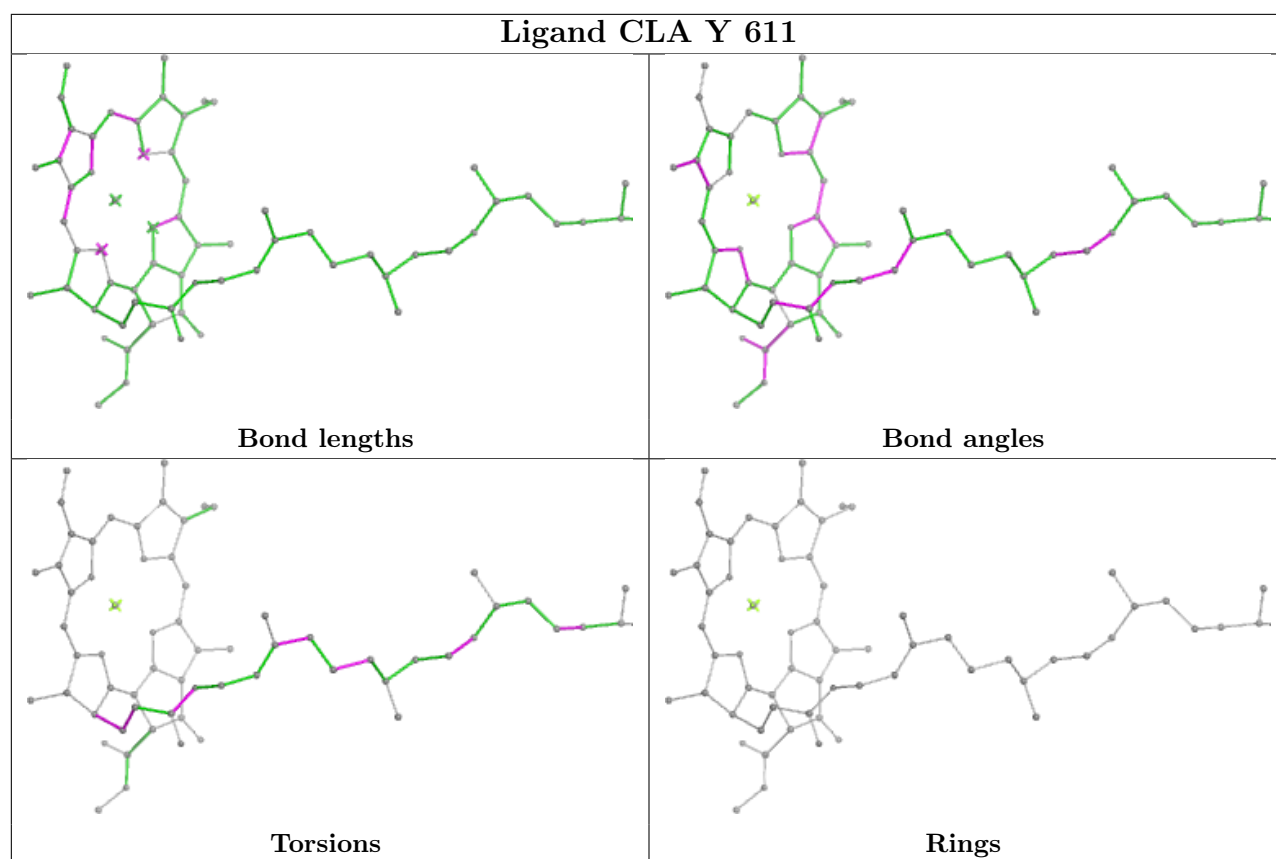
Bond angles

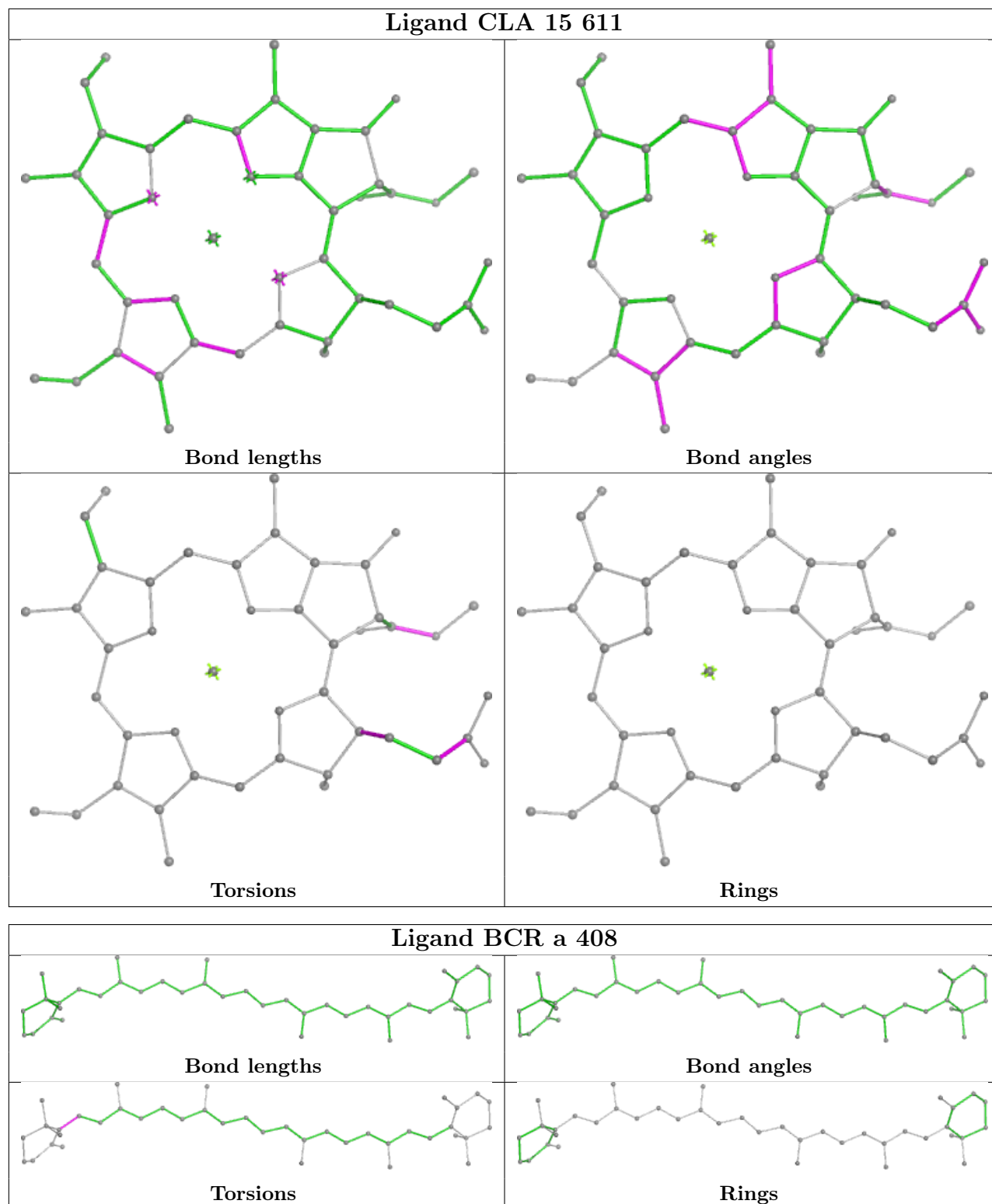


Torsions

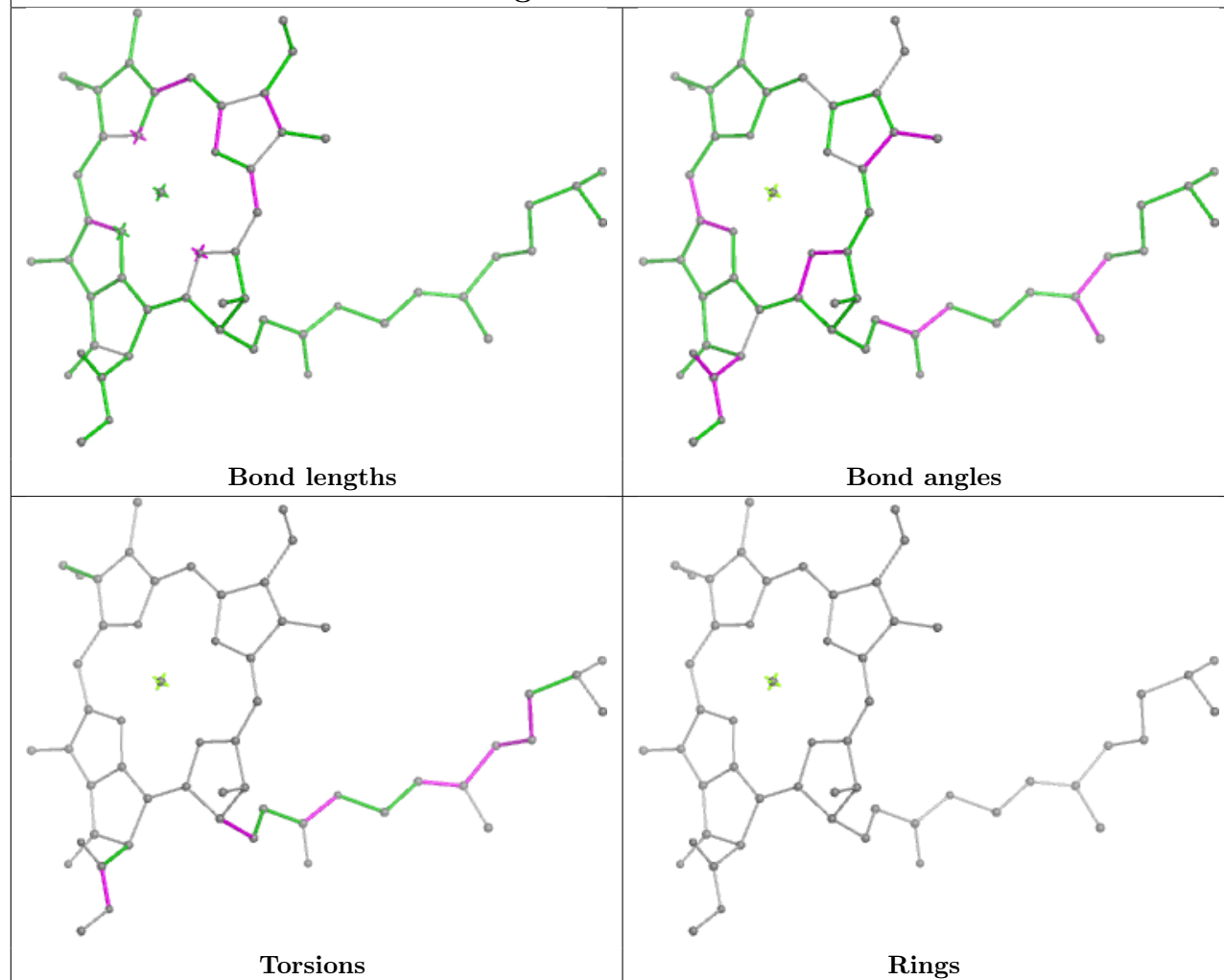


Rings

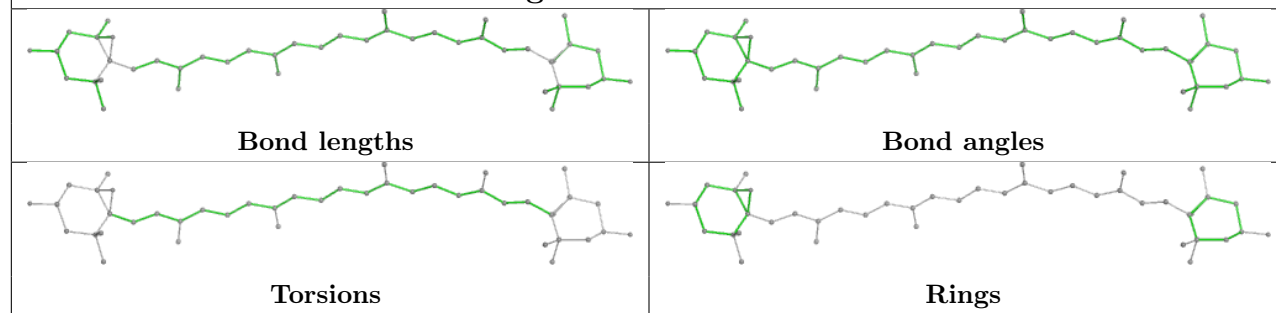




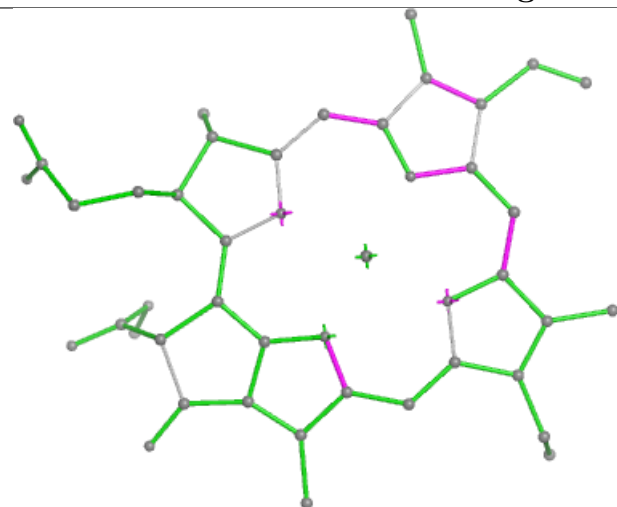
Ligand CLA a 407



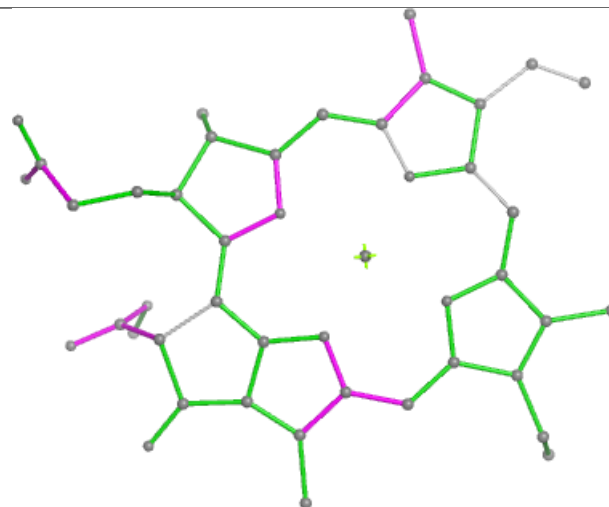
Ligand XAT 11 619



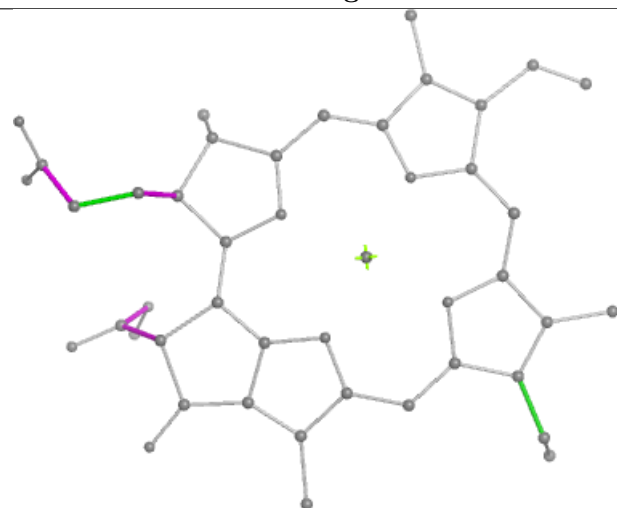
Ligand CLA N 612



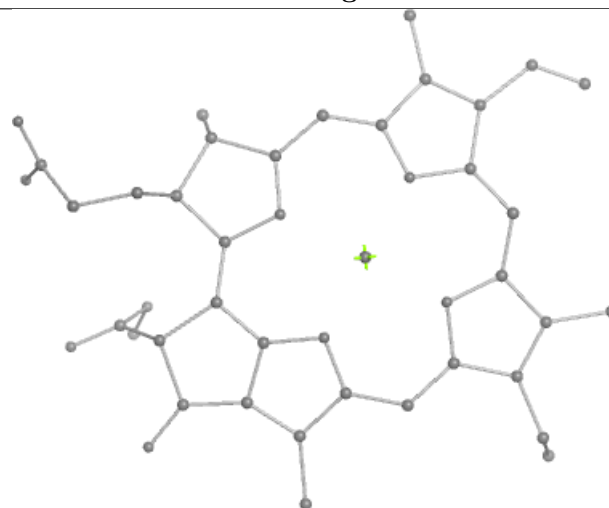
Bond lengths



Bond angles

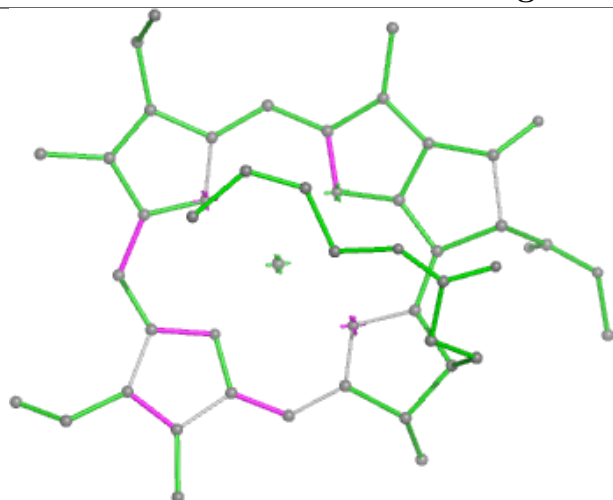


Torsions

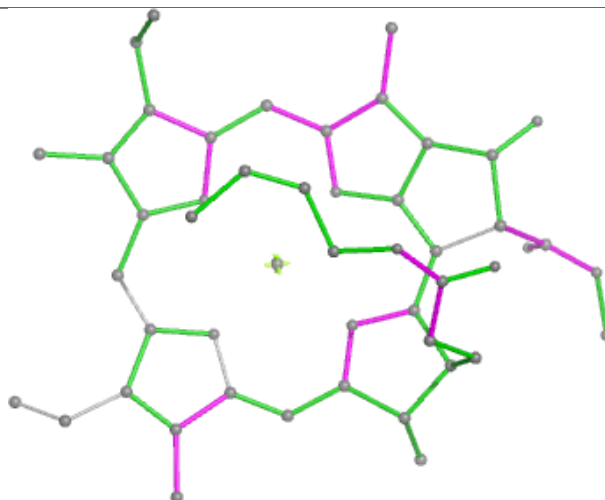


Rings

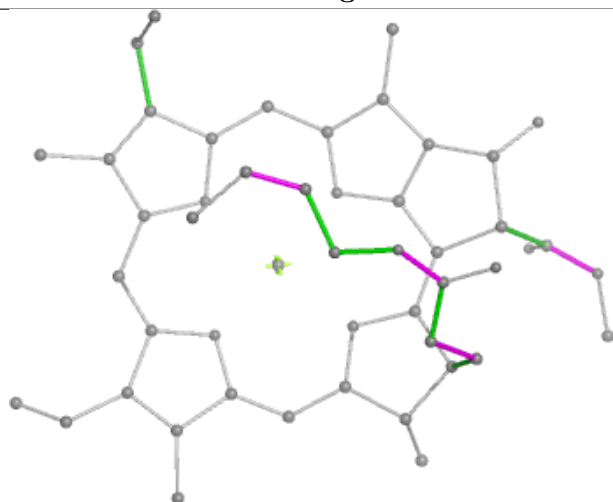
Ligand CLA S 613



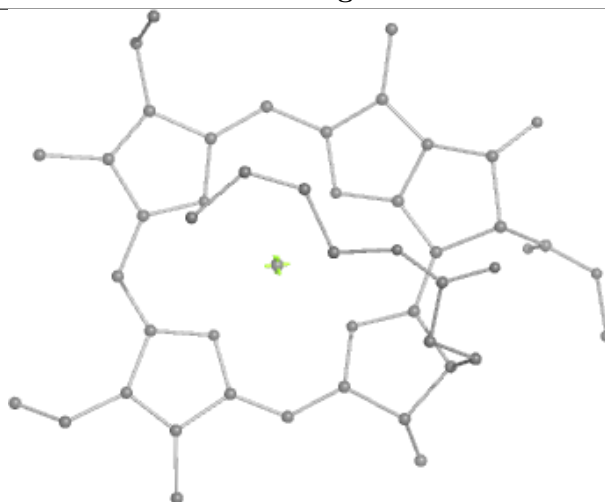
Bond lengths



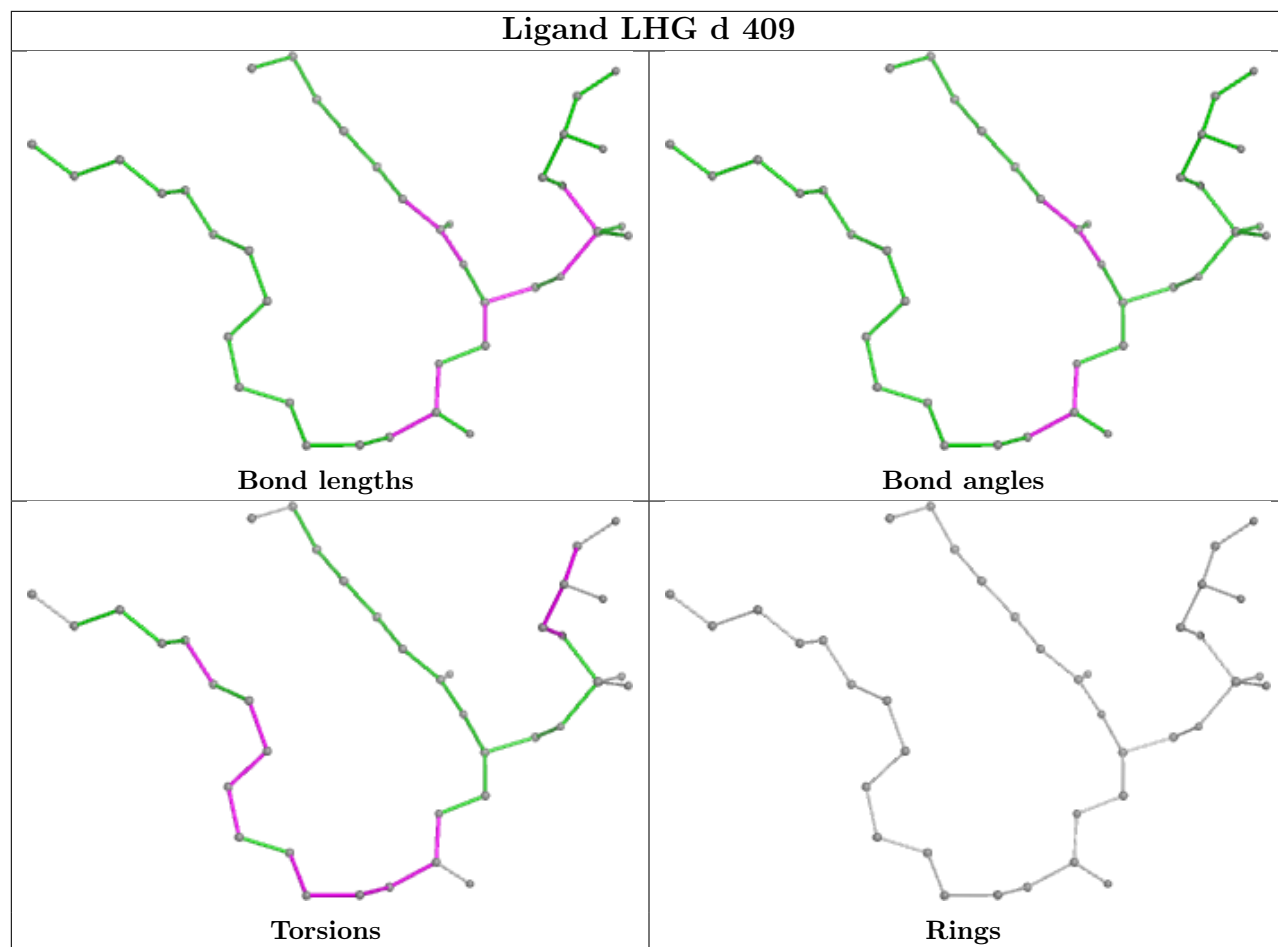
Bond angles



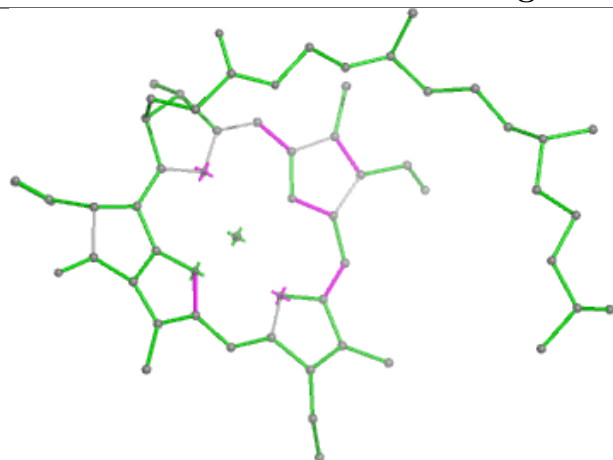
Torsions



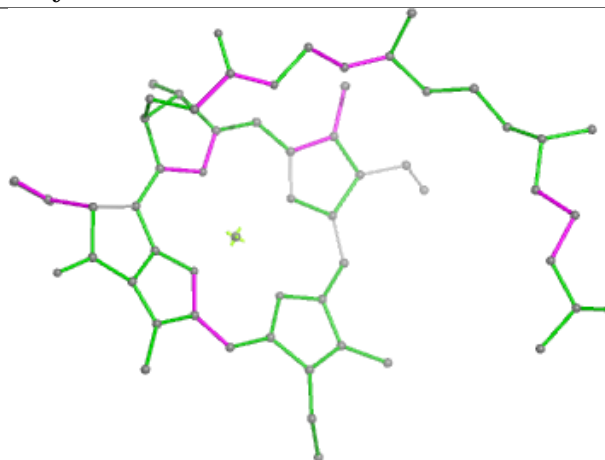
Rings



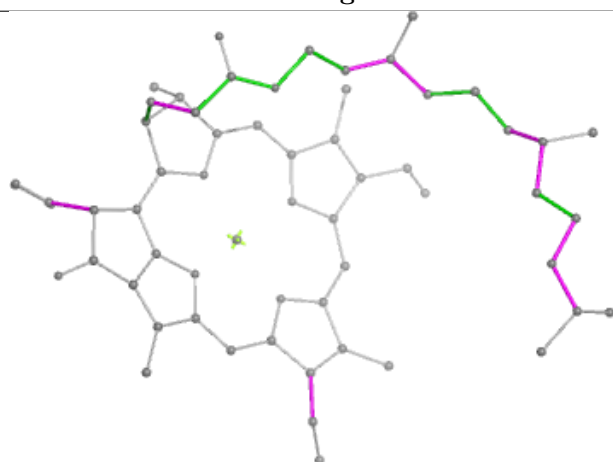
Ligand CLA y 602



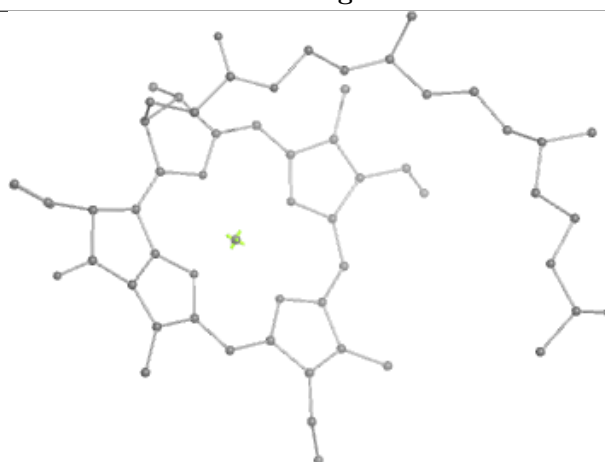
Bond lengths



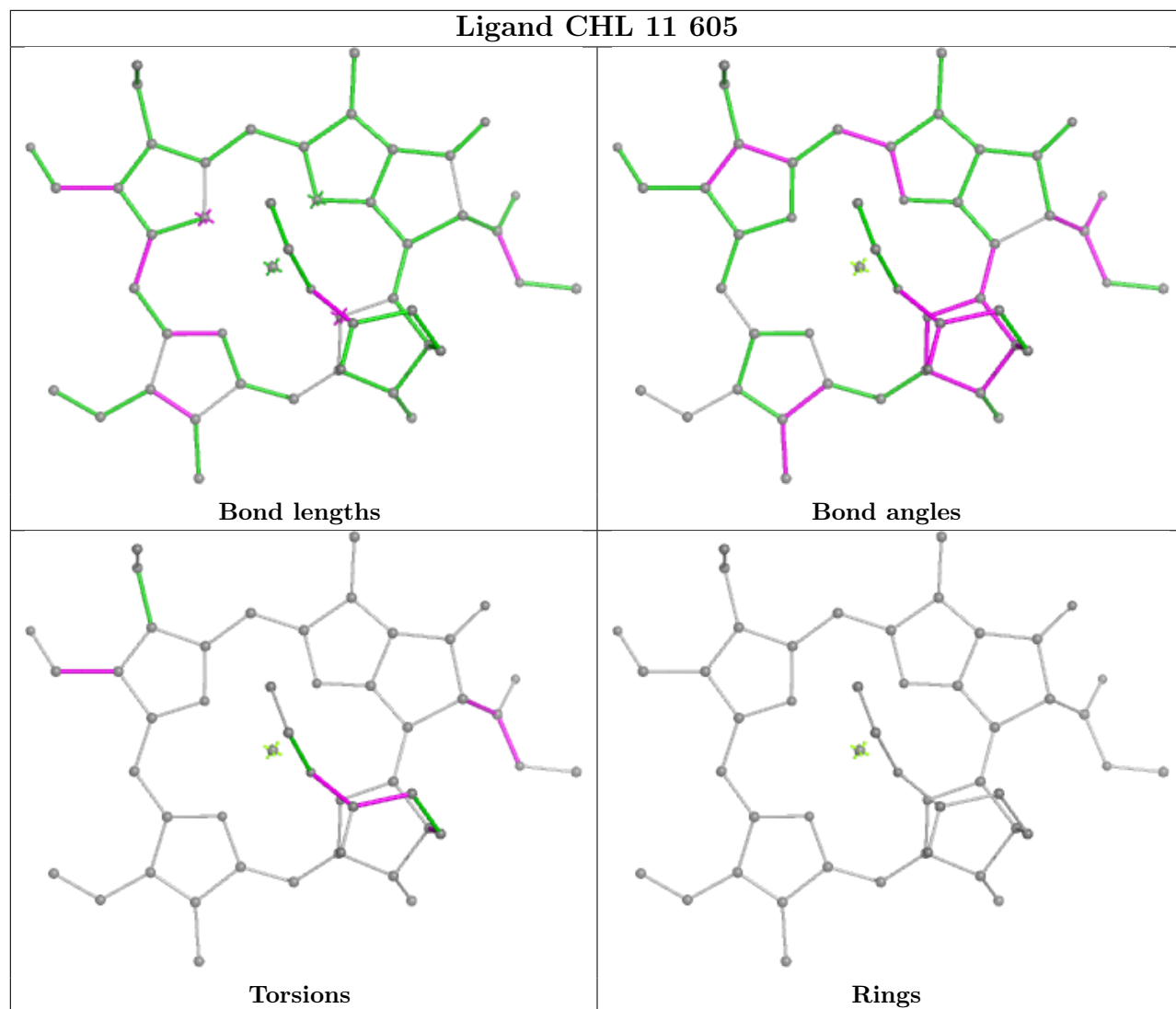
Bond angles

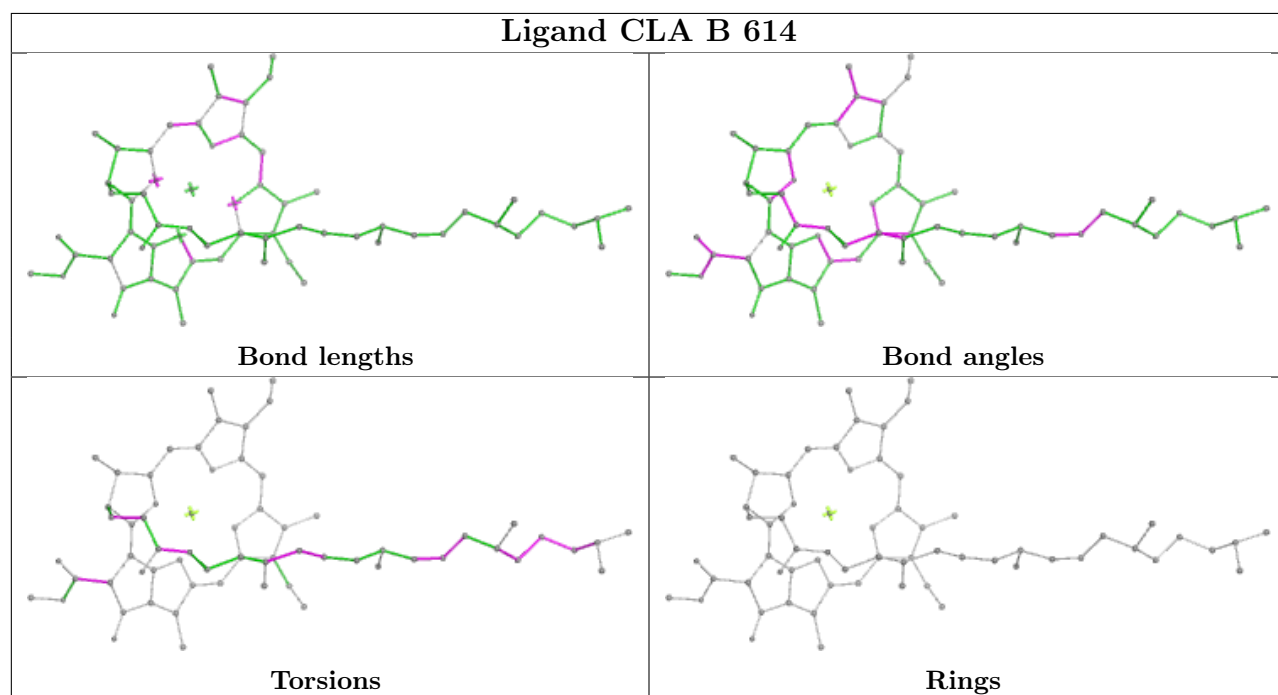
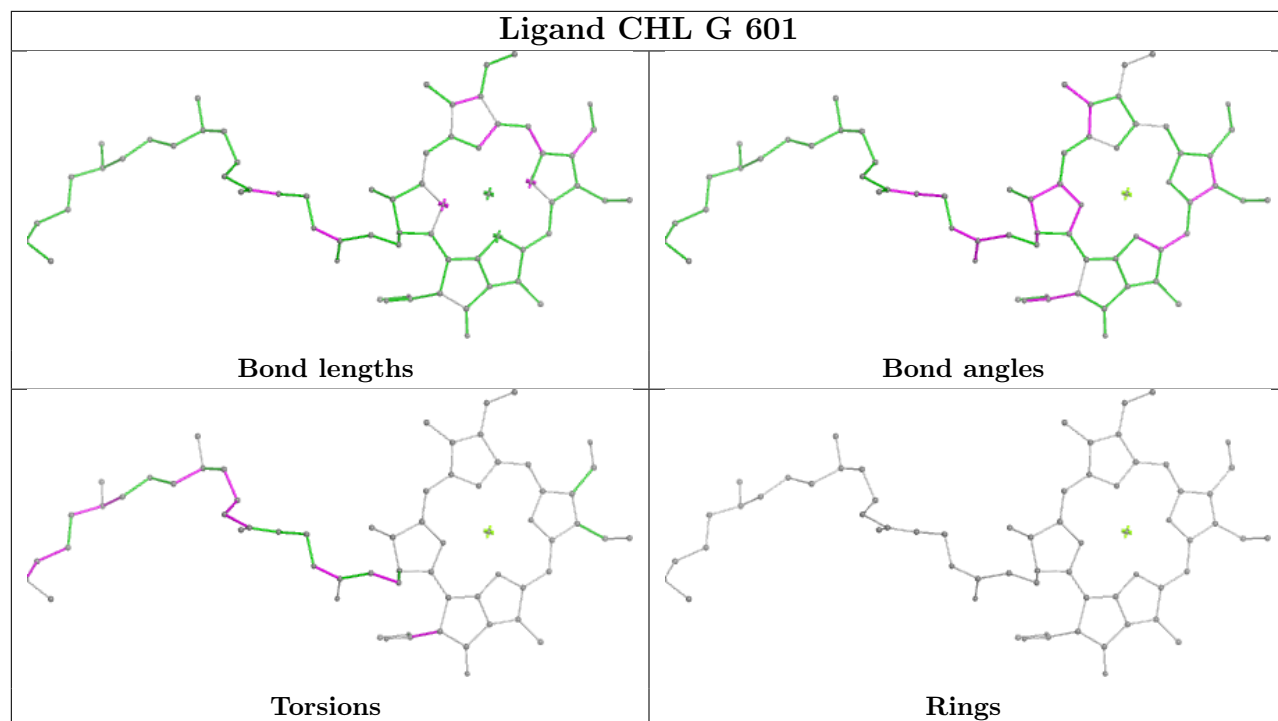


Torsions

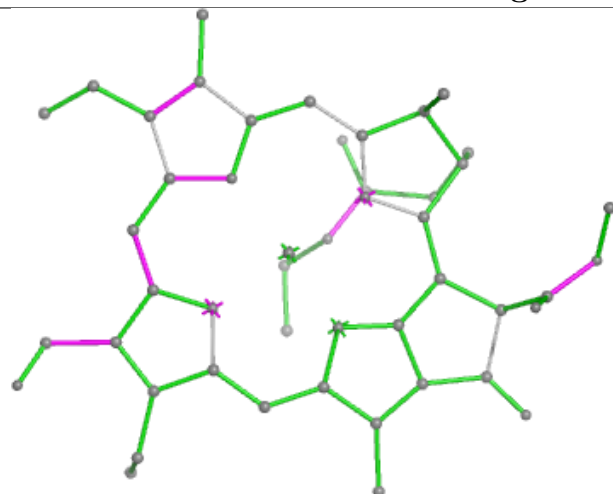


Rings

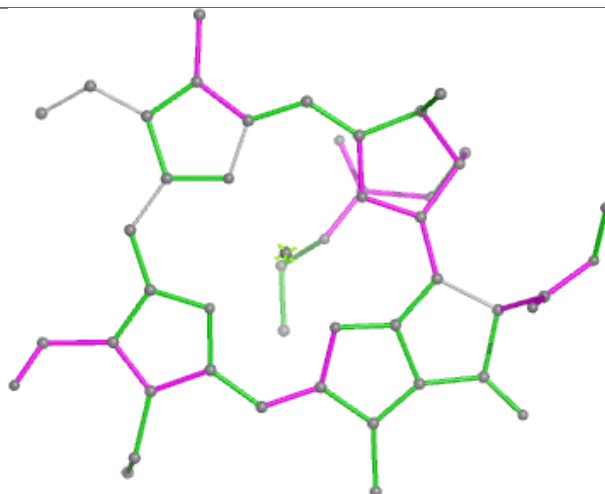




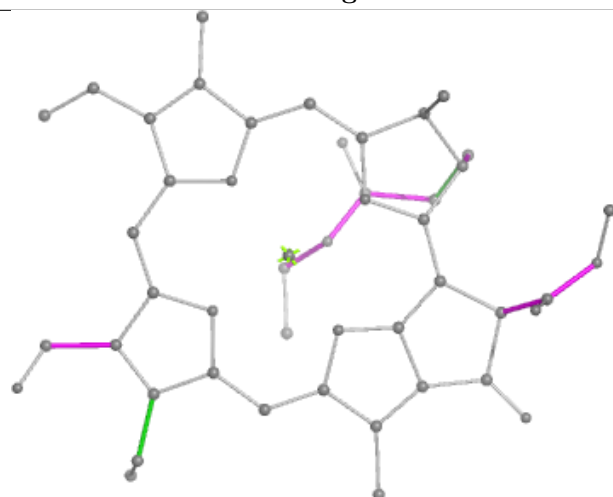
Ligand CHL 14 605



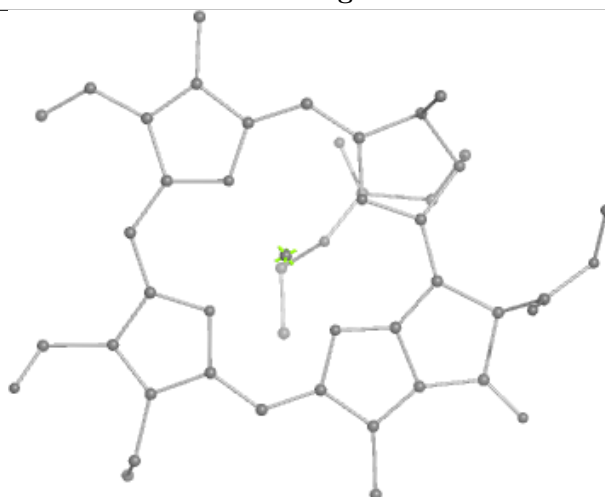
Bond lengths



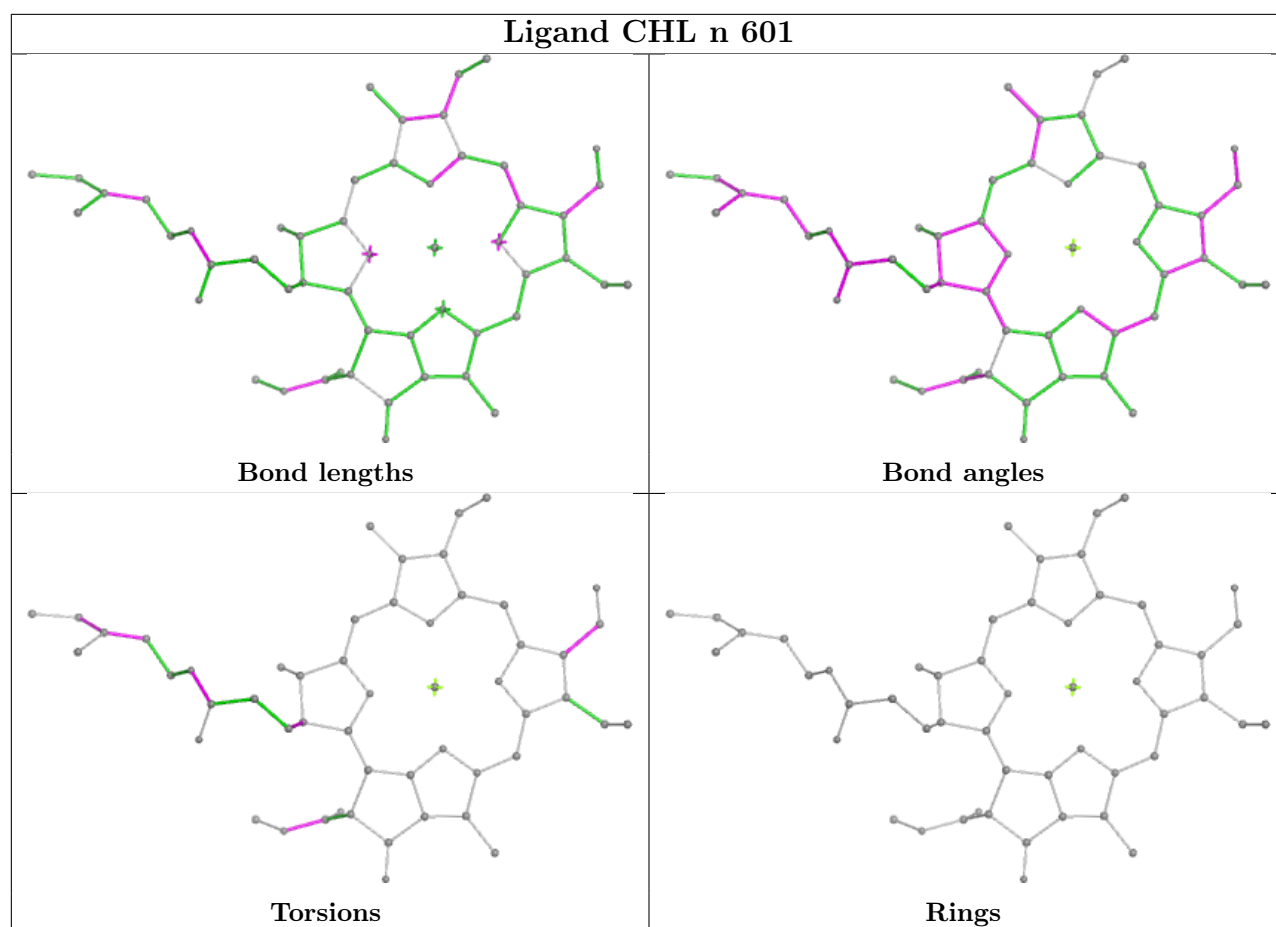
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

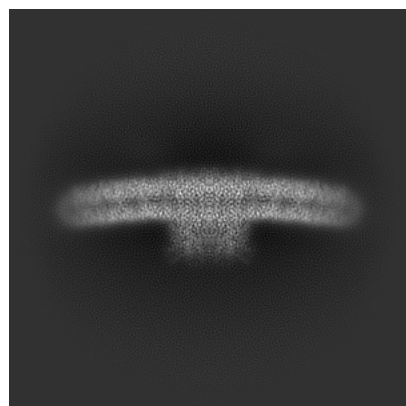
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52056. These allow visual inspection of the internal detail of the map and identification of artifacts.

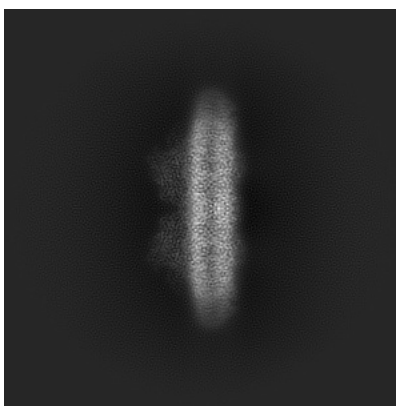
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

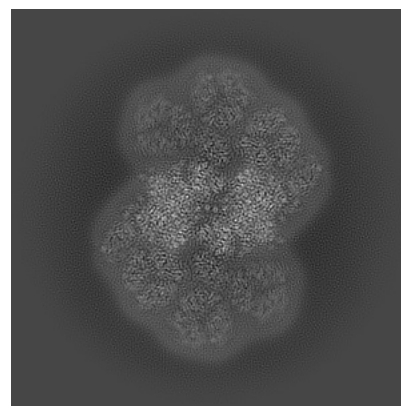
6.1.1 Primary map



X

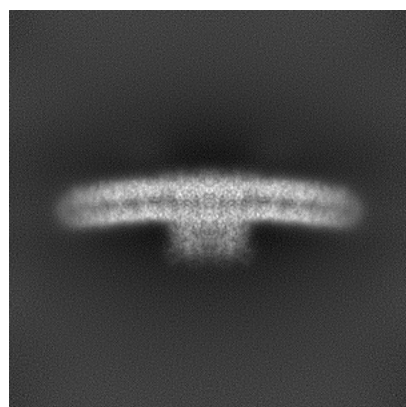


Y

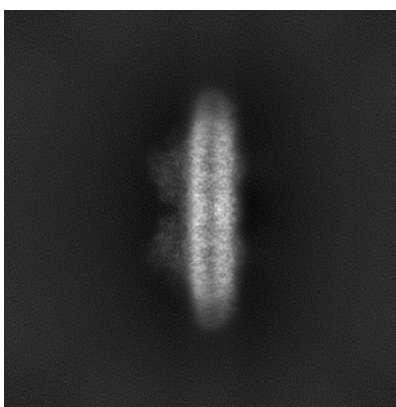


Z

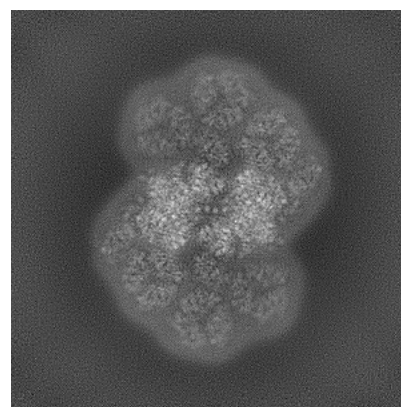
6.1.2 Raw map



X



Y

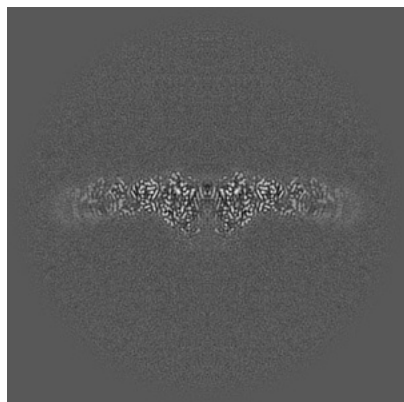


Z

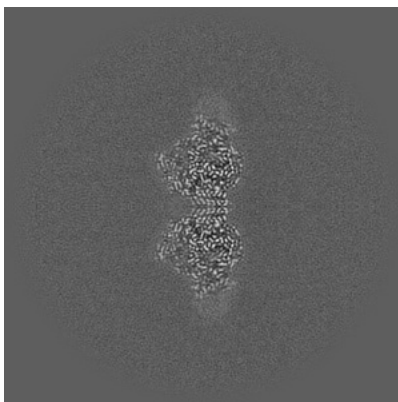
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

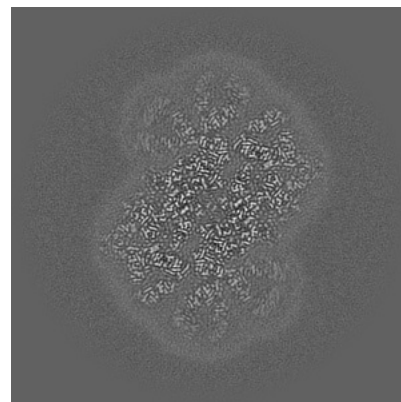
6.2.1 Primary map



X Index: 240

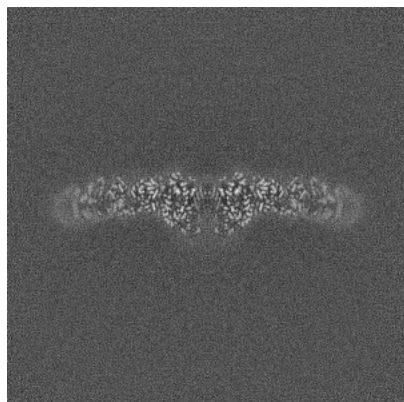


Y Index: 240

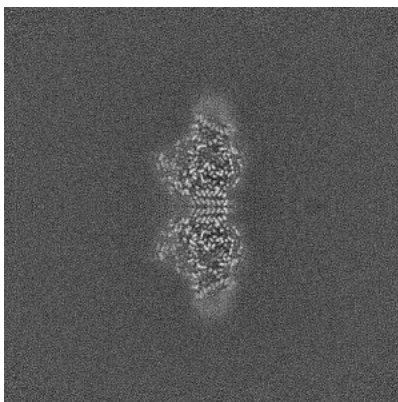


Z Index: 240

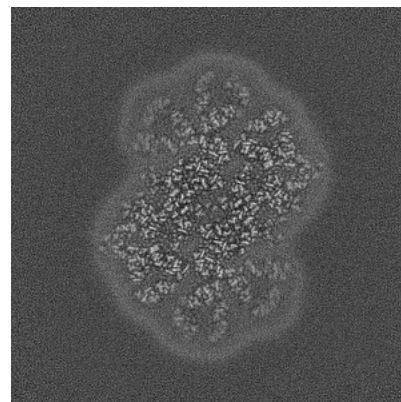
6.2.2 Raw map



X Index: 240



Y Index: 240

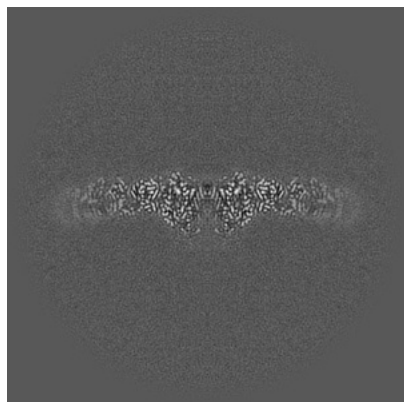


Z Index: 240

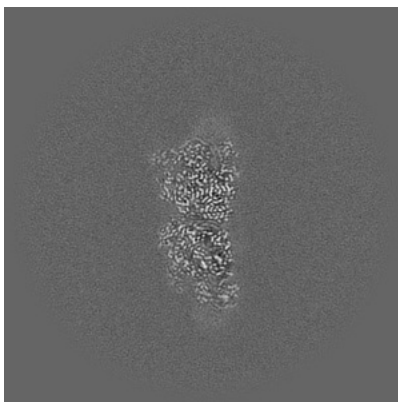
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

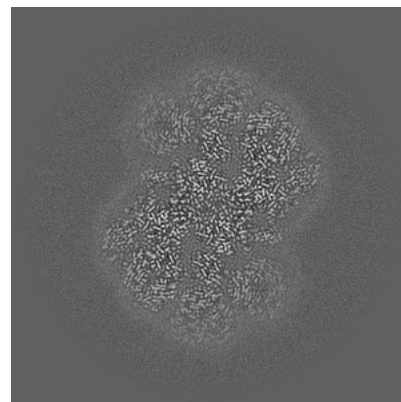
6.3.1 Primary map



X Index: 240

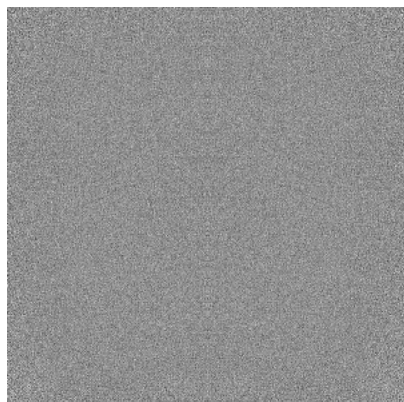


Y Index: 214

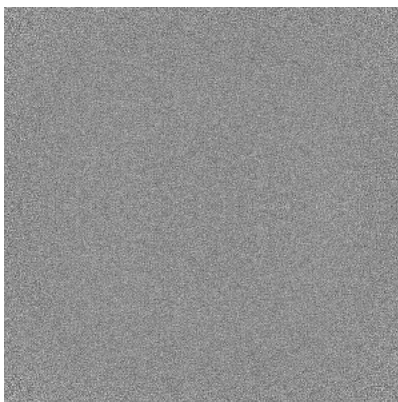


Z Index: 259

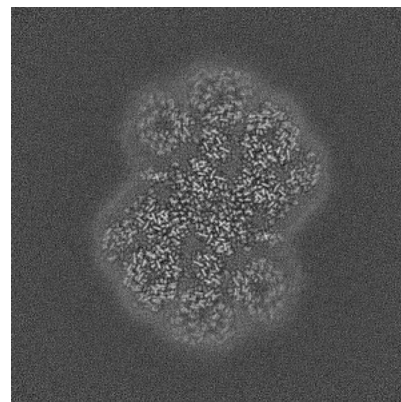
6.3.2 Raw map



X Index: 0



Y Index: 0

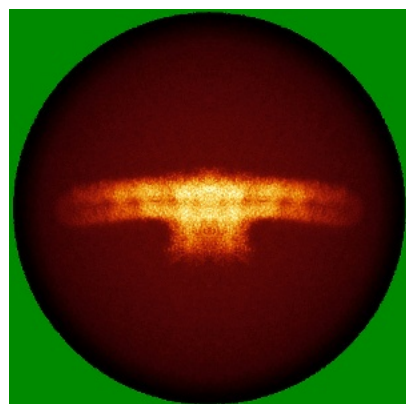


Z Index: 259

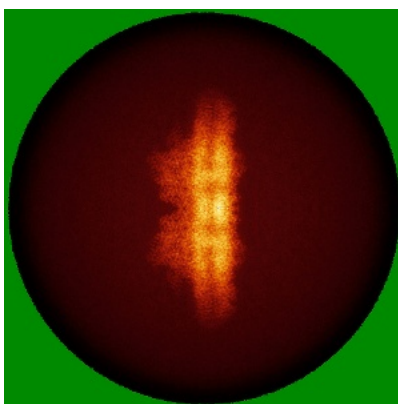
The images above show the largest variance slices of the map in three orthogonal directions.

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

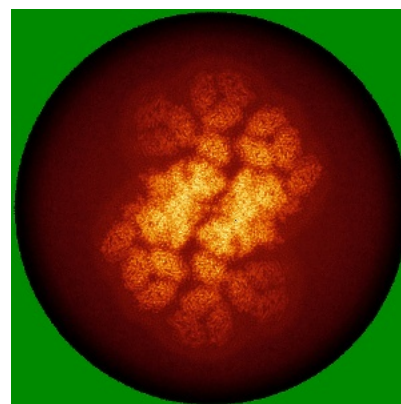
6.4.1 Primary map



X

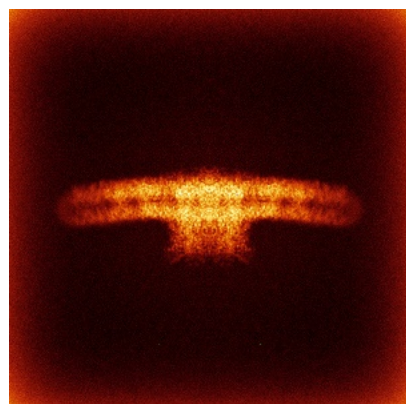


Y

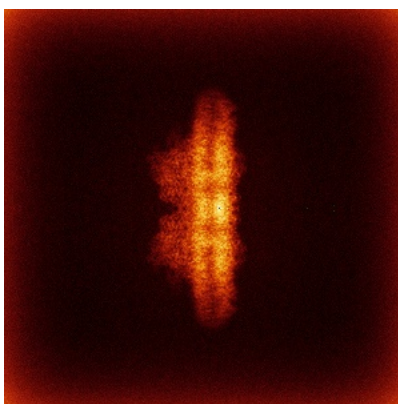


Z

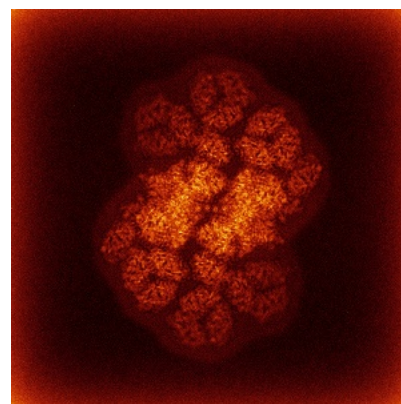
6.4.2 Raw map



X



Y

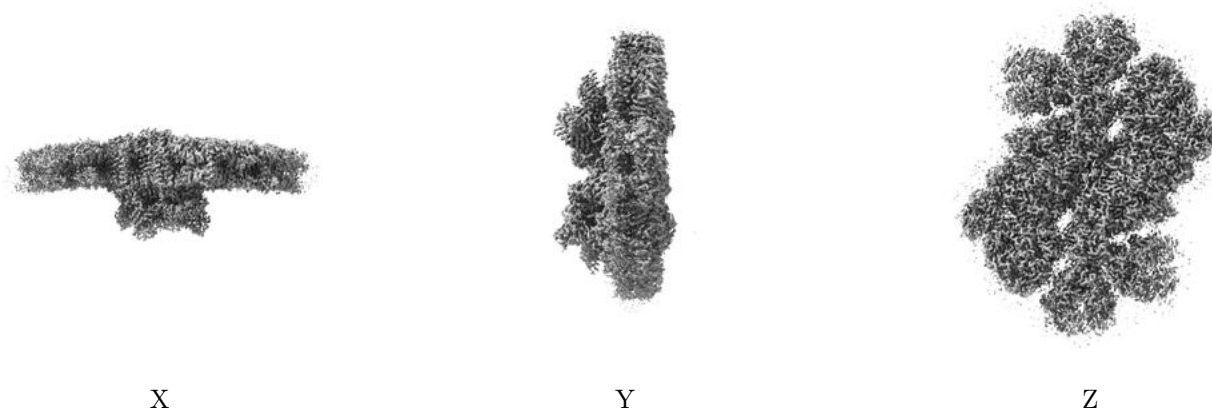


Z

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

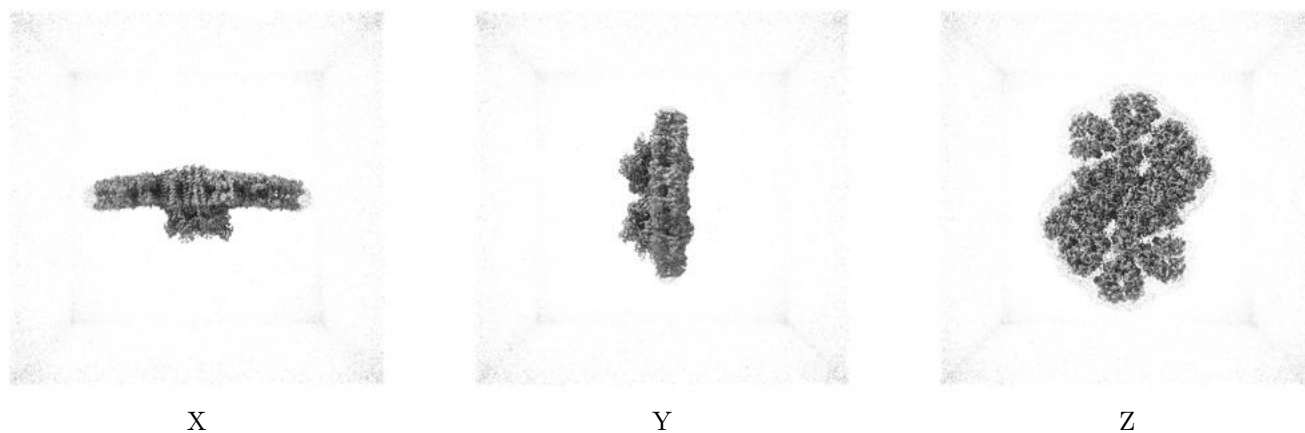
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

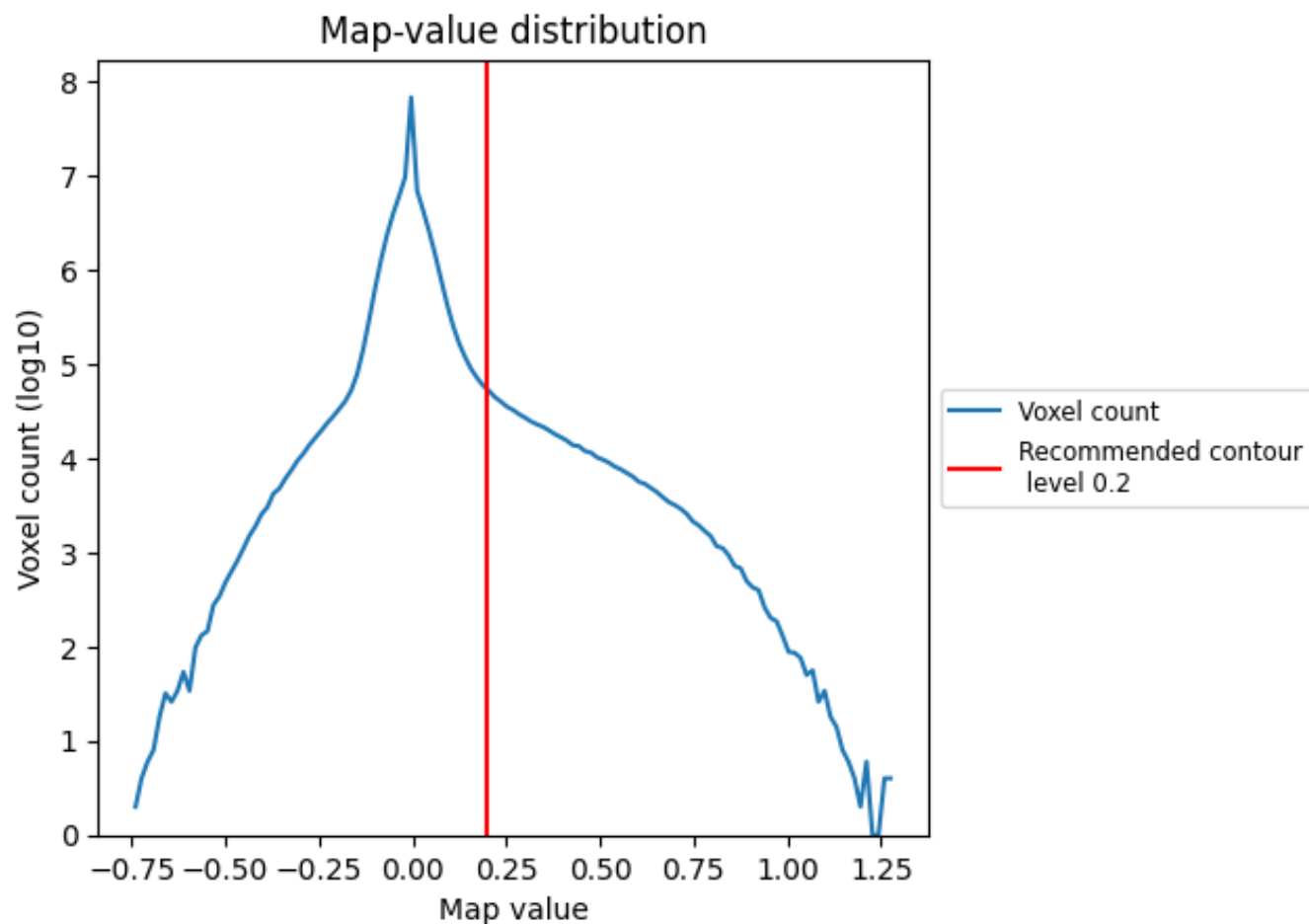
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

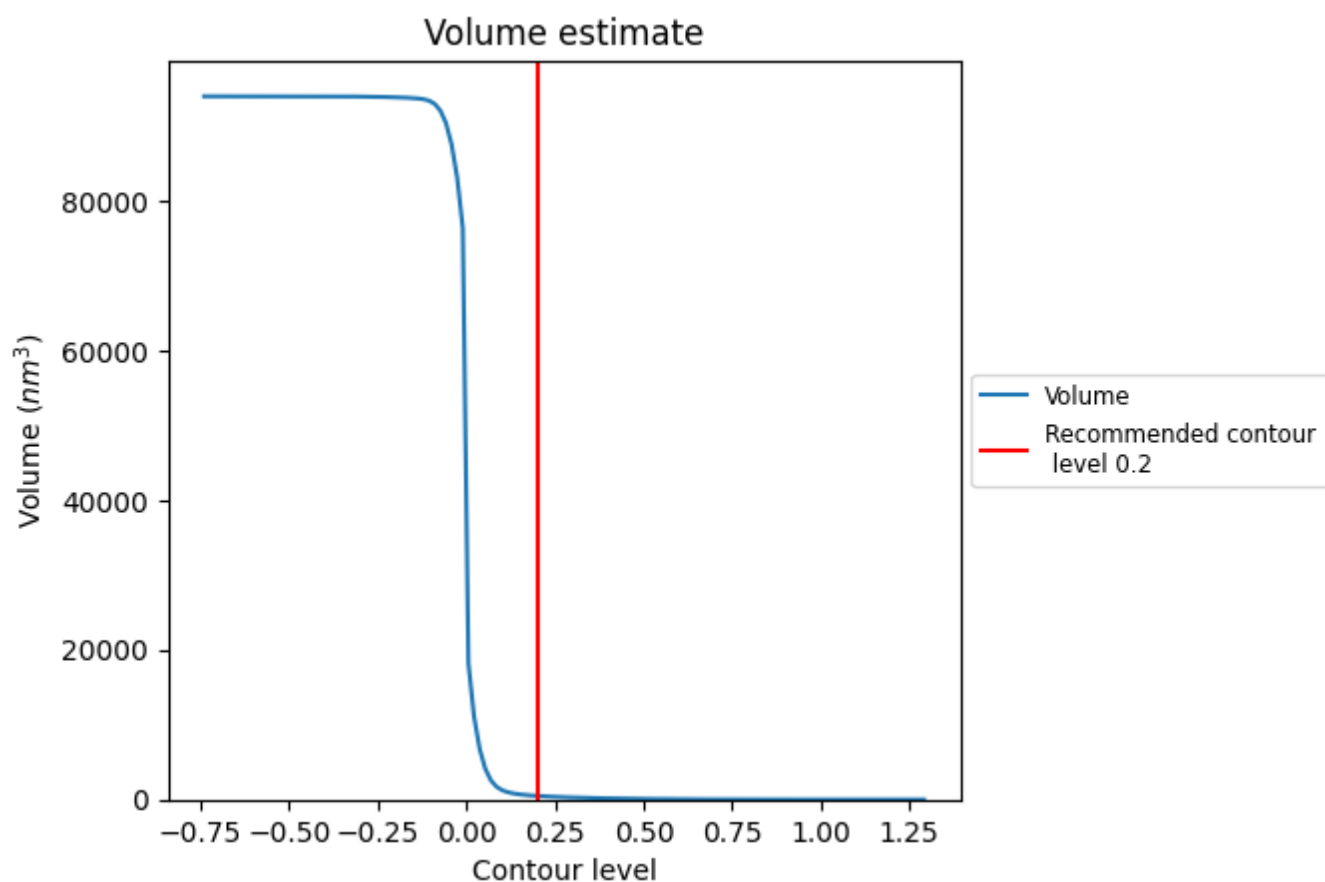
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

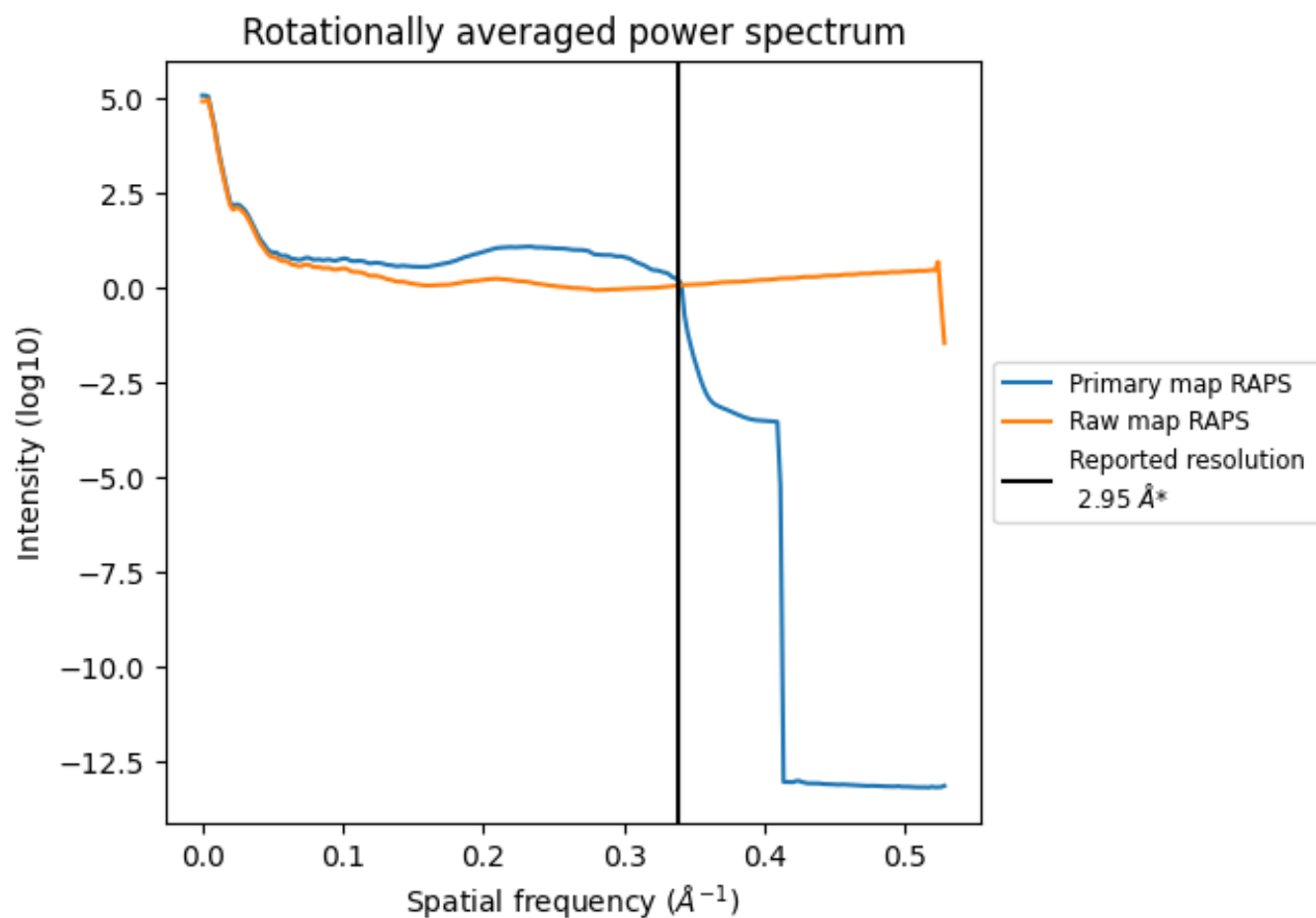
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 486 nm³; this corresponds to an approximate mass of 439 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 ⓘ

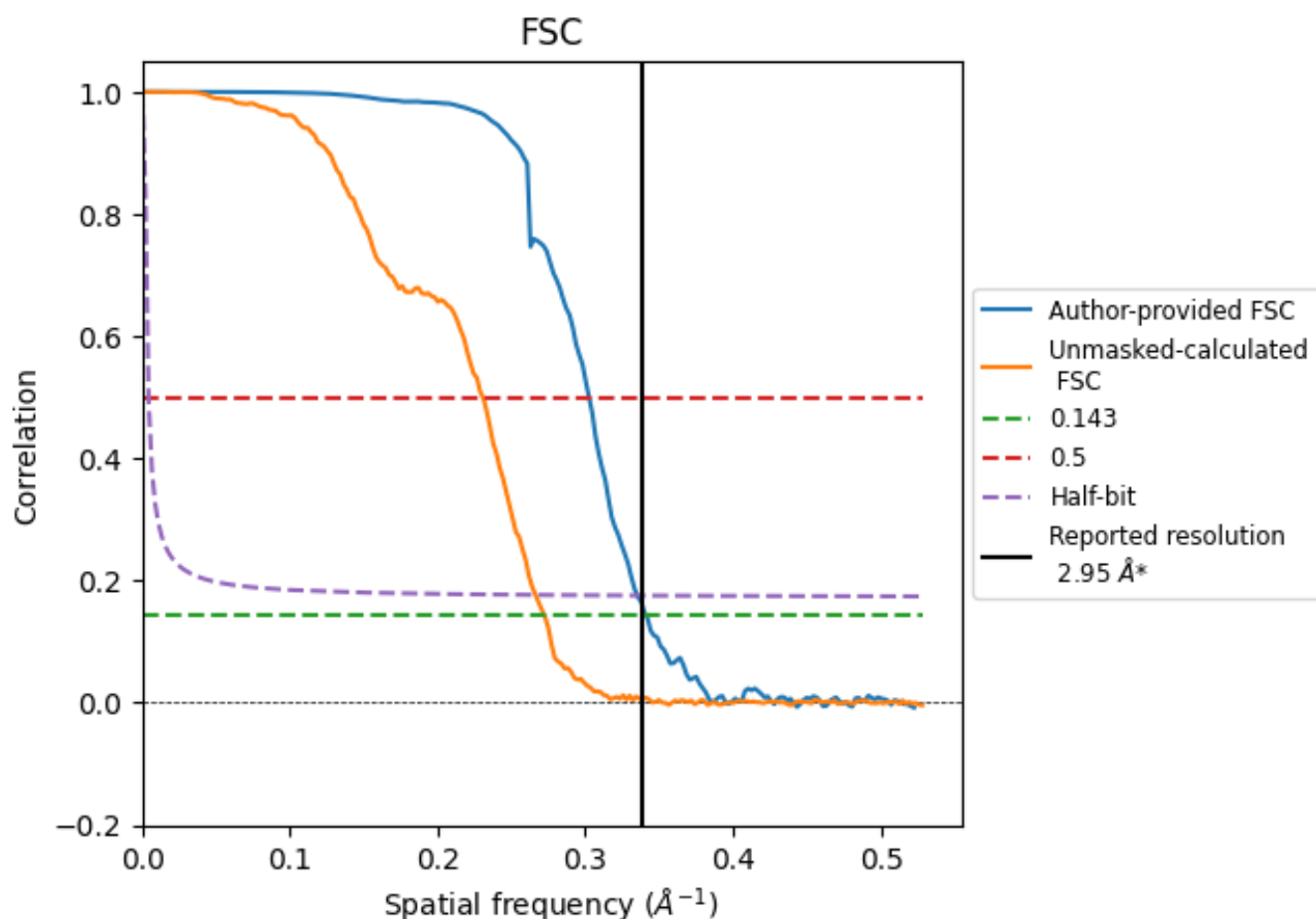


*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

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 0.339\AA^{-1}

8.2 Resolution estimates [i](#)

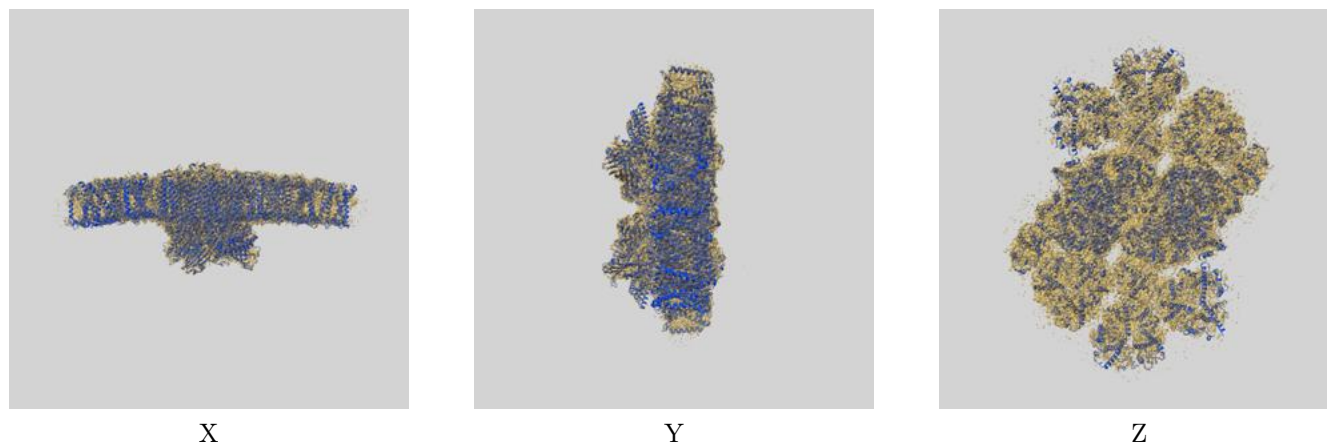
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.93	3.31	2.98
Unmasked-calculated*	3.67	4.33	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

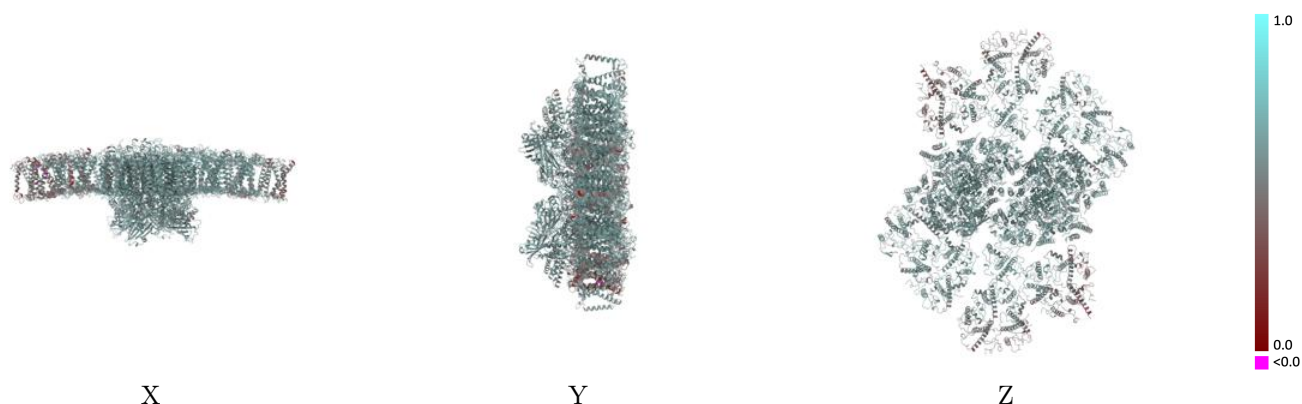
This section contains information regarding the fit between EMDB map EMD-52056 and PDB model 9HD7. Per-residue inclusion information can be found in [section 3](#) on [page 60](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



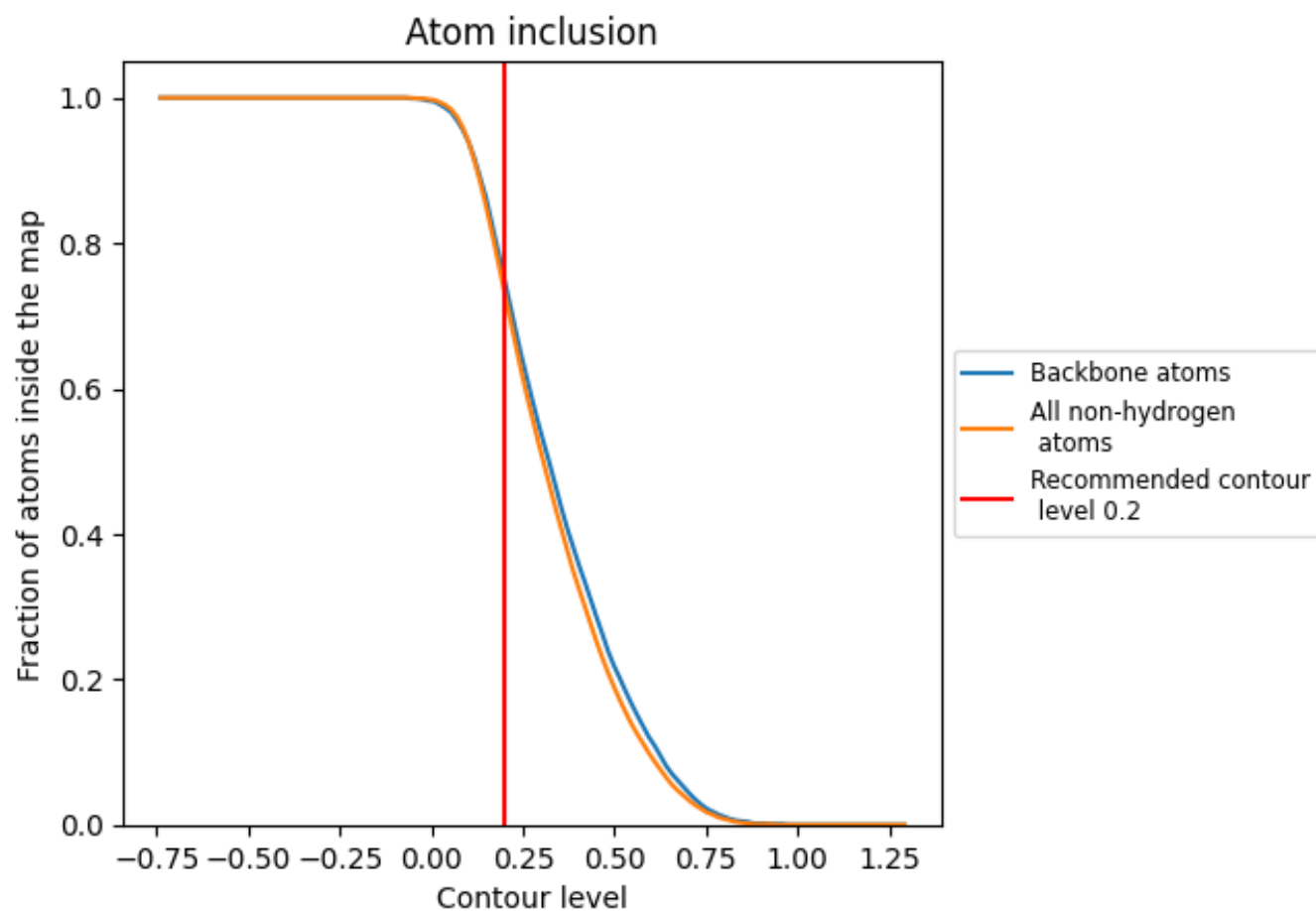
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 73% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.5760
1	 0.4700	 0.5130
11	 0.4260	 0.4850
12	 0.2500	 0.4300
13	 0.6560	 0.5560
14	 0.4220	 0.4860
15	 0.2480	 0.4320
16	 0.6510	 0.5550
2	 0.3760	 0.4700
3	 0.7550	 0.5810
4	 0.4620	 0.5080
5	 0.3760	 0.4760
6	 0.7570	 0.5790
7	 0.6010	 0.5670
8	 0.6000	 0.5670
A	 0.8840	 0.6170
B	 0.8780	 0.6130
C	 0.8840	 0.6110
D	 0.8990	 0.6200
E	 0.8340	 0.6050
F	 0.8600	 0.6090
G	 0.7700	 0.5830
H	 0.8650	 0.6040
I	 0.8970	 0.6150
J	 0.7330	 0.5830
K	 0.7920	 0.5790
L	 0.8230	 0.5940
M	 0.7750	 0.5830
N	 0.7950	 0.5870
O	 0.7220	 0.5880
P	 0.6690	 0.5880
Q	 0.5370	 0.5550
R	 0.8390	 0.6050
S	 0.7130	 0.5740
T	 0.7730	 0.5840



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Chain	Atom inclusion	Q-score
U	 0.4520	 0.5170
V	 0.5520	 0.5230
W	 0.8050	 0.6020
X	 0.8100	 0.6010
Y	 0.8720	 0.6150
Z	 0.7120	 0.5670
a	 0.8900	 0.6180
b	 0.8820	 0.6160
c	 0.8820	 0.6110
d	 0.8970	 0.6190
e	 0.8380	 0.6050
f	 0.8510	 0.6090
g	 0.7660	 0.5830
h	 0.8700	 0.6070
i	 0.9000	 0.6140
j	 0.7420	 0.5820
k	 0.8320	 0.5760
l	 0.8230	 0.5950
m	 0.7800	 0.5820
n	 0.7960	 0.5850
o	 0.7230	 0.5880
p	 0.6770	 0.5890
q	 0.5380	 0.5530
r	 0.8360	 0.6070
s	 0.7150	 0.5760
t	 0.8090	 0.5910
u	 0.4570	 0.5240
v	 0.5660	 0.5370
w	 0.8060	 0.6010
x	 0.7990	 0.6060
y	 0.8730	 0.6140
z	 0.7040	 0.5670