



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 04:18 AM JST

PDB ID : 6KAF
EMDB ID : EMD-9957
Title : C2S2M2N2-type PSII-LHCII
Authors : Chang, S.H.; Shen, L.L.; Huang, Z.H.; Wang, W.D.; Han, G.Y.; Shen, J.R.;
Zhang, X.
Deposited on : 2019-06-22
Resolution : 3.73 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

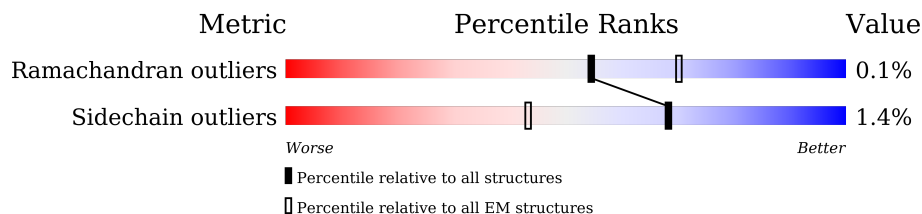
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.73 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	R	280	
1	r	280	
2	A	352	
2	a	352	
3	D	352	
3	d	352	
4	F	44	
4	f	44	
5	H	88	

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Mol	Chain	Length	Quality of chain
5	h	88	73% 27%
6	I	37	86% 5% 8%
6	i	37	86% 5% 8%
7	J	50	32% 62% 38%
7	j	50	32% 62% 38%
8	K	46	78% 22%
8	k	46	78% 22%
9	L	38	5% 97%
9	l	38	5% 97%
10	M	34	94% 6%
10	m	34	6% 94% 6%
11	O	291	7% 72% 28%
11	o	291	8% 71% 28%
12	T	31	97%
12	t	31	97%
13	W	115	47% 53%
13	w	115	47% 53%
14	X	101	35% 65%
14	x	101	35% 65%
15	Z	62	100%
15	z	62	100%
16	Y	33	9% 91% 9%
16	y	33	9% 91% 9%
17	E	82	82% 17%
17	e	82	82% 17%

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Mol	Chain	Length	Quality of chain
18	1	257	30% 82% 15%
18	2	257	63% 81% 15%
18	3	257	58% 82% 15%
18	4	257	30% 82% 15%
18	5	257	63% 82% 15%
18	6	257	57% 83% 15%
18	G	257	6% 83% 15%
18	N	257	81% 16%
18	P	257	61% 82% 15%
18	Q	257	80% 83% 15%
18	U	257	82% 15%
18	V	257	69% 82% 15%
18	g	257	7% 83% 15%
18	n	257	82% 15%
18	p	257	60% 81% 15%
18	q	257	80% 83% 15%
18	u	257	83% 15%
18	v	257	68% 82% 15%
19	S	289	81% 18%
19	s	289	81% 18%
20	C	461	97% .
20	c	461	97% .
21	B	508	98% ..
21	b	508	5% 98% ..

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	2	301	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	305	X	-	-	-
22	CLA	2	306	X	-	-	-
22	CLA	2	307	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	306	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	4	301	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	305	X	-	-	-
22	CLA	4	306	X	-	-	-
22	CLA	4	307	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	303	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	306	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	6	302	X	-	-	-
22	CLA	6	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	306	X	-	-	-
22	CLA	6	307	X	-	-	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	G	301	X	-	-	-
22	CLA	G	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	303	X	-	-	-
22	CLA	G	304	X	-	-	-
22	CLA	G	305	X	-	-	-
22	CLA	G	306	X	-	-	-
22	CLA	G	307	X	-	-	-
22	CLA	G	308	X	-	-	-
22	CLA	N	301	X	-	-	-
22	CLA	N	302	X	-	-	-
22	CLA	N	303	X	-	-	-
22	CLA	N	304	X	-	-	-
22	CLA	N	305	X	-	-	-
22	CLA	N	306	X	-	-	-
22	CLA	N	307	X	-	-	-
22	CLA	N	308	X	-	-	-
22	CLA	P	302	X	-	-	-
22	CLA	P	303	X	-	-	-
22	CLA	P	304	X	-	-	-
22	CLA	P	305	X	-	-	-
22	CLA	P	306	X	-	-	-
22	CLA	P	307	X	-	-	-
22	CLA	P	308	X	-	-	-
22	CLA	P	309	X	-	-	-
22	CLA	Q	301	X	-	-	-
22	CLA	Q	302	X	-	-	-
22	CLA	Q	303	X	-	-	-
22	CLA	Q	304	X	-	-	-
22	CLA	Q	305	X	-	-	-
22	CLA	Q	306	X	-	-	-
22	CLA	Q	307	X	-	-	-
22	CLA	Q	308	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-
22	CLA	R	305	X	-	-	-
22	CLA	R	306	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	301	X	-	-	-
22	CLA	S	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	306	X	-	-	-
22	CLA	S	307	X	-	-	-
22	CLA	S	308	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	U	302	X	-	-	-
22	CLA	U	303	X	-	-	-
22	CLA	U	304	X	-	-	-
22	CLA	U	305	X	-	-	-
22	CLA	U	306	X	-	-	-
22	CLA	U	307	X	-	-	-
22	CLA	U	308	X	-	-	-
22	CLA	V	302	X	-	-	-
22	CLA	V	303	X	-	-	-
22	CLA	V	304	X	-	-	-
22	CLA	V	305	X	-	-	-
22	CLA	V	306	X	-	-	-
22	CLA	V	307	X	-	-	-
22	CLA	V	308	X	-	-	-
22	CLA	X	202	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	g	301	X	-	-	-
22	CLA	g	302	X	-	-	-
22	CLA	g	303	X	-	-	-
22	CLA	g	304	X	-	-	-
22	CLA	g	305	X	-	-	-
22	CLA	g	306	X	-	-	-
22	CLA	g	307	X	-	-	-
22	CLA	g	308	X	-	-	-
22	CLA	n	301	X	-	-	-
22	CLA	n	302	X	-	-	-
22	CLA	n	303	X	-	-	-
22	CLA	n	304	X	-	-	-
22	CLA	n	305	X	-	-	-
22	CLA	n	306	X	-	-	-
22	CLA	n	307	X	-	-	-
22	CLA	n	308	X	-	-	-
22	CLA	p	302	X	-	-	-
22	CLA	p	303	X	-	-	-
22	CLA	p	304	X	-	-	-
22	CLA	p	305	X	-	-	-
22	CLA	p	306	X	-	-	-
22	CLA	p	307	X	-	-	-
22	CLA	p	308	X	-	-	-
22	CLA	p	309	X	-	-	-
22	CLA	q	302	X	-	-	-
22	CLA	q	303	X	-	-	-
22	CLA	q	304	X	-	-	-
22	CLA	q	305	X	-	-	-
22	CLA	q	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	q	307	X	-	-	-
22	CLA	q	308	X	-	-	-
22	CLA	r	601	X	-	-	-
22	CLA	r	602	X	-	-	-
22	CLA	r	603	X	-	-	-
22	CLA	r	604	X	-	-	-
22	CLA	r	605	X	-	-	-
22	CLA	r	606	X	-	-	-
22	CLA	r	607	X	-	-	-
22	CLA	r	608	X	-	-	-
22	CLA	r	609	X	-	-	-
22	CLA	r	610	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	302	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	306	X	-	-	-
22	CLA	s	307	X	-	-	-
22	CLA	s	308	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	u	302	X	-	-	-
22	CLA	u	303	X	-	-	-
22	CLA	u	304	X	-	-	-
22	CLA	u	305	X	-	-	-
22	CLA	u	306	X	-	-	-
22	CLA	u	307	X	-	-	-
22	CLA	u	308	X	-	-	-
22	CLA	v	302	X	-	-	-
22	CLA	v	303	X	-	-	-
22	CLA	v	304	X	-	-	-
22	CLA	v	305	X	-	-	-
22	CLA	v	306	X	-	-	-
22	CLA	v	307	X	-	-	-
22	CLA	v	308	X	-	-	-
22	CLA	x	201	X	-	-	-
26	CHL	1	313	X	-	-	-
26	CHL	1	314	X	-	-	-
26	CHL	1	315	X	-	-	-
26	CHL	1	316	X	-	-	-
26	CHL	1	317	X	-	-	-
26	CHL	1	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	2	313	X	-	-	-
26	CHL	2	314	X	-	-	-
26	CHL	2	315	X	-	-	-
26	CHL	2	316	X	-	-	-
26	CHL	2	317	X	-	-	-
26	CHL	2	318	X	-	-	-
26	CHL	3	311	X	-	-	-
26	CHL	3	312	X	-	-	-
26	CHL	3	313	X	-	-	-
26	CHL	3	314	X	-	-	-
26	CHL	3	315	X	-	-	-
26	CHL	3	316	X	-	-	-
26	CHL	4	313	X	-	-	-
26	CHL	4	314	X	-	-	-
26	CHL	4	315	X	-	-	-
26	CHL	4	316	X	-	-	-
26	CHL	4	317	X	-	-	-
26	CHL	5	313	X	-	-	-
26	CHL	5	314	X	-	-	-
26	CHL	5	315	X	-	-	-
26	CHL	5	316	X	-	-	-
26	CHL	5	317	X	-	-	-
26	CHL	5	318	X	-	-	-
26	CHL	6	301	X	-	-	-
26	CHL	6	312	X	-	-	-
26	CHL	6	313	X	-	-	-
26	CHL	6	314	X	-	-	-
26	CHL	6	315	X	-	-	-
26	CHL	6	316	X	-	-	-
26	CHL	6	317	X	-	-	-
26	CHL	G	311	X	-	-	-
26	CHL	G	312	X	-	-	-
26	CHL	G	313	X	-	-	-
26	CHL	G	314	X	-	-	-
26	CHL	G	315	X	-	-	-
26	CHL	G	316	X	-	-	-
26	CHL	N	313	X	-	-	-
26	CHL	N	314	X	-	-	-
26	CHL	N	315	X	-	-	-
26	CHL	N	316	X	-	-	-
26	CHL	N	317	X	-	-	-
26	CHL	P	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	P	315	X	-	-	-
26	CHL	P	316	X	-	-	-
26	CHL	P	317	X	-	-	-
26	CHL	P	318	X	-	-	-
26	CHL	P	319	X	-	-	-
26	CHL	Q	311	X	-	-	-
26	CHL	Q	312	X	-	-	-
26	CHL	Q	313	X	-	-	-
26	CHL	Q	314	X	-	-	-
26	CHL	Q	315	X	-	-	-
26	CHL	Q	316	X	-	-	-
26	CHL	R	315	X	-	-	-
26	CHL	R	316	X	-	-	-
26	CHL	R	317	X	-	-	-
26	CHL	S	313	X	-	-	-
26	CHL	S	314	X	-	-	-
26	CHL	S	315	X	-	-	-
26	CHL	S	316	X	-	-	-
26	CHL	U	313	X	-	-	-
26	CHL	U	314	X	-	-	-
26	CHL	U	315	X	-	-	-
26	CHL	U	316	X	-	-	-
26	CHL	U	317	X	-	-	-
26	CHL	U	319	X	-	-	-
26	CHL	V	313	X	-	-	-
26	CHL	V	314	X	-	-	-
26	CHL	V	315	X	-	-	-
26	CHL	V	316	X	-	-	-
26	CHL	V	317	X	-	-	-
26	CHL	V	318	X	-	-	-
26	CHL	g	311	X	-	-	-
26	CHL	g	312	X	-	-	-
26	CHL	g	313	X	-	-	-
26	CHL	g	314	X	-	-	-
26	CHL	g	315	X	-	-	-
26	CHL	g	316	X	-	-	-
26	CHL	n	313	X	-	-	-
26	CHL	n	314	X	-	-	-
26	CHL	n	315	X	-	-	-
26	CHL	n	316	X	-	-	-
26	CHL	n	317	X	-	-	-
26	CHL	n	318	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CHL	p	314	X	-	-	-
26	CHL	p	315	X	-	-	-
26	CHL	p	316	X	-	-	-
26	CHL	p	317	X	-	-	-
26	CHL	p	318	X	-	-	-
26	CHL	p	319	X	-	-	-
26	CHL	p	320	X	-	-	-
26	CHL	q	311	X	-	-	-
26	CHL	q	312	X	-	-	-
26	CHL	q	313	X	-	-	-
26	CHL	q	314	X	-	-	-
26	CHL	q	315	X	-	-	-
26	CHL	r	614	X	-	-	-
26	CHL	r	615	X	-	-	-
26	CHL	r	616	X	-	-	-
26	CHL	r	619	X	-	-	-
26	CHL	s	313	X	-	-	-
26	CHL	s	314	X	-	-	-
26	CHL	s	315	X	-	-	-
26	CHL	s	316	X	-	-	-
26	CHL	u	313	X	-	-	-
26	CHL	u	314	X	-	-	-
26	CHL	u	315	X	-	-	-
26	CHL	u	316	X	-	-	-
26	CHL	u	317	X	-	-	-
26	CHL	u	318	X	-	-	-
26	CHL	v	313	X	-	-	-
26	CHL	v	314	X	-	-	-
26	CHL	v	315	X	-	-	-
26	CHL	v	316	X	-	-	-
26	CHL	v	317	X	-	-	-
26	CHL	v	318	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 104363 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 CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	r	223	Total	C	N	O	S	0	0
			1701	1081	286	329	5		
1	R	223	Total	C	N	O	S	0	0
			1698	1080	285	328	5		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	333	Total	C	N	O	S	0	0
			2614	1707	430	462	15		
2	A	333	Total	C	N	O	S	0	0
			2614	1707	430	462	15		

- Molecule 3 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	341	Total	C	N	O	S	0	0
			2714	1791	447	464	12		
3	D	341	Total	C	N	O	S	0	0
			2714	1791	447	464	12		

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	30	Total	C	N	O	S	0	0
			243	165	41	36	1		
4	F	30	Total	C	N	O	S	0	0
			243	165	41	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	64	Total	C	N	O	S	0	0
			488	327	72	87	2		
5	H	64	Total	C	N	O	S	0	0
			488	327	72	87	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		
6	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- Molecule 7 is a protein called Photosystem II reaction center protein J, PsbJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	31	Total	C	N	O	S	0	0
			245	168	36	39	2		
7	J	31	Total	C	N	O	S	0	0
			245	168	36	39	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	k	36	Total	C	N	O	0	0
			288	203	41	44		
8	K	36	Total	C	N	O	0	0
			288	203	41	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	l	37	Total	C	N	O	0	0
			306	205	50	51		
9	L	37	Total	C	N	O	0	0
			306	205	50	51		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	m	32	Total	C	N	O	0	0
			248	168	35	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	M	32	248	168	35	45	0	0

- Molecule 11 is a protein called Oxygen-evolving enhancer protein 1 of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	210	1592	1016	254	318	4	0	0
11	O	210	1592	1016	254	318	4	0	0

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

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

- Molecule 13 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	w	54	417	269	67	79	2	0	0
13	W	54	417	269	67	79	2	0	0

- Molecule 14 is a protein called 4.1 kDa photosystem II subunit.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	z	62	465	319	69	76	1	0	0
15	Z	62	465	319	69	76	1	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein 30, Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	30	Total	C	N	O	0	0
			208	137	34	37		
16	y	30	Total	C	N	O	0	0
			208	137	34	37		

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	E	68	Total	C	N	O	0	0
			555	366	90	99		
17	e	68	Total	C	N	O	0	0
			555	366	90	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	2	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	3	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	4	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	5	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	6	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	v	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	p	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	q	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	V	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	P	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	Q	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	U	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
18	G	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	u	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	n	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	g	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	236	Total	C	N	O	S	0	0
			1797	1166	290	337	4		
19	s	236	Total	C	N	O	S	0	0
			1797	1166	290	337	4		

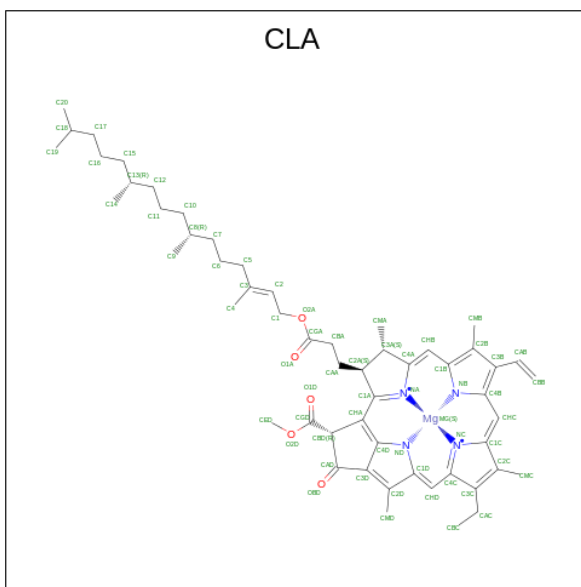
- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	450	Total	C	N	O	S	0	0
			3502	2290	585	610	17		
20	c	450	Total	C	N	O	S	0	0
			3502	2290	585	610	17		

- Molecule 21 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	503	Total	C	N	O	S	0	0
			3937	2575	658	692	12		
21	b	503	Total	C	N	O	S	0	0
			3937	2575	658	692	12		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
22	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
22	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
22	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	A	1	Total 240	C 200	Mg 4	N 16	O 20	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	1	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	2	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	3	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	4	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	5	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	6	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	v	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	p	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	V	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	P	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	Q	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	U	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	G	1	Total 477	C 397	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	u	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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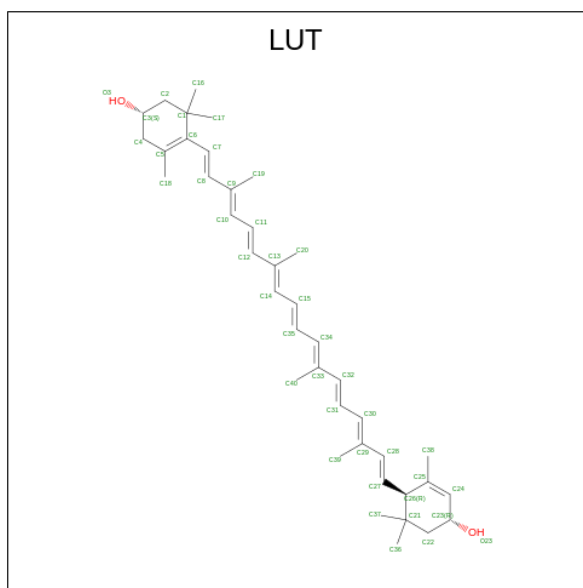
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
22	s	1	Total 465	C 375	Mg 9	N 36	O 45	0

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	r	1	Total 42	C 40	O 2	0
23	1	1	Total 84	C 80	O 4	0
23	1	1	Total 84	C 80	O 4	0
23	2	1	Total 84	C 80	O 4	0

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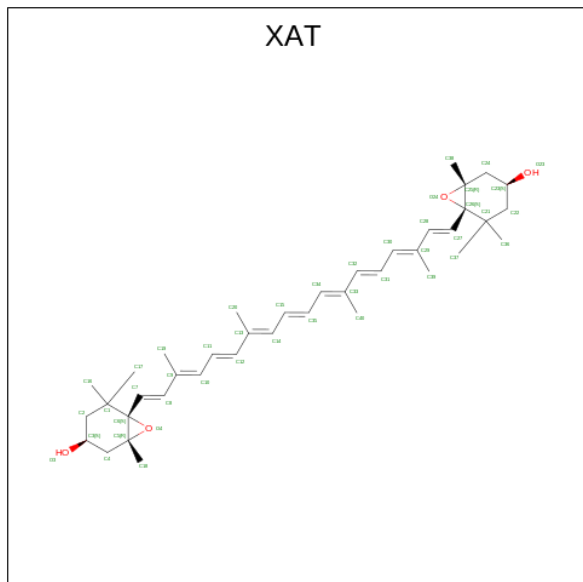
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	2	1	84	80	4	0
23	4	1	84	80	4	0
23	4	1	84	80	4	0
23	5	1	84	80	4	0
23	5	1	84	80	4	0
23	v	1	84	80	4	0
23	v	1	84	80	4	0
23	p	1	84	80	4	0
23	p	1	84	80	4	0
23	V	1	84	80	4	0
23	V	1	84	80	4	0
23	P	1	84	80	4	0
23	P	1	84	80	4	0
23	U	1	84	80	4	0
23	U	1	84	80	4	0
23	N	1	84	80	4	0
23	N	1	84	80	4	0
23	u	1	84	80	4	0
23	u	1	84	80	4	0
23	n	1	84	80	4	0
23	n	1	84	80	4	0

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Mol	Chain	Residues	Atoms			AltConf
23	R	1	Total	C	O	0
			42	40	2	
23	S	1	Total	C	O	0
			84	80	4	
23	S	1	Total	C	O	0
			84	80	4	
23	s	1	Total	C	O	0
			84	80	4	
23	s	1	Total	C	O	0
			84	80	4	

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



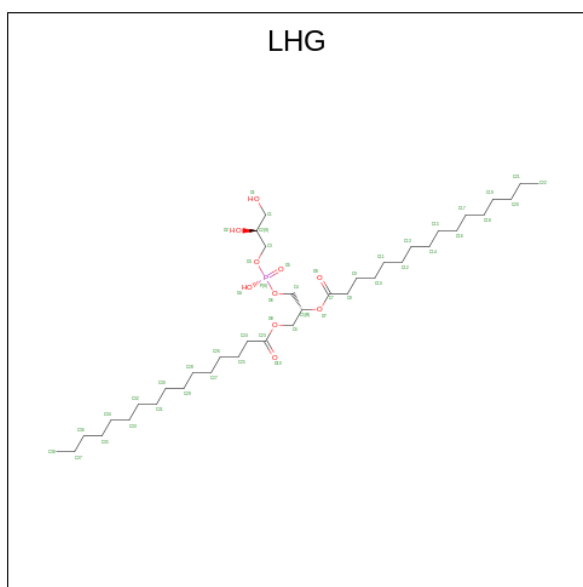
Mol	Chain	Residues	Atoms			AltConf
24	r	1	Total	C	O	0
			44	40	4	
24	1	1	Total	C	O	0
			44	40	4	
24	2	1	Total	C	O	0
			44	40	4	
24	3	1	Total	C	O	0
			44	40	4	
24	4	1	Total	C	O	0
			44	40	4	
24	5	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	6	1	44	40	4	0
24	v	1	44	40	4	0
24	p	1	44	40	4	0
24	q	1	44	40	4	0
24	V	1	44	40	4	0
24	P	1	44	40	4	0
24	Q	1	44	40	4	0
24	U	1	44	40	4	0
24	N	1	44	40	4	0
24	G	1	44	40	4	0
24	u	1	44	40	4	0
24	n	1	44	40	4	0
24	g	1	44	40	4	0
24	R	1	44	40	4	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	r	1	Total 42	C 31	O 10	P 1	0
25	a	1	Total 43	C 32	O 10	P 1	0
25	d	1	Total 95	C 73	O 20	P 2	0
25	d	1	Total 95	C 73	O 20	P 2	0
25	l	1	Total 49	C 38	O 10	P 1	0
25	A	1	Total 43	C 32	O 10	P 1	0
25	L	1	Total 49	C 38	O 10	P 1	0
25	1	1	Total 49	C 38	O 10	P 1	0
25	2	1	Total 49	C 38	O 10	P 1	0
25	3	1	Total 49	C 38	O 10	P 1	0
25	4	1	Total 49	C 38	O 10	P 1	0
25	5	1	Total 49	C 38	O 10	P 1	0
25	6	1	Total 49	C 38	O 10	P 1	0
25	v	1	Total 49	C 38	O 10	P 1	0

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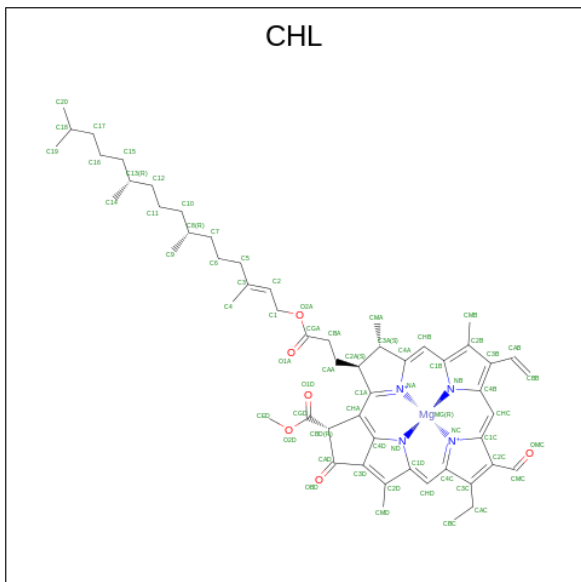
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	p	1	49	38	10	1	0
25	q	1	49	38	10	1	0
25	V	1	49	38	10	1	0
25	P	1	49	38	10	1	0
25	Q	1	49	38	10	1	0
25	U	1	49	38	10	1	0
25	N	1	49	38	10	1	0
25	G	1	49	38	10	1	0
25	u	1	49	38	10	1	0
25	n	1	49	38	10	1	0
25	g	1	49	38	10	1	0
25	R	1	42	31	10	1	0
25	S	1	49	38	10	1	0
25	C	1	147	114	30	3	0
25	C	1	147	114	30	3	0
25	C	1	147	114	30	3	0
25	B	1	96	74	20	2	0
25	B	1	96	74	20	2	0
25	D	1	95	73	20	2	0
25	D	1	95	73	20	2	0
25	b	1	96	74	20	2	0

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Mol	Chain	Residues	Atoms				AltConf
25	b	1	Total	C	O	P	0
			96	74	20	2	
25	c	1	Total	C	O	P	0
			147	114	30	3	
25	c	1	Total	C	O	P	0
			147	114	30	3	
25	c	1	Total	C	O	P	0
			147	114	30	3	
25	s	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
26	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
26	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
26	r	1	Total	C	Mg	N	O	0
			231	187	4	16	24	
26	1	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
26	1	1	Total	C	Mg	N	O	0
			362	296	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	1	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	1	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	1	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	1	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	2	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	3	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	4	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	4	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	4	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	4	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	4	1	Total 296	C 241	Mg 5	N 20	O 30	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	5	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	6	1	Total 423	C 346	Mg 7	N 28	O 42	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	v	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	p	1	Total 428	C 351	Mg 7	N 28	O 42	0
26	q	1	Total 291	C 236	Mg 5	N 20	O 30	0
26	q	1	Total 291	C 236	Mg 5	N 20	O 30	0
26	q	1	Total 291	C 236	Mg 5	N 20	O 30	0
26	q	1	Total 291	C 236	Mg 5	N 20	O 30	0
26	q	1	Total 291	C 236	Mg 5	N 20	O 30	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	V	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	P	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	Q	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	U	1	Total 380	C 314	Mg 6	N 24	O 36	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	N	1	Total 296	C 241	Mg 5	N 20	O 30	0
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0

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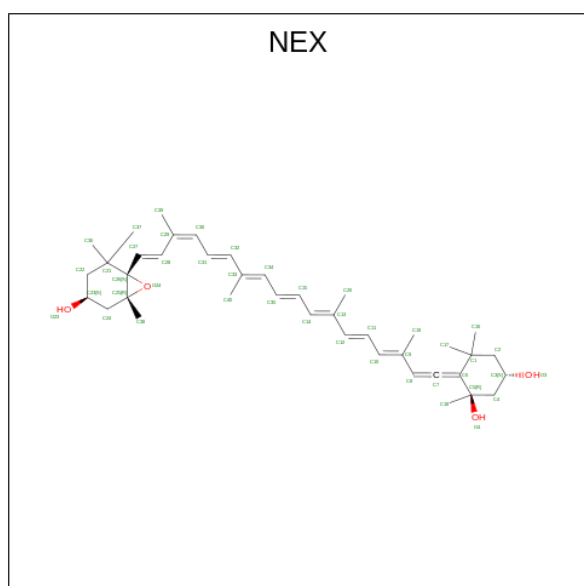
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	G	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	u	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0
26	g	1	Total 357	C 291	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
26	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
26	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
26	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
26	s	1	Total 196	C 152	Mg 4	N 16	O 24	0

- Molecule 27 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
27	r	1	Total	C	O	0
			88	80	8	
27	r	1	Total	C	O	0
			88	80	8	
27	2	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	v	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	V	1	Total	C	O	0
			44	40	4	
27	P	1	Total	C	O	0
			44	40	4	
27	U	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	u	1	Total	C	O	0
			88	80	8	
27	u	1	Total	C	O	0
			88	80	8	
27	n	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	S	1	Total	C	O	0
			44	40	4	
27	s	1	Total	C	O	0
			44	40	4	

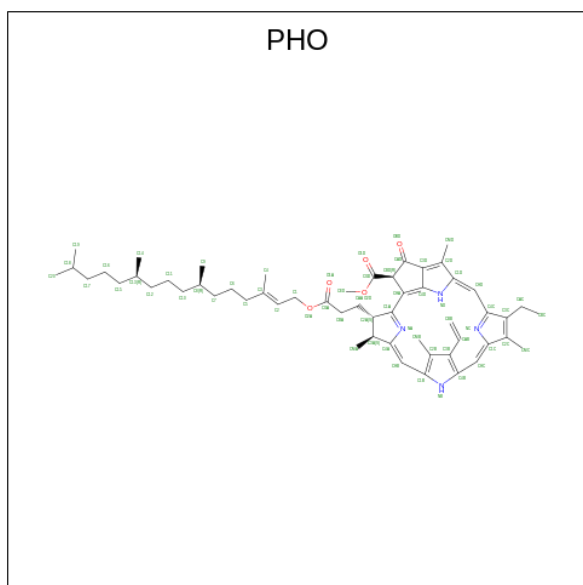
- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 29 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

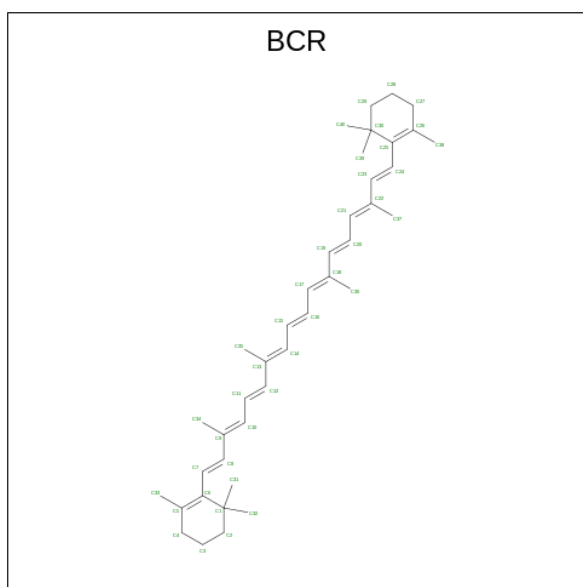
Mol	Chain	Residues	Atoms	AltConf
29	a	2	Total Cl 2 2	0
29	A	2	Total Cl 2 2	0

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



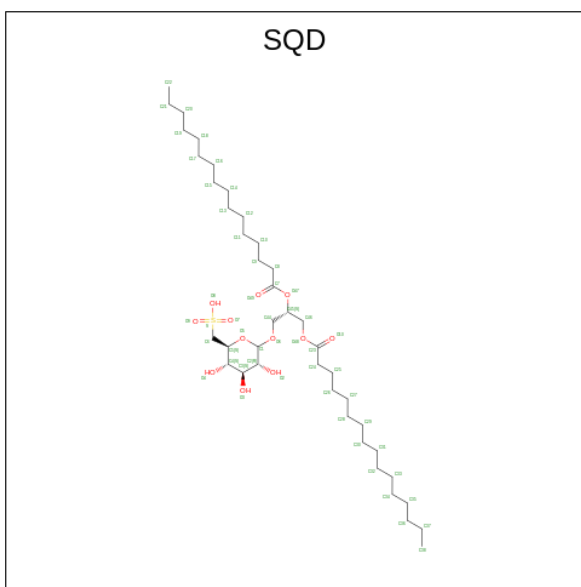
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	t	1	Total C 40 40	0
31	x	1	Total C 40 40	0
31	z	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	C	1	Total C 120 120	0
31	C	1	Total C 120 120	0
31	C	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0

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Mol	Chain	Residues	Atoms		AltConf
31	B	1	Total	C	0
			120	120	
31	D	1	Total	C	0
			40	40	
31	X	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			120	120	
31	b	1	Total	C	0
			120	120	
31	b	1	Total	C	0
			120	120	
31	c	1	Total	C	0
			80	80	
31	c	1	Total	C	0
			80	80	

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



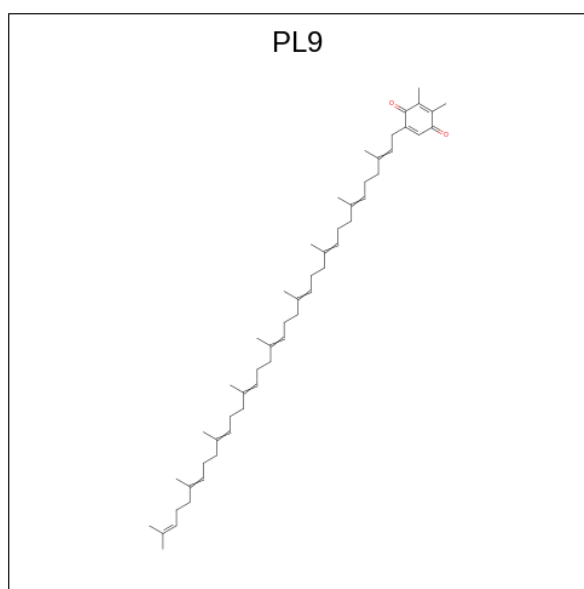
Mol	Chain	Residues	Atoms				AltConf
32	a	1	Total	C	O	S	0
			104	78	24	2	
32	a	1	Total	C	O	S	0
			104	78	24	2	
32	1	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	m	1	Total 42	C 29	O 12	S 1	0
32	A	1	Total 54	C 41	O 12	S 1	0
32	L	1	Total 54	C 41	O 12	S 1	0
32	M	1	Total 42	C 29	O 12	S 1	0
32	C	1	Total 50	C 37	O 12	S 1	0

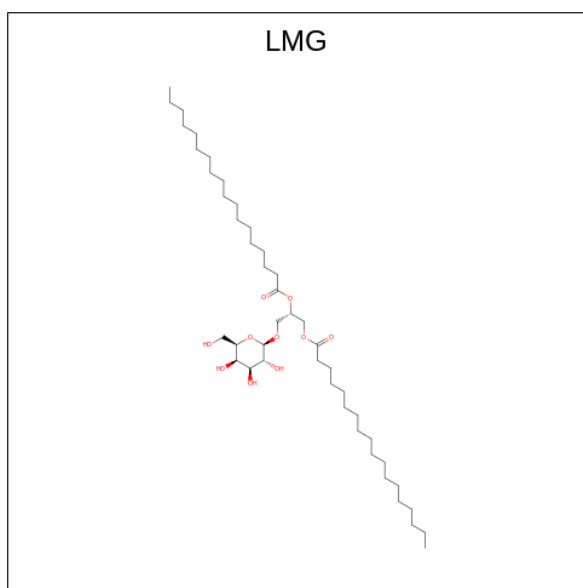
- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C₄₅H₈₆O₁₀).



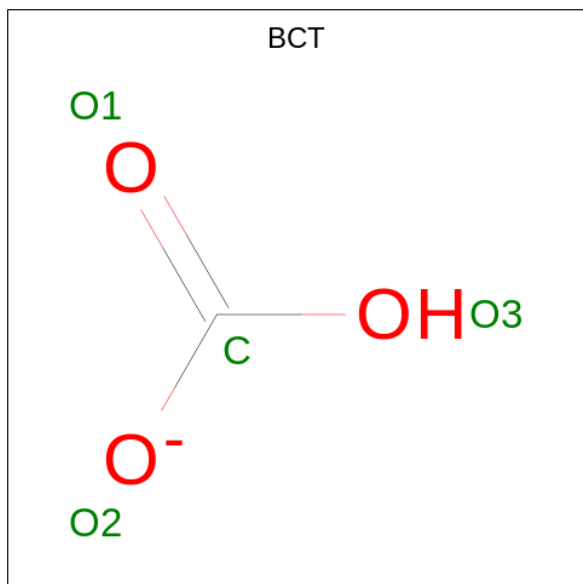
Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			40	30	10	
34	d	1	Total	C	O	0
			46	36	10	
34	w	1	Total	C	O	0
			48	38	10	
34	A	1	Total	C	O	0
			40	30	10	
34	W	1	Total	C	O	0
			48	38	10	
34	C	1	Total	C	O	0
			102	82	20	
34	C	1	Total	C	O	0
			102	82	20	
34	B	1	Total	C	O	0
			106	86	20	
34	B	1	Total	C	O	0
			106	86	20	
34	D	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			106	86	20	
34	b	1	Total	C	O	0
			106	86	20	
34	c	1	Total	C	O	0
			102	82	20	

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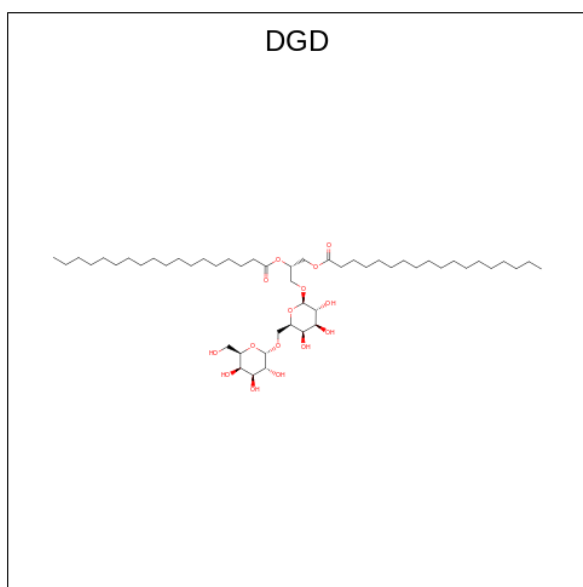
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	c	1	102	82	20	0

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



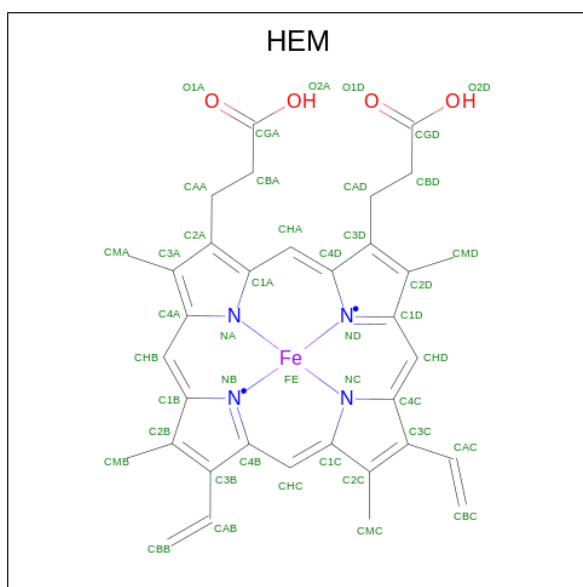
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	a	1	4	1	3	0
35	D	1	4	1	3	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	a	1	59	44	15	0
36	A	1	59	44	15	0
36	J	1	60	45	15	0
36	C	1	117	87	30	0
36	C	1	117	87	30	0
36	B	1	62	47	15	0
36	b	1	62	47	15	0
36	c	1	177	132	45	0
36	c	1	177	132	45	0
36	c	1	177	132	45	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

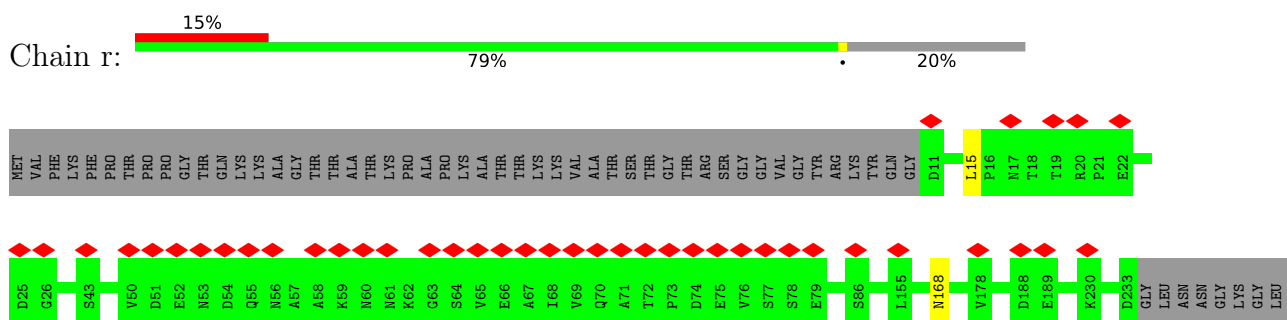


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
37	E	1	43	34	1	4	4	0
37	e	1	43	34	1	4	4	0

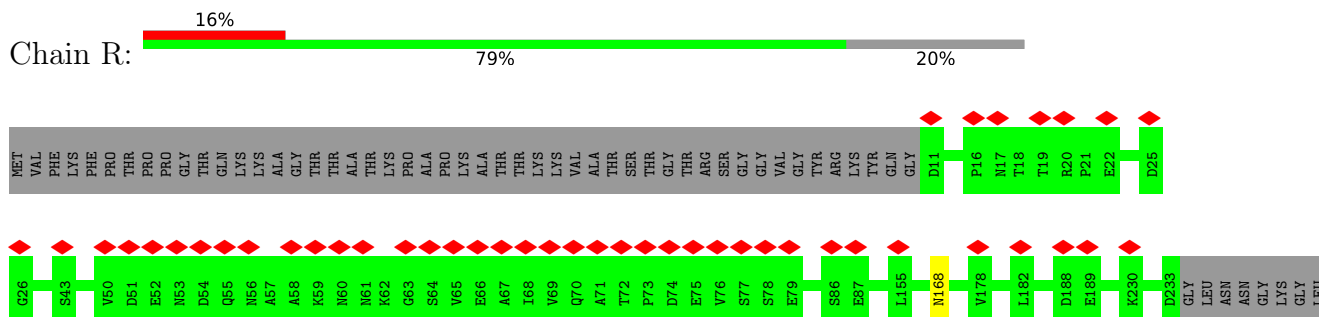
3 Residue-property plots [i](#)

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

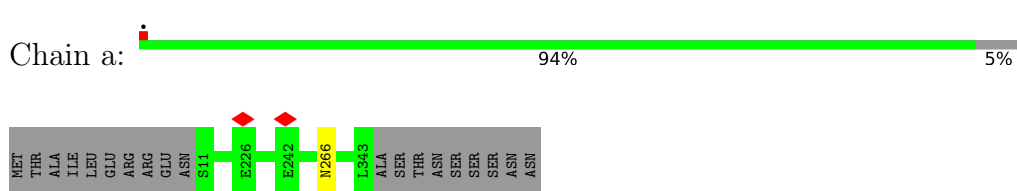
- Molecule 1: Chlorophyll a-b binding protein CP29



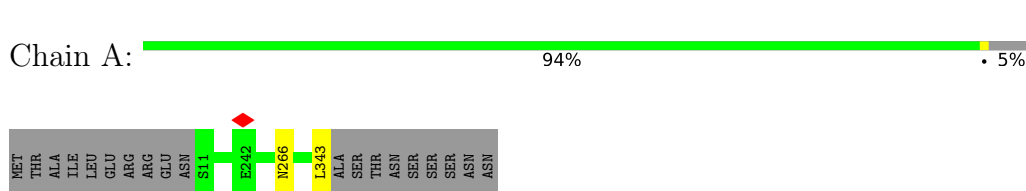
- Molecule 1: Chlorophyll a-b binding protein CP29



- Molecule 2: Photosystem II protein D1



- Molecule 2: Photosystem II protein D1



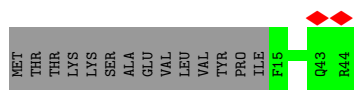
• Molecule 3: Photosystem II D2 protein



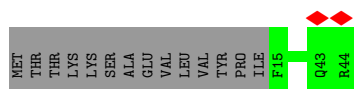
• Molecule 3: Photosystem II D2 protein



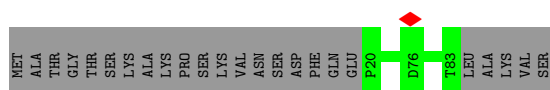
• Molecule 4: Cytochrome b559 subunit beta



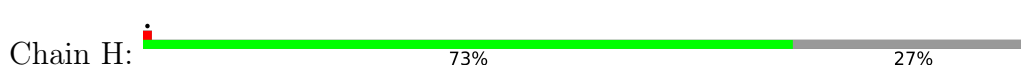
• Molecule 4: Cytochrome b559 subunit beta



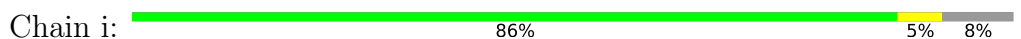
• Molecule 5: Photosystem II reaction center protein H



• Molecule 5: Photosystem II reaction center protein H

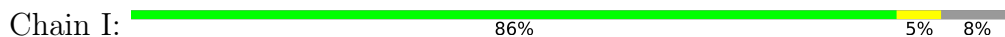


• Molecule 6: Photosystem II reaction center protein I

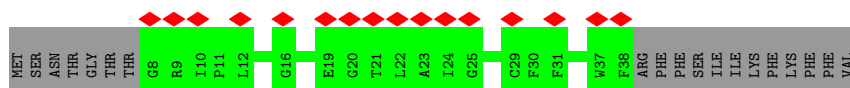




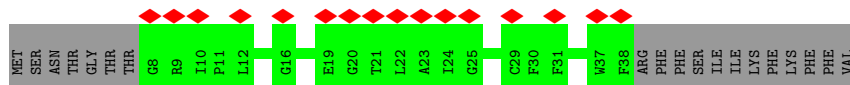
• Molecule 6: Photosystem II reaction center protein I



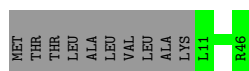
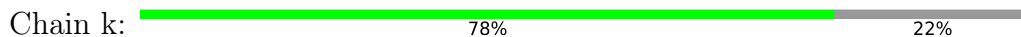
• Molecule 7: Photosystem II reaction center protein J, PsbJ



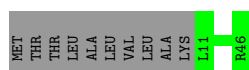
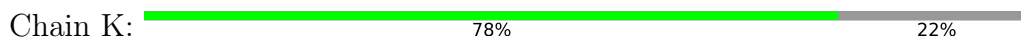
• Molecule 7: Photosystem II reaction center protein J, PsbJ



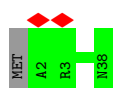
• Molecule 8: Photosystem II reaction center protein K



• Molecule 8: Photosystem II reaction center protein K

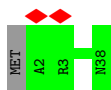


• Molecule 9: Photosystem II reaction center protein L

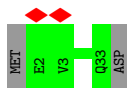


• Molecule 9: Photosystem II reaction center protein L

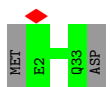




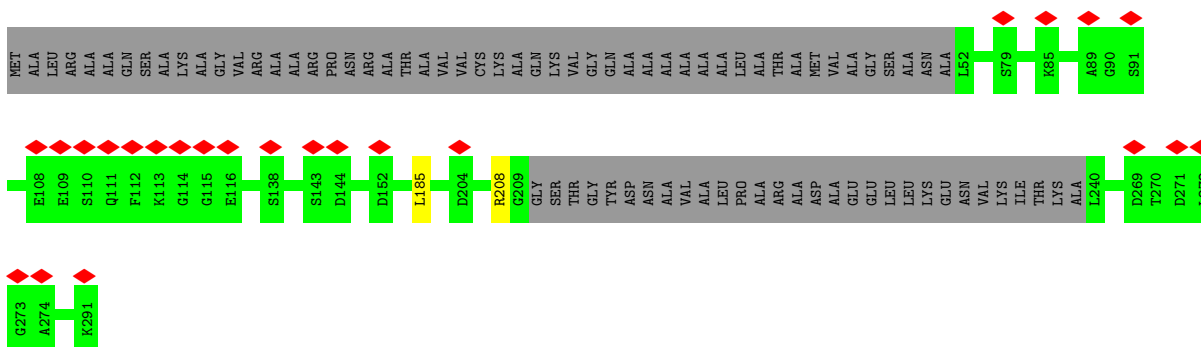
- Molecule 10: Photosystem II reaction center protein M



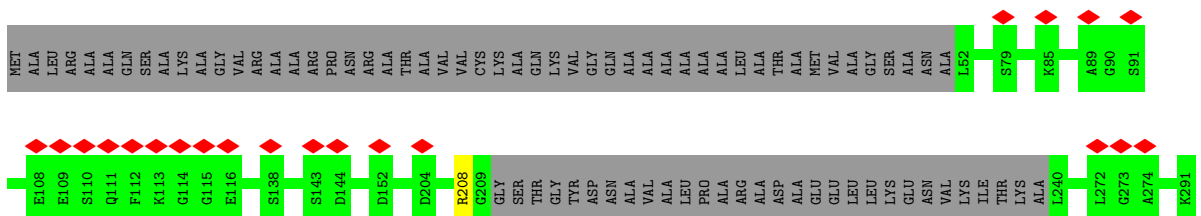
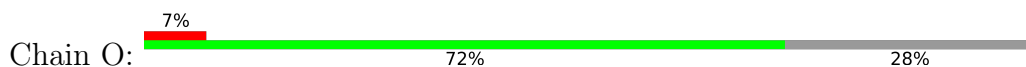
- Molecule 10: Photosystem II reaction center protein M



- Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II



- Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II



- Molecule 12: Photosystem II reaction center protein T

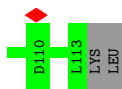
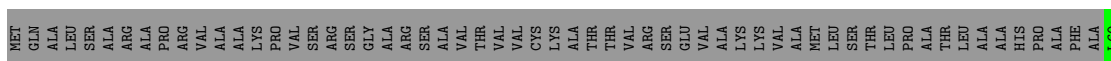




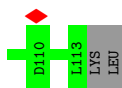
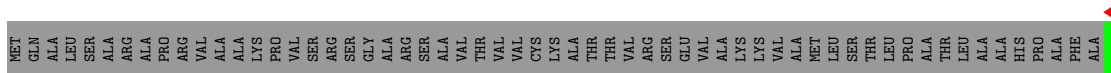
- Molecule 12: Photosystem II reaction center protein T



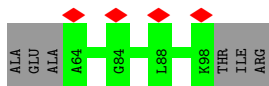
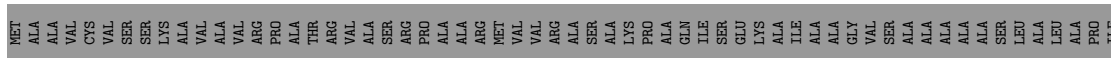
- Molecule 13: Photosystem II reaction center W protein, chloroplastic



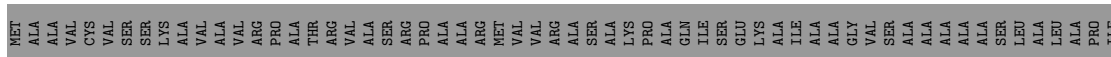
- Molecule 13: Photosystem II reaction center W protein, chloroplastic

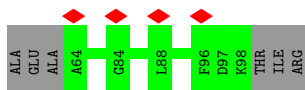


- Molecule 14: 4.1 kDa photosystem II subunit



- Molecule 14: 4.1 kDa photosystem II subunit





- Molecule 15: Photosystem II reaction center protein Z

Chain z: 100%

There are no outlier residues recorded for this chain.

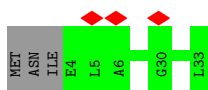
- Molecule 15: Photosystem II reaction center protein Z

Chain Z: 100%

There are no outlier residues recorded for this chain.

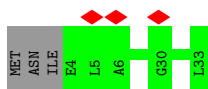
- Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain Y: 9% 91% 9%



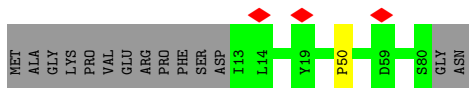
- Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain y: 9% 91% 9%



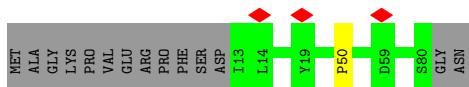
- Molecule 17: Cytochrome b559 subunit alpha

Chain E: 1% 82% 17%



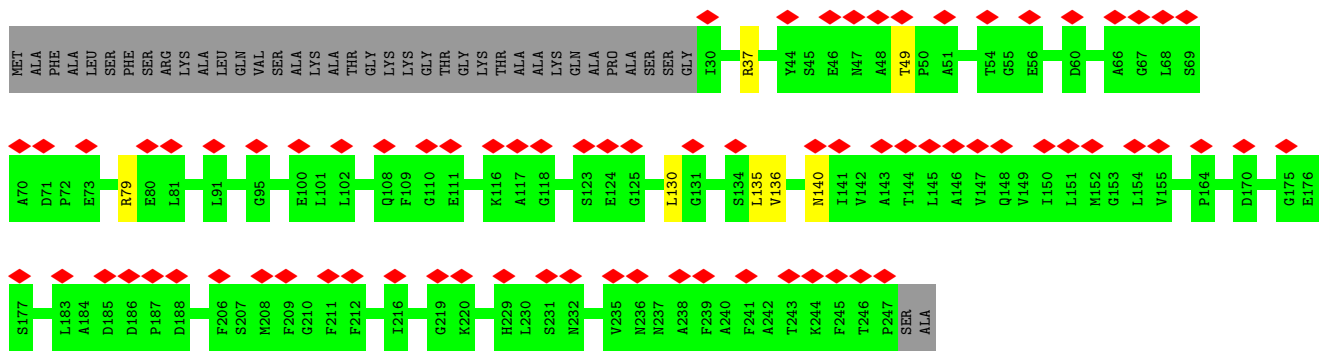
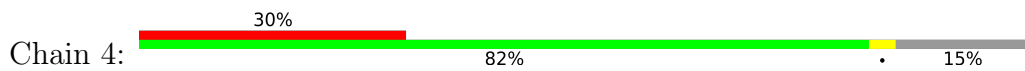
- Molecule 17: Cytochrome b559 subunit alpha

Chain e: 1% 82% 17%

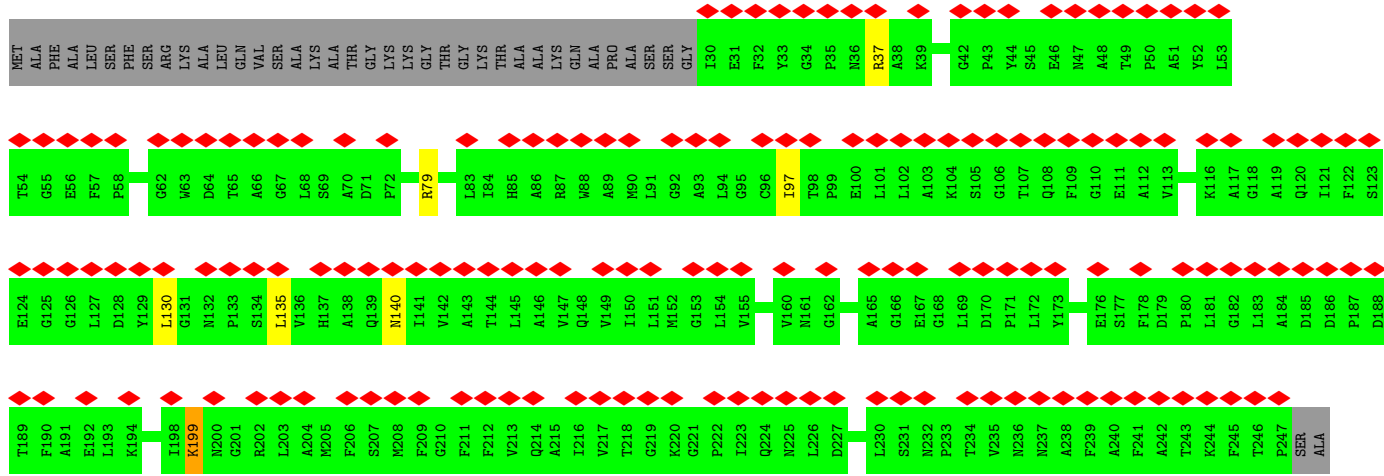
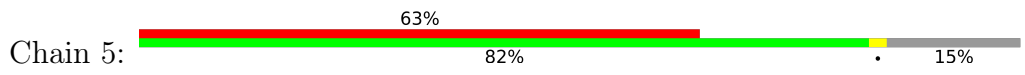


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

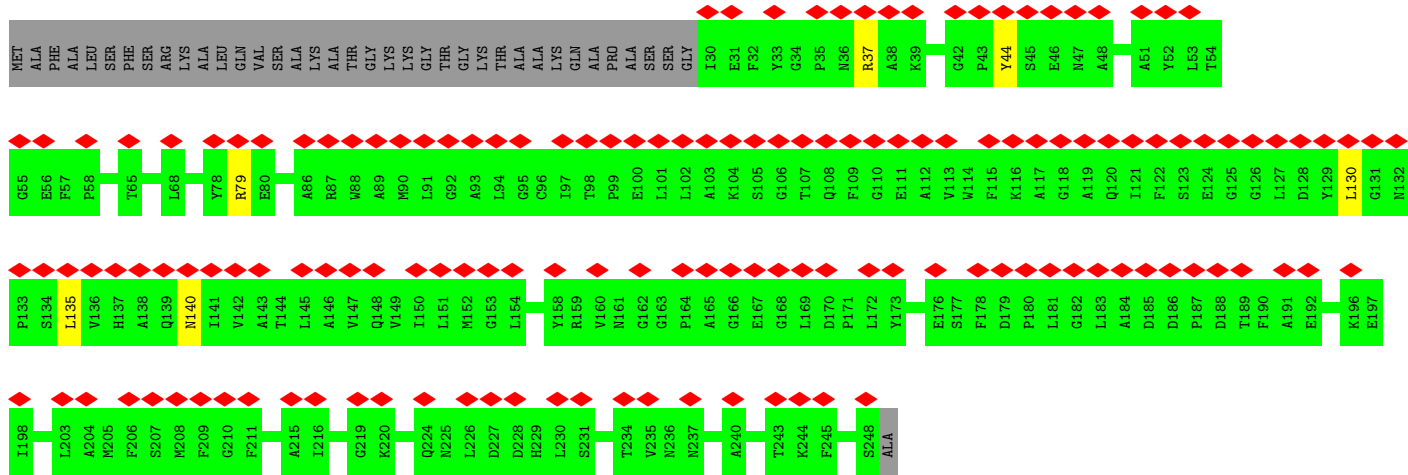
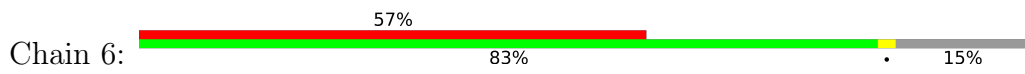
Chain 1: 30% 82% 15%



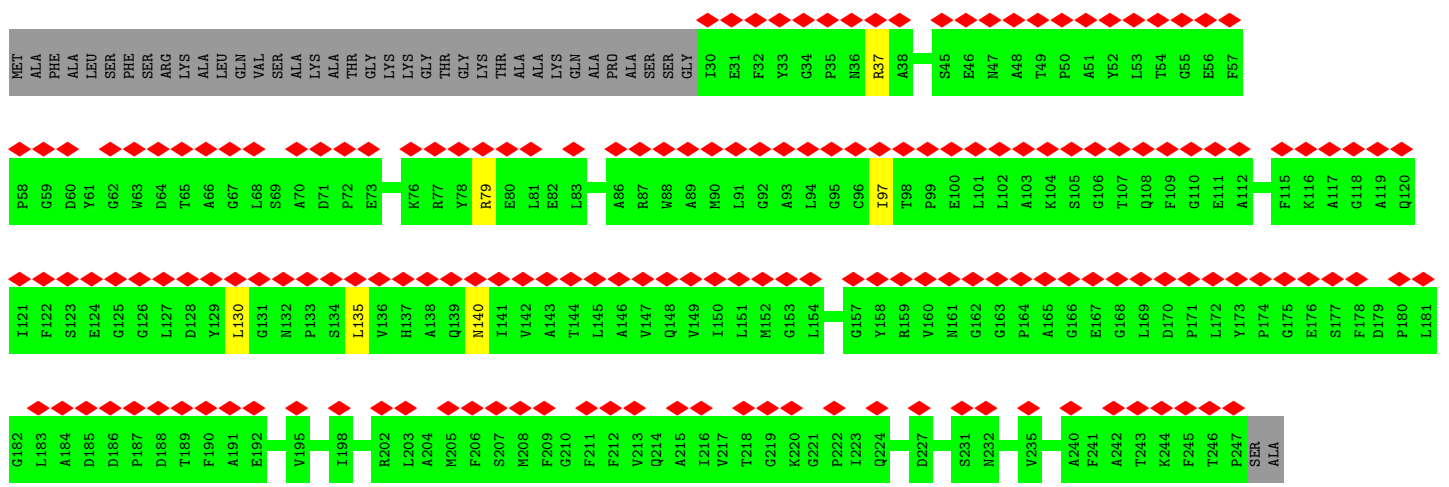
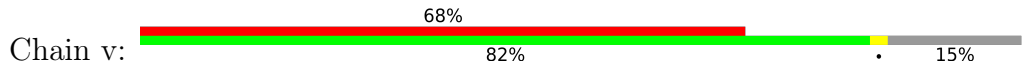
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



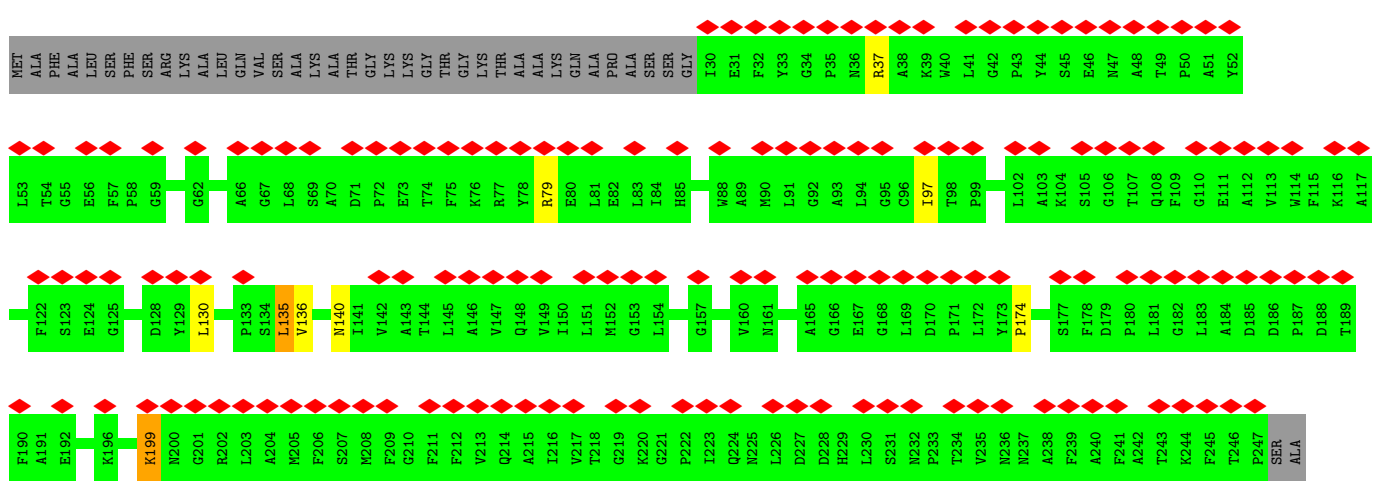
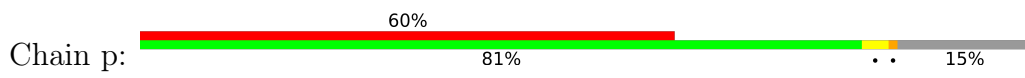
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



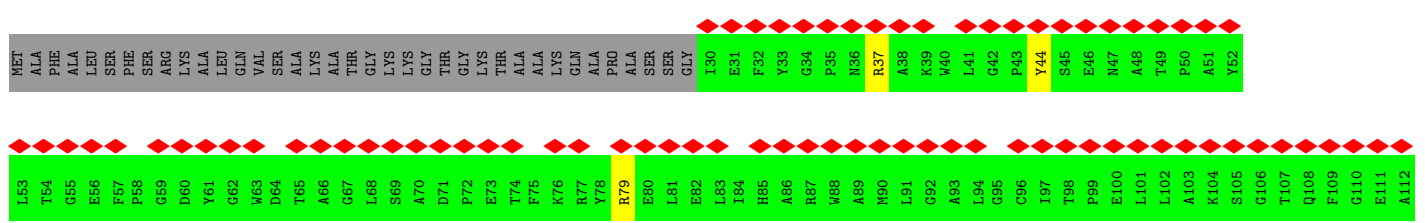
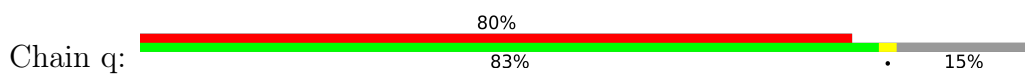
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

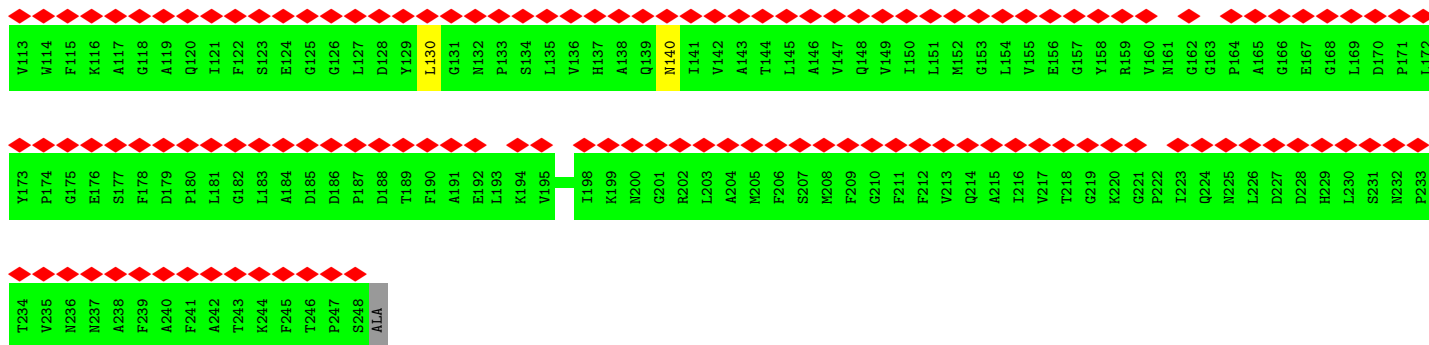


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

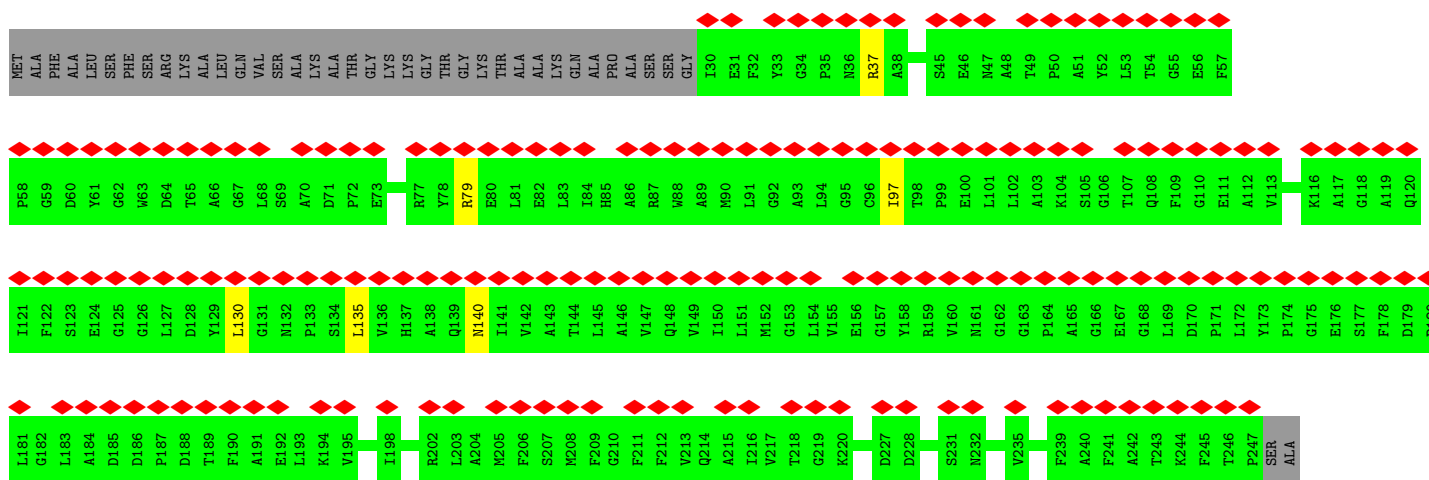
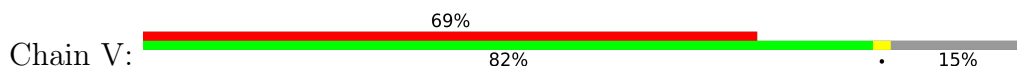


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

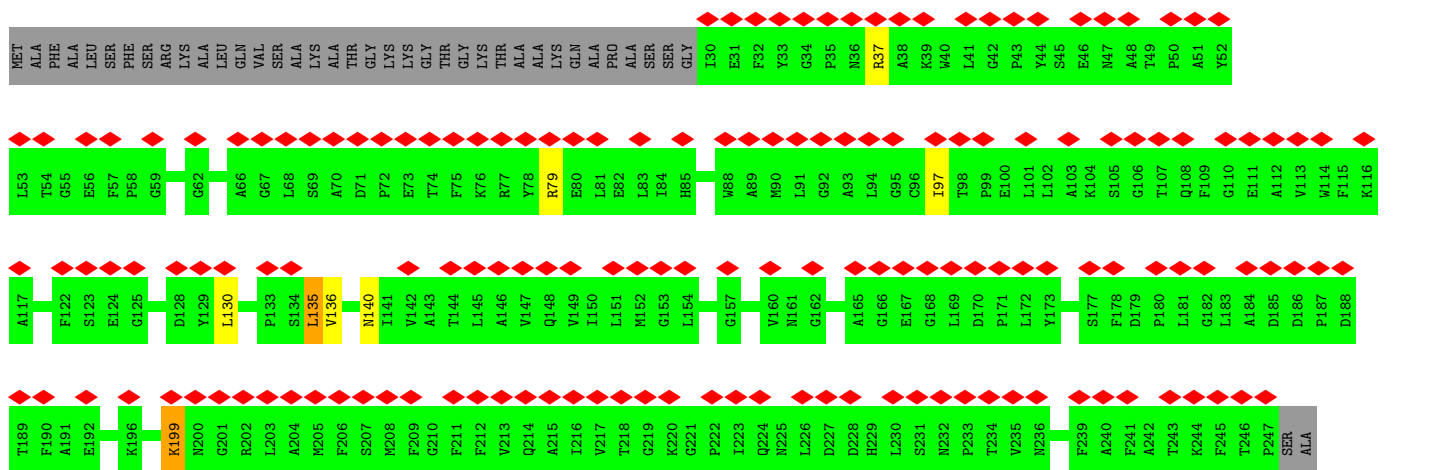
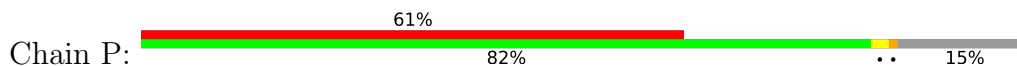




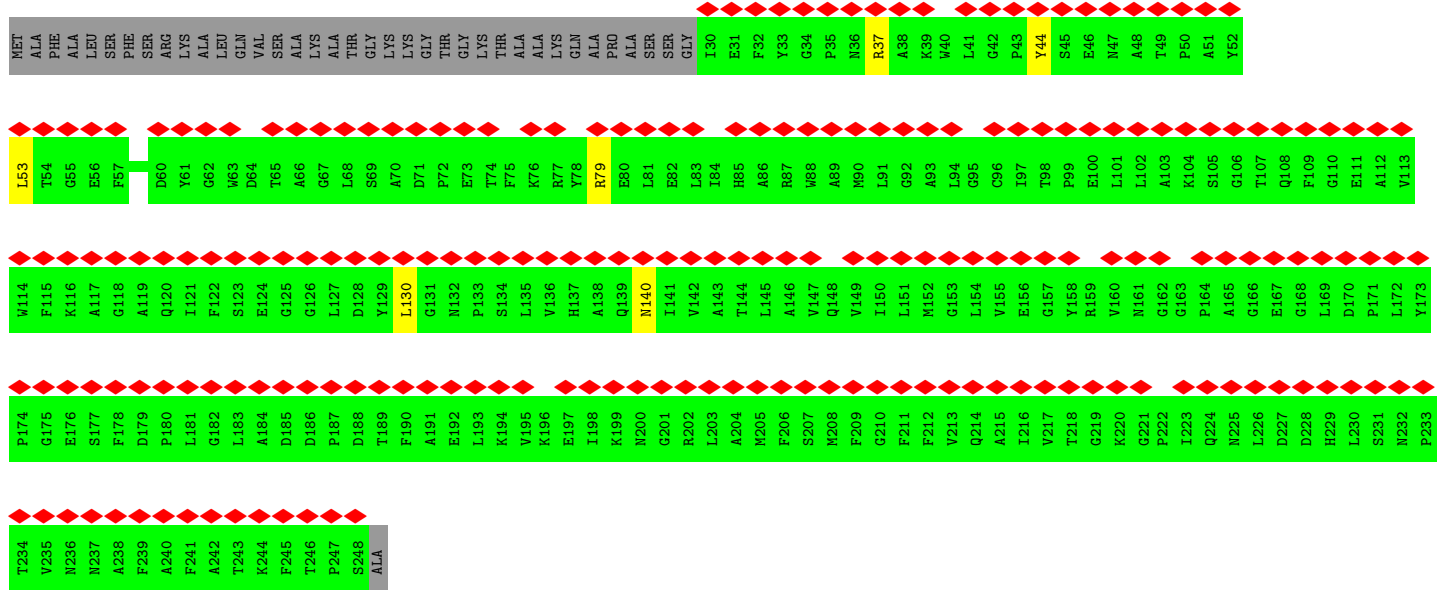
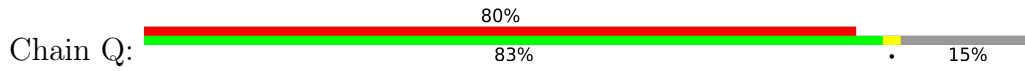
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



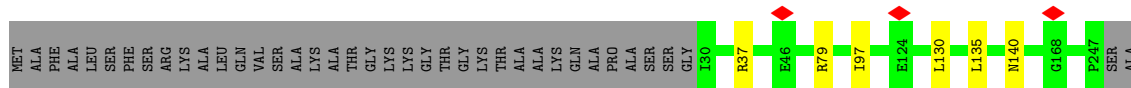
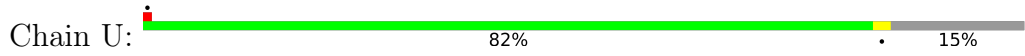
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



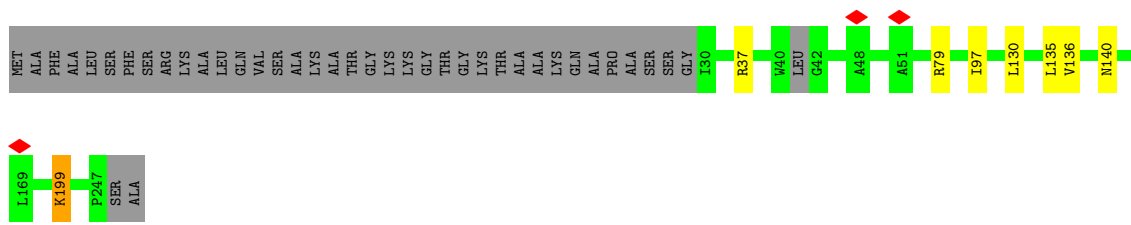
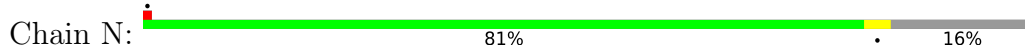
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



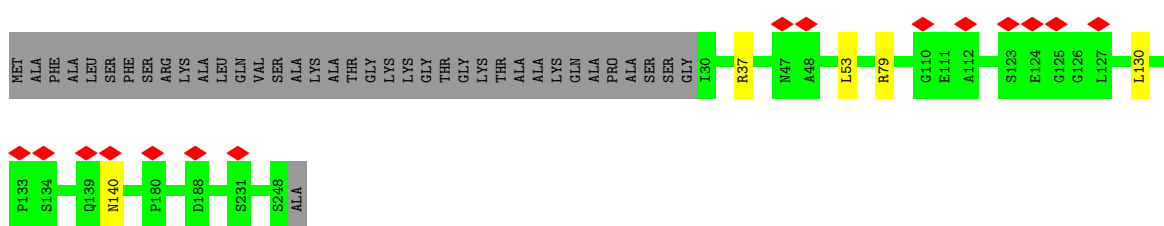
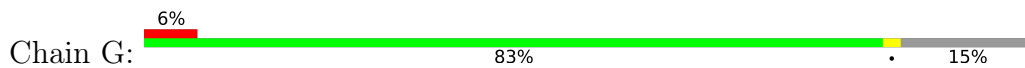
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



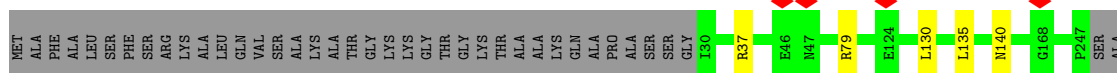
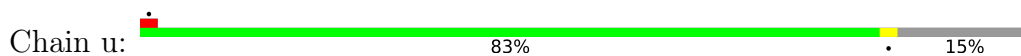
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



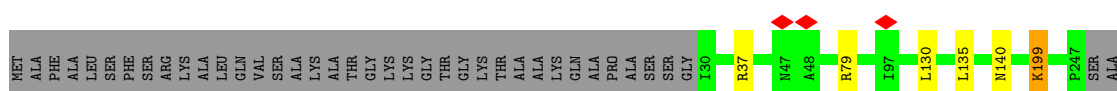
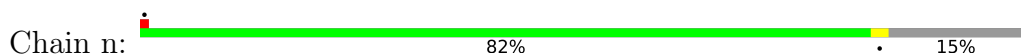
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



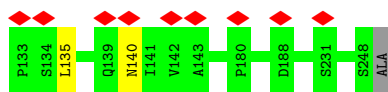
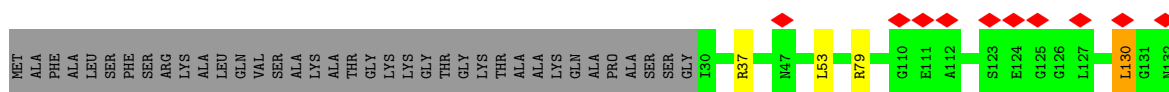
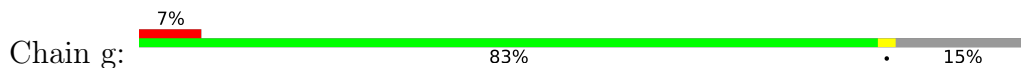
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



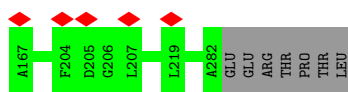
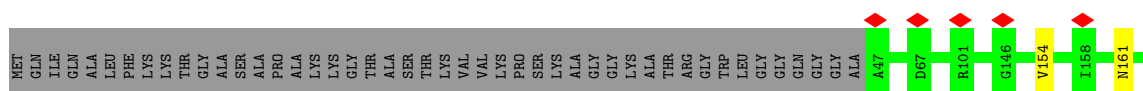
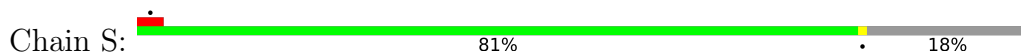
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



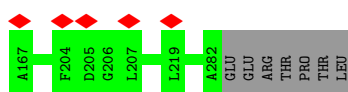
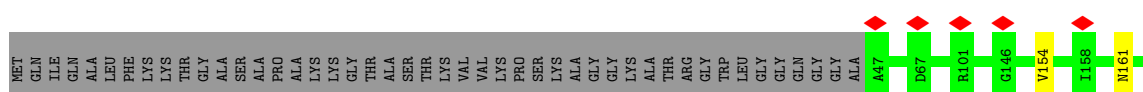
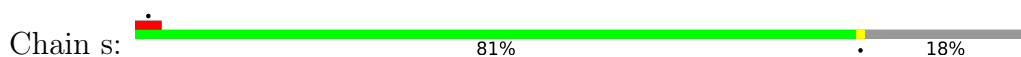
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

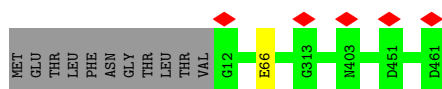


- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



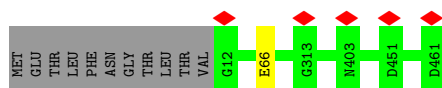
- Molecule 20: Photosystem II CP43 reaction center protein

Chain C:  97%



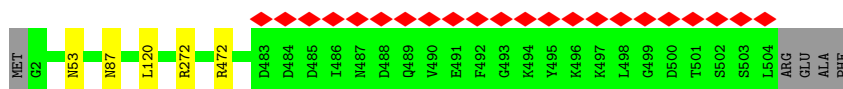
- Molecule 20: Photosystem II CP43 reaction center protein

Chain c:  97%



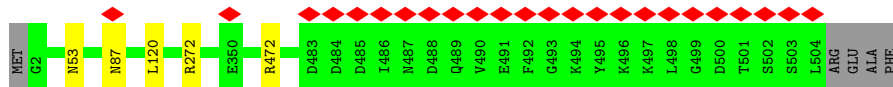
- Molecule 21: Photosystem II CP47 reaction center protein

Chain B:  98%



- Molecule 21: Photosystem II CP47 reaction center protein

Chain b:  5%  98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.181	Depositor
Minimum map value	-1.592	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	392.1, 392.1, 392.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.29	0/1736	0.55	0/2357
1	r	0.29	0/1739	0.55	0/2361
2	A	0.37	0/2696	0.55	1/3676 (0.0%)
2	a	0.37	0/2696	0.55	0/3676
3	D	0.38	0/2808	0.60	1/3830 (0.0%)
3	d	0.38	0/2808	0.60	1/3830 (0.0%)
4	F	0.31	0/250	0.51	0/338
4	f	0.32	0/250	0.52	0/338
5	H	0.33	0/499	0.55	0/683
5	h	0.32	0/499	0.55	0/683
6	I	0.42	0/283	0.58	0/383
6	i	0.42	0/283	0.58	0/383
7	J	0.28	0/254	0.49	0/345
7	j	0.27	0/254	0.48	0/345
8	K	0.40	0/300	0.65	0/414
8	k	0.40	0/300	0.64	0/414
9	L	0.33	0/314	0.51	0/427
9	l	0.33	0/314	0.51	0/427
10	M	0.30	0/252	0.53	0/345
10	m	0.30	0/252	0.54	0/345
11	O	0.30	0/1620	0.59	0/2184
11	o	0.30	0/1620	0.59	1/2184 (0.0%)
12	T	0.33	0/254	0.48	0/343
12	t	0.33	0/254	0.48	0/343
13	W	0.31	0/428	0.49	0/581
13	w	0.31	0/428	0.49	0/581
14	X	0.30	0/244	0.42	0/330
14	x	0.30	0/244	0.42	0/330
15	Z	0.29	0/476	0.49	0/654
15	z	0.29	0/476	0.49	0/654
16	Y	0.27	0/208	0.63	0/285
16	y	0.27	0/208	0.63	0/285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	E	0.32	0/571	0.55	1/780 (0.1%)
17	e	0.32	0/571	0.56	1/780 (0.1%)
18	1	0.31	0/1717	0.56	1/2337 (0.0%)
18	2	0.33	0/1717	0.64	3/2337 (0.1%)
18	3	0.30	0/1723	0.57	2/2345 (0.1%)
18	4	0.31	0/1717	0.57	1/2337 (0.0%)
18	5	0.32	0/1717	0.60	2/2337 (0.1%)
18	6	0.31	0/1723	0.57	1/2345 (0.0%)
18	G	0.31	0/1723	0.59	2/2345 (0.1%)
18	N	0.33	0/1708	0.60	2/2323 (0.1%)
18	P	0.32	0/1717	0.60	3/2337 (0.1%)
18	Q	0.30	0/1723	0.58	2/2345 (0.1%)
18	U	0.33	0/1717	0.61	1/2337 (0.0%)
18	V	0.31	0/1717	0.57	1/2337 (0.0%)
18	g	0.31	0/1723	0.61	2/2345 (0.1%)
18	n	0.33	0/1717	0.62	2/2337 (0.1%)
18	p	0.32	0/1717	0.61	3/2337 (0.1%)
18	q	0.30	0/1723	0.58	1/2345 (0.0%)
18	u	0.33	0/1717	0.62	1/2337 (0.0%)
18	v	0.31	0/1717	0.58	1/2337 (0.0%)
19	S	0.33	0/1849	0.60	0/2521
19	s	0.33	0/1849	0.61	0/2521
20	C	0.34	0/3623	0.51	1/4936 (0.0%)
20	c	0.34	0/3623	0.51	1/4936 (0.0%)
21	B	0.33	0/4067	0.50	0/5533
21	b	0.33	0/4067	0.50	0/5533
All	All	0.33	0/76400	0.57	39/103994 (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
1	r	0	1
18	1	0	1
18	2	0	2
18	3	0	1
18	4	0	2
18	5	0	1
18	6	0	2
18	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	1
18	Q	0	1
18	U	0	1
18	V	0	1
18	g	0	1
18	n	0	1
18	p	0	1
18	q	0	1
18	u	0	1
18	v	0	1
All	All	0	21

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	199	LYS	CD-CE-NZ	-8.78	91.50	111.70
18	5	199	LYS	CD-CE-NZ	-8.57	91.99	111.70
18	n	199	LYS	CD-CE-NZ	-8.17	92.92	111.70
18	p	199	LYS	CD-CE-NZ	-7.90	93.54	111.70
18	2	53	LEU	CA-CB-CG	7.88	133.43	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	1	135	LEU	Peptide
18	2	51	ALA	Peptide
18	2	52	TYR	Peptide
18	3	135	LEU	Peptide
1	r	15	LEU	Peptide

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	221/280 (79%)	201 (91%)	20 (9%)	0	100	100
1	r	221/280 (79%)	197 (89%)	24 (11%)	0	100	100
2	A	331/352 (94%)	314 (95%)	17 (5%)	0	100	100
2	a	331/352 (94%)	316 (96%)	15 (4%)	0	100	100
3	D	339/352 (96%)	304 (90%)	35 (10%)	0	100	100
3	d	339/352 (96%)	307 (91%)	32 (9%)	0	100	100
4	F	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
4	f	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
5	H	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
5	h	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
6	I	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
6	i	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
7	J	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
7	j	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
8	K	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
8	k	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
9	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
10	M	30/34 (88%)	30 (100%)	0	0	100	100
10	m	30/34 (88%)	30 (100%)	0	0	100	100
11	O	206/291 (71%)	176 (85%)	30 (15%)	0	100	100
11	o	206/291 (71%)	175 (85%)	31 (15%)	0	100	100
12	T	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
12	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
13	W	52/115 (45%)	49 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	w	52/115 (45%)	49 (94%)	3 (6%)	0	100	100
14	X	33/101 (33%)	33 (100%)	0	0	100	100
14	x	33/101 (33%)	33 (100%)	0	0	100	100
15	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
15	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
16	Y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
16	y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
17	E	66/82 (80%)	58 (88%)	8 (12%)	0	100	100
17	e	66/82 (80%)	57 (86%)	9 (14%)	0	100	100
18	1	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	29	65
18	2	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	29	65
18	3	217/257 (84%)	191 (88%)	26 (12%)	0	100	100
18	4	216/257 (84%)	189 (88%)	26 (12%)	1 (0%)	29	65
18	5	216/257 (84%)	190 (88%)	26 (12%)	0	100	100
18	6	217/257 (84%)	190 (88%)	27 (12%)	0	100	100
18	G	217/257 (84%)	185 (85%)	32 (15%)	0	100	100
18	N	213/257 (83%)	188 (88%)	24 (11%)	1 (0%)	29	65
18	P	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	29	65
18	Q	217/257 (84%)	184 (85%)	33 (15%)	0	100	100
18	U	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	V	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	g	217/257 (84%)	183 (84%)	34 (16%)	0	100	100
18	n	216/257 (84%)	184 (85%)	32 (15%)	0	100	100
18	p	216/257 (84%)	186 (86%)	28 (13%)	2 (1%)	17	53
18	q	217/257 (84%)	186 (86%)	31 (14%)	0	100	100
18	u	216/257 (84%)	183 (85%)	33 (15%)	0	100	100
18	v	216/257 (84%)	186 (86%)	30 (14%)	0	100	100
19	S	234/289 (81%)	201 (86%)	33 (14%)	0	100	100
19	s	234/289 (81%)	202 (86%)	32 (14%)	0	100	100
20	C	448/461 (97%)	429 (96%)	19 (4%)	0	100	100
20	c	448/461 (97%)	430 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	B	501/508 (99%)	472 (94%)	29 (6%)	0	100	100
21	b	501/508 (99%)	470 (94%)	31 (6%)	0	100	100
All	All	9485/11214 (85%)	8533 (90%)	945 (10%)	7 (0%)	54	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	2	52	TYR
18	p	136	VAL
18	P	136	VAL
18	1	136	VAL
18	N	136	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	175/218 (80%)	174 (99%)	1 (1%)	86	92
1	r	176/218 (81%)	175 (99%)	1 (1%)	86	92
2	A	272/289 (94%)	271 (100%)	1 (0%)	91	95
2	a	272/289 (94%)	271 (100%)	1 (0%)	91	95
3	D	272/281 (97%)	265 (97%)	7 (3%)	46	69
3	d	272/281 (97%)	265 (97%)	7 (3%)	46	69
4	F	24/37 (65%)	24 (100%)	0	100	100
4	f	24/37 (65%)	24 (100%)	0	100	100
5	H	55/75 (73%)	55 (100%)	0	100	100
5	h	55/75 (73%)	55 (100%)	0	100	100
6	I	31/34 (91%)	29 (94%)	2 (6%)	17	48
6	i	31/34 (91%)	29 (94%)	2 (6%)	17	48
7	J	24/42 (57%)	24 (100%)	0	100	100
7	j	24/42 (57%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	30/38 (79%)	30 (100%)	0	100	100
8	k	30/38 (79%)	30 (100%)	0	100	100
9	L	34/35 (97%)	34 (100%)	0	100	100
9	l	34/35 (97%)	34 (100%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	100	100
10	m	28/30 (93%)	28 (100%)	0	100	100
11	O	174/223 (78%)	173 (99%)	1 (1%)	86	92
11	o	174/223 (78%)	173 (99%)	1 (1%)	86	92
12	T	27/28 (96%)	27 (100%)	0	100	100
12	t	27/28 (96%)	27 (100%)	0	100	100
13	W	42/87 (48%)	42 (100%)	0	100	100
13	w	42/87 (48%)	42 (100%)	0	100	100
14	X	25/67 (37%)	25 (100%)	0	100	100
14	x	25/67 (37%)	25 (100%)	0	100	100
15	Z	52/52 (100%)	52 (100%)	0	100	100
15	z	52/52 (100%)	52 (100%)	0	100	100
16	Y	24/27 (89%)	24 (100%)	0	100	100
16	y	24/27 (89%)	24 (100%)	0	100	100
17	E	60/71 (84%)	60 (100%)	0	100	100
17	e	60/71 (84%)	60 (100%)	0	100	100
18	1	169/194 (87%)	166 (98%)	3 (2%)	59	77
18	2	169/194 (87%)	164 (97%)	5 (3%)	41	65
18	3	170/194 (88%)	166 (98%)	4 (2%)	49	71
18	4	169/194 (87%)	166 (98%)	3 (2%)	59	77
18	5	169/194 (87%)	164 (97%)	5 (3%)	41	65
18	6	170/194 (88%)	167 (98%)	3 (2%)	59	77
18	G	170/194 (88%)	167 (98%)	3 (2%)	59	77
18	N	168/194 (87%)	163 (97%)	5 (3%)	41	65
18	P	169/194 (87%)	164 (97%)	5 (3%)	41	65
18	Q	170/194 (88%)	167 (98%)	3 (2%)	59	77
18	U	169/194 (87%)	165 (98%)	4 (2%)	49	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	V	169/194 (87%)	165 (98%)	4 (2%)	49	71
18	g	170/194 (88%)	166 (98%)	4 (2%)	49	71
18	n	169/194 (87%)	165 (98%)	4 (2%)	49	71
18	p	169/194 (87%)	164 (97%)	5 (3%)	41	65
18	q	170/194 (88%)	167 (98%)	3 (2%)	59	77
18	u	169/194 (87%)	166 (98%)	3 (2%)	59	77
18	v	169/194 (87%)	165 (98%)	4 (2%)	49	71
19	S	181/217 (83%)	179 (99%)	2 (1%)	73	85
19	s	181/217 (83%)	179 (99%)	2 (1%)	73	85
20	C	352/362 (97%)	352 (100%)	0	100	100
20	c	352/362 (97%)	352 (100%)	0	100	100
21	B	403/407 (99%)	398 (99%)	5 (1%)	71	84
21	b	403/407 (99%)	398 (99%)	5 (1%)	71	84
All	All	7618/8732 (87%)	7510 (99%)	108 (1%)	68	82

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	P	140	ASN
18	G	37	ARG
3	D	236	ASN
18	Q	37	ARG
18	U	140	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	229	HIS
1	R	56	ASN
21	b	114	HIS
18	U	140	ASN
18	u	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 552 ligands modelled in this entry, 6 are monoatomic - leaving 546 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
27	NEX	v	319	-	38,46,46	0.89	1 (2%)	50,70,70	2.45	14 (28%)
22	CLA	s	308	-	55,63,73	1.58	8 (14%)	64,101,113	1.51	7 (10%)
31	BCR	B	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.26	22 (39%)
26	CHL	U	316	18	66,74,74	1.87	15 (22%)	73,114,114	2.56	24 (32%)
25	LHG	C	522	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	u	317	18	66,74,74	1.86	15 (22%)	73,114,114	2.52	24 (32%)
23	LUT	l	309	-	42,43,43	0.72	0	51,60,60	1.57	10 (19%)
32	SQD	l	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
26	CHL	R	316	-	56,64,74	2.05	14 (25%)	61,102,114	2.62	21 (34%)
22	CLA	b	609	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	6 (7%)
23	LUT	p	311	-	42,43,43	0.76	0	51,60,60	1.54	12 (23%)
24	XAT	G	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.82	19 (35%)
22	CLA	C	511	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	11 (14%)
27	NEX	R	301	22,1	38,46,46	1.03	2 (5%)	50,70,70	2.42	13 (26%)
25	LHG	d	405	3	45,45,48	0.92	4 (8%)	48,51,54	1.07	2 (4%)
26	CHL	U	315	-	66,74,74	1.85	14 (21%)	73,114,114	2.47	23 (31%)
22	CLA	U	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	b	617	21	65,73,73	1.51	10 (15%)	76,113,113	1.56	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PL9	D	405	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
22	CLA	R	310	-	60,68,73	1.54	5 (8%)	70,107,113	1.55	9 (12%)
22	CLA	S	308	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	7 (10%)
22	CLA	p	307	-	60,68,73	1.52	5 (8%)	70,107,113	1.46	8 (11%)
25	LHG	3	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	p	306	18	60,68,73	1.49	6 (10%)	70,107,113	2.10	16 (22%)
22	CLA	u	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.37	7 (9%)
24	XAT	R	313	-	39,47,47	2.54	17 (43%)	54,74,74	11.48	22 (40%)
26	CHL	q	313	-	50,58,74	2.18	16 (32%)	52,94,114	2.73	19 (36%)
26	CHL	n	313	18	66,74,74	1.94	16 (24%)	73,114,114	2.40	24 (32%)
32	SQD	a	410	-	49,50,54	1.01	5 (10%)	58,61,65	1.74	11 (18%)
30	PHO	d	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
36	DGD	C	519	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
22	CLA	B	610	-	65,73,73	1.48	8 (12%)	76,113,113	1.46	9 (11%)
26	CHL	V	314	-	48,56,74	2.30	17 (35%)	51,92,114	2.79	21 (41%)
22	CLA	q	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.64	9 (15%)
23	LUT	S	310	-	42,43,43	0.77	0	51,60,60	1.69	14 (27%)
34	LMG	A	411	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
26	CHL	3	315	18	66,74,74	1.89	16 (24%)	73,114,114	2.44	20 (27%)
26	CHL	Q	314	-	66,74,74	1.93	16 (24%)	73,114,114	2.36	22 (30%)
26	CHL	u	313	-	66,74,74	1.94	17 (25%)	73,114,114	2.37	23 (31%)
25	LHG	1	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	G	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.58	7 (12%)
26	CHL	s	316	-	46,54,74	2.37	16 (34%)	49,90,114	2.82	20 (40%)
32	SQD	a	413	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
27	NEX	r	617	-	38,46,46	1.01	3 (7%)	50,70,70	2.42	17 (34%)
22	CLA	g	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	7 (9%)
30	PHO	A	407	-	51,69,69	1.09	5 (9%)	47,99,99	1.23	6 (12%)
22	CLA	U	306	-	60,68,73	1.57	9 (15%)	70,107,113	1.43	8 (11%)
26	CHL	N	314	-	48,56,74	2.33	16 (33%)	51,92,114	2.82	20 (39%)
27	NEX	5	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.43	16 (32%)
23	LUT	n	310	-	42,43,43	0.79	0	51,60,60	1.75	14 (27%)
26	CHL	2	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.37	20 (27%)
22	CLA	q	302	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	p	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	n	302	-	65,73,73	1.52	7 (10%)	76,113,113	1.37	7 (9%)
26	CHL	6	312	-	66,74,74	1.90	15 (22%)	73,114,114	2.48	23 (31%)
22	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	7 (9%)
23	LUT	u	309	-	42,43,43	0.75	0	51,60,60	1.52	10 (19%)
22	CLA	Q	301	-	65,73,73	1.49	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	6	309	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	C	503	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	9 (11%)
22	CLA	C	513	-	65,73,73	1.47	9 (13%)	76,113,113	1.53	9 (11%)
36	DGD	c	517	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
22	CLA	c	503	-	65,73,73	1.49	10 (15%)	76,113,113	1.51	7 (9%)
22	CLA	3	305	22	60,68,73	1.51	6 (10%)	70,107,113	1.52	10 (14%)
26	CHL	p	316	-	50,58,74	2.23	16 (32%)	52,94,114	2.72	22 (42%)
31	BCR	k	101	-	41,41,41	4.73	25 (60%)	56,56,56	2.52	19 (33%)
25	LHG	s	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.14	3 (5%)
22	CLA	V	306	-	60,68,73	1.56	7 (11%)	70,107,113	1.43	8 (11%)
22	CLA	N	304	18	65,73,73	1.43	7 (10%)	76,113,113	1.53	9 (11%)
22	CLA	G	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
26	CHL	3	312	-	48,56,74	2.38	17 (35%)	51,92,114	2.80	23 (45%)
37	HEM	E	101	17,4	41,50,50	1.60	6 (14%)	45,82,82	1.15	2 (4%)
24	XAT	2	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
26	CHL	S	316	-	46,54,74	2.36	16 (34%)	49,90,114	2.81	20 (40%)
22	CLA	p	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.50	6 (8%)
22	CLA	4	301	-	65,73,73	1.47	9 (13%)	76,113,113	1.44	7 (9%)
26	CHL	r	615	-	56,64,74	2.05	15 (26%)	61,102,114	2.61	21 (34%)
22	CLA	N	305	18	60,68,73	1.49	6 (10%)	70,107,113	1.93	13 (18%)
22	CLA	c	509	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)
26	CHL	Q	311	-	66,74,74	1.90	16 (24%)	73,114,114	2.44	23 (31%)
25	LHG	n	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.03	2 (3%)
26	CHL	u	314	-	48,56,74	2.22	16 (33%)	51,92,114	2.79	21 (41%)
22	CLA	s	305	-	55,63,73	1.58	7 (12%)	64,101,113	1.49	8 (12%)
22	CLA	r	602	-	60,68,73	1.53	6 (10%)	70,107,113	1.47	7 (10%)
26	CHL	p	320	-	66,74,74	1.87	14 (21%)	73,114,114	2.42	21 (28%)
22	CLA	r	603	-	60,68,73	1.53	6 (10%)	70,107,113	1.46	6 (8%)
22	CLA	C	509	20	65,73,73	1.46	9 (13%)	76,113,113	1.53	10 (13%)
22	CLA	q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	611	-	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
22	CLA	G	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.53	9 (12%)
36	DGD	B	601	21	63,63,67	1.22	7 (11%)	77,77,81	1.07	3 (3%)
22	CLA	r	605	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
26	CHL	g	314	-	66,74,74	1.96	16 (24%)	73,114,114	2.41	23 (31%)
26	CHL	2	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
22	CLA	1	305	-	60,68,73	1.49	6 (10%)	70,107,113	1.45	8 (11%)
25	LHG	u	312	-	48,48,48	0.88	4 (8%)	51,54,54	1.13	3 (5%)
26	CHL	v	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.52	25 (34%)
23	LUT	P	310	-	42,43,43	0.73	0	51,60,60	1.67	14 (27%)
34	LMG	w	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
26	CHL	Q	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.47	21 (28%)
22	CLA	R	306	-	58,66,73	1.56	6 (10%)	67,104,113	1.53	6 (8%)
22	CLA	p	304	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	8 (13%)
22	CLA	c	513	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	8 (10%)
22	CLA	b	602	-	65,73,73	1.42	9 (13%)	76,113,113	1.44	7 (9%)
22	CLA	C	515	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	9 (11%)
22	CLA	c	511	8,20	65,73,73	1.48	9 (13%)	76,113,113	1.29	7 (9%)
26	CHL	g	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.40	22 (30%)
23	LUT	S	311	-	42,43,43	0.77	0	51,60,60	1.64	17 (33%)
26	CHL	4	316	18	66,74,74	1.91	15 (22%)	73,114,114	2.48	26 (35%)
26	CHL	u	315	-	50,58,74	2.14	13 (26%)	52,94,114	2.65	20 (38%)
26	CHL	V	317	18	66,74,74	1.91	15 (22%)	73,114,114	2.51	25 (34%)
34	LMG	b	624	21	55,55,55	1.17	6 (10%)	63,63,63	1.07	2 (3%)
22	CLA	a	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	8 (13%)
22	CLA	q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.63	8 (10%)
22	CLA	n	304	18	65,73,73	1.42	7 (10%)	76,113,113	1.54	9 (11%)
23	LUT	2	310	-	42,43,43	0.78	0	51,60,60	1.64	12 (23%)
22	CLA	R	303	-	60,68,73	1.52	6 (10%)	70,107,113	1.48	8 (11%)
32	SQD	C	501	-	49,50,54	1.00	5 (10%)	58,61,65	1.75	11 (18%)
22	CLA	A	404	-	65,73,73	1.41	8 (12%)	76,113,113	1.59	8 (10%)
22	CLA	B	615	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	7 (9%)
26	CHL	U	317	-	66,74,74	1.86	14 (21%)	73,114,114	2.38	19 (26%)
26	CHL	6	315	-	66,74,74	1.96	17 (25%)	73,114,114	2.39	22 (30%)
22	CLA	C	507	-	65,73,73	1.39	7 (10%)	76,113,113	1.64	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	408	-	60,68,73	1.45	8 (13%)	70,107,113	1.67	8 (11%)
22	CLA	b	604	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
27	NEX	S	317	19	38,46,46	0.88	1 (2%)	50,70,70	2.45	17 (34%)
34	LMG	b	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	7 (11%)
25	LHG	q	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.05	2 (3%)
33	PL9	d	404	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
26	CHL	R	317	-	61,69,74	2.01	17 (27%)	67,108,114	2.38	20 (29%)
26	CHL	v	314	-	48,56,74	2.23	15 (31%)	51,92,114	2.84	21 (41%)
22	CLA	U	303	-	50,58,73	1.68	9 (18%)	58,95,113	1.56	7 (12%)
22	CLA	q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	8 (14%)
25	LHG	D	407	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
22	CLA	C	512	8,20	65,73,73	1.48	9 (13%)	76,113,113	1.28	7 (9%)
27	NEX	P	301	18	38,46,46	0.94	1 (2%)	50,70,70	2.35	18 (36%)
25	LHG	r	613	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
32	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.50	10 (16%)
22	CLA	R	308	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	8 (14%)
22	CLA	b	615	-	65,73,73	1.43	8 (12%)	76,113,113	1.49	7 (9%)
22	CLA	S	309	-	49,57,73	1.69	8 (16%)	55,93,113	1.55	6 (10%)
31	BCR	b	620	-	41,41,41	4.77	24 (58%)	56,56,56	2.21	21 (37%)
26	CHL	5	315	-	50,58,74	2.17	15 (30%)	52,94,114	2.79	20 (38%)
22	CLA	G	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.53	8 (11%)
22	CLA	S	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	8 (12%)
22	CLA	U	307	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	v	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.35	6 (7%)
26	CHL	n	318	-	66,74,74	1.95	16 (24%)	73,114,114	2.35	23 (31%)
26	CHL	G	312	-	48,56,74	2.32	18 (37%)	51,92,114	2.82	20 (39%)
26	CHL	v	318	-	66,74,74	1.92	16 (24%)	73,114,114	2.32	21 (28%)
26	CHL	2	314	-	48,56,74	2.38	17 (35%)	51,92,114	2.95	21 (41%)
37	HEM	e	101	17,4	41,50,50	1.59	5 (12%)	45,82,82	1.14	2 (4%)
26	CHL	2	317	-	66,74,74	1.86	13 (19%)	73,114,114	2.45	23 (31%)
22	CLA	c	506	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
26	CHL	N	315	-	50,58,74	2.17	16 (32%)	52,94,114	2.72	21 (40%)
22	CLA	R	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
35	BCT	D	402	-	2,3,3	1.35	0	2,3,3	0.19	0
36	DGD	b	601	21	63,63,67	1.23	7 (11%)	77,77,81	1.06	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	XAT	6	310	-	39,47,47	2.56	18 (46%)	54,74,74	11.74	17 (31%)
22	CLA	C	506	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	r	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
26	CHL	v	313	-	66,74,74	1.92	16 (24%)	73,114,114	2.45	23 (31%)
23	LUT	r	611	1	42,43,43	0.75	0	51,60,60	1.66	10 (19%)
26	CHL	U	319	-	66,74,74	1.92	15 (22%)	73,114,114	2.39	21 (28%)
26	CHL	s	313	-	46,54,74	2.34	16 (34%)	49,90,114	2.82	20 (40%)
25	LHG	l	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
26	CHL	g	316	-	61,69,74	1.97	16 (26%)	67,108,114	2.48	25 (37%)
26	CHL	S	314	-	46,54,74	2.28	16 (34%)	49,90,114	2.86	18 (36%)
24	XAT	g	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.71	20 (37%)
26	CHL	6	316	18	66,74,74	1.89	17 (25%)	73,114,114	2.47	19 (26%)
22	CLA	3	301	-	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
25	LHG	R	314	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
31	BCR	B	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.45	22 (39%)
23	LUT	N	310	-	42,43,43	0.78	0	51,60,60	1.69	15 (29%)
22	CLA	p	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.46	8 (10%)
22	CLA	b	616	21	65,73,73	1.43	9 (13%)	76,113,113	1.46	9 (11%)
22	CLA	s	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.64	8 (14%)
25	LHG	d	406	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
26	CHL	4	314	-	48,56,74	2.20	14 (29%)	51,92,114	2.87	21 (41%)
31	BCR	X	201	-	41,41,41	4.79	24 (58%)	56,56,56	2.26	17 (30%)
22	CLA	2	303	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
26	CHL	U	314	-	50,58,74	2.15	14 (28%)	52,94,114	2.70	20 (38%)
22	CLA	6	306	22	60,68,73	1.51	6 (10%)	70,107,113	1.51	10 (14%)
22	CLA	B	611	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	8 (10%)
22	CLA	C	508	-	65,73,73	1.51	9 (13%)	76,113,113	1.43	7 (9%)
26	CHL	6	317	-	61,69,74	1.99	13 (21%)	67,108,114	2.52	22 (32%)
22	CLA	A	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	10 (13%)
22	CLA	g	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
26	CHL	G	311	-	66,74,74	1.87	15 (22%)	73,114,114	2.46	23 (31%)
26	CHL	G	315	18	66,74,74	1.87	16 (24%)	73,114,114	2.42	20 (27%)
22	CLA	s	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
26	CHL	V	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.38	22 (30%)
22	CLA	c	505	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.51	8 (10%)
26	CHL	n	317	-	66,74,74	1.92	17 (25%)	73,114,114	2.48	22 (30%)
22	CLA	n	308	-	48,56,73	1.75	6 (12%)	55,92,113	1.65	9 (16%)
36	DGD	A	414	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
22	CLA	S	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.63	8 (13%)
22	CLA	2	307	-	60,68,73	1.51	6 (10%)	70,107,113	1.50	7 (10%)
22	CLA	P	309	-	48,56,73	1.69	6 (12%)	55,92,113	1.57	7 (12%)
24	XAT	4	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.07	21 (38%)
22	CLA	c	502	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
26	CHL	q	315	-	61,69,74	2.01	16 (26%)	67,108,114	2.49	23 (34%)
22	CLA	n	303	-	50,58,73	1.69	6 (12%)	58,95,113	1.61	8 (13%)
34	LMG	W	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
26	CHL	P	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.42	22 (30%)
22	CLA	P	306	18	60,68,73	1.48	6 (10%)	70,107,113	2.01	12 (17%)
22	CLA	u	303	-	50,58,73	1.69	8 (16%)	58,95,113	1.59	8 (13%)
23	LUT	4	310	-	42,43,43	0.83	1 (2%)	51,60,60	1.79	14 (27%)
22	CLA	S	307	-	49,57,73	1.66	7 (14%)	55,93,113	1.65	8 (14%)
25	LHG	b	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.04	2 (4%)
22	CLA	6	307	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
31	BCR	x	202	-	41,41,41	4.78	24 (58%)	56,56,56	2.27	18 (32%)
33	PL9	A	410	-	13,13,55	3.64	7 (53%)	17,17,69	1.47	3 (17%)
24	XAT	U	311	-	39,47,47	2.51	17 (43%)	54,74,74	11.93	20 (37%)
26	CHL	3	314	-	66,74,74	1.96	17 (25%)	73,114,114	2.38	20 (27%)
26	CHL	p	315	-	48,56,74	2.41	17 (35%)	51,92,114	2.76	19 (37%)
22	CLA	6	308	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
23	LUT	n	309	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
24	XAT	v	311	-	39,47,47	2.56	18 (46%)	54,74,74	12.01	19 (35%)
23	LUT	u	310	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	R	309	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	9 (16%)
36	DGD	C	520	-	63,63,67	1.22	6 (9%)	77,77,81	1.16	4 (5%)
22	CLA	n	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
22	CLA	V	301	-	65,73,73	1.51	9 (13%)	76,113,113	1.33	6 (7%)
25	LHG	2	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	V	315	-	50,58,74	2.29	16 (32%)	52,94,114	2.69	20 (38%)
26	CHL	V	318	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	u	316	-	66,74,74	1.90	14 (21%)	73,114,114	2.52	27 (36%)
26	CHL	G	316	-	61,69,74	1.95	15 (24%)	67,108,114	2.49	22 (32%)
22	CLA	u	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	8 (10%)
22	CLA	B	602	-	65,73,73	1.43	9 (13%)	76,113,113	1.45	10 (13%)
24	XAT	V	311	-	39,47,47	2.58	18 (46%)	54,74,74	12.00	18 (33%)
26	CHL	5	316	-	66,74,74	1.94	16 (24%)	73,114,114	2.36	21 (28%)
22	CLA	r	601	27	49,57,73	1.73	7 (14%)	55,93,113	1.63	8 (14%)
22	CLA	R	305	-	48,56,73	1.73	6 (12%)	55,92,113	1.63	8 (14%)
22	CLA	4	304	-	60,68,73	1.50	8 (13%)	70,107,113	1.46	6 (8%)
31	BCR	b	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.46	23 (41%)
26	CHL	Q	313	-	50,58,74	2.20	16 (32%)	52,94,114	2.72	20 (38%)
34	LMG	B	624	21	55,55,55	1.16	6 (10%)	63,63,63	1.07	2 (3%)
34	LMG	c	520	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	2 (3%)
25	LHG	P	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
26	CHL	q	311	-	66,74,74	1.89	15 (22%)	73,114,114	2.43	22 (30%)
22	CLA	v	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	8 (10%)
26	CHL	1	314	22	48,56,74	2.25	14 (29%)	51,92,114	2.82	20 (39%)
22	CLA	Q	303	-	50,58,73	1.70	6 (12%)	58,95,113	1.58	8 (13%)
26	CHL	1	317	18	66,74,74	1.90	15 (22%)	73,114,114	2.52	26 (35%)
22	CLA	N	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	6 (7%)
22	CLA	B	608	-	65,73,73	1.43	7 (10%)	76,113,113	1.52	7 (9%)
22	CLA	P	308	-	60,68,73	1.53	7 (11%)	70,107,113	1.47	6 (8%)
26	CHL	3	311	-	66,74,74	1.89	14 (21%)	73,114,114	2.46	23 (31%)
24	XAT	P	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.98	19 (35%)
25	LHG	D	406	3	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
26	CHL	g	315	18	66,74,74	1.87	14 (21%)	73,114,114	2.44	20 (27%)
22	CLA	B	614	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
32	SQD	L	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
26	CHL	r	619	1	48,56,74	2.20	15 (31%)	51,92,114	2.82	19 (37%)
24	XAT	q	309	-	39,47,47	2.58	18 (46%)	54,74,74	11.94	18 (33%)
22	CLA	Q	302	-	65,73,73	1.45	6 (9%)	76,113,113	1.36	7 (9%)
22	CLA	u	301	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	6 (7%)
22	CLA	S	301	19	61,69,73	1.48	7 (11%)	71,108,113	1.52	10 (14%)
26	CHL	S	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.44	20 (31%)
27	NEX	N	318	-	38,46,46	0.93	2 (5%)	50,70,70	2.40	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	s	309	-	49,57,73	1.67	8 (16%)	55,93,113	1.56	6 (10%)
27	NEX	V	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.46	16 (32%)
25	LHG	a	415	2	42,42,48	0.93	3 (7%)	45,48,54	1.10	2 (4%)
22	CLA	6	304	-	50,58,73	1.68	7 (14%)	58,95,113	1.60	8 (13%)
23	LUT	v	310	-	42,43,43	0.77	0	51,60,60	1.63	10 (19%)
22	CLA	5	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	u	305	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	7 (10%)
22	CLA	g	303	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	7 (12%)
22	CLA	3	302	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
26	CHL	5	318	-	66,74,74	1.88	14 (21%)	73,114,114	2.37	23 (31%)
22	CLA	R	311	-	45,53,73	1.78	6 (13%)	52,89,113	1.65	6 (11%)
25	LHG	4	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
26	CHL	1	318	-	66,74,74	1.89	15 (22%)	73,114,114	2.39	22 (30%)
22	CLA	N	306	-	60,68,73	1.50	6 (10%)	70,107,113	1.55	8 (11%)
26	CHL	p	319	-	66,74,74	1.90	15 (22%)	73,114,114	2.37	22 (30%)
22	CLA	G	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.51	6 (7%)
22	CLA	1	307	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	9 (11%)
26	CHL	6	301	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
26	CHL	4	317	-	66,74,74	1.88	15 (22%)	73,114,114	2.41	22 (30%)
25	LHG	v	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
22	CLA	6	305	18	64,72,73	1.47	7 (10%)	74,111,113	1.50	9 (12%)
35	BCT	a	414	-	2,3,3	1.35	0	2,3,3	0.20	0
25	LHG	c	521	-	48,48,48	0.90	4 (8%)	51,54,54	1.08	2 (3%)
22	CLA	1	306	-	60,68,73	1.52	9 (15%)	70,107,113	1.45	9 (12%)
31	BCR	A	409	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	22 (39%)
36	DGD	J	101	-	61,61,67	1.26	6 (9%)	75,75,81	1.17	3 (4%)
24	XAT	Q	309	-	39,47,47	2.60	18 (46%)	54,74,74	11.94	19 (35%)
22	CLA	4	305	-	60,68,73	1.51	7 (11%)	70,107,113	1.42	8 (11%)
22	CLA	d	402	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
22	CLA	g	307	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	Q	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	n	305	18	60,68,73	1.51	7 (11%)	70,107,113	2.08	16 (22%)
22	CLA	6	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	7 (9%)
31	BCR	T	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
26	CHL	p	318	-	66,74,74	1.84	14 (21%)	73,114,114	2.44	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	s	315	19	58,66,74	2.14	16 (27%)	63,104,114	2.45	20 (31%)
26	CHL	G	314	-	66,74,74	1.94	16 (24%)	73,114,114	2.32	21 (28%)
22	CLA	V	302	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
22	CLA	Q	306	22	60,68,73	1.54	5 (8%)	70,107,113	1.40	6 (8%)
22	CLA	g	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.56	7 (12%)
22	CLA	r	607	1	49,57,73	1.68	6 (12%)	55,93,113	1.66	9 (16%)
22	CLA	u	304	-	60,68,73	1.48	7 (11%)	70,107,113	1.55	7 (10%)
22	CLA	r	608	-	49,57,73	1.68	6 (12%)	55,93,113	1.65	8 (14%)
22	CLA	q	301	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	b	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.75	11 (14%)
26	CHL	g	313	-	50,58,74	2.19	14 (28%)	52,94,114	2.75	18 (34%)
26	CHL	u	318	-	66,74,74	1.85	14 (21%)	73,114,114	2.38	21 (28%)
24	XAT	3	309	-	39,47,47	2.56	18 (46%)	54,74,74	11.80	17 (31%)
22	CLA	B	612	-	65,73,73	1.49	7 (10%)	76,113,113	1.55	7 (9%)
26	CHL	V	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.43	21 (28%)
31	BCR	b	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.27	20 (35%)
26	CHL	2	315	-	50,58,74	2.18	15 (30%)	52,94,114	2.77	19 (36%)
22	CLA	U	302	-	65,73,73	1.47	8 (12%)	76,113,113	1.39	6 (7%)
22	CLA	g	306	22	60,68,73	1.56	7 (11%)	70,107,113	1.39	6 (8%)
22	CLA	V	303	-	50,58,73	1.66	8 (16%)	58,95,113	1.66	8 (13%)
31	BCR	K	101	-	41,41,41	4.72	24 (58%)	56,56,56	2.53	19 (33%)
26	CHL	l	316	-	66,74,74	1.91	16 (24%)	73,114,114	2.45	22 (30%)
31	BCR	t	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
26	CHL	S	313	-	46,54,74	2.33	16 (34%)	49,90,114	2.84	20 (40%)
22	CLA	C	514	-	65,73,73	1.44	10 (15%)	76,113,113	1.41	7 (9%)
26	CHL	n	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.84	20 (39%)
26	CHL	R	315	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
22	CLA	r	604	-	48,56,73	1.72	6 (12%)	55,92,113	1.63	8 (14%)
31	BCR	d	403	3	41,41,41	4.76	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	b	614	-	65,73,73	1.43	9 (13%)	76,113,113	1.42	7 (9%)
25	LHG	S	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.13	3 (5%)
22	CLA	N	302	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	7 (9%)
34	LMG	d	407	3	46,46,55	1.26	6 (13%)	54,54,63	1.01	2 (3%)
31	BCR	C	518	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	19 (33%)
26	CHL	p	314	18	66,74,74	1.93	16 (24%)	73,114,114	2.42	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	Q	316	-	61,69,74	2.00	16 (26%)	67,108,114	2.48	22 (32%)
24	XAT	5	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
26	CHL	r	614	-	66,74,74	1.88	13 (19%)	73,114,114	2.43	22 (30%)
26	CHL	6	314	-	50,58,74	2.29	16 (32%)	52,94,114	2.62	22 (42%)
26	CHL	5	314	-	48,56,74	2.35	17 (35%)	51,92,114	2.83	20 (39%)
22	CLA	A	406	-	50,58,73	1.65	10 (20%)	58,95,113	1.56	7 (12%)
26	CHL	G	313	-	50,58,74	2.19	15 (30%)	52,94,114	2.72	18 (34%)
22	CLA	v	303	-	50,58,73	1.67	7 (14%)	58,95,113	1.62	6 (10%)
22	CLA	Q	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.54	8 (14%)
22	CLA	b	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.45	9 (11%)
26	CHL	p	317	-	66,74,74	1.91	16 (24%)	73,114,114	2.41	21 (28%)
23	LUT	5	310	-	42,43,43	0.77	0	51,60,60	1.64	12 (23%)
22	CLA	B	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	6 (7%)
22	CLA	2	302	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	7 (9%)
23	LUT	s	311	-	42,43,43	0.76	0	51,60,60	1.65	16 (31%)
22	CLA	R	302	27	49,57,73	1.73	7 (14%)	55,93,113	1.62	8 (14%)
30	PHO	a	407	-	51,69,69	1.08	5 (9%)	47,99,99	1.23	6 (12%)
22	CLA	b	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
22	CLA	4	306	-	60,68,73	1.56	8 (13%)	70,107,113	1.42	8 (11%)
22	CLA	B	609	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	6 (7%)
24	XAT	r	612	-	39,47,47	2.52	17 (43%)	54,74,74	11.45	25 (46%)
22	CLA	v	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
26	CHL	U	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.41	22 (30%)
25	LHG	C	524	-	48,48,48	0.90	4 (8%)	51,54,54	1.13	2 (3%)
26	CHL	q	314	18	66,74,74	1.88	17 (25%)	73,114,114	2.48	20 (27%)
22	CLA	a	408	-	60,68,73	1.46	8 (13%)	70,107,113	1.68	8 (11%)
22	CLA	v	306	-	60,68,73	1.55	8 (13%)	70,107,113	1.46	9 (12%)
25	LHG	V	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
25	LHG	b	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
23	LUT	V	309	-	42,43,43	0.78	0	51,60,60	1.63	13 (25%)
22	CLA	S	302	-	45,53,73	1.81	6 (13%)	52,89,113	1.61	7 (13%)
22	CLA	B	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.50	9 (11%)
22	CLA	U	301	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	7 (9%)
22	CLA	4	303	-	50,58,73	1.68	8 (16%)	58,95,113	1.56	8 (13%)
22	CLA	1	301	-	65,73,73	1.48	9 (13%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	N	313	-	66,74,74	1.92	15 (22%)	73,114,114	2.41	22 (30%)
23	LUT	U	309	-	42,43,43	0.74	0	51,60,60	1.54	10 (19%)
31	BCR	a	409	-	41,41,41	4.73	24 (58%)	56,56,56	2.22	22 (39%)
32	SQD	m	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.75	11 (22%)
30	PHO	D	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.32	6 (12%)
31	BCR	B	620	-	41,41,41	4.75	24 (58%)	56,56,56	2.28	23 (41%)
26	CHL	n	315	-	50,58,74	2.22	16 (32%)	52,94,114	2.72	21 (40%)
22	CLA	b	612	-	65,73,73	1.48	7 (10%)	76,113,113	1.54	7 (9%)
22	CLA	v	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	7 (10%)
22	CLA	2	306	-	60,68,73	1.48	7 (11%)	70,107,113	1.56	8 (11%)
25	LHG	Q	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
23	LUT	5	309	-	42,43,43	0.76	0	51,60,60	1.75	13 (25%)
22	CLA	4	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.49	9 (11%)
22	CLA	p	302	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	7 (9%)
25	LHG	N	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	g	304	18	64,72,73	1.48	7 (10%)	74,111,113	1.50	8 (10%)
23	LUT	1	310	-	42,43,43	0.80	0	51,60,60	1.74	14 (27%)
36	DGD	c	519	-	61,61,67	1.25	6 (9%)	75,75,81	1.17	3 (4%)
26	CHL	N	316	-	66,74,74	1.86	15 (22%)	73,114,114	2.48	21 (28%)
26	CHL	2	313	18	66,74,74	1.99	17 (25%)	73,114,114	2.38	22 (30%)
22	CLA	4	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.60	7 (12%)
22	CLA	V	304	-	60,68,73	1.50	6 (10%)	70,107,113	1.52	8 (11%)
26	CHL	q	312	-	48,56,74	2.36	17 (35%)	51,92,114	2.82	21 (41%)
25	LHG	g	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	4	302	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	7 (9%)
22	CLA	v	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	6 (10%)
22	CLA	g	305	22	60,68,73	1.52	8 (13%)	70,107,113	1.50	10 (14%)
22	CLA	U	304	-	60,68,73	1.50	9 (15%)	70,107,113	1.48	8 (11%)
22	CLA	5	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.51	10 (13%)
22	CLA	q	306	22	60,68,73	1.53	5 (8%)	70,107,113	1.44	7 (10%)
36	DGD	a	416	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
26	CHL	1	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.67	19 (36%)
25	LHG	5	312	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
24	XAT	N	311	-	39,47,47	2.53	17 (43%)	54,74,74	11.91	18 (33%)
22	CLA	V	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.48	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
22	CLA	R	304	-	60,68,73	1.53	5 (8%)	70,107,113	1.48	6 (8%)
22	CLA	q	305	22	60,68,73	1.51	7 (11%)	70,107,113	1.44	6 (8%)
26	CHL	5	317	-	66,74,74	1.86	12 (18%)	73,114,114	2.45	22 (30%)
31	BCR	C	517	-	41,41,41	4.69	24 (58%)	56,56,56	2.67	24 (42%)
34	LMG	C	502	-	51,51,55	1.15	4 (7%)	59,59,63	1.16	3 (5%)
22	CLA	b	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.42	7 (9%)
22	CLA	G	302	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	P	304	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
23	LUT	P	311	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
26	CHL	P	317	-	66,74,74	1.93	17 (25%)	73,114,114	2.42	24 (32%)
27	NEX	U	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	12 (24%)
32	SQD	M	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.74	11 (22%)
23	LUT	4	309	-	42,43,43	0.73	0	51,60,60	1.60	11 (21%)
22	CLA	B	604	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
26	CHL	Q	312	-	48,56,74	2.29	15 (31%)	51,92,114	2.76	21 (41%)
26	CHL	6	313	-	48,56,74	2.37	17 (35%)	51,92,114	2.83	23 (45%)
22	CLA	2	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.59	7 (12%)
22	CLA	5	305	18	60,68,73	1.52	7 (11%)	70,107,113	2.04	13 (18%)
24	XAT	p	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.83	18 (33%)
27	NEX	n	319	-	38,46,46	0.96	2 (5%)	50,70,70	2.64	17 (34%)
22	CLA	3	303	-	50,58,73	1.68	7 (14%)	58,95,113	1.62	8 (13%)
25	LHG	B	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
25	LHG	G	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.10	2 (3%)
22	CLA	s	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
22	CLA	s	301	19	61,69,73	1.49	8 (13%)	71,108,113	1.53	11 (15%)
22	CLA	r	609	26	60,68,73	1.54	6 (10%)	70,107,113	1.58	11 (15%)
31	BCR	z	101	-	41,41,41	4.76	24 (58%)	56,56,56	2.32	20 (35%)
22	CLA	c	507	-	65,73,73	1.52	9 (13%)	76,113,113	1.45	8 (10%)
26	CHL	n	316	-	66,74,74	1.91	15 (22%)	73,114,114	2.35	21 (28%)
22	CLA	x	201	14	65,73,73	1.40	7 (10%)	76,113,113	1.53	8 (10%)
22	CLA	B	613	-	65,73,73	1.43	8 (12%)	76,113,113	1.46	10 (13%)
22	CLA	B	616	21	65,73,73	1.42	9 (13%)	76,113,113	1.45	9 (11%)
22	CLA	2	304	18	65,73,73	1.45	9 (13%)	76,113,113	1.48	9 (11%)
22	CLA	Q	305	22	60,68,73	1.52	7 (11%)	70,107,113	1.41	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	404	-	65,73,73	1.40	8 (12%)	76,113,113	1.60	8 (10%)
22	CLA	3	307	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
34	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.07	2 (3%)
27	NEX	p	301	18	38,46,46	0.98	2 (5%)	50,70,70	2.43	19 (38%)
22	CLA	P	303	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	7 (9%)
31	BCR	c	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	21 (37%)
22	CLA	3	306	22	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
33	PL9	a	411	-	13,13,55	3.63	7 (53%)	17,17,69	1.48	3 (17%)
22	CLA	2	301	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
22	CLA	U	308	-	48,56,73	1.71	8 (16%)	55,92,113	1.58	7 (12%)
22	CLA	r	610	-	45,53,73	1.79	6 (13%)	52,89,113	1.65	6 (11%)
22	CLA	C	510	-	65,73,73	1.53	9 (13%)	76,113,113	1.52	9 (11%)
25	LHG	A	413	2	42,42,48	0.93	3 (7%)	45,48,54	1.11	2 (4%)
22	CLA	S	305	-	55,63,73	1.57	7 (12%)	64,101,113	1.49	7 (10%)
23	LUT	s	310	19	42,43,43	0.79	0	51,60,60	1.72	13 (25%)
34	LMG	a	412	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
23	LUT	v	309	-	42,43,43	0.79	0	51,60,60	1.65	12 (23%)
31	BCR	C	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	20 (35%)
24	XAT	u	311	-	39,47,47	2.54	18 (46%)	54,74,74	11.77	18 (33%)
22	CLA	S	304	19	45,53,73	1.75	6 (13%)	52,89,113	1.58	6 (11%)
22	CLA	P	302	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
22	CLA	v	305	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	7 (10%)
26	CHL	P	319	-	66,74,74	1.88	14 (21%)	73,114,114	2.40	20 (27%)
22	CLA	D	403	3	65,73,73	1.43	9 (13%)	76,113,113	1.39	8 (10%)
26	CHL	3	313	-	50,58,74	2.26	16 (32%)	52,94,114	2.63	21 (40%)
26	CHL	g	312	-	48,56,74	2.27	14 (29%)	51,92,114	2.77	21 (41%)
22	CLA	n	301	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	7 (9%)
26	CHL	r	616	-	61,69,74	2.02	17 (27%)	67,108,114	2.36	19 (28%)
27	NEX	2	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	14 (28%)
22	CLA	V	308	-	48,56,73	1.69	6 (12%)	55,92,113	1.58	6 (10%)
22	CLA	u	306	-	60,68,73	1.54	10 (16%)	70,107,113	1.44	7 (10%)
22	CLA	B	603	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	6 (7%)
22	CLA	6	303	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
23	LUT	2	309	-	42,43,43	0.76	0	51,60,60	1.68	14 (27%)
25	LHG	C	523	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CHL	3	316	-	61,69,74	2.00	14 (22%)	67,108,114	2.48	23 (34%)
25	LHG	c	523	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
26	CHL	v	315	-	50,58,74	2.23	16 (32%)	52,94,114	2.70	21 (40%)
36	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.15	5 (6%)
26	CHL	P	314	18	66,74,74	1.98	16 (24%)	73,114,114	2.40	22 (30%)
25	LHG	B	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.06	2 (4%)
23	LUT	p	310	-	42,43,43	0.74	0	51,60,60	1.72	14 (27%)
22	CLA	5	306	-	60,68,73	1.47	7 (11%)	70,107,113	1.55	7 (10%)
34	LMG	D	408	3	46,46,55	1.26	6 (13%)	54,54,63	1.02	2 (3%)
22	CLA	a	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
31	BCR	D	404	3	41,41,41	4.77	24 (58%)	56,56,56	2.26	23 (41%)
22	CLA	B	617	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	8 (10%)
22	CLA	3	308	-	48,56,73	1.71	6 (12%)	55,92,113	1.58	7 (12%)
26	CHL	1	313	-	66,74,74	1.94	15 (22%)	73,114,114	2.37	23 (31%)
26	CHL	s	314	-	46,54,74	2.29	16 (34%)	49,90,114	2.86	19 (38%)
27	NEX	u	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	18 (36%)
26	CHL	N	317	-	66,74,74	1.93	16 (24%)	73,114,114	2.33	22 (30%)
22	CLA	P	307	-	60,68,73	1.48	6 (10%)	70,107,113	1.50	8 (11%)
22	CLA	c	514	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
22	CLA	c	504	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	7 (9%)
22	CLA	V	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
34	LMG	B	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	6 (10%)
22	CLA	5	303	-	50,58,73	1.67	8 (16%)	58,95,113	1.58	8 (13%)
22	CLA	n	306	-	60,68,73	1.49	6 (10%)	70,107,113	1.55	8 (11%)
25	LHG	U	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.17	3 (5%)
31	BCR	c	515	-	41,41,41	4.70	24 (58%)	56,56,56	2.67	23 (41%)
22	CLA	N	308	-	48,56,73	1.74	6 (12%)	55,92,113	1.54	7 (12%)
22	CLA	s	306	-	56,64,73	1.59	8 (14%)	65,102,113	1.51	10 (15%)
34	LMG	c	501	-	51,51,55	1.15	5 (9%)	59,59,63	1.16	3 (5%)
22	CLA	C	504	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	N	303	-	50,58,73	1.65	7 (14%)	58,95,113	1.69	7 (12%)
22	CLA	Q	304	18	64,72,73	1.47	7 (10%)	74,111,113	1.53	9 (12%)
22	CLA	1	308	-	48,56,73	1.68	6 (12%)	55,92,113	1.58	7 (12%)
26	CHL	4	315	-	50,58,74	2.25	16 (32%)	52,94,114	2.67	19 (36%)
22	CLA	c	510	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	XAT	1	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.16	18 (33%)
22	CLA	3	304	18	64,72,73	1.47	8 (12%)	74,111,113	1.52	9 (12%)
22	CLA	u	308	-	48,56,73	1.70	8 (16%)	55,92,113	1.57	7 (12%)
22	CLA	1	303	-	50,58,73	1.66	9 (18%)	58,95,113	1.58	8 (13%)
22	CLA	5	307	-	60,68,73	1.51	7 (11%)	70,107,113	1.48	7 (10%)
22	CLA	X	202	14	65,73,73	1.40	7 (10%)	76,113,113	1.52	8 (10%)
22	CLA	b	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.52	7 (9%)
22	CLA	s	303	19	50,58,73	1.67	7 (14%)	58,95,113	1.64	8 (13%)
27	NEX	s	317	19	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
26	CHL	v	316	-	66,74,74	1.89	16 (24%)	73,114,114	2.46	24 (32%)
26	CHL	4	313	-	66,74,74	1.95	16 (24%)	73,114,114	2.33	22 (30%)
22	CLA	c	512	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)
25	LHG	p	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.04	2 (3%)
22	CLA	2	305	18	60,68,73	1.50	7 (11%)	70,107,113	2.03	15 (21%)
22	CLA	5	308	-	48,56,73	1.70	6 (12%)	55,92,113	1.57	7 (12%)
22	CLA	N	307	-	60,68,73	1.52	7 (11%)	70,107,113	1.48	7 (10%)
22	CLA	G	307	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
23	LUT	V	310	-	42,43,43	0.78	0	51,60,60	1.62	12 (23%)
24	XAT	n	311	-	39,47,47	2.53	18 (46%)	54,74,74	11.76	23 (42%)
23	LUT	R	312	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
26	CHL	P	316	-	50,58,74	2.24	16 (32%)	52,94,114	2.70	20 (38%)
22	CLA	G	306	22	60,68,73	1.54	6 (10%)	70,107,113	1.39	6 (8%)
22	CLA	5	302	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
22	CLA	1	302	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	7 (9%)
22	CLA	c	508	20	65,73,73	1.47	9 (13%)	76,113,113	1.52	10 (13%)
25	LHG	c	522	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
22	CLA	1	304	-	60,68,73	1.49	8 (13%)	70,107,113	1.45	6 (8%)
22	CLA	P	305	18	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
26	CHL	P	315	-	48,56,74	2.46	16 (33%)	51,92,114	2.76	19 (37%)
23	LUT	U	310	-	42,43,43	0.79	0	51,60,60	1.61	9 (17%)
22	CLA	p	303	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	8 (10%)
22	CLA	B	605	21	65,73,73	1.46	9 (13%)	76,113,113	1.76	13 (17%)
22	CLA	b	613	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	10 (13%)
25	LHG	6	311	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
26	CHL	5	313	18	66,74,74	2.00	17 (25%)	73,114,114	2.39	21 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LUT	N	309	-	42,43,43	0.72	0	51,60,60	1.55	11 (21%)
27	NEX	r	618	22,1	38,46,46	1.04	2 (5%)	50,70,70	2.49	16 (32%)
27	NEX	u	320	-	38,46,46	0.89	2 (5%)	50,70,70	2.32	18 (36%)

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
27	NEX	v	319	-	-	4/27/83/83	0/3/3/3
22	CLA	s	308	-	1/1/13/20	7/25/103/115	-
31	BCR	B	619	-	-	14/29/63/63	0/2/2/2
26	CHL	U	316	18	3/3/20/26	11/39/137/137	-
25	LHG	C	522	-	-	16/53/53/53	-
26	CHL	u	317	18	3/3/20/26	11/39/137/137	-
23	LUT	l	309	-	-	2/29/67/67	0/2/2/2
32	SQD	l	102	9	-	21/49/69/69	0/1/1/1
26	CHL	R	316	-	3/3/18/26	11/27/125/137	-
22	CLA	b	609	-	1/1/15/20	12/37/115/115	-
23	LUT	p	311	-	-	3/29/67/67	0/2/2/2
24	XAT	G	309	-	-	10/31/93/93	0/4/4/4
22	CLA	C	511	-	1/1/15/20	14/37/115/115	-
27	NEX	R	301	22,1	-	10/27/83/83	0/3/3/3
25	LHG	d	405	3	-	26/50/50/53	-
26	CHL	U	315	-	3/3/20/26	14/39/137/137	-
22	CLA	U	305	-	1/1/14/20	10/31/109/115	-
22	CLA	b	617	21	1/1/15/20	12/37/115/115	-
33	PL9	D	405	-	-	9/53/73/73	0/1/1/1
22	CLA	R	310	-	1/1/14/20	10/31/109/115	-
22	CLA	S	308	-	1/1/13/20	7/25/103/115	-
22	CLA	p	307	-	1/1/14/20	7/31/109/115	-
25	LHG	3	310	-	-	18/53/53/53	-
22	CLA	p	306	18	1/1/14/20	11/31/109/115	-
22	CLA	u	302	-	1/1/15/20	14/37/115/115	-
24	XAT	R	313	-	-	8/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	q	313	-	3/3/16/26	9/20/118/137	-
26	CHL	n	313	18	3/3/20/26	19/39/137/137	-
32	SQD	a	410	-	-	25/45/65/69	0/1/1/1
30	PHO	d	401	-	-	11/37/103/103	0/5/6/6
36	DGD	C	519	-	-	23/44/84/95	0/2/2/2
22	CLA	B	610	-	1/1/15/20	16/37/115/115	-
26	CHL	V	314	-	3/3/16/26	11/18/116/137	-
22	CLA	q	303	-	1/1/12/20	8/19/97/115	-
23	LUT	S	310	-	-	2/29/67/67	0/2/2/2
34	LMG	A	411	-	-	11/35/55/70	0/1/1/1
26	CHL	3	315	18	3/3/20/26	21/39/137/137	-
26	CHL	Q	314	-	3/3/20/26	20/39/137/137	-
26	CHL	u	313	-	3/3/20/26	14/39/137/137	-
25	LHG	l	312	-	-	14/53/53/53	-
22	CLA	G	308	-	1/1/11/20	9/17/95/115	-
26	CHL	s	316	-	3/3/16/26	11/15/113/137	-
32	SQD	a	413	-	-	22/49/69/69	0/1/1/1
27	NEX	r	617	-	-	2/27/83/83	0/3/3/3
22	CLA	g	301	-	1/1/15/20	14/37/115/115	-
30	PHO	A	407	-	-	10/37/103/103	0/5/6/6
22	CLA	U	306	-	1/1/14/20	10/31/109/115	-
26	CHL	N	314	-	3/3/16/26	10/18/116/137	-
27	NEX	5	319	-	-	8/27/83/83	0/3/3/3
23	LUT	n	310	-	-	3/29/67/67	0/2/2/2
26	CHL	2	316	-	3/3/20/26	17/39/137/137	-
22	CLA	q	302	-	1/1/15/20	11/37/115/115	-
22	CLA	p	309	-	1/1/11/20	6/17/95/115	-
22	CLA	n	302	-	1/1/15/20	16/37/115/115	-
26	CHL	6	312	-	3/3/20/26	16/39/137/137	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
23	LUT	u	309	-	-	2/29/67/67	0/2/2/2
22	CLA	Q	301	-	1/1/15/20	14/37/115/115	-
22	CLA	6	309	-	1/1/11/20	10/17/95/115	-
22	CLA	C	503	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	513	-	1/1/15/20	10/37/115/115	-
36	DGD	c	517	-	-	22/44/84/95	0/2/2/2
22	CLA	c	503	-	1/1/15/20	20/37/115/115	-
22	CLA	3	305	22	1/1/14/20	9/31/109/115	-
26	CHL	p	316	-	3/3/16/26	7/20/118/137	-
31	BCR	k	101	-	-	13/29/63/63	0/2/2/2
25	LHG	s	312	19	-	17/53/53/53	-
22	CLA	V	306	-	1/1/14/20	7/31/109/115	-
22	CLA	N	304	18	1/1/15/20	17/37/115/115	-
22	CLA	G	303	-	1/1/12/20	10/19/97/115	-
26	CHL	3	312	-	3/3/16/26	8/18/116/137	-
37	HEM	E	101	17,4	-	2/12/54/54	-
24	XAT	2	311	-	-	6/31/93/93	0/4/4/4
26	CHL	S	316	-	3/3/16/26	11/15/113/137	-
22	CLA	p	308	-	1/1/14/20	11/31/109/115	-
22	CLA	4	301	-	1/1/15/20	7/37/115/115	-
26	CHL	r	615	-	3/3/18/26	10/27/125/137	-
22	CLA	N	305	18	1/1/14/20	12/31/109/115	-
22	CLA	c	509	-	1/1/15/20	9/37/115/115	-
26	CHL	Q	311	-	3/3/20/26	19/39/137/137	-
25	LHG	n	312	-	-	19/53/53/53	-
26	CHL	u	314	-	3/3/16/26	11/18/116/137	-
22	CLA	s	305	-	1/1/13/20	5/25/103/115	-
22	CLA	r	602	-	1/1/14/20	7/31/109/115	-
26	CHL	p	320	-	3/3/20/26	18/39/137/137	-
22	CLA	r	603	-	1/1/14/20	11/31/109/115	-
22	CLA	C	509	20	1/1/15/20	14/37/115/115	-
22	CLA	q	307	-	1/1/15/20	15/37/115/115	-
22	CLA	b	611	-	1/1/15/20	14/37/115/115	-
22	CLA	G	304	18	1/1/14/20	10/36/114/115	-
36	DGD	B	601	21	-	22/51/91/95	0/2/2/2
22	CLA	r	605	-	1/1/13/20	7/29/107/115	-
26	CHL	g	314	-	3/3/20/26	20/39/137/137	-
26	CHL	2	318	-	3/3/20/26	18/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	305	-	1/1/14/20	8/31/109/115	-
25	LHG	u	312	-	-	25/53/53/53	-
26	CHL	v	317	18	3/3/20/26	12/39/137/137	-
23	LUT	P	310	-	-	2/29/67/67	0/2/2/2
34	LMG	w	201	-	-	22/43/63/70	0/1/1/1
26	CHL	Q	315	18	3/3/20/26	20/39/137/137	-
22	CLA	R	306	-	1/1/13/20	7/29/107/115	-
22	CLA	p	304	-	1/1/12/20	10/19/97/115	-
22	CLA	c	513	-	1/1/15/20	8/37/115/115	-
22	CLA	b	602	-	1/1/15/20	17/37/115/115	-
22	CLA	C	515	-	1/1/15/20	10/37/115/115	-
22	CLA	c	511	8,20	1/1/15/20	18/37/115/115	-
26	CHL	g	311	-	3/3/20/26	21/39/137/137	-
23	LUT	S	311	-	-	8/29/67/67	0/2/2/2
26	CHL	4	316	18	3/3/20/26	14/39/137/137	-
26	CHL	u	315	-	3/3/16/26	8/20/118/137	-
26	CHL	V	317	18	3/3/20/26	14/39/137/137	-
34	LMG	b	624	21	-	22/50/70/70	0/1/1/1
22	CLA	a	406	-	1/1/12/20	8/19/97/115	-
22	CLA	q	304	18	1/1/14/20	15/36/114/115	-
22	CLA	n	304	18	1/1/15/20	14/37/115/115	-
23	LUT	2	310	-	-	1/29/67/67	0/2/2/2
22	CLA	R	303	-	1/1/14/20	7/31/109/115	-
32	SQD	C	501	-	-	27/45/65/69	0/1/1/1
22	CLA	A	404	-	1/1/15/20	15/37/115/115	-
22	CLA	B	615	-	1/1/15/20	17/37/115/115	-
26	CHL	U	317	-	3/3/20/26	18/39/137/137	-
26	CHL	6	315	-	3/3/20/26	15/39/137/137	-
22	CLA	C	507	-	1/1/15/20	19/37/115/115	-
22	CLA	A	408	-	1/1/14/20	12/31/109/115	-
22	CLA	b	604	-	1/1/15/20	16/37/115/115	-
27	NEX	S	317	19	-	4/27/83/83	0/3/3/3
34	LMG	b	621	-	-	24/46/66/70	0/1/1/1
25	LHG	q	310	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PL9	d	404	-	-	9/53/73/73	0/1/1/1
26	CHL	R	317	-	3/3/19/26	16/33/131/137	-
26	CHL	v	314	-	3/3/16/26	12/18/116/137	-
22	CLA	U	303	-	1/1/12/20	5/19/97/115	-
22	CLA	q	308	-	1/1/11/20	11/17/95/115	-
25	LHG	D	407	3	-	18/53/53/53	-
22	CLA	C	512	8,20	1/1/15/20	20/37/115/115	-
27	NEX	P	301	18	-	3/27/83/83	0/3/3/3
25	LHG	r	613	-	-	19/46/46/53	-
32	SQD	A	412	-	-	21/49/69/69	0/1/1/1
22	CLA	R	308	1	1/1/11/20	10/18/96/115	-
22	CLA	b	615	-	1/1/15/20	18/37/115/115	-
22	CLA	S	309	-	1/1/11/20	2/18/96/115	-
31	BCR	b	620	-	-	12/29/63/63	0/2/2/2
26	CHL	5	315	-	3/3/16/26	6/20/118/137	-
22	CLA	G	305	22	1/1/14/20	10/31/109/115	-
22	CLA	S	306	-	1/1/13/20	6/27/105/115	-
22	CLA	U	307	-	1/1/15/20	15/37/115/115	-
22	CLA	v	301	-	-	11/37/115/115	-
26	CHL	n	318	-	3/3/20/26	23/39/137/137	-
26	CHL	G	312	-	3/3/16/26	6/18/116/137	-
26	CHL	v	318	-	3/3/20/26	20/39/137/137	-
26	CHL	2	314	-	3/3/16/26	9/18/116/137	-
37	HEM	e	101	17,4	-	3/12/54/54	-
26	CHL	2	317	-	3/3/20/26	11/39/137/137	-
22	CLA	c	506	-	1/1/15/20	19/37/115/115	-
26	CHL	N	315	-	3/3/16/26	7/20/118/137	-
22	CLA	R	307	-	1/1/15/20	16/37/115/115	-
36	DGD	b	601	21	-	21/51/91/95	0/2/2/2
24	XAT	6	310	-	-	8/31/93/93	0/4/4/4
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
22	CLA	r	606	-	1/1/15/20	16/37/115/115	-
26	CHL	v	313	-	3/3/20/26	16/39/137/137	-
23	LUT	r	611	1	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	U	319	-	3/3/20/26	20/39/137/137	-
26	CHL	s	313	-	3/3/16/26	7/15/113/137	-
25	LHG	l	101	-	-	27/53/53/53	-
26	CHL	g	316	-	3/3/19/26	15/33/131/137	-
26	CHL	S	314	-	3/3/16/26	7/15/113/137	-
24	XAT	g	309	-	-	10/31/93/93	0/4/4/4
26	CHL	6	316	18	3/3/20/26	23/39/137/137	-
22	CLA	3	301	-	1/1/15/20	14/37/115/115	-
25	LHG	R	314	-	-	24/46/46/53	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
23	LUT	N	310	-	-	1/29/67/67	0/2/2/2
22	CLA	p	305	18	1/1/15/20	11/37/115/115	-
22	CLA	b	616	21	1/1/15/20	9/37/115/115	-
22	CLA	s	307	-	1/1/11/20	6/18/96/115	-
26	CHL	4	314	-	3/3/16/26	10/18/116/137	-
25	LHG	d	406	3	-	19/53/53/53	-
31	BCR	X	201	-	-	9/29/63/63	0/2/2/2
22	CLA	2	303	-	1/1/12/20	6/19/97/115	-
26	CHL	U	314	-	3/3/16/26	10/20/118/137	-
22	CLA	6	306	22	1/1/14/20	13/31/109/115	-
22	CLA	B	611	-	1/1/15/20	14/37/115/115	-
22	CLA	C	508	-	1/1/15/20	20/37/115/115	-
26	CHL	6	317	-	3/3/19/26	16/33/131/137	-
22	CLA	A	405	-	1/1/15/20	10/37/115/115	-
22	CLA	g	302	-	1/1/15/20	13/37/115/115	-
26	CHL	G	311	-	3/3/20/26	18/39/137/137	-
26	CHL	G	315	18	3/3/20/26	19/39/137/137	-
22	CLA	s	302	-	1/1/11/20	6/13/91/115	-
26	CHL	V	316	-	3/3/20/26	17/39/137/137	-
22	CLA	c	505	-	1/1/15/20	9/37/115/115	-
22	CLA	b	607	-	-	13/37/115/115	-
26	CHL	n	317	-	3/3/20/26	17/39/137/137	-
22	CLA	n	308	-	1/1/11/20	11/17/95/115	-
36	DGD	A	414	-	-	22/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	S	303	19	1/1/12/20	6/19/97/115	-
22	CLA	2	307	-	1/1/14/20	8/31/109/115	-
22	CLA	P	309	-	1/1/11/20	10/17/95/115	-
24	XAT	4	311	-	-	8/31/93/93	0/4/4/4
22	CLA	c	502	-	1/1/15/20	8/37/115/115	-
26	CHL	q	315	-	3/3/19/26	12/33/131/137	-
22	CLA	n	303	-	1/1/12/20	7/19/97/115	-
34	LMG	W	201	-	-	21/43/63/70	0/1/1/1
26	CHL	P	318	-	3/3/20/26	17/39/137/137	-
22	CLA	P	306	18	1/1/14/20	10/31/109/115	-
22	CLA	u	303	-	1/1/12/20	6/19/97/115	-
23	LUT	4	310	-	-	0/29/67/67	0/2/2/2
22	CLA	S	307	-	1/1/11/20	6/18/96/115	-
25	LHG	b	622	-	-	22/51/51/53	-
22	CLA	6	307	22	1/1/14/20	16/31/109/115	-
31	BCR	x	202	-	-	9/29/63/63	0/2/2/2
33	PL9	A	410	-	-	0/5/18/73	0/1/1/1
24	XAT	U	311	-	-	7/31/93/93	0/4/4/4
26	CHL	3	314	-	3/3/20/26	16/39/137/137	-
26	CHL	p	315	-	3/3/16/26	8/18/116/137	-
22	CLA	6	308	-	1/1/15/20	10/37/115/115	-
23	LUT	n	309	-	-	0/29/67/67	0/2/2/2
24	XAT	v	311	-	-	11/31/93/93	0/4/4/4
23	LUT	u	310	-	-	2/29/67/67	0/2/2/2
22	CLA	R	309	-	1/1/11/20	7/18/96/115	-
36	DGD	C	520	-	-	31/51/91/95	0/2/2/2
22	CLA	n	307	-	1/1/14/20	11/31/109/115	-
22	CLA	V	301	-	-	12/37/115/115	-
25	LHG	2	312	-	-	24/53/53/53	-
26	CHL	V	315	-	3/3/16/26	6/20/118/137	-
26	CHL	V	318	-	3/3/20/26	17/39/137/137	-
26	CHL	u	316	-	3/3/20/26	23/39/137/137	-
26	CHL	G	316	-	3/3/19/26	13/33/131/137	-
22	CLA	u	307	-	1/1/15/20	14/37/115/115	-
22	CLA	B	602	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	XAT	V	311	-	-	11/31/93/93	0/4/4/4
26	CHL	5	316	-	3/3/20/26	18/39/137/137	-
22	CLA	r	601	27	1/1/11/20	7/18/96/115	-
22	CLA	R	305	-	1/1/11/20	7/17/95/115	-
22	CLA	4	304	-	1/1/14/20	9/31/109/115	-
31	BCR	b	618	-	-	8/29/63/63	0/2/2/2
26	CHL	Q	313	-	3/3/16/26	9/20/118/137	-
34	LMG	B	624	21	-	21/50/70/70	0/1/1/1
34	LMG	c	520	-	-	21/46/66/70	0/1/1/1
25	LHG	P	313	-	-	24/53/53/53	-
26	CHL	q	311	-	3/3/20/26	17/39/137/137	-
22	CLA	v	302	-	1/1/15/20	12/37/115/115	-
26	CHL	l	314	22	3/3/16/26	14/18/116/137	-
22	CLA	Q	303	-	1/1/12/20	10/19/97/115	-
26	CHL	l	317	18	3/3/20/26	19/39/137/137	-
22	CLA	N	301	-	1/1/15/20	13/37/115/115	-
22	CLA	B	608	-	1/1/15/20	14/37/115/115	-
22	CLA	P	308	-	1/1/14/20	13/31/109/115	-
26	CHL	3	311	-	3/3/20/26	16/39/137/137	-
24	XAT	P	312	-	-	8/31/93/93	0/4/4/4
25	LHG	D	406	3	-	28/50/50/53	-
26	CHL	g	315	18	3/3/20/26	23/39/137/137	-
22	CLA	B	614	-	1/1/15/20	14/37/115/115	-
32	SQD	L	102	9	-	21/49/69/69	0/1/1/1
26	CHL	r	619	1	3/3/16/26	8/18/116/137	-
24	XAT	q	309	-	-	12/31/93/93	0/4/4/4
22	CLA	Q	302	-	1/1/15/20	11/37/115/115	-
22	CLA	u	301	-	-	7/37/115/115	-
22	CLA	S	301	19	1/1/14/20	16/33/111/115	-
26	CHL	S	315	19	3/3/18/26	15/30/128/137	-
27	NEX	N	318	-	-	9/27/83/83	0/3/3/3
22	CLA	s	309	-	1/1/11/20	2/18/96/115	-
27	NEX	V	319	-	-	6/27/83/83	0/3/3/3
25	LHG	a	415	2	-	26/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	304	-	1/1/12/20	11/19/97/115	-
23	LUT	v	310	-	-	0/29/67/67	0/2/2/2
22	CLA	5	301	-	1/1/15/20	10/37/115/115	-
22	CLA	u	305	-	1/1/14/20	12/31/109/115	-
22	CLA	g	303	-	1/1/12/20	11/19/97/115	-
22	CLA	3	302	-	1/1/15/20	13/37/115/115	-
26	CHL	5	318	-	3/3/20/26	16/39/137/137	-
22	CLA	R	311	-	1/1/11/20	8/13/91/115	-
25	LHG	4	312	-	-	18/53/53/53	-
26	CHL	1	318	-	3/3/20/26	14/39/137/137	-
22	CLA	N	306	-	1/1/14/20	9/31/109/115	-
26	CHL	p	319	-	3/3/20/26	15/39/137/137	-
22	CLA	G	301	-	1/1/15/20	19/37/115/115	-
22	CLA	1	307	-	1/1/15/20	11/37/115/115	-
26	CHL	6	301	-	3/3/20/26	20/39/137/137	-
26	CHL	4	317	-	3/3/20/26	14/39/137/137	-
25	LHG	v	312	-	-	19/53/53/53	-
22	CLA	6	305	18	1/1/14/20	19/36/114/115	-
25	LHG	c	521	-	-	14/53/53/53	-
22	CLA	1	306	-	1/1/14/20	14/31/109/115	-
31	BCR	A	409	-	-	3/29/63/63	0/2/2/2
36	DGD	J	101	-	-	21/49/89/95	0/2/2/2
24	XAT	Q	309	-	-	10/31/93/93	0/4/4/4
22	CLA	4	305	-	1/1/14/20	6/31/109/115	-
22	CLA	d	402	3	1/1/15/20	13/37/115/115	-
22	CLA	g	307	-	1/1/15/20	12/37/115/115	-
22	CLA	Q	307	-	1/1/15/20	10/37/115/115	-
22	CLA	n	305	18	1/1/14/20	11/31/109/115	-
22	CLA	6	302	-	1/1/15/20	17/37/115/115	-
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
26	CHL	p	318	-	3/3/20/26	17/39/137/137	-
26	CHL	s	315	19	3/3/18/26	15/30/128/137	-
26	CHL	G	314	-	3/3/20/26	15/39/137/137	-
22	CLA	V	302	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	306	22	1/1/14/20	11/31/109/115	-
22	CLA	g	308	-	1/1/11/20	8/17/95/115	-
22	CLA	r	607	1	1/1/11/20	9/18/96/115	-
22	CLA	u	304	-	1/1/14/20	5/31/109/115	-
22	CLA	r	608	-	1/1/11/20	7/18/96/115	-
22	CLA	q	301	-	-	15/37/115/115	-
22	CLA	b	605	21	1/1/15/20	16/37/115/115	-
26	CHL	g	313	-	3/3/16/26	8/20/118/137	-
26	CHL	u	318	-	3/3/20/26	20/39/137/137	-
24	XAT	3	309	-	-	8/31/93/93	0/4/4/4
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
26	CHL	V	313	-	3/3/20/26	19/39/137/137	-
31	BCR	b	619	-	-	14/29/63/63	0/2/2/2
26	CHL	2	315	-	3/3/16/26	5/20/118/137	-
22	CLA	U	302	-	1/1/15/20	12/37/115/115	-
22	CLA	g	306	22	1/1/14/20	13/31/109/115	-
22	CLA	V	303	-	1/1/12/20	6/19/97/115	-
31	BCR	K	101	-	-	13/29/63/63	0/2/2/2
26	CHL	1	316	-	3/3/20/26	21/39/137/137	-
31	BCR	t	101	-	-	12/29/63/63	0/2/2/2
26	CHL	S	313	-	3/3/16/26	7/15/113/137	-
22	CLA	C	514	-	1/1/15/20	12/37/115/115	-
26	CHL	n	314	-	3/3/16/26	10/18/116/137	-
26	CHL	R	315	-	3/3/20/26	20/39/137/137	-
22	CLA	r	604	-	1/1/11/20	7/17/95/115	-
31	BCR	d	403	3	-	12/29/63/63	0/2/2/2
22	CLA	b	614	-	1/1/15/20	16/37/115/115	-
25	LHG	S	312	19	-	17/53/53/53	-
22	CLA	N	302	-	1/1/15/20	20/37/115/115	-
34	LMG	d	407	3	-	17/41/61/70	0/1/1/1
31	BCR	C	518	-	-	11/29/63/63	0/2/2/2
26	CHL	p	314	18	3/3/20/26	13/39/137/137	-
26	CHL	Q	316	-	3/3/19/26	12/33/131/137	-
24	XAT	5	311	-	-	6/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	r	614	-	3/3/20/26	20/39/137/137	-
26	CHL	6	314	-	3/3/16/26	11/20/118/137	-
26	CHL	5	314	-	3/3/16/26	11/18/116/137	-
22	CLA	A	406	-	1/1/12/20	7/19/97/115	-
26	CHL	G	313	-	3/3/16/26	7/20/118/137	-
22	CLA	v	303	-	1/1/12/20	7/19/97/115	-
22	CLA	Q	308	-	1/1/11/20	9/17/95/115	-
22	CLA	b	610	-	1/1/15/20	16/37/115/115	-
26	CHL	p	317	-	3/3/20/26	14/39/137/137	-
23	LUT	5	310	-	-	1/29/67/67	0/2/2/2
22	CLA	B	606	-	1/1/15/20	18/37/115/115	-
22	CLA	2	302	-	1/1/15/20	14/37/115/115	-
23	LUT	s	311	-	-	7/29/67/67	0/2/2/2
22	CLA	R	302	27	1/1/11/20	8/18/96/115	-
30	PHO	a	407	-	-	10/37/103/103	0/5/6/6
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
22	CLA	4	306	-	1/1/14/20	16/31/109/115	-
22	CLA	B	609	-	1/1/15/20	12/37/115/115	-
24	XAT	r	612	-	-	7/31/93/93	0/4/4/4
22	CLA	v	307	-	1/1/15/20	10/37/115/115	-
26	CHL	U	313	-	3/3/20/26	15/39/137/137	-
25	LHG	C	524	-	-	13/53/53/53	-
26	CHL	q	314	18	3/3/20/26	23/39/137/137	-
22	CLA	a	408	-	1/1/14/20	11/31/109/115	-
22	CLA	v	306	-	1/1/14/20	13/31/109/115	-
25	LHG	V	312	-	-	18/53/53/53	-
25	LHG	b	623	21	-	24/53/53/53	-
22	CLA	S	302	-	1/1/11/20	6/13/91/115	-
22	CLA	B	607	-	1/1/15/20	13/37/115/115	-
23	LUT	V	309	-	-	2/29/67/67	0/2/2/2
22	CLA	U	301	-	-	8/37/115/115	-
22	CLA	4	303	-	1/1/12/20	9/19/97/115	-
22	CLA	1	301	-	1/1/15/20	7/37/115/115	-
26	CHL	N	313	-	3/3/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	U	309	-	-	4/29/67/67	0/2/2/2
31	BCR	a	409	-	-	2/29/63/63	0/2/2/2
32	SQD	m	101	-	-	21/37/57/69	0/1/1/1
30	PHO	D	401	-	-	11/37/103/103	0/5/6/6
31	BCR	B	620	-	-	12/29/63/63	0/2/2/2
26	CHL	n	315	-	3/3/16/26	10/20/118/137	-
22	CLA	b	612	-	1/1/15/20	13/37/115/115	-
22	CLA	v	304	-	1/1/14/20	14/31/109/115	-
22	CLA	2	306	-	1/1/14/20	11/31/109/115	-
25	LHG	Q	310	-	-	19/53/53/53	-
23	LUT	5	309	-	-	4/29/67/67	0/2/2/2
22	CLA	4	307	-	1/1/15/20	7/37/115/115	-
22	CLA	p	302	-	1/1/15/20	15/37/115/115	-
25	LHG	N	312	-	-	16/53/53/53	-
22	CLA	g	304	18	1/1/14/20	8/36/114/115	-
23	LUT	1	310	-	-	0/29/67/67	0/2/2/2
36	DGD	c	519	-	-	21/49/89/95	0/2/2/2
26	CHL	N	316	-	3/3/20/26	17/39/137/137	-
26	CHL	2	313	18	3/3/20/26	20/39/137/137	-
22	CLA	4	308	-	1/1/11/20	11/17/95/115	-
22	CLA	V	304	-	1/1/14/20	12/31/109/115	-
26	CHL	q	312	-	3/3/16/26	12/18/116/137	-
25	LHG	g	310	-	-	20/53/53/53	-
22	CLA	4	302	-	1/1/15/20	15/37/115/115	-
22	CLA	v	308	-	1/1/11/20	9/17/95/115	-
22	CLA	g	305	22	1/1/14/20	10/31/109/115	-
22	CLA	U	304	-	1/1/14/20	5/31/109/115	-
22	CLA	5	304	18	1/1/15/20	12/37/115/115	-
22	CLA	q	306	22	1/1/14/20	12/31/109/115	-
36	DGD	a	416	-	-	24/48/88/95	0/2/2/2
26	CHL	1	315	-	3/3/16/26	6/20/118/137	-
25	LHG	5	312	-	-	23/53/53/53	-
24	XAT	N	311	-	-	8/31/93/93	0/4/4/4
22	CLA	V	305	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	L	101	-	-	28/53/53/53	-
22	CLA	R	304	-	1/1/14/20	11/31/109/115	-
22	CLA	q	305	22	1/1/14/20	12/31/109/115	-
26	CHL	5	317	-	3/3/20/26	15/39/137/137	-
31	BCR	C	517	-	-	14/29/63/63	0/2/2/2
34	LMG	C	502	-	-	26/46/66/70	0/1/1/1
22	CLA	b	606	-	1/1/15/20	18/37/115/115	-
22	CLA	G	302	-	1/1/15/20	17/37/115/115	-
22	CLA	P	304	-	1/1/12/20	10/19/97/115	-
26	CHL	P	317	-	3/3/20/26	15/39/137/137	-
23	LUT	P	311	-	-	3/29/67/67	0/2/2/2
27	NEX	U	318	-	-	3/27/83/83	0/3/3/3
32	SQD	M	101	-	-	22/37/57/69	0/1/1/1
23	LUT	4	309	-	-	2/29/67/67	0/2/2/2
22	CLA	B	604	-	1/1/15/20	15/37/115/115	-
26	CHL	Q	312	-	3/3/16/26	14/18/116/137	-
26	CHL	6	313	-	3/3/16/26	8/18/116/137	-
22	CLA	2	308	-	1/1/11/20	6/17/95/115	-
22	CLA	5	305	18	1/1/14/20	11/31/109/115	-
24	XAT	p	312	-	-	7/31/93/93	0/4/4/4
27	NEX	n	319	-	-	7/27/83/83	0/3/3/3
22	CLA	3	303	-	1/1/12/20	10/19/97/115	-
25	LHG	B	623	21	-	21/53/53/53	-
25	LHG	G	310	-	-	19/53/53/53	-
22	CLA	s	304	19	1/1/11/20	9/13/91/115	-
22	CLA	s	301	19	1/1/14/20	16/33/111/115	-
22	CLA	r	609	26	1/1/14/20	10/31/109/115	-
31	BCR	z	101	-	-	8/29/63/63	0/2/2/2
22	CLA	c	507	-	1/1/15/20	20/37/115/115	-
26	CHL	n	316	-	3/3/20/26	25/39/137/137	-
22	CLA	x	201	14	1/1/15/20	10/37/115/115	-
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
22	CLA	B	616	21	1/1/15/20	6/37/115/115	-
22	CLA	2	304	18	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	305	22	1/1/14/20	16/31/109/115	-
22	CLA	a	404	-	1/1/15/20	15/37/115/115	-
22	CLA	3	307	-	1/1/15/20	10/37/115/115	-
34	LMG	C	521	-	-	19/46/66/70	0/1/1/1
27	NEX	p	301	18	-	3/27/83/83	0/3/3/3
22	CLA	P	303	-	1/1/15/20	13/37/115/115	-
31	BCR	c	516	-	-	11/29/63/63	0/2/2/2
22	CLA	3	306	22	1/1/14/20	16/31/109/115	-
33	PL9	a	411	-	-	0/5/18/73	0/1/1/1
22	CLA	2	301	-	1/1/15/20	11/37/115/115	-
22	CLA	U	308	-	1/1/11/20	10/17/95/115	-
22	CLA	r	610	-	1/1/11/20	8/13/91/115	-
22	CLA	C	510	-	1/1/15/20	8/37/115/115	-
25	LHG	A	413	2	-	27/47/47/53	-
22	CLA	S	305	-	1/1/13/20	6/25/103/115	-
23	LUT	s	310	19	-	2/29/67/67	0/2/2/2
34	LMG	a	412	-	-	8/35/55/70	0/1/1/1
23	LUT	v	309	-	-	2/29/67/67	0/2/2/2
31	BCR	C	516	-	-	8/29/63/63	0/2/2/2
24	XAT	u	311	-	-	7/31/93/93	0/4/4/4
22	CLA	S	304	19	1/1/11/20	9/13/91/115	-
22	CLA	P	302	-	1/1/15/20	16/37/115/115	-
22	CLA	v	305	-	1/1/14/20	7/31/109/115	-
26	CHL	P	319	-	3/3/20/26	20/39/137/137	-
22	CLA	D	403	3	1/1/15/20	15/37/115/115	-
26	CHL	3	313	-	3/3/16/26	14/20/118/137	-
26	CHL	g	312	-	3/3/16/26	10/18/116/137	-
22	CLA	n	301	-	1/1/15/20	13/37/115/115	-
26	CHL	r	616	-	3/3/19/26	16/33/131/137	-
27	NEX	2	319	-	-	7/27/83/83	0/3/3/3
22	CLA	V	308	-	1/1/11/20	9/17/95/115	-
22	CLA	u	306	-	1/1/14/20	10/31/109/115	-
22	CLA	B	603	-	1/1/15/20	14/37/115/115	-
22	CLA	6	303	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	2	309	-	-	4/29/67/67	0/2/2/2
25	LHG	C	523	-	-	24/53/53/53	-
26	CHL	3	316	-	3/3/19/26	16/33/131/137	-
25	LHG	c	523	-	-	17/53/53/53	-
26	CHL	v	315	-	3/3/16/26	8/20/118/137	-
36	DGD	c	518	-	-	31/51/91/95	0/2/2/2
26	CHL	P	314	18	3/3/20/26	14/39/137/137	-
25	LHG	B	622	-	-	21/51/51/53	-
23	LUT	p	310	-	-	2/29/67/67	0/2/2/2
22	CLA	5	306	-	1/1/14/20	13/31/109/115	-
34	LMG	D	408	3	-	17/41/61/70	0/1/1/1
22	CLA	a	405	-	1/1/15/20	10/37/115/115	-
31	BCR	D	404	3	-	13/29/63/63	0/2/2/2
22	CLA	B	617	-	1/1/15/20	11/37/115/115	-
22	CLA	3	308	-	1/1/11/20	10/17/95/115	-
26	CHL	1	313	-	3/3/20/26	12/39/137/137	-
26	CHL	s	314	-	3/3/16/26	6/15/113/137	-
27	NEX	u	319	-	-	7/27/83/83	0/3/3/3
26	CHL	N	317	-	3/3/20/26	20/39/137/137	-
22	CLA	P	307	-	1/1/14/20	12/31/109/115	-
22	CLA	c	514	-	1/1/15/20	9/37/115/115	-
22	CLA	c	504	-	1/1/15/20	17/37/115/115	-
22	CLA	V	307	-	1/1/15/20	8/37/115/115	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
22	CLA	5	303	-	1/1/12/20	5/19/97/115	-
22	CLA	n	306	-	1/1/14/20	9/31/109/115	-
25	LHG	U	312	-	-	29/53/53/53	-
31	BCR	c	515	-	-	14/29/63/63	0/2/2/2
22	CLA	N	308	-	1/1/11/20	14/17/95/115	-
22	CLA	s	306	-	1/1/13/20	5/27/105/115	-
34	LMG	c	501	-	-	25/46/66/70	0/1/1/1
22	CLA	C	504	-	1/1/15/20	21/37/115/115	-
22	CLA	N	303	-	1/1/12/20	5/19/97/115	-
22	CLA	Q	304	18	1/1/14/20	14/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	308	-	1/1/11/20	11/17/95/115	-
26	CHL	4	315	-	3/3/16/26	6/20/118/137	-
22	CLA	c	510	-	1/1/15/20	15/37/115/115	-
24	XAT	1	311	-	-	7/31/93/93	0/4/4/4
22	CLA	3	304	18	1/1/14/20	15/36/114/115	-
22	CLA	u	308	-	1/1/11/20	10/17/95/115	-
22	CLA	1	303	-	1/1/12/20	8/19/97/115	-
22	CLA	5	307	-	1/1/14/20	10/31/109/115	-
22	CLA	X	202	14	1/1/15/20	9/37/115/115	-
22	CLA	b	608	-	1/1/15/20	11/37/115/115	-
22	CLA	s	303	19	1/1/12/20	6/19/97/115	-
27	NEX	s	317	19	-	4/27/83/83	0/3/3/3
26	CHL	v	316	-	3/3/20/26	15/39/137/137	-
26	CHL	4	313	-	3/3/20/26	16/39/137/137	-
22	CLA	c	512	-	1/1/15/20	9/37/115/115	-
25	LHG	p	313	-	-	22/53/53/53	-
22	CLA	2	305	18	1/1/14/20	11/31/109/115	-
22	CLA	5	308	-	1/1/11/20	3/17/95/115	-
22	CLA	N	307	-	1/1/14/20	13/31/109/115	-
22	CLA	G	307	-	1/1/15/20	12/37/115/115	-
23	LUT	V	310	-	-	0/29/67/67	0/2/2/2
26	CHL	P	316	-	3/3/16/26	7/20/118/137	-
23	LUT	R	312	-	-	4/29/67/67	0/2/2/2
24	XAT	n	311	-	-	9/31/93/93	0/4/4/4
22	CLA	G	306	22	1/1/14/20	9/31/109/115	-
22	CLA	5	302	-	1/1/15/20	16/37/115/115	-
22	CLA	1	302	-	1/1/15/20	14/37/115/115	-
22	CLA	c	508	20	1/1/15/20	14/37/115/115	-
25	LHG	c	522	-	-	24/53/53/53	-
22	CLA	1	304	-	1/1/14/20	7/31/109/115	-
22	CLA	P	305	18	1/1/15/20	10/37/115/115	-
26	CHL	P	315	-	3/3/16/26	9/18/116/137	-
23	LUT	U	310	-	-	3/29/67/67	0/2/2/2
22	CLA	p	303	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	21	1/1/15/20	18/37/115/115	-
22	CLA	b	613	-	1/1/15/20	16/37/115/115	-
25	LHG	6	311	-	-	19/53/53/53	-
26	CHL	5	313	18	3/3/20/26	21/39/137/137	-
23	LUT	N	309	-	-	2/29/67/67	0/2/2/2
27	NEX	r	618	22,1	-	7/27/83/83	0/3/3/3
27	NEX	u	320	-	-	2/27/83/83	0/3/3/3

The worst 5 of 5049 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C26-C25	15.51	1.61	1.34
31	a	409	BCR	C26-C25	15.51	1.61	1.34
31	b	619	BCR	C5-C6	15.49	1.61	1.34
31	B	619	BCR	C5-C6	15.47	1.61	1.34
31	x	202	BCR	C5-C6	15.45	1.61	1.34

The worst 5 of 6389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	311	XAT	O4-C5-C4	60.27	158.66	113.38
24	2	311	XAT	O4-C5-C4	60.01	158.46	113.38
24	n	311	XAT	O24-C25-C24	59.81	158.31	113.38
24	N	311	XAT	O24-C25-C24	59.80	158.31	113.38
24	4	311	XAT	O4-C5-C4	59.80	158.31	113.38

5 of 612 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	r	601	CLA	ND
22	r	602	CLA	ND
22	r	603	CLA	ND
22	r	604	CLA	ND
22	r	605	CLA	ND

5 of 6713 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	r	604	CLA	C1A-C2A-CAA-CBA
22	r	606	CLA	CBD-CGD-O2D-CED

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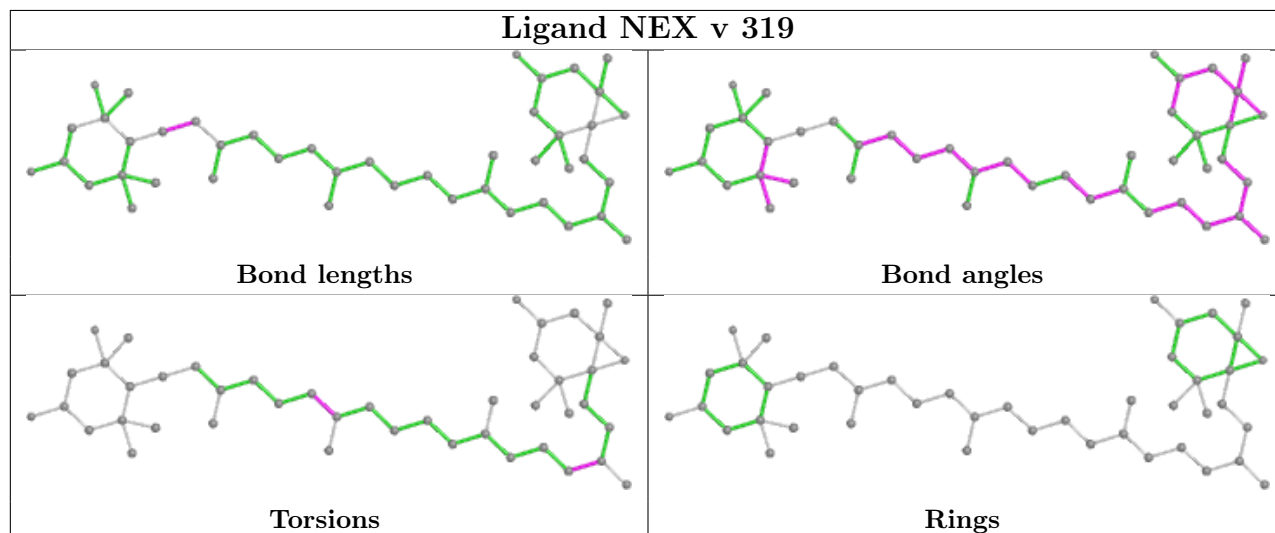
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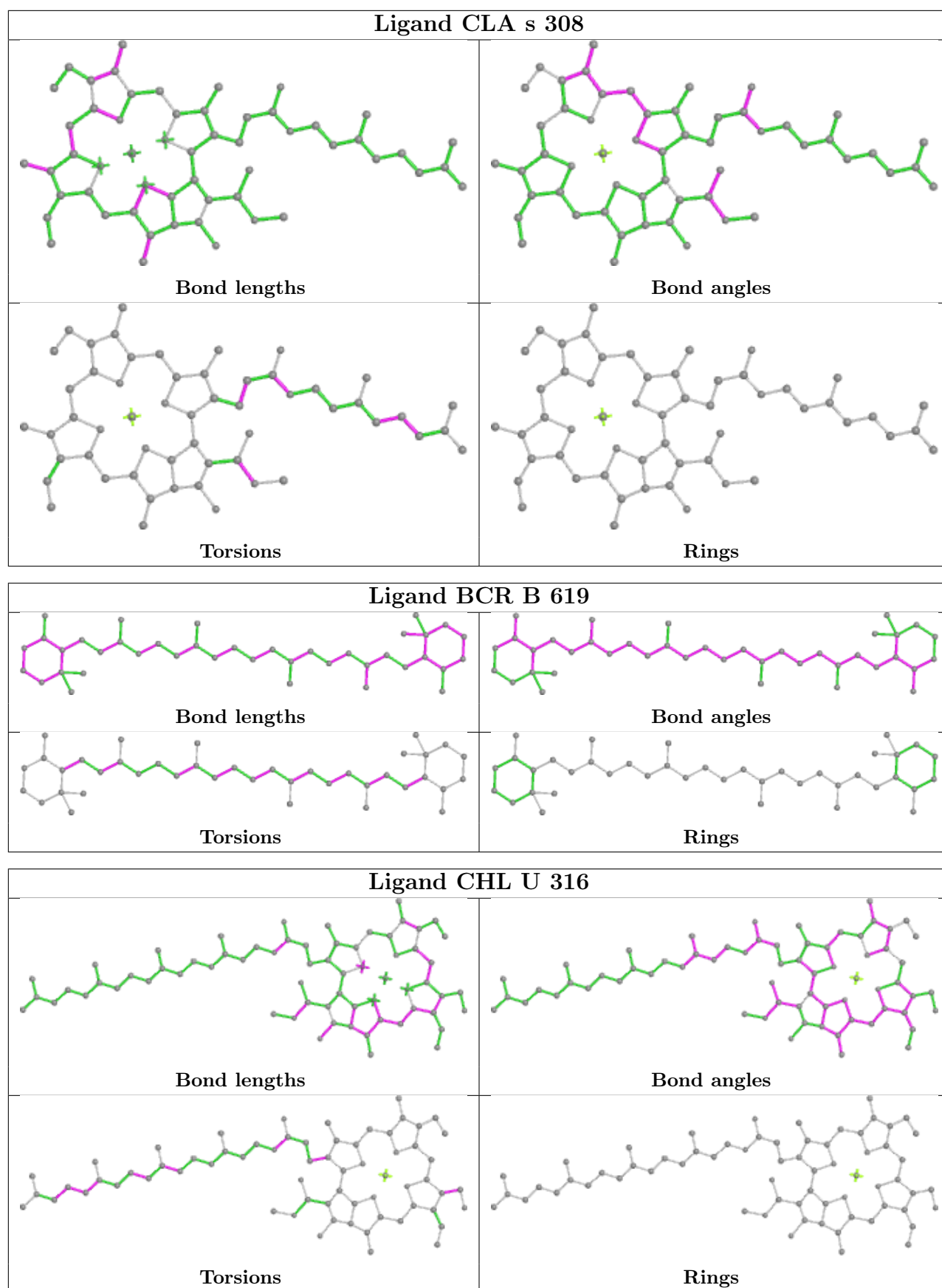
Mol	Chain	Res	Type	Atoms
22	r	606	CLA	C2-C3-C5-C6
22	r	606	CLA	C4-C3-C5-C6
22	r	607	CLA	C1A-C2A-CAA-CBA

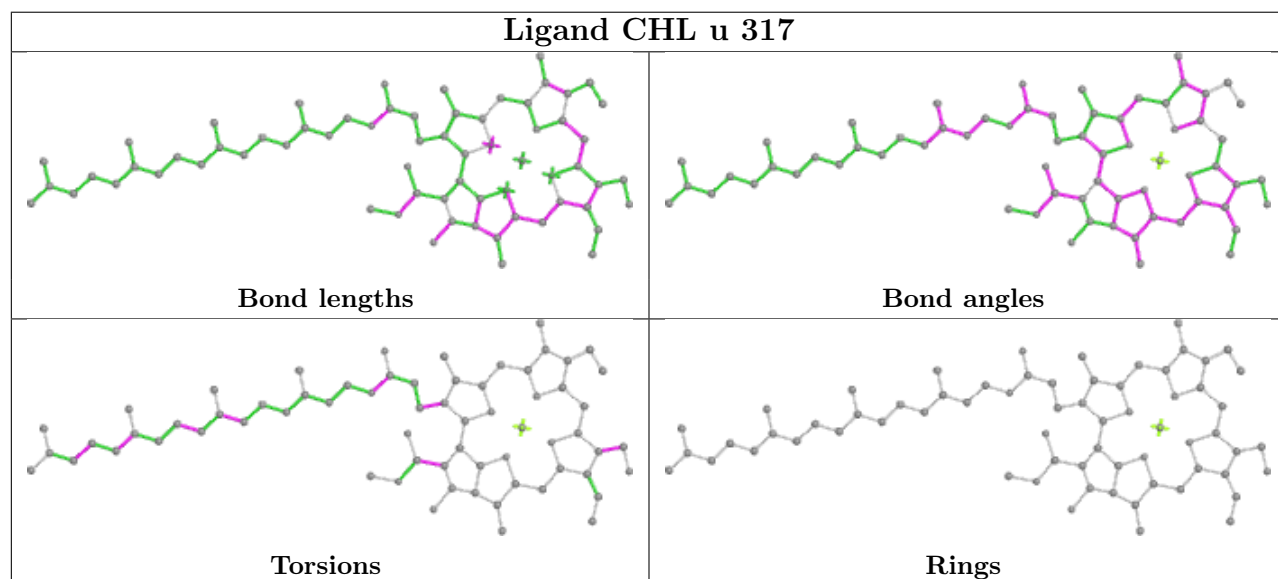
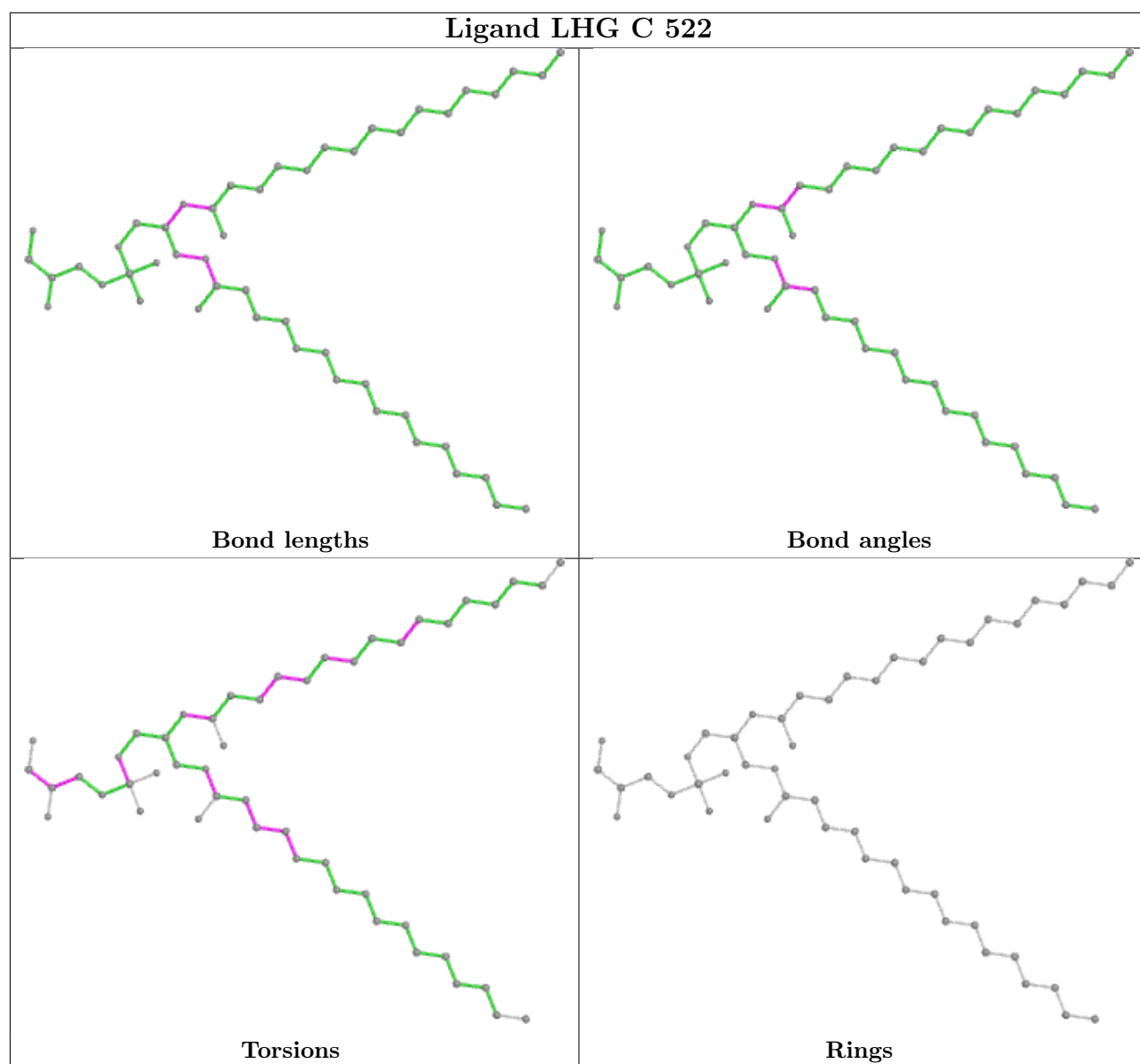
There are no ring outliers.

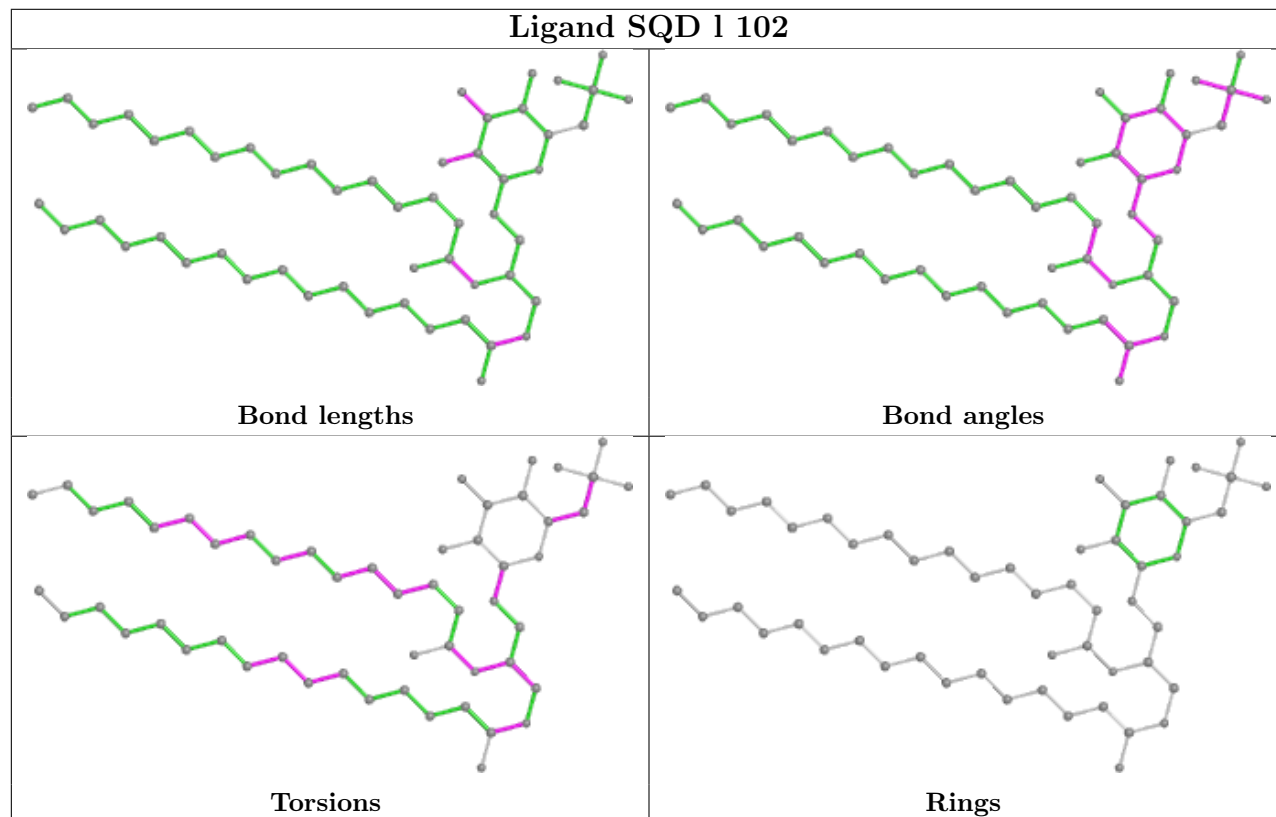
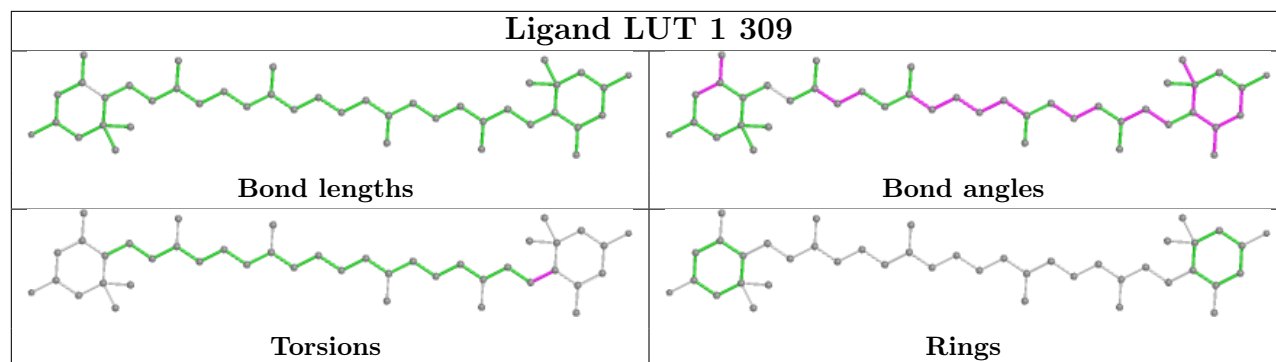
No monomer is involved in short contacts.

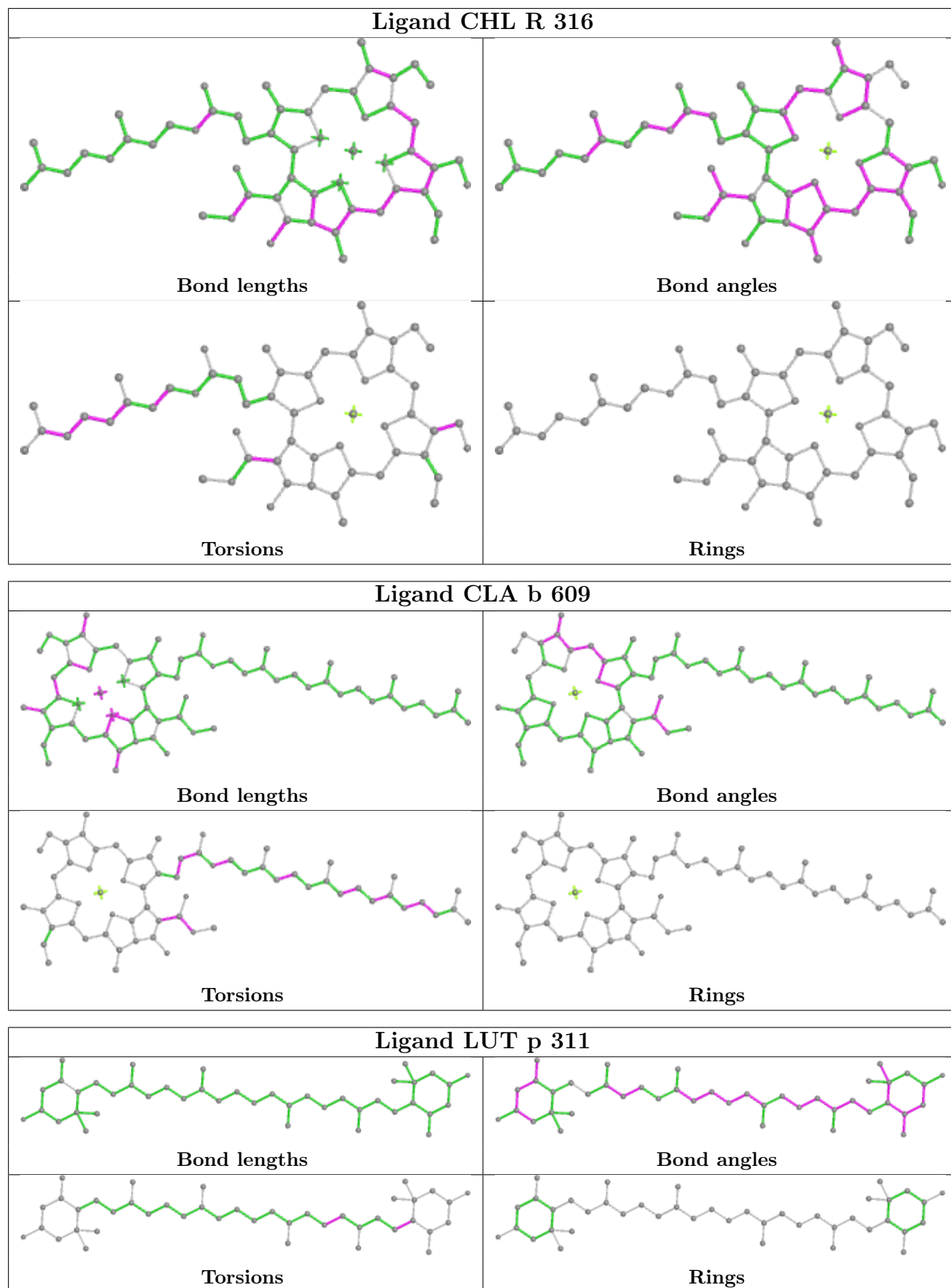
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

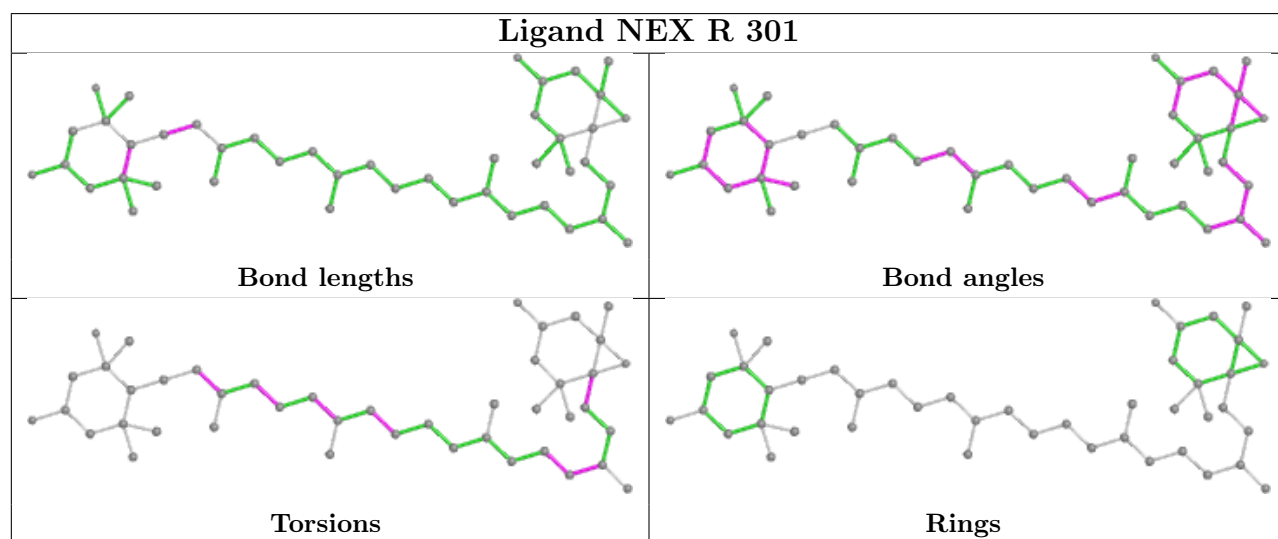
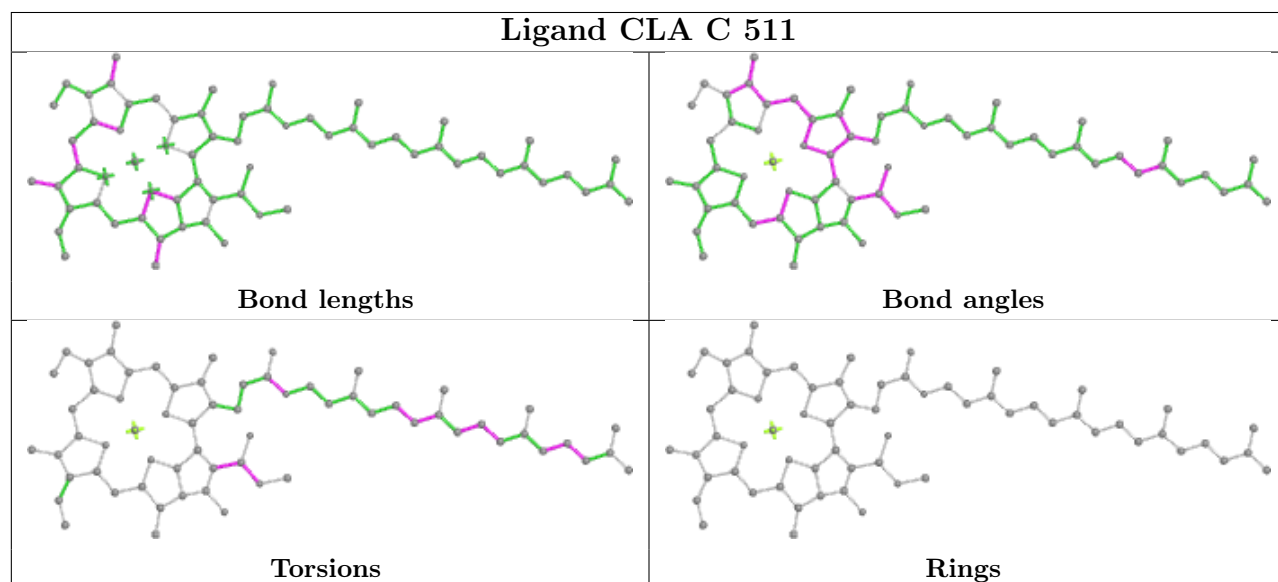
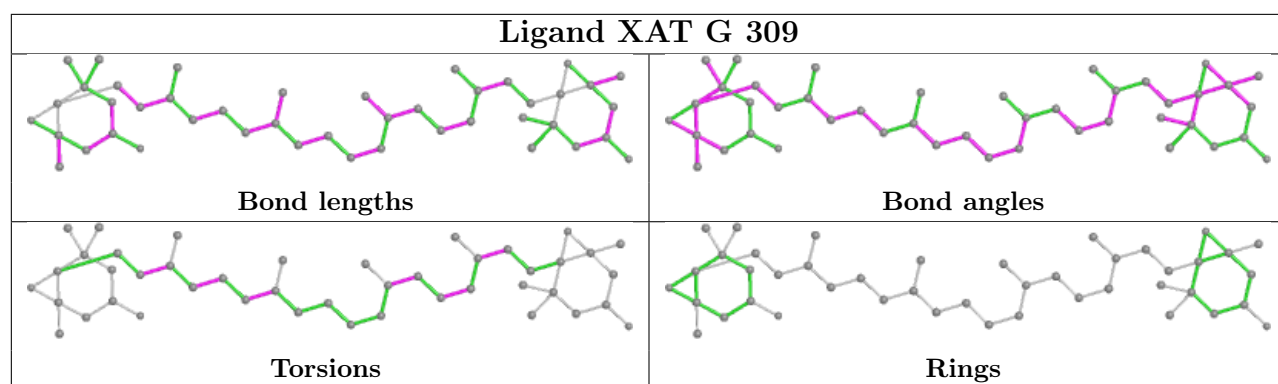


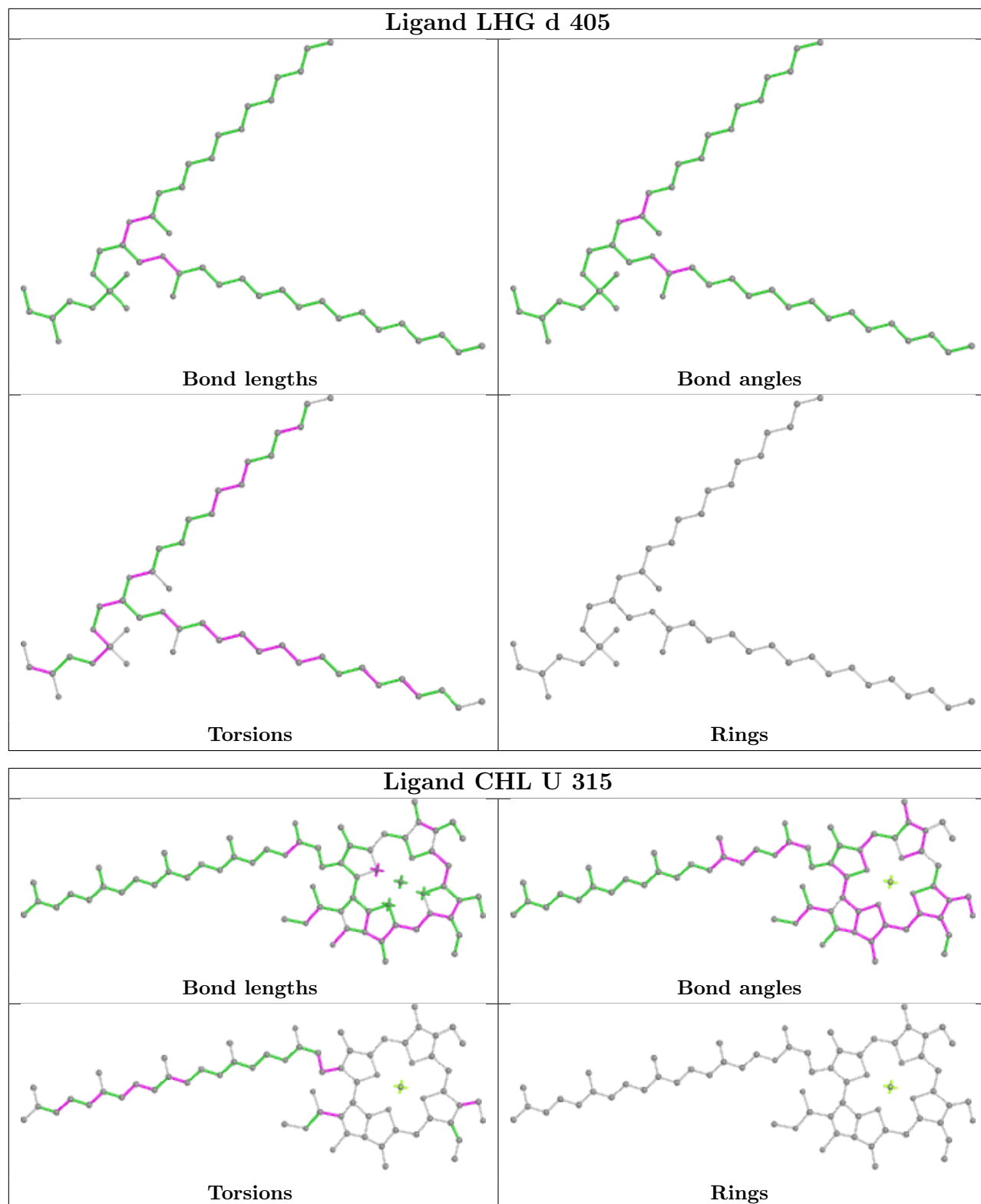


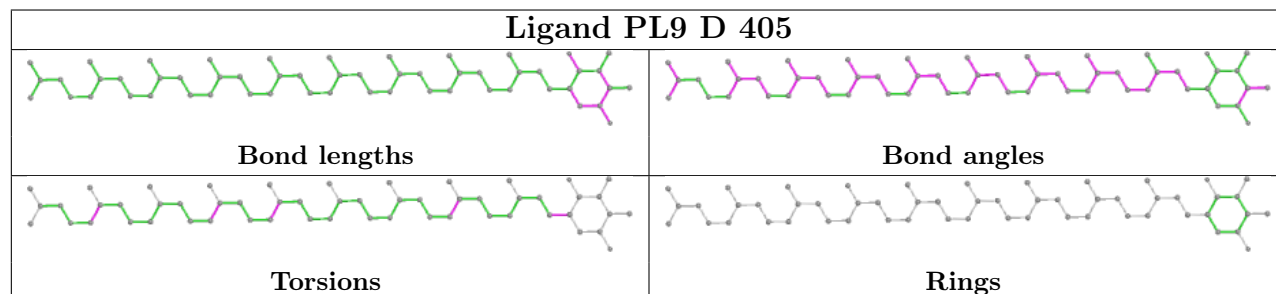
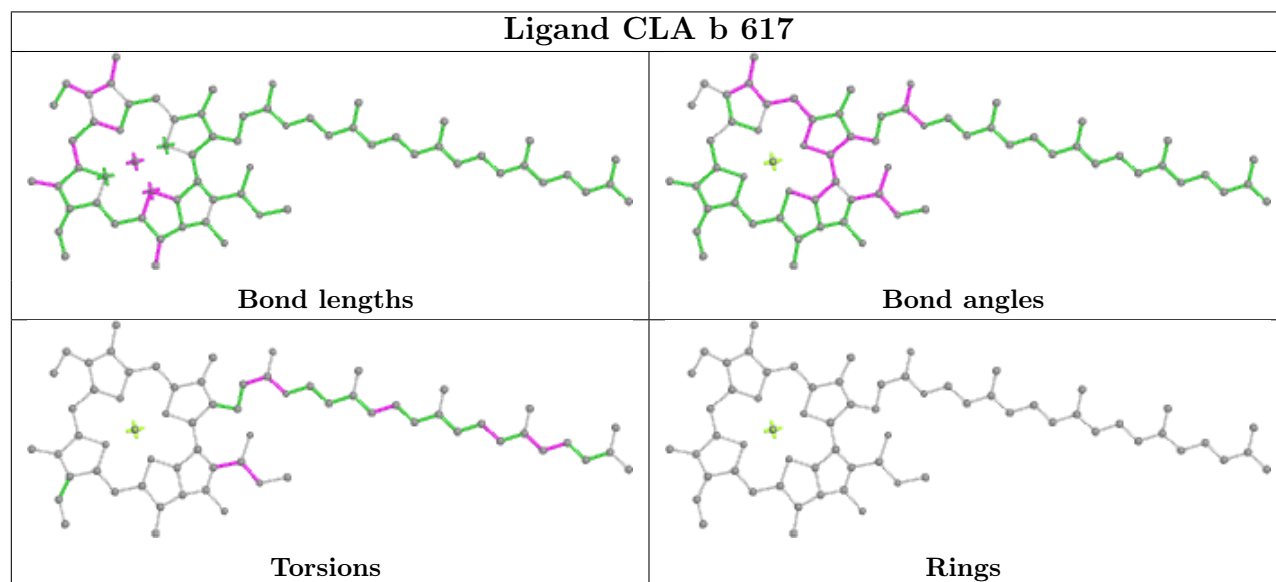
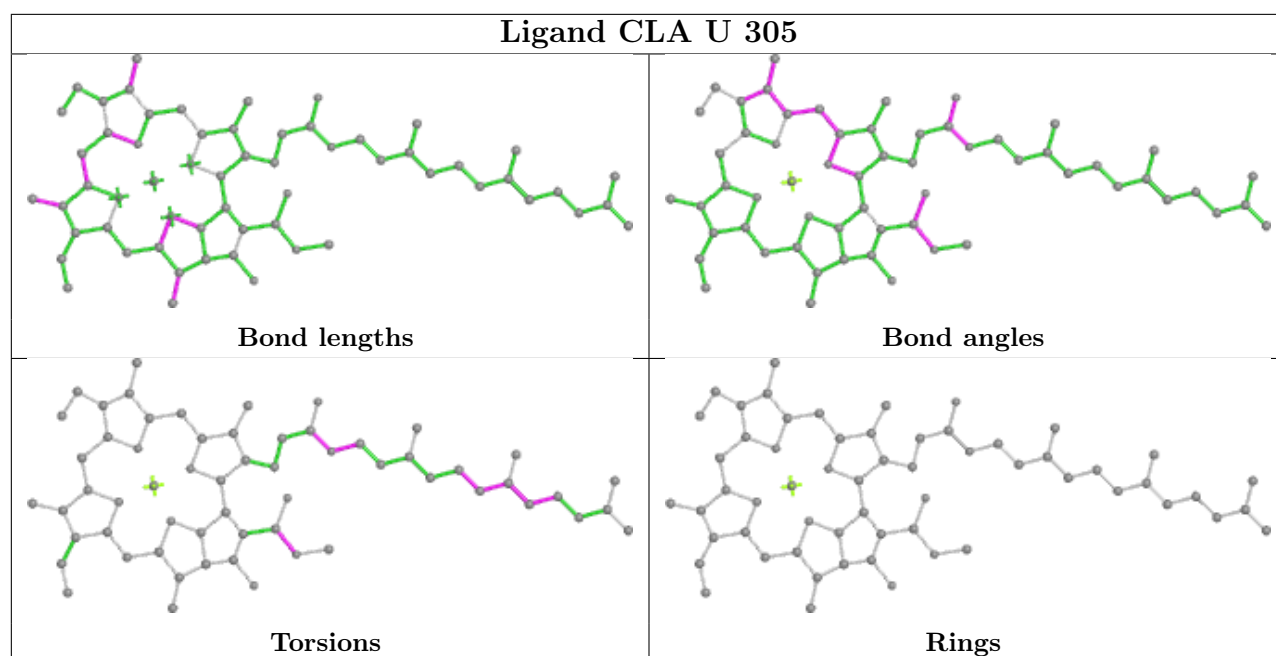


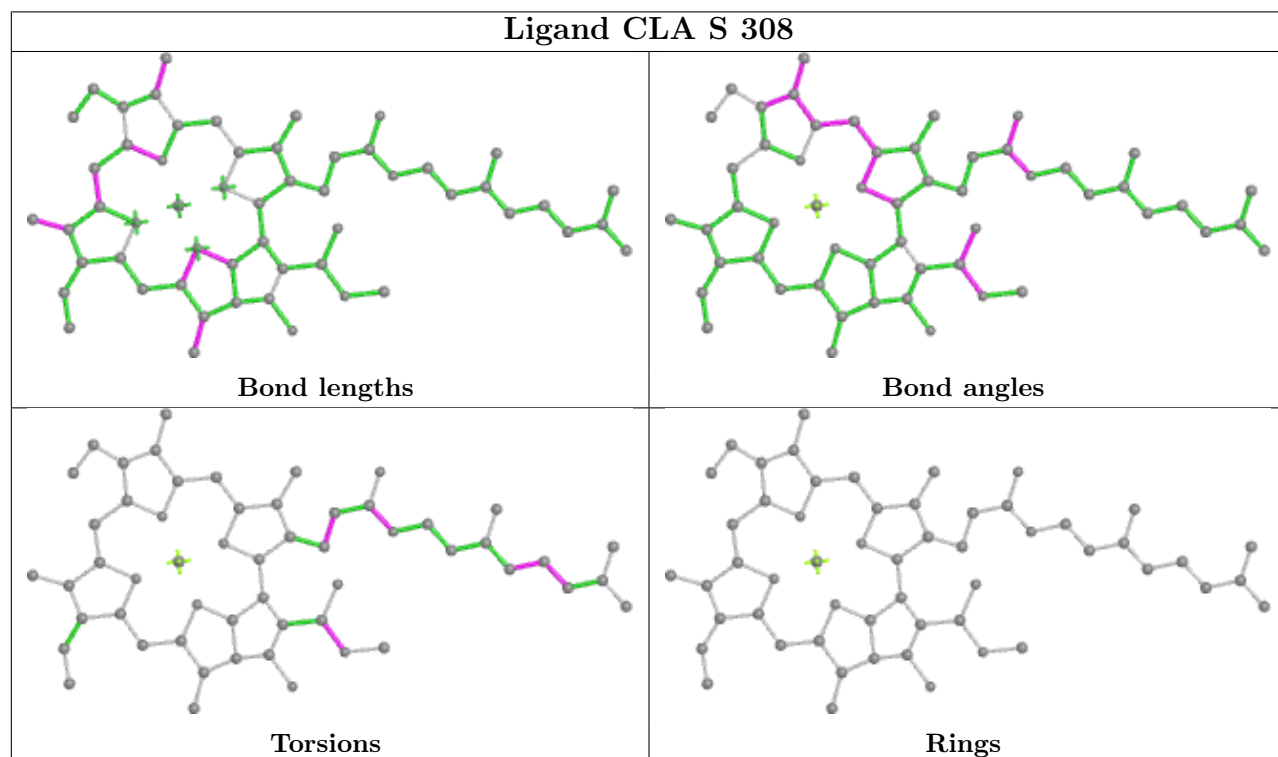
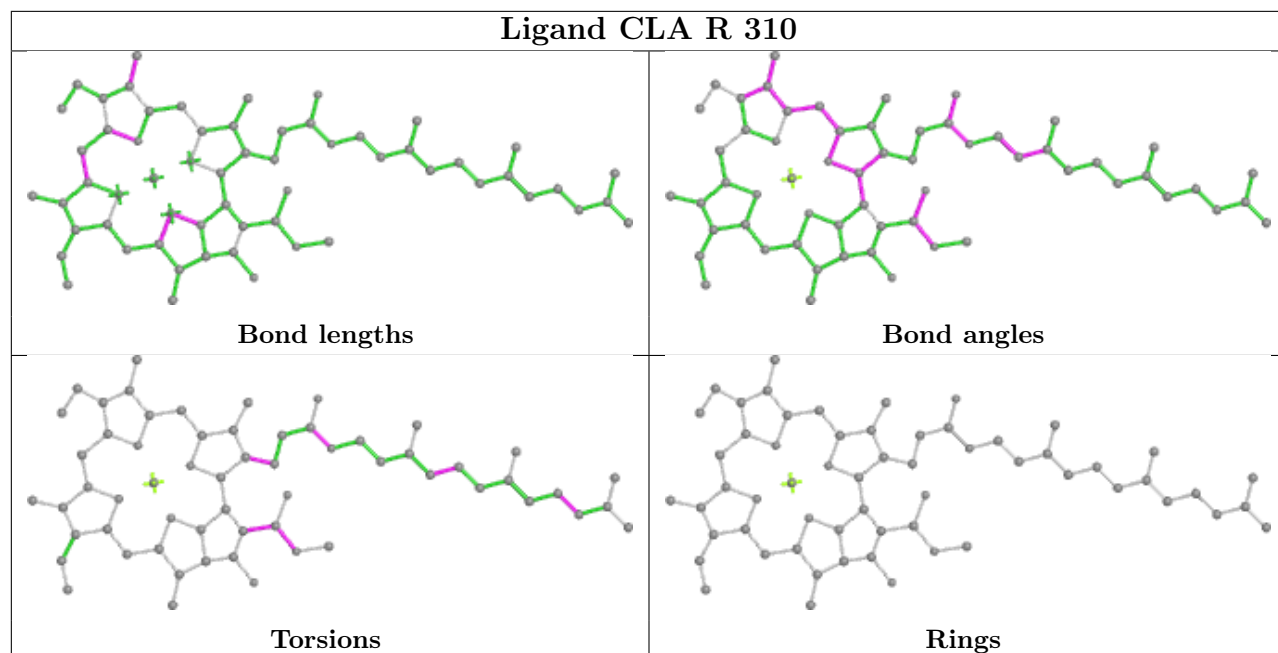


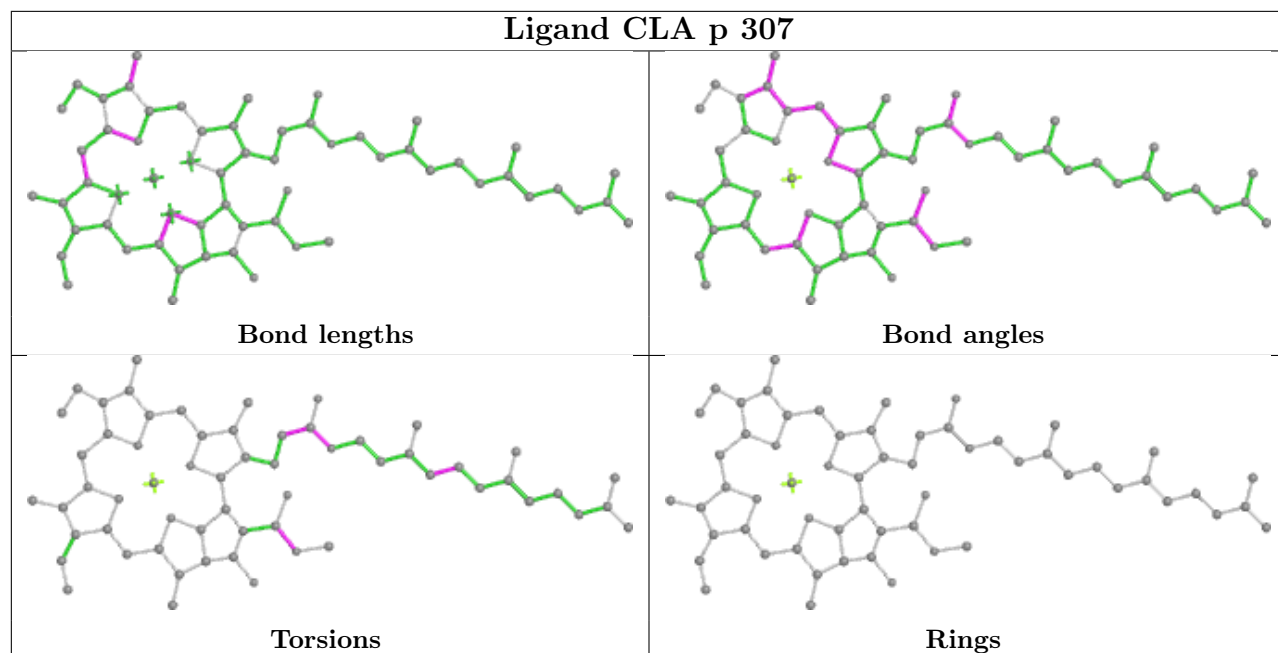


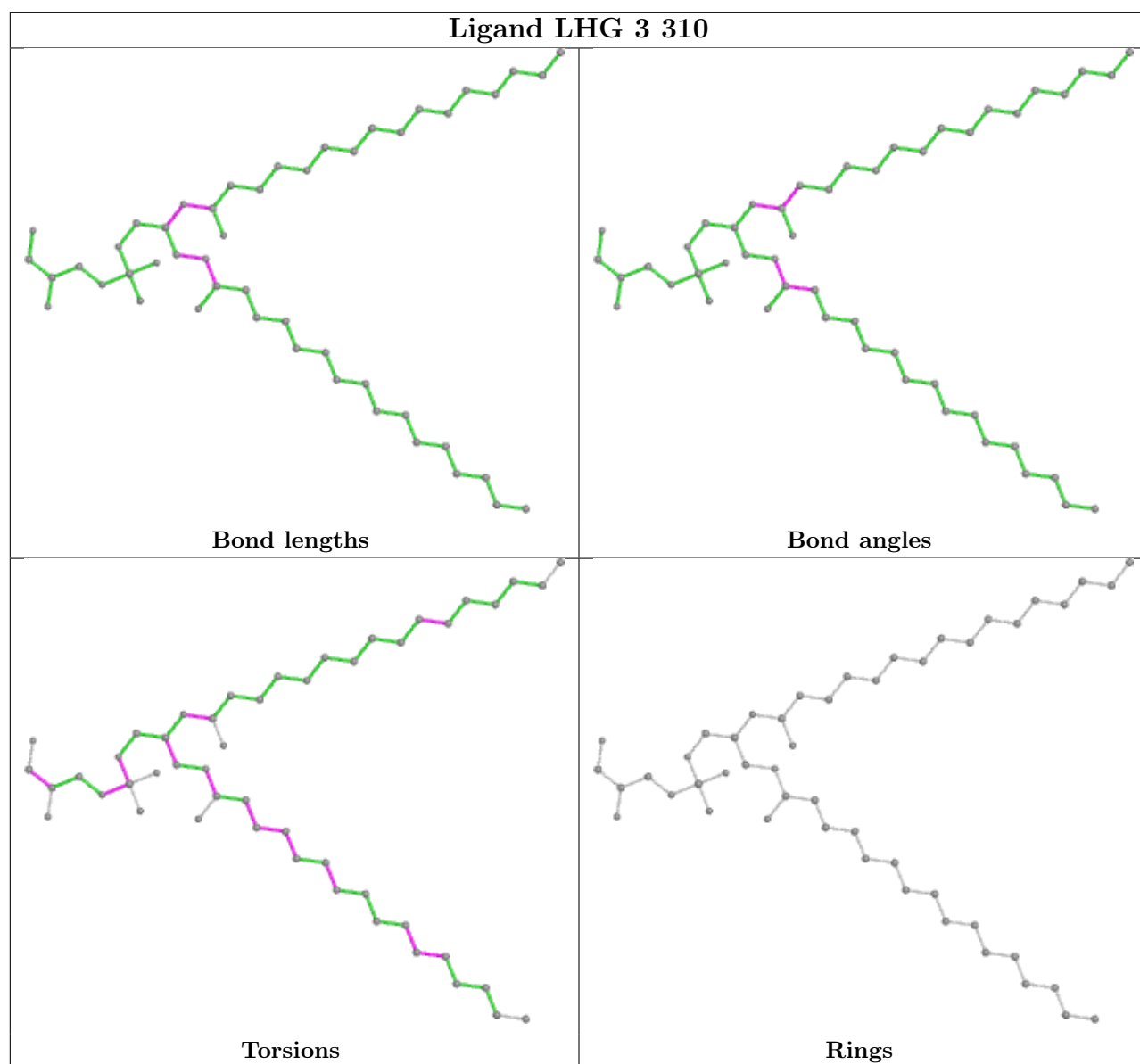


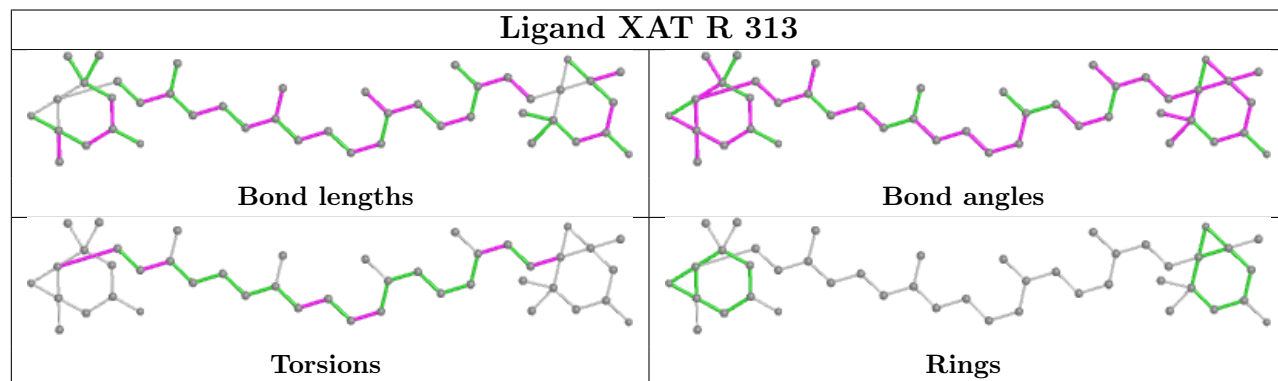
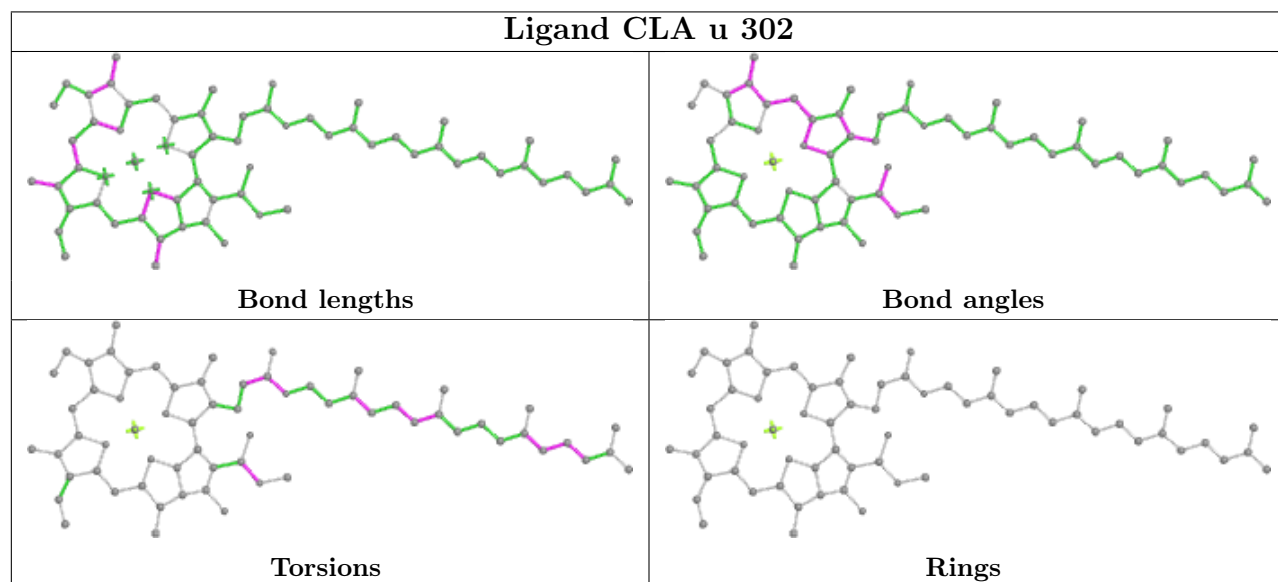
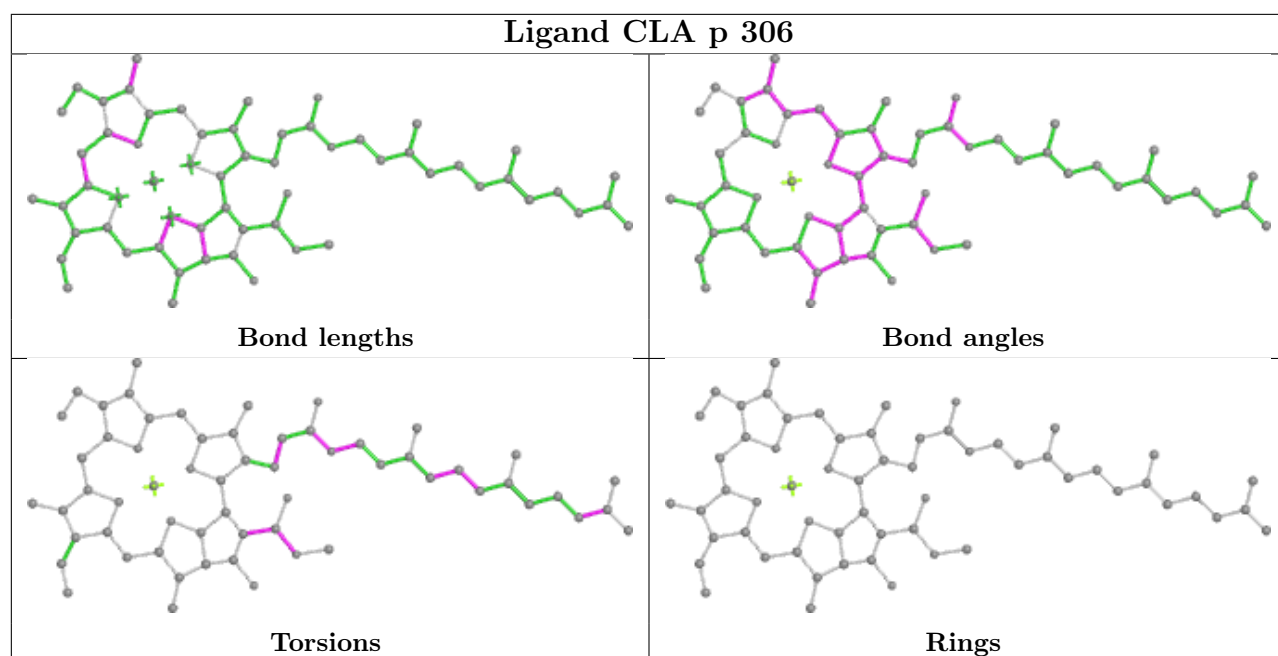


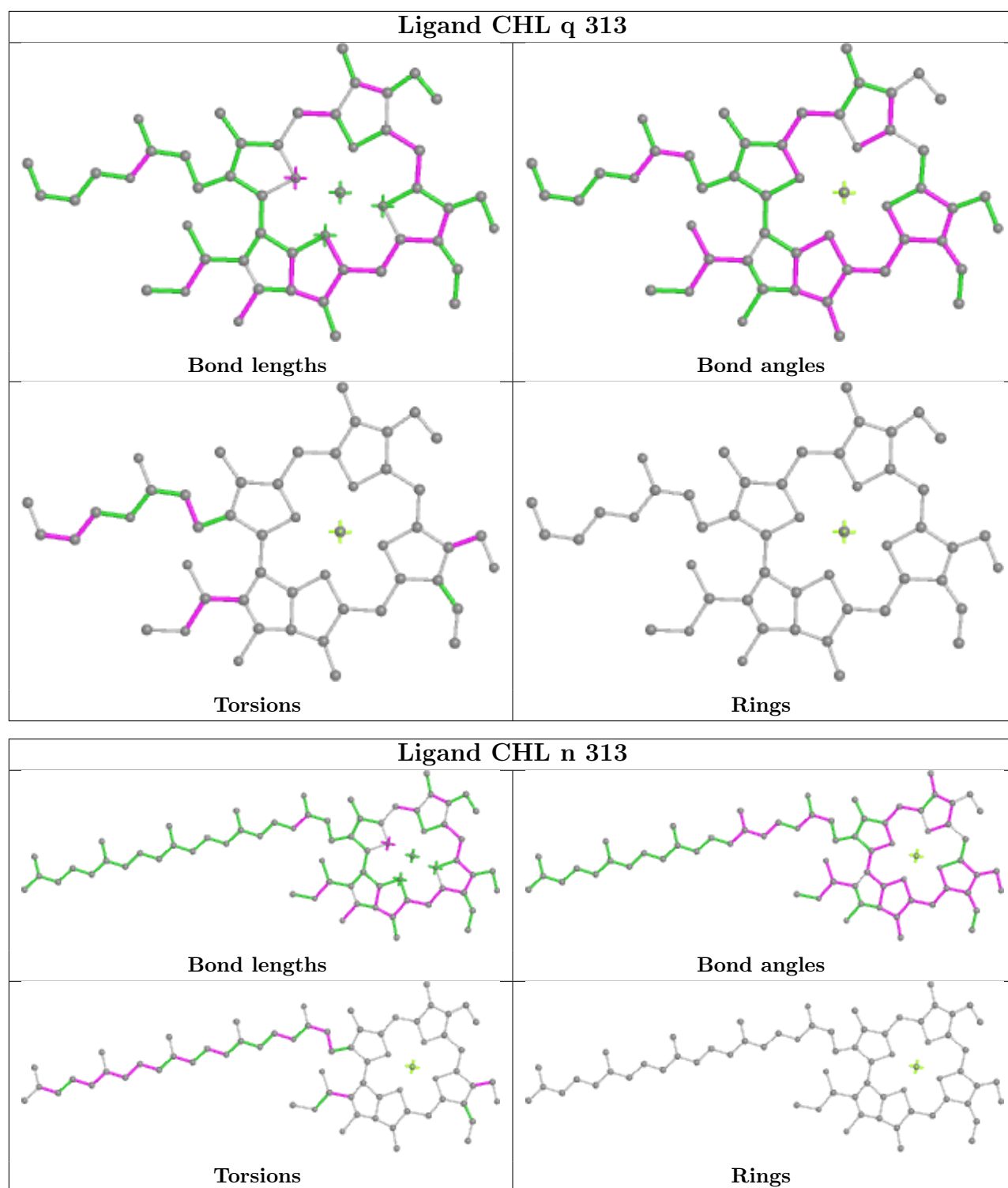


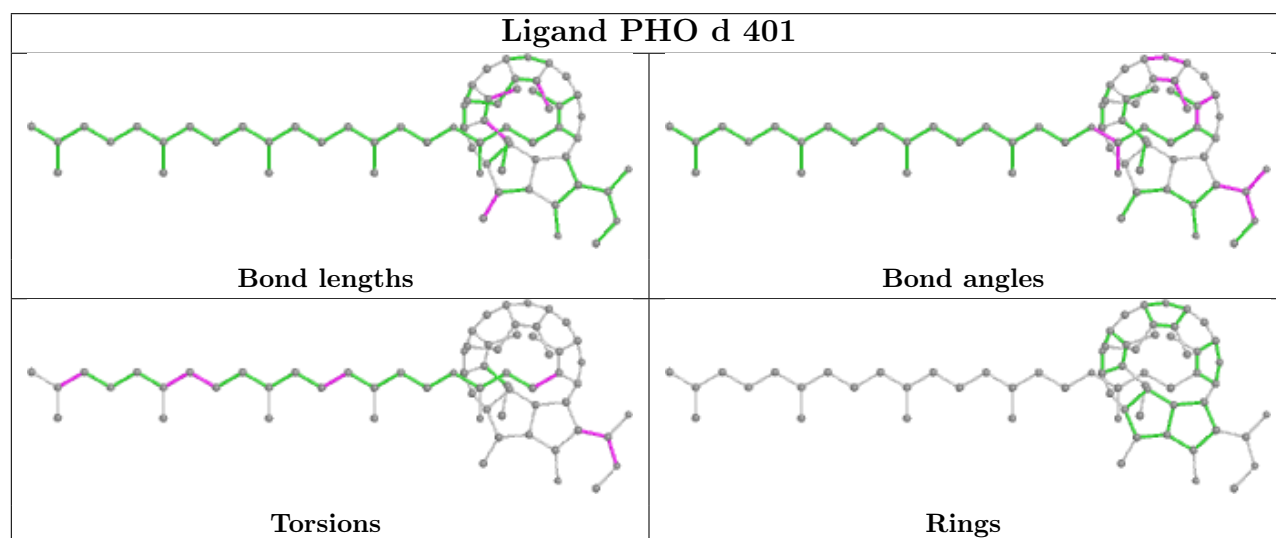
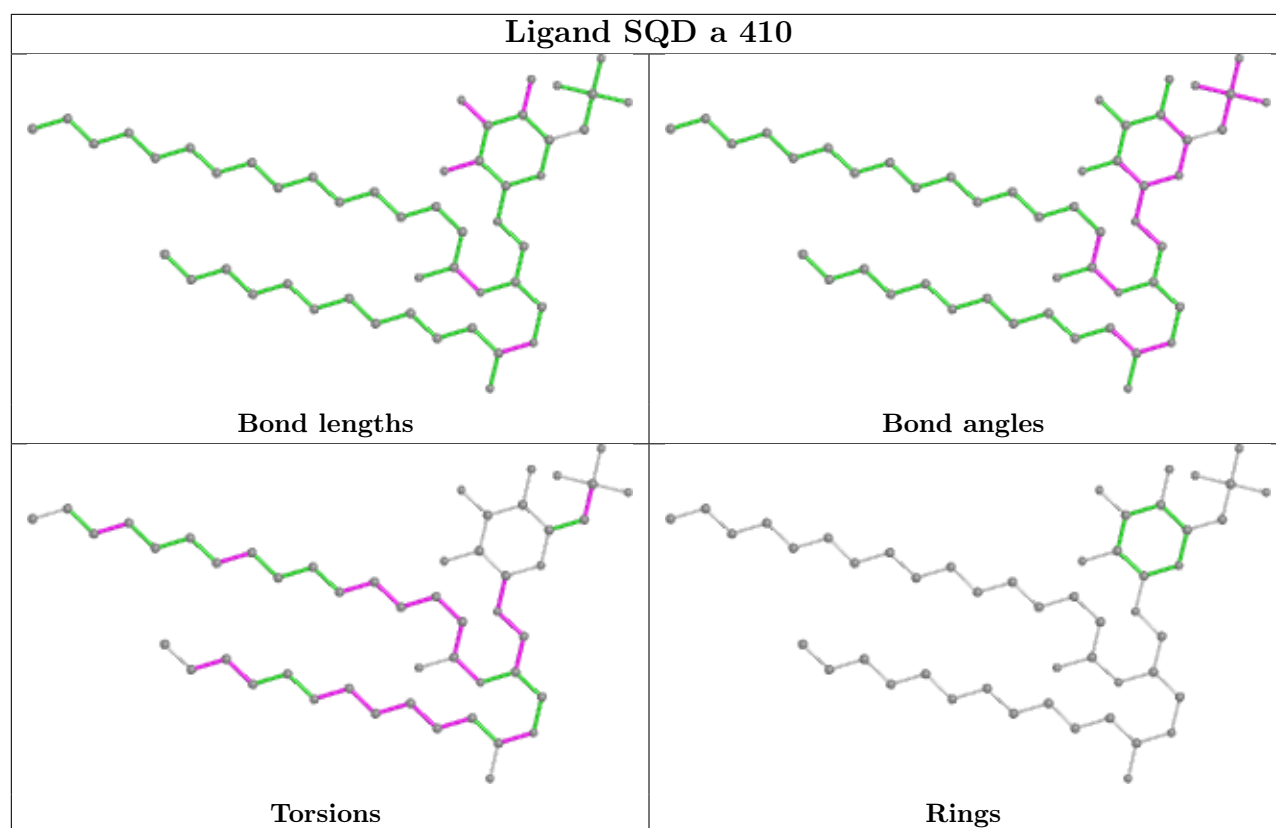


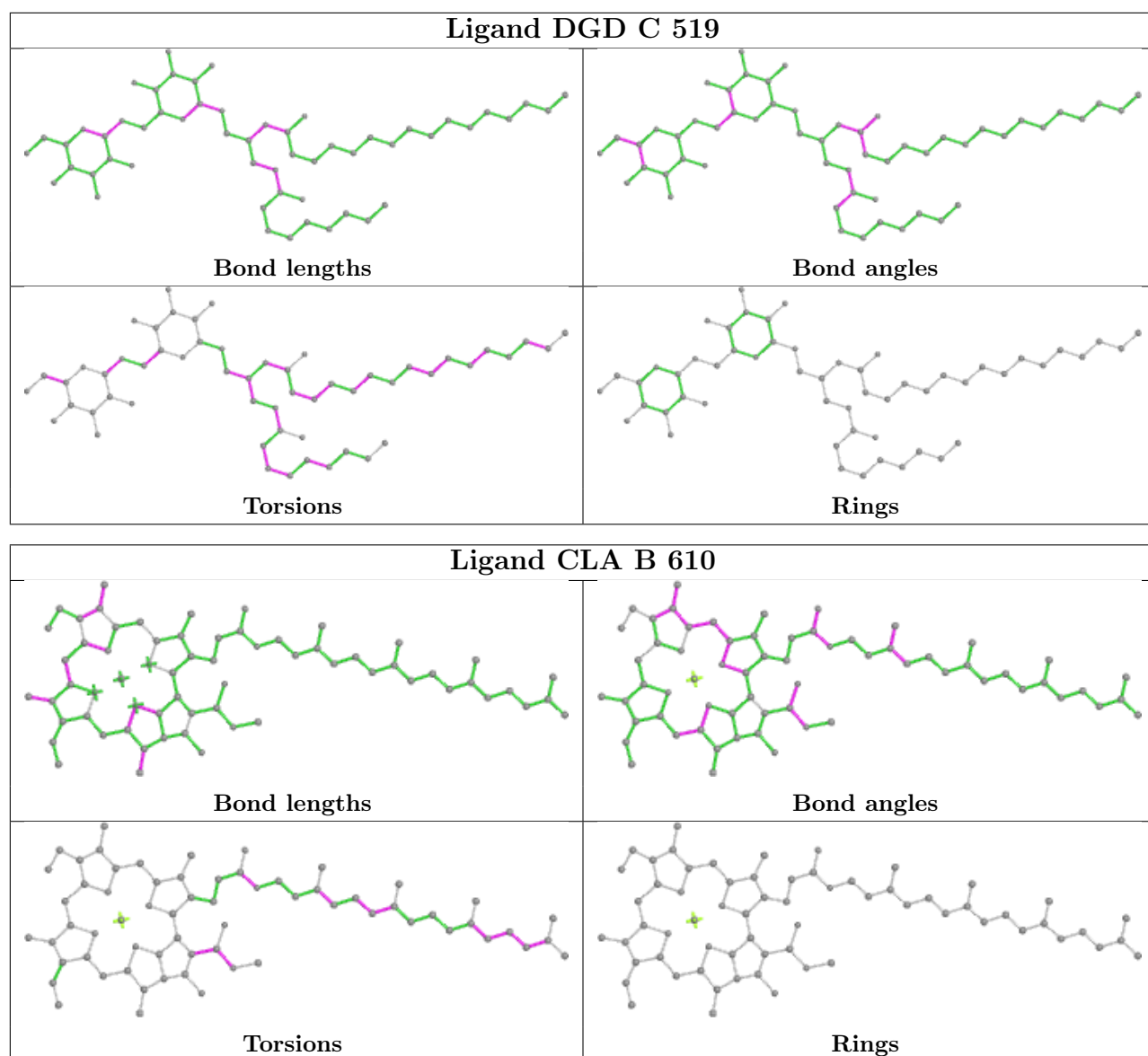


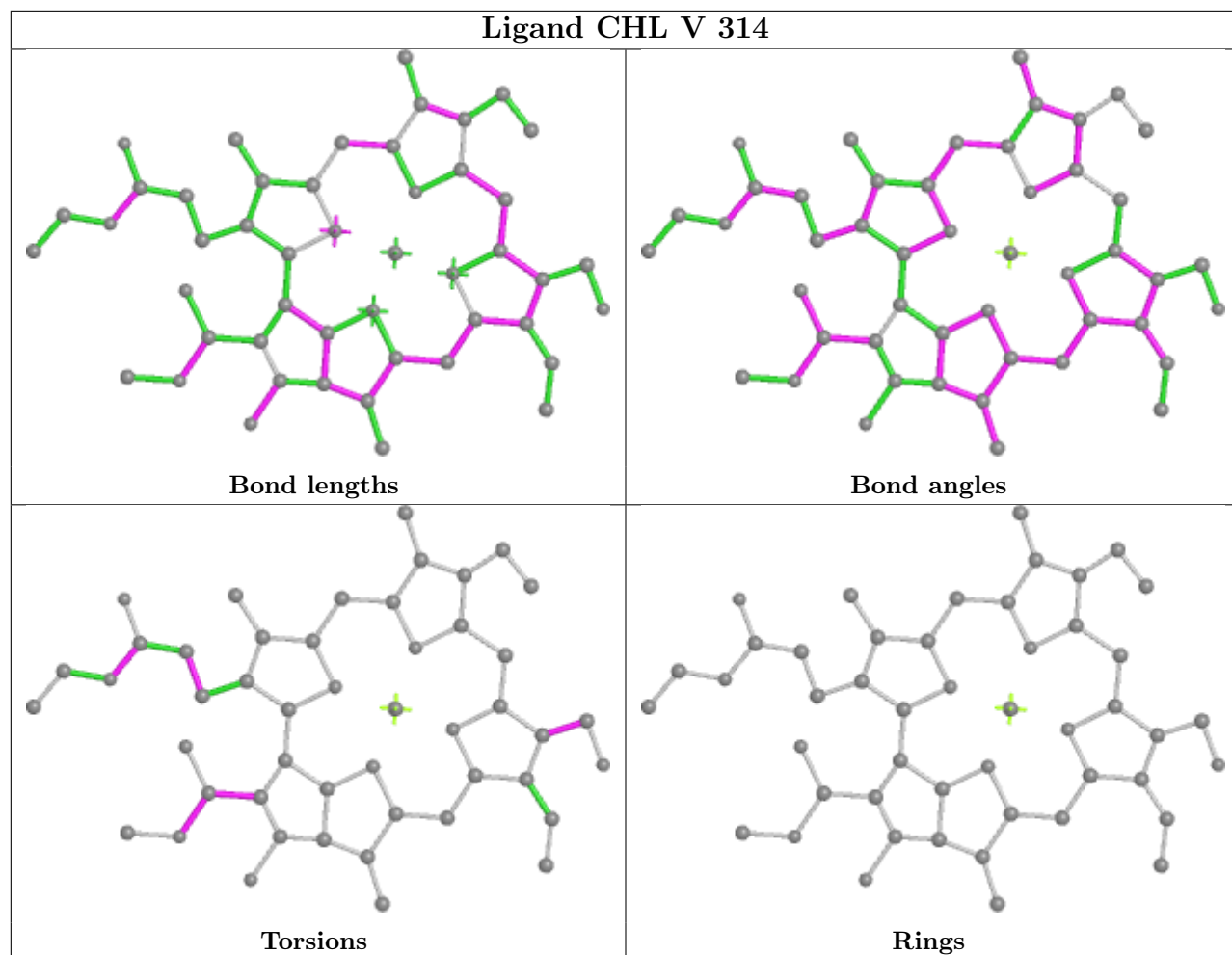


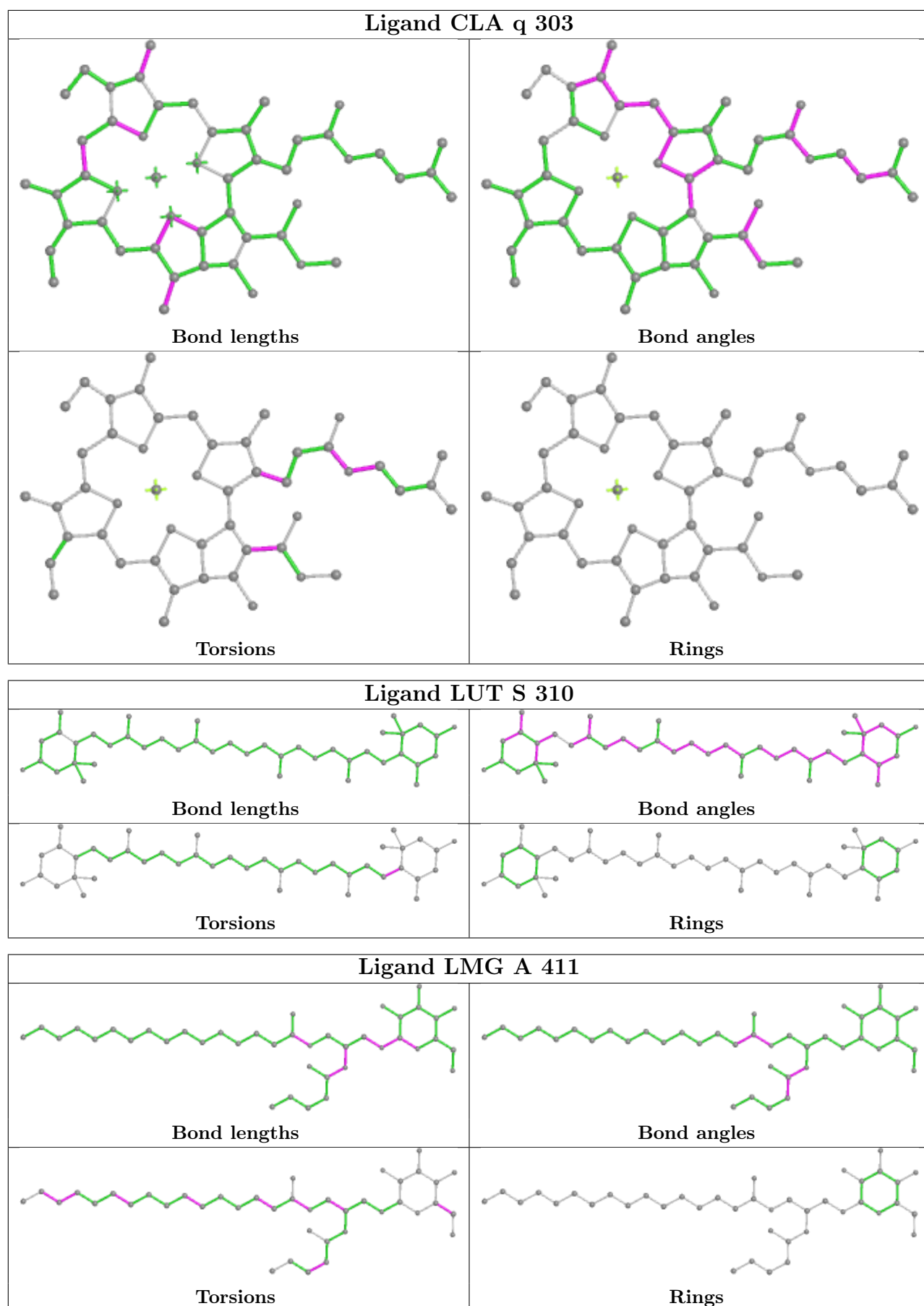


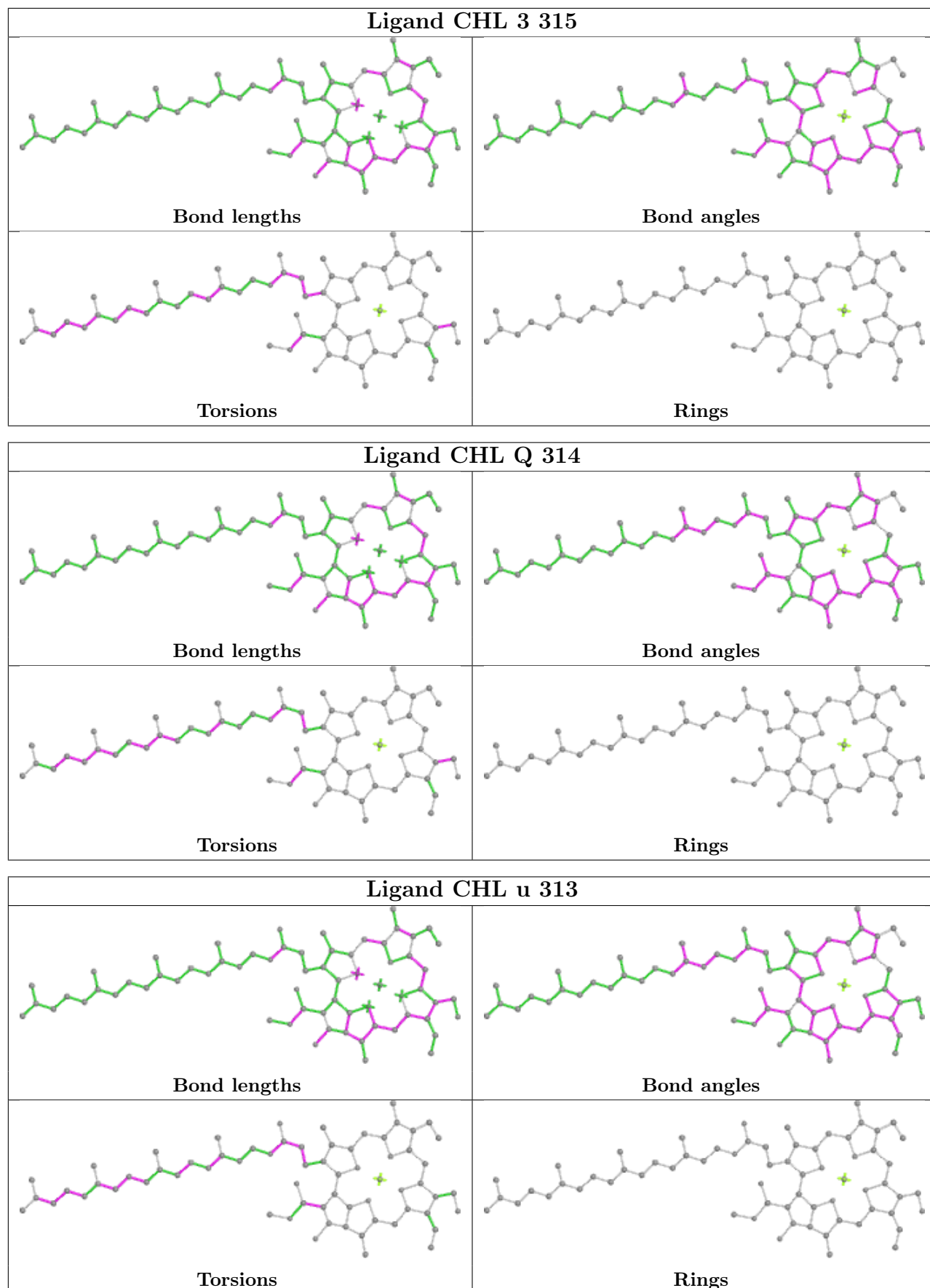


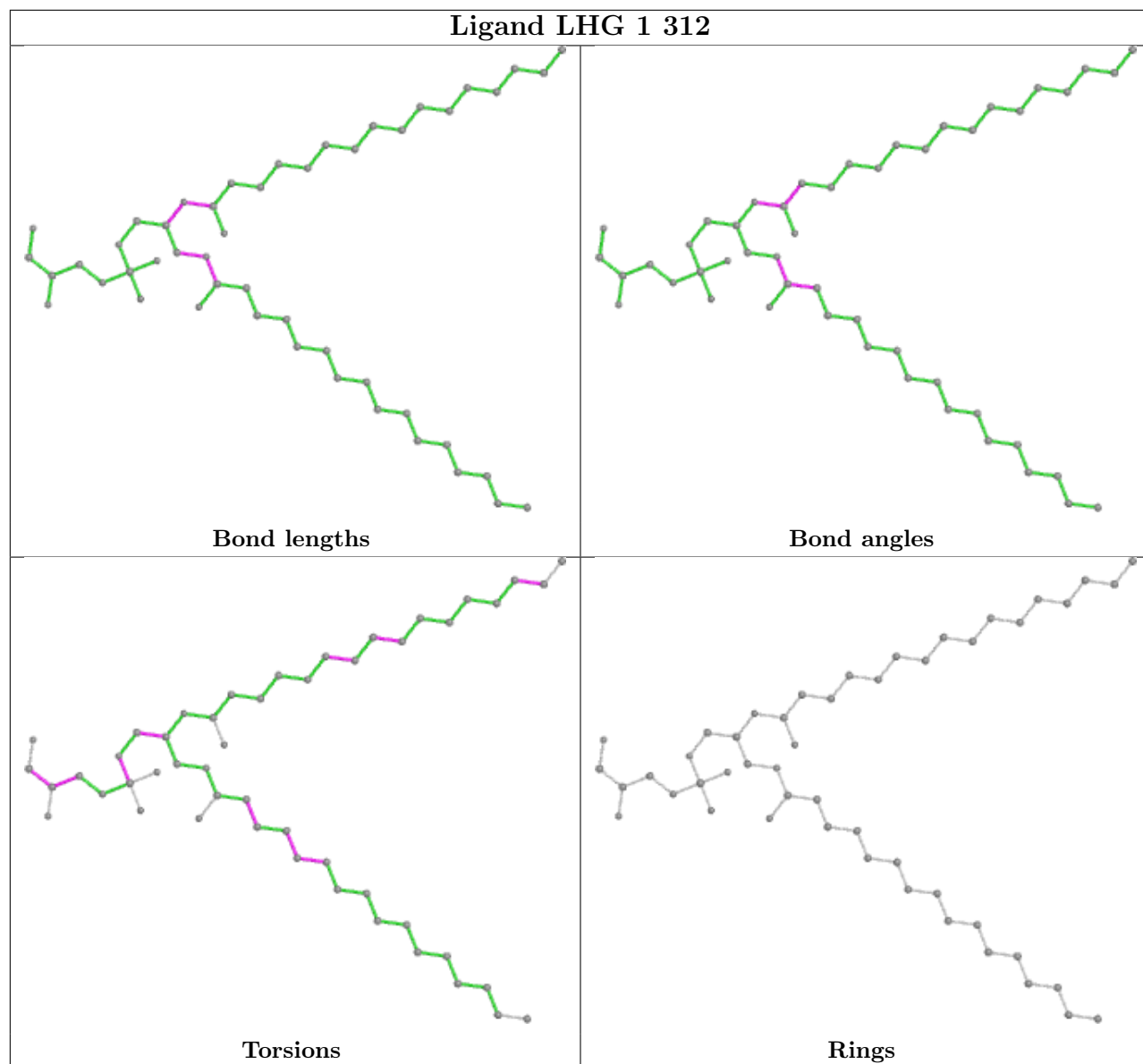


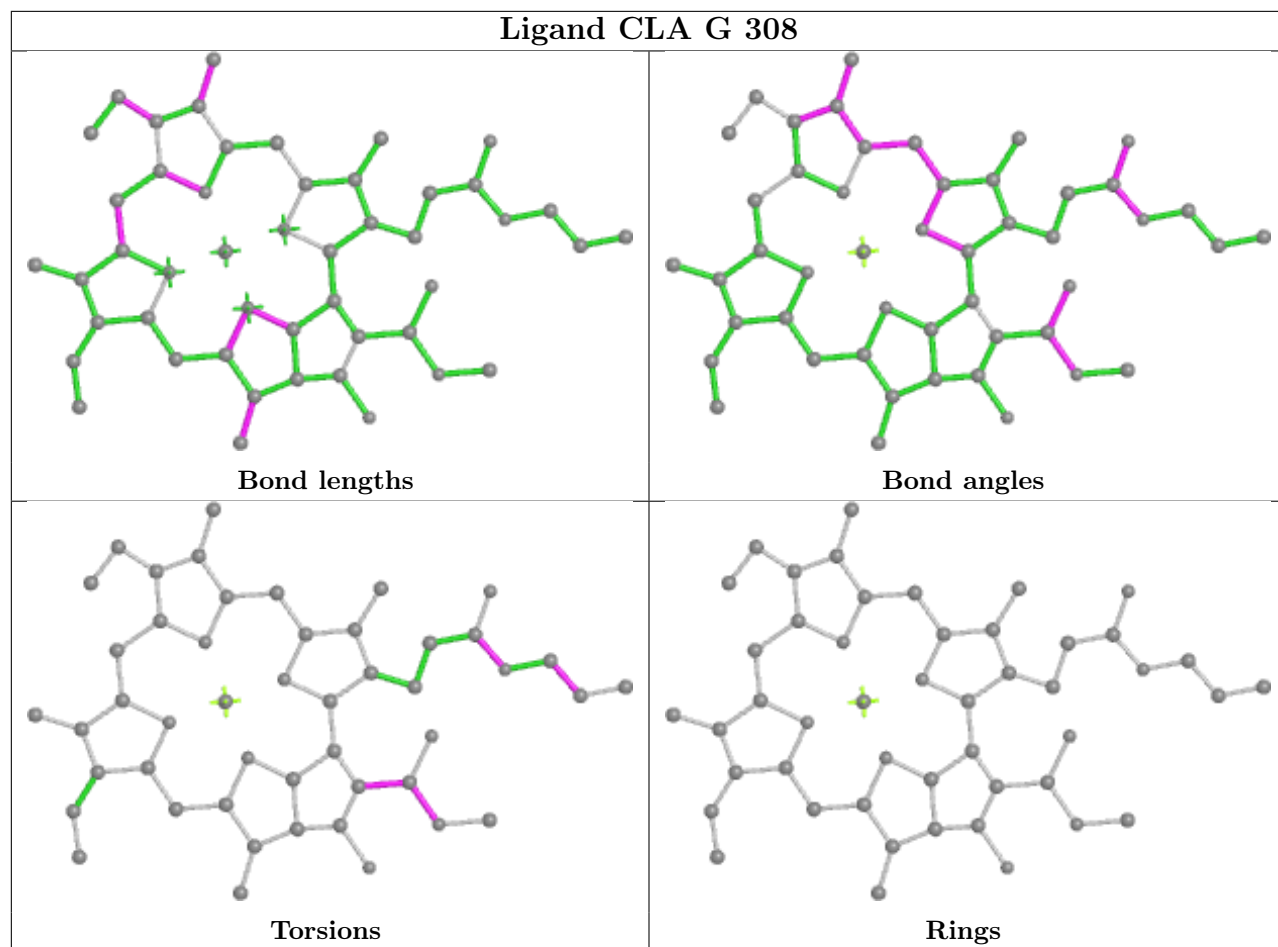


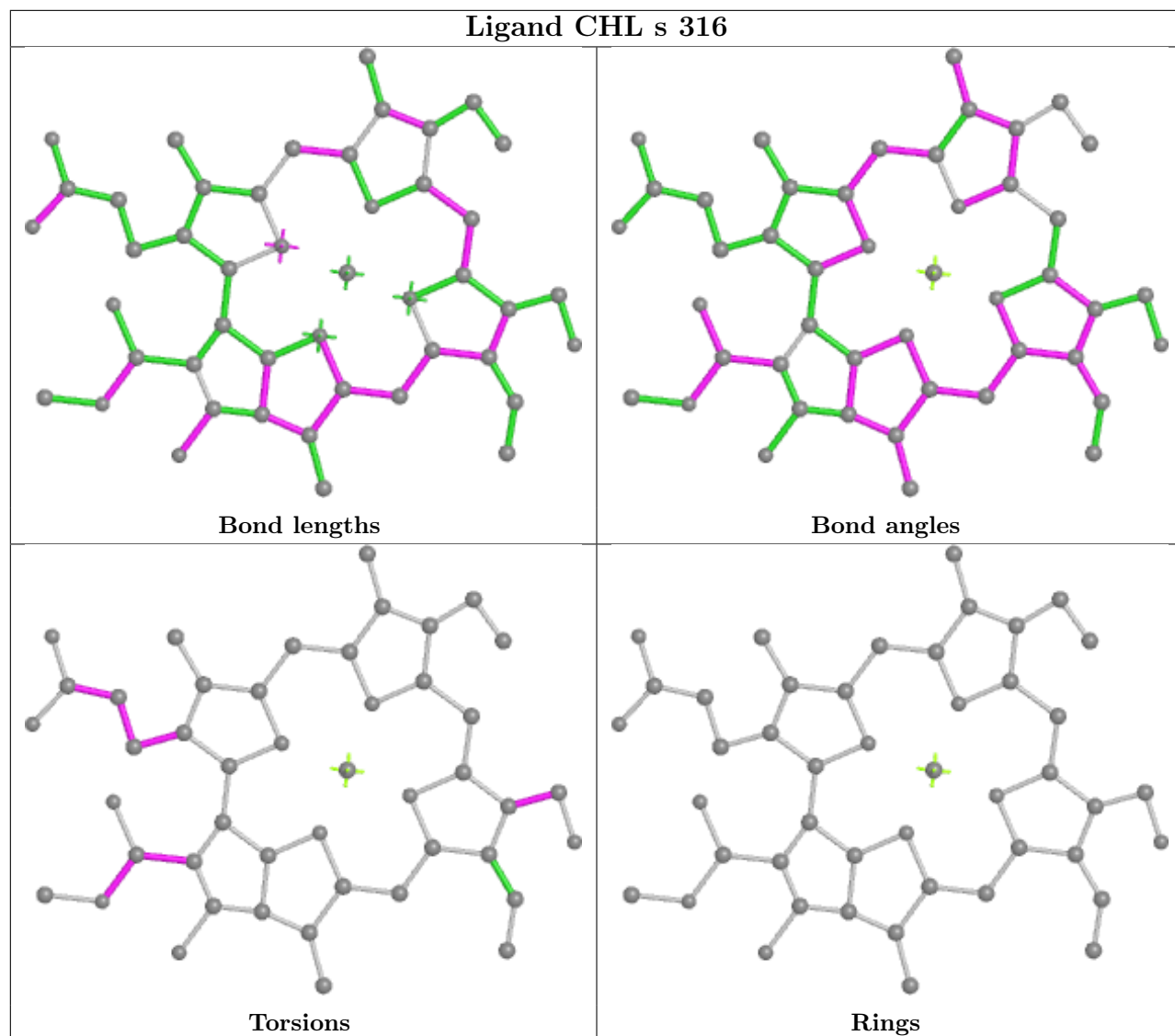


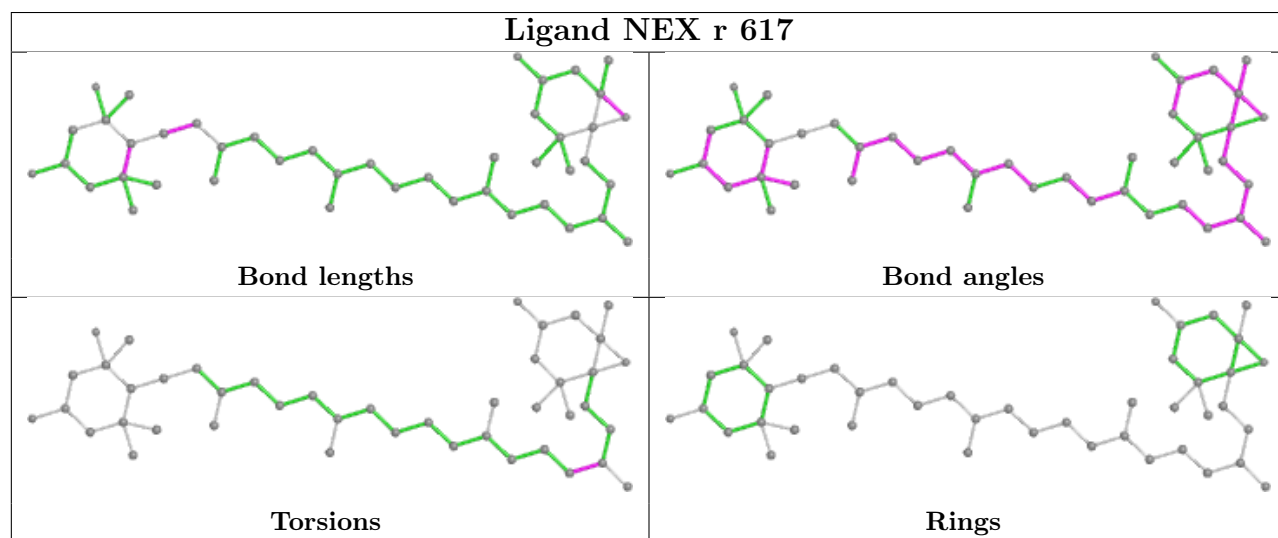
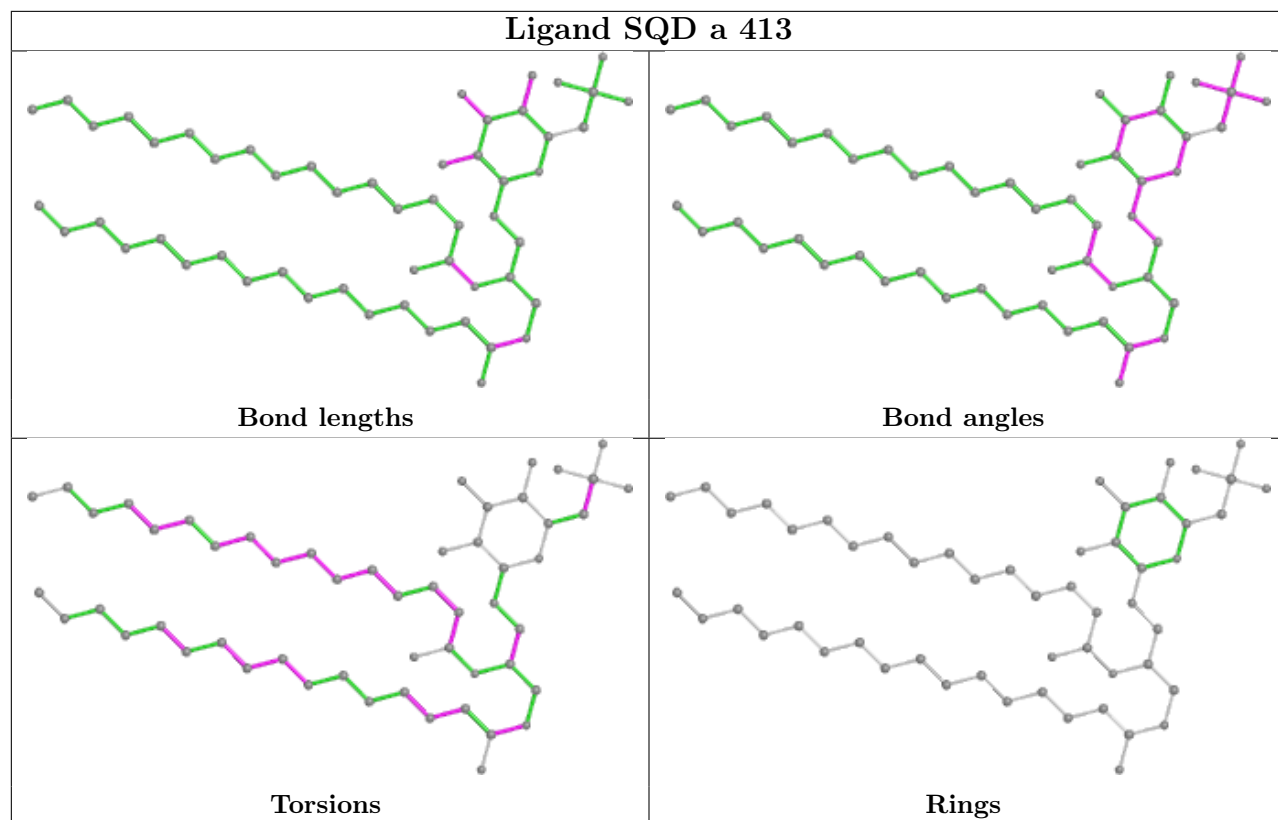


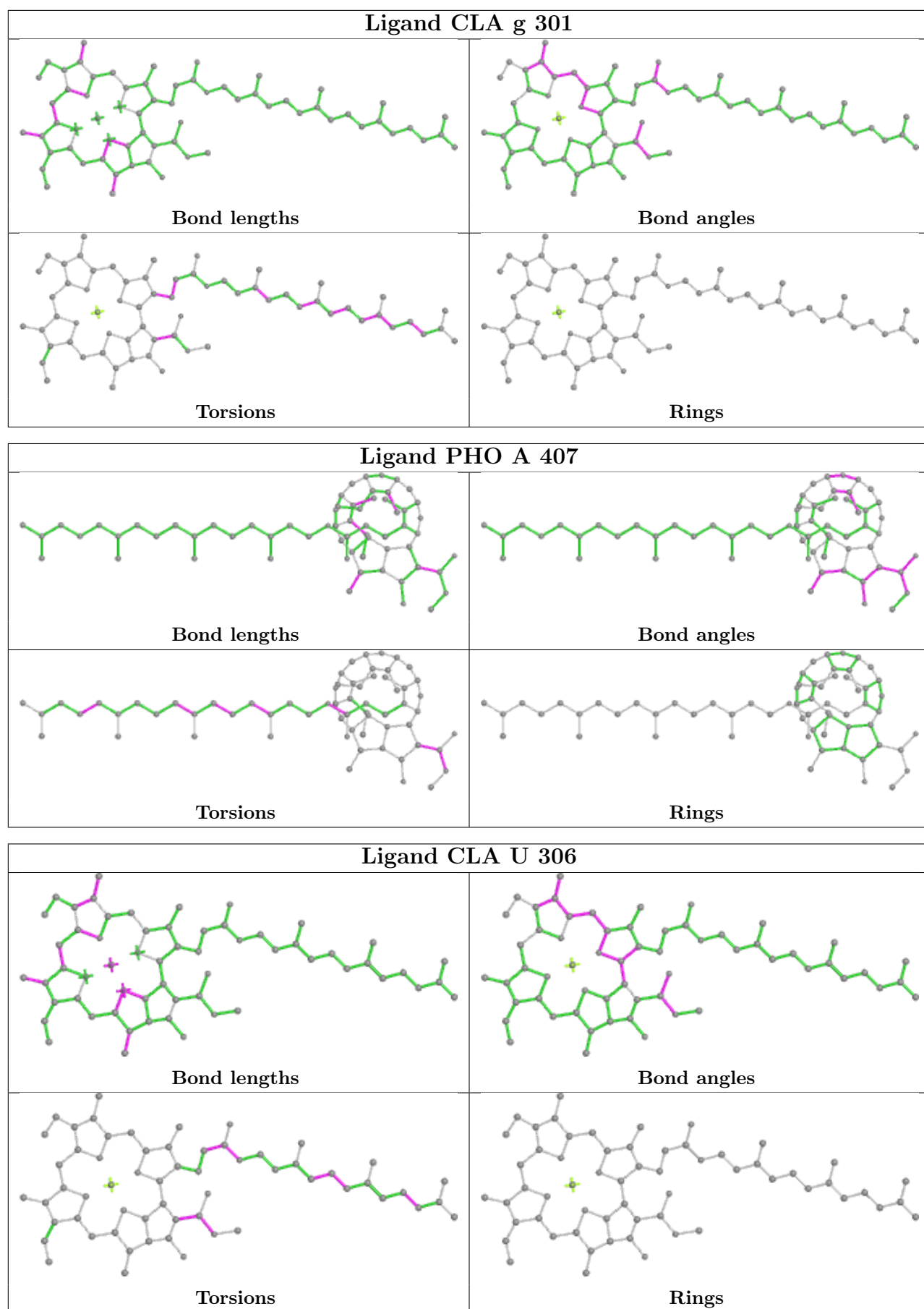


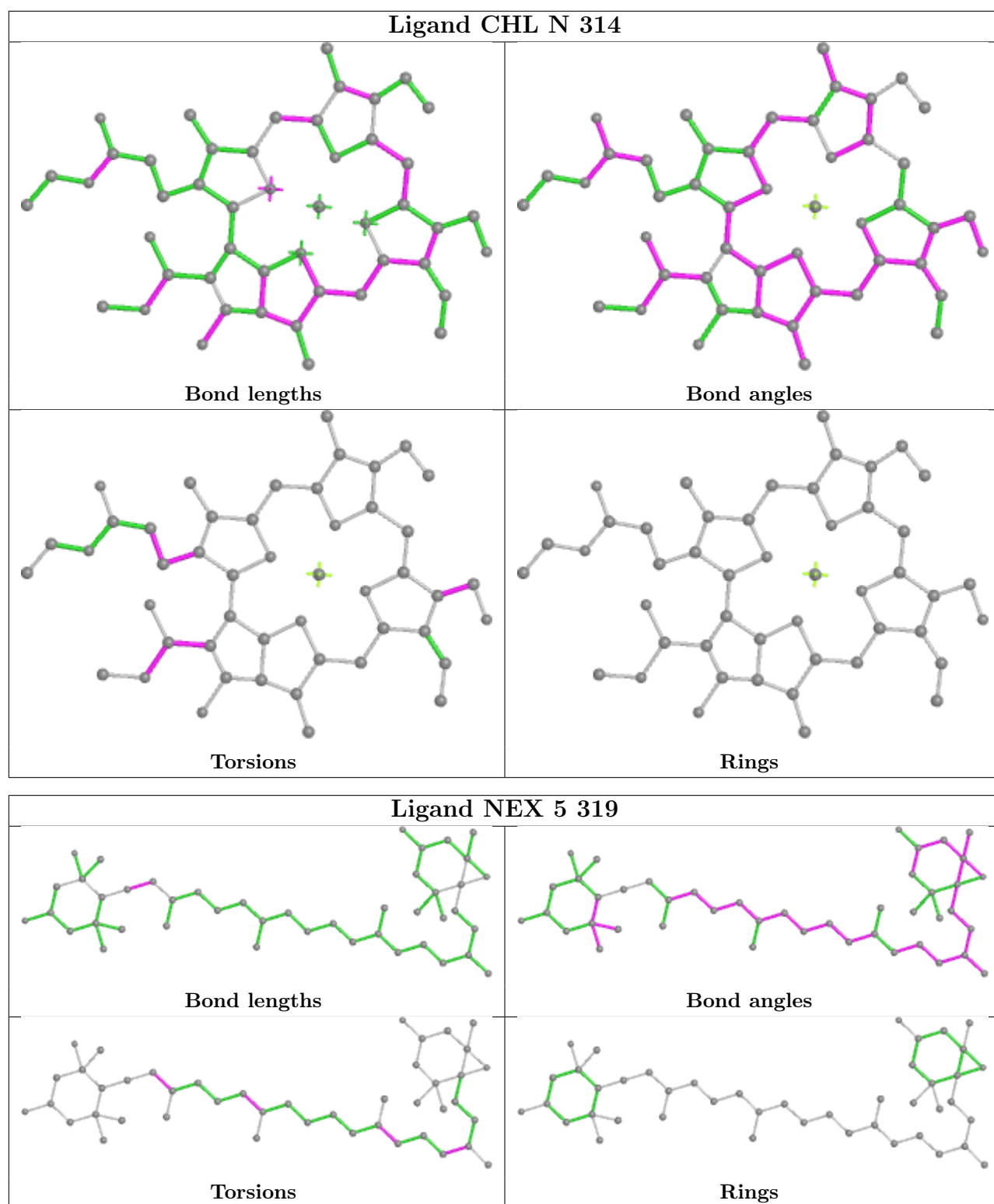


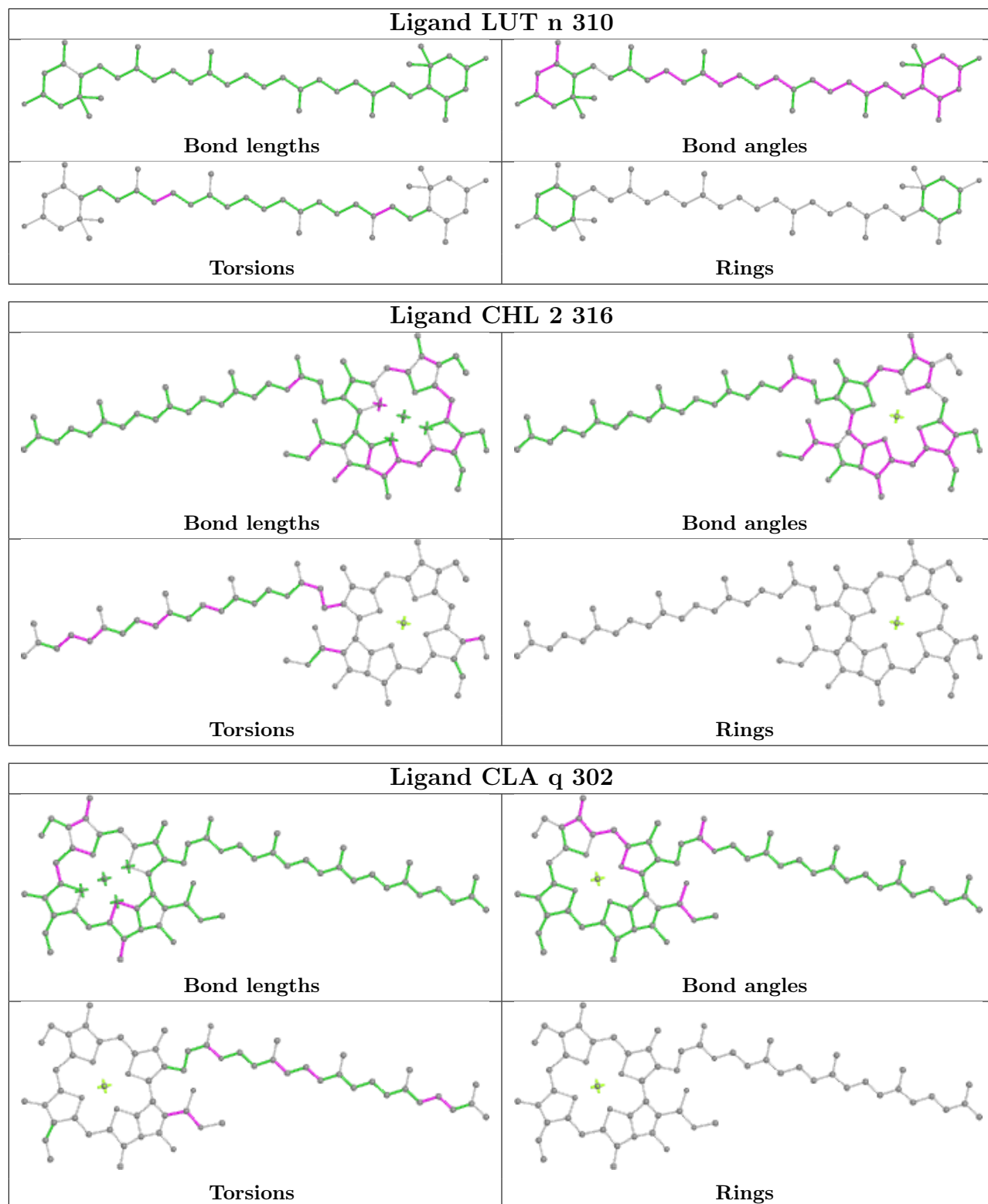


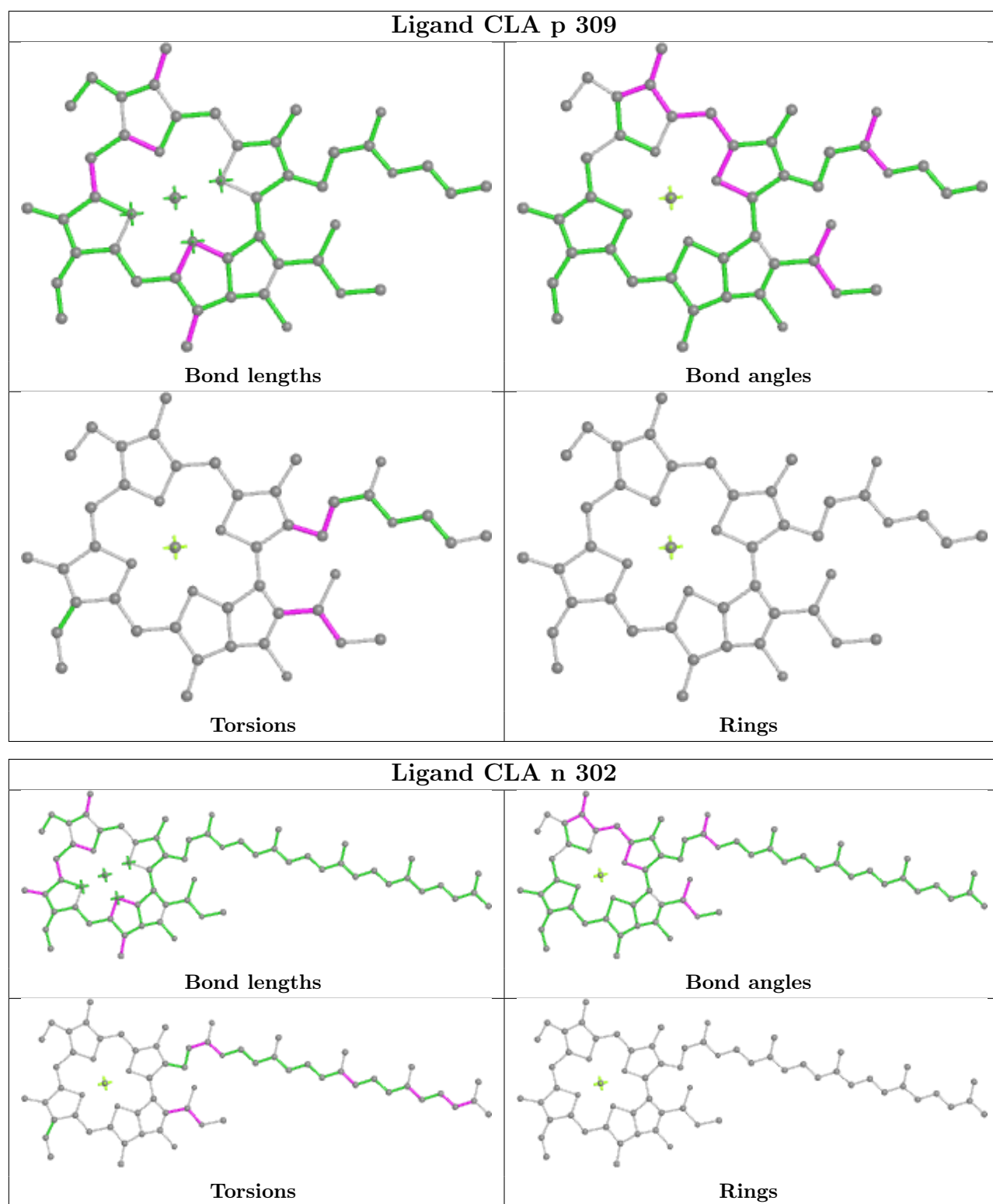


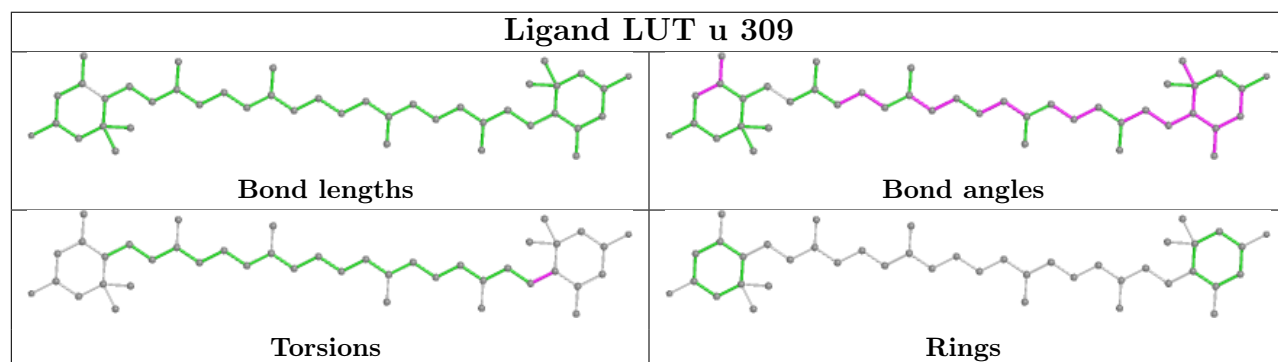
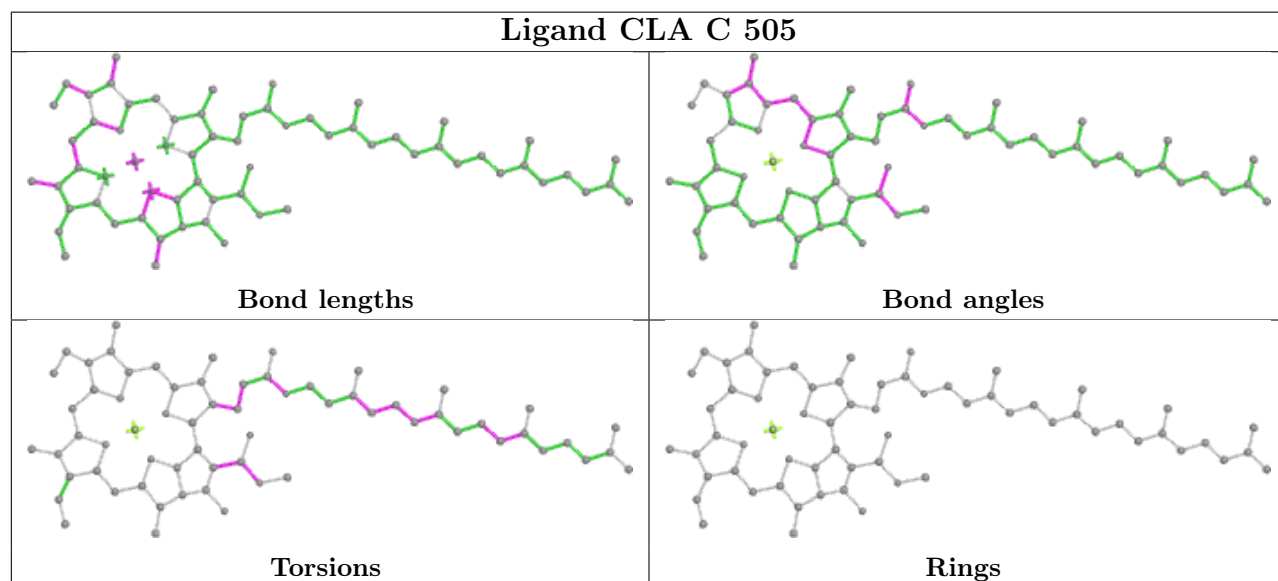
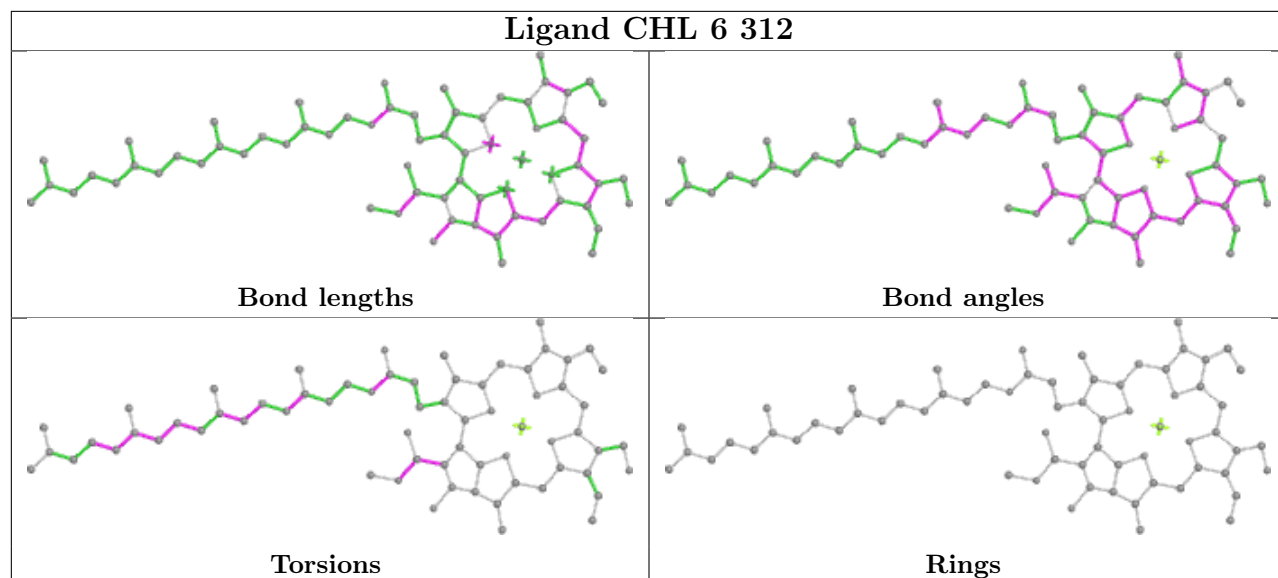


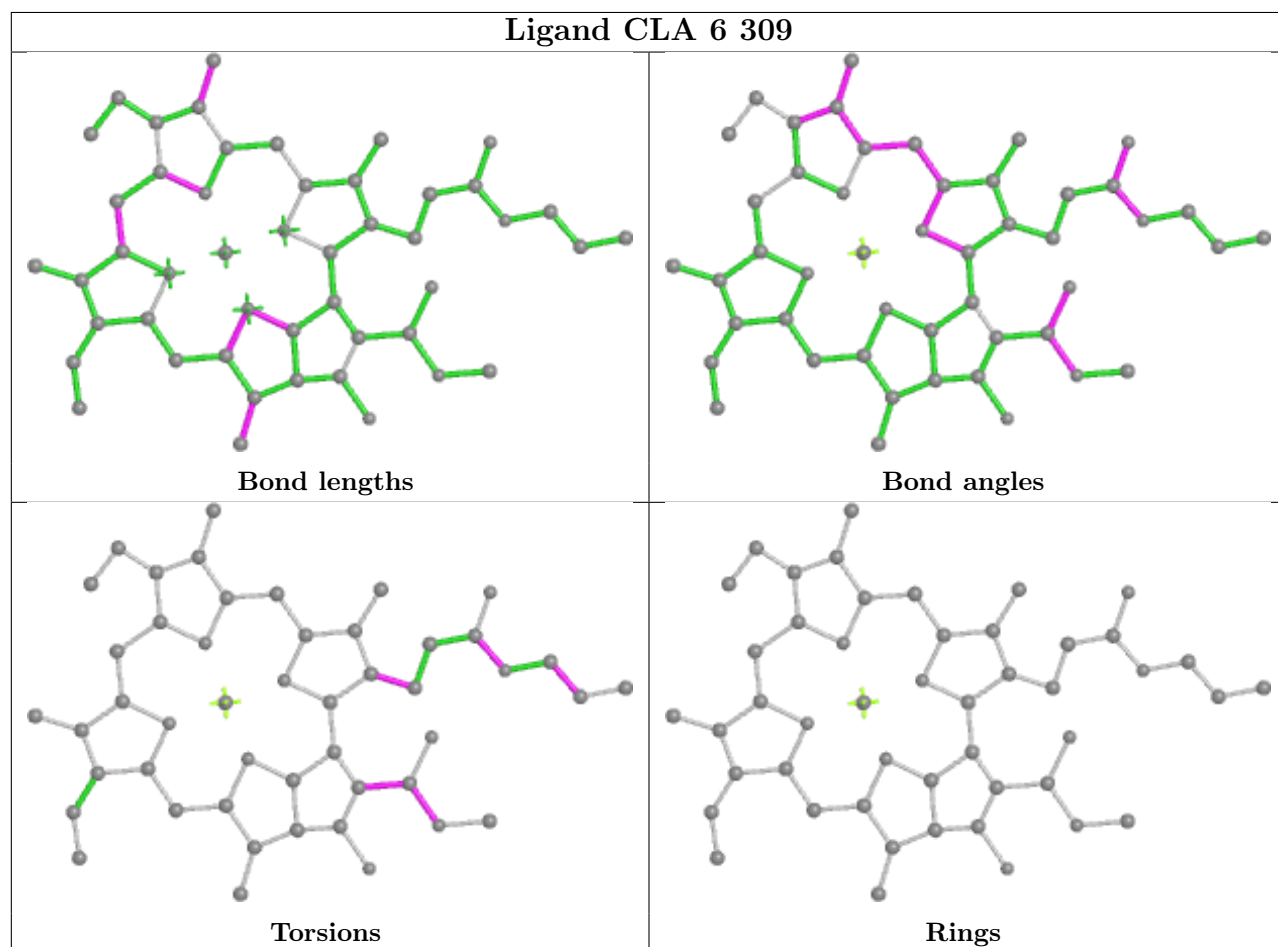
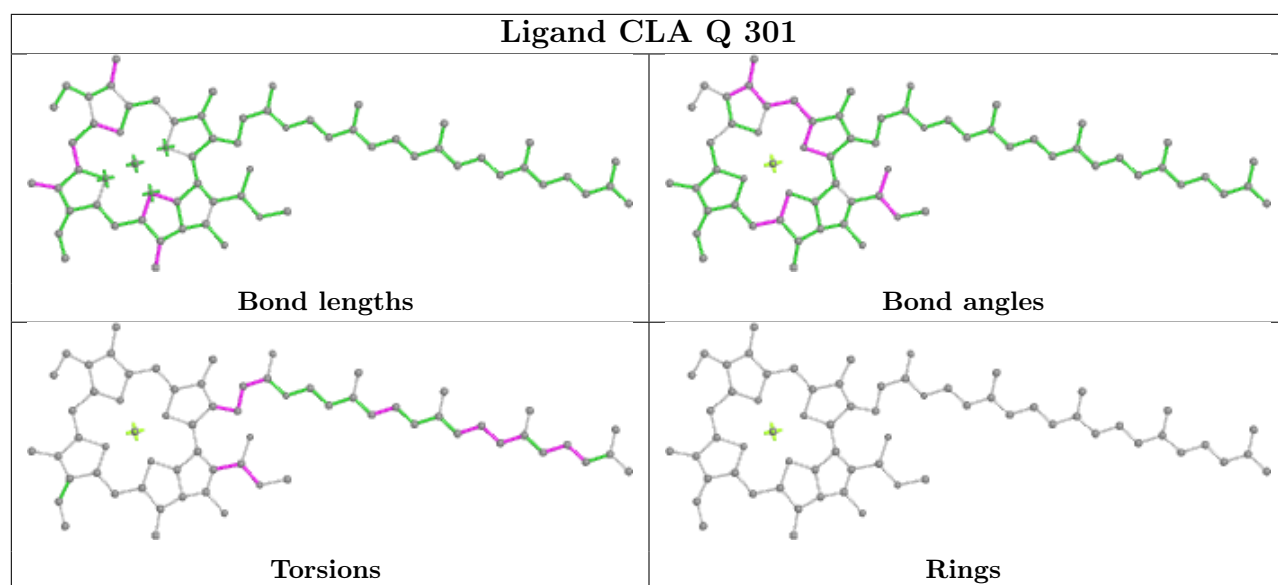


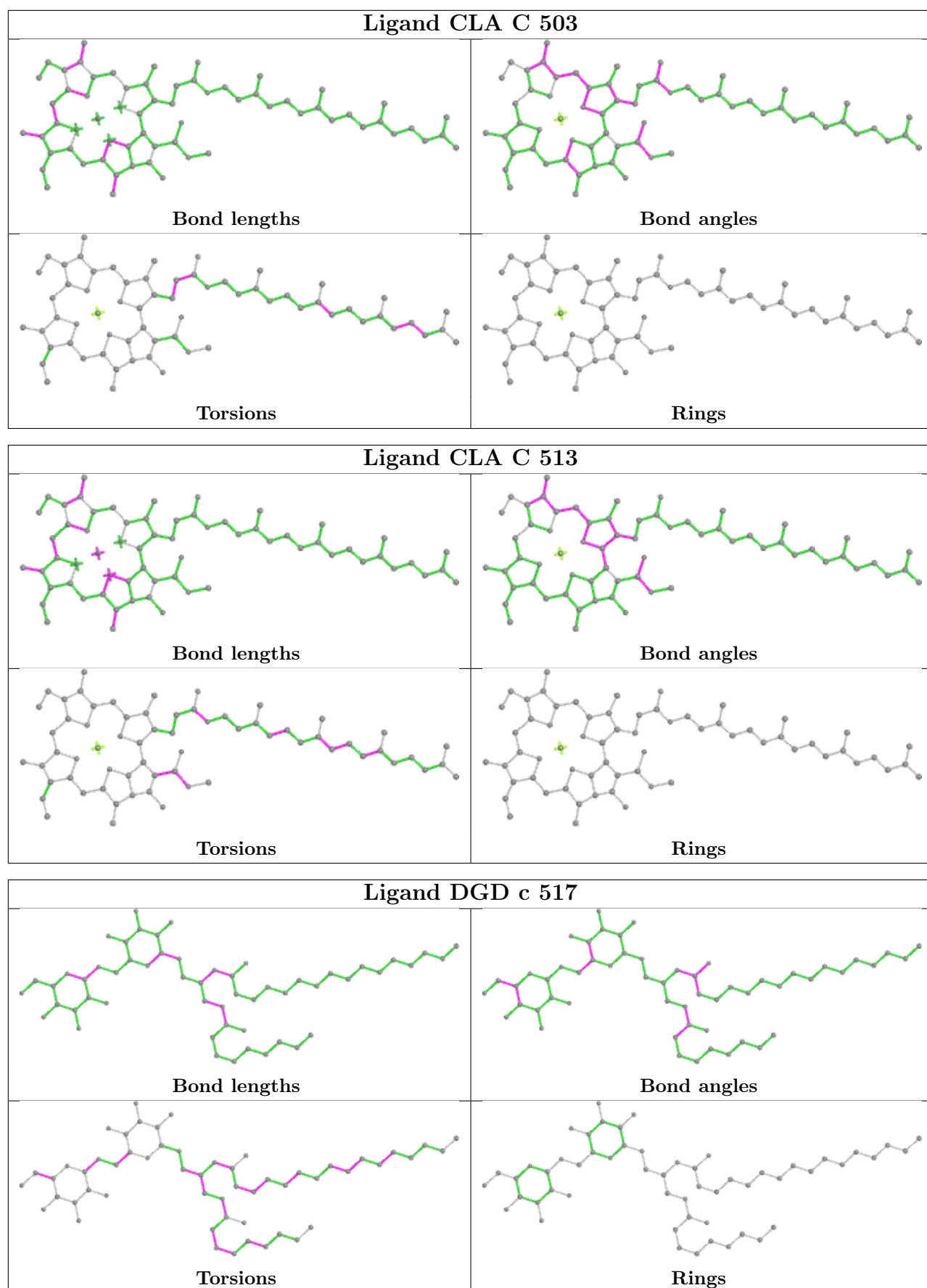


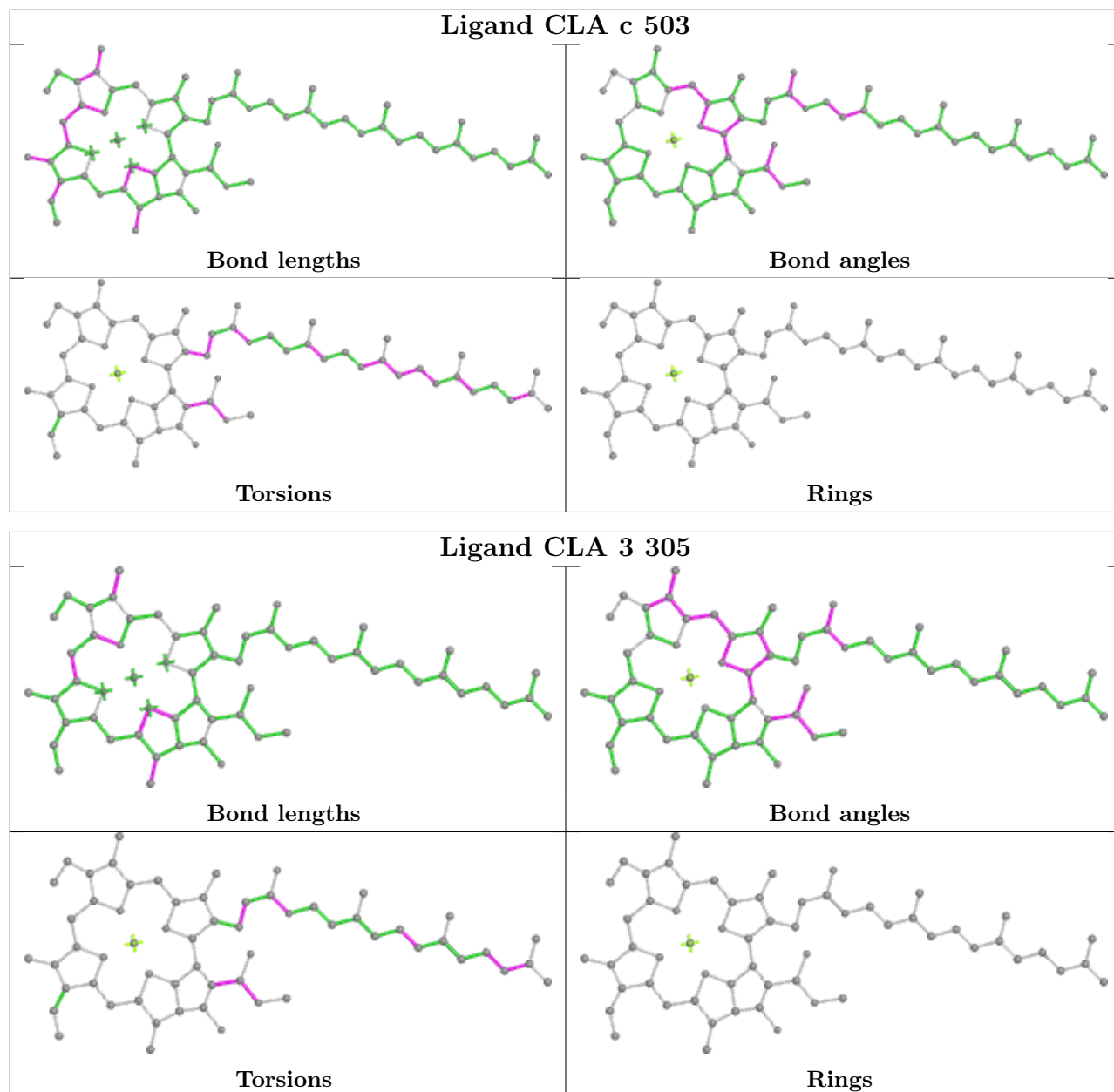


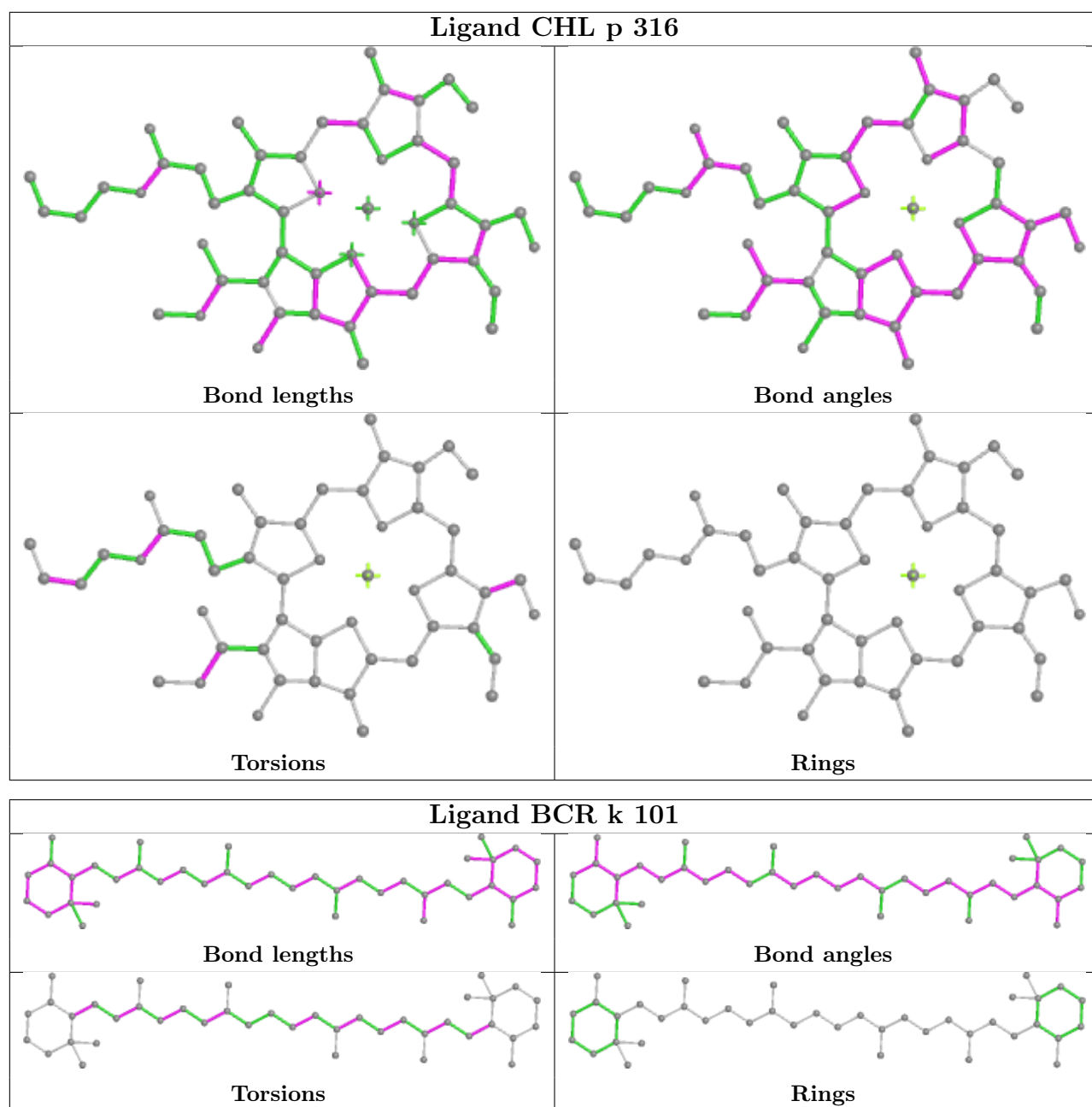


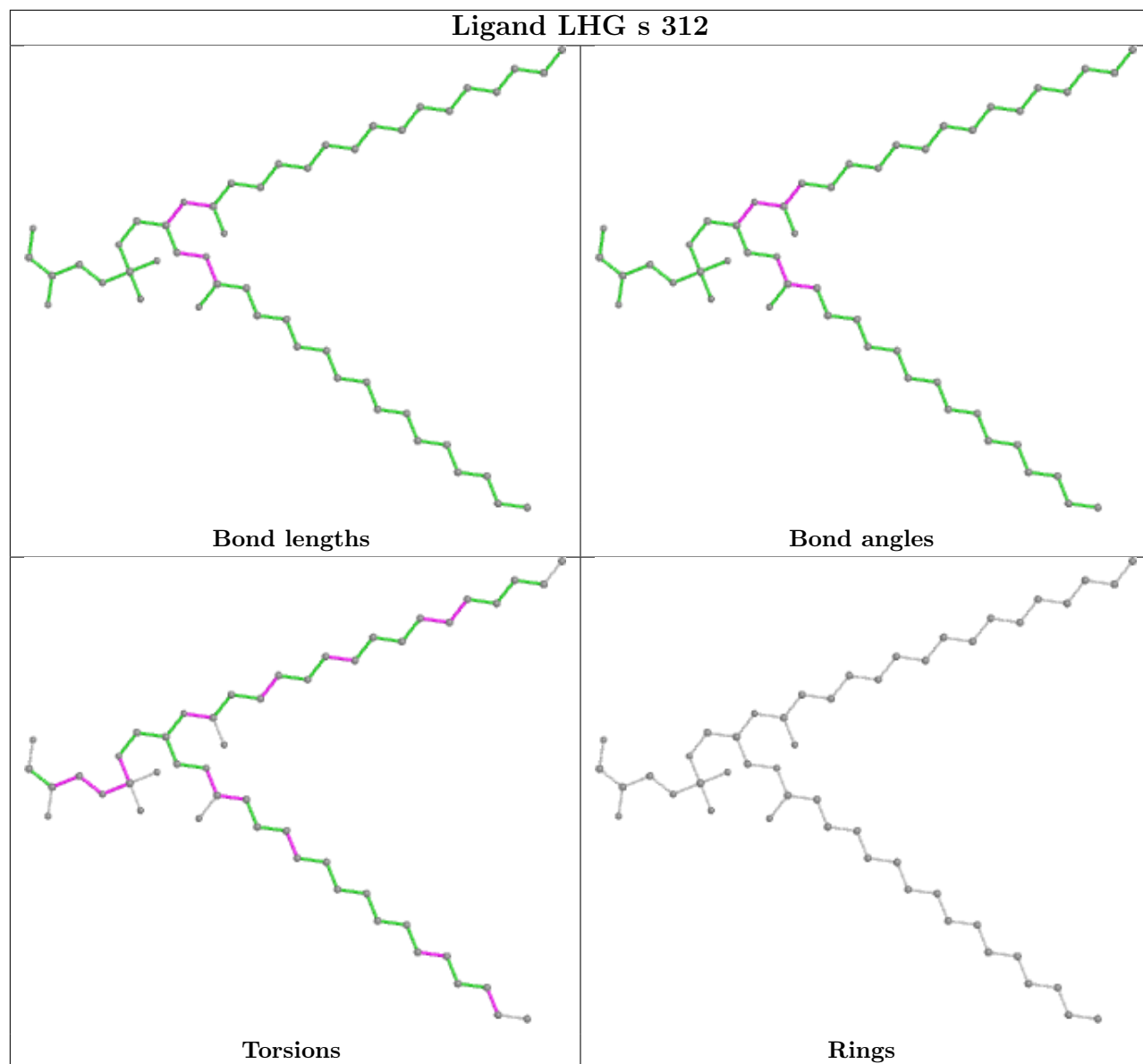


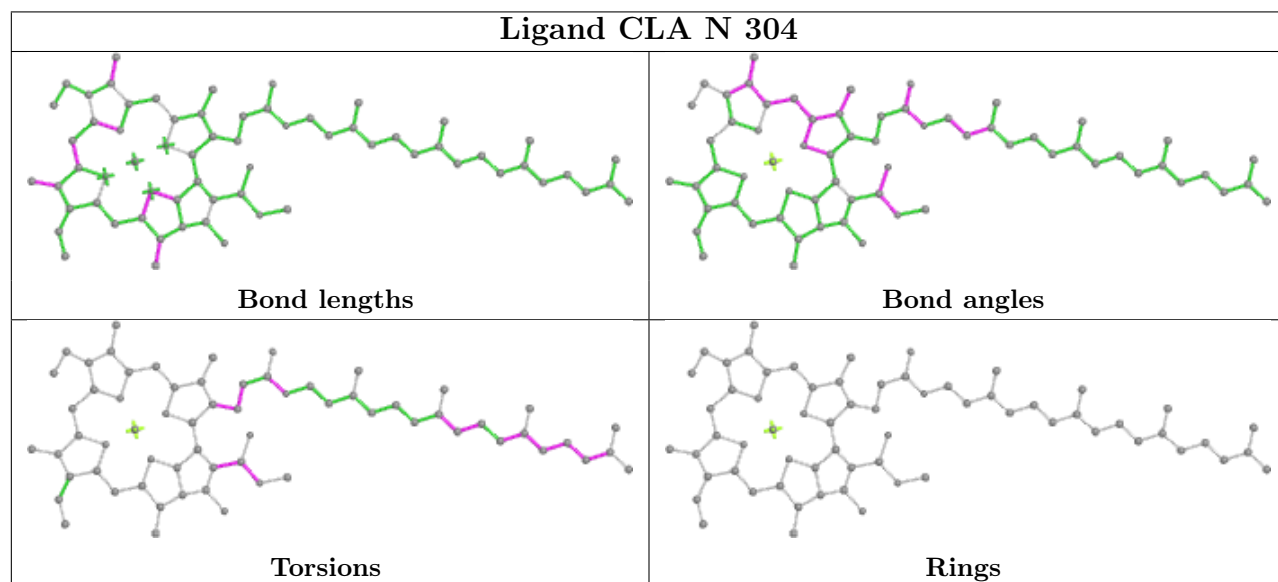
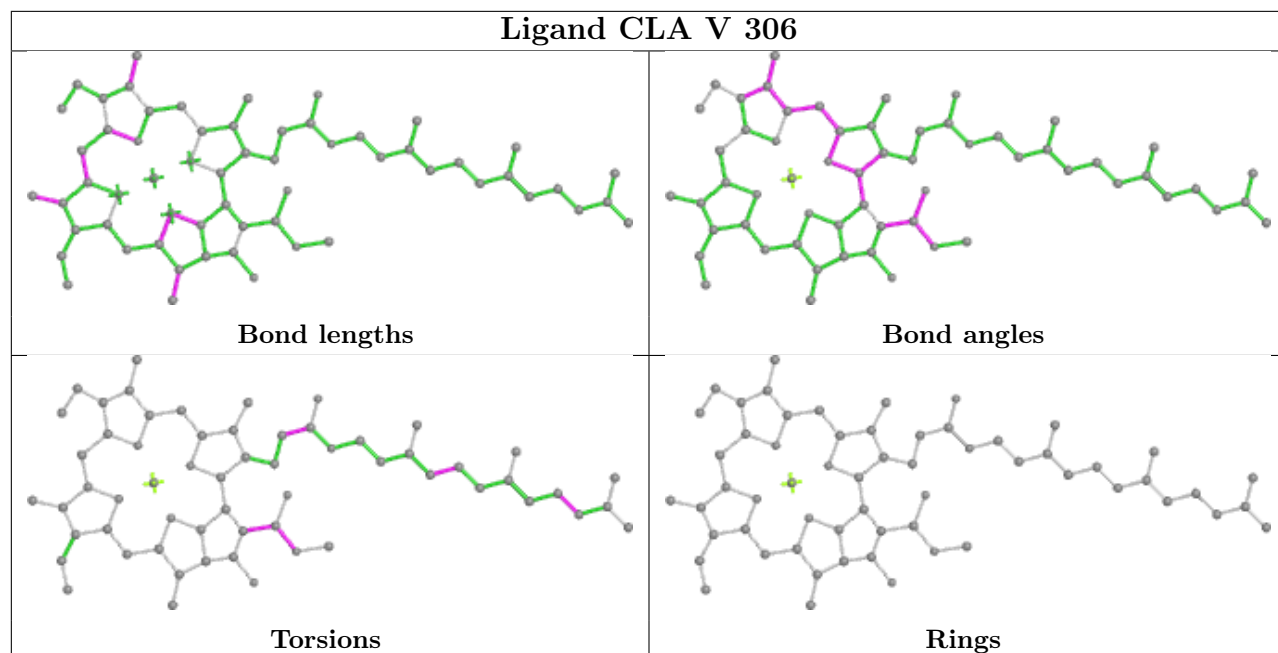


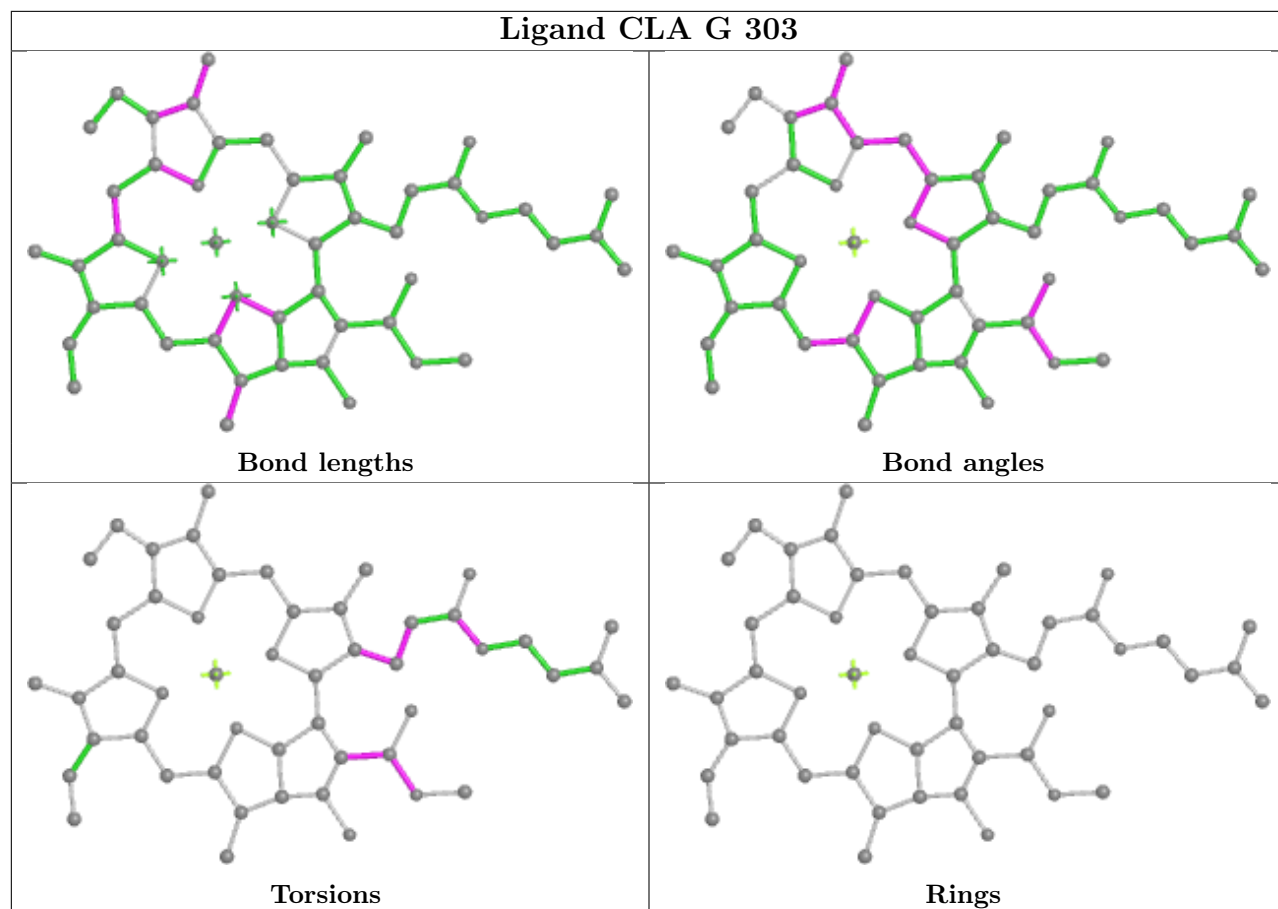


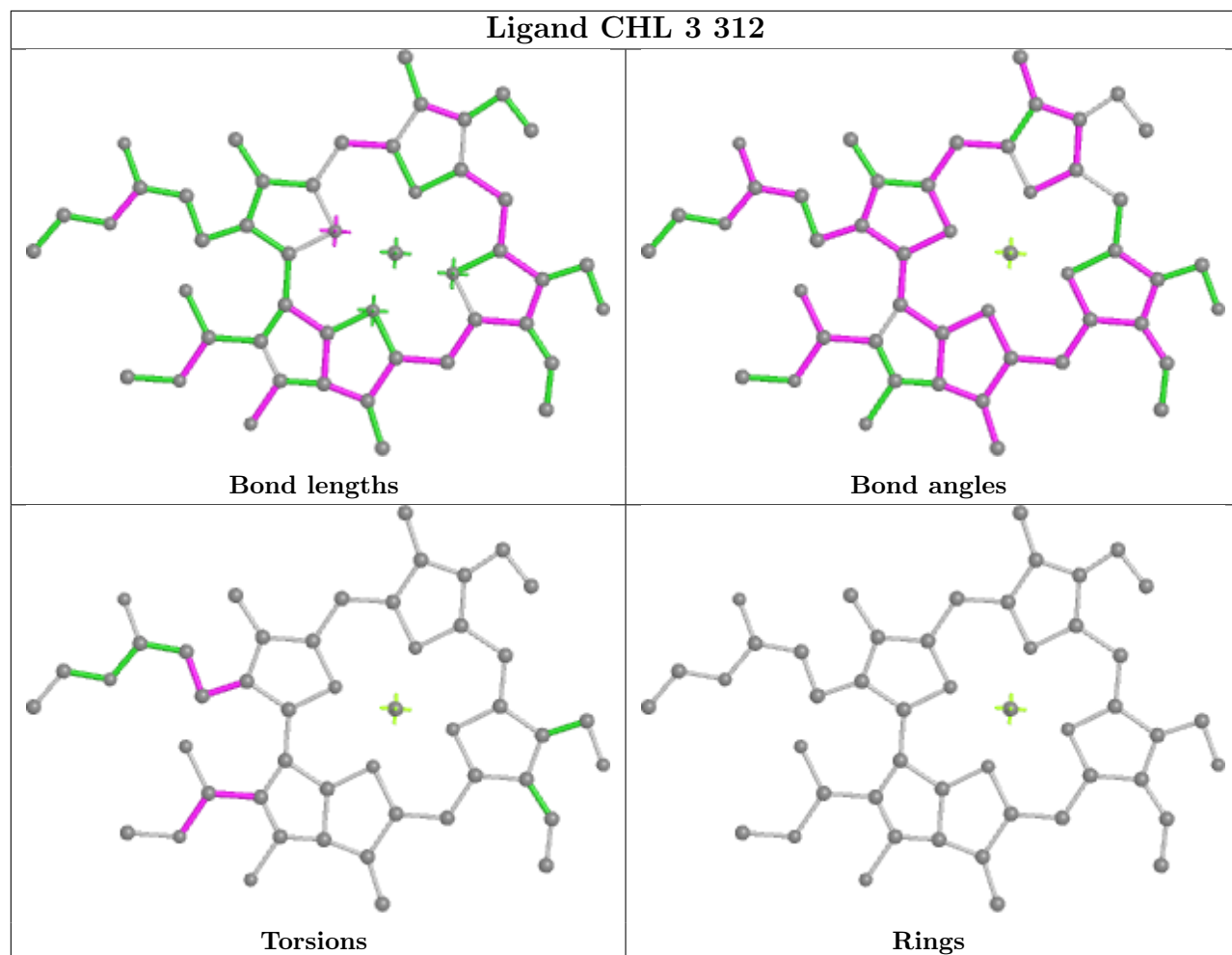


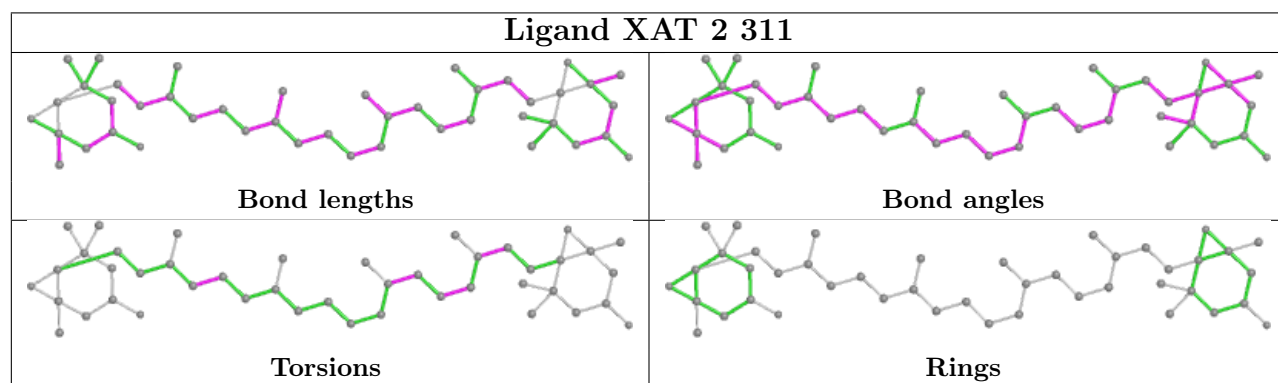
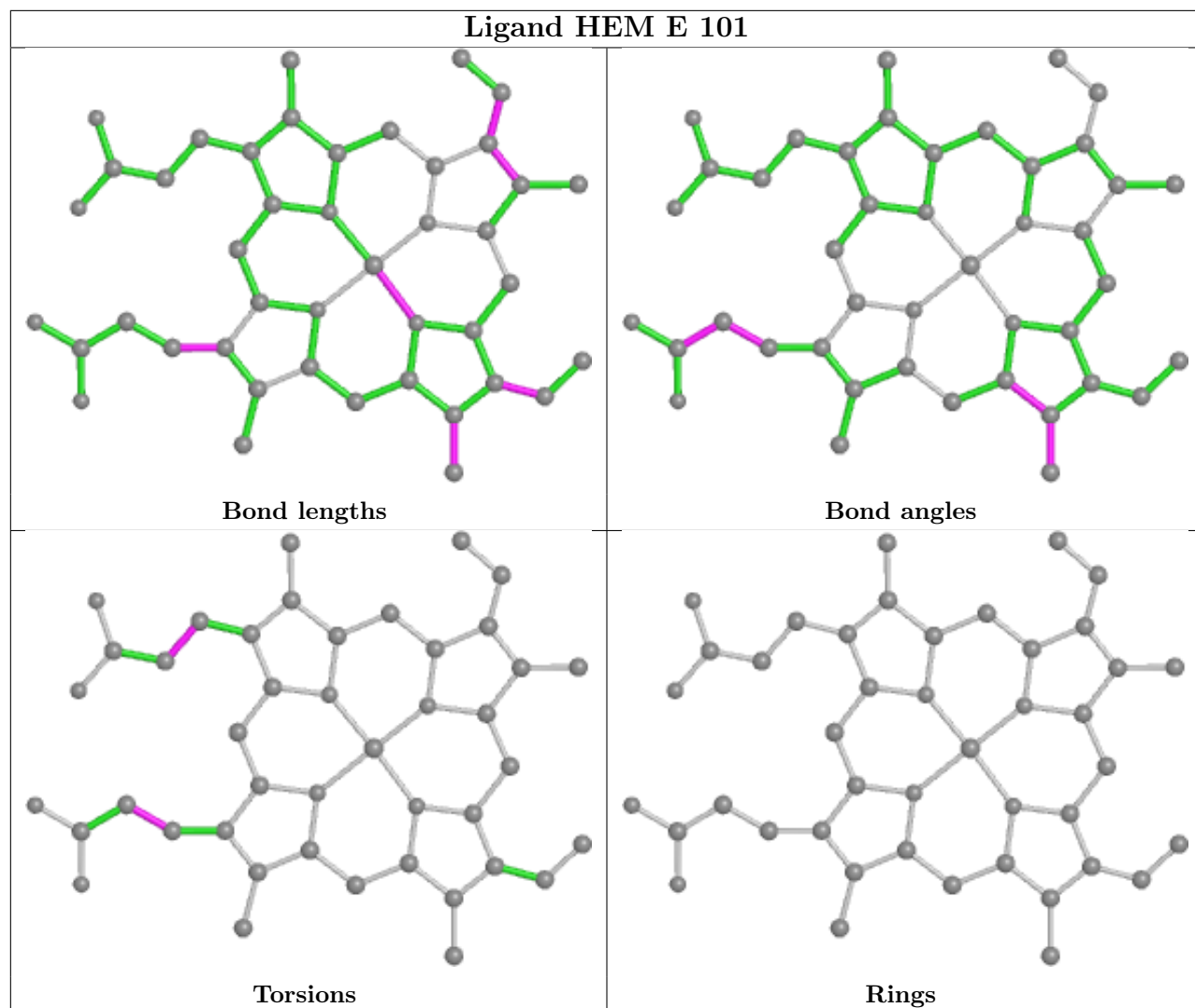


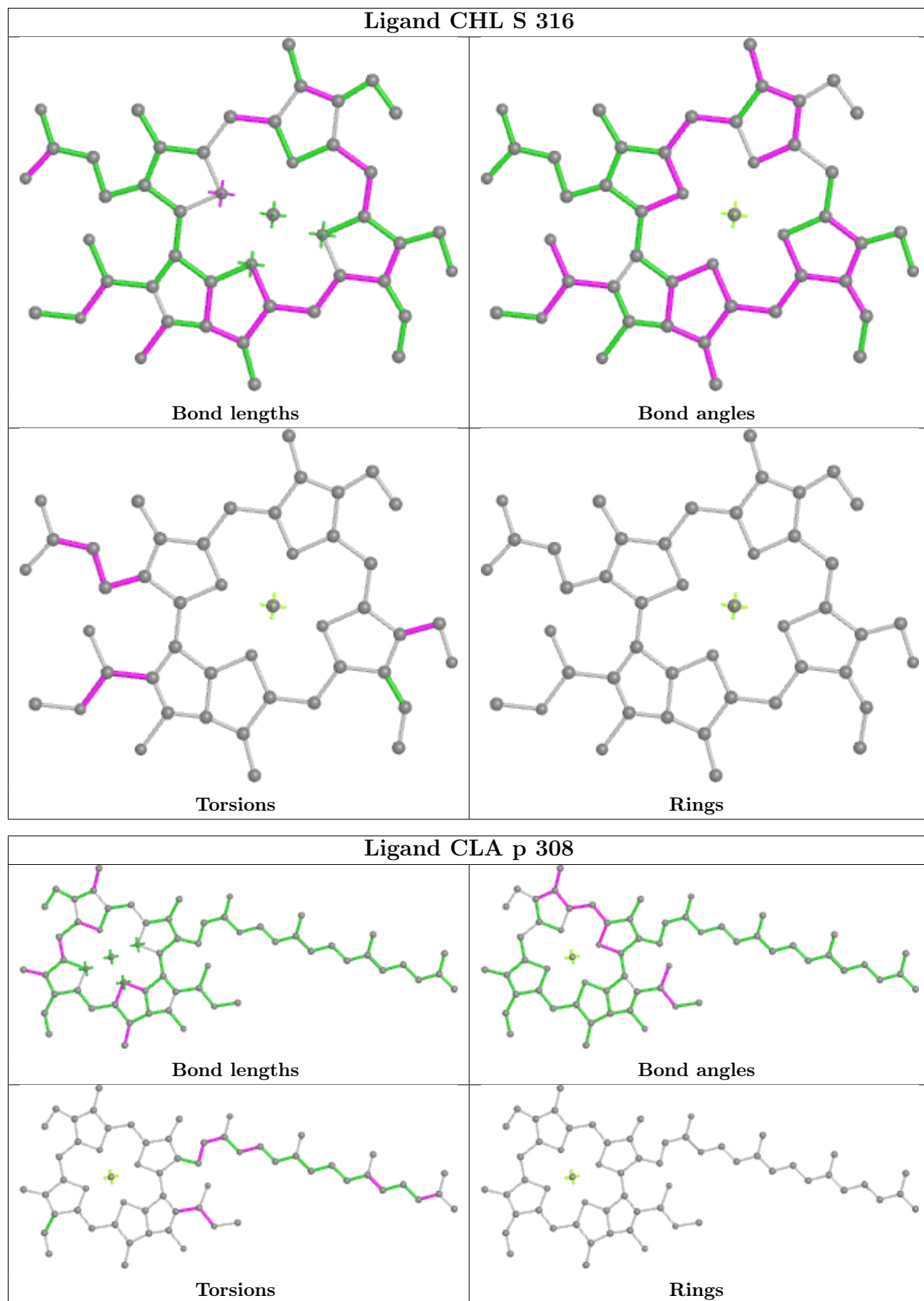


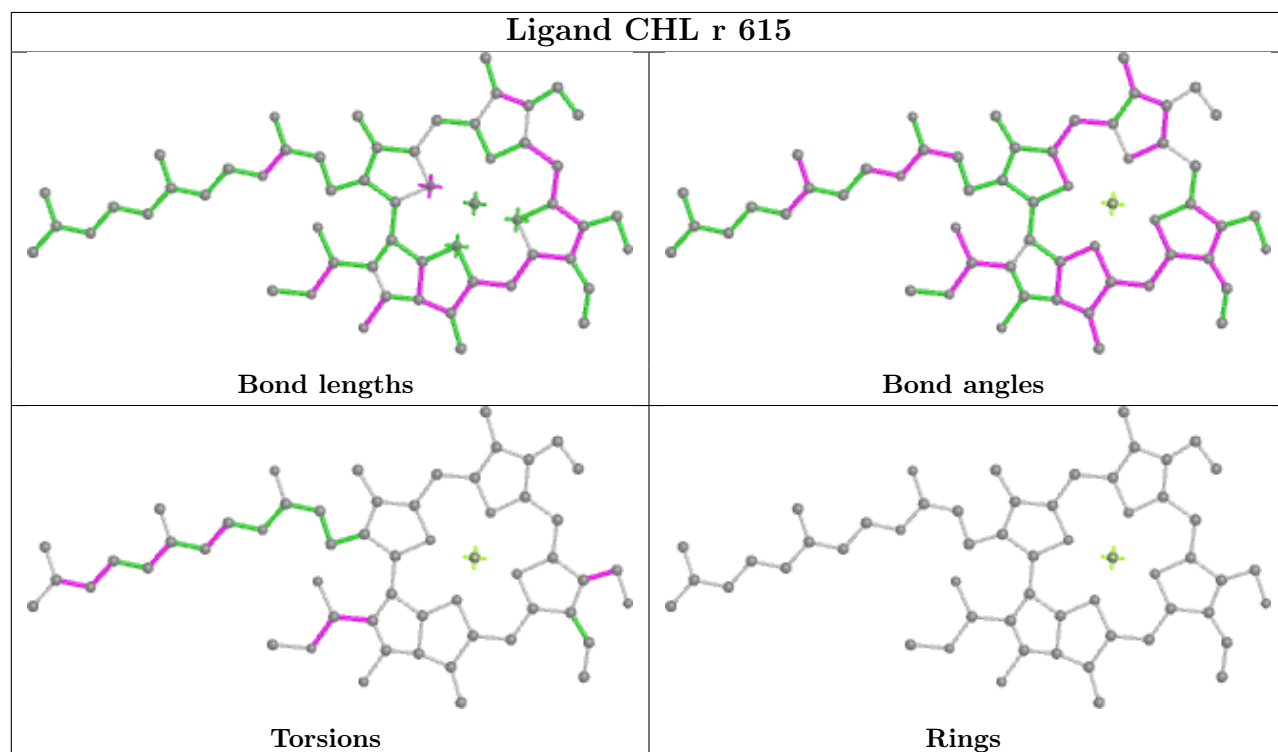
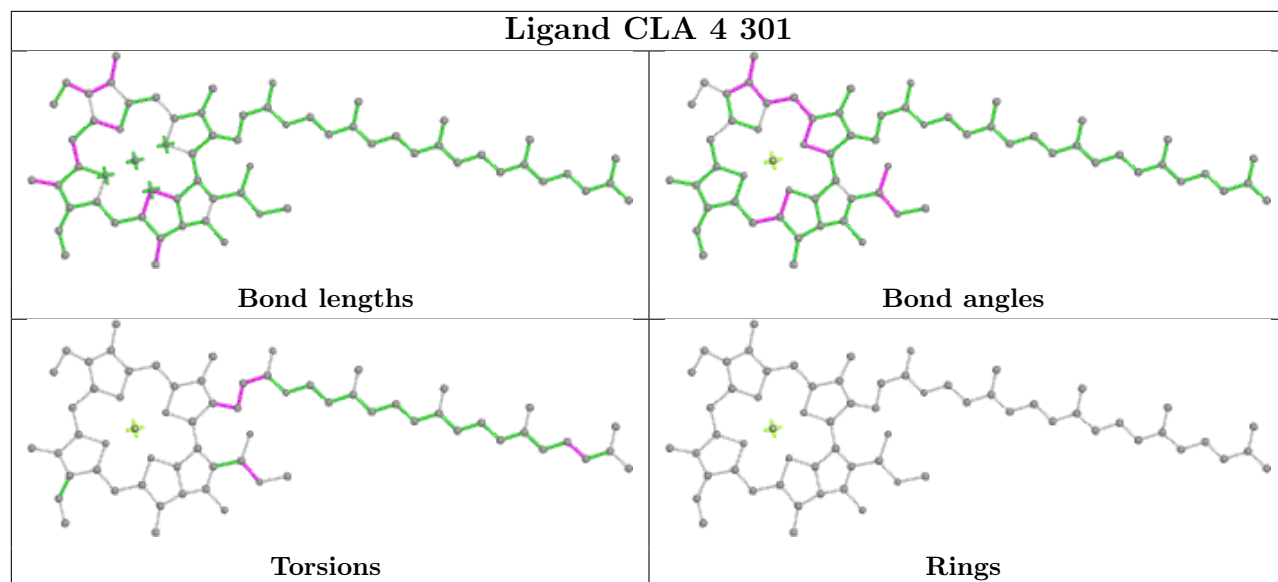


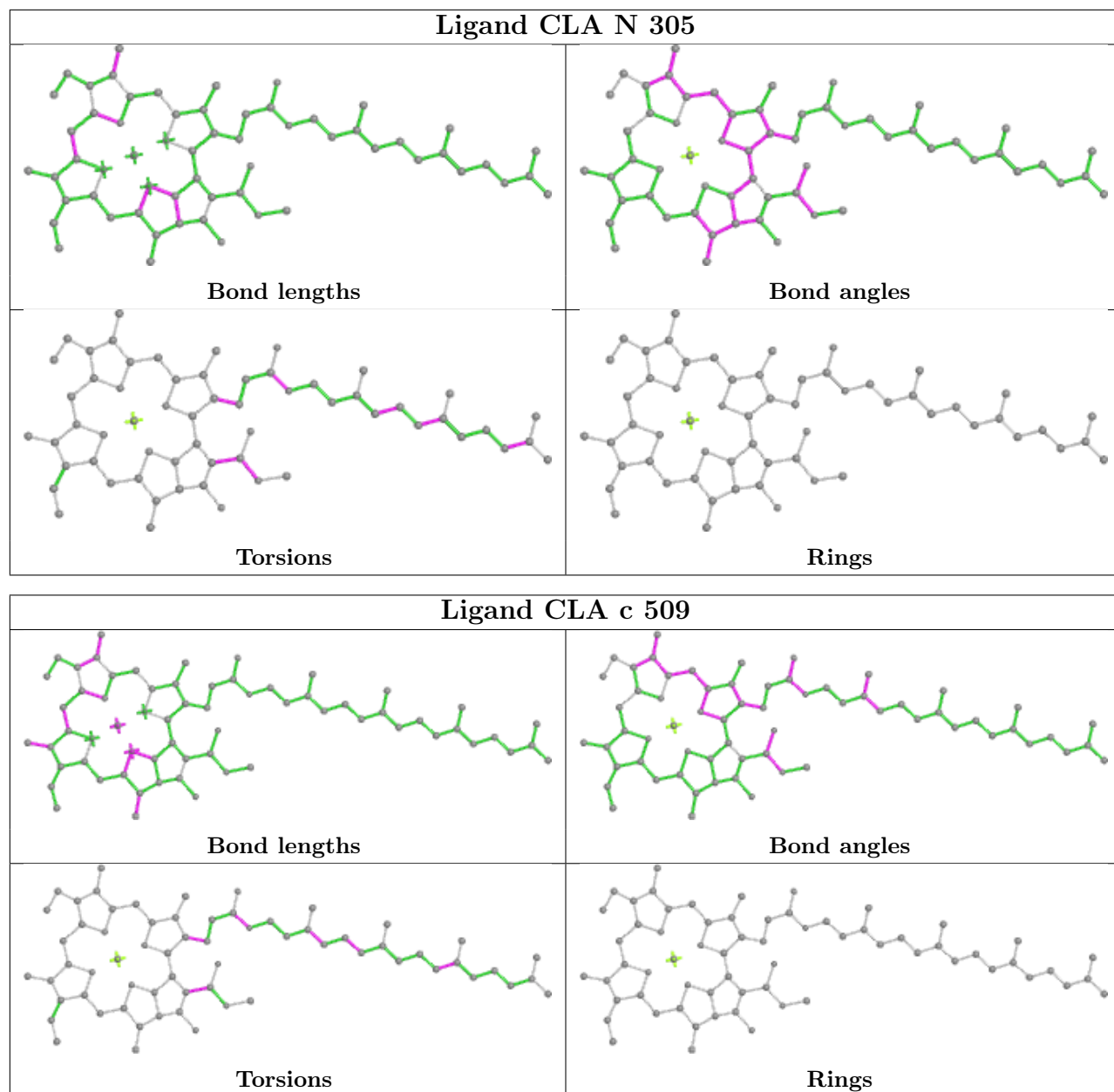


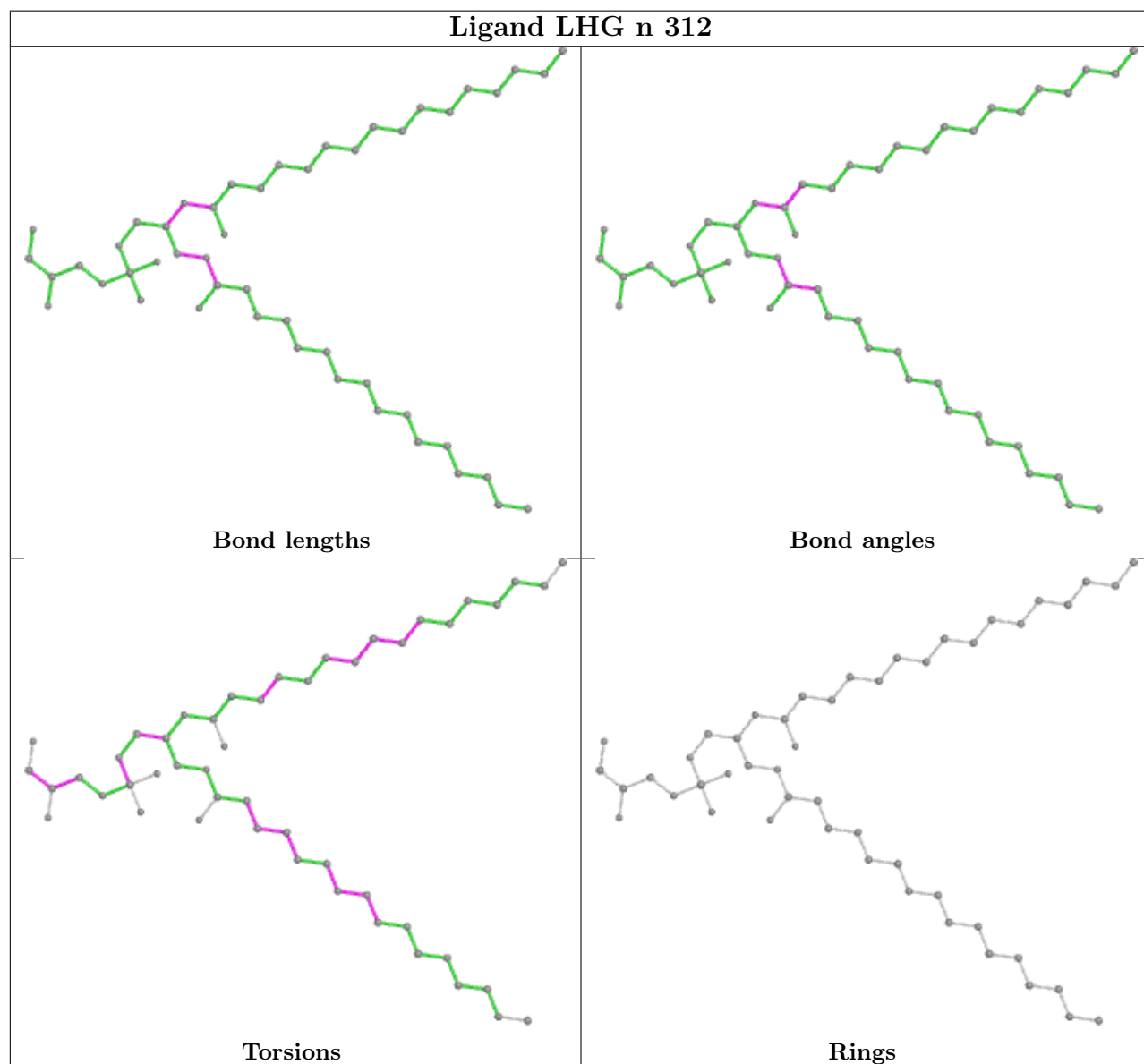
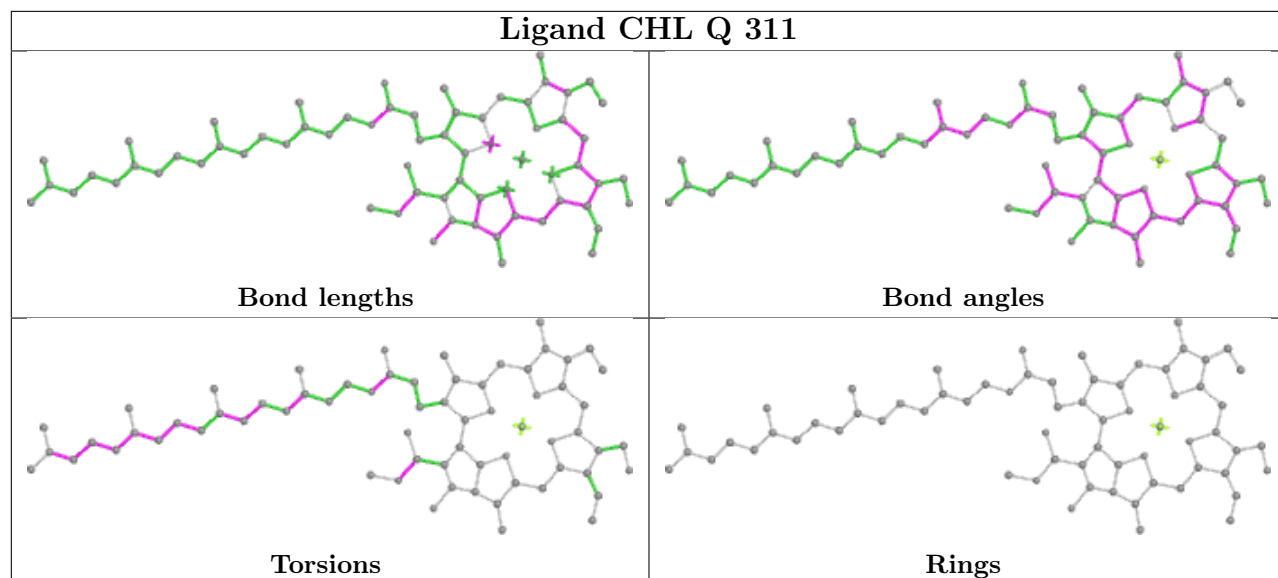


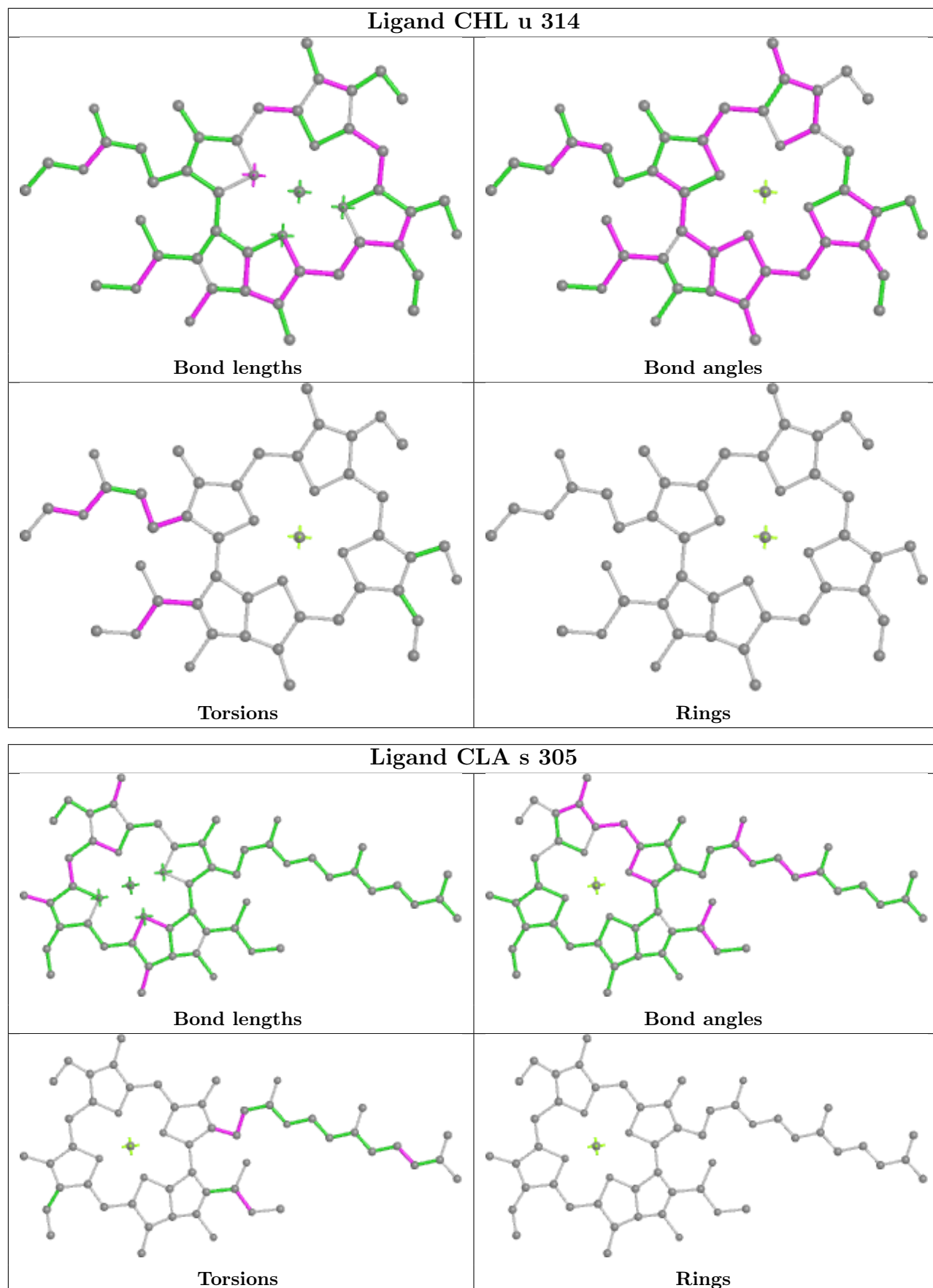


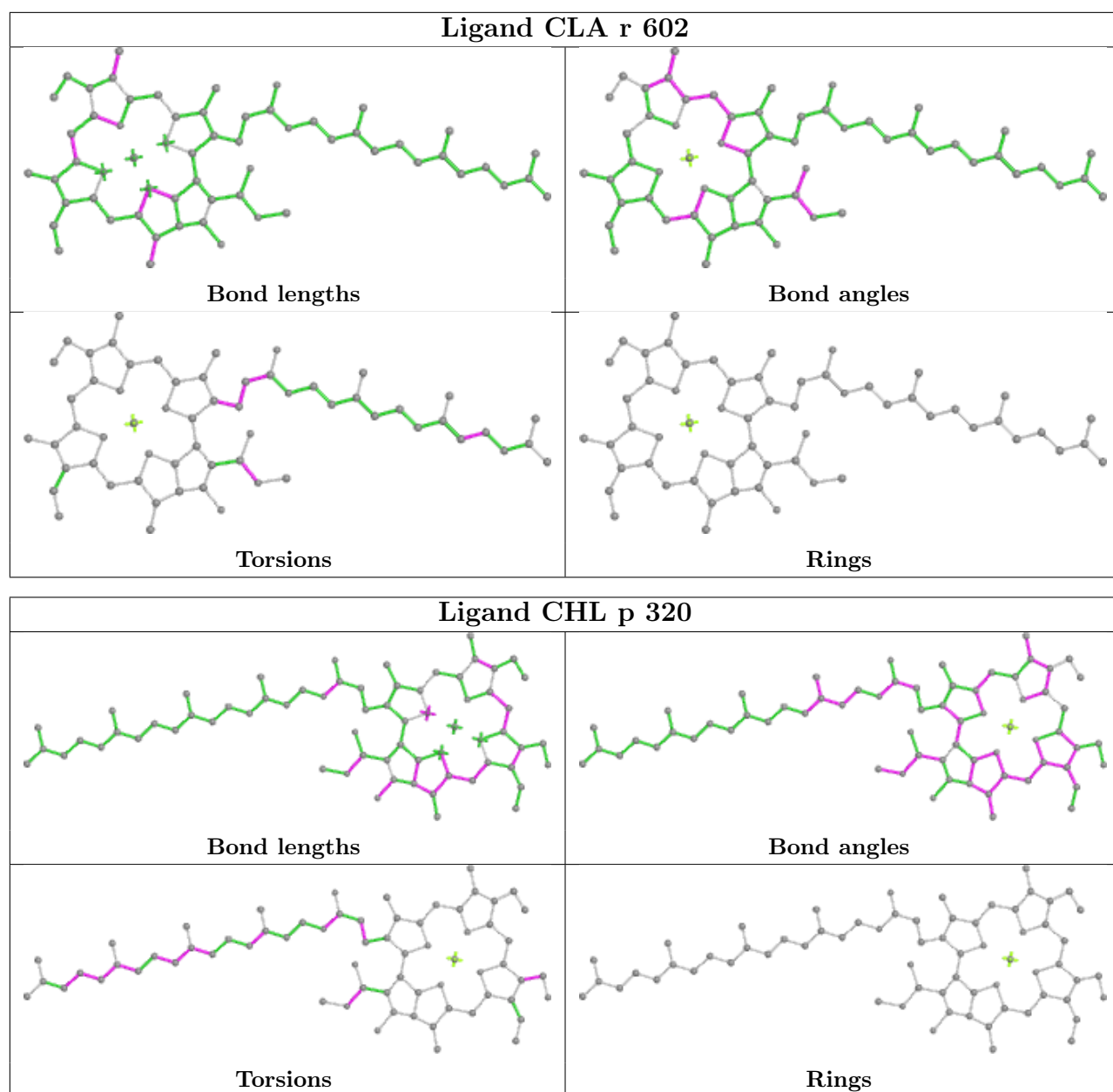


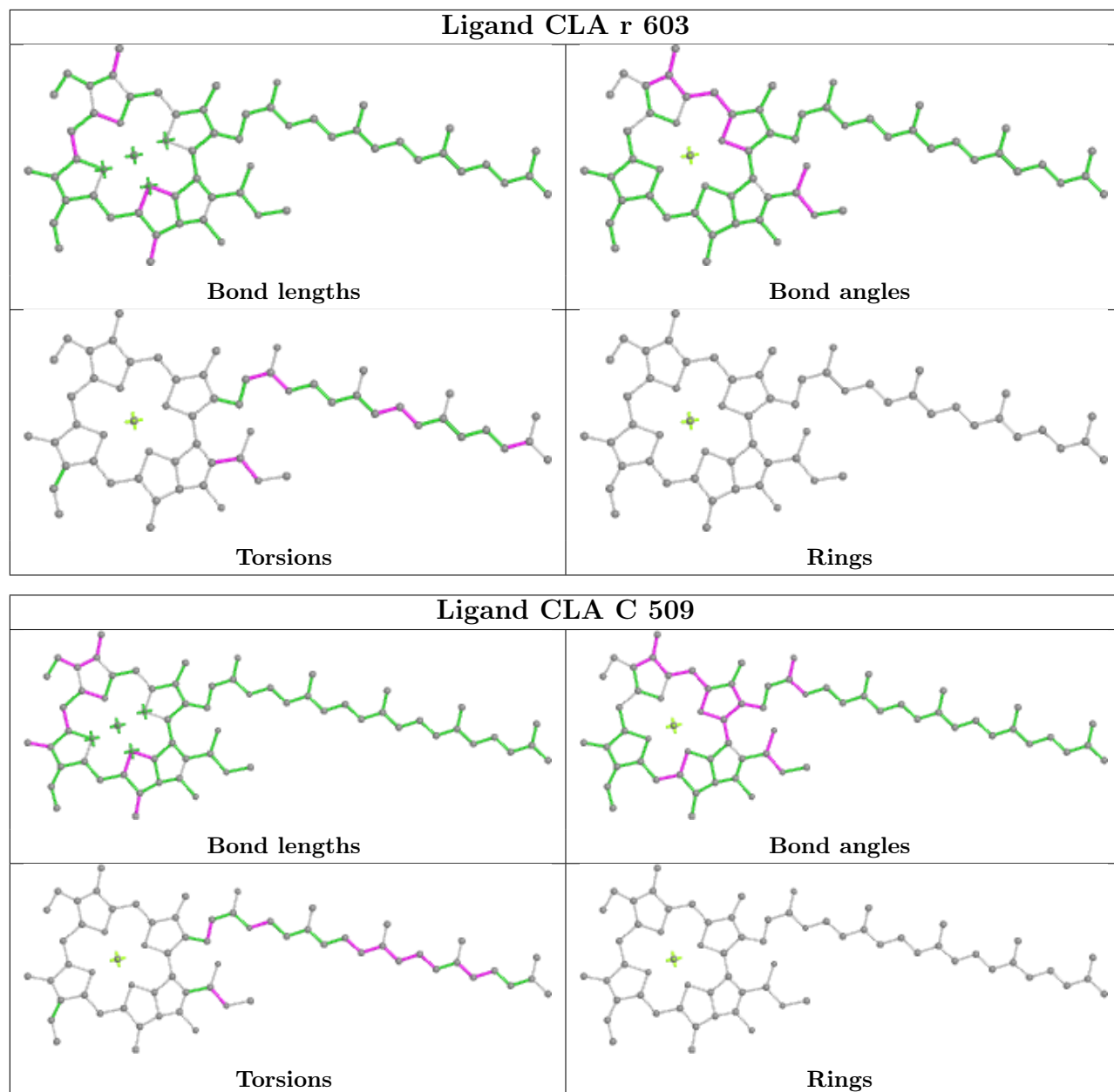


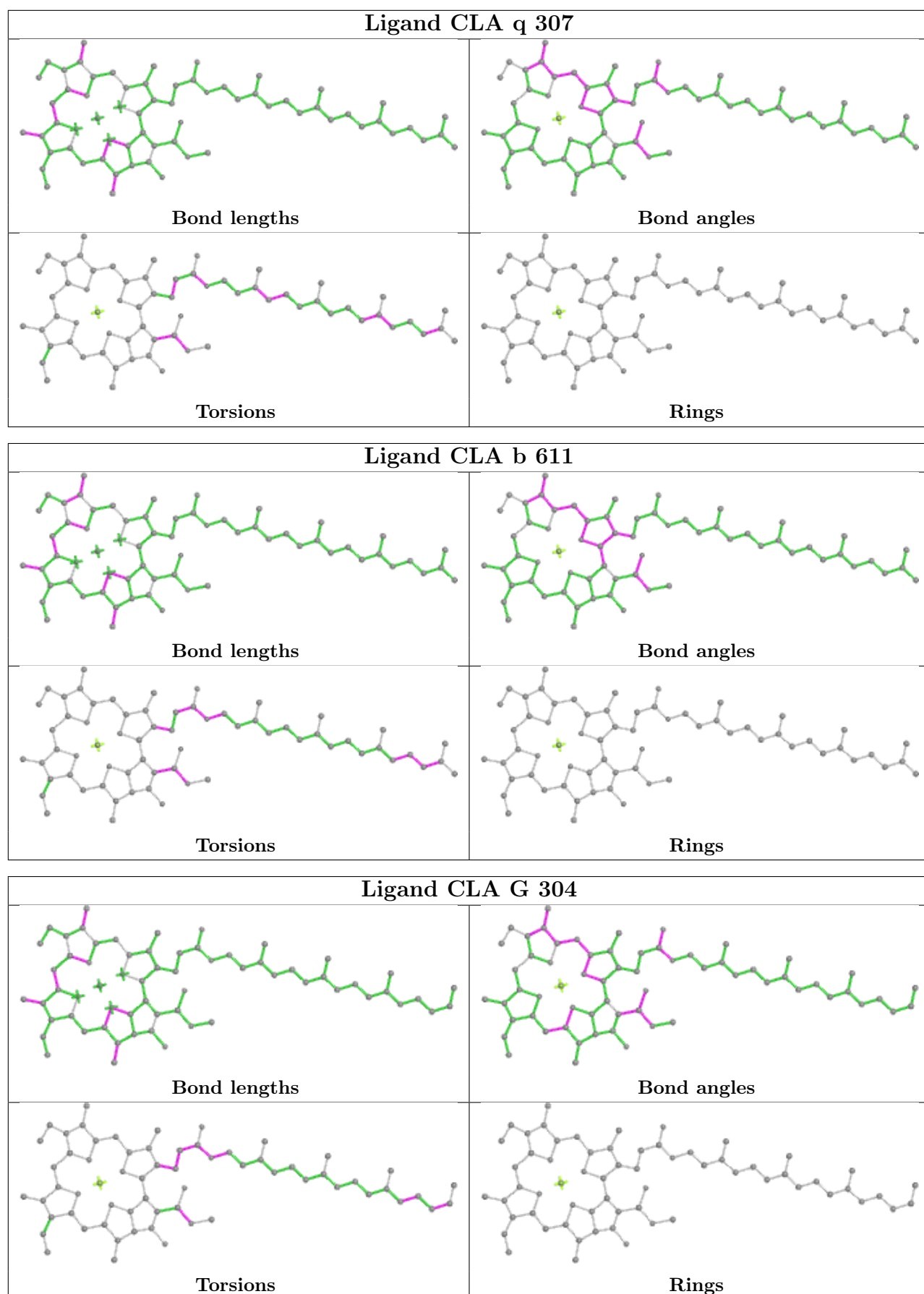


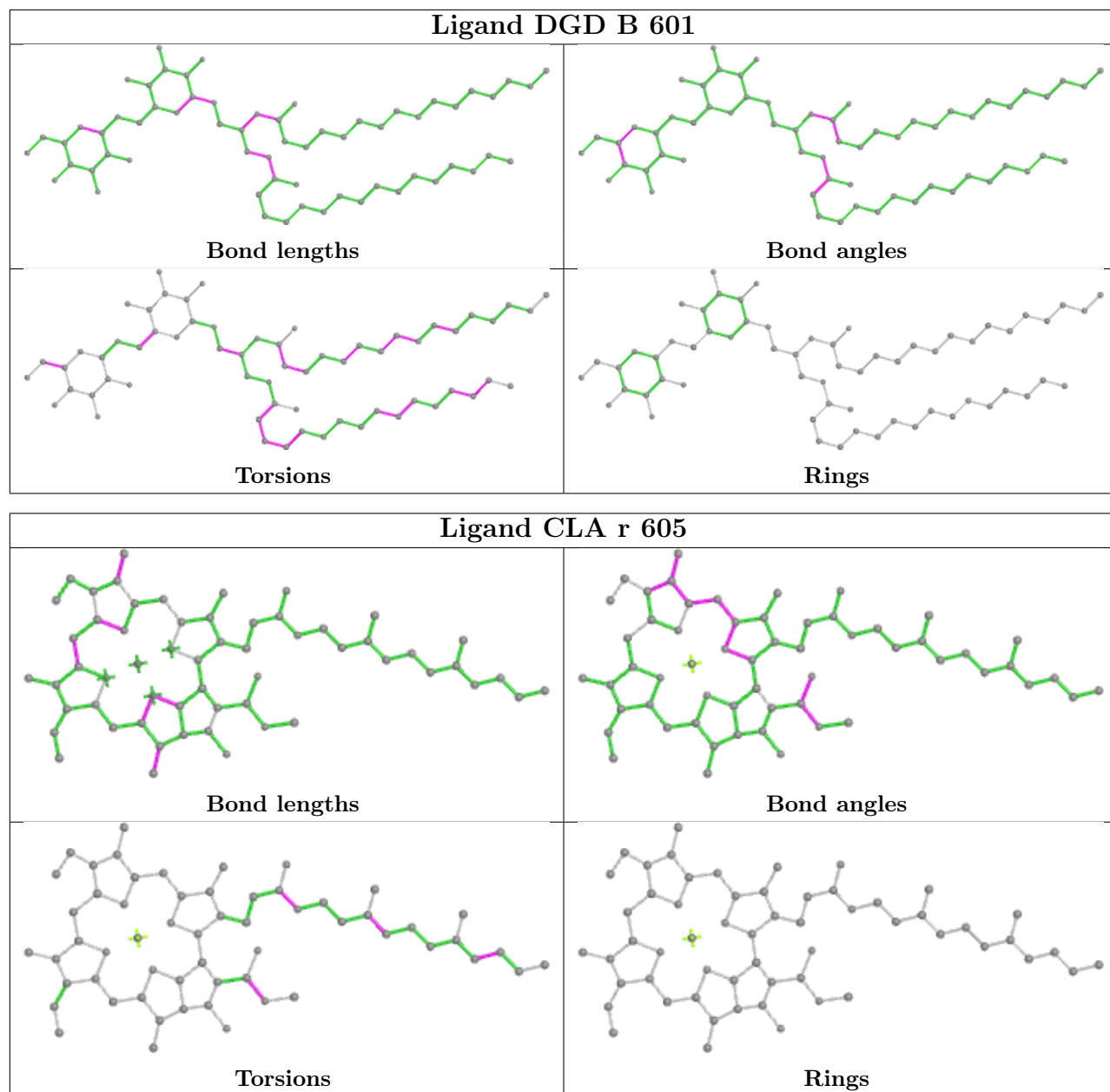


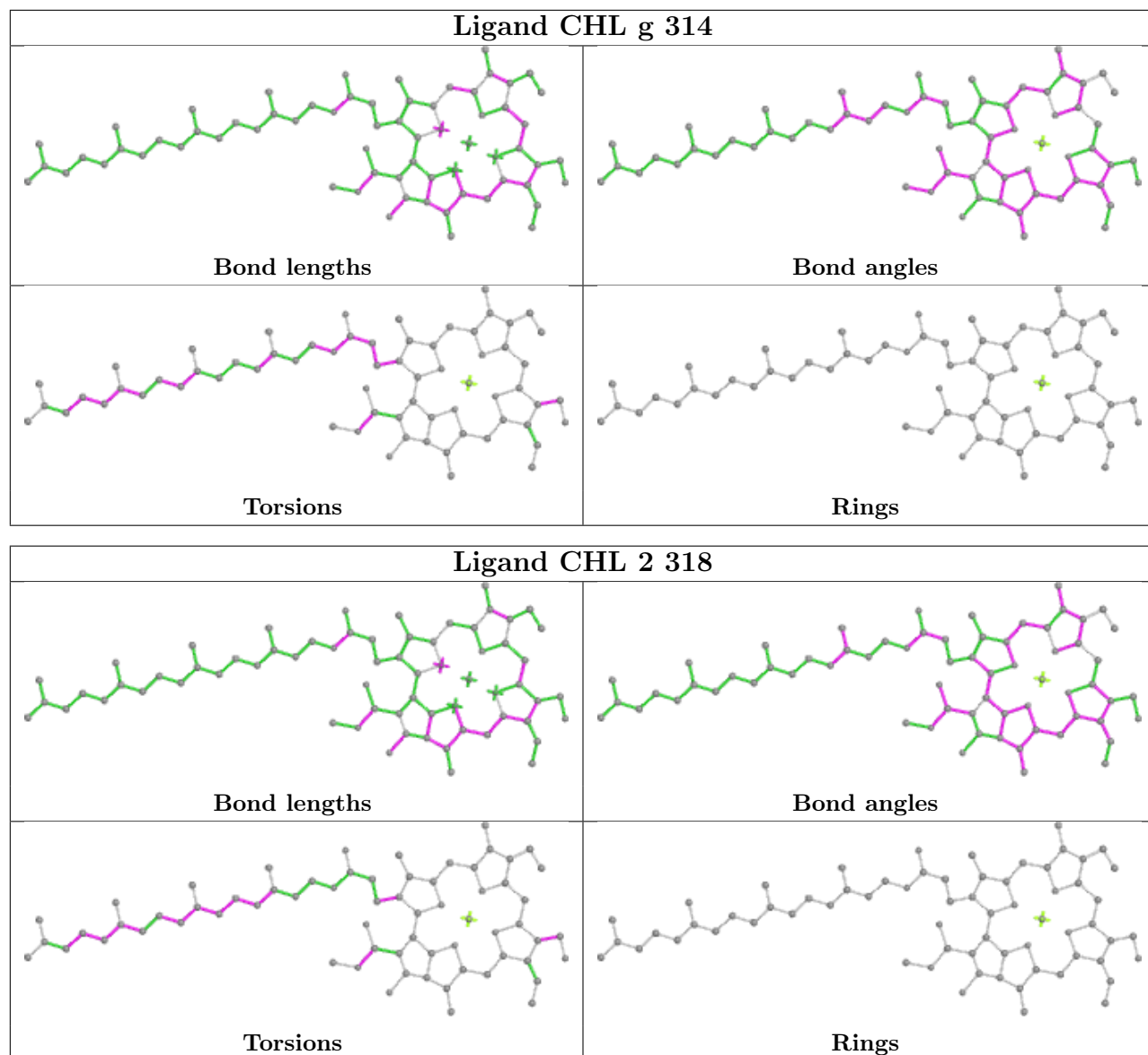


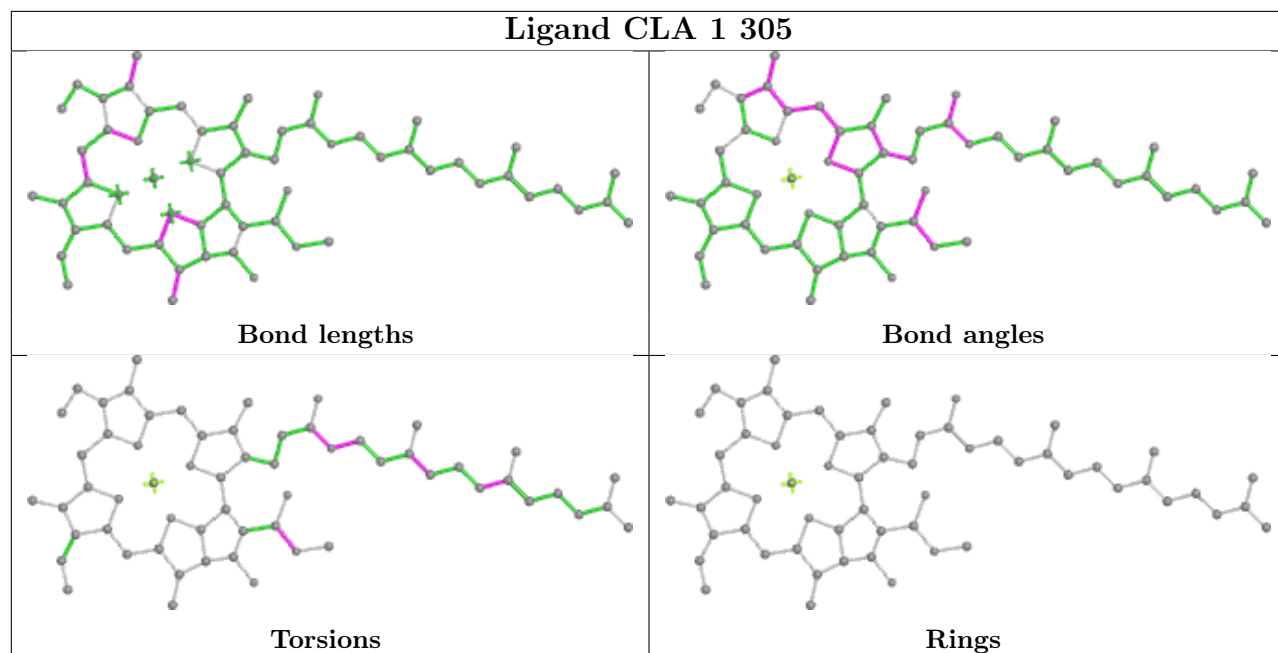


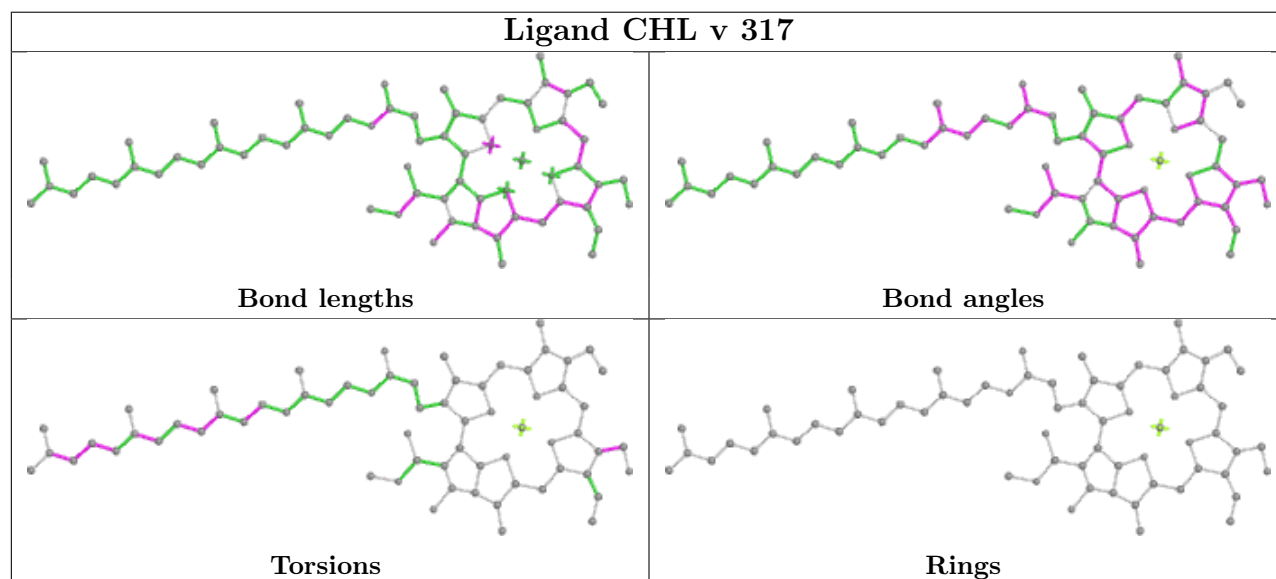
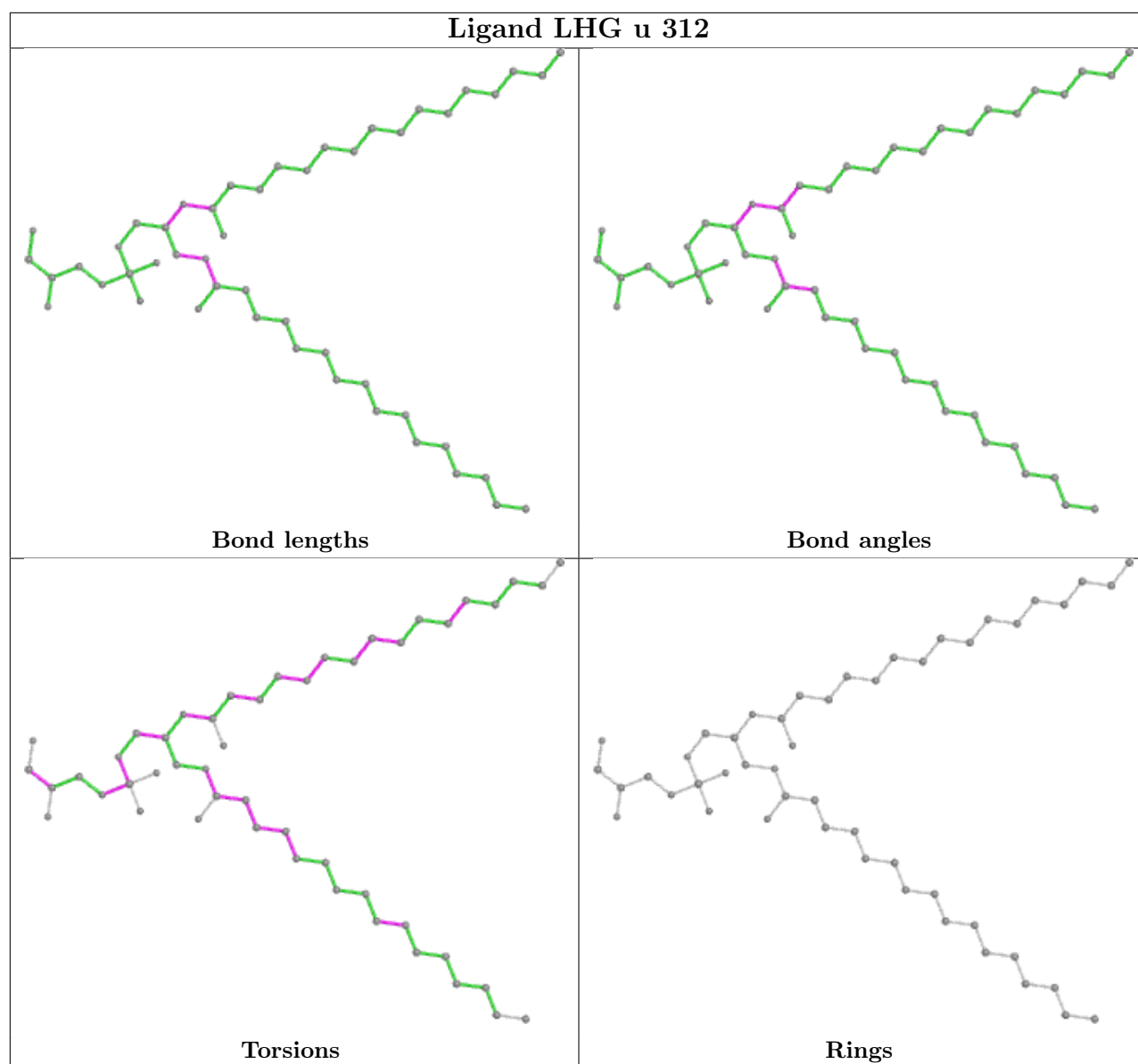


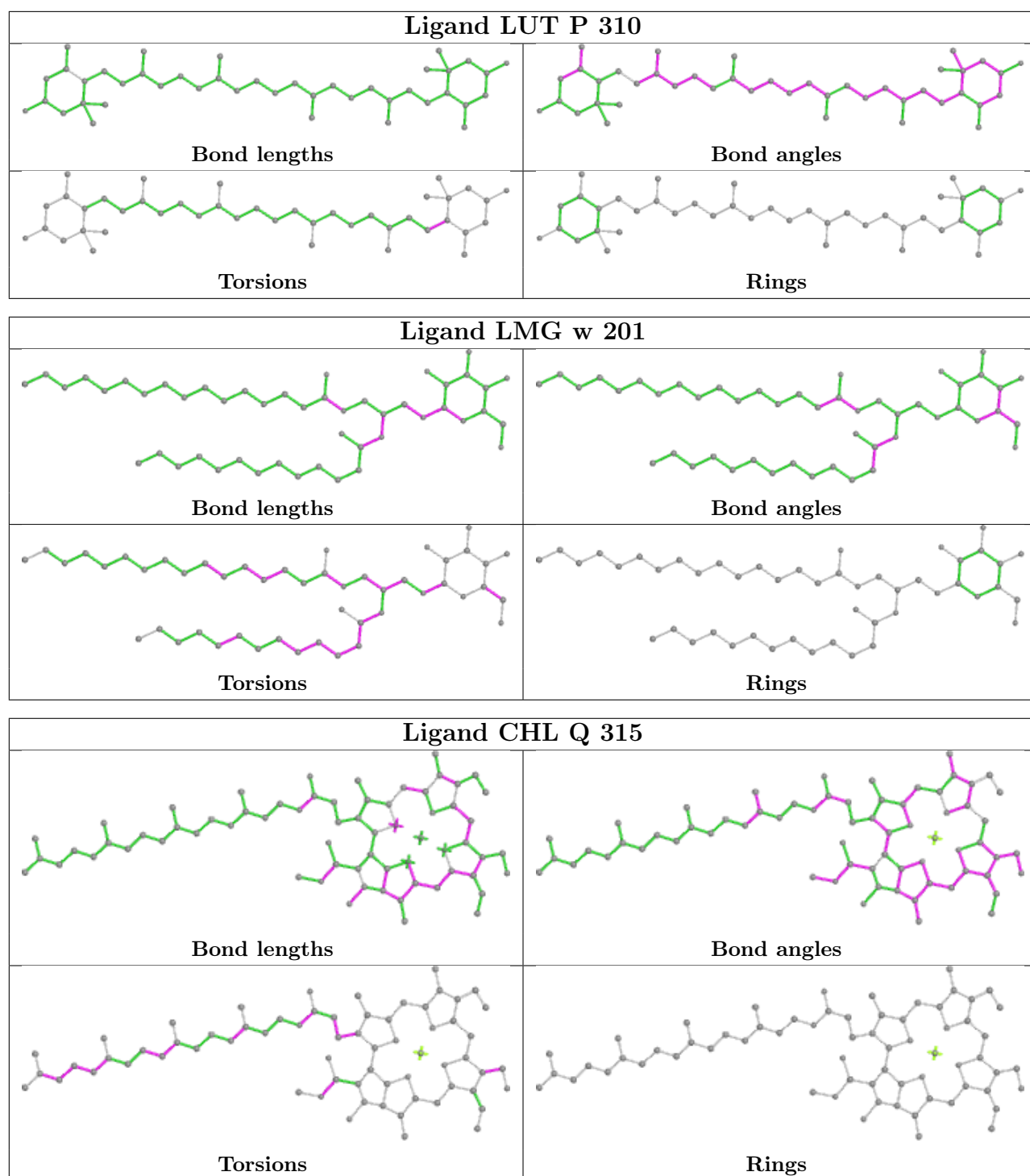


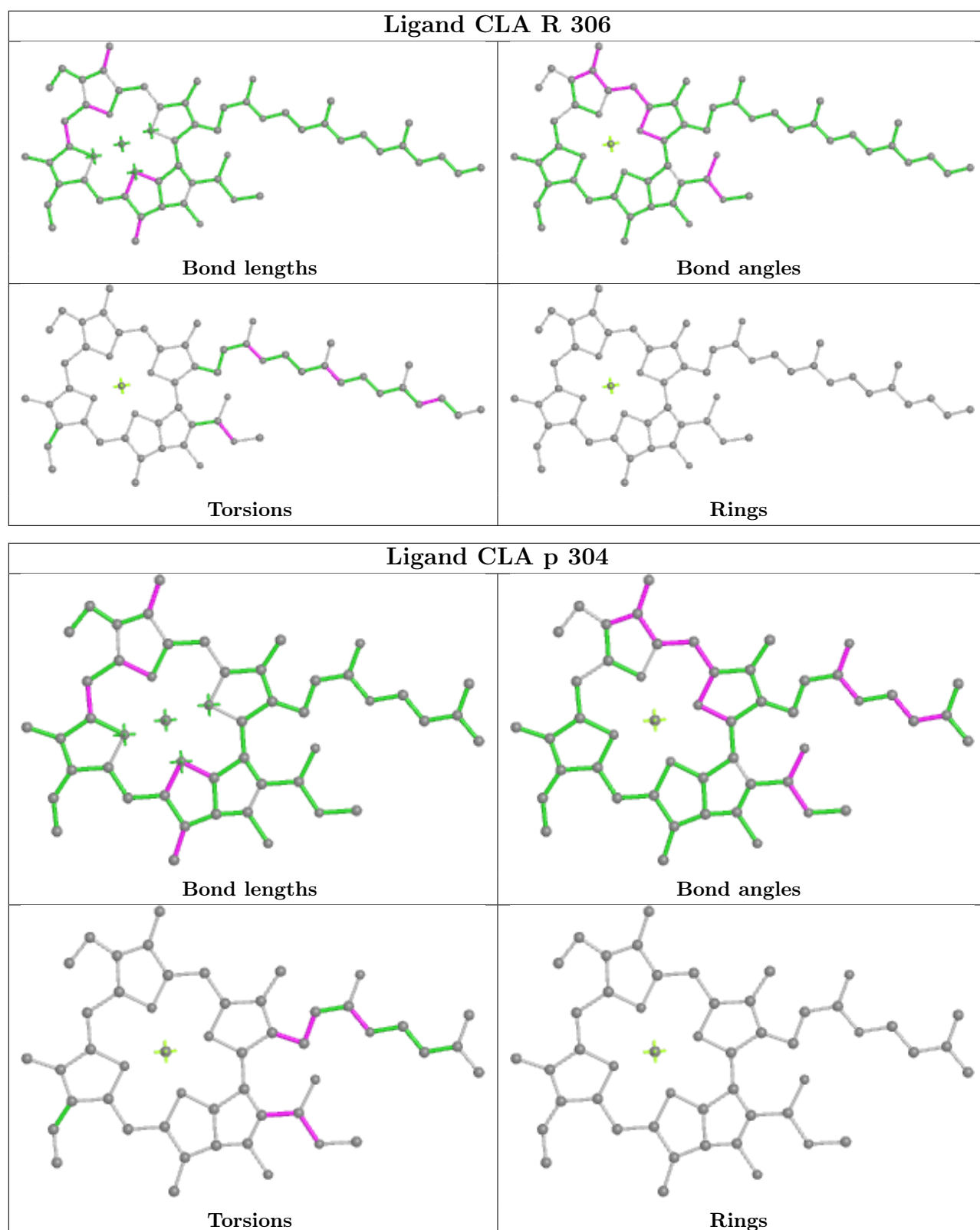


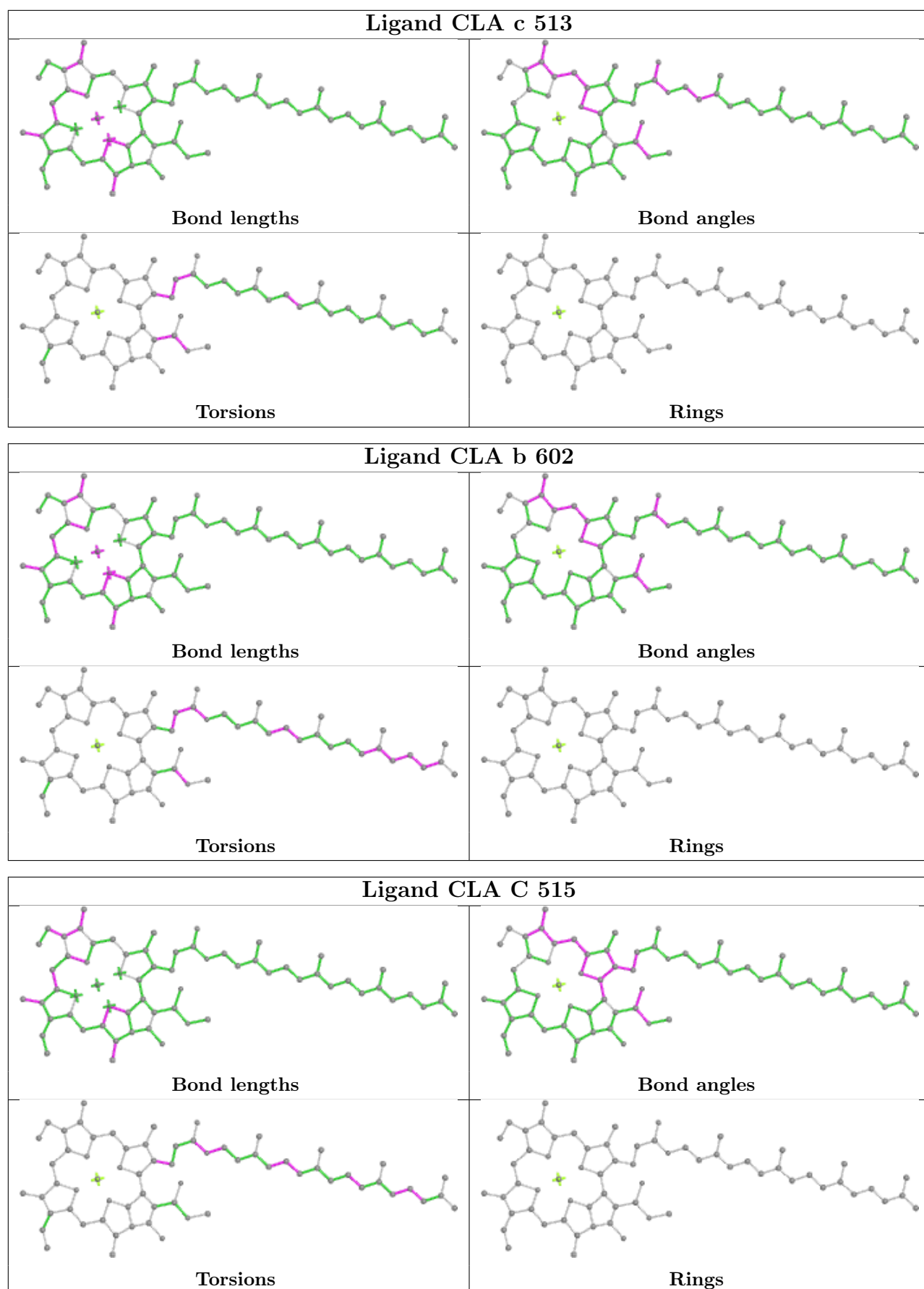


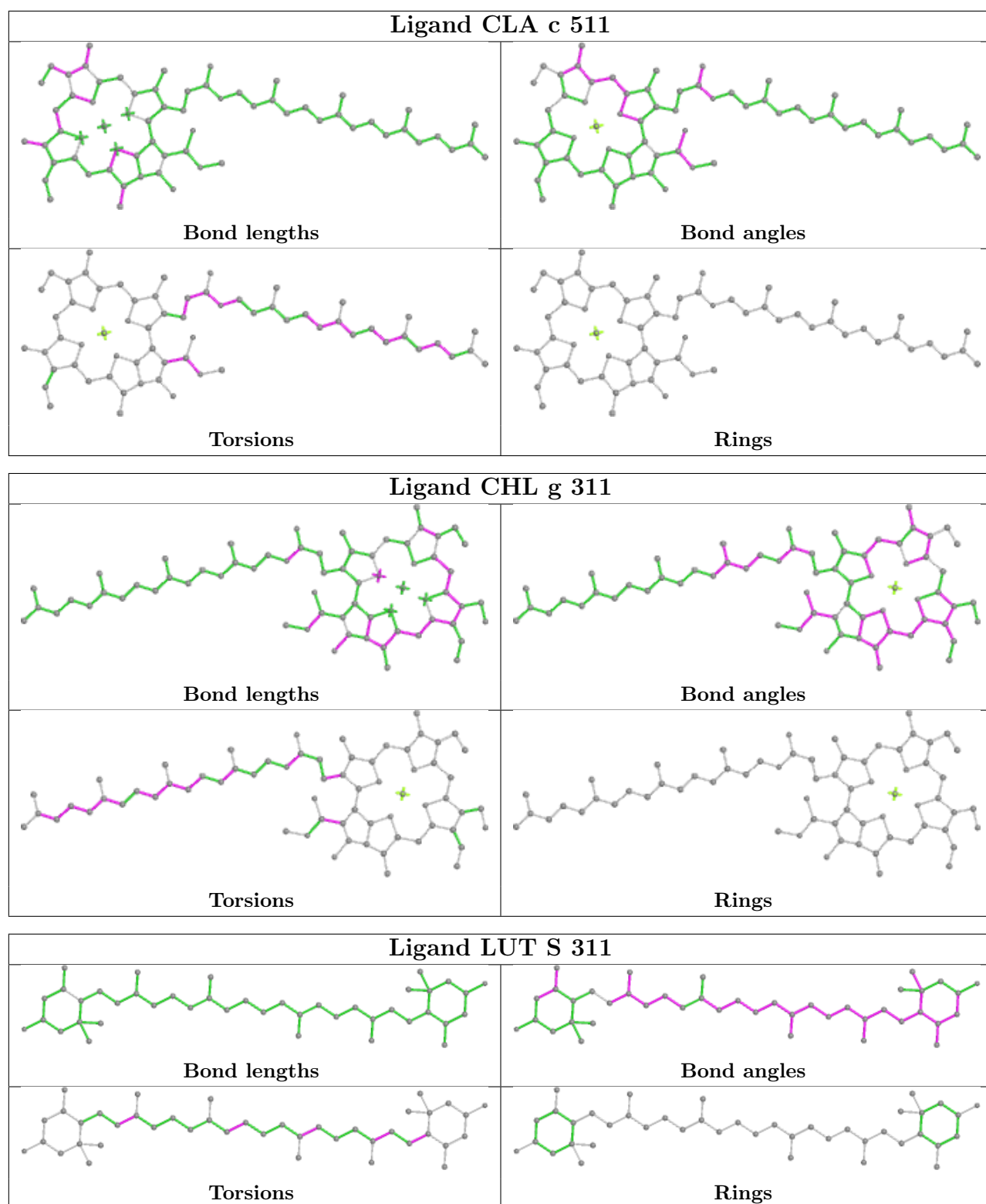


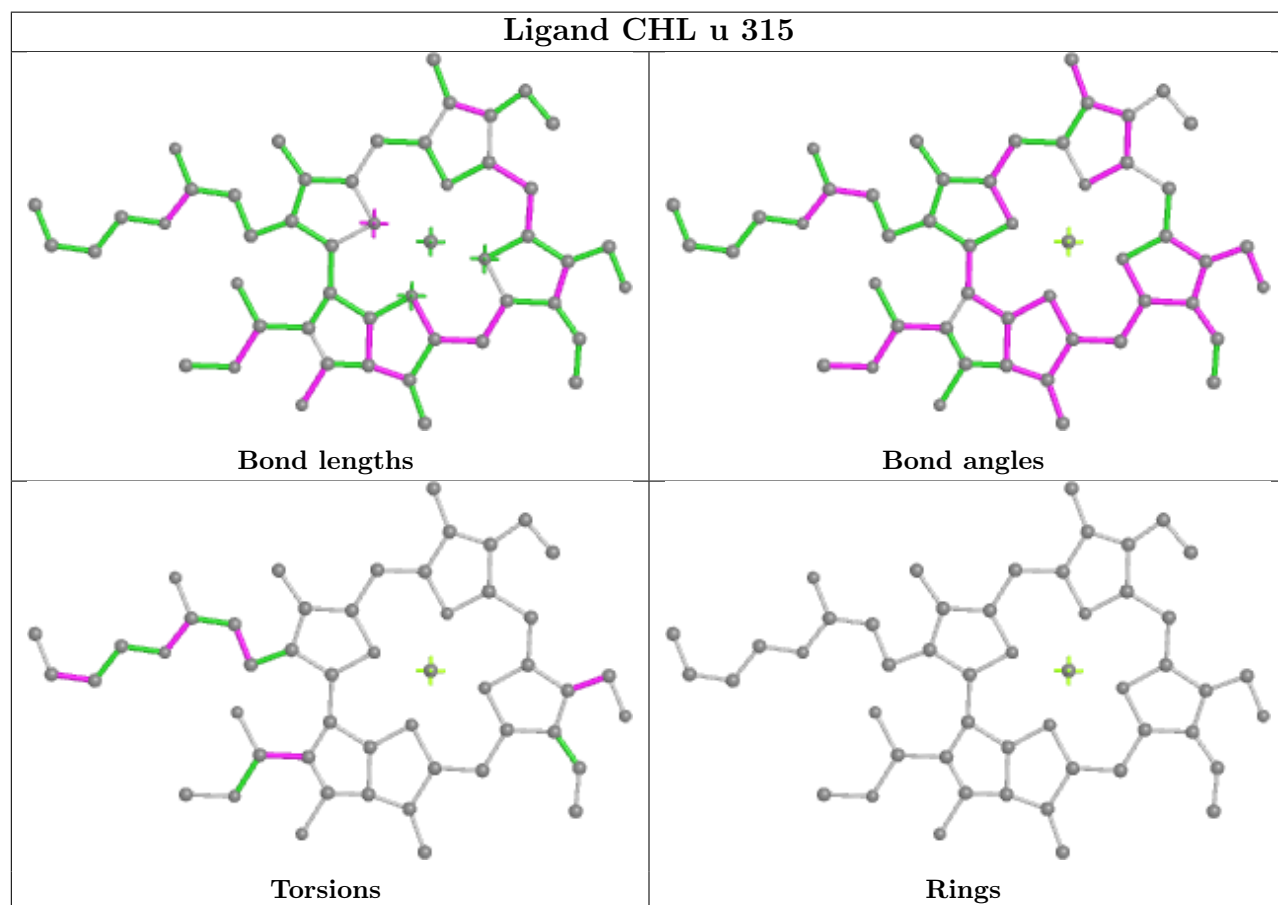
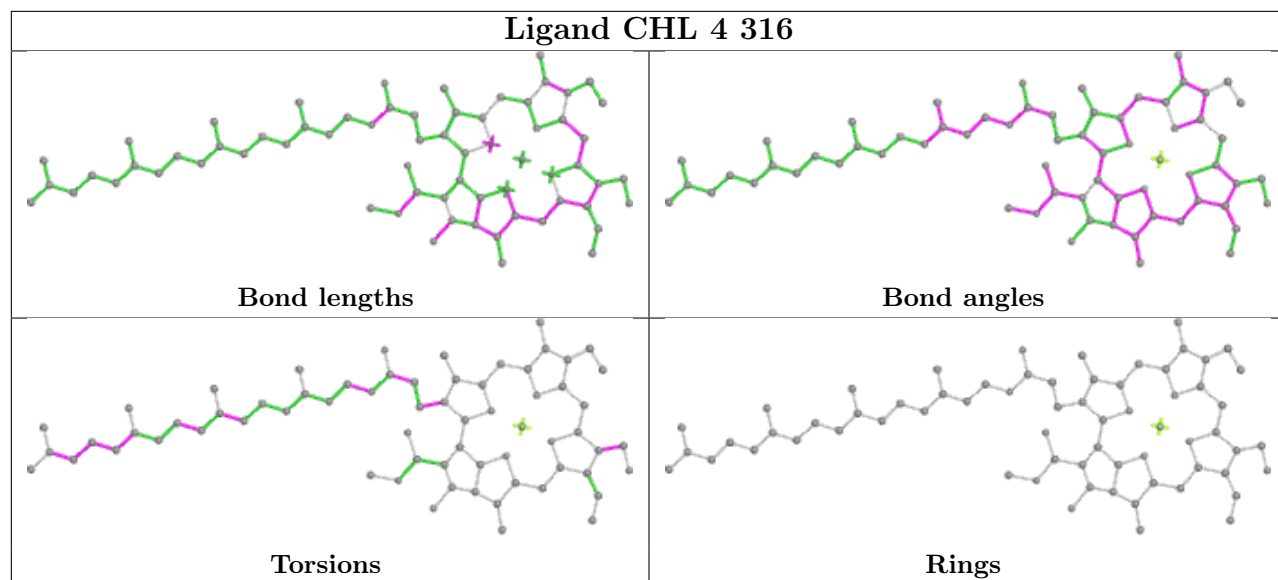


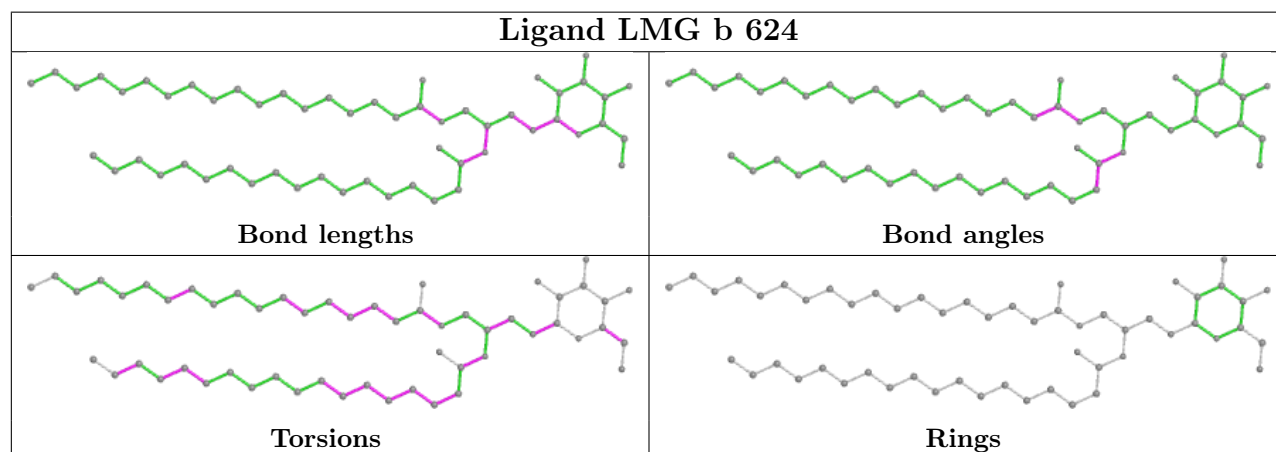
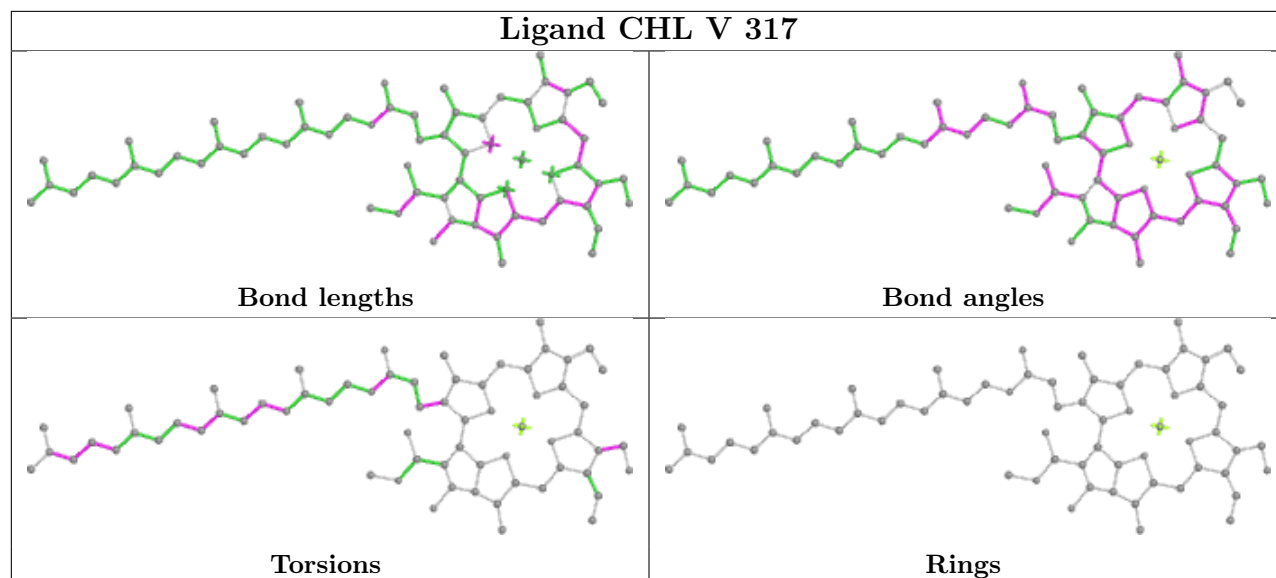


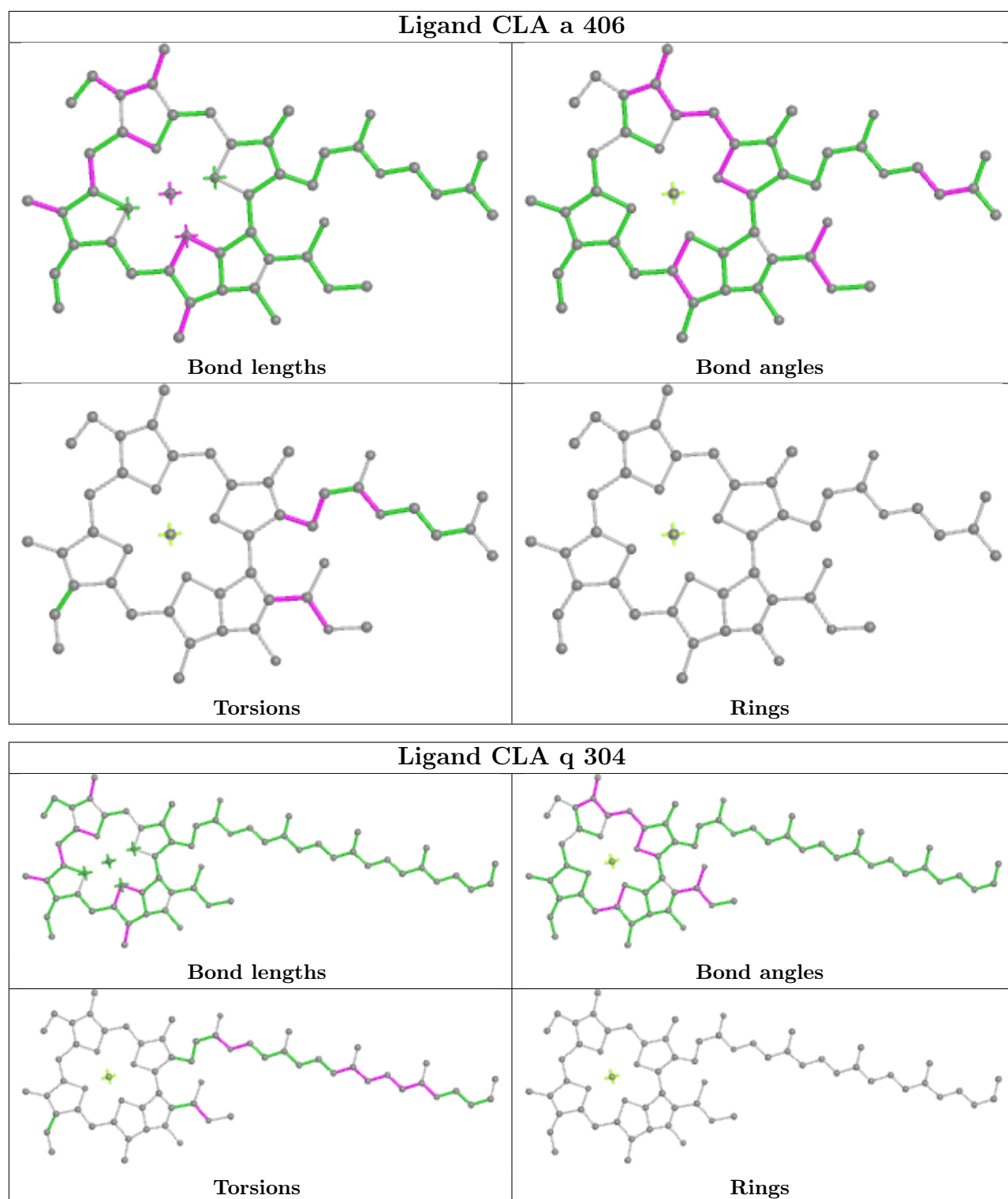


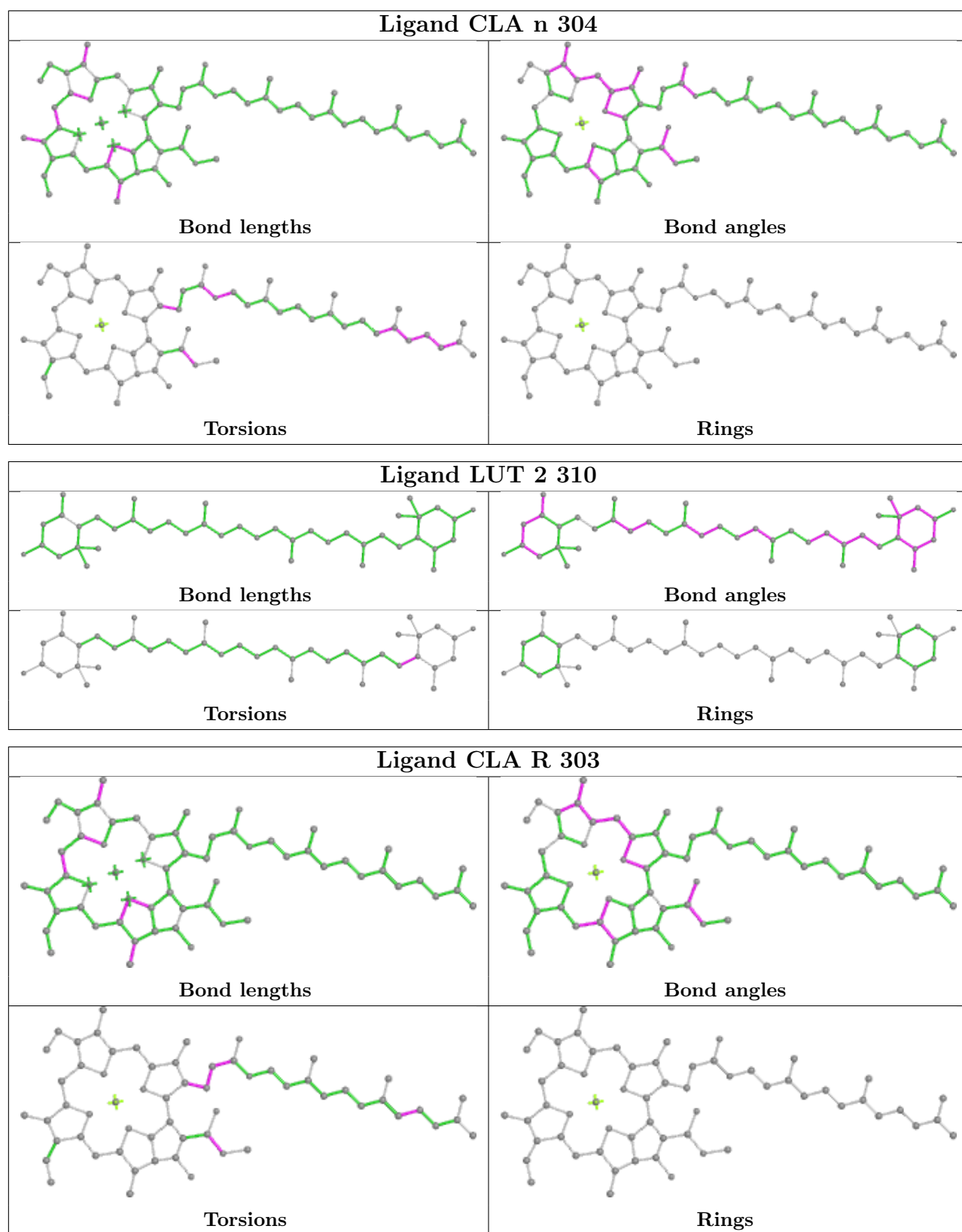


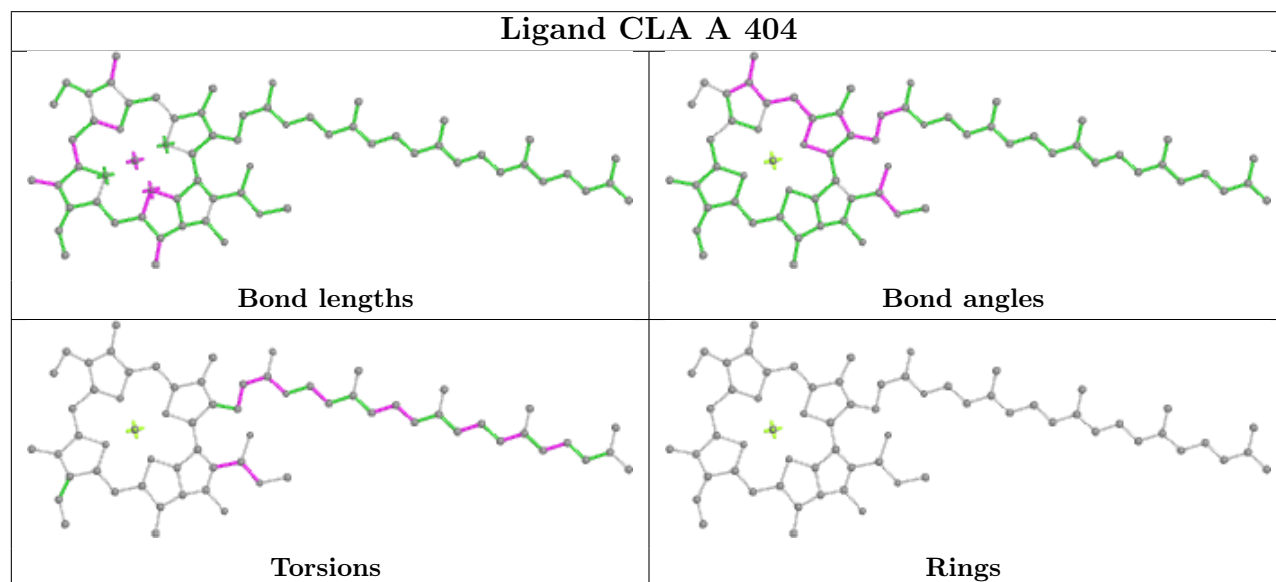
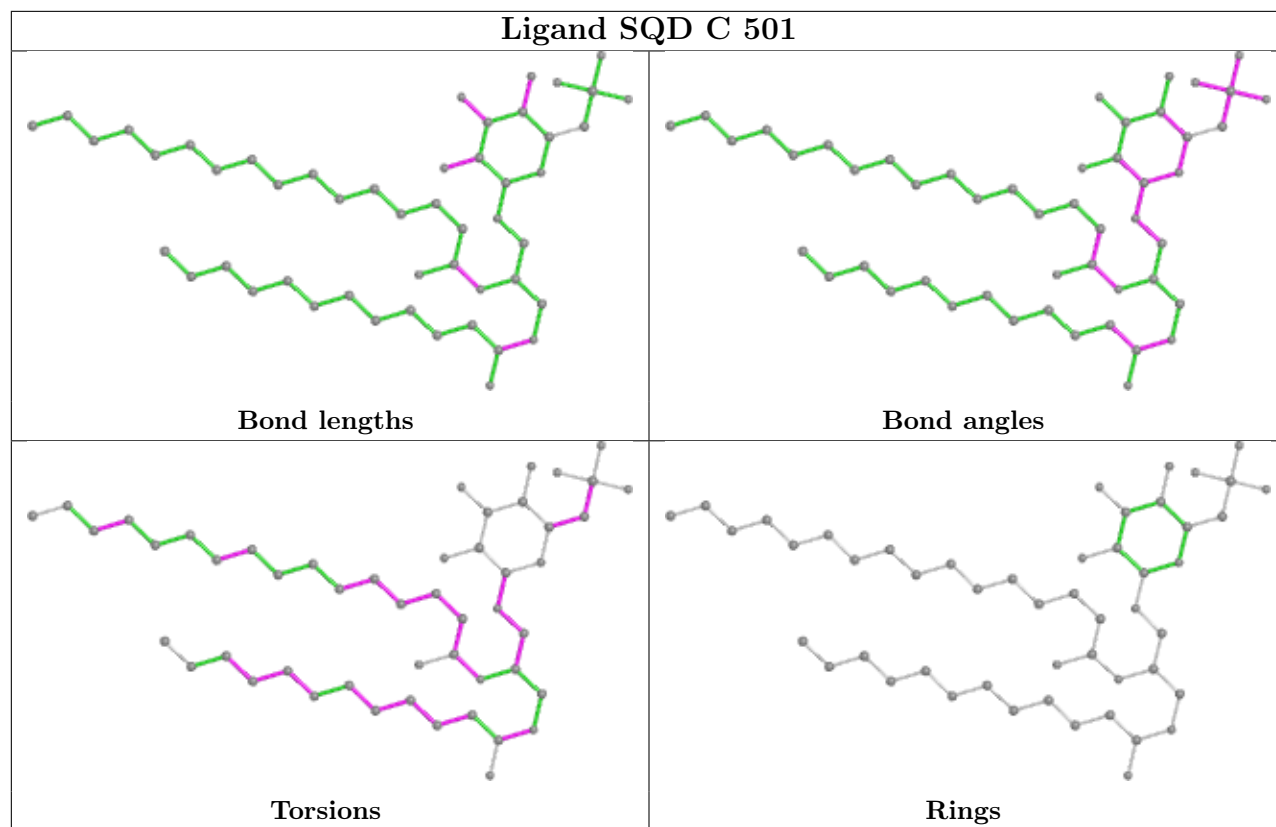


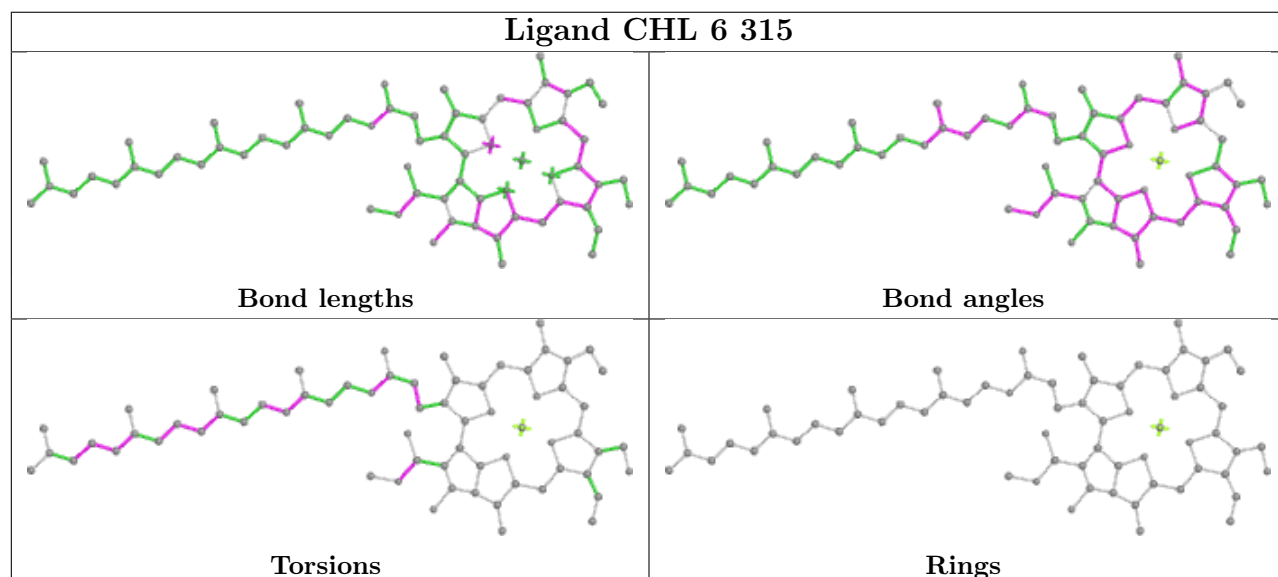
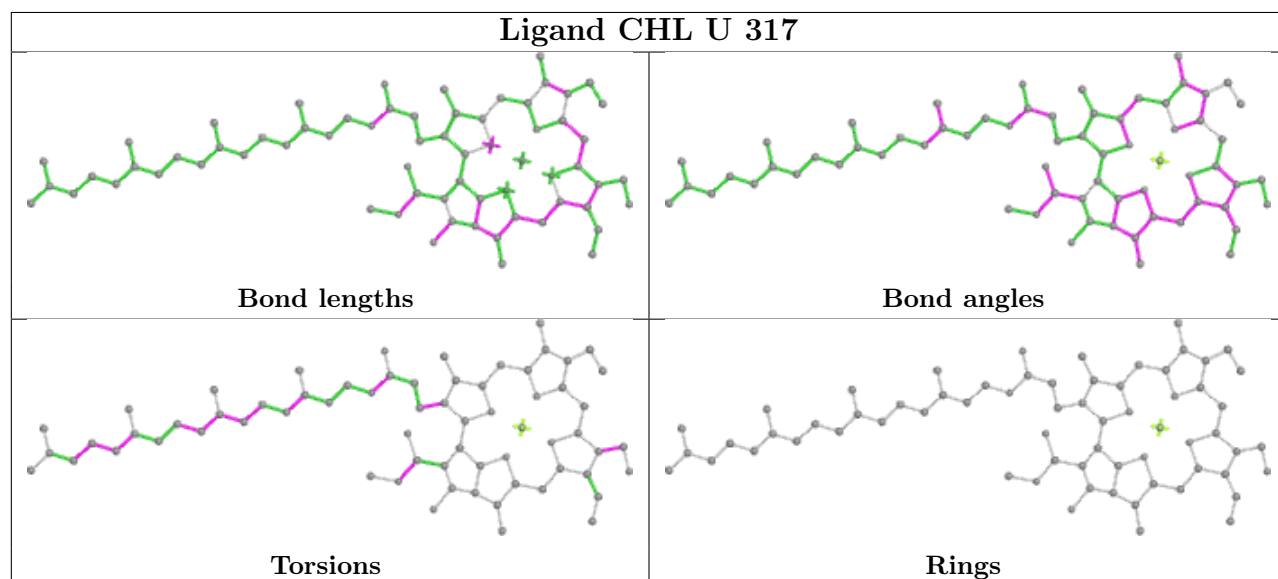
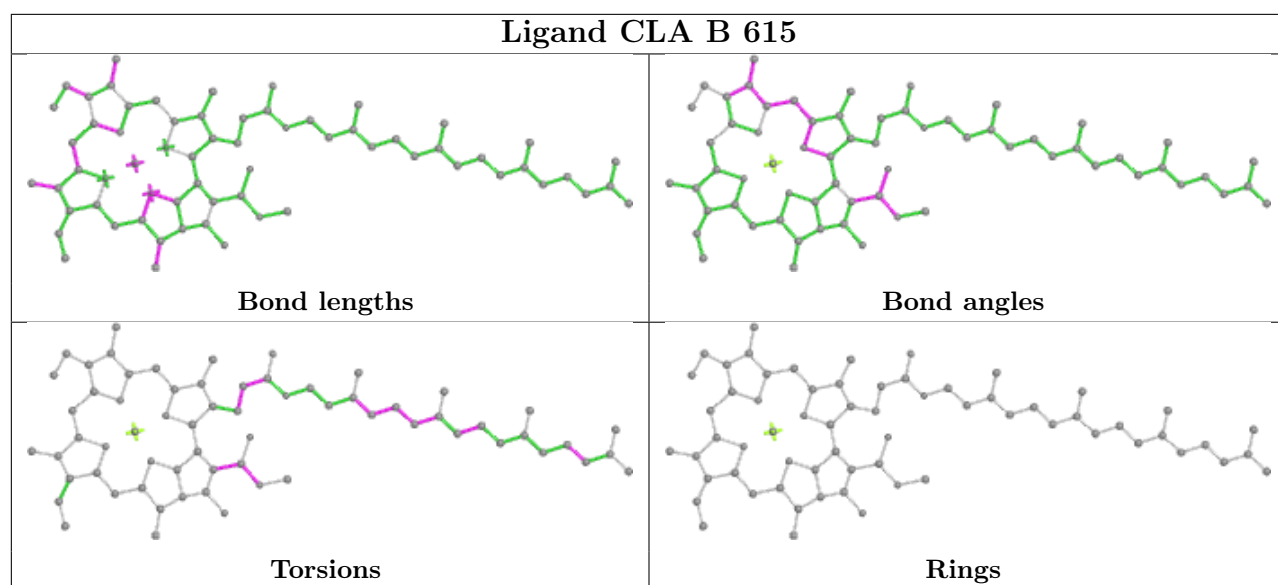


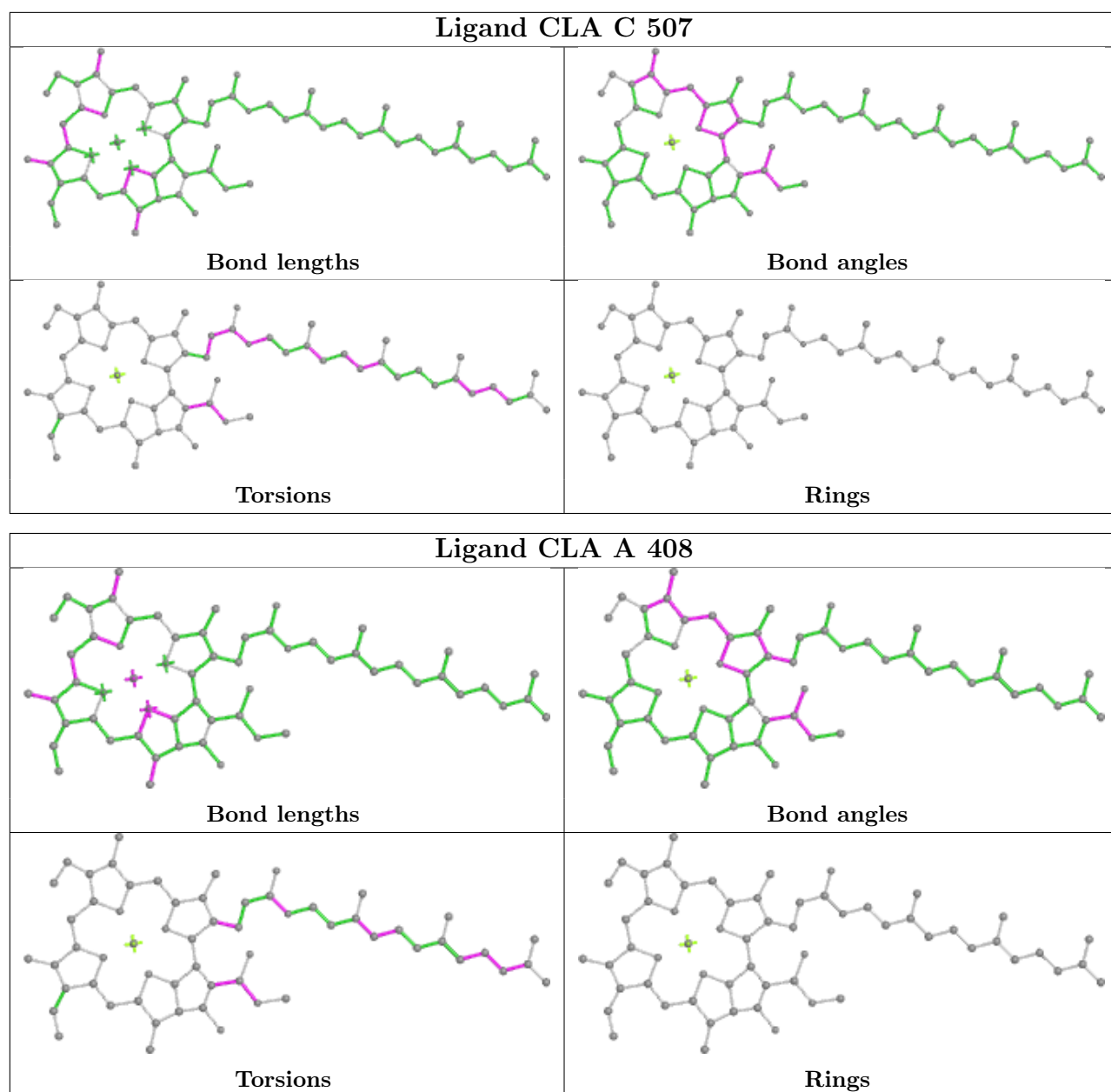


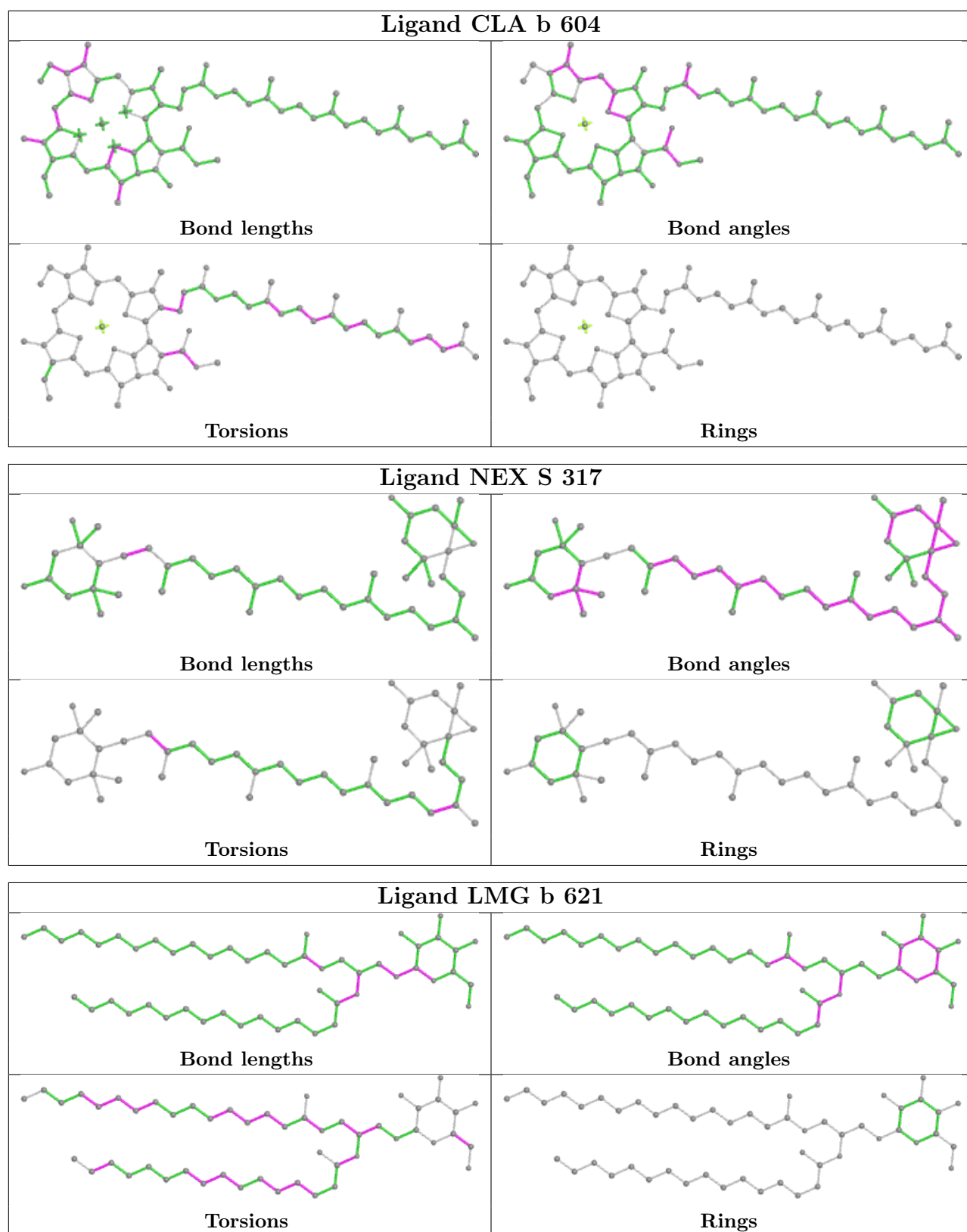


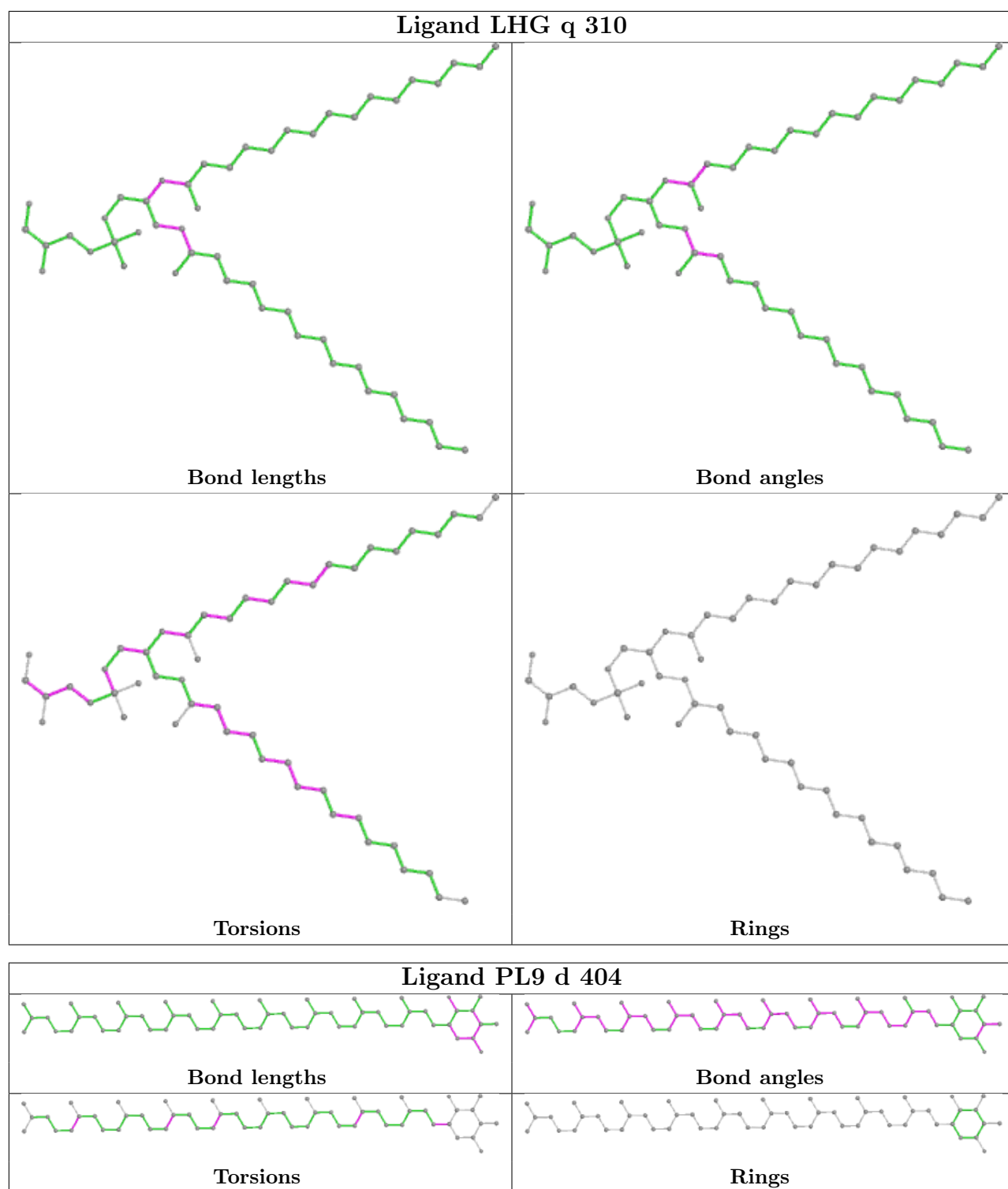


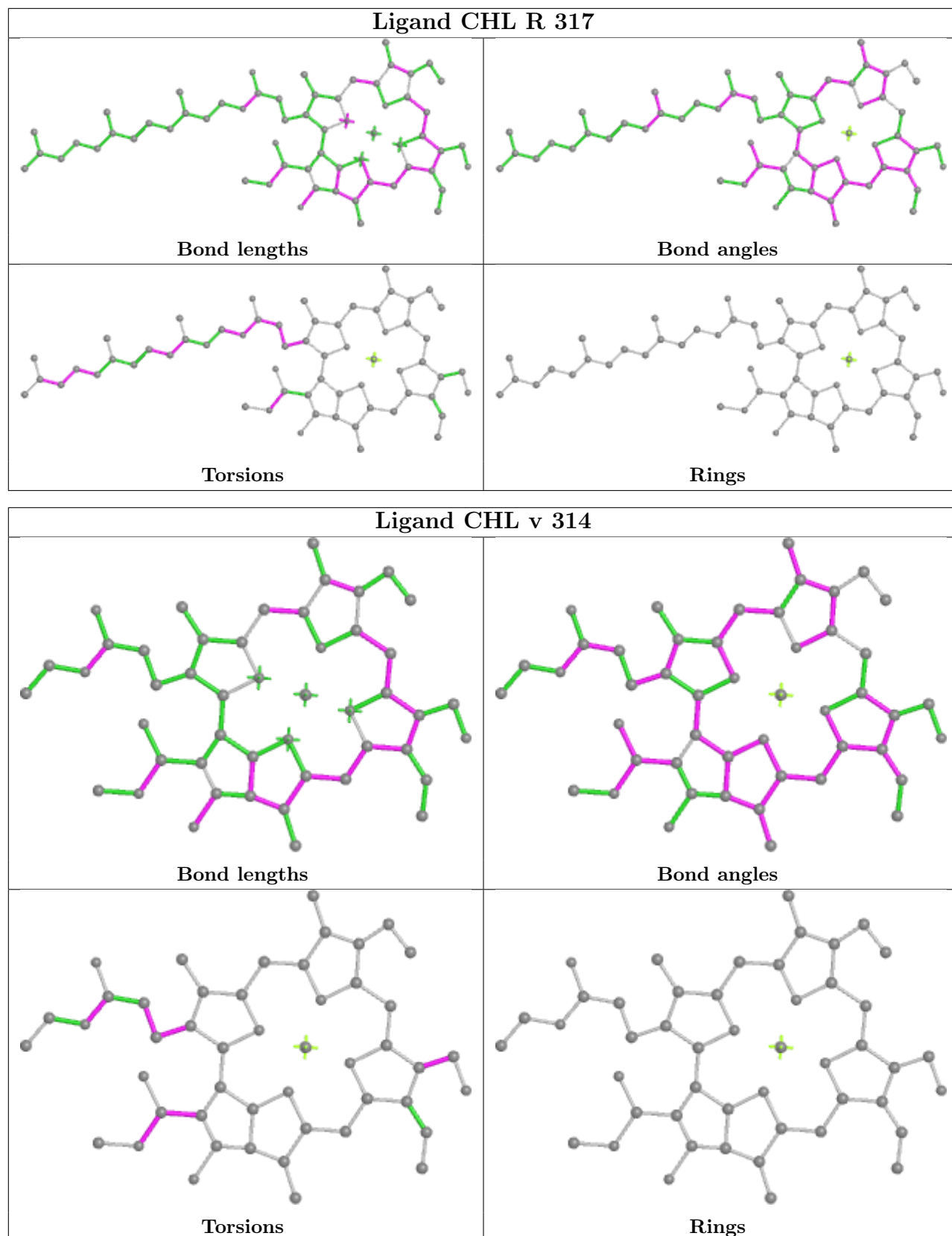


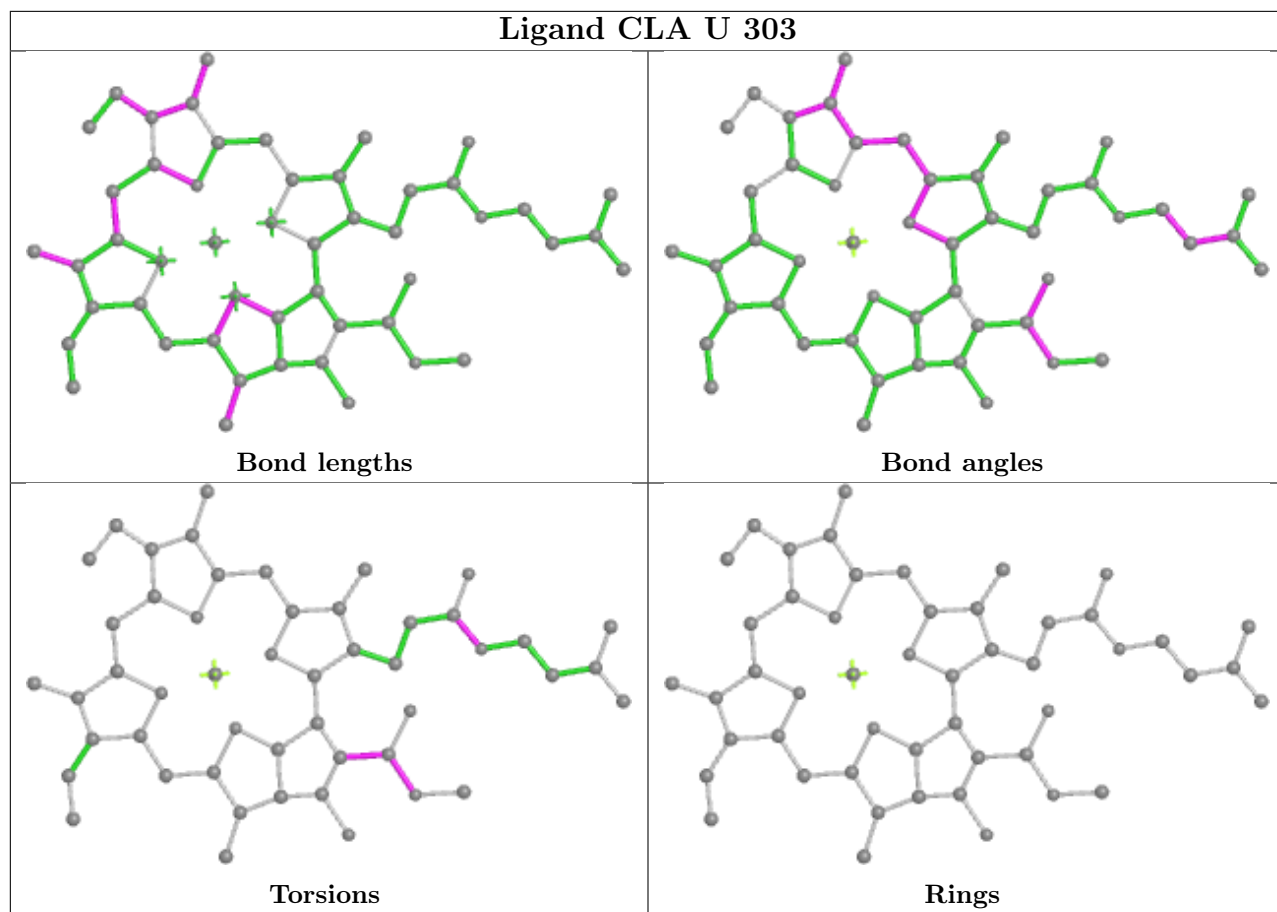


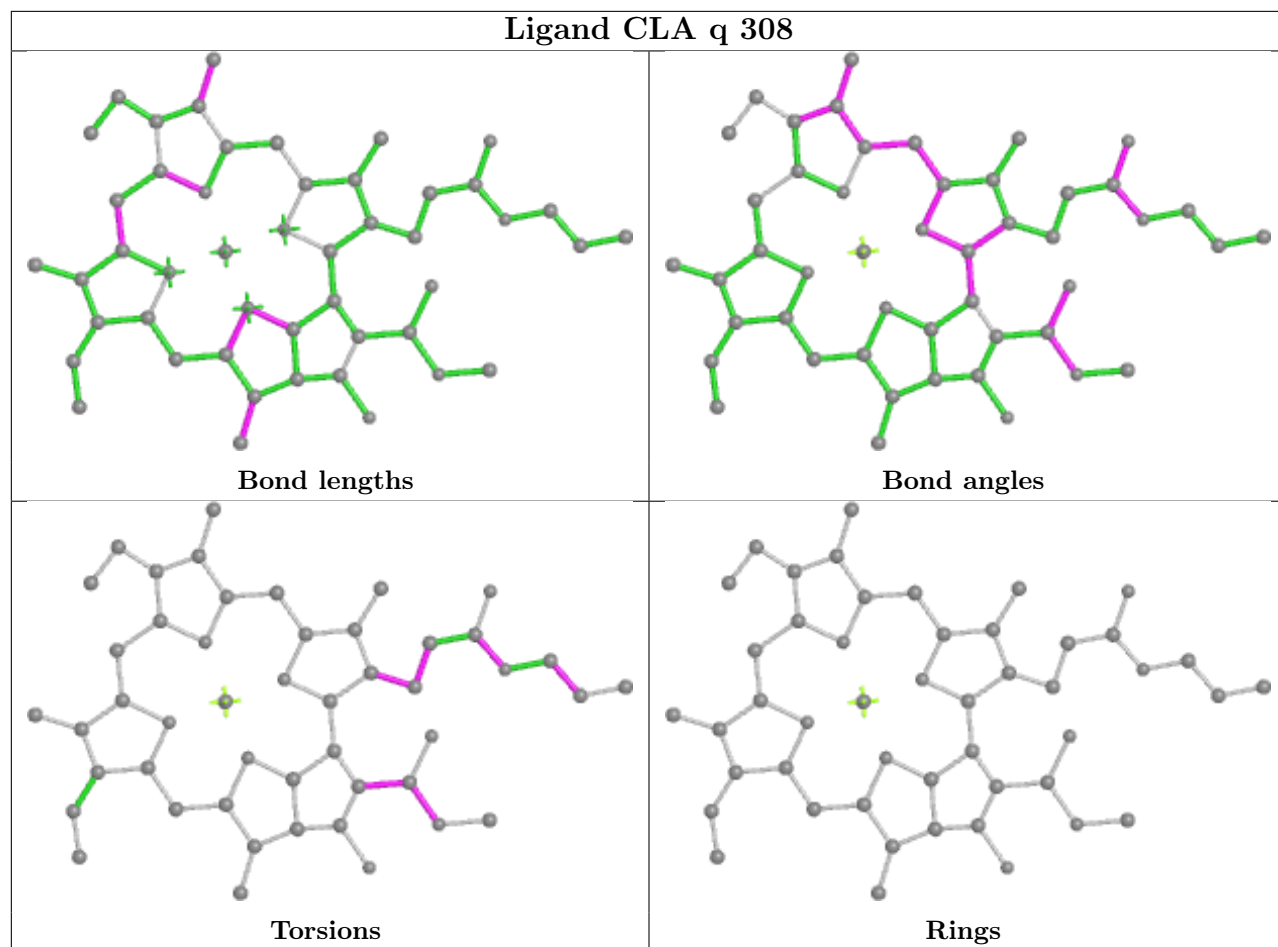


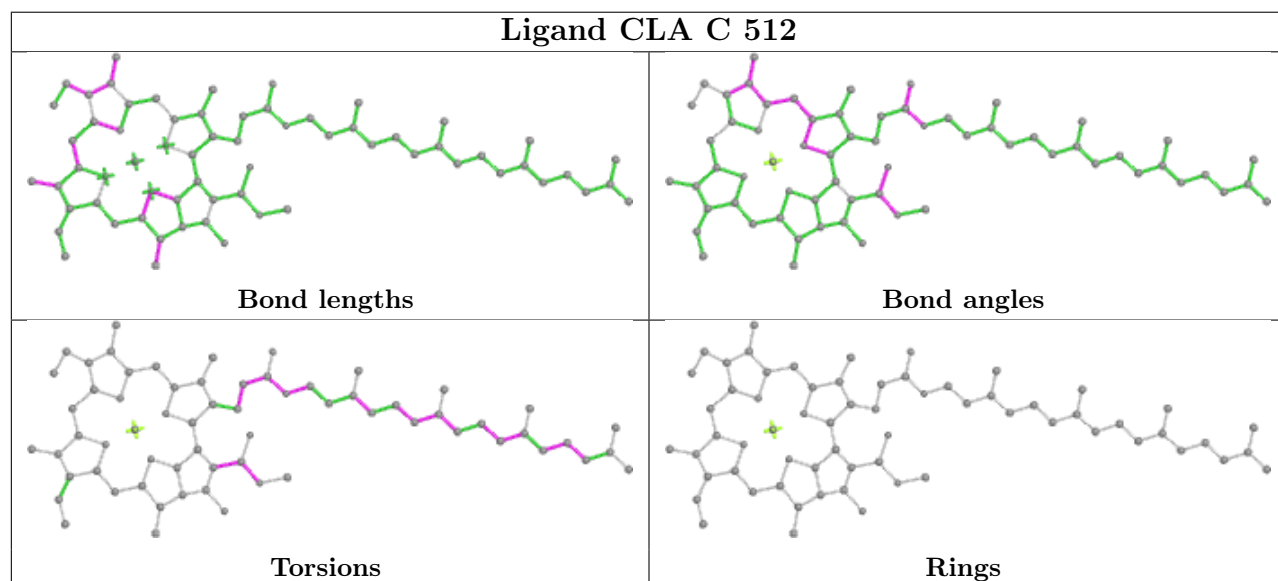
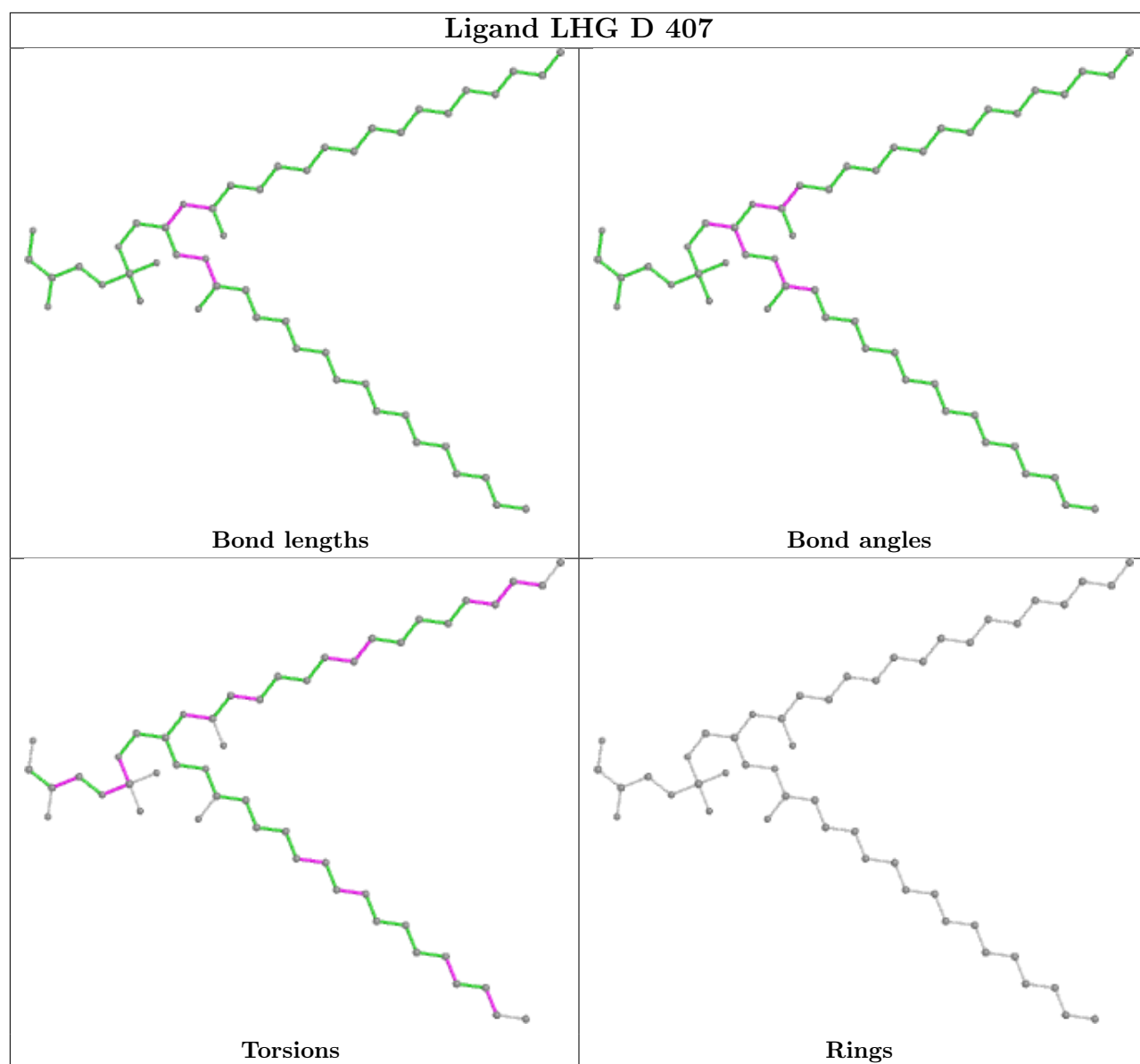


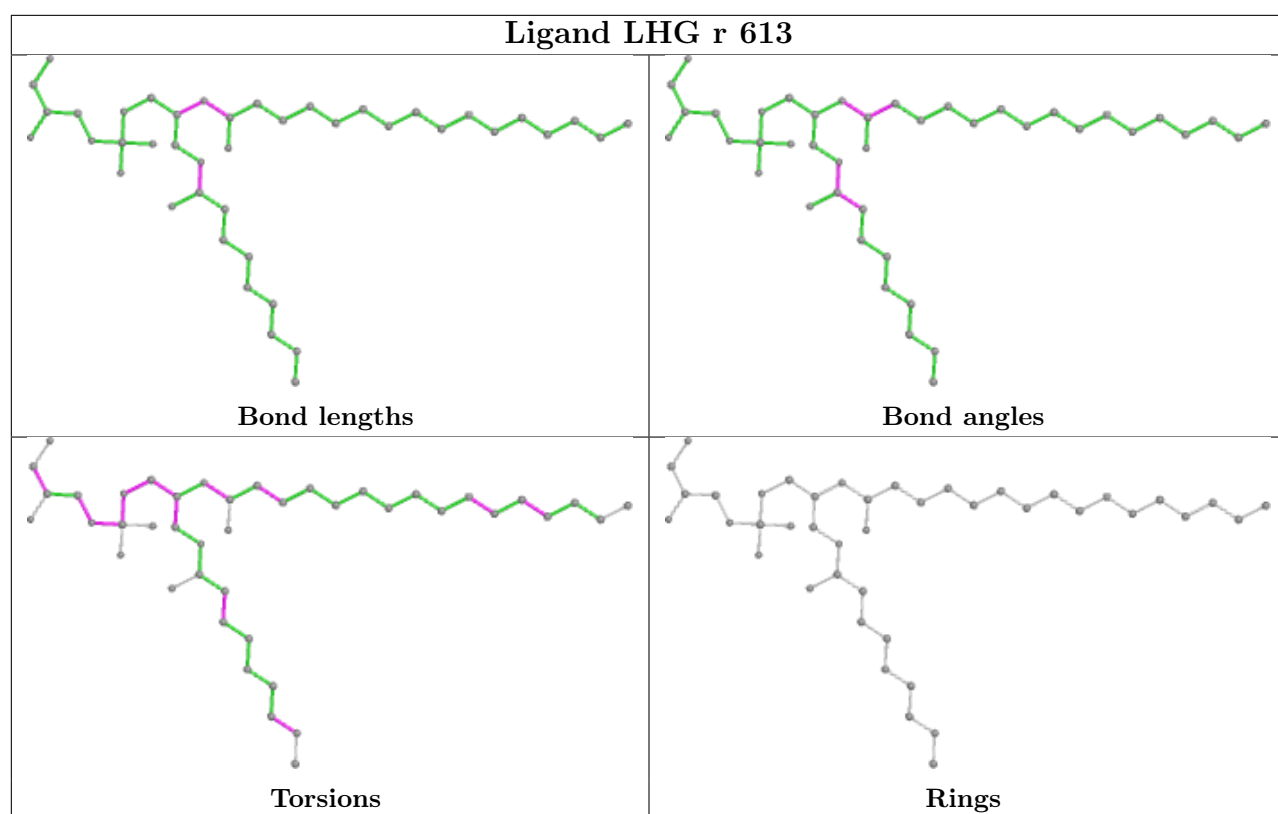
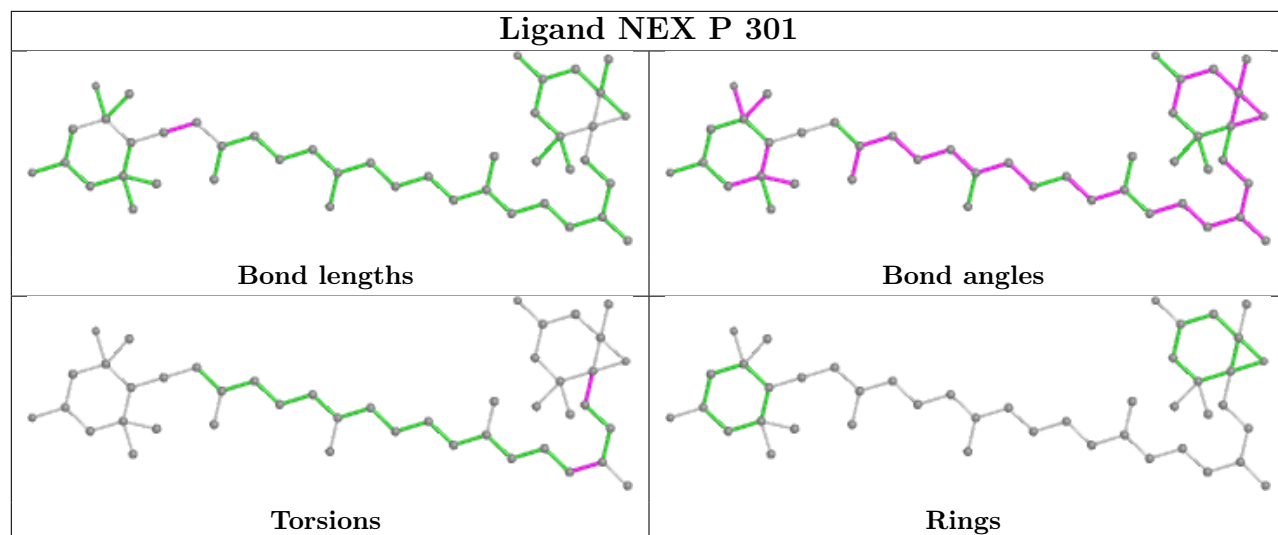


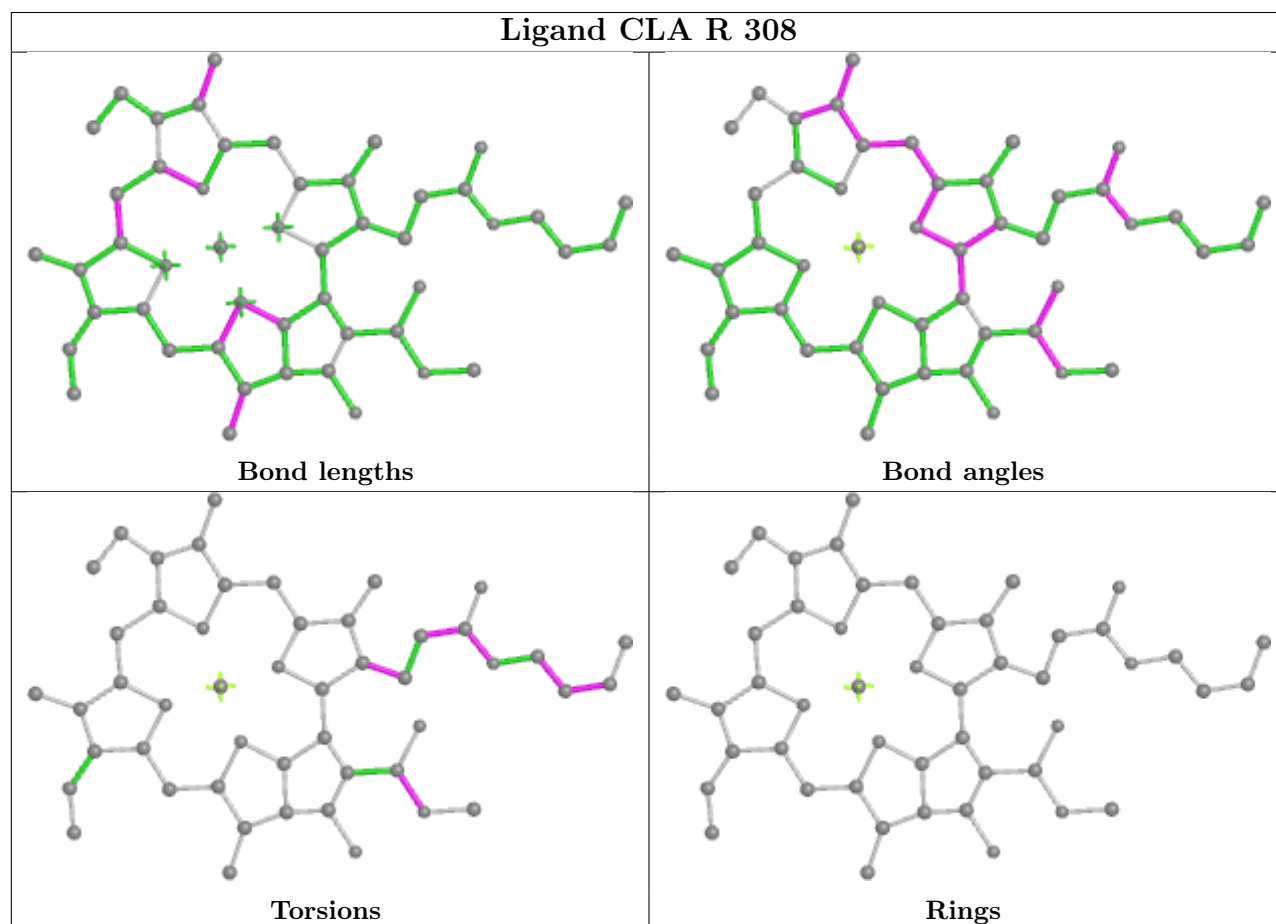
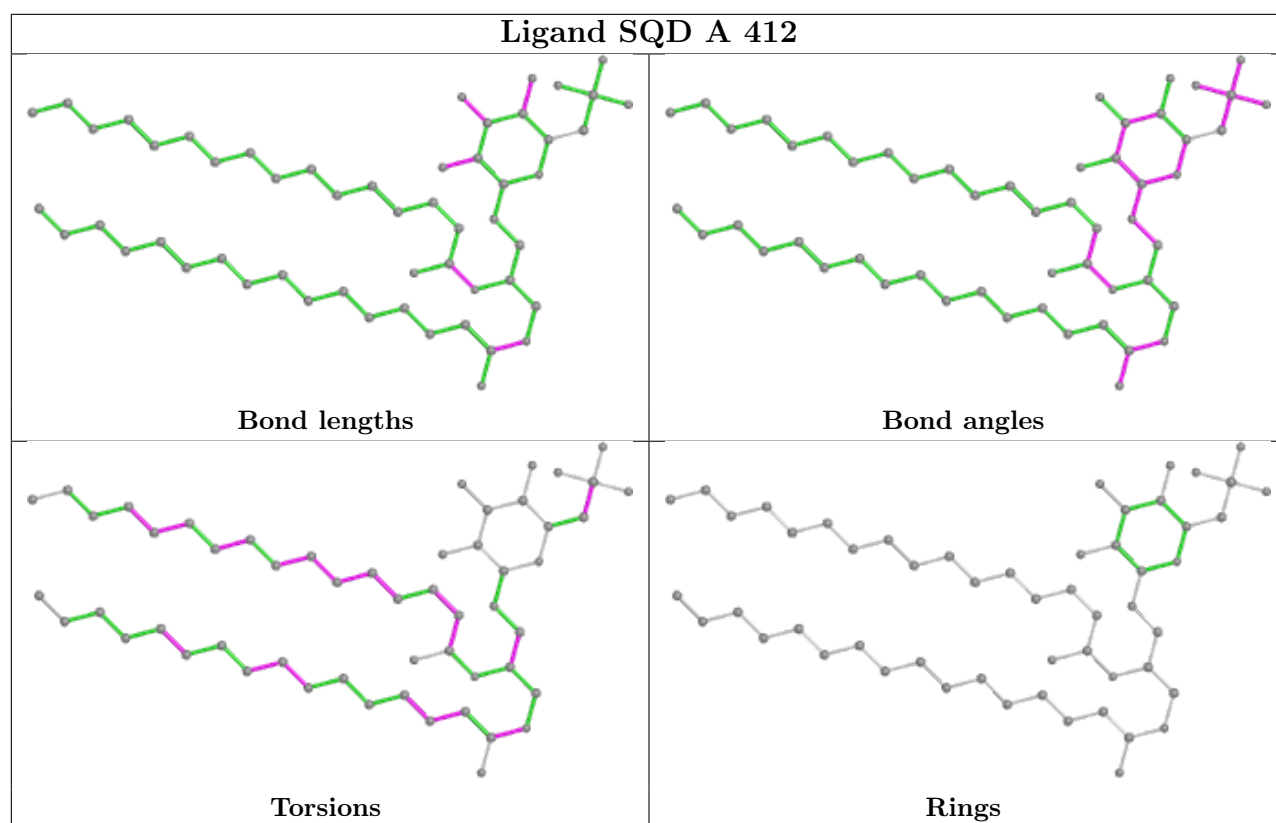


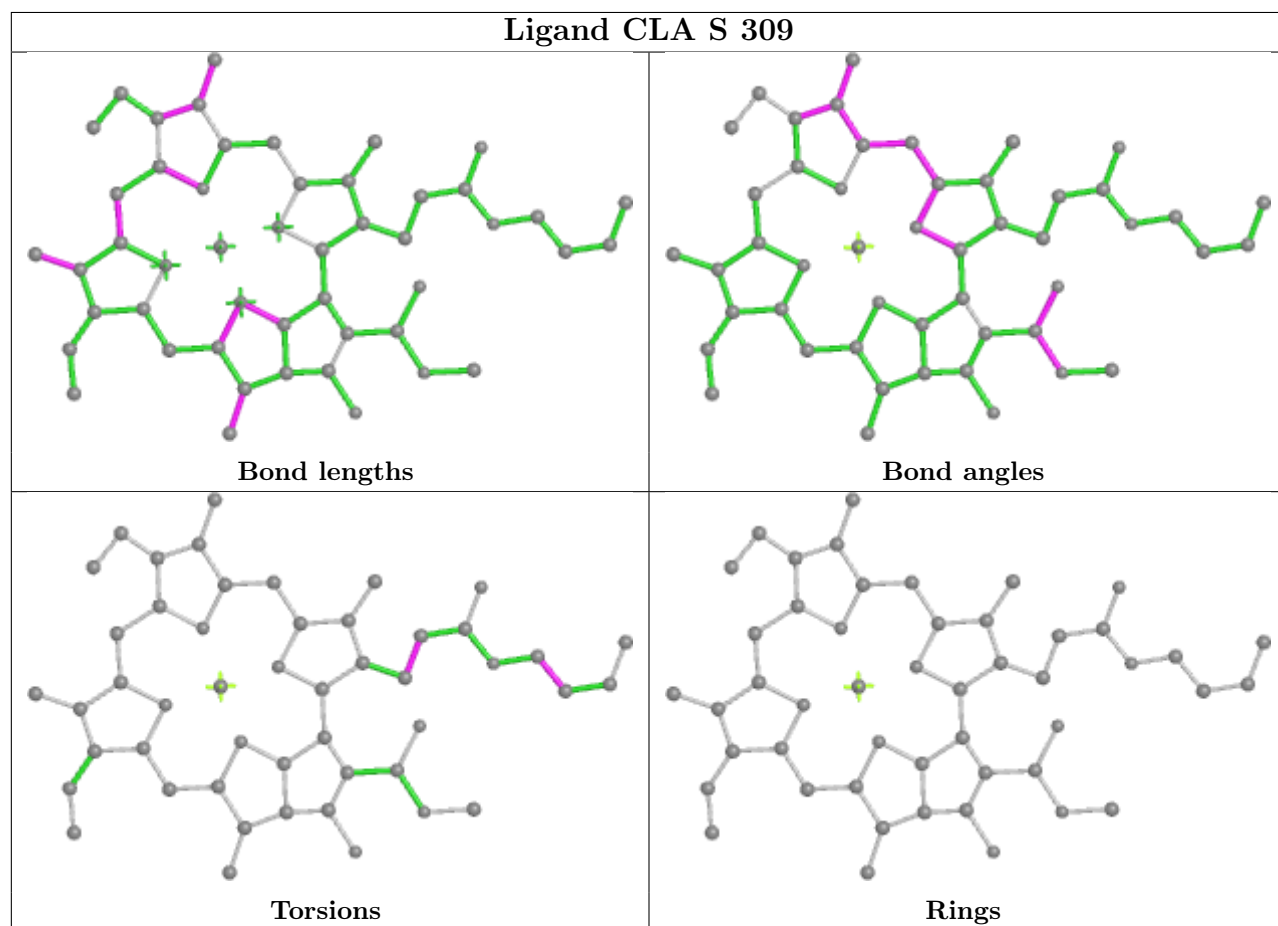
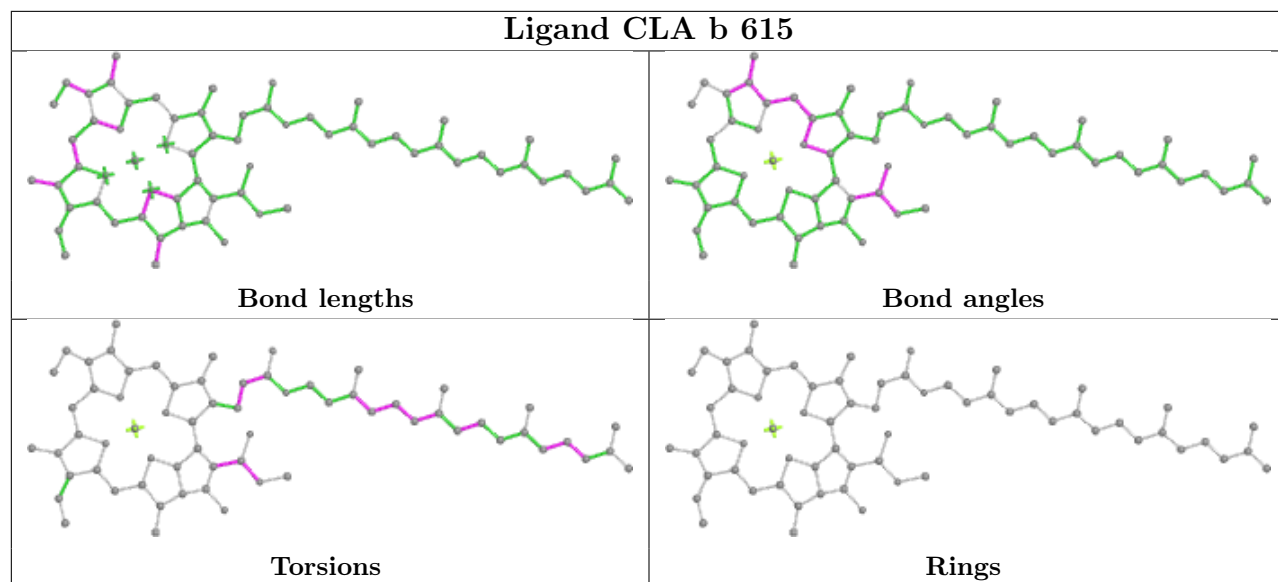


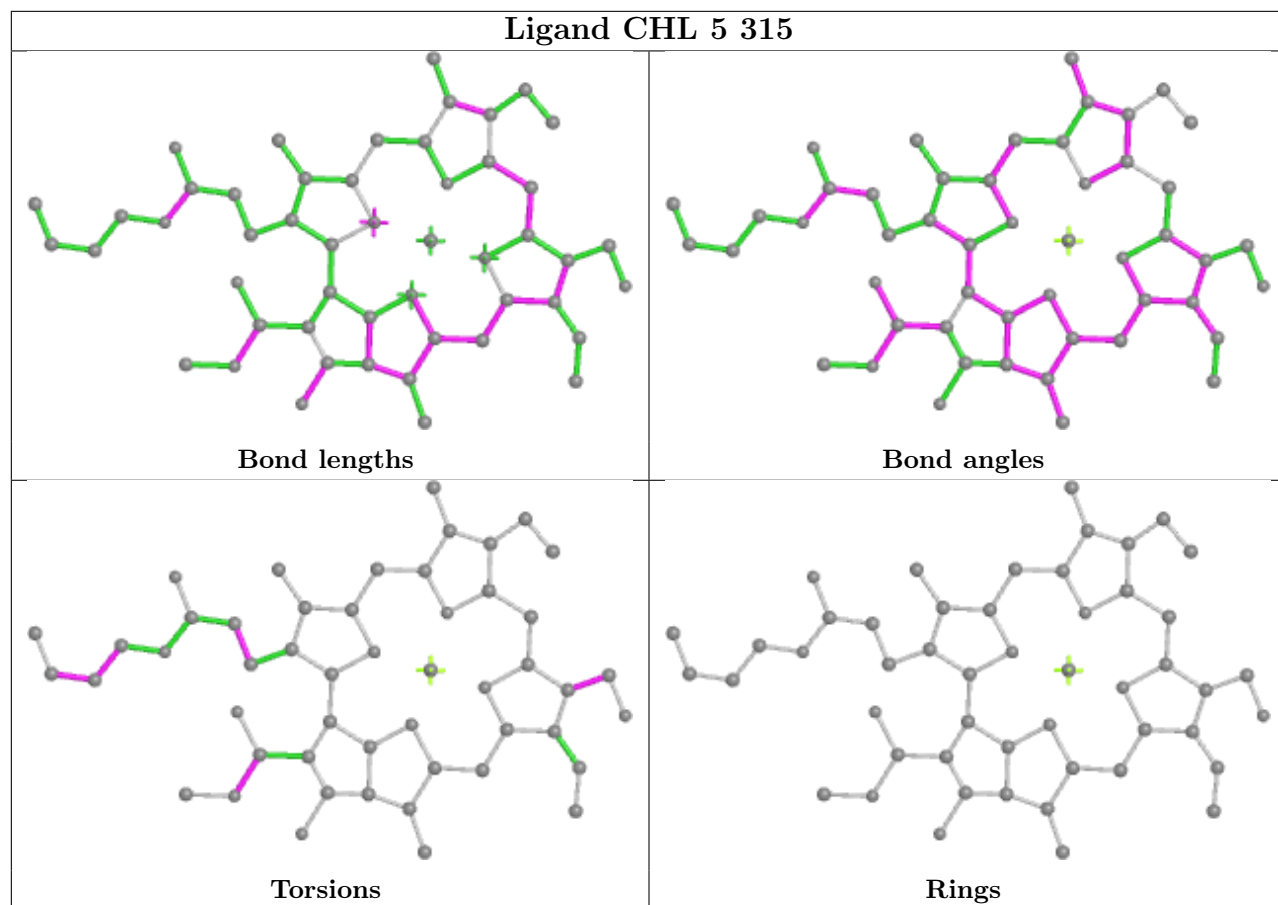
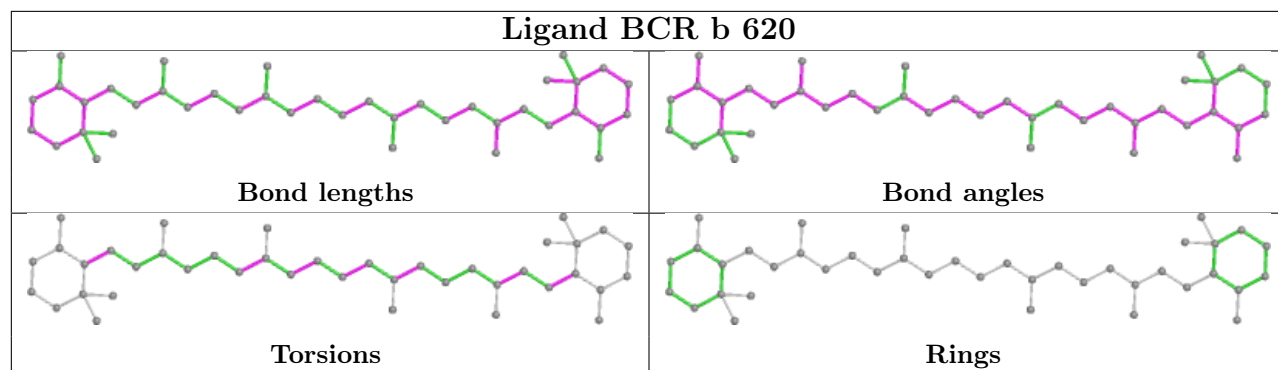


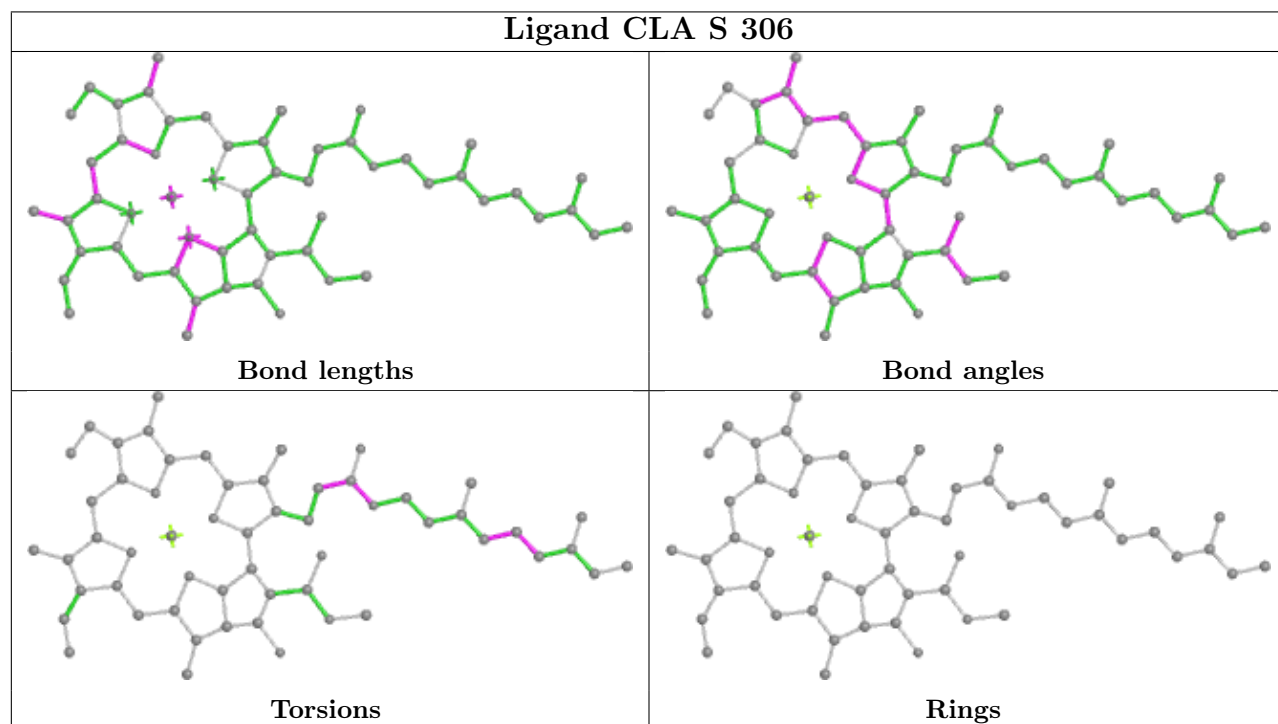
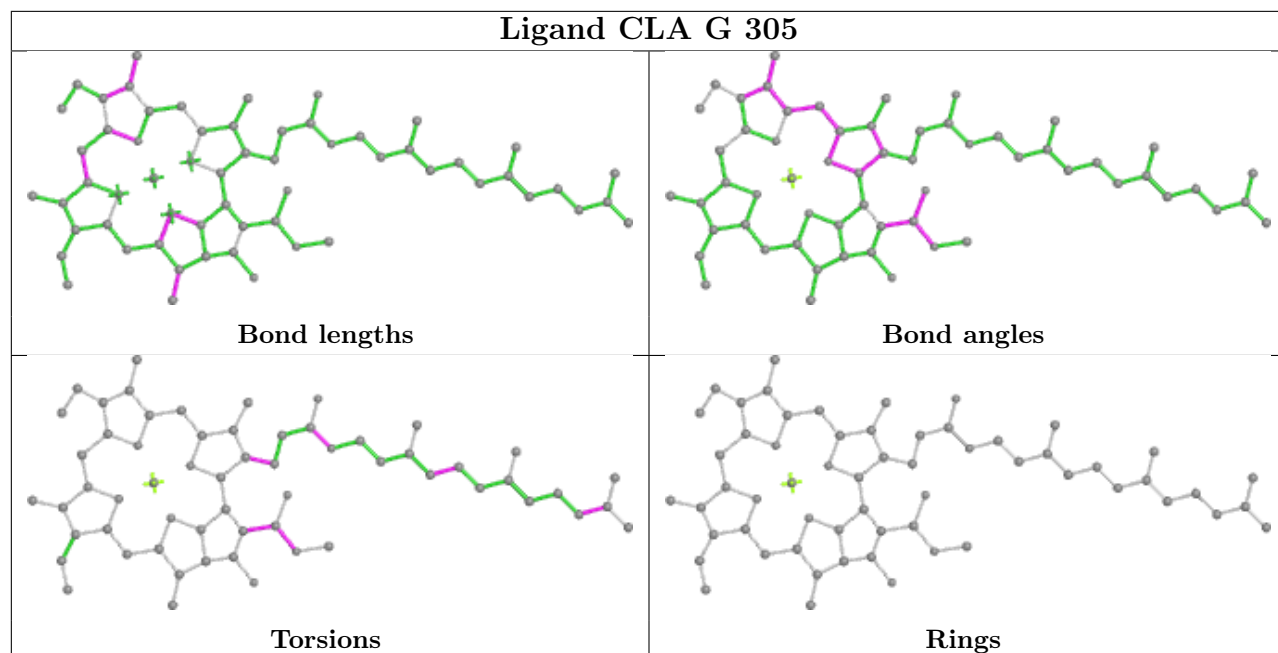


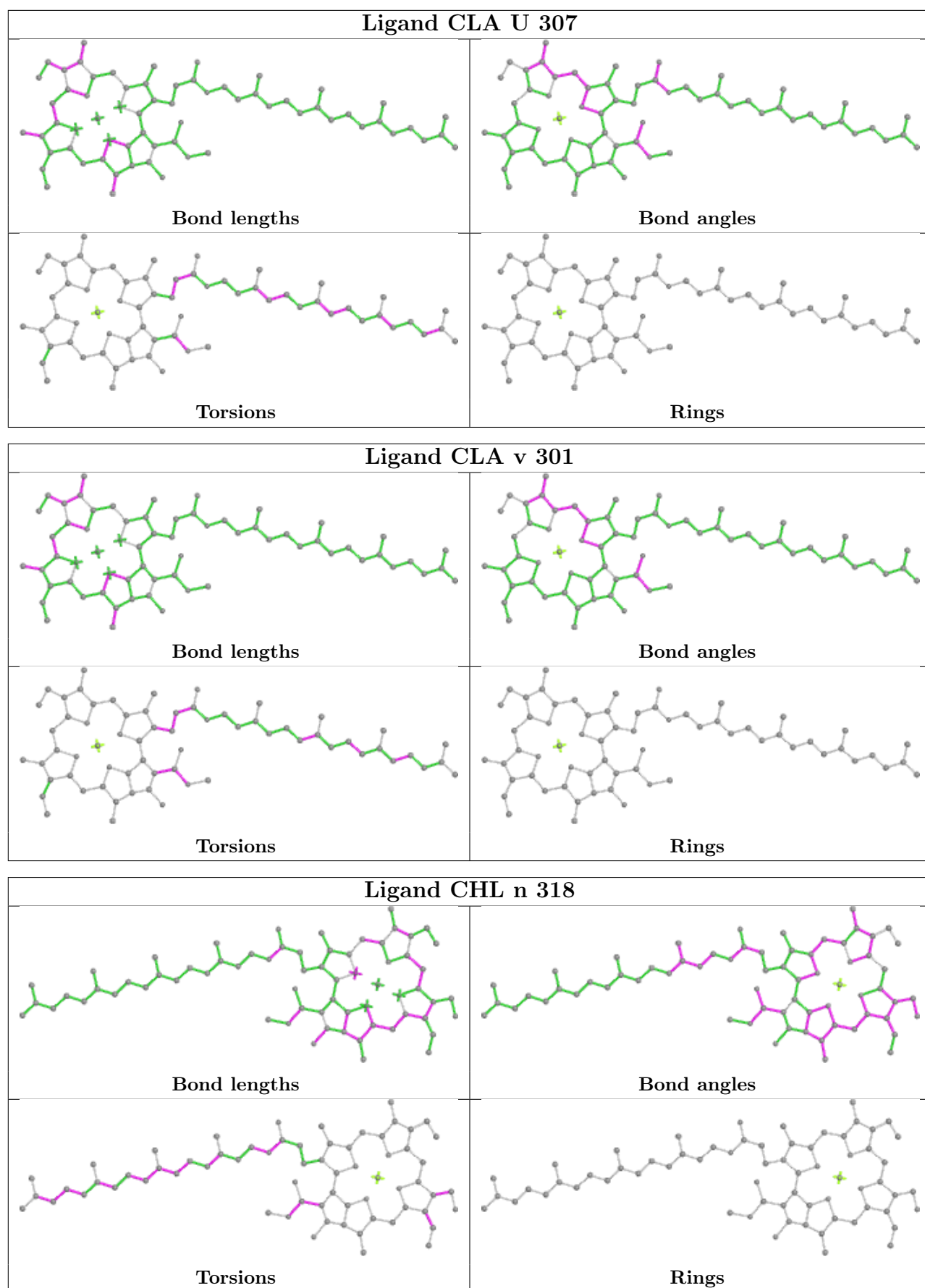


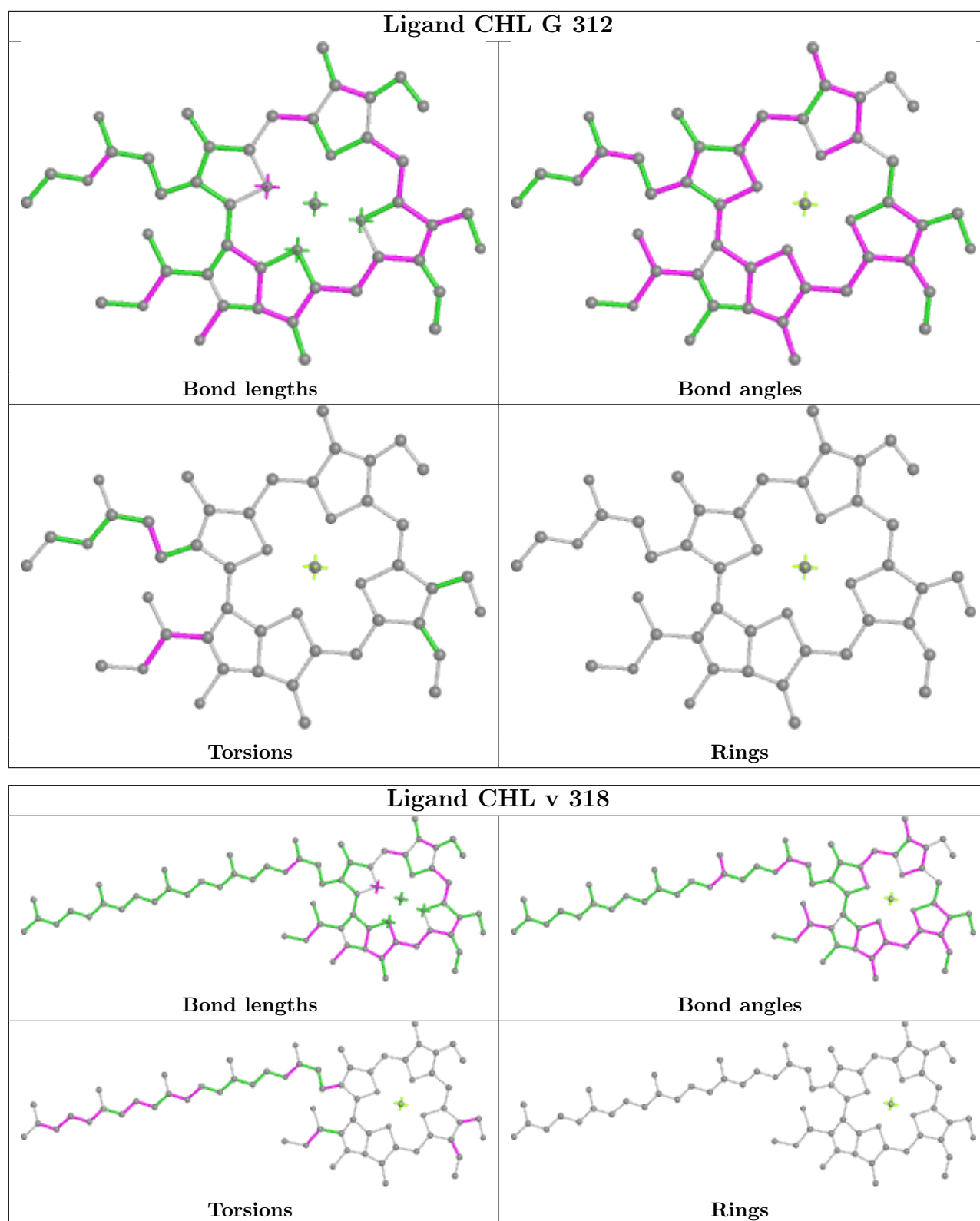


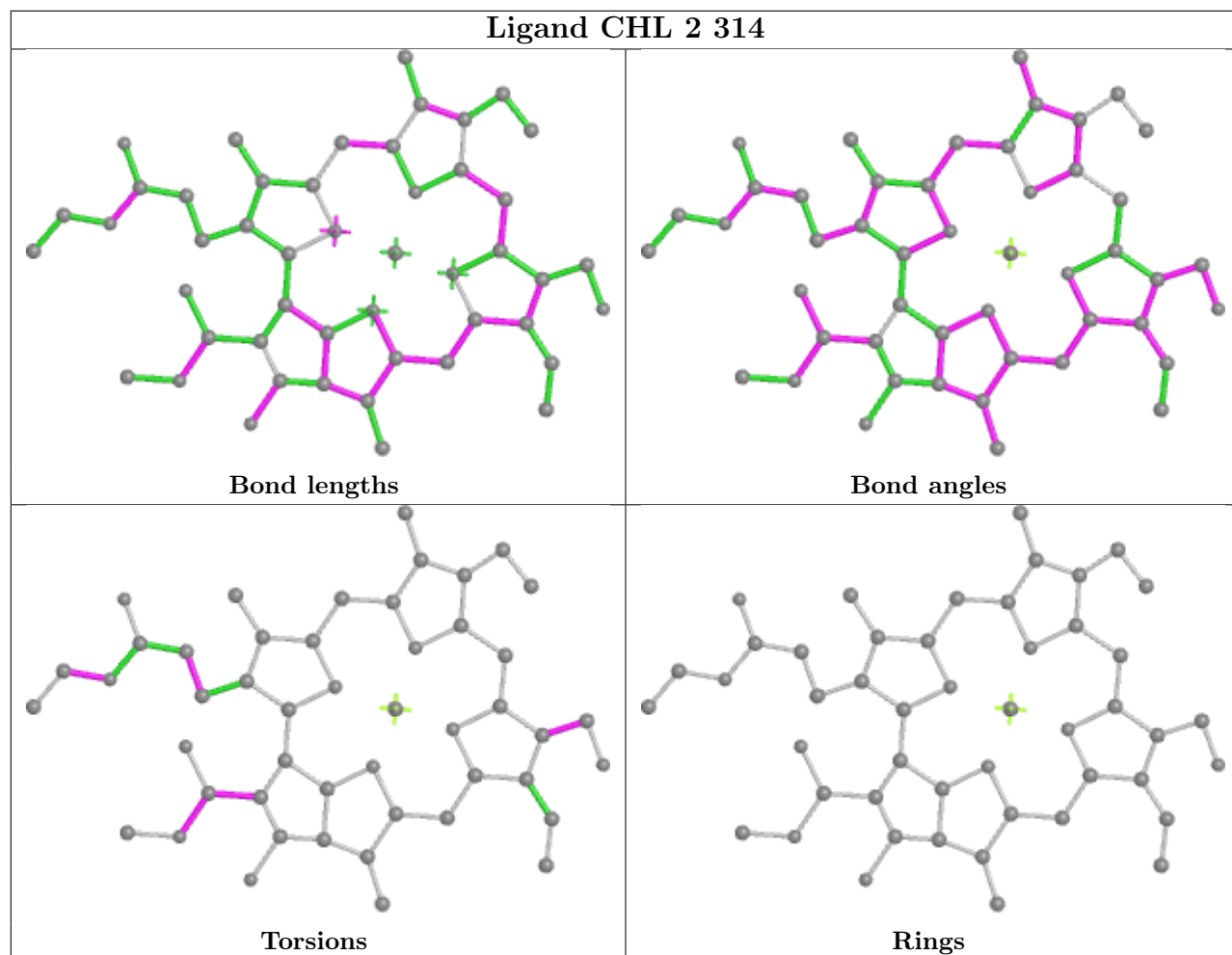


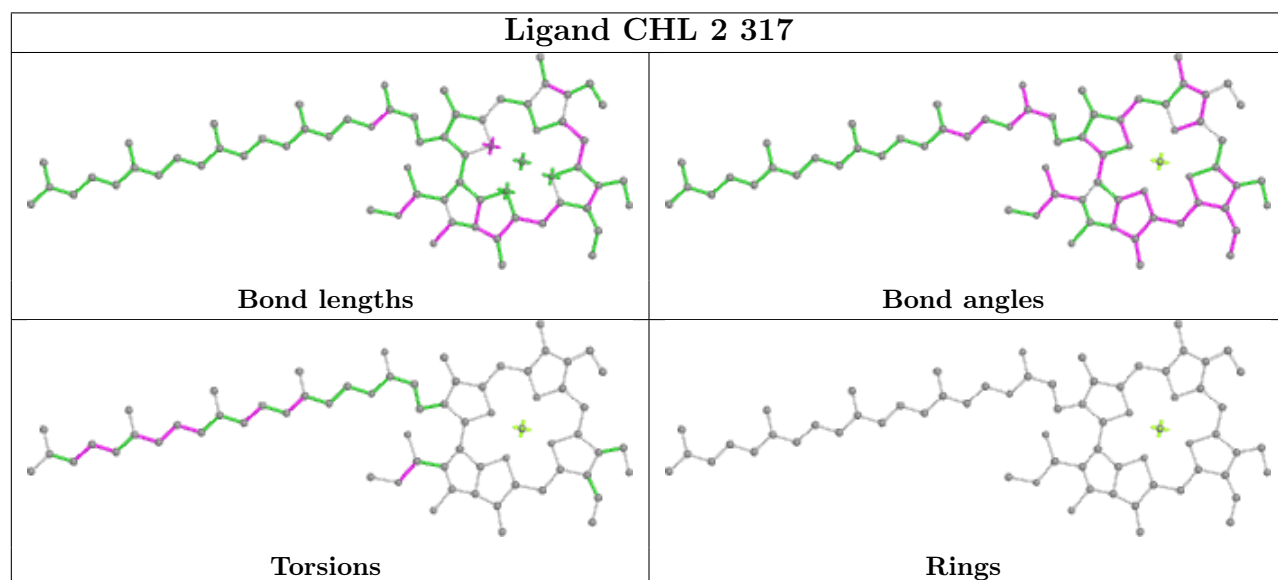
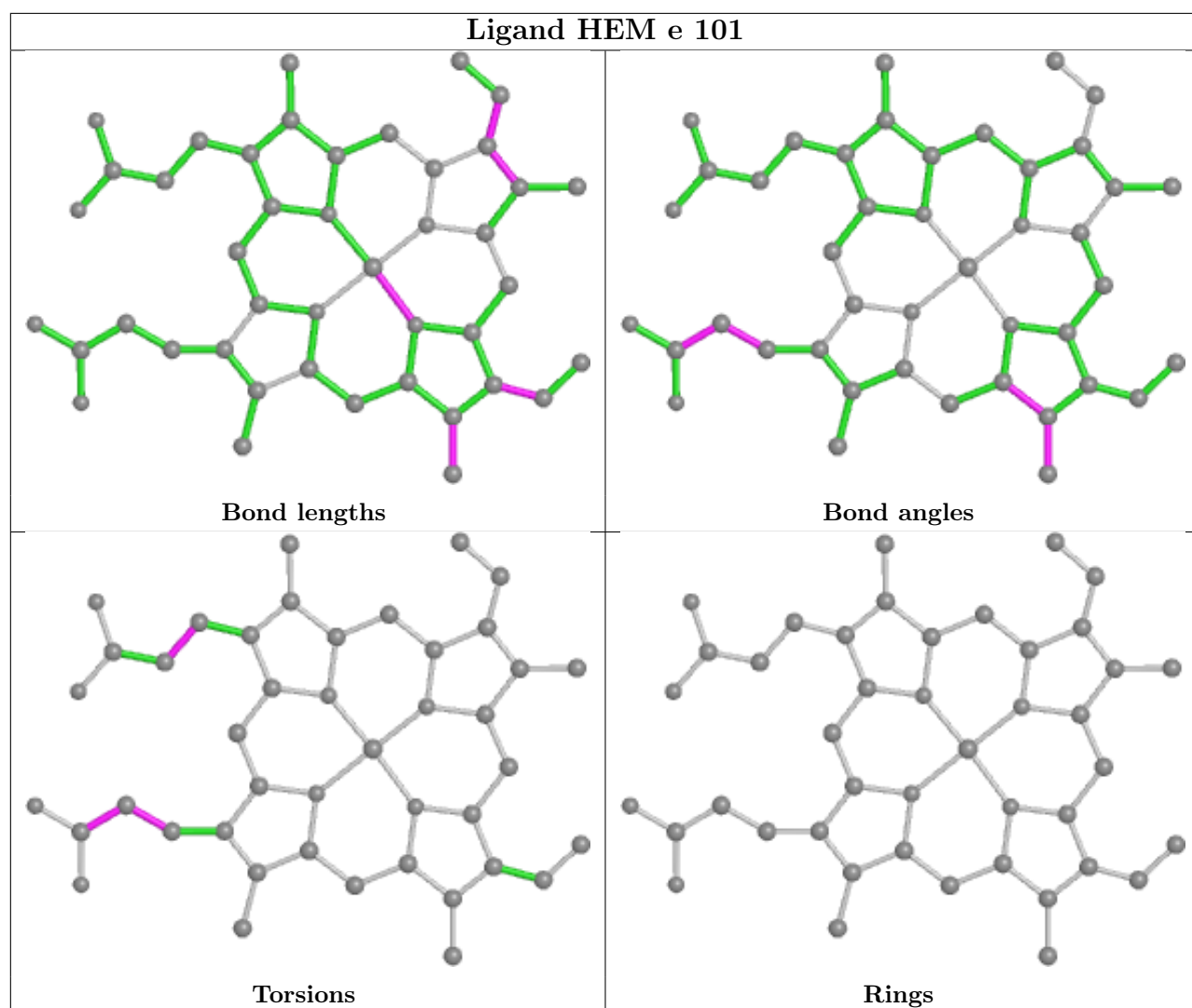


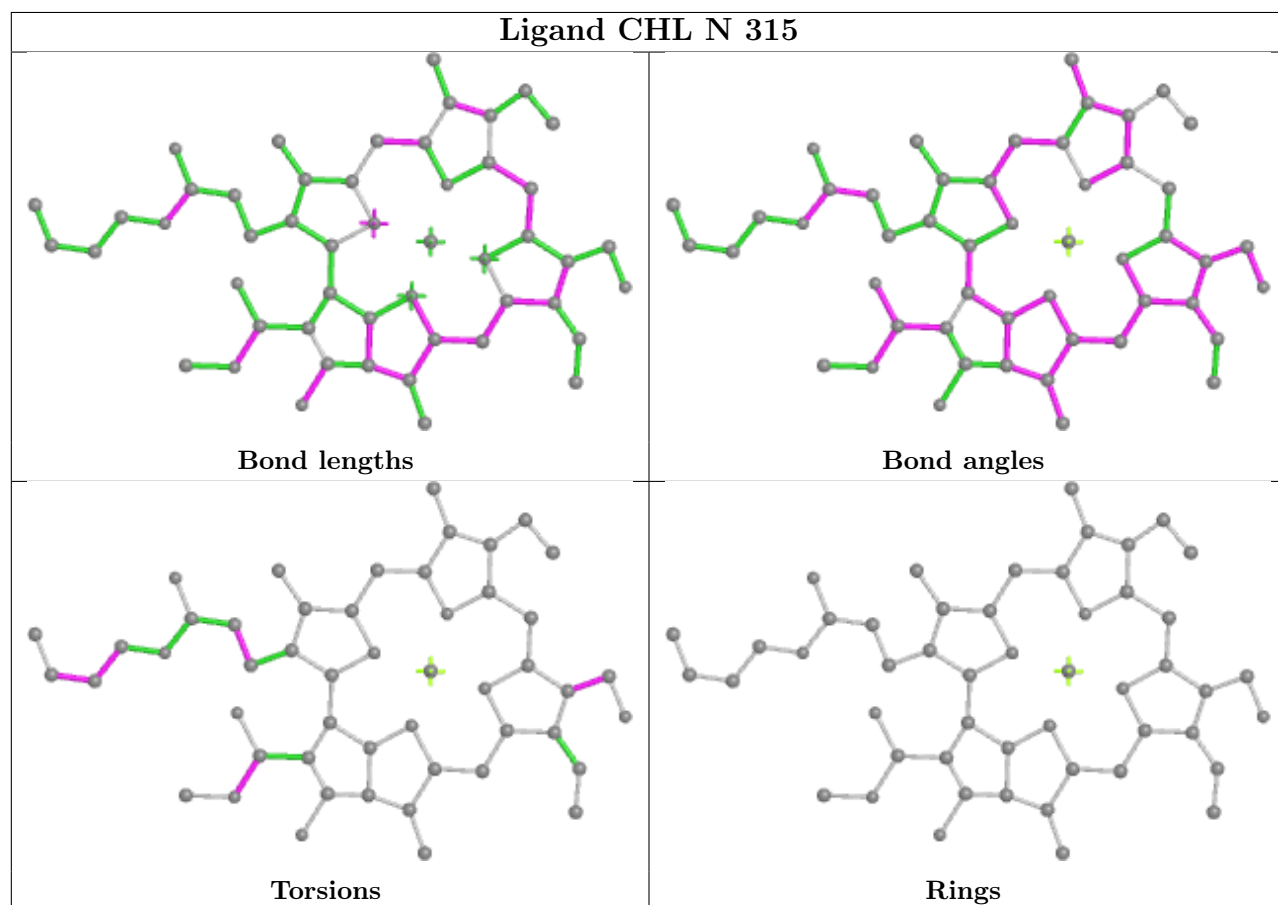
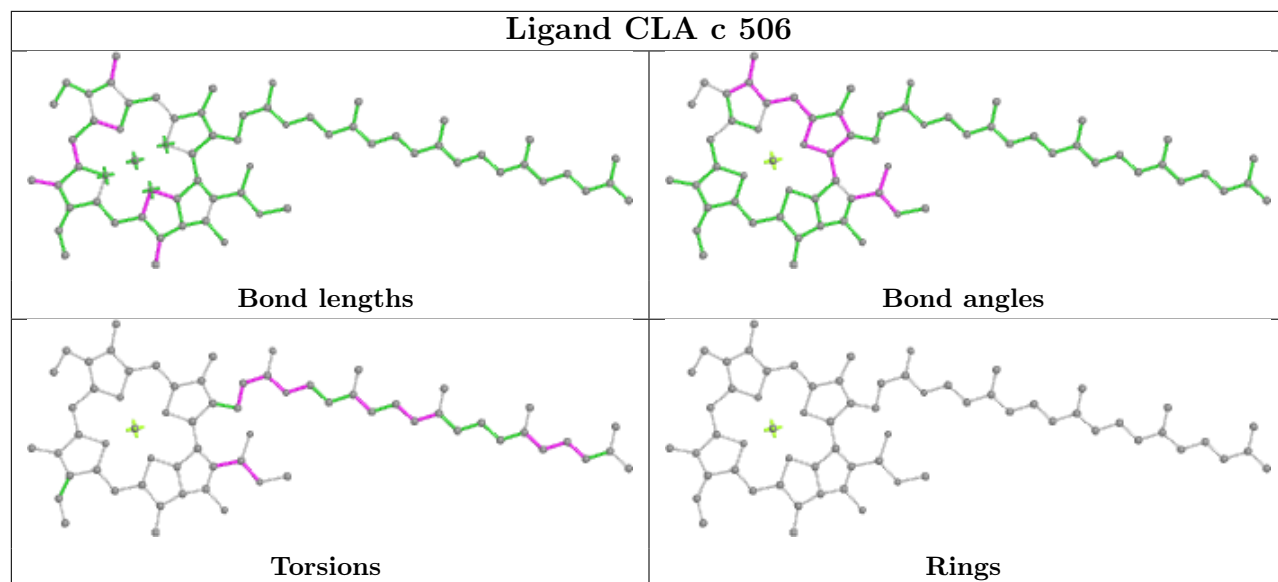


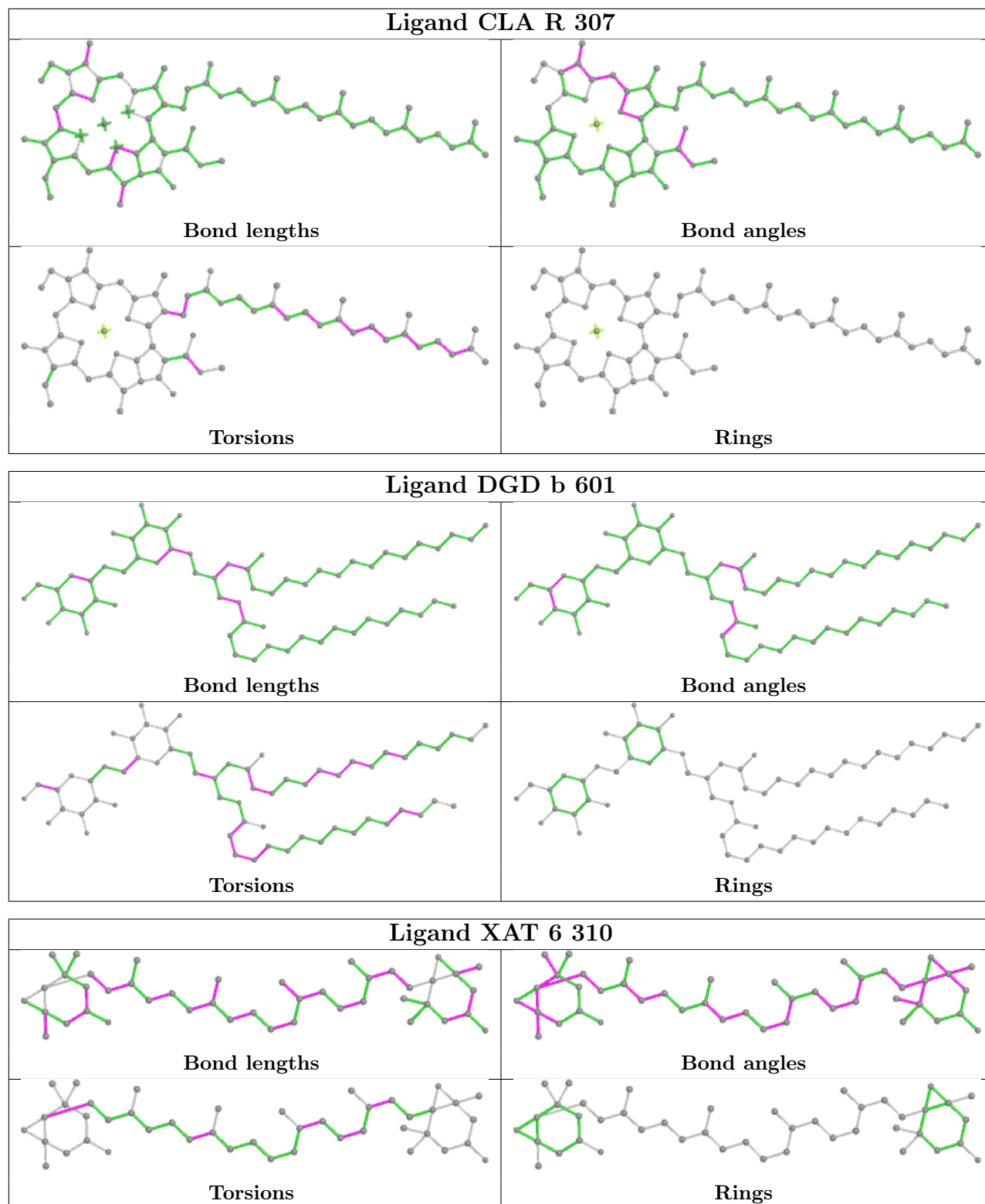


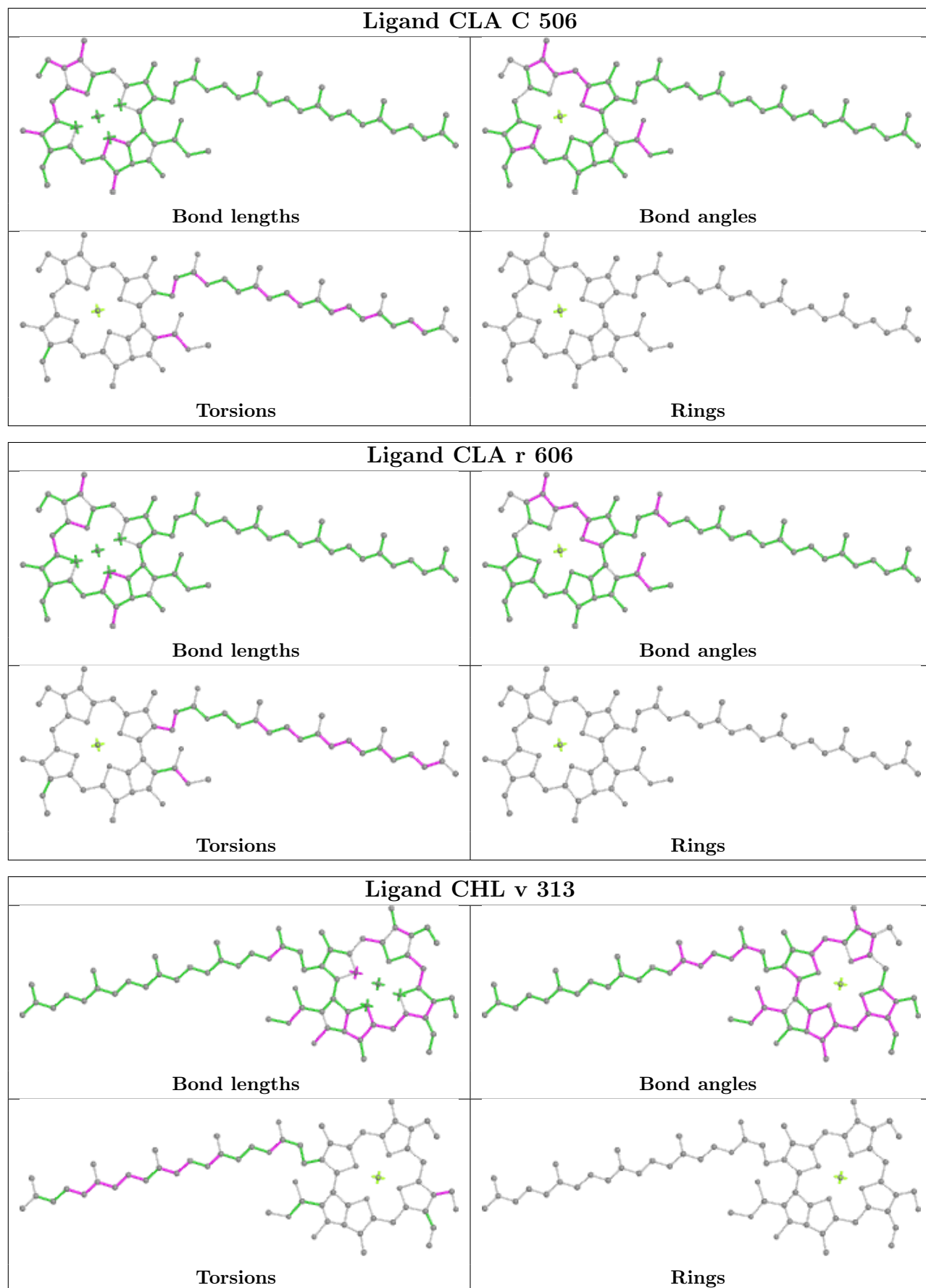


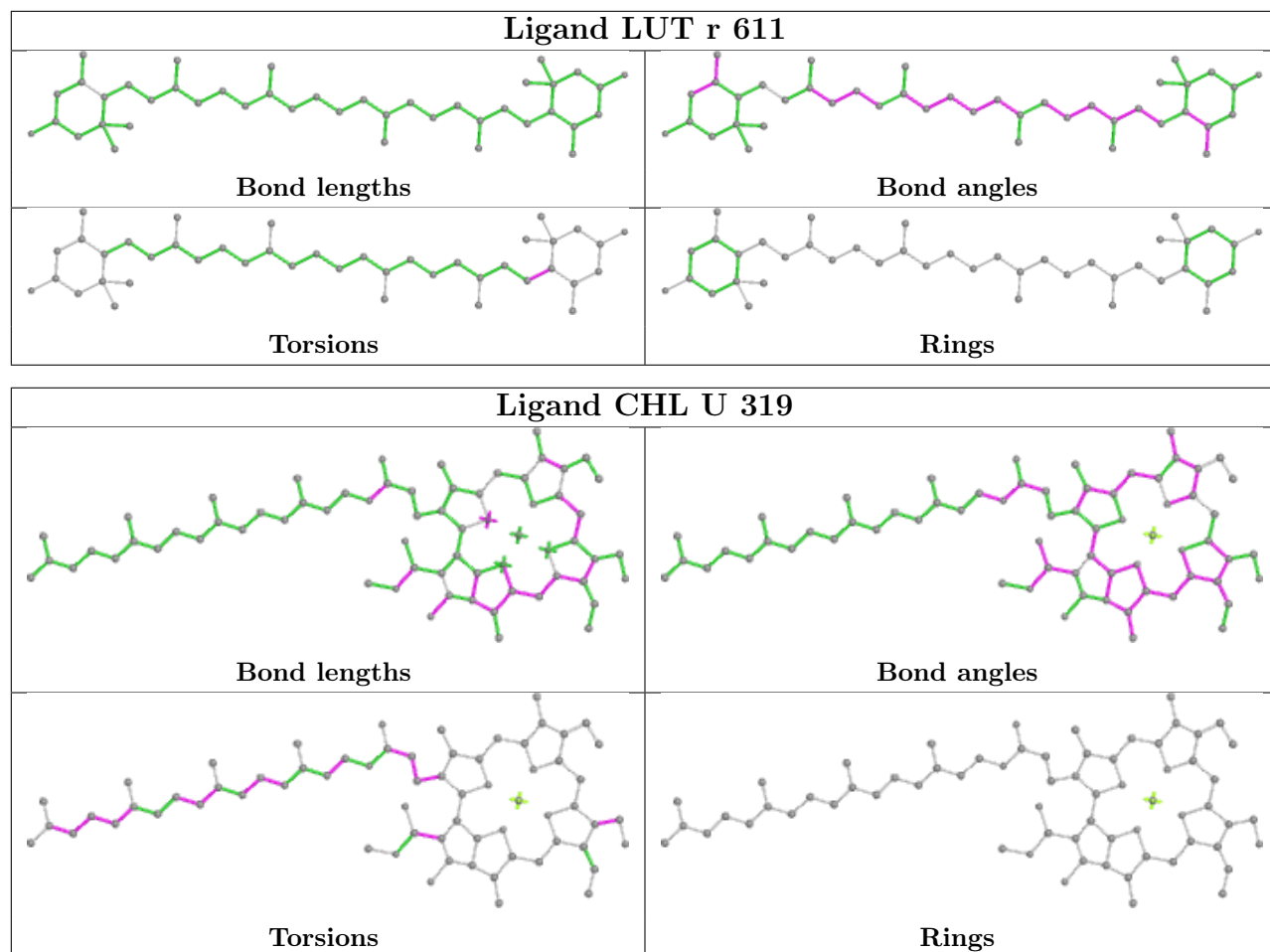


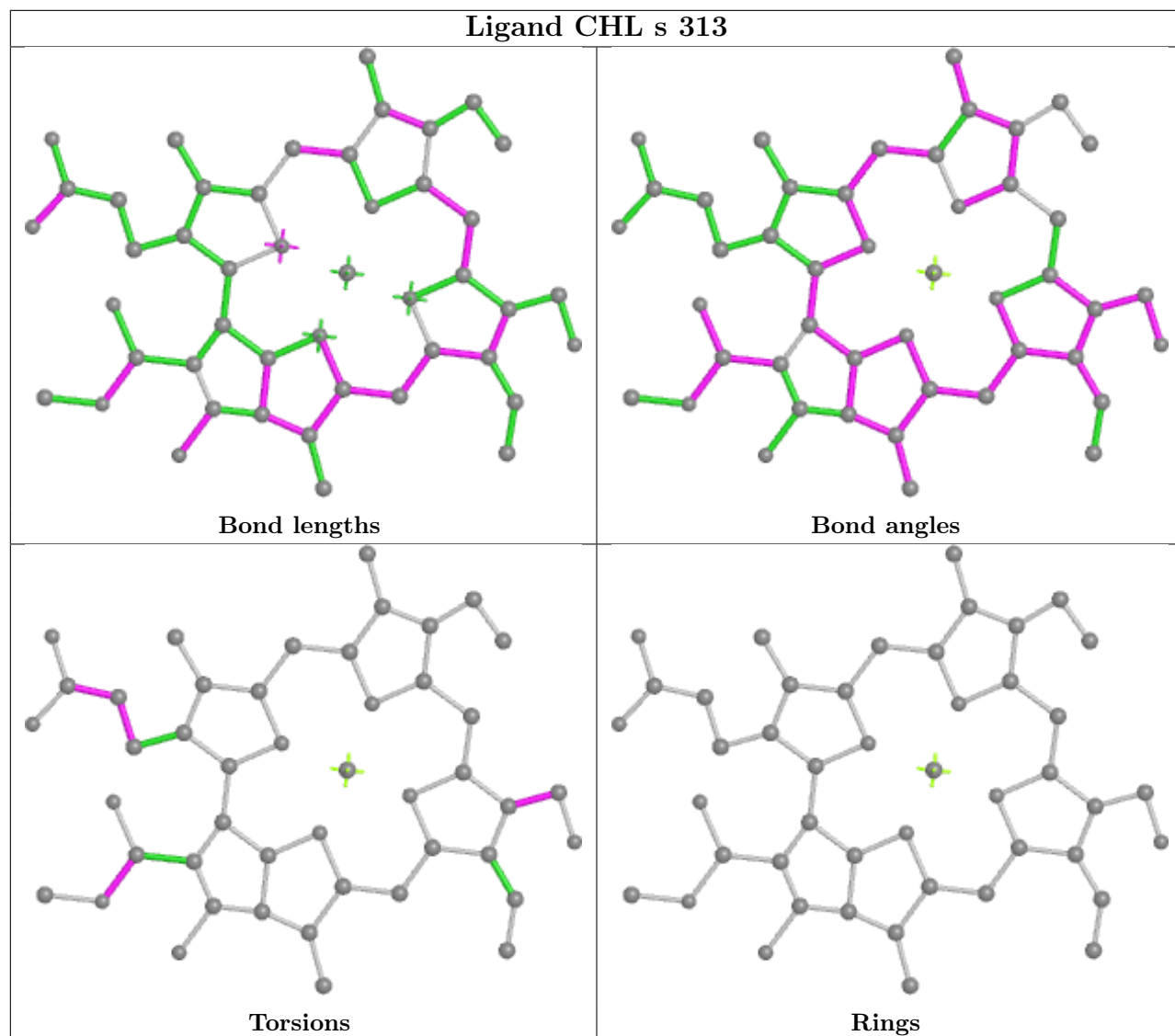


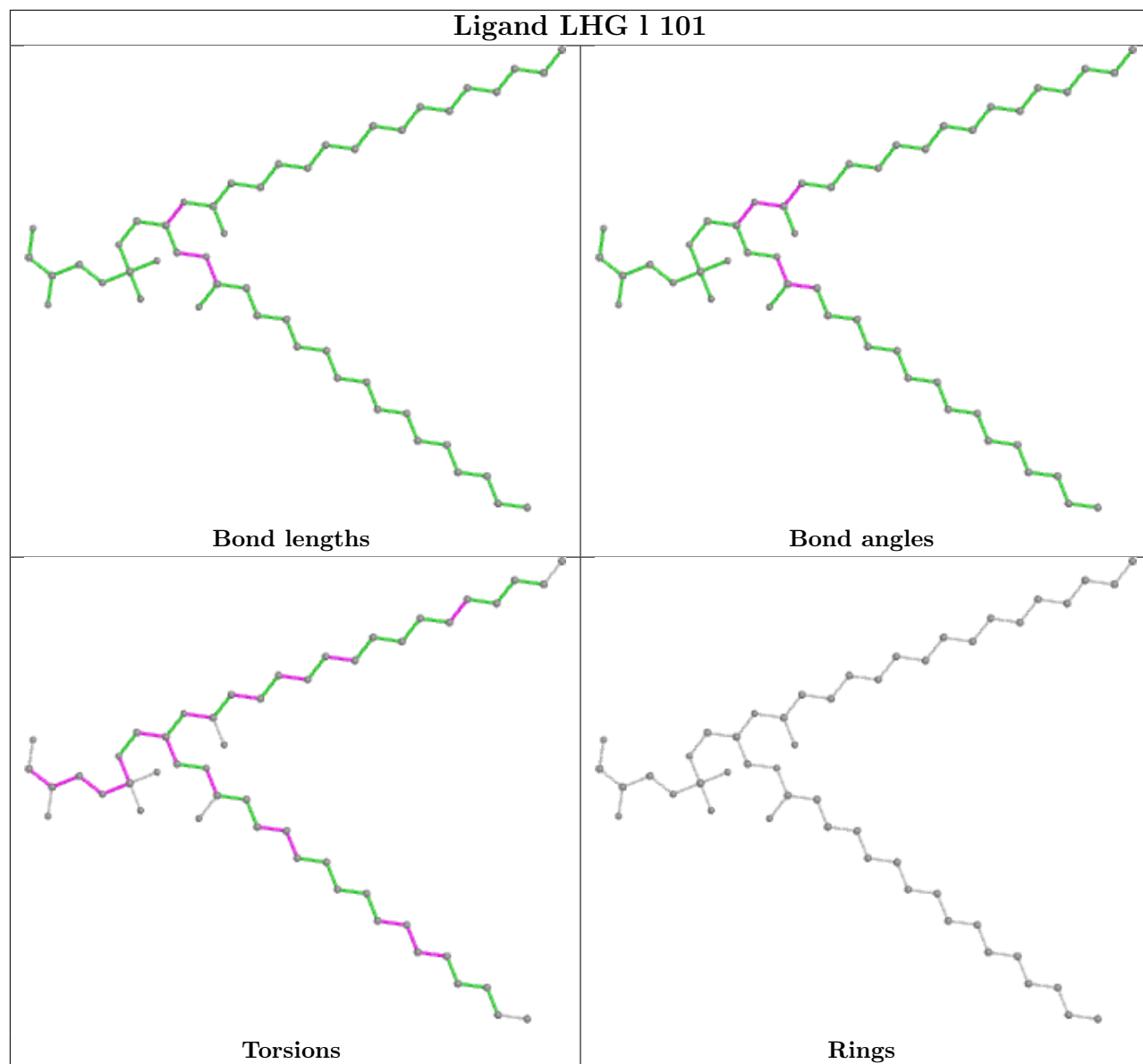


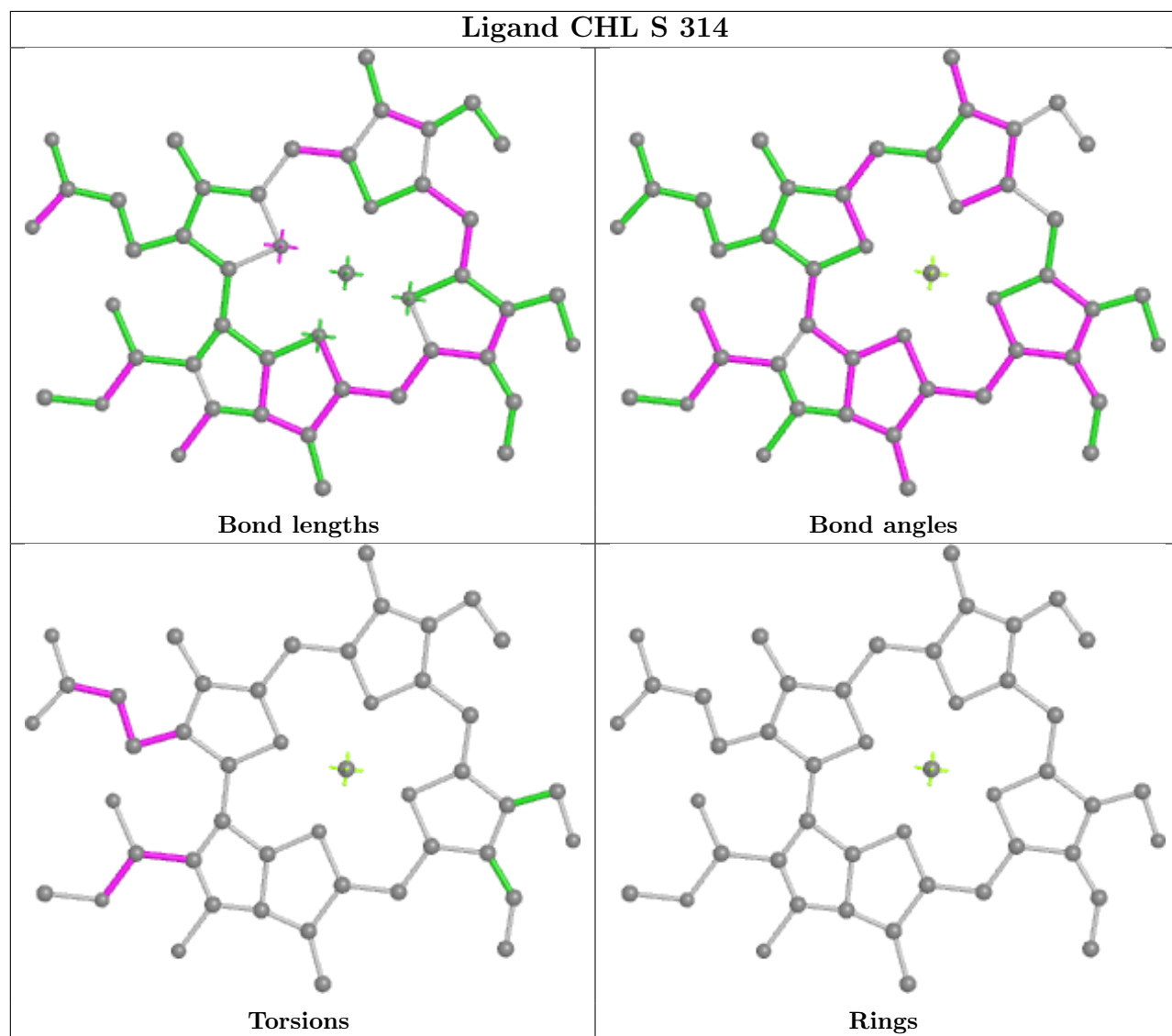
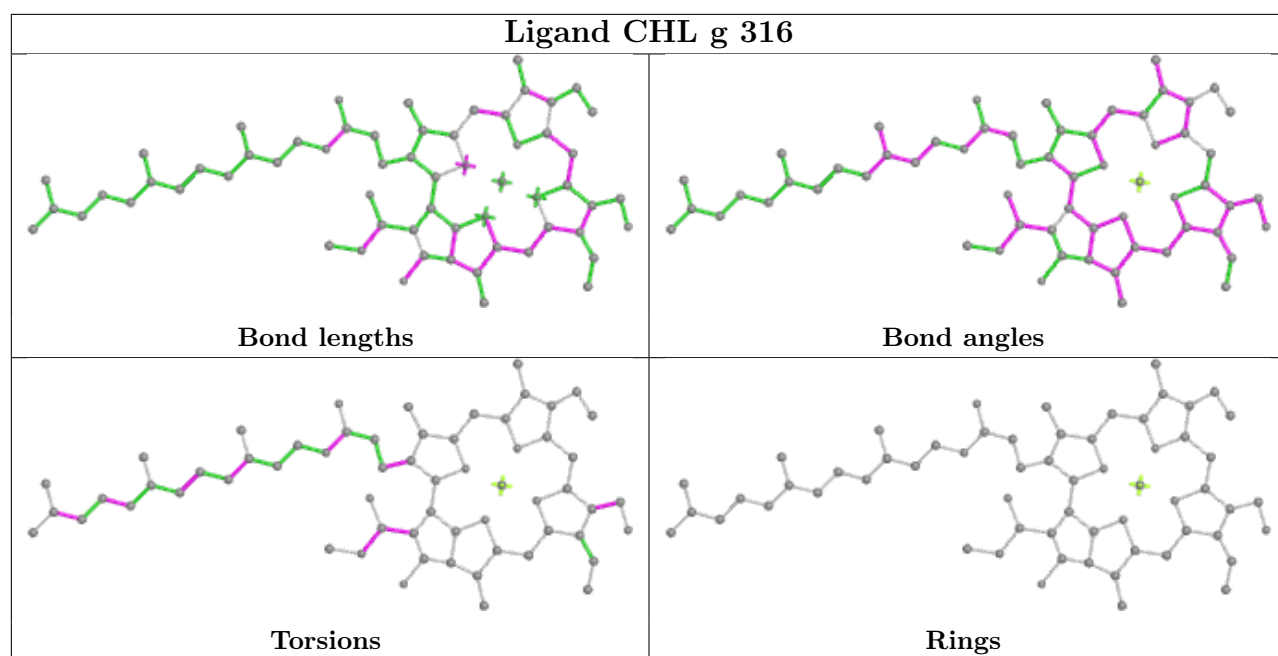


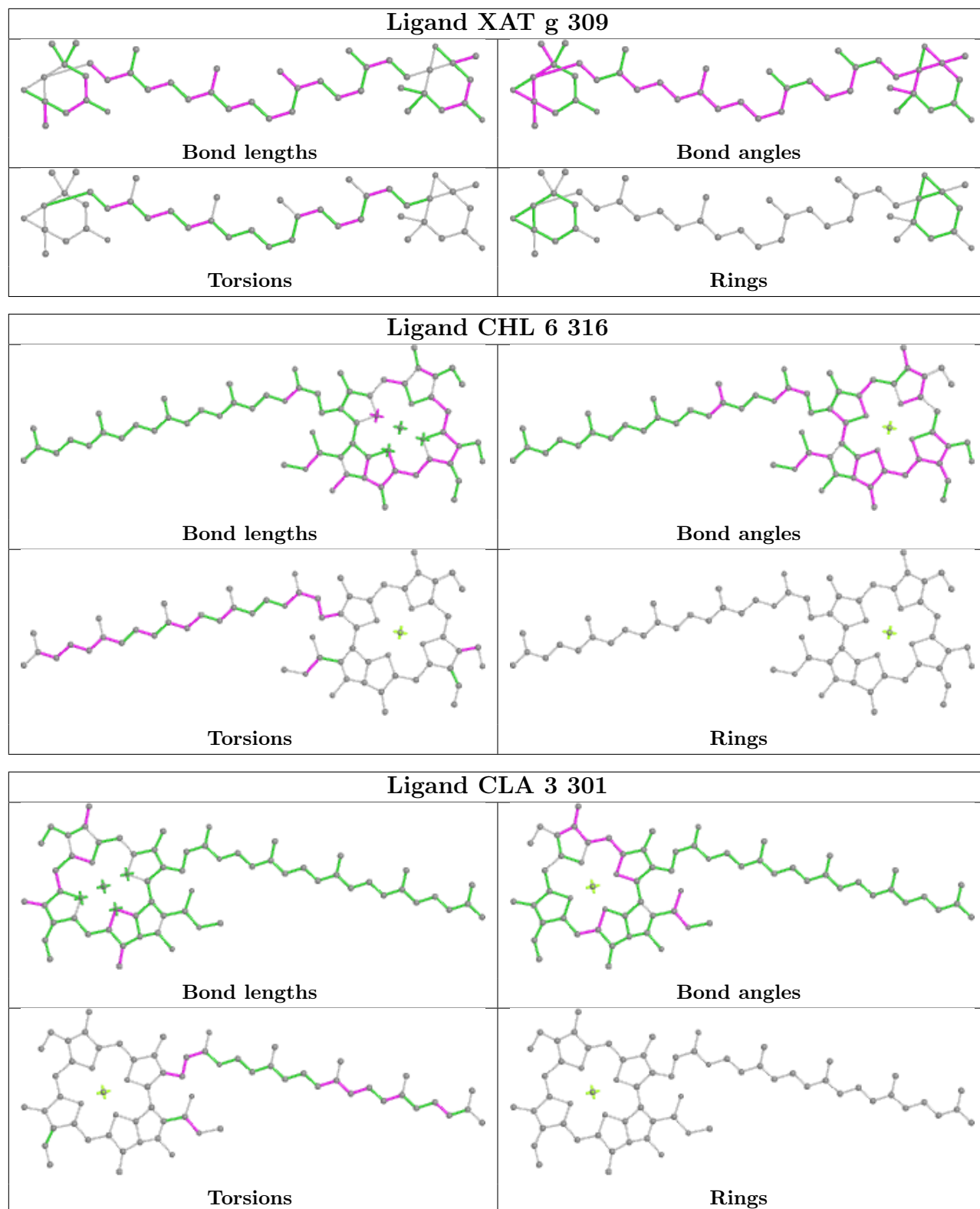


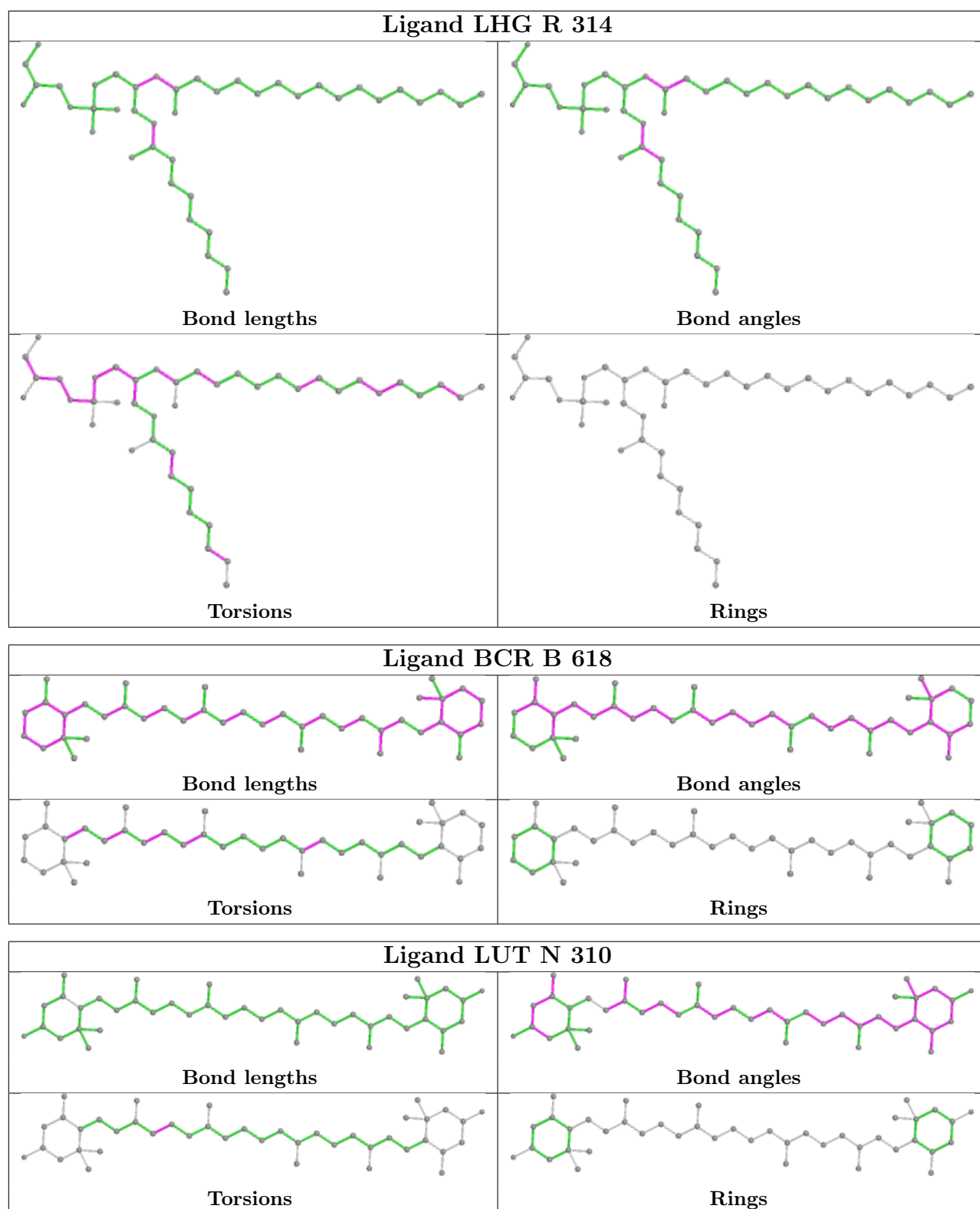


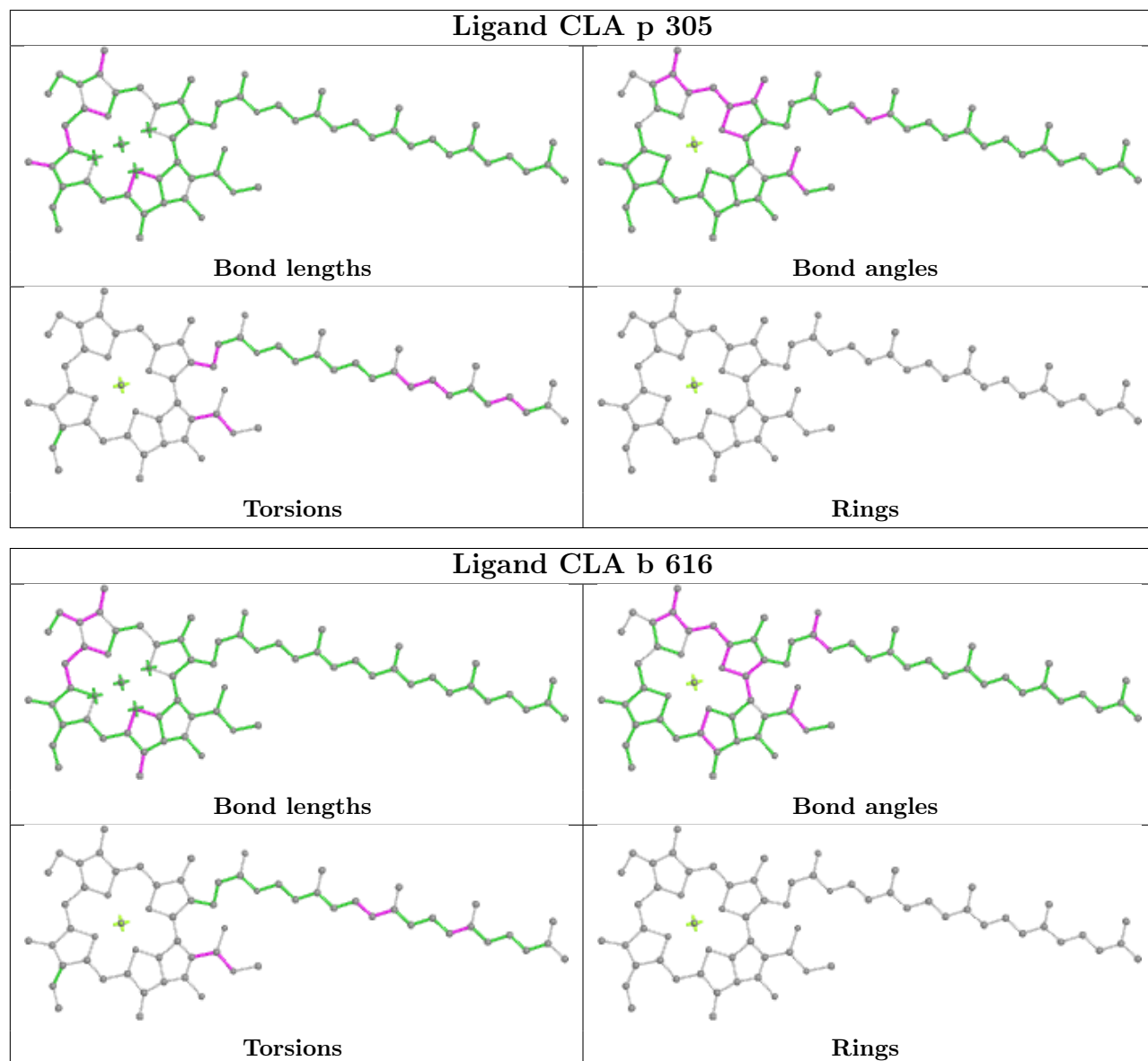


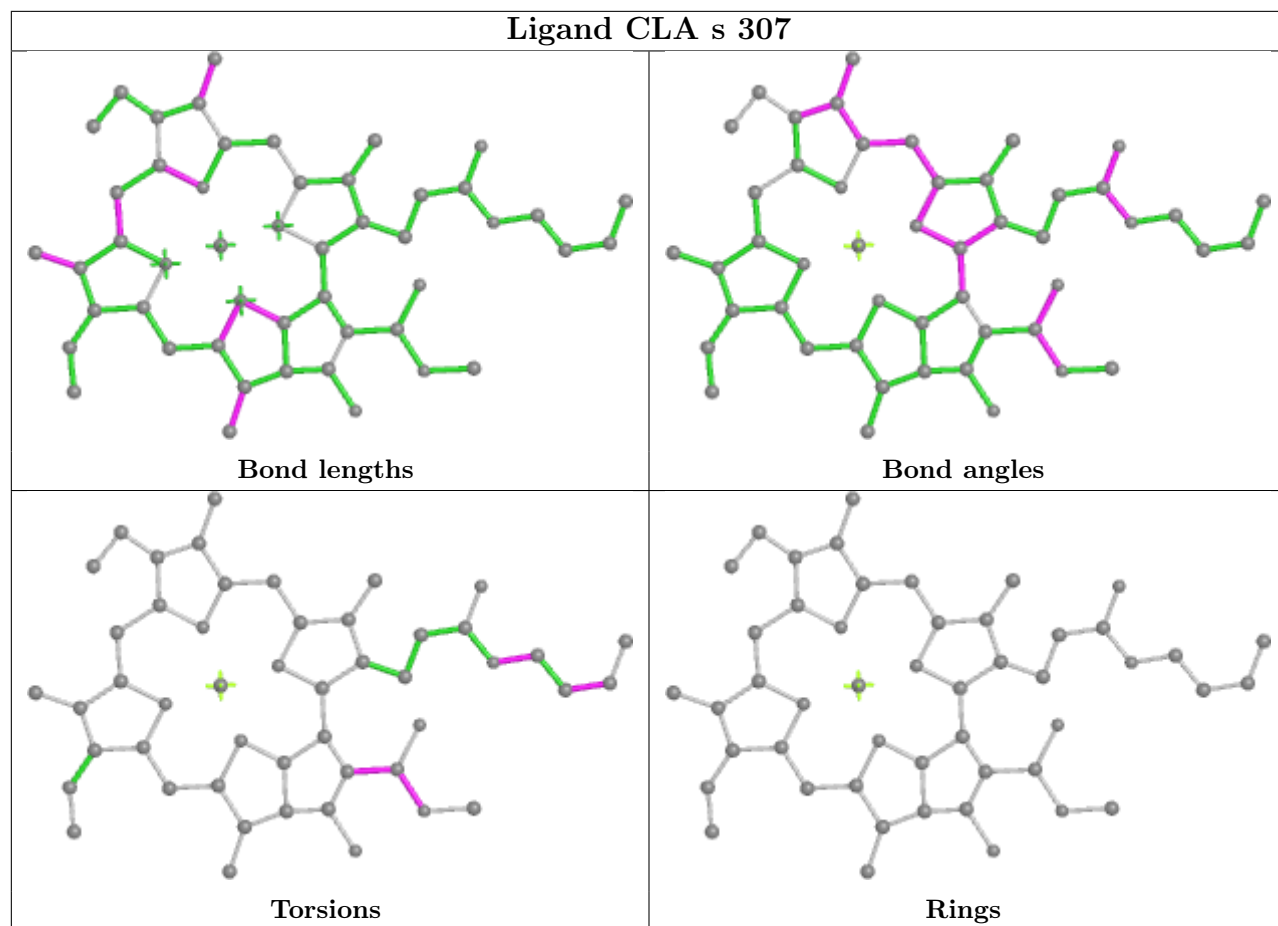


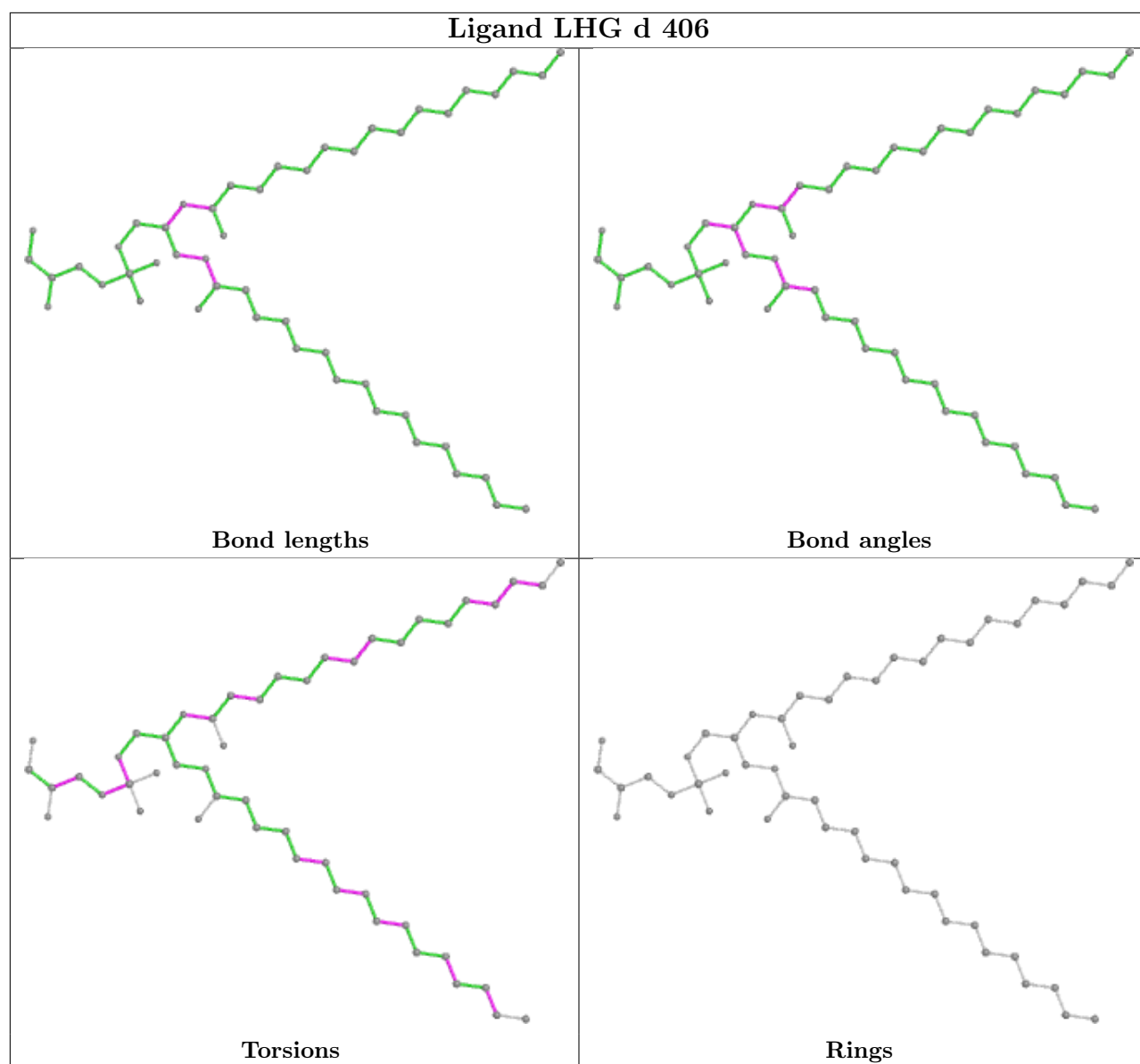


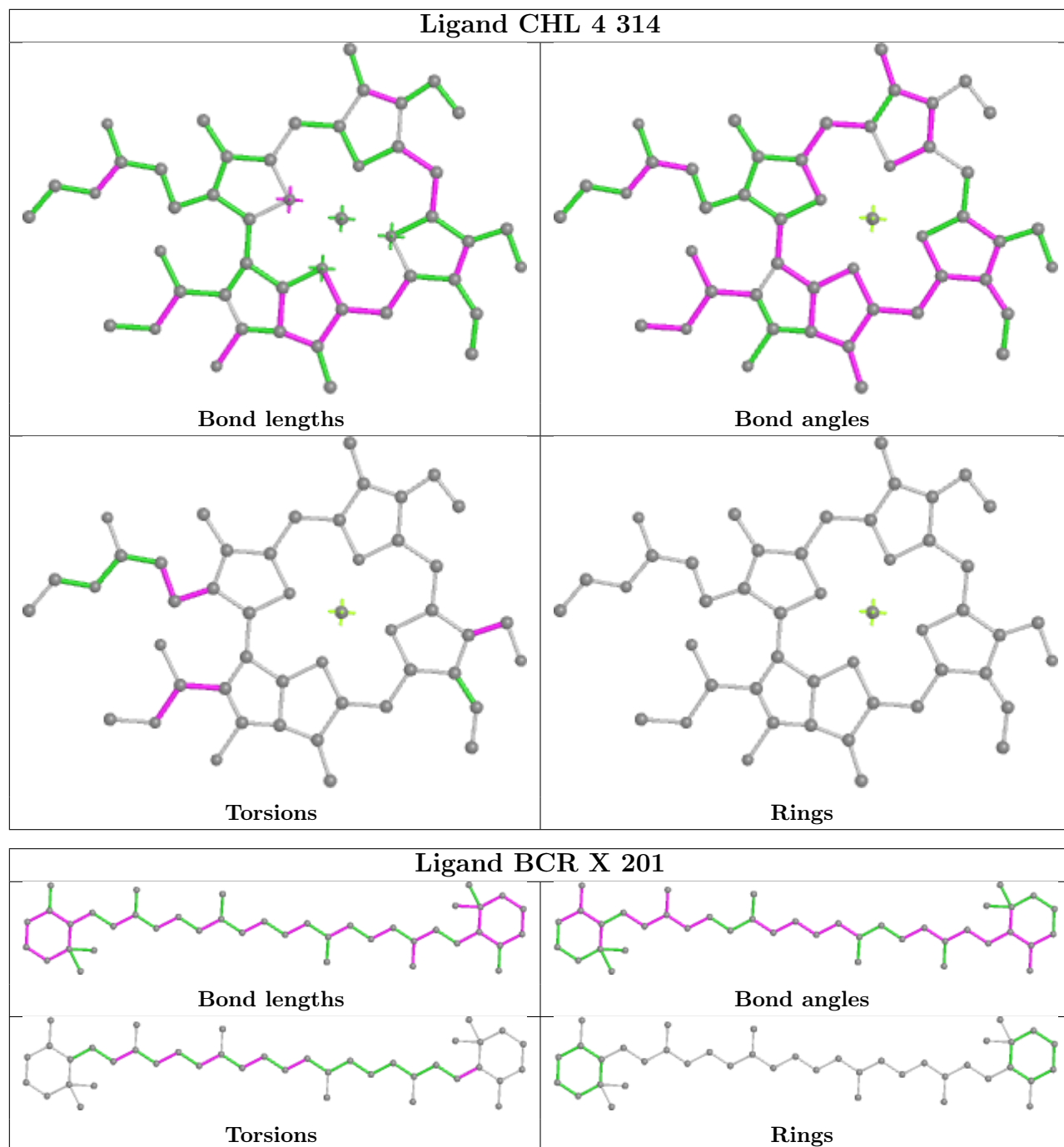


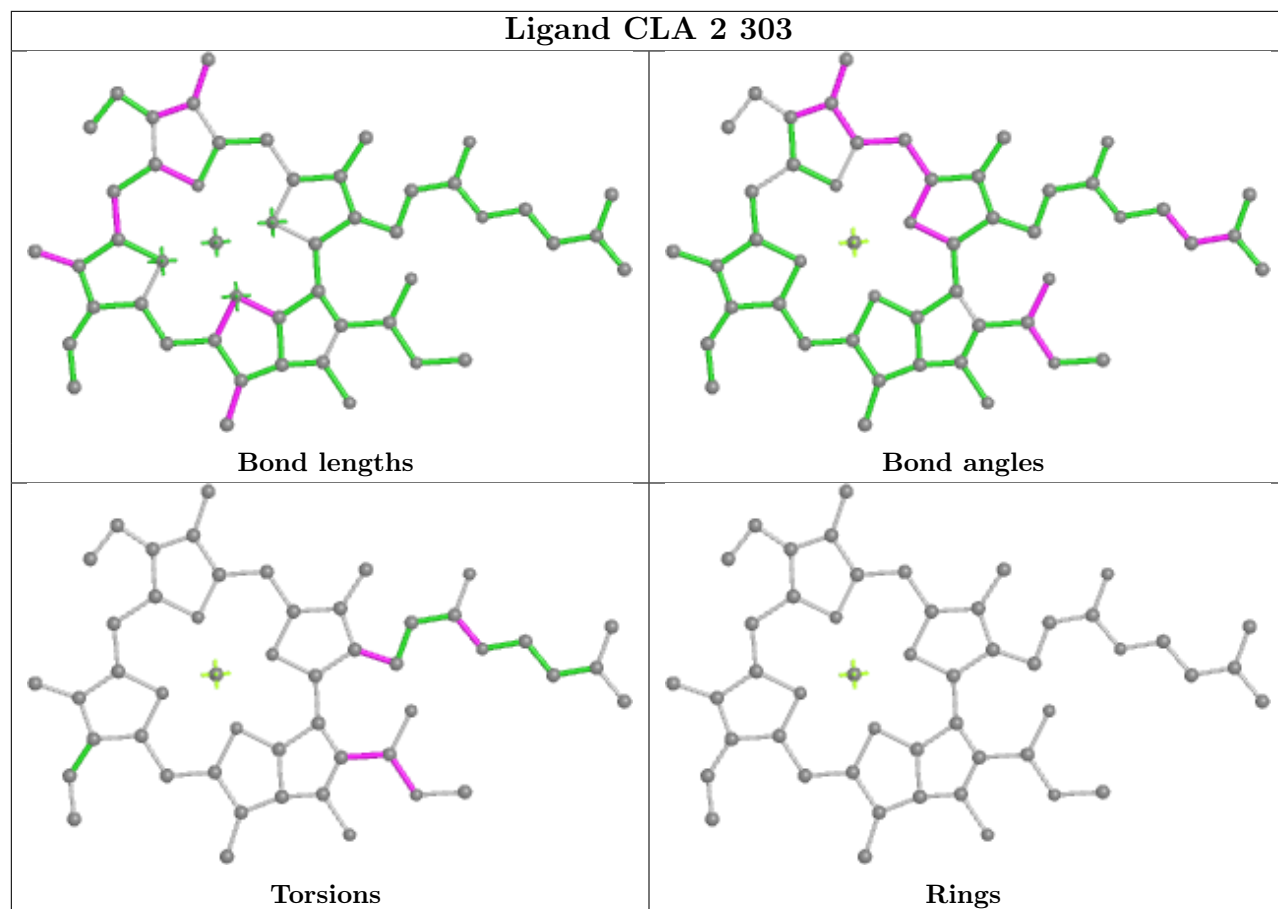


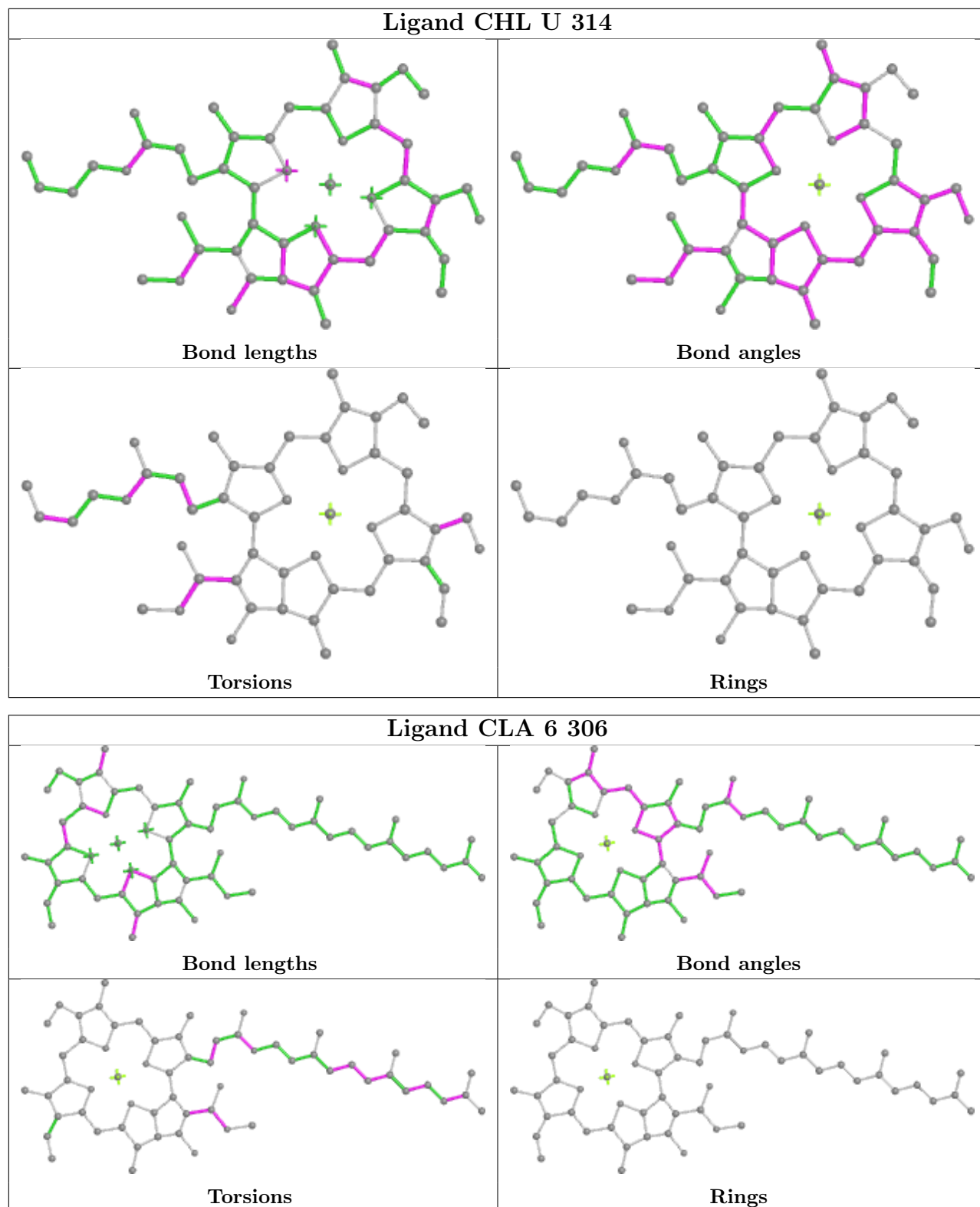


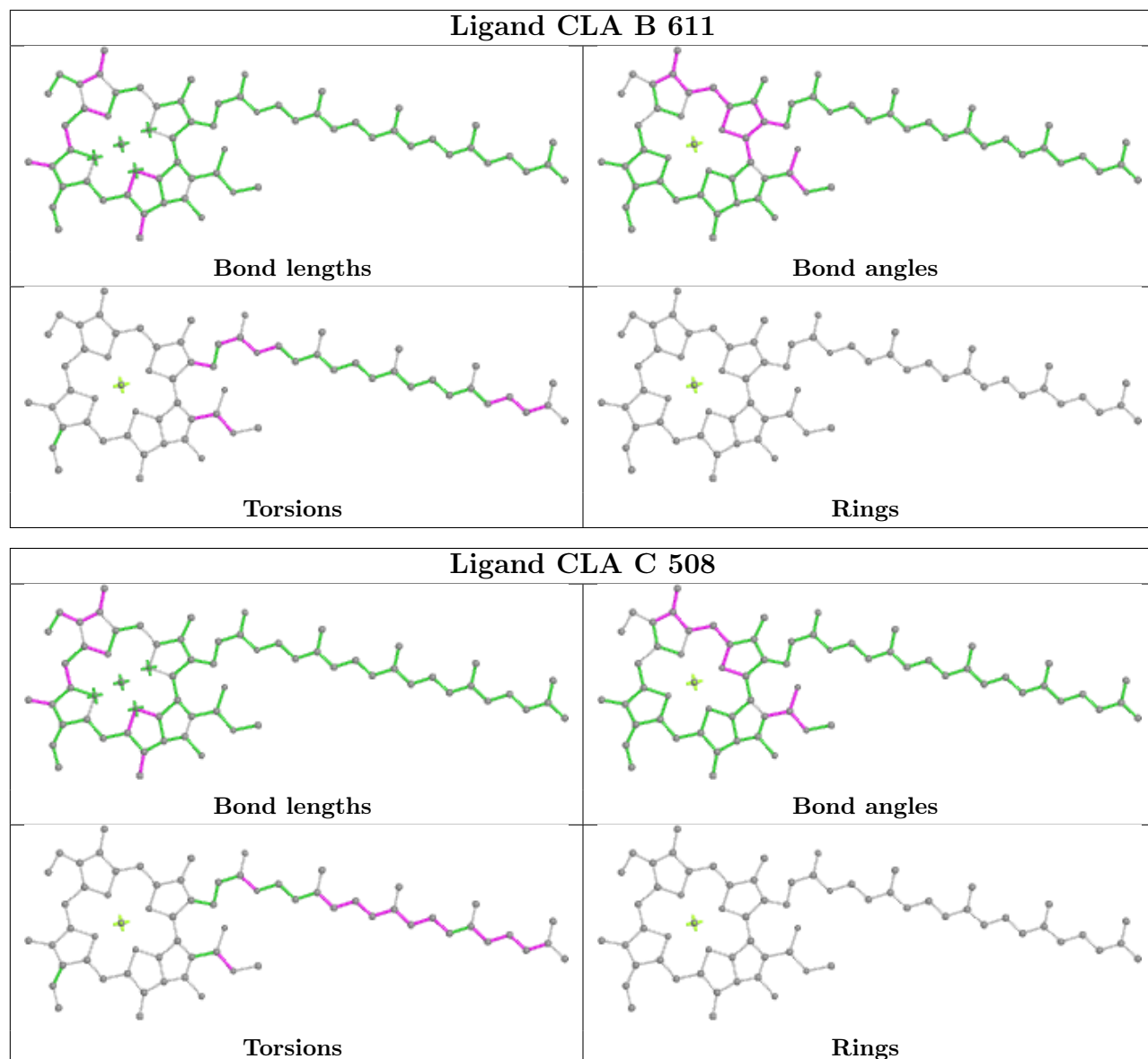


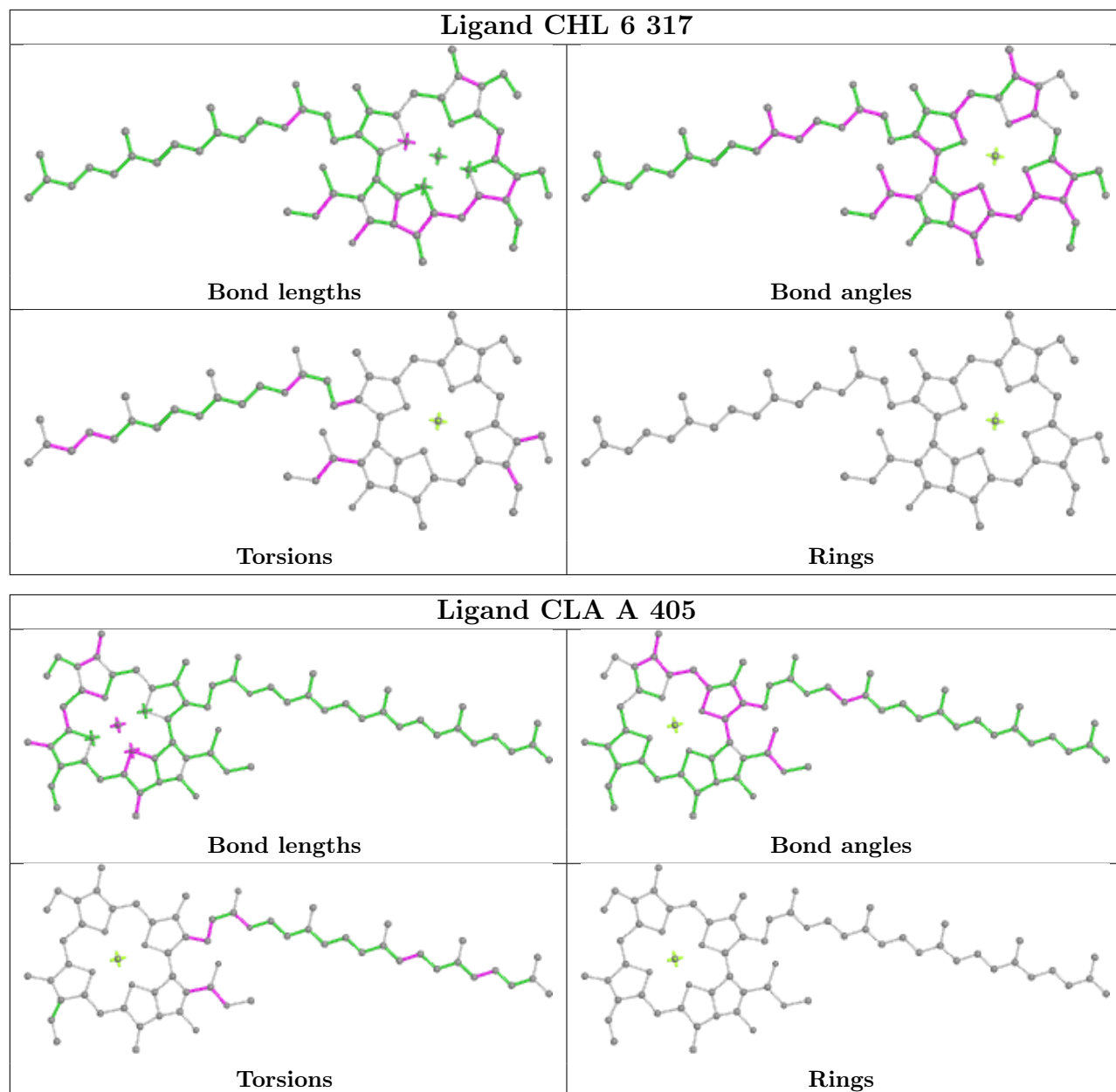


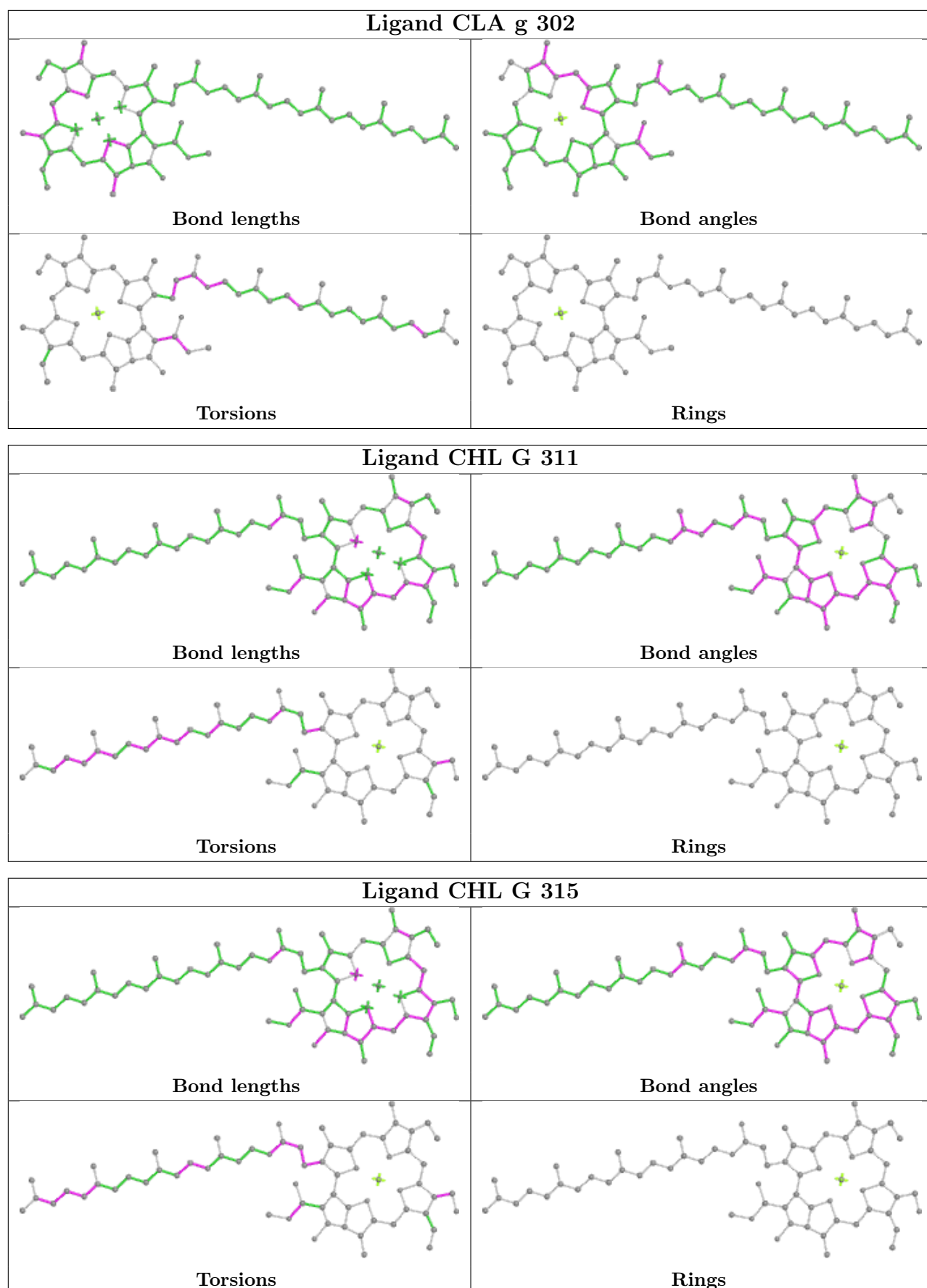


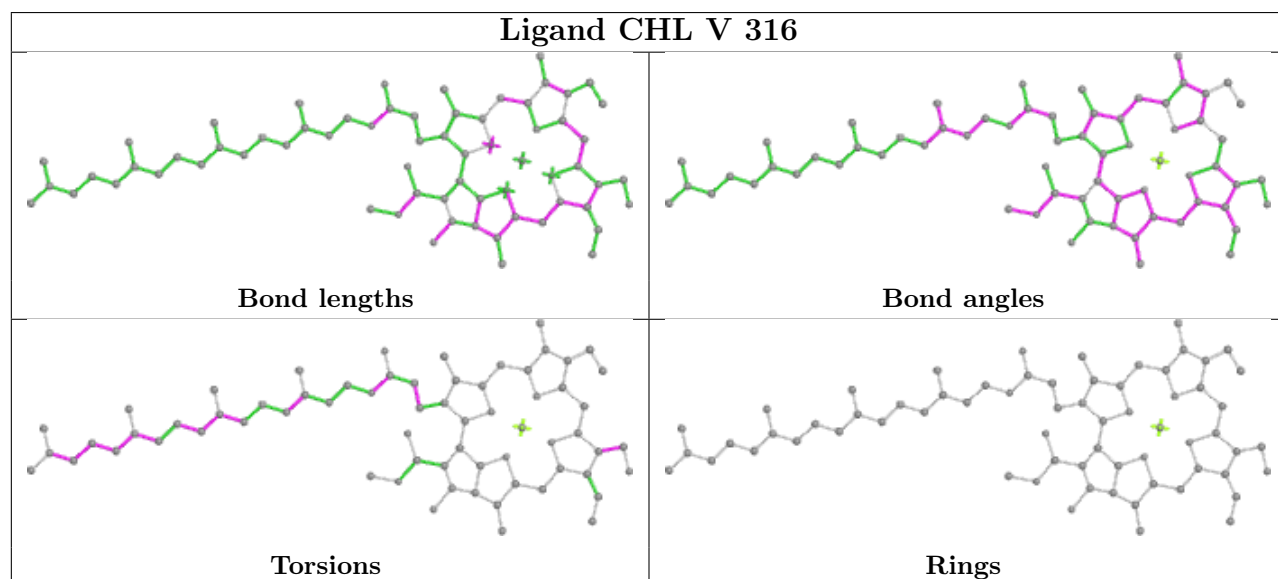
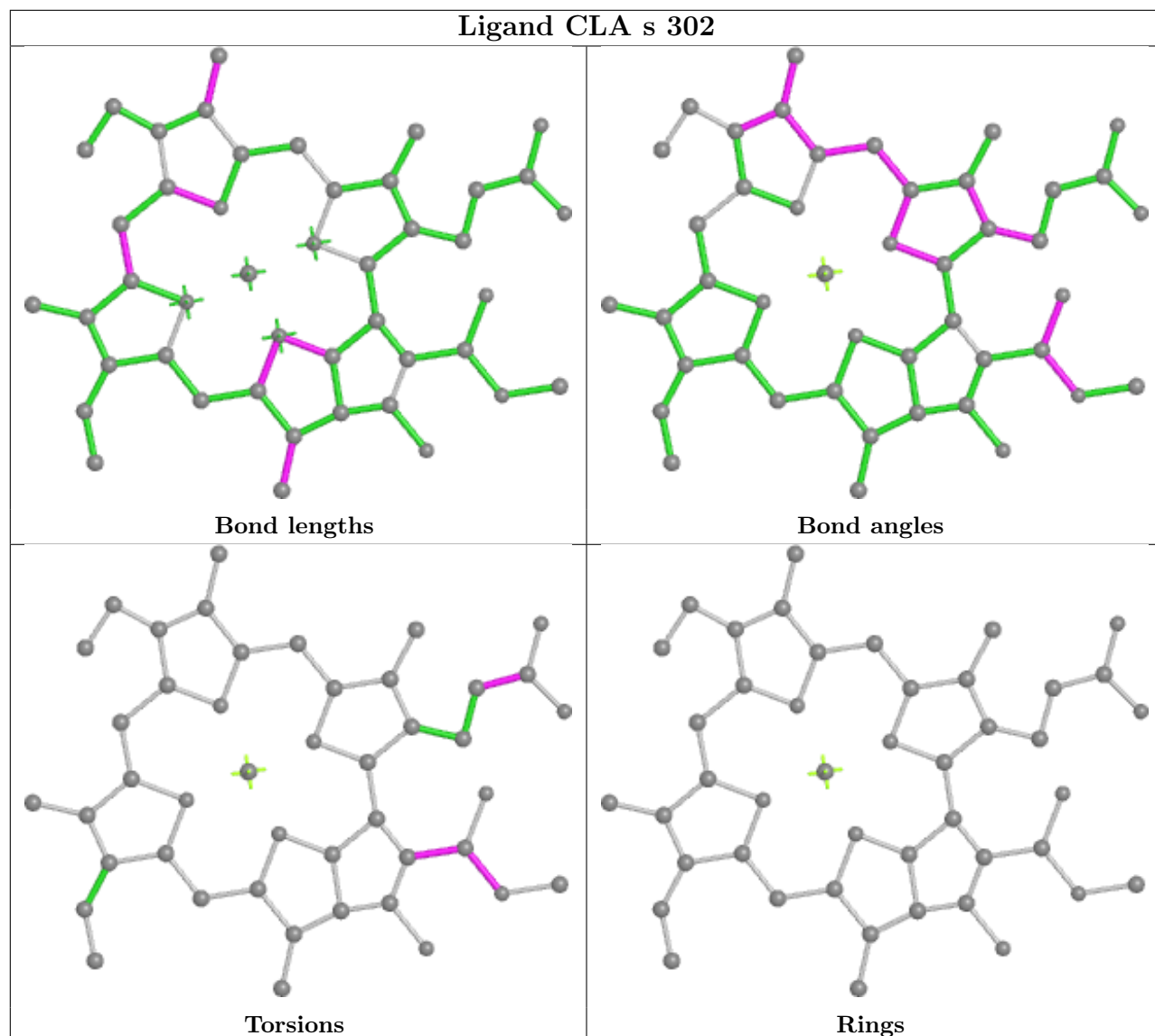


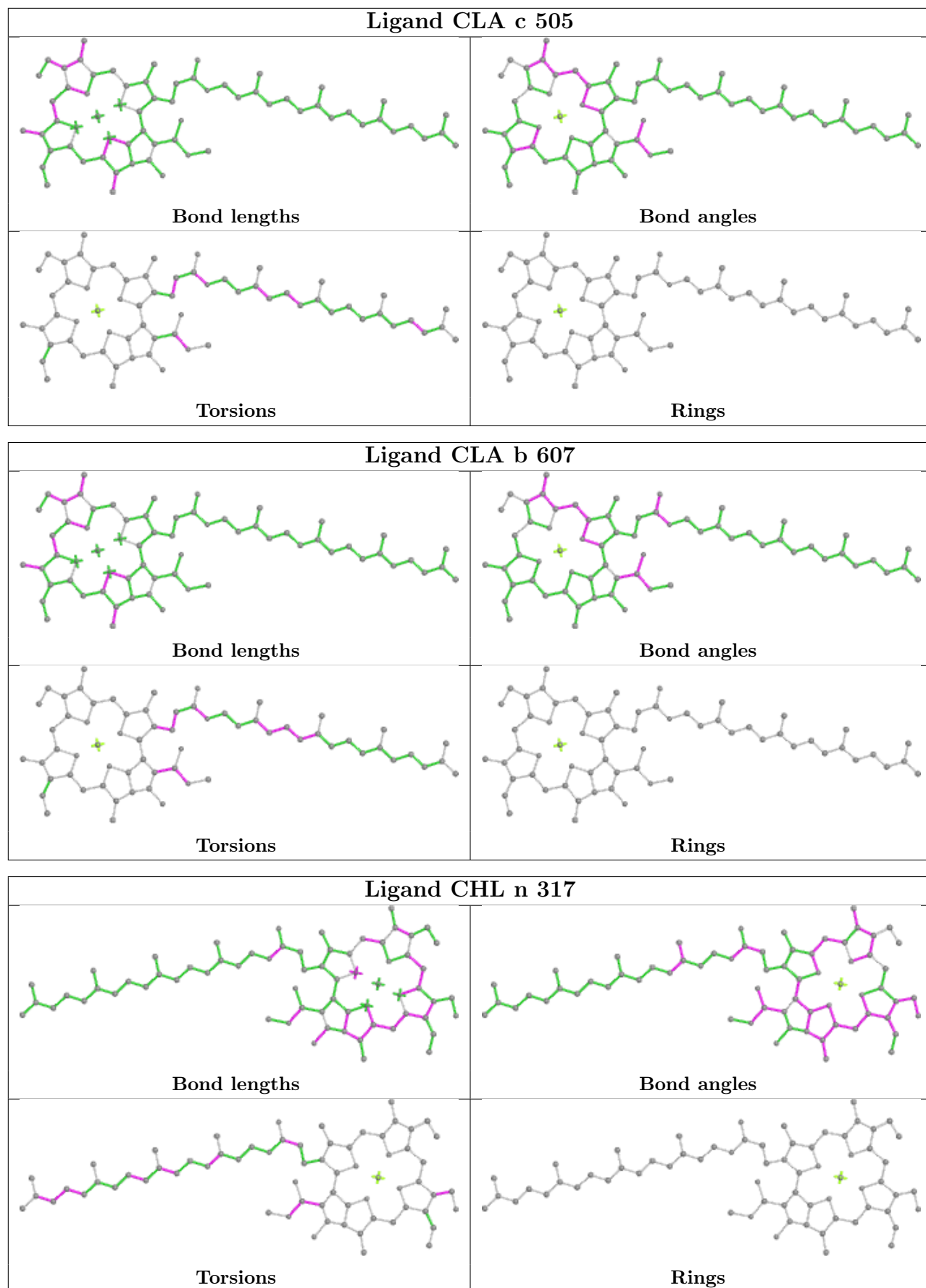


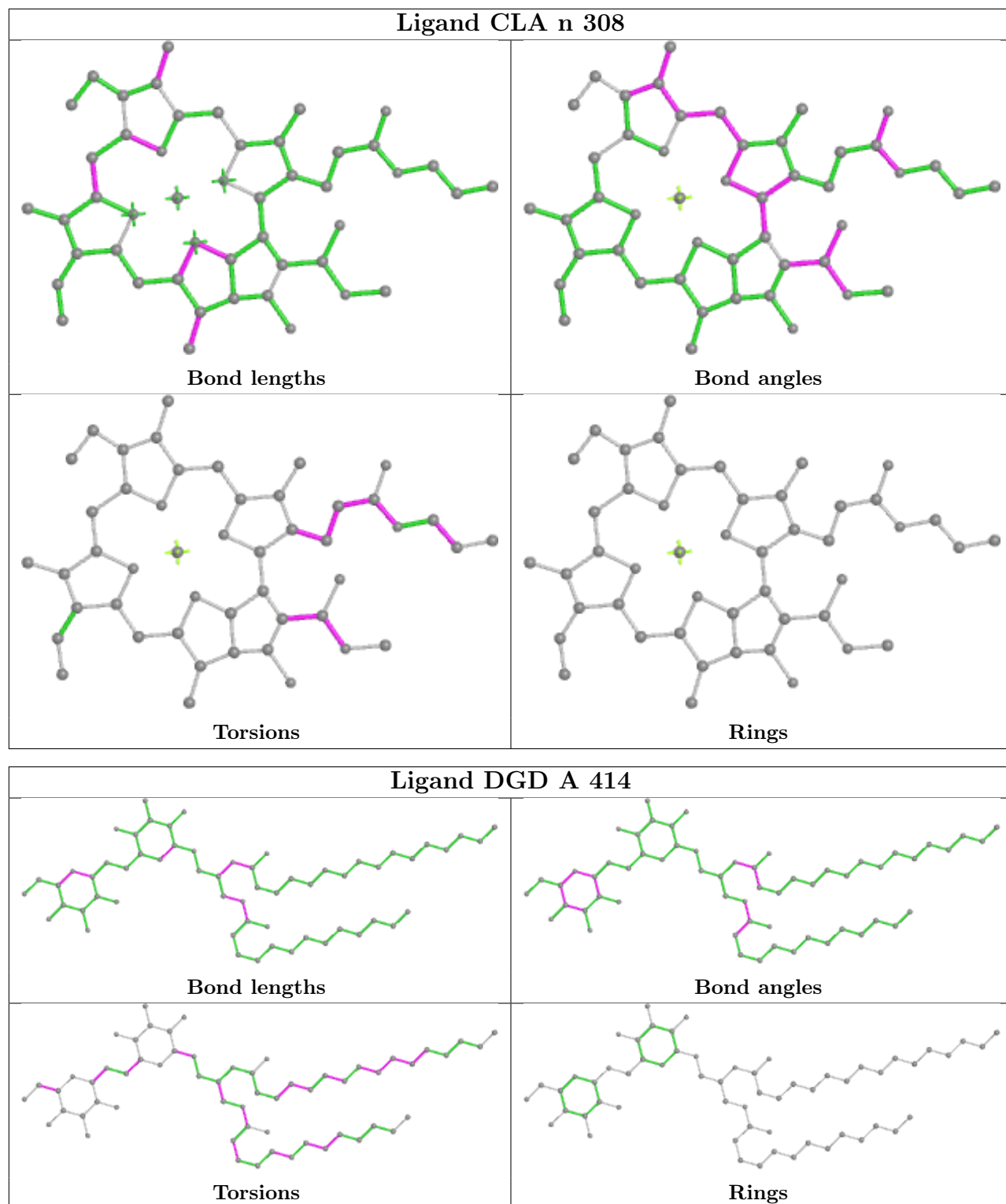


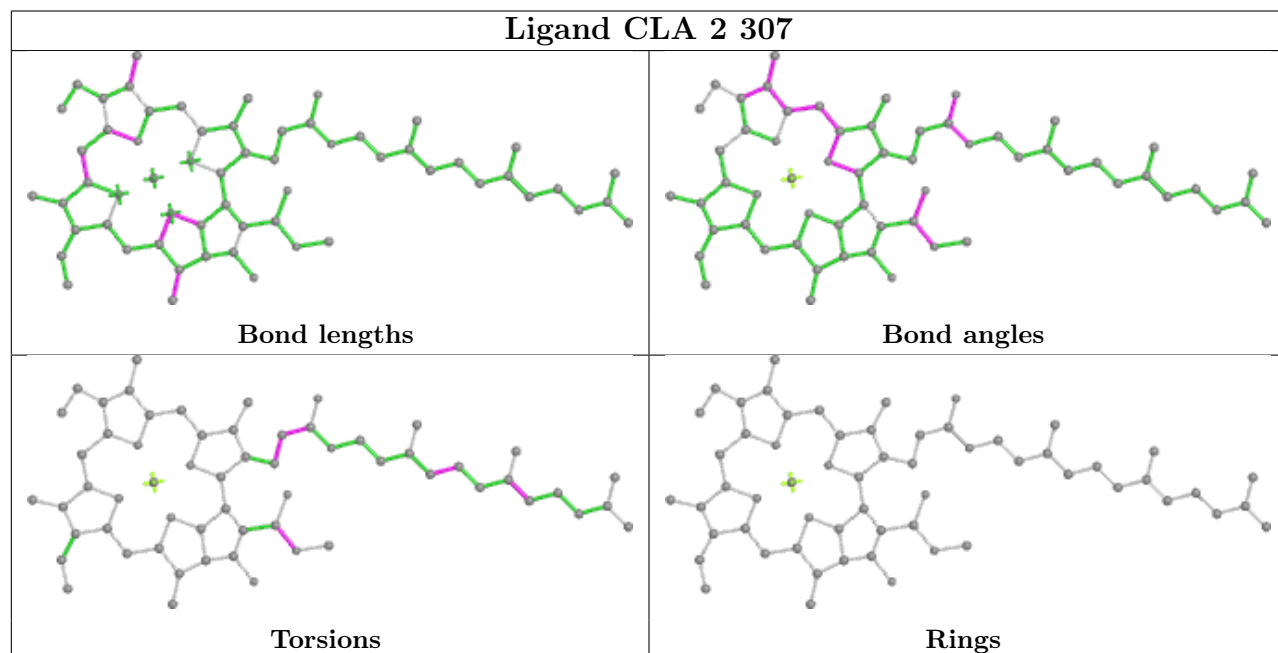
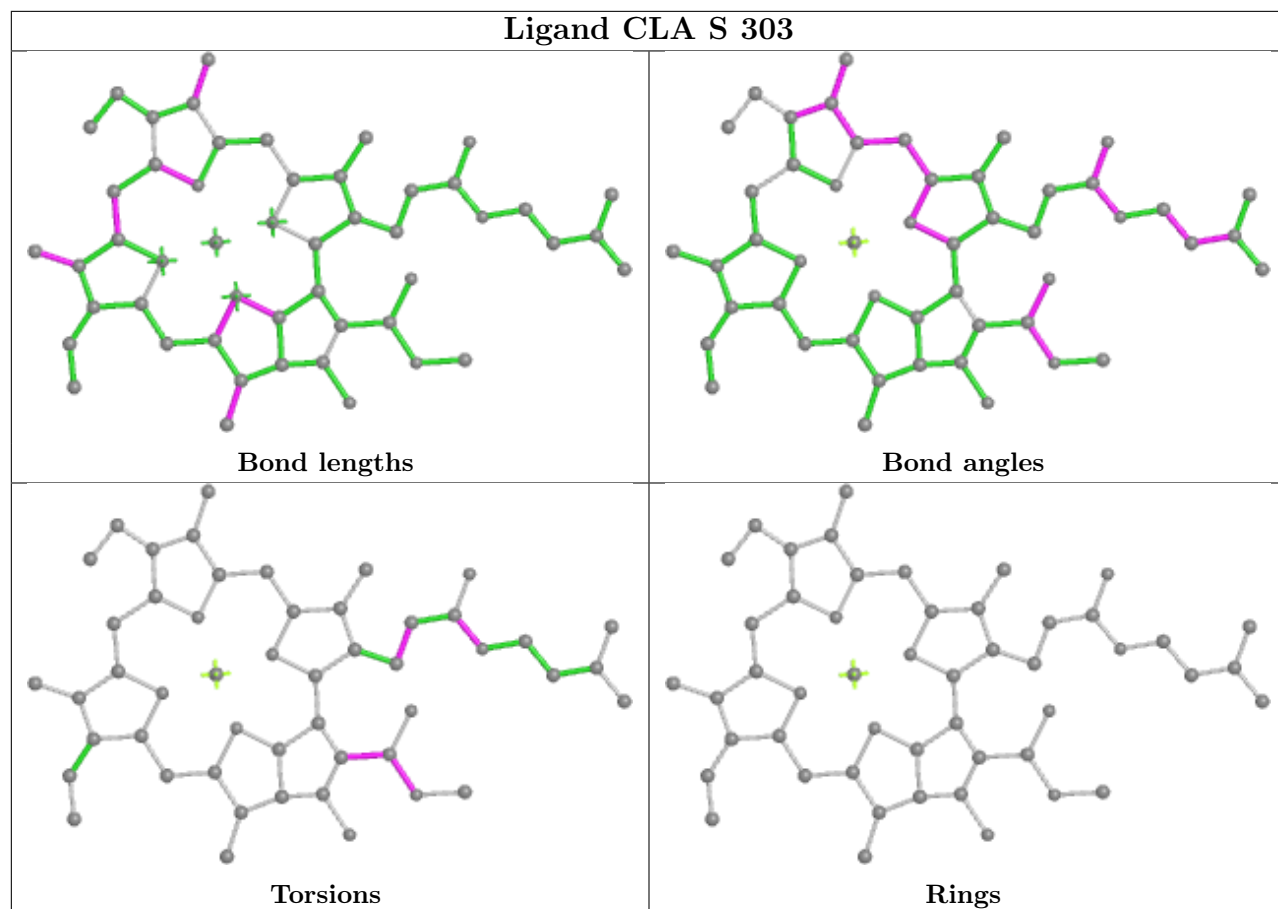


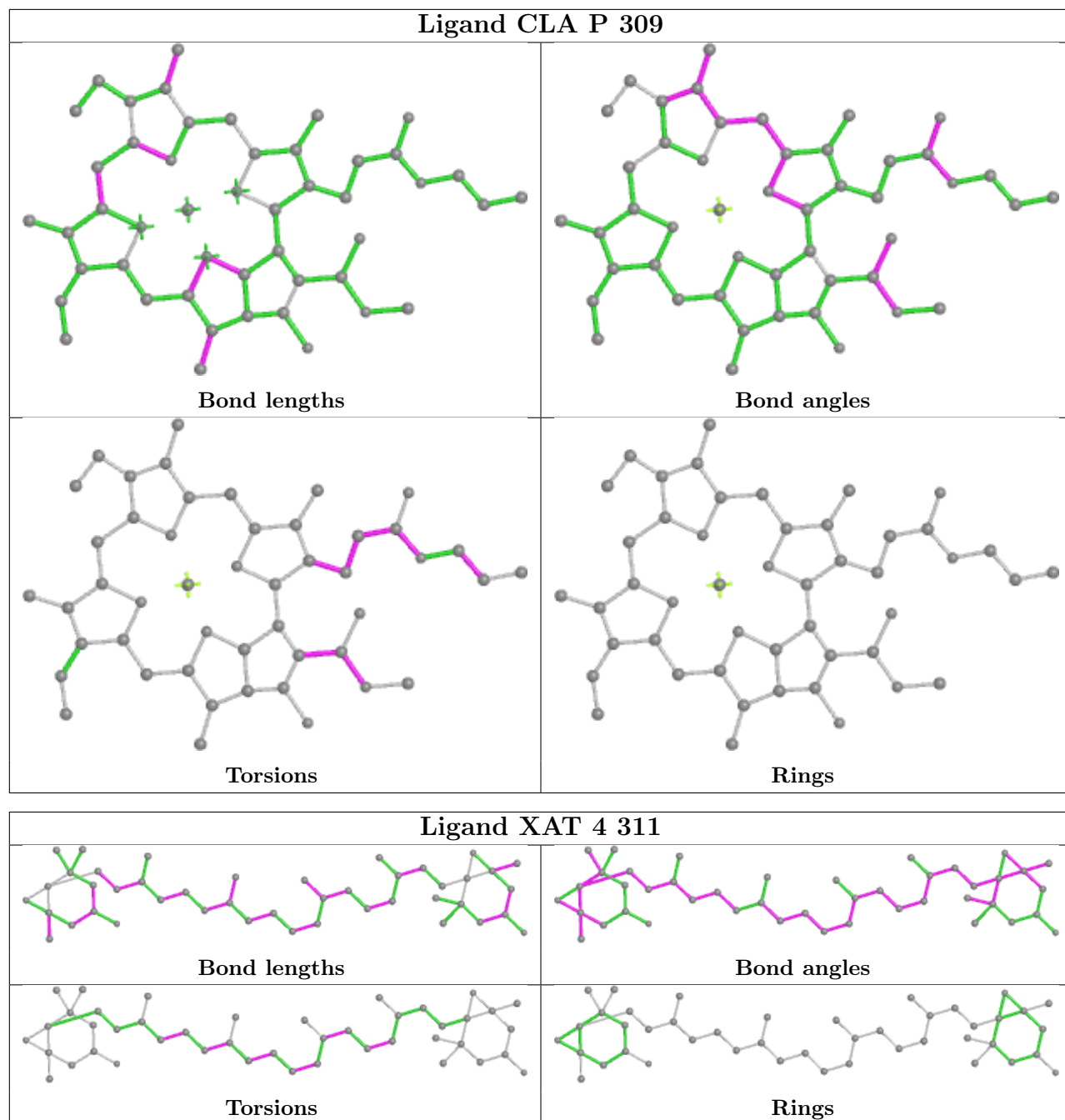


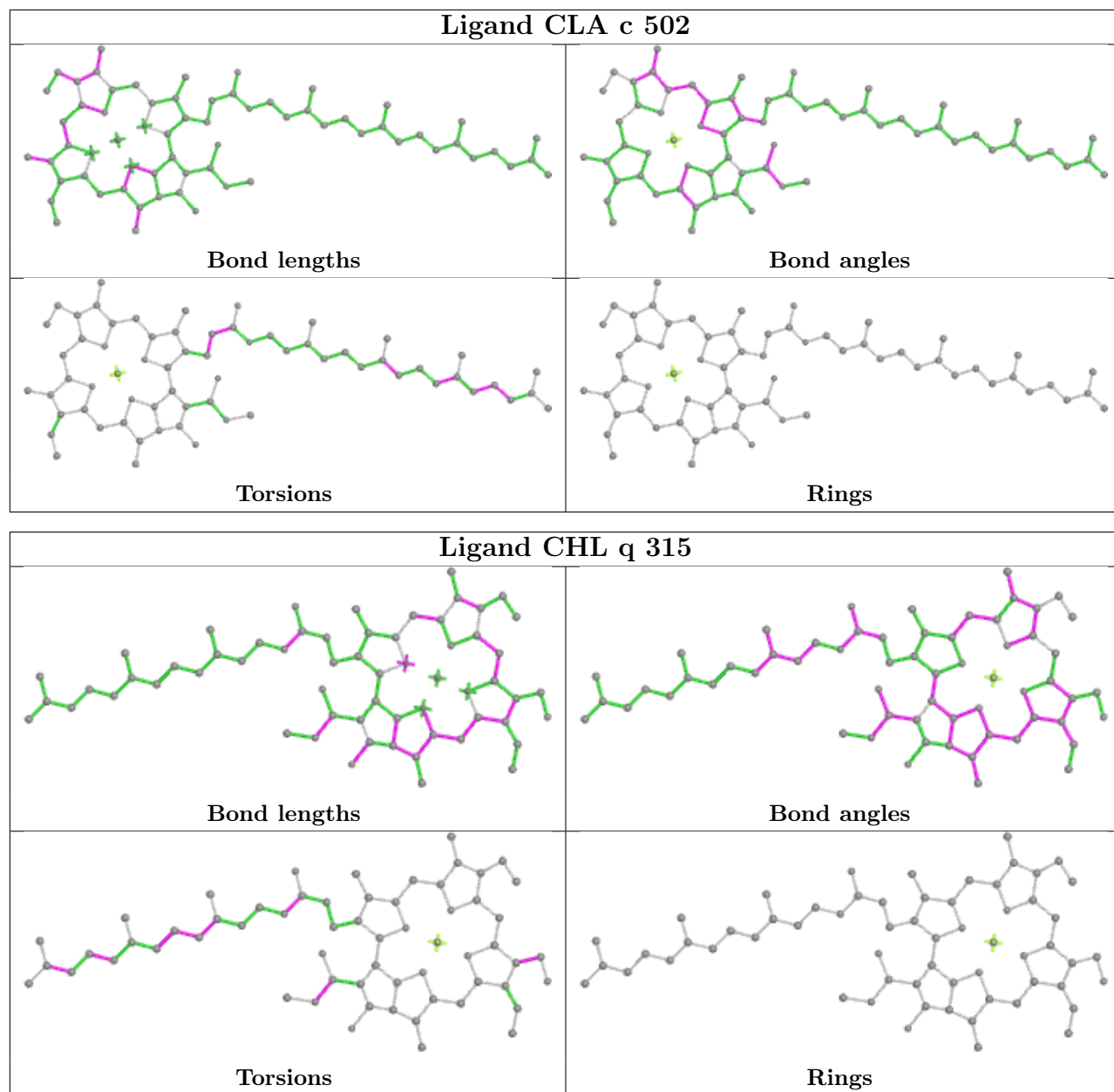


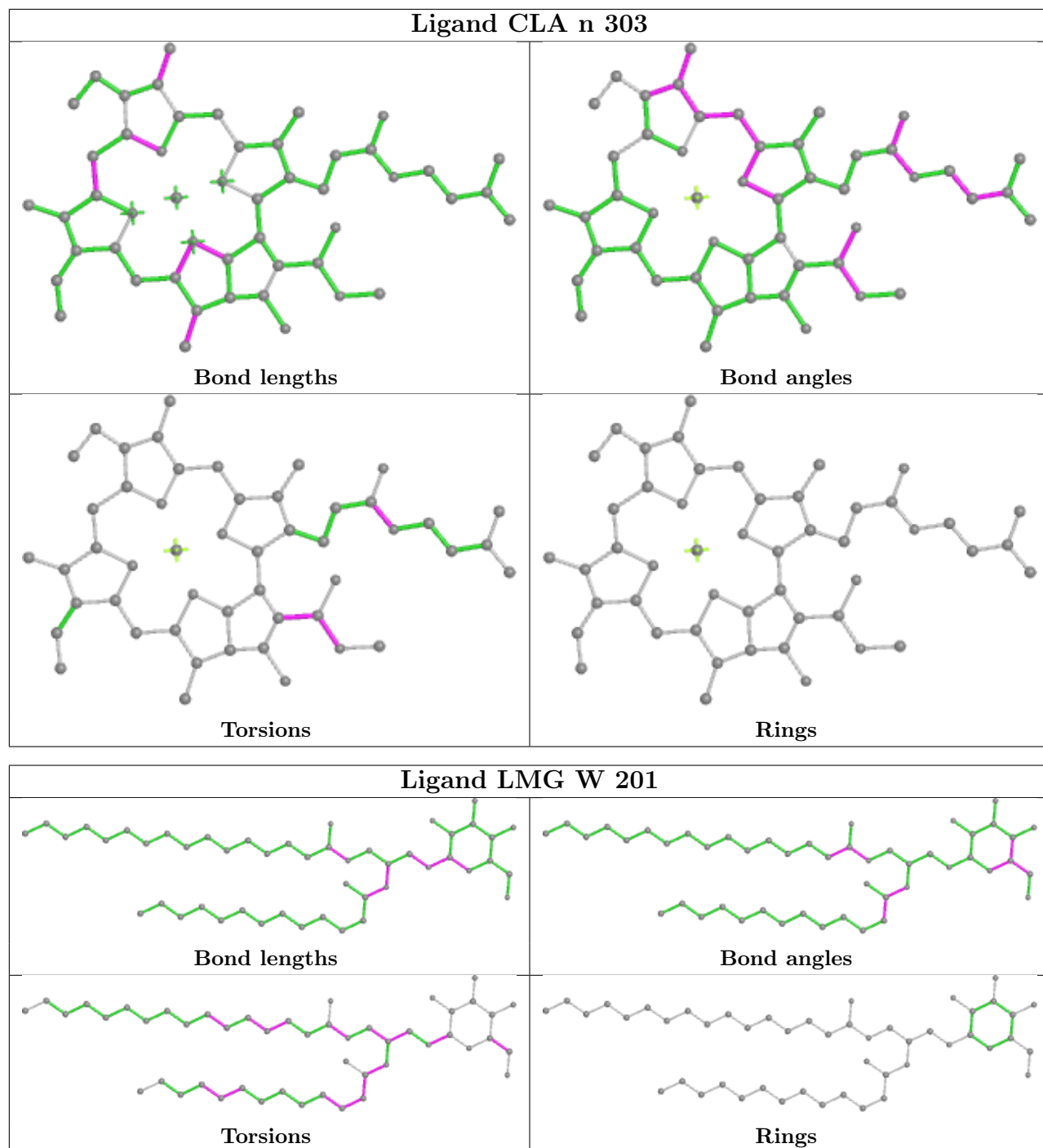


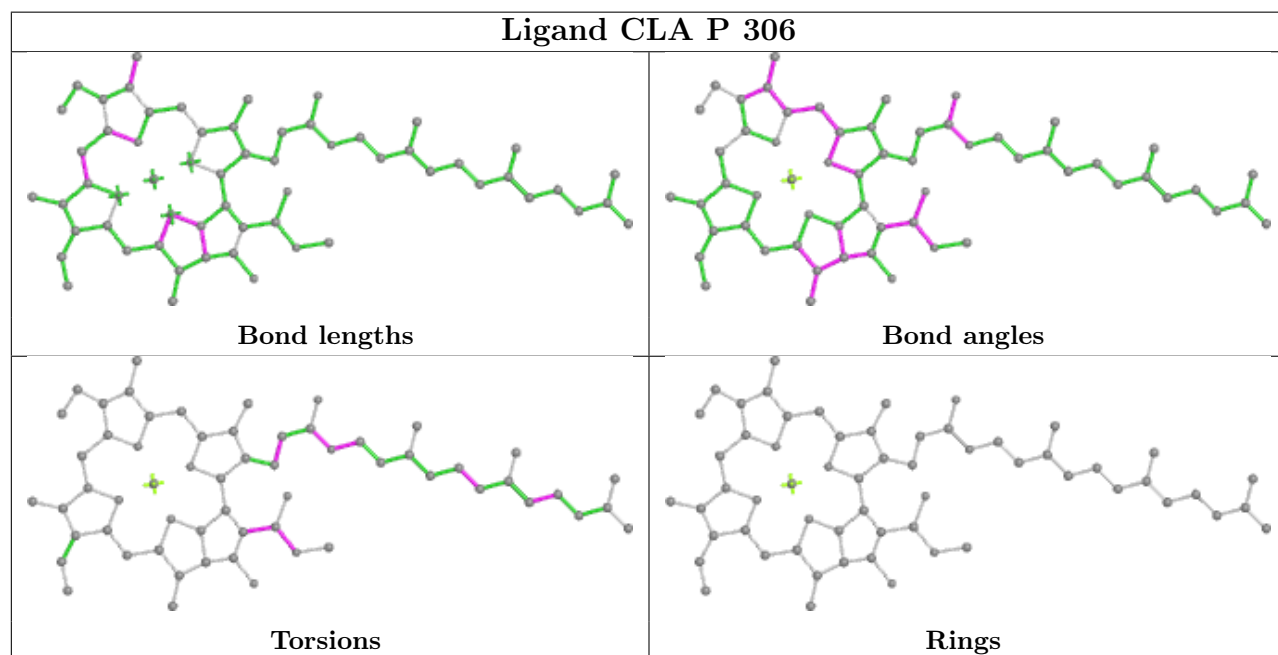
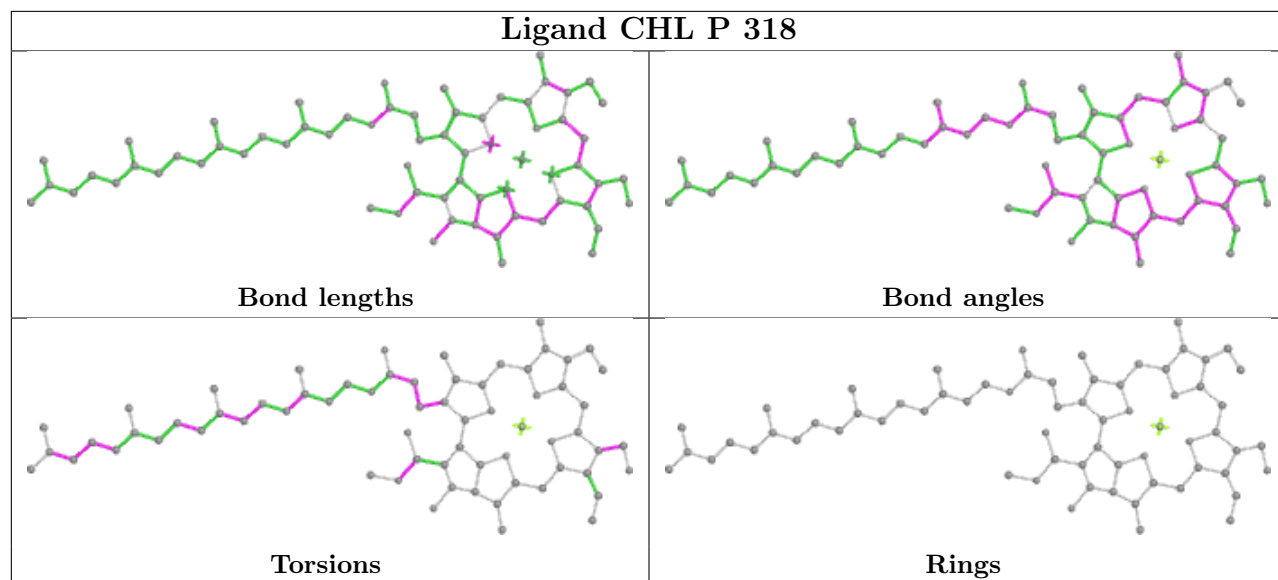


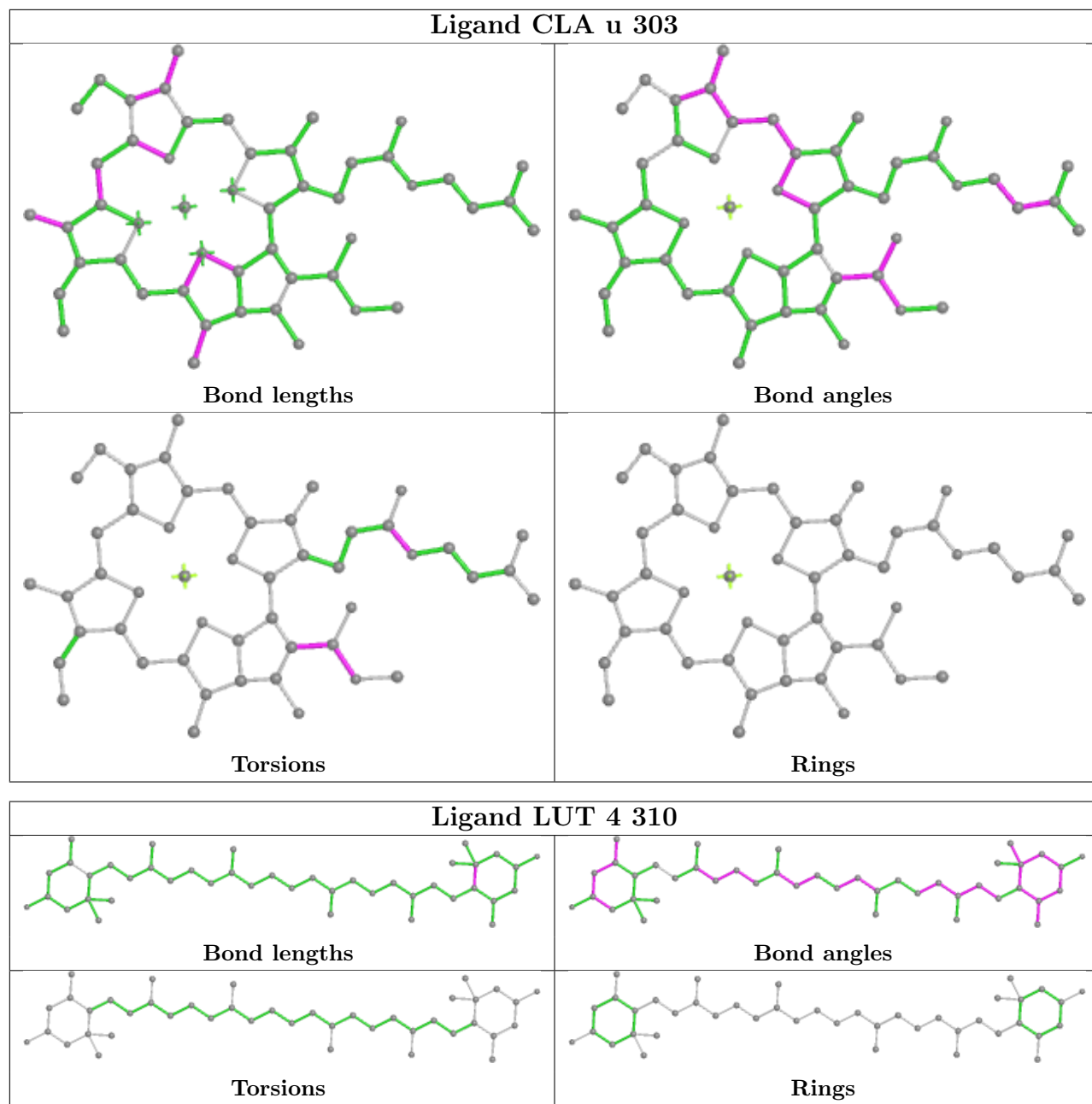


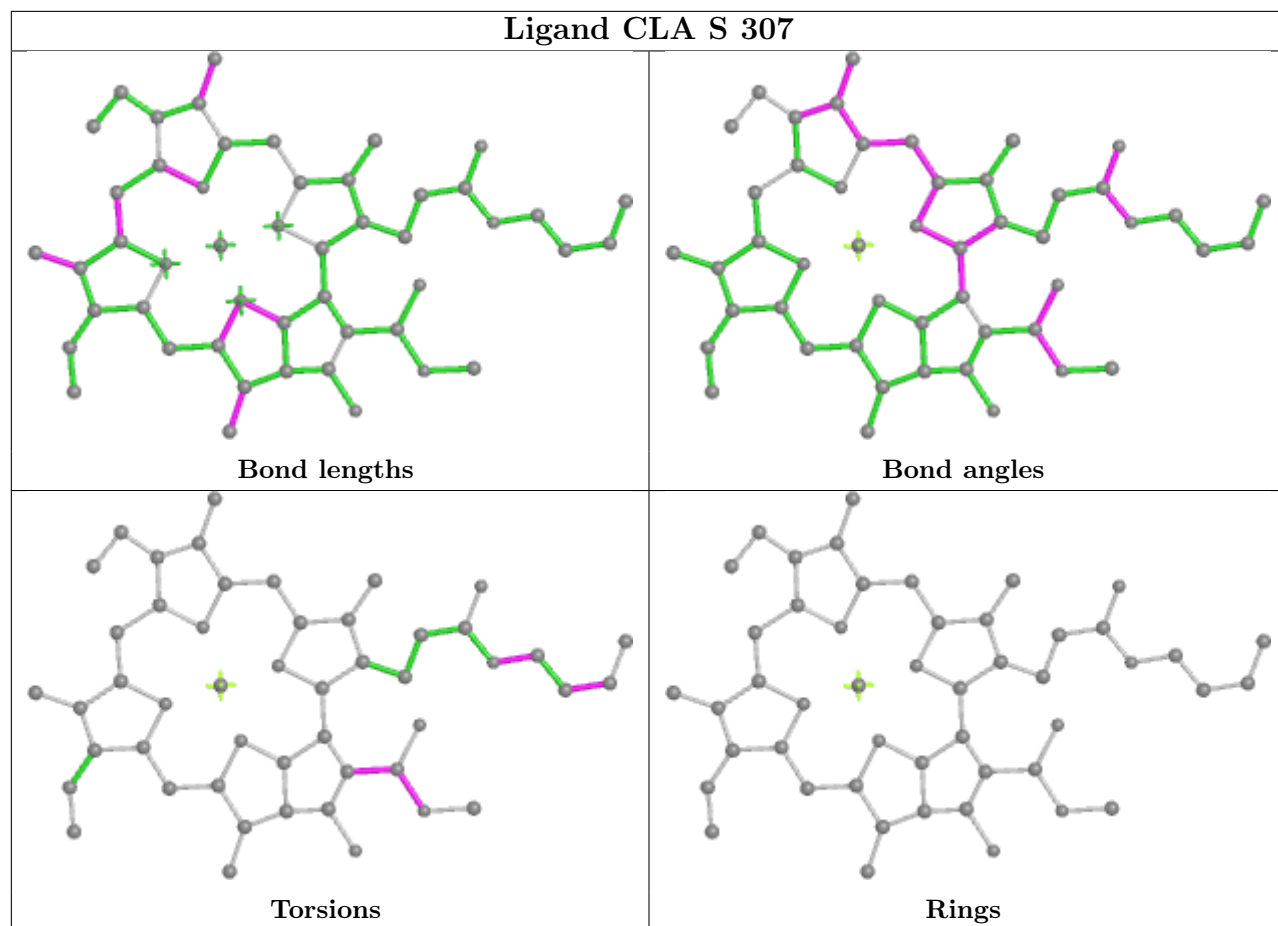


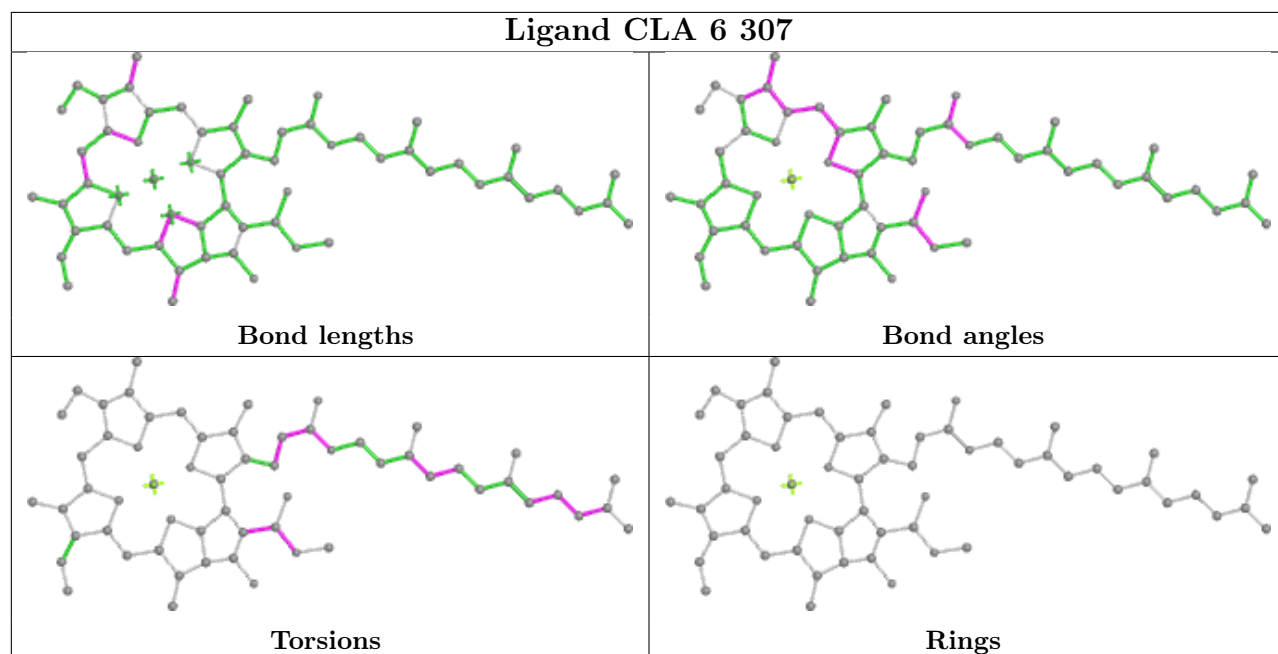
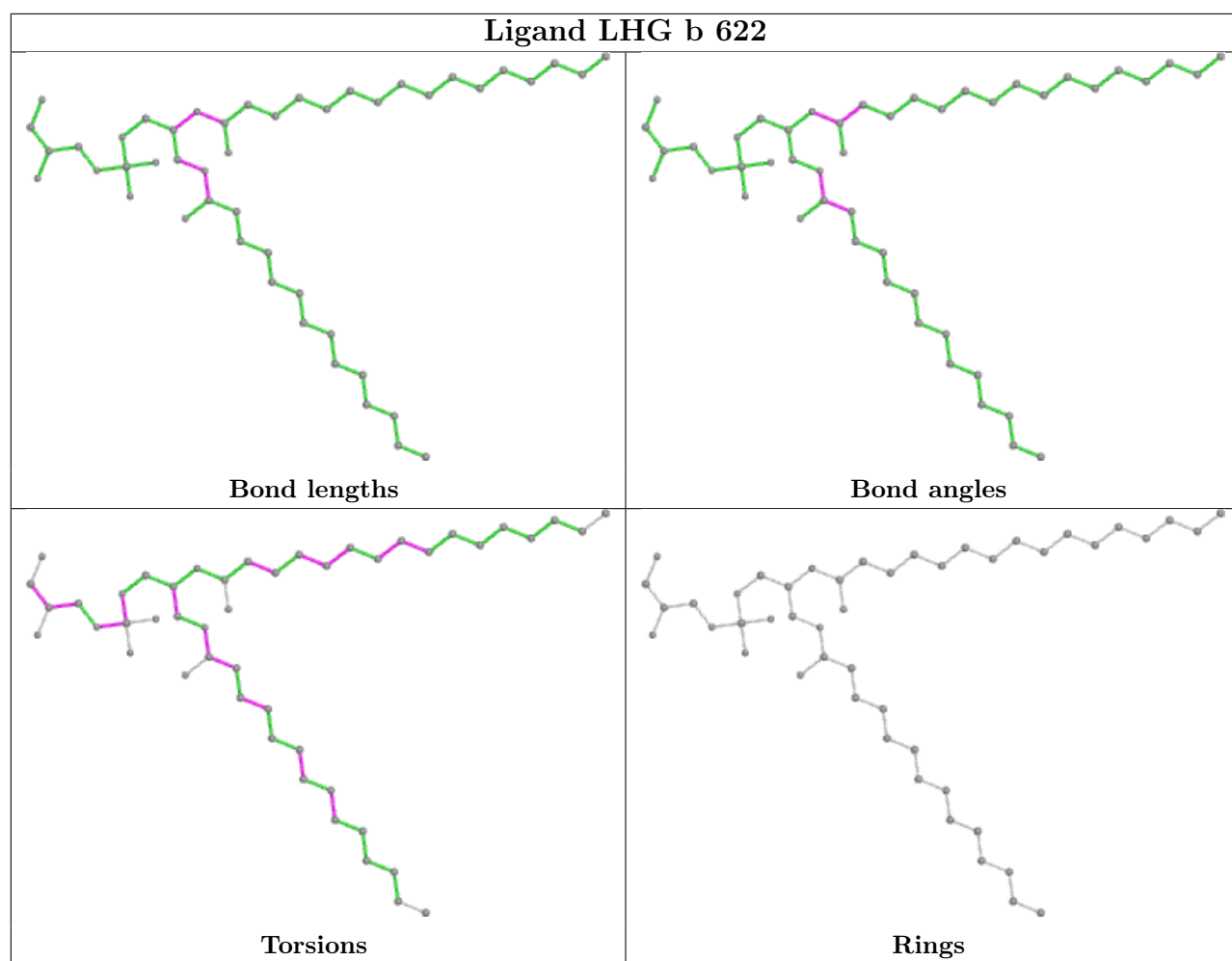


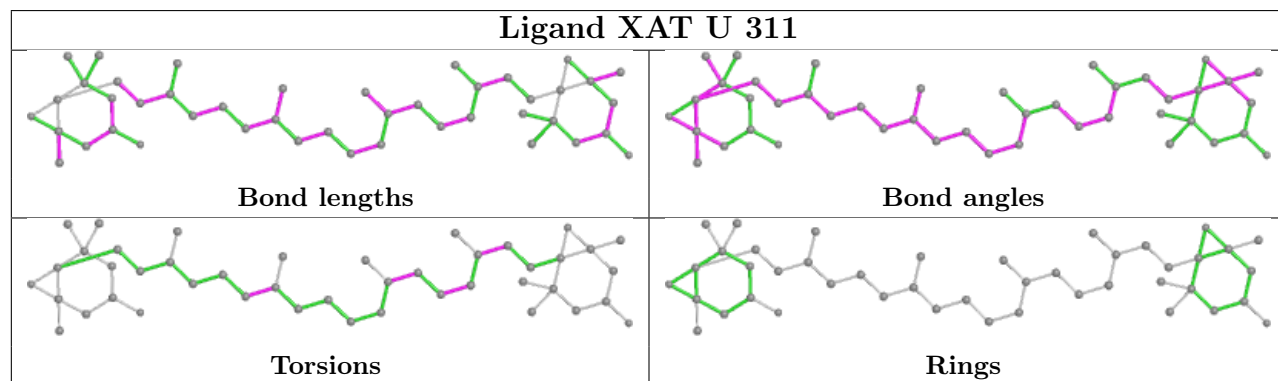
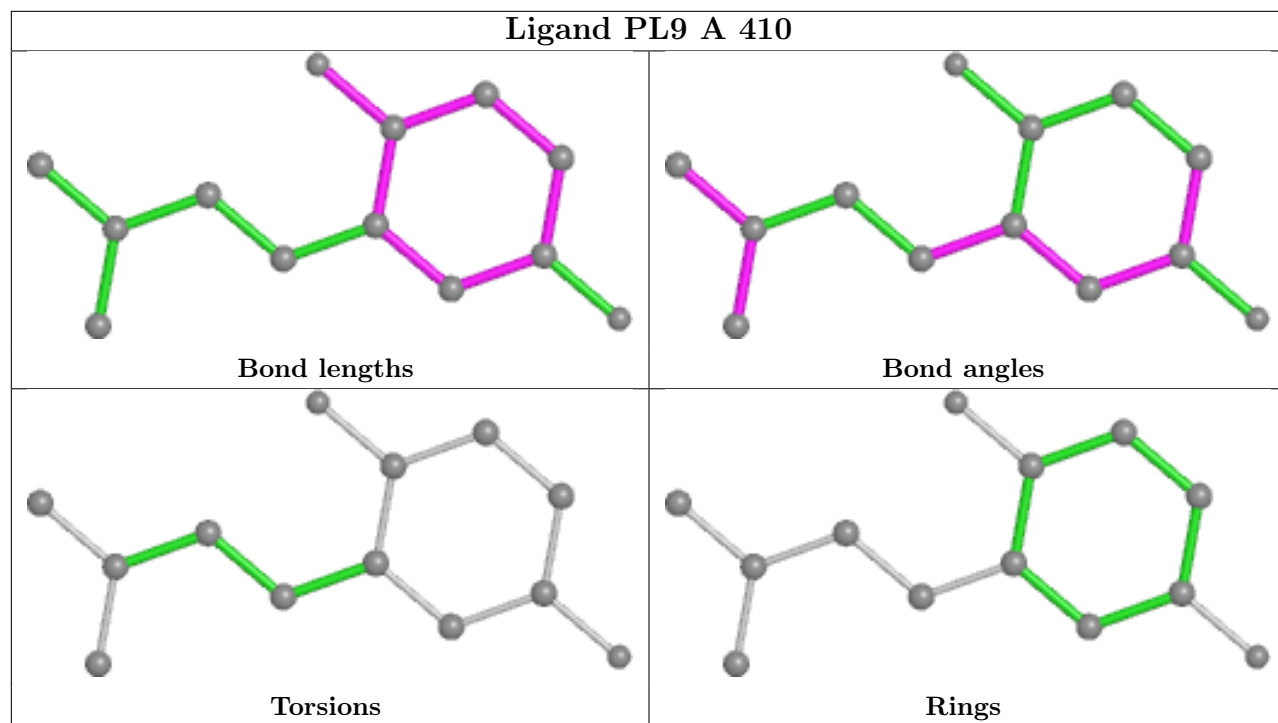
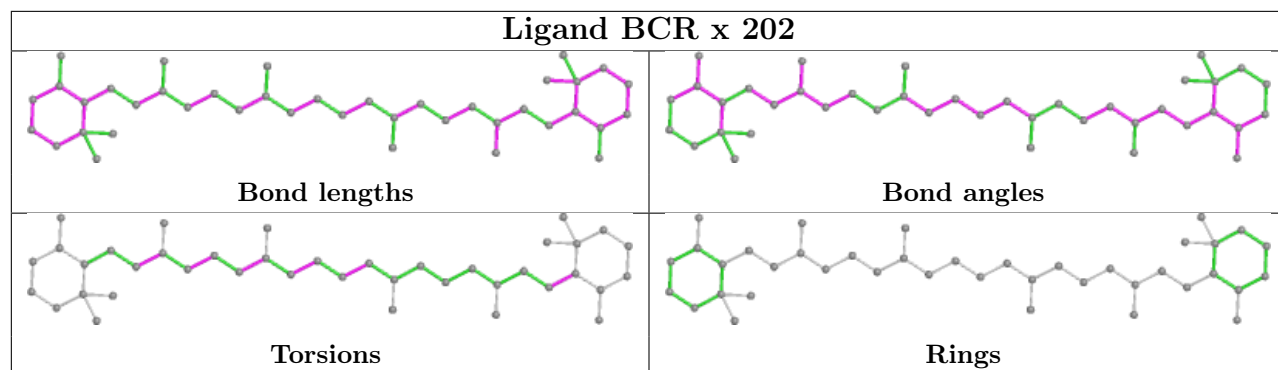


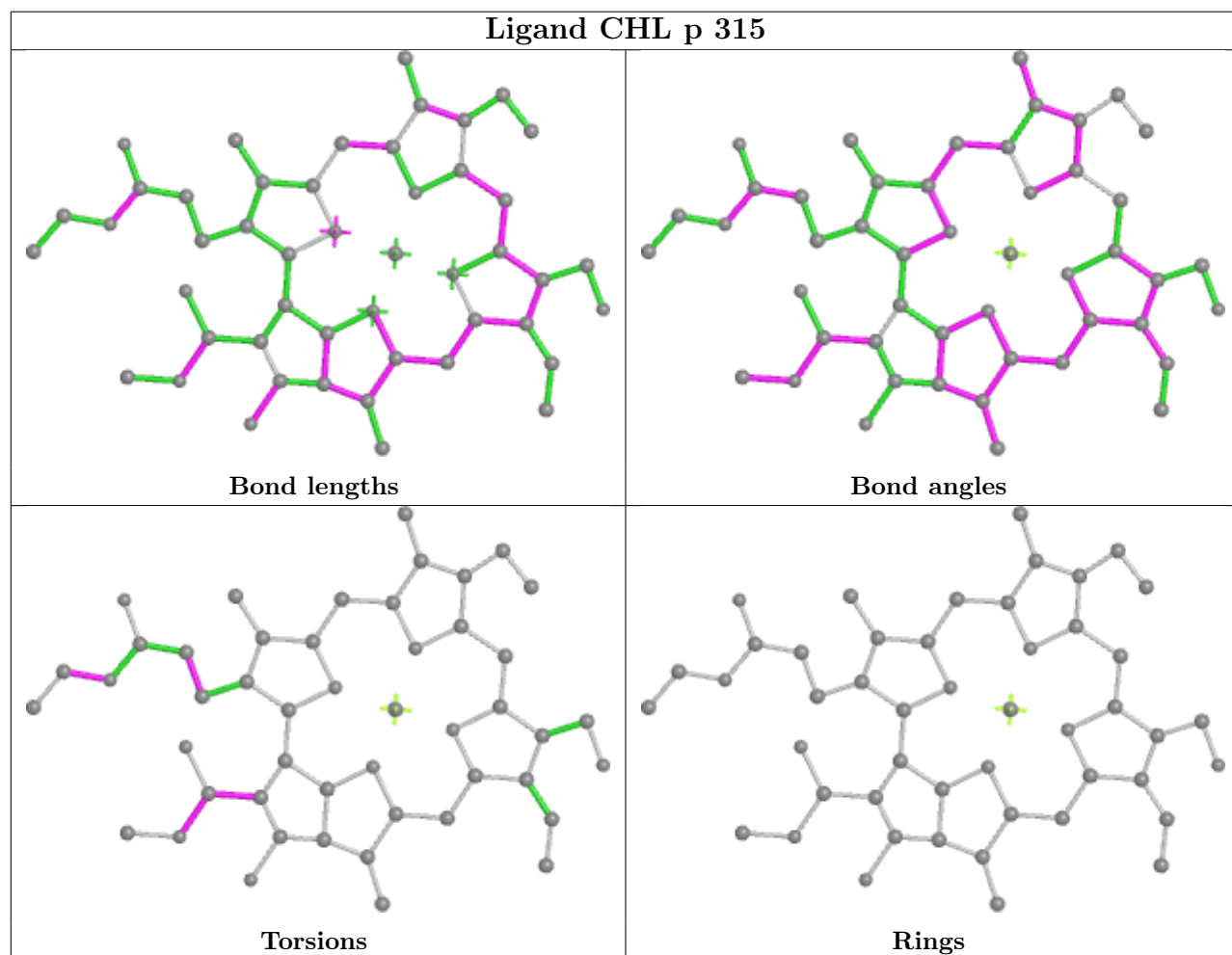
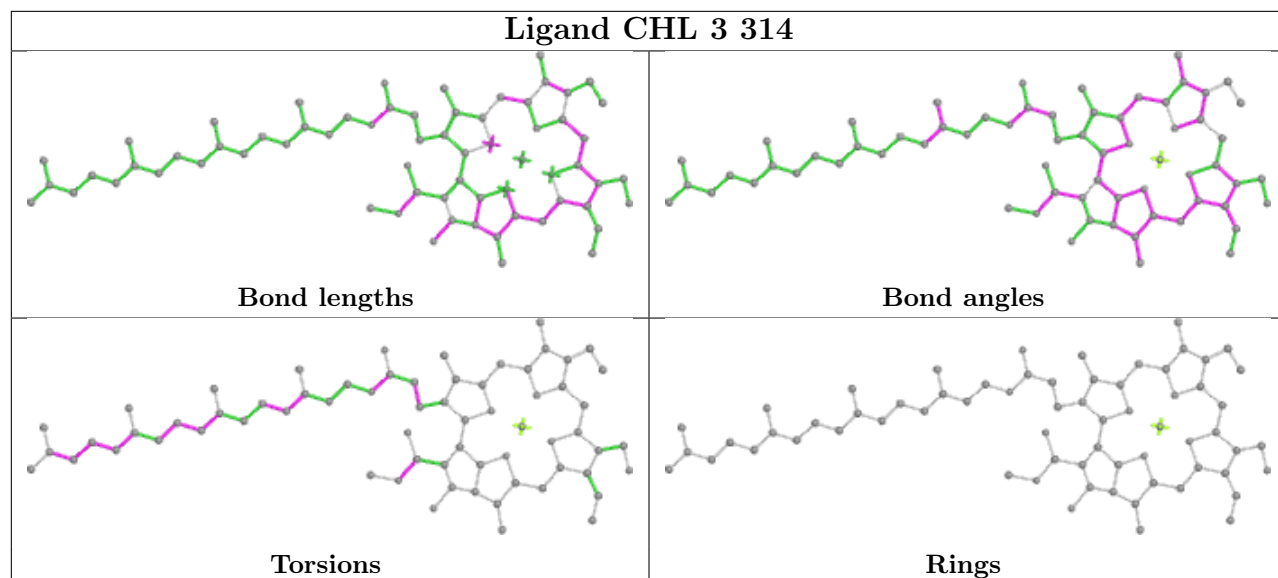


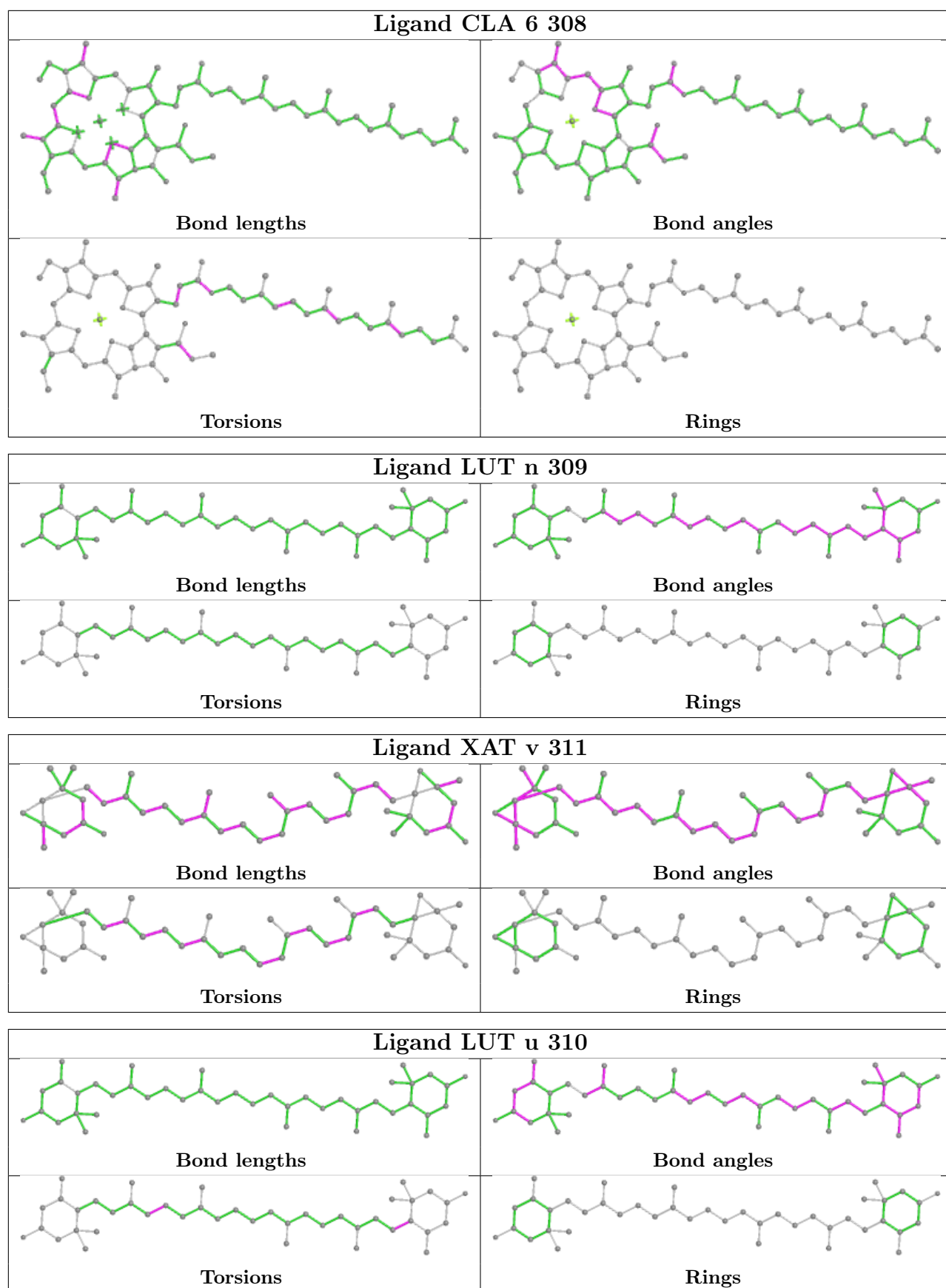


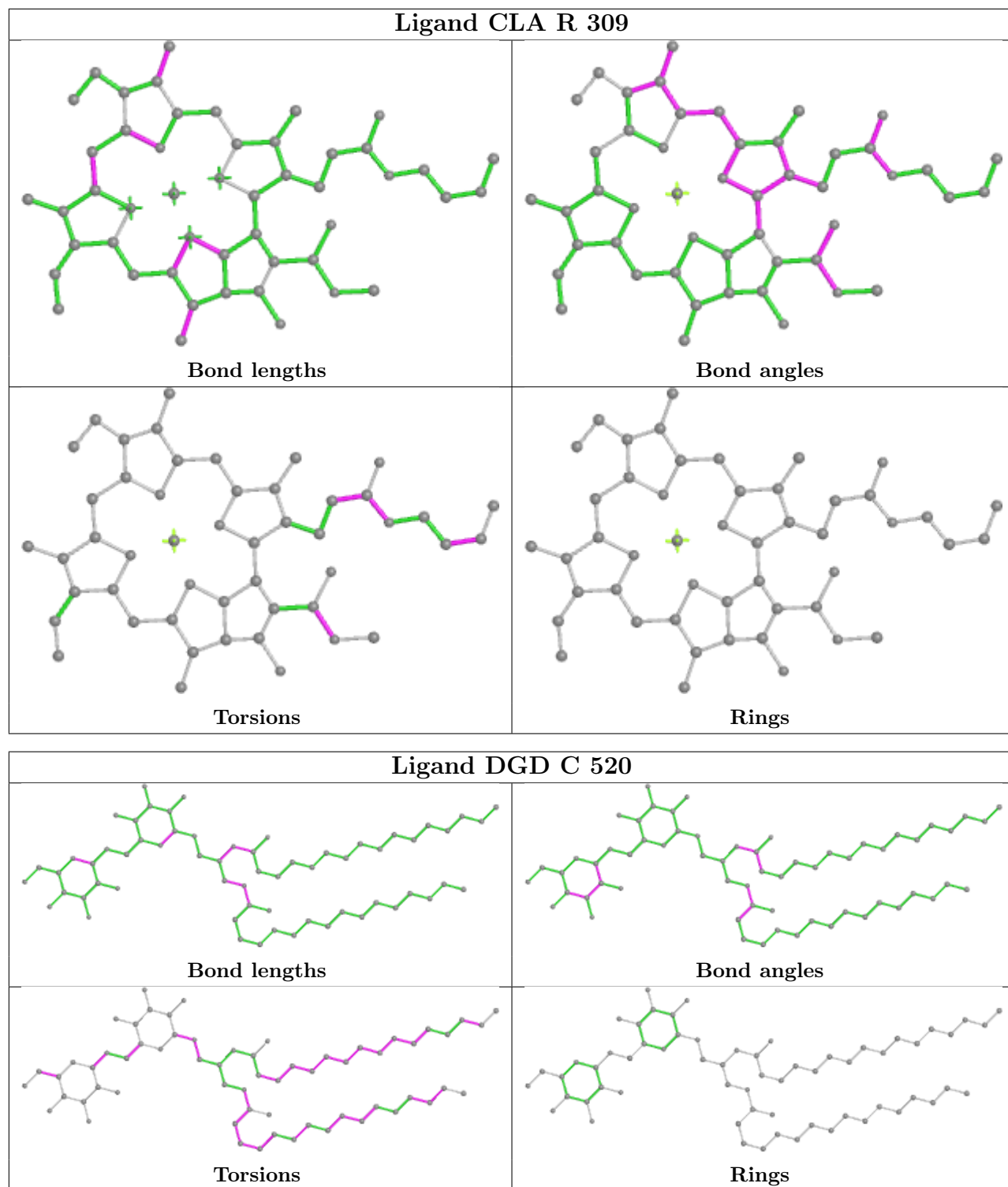


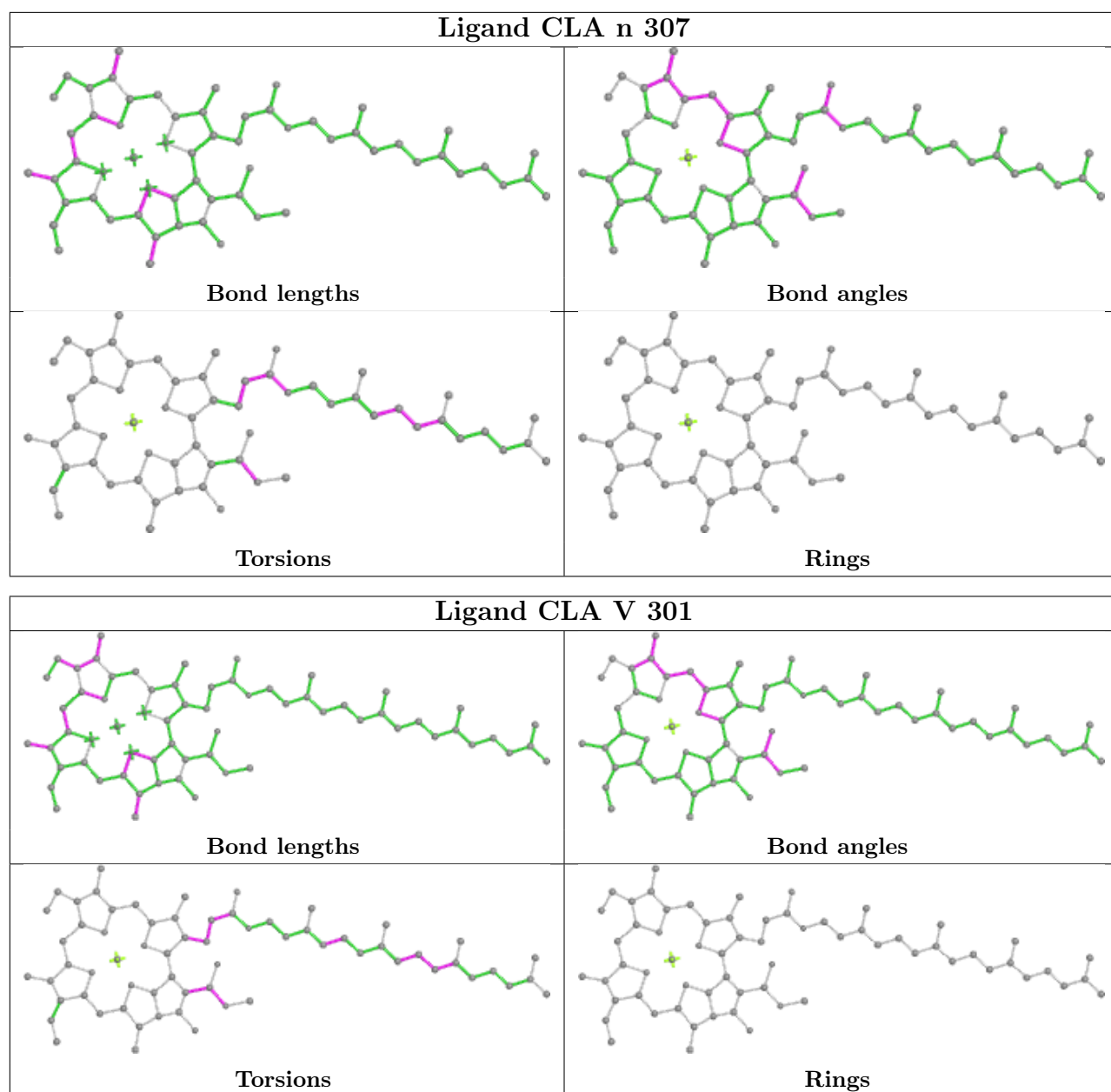


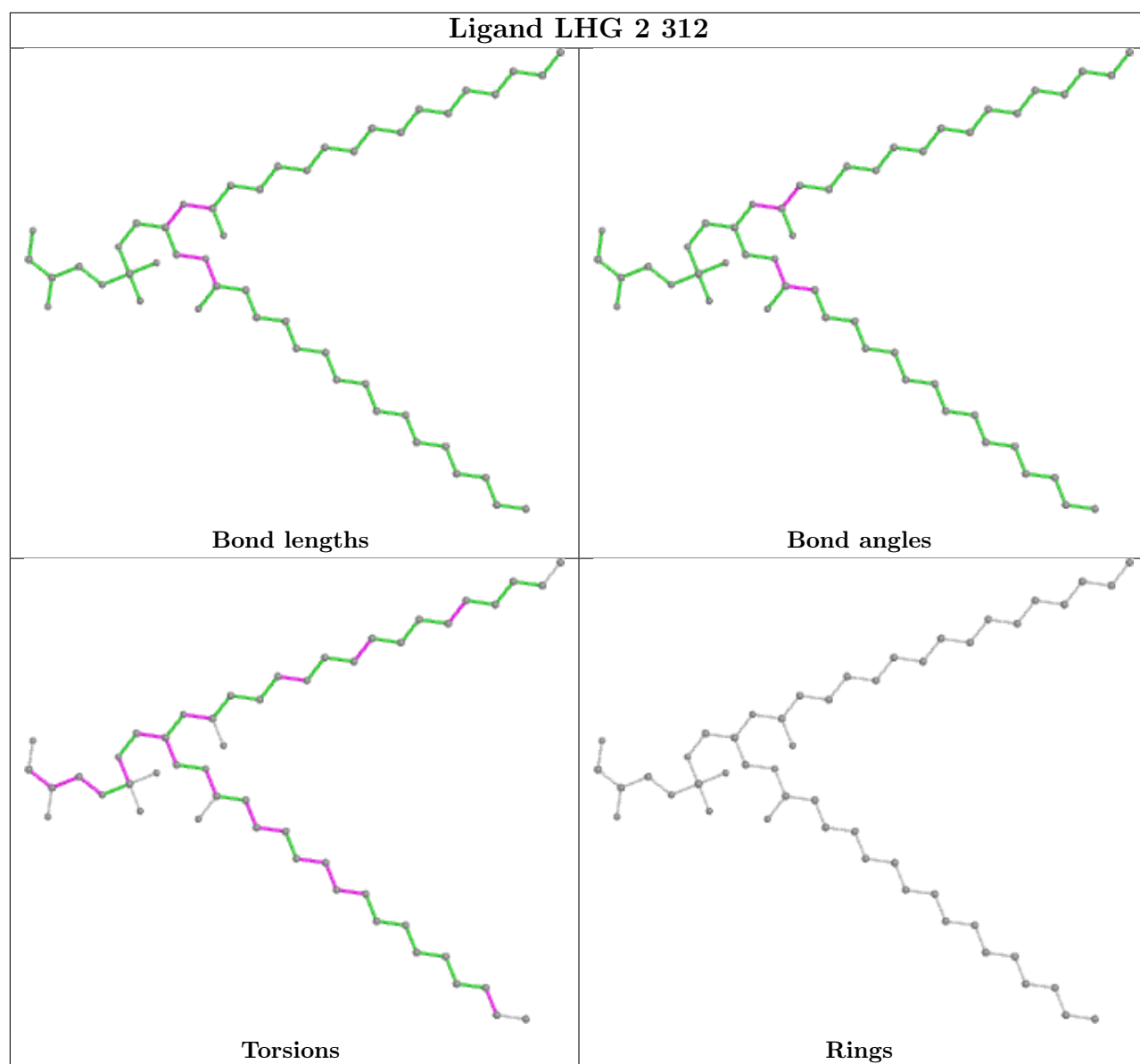


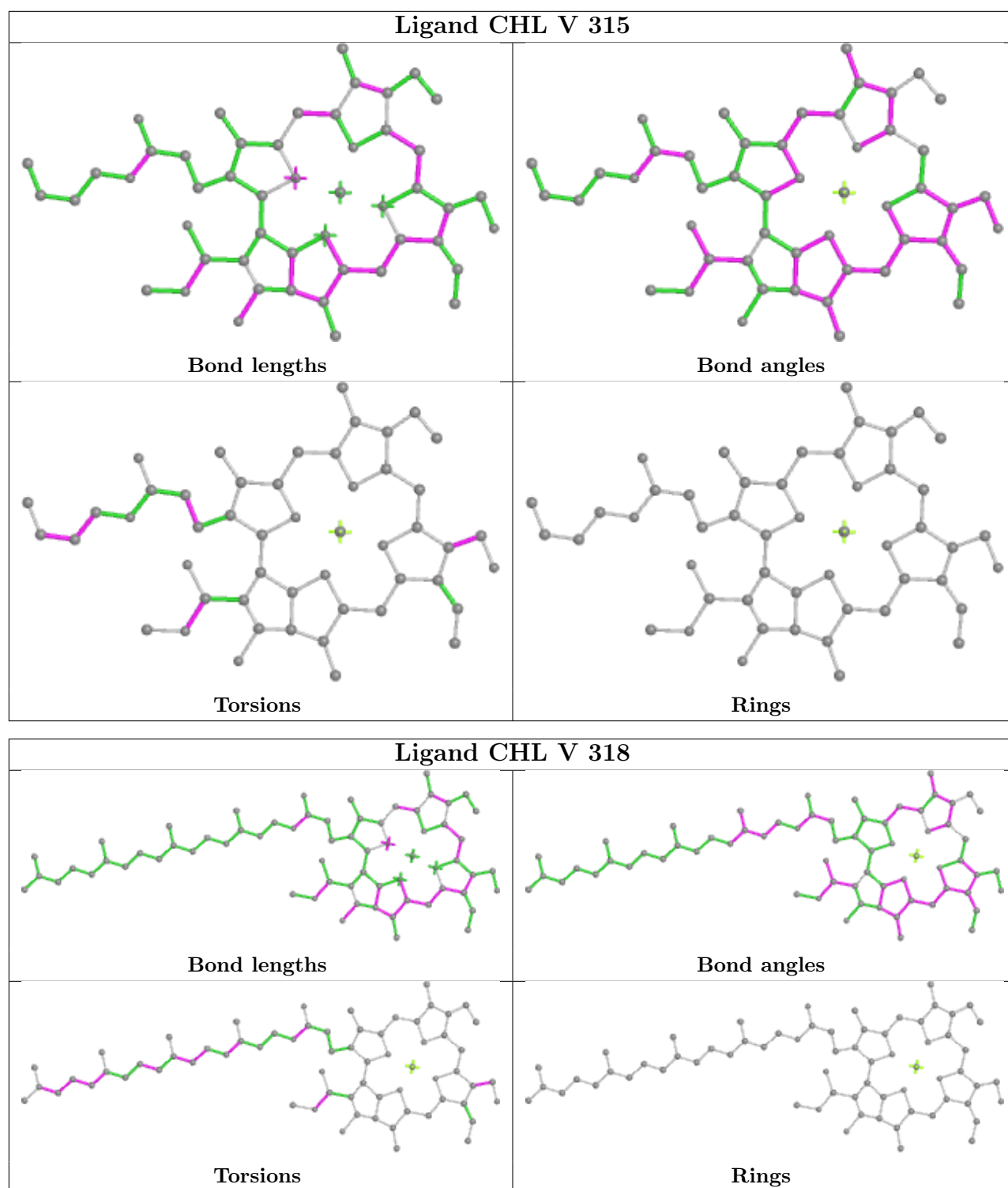


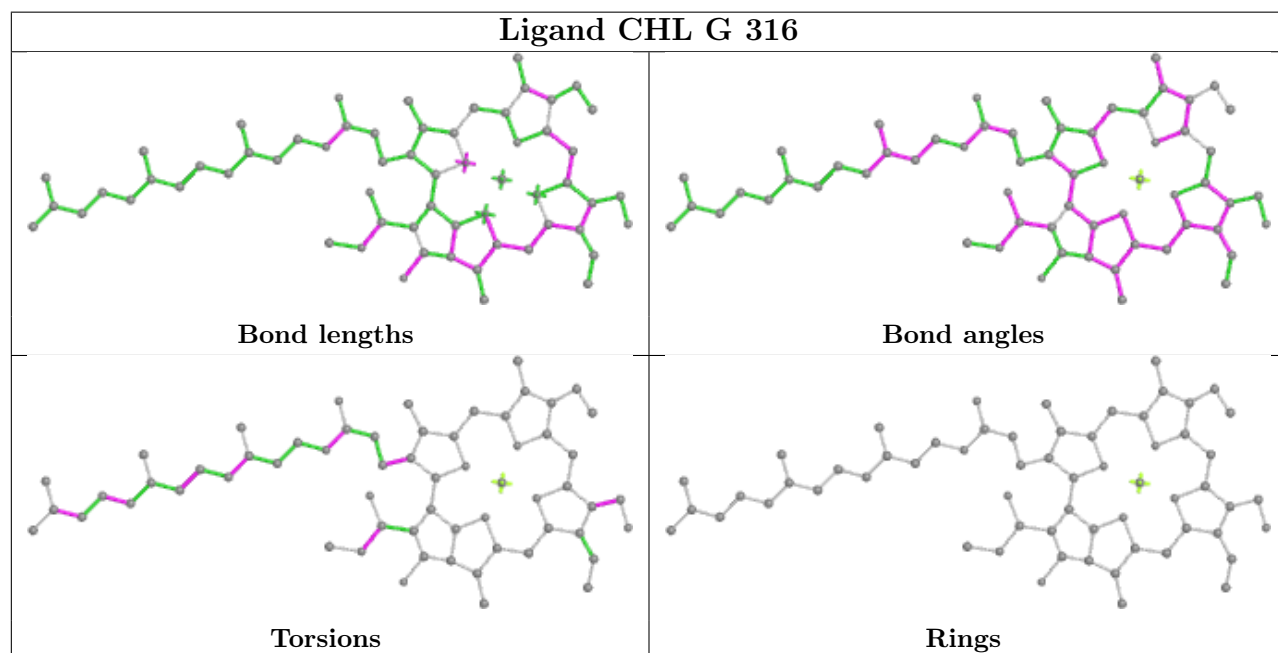
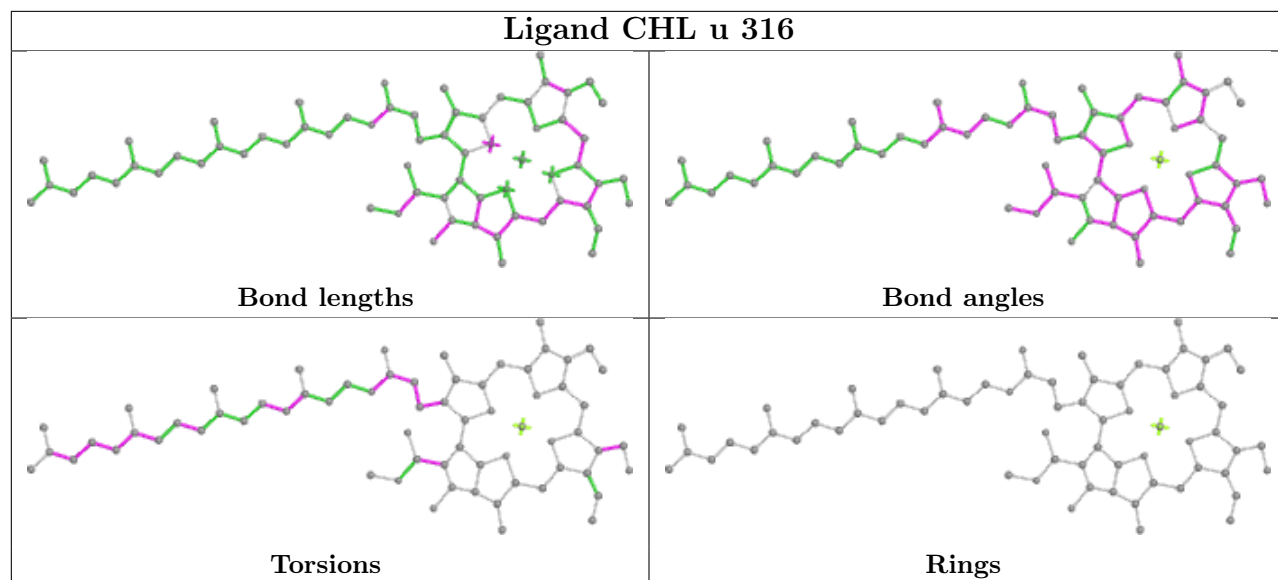


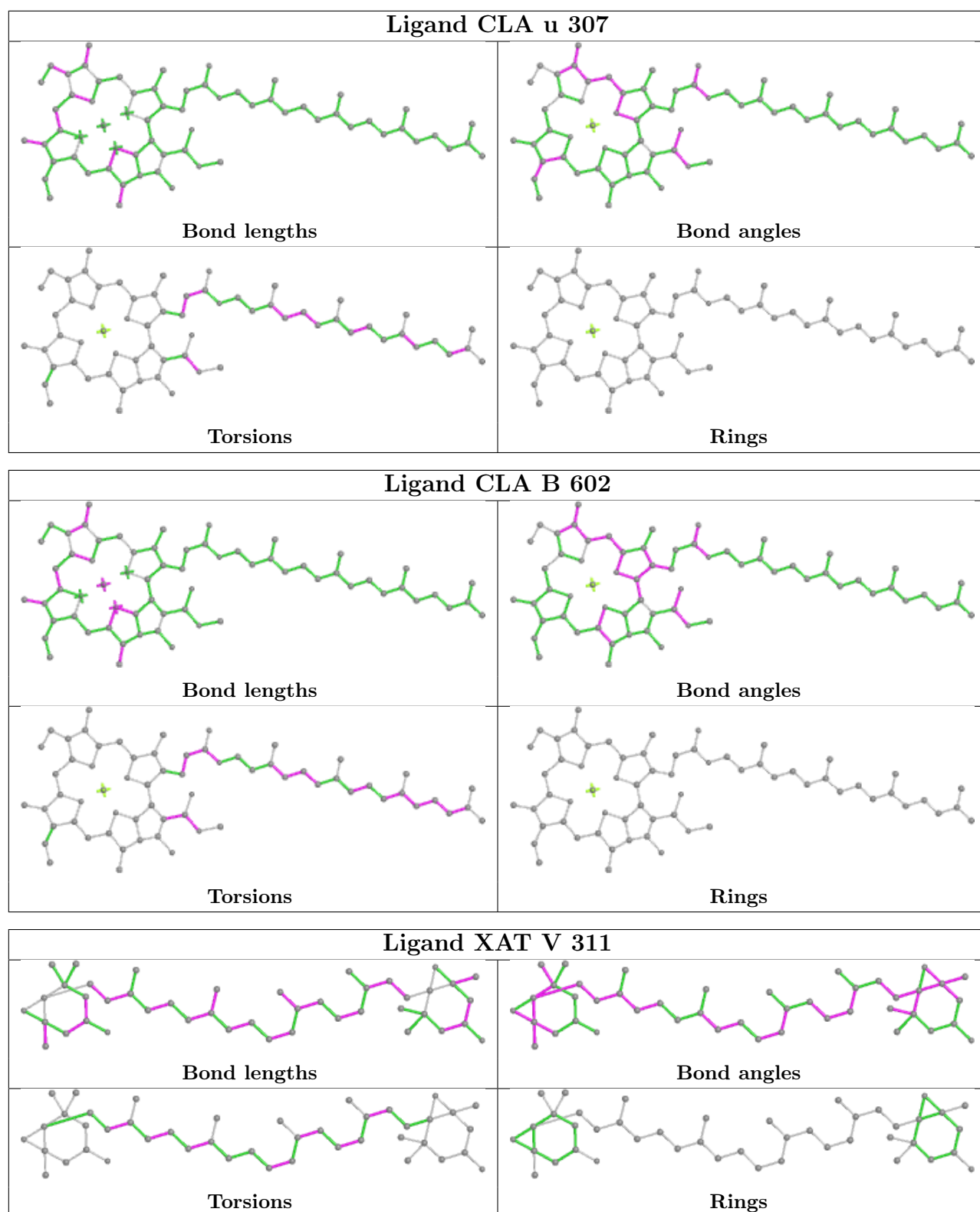


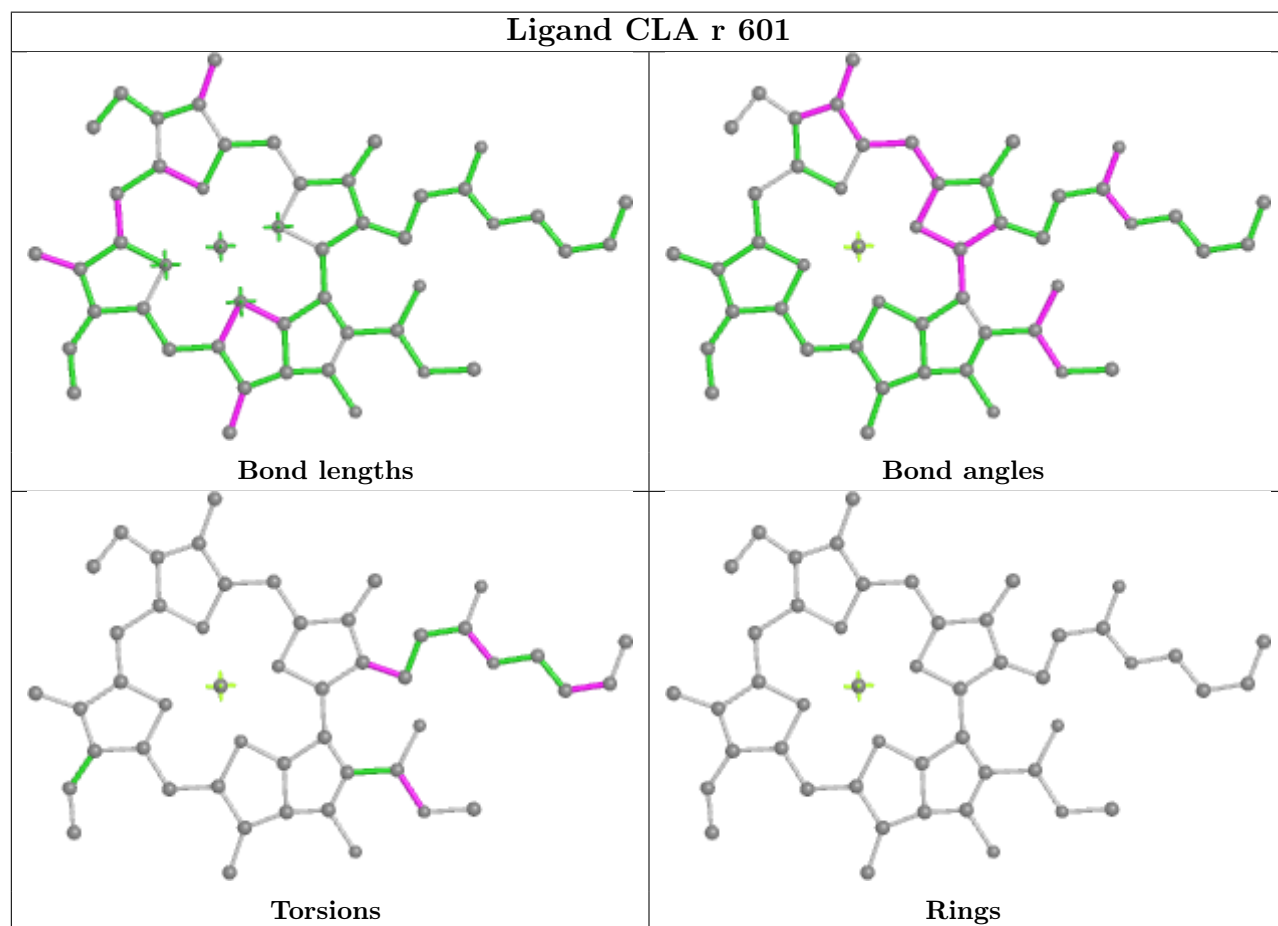
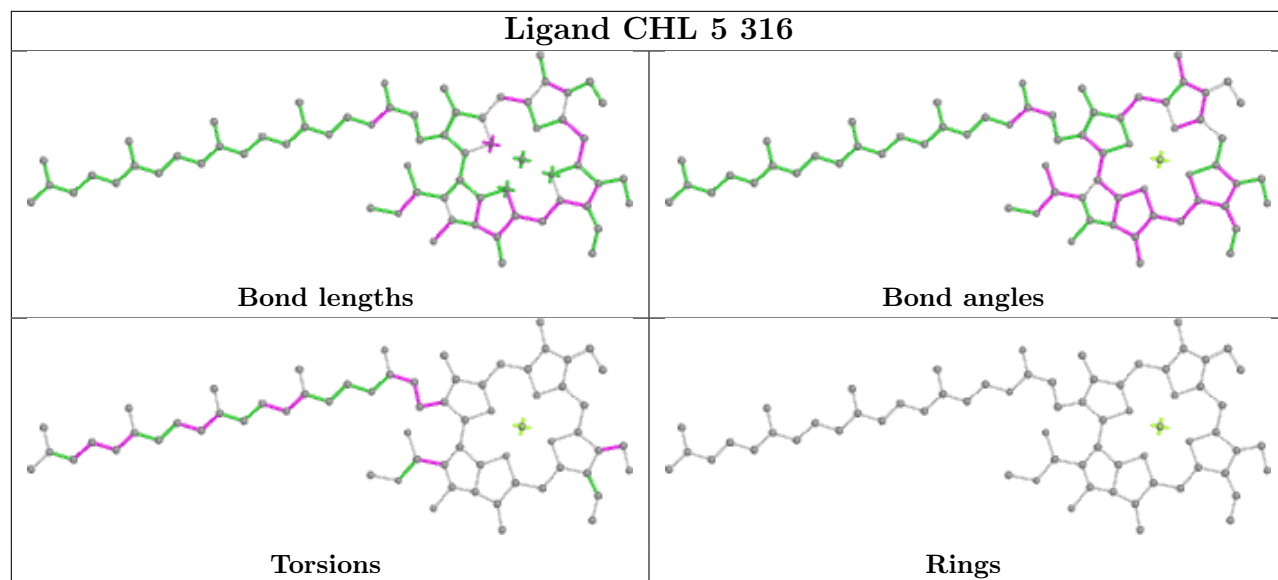


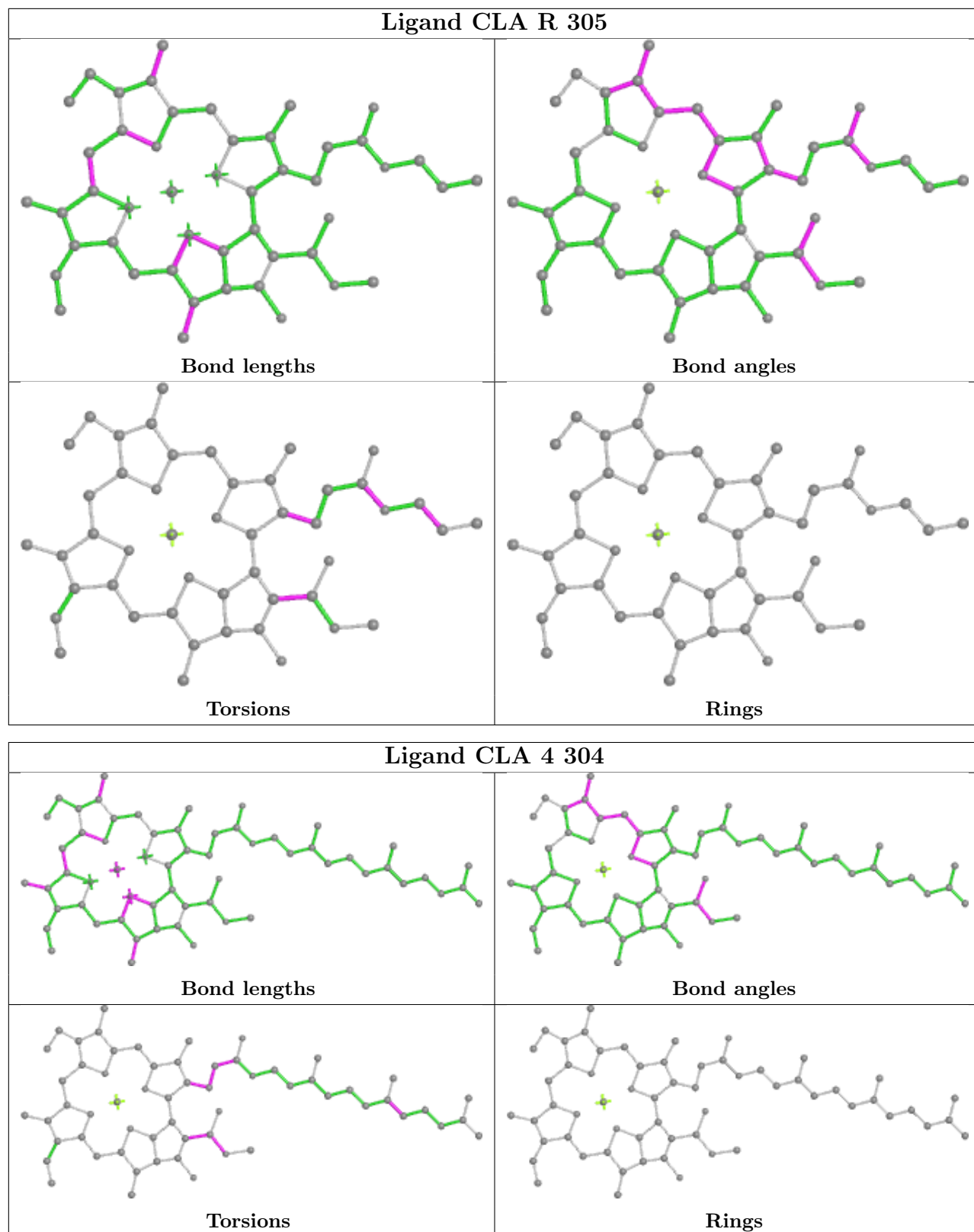


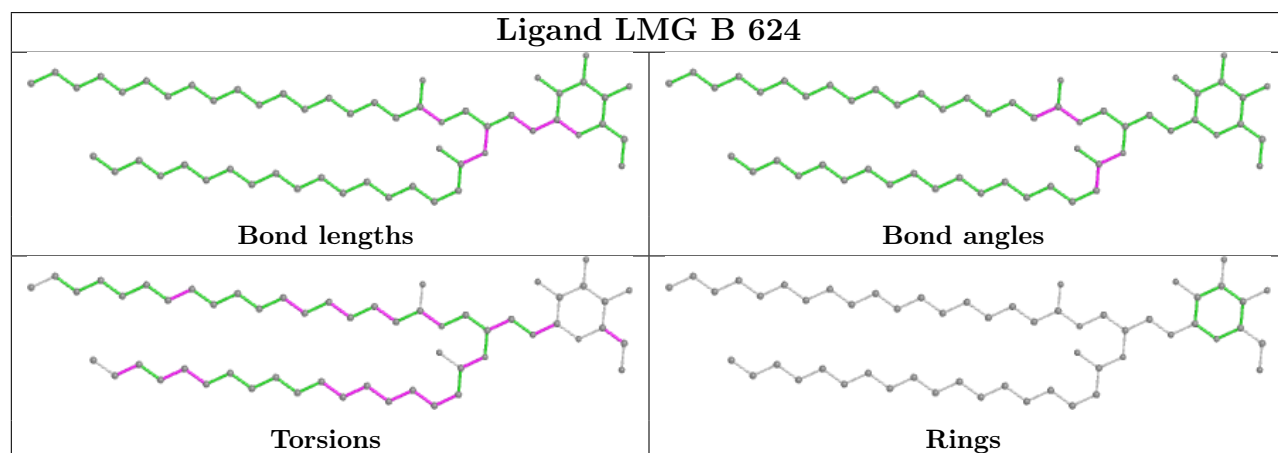
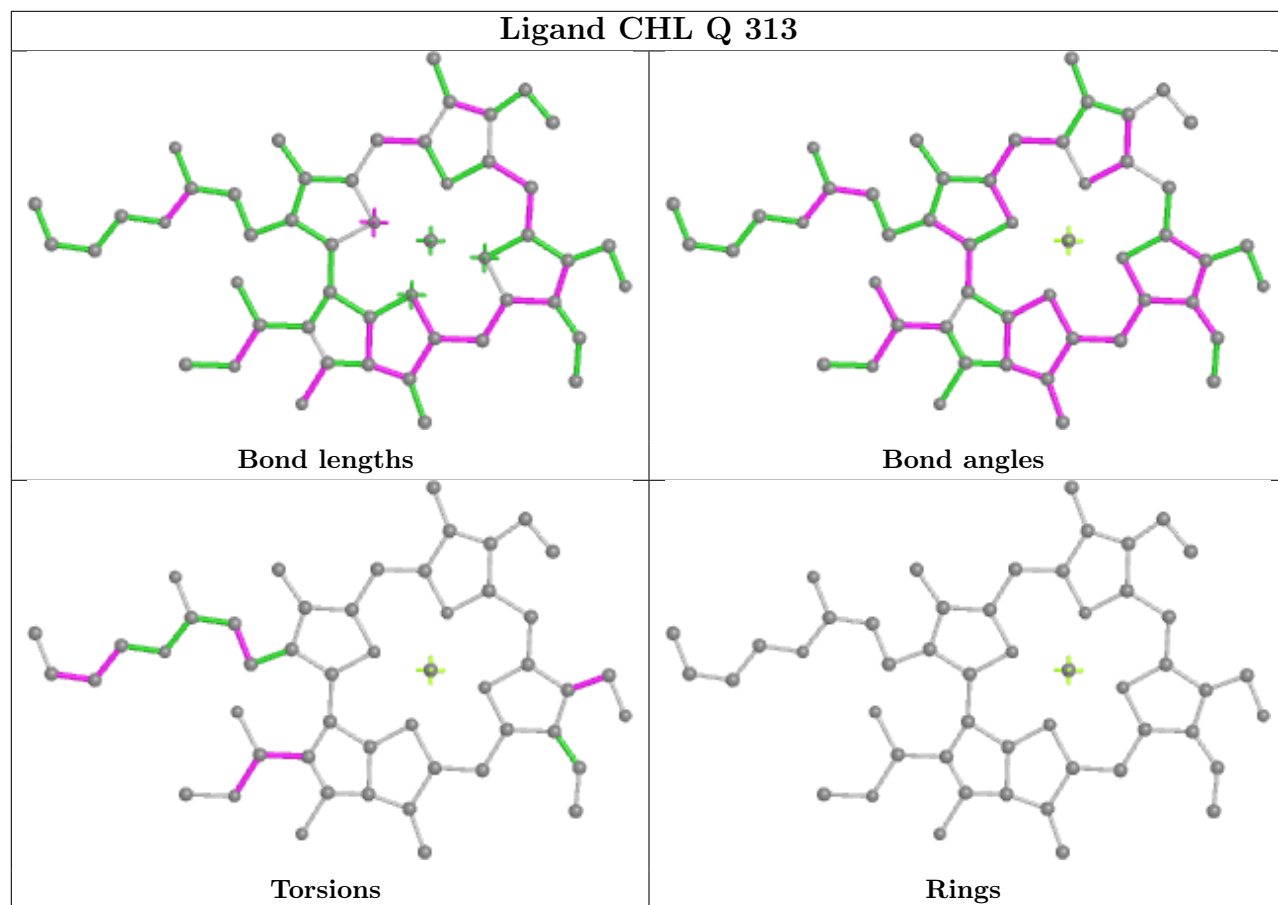
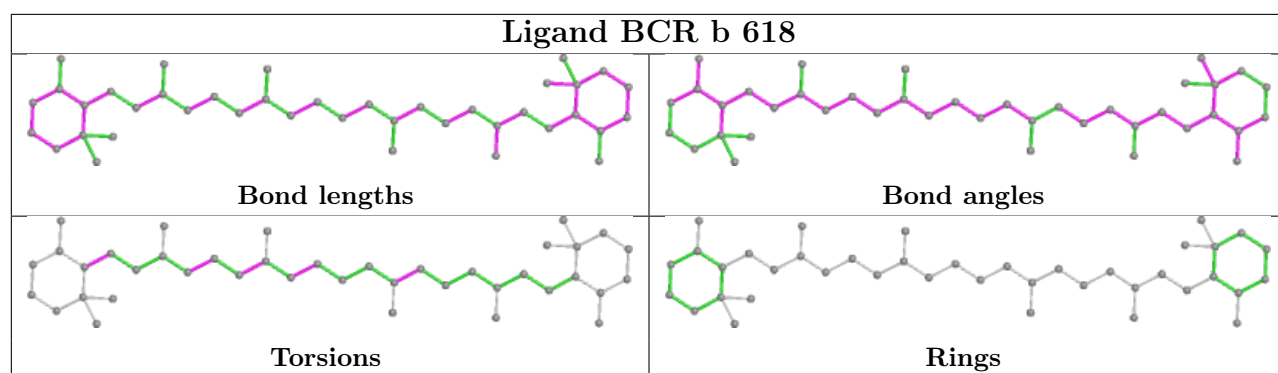


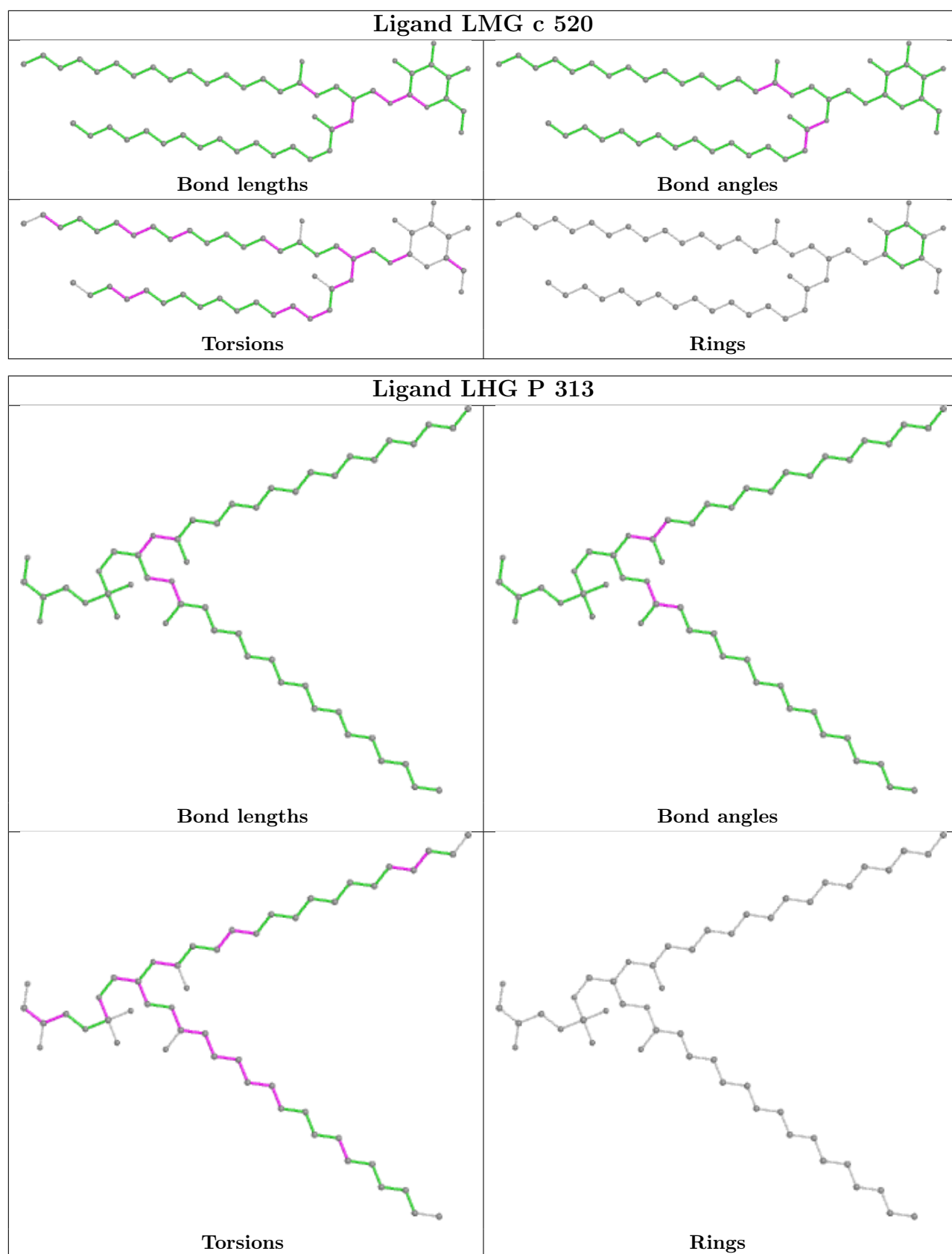


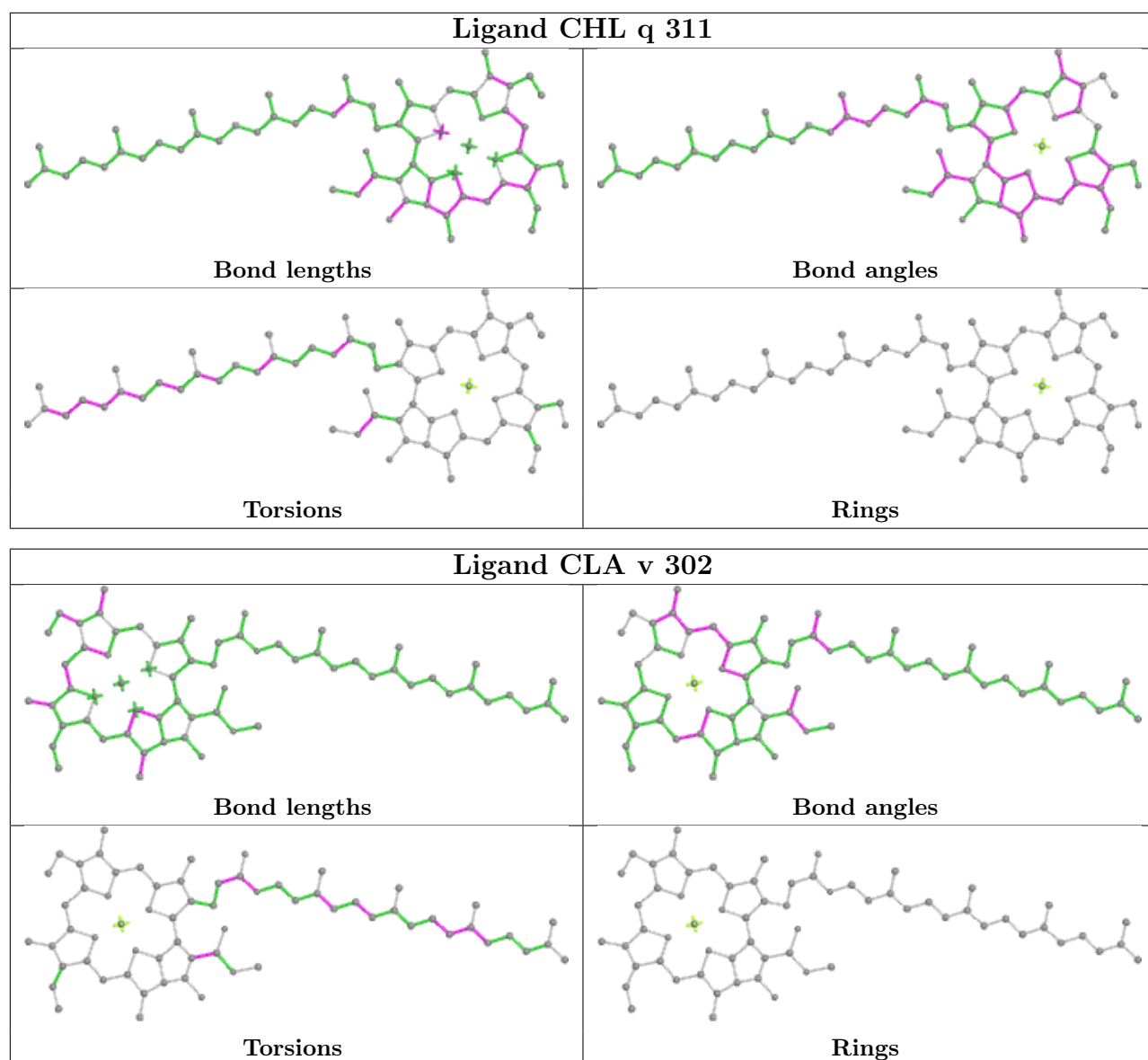


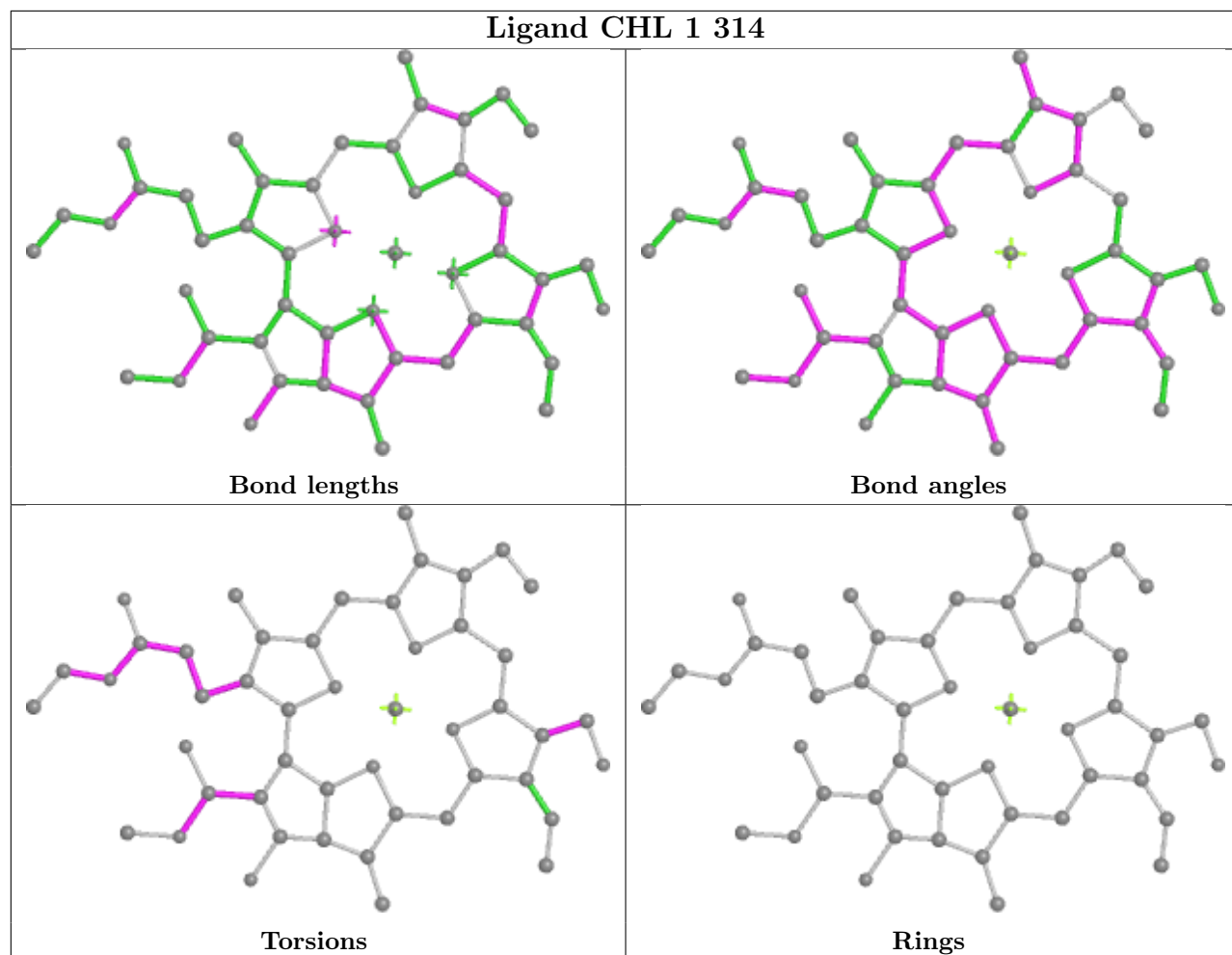


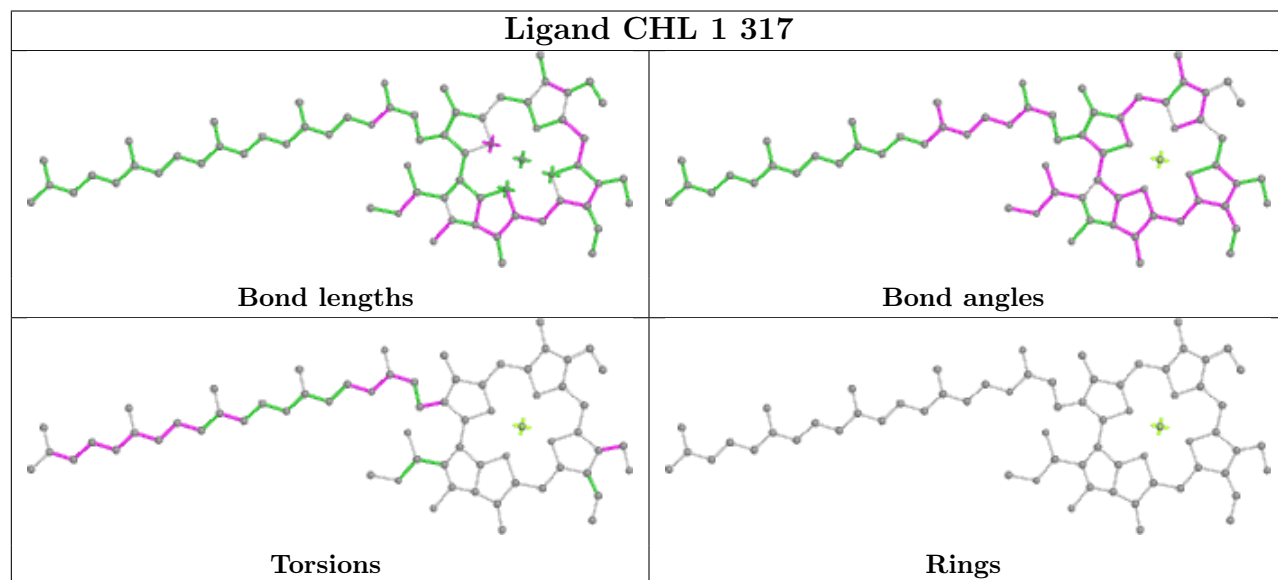
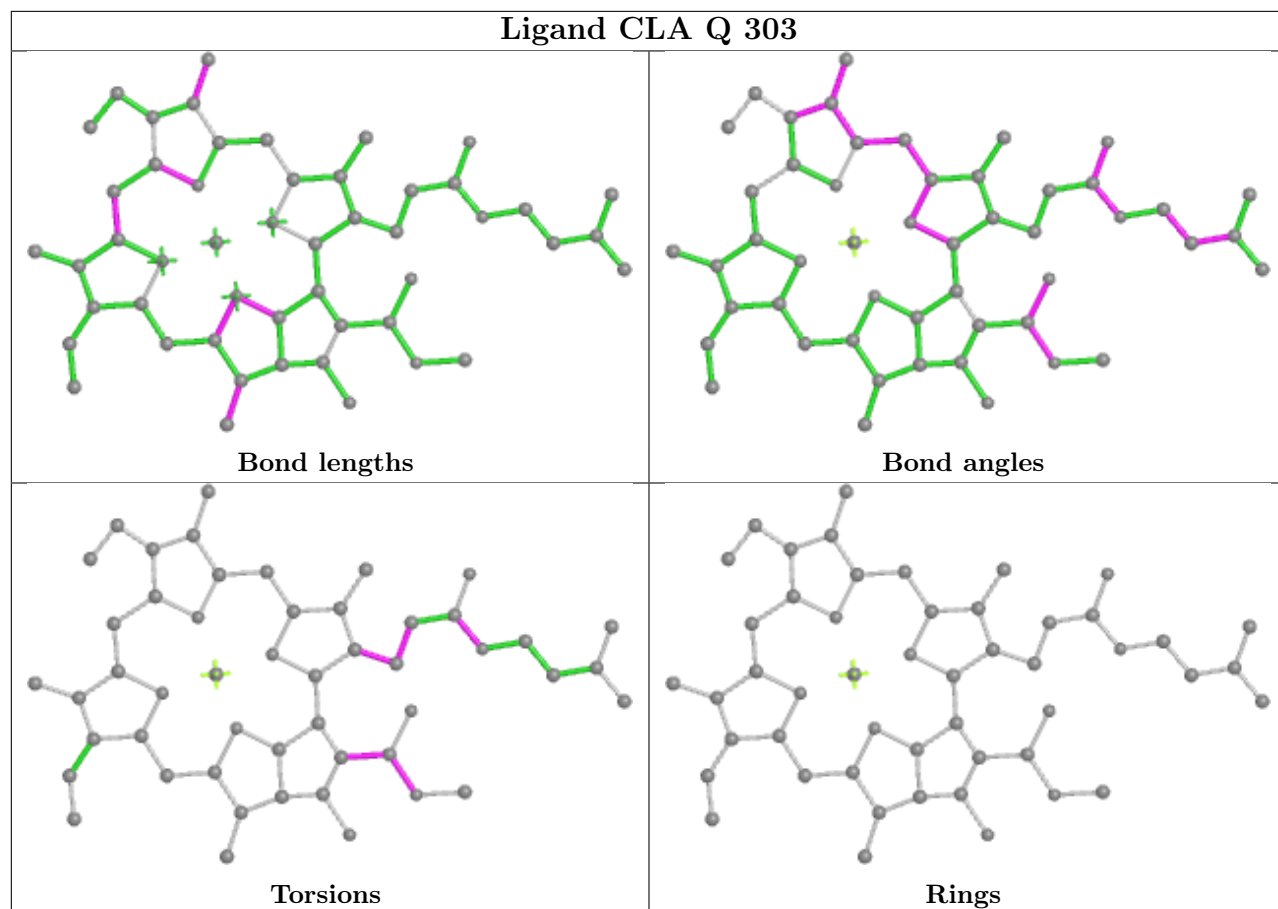


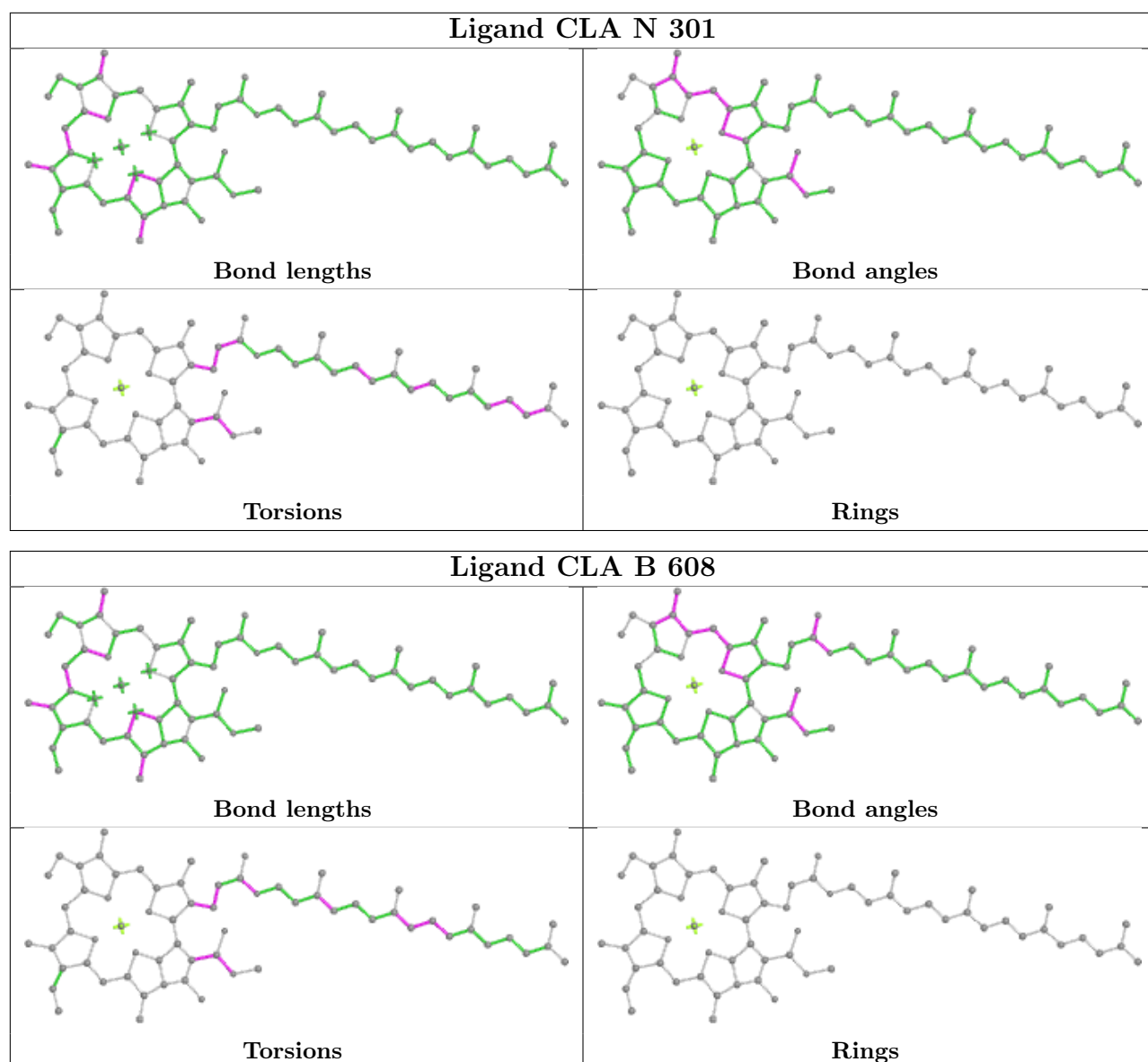


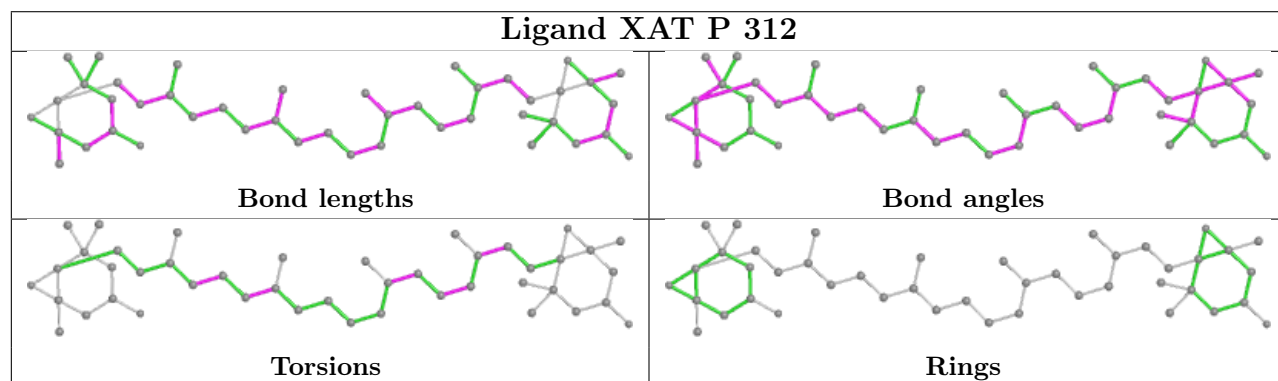
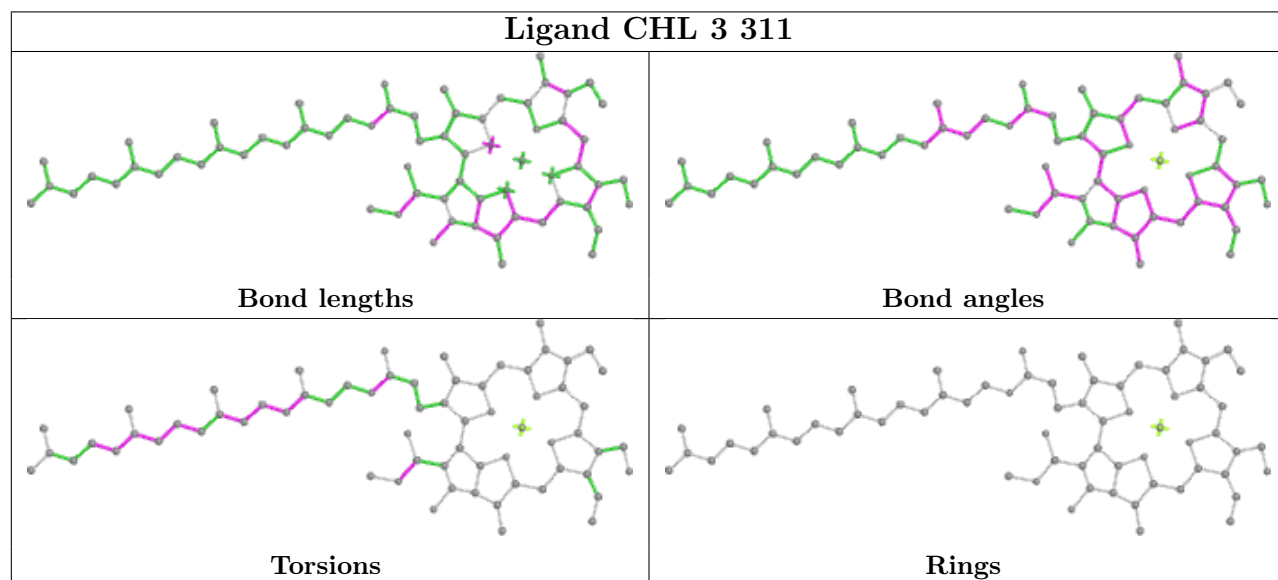
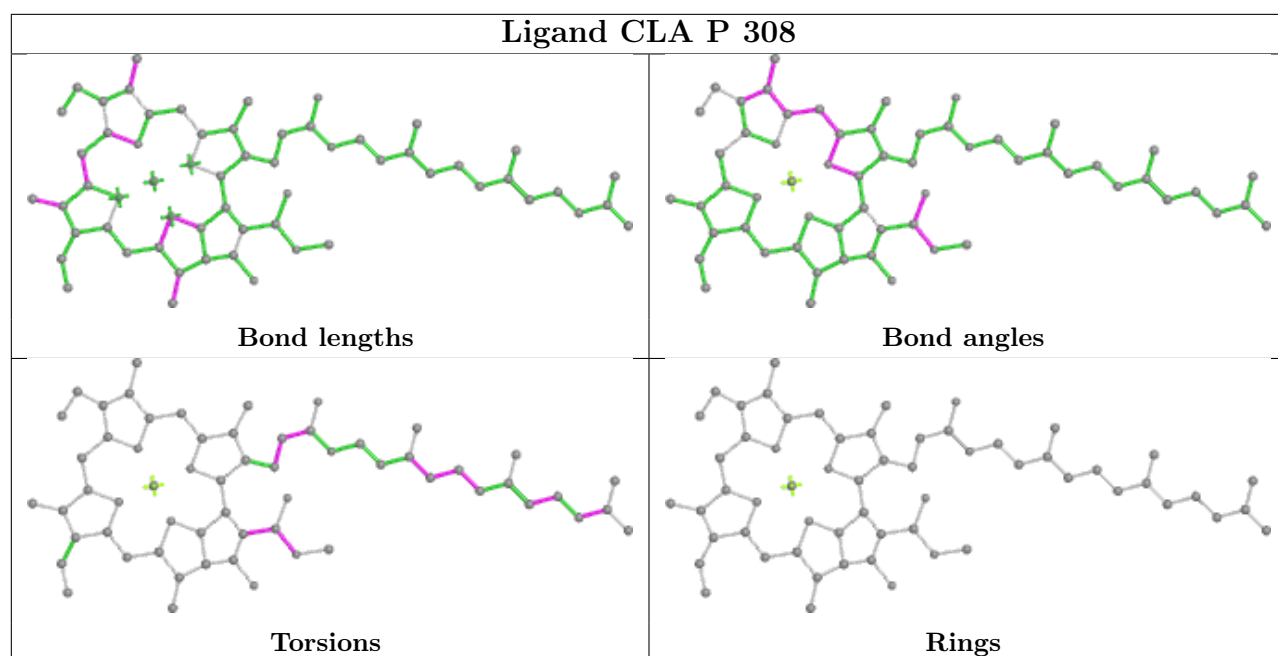


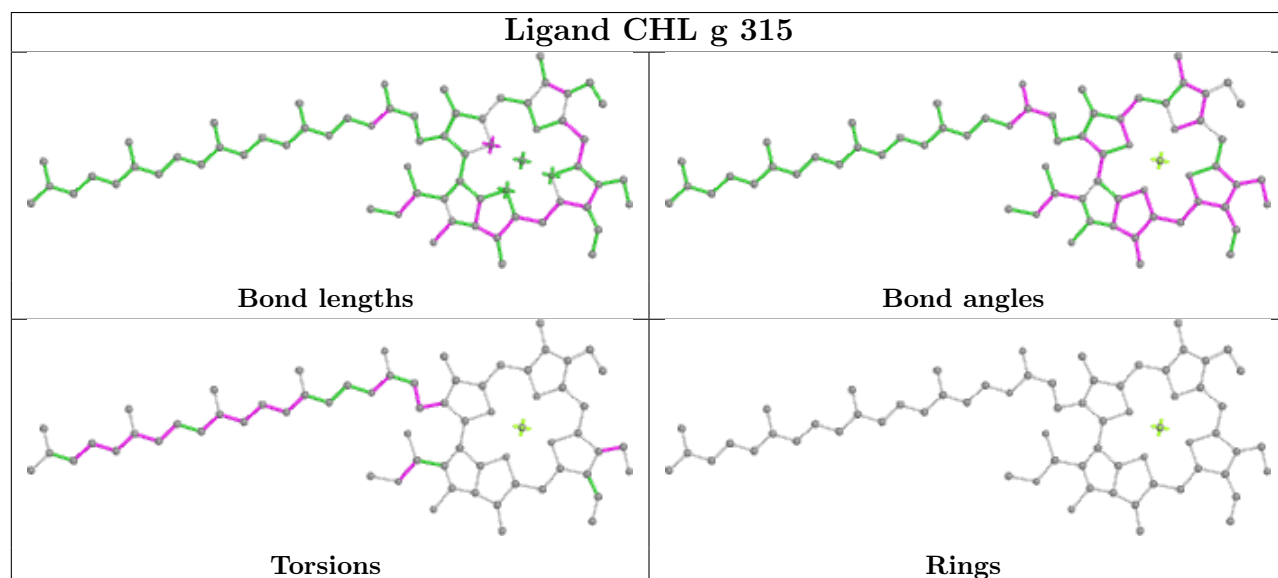
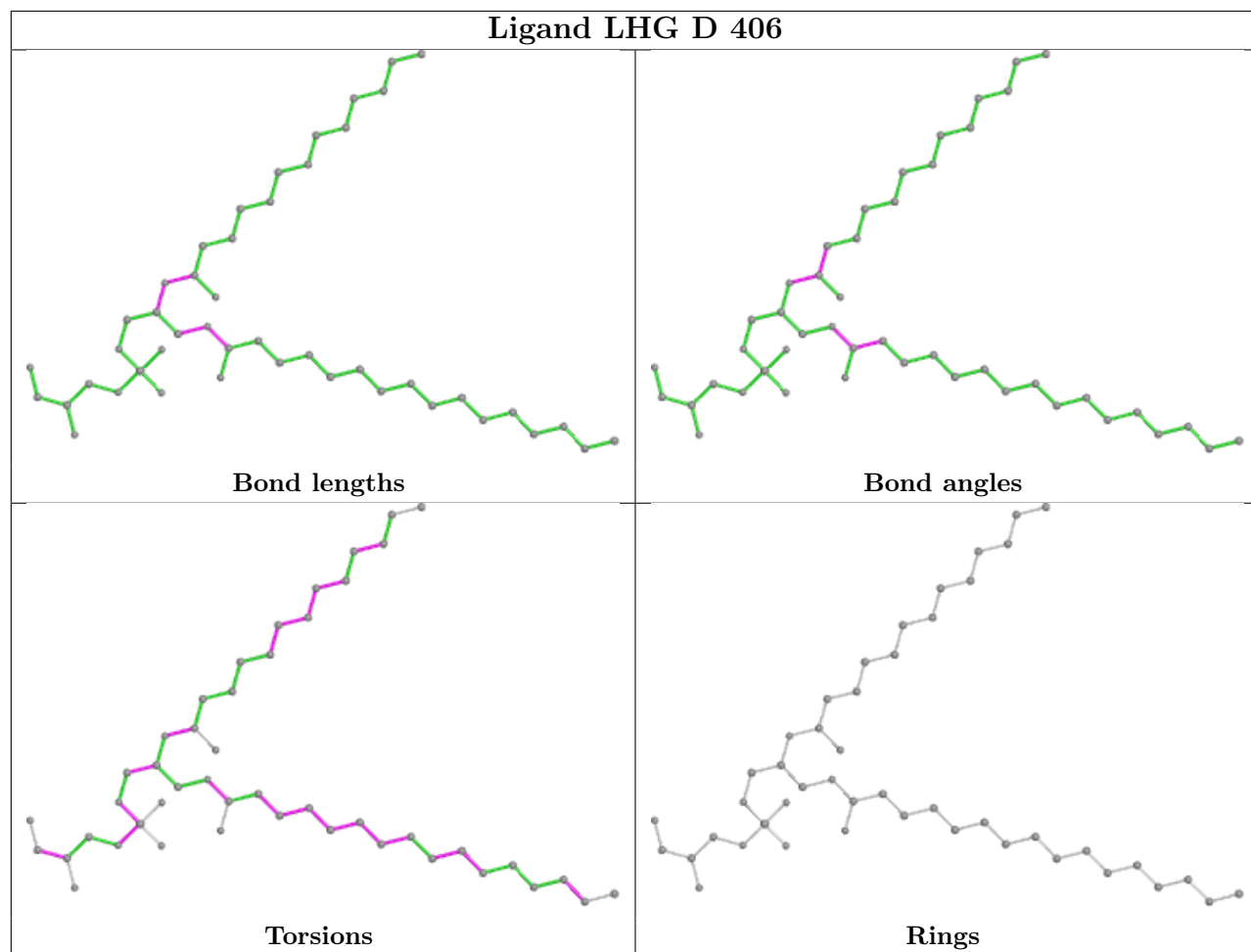


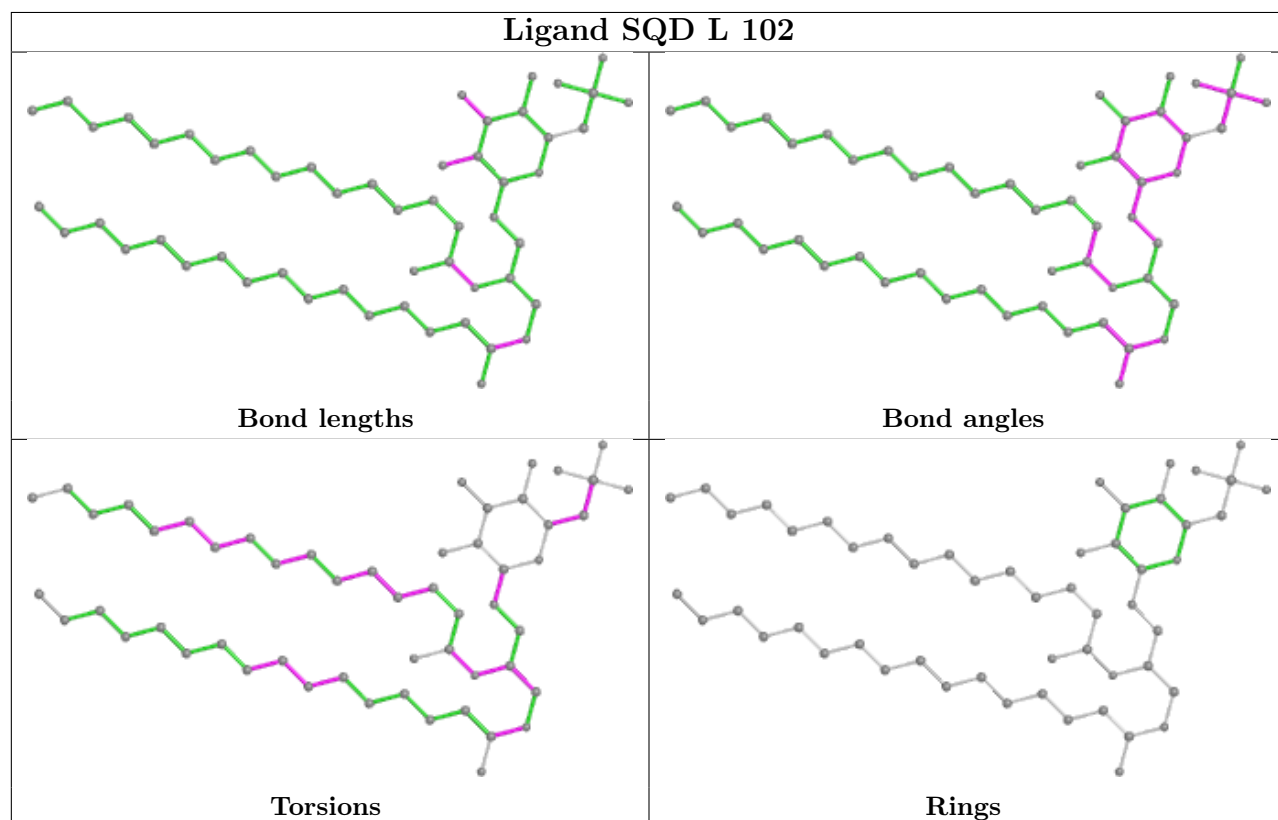
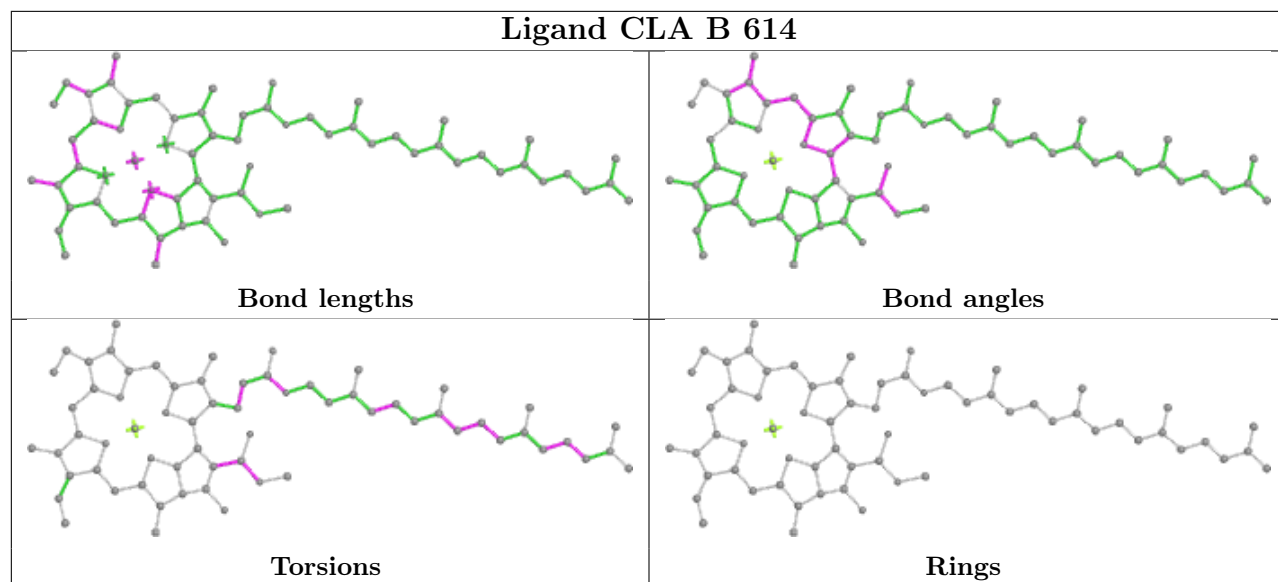


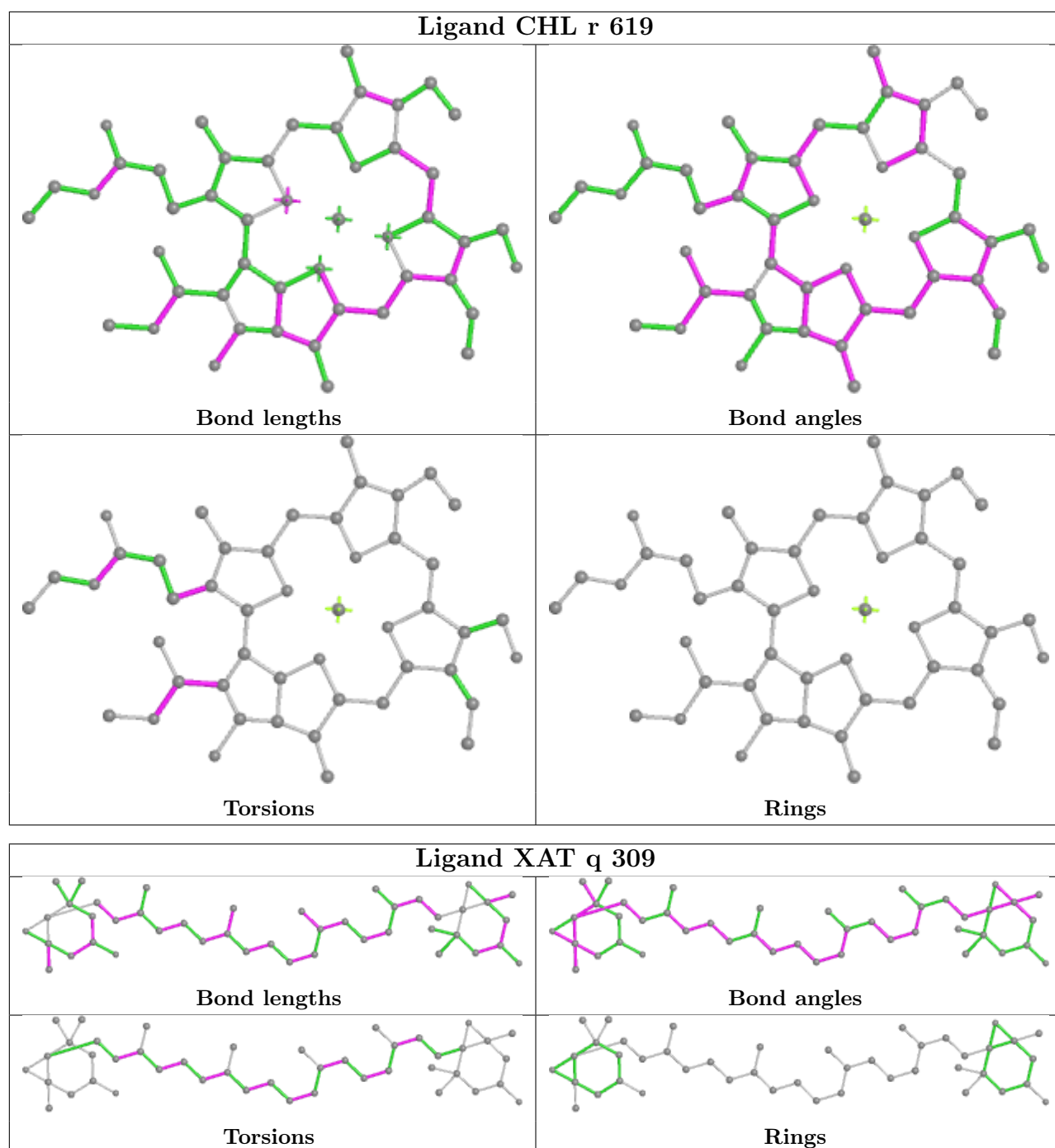


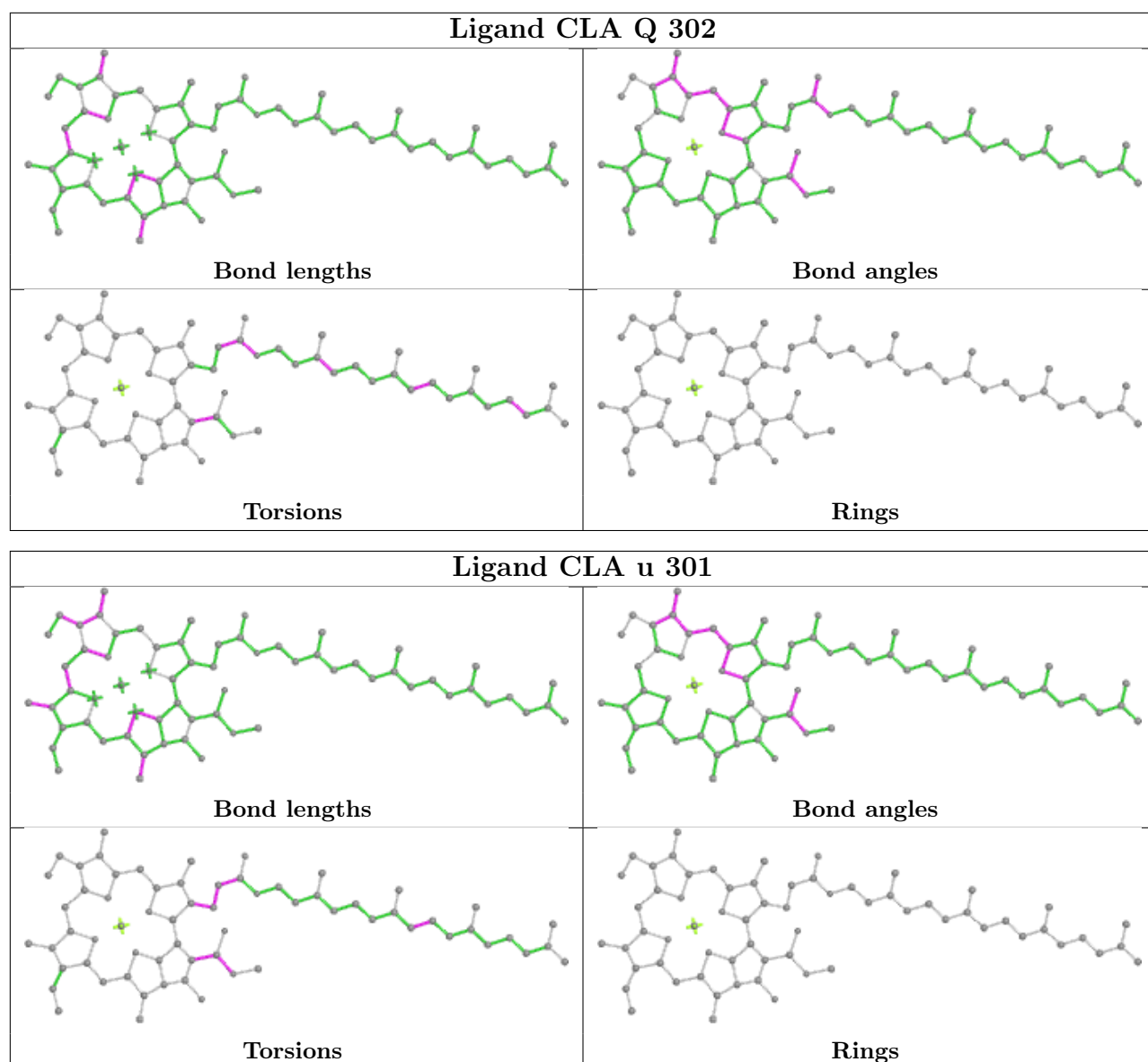


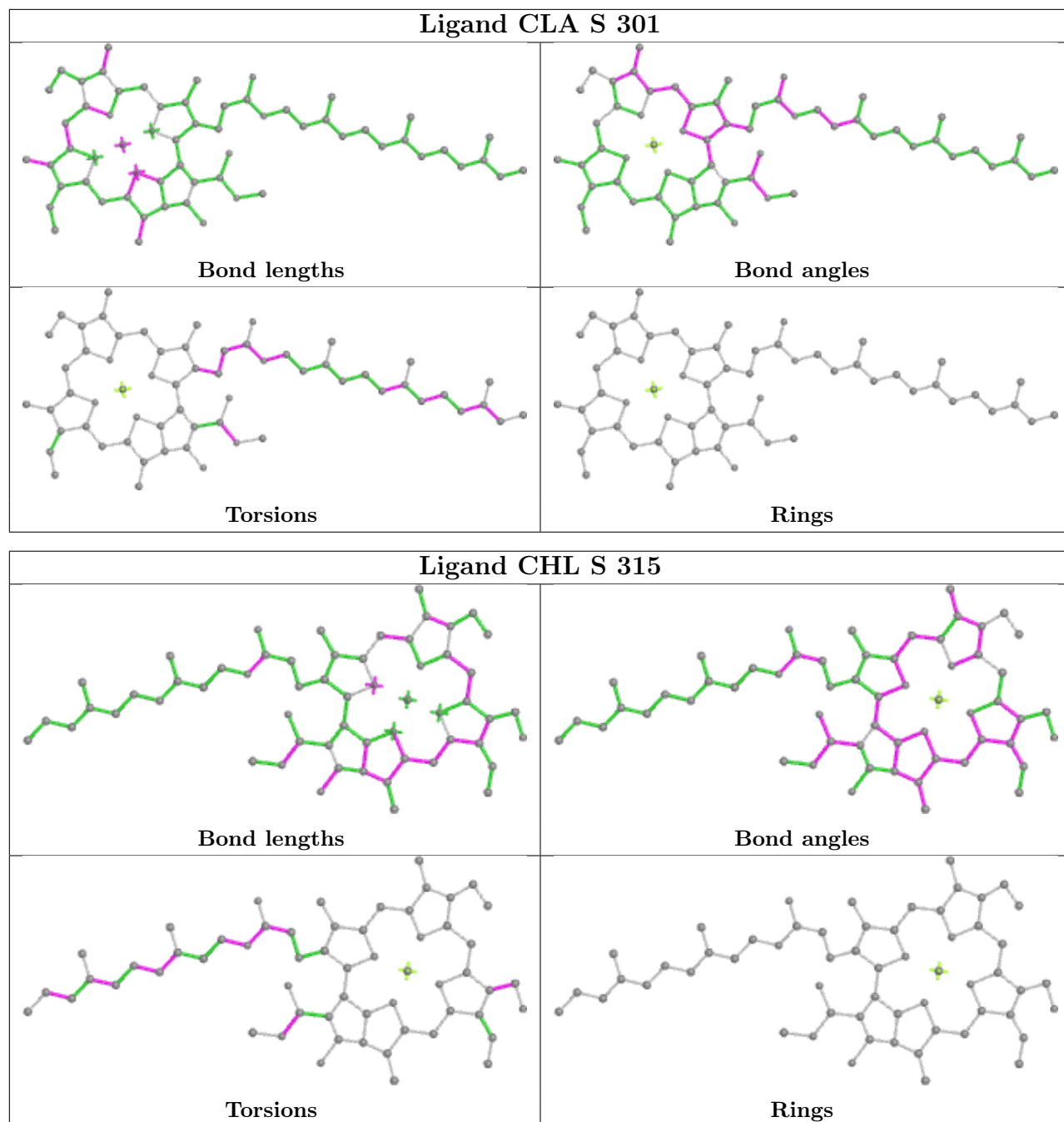


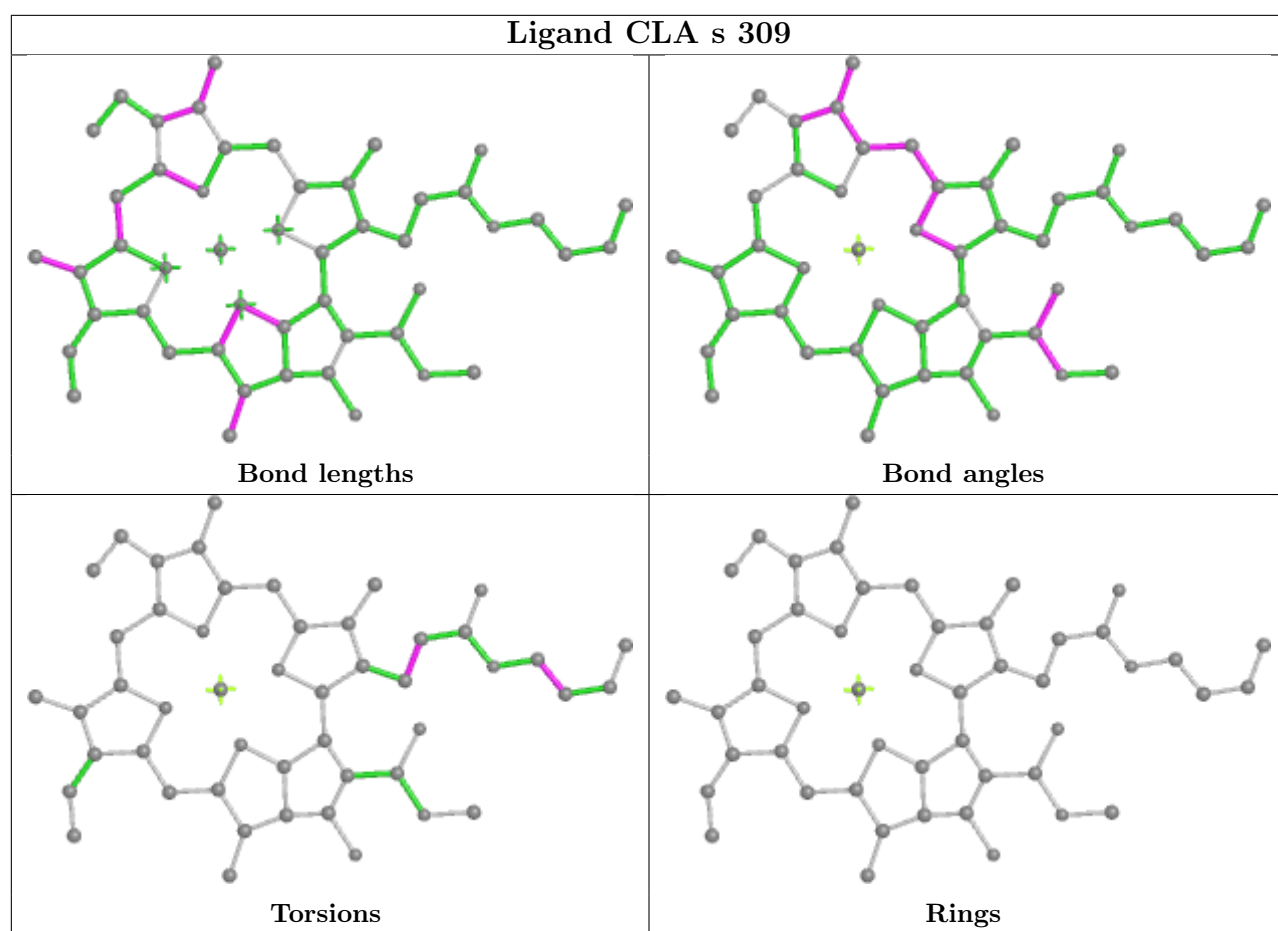
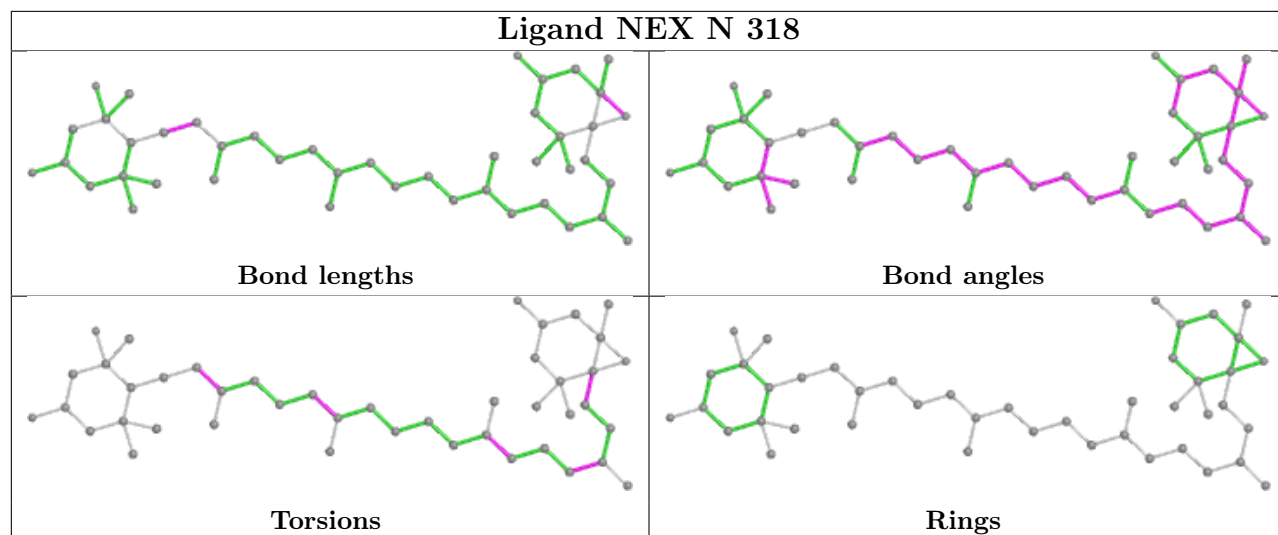


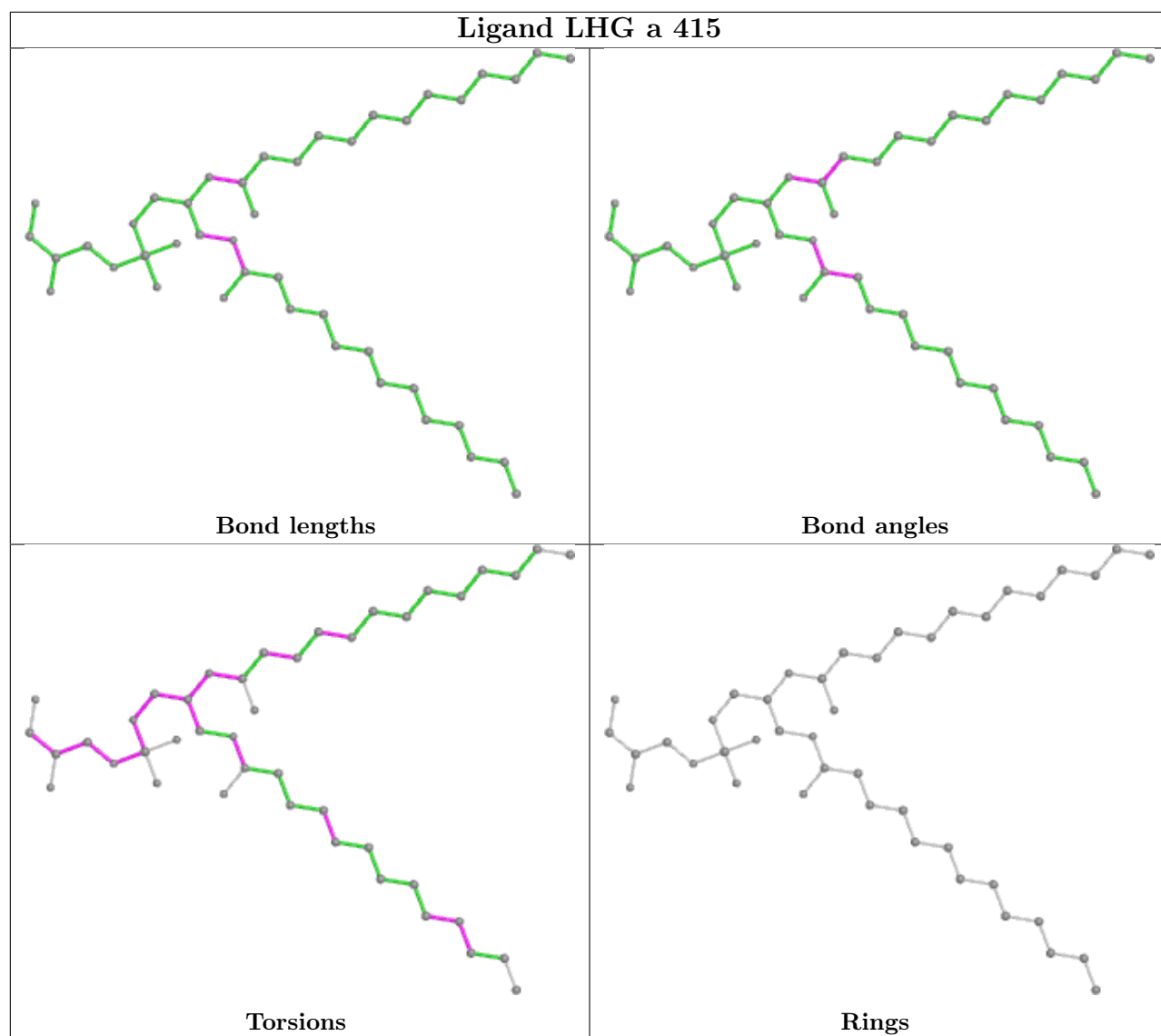
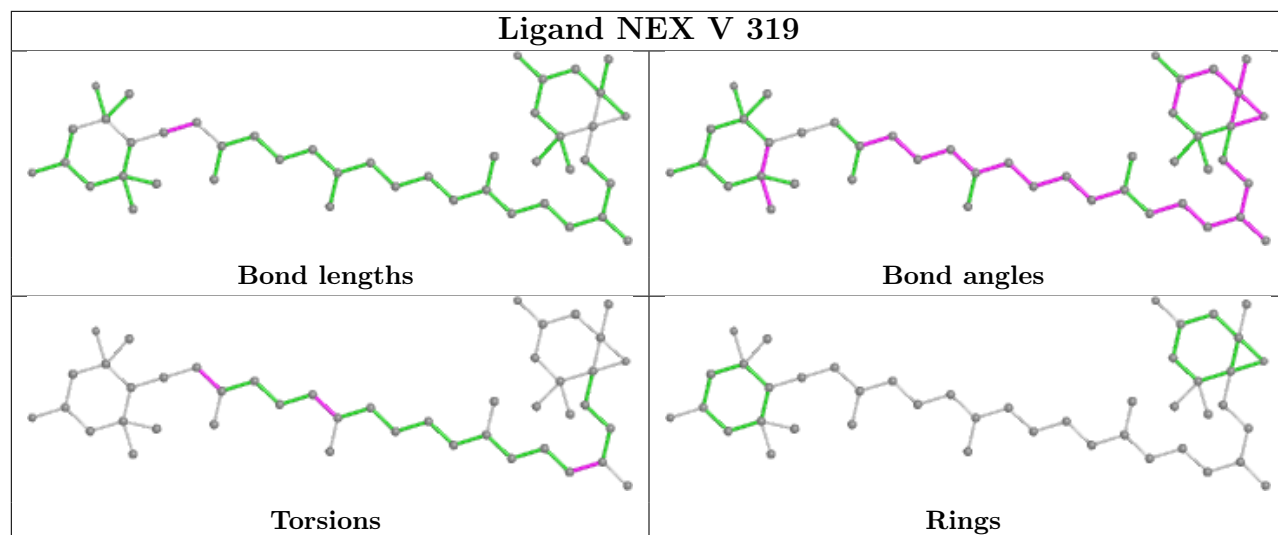


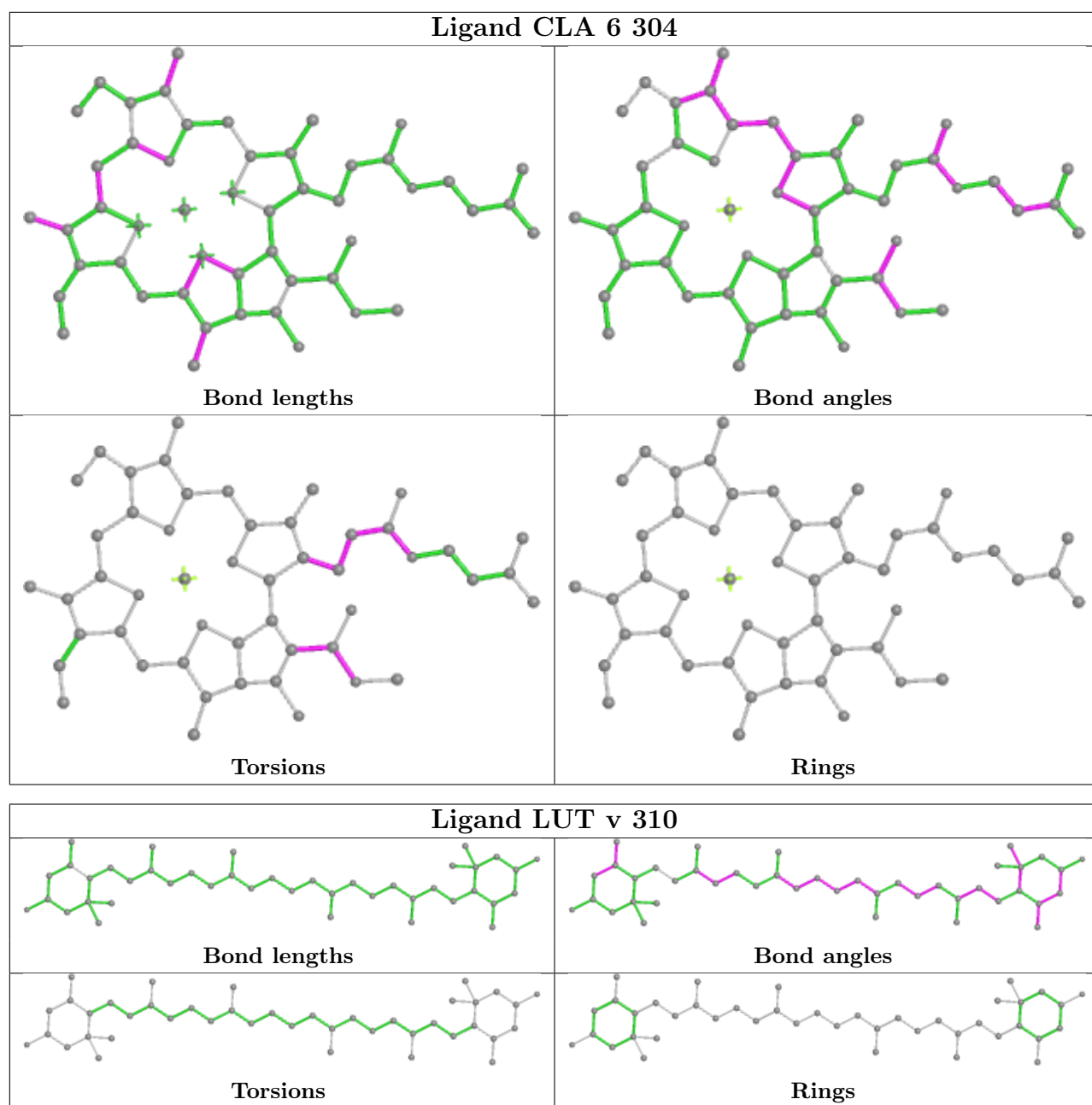


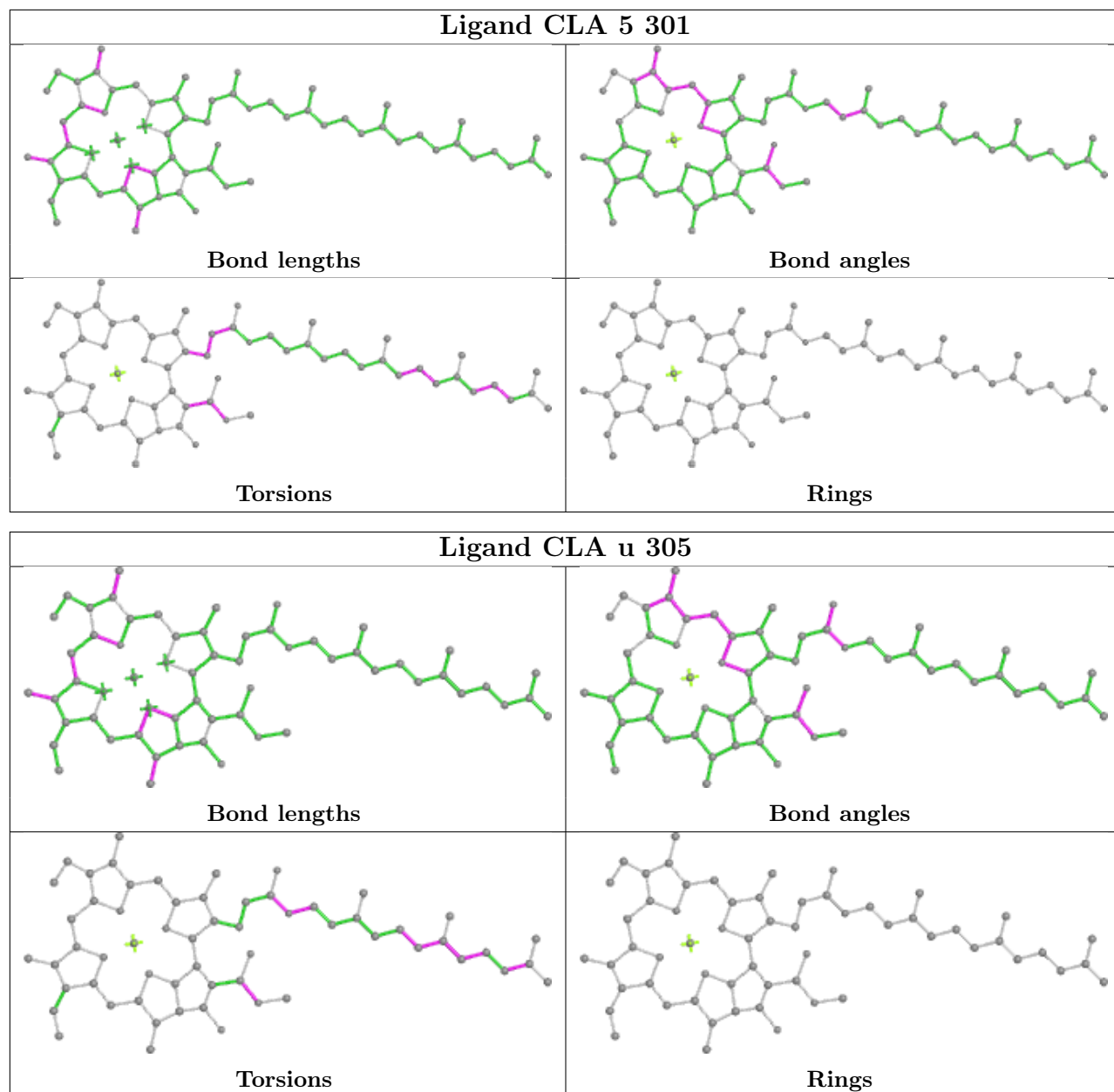


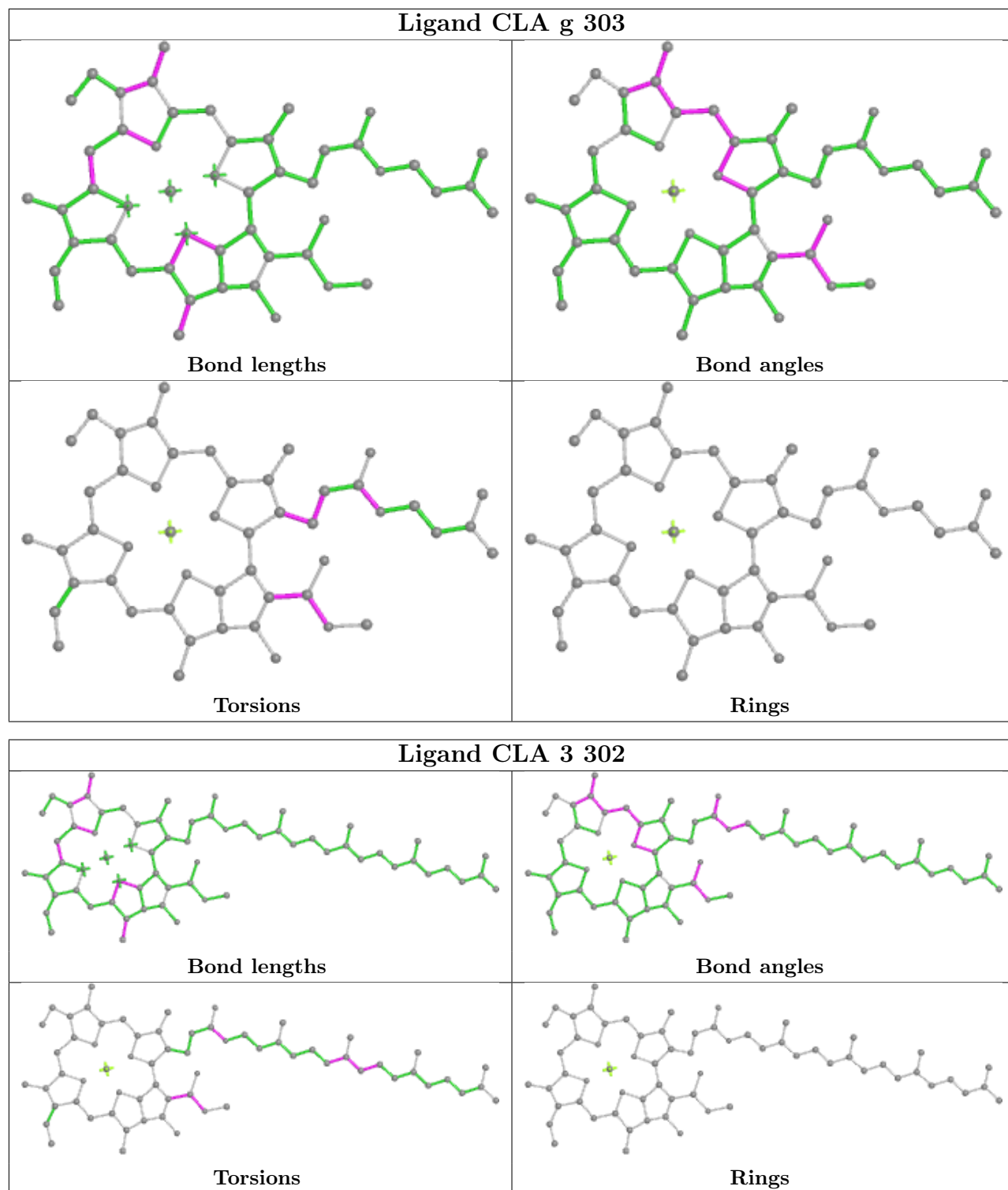


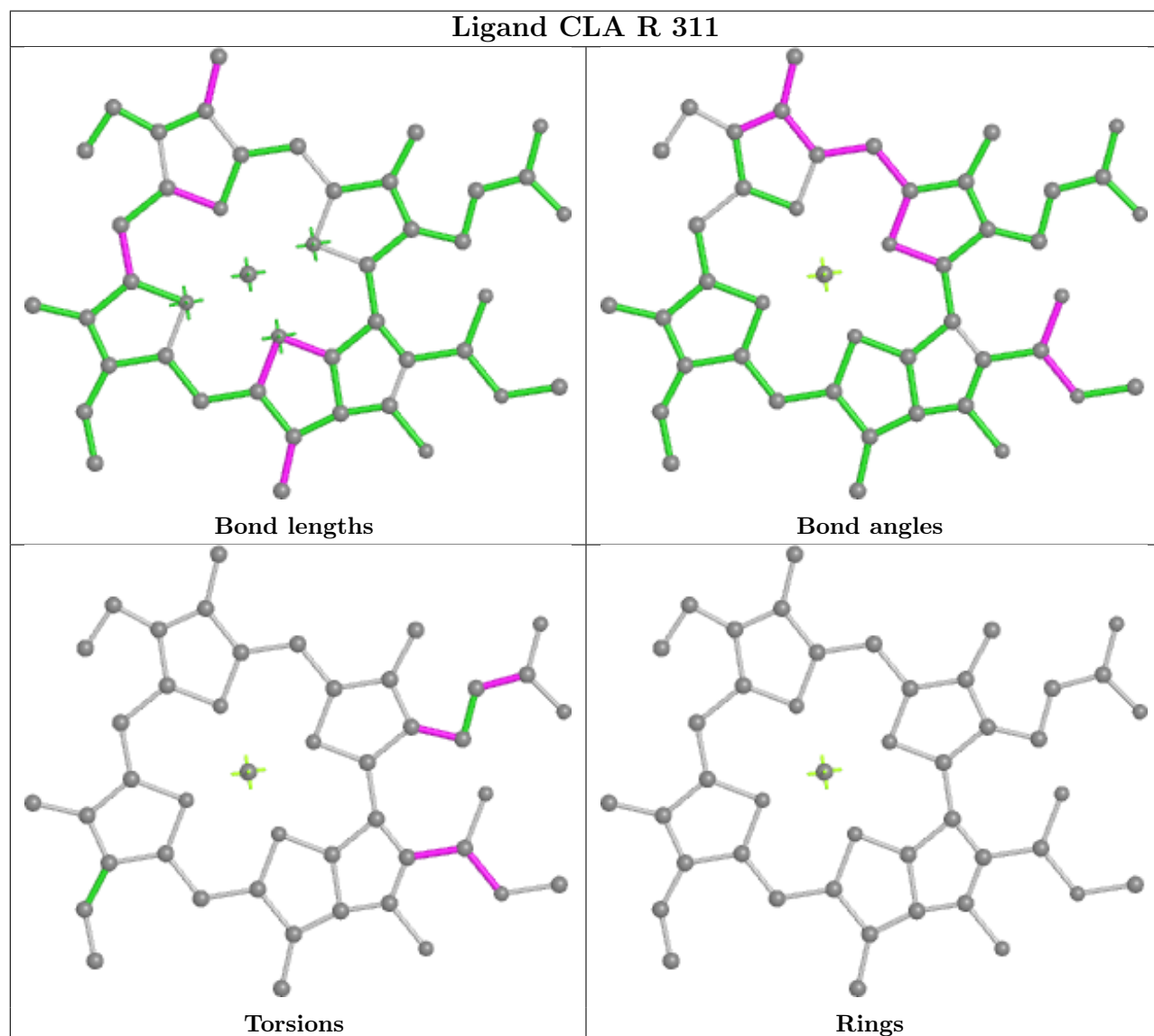
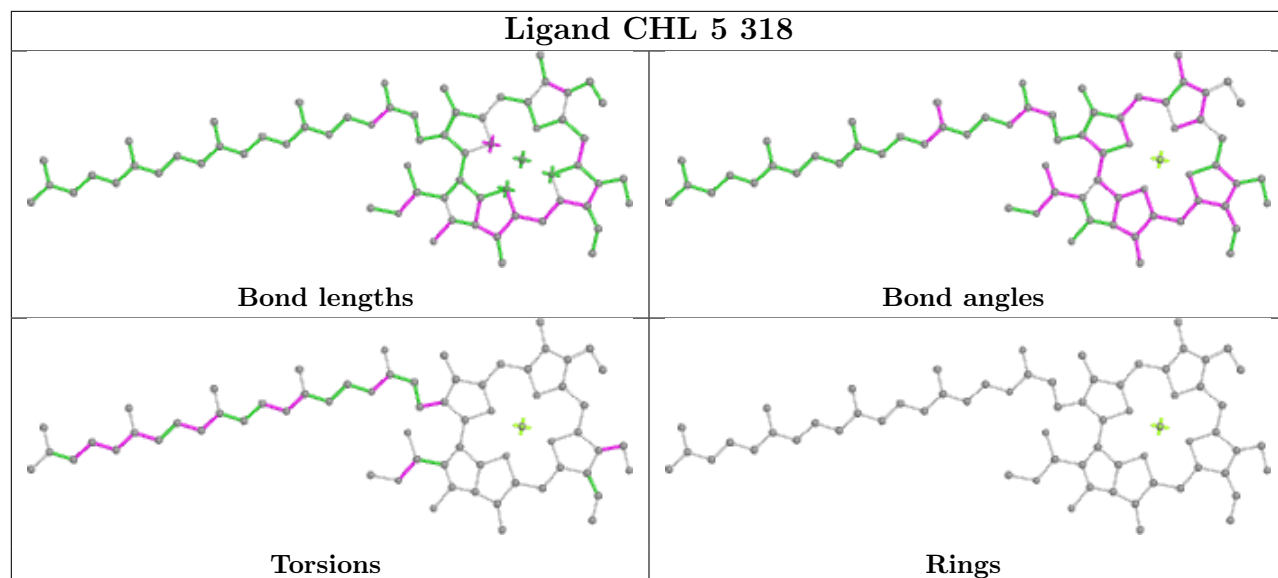


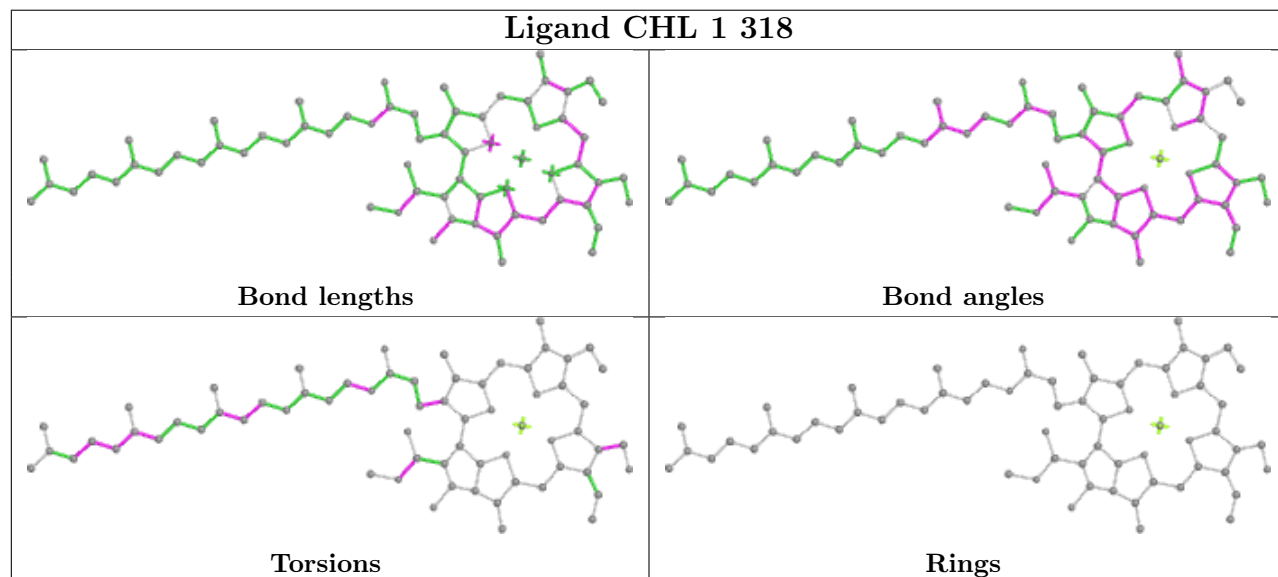
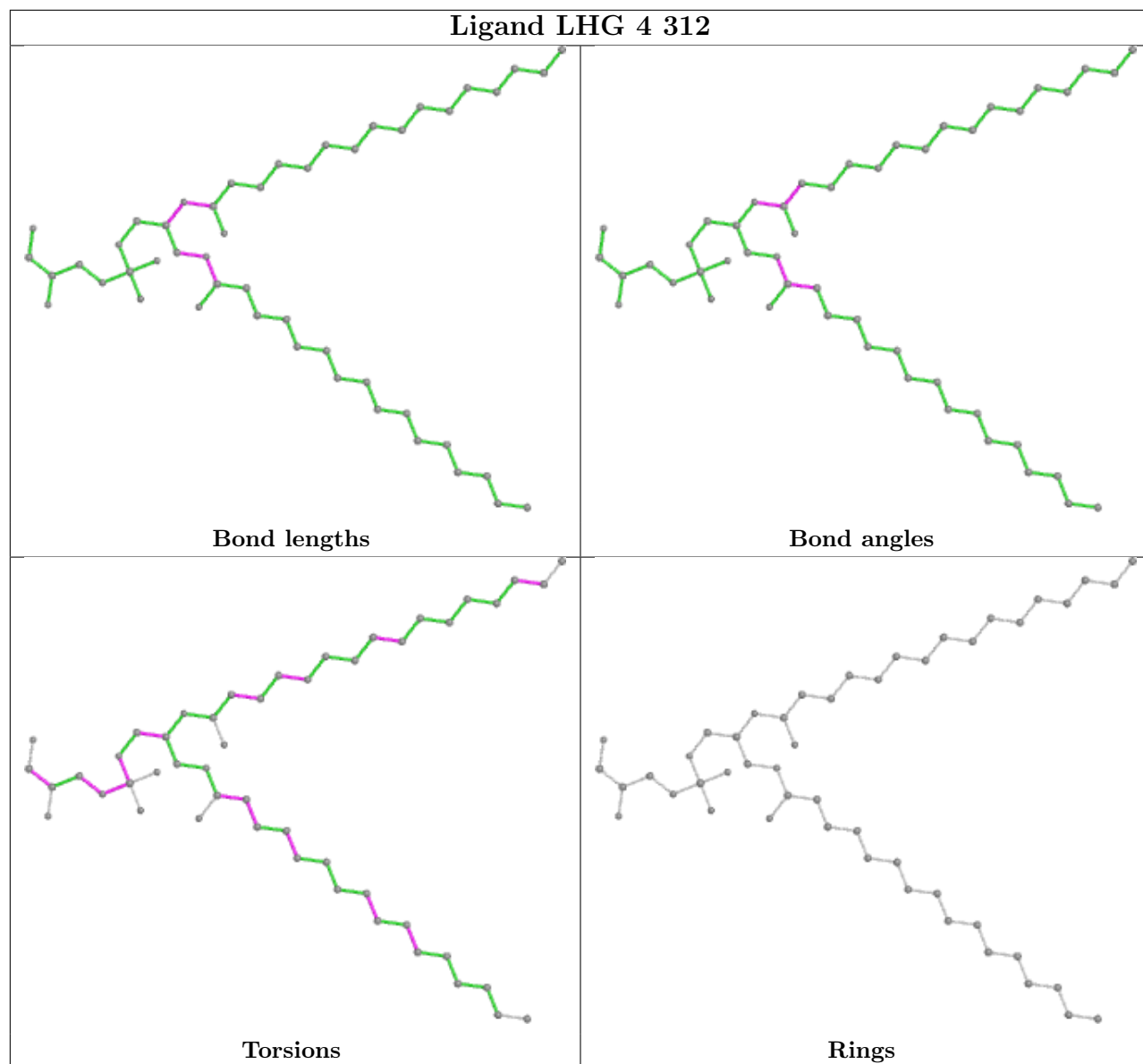


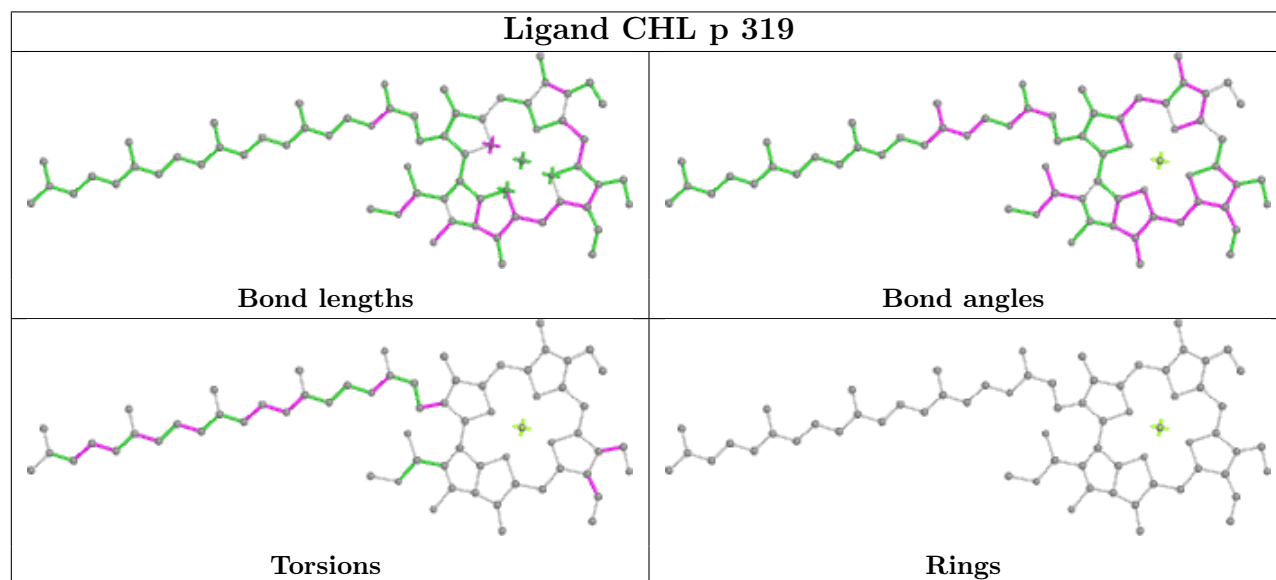
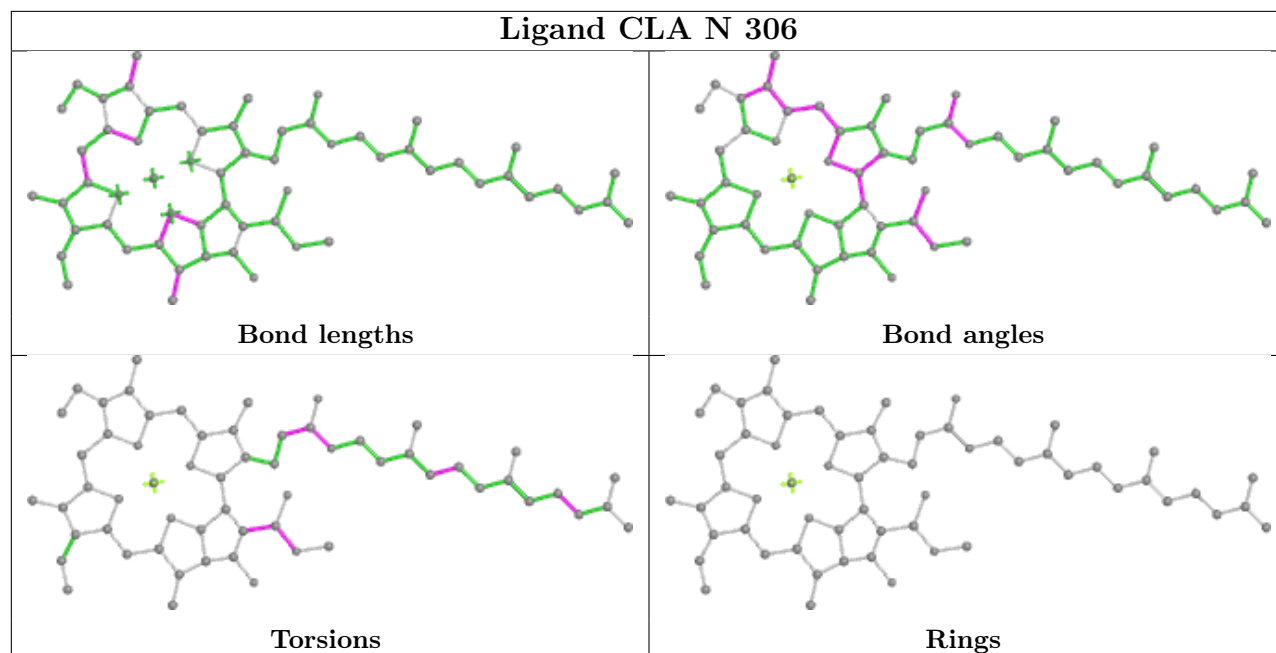


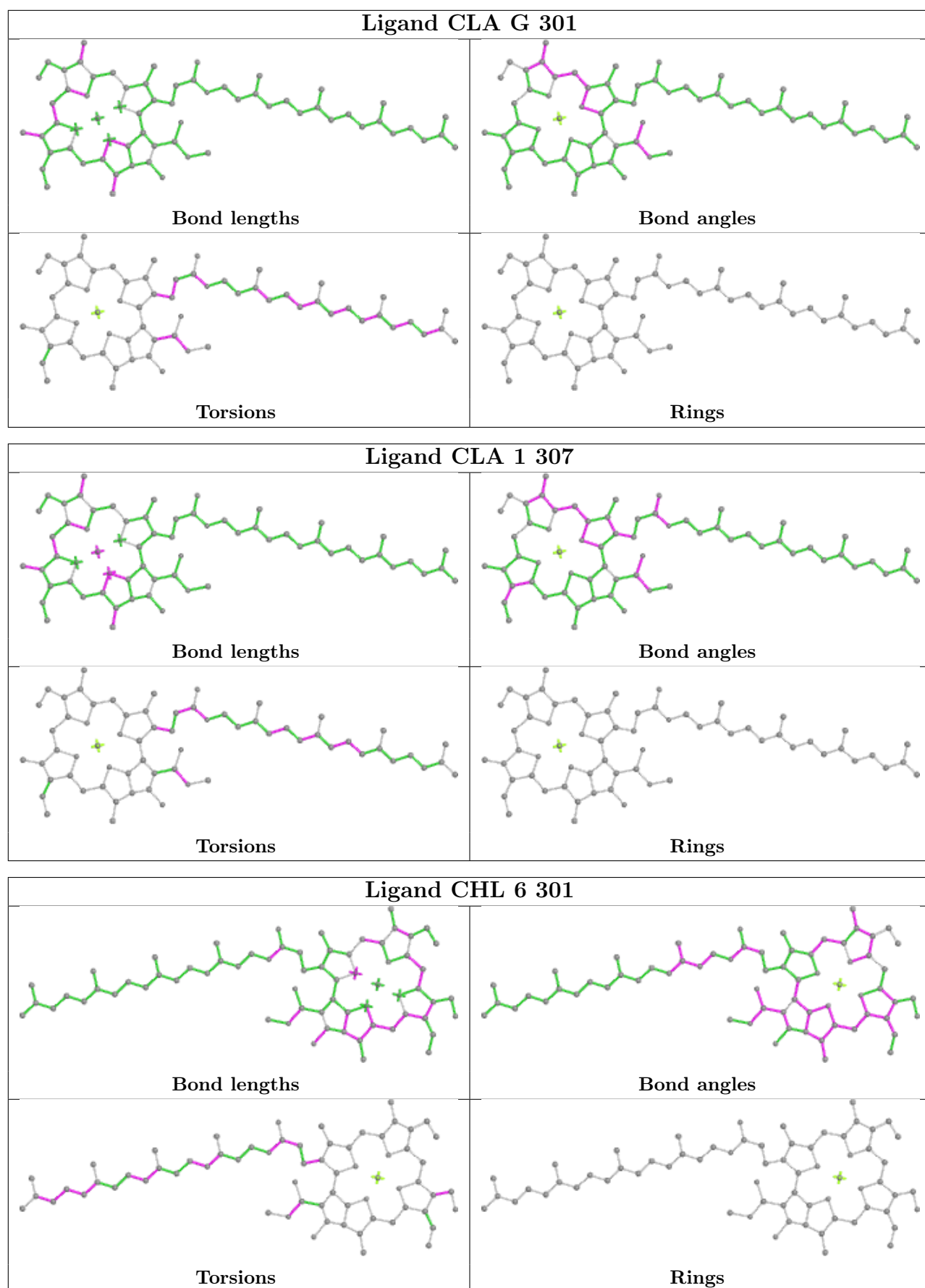


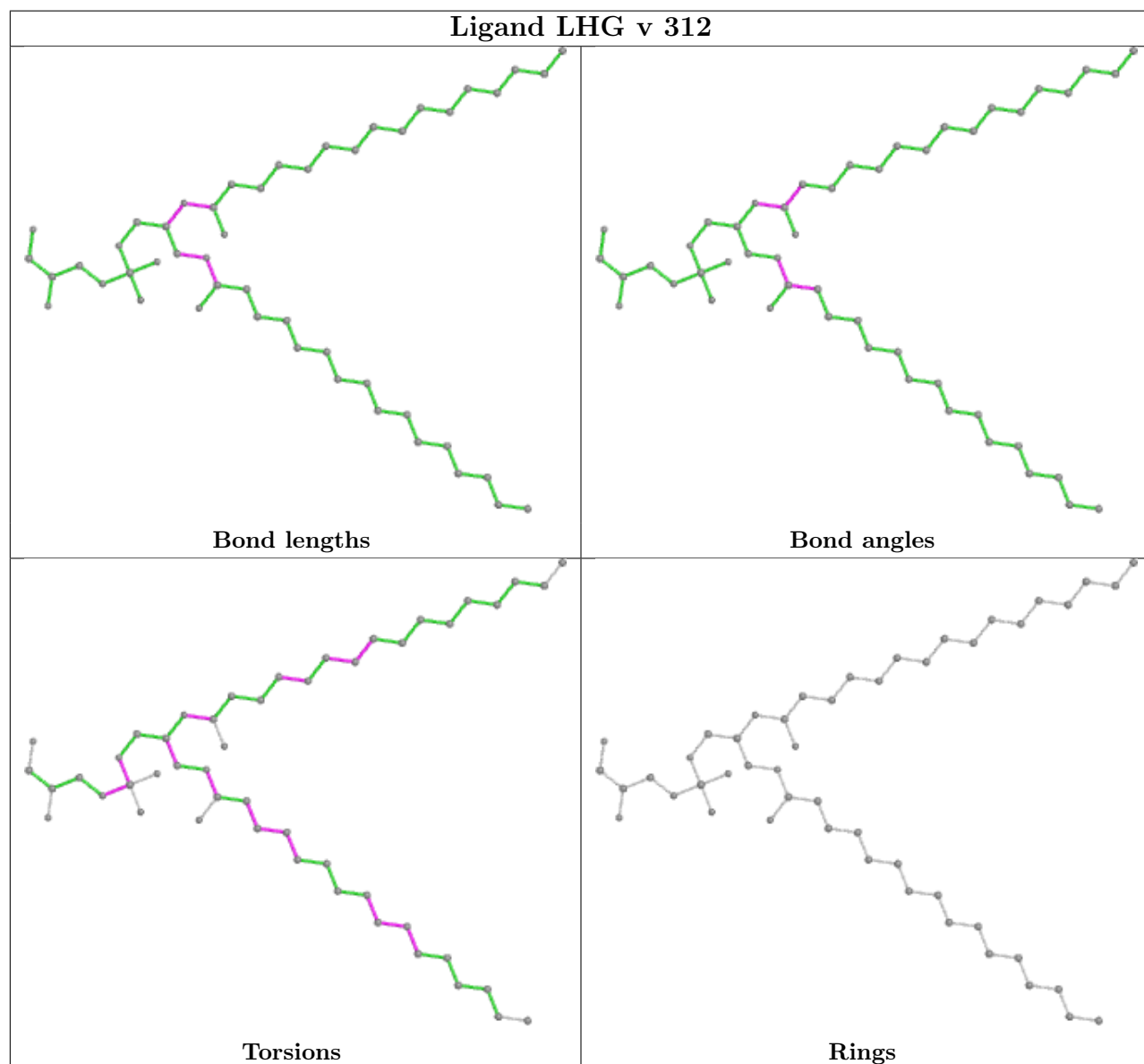
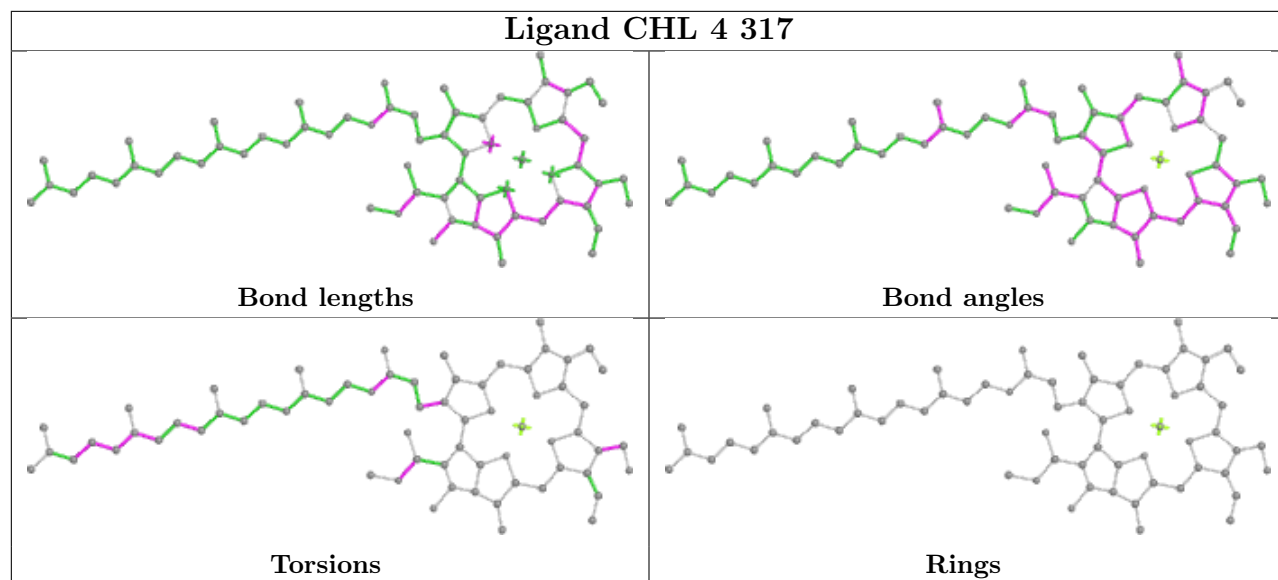


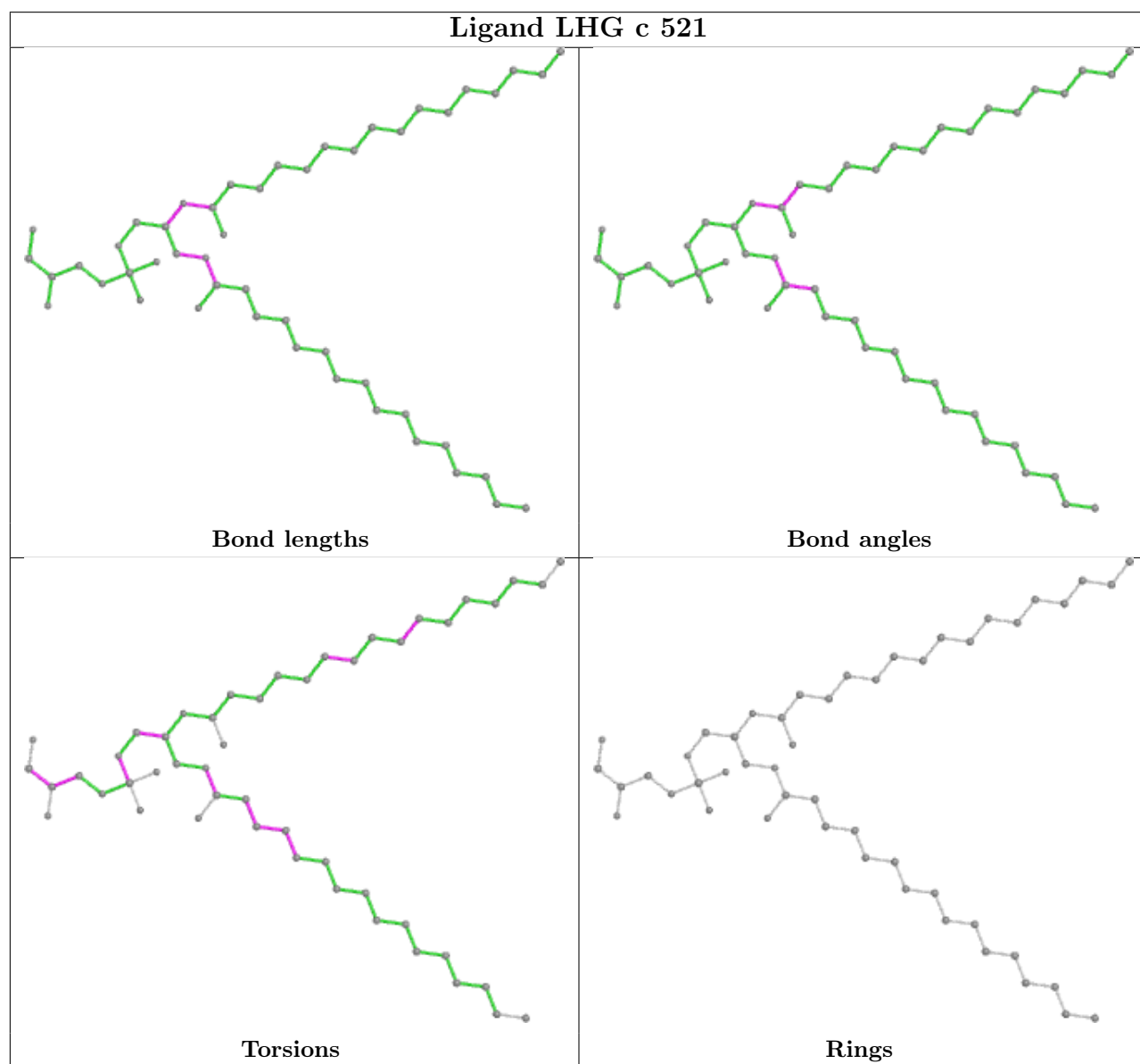
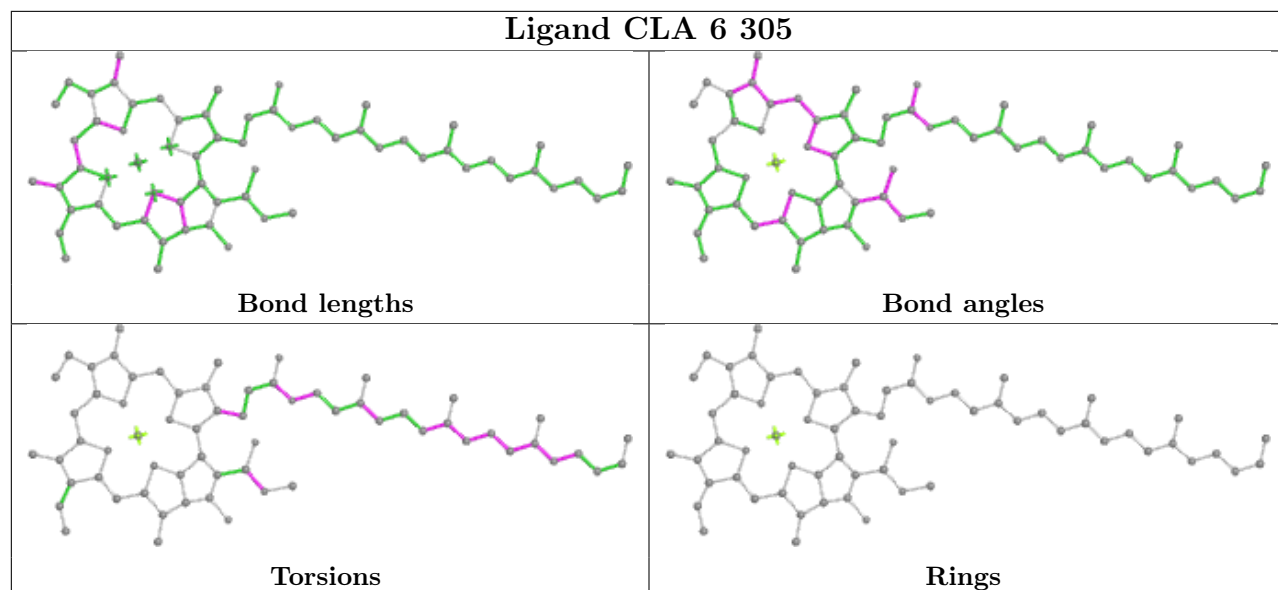


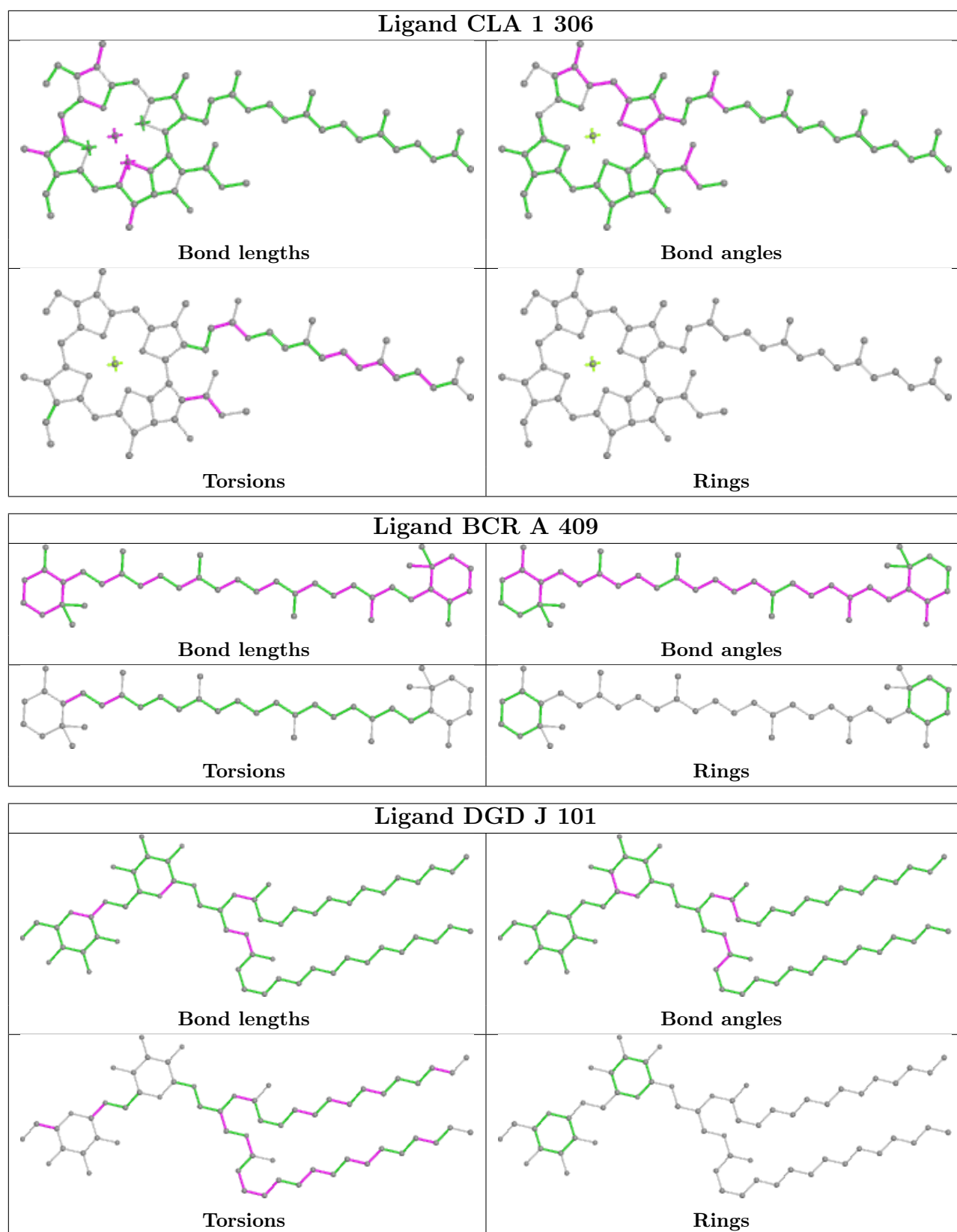


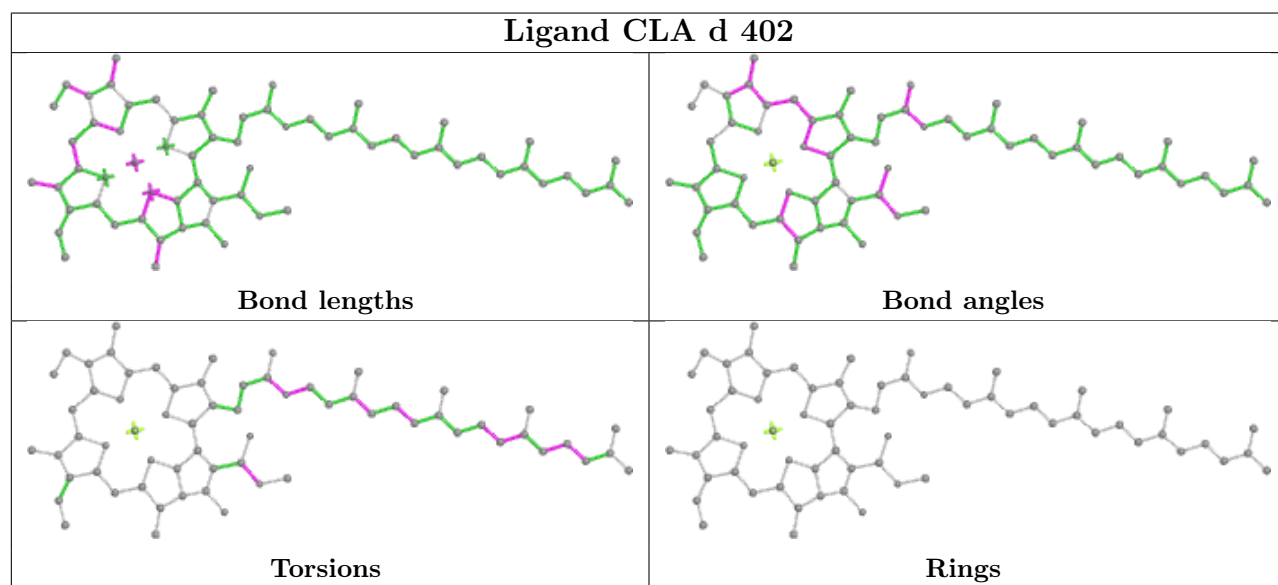
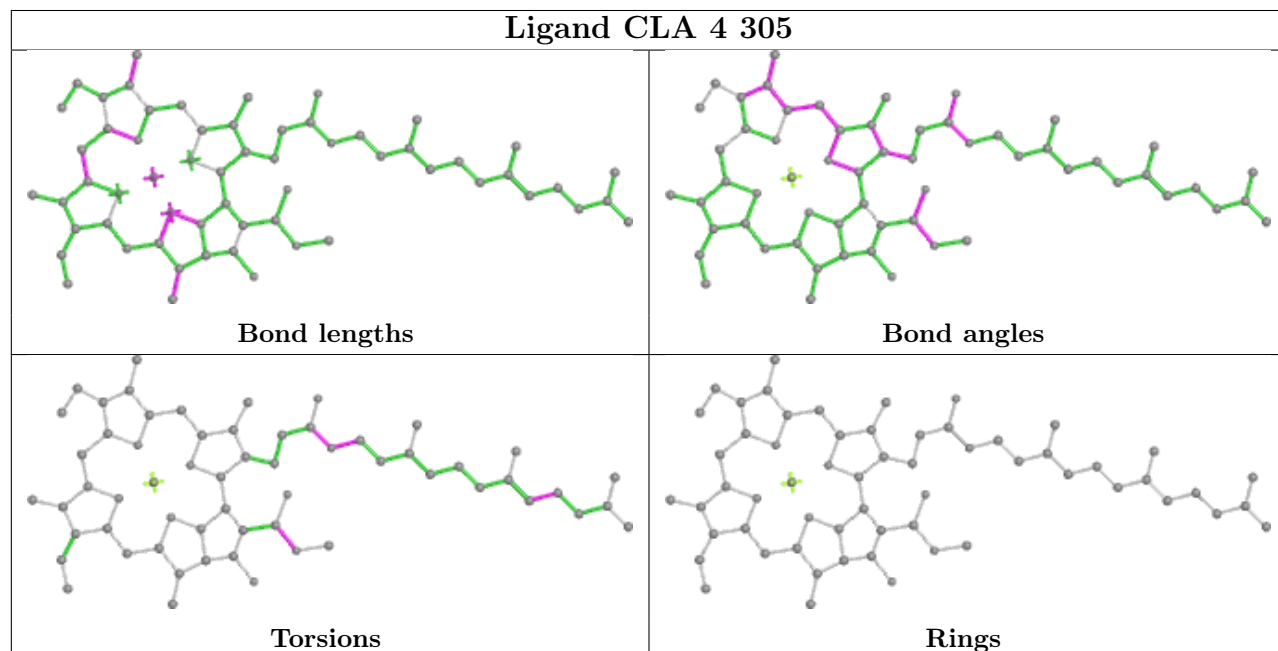
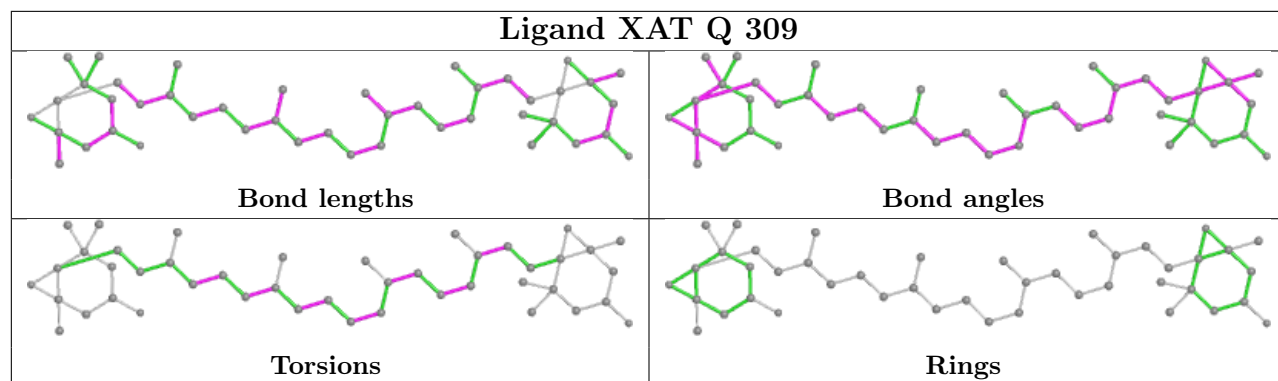


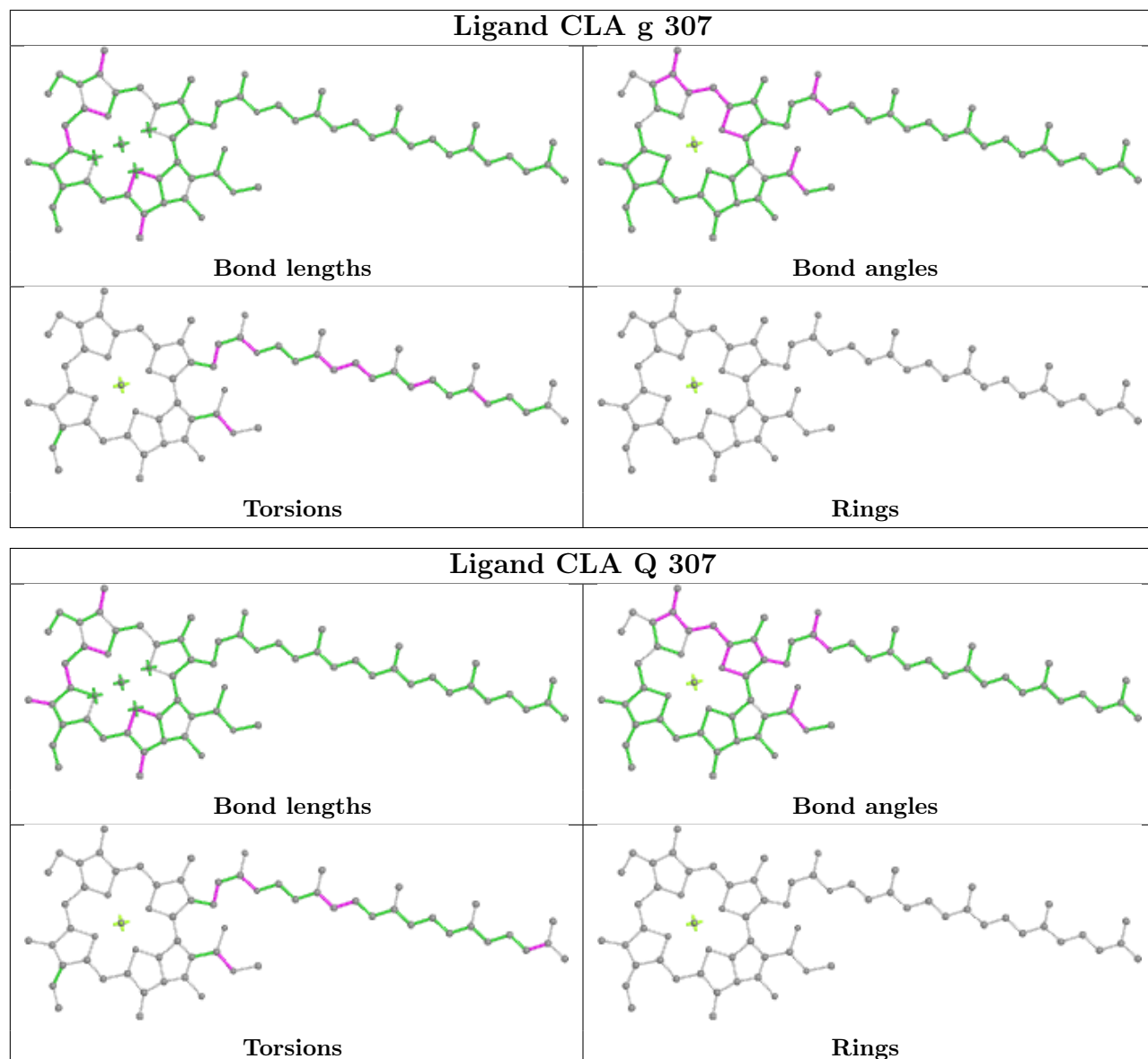


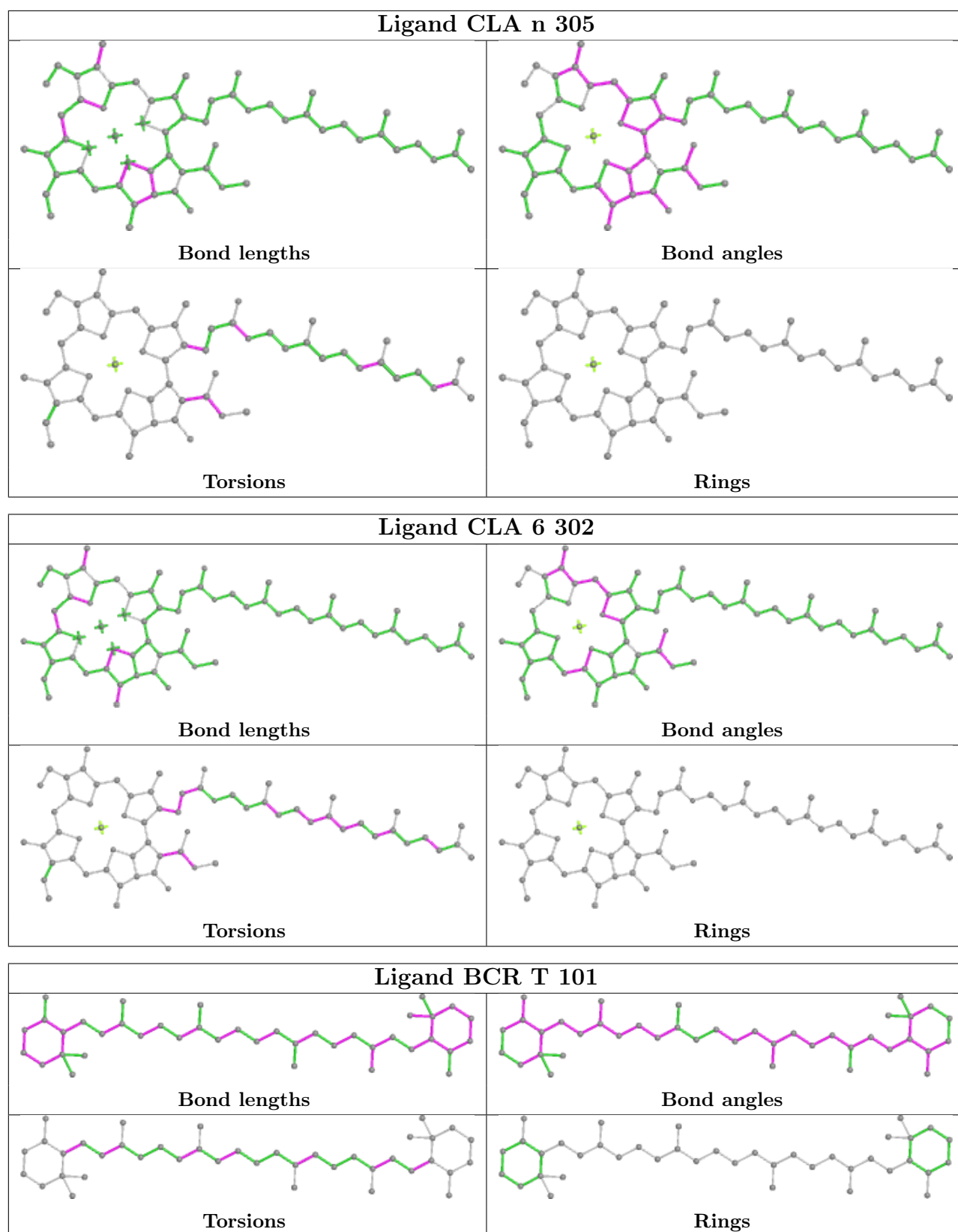


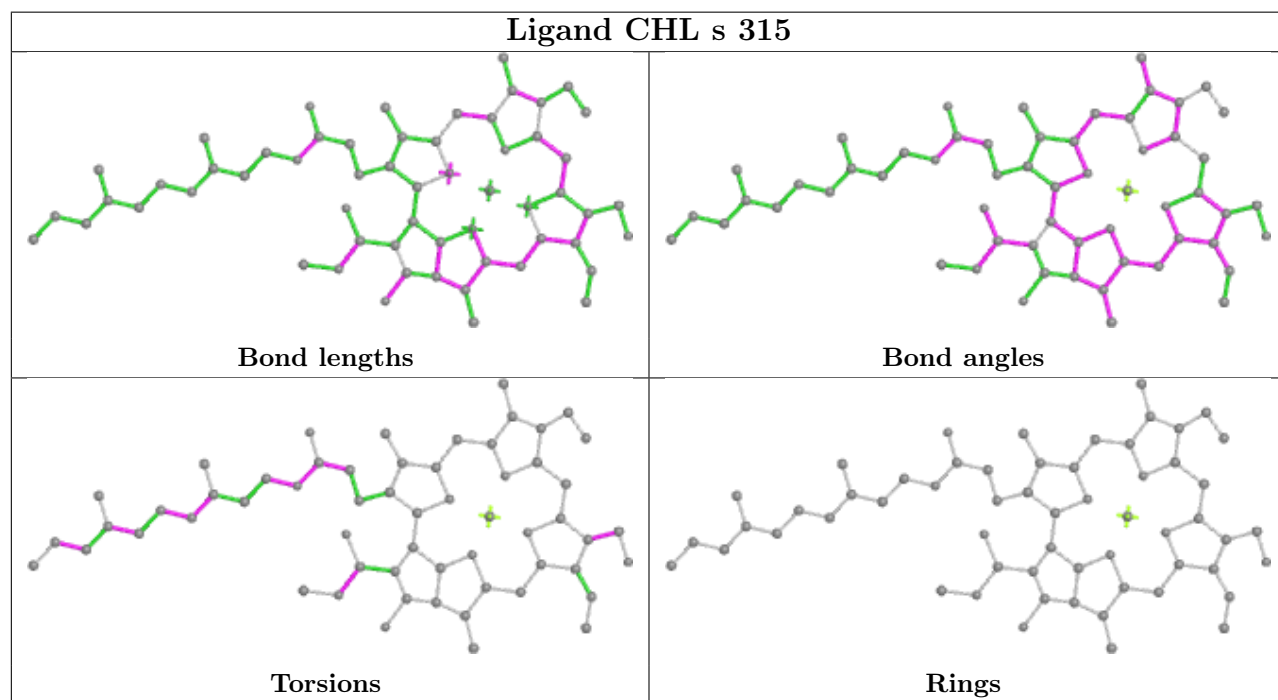
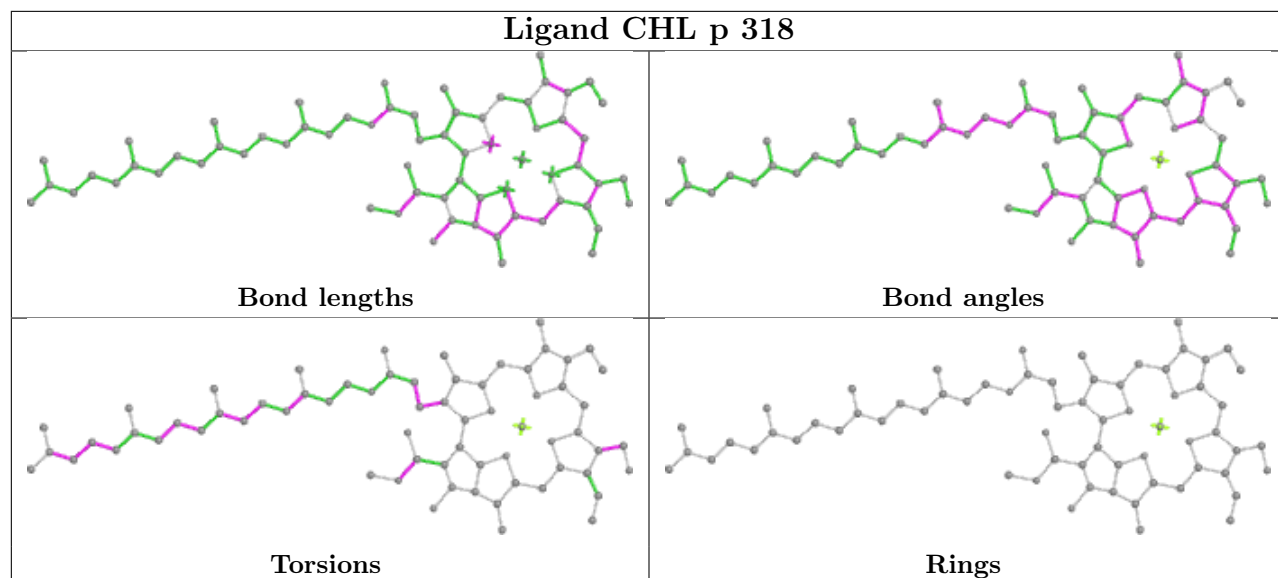


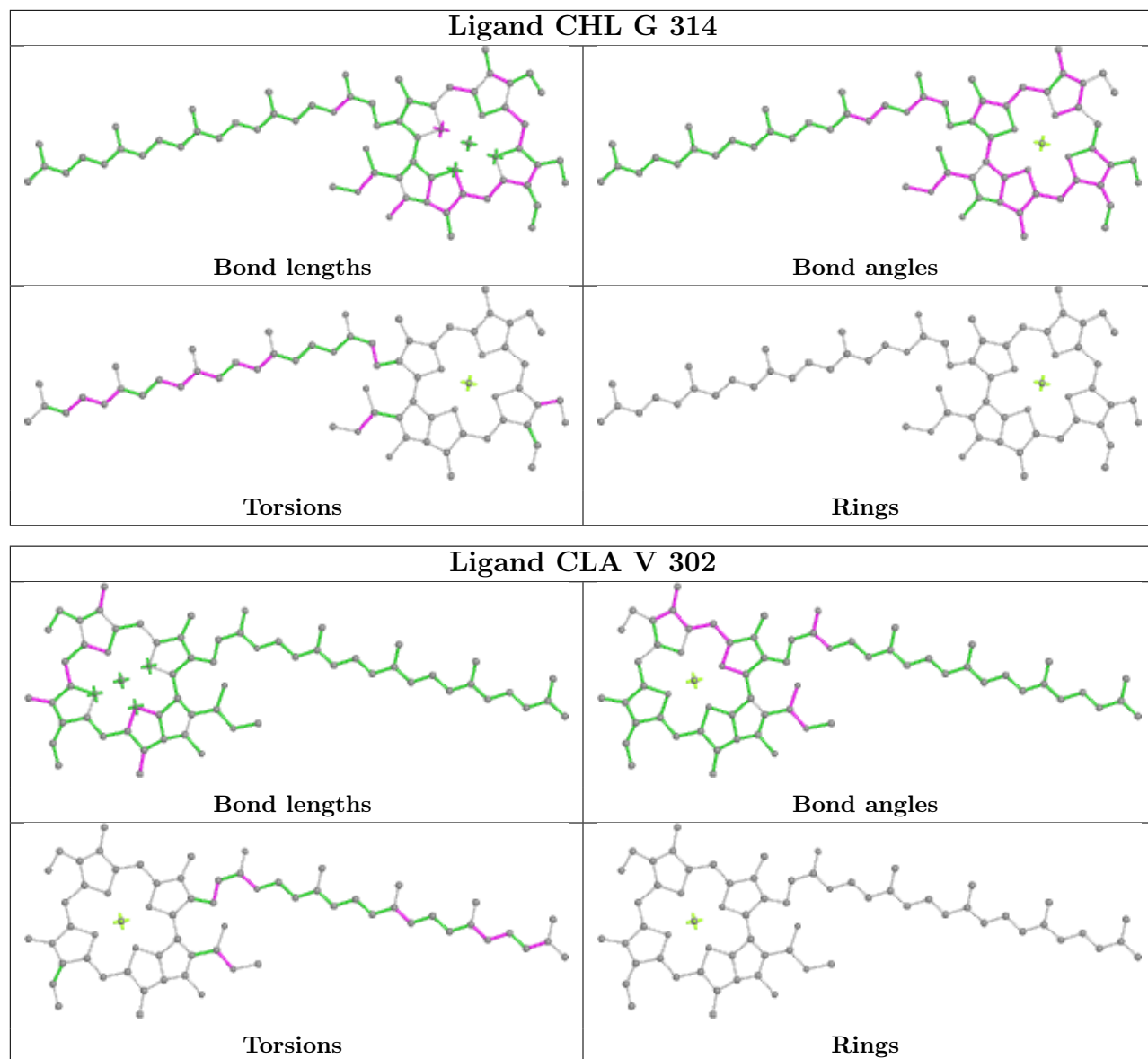


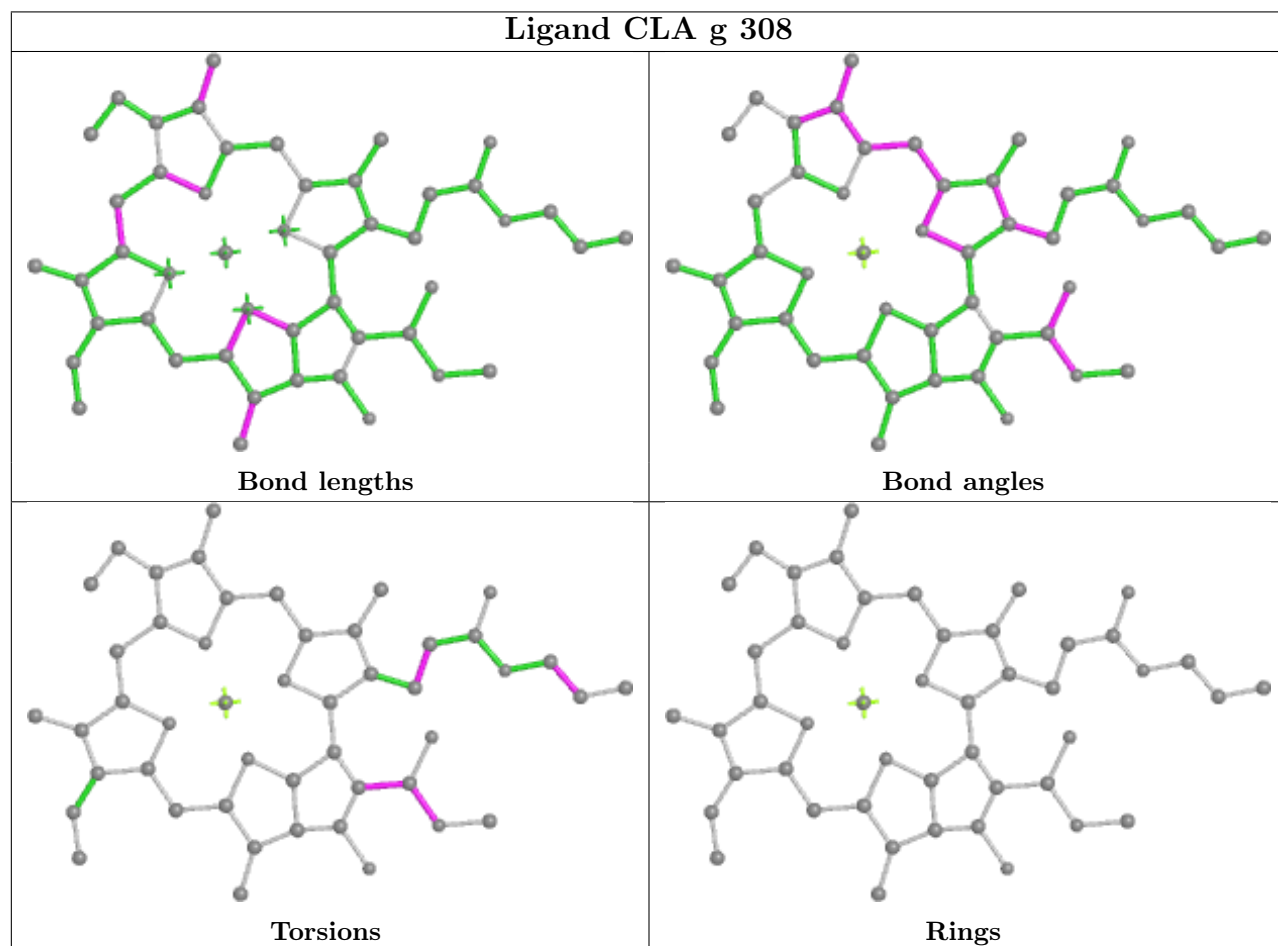
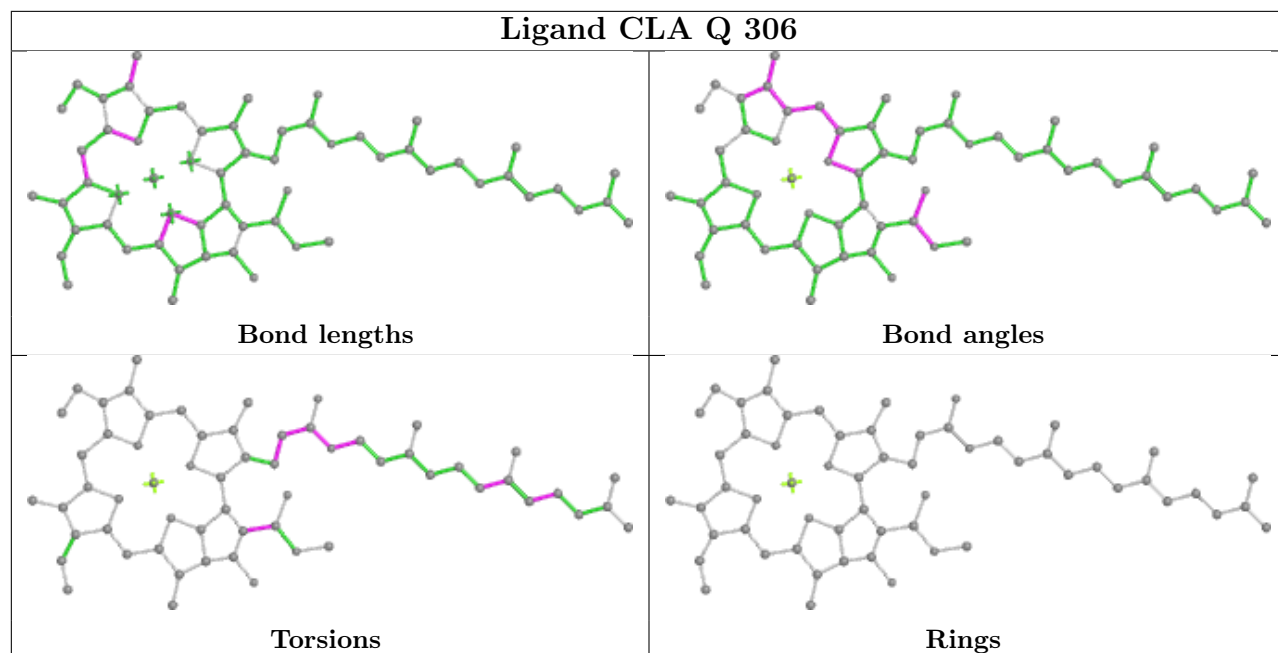


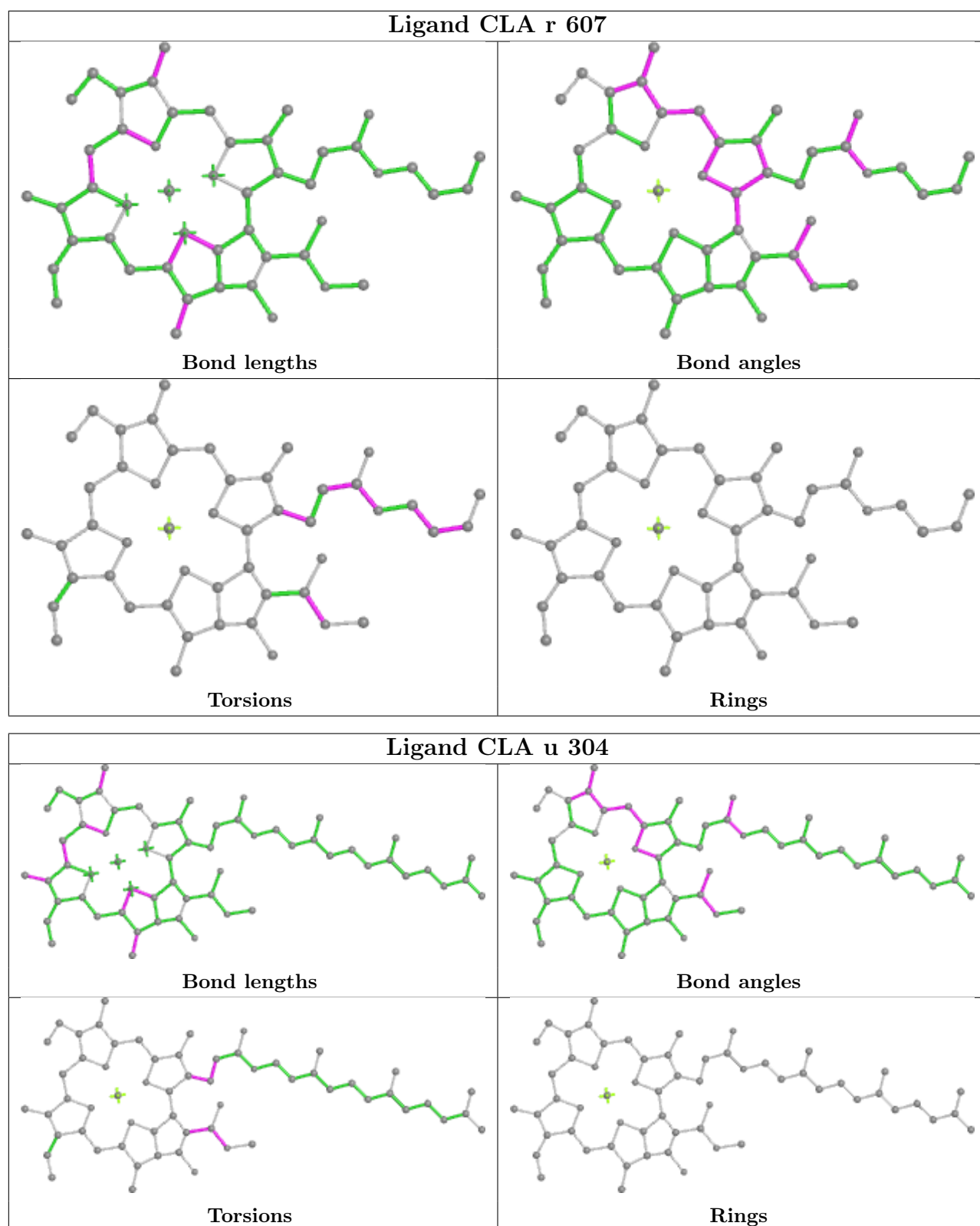


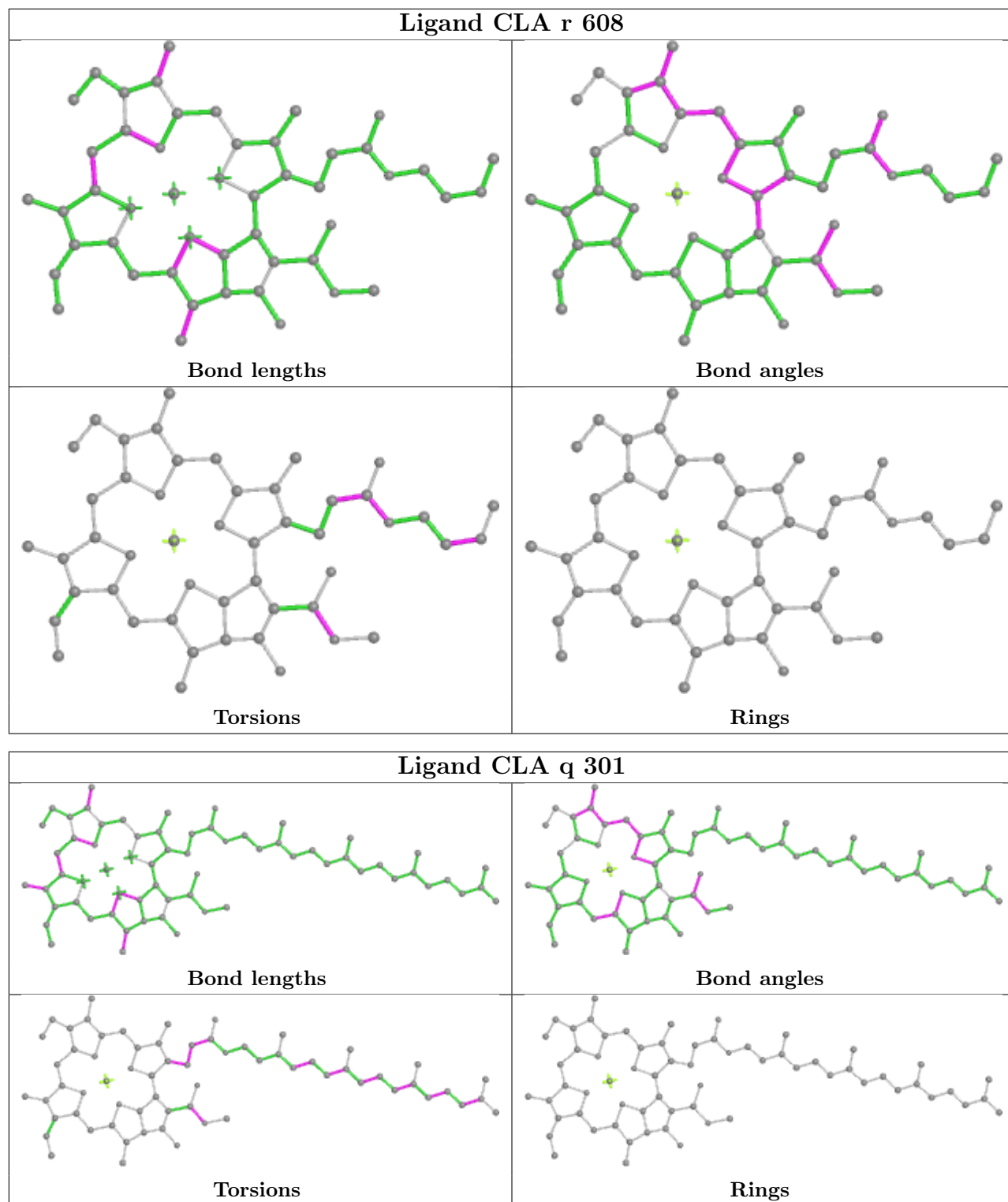


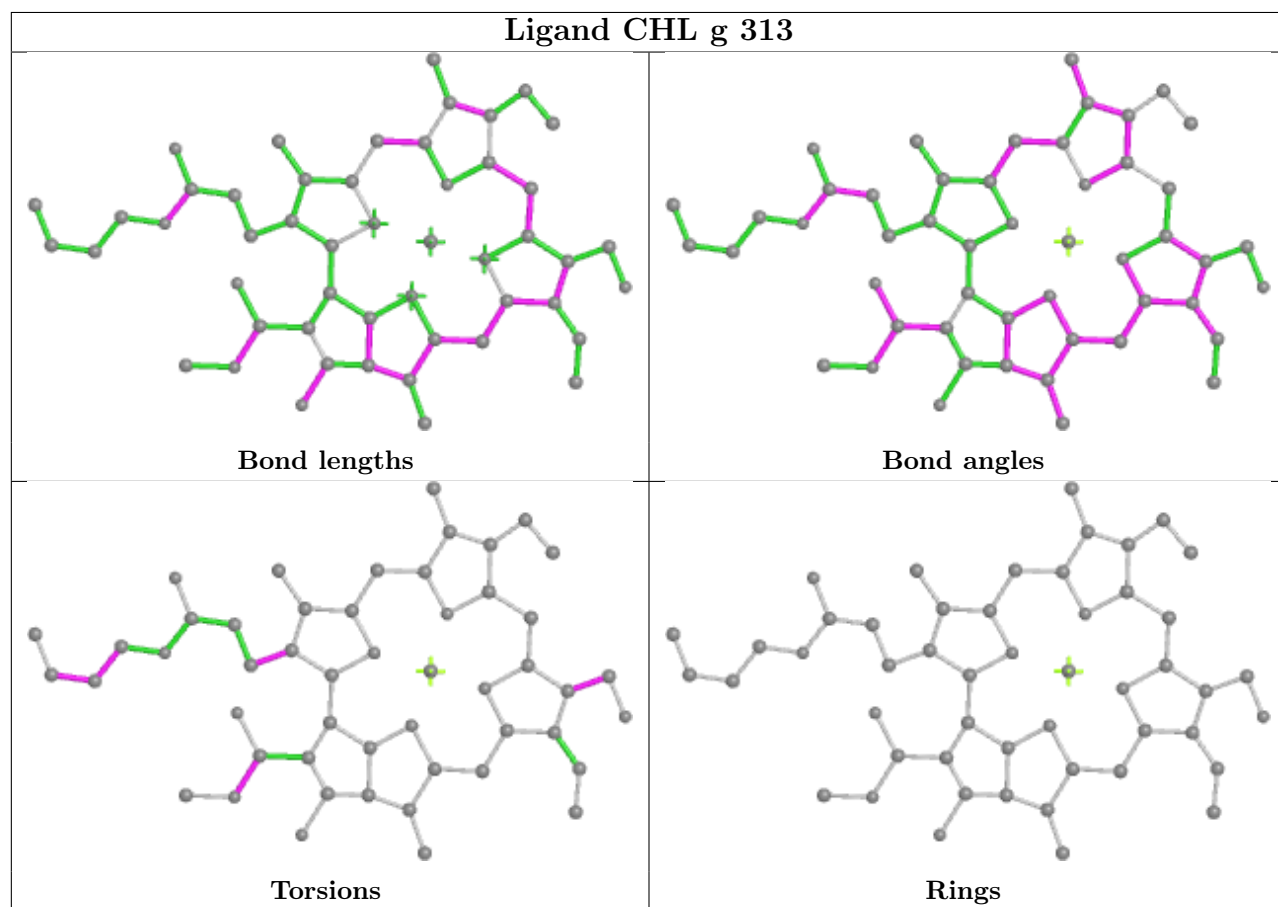
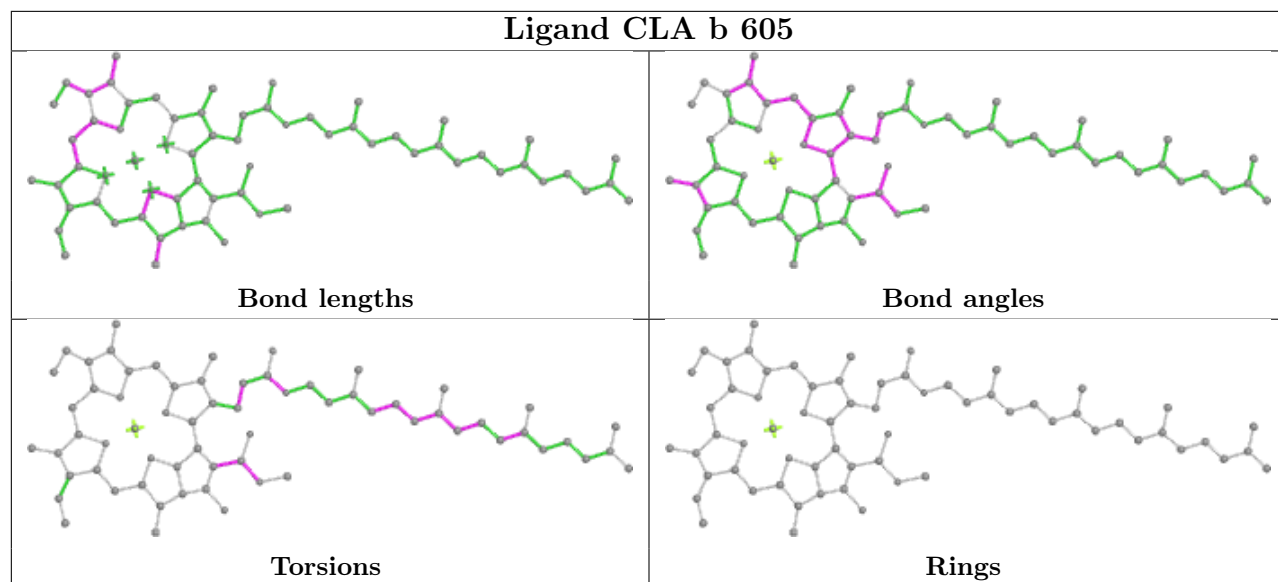


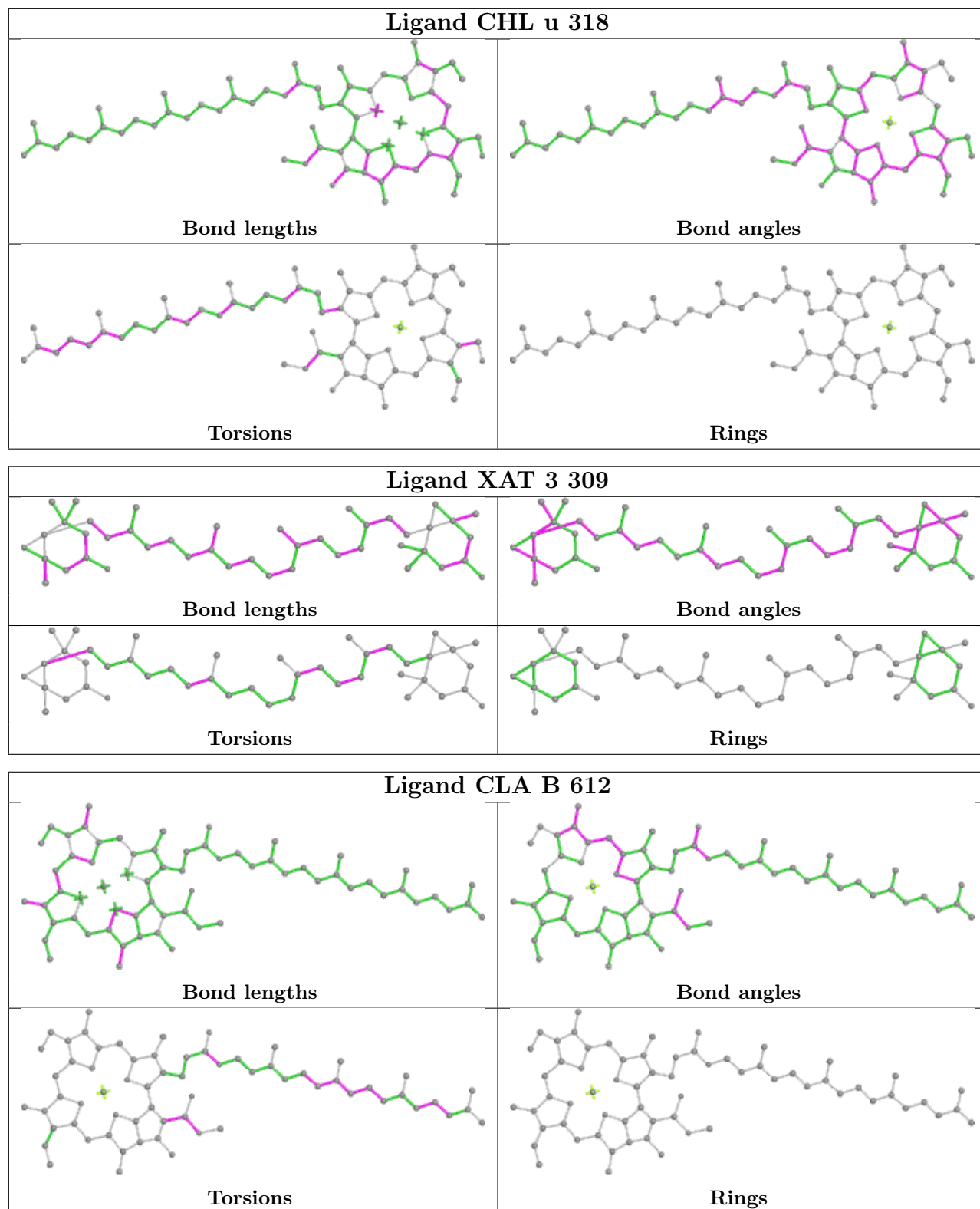


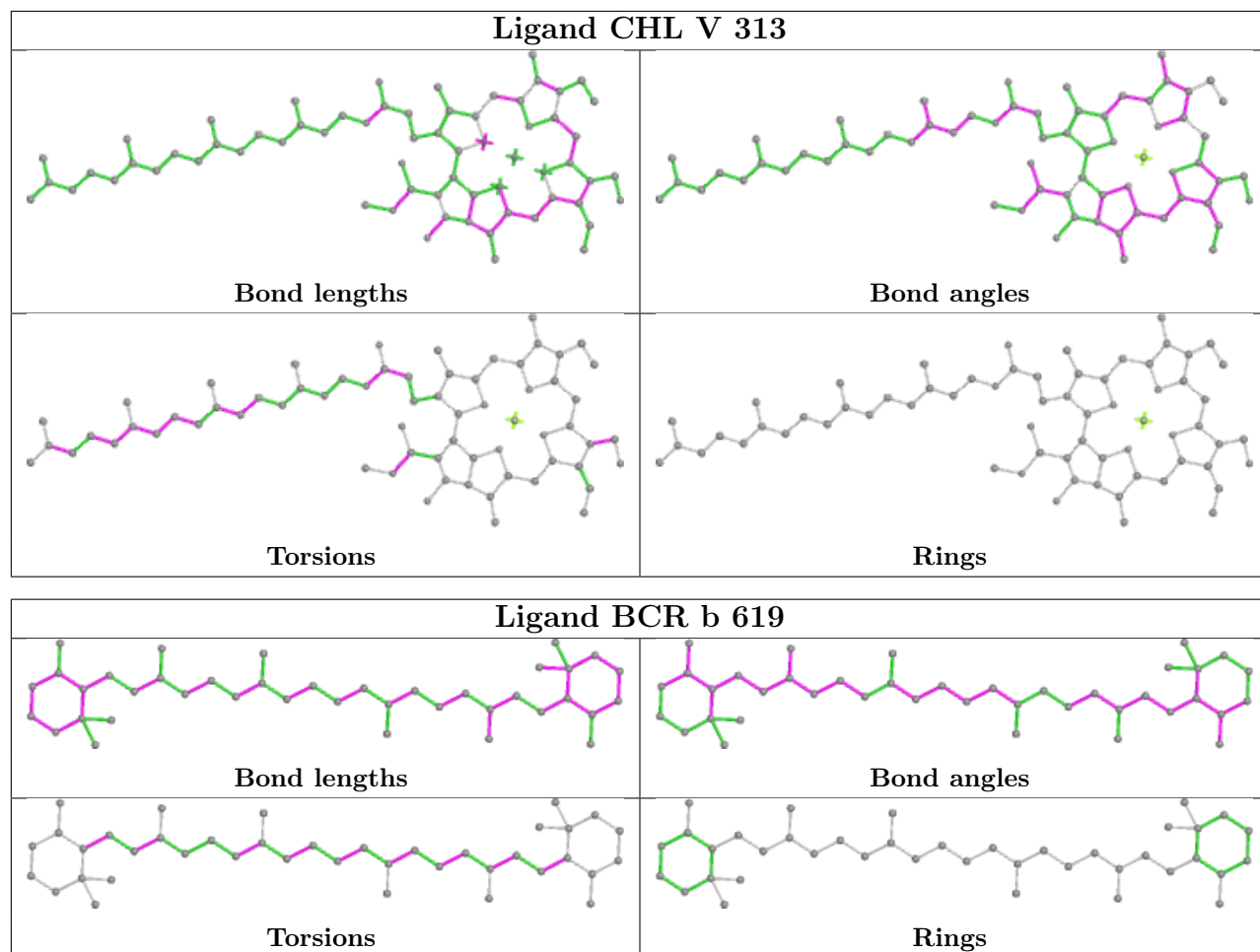


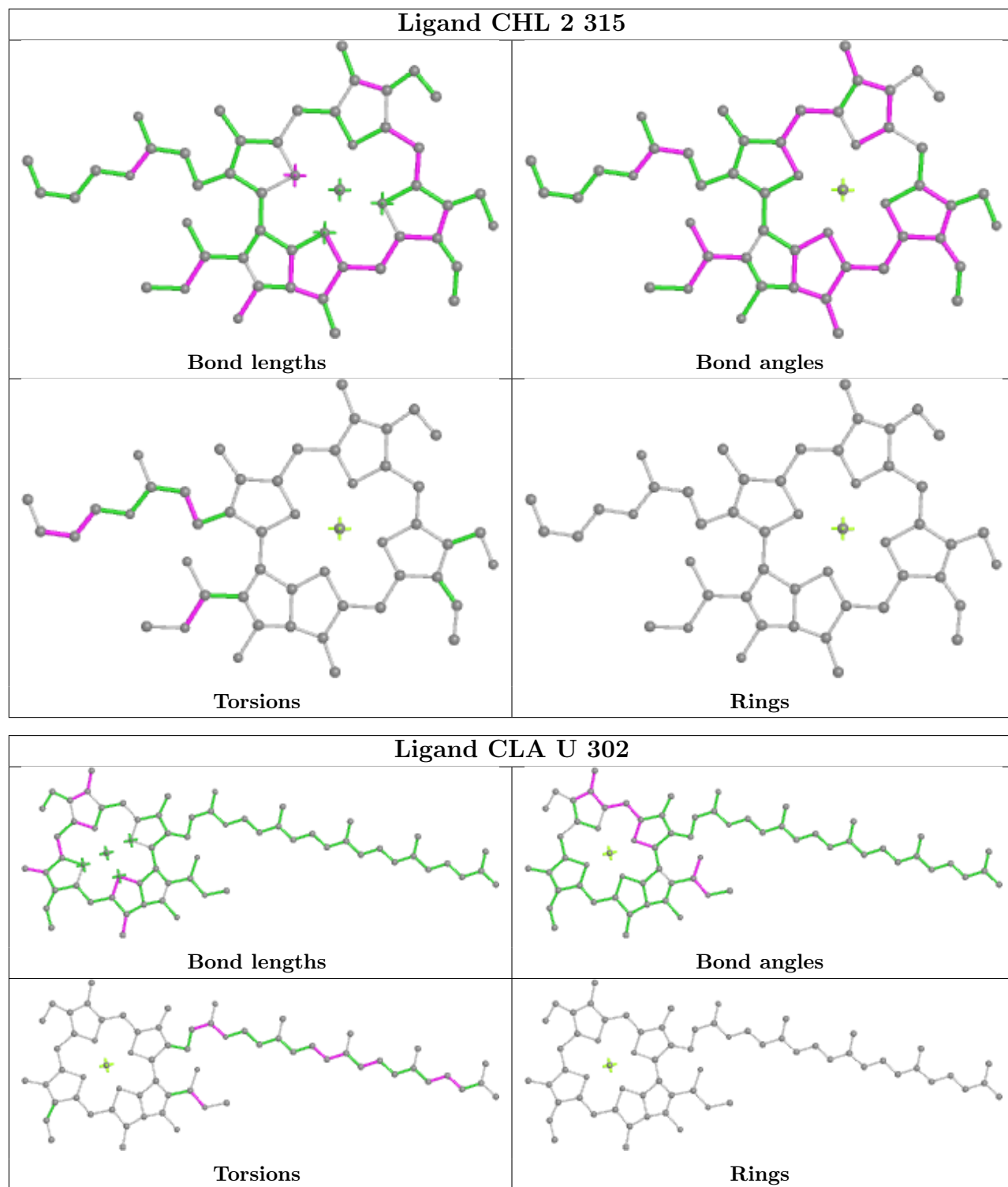


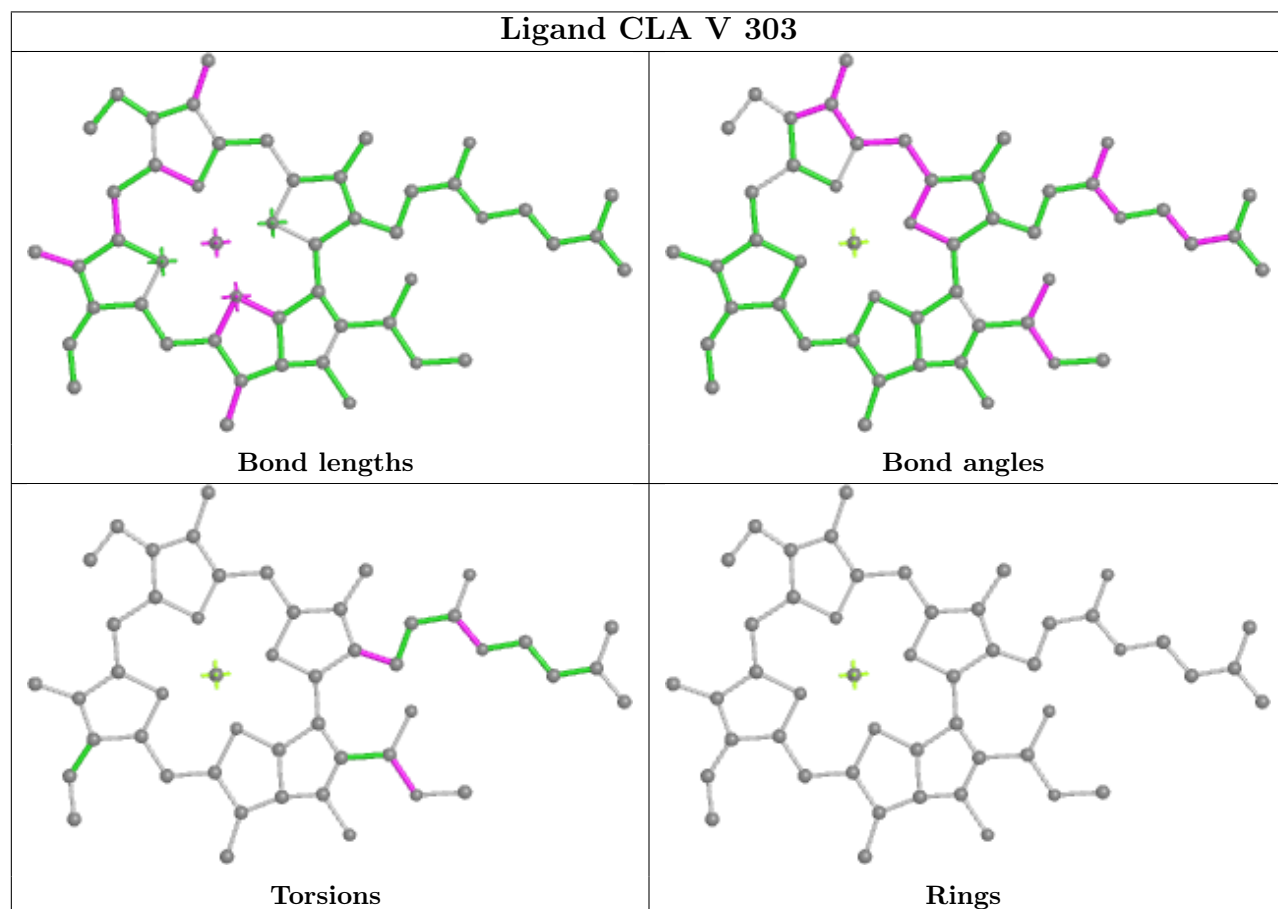
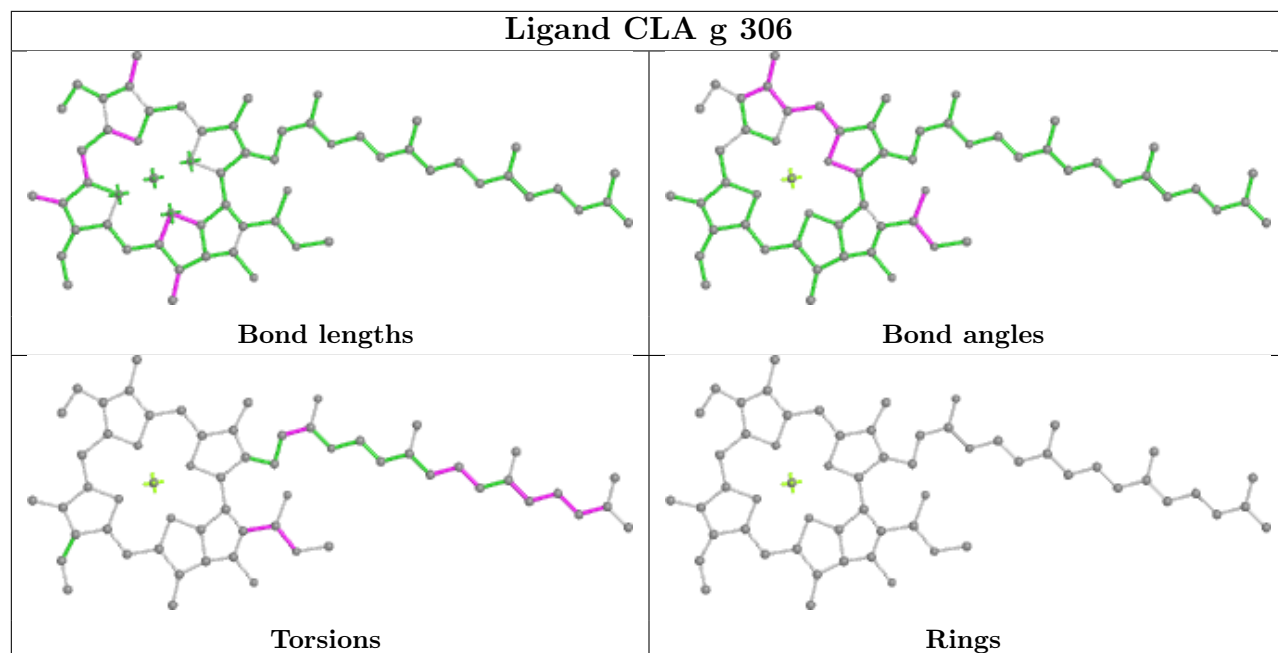


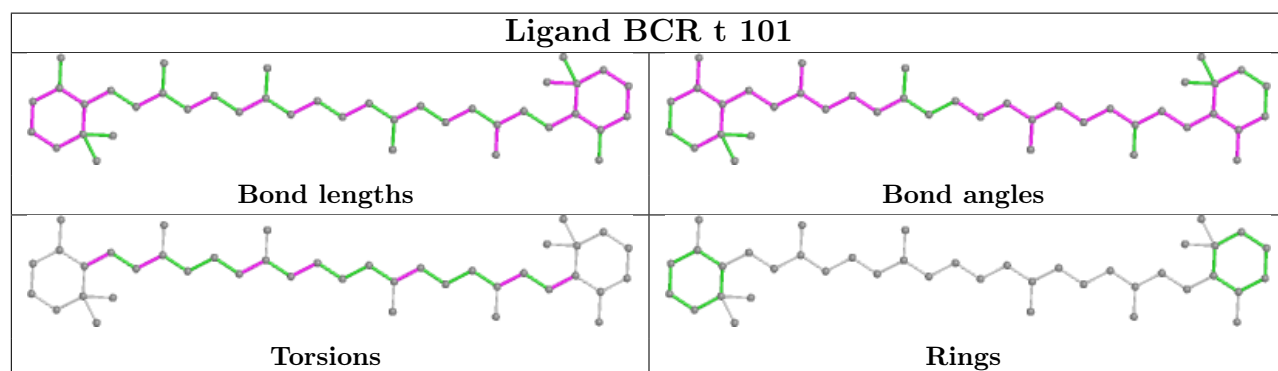
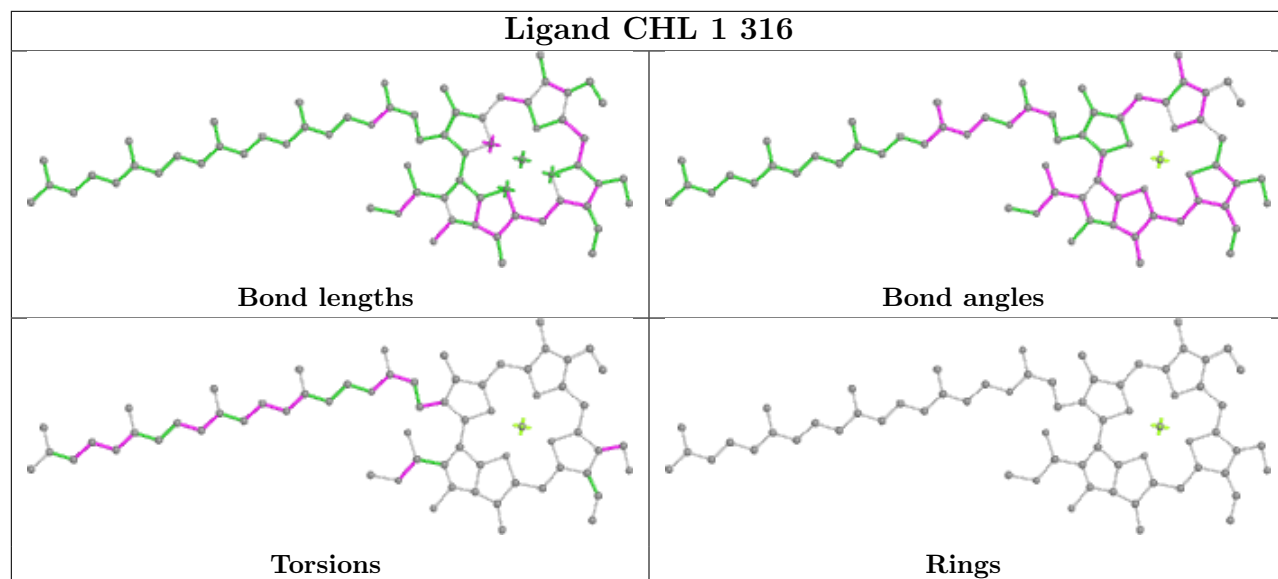
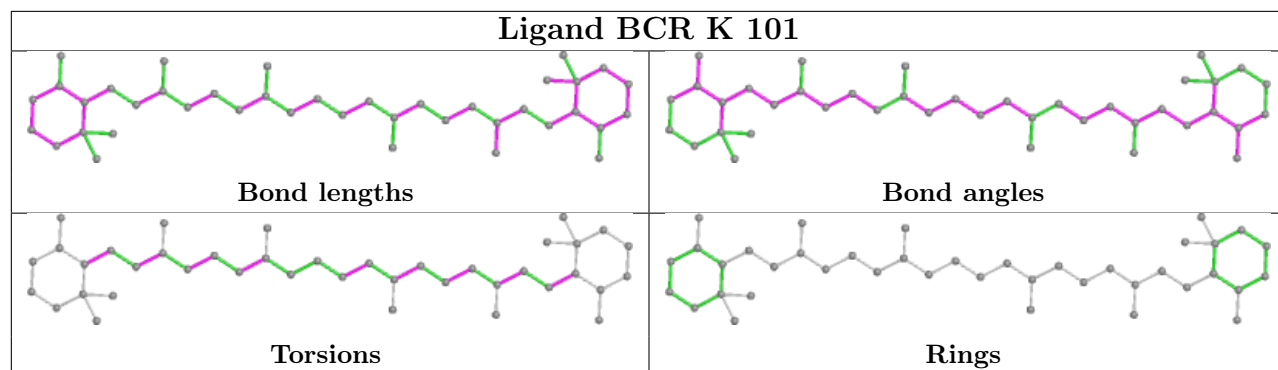


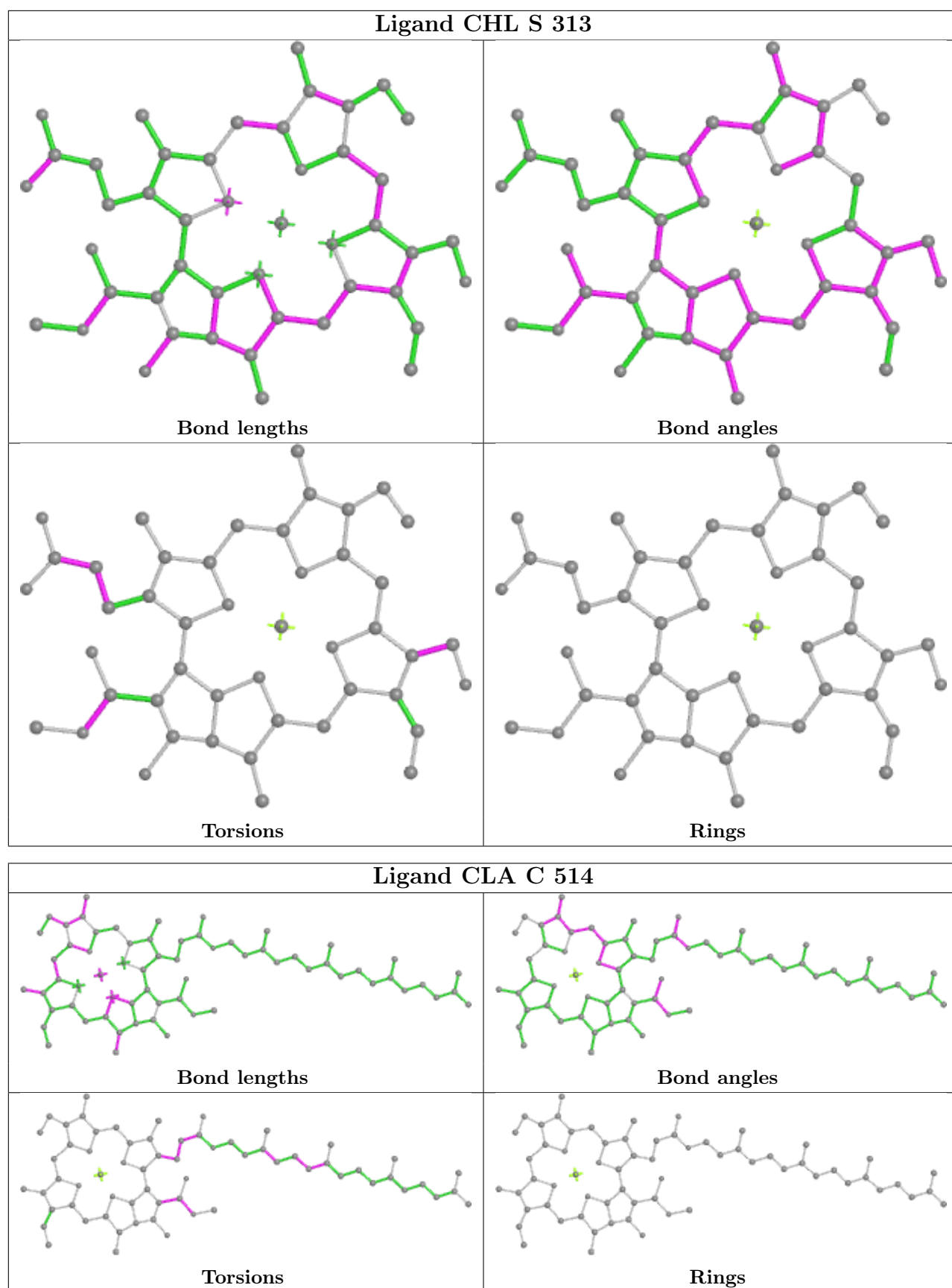


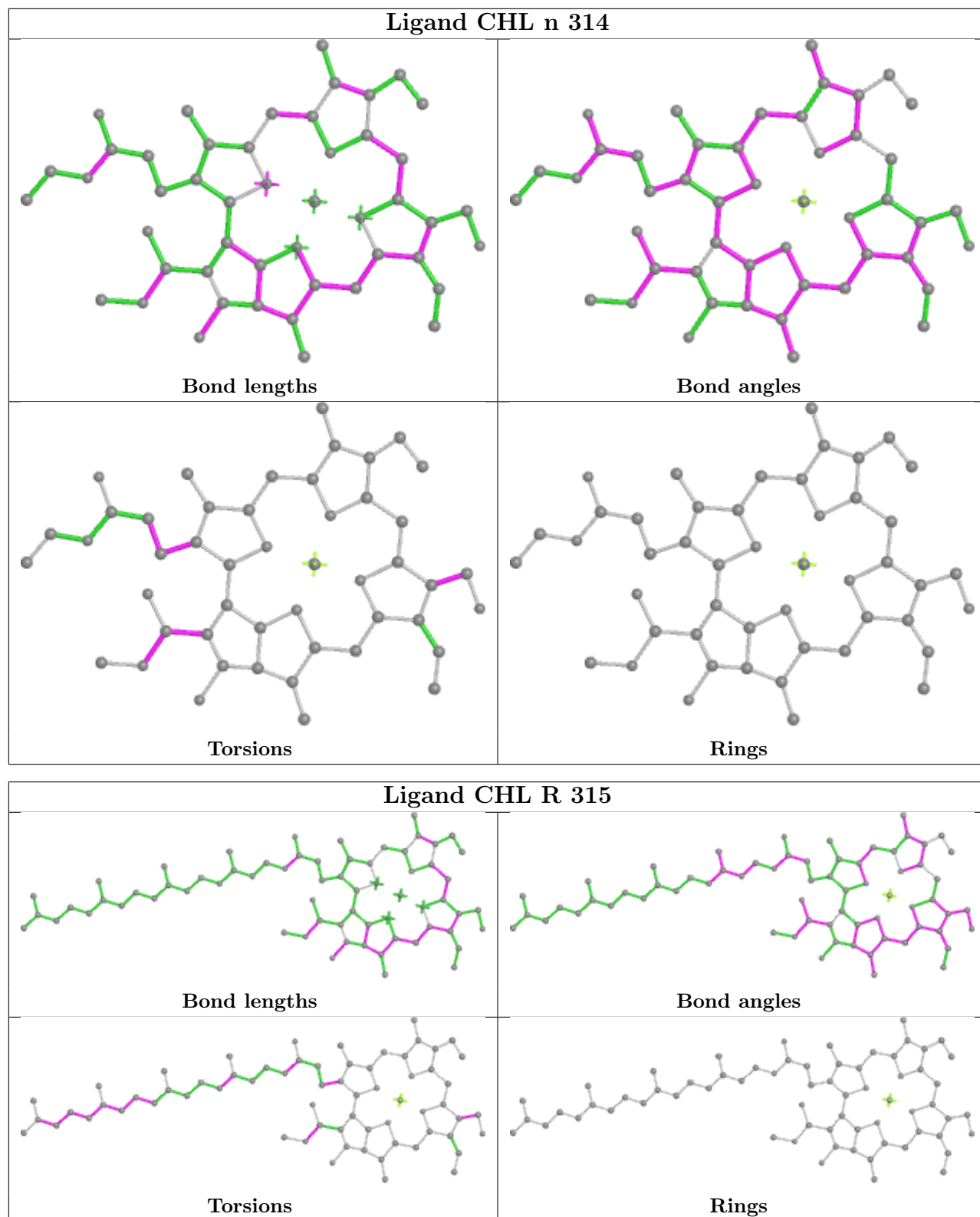


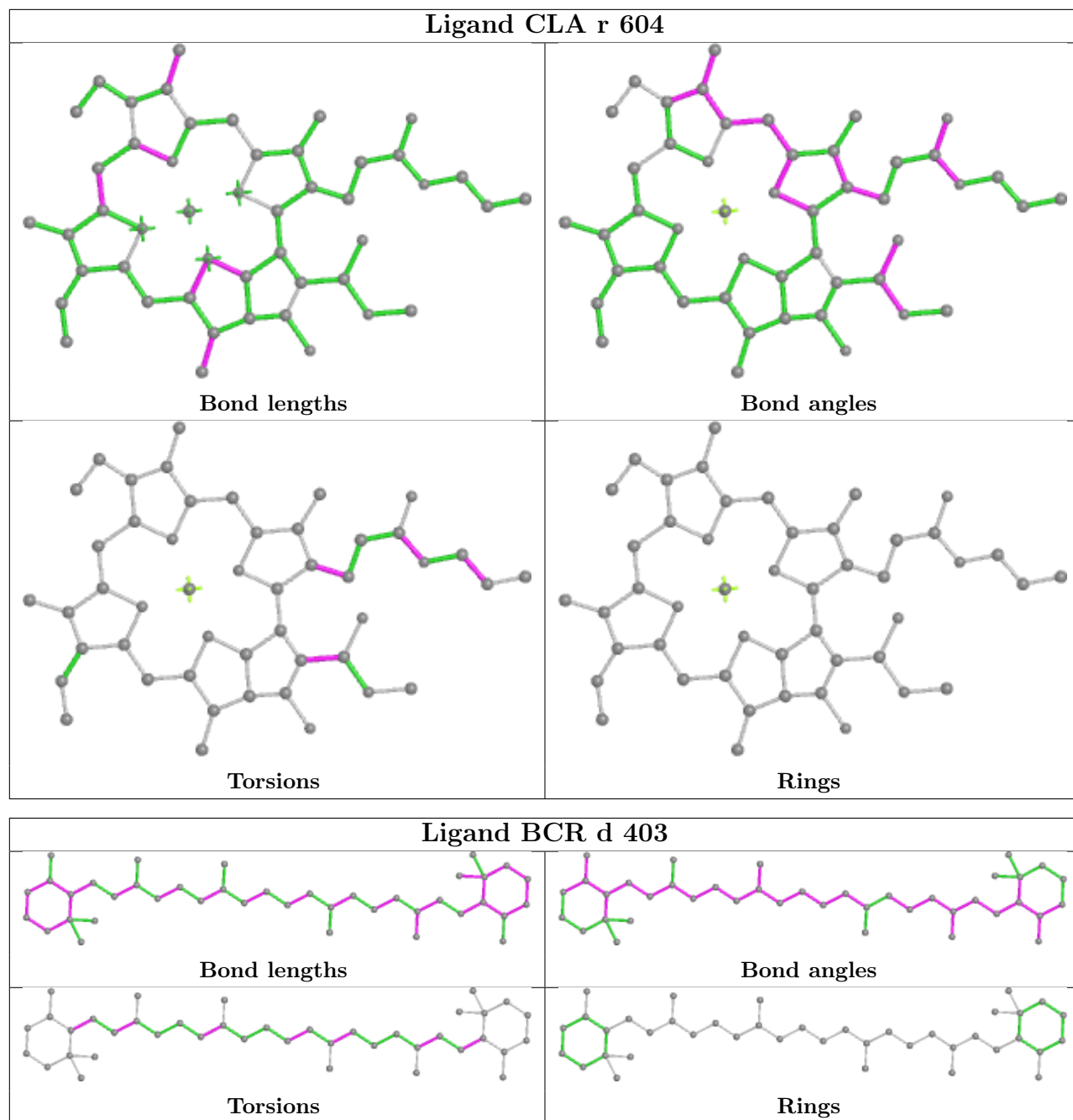


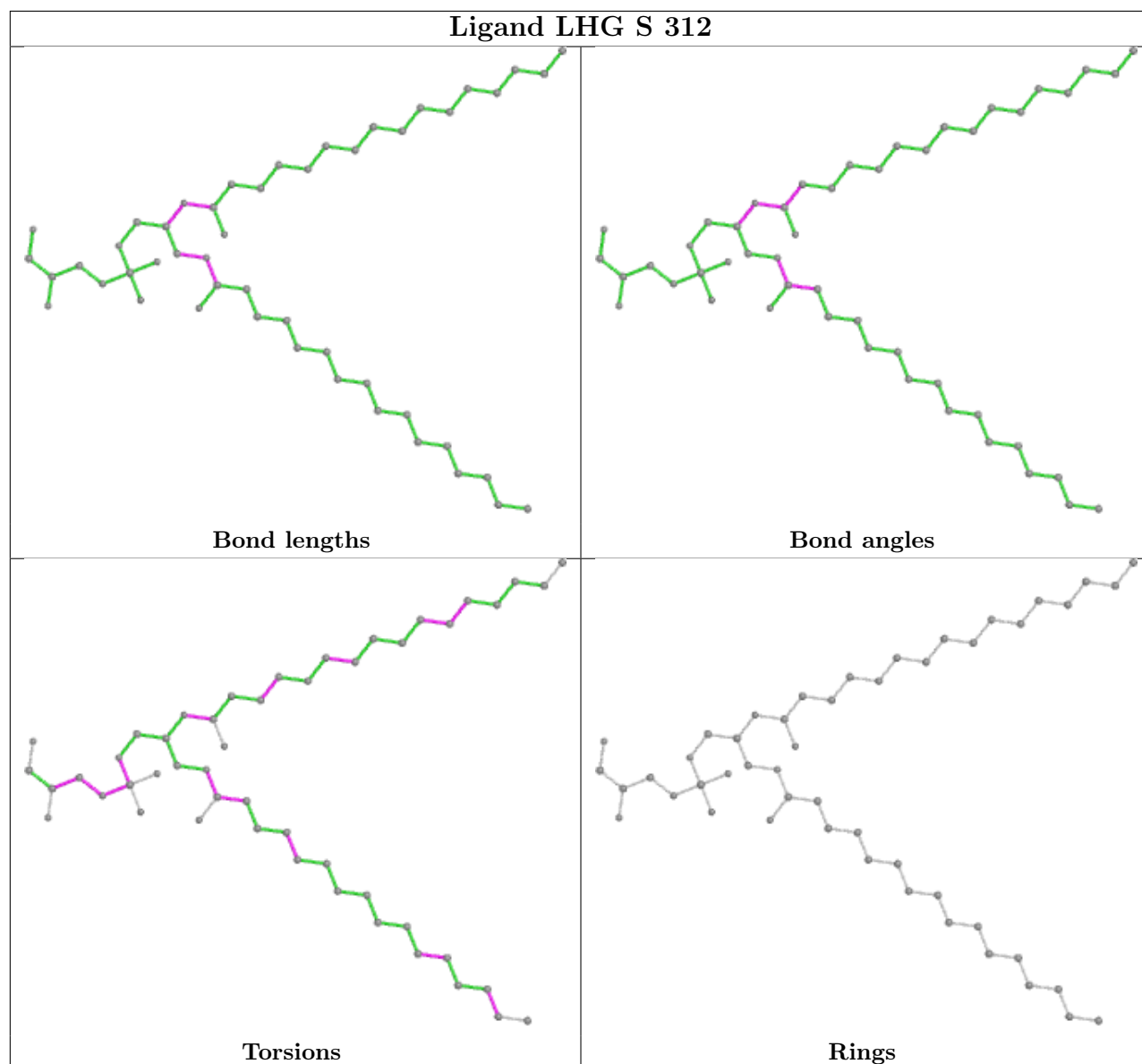
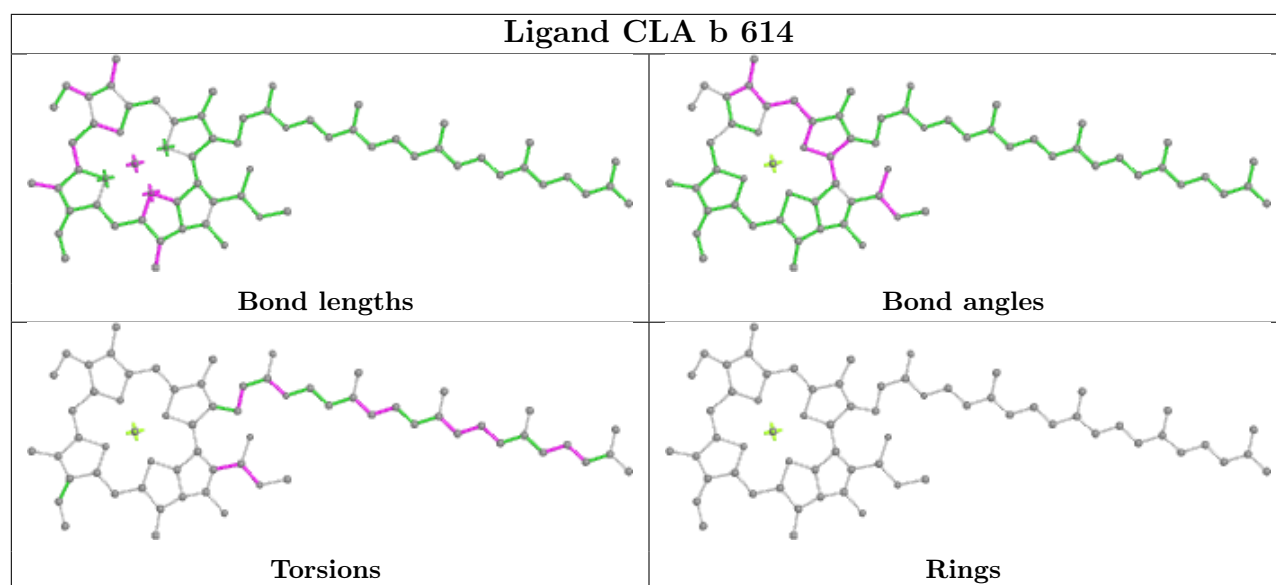


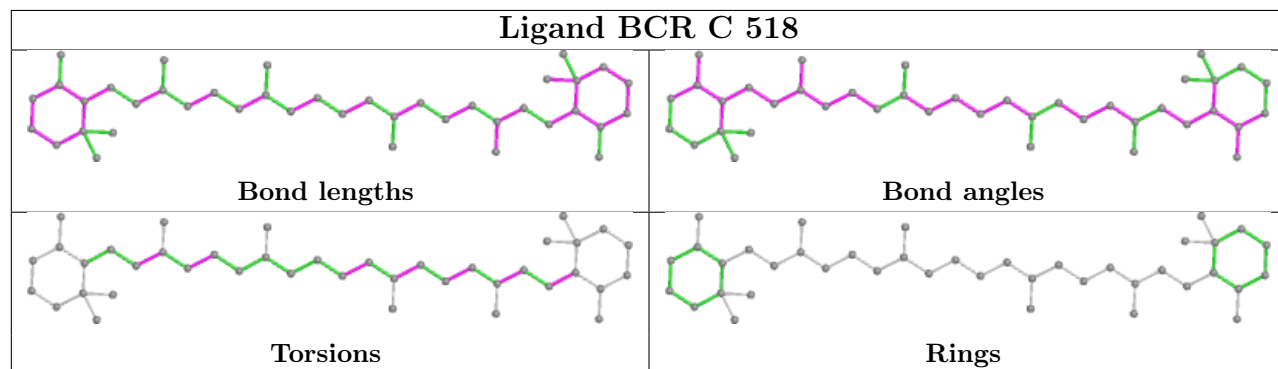
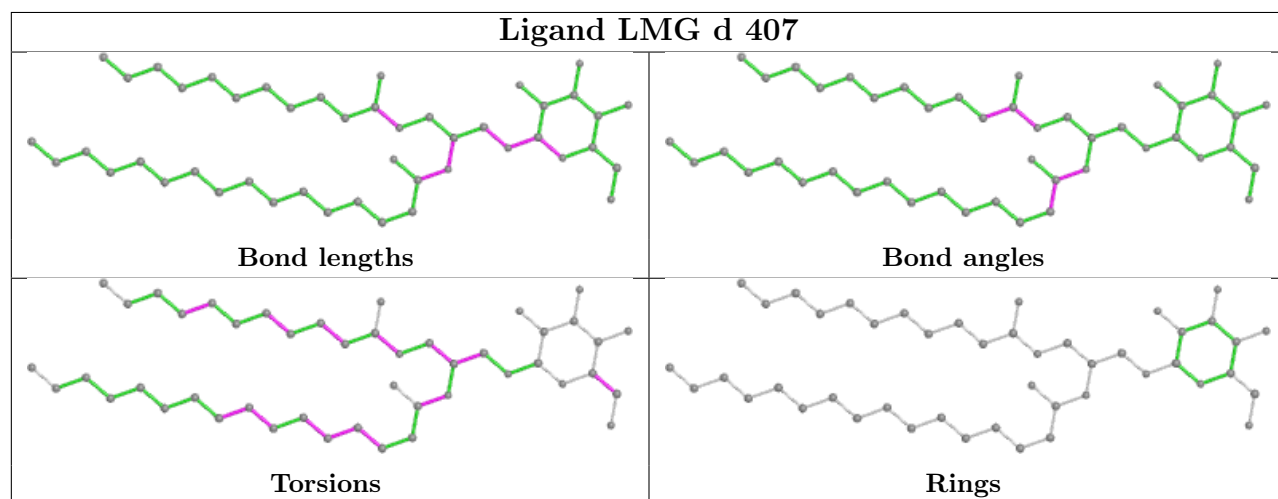
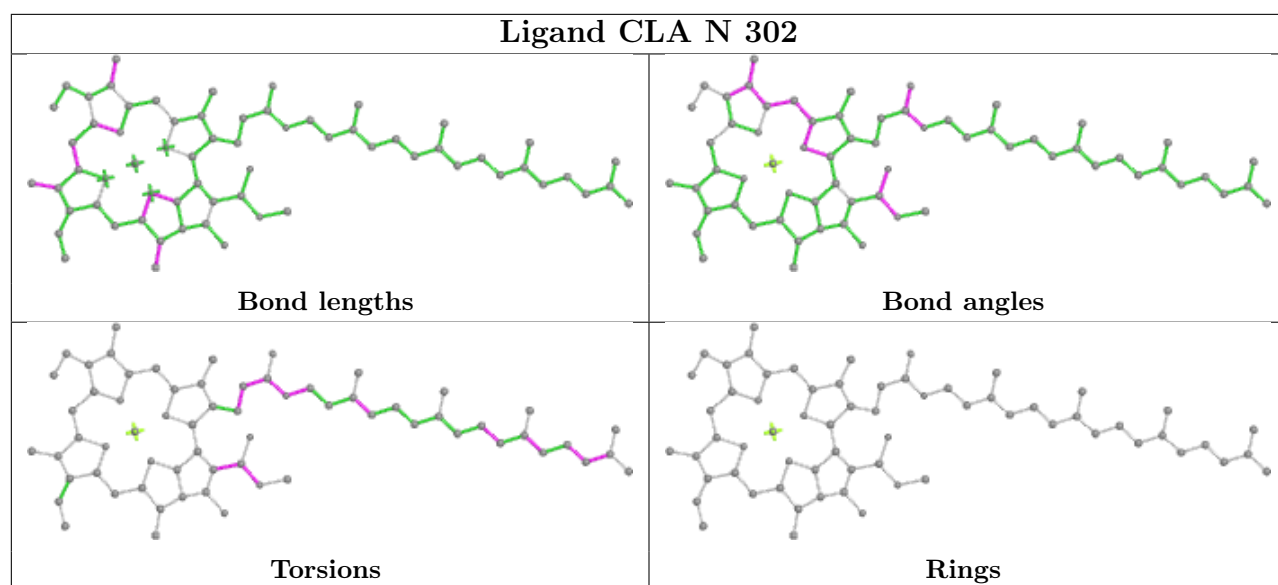


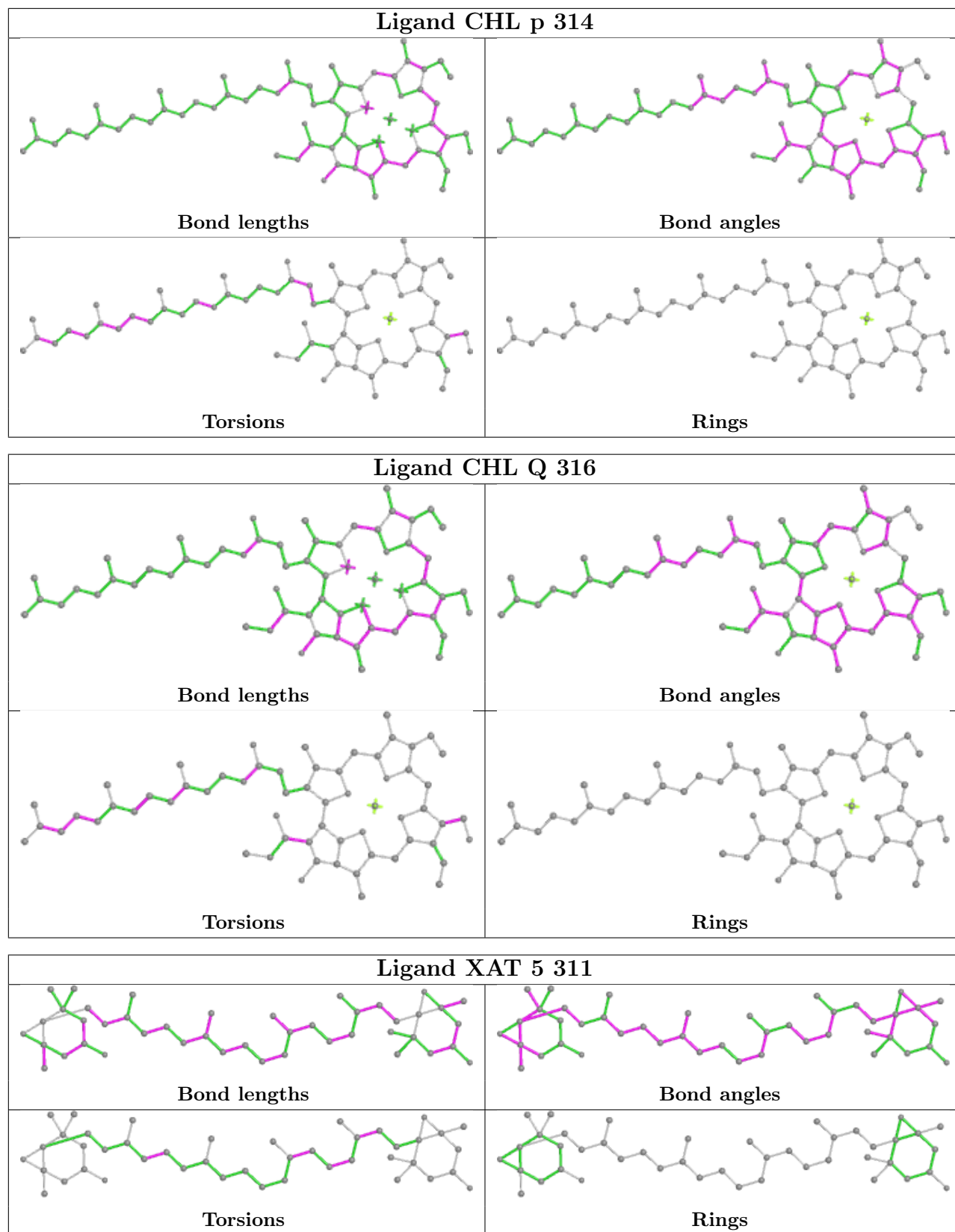


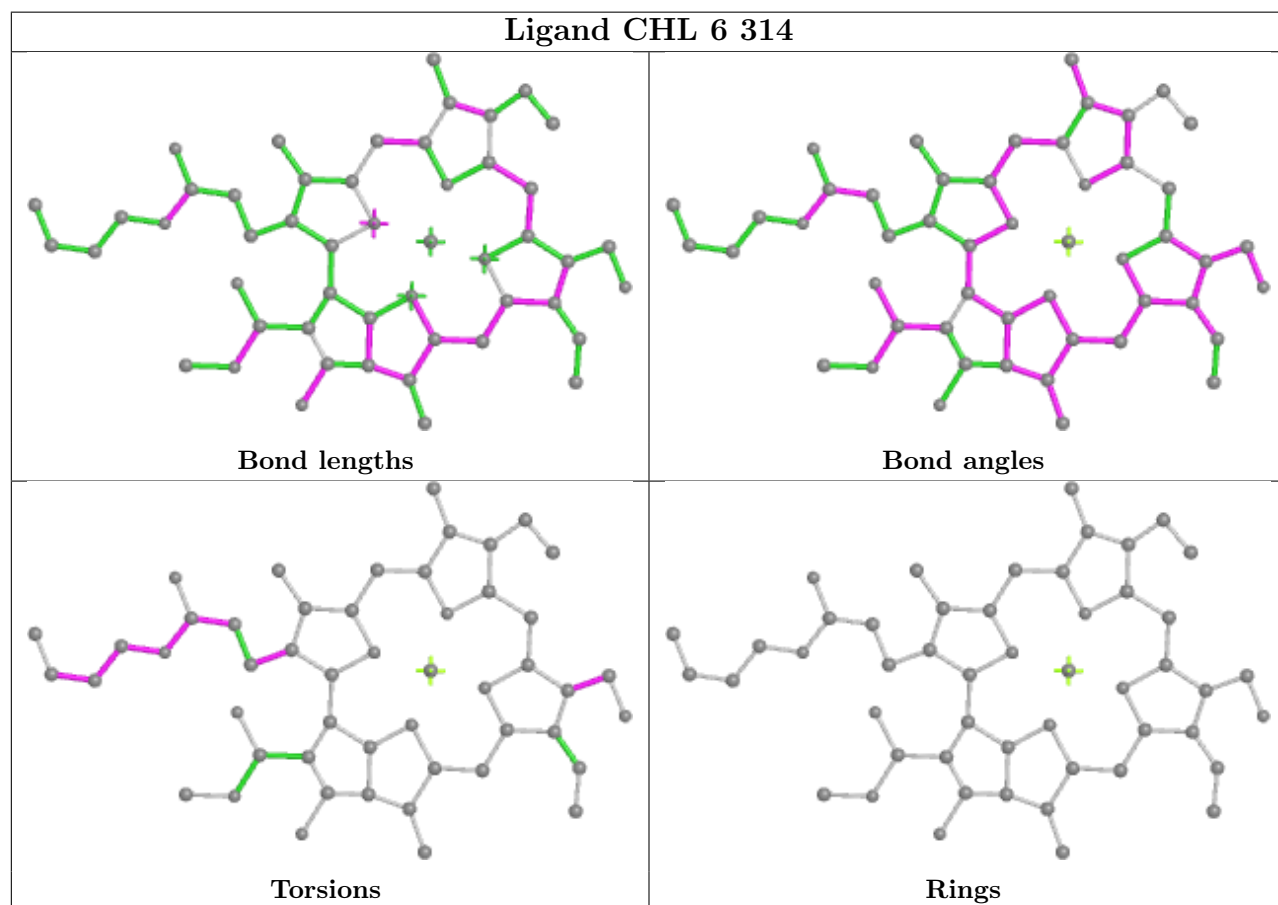
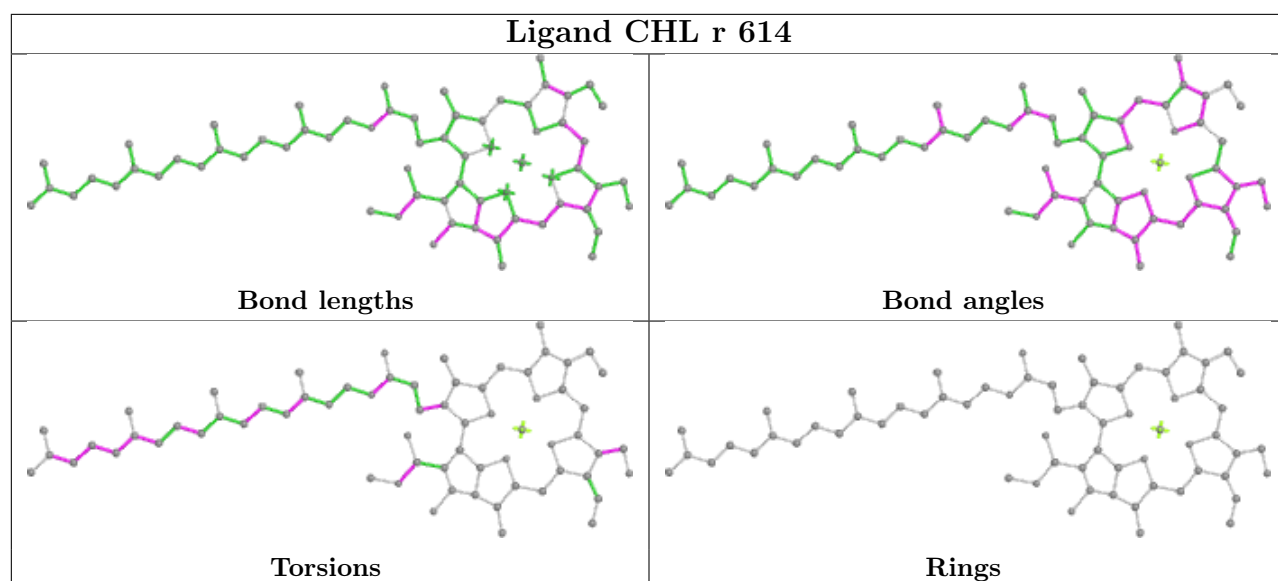


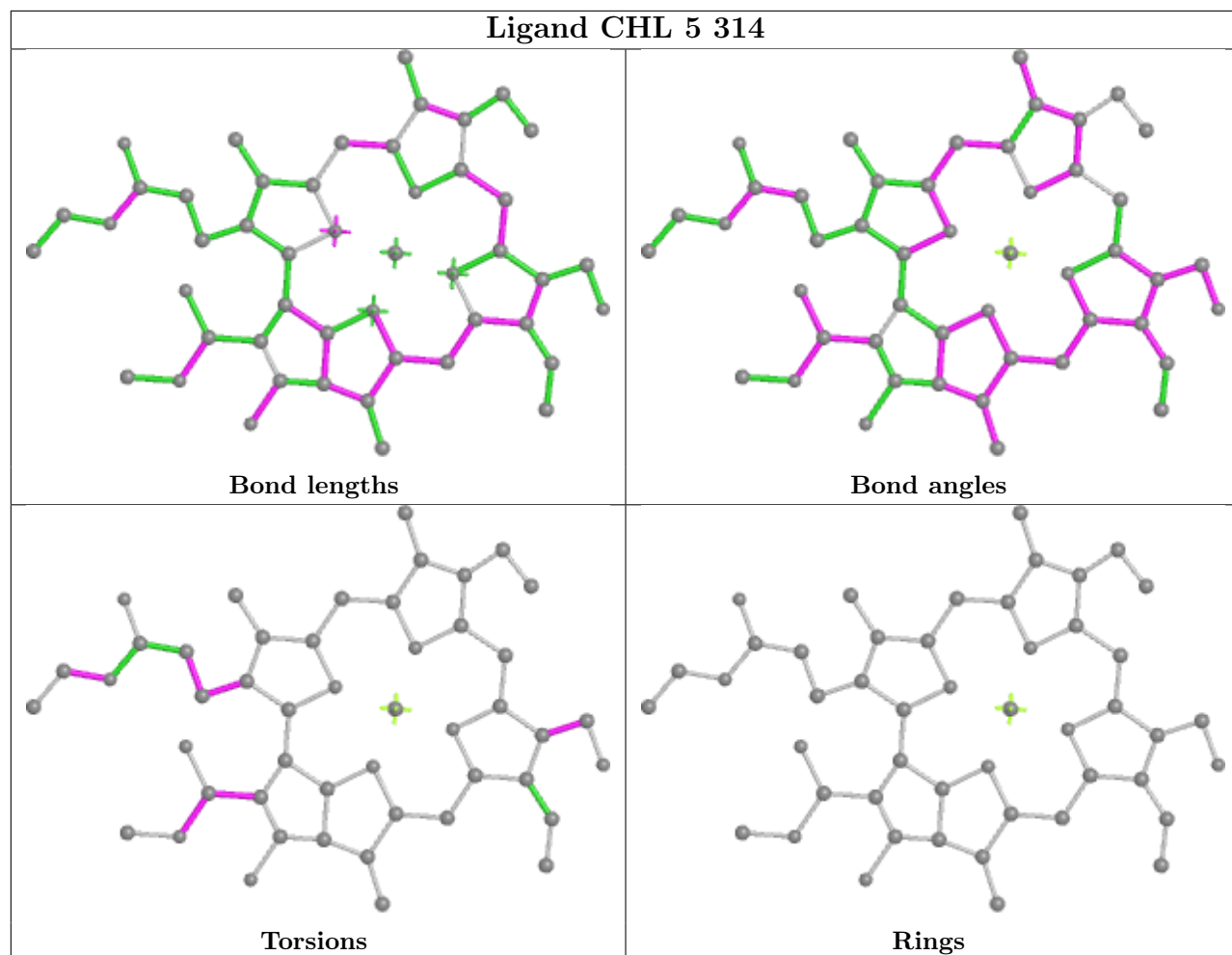


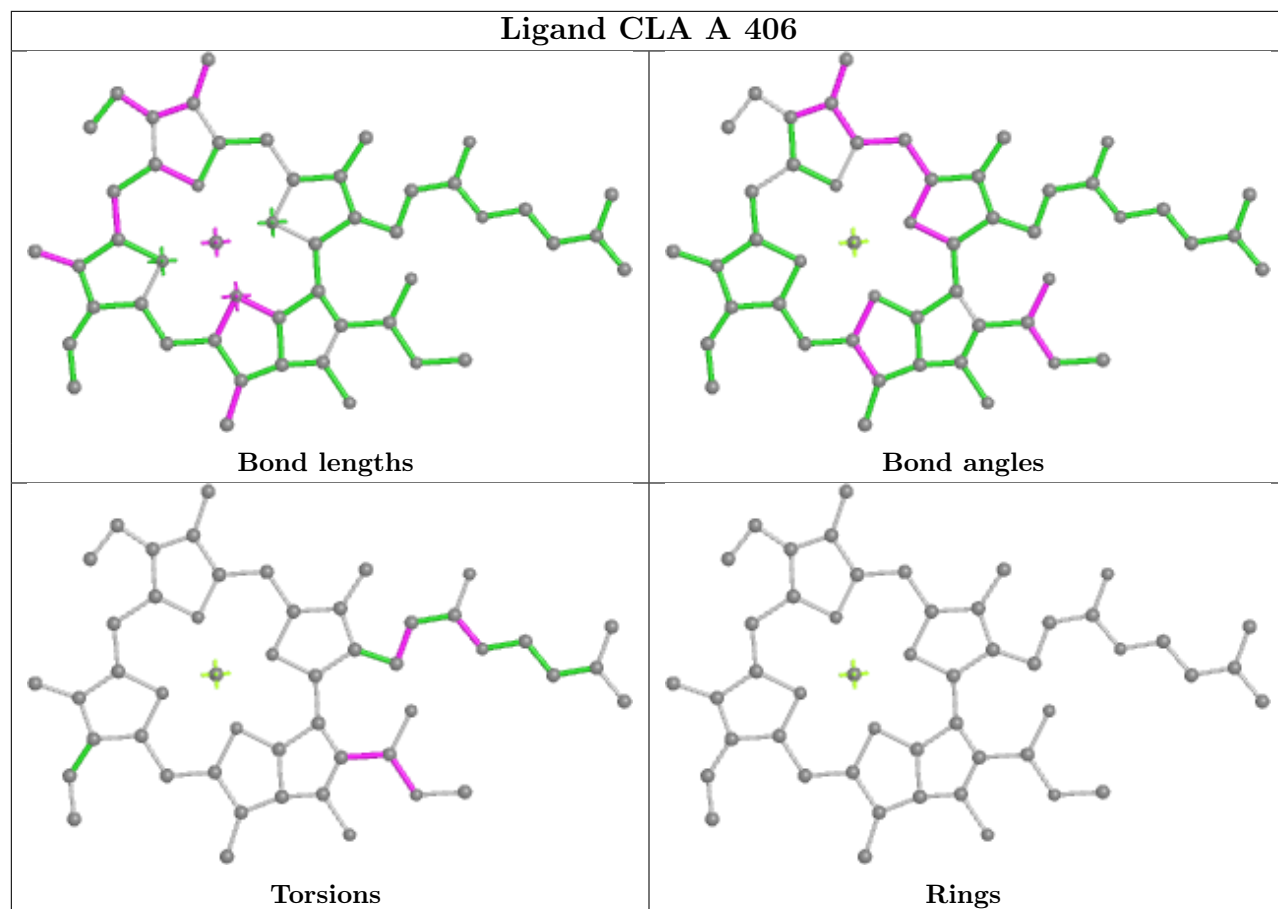


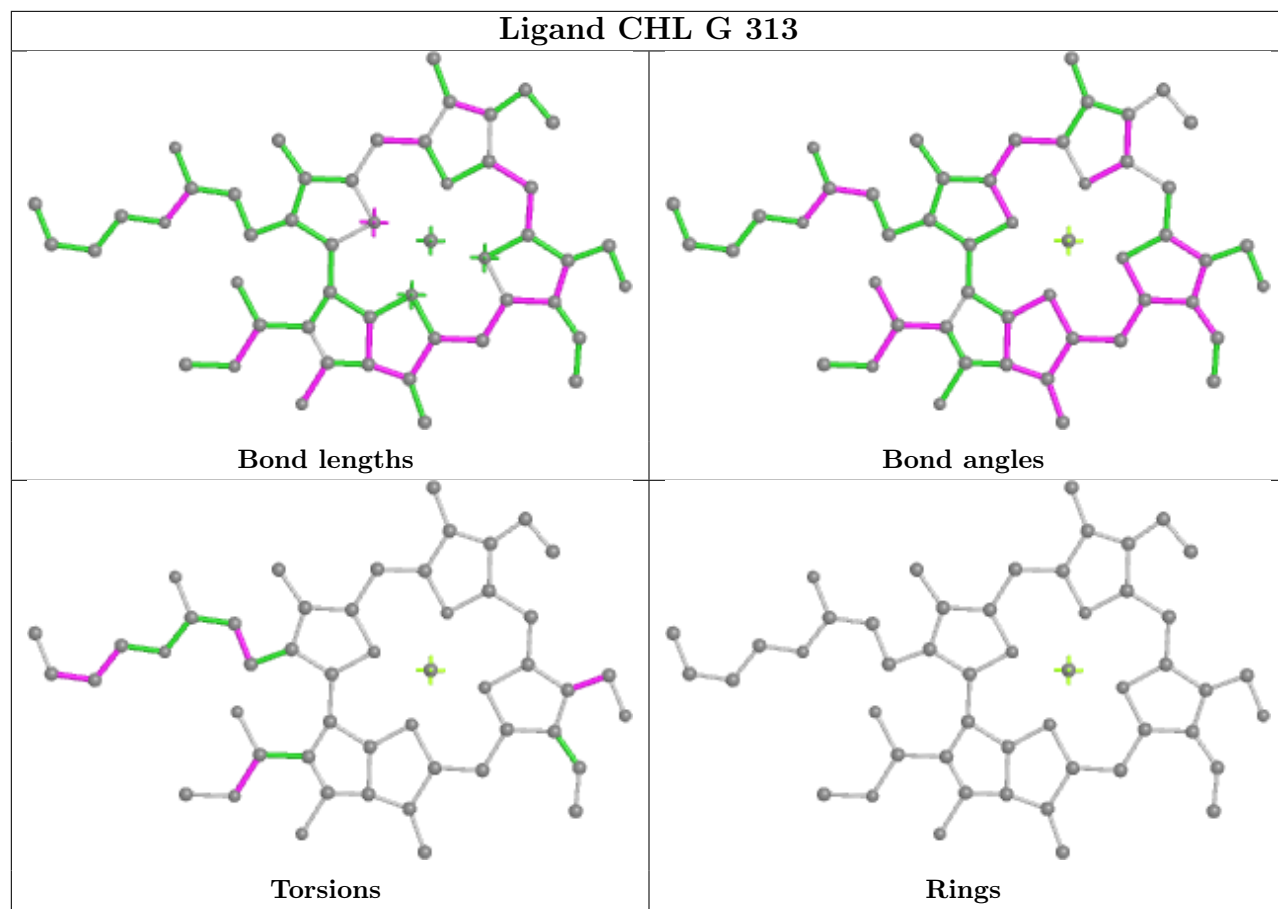


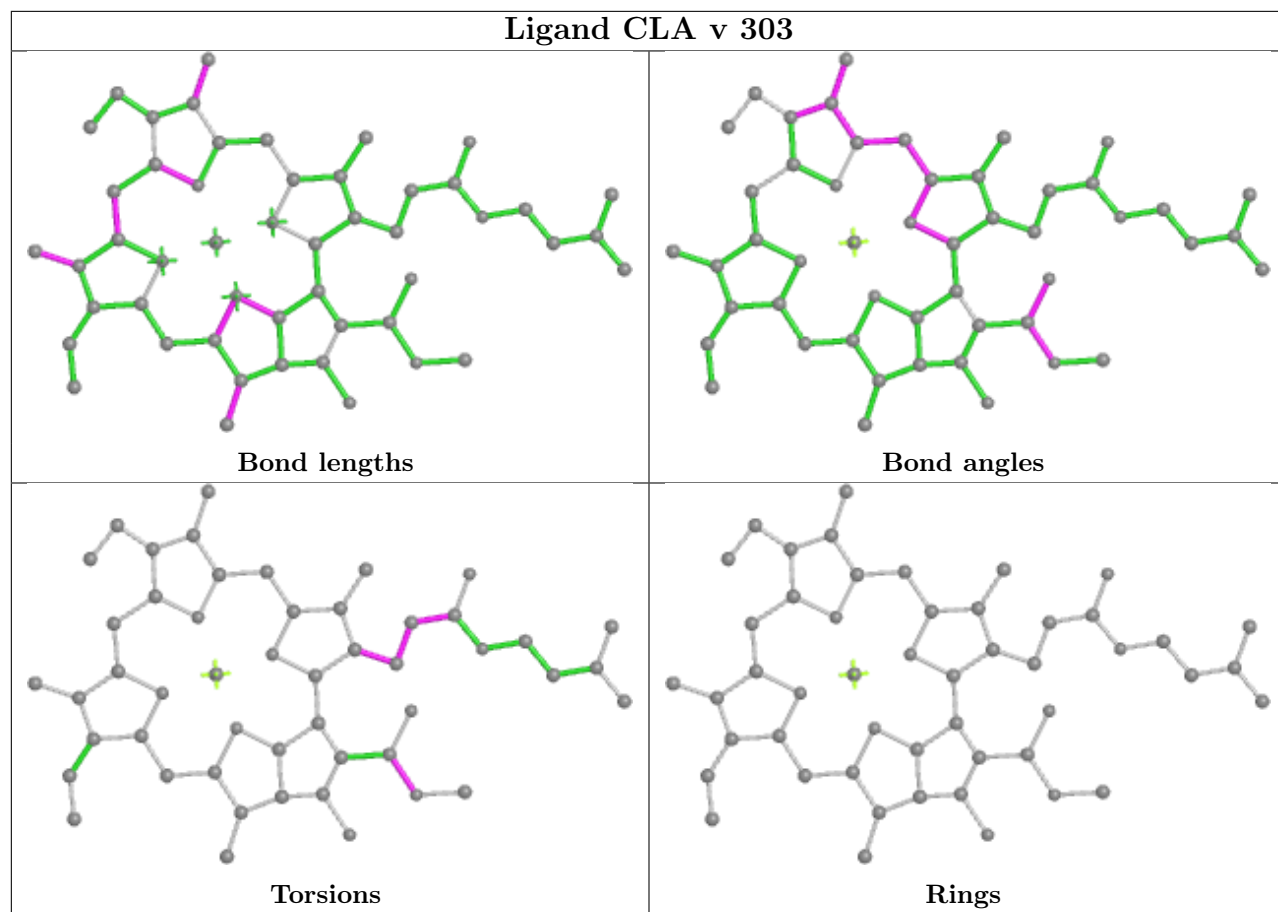


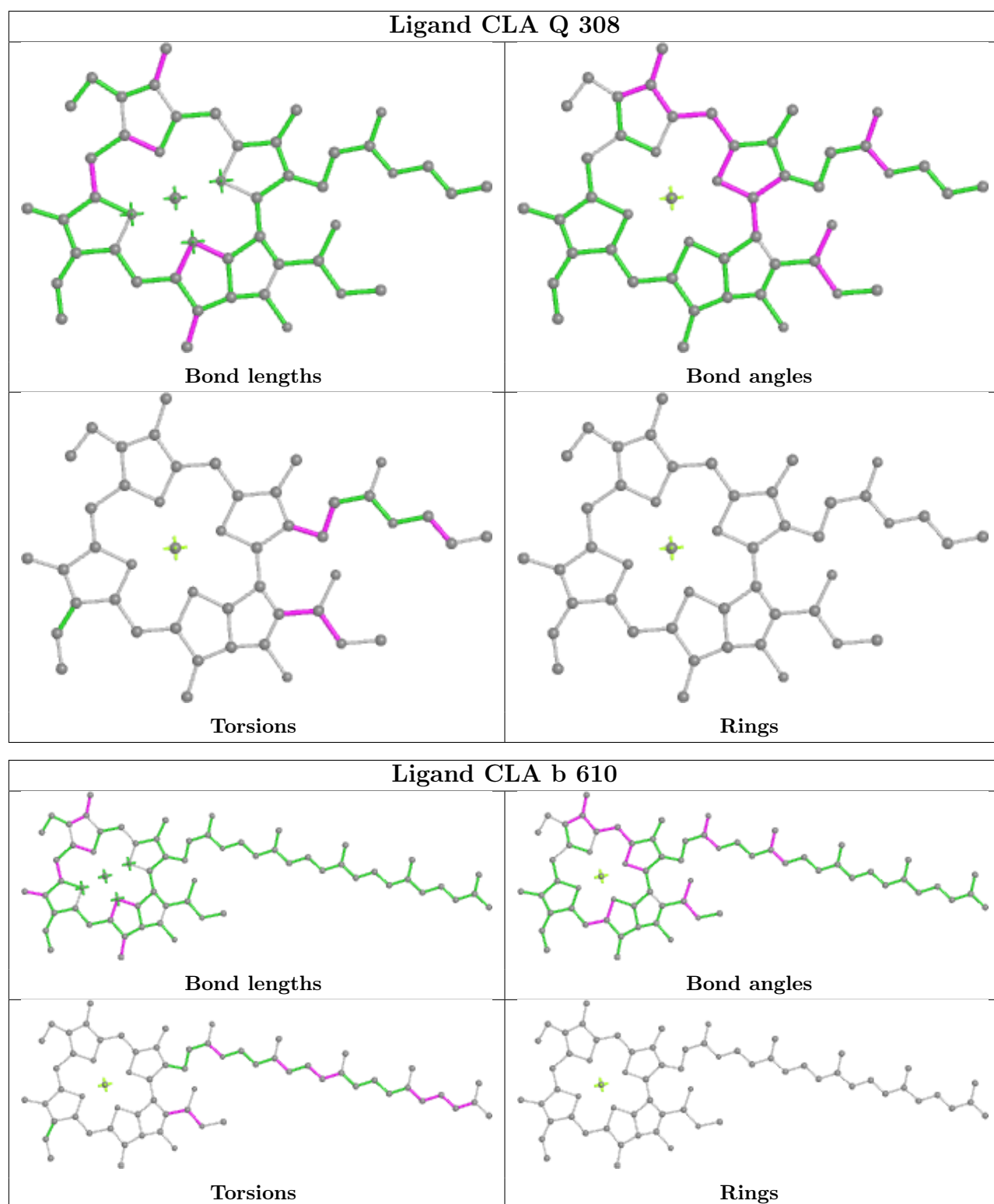


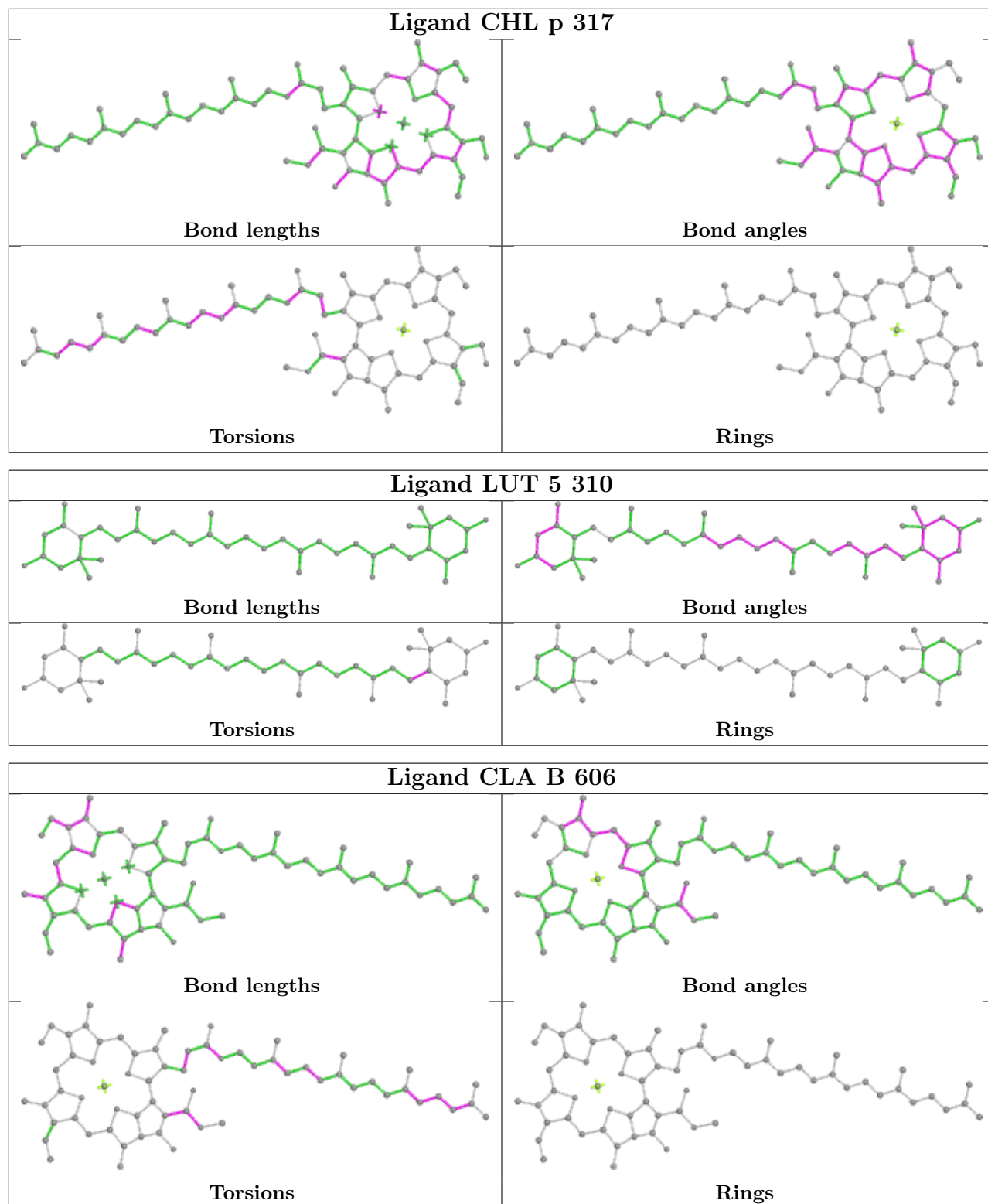


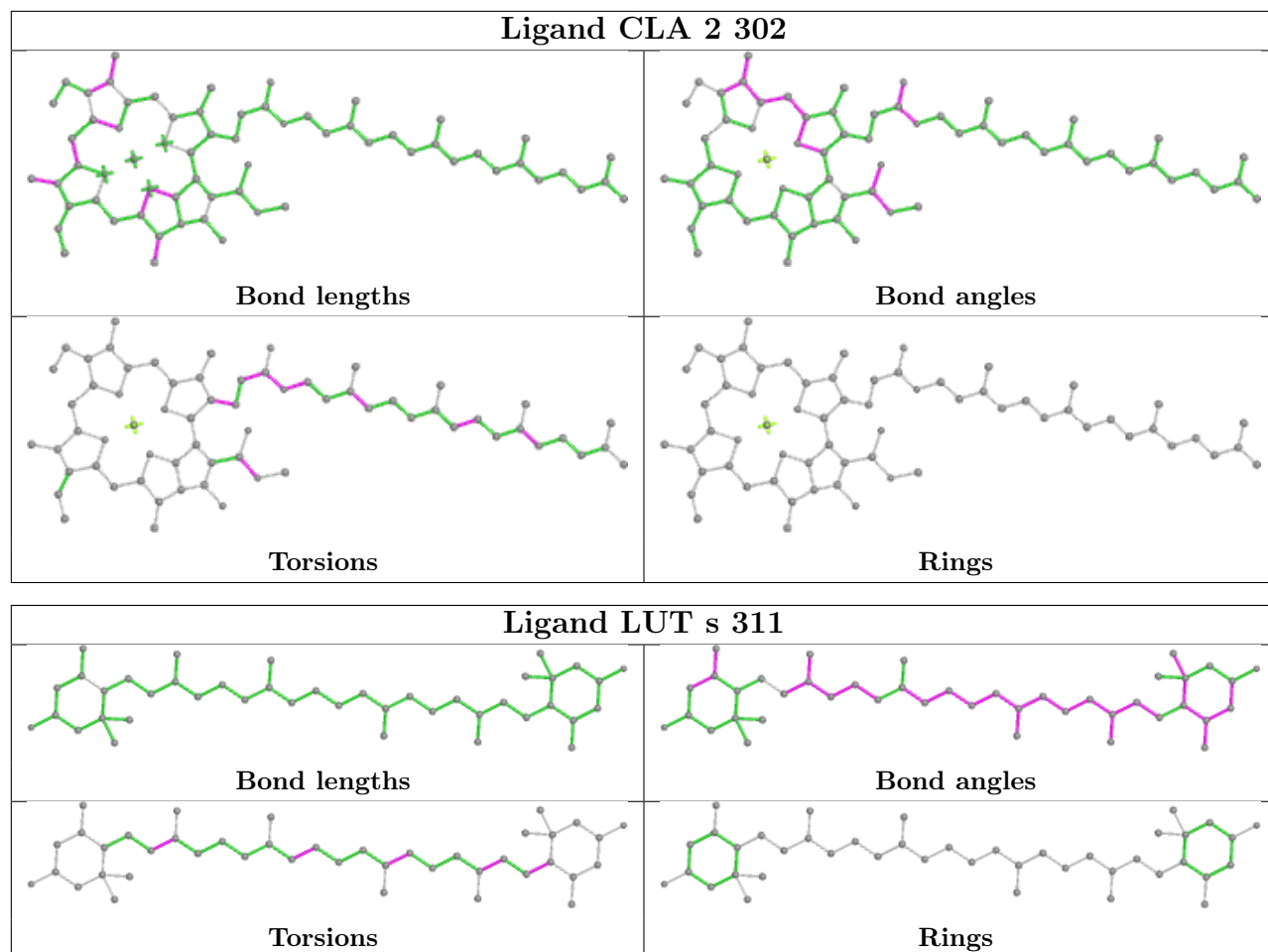


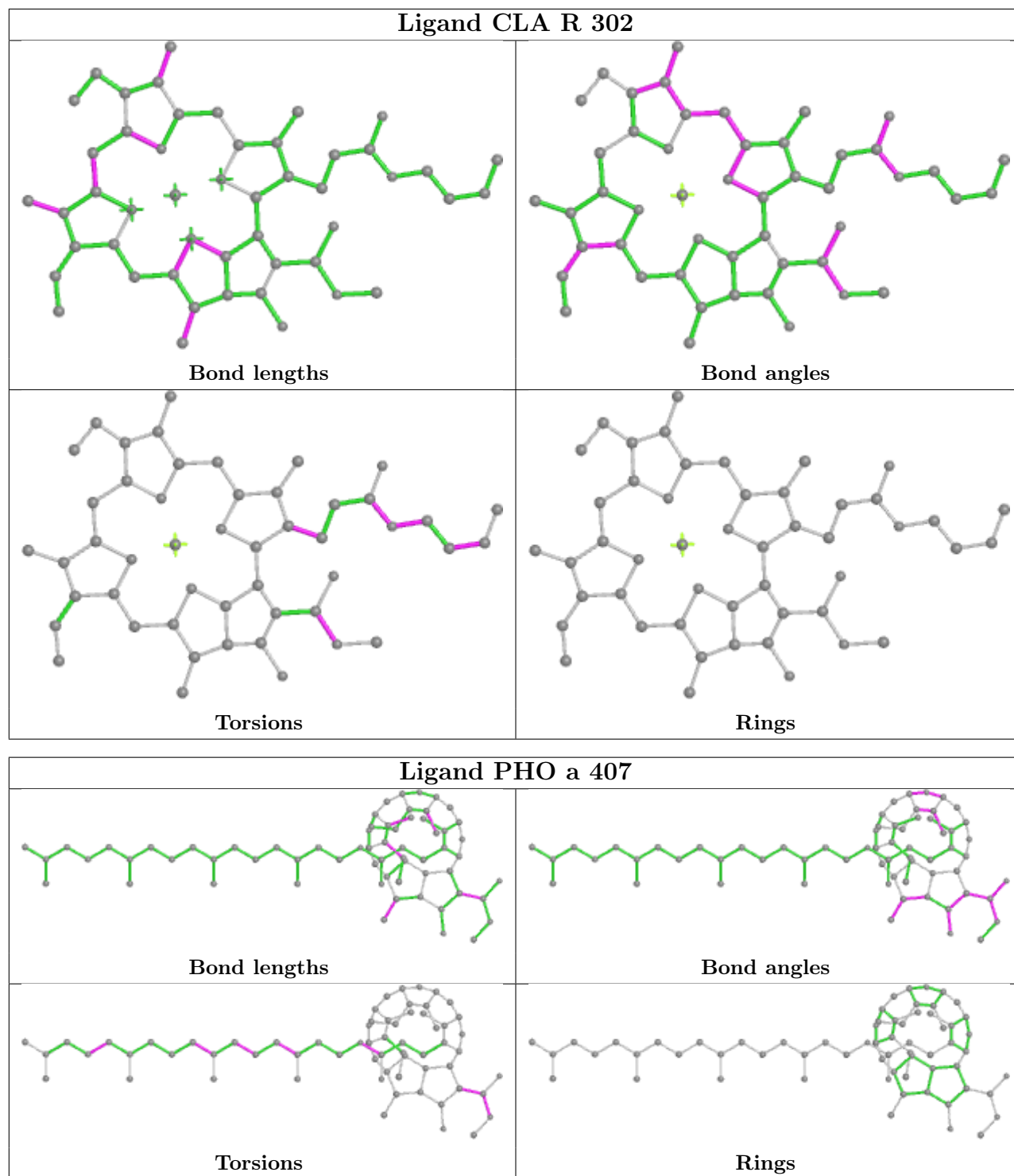


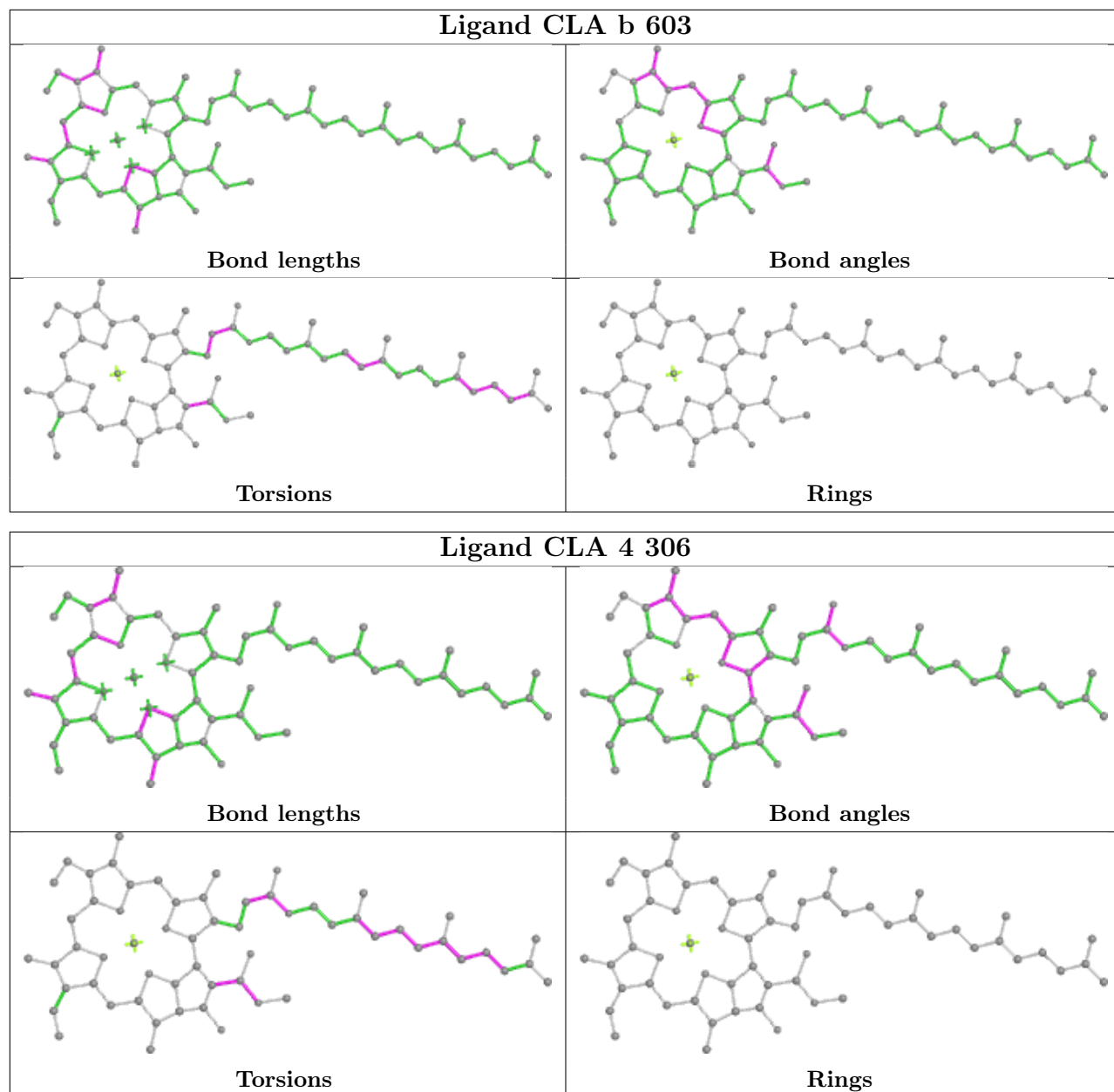


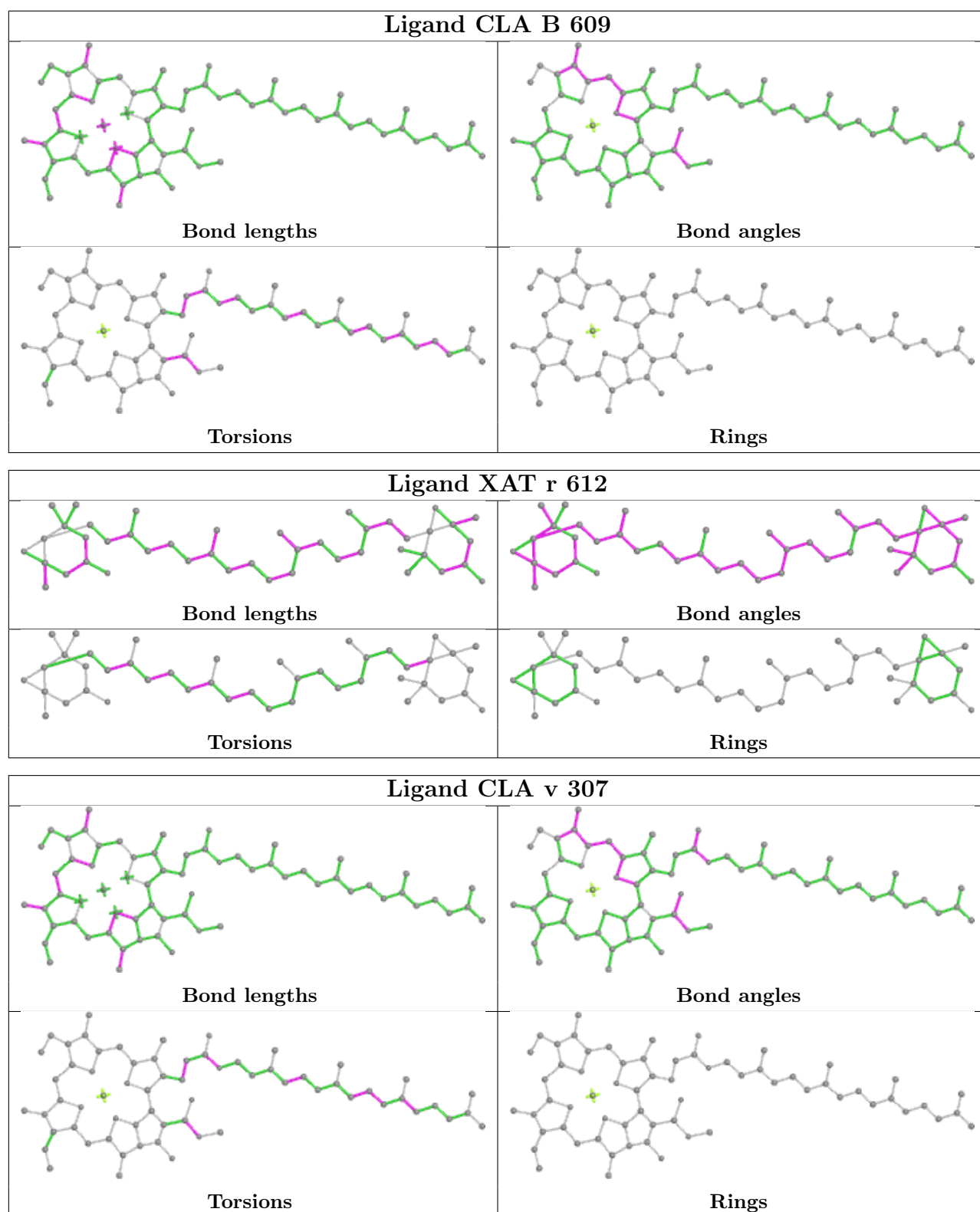


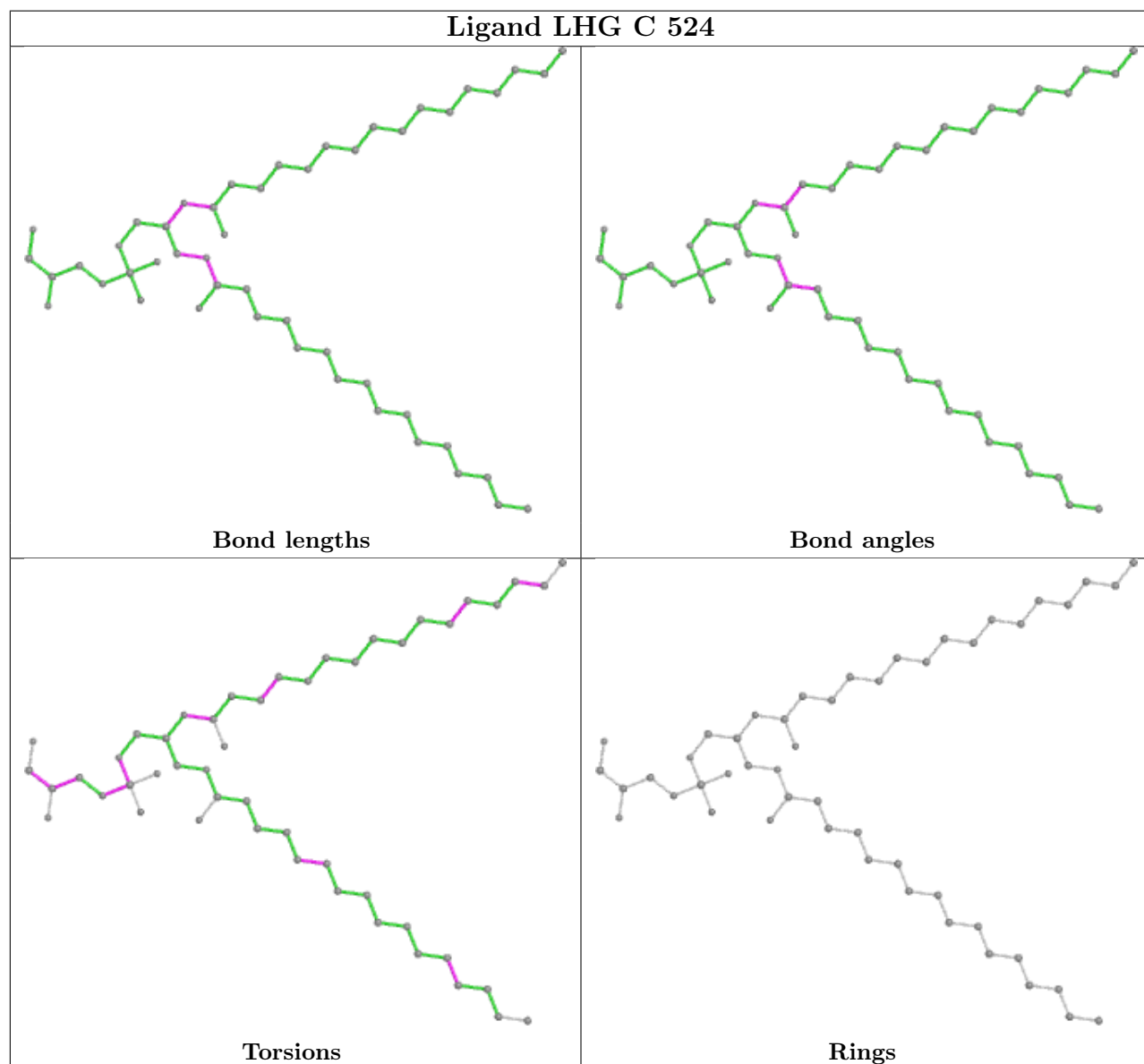
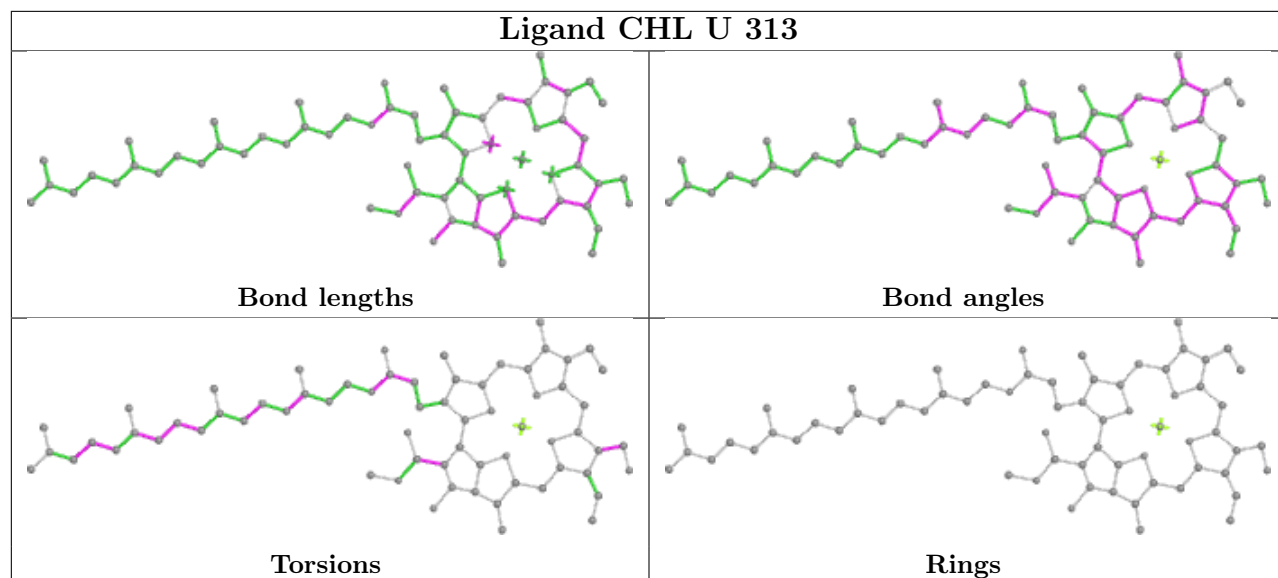


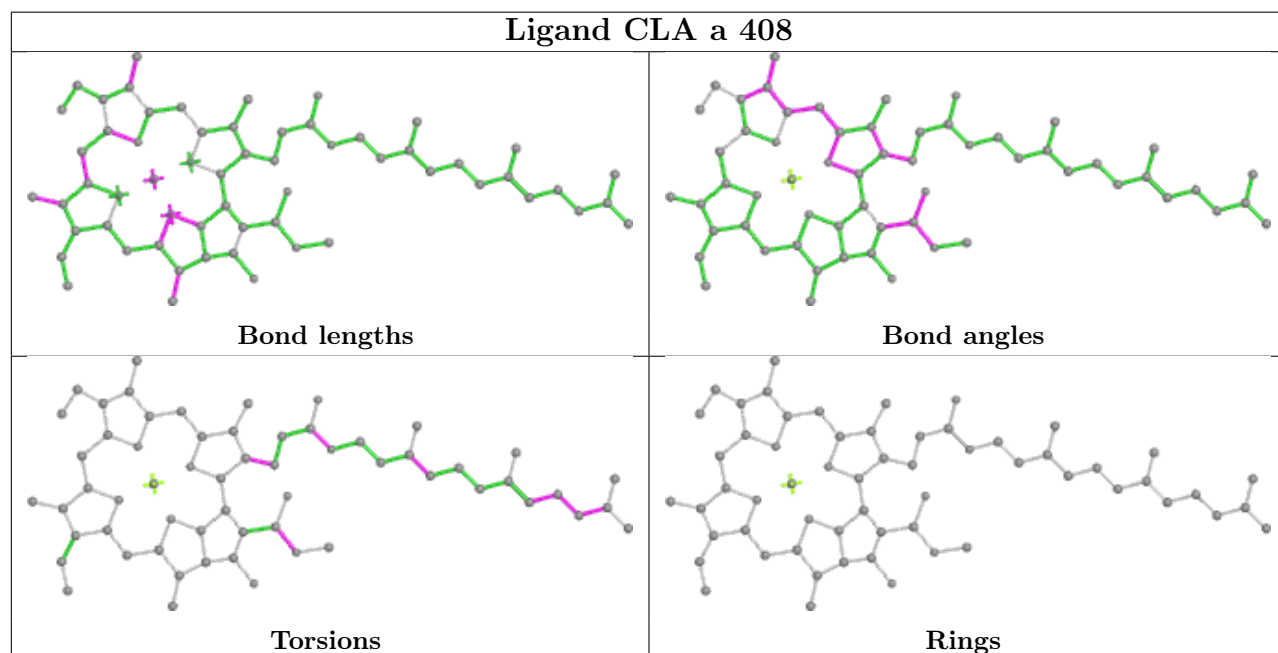
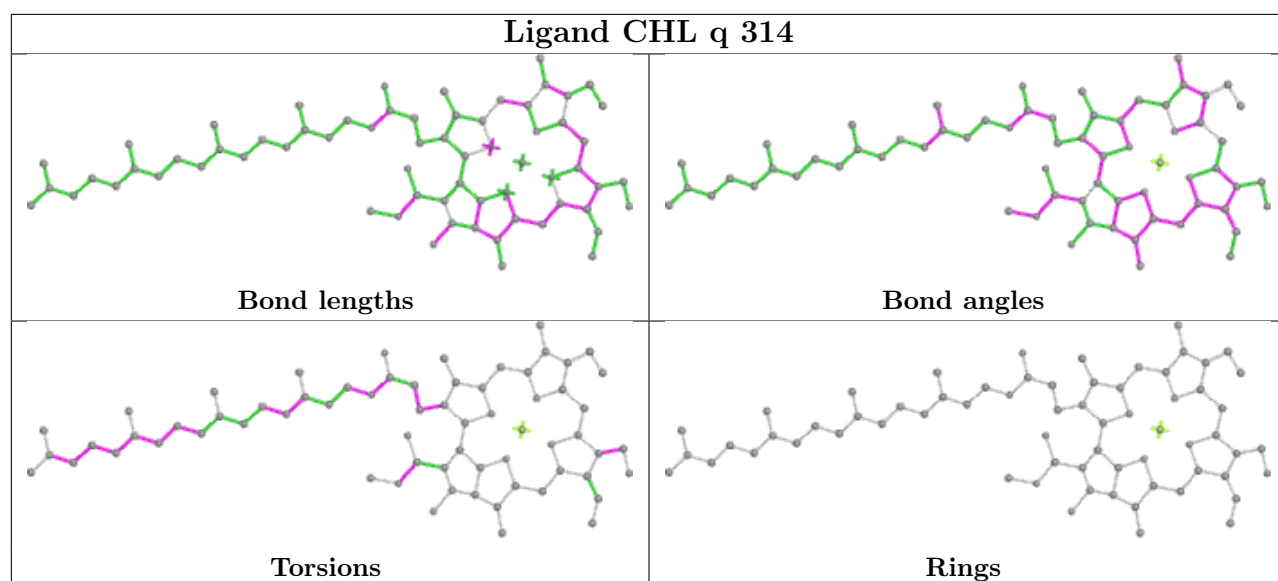


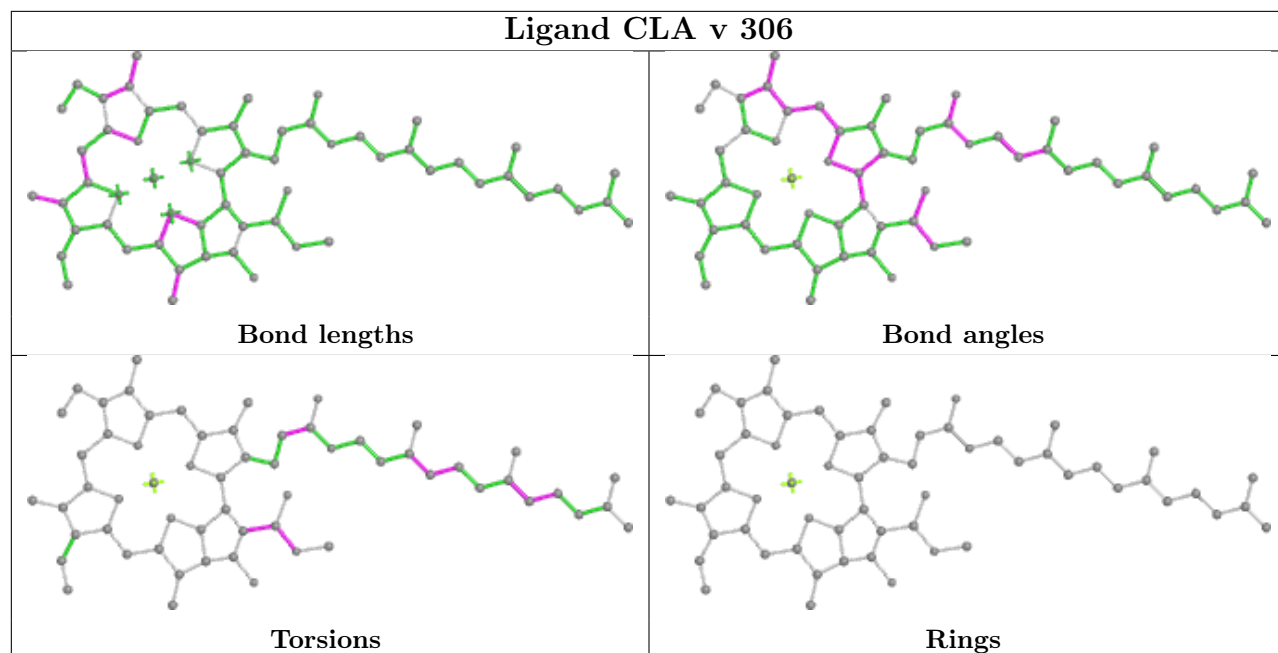


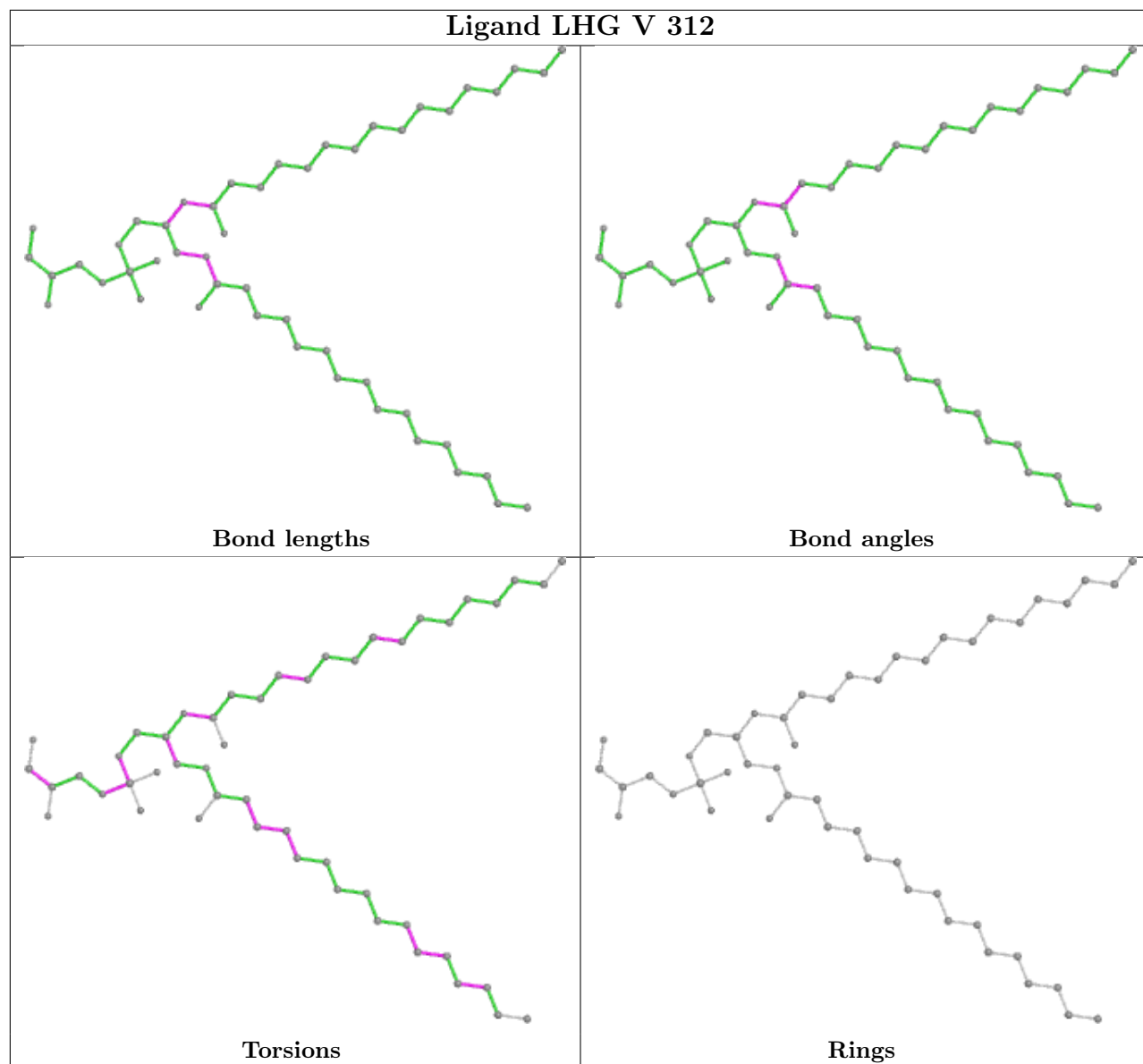


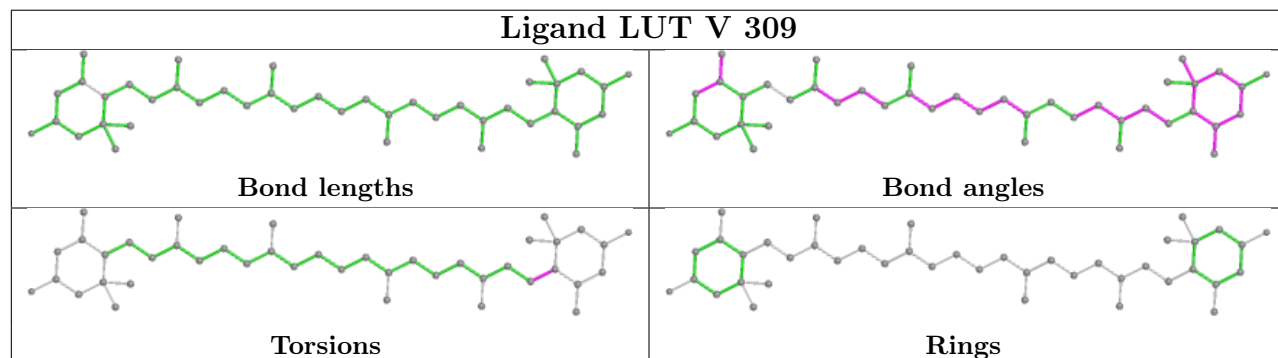
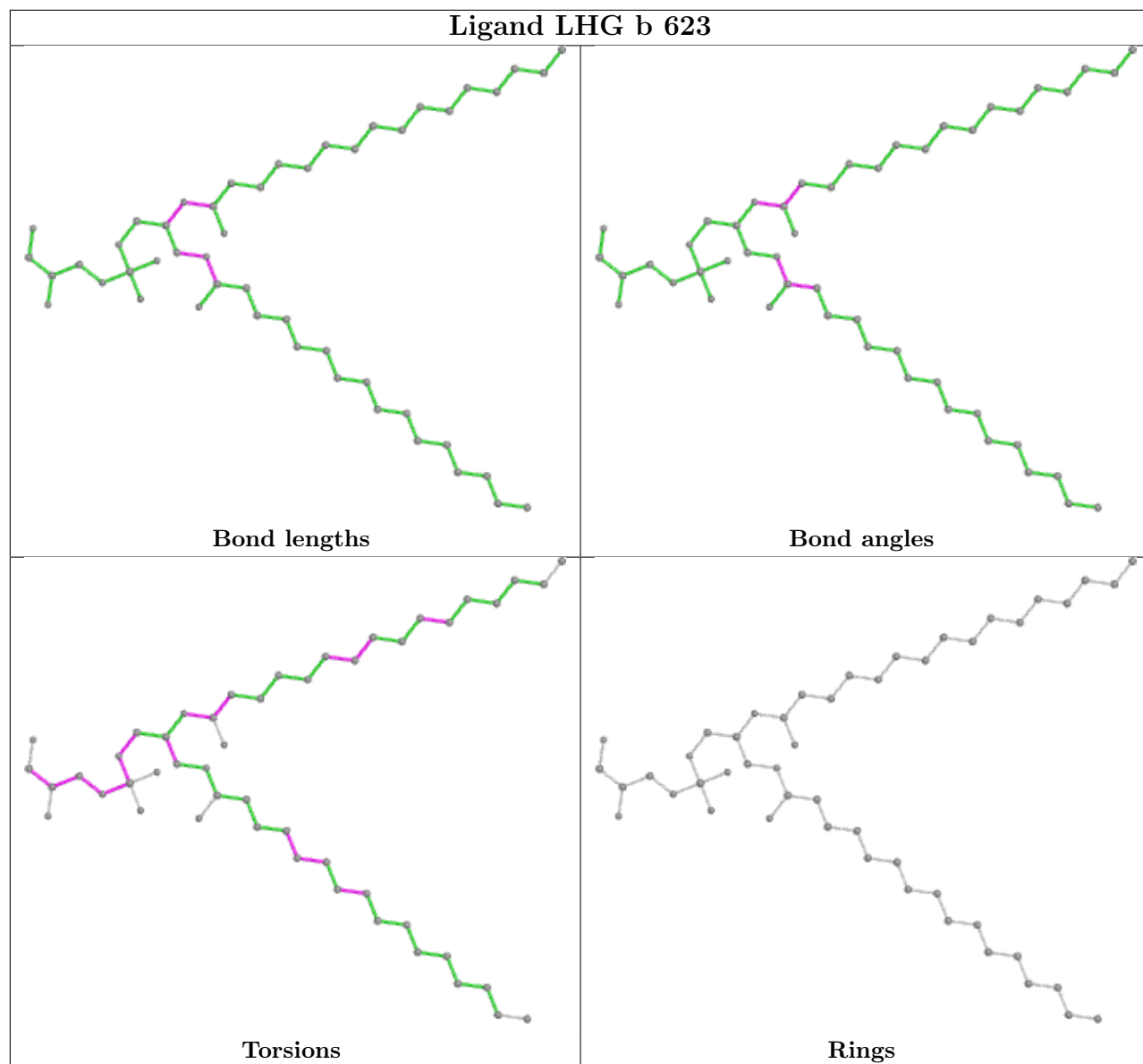


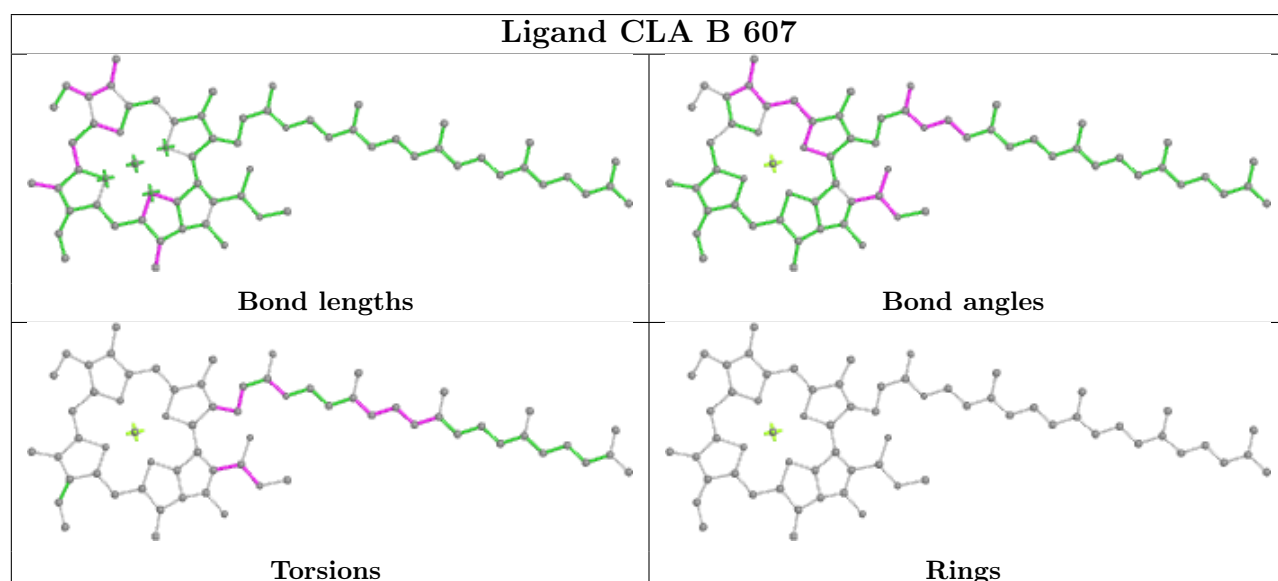
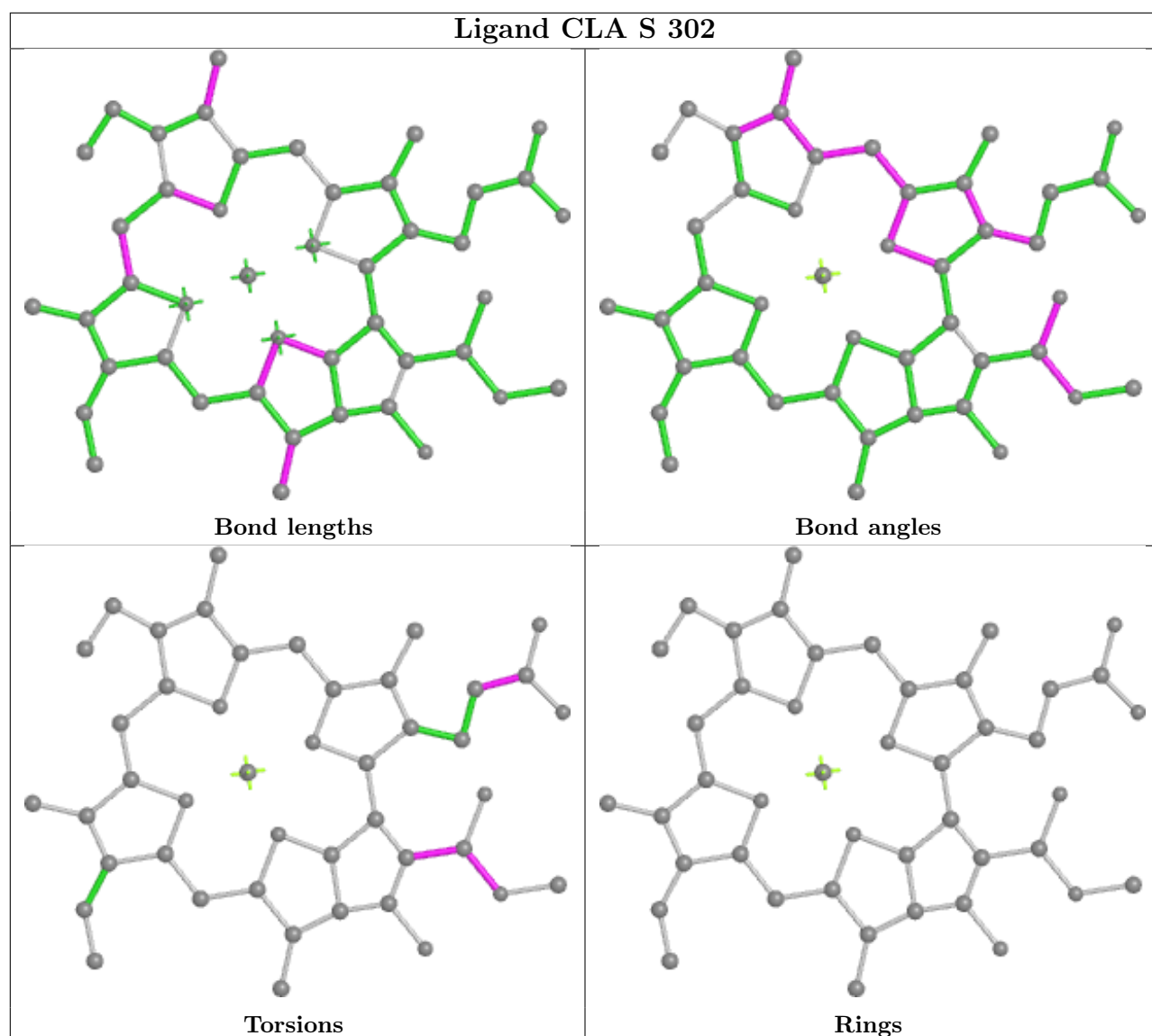


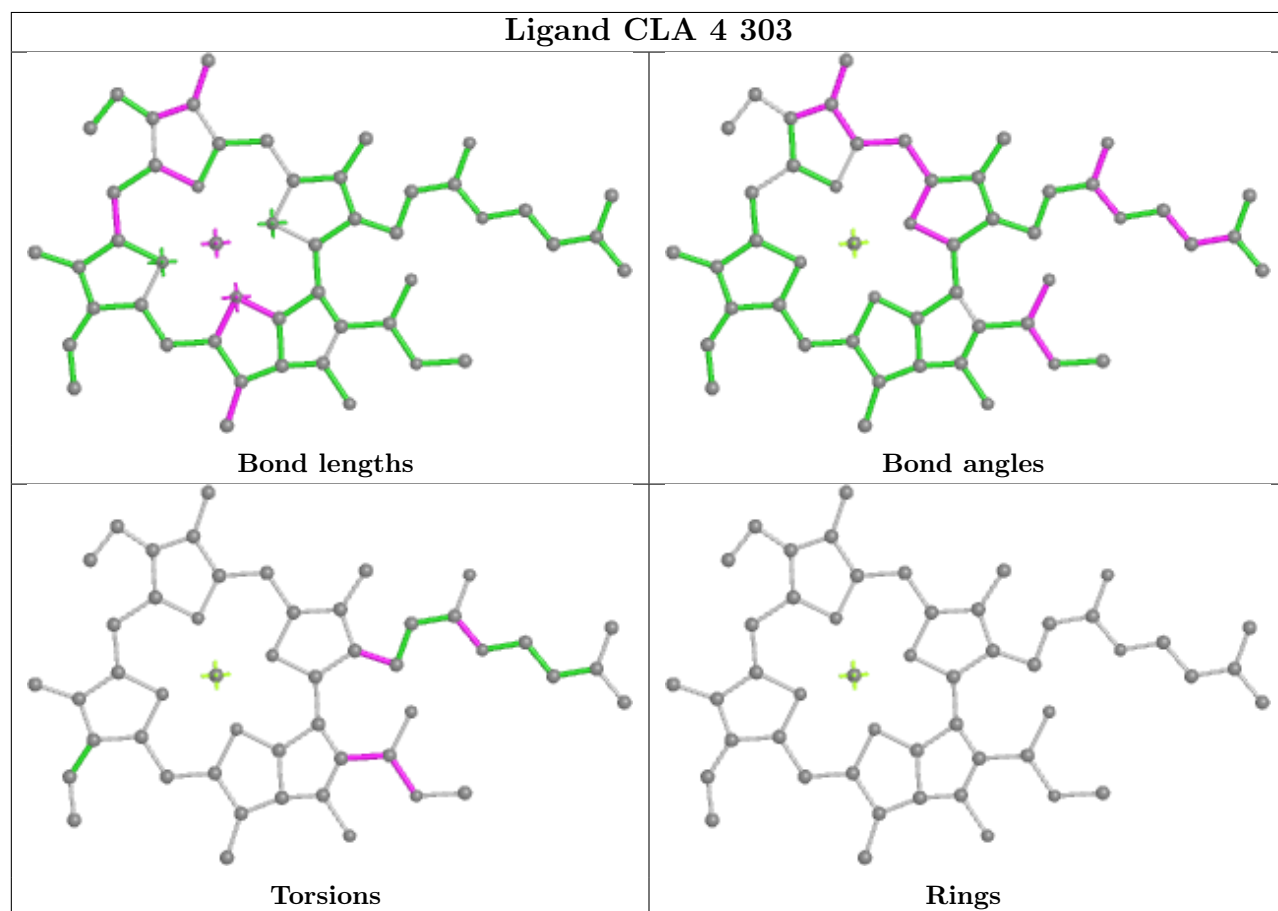
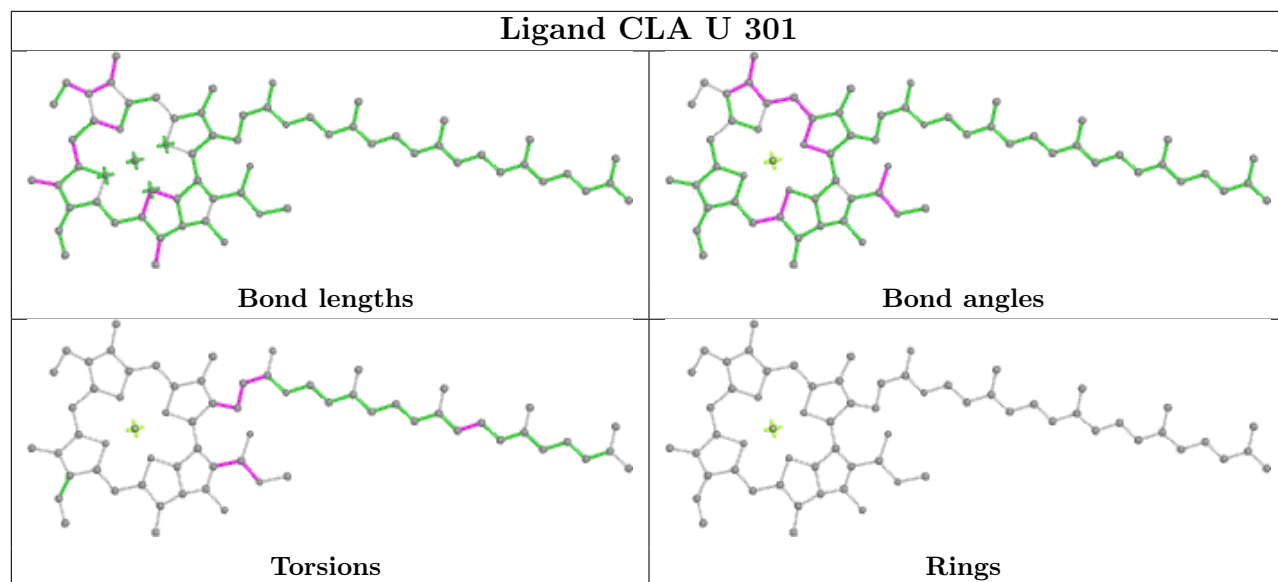


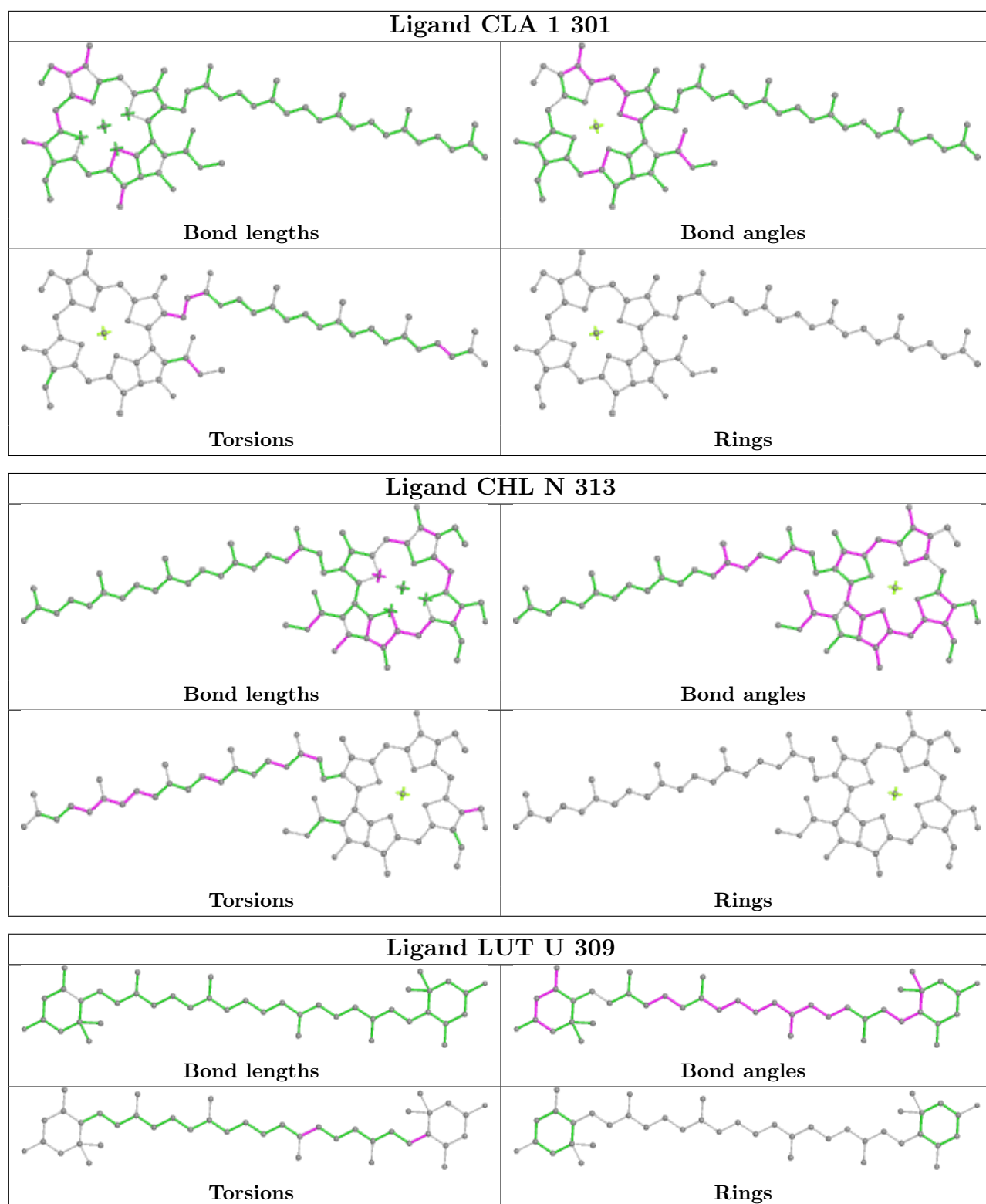


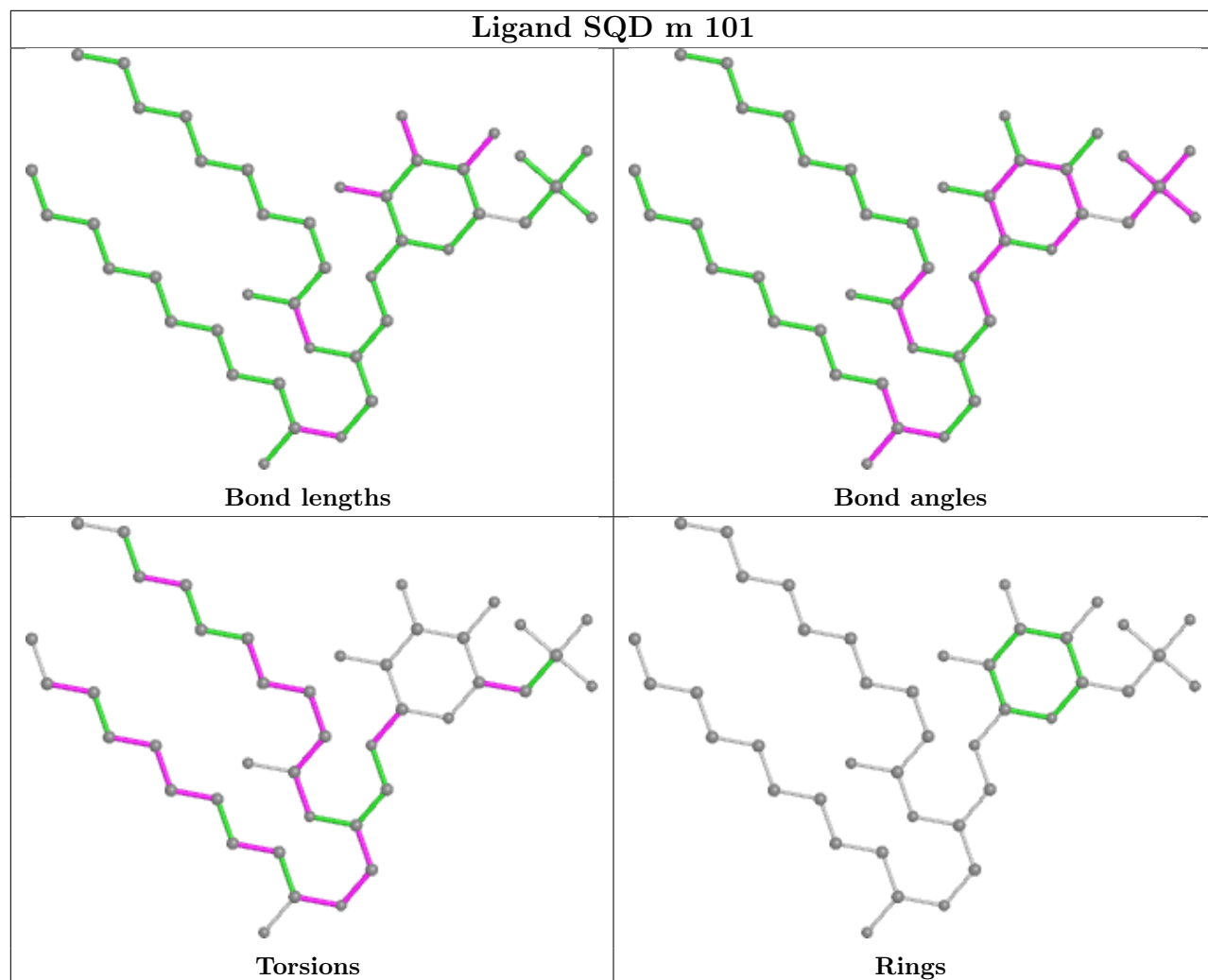
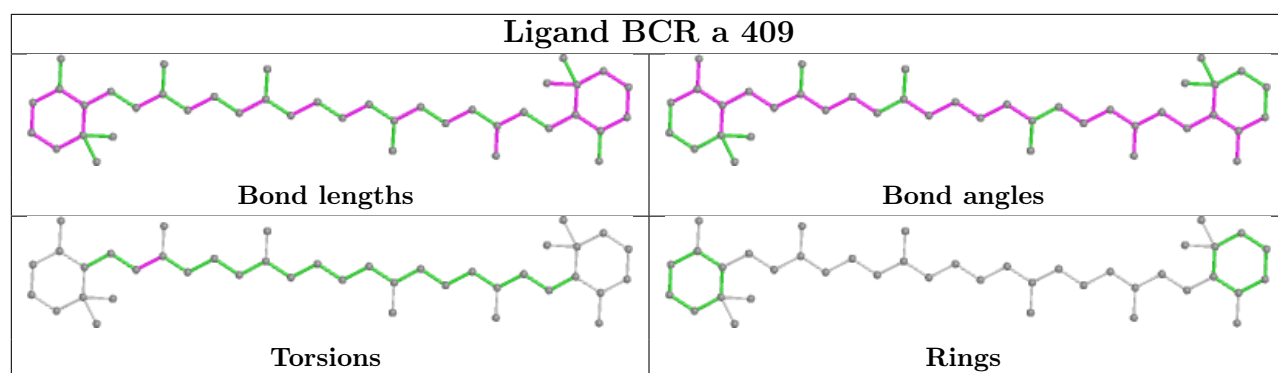


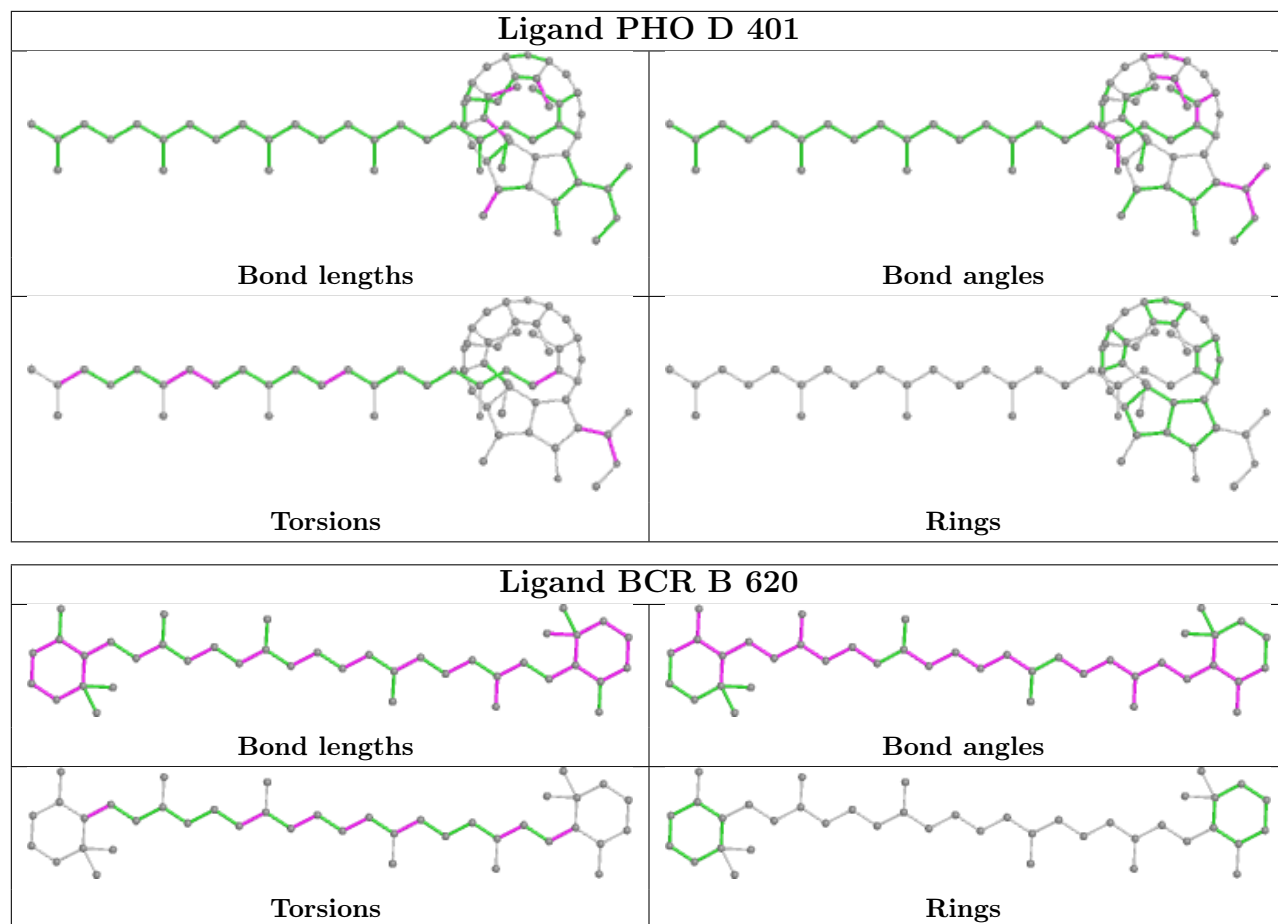


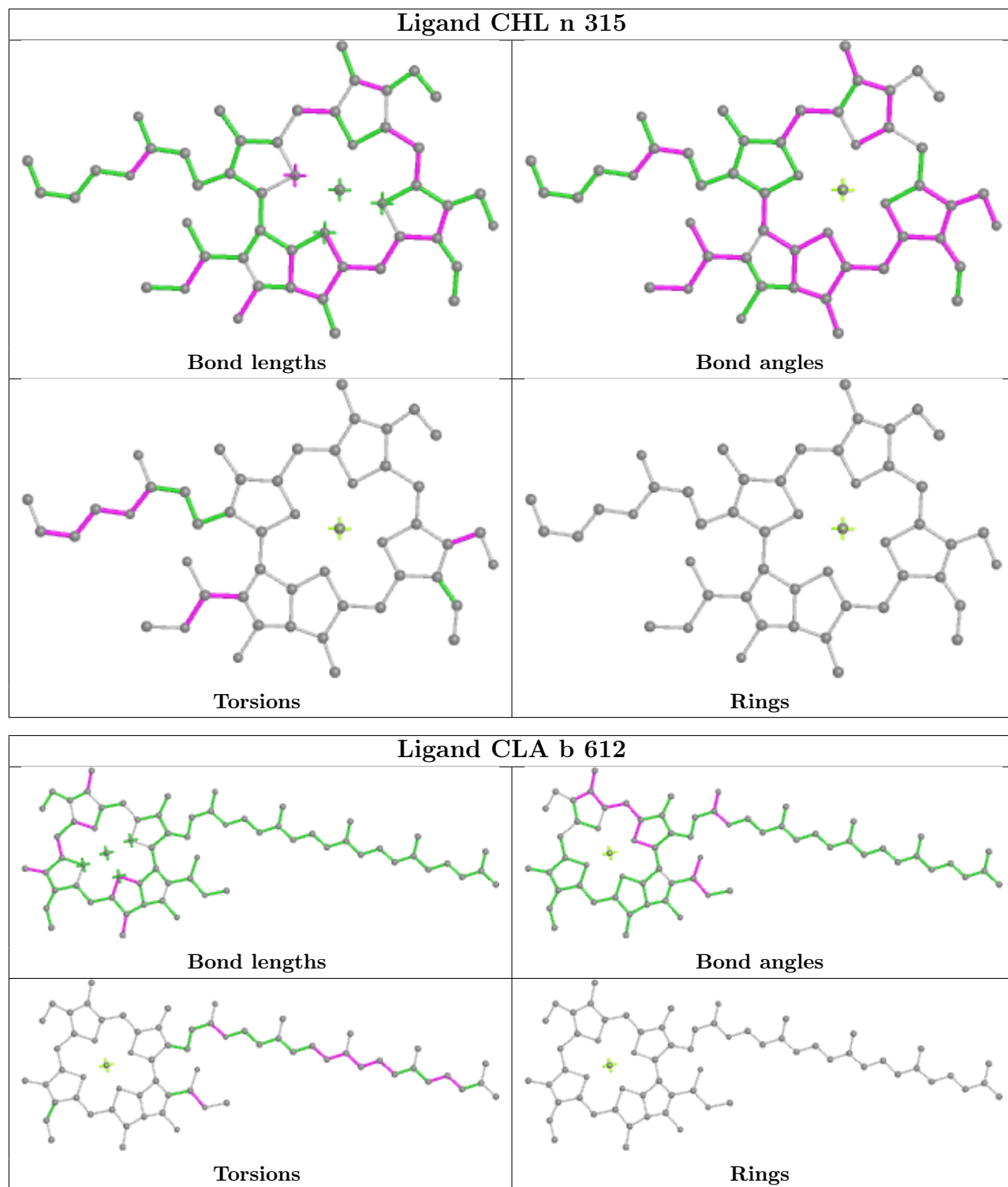


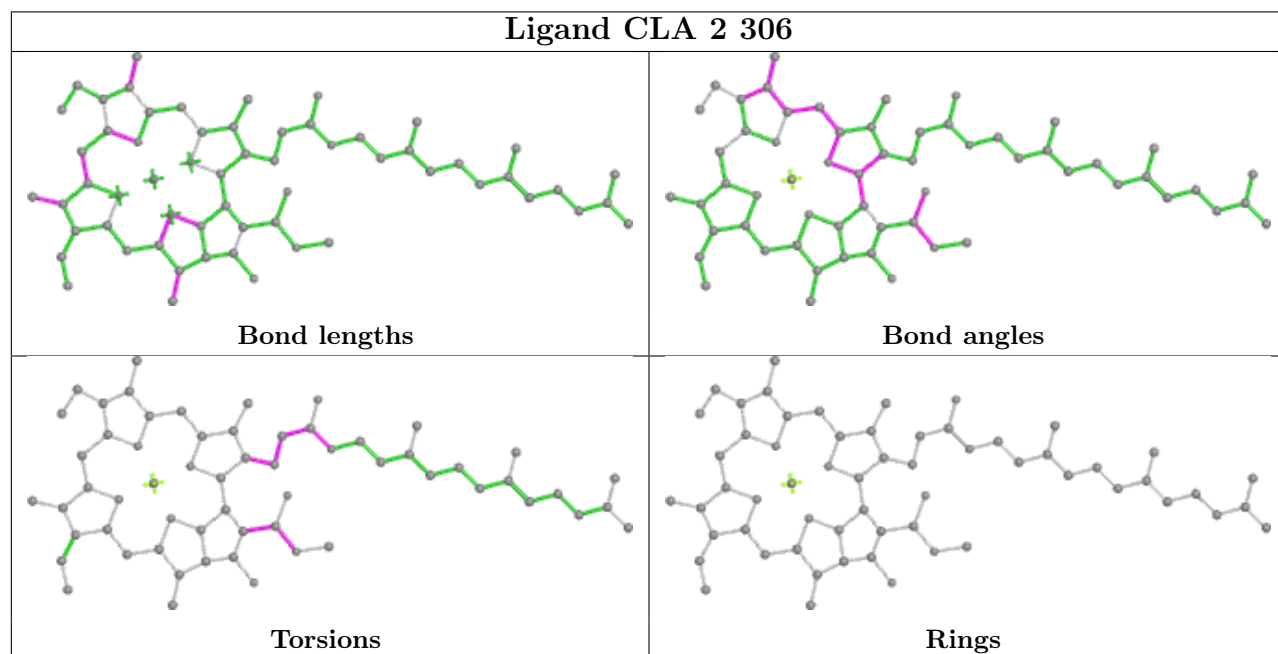
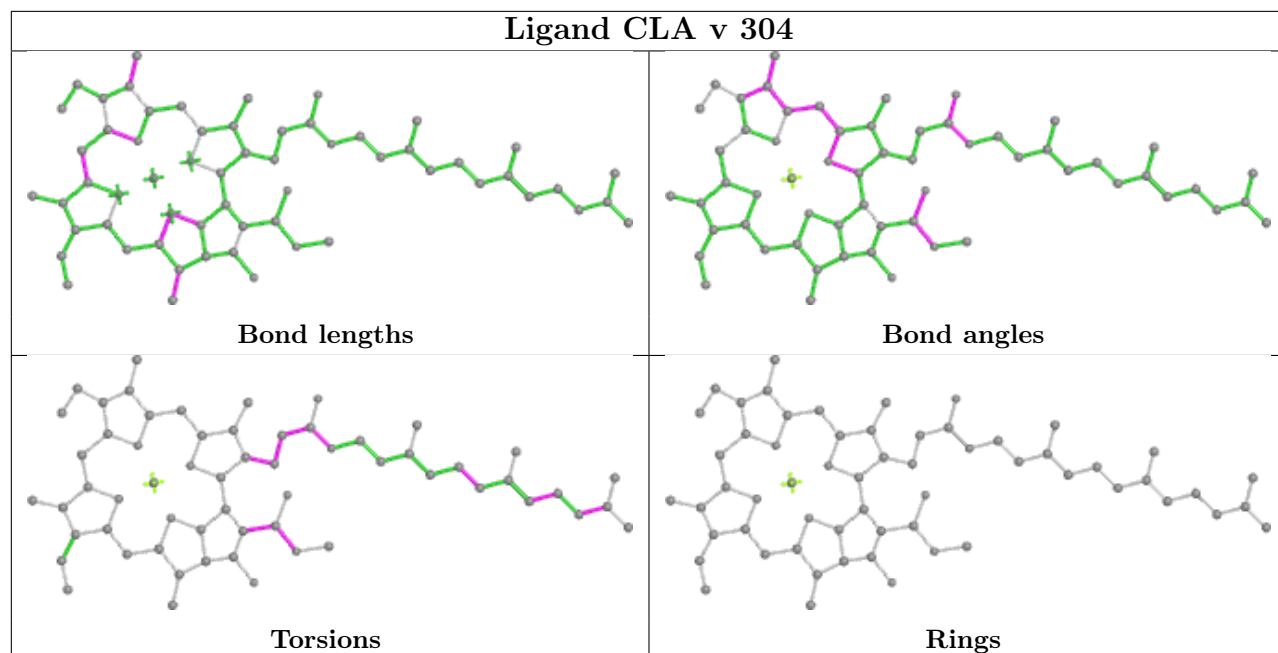


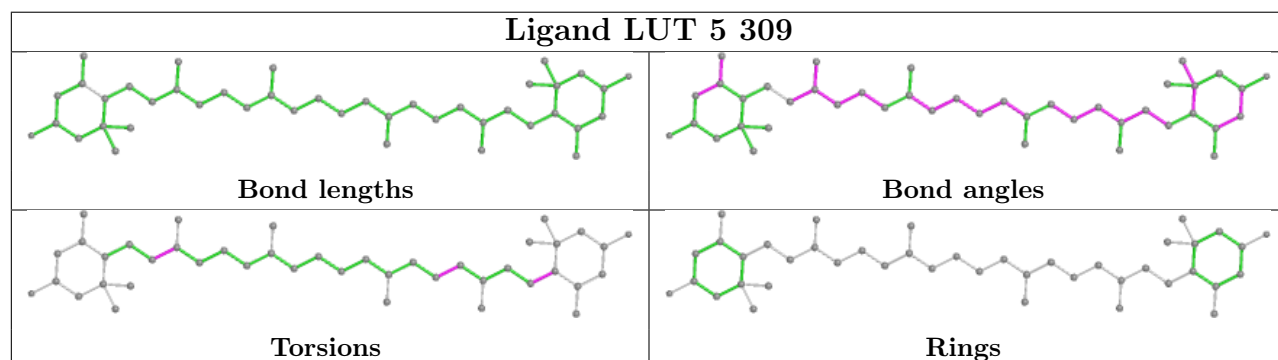
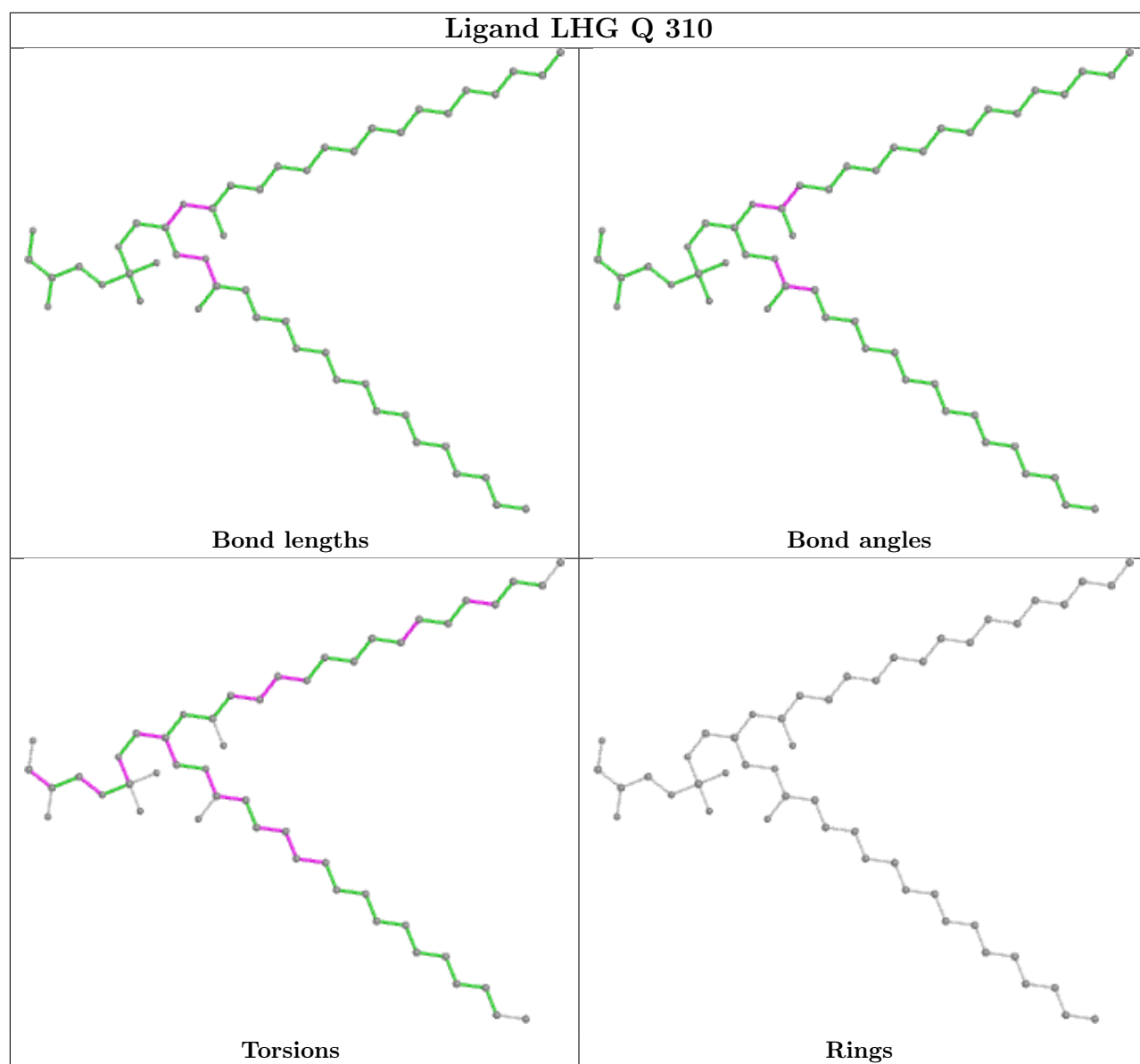


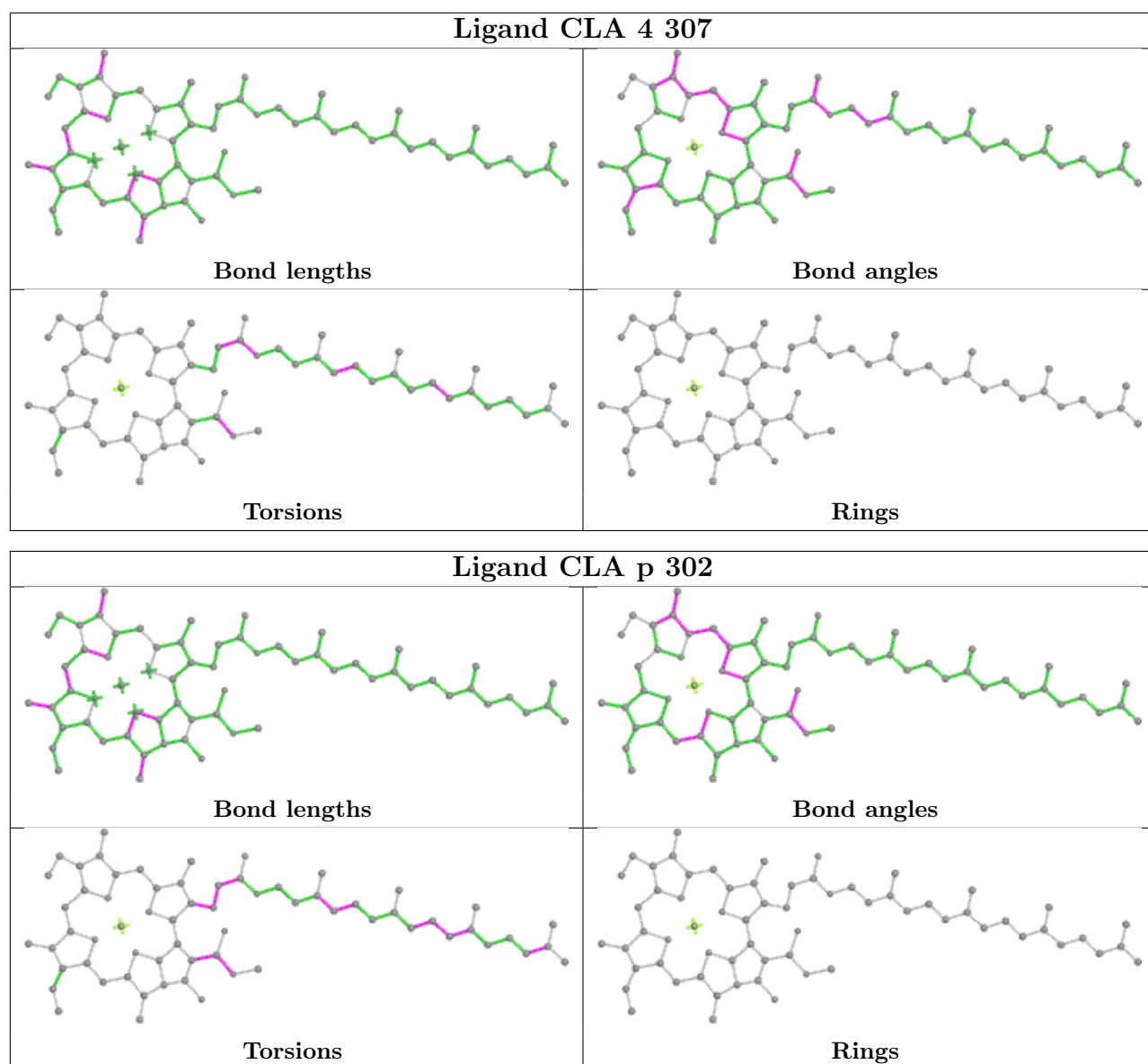


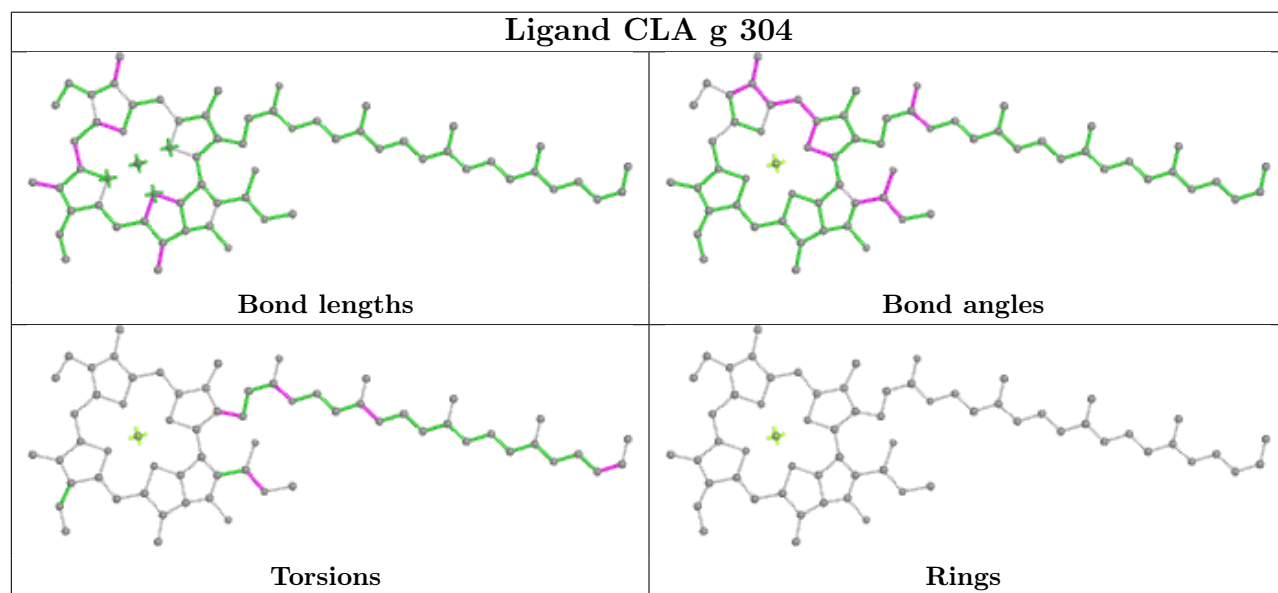
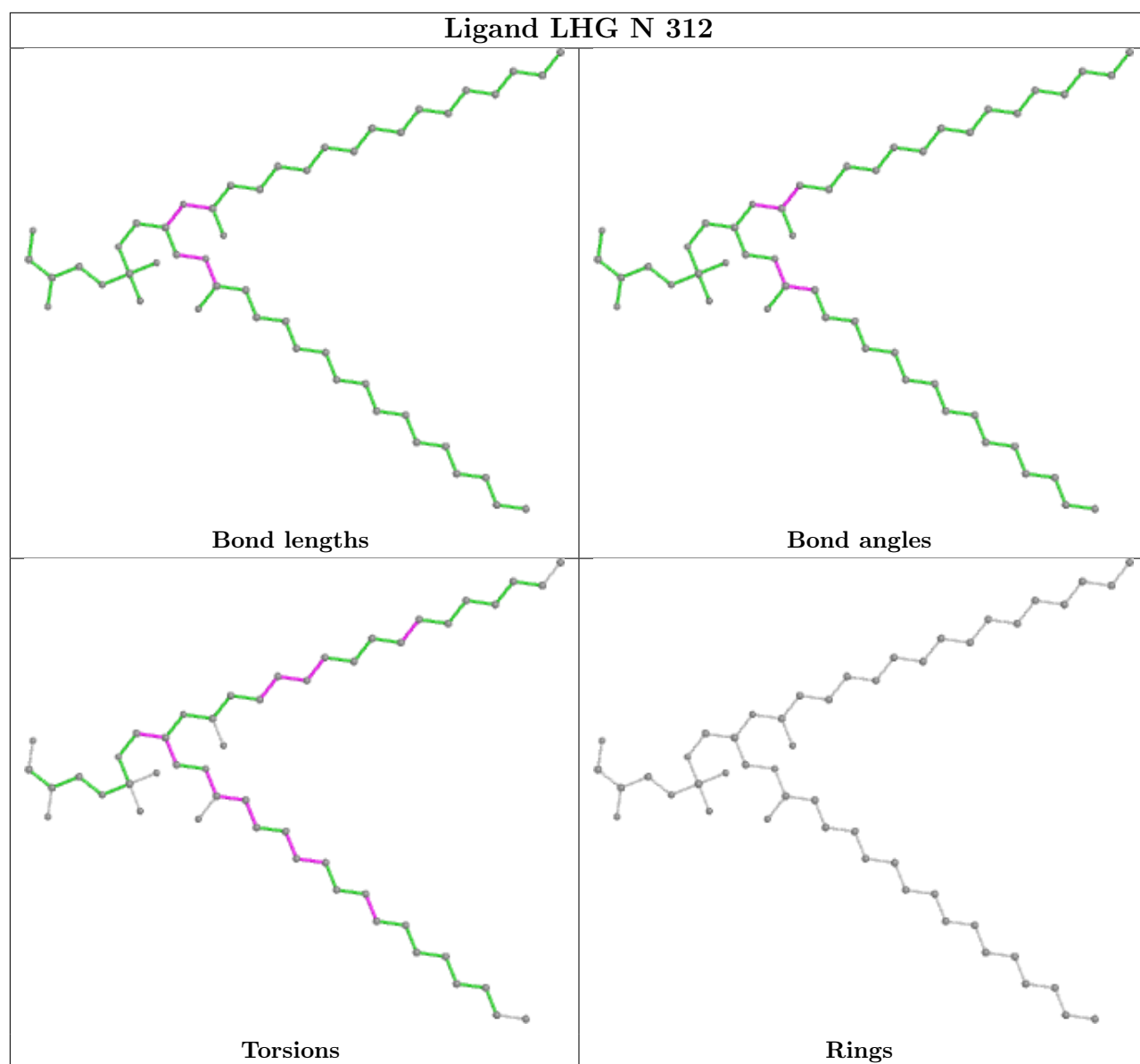


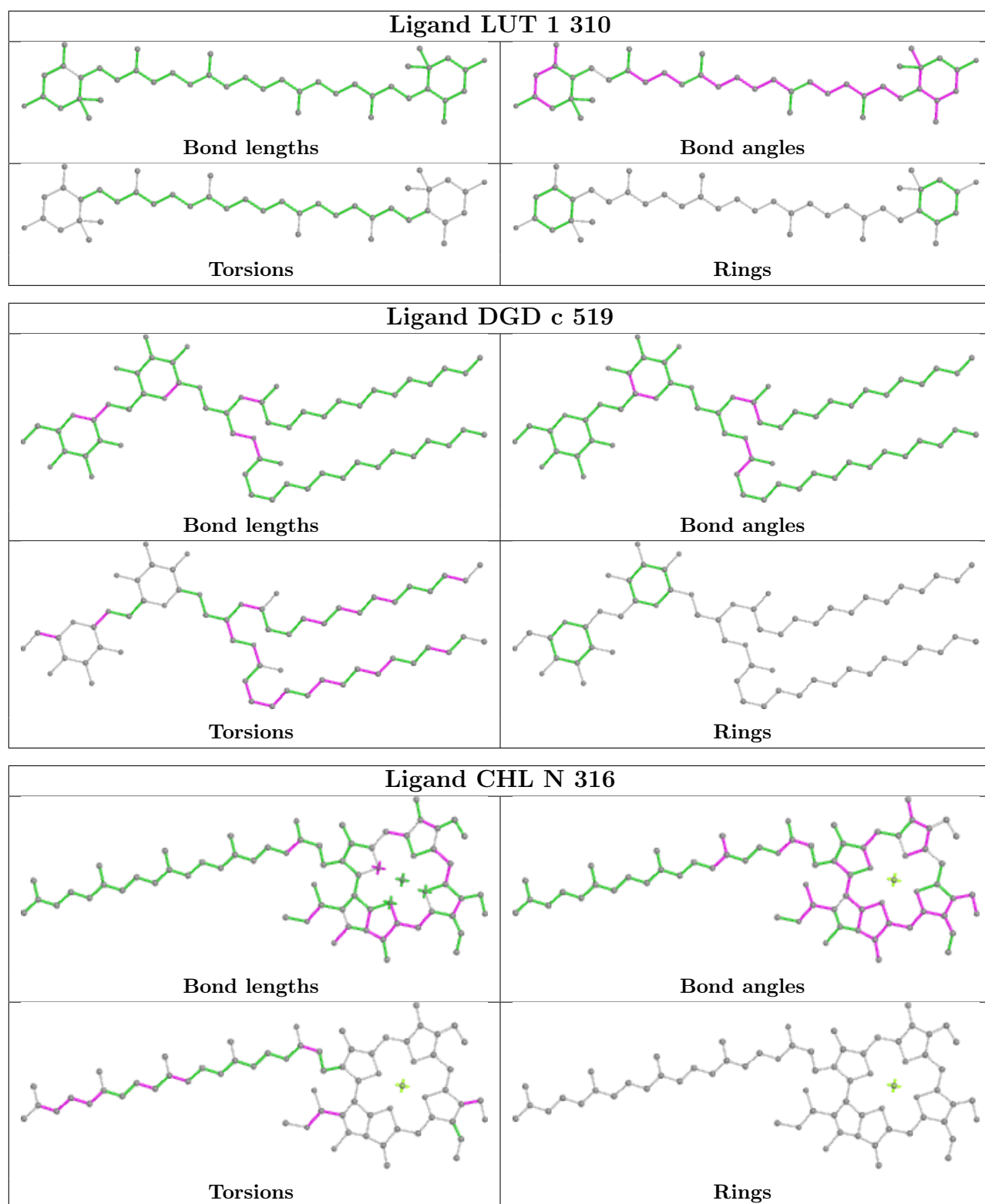


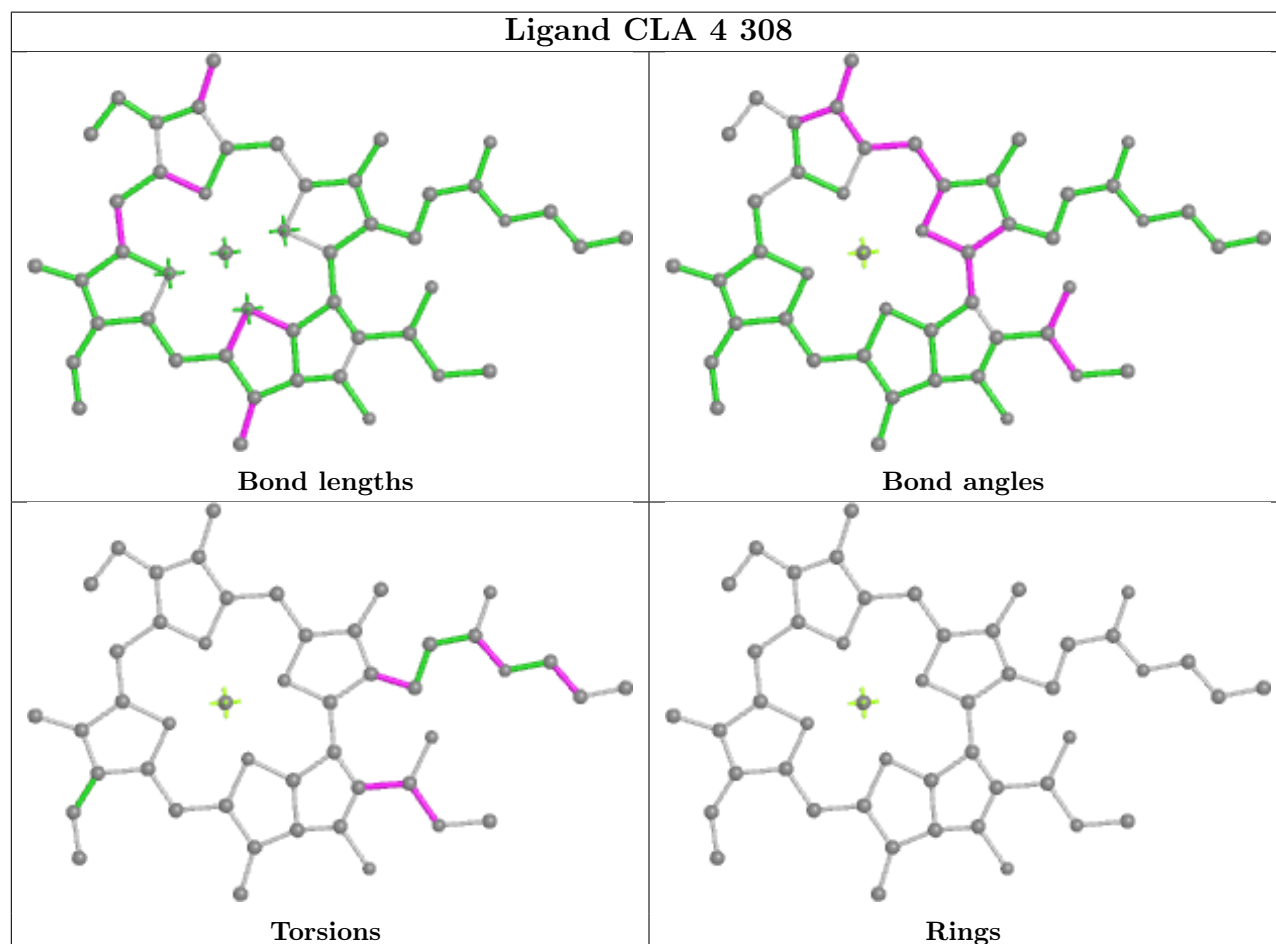
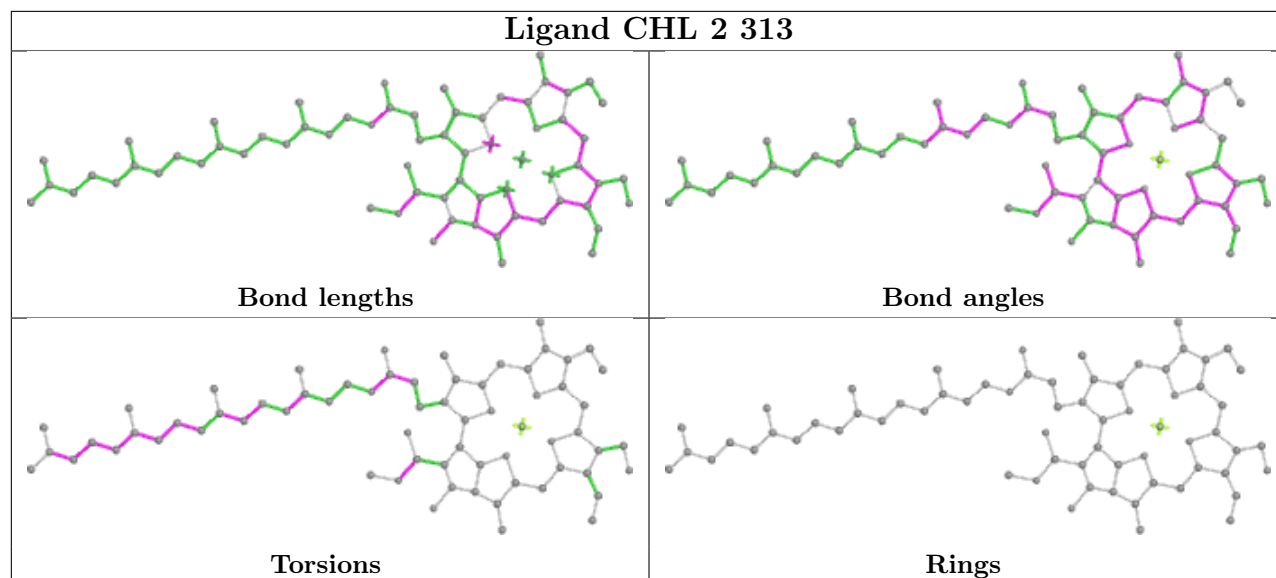


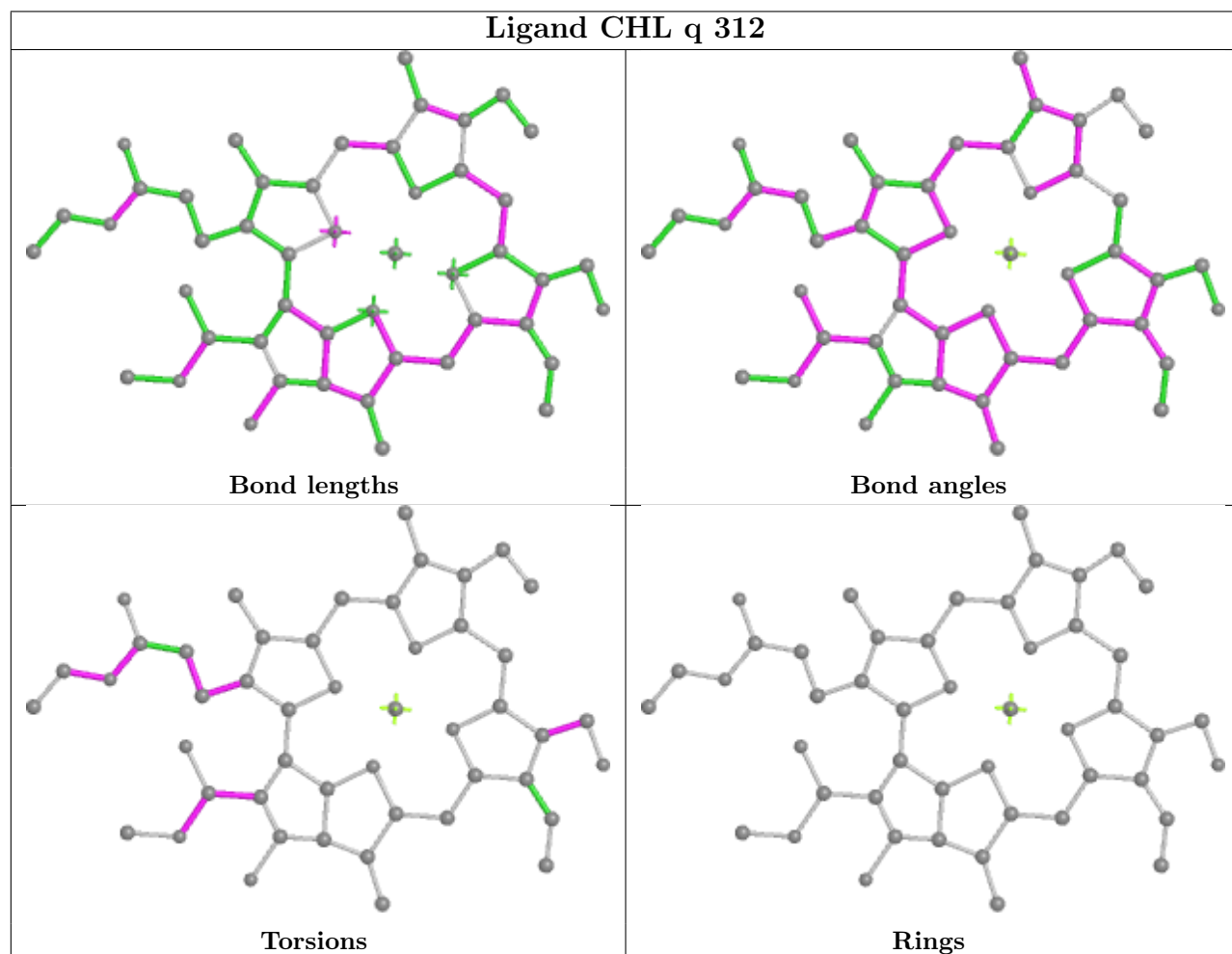
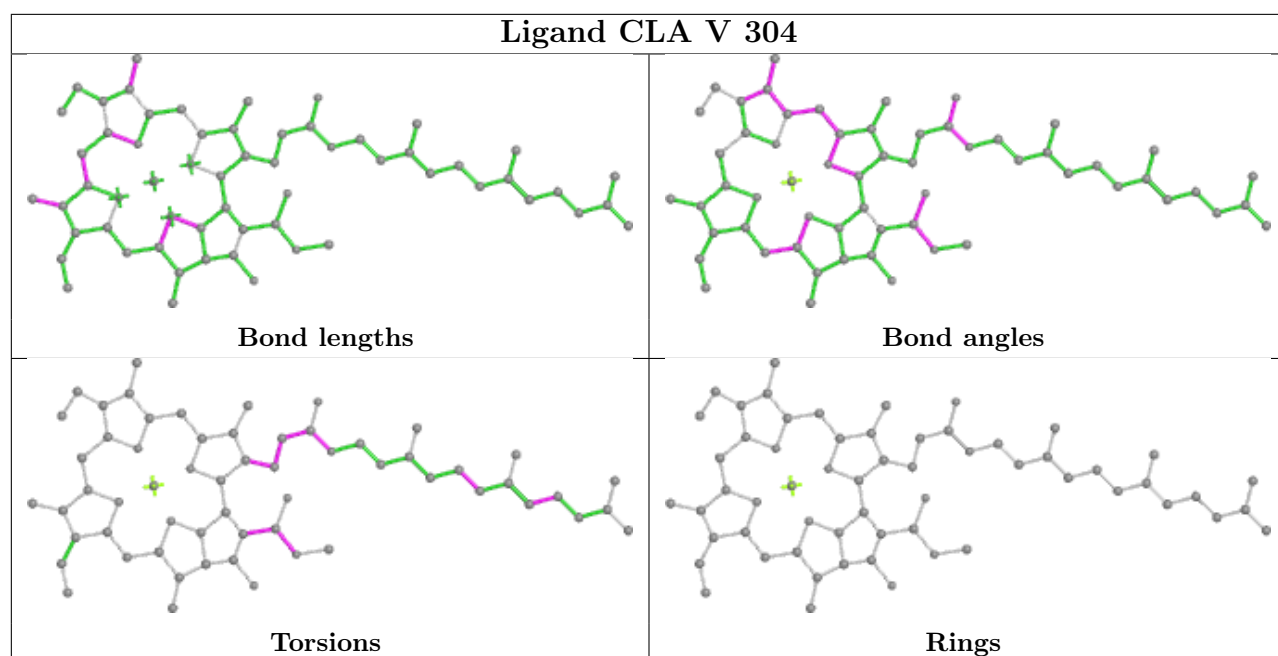


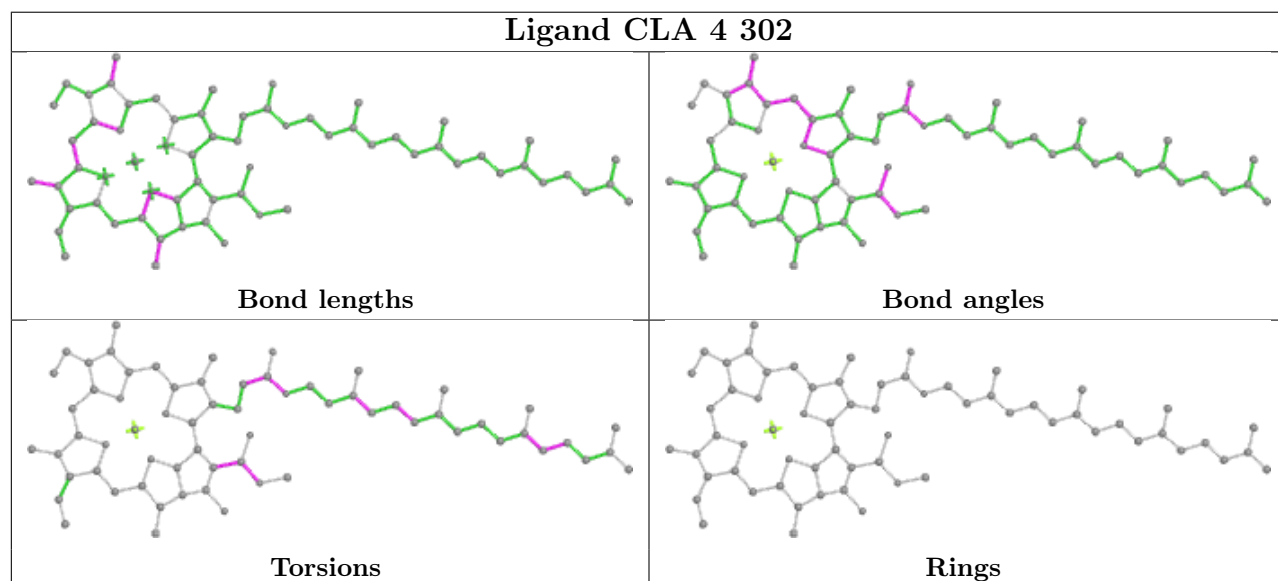
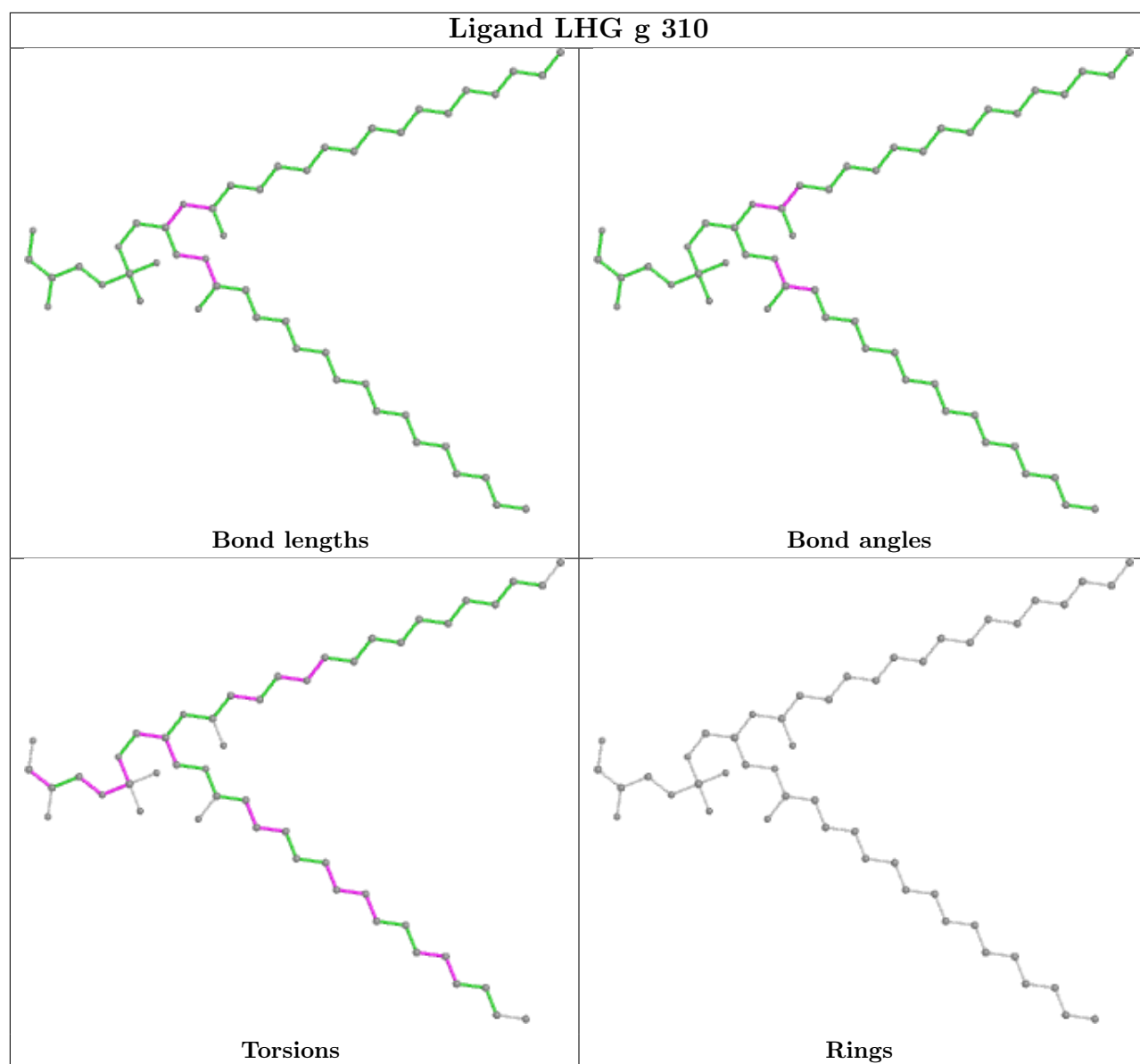


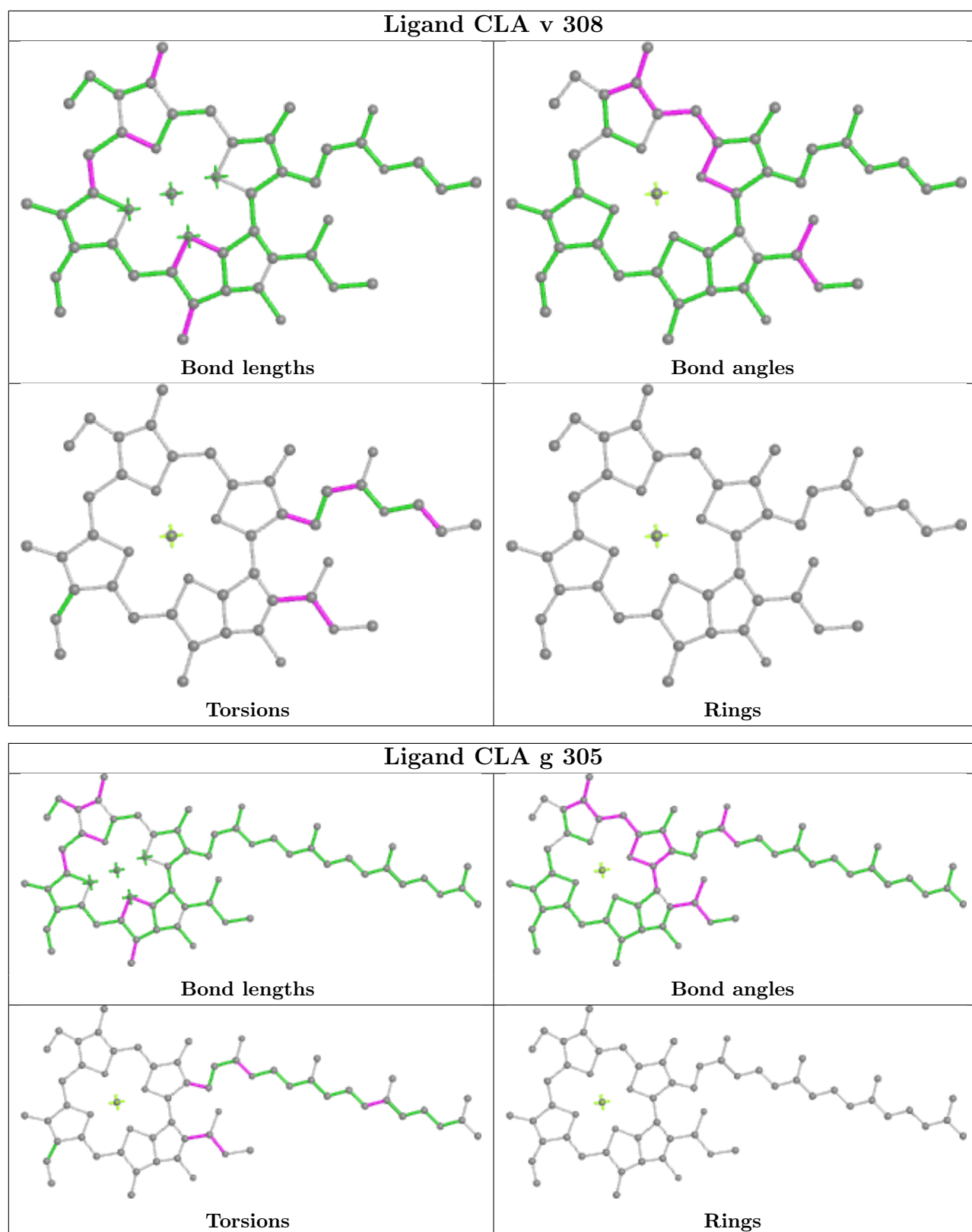


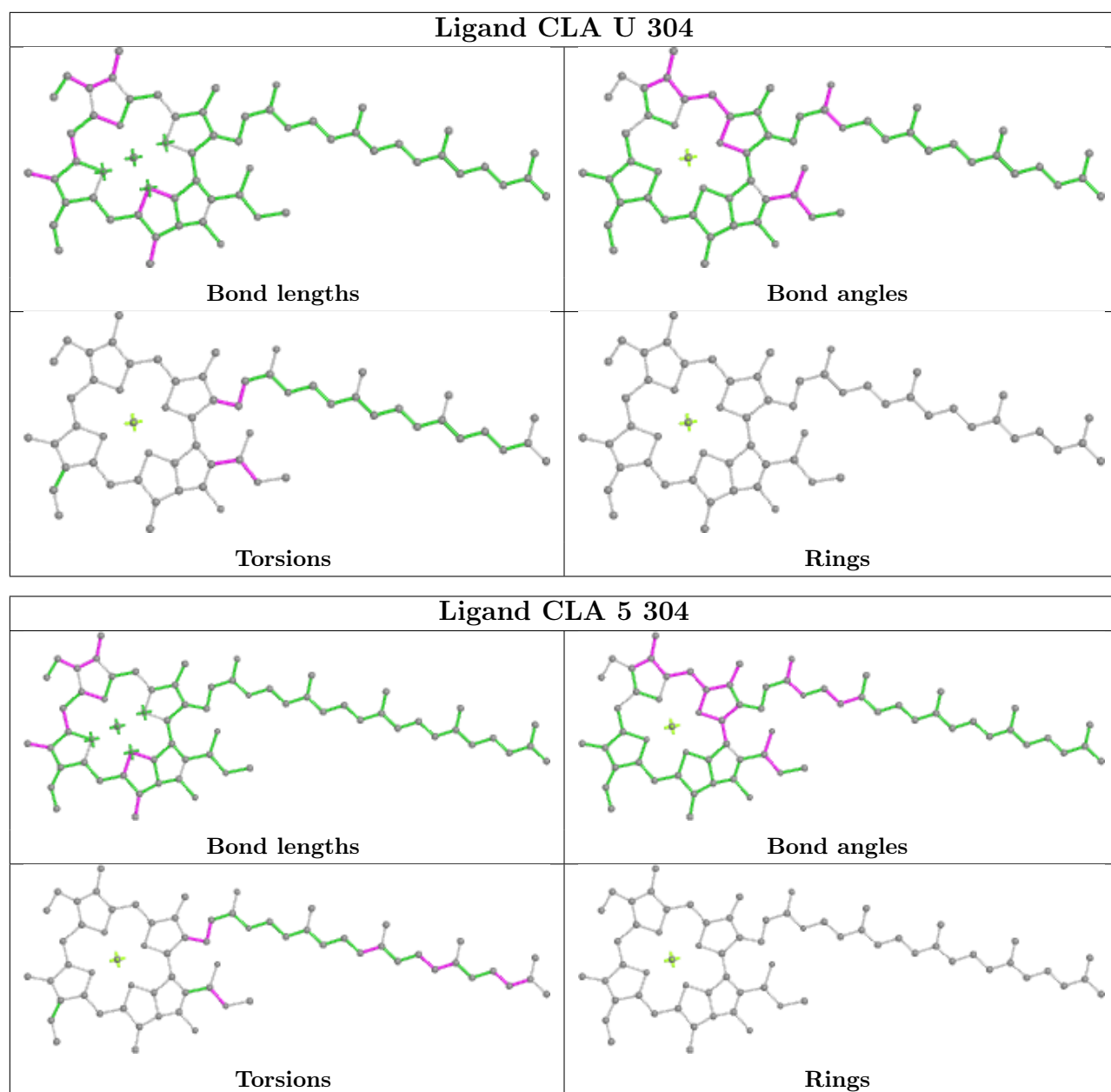


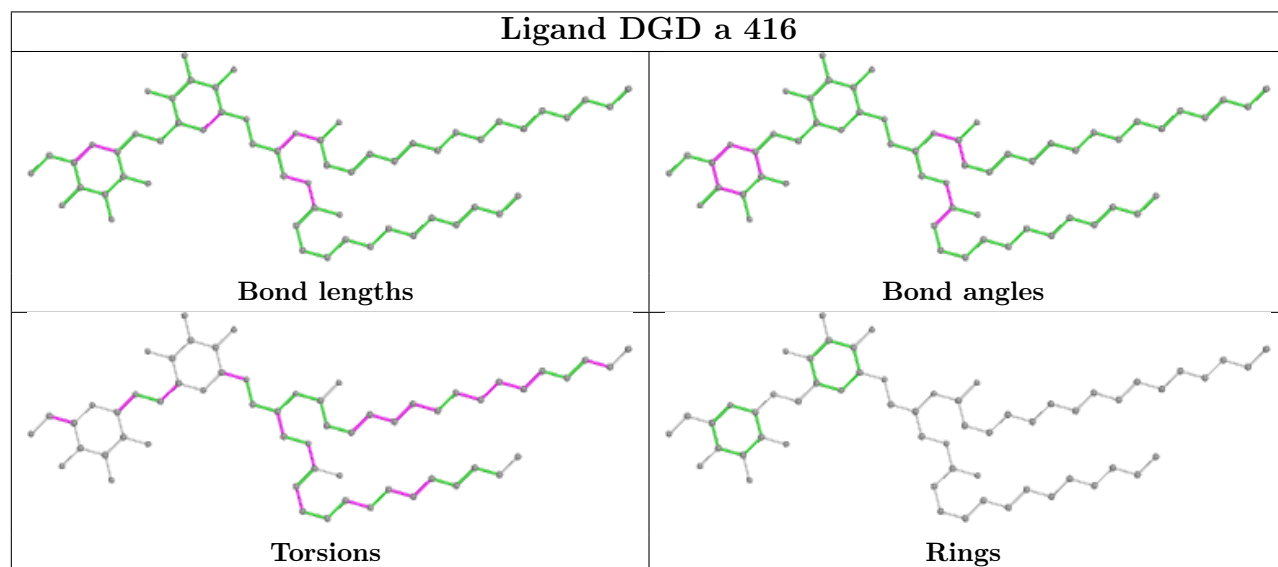
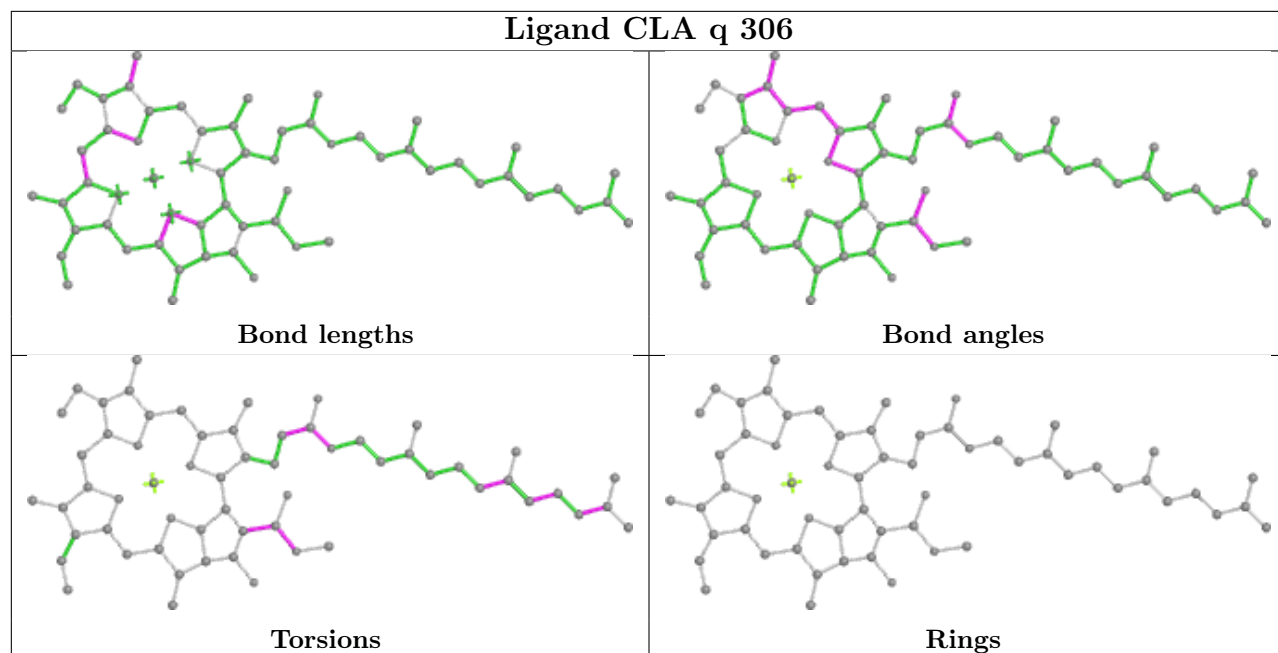


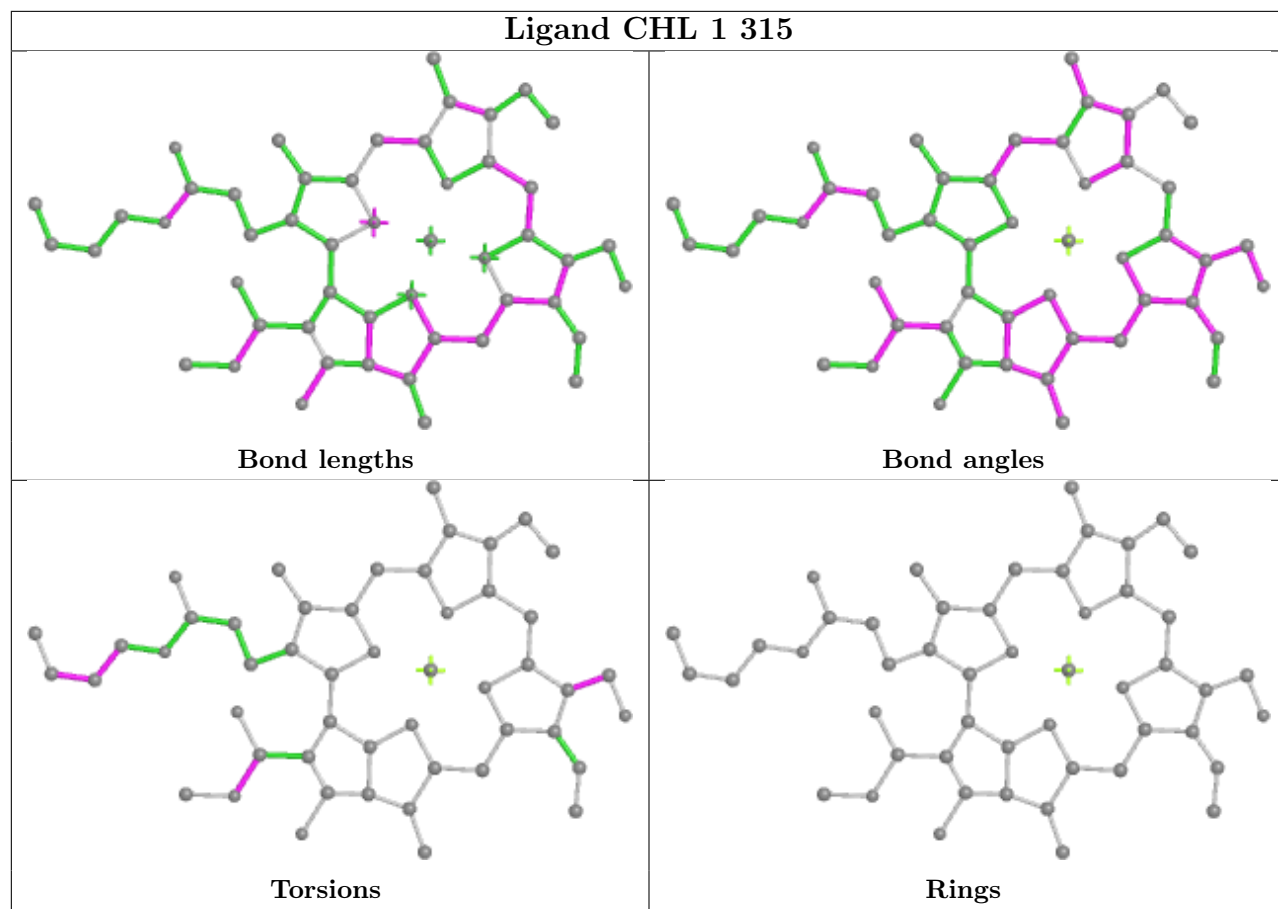


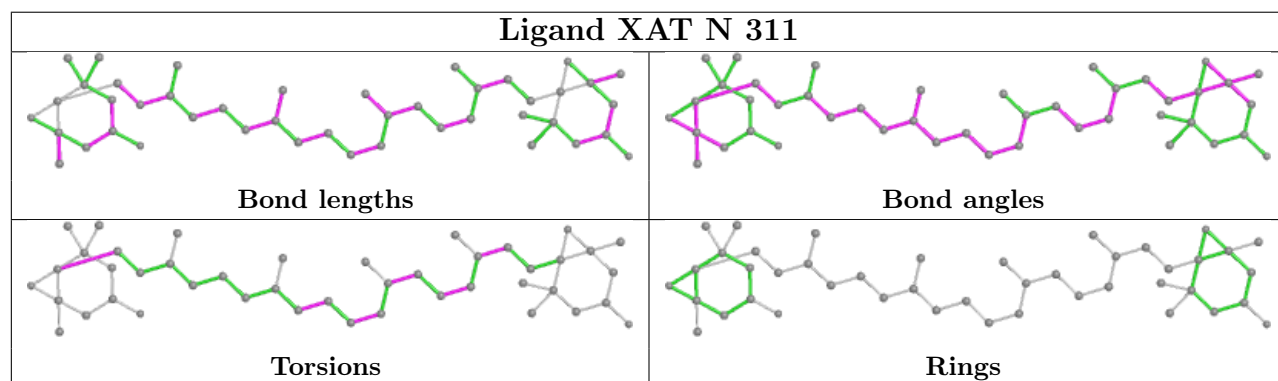
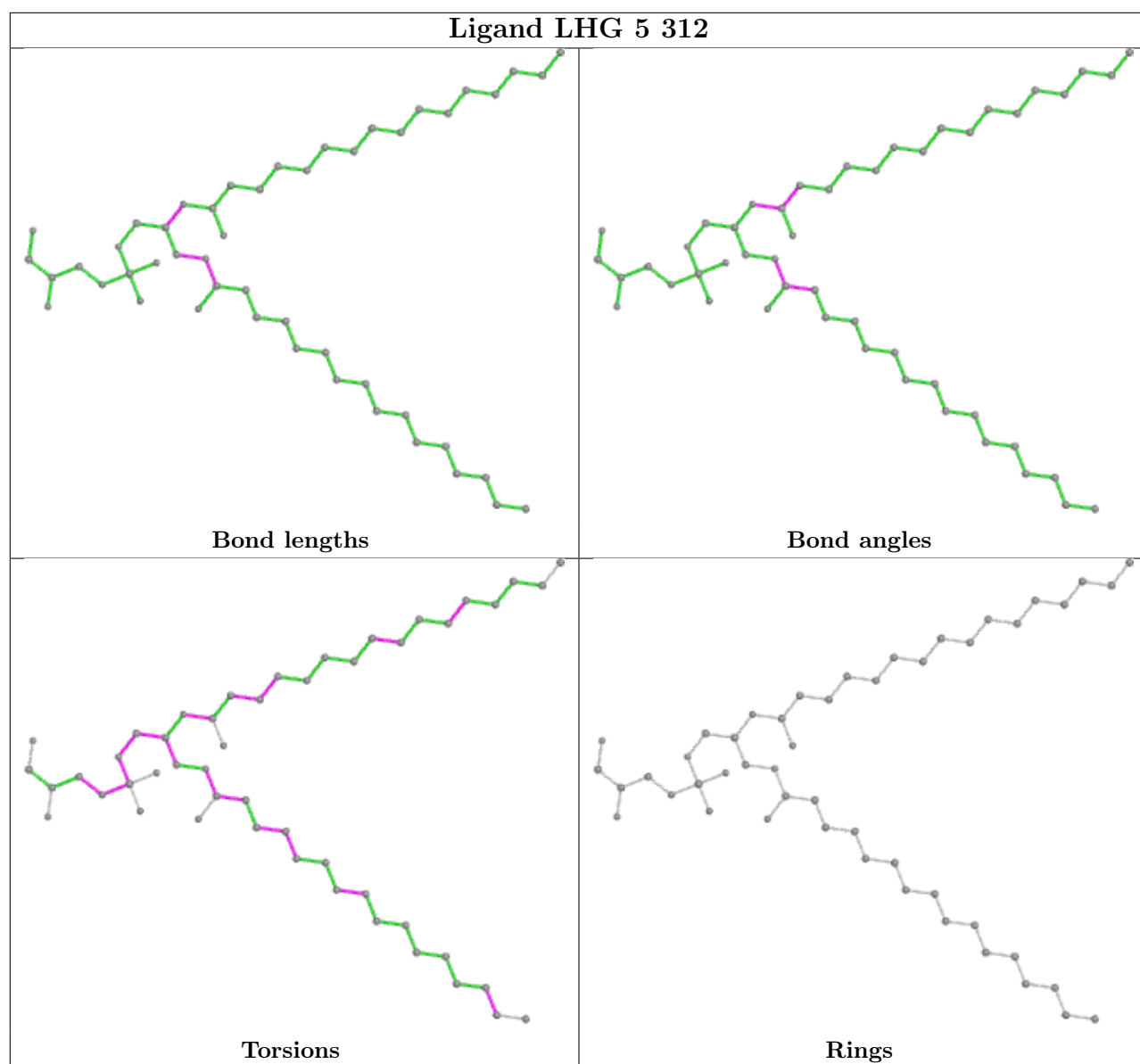


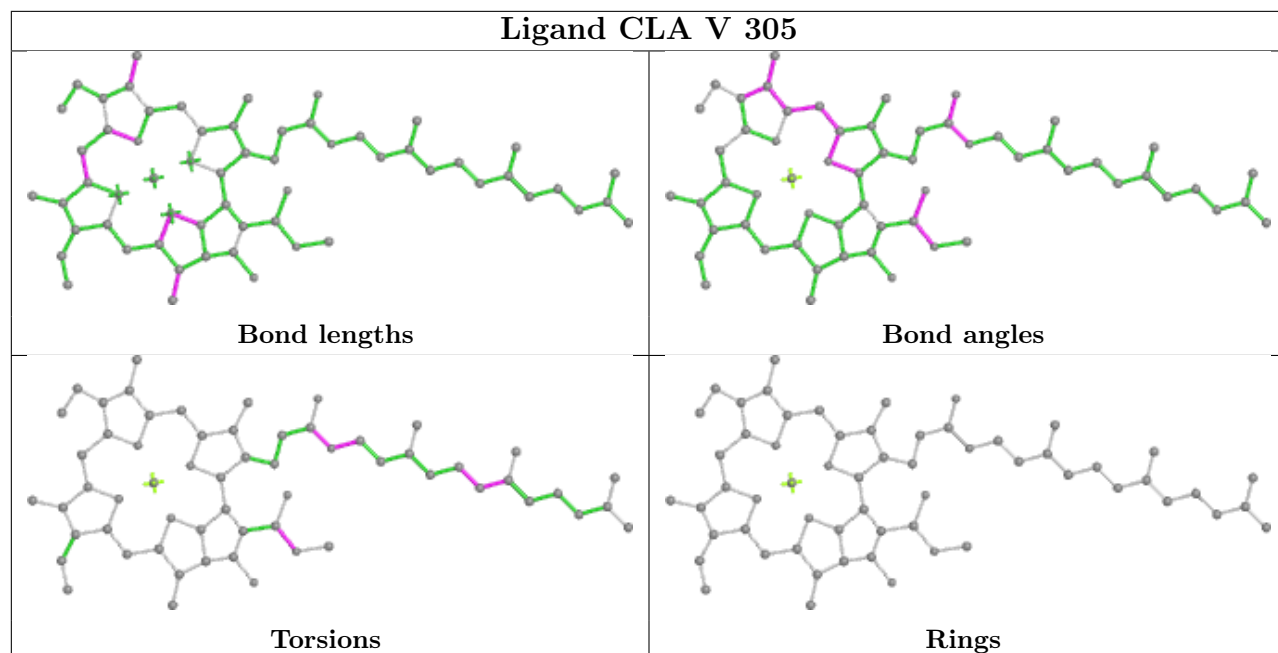


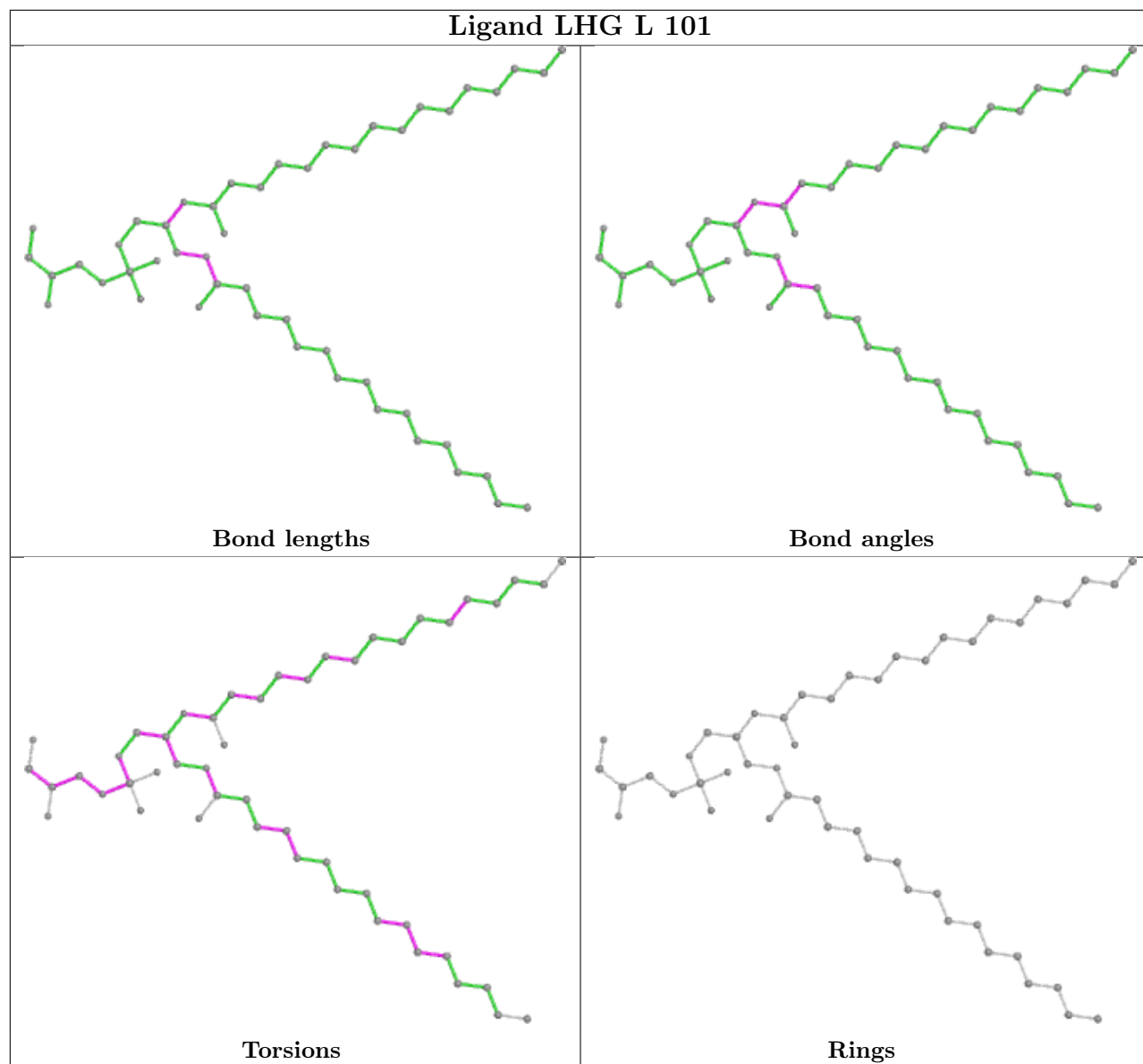


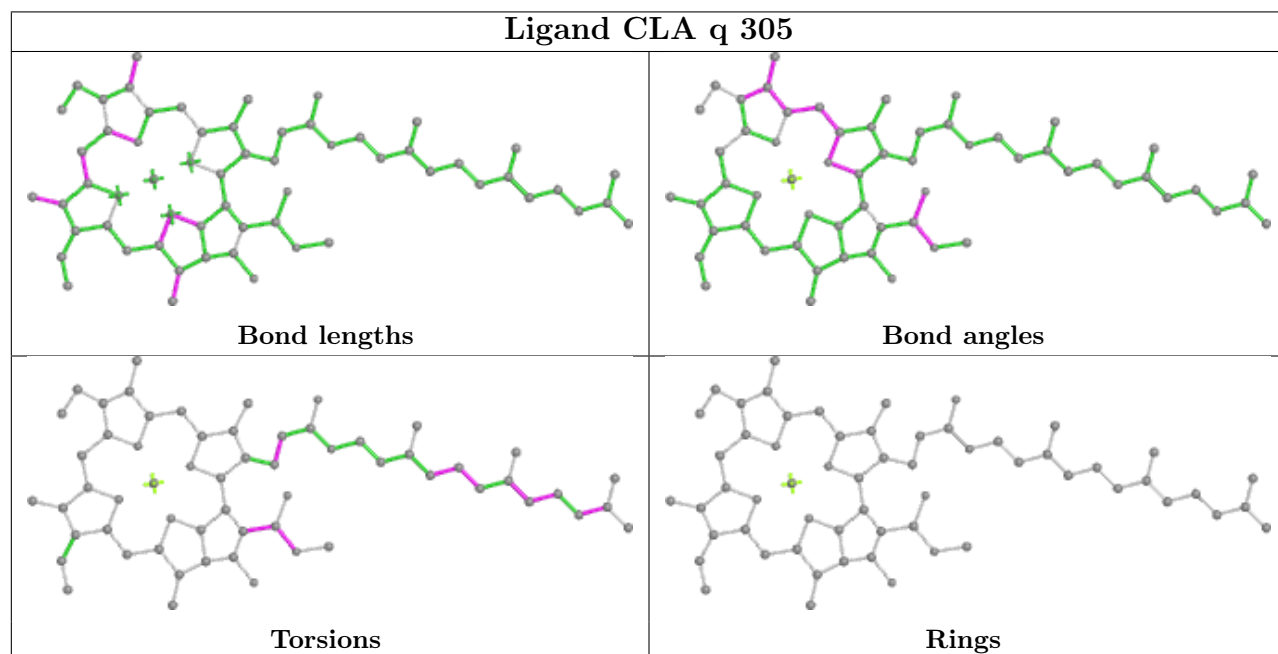
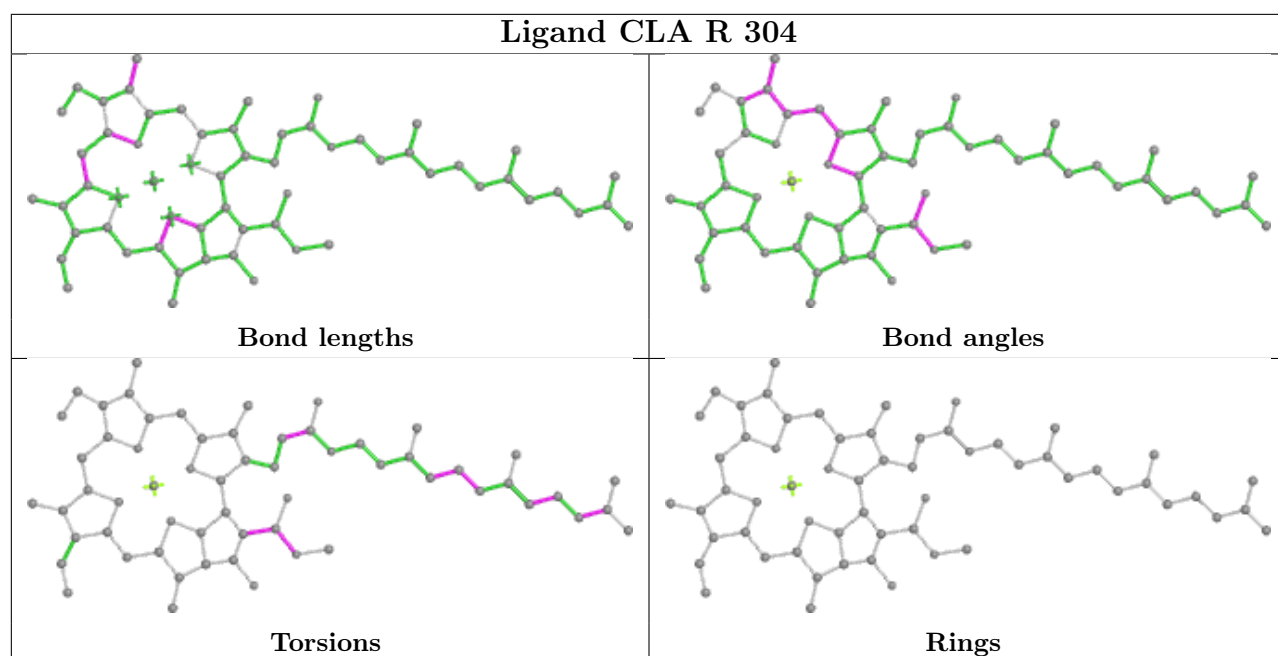


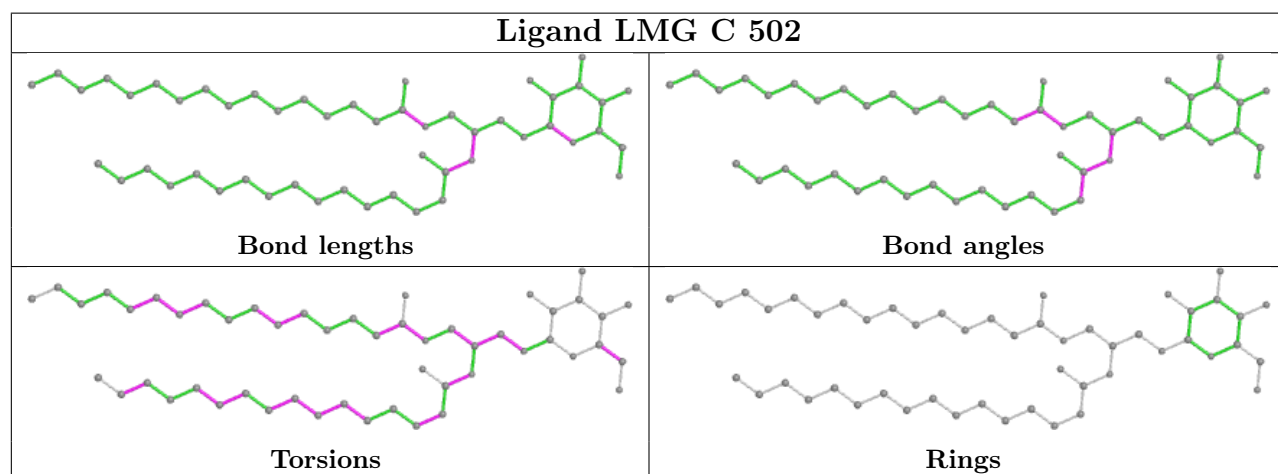
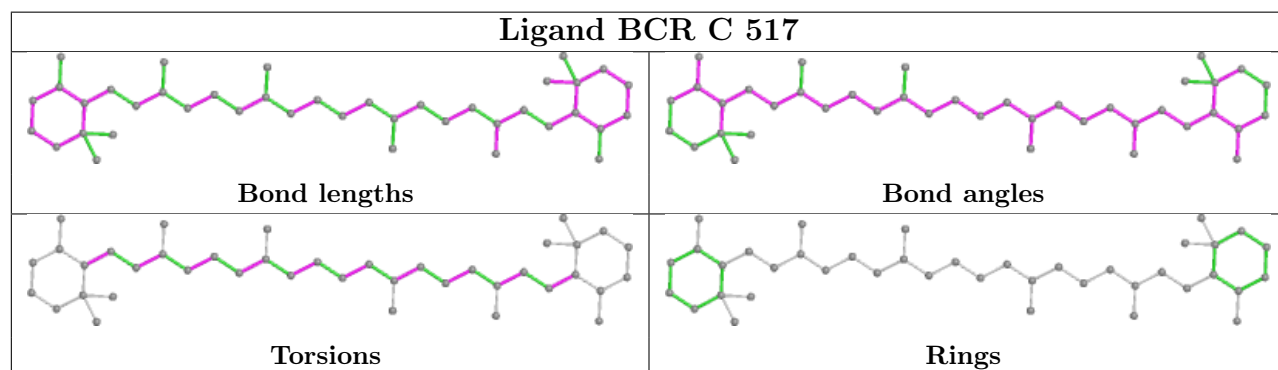
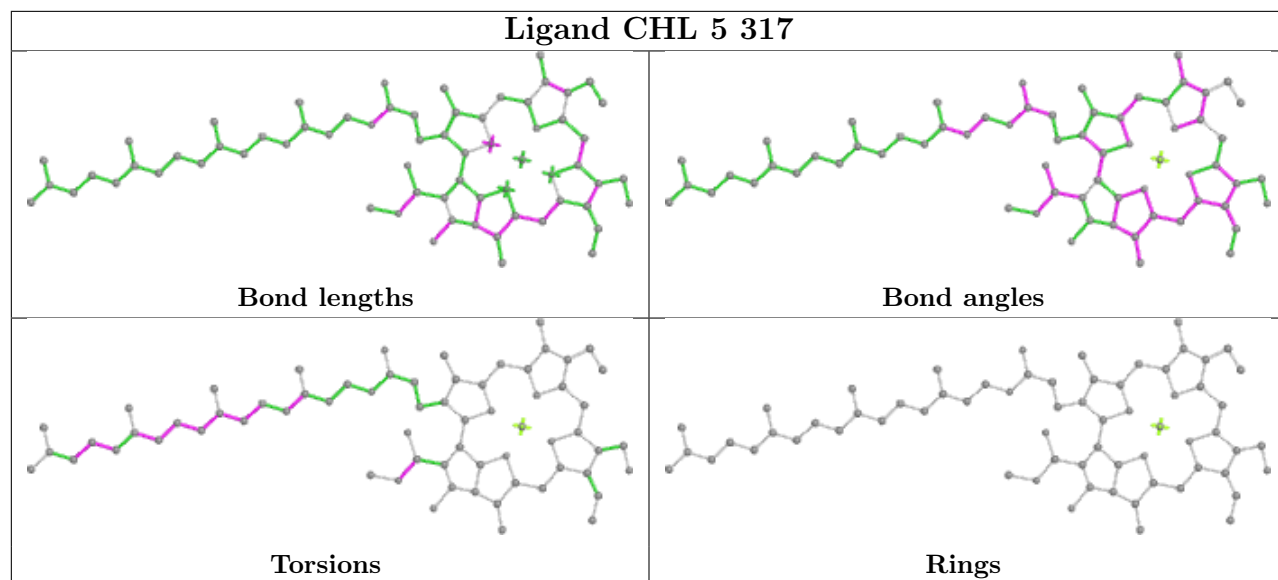


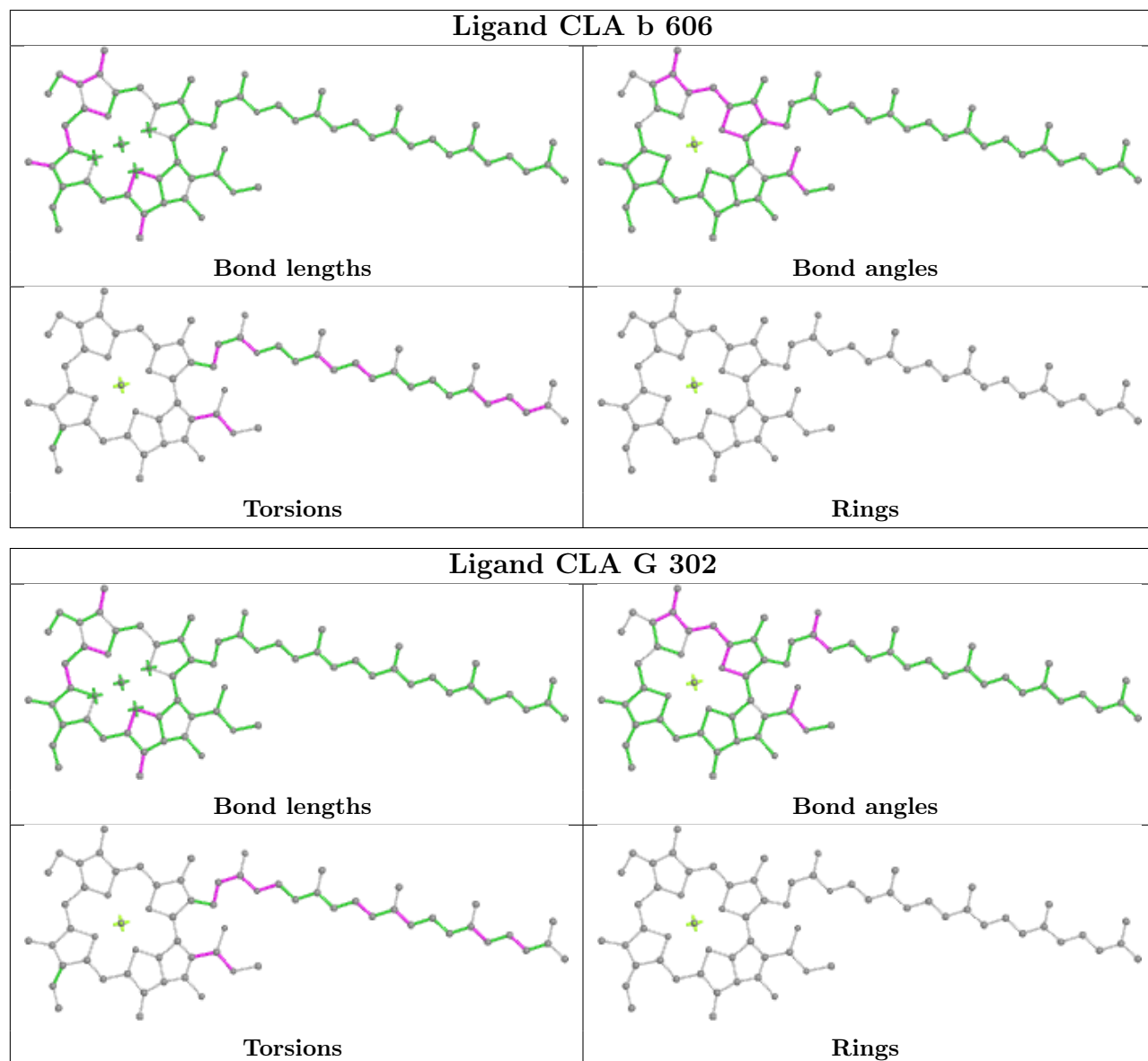


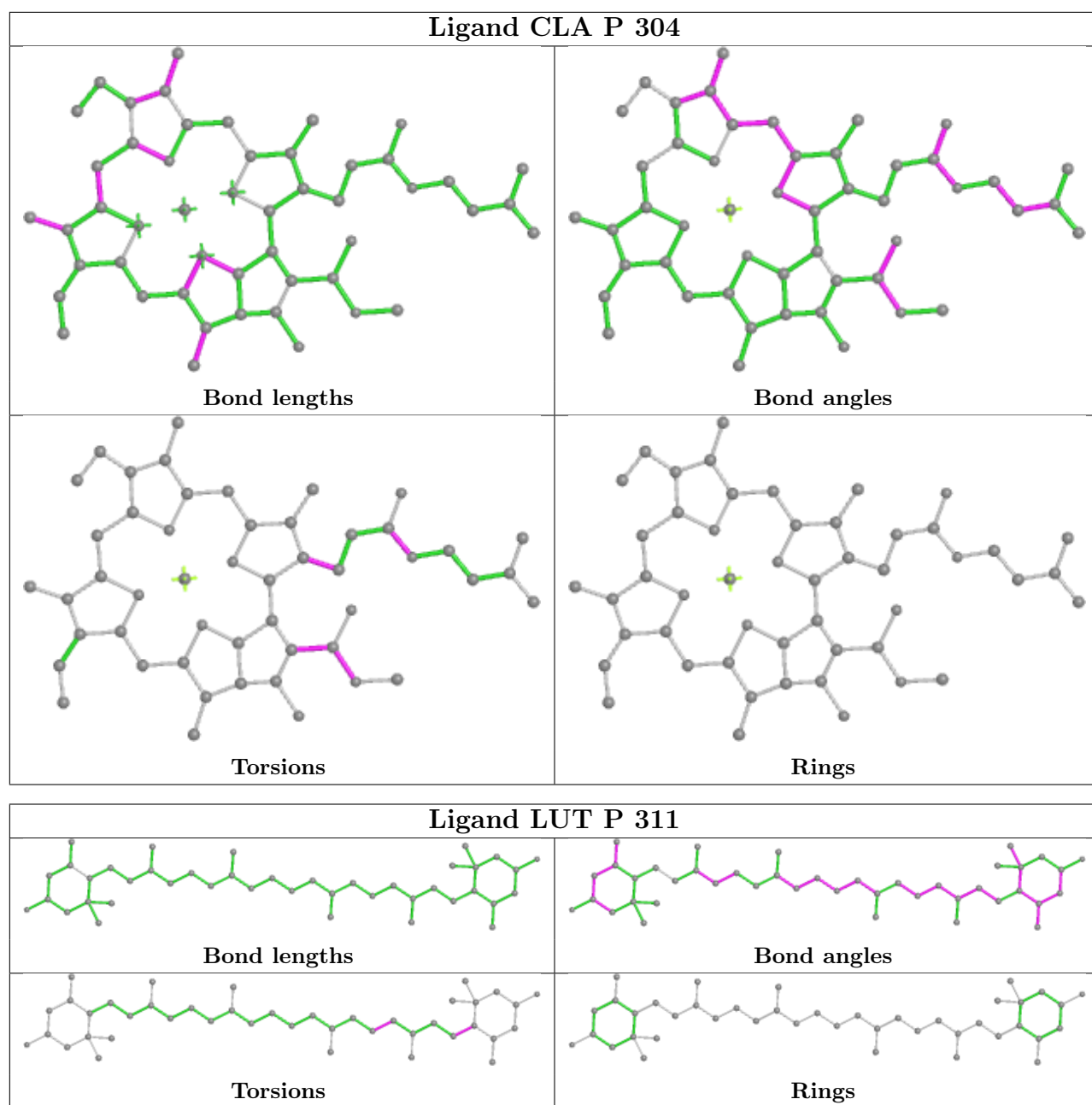


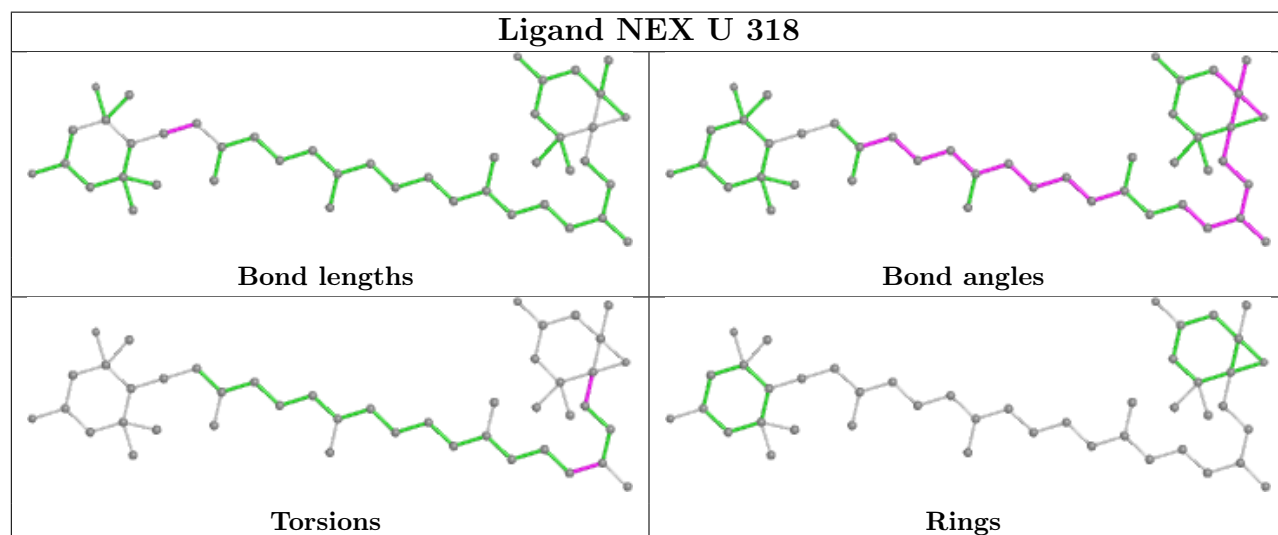
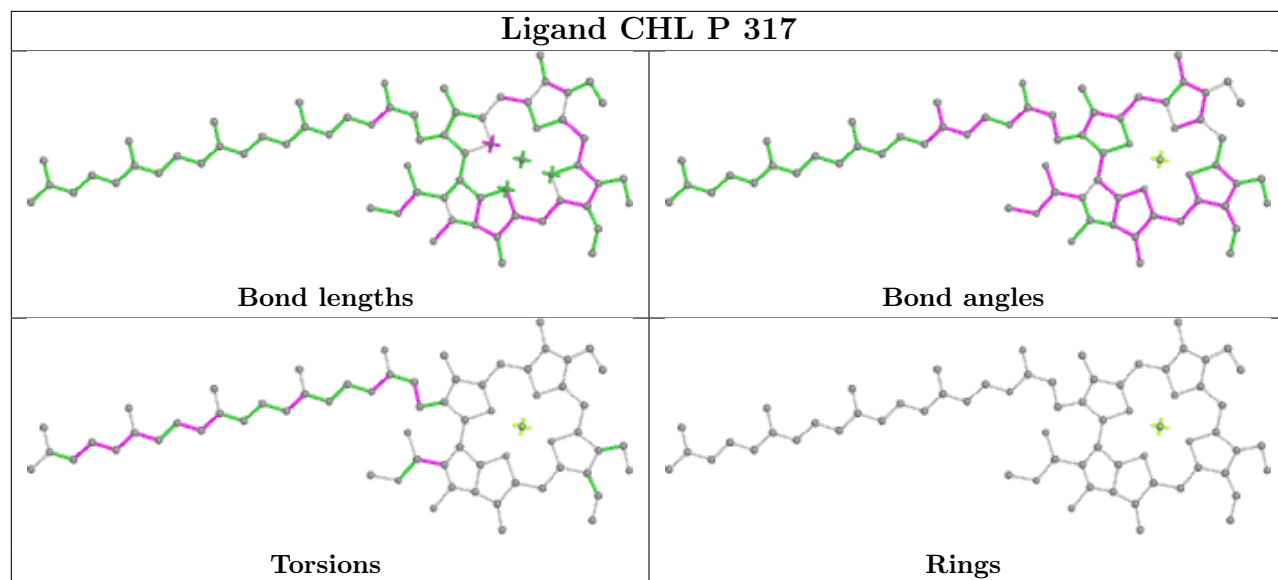


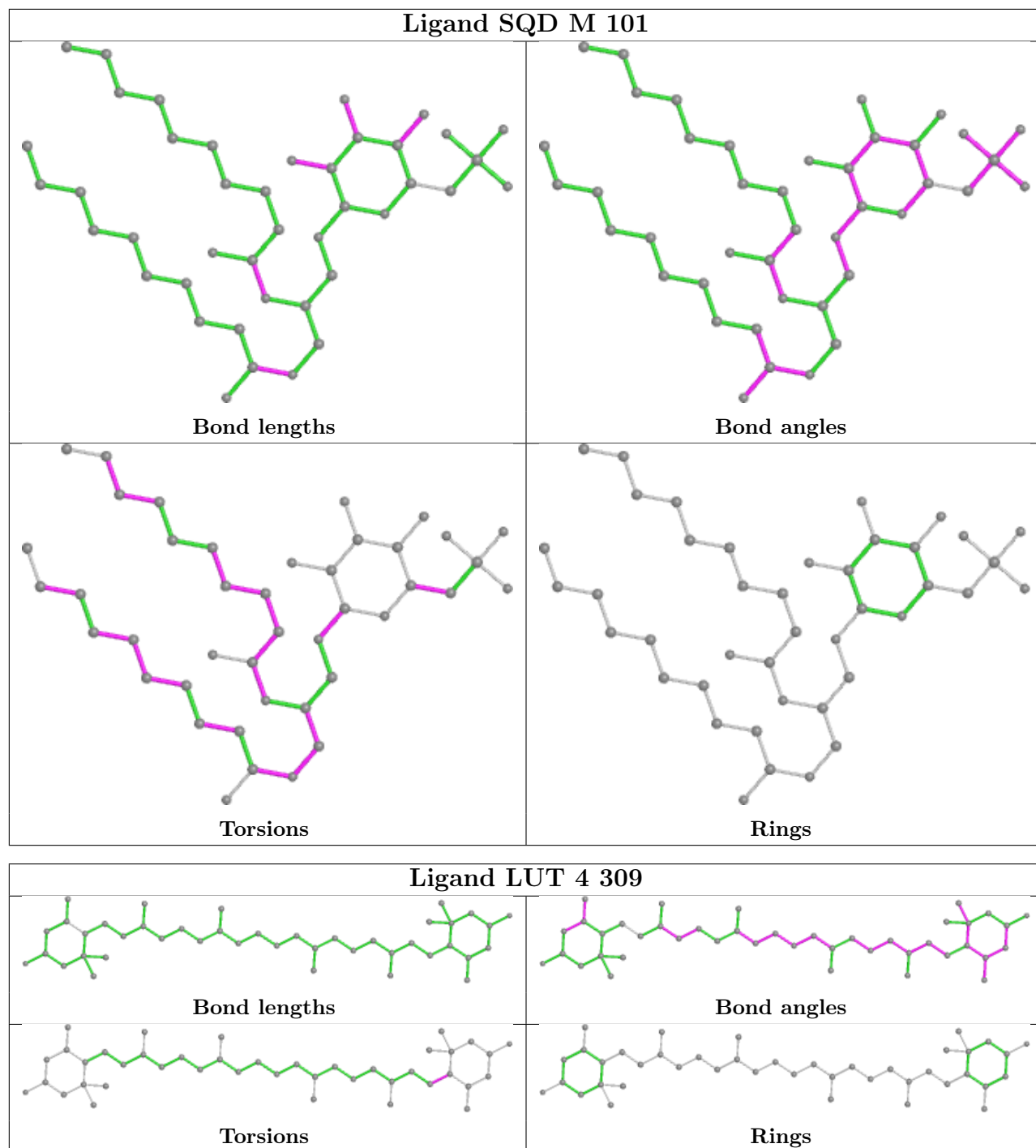


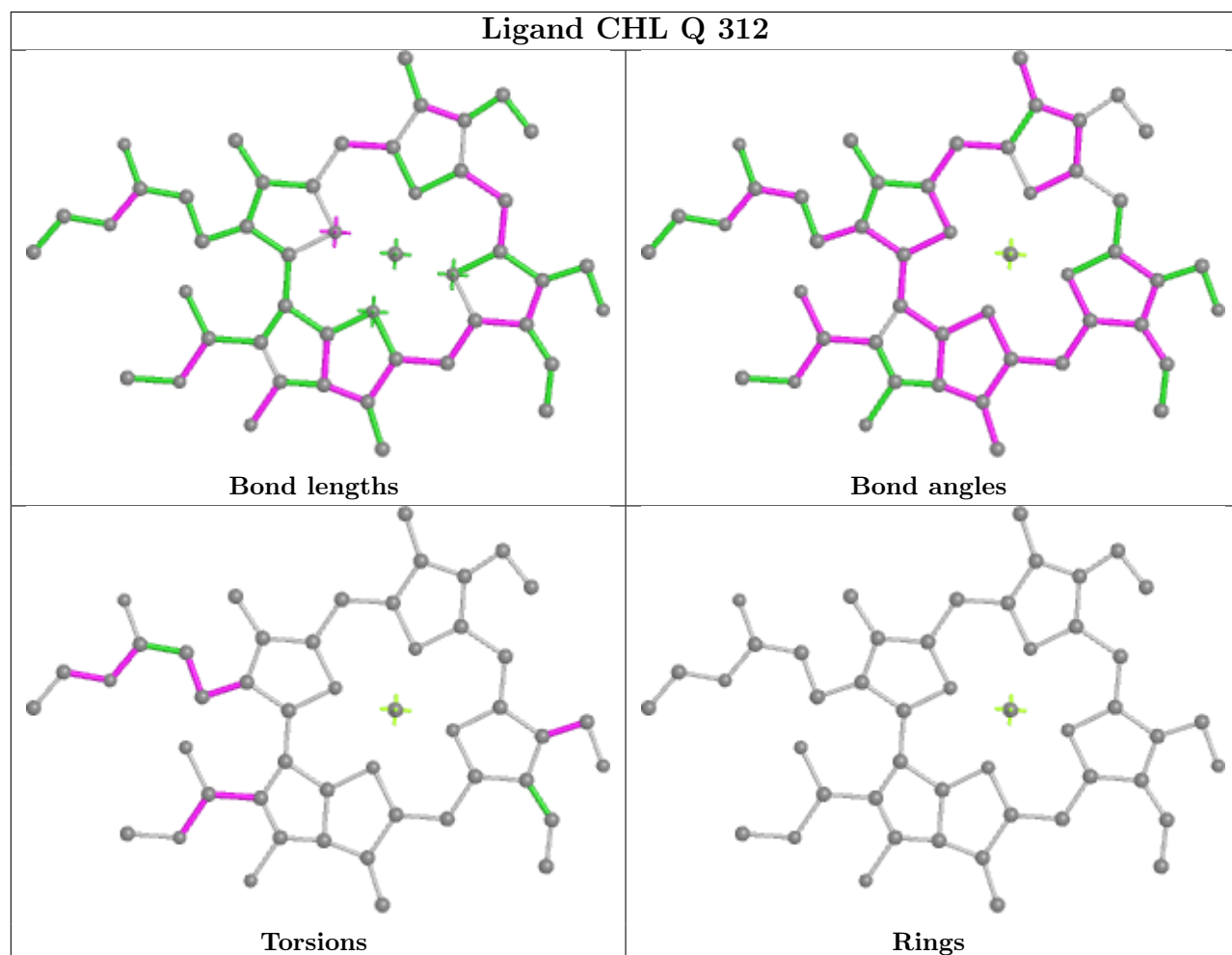
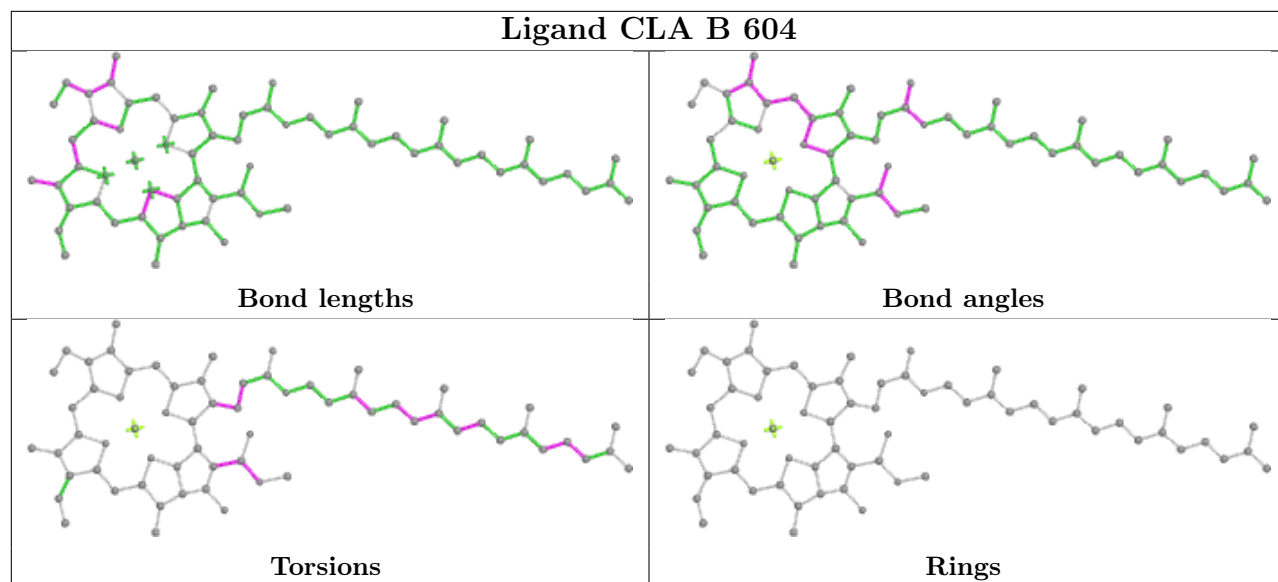


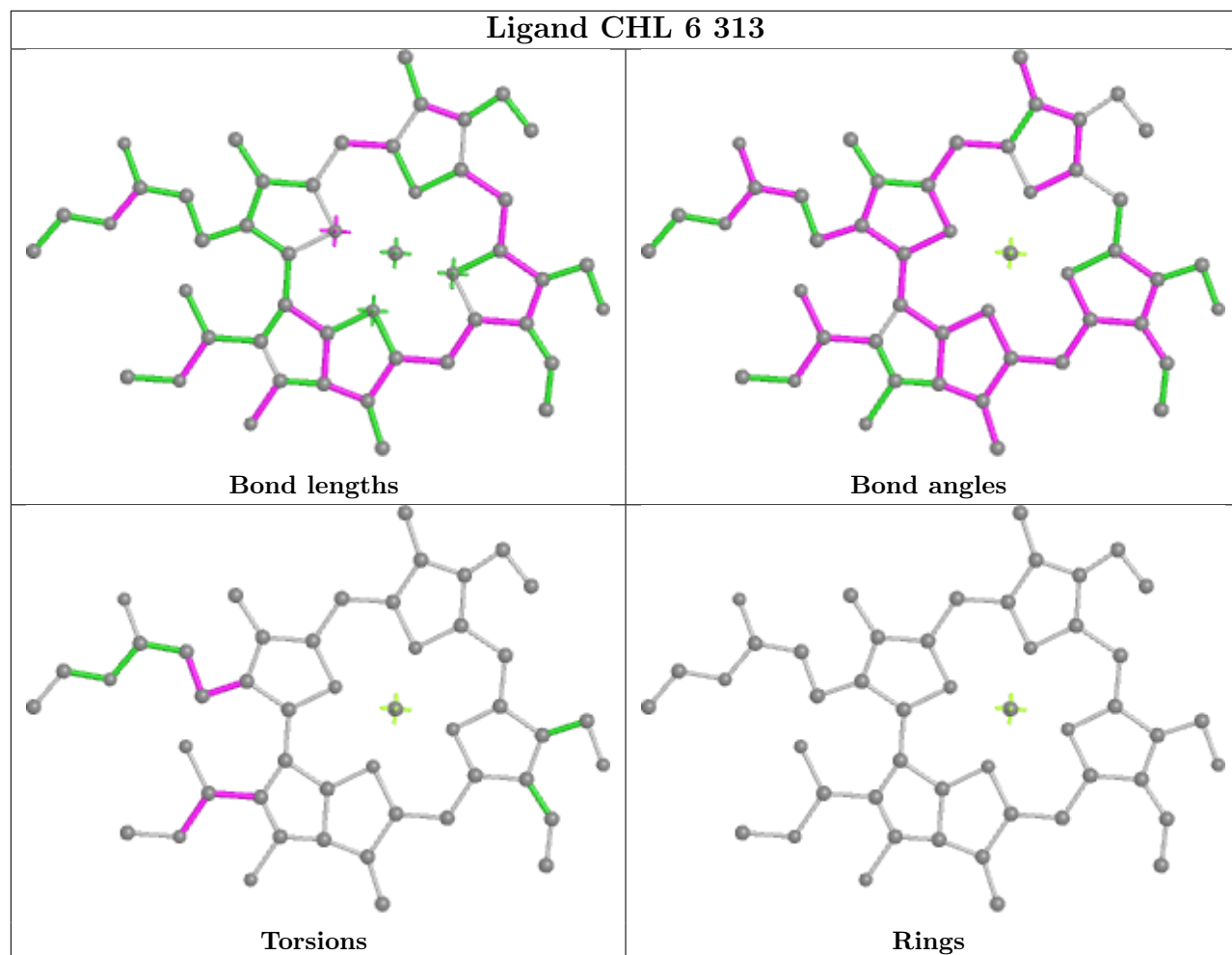


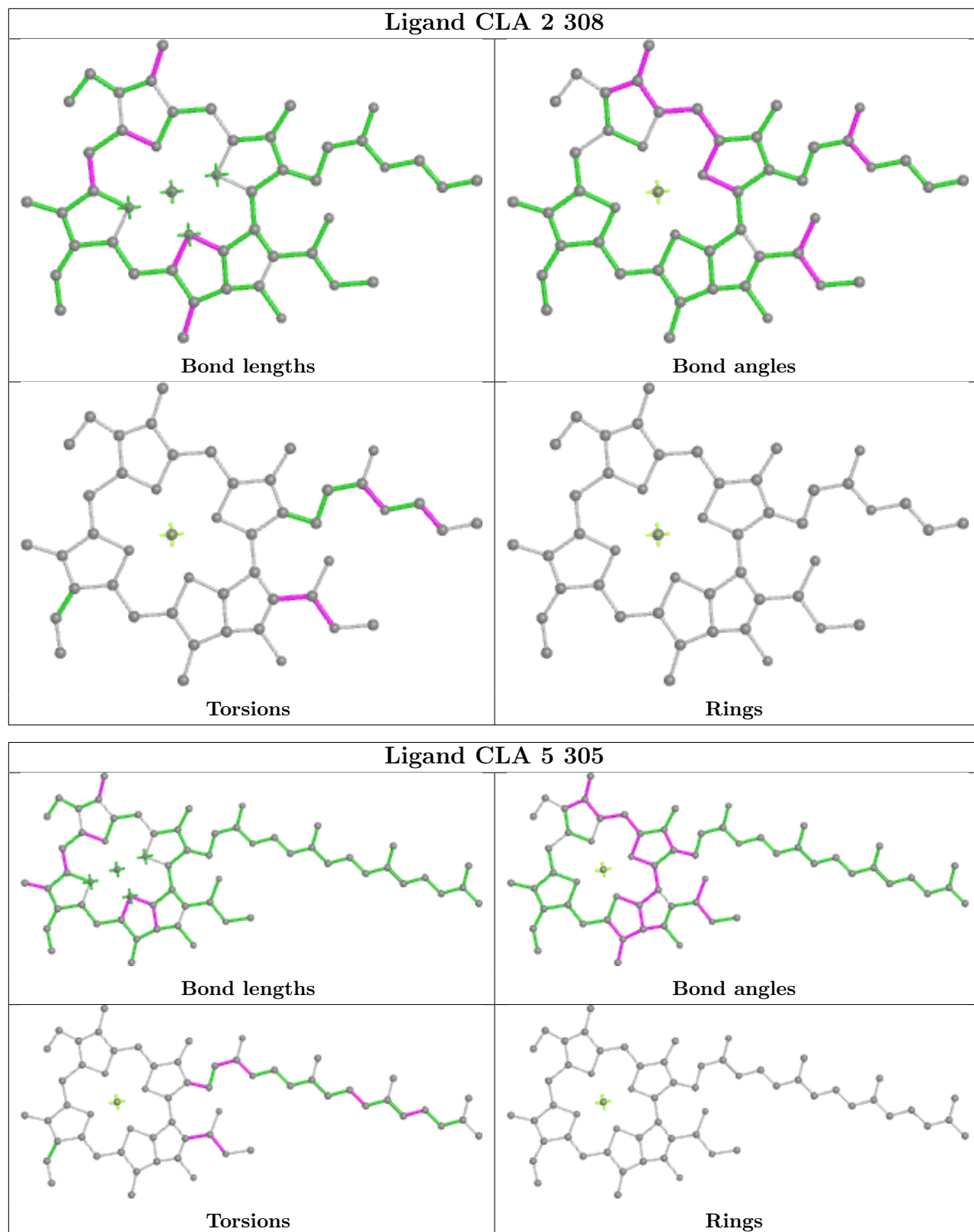


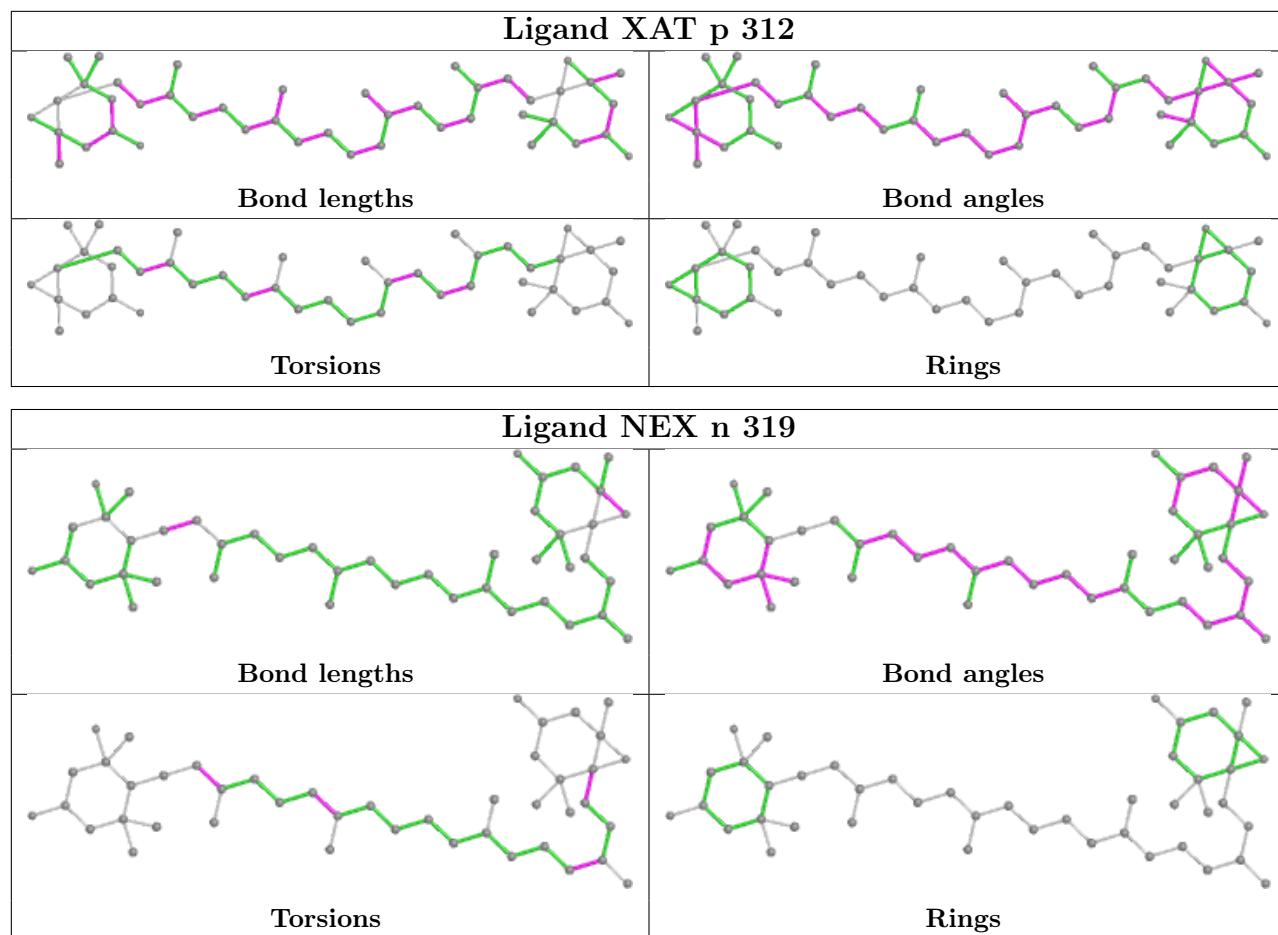


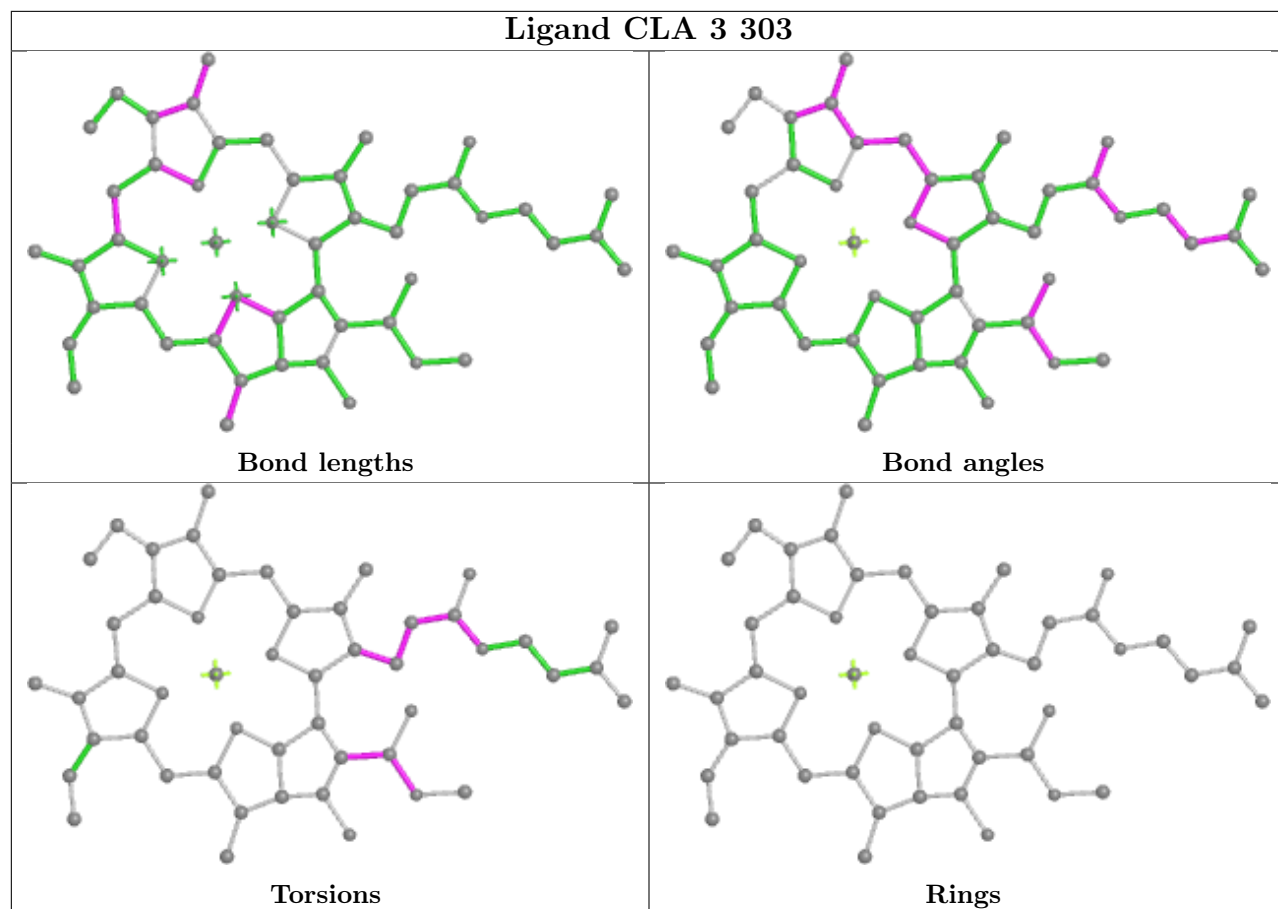


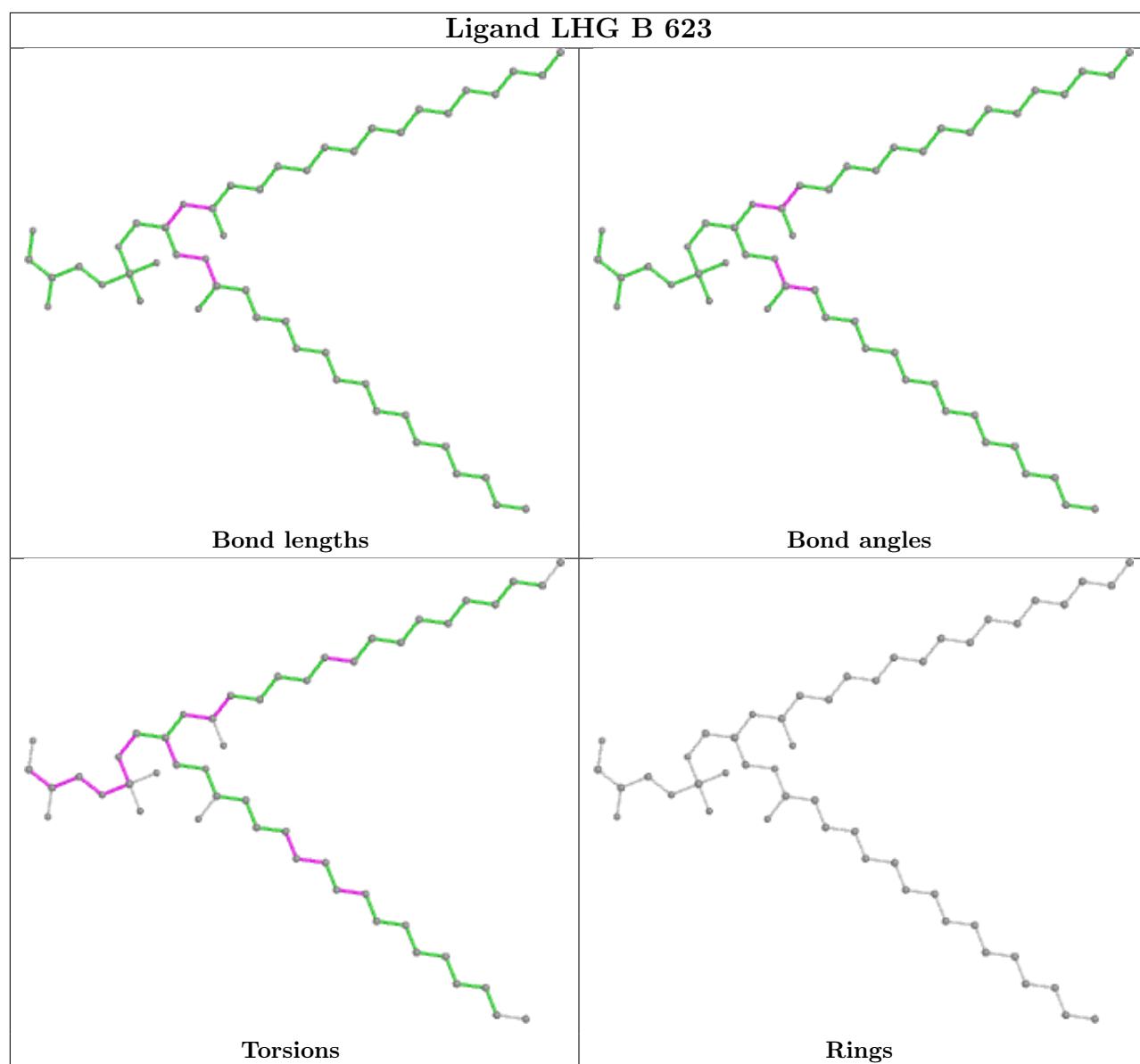


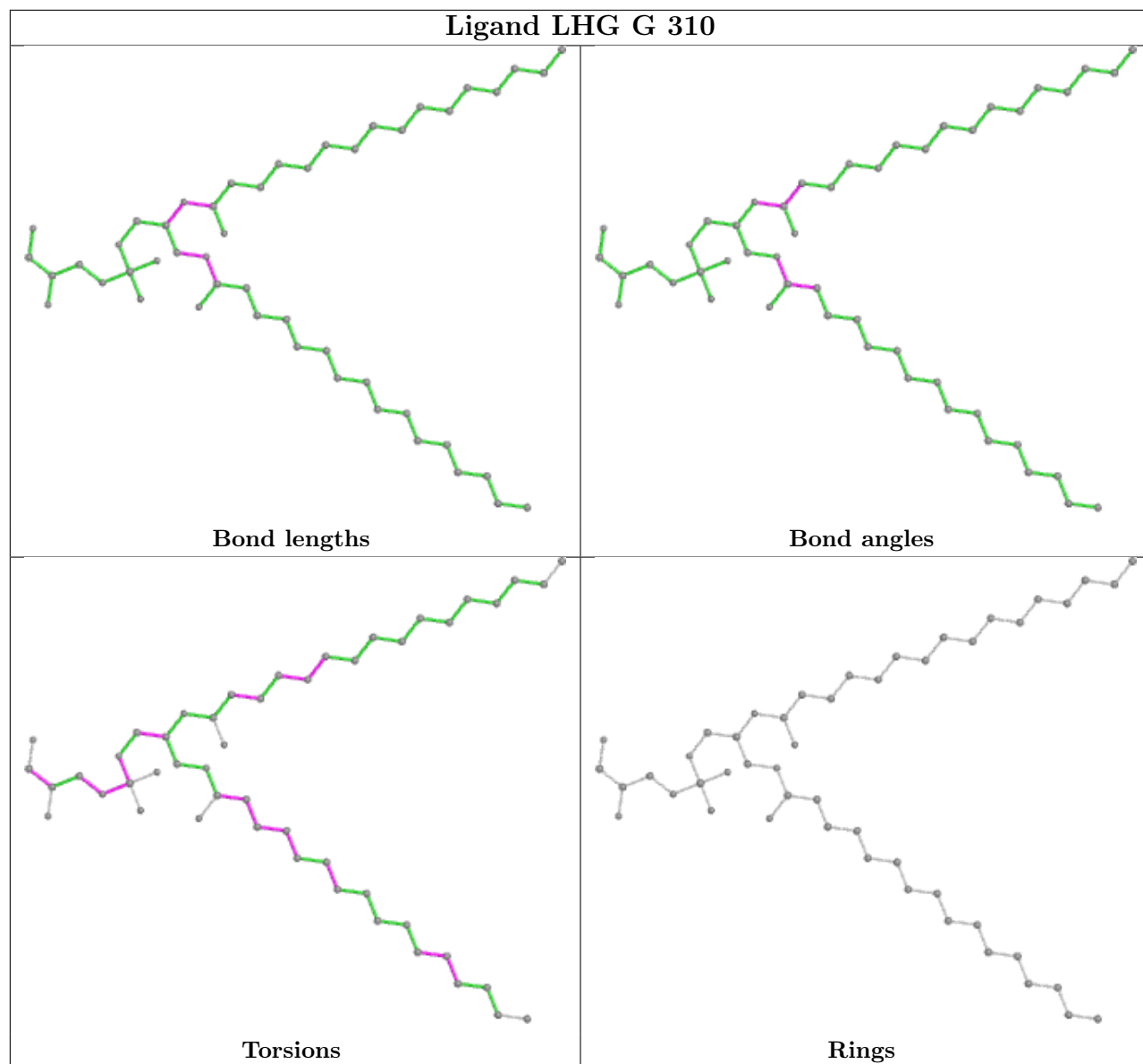


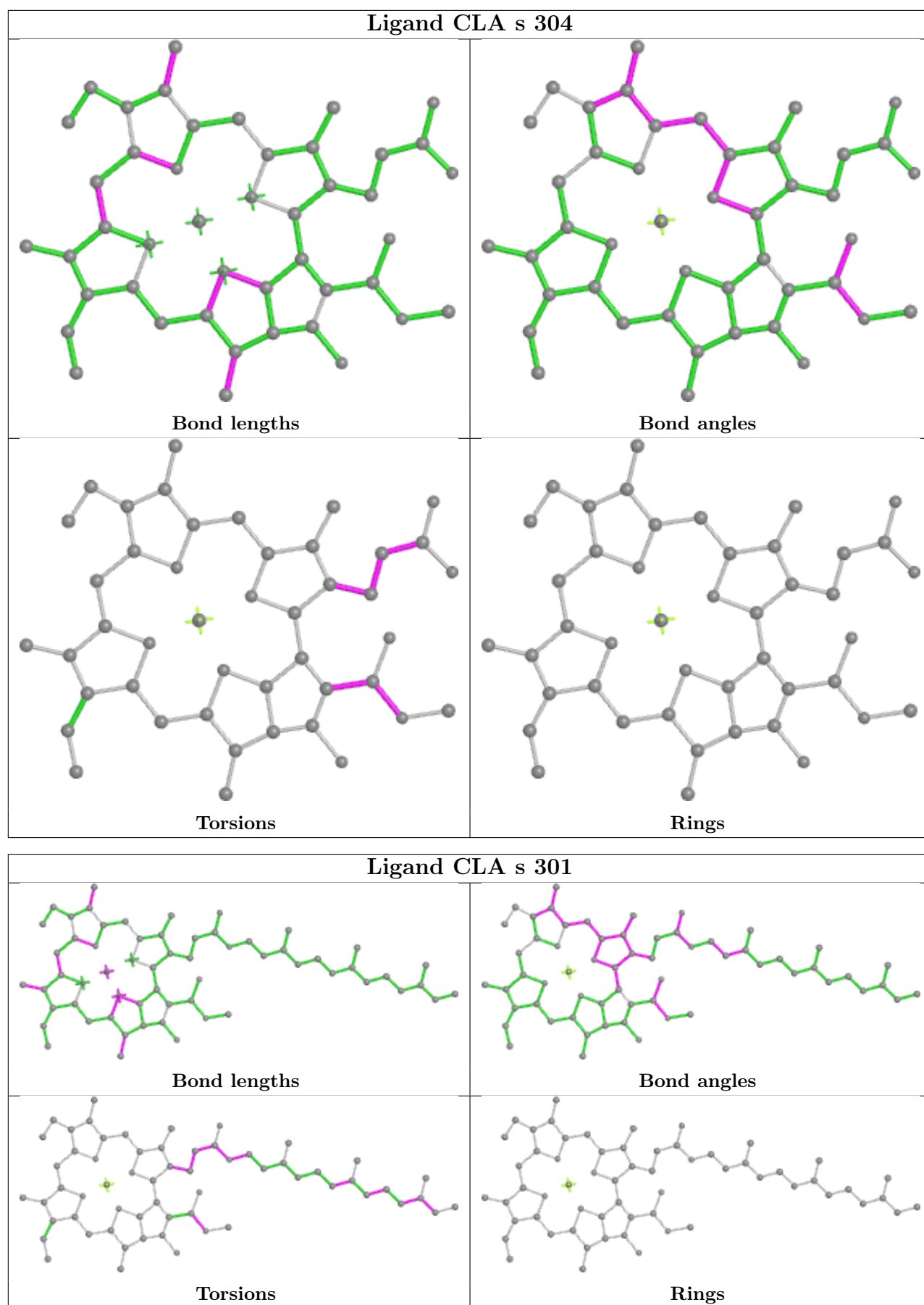


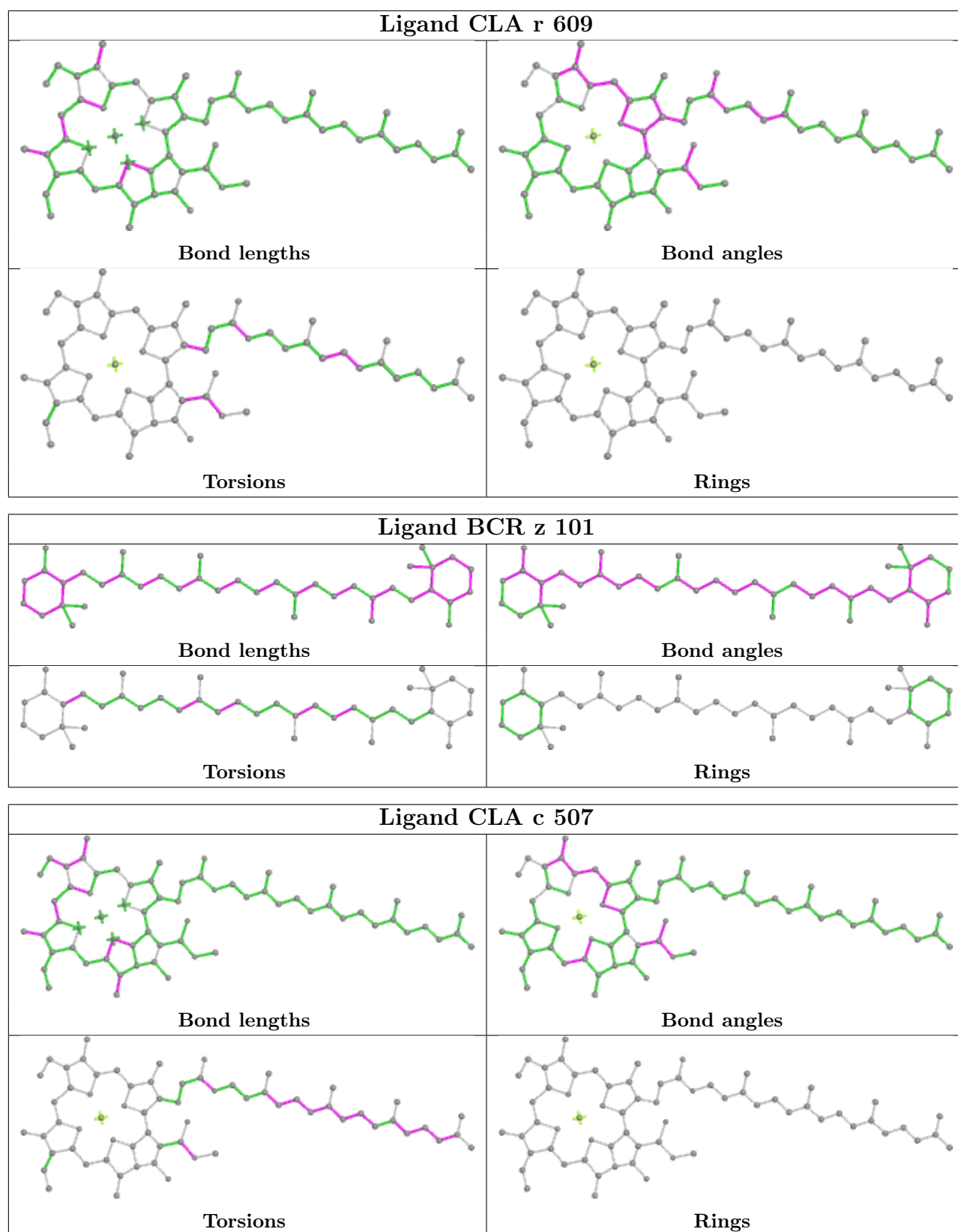


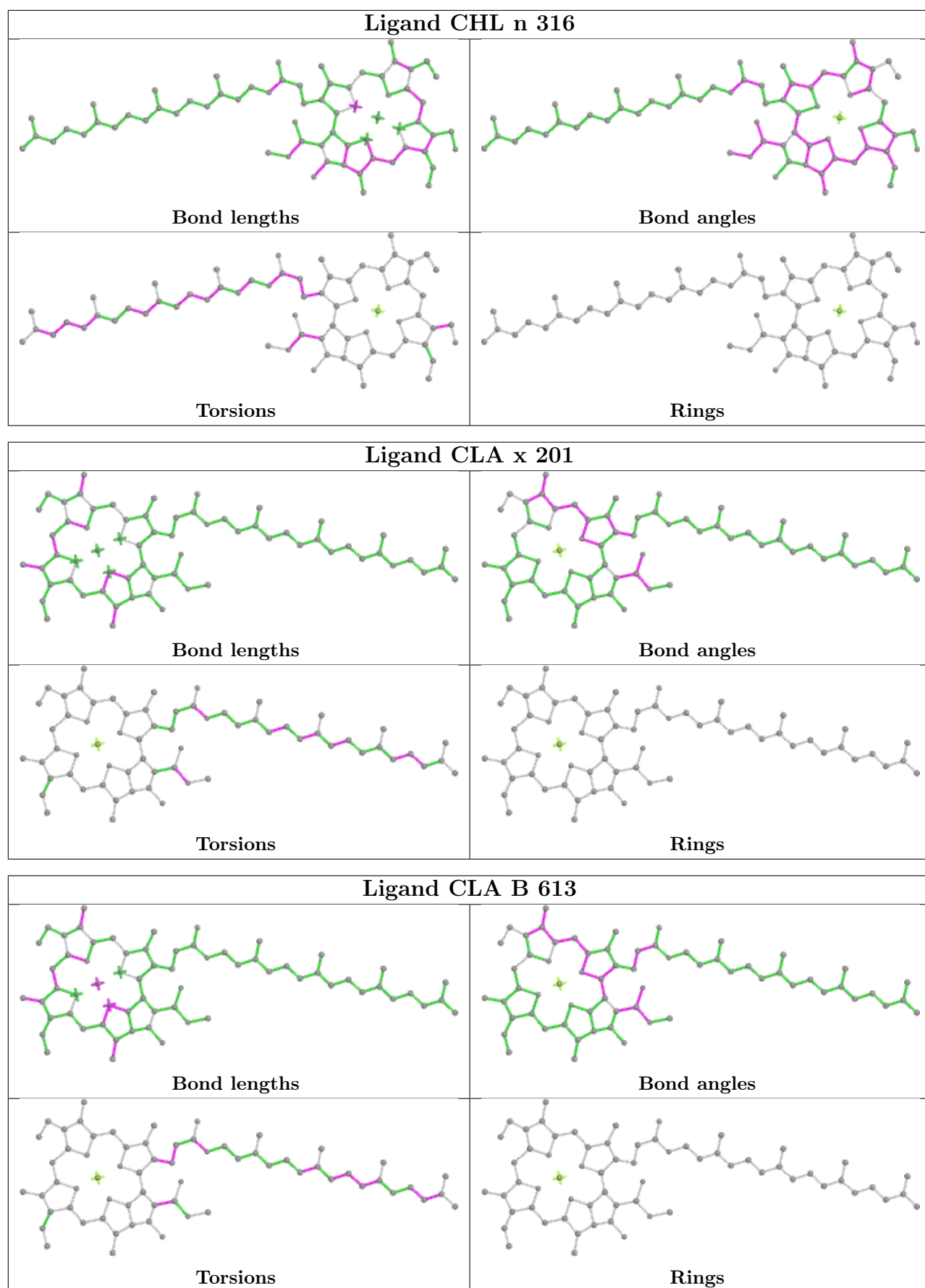


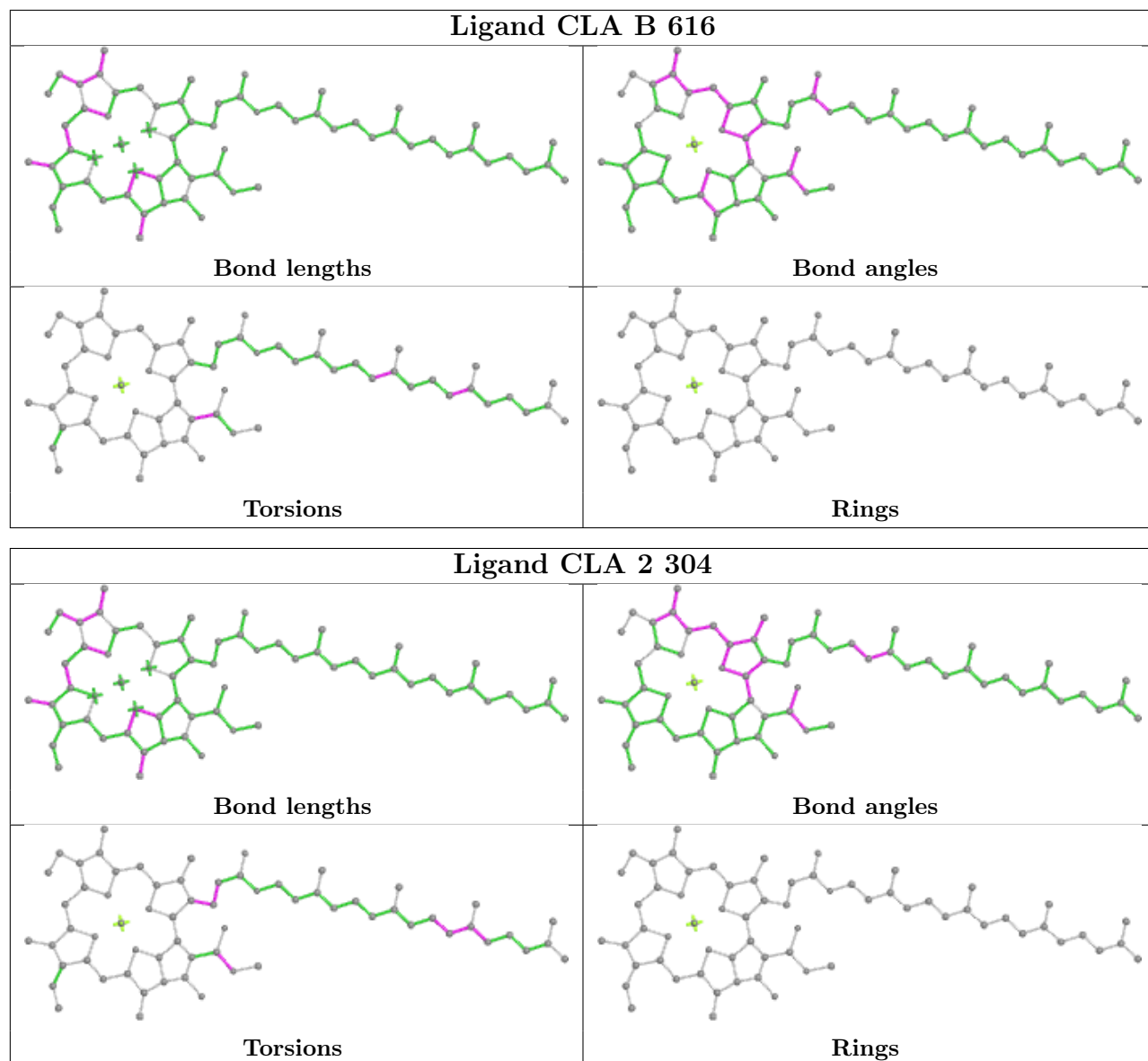


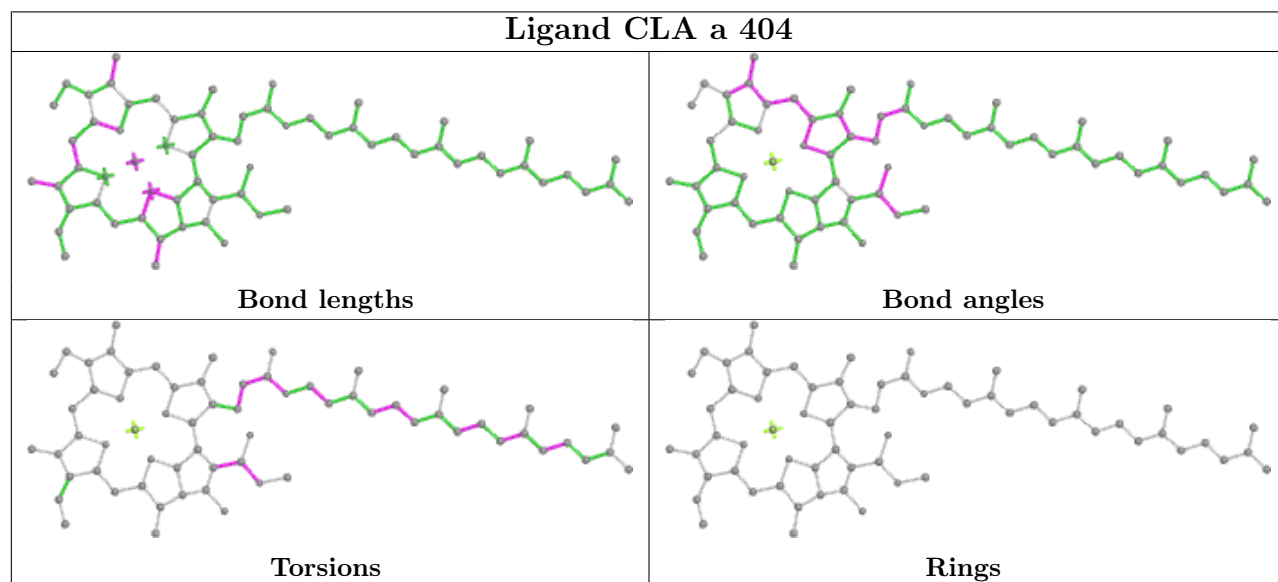
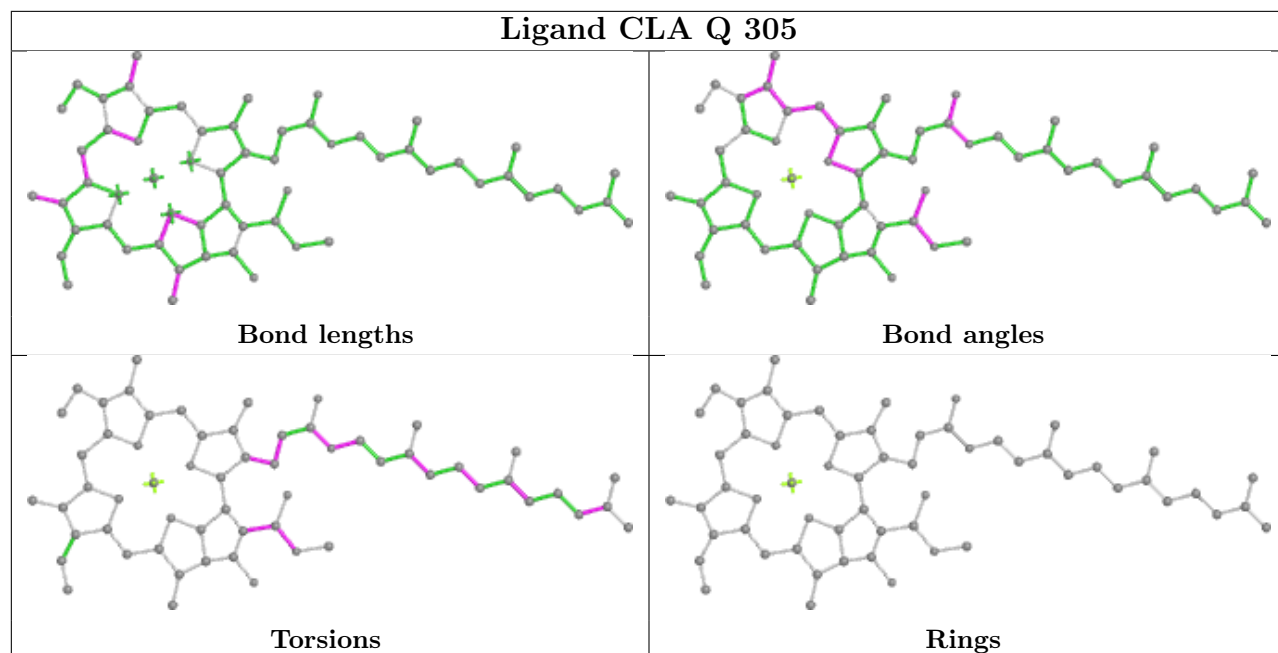


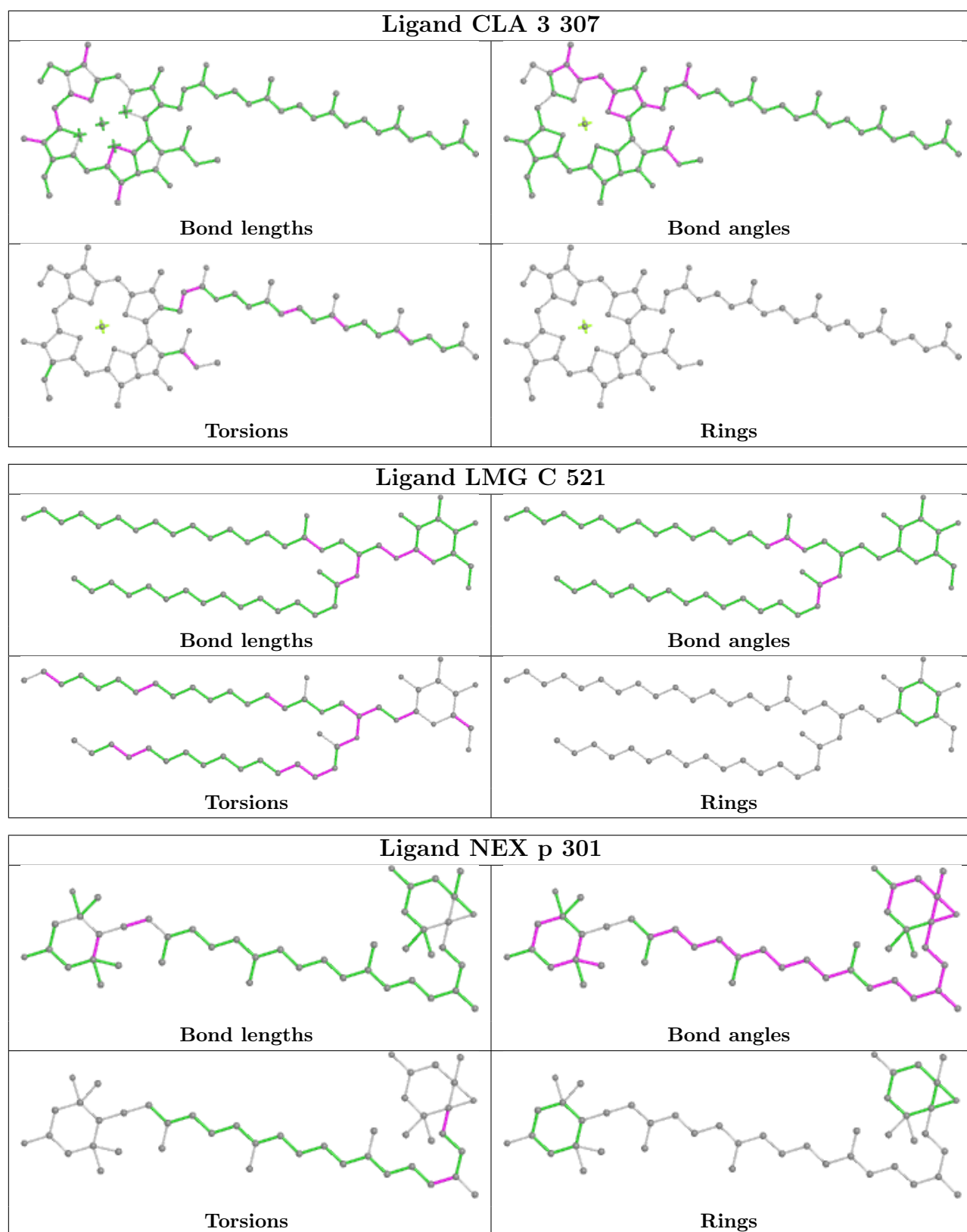


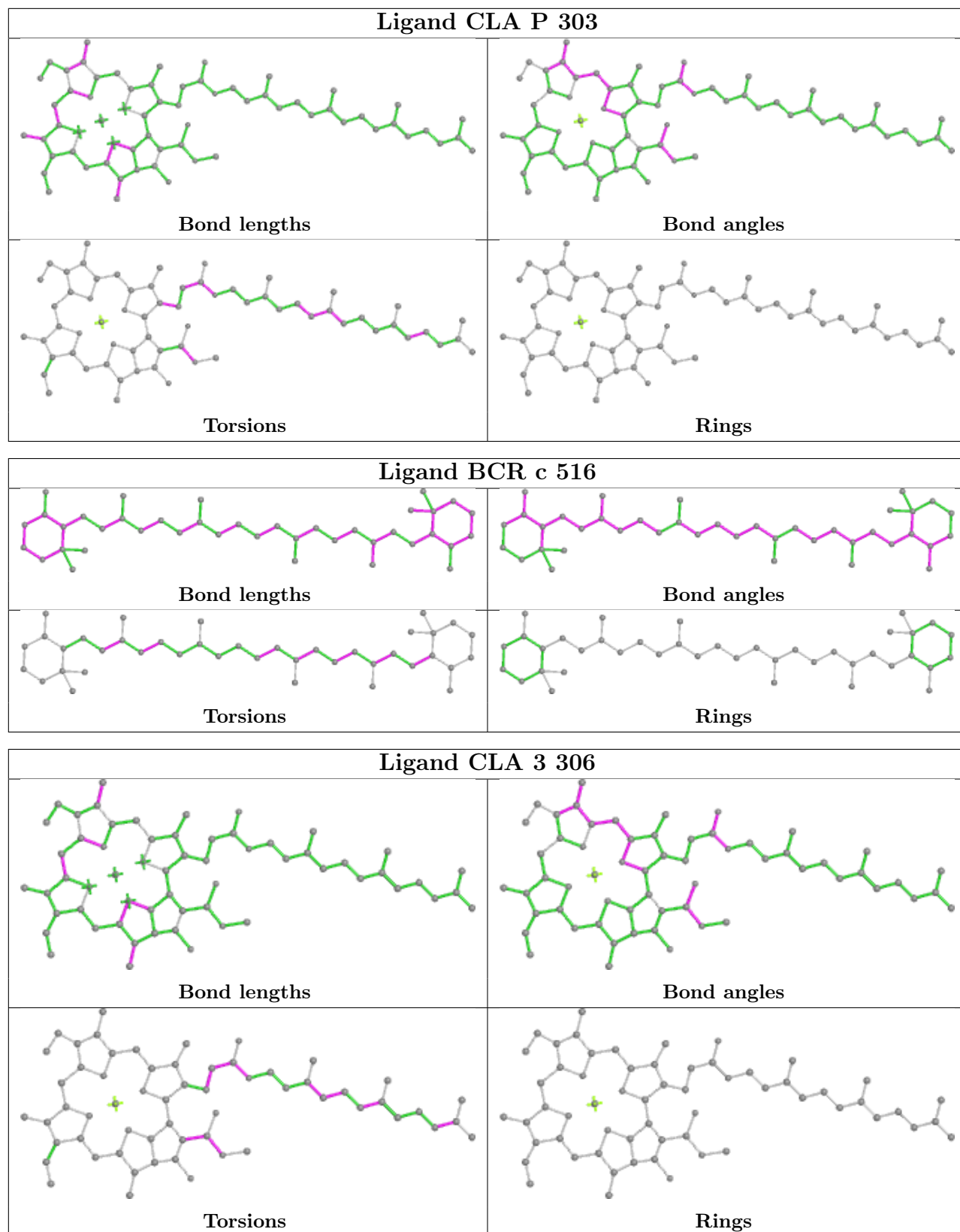


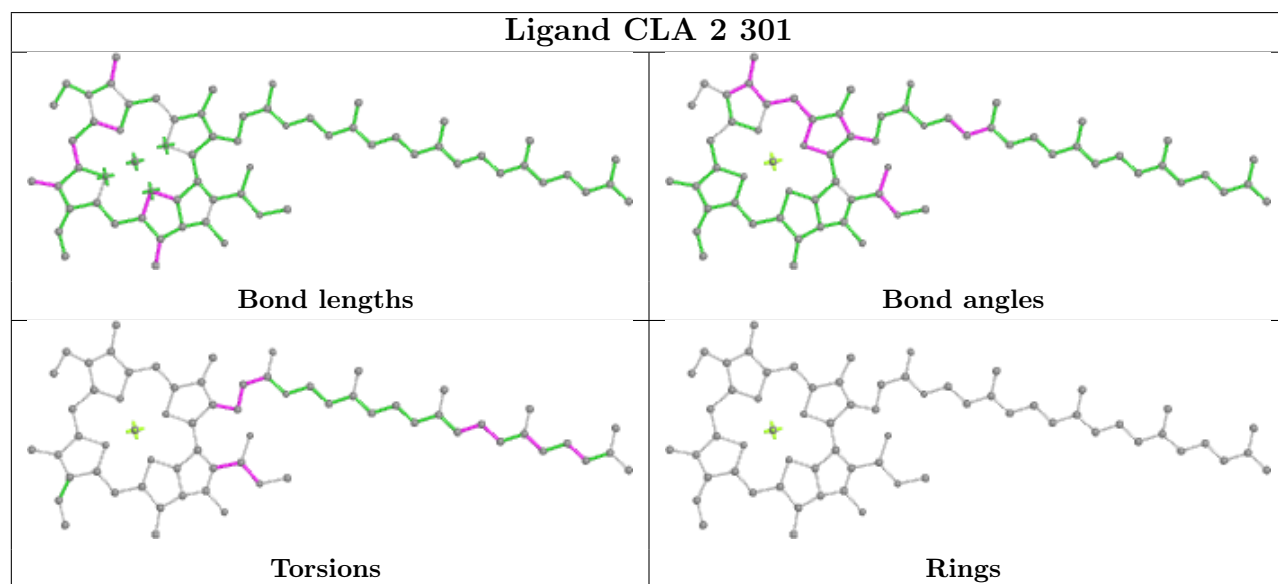
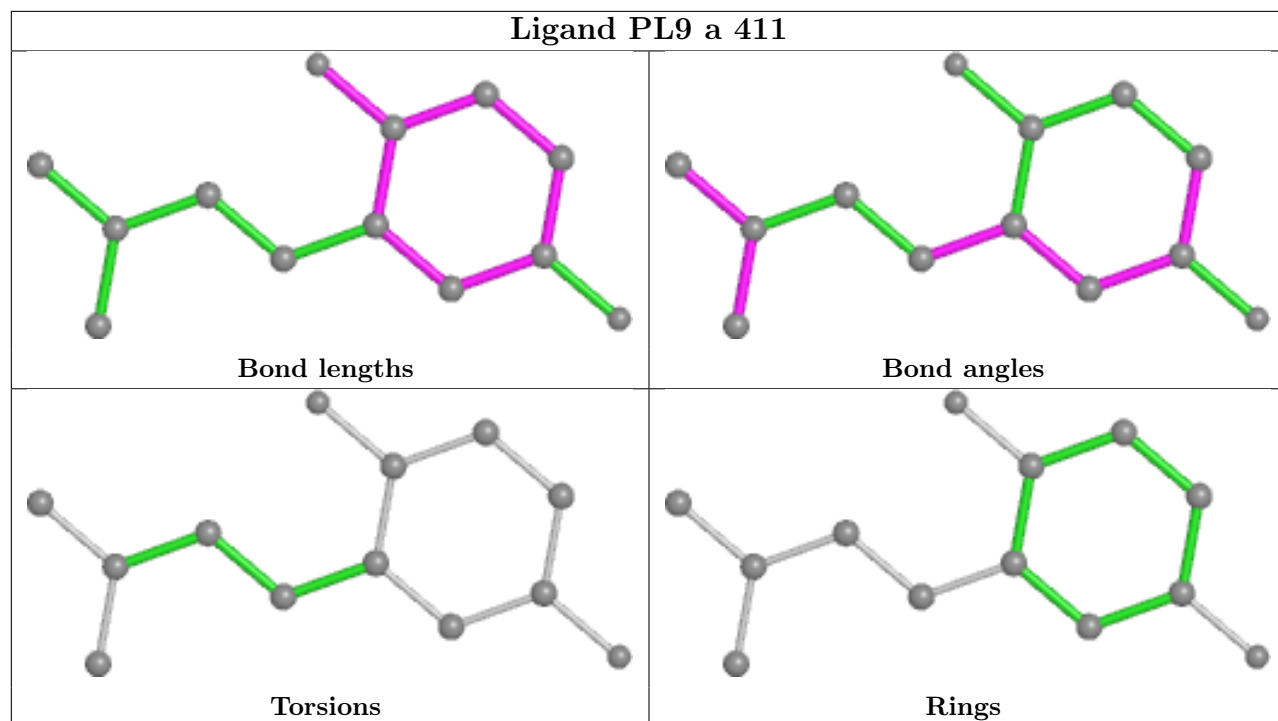


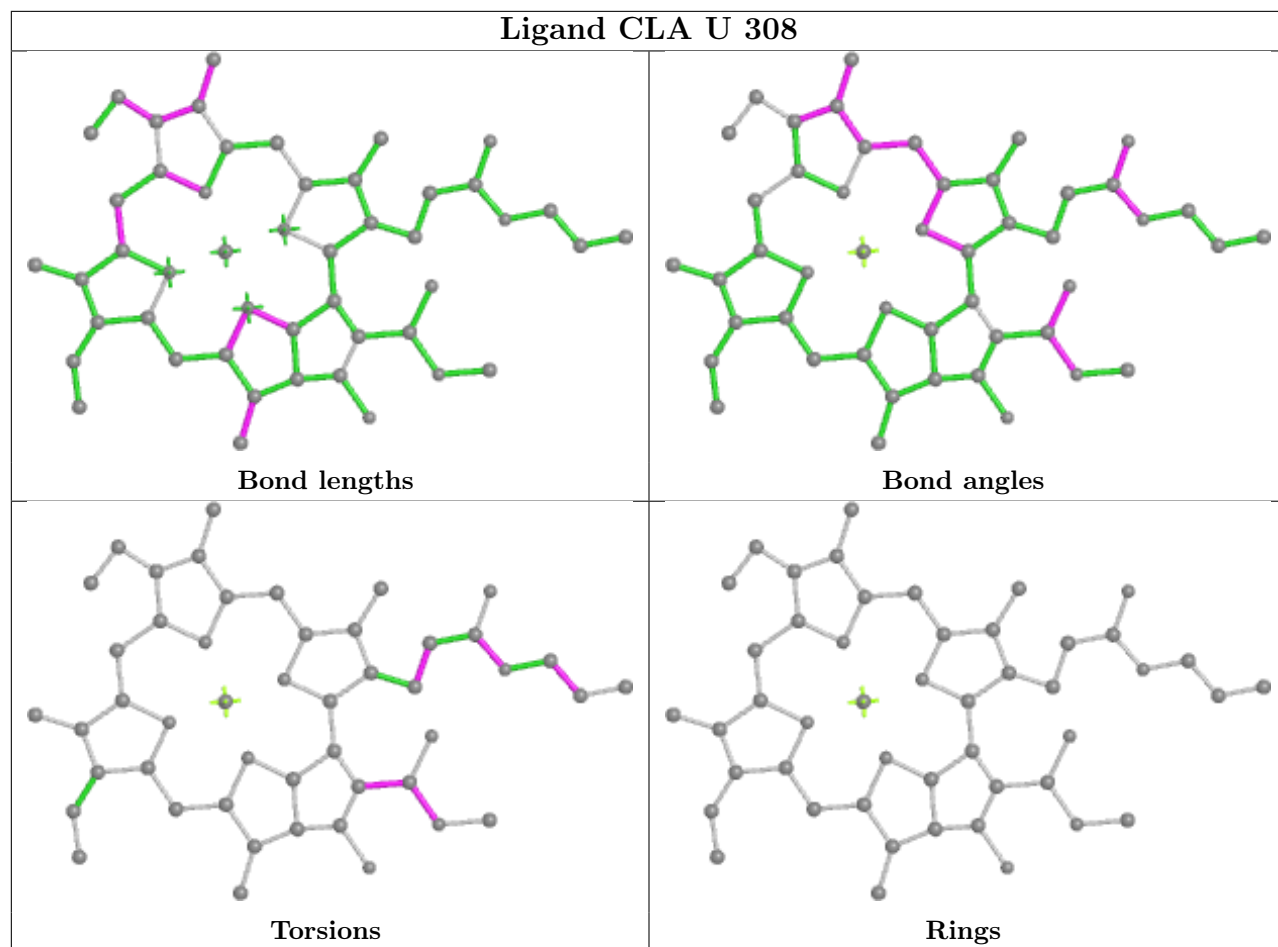


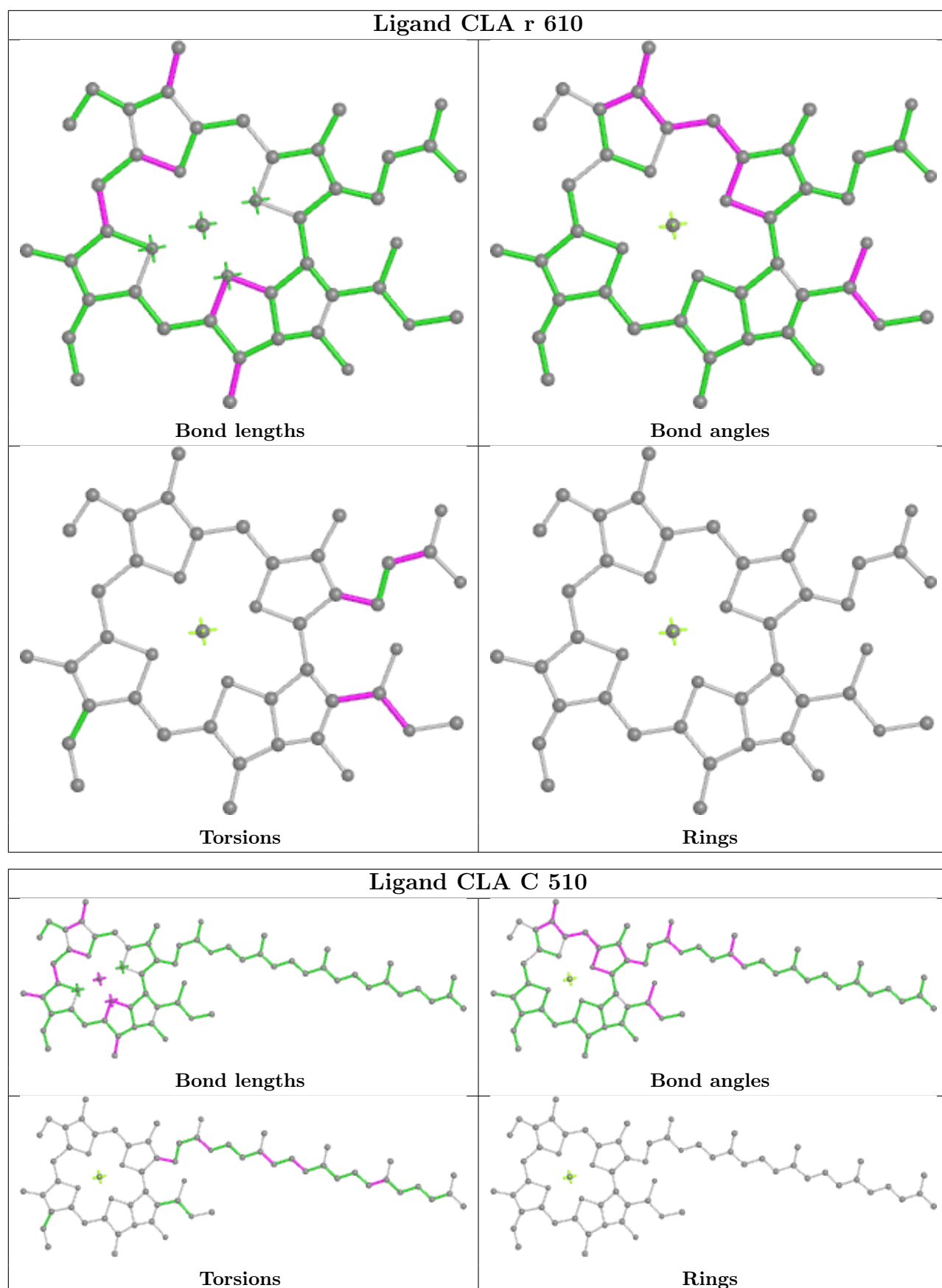


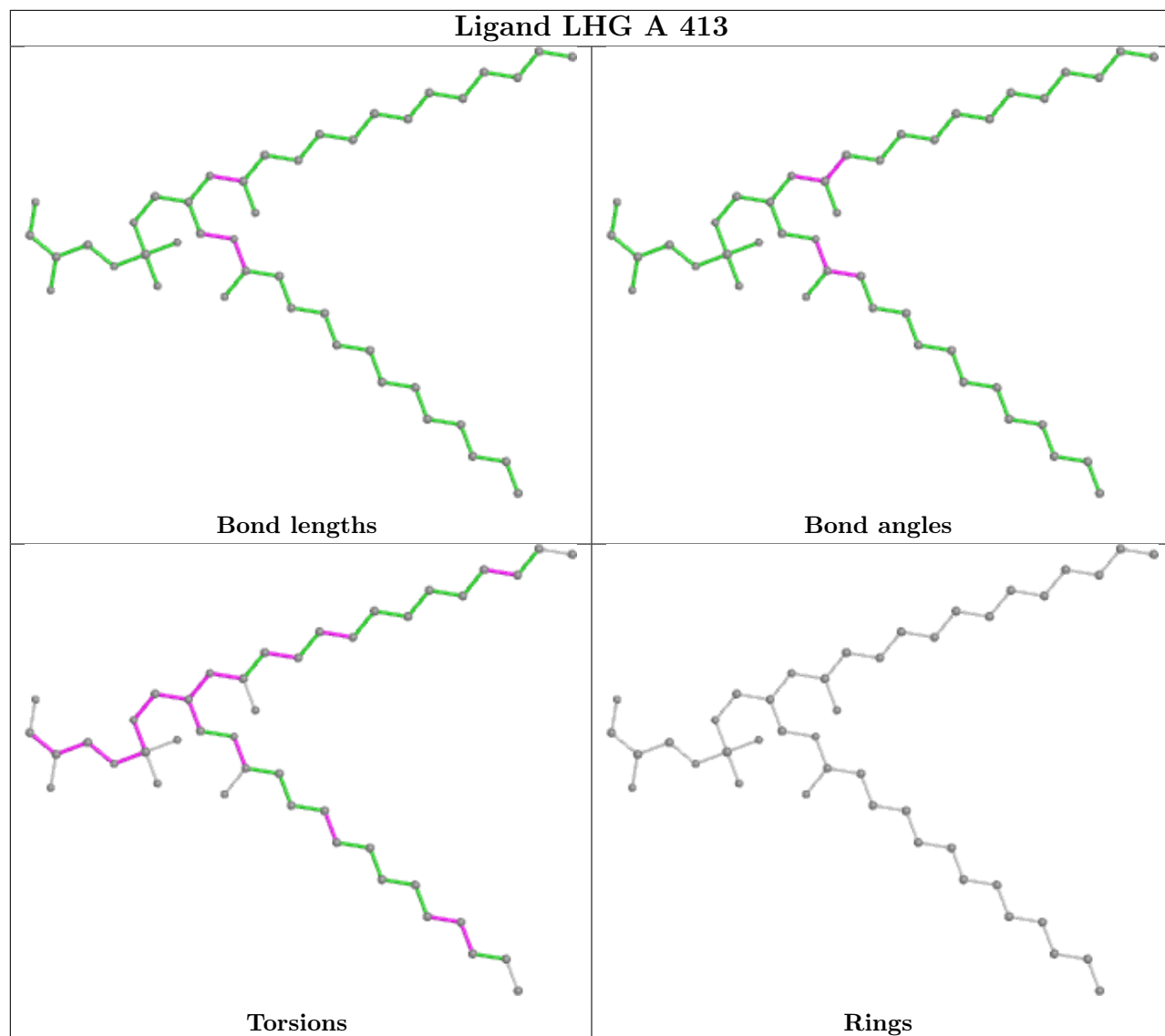


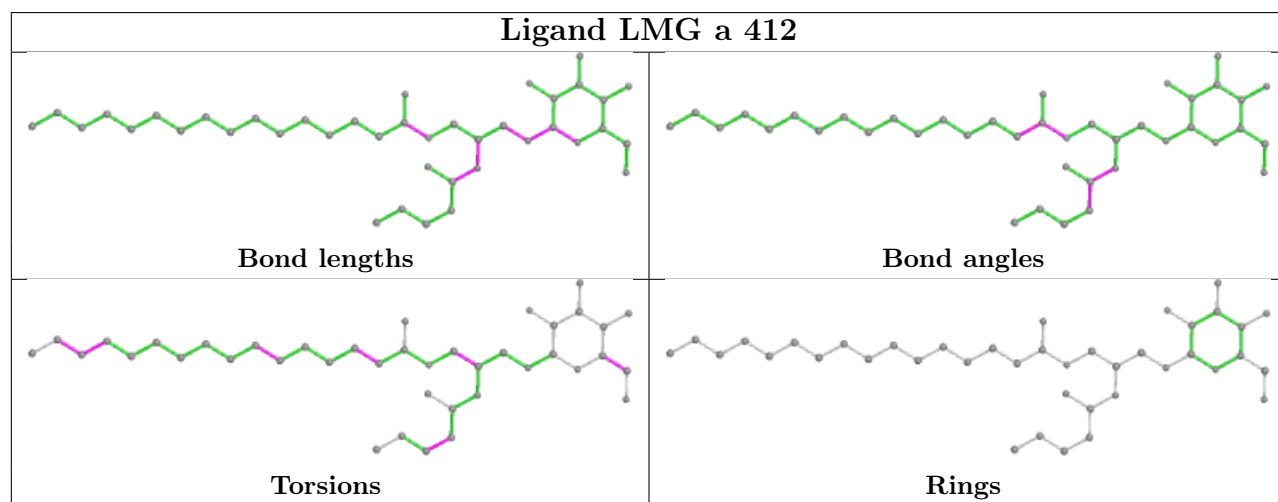
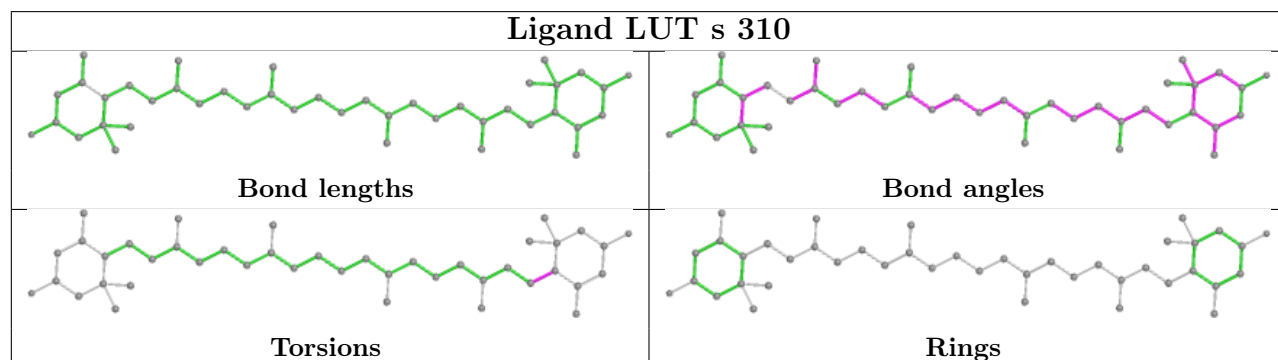
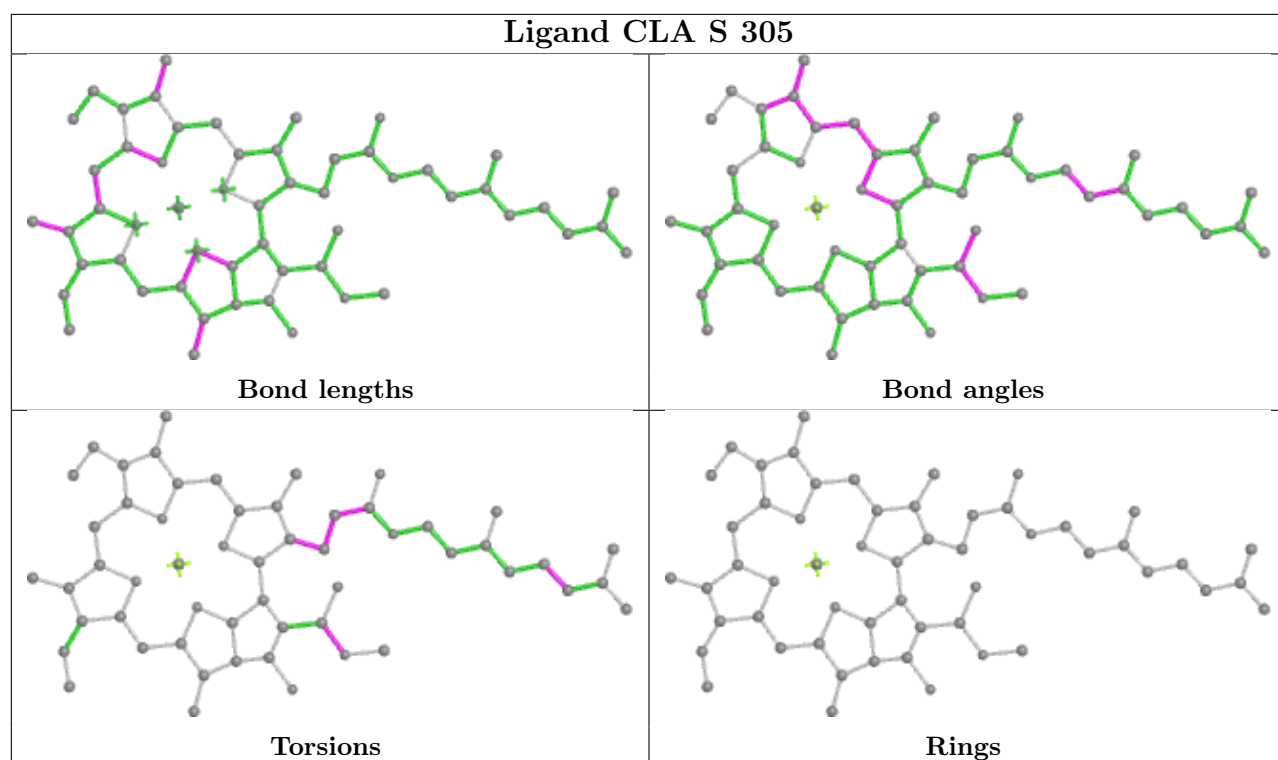


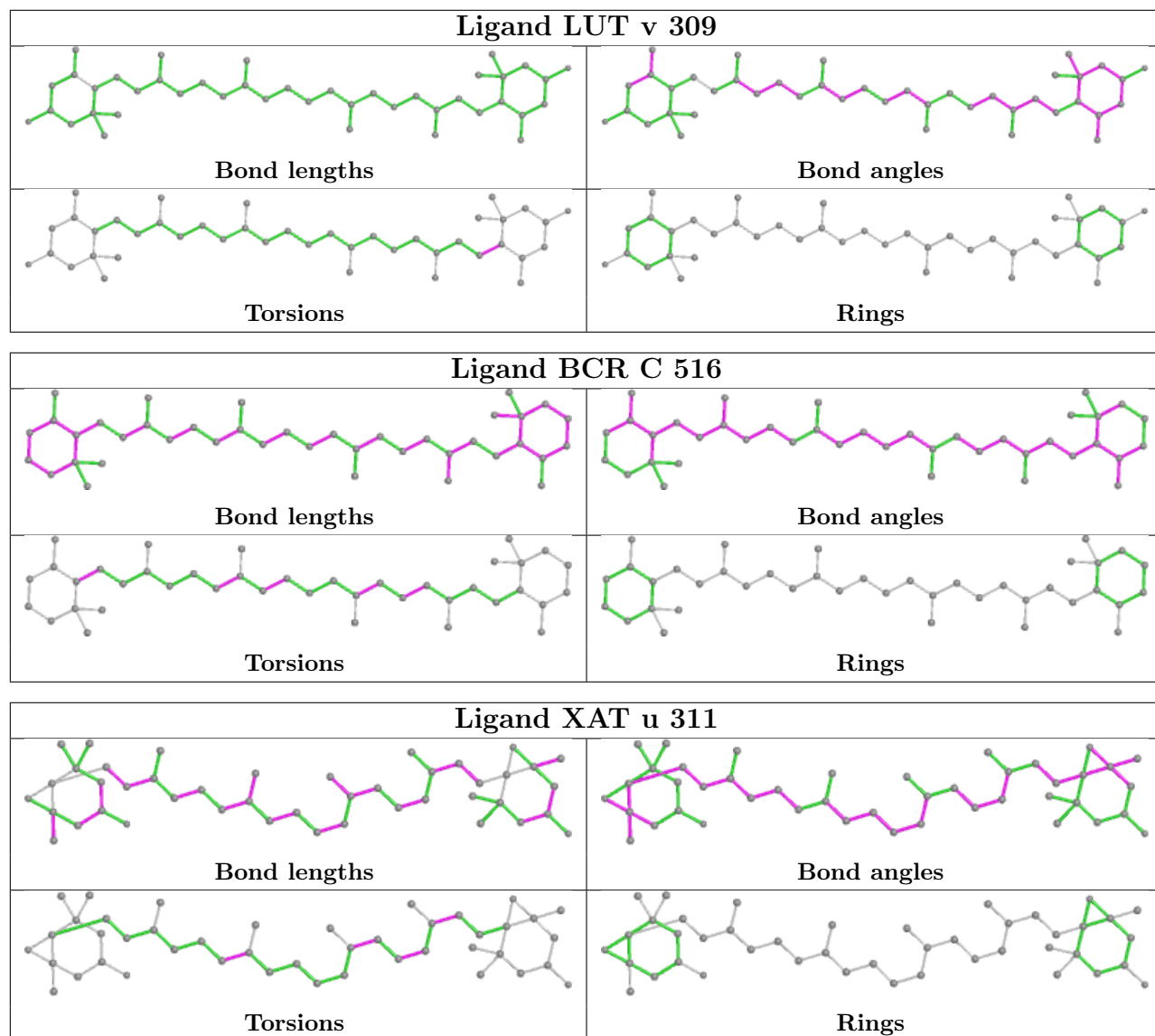


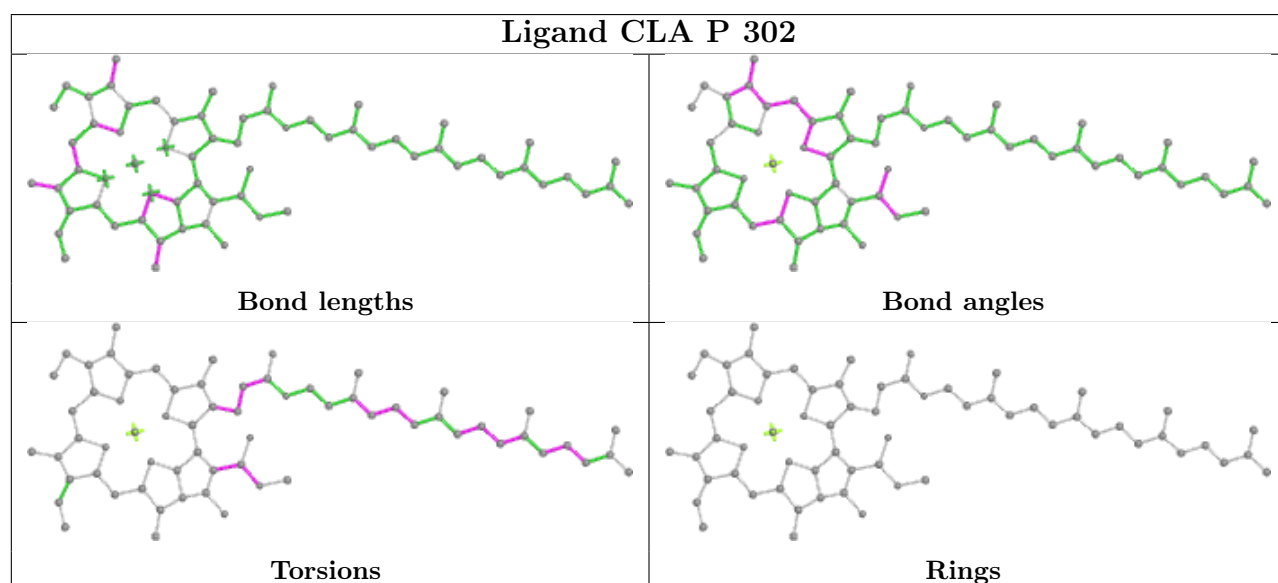
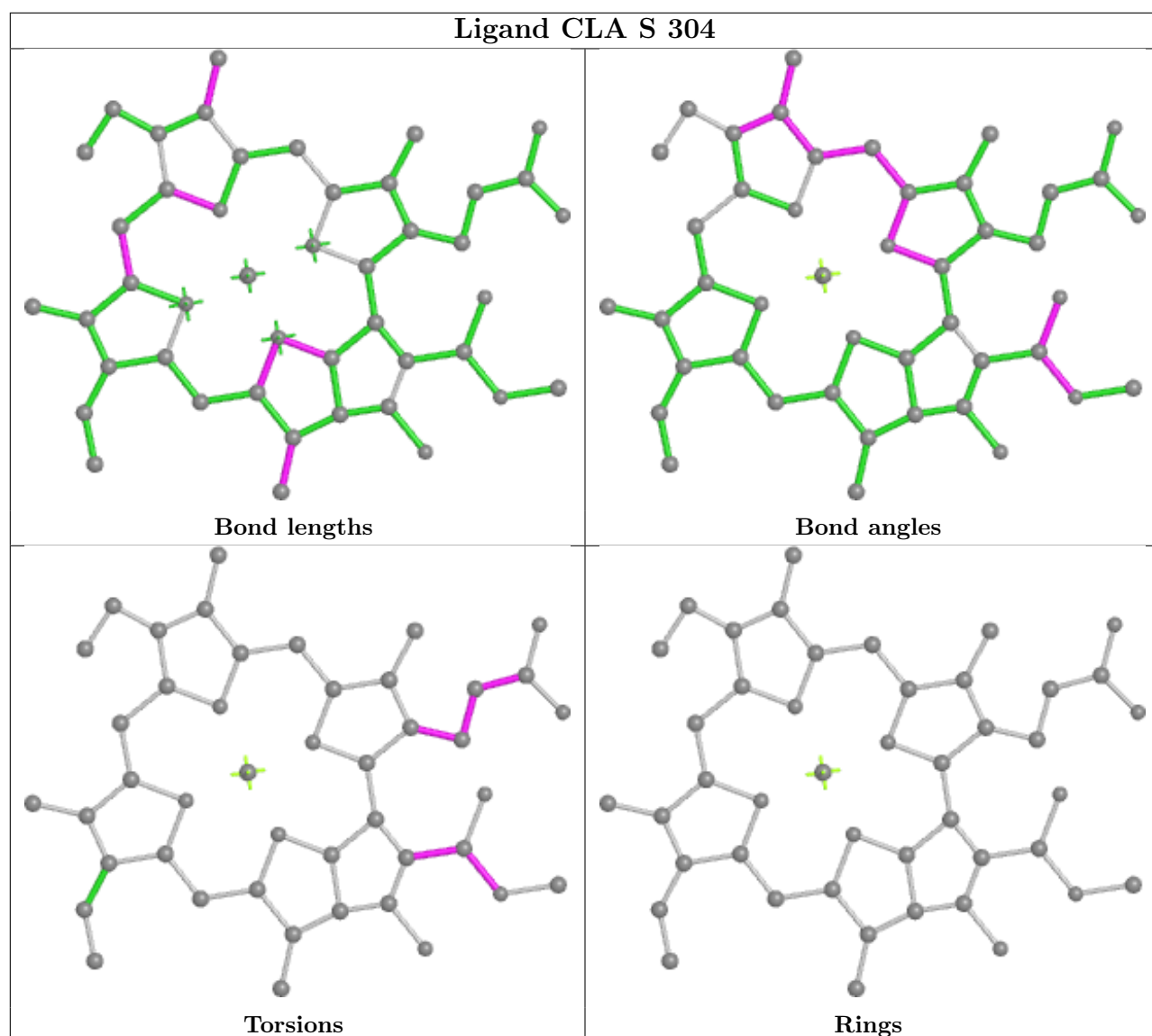


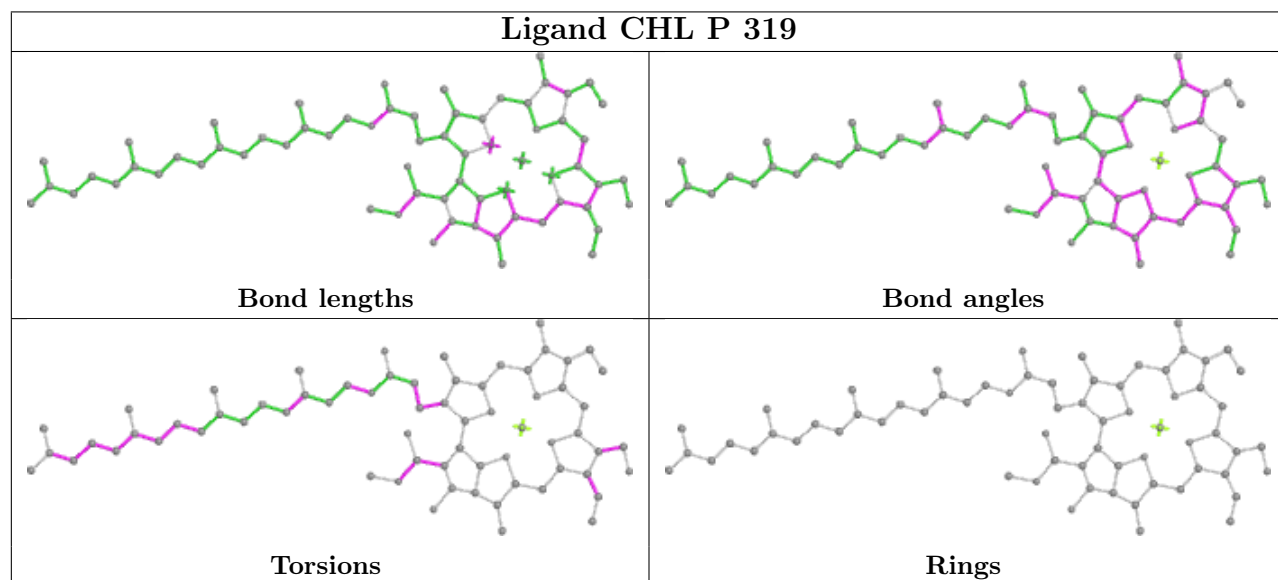
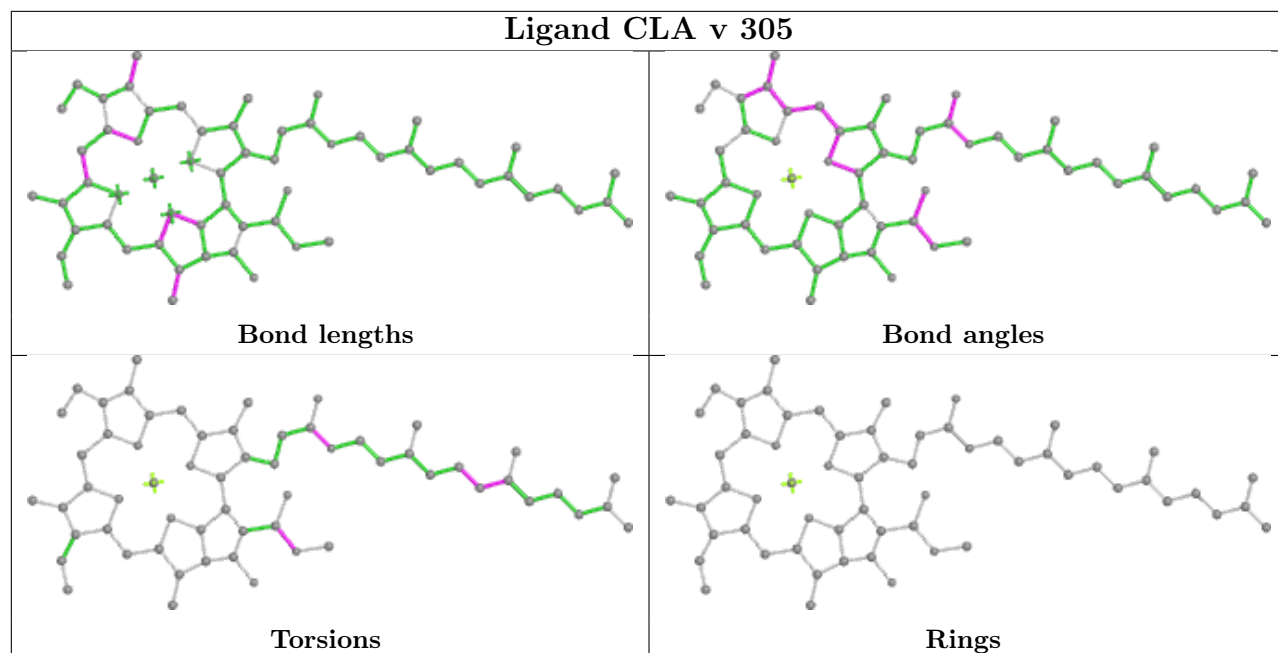


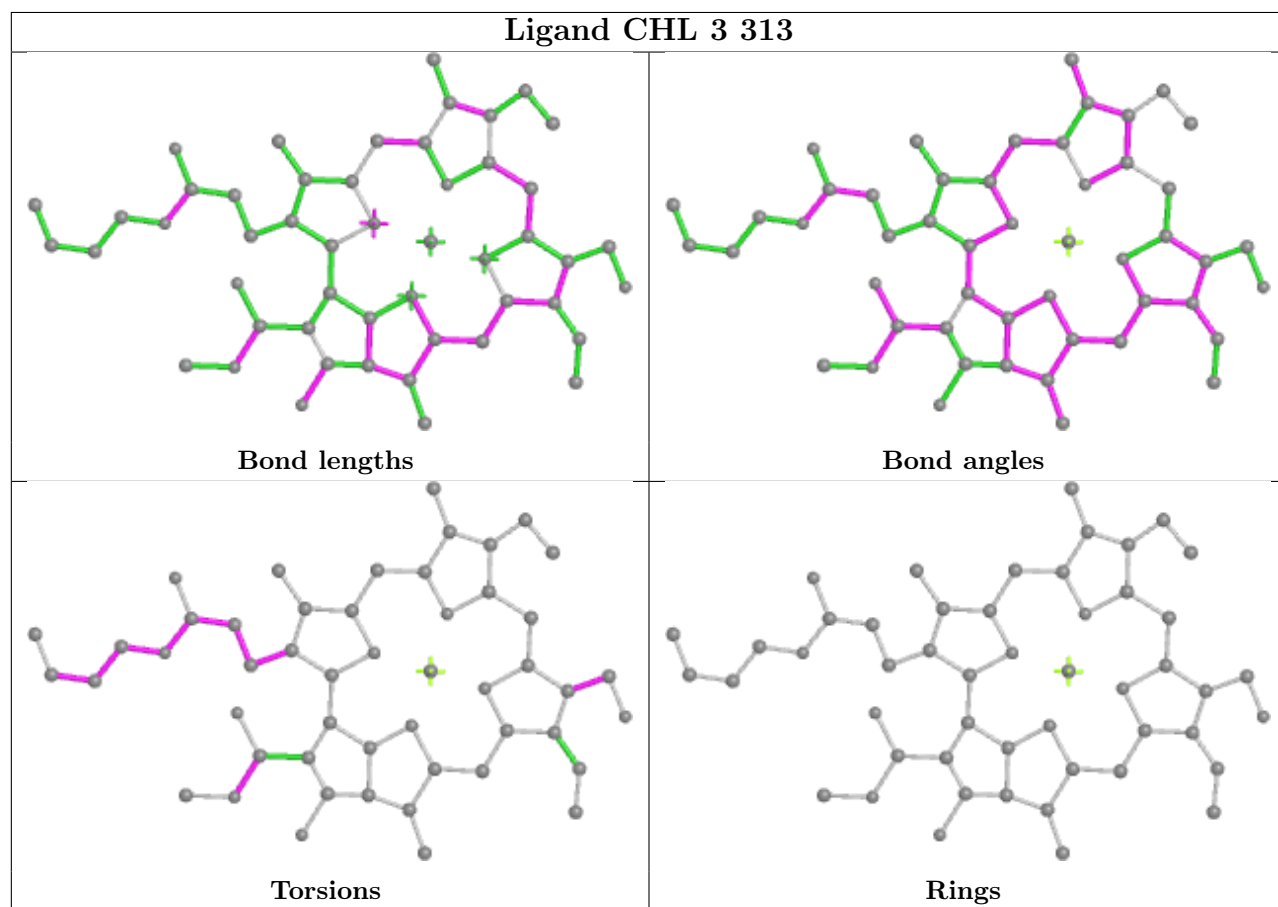
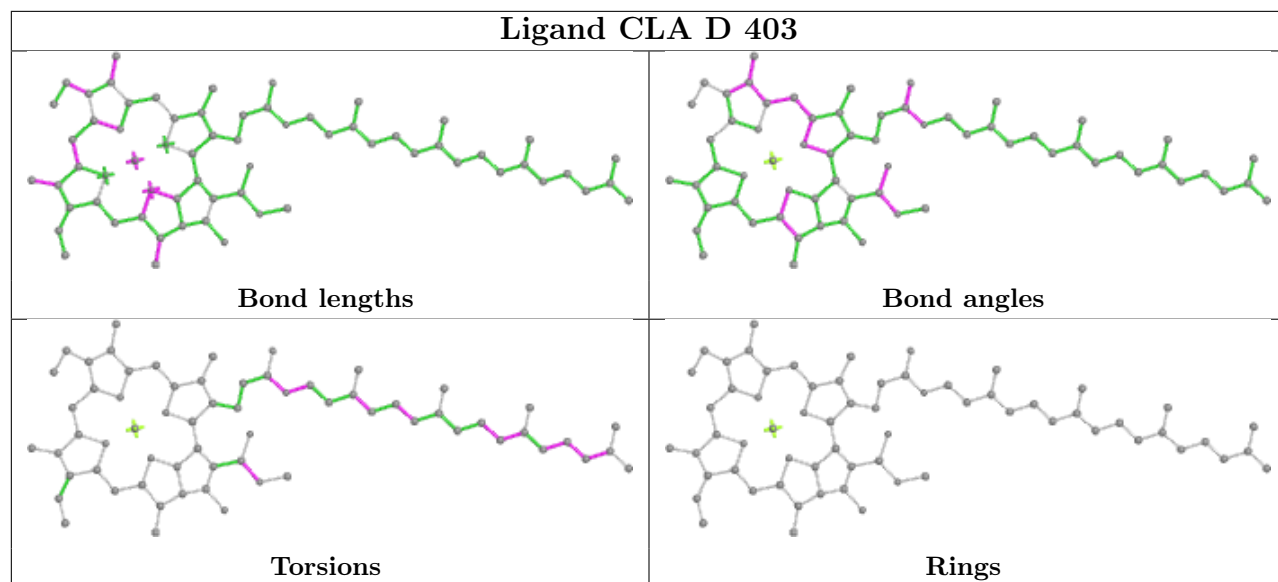


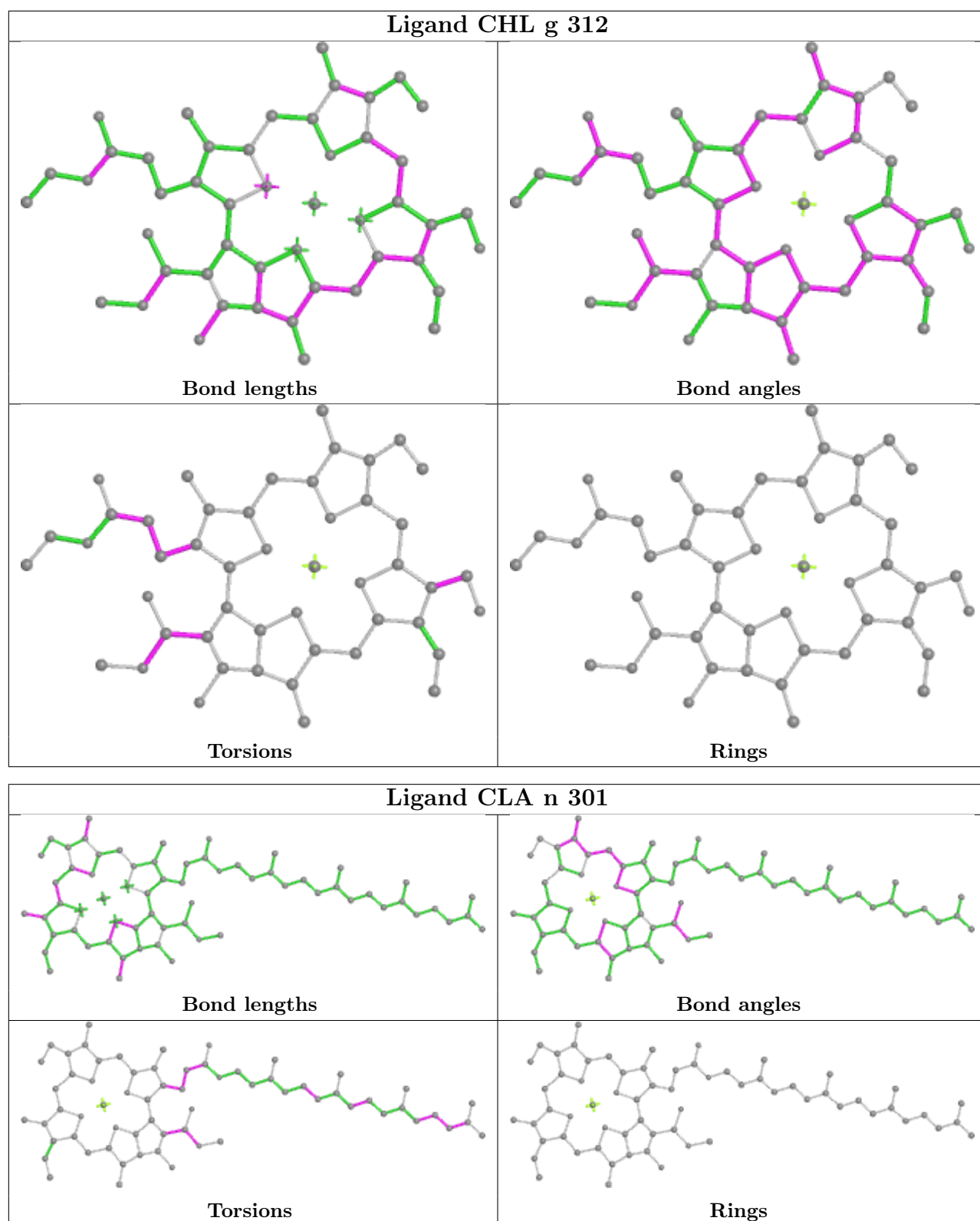


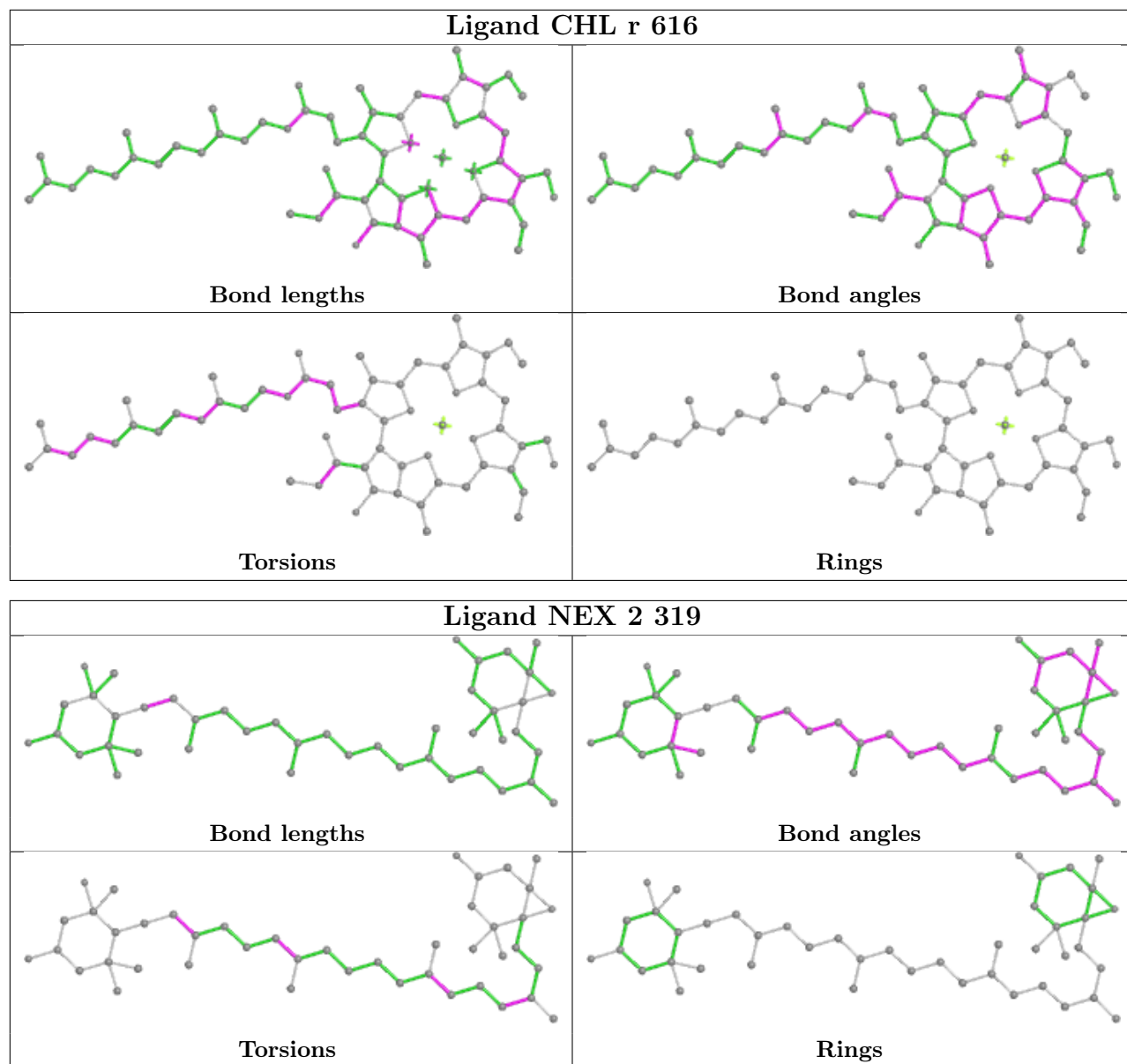


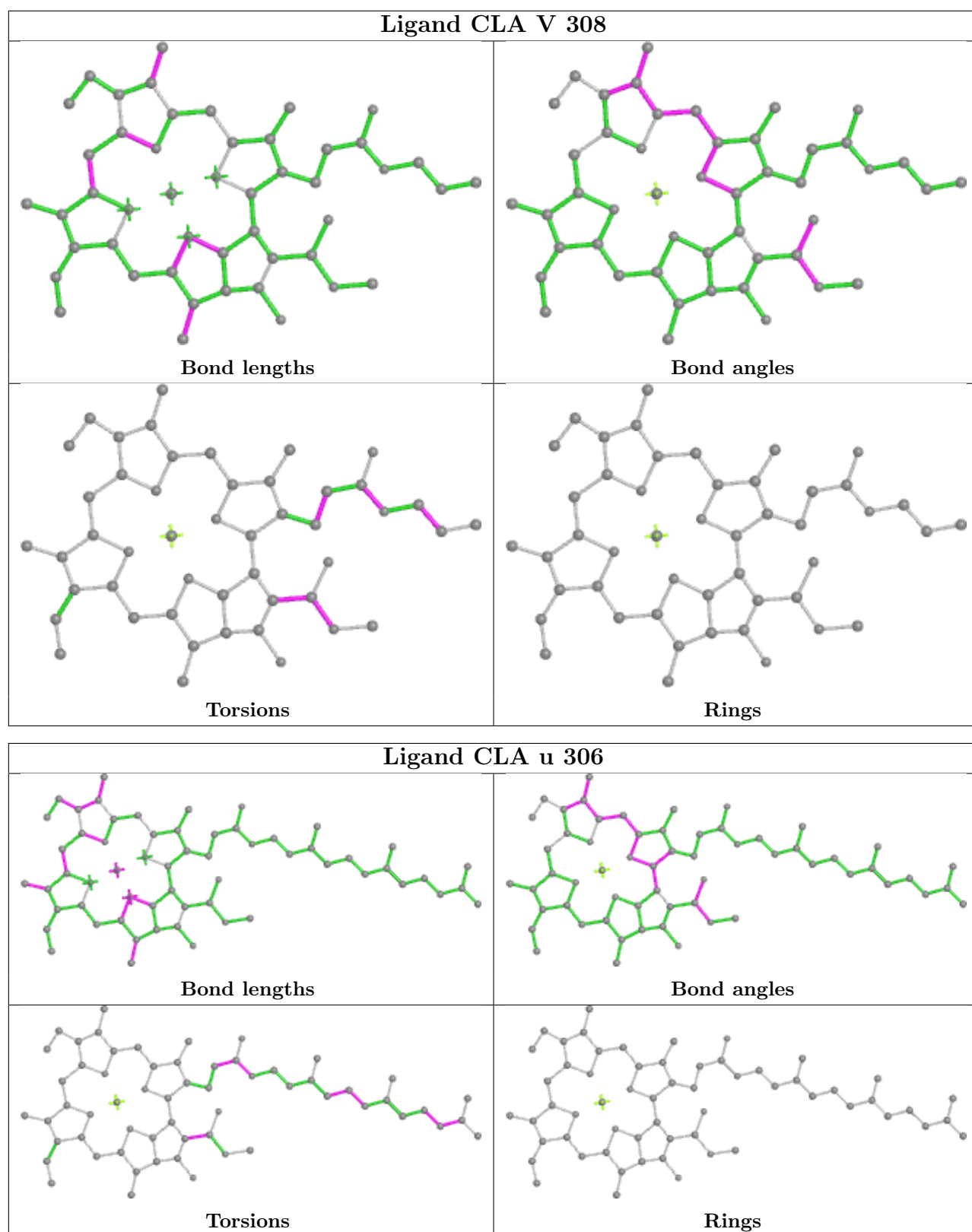


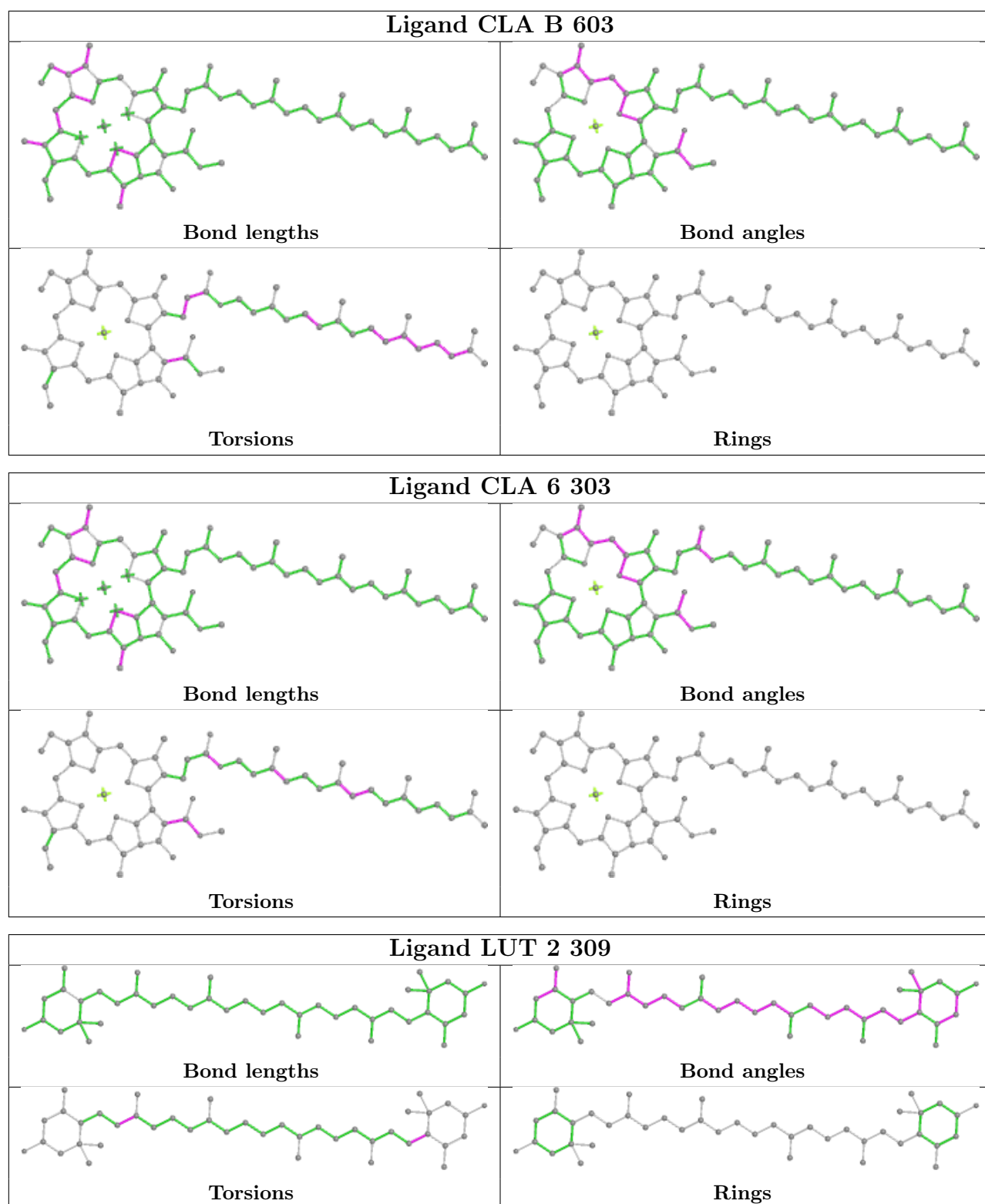


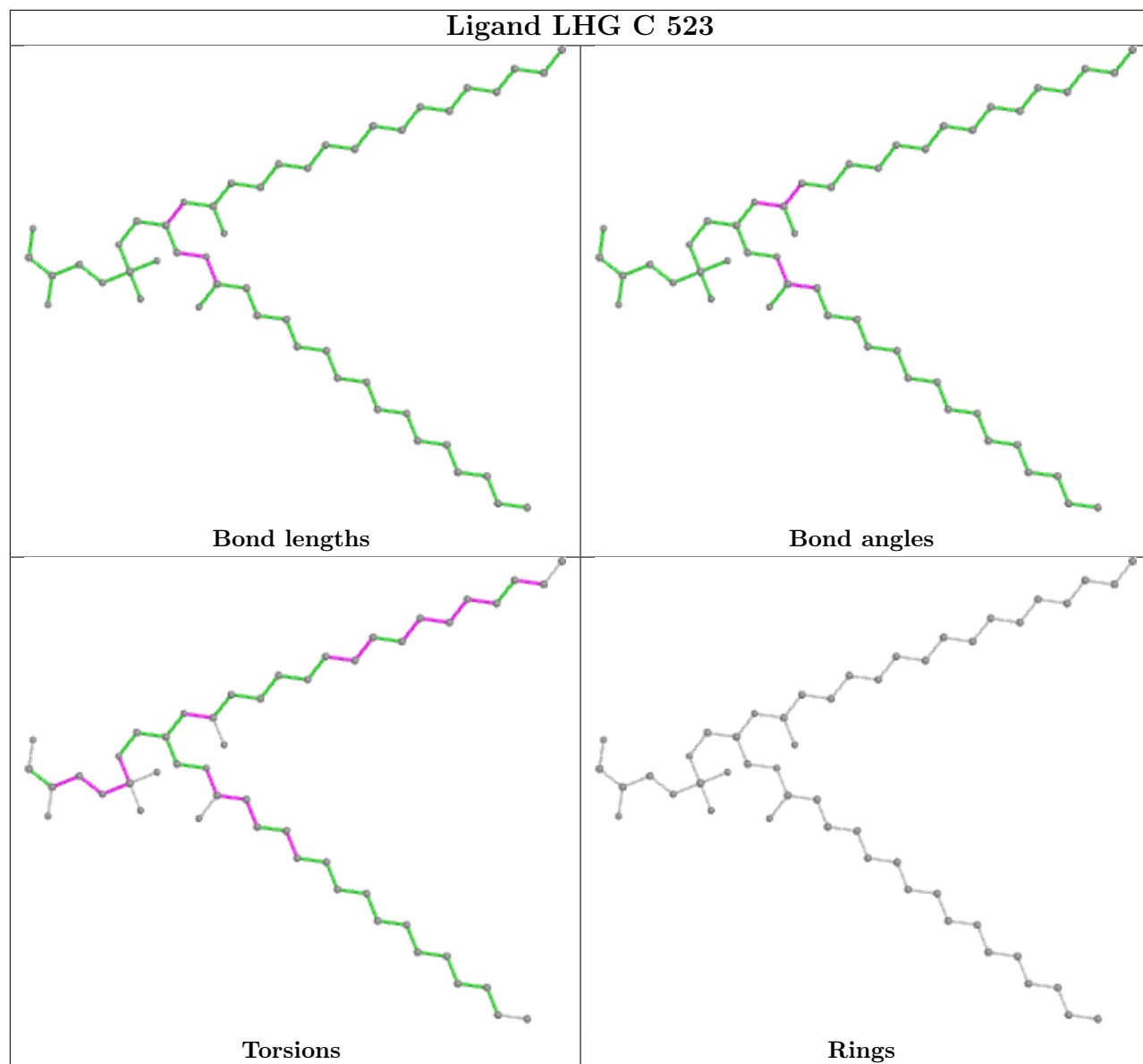


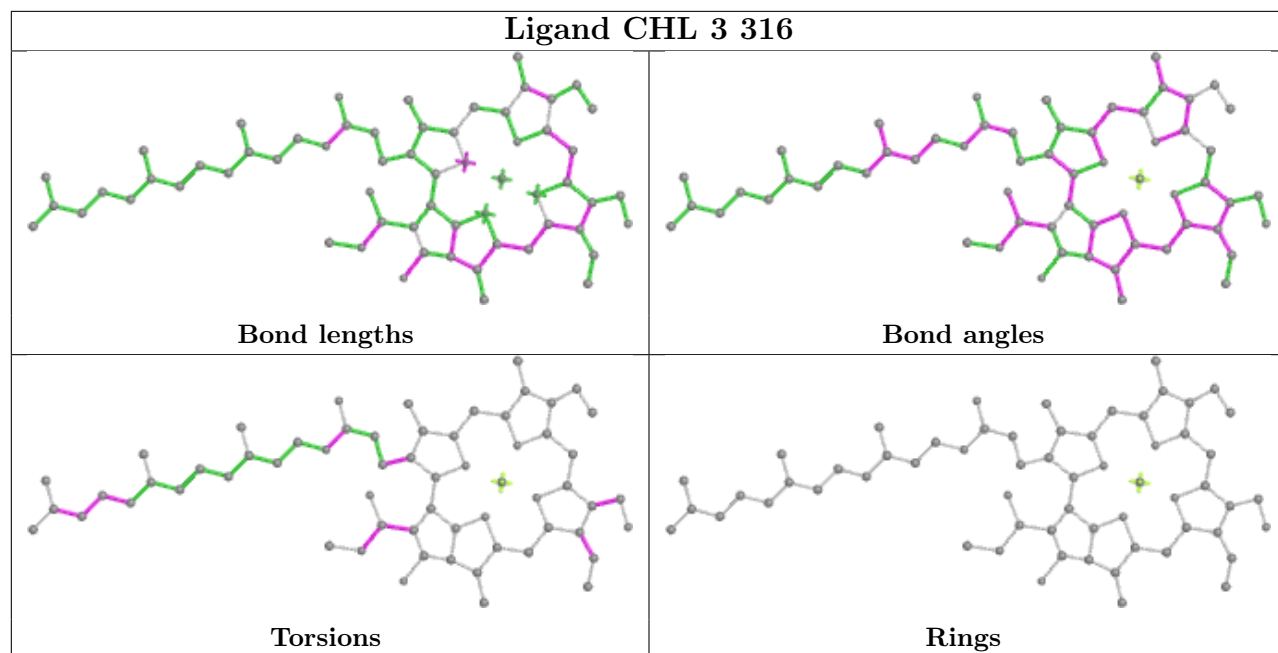


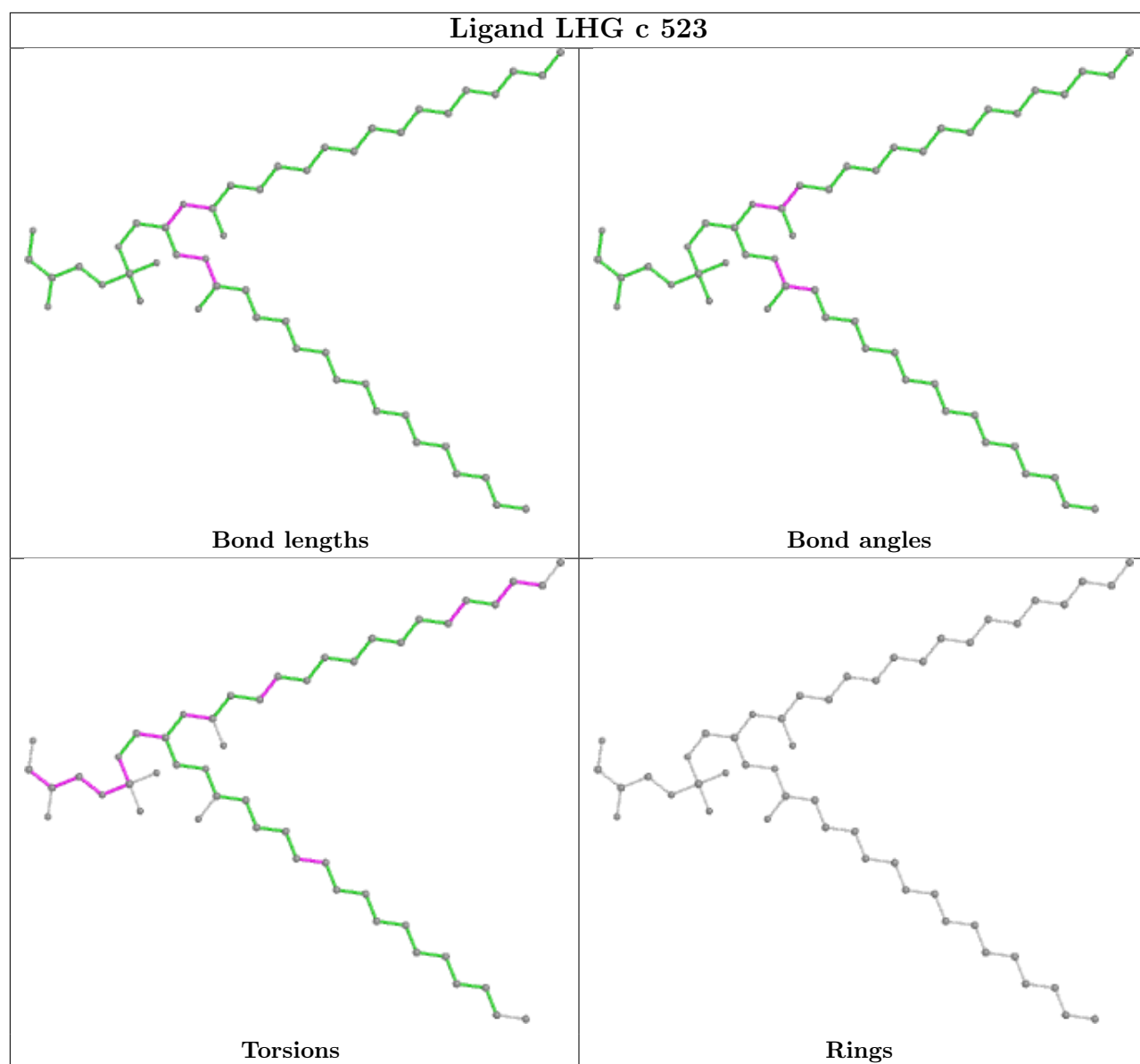


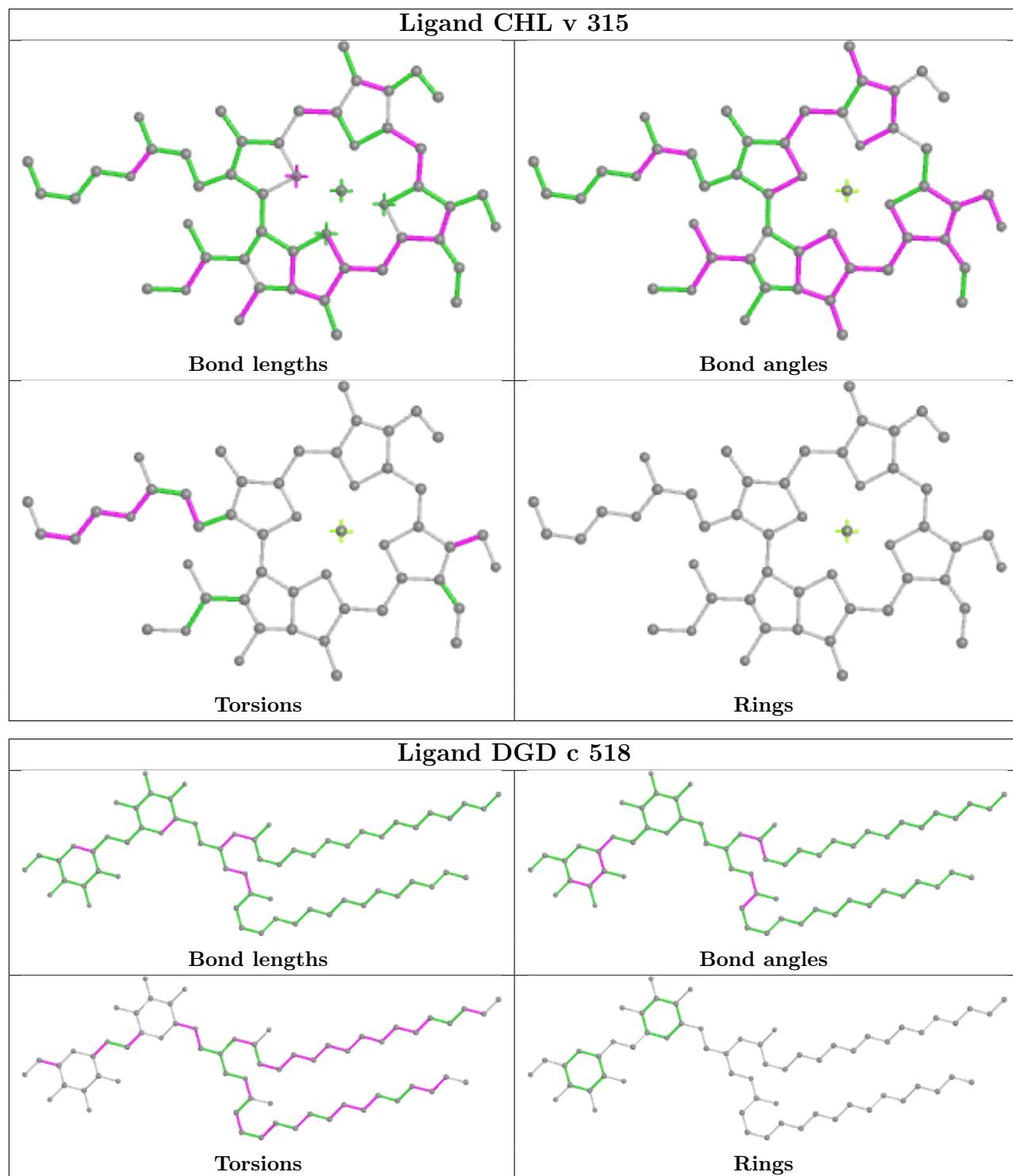


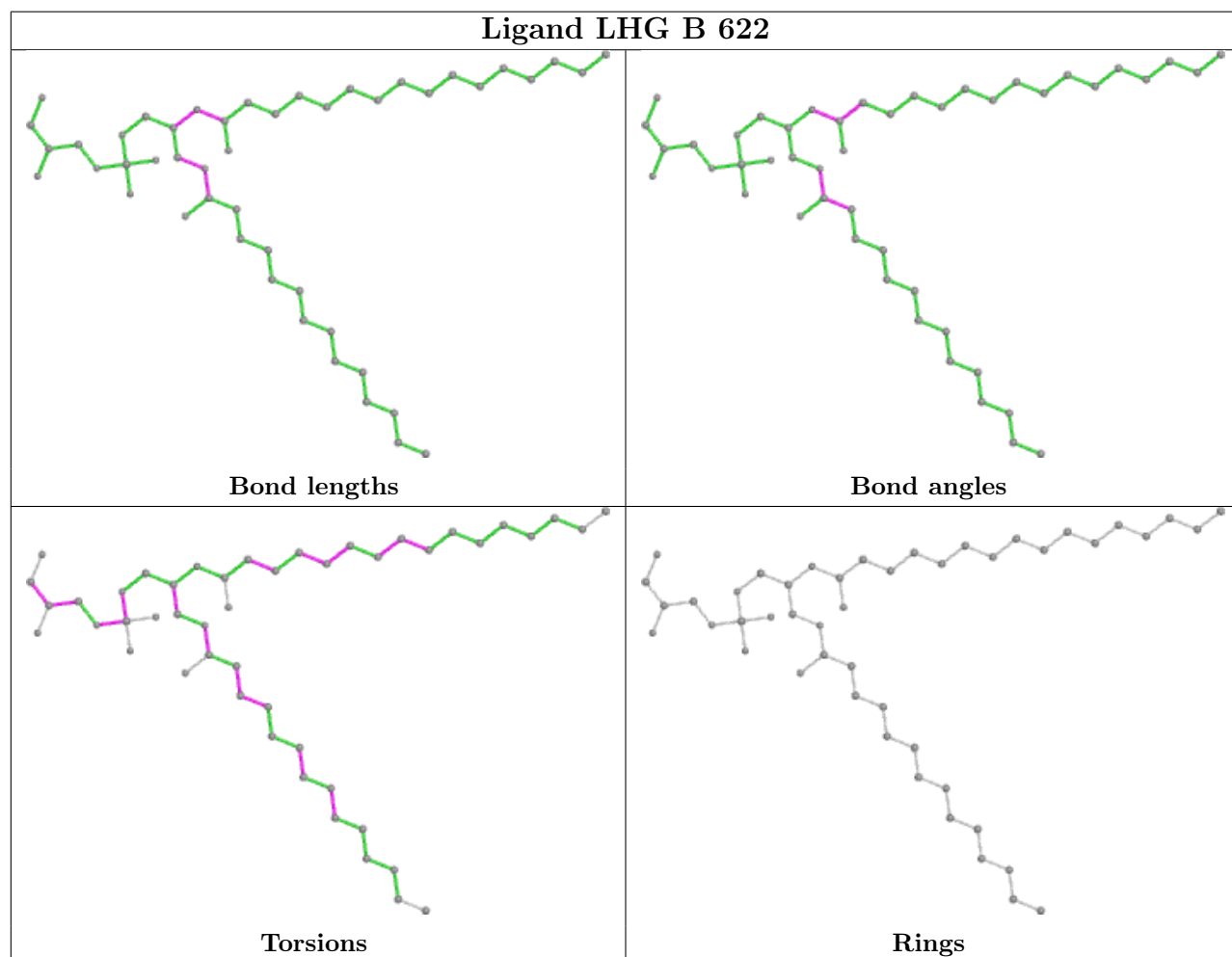
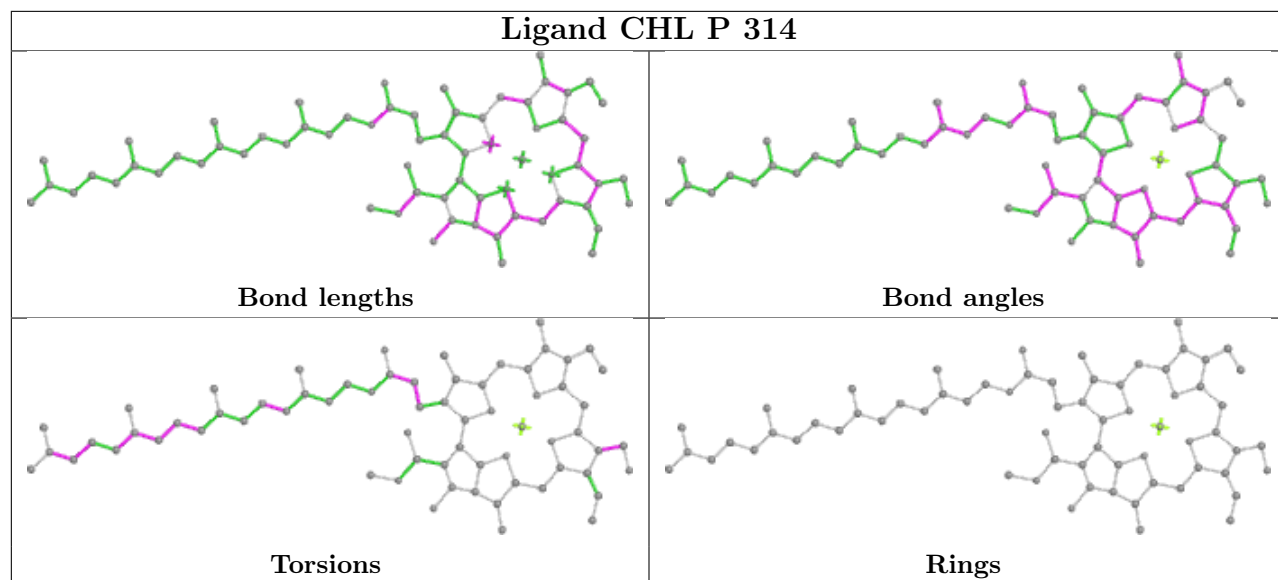


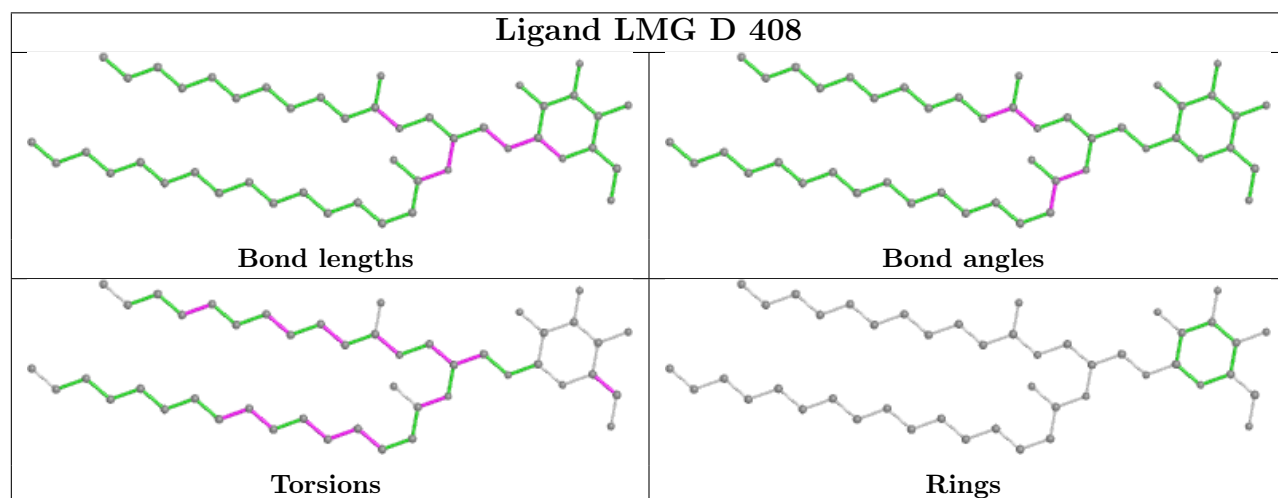
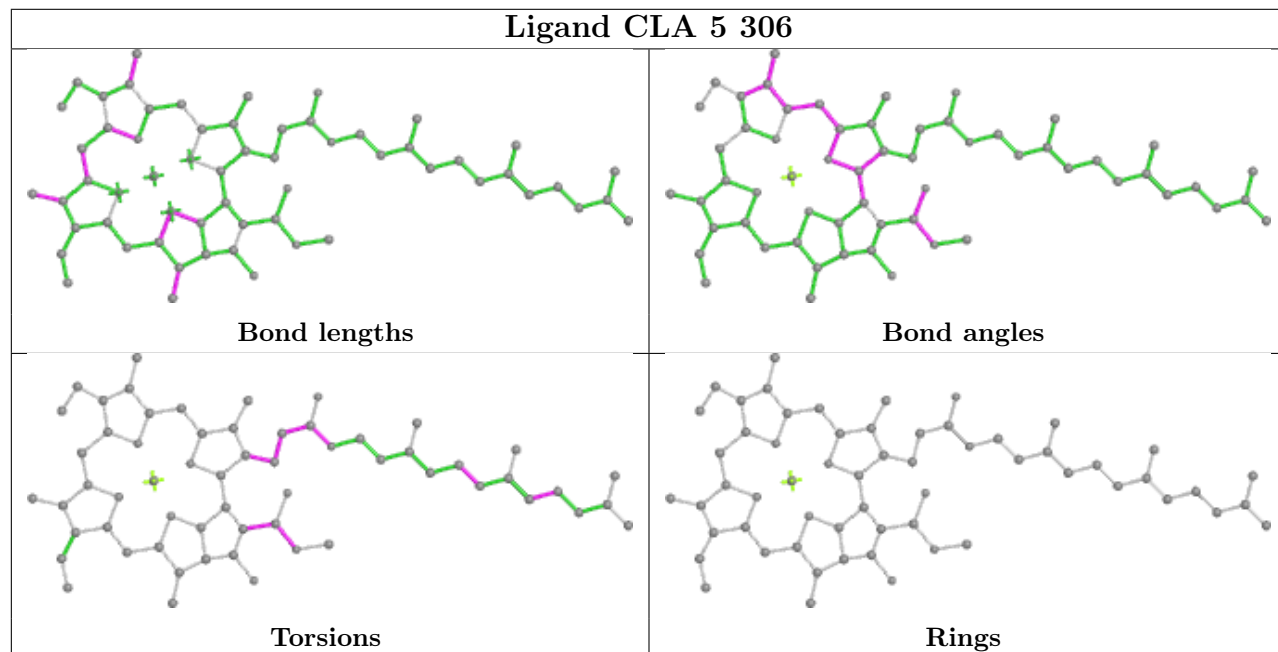
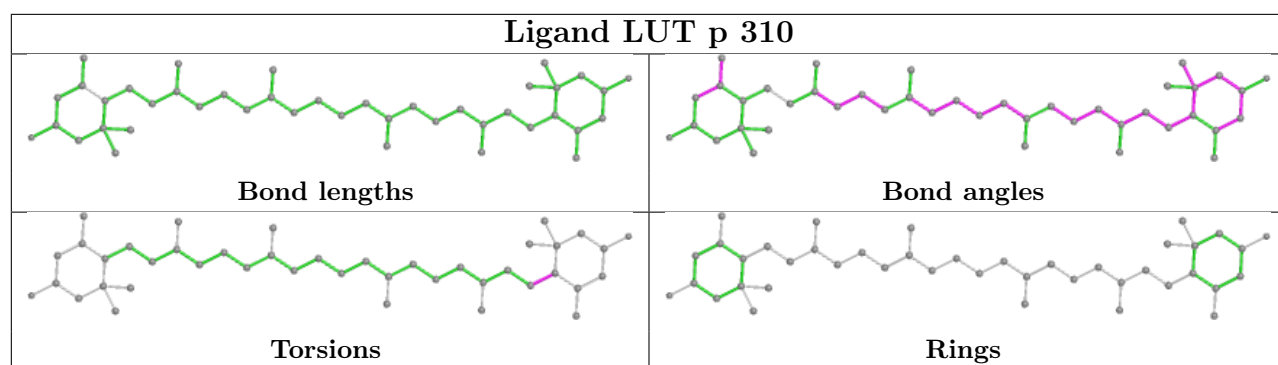


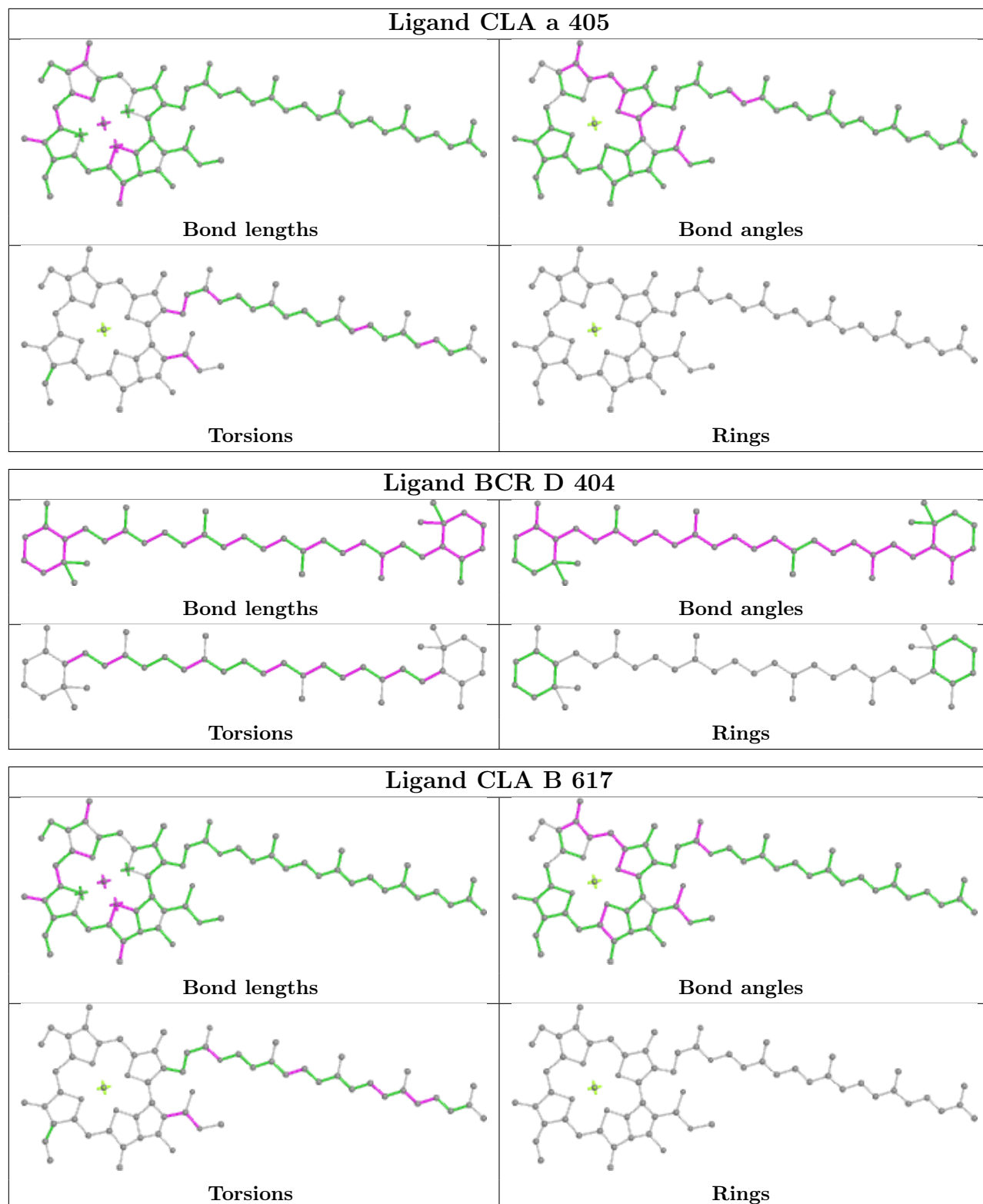


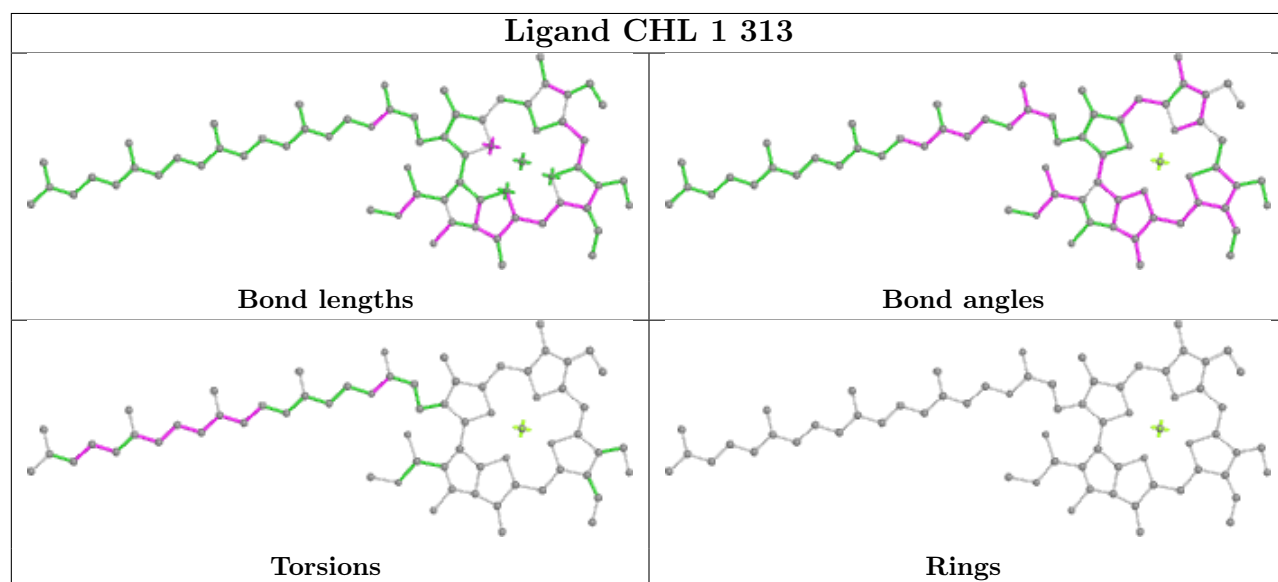
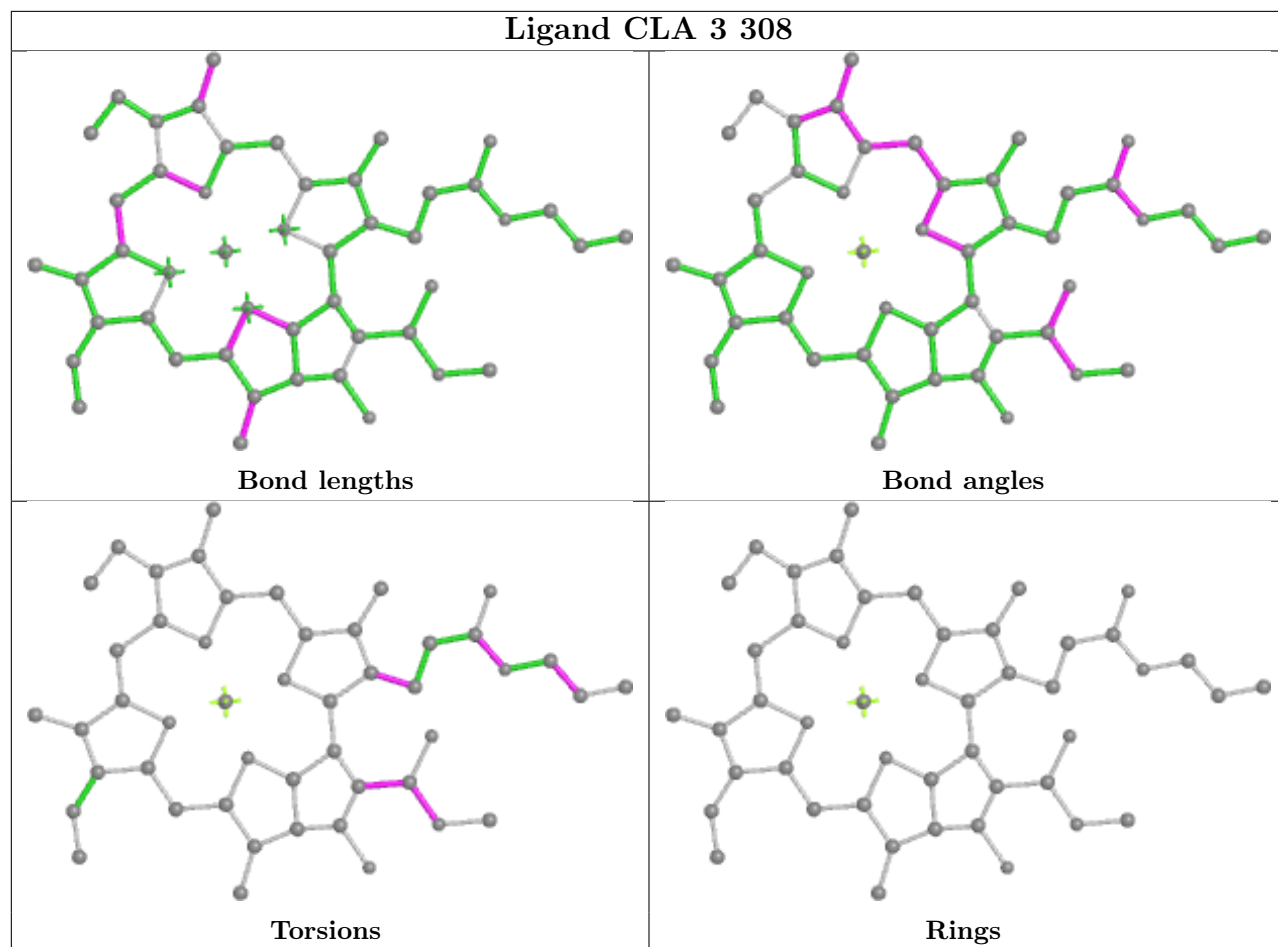


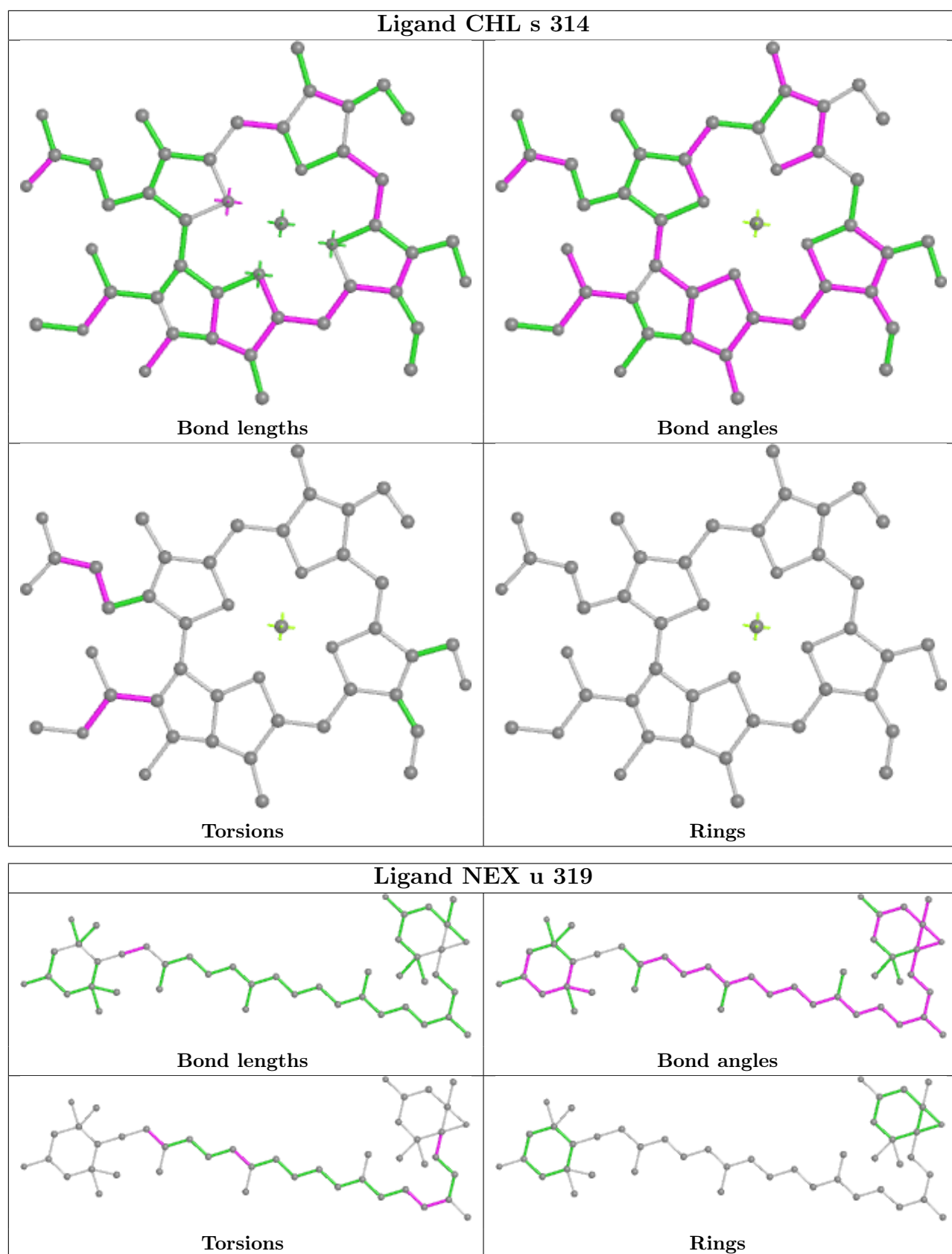


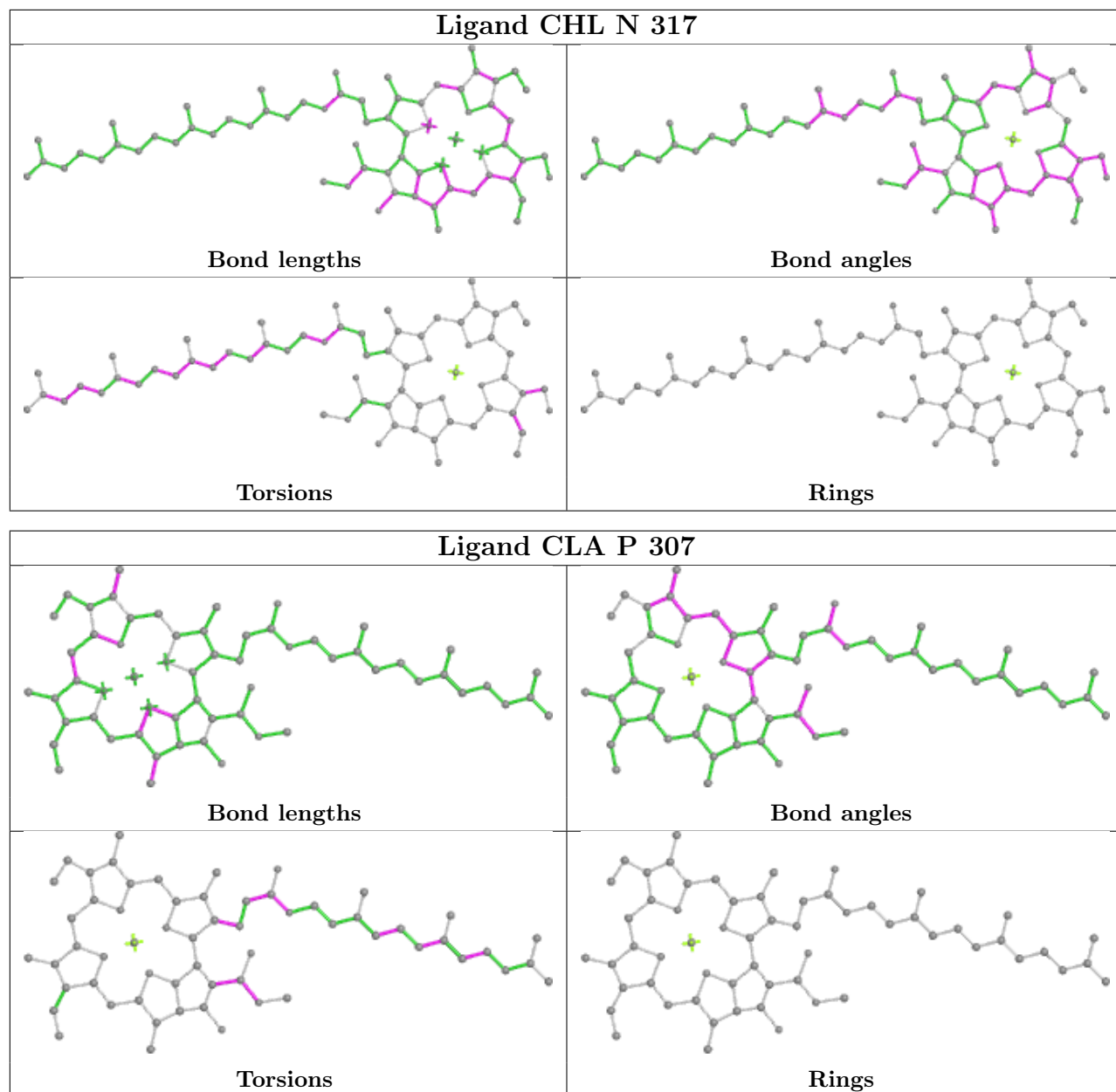


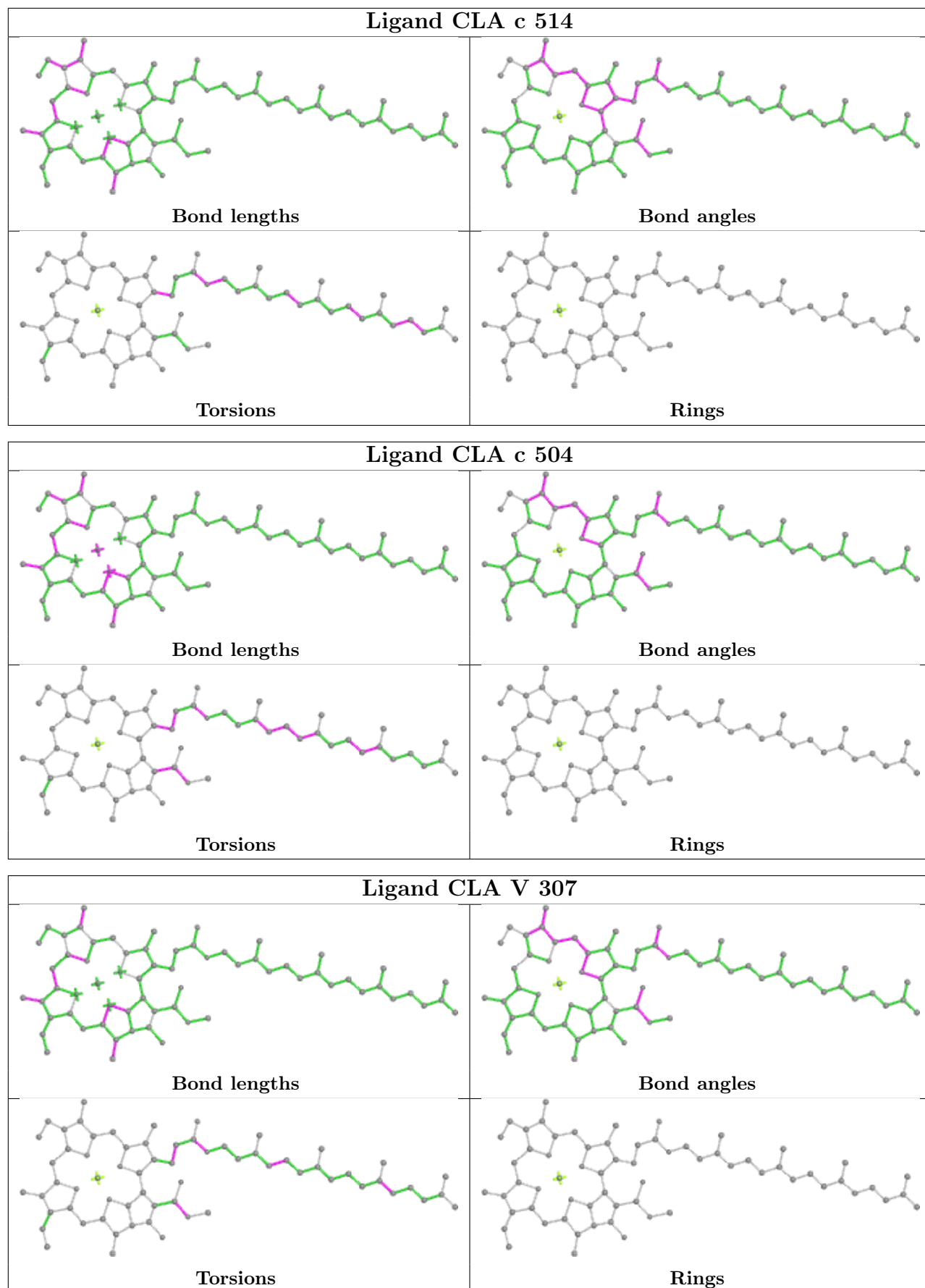


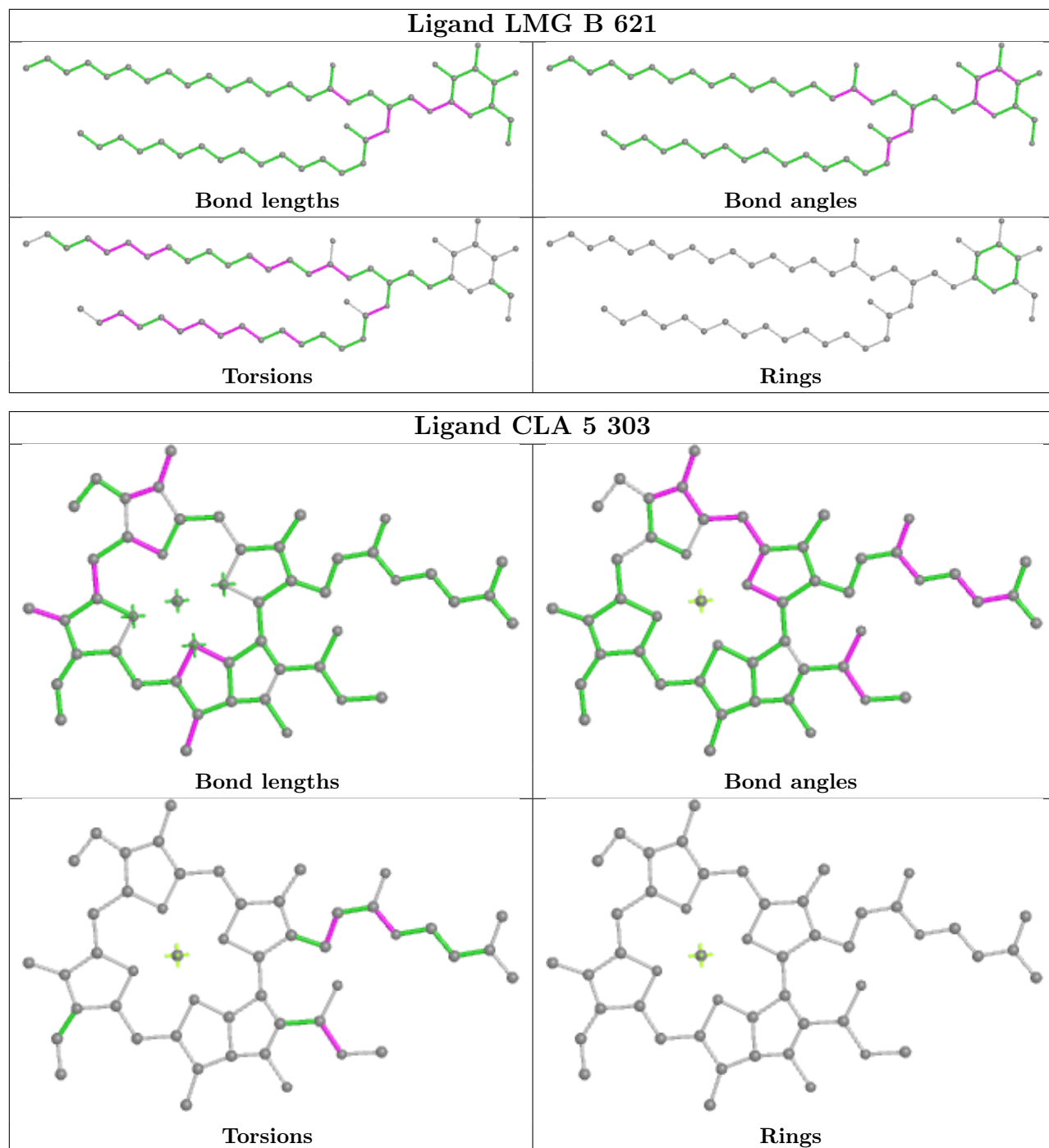


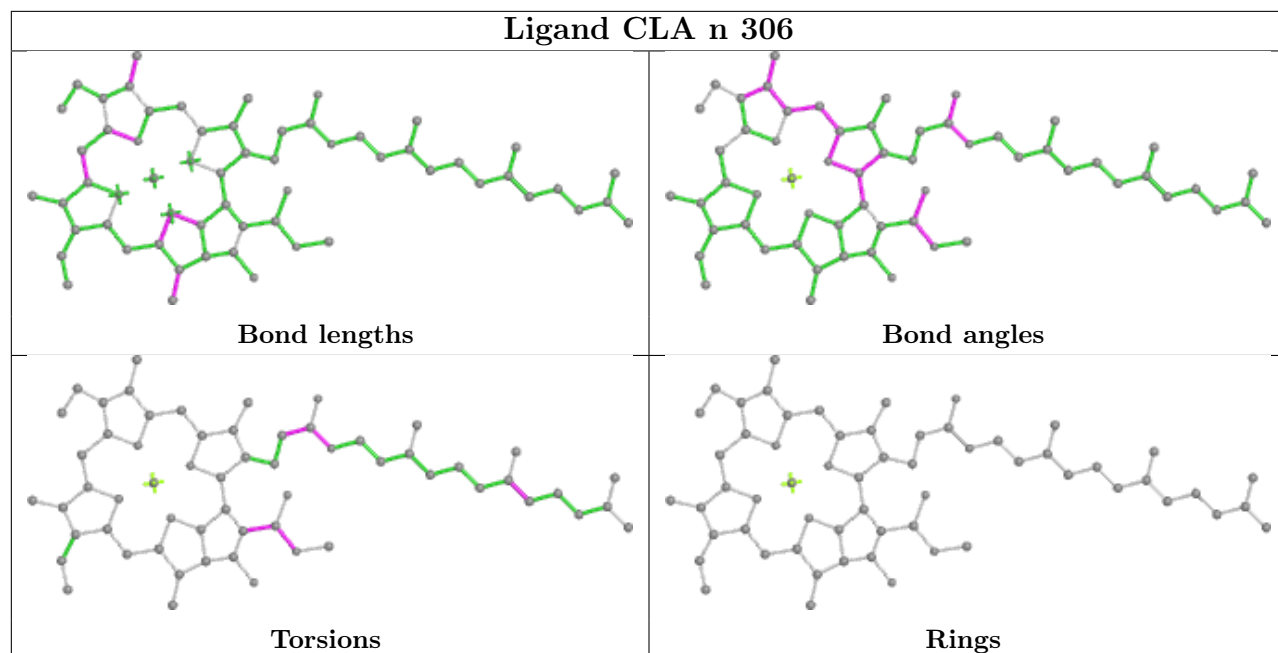


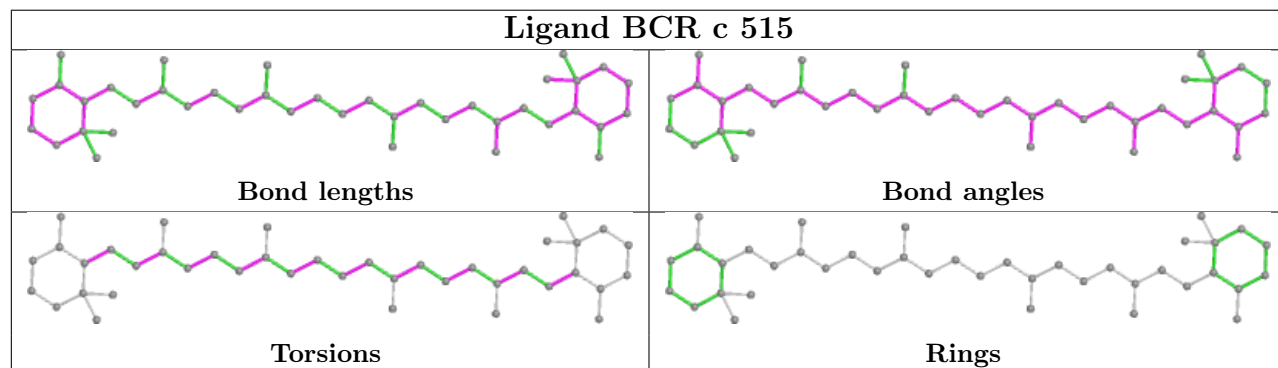
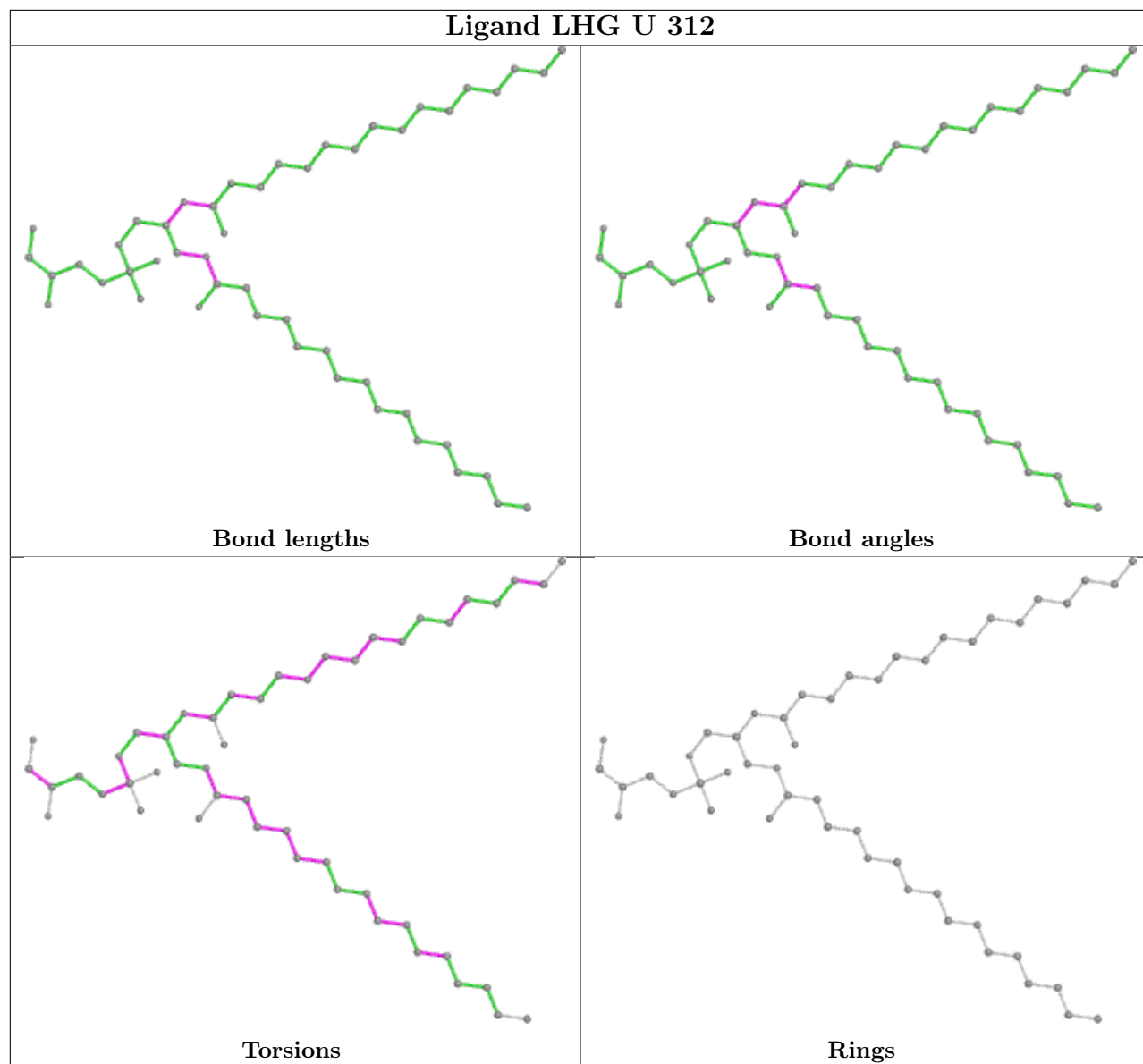


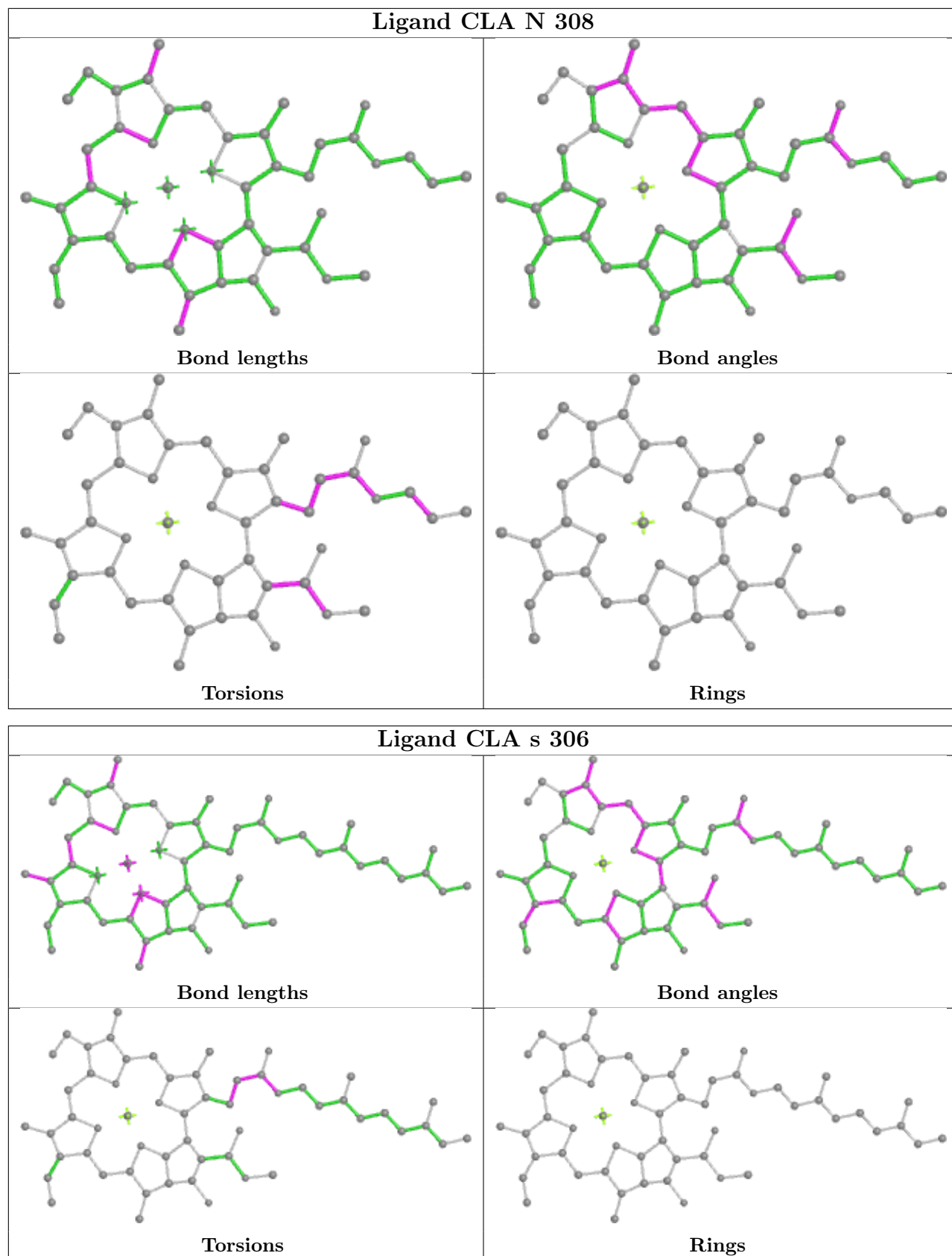


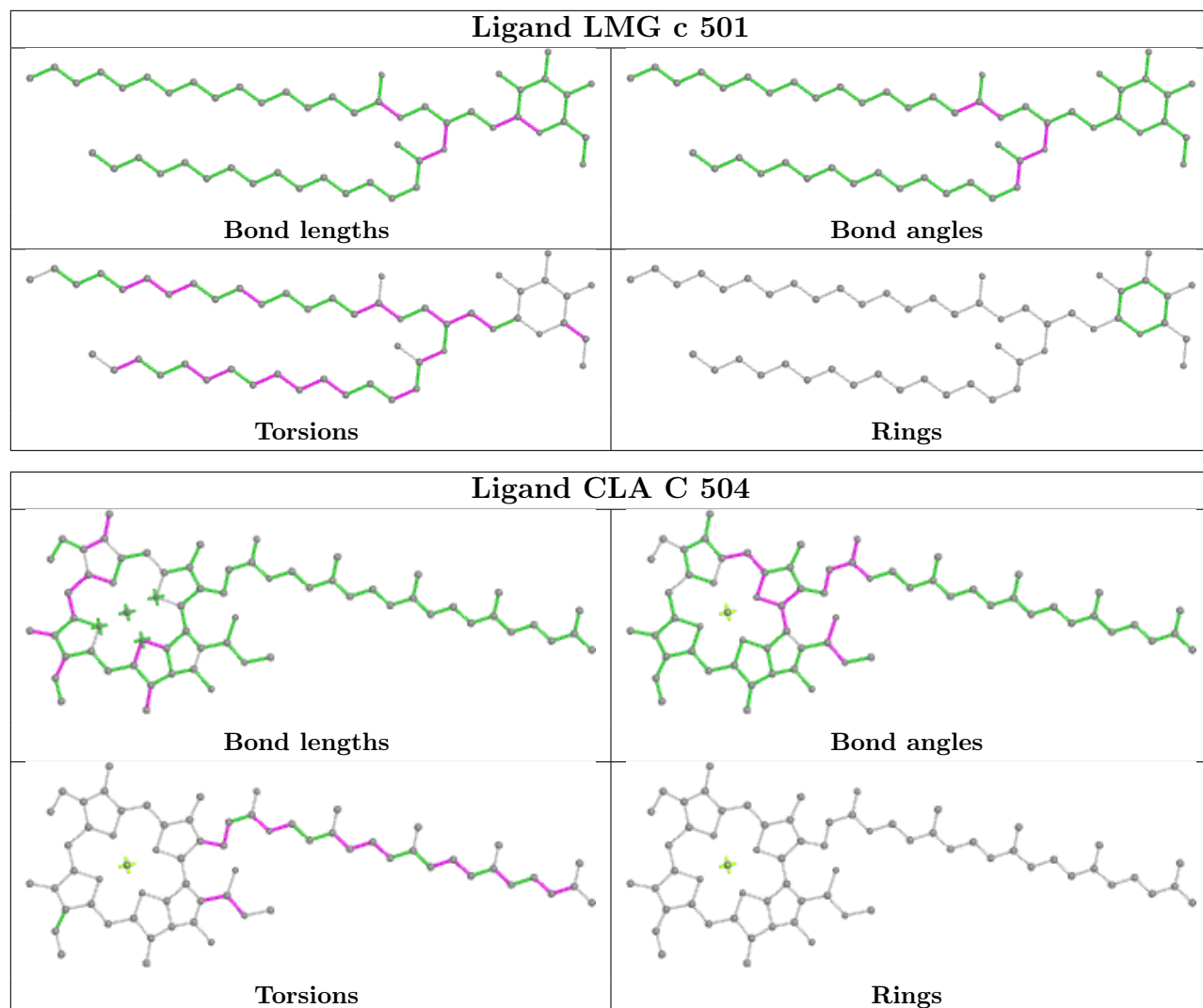


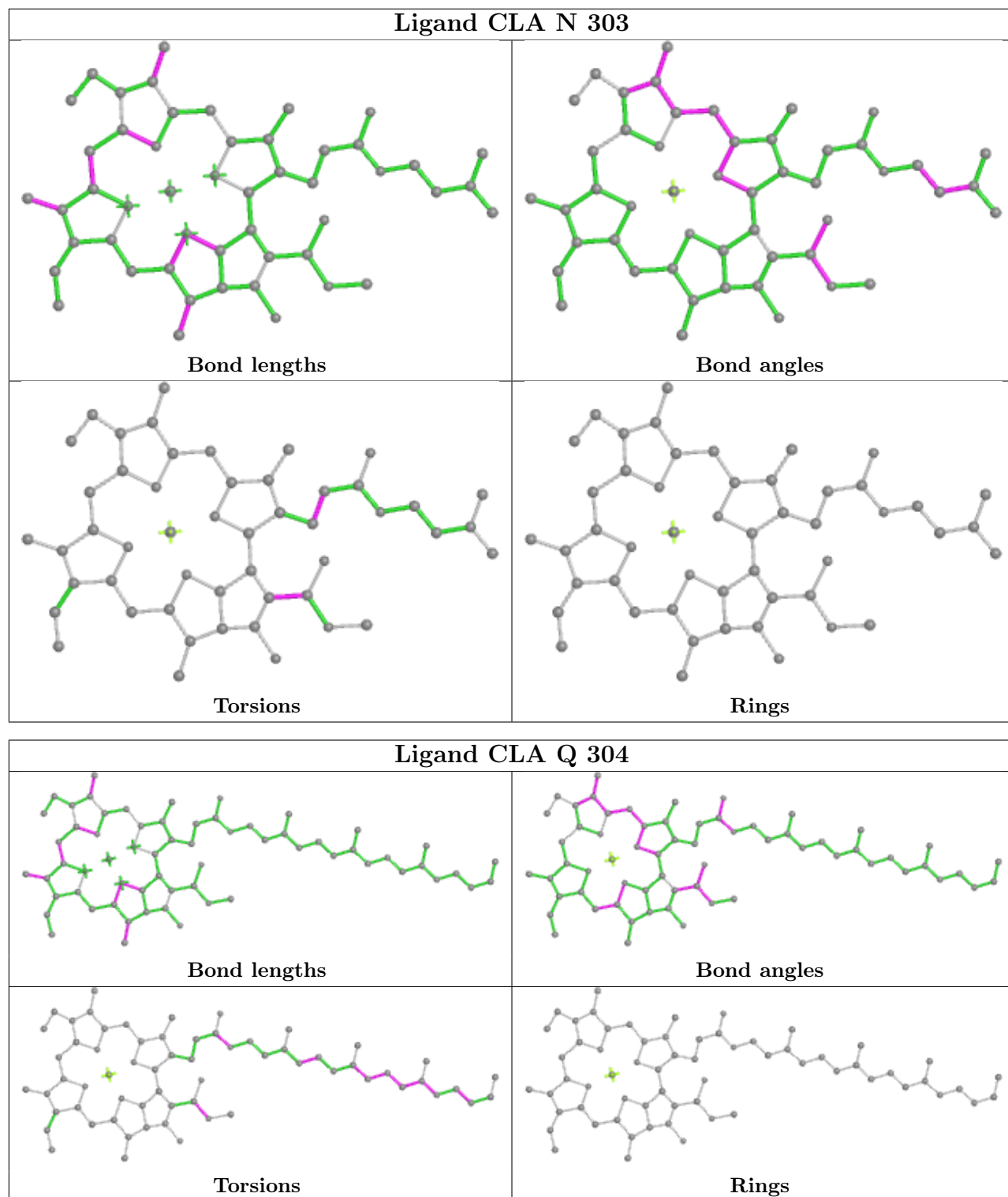


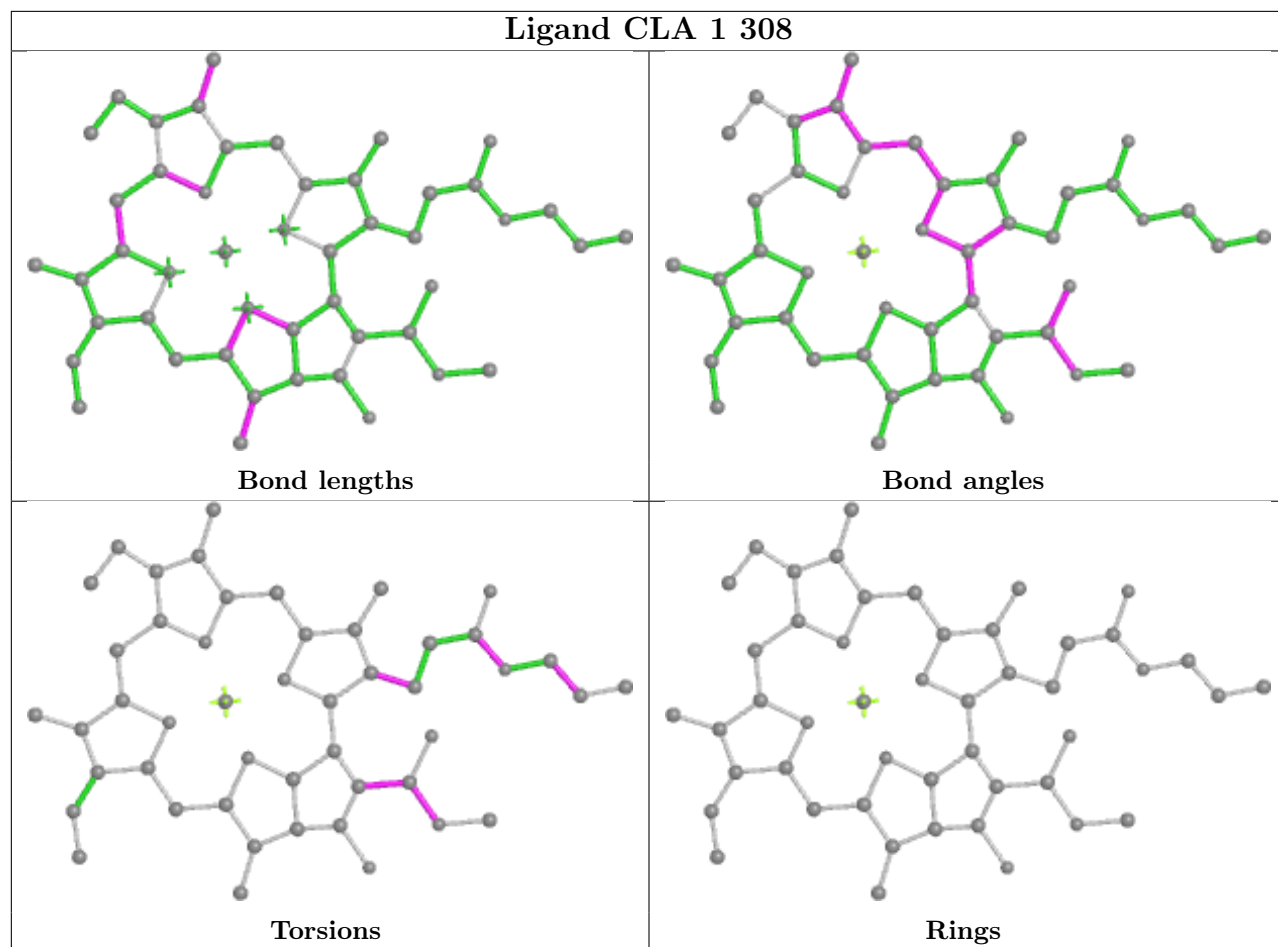


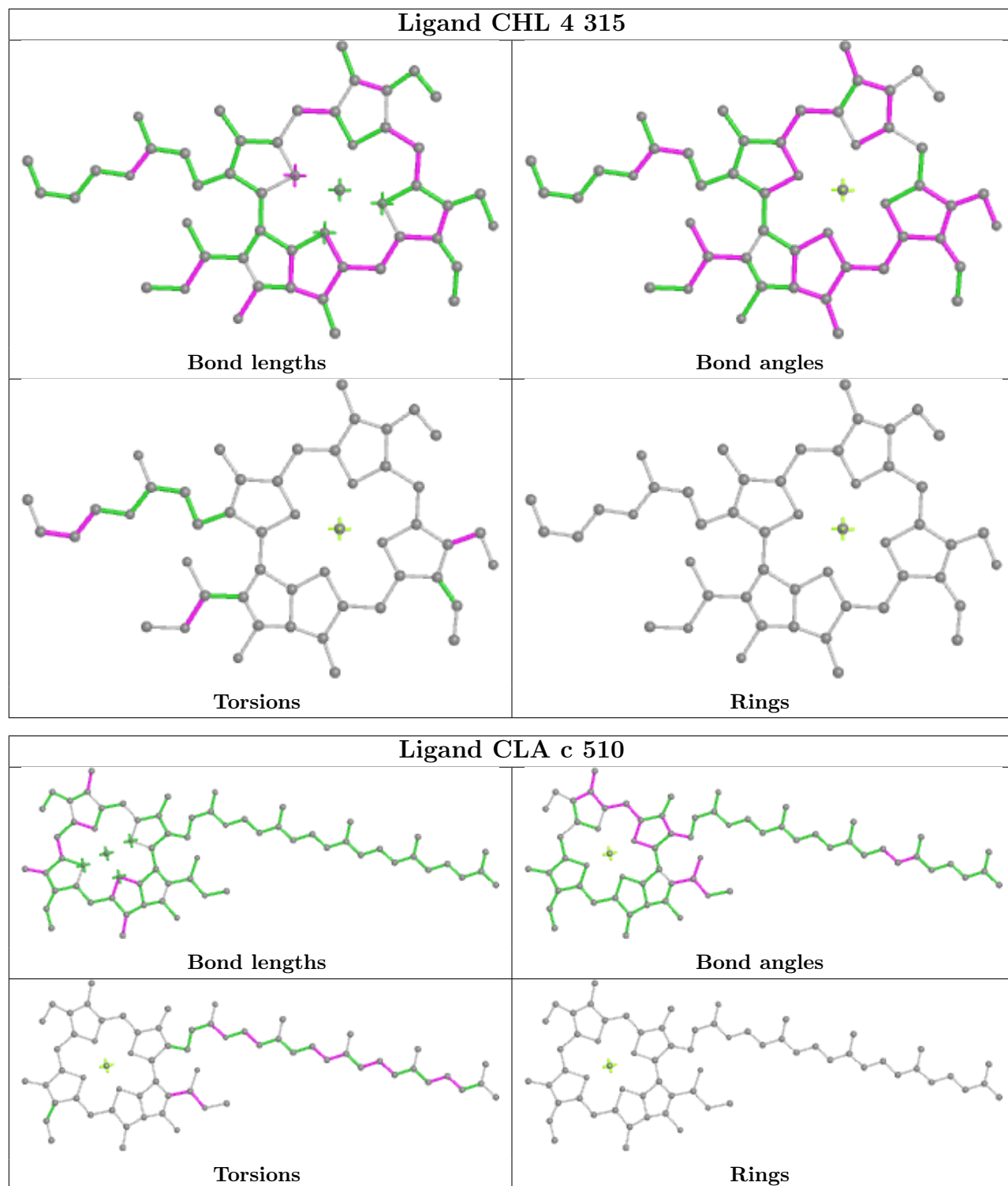


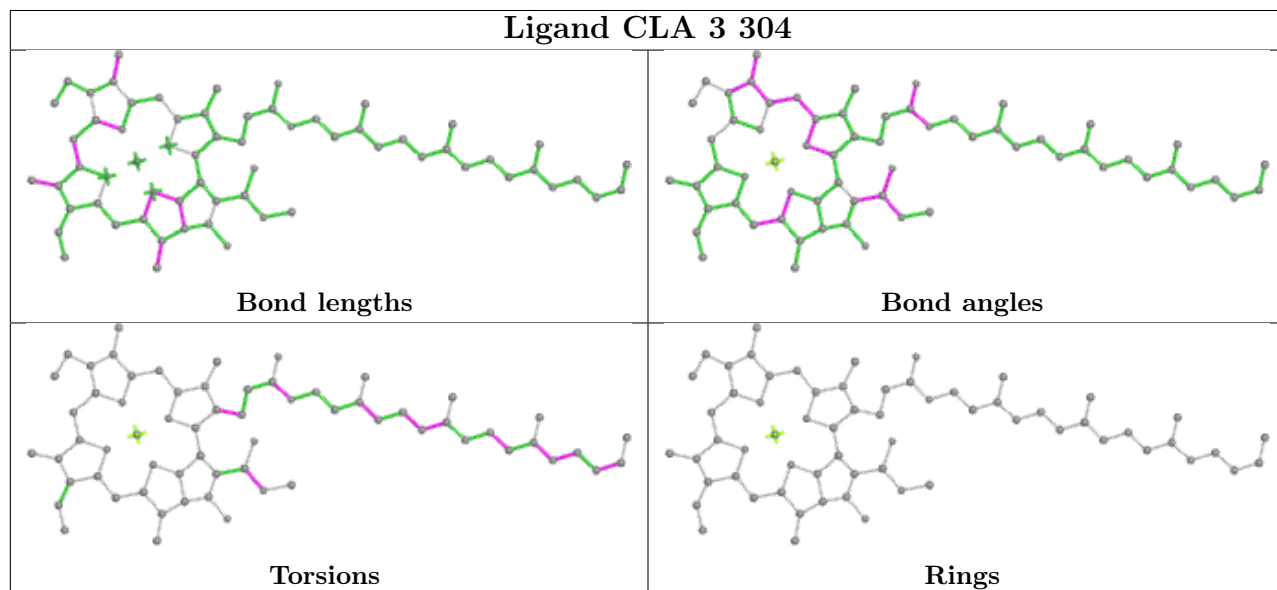
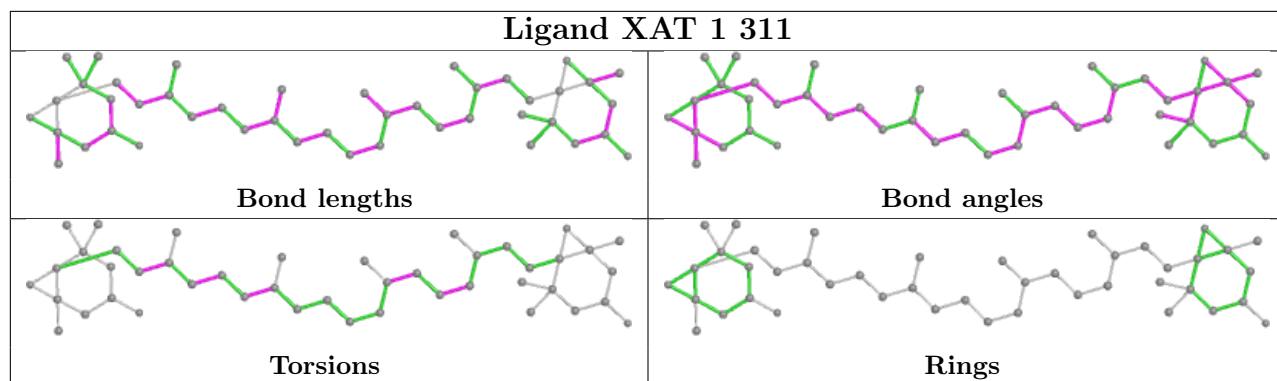


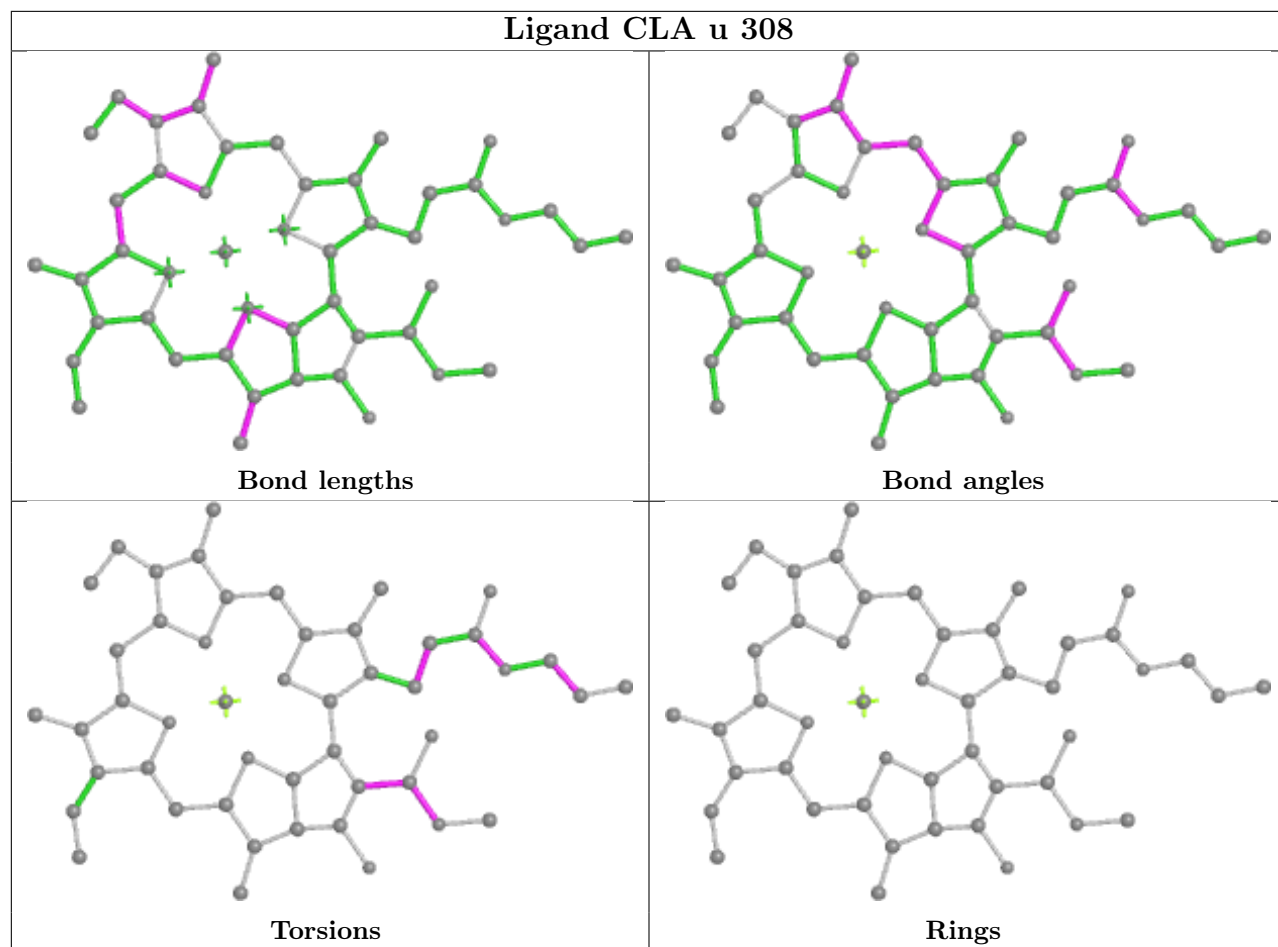


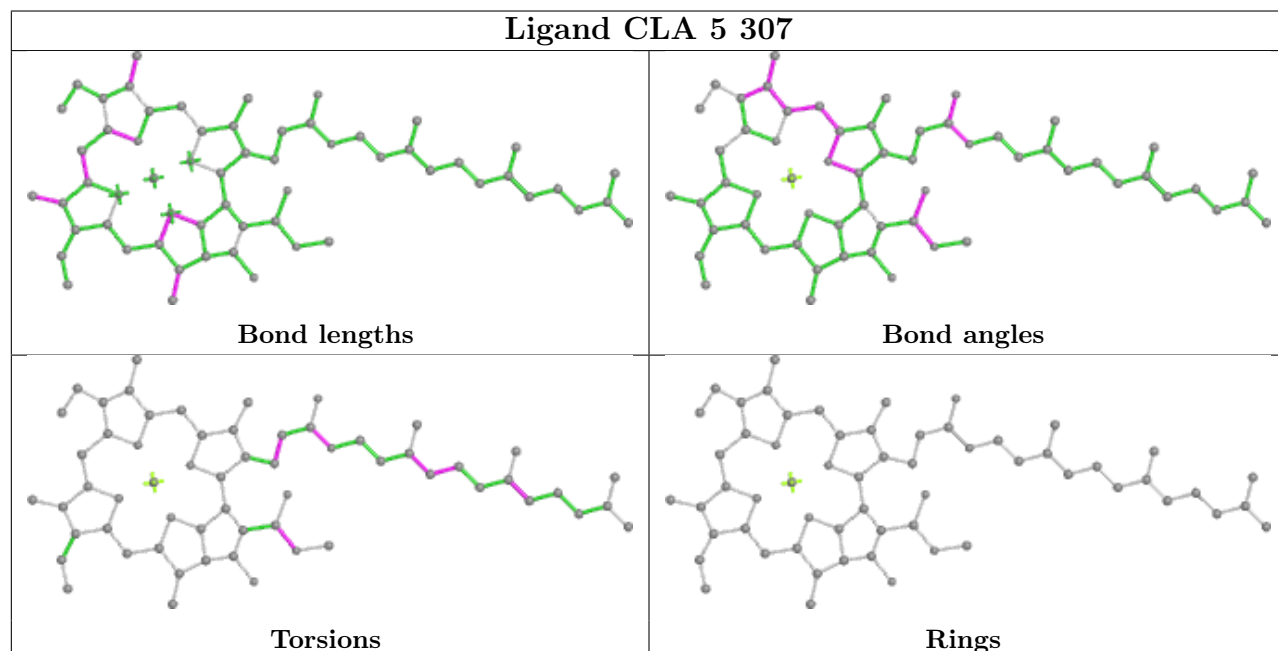
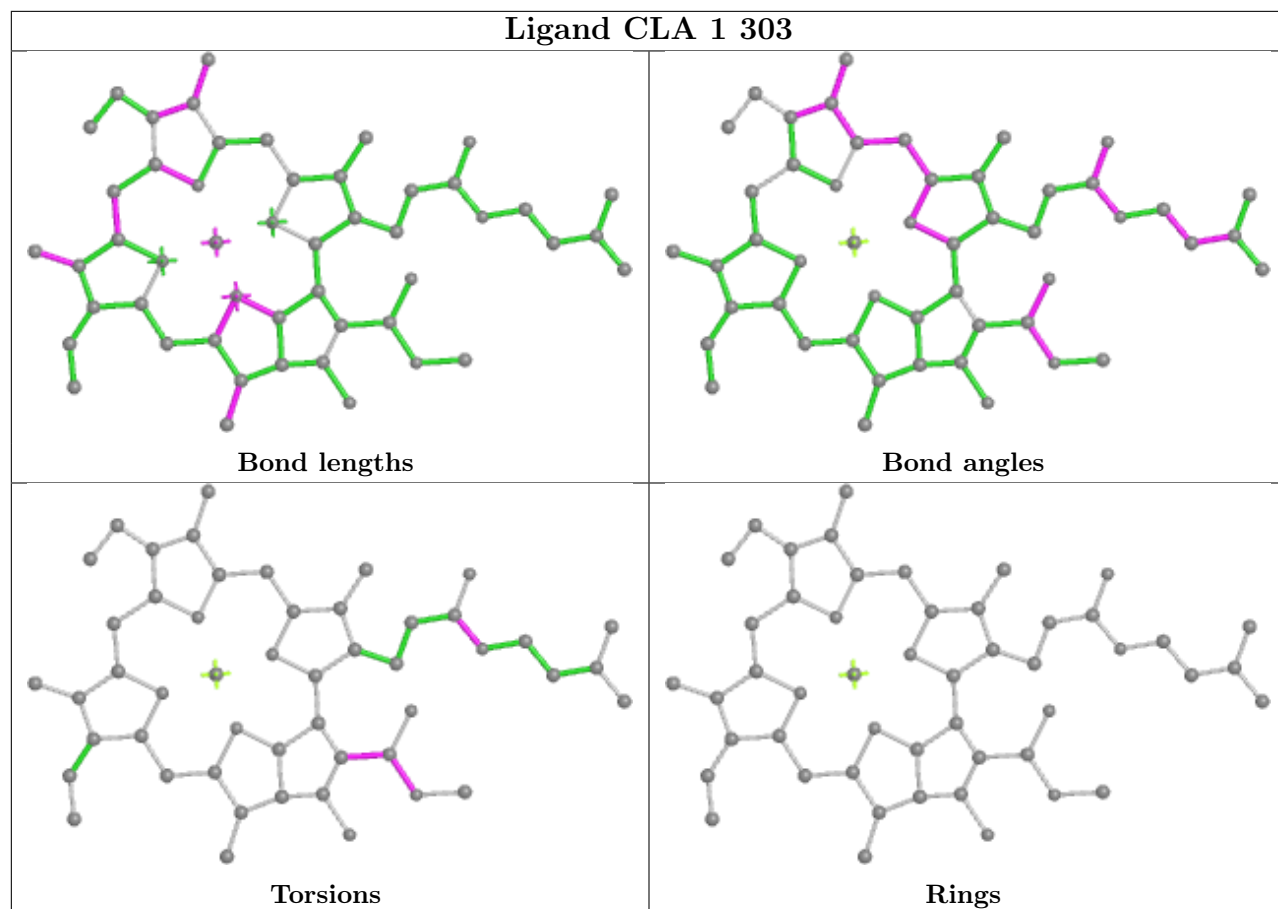


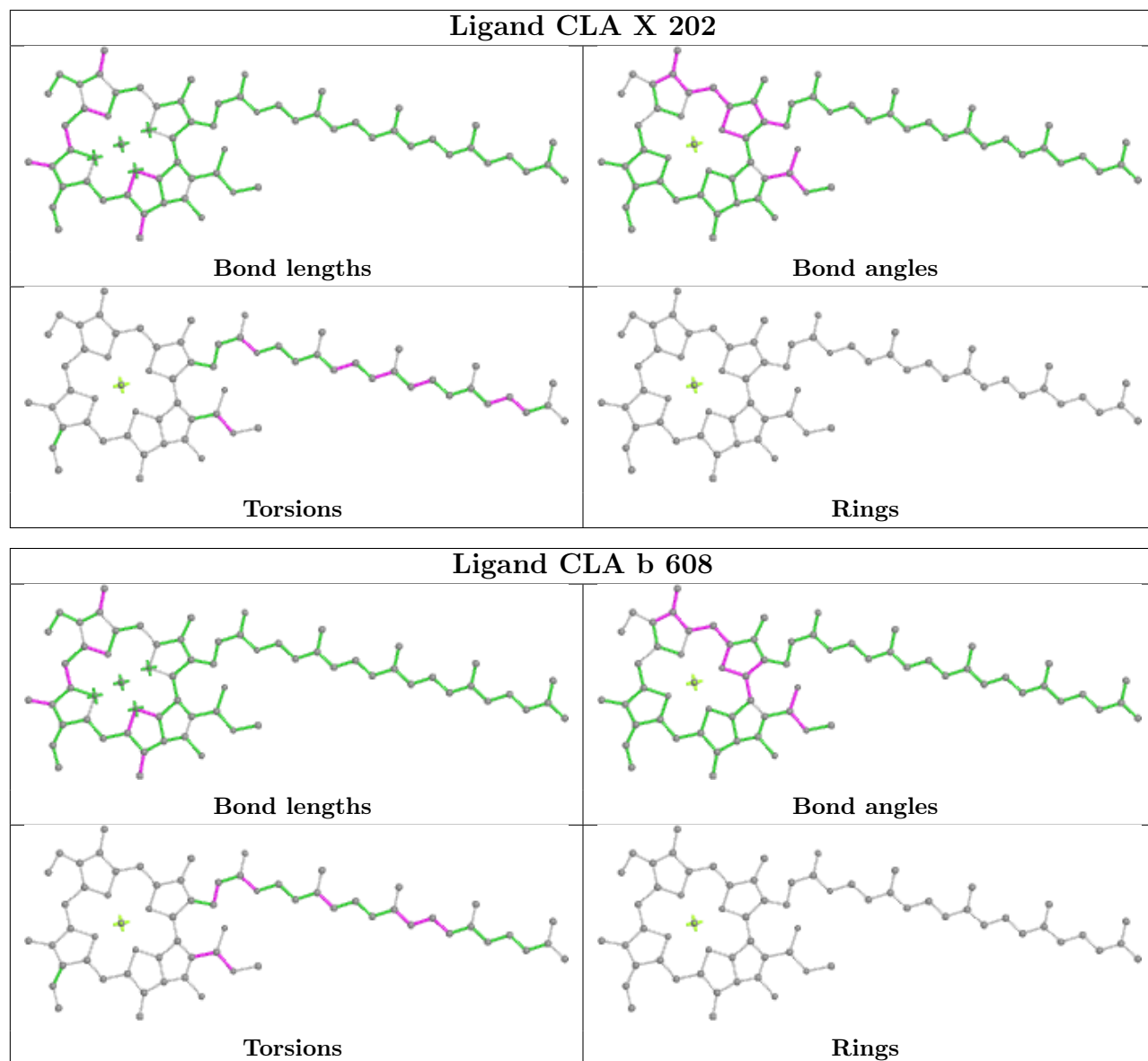


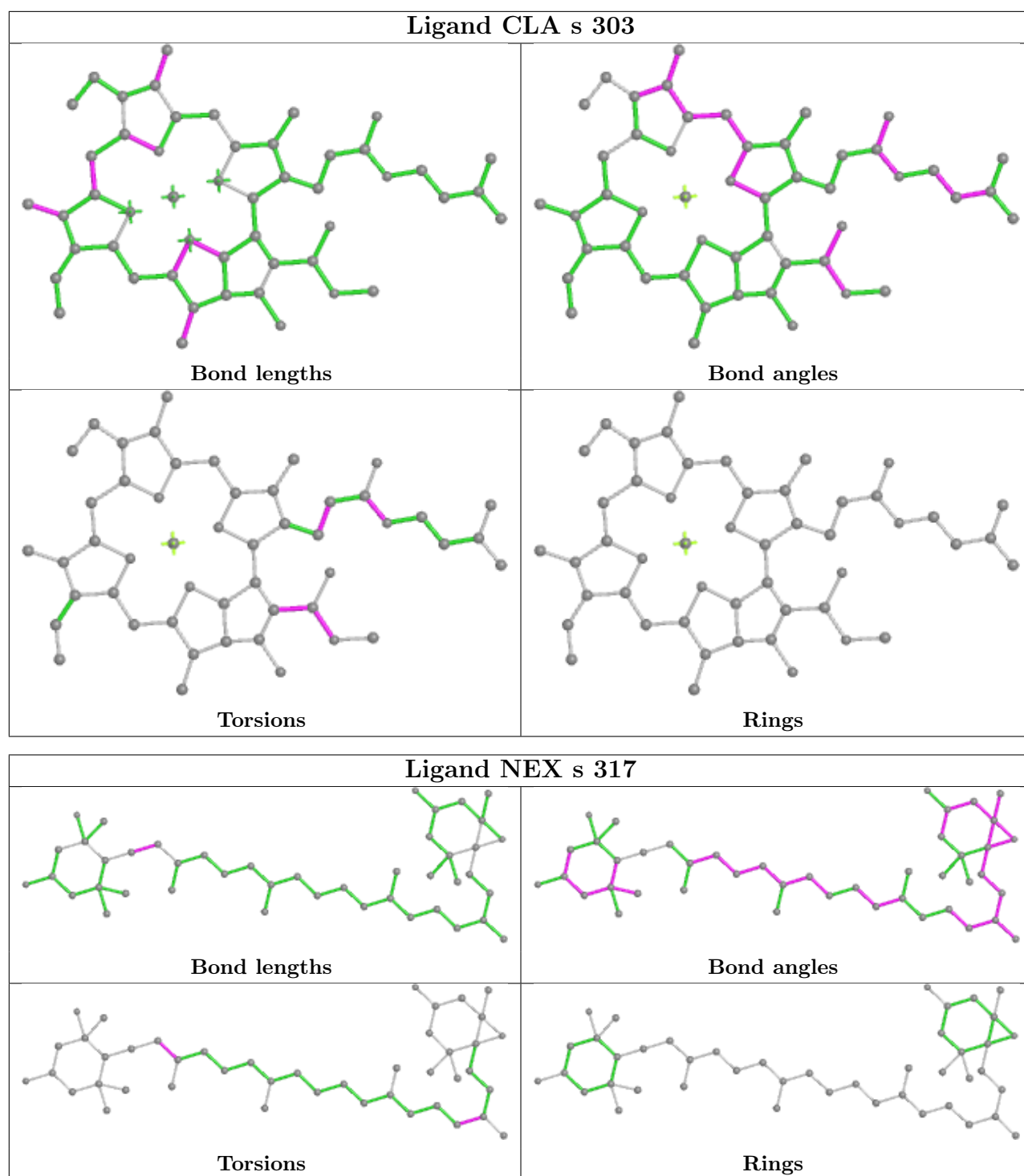


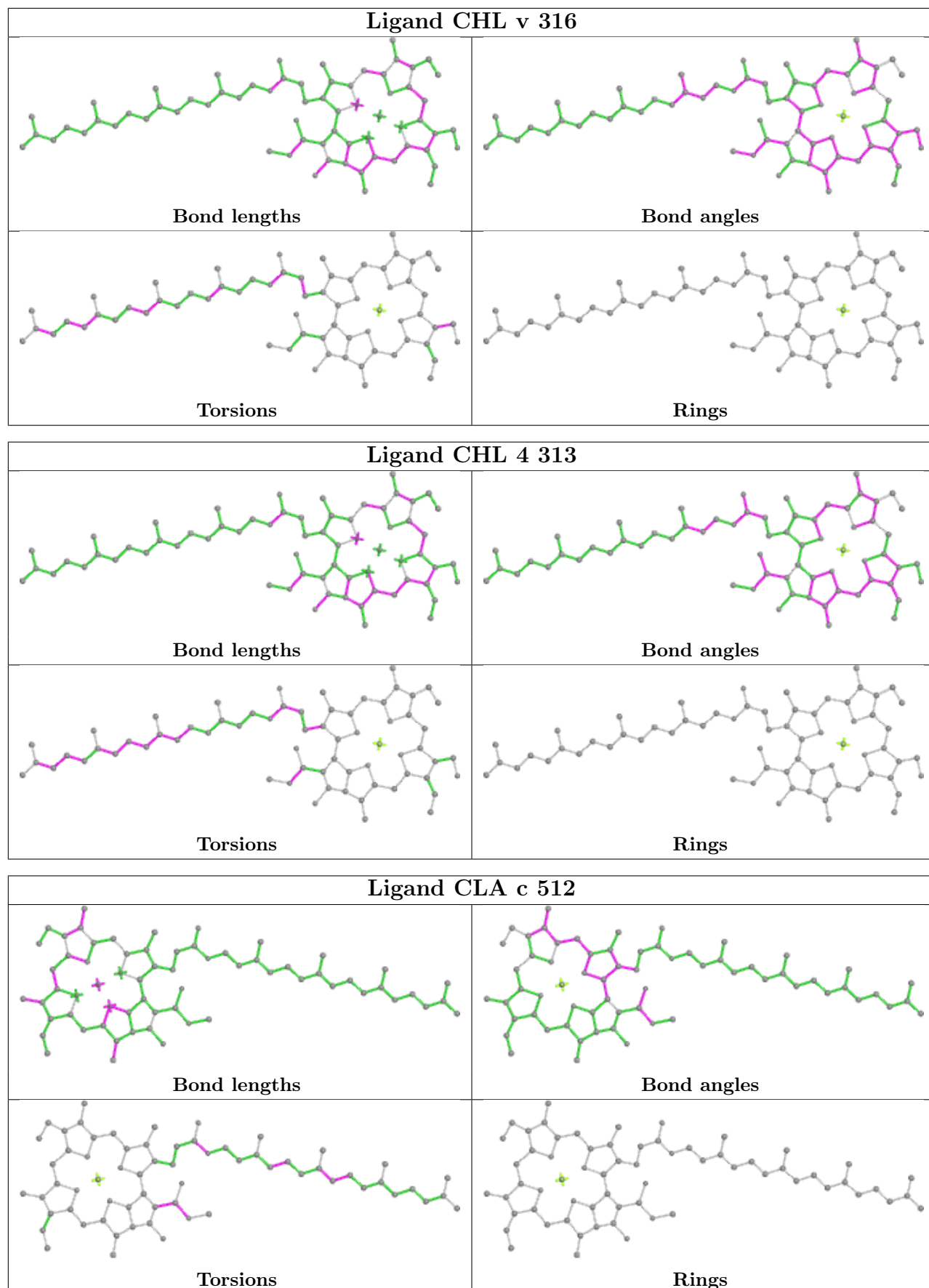


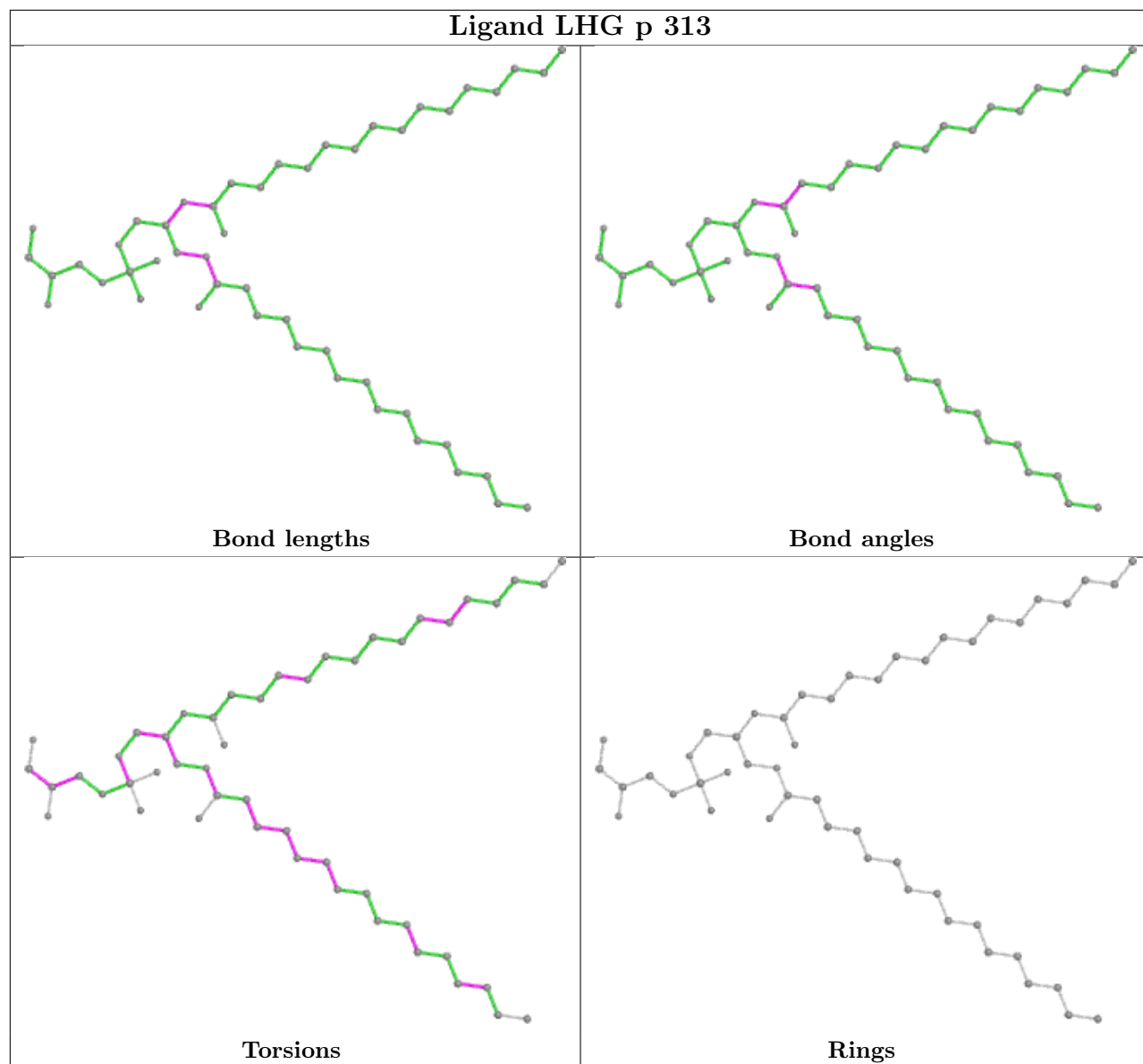


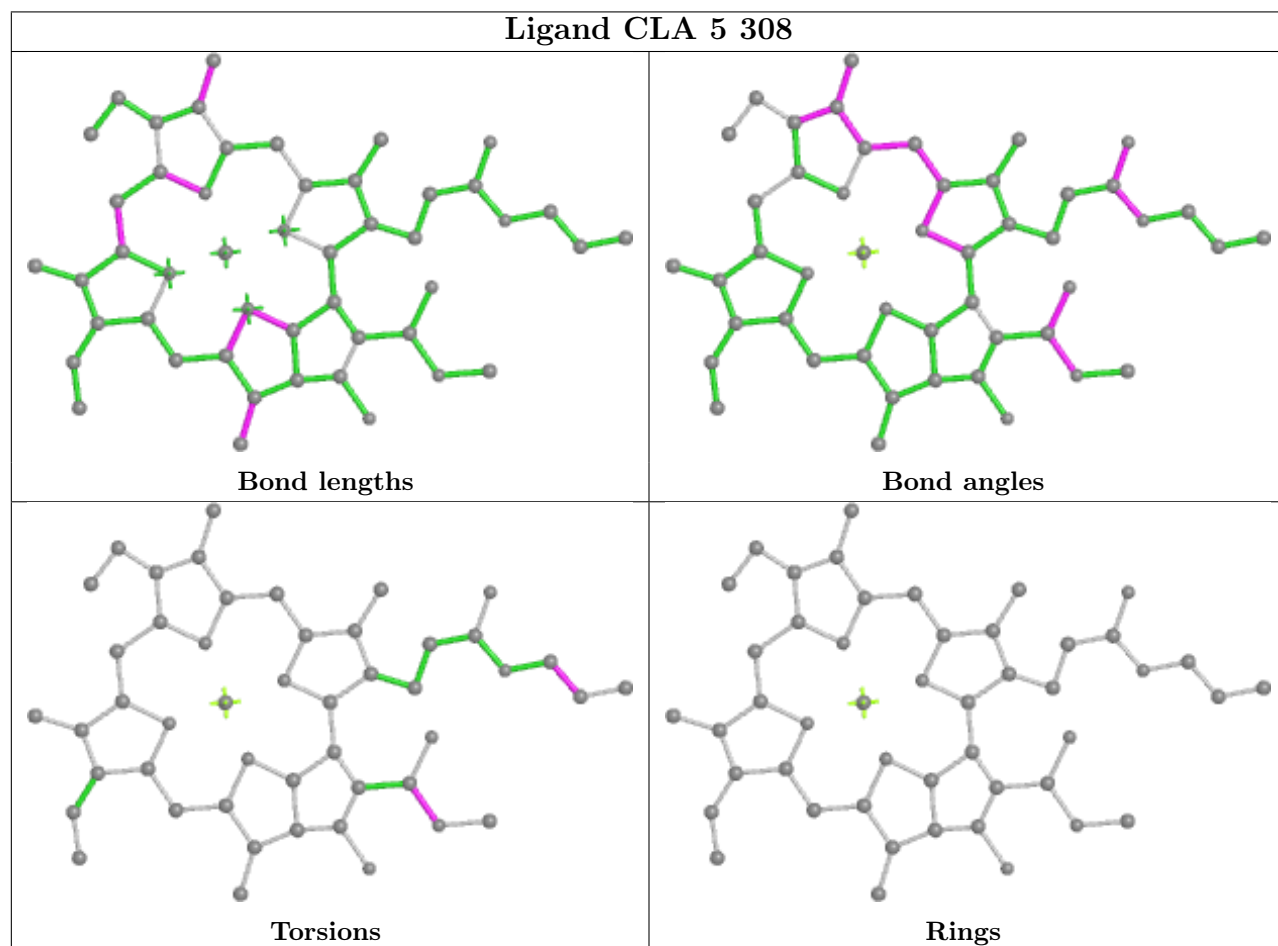
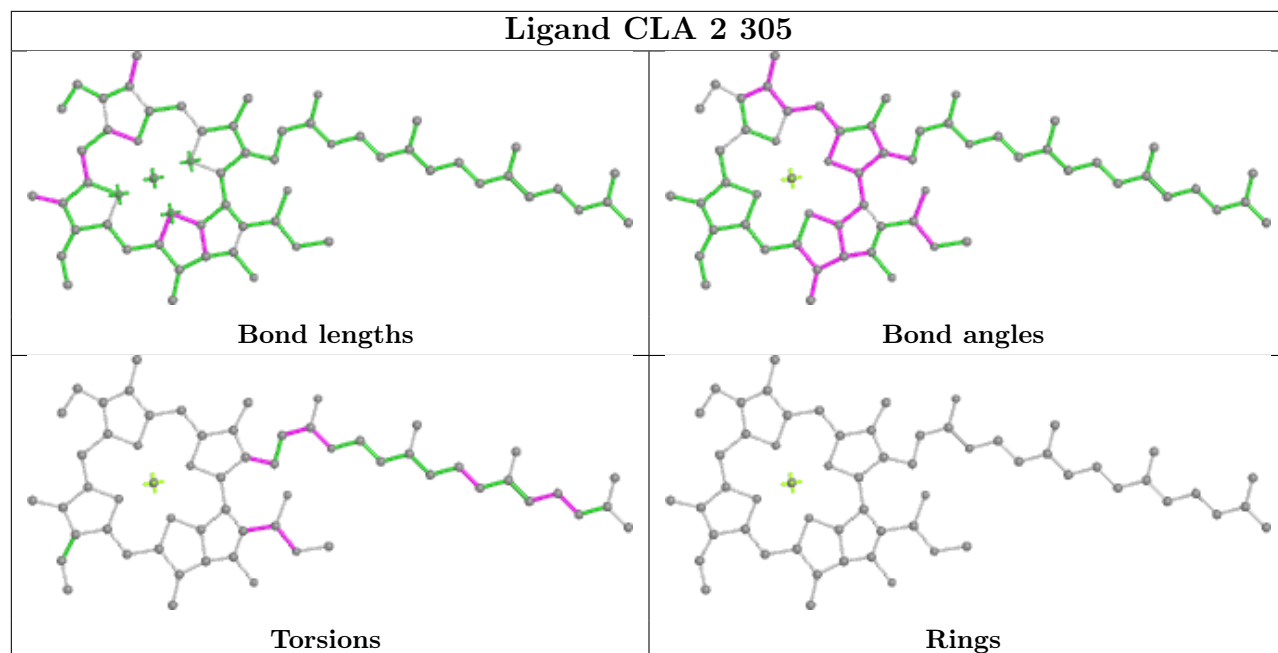


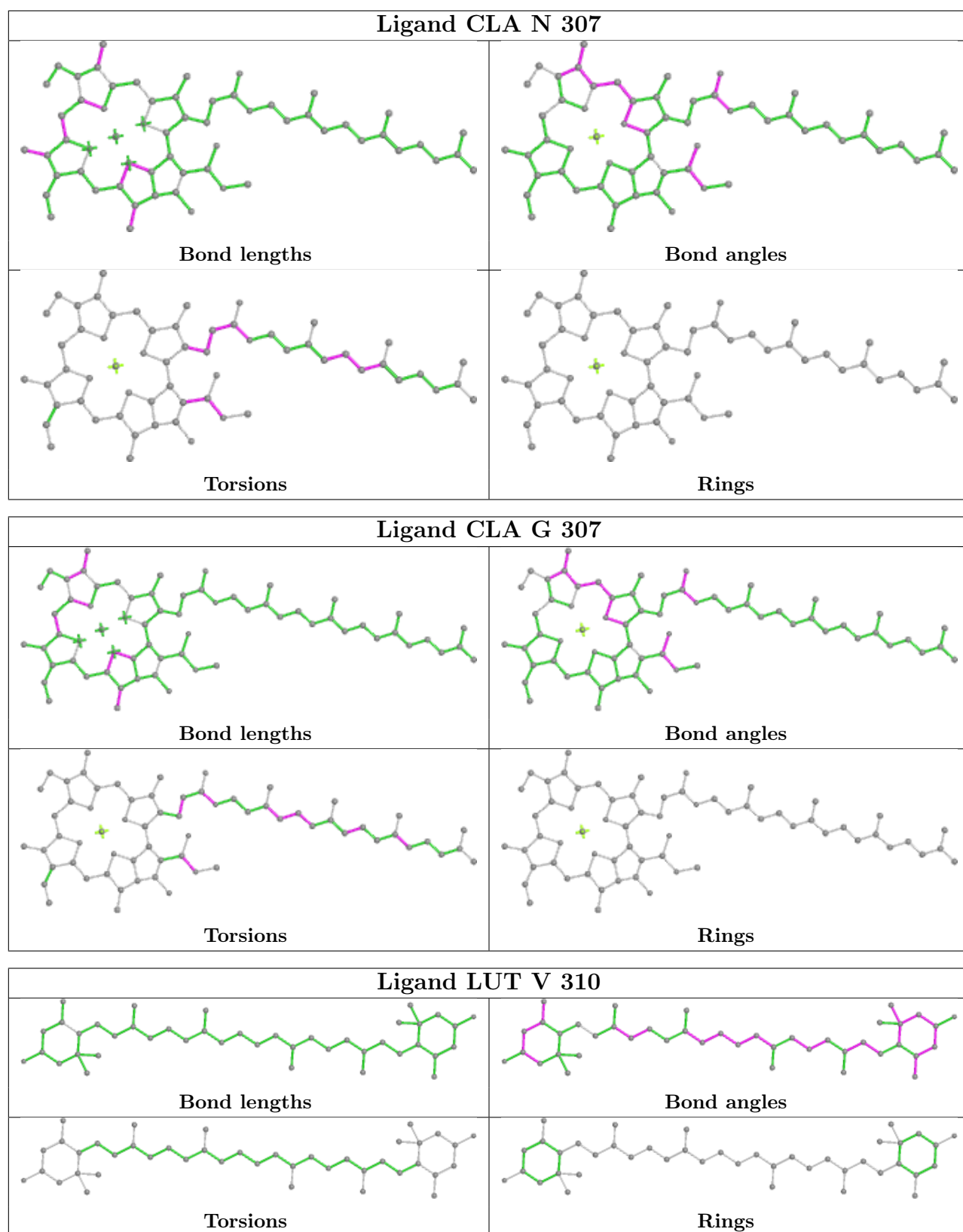


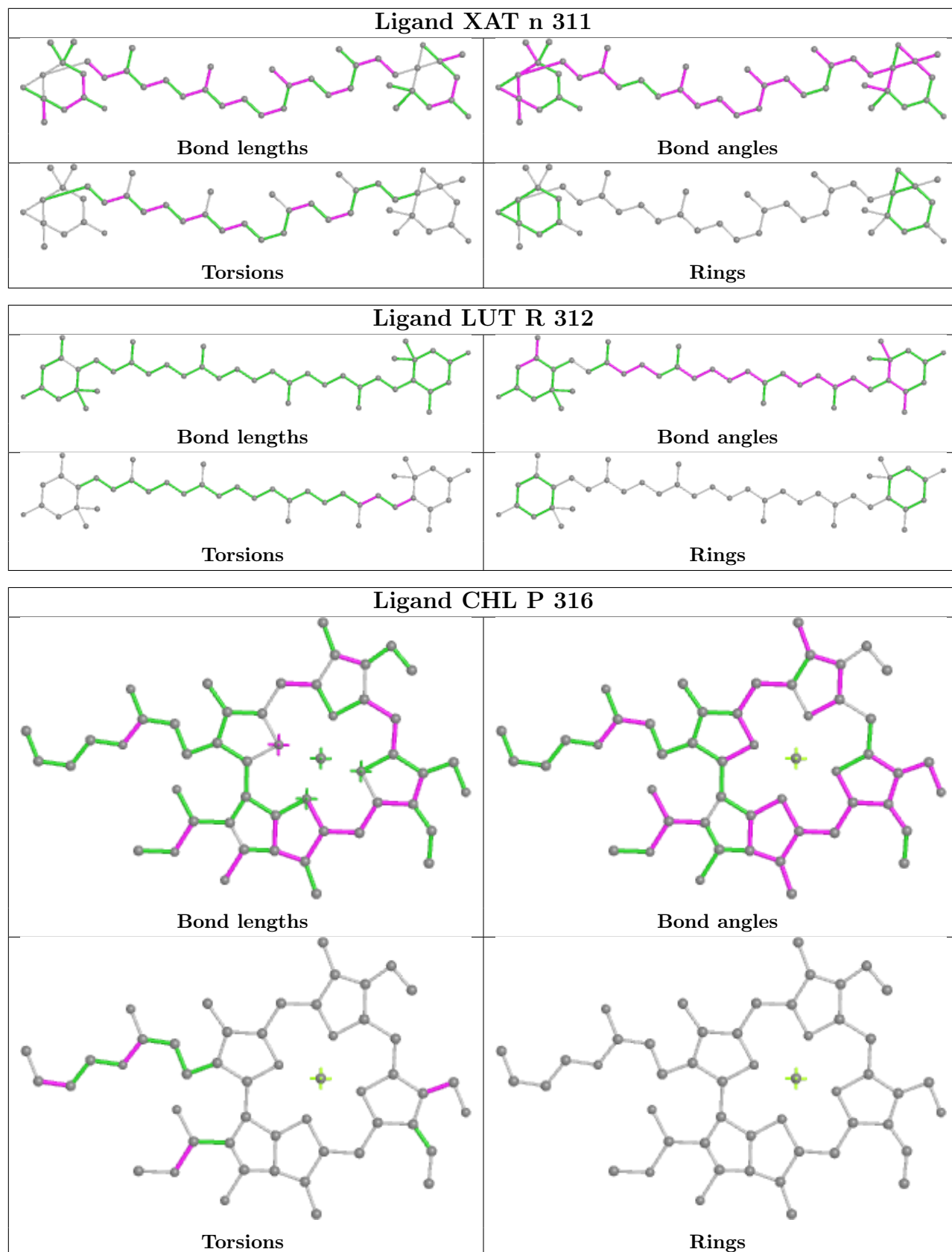


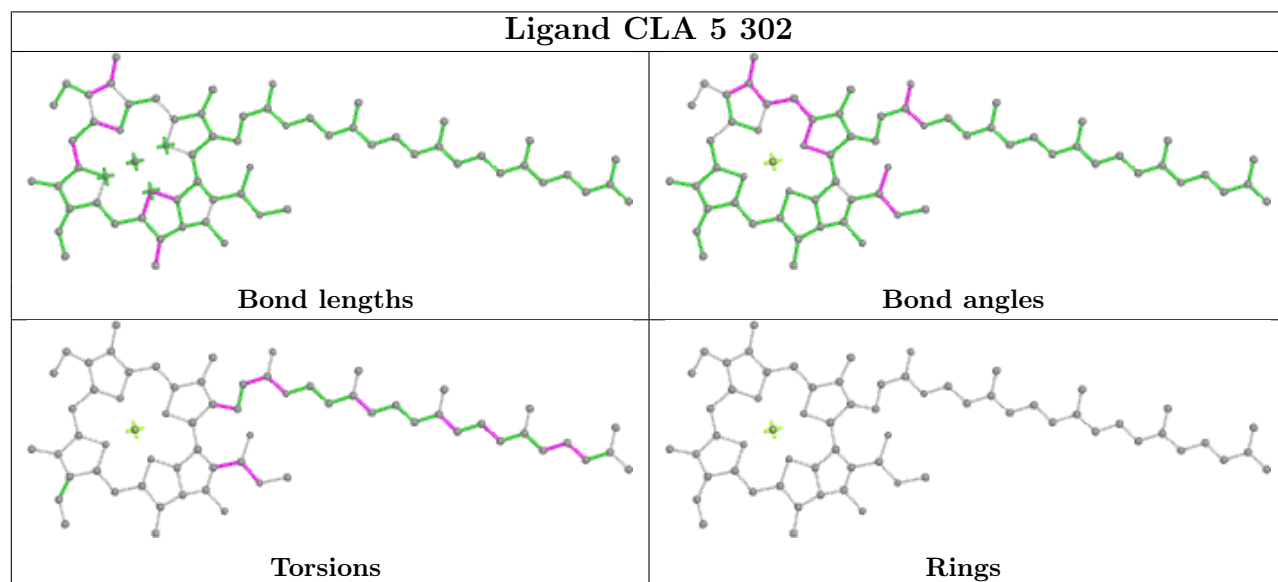
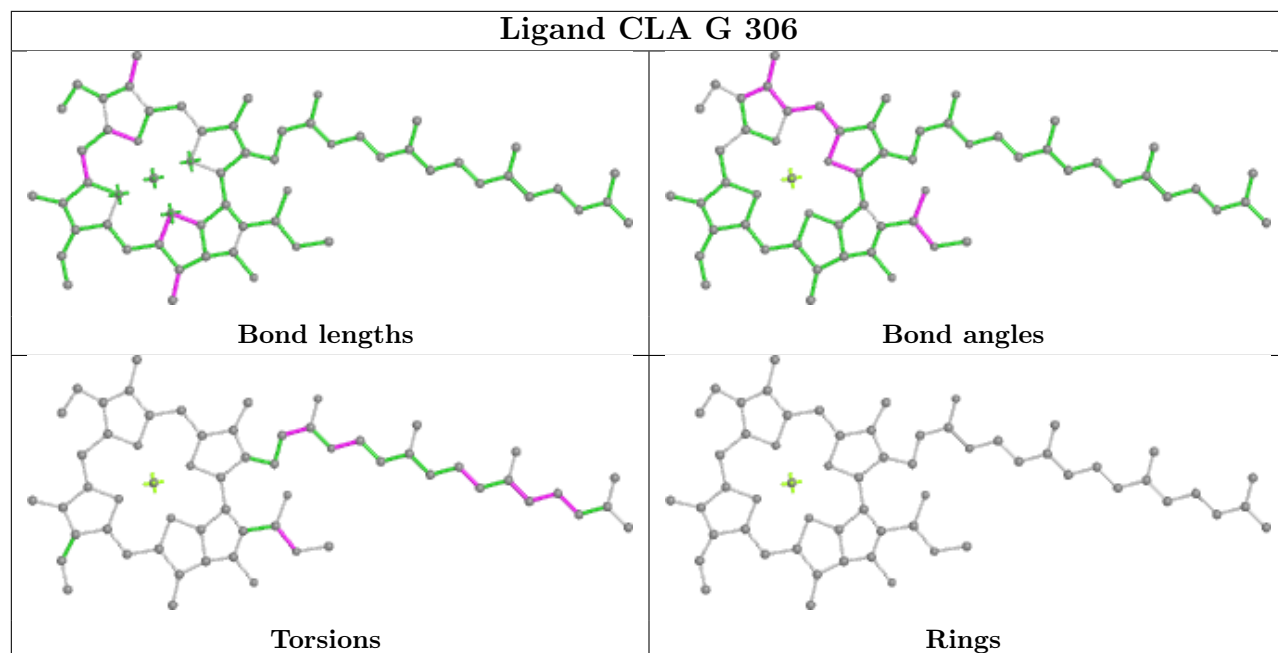


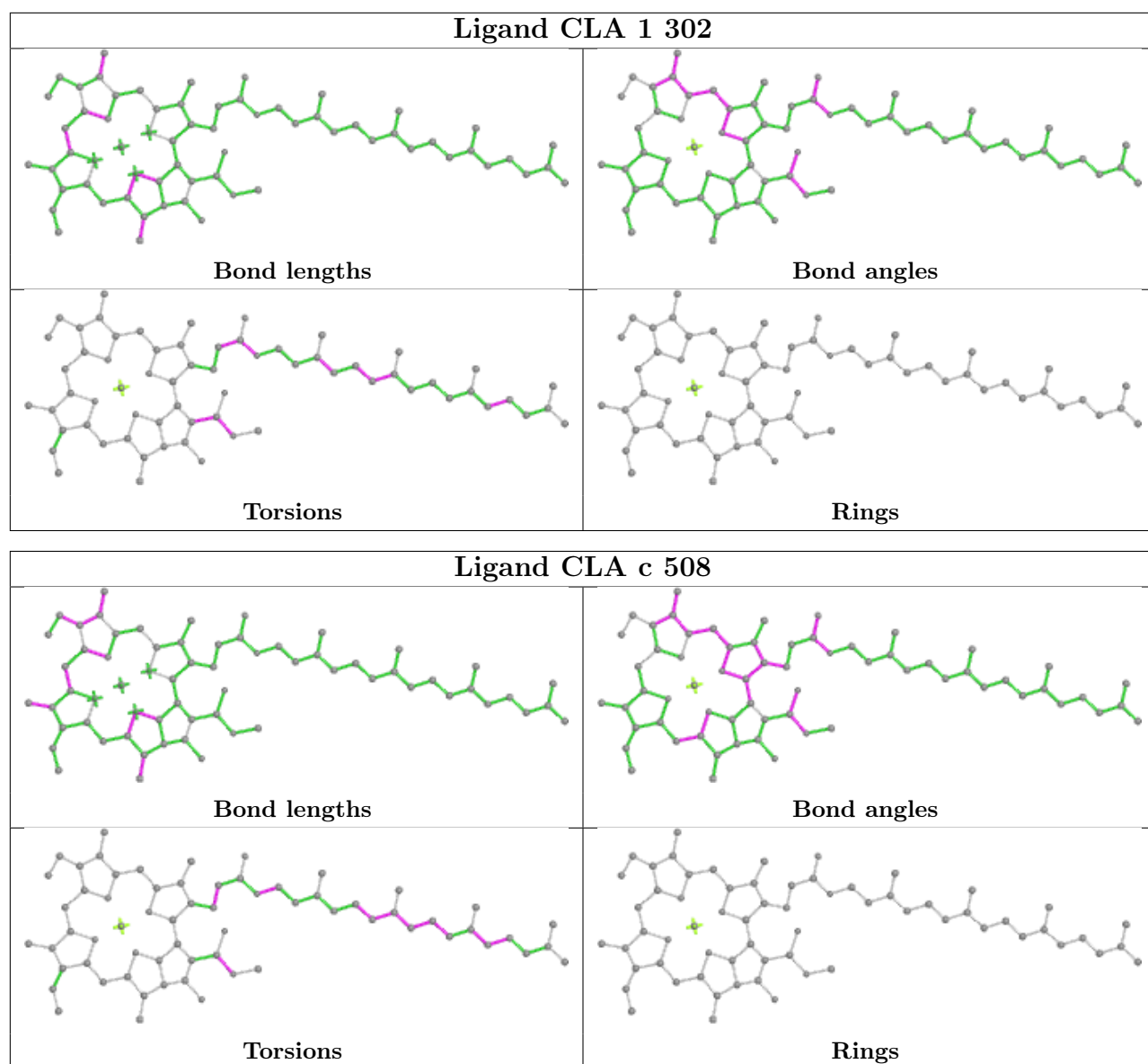


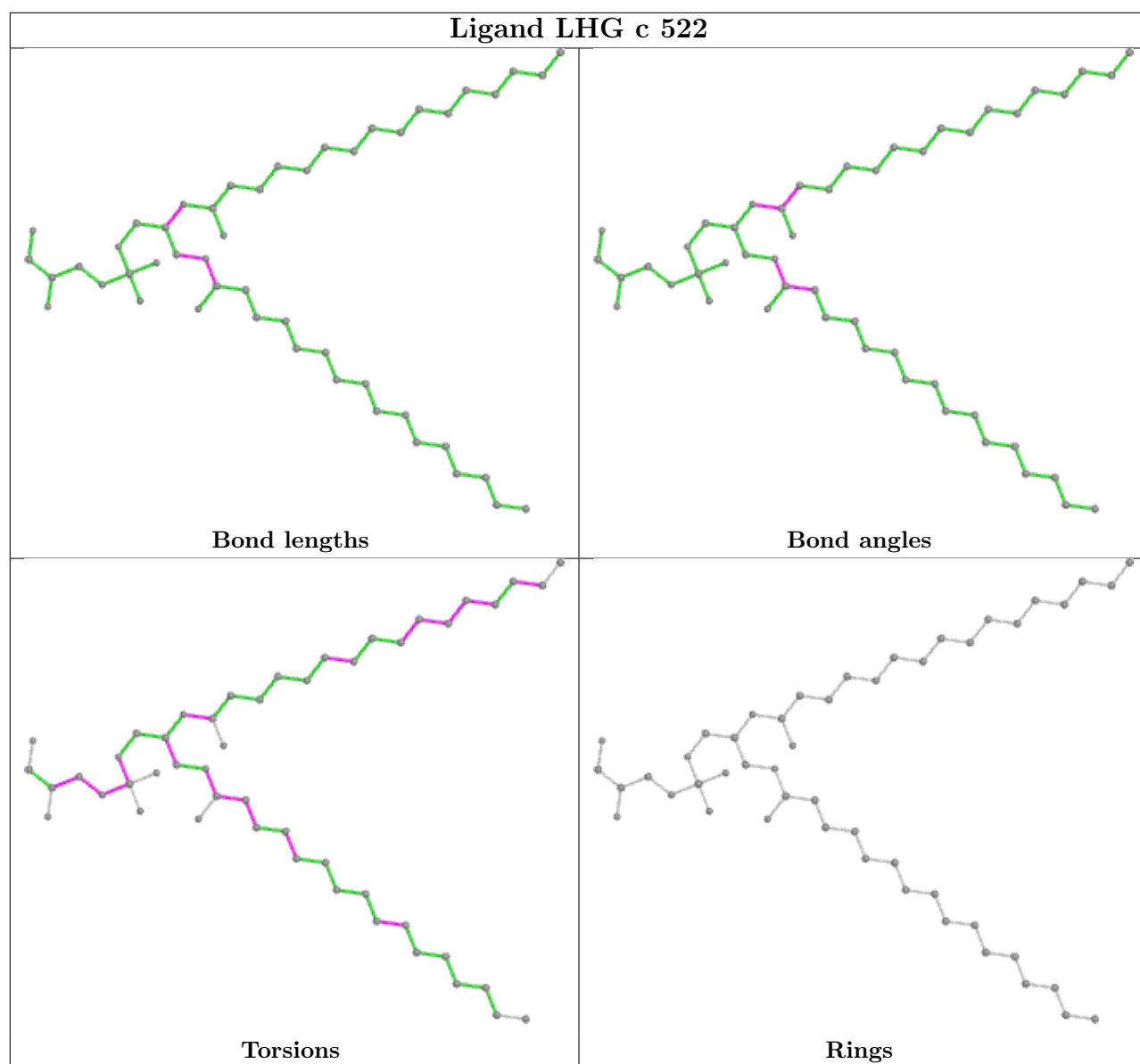


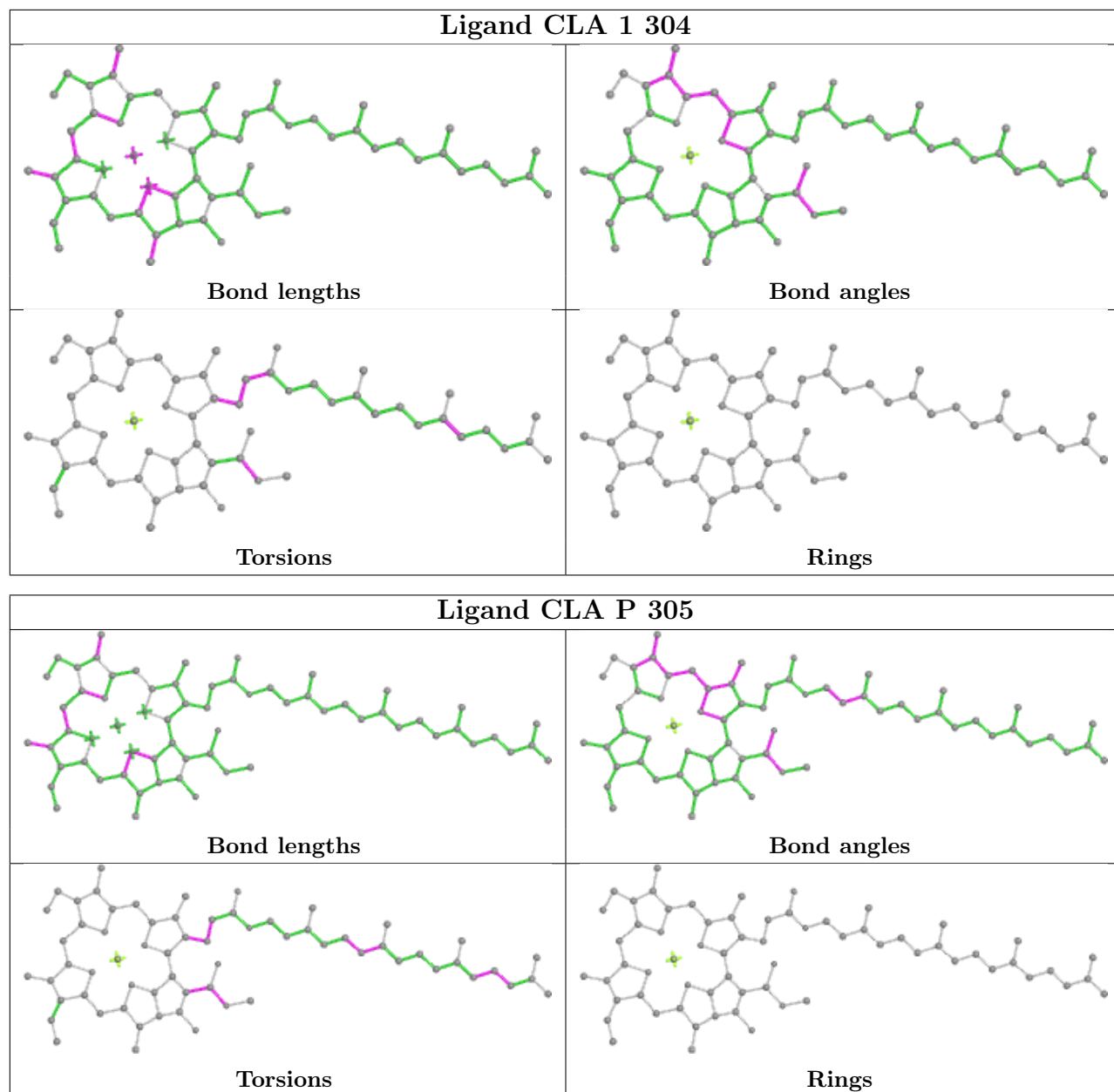


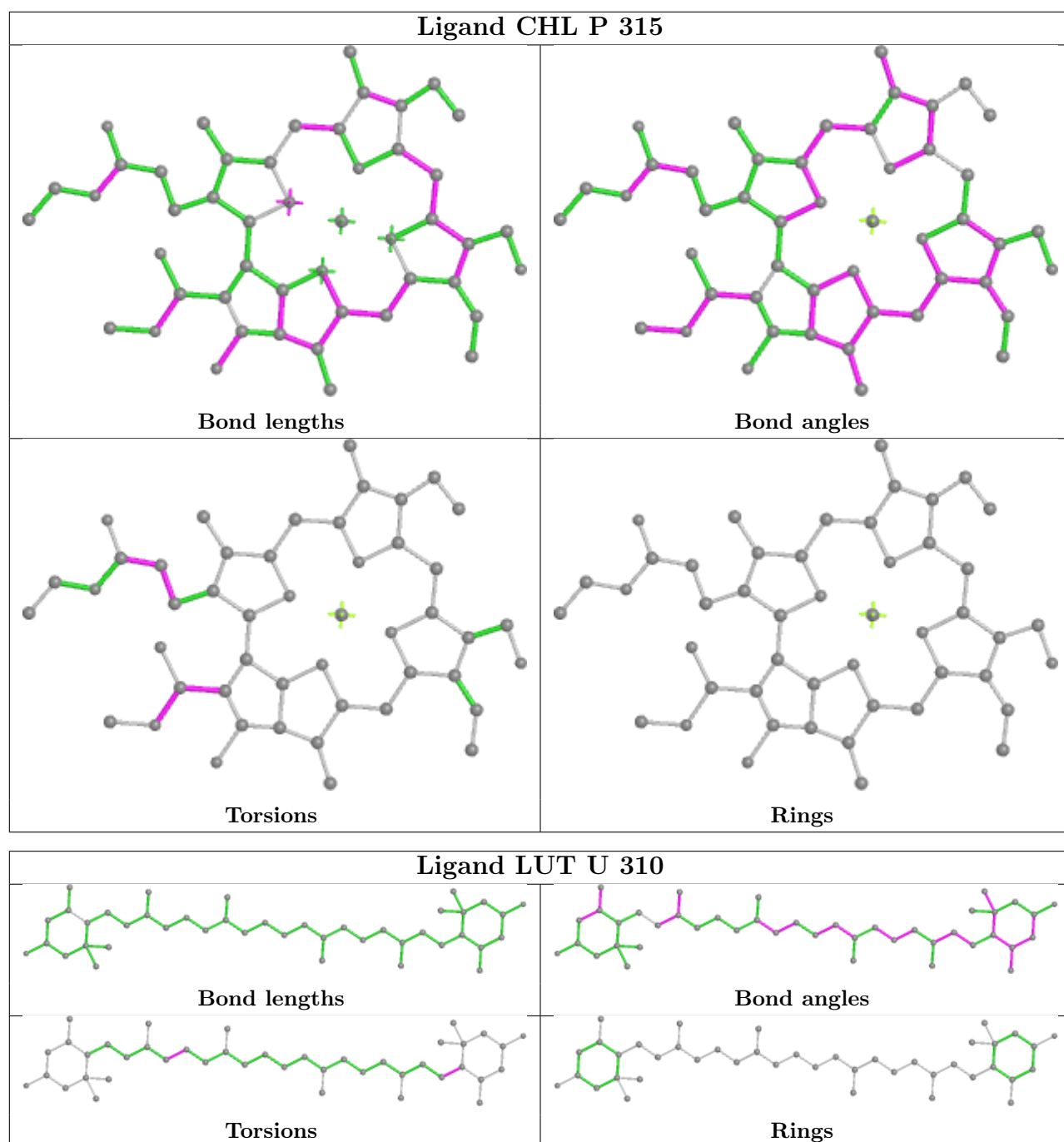


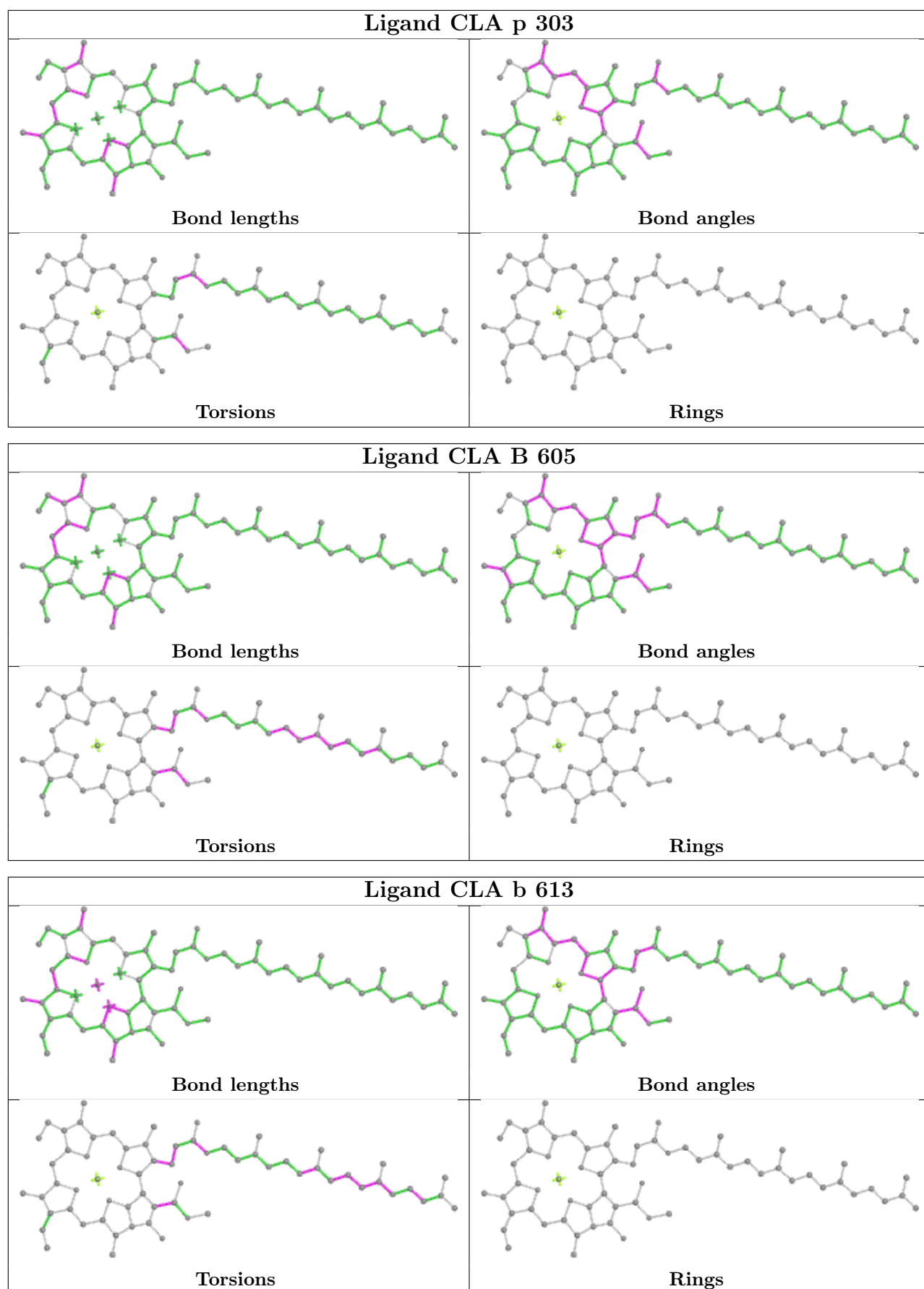


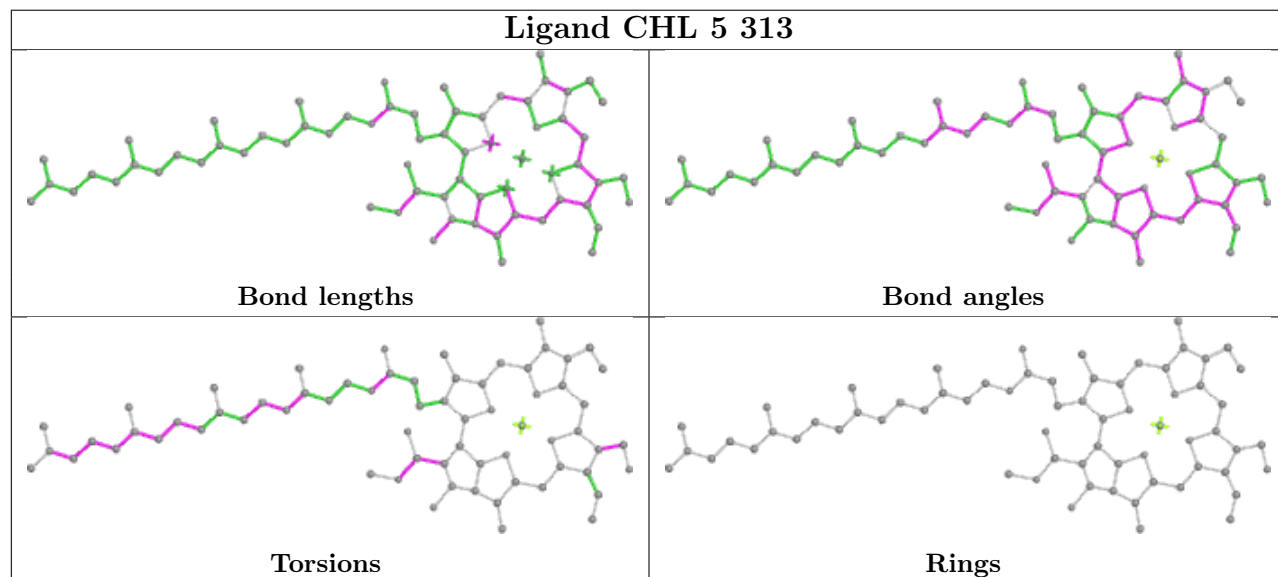
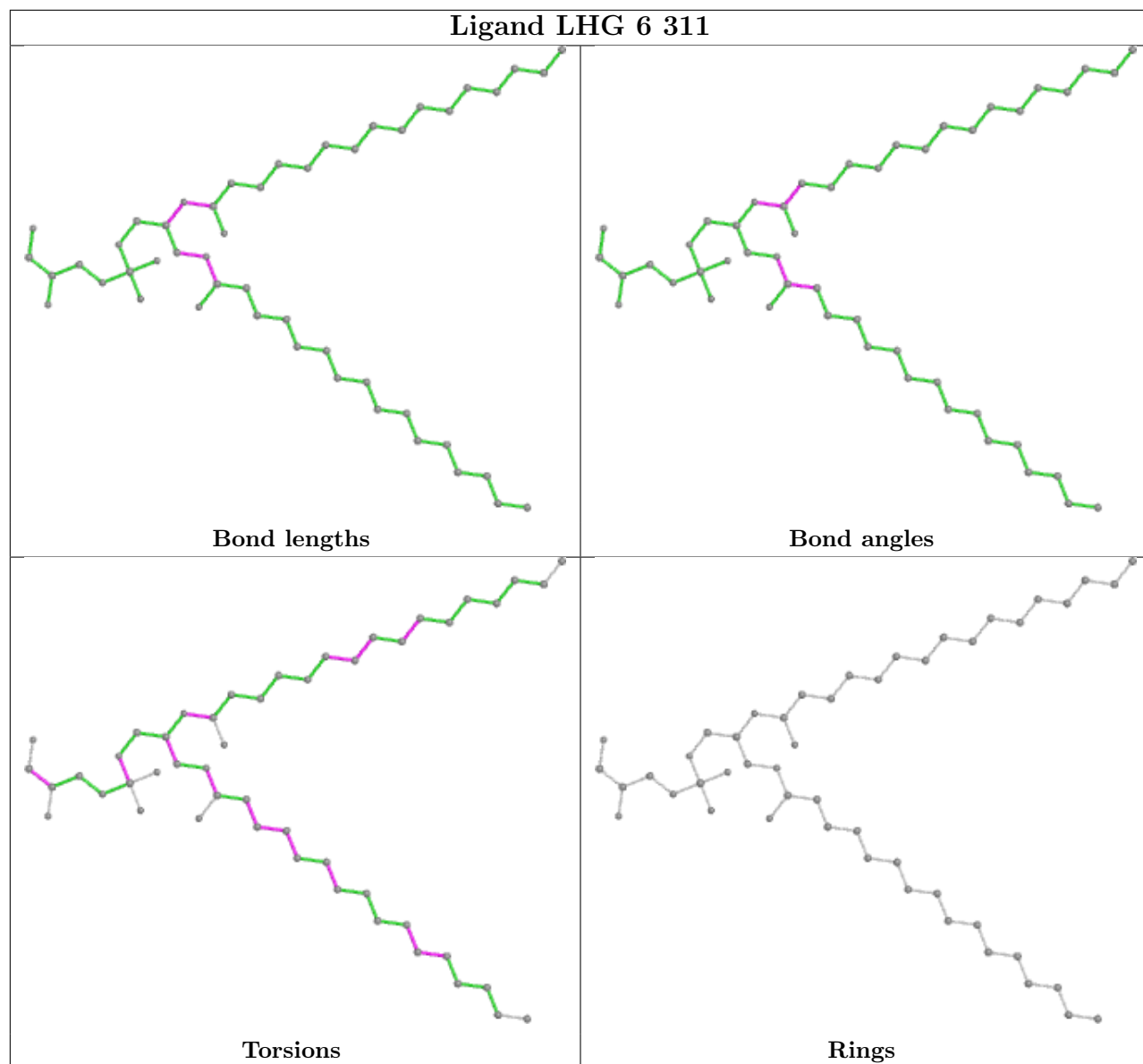


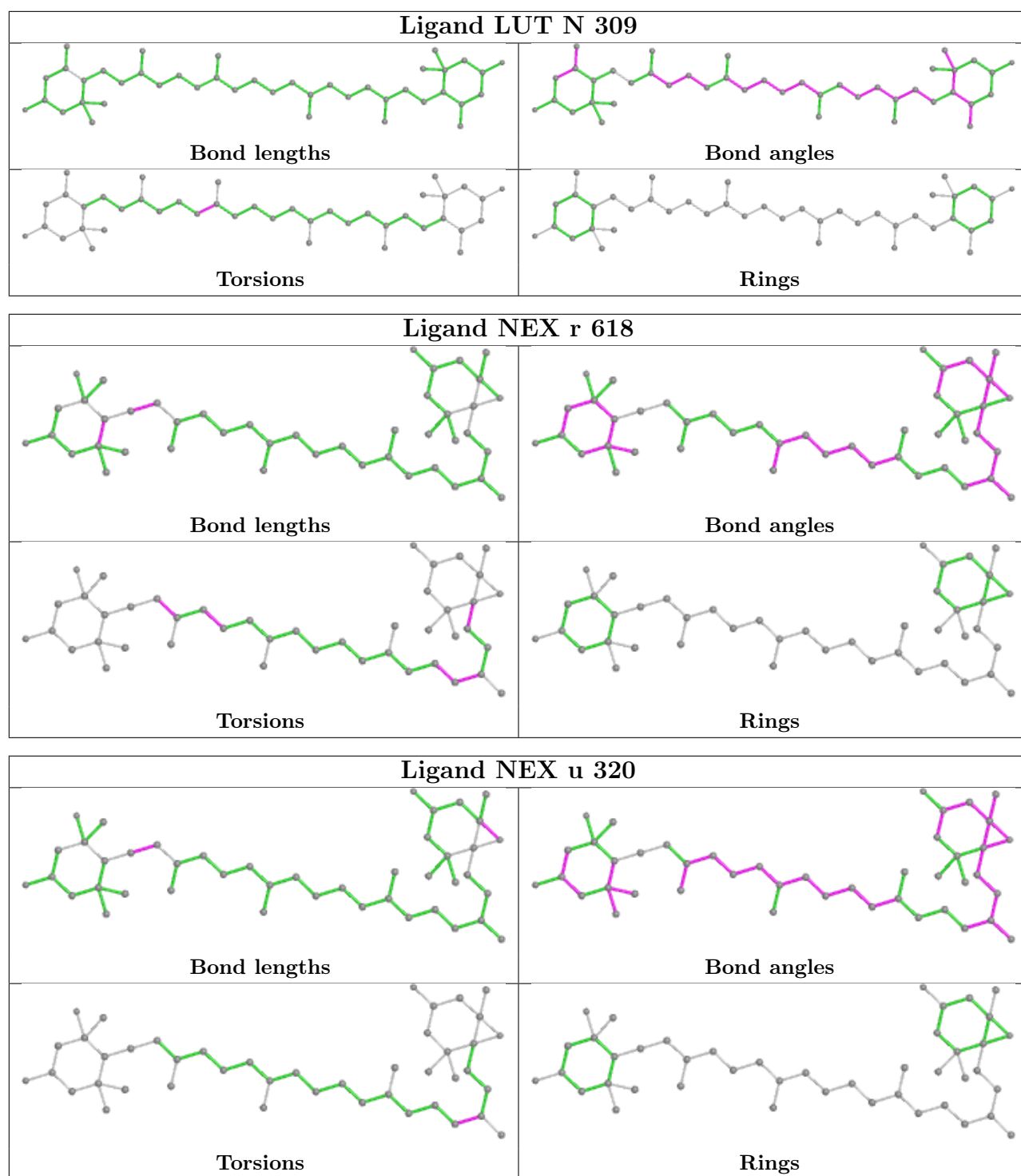












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

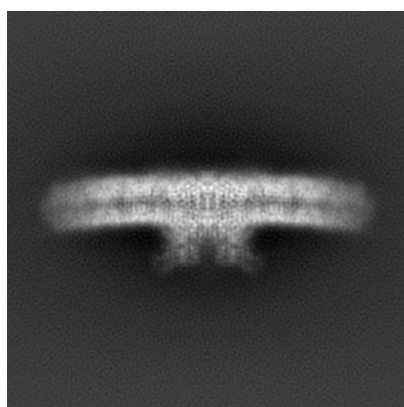
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9957. These allow visual inspection of the internal detail of the map and identification of artifacts.

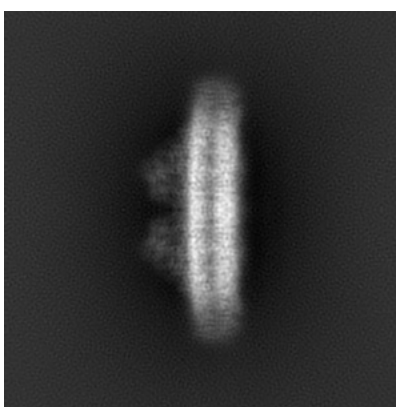
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

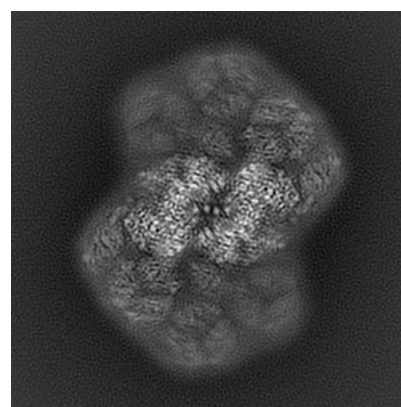
6.1.1 Primary map



X



Y

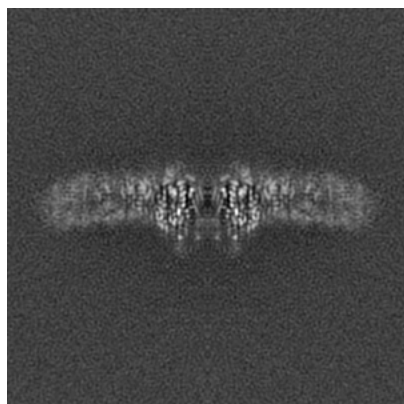


Z

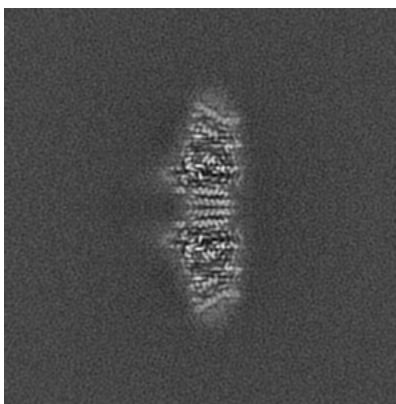
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

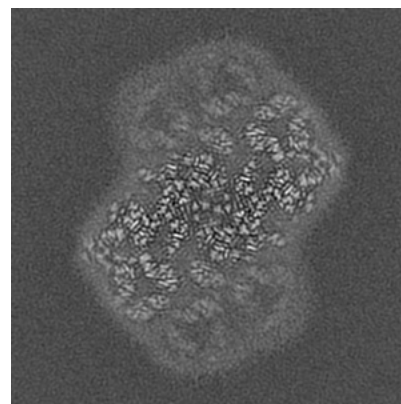
6.2.1 Primary map



X Index: 150



Y Index: 150

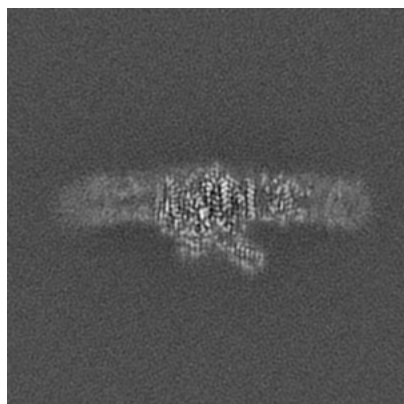


Z Index: 150

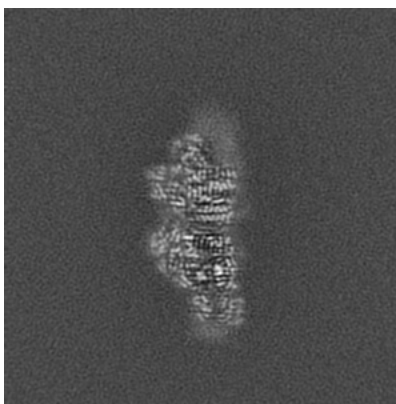
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

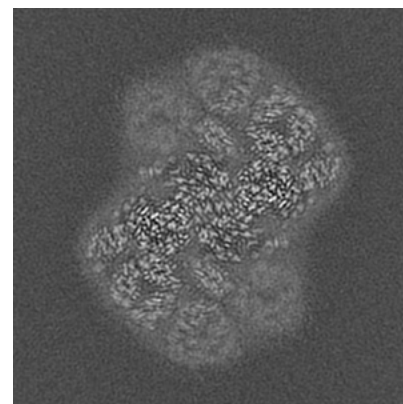
6.3.1 Primary map



X Index: 180



Y Index: 131



Z Index: 164

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

6.4 Orthogonal surface views [i](#)

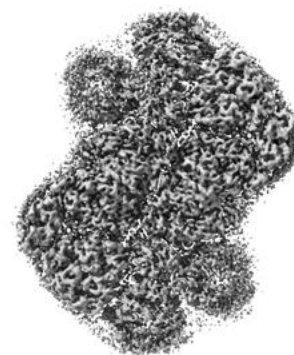
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

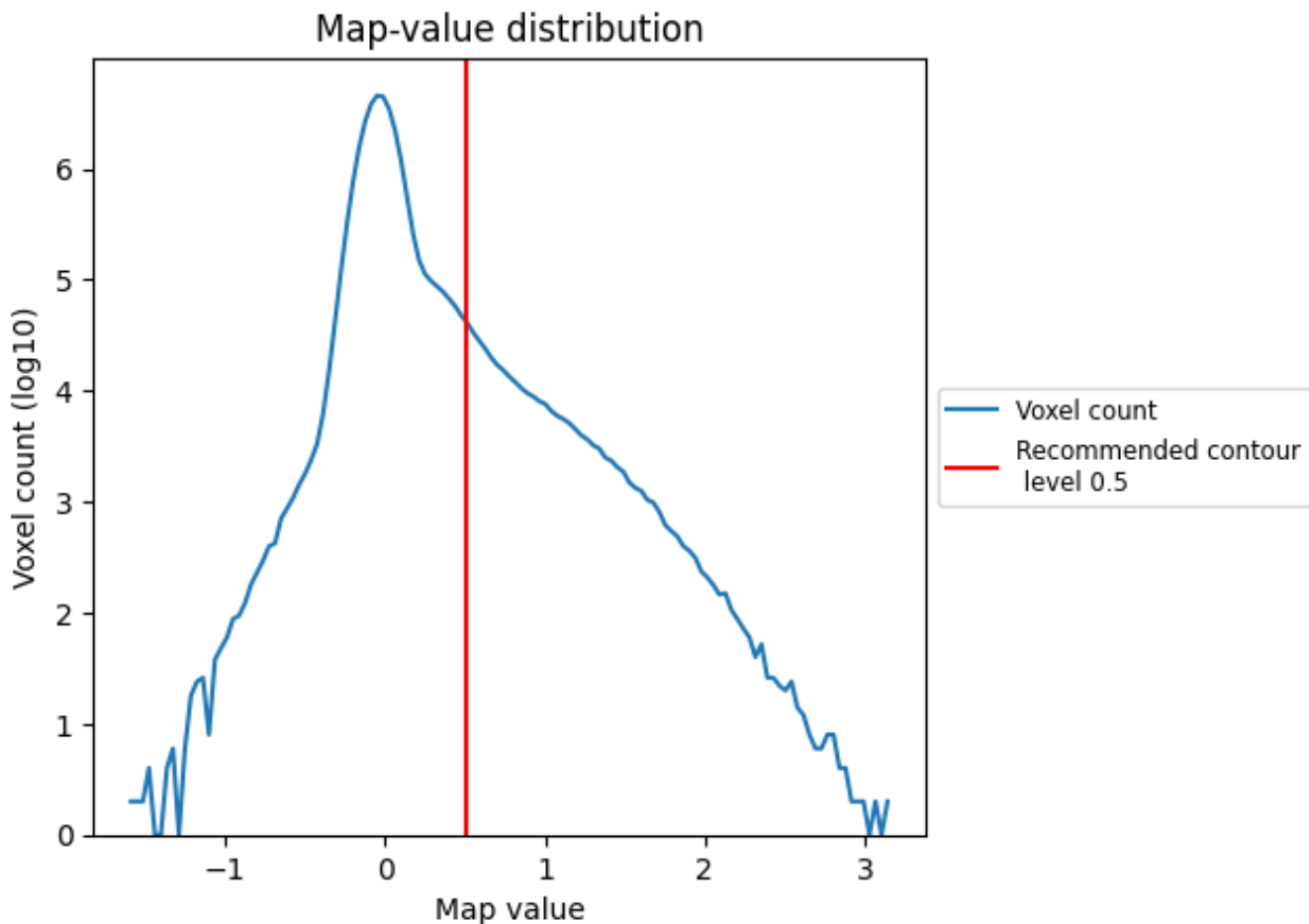
6.5 Mask visualisation

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

7 Map analysis [i](#)

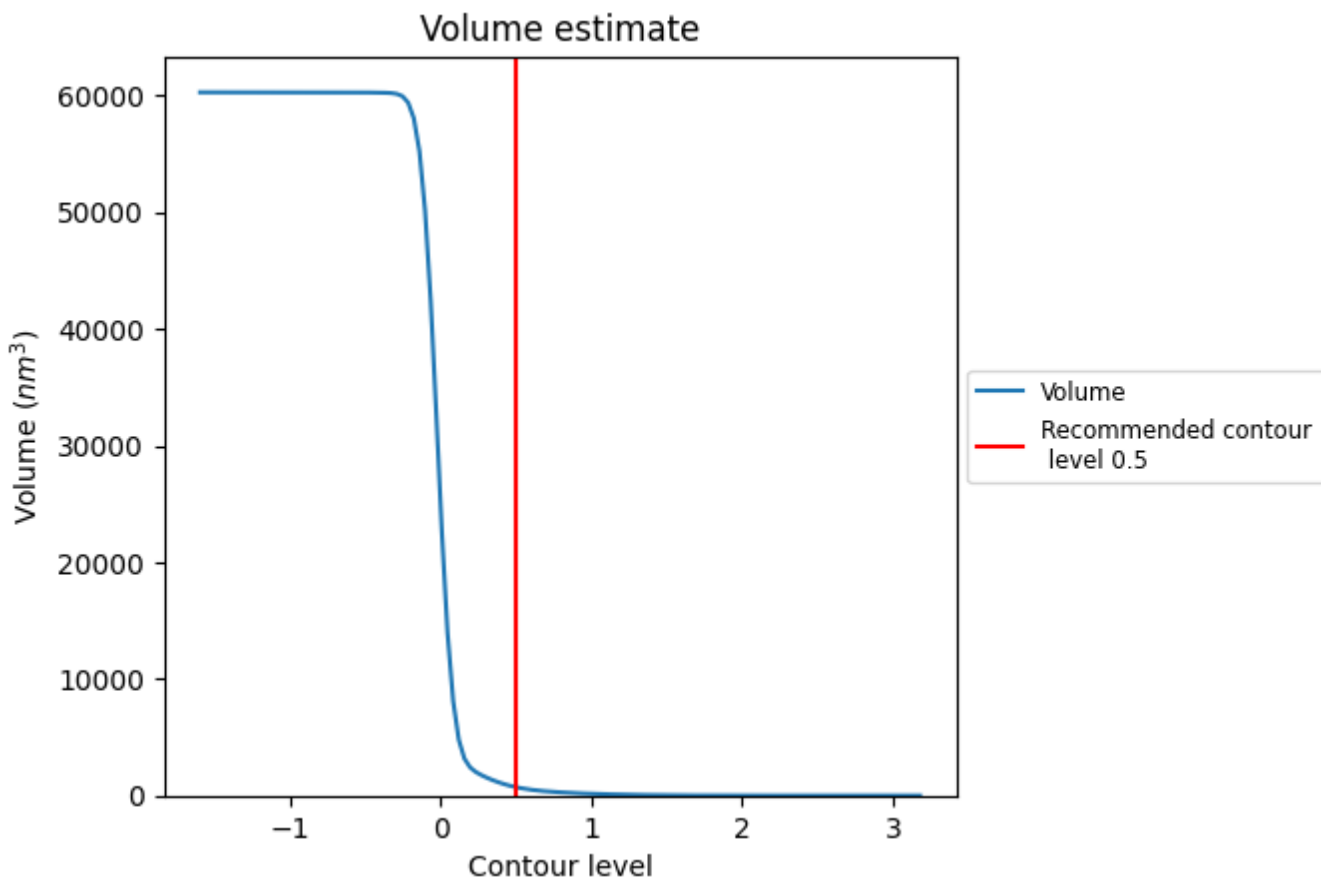
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

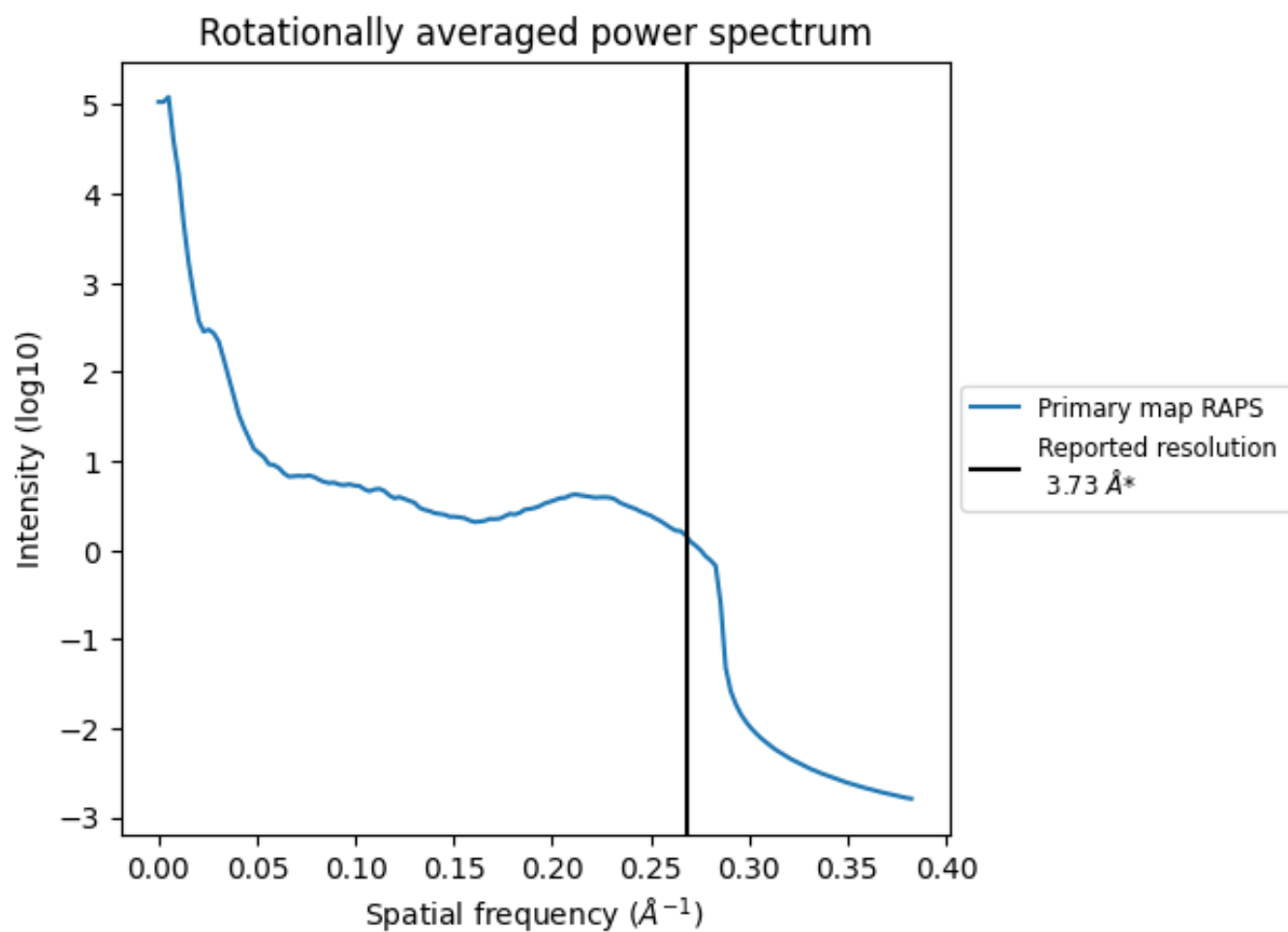
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 727 nm^3 ; this corresponds to an approximate mass of 657 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.268\AA^{-1}

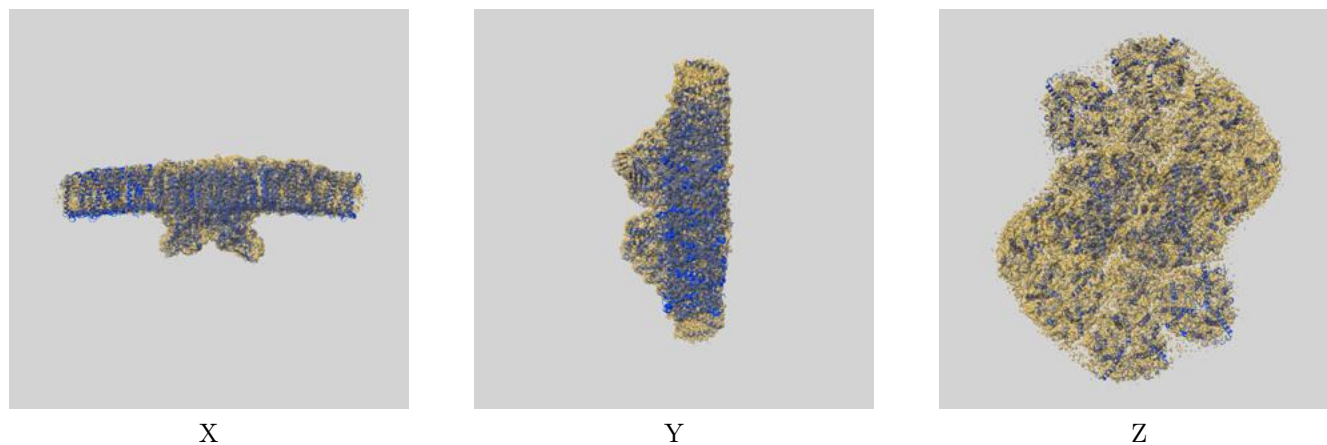
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

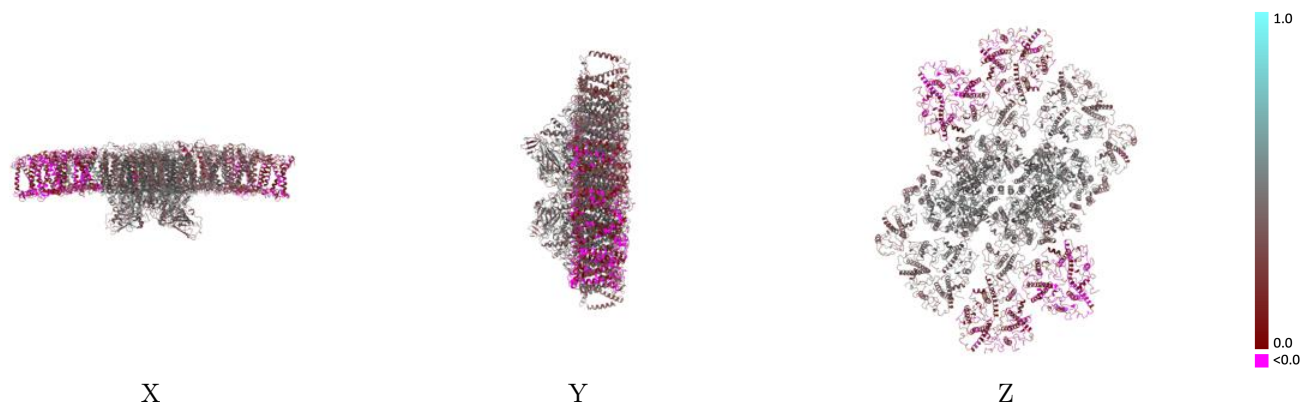
This section contains information regarding the fit between EMDB map EMD-9957 and PDB model 6KAF. Per-residue inclusion information can be found in section 3 on page 53.

9.1 Map-model overlay [i](#)



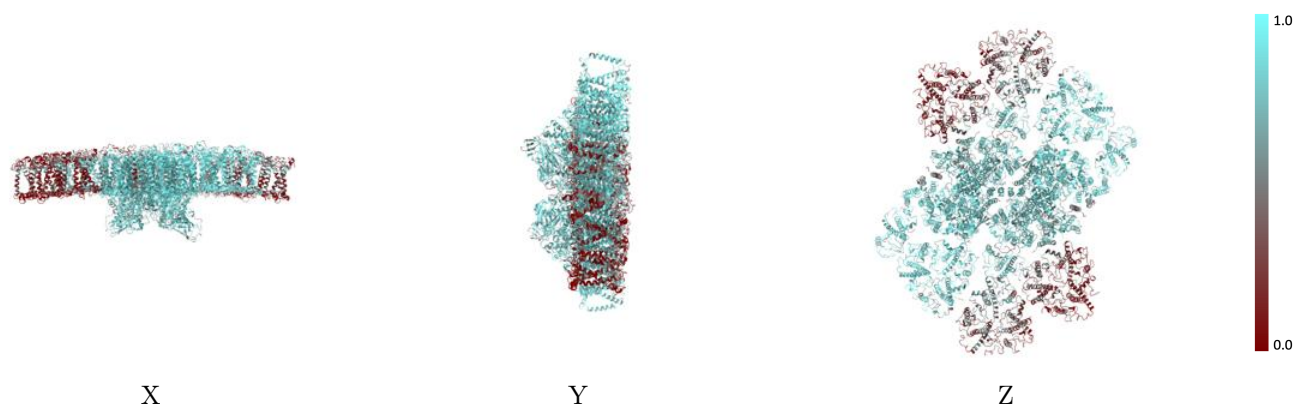
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



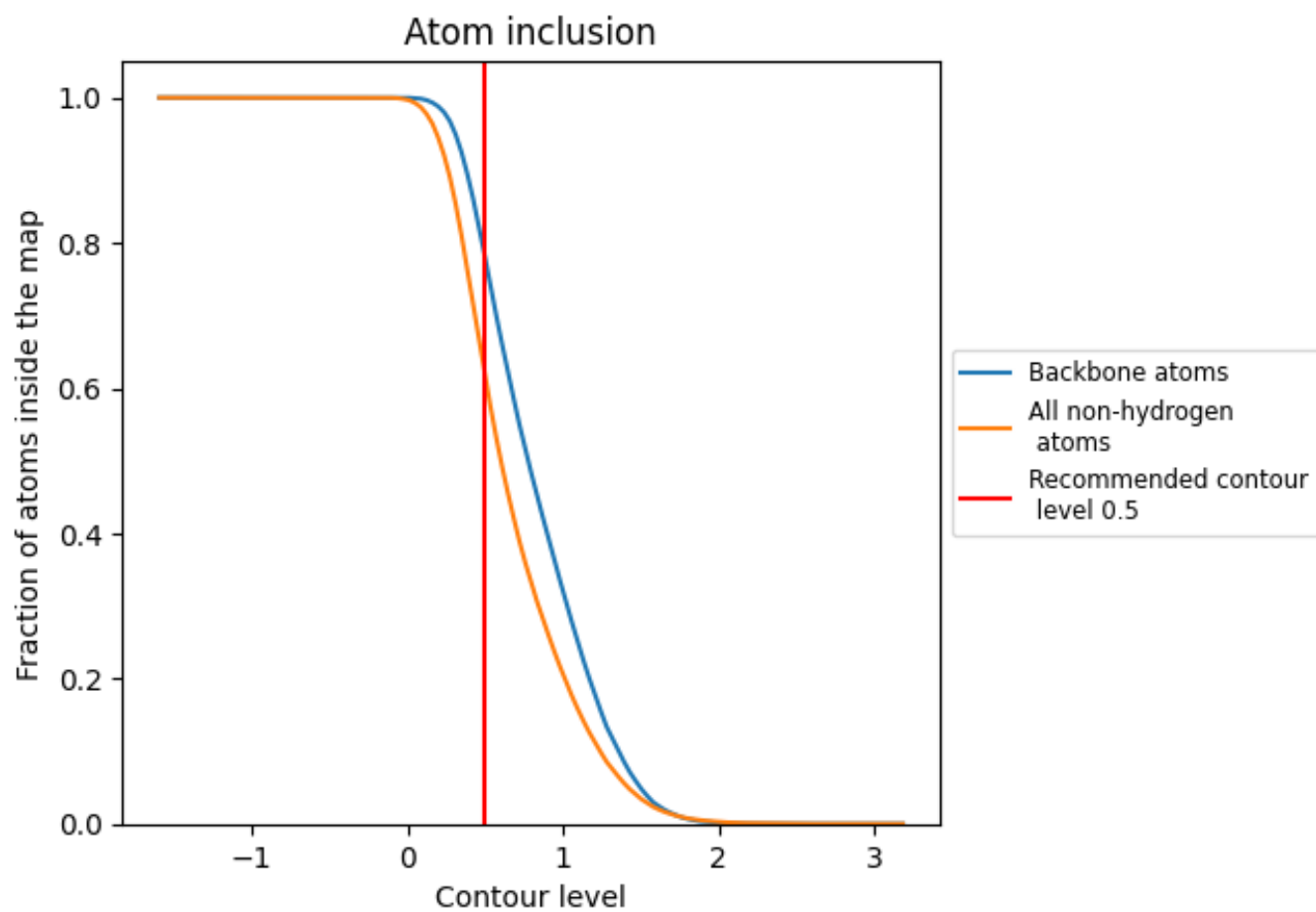
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6153	 0.3260
1	 0.4694	 0.2180
2	 0.2684	 0.1130
3	 0.2684	 0.1030
4	 0.4797	 0.2330
5	 0.2692	 0.1100
6	 0.2767	 0.1120
A	 0.8494	 0.4710
B	 0.7776	 0.4420
C	 0.8258	 0.4680
D	 0.8309	 0.4580
E	 0.7556	 0.3920
F	 0.7563	 0.3190
G	 0.7133	 0.3870
H	 0.8095	 0.4290
I	 0.9007	 0.4840
J	 0.4167	 0.2730
K	 0.8148	 0.4280
L	 0.7388	 0.4530
M	 0.7014	 0.4110
N	 0.7720	 0.4060
O	 0.7115	 0.3810
P	 0.2556	 0.0890
Q	 0.1055	 0.0300
R	 0.6318	 0.3760
S	 0.7691	 0.3680
T	 0.6879	 0.4350
U	 0.7826	 0.4490
V	 0.2129	 0.0700
W	 0.7838	 0.4360
X	 0.6851	 0.3900
Y	 0.6117	 0.3520
Z	 0.7732	 0.3730
a	 0.8460	 0.4710
b	 0.7771	 0.4400



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Chain	Atom inclusion	Q-score
c	 0.8222	 0.4660
d	 0.8316	 0.4570
e	 0.7539	 0.3870
f	 0.7605	 0.3190
g	 0.7078	 0.3760
h	 0.8157	 0.4260
i	 0.9007	 0.4870
j	 0.4125	 0.2370
k	 0.8148	 0.4320
l	 0.7363	 0.4490
m	 0.7014	 0.4070
n	 0.7641	 0.3960
o	 0.7115	 0.3830
p	 0.2401	 0.0800
q	 0.1077	 0.0270
r	 0.6393	 0.3800
s	 0.7683	 0.3660
t	 0.6879	 0.4350
u	 0.7851	 0.4490
v	 0.2155	 0.0810
w	 0.7795	 0.4320
x	 0.6851	 0.3940
y	 0.6117	 0.3550
z	 0.7634	 0.3830