



## wwPDB EM Validation Summary Report ⓘ

Jun 29, 2025 – 01:33 am BST

PDB ID : 6YP7 / pdb\_00006yp7  
EMDB ID : EMD-10865  
Title : PSII-LHCII C2S2 supercomplex from *Pisum sativum* grown in high light conditions  
Authors : Grinzato, A.; Albanese, P.; Zanotti, G.; Pagliano, C.  
Deposited on : 2020-04-15  
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

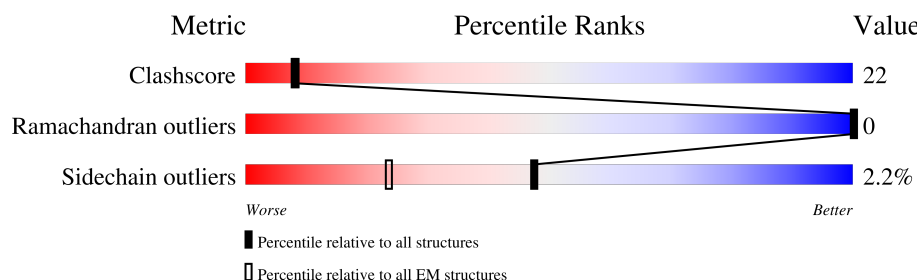
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	G	219	<div> <div>33%</div> <div>66%</div> <div>32%</div> </div>
1	N	219	<div> <div>25%</div> <div>65%</div> <div>33%</div> </div>
1	Y	219	<div> <div>13%</div> <div>64%</div> <div>35%</div> </div>
1	g	219	<div> <div>34%</div> <div>65%</div> <div>33%</div> </div>
1	n	219	<div> <div>22%</div> <div>63%</div> <div>35%</div> </div>
1	y	219	<div> <div>11%</div> <div>66%</div> <div>32%</div> </div>
2	A	334	<div> <div>5%</div> <div>76%</div> <div>24%</div> </div>
2	a	334	<div> <div>79%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	503	
3	b	503	
4	C	450	
4	c	450	
5	D	341	
5	d	341	
6	E	75	
6	e	75	
7	F	30	
7	f	30	
8	H	60	
8	h	60	
9	I	34	
9	i	34	
10	J	35	
10	j	35	
11	K	37	
11	k	37	
12	L	37	
12	l	37	
13	M	33	
13	m	33	
14	O	248	
14	o	248	
15	T	32	

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Mol	Chain	Length	Quality of chain
15	t	32	
16	W	54	
16	w	54	
17	X	39	
17	x	39	
18	Z	62	
18	z	62	
19	R	222	
19	r	222	
20	S	218	
20	s	218	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	G	601	X	-	X	-
21	CHL	G	605	X	-	-	-
21	CHL	G	606	X	-	X	-
21	CHL	G	607	X	-	X	-
21	CHL	G	608	X	-	X	-
21	CHL	G	609	X	-	X	-
21	CHL	N	601	X	-	X	-
21	CHL	N	605	X	-	X	-
21	CHL	N	606	X	-	X	-
21	CHL	N	607	X	-	X	-
21	CHL	N	608	X	-	X	-
21	CHL	R	305	X	-	X	-
21	CHL	R	306	X	-	X	-
21	CHL	R	307	X	-	-	-
21	CHL	S	301	X	-	X	-
21	CHL	S	302	X	-	-	-
21	CHL	S	306	X	-	-	-
21	CHL	S	307	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	Y	601	X	-	X	-
21	CHL	Y	605	X	-	X	-
21	CHL	Y	606	X	-	X	-
21	CHL	Y	607	X	-	X	-
21	CHL	Y	608	X	-	X	-
21	CHL	g	601	X	-	X	-
21	CHL	g	605	X	-	-	-
21	CHL	g	606	X	-	X	-
21	CHL	g	607	X	-	X	-
21	CHL	g	608	X	-	X	-
21	CHL	g	609	X	-	X	-
21	CHL	n	601	X	-	X	-
21	CHL	n	605	X	-	X	-
21	CHL	n	606	X	-	-	-
21	CHL	n	607	X	-	X	-
21	CHL	n	608	X	-	X	-
21	CHL	r	301	X	-	X	-
21	CHL	r	306	X	-	X	-
21	CHL	r	307	X	-	X	-
21	CHL	r	308	X	-	-	-
21	CHL	s	301	X	-	X	-
21	CHL	s	302	X	-	-	-
21	CHL	s	306	X	-	-	-
21	CHL	s	307	X	-	X	-
21	CHL	y	601	X	-	X	-
21	CHL	y	605	X	-	X	-
21	CHL	y	606	X	-	X	-
21	CHL	y	607	X	-	-	-
21	CHL	y	608	X	-	X	-
21	CHL	y	609	X	-	X	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	A	409	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B	618	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	-	X	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	609	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	R	302	X	-	-	-
22	CLA	R	303	X	-	-	-
22	CLA	R	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	W	101	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	609	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	X	-
22	CLA	Y	612	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	601	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	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	X	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	609	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	304	X	-	-	-
22	CLA	r	305	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	s	313	X	-	-	-
22	CLA	w	101	X	-	-	-
22	CLA	x	101	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	X	-
22	CLA	y	613	X	-	-	-
24	XAT	G	617	X	-	-	-
24	XAT	N	616	X	-	-	-
24	XAT	R	313	X	-	-	-
24	XAT	Y	615	X	-	-	-
24	XAT	g	617	X	-	-	-
24	XAT	n	615	X	-	-	-
24	XAT	r	314	X	-	-	-
24	XAT	y	615	X	-	-	-
25	NEX	N	617	X	-	-	-
25	NEX	Y	616	X	-	-	-
25	NEX	g	618	X	-	-	-
25	NEX	n	616	X	-	-	-
25	NEX	r	315	X	-	-	-
25	NEX	y	616	X	-	-	-
25	NEX	y	618	X	-	-	-
33	SQD	D	402	X	-	-	-
33	SQD	d	402	X	-	-	-
34	BCT	D	403	-	-	X	-
34	BCT	a	412	-	-	X	-
36	LMG	B	623	-	-	X	-
36	LMG	b	620	-	-	X	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 71784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

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

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

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

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

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

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

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
5	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

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

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	26	PHE	SER	conflict	UNP P62096
F	26	PHE	SER	conflict	UNP P62096

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	35	Total	C	N	O	0	0
			256	174	39	43		
10	J	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
11	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

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

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

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

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
14	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

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

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

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

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

- Molecule 17 is a protein called Ultraviolet-B-repressible protein.

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

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	222	Total	C	N	O	S	0	0
			1732	1133	281	314	4		

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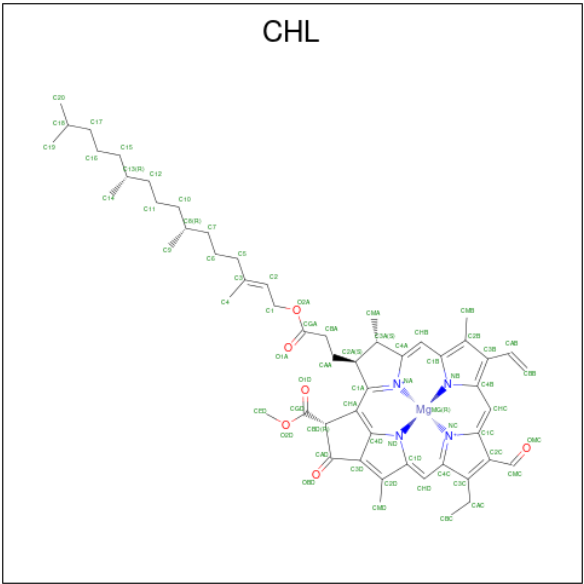
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Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	222	Total	C	N	O	S	0	0
			1732	1133	281	314	4		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	218	Total	C	N	O	S	0	0
			1688	1105	271	308	4		
20	S	218	Total	C	N	O	S	0	0
			1688	1105	271	308	4		

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
21	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
21	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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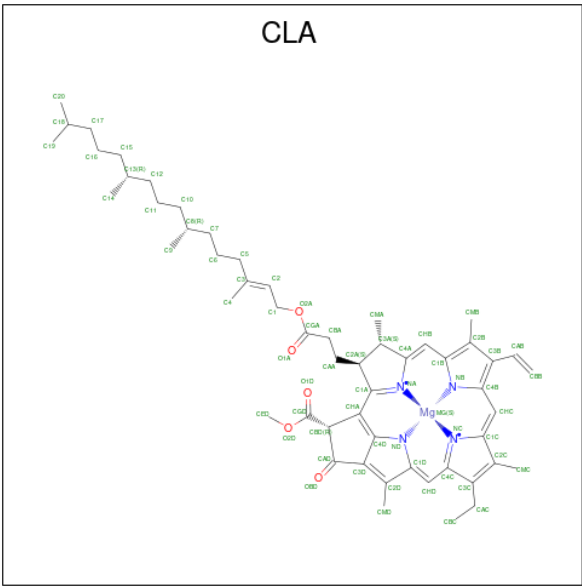
Mol	Chain	Residues	Atoms					AltConf
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	r	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	r	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	r	1	Total 61	C 50	Mg 1	N 4	O 6	0
21	s	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 48	C 37	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
21	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
21	R	1	Total 56	C 45	Mg 1	N 4	O 6	0
21	R	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	w	1	Total 60	C 50	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 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0

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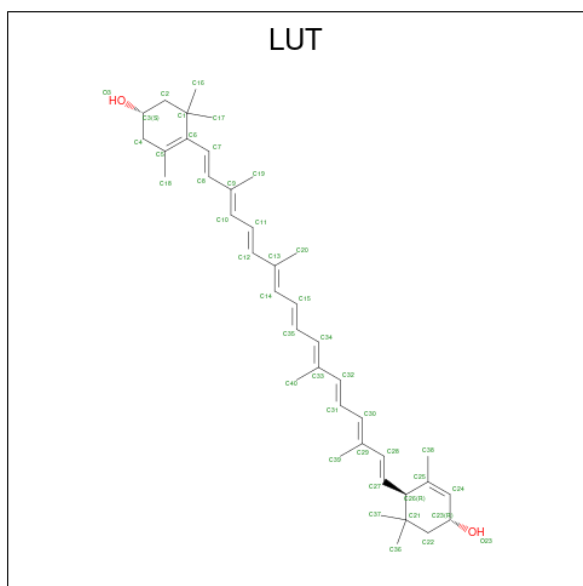
Mol	Chain	Residues	Atoms					AltConf
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
22	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	s	1	Total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

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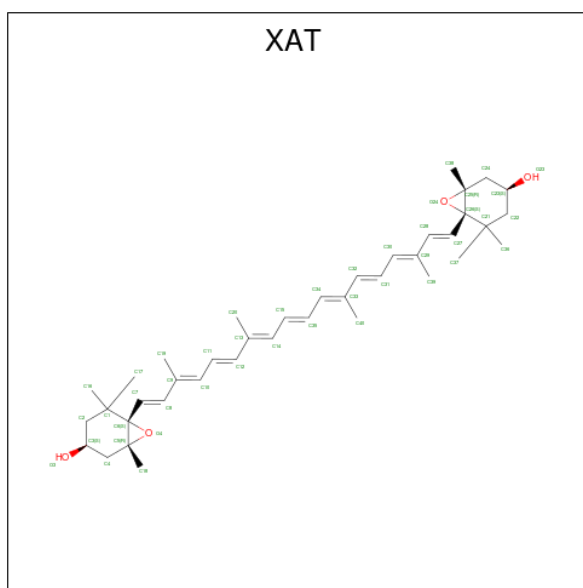
Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0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

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



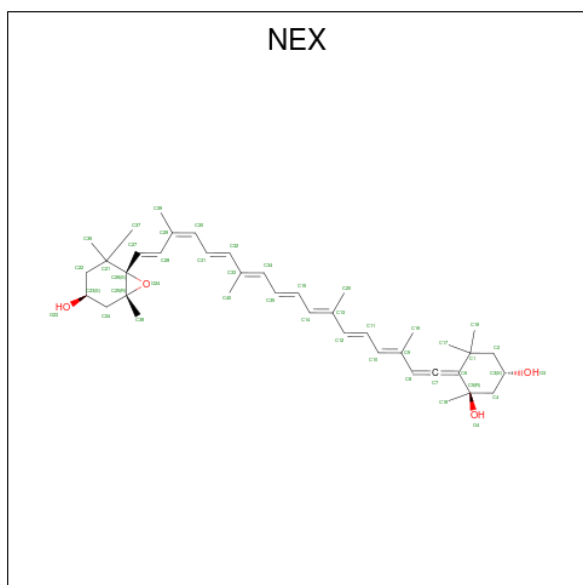
Mol	Chain	Residues	Atoms			AltConf
23	g	1	Total	C	O	0
			42	40	2	
23	g	1	Total	C	O	0
			42	40	2	
23	n	1	Total	C	O	0
			42	40	2	
23	y	1	Total	C	O	0
			42	40	2	
23	G	1	Total	C	O	0
			42	40	2	
23	G	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	Y	1	Total	C	O	0
			42	40	2	
23	r	1	Total	C	O	0
			42	40	2	
23	R	1	Total	C	O	0
			42	40	2	

- 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 (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
24	g	1	Total	C	O	0
			44	40	4	
24	n	1	Total	C	O	0
			44	40	4	
24	y	1	Total	C	O	0
			44	40	4	
24	G	1	Total	C	O	0
			44	40	4	
24	N	1	Total	C	O	0
			44	40	4	
24	Y	1	Total	C	O	0
			44	40	4	
24	r	1	Total	C	O	0
			44	40	4	
24	R	1	Total	C	O	0
			44	40	4	

- Molecule 25 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



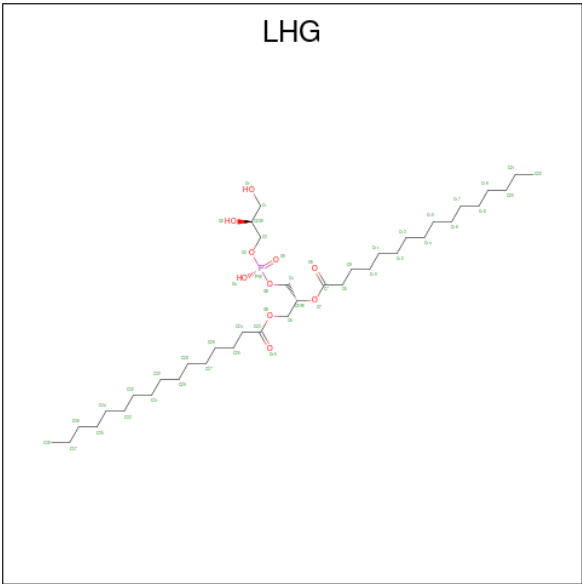
Mol	Chain	Residues	Atoms			AltConf
25	g	1	Total	C	O	0
			44	40	4	
25	n	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
25	y	1	Total	C	O	0
			44	40	4	
25	y	1	Total	C	O	0
			44	40	4	
25	N	1	Total	C	O	0
			44	40	4	
25	Y	1	Total	C	O	0
			44	40	4	
25	r	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



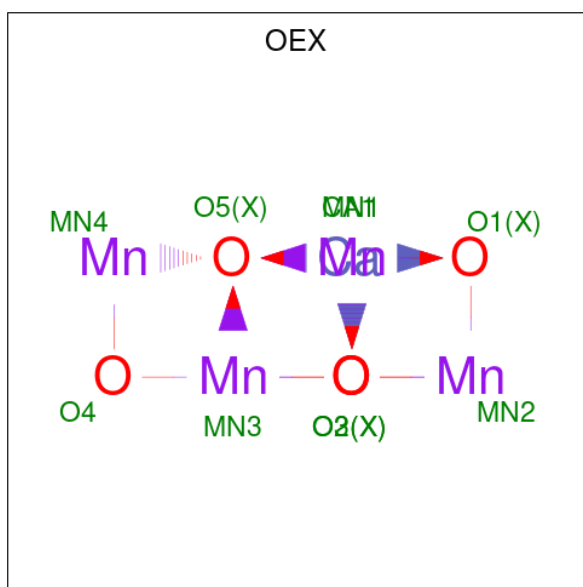
Mol	Chain	Residues	Atoms				AltConf
26	g	1	Total	C	O	P	0
			49	38	10	1	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	G	1	Total	C	O	P	0
			49	38	10	1	
26	N	1	Total	C	O	P	0
			49	38	10	1	
26	Y	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	b	1	Total 49	C 38	O 10	P 1	0
26	c	1	Total 49	C 38	O 10	P 1	0
26	c	1	Total 49	C 38	O 10	P 1	0
26	c	1	Total 49	C 38	O 10	P 1	0
26	d	1	Total 46	C 35	O 10	P 1	0
26	d	1	Total 49	C 38	O 10	P 1	0
26	d	1	Total 43	C 32	O 10	P 1	0
26	l	1	Total 49	C 38	O 10	P 1	0
26	B	1	Total 49	C 38	O 10	P 1	0
26	C	1	Total 49	C 38	O 10	P 1	0
26	C	1	Total 49	C 38	O 10	P 1	0
26	C	1	Total 49	C 38	O 10	P 1	0
26	D	1	Total 46	C 35	O 10	P 1	0
26	D	1	Total 49	C 38	O 10	P 1	0
26	D	1	Total 43	C 32	O 10	P 1	0
26	L	1	Total 49	C 38	O 10	P 1	0
26	r	1	Total 47	C 36	O 10	P 1	0
26	s	1	Total 49	C 38	O 10	P 1	0
26	S	1	Total 49	C 38	O 10	P 1	0
26	R	1	Total 47	C 36	O 10	P 1	0

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

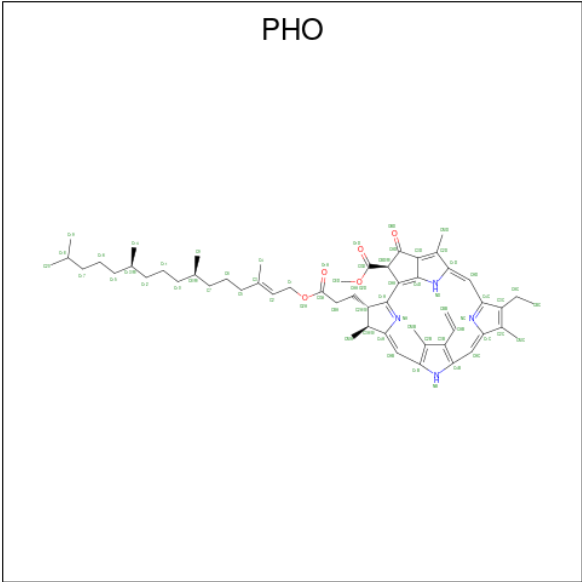
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

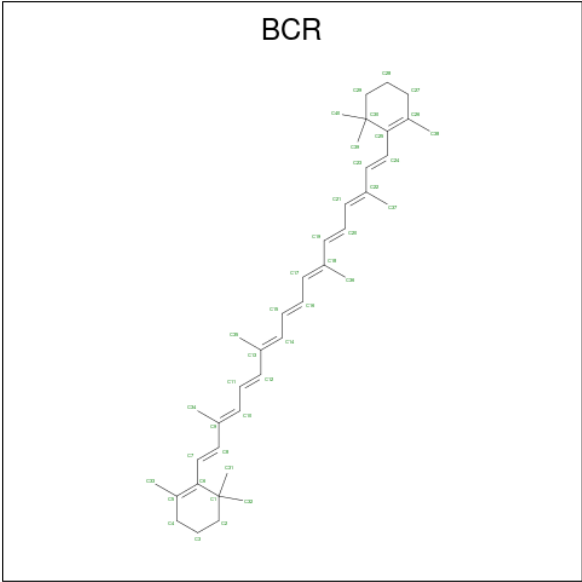
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Cl	0
			1	1	
29	c	1	Total	Cl	0
			1	1	
29	A	1	Total	Cl	0
			1	1	
29	C	1	Total	Cl	0
			1	1	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



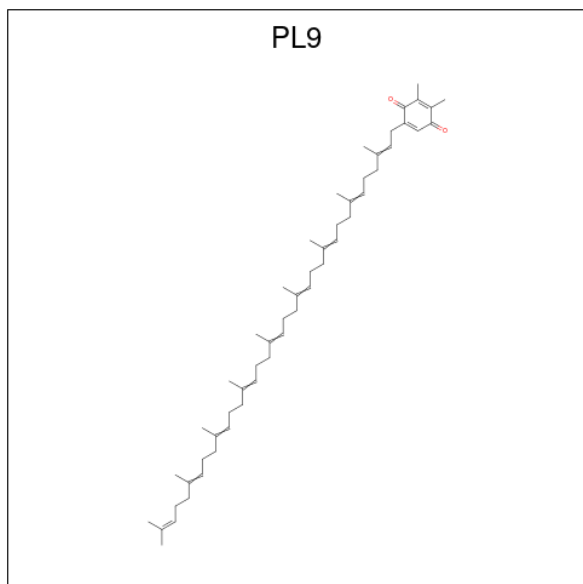
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	d	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



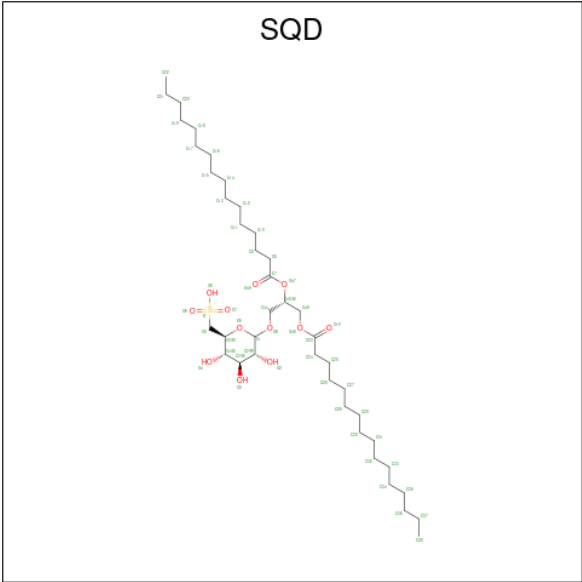
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	h	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	T	1	Total C 40 40	0

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



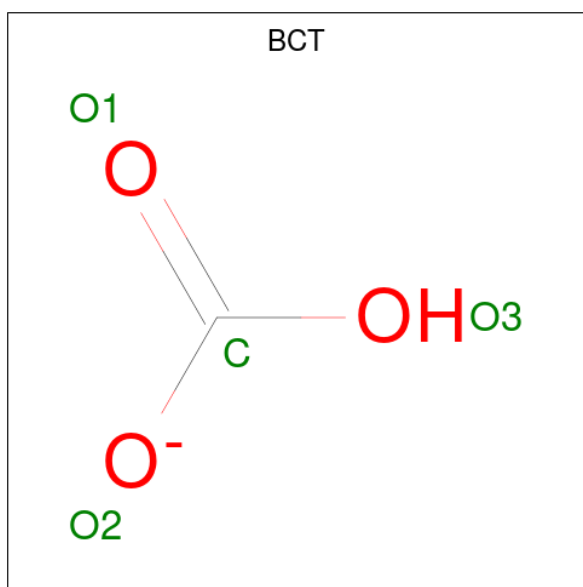
Mol	Chain	Residues	Atoms			AltConf
32	a	1	Total	C	O	0
			13	11	2	
32	d	1	Total	C	O	0
			55	53	2	
32	A	1	Total	C	O	0
			13	11	2	
32	D	1	Total	C	O	0
			55	53	2	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



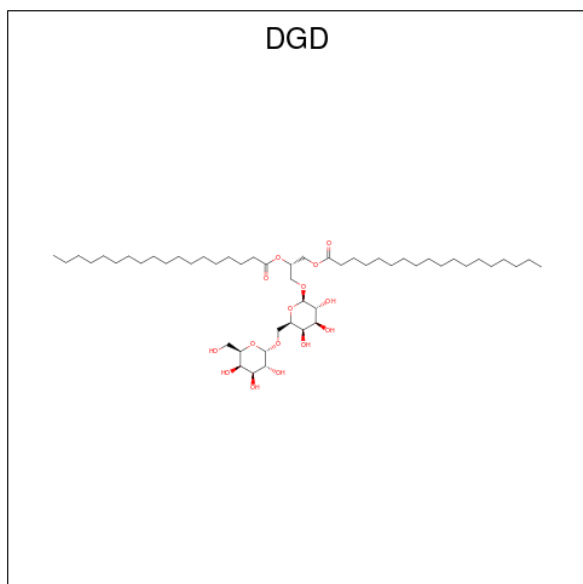
Mol	Chain	Residues	Atoms				AltConf
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	d	1	Total	C	O	S	0
			50	37	12	1	
33	l	1	Total	C	O	S	0
			42	29	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	D	1	Total	C	O	S	0
			50	37	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	L	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



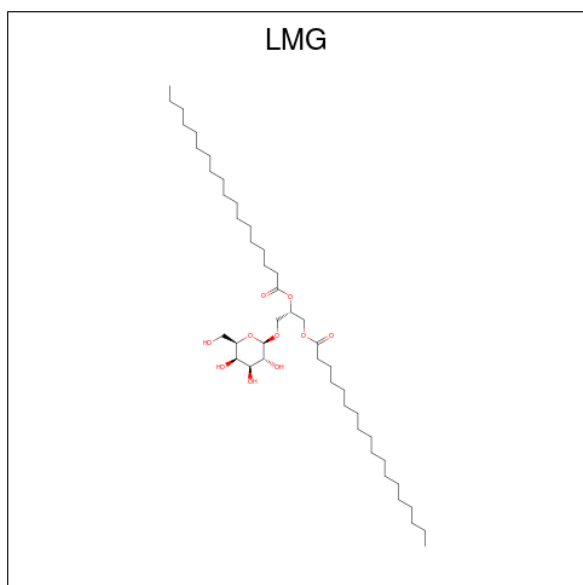
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			59	44	15	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			60	45	15	
35	h	1	Total	C	O	0
			62	47	15	
35	A	1	Total	C	O	0
			59	44	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	H	1	Total	C	O	0
			62	47	15	
35	J	1	Total	C	O	0
			60	45	15	

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



Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	C	O	0
			55	45	10	
36	c	1	Total	C	O	0
			51	41	10	

*Continued on next page...*

Mol	Chain	Residues	Atoms			AltConf
36	d	1	Total 46	C 36	O 10	0
36	k	1	Total 51	C 41	O 10	0
36	w	1	Total 48	C 38	O 10	0
36	B	1	Total 40	C 30	O 10	0
36	B	1	Total 55	C 45	O 10	0
36	C	1	Total 48	C 38	O 10	0
36	C	1	Total 51	C 41	O 10	0
36	D	1	Total 46	C 36	O 10	0
36	I	1	Total 40	C 30	O 10	0
36	K	1	Total 51	C 41	O 10	0
36	M	1	Total 51	C 41	O 10	0
36	T	1	Total 51	C 41	O 10	0

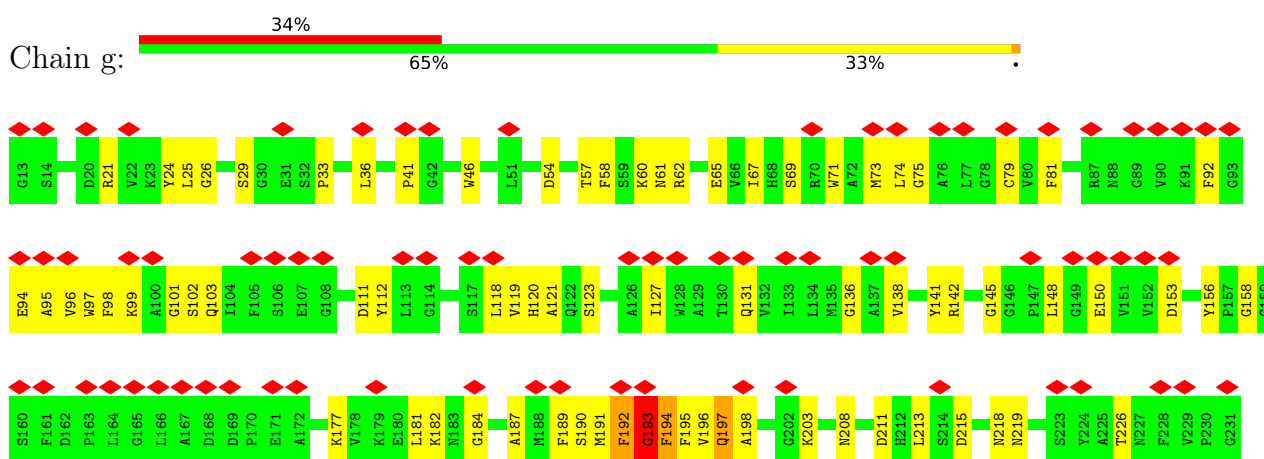
- # HEM

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

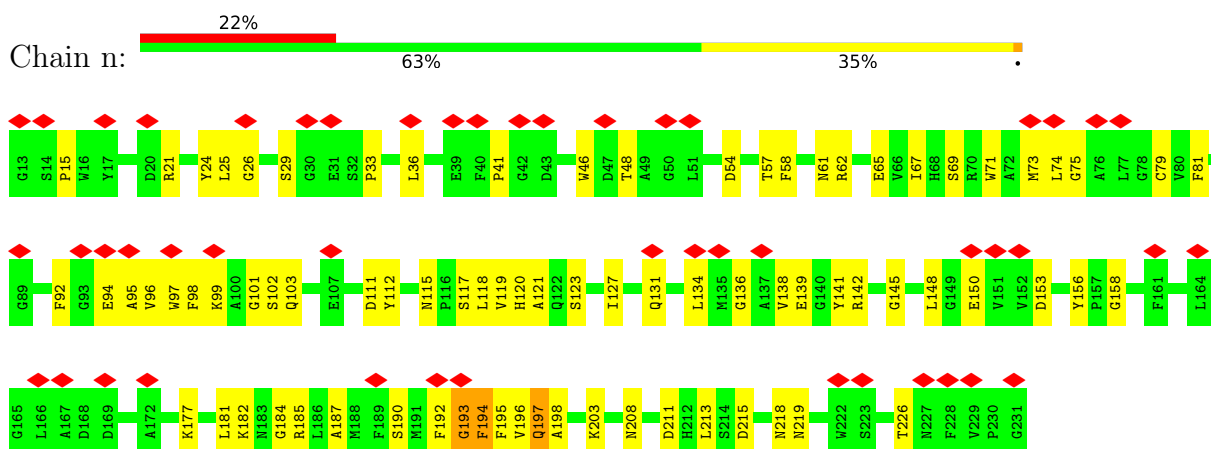
### 3 Residue-property plots

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

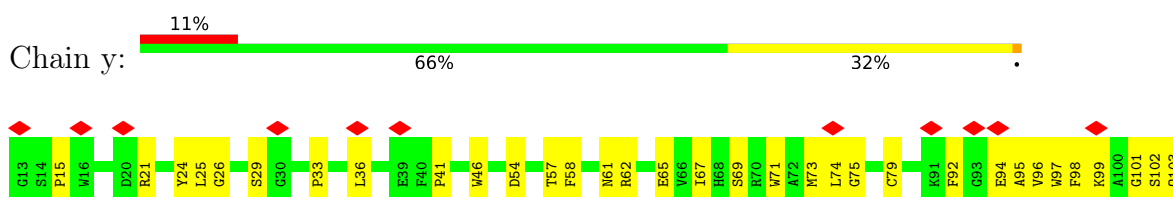
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

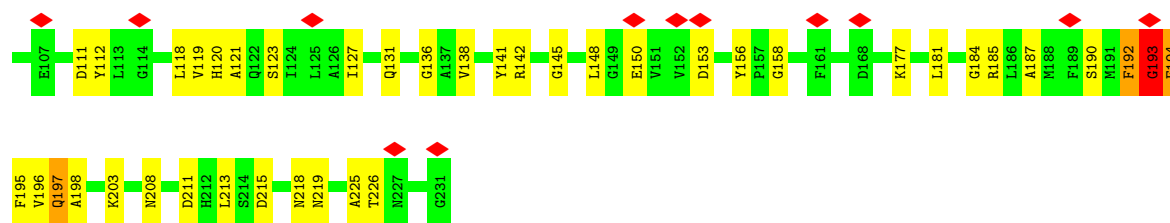


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

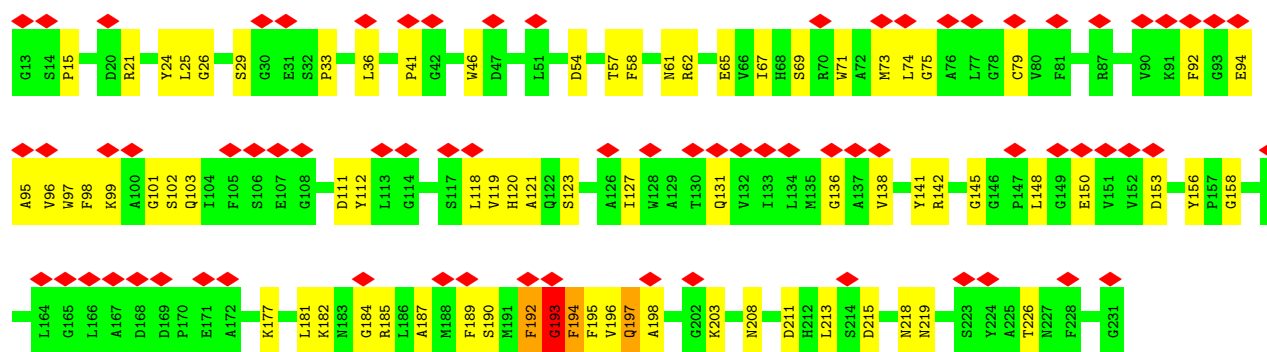


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

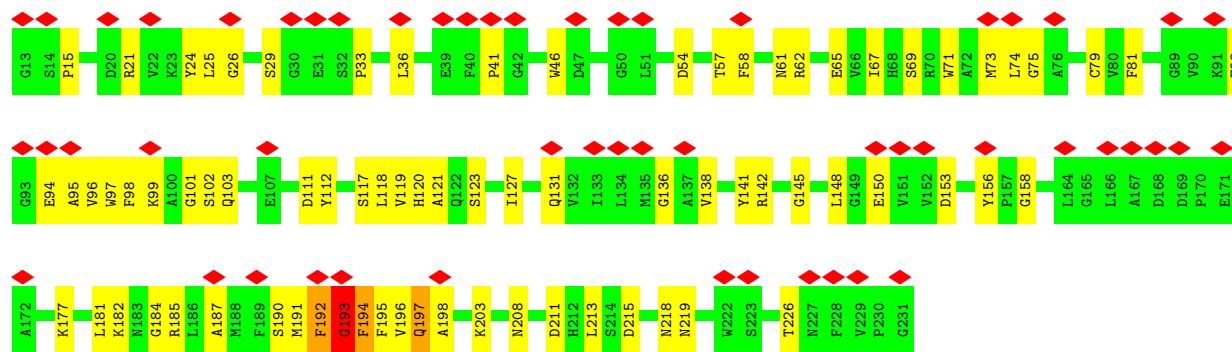




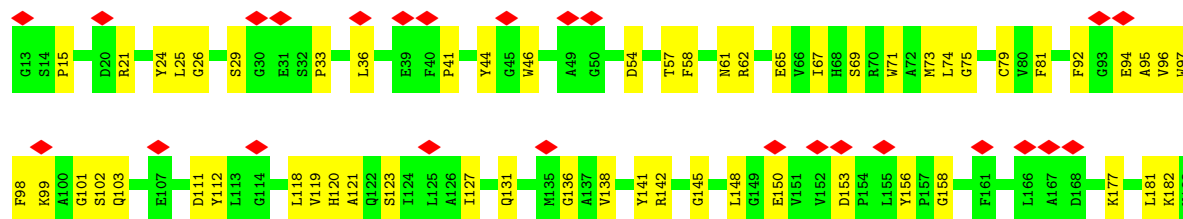
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



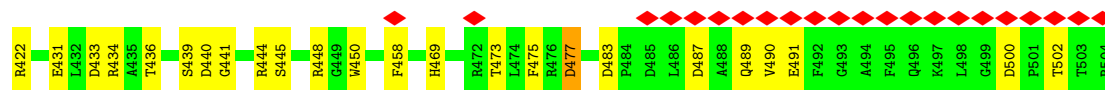
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



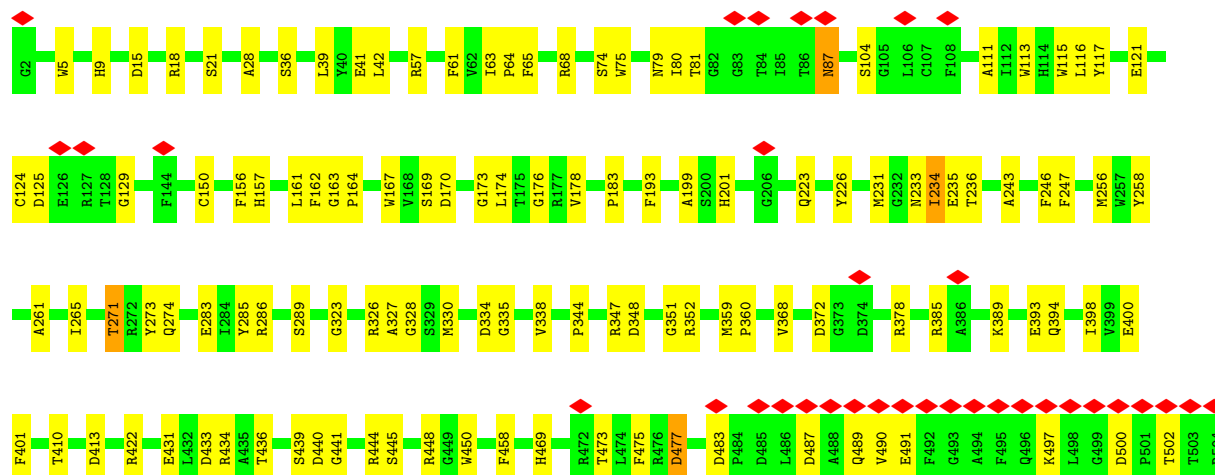
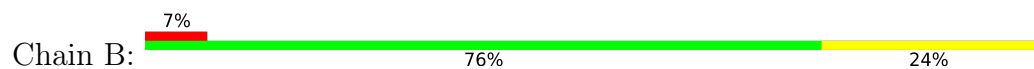
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



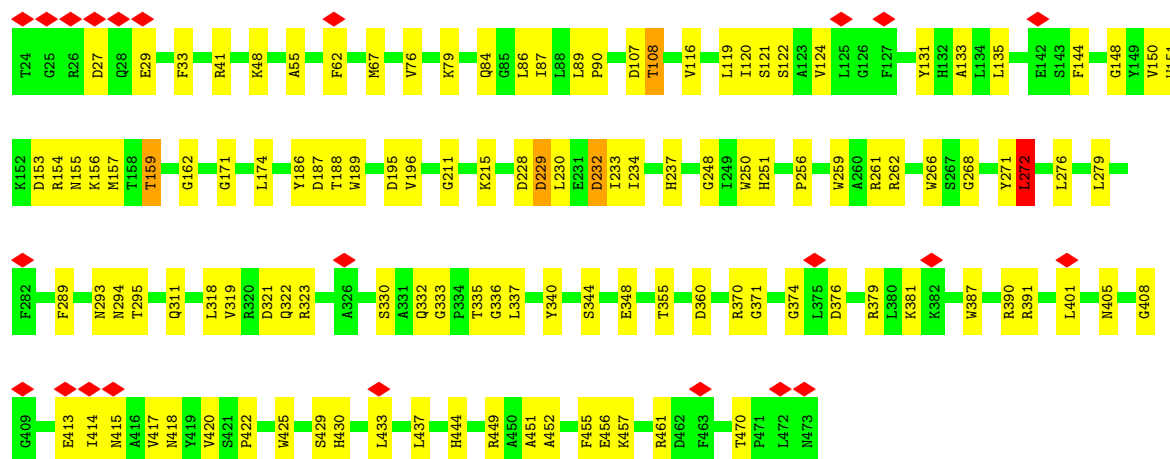




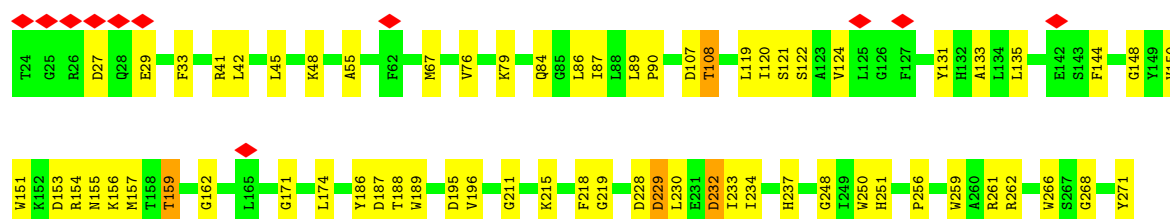
• Molecule 3: Photosystem II CP47 reaction center protein

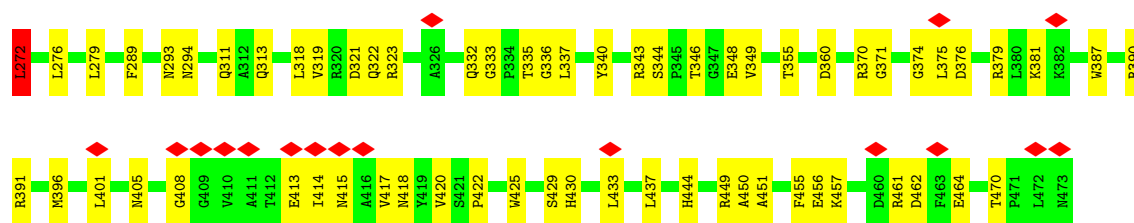


• Molecule 4: Photosystem II CP43 reaction center protein

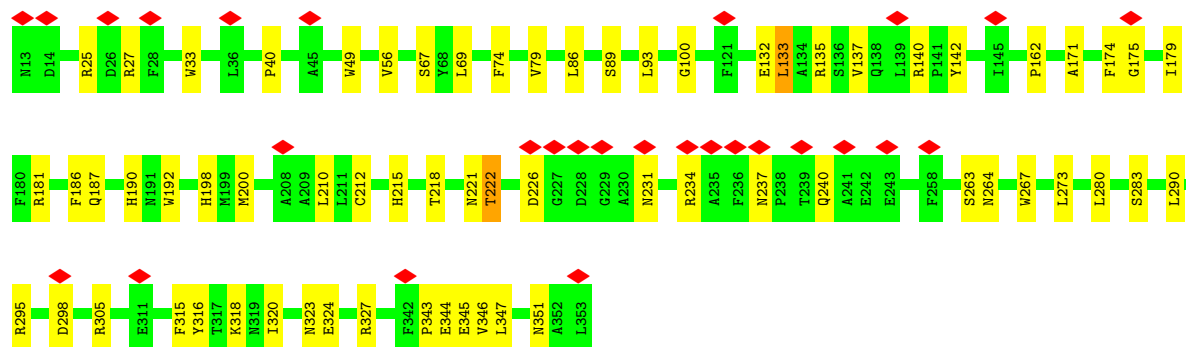
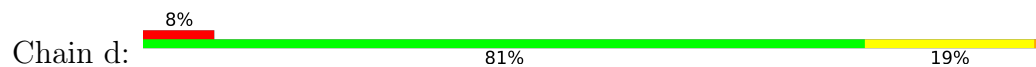


• Molecule 4: Photosystem II CP43 reaction center protein

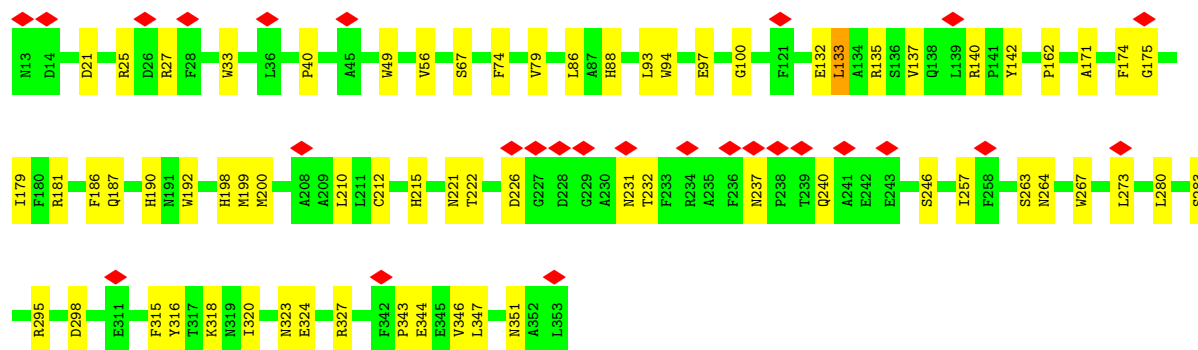
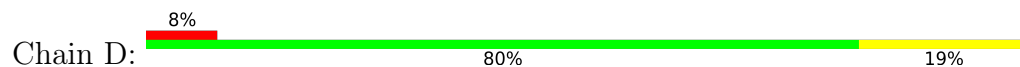




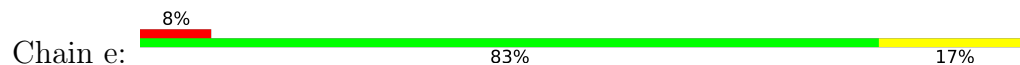
• Molecule 5: Photosystem II D2 protein



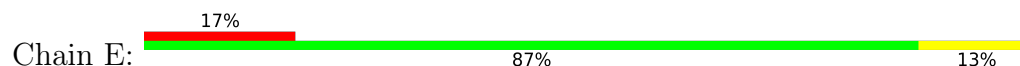
• Molecule 5: Photosystem II D2 protein

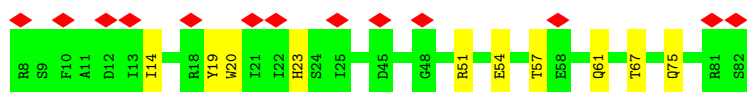


• Molecule 6: Cytochrome b559 subunit alpha

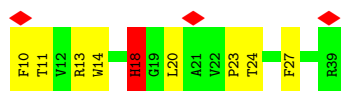


• Molecule 6: Cytochrome b559 subunit alpha

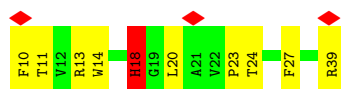




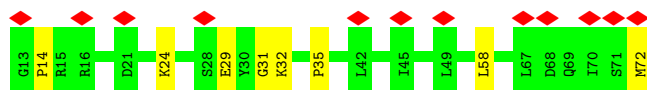
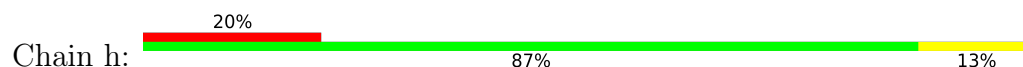
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 7: Cytochrome b559 subunit beta



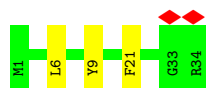
- Molecule 8: Photosystem II reaction center protein H



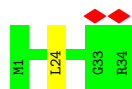
- Molecule 8: Photosystem II reaction center protein H



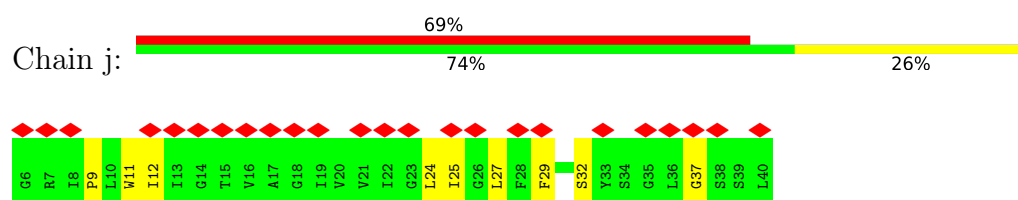
- Molecule 9: Photosystem II reaction center protein I



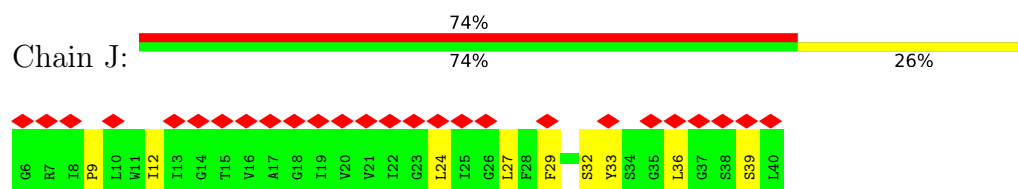
- Molecule 9: Photosystem II reaction center protein I



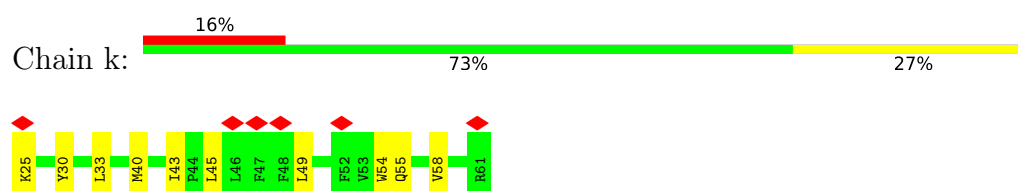
- Molecule 10: Photosystem II reaction center protein J



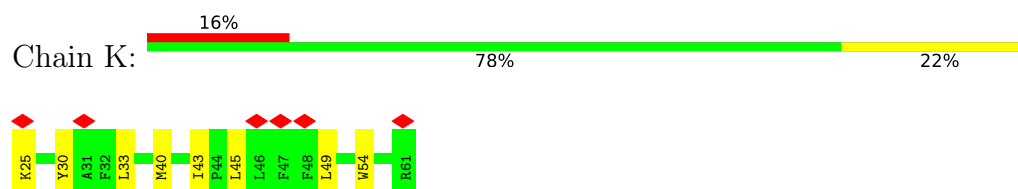
- Molecule 10: Photosystem II reaction center protein J



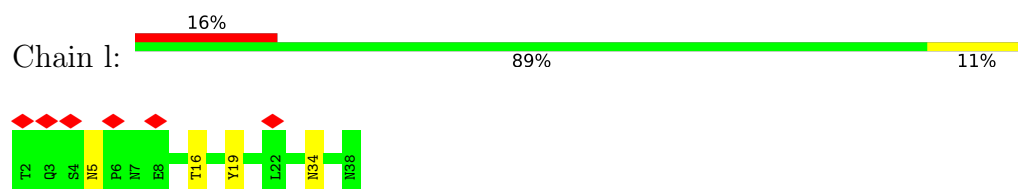
- Molecule 11: Photosystem II reaction center protein K



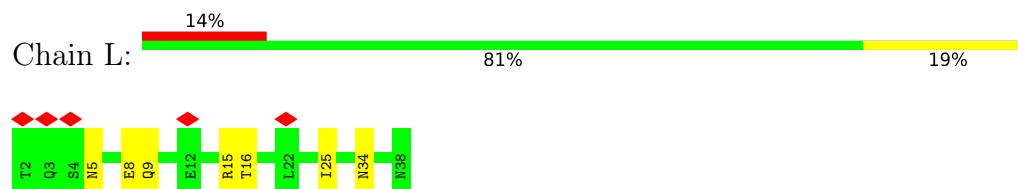
- Molecule 11: Photosystem II reaction center protein K



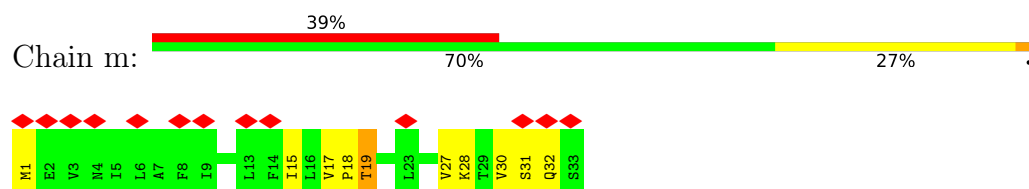
- Molecule 12: Photosystem II reaction center protein L



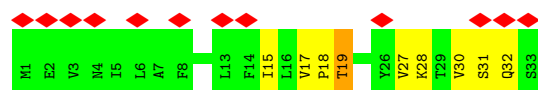
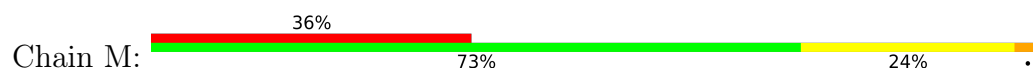
- Molecule 12: Photosystem II reaction center protein L



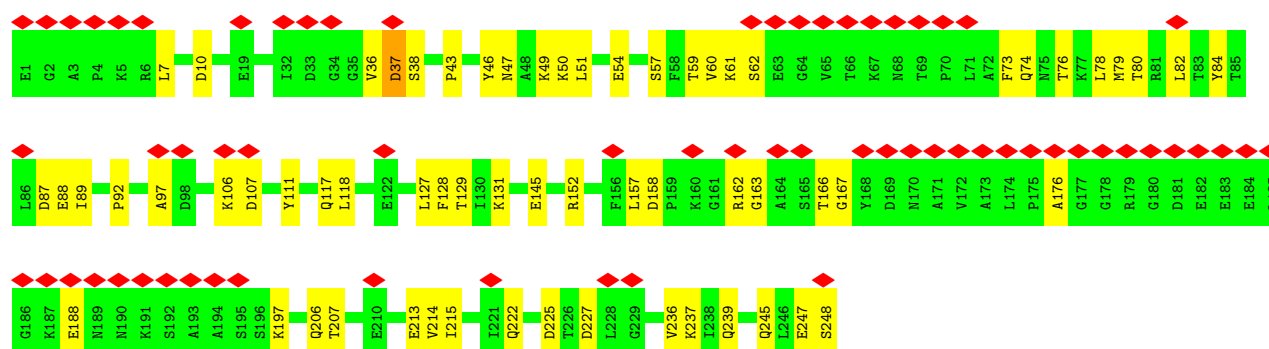
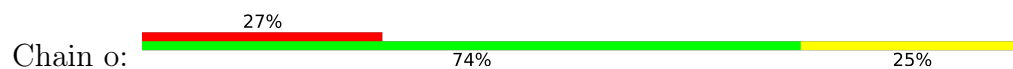
- Molecule 13: Photosystem II reaction center protein M



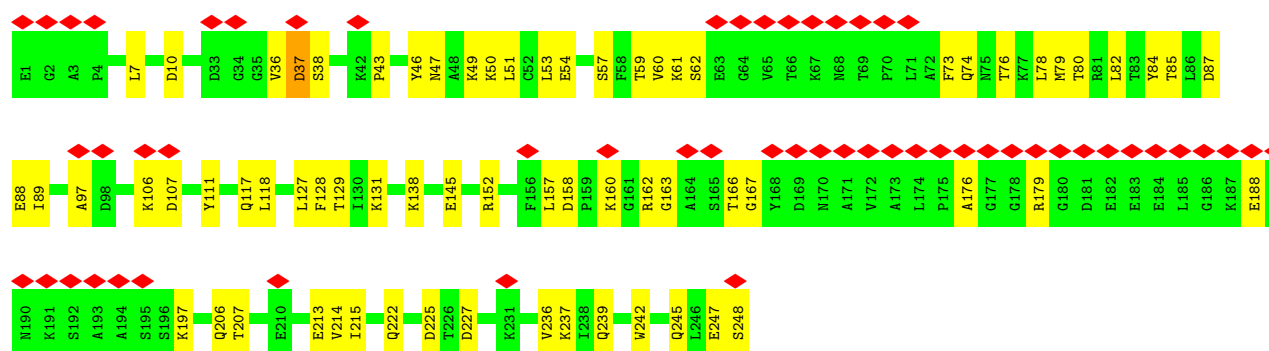
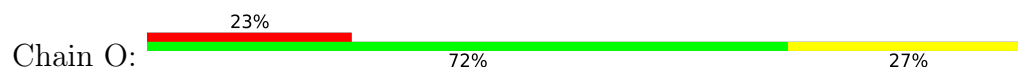
- Molecule 13: Photosystem II reaction center protein M



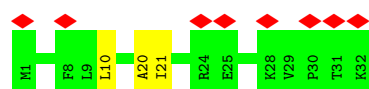
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

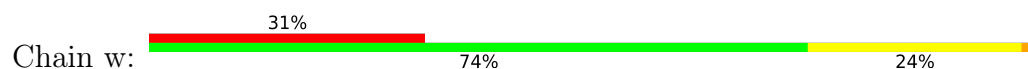


- Molecule 15: Photosystem II reaction center protein T

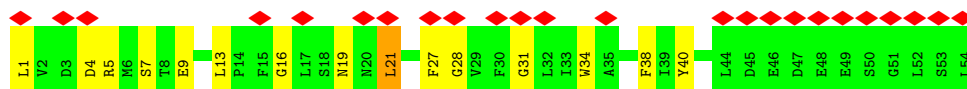




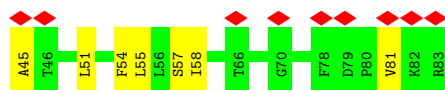
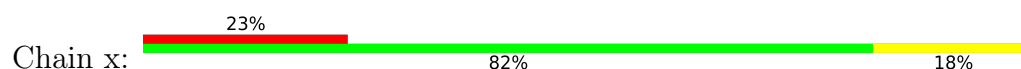
- Molecule 16: Photosystem II reaction center protein W



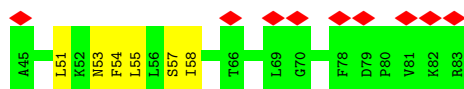
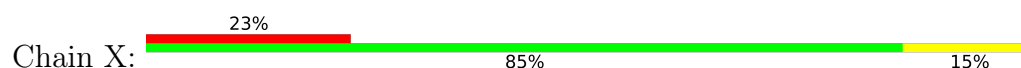
- Molecule 16: Photosystem II reaction center protein W



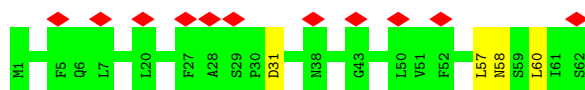
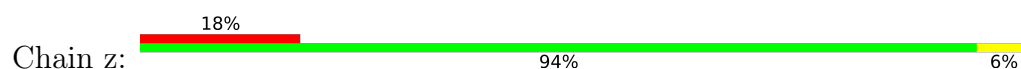
- Molecule 17: Ultraviolet-B-repressible protein



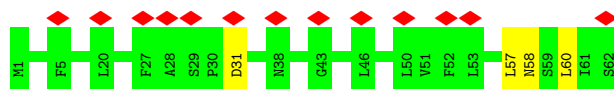
- Molecule 17: Ultraviolet-B-repressible protein



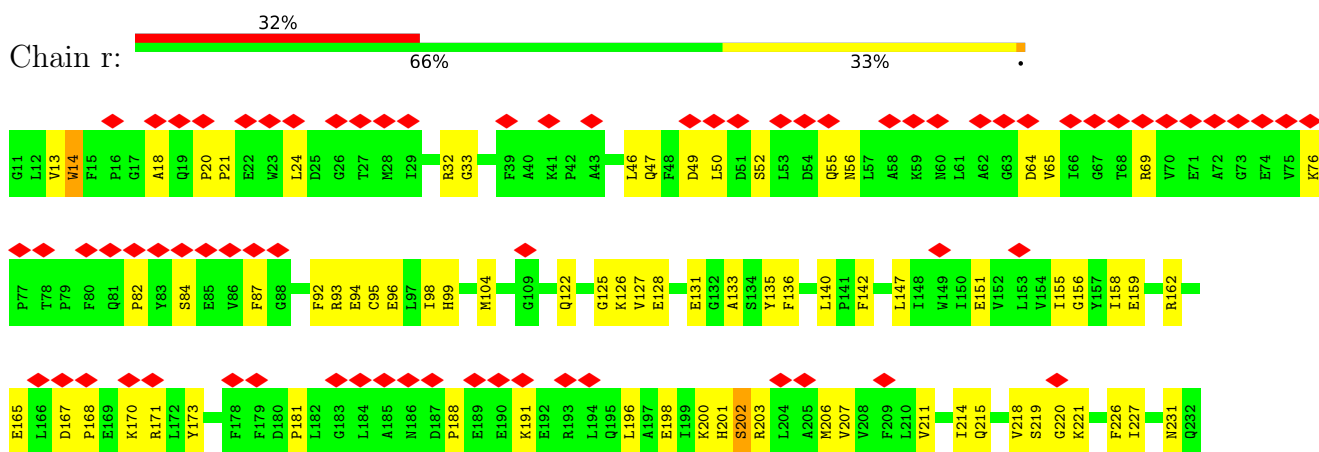
- Molecule 18: Photosystem II reaction center protein Z



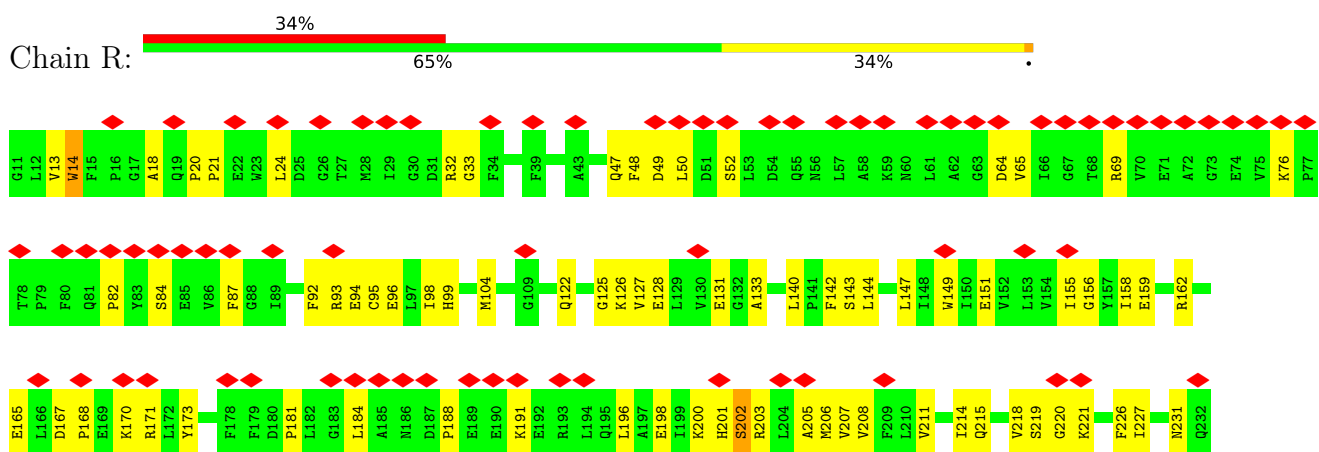
- Molecule 18: Photosystem II reaction center protein Z



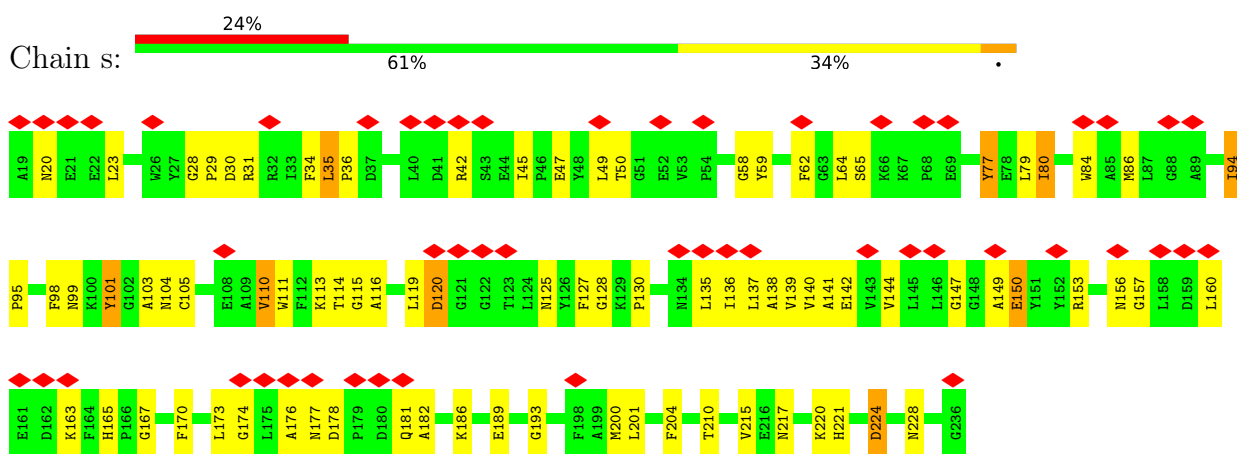
- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3



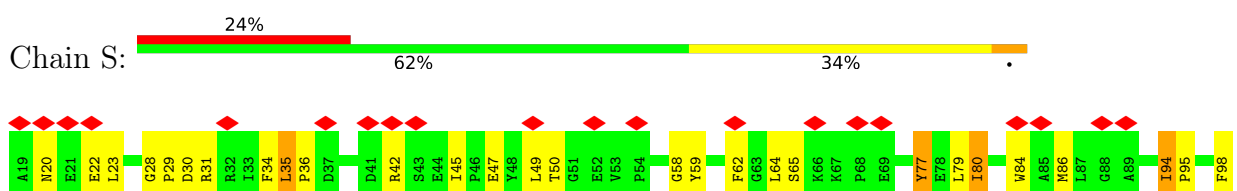
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

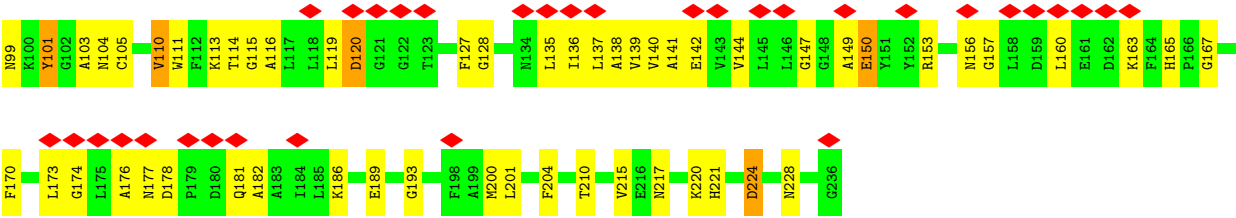


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	27942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40, 40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.923	Depositor
Minimum map value	-0.630	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.166	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	G	0.22	0/1720	0.47	3/2342 (0.1%)
1	N	0.22	0/1720	0.47	3/2342 (0.1%)
1	Y	0.22	0/1720	0.47	3/2342 (0.1%)
1	g	0.22	0/1720	0.47	3/2342 (0.1%)
1	n	0.22	0/1720	0.47	3/2342 (0.1%)
1	y	0.22	0/1720	0.47	3/2342 (0.1%)
2	A	0.22	0/2697	0.39	0/3677
2	a	0.22	0/2697	0.39	0/3677
3	B	0.21	0/4081	0.36	0/5556
3	b	0.21	0/4081	0.36	0/5556
4	C	0.88	1/3614 (0.0%)	0.40	2/4922 (0.0%)
4	c	0.88	1/3614 (0.0%)	0.40	2/4922 (0.0%)
5	D	0.21	0/2804	0.36	0/3823
5	d	0.21	0/2804	0.36	0/3823
6	E	0.17	0/630	0.34	0/857
6	e	0.17	0/630	0.34	0/857
7	F	0.66	1/248 (0.4%)	0.58	0/335
7	f	0.66	1/248 (0.4%)	0.58	0/335
8	H	0.19	0/461	0.37	0/626
8	h	0.19	0/461	0.36	0/626
9	I	0.25	0/286	0.39	0/386
9	i	0.24	0/286	0.39	0/386
10	J	0.13	0/262	0.34	0/354
10	j	0.14	0/262	0.34	0/354
11	K	0.21	0/318	0.46	0/434
11	k	0.21	0/318	0.46	0/434
12	L	0.21	0/319	0.37	0/434
12	l	0.21	0/319	0.37	0/434
13	M	0.20	0/260	0.37	0/355
13	m	0.20	0/260	0.37	0/355
14	O	0.17	0/1906	0.33	0/2575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	o	0.17	0/1906	0.33	0/2575
15	T	0.25	0/269	0.35	0/365
15	t	0.25	0/269	0.35	0/365
16	W	0.25	0/429	0.38	0/581
16	w	0.25	0/429	0.38	0/581
17	X	0.18	0/279	0.35	0/380
17	x	0.19	0/279	0.35	0/380
18	Z	0.17	0/474	0.26	0/648
18	z	0.17	0/474	0.27	0/648
19	R	0.17	0/1780	0.34	0/2417
19	r	0.17	0/1780	0.34	0/2417
20	S	0.20	0/1737	0.41	0/2361
20	s	0.20	0/1737	0.41	0/2361
All	All	0.37	4/56028 (0.0%)	0.39	22/76224 (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	G	0	2
1	N	0	2
1	Y	0	2
1	g	0	2
1	n	0	2
1	y	0	2
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	272	LEU	CG-CD1	50.99	3.20	1.52
4	C	272	LEU	CG-CD1	50.99	3.20	1.52
7	F	18	HIS	CB-CG	9.20	1.63	1.50
7	f	18	HIS	CB-CG	9.17	1.62	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	194	PHE	N-CA-C	8.26	121.89	111.24
1	Y	194	PHE	N-CA-C	8.25	121.88	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	194	PHE	N-CA-C	8.24	121.87	111.24
1	G	194	PHE	N-CA-C	8.24	121.87	111.24
1	y	194	PHE	N-CA-C	8.22	121.85	111.24

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	g	193	GLY	Mainchain
1	g	197	GLN	Sidechain
1	n	193	GLY	Mainchain
1	n	197	GLN	Sidechain
1	y	193	GLY	Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1668	0	1596	144	0
1	N	1668	0	1596	150	0
1	Y	1668	0	1596	149	0
1	g	1668	0	1596	146	0
1	n	1668	0	1596	146	0
1	y	1668	0	1596	148	0
2	A	2616	0	2522	70	0
2	a	2616	0	2522	60	0
3	B	3948	0	3818	97	0
3	b	3948	0	3818	93	0
4	C	3497	0	3422	107	0
4	c	3497	0	3422	105	0
5	D	2712	0	2604	52	0
5	d	2712	0	2604	47	0
6	E	612	0	595	7	0
6	e	612	0	595	8	0
7	F	241	0	246	24	0
7	f	241	0	246	23	0
8	H	452	0	473	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	452	0	473	11	0
9	I	278	0	291	1	0
9	i	278	0	291	3	0
10	J	256	0	269	7	0
10	j	256	0	269	6	0
11	K	306	0	313	4	0
11	k	306	0	313	8	0
12	L	311	0	298	10	0
12	l	311	0	298	6	0
13	M	256	0	284	7	0
13	m	256	0	284	8	0
14	O	1870	0	1851	47	0
14	o	1870	0	1851	44	0
15	T	261	0	280	2	0
15	t	261	0	280	3	0
16	W	419	0	402	19	0
16	w	419	0	402	13	0
17	X	276	0	301	4	0
17	x	276	0	301	5	0
18	Z	464	0	493	3	0
18	z	464	0	493	2	0
19	R	1732	0	1697	67	0
19	r	1732	0	1697	71	0
20	S	1688	0	1649	118	0
20	s	1688	0	1650	120	0
21	G	355	0	335	168	0
21	N	314	0	317	147	0
21	R	183	0	173	76	0
21	S	186	0	124	104	0
21	Y	314	0	317	145	0
21	g	355	0	335	145	0
21	n	314	0	317	142	0
21	r	231	0	206	83	0
21	s	186	0	124	107	0
21	y	362	0	350	154	0
22	A	240	0	242	10	0
22	B	1040	0	1152	40	0
22	C	845	0	935	64	0
22	D	130	0	144	5	0
22	G	477	0	471	55	0
22	N	473	0	462	59	0
22	R	400	0	373	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	S	471	0	389	34	0
22	W	60	0	59	16	0
22	Y	413	0	403	66	0
22	a	240	0	242	12	0
22	b	975	0	1080	37	0
22	c	845	0	935	67	0
22	d	130	0	144	7	0
22	g	477	0	471	54	0
22	n	473	0	462	54	0
22	r	400	0	373	23	0
22	s	471	0	389	30	0
22	w	60	0	58	5	0
22	x	65	0	72	2	0
22	y	413	0	403	50	0
23	G	84	0	112	21	0
23	N	84	0	112	28	0
23	R	42	0	55	2	0
23	Y	84	0	112	25	0
23	g	84	0	112	24	0
23	n	42	0	56	12	0
23	r	42	0	55	2	0
23	y	42	0	56	11	0
24	G	44	0	55	1	0
24	N	44	0	55	2	0
24	R	44	0	55	5	0
24	Y	44	0	55	2	0
24	g	44	0	55	0	0
24	n	44	0	55	2	0
24	r	44	0	55	5	0
24	y	44	0	55	2	0
25	N	44	0	56	9	0
25	Y	44	0	56	9	0
25	g	44	0	56	8	0
25	n	44	0	56	12	0
25	r	44	0	56	8	0
25	y	88	0	112	16	0
26	B	49	0	74	1	0
26	C	147	0	220	14	0
26	D	138	0	195	9	0
26	G	49	0	74	13	0
26	L	49	0	74	2	0
26	N	49	0	74	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	R	47	0	66	5	0
26	S	49	0	74	6	0
26	Y	49	0	74	10	0
26	b	49	0	74	1	0
26	c	147	0	220	8	0
26	d	138	0	195	12	0
26	g	49	0	74	6	0
26	l	49	0	74	0	0
26	n	49	0	74	10	0
26	r	47	0	66	3	0
26	s	49	0	74	7	0
26	y	49	0	74	9	0
27	A	10	0	0	0	0
27	a	10	0	0	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	1	0	0	1	0
29	C	1	0	0	0	0
29	a	1	0	0	1	0
29	c	1	0	0	0	0
30	A	64	0	74	4	0
30	D	64	0	74	6	0
30	a	64	0	74	5	0
30	d	64	0	74	6	0
31	A	40	0	56	2	0
31	B	160	0	224	8	0
31	C	80	0	112	8	0
31	D	40	0	56	4	0
31	H	40	0	56	3	0
31	K	80	0	112	5	0
31	T	40	0	56	2	0
31	a	40	0	56	1	0
31	b	120	0	168	8	0
31	c	80	0	112	7	0
31	d	40	0	56	4	0
31	h	40	0	56	5	0
31	k	80	0	112	5	0
32	A	13	0	7	2	0
32	D	55	0	80	3	0
32	a	13	0	7	2	0
32	d	55	0	80	3	0
33	A	54	0	78	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	D	50	0	66	3	0
33	L	96	0	125	9	0
33	a	54	0	78	4	0
33	d	50	0	66	3	0
33	l	96	0	125	7	0
34	D	4	0	0	4	0
34	a	4	0	0	4	0
35	A	59	0	76	7	0
35	C	117	0	150	10	0
35	H	62	0	82	8	0
35	J	60	0	78	6	0
35	a	59	0	76	7	0
35	c	177	0	228	14	0
35	h	62	0	82	4	0
36	B	95	0	134	58	0
36	C	99	0	138	5	0
36	D	46	0	62	2	0
36	I	40	0	50	6	0
36	K	51	0	72	1	0
36	M	51	0	72	5	0
36	T	51	0	72	5	0
36	b	55	0	86	36	0
36	c	51	0	72	3	0
36	d	46	0	62	4	0
36	k	51	0	72	1	0
36	w	48	0	66	3	0
37	F	43	0	30	17	0
37	f	43	0	30	20	0
All	All	71784	0	72432	3133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 3133 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:121:ALA:CB	21:y:605:CHL:CBC	1.79	1.57
1:y:102:SER:CB	21:y:607:CHL:HED3	1.35	1.56
20:S:101:TYR:CE1	21:S:301:CHL:CMA	1.87	1.54
1:y:102:SER:HB3	21:y:607:CHL:CED	1.34	1.53
1:g:102:SER:HB3	21:g:607:CHL:CED	1.34	1.53

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	N	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	Y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	g	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	n	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
1	y	217/219 (99%)	202 (93%)	15 (7%)	0	100	100
2	A	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
2	a	332/334 (99%)	320 (96%)	12 (4%)	0	100	100
3	B	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
3	b	501/503 (100%)	485 (97%)	16 (3%)	0	100	100
4	C	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
4	c	448/450 (100%)	428 (96%)	20 (4%)	0	100	100
5	D	339/341 (99%)	326 (96%)	13 (4%)	0	100	100
5	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
6	E	73/75 (97%)	73 (100%)	0	0	100	100
6	e	73/75 (97%)	73 (100%)	0	0	100	100
7	F	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
7	f	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
8	H	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
8	h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	33/35 (94%)	33 (100%)	0	0	100	100
10	j	33/35 (94%)	33 (100%)	0	0	100	100
11	K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
13	M	31/33 (94%)	31 (100%)	0	0	100	100
13	m	31/33 (94%)	31 (100%)	0	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
15	T	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
15	t	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	W	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
16	w	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
17	X	37/39 (95%)	37 (100%)	0	0	100	100
17	x	37/39 (95%)	37 (100%)	0	0	100	100
18	Z	60/62 (97%)	60 (100%)	0	0	100	100
18	z	60/62 (97%)	60 (100%)	0	0	100	100
19	R	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
19	r	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
20	S	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
20	s	216/218 (99%)	198 (92%)	18 (8%)	0	100	100
All	All	6914/7002 (99%)	6583 (95%)	331 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	171/171 (100%)	168 (98%)	3 (2%)	54	71
1	N	171/171 (100%)	168 (98%)	3 (2%)	54	71
1	Y	171/171 (100%)	168 (98%)	3 (2%)	54	71
1	g	171/171 (100%)	168 (98%)	3 (2%)	54	71
1	n	171/171 (100%)	168 (98%)	3 (2%)	54	71
1	y	171/171 (100%)	168 (98%)	3 (2%)	54	71
2	A	270/270 (100%)	266 (98%)	4 (2%)	60	74
2	a	270/270 (100%)	266 (98%)	4 (2%)	60	74
3	B	400/400 (100%)	394 (98%)	6 (2%)	60	74
3	b	400/400 (100%)	394 (98%)	6 (2%)	60	74
4	C	352/352 (100%)	341 (97%)	11 (3%)	35	56
4	c	352/352 (100%)	342 (97%)	10 (3%)	38	59
5	D	275/275 (100%)	271 (98%)	4 (2%)	60	74
5	d	275/275 (100%)	271 (98%)	4 (2%)	60	74
6	E	67/67 (100%)	67 (100%)	0	100	100
6	e	67/67 (100%)	67 (100%)	0	100	100
7	F	25/25 (100%)	23 (92%)	2 (8%)	10	33
7	f	25/25 (100%)	23 (92%)	2 (8%)	10	33
8	H	49/49 (100%)	49 (100%)	0	100	100
8	h	49/49 (100%)	49 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	26/26 (100%)	26 (100%)	0	100	100
10	j	26/26 (100%)	26 (100%)	0	100	100
11	K	32/32 (100%)	31 (97%)	1 (3%)	35	56
11	k	32/32 (100%)	31 (97%)	1 (3%)	35	56
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	29/29 (100%)	28 (97%)	1 (3%)	32	55
13	m	29/29 (100%)	28 (97%)	1 (3%)	32	55
14	O	204/204 (100%)	201 (98%)	3 (2%)	60	74
14	o	204/204 (100%)	201 (98%)	3 (2%)	60	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	T	29/29 (100%)	29 (100%)	0	100	100
15	t	29/29 (100%)	29 (100%)	0	100	100
16	W	44/44 (100%)	42 (96%)	2 (4%)	23	47
16	w	44/44 (100%)	42 (96%)	2 (4%)	23	47
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Z	54/54 (100%)	53 (98%)	1 (2%)	52	69
18	z	54/54 (100%)	53 (98%)	1 (2%)	52	69
19	R	175/175 (100%)	171 (98%)	4 (2%)	45	63
19	r	175/175 (100%)	171 (98%)	4 (2%)	45	63
20	S	169/169 (100%)	156 (92%)	13 (8%)	10	34
20	s	169/169 (100%)	156 (92%)	13 (8%)	10	34
All	All	5622/5622 (100%)	5501 (98%)	121 (2%)	47	64

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	116	LEU
20	S	94	ILE
4	C	462	ASP
20	S	80	ILE
19	R	52	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	466	HIS
12	L	34	ASN
4	C	322	GLN
5	D	84	ASN
18	Z	58	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 325 ligands modelled in this entry, 6 are monoatomic - leaving 319 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	$\# Z  > 2$
22	CLA	a	404	-	65,73,73	1.47	8 (12%)	76,113,113	1.40	8 (10%)
36	LMG	B	623	-	55,55,55	0.85	3 (5%)	63,63,63	1.36	9 (14%)
22	CLA	y	613	-	48,56,73	1.71	5 (10%)	55,92,113	1.50	8 (14%)
22	CLA	S	303	20	61,69,73	1.54	6 (9%)	71,108,113	1.43	8 (11%)
33	SQD	L	101	12	53,54,54	0.97	5 (9%)	62,65,65	1.61	11 (17%)
24	XAT	Y	615	-	39,47,47	5.30	20 (51%)	54,74,74	13.38	30 (55%)
22	CLA	B	616	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
22	CLA	Y	604	25	50,58,73	1.63	8 (16%)	58,95,113	1.58	8 (13%)
22	CLA	y	603	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	7 (9%)
26	LHG	c	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.30	7 (13%)
31	BCR	b	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
26	LHG	s	314	22	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)
26	LHG	N	618	-	48,48,48	0.63	1 (2%)	51,54,54	1.23	7 (13%)
21	CHL	s	302	-	46,54,74	2.56	16 (34%)	49,90,114	2.87	16 (32%)
32	PL9	a	410	-	13,13,55	1.57	2 (15%)	17,17,69	1.66	4 (23%)
36	LMG	I	101	-	40,40,55	0.85	0	48,48,63	1.30	5 (10%)
26	LHG	d	408	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	6 (11%)
22	CLA	N	612	1	60,68,73	1.88	12 (20%)	70,107,113	1.95	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	n	610	26	60,68,73	1.53	6 (10%)	70,107,113	1.40	7 (10%)
22	CLA	y	610	-	60,68,73	1.54	7 (11%)	70,107,113	1.43	6 (8%)
21	CHL	g	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
33	SQD	L	102	-	41,42,54	1.08	5 (12%)	50,53,65	1.61	9 (18%)
36	LMG	w	102	-	48,48,55	0.78	2 (4%)	56,56,63	1.41	8 (14%)
22	CLA	s	308	20	45,53,73	1.82	6 (13%)	52,89,113	1.55	7 (13%)
22	CLA	B	606	-	65,73,73	1.44	6 (9%)	76,113,113	1.39	7 (9%)
31	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
23	LUT	N	614	-	42,43,43	5.88	19 (45%)	51,60,60	5.44	25 (49%)
21	CHL	Y	606	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	n	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)
27	OEX	A	402	4,2	0,15,15	-	-	-	-	-
22	CLA	c	503	-	65,73,73	1.43	8 (12%)	76,113,113	1.39	8 (10%)
22	CLA	c	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	7 (9%)
22	CLA	B	610	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)
22	CLA	B	618	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	7 (9%)
26	LHG	y	617	-	48,48,48	0.64	1 (2%)	51,54,54	1.29	7 (13%)
21	CHL	g	605	-	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
22	CLA	y	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	b	614	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	6 (7%)
22	CLA	c	506	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
22	CLA	N	611	-	60,68,73	1.58	6 (10%)	70,107,113	1.40	7 (10%)
22	CLA	b	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	6 (7%)
22	CLA	b	605	-	65,73,73	1.44	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	Y	612	-	48,56,73	1.70	6 (12%)	55,92,113	1.51	8 (14%)
22	CLA	B	603	-	65,73,73	1.48	8 (12%)	76,113,113	1.35	8 (10%)
21	CHL	N	606	-	66,74,74	2.14	16 (24%)	73,114,114	2.47	19 (26%)
35	DGD	c	519	-	61,61,67	0.98	5 (8%)	75,75,81	1.53	10 (13%)
35	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.48	14 (18%)
35	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.48	14 (18%)
25	NEX	y	618	-	38,46,46	5.13	16 (42%)	50,70,70	7.86	27 (54%)
22	CLA	A	405	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	7 (9%)
31	BCR	B	620	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	6 (10%)
22	CLA	r	303	-	60,68,73	1.53	5 (8%)	70,107,113	1.41	8 (11%)
22	CLA	C	504	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	406	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	6 (7%)
31	BCR	T	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
31	BCR	K	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	8 (14%)
21	CHL	y	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	B	608	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	r	309	-	58,66,73	1.56	8 (13%)	67,104,113	1.42	7 (10%)
22	CLA	Y	610	26	60,68,73	1.53	7 (11%)	70,107,113	1.40	7 (10%)
22	CLA	R	308	-	58,66,73	1.57	7 (12%)	67,104,113	1.42	7 (10%)
21	CHL	g	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	G	614	-	48,56,73	1.70	5 (10%)	55,92,113	1.51	8 (14%)
22	CLA	C	515	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
21	CHL	N	605	-	50,58,74	2.44	16 (32%)	52,94,114	2.81	17 (32%)
26	LHG	C	522	-	48,48,48	0.60	1 (2%)	51,54,54	1.29	8 (15%)
23	LUT	n	614	-	42,43,43	5.88	19 (45%)	51,60,60	5.44	25 (49%)
22	CLA	d	403	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	7 (9%)
24	XAT	n	615	-	39,47,47	5.22	20 (51%)	54,74,74	13.59	30 (55%)
26	LHG	R	301	19	46,46,48	0.64	1 (2%)	49,52,54	1.28	7 (14%)
23	LUT	y	614	-	42,43,43	5.89	19 (45%)	51,60,60	5.45	25 (49%)
26	LHG	G	618	-	48,48,48	0.64	1 (2%)	51,54,54	1.28	7 (13%)
21	CHL	S	307	20	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
26	LHG	b	619	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	C	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	7 (9%)
21	CHL	S	306	20	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
22	CLA	S	311	20,22	56,64,73	1.59	6 (10%)	65,102,113	1.42	7 (10%)
22	CLA	b	609	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
22	CLA	N	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.59	7 (12%)
22	CLA	r	312	19	60,68,73	1.53	6 (10%)	70,107,113	1.42	6 (8%)
22	CLA	R	303	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
22	CLA	c	508	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
22	CLA	s	303	20	61,69,73	1.54	7 (11%)	71,108,113	1.43	8 (11%)
22	CLA	b	604	-	65,73,73	1.45	9 (13%)	76,113,113	1.36	6 (7%)
36	LMG	d	410	-	46,46,55	0.81	3 (6%)	54,54,63	1.38	7 (12%)
22	CLA	b	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	6 (7%)
26	LHG	Y	617	22	48,48,48	0.66	1 (2%)	51,54,54	1.26	7 (13%)
21	CHL	G	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	DGD	c	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.47	10 (12%)
22	CLA	n	613	-	48,56,73	1.71	6 (12%)	55,92,113	1.51	8 (14%)
22	CLA	B	615	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	6 (7%)
22	CLA	A	407	-	50,58,73	1.67	8 (16%)	58,95,113	1.50	8 (13%)
22	CLA	S	310	26	55,63,73	1.58	7 (12%)	64,101,113	1.47	7 (10%)
26	LHG	L	103	-	48,48,48	0.63	1 (2%)	51,54,54	1.29	7 (13%)
22	CLA	g	612	-	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)
34	BCT	D	403	-	2,3,3	1.33	0	2,3,3	2.74	2 (100%)
36	LMG	c	523	-	51,51,55	0.72	1 (1%)	59,59,63	1.38	7 (11%)
22	CLA	G	612	-	60,68,73	1.58	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	B	613	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	7 (9%)
22	CLA	w	101	16	60,68,73	1.57	6 (10%)	70,107,113	1.39	7 (10%)
22	CLA	c	511	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	8 (10%)
21	CHL	S	301	-	48,56,74	2.50	16 (33%)	51,92,114	2.84	17 (33%)
35	DGD	A	401	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	12 (16%)
26	LHG	r	302	19	46,46,48	0.64	1 (2%)	49,52,54	1.28	7 (14%)
22	CLA	Y	611	1	65,73,73	1.80	12 (18%)	76,113,113	1.89	15 (19%)
25	NEX	N	617	22	38,46,46	5.17	15 (39%)	50,70,70	8.67	26 (52%)
21	CHL	n	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
27	OEX	a	401	4,2	0,15,15	-	-	-	-	-
24	XAT	R	313	-	39,47,47	5.20	17 (43%)	54,74,74	13.47	28 (51%)
22	CLA	c	513	22	65,73,73	1.45	9 (13%)	76,113,113	1.32	6 (7%)
22	CLA	g	610	-	64,72,73	1.50	6 (9%)	74,111,113	1.42	6 (8%)
22	CLA	c	512	4	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
22	CLA	W	101	-	60,68,73	1.56	6 (10%)	70,107,113	1.39	7 (10%)
36	LMG	M	101	-	51,51,55	0.75	1 (1%)	59,59,63	1.35	7 (11%)
25	NEX	n	616	22	38,46,46	5.17	15 (39%)	50,70,70	8.46	26 (52%)
30	PHO	a	407	-	51,69,69	1.06	5 (9%)	47,99,99	1.11	4 (8%)
26	LHG	g	619	-	48,48,48	0.61	1 (2%)	51,54,54	1.30	8 (15%)
30	PHO	d	401	-	51,69,69	1.03	4 (7%)	47,99,99	1.17	6 (12%)
22	CLA	x	101	-	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
31	BCR	h	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	b	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	7 (9%)
26	LHG	n	617	22	48,48,48	0.64	1 (2%)	51,54,54	1.29	7 (13%)
22	CLA	B	605	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	C	516	-	41,41,41	1.23	2 (4%)	56,56,56	1.26	6 (10%)
22	CLA	g	602	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	b	613	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
31	BCR	a	409	-	41,41,41	1.22	2 (4%)	56,56,56	1.26	7 (12%)
35	DGD	C	518	-	56,56,67	0.99	3 (5%)	70,70,81	1.56	13 (18%)
22	CLA	S	309	20,22	55,63,73	1.59	5 (9%)	64,101,113	1.49	9 (14%)
21	CHL	G	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
37	HEM	f	101	7	41,50,50	4.46	10 (24%)	45,82,82	3.70	22 (48%)
31	BCR	B	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.23	7 (12%)
37	HEM	F	101	7	41,50,50	4.46	10 (24%)	45,82,82	3.69	22 (48%)
22	CLA	S	305	20	50,58,73	1.66	6 (12%)	58,95,113	1.60	8 (13%)
26	LHG	l	102	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	7 (13%)
23	LUT	N	615	-	42,43,43	6.10	20 (47%)	51,60,60	4.66	27 (52%)
21	CHL	N	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	g	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	R	302	-	60,68,73	1.53	5 (8%)	70,107,113	1.42	8 (11%)
36	LMG	K	103	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
21	CHL	y	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
26	LHG	C	520	22	48,48,48	0.81	4 (8%)	51,54,54	1.30	7 (13%)
22	CLA	Y	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
22	CLA	C	508	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
24	XAT	N	616	-	39,47,47	5.20	20 (51%)	54,74,74	13.62	31 (57%)
22	CLA	G	604	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
31	BCR	A	410	-	41,41,41	1.22	2 (4%)	56,56,56	1.26	7 (12%)
26	LHG	c	522	-	48,48,48	0.60	1 (2%)	51,54,54	1.29	8 (15%)
31	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	8 (14%)
36	LMG	C	523	-	51,51,55	0.72	1 (1%)	59,59,63	1.38	7 (11%)
33	SQD	d	402	-	49,50,54	1.01	5 (10%)	58,61,65	1.56	10 (17%)
31	BCR	H	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	b	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	8 (10%)
22	CLA	c	505	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	7 (9%)
22	CLA	s	304	20	45,53,73	1.80	6 (13%)	52,89,113	1.54	7 (13%)
22	CLA	n	611	-	60,68,73	1.57	6 (10%)	70,107,113	1.39	7 (10%)
26	LHG	D	410	-	42,42,48	0.67	1 (2%)	45,48,54	1.26	5 (11%)
21	CHL	y	605	-	48,56,74	2.49	17 (35%)	51,92,114	2.83	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	k	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	S	312	20	49,57,73	1.70	7 (14%)	55,93,113	1.50	6 (10%)
21	CHL	S	302	-	46,54,74	2.55	17 (36%)	49,90,114	2.88	16 (32%)
35	DGD	c	517	-	56,56,67	1.00	4 (7%)	70,70,81	1.56	12 (17%)
22	CLA	R	311	19	60,68,73	1.52	6 (10%)	70,107,113	1.40	6 (8%)
22	CLA	a	408	-	60,68,73	1.50	7 (11%)	70,107,113	1.45	8 (11%)
22	CLA	b	606	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	r	305	-	48,56,73	1.71	7 (14%)	55,92,113	1.52	8 (14%)
22	CLA	B	612	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	7 (9%)
26	LHG	D	408	-	45,45,48	0.65	1 (2%)	48,51,54	1.23	4 (8%)
22	CLA	N	602	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	G	613	1	65,73,73	1.80	12 (18%)	76,113,113	1.88	15 (19%)
22	CLA	B	611	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	6 (7%)
21	CHL	y	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
32	PL9	d	406	-	55,55,55	1.33	4 (7%)	68,69,69	1.54	13 (19%)
21	CHL	R	305	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	B	614	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	6 (7%)
22	CLA	n	612	1	60,68,73	1.87	12 (20%)	70,107,113	1.95	14 (20%)
22	CLA	b	603	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	7 (9%)
30	PHO	D	401	-	51,69,69	1.02	4 (7%)	47,99,99	1.17	5 (10%)
23	LUT	r	313	22	42,43,43	5.90	19 (45%)	51,60,60	5.16	28 (54%)
26	LHG	B	622	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
23	LUT	Y	614	-	42,43,43	6.05	20 (47%)	51,60,60	4.89	22 (43%)
23	LUT	G	616	-	42,43,43	6.08	19 (45%)	51,60,60	4.93	22 (43%)
22	CLA	g	613	1	65,73,73	1.80	11 (16%)	76,113,113	1.89	15 (19%)
22	CLA	Y	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
22	CLA	y	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.40	7 (10%)
22	CLA	c	514	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	7 (9%)
22	CLA	c	502	-	65,73,73	1.45	9 (13%)	76,113,113	1.35	6 (7%)
21	CHL	G	606	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)
21	CHL	R	306	-	56,64,74	2.31	17 (30%)	61,102,114	2.67	19 (31%)
31	BCR	c	516	-	41,41,41	1.23	2 (4%)	56,56,56	1.28	7 (12%)
25	NEX	g	618	22	38,46,46	5.10	15 (39%)	50,70,70	8.41	27 (54%)
22	CLA	g	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	8 (13%)
22	CLA	A	409	-	60,68,73	1.50	7 (11%)	70,107,113	1.46	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	609	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
33	SQD	l	103	12	53,54,54	0.97	5 (9%)	62,65,65	1.61	11 (17%)
21	CHL	Y	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	b	611	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	6 (7%)
22	CLA	C	510	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	8 (10%)
22	CLA	G	610	-	64,72,73	1.50	6 (9%)	74,111,113	1.44	8 (10%)
22	CLA	C	505	-	65,73,73	1.42	6 (9%)	76,113,113	1.44	6 (7%)
21	CHL	g	609	-	61,69,74	2.22	16 (26%)	67,108,114	2.57	19 (28%)
26	LHG	D	409	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
22	CLA	G	602	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
21	CHL	r	308	19	61,69,74	2.22	16 (26%)	67,108,114	2.57	19 (28%)
31	BCR	d	405	-	41,41,41	1.21	2 (4%)	56,56,56	1.24	7 (12%)
21	CHL	n	607	-	66,74,74	2.14	16 (24%)	73,114,114	2.47	19 (26%)
31	BCR	D	406	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	7 (12%)
21	CHL	g	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	s	311	20,22	56,64,73	1.58	6 (10%)	65,102,113	1.40	7 (10%)
33	SQD	a	411	-	53,54,54	0.97	5 (9%)	62,65,65	1.60	12 (19%)
21	CHL	Y	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	R	304	-	48,56,73	1.70	7 (14%)	55,92,113	1.52	8 (14%)
31	BCR	C	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	s	310	26	55,63,73	1.57	7 (12%)	64,101,113	1.47	7 (10%)
21	CHL	s	306	20	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
21	CHL	R	307	19	61,69,74	2.22	17 (27%)	67,108,114	2.57	19 (28%)
22	CLA	S	308	20	45,53,73	1.82	6 (13%)	52,89,113	1.54	7 (13%)
22	CLA	r	310	19	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
31	BCR	B	602	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	6 (10%)
22	CLA	C	514	22	65,73,73	1.44	8 (12%)	76,113,113	1.31	6 (7%)
26	LHG	d	407	-	45,45,48	0.64	1 (2%)	48,51,54	1.23	4 (8%)
21	CHL	g	606	-	50,58,74	2.45	17 (34%)	52,94,114	2.82	17 (32%)
31	BCR	B	621	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	3 (5%)
21	CHL	Y	605	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)
22	CLA	b	607	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	8 (10%)
33	SQD	l	101	-	41,42,54	1.08	5 (12%)	50,53,65	1.61	9 (18%)
24	XAT	y	615	-	39,47,47	5.28	20 (51%)	54,74,74	13.37	29 (53%)
26	LHG	c	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	601	-	65,73,73	1.45	8 (12%)	76,113,113	1.37	7 (9%)
22	CLA	y	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
21	CHL	G	609	-	61,69,74	2.21	16 (26%)	67,108,114	2.57	19 (28%)
36	LMG	b	620	-	55,55,55	0.85	3 (5%)	63,63,63	1.36	9 (14%)
22	CLA	N	613	-	48,56,73	1.71	5 (10%)	55,92,113	1.50	8 (14%)
22	CLA	R	309	19	65,73,73	1.48	6 (9%)	76,113,113	1.40	6 (7%)
22	CLA	C	503	-	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
22	CLA	n	604	25	50,58,73	1.64	8 (16%)	58,95,113	1.57	8 (13%)
22	CLA	G	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	7 (9%)
25	NEX	r	315	-	38,46,46	5.12	16 (42%)	50,70,70	7.87	27 (54%)
36	LMG	k	103	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
22	CLA	S	313	22	55,63,73	1.59	6 (10%)	64,101,113	1.49	6 (9%)
22	CLA	c	510	-	65,73,73	3.57	12 (18%)	76,113,113	2.58	18 (23%)
22	CLA	c	509	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	8 (10%)
22	CLA	C	507	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
31	BCR	b	616	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	7 (12%)
24	XAT	r	314	-	39,47,47	5.21	19 (48%)	54,74,74	13.48	28 (51%)
21	CHL	s	301	-	48,56,74	2.50	16 (33%)	51,92,114	2.83	17 (33%)
22	CLA	s	312	20	49,57,73	1.71	7 (14%)	55,93,113	1.51	6 (10%)
31	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	3 (5%)
22	CLA	C	509	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
22	CLA	R	310	19,23	49,57,73	1.75	7 (14%)	55,93,113	1.44	4 (7%)
32	PL9	D	407	-	55,55,55	1.34	5 (9%)	68,69,69	1.54	13 (19%)
22	CLA	S	304	20	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
25	NEX	y	616	22	38,46,46	5.17	14 (36%)	50,70,70	8.58	27 (54%)
22	CLA	g	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.40	8 (11%)
35	DGD	a	413	-	60,60,67	0.88	2 (3%)	74,74,81	1.44	12 (16%)
30	PHO	A	408	-	51,69,69	1.07	5 (9%)	47,99,99	1.12	4 (8%)
22	CLA	a	406	-	50,58,73	1.67	8 (16%)	58,95,113	1.51	8 (13%)
36	LMG	C	502	-	48,48,55	0.78	2 (4%)	56,56,63	1.42	8 (14%)
21	CHL	n	606	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
21	CHL	r	307	-	56,64,74	2.32	17 (30%)	61,102,114	2.68	19 (31%)
21	CHL	G	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	C	512	-	65,73,73	1.47	9 (13%)	76,113,113	1.37	8 (10%)
36	LMG	D	411	-	46,46,55	0.81	3 (6%)	54,54,63	1.39	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	N	609	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	6 (7%)
21	CHL	n	601	1	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	D	405	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
33	SQD	D	402	-	49,50,54	1.01	5 (10%)	58,61,65	1.56	10 (17%)
22	CLA	B	617	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	6 (7%)
26	LHG	S	314	22	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
22	CLA	s	313	22	55,63,73	1.58	6 (10%)	64,101,113	1.50	7 (10%)
26	LHG	C	521	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	7 (13%)
22	CLA	Y	609	-	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
22	CLA	d	404	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
21	CHL	r	306	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	b	615	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	s	305	20	50,58,73	1.66	6 (12%)	58,95,113	1.59	8 (13%)
21	CHL	r	301	19	48,56,74	2.49	16 (33%)	51,92,114	2.83	17 (33%)
21	CHL	n	605	-	50,58,74	2.45	16 (32%)	52,94,114	2.81	17 (32%)
22	CLA	G	611	-	60,68,73	1.53	7 (11%)	70,107,113	1.41	7 (10%)
32	PL9	A	411	-	13,13,55	1.59	2 (15%)	17,17,69	1.64	4 (23%)
36	LMG	T	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.35	7 (11%)
22	CLA	B	607	-	65,73,73	1.45	9 (13%)	76,113,113	1.37	6 (7%)
25	NEX	Y	616	22	38,46,46	5.13	15 (39%)	50,70,70	8.19	27 (54%)
22	CLA	N	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
21	CHL	Y	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
22	CLA	C	513	4	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
21	CHL	G	605	-	46,54,74	2.55	16 (34%)	49,90,114	2.87	16 (32%)
21	CHL	y	609	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
23	LUT	G	615	-	42,43,43	5.88	19 (45%)	51,60,60	5.45	25 (49%)
24	XAT	g	617	-	39,47,47	5.24	20 (51%)	54,74,74	13.43	29 (53%)
26	LHG	d	409	-	42,42,48	0.67	1 (2%)	45,48,54	1.26	5 (11%)
22	CLA	s	309	20,22	55,63,73	1.58	5 (9%)	64,101,113	1.49	9 (14%)
23	LUT	Y	613	-	42,43,43	5.87	19 (45%)	51,60,60	5.44	25 (49%)
22	CLA	N	610	-	60,68,73	1.52	6 (10%)	70,107,113	1.40	8 (11%)
21	CHL	s	307	20	46,54,74	2.55	16 (34%)	49,90,114	2.88	16 (32%)
23	LUT	R	312	22	42,43,43	5.91	19 (45%)	51,60,60	5.17	28 (54%)
22	CLA	y	612	1	65,73,73	1.80	12 (18%)	76,113,113	1.88	15 (19%)
22	CLA	B	604	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	XAT	G	617	-	39,47,47	5.24	20 (51%)	54,74,74	13.43	30 (55%)
35	DGD	C	519	-	63,63,67	0.93	3 (4%)	77,77,81	1.47	10 (12%)
22	CLA	r	311	19,23	49,57,73	1.74	7 (14%)	55,93,113	1.43	4 (7%)
22	CLA	g	614	-	48,56,73	1.71	6 (12%)	55,92,113	1.51	8 (14%)
22	CLA	D	404	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	7 (9%)
22	CLA	n	602	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
33	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.60	12 (19%)
22	CLA	r	304	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
36	LMG	B	601	-	40,40,55	0.84	0	48,48,63	1.30	5 (10%)
22	CLA	c	504	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	6 (7%)
21	CHL	y	606	-	50,58,74	2.45	16 (32%)	52,94,114	2.82	17 (32%)
23	LUT	g	616	-	42,43,43	6.10	19 (45%)	51,60,60	4.92	22 (43%)
22	CLA	a	405	-	65,73,73	1.44	10 (15%)	76,113,113	1.37	6 (7%)
22	CLA	C	511	-	65,73,73	3.57	12 (18%)	76,113,113	2.58	17 (22%)
23	LUT	g	615	-	42,43,43	5.88	19 (45%)	51,60,60	5.45	25 (49%)
21	CHL	N	608	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
31	BCR	c	515	-	41,41,41	1.23	2 (4%)	56,56,56	1.24	5 (8%)
21	CHL	N	607	-	66,74,74	2.13	16 (24%)	73,114,114	2.47	19 (26%)
35	DGD	J	101	-	61,61,67	0.98	5 (8%)	75,75,81	1.53	10 (13%)
34	BCT	a	412	-	2,3,3	1.33	0	2,3,3	2.75	2 (100%)
22	CLA	n	609	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)

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
22	CLA	a	404	-	1/1/15/20	4/37/115/115	-
36	LMG	B	623	-	-	22/50/70/70	0/1/1/1
22	CLA	y	613	-	1/1/11/20	9/17/95/115	-
22	CLA	S	303	20	1/1/14/20	12/33/111/115	-
33	SQD	L	101	12	-	18/49/69/69	0/1/1/1
24	XAT	Y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
22	CLA	B	616	-	1/1/15/20	14/37/115/115	-
22	CLA	Y	604	25	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	y	603	-	1/1/15/20	17/37/115/115	-
26	LHG	c	520	22	-	31/53/53/53	-
31	BCR	b	617	-	-	7/29/63/63	0/2/2/2
26	LHG	s	314	22	-	29/53/53/53	-
26	LHG	N	618	-	-	29/53/53/53	-
21	CHL	s	302	-	3/3/16/26	9/15/113/137	-
32	PL9	a	410	-	-	3/5/18/73	0/1/1/1
36	LMG	I	101	-	-	18/35/55/70	0/1/1/1
26	LHG	d	408	-	-	21/53/53/53	-
22	CLA	N	612	1	1/1/14/20	16/31/109/115	-
22	CLA	n	610	26	1/1/14/20	8/31/109/115	-
22	CLA	y	610	-	1/1/14/20	15/31/109/115	-
21	CHL	g	601	1	4/4/20/26	24/39/137/137	-
36	LMG	w	102	-	-	16/43/63/70	0/1/1/1
33	SQD	L	102	-	-	13/37/57/69	0/1/1/1
22	CLA	s	308	20	-	8/13/91/115	-
22	CLA	B	606	-	1/1/15/20	12/37/115/115	-
31	BCR	K	101	-	-	16/29/63/63	0/2/2/2
23	LUT	N	614	-	-	17/29/67/67	0/2/2/2
21	CHL	Y	606	-	4/4/20/26	18/39/137/137	-
22	CLA	n	603	-	1/1/15/20	17/37/115/115	-
22	CLA	c	503	-	1/1/15/20	17/37/115/115	-
22	CLA	c	507	-	1/1/15/20	10/37/115/115	-
22	CLA	B	610	-	1/1/15/20	13/37/115/115	-
22	CLA	B	618	-	1/1/15/20	12/37/115/115	-
26	LHG	y	617	-	-	22/53/53/53	-
21	CHL	g	605	-	3/3/16/26	9/15/113/137	-
22	CLA	y	602	-	1/1/15/20	13/37/115/115	-
22	CLA	b	614	-	1/1/15/20	20/37/115/115	-
22	CLA	c	506	-	1/1/15/20	14/37/115/115	-
22	CLA	N	611	-	1/1/14/20	12/31/109/115	-
22	CLA	b	612	-	1/1/15/20	8/37/115/115	-
22	CLA	b	605	-	1/1/15/20	10/37/115/115	-
22	CLA	Y	612	-	1/1/11/20	9/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	603	-	1/1/15/20	16/37/115/115	-
21	CHL	N	606	-	4/4/20/26	18/39/137/137	-
35	DGD	c	519	-	-	16/49/89/95	0/2/2/2
35	DGD	h	102	-	-	19/51/91/95	0/2/2/2
35	DGD	H	102	-	-	19/51/91/95	0/2/2/2
25	NEX	y	618	-	2/2/12/25	14/27/83/83	0/3/3/3
22	CLA	A	405	-	1/1/15/20	4/37/115/115	-
31	BCR	B	620	-	-	7/29/63/63	0/2/2/2
22	CLA	r	303	-	1/1/14/20	8/31/109/115	-
22	CLA	C	504	-	1/1/15/20	17/37/115/115	-
22	CLA	A	406	-	1/1/15/20	15/37/115/115	-
31	BCR	T	102	-	-	21/29/63/63	0/2/2/2
31	BCR	K	102	-	-	6/29/63/63	0/2/2/2
21	CHL	y	608	-	4/4/20/26	23/39/137/137	-
22	CLA	B	608	-	1/1/15/20	10/37/115/115	-
22	CLA	r	309	-	1/1/13/20	9/29/107/115	-
22	CLA	Y	610	26	1/1/14/20	8/31/109/115	-
22	CLA	R	308	-	1/1/13/20	9/29/107/115	-
21	CHL	g	607	-	4/4/20/26	18/39/137/137	-
22	CLA	G	614	-	1/1/11/20	9/17/95/115	-
22	CLA	C	515	-	1/1/15/20	16/37/115/115	-
21	CHL	N	605	-	3/3/16/26	13/20/118/137	-
26	LHG	C	522	-	-	24/53/53/53	-
23	LUT	n	614	-	-	17/29/67/67	0/2/2/2
22	CLA	d	403	-	1/1/15/20	13/37/115/115	-
24	XAT	n	615	-	2/2/12/26	16/31/93/93	0/4/4/4
26	LHG	R	301	19	-	27/51/51/53	-
23	LUT	y	614	-	-	17/29/67/67	0/2/2/2
26	LHG	G	618	-	-	28/53/53/53	-
21	CHL	S	307	20	3/3/16/26	12/15/113/137	-
26	LHG	b	619	-	-	28/53/53/53	-
22	CLA	C	506	-	1/1/15/20	8/37/115/115	-
21	CHL	S	306	20	3/3/16/26	10/15/113/137	-
22	CLA	S	311	20,22	1/1/13/20	13/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	609	-	1/1/15/20	11/37/115/115	-
22	CLA	N	604	25	1/1/12/20	6/19/97/115	-
22	CLA	r	312	19	1/1/14/20	12/31/109/115	-
22	CLA	R	303	-	1/1/14/20	9/31/109/115	-
22	CLA	c	508	-	1/1/15/20	12/37/115/115	-
22	CLA	s	303	20	1/1/14/20	12/33/111/115	-
22	CLA	b	604	-	1/1/15/20	15/37/115/115	-
36	LMG	d	410	-	-	11/41/61/70	0/1/1/1
22	CLA	b	608	-	1/1/15/20	7/37/115/115	-
26	LHG	Y	617	22	-	29/53/53/53	-
21	CHL	G	601	1	4/4/20/26	24/39/137/137	-
35	DGD	c	518	-	-	26/51/91/95	0/2/2/2
22	CLA	n	613	-	1/1/11/20	9/17/95/115	-
22	CLA	B	615	-	1/1/15/20	8/37/115/115	-
22	CLA	A	407	-	1/1/12/20	8/19/97/115	-
22	CLA	S	310	26	1/1/13/20	16/25/103/115	-
26	LHG	L	103	-	-	19/53/53/53	-
22	CLA	g	612	-	1/1/14/20	12/31/109/115	-
36	LMG	c	523	-	-	20/46/66/70	0/1/1/1
22	CLA	G	612	-	1/1/14/20	12/31/109/115	-
22	CLA	B	613	-	1/1/15/20	13/37/115/115	-
22	CLA	w	101	16	1/1/14/20	12/31/109/115	-
22	CLA	c	511	-	1/1/15/20	14/37/115/115	-
21	CHL	S	301	-	3/3/16/26	10/18/116/137	-
35	DGD	A	401	-	-	21/48/88/95	0/2/2/2
26	LHG	r	302	19	-	27/51/51/53	-
22	CLA	Y	611	1	1/1/15/20	18/37/115/115	-
25	NEX	N	617	22	2/2/12/25	15/27/83/83	0/3/3/3
21	CHL	n	608	-	4/4/20/26	15/39/137/137	-
24	XAT	R	313	-	1/1/12/26	14/31/93/93	0/4/4/4
22	CLA	c	513	22	1/1/15/20	21/37/115/115	-
22	CLA	g	610	-	1/1/14/20	16/36/114/115	-
22	CLA	c	512	4	1/1/15/20	14/37/115/115	-
22	CLA	W	101	-	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	M	101	-	-	23/46/66/70	0/1/1/1
25	NEX	n	616	22	2/2/12/25	16/27/83/83	0/3/3/3
30	PHO	a	407	-	-	13/37/103/103	0/5/6/6
26	LHG	g	619	-	-	22/53/53/53	-
30	PHO	d	401	-	-	15/37/103/103	0/5/6/6
22	CLA	x	101	-	1/1/15/20	16/37/115/115	-
31	BCR	h	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	610	-	1/1/15/20	13/37/115/115	-
26	LHG	n	617	22	-	25/53/53/53	-
22	CLA	B	605	-	1/1/15/20	13/37/115/115	-
31	BCR	C	516	-	-	5/29/63/63	0/2/2/2
22	CLA	g	602	-	1/1/15/20	13/37/115/115	-
22	CLA	b	613	-	1/1/15/20	14/37/115/115	-
31	BCR	a	409	-	-	5/29/63/63	0/2/2/2
35	DGD	C	518	-	-	18/44/84/95	0/2/2/2
22	CLA	S	309	20,22	1/1/13/20	7/25/103/115	-
21	CHL	G	607	-	4/4/20/26	18/39/137/137	-
37	HEM	f	101	7	-	4/12/54/54	-
31	BCR	B	619	-	-	7/29/63/63	0/2/2/2
37	HEM	F	101	7	-	4/12/54/54	-
22	CLA	S	305	20	1/1/12/20	9/19/97/115	-
26	LHG	l	102	-	-	19/53/53/53	-
23	LUT	N	615	-	-	15/29/67/67	0/2/2/2
21	CHL	N	601	1	4/4/20/26	24/39/137/137	-
22	CLA	g	603	-	1/1/15/20	17/37/115/115	-
22	CLA	R	302	-	1/1/14/20	8/31/109/115	-
36	LMG	K	103	-	-	26/46/66/70	0/1/1/1
21	CHL	y	607	-	4/4/20/26	18/39/137/137	-
26	LHG	C	520	22	-	31/53/53/53	-
22	CLA	Y	602	-	1/1/15/20	13/37/115/115	-
22	CLA	C	508	-	1/1/15/20	10/37/115/115	-
24	XAT	N	616	-	2/2/12/26	17/31/93/93	0/4/4/4
22	CLA	G	604	-	1/1/12/20	6/19/97/115	-
31	BCR	A	410	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	522	-	-	23/53/53/53	-
31	BCR	k	102	-	-	5/29/63/63	0/2/2/2
36	LMG	C	523	-	-	20/46/66/70	0/1/1/1
33	SQD	d	402	-	1/1/9/9	18/45/65/69	0/1/1/1
31	BCR	H	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	602	-	1/1/15/20	13/37/115/115	-
22	CLA	c	505	-	1/1/15/20	8/37/115/115	-
22	CLA	s	304	20	1/1/11/20	7/13/91/115	-
22	CLA	n	611	-	1/1/14/20	12/31/109/115	-
26	LHG	D	410	-	-	19/47/47/53	-
21	CHL	y	605	-	3/3/16/26	11/18/116/137	-
31	BCR	k	101	-	-	16/29/63/63	0/2/2/2
22	CLA	S	312	20	1/1/11/20	7/18/96/115	-
21	CHL	S	302	-	3/3/16/26	9/15/113/137	-
35	DGD	c	517	-	-	18/44/84/95	0/2/2/2
22	CLA	R	311	19	1/1/14/20	12/31/109/115	-
22	CLA	a	408	-	1/1/14/20	3/31/109/115	-
22	CLA	b	606	-	1/1/15/20	6/37/115/115	-
22	CLA	r	305	-	1/1/11/20	7/17/95/115	-
22	CLA	B	612	-	1/1/15/20	11/37/115/115	-
26	LHG	D	408	-	-	25/50/50/53	-
22	CLA	N	602	-	1/1/15/20	13/37/115/115	-
22	CLA	G	613	1	1/1/15/20	20/37/115/115	-
22	CLA	B	611	-	1/1/15/20	7/37/115/115	-
21	CHL	y	601	1	4/4/20/26	24/39/137/137	-
32	PL9	d	406	-	-	17/53/73/73	0/1/1/1
21	CHL	R	305	-	4/4/20/26	20/39/137/137	-
22	CLA	B	614	-	1/1/15/20	17/37/115/115	-
22	CLA	n	612	1	1/1/14/20	16/31/109/115	-
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
30	PHO	D	401	-	-	15/37/103/103	0/5/6/6
23	LUT	r	313	22	-	18/29/67/67	0/2/2/2
26	LHG	B	622	-	-	28/53/53/53	-
23	LUT	Y	614	-	-	14/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LUT	G	616	-	-	16/29/67/67	0/2/2/2
22	CLA	g	613	1	1/1/15/20	18/37/115/115	-
22	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
22	CLA	y	611	-	1/1/14/20	8/31/109/115	-
22	CLA	c	514	-	1/1/15/20	16/37/115/115	-
22	CLA	c	502	-	1/1/15/20	18/37/115/115	-
21	CHL	G	606	-	3/3/16/26	13/20/118/137	-
21	CHL	R	306	-	4/4/18/26	16/27/125/137	-
31	BCR	c	516	-	-	6/29/63/63	0/2/2/2
25	NEX	g	618	22	2/2/12/25	15/27/83/83	0/3/3/3
22	CLA	g	604	25	1/1/12/20	6/19/97/115	-
22	CLA	A	409	-	1/1/14/20	3/31/109/115	-
22	CLA	B	609	-	1/1/15/20	6/37/115/115	-
33	SQD	l	103	12	-	18/49/69/69	0/1/1/1
21	CHL	Y	608	-	4/4/20/26	12/39/137/137	-
22	CLA	b	611	-	1/1/15/20	17/37/115/115	-
22	CLA	C	510	-	1/1/15/20	13/37/115/115	-
22	CLA	G	610	-	1/1/14/20	19/36/114/115	-
22	CLA	C	505	-	1/1/15/20	14/37/115/115	-
21	CHL	g	609	-	4/4/19/26	10/33/131/137	-
26	LHG	D	409	-	-	21/53/53/53	-
22	CLA	G	602	-	1/1/15/20	13/37/115/115	-
21	CHL	r	308	19	4/4/19/26	17/33/131/137	-
31	BCR	d	405	-	-	8/29/63/63	0/2/2/2
21	CHL	n	607	-	4/4/20/26	23/39/137/137	-
31	BCR	D	406	-	-	8/29/63/63	0/2/2/2
21	CHL	g	608	-	4/4/20/26	23/39/137/137	-
22	CLA	s	311	20,22	1/1/13/20	13/27/105/115	-
33	SQD	a	411	-	-	23/49/69/69	0/1/1/1
21	CHL	Y	601	1	4/4/20/26	24/39/137/137	-
22	CLA	R	304	-	1/1/11/20	7/17/95/115	-
31	BCR	C	517	-	-	6/29/63/63	0/2/2/2
22	CLA	s	310	26	1/1/13/20	16/25/103/115	-
21	CHL	s	306	20	3/3/16/26	10/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHL	R	307	19	4/4/19/26	17/33/131/137	-
22	CLA	S	308	20	-	8/13/91/115	-
22	CLA	r	310	19	1/1/15/20	18/37/115/115	-
31	BCR	B	602	-	-	20/29/63/63	0/2/2/2
22	CLA	C	514	22	1/1/15/20	21/37/115/115	-
26	LHG	d	407	-	-	25/50/50/53	-
21	CHL	g	606	-	3/3/16/26	13/20/118/137	-
31	BCR	B	621	-	-	5/29/63/63	0/2/2/2
21	CHL	Y	605	-	3/3/16/26	13/20/118/137	-
22	CLA	b	607	-	1/1/15/20	13/37/115/115	-
33	SQD	l	101	-	-	13/37/57/69	0/1/1/1
24	XAT	y	615	-	2/2/12/26	18/31/93/93	0/4/4/4
26	LHG	c	521	-	-	21/53/53/53	-
22	CLA	b	601	-	1/1/15/20	18/37/115/115	-
22	CLA	y	604	25	1/1/12/20	6/19/97/115	-
21	CHL	G	609	-	4/4/19/26	10/33/131/137	-
36	LMG	b	620	-	-	22/50/70/70	0/1/1/1
22	CLA	N	613	-	1/1/11/20	9/17/95/115	-
22	CLA	R	309	19	1/1/15/20	18/37/115/115	-
22	CLA	C	503	-	1/1/15/20	18/37/115/115	-
22	CLA	n	604	25	1/1/12/20	6/19/97/115	-
22	CLA	G	603	-	1/1/15/20	17/37/115/115	-
25	NEX	r	315	-	2/2/12/25	14/27/83/83	0/3/3/3
36	LMG	k	103	-	-	26/46/66/70	0/1/1/1
22	CLA	S	313	22	1/1/13/20	12/25/103/115	-
22	CLA	c	510	-	1/1/15/20	11/37/115/115	-
22	CLA	c	509	-	1/1/15/20	13/37/115/115	-
22	CLA	C	507	-	1/1/15/20	14/37/115/115	-
31	BCR	b	616	-	-	7/29/63/63	0/2/2/2
24	XAT	r	314	-	1/1/12/26	14/31/93/93	0/4/4/4
21	CHL	s	301	-	3/3/16/26	10/18/116/137	-
22	CLA	s	312	20	1/1/11/20	7/18/96/115	-
31	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	R	310	19,23	1/1/11/20	11/18/96/115	-
32	PL9	D	407	-	-	17/53/73/73	0/1/1/1
22	CLA	S	304	20	1/1/11/20	7/13/91/115	-
25	NEX	y	616	22	2/2/12/25	15/27/83/83	0/3/3/3
22	CLA	g	611	-	1/1/14/20	8/31/109/115	-
35	DGD	a	413	-	-	21/48/88/95	0/2/2/2
30	PHO	A	408	-	-	13/37/103/103	0/5/6/6
22	CLA	a	406	-	1/1/12/20	8/19/97/115	-
36	LMG	C	502	-	-	16/43/63/70	0/1/1/1
21	CHL	n	606	-	4/4/20/26	18/39/137/137	-
21	CHL	r	307	-	4/4/18/26	16/27/125/137	-
21	CHL	G	608	-	4/4/20/26	23/39/137/137	-
22	CLA	C	512	-	1/1/15/20	14/37/115/115	-
36	LMG	D	411	-	-	12/41/61/70	0/1/1/1
22	CLA	N	609	-	1/1/15/20	16/37/115/115	-
21	CHL	n	601	1	4/4/20/26	24/39/137/137	-
22	CLA	D	405	-	1/1/15/20	12/37/115/115	-
33	SQD	D	402	-	1/1/9/9	18/45/65/69	0/1/1/1
22	CLA	B	617	-	1/1/15/20	20/37/115/115	-
26	LHG	S	314	22	-	29/53/53/53	-
22	CLA	s	313	22	1/1/13/20	12/25/103/115	-
26	LHG	C	521	-	-	21/53/53/53	-
22	CLA	Y	609	-	1/1/14/20	15/31/109/115	-
22	CLA	d	404	-	1/1/15/20	12/37/115/115	-
21	CHL	r	306	-	4/4/20/26	20/39/137/137	-
22	CLA	b	615	-	1/1/15/20	12/37/115/115	-
22	CLA	s	305	20	1/1/12/20	9/19/97/115	-
21	CHL	r	301	19	3/3/16/26	8/18/116/137	-
21	CHL	n	605	-	3/3/16/26	13/20/118/137	-
22	CLA	G	611	-	1/1/14/20	8/31/109/115	-
32	PL9	A	411	-	-	3/5/18/73	0/1/1/1
36	LMG	T	101	-	-	23/46/66/70	0/1/1/1
22	CLA	B	607	-	1/1/15/20	15/37/115/115	-
25	NEX	Y	616	22	2/2/12/25	14/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	N	603	-	1/1/15/20	17/37/115/115	-
21	CHL	Y	607	-	4/4/20/26	23/39/137/137	-
22	CLA	C	513	4	1/1/15/20	14/37/115/115	-
21	CHL	G	605	-	3/3/16/26	9/15/113/137	-
21	CHL	y	609	-	4/4/20/26	14/39/137/137	-
23	LUT	G	615	-	-	17/29/67/67	0/2/2/2
24	XAT	g	617	-	2/2/12/26	17/31/93/93	0/4/4/4
26	LHG	d	409	-	-	19/47/47/53	-
22	CLA	s	309	20,22	1/1/13/20	7/25/103/115	-
23	LUT	Y	613	-	-	17/29/67/67	0/2/2/2
22	CLA	N	610	-	1/1/14/20	8/31/109/115	-
21	CHL	s	307	20	3/3/16/26	12/15/113/137	-
23	LUT	R	312	22	-	18/29/67/67	0/2/2/2
22	CLA	y	612	1	1/1/15/20	20/37/115/115	-
22	CLA	B	604	-	1/1/15/20	18/37/115/115	-
24	XAT	G	617	-	3/3/12/26	17/31/93/93	0/4/4/4
35	DGD	C	519	-	-	26/51/91/95	0/2/2/2
22	CLA	r	311	19,23	1/1/11/20	11/18/96/115	-
22	CLA	g	614	-	1/1/11/20	9/17/95/115	-
22	CLA	D	404	-	1/1/15/20	13/37/115/115	-
22	CLA	n	602	-	1/1/15/20	13/37/115/115	-
33	SQD	A	412	-	-	23/49/69/69	0/1/1/1
22	CLA	r	304	-	1/1/14/20	9/31/109/115	-
36	LMG	B	601	-	-	18/35/55/70	0/1/1/1
22	CLA	c	504	-	1/1/15/20	14/37/115/115	-
21	CHL	y	606	-	3/3/16/26	13/20/118/137	-
23	LUT	g	616	-	-	15/29/67/67	0/2/2/2
22	CLA	a	405	-	1/1/15/20	15/37/115/115	-
22	CLA	C	511	-	1/1/15/20	11/37/115/115	-
23	LUT	g	615	-	-	17/29/67/67	0/2/2/2
21	CHL	N	608	-	4/4/20/26	15/39/137/137	-
31	BCR	c	515	-	-	5/29/63/63	0/2/2/2
21	CHL	N	607	-	4/4/20/26	23/39/137/137	-
35	DGD	J	101	-	-	16/49/89/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	n	609	-	1/1/15/20	18/37/115/115	-

The worst 5 of 2557 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	f	101	HEM	FE-NB	25.25	3.21	1.96
37	F	101	HEM	FE-NB	25.23	3.21	1.96
23	N	615	LUT	C24-C25	17.30	1.54	1.33
23	N	614	LUT	C24-C25	17.28	1.54	1.33
23	n	614	LUT	C24-C25	17.28	1.54	1.33

The worst 5 of 3429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	617	XAT	O24-C25-C24	-78.18	54.66	113.38
24	N	616	XAT	O24-C25-C24	-78.01	54.78	113.38
24	R	313	XAT	O24-C25-C24	-77.64	55.06	113.38
24	r	314	XAT	O24-C25-C24	-77.61	55.08	113.38
24	g	617	XAT	O24-C25-C24	-77.46	55.19	113.38

5 of 353 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	g	601	CHL	C8
21	g	601	CHL	ND
21	g	601	CHL	NC
21	g	601	CHL	NA
21	g	605	CHL	ND

5 of 4559 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	g	601	CHL	C1A-C2A-CAA-CBA
21	g	601	CHL	C1C-C2C-CMC-OMC
21	g	601	CHL	C3C-C2C-CMC-OMC
21	g	605	CHL	C1C-C2C-CMC-OMC
21	g	605	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

311 monomers are involved in 2203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	404	CLA	4	0
36	B	623	LMG	53	0
22	y	613	CLA	3	0
22	S	303	CLA	3	0
33	L	101	SQD	4	0
24	Y	615	XAT	2	0
22	B	616	CLA	3	0
22	Y	604	CLA	14	0
22	y	603	CLA	3	0
26	c	520	LHG	4	0
31	b	617	BCR	1	0
26	s	314	LHG	7	0
26	N	618	LHG	9	0
21	s	302	CHL	19	0
32	a	410	PL9	2	0
36	I	101	LMG	6	0
26	d	408	LHG	7	0
22	N	612	CLA	17	0
22	n	610	CLA	2	0
22	y	610	CLA	6	0
21	g	601	CHL	23	0
33	L	102	SQD	5	0
36	w	102	LMG	3	0
22	s	308	CLA	2	0
22	B	606	CLA	6	0
31	K	101	BCR	2	0
23	N	614	LUT	16	0
21	Y	606	CHL	24	0
22	n	603	CLA	3	0
22	c	503	CLA	3	0
22	c	507	CLA	1	0
22	B	610	CLA	2	0
22	B	618	CLA	3	0
26	y	617	LHG	9	0
21	g	605	CHL	20	0
22	y	602	CLA	3	0
22	b	614	CLA	3	0
22	c	506	CLA	5	0
22	N	611	CLA	8	0
22	b	612	CLA	3	0
22	b	605	CLA	2	0
22	Y	612	CLA	3	0
22	B	603	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	606	CHL	23	0
35	c	519	DGD	4	0
35	h	102	DGD	4	0
35	H	102	DGD	8	0
25	y	618	NEX	9	0
22	A	405	CLA	3	0
31	B	620	BCR	2	0
22	r	303	CLA	2	0
22	C	504	CLA	3	0
22	A	406	CLA	3	0
31	T	102	BCR	2	0
31	K	102	BCR	4	0
21	y	608	CHL	37	0
22	B	608	CLA	2	0
22	r	309	CLA	6	0
22	Y	610	CLA	4	0
22	R	308	CLA	8	0
21	g	607	CHL	22	0
22	G	614	CLA	3	0
22	C	515	CLA	8	0
21	N	605	CHL	24	0
26	C	522	LHG	3	0
23	n	614	LUT	12	0
22	d	403	CLA	4	0
24	n	615	XAT	2	0
26	R	301	LHG	5	0
23	y	614	LUT	11	0
26	G	618	LHG	13	0
21	S	307	CHL	25	0
26	b	619	LHG	1	0
22	C	506	CLA	6	0
21	S	306	CHL	16	0
22	S	311	CLA	3	0
22	b	609	CLA	3	0
22	N	604	CLA	13	0
22	r	312	CLA	4	0
22	R	303	CLA	5	0
22	c	508	CLA	4	0
22	s	303	CLA	4	0
22	b	604	CLA	2	0
36	d	410	LMG	4	0
22	b	608	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	617	LHG	10	0
21	G	601	CHL	42	0
35	c	518	DGD	10	0
22	n	613	CLA	1	0
22	B	615	CLA	3	0
22	A	407	CLA	2	0
22	S	310	CLA	8	0
26	L	103	LHG	2	0
22	g	612	CLA	7	0
34	D	403	BCT	4	0
36	c	523	LMG	3	0
22	G	612	CLA	6	0
22	B	613	CLA	1	0
22	w	101	CLA	5	0
22	c	511	CLA	5	0
21	S	301	CHL	48	0
35	A	401	DGD	7	0
26	r	302	LHG	3	0
22	Y	611	CLA	21	0
25	N	617	NEX	9	0
21	n	608	CHL	28	0
24	R	313	XAT	5	0
22	c	513	CLA	4	0
22	g	610	CLA	6	0
22	c	512	CLA	5	0
22	W	101	CLA	16	0
36	M	101	LMG	5	0
25	n	616	NEX	12	0
30	a	407	PHO	5	0
26	g	619	LHG	6	0
30	d	401	PHO	6	0
22	x	101	CLA	2	0
31	h	101	BCR	5	0
22	b	610	CLA	1	0
26	n	617	LHG	10	0
22	B	605	CLA	7	0
31	C	516	BCR	6	0
22	g	602	CLA	3	0
22	b	613	CLA	3	0
31	a	409	BCR	1	0
35	C	518	DGD	1	0
22	S	309	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	607	CHL	22	0
37	f	101	HEM	20	0
31	B	619	BCR	4	0
37	F	101	HEM	17	0
22	S	305	CLA	9	0
23	N	615	LUT	17	0
21	N	601	CHL	32	0
22	g	603	CLA	7	0
22	R	302	CLA	2	0
36	K	103	LMG	1	0
21	y	607	CHL	19	0
26	C	520	LHG	7	0
22	Y	602	CLA	5	0
22	C	508	CLA	1	0
24	N	616	XAT	2	0
22	G	604	CLA	12	0
31	A	410	BCR	2	0
26	c	522	LHG	3	0
31	k	102	BCR	4	0
36	C	523	LMG	3	0
33	d	402	SQD	3	0
31	H	101	BCR	3	0
22	b	602	CLA	5	0
22	c	505	CLA	6	0
22	s	304	CLA	1	0
22	n	611	CLA	7	0
26	D	410	LHG	4	0
21	y	605	CHL	26	0
31	k	101	BCR	2	0
21	S	302	CHL	17	0
35	c	517	DGD	1	0
22	R	311	CLA	5	0
22	a	408	CLA	3	0
22	b	606	CLA	3	0
22	r	305	CLA	2	0
22	B	612	CLA	3	0
26	D	408	LHG	1	0
22	N	602	CLA	4	0
22	G	613	CLA	18	0
22	B	611	CLA	1	0
21	y	601	CHL	26	0
32	d	406	PL9	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	R	305	CHL	33	0
22	B	614	CLA	4	0
22	n	612	CLA	18	0
22	b	603	CLA	6	0
30	D	401	PHO	6	0
23	r	313	LUT	2	0
26	B	622	LHG	1	0
23	Y	614	LUT	14	0
23	G	616	LUT	11	0
22	g	613	CLA	18	0
22	Y	603	CLA	14	0
22	y	611	CLA	2	0
22	c	514	CLA	7	0
22	c	502	CLA	7	0
21	G	606	CHL	23	0
21	R	306	CHL	39	0
25	g	618	NEX	8	0
22	g	604	CLA	13	0
22	A	409	CLA	2	0
22	B	609	CLA	2	0
33	l	103	SQD	4	0
21	Y	608	CHL	32	0
22	b	611	CLA	3	0
22	C	510	CLA	4	0
22	G	610	CLA	7	0
22	C	505	CLA	5	0
21	g	609	CHL	25	0
26	D	409	LHG	4	0
22	G	602	CLA	4	0
21	r	308	CHL	4	0
31	d	405	BCR	4	0
21	n	607	CHL	38	0
31	D	406	BCR	4	0
21	g	608	CHL	35	0
22	s	311	CLA	2	0
33	a	411	SQD	4	0
21	Y	601	CHL	23	0
22	R	304	CLA	3	0
31	C	517	BCR	2	0
22	s	310	CLA	6	0
21	s	306	CHL	15	0
21	R	307	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	S	308	CLA	2	0
22	r	310	CLA	3	0
31	B	602	BCR	2	0
22	C	514	CLA	5	0
21	g	606	CHL	28	0
31	B	621	BCR	1	0
21	Y	605	CHL	29	0
22	b	607	CLA	2	0
33	l	101	SQD	3	0
24	y	615	XAT	2	0
26	c	521	LHG	2	0
22	b	601	CLA	6	0
22	y	604	CLA	13	0
21	G	609	CHL	34	0
36	b	620	LMG	36	0
22	N	613	CLA	3	0
22	R	309	CLA	5	0
22	C	503	CLA	4	0
22	n	604	CLA	16	0
22	G	603	CLA	6	0
25	r	315	NEX	8	0
36	k	103	LMG	1	0
22	S	313	CLA	5	0
22	c	510	CLA	21	0
22	c	509	CLA	3	0
22	C	507	CLA	4	0
31	b	616	BCR	4	0
24	r	314	XAT	5	0
21	s	301	CHL	51	0
31	b	618	BCR	3	0
22	C	509	CLA	2	0
22	R	310	CLA	3	0
32	D	407	PL9	3	0
22	S	304	CLA	1	0
25	y	616	NEX	7	0
22	g	611	CLA	2	0
35	a	413	DGD	7	0
30	A	408	PHO	4	0
22	a	406	CLA	2	0
36	C	502	LMG	2	0
21	n	606	CHL	17	0
21	r	307	CHL	28	0

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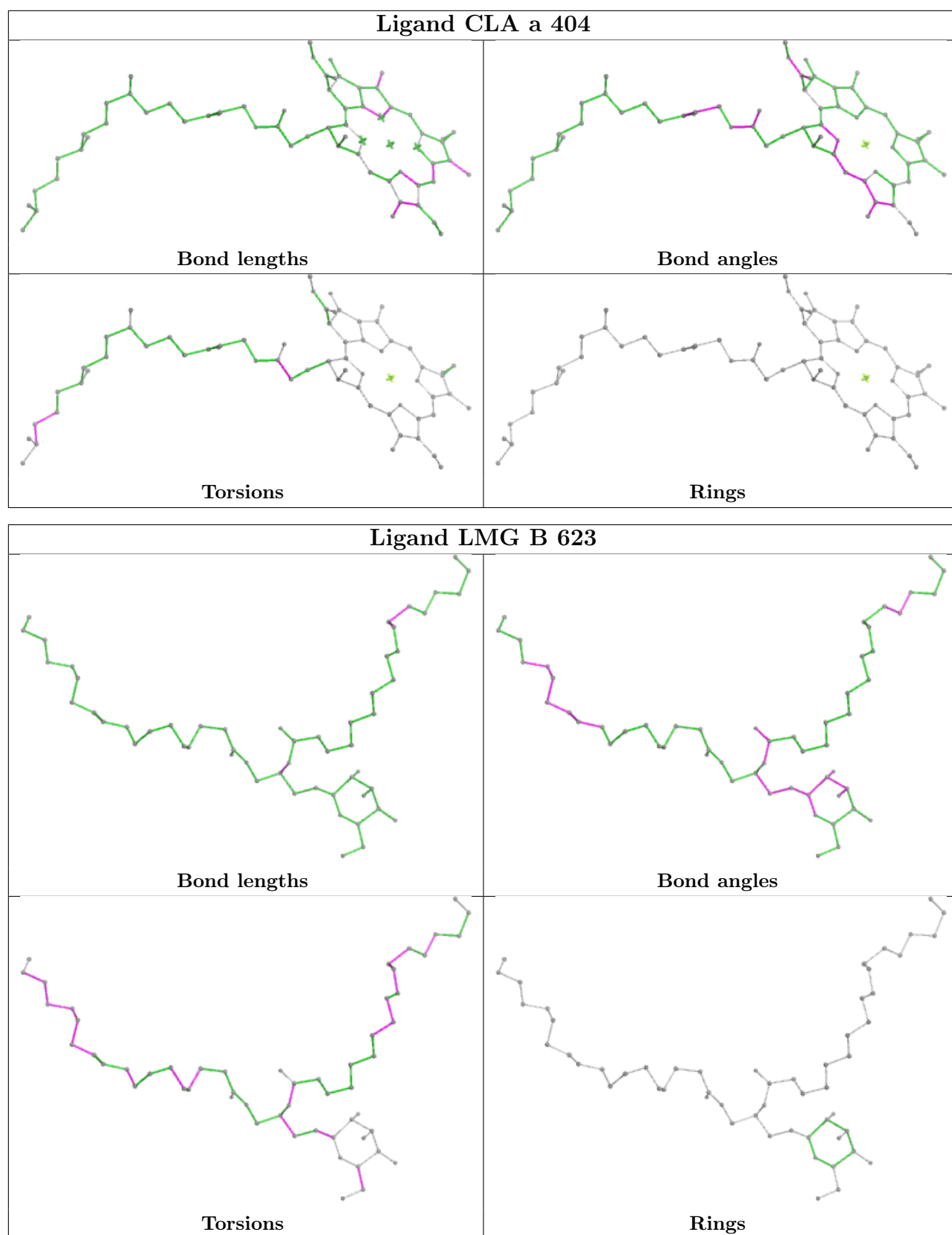
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	608	CHL	35	0
22	C	512	CLA	5	0
36	D	411	LMG	2	0
22	N	609	CLA	7	0
21	n	601	CHL	28	0
22	D	405	CLA	3	0
33	D	402	SQD	3	0
22	B	617	CLA	3	0
26	S	314	LHG	6	0
22	s	313	CLA	5	0
26	C	521	LHG	5	0
22	Y	609	CLA	6	0
22	d	404	CLA	3	0
21	r	306	CHL	25	0
22	b	615	CLA	1	0
22	s	305	CLA	8	0
21	r	301	CHL	26	0
21	n	605	CHL	31	0
22	G	611	CLA	2	0
32	A	411	PL9	2	0
36	T	101	LMG	5	0
22	B	607	CLA	4	0
25	Y	616	NEX	9	0
22	N	603	CLA	9	0
21	Y	607	CHL	37	0
22	C	513	CLA	4	0
21	G	605	CHL	20	0
21	y	609	CHL	26	0
23	G	615	LUT	14	0
26	d	409	LHG	5	0
22	s	309	CLA	2	0
23	Y	613	LUT	16	0
22	N	610	CLA	2	0
21	s	307	CHL	24	0
23	R	312	LUT	2	0
22	y	612	CLA	21	0
22	B	604	CLA	3	0
24	G	617	XAT	1	0
35	C	519	DGD	9	0
22	r	311	CLA	3	0
22	g	614	CLA	1	0
22	D	404	CLA	2	0

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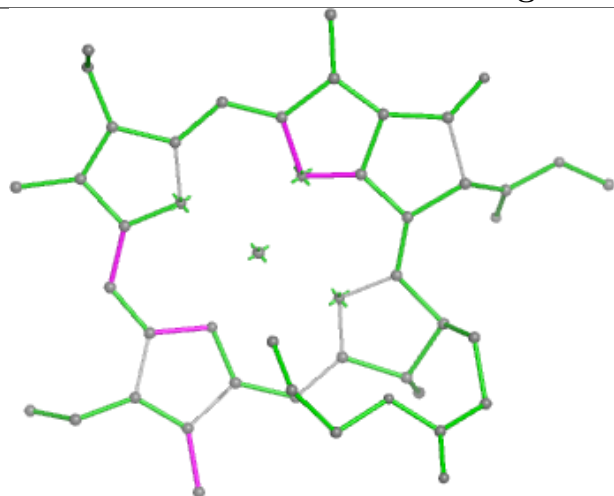
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	n	602	CLA	4	0
33	A	412	SQD	4	0
22	r	304	CLA	5	0
36	B	601	LMG	5	0
22	c	504	CLA	5	0
21	y	606	CHL	28	0
23	g	616	LUT	13	0
22	a	405	CLA	3	0
22	C	511	CLA	21	0
23	g	615	LUT	16	0
21	N	608	CHL	27	0
31	c	515	BCR	7	0
21	N	607	CHL	41	0
35	J	101	DGD	6	0
34	a	412	BCT	4	0
22	n	609	CLA	6	0

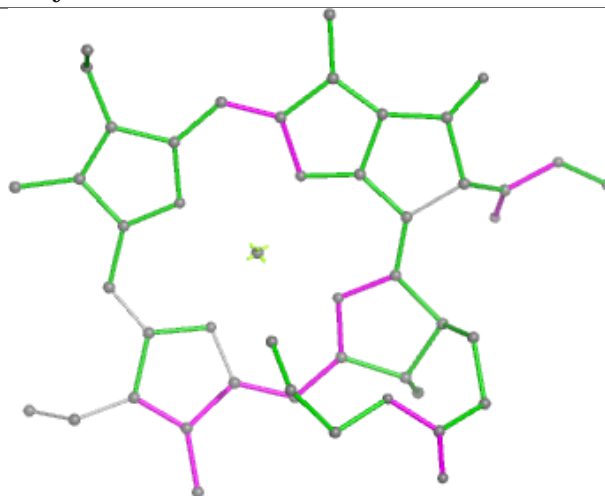
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



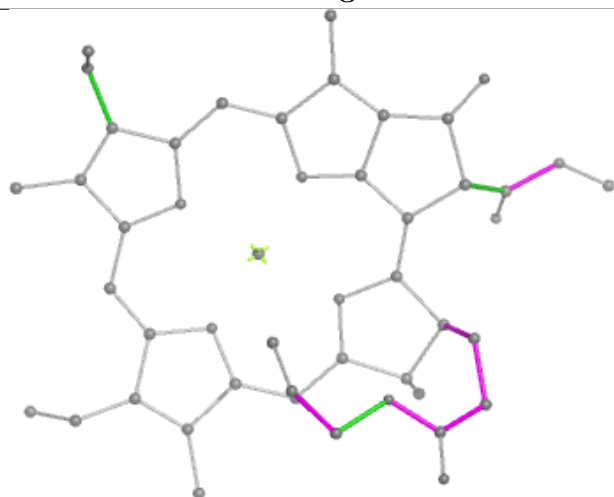
## Ligand CLA y 613



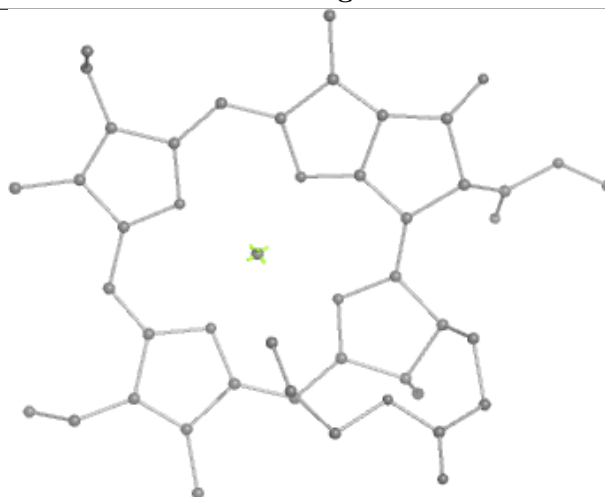
Bond lengths



Bond angles

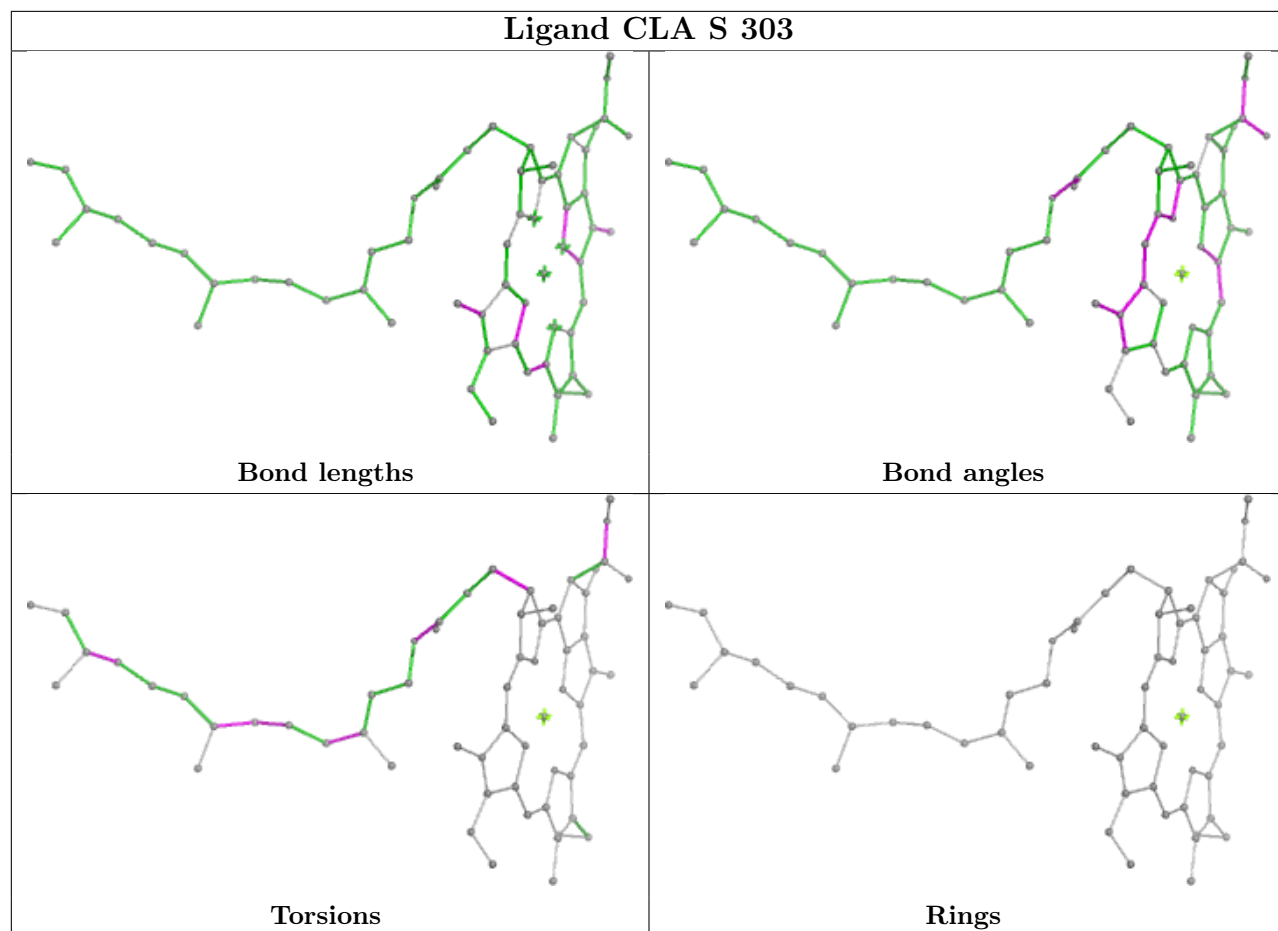


Torsions

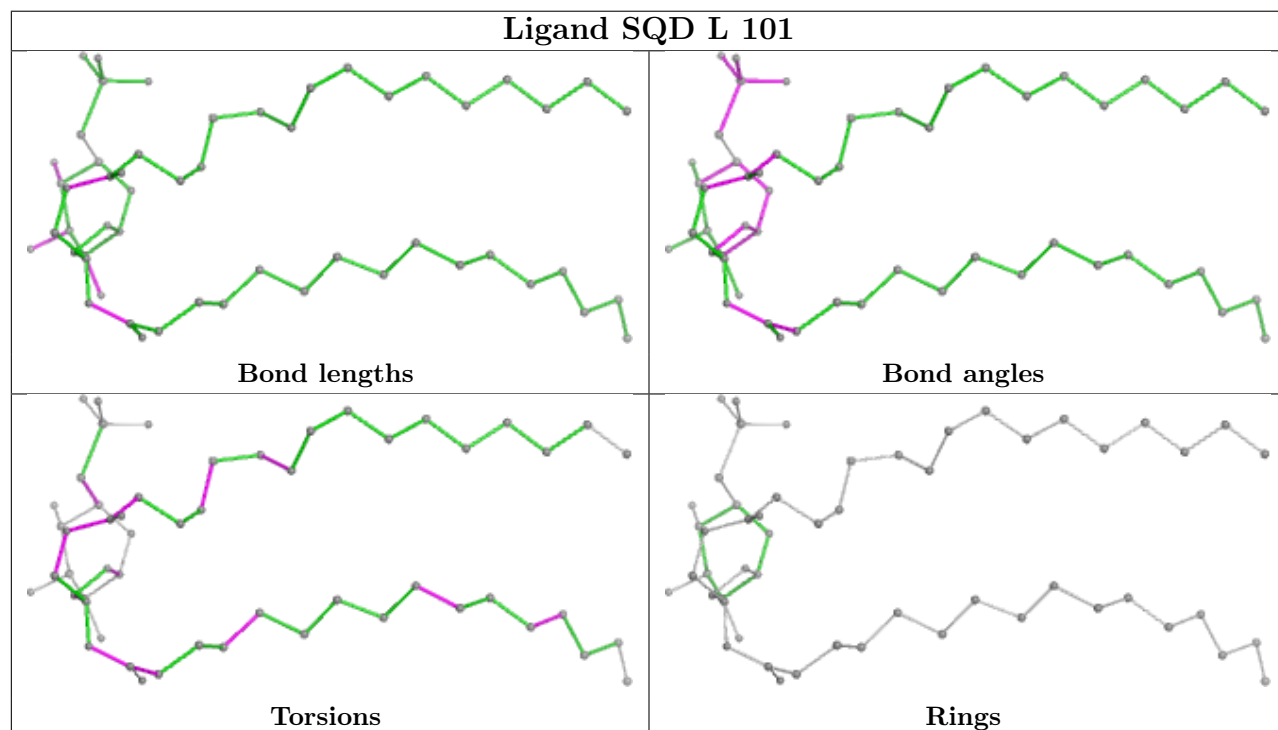


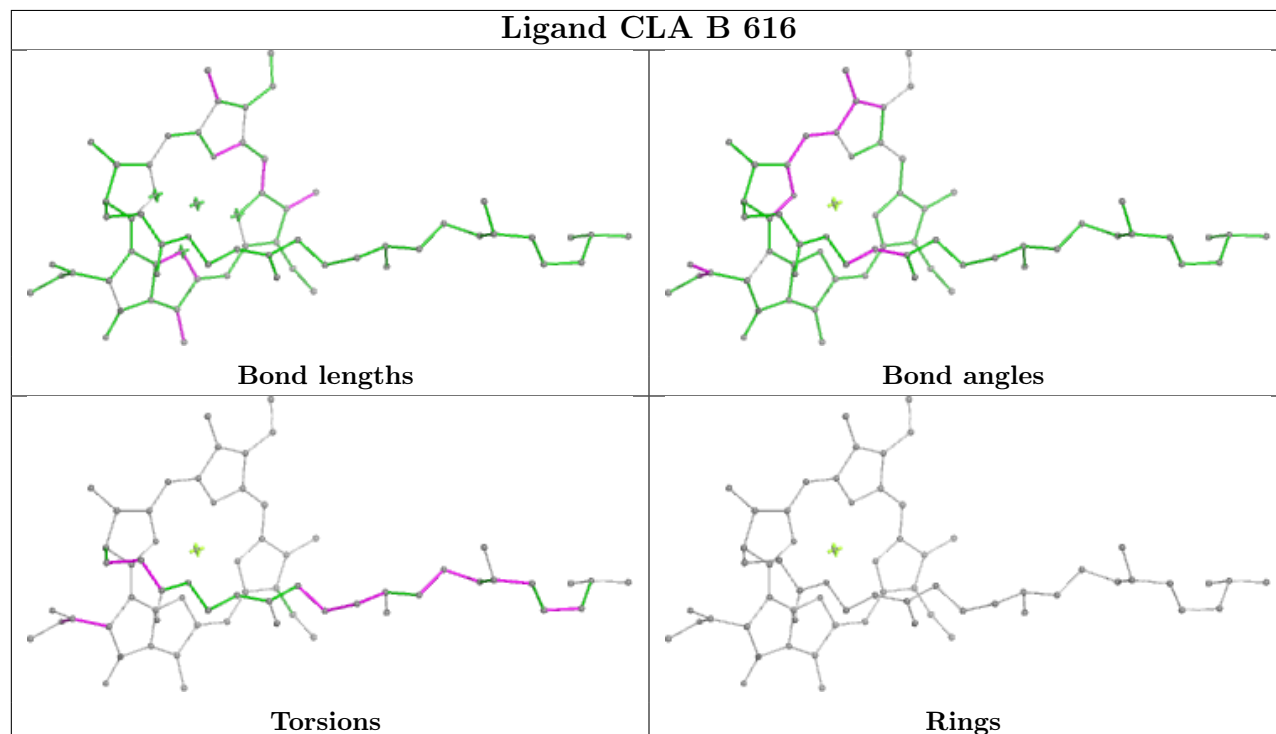
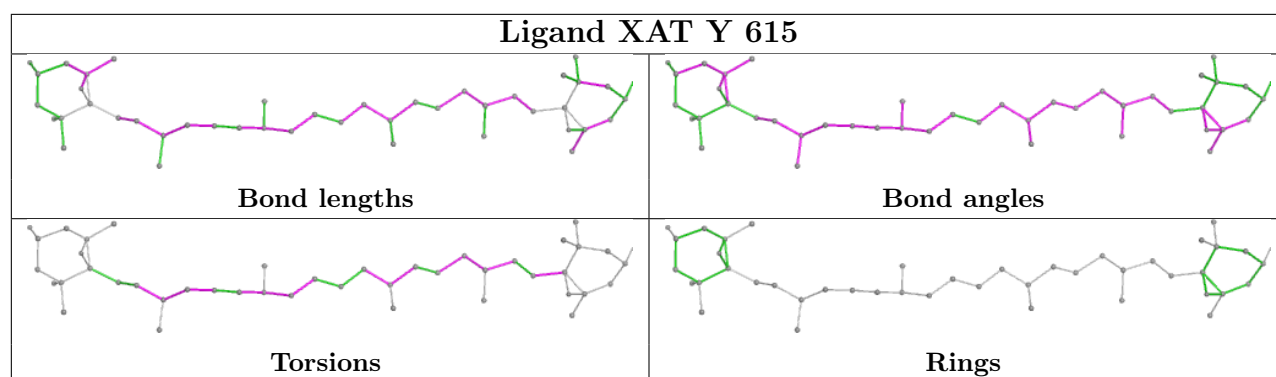
Rings

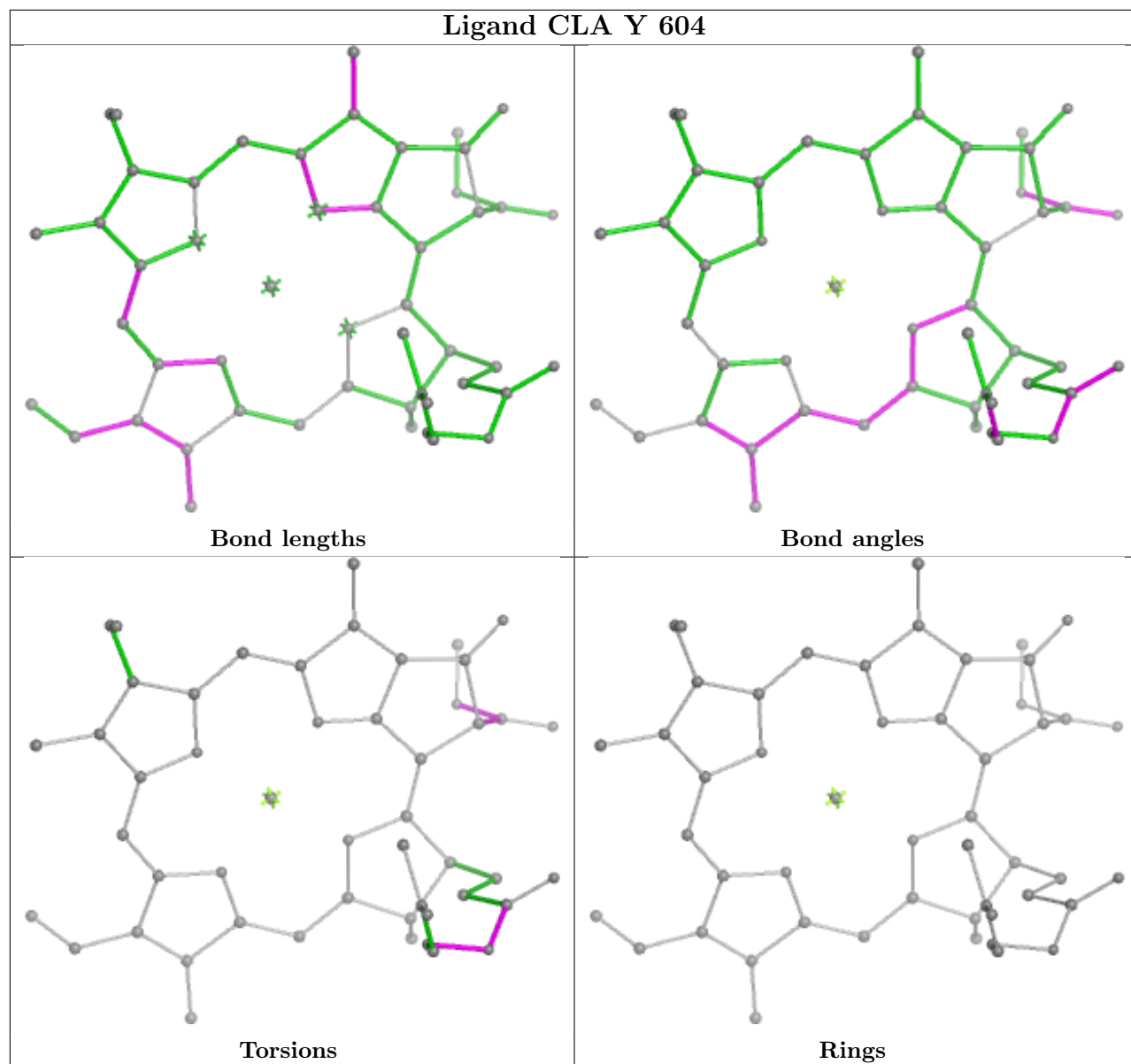
## Ligand CLA S 303

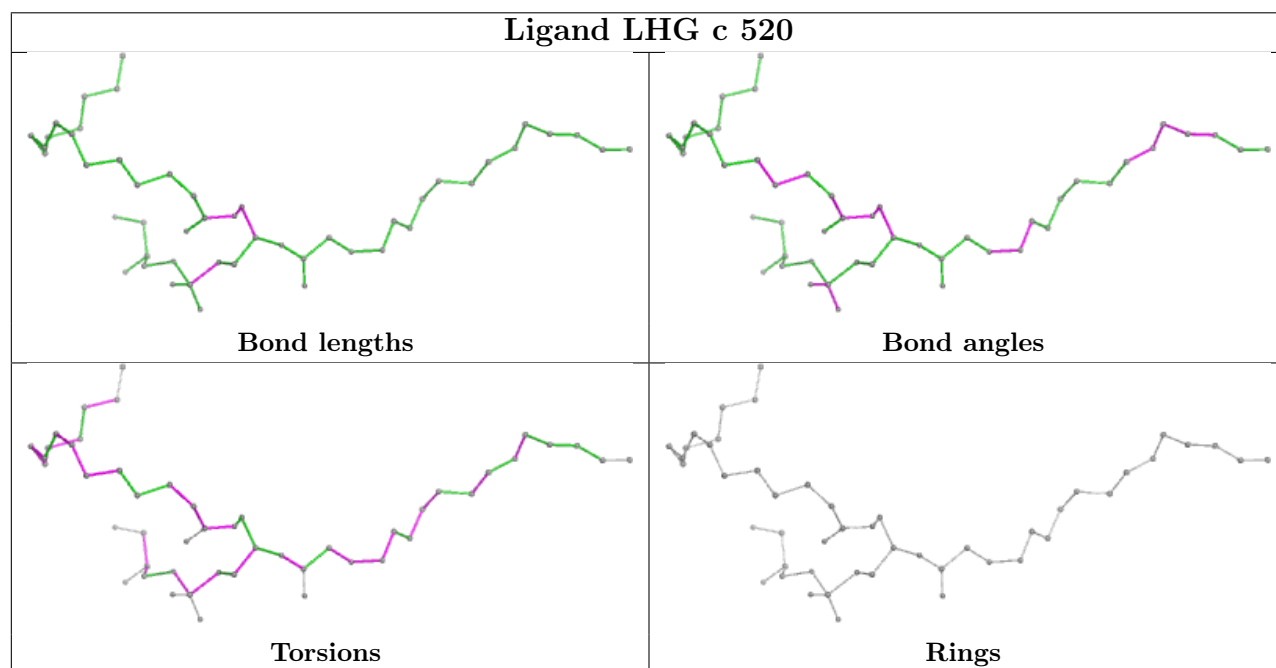
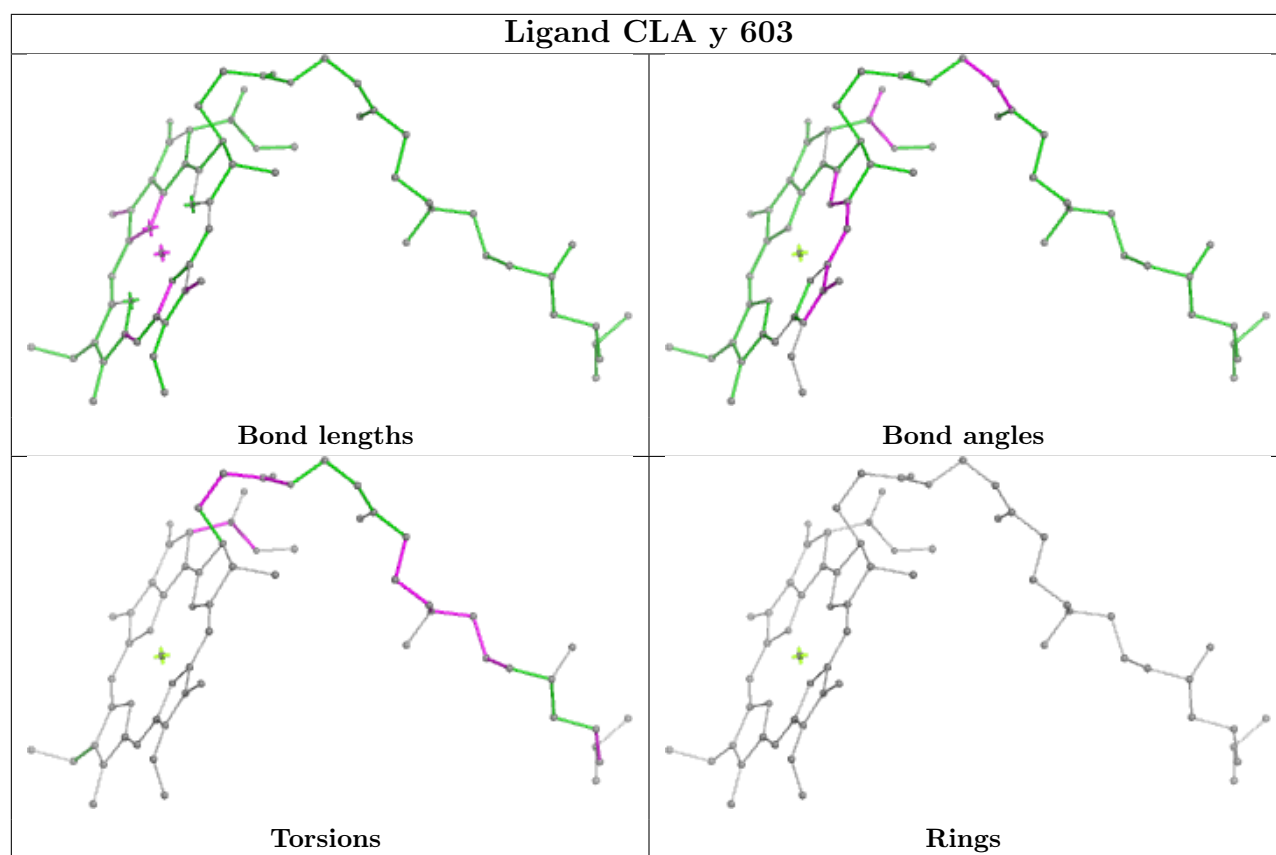


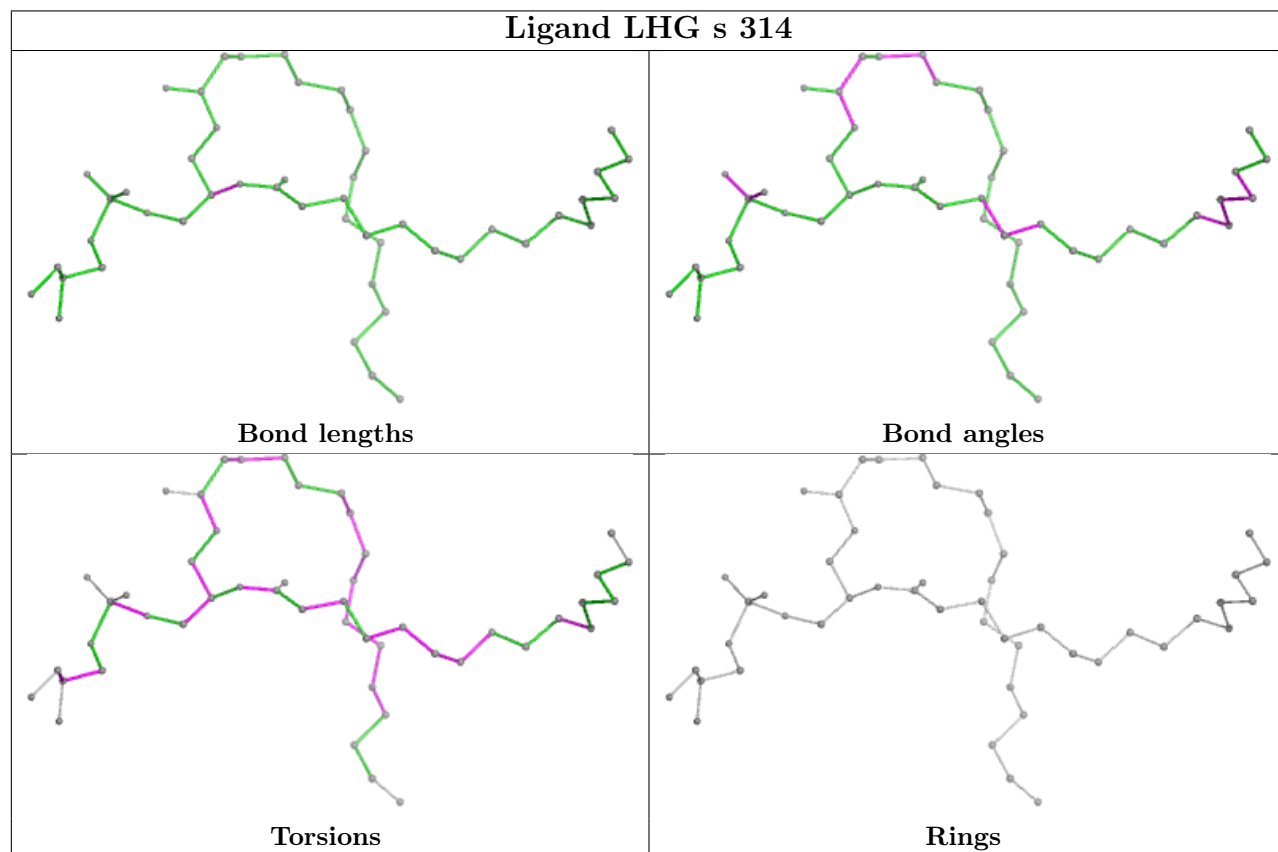
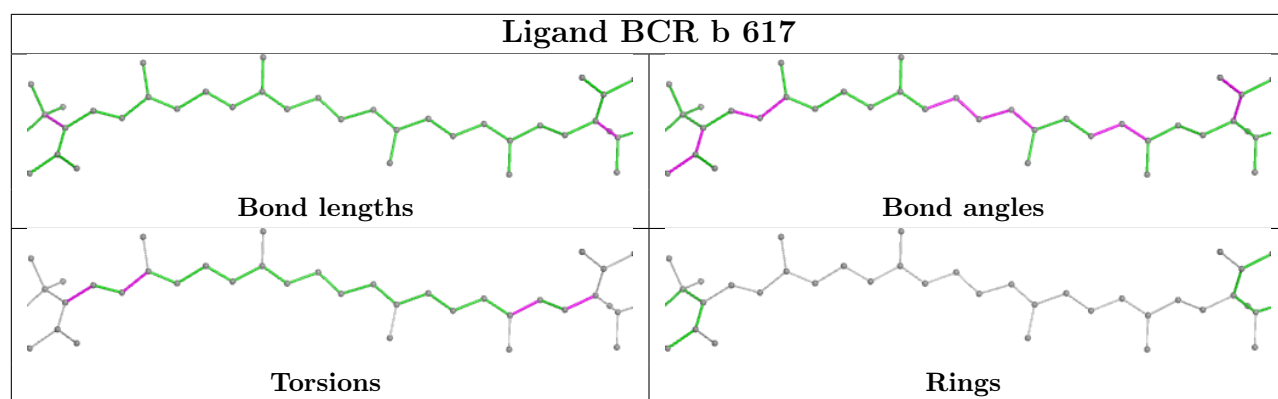
## Ligand SQD L 101

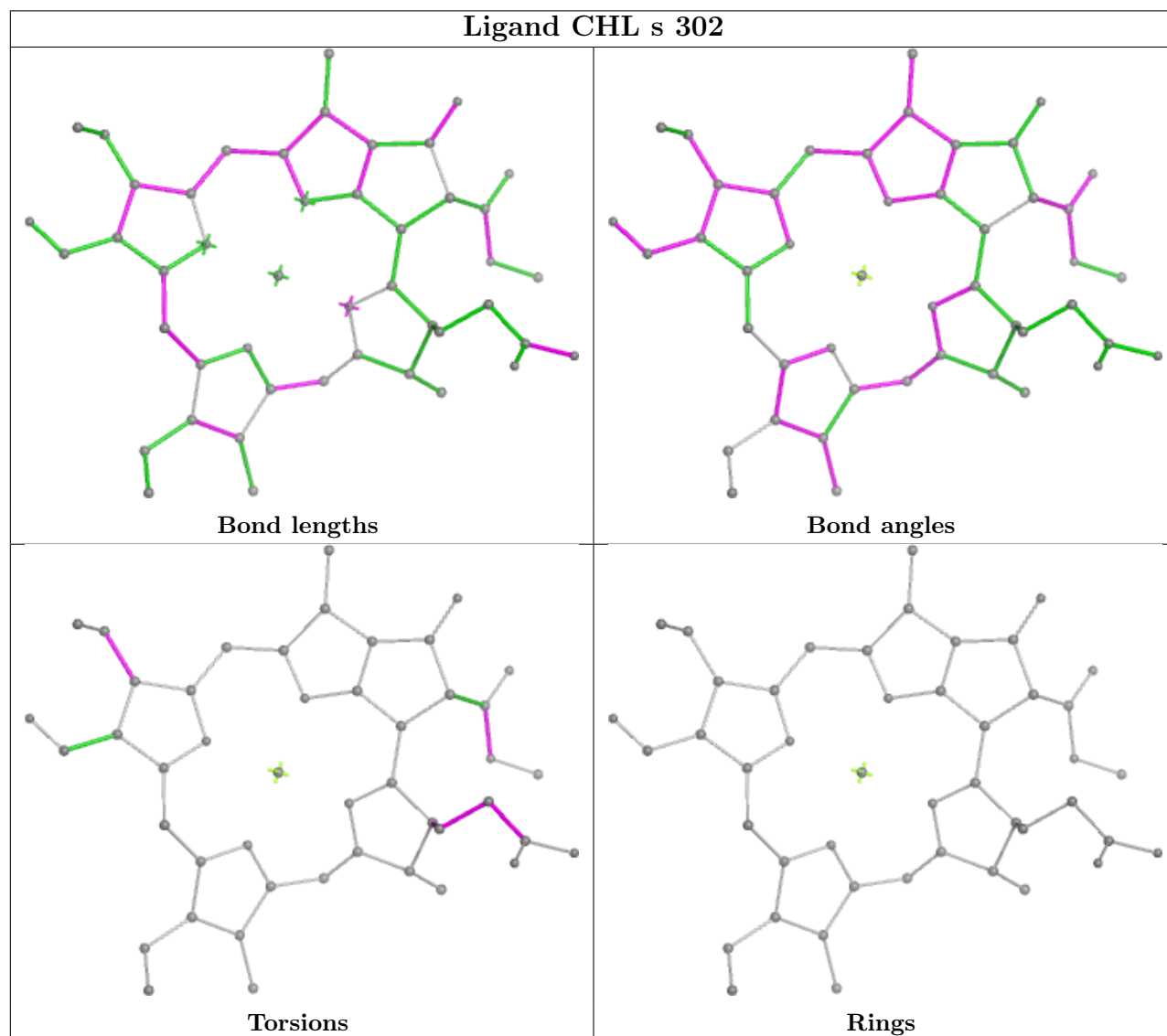
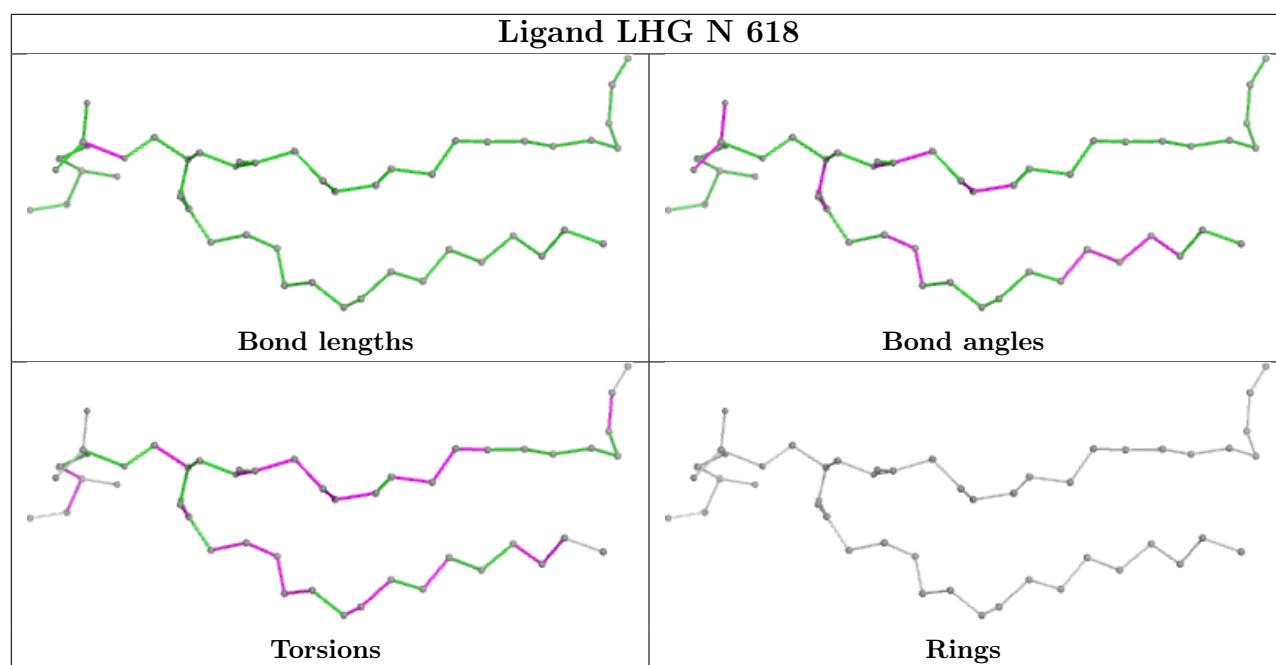


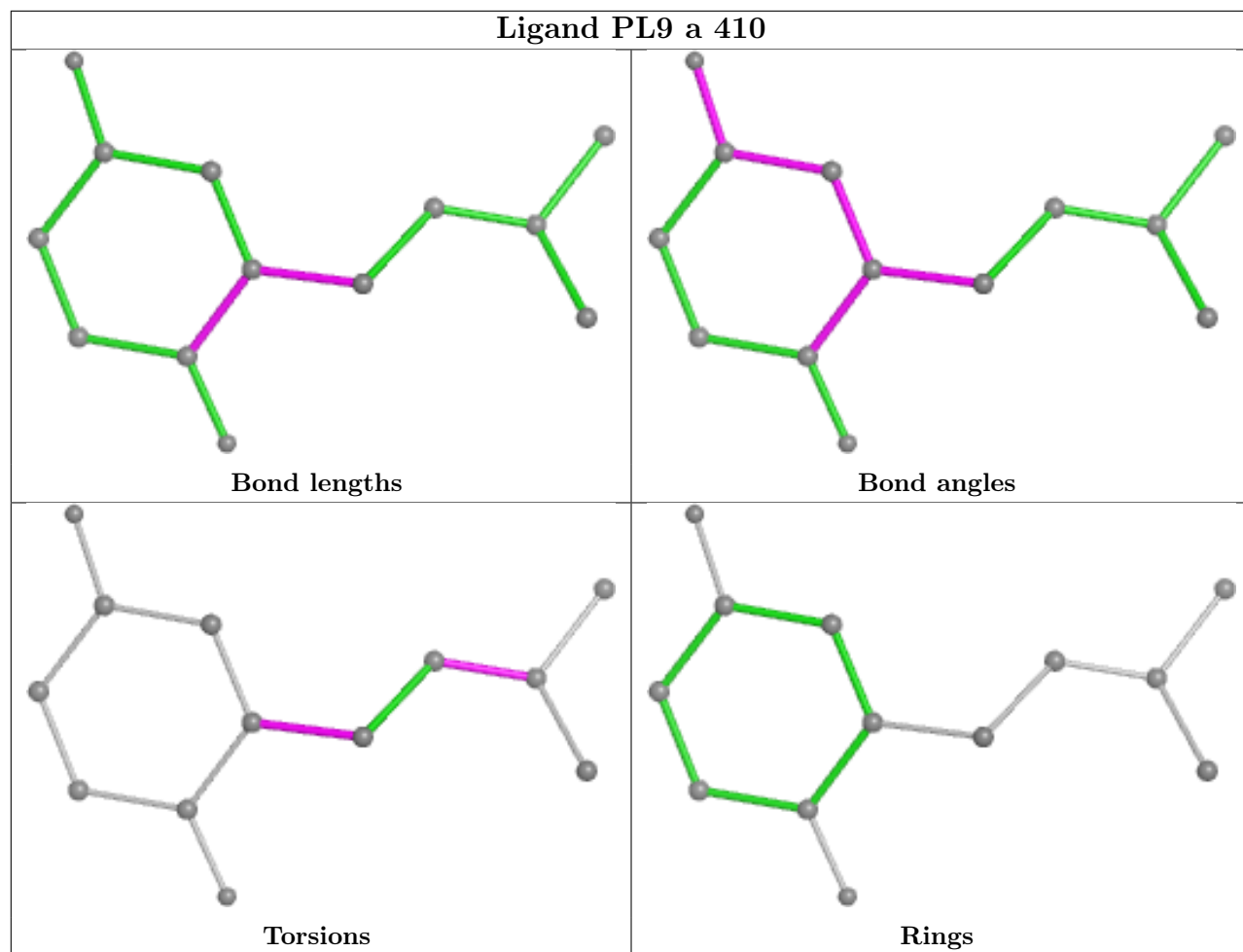


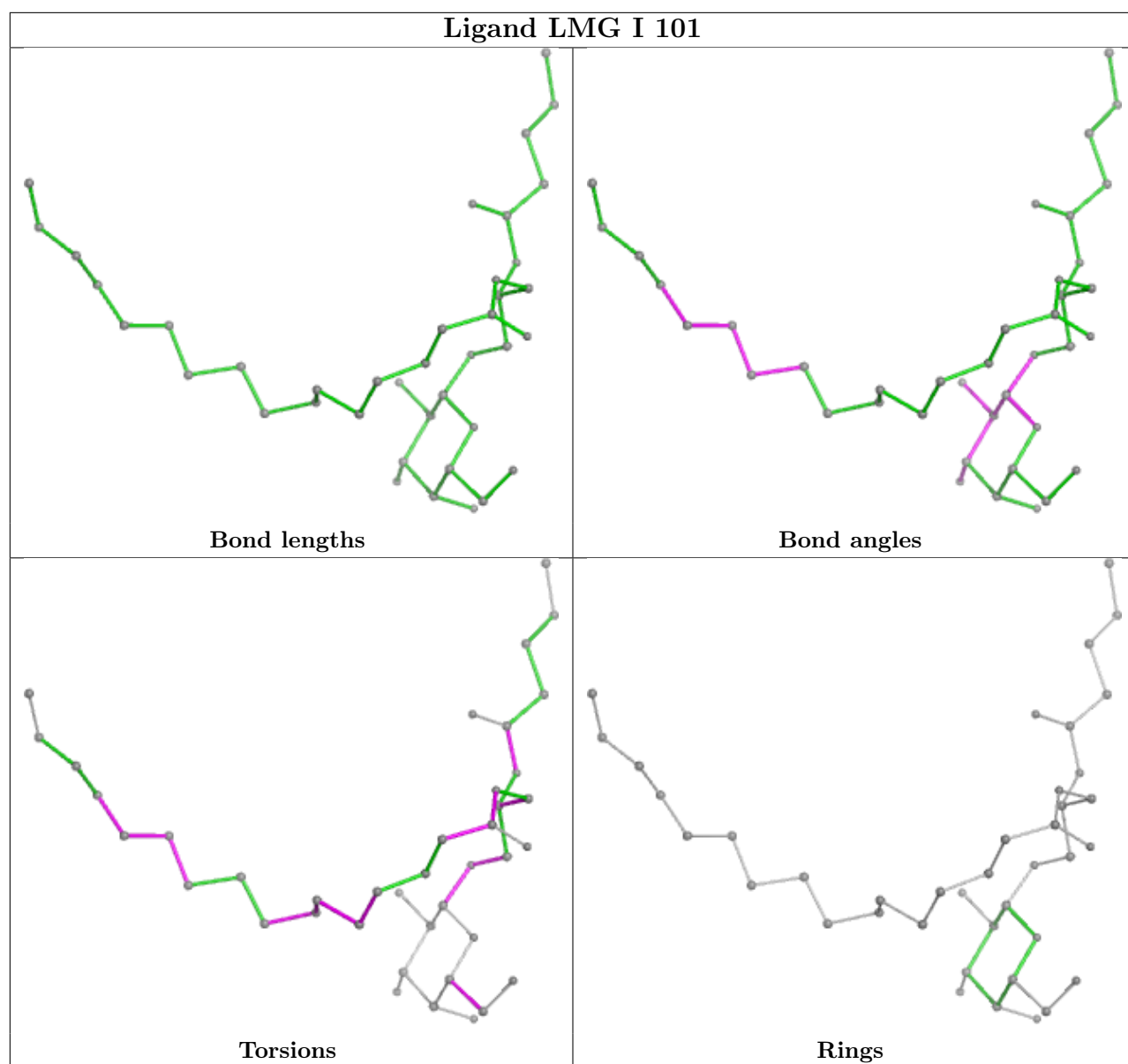


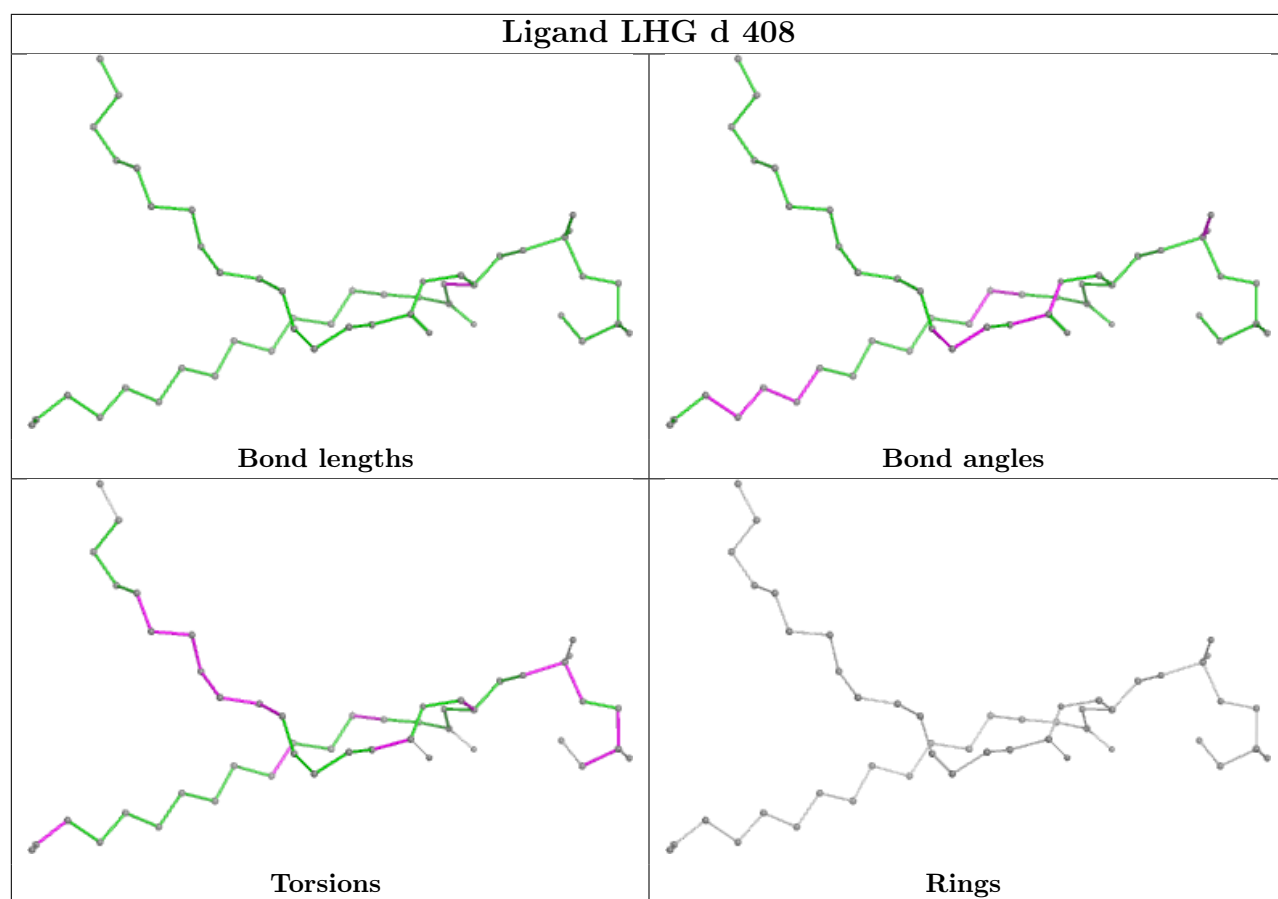


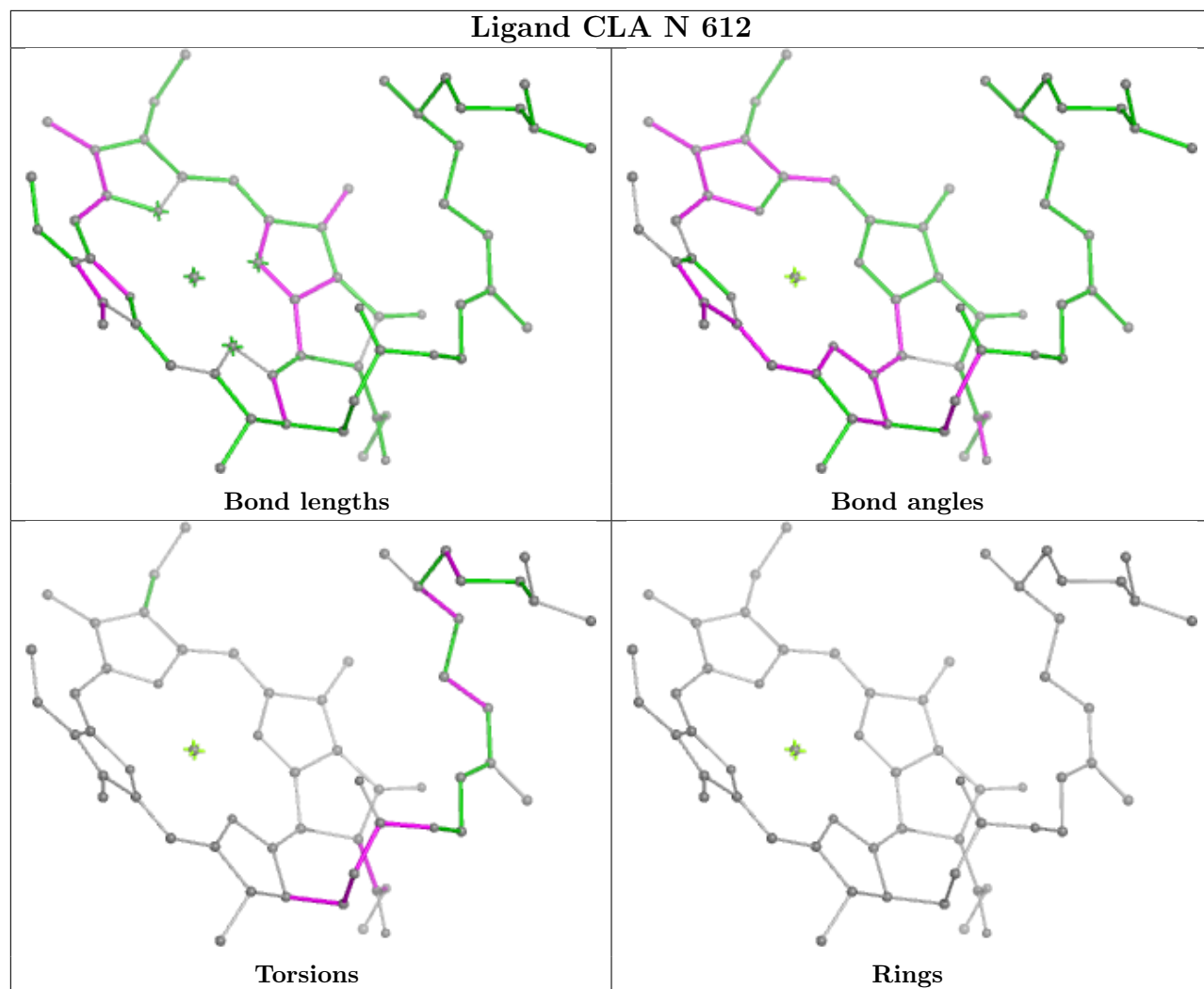


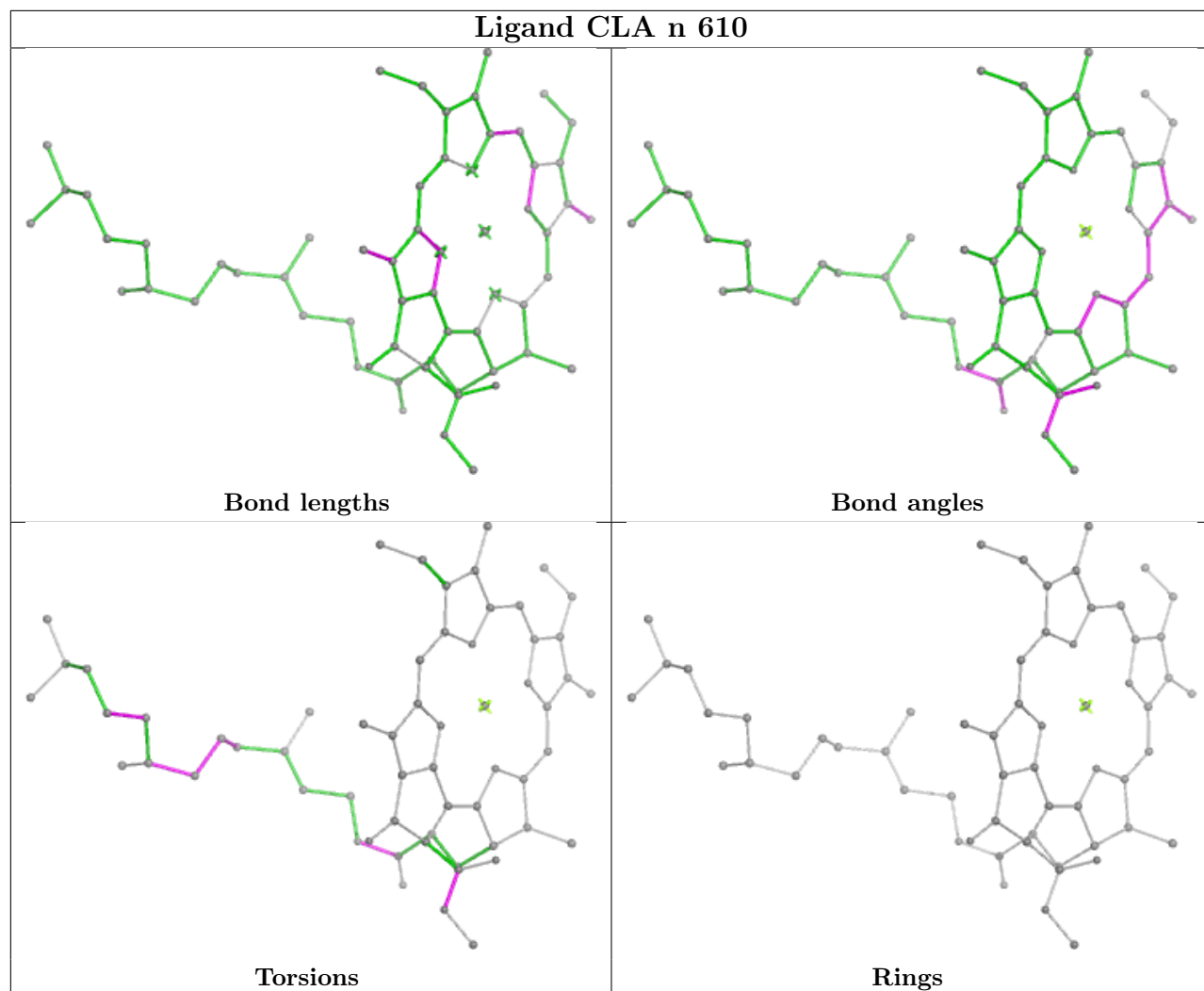




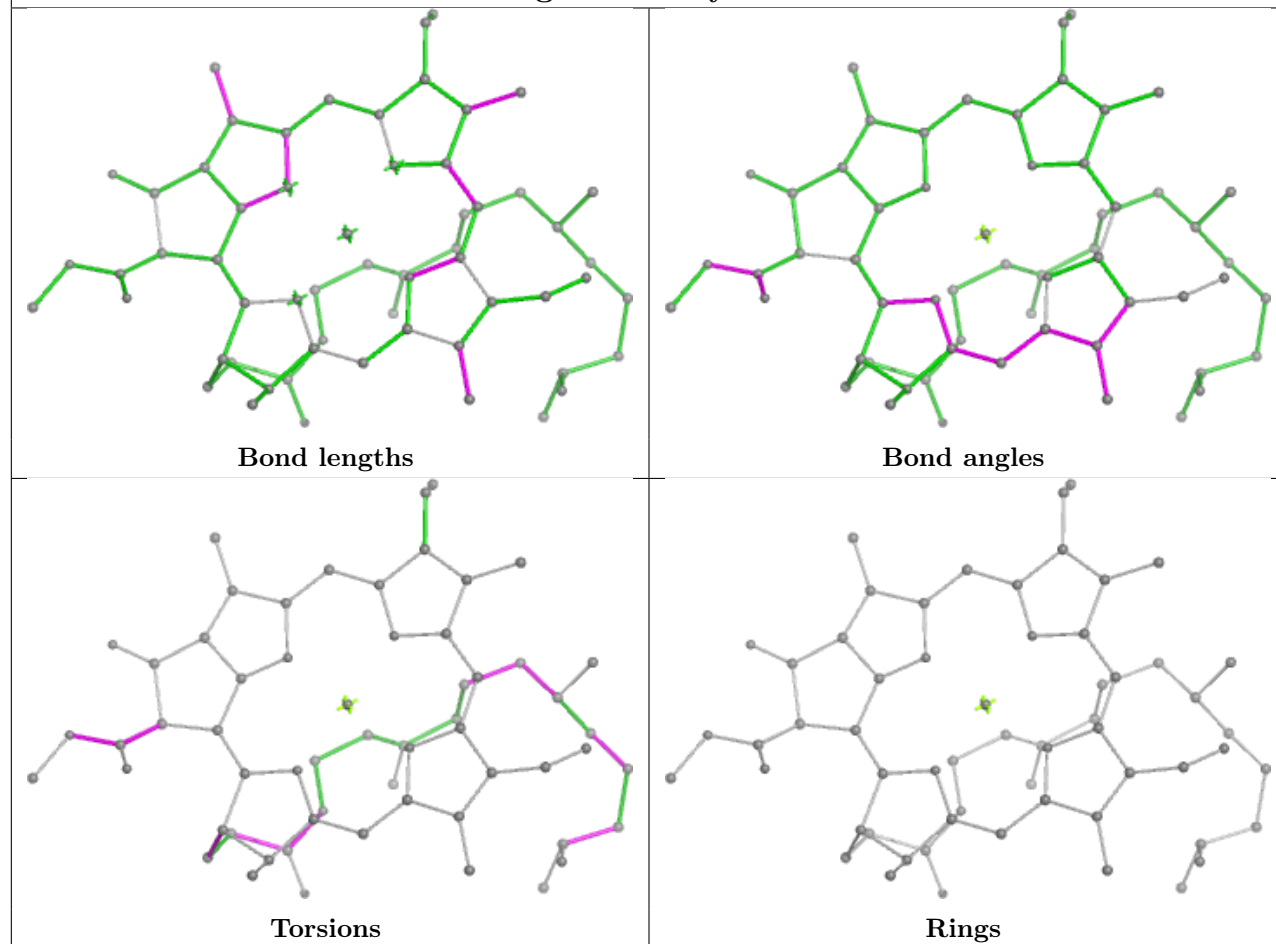




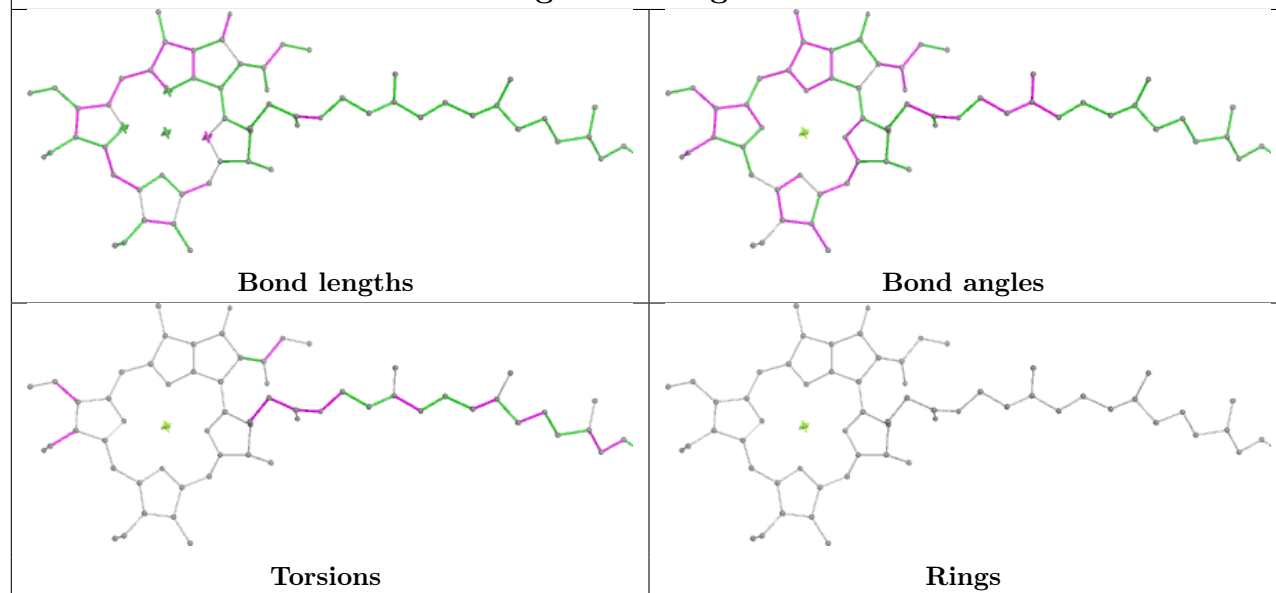


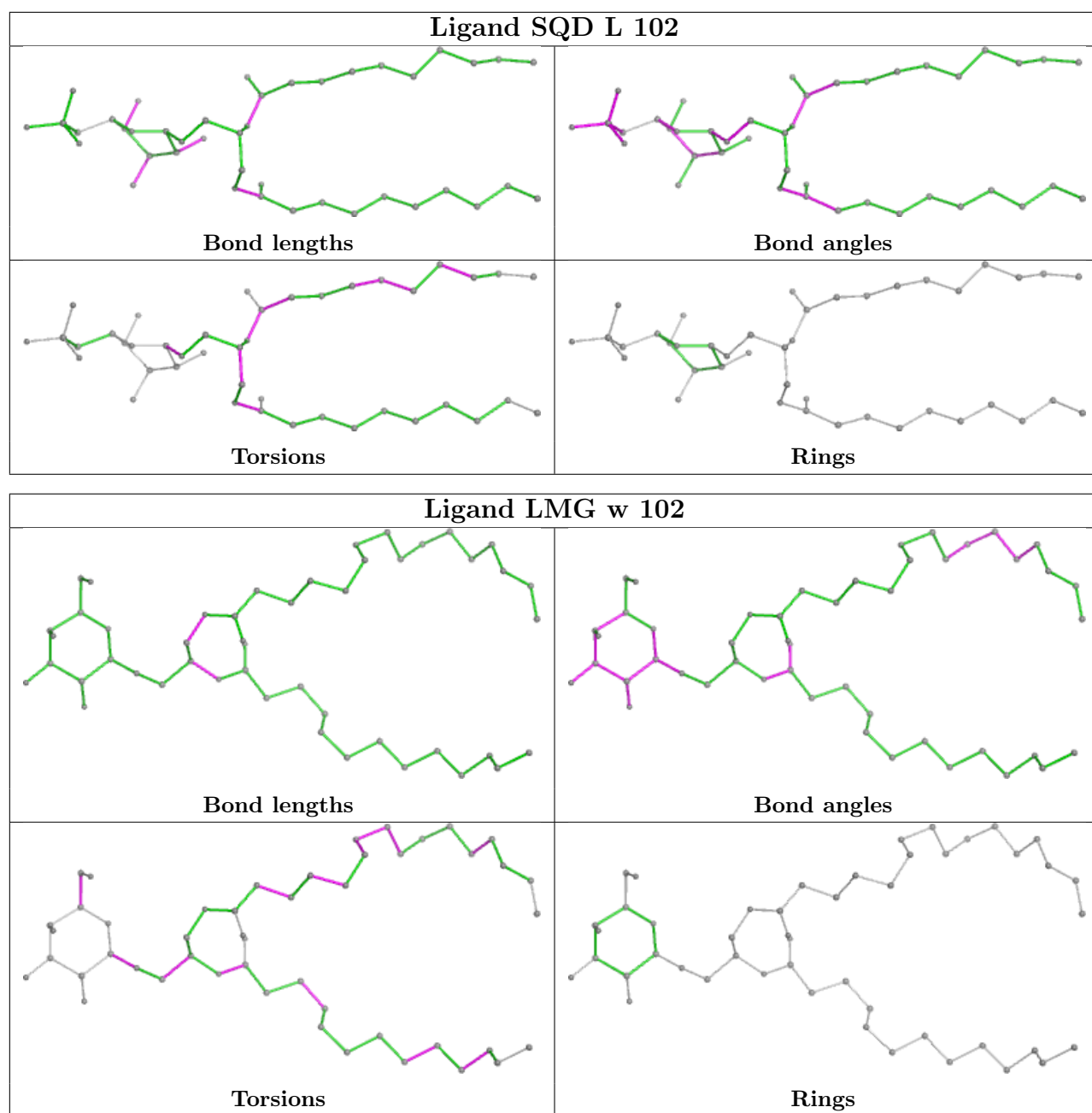


## Ligand CLA y 610

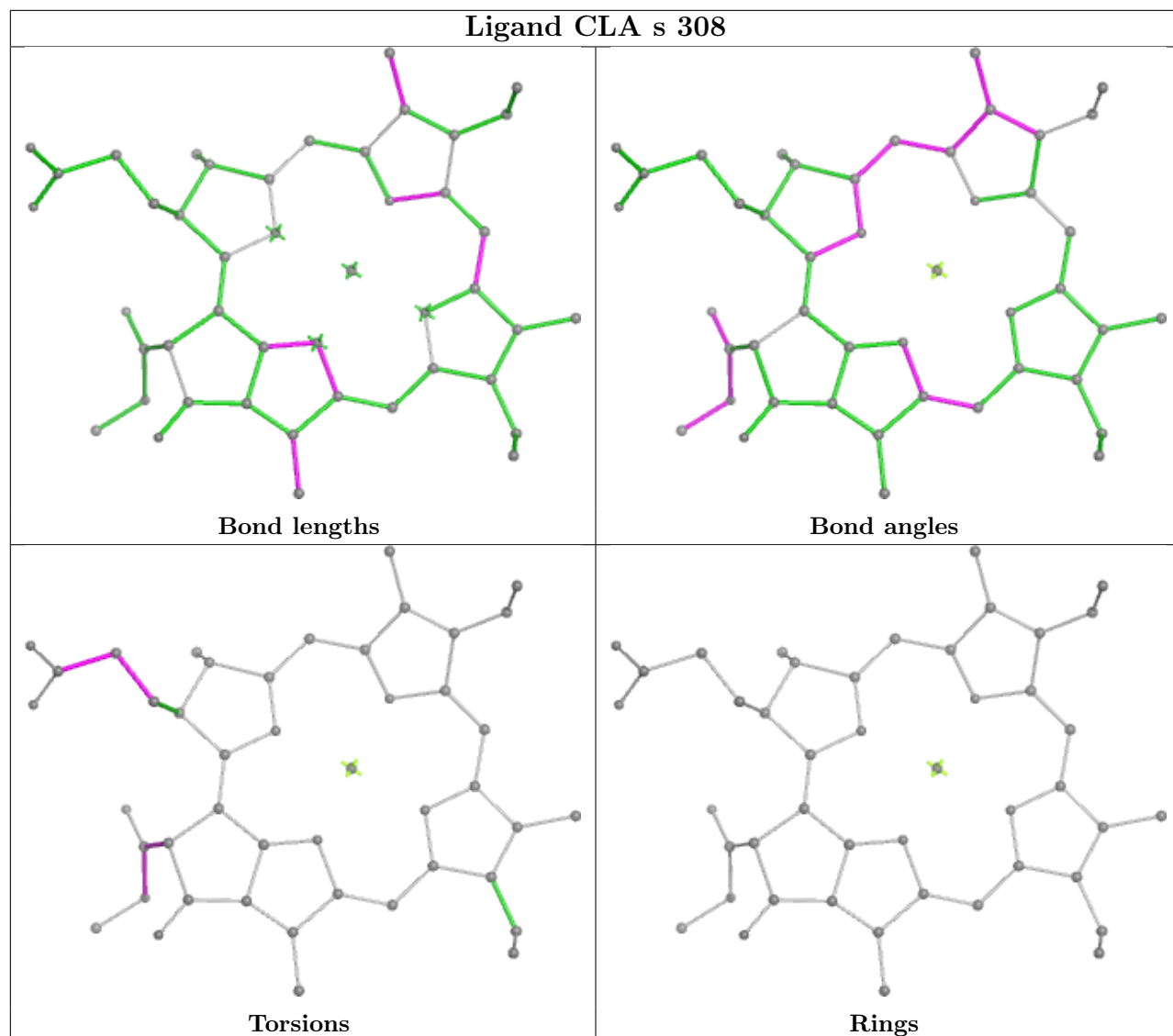


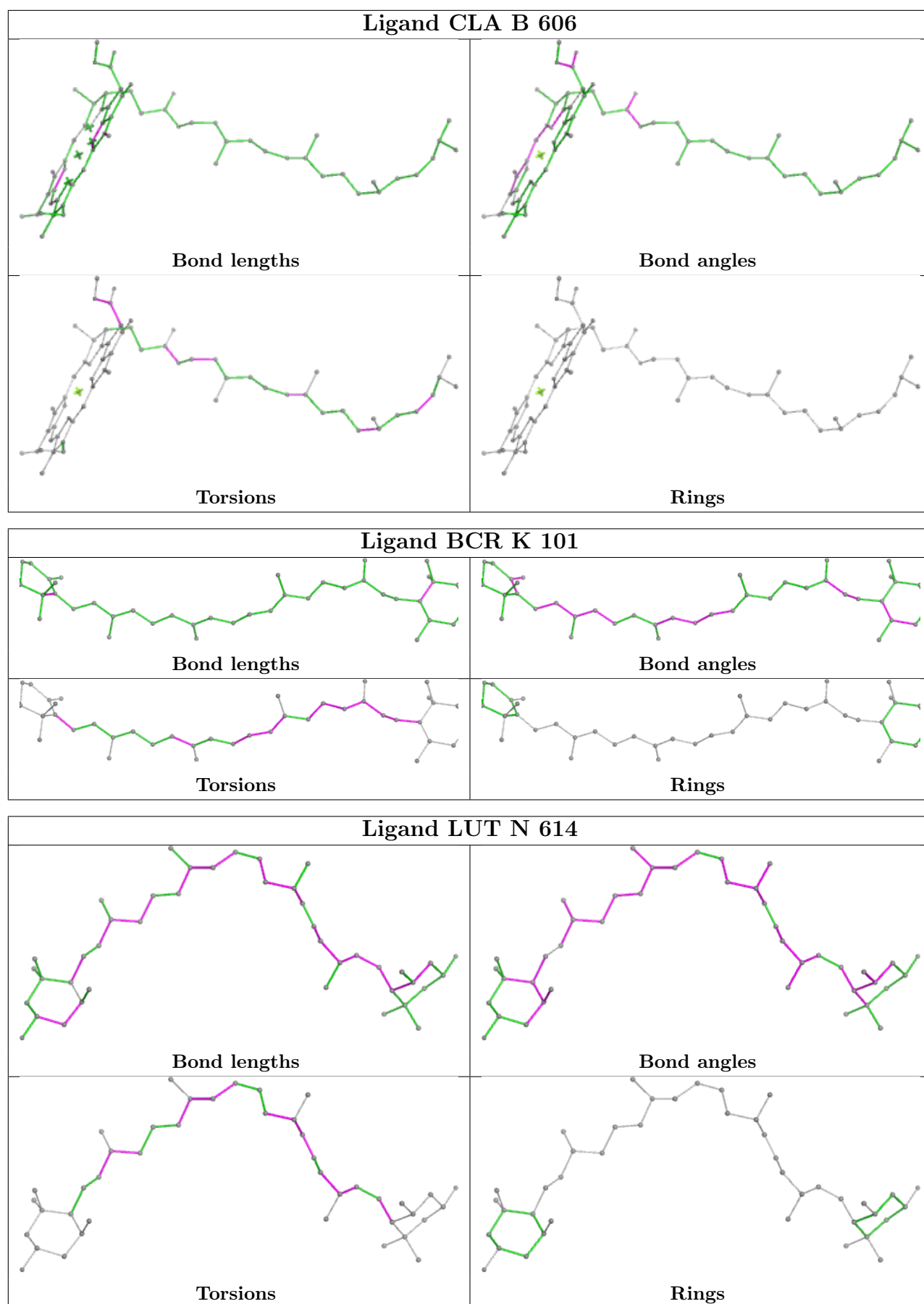
## Ligand CHL g 601

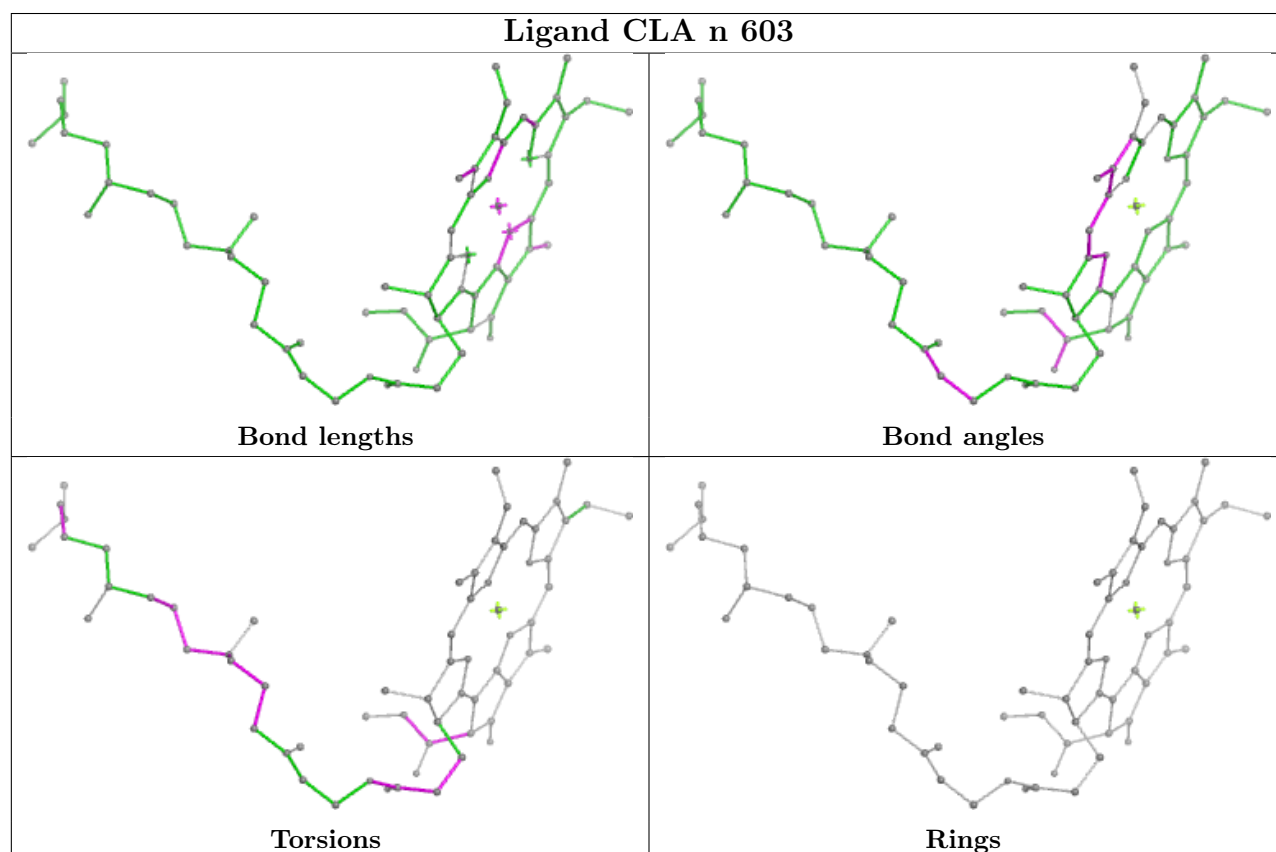
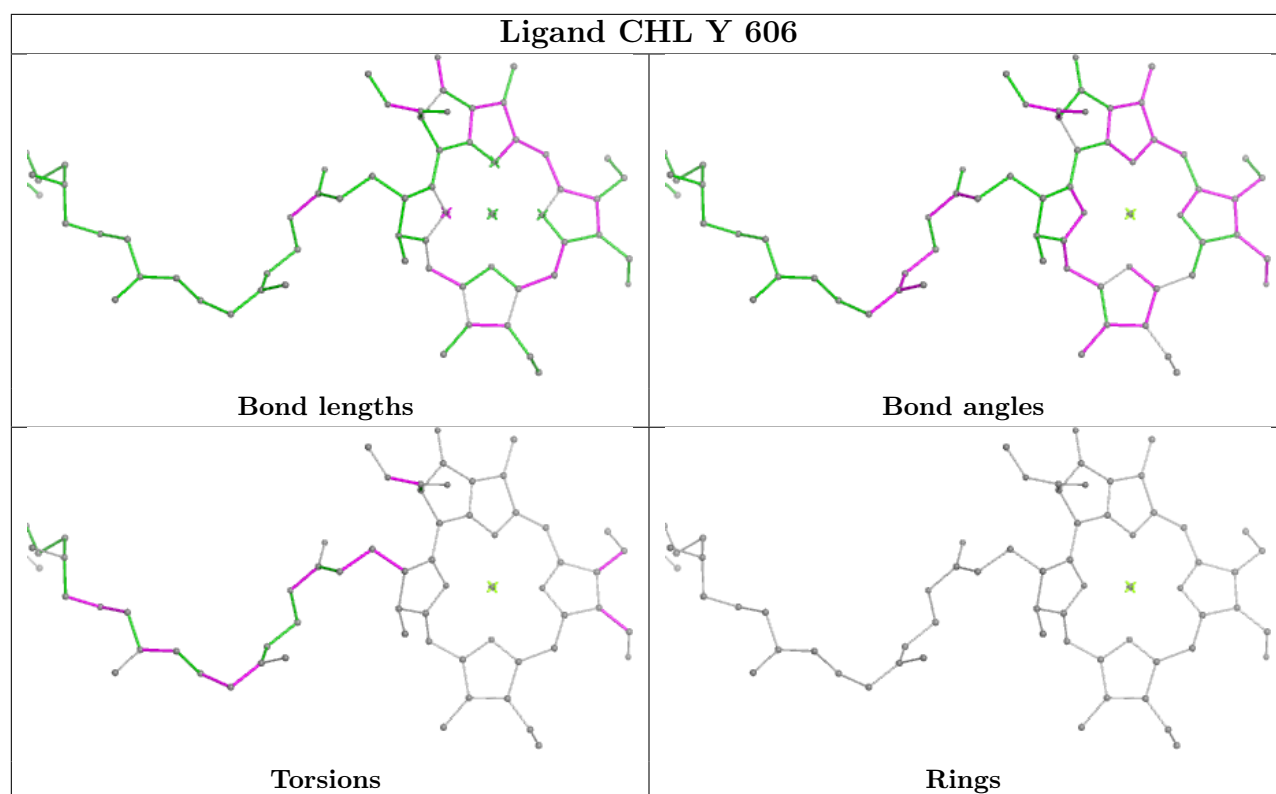


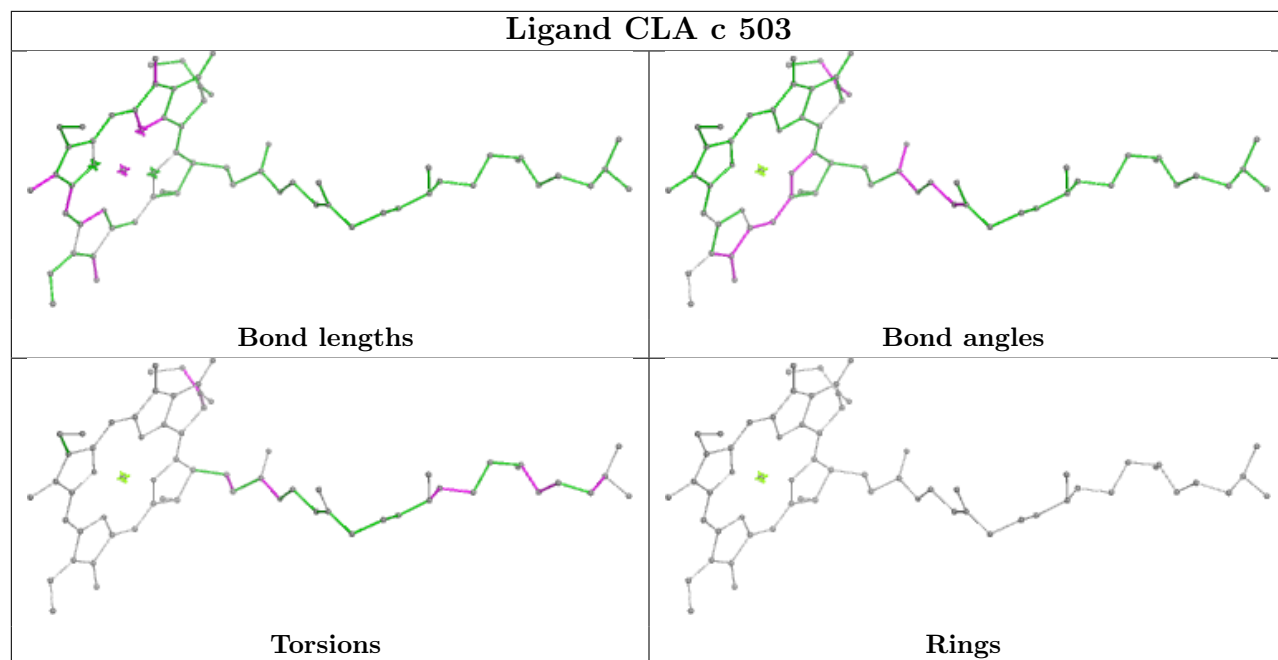
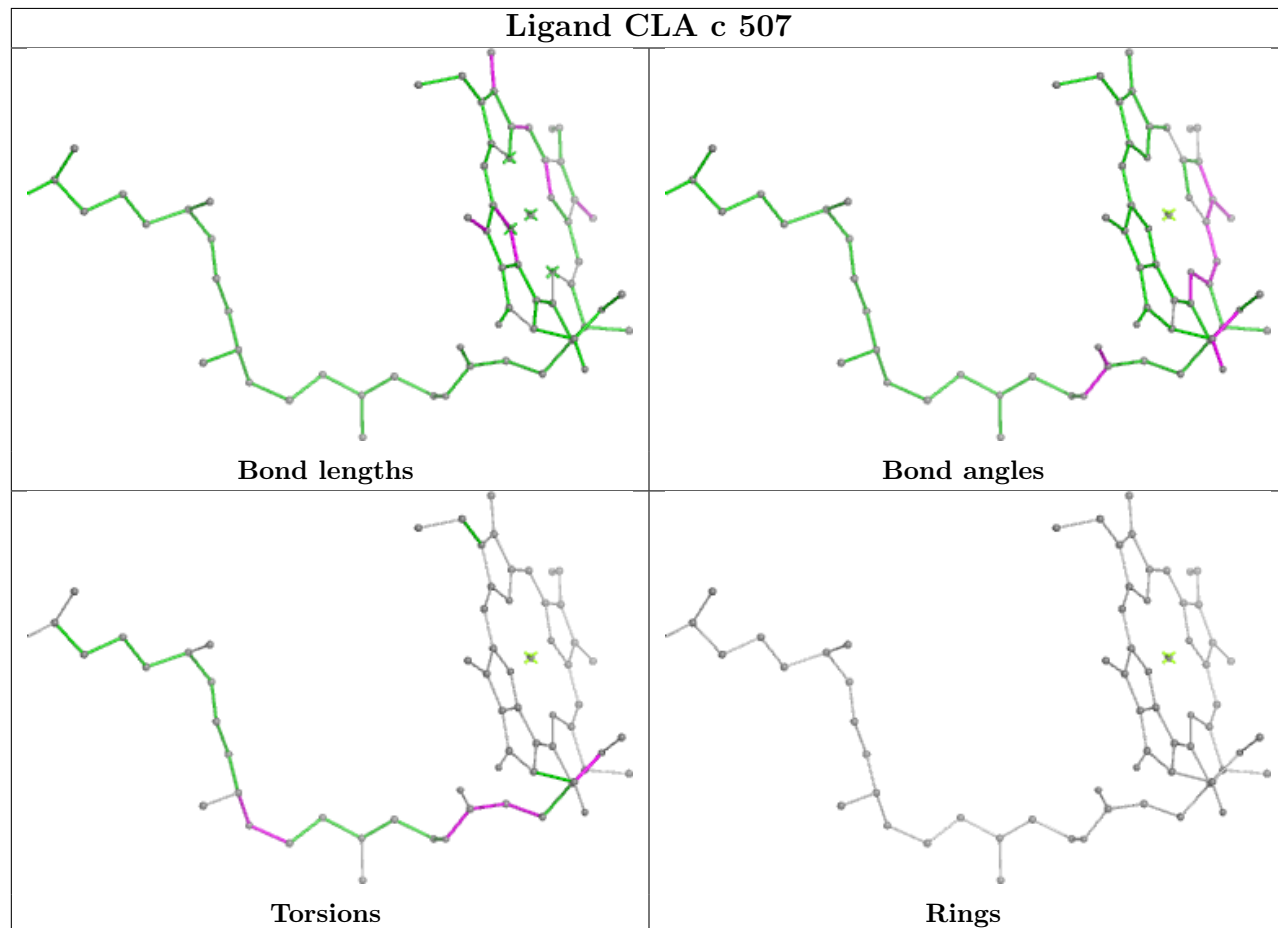


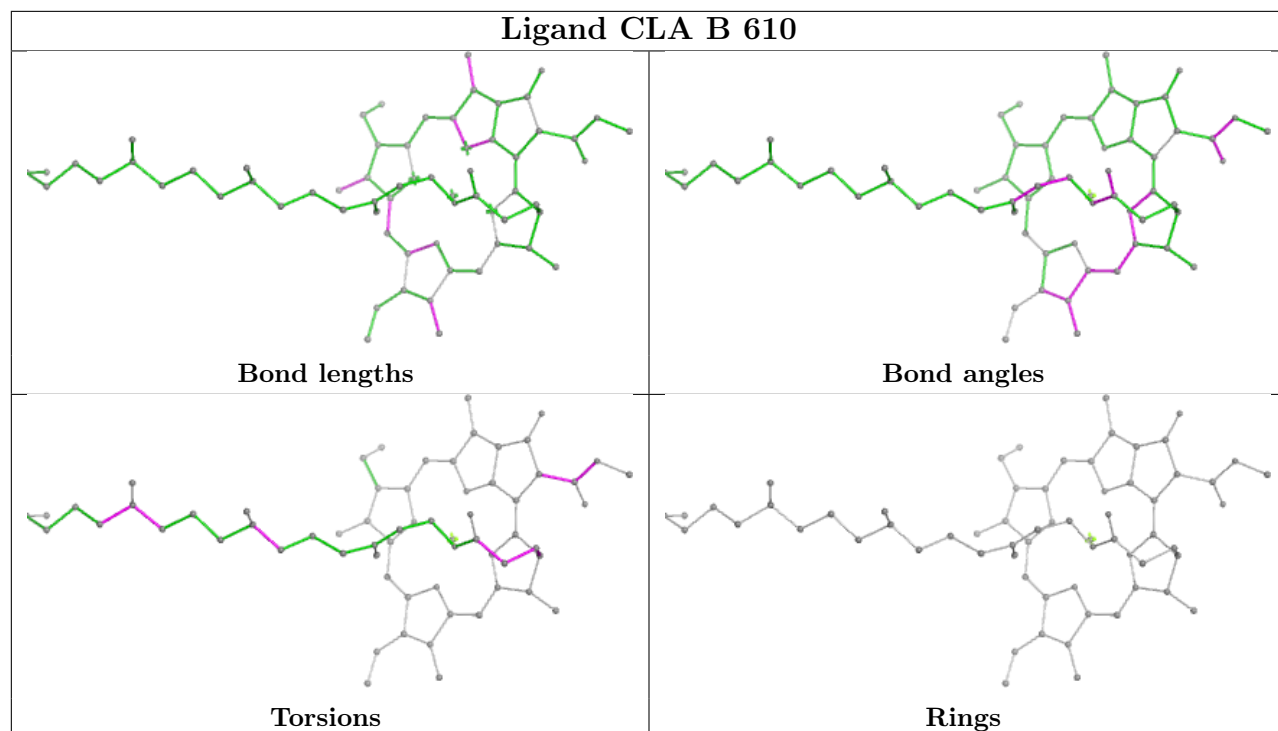
## Ligand CLA s 308



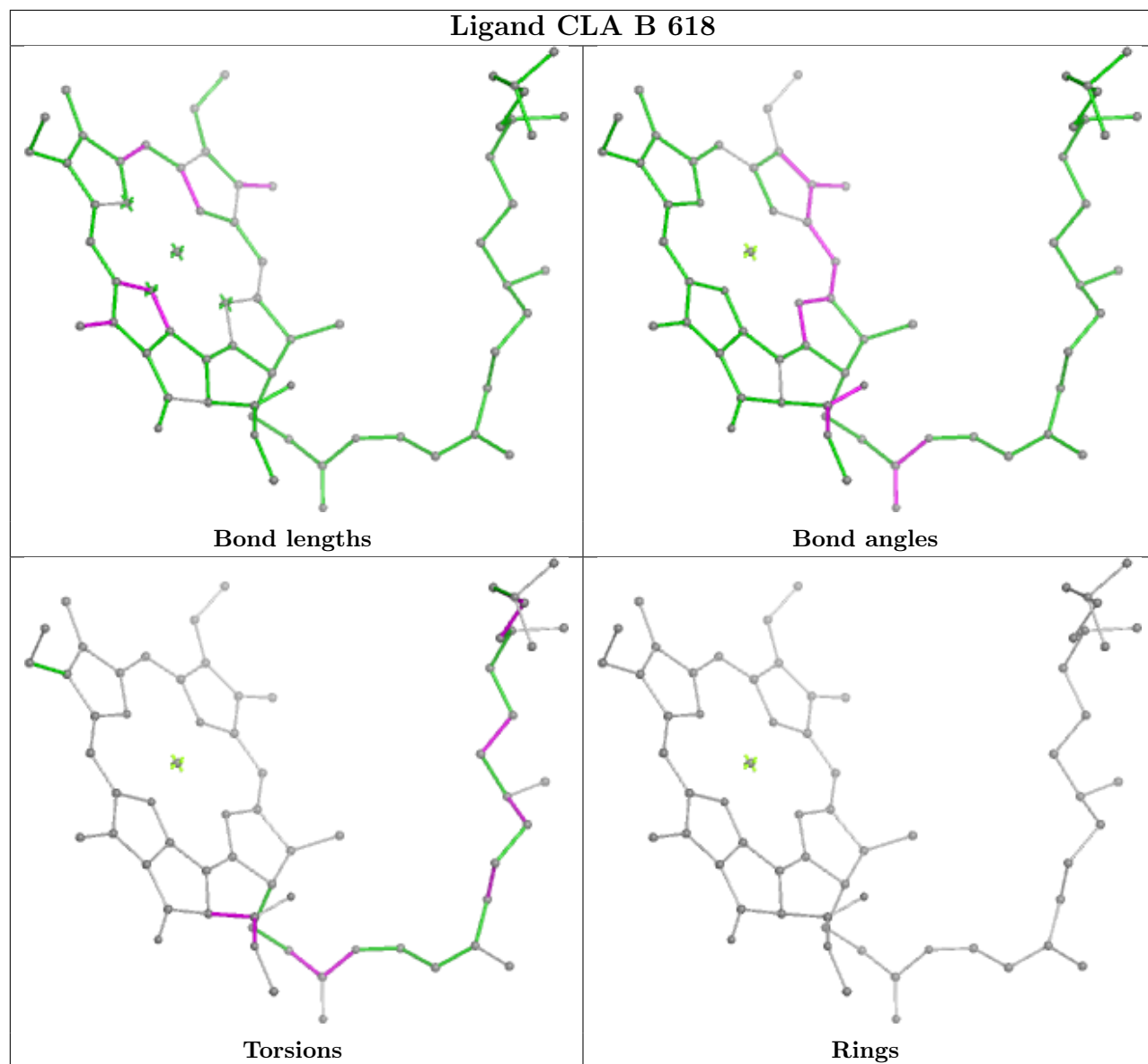


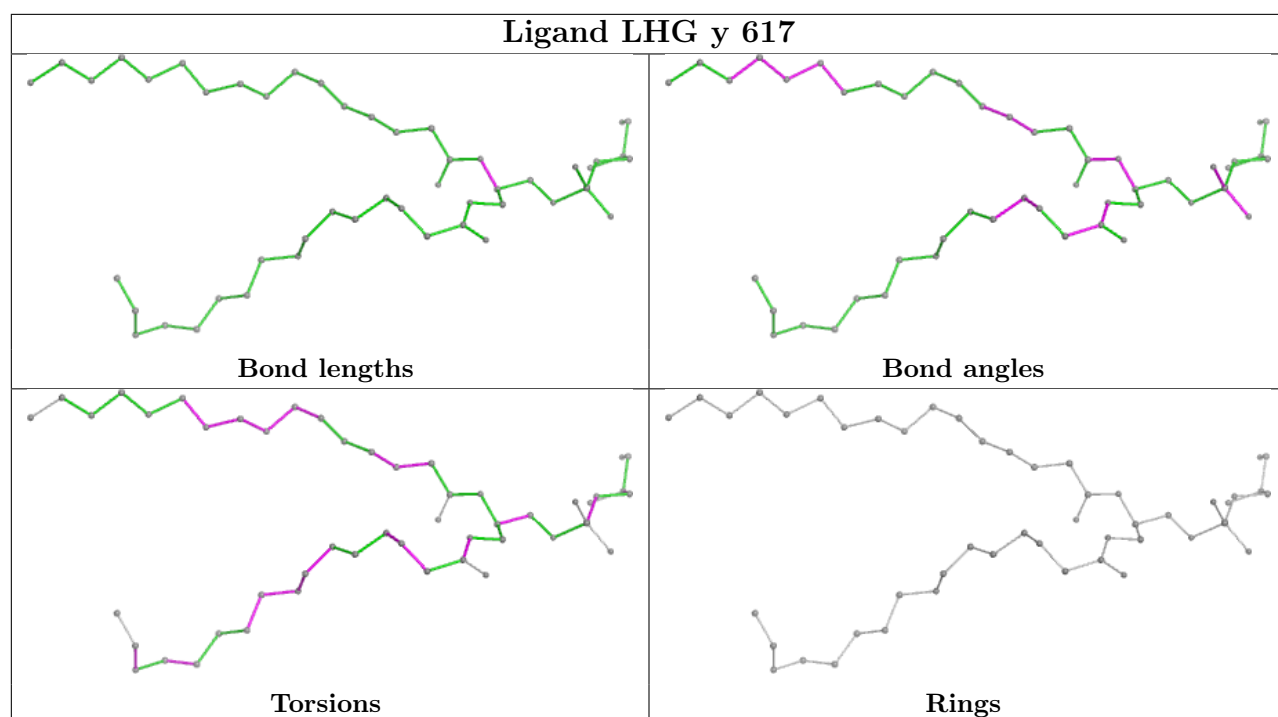


**Ligand CLA c 503****Ligand CLA c 507**

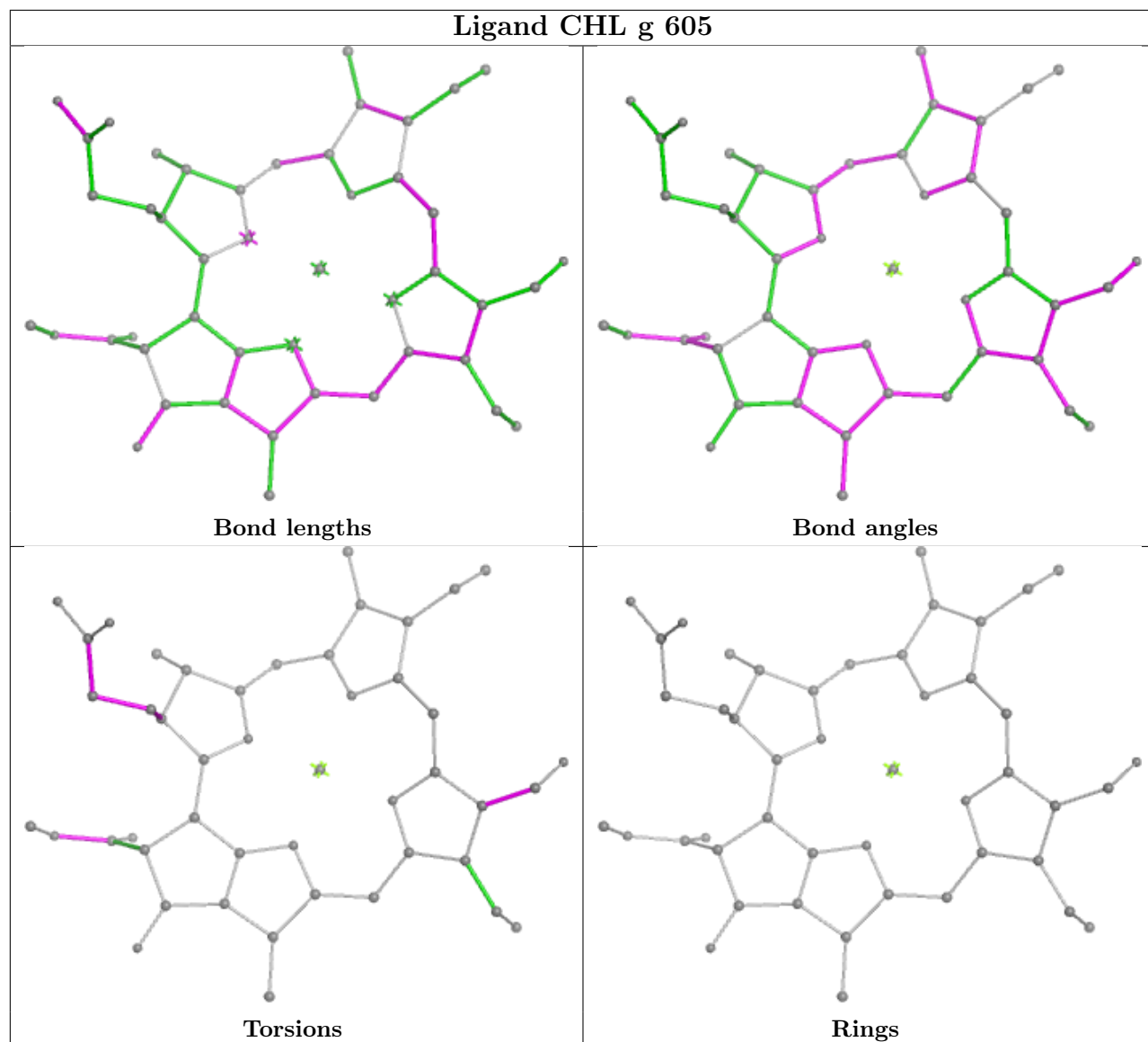


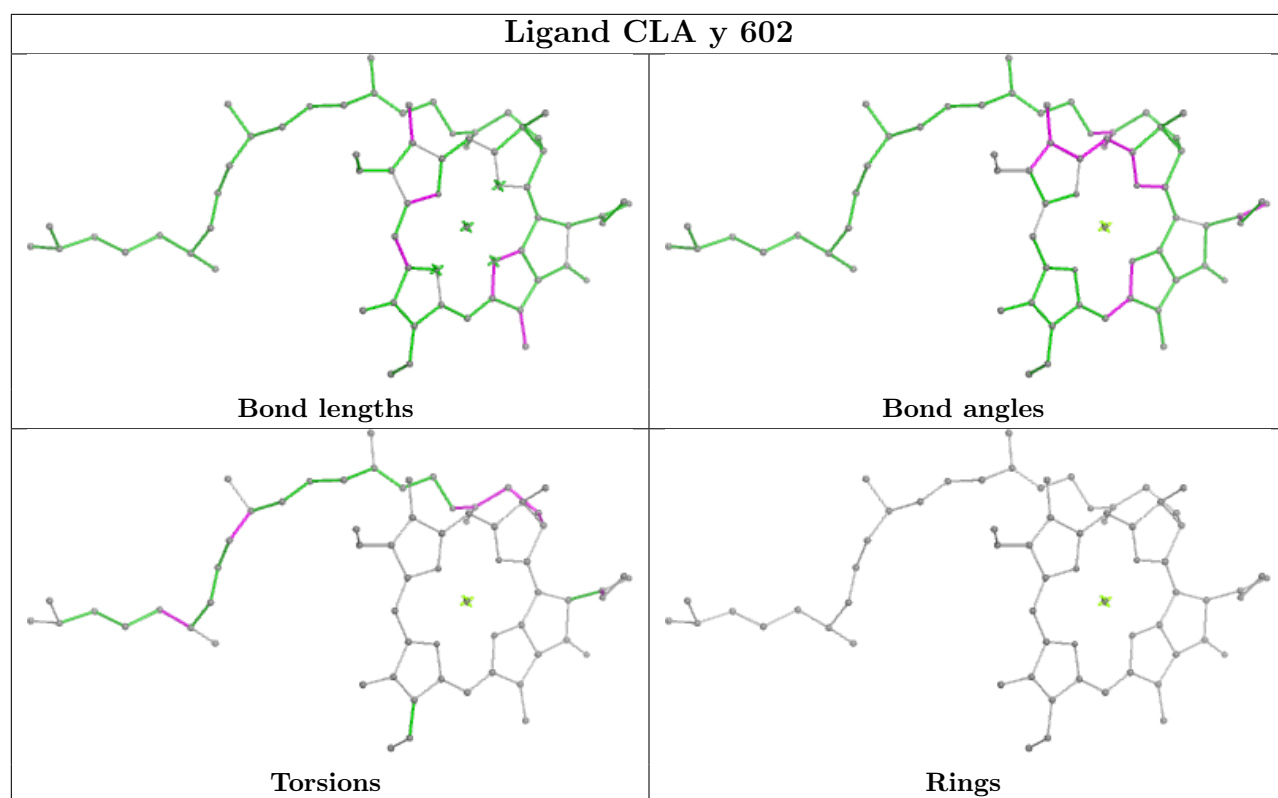
## Ligand CLA B 618



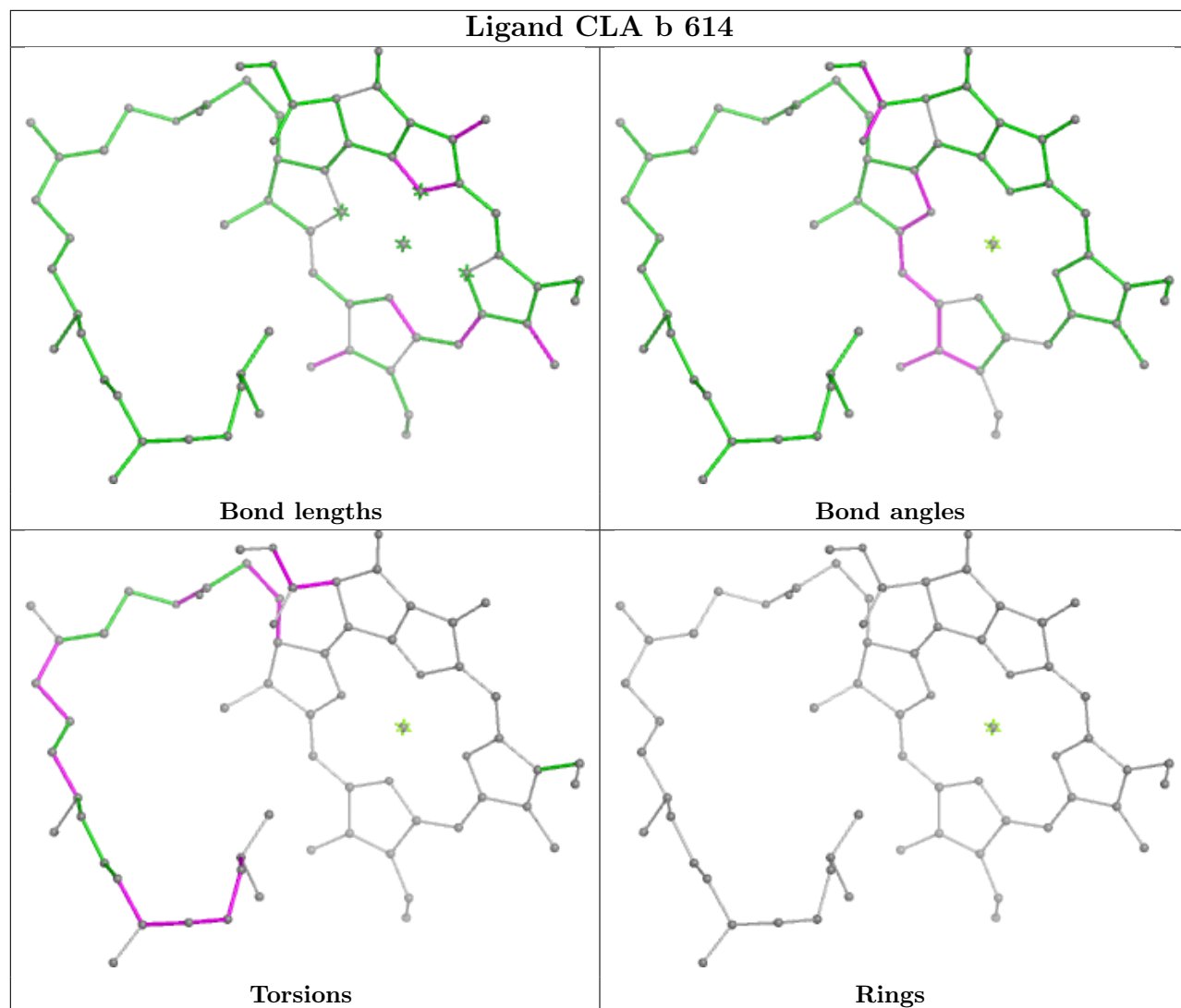


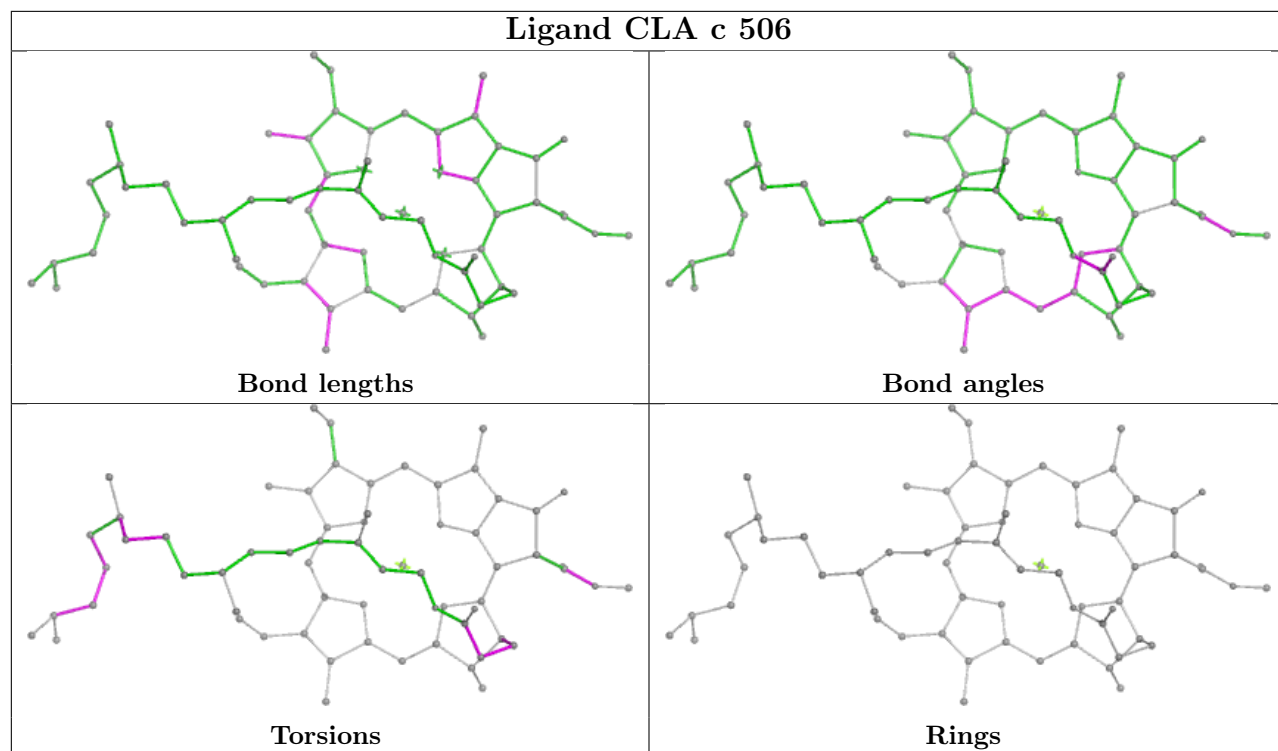
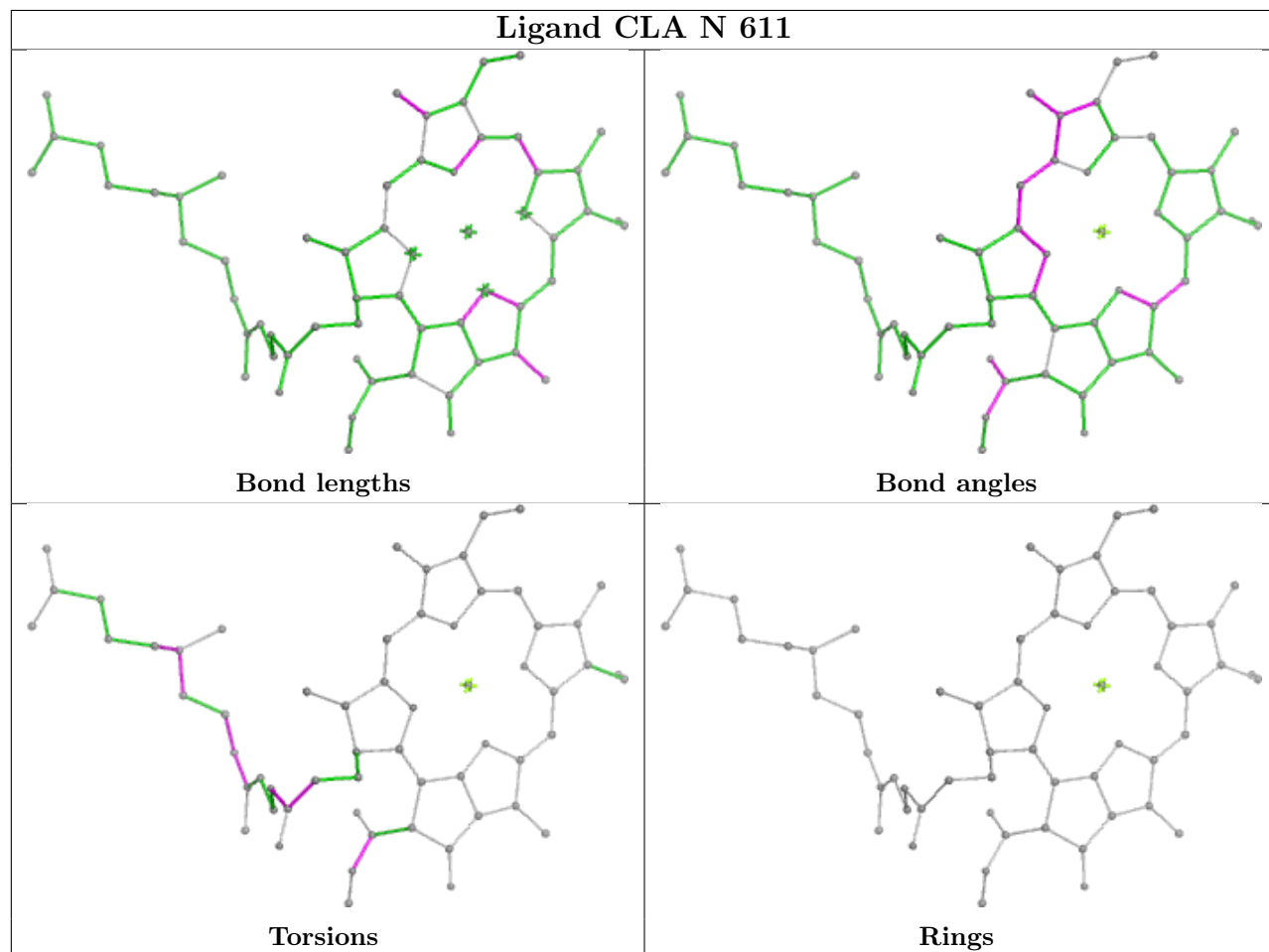
## Ligand CHL g 605

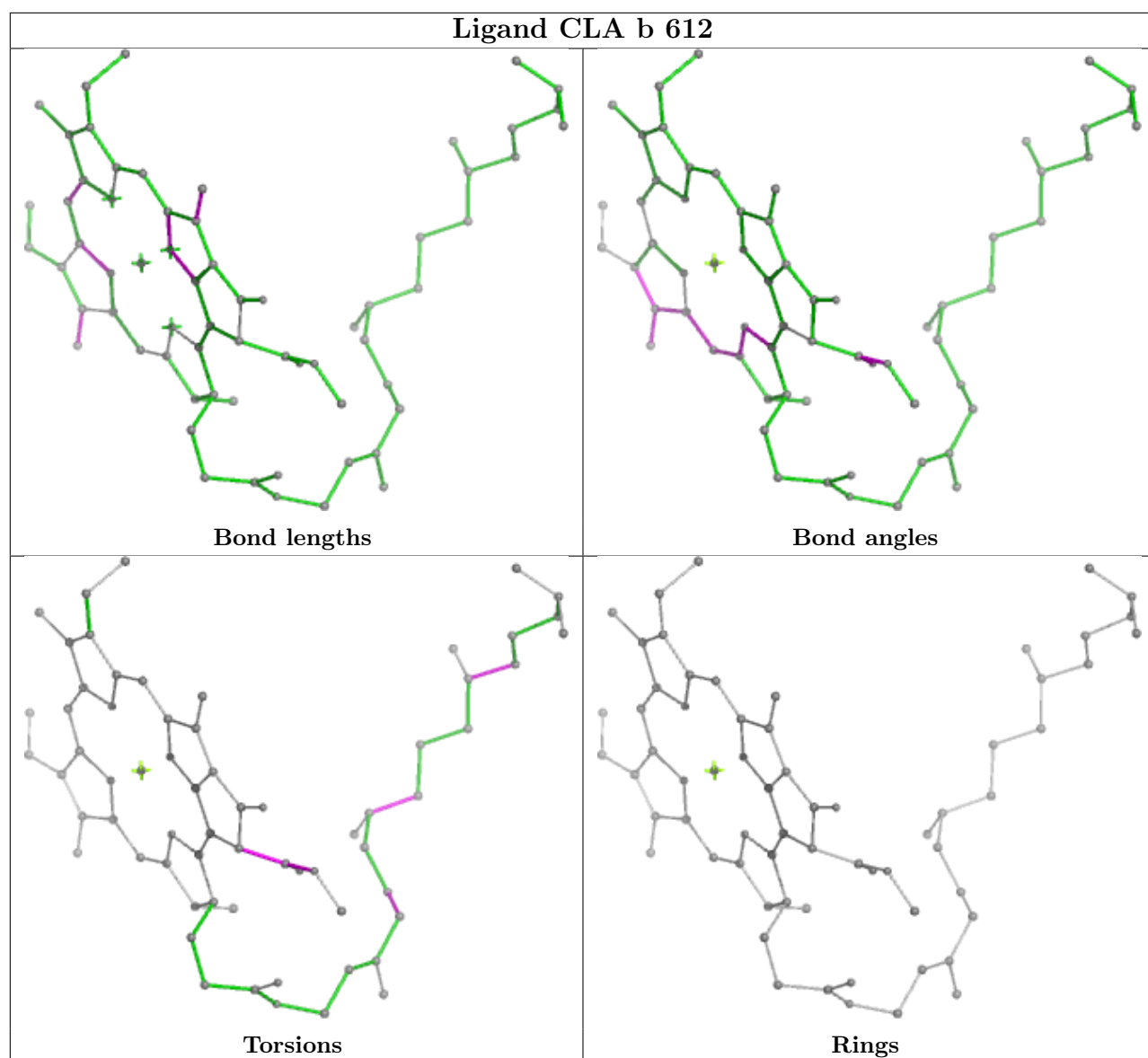


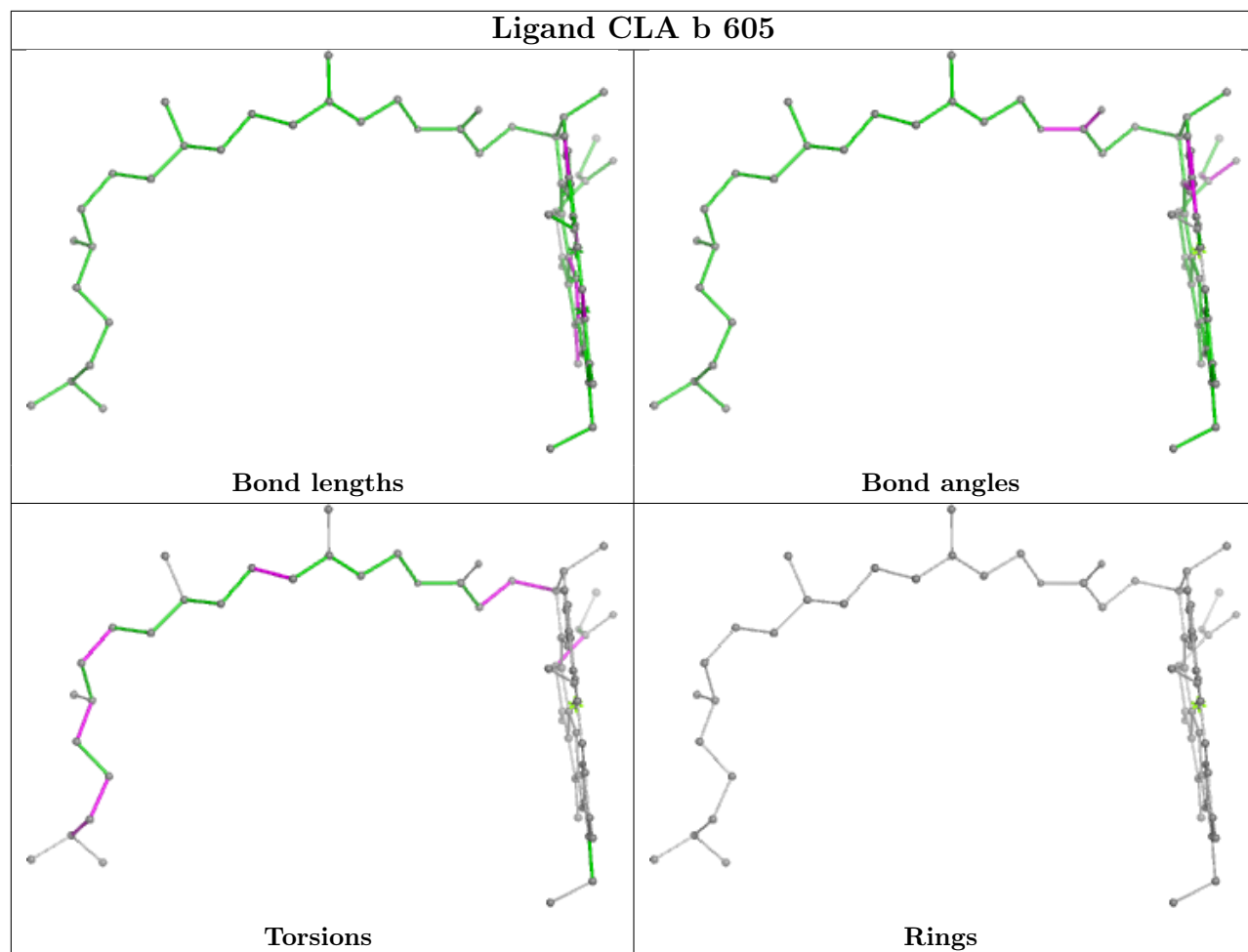


## Ligand CLA b 614

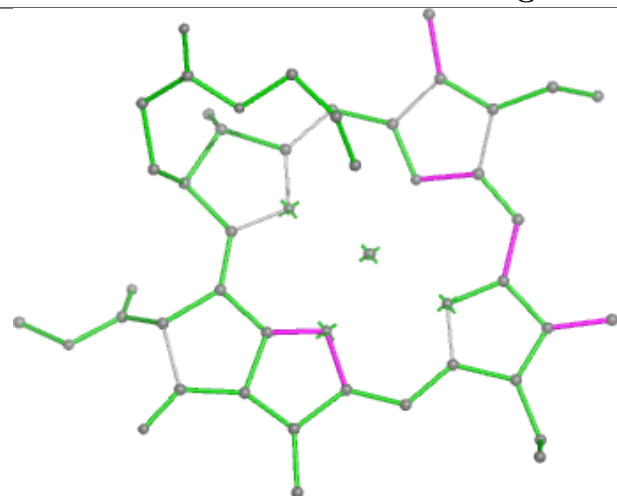


**Ligand CLA c 506****Ligand CLA N 611**

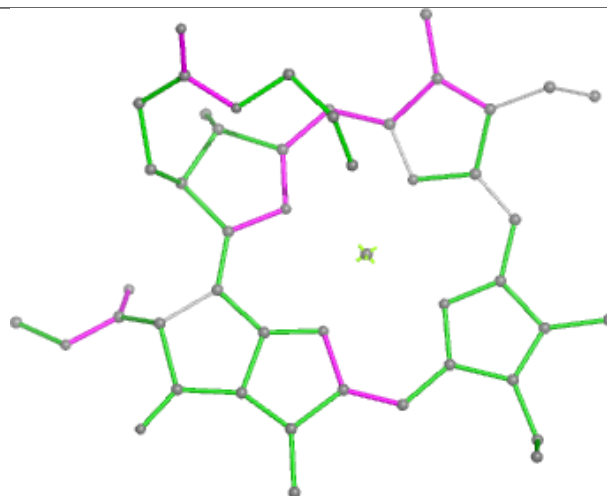




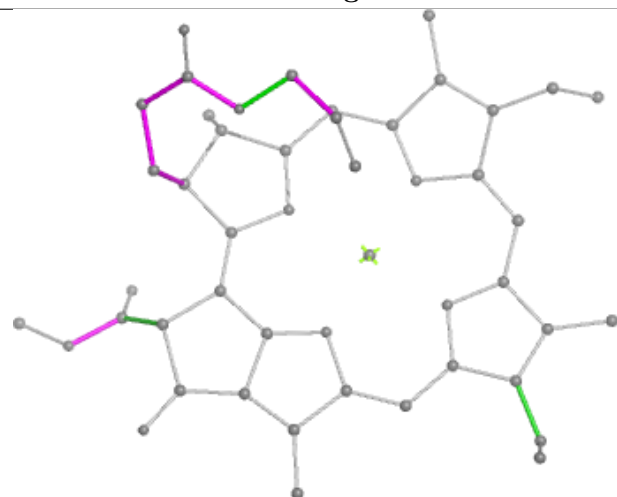
## Ligand CLA Y 612



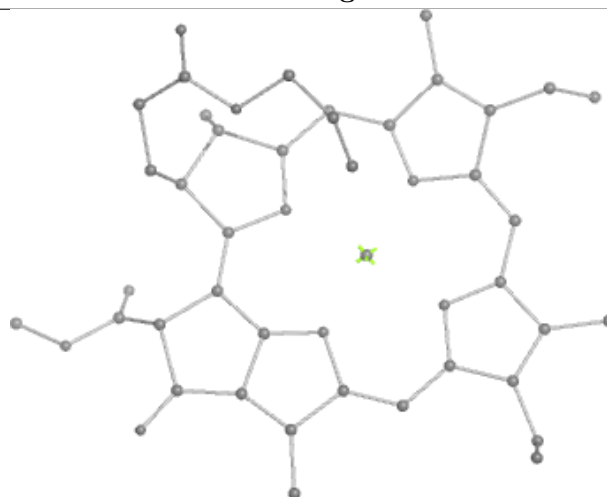
Bond lengths



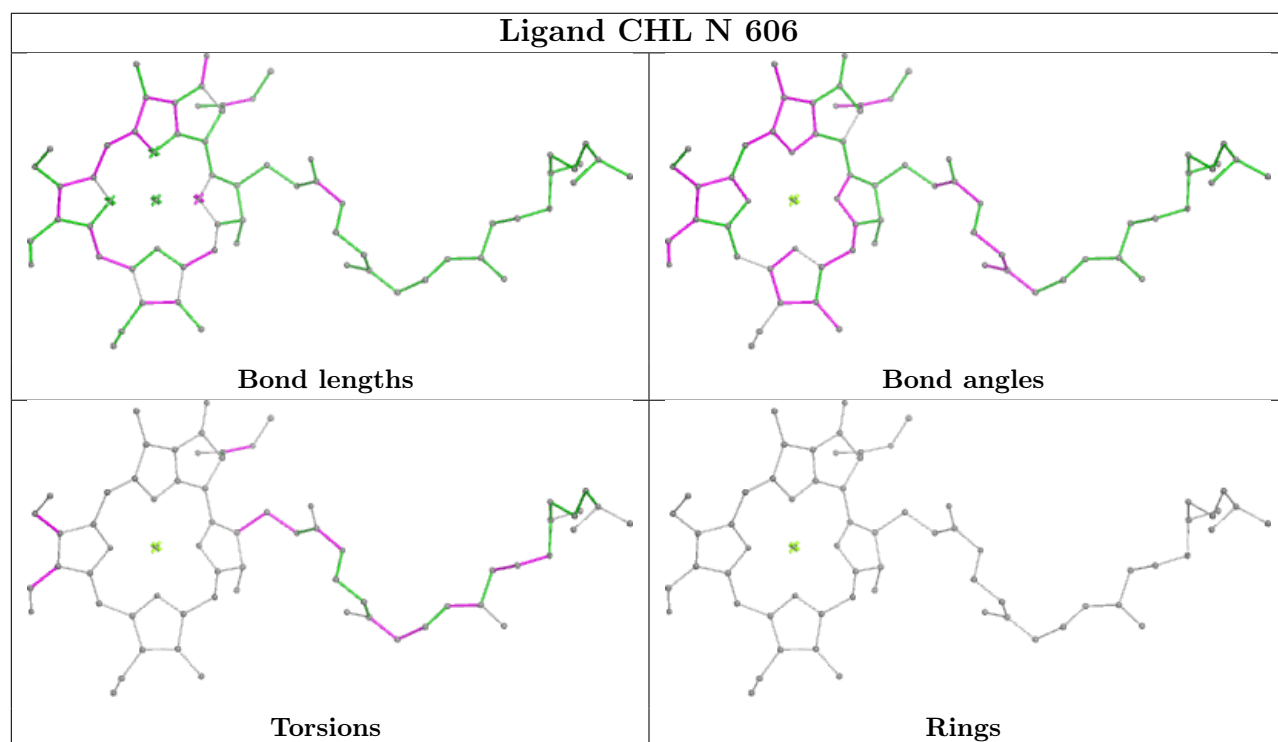
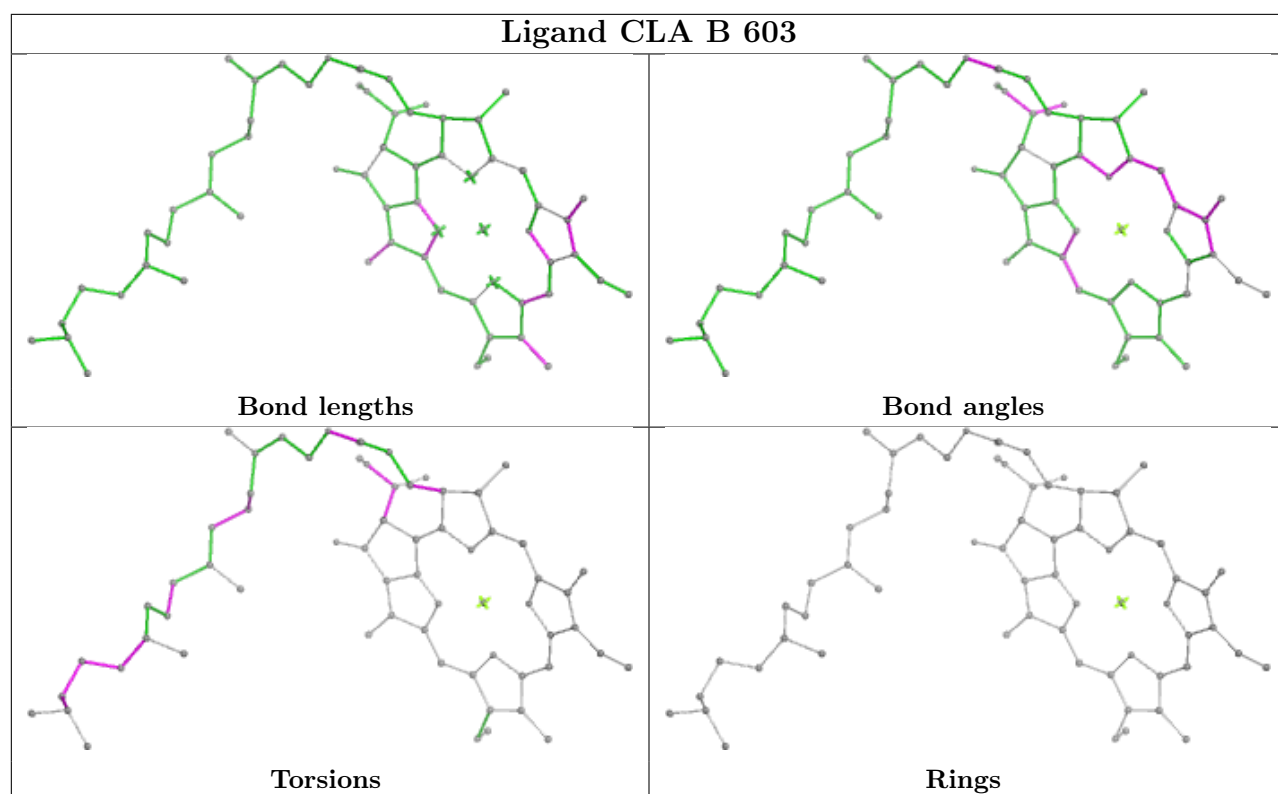
Bond angles

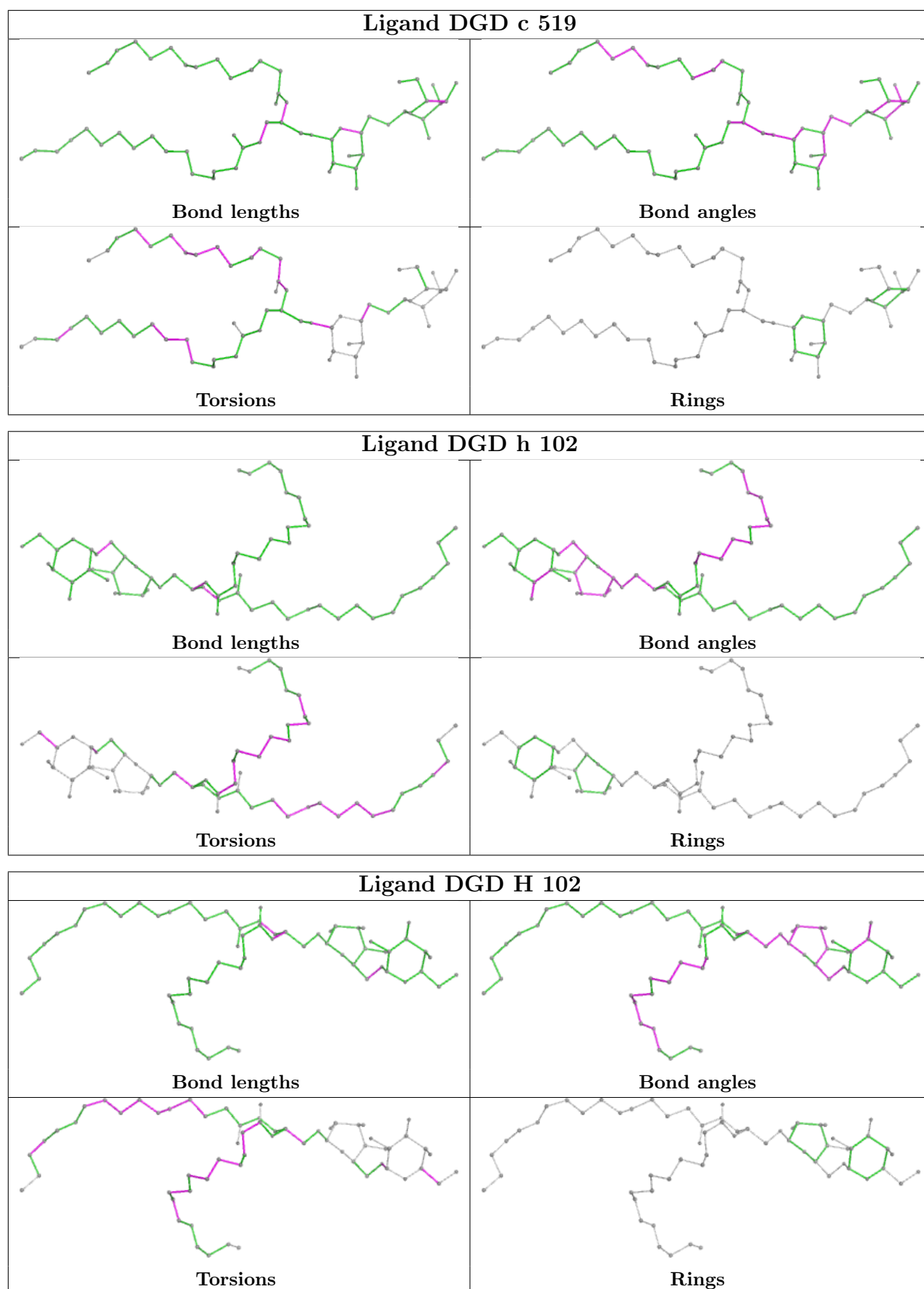


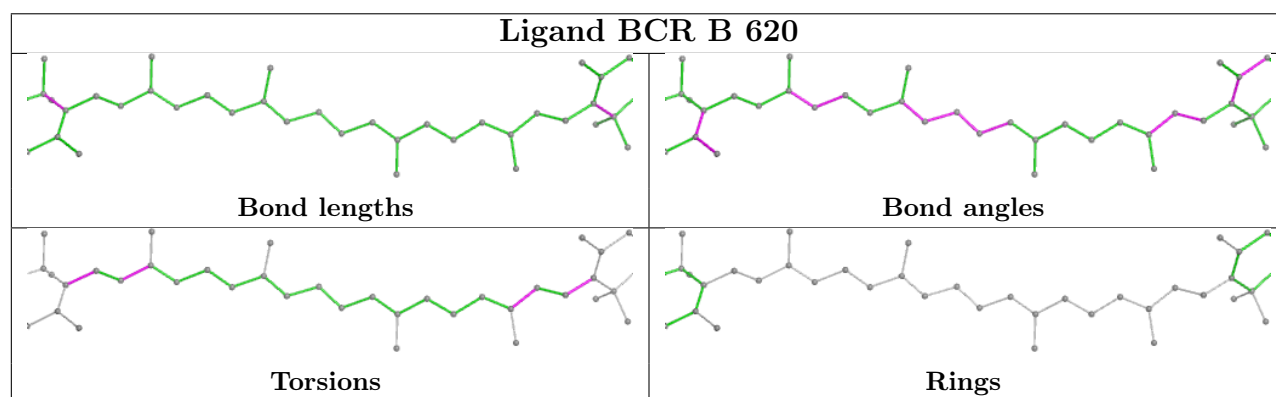
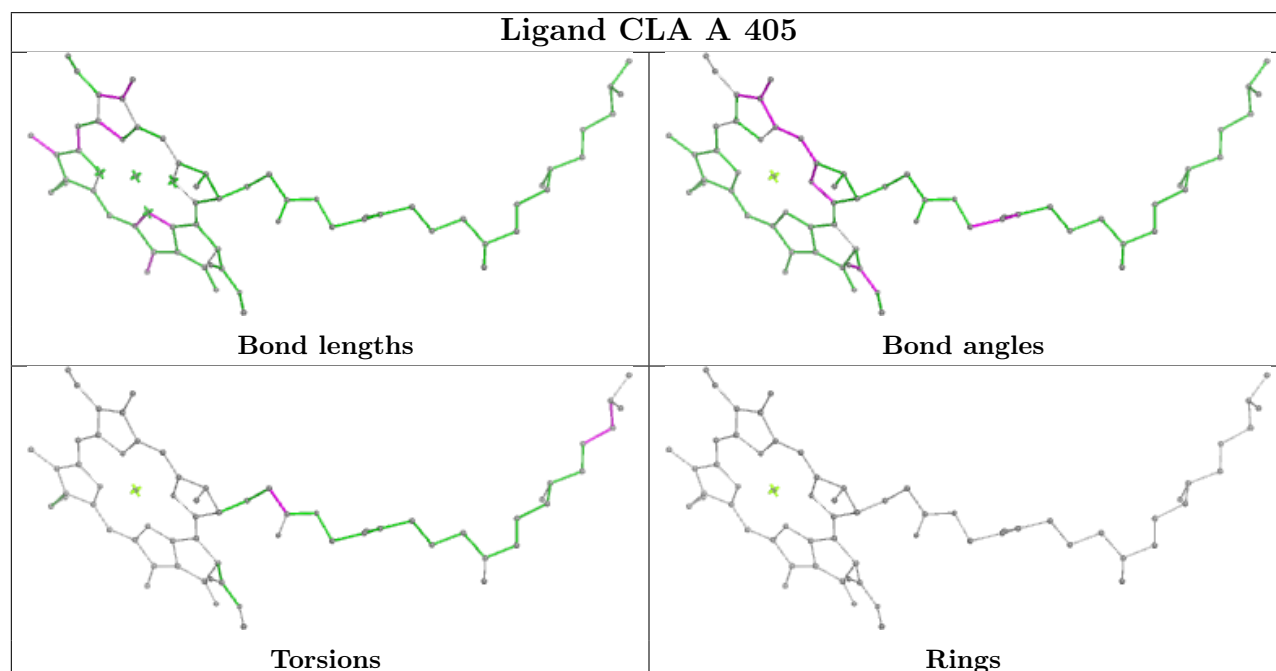
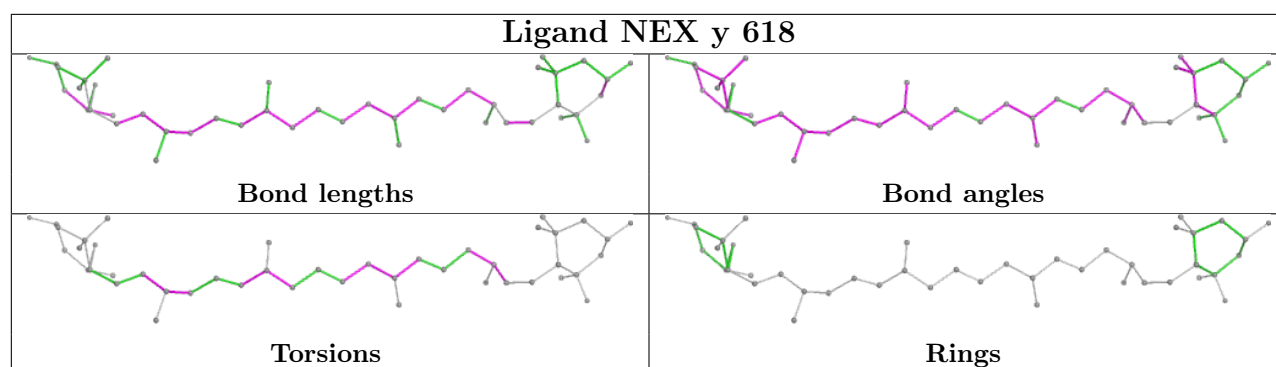
Torsions



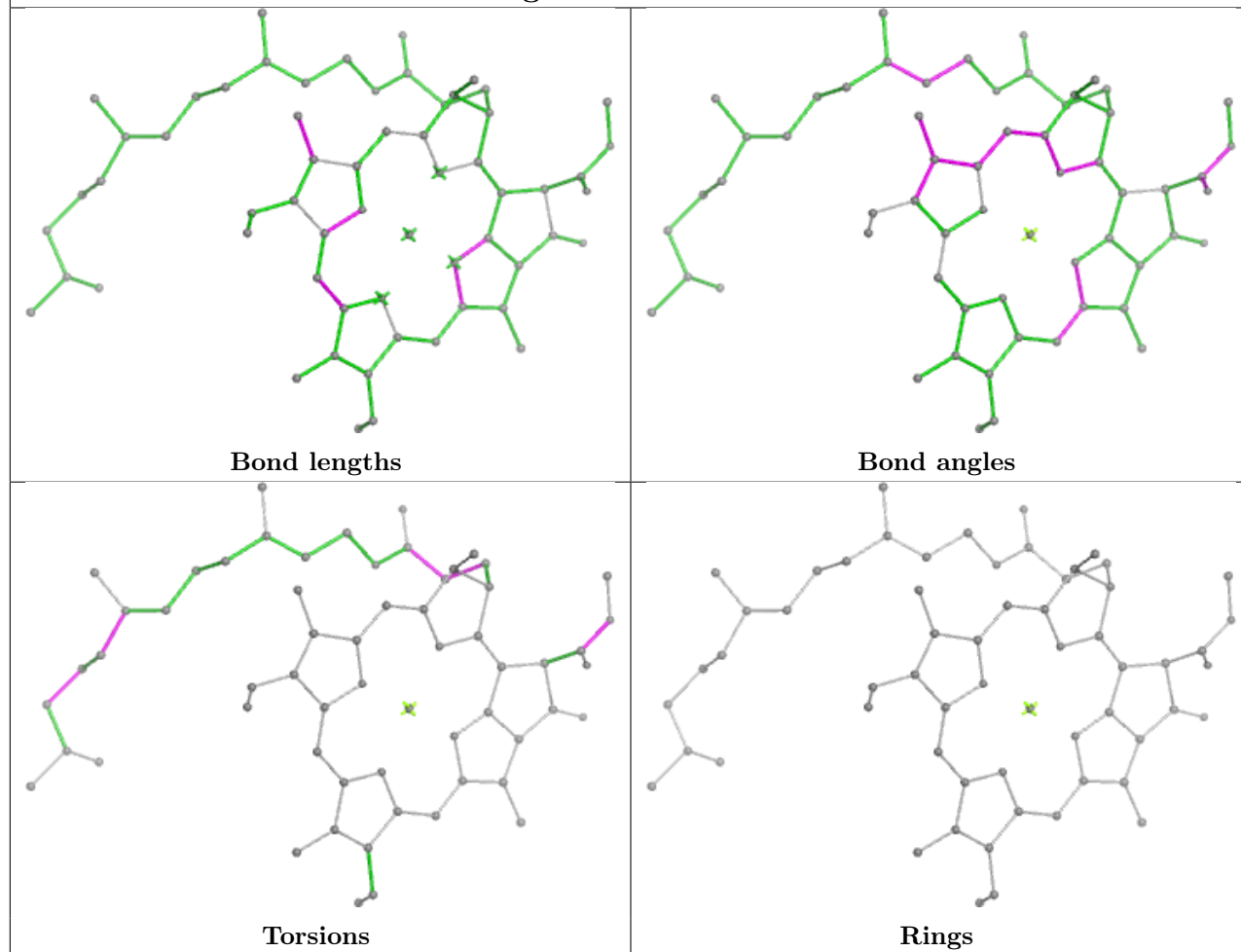
Rings



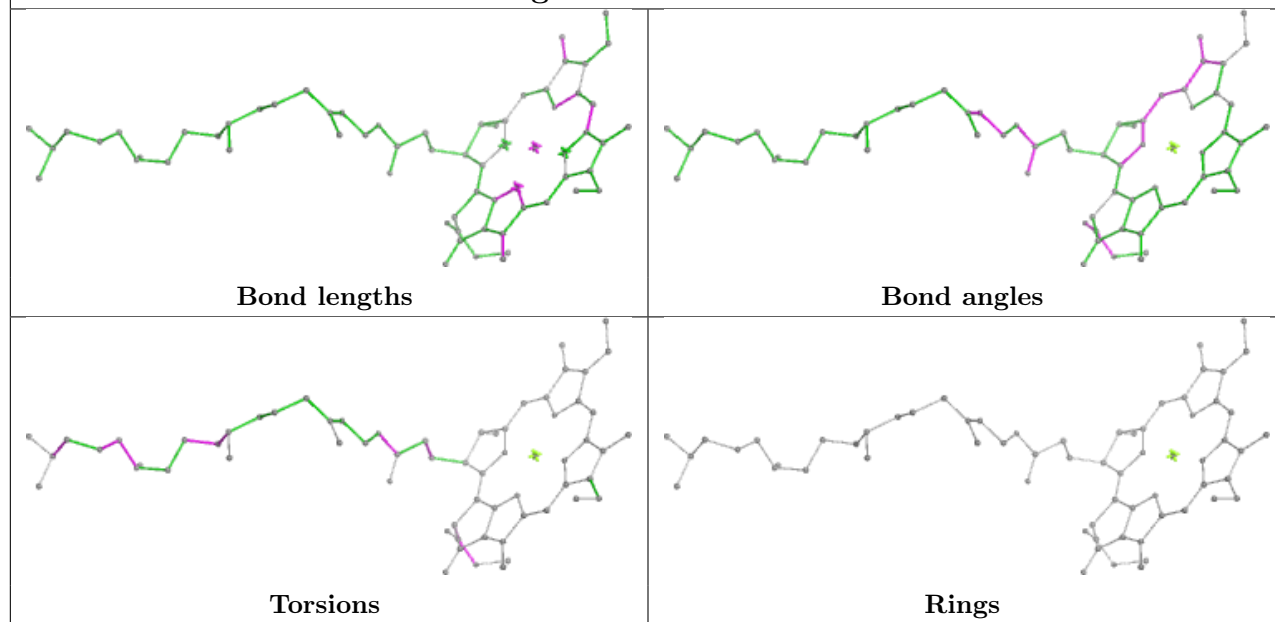


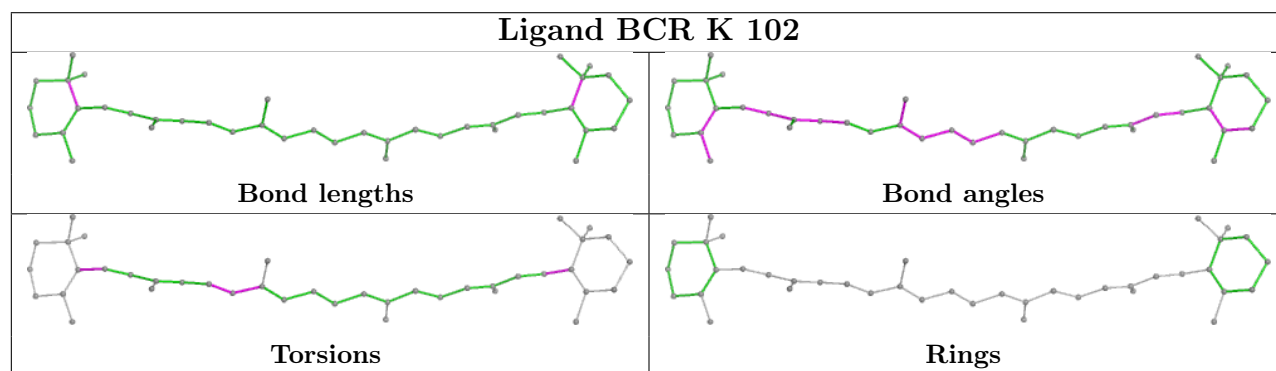
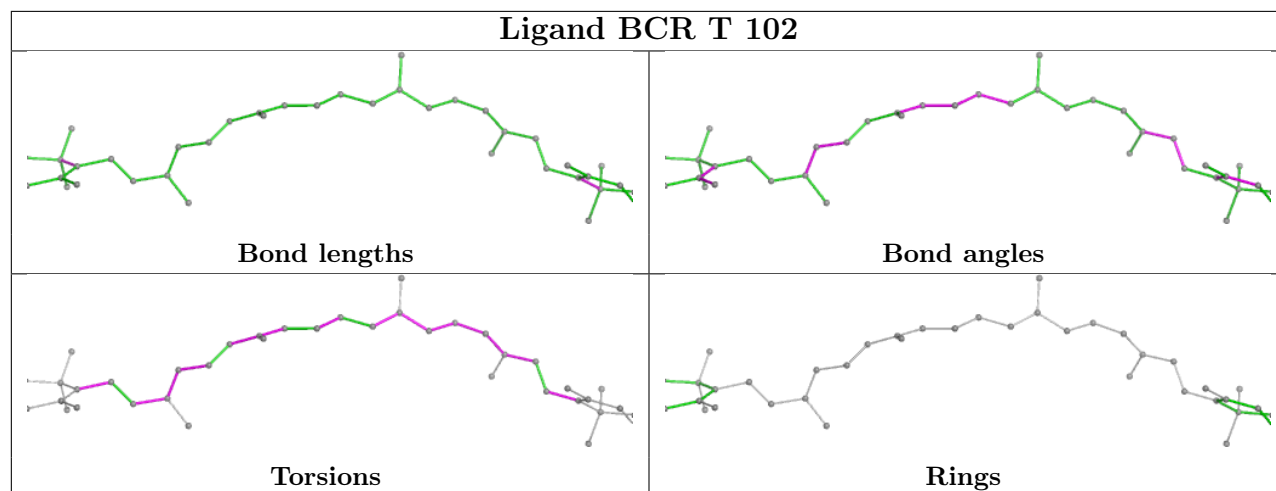
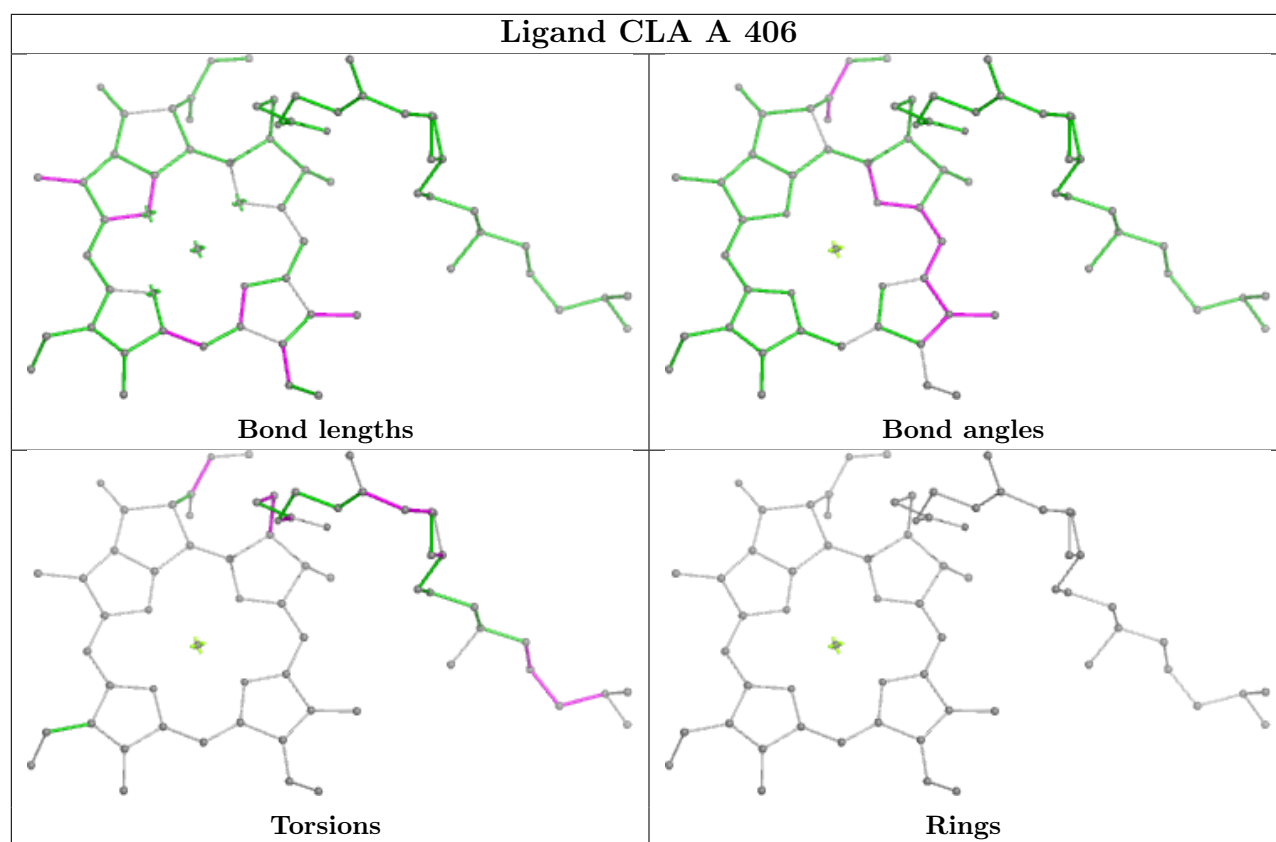


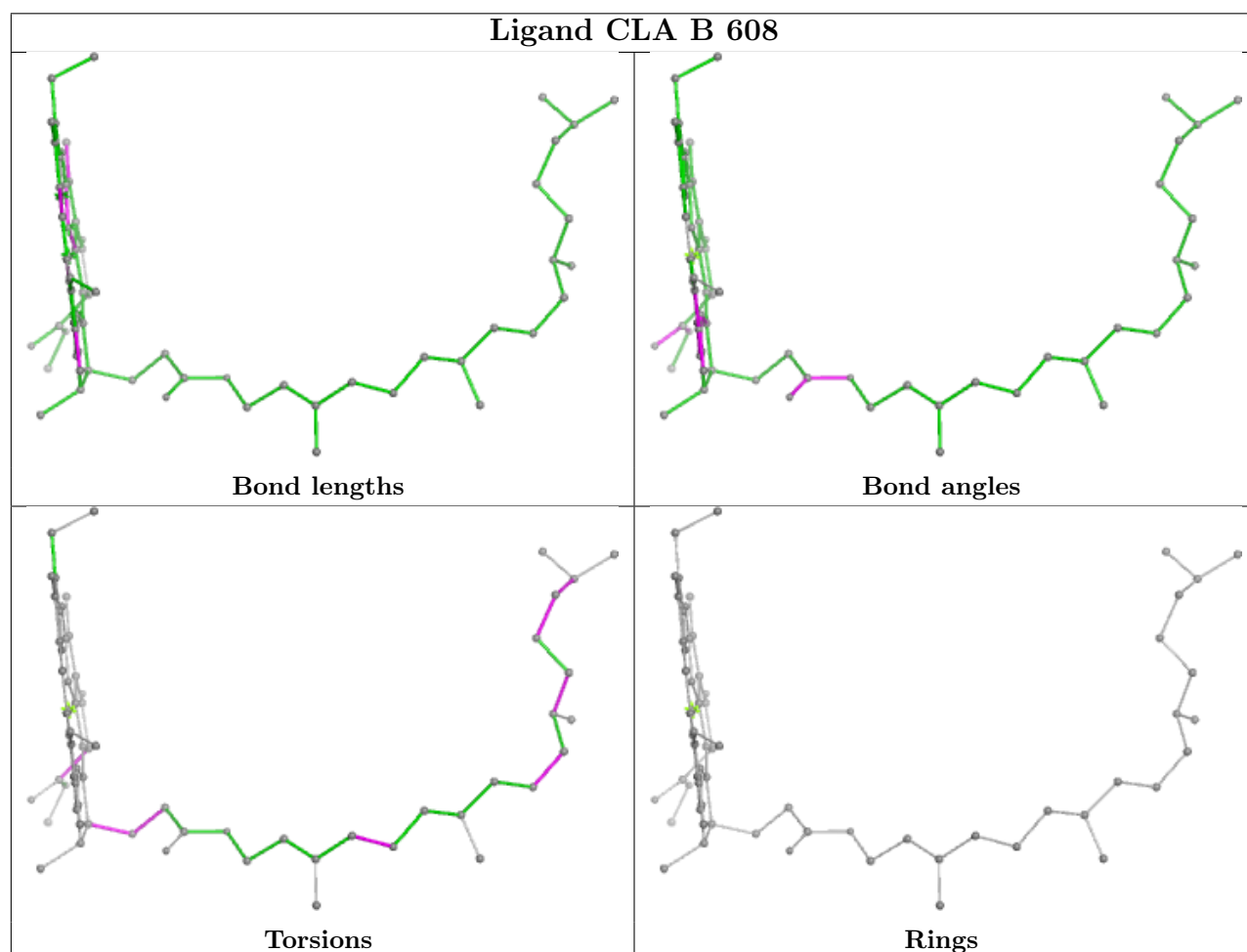
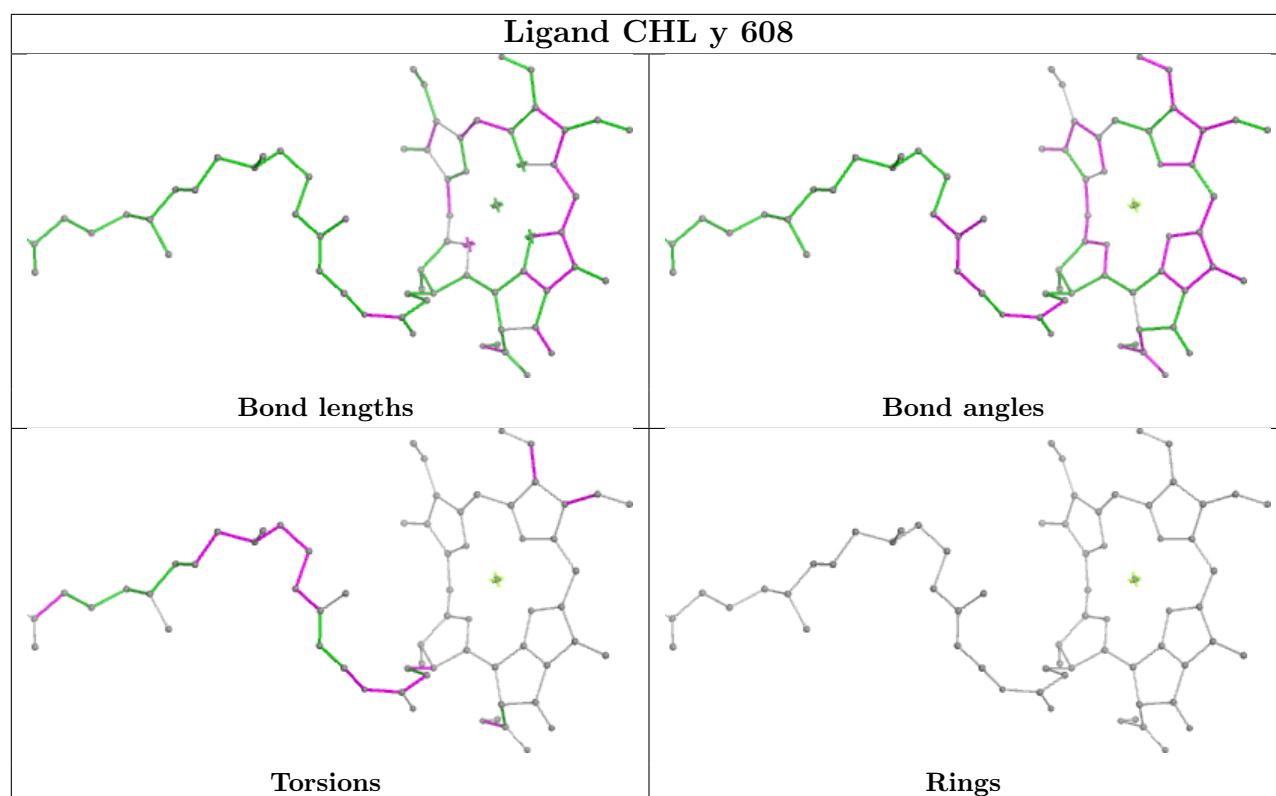
## Ligand CLA r 303



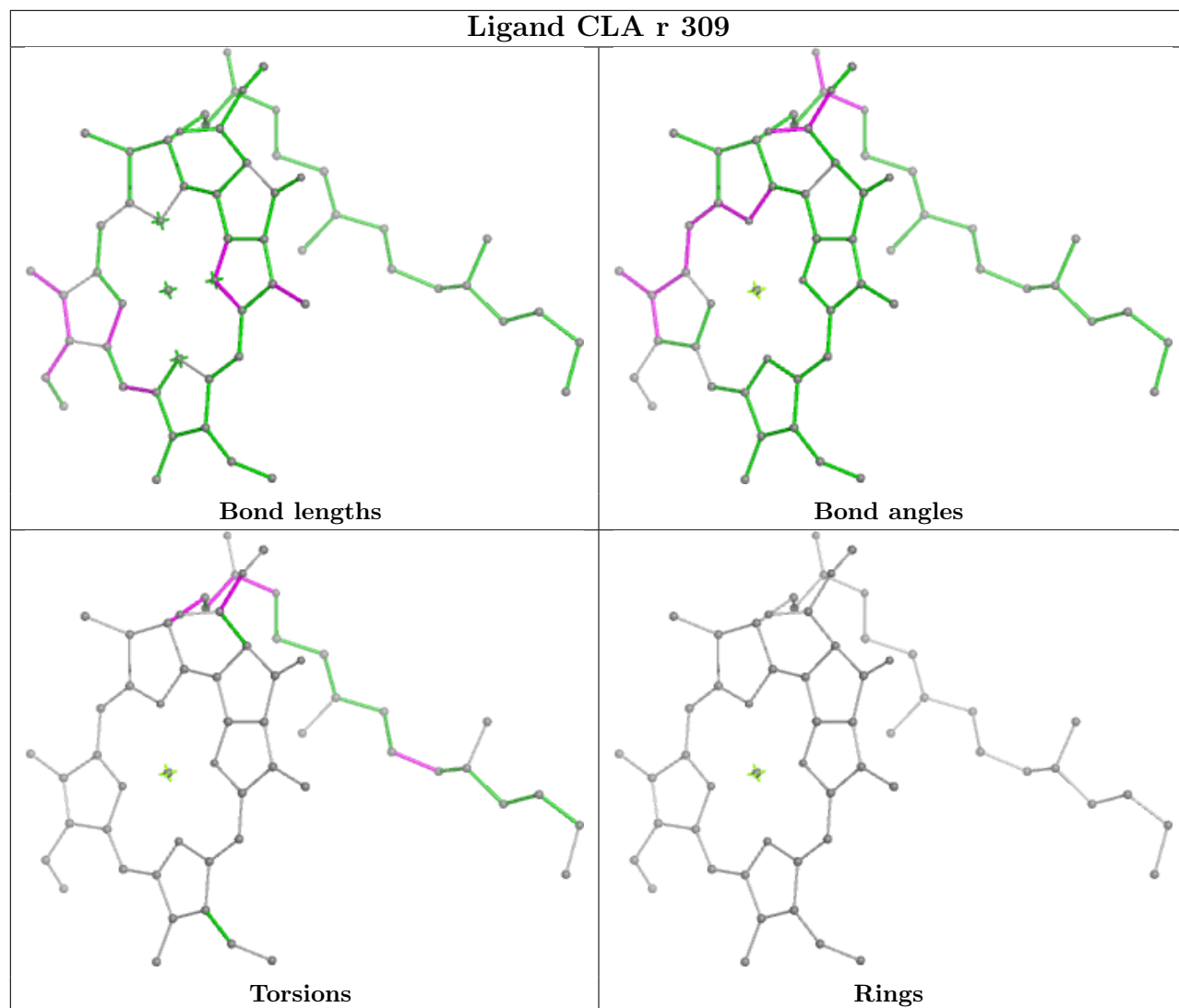
## Ligand CLA C 504

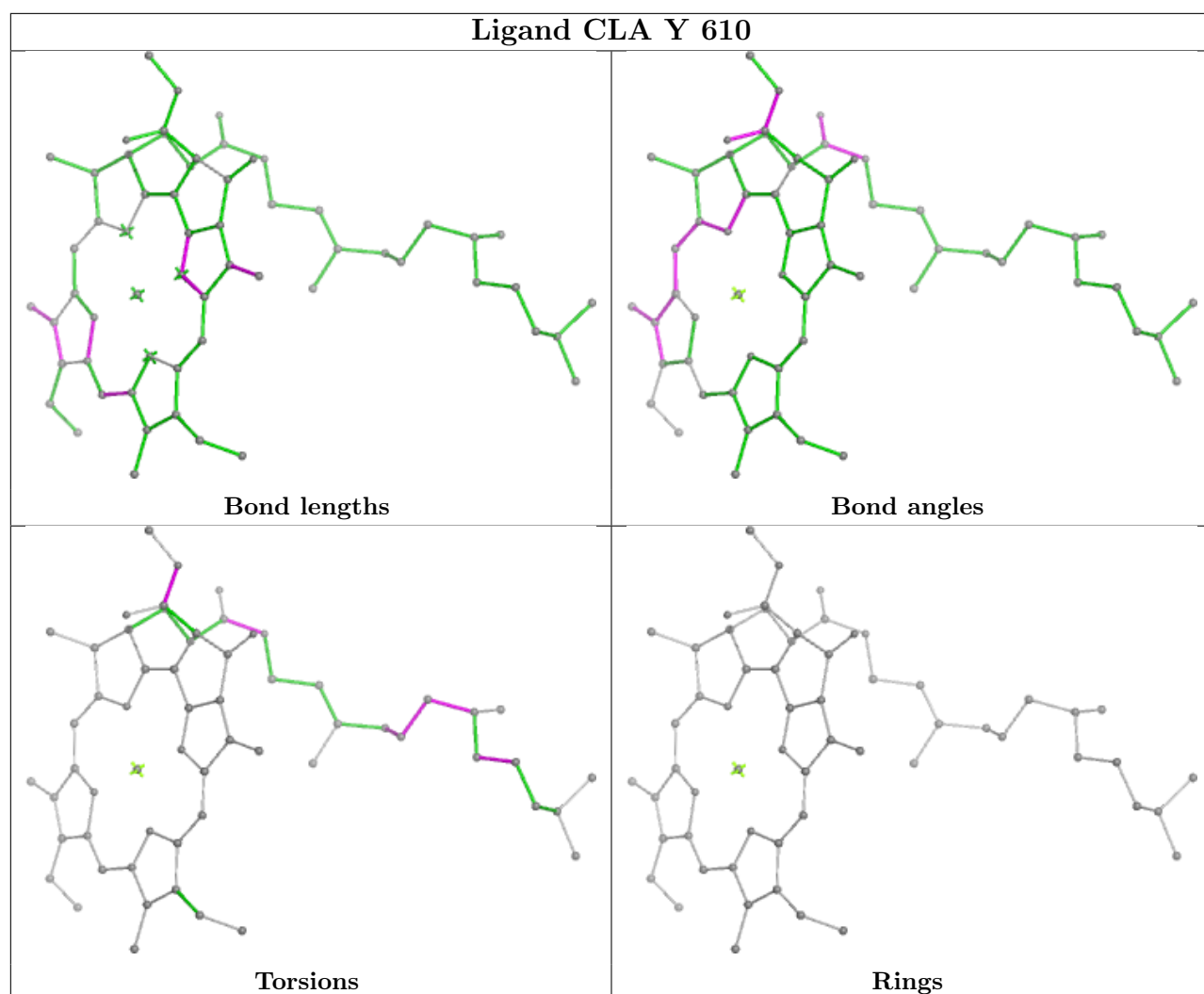


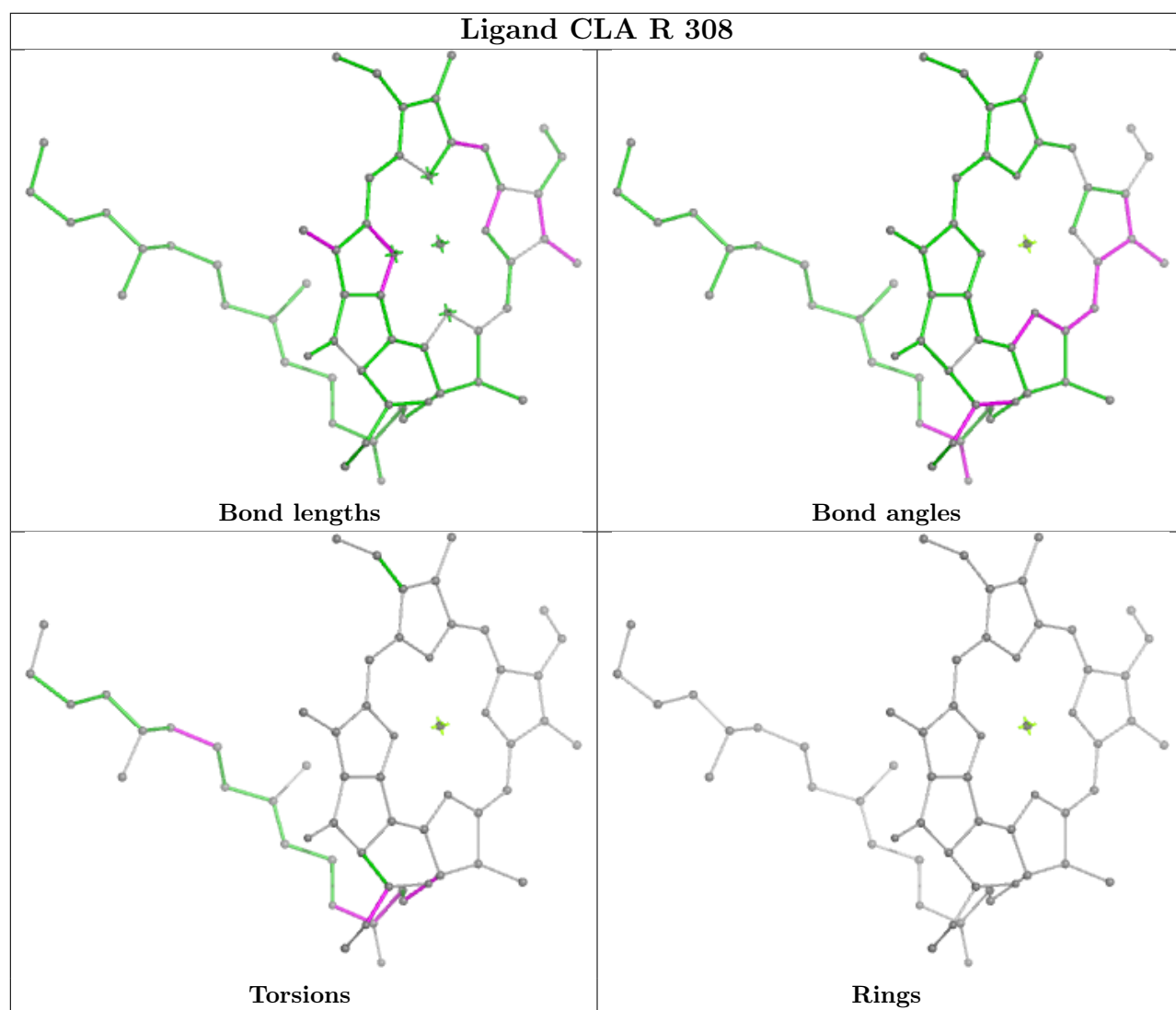


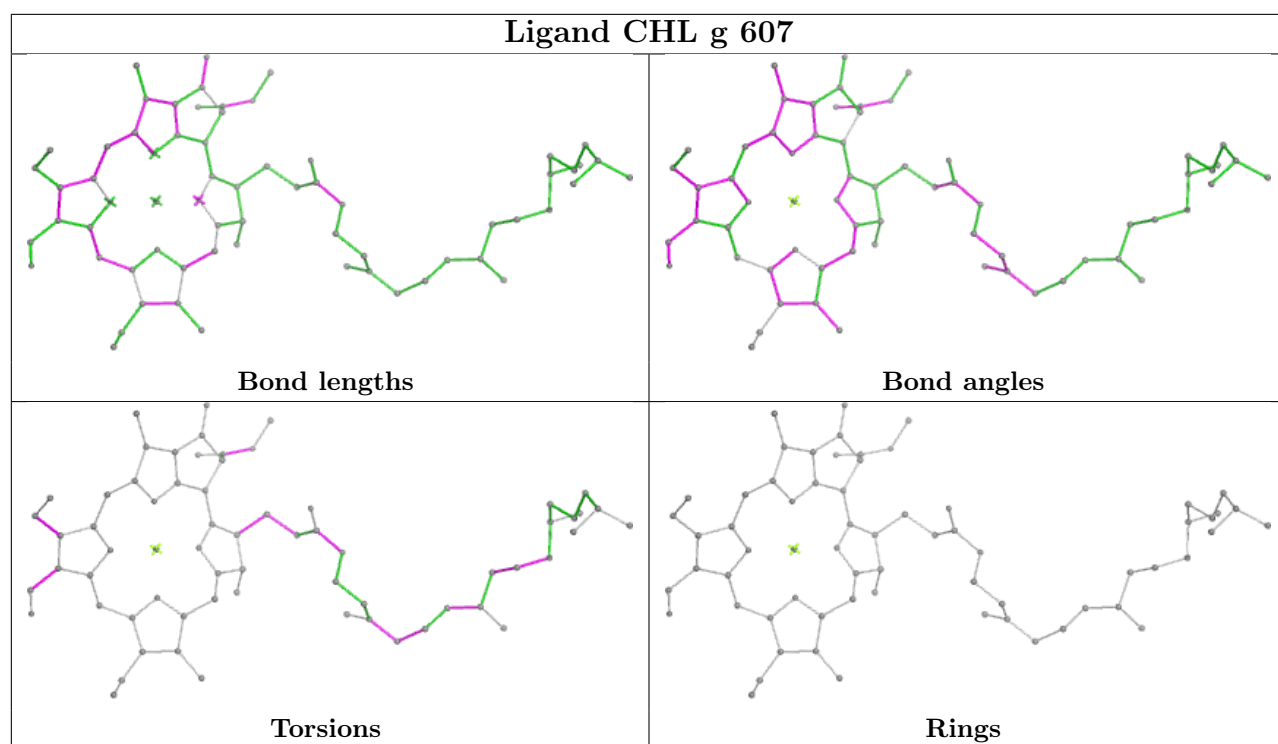


## Ligand CLA r 309

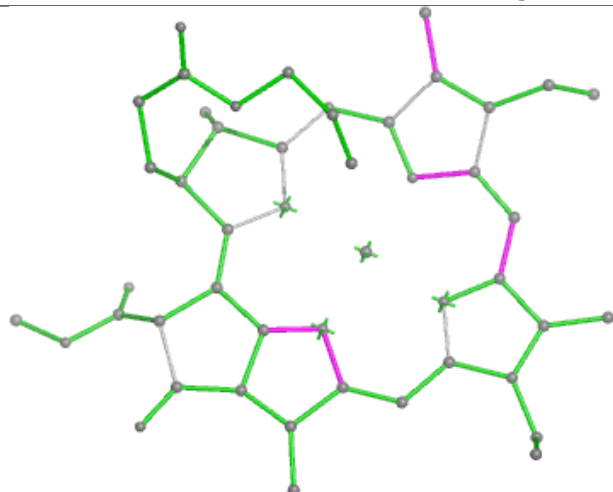




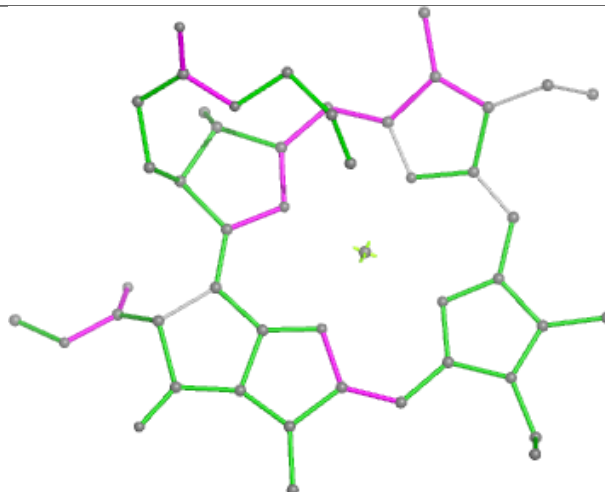




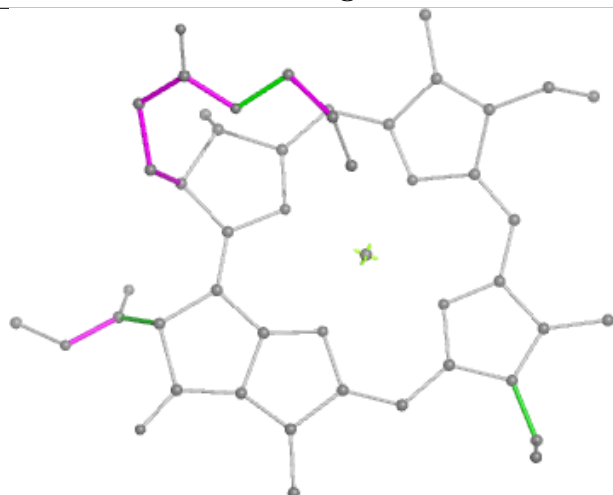
## Ligand CLA G 614



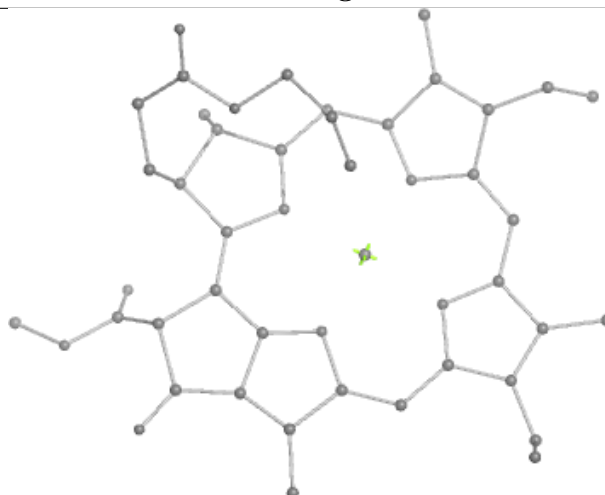
Bond lengths



Bond angles

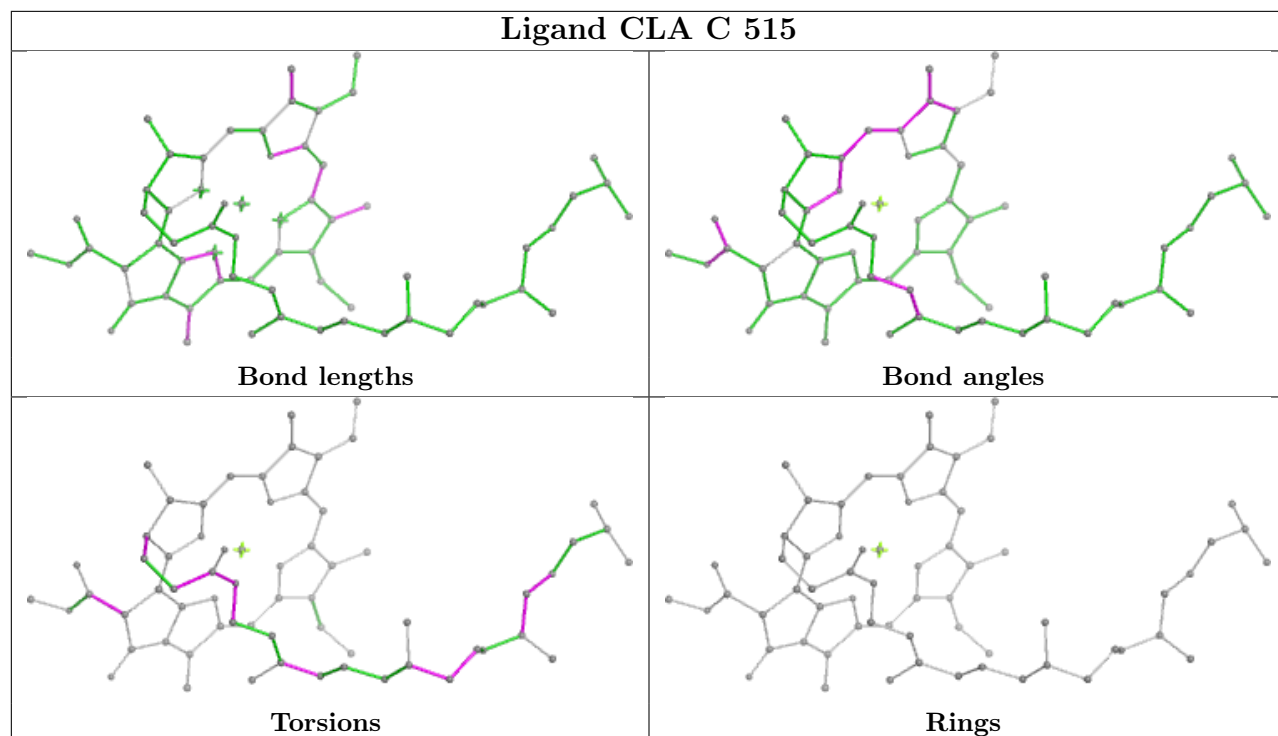


Torsions

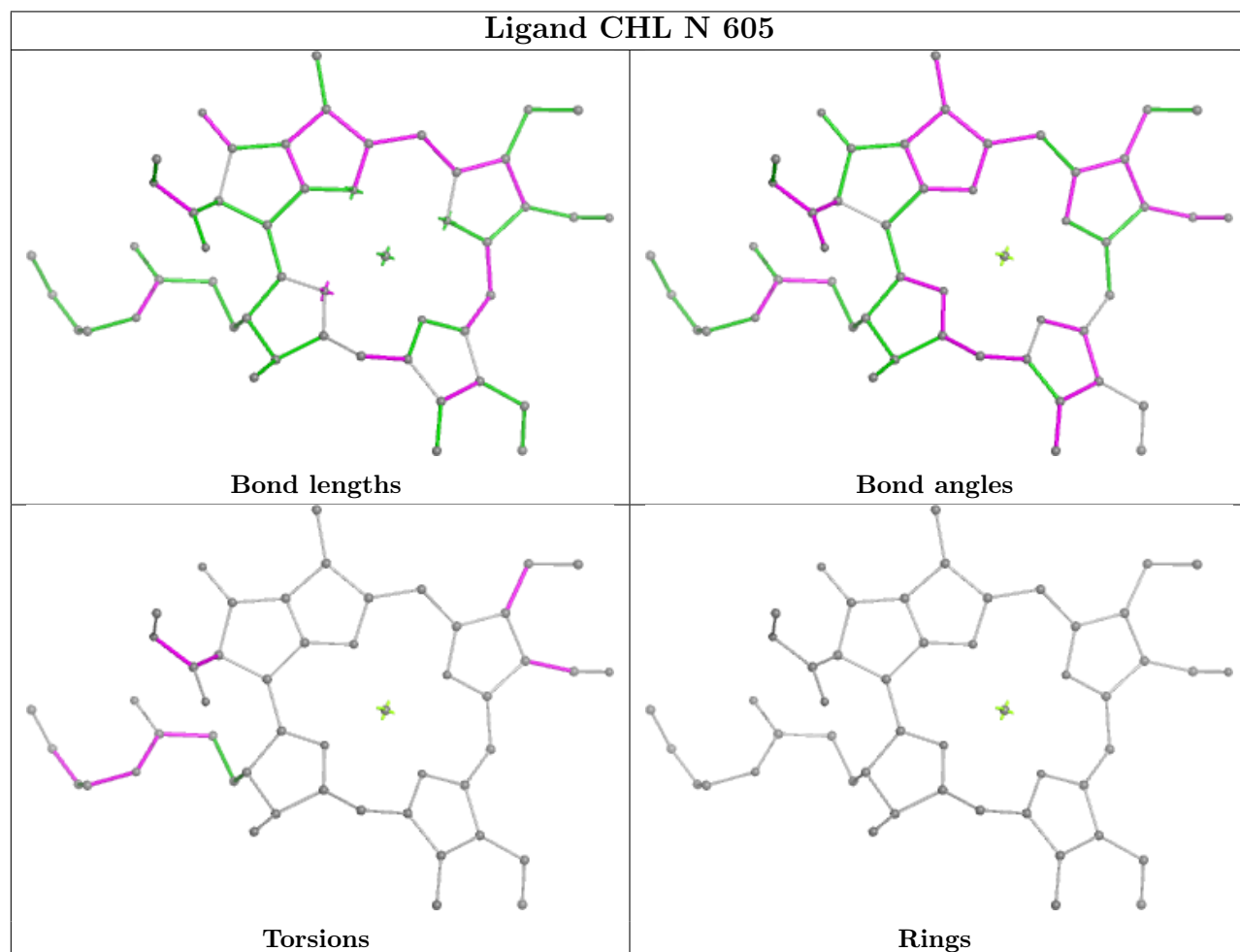


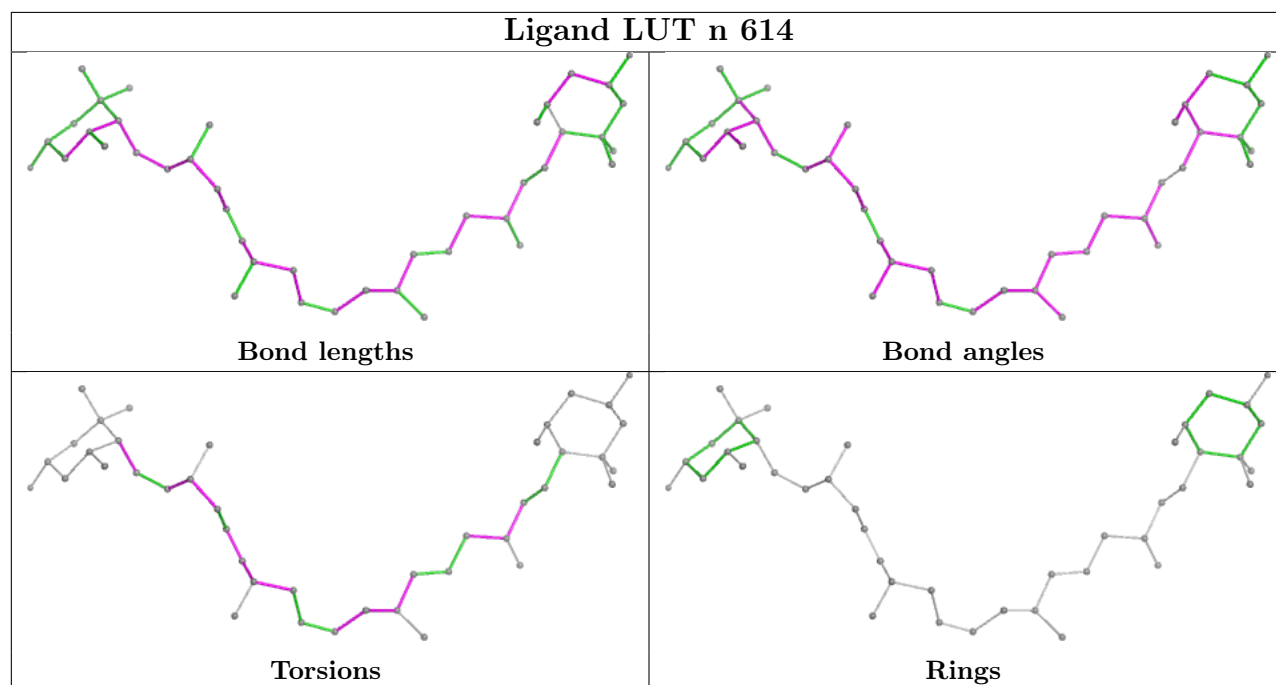
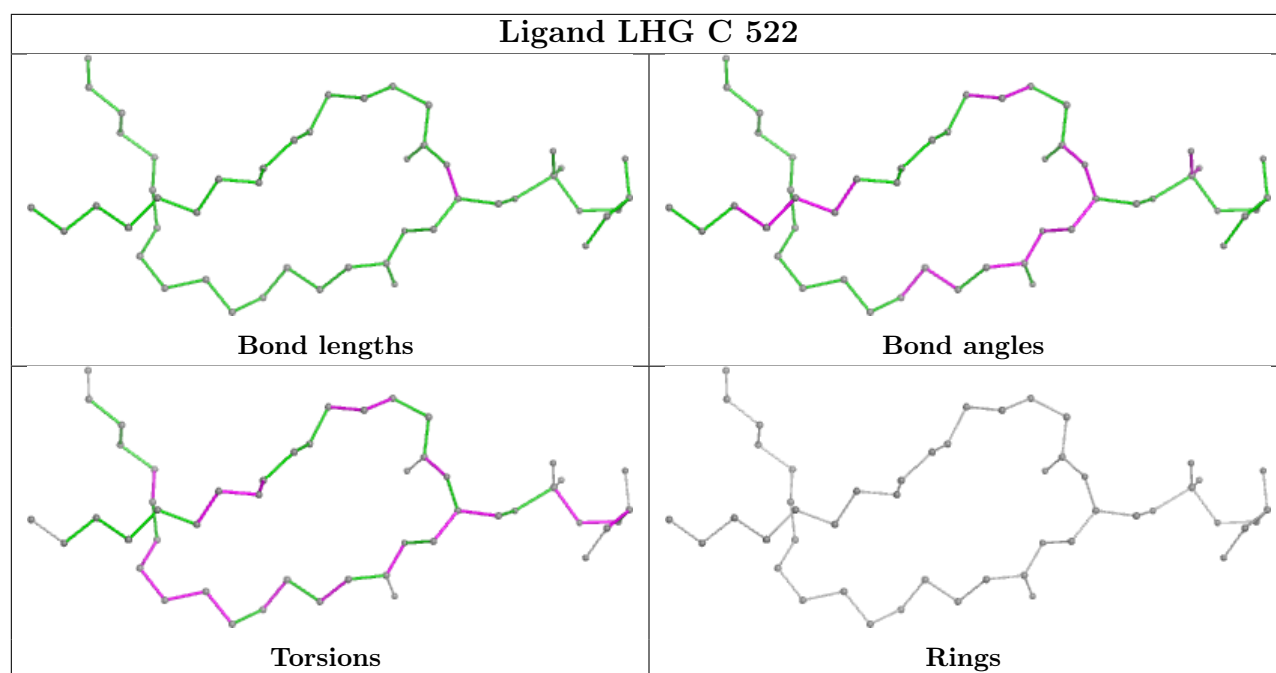
Rings

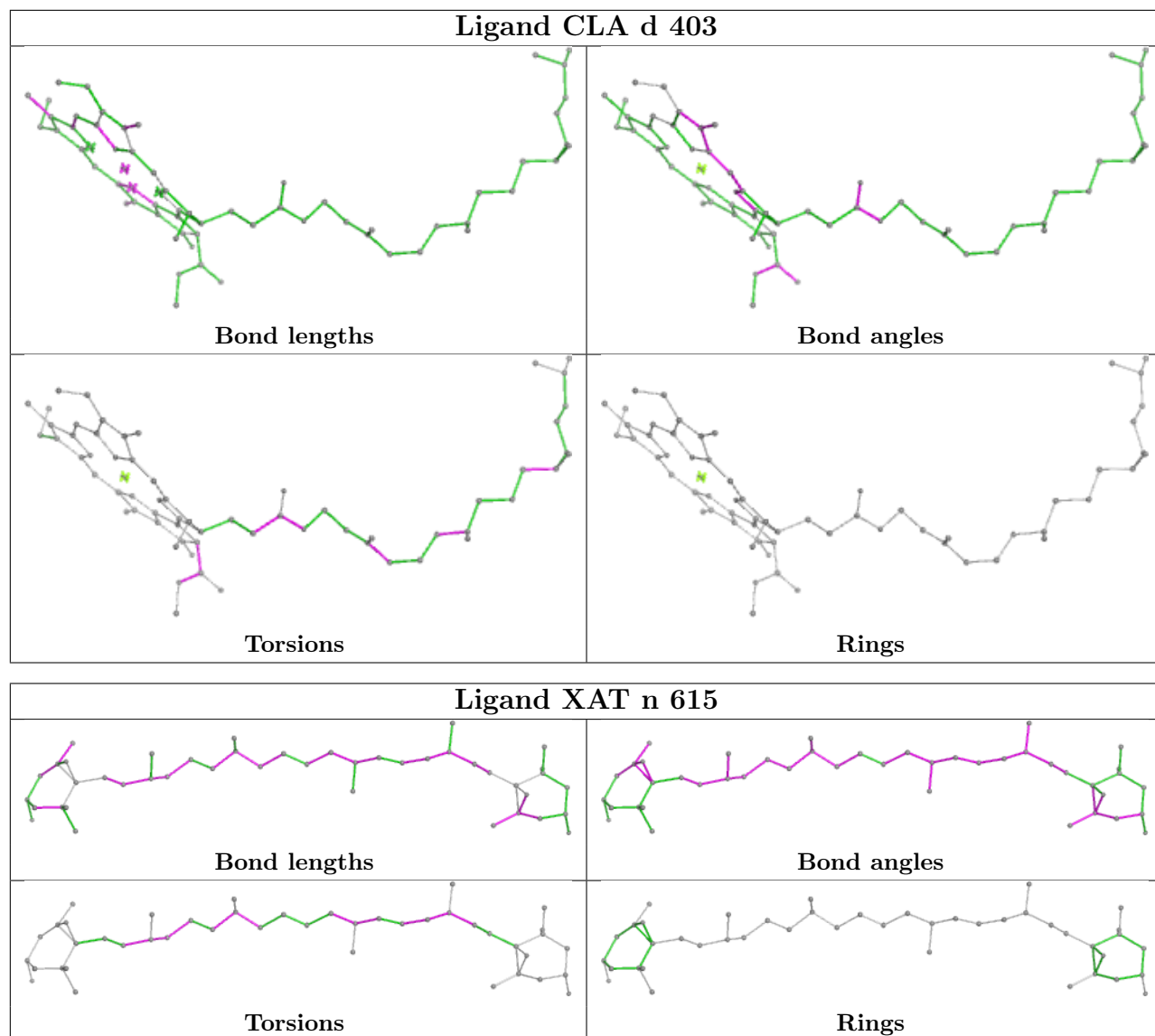
## Ligand CLA C 515

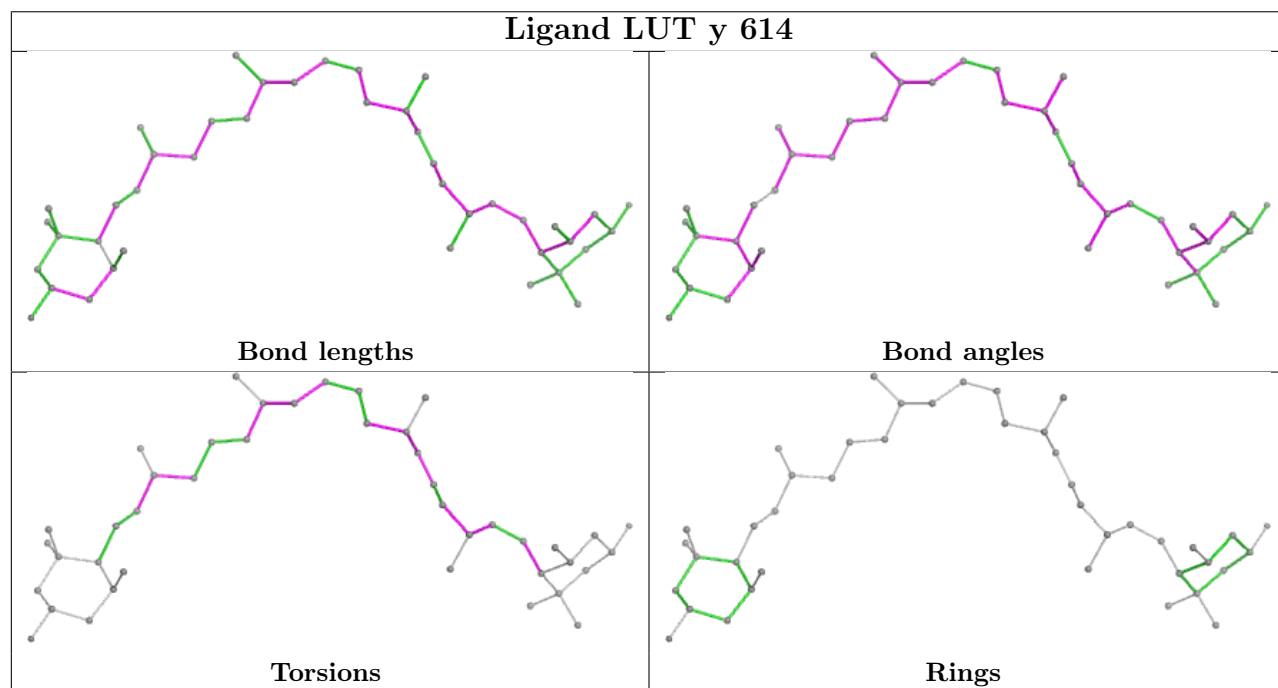
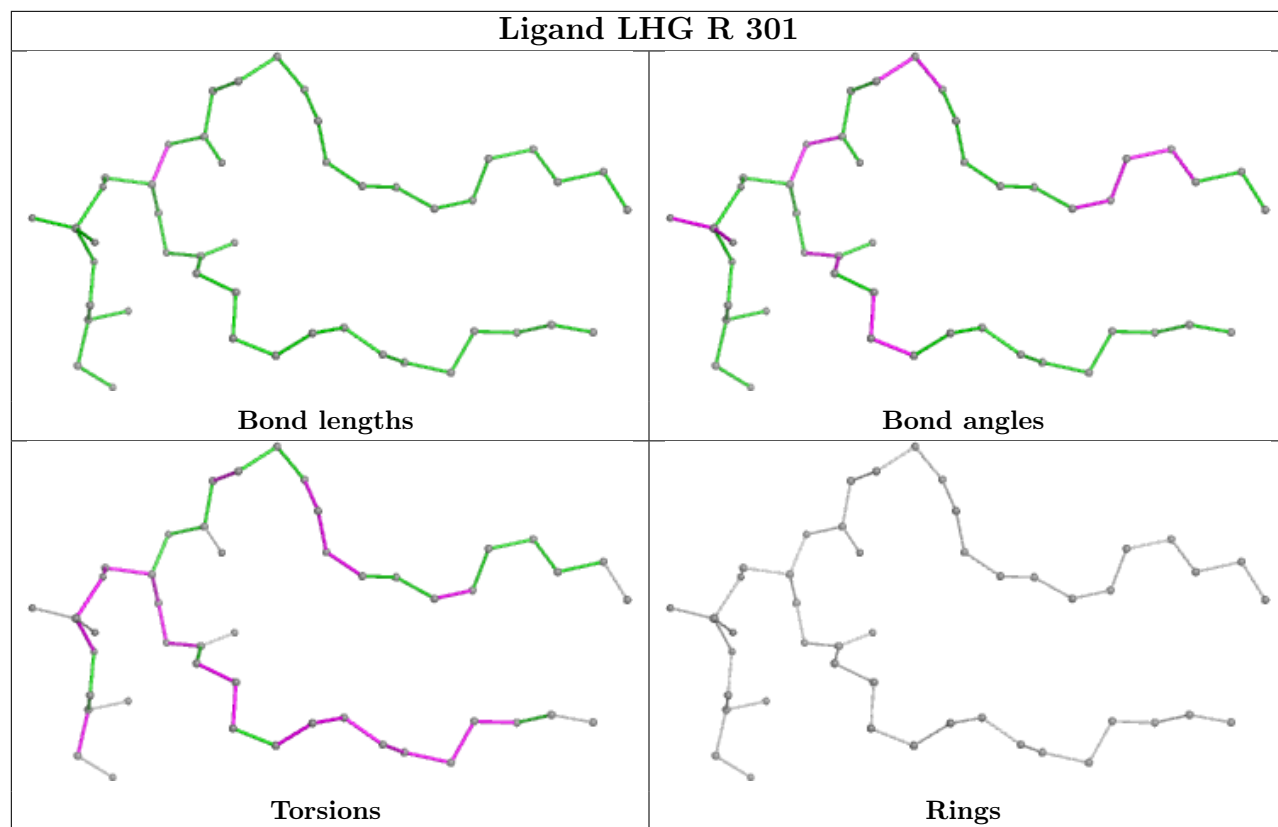


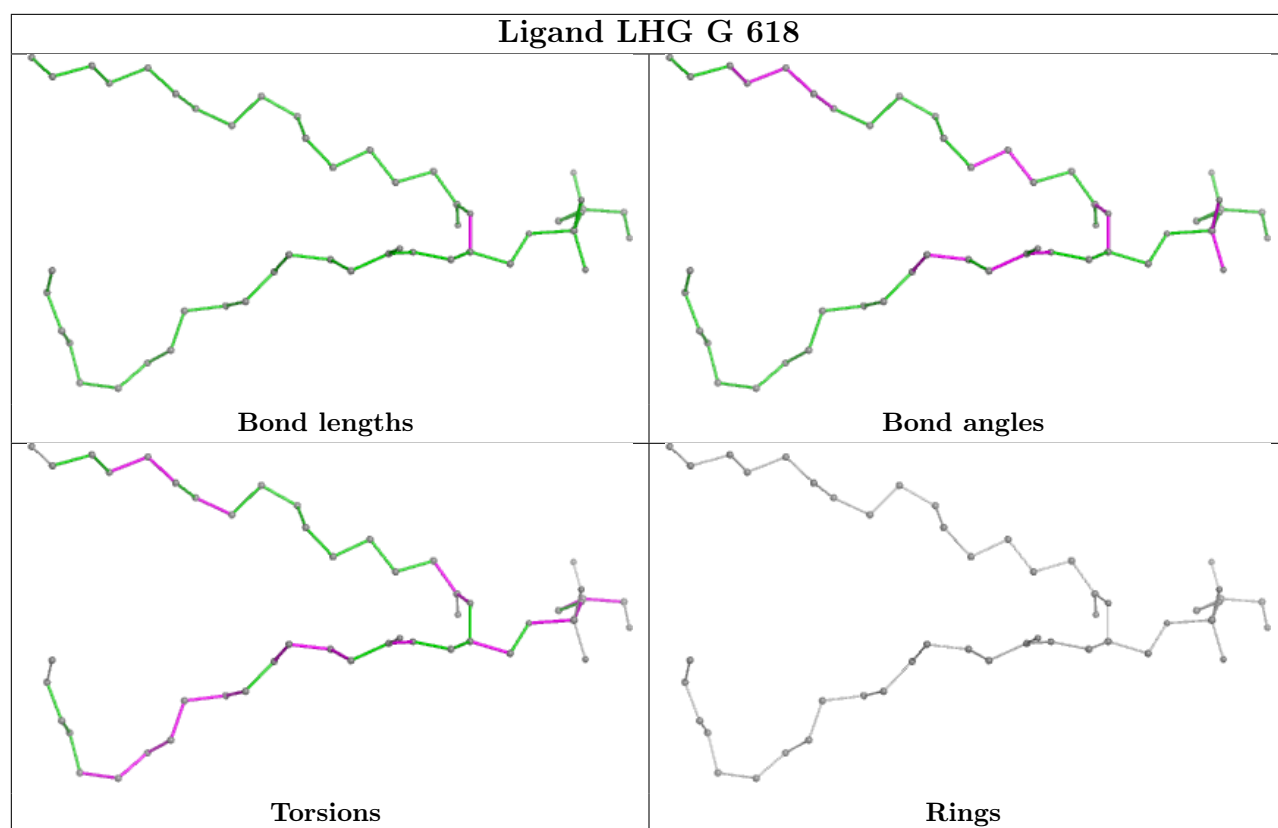
## Ligand CHL N 605



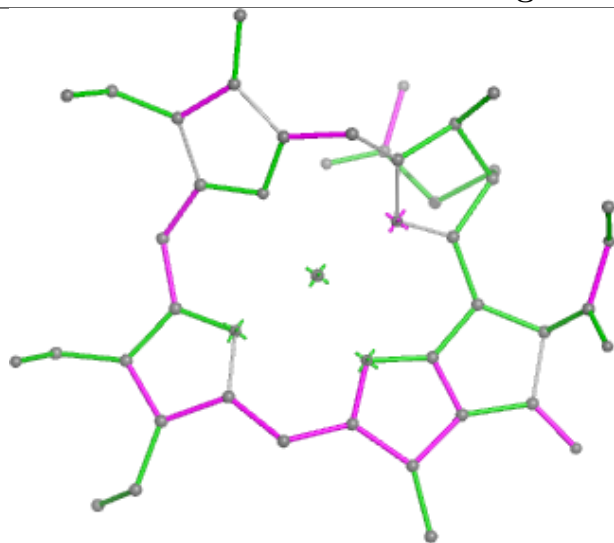




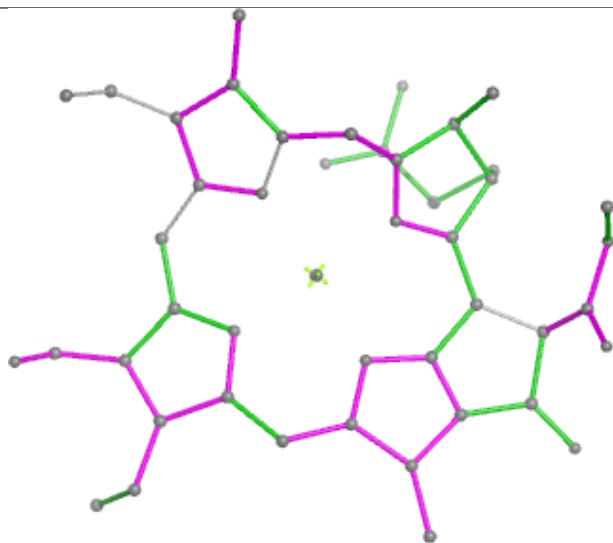




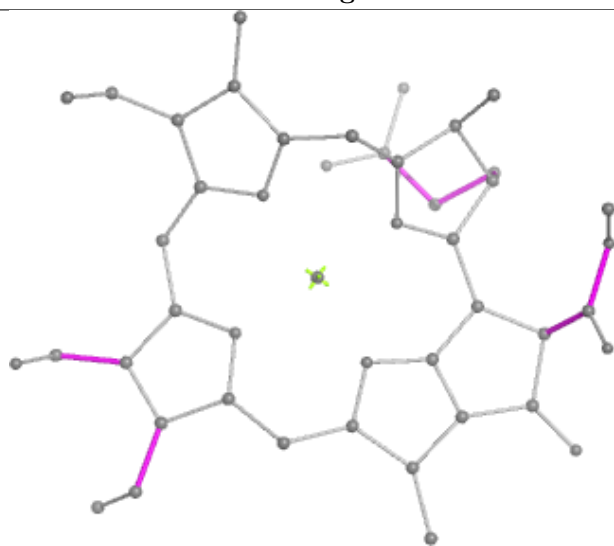
## Ligand CHL S 307



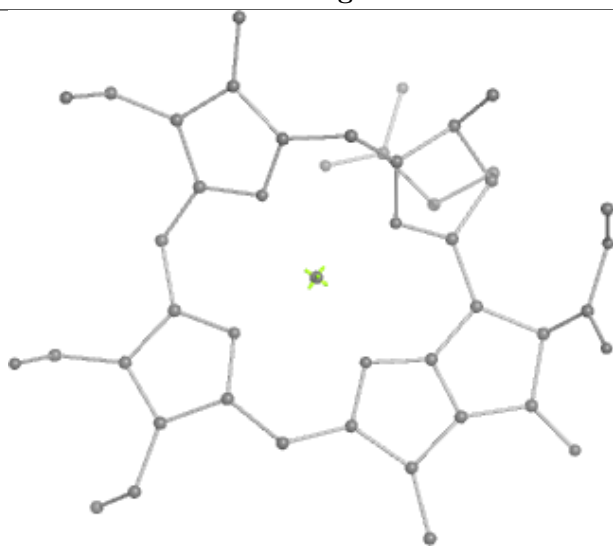
Bond lengths



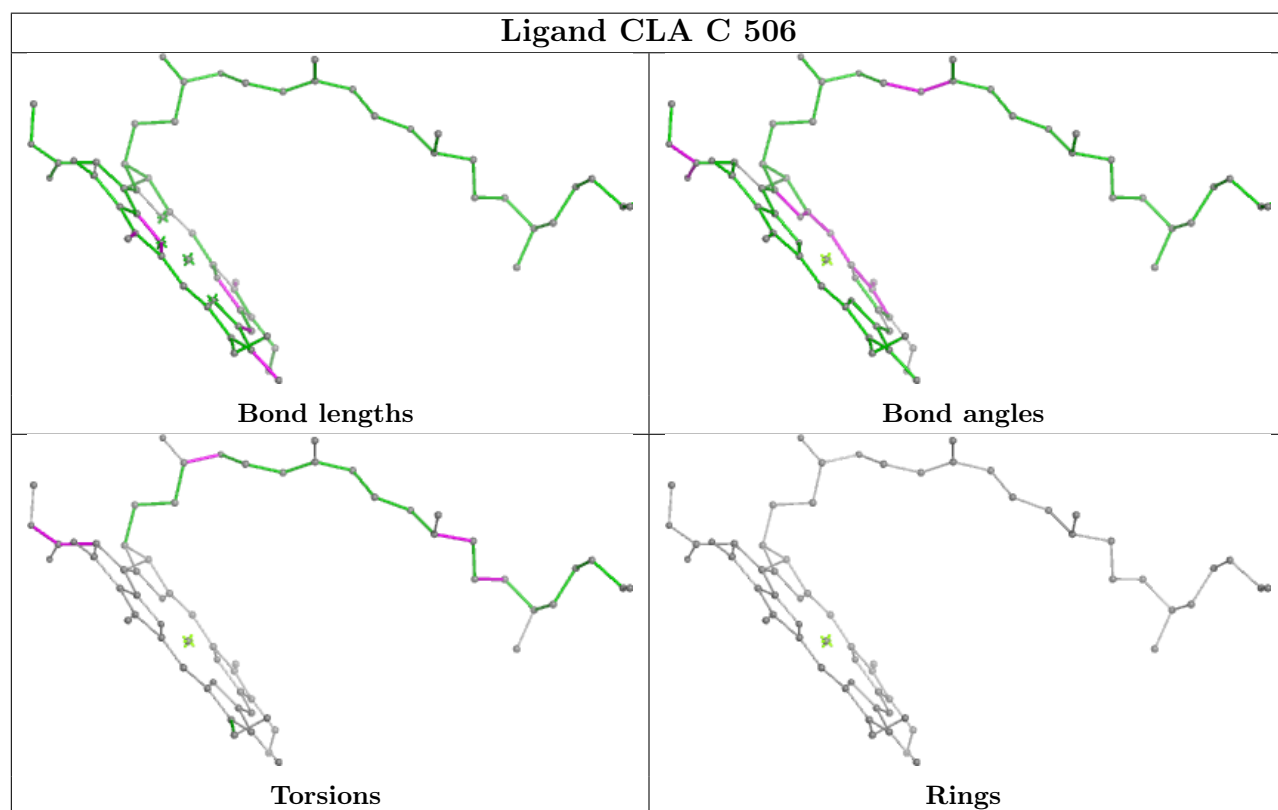
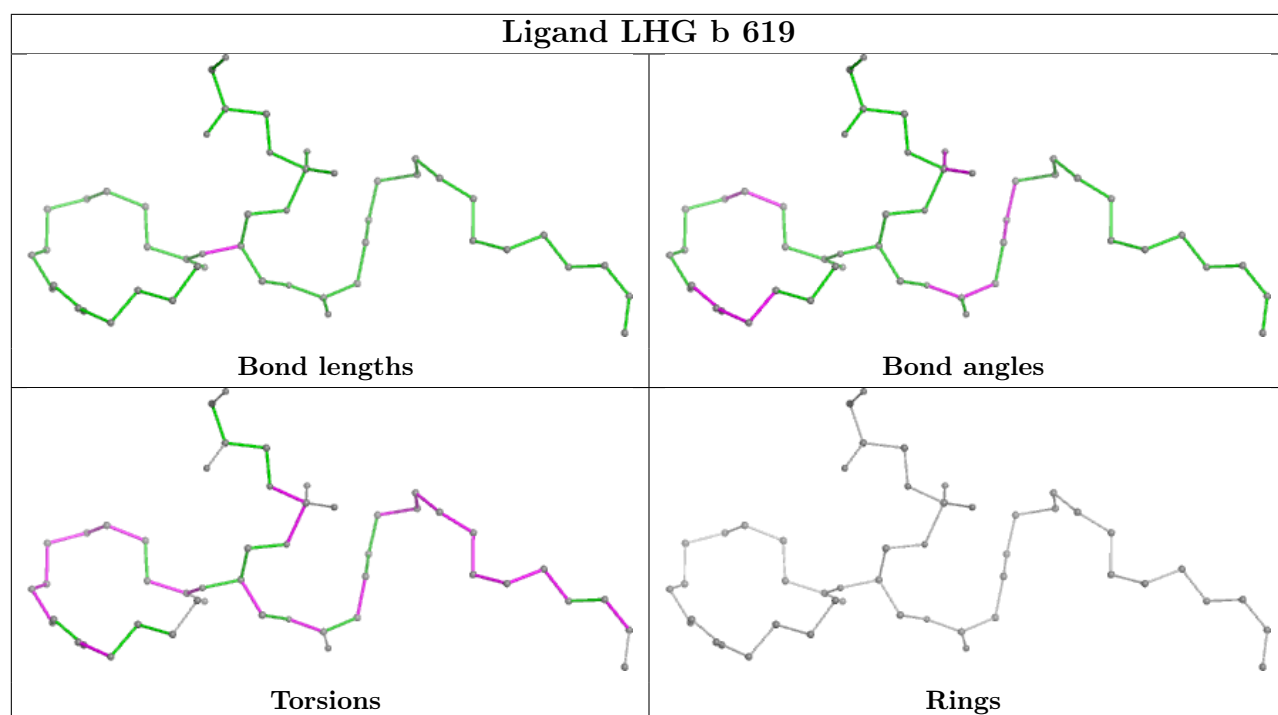
Bond angles



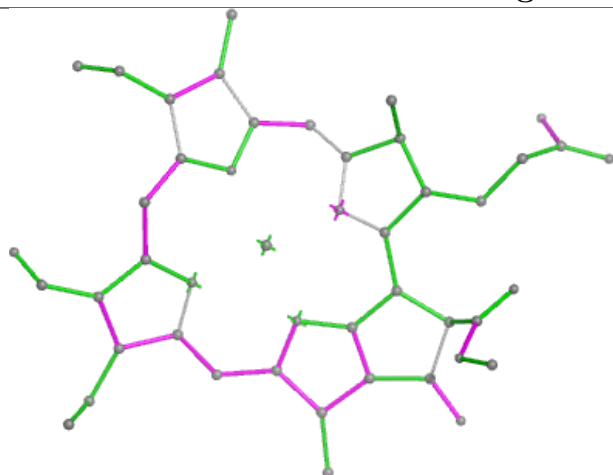
Torsions



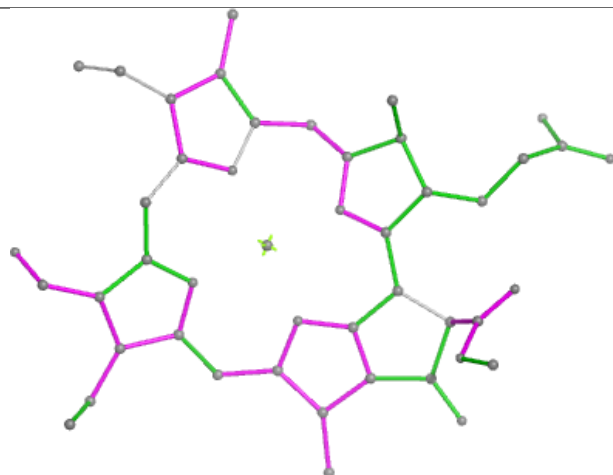
Rings



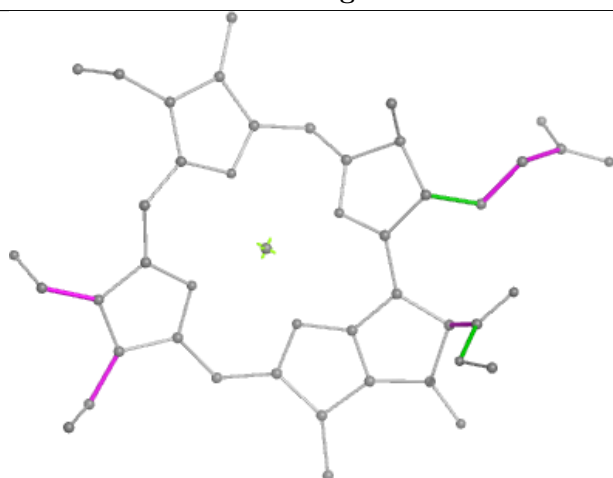
## Ligand CHL S 306



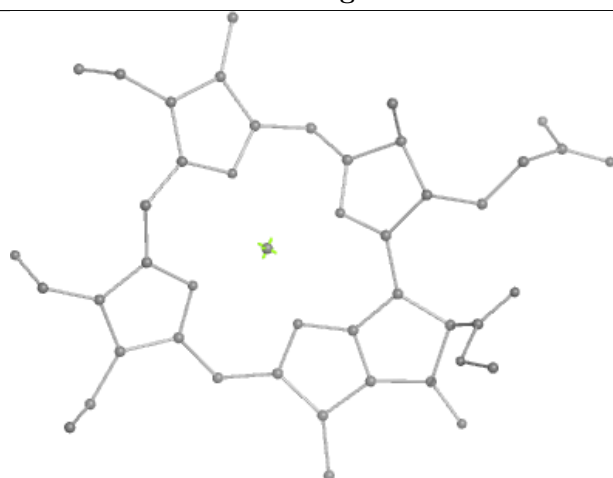
Bond lengths



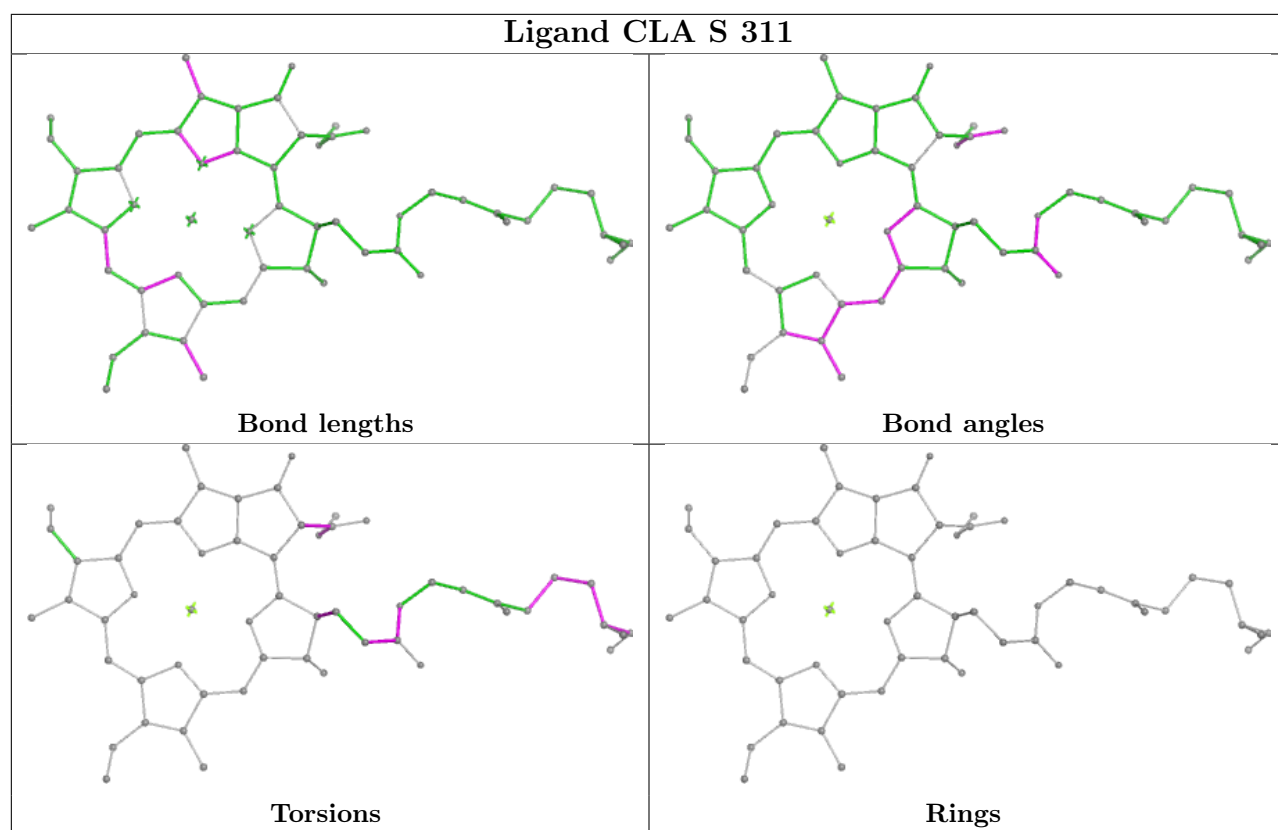
Bond angles

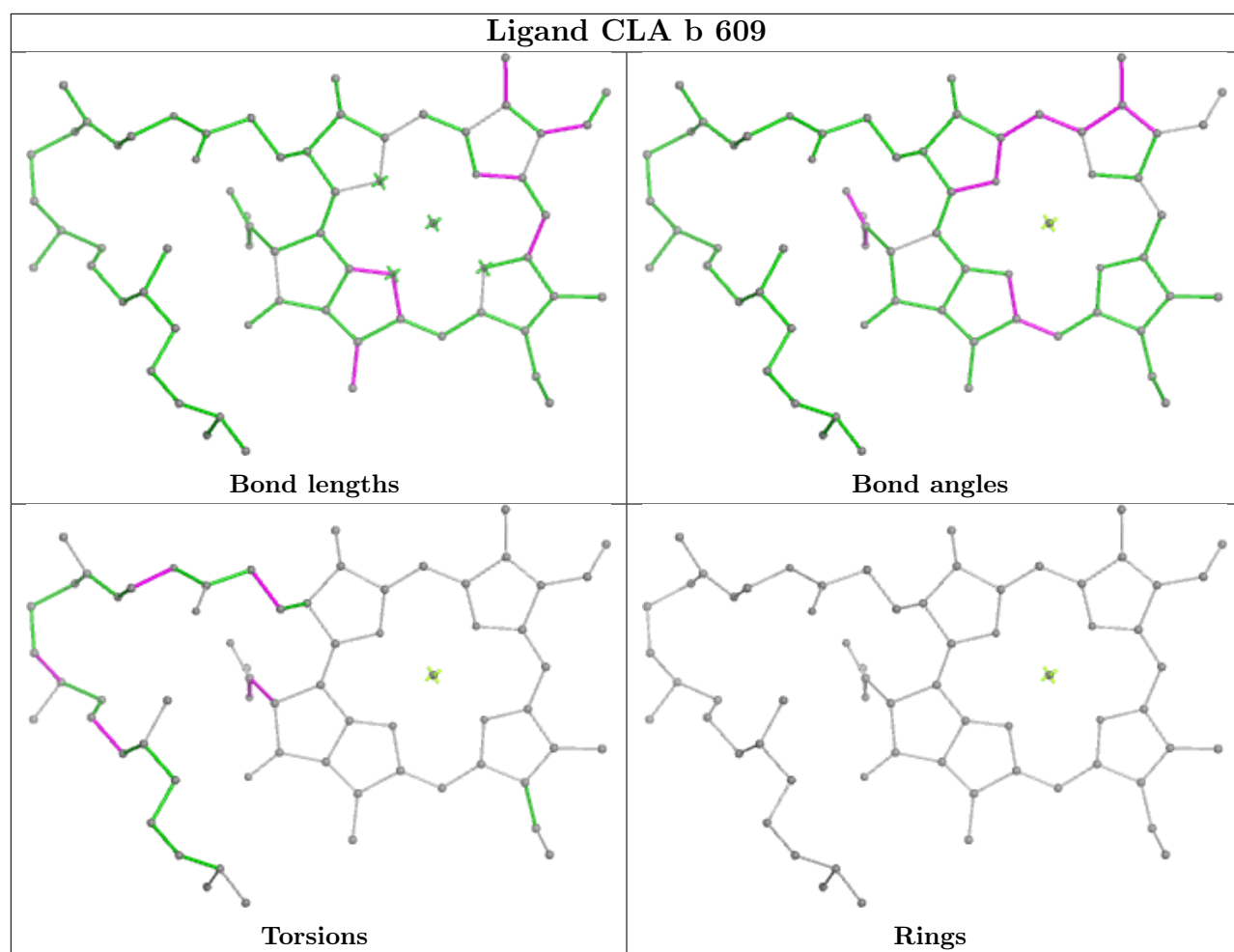


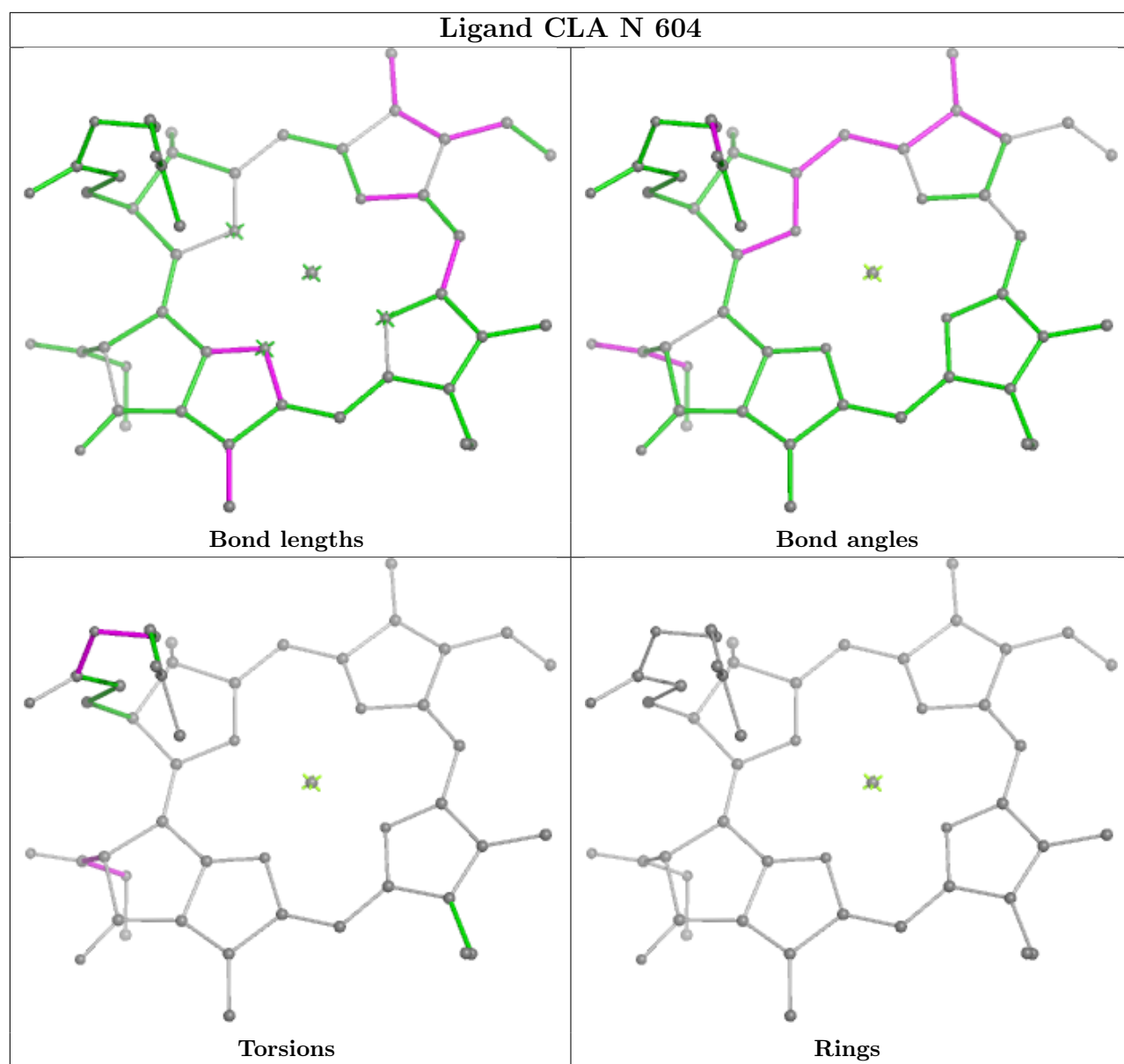
Torsions



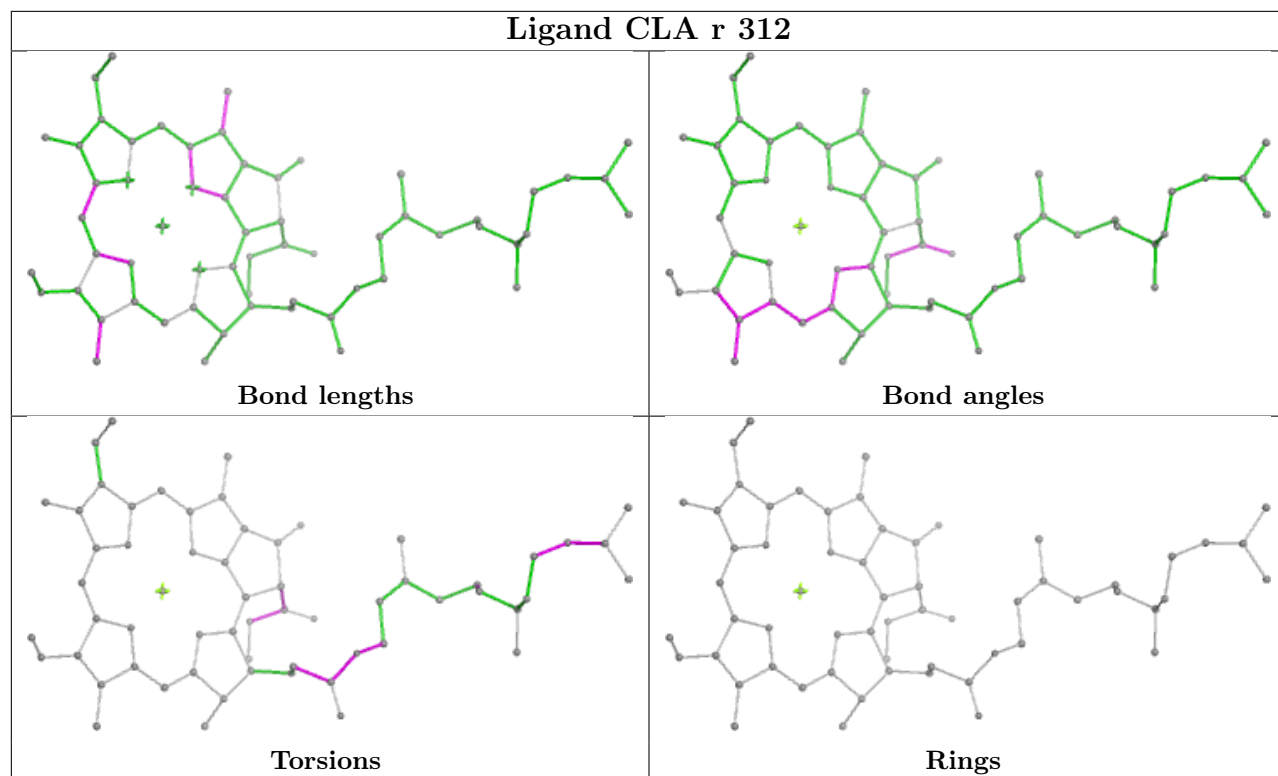
Rings



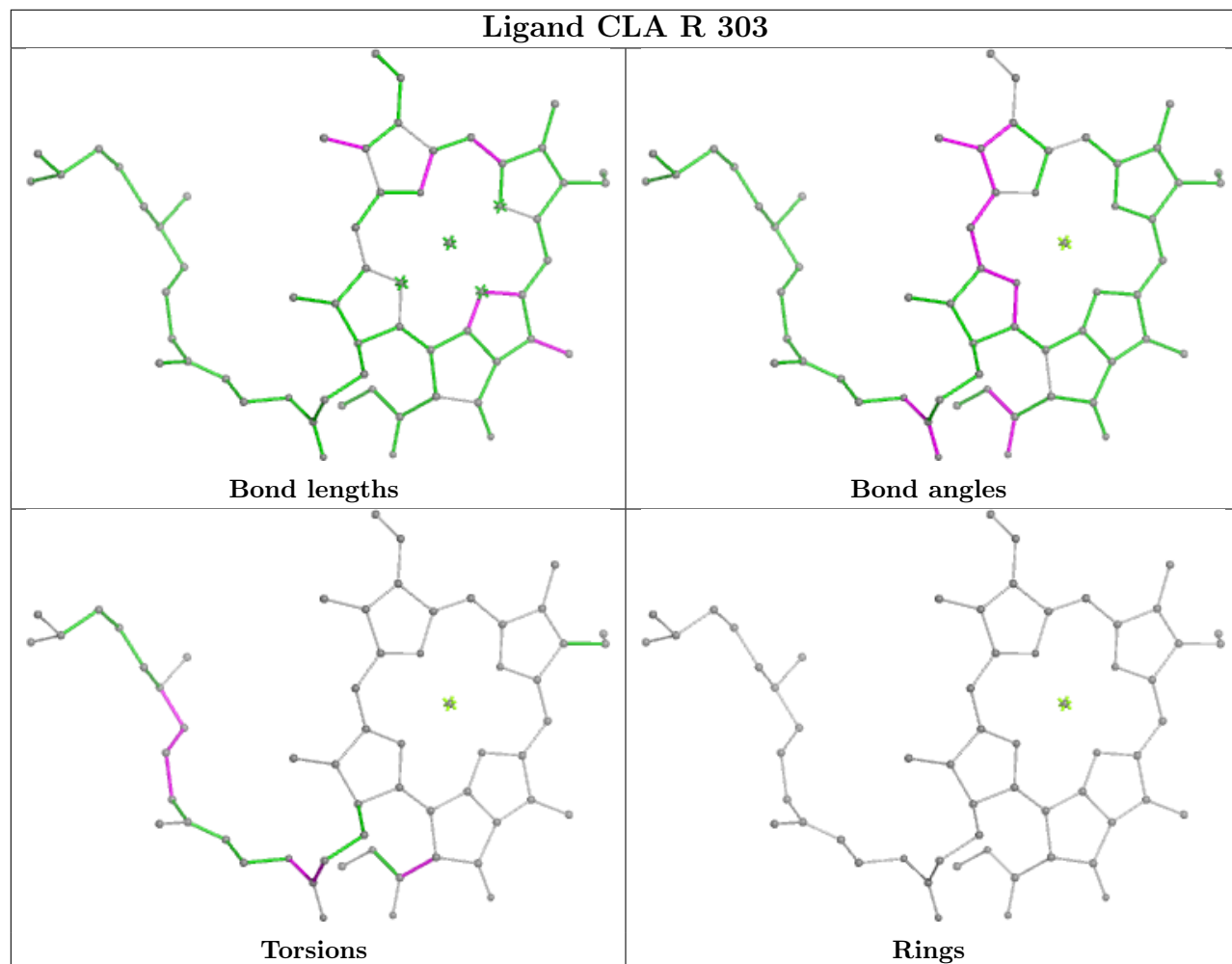




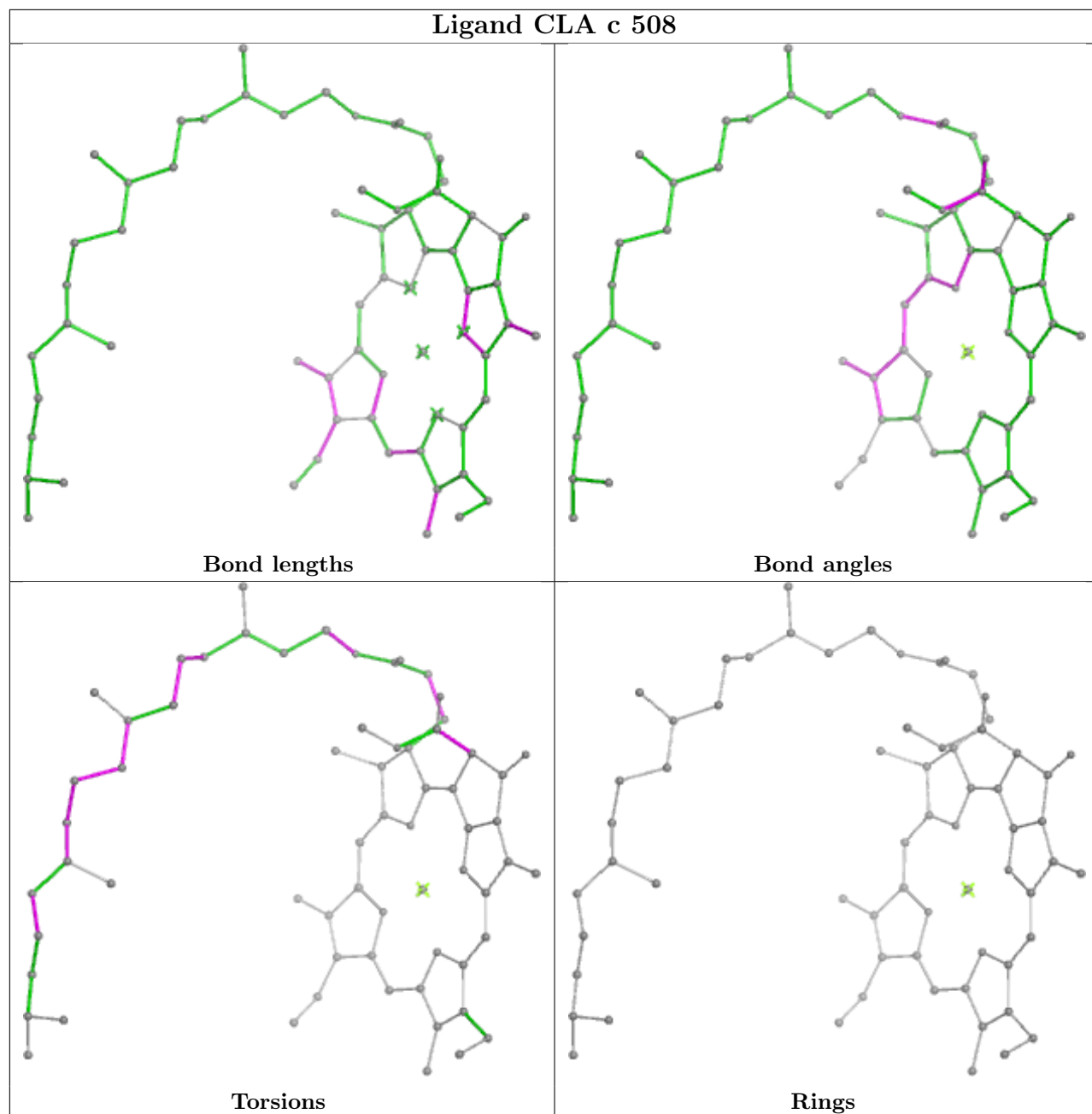
## Ligand CLA r 312



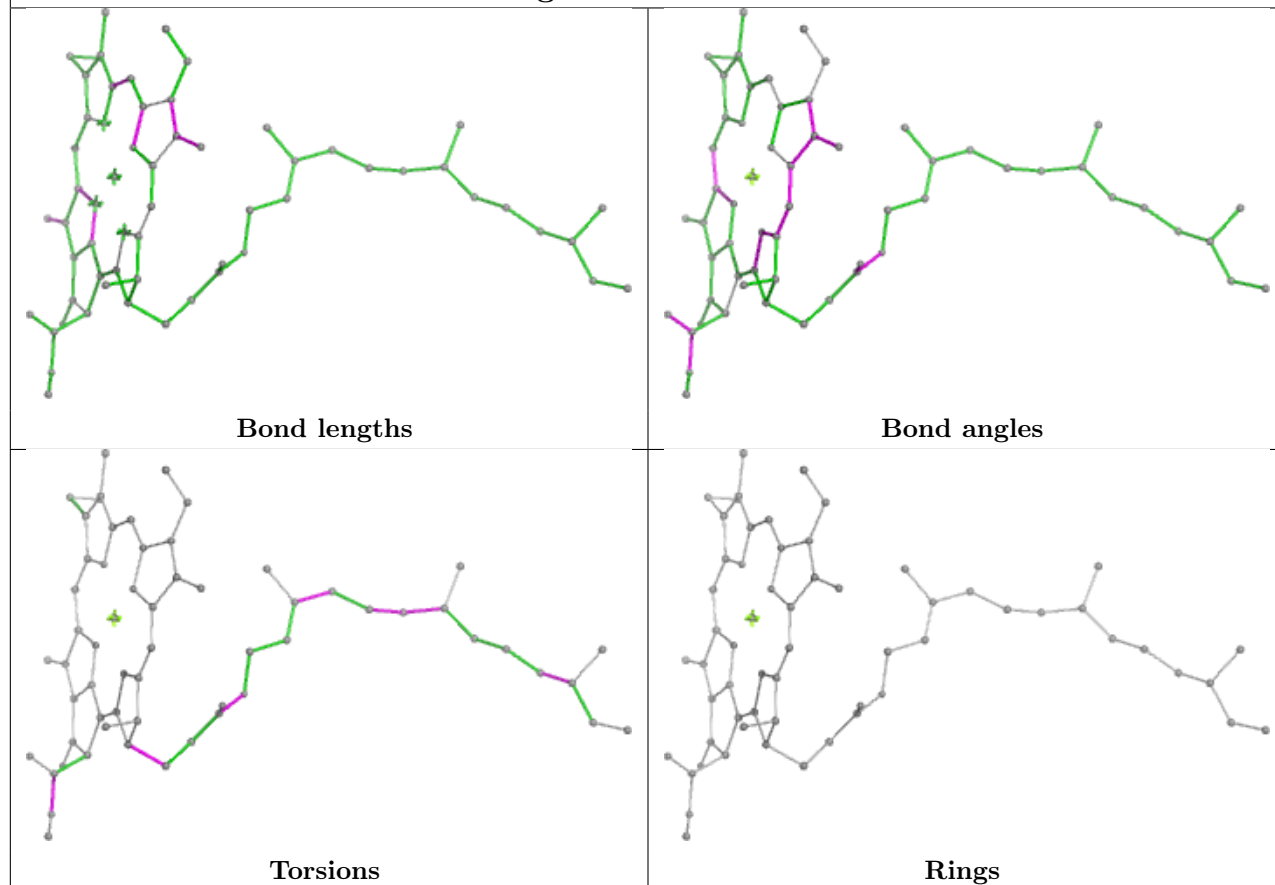
## Ligand CLA R 303



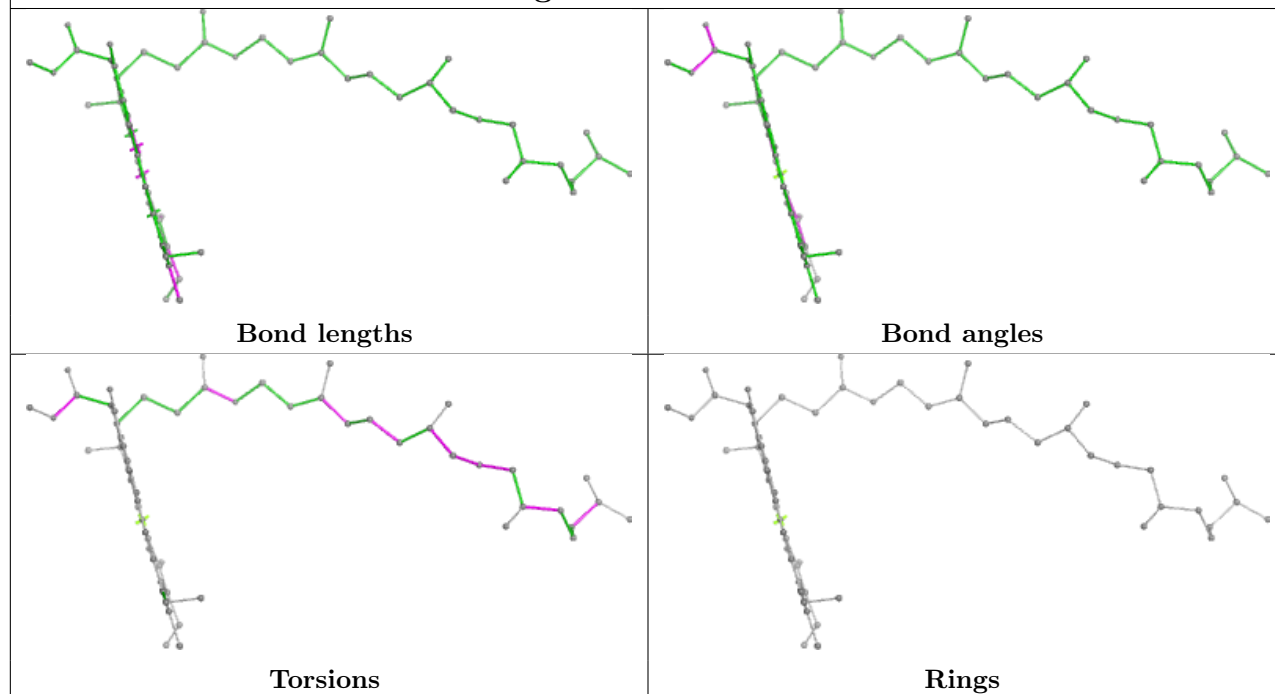
## Ligand CLA c 508

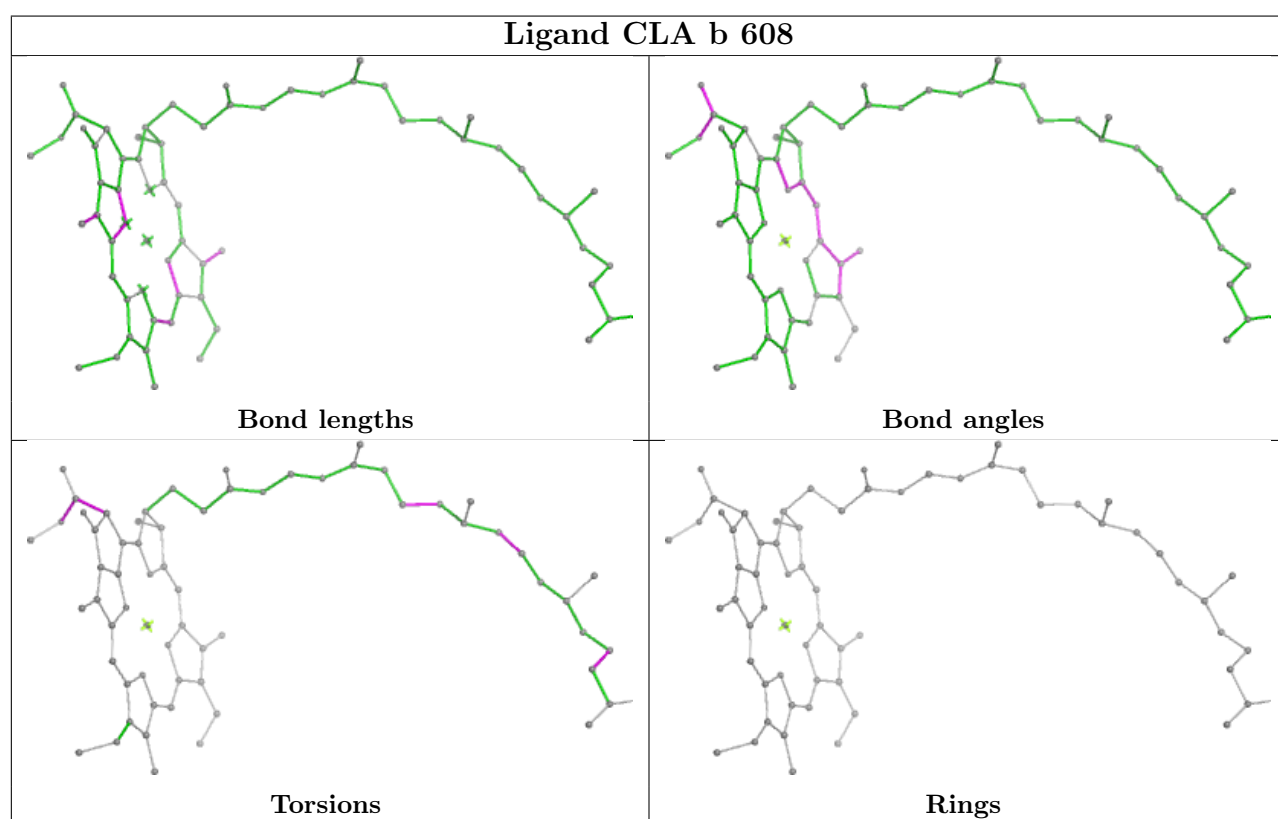
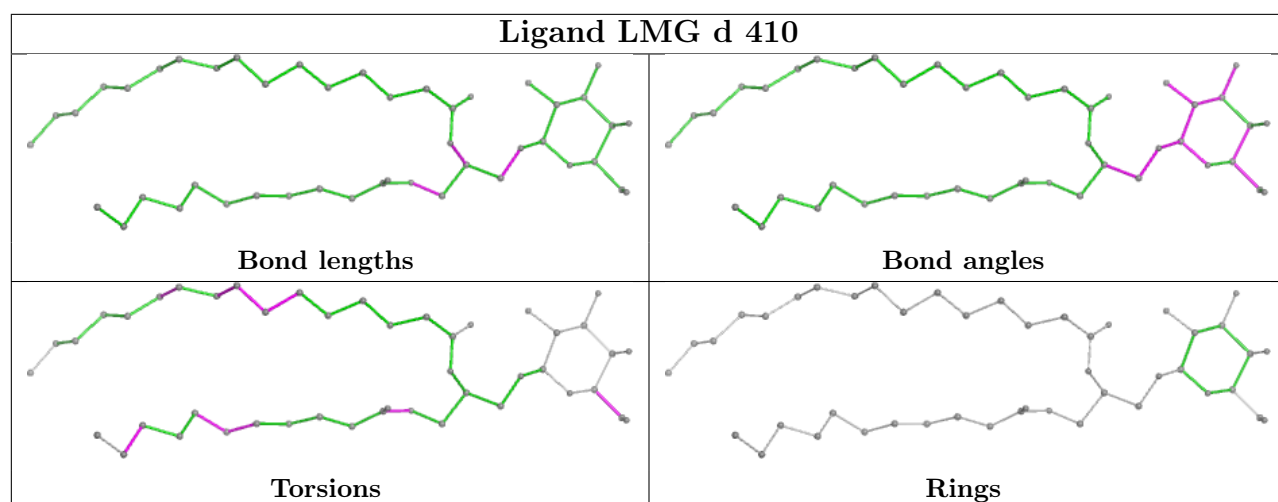


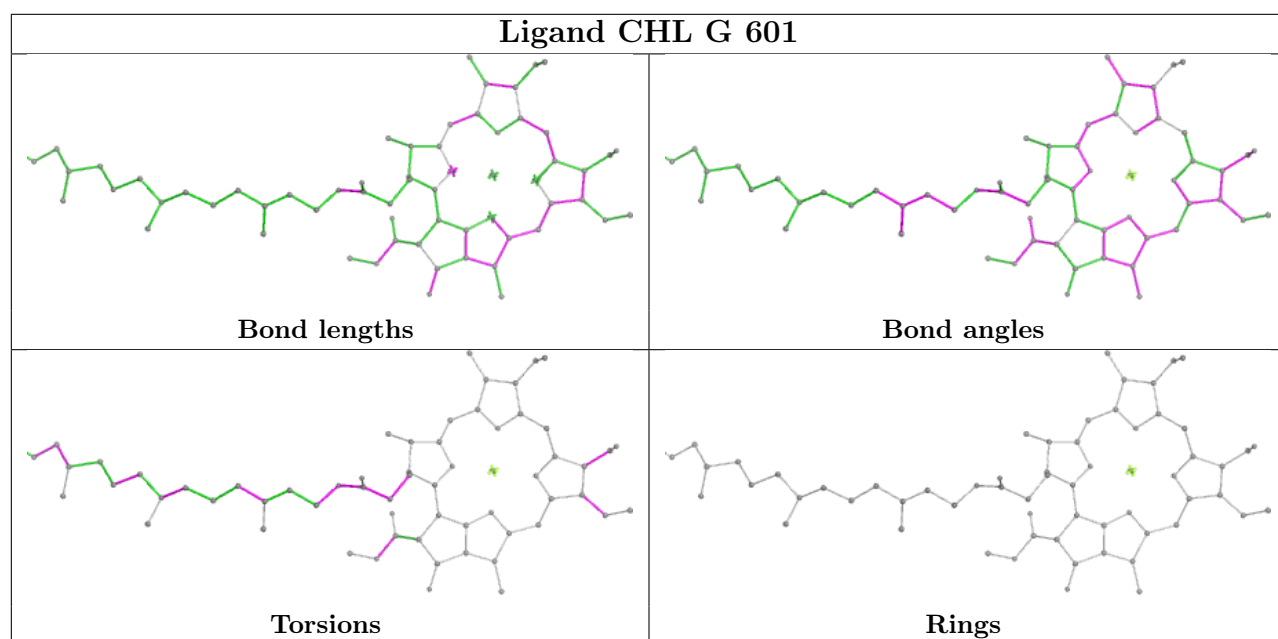
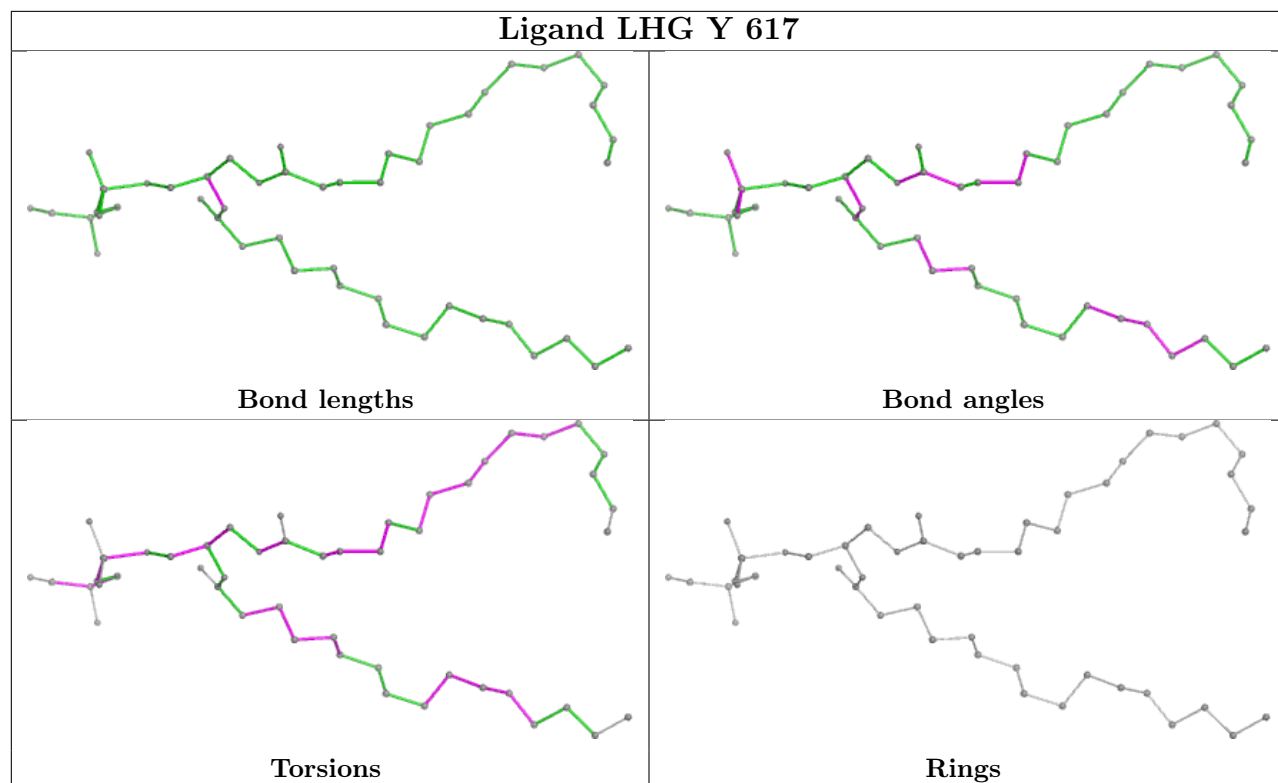
## Ligand CLA s 303

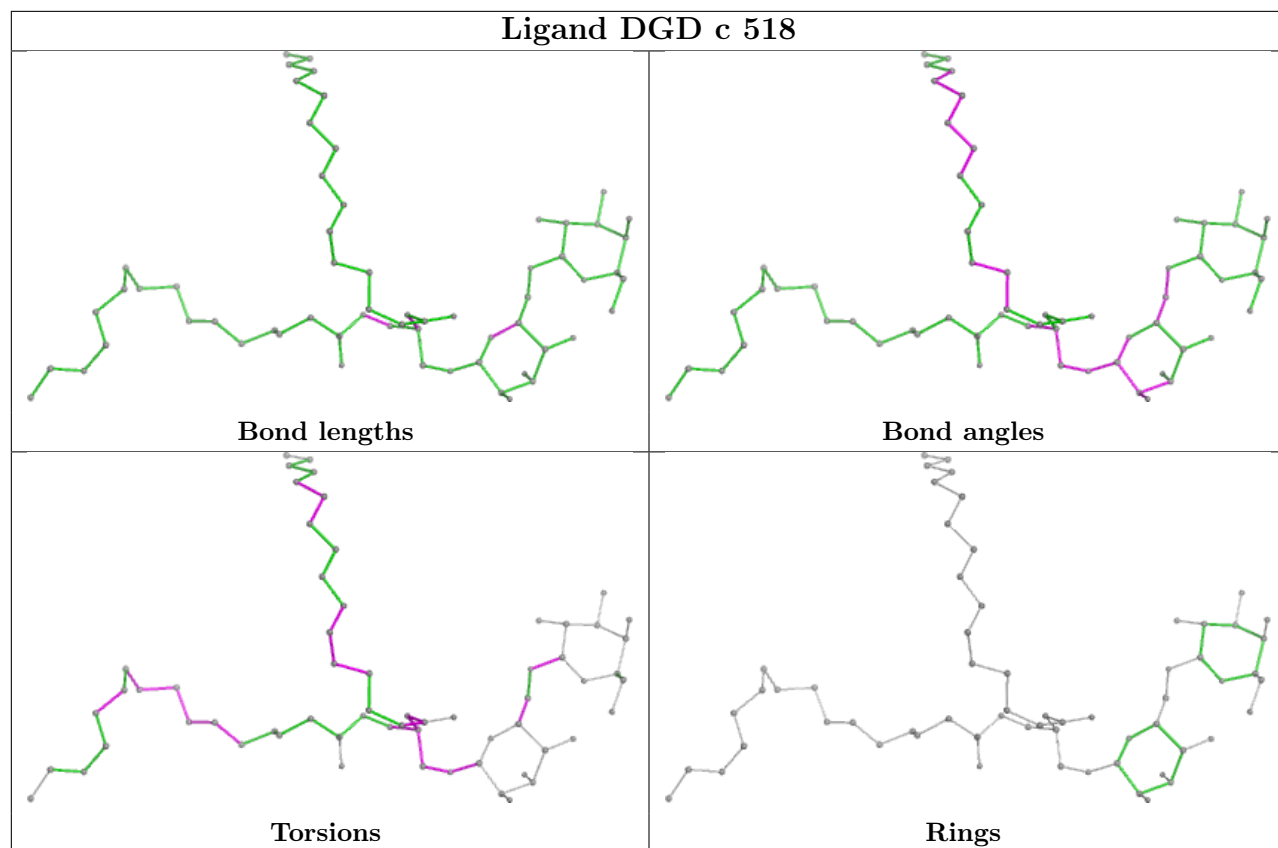


## Ligand CLA b 604

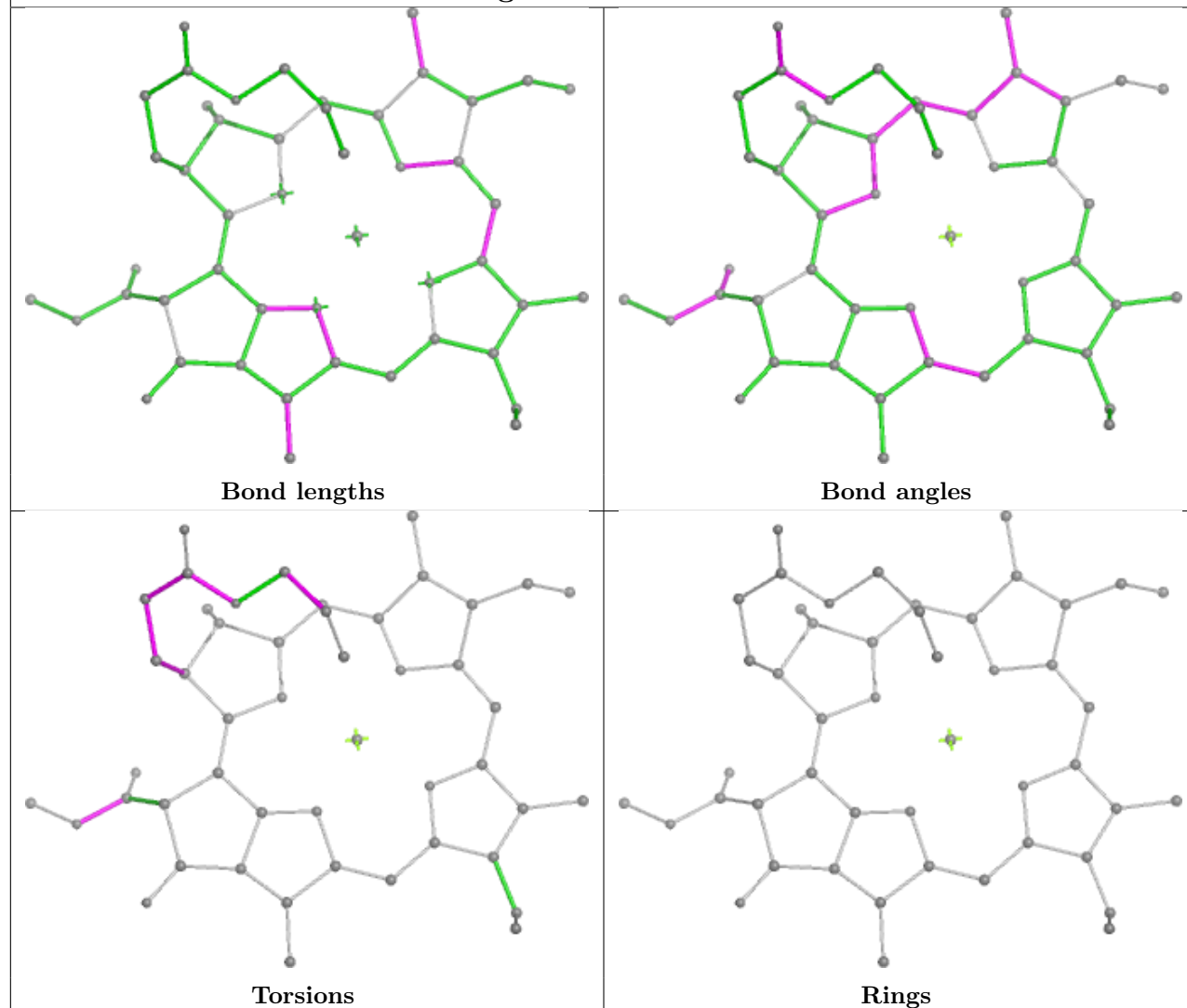


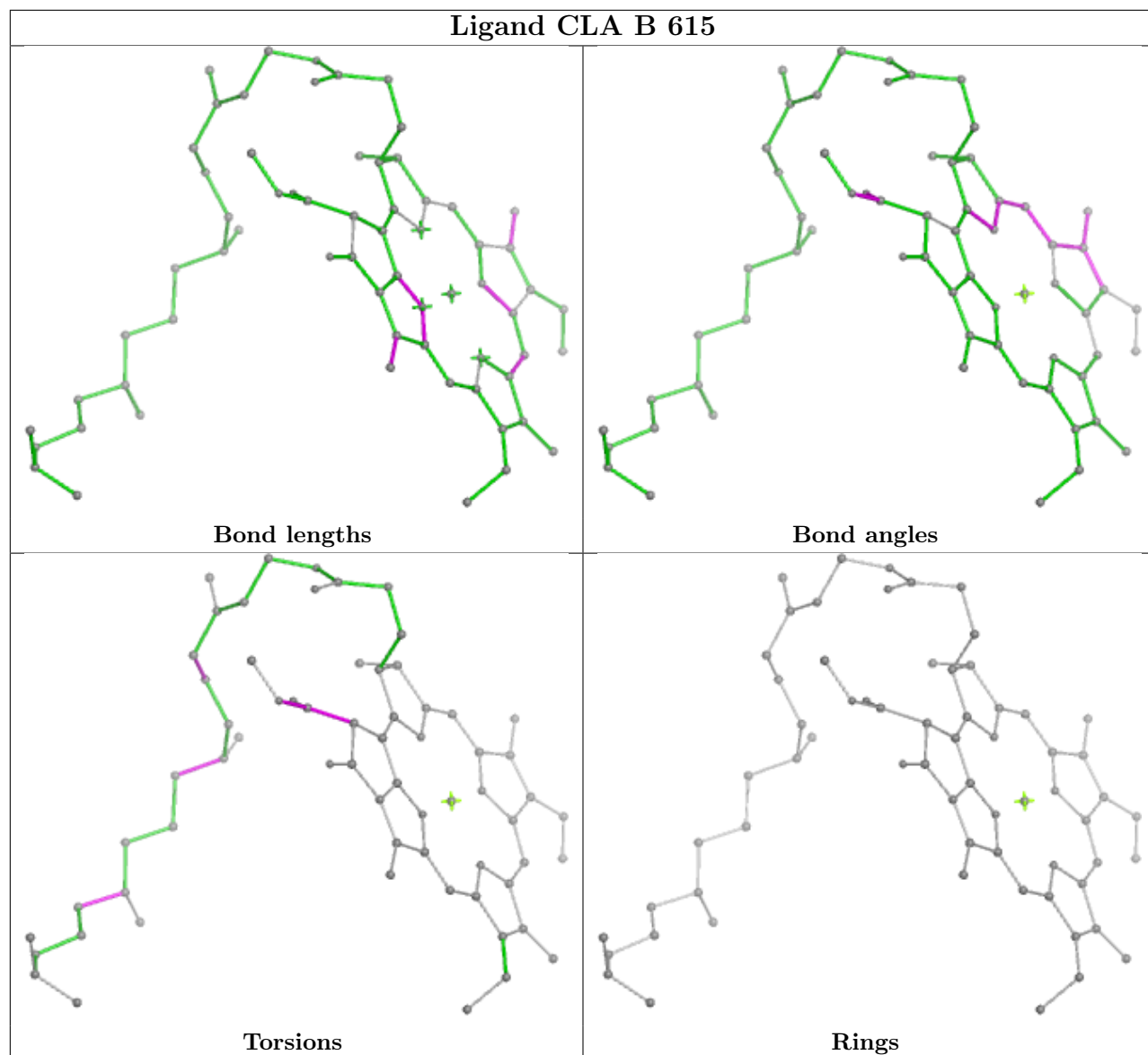




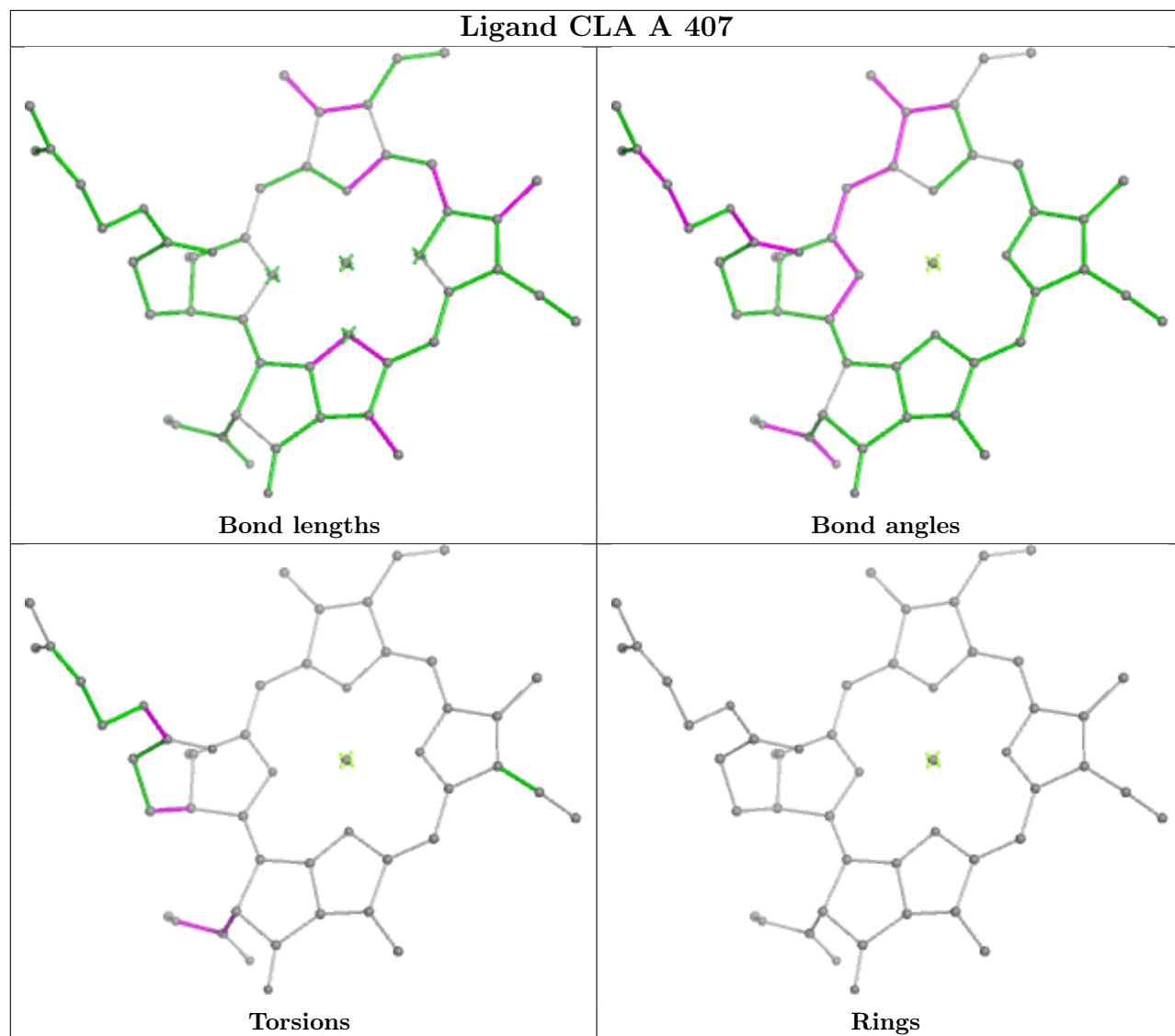


## Ligand CLA n 613

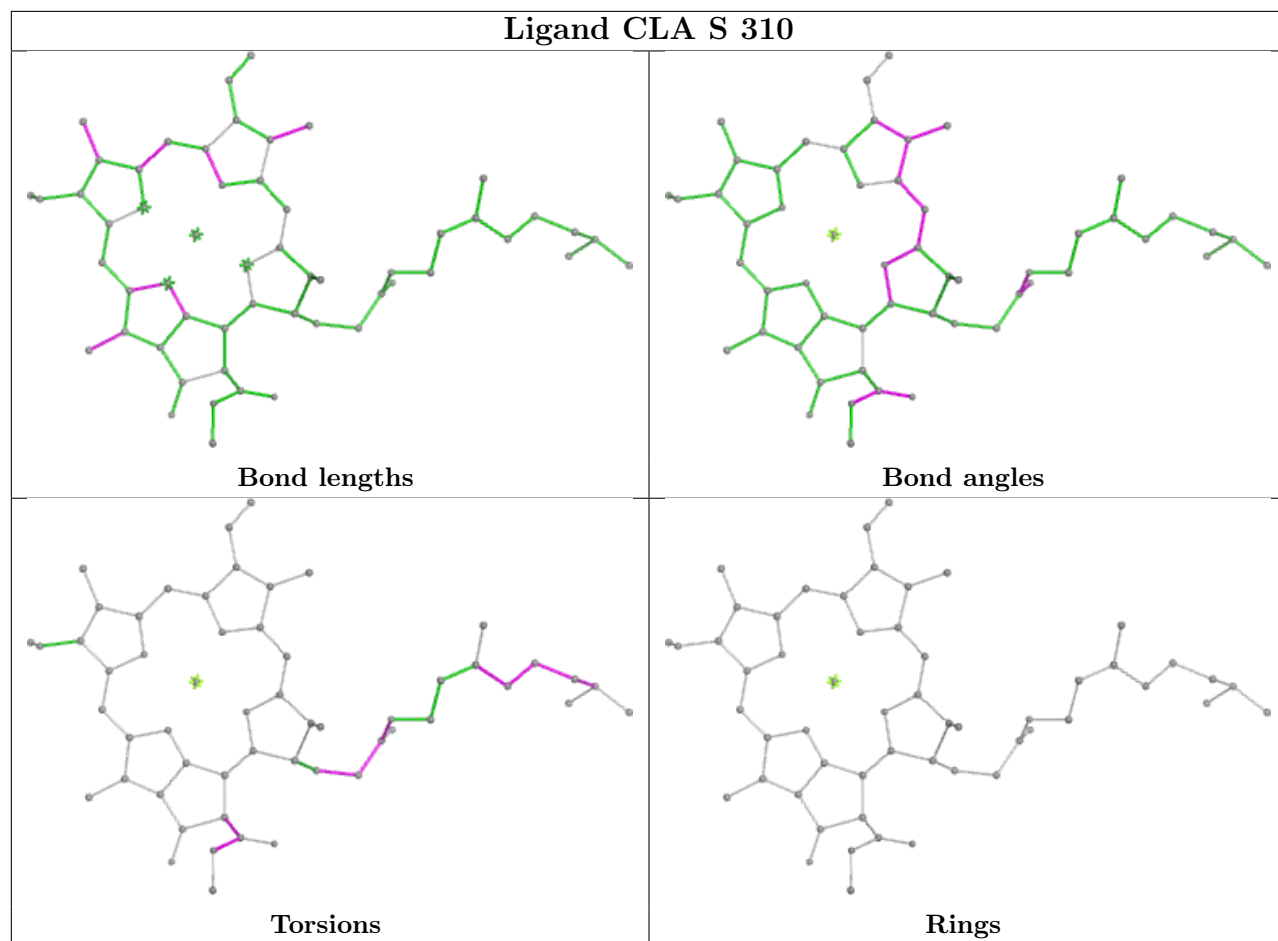


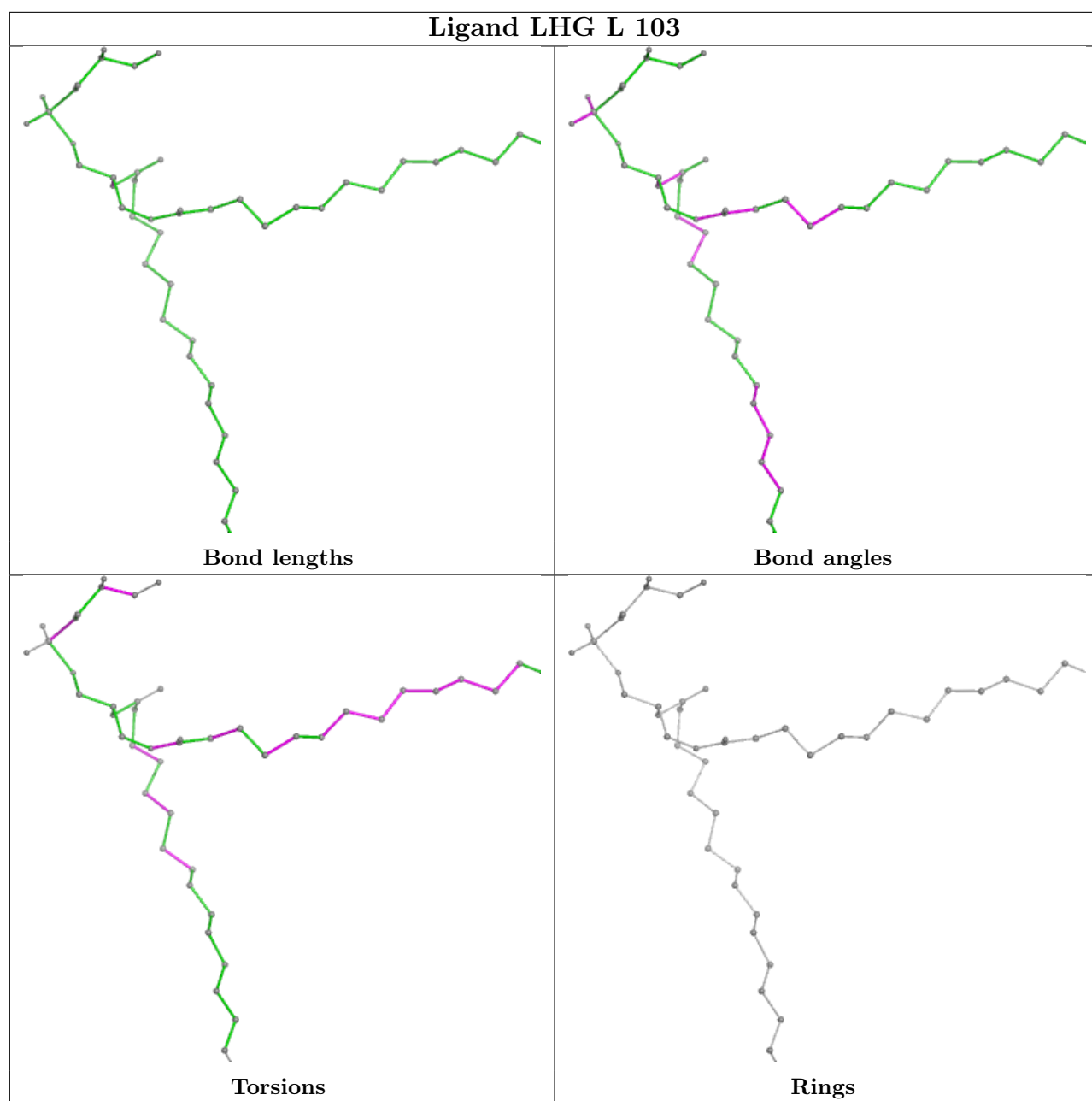


## Ligand CLA A 407

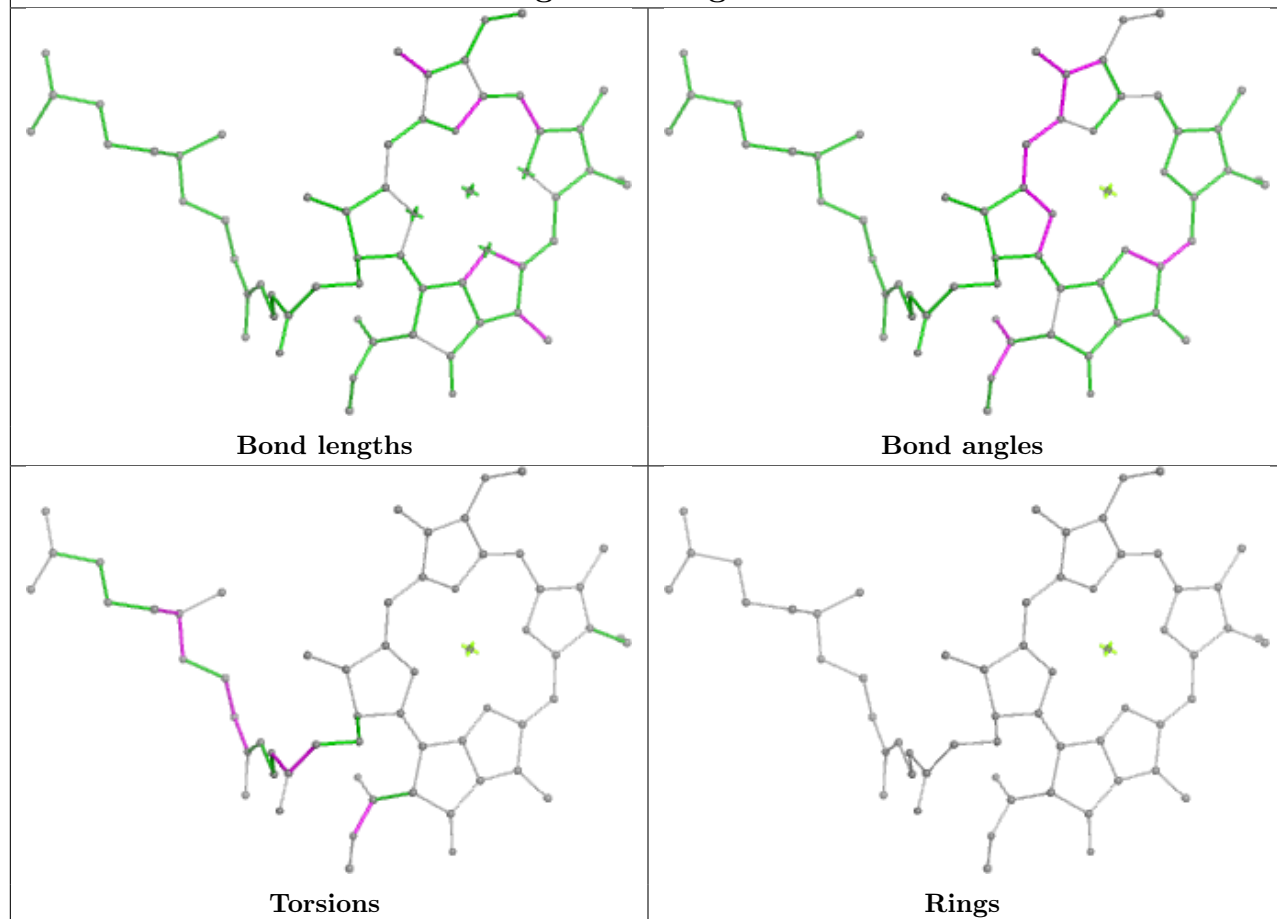


## Ligand CLA S 310

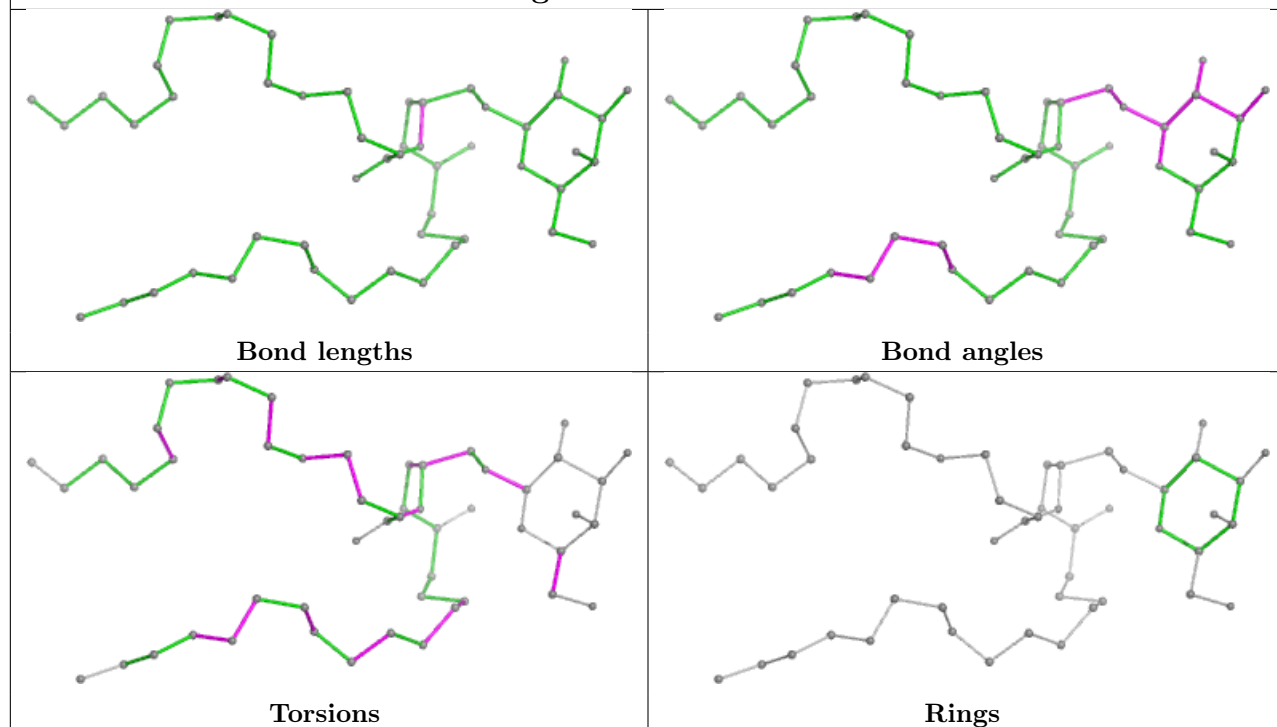


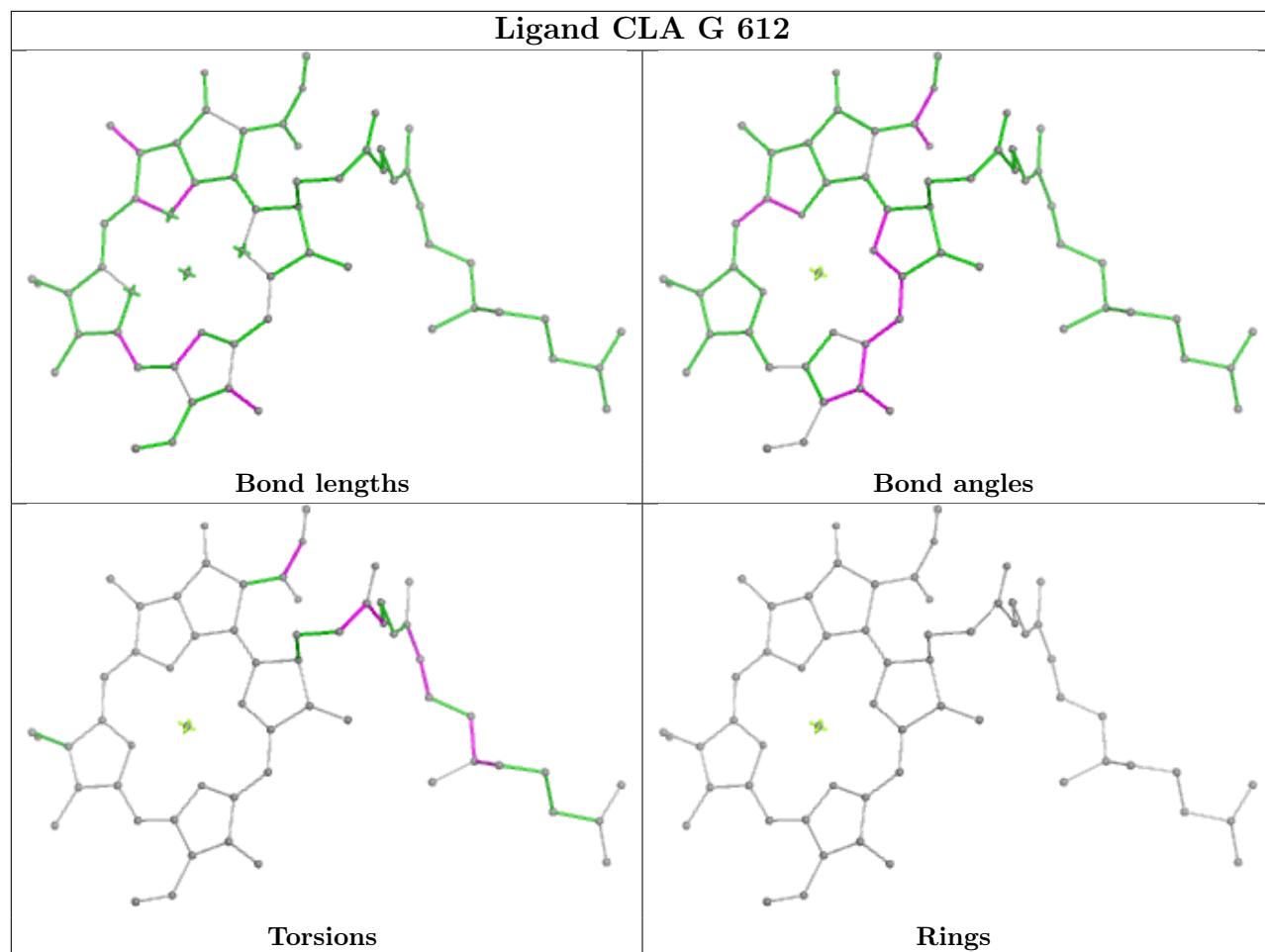


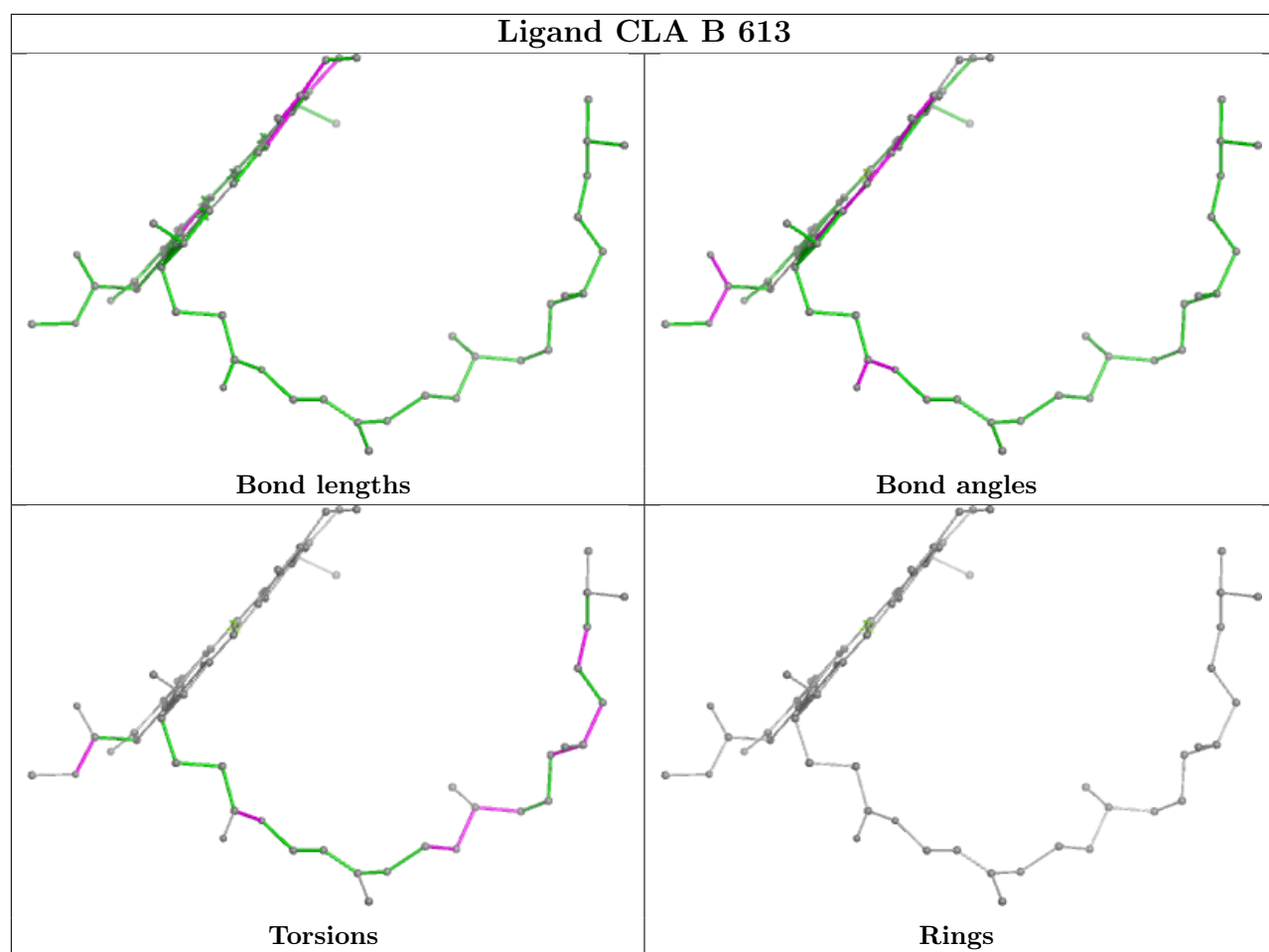
## Ligand CLA g 612

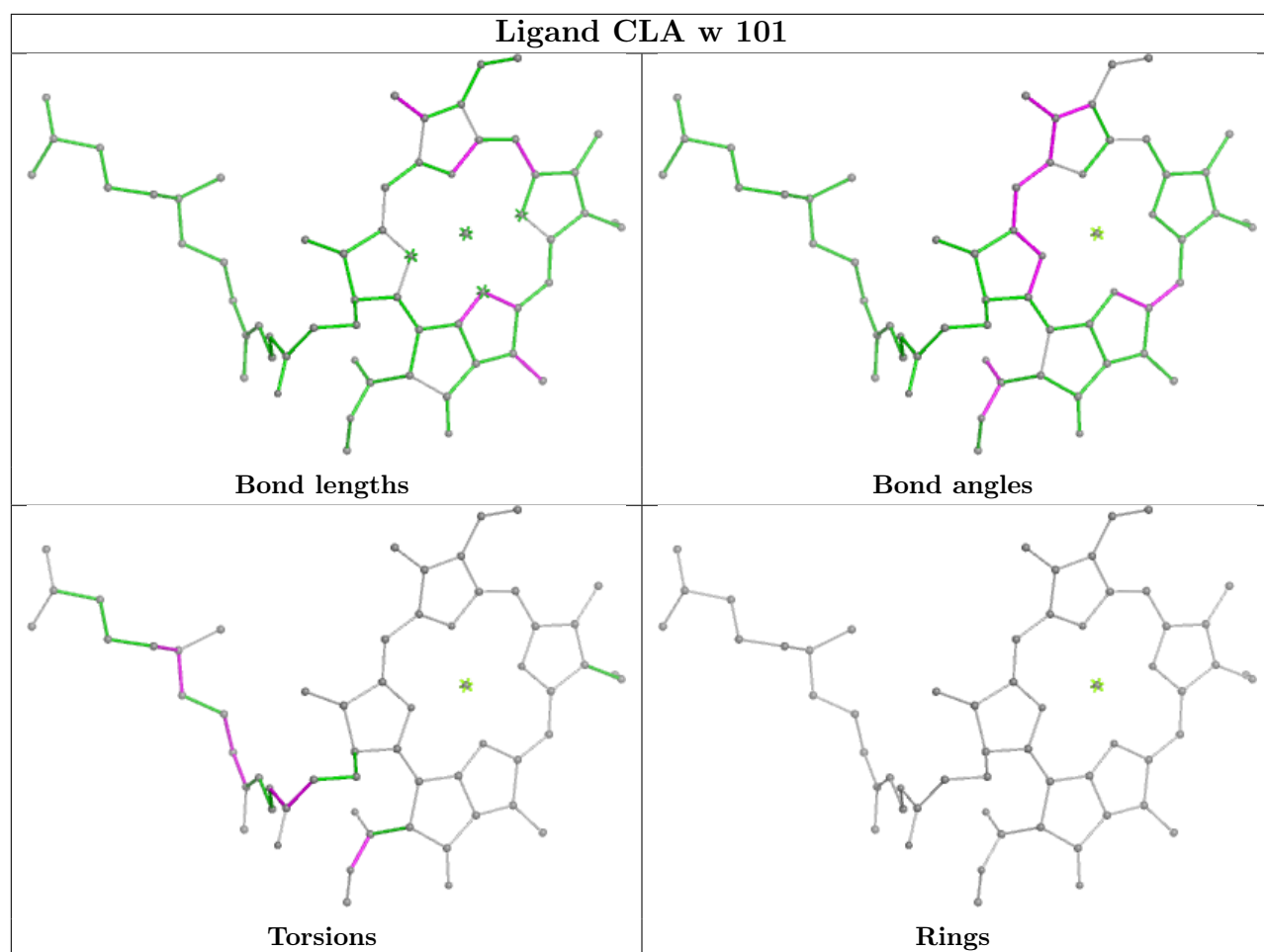


## Ligand LMG c 523

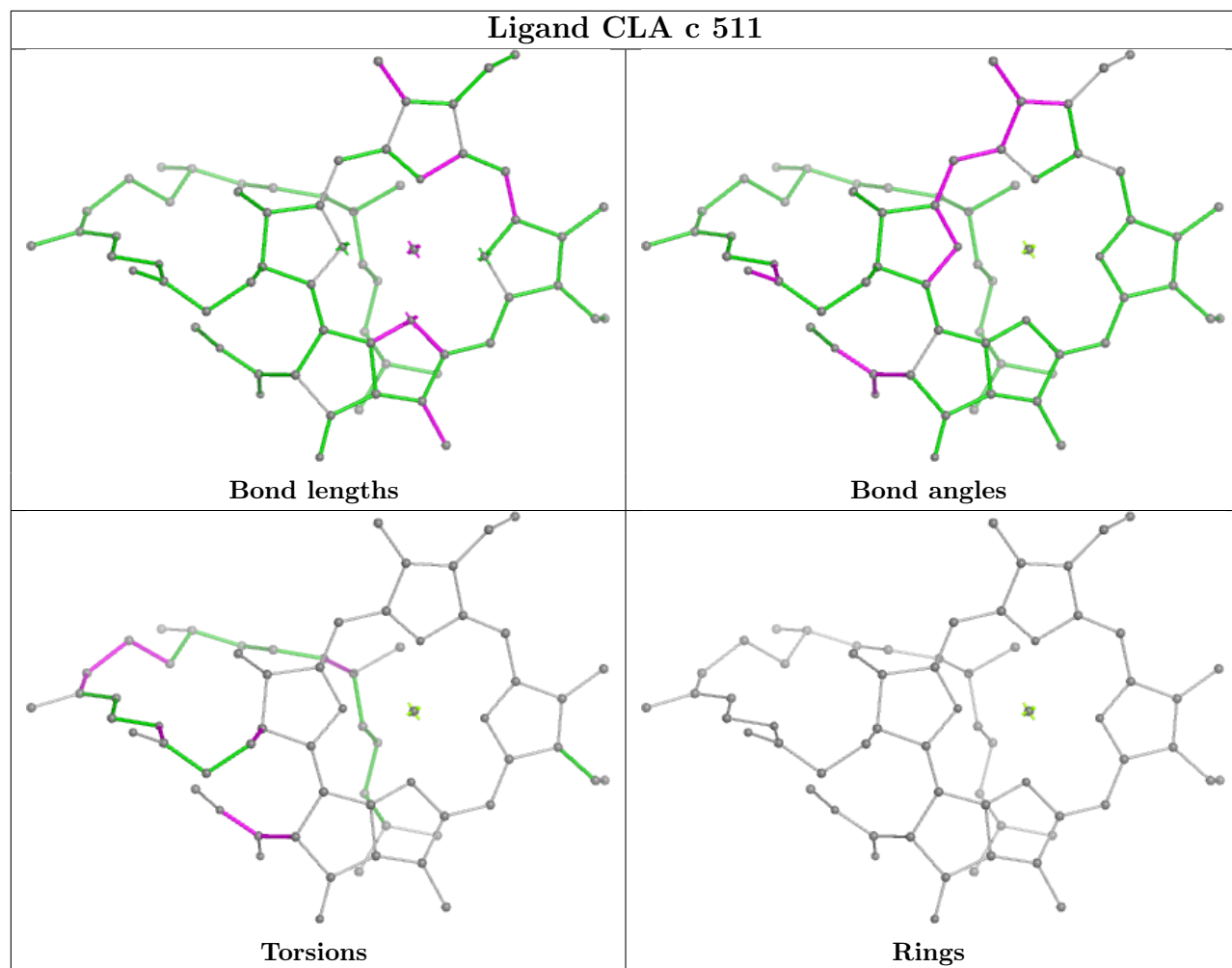




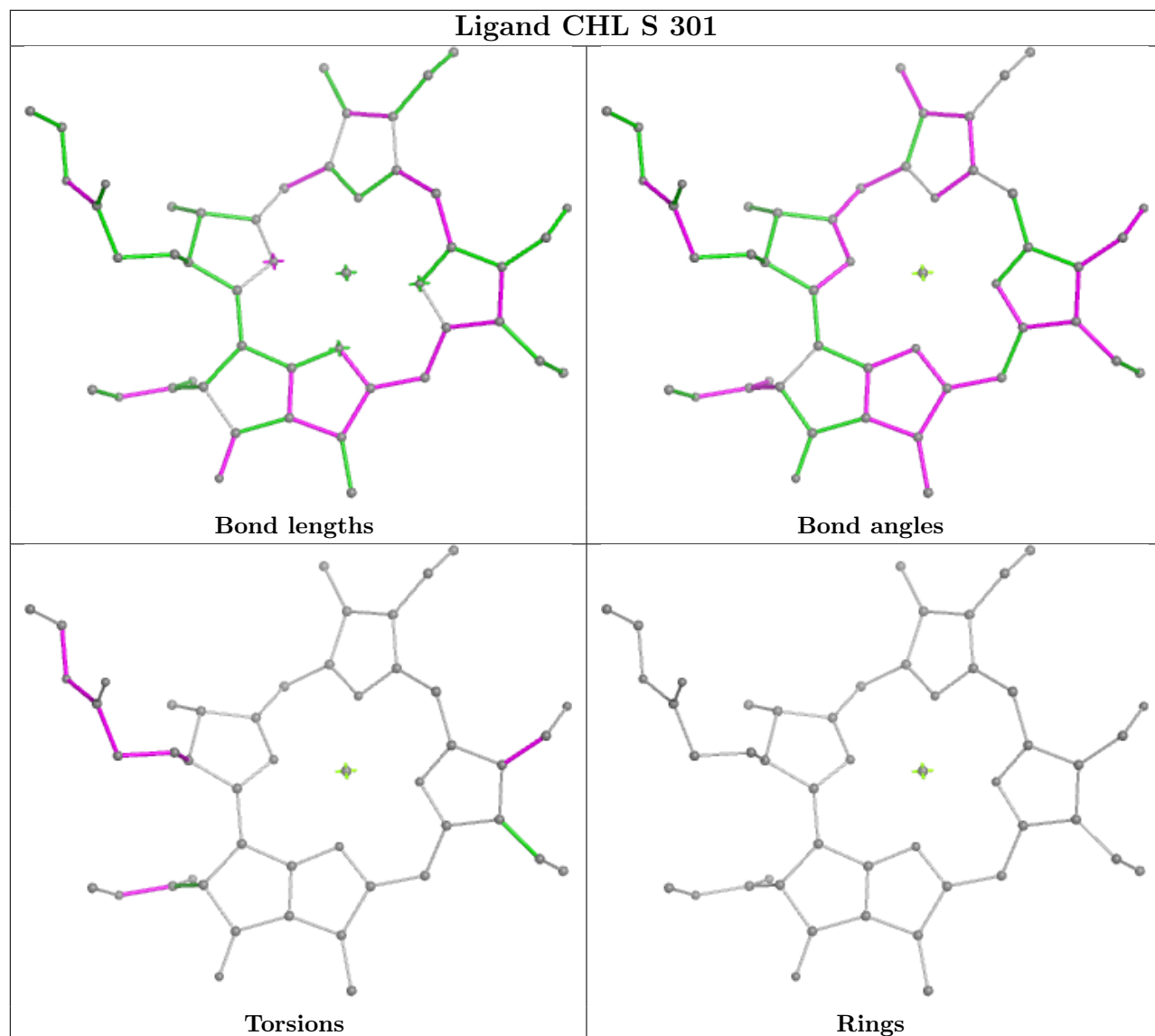


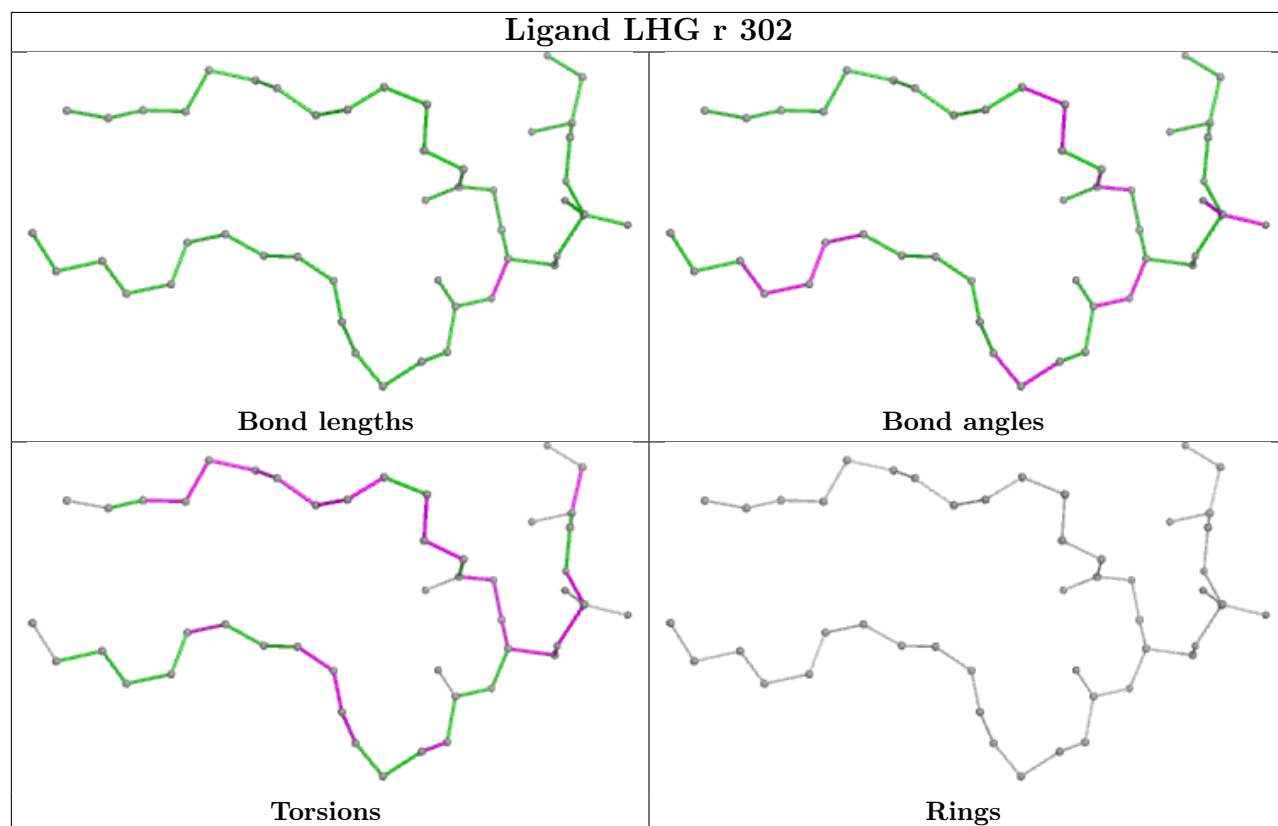
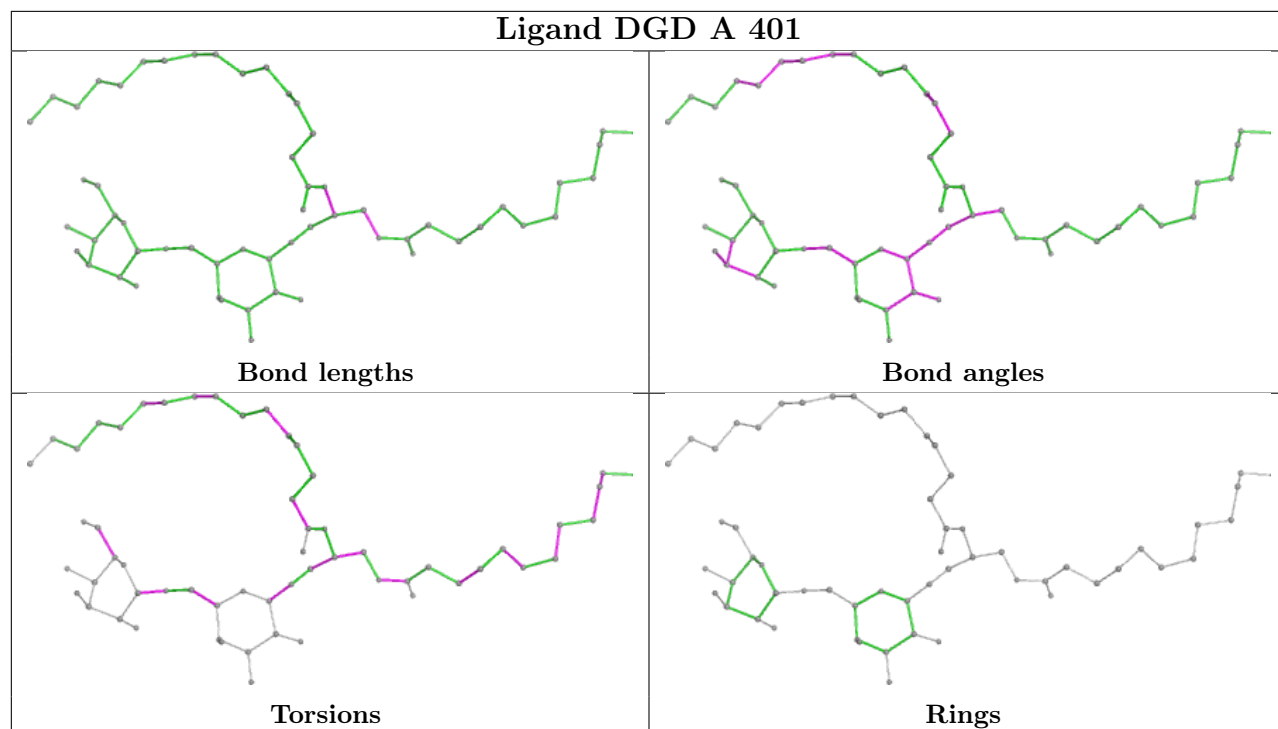


## Ligand CLA c 511

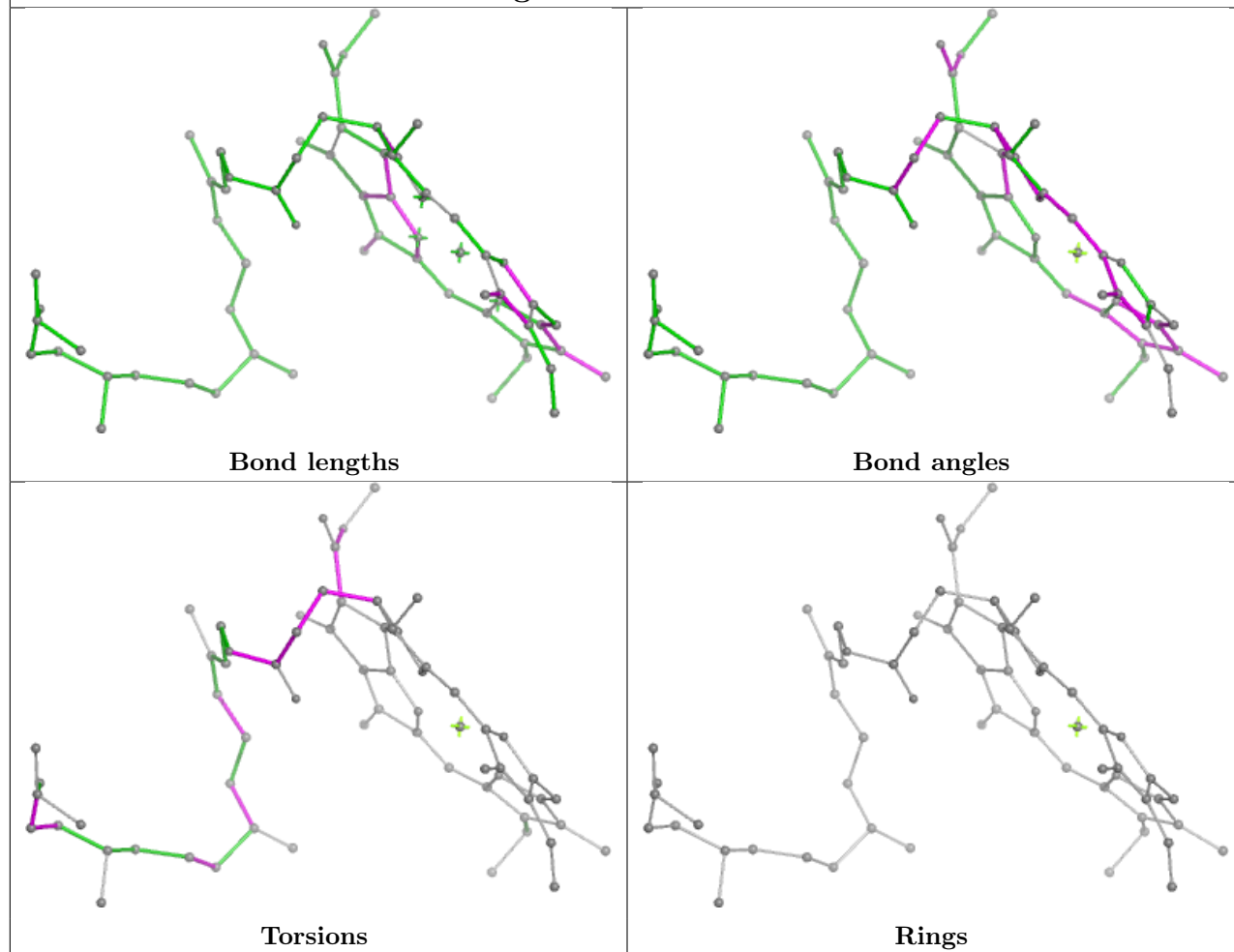


## Ligand CHL S 301

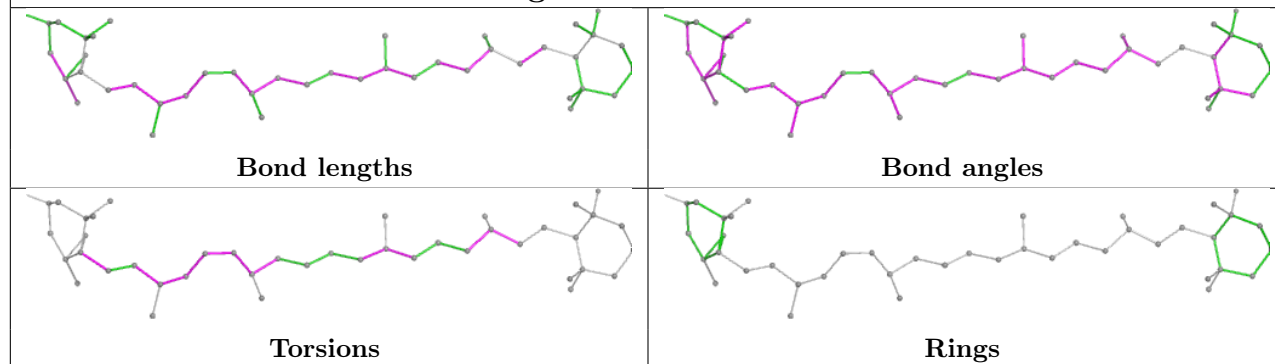


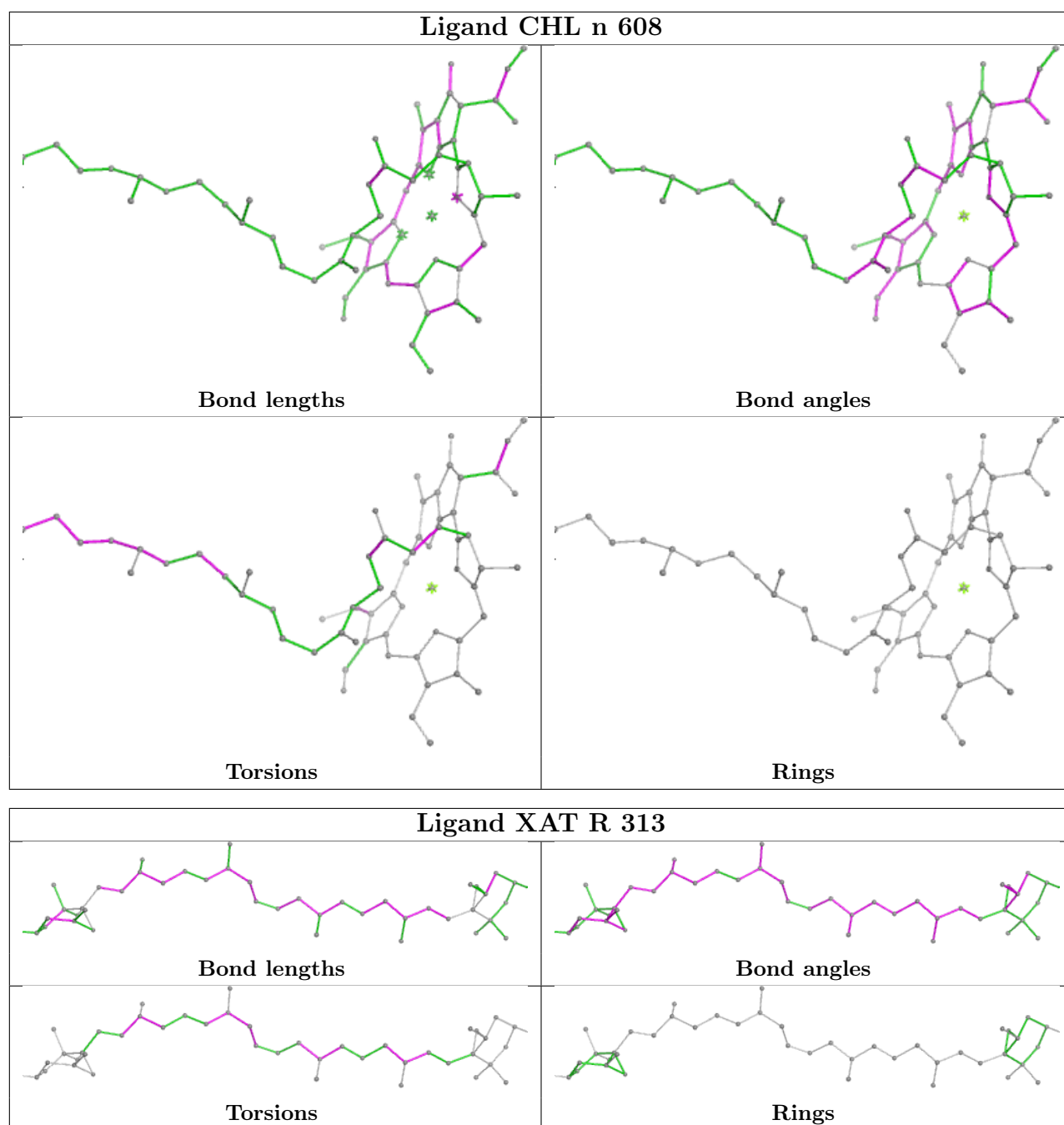


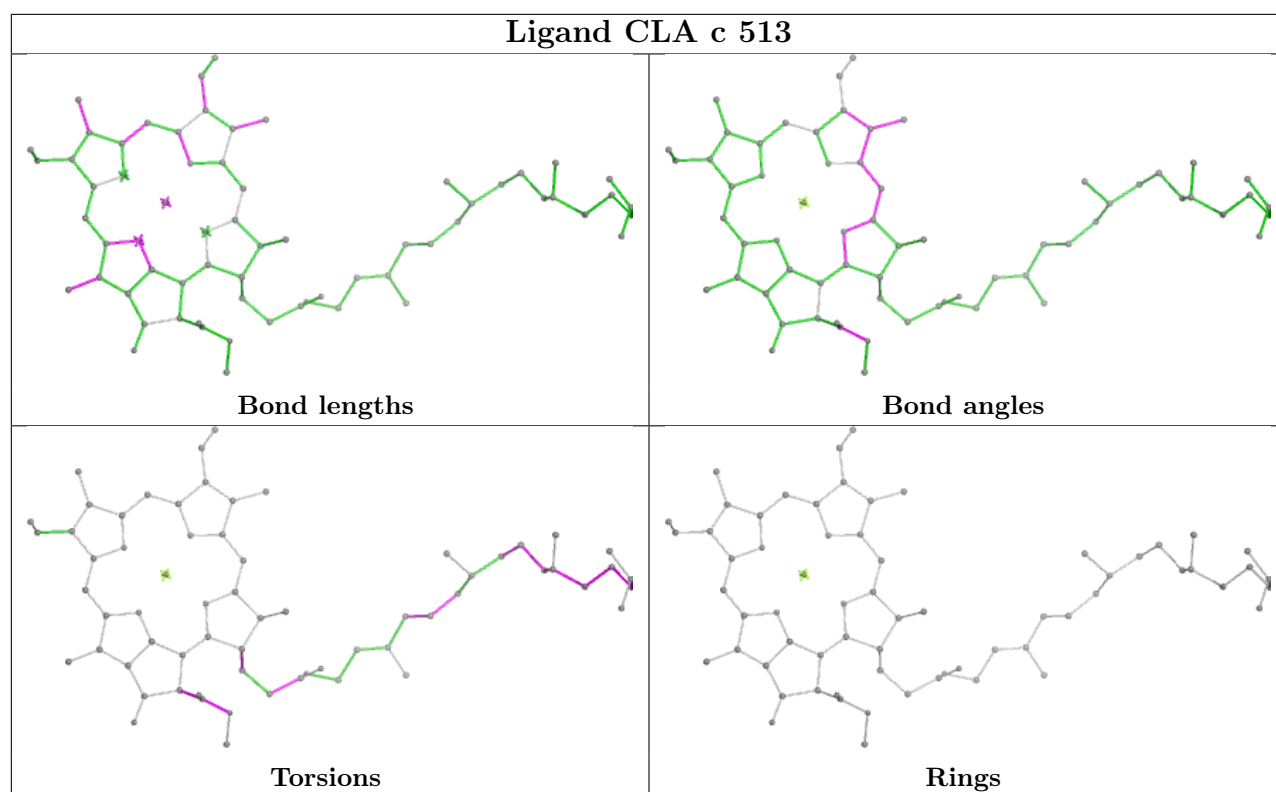
## Ligand CLA Y 611

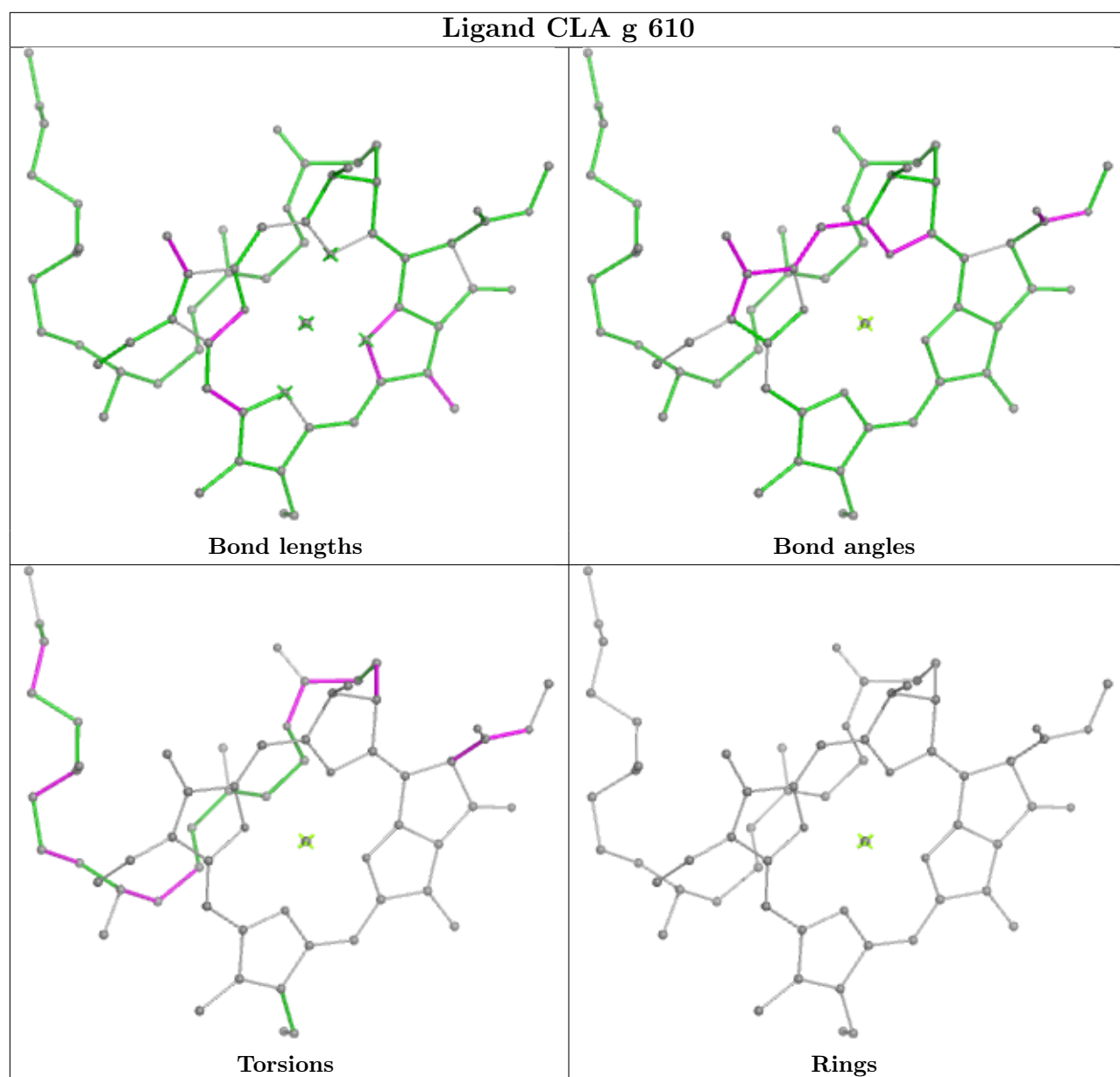


## Ligand NEX N 617

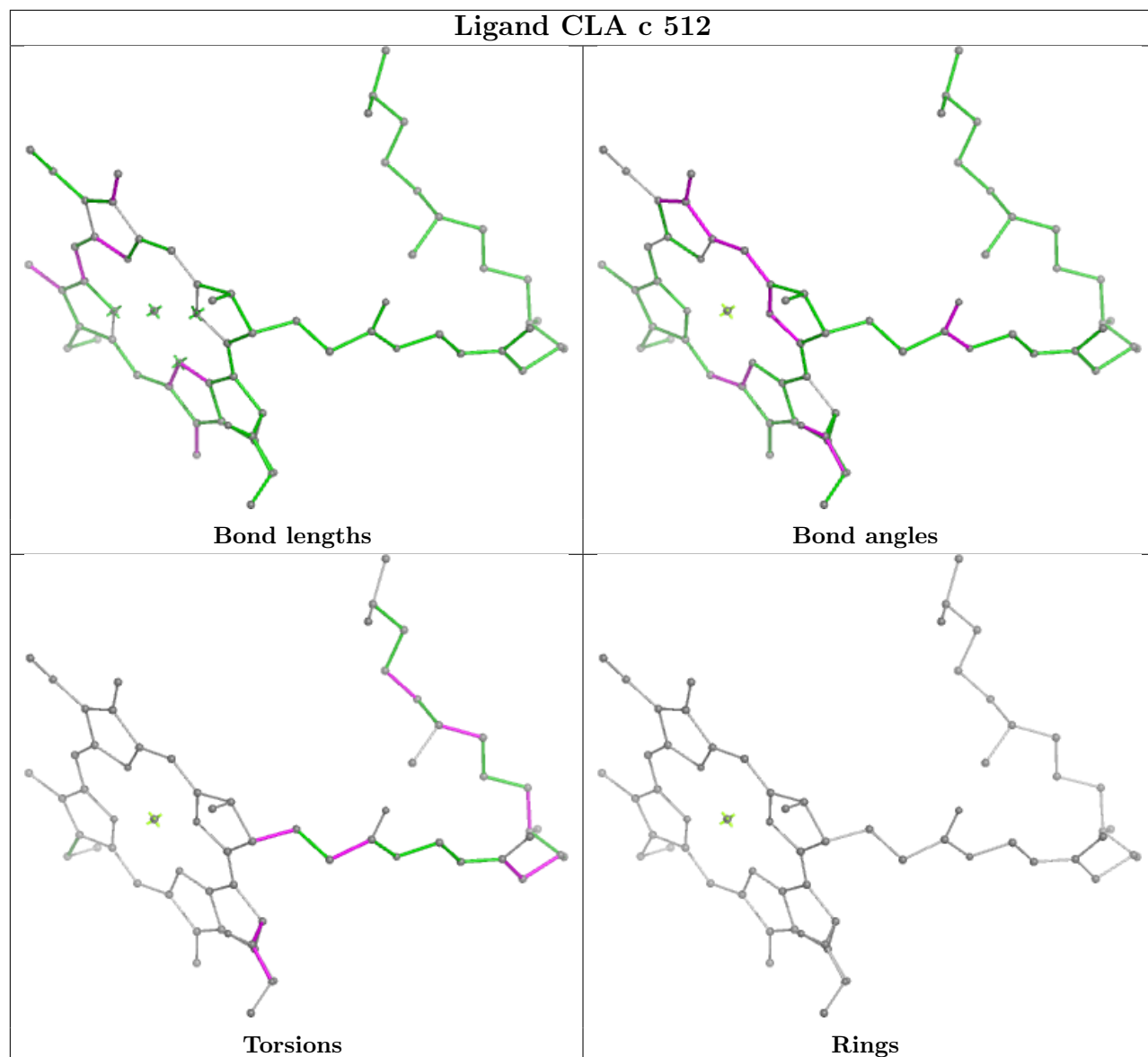


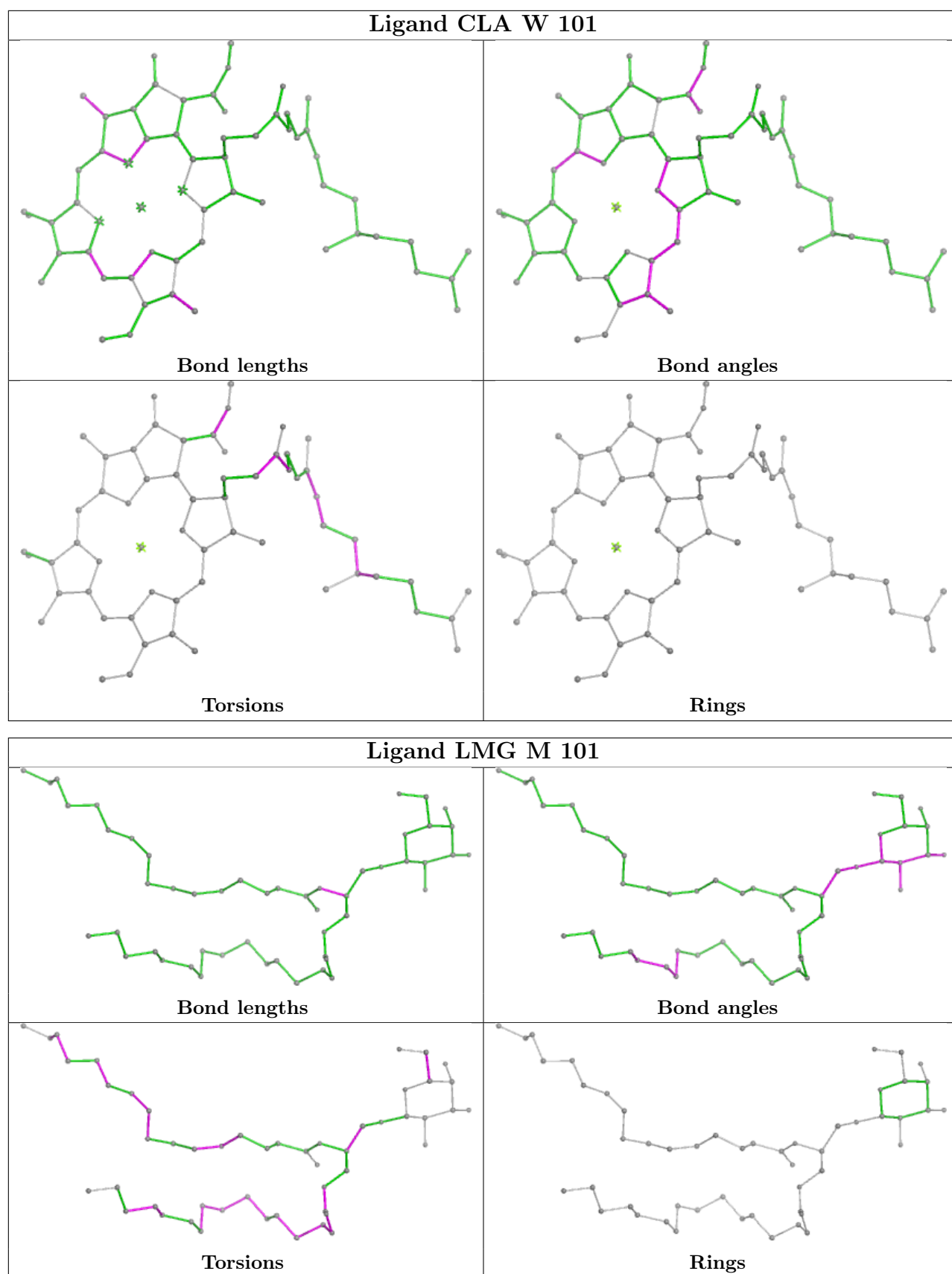


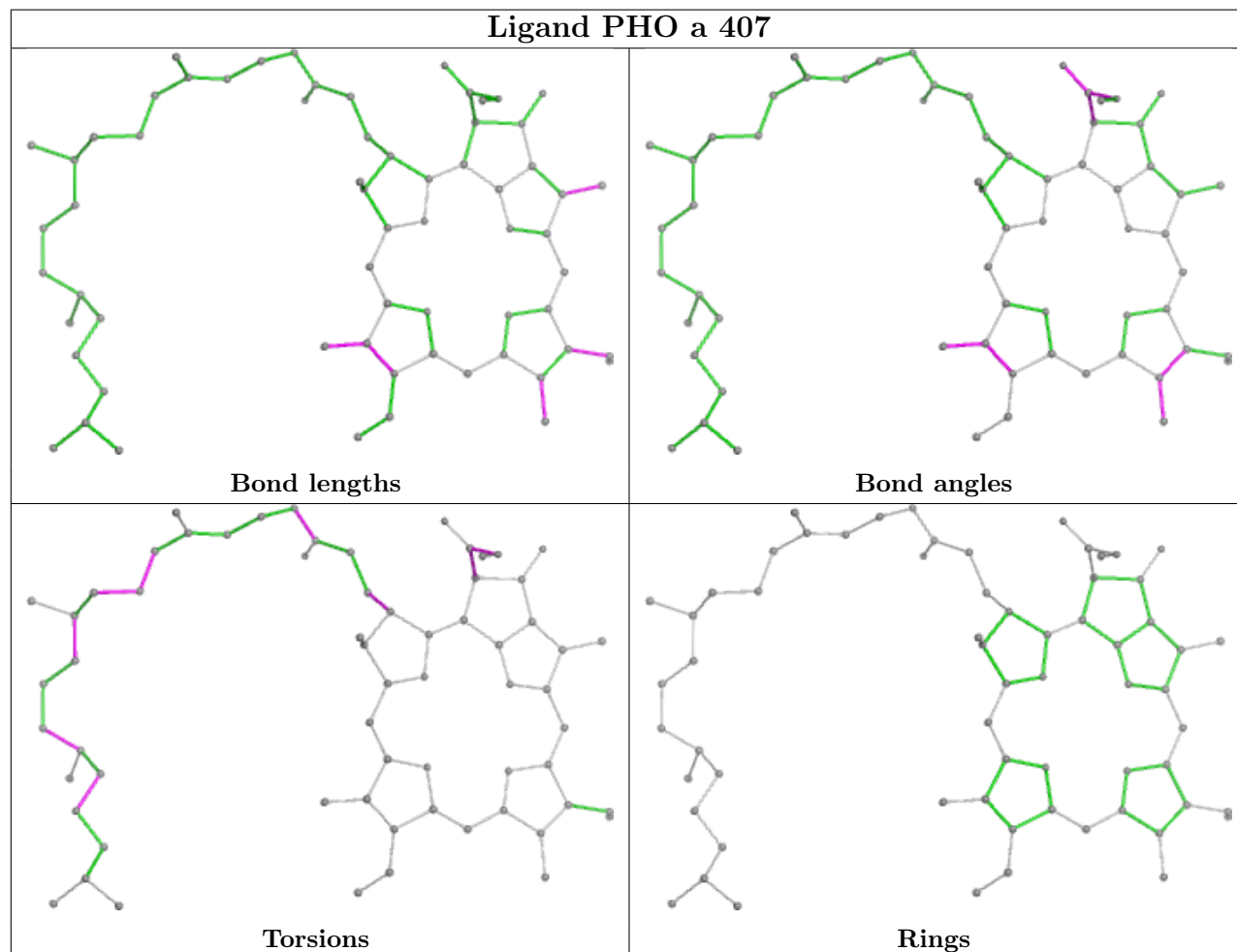
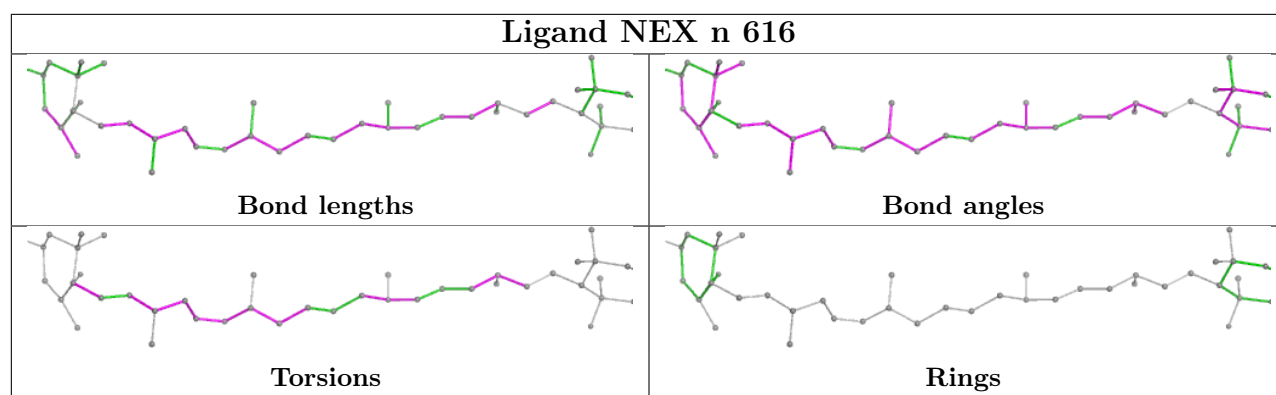


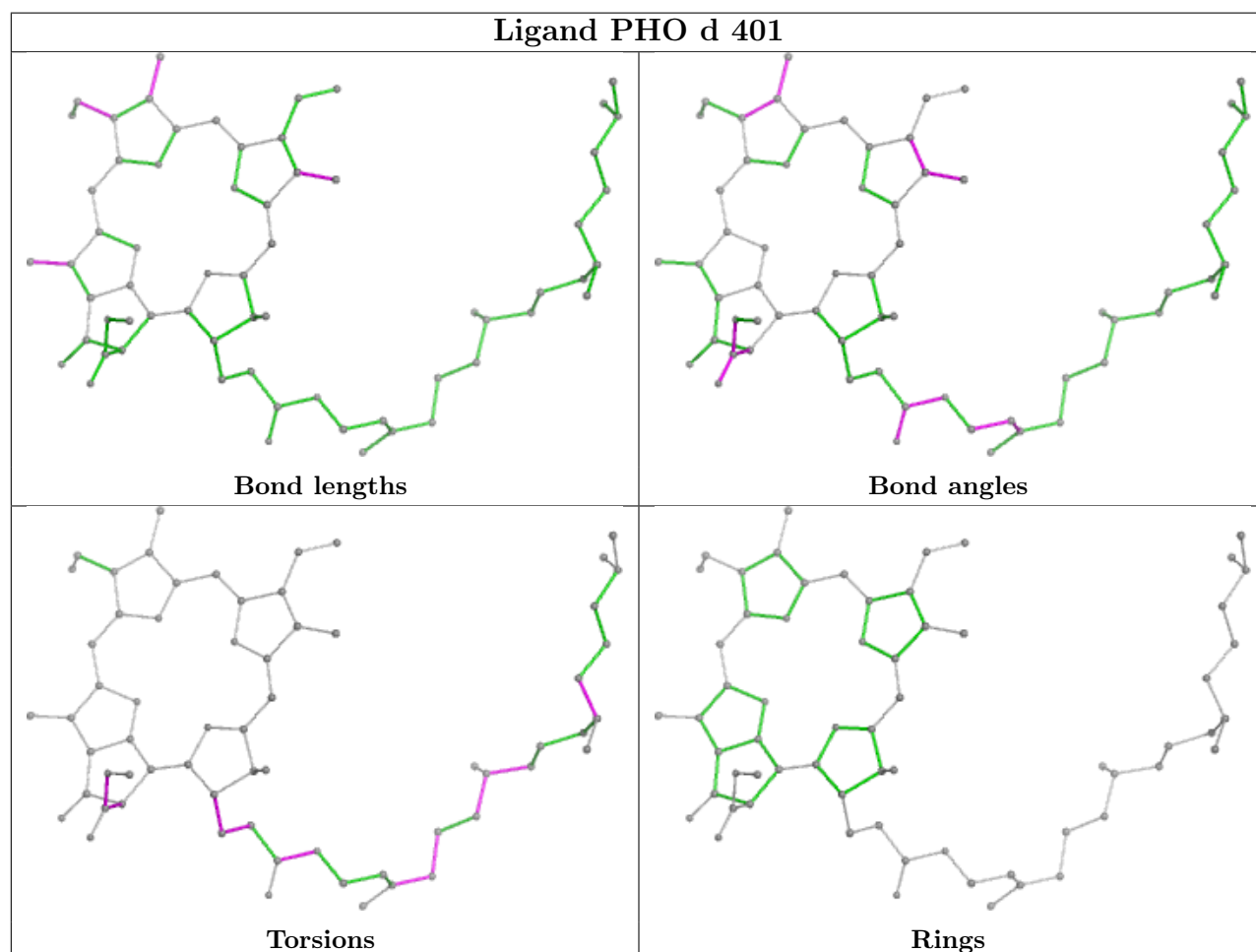
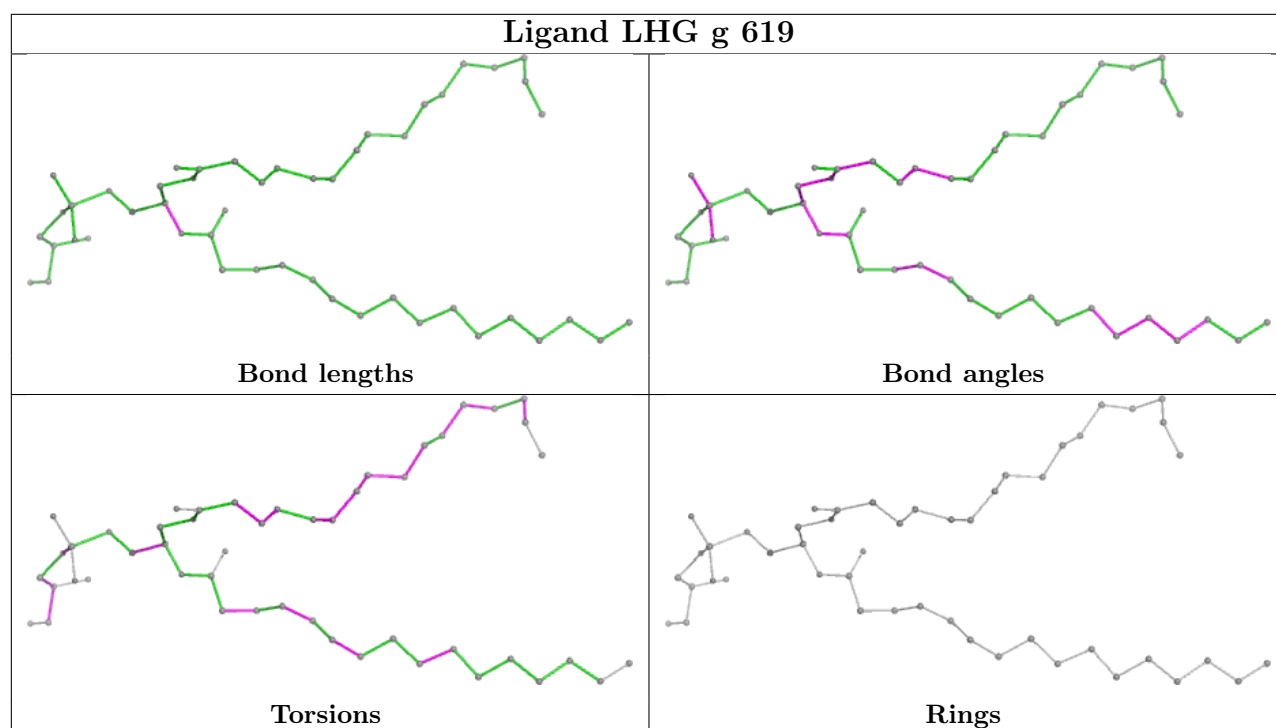


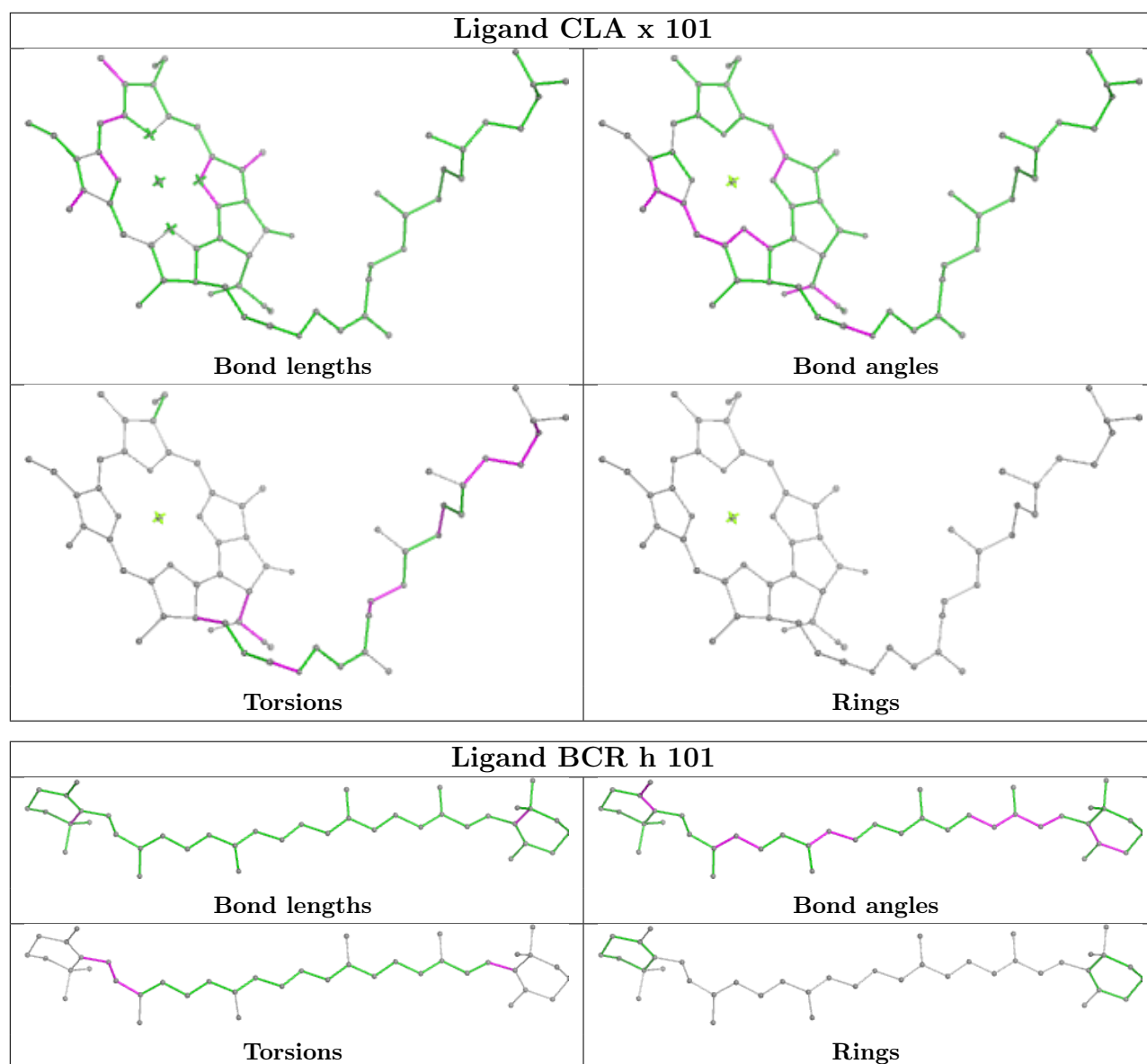
## Ligand CLA c 512

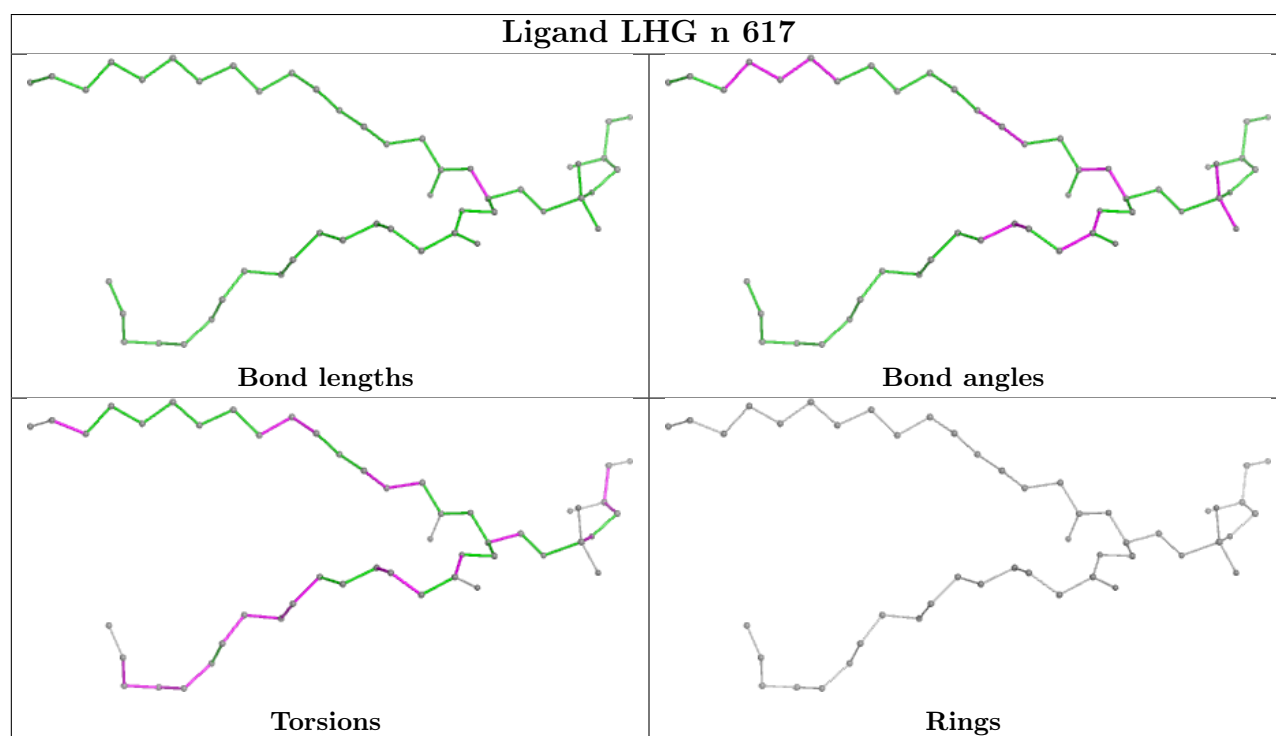
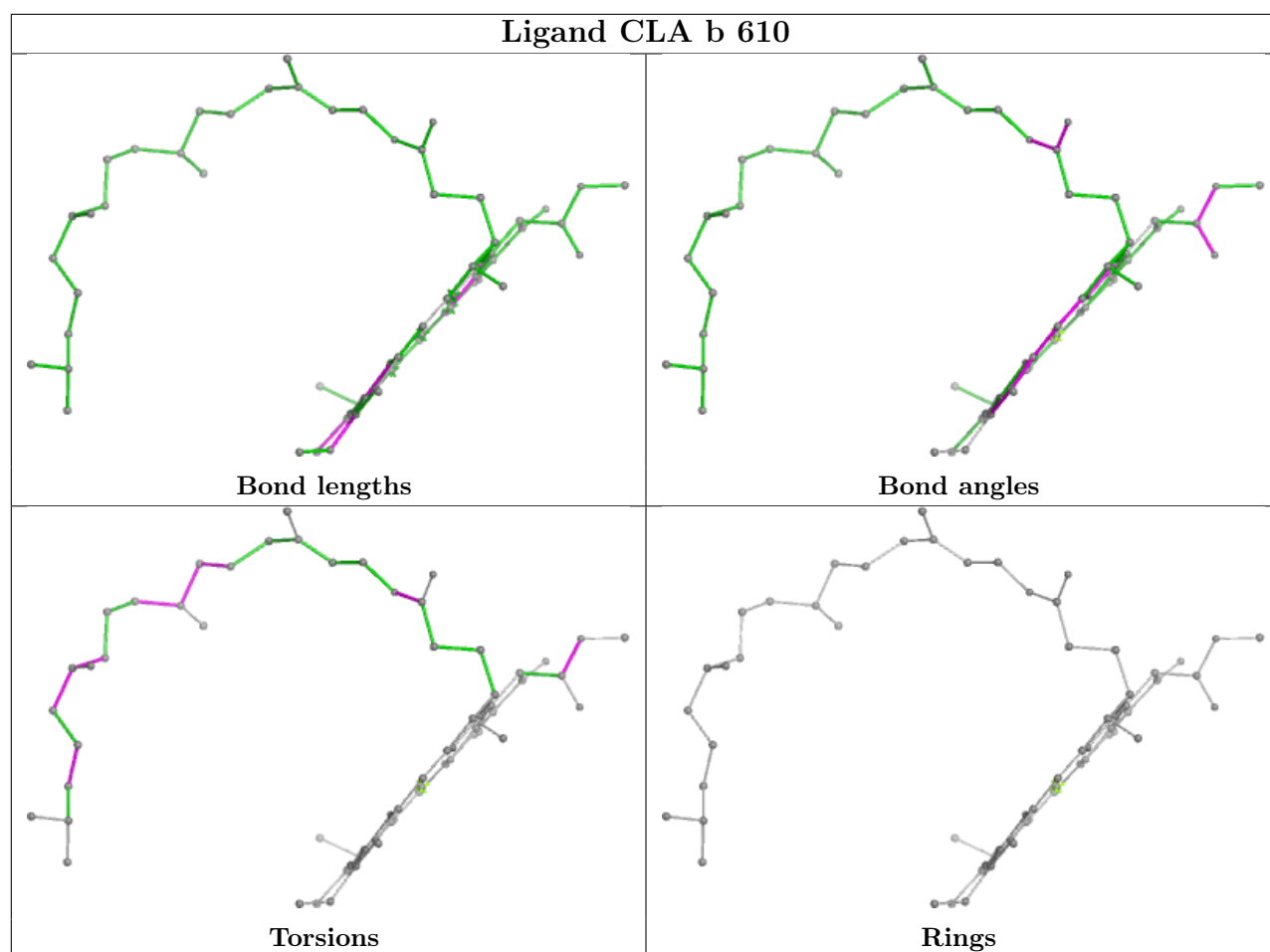


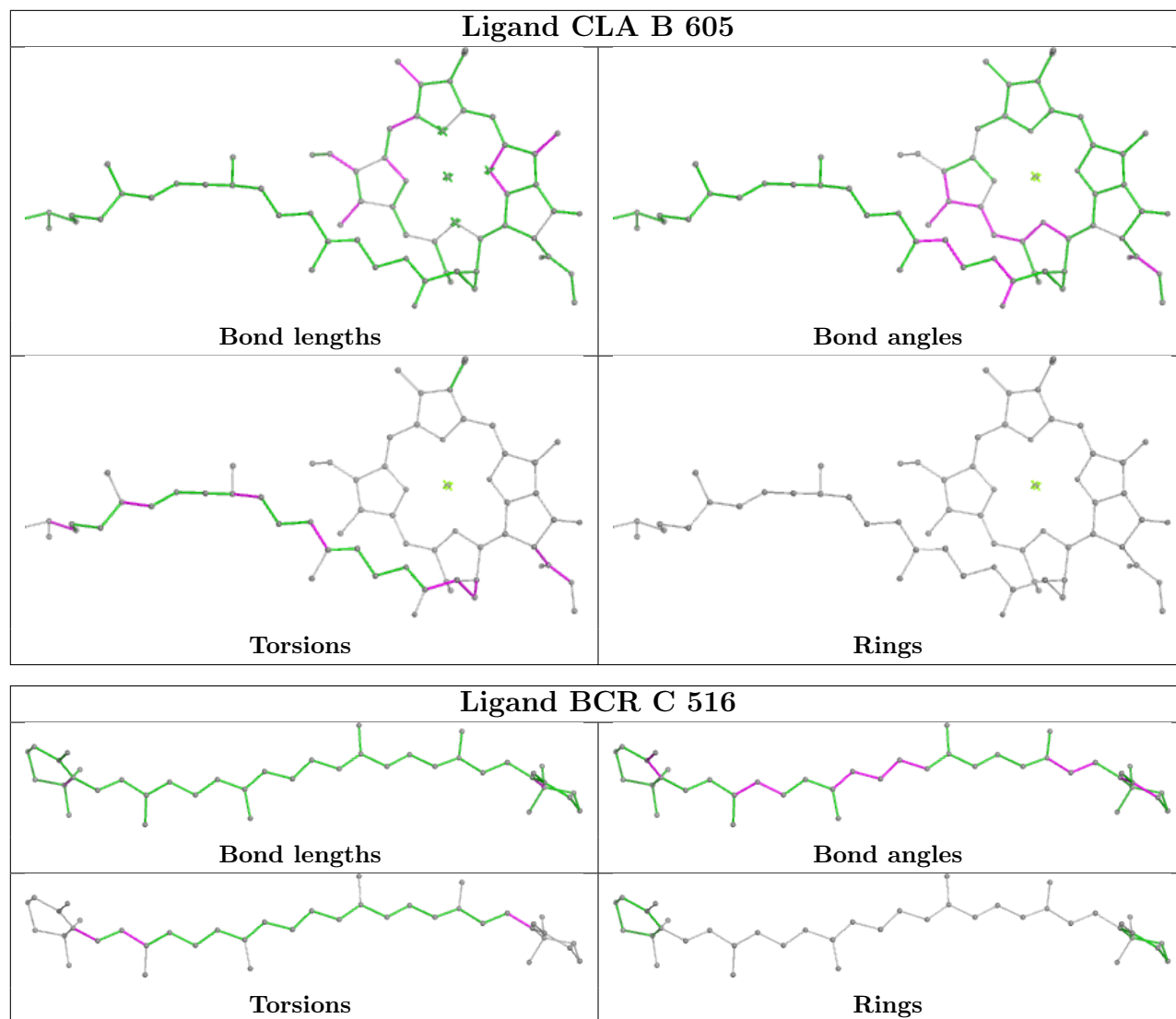


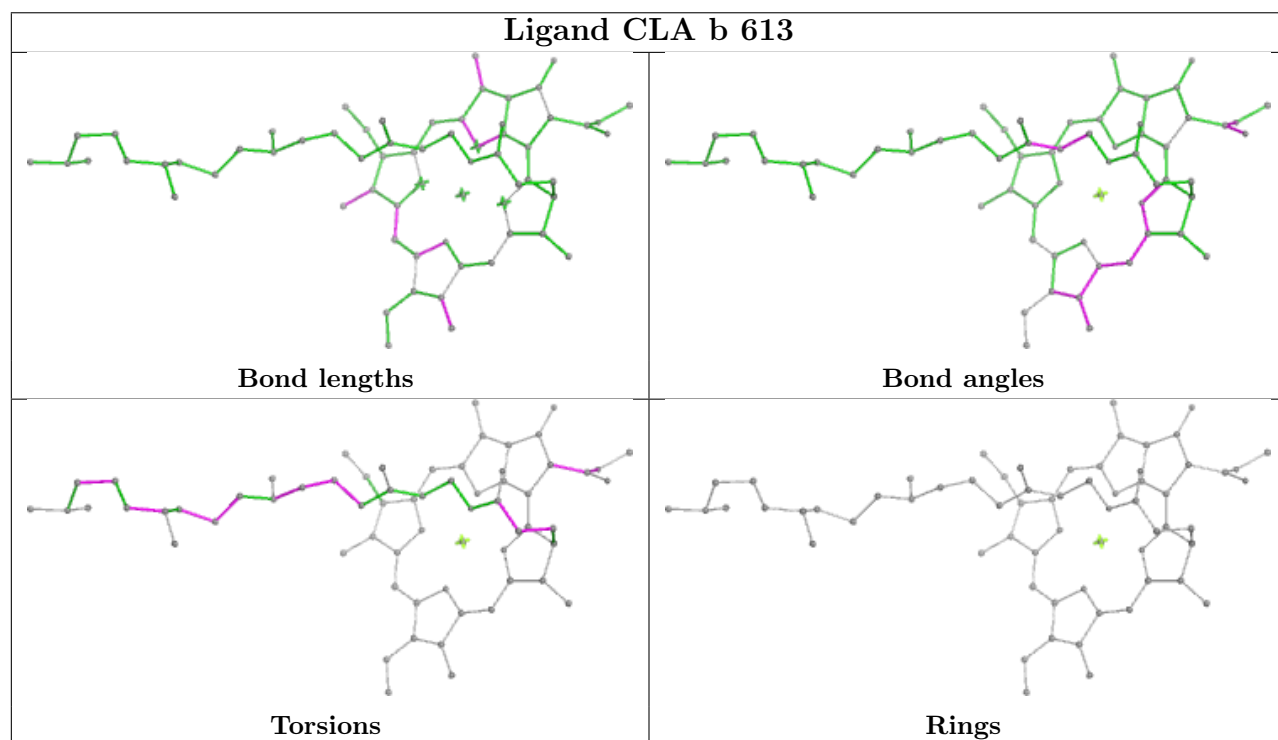
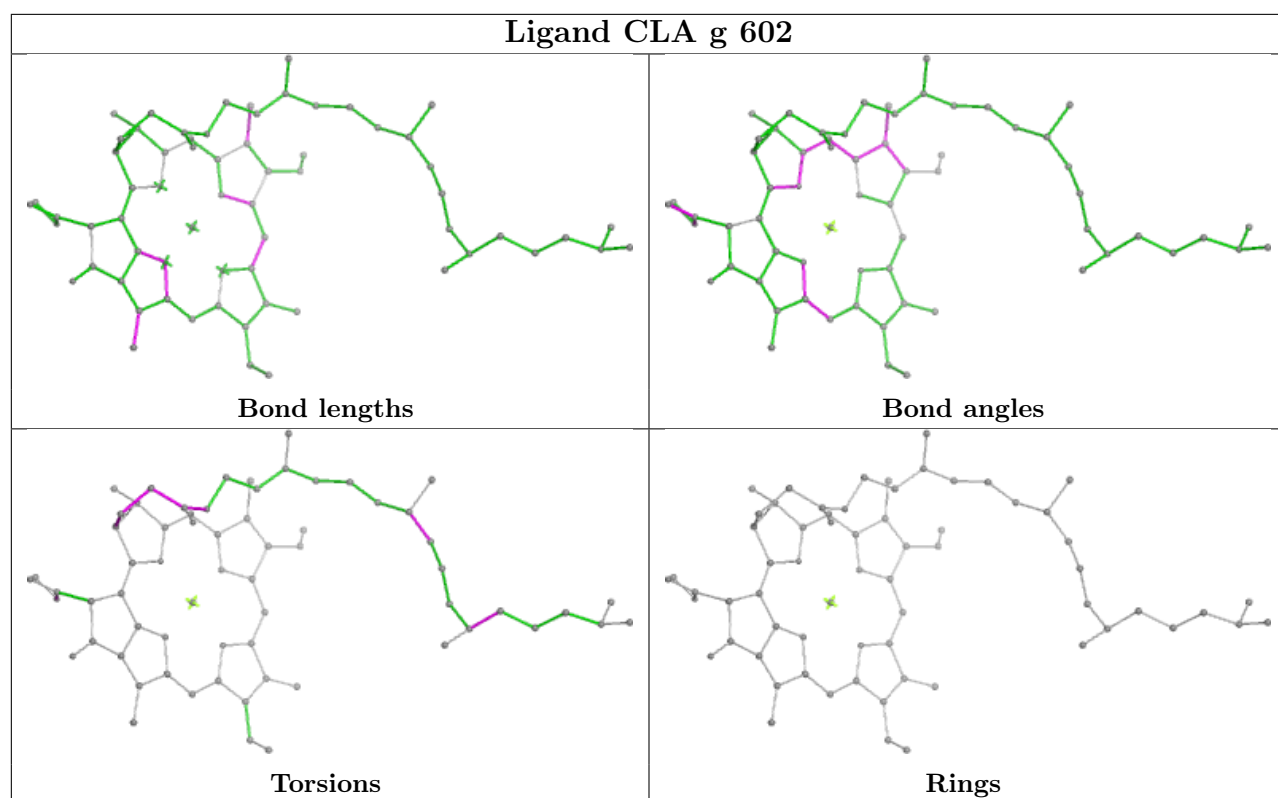


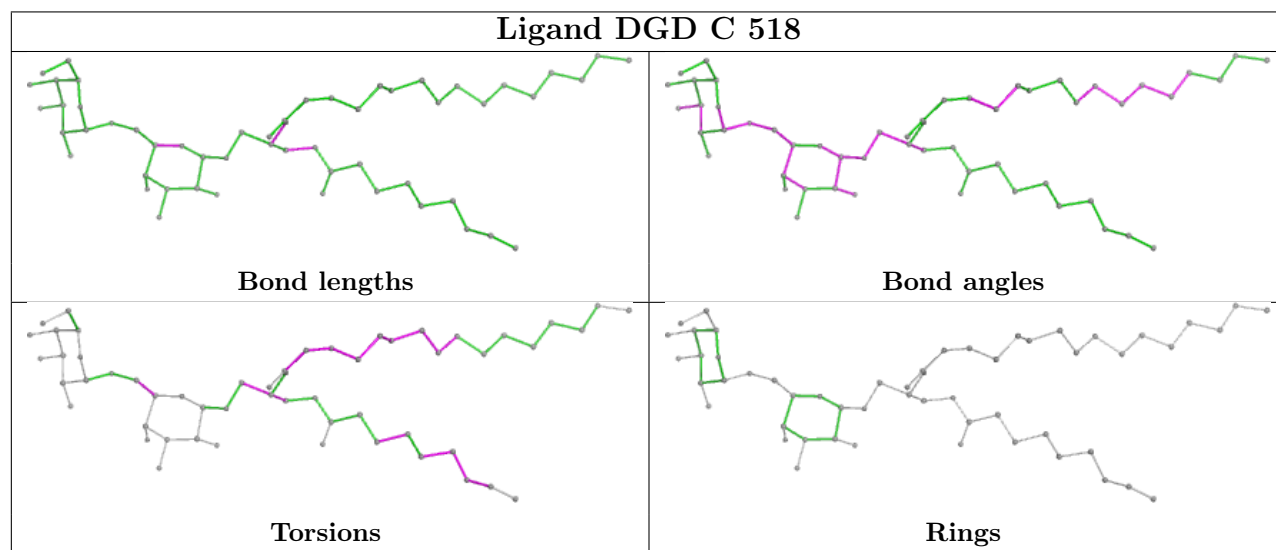
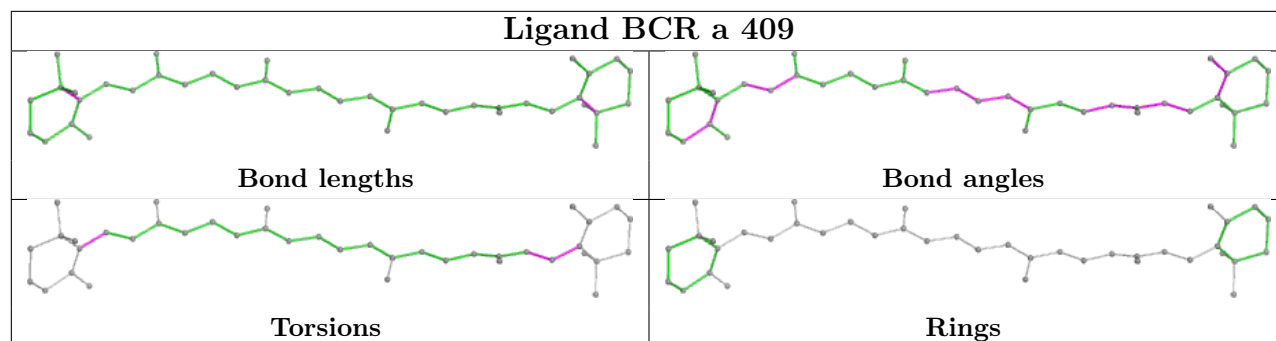




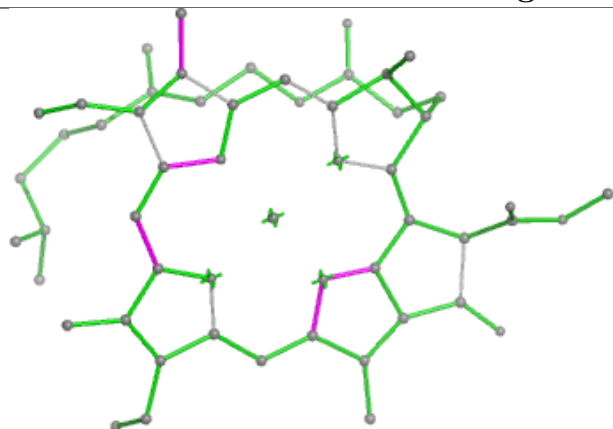




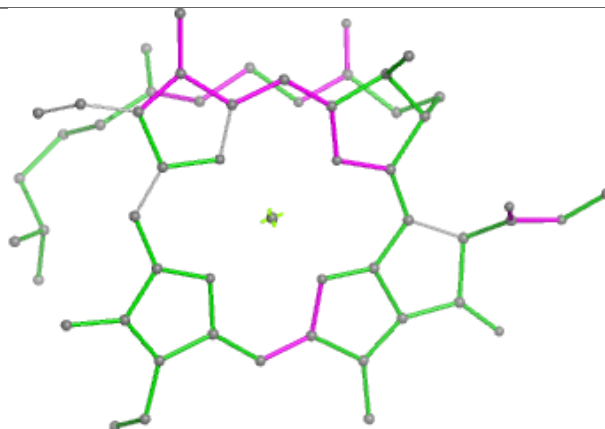




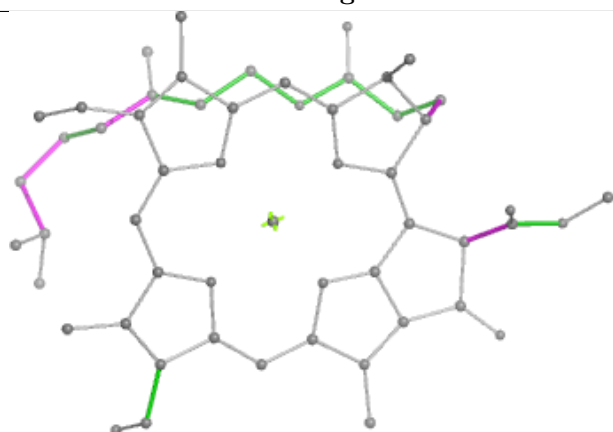
## Ligand CLA S 309



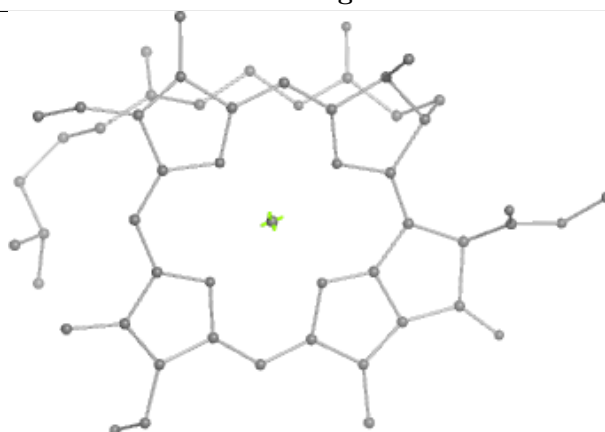
Bond lengths



Bond angles

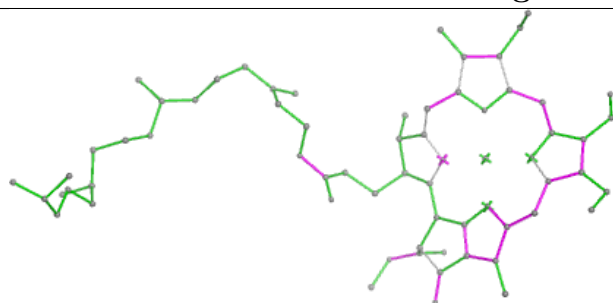


Torsions

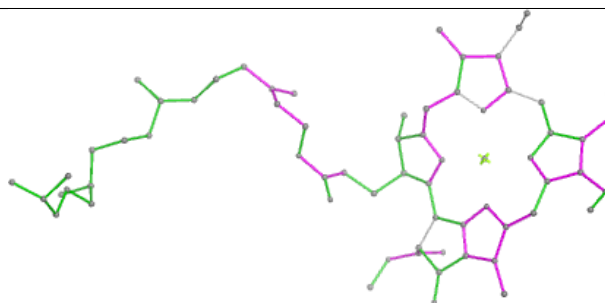


Rings

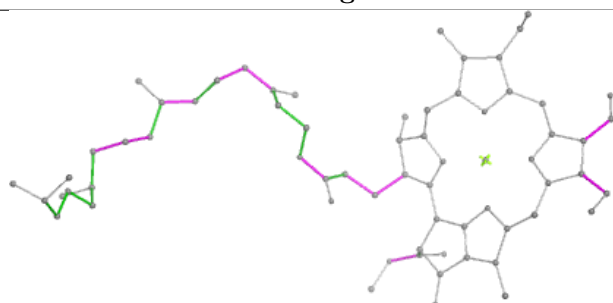
## Ligand CHL G 607



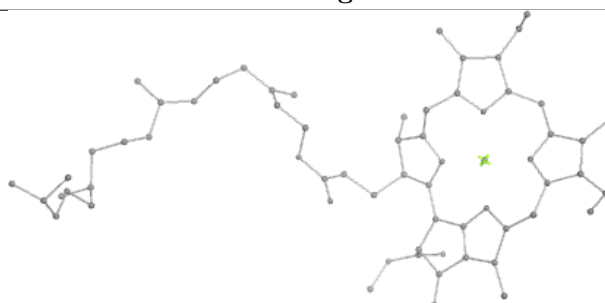
Bond lengths



Bond angles

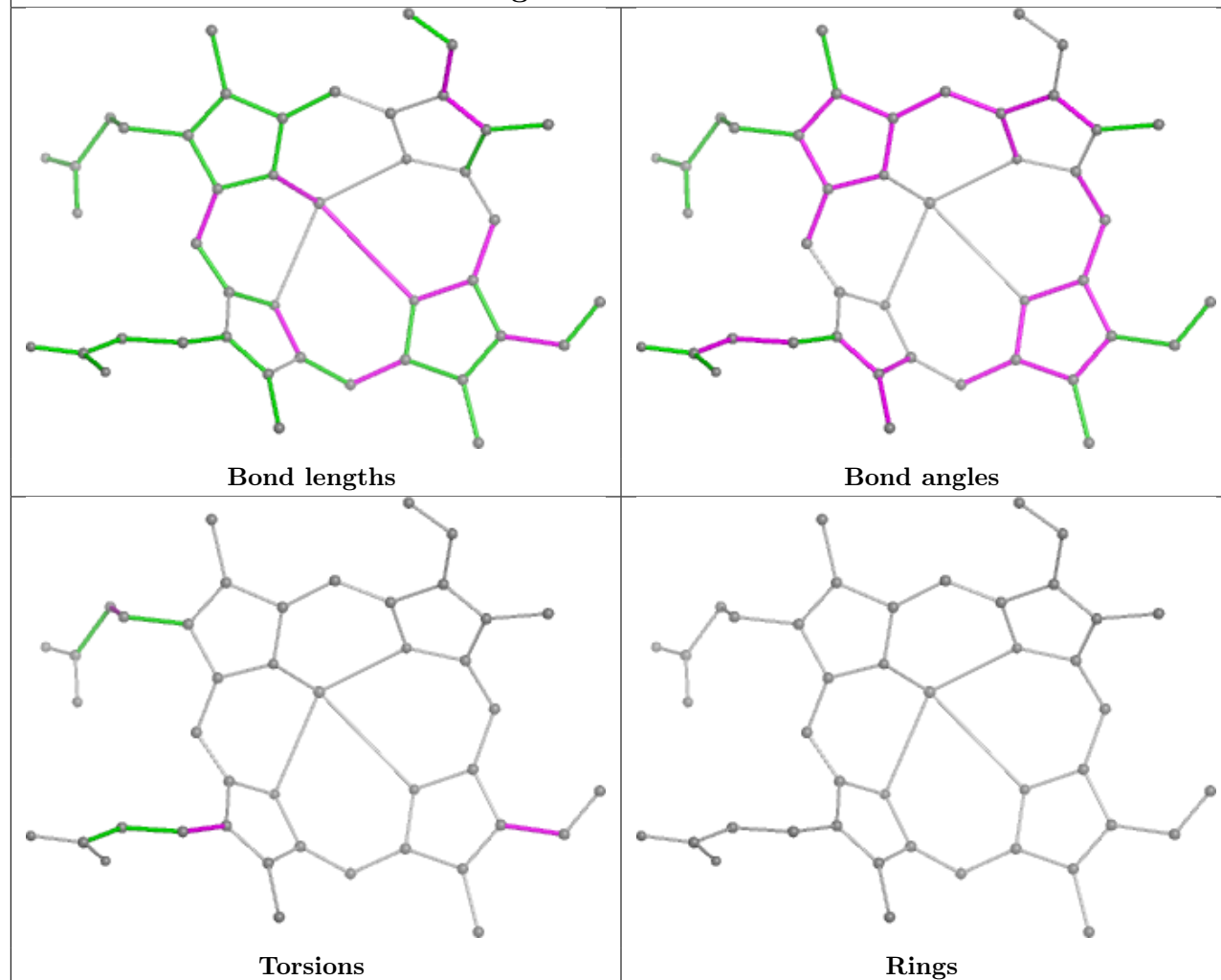


Torsions

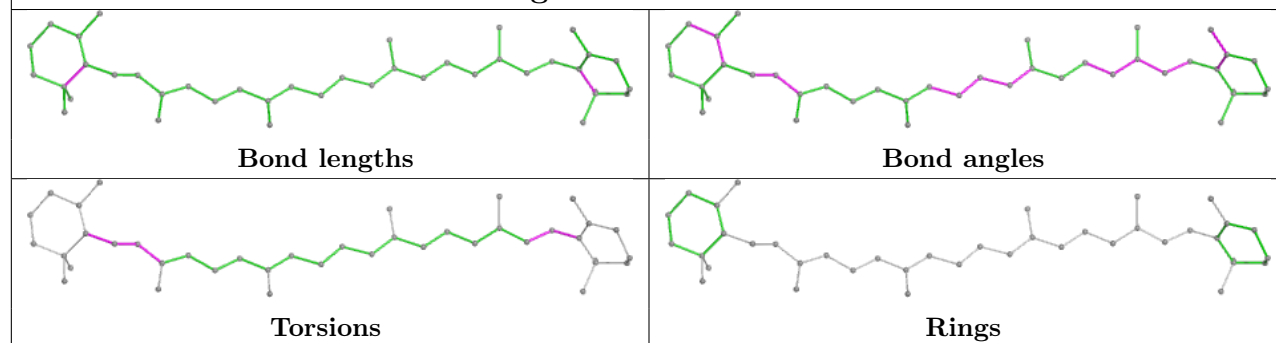


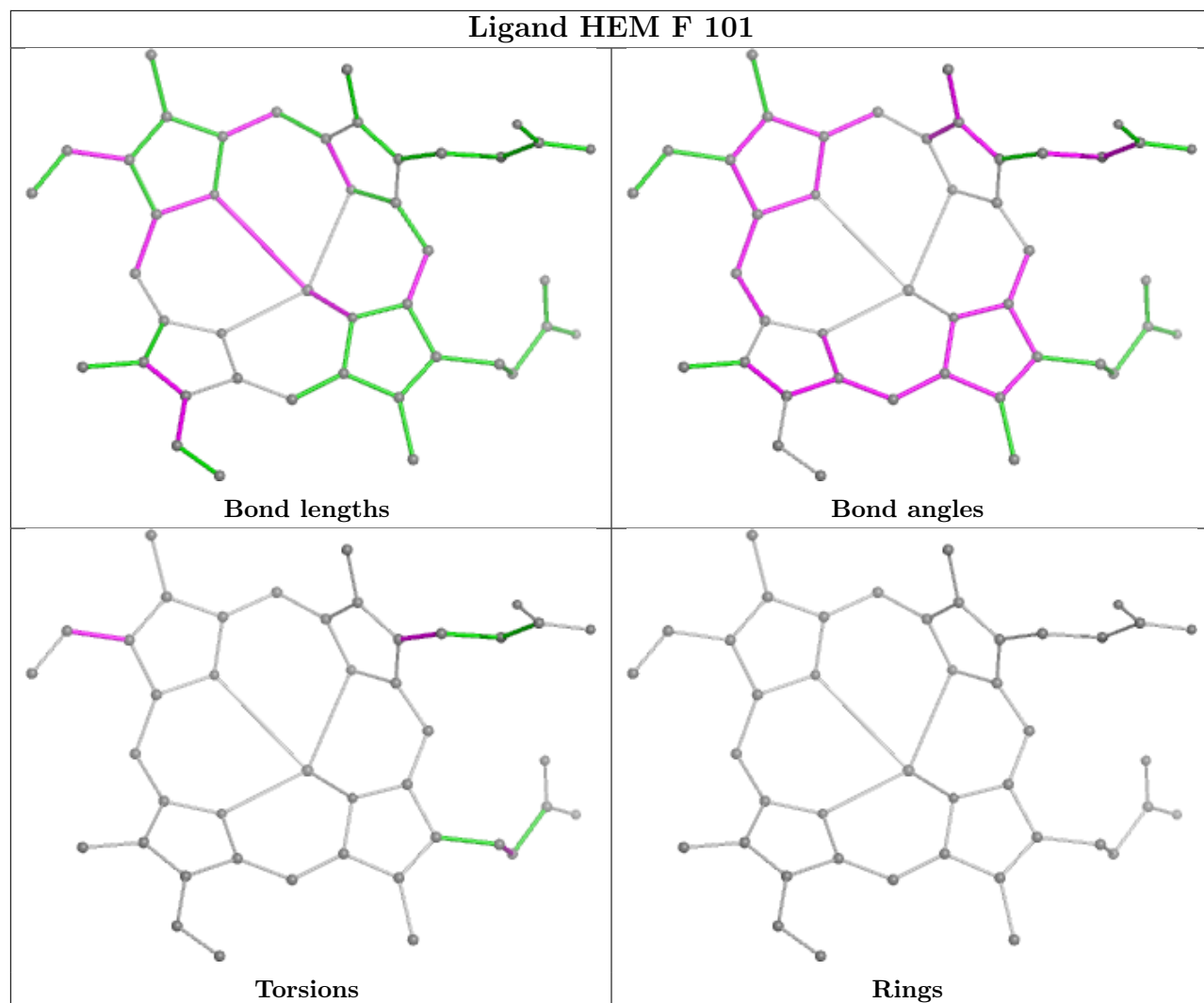
Rings

## Ligand HEM f 101

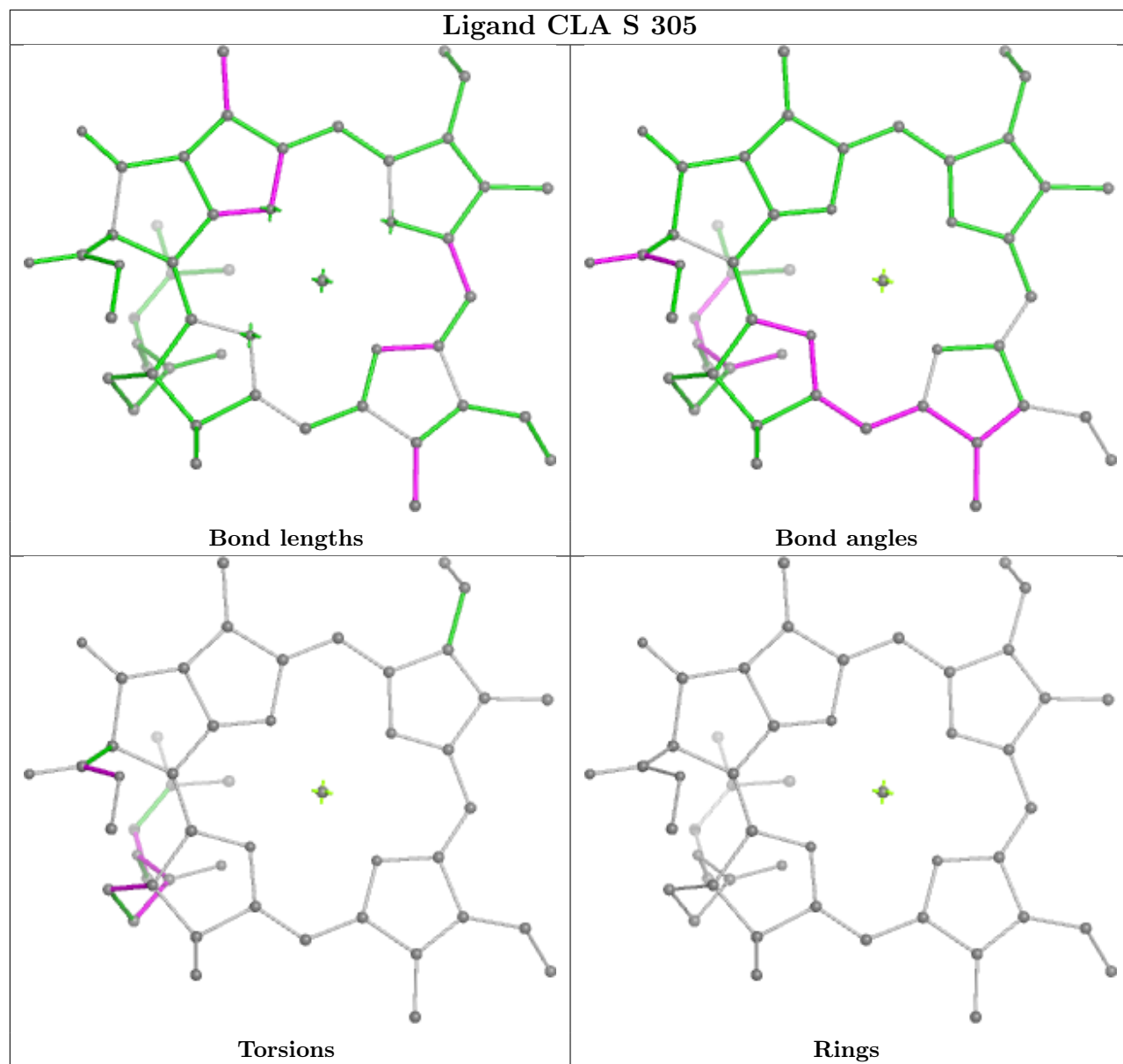


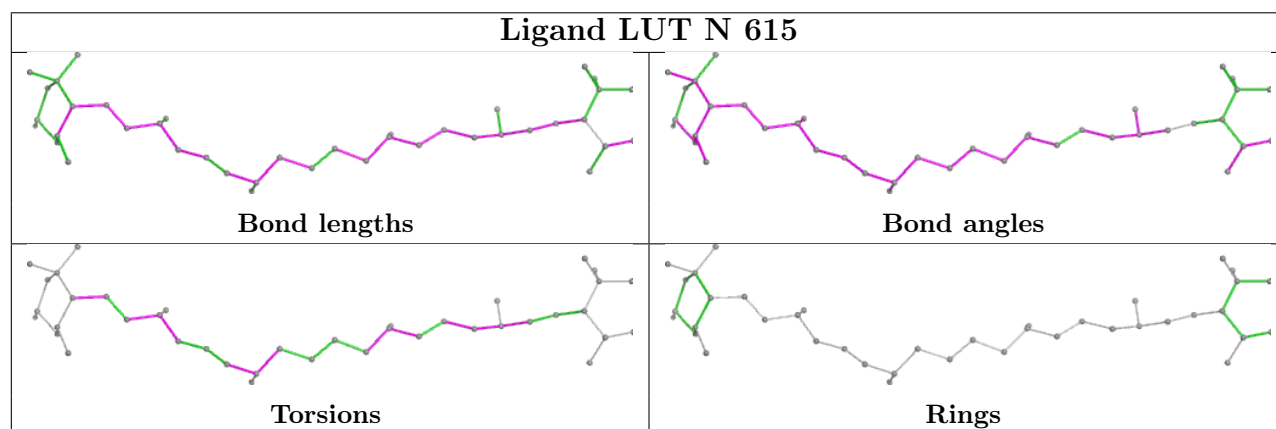
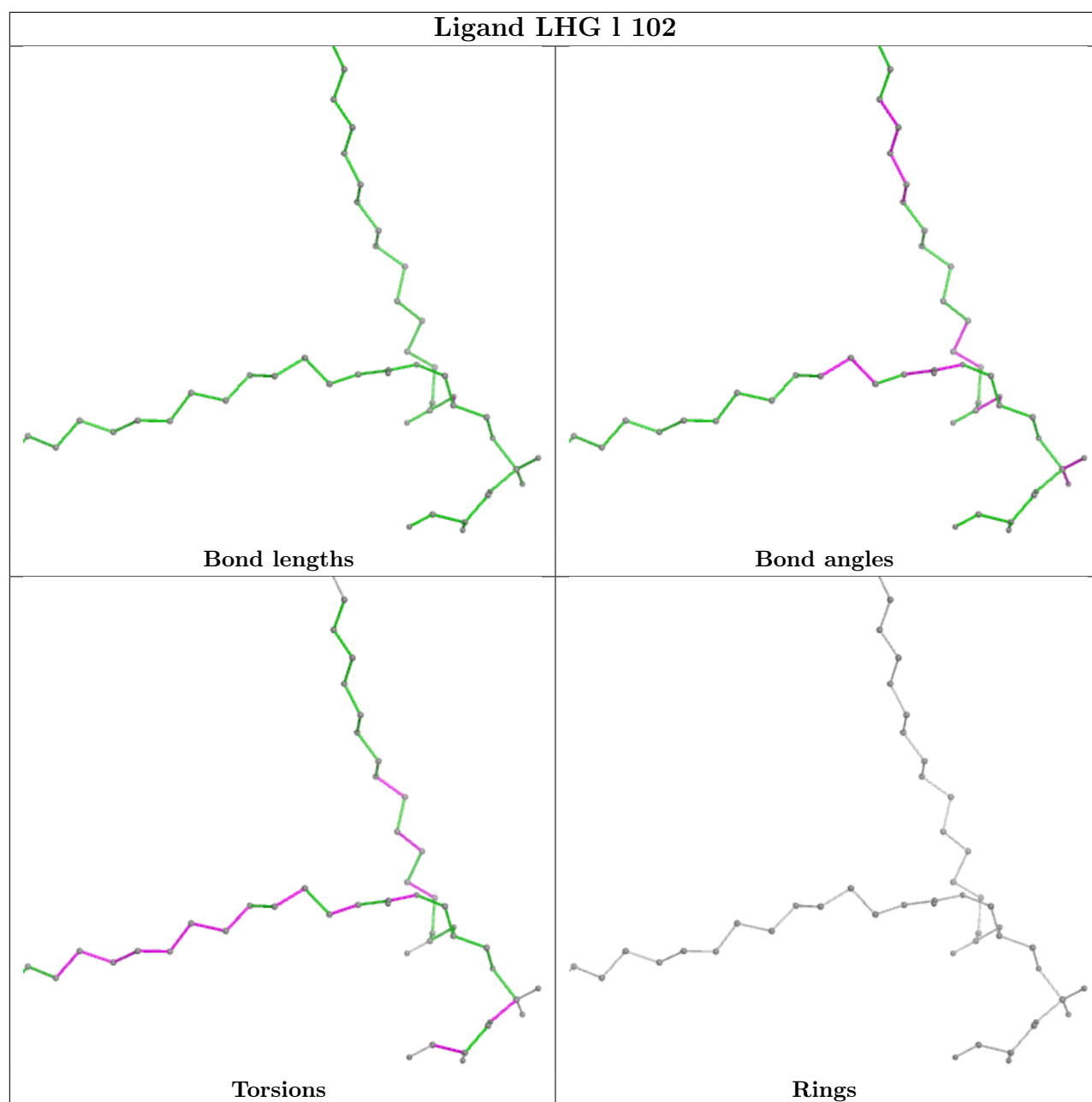
## Ligand BCR B 619

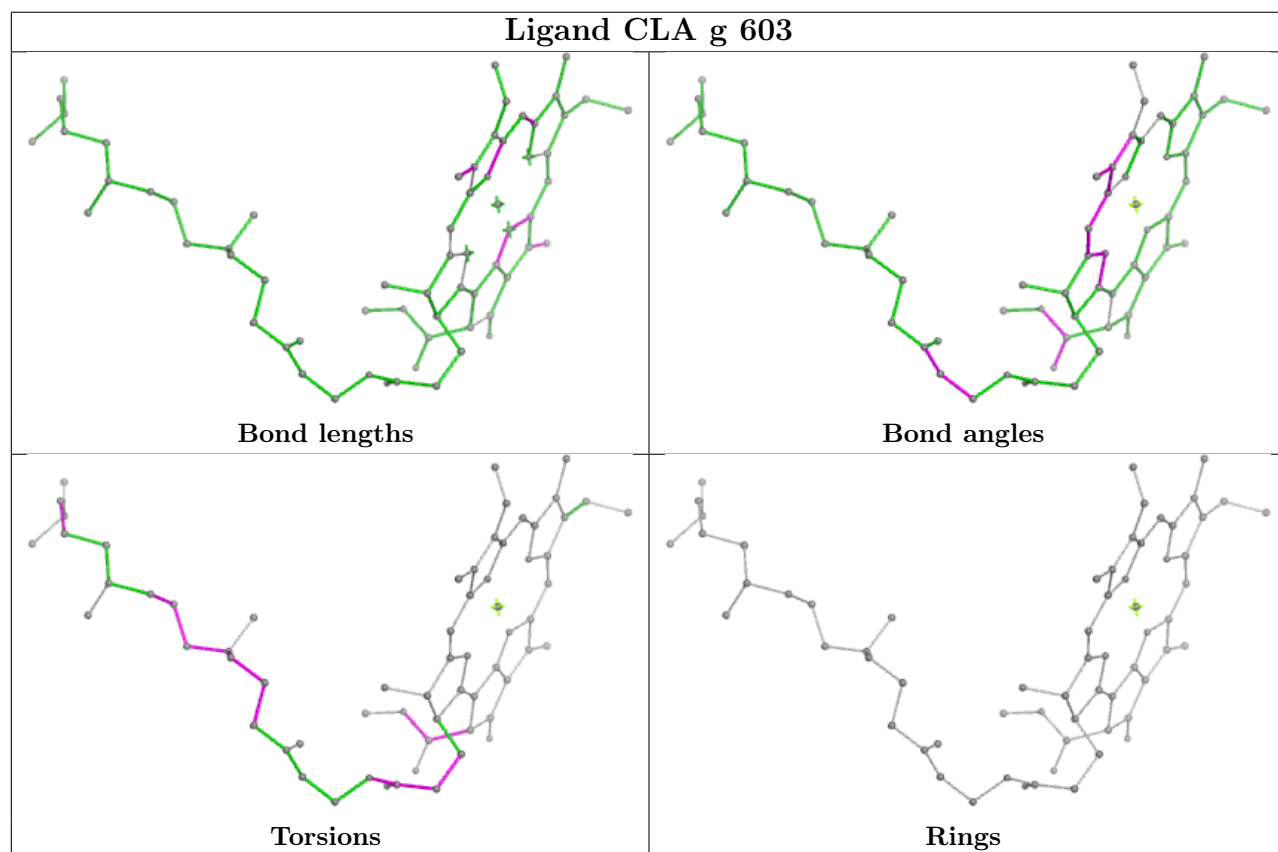
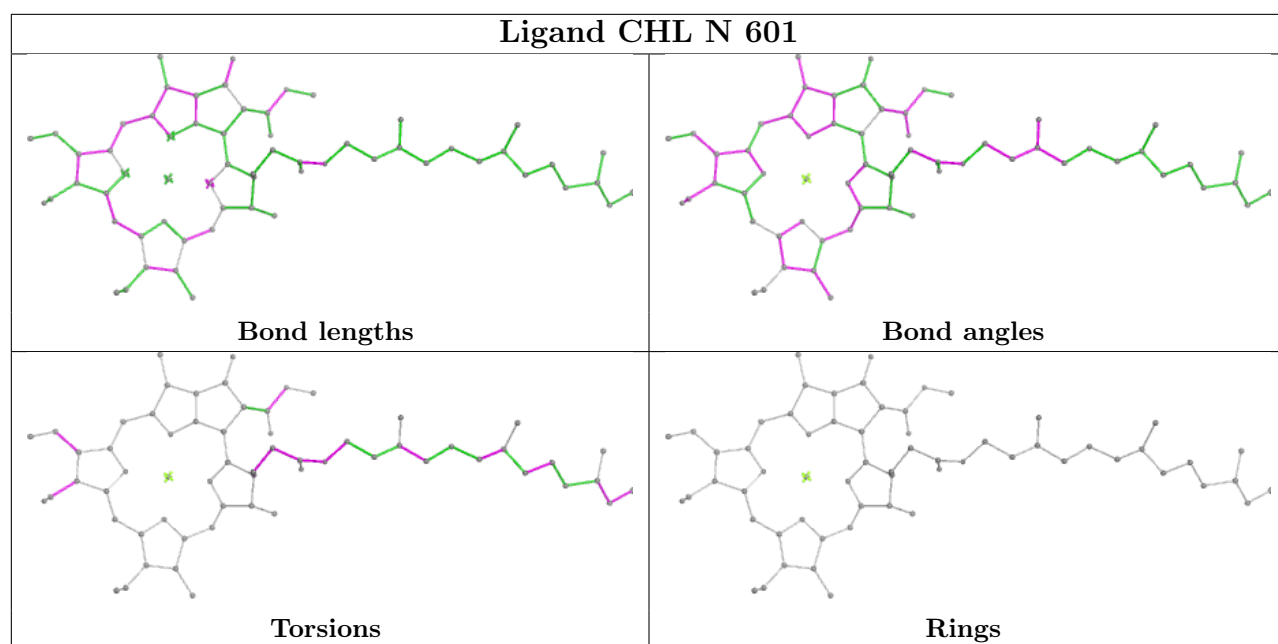


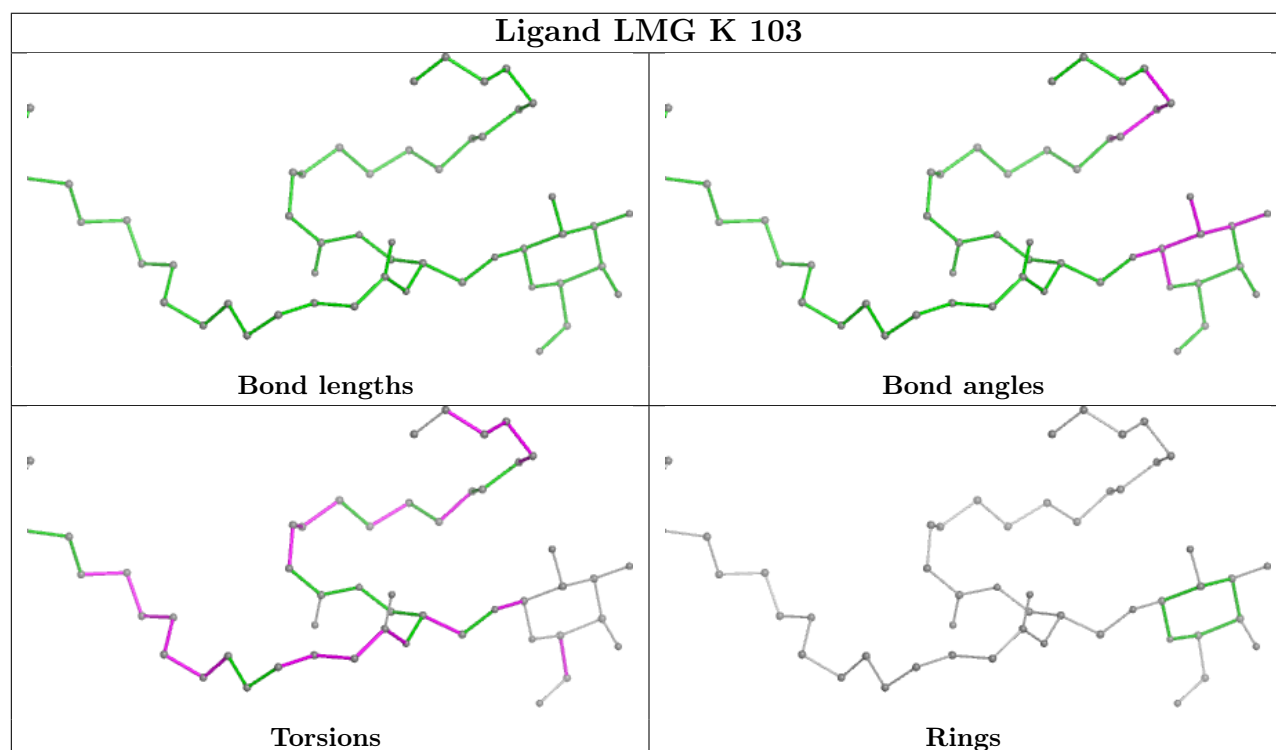
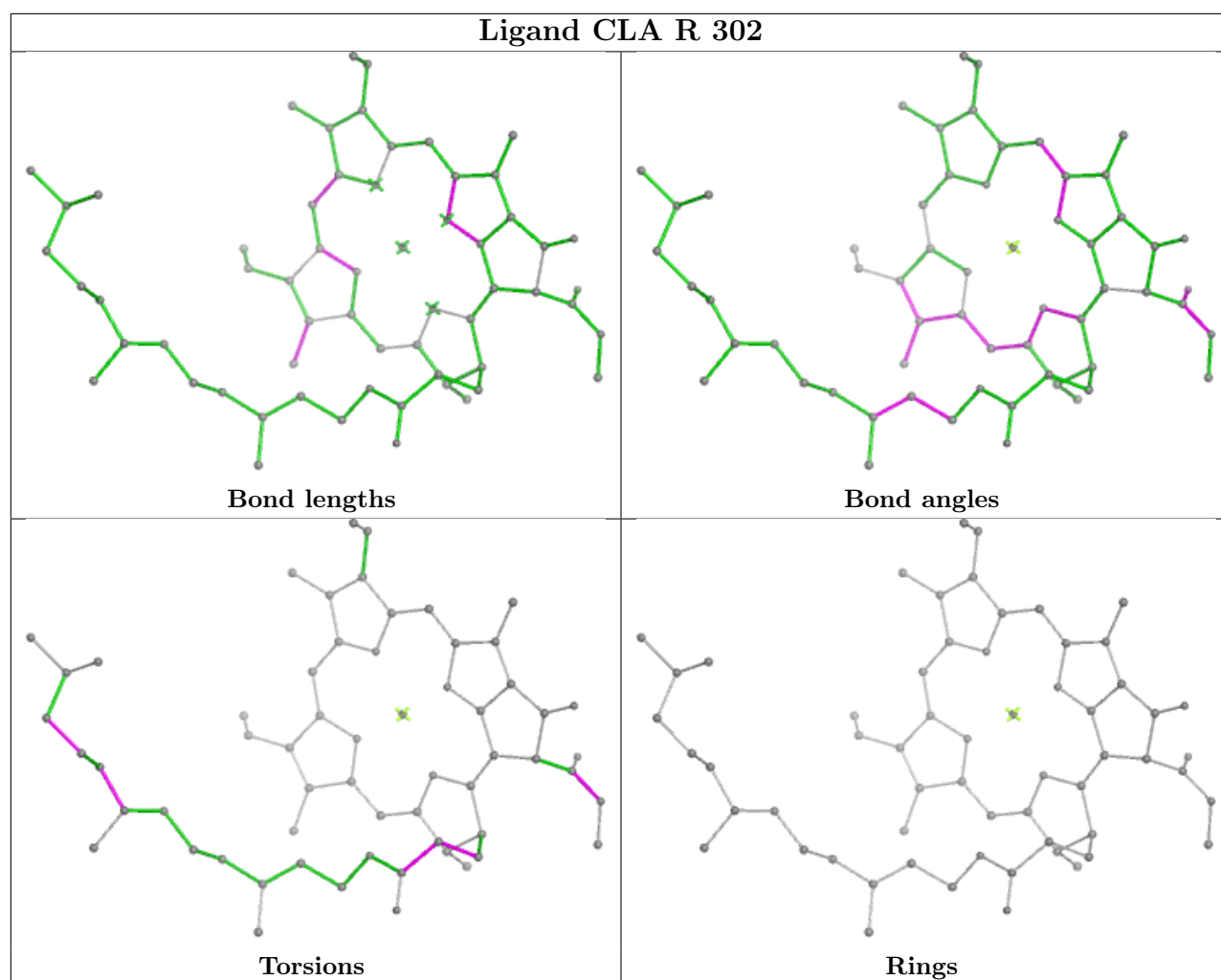


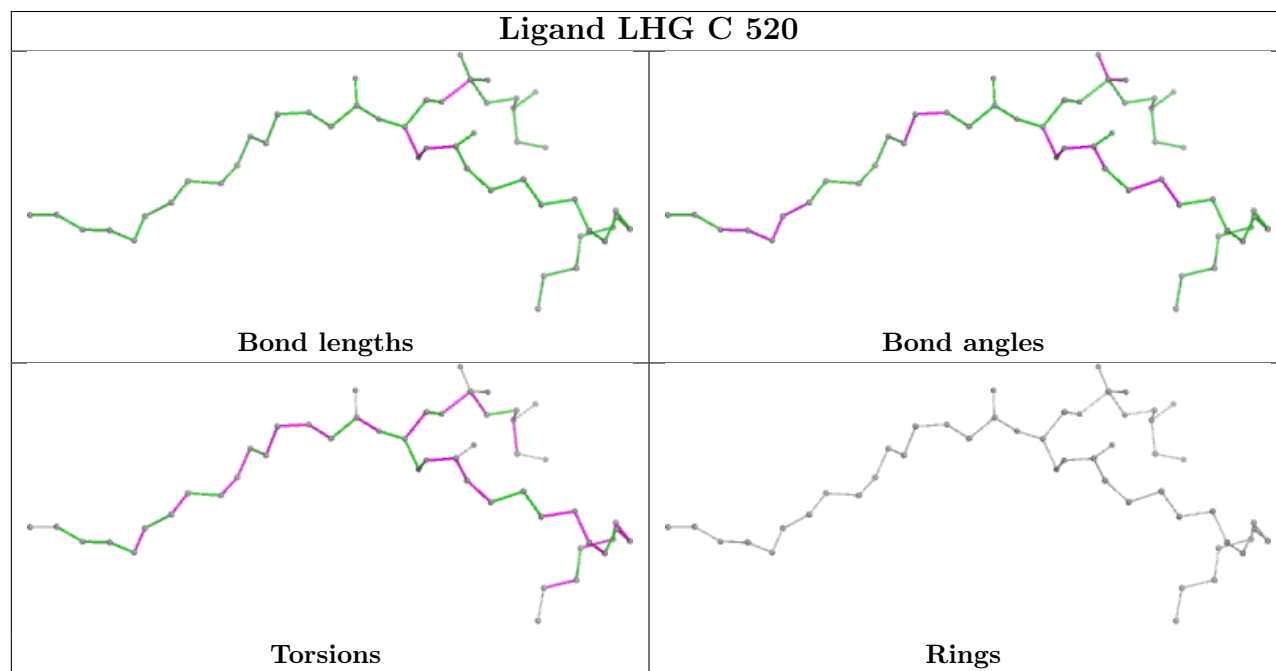
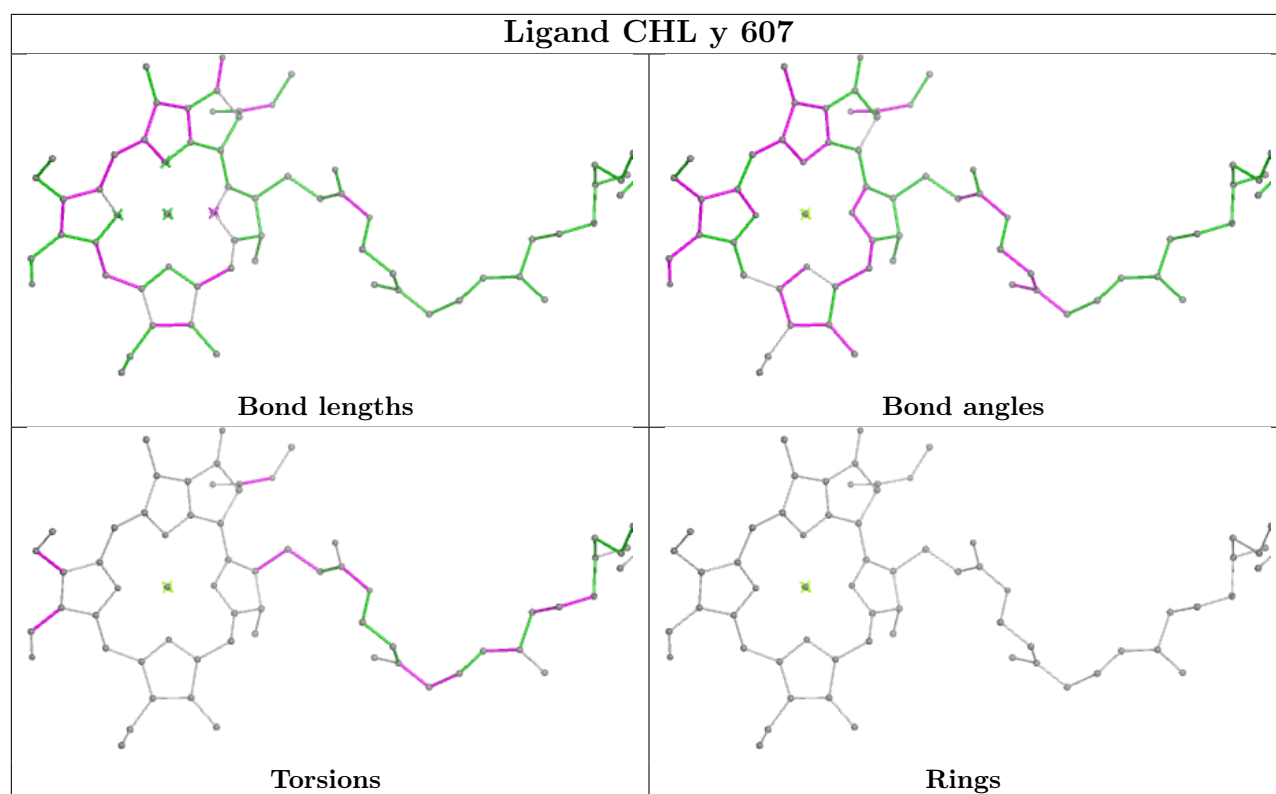
## Ligand CLA S 305

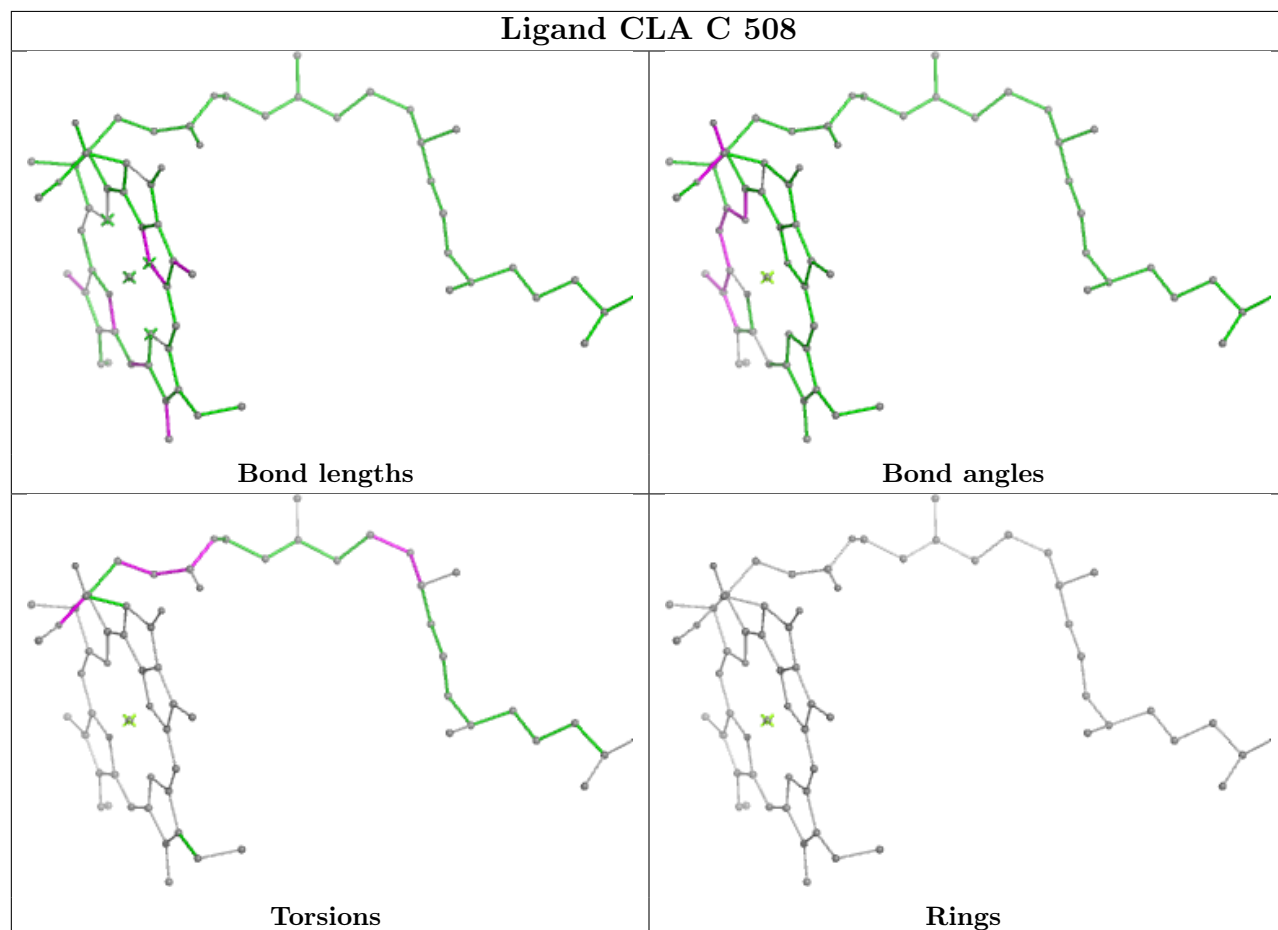
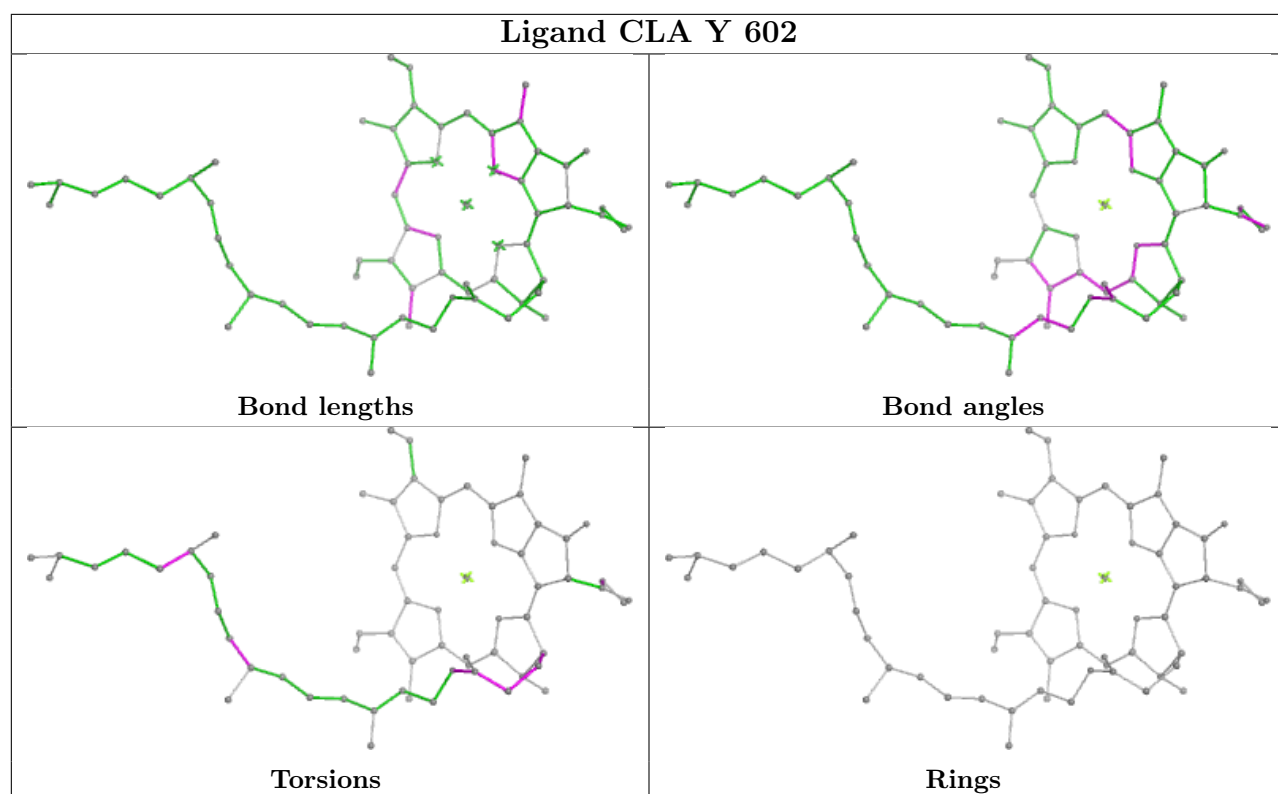


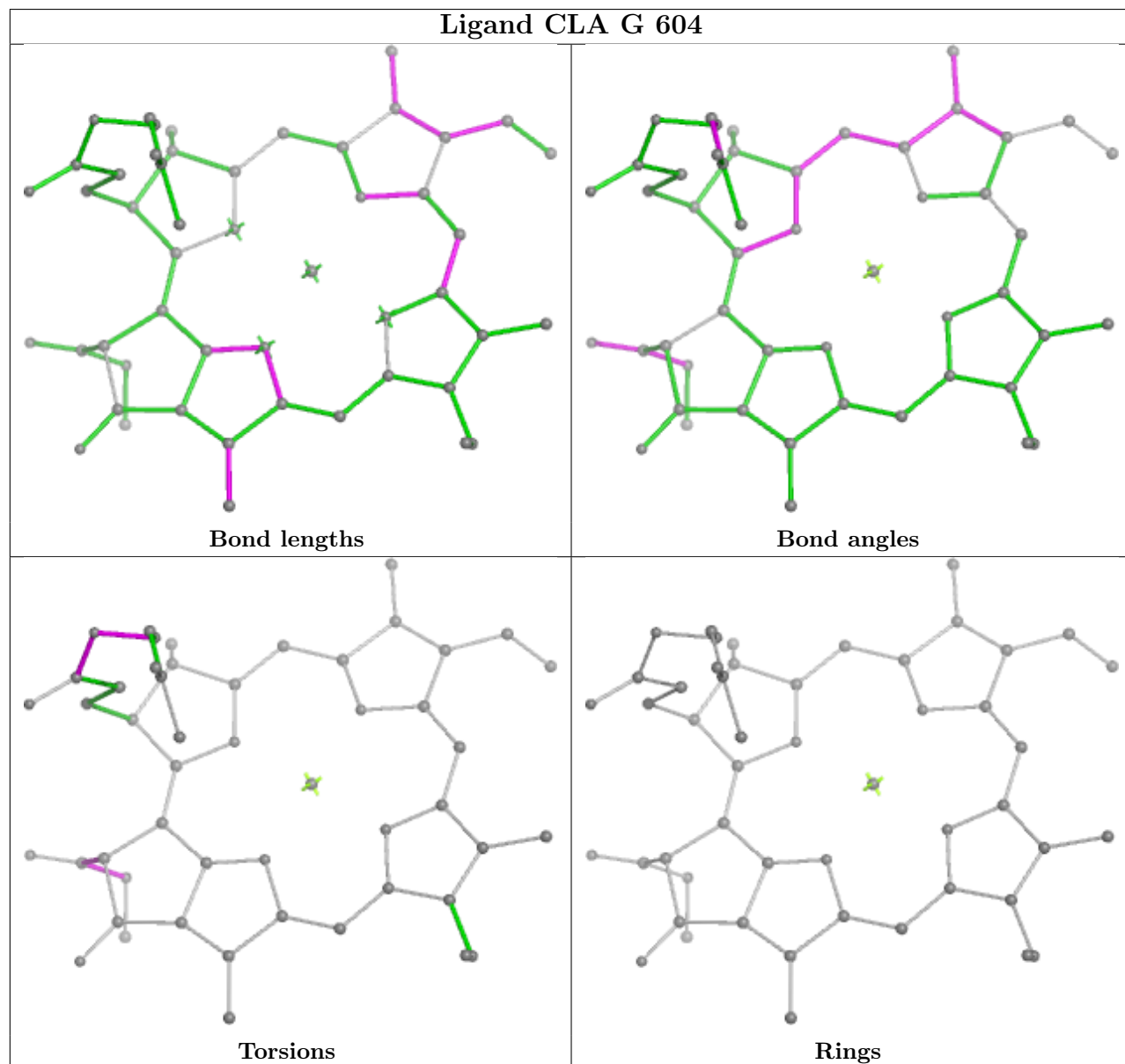
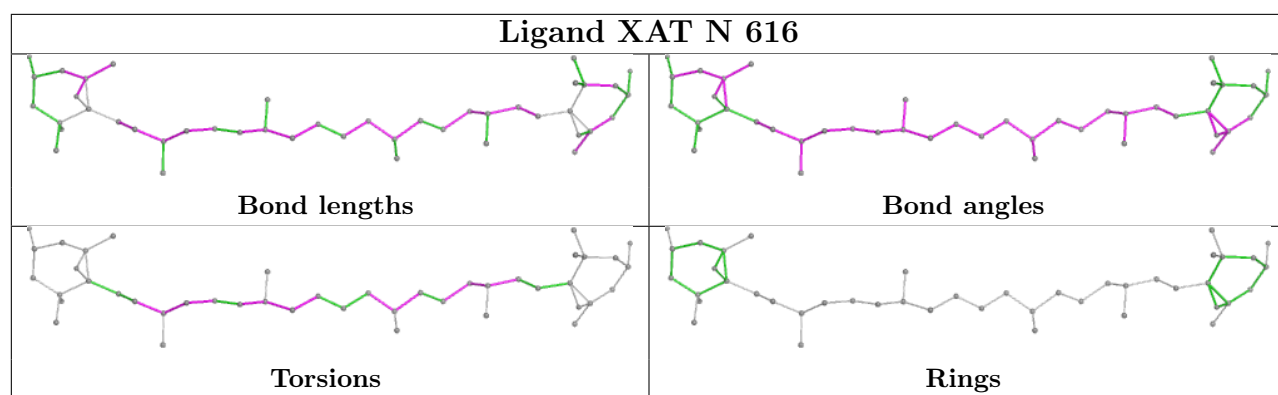


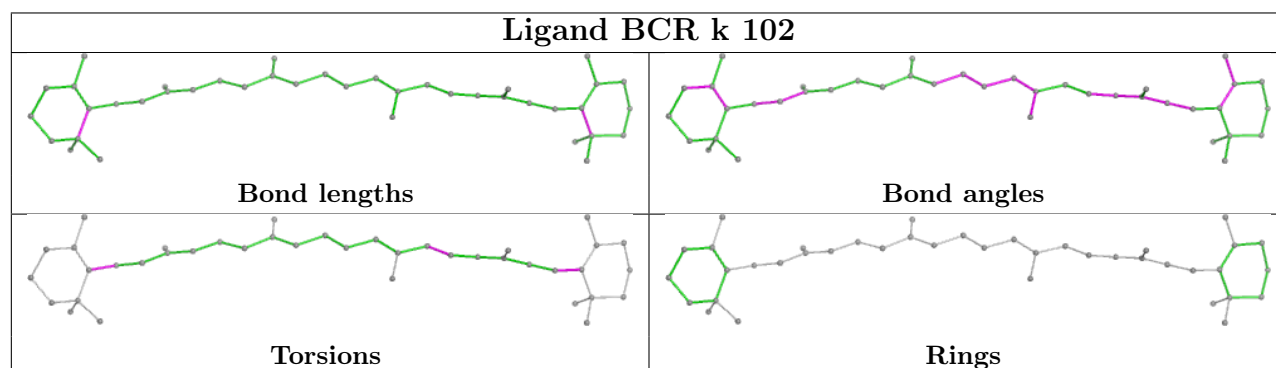
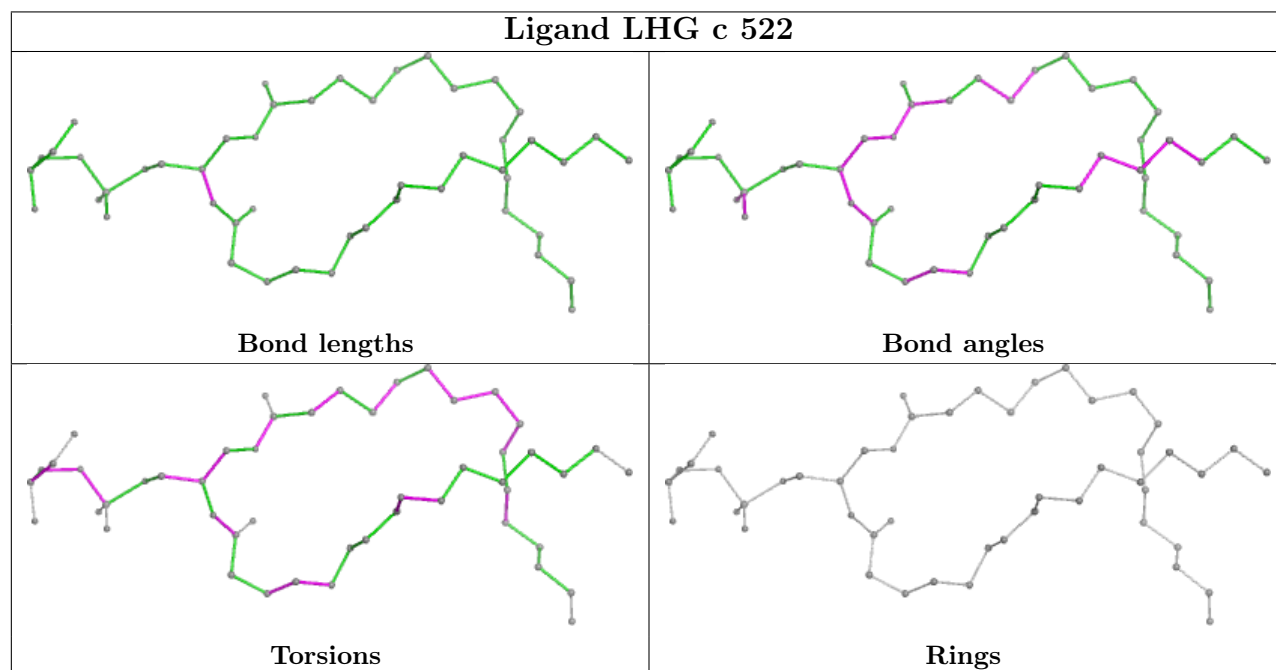
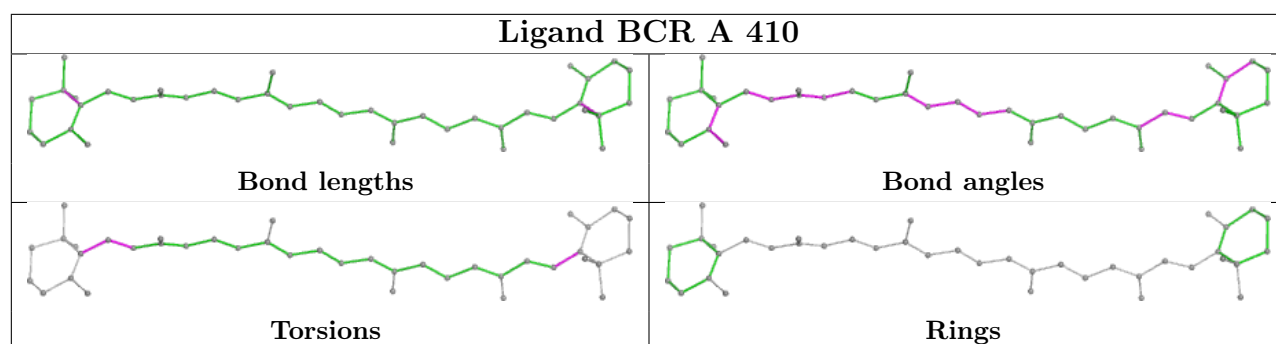


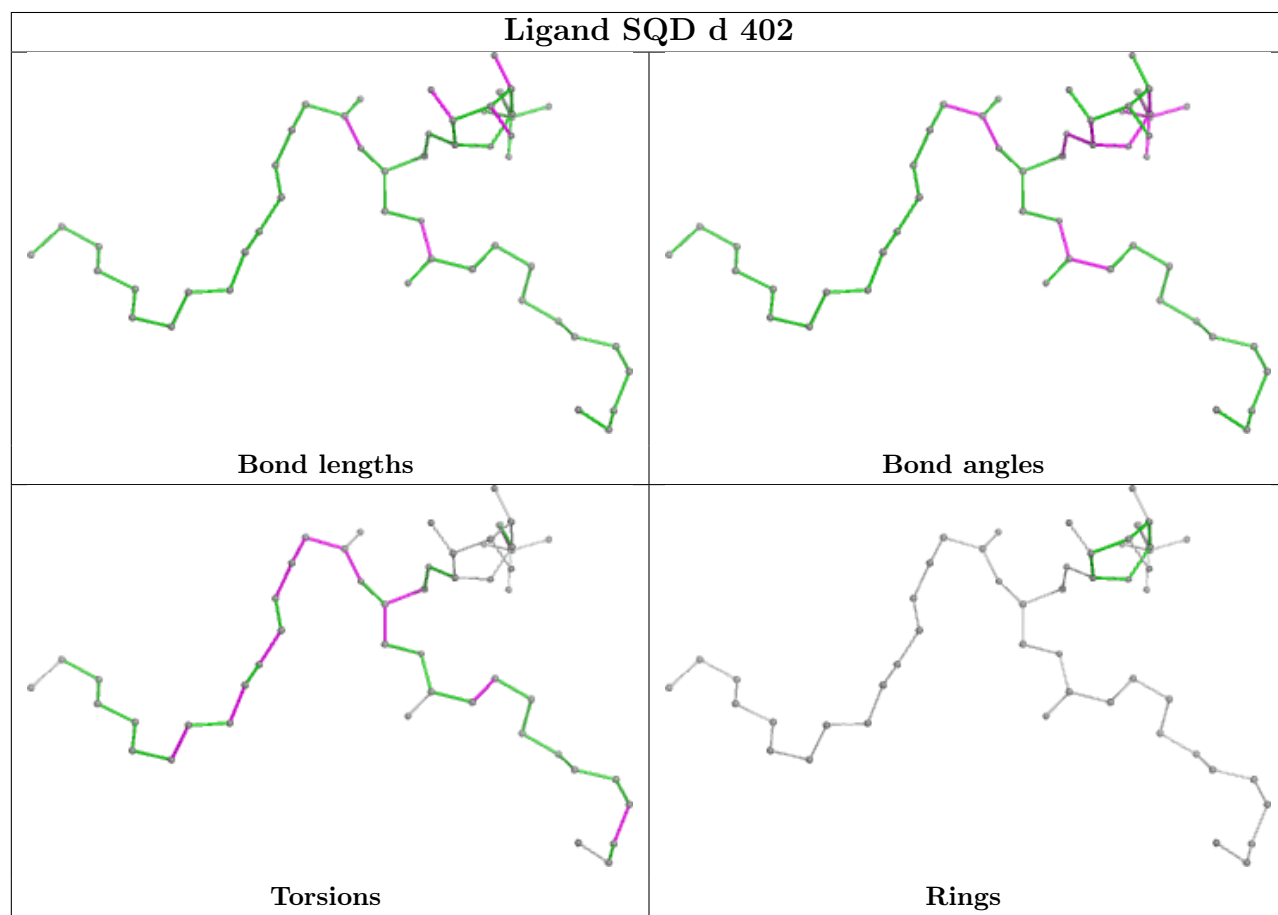
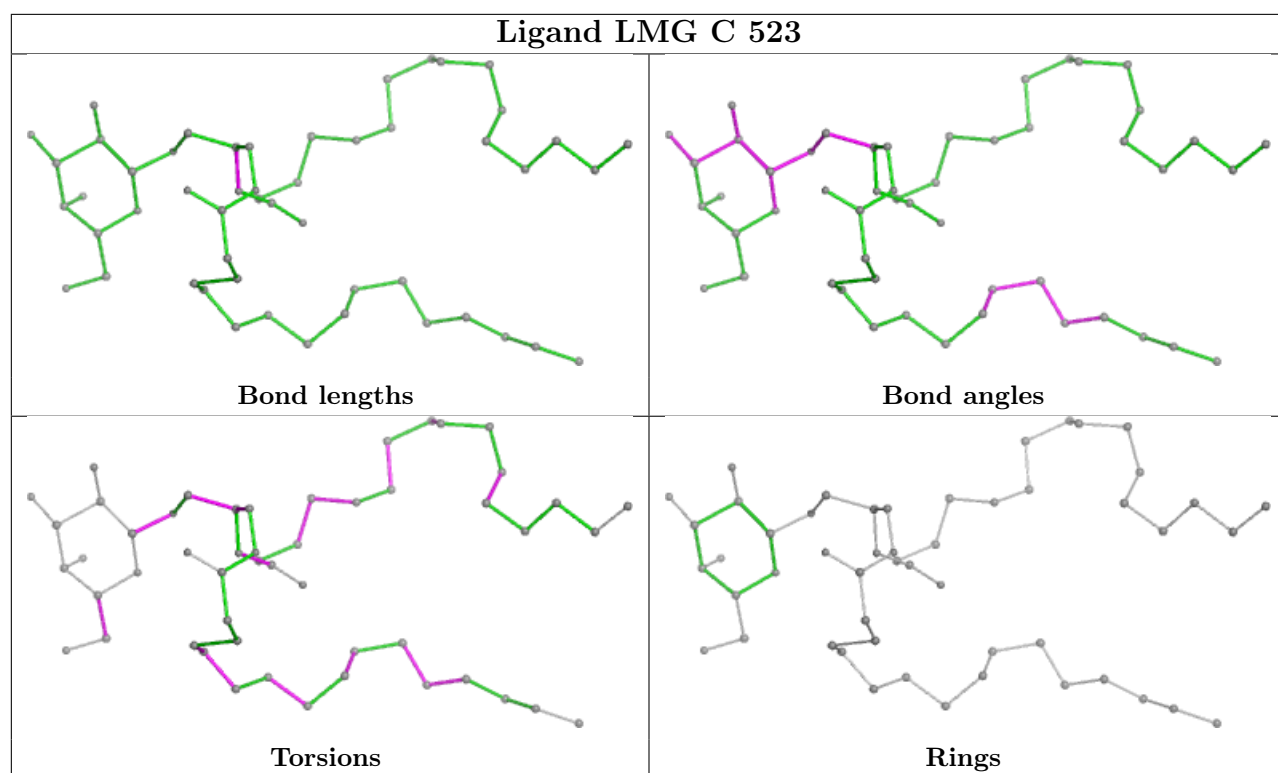


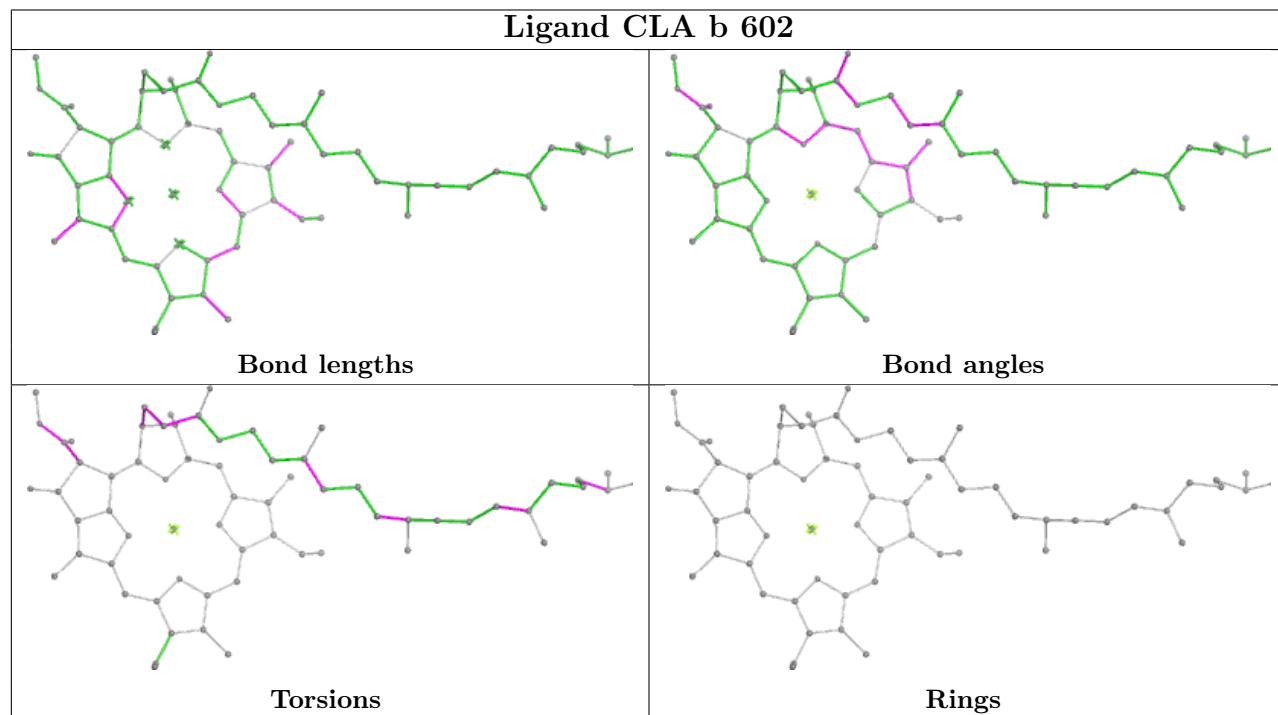
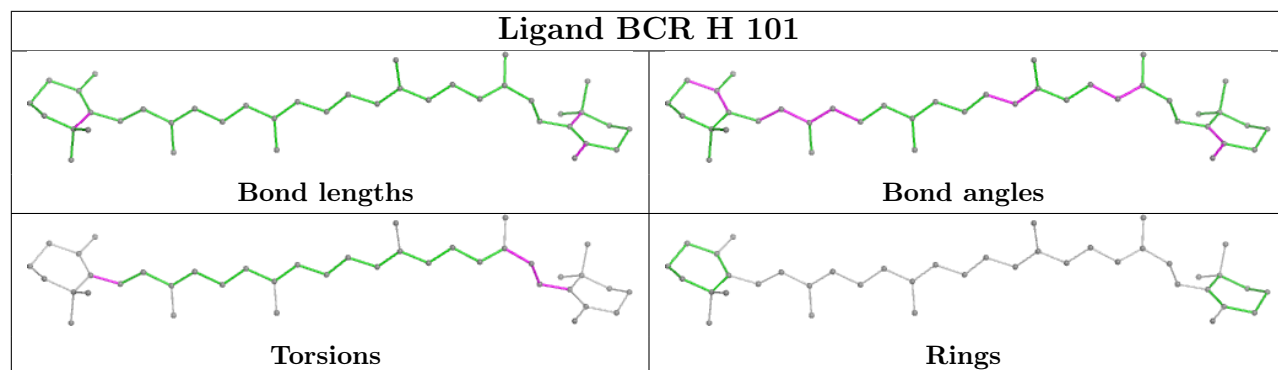


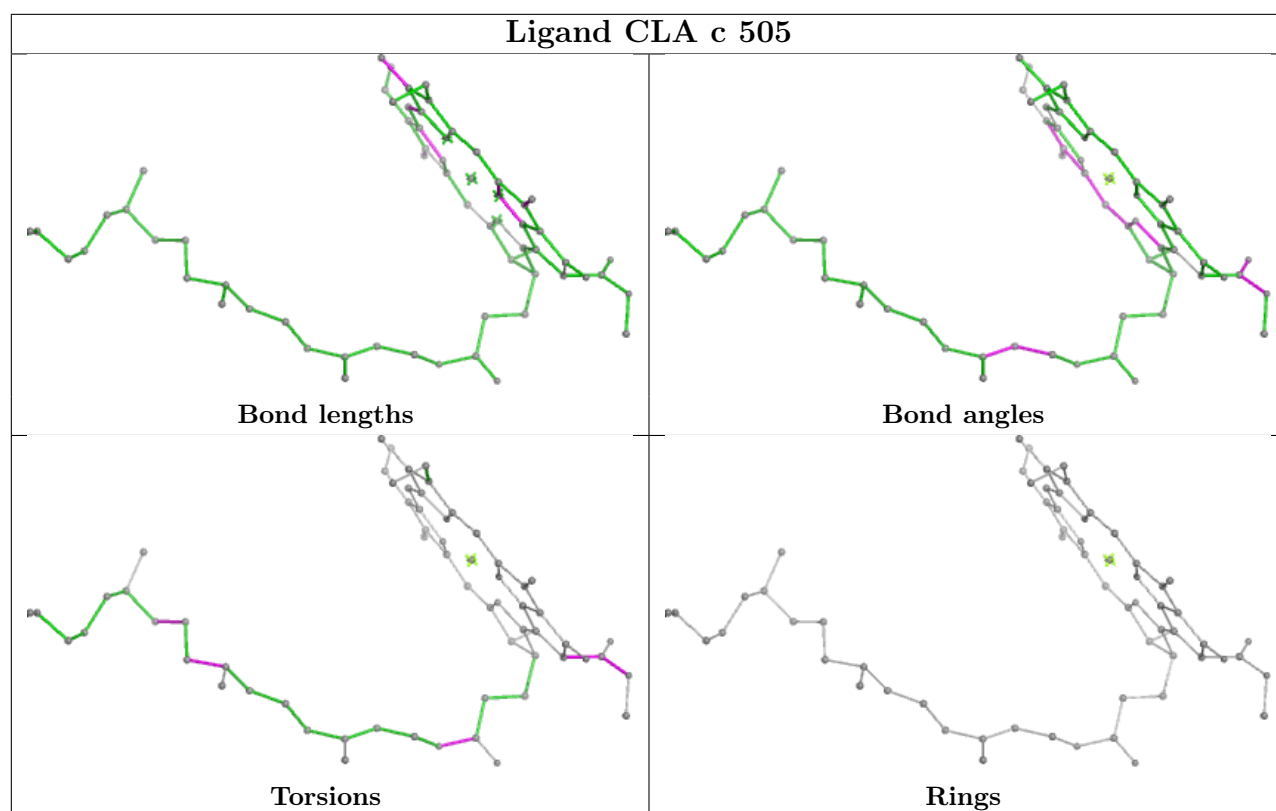




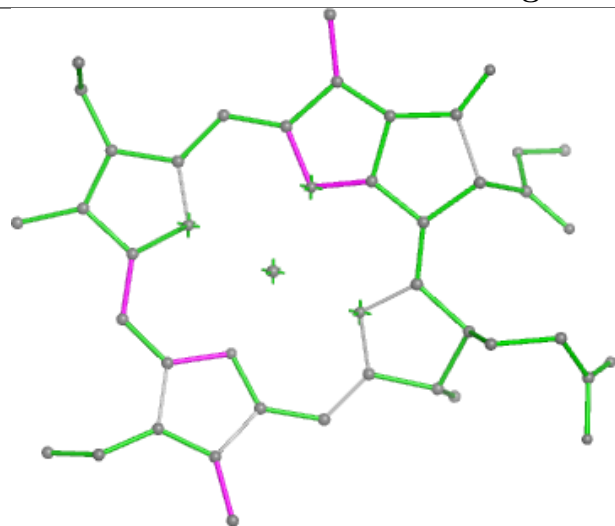




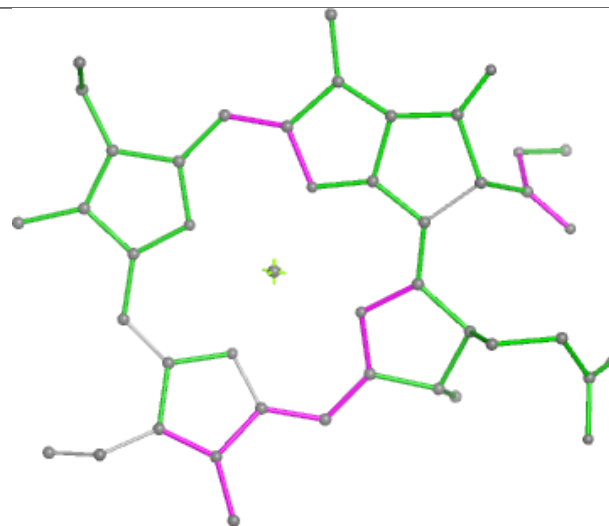




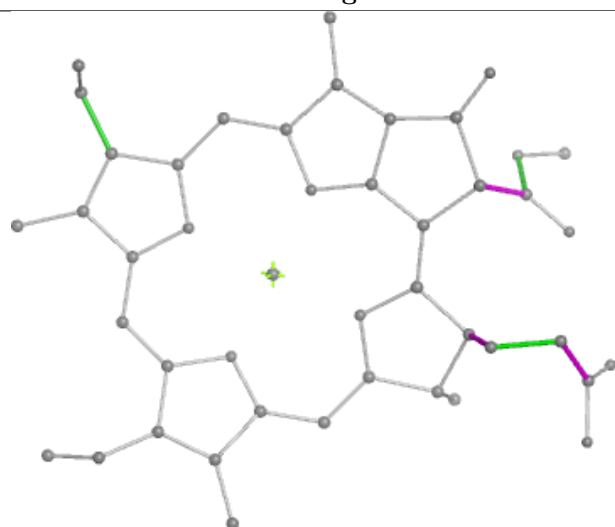
## Ligand CLA s 304



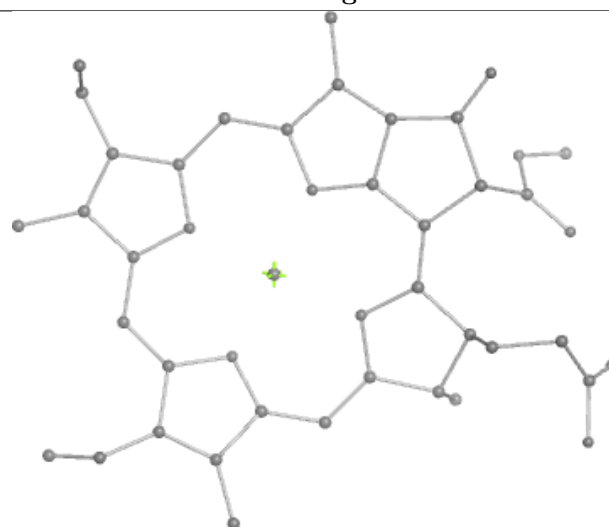
Bond lengths



Bond angles

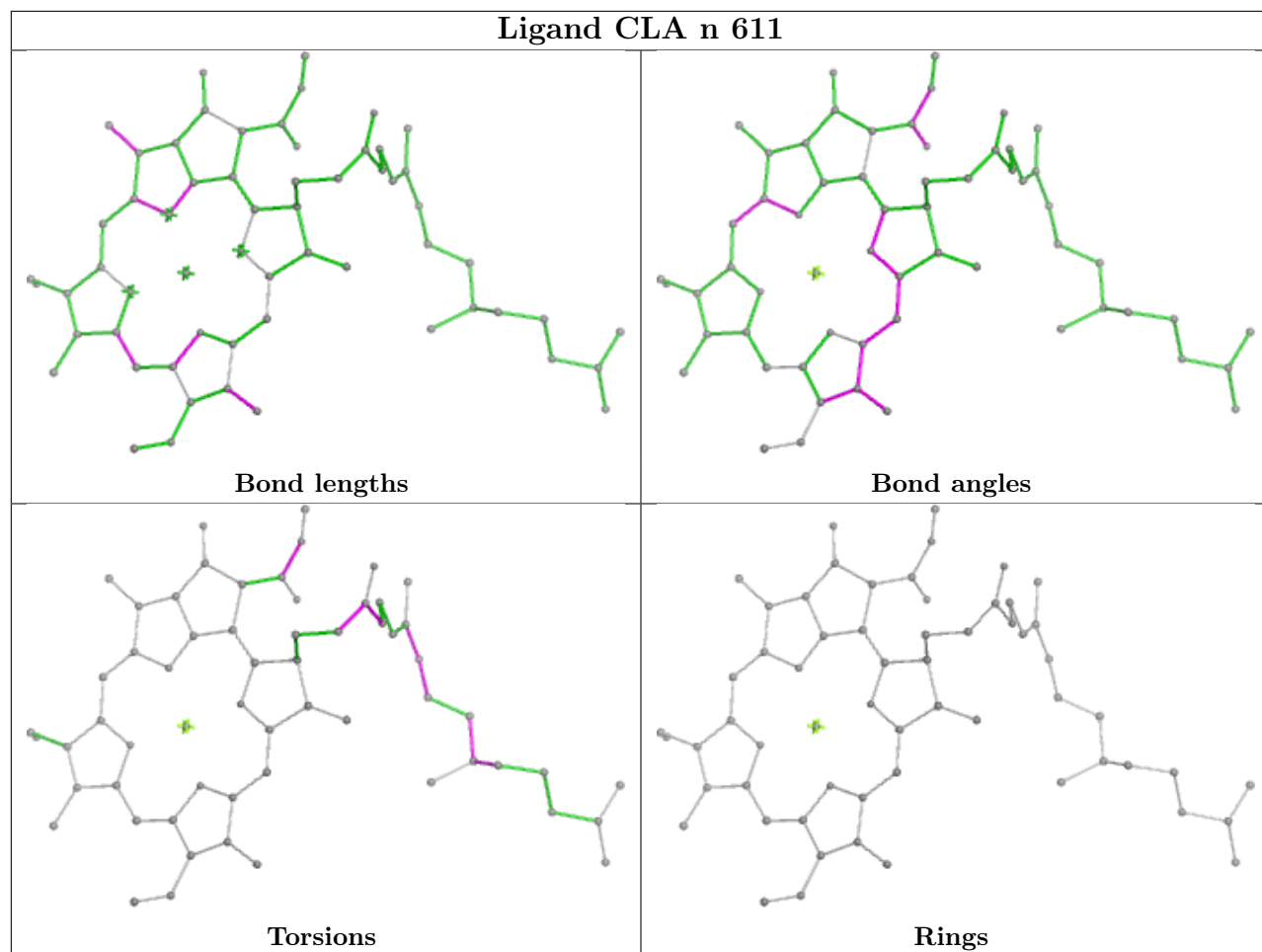


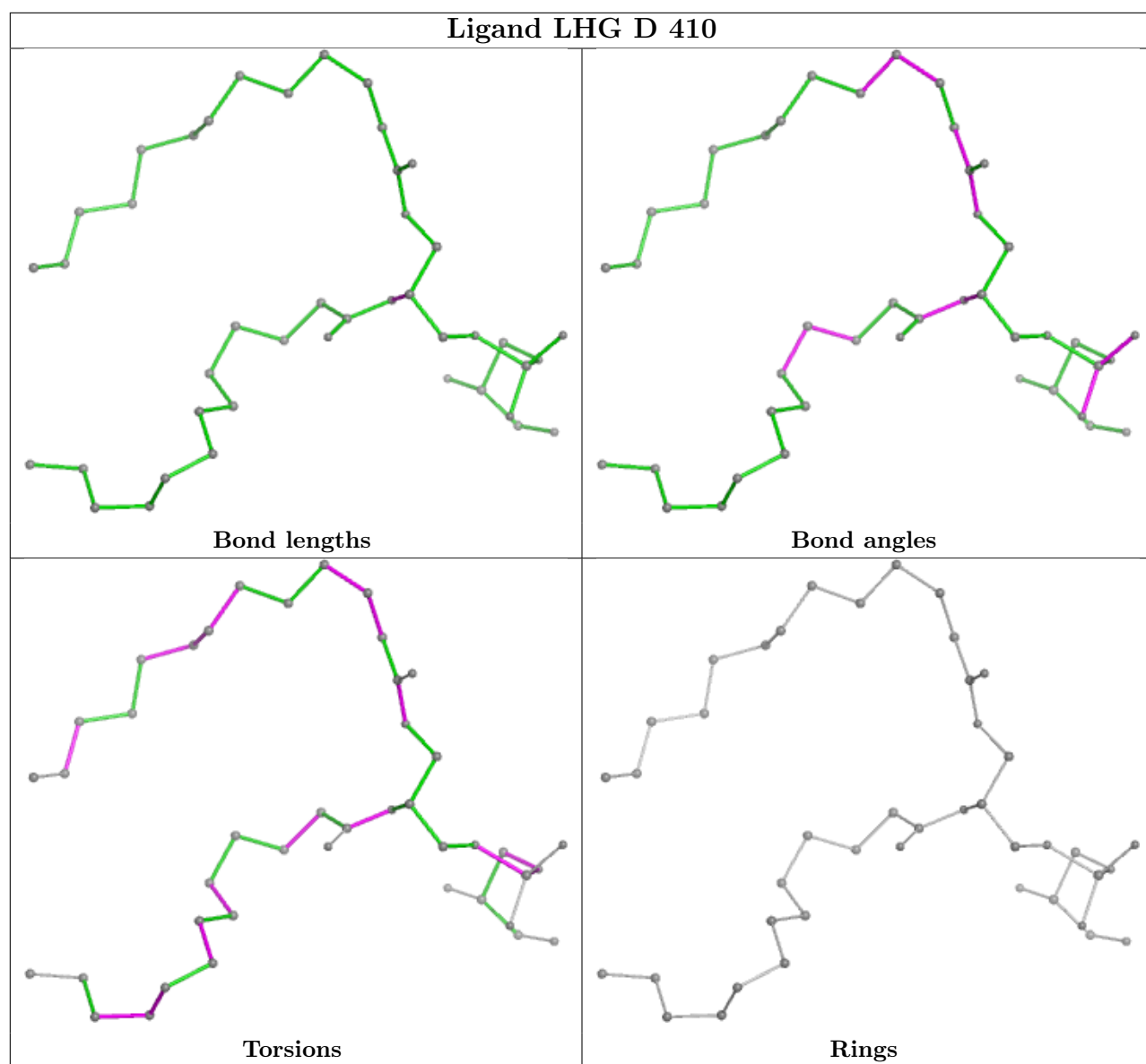
Torsions

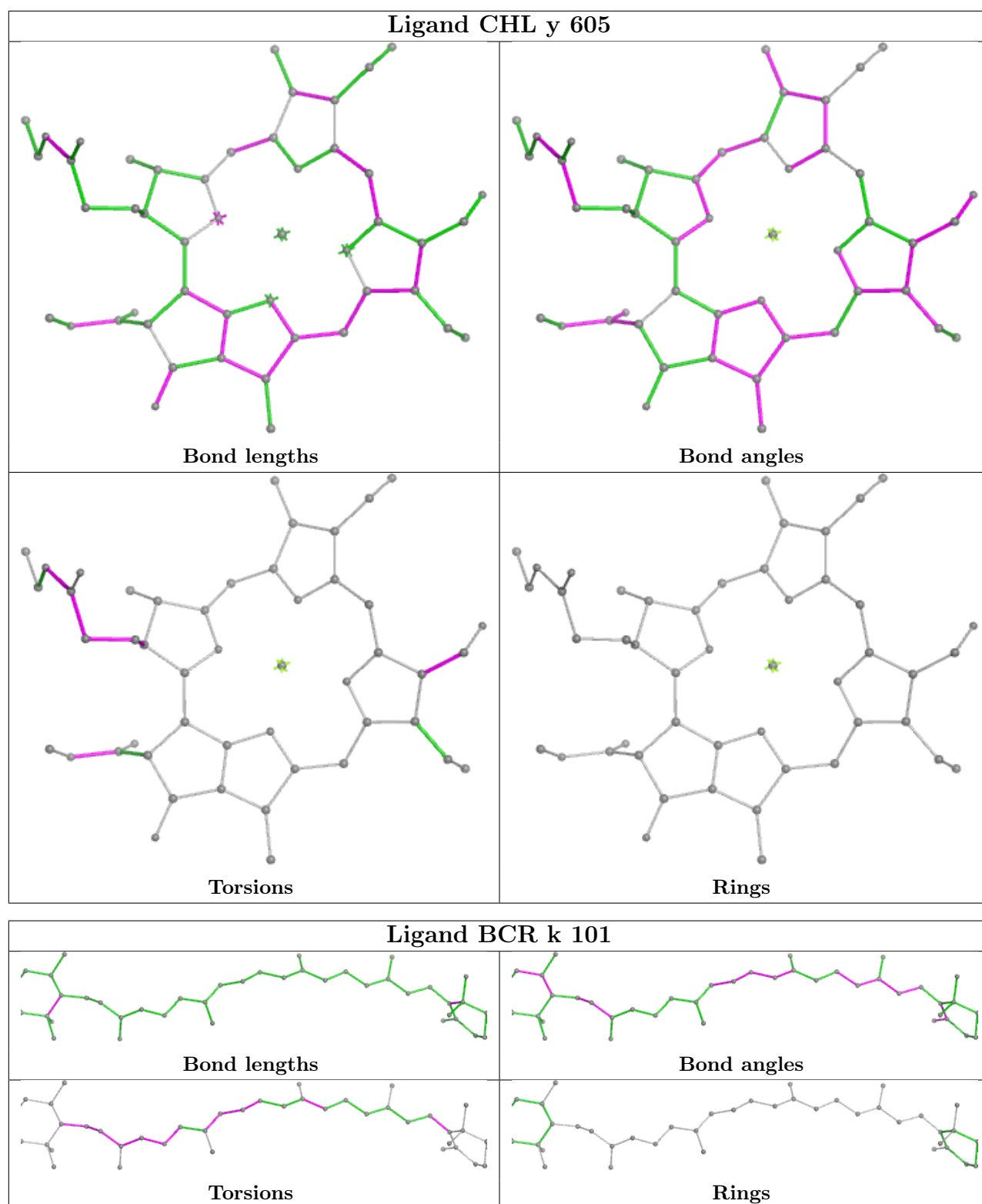


Rings

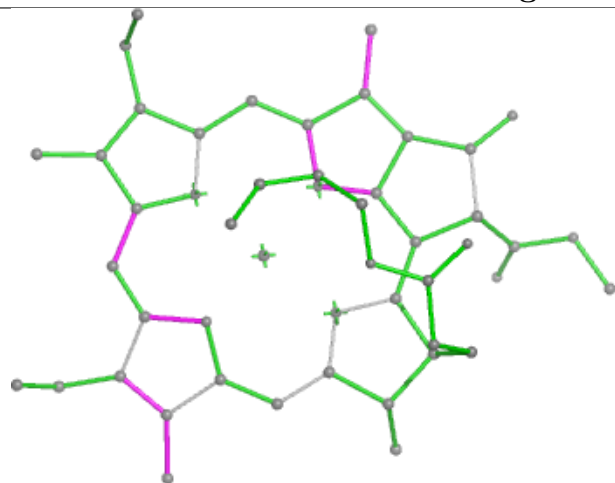
## Ligand CLA n 611



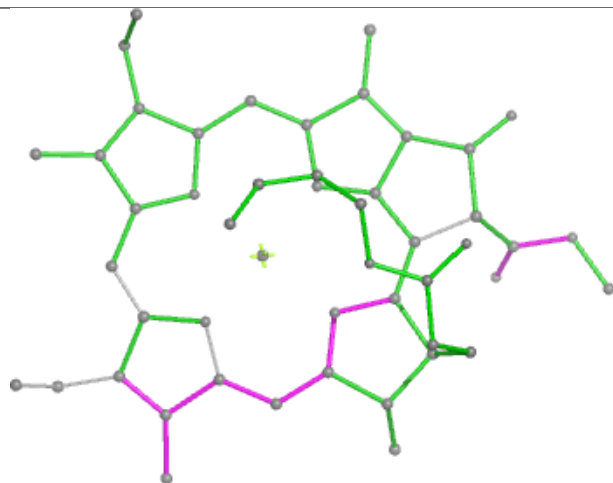




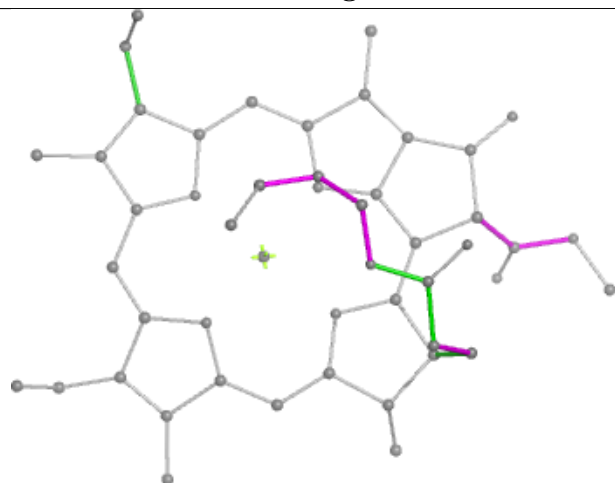
## Ligand CLA S 312



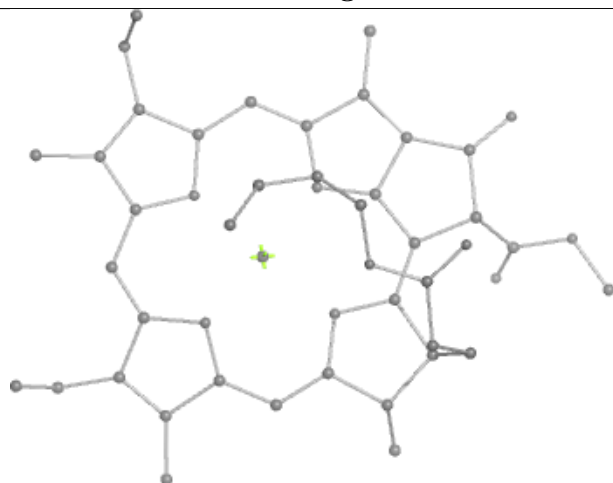
Bond lengths



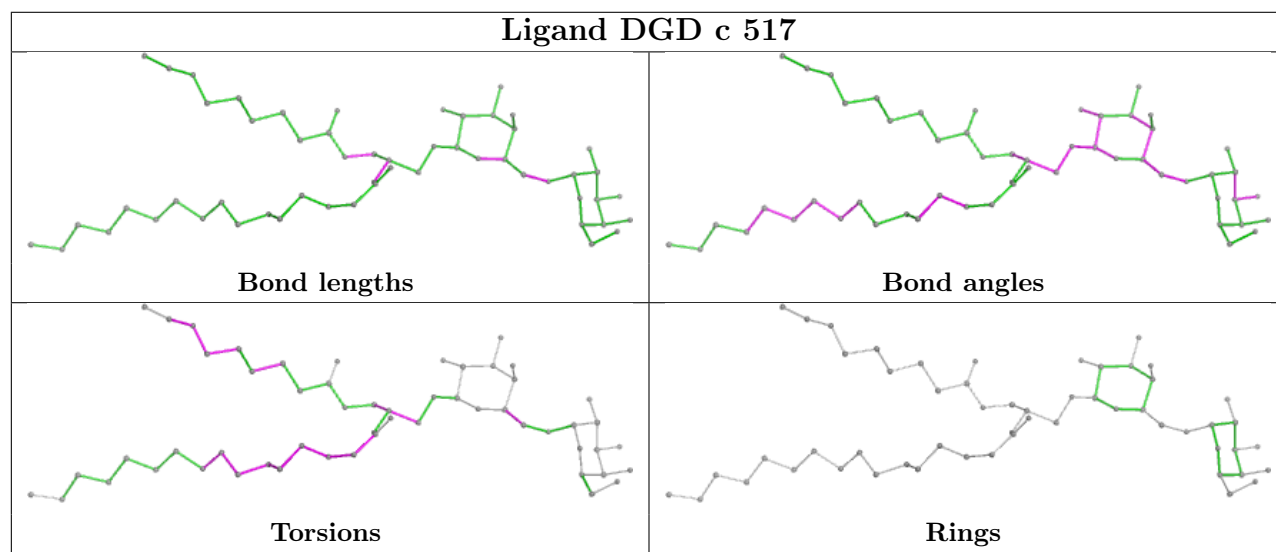
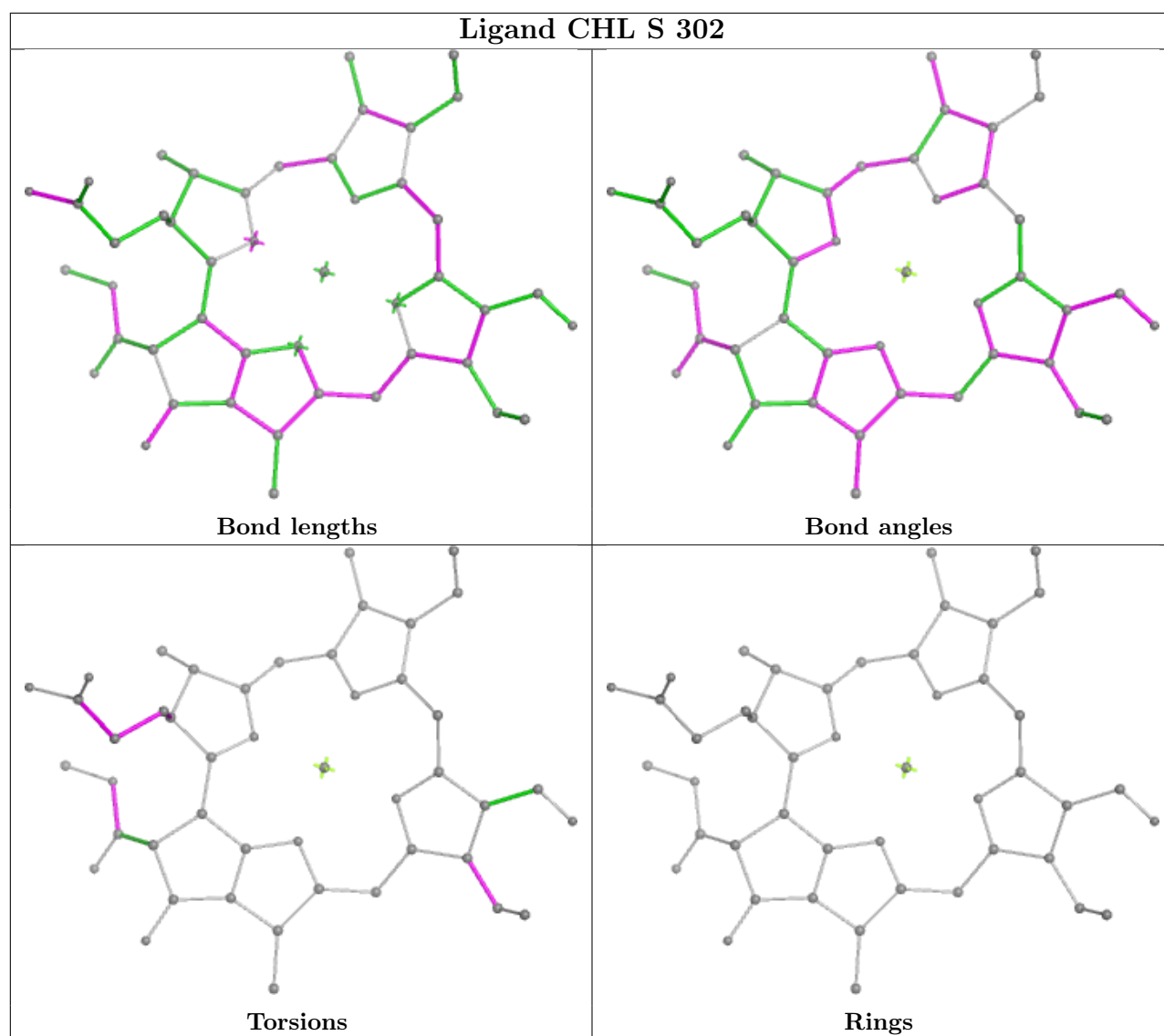
Bond angles

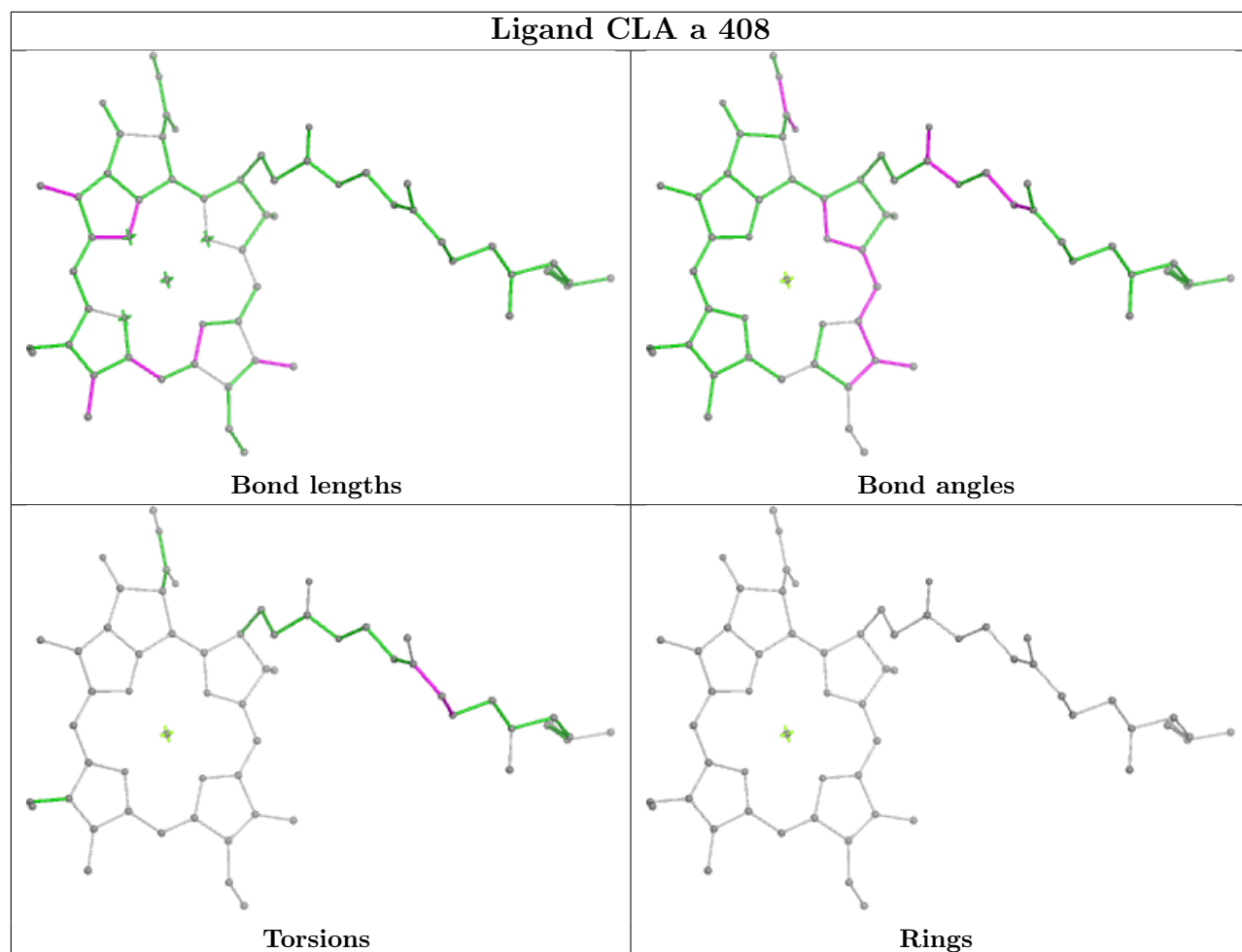
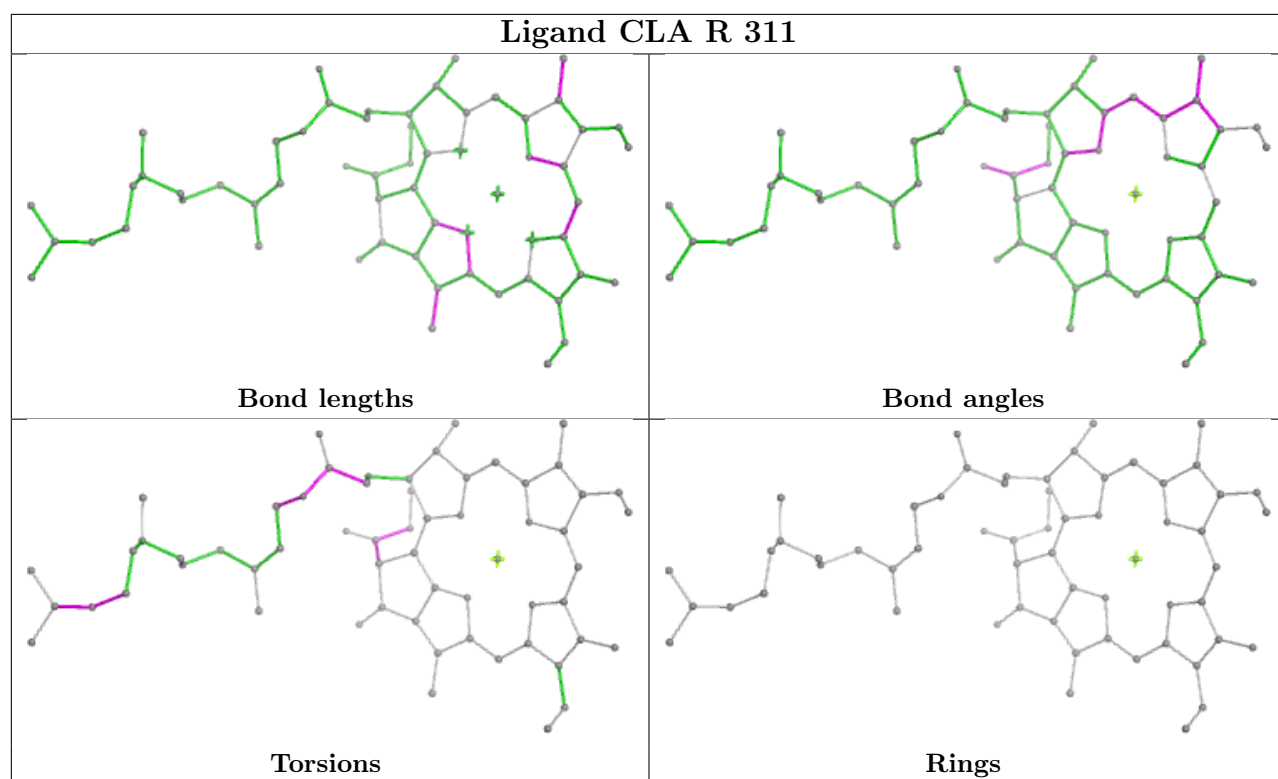


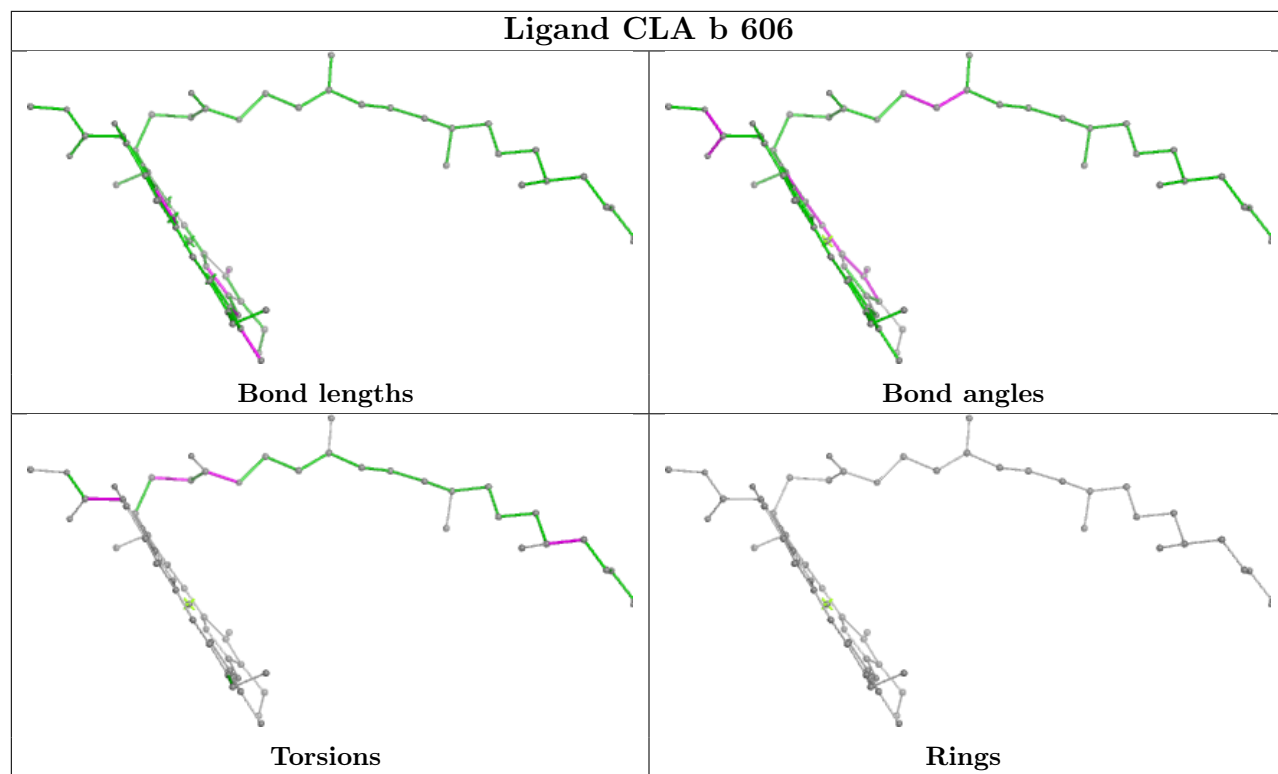
Torsions



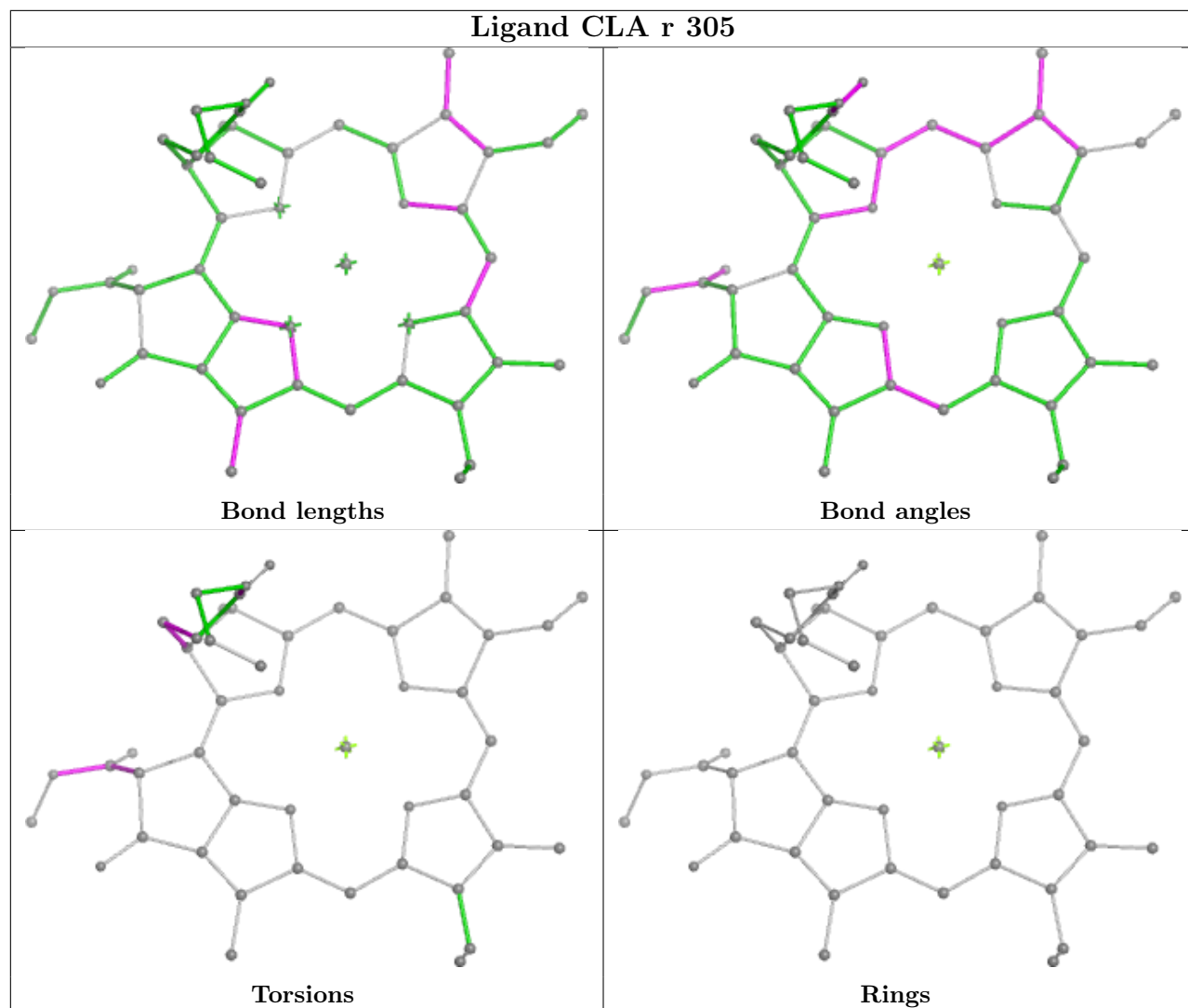
Rings

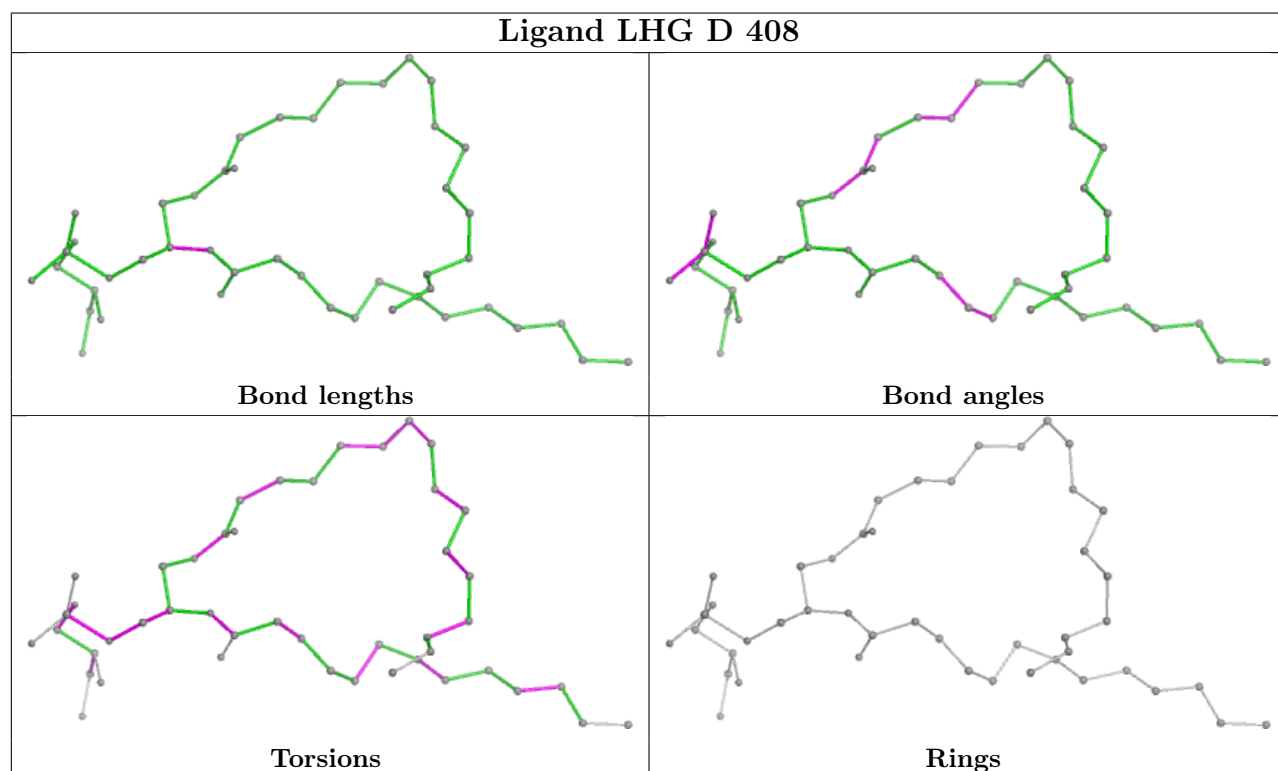
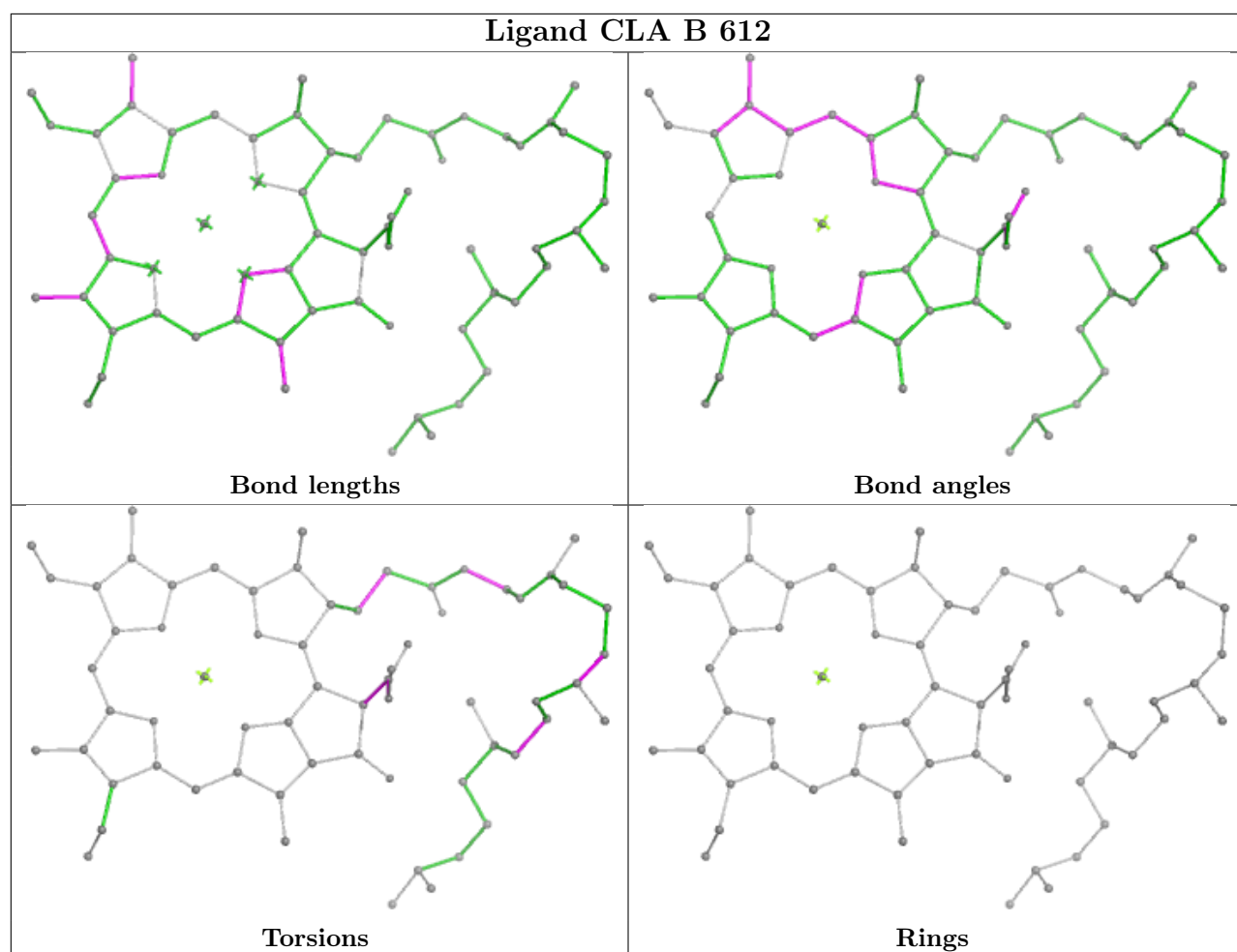


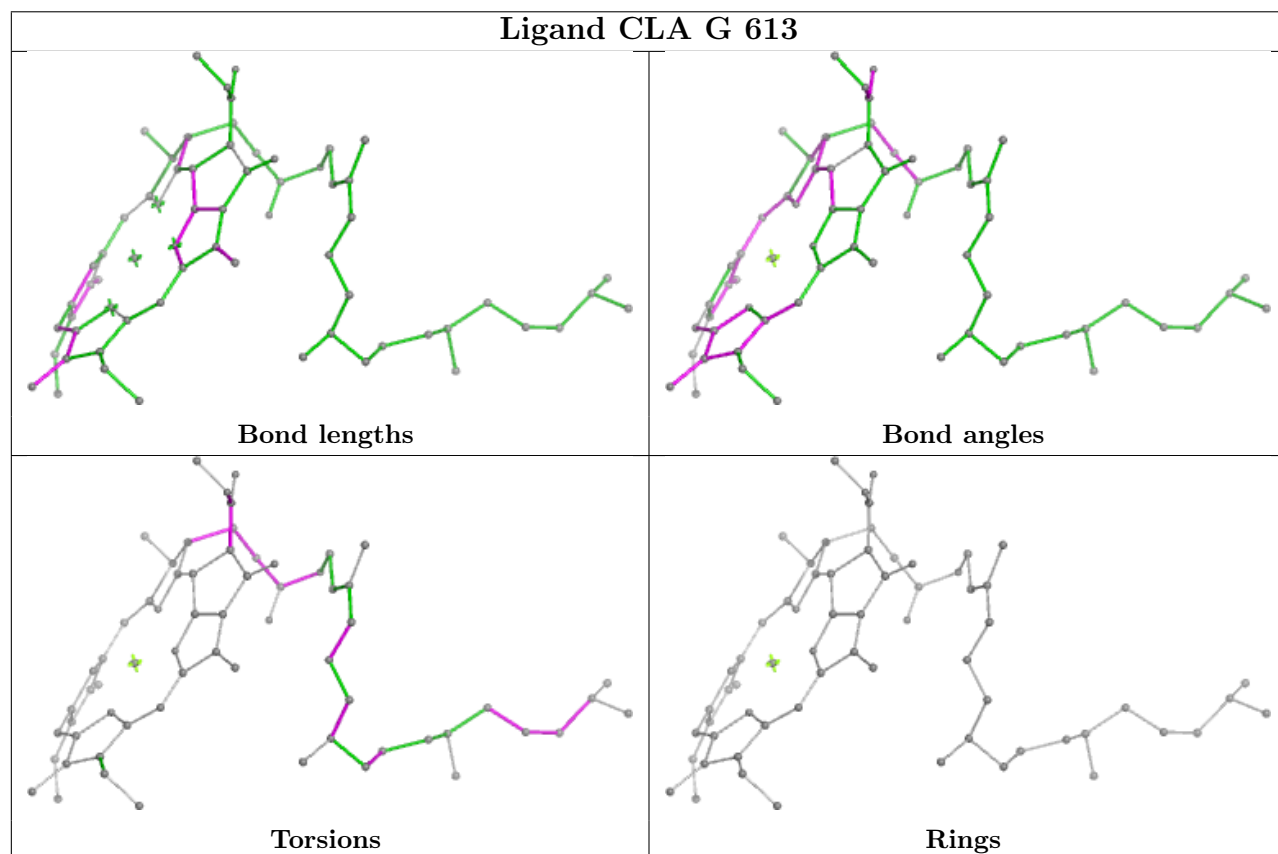
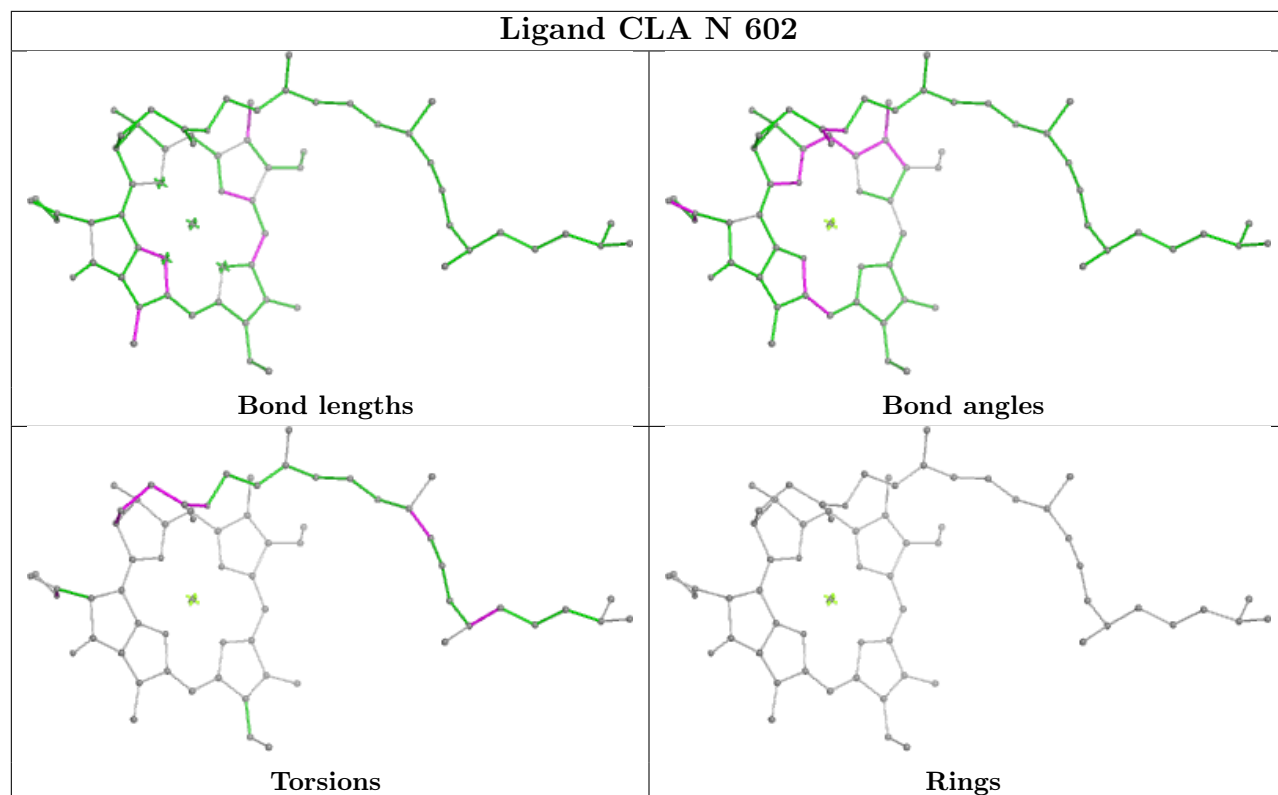


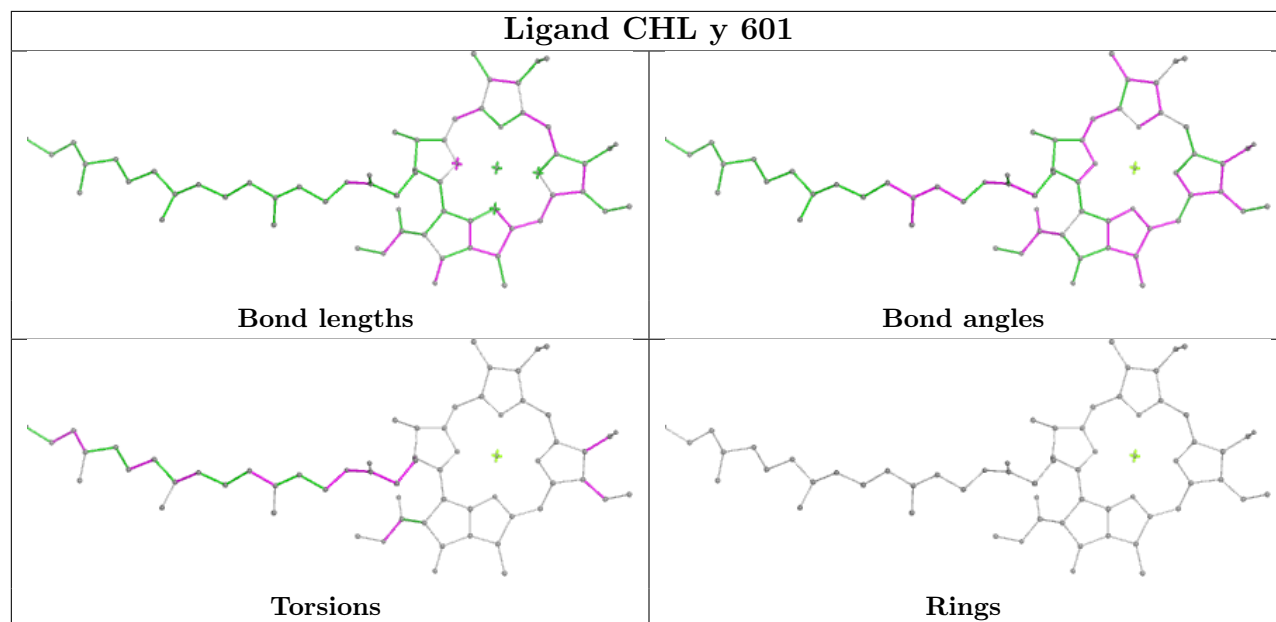
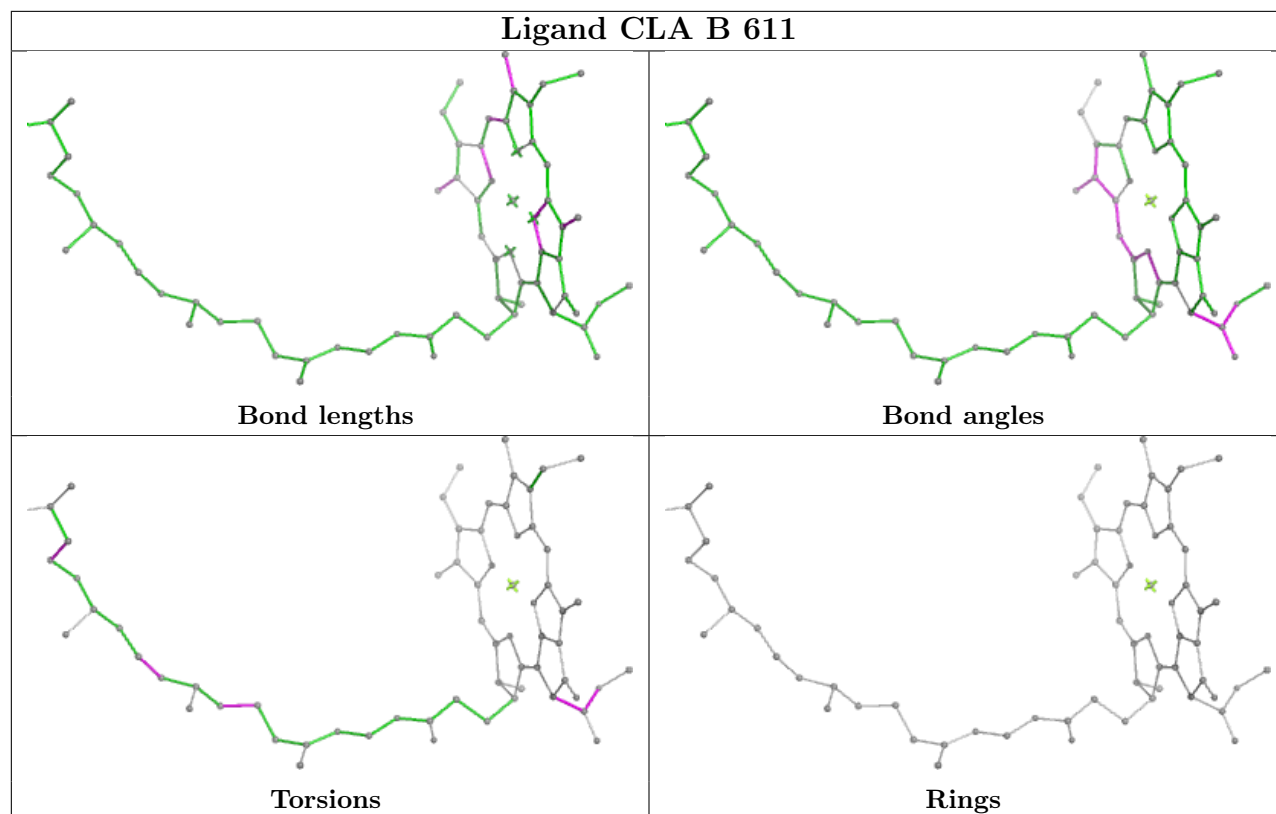


## Ligand CLA r 305

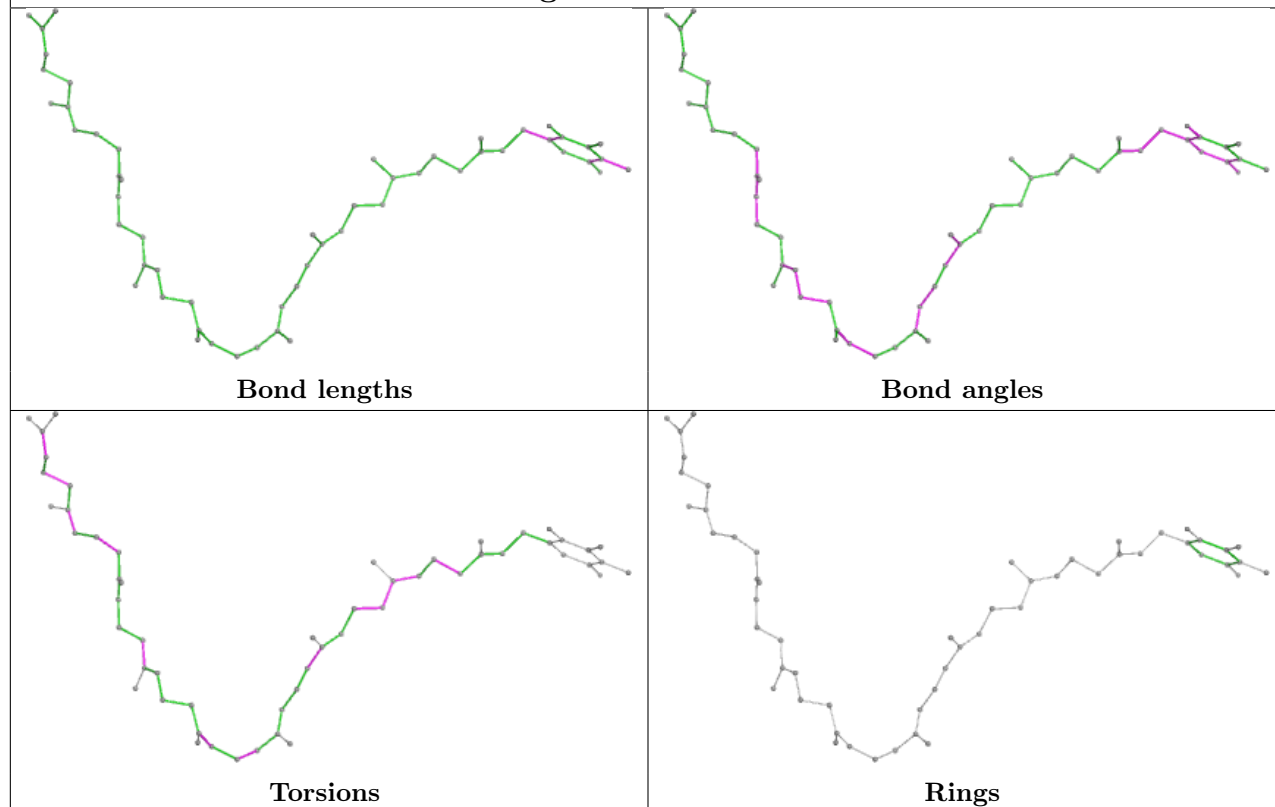




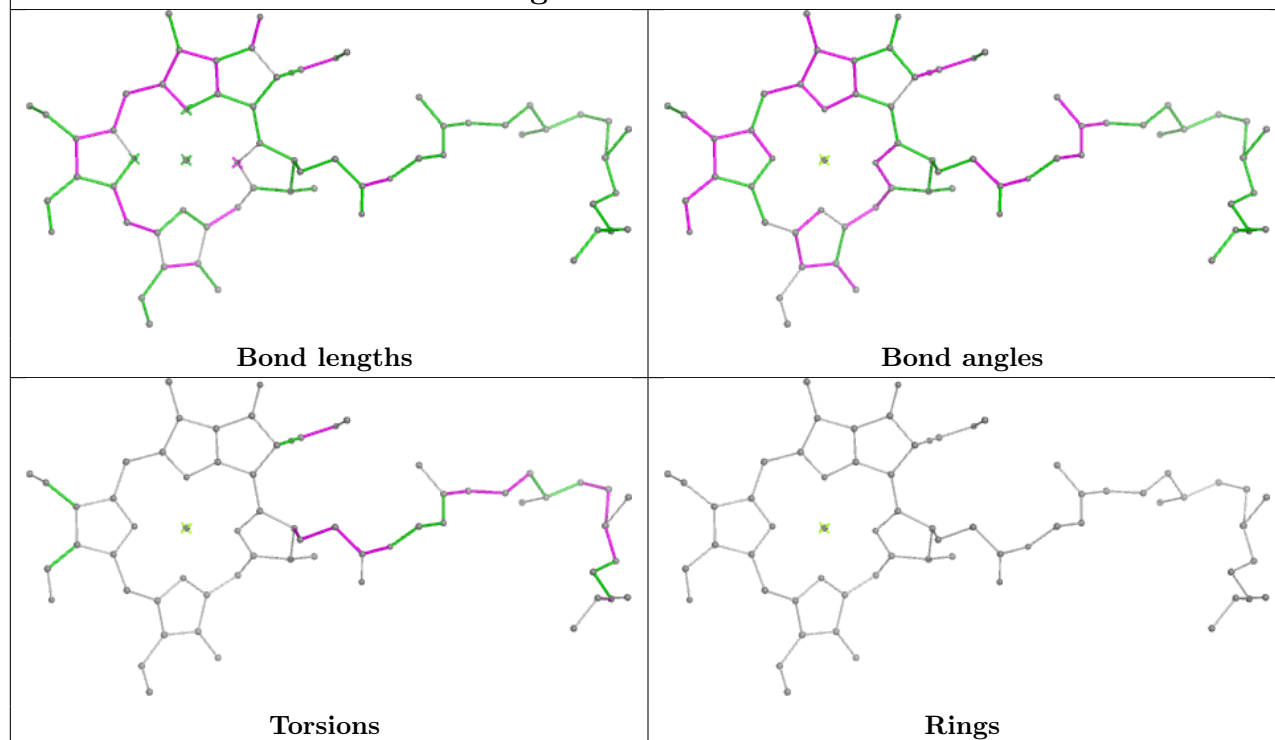


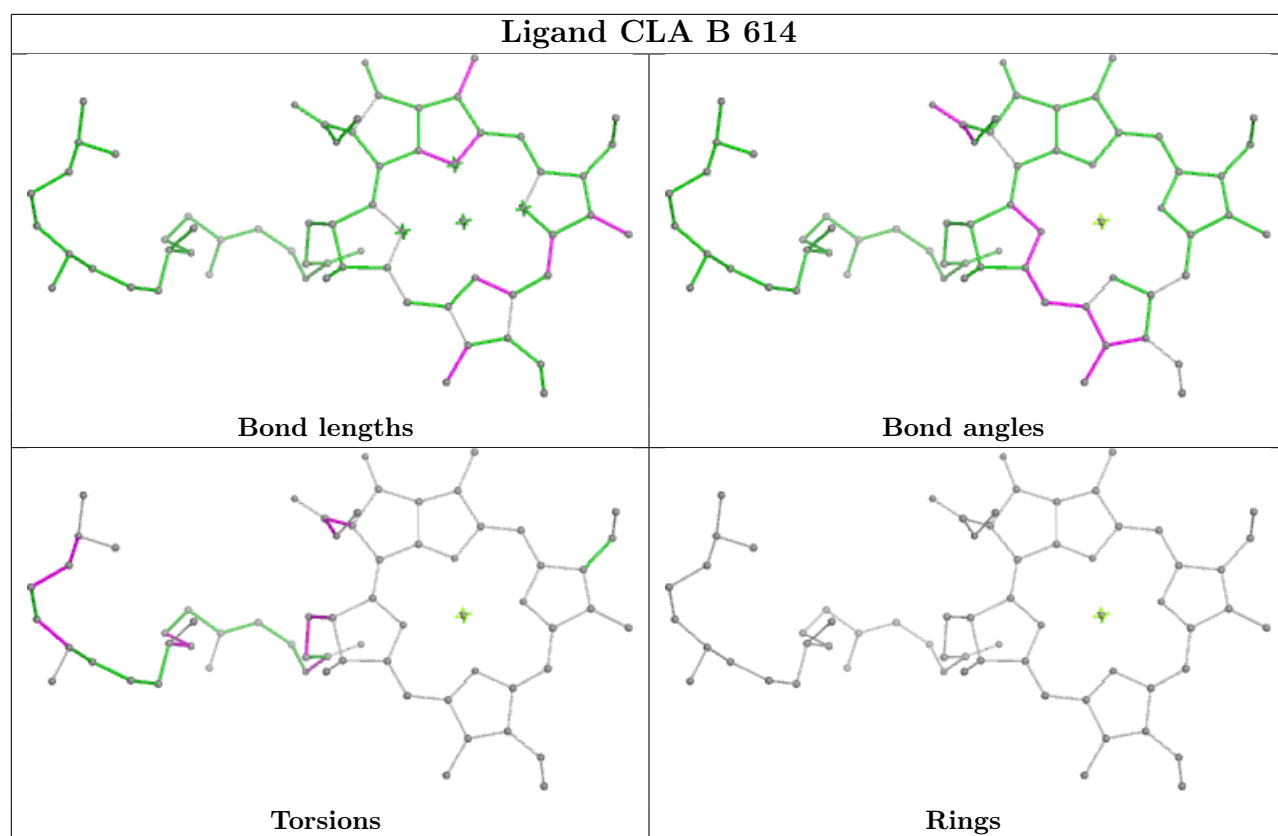


## Ligand PL9 d 406

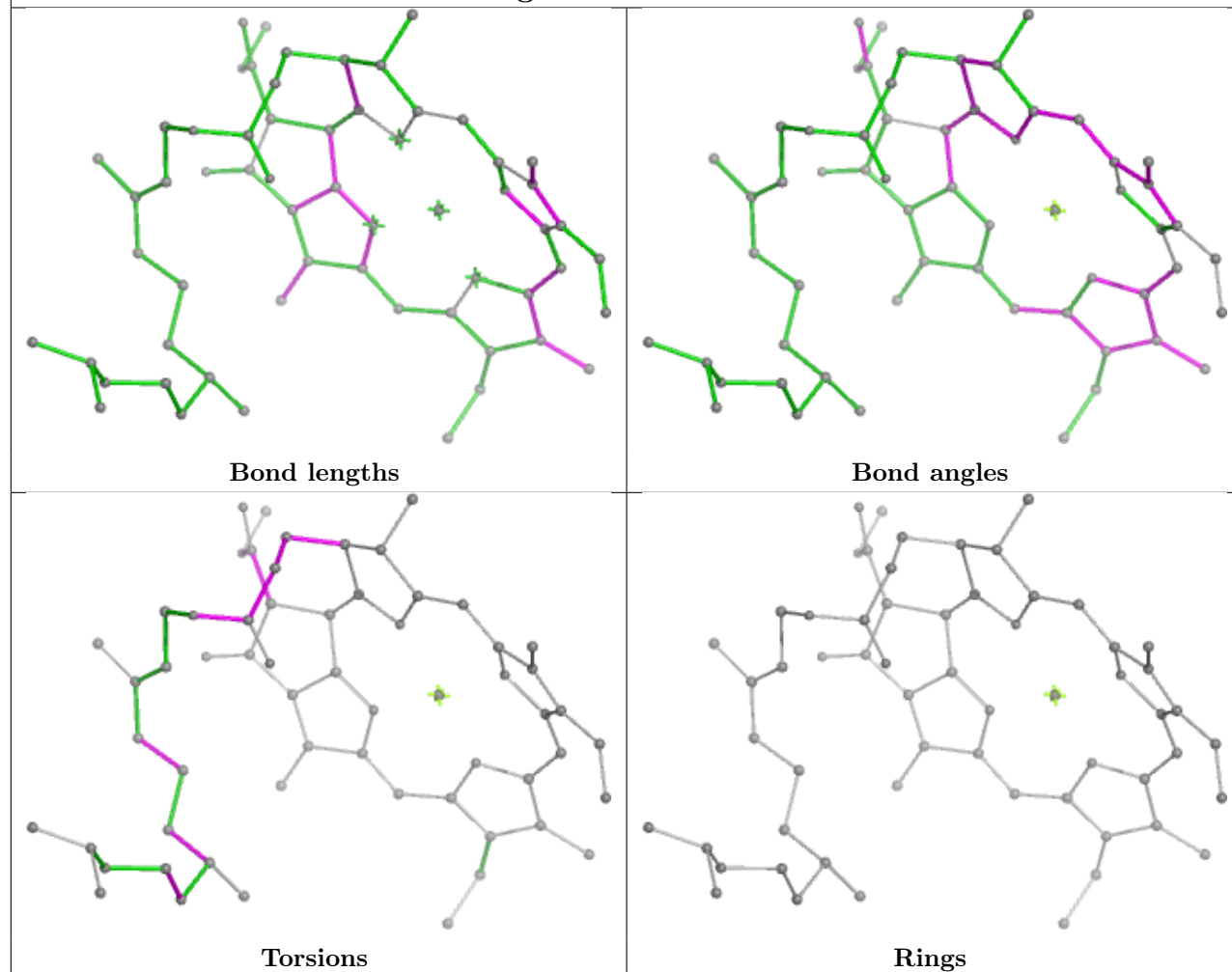


## Ligand CHL R 305

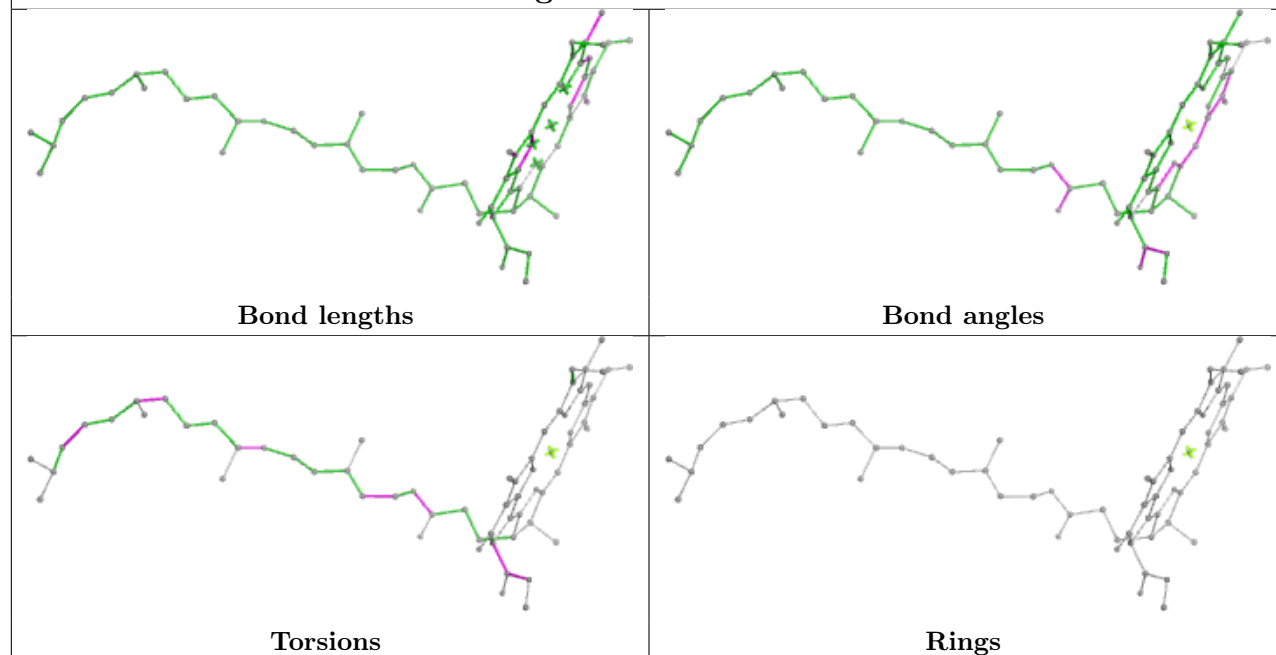


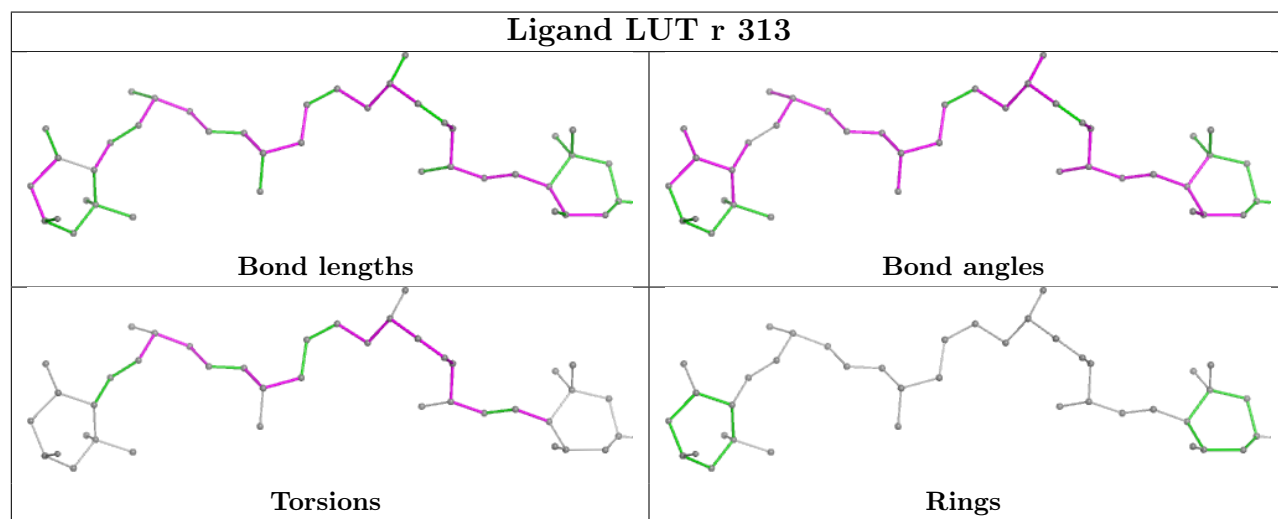
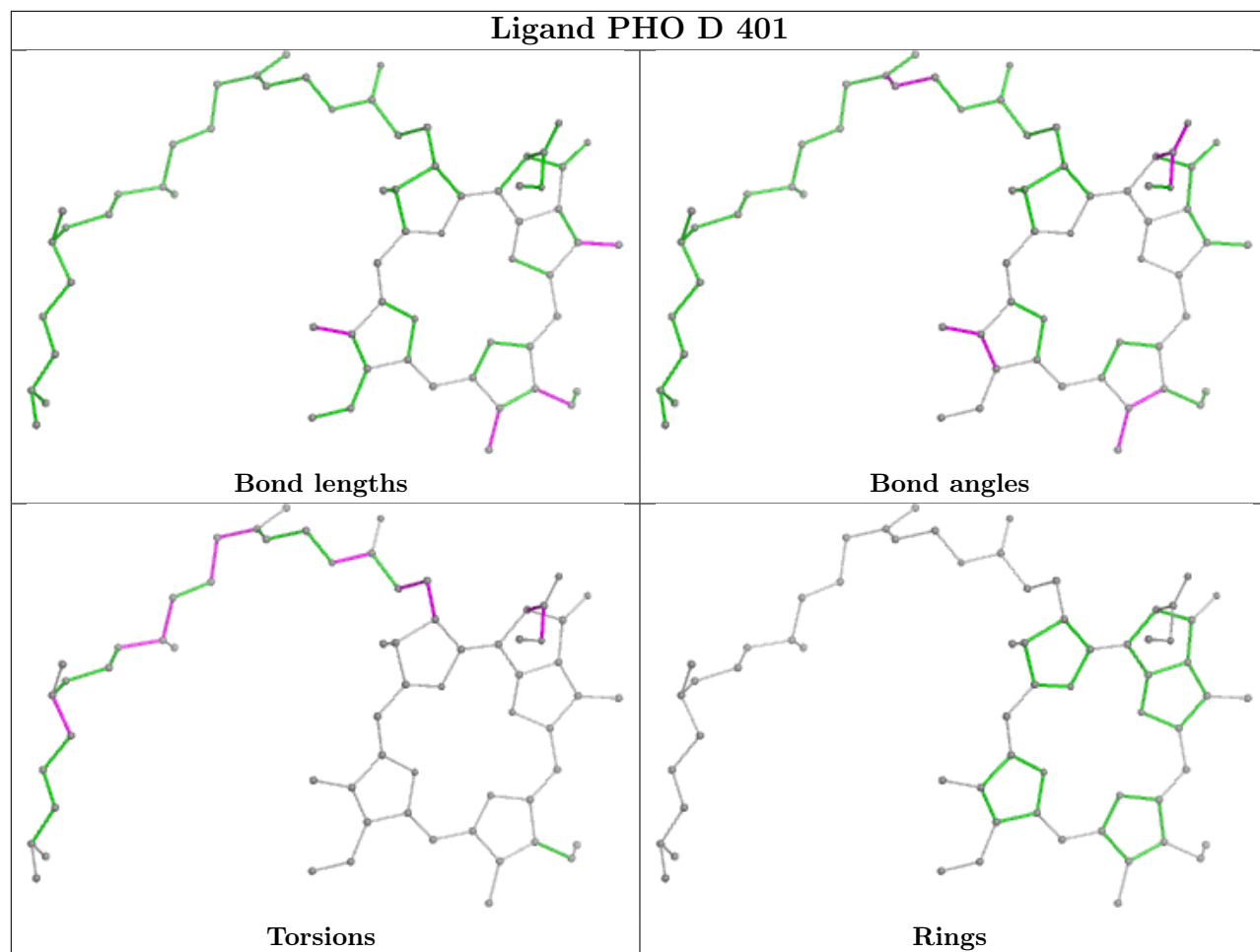


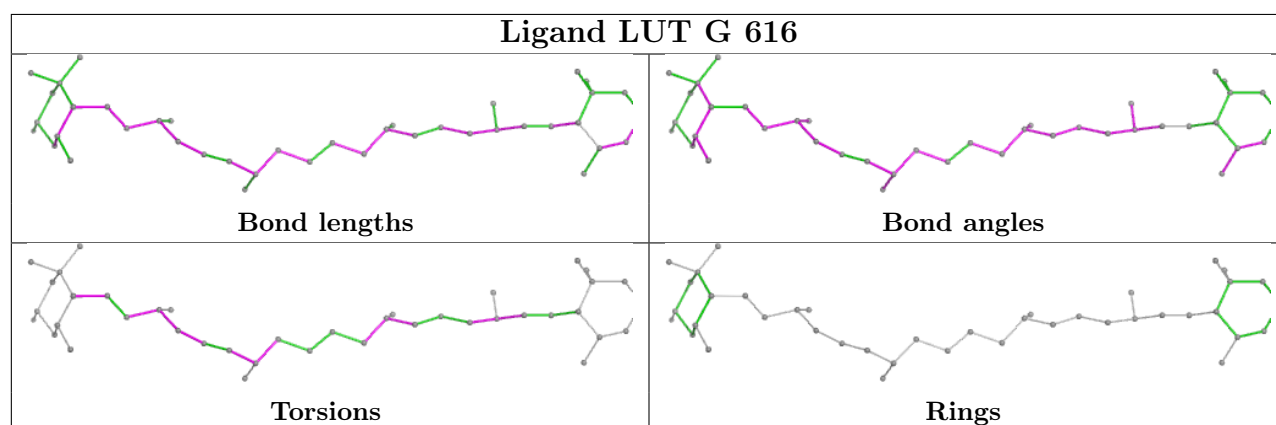
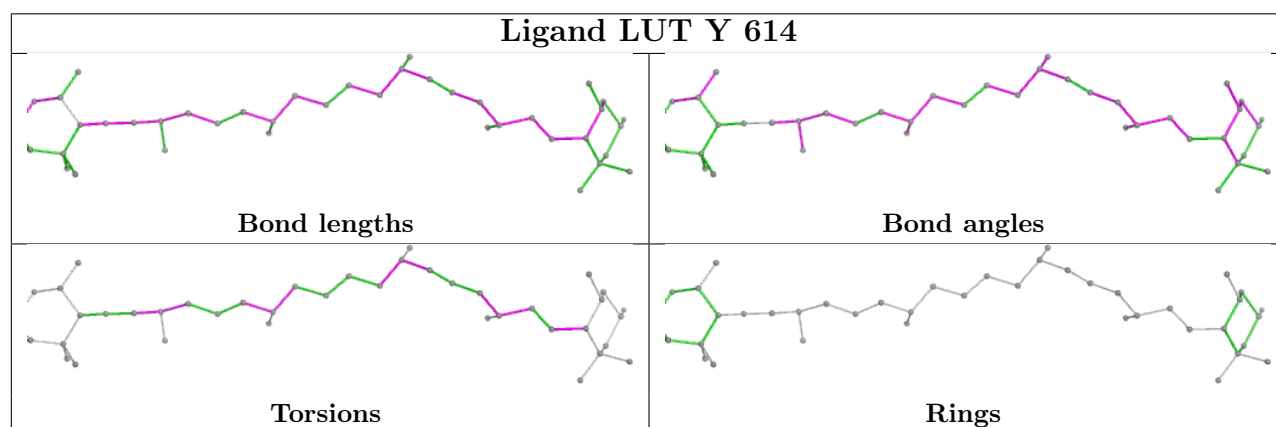
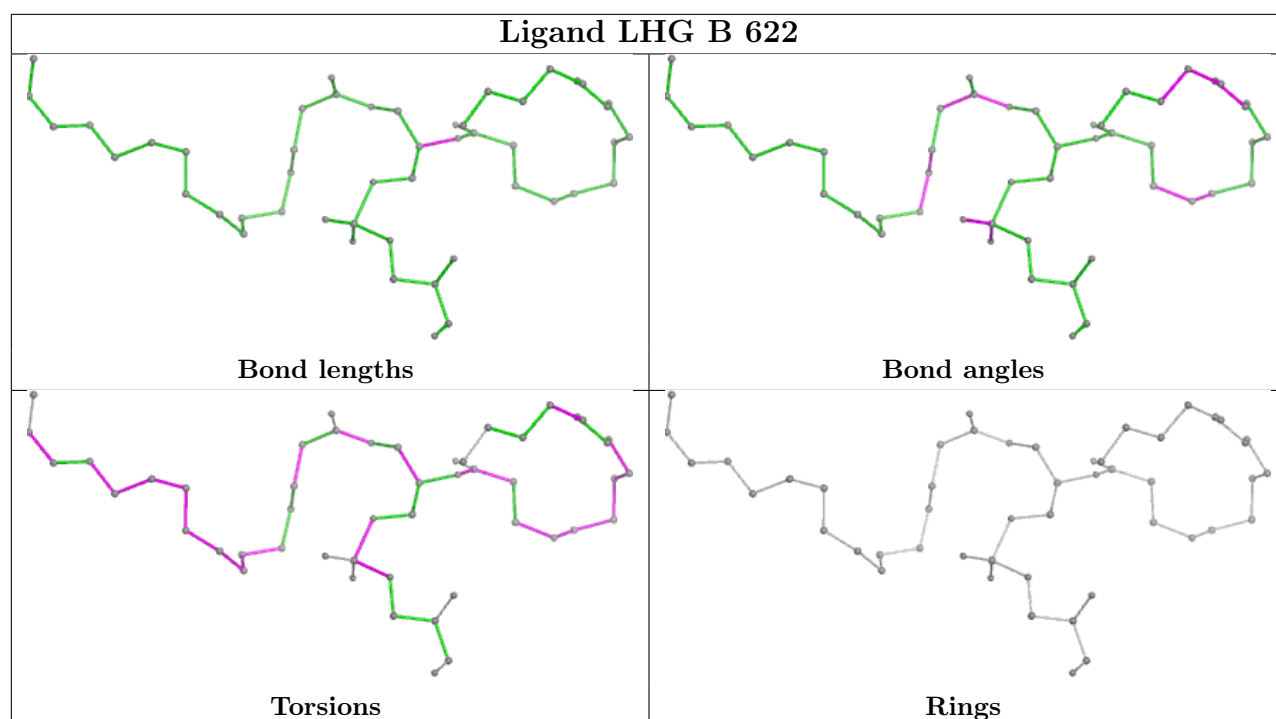
## Ligand CLA n 612



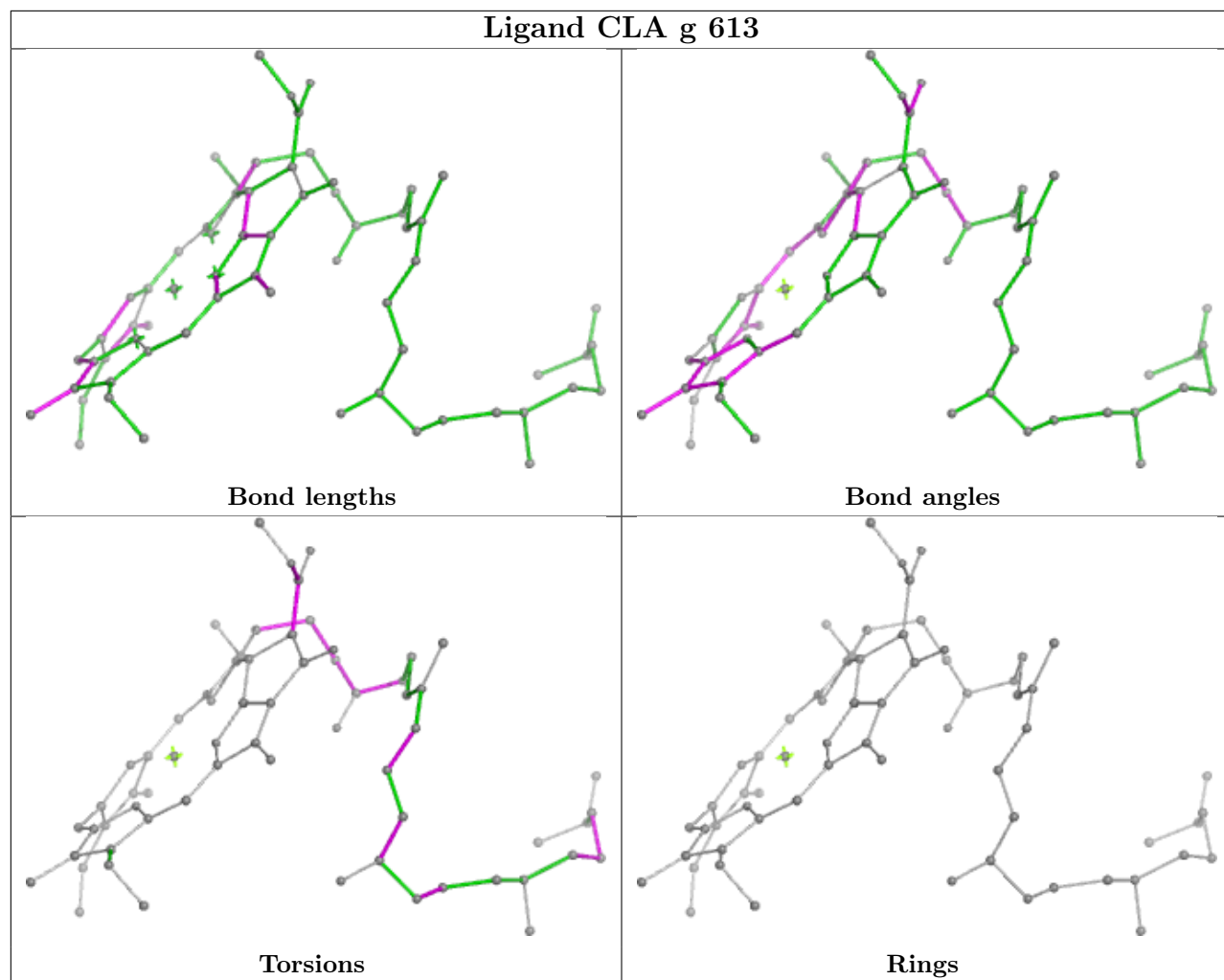
## Ligand CLA b 603

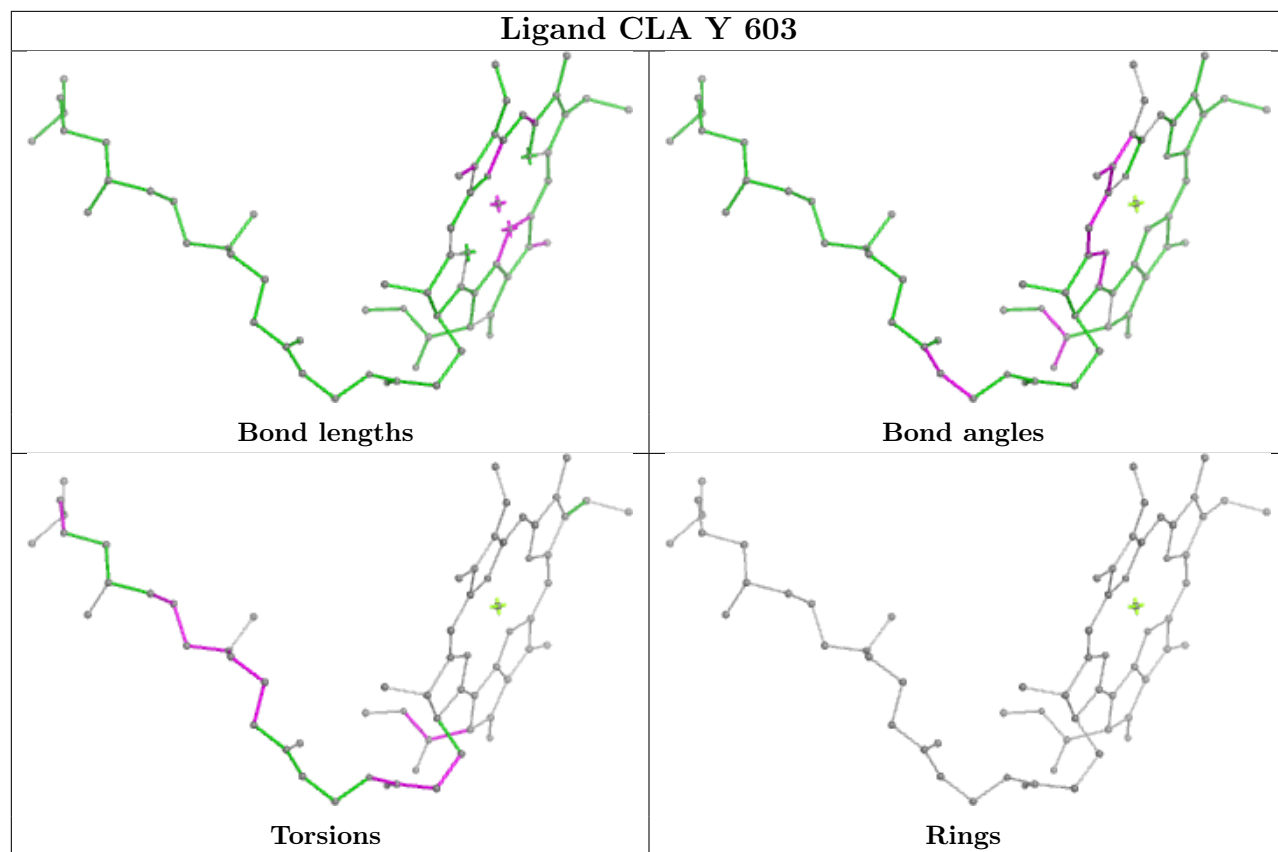




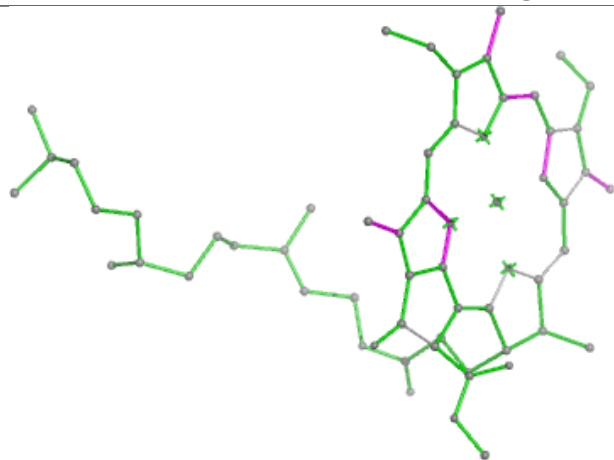


## Ligand CLA g 613

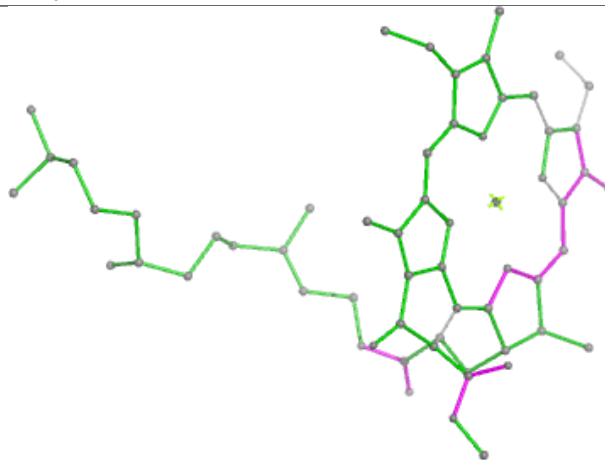




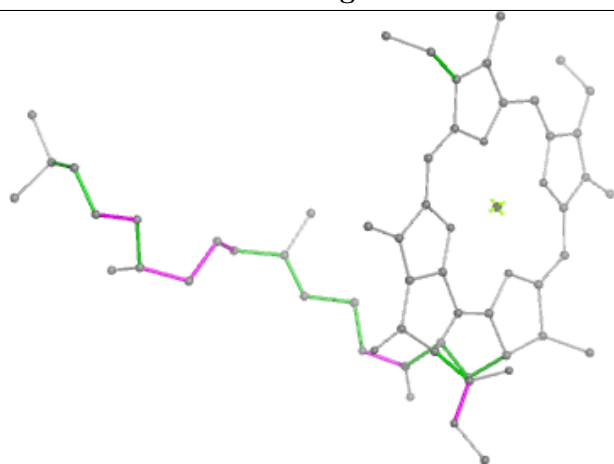
## Ligand CLA y 611



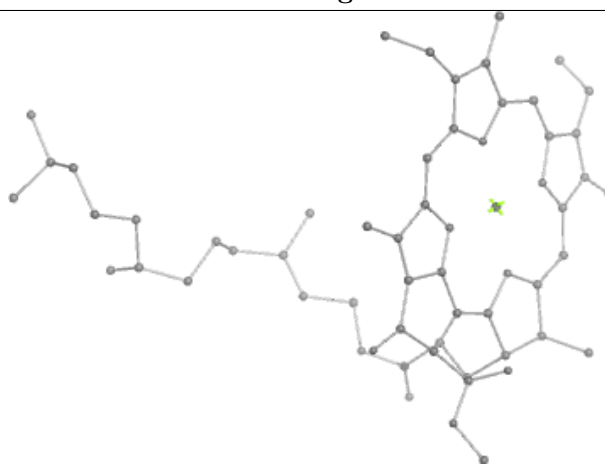
Bond lengths



Bond angles

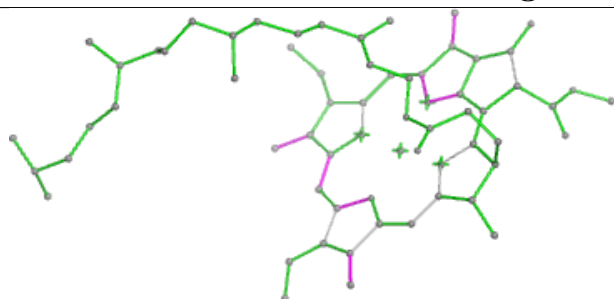


Torsions

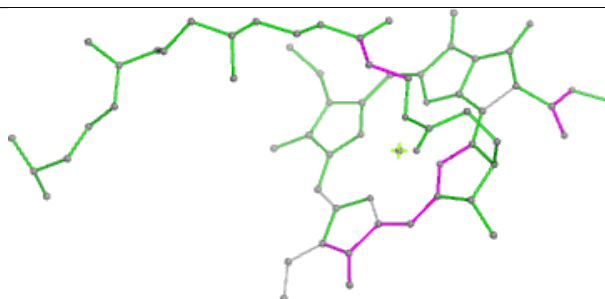


Rings

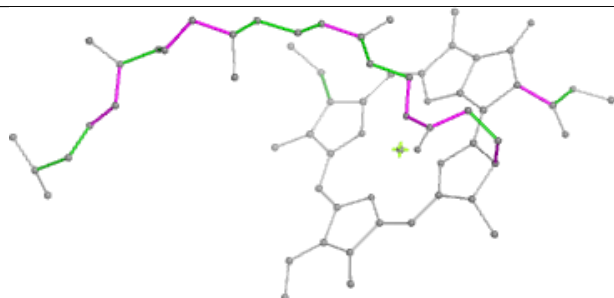
## Ligand CLA c 514



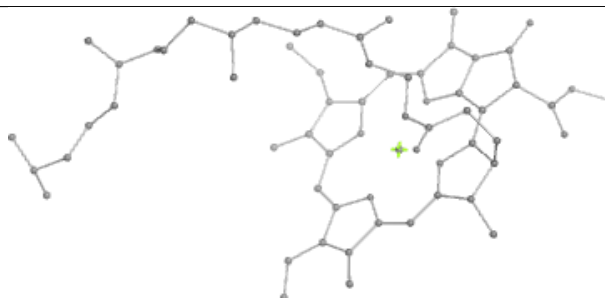
Bond lengths



Bond angles

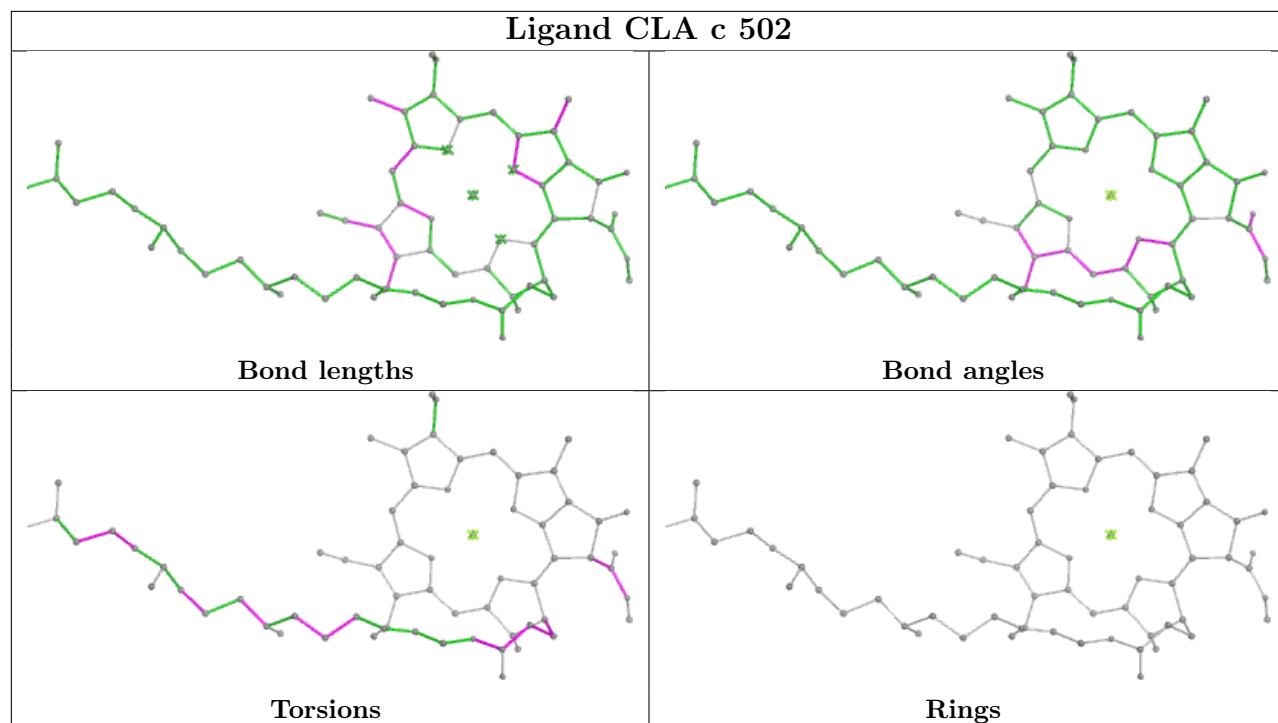


Torsions

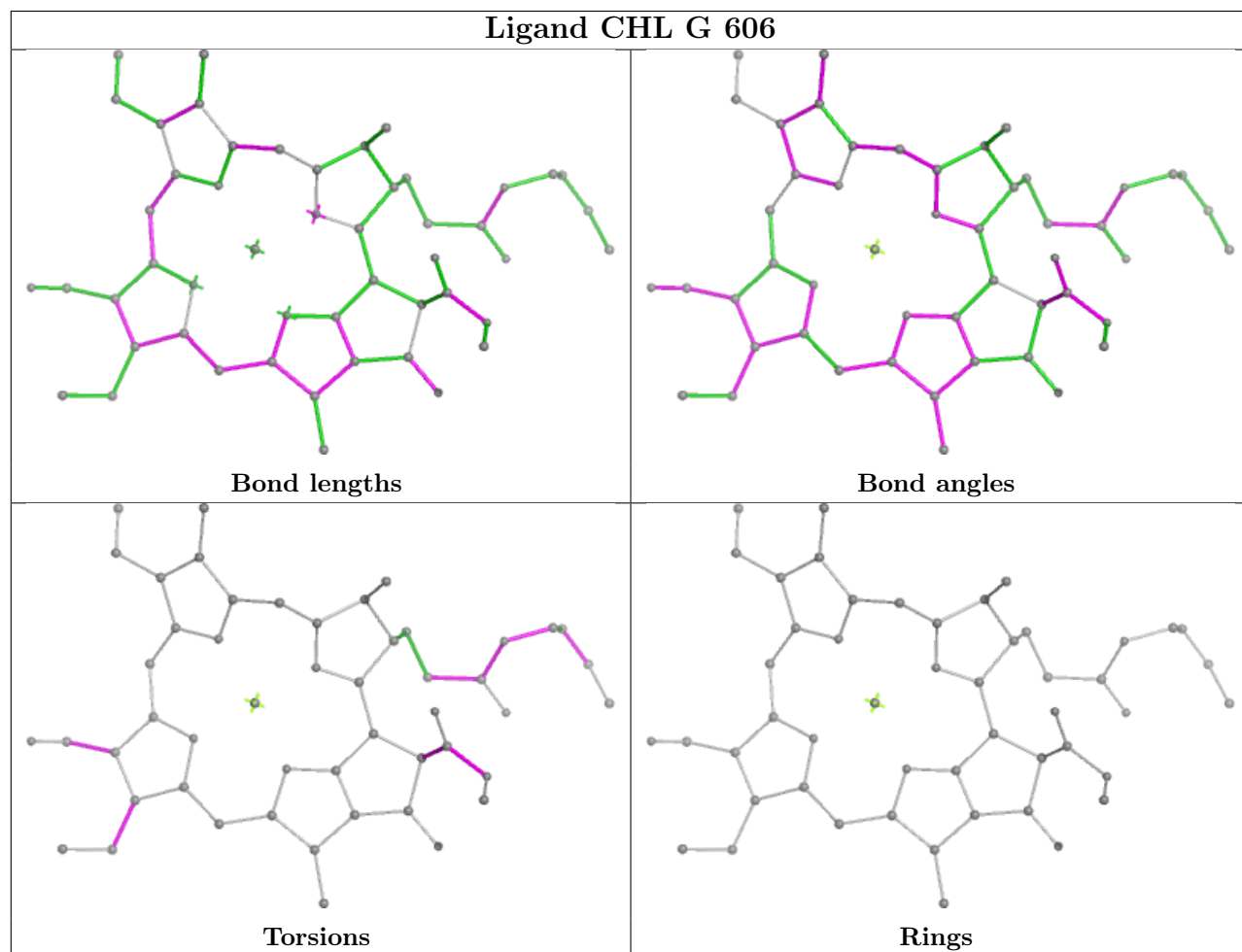


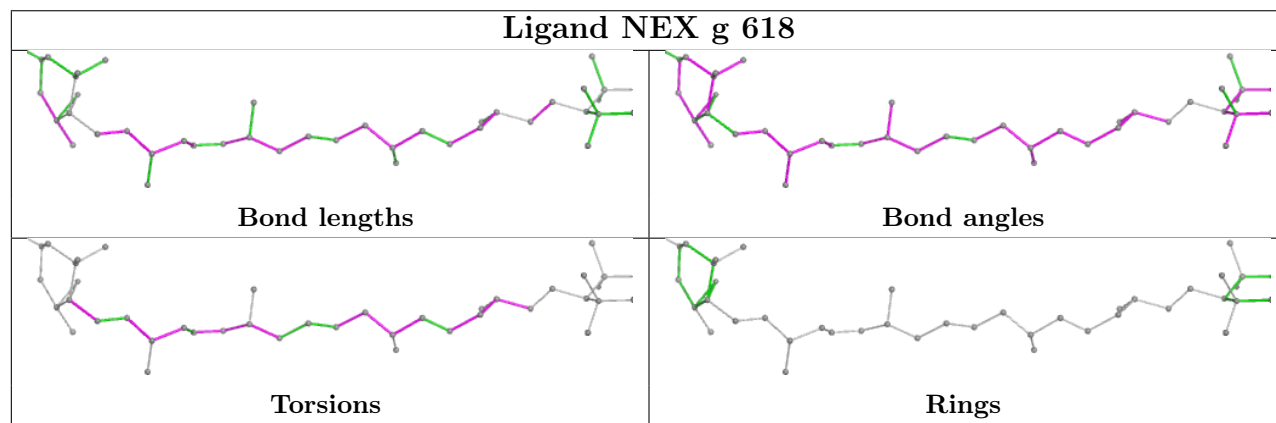
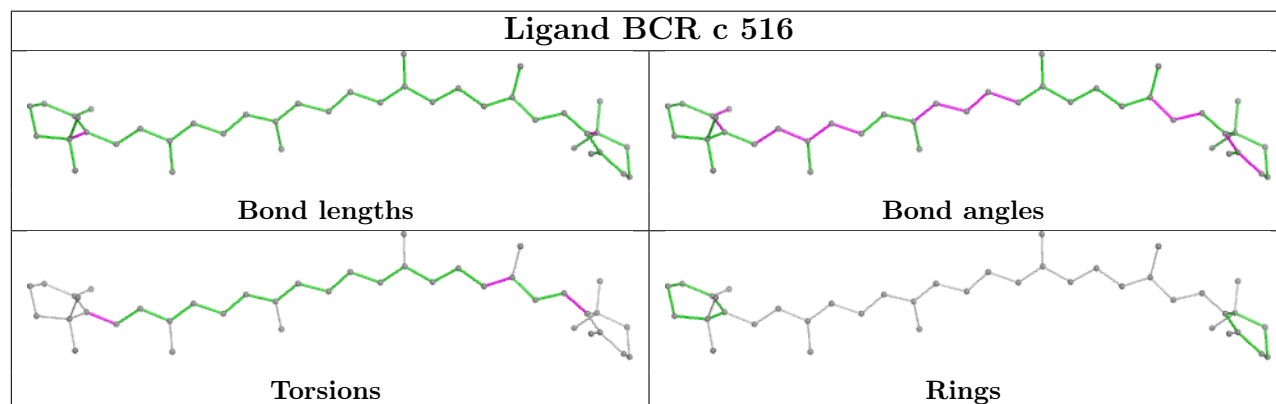
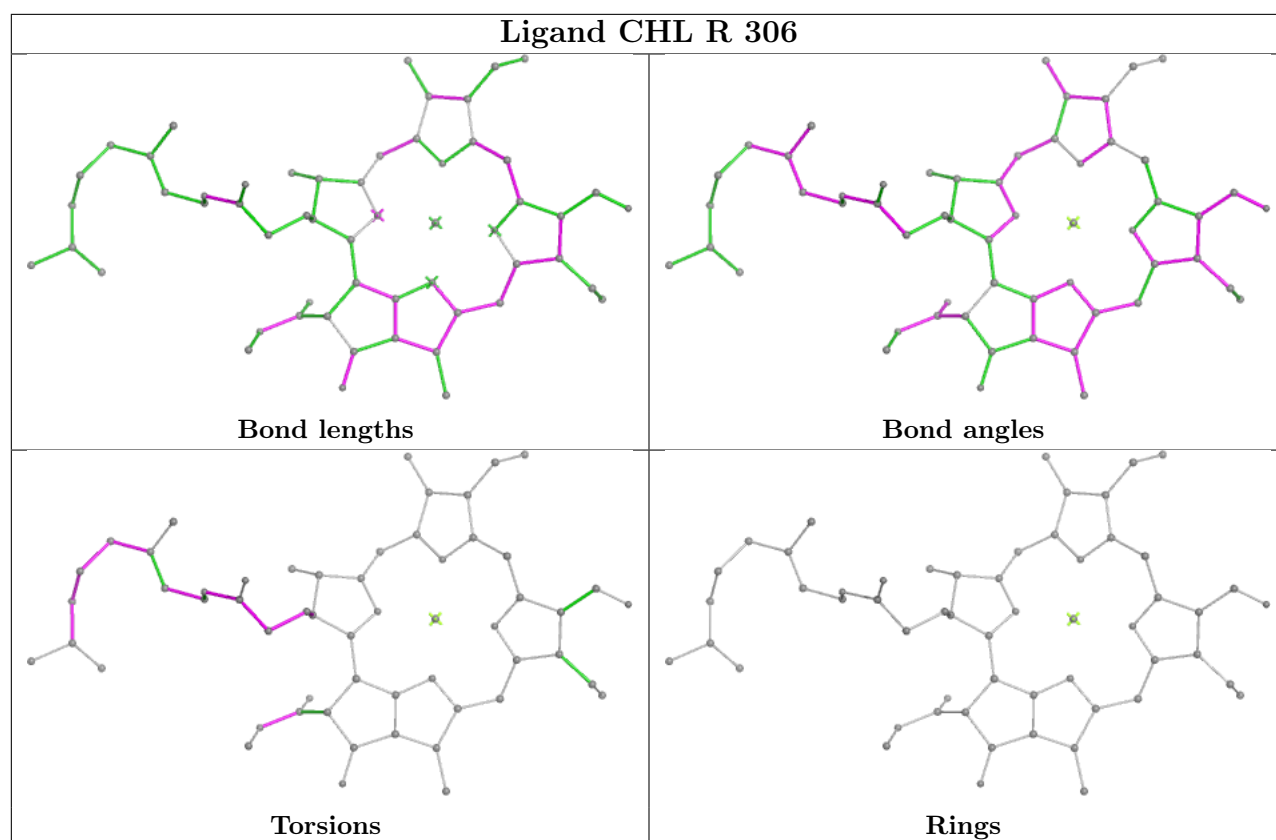
Rings

## Ligand CLA c 502

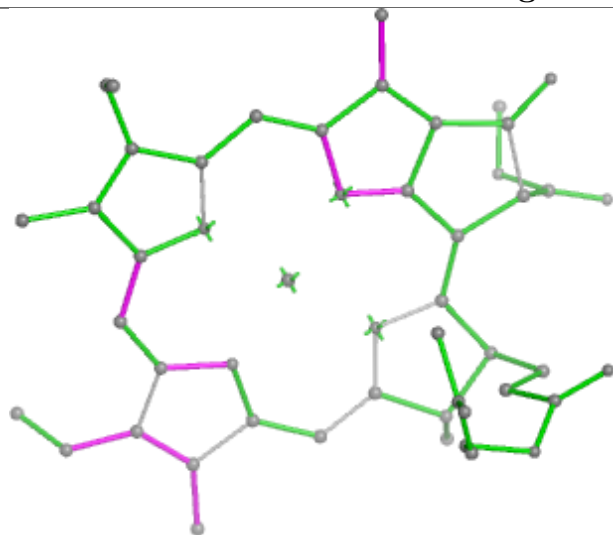


## Ligand CHL G 606

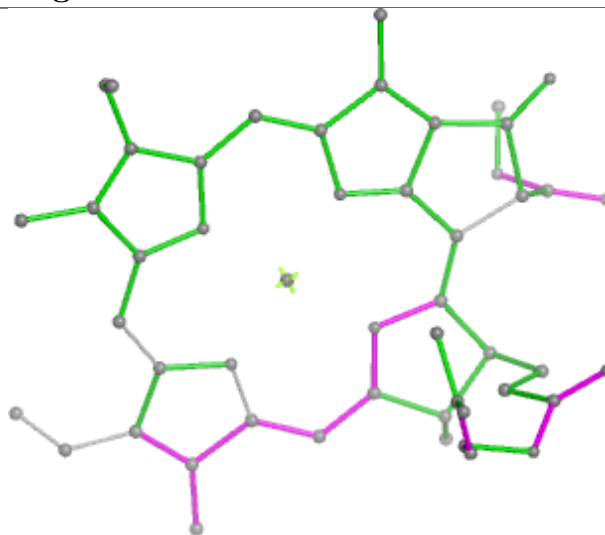




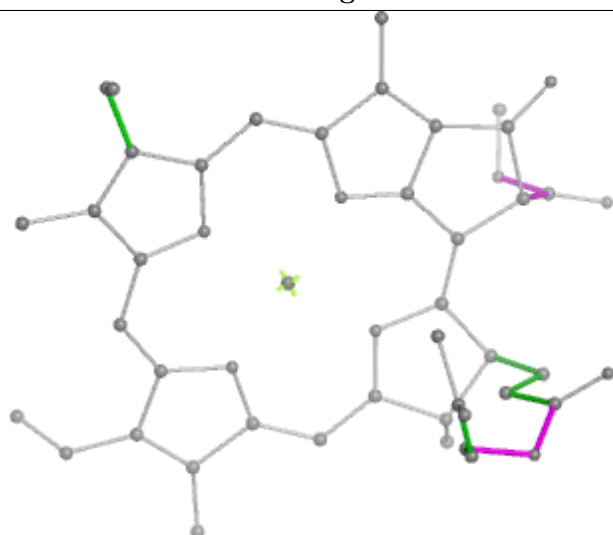
## Ligand CLA g 604



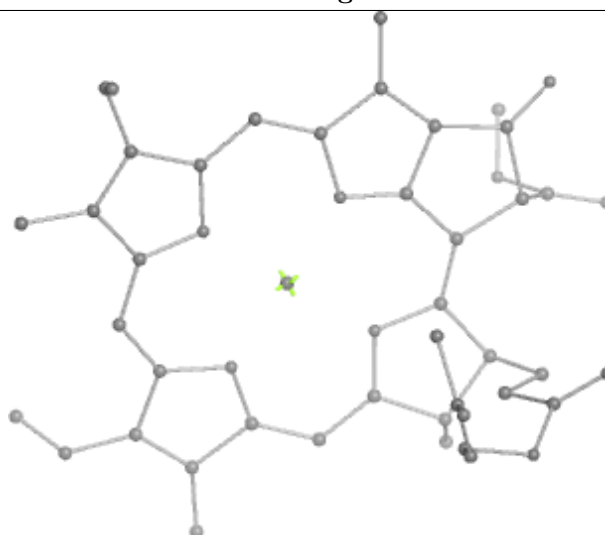
Bond lengths



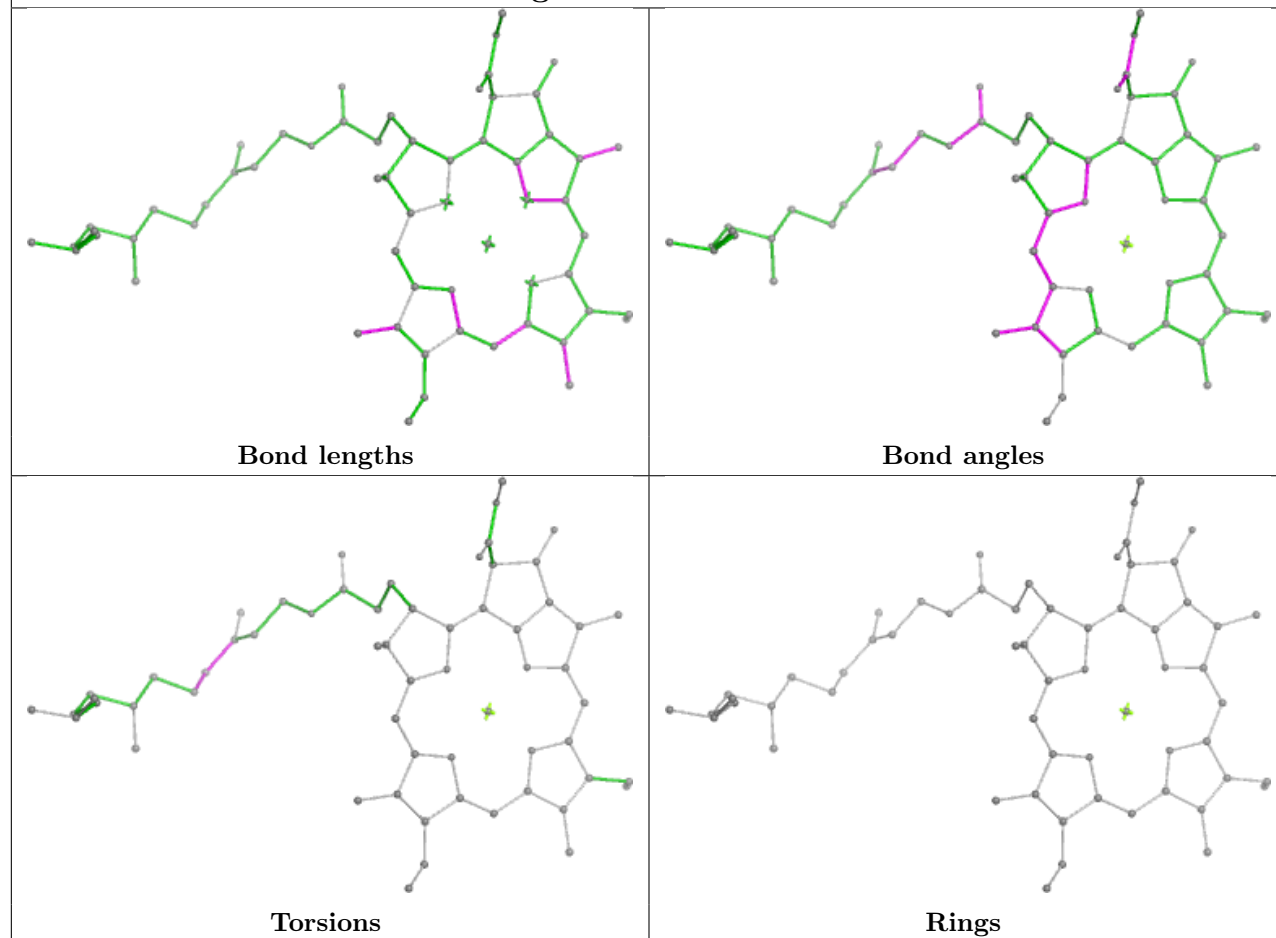
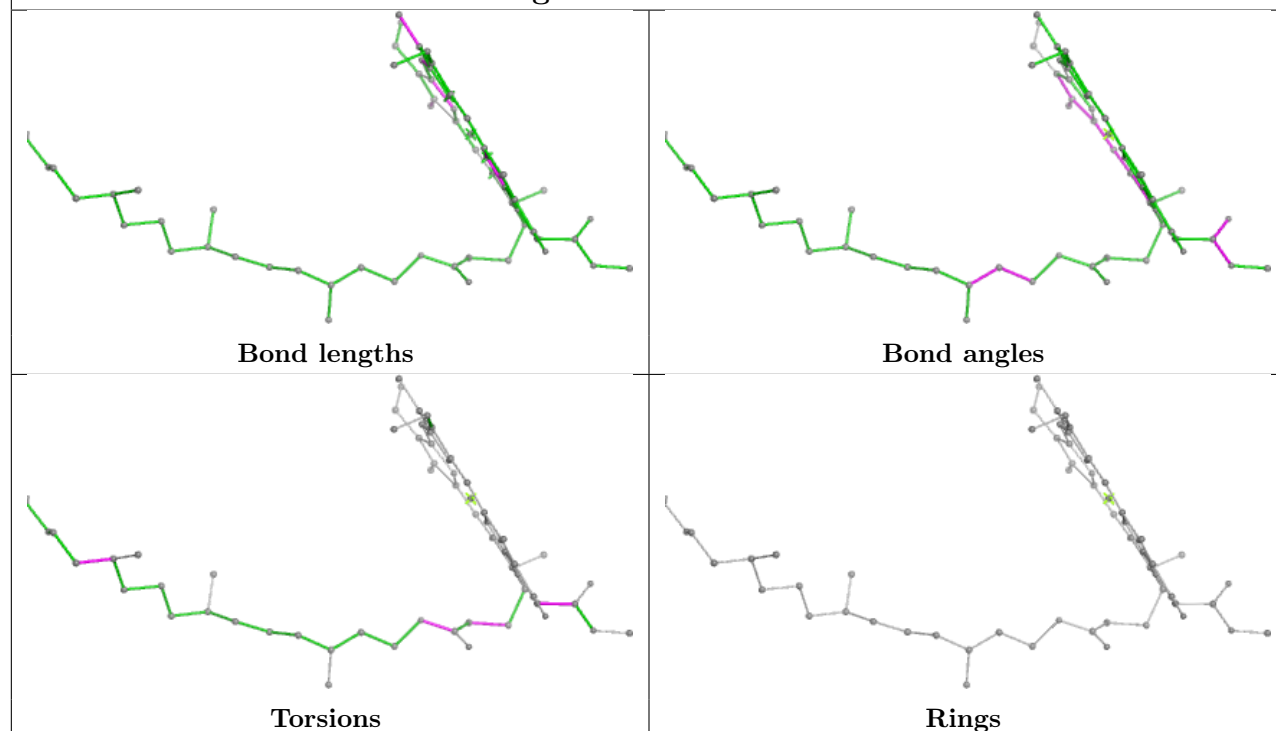
Bond angles

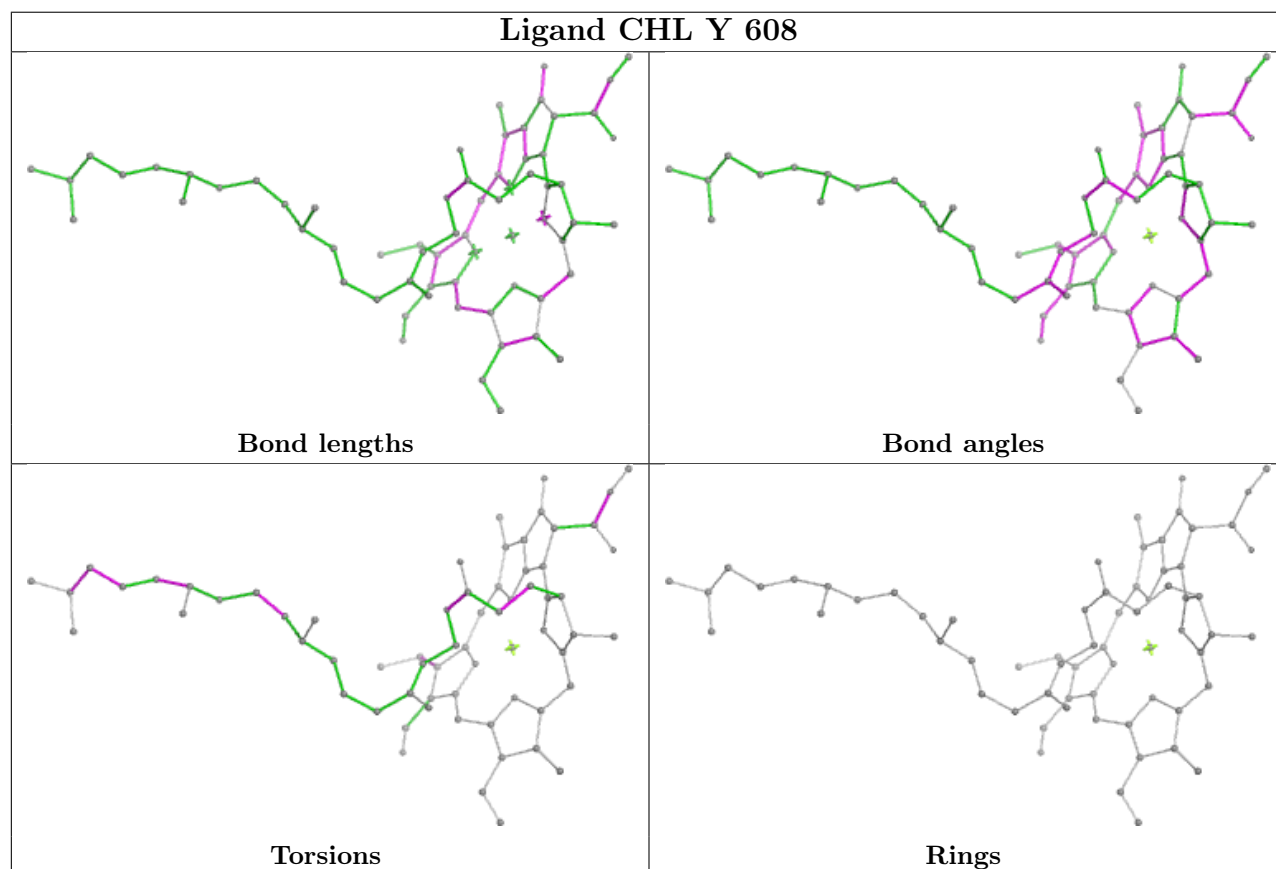
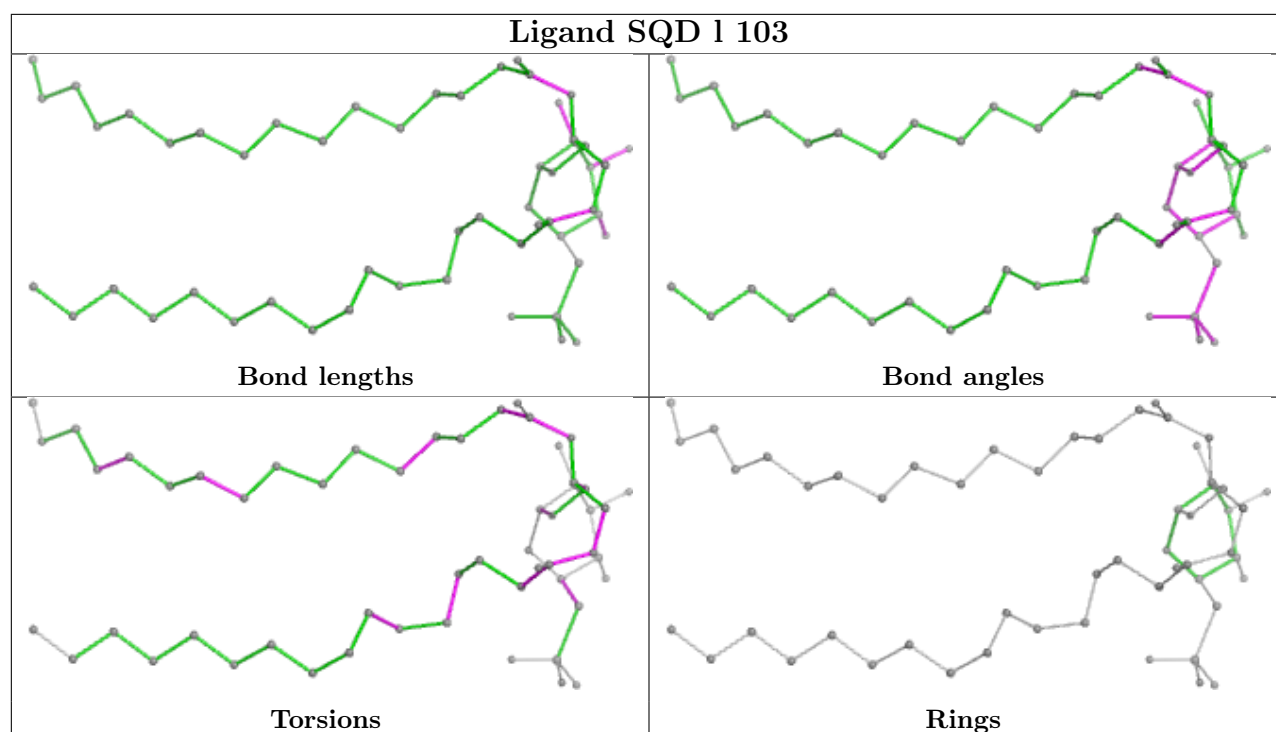


Torsions

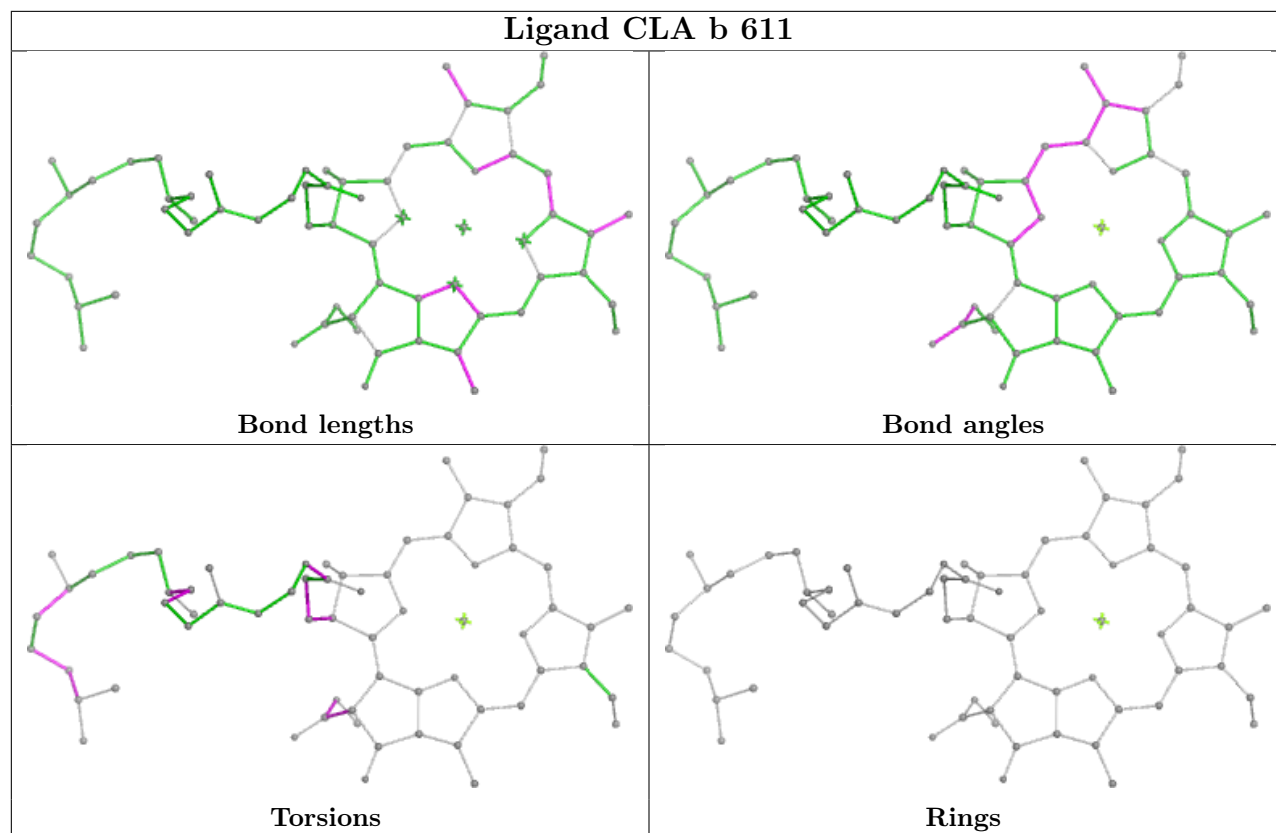


Rings

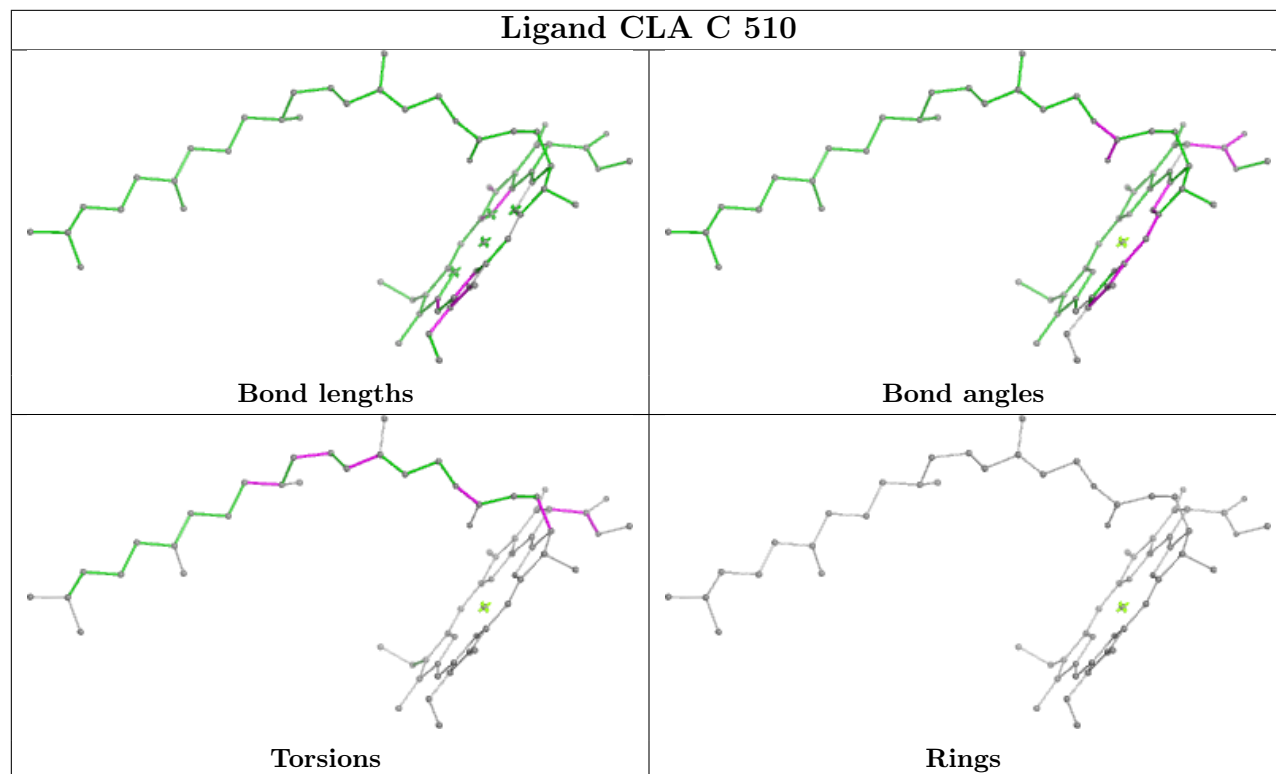
**Ligand CLA A 409****Ligand CLA B 609**

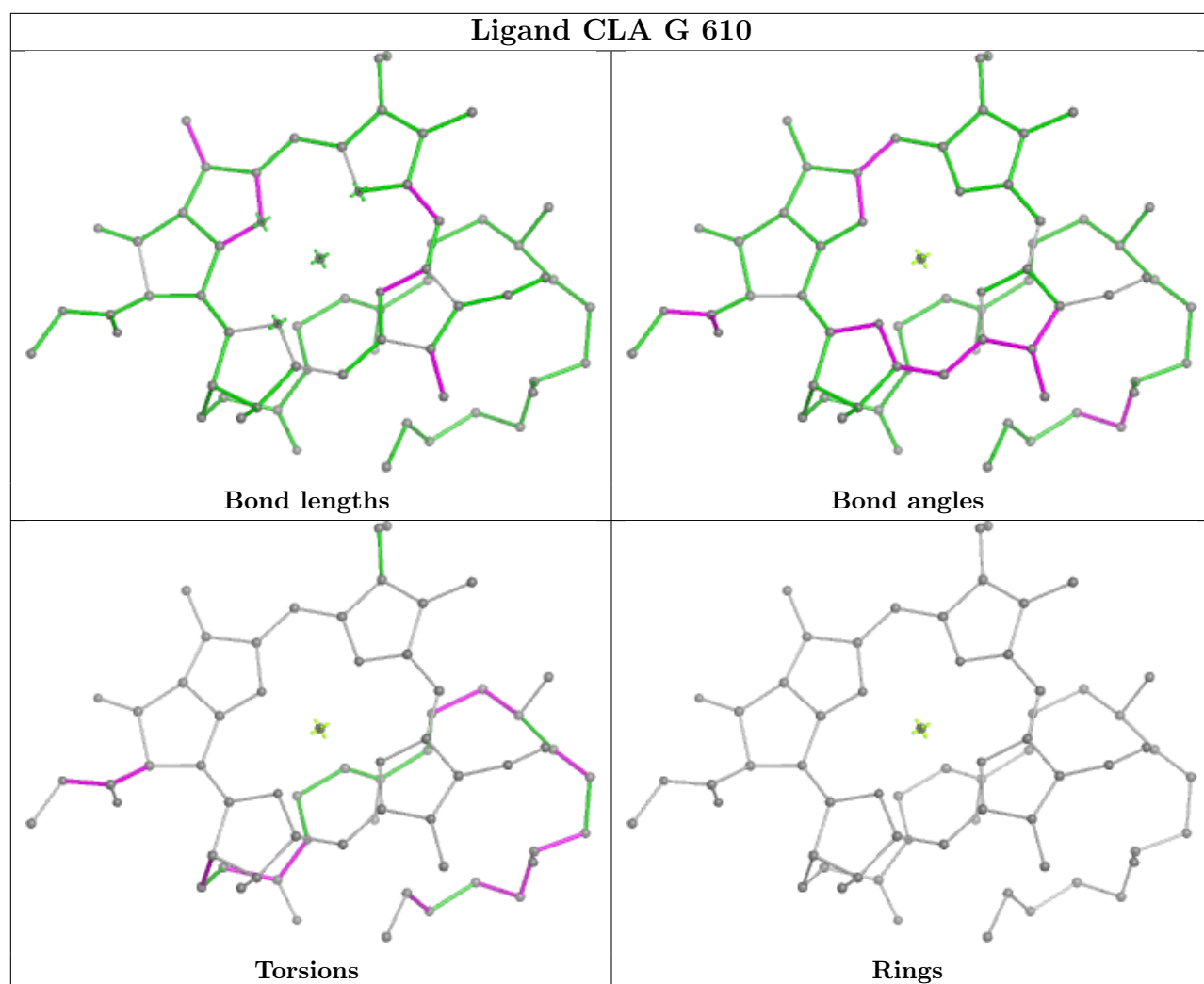


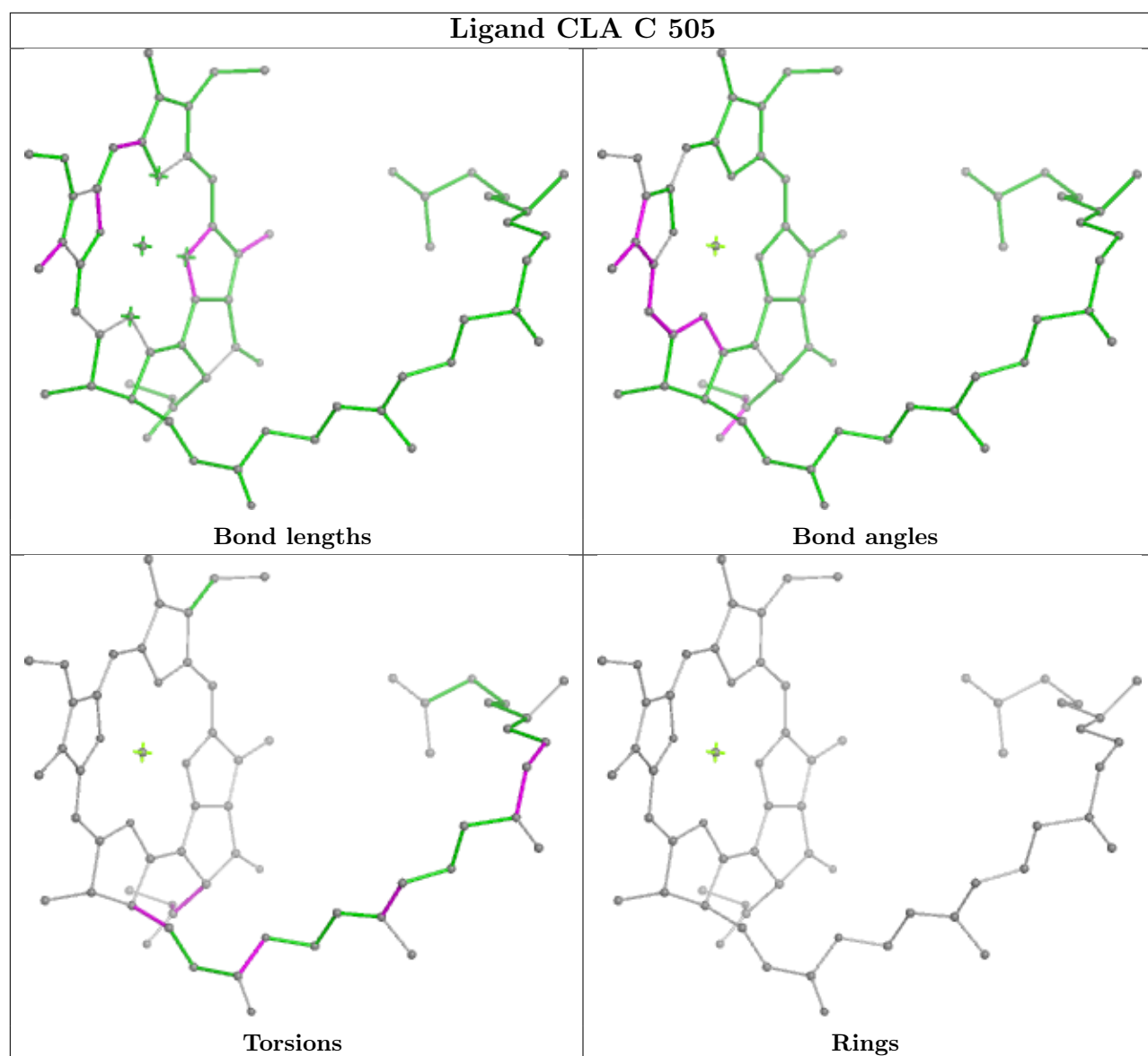
## Ligand CLA b 611



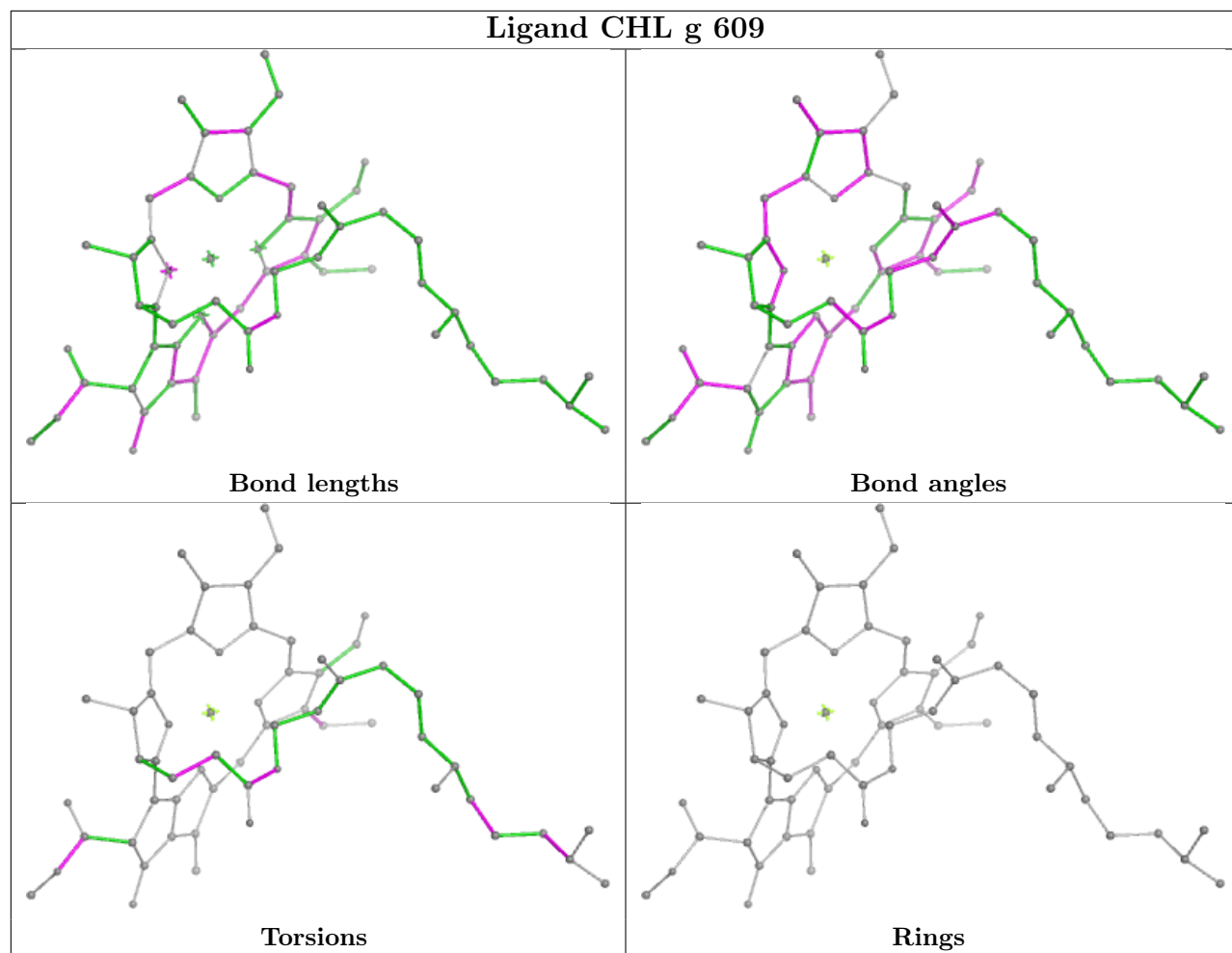
## Ligand CLA C 510

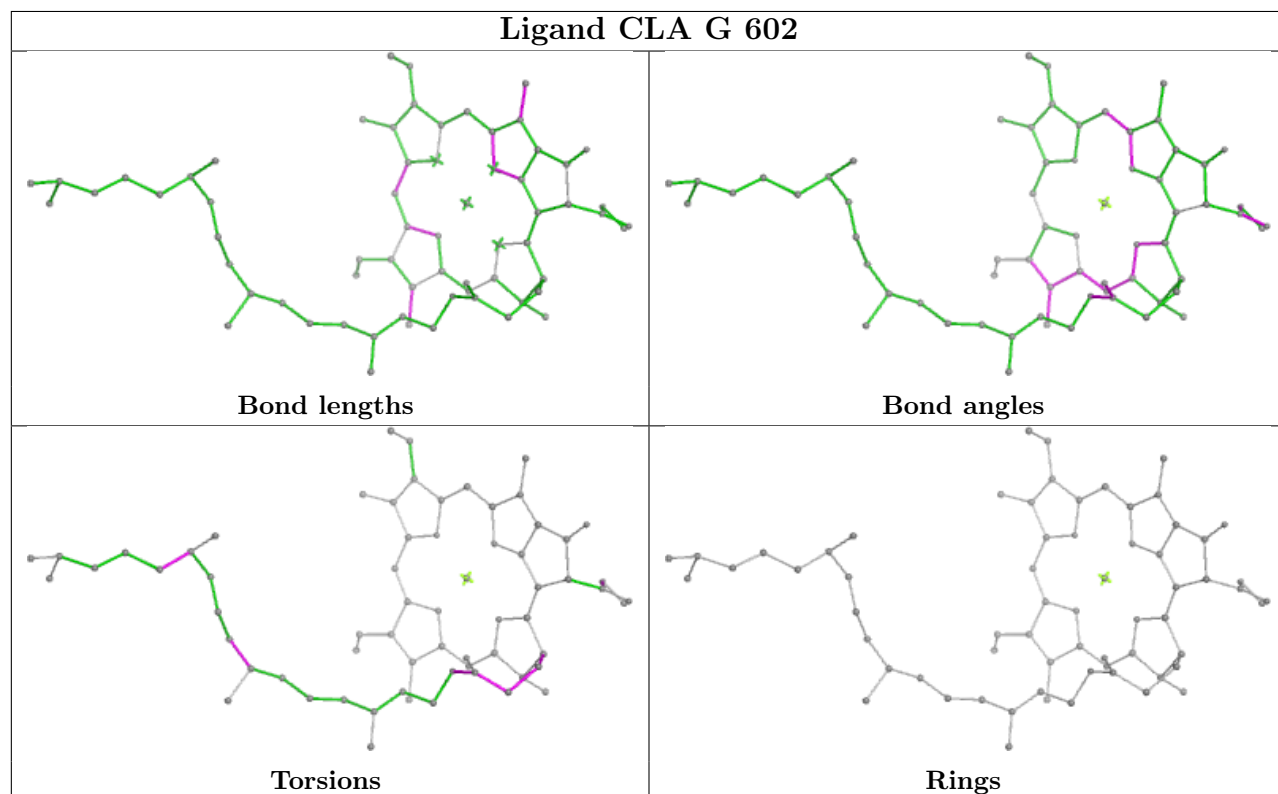
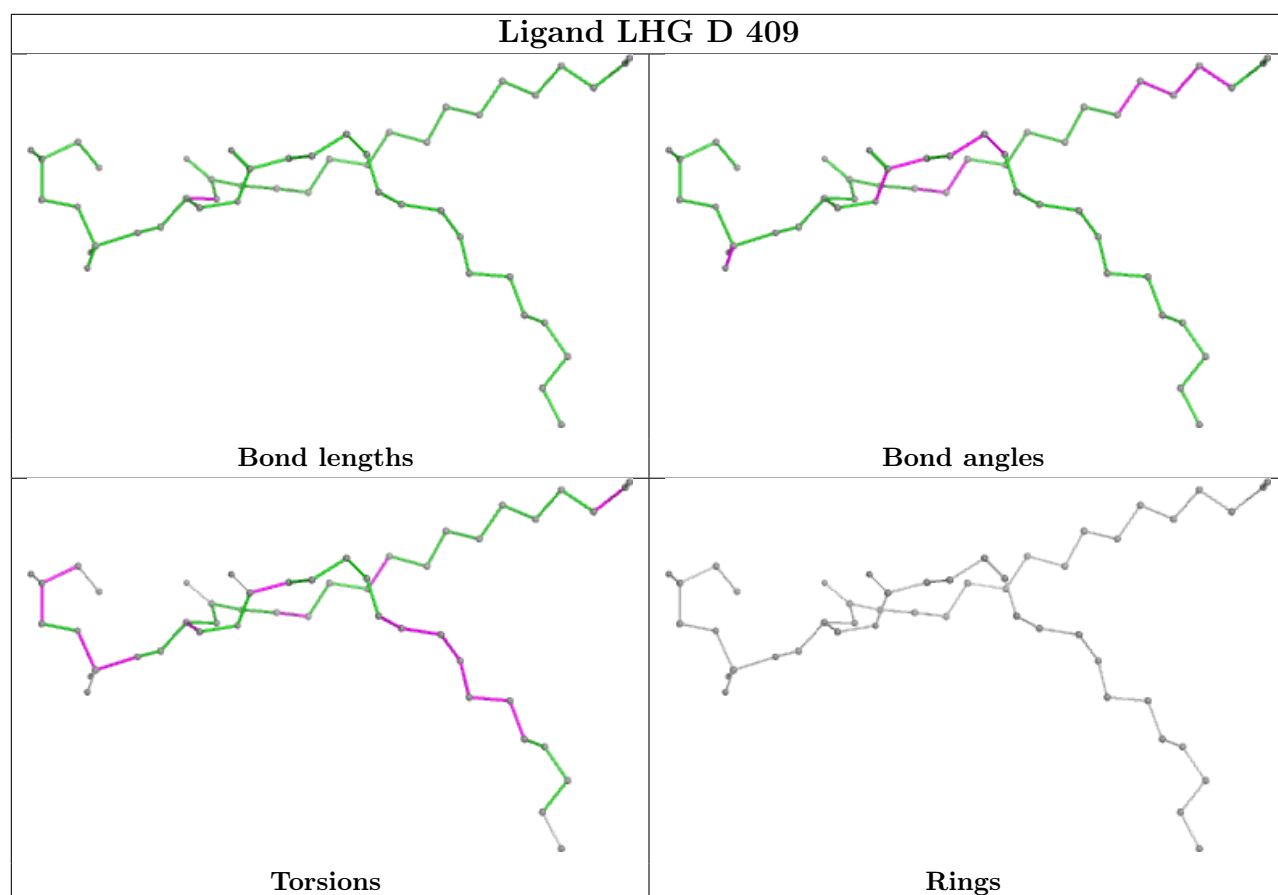




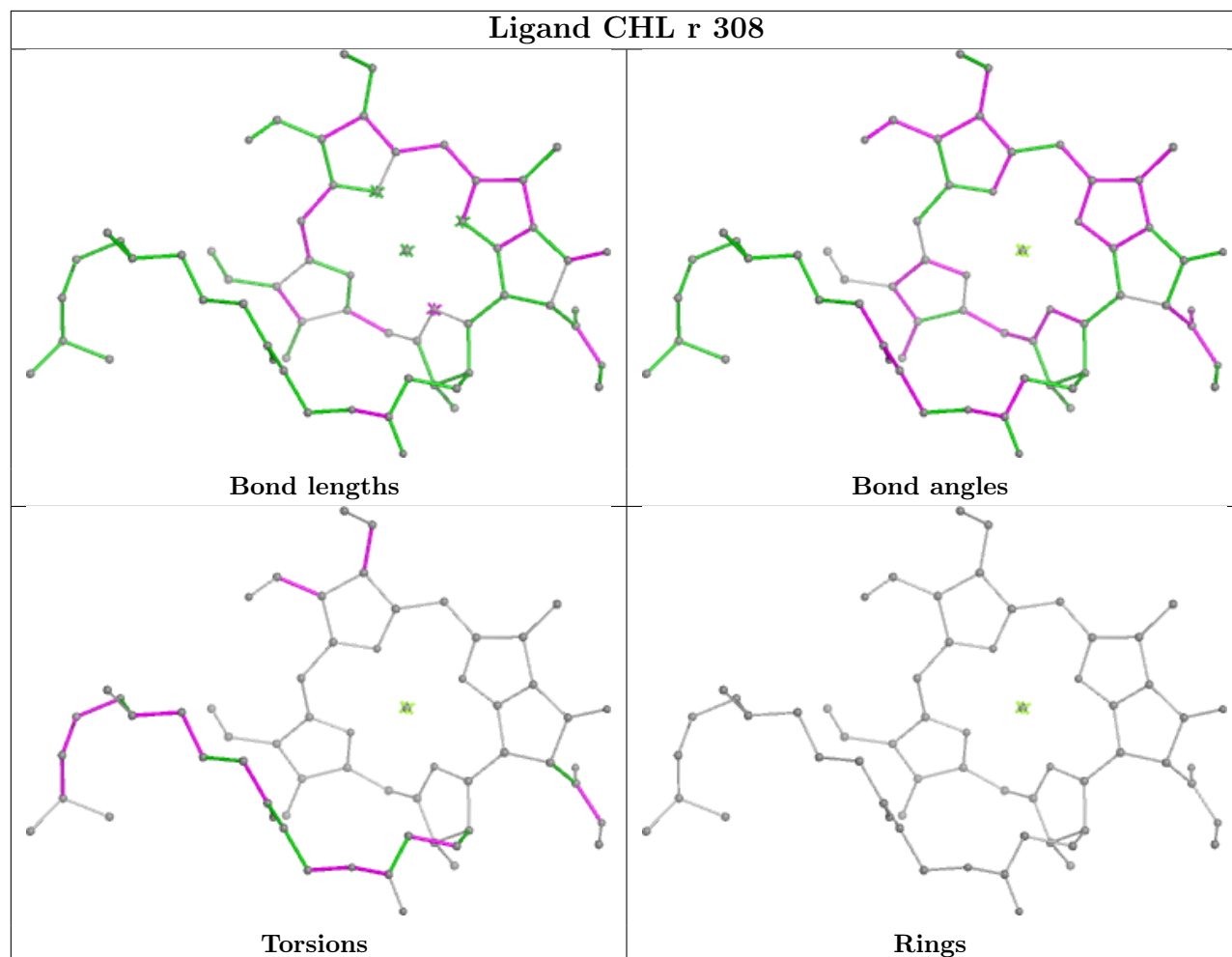


## Ligand CHL g 609

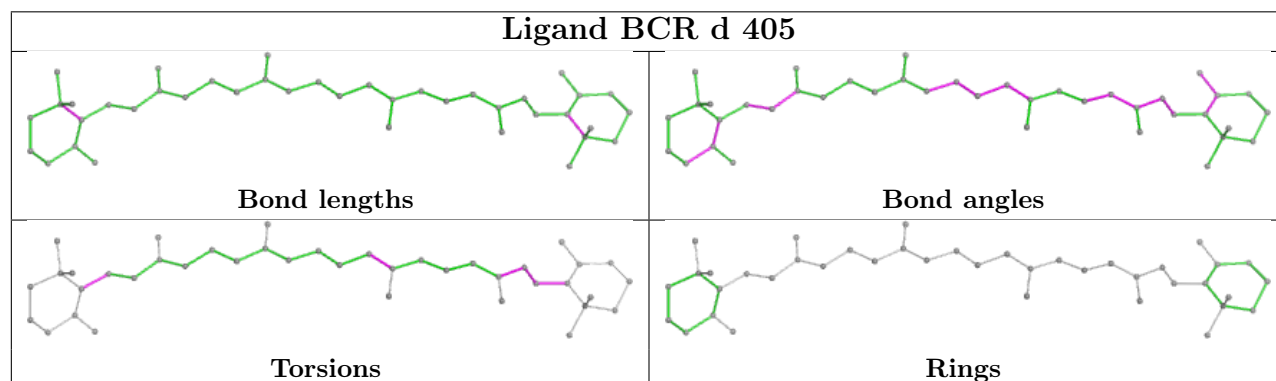


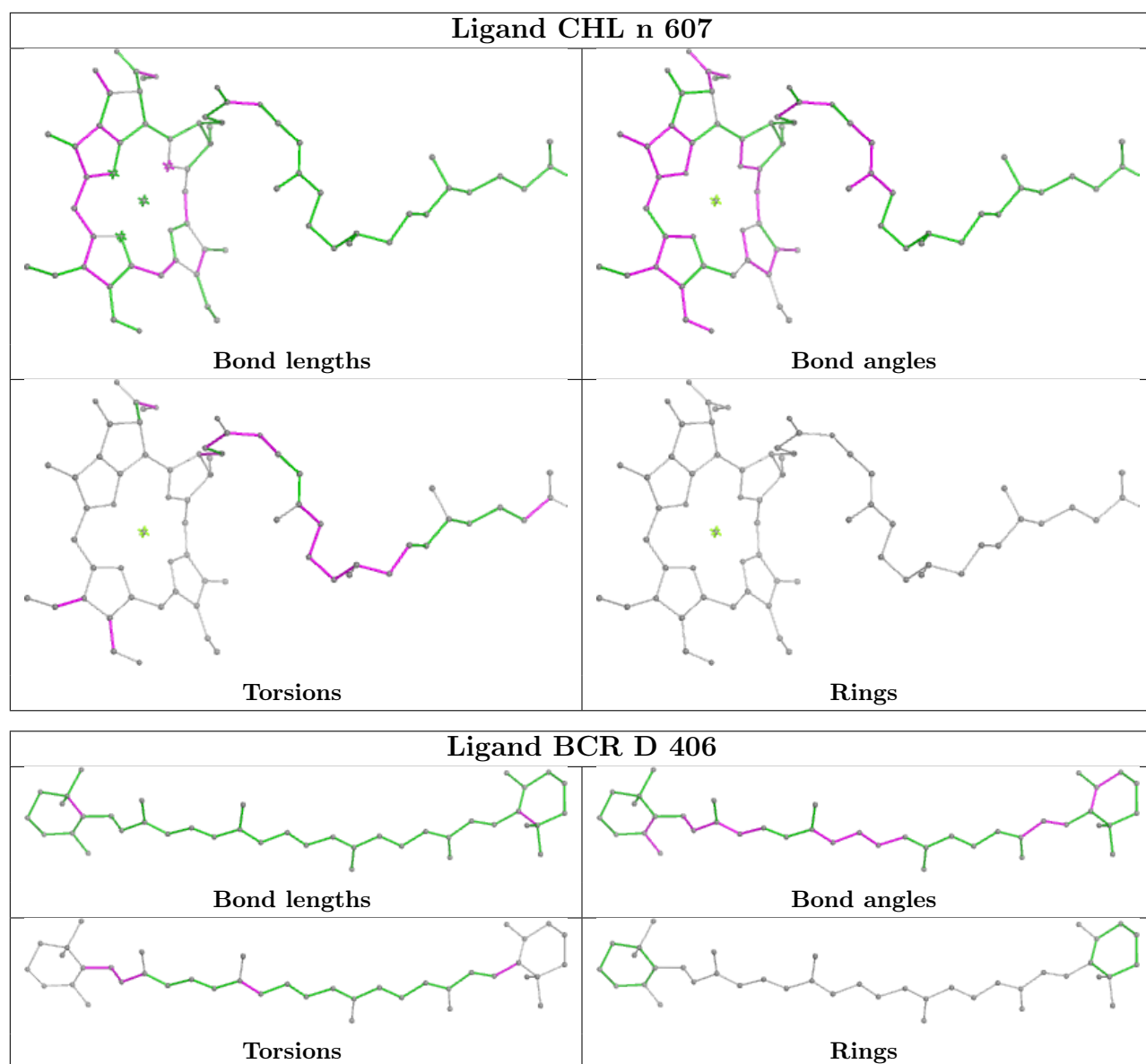


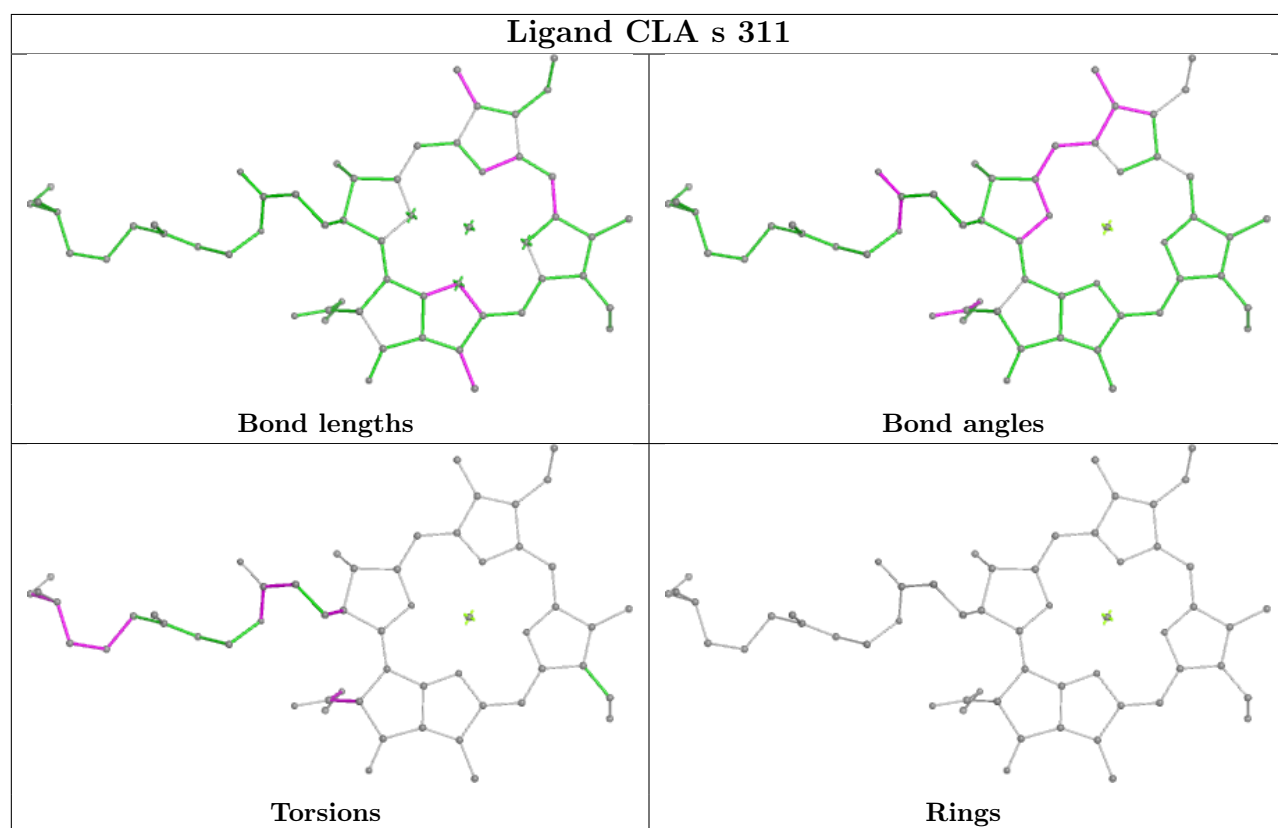
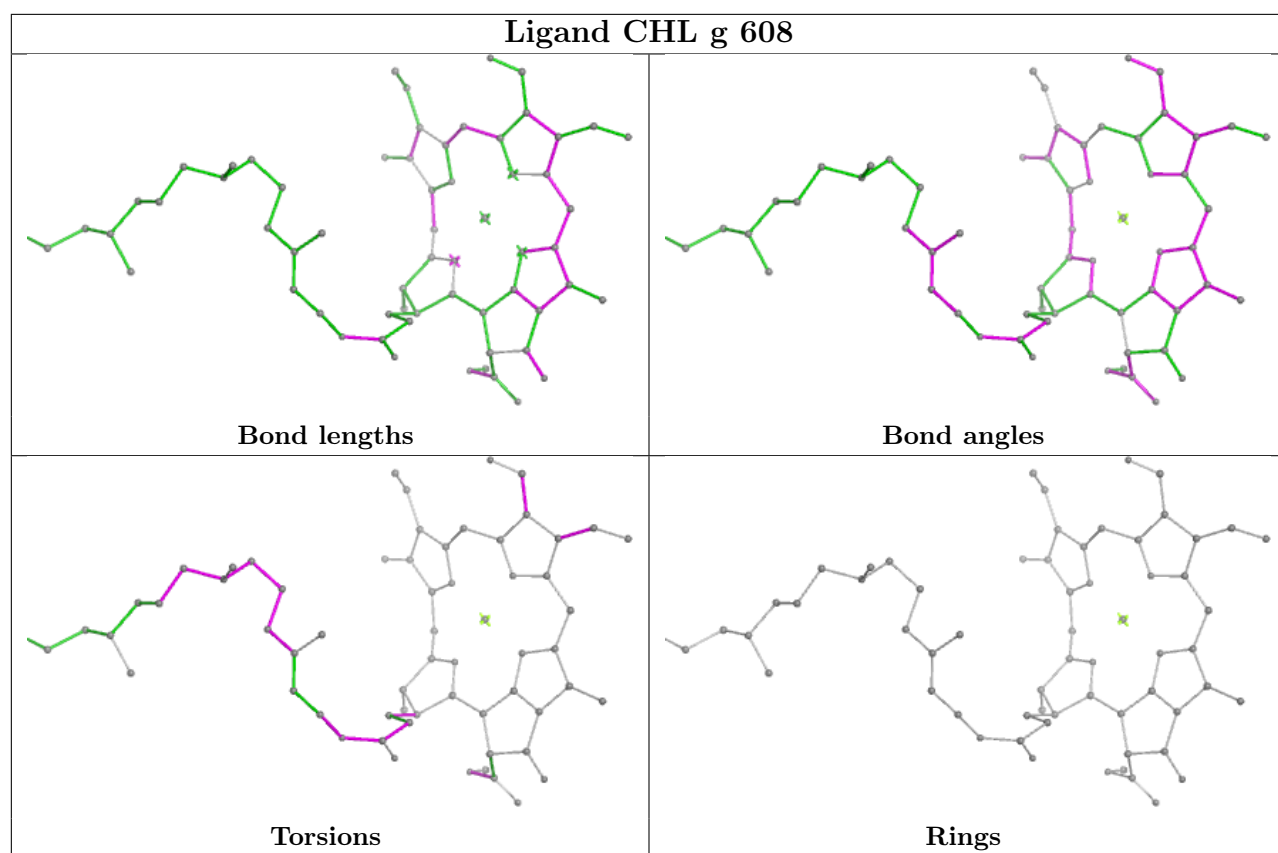
## Ligand CHL r 308

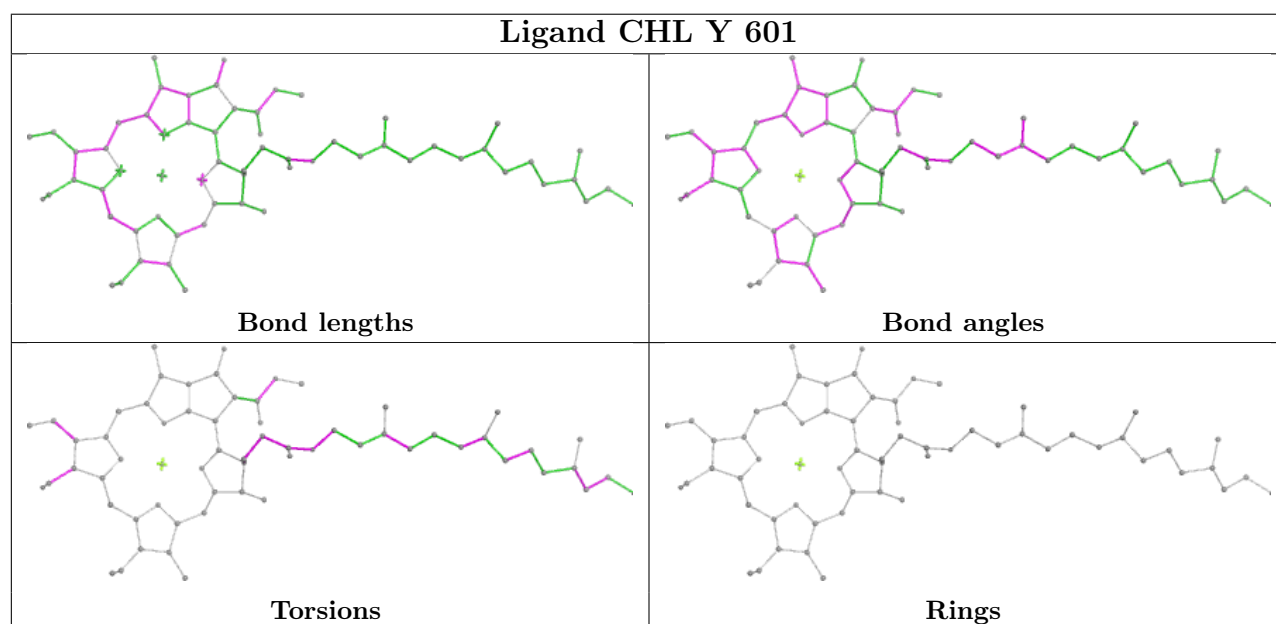
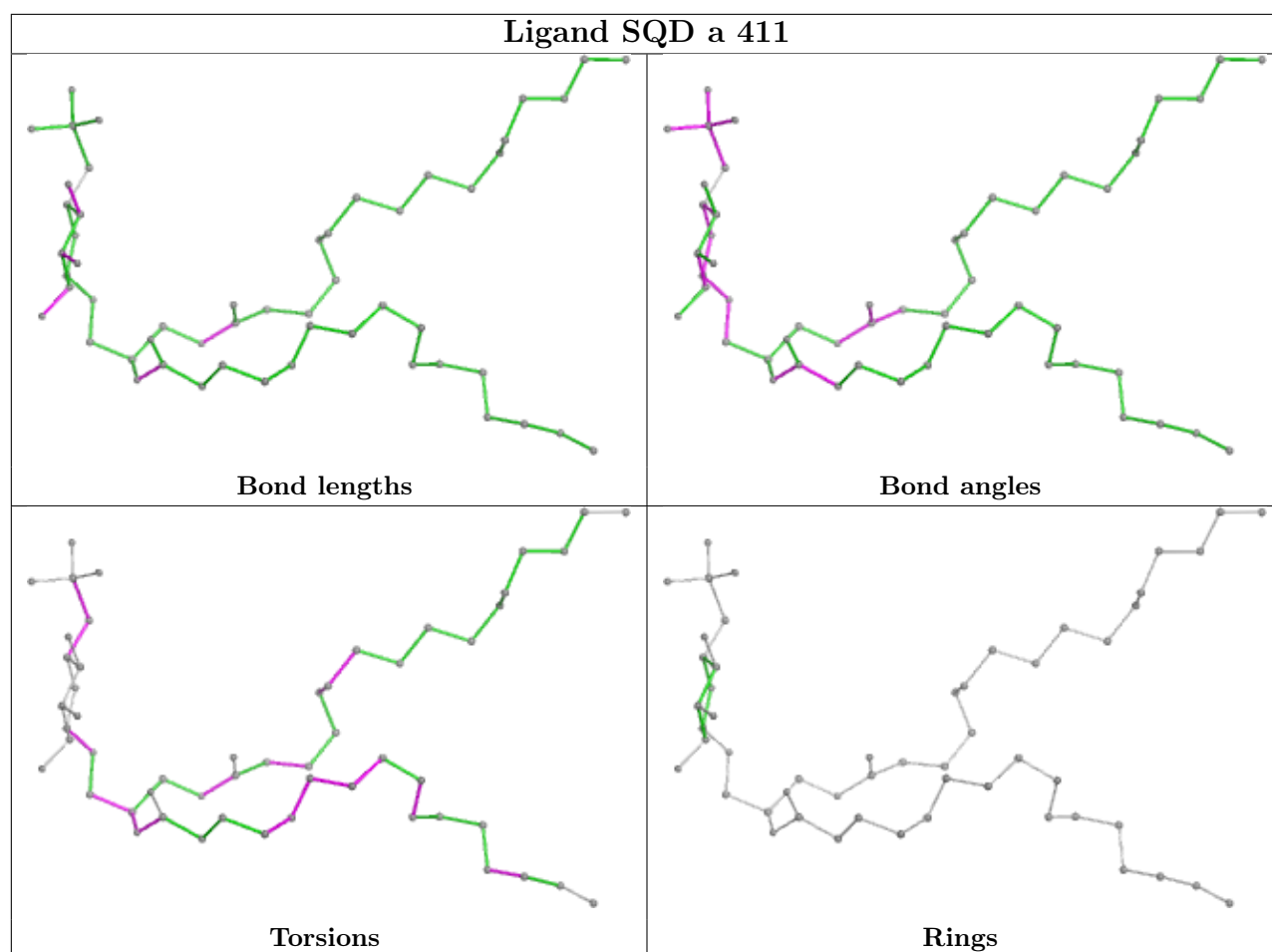


## Ligand BCR d 405

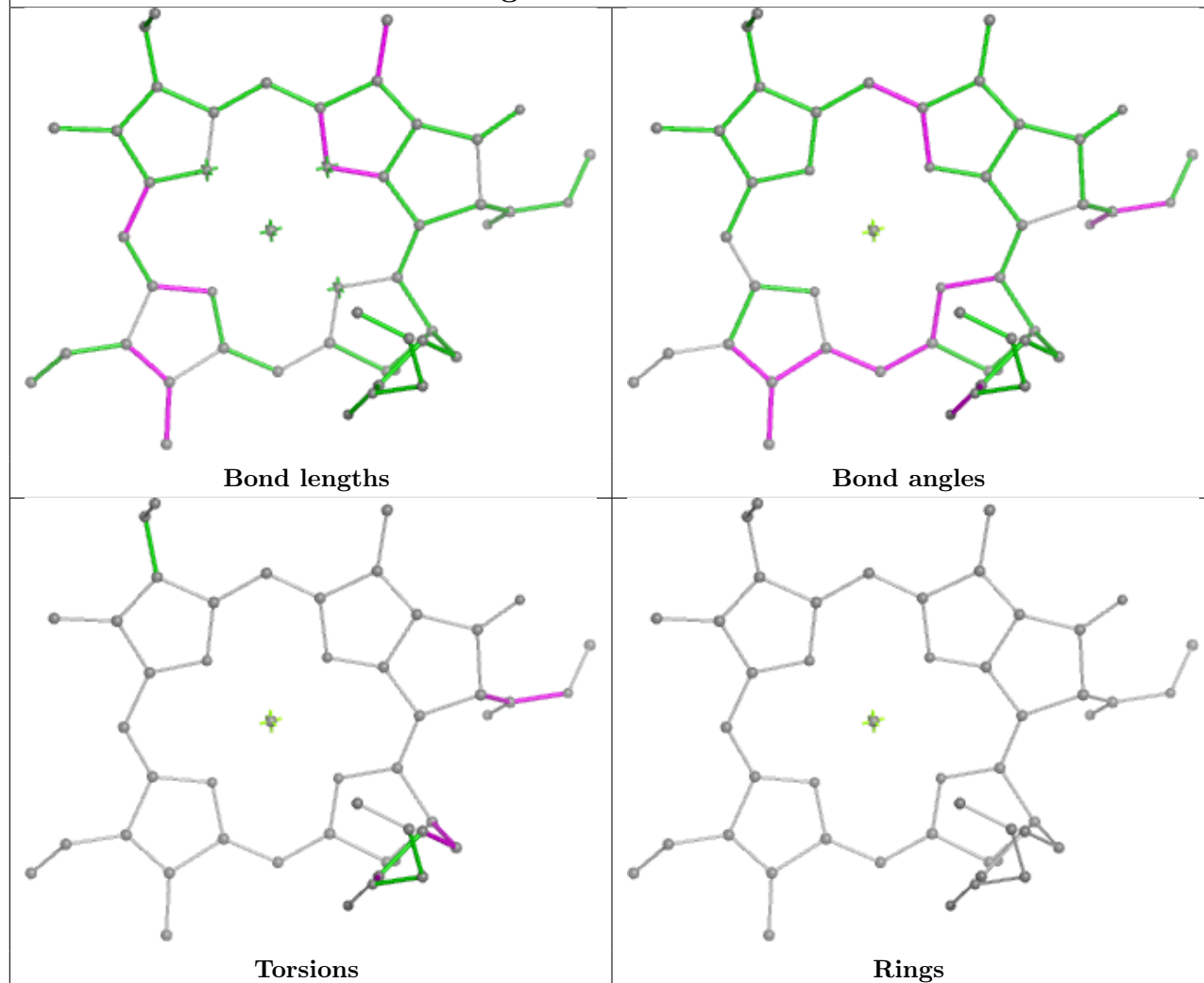




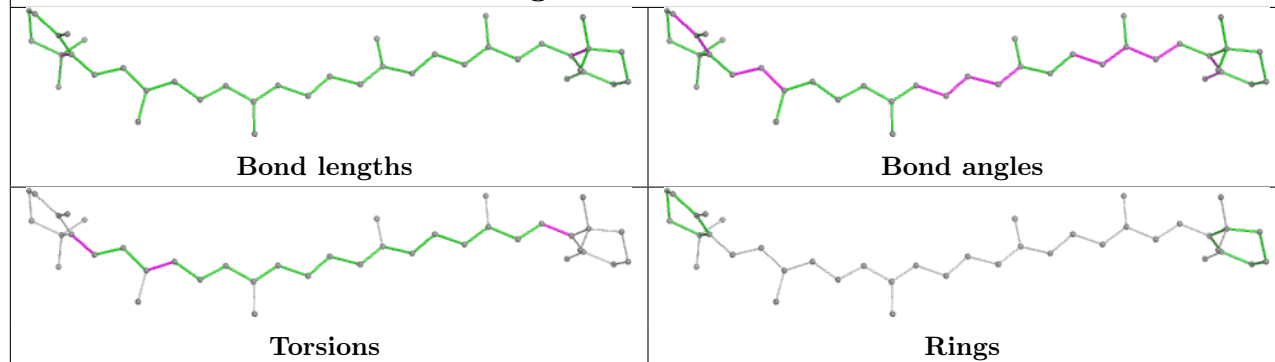




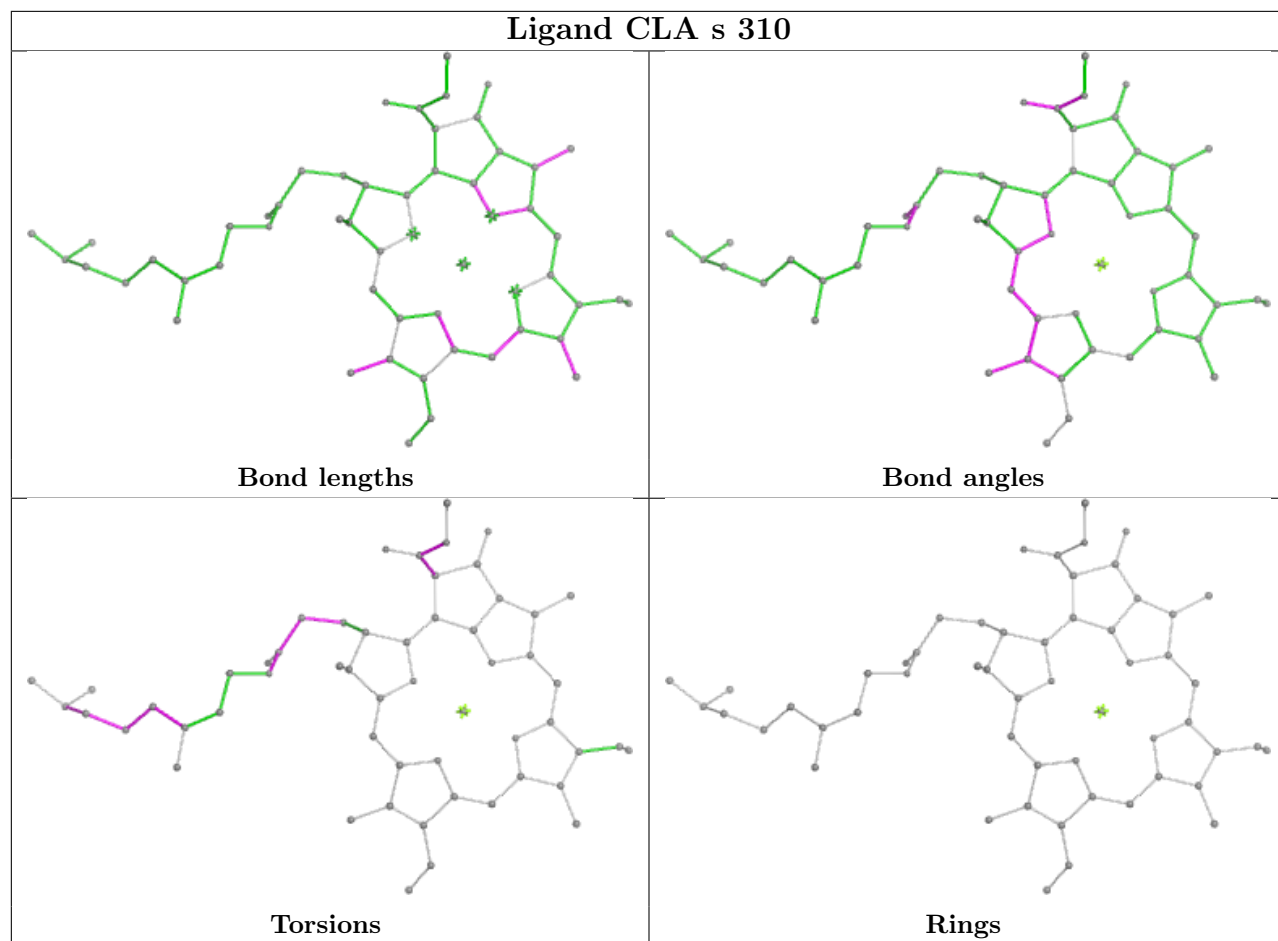
## Ligand CLA R 304



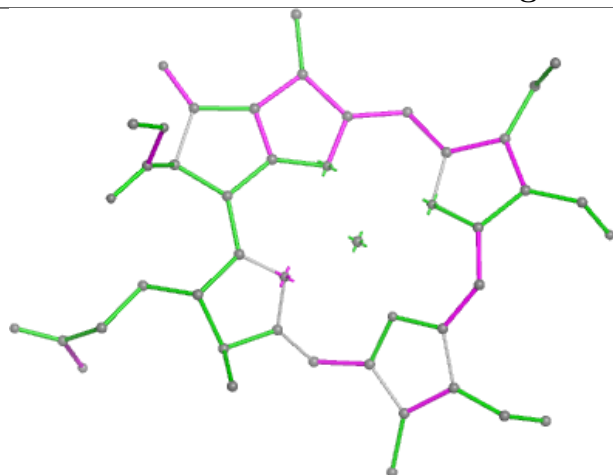
## Ligand BCR C 517



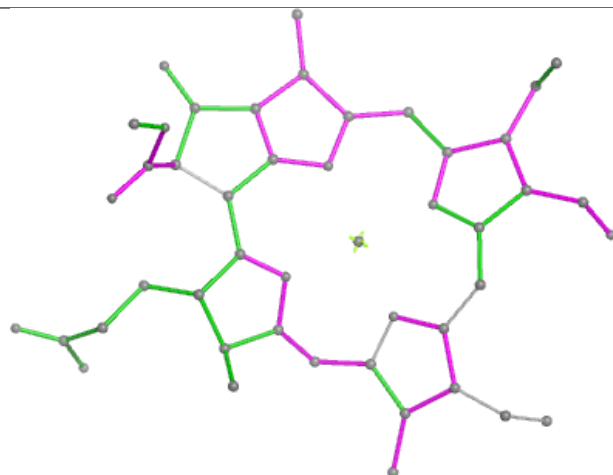
## Ligand CLA s 310



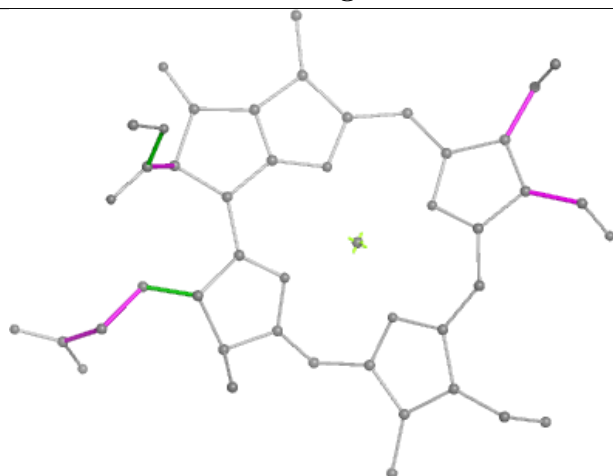
## Ligand CHL s 306



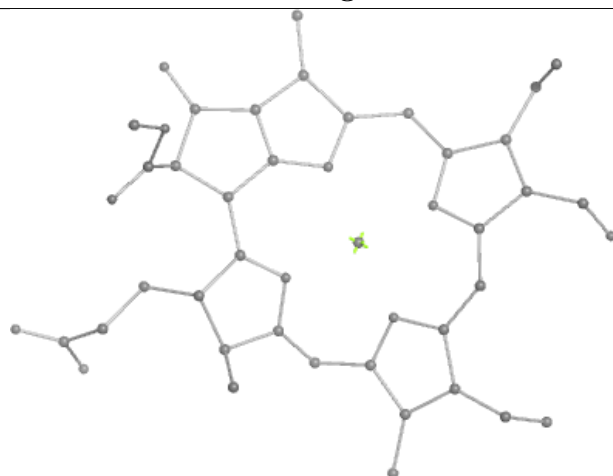
Bond lengths



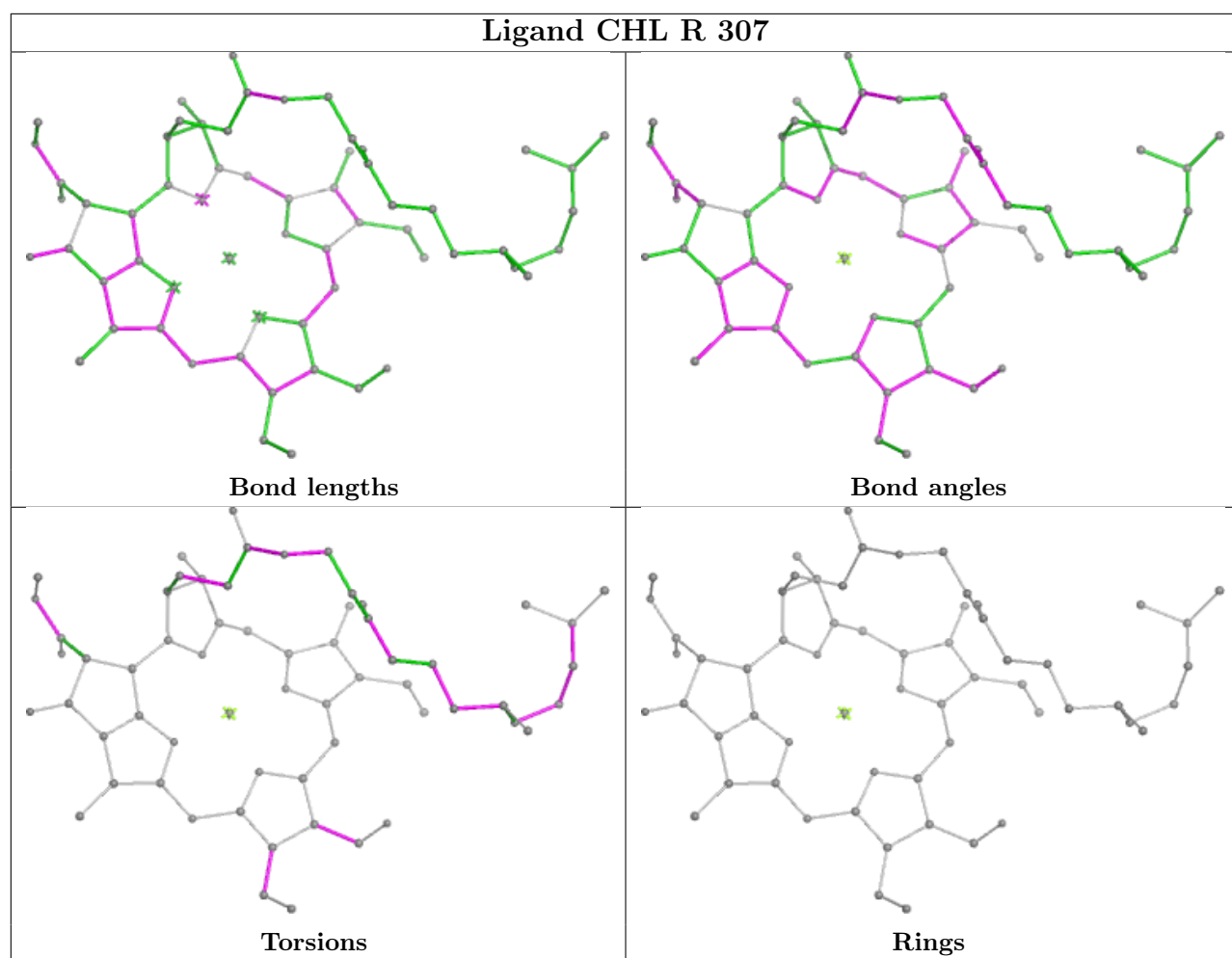
Bond angles



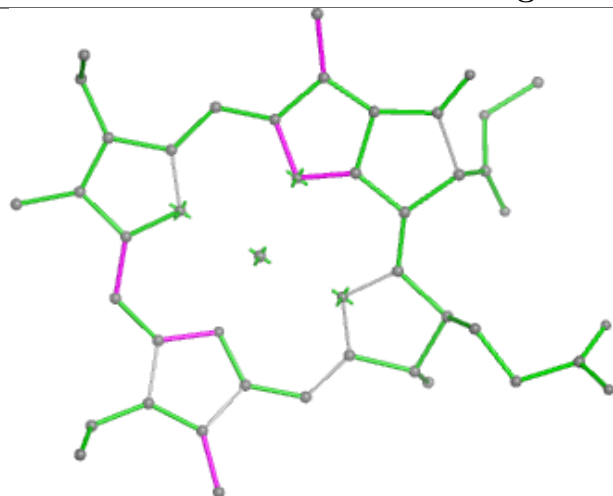
Torsions



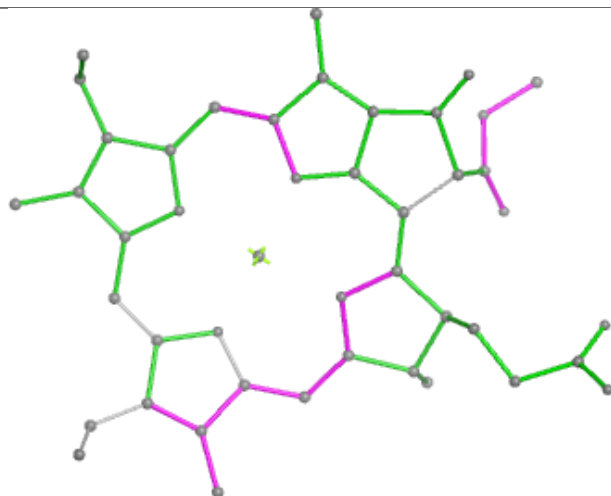
Rings



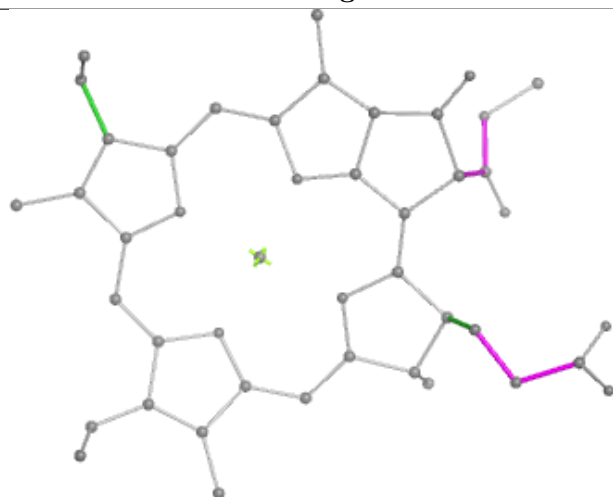
## Ligand CLA S 308



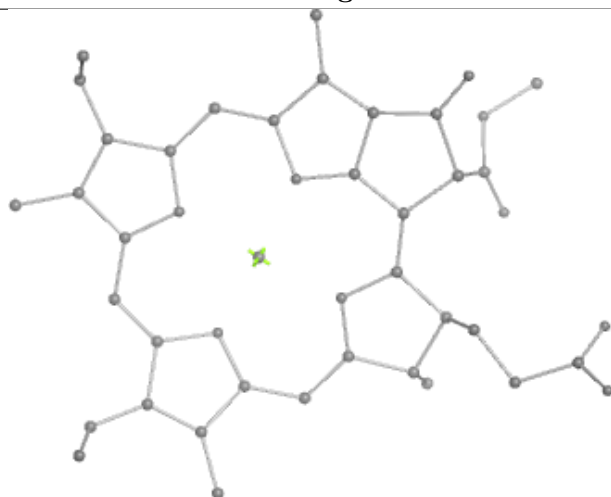
Bond lengths



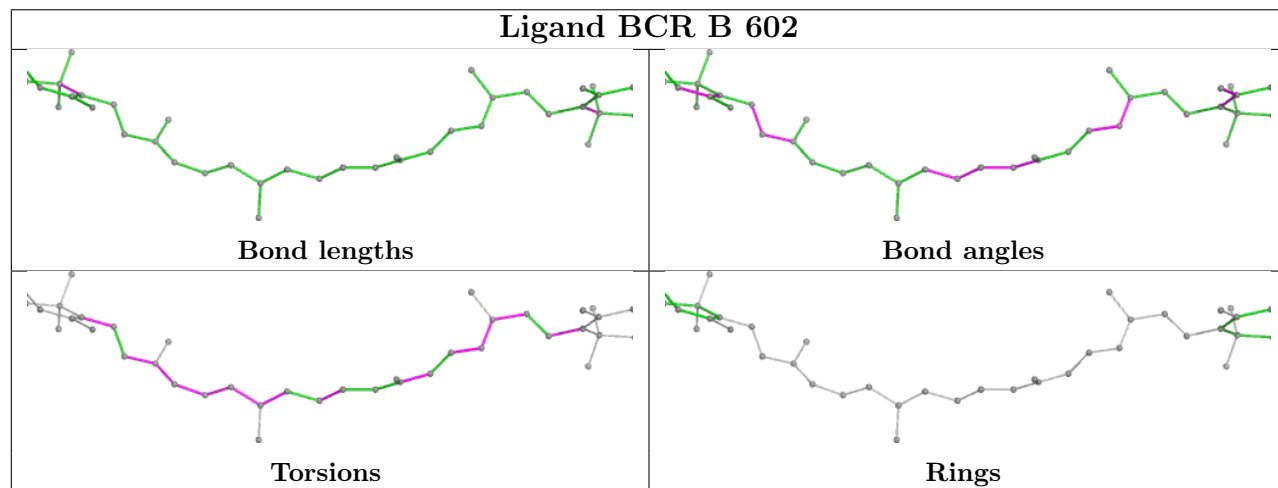
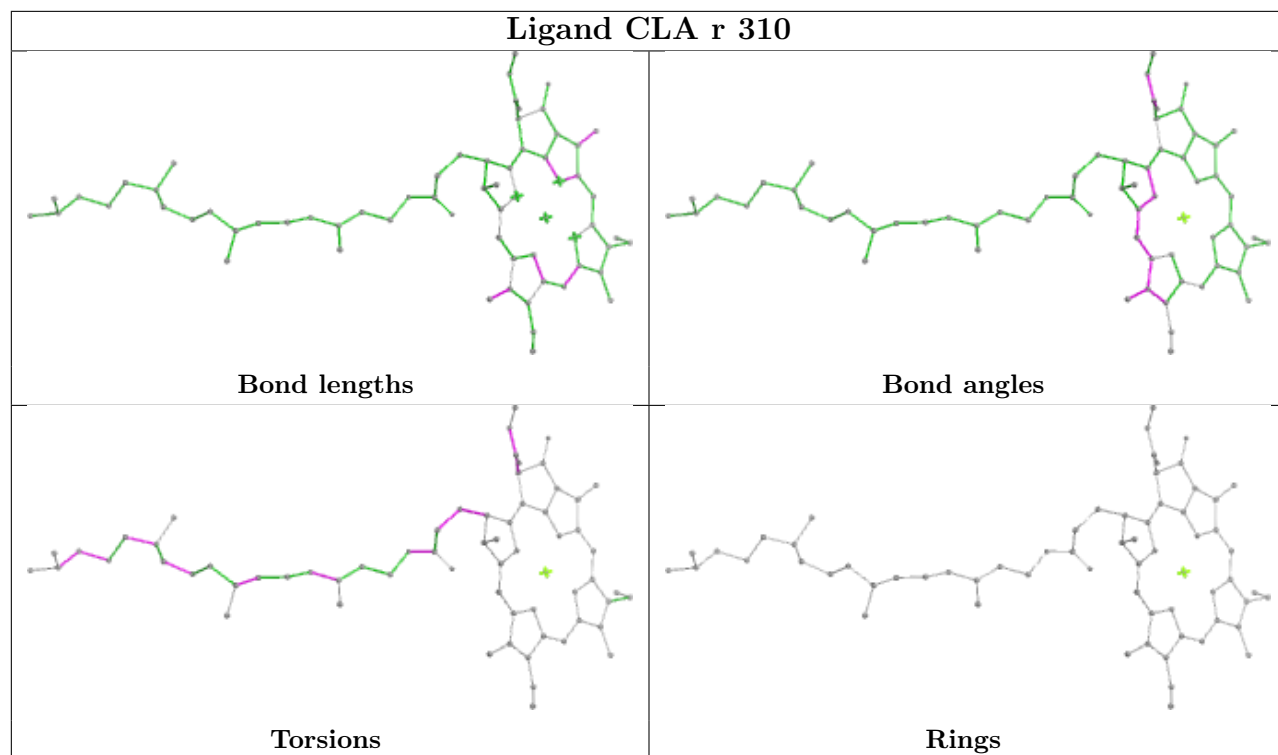
Bond angles

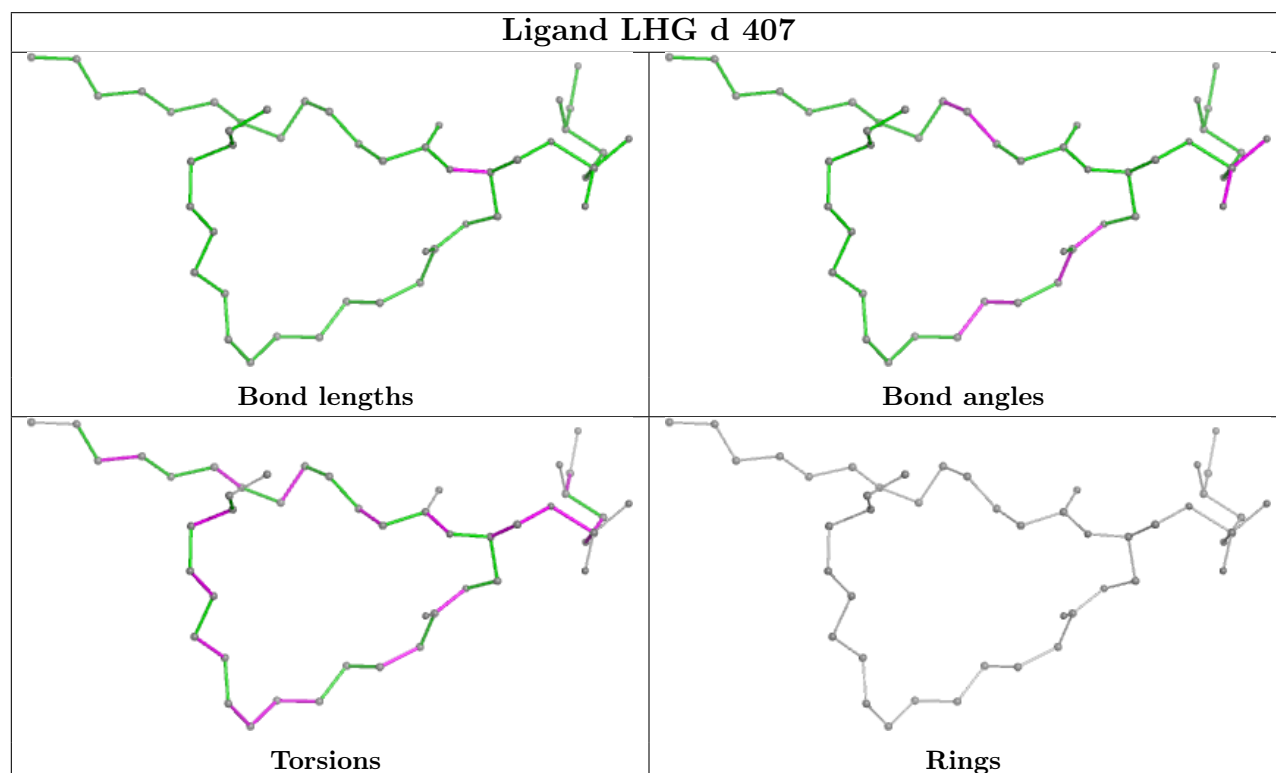
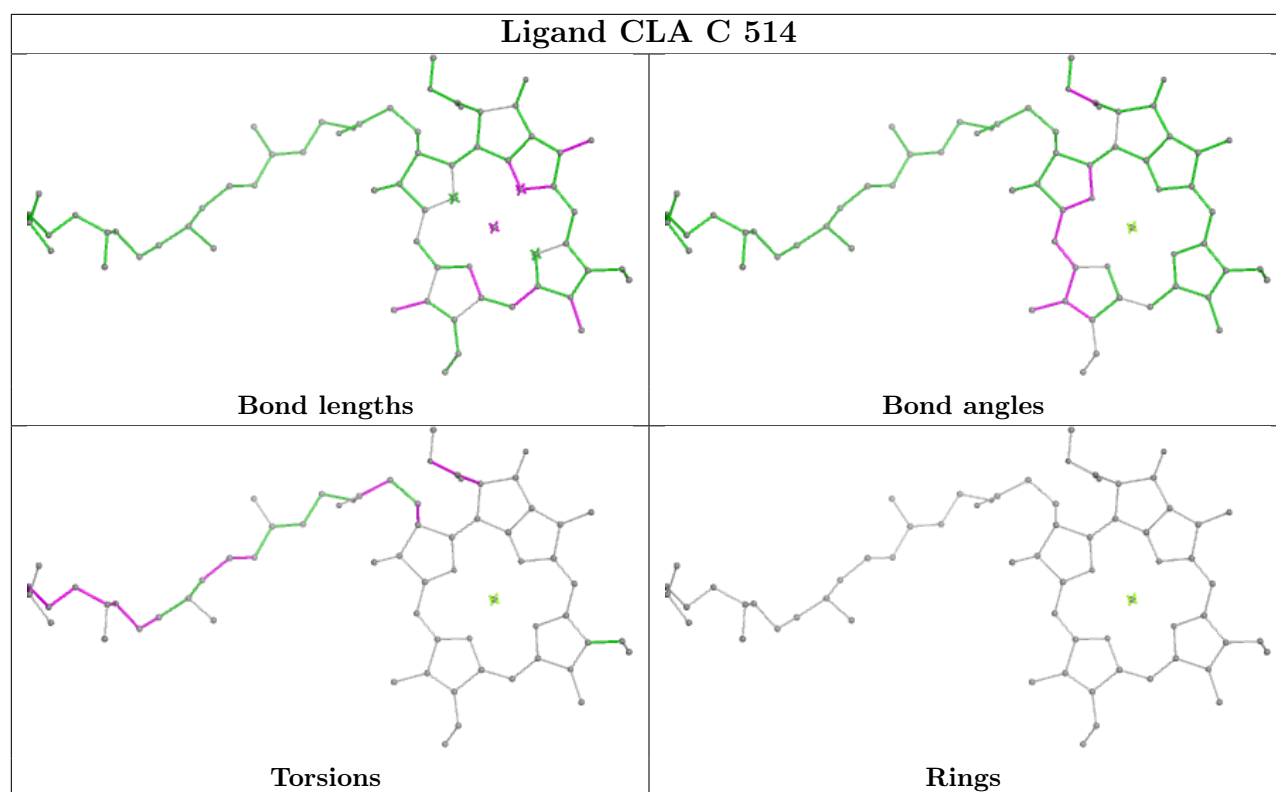


Torsions

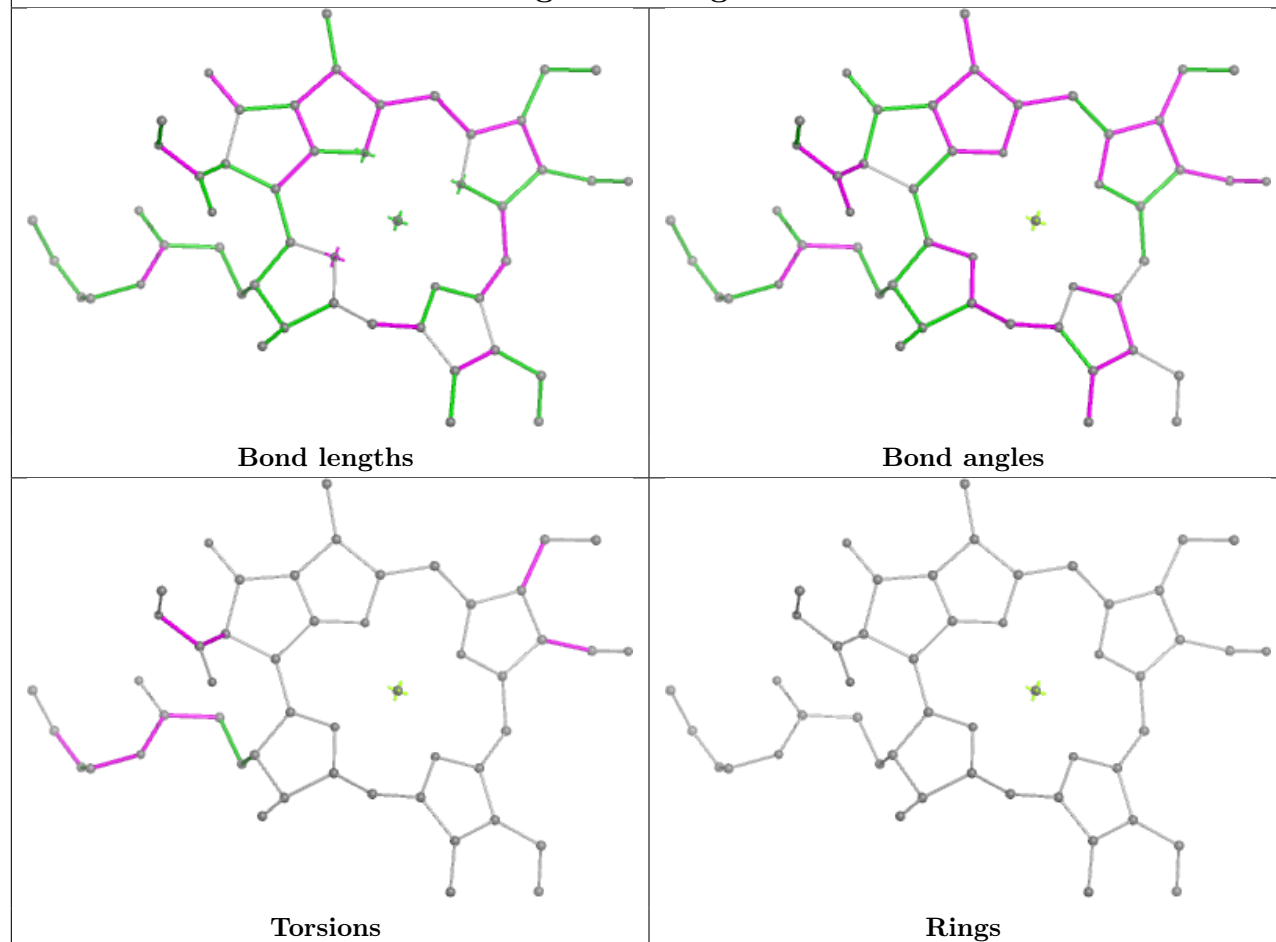


Rings

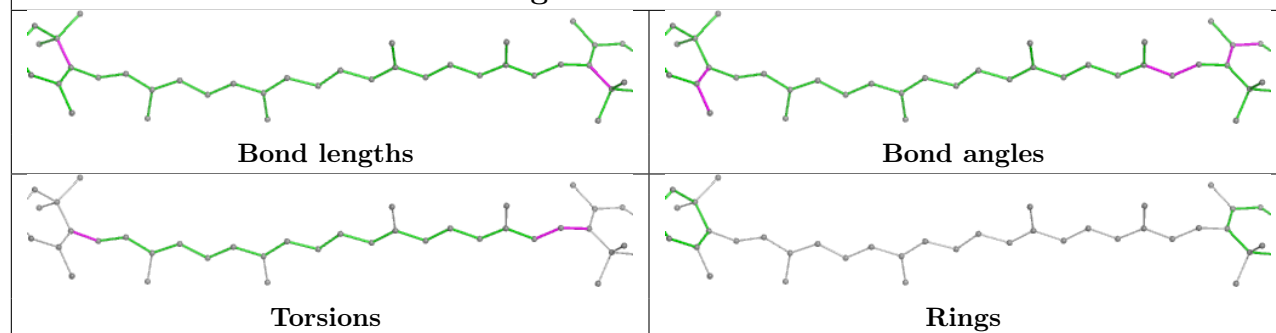




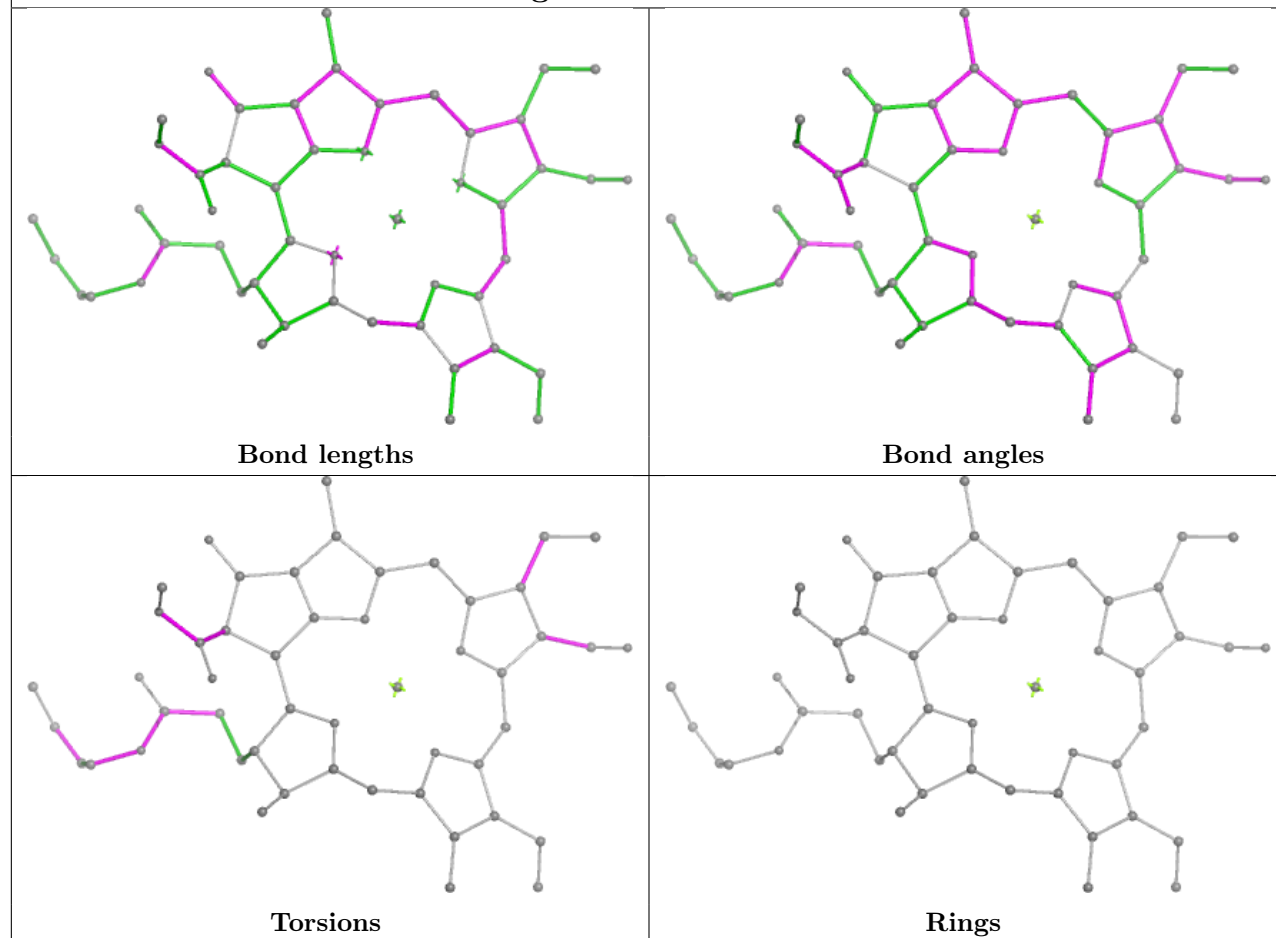
## Ligand CHL g 606



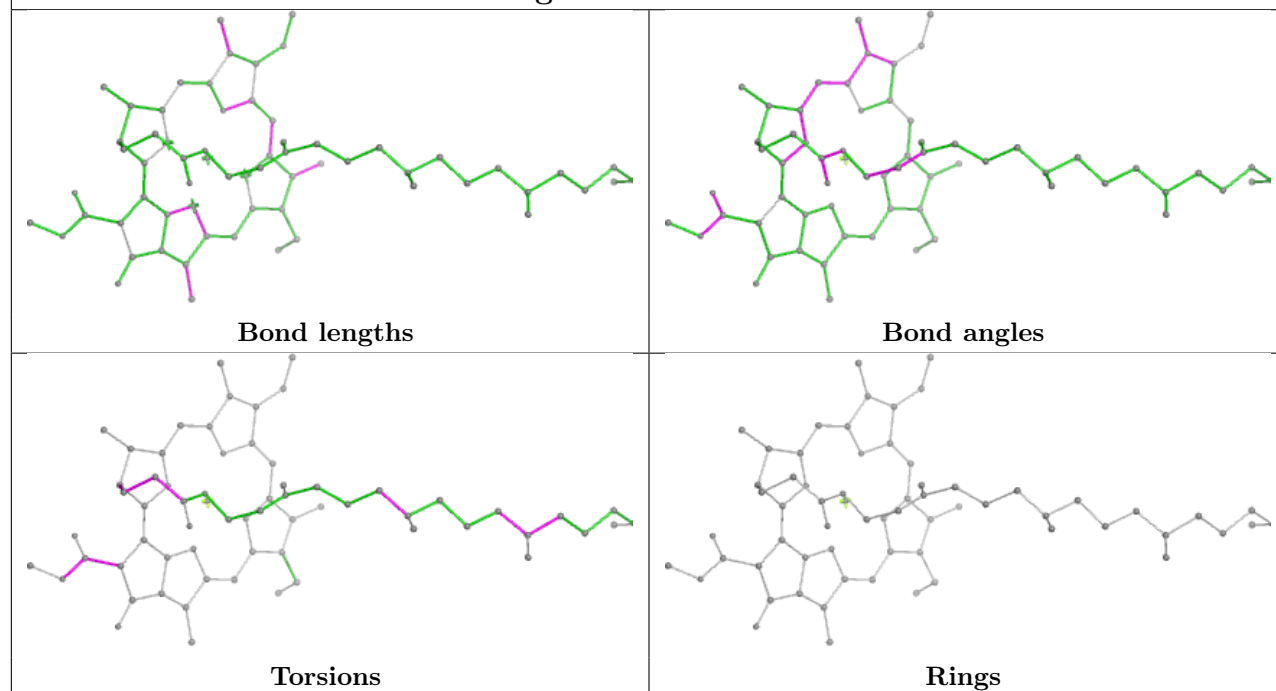
## Ligand BCR B 621

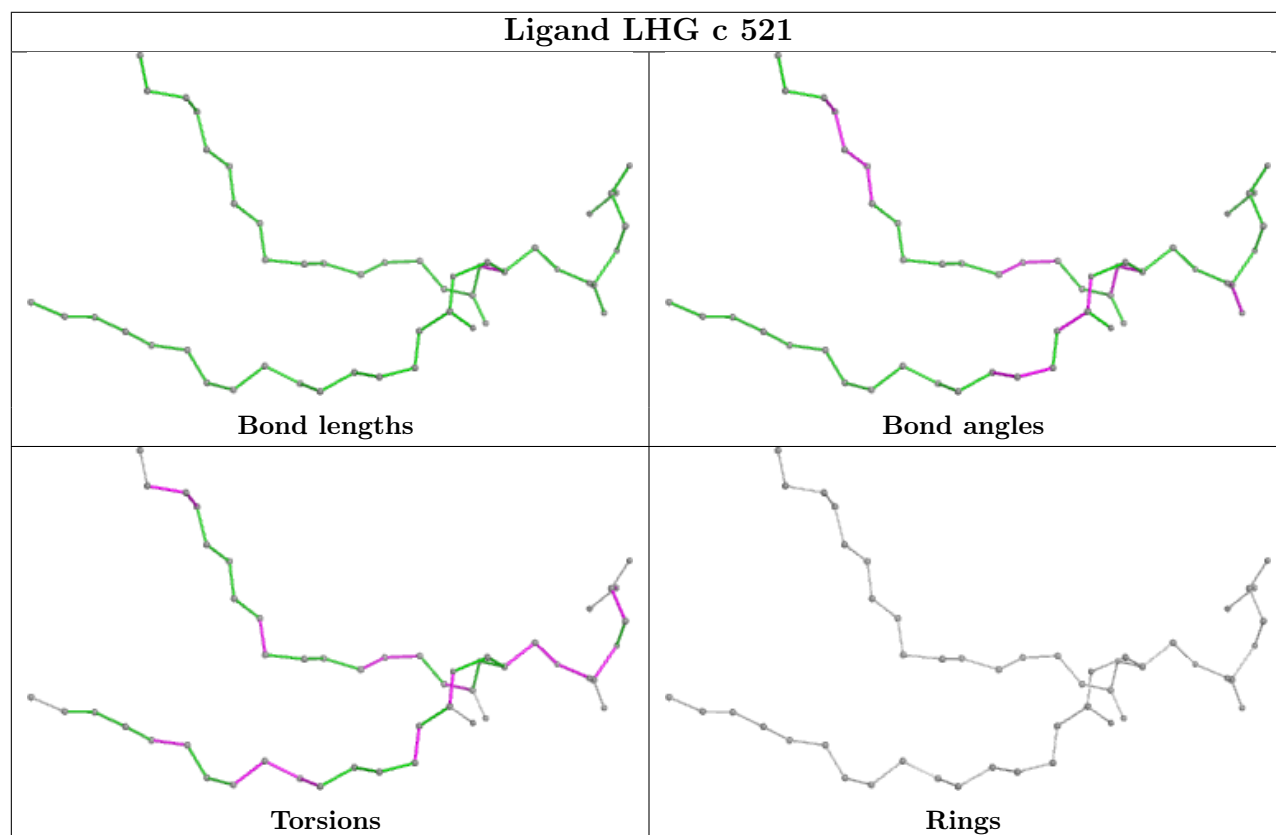
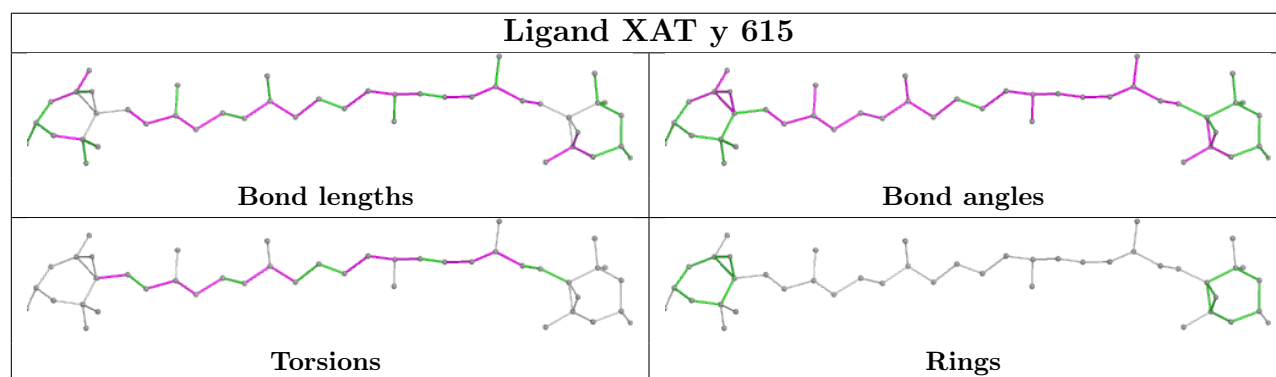
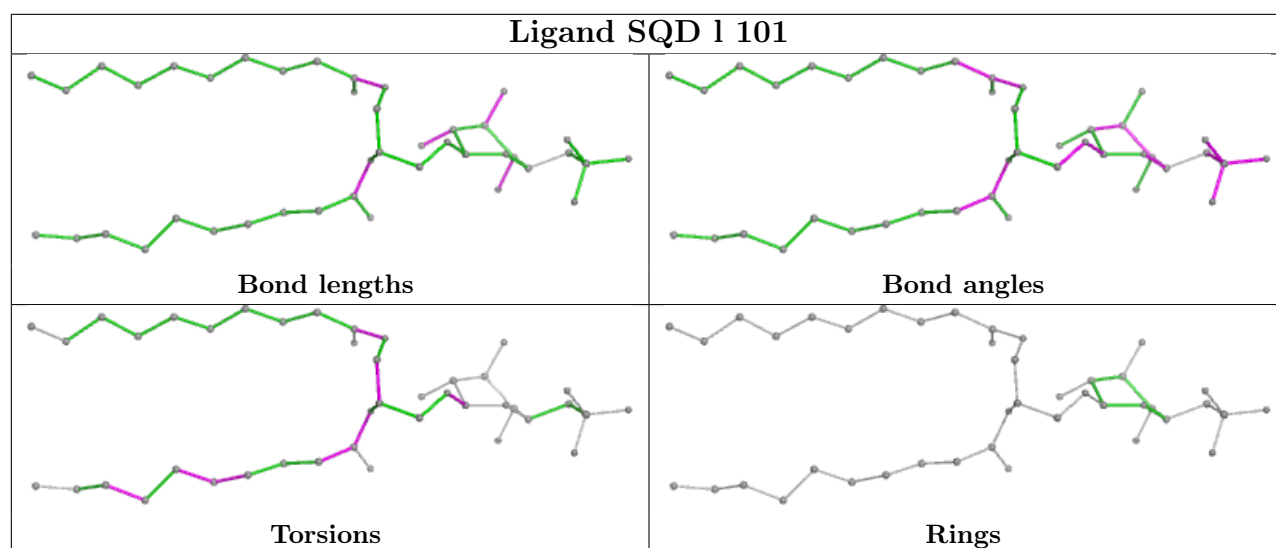


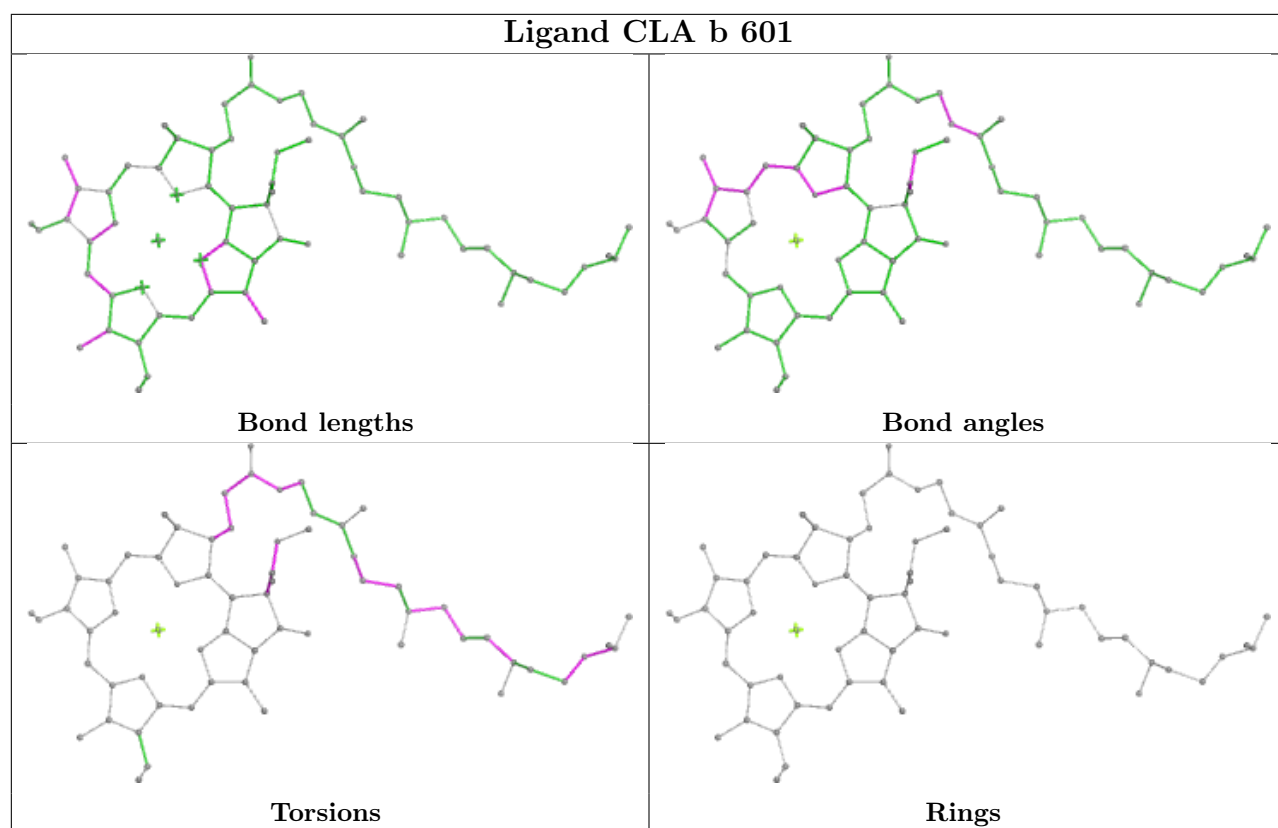
## Ligand CHL Y 605



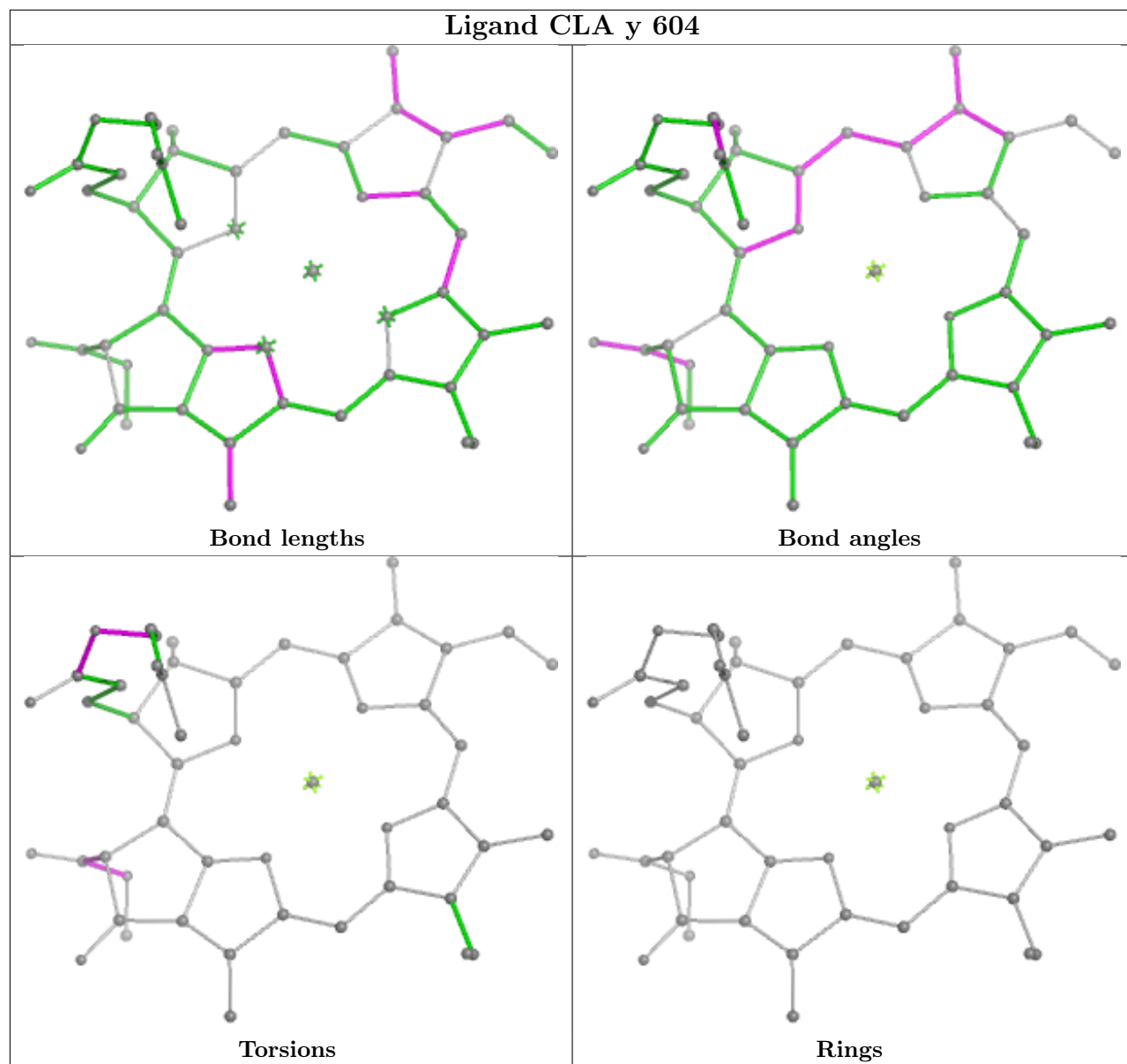
## Ligand CLA b 607

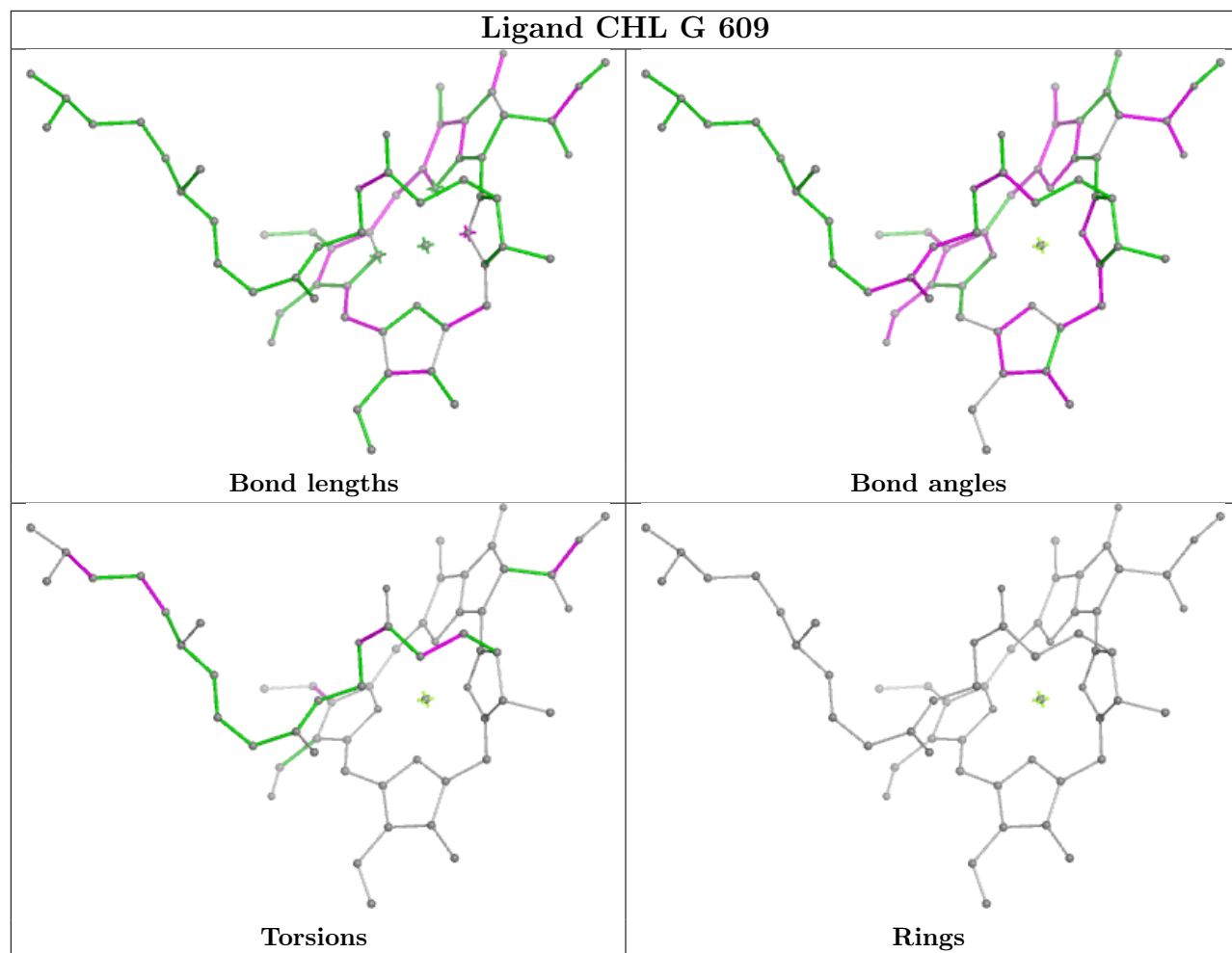


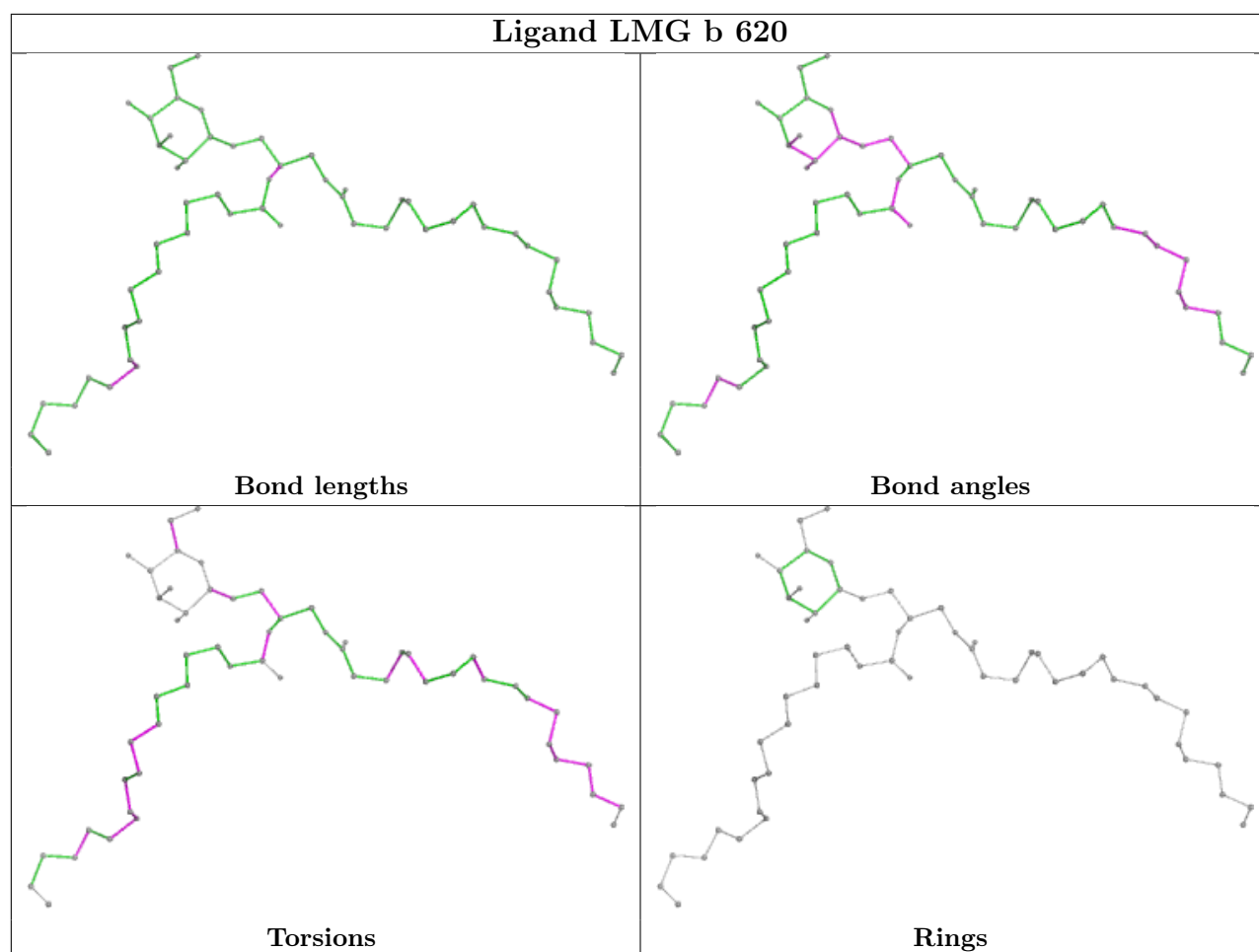




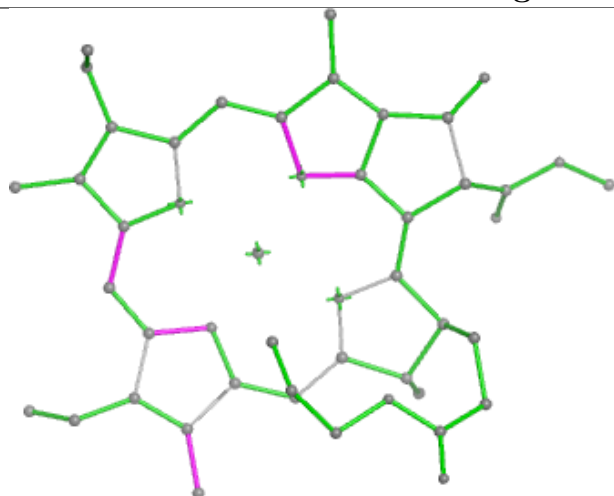
## Ligand CLA y 604



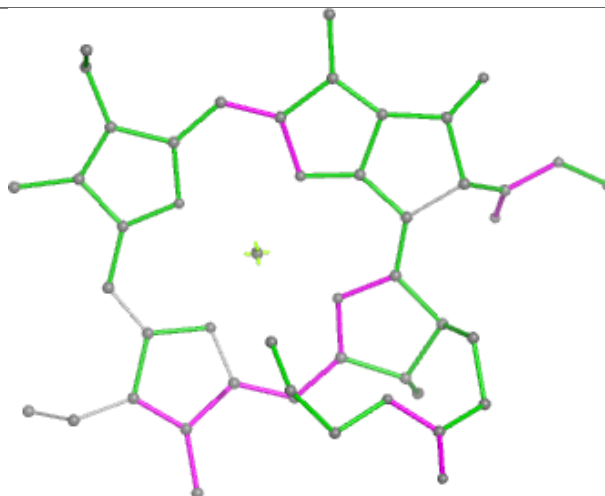




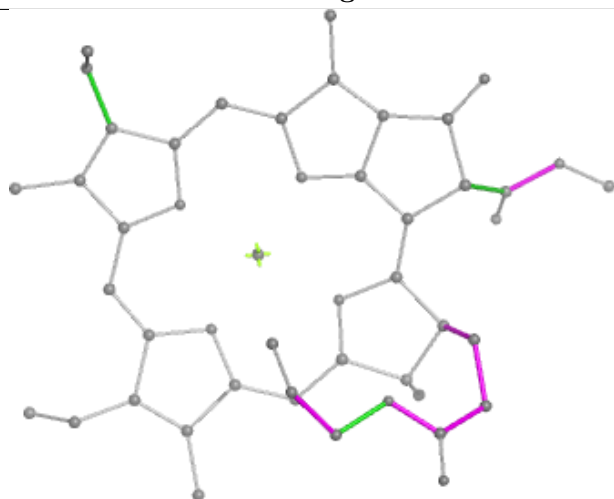
## Ligand CLA N 613



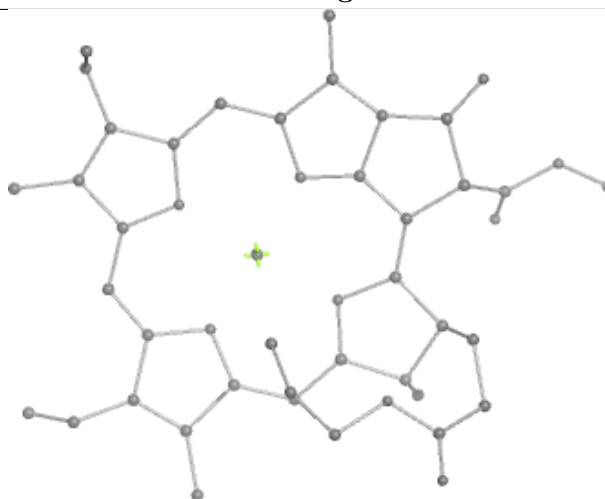
Bond lengths



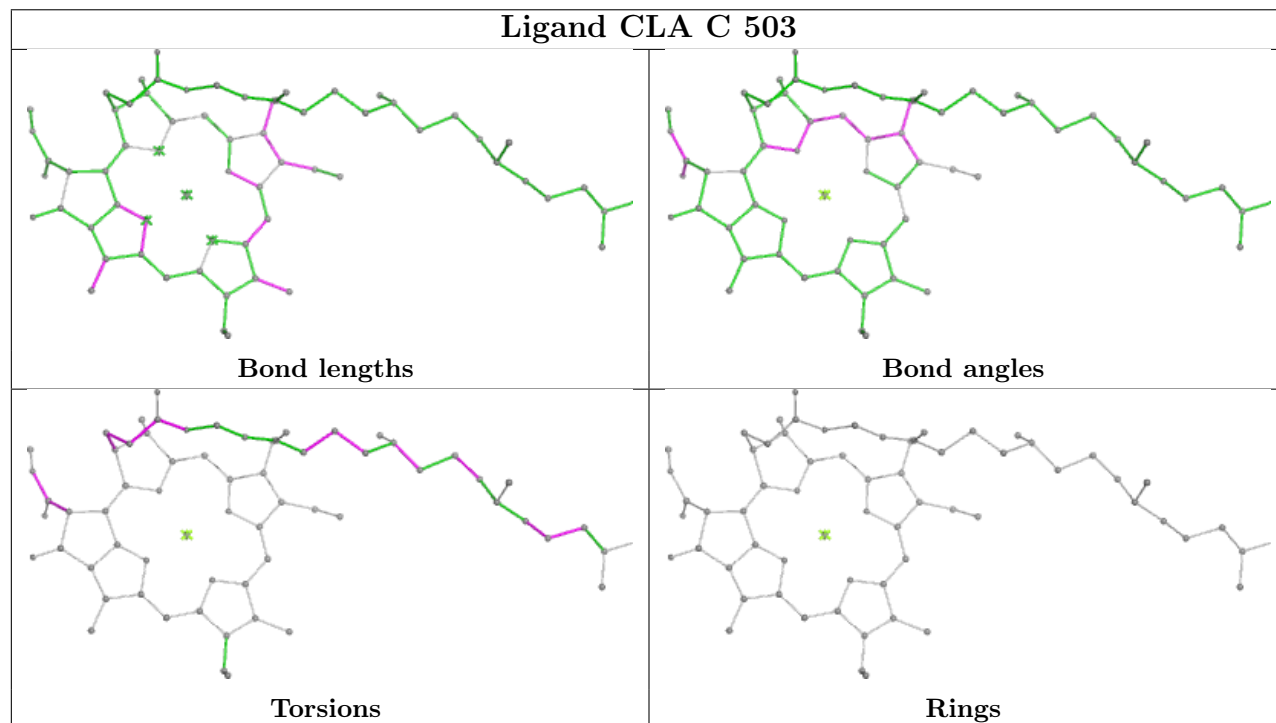
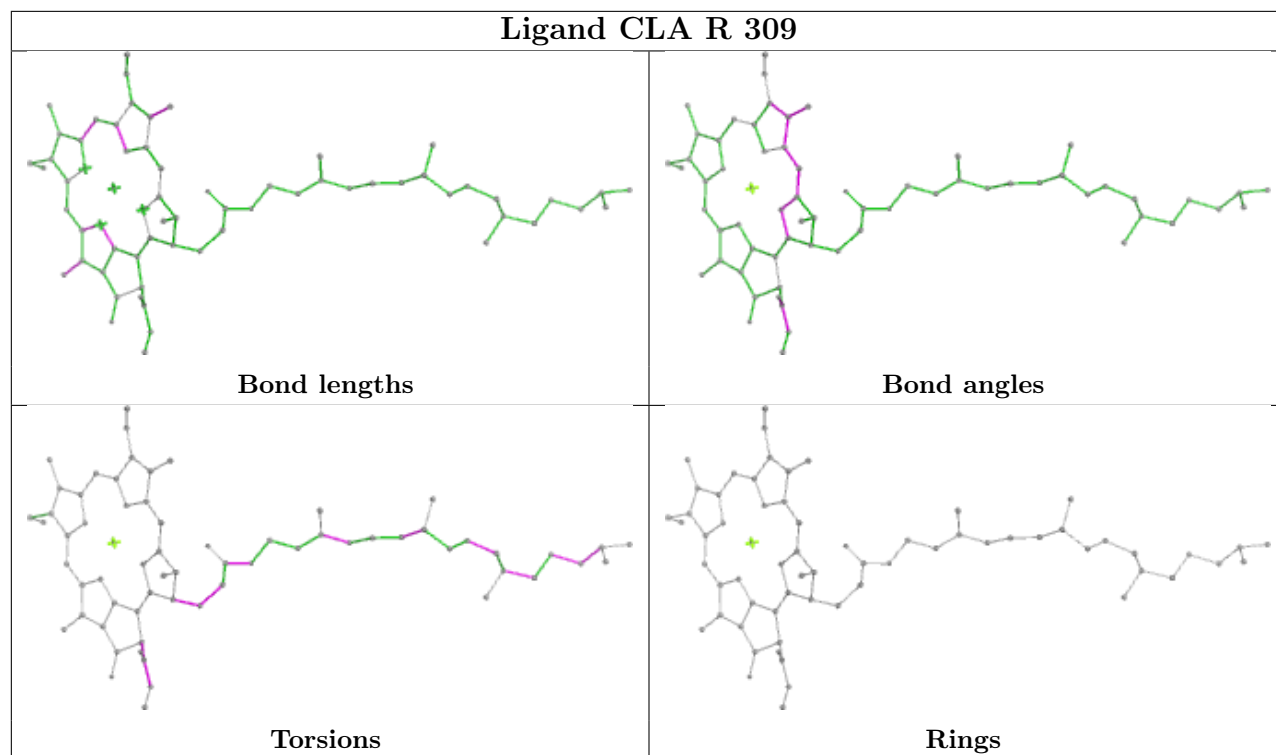
Bond angles



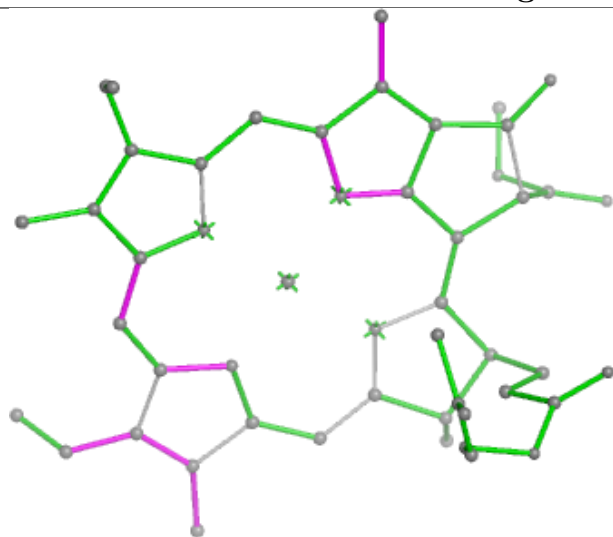
Torsions



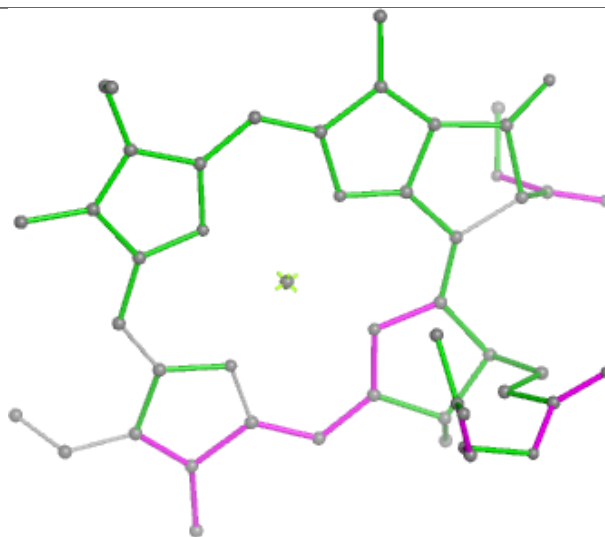
Rings



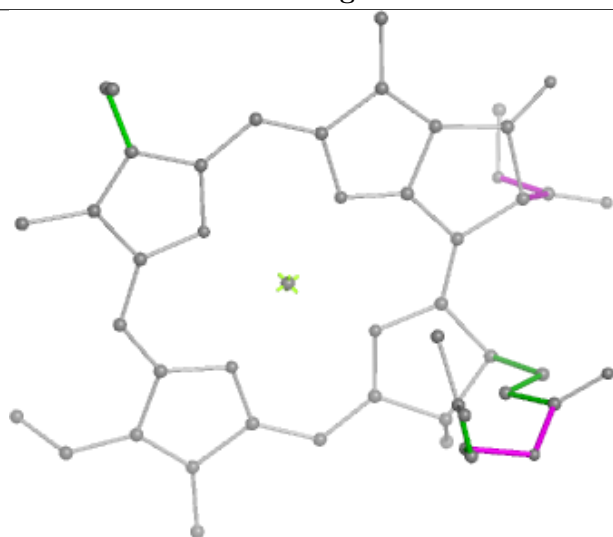
## Ligand CLA n 604



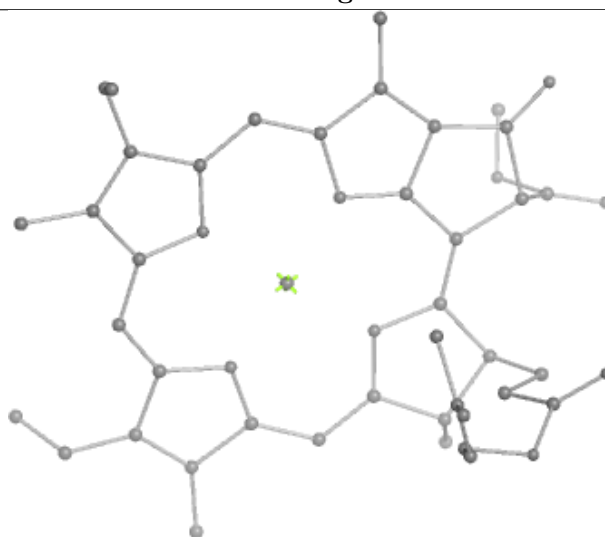
Bond lengths



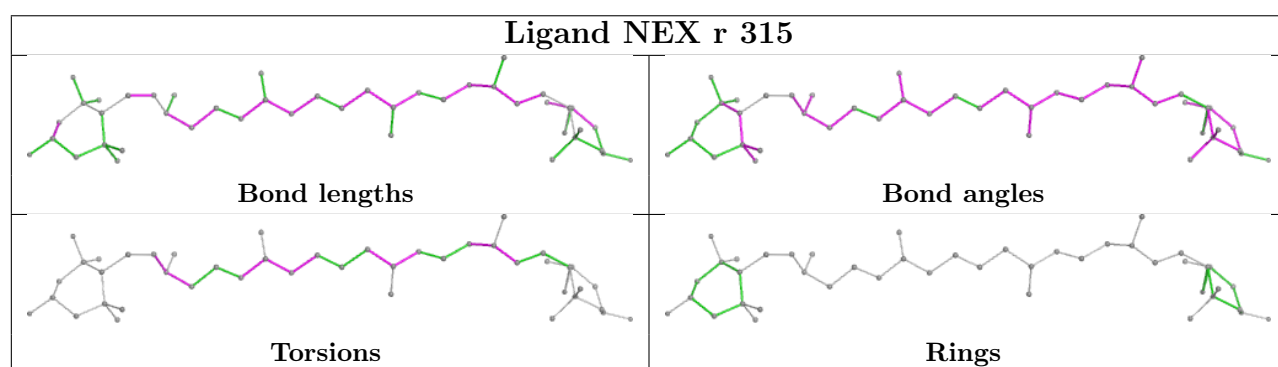
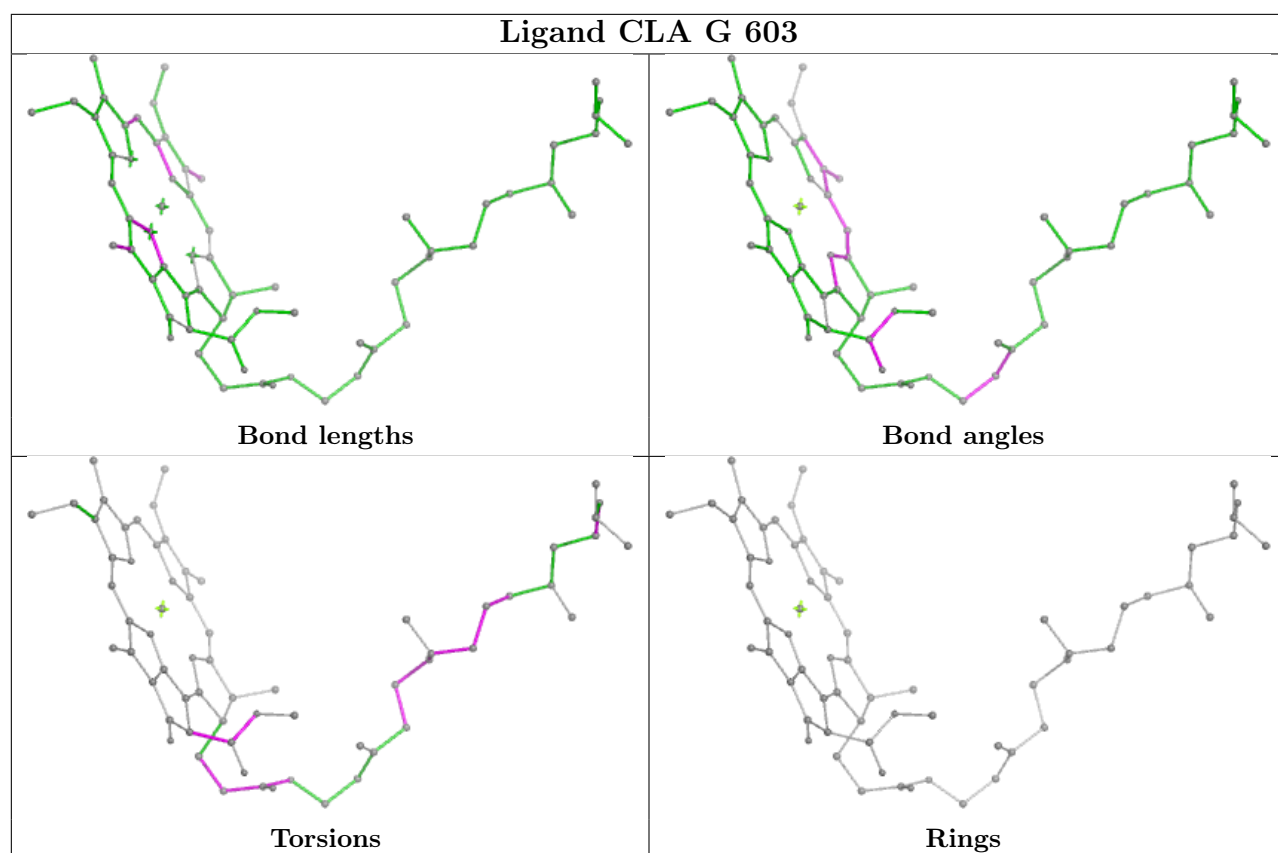
Bond angles

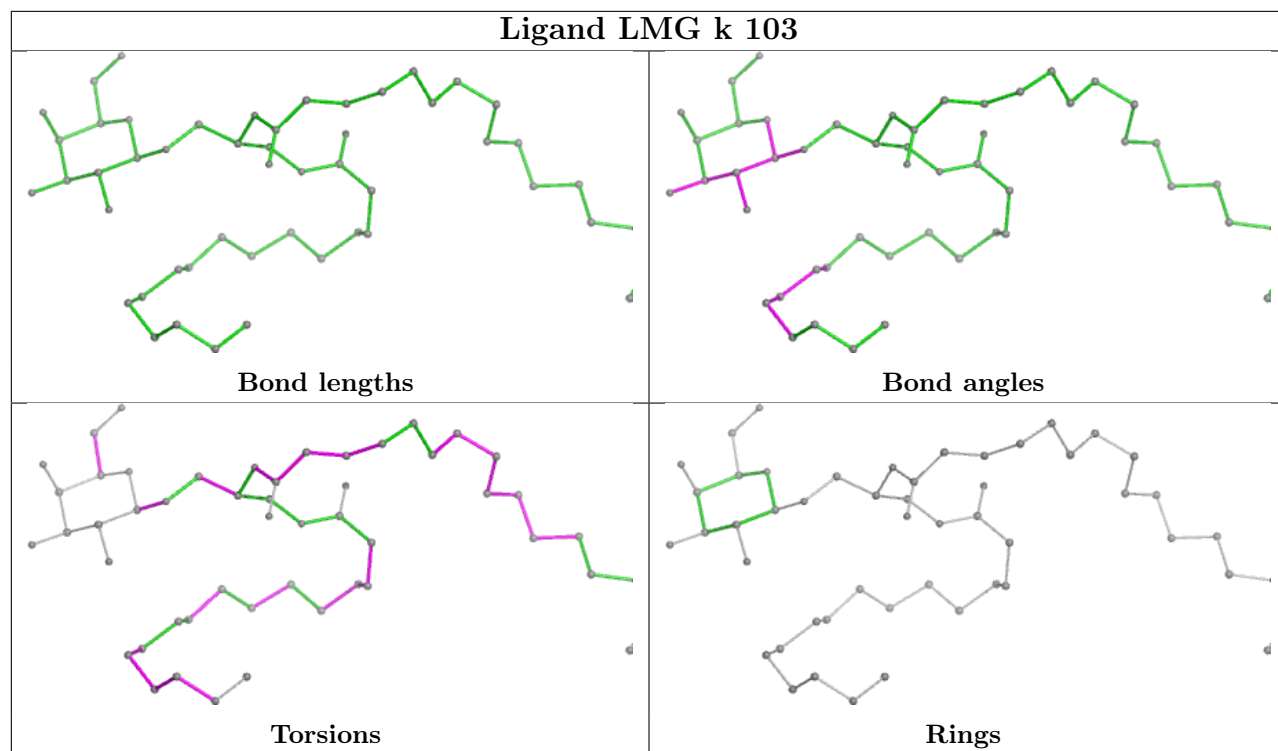


Torsions

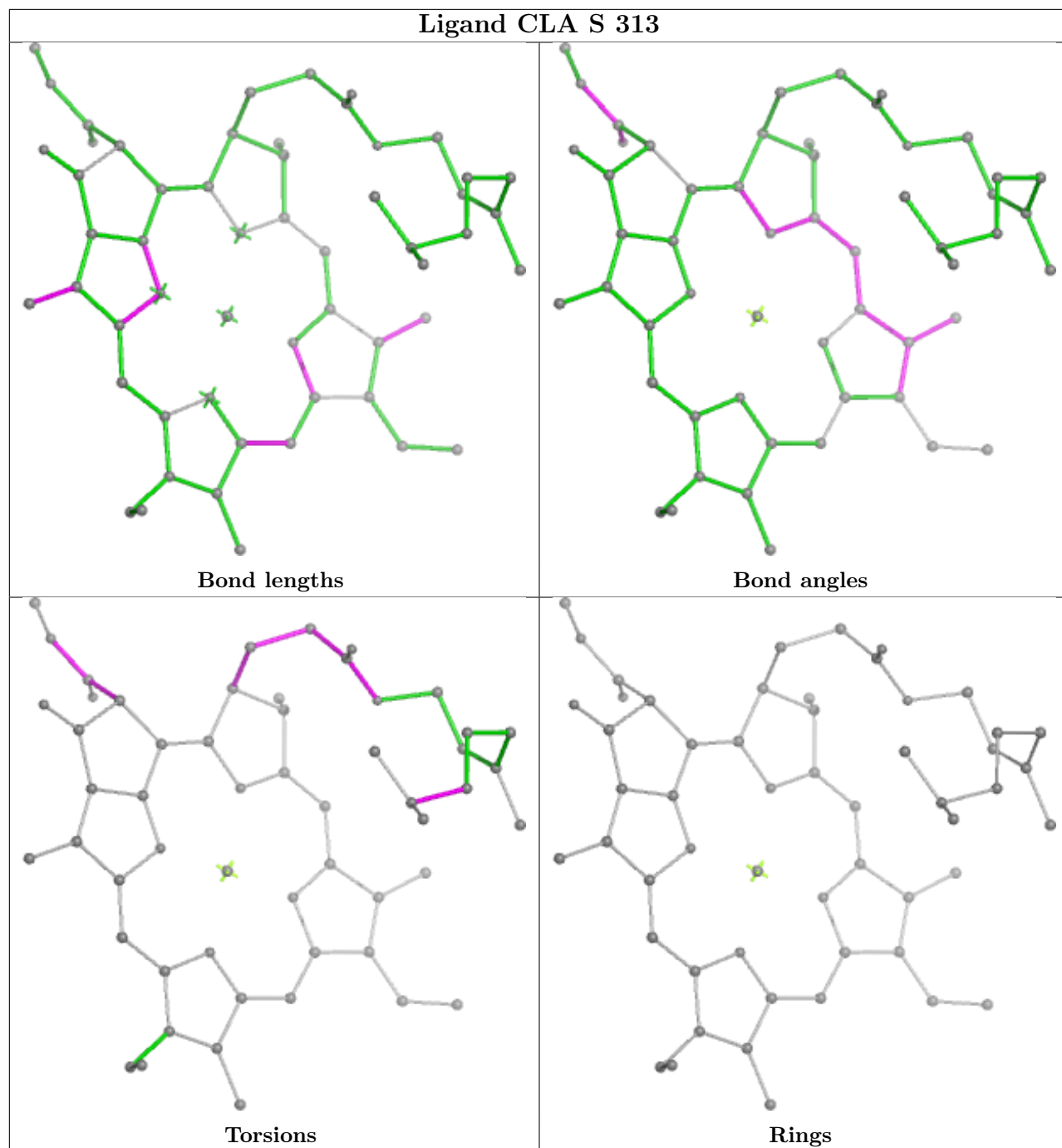


Rings

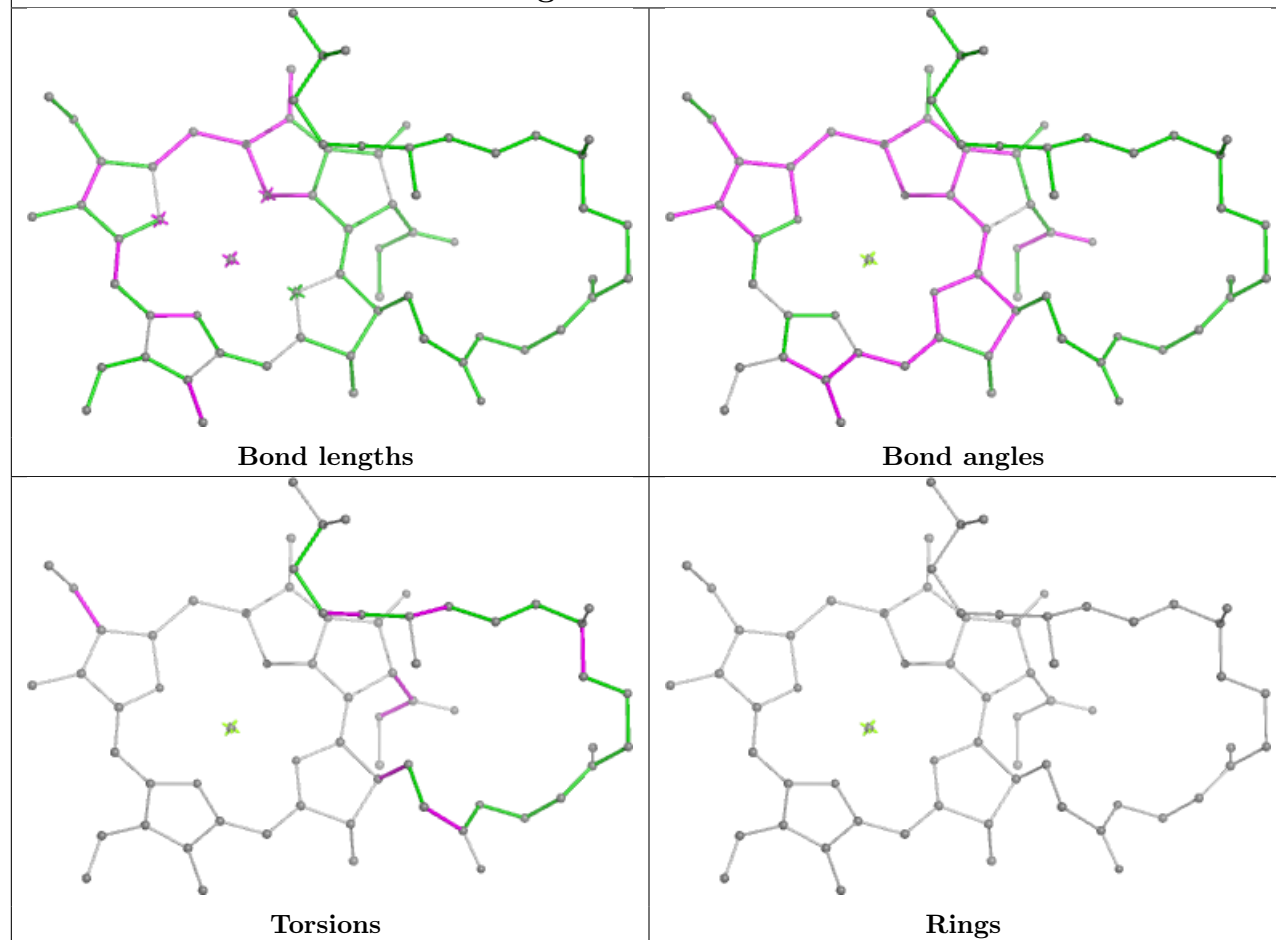




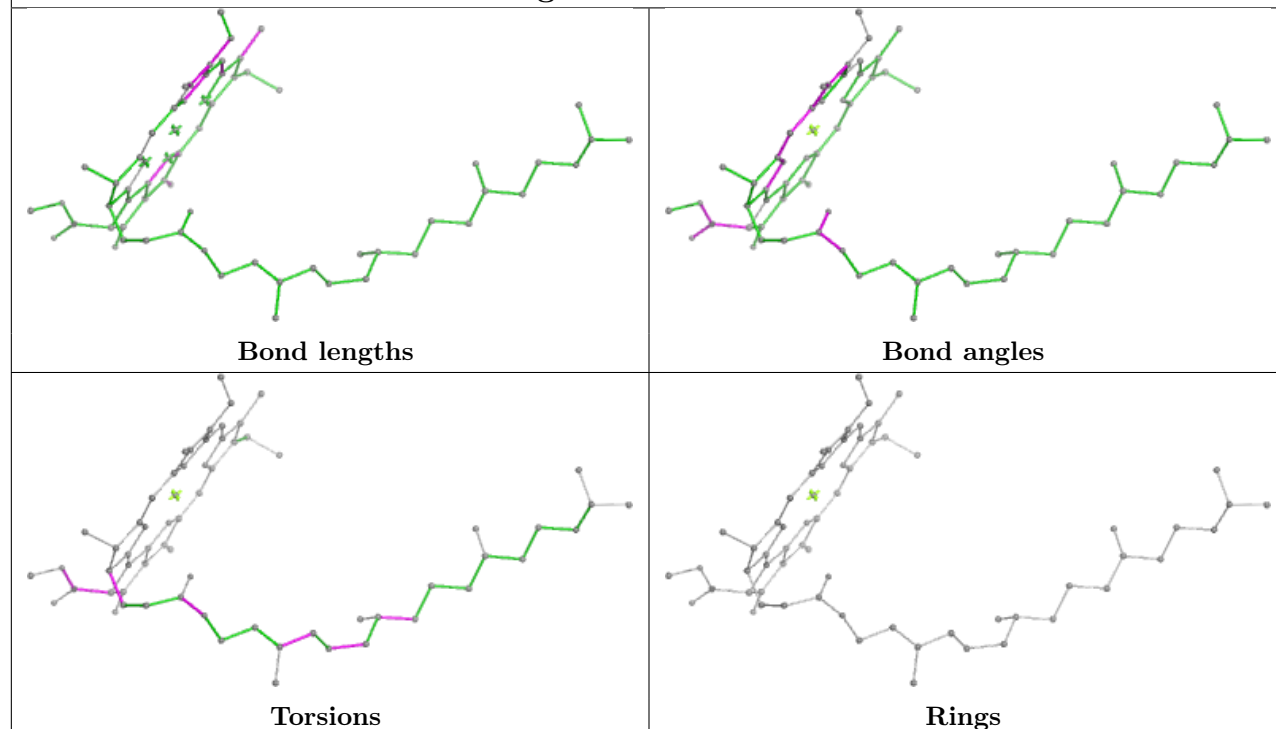
## Ligand CLA S 313

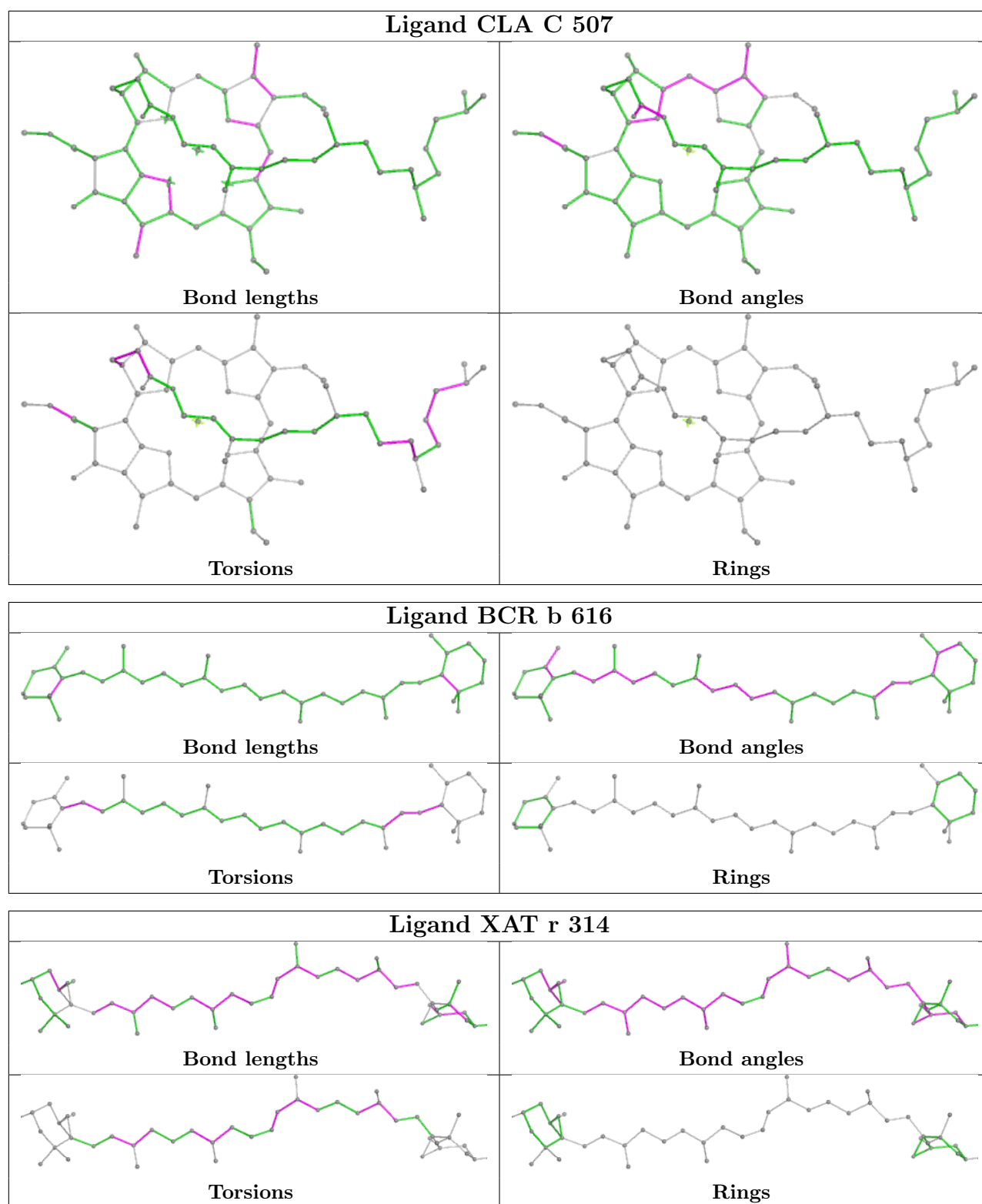


## Ligand CLA c 510

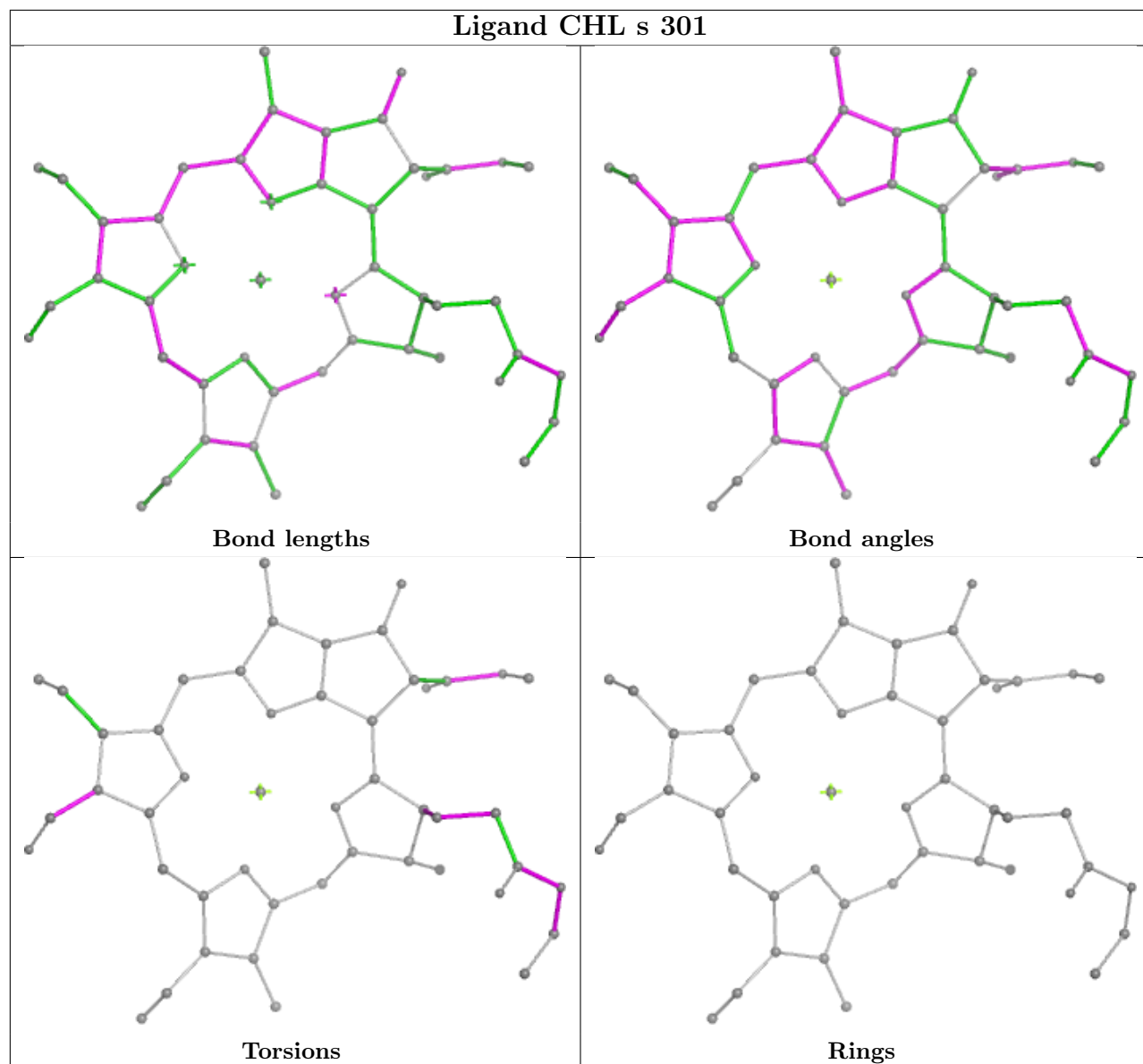


## Ligand CLA c 509

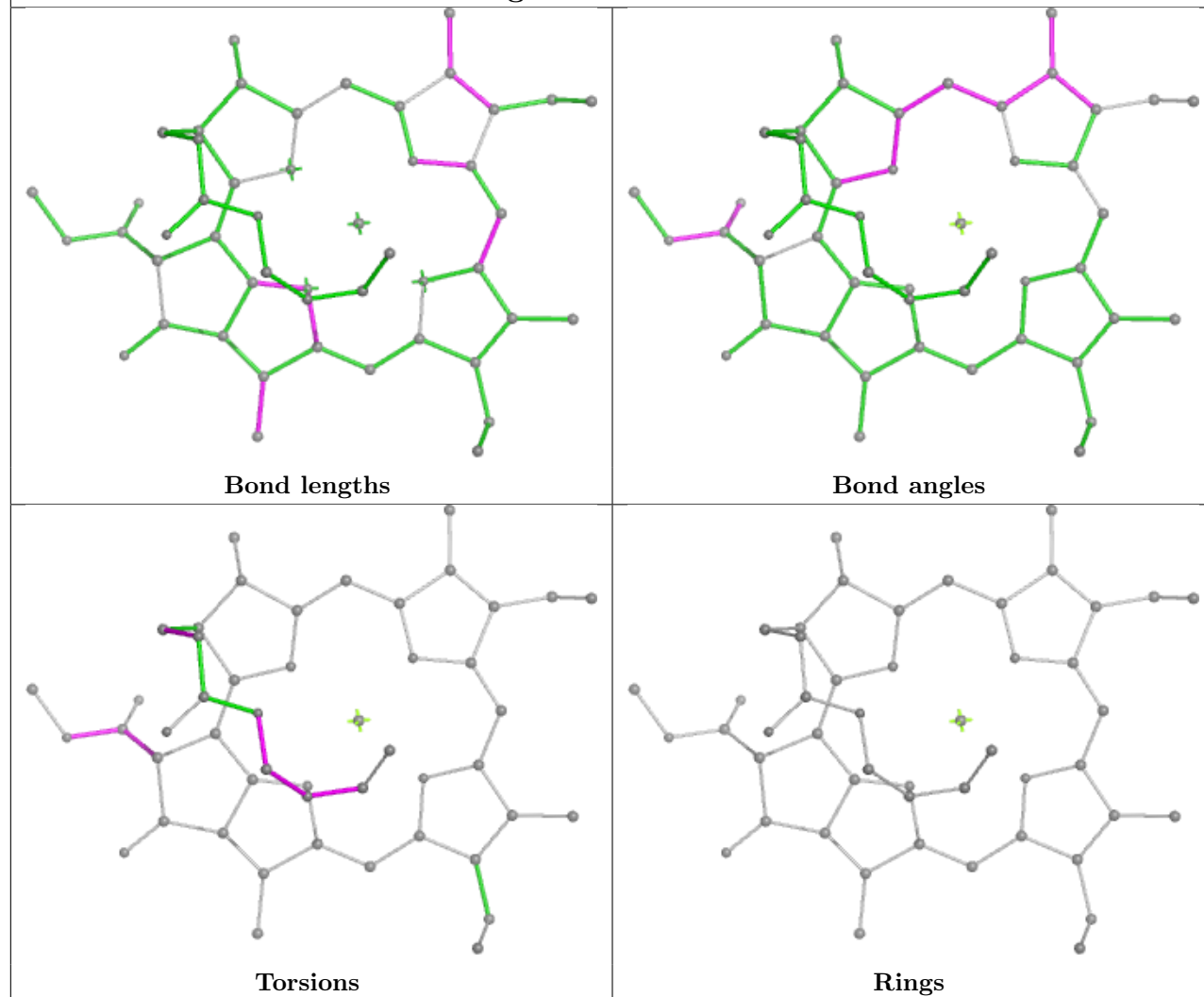




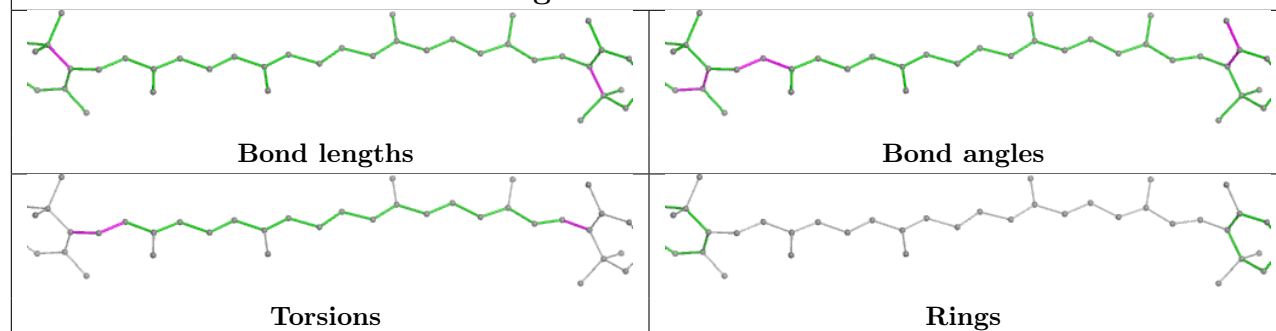
## Ligand CHL s 301



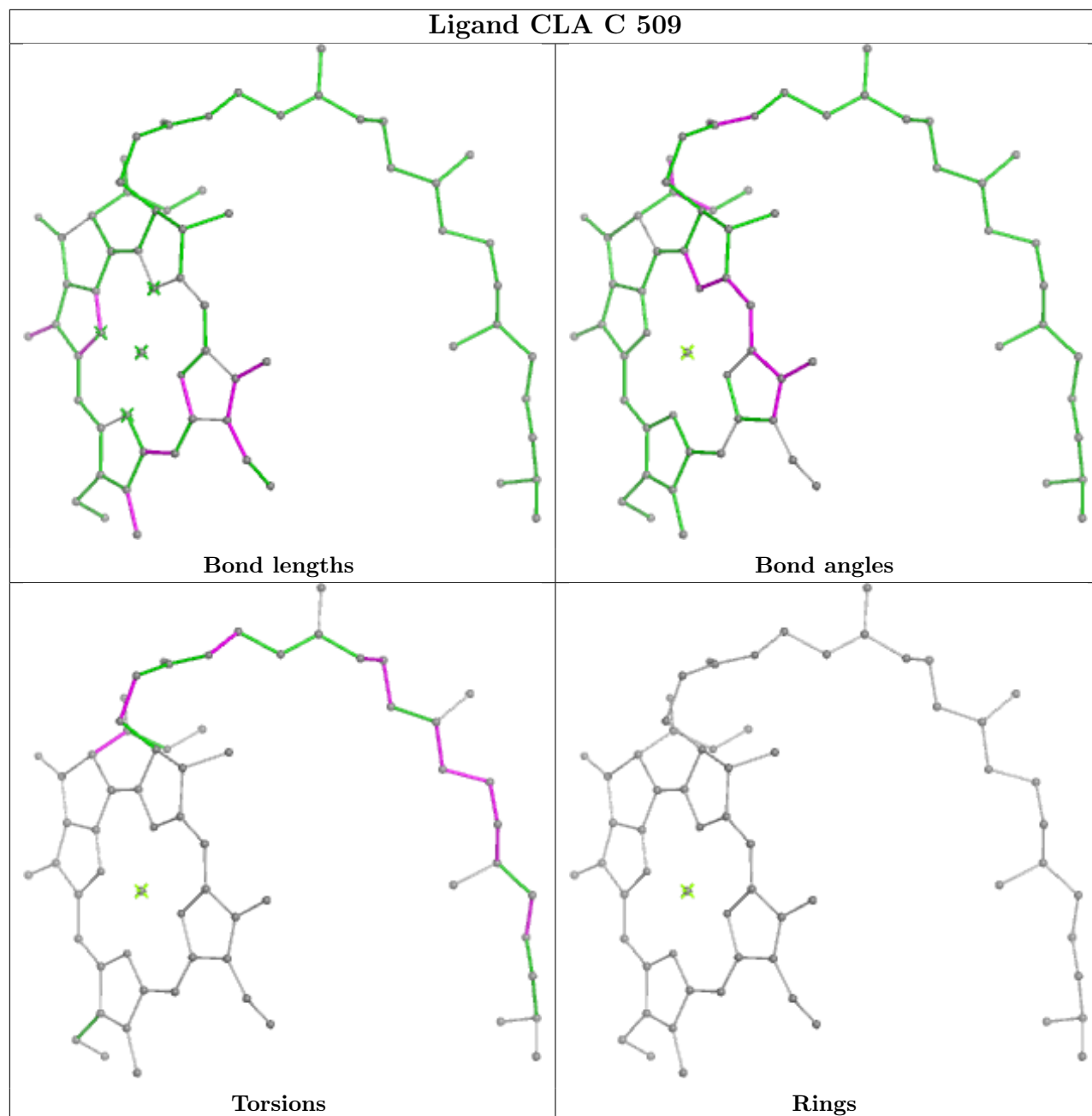
## Ligand CLA s 312



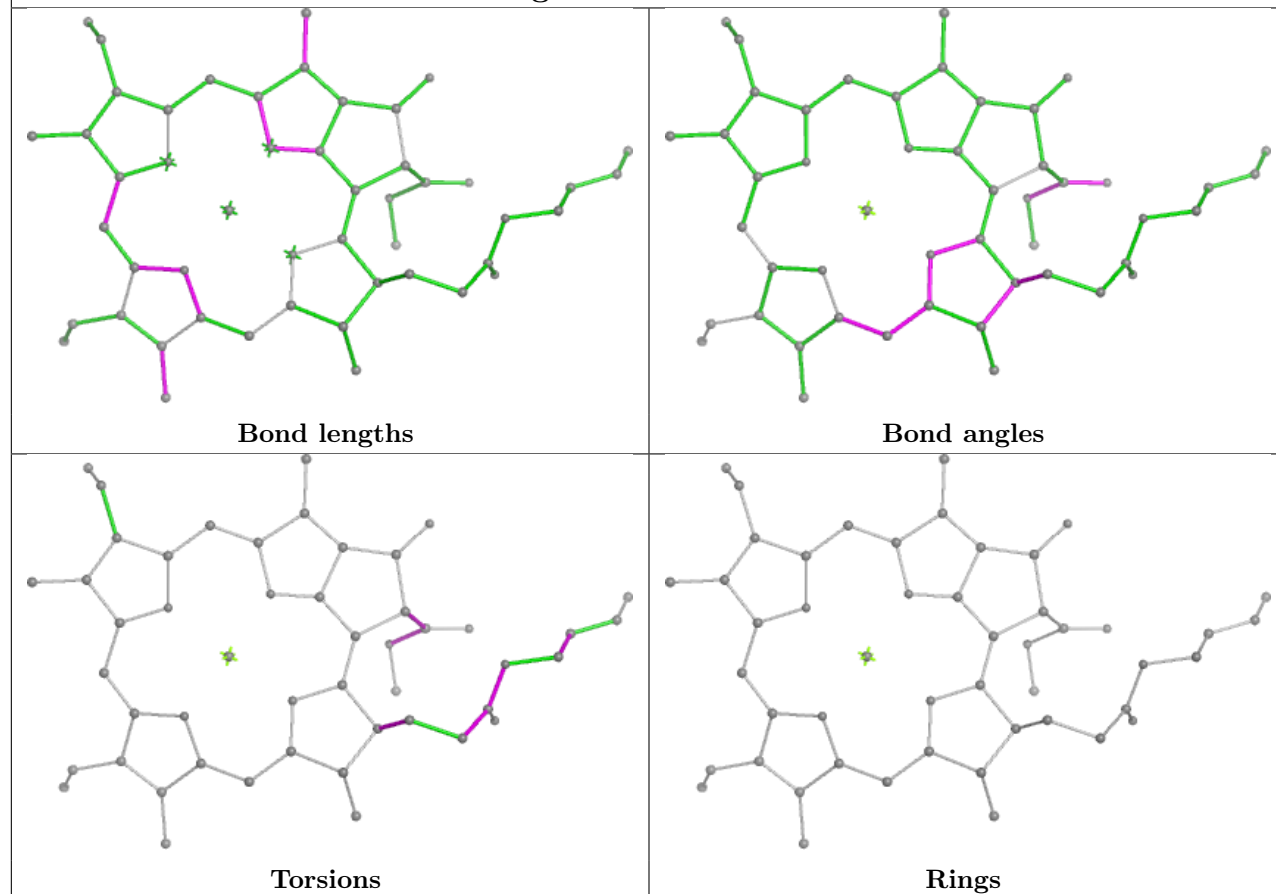
## Ligand BCR b 618



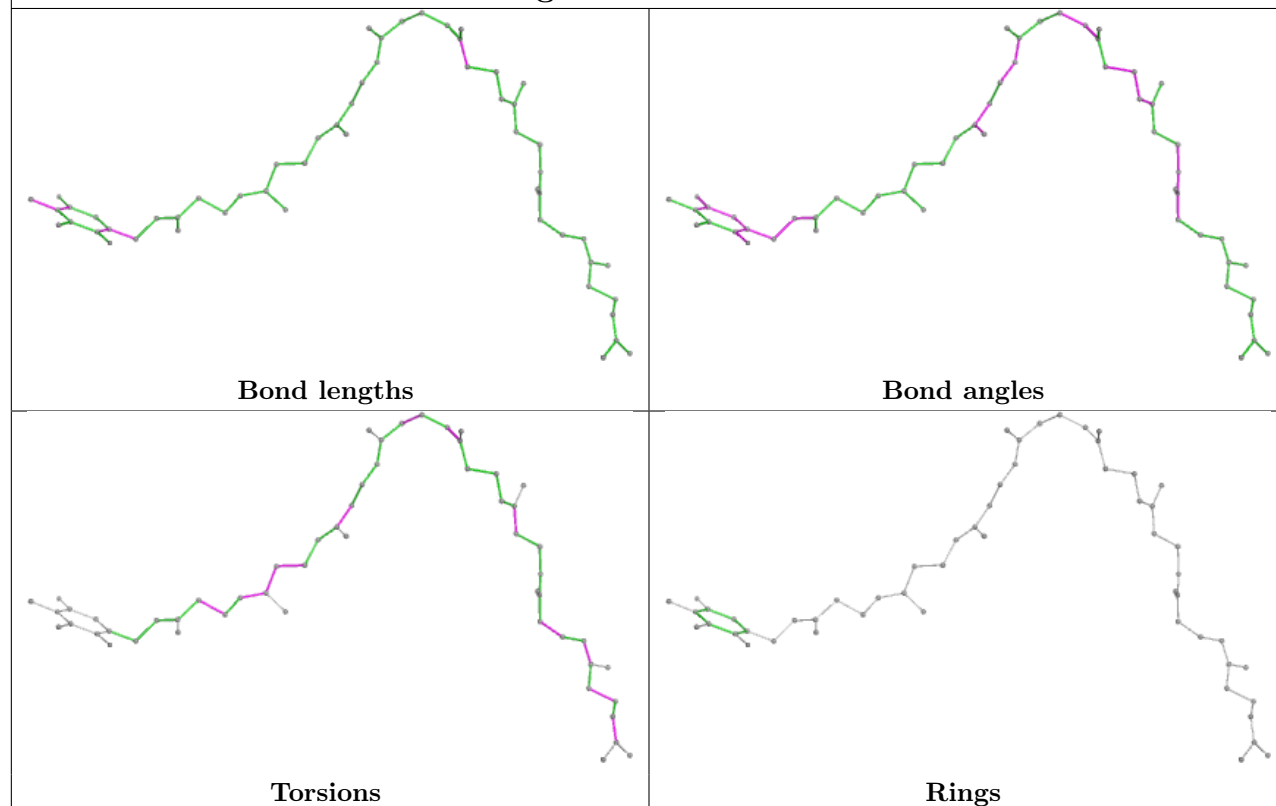
## Ligand CLA C 509



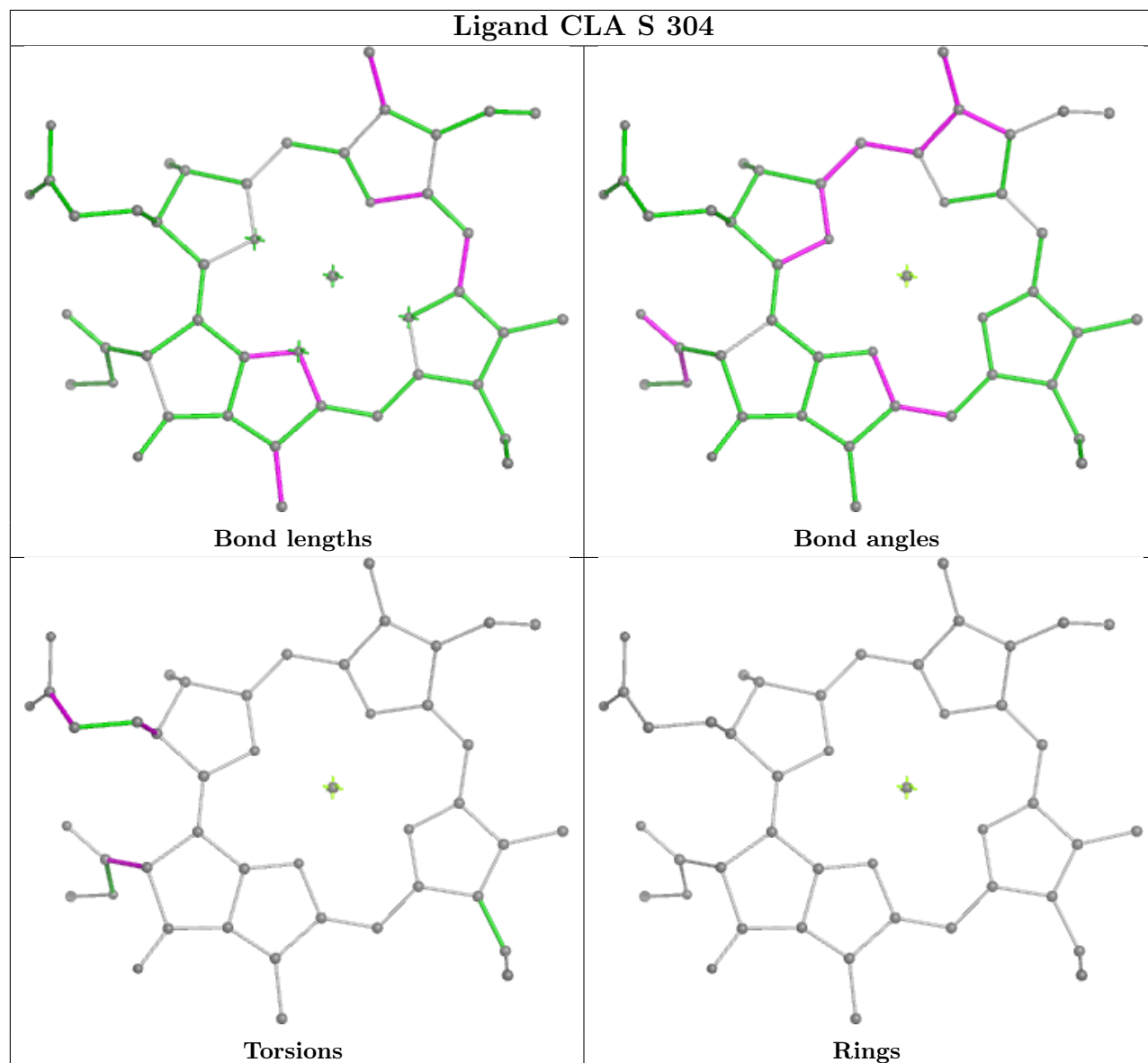
## Ligand CLA R 310



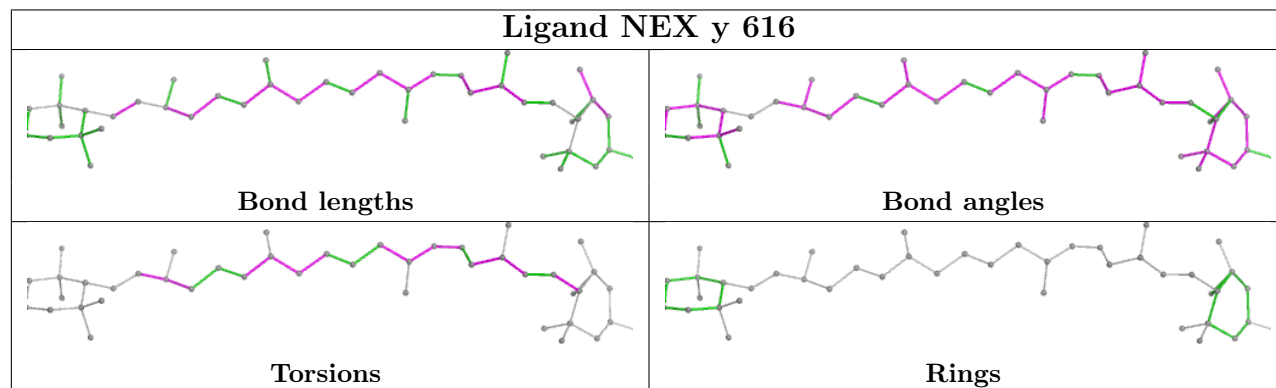
## Ligand PL9 D 407



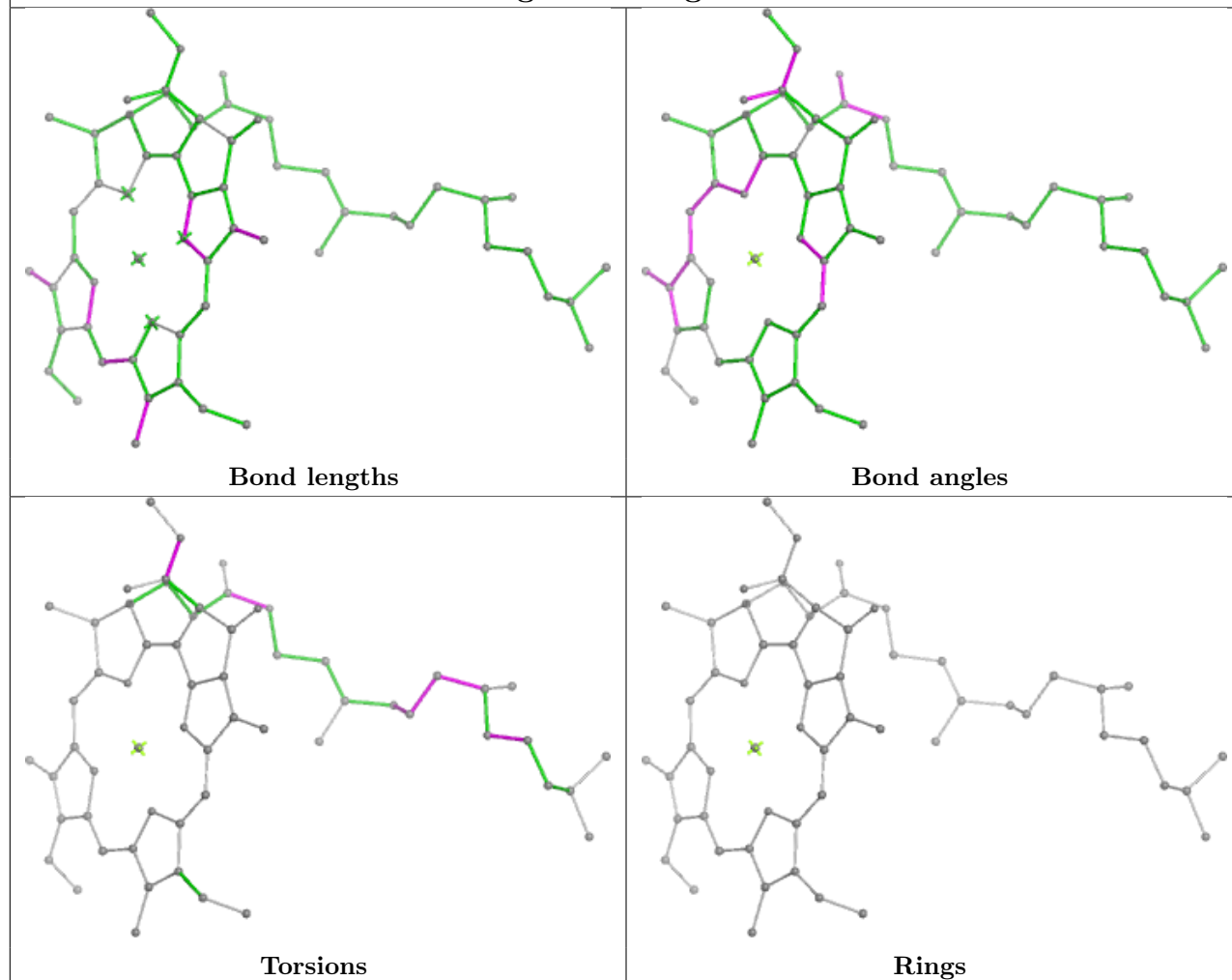
## Ligand CLA S 304



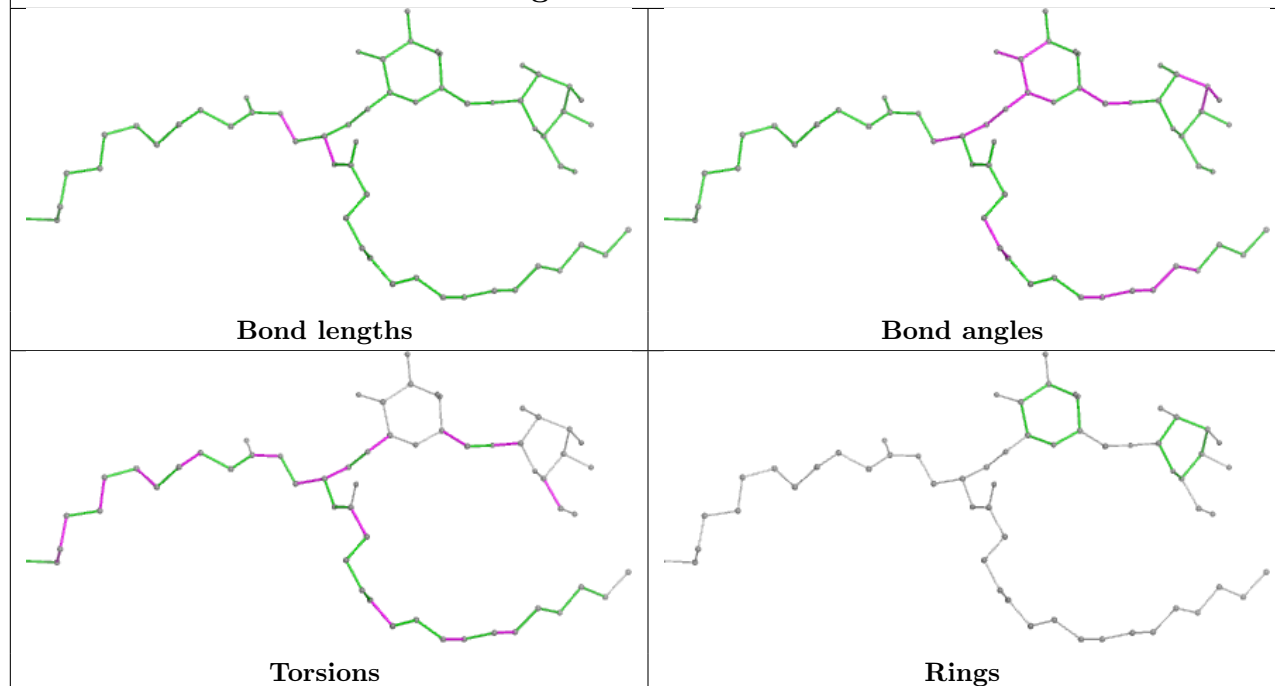
## Ligand NEX y 616

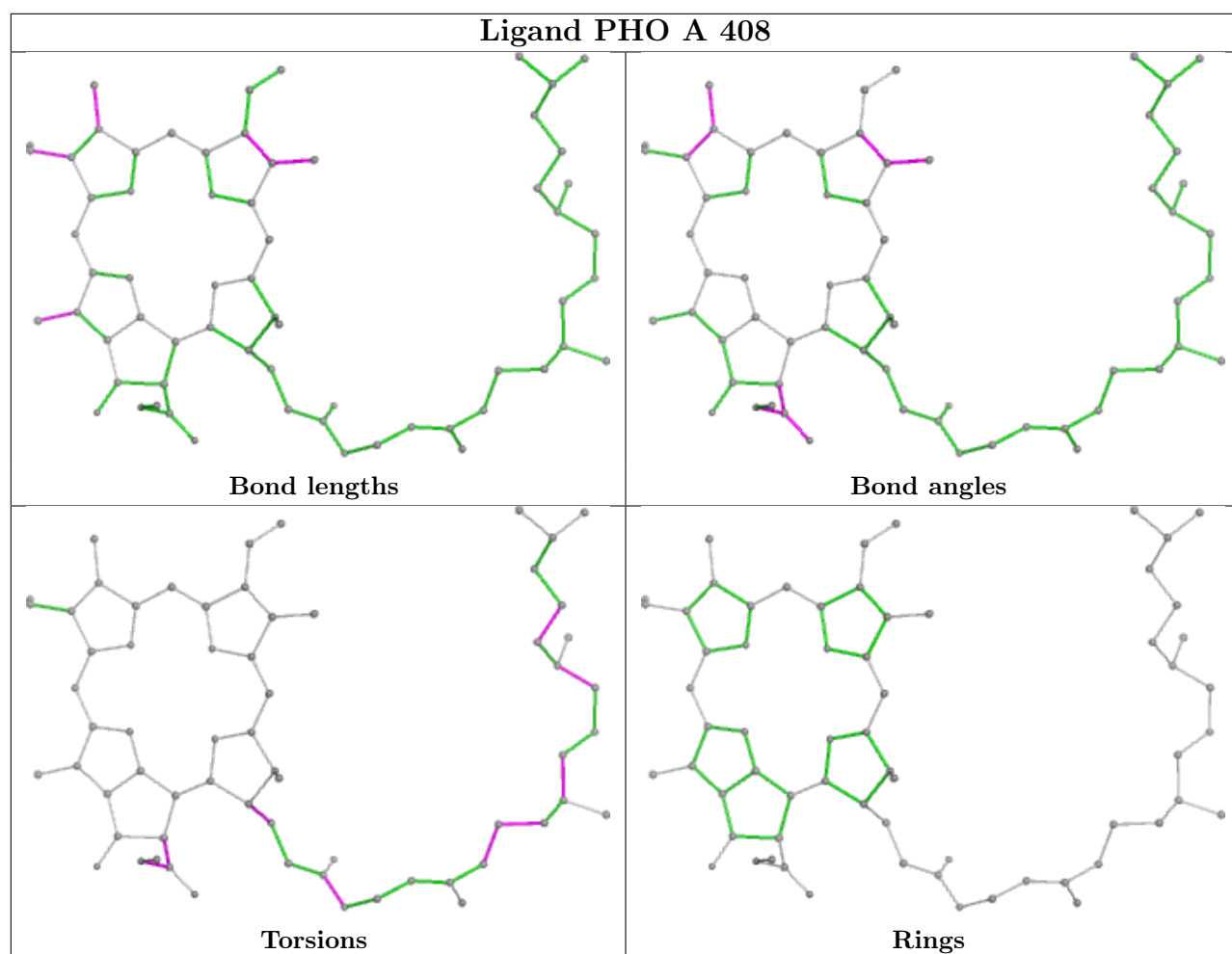


## Ligand CLA g 611

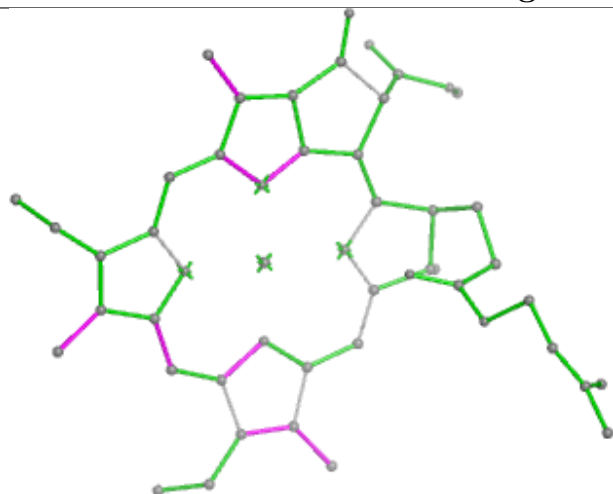


## Ligand DGD a 413

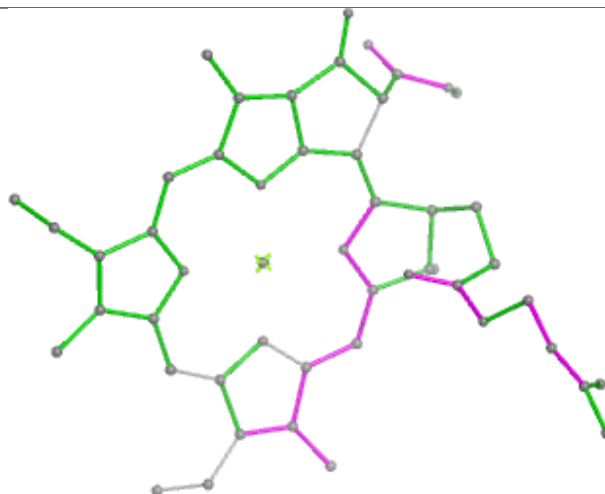




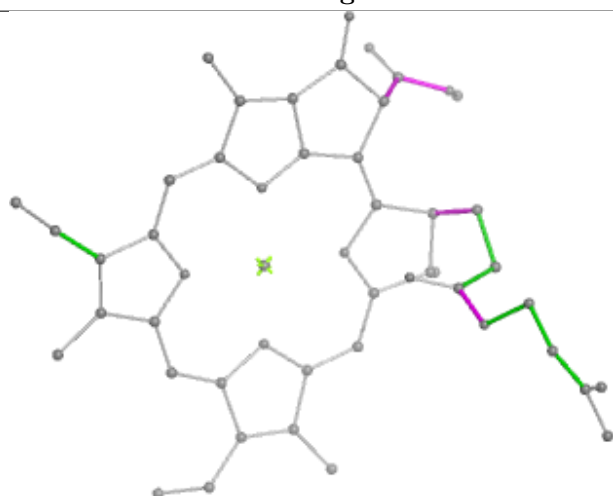
## Ligand CLA a 406



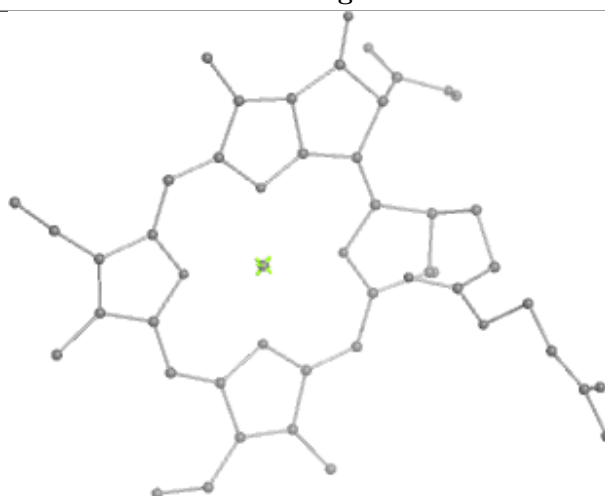
Bond lengths



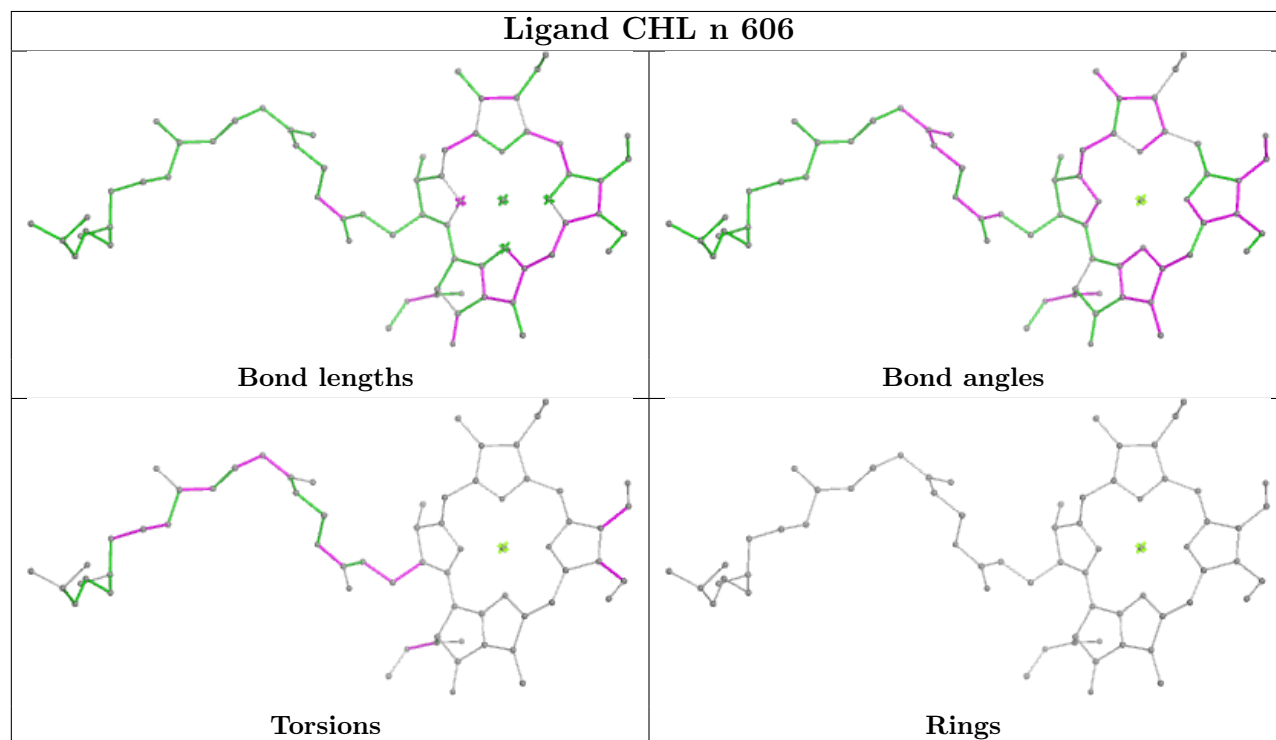
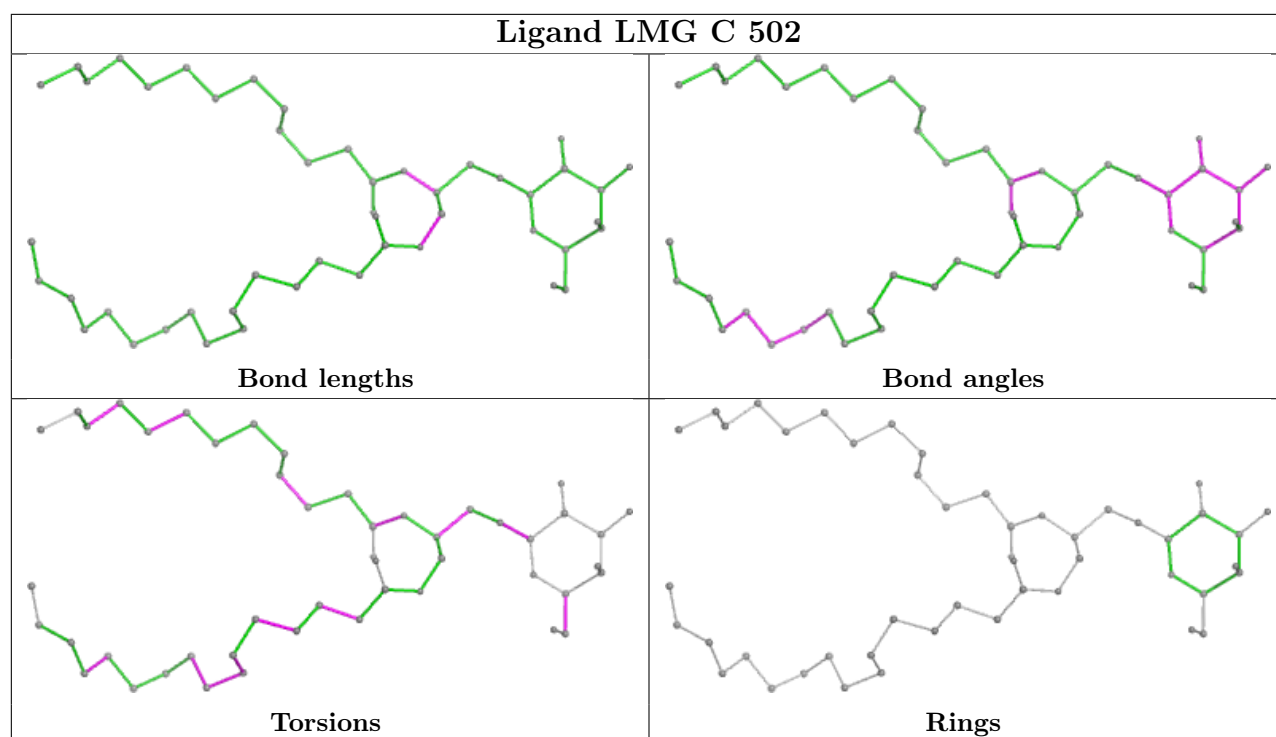
Bond angles



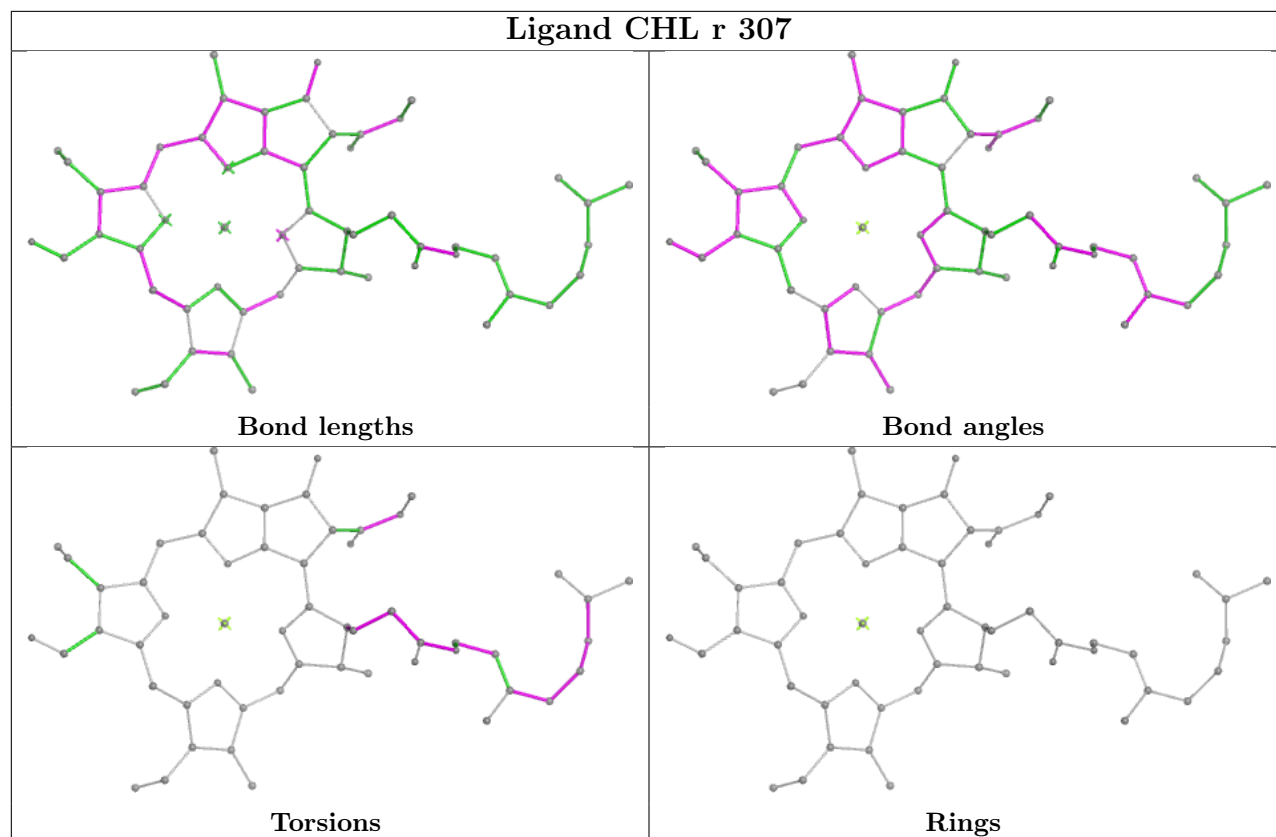
Torsions



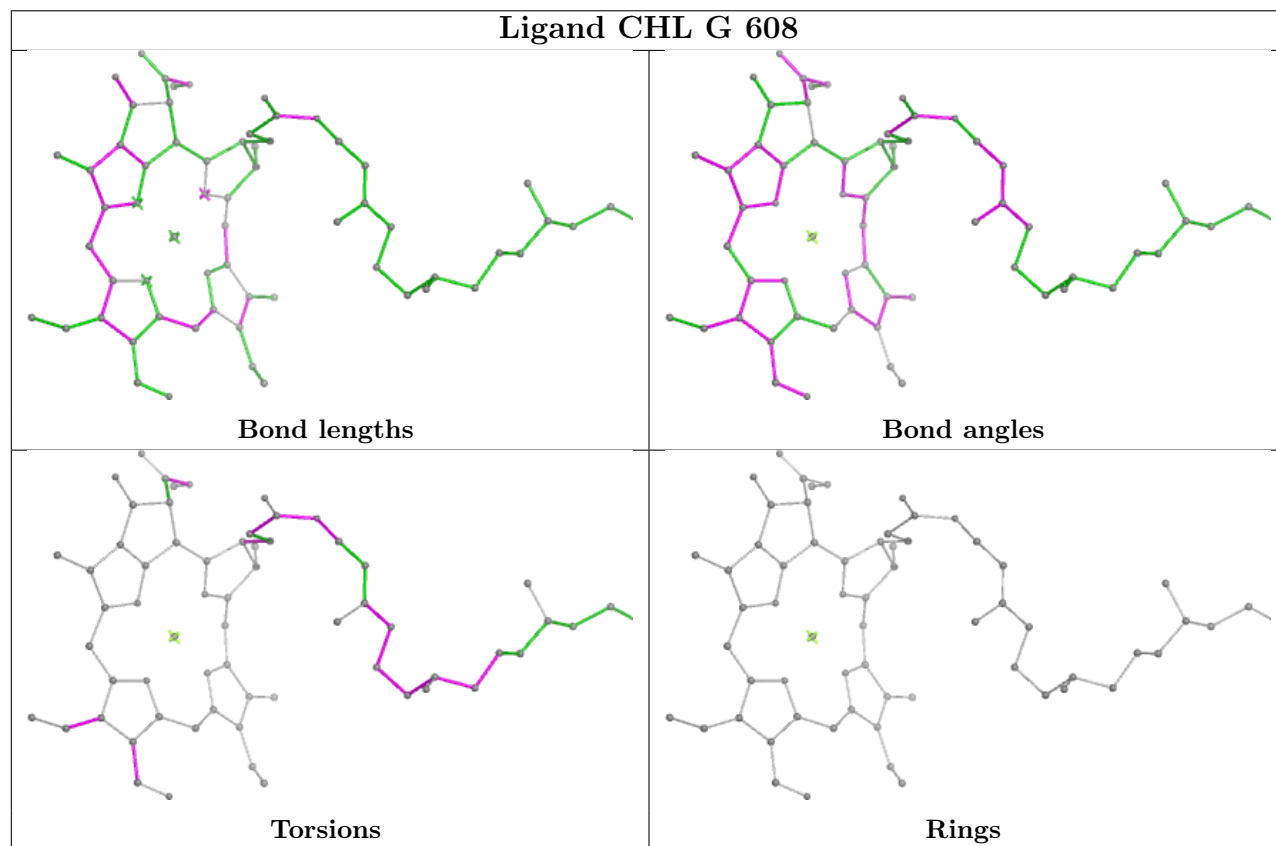
Rings



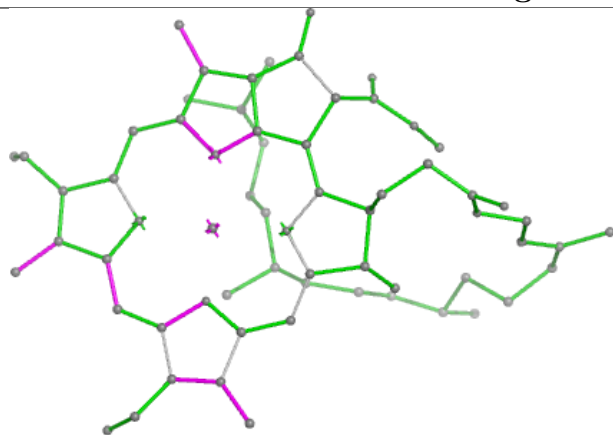
## Ligand CHL r 307



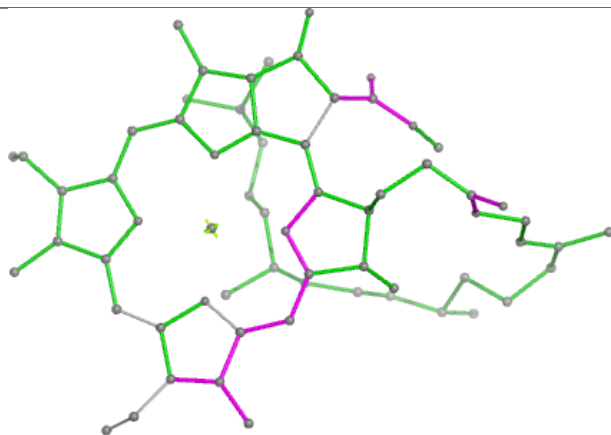
## Ligand CHL G 608



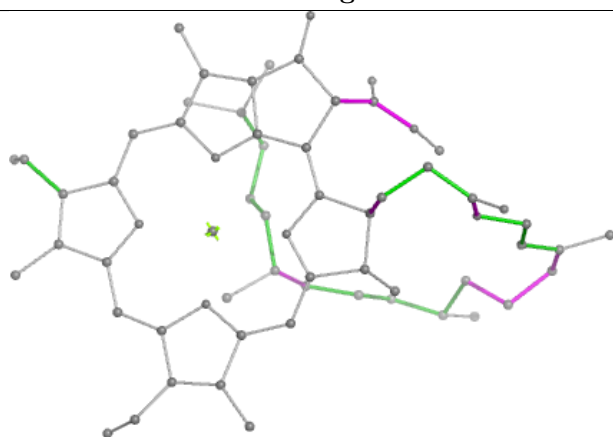
## Ligand CLA C 512



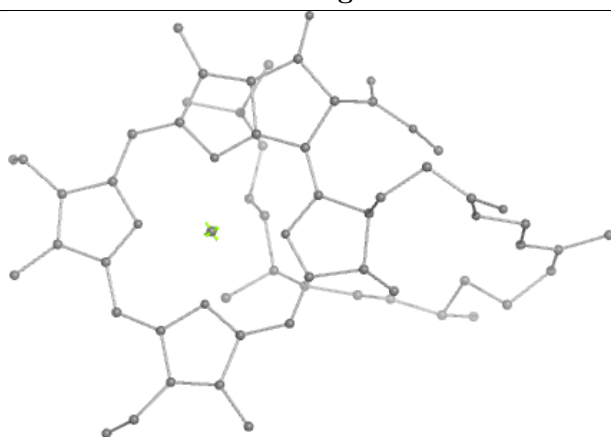
Bond lengths



Bond angles

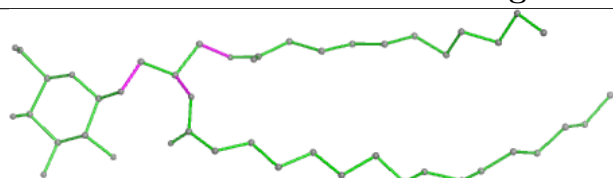


Torsions

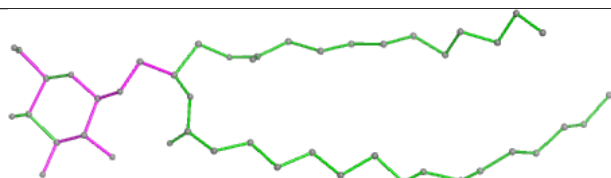


Rings

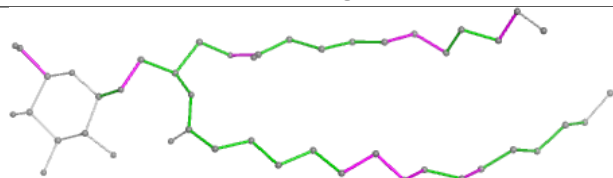
## Ligand LMG D 411



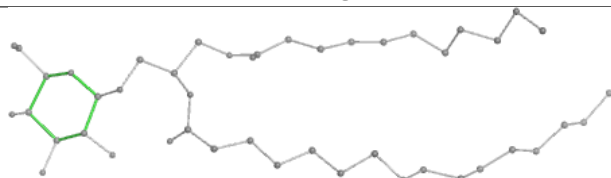
Bond lengths



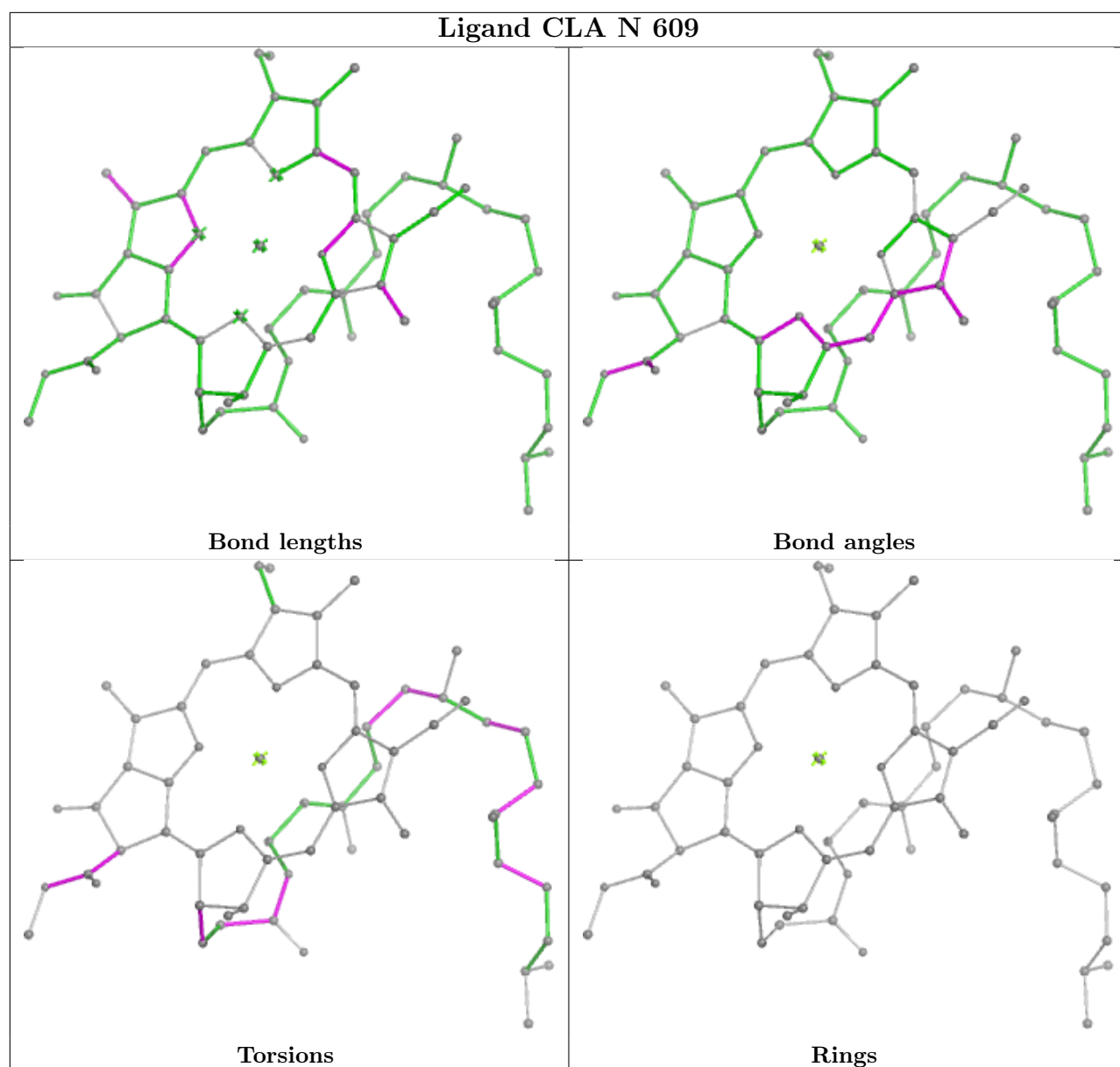
Bond angles

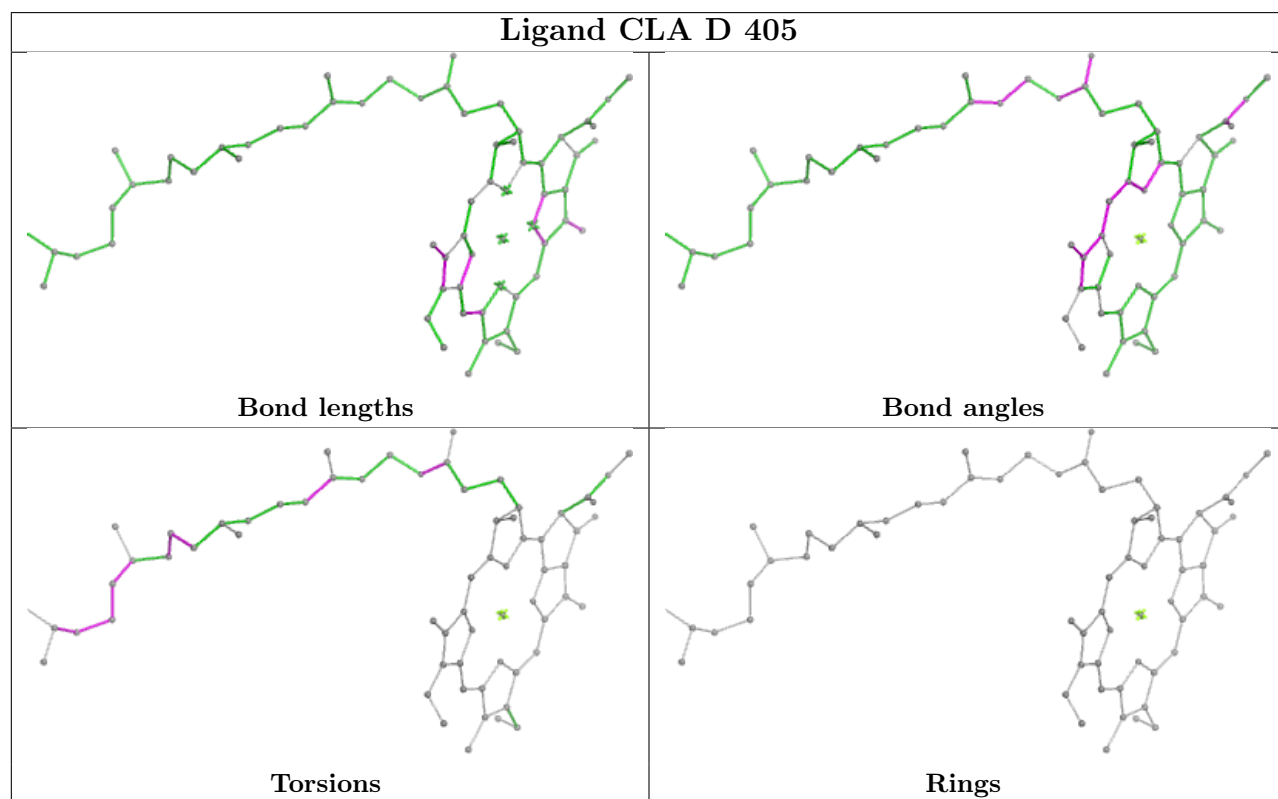
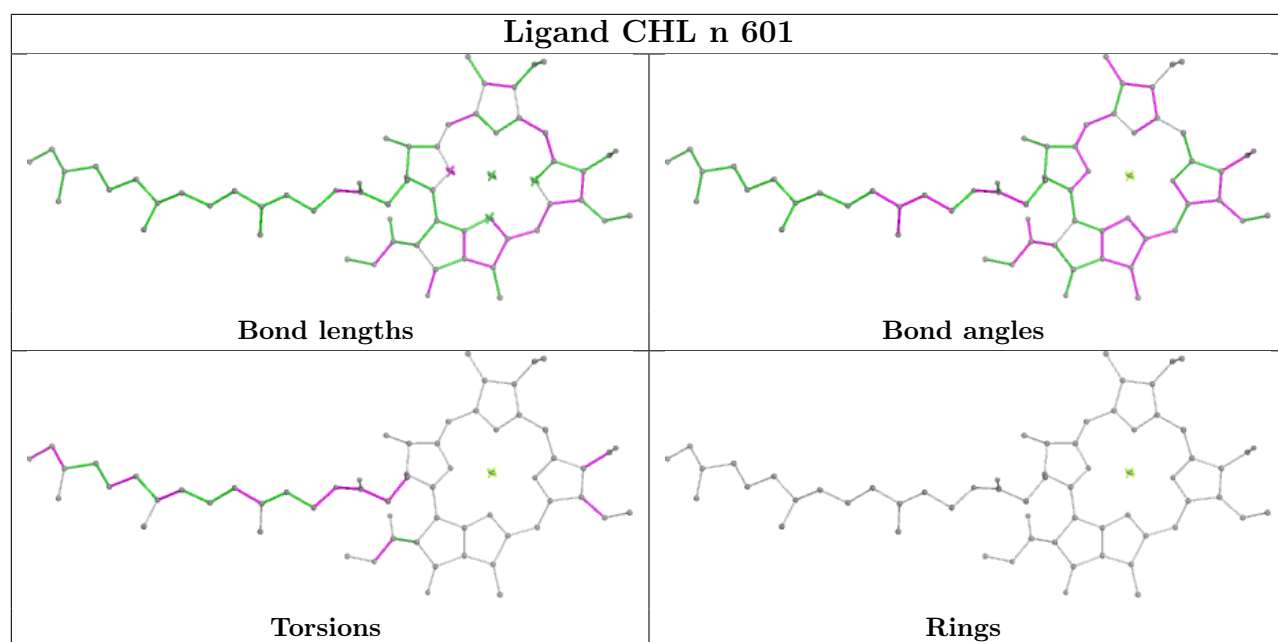


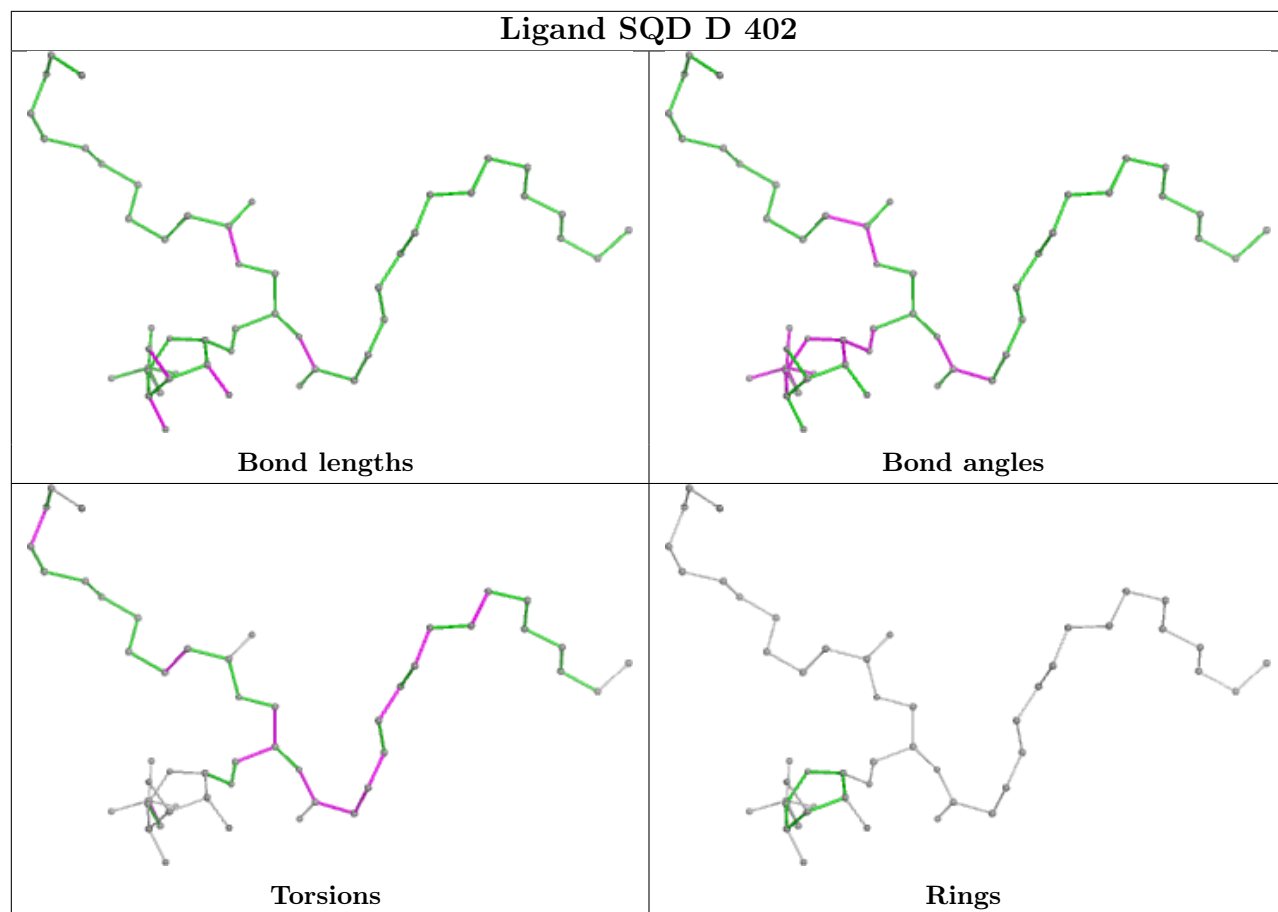
Torsions



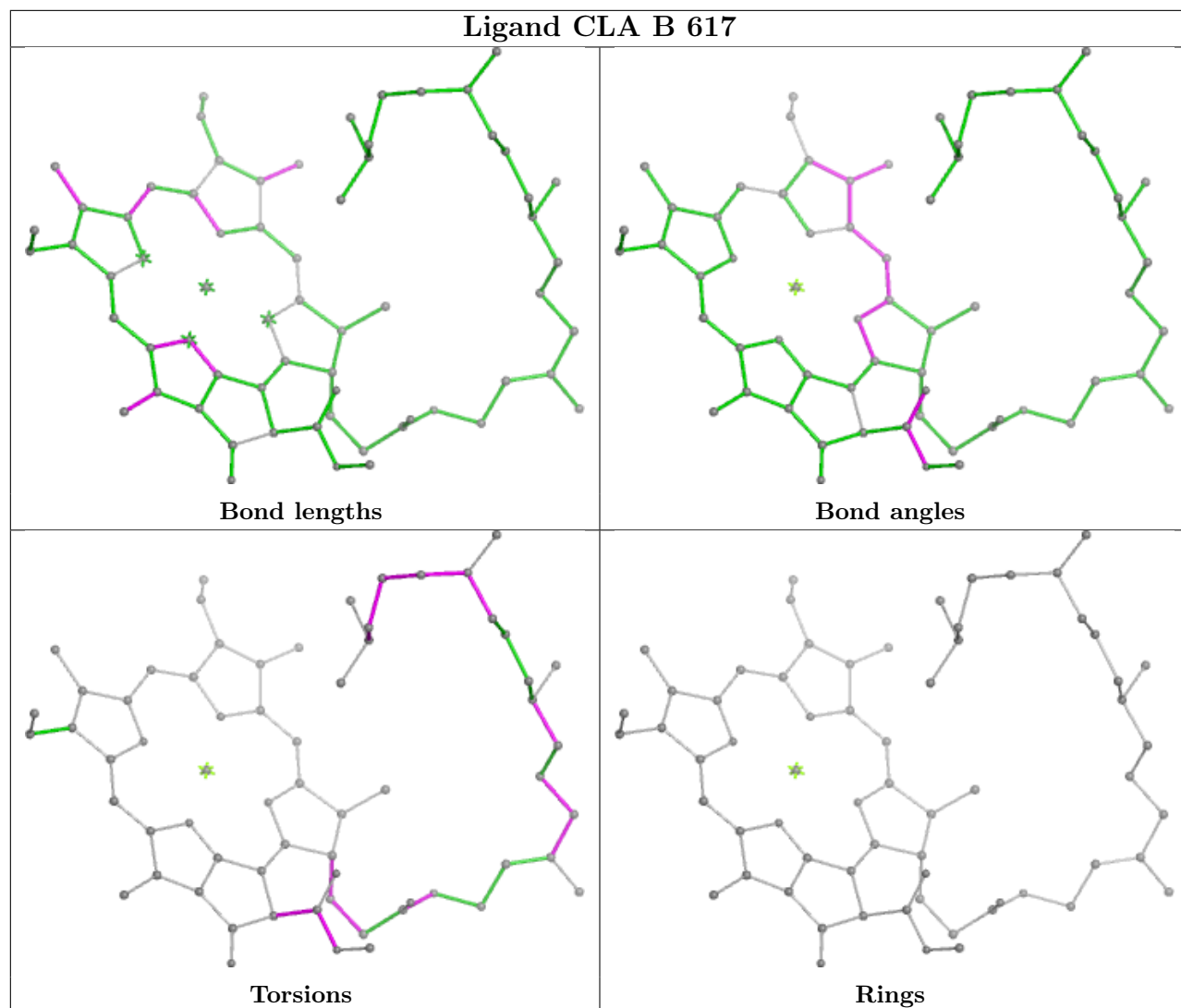
Rings

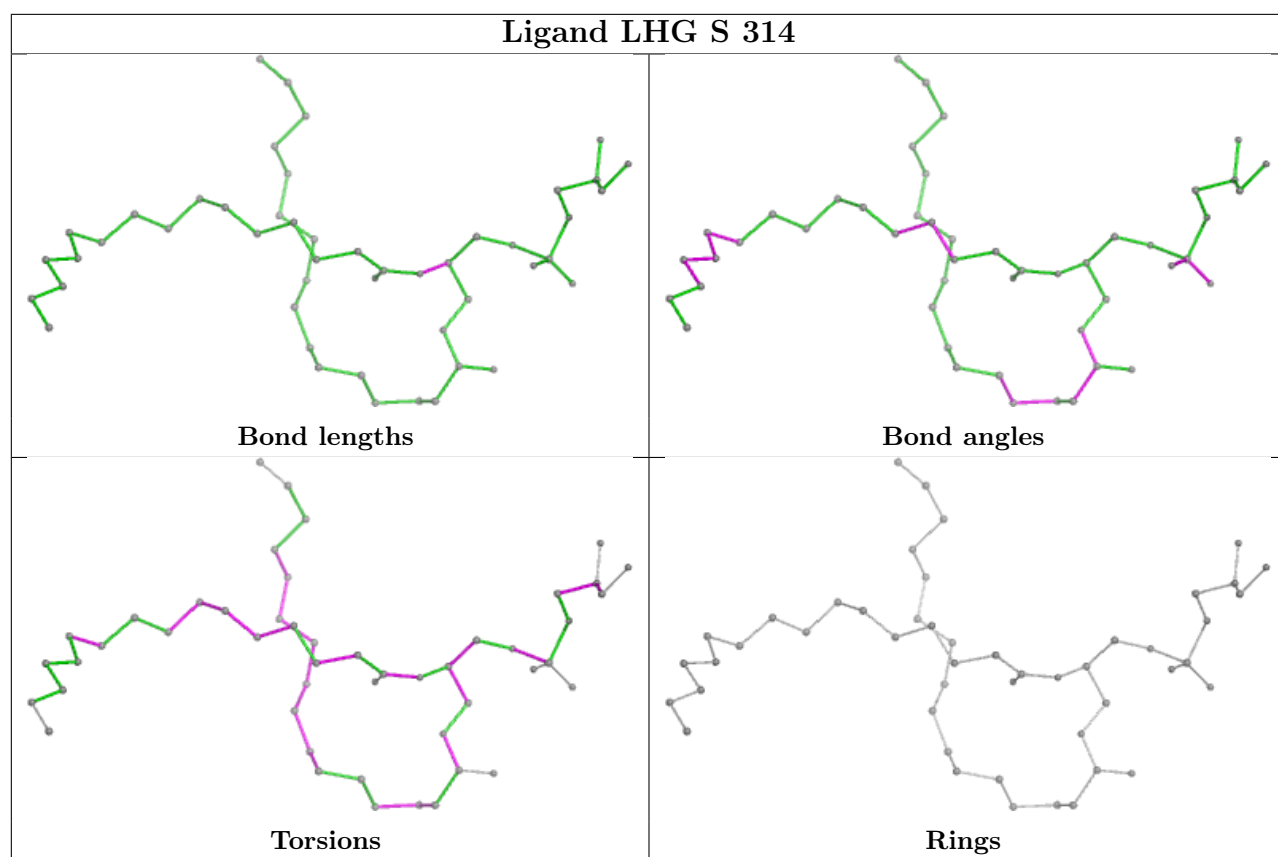




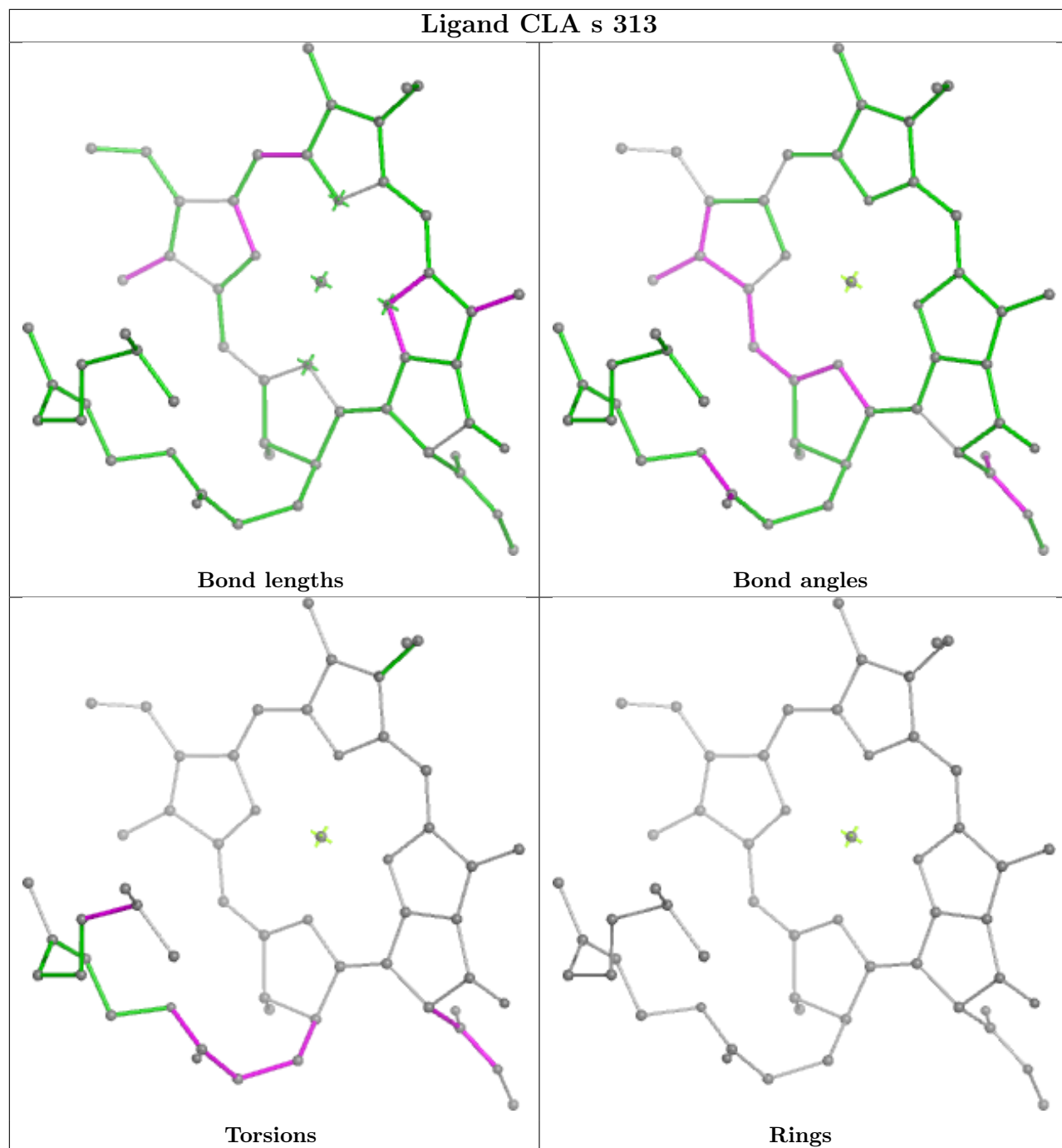


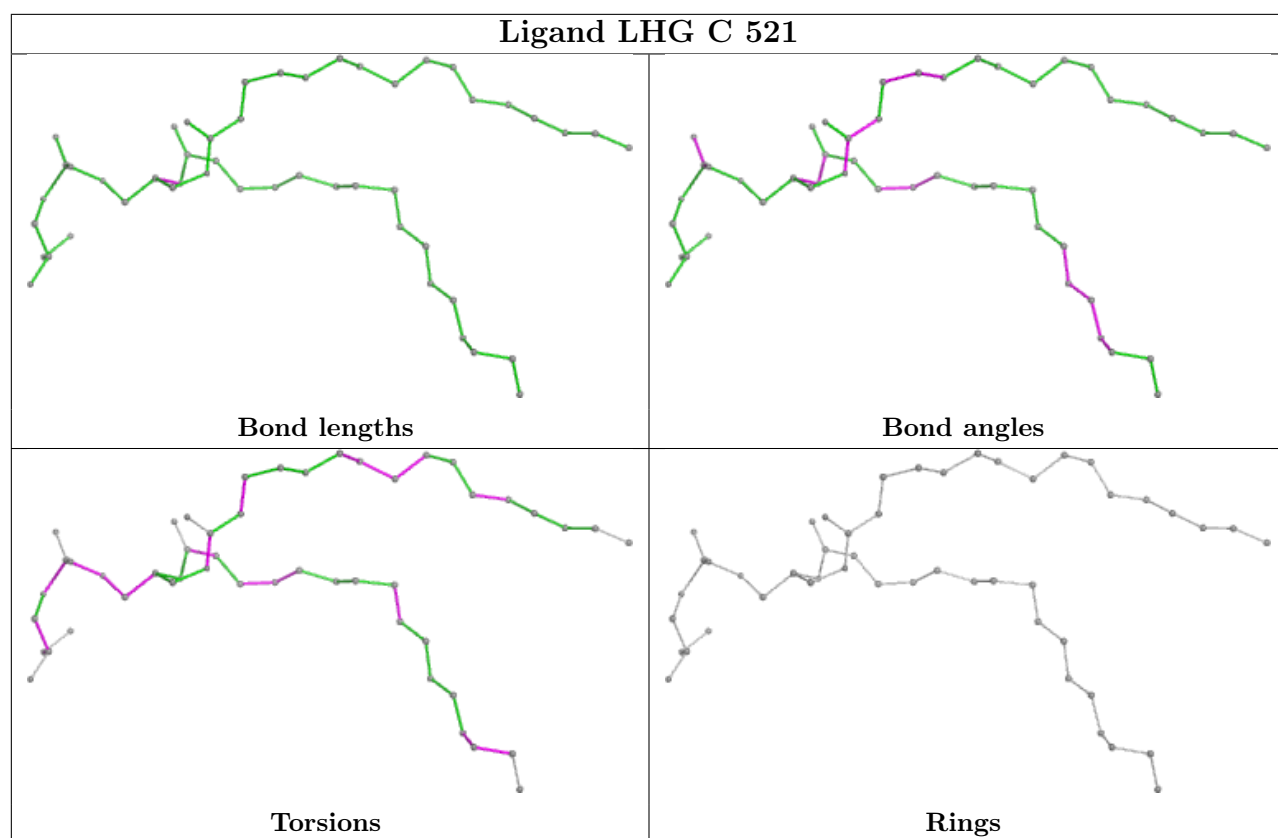
## Ligand CLA B 617



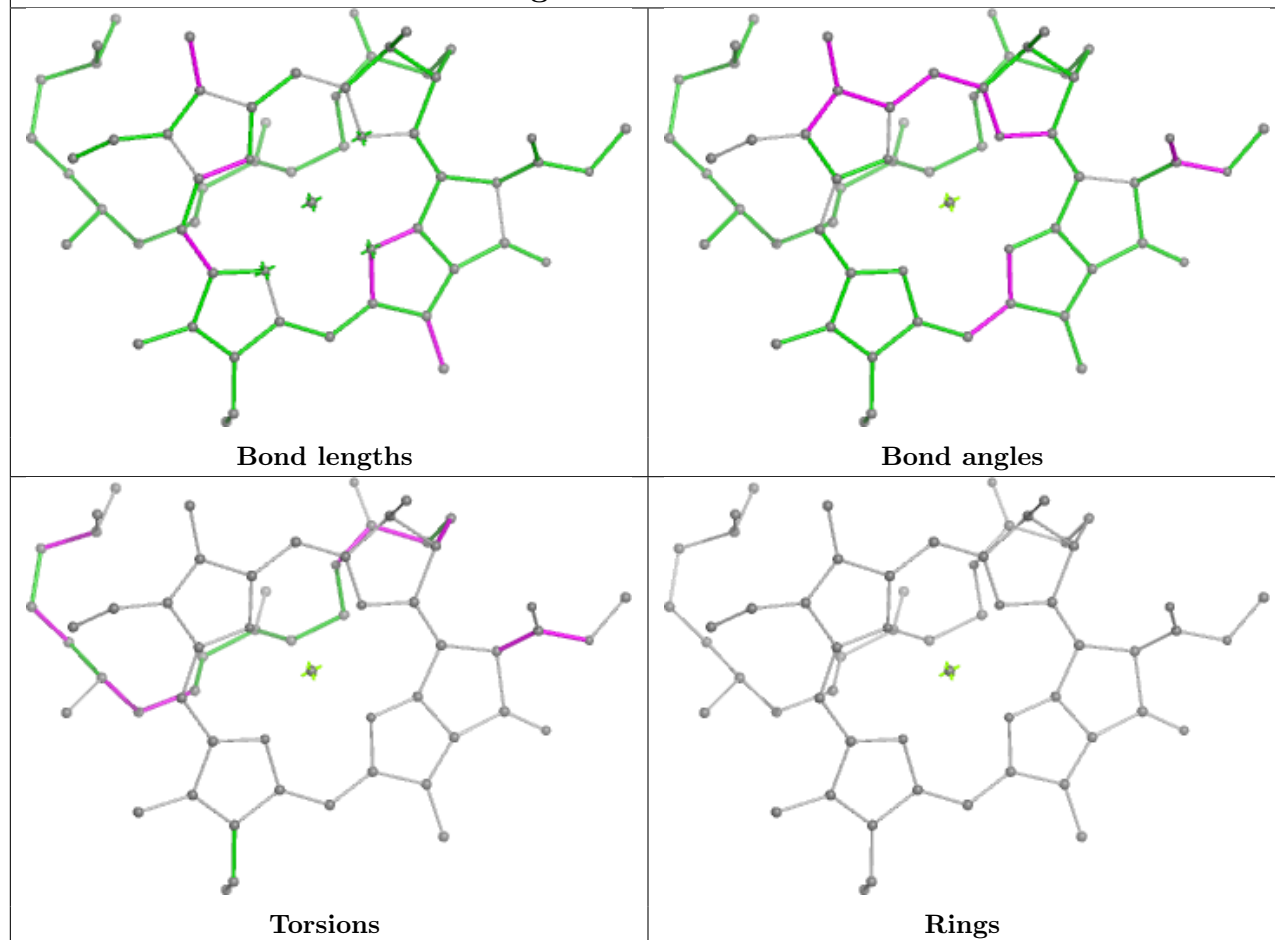


## Ligand CLA s 313

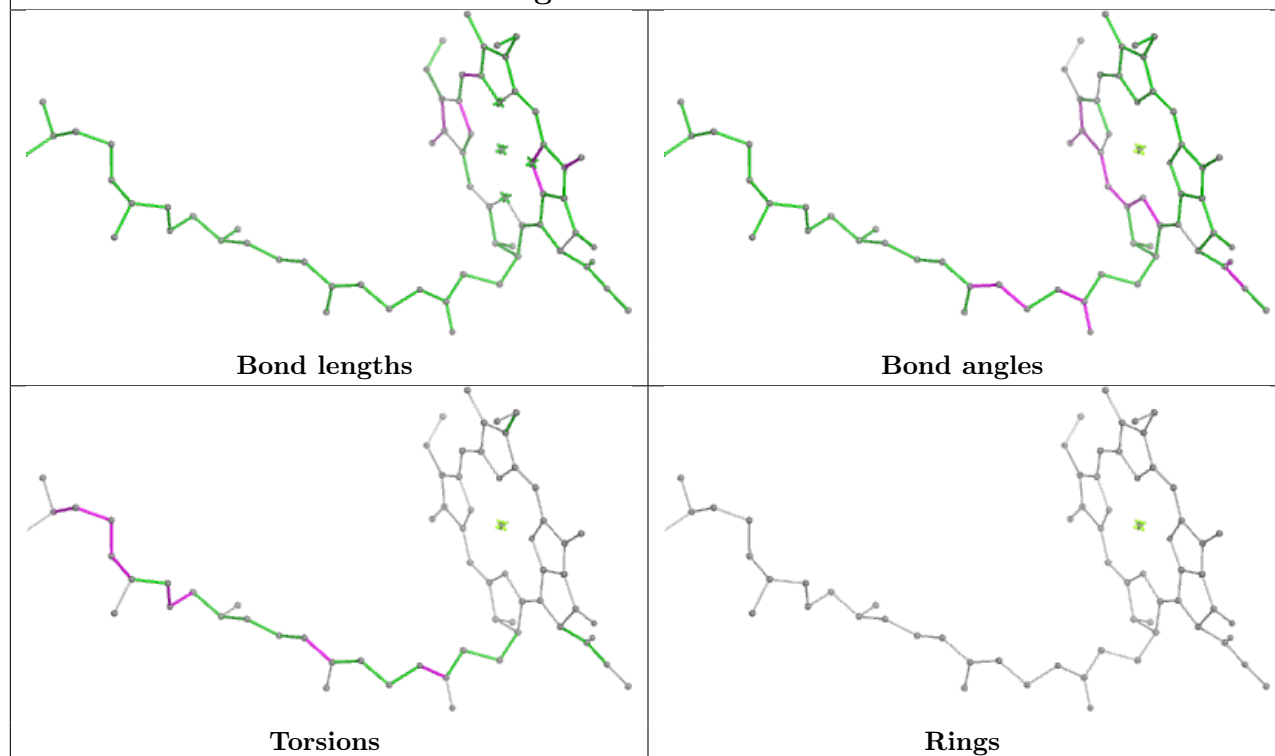


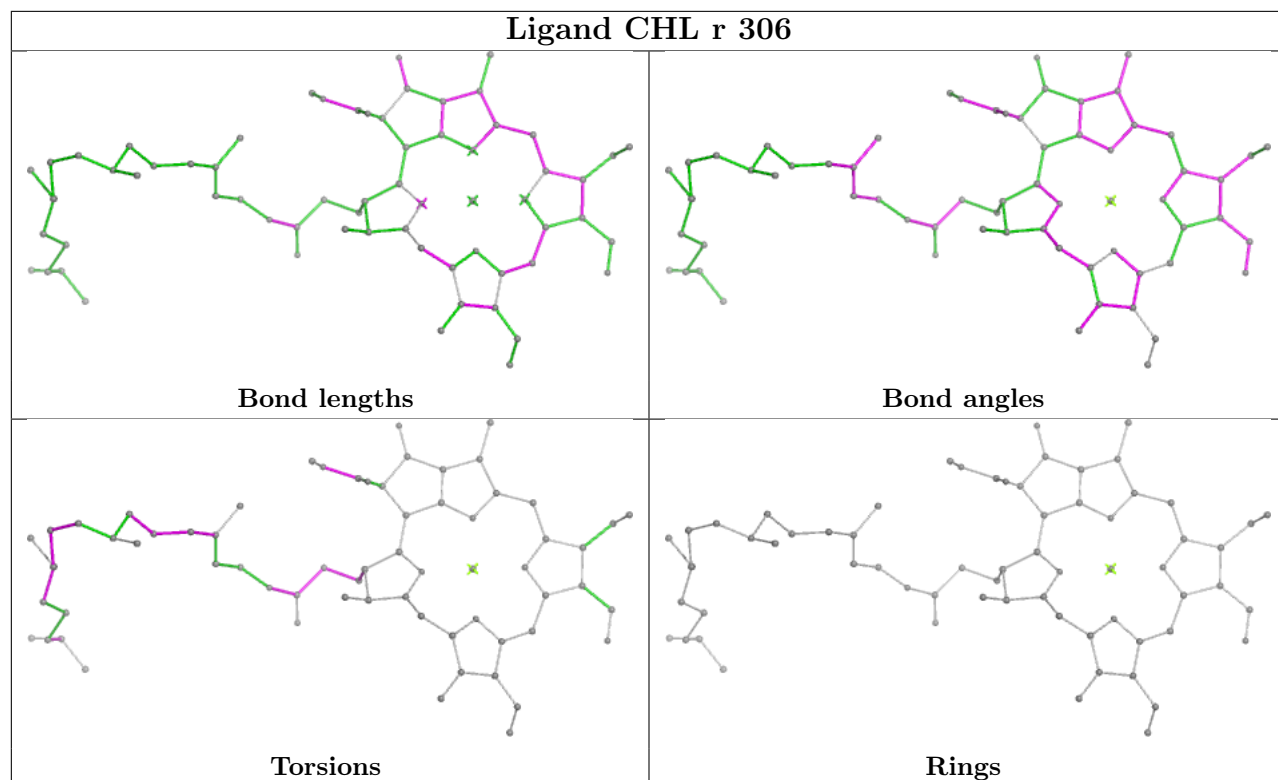


## Ligand CLA Y 609

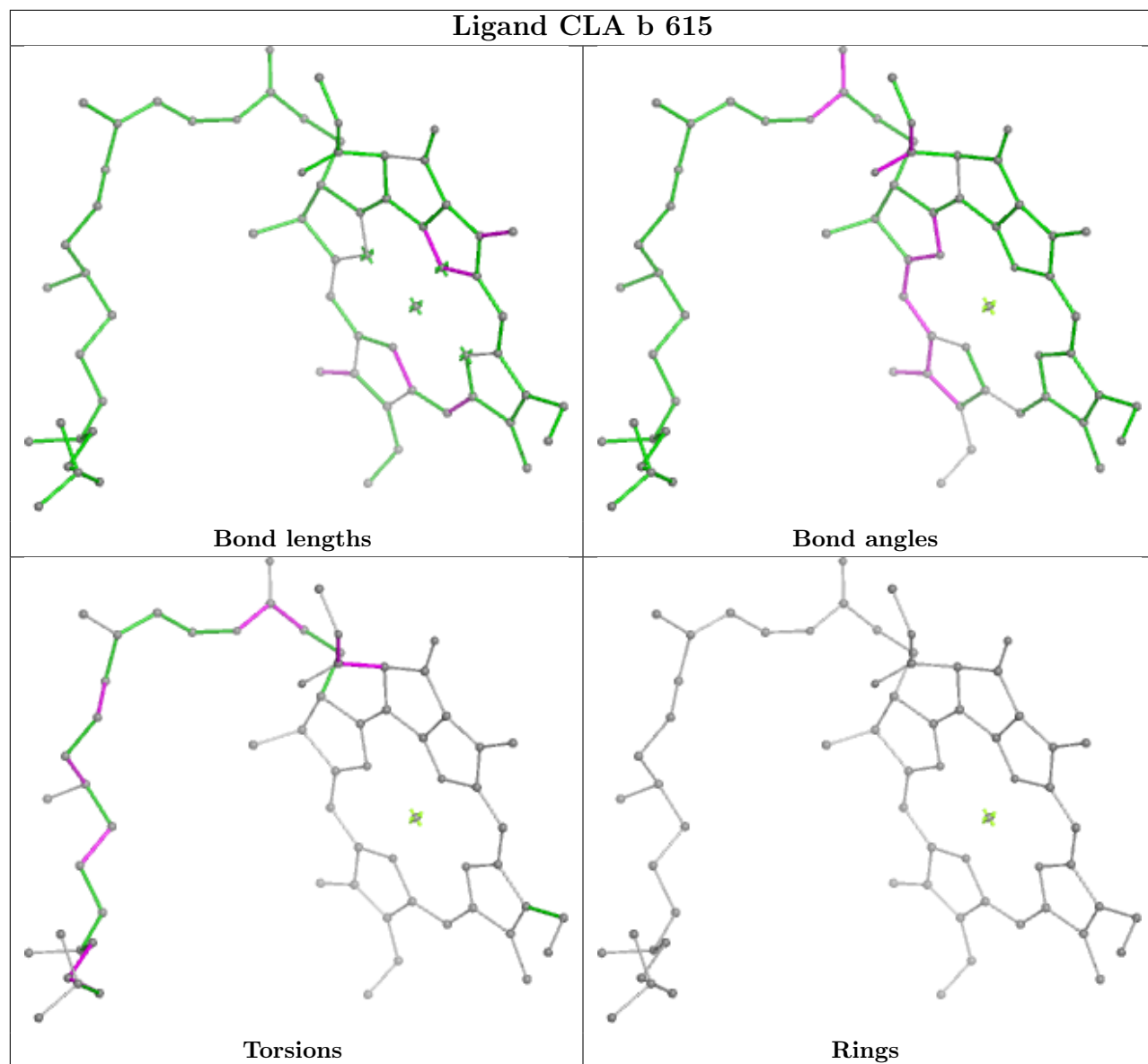


## Ligand CLA d 404

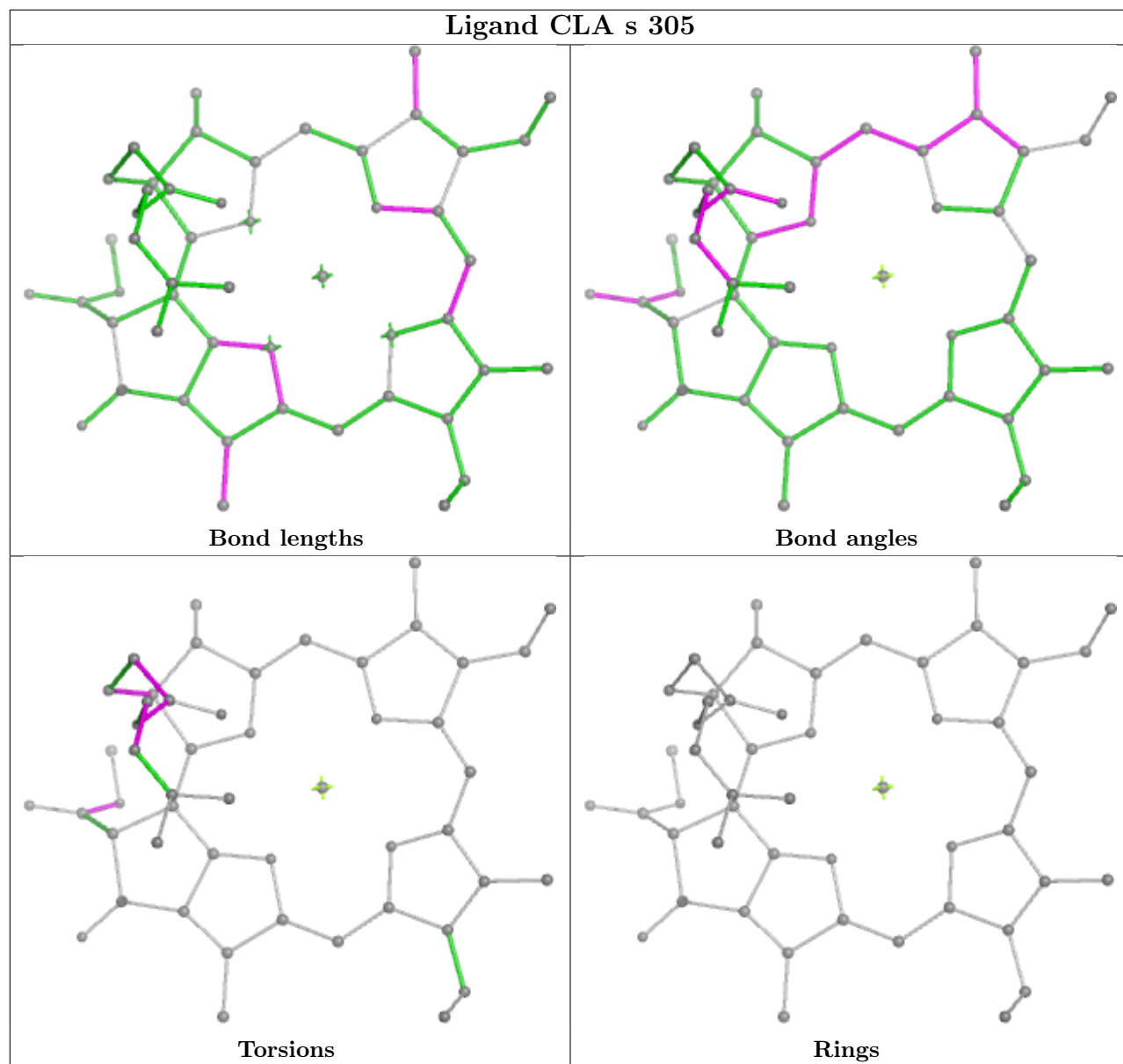




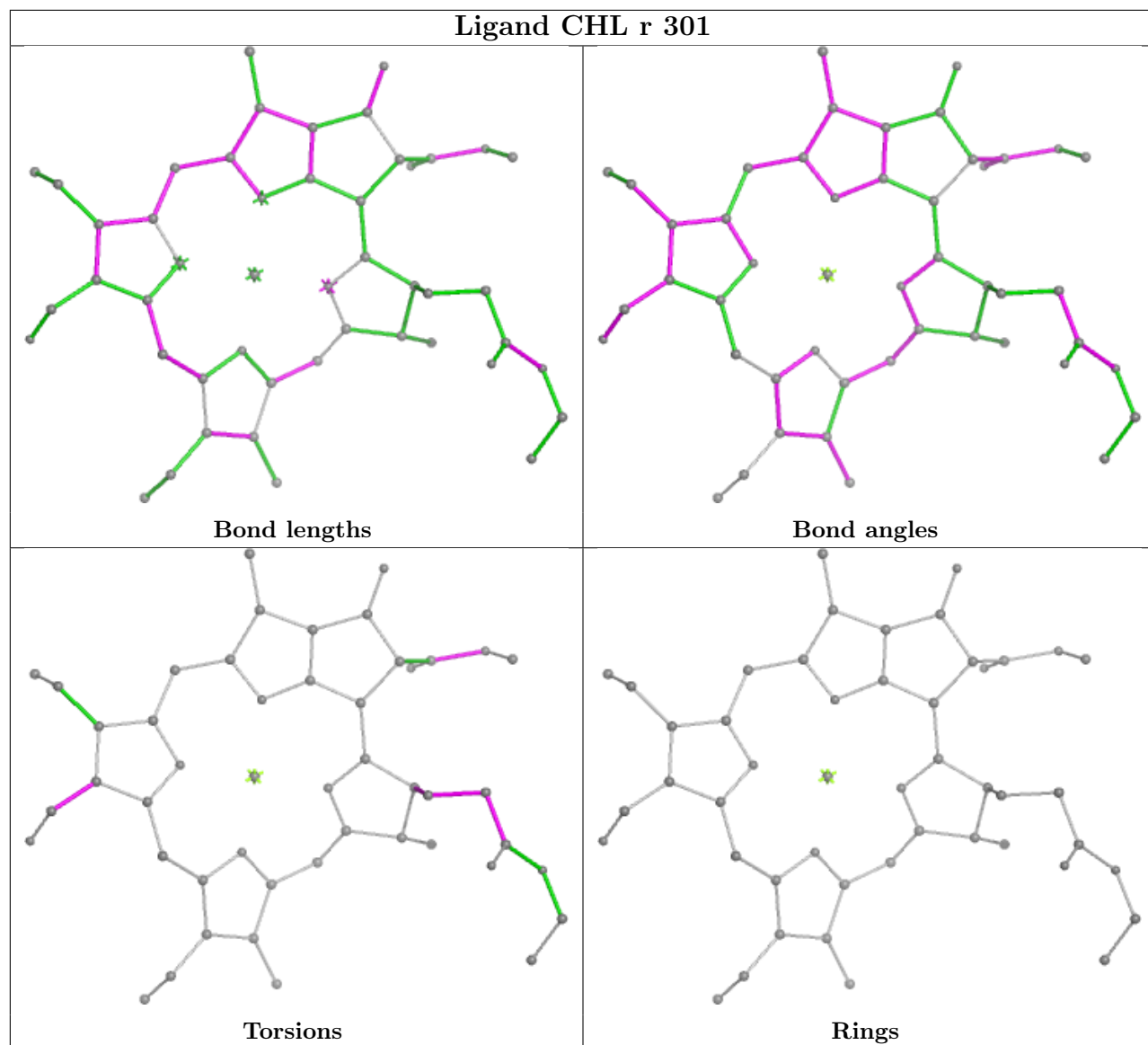
## Ligand CLA b 615



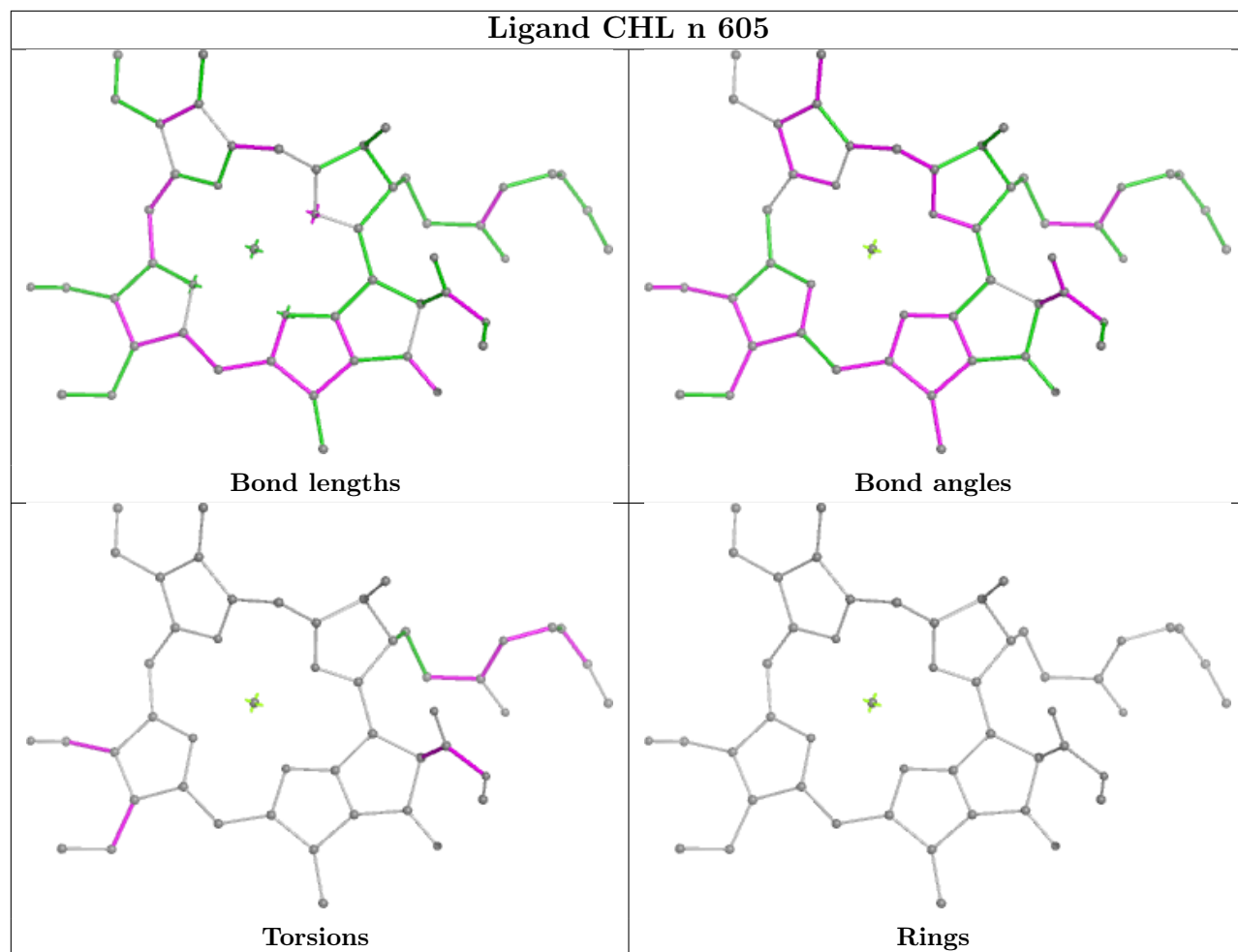
## Ligand CLA s 305

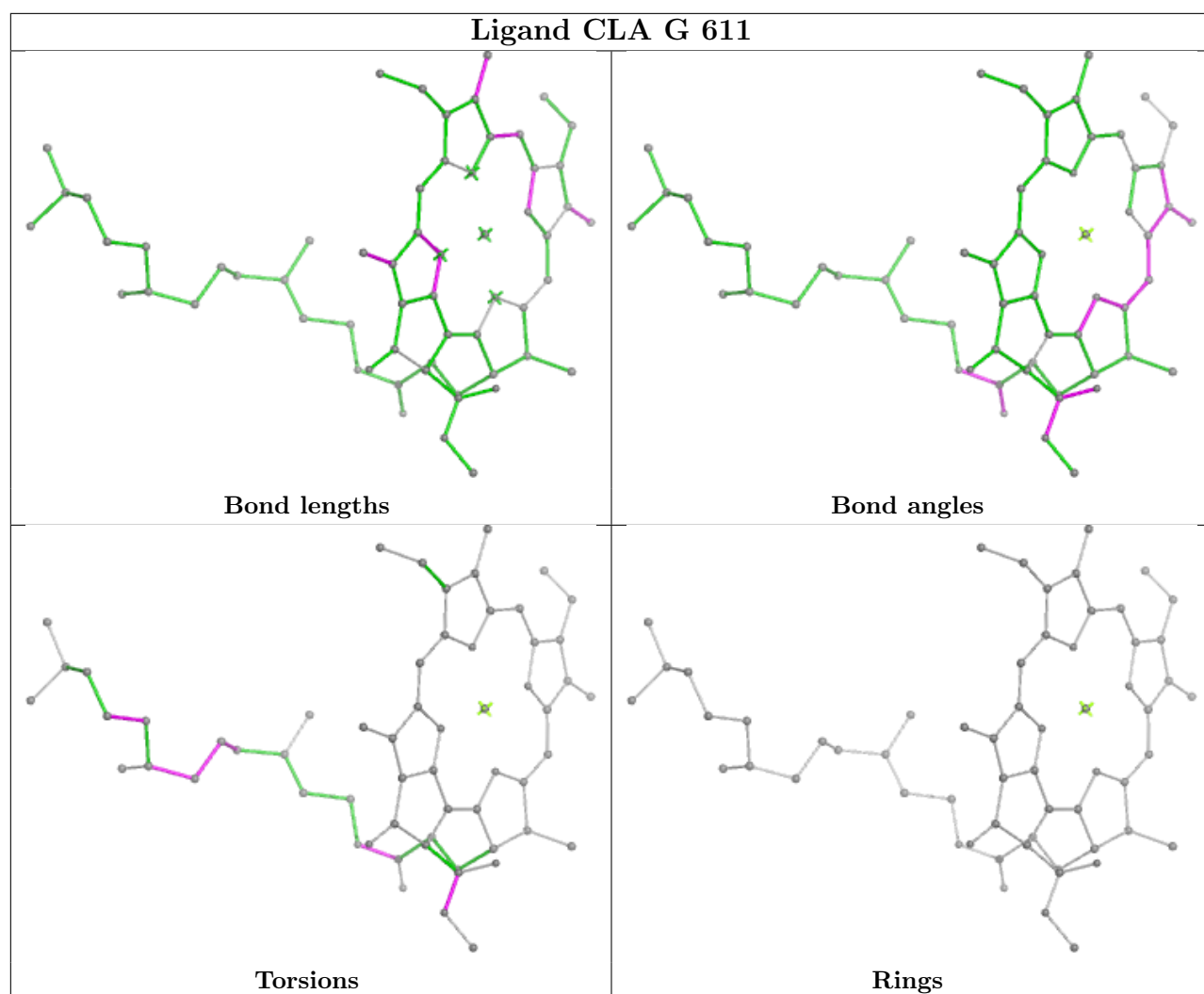


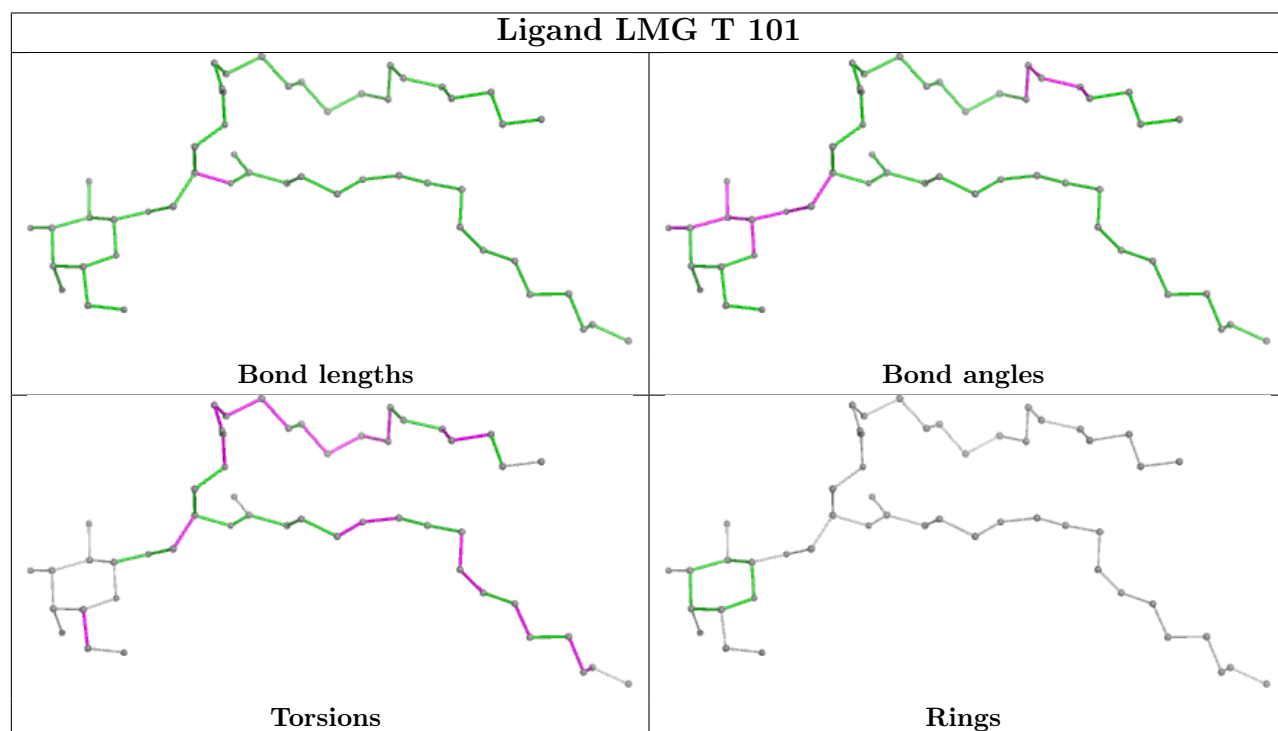
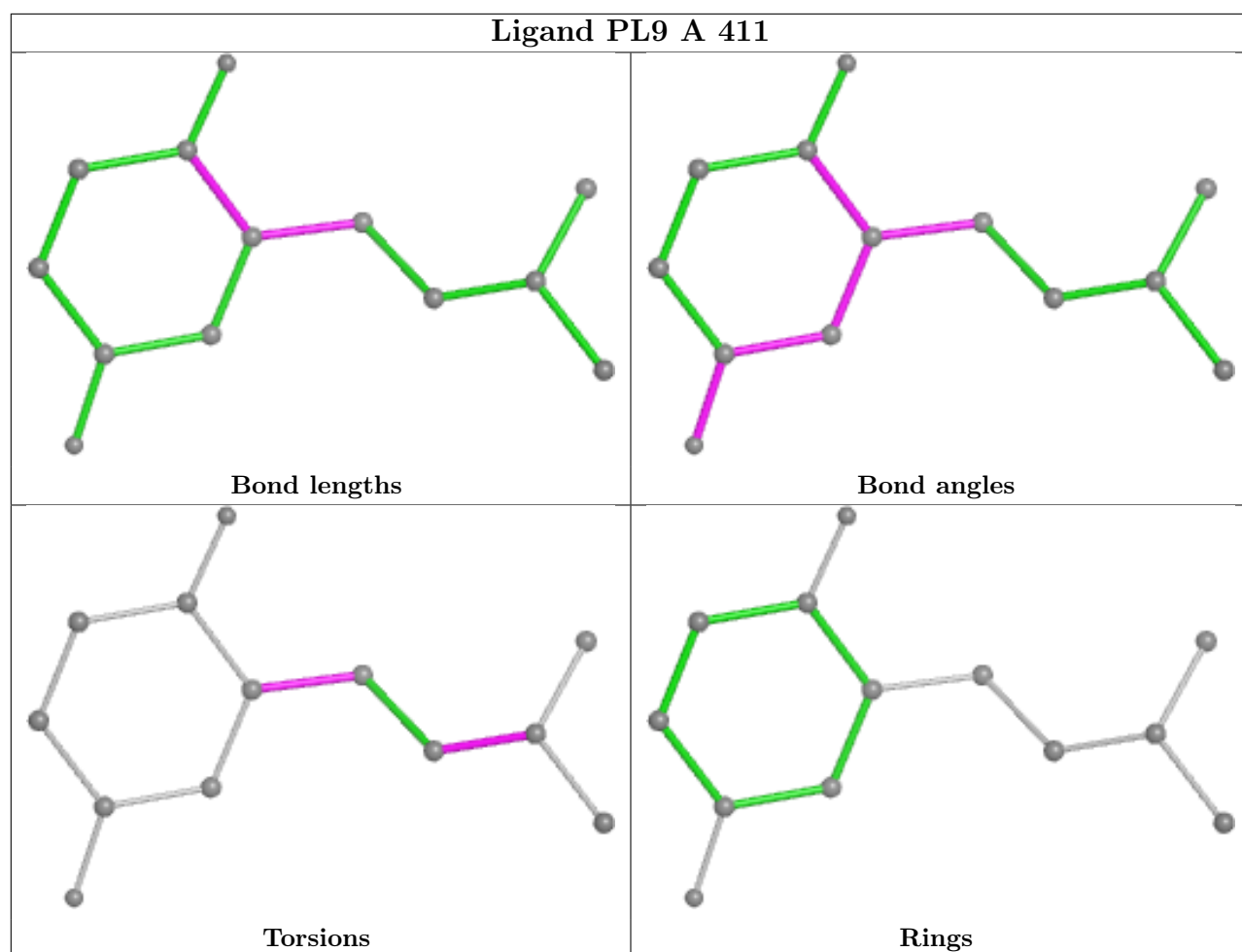
## Ligand CHL r 301

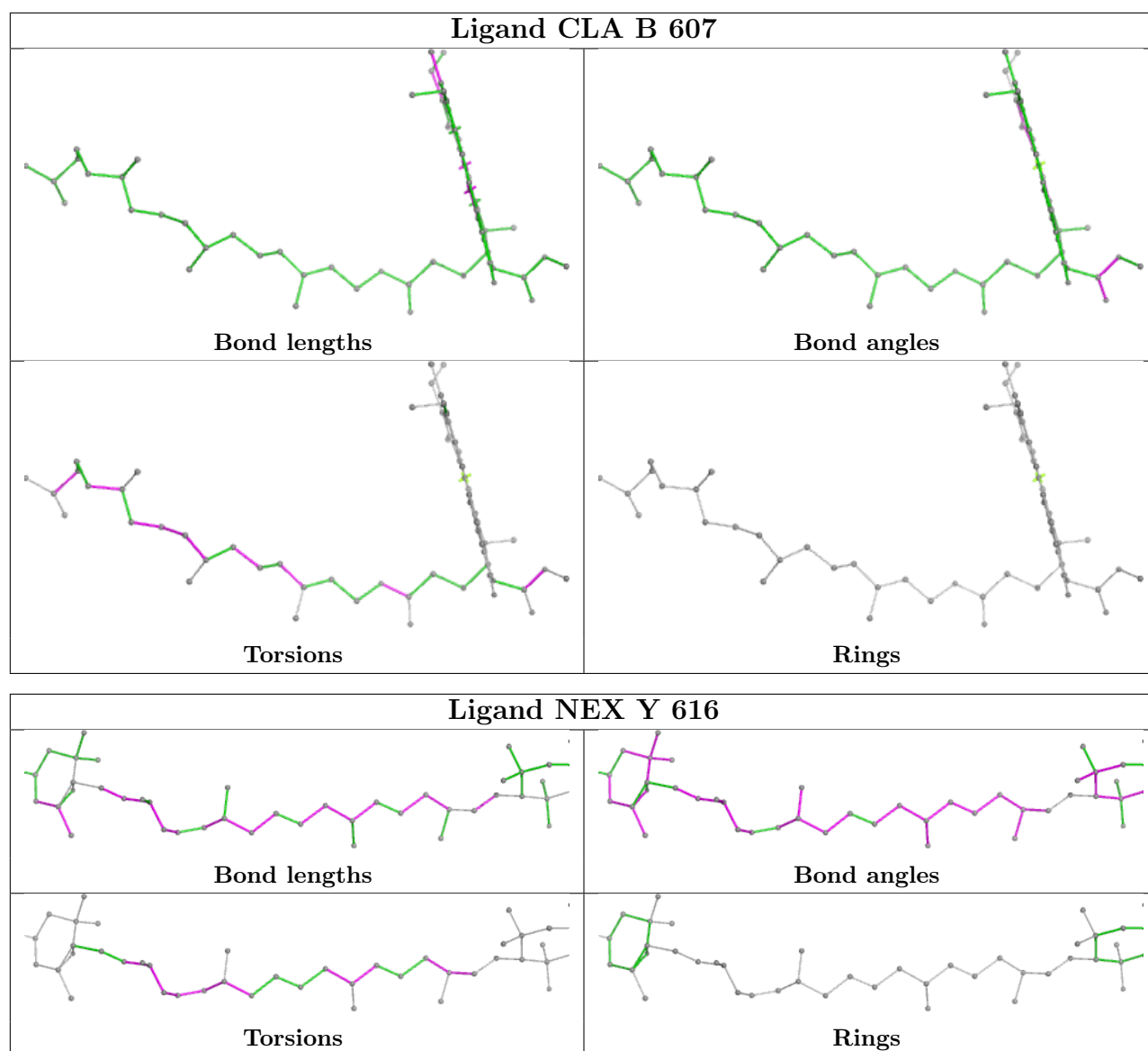


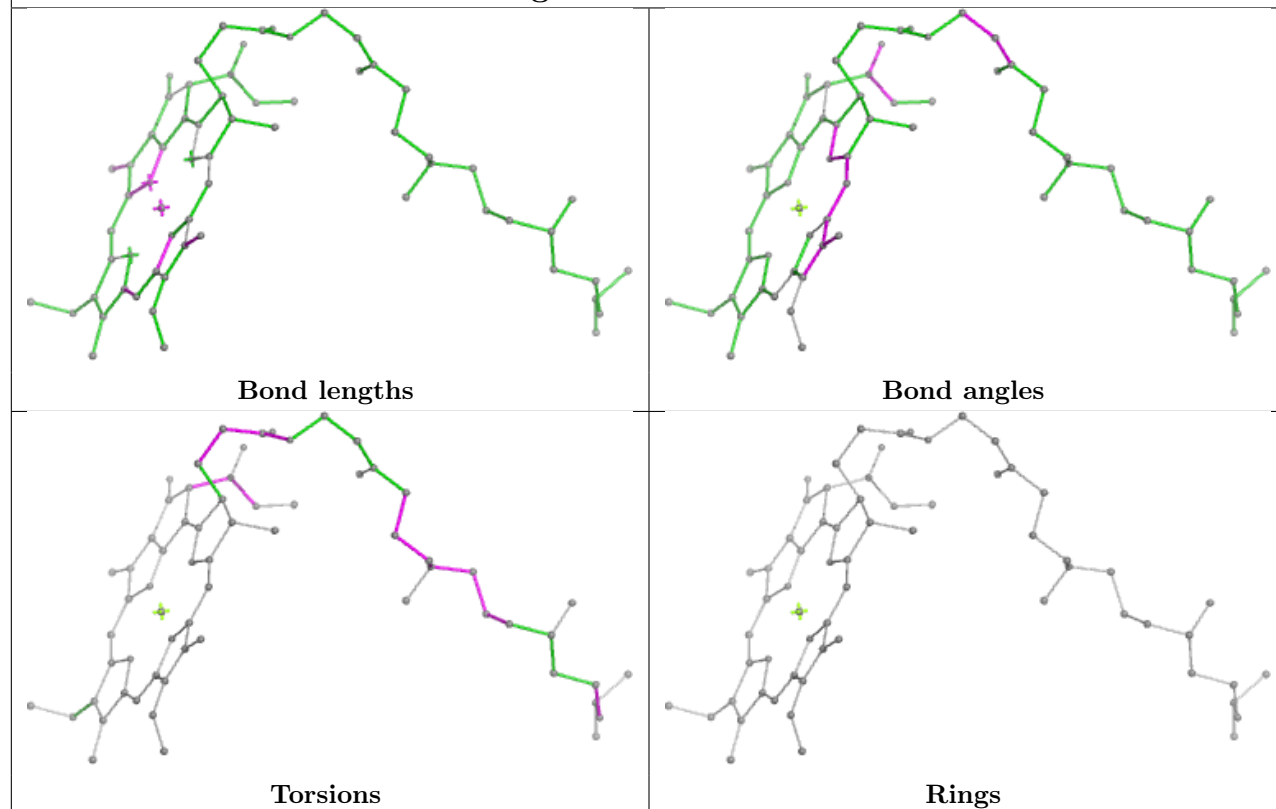
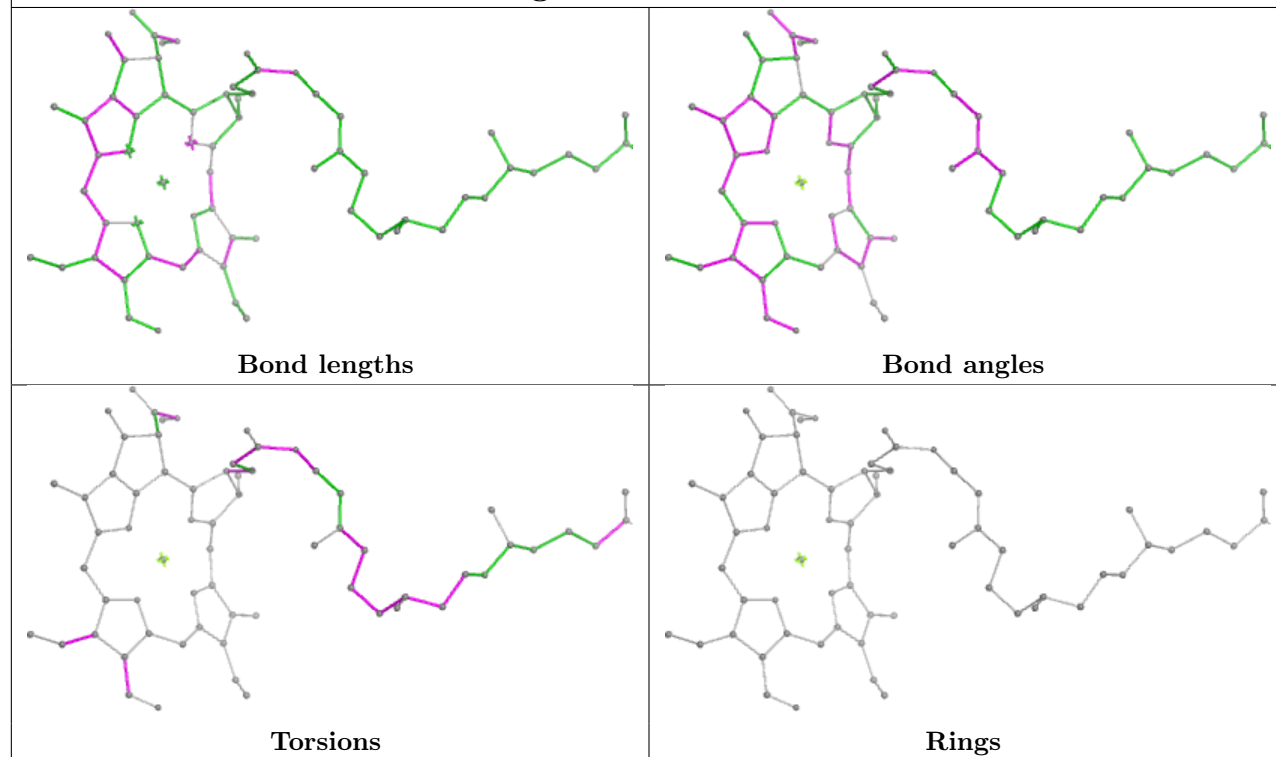
## Ligand CHL n 605

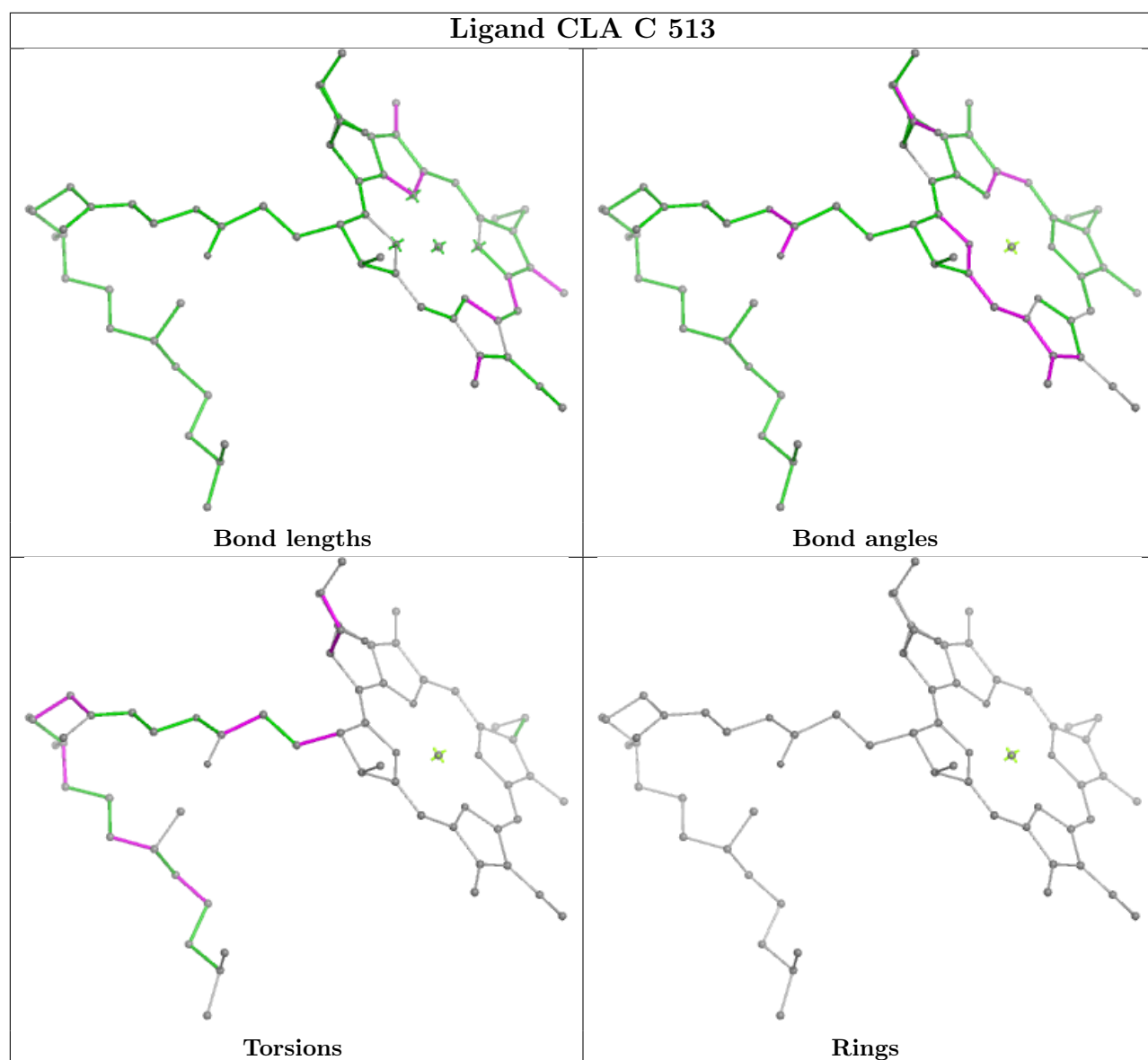


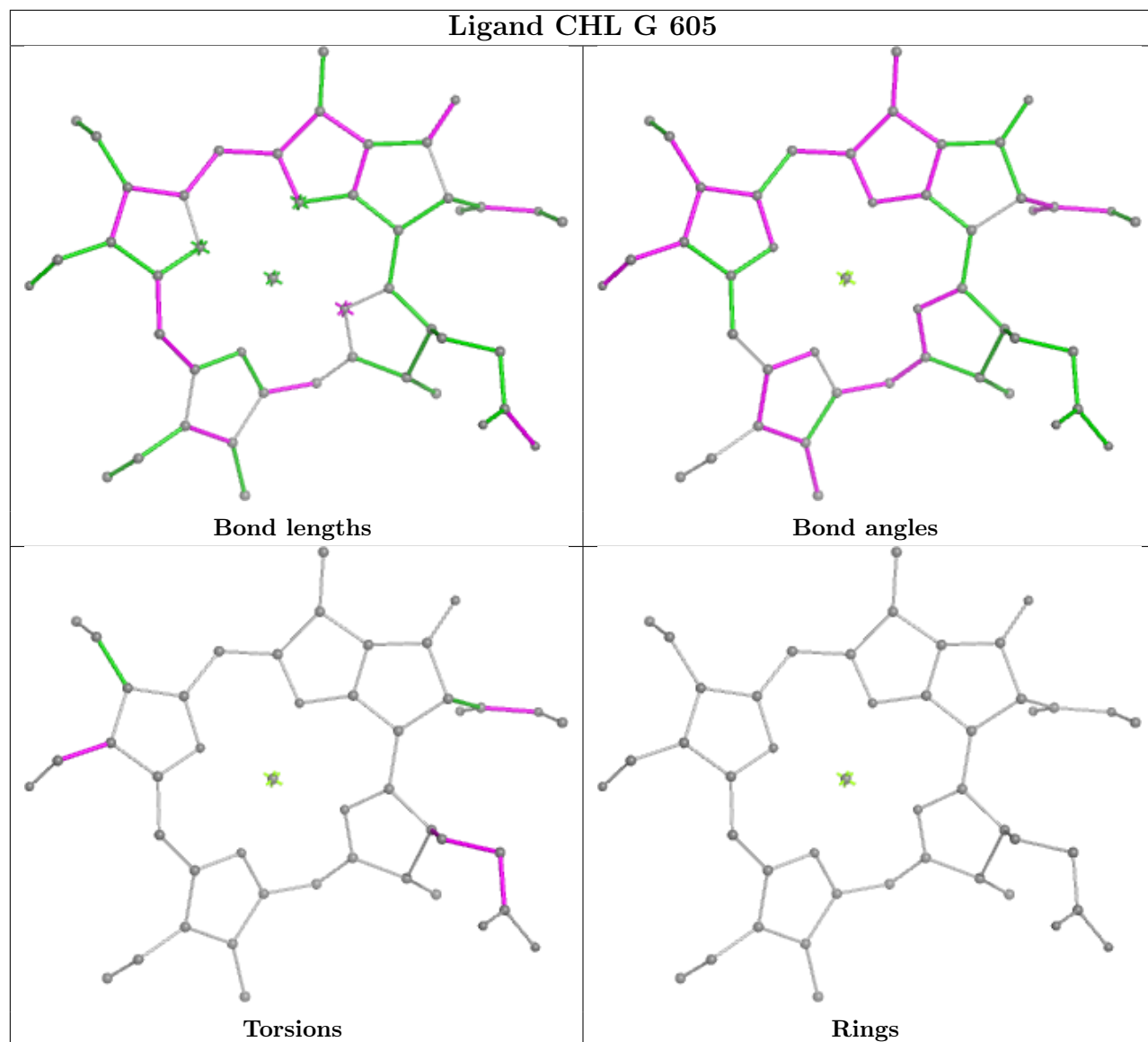


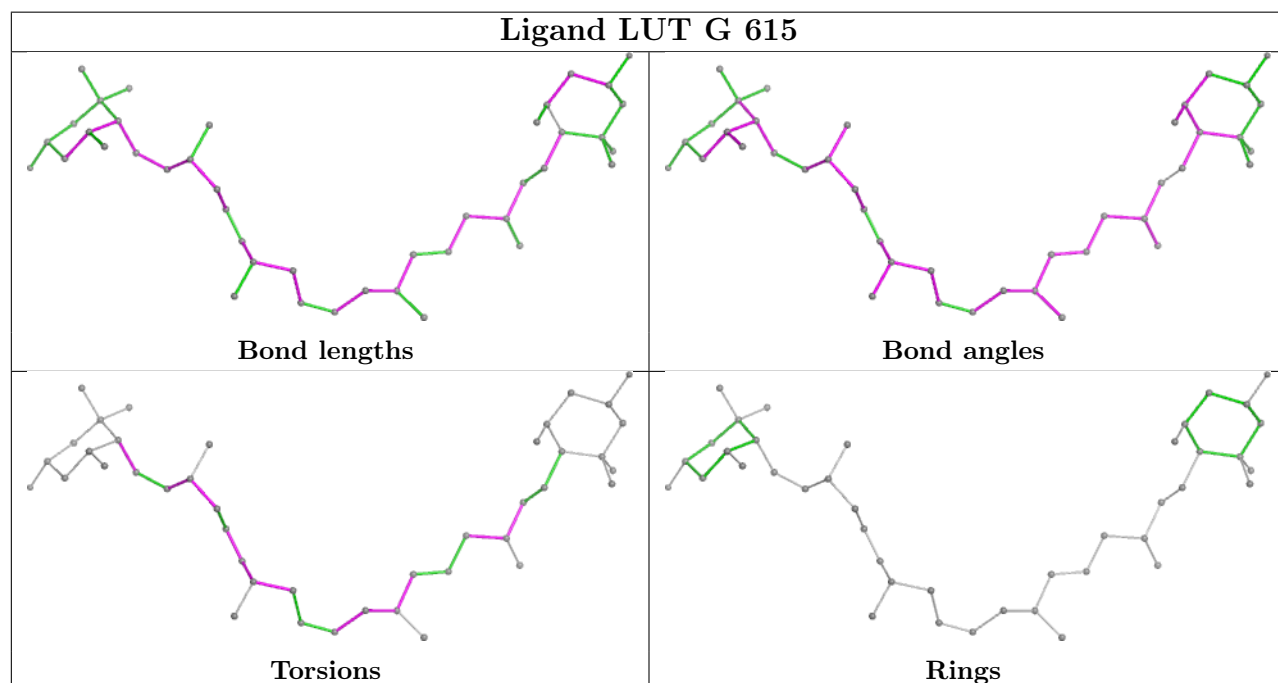
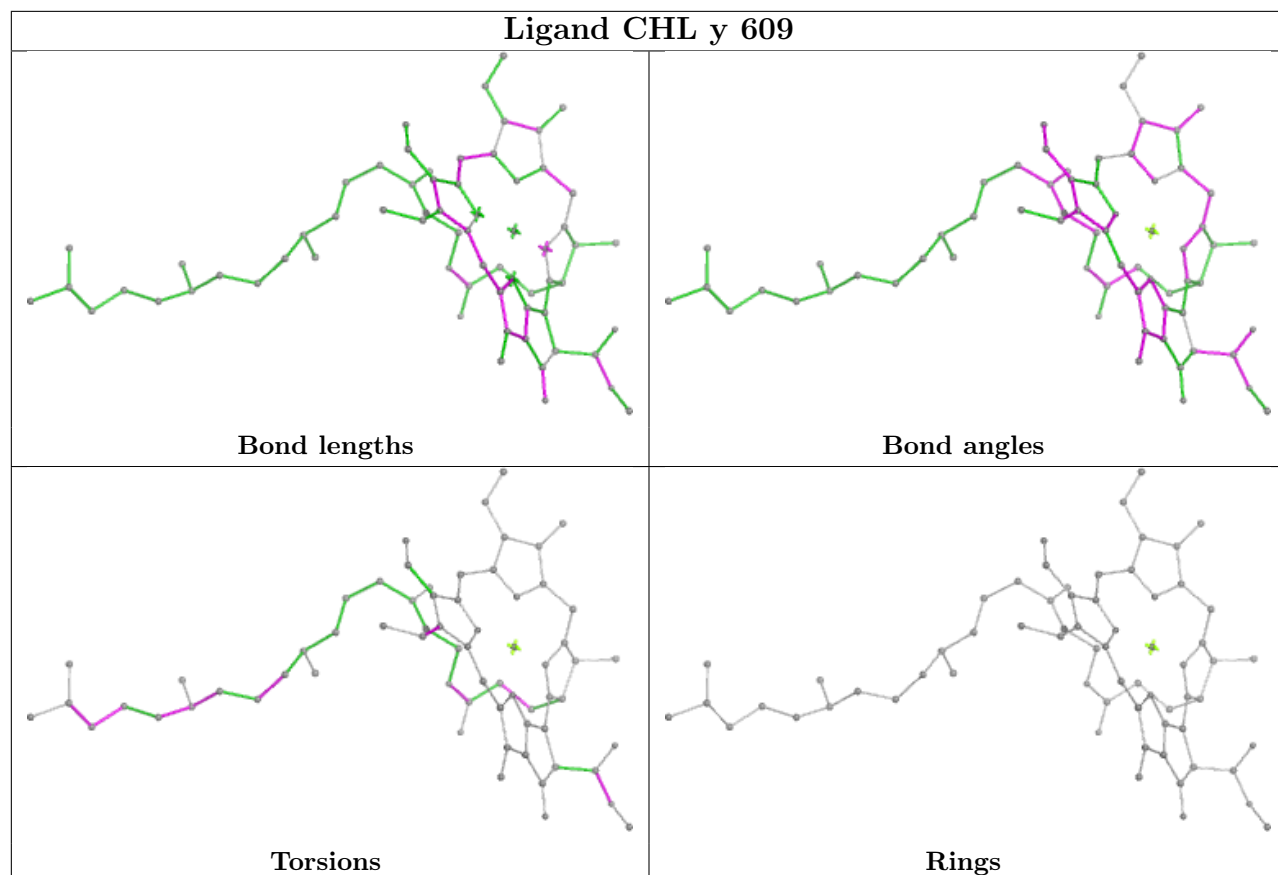


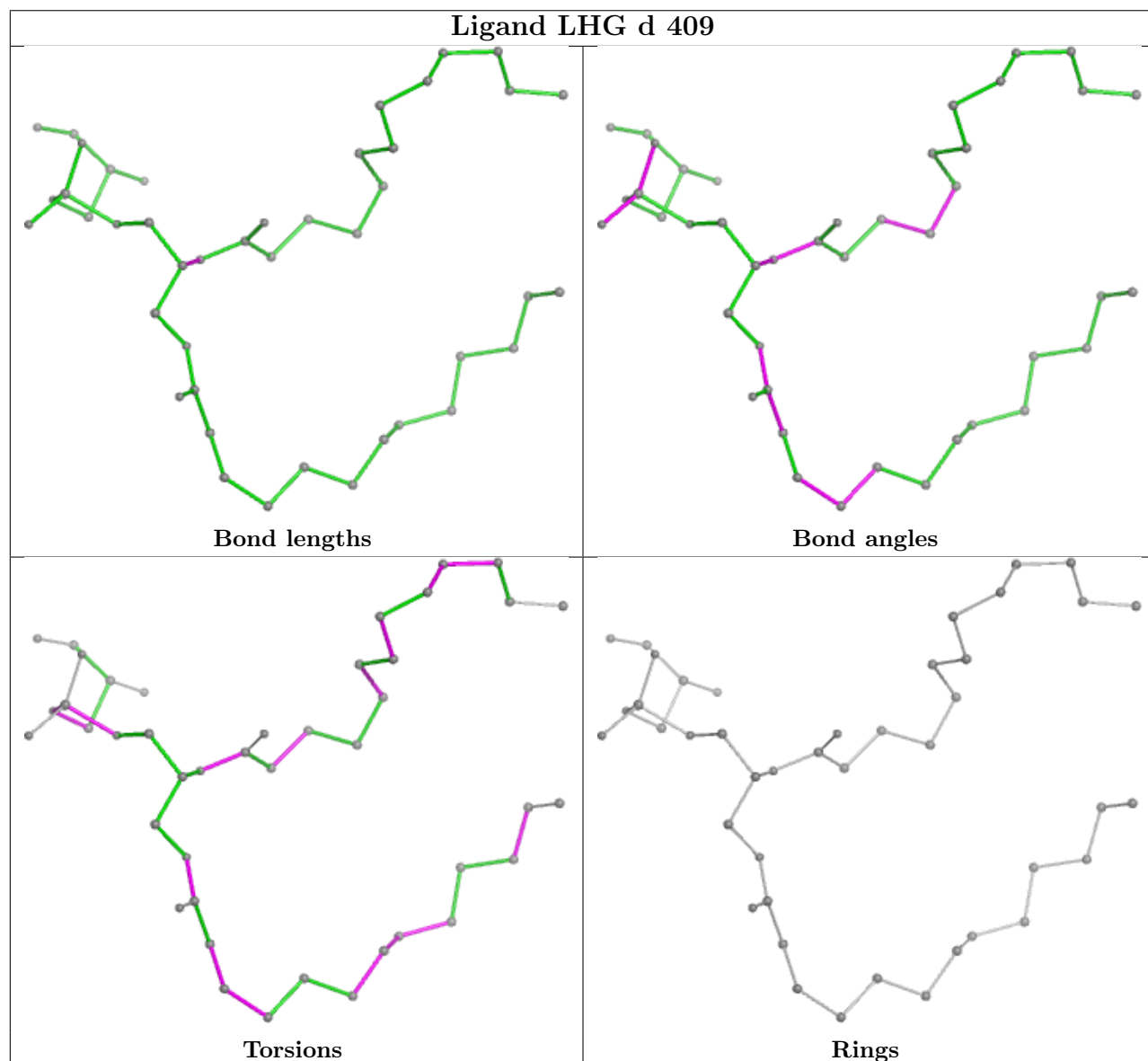
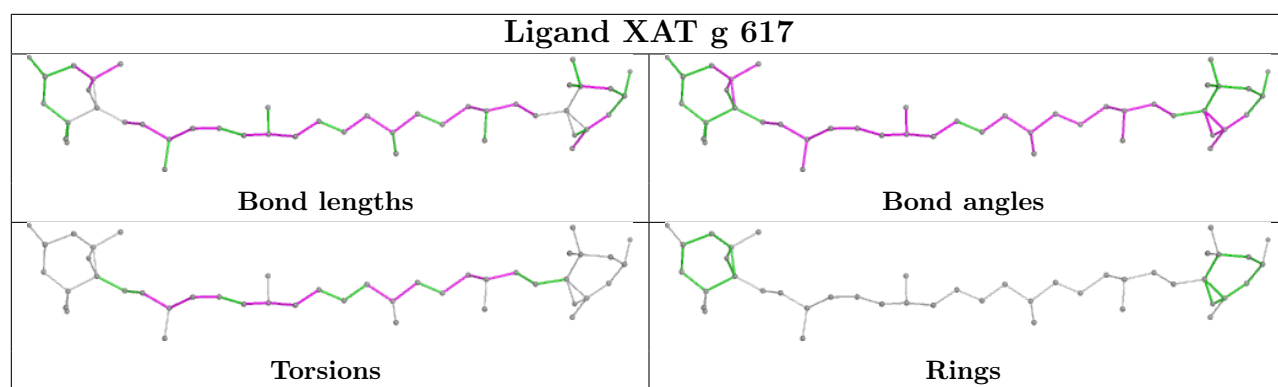


**Ligand CLA N 603****Ligand CHL Y 607**

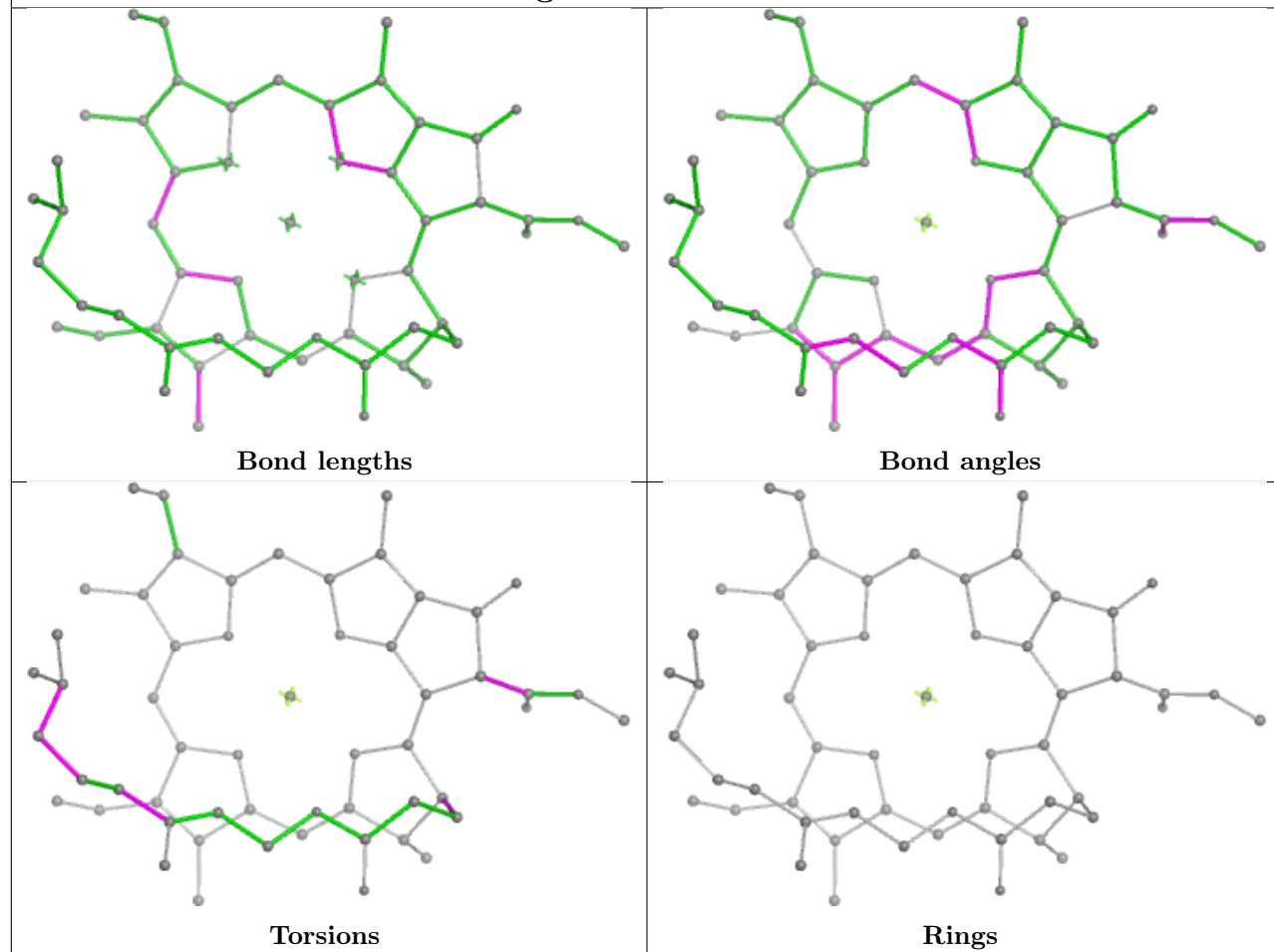




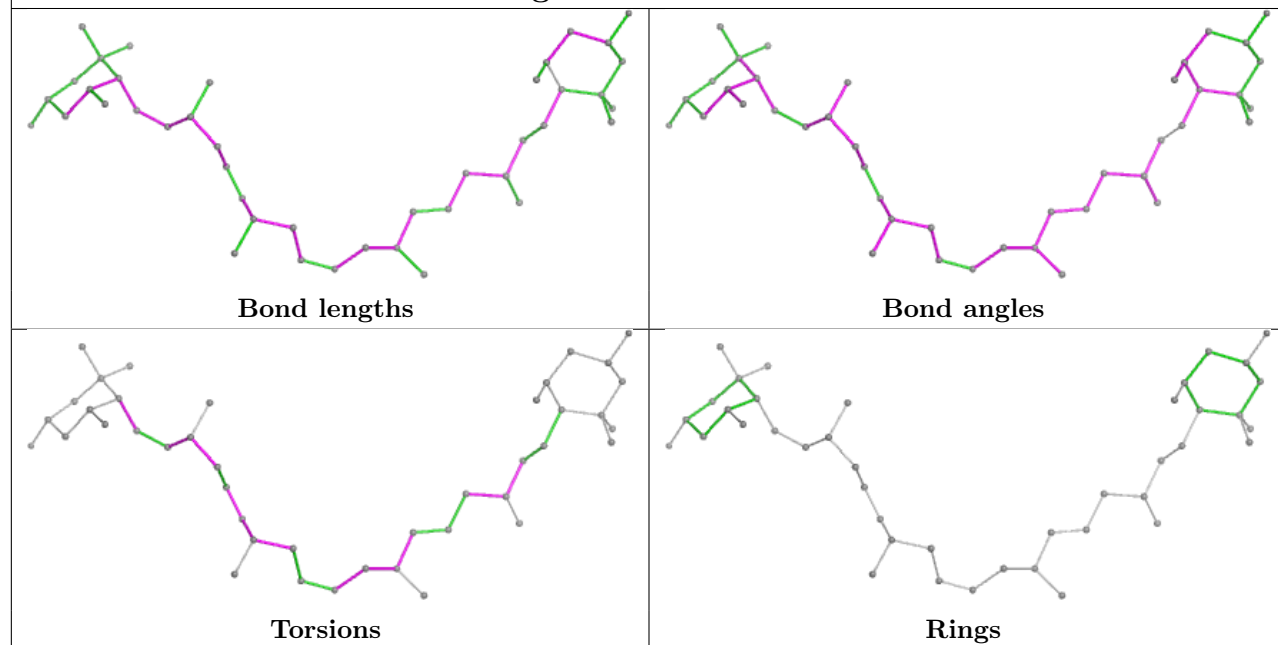




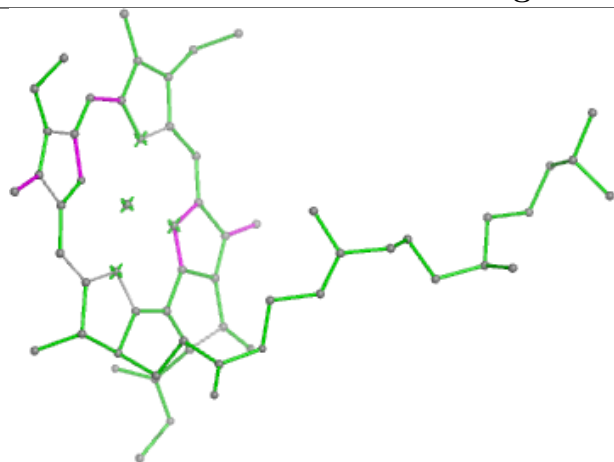
## Ligand CLA s 309



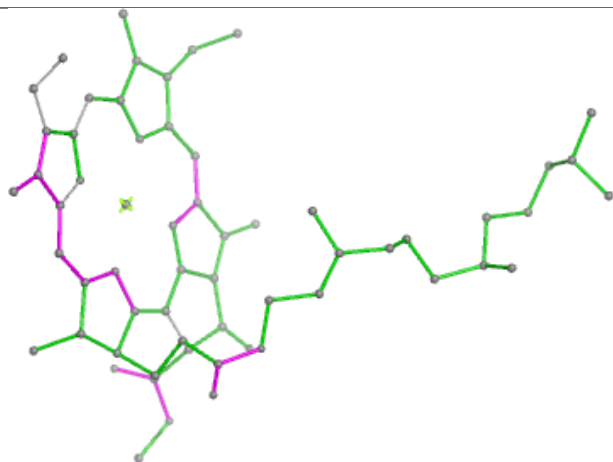
## Ligand LUT Y 613



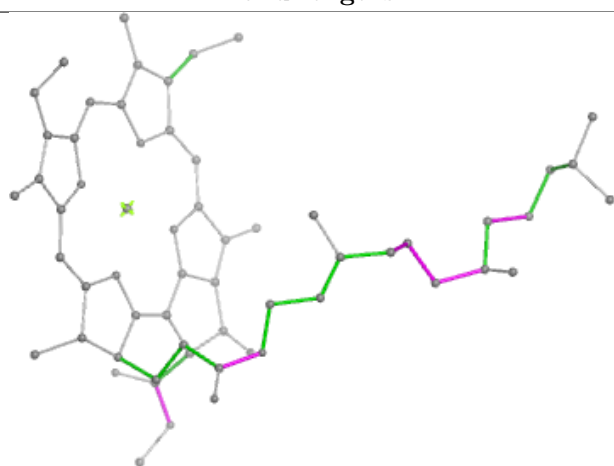
## Ligand CLA N 610



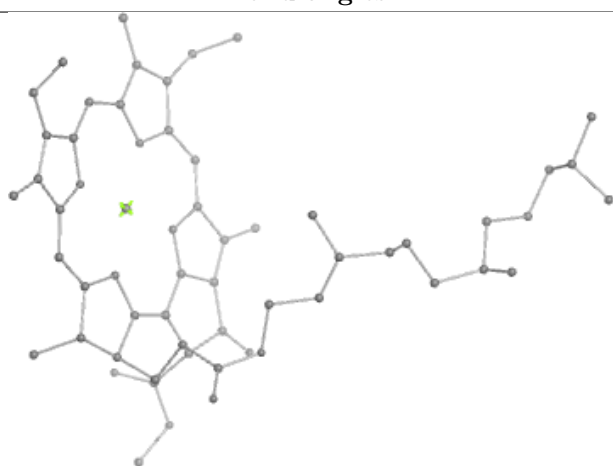
Bond lengths



Bond angles

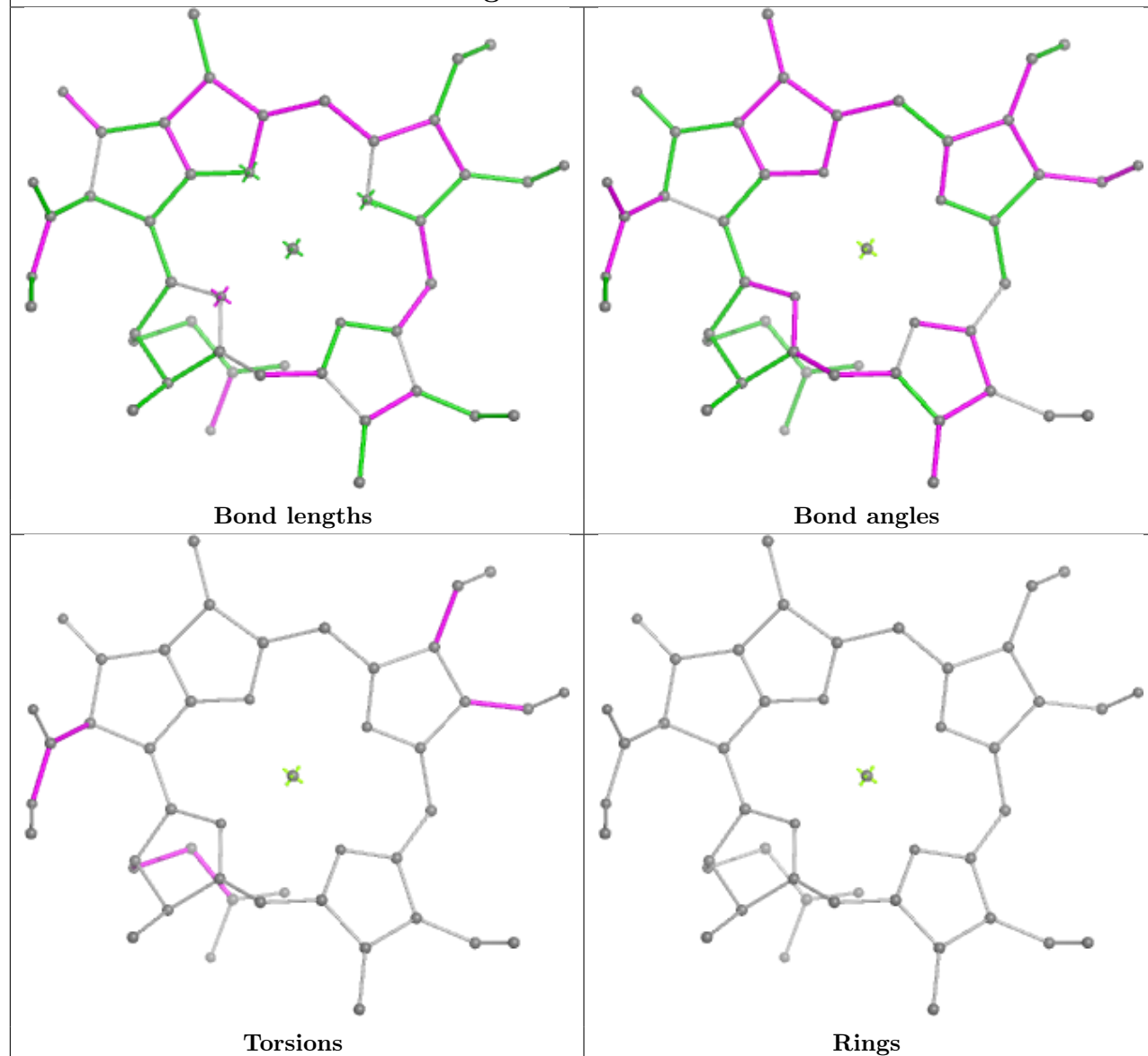


Torsions

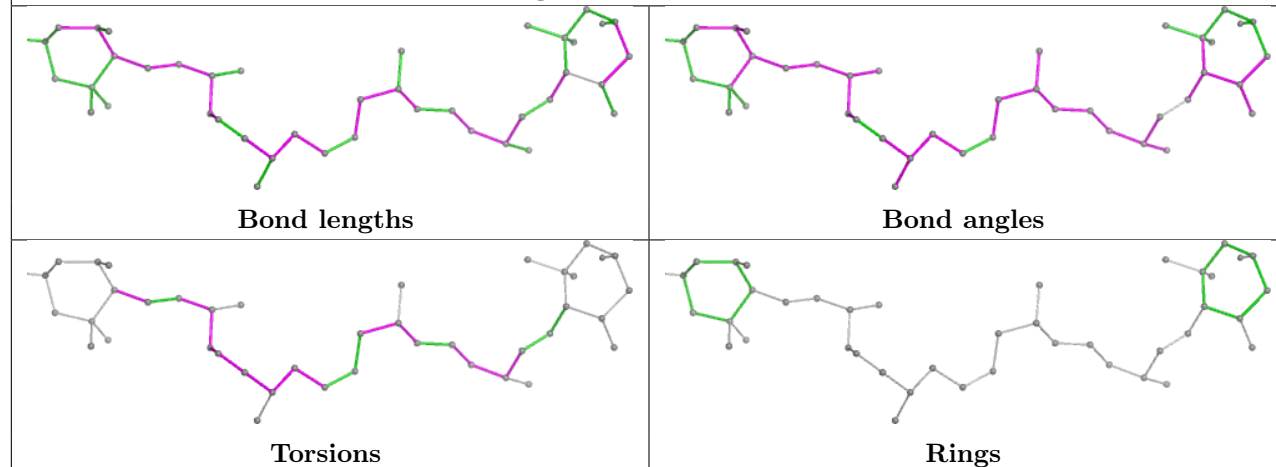


Rings

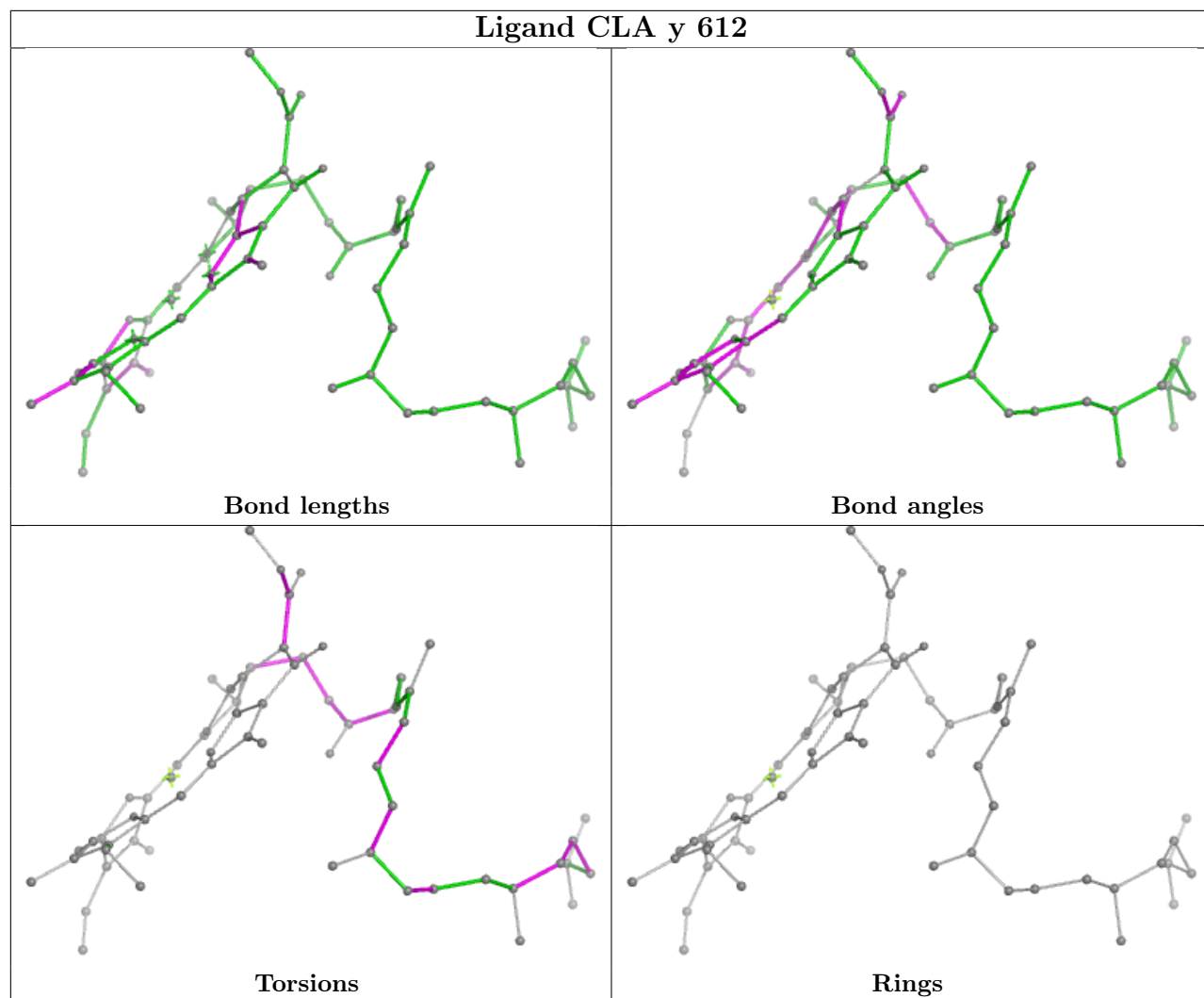
## Ligand CHL s 307

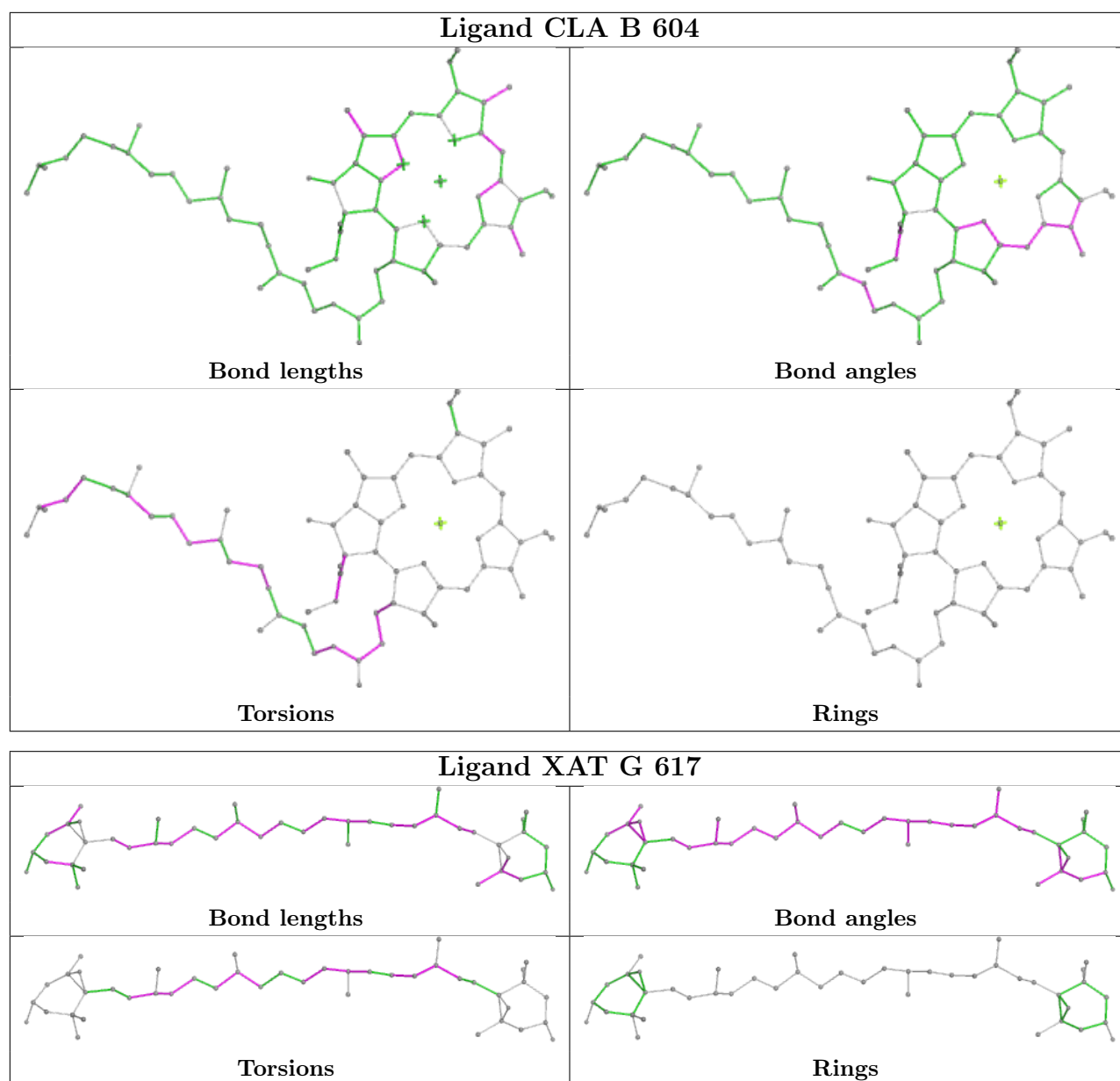


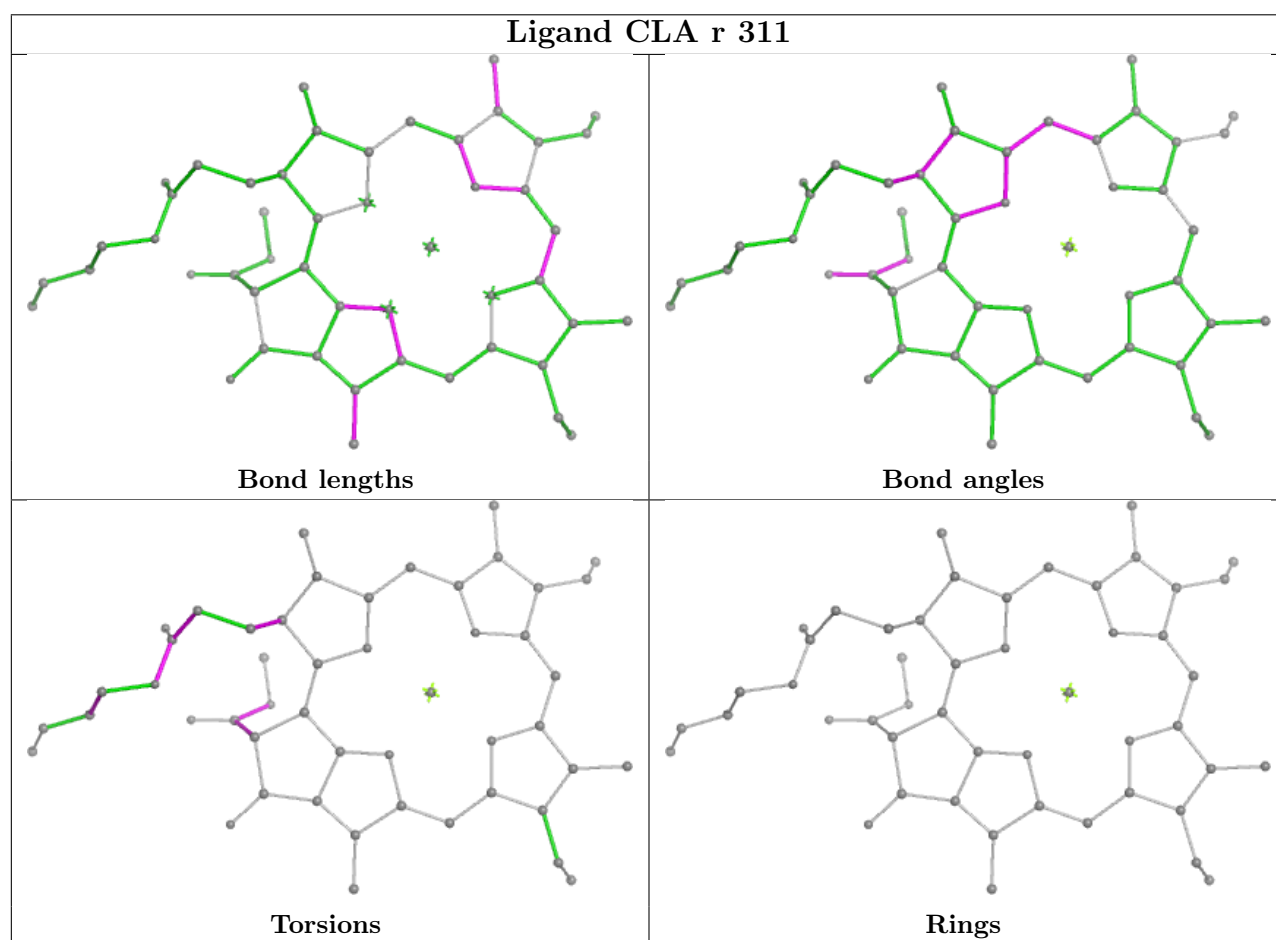
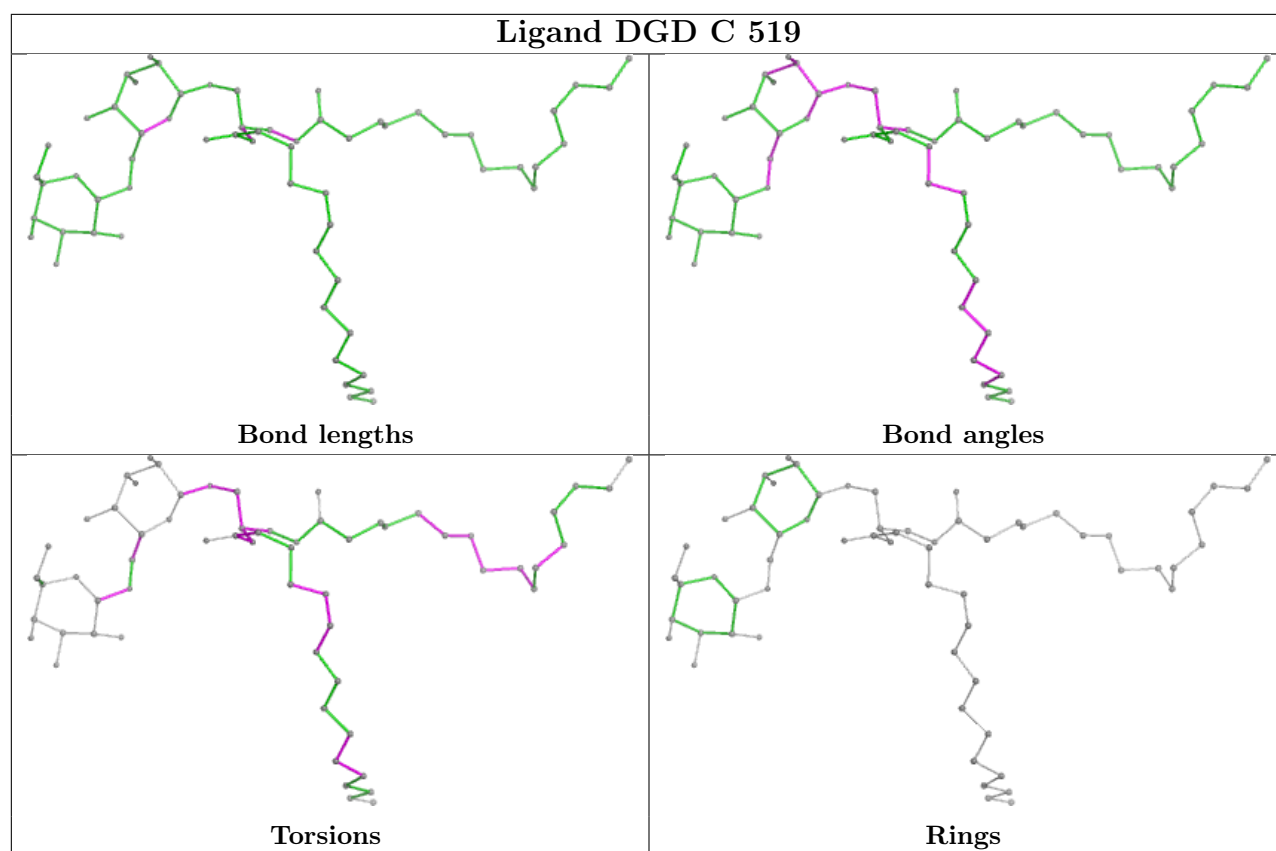
## Ligand LUT R 312



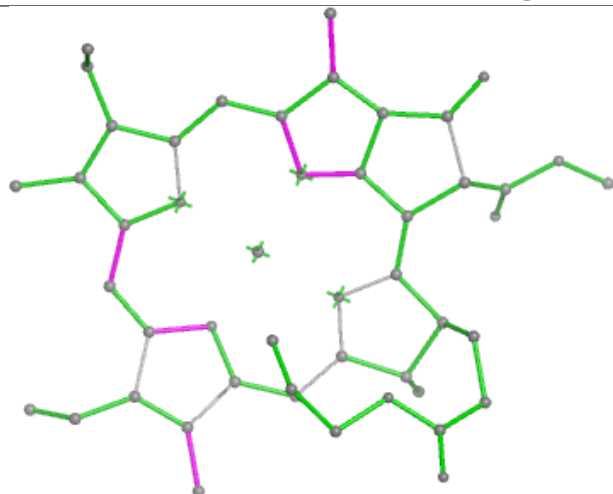
## Ligand CLA y 612



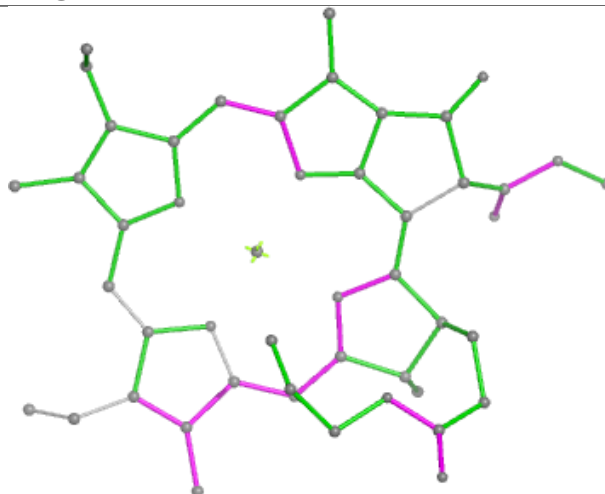




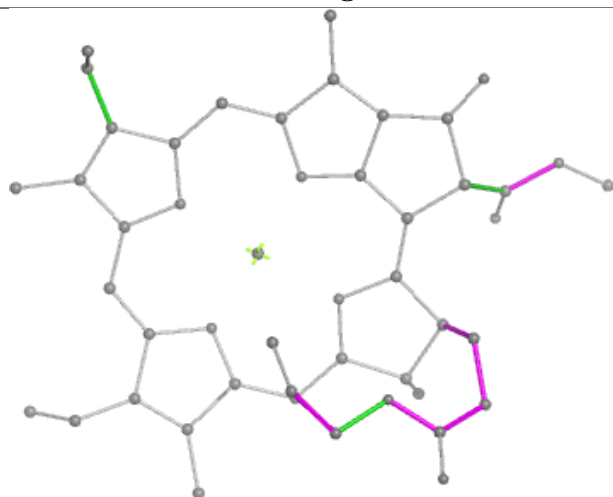
## Ligand CLA g 614



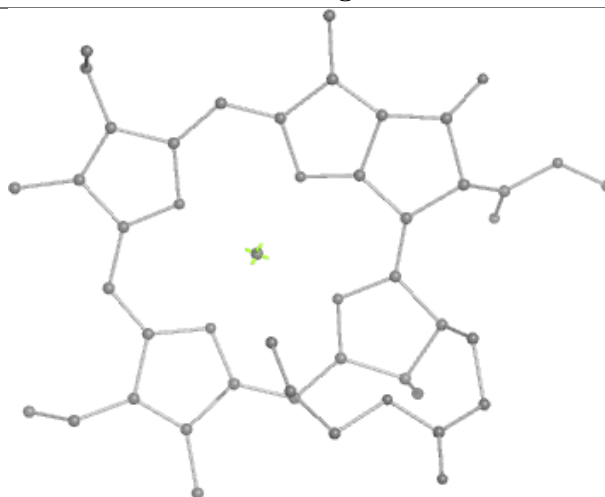
Bond lengths



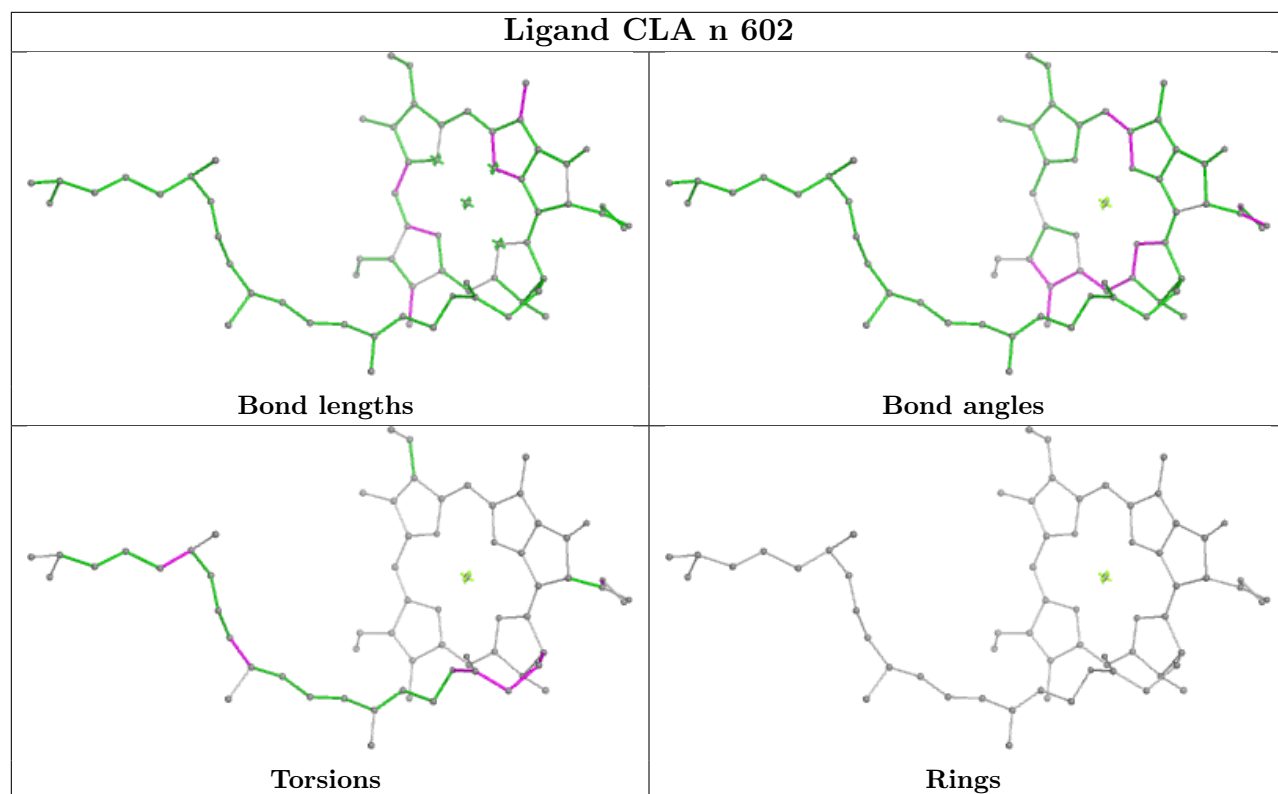
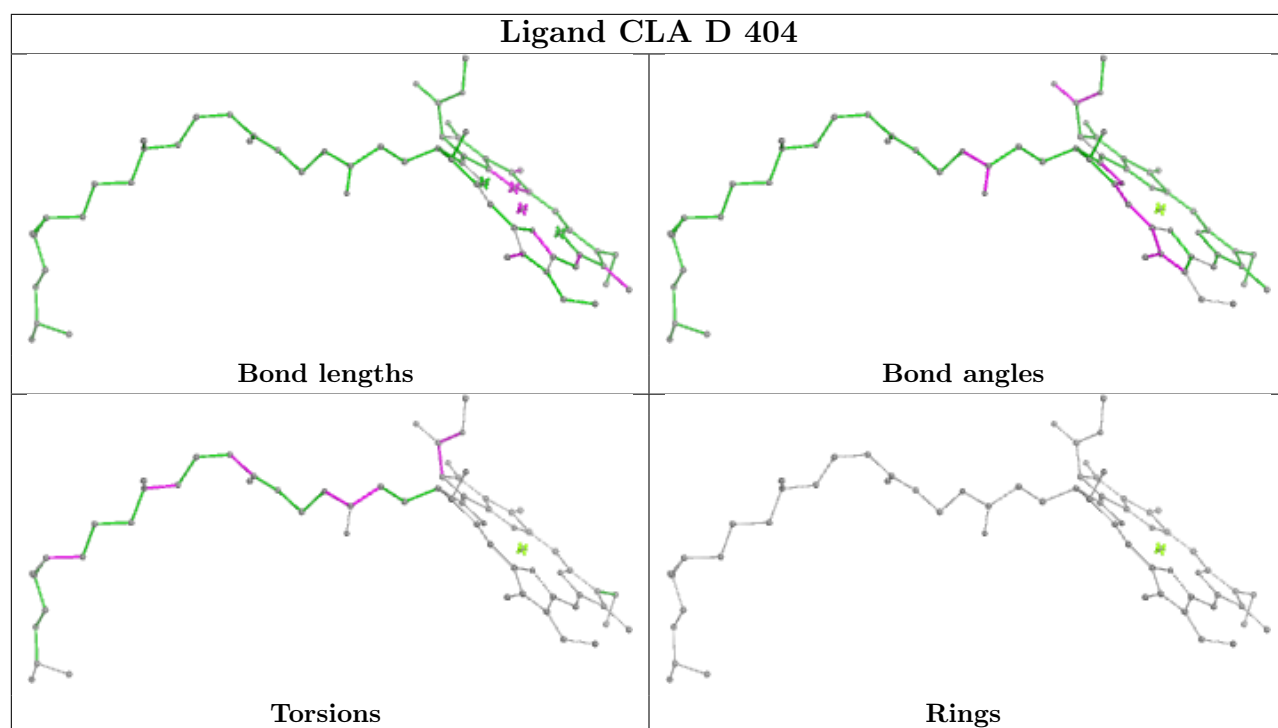
Bond angles

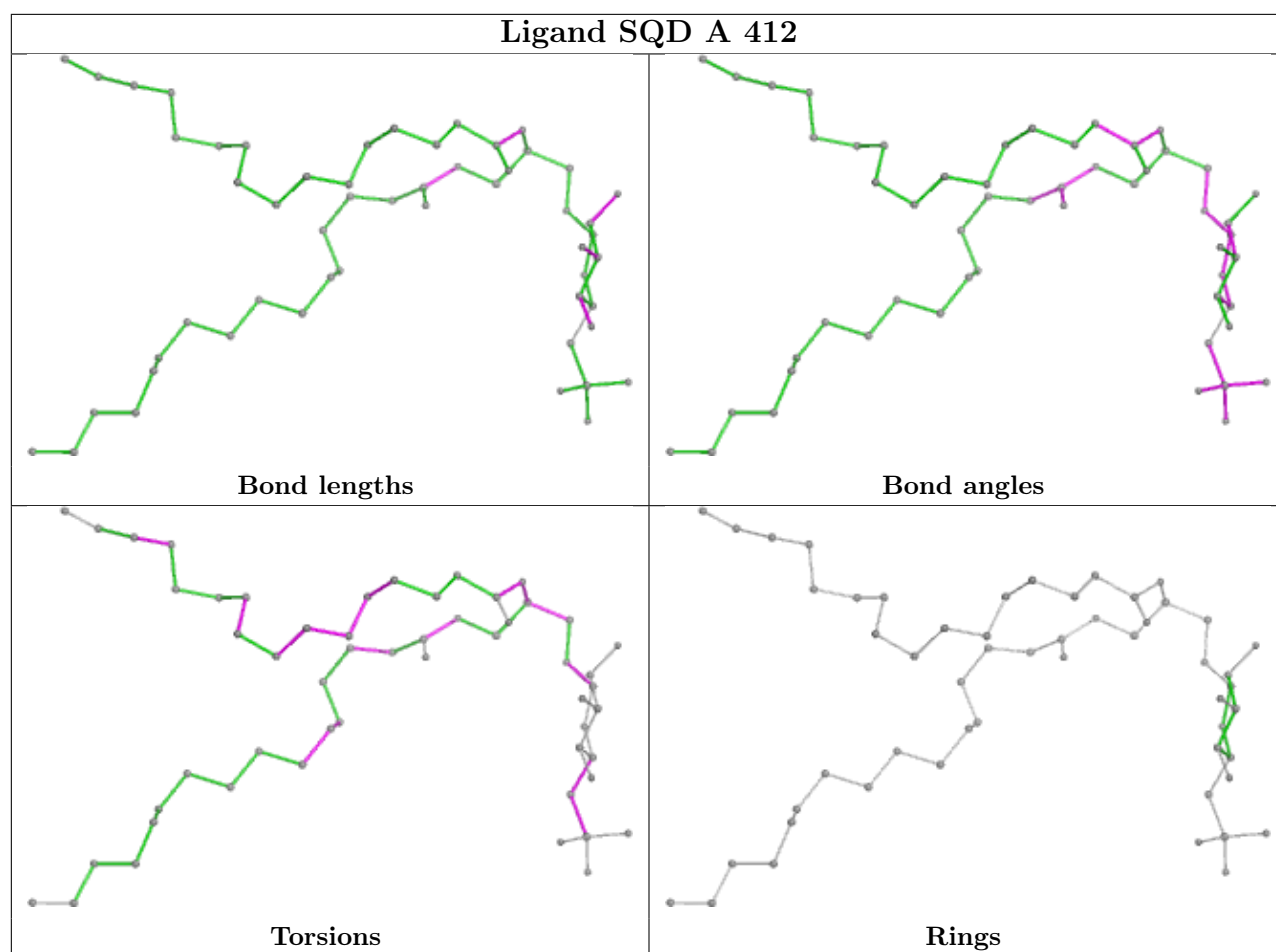


Torsions

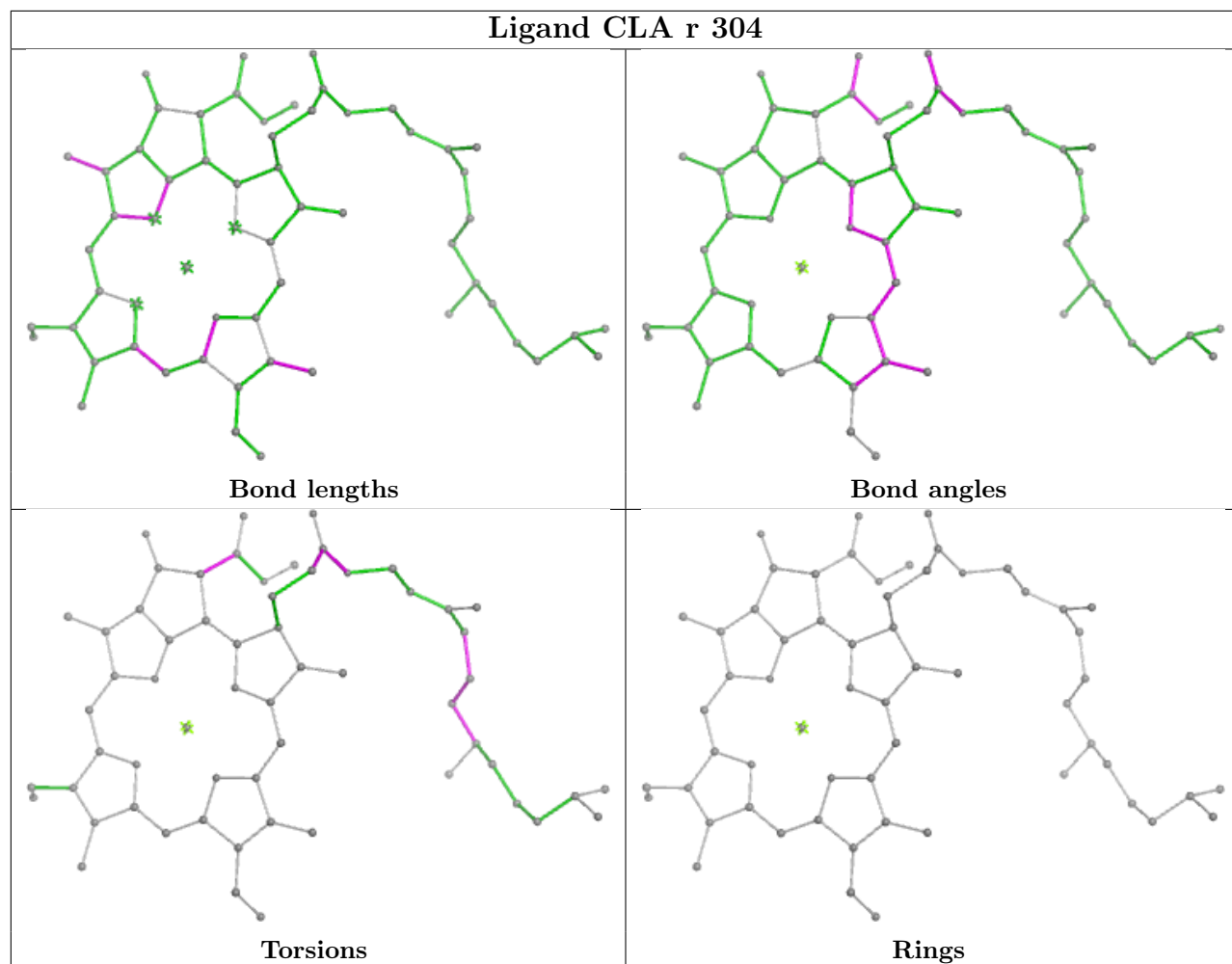


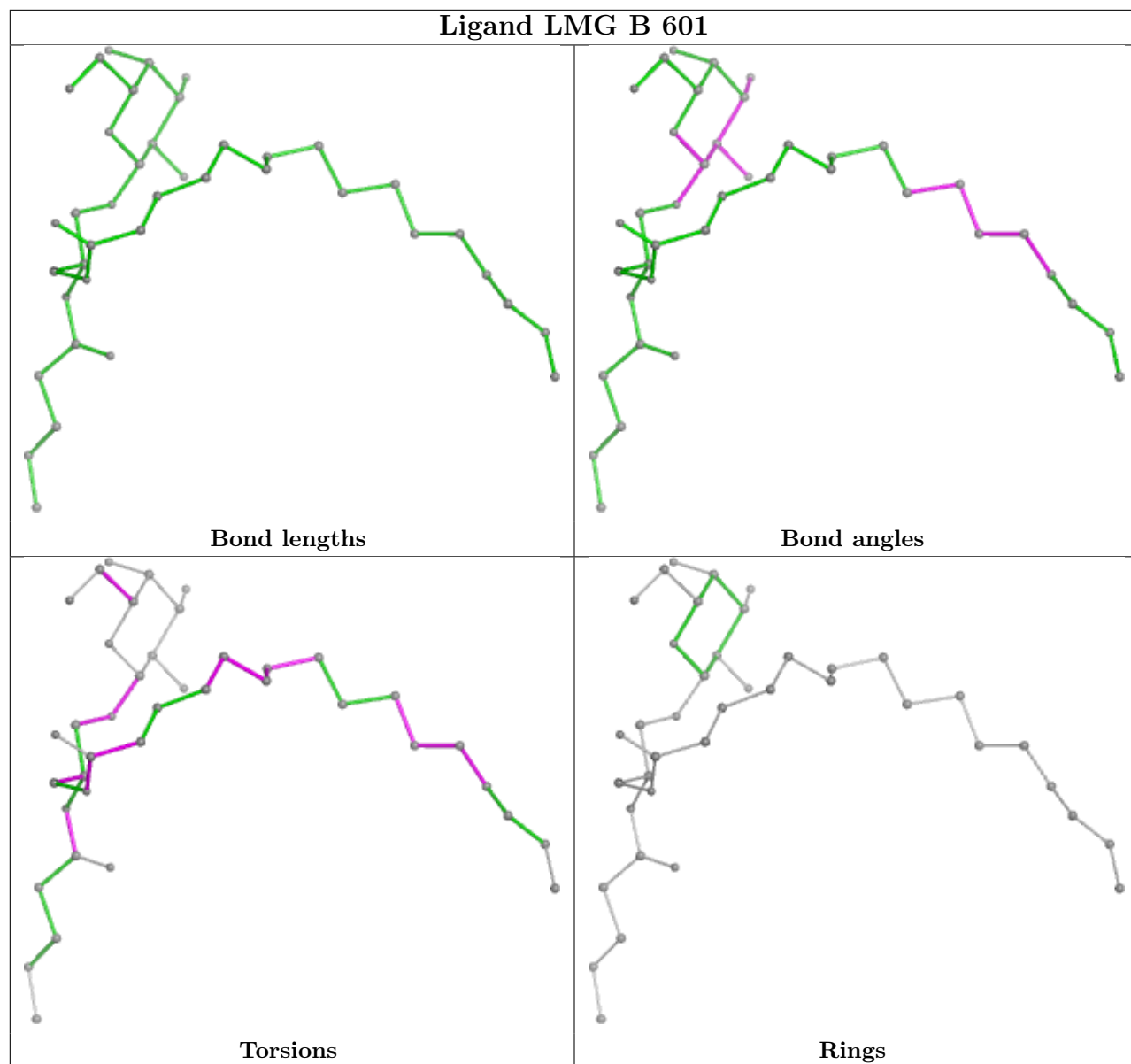
Rings



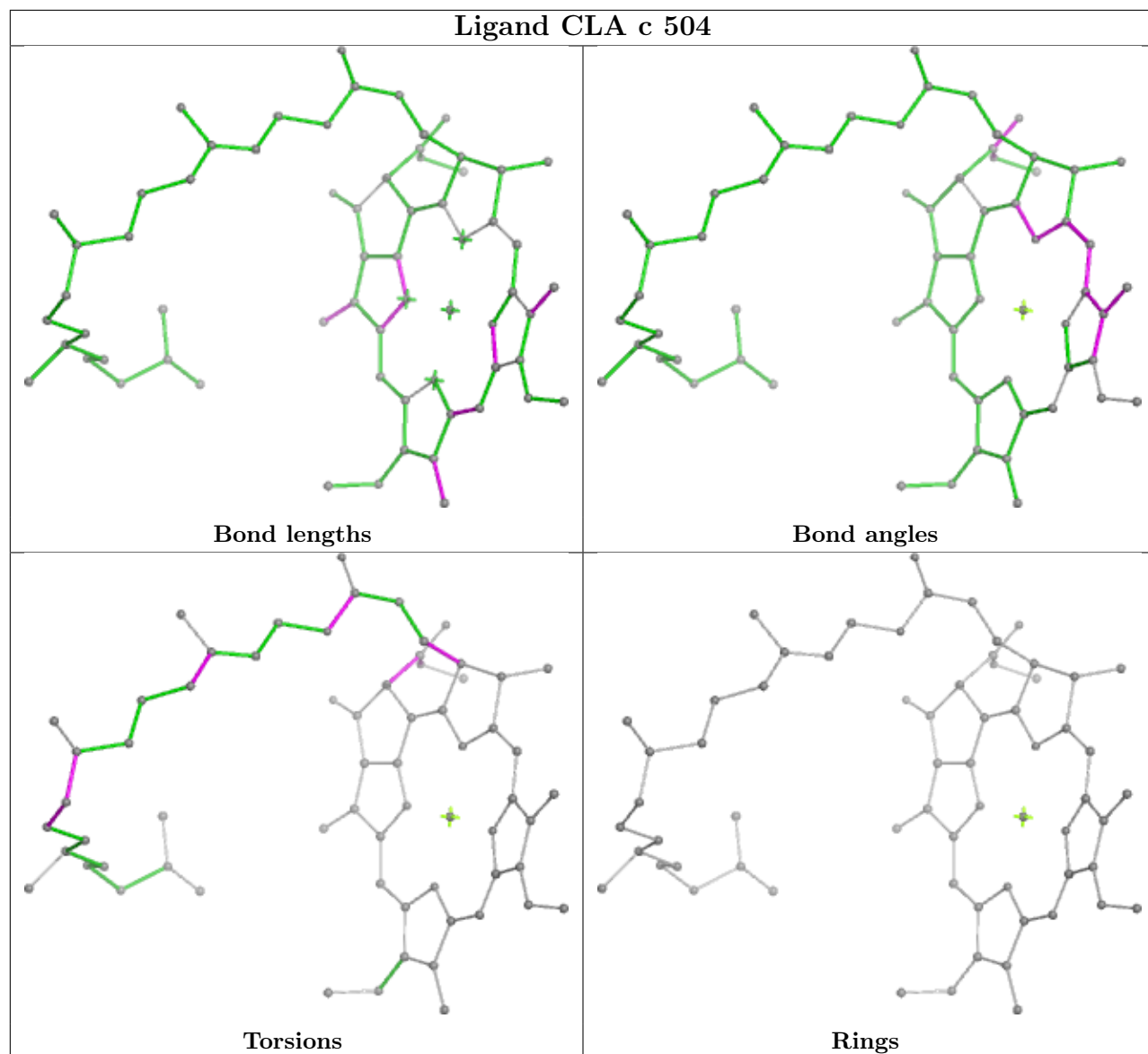


## Ligand CLA r 304

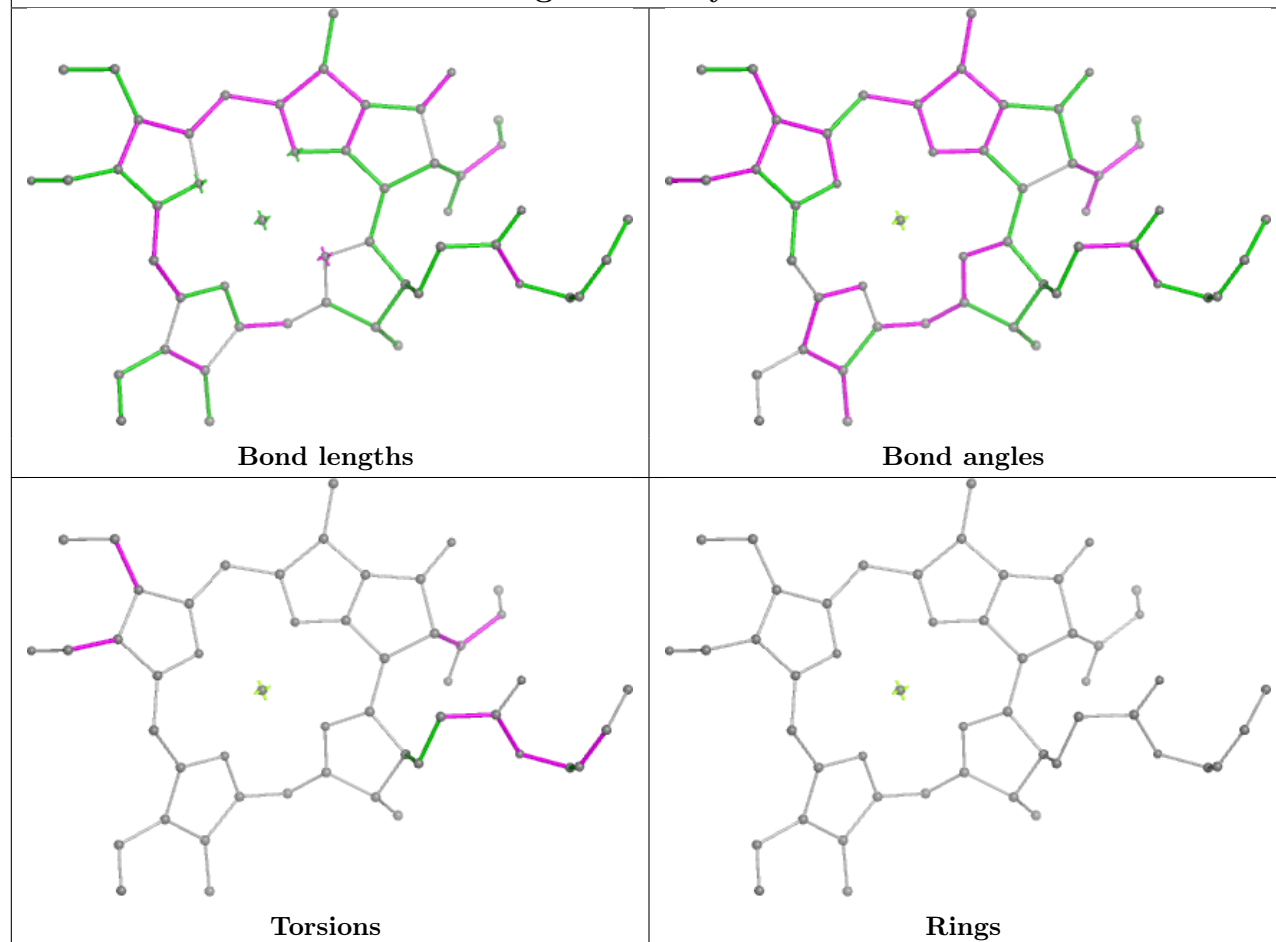




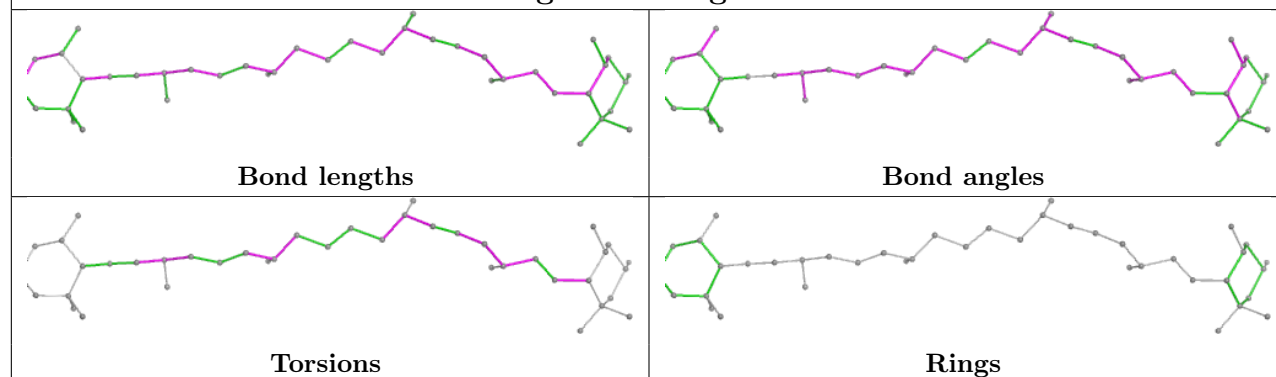
## Ligand CLA c 504

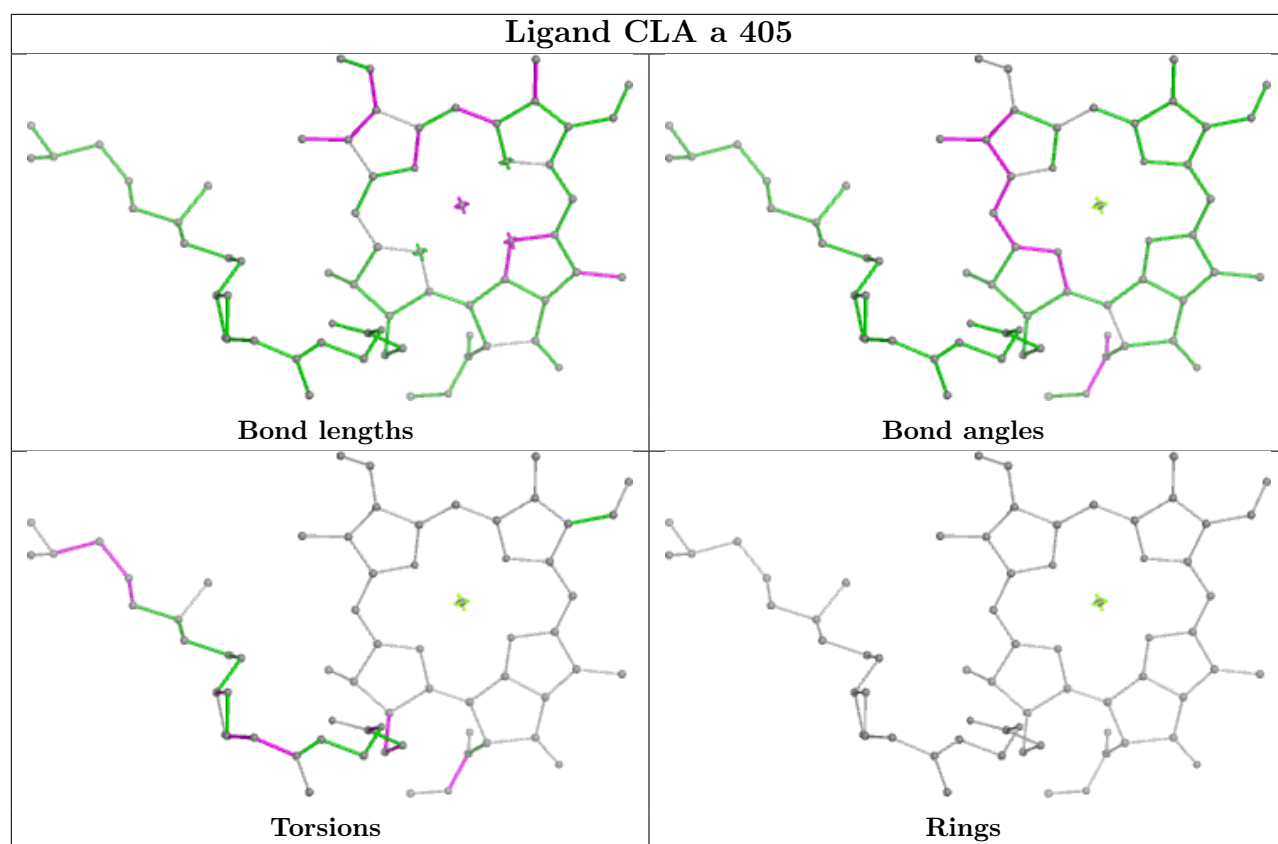


## Ligand CHL y 606

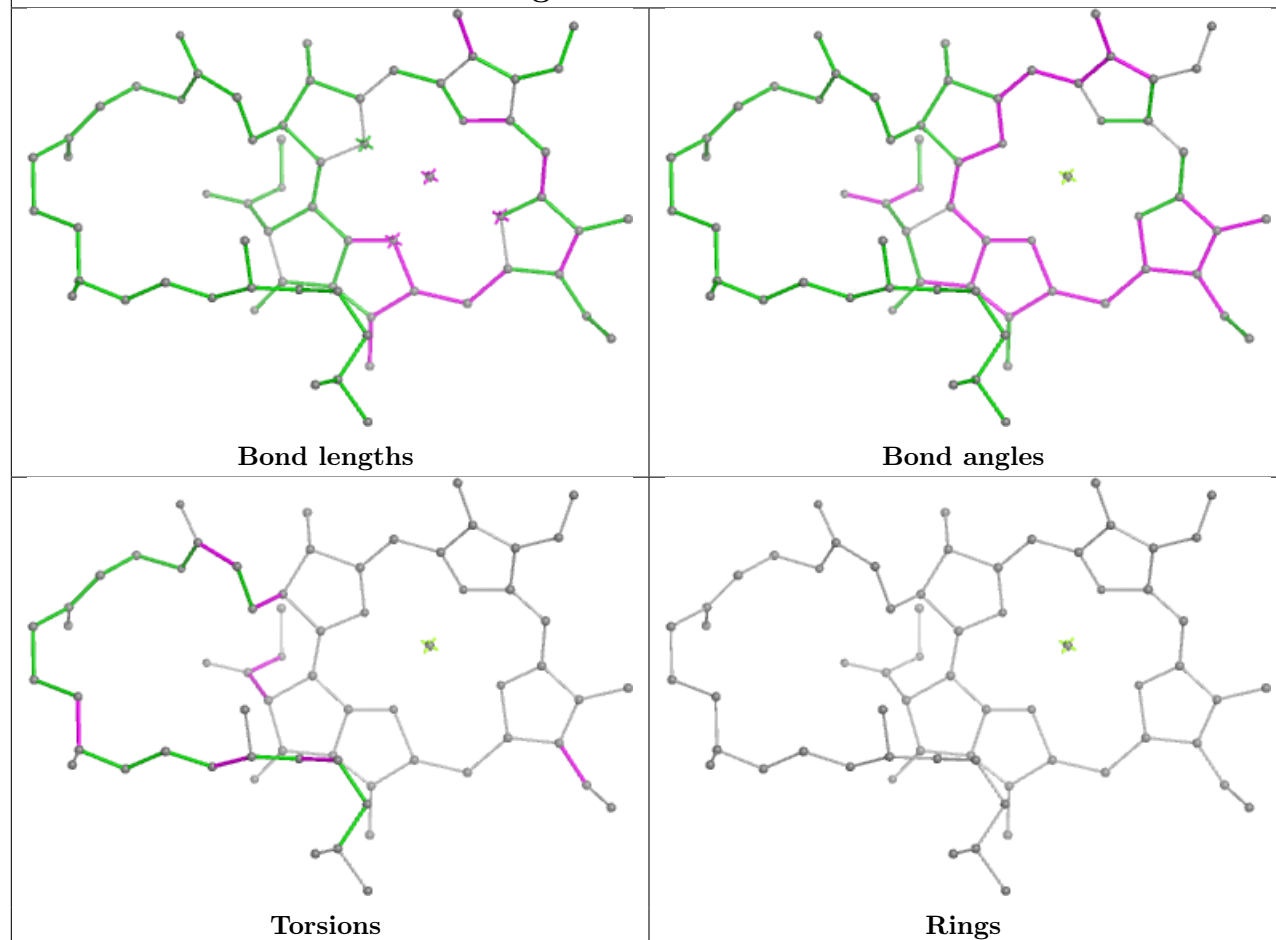


## Ligand LUT g 616

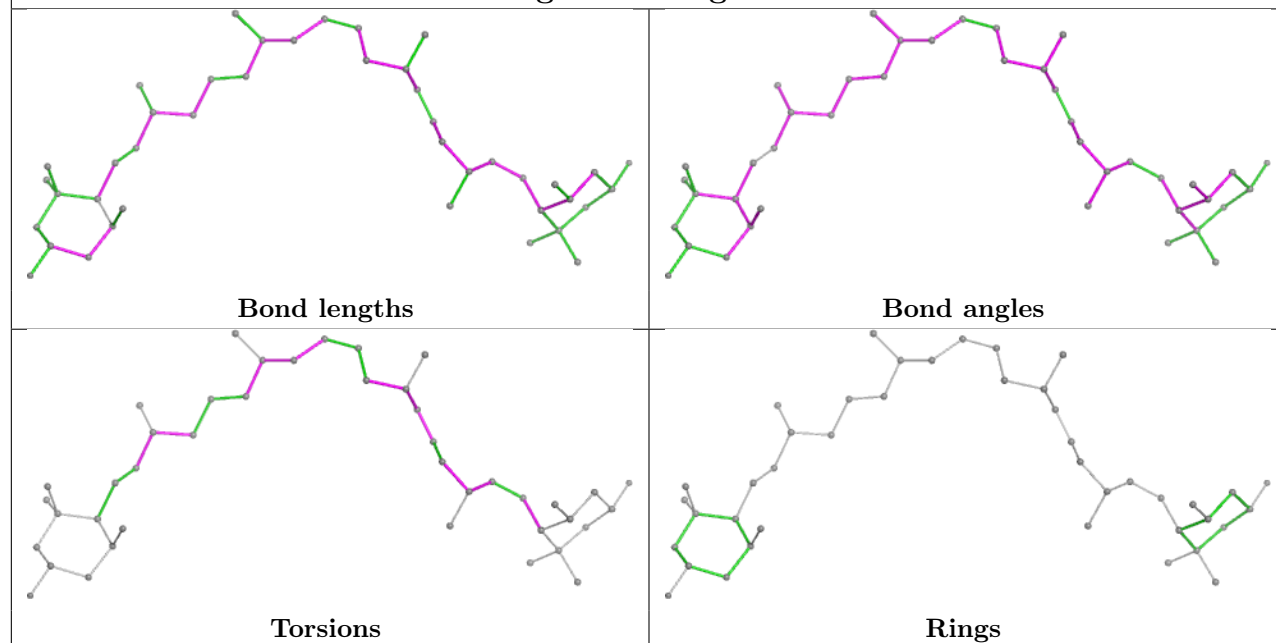


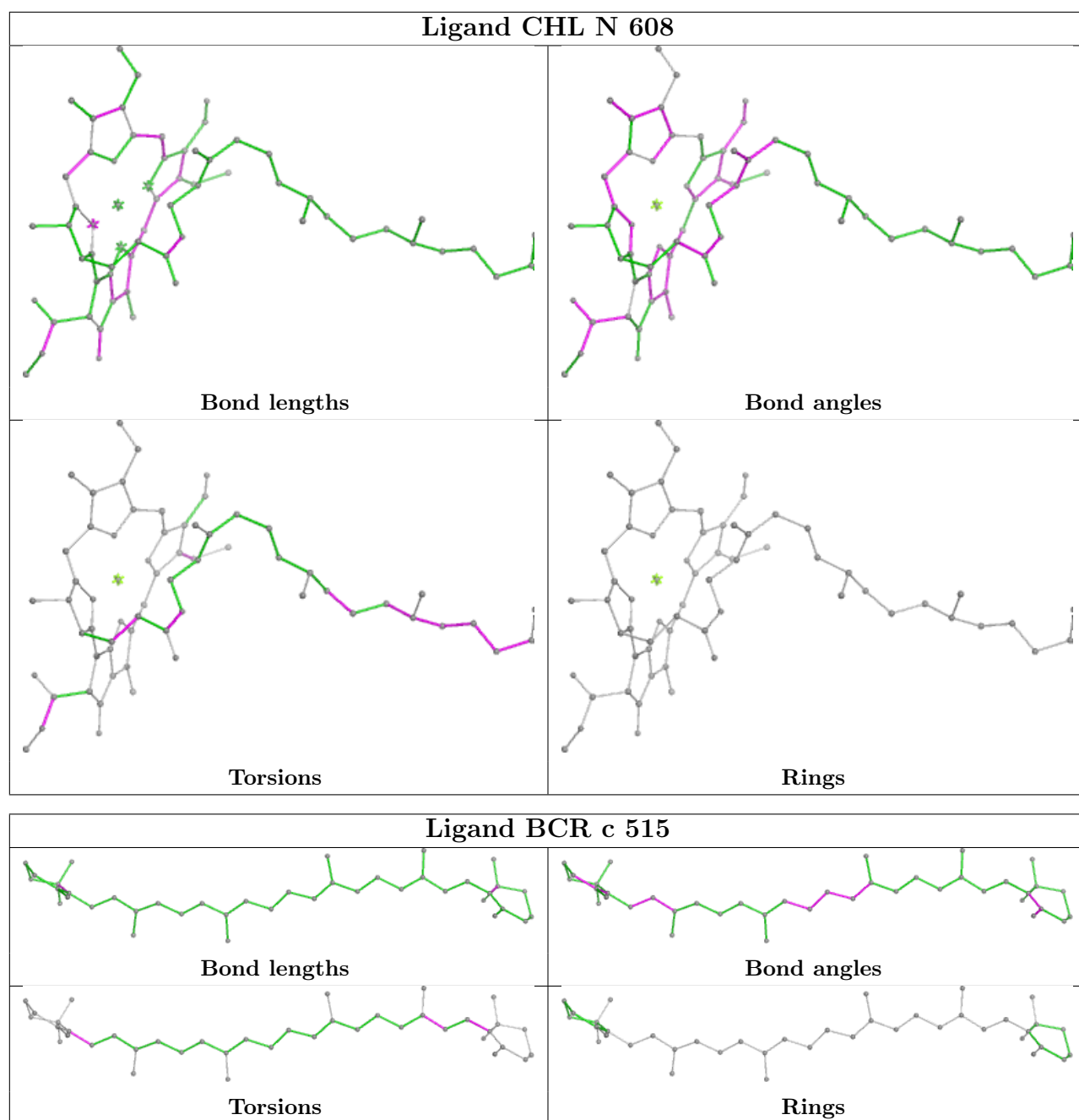


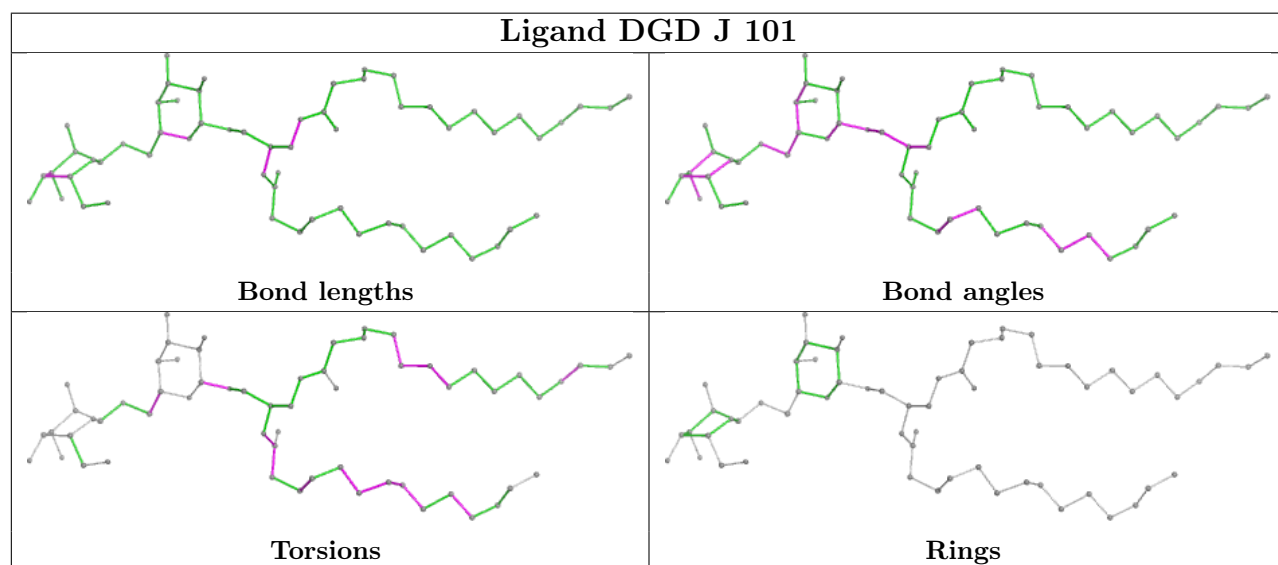
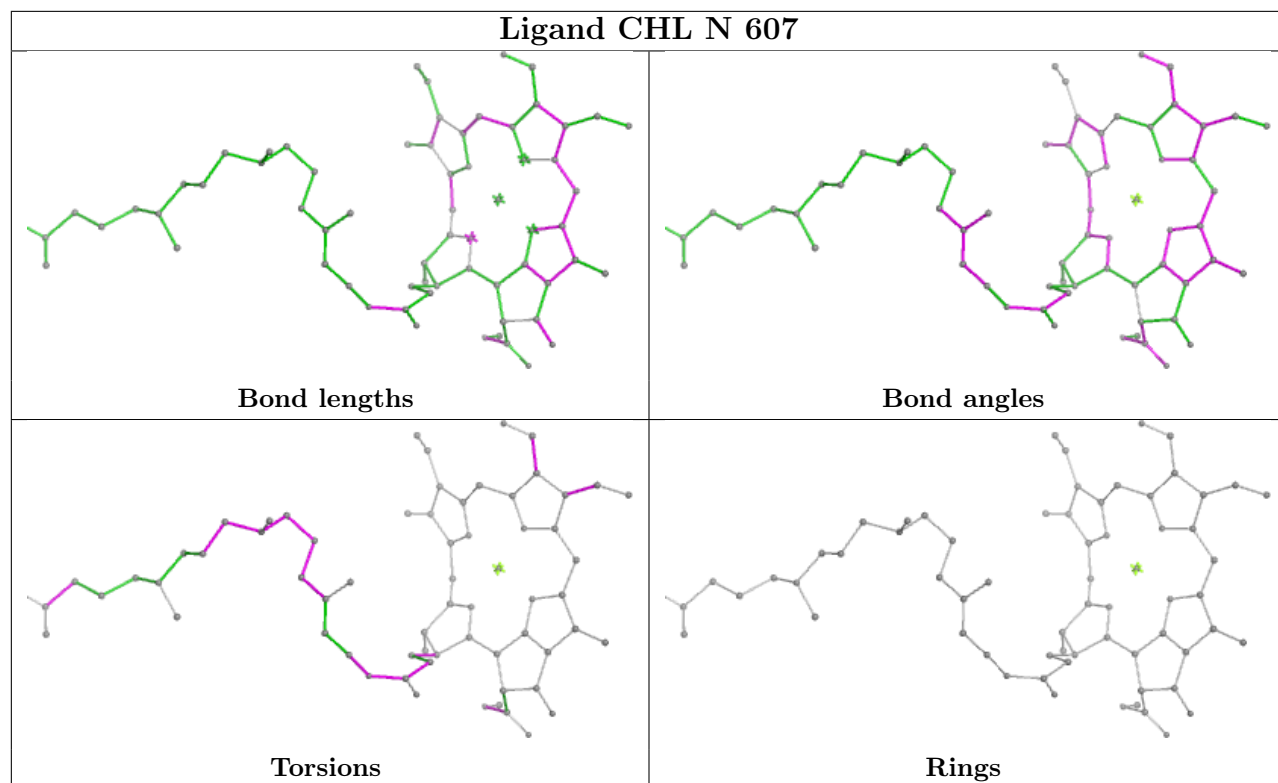
## Ligand CLA C 511

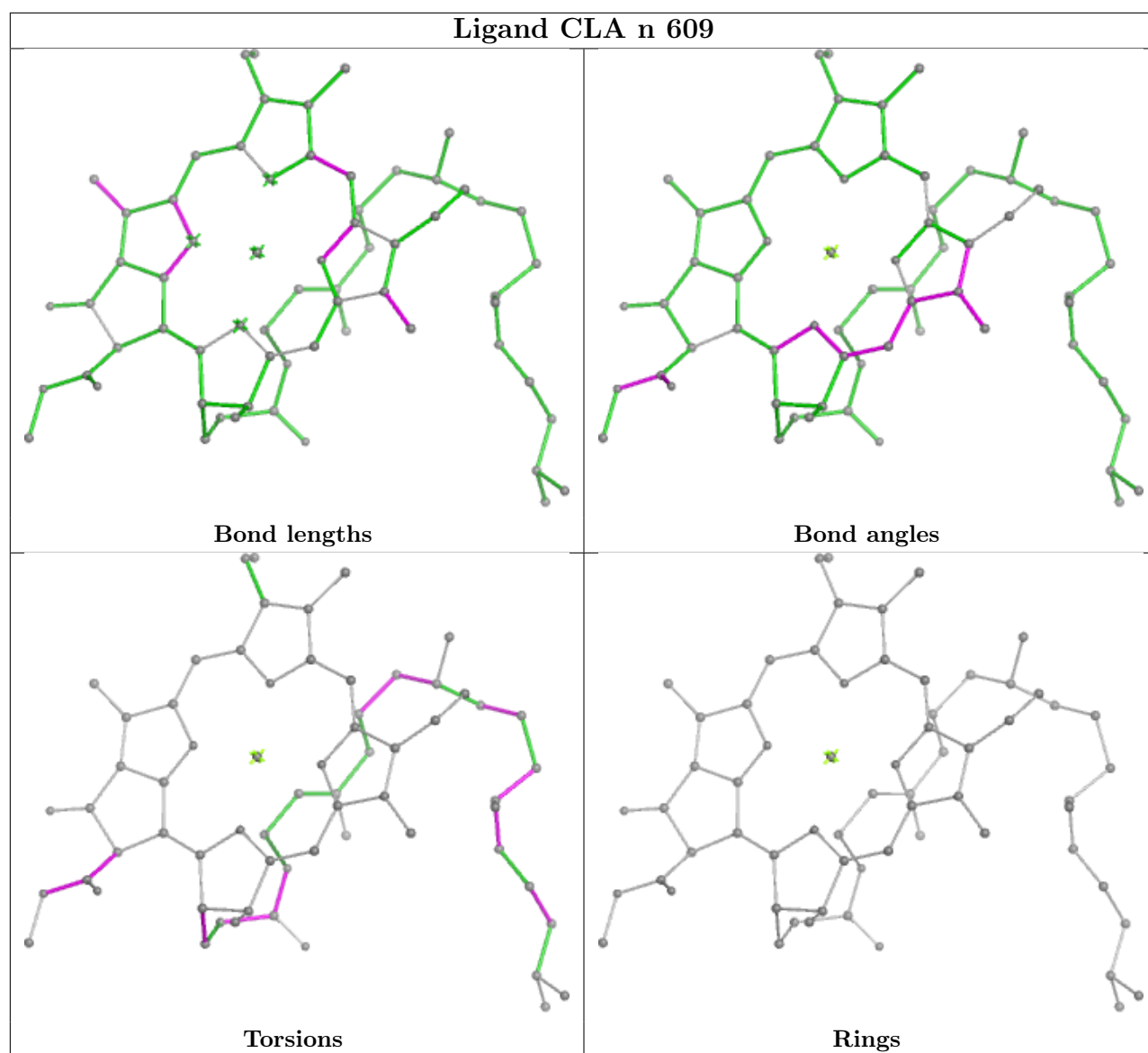


## Ligand LUT g 615









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

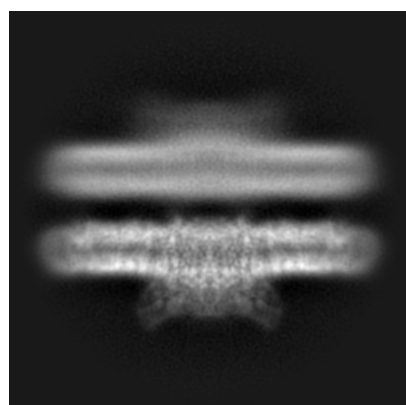
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10865. These allow visual inspection of the internal detail of the map and identification of artifacts.

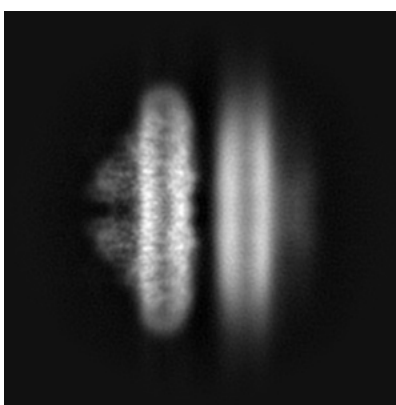
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

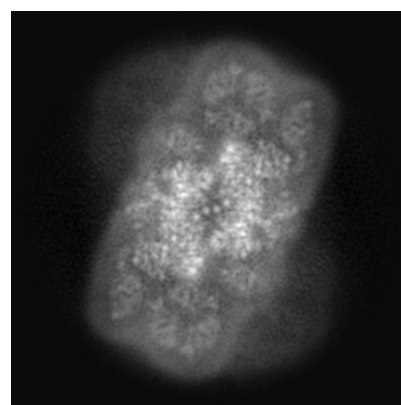
#### 6.1.1 Primary map



X



Y

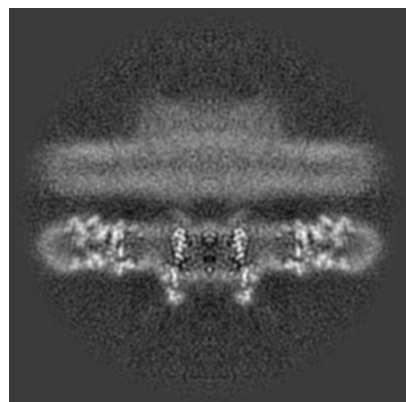


Z

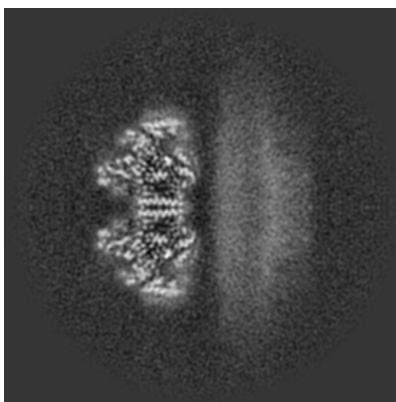
The images above show the map projected in three orthogonal directions.

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

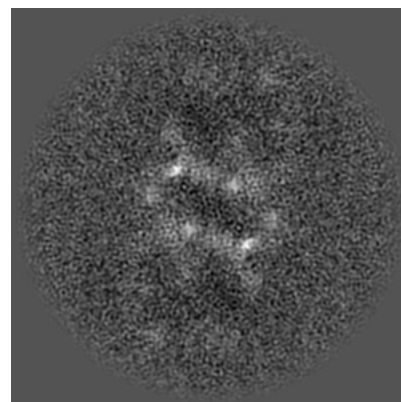
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

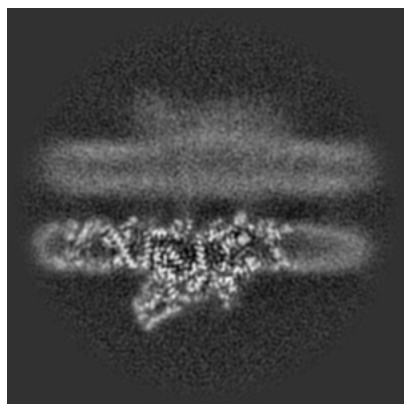


Z Index: 170

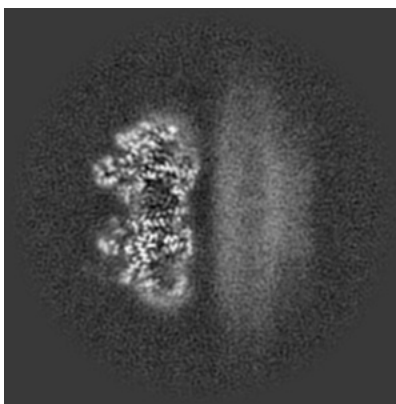
The images above show central slices of the map in three orthogonal directions.

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

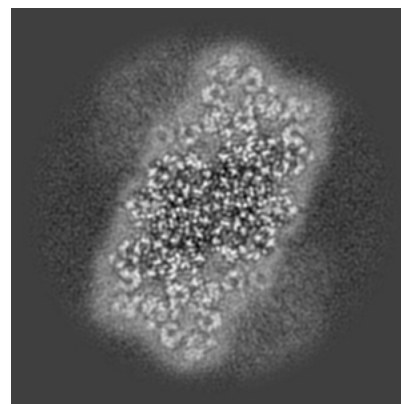
### 6.3.1 Primary map



X Index: 156



Y Index: 166

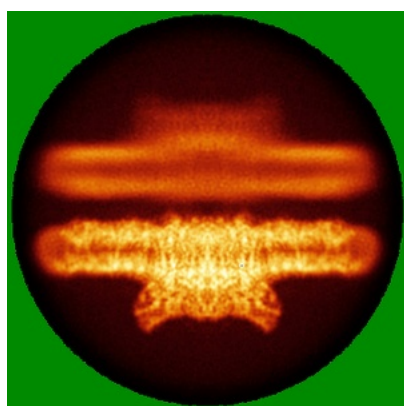


Z Index: 121

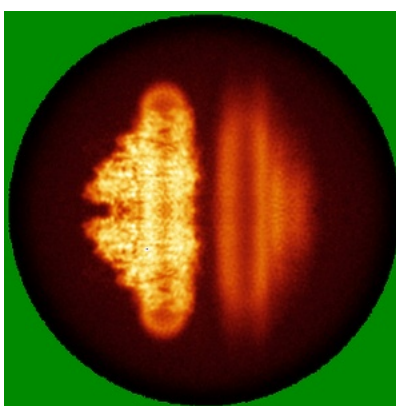
The images above show the largest variance slices of the map in three orthogonal directions.

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

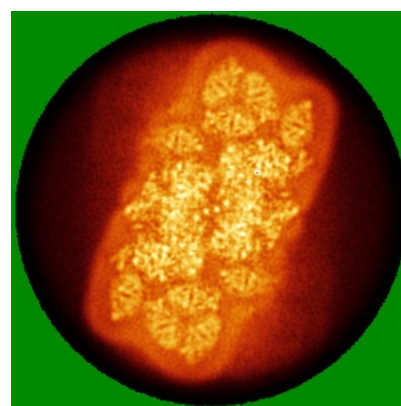
### 6.4.1 Primary map



X



Y

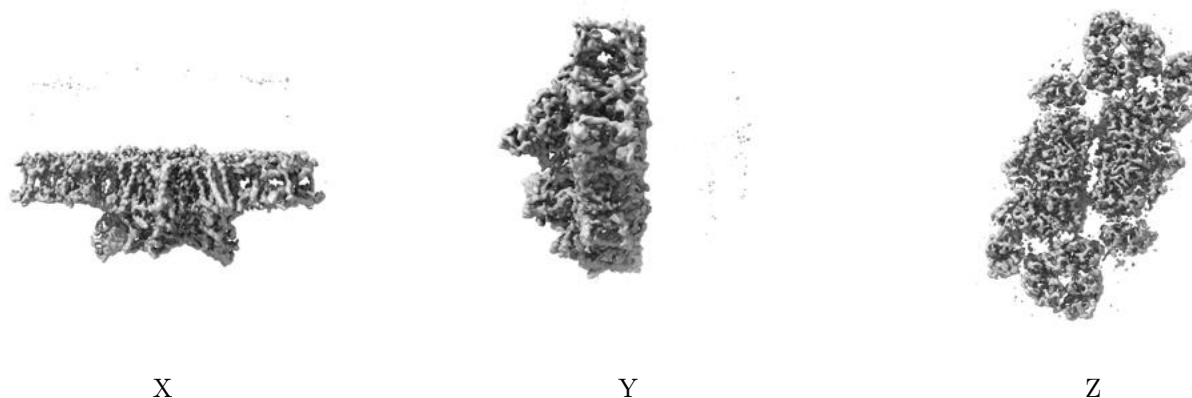


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

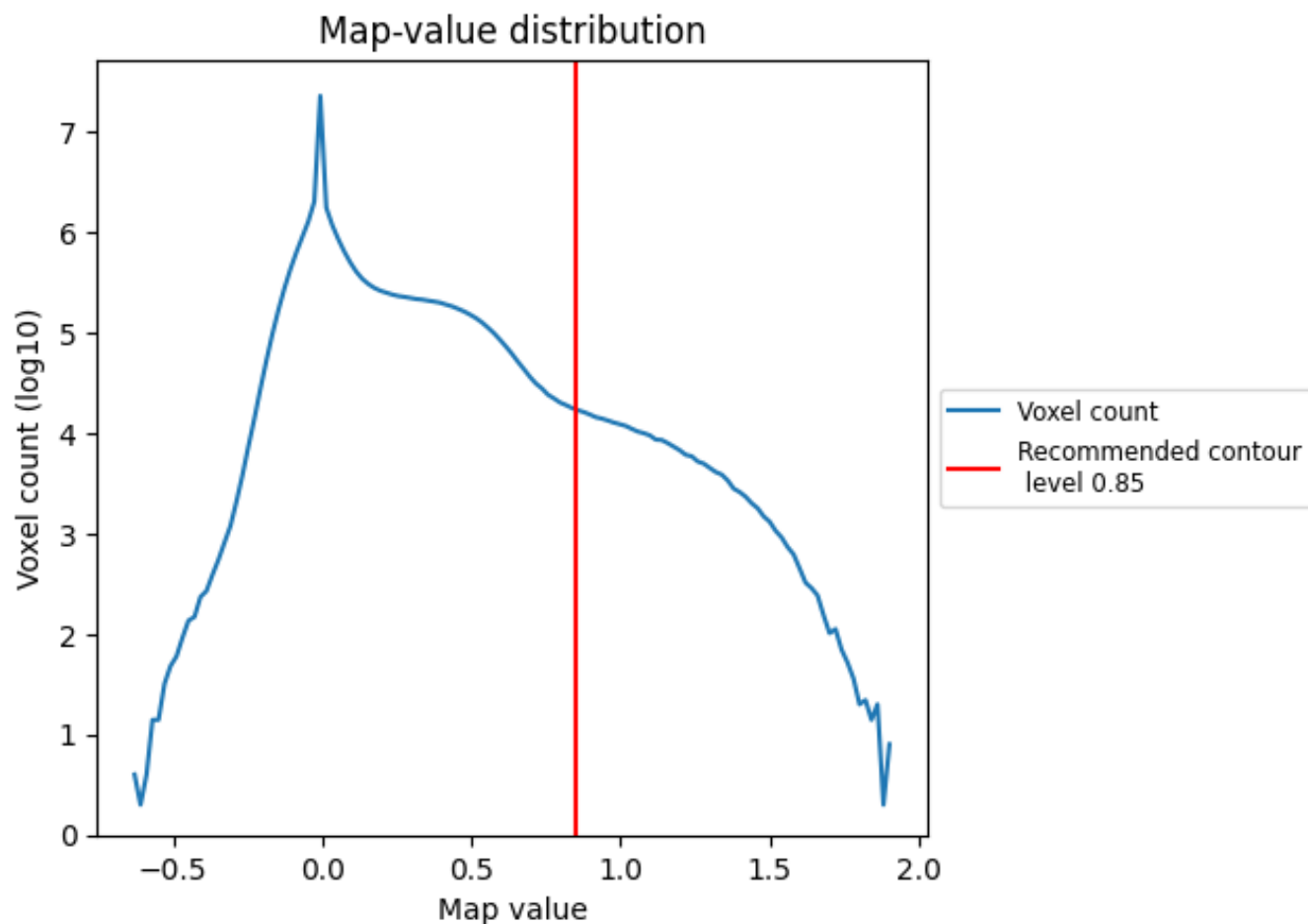
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

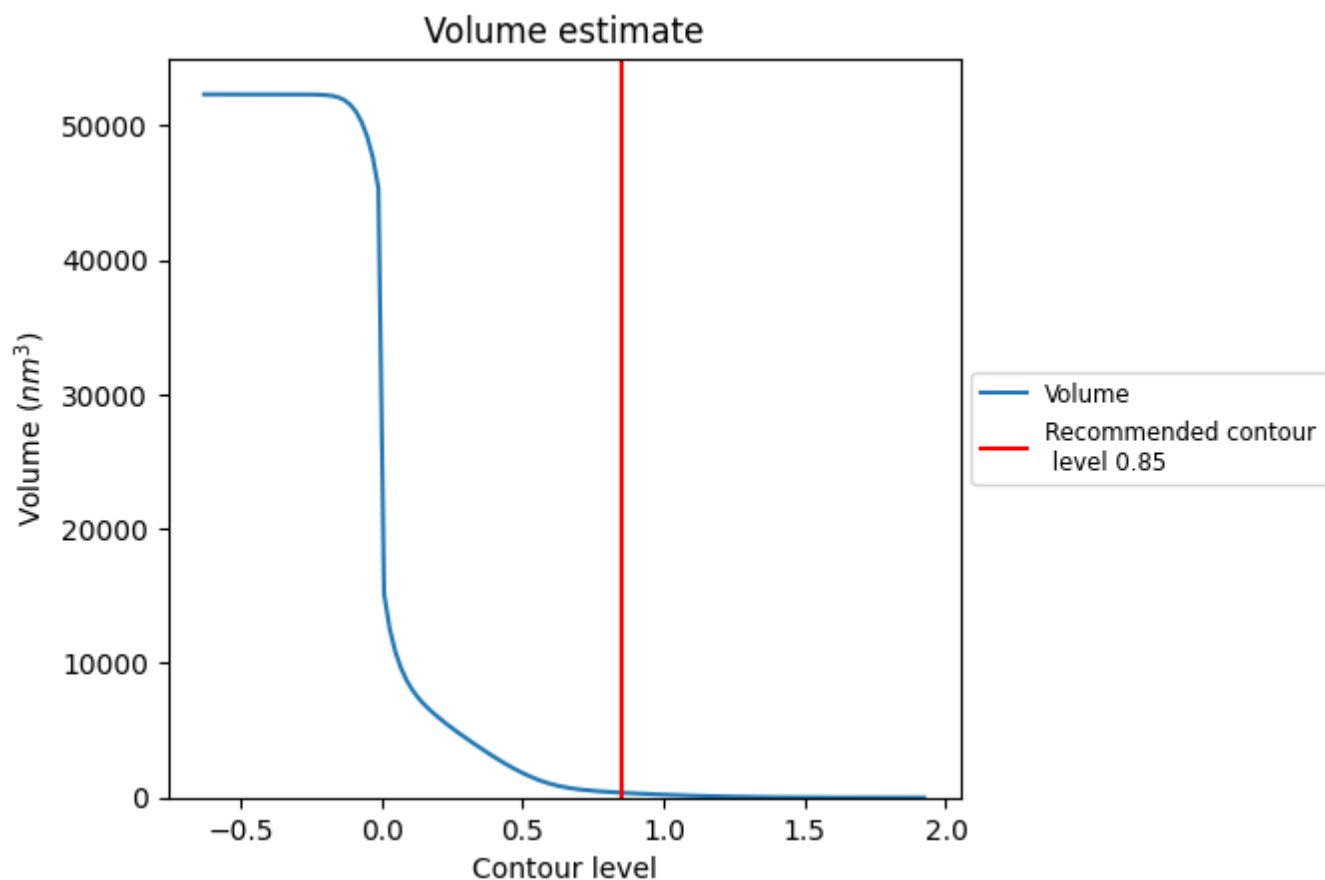
This section contains the results of statistical analysis of the map.

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



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

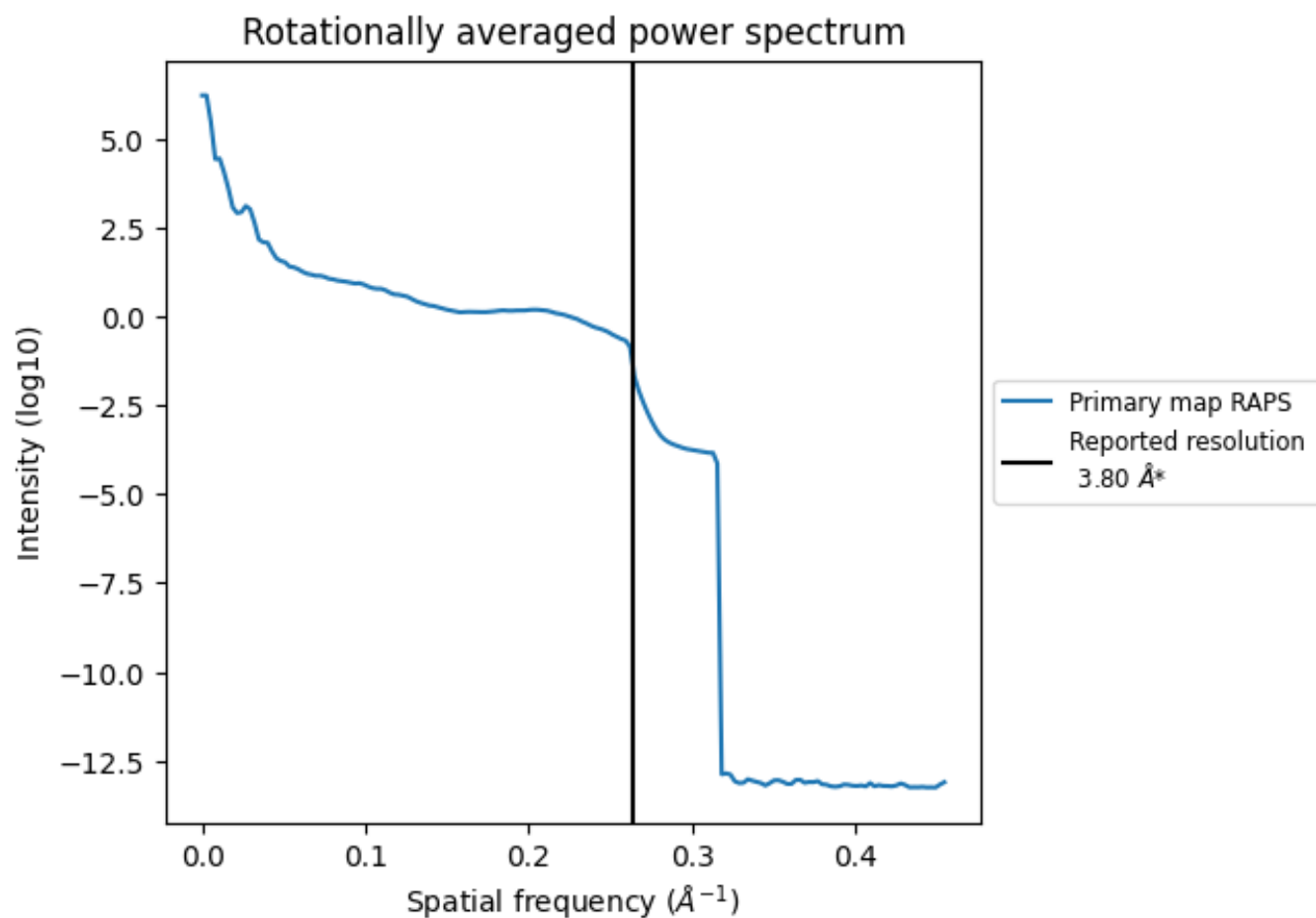
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm<sup>3</sup>; this corresponds to an approximate mass of 325 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

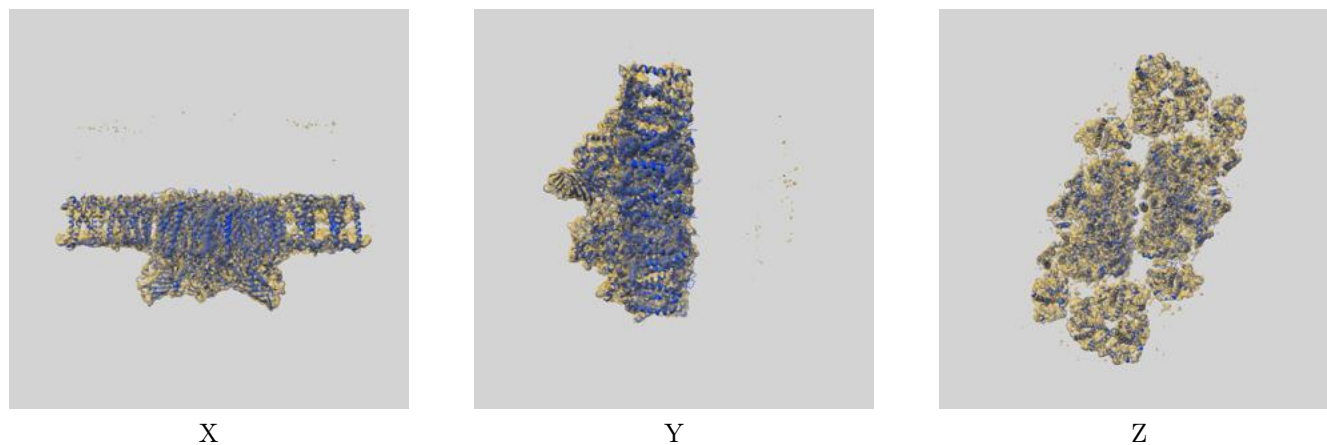
## 8 Fourier-Shell correlation

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

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

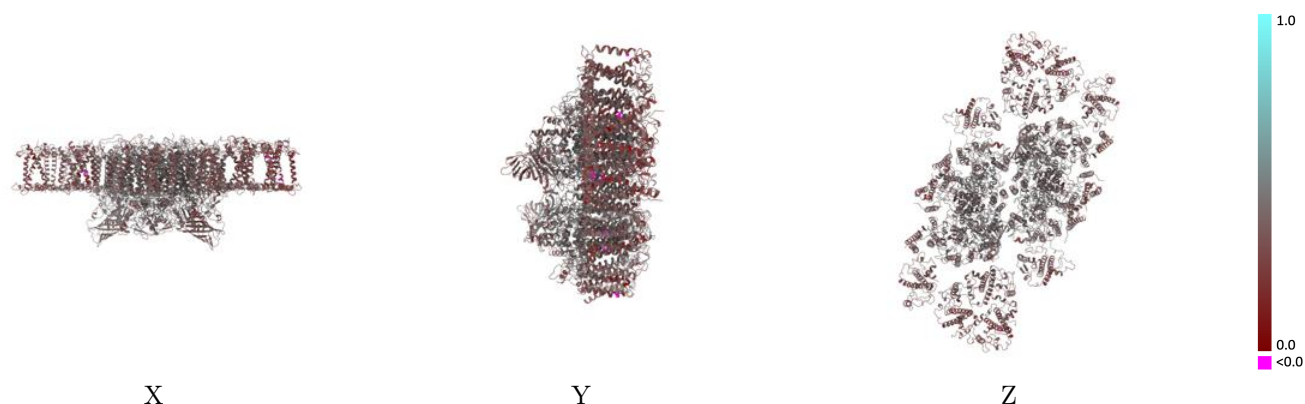
This section contains information regarding the fit between EMDB map EMD-10865 and PDB model 6YP7. Per-residue inclusion information can be found in section [3](#) on page [38](#).

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



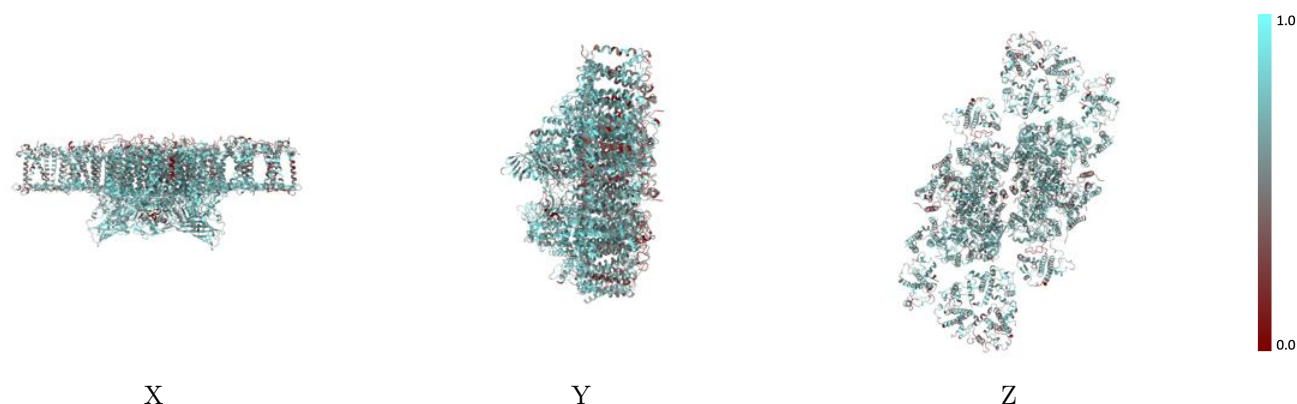
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



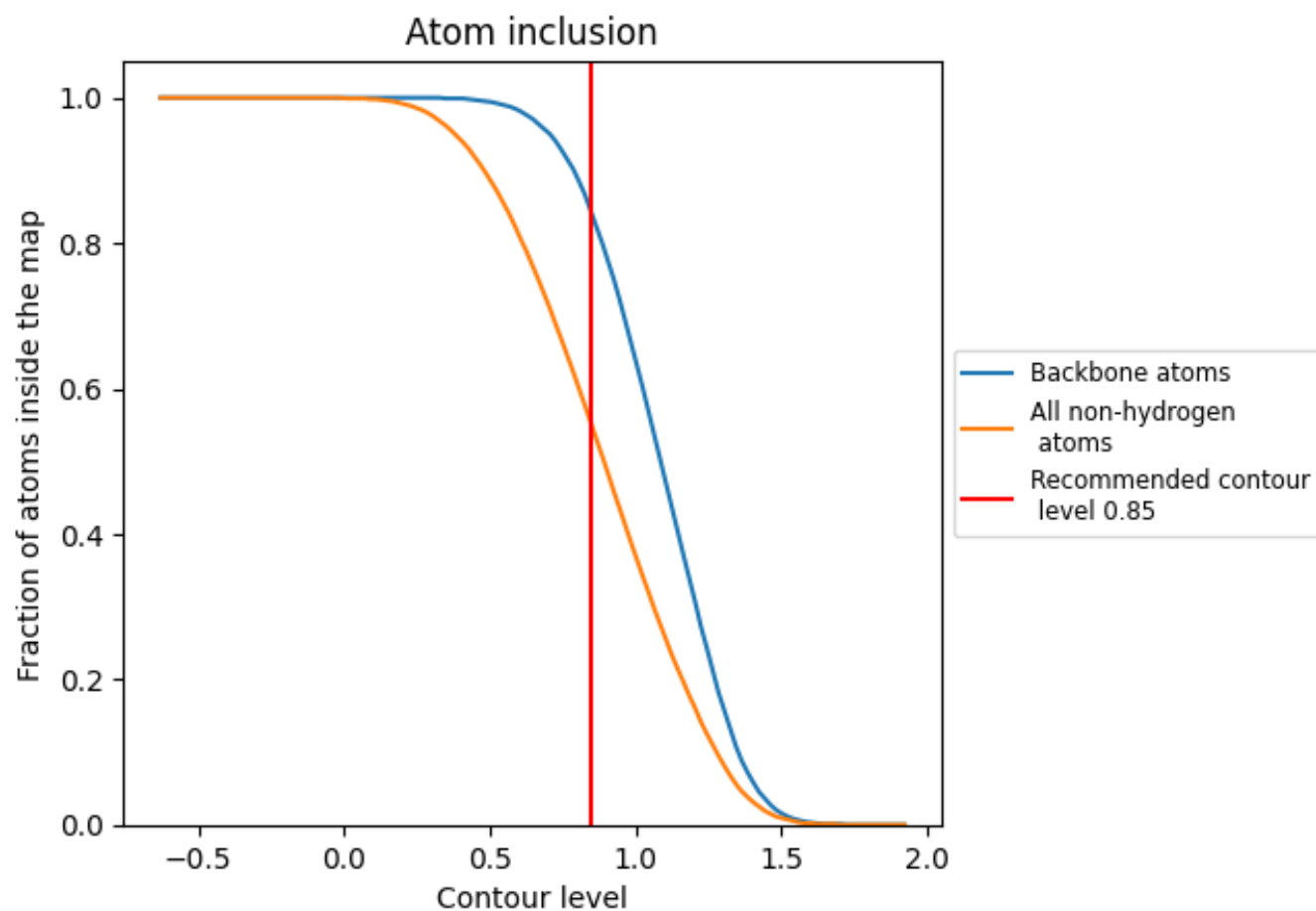
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.85).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 55% 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 (0.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5490	 0.3820
A	 0.6070	 0.4440
B	 0.6110	 0.4330
C	 0.6010	 0.4200
D	 0.5870	 0.4380
E	 0.6390	 0.3060
F	 0.5960	 0.3180
G	 0.4520	 0.2780
H	 0.5190	 0.3920
I	 0.5270	 0.4460
J	 0.2670	 0.3740
K	 0.4340	 0.4020
L	 0.4010	 0.4420
M	 0.3530	 0.3940
N	 0.4790	 0.2880
O	 0.5690	 0.4020
R	 0.4710	 0.3470
S	 0.5430	 0.3340
T	 0.3670	 0.4390
W	 0.4440	 0.3460
X	 0.5220	 0.3380
Y	 0.5450	 0.3440
Z	 0.5280	 0.3270
a	 0.6190	 0.4440
b	 0.6220	 0.4350
c	 0.6050	 0.4220
d	 0.5890	 0.4410
e	 0.6740	 0.3500
f	 0.5960	 0.3260
g	 0.4420	 0.2710
h	 0.5360	 0.4140
i	 0.6040	 0.4440
j	 0.2790	 0.3520
k	 0.4300	 0.4000
l	 0.3950	 0.4490



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
m	 0.4160	 0.3850
n	 0.4890	 0.2920
o	 0.5420	 0.3560
r	 0.4680	 0.3520
s	 0.5430	 0.3330
t	 0.4960	 0.4360
w	 0.4700	 0.4050
x	 0.5250	 0.3640
y	 0.5440	 0.3470
z	 0.5410	 0.3310