



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:18 PM UTC

PDB ID : 9IFM / pdb\_00009ifm  
EMDB ID : EMD-52846  
Title : STRUCTURE OF UNSTACKED C2S2-TYPE PSII-LHCII SUPERCOM-  
PLEX FROM PISUM SATIVUM  
Authors : Klaiman, D.; Fadeeva, M.; Kandiah, E.; Nelson, N.  
Deposited on : 2025-02-18  
Resolution : 2.20 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:

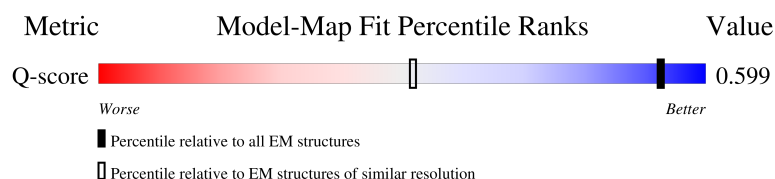
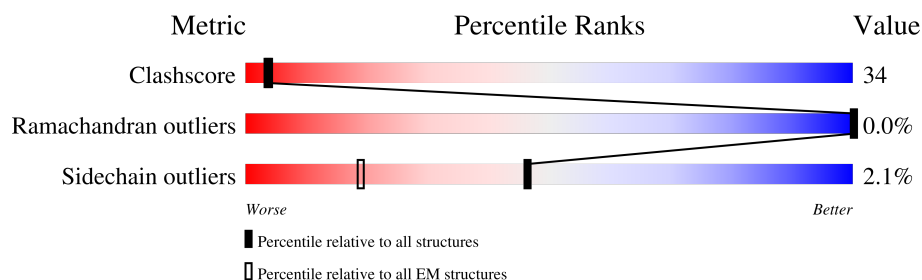
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 Å.

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







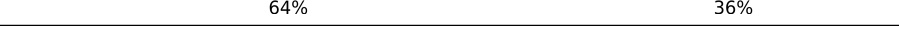
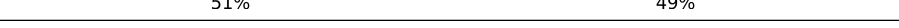

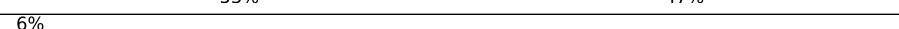
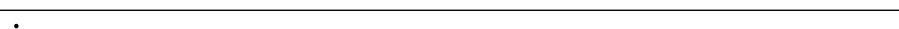
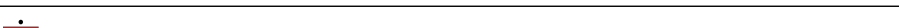




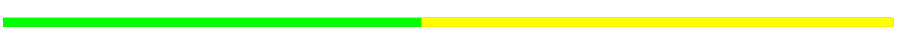



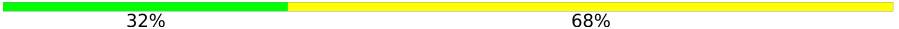






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 ( 1.71 - 2.70 )

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	A	334	
1	a	334	
2	B	503	
2	b	503	



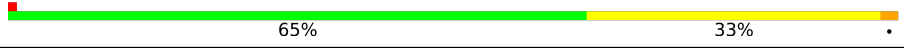
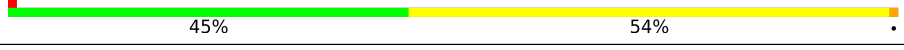



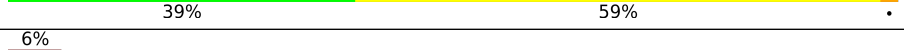
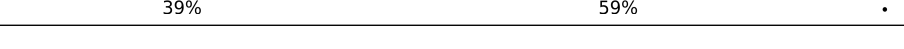
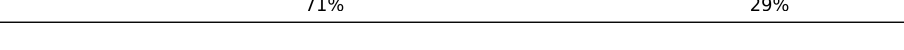

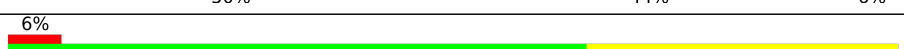









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Mol	Chain	Length	Quality of chain
3	C	450	
3	c	450	
4	D	352	
4	d	352	
5	E	75	
5	e	75	
6	F	30	
6	f	30	
7	G	216	
7	N	216	
7	g	216	
7	n	216	
8	H	60	
8	h	60	
9	I	34	
9	i	34	
10	J	35	
10	j	35	
11	K	37	
11	k	37	
12	L	36	
12	l	36	
13	M	33	
13	m	33	
14	O	248	

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Mol	Chain	Length	Quality of chain
14	o	248	
15	P	186	
15	p	186	
16	Q	148	
16	q	148	
17	R	224	
17	r	224	
18	S	218	
18	s	218	
19	T	31	
19	t	31	
20	W	54	
20	w	54	
21	X	39	
21	x	39	
22	Y	219	
22	y	219	
23	Z	61	
23	z	61	
24	U	28	
24	u	28	

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
28	CLA	A	405	X	-	-	-
28	CLA	A	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	408	X	-	-	-
28	CLA	B	601	X	-	-	-
28	CLA	B	602	X	-	-	-
28	CLA	B	603	X	-	X	-
28	CLA	B	604	X	-	-	-
28	CLA	B	605	X	-	-	-
28	CLA	B	606	X	-	-	-
28	CLA	B	607	X	-	-	-
28	CLA	B	608	X	-	-	-
28	CLA	B	609	X	-	-	-
28	CLA	B	610	X	-	-	-
28	CLA	B	611	X	-	-	-
28	CLA	B	612	X	-	-	-
28	CLA	B	613	X	-	-	-
28	CLA	B	614	X	-	-	-
28	CLA	B	615	X	-	-	-
28	CLA	B	616	X	-	-	-
28	CLA	C	501	X	-	-	-
28	CLA	C	502	X	-	-	-
28	CLA	C	503	X	-	-	-
28	CLA	C	504	X	-	-	-
28	CLA	C	505	X	-	-	-
28	CLA	C	506	X	-	X	-
28	CLA	C	507	X	-	X	-
28	CLA	C	508	X	-	-	-
28	CLA	C	509	X	-	-	-
28	CLA	C	510	X	-	-	-
28	CLA	C	511	X	-	-	-
28	CLA	C	512	X	-	-	-
28	CLA	C	513	X	-	-	-
28	CLA	D	401	X	-	-	-
28	CLA	D	403	X	-	-	-
28	CLA	D	404	X	-	-	-
28	CLA	G	602	X	-	-	-
28	CLA	G	603	X	-	-	-
28	CLA	G	604	X	-	-	-
28	CLA	G	610	X	-	X	-
28	CLA	G	611	X	-	-	-
28	CLA	G	612	X	-	-	-
28	CLA	G	613	X	-	X	-
28	CLA	G	614	X	-	-	-
28	CLA	N	602	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	N	603	X	-	-	-
28	CLA	N	604	X	-	-	-
28	CLA	N	610	X	-	-	-
28	CLA	N	611	X	-	-	-
28	CLA	N	612	X	-	-	-
28	CLA	N	613	X	-	-	-
28	CLA	N	614	X	-	-	-
28	CLA	R	601	X	-	-	-
28	CLA	R	602	X	-	-	-
28	CLA	R	603	X	-	-	-
28	CLA	R	604	X	-	-	-
28	CLA	R	608	X	-	-	-
28	CLA	R	609	X	-	-	-
28	CLA	R	610	X	-	-	-
28	CLA	R	611	X	-	-	-
28	CLA	R	612	X	-	-	-
28	CLA	R	613	X	-	-	-
28	CLA	S	303	X	-	X	-
28	CLA	S	304	X	-	-	-
28	CLA	S	305	X	-	-	-
28	CLA	S	309	X	-	-	-
28	CLA	S	310	X	-	X	-
28	CLA	S	311	X	-	-	-
28	CLA	S	312	X	-	-	-
28	CLA	S	313	X	-	-	-
28	CLA	S	314	X	-	-	-
28	CLA	Y	602	X	-	-	-
28	CLA	Y	603	X	-	-	-
28	CLA	Y	604	X	-	-	-
28	CLA	Y	610	X	-	-	-
28	CLA	Y	611	X	-	-	-
28	CLA	Y	612	X	-	-	-
28	CLA	Y	613	X	-	-	-
28	CLA	Y	614	X	-	-	-
28	CLA	a	406	X	-	-	-
28	CLA	a	407	X	-	-	-
28	CLA	a	409	X	-	-	-
28	CLA	b	601	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	604	X	-	-	-
28	CLA	b	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	b	606	X	-	-	-
28	CLA	b	607	X	-	-	-
28	CLA	b	608	X	-	-	-
28	CLA	b	609	X	-	-	-
28	CLA	b	610	X	-	-	-
28	CLA	b	611	X	-	-	-
28	CLA	b	612	X	-	-	-
28	CLA	b	613	X	-	-	-
28	CLA	b	614	X	-	-	-
28	CLA	b	615	X	-	-	-
28	CLA	b	616	X	-	-	-
28	CLA	c	501	X	-	-	-
28	CLA	c	502	X	-	-	-
28	CLA	c	503	X	-	-	-
28	CLA	c	504	X	-	-	-
28	CLA	c	505	X	-	-	-
28	CLA	c	506	X	-	-	-
28	CLA	c	507	X	-	-	-
28	CLA	c	508	X	-	-	-
28	CLA	c	509	X	-	-	-
28	CLA	c	510	X	-	-	-
28	CLA	c	511	X	-	-	-
28	CLA	c	512	X	-	-	-
28	CLA	c	513	X	-	-	-
28	CLA	d	401	X	-	-	-
28	CLA	d	404	X	-	-	-
28	CLA	d	405	X	-	-	-
28	CLA	g	602	X	-	-	-
28	CLA	g	603	X	-	-	-
28	CLA	g	604	X	-	-	-
28	CLA	g	610	X	-	-	-
28	CLA	g	611	X	-	-	-
28	CLA	g	612	X	-	-	-
28	CLA	g	613	X	-	-	-
28	CLA	g	614	X	-	-	-
28	CLA	n	602	X	-	-	-
28	CLA	n	603	X	-	X	-
28	CLA	n	604	X	-	-	-
28	CLA	n	610	X	-	X	-
28	CLA	n	611	X	-	-	-
28	CLA	n	612	X	-	-	-
28	CLA	n	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	n	614	X	-	-	-
28	CLA	r	601	X	-	-	-
28	CLA	r	602	X	-	-	-
28	CLA	r	603	X	-	-	-
28	CLA	r	604	X	-	-	-
28	CLA	r	608	X	-	-	-
28	CLA	r	609	X	-	-	-
28	CLA	r	610	X	-	-	-
28	CLA	r	611	X	-	-	-
28	CLA	r	612	X	-	-	-
28	CLA	r	613	X	-	-	-
28	CLA	s	602	X	-	-	-
28	CLA	s	603	X	-	-	-
28	CLA	s	604	X	-	-	-
28	CLA	s	608	X	-	-	-
28	CLA	s	609	X	-	-	-
28	CLA	s	610	X	-	-	-
28	CLA	s	611	X	-	-	-
28	CLA	s	612	X	-	-	-
28	CLA	s	613	X	-	-	-
28	CLA	y	303	X	-	-	-
28	CLA	y	304	X	-	X	-
28	CLA	y	305	X	-	-	-
28	CLA	y	310	X	-	-	-
28	CLA	y	311	X	-	-	-
28	CLA	y	312	X	-	-	-
28	CLA	y	313	X	-	-	-
28	CLA	y	314	X	-	-	-
30	BCR	B	619	-	-	X	-
30	BCR	C	514	-	X	-	-
30	BCR	C	516	-	-	X	-
30	BCR	a	410	-	-	X	-
35	LHG	S	317	-	-	X	-
36	DGD	C	518	-	-	X	-
38	CHL	G	601	X	-	-	-
38	CHL	G	605	X	-	-	-
38	CHL	G	606	X	-	-	-
38	CHL	G	607	X	-	-	-
38	CHL	G	608	X	-	-	-
38	CHL	G	609	X	-	-	-
38	CHL	N	601	X	-	-	-
38	CHL	N	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	CHL	N	606	X	-	-	-
38	CHL	N	607	X	-	-	-
38	CHL	N	608	X	-	-	-
38	CHL	N	609	X	-	-	-
38	CHL	R	605	X	-	-	-
38	CHL	R	606	X	-	-	-
38	CHL	R	607	X	-	-	-
38	CHL	S	302	X	-	-	-
38	CHL	S	306	X	-	-	-
38	CHL	S	307	X	-	-	-
38	CHL	S	308	X	-	-	-
38	CHL	Y	601	X	-	-	-
38	CHL	Y	605	X	-	-	-
38	CHL	Y	606	X	-	-	-
38	CHL	Y	607	X	-	X	-
38	CHL	Y	608	X	-	-	-
38	CHL	Y	609	X	-	-	-
38	CHL	g	601	X	-	X	-
38	CHL	g	605	X	-	-	-
38	CHL	g	606	X	-	-	-
38	CHL	g	607	X	-	-	-
38	CHL	g	608	X	-	-	-
38	CHL	g	609	X	-	-	-
38	CHL	g	619	X	-	-	-
38	CHL	n	601	X	-	-	-
38	CHL	n	605	X	-	-	-
38	CHL	n	606	X	-	-	-
38	CHL	n	607	X	-	X	-
38	CHL	n	608	X	-	-	-
38	CHL	n	609	X	-	X	-
38	CHL	r	605	X	-	-	-
38	CHL	r	606	X	-	-	-
38	CHL	r	607	X	-	-	-
38	CHL	s	601	X	-	-	-
38	CHL	s	605	X	-	-	-
38	CHL	s	606	X	-	-	-
38	CHL	s	607	X	-	-	-
38	CHL	y	302	X	-	-	-
38	CHL	y	306	X	-	-	-
38	CHL	y	307	X	-	-	-
38	CHL	y	308	X	-	-	-
38	CHL	y	309	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	LUT	G	615	-	-	X	-
39	LUT	S	315	-	-	X	-

## 2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 79416 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 Photosystem II protein D1.

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

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		
2	b	503	Total	C	N	O	S	0	0
			3939	2577	665	685	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
3	c	450	Total	C	N	O	S	0	0
			3496	2300	583	603	10		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		
4	d	352	Total	C	N	O	S	0	0
			2797	1845	458	482	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
6	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 7 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	216	Total	C	N	O	S	0	0
			1650	1069	267	309	5		
7	N	216	Total	C	N	O	S	0	0
			1649	1068	267	309	5		
7	g	216	Total	C	N	O	S	0	0
			1650	1069	267	309	5		
7	n	216	Total	C	N	O	S	0	0
			1650	1069	267	309	5		

- 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	S	0	0
			256	174	39	43			
10	j	35	Total	C	N	O	S	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	36	Total	C	N	O	S	0	0
			304	201	48	55			
12	l	36	Total	C	N	O	S	0	0
			304	201	48	55			

- 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		

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

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		
15	p	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1157	742	197	218			
16	q	148	Total	C	N	O	S	0	0
			1157	742	197	218			

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	224	Total	C	N	O	S	0	0
			1755	1142	285	325	3		
17	r	224	Total	C	N	O	S	0	0
			1755	1142	285	325	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	31	Total	C	N	O	S	0	0
			252	176	35	40	1		
19	t	31	Total	C	N	O	S	0	0
			252	176	35	40	1		

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

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

- Molecule 21 is a protein called Ultraviolet-B-repressible protein.

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

- Molecule 22 is a protein called Chlorophyll a-b binding protein AB80, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		
22	y	219	Total	C	N	O	S	0	0
			1667	1081	270	311	5		

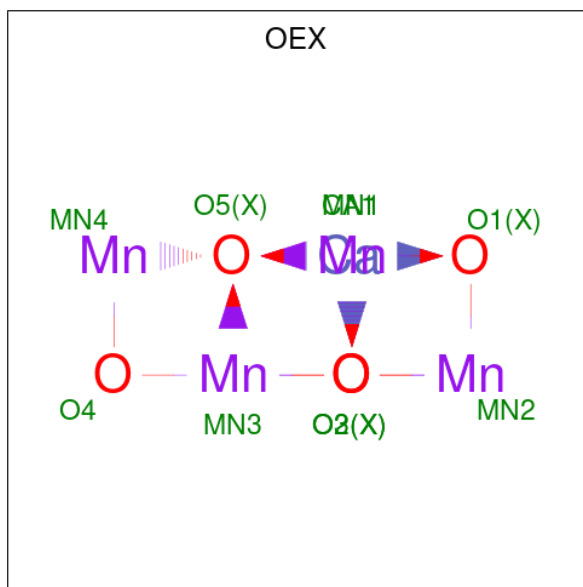
- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		
23	z	61	Total	C	N	O	S	0	0
			457	309	68	79	1		

- Molecule 24 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	28	Total	C	N	O	S	0	0
			212	131	41	37	3		
24	u	28	Total	C	N	O	S	0	0
			212	131	41	37	3		

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

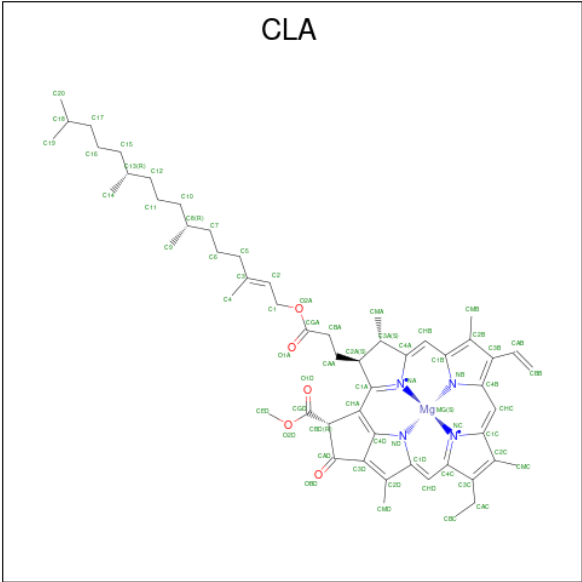
- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 28 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
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
28	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	N	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	R	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	c	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	g	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

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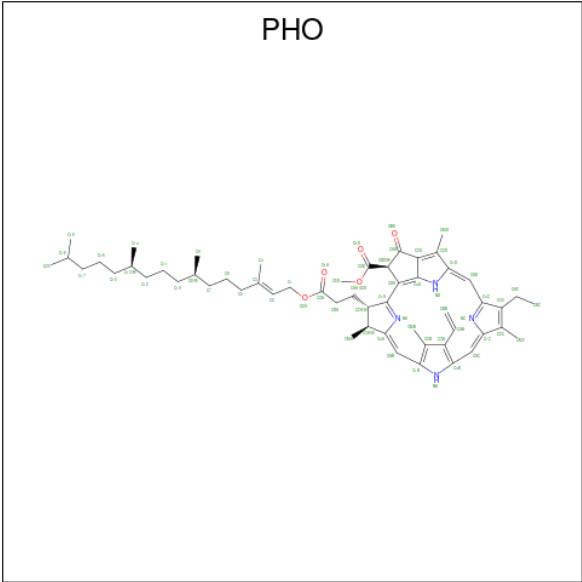
Mol	Chain	Residues	Atoms					AltConf
28	g	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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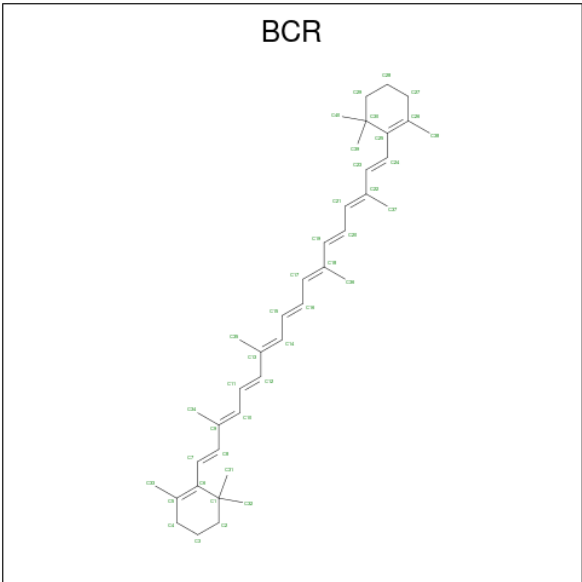
Mol	Chain	Residues	Atoms					AltConf
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	y	1	Total 48	C 38	Mg 1	N 4	O 5	0

- Molecule 29 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



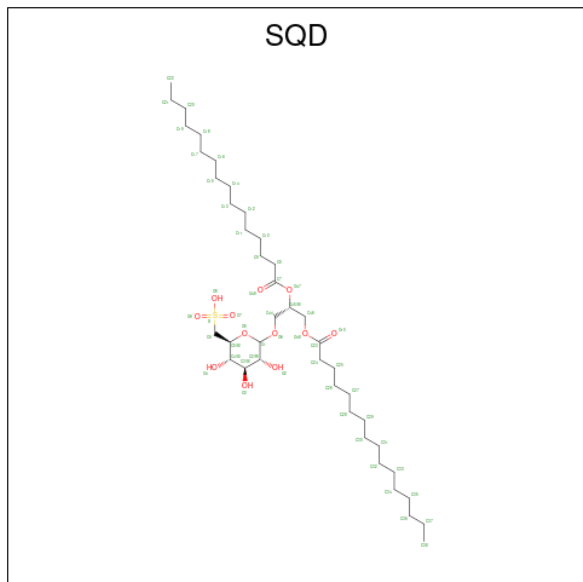
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	D	1	Total	C	N	O	0
			64	55	4	5	
29	a	1	Total	C	N	O	0
			64	55	4	5	
29	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



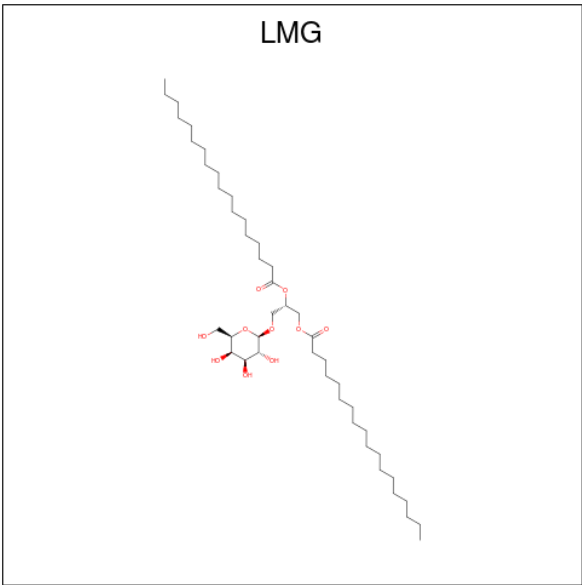
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	a	1	Total C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

- Molecule 31 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
31	A	1	Total	C	O	S	0
			50	37	12	1	
31	A	1	Total	C	O	S	0
			54	41	12	1	
31	B	1	Total	C	O	S	0
			54	41	12	1	
31	L	1	Total	C	O	S	0
			42	29	12	1	
31	L	1	Total	C	O	S	0
			54	41	12	1	
31	M	1	Total	C	O	S	0
			42	29	12	1	
31	a	1	Total	C	O	S	0
			50	37	12	1	
31	a	1	Total	C	O	S	0
			54	41	12	1	

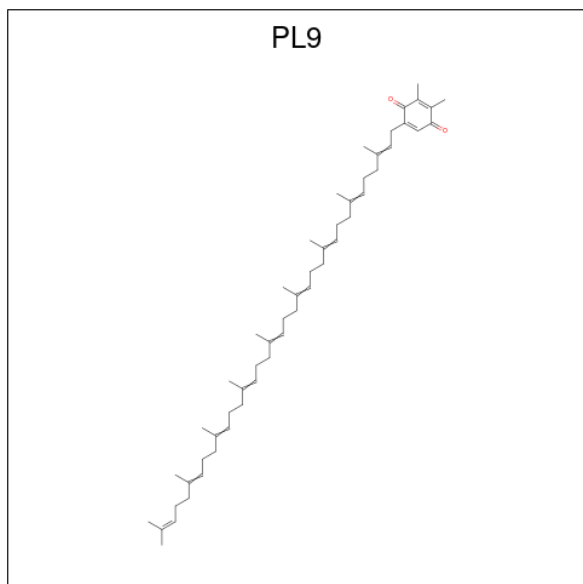
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			48	38	10	
32	A	1	Total	C	O	0
			40	30	10	
32	B	1	Total	C	O	0
			51	41	10	
32	B	1	Total	C	O	0
			31	21	10	
32	C	1	Total	C	O	0
			51	41	10	
32	C	1	Total	C	O	0
			44	34	10	
32	D	1	Total	C	O	0
			46	36	10	
32	a	1	Total	C	O	0
			40	30	10	
32	b	1	Total	C	O	0
			51	41	10	
32	b	1	Total	C	O	0
			50	40	10	
32	c	1	Total	C	O	0
			51	41	10	
32	d	1	Total	C	O	0
			46	36	10	
32	k	1	Total	C	O	0
			51	41	10	
32	w	1	Total	C	O	0
			48	38	10	

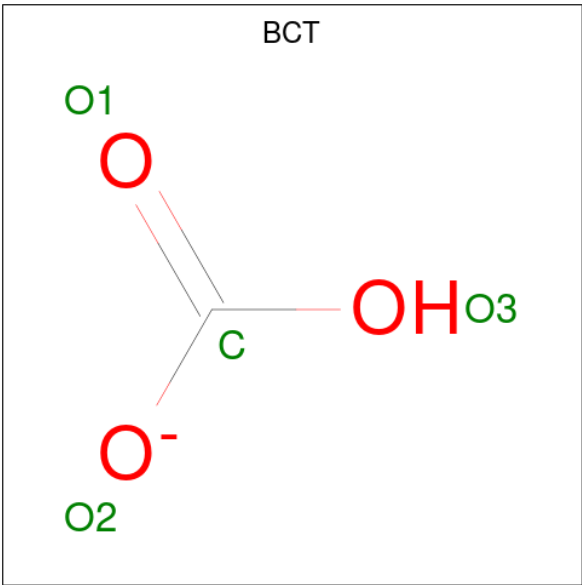


- Molecule 33 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



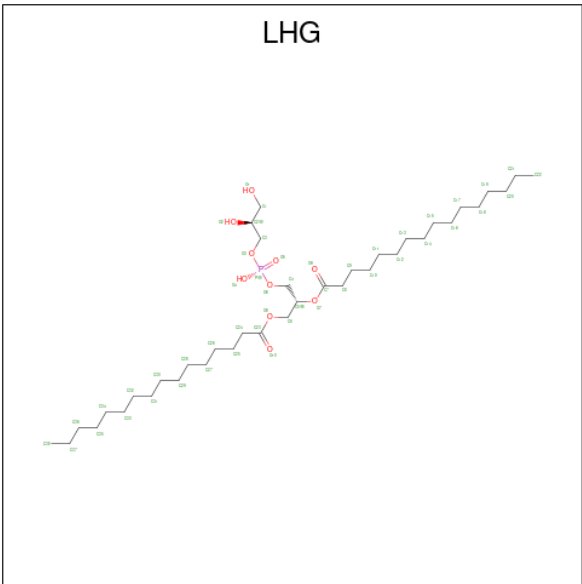
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			13	11	2	
33	D	1	Total	C	O	0
			55	53	2	
33	a	1	Total	C	O	0
			13	11	2	
33	d	1	Total	C	O	0
			55	53	2	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $CHO_3$ ).



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 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
35	A	1	Total	C	O	P	0
			43	32	10	1	

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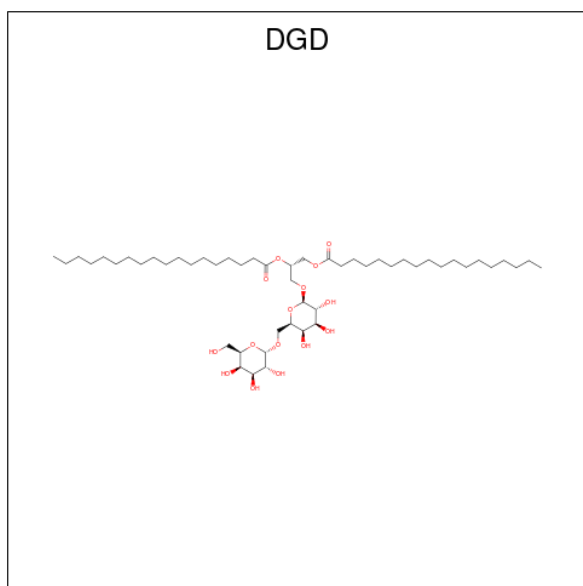
Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			30	19	10	1	
35	B	1	Total	C	O	P	0
			41	30	10	1	
35	B	1	Total	C	O	P	0
			46	35	10	1	
35	C	1	Total	C	O	P	0
			49	38	10	1	
35	D	1	Total	C	O	P	0
			49	38	10	1	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			31	20	10	1	
35	R	1	Total	C	O	P	0
			25	14	10	1	
35	S	1	Total	C	O	P	0
			34	23	10	1	
35	S	1	Total	C	O	P	0
			43	32	10	1	
35	W	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			43	32	10	1	
35	b	1	Total	C	O	P	0
			34	23	10	1	
35	b	1	Total	C	O	P	0
			41	30	10	1	
35	b	1	Total	C	O	P	0
			46	35	10	1	
35	c	1	Total	C	O	P	0
			32	21	10	1	
35	c	1	Total	C	O	P	0
			40	29	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	g	1	Total	C	O	P	0
			41	30	10	1	

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Mol	Chain	Residues	Atoms				AltConf
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			32	21	10	1	
35	r	1	Total	C	O	P	0
			30	19	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	w	1	Total	C	O	P	0
			39	28	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



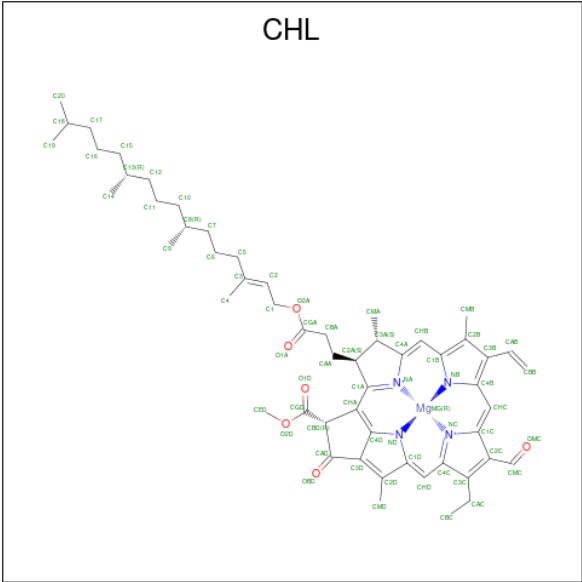
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			59	44	15	
36	B	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			55	40	15	
36	C	1	Total	C	O	0
			62	47	15	
36	C	1	Total	C	O	0
			60	45	15	

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Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total 59	C 44	O 15	0
36	b	1	Total 62	C 47	O 15	0
36	c	1	Total 55	C 40	O 15	0
36	c	1	Total 54	C 39	O 15	0
36	c	1	Total 59	C 44	O 15	0

- # HEM

- Molecule 38 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $\text{C}_{55}\text{H}_{70}\text{MgN}_4\text{O}_6$ ).



Mol	Chain	Residues	Atoms					AltConf
38	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
38	G	1	Total 56	C 45	Mg 1	N 4	O 6	0
38	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	G	1	Total 55	C 44	Mg 1	N 4	O 6	0
38	N	1	Total 52	C 41	Mg 1	N 4	O 6	0
38	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
38	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
38	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	N	1	Total 65	C 54	Mg 1	N 4	O 6	0
38	R	1	Total 47	C 36	Mg 1	N 4	O 6	0
38	R	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
38	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
38	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	S	1	Total 58	C 47	Mg 1	N 4	O 6	0
38	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
38	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
38	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
38	g	1	Total 57	C 46	Mg 1	N 4	O 6	0
38	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
38	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	n	1	Total 54	C 43	Mg 1	N 4	O 6	0
38	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
38	n	1	Total 50	C 39	Mg 1	N 4	O 6	0

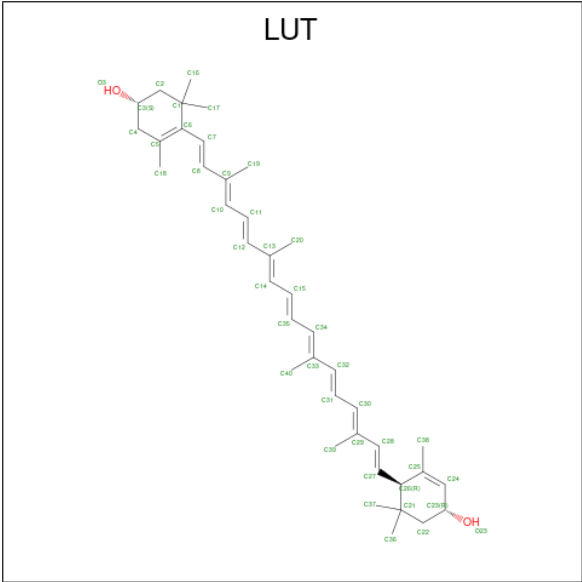
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Mol	Chain	Residues	Atoms					AltConf
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
38	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
38	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
38	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 39 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>).





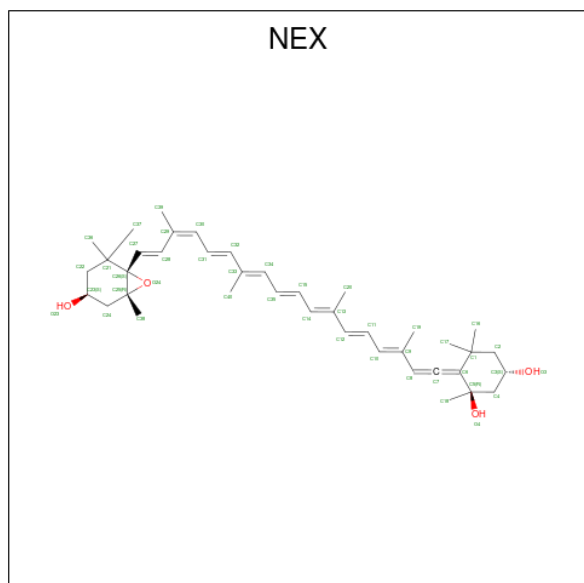
Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
39	s	1	Total	C	O	0
			42	40	2	
39	s	1	Total	C	O	0
			42	40	2	
39	y	1	Total	C	O	0
			42	40	2	
39	y	1	Total	C	O	0
			42	40	2	

- Molecule 40 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-TETRAMETHYLOCTADEC-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>).



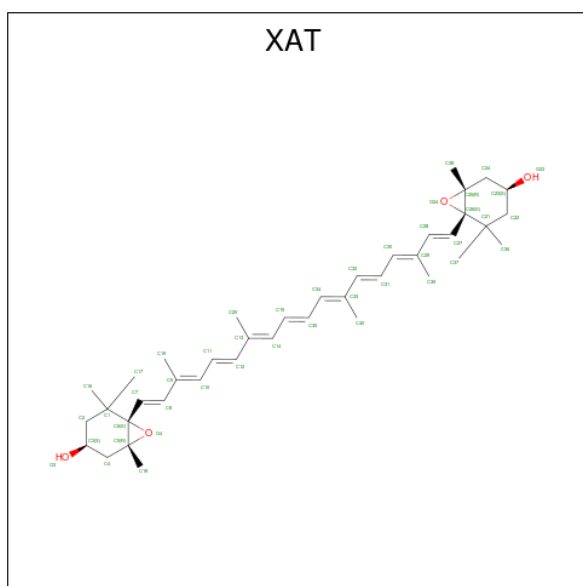
Mol	Chain	Residues	Atoms			AltConf
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
40	s	1	Total	C	O	0
			44	40	4	
40	y	1	Total	C	O	0
			44	40	4	
40	y	1	Total	C	O	0
			44	40	4	

- Molecule 41 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
41	R	1	Total	C	O	0
			44	40	4	
41	Y	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	
41	y	1	Total	C	O	0
			44	40	4	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	92	Total	O	0
			92	92	
42	B	151	Total	O	0
			151	151	

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Mol	Chain	Residues	Atoms		AltConf
42	C	134	Total 134	O 134	0
42	D	101	Total 101	O 101	0
42	E	14	Total 14	O 14	0
42	F	6	Total 6	O 6	0
42	G	26	Total 26	O 26	0
42	H	16	Total 16	O 16	0
42	I	3	Total 3	O 3	0
42	J	5	Total 5	O 5	0
42	K	6	Total 6	O 6	0
42	L	8	Total 8	O 8	0
42	M	6	Total 6	O 6	0
42	N	28	Total 28	O 28	0
42	O	69	Total 69	O 69	0
42	P	52	Total 52	O 52	0
42	Q	28	Total 28	O 28	0
42	R	40	Total 40	O 40	0
42	S	24	Total 24	O 24	0
42	T	7	Total 7	O 7	0
42	W	11	Total 11	O 11	0
42	X	10	Total 10	O 10	0
42	Y	45	Total 45	O 45	0

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Mol	Chain	Residues	Atoms		AltConf
42	Z	6	Total 6	O 6	0
42	U	1	Total 1	O 1	0
42	a	100	Total 100	O 100	0
42	b	167	Total 167	O 167	0
42	c	128	Total 128	O 128	0
42	d	85	Total 85	O 85	0
42	e	21	Total 21	O 21	0
42	f	3	Total 3	O 3	0
42	g	23	Total 23	O 23	0
42	h	14	Total 14	O 14	0
42	i	2	Total 2	O 2	0
42	j	4	Total 4	O 4	0
42	k	4	Total 4	O 4	0
42	l	8	Total 8	O 8	0
42	m	2	Total 2	O 2	0
42	n	23	Total 23	O 23	0
42	o	67	Total 67	O 67	0
42	p	43	Total 43	O 43	0
42	q	18	Total 18	O 18	0
42	r	33	Total 33	O 33	0
42	s	19	Total 19	O 19	0

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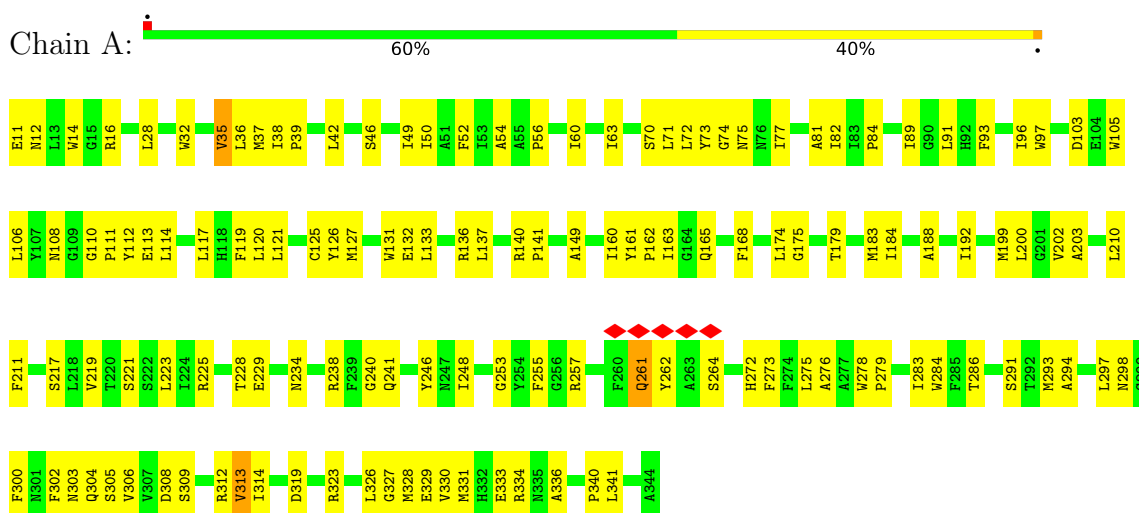
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Mol	Chain	Residues	Atoms		AltConf
42	t	3	Total 3	O 3	0
42	w	11	Total 11	O 11	0
42	x	7	Total 7	O 7	0
42	y	31	Total 31	O 31	0
42	z	2	Total 2	O 2	0
42	u	4	Total 4	O 4	0

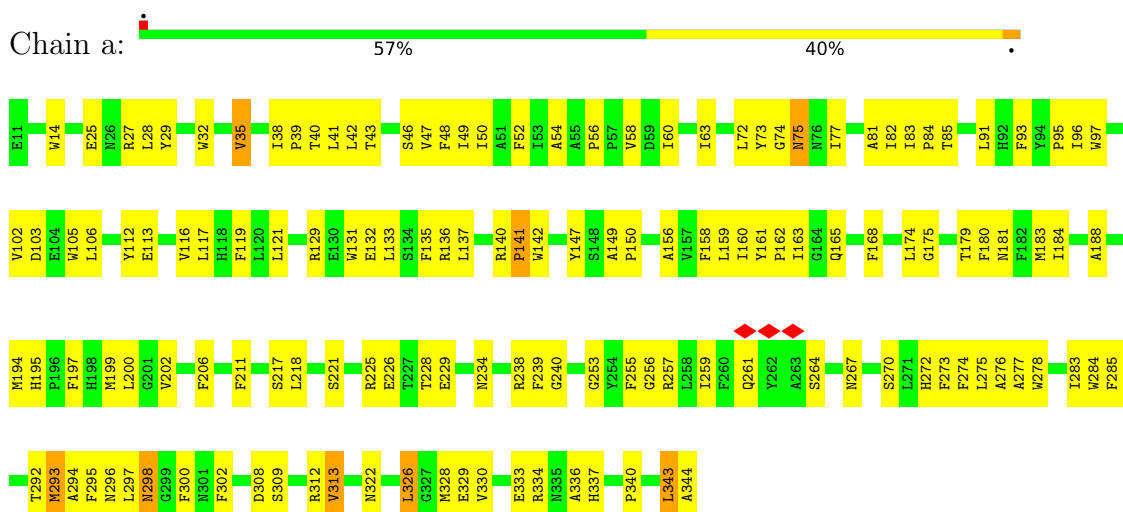
### 3 Residue-property plots

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: Photosystem II protein D1

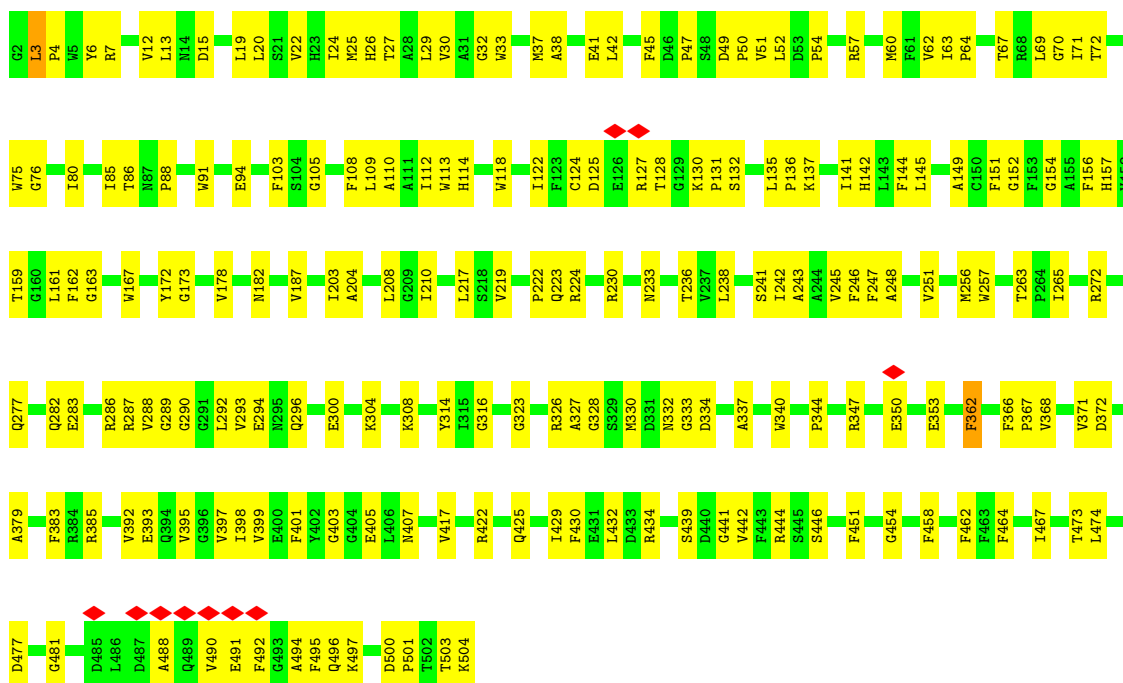


#### • Molecule 1: Photosystem II protein D1

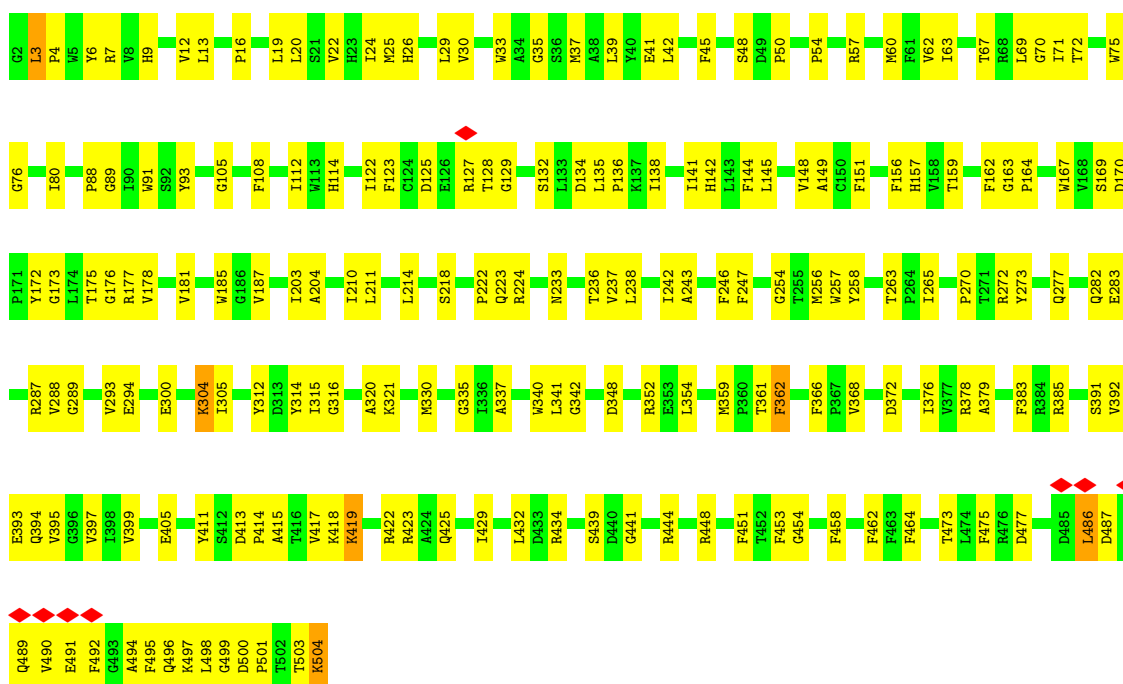


#### • Molecule 2: Photosystem II CP47 reaction center protein





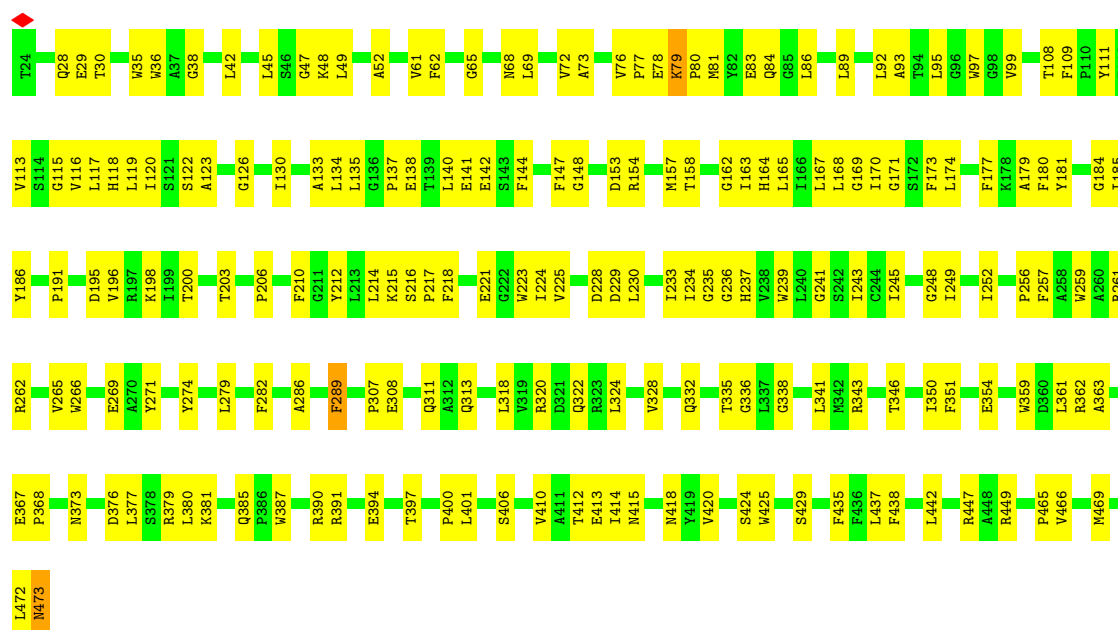
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

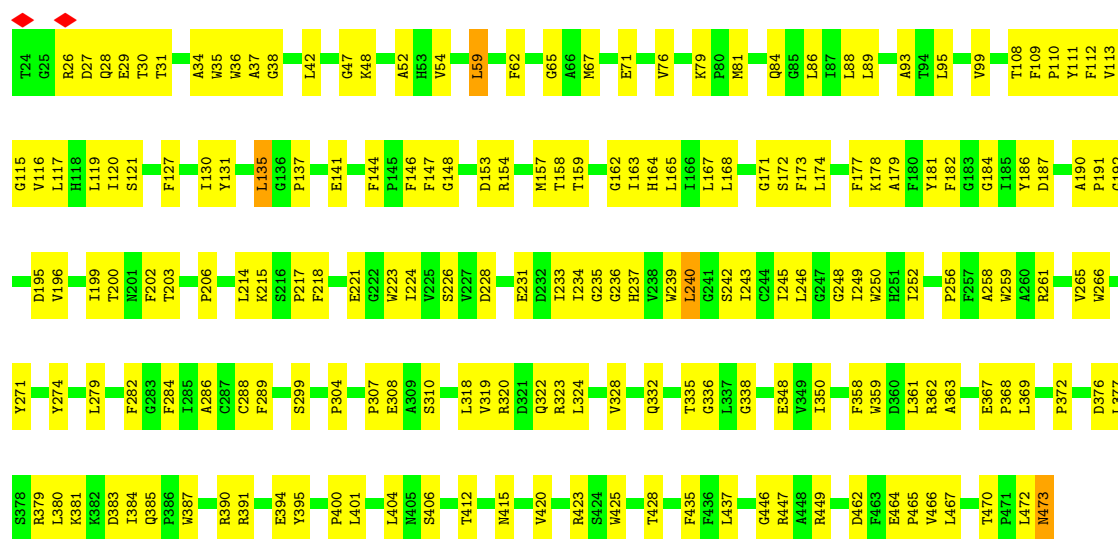






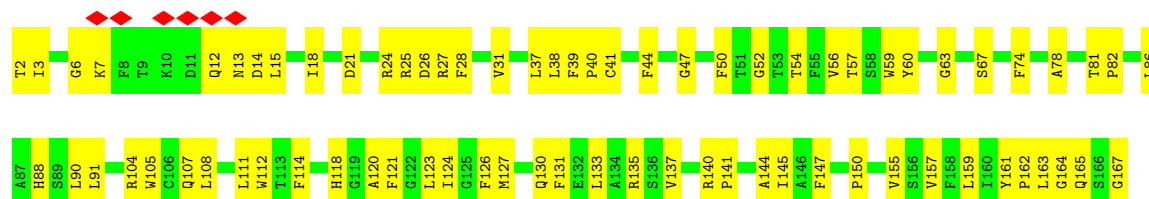
• Molecule 3: Photosystem II CP43 reaction center protein

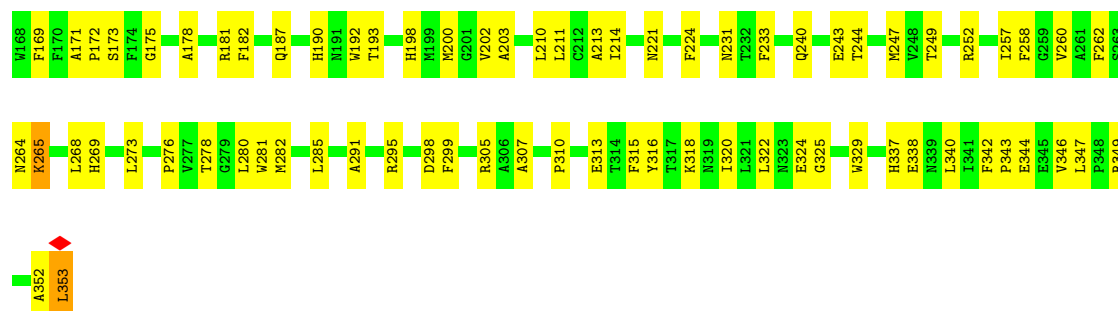
Chain c: 58% 41% .



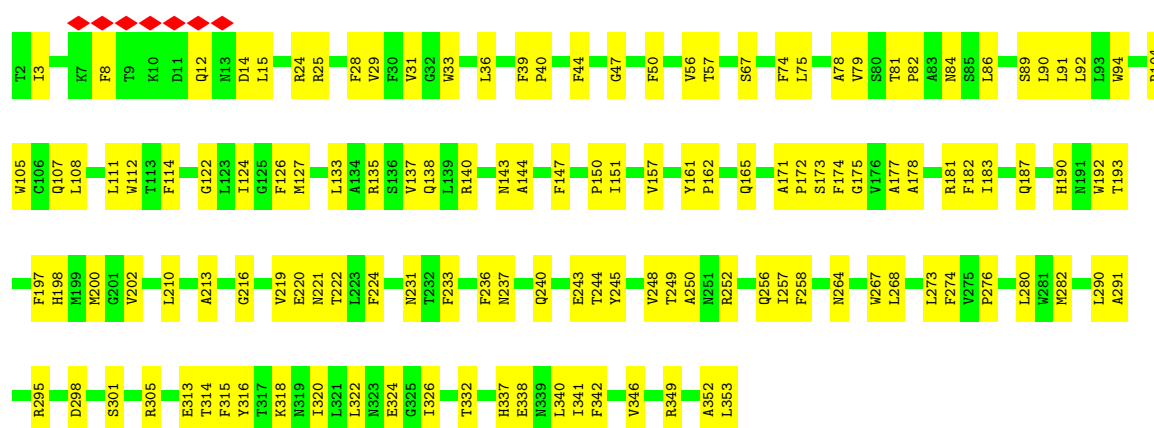
• Molecule 4: Photosystem II D2 protein

Chain D: 59% 41% .





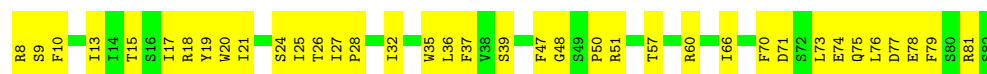
• Molecule 4: Photosystem II D2 protein



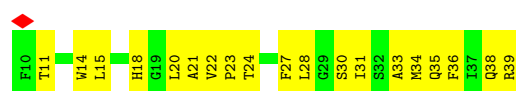
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

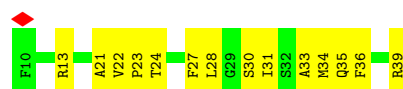


• Molecule 6: Cytochrome b559 subunit beta




• Molecule 6: Cytochrome b559 subunit beta

Chain f:  53% 47%



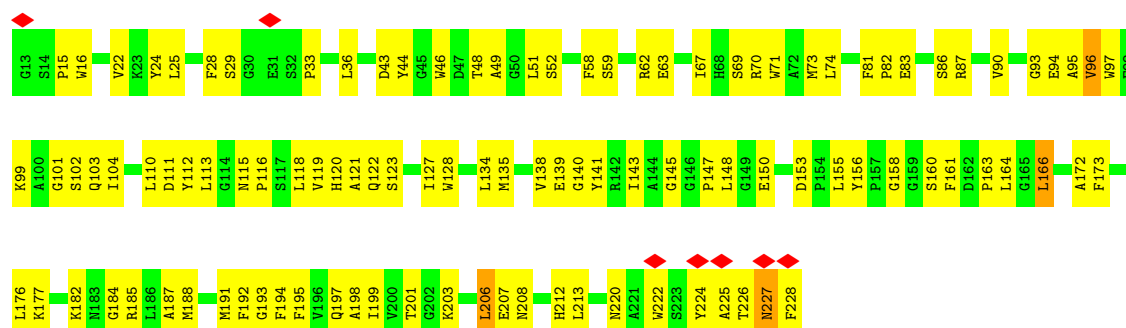
• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:  6% 43% 56%



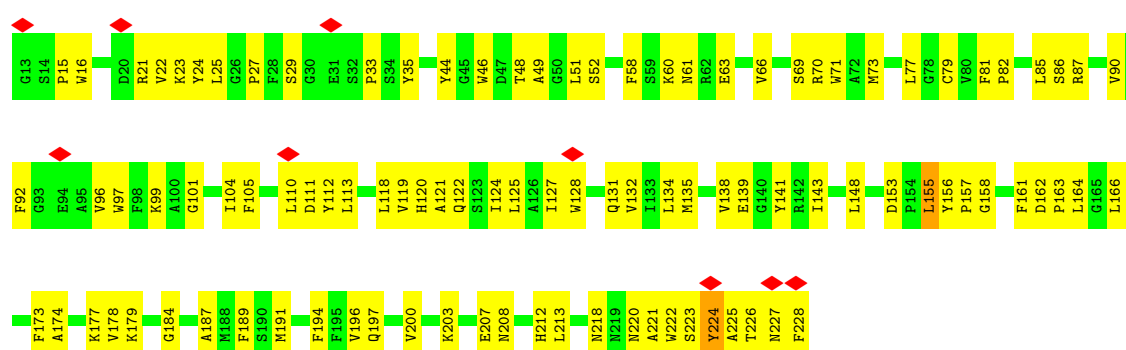
• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:  50% 48%



• Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic

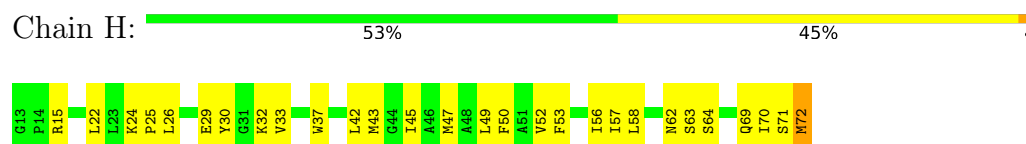
Chain g:  53% 46%



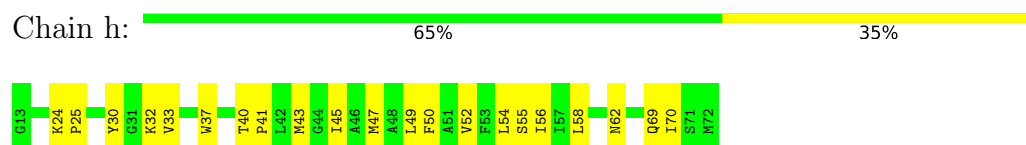
- Molecule 7: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 8: Photosystem II reaction center protein H



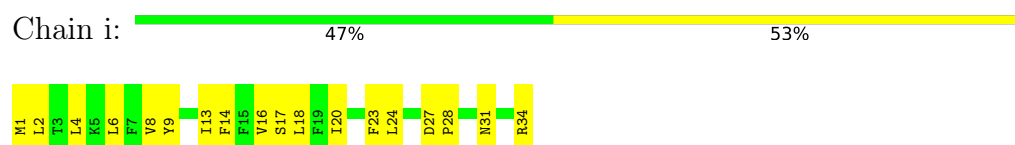
- Molecule 8: Photosystem II reaction center protein H



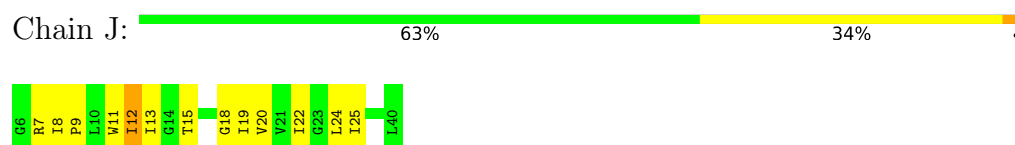
- Molecule 9: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J

Chain j:  54% 40% 6%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  35% 65%



- Molecule 11: Photosystem II reaction center protein K

Chain k:  32% 68%



- Molecule 12: Photosystem II reaction center protein L

Chain L:  50% 47% .



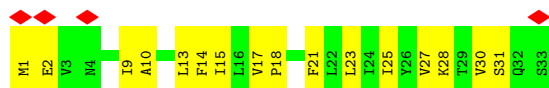
- Molecule 12: Photosystem II reaction center protein L

Chain l:  64% 33% .



- Molecule 13: Photosystem II reaction center protein M

Chain M:  12% 52% 48%



- Molecule 13: Photosystem II reaction center protein M

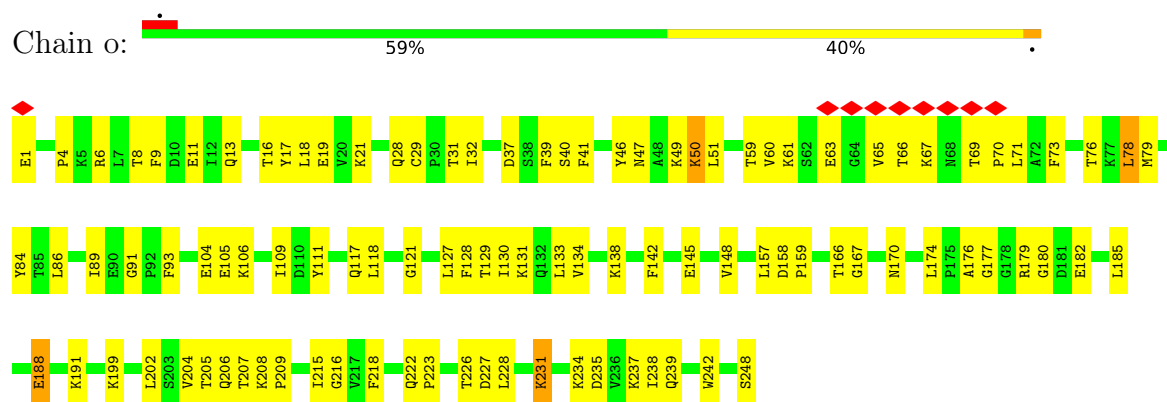
Chain m:  12% 55% 45%



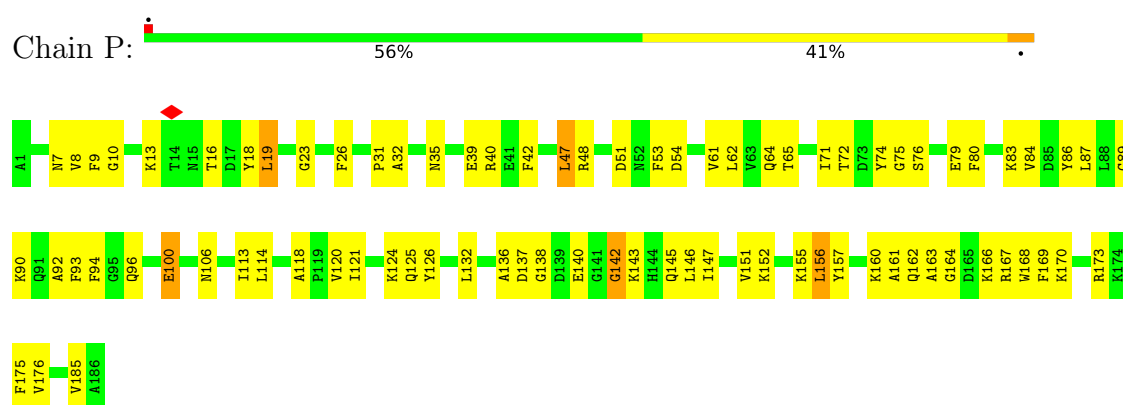
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



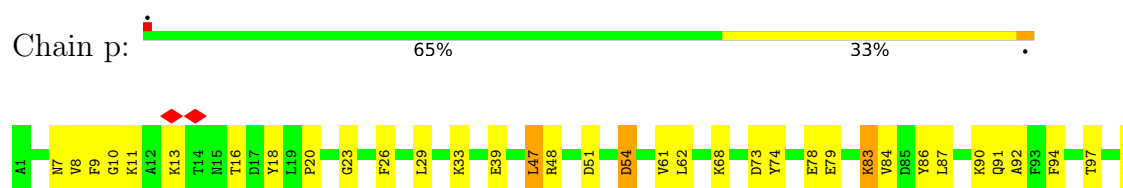
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic





• Molecule 16: Oxygen-evolving enhancer protein 3



• Molecule 16: Oxygen-evolving enhancer protein 3



• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

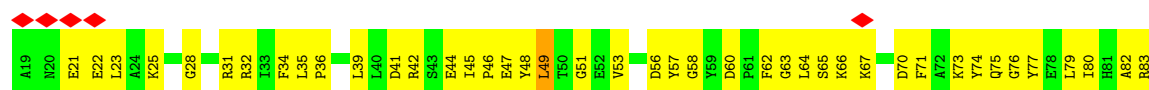


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

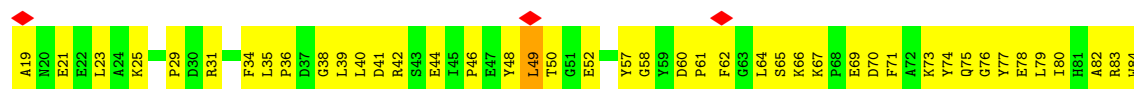




- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 19: Photosystem II reaction center protein T



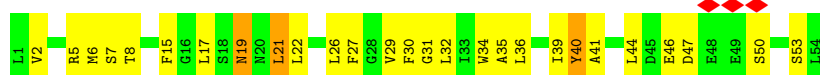
- Molecule 19: Photosystem II reaction center protein T



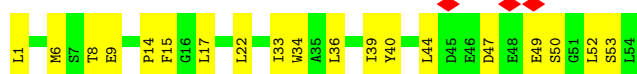




- Molecule 20: Photosystem II reaction center protein W



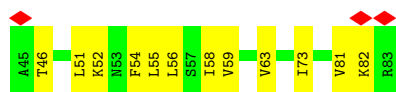
- Molecule 20: Photosystem II reaction center protein W



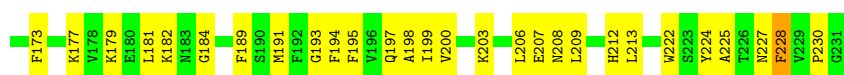
- Molecule 21: Ultraviolet-B-repressible protein



- Molecule 21: Ultraviolet-B-repressible protein

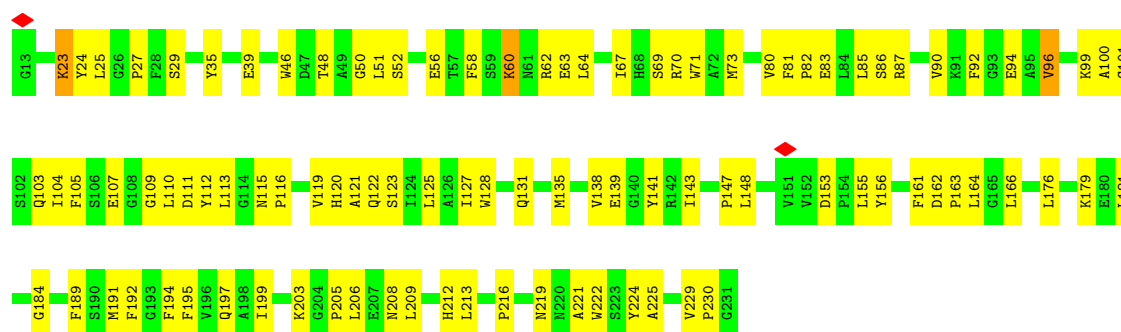


- Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic

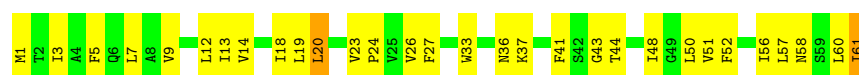


- Molecule 22: Chlorophyll a-b binding protein AB80, chloroplastic





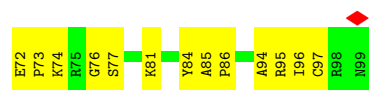
• Molecule 23: Photosystem II reaction center protein Z



• Molecule 23: Photosystem II reaction center protein Z



• Molecule 24: Photosystem II 5 kDa protein, chloroplastic



• Molecule 24: Photosystem II 5 kDa protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	200827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size ( $\text{\AA}$ )	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.84, 0.84, 0.84	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	A	0.95	0/2697	1.13	0/3677
1	a	0.95	0/2697	1.12	1/3677 (0.0%)
2	B	0.95	0/4071	1.13	0/5542
2	b	0.95	0/4071	1.13	2/5542 (0.0%)
3	C	0.94	1/3614 (0.0%)	1.13	0/4922
3	c	0.94	0/3613	1.12	0/4920
4	D	0.92	0/2890	1.12	0/3938
4	d	0.92	0/2890	1.12	0/3938
5	E	0.93	0/630	1.13	0/857
5	e	0.92	0/630	1.14	0/857
6	F	0.92	0/248	1.14	0/335
6	f	0.92	0/248	1.14	0/335
7	G	0.93	0/1701	1.17	0/2315
7	N	0.93	0/1700	1.16	2/2313 (0.1%)
7	g	0.93	0/1701	1.16	0/2315
7	n	0.93	0/1701	1.18	1/2315 (0.0%)
8	H	0.97	0/461	1.18	0/626
8	h	0.96	0/461	1.15	0/626
9	I	0.91	0/286	1.13	0/386
9	i	0.91	0/286	1.14	0/386
10	J	0.95	0/262	1.19	0/354
10	j	0.94	0/262	1.20	0/354
11	K	0.90	0/318	1.05	0/434
11	k	0.90	0/318	1.06	0/434
12	L	0.89	0/312	1.06	0/424
12	l	0.90	0/312	1.05	0/424
13	M	0.94	0/260	1.18	0/355
13	m	0.94	0/260	1.14	0/355
14	O	0.99	0/1906	1.09	0/2575
14	o	0.99	0/1906	1.10	0/2575
15	P	0.97	0/1464	1.08	2/1978 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	p	0.98	0/1464	1.08	1/1978 (0.1%)
16	Q	0.95	0/1179	1.17	0/1591
16	q	0.96	0/1179	1.18	0/1591
17	R	0.93	0/1804	1.14	1/2456 (0.0%)
17	r	0.92	0/1804	1.15	0/2456
18	S	0.93	0/1737	1.14	0/2361
18	s	0.91	0/1737	1.15	0/2361
19	T	0.90	0/260	1.10	0/354
19	t	0.89	0/260	1.12	0/354
20	W	0.92	0/429	1.11	0/581
20	w	0.92	0/429	1.13	0/581
21	X	0.97	0/279	1.28	0/380
21	x	0.98	0/279	1.27	0/380
22	Y	0.93	0/1719	1.17	0/2341
22	y	0.94	0/1719	1.16	0/2341
23	Z	0.97	0/467	1.23	0/640
23	z	0.96	0/467	1.22	0/640
24	U	0.94	0/216	1.21	0/291
24	u	0.94	0/216	1.17	0/291
All	All	0.94	1/61820 (0.0%)	1.14	10/84052 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	76	VAL	N-CA	5.10	1.49	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	145	GLY	CA-C-O	-6.09	118.03	122.23
15	P	89	GLY	CA-C-O	-5.92	118.05	122.37
2	b	89	GLY	CA-C-O	-5.92	118.15	122.23
17	R	132	GLY	CA-C-O	-5.89	118.17	122.23
15	p	142	GLY	CA-C-O	-5.85	118.19	122.23

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2522	138	0
1	a	2616	0	2522	178	0
2	B	3939	0	3814	208	0
2	b	3939	0	3814	180	0
3	C	3497	0	3422	198	0
3	c	3496	0	3422	208	0
4	D	2797	0	2695	152	0
4	d	2797	0	2695	134	0
5	E	612	0	595	33	0
5	e	612	0	595	38	0
6	F	241	0	246	22	0
6	f	241	0	246	18	0
7	G	1650	0	1577	168	0
7	N	1649	0	1573	135	0
7	g	1650	0	1577	137	0
7	n	1650	0	1577	136	0
8	H	452	0	473	34	0
8	h	452	0	473	31	0
9	I	278	0	291	16	0
9	i	278	0	291	17	0
10	J	256	0	269	11	0
10	j	256	0	269	15	0
11	K	306	0	313	41	0
11	k	306	0	313	32	0
12	L	304	0	292	24	0
12	l	304	0	292	12	0
13	M	256	0	284	23	0
13	m	256	0	284	22	0
14	O	1870	0	1849	86	0
14	o	1870	0	1851	92	0
15	P	1434	0	1392	80	0
15	p	1434	0	1392	51	0
16	Q	1157	0	1210	77	0
16	q	1157	0	1210	63	0
17	R	1755	0	1722	110	0
17	r	1755	0	1722	121	0
18	S	1688	0	1652	188	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1688	0	1652	148	0
19	T	252	0	267	13	0
19	t	252	0	267	24	0
20	W	419	0	402	34	0
20	w	419	0	402	28	0
21	X	276	0	301	23	0
21	x	276	0	301	17	0
22	Y	1667	0	1596	120	0
22	y	1667	0	1596	110	0
23	Z	457	0	488	31	0
23	z	457	0	488	40	0
24	U	212	0	220	8	0
24	u	212	0	223	16	0
25	A	10	0	0	0	0
25	a	10	0	0	0	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0
27	A	2	0	0	0	0
27	a	2	0	0	1	0
28	A	175	0	168	31	0
28	B	1040	0	1142	177	0
28	C	837	0	908	164	0
28	D	195	0	214	23	0
28	G	465	0	443	105	0
28	N	456	0	426	88	0
28	R	554	0	507	99	0
28	S	465	0	387	113	0
28	Y	463	0	440	79	0
28	a	175	0	169	32	0
28	b	1040	0	1144	176	0
28	c	808	0	837	127	0
28	d	195	0	214	34	0
28	g	440	0	402	81	0
28	n	465	0	450	97	0
28	r	563	0	524	107	0
28	s	465	0	387	84	0
28	y	473	0	463	88	0
29	A	64	0	74	9	0
29	D	64	0	74	9	0
29	a	64	0	74	12	0
29	d	64	0	74	12	0
30	A	40	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	120	0	168	51	0
30	C	120	0	168	50	0
30	D	40	0	56	11	0
30	H	40	0	56	14	0
30	K	40	0	56	13	0
30	T	40	0	56	13	0
30	a	40	0	56	22	0
30	b	120	0	168	34	0
30	c	80	0	112	30	0
30	d	40	0	56	20	0
30	h	40	0	56	19	0
30	i	40	0	56	8	0
30	k	40	0	56	16	0
30	t	40	0	56	10	0
31	A	104	0	143	23	0
31	B	54	0	77	12	0
31	L	96	0	124	21	0
31	M	42	0	47	5	0
31	a	104	0	143	30	0
32	A	88	0	116	31	0
32	B	82	0	104	23	0
32	C	95	0	130	24	0
32	D	46	0	62	15	0
32	a	40	0	50	14	0
32	b	101	0	145	22	0
32	c	51	0	72	15	0
32	d	46	0	62	20	0
32	k	51	0	72	15	0
32	w	48	0	66	13	0
33	A	13	0	7	0	0
33	D	55	0	80	8	0
33	a	13	0	7	0	0
33	d	55	0	80	6	0
34	A	4	0	0	0	0
34	d	4	0	0	0	0
35	A	43	0	56	4	0
35	B	117	0	150	30	0
35	C	49	0	74	11	0
35	D	49	0	74	13	0
35	G	49	0	74	7	0
35	L	49	0	74	6	0
35	N	31	0	32	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	25	0	20	5	0
35	S	77	0	97	26	0
35	W	49	0	74	20	0
35	Y	49	0	74	5	0
35	a	43	0	56	10	0
35	b	121	0	158	23	0
35	c	72	0	83	14	0
35	d	49	0	74	12	0
35	g	41	0	55	9	0
35	l	49	0	74	5	0
35	n	32	0	34	6	0
35	r	30	0	30	5	0
35	s	49	0	74	16	0
35	w	39	0	51	8	0
35	y	49	0	74	6	0
36	A	59	0	76	10	0
36	B	62	0	82	11	0
36	C	177	0	228	48	0
36	a	59	0	76	17	0
36	b	62	0	82	11	0
36	c	168	0	210	45	0
37	E	43	0	30	7	0
37	f	43	0	30	6	0
38	G	339	0	295	75	0
38	N	347	0	310	78	0
38	R	154	0	116	25	0
38	S	196	0	140	47	0
38	Y	362	0	345	93	0
38	g	412	0	378	99	0
38	n	350	0	317	86	0
38	r	183	0	171	37	0
38	s	196	0	140	36	0
38	y	296	0	276	67	0
39	G	84	0	112	39	0
39	N	84	0	112	27	0
39	R	42	0	56	14	0
39	S	84	0	112	43	0
39	Y	84	0	112	15	0
39	g	84	0	112	36	0
39	n	84	0	112	21	0
39	r	42	0	56	15	0
39	s	84	0	112	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	y	84	0	112	17	0
40	G	44	0	54	11	0
40	N	44	0	54	9	0
40	Y	44	0	54	9	0
40	g	44	0	55	9	0
40	n	44	0	54	8	0
40	r	44	0	54	13	0
40	s	44	0	54	7	0
40	y	88	0	108	10	0
41	R	44	0	56	13	0
41	Y	44	0	56	17	0
41	r	44	0	56	9	0
41	y	44	0	56	11	0
42	A	92	0	0	4	0
42	B	151	0	0	2	0
42	C	134	0	0	0	0
42	D	101	0	0	2	0
42	E	14	0	0	0	0
42	F	6	0	0	0	0
42	G	26	0	0	2	0
42	H	16	0	0	2	0
42	I	3	0	0	0	0
42	J	5	0	0	0	0
42	K	6	0	0	0	0
42	L	8	0	0	0	0
42	M	6	0	0	0	0
42	N	28	0	0	1	0
42	O	69	0	0	1	0
42	P	52	0	0	2	0
42	Q	28	0	0	2	0
42	R	40	0	0	3	0
42	S	24	0	0	3	0
42	T	7	0	0	2	0
42	U	1	0	0	0	0
42	W	11	0	0	0	0
42	X	10	0	0	0	0
42	Y	45	0	0	1	0
42	Z	6	0	0	0	0
42	a	100	0	0	5	0
42	b	167	0	0	1	0
42	c	128	0	0	2	0
42	d	85	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	e	21	0	0	1	0
42	f	3	0	0	0	0
42	g	23	0	0	0	0
42	h	14	0	0	0	0
42	i	2	0	0	0	0
42	j	4	0	0	0	0
42	k	4	0	0	1	0
42	l	8	0	0	0	0
42	m	2	0	0	0	0
42	n	23	0	0	2	0
42	o	67	0	0	0	0
42	p	43	0	0	1	0
42	q	18	0	0	0	0
42	r	33	0	0	1	0
42	s	19	0	0	1	0
42	t	3	0	0	0	0
42	u	4	0	0	0	0
42	w	11	0	0	0	0
42	x	7	0	0	0	0
42	y	31	0	0	1	0
42	z	2	0	0	0	0
All	All	79416	0	77862	5285	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 34.

The worst 5 of 5285 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)
28:B:601:CLA:H152	30:H:101:BCR:H17C	1.34	1.09
16:Q:13:LEU:HD22	16:Q:18:PRO:HA	1.40	1.04
1:a:42:LEU:HB3	30:a:410:BCR:H353	1.38	1.04
36:a:401:DGD:HA92	32:a:413:LMG:H352	1.39	1.04
14:O:65:VAL:HA	14:O:71:LEU:HD21	1.39	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	36	42
1	a	332/334 (99%)	317 (96%)	14 (4%)	1 (0%)	36	42
2	B	501/503 (100%)	489 (98%)	12 (2%)	0	100	100
2	b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
3	C	448/450 (100%)	432 (96%)	16 (4%)	0	100	100
3	c	448/450 (100%)	429 (96%)	19 (4%)	0	100	100
4	D	350/352 (99%)	334 (95%)	16 (5%)	0	100	100
4	d	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
5	e	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
6	F	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
6	f	28/30 (93%)	28 (100%)	0	0	100	100
7	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
7	N	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	g	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
7	n	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
8	H	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
8	h	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
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%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/36 (94%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	34/36 (94%)	34 (100%)	0	0	100	100
13	M	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
13	m	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
14	O	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
14	o	246/248 (99%)	234 (95%)	12 (5%)	0	100	100
15	P	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
15	p	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
16	Q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
16	q	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
17	R	222/224 (99%)	215 (97%)	7 (3%)	0	100	100
17	r	222/224 (99%)	216 (97%)	6 (3%)	0	100	100
18	S	216/218 (99%)	204 (94%)	11 (5%)	1 (0%)	24	27
18	s	216/218 (99%)	202 (94%)	14 (6%)	0	100	100
19	T	29/31 (94%)	29 (100%)	0	0	100	100
19	t	29/31 (94%)	29 (100%)	0	0	100	100
20	W	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
20	w	52/54 (96%)	52 (100%)	0	0	100	100
21	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
21	x	37/39 (95%)	37 (100%)	0	0	100	100
22	Y	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
22	y	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
23	Z	59/61 (97%)	59 (100%)	0	0	100	100
23	z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
24	U	26/28 (93%)	26 (100%)	0	0	100	100
24	u	26/28 (93%)	26 (100%)	0	0	100	100
All	All	7634/7734 (99%)	7353 (96%)	278 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	161	GLU
1	a	141	PRO
1	A	141	PRO

### 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	A	270/270 (100%)	265 (98%)	5 (2%)	50	66
1	a	270/270 (100%)	262 (97%)	8 (3%)	36	49
2	B	399/399 (100%)	396 (99%)	3 (1%)	73	85
2	b	399/399 (100%)	391 (98%)	8 (2%)	48	64
3	C	352/352 (100%)	348 (99%)	4 (1%)	65	79
3	c	352/352 (100%)	345 (98%)	7 (2%)	48	64
4	D	284/284 (100%)	281 (99%)	3 (1%)	65	79
4	d	284/284 (100%)	281 (99%)	3 (1%)	65	79
5	E	67/67 (100%)	67 (100%)	0	100	100
5	e	67/67 (100%)	67 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100
6	f	25/25 (100%)	25 (100%)	0	100	100
7	G	169/169 (100%)	166 (98%)	3 (2%)	51	68
7	N	168/169 (99%)	162 (96%)	6 (4%)	31	42
7	g	169/169 (100%)	166 (98%)	3 (2%)	51	68
7	n	169/169 (100%)	161 (95%)	8 (5%)	23	31
8	H	49/49 (100%)	46 (94%)	3 (6%)	17	20
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%)	30 (97%)	1 (3%)	34	47
10	J	26/26 (100%)	25 (96%)	1 (4%)	29	40
10	j	26/26 (100%)	24 (92%)	2 (8%)	12	13
11	K	32/32 (100%)	31 (97%)	1 (3%)	35	48
11	k	32/32 (100%)	32 (100%)	0	100	100
12	L	34/34 (100%)	33 (97%)	1 (3%)	37	51
12	l	34/34 (100%)	33 (97%)	1 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	29/29 (100%)	29 (100%)	0	100	100
13	m	29/29 (100%)	29 (100%)	0	100	100
14	O	204/204 (100%)	201 (98%)	3 (2%)	57	73
14	o	204/204 (100%)	200 (98%)	4 (2%)	48	64
15	P	150/150 (100%)	145 (97%)	5 (3%)	33	45
15	p	150/150 (100%)	147 (98%)	3 (2%)	48	64
16	Q	125/125 (100%)	122 (98%)	3 (2%)	43	58
16	q	125/125 (100%)	124 (99%)	1 (1%)	73	85
17	R	181/181 (100%)	178 (98%)	3 (2%)	53	69
17	r	181/181 (100%)	174 (96%)	7 (4%)	28	39
18	S	169/169 (100%)	165 (98%)	4 (2%)	43	58
18	s	169/169 (100%)	164 (97%)	5 (3%)	36	49
19	T	28/28 (100%)	28 (100%)	0	100	100
19	t	28/28 (100%)	28 (100%)	0	100	100
20	W	44/44 (100%)	41 (93%)	3 (7%)	14	17
20	w	44/44 (100%)	43 (98%)	1 (2%)	44	59
21	X	32/32 (100%)	32 (100%)	0	100	100
21	x	32/32 (100%)	32 (100%)	0	100	100
22	Y	170/170 (100%)	166 (98%)	4 (2%)	43	58
22	y	170/170 (100%)	165 (97%)	5 (3%)	37	51
23	Z	53/53 (100%)	51 (96%)	2 (4%)	29	40
23	z	53/53 (100%)	50 (94%)	3 (6%)	18	23
24	U	23/23 (100%)	23 (100%)	0	100	100
24	u	23/23 (100%)	21 (91%)	2 (9%)	9	10
All	All	6229/6230 (100%)	6100 (98%)	129 (2%)	46	63

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	s	124	LEU
22	y	23	LYS
20	W	19	ASN
18	S	185	LEU
22	y	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
13	m	32	GLN
22	y	88	ASN
7	n	208	ASN
16	q	112	GLN
7	N	220	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 339 ligands modelled in this entry, 6 are monoatomic - leaving 333 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	$\# Z  > 2$
28	CLA	b	602	2	69,73,73	1.34	7 (10%)	82,113,113	1.87	19 (23%)
35	LHG	S	301	-	33,33,48	0.46	0	36,39,54	1.15	3 (8%)
38	CHL	N	608	42	60,74,74	1.42	9 (15%)	58,114,114	1.67	13 (22%)
28	CLA	N	613	7	57,61,73	1.48	6 (10%)	67,98,113	2.03	19 (28%)
32	LMG	D	408	-	46,46,55	1.04	4 (8%)	54,54,63	1.03	2 (3%)
38	CHL	R	605	42	41,55,74	1.82	8 (19%)	35,91,114	2.07	11 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	CLA	D	404	4	69,73,73	1.35	6 (8%)	82,113,113	1.95	21 (25%)
28	CLA	S	304	18	49,53,73	1.59	5 (10%)	58,89,113	2.09	17 (29%)
28	CLA	S	310	18	59,63,73	1.46	6 (10%)	70,101,113	2.05	21 (30%)
38	CHL	S	306	42	40,54,74	1.75	9 (22%)	34,90,114	1.99	10 (29%)
28	CLA	A	405	1	69,73,73	1.35	5 (7%)	82,113,113	1.84	19 (23%)
35	LHG	n	618	28	31,31,48	0.51	0	34,37,54	1.20	3 (8%)
28	CLA	g	611	35	64,68,73	1.42	6 (9%)	76,107,113	1.96	16 (21%)
35	LHG	A	416	-	42,42,48	0.41	0	45,48,54	1.10	3 (6%)
38	CHL	G	606	42	44,58,74	1.76	9 (20%)	37,94,114	1.94	10 (27%)
28	CLA	C	503	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	20 (24%)
30	BCR	b	618	-	41,41,41	4.95	27 (65%)	56,56,56	2.25	18 (32%)
28	CLA	C	508	3	69,73,73	1.35	5 (7%)	82,113,113	1.89	19 (23%)
38	CHL	n	601	7	48,62,74	1.45	9 (18%)	43,99,114	1.94	11 (25%)
28	CLA	g	610	7	62,66,73	1.43	6 (9%)	73,104,113	2.22	22 (30%)
28	CLA	B	612	2	69,73,73	1.35	6 (8%)	82,113,113	1.90	18 (21%)
28	CLA	y	305	42	54,58,73	1.52	7 (12%)	64,95,113	2.08	17 (26%)
28	CLA	y	303	22	69,73,73	1.35	7 (10%)	82,113,113	1.91	22 (26%)
38	CHL	S	308	-	40,54,74	1.61	8 (20%)	34,90,114	2.02	10 (29%)
28	CLA	R	612	17	59,63,73	1.46	7 (11%)	70,101,113	2.04	19 (27%)
35	LHG	w	102	-	38,38,48	0.43	0	41,44,54	1.05	3 (7%)
28	CLA	r	609	17	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
32	LMG	A	413	-	40,40,55	1.03	3 (7%)	48,48,63	1.12	3 (6%)
28	CLA	B	614	2	69,73,73	1.34	7 (10%)	82,113,113	1.89	19 (23%)
28	CLA	b	610	42	69,73,73	1.35	7 (10%)	82,113,113	1.88	19 (23%)
28	CLA	s	604	42	54,58,73	1.51	6 (11%)	64,95,113	2.10	17 (26%)
38	CHL	n	607	42	60,74,74	1.23	8 (13%)	58,114,114	1.66	11 (18%)
28	CLA	n	613	7	59,63,73	1.48	6 (10%)	70,101,113	2.11	18 (25%)
31	SQD	M	101	-	40,42,54	0.85	0	50,53,65	0.90	2 (4%)
28	CLA	r	601	17	53,57,73	1.53	7 (13%)	61,93,113	2.12	17 (27%)
28	CLA	c	512	3	61,65,73	1.43	6 (9%)	72,103,113	2.04	19 (26%)
28	CLA	N	612	7	64,68,73	1.40	7 (10%)	76,107,113	1.93	20 (26%)
38	CHL	n	608	42	60,74,74	1.38	9 (15%)	58,114,114	1.68	13 (22%)
28	CLA	b	601	42	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
39	LUT	g	616	-	42,43,43	6.36	27 (64%)	51,60,60	2.08	13 (25%)
28	CLA	S	305	42	54,58,73	1.56	6 (11%)	64,95,113	2.12	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	CLA	s	603	18	49,53,73	1.60	7 (14%)	58,89,113	2.06	15 (25%)
28	CLA	B	606	2	69,73,73	1.34	6 (8%)	82,113,113	1.87	18 (21%)
37	HEM	E	101	6,5	50,50,50	1.57	9 (18%)	67,82,82	1.70	12 (17%)
36	DGD	B	626	-	63,63,67	1.24	7 (11%)	77,77,81	0.95	2 (2%)
25	OEX	a	402	3,1,42	0,15,15	-	-	-	-	-
30	BCR	H	101	-	41,41,41	4.94	27 (65%)	56,56,56	2.45	18 (32%)
36	DGD	A	417	-	60,60,67	1.17	6 (10%)	74,74,81	1.04	5 (6%)
38	CHL	y	302	22	60,74,74	1.19	8 (13%)	58,114,114	1.64	11 (18%)
39	LUT	N	616	-	42,43,43	6.31	26 (61%)	51,60,60	2.21	18 (35%)
32	LMG	B	621	-	51,51,55	1.21	6 (11%)	59,59,63	1.25	5 (8%)
28	CLA	s	612	18	59,63,73	1.45	5 (8%)	70,101,113	1.97	19 (27%)
28	CLA	N	602	7	69,73,73	1.35	7 (10%)	82,113,113	1.91	20 (24%)
28	CLA	Y	611	35	64,68,73	1.39	6 (9%)	76,107,113	1.96	18 (23%)
30	BCR	C	515	-	41,41,41	4.95	27 (65%)	56,56,56	2.33	18 (32%)
28	CLA	B	615	2	69,73,73	1.34	6 (8%)	82,113,113	1.89	20 (24%)
35	LHG	N	618	28	30,30,48	0.49	0	33,36,54	1.40	4 (12%)
39	LUT	y	316	-	42,43,43	6.41	26 (61%)	51,60,60	2.04	17 (33%)
28	CLA	b	607	42	69,73,73	1.35	6 (8%)	82,113,113	1.90	20 (24%)
38	CHL	s	605	42	40,54,74	1.72	8 (20%)	34,90,114	1.98	10 (29%)
38	CHL	g	607	42	51,65,74	1.45	9 (17%)	47,103,114	1.89	12 (25%)
40	NEX	r	616	28	40,46,46	2.71	12 (30%)	50,70,70	1.58	5 (10%)
28	CLA	N	614	7	52,56,73	1.55	6 (11%)	61,92,113	2.07	18 (29%)
32	LMG	d	409	-	46,46,55	1.03	4 (8%)	54,54,63	1.04	3 (5%)
28	CLA	y	312	22	64,68,73	1.39	7 (10%)	76,107,113	1.96	18 (23%)
28	CLA	Y	603	22	59,63,73	1.45	6 (10%)	70,101,113	2.05	20 (28%)
29	PHO	A	407	-	58,69,69	0.81	3 (5%)	55,99,99	0.87	2 (3%)
38	CHL	R	607	42	55,69,74	1.32	9 (16%)	52,108,114	1.74	11 (21%)
38	CHL	g	619	42	60,74,74	1.35	9 (15%)	58,114,114	1.66	13 (22%)
33	PL9	D	406	-	55,55,55	0.73	1 (1%)	68,69,69	0.61	2 (2%)
38	CHL	y	307	42	44,58,74	1.66	8 (18%)	37,94,114	1.94	10 (27%)
40	NEX	y	318	-	40,46,46	2.69	12 (30%)	50,70,70	1.70	11 (22%)
28	CLA	B	611	2	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
28	CLA	b	616	2	69,73,73	1.35	6 (8%)	82,113,113	1.87	18 (21%)
28	CLA	R	608	17	62,66,73	1.42	5 (8%)	73,104,113	1.99	18 (24%)
28	CLA	C	507	42	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	CHL	s	606	42	52,66,74	1.34	9 (17%)	48,104,114	1.87	11 (22%)
41	XAT	y	317	-	41,47,47	0.67	0	54,74,74	1.89	10 (18%)
39	LUT	G	615	-	42,43,43	6.40	26 (61%)	51,60,60	2.82	18 (35%)
28	CLA	B	602	2	69,73,73	1.35	7 (10%)	82,113,113	1.91	18 (21%)
39	LUT	S	315	-	42,43,43	6.39	27 (64%)	51,60,60	1.99	14 (27%)
38	CHL	N	606	42	44,58,74	1.73	9 (20%)	37,94,114	1.95	10 (27%)
35	LHG	G	618	28	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
30	BCR	b	619	-	41,41,41	4.86	25 (60%)	56,56,56	2.47	23 (41%)
28	CLA	a	409	1	64,68,73	1.40	5 (7%)	76,107,113	1.99	19 (25%)
30	BCR	a	410	-	41,41,41	4.93	27 (65%)	56,56,56	2.33	18 (32%)
28	CLA	B	613	2	69,73,73	1.35	6 (8%)	82,113,113	1.87	17 (20%)
28	CLA	b	613	2	69,73,73	1.35	6 (8%)	82,113,113	1.85	18 (21%)
38	CHL	r	606	42	50,64,74	1.61	8 (16%)	46,102,114	1.87	12 (26%)
30	BCR	h	101	-	41,41,41	4.98	27 (65%)	56,56,56	2.27	18 (32%)
32	LMG	C	522	-	44,44,55	0.97	3 (6%)	52,52,63	1.11	2 (3%)
28	CLA	s	610	35	60,64,73	1.44	6 (10%)	71,102,113	1.99	19 (26%)
38	CHL	y	308	42	60,74,74	1.42	9 (15%)	58,114,114	1.65	12 (20%)
28	CLA	Y	602	22	69,73,73	1.43	7 (10%)	82,113,113	1.87	21 (25%)
38	CHL	Y	606	42	44,58,74	1.68	9 (20%)	37,94,114	1.94	10 (27%)
28	CLA	B	605	2	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
28	CLA	c	507	42	69,73,73	1.35	5 (7%)	82,113,113	1.94	18 (21%)
38	CHL	G	608	42	60,74,74	1.44	9 (15%)	58,114,114	1.64	12 (20%)
32	LMG	b	623	-	50,50,55	1.16	5 (10%)	58,58,63	0.97	2 (3%)
35	LHG	a	415	-	42,42,48	0.41	0	45,48,54	1.10	3 (6%)
36	DGD	c	516	-	56,56,67	1.06	4 (7%)	70,70,81	0.98	3 (4%)
30	BCR	T	101	-	41,41,41	4.91	26 (63%)	56,56,56	2.63	20 (35%)
38	CHL	S	307	42	52,66,74	1.35	8 (15%)	48,104,114	1.83	11 (22%)
28	CLA	r	604	40,42	52,56,73	1.54	7 (13%)	61,92,113	2.10	18 (29%)
31	SQD	A	414	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
28	CLA	B	601	42	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
28	CLA	C	509	3	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
28	CLA	g	612	7	49,53,73	1.60	7 (14%)	58,89,113	2.06	17 (29%)
38	CHL	g	601	7	60,74,74	1.30	8 (13%)	58,114,114	1.66	12 (20%)
28	CLA	S	313	18	59,63,73	1.45	6 (10%)	70,101,113	1.97	20 (28%)
29	PHO	a	408	-	58,69,69	0.81	3 (5%)	55,99,99	0.88	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	CHL	Y	608	42	60,74,74	1.33	8 (13%)	58,114,114	1.62	10 (17%)
28	CLA	S	314	18	53,57,73	1.54	6 (11%)	61,93,113	2.14	18 (29%)
33	PL9	a	412	-	13,13,55	1.56	1 (7%)	17,17,69	1.13	1 (5%)
32	LMG	k	102	-	51,51,55	1.21	6 (11%)	59,59,63	1.10	3 (5%)
32	LMG	C	520	-	51,51,55	1.21	6 (11%)	59,59,63	1.12	3 (5%)
28	CLA	R	609	17	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
28	CLA	B	609	2	69,73,73	1.35	5 (7%)	82,113,113	1.91	18 (21%)
28	CLA	b	609	-	69,73,73	1.34	5 (7%)	82,113,113	1.92	17 (20%)
28	CLA	n	612	7	64,68,73	1.42	6 (9%)	76,107,113	1.95	18 (23%)
40	NEX	Y	618	28	40,46,46	2.69	12 (30%)	50,70,70	1.52	8 (16%)
32	LMG	w	101	-	48,48,55	1.12	5 (10%)	56,56,63	1.18	4 (7%)
36	DGD	a	401	-	60,60,67	1.16	6 (10%)	74,74,81	0.93	2 (2%)
30	BCR	d	406	-	41,41,41	4.91	27 (65%)	56,56,56	2.56	20 (35%)
28	CLA	N	610	7	69,73,73	1.34	7 (10%)	82,113,113	1.88	18 (21%)
28	CLA	D	403	4	69,73,73	1.35	7 (10%)	82,113,113	1.87	18 (21%)
28	CLA	A	408	1	64,68,73	1.40	6 (9%)	76,107,113	1.91	20 (26%)
28	CLA	s	609	18	59,63,73	1.46	6 (10%)	70,101,113	1.99	19 (27%)
38	CHL	G	605	7	40,54,74	1.49	7 (17%)	34,90,114	2.02	9 (26%)
35	LHG	g	618	28	40,40,48	0.41	0	43,46,54	1.16	3 (6%)
28	CLA	N	611	35	64,68,73	1.40	6 (9%)	76,107,113	1.91	18 (23%)
30	BCR	t	101	-	41,41,41	4.92	27 (65%)	56,56,56	2.61	20 (35%)
35	LHG	W	101	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
38	CHL	Y	601	22	60,74,74	1.32	8 (13%)	58,114,114	1.72	12 (20%)
28	CLA	c	502	3	69,73,73	1.34	6 (8%)	82,113,113	1.89	19 (23%)
32	LMG	A	411	-	48,48,55	1.12	5 (10%)	56,56,63	1.17	4 (7%)
30	BCR	c	514	-	41,41,41	4.91	27 (65%)	56,56,56	2.57	21 (37%)
28	CLA	c	501	3	69,73,73	1.35	6 (8%)	82,113,113	1.85	19 (23%)
28	CLA	G	612	-	64,68,73	1.39	6 (9%)	76,107,113	2.00	21 (27%)
28	CLA	a	407	42	54,58,73	1.52	5 (9%)	64,95,113	2.08	19 (29%)
28	CLA	B	603	2	69,73,73	1.35	6 (8%)	82,113,113	1.85	19 (23%)
28	CLA	r	603	17	64,68,73	1.41	6 (9%)	76,107,113	1.91	17 (22%)
30	BCR	D	405	-	41,41,41	4.91	27 (65%)	56,56,56	2.55	19 (33%)
30	BCR	c	515	-	41,41,41	4.95	27 (65%)	56,56,56	2.28	19 (33%)
28	CLA	n	602	7	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
39	LUT	n	615	-	42,43,43	6.40	26 (61%)	51,60,60	2.12	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	CHL	G	601	7	60,74,74	1.27	8 (13%)	58,114,114	1.65	11 (18%)
38	CHL	r	605	42	60,74,74	1.54	8 (13%)	58,114,114	1.60	11 (18%)
28	CLA	d	405	4	69,73,73	1.35	5 (7%)	82,113,113	1.92	19 (23%)
28	CLA	b	614	2	69,73,73	1.34	7 (10%)	82,113,113	1.92	19 (23%)
28	CLA	y	313	22	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
28	CLA	S	309	18	49,53,73	1.59	5 (10%)	58,89,113	2.09	16 (27%)
28	CLA	Y	612	22	64,68,73	1.39	7 (10%)	76,107,113	1.94	19 (25%)
28	CLA	g	603	7	69,73,73	1.36	6 (8%)	82,113,113	1.87	17 (20%)
32	LMG	a	413	-	40,40,55	1.02	3 (7%)	48,48,63	1.10	4 (8%)
35	LHG	c	519	-	30,30,48	0.48	0	32,35,54	1.28	3 (9%)
31	SQD	a	411	-	48,50,54	0.80	1 (2%)	58,61,65	0.89	2 (3%)
28	CLA	c	511	3	69,73,73	1.35	6 (8%)	82,113,113	1.91	20 (24%)
28	CLA	g	604	42	54,58,73	1.58	7 (12%)	64,95,113	2.13	18 (28%)
28	CLA	S	303	18	65,69,73	1.38	7 (10%)	77,108,113	1.96	20 (25%)
35	LHG	l	101	-	48,48,48	0.43	0	51,54,54	1.11	4 (7%)
30	BCR	A	409	-	41,41,41	4.93	27 (65%)	56,56,56	2.25	18 (32%)
35	LHG	C	521	-	48,48,48	0.38	0	51,54,54	1.10	3 (5%)
38	CHL	n	605	7	42,56,74	1.47	9 (21%)	36,92,114	2.04	11 (30%)
28	CLA	Y	614	22	52,56,73	1.55	6 (11%)	61,92,113	2.09	17 (27%)
28	CLA	n	604	40,42	54,58,73	1.53	7 (12%)	64,95,113	2.12	18 (28%)
28	CLA	C	510	3	69,73,73	1.34	7 (10%)	82,113,113	1.85	18 (21%)
35	LHG	D	407	-	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
28	CLA	B	607	42	69,73,73	1.34	6 (8%)	82,113,113	1.90	18 (21%)
31	SQD	B	620	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
28	CLA	c	503	3	69,73,73	1.35	6 (8%)	82,113,113	1.87	19 (23%)
30	BCR	C	516	-	41,41,41	4.94	27 (65%)	56,56,56	2.46	19 (33%)
28	CLA	Y	610	22	64,68,73	1.44	6 (9%)	76,107,113	1.92	20 (26%)
41	XAT	R	615	-	41,47,47	0.65	0	54,74,74	1.90	12 (22%)
30	BCR	B	617	-	41,41,41	4.95	27 (65%)	56,56,56	2.23	20 (35%)
30	BCR	b	617	-	41,41,41	4.95	27 (65%)	56,56,56	2.28	21 (37%)
28	CLA	R	603	17	64,68,73	1.44	6 (9%)	76,107,113	1.92	19 (25%)
35	LHG	b	624	-	45,45,48	0.41	0	48,51,54	1.13	4 (8%)
31	SQD	a	414	-	52,54,54	0.77	0	62,65,65	0.84	2 (3%)
28	CLA	c	508	3	69,73,73	1.37	6 (8%)	82,113,113	1.88	19 (23%)
28	CLA	R	611	17	53,57,73	1.54	6 (11%)	61,93,113	2.17	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	LMG	B	624	-	31,31,55	0.53	0	39,39,63	1.30	3 (7%)
28	CLA	d	404	4	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
28	CLA	r	608	17	62,66,73	1.42	6 (9%)	73,104,113	2.00	17 (23%)
40	NEX	g	617	-	40,46,46	2.76	12 (30%)	50,70,70	1.51	7 (14%)
28	CLA	r	610	35	53,57,73	1.53	6 (11%)	61,93,113	2.14	17 (27%)
38	CHL	n	609	7	60,74,74	1.43	9 (15%)	58,114,114	1.67	12 (20%)
28	CLA	R	604	42	52,56,73	1.60	9 (17%)	61,92,113	2.15	18 (29%)
38	CHL	s	601	18	40,54,74	1.69	8 (20%)	34,90,114	2.03	11 (32%)
28	CLA	b	606	2	69,73,73	1.35	6 (8%)	82,113,113	1.85	21 (25%)
28	CLA	B	608	2	69,73,73	1.35	7 (10%)	82,113,113	1.85	19 (23%)
28	CLA	n	603	7	69,73,73	1.34	7 (10%)	82,113,113	1.96	21 (25%)
40	NEX	s	616	-	40,46,46	2.73	12 (30%)	50,70,70	1.54	7 (14%)
40	NEX	G	617	28	40,46,46	2.81	12 (30%)	50,70,70	1.93	8 (16%)
39	LUT	R	614	-	42,43,43	6.36	26 (61%)	51,60,60	2.34	17 (33%)
38	CHL	g	605	7	40,54,74	1.48	8 (20%)	34,90,114	2.08	11 (32%)
28	CLA	c	506	3	60,64,73	1.45	7 (11%)	71,102,113	1.98	19 (26%)
35	LHG	B	625	-	45,45,48	0.41	0	48,51,54	1.03	3 (6%)
35	LHG	y	319	28	48,48,48	0.49	1 (2%)	51,54,54	1.13	3 (5%)
28	CLA	g	602	7	69,73,73	1.34	6 (8%)	82,113,113	1.90	20 (24%)
30	BCR	B	619	-	41,41,41	4.94	27 (65%)	56,56,56	2.46	22 (39%)
39	LUT	g	615	-	42,43,43	6.40	25 (59%)	51,60,60	2.09	12 (23%)
28	CLA	Y	604	40,42	54,58,73	1.52	7 (12%)	64,95,113	2.09	18 (28%)
31	SQD	A	410	-	48,50,54	0.80	1 (2%)	58,61,65	0.87	2 (3%)
36	DGD	C	519	-	61,61,67	1.18	6 (9%)	75,75,81	0.94	3 (4%)
30	BCR	k	101	-	41,41,41	4.95	27 (65%)	56,56,56	2.34	19 (33%)
33	PL9	d	407	-	55,55,55	0.73	1 (1%)	68,69,69	0.61	2 (2%)
28	CLA	G	611	35	64,68,73	1.39	6 (9%)	76,107,113	1.92	16 (21%)
28	CLA	R	602	17	64,68,73	1.45	6 (9%)	76,107,113	1.96	19 (25%)
35	LHG	c	520	-	39,39,48	0.42	0	42,45,54	1.21	4 (9%)
36	DGD	b	625	-	63,63,67	1.23	7 (11%)	77,77,81	0.97	2 (2%)
28	CLA	s	611	-	53,57,73	1.54	7 (13%)	61,93,113	2.09	18 (29%)
35	LHG	r	617	28	29,29,48	0.49	0	32,35,54	1.37	4 (12%)
38	CHL	s	607	-	40,54,74	1.61	9 (22%)	34,90,114	2.05	9 (26%)
40	NEX	n	617	28	40,46,46	2.80	12 (30%)	50,70,70	1.68	9 (18%)
38	CHL	y	309	22	60,74,74	1.51	8 (13%)	58,114,114	1.67	12 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	CLA	G	602	7	69,73,73	1.35	6 (8%)	82,113,113	1.92	21 (25%)
38	CHL	Y	609	22	60,74,74	1.52	9 (15%)	58,114,114	1.68	13 (22%)
33	PL9	A	412	-	13,13,55	1.58	1 (7%)	17,17,69	1.11	2 (11%)
38	CHL	g	608	42	60,74,74	1.39	8 (13%)	58,114,114	1.68	11 (18%)
28	CLA	R	601	17	49,53,73	1.60	6 (12%)	58,89,113	2.10	17 (29%)
30	BCR	B	618	-	41,41,41	4.95	27 (65%)	56,56,56	2.26	19 (33%)
38	CHL	r	607	42	55,69,74	1.28	8 (14%)	52,108,114	1.72	9 (17%)
28	CLA	c	505	3	61,65,73	1.43	6 (9%)	72,103,113	1.96	19 (26%)
28	CLA	C	505	3	69,73,73	1.35	6 (8%)	82,113,113	1.86	18 (21%)
28	CLA	B	604	2	69,73,73	1.35	7 (10%)	82,113,113	1.91	19 (23%)
28	CLA	b	604	2	69,73,73	1.35	6 (8%)	82,113,113	1.95	19 (23%)
39	LUT	Y	615	-	42,43,43	6.20	26 (61%)	51,60,60	2.25	21 (41%)
28	CLA	G	603	7	57,61,73	1.49	6 (10%)	67,98,113	2.07	19 (28%)
39	LUT	y	315	-	42,43,43	6.40	25 (59%)	51,60,60	1.94	17 (33%)
38	CHL	Y	607	42	60,74,74	1.30	8 (13%)	58,114,114	1.52	9 (15%)
28	CLA	C	511	3	69,73,73	1.35	6 (8%)	82,113,113	1.94	21 (25%)
28	CLA	S	312	18	53,57,73	1.54	6 (11%)	61,93,113	2.13	16 (26%)
34	BCT	A	415	26	3,3,3	1.02	0	2,3,3	1.66	1 (50%)
39	LUT	S	316	-	42,43,43	6.43	27 (64%)	51,60,60	2.15	12 (23%)
28	CLA	C	501	3	69,73,73	1.35	6 (8%)	82,113,113	1.85	19 (23%)
35	LHG	b	621	-	33,33,48	0.46	0	36,39,54	1.14	3 (8%)
28	CLA	c	513	3	61,65,73	1.43	7 (11%)	72,103,113	2.01	19 (26%)
28	CLA	G	604	40	54,58,73	1.53	6 (11%)	64,95,113	2.08	18 (28%)
39	LUT	s	615	-	42,43,43	6.36	27 (64%)	51,60,60	2.24	15 (29%)
28	CLA	C	512	3	61,65,73	1.42	6 (9%)	72,103,113	1.98	20 (27%)
32	LMG	b	620	-	51,51,55	1.21	6 (11%)	59,59,63	1.06	3 (5%)
35	LHG	d	408	-	48,48,48	0.40	0	51,54,54	1.10	4 (7%)
28	CLA	g	614	7	49,53,73	1.59	7 (14%)	58,89,113	2.11	16 (27%)
30	BCR	i	101	-	41,41,41	4.96	27 (65%)	56,56,56	2.45	20 (35%)
28	CLA	r	613	17	69,73,73	1.34	5 (7%)	82,113,113	1.89	19 (23%)
35	LHG	L	102	-	48,48,48	0.38	0	51,54,54	0.99	2 (3%)
28	CLA	b	611	2	69,73,73	1.35	6 (8%)	82,113,113	1.90	20 (24%)
34	BCT	d	403	26	3,3,3	1.00	0	2,3,3	1.68	1 (50%)
38	CHL	N	605	7	42,56,74	1.54	8 (19%)	36,92,114	1.98	10 (27%)
28	CLA	D	401	42	69,73,73	1.35	6 (8%)	82,113,113	1.86	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LHG	B	623	-	40,40,48	0.42	0	43,46,54	1.11	3 (6%)
38	CHL	Y	605	22	42,56,74	1.58	8 (19%)	36,92,114	2.02	12 (33%)
28	CLA	R	613	17	69,73,73	1.34	5 (7%)	82,113,113	1.86	19 (23%)
36	DGD	c	517	-	55,55,67	1.08	4 (7%)	69,69,81	1.01	4 (5%)
39	LUT	n	616	-	42,43,43	6.29	25 (59%)	51,60,60	2.26	16 (31%)
28	CLA	B	616	2	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
28	CLA	C	504	42	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
29	PHO	D	402	-	58,69,69	0.80	3 (5%)	55,99,99	0.88	2 (3%)
38	CHL	g	606	42	44,58,74	1.76	9 (20%)	37,94,114	1.80	9 (24%)
38	CHL	N	601	7	46,60,74	1.45	8 (17%)	40,97,114	2.03	12 (30%)
28	CLA	y	304	22	69,73,73	1.34	5 (7%)	82,113,113	1.94	20 (24%)
28	CLA	C	513	3	69,73,73	1.35	6 (8%)	82,113,113	1.94	19 (23%)
28	CLA	y	310	22	64,68,73	1.40	6 (9%)	76,107,113	1.97	19 (25%)
38	CHL	S	302	18	40,54,74	1.73	8 (20%)	34,90,114	2.02	11 (32%)
38	CHL	y	306	22	42,56,74	1.46	7 (16%)	36,92,114	1.99	9 (25%)
35	LHG	b	622	-	40,40,48	0.41	0	43,46,54	1.13	3 (6%)
28	CLA	b	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	19 (23%)
28	CLA	A	406	42	54,58,73	1.52	6 (11%)	64,95,113	2.09	19 (29%)
38	CHL	n	606	42	44,58,74	1.62	7 (15%)	37,94,114	1.97	11 (29%)
28	CLA	c	509	3	69,73,73	1.38	6 (8%)	82,113,113	1.95	21 (25%)
28	CLA	s	602	18	65,69,73	1.39	7 (10%)	77,108,113	1.96	19 (24%)
28	CLA	g	613	7	56,60,73	1.49	6 (10%)	65,97,113	2.12	18 (27%)
38	CHL	G	609	7	49,63,74	1.65	9 (18%)	44,100,114	1.91	12 (27%)
28	CLA	b	612	2	69,73,73	1.33	6 (8%)	82,113,113	1.94	20 (24%)
28	CLA	C	502	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	20 (24%)
36	DGD	C	517	-	56,56,67	1.07	4 (7%)	70,70,81	1.01	3 (4%)
28	CLA	G	613	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	18 (21%)
35	LHG	s	617	28	48,48,48	0.39	0	51,54,54	1.04	4 (7%)
41	XAT	r	615	-	41,47,47	0.64	0	54,74,74	1.91	12 (22%)
28	CLA	C	506	3	69,73,73	1.35	6 (8%)	82,113,113	1.89	19 (23%)
28	CLA	R	610	35	53,57,73	1.53	6 (11%)	61,93,113	2.15	18 (29%)
28	CLA	s	613	18	53,57,73	1.54	6 (11%)	61,93,113	2.13	19 (31%)
28	CLA	r	611	17	53,57,73	1.59	5 (9%)	61,93,113	2.25	19 (31%)
28	CLA	r	612	17	64,68,73	1.40	6 (9%)	76,107,113	1.97	18 (23%)
39	LUT	N	615	-	42,43,43	6.36	25 (59%)	51,60,60	2.09	15 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LHG	S	317	28	42,42,48	0.41	0	45,48,54	1.10	3 (6%)
39	LUT	r	614	-	42,43,43	6.37	25 (59%)	51,60,60	3.41	21 (41%)
28	CLA	b	615	2	69,73,73	1.35	7 (10%)	82,113,113	1.86	19 (23%)
38	CHL	R	606	42	40,54,74	1.69	8 (20%)	34,90,114	1.98	10 (29%)
39	LUT	G	616	-	42,43,43	6.31	25 (59%)	51,60,60	2.29	14 (27%)
28	CLA	c	504	42	63,67,73	1.41	6 (9%)	74,105,113	1.92	21 (28%)
28	CLA	G	614	7	52,56,73	1.55	6 (11%)	61,92,113	2.06	18 (29%)
35	LHG	Y	619	28	48,48,48	0.48	1 (2%)	51,54,54	1.08	3 (5%)
28	CLA	N	603	7	59,63,73	1.45	6 (10%)	70,101,113	2.02	19 (27%)
28	CLA	S	311	35	60,64,73	1.44	6 (10%)	71,102,113	2.05	20 (28%)
28	CLA	Y	613	22	69,73,73	1.35	7 (10%)	82,113,113	1.85	19 (23%)
38	CHL	G	607	42	50,64,74	1.37	9 (18%)	46,102,114	1.86	12 (26%)
25	OEX	A	401	3,1,42	0,15,15	-	-	-	-	-
28	CLA	n	614	7	49,53,73	1.59	6 (12%)	58,89,113	2.04	16 (27%)
31	SQD	L	101	-	40,42,54	0.86	1 (2%)	50,53,65	0.92	2 (4%)
28	CLA	n	611	35	64,68,73	1.43	7 (10%)	76,107,113	1.99	21 (27%)
36	DGD	c	518	-	60,60,67	5.14	7 (11%)	74,74,81	1.18	4 (5%)
28	CLA	s	608	-	49,53,73	1.59	5 (10%)	58,89,113	2.05	16 (27%)
39	LUT	Y	616	-	42,43,43	6.39	25 (59%)	51,60,60	2.00	15 (29%)
40	NEX	N	617	28	40,46,46	2.72	12 (30%)	50,70,70	1.55	9 (18%)
28	CLA	r	602	17	64,68,73	1.40	6 (9%)	76,107,113	1.94	20 (26%)
36	DGD	C	518	-	63,63,67	1.23	7 (11%)	77,77,81	0.92	3 (3%)
38	CHL	g	609	-	55,69,74	1.54	8 (14%)	52,108,114	1.74	12 (23%)
38	CHL	N	607	42	60,74,74	1.28	9 (15%)	58,114,114	1.61	10 (17%)
35	LHG	B	622	-	29,29,48	0.48	0	32,35,54	1.22	3 (9%)
40	NEX	y	301	-	40,46,46	2.78	12 (30%)	50,70,70	1.43	9 (18%)
28	CLA	a	406	1	69,73,73	1.34	6 (8%)	82,113,113	1.85	18 (21%)
28	CLA	n	610	7	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
31	SQD	L	103	-	52,54,54	0.78	0	62,65,65	0.86	2 (3%)
28	CLA	c	510	3	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
41	XAT	Y	617	-	41,47,47	0.65	0	54,74,74	2.00	13 (24%)
35	LHG	R	616	28	24,24,48	0.51	0	27,30,54	1.17	2 (7%)
28	CLA	b	608	2	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
28	CLA	y	311	35	64,68,73	1.39	5 (7%)	76,107,113	1.94	18 (23%)
28	CLA	B	610	42	69,73,73	1.35	6 (8%)	82,113,113	1.86	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	PHO	d	402	-	58,69,69	0.80	3 (5%)	55,99,99	0.90	2 (3%)
28	CLA	d	401	42	69,73,73	1.35	6 (8%)	82,113,113	1.85	20 (24%)
28	CLA	N	604	40,42	54,58,73	1.52	6 (11%)	64,95,113	2.12	18 (28%)
30	BCR	C	514	-	41,41,41	4.93	27 (65%)	56,56,56	3.66	27 (48%)
38	CHL	N	609	7	58,72,74	1.40	9 (15%)	55,111,114	1.62	9 (16%)
30	BCR	K	101	-	41,41,41	4.92	27 (65%)	56,56,56	2.45	22 (39%)
39	LUT	s	614	-	42,43,43	6.39	27 (64%)	51,60,60	2.15	14 (27%)
28	CLA	G	610	7	68,72,73	1.36	6 (8%)	80,111,113	1.94	19 (23%)
28	CLA	b	605	2	69,73,73	1.40	6 (8%)	82,113,113	1.96	18 (21%)
37	HEM	f	101	6,5	50,50,50	1.57	9 (18%)	67,82,82	1.64	10 (14%)
32	LMG	c	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.05	3 (5%)
28	CLA	y	314	22	52,56,73	1.55	6 (11%)	61,92,113	2.07	17 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	602	2	1/1/15/20	18/39/115/115	-
35	LHG	S	301	-	-	27/38/38/53	-
38	CHL	N	608	42	3/3/20/26	10/39/137/137	-
28	CLA	N	613	7	1/1/12/20	5/25/101/115	-
32	LMG	D	408	-	-	7/41/61/70	0/1/1/1
38	CHL	R	605	42	3/3/16/26	1/17/115/137	-
28	CLA	D	404	4	1/1/15/20	12/39/115/115	-
28	CLA	S	304	18	1/1/11/20	8/15/91/115	-
28	CLA	S	310	18	1/1/13/20	9/27/103/115	-
38	CHL	S	306	42	3/3/16/26	2/15/113/137	-
28	CLA	A	405	1	1/1/15/20	13/39/115/115	-
35	LHG	n	618	28	-	22/36/36/53	-
28	CLA	g	611	35	1/1/14/20	15/33/109/115	-
38	CHL	G	606	42	3/3/16/26	3/20/118/137	-
35	LHG	A	416	-	-	29/47/47/53	-
28	CLA	C	503	-	1/1/15/20	16/39/115/115	-
30	BCR	b	618	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	C	508	3	1/1/15/20	11/39/115/115	-
38	CHL	n	601	7	3/3/17/26	2/25/123/137	-
28	CLA	g	610	7	1/1/13/20	10/31/107/115	-
28	CLA	B	612	2	1/1/15/20	15/39/115/115	-
28	CLA	y	305	42	1/1/12/20	10/21/97/115	-
28	CLA	y	303	22	1/1/15/20	13/39/115/115	-
38	CHL	S	308	-	3/3/16/26	7/15/113/137	-
28	CLA	R	612	17	1/1/13/20	6/27/103/115	-
35	LHG	w	102	-	-	27/43/43/53	-
28	CLA	r	609	17	1/1/15/20	13/39/115/115	-
32	LMG	A	413	-	-	7/35/55/70	0/1/1/1
28	CLA	B	614	2	1/1/15/20	15/39/115/115	-
28	CLA	b	610	42	1/1/15/20	5/39/115/115	-
28	CLA	s	604	42	1/1/12/20	8/21/97/115	-
38	CHL	n	607	42	3/3/20/26	9/39/137/137	-
28	CLA	n	613	7	1/1/13/20	5/27/103/115	-
31	SQD	M	101	-	-	13/37/57/69	0/1/1/1
28	CLA	r	601	17	1/1/11/20	6/20/96/115	-
28	CLA	c	512	3	1/1/13/20	17/30/106/115	-
28	CLA	N	612	7	1/1/14/20	13/33/109/115	-
38	CHL	n	608	42	3/3/20/26	16/39/137/137	-
28	CLA	b	601	42	1/1/15/20	14/39/115/115	-
39	LUT	g	616	-	-	7/29/67/67	0/2/2/2
28	CLA	S	305	42	1/1/12/20	9/21/97/115	-
28	CLA	s	603	18	1/1/11/20	6/15/91/115	-
28	CLA	B	606	2	1/1/15/20	11/39/115/115	-
37	HEM	E	101	6,5	-	7/14/54/54	-
36	DGD	B	626	-	-	9/51/91/95	0/2/2/2
30	BCR	H	101	-	-	13/29/63/63	0/2/2/2
38	CHL	y	302	22	3/3/20/26	20/39/137/137	-
36	DGD	A	417	-	-	16/48/88/95	0/2/2/2
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
32	LMG	B	621	-	-	9/46/66/70	0/1/1/1
28	CLA	s	612	18	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	N	602	7	1/1/15/20	15/39/115/115	-
28	CLA	Y	611	35	1/1/14/20	12/33/109/115	-
30	BCR	C	515	-	-	14/29/63/63	0/2/2/2
28	CLA	B	615	2	1/1/15/20	15/39/115/115	-
35	LHG	N	618	28	-	23/35/35/53	-
39	LUT	y	316	-	-	7/29/67/67	0/2/2/2
28	CLA	b	607	42	1/1/15/20	16/39/115/115	-
38	CHL	s	605	42	3/3/16/26	6/15/113/137	-
38	CHL	g	607	42	3/3/18/26	12/29/127/137	-
40	NEX	r	616	28	-	6/27/83/83	0/3/3/3
28	CLA	N	614	7	1/1/11/20	8/19/95/115	-
32	LMG	d	409	-	-	4/41/61/70	0/1/1/1
28	CLA	y	312	22	1/1/14/20	13/33/109/115	-
28	CLA	Y	603	22	1/1/13/20	12/27/103/115	-
38	CHL	R	607	42	3/3/19/26	12/33/131/137	-
29	PHO	A	407	-	-	6/37/103/103	0/5/6/6
38	CHL	g	619	42	3/3/20/26	17/39/137/137	-
33	PL9	D	406	-	-	7/53/73/73	0/1/1/1
38	CHL	y	307	42	3/3/16/26	5/20/118/137	-
40	NEX	y	318	-	-	8/27/83/83	0/3/3/3
28	CLA	B	611	2	1/1/15/20	14/39/115/115	-
28	CLA	b	616	2	1/1/15/20	17/39/115/115	-
28	CLA	R	608	17	1/1/13/20	12/31/107/115	-
28	CLA	C	507	42	1/1/15/20	15/39/115/115	-
38	CHL	s	606	42	3/3/18/26	8/30/128/137	-
41	XAT	y	317	-	-	2/31/93/93	0/4/4/4
39	LUT	G	615	-	-	10/29/67/67	0/2/2/2
28	CLA	B	602	2	1/1/15/20	14/39/115/115	-
39	LUT	S	315	-	-	7/29/67/67	0/2/2/2
38	CHL	N	606	42	3/3/16/26	4/20/118/137	-
35	LHG	G	618	28	-	31/53/53/53	-
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
28	CLA	a	409	1	1/1/14/20	9/33/109/115	-
30	BCR	a	410	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	613	2	1/1/15/20	11/39/115/115	-
28	CLA	b	613	2	1/1/15/20	8/39/115/115	-
38	CHL	r	606	42	3/3/18/26	4/27/125/137	-
30	BCR	h	101	-	-	14/29/63/63	0/2/2/2
32	LMG	C	522	-	-	14/39/59/70	0/1/1/1
28	CLA	s	610	35	1/1/13/20	10/29/105/115	-
38	CHL	y	308	42	3/3/20/26	14/39/137/137	-
28	CLA	Y	602	22	1/1/15/20	12/39/115/115	-
38	CHL	Y	606	42	3/3/16/26	1/20/118/137	-
28	CLA	B	605	2	1/1/15/20	16/39/115/115	-
28	CLA	c	507	42	1/1/15/20	10/39/115/115	-
38	CHL	G	608	42	3/3/20/26	8/39/137/137	-
32	LMG	b	623	-	-	13/45/65/70	0/1/1/1
35	LHG	a	415	-	-	29/47/47/53	-
36	DGD	c	516	-	-	6/44/84/95	0/2/2/2
30	BCR	T	101	-	-	9/29/63/63	0/2/2/2
38	CHL	S	307	42	3/3/18/26	11/30/128/137	-
28	CLA	r	604	40,42	1/1/11/20	10/19/95/115	-
31	SQD	A	414	-	-	11/49/69/69	0/1/1/1
28	CLA	B	601	42	1/1/15/20	12/39/115/115	-
28	CLA	C	509	3	1/1/15/20	15/39/115/115	-
28	CLA	g	612	7	1/1/11/20	6/15/91/115	-
38	CHL	g	601	7	3/3/20/26	10/39/137/137	-
28	CLA	S	313	18	1/1/13/20	8/27/103/115	-
29	PHO	a	408	-	-	5/37/103/103	0/5/6/6
38	CHL	Y	608	42	3/3/20/26	13/39/137/137	-
28	CLA	S	314	18	1/1/11/20	3/20/96/115	-
33	PL9	a	412	-	-	0/5/18/73	0/1/1/1
32	LMG	k	102	-	-	7/46/66/70	0/1/1/1
32	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	CLA	R	609	17	1/1/15/20	12/39/115/115	-
28	CLA	B	609	2	1/1/15/20	12/39/115/115	-
28	CLA	b	609	-	1/1/15/20	10/39/115/115	-
28	CLA	n	612	7	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	NEX	Y	618	28	-	3/27/83/83	0/3/3/3
32	LMG	w	101	-	-	7/43/63/70	0/1/1/1
36	DGD	a	401	-	-	11/48/88/95	0/2/2/2
30	BCR	d	406	-	-	10/29/63/63	0/2/2/2
28	CLA	N	610	7	1/1/15/20	17/39/115/115	-
28	CLA	D	403	4	1/1/15/20	11/39/115/115	-
28	CLA	A	408	1	1/1/14/20	18/33/109/115	-
28	CLA	s	609	18	1/1/13/20	9/27/103/115	-
38	CHL	G	605	7	3/3/16/26	7/15/113/137	-
35	LHG	g	618	28	-	27/45/45/53	-
28	CLA	N	611	35	1/1/14/20	14/33/109/115	-
30	BCR	t	101	-	-	14/29/63/63	0/2/2/2
35	LHG	W	101	-	-	35/53/53/53	-
38	CHL	Y	601	22	3/3/20/26	8/39/137/137	-
28	CLA	c	502	3	1/1/15/20	15/39/115/115	-
32	LMG	A	411	-	-	6/43/63/70	0/1/1/1
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
28	CLA	c	501	3	1/1/15/20	9/39/115/115	-
28	CLA	G	612	-	1/1/14/20	12/33/109/115	-
28	CLA	a	407	42	1/1/12/20	3/21/97/115	-
28	CLA	B	603	2	1/1/15/20	13/39/115/115	-
28	CLA	r	603	17	1/1/14/20	16/33/109/115	-
30	BCR	D	405	-	-	15/29/63/63	0/2/2/2
30	BCR	c	515	-	-	13/29/63/63	0/2/2/2
28	CLA	n	602	7	1/1/15/20	20/39/115/115	-
39	LUT	n	615	-	-	7/29/67/67	0/2/2/2
38	CHL	G	601	7	3/3/20/26	9/39/137/137	-
38	CHL	r	605	42	3/3/20/26	5/39/137/137	-
28	CLA	d	405	4	1/1/15/20	16/39/115/115	-
28	CLA	b	614	2	1/1/15/20	13/39/115/115	-
28	CLA	y	313	22	1/1/15/20	8/39/115/115	-
28	CLA	S	309	18	1/1/11/20	8/15/91/115	-
28	CLA	Y	612	22	1/1/14/20	11/33/109/115	-
28	CLA	g	603	7	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	a	413	-	-	5/35/55/70	0/1/1/1
35	LHG	c	519	-	-	23/34/34/53	-
31	SQD	a	411	-	-	10/45/65/69	0/1/1/1
28	CLA	c	511	3	1/1/15/20	12/39/115/115	-
28	CLA	g	604	42	1/1/12/20	7/21/97/115	-
28	CLA	S	303	18	1/1/14/20	16/35/111/115	-
35	LHG	l	101	-	-	24/53/53/53	-
30	BCR	A	409	-	-	14/29/63/63	0/2/2/2
35	LHG	C	521	-	-	35/53/53/53	-
38	CHL	n	605	7	3/3/16/26	6/18/116/137	-
28	CLA	Y	614	22	1/1/11/20	6/19/95/115	-
28	CLA	n	604	40,42	1/1/12/20	9/21/97/115	-
28	CLA	C	510	3	1/1/15/20	16/39/115/115	-
35	LHG	D	407	-	-	36/53/53/53	-
28	CLA	B	607	42	1/1/15/20	18/39/115/115	-
31	SQD	B	620	-	-	7/49/69/69	0/1/1/1
28	CLA	c	503	3	1/1/15/20	15/39/115/115	-
30	BCR	C	516	-	-	16/29/63/63	0/2/2/2
28	CLA	Y	610	22	1/1/14/20	13/33/109/115	-
41	XAT	R	615	-	-	7/31/93/93	0/4/4/4
30	BCR	B	617	-	-	14/29/63/63	0/2/2/2
30	BCR	b	617	-	-	14/29/63/63	0/2/2/2
28	CLA	R	603	17	1/1/14/20	11/33/109/115	-
35	LHG	b	624	-	-	31/50/50/53	-
31	SQD	a	414	-	-	10/49/69/69	0/1/1/1
28	CLA	c	508	3	1/1/15/20	16/39/115/115	-
28	CLA	R	611	17	1/1/11/20	6/20/96/115	-
32	LMG	B	624	-	-	14/26/46/70	0/1/1/1
28	CLA	d	404	4	1/1/15/20	10/39/115/115	-
28	CLA	r	608	17	1/1/13/20	12/31/107/115	-
40	NEX	g	617	-	-	18/27/83/83	0/3/3/3
28	CLA	r	610	35	1/1/11/20	11/20/96/115	-
38	CHL	n	609	7	3/3/20/26	9/39/137/137	-
28	CLA	R	604	42	1/1/11/20	6/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	s	601	18	3/3/16/26	7/15/113/137	-
28	CLA	b	606	2	1/1/15/20	14/39/115/115	-
28	CLA	B	608	2	1/1/15/20	9/39/115/115	-
28	CLA	n	603	7	1/1/15/20	18/39/115/115	-
40	NEX	s	616	-	-	8/27/83/83	0/3/3/3
40	NEX	G	617	28	-	8/27/83/83	0/3/3/3
39	LUT	R	614	-	-	5/29/67/67	0/2/2/2
38	CHL	g	605	7	3/3/16/26	5/15/113/137	-
28	CLA	c	506	3	1/1/13/20	10/29/105/115	-
35	LHG	B	625	-	-	31/50/50/53	-
35	LHG	y	319	28	-	33/53/53/53	-
28	CLA	g	602	7	1/1/15/20	17/39/115/115	-
30	BCR	B	619	-	-	14/29/63/63	0/2/2/2
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
28	CLA	Y	604	40,42	1/1/12/20	9/21/97/115	-
31	SQD	A	410	-	-	9/45/65/69	0/1/1/1
36	DGD	C	519	-	-	11/49/89/95	0/2/2/2
30	BCR	k	101	-	-	13/29/63/63	0/2/2/2
33	PL9	d	407	-	-	7/53/73/73	0/1/1/1
28	CLA	G	611	35	1/1/14/20	13/33/109/115	-
28	CLA	R	602	17	1/1/14/20	10/33/109/115	-
35	LHG	c	520	-	-	27/44/44/53	-
36	DGD	b	625	-	-	6/51/91/95	0/2/2/2
28	CLA	s	611	-	1/1/11/20	7/20/96/115	-
38	CHL	s	607	-	3/3/16/26	4/15/113/137	-
35	LHG	r	617	28	-	22/34/34/53	-
40	NEX	n	617	28	-	13/27/83/83	0/3/3/3
38	CHL	y	309	22	3/3/20/26	6/39/137/137	-
28	CLA	G	602	7	1/1/15/20	16/39/115/115	-
38	CHL	Y	609	22	3/3/20/26	9/39/137/137	-
33	PL9	A	412	-	-	0/5/18/73	0/1/1/1
38	CHL	g	608	42	3/3/20/26	14/39/137/137	-
28	CLA	R	601	17	1/1/11/20	6/15/91/115	-
30	BCR	B	618	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	r	607	42	3/3/19/26	15/33/131/137	-
28	CLA	c	505	3	1/1/13/20	14/30/106/115	-
28	CLA	C	505	3	1/1/15/20	8/39/115/115	-
28	CLA	B	604	2	1/1/15/20	16/39/115/115	-
28	CLA	b	604	2	1/1/15/20	14/39/115/115	-
39	LUT	Y	615	-	-	3/29/67/67	0/2/2/2
28	CLA	G	603	7	1/1/12/20	9/25/101/115	-
39	LUT	y	315	-	-	4/29/67/67	0/2/2/2
38	CHL	Y	607	42	3/3/20/26	17/39/137/137	-
28	CLA	C	511	3	1/1/15/20	13/39/115/115	-
28	CLA	S	312	18	1/1/11/20	8/20/96/115	-
39	LUT	S	316	-	-	6/29/67/67	0/2/2/2
28	CLA	C	501	3	1/1/15/20	9/39/115/115	-
35	LHG	b	621	-	-	22/38/38/53	-
28	CLA	c	513	3	1/1/13/20	8/30/106/115	-
28	CLA	G	604	40	1/1/12/20	8/21/97/115	-
39	LUT	s	615	-	-	6/29/67/67	0/2/2/2
28	CLA	C	512	3	1/1/13/20	17/30/106/115	-
32	LMG	b	620	-	-	12/46/66/70	0/1/1/1
35	LHG	d	408	-	-	30/53/53/53	-
28	CLA	g	614	7	1/1/11/20	4/15/91/115	-
30	BCR	i	101	-	-	14/29/63/63	0/2/2/2
28	CLA	r	613	17	1/1/15/20	12/39/115/115	-
35	LHG	L	102	-	-	30/53/53/53	-
28	CLA	b	611	2	1/1/15/20	17/39/115/115	-
38	CHL	N	605	7	3/3/16/26	4/18/116/137	-
28	CLA	D	401	42	1/1/15/20	14/39/115/115	-
35	LHG	B	623	-	-	26/45/45/53	-
38	CHL	Y	605	22	3/3/16/26	4/18/116/137	-
28	CLA	R	613	17	1/1/15/20	10/39/115/115	-
36	DGD	c	517	-	-	13/43/83/95	0/2/2/2
39	LUT	n	616	-	-	3/29/67/67	0/2/2/2
28	CLA	B	616	2	1/1/15/20	14/39/115/115	-
28	CLA	C	504	42	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PHO	D	402	-	-	3/37/103/103	0/5/6/6
38	CHL	g	606	42	3/3/16/26	5/20/118/137	-
38	CHL	N	601	7	3/3/17/26	2/23/121/137	-
28	CLA	y	304	22	1/1/15/20	10/39/115/115	-
28	CLA	C	513	3	1/1/15/20	10/39/115/115	-
28	CLA	y	310	22	1/1/14/20	11/33/109/115	-
38	CHL	S	302	18	3/3/16/26	0/15/113/137	-
38	CHL	y	306	22	3/3/16/26	1/18/116/137	-
35	LHG	b	622	-	-	26/45/45/53	-
28	CLA	b	603	-	1/1/15/20	14/39/115/115	-
28	CLA	A	406	42	1/1/12/20	8/21/97/115	-
38	CHL	n	606	42	3/3/16/26	4/20/118/137	-
28	CLA	c	509	3	1/1/15/20	10/39/115/115	-
28	CLA	s	602	18	1/1/14/20	14/35/111/115	-
28	CLA	g	613	7	1/1/12/20	6/24/100/115	-
38	CHL	G	609	7	3/3/17/26	8/26/124/137	-
28	CLA	b	612	2	1/1/15/20	18/39/115/115	-
28	CLA	C	502	-	1/1/15/20	16/39/115/115	-
36	DGD	C	517	-	-	5/44/84/95	0/2/2/2
28	CLA	G	613	-	1/1/15/20	18/39/115/115	-
35	LHG	s	617	28	-	34/53/53/53	-
41	XAT	r	615	-	-	7/31/93/93	0/4/4/4
28	CLA	C	506	3	1/1/15/20	17/39/115/115	-
28	CLA	R	610	35	1/1/11/20	10/20/96/115	-
28	CLA	s	613	18	1/1/11/20	6/20/96/115	-
28	CLA	r	611	17	1/1/11/20	6/20/96/115	-
28	CLA	r	612	17	1/1/14/20	15/33/109/115	-
39	LUT	N	615	-	-	4/29/67/67	0/2/2/2
35	LHG	S	317	28	-	27/47/47/53	-
39	LUT	r	614	-	-	7/29/67/67	0/2/2/2
28	CLA	b	615	2	1/1/15/20	11/39/115/115	-
38	CHL	R	606	42	3/3/16/26	3/15/113/137	-
39	LUT	G	616	-	-	5/29/67/67	0/2/2/2
28	CLA	c	504	42	1/1/14/20	13/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	G	614	7	1/1/11/20	7/19/95/115	-
35	LHG	Y	619	28	-	33/53/53/53	-
28	CLA	N	603	7	1/1/13/20	11/27/103/115	-
28	CLA	S	311	35	1/1/13/20	13/29/105/115	-
28	CLA	Y	613	22	1/1/15/20	9/39/115/115	-
38	CHL	G	607	42	3/3/18/26	10/27/125/137	-
28	CLA	n	614	7	1/1/11/20	5/15/91/115	-
31	SQD	L	101	-	-	5/37/57/69	0/1/1/1
28	CLA	n	611	35	1/1/14/20	17/33/109/115	-
36	DGD	c	518	-	-	13/48/88/95	0/2/2/2
28	CLA	s	608	-	1/1/11/20	6/15/91/115	-
39	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
40	NEX	N	617	28	-	5/27/83/83	0/3/3/3
28	CLA	r	602	17	1/1/14/20	9/33/109/115	-
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
38	CHL	g	609	-	3/3/19/26	14/33/131/137	-
38	CHL	N	607	42	3/3/20/26	11/39/137/137	-
35	LHG	B	622	-	-	26/34/34/53	-
40	NEX	y	301	-	-	13/27/83/83	0/3/3/3
28	CLA	a	406	1	1/1/15/20	11/39/115/115	-
28	CLA	n	610	7	1/1/15/20	20/39/115/115	-
31	SQD	L	103	-	-	9/49/69/69	0/1/1/1
28	CLA	c	510	3	1/1/15/20	14/39/115/115	-
41	XAT	Y	617	-	-	4/31/93/93	0/4/4/4
35	LHG	R	616	28	-	16/29/29/53	-
28	CLA	b	608	2	1/1/15/20	5/39/115/115	-
28	CLA	y	311	35	1/1/14/20	12/33/109/115	-
28	CLA	B	610	42	1/1/15/20	17/39/115/115	-
29	PHO	d	402	-	-	2/37/103/103	0/5/6/6
28	CLA	d	401	42	1/1/15/20	13/39/115/115	-
28	CLA	N	604	40,42	1/1/12/20	7/21/97/115	-
38	CHL	N	609	7	3/3/20/26	13/33/131/137	-
30	BCR	C	514	-	-	13/29/63/63	0/2/2/2
30	BCR	K	101	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LUT	s	614	-	-	8/29/67/67	0/2/2/2
28	CLA	G	610	7	1/1/14/20	11/38/114/115	-
28	CLA	b	605	2	1/1/15/20	8/39/115/115	-
37	HEM	f	101	6,5	-	6/14/54/54	-
32	LMG	c	521	-	-	14/46/66/70	0/1/1/1
28	CLA	y	314	22	1/1/11/20	7/19/95/115	-

The worst 5 of 2705 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	518	DGD	C6B-C5B	38.69	3.44	1.51
39	S	316	LUT	C24-C25	24.53	1.62	1.33
39	n	615	LUT	C24-C25	24.34	1.62	1.33
39	y	315	LUT	C24-C25	24.34	1.62	1.33
39	g	615	LUT	C24-C25	24.33	1.62	1.33

The worst 5 of 4534 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	614	LUT	C15-C14-C13	-13.38	108.51	127.28
28	r	611	CLA	C4A-NA-C1A	10.28	111.37	106.68
30	C	514	BCR	C16-C17-C18	-10.10	113.12	127.28
30	C	514	BCR	C15-C14-C13	-9.96	113.30	127.28
39	G	615	LUT	C31-C30-C29	-9.76	113.59	127.28

5 of 306 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	405	CLA	ND
28	A	406	CLA	ND
28	A	408	CLA	ND
28	B	601	CLA	ND
28	B	602	CLA	ND

5 of 3806 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	405	CLA	C6-C7-C8-C9
28	A	406	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	B	601	CLA	O1A-CGA-O2A-C1
28	B	601	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

327 monomers are involved in 3043 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	602	CLA	8	0
35	S	301	LHG	5	0
38	N	608	CHL	16	0
28	N	613	CLA	7	0
32	D	408	LMG	15	0
38	R	605	CHL	11	0
28	D	404	CLA	9	0
28	S	304	CLA	11	0
28	S	310	CLA	26	0
38	S	306	CHL	11	0
28	A	405	CLA	6	0
35	n	618	LHG	6	0
28	g	611	CLA	5	0
35	A	416	LHG	4	0
38	G	606	CHL	11	0
28	C	503	CLA	9	0
30	b	618	BCR	15	0
28	C	508	CLA	18	0
38	n	601	CHL	11	0
28	g	610	CLA	15	0
28	B	612	CLA	10	0
28	y	305	CLA	6	0
28	y	303	CLA	7	0
38	S	308	CHL	9	0
28	R	612	CLA	12	0
35	w	102	LHG	8	0
28	r	609	CLA	19	0
32	A	413	LMG	11	0
28	B	614	CLA	15	0
28	b	610	CLA	13	0
28	s	604	CLA	11	0
38	n	607	CHL	21	0
28	n	613	CLA	12	0
31	M	101	SQD	5	0
28	r	601	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	c	512	CLA	10	0
28	N	612	CLA	17	0
38	n	608	CHL	13	0
28	b	601	CLA	16	0
39	g	616	LUT	18	0
28	S	305	CLA	8	0
28	s	603	CLA	7	0
28	B	606	CLA	16	0
37	E	101	HEM	7	0
36	B	626	DGD	11	0
30	H	101	BCR	14	0
36	A	417	DGD	10	0
38	y	302	CHL	13	0
39	N	616	LUT	17	0
32	B	621	LMG	18	0
28	s	612	CLA	10	0
28	N	602	CLA	21	0
28	Y	611	CLA	12	0
30	C	515	BCR	10	0
28	B	615	CLA	12	0
35	N	618	LHG	8	0
39	y	316	LUT	6	0
28	b	607	CLA	8	0
38	s	605	CHL	9	0
38	g	607	CHL	5	0
40	r	616	NEX	13	0
28	N	614	CLA	6	0
32	d	409	LMG	20	0
28	y	312	CLA	16	0
28	Y	603	CLA	16	0
29	A	407	PHO	9	0
38	R	607	CHL	4	0
38	g	619	CHL	20	0
33	D	406	PL9	8	0
38	y	307	CHL	10	0
40	y	318	NEX	6	0
28	B	611	CLA	15	0
28	b	616	CLA	16	0
28	R	608	CLA	20	0
28	C	507	CLA	21	0
38	s	606	CHL	10	0
41	y	317	XAT	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	G	615	LUT	28	0
28	B	602	CLA	12	0
39	S	315	LUT	24	0
38	N	606	CHL	11	0
35	G	618	LHG	7	0
30	b	619	BCR	10	0
28	a	409	CLA	11	0
30	a	410	BCR	22	0
28	B	613	CLA	16	0
28	b	613	CLA	12	0
38	r	606	CHL	11	0
30	h	101	BCR	19	0
32	C	522	LMG	7	0
28	s	610	CLA	7	0
38	y	308	CHL	13	0
28	Y	602	CLA	11	0
38	Y	606	CHL	10	0
28	B	605	CLA	19	0
28	c	507	CLA	15	0
38	G	608	CHL	19	0
32	b	623	LMG	8	0
35	a	415	LHG	10	0
36	c	516	DGD	12	0
30	T	101	BCR	13	0
38	S	307	CHL	14	0
28	r	604	CLA	11	0
31	A	414	SQD	14	0
28	B	601	CLA	14	0
28	C	509	CLA	13	0
28	g	612	CLA	10	0
38	g	601	CHL	23	0
28	S	313	CLA	9	0
29	a	408	PHO	12	0
38	Y	608	CHL	12	0
28	S	314	CLA	6	0
32	k	102	LMG	15	0
32	C	520	LMG	17	0
28	R	609	CLA	14	0
28	B	609	CLA	13	0
28	b	609	CLA	12	0
28	n	612	CLA	15	0
40	Y	618	NEX	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	w	101	LMG	13	0
36	a	401	DGD	17	0
30	d	406	BCR	20	0
28	N	610	CLA	15	0
28	D	403	CLA	7	0
28	A	408	CLA	16	0
28	s	609	CLA	18	0
38	G	605	CHL	10	0
35	g	618	LHG	9	0
28	N	611	CLA	13	0
30	t	101	BCR	10	0
35	W	101	LHG	20	0
38	Y	601	CHL	16	0
28	c	502	CLA	6	0
32	A	411	LMG	20	0
30	c	514	BCR	19	0
28	c	501	CLA	15	0
28	G	612	CLA	19	0
28	a	407	CLA	8	0
28	B	603	CLA	21	0
28	r	603	CLA	18	0
30	D	405	BCR	11	0
30	c	515	BCR	11	0
28	n	602	CLA	15	0
39	n	615	LUT	14	0
38	G	601	CHL	12	0
38	r	605	CHL	17	0
28	d	405	CLA	9	0
28	b	614	CLA	12	0
28	y	313	CLA	10	0
28	S	309	CLA	13	0
28	Y	612	CLA	13	0
28	g	603	CLA	9	0
32	a	413	LMG	14	0
35	c	519	LHG	5	0
31	a	411	SQD	20	0
28	c	511	CLA	17	0
28	g	604	CLA	14	0
28	S	303	CLA	23	0
35	l	101	LHG	5	0
30	A	409	BCR	12	0
35	C	521	LHG	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	n	605	CHL	12	0
28	Y	614	CLA	7	0
28	n	604	CLA	6	0
28	C	510	CLA	16	0
35	D	407	LHG	13	0
28	B	607	CLA	8	0
31	B	620	SQD	12	0
28	c	503	CLA	9	0
30	C	516	BCR	22	0
28	Y	610	CLA	6	0
41	R	615	XAT	13	0
30	B	617	BCR	16	0
30	b	617	BCR	9	0
28	R	603	CLA	9	0
35	b	624	LHG	10	0
31	a	414	SQD	10	0
28	c	508	CLA	11	0
28	R	611	CLA	5	0
32	B	624	LMG	5	0
28	d	404	CLA	9	0
28	r	608	CLA	19	0
40	g	617	NEX	9	0
28	r	610	CLA	8	0
38	n	609	CHL	21	0
28	R	604	CLA	11	0
38	s	601	CHL	14	0
28	b	606	CLA	17	0
28	B	608	CLA	11	0
28	n	603	CLA	23	0
40	s	616	NEX	7	0
40	G	617	NEX	11	0
39	R	614	LUT	14	0
38	g	605	CHL	11	0
28	c	506	CLA	12	0
35	B	625	LHG	8	0
35	y	319	LHG	6	0
28	g	602	CLA	18	0
30	B	619	BCR	21	0
39	g	615	LUT	18	0
28	Y	604	CLA	14	0
31	A	410	SQD	9	0
36	C	519	DGD	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	k	101	BCR	16	0
33	d	407	PL9	6	0
28	G	611	CLA	13	0
28	R	602	CLA	9	0
35	c	520	LHG	9	0
36	b	625	DGD	11	0
28	s	611	CLA	8	0
35	r	617	LHG	5	0
38	s	607	CHL	5	0
40	n	617	NEX	8	0
38	y	309	CHL	24	0
28	G	602	CLA	10	0
38	Y	609	CHL	15	0
38	g	608	CHL	14	0
28	R	601	CLA	12	0
30	B	618	BCR	14	0
38	r	607	CHL	13	0
28	c	505	CLA	10	0
28	C	505	CLA	15	0
28	B	604	CLA	7	0
28	b	604	CLA	15	0
39	Y	615	LUT	8	0
28	G	603	CLA	10	0
39	y	315	LUT	11	0
38	Y	607	CHL	31	0
28	C	511	CLA	16	0
28	S	312	CLA	12	0
39	S	316	LUT	19	0
28	C	501	CLA	13	0
35	b	621	LHG	3	0
28	c	513	CLA	12	0
28	G	604	CLA	7	0
39	s	615	LUT	17	0
28	C	512	CLA	17	0
32	b	620	LMG	14	0
35	d	408	LHG	12	0
28	g	614	CLA	7	0
30	i	101	BCR	8	0
28	r	613	CLA	19	0
35	L	102	LHG	6	0
28	b	611	CLA	15	0
38	N	605	CHL	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	D	401	CLA	7	0
35	B	623	LHG	14	0
38	Y	605	CHL	11	0
28	R	613	CLA	15	0
36	c	517	DGD	18	0
39	n	616	LUT	7	0
28	B	616	CLA	16	0
28	C	504	CLA	10	0
29	D	402	PHO	9	0
38	g	606	CHL	18	0
38	N	601	CHL	13	0
28	y	304	CLA	28	0
28	C	513	CLA	13	0
28	y	310	CLA	11	0
38	S	302	CHL	15	0
38	y	306	CHL	8	0
35	b	622	LHG	10	0
28	b	603	CLA	14	0
28	A	406	CLA	9	0
38	n	606	CHL	12	0
28	c	509	CLA	7	0
28	s	602	CLA	16	0
28	g	613	CLA	8	0
38	G	609	CHL	15	0
28	b	612	CLA	15	0
28	C	502	CLA	11	0
36	C	517	DGD	7	0
28	G	613	CLA	23	0
35	s	617	LHG	16	0
41	r	615	XAT	9	0
28	C	506	CLA	23	0
28	R	610	CLA	9	0
28	s	613	CLA	5	0
28	r	611	CLA	5	0
28	r	612	CLA	11	0
39	N	615	LUT	10	0
35	S	317	LHG	21	0
39	r	614	LUT	15	0
28	b	615	CLA	17	0
38	R	606	CHL	12	0
39	G	616	LUT	11	0
28	c	504	CLA	16	0

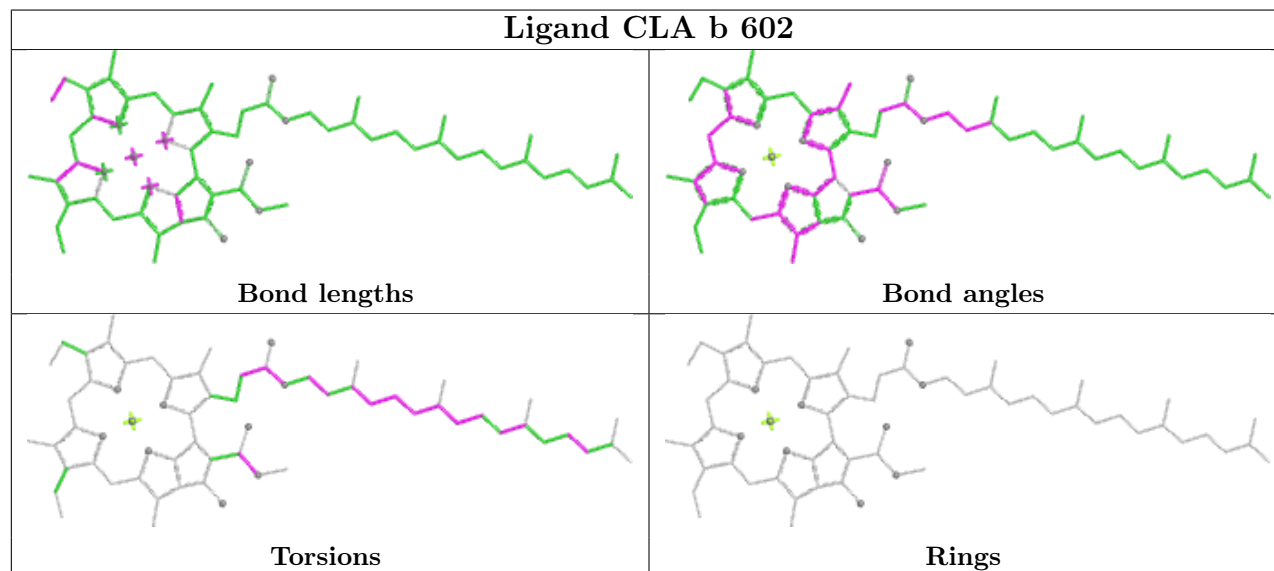
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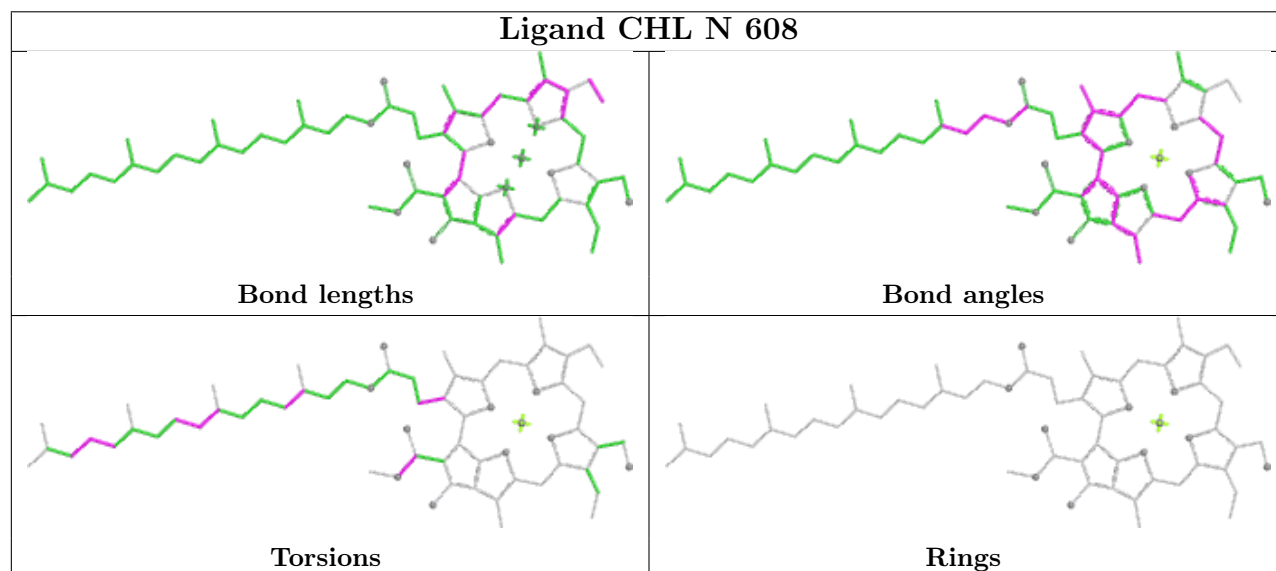
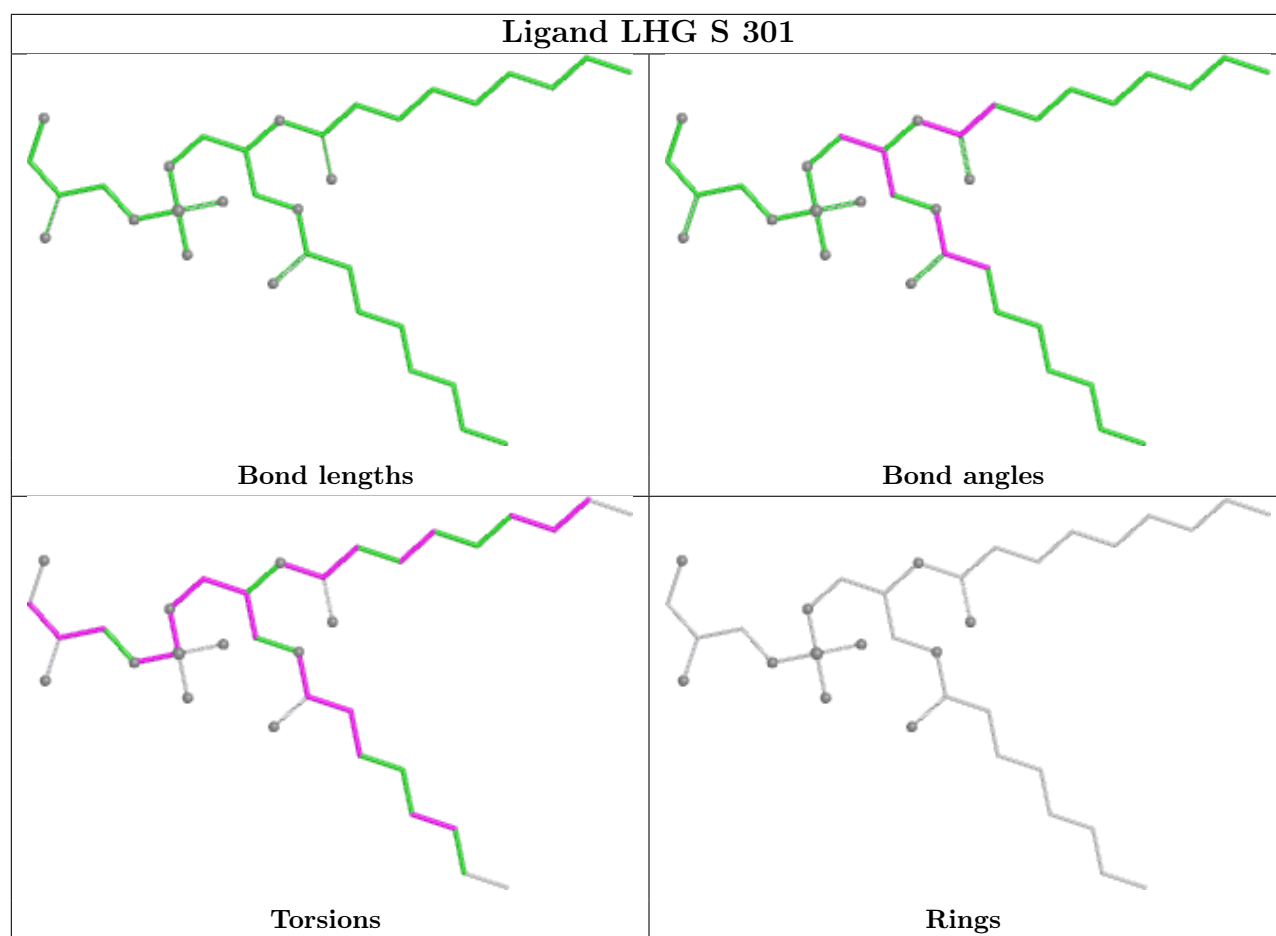
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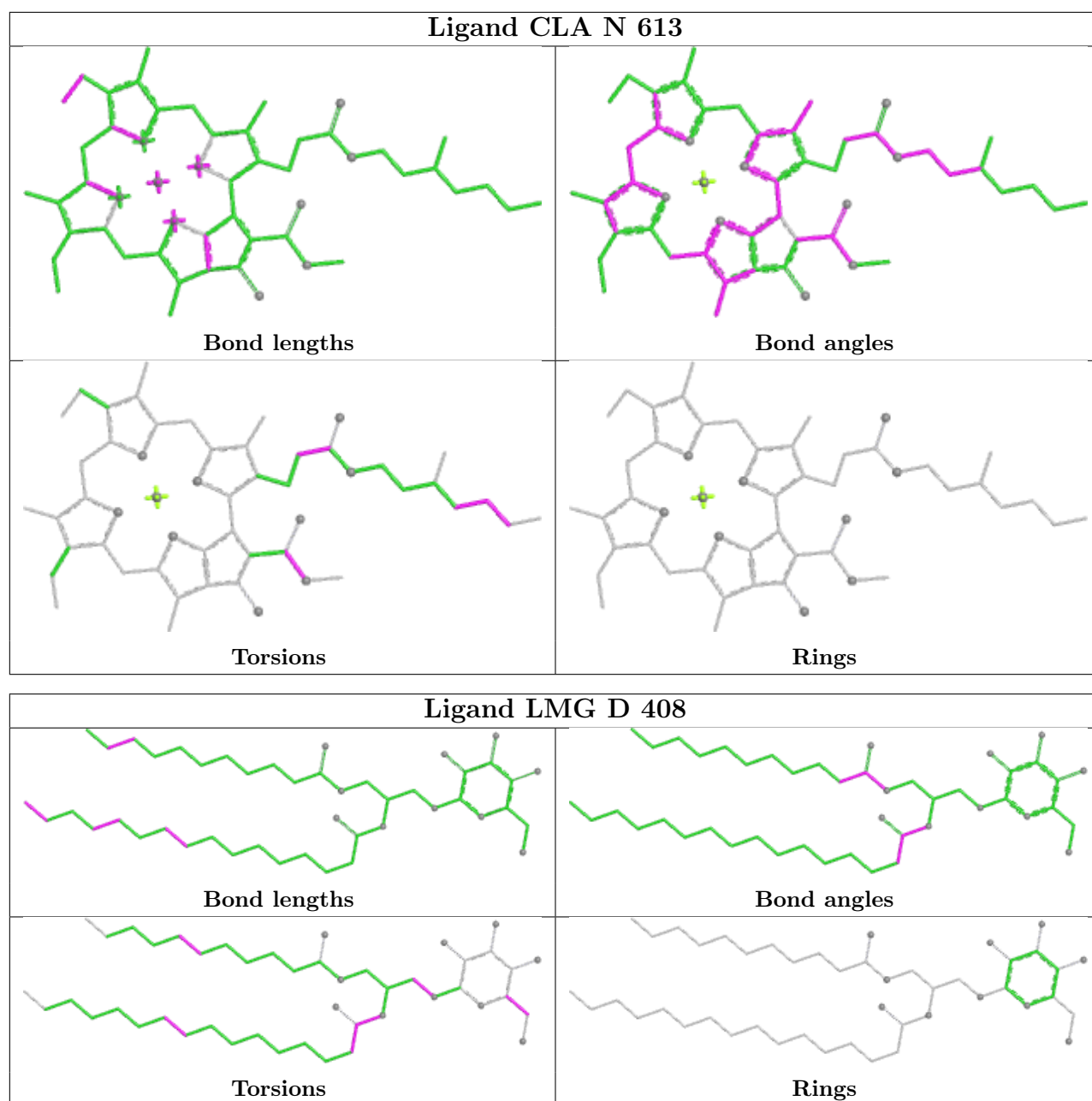
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	614	CLA	9	0
35	Y	619	LHG	5	0
28	N	603	CLA	10	0
28	S	311	CLA	16	0
28	Y	613	CLA	13	0
38	G	607	CHL	11	0
28	n	614	CLA	3	0
31	L	101	SQD	11	0
28	n	611	CLA	13	0
36	c	518	DGD	15	0
28	s	608	CLA	8	0
39	Y	616	LUT	7	0
40	N	617	NEX	9	0
28	r	602	CLA	7	0
36	C	518	DGD	28	0
38	g	609	CHL	14	0
38	N	607	CHL	13	0
35	B	622	LHG	8	0
40	y	301	NEX	4	0
28	a	406	CLA	13	0
28	n	610	CLA	24	0
31	L	103	SQD	10	0
28	c	510	CLA	11	0
41	Y	617	XAT	17	0
35	R	616	LHG	5	0
28	b	608	CLA	18	0
28	y	311	CLA	12	0
28	B	610	CLA	5	0
29	d	402	PHO	12	0
28	d	401	CLA	16	0
28	N	604	CLA	10	0
30	C	514	BCR	18	0
38	N	609	CHL	19	0
30	K	101	BCR	13	0
39	s	614	LUT	16	0
28	G	610	CLA	30	0
28	b	605	CLA	14	0
37	f	101	HEM	6	0
32	c	521	LMG	15	0
28	y	314	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

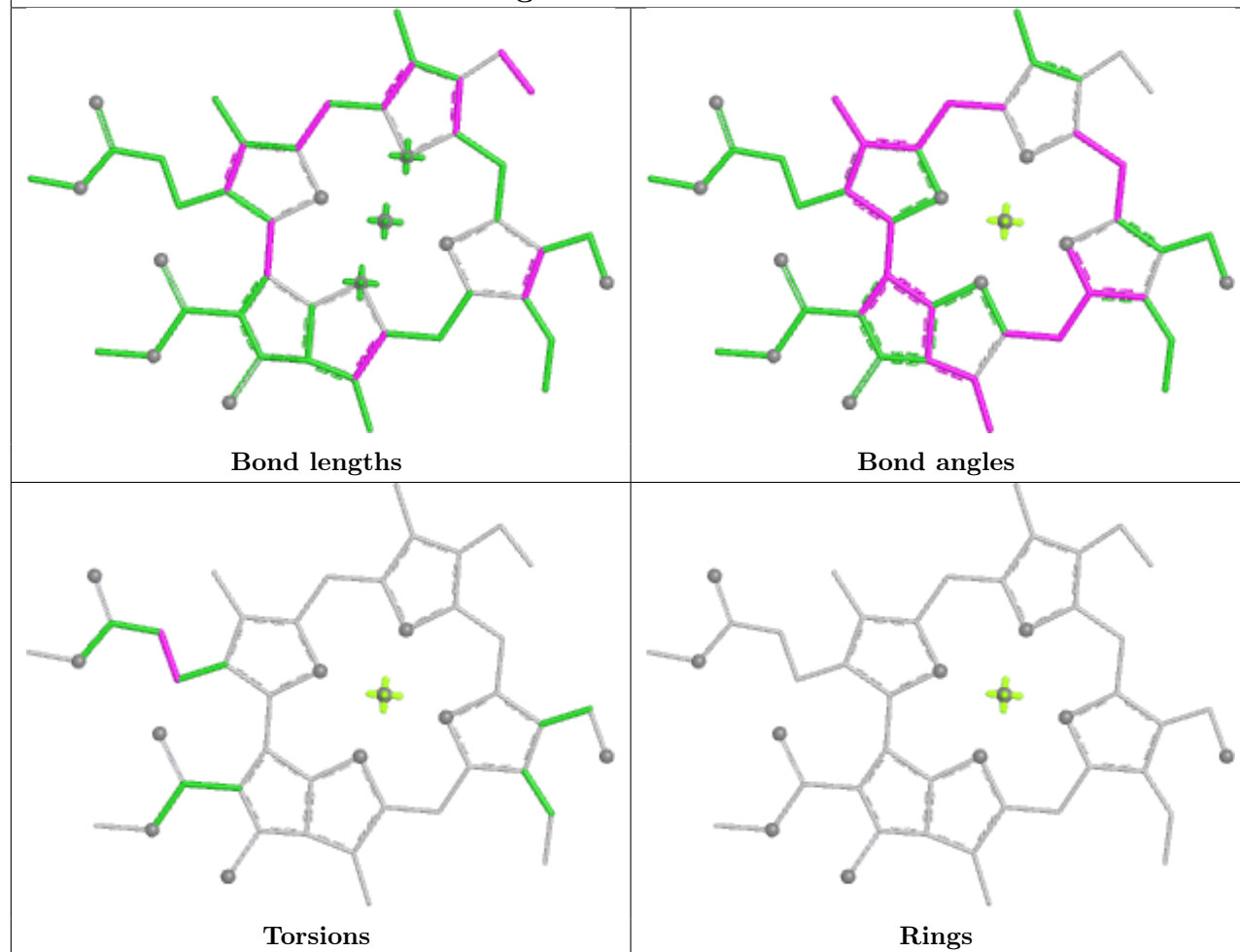
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



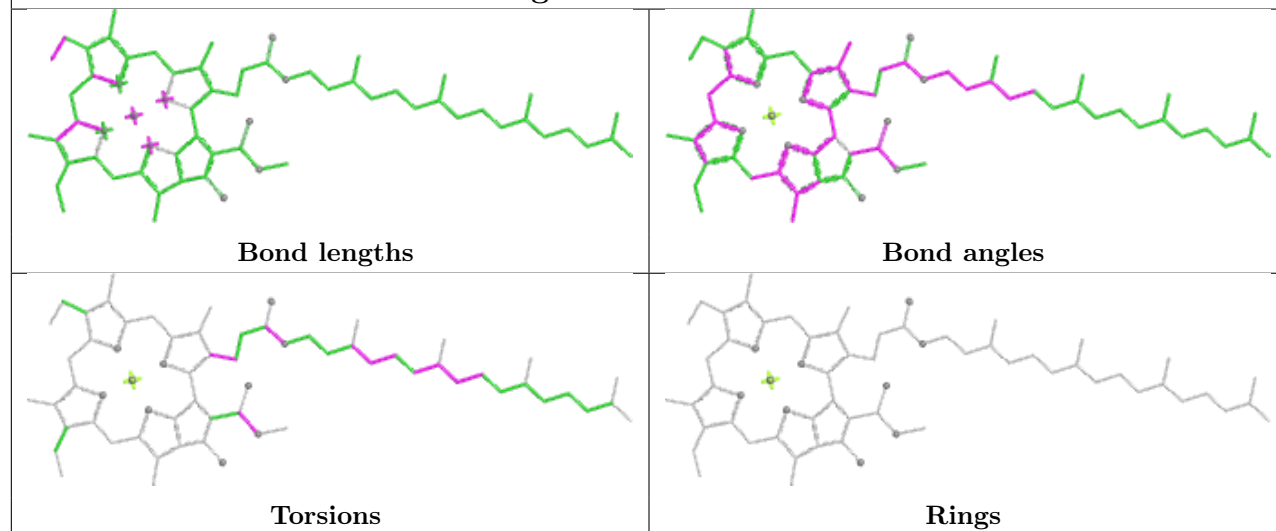




## Ligand CHL R 605

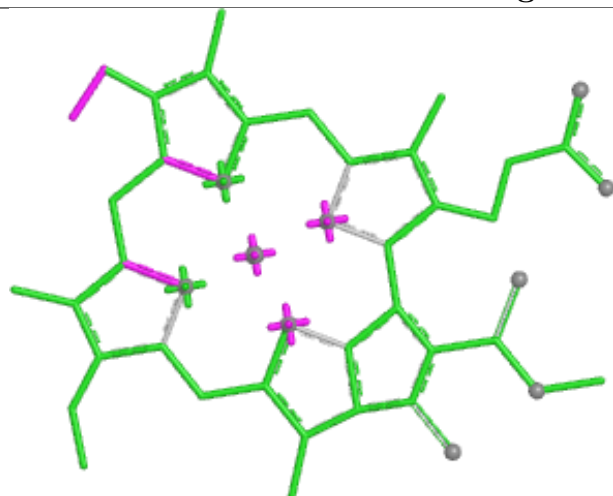


## Ligand CLA D 404

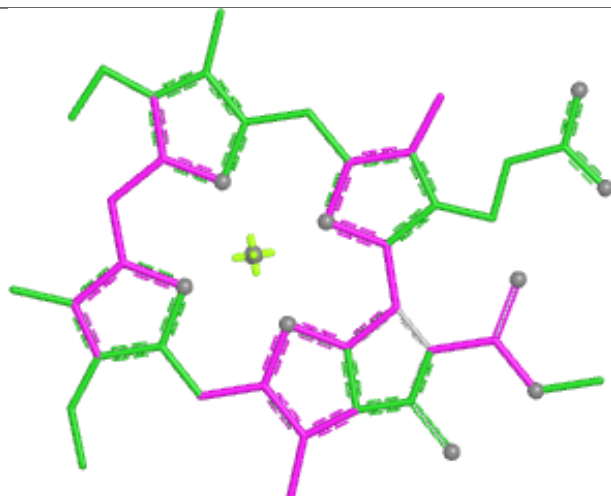




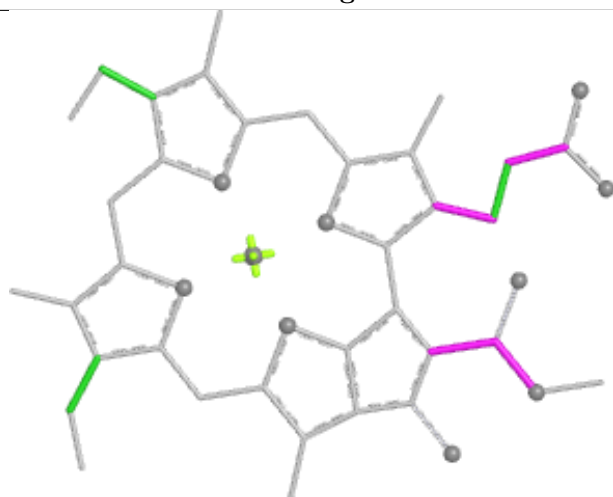
## Ligand CLA S 304



Bond lengths



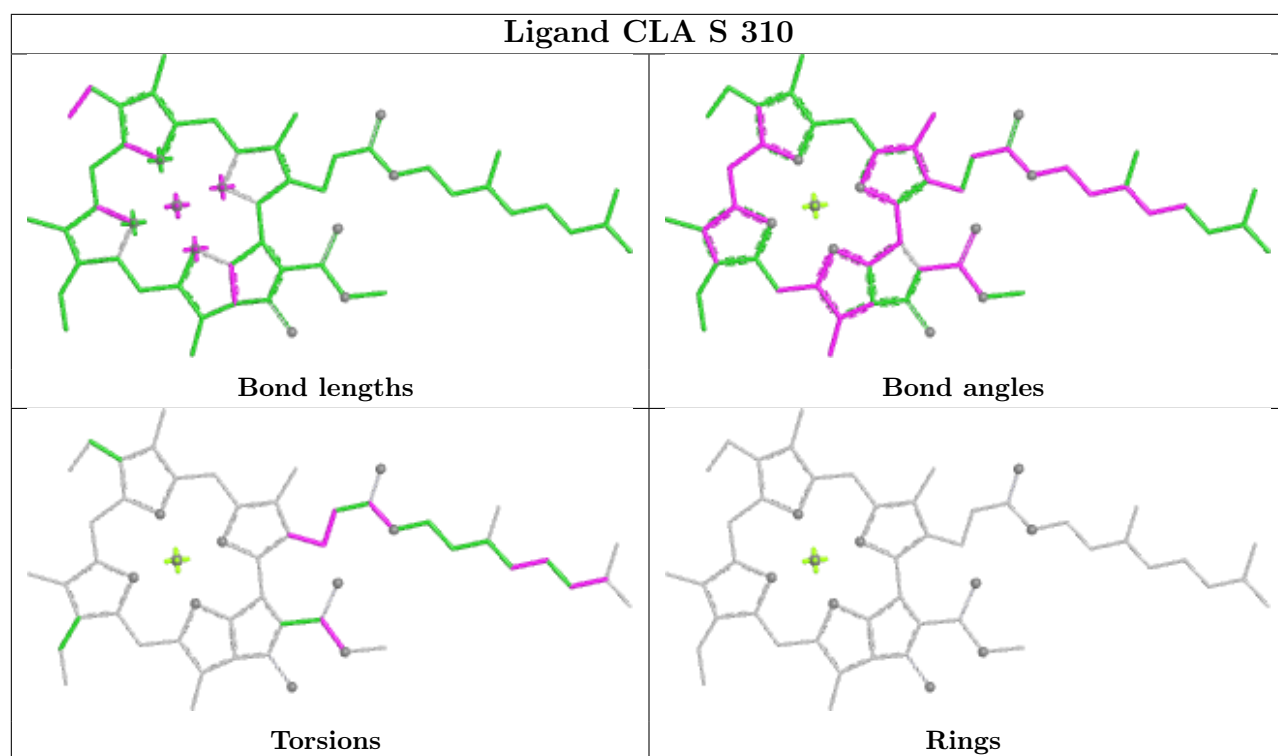
Bond angles



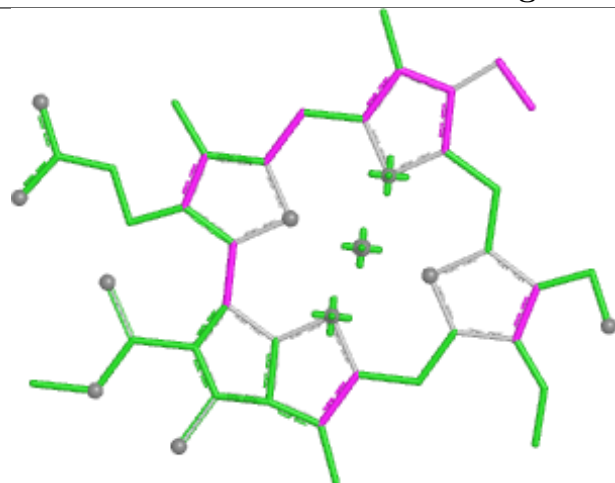
Torsions



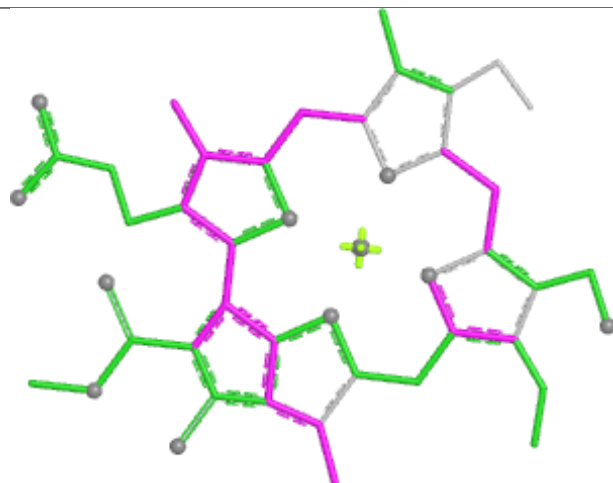
Rings



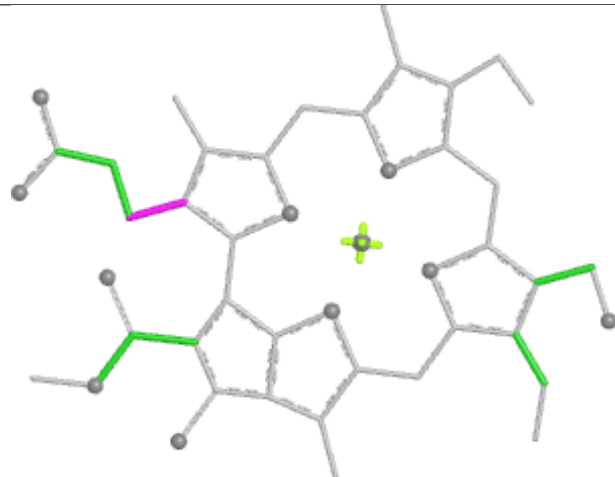
## Ligand CHL S 306



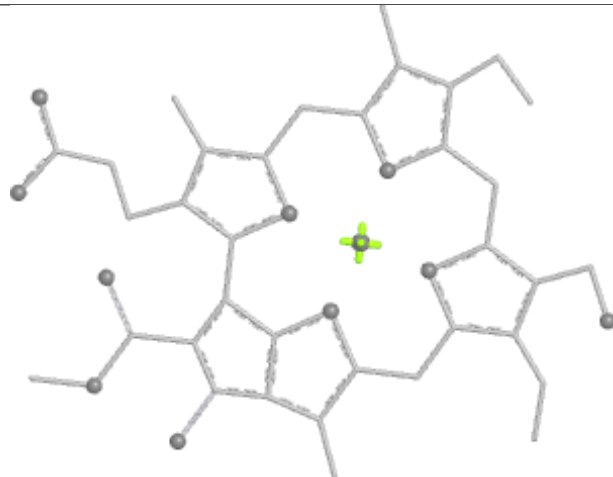
Bond lengths



Bond angles

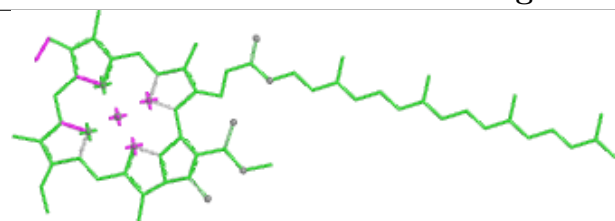


Torsions

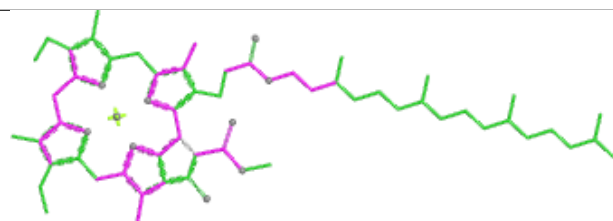


Rings

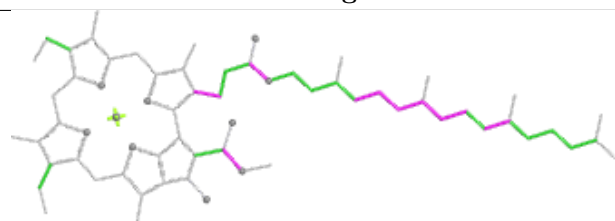
## Ligand CLA A 405



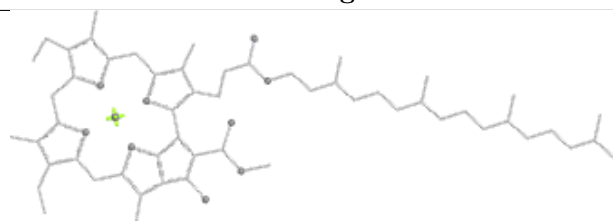
Bond lengths



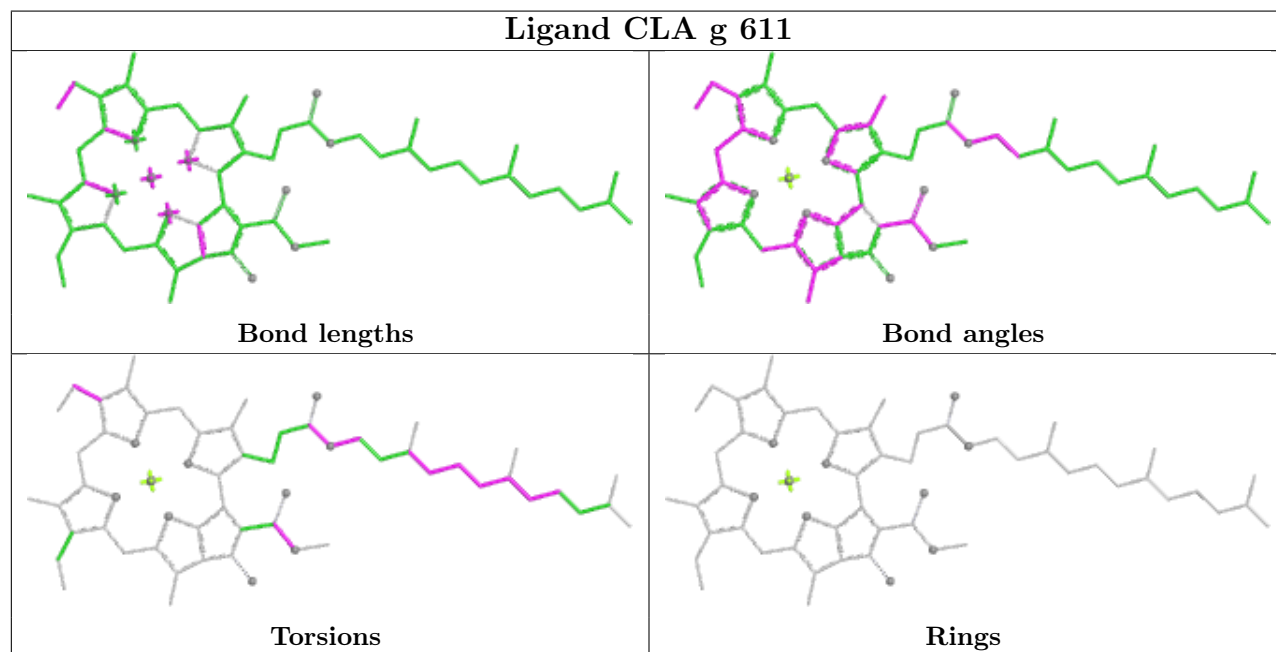
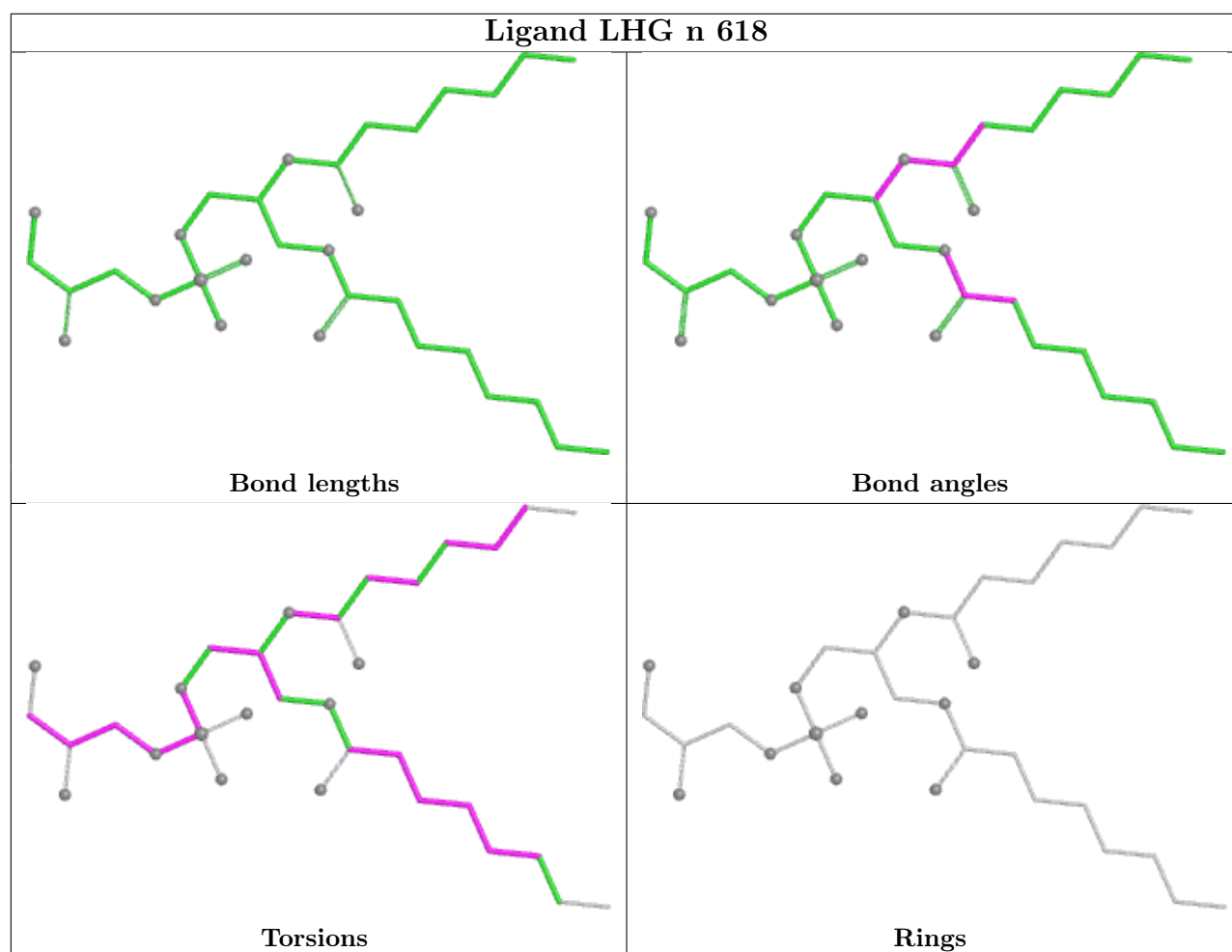
Bond angles

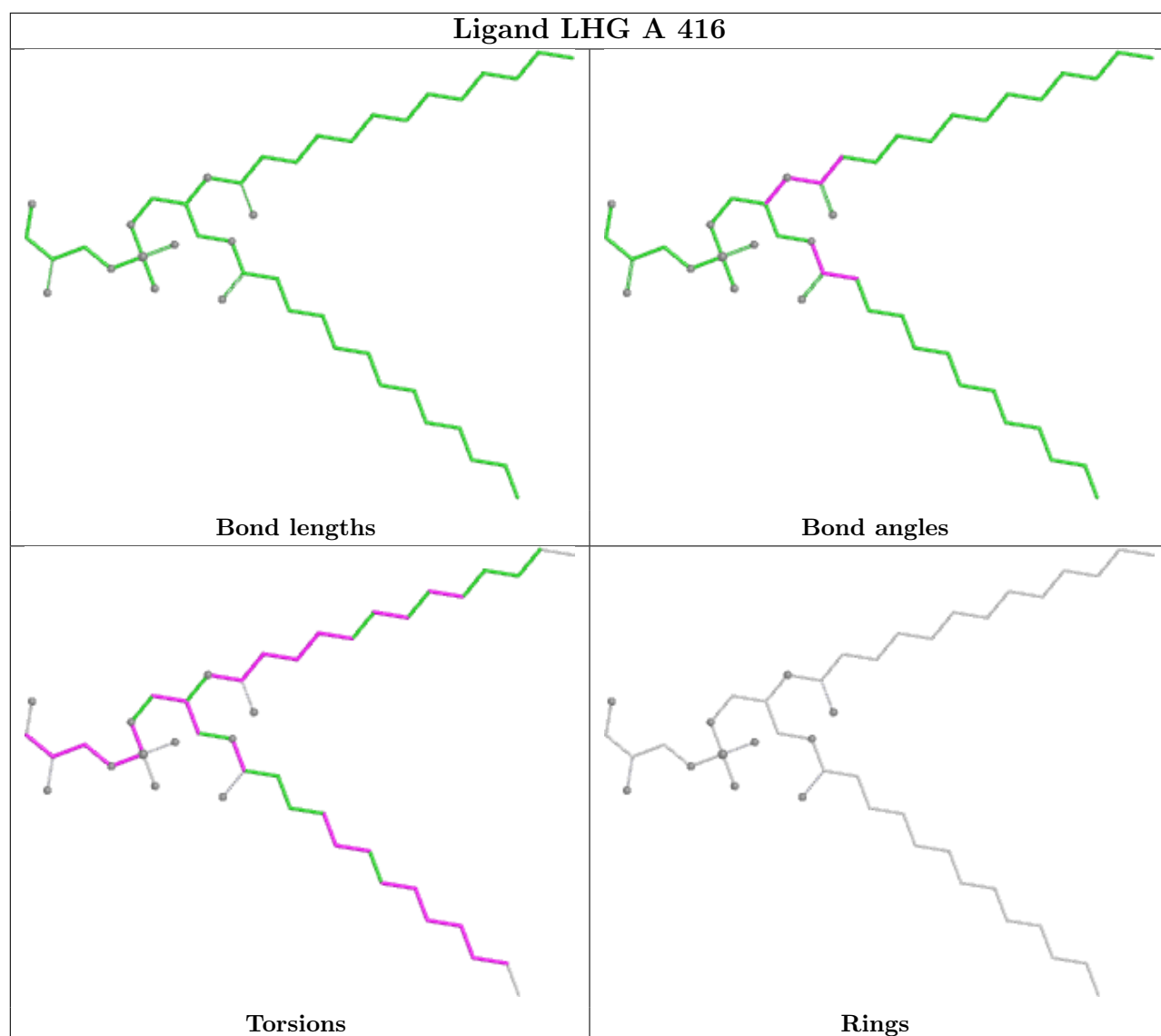


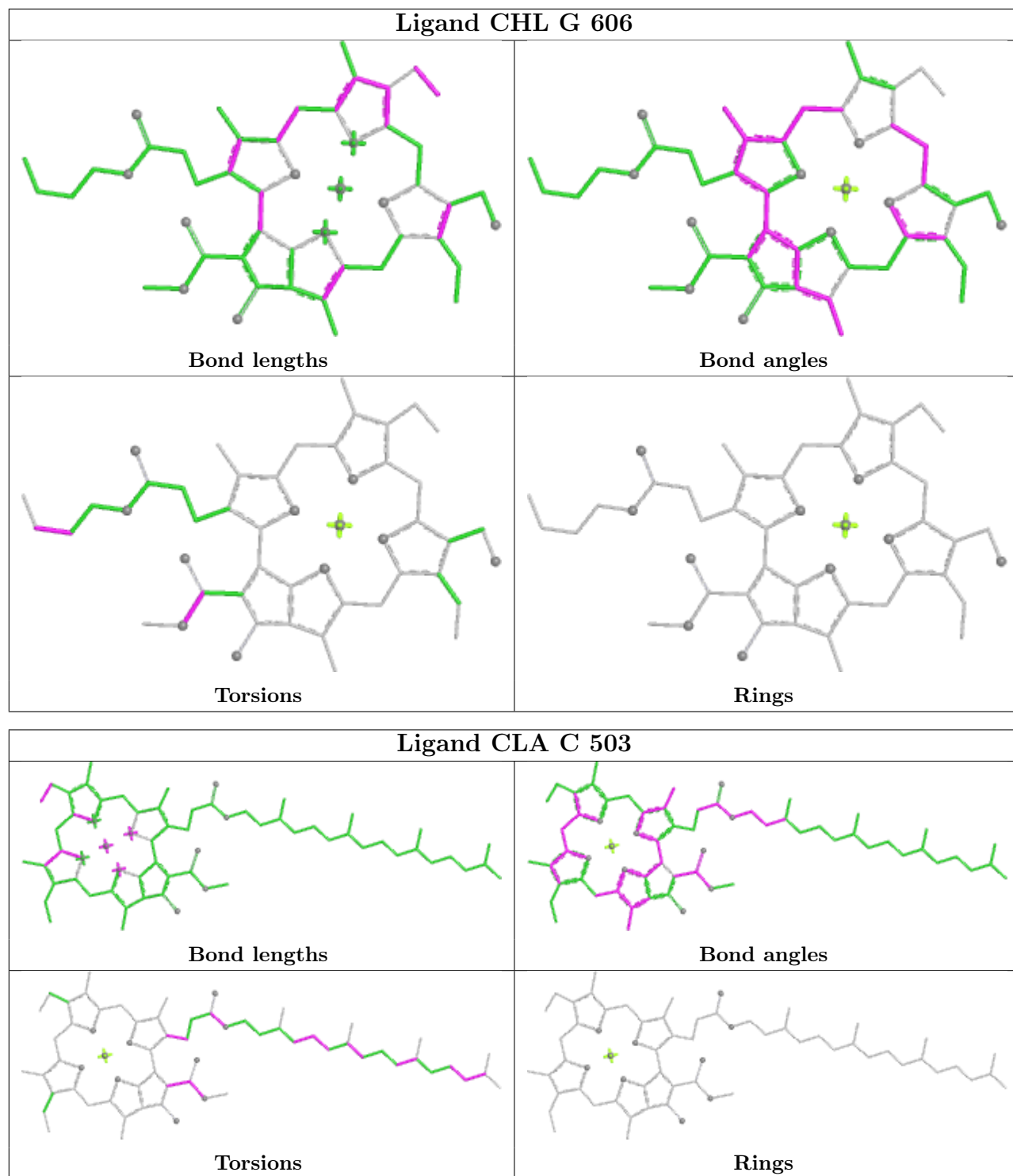
Torsions

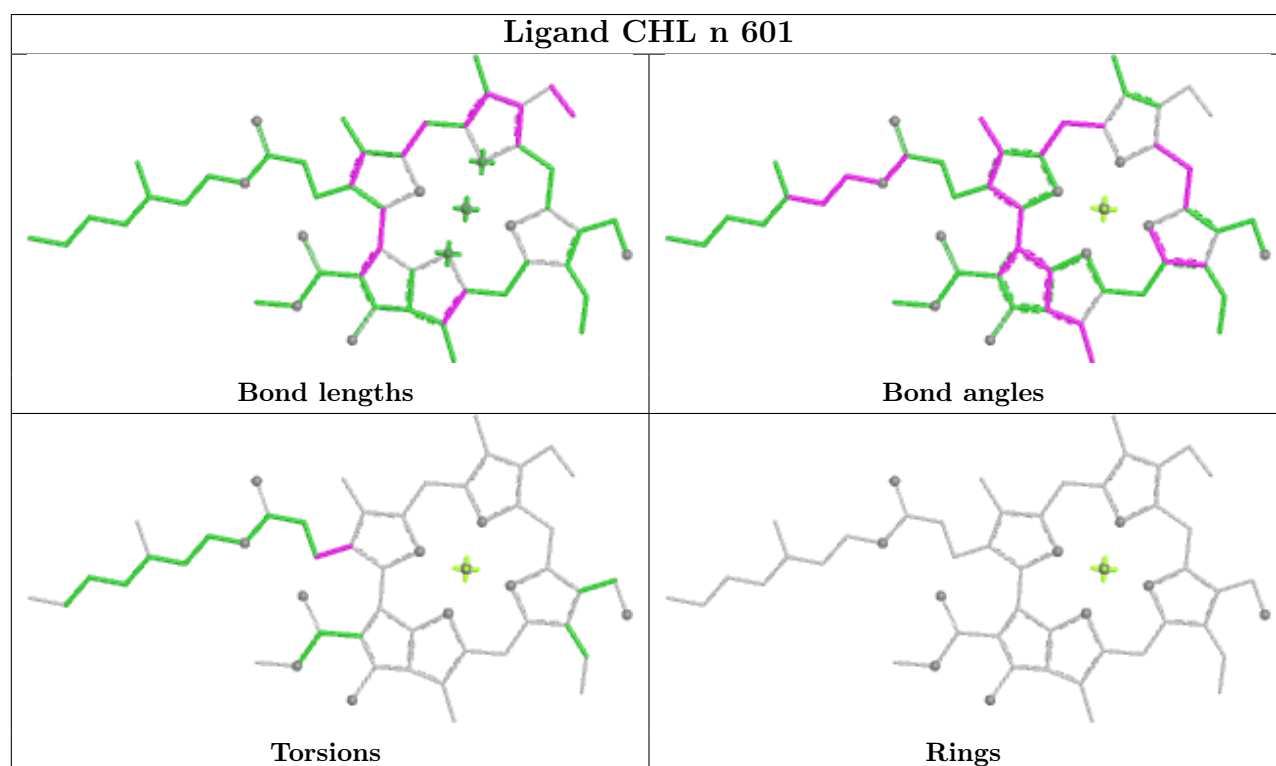
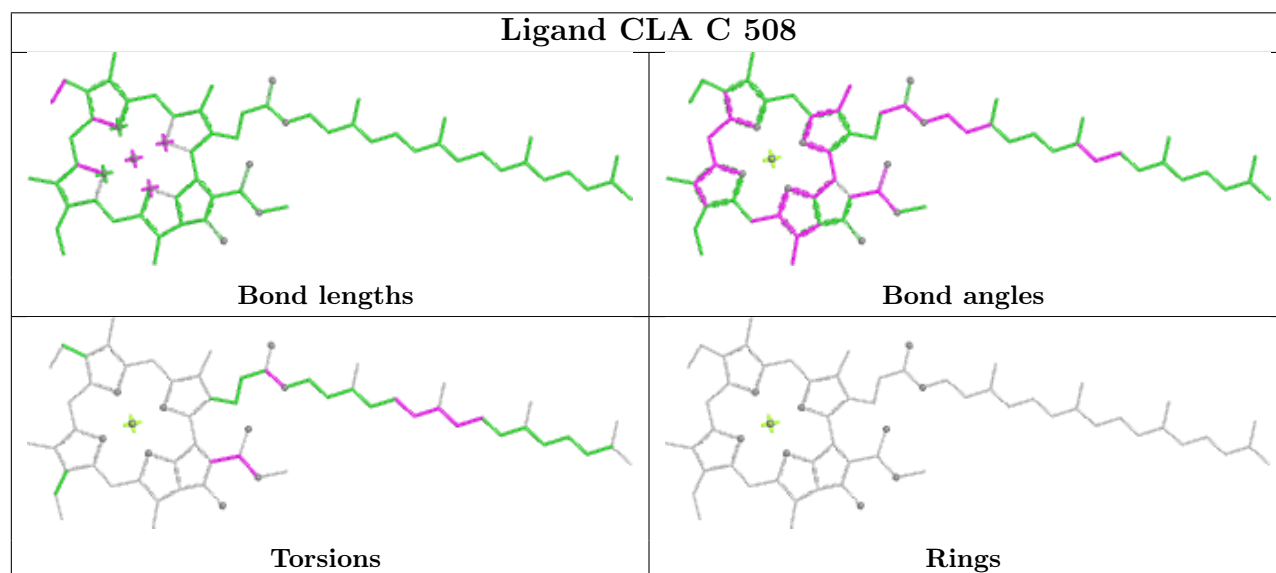
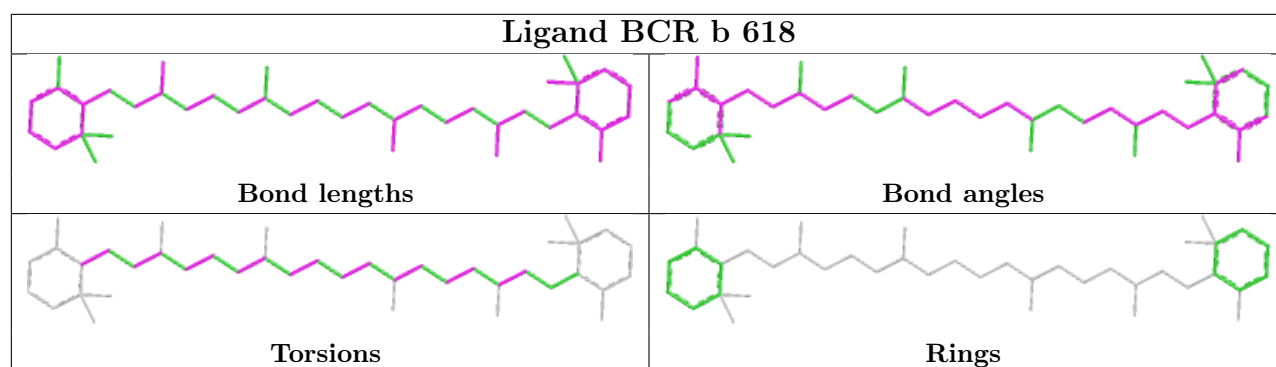


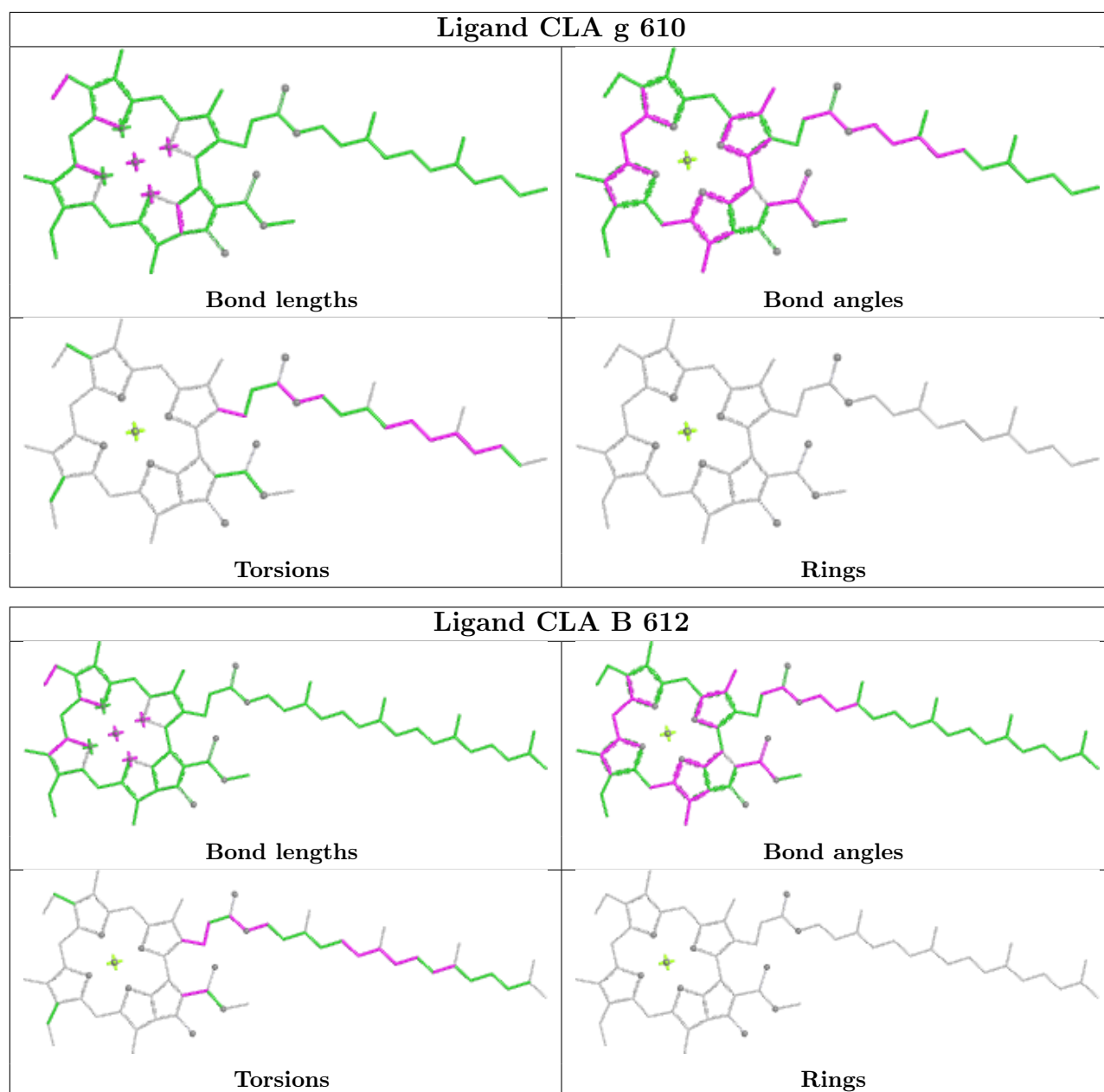
Rings





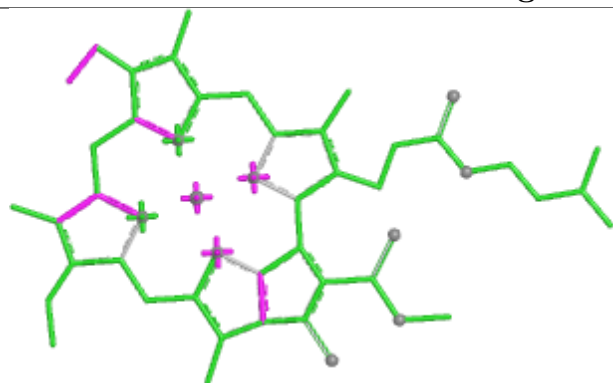




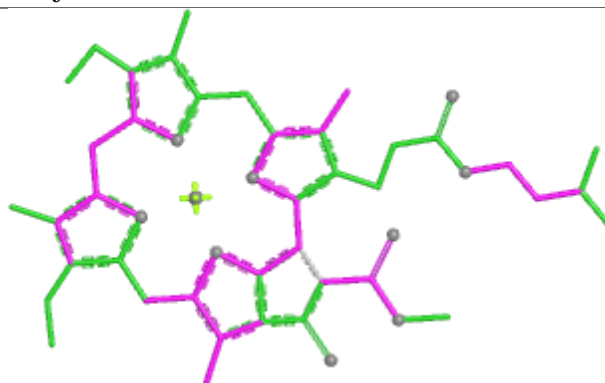




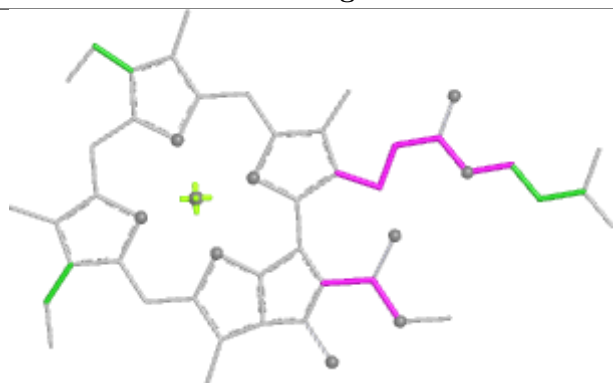
## Ligand CLA y 305



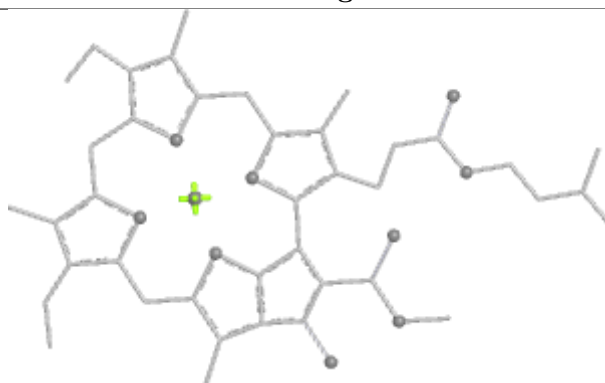
Bond lengths



Bond angles

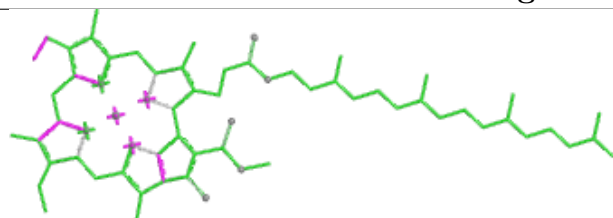


Torsions

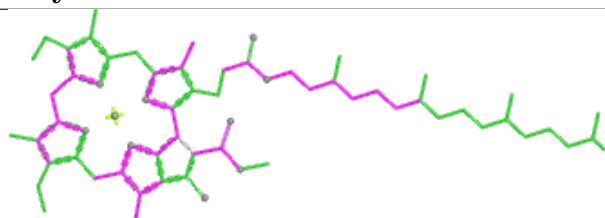


Rings

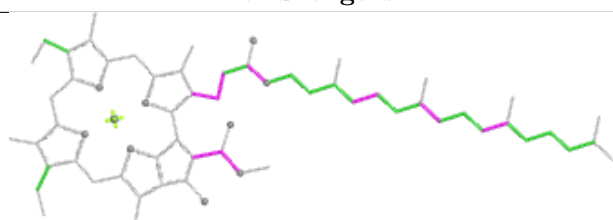
## Ligand CLA y 303



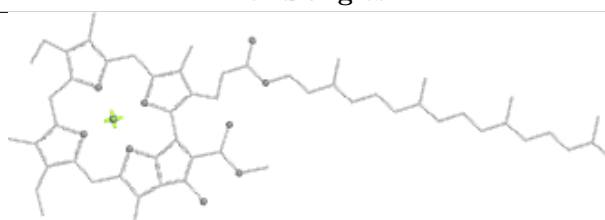
Bond lengths



Bond angles

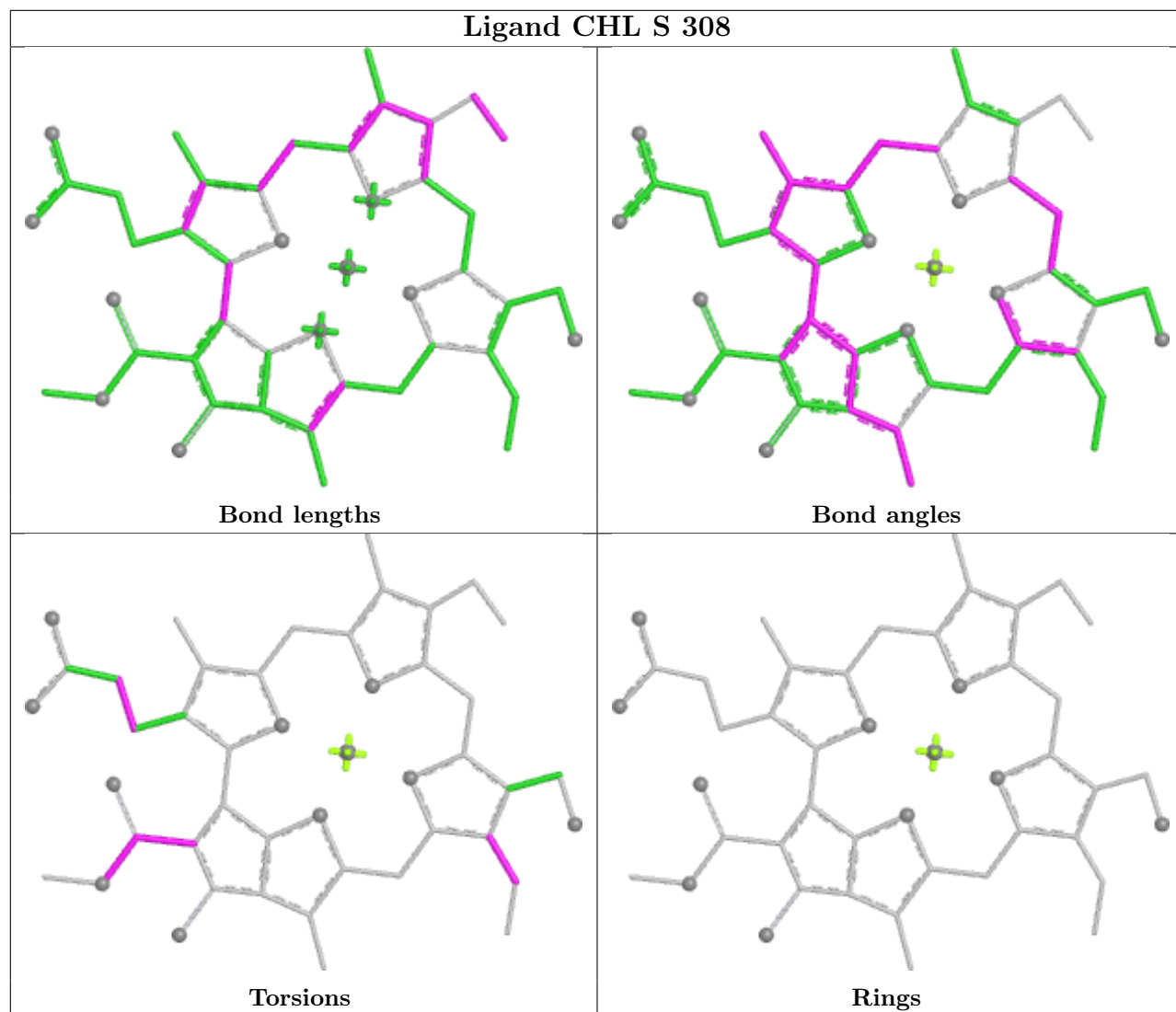


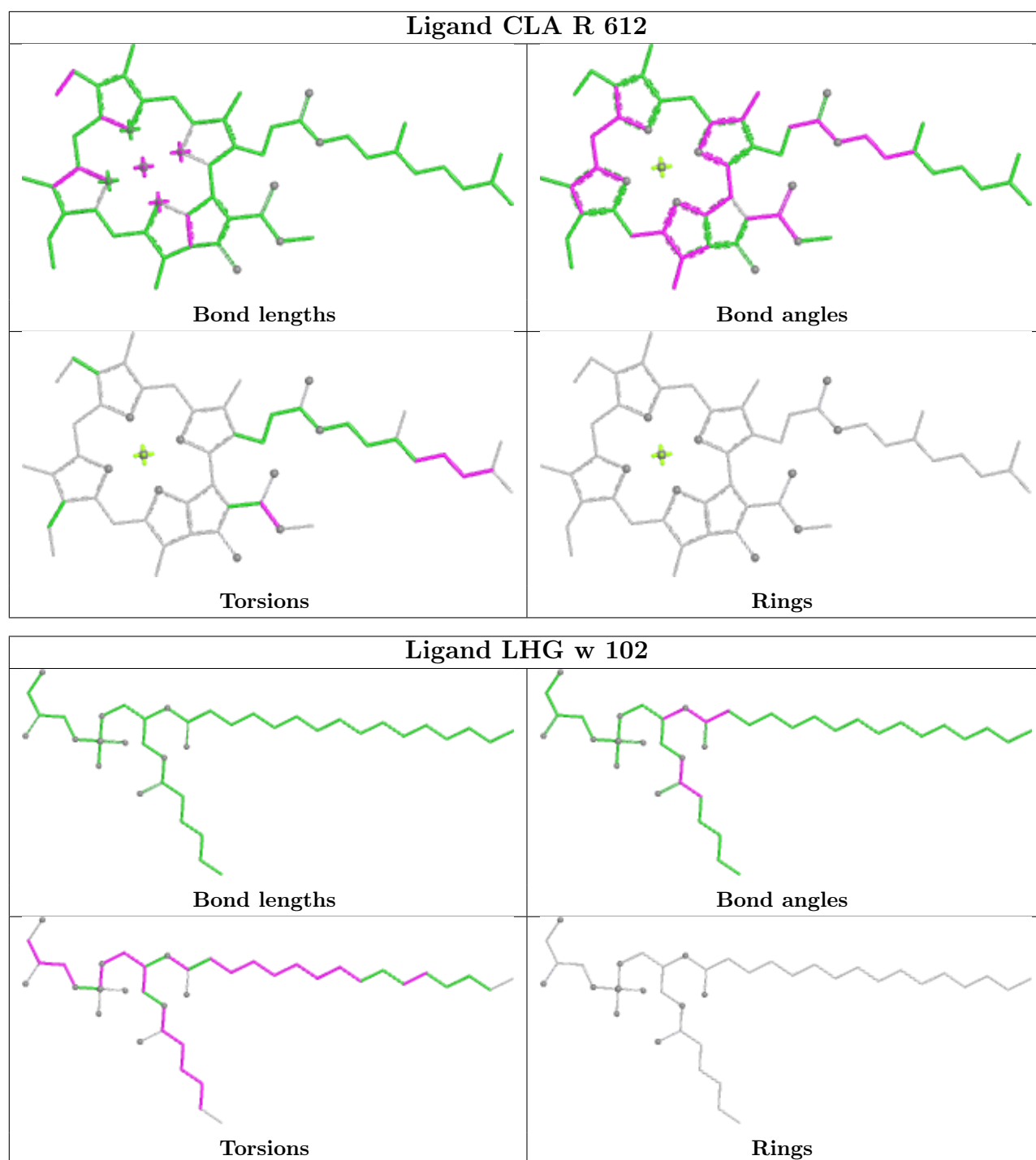
Torsions

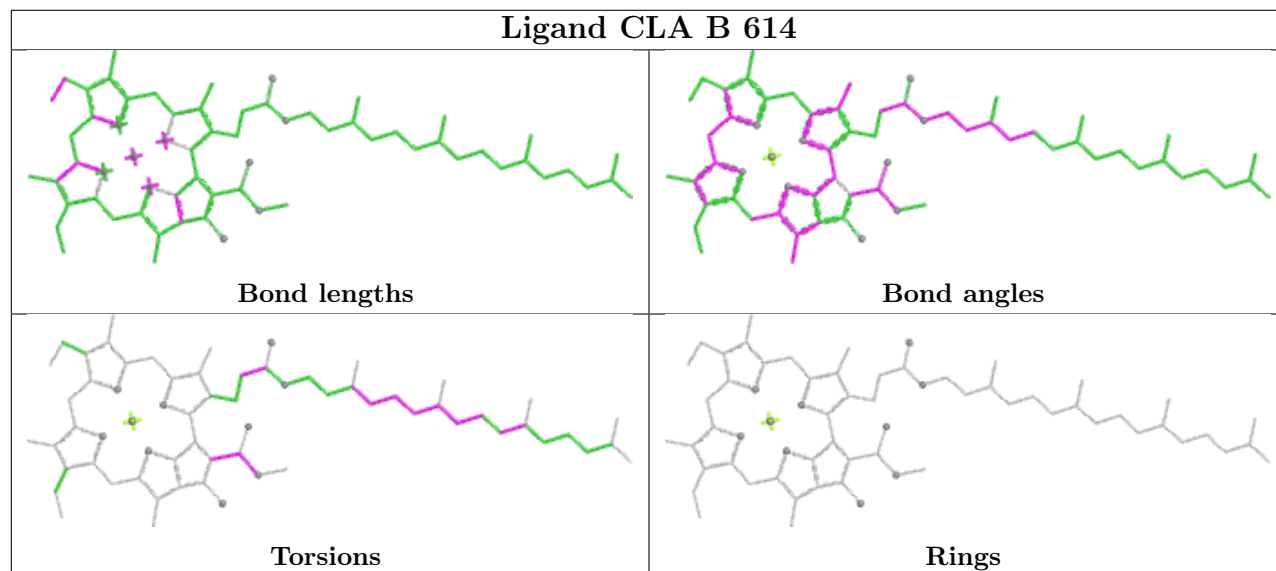
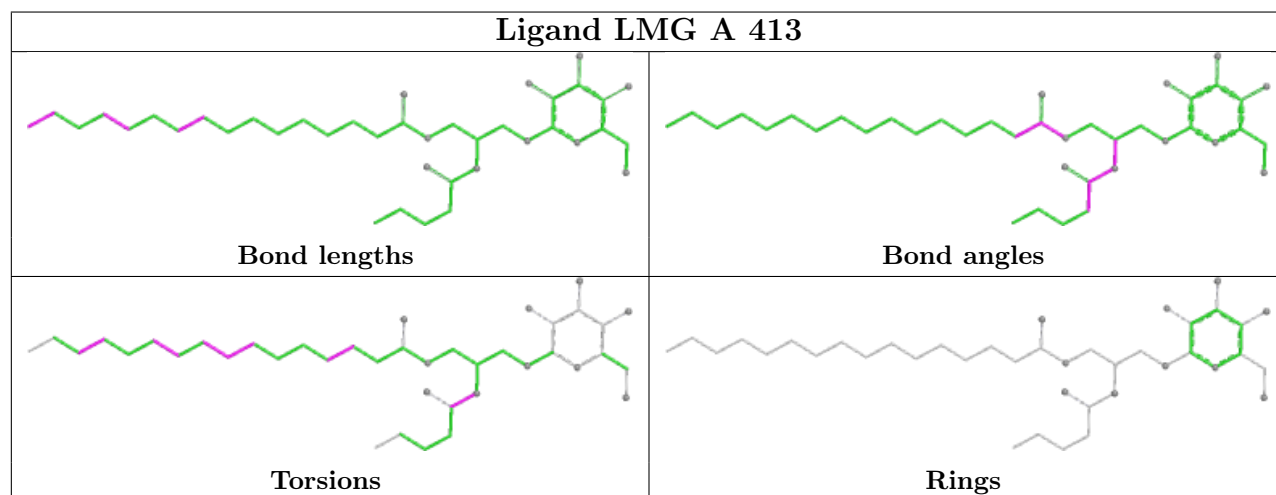
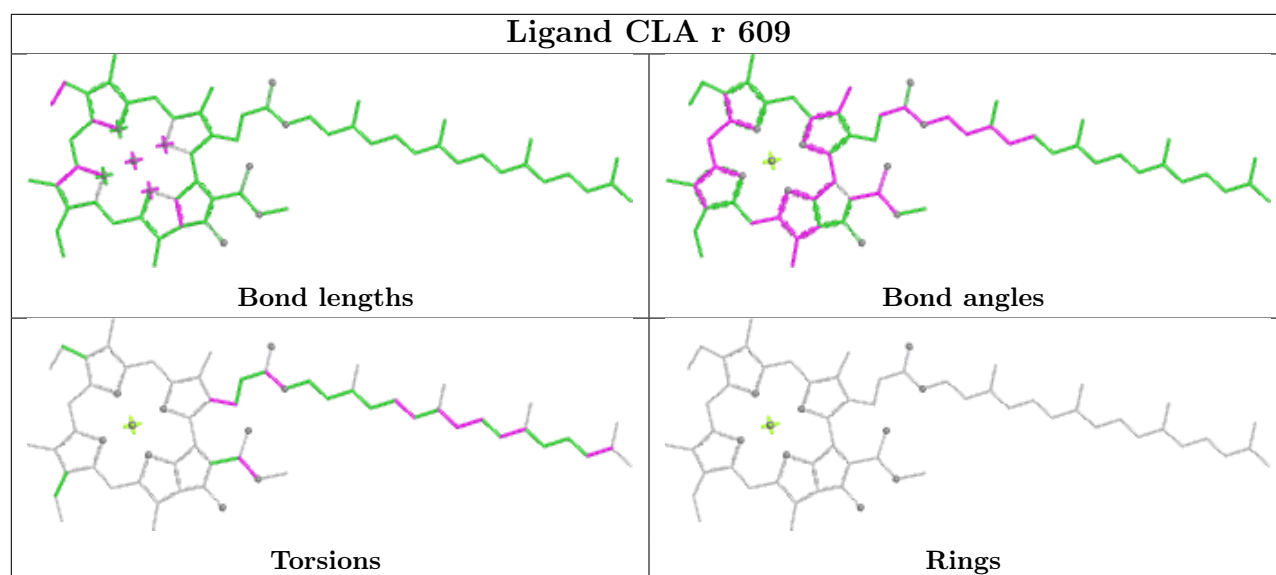


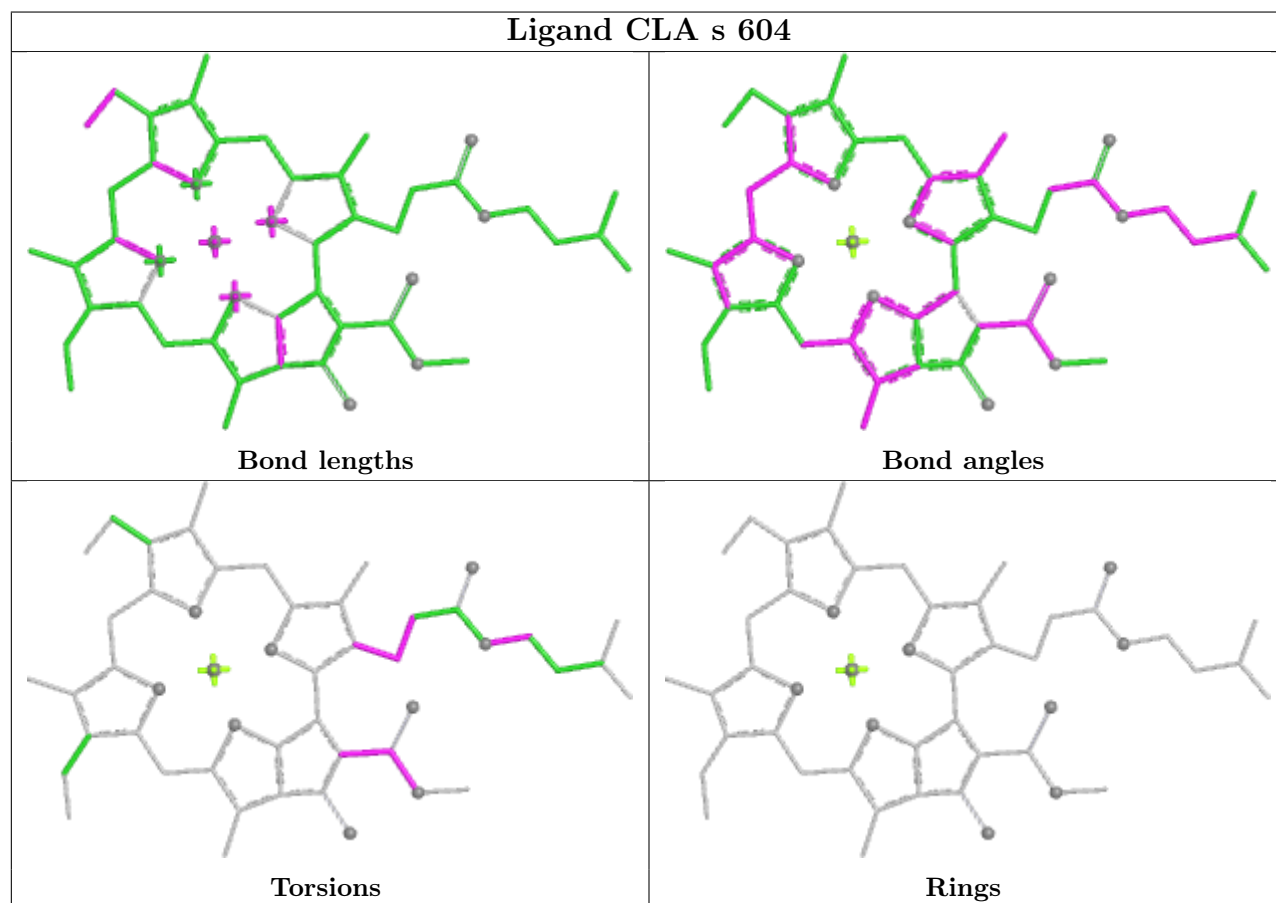
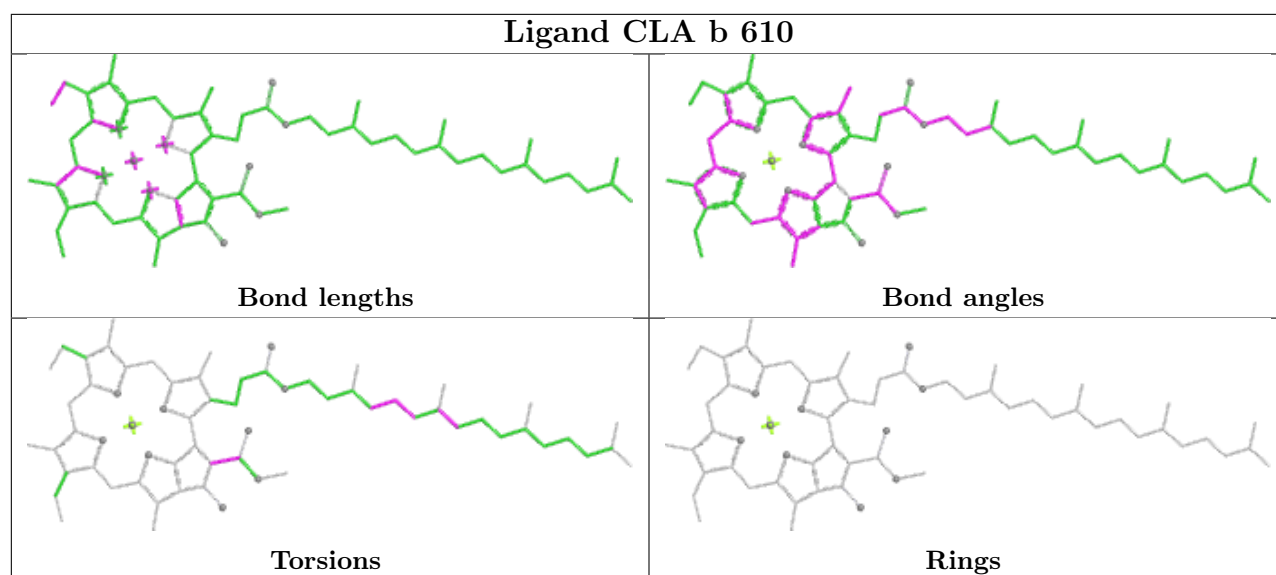
Rings

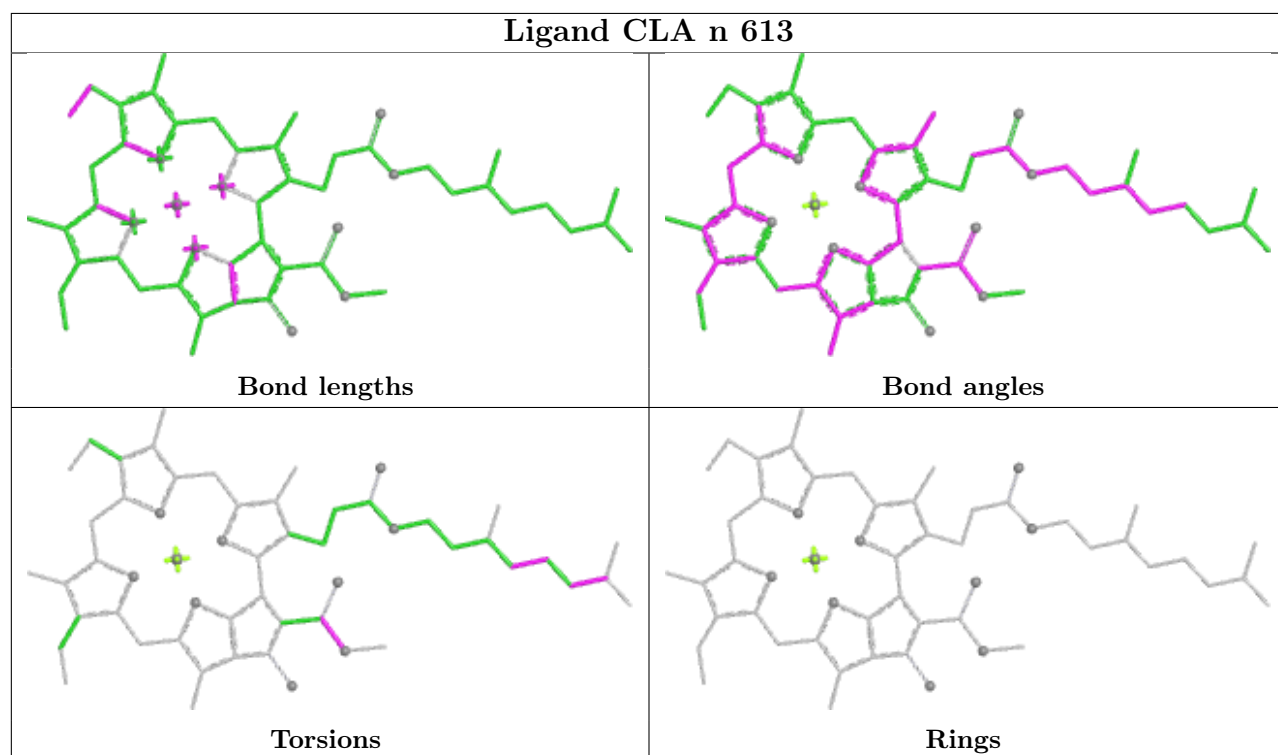
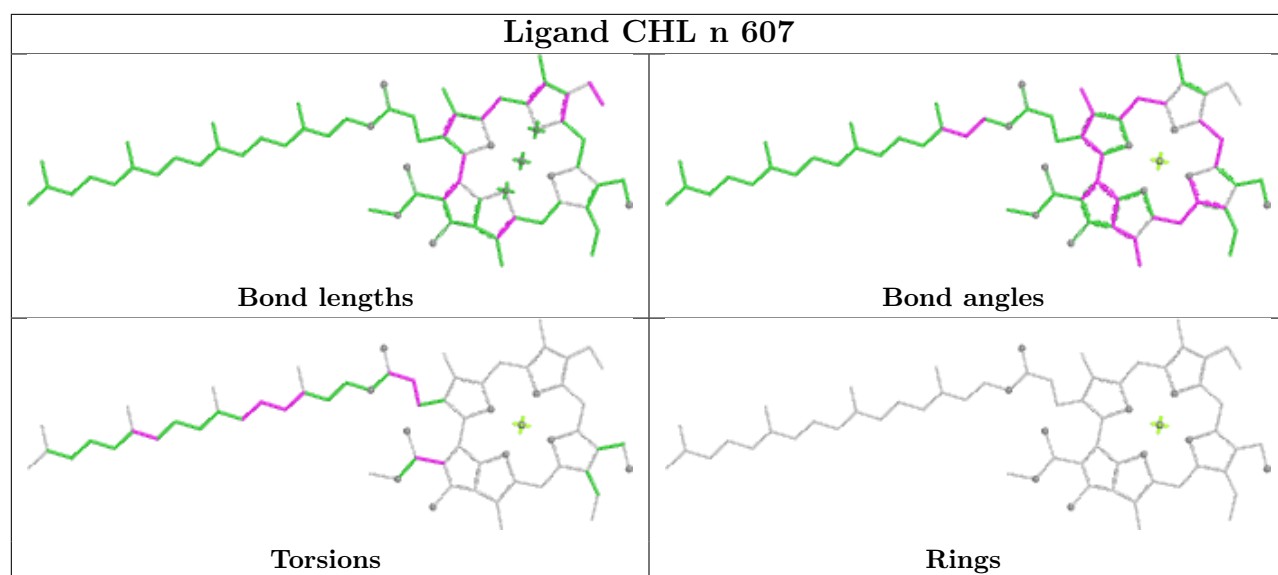
## Ligand CHL S 308

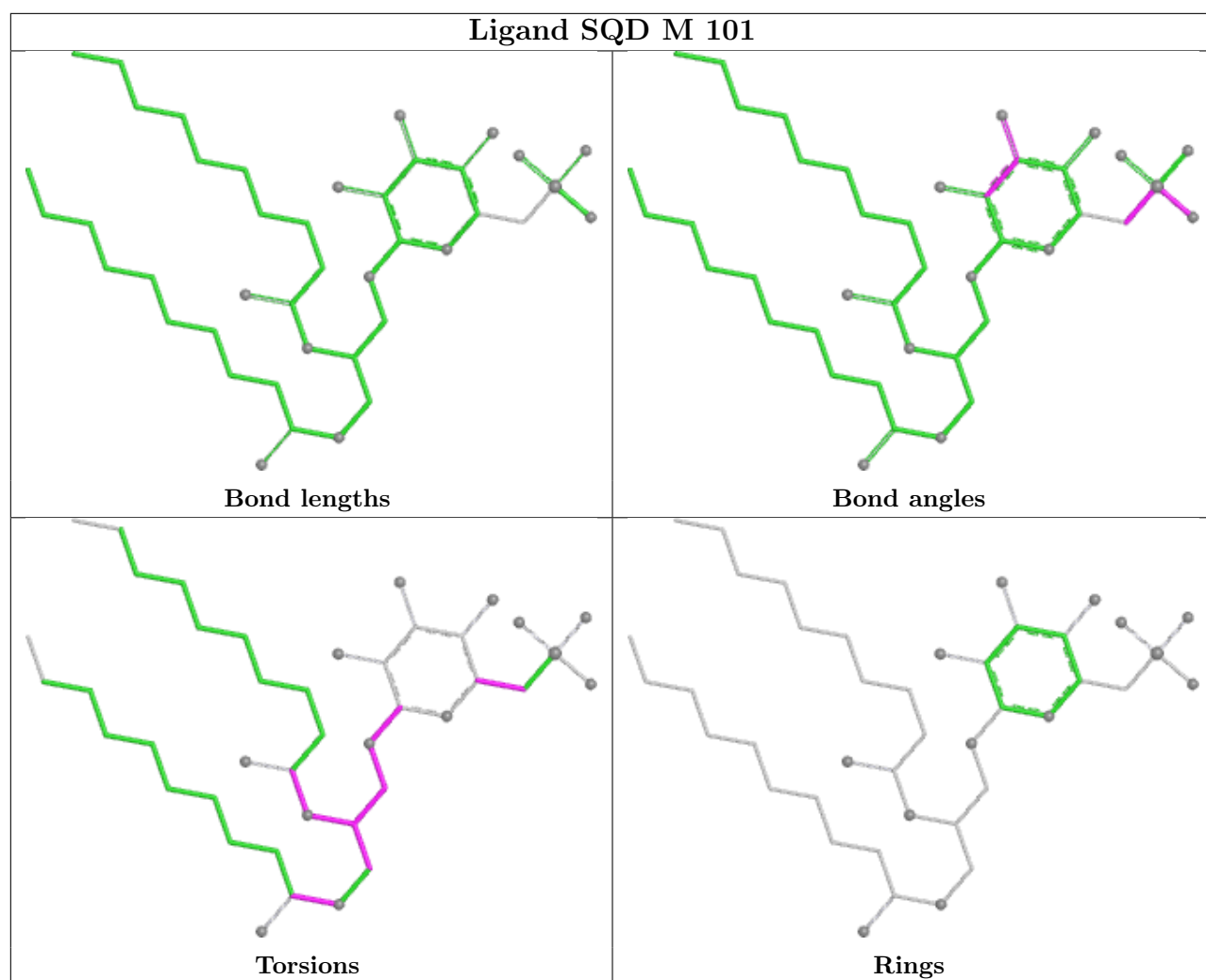




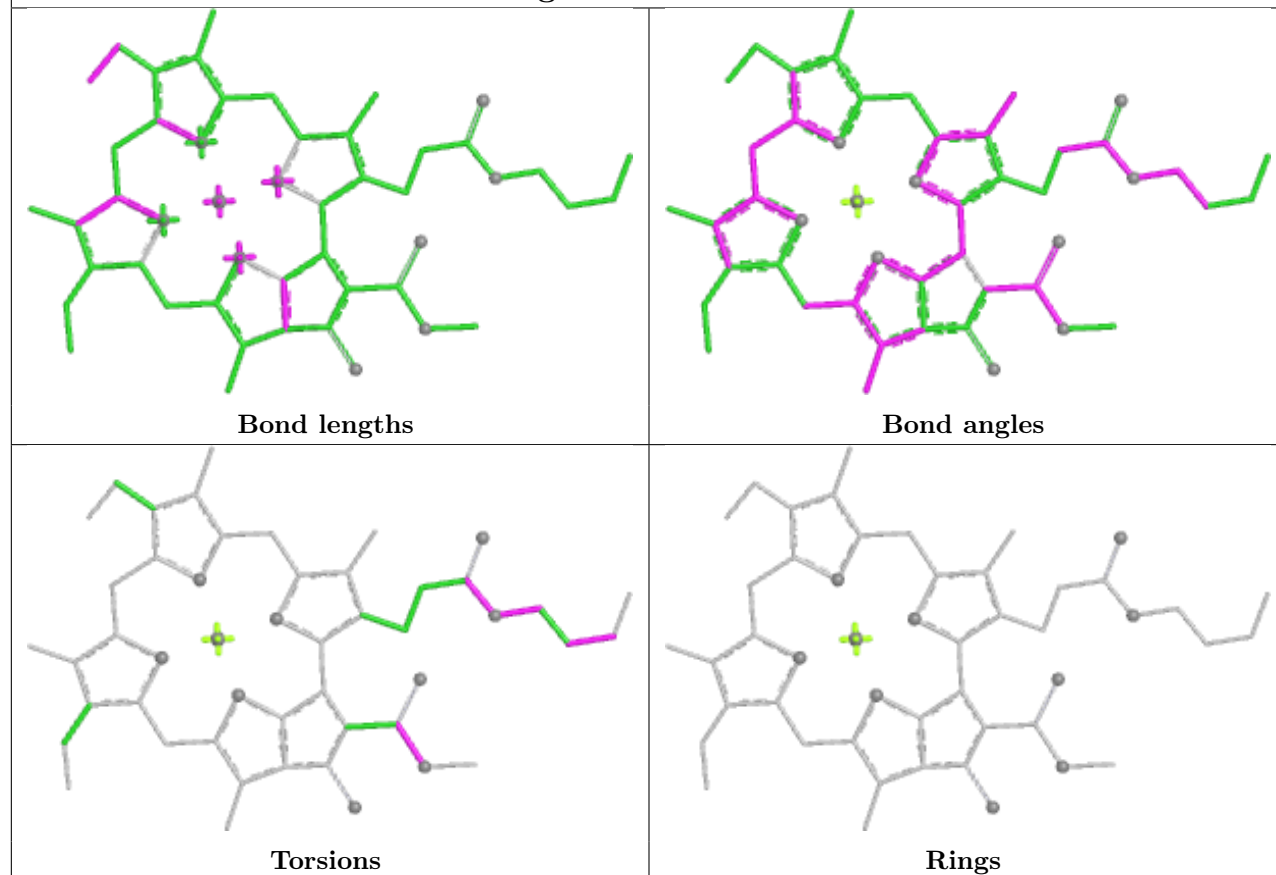




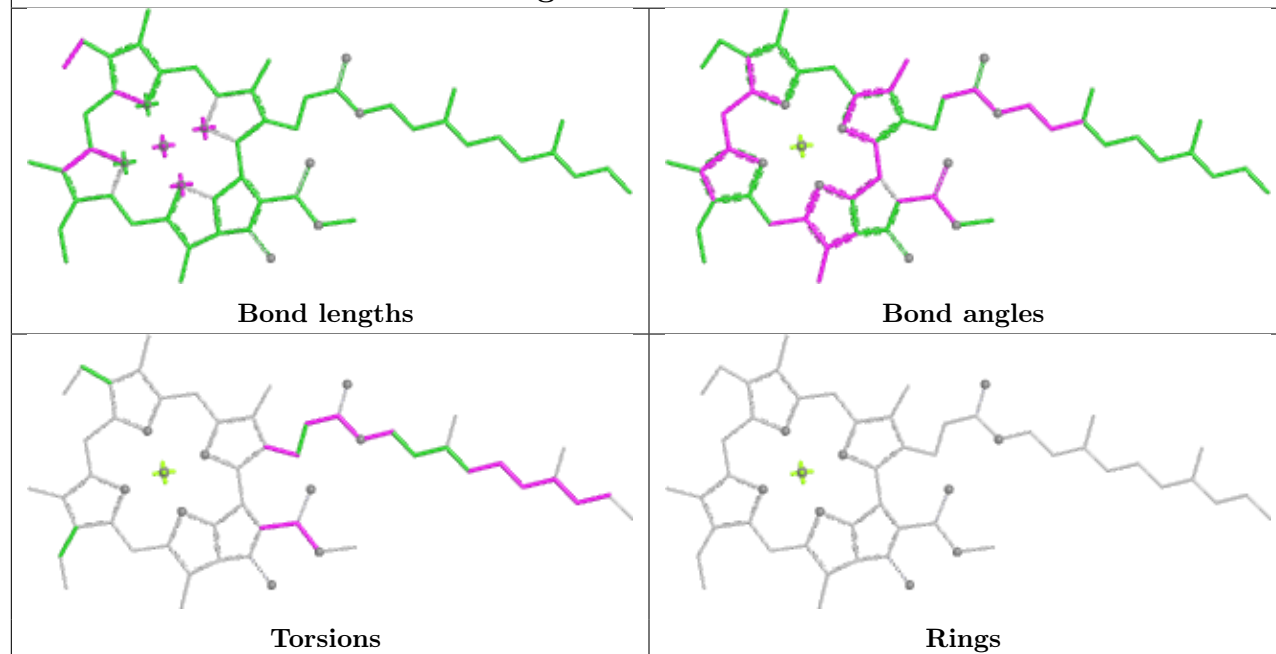




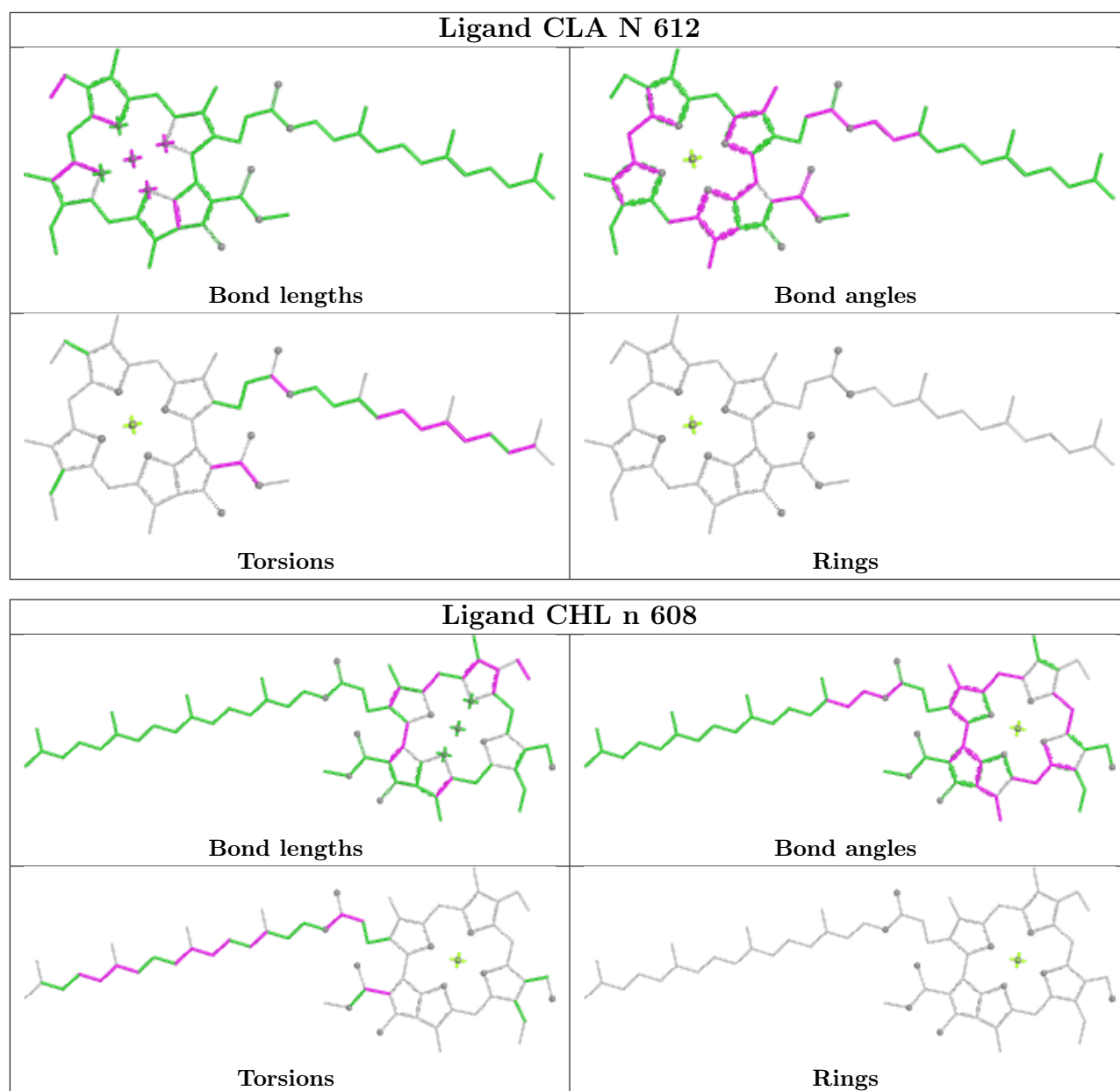
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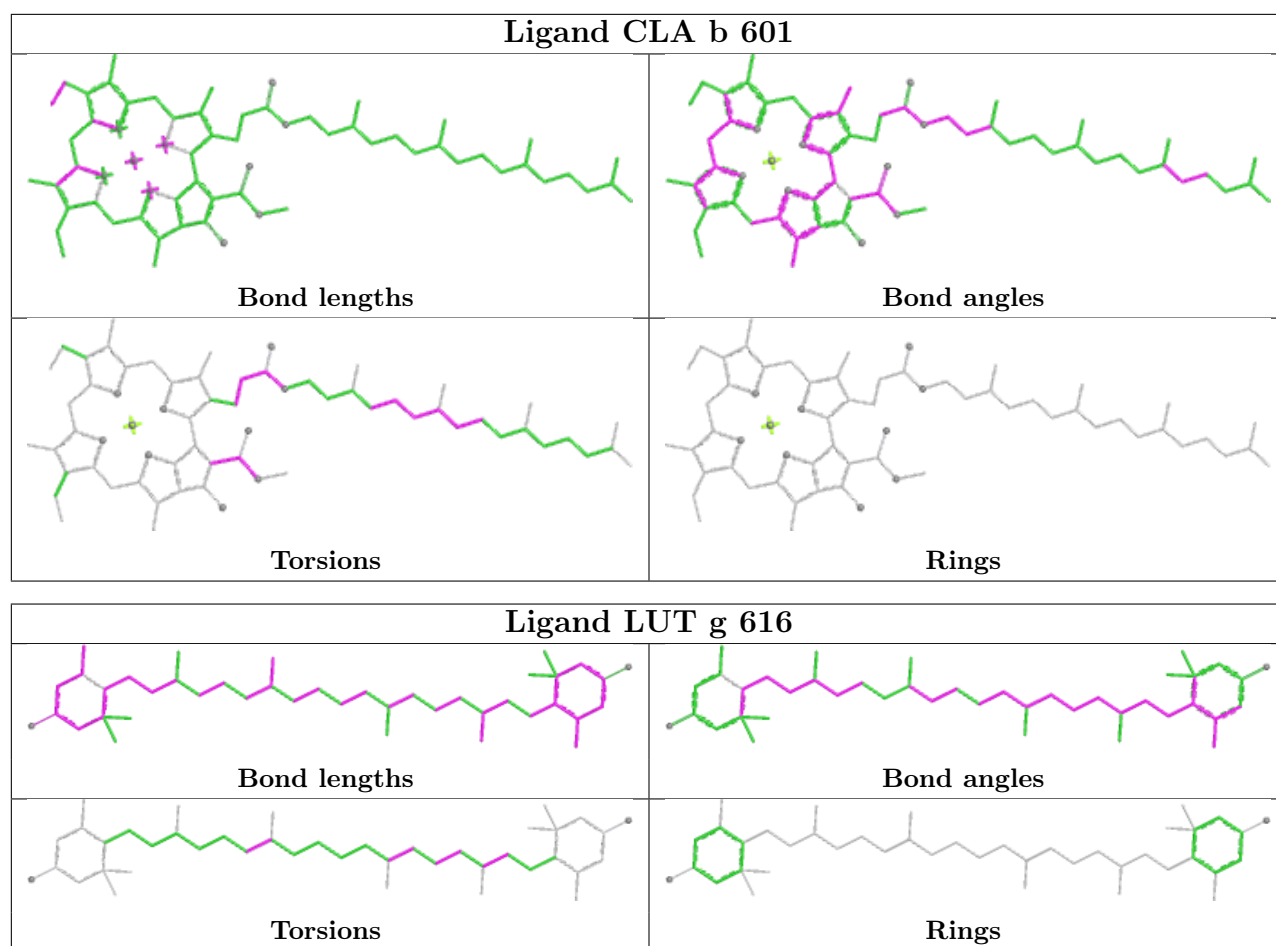


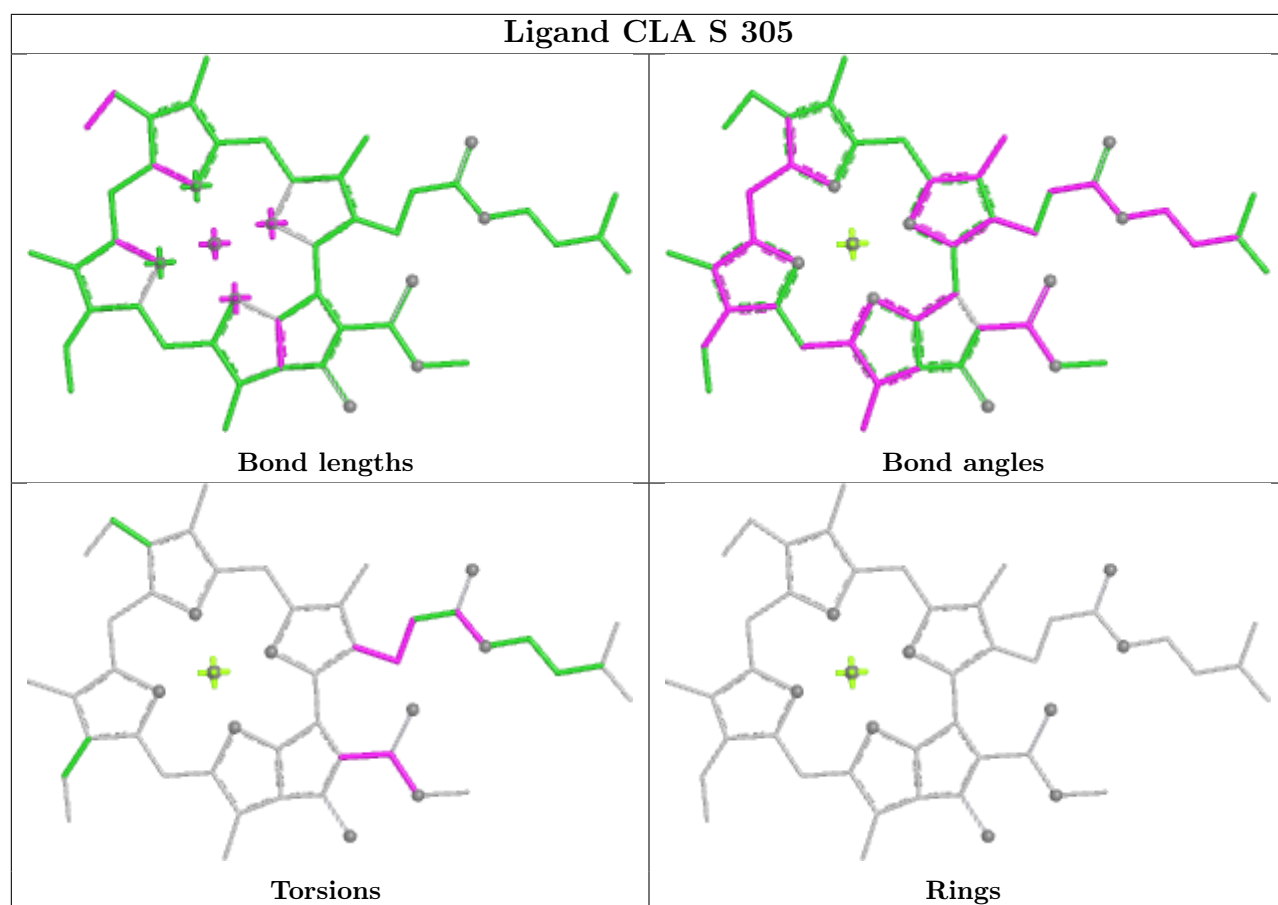
## Ligand CLA c 512

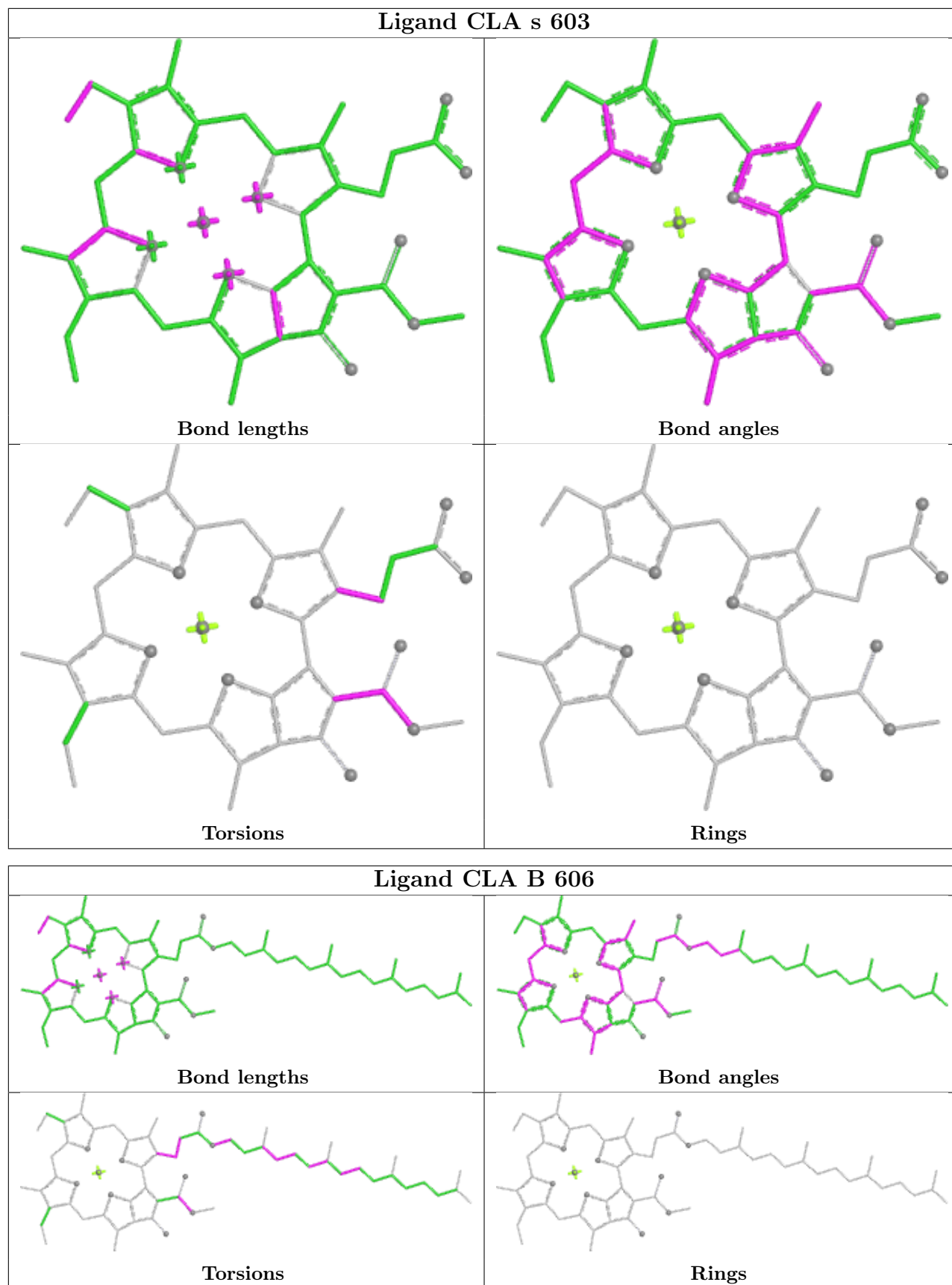


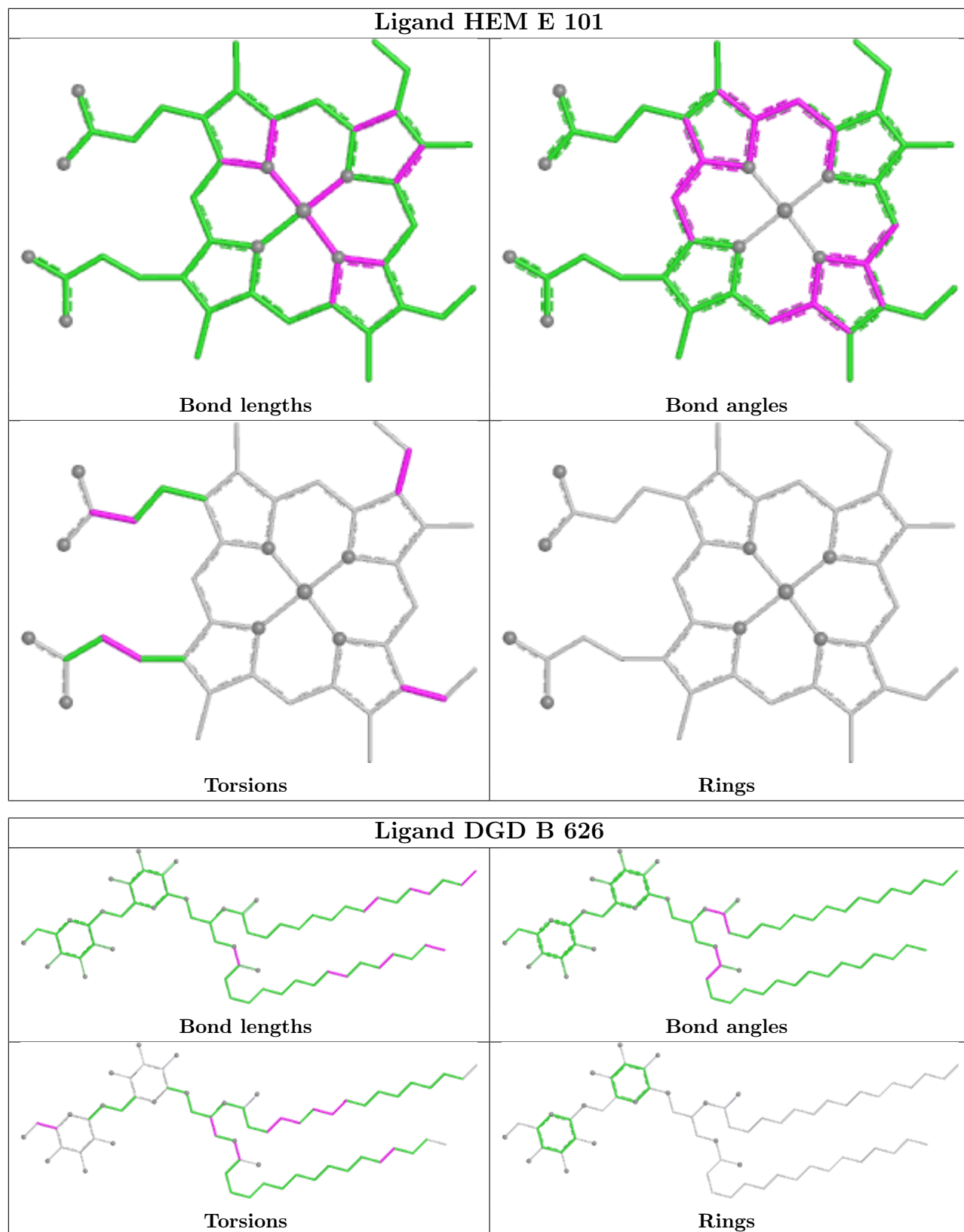


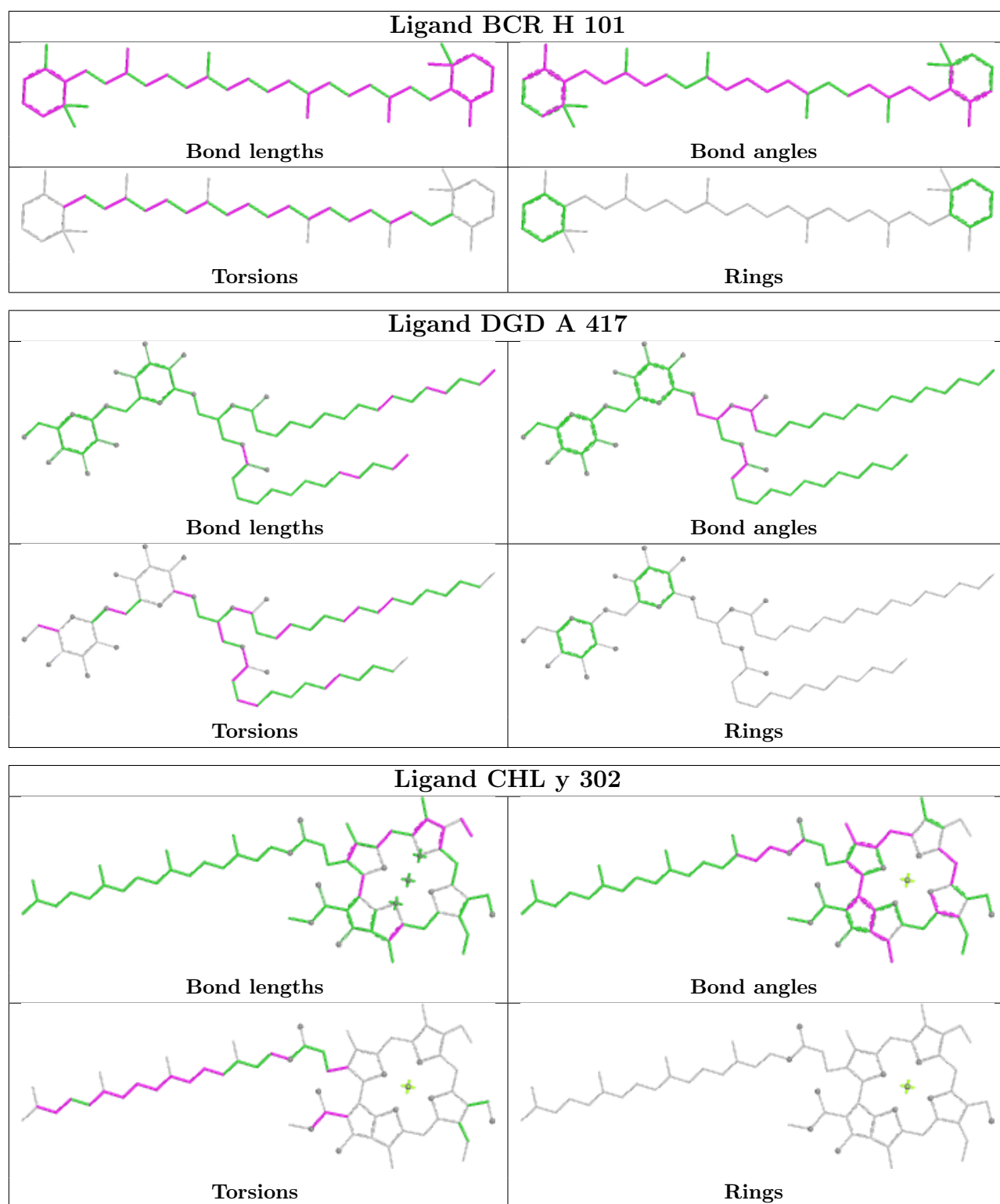


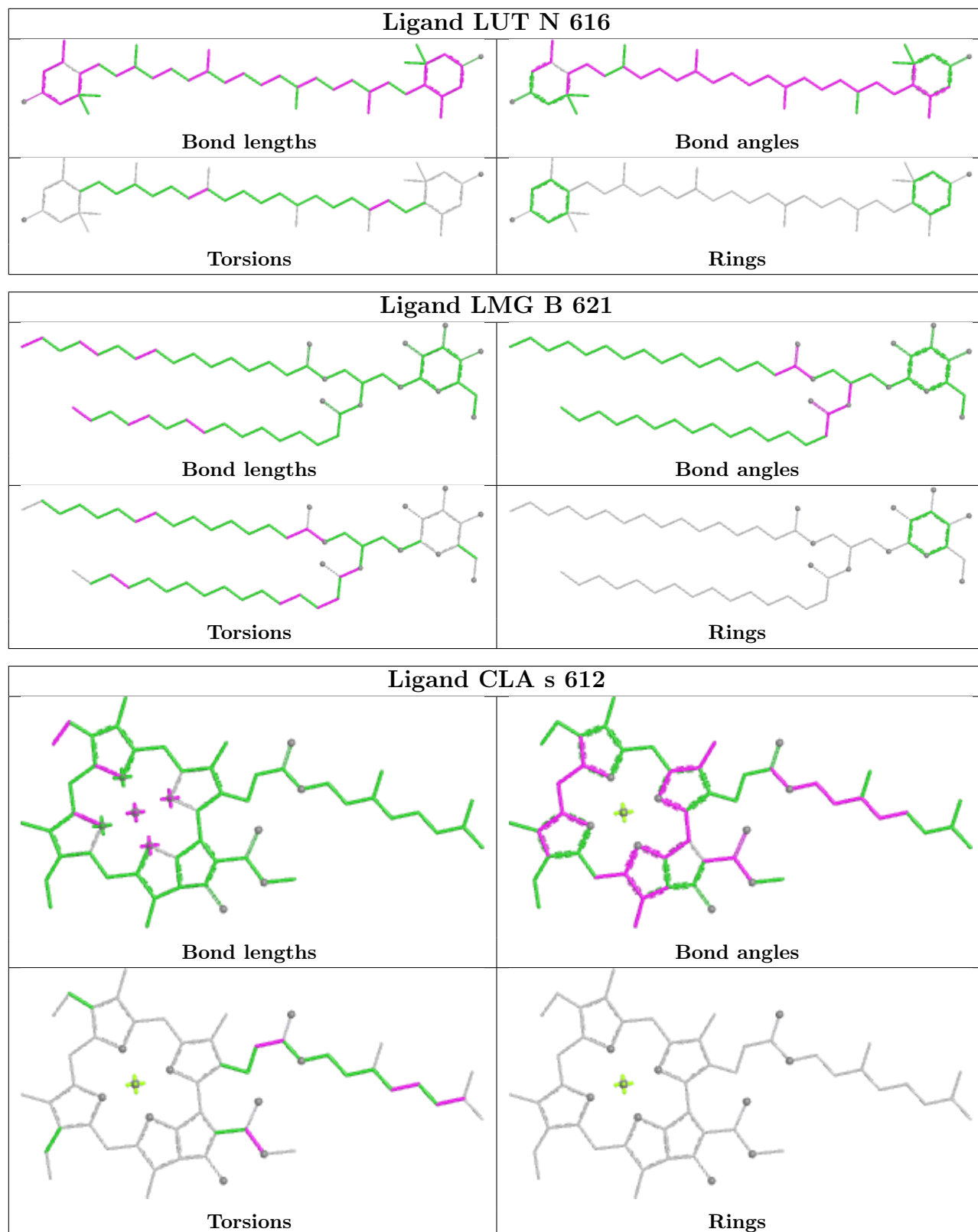


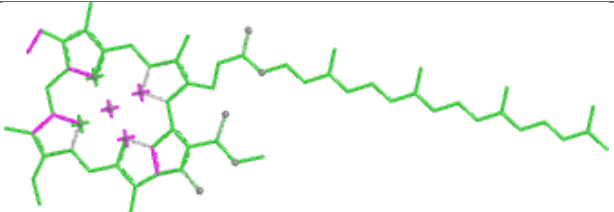
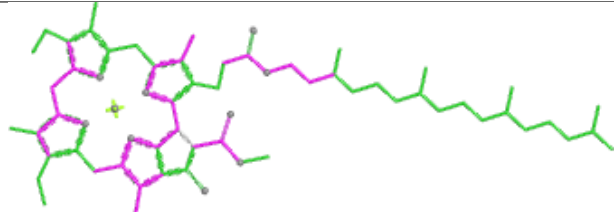
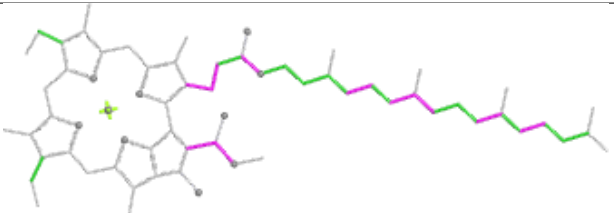
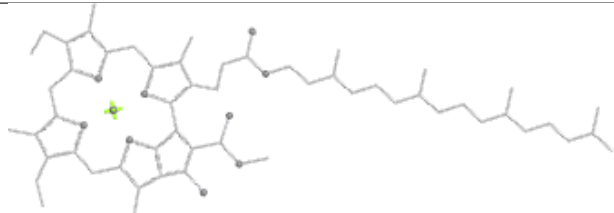


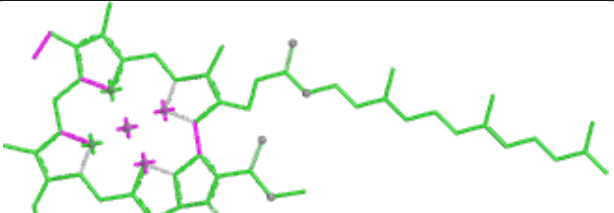
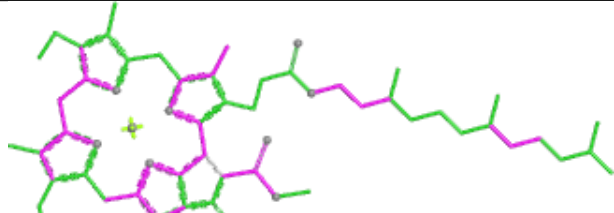
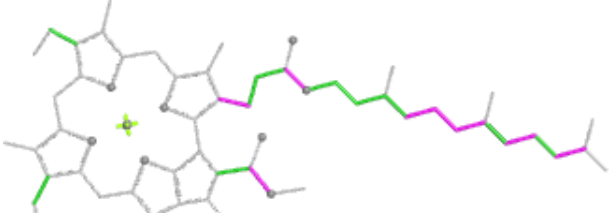
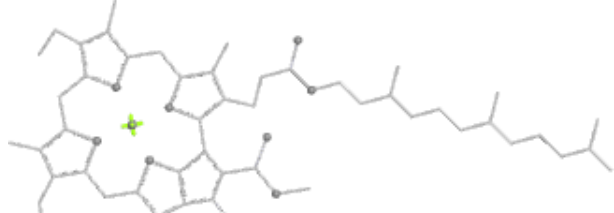



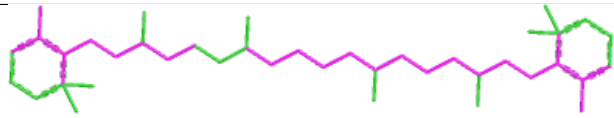
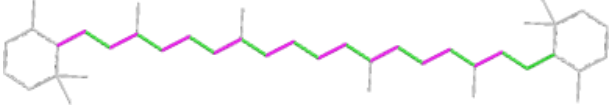
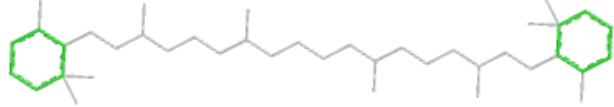




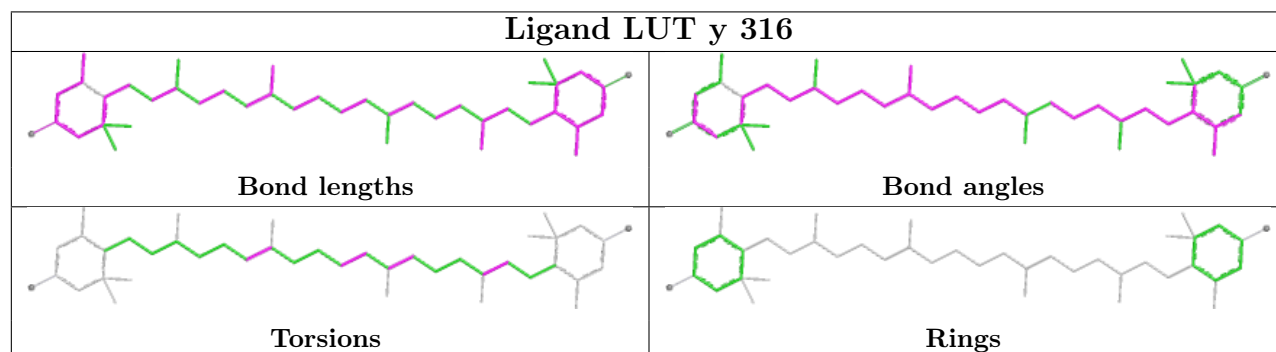
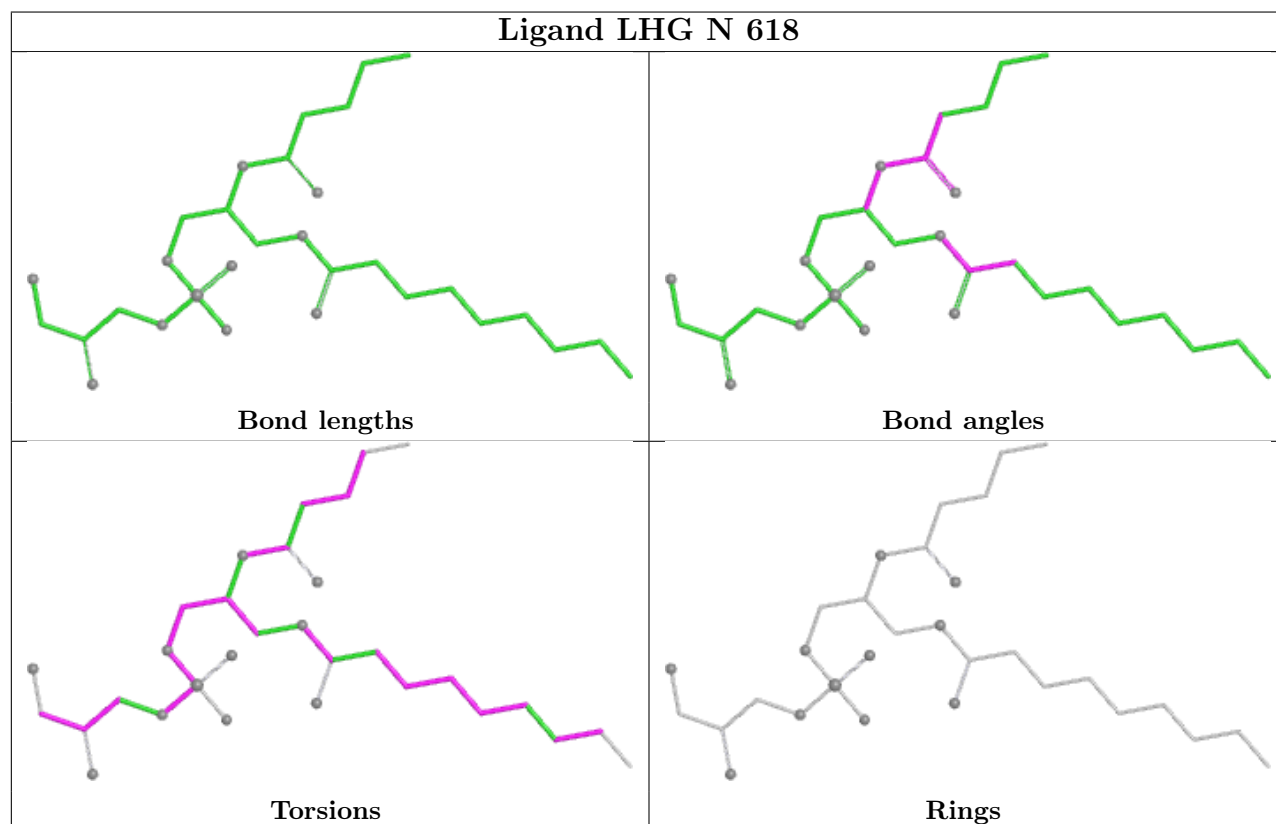
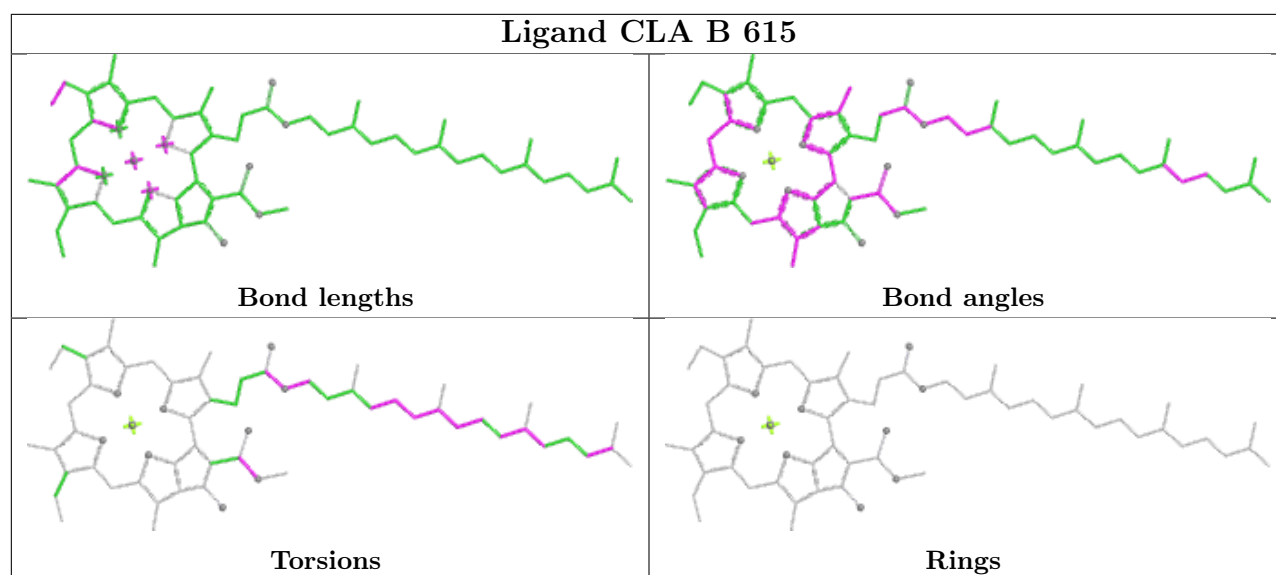


Ligand CLA N 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

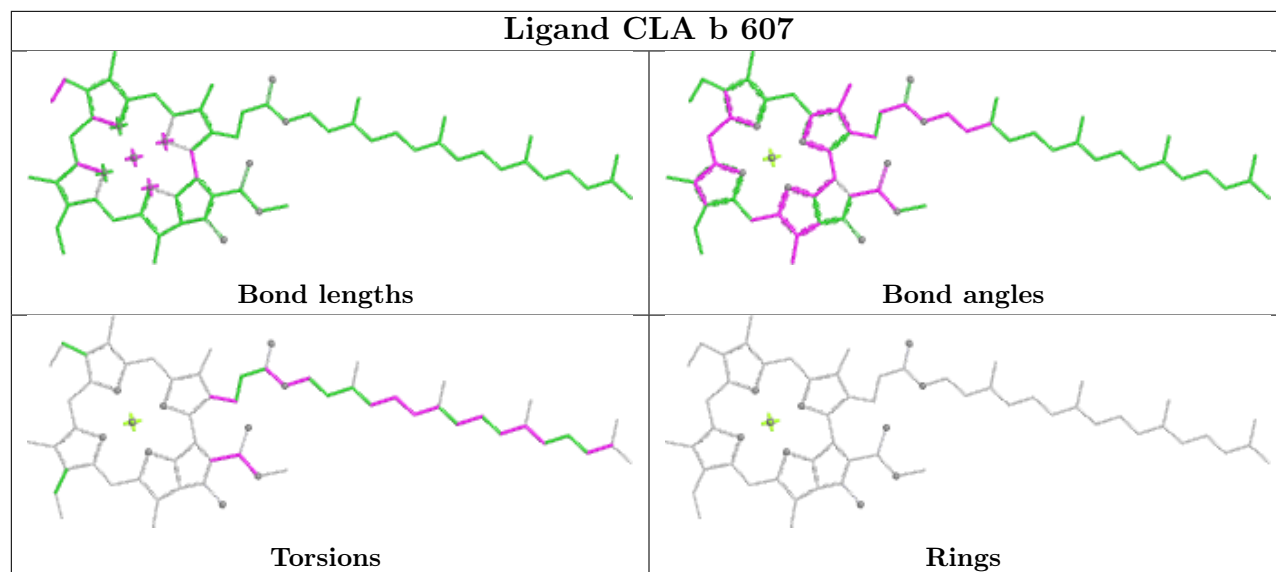
Ligand CLA Y 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

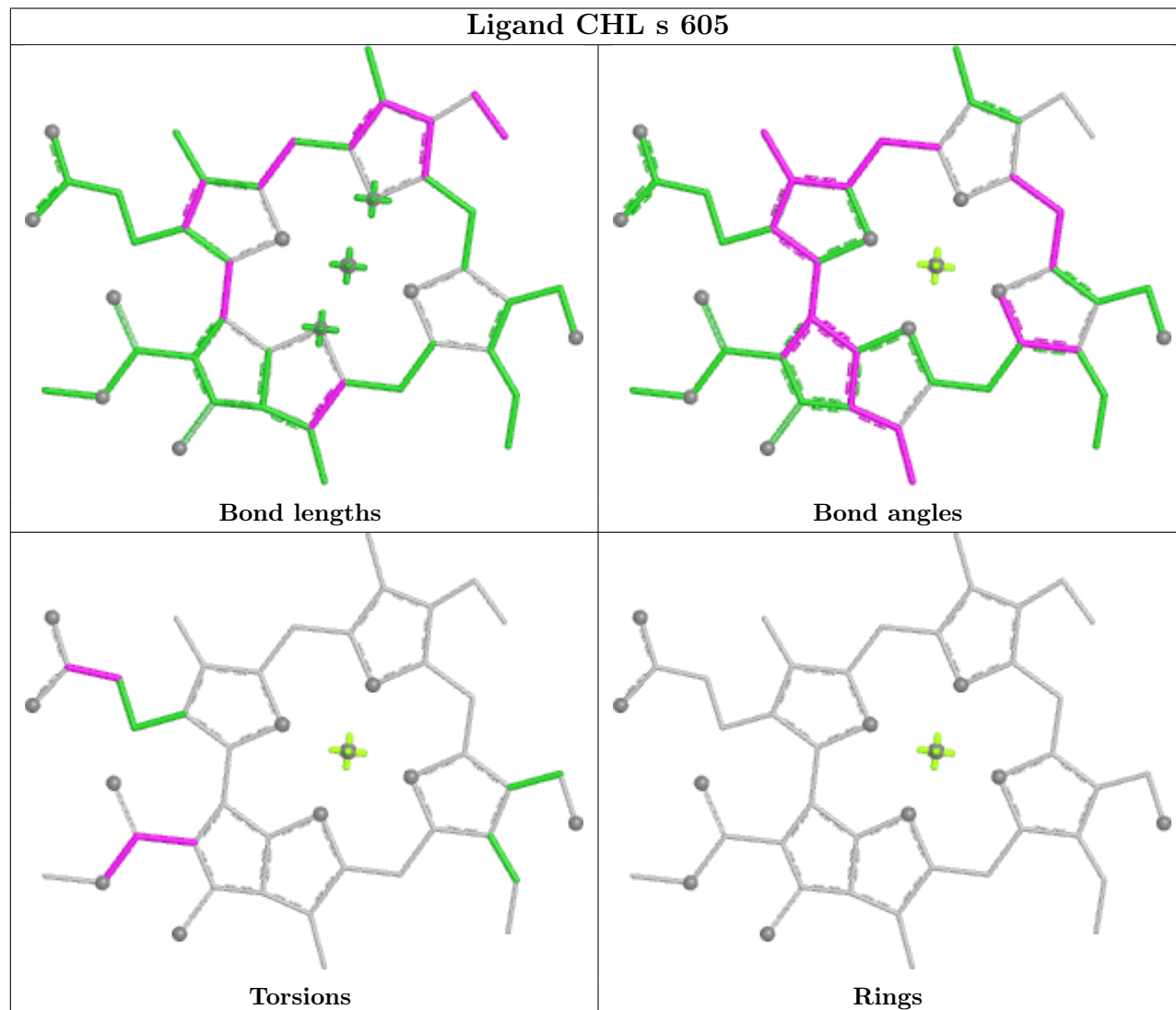


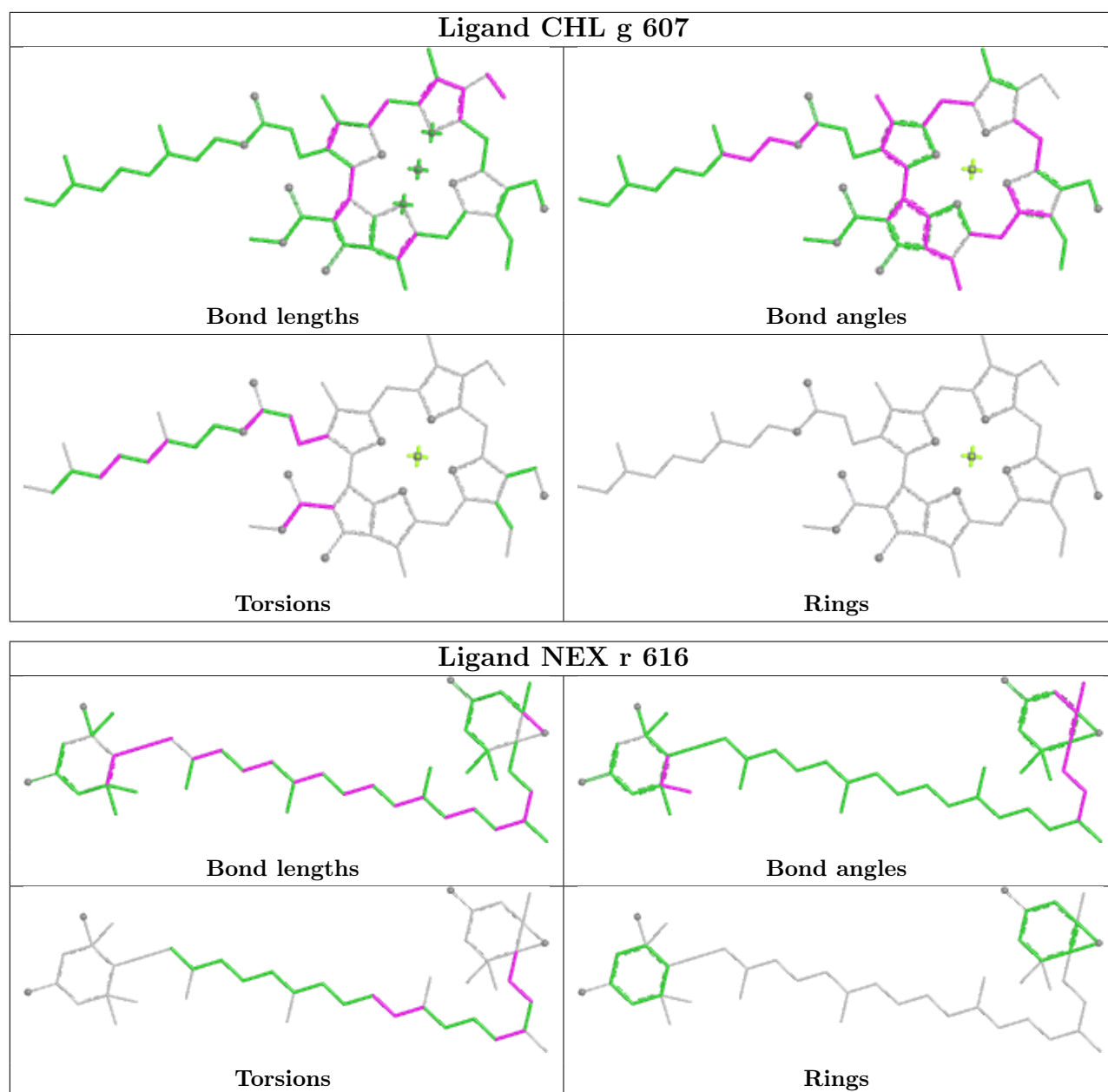


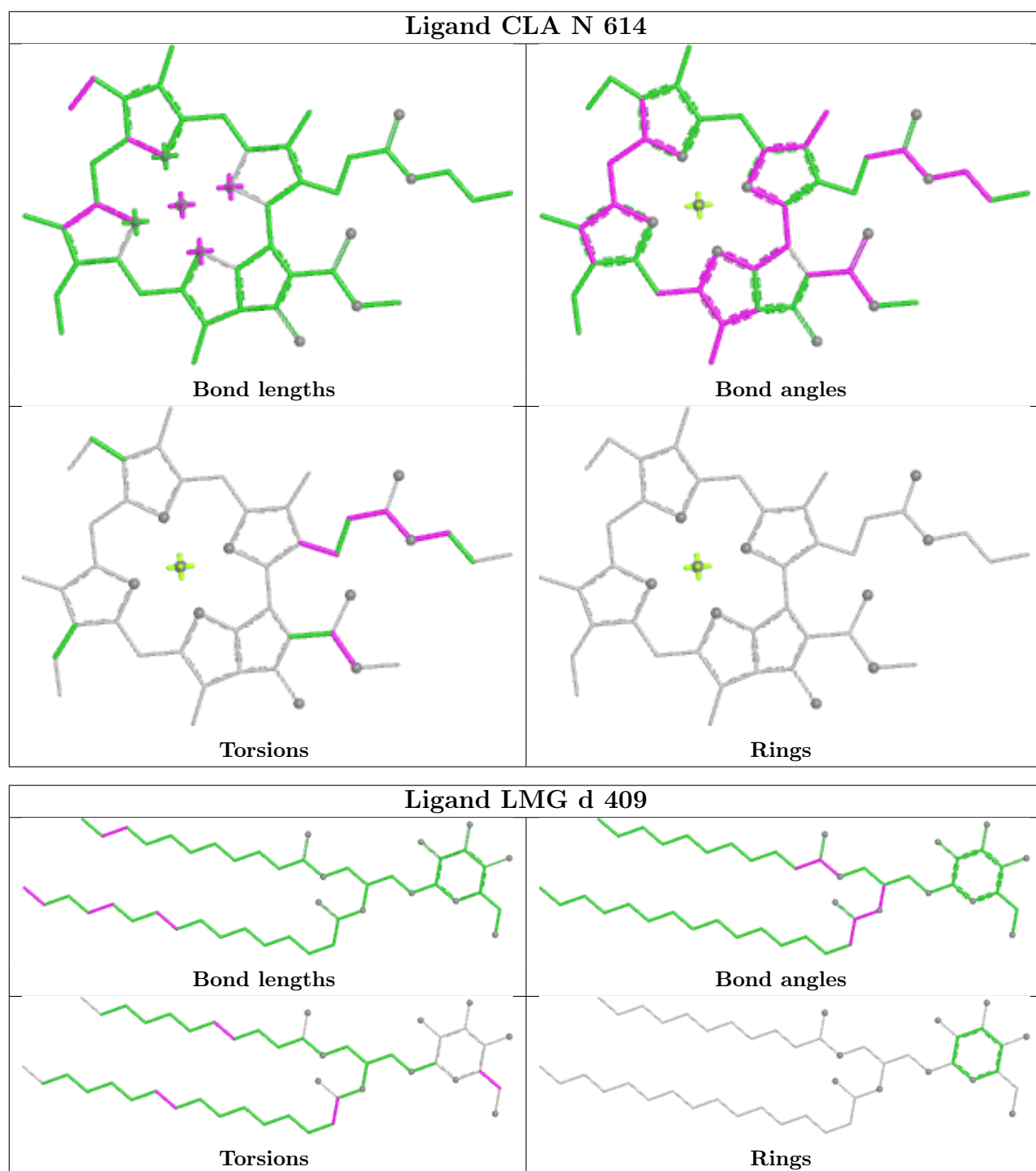
## Ligand CLA b 607

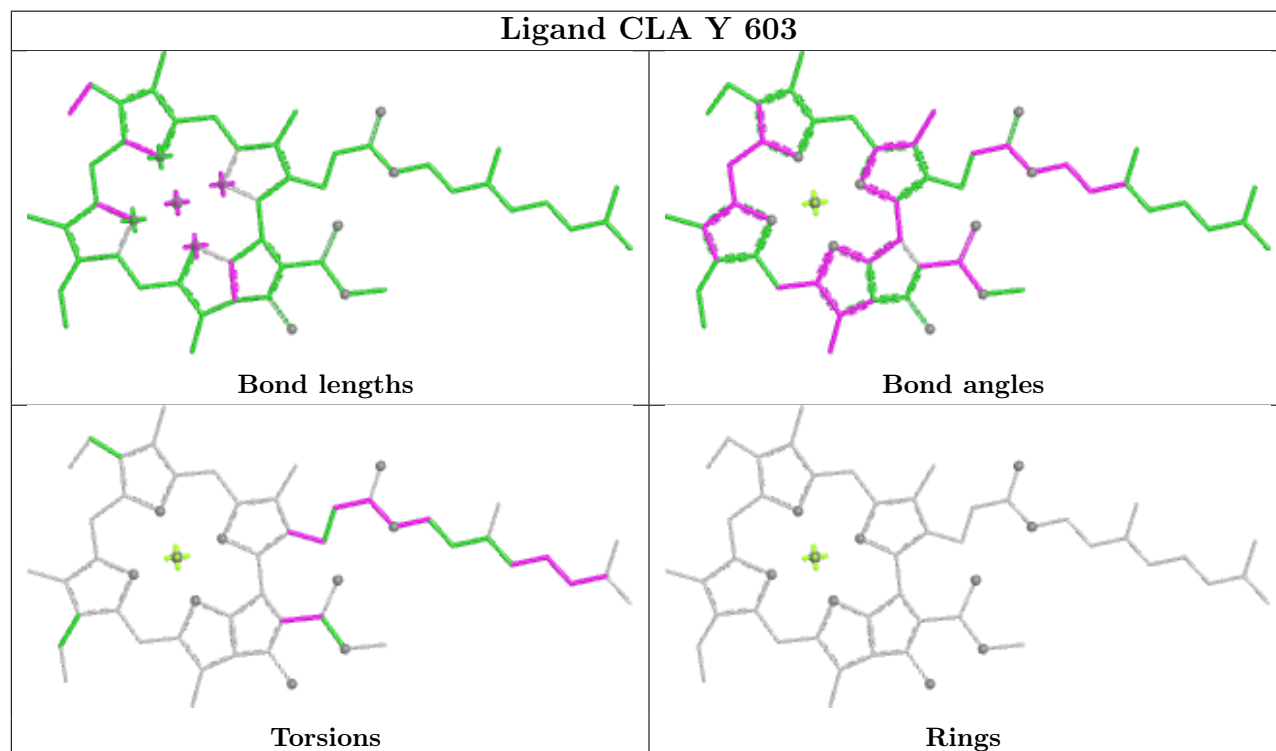
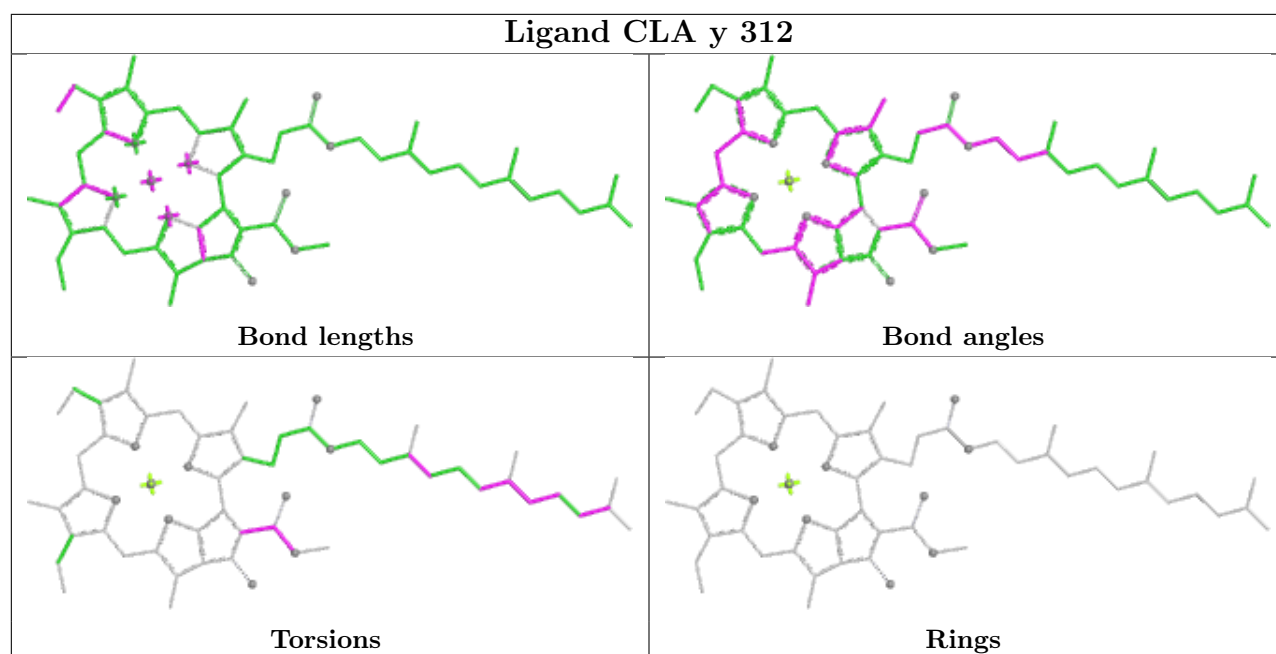


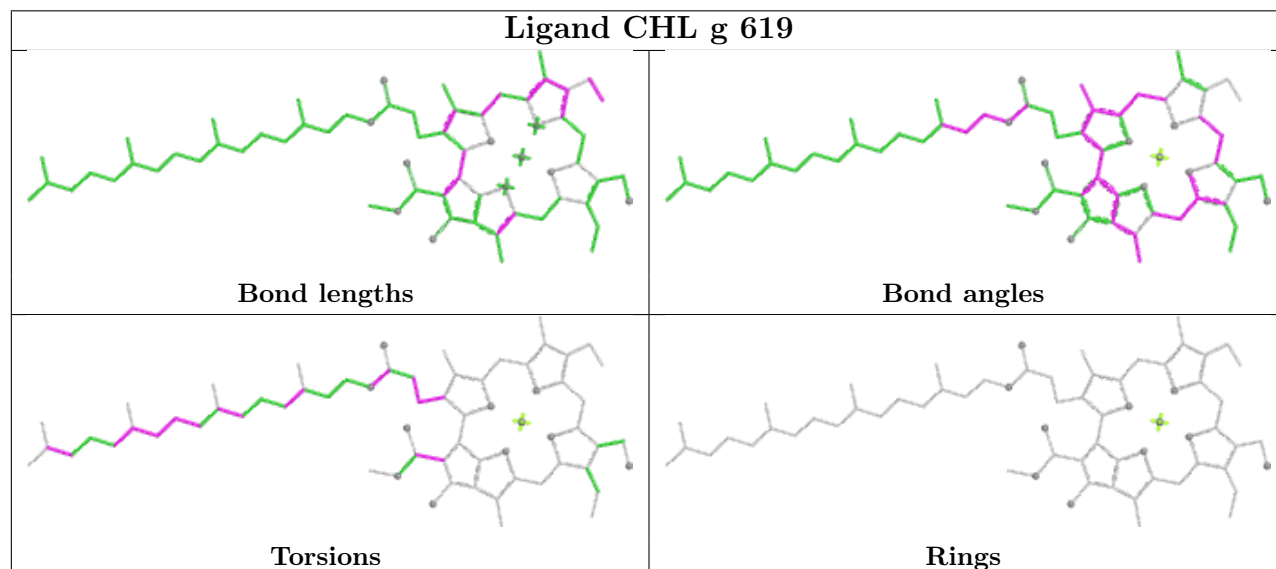
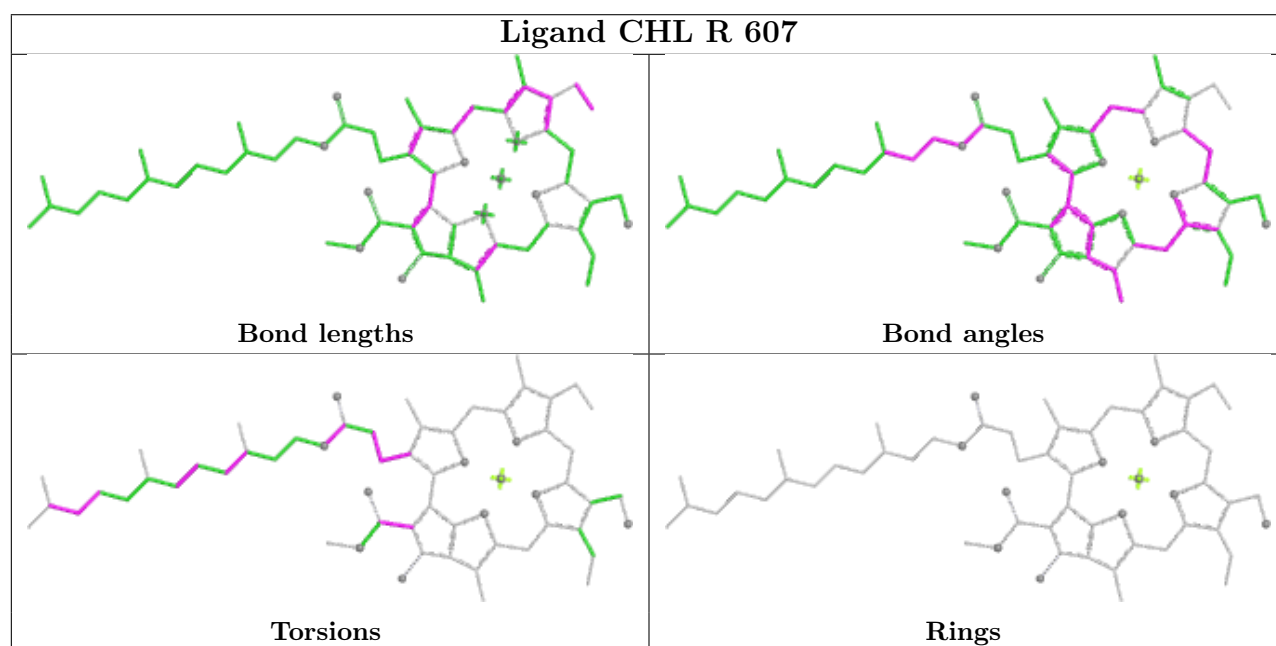
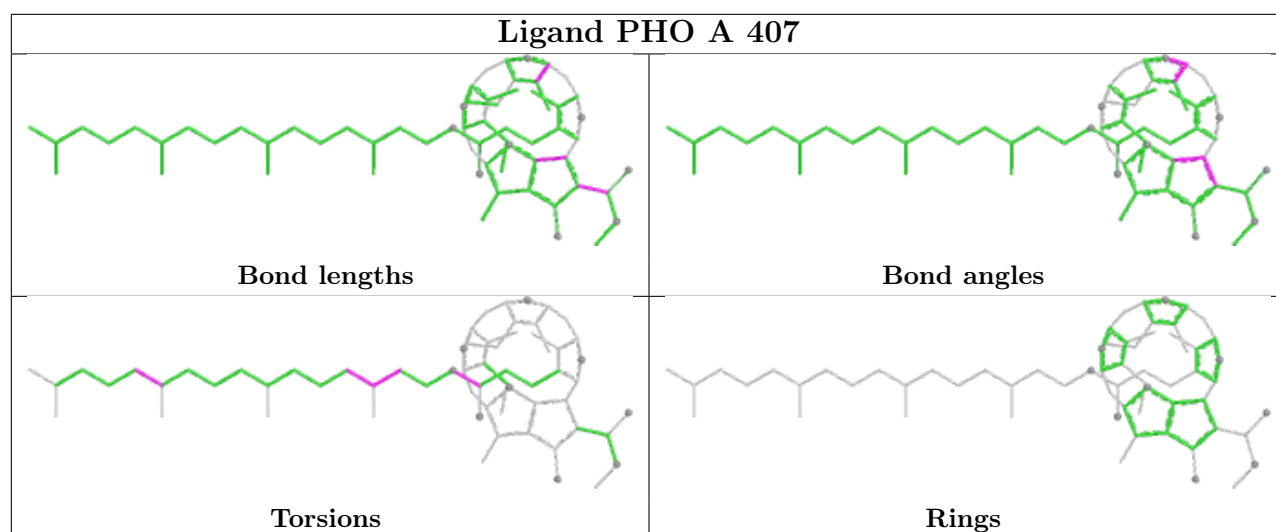
## Ligand CHL s 605

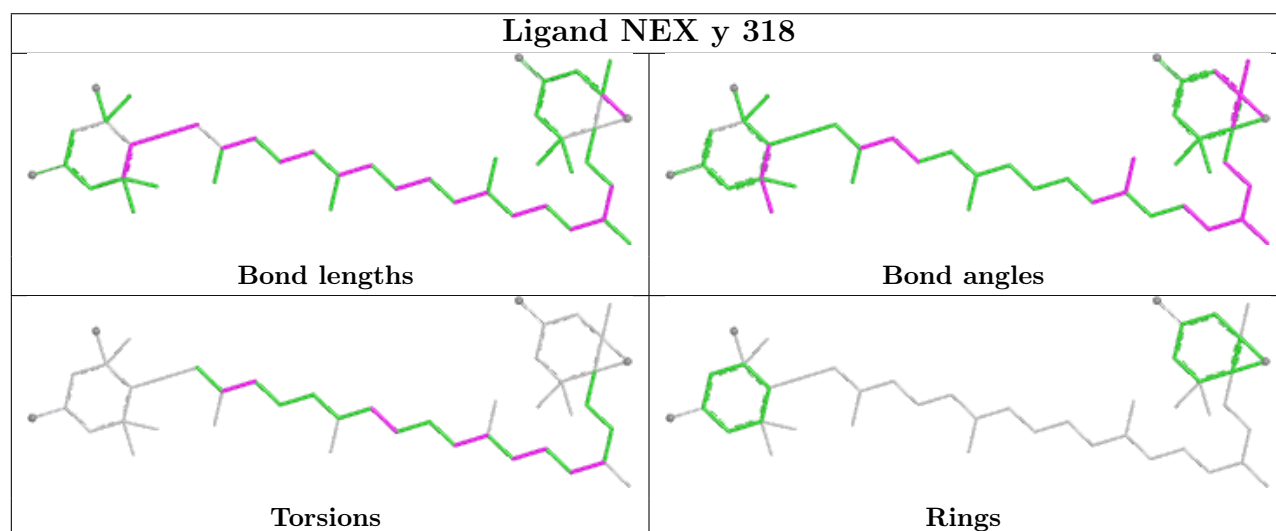
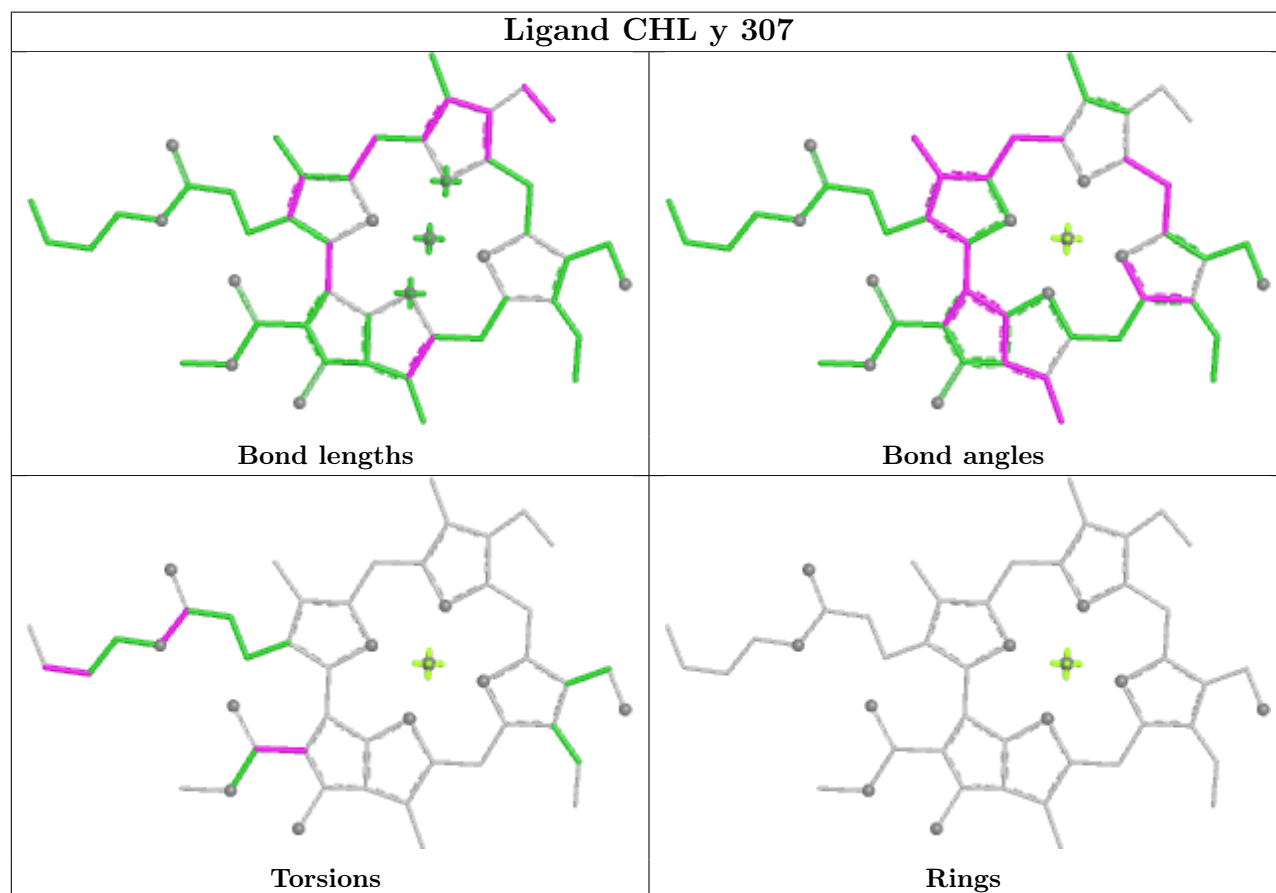
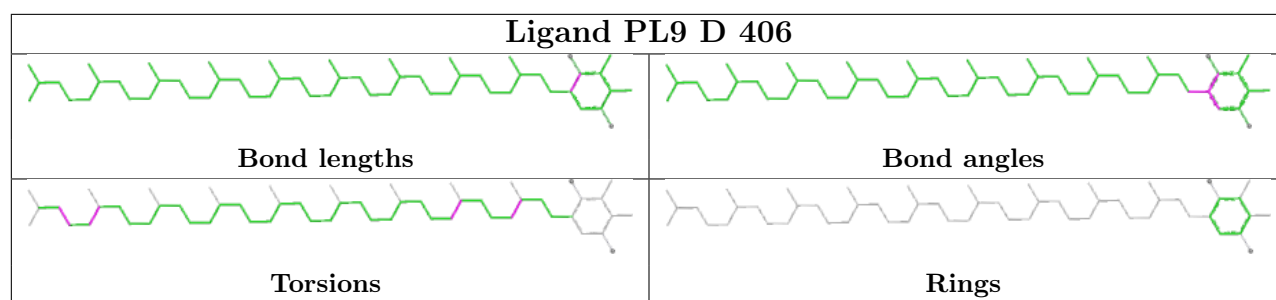


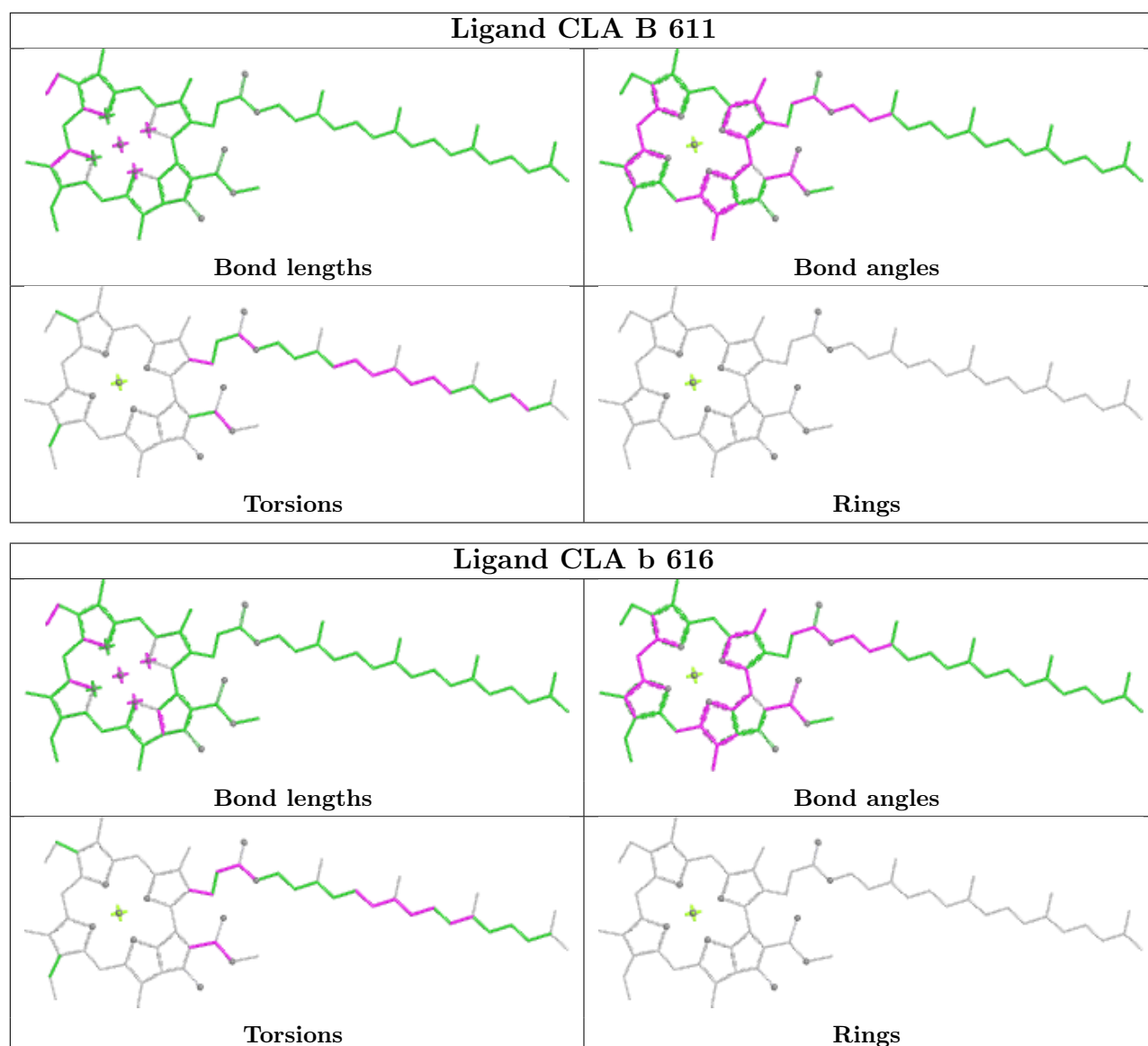




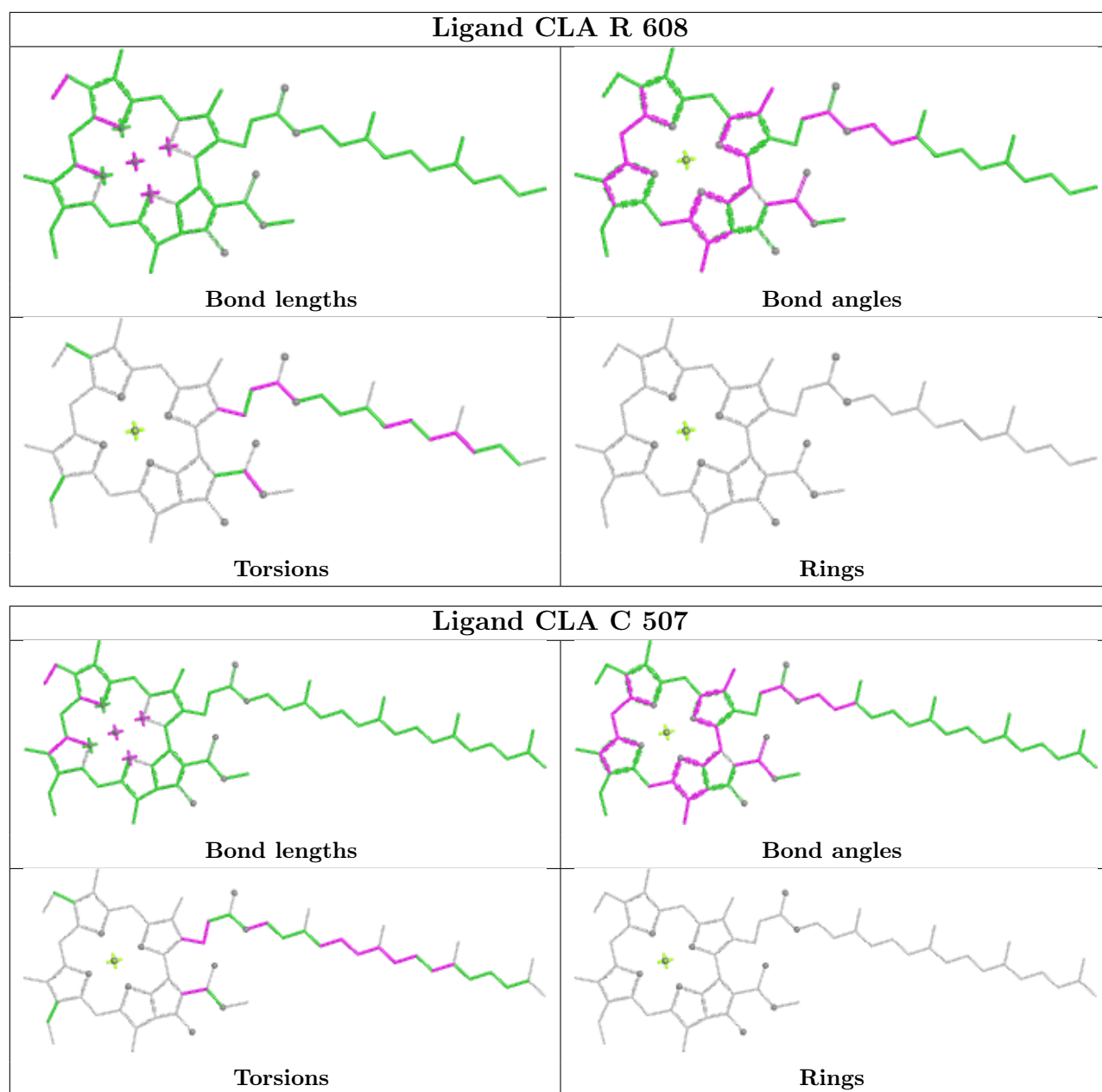


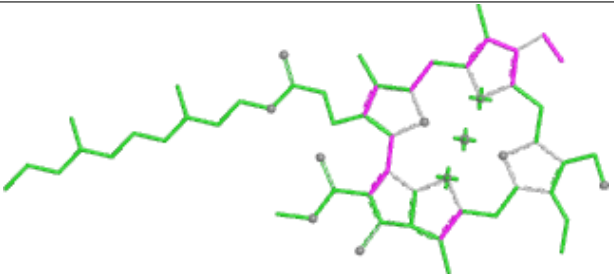
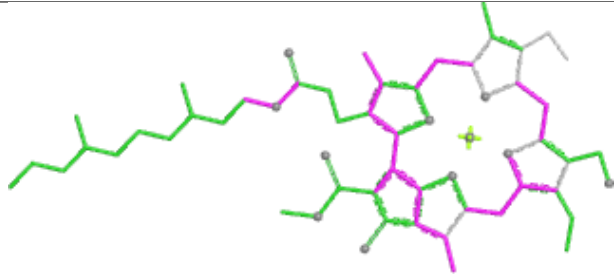
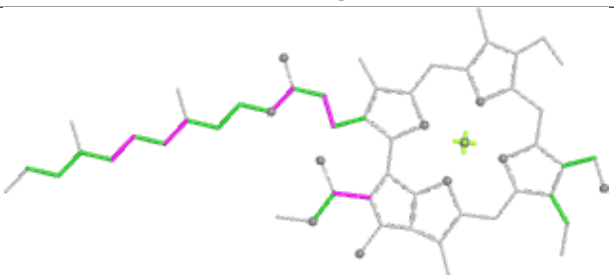
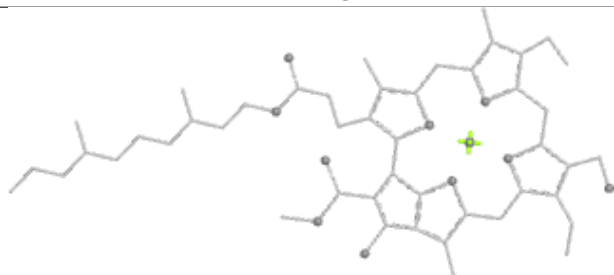


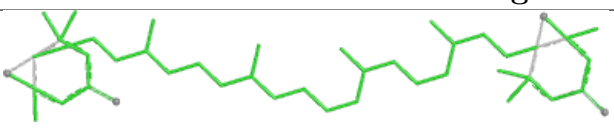
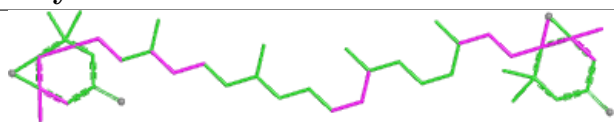
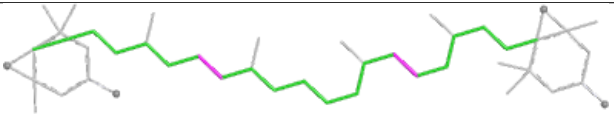
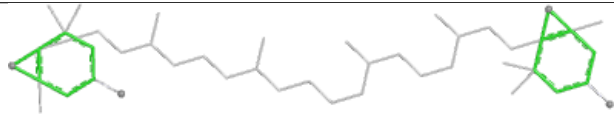


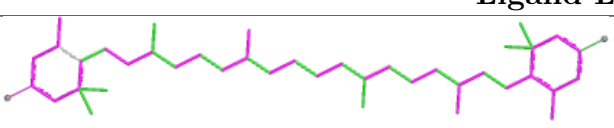
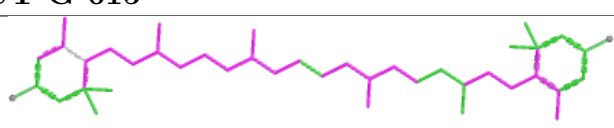
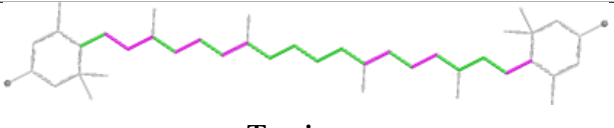
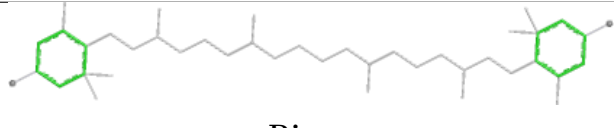


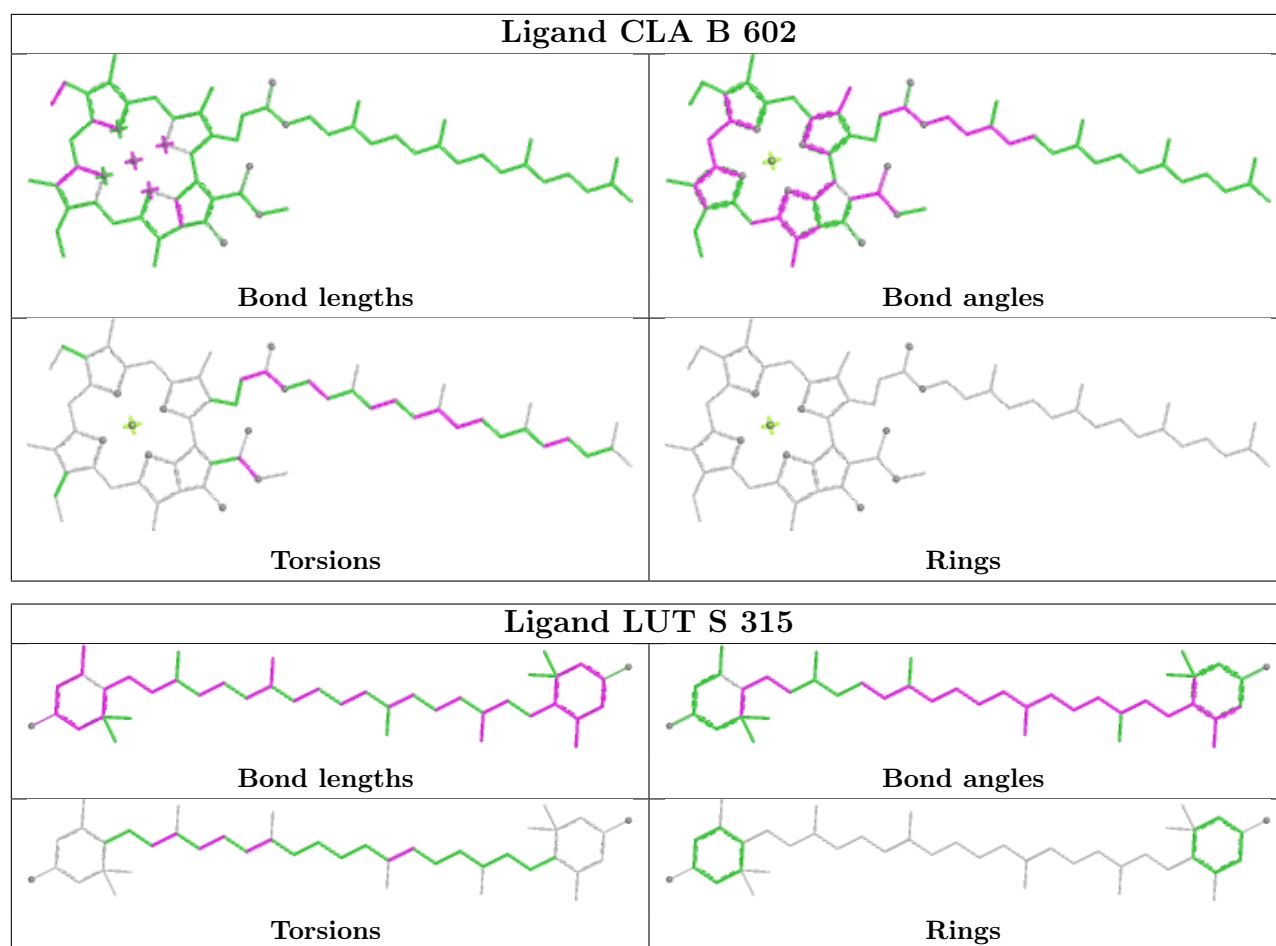


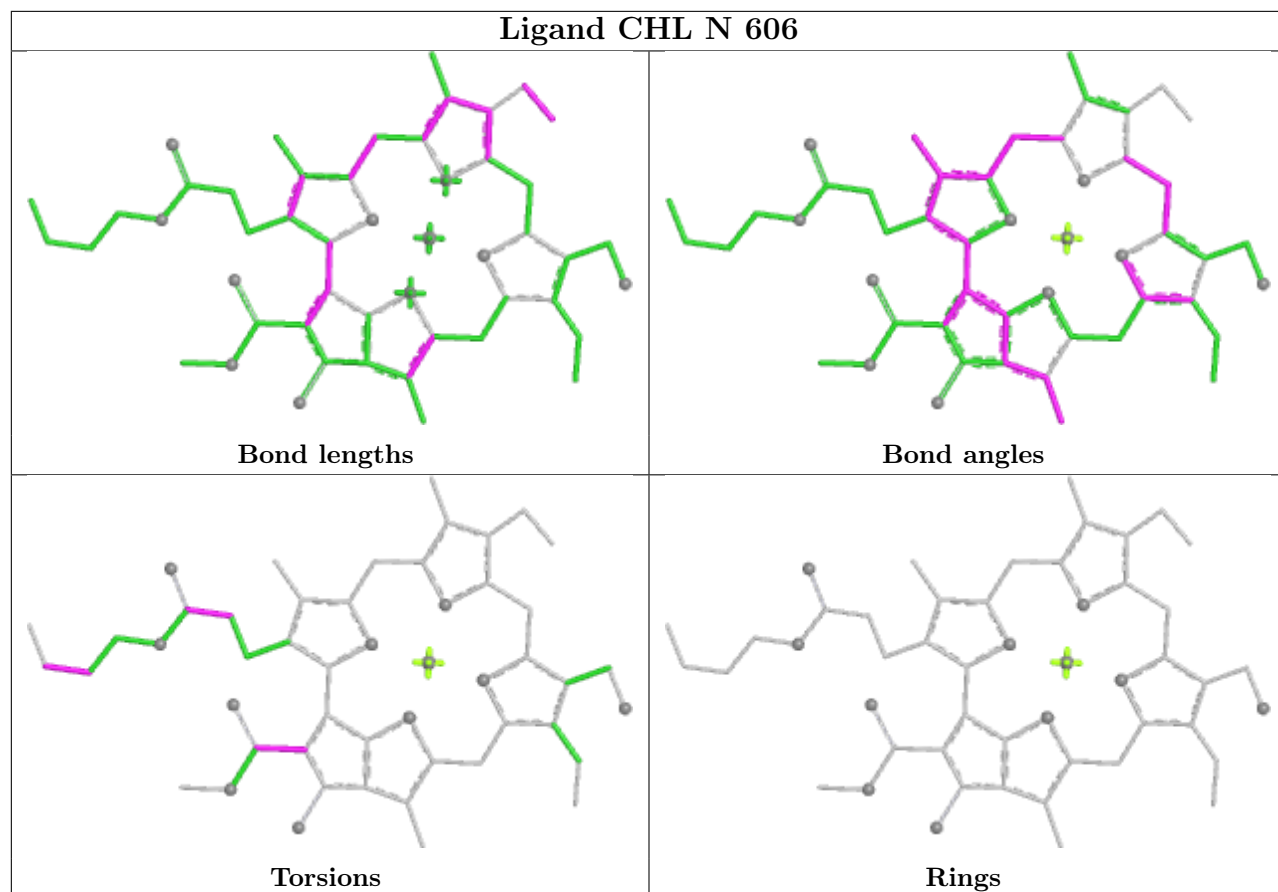


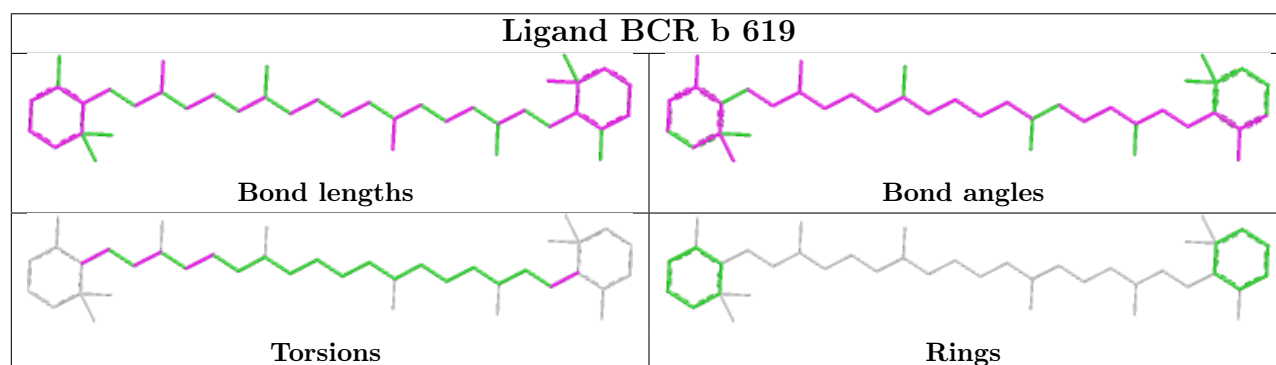
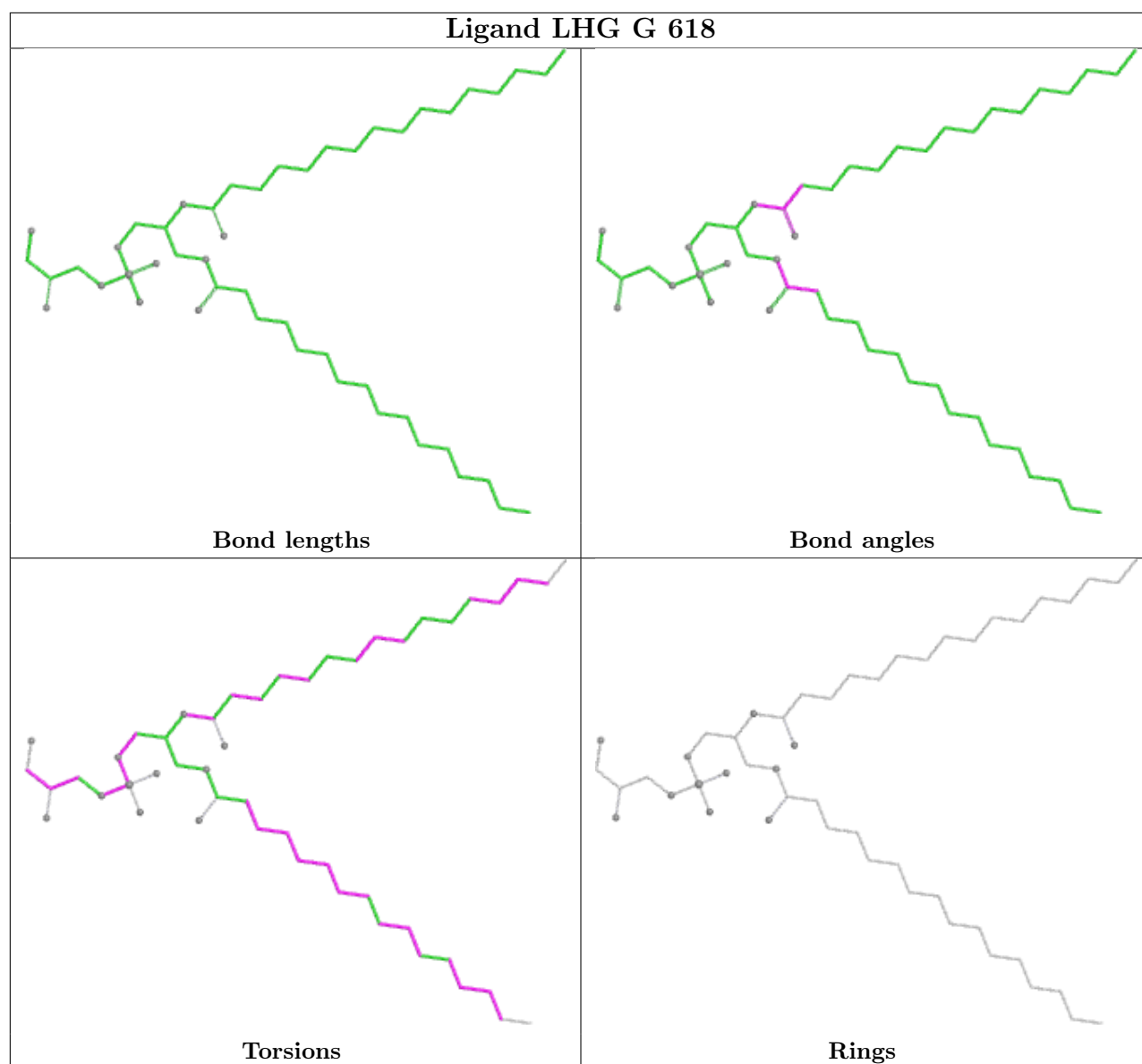
Ligand CHL s 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

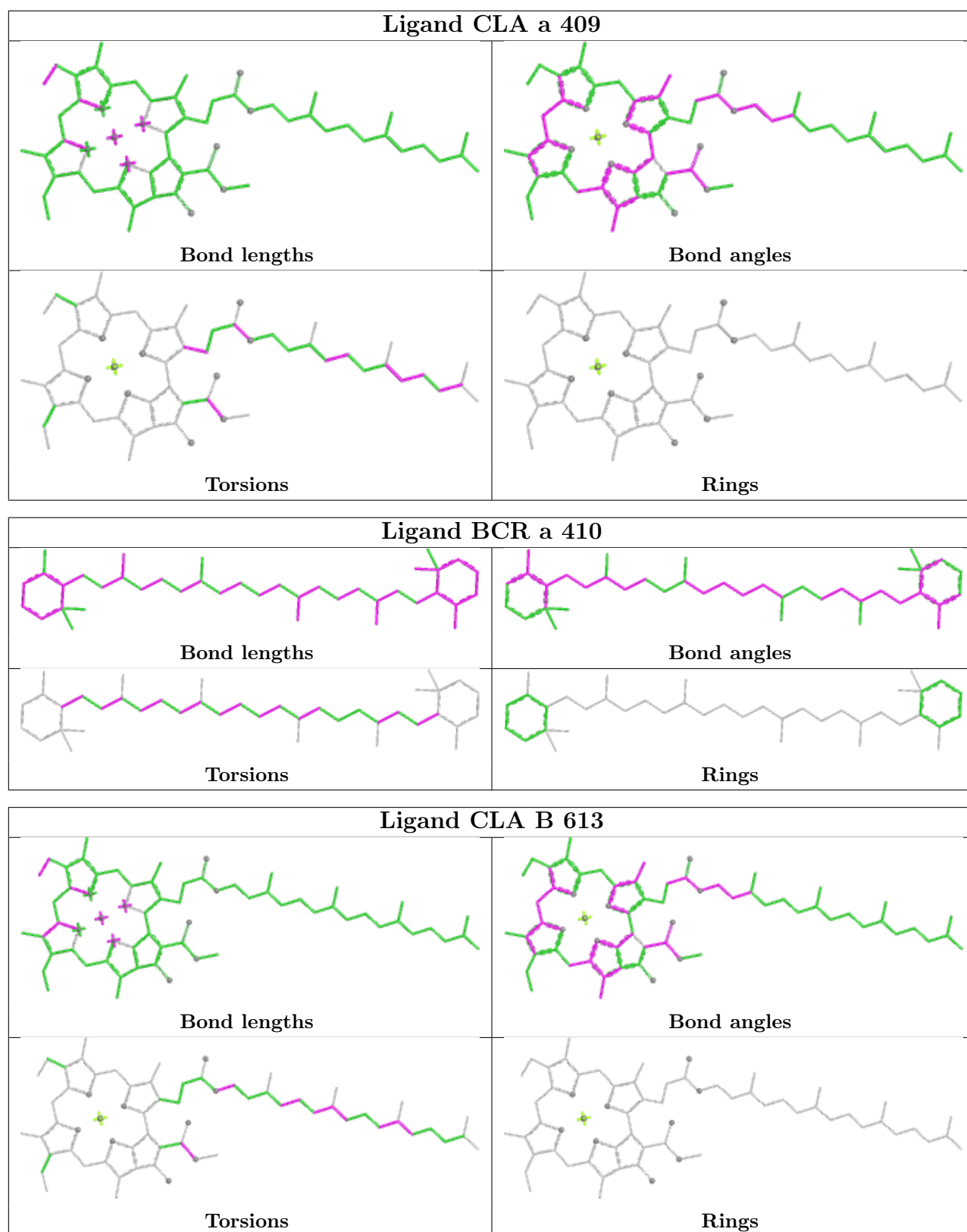
Ligand XAT y 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

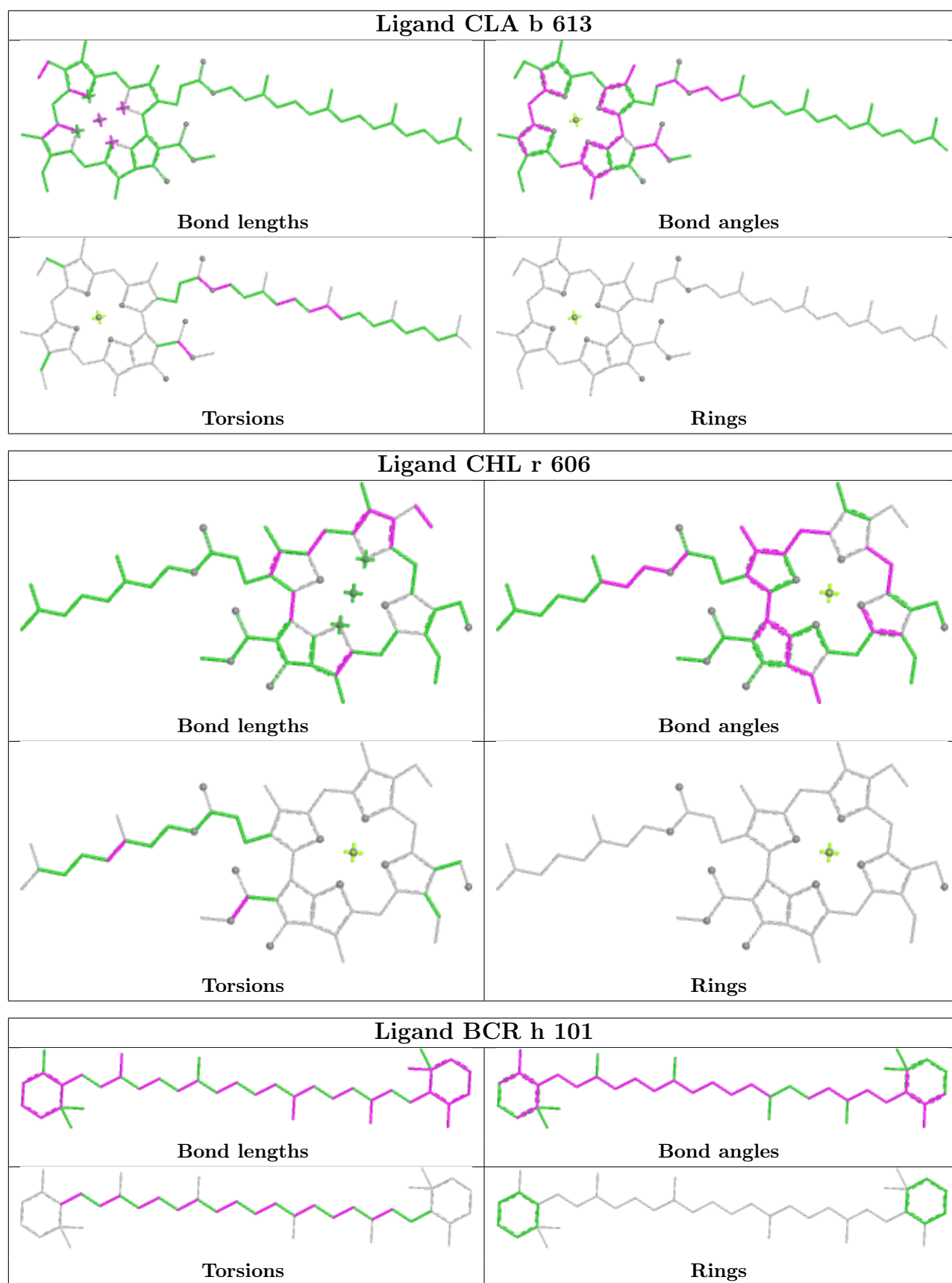
Ligand LUT G 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

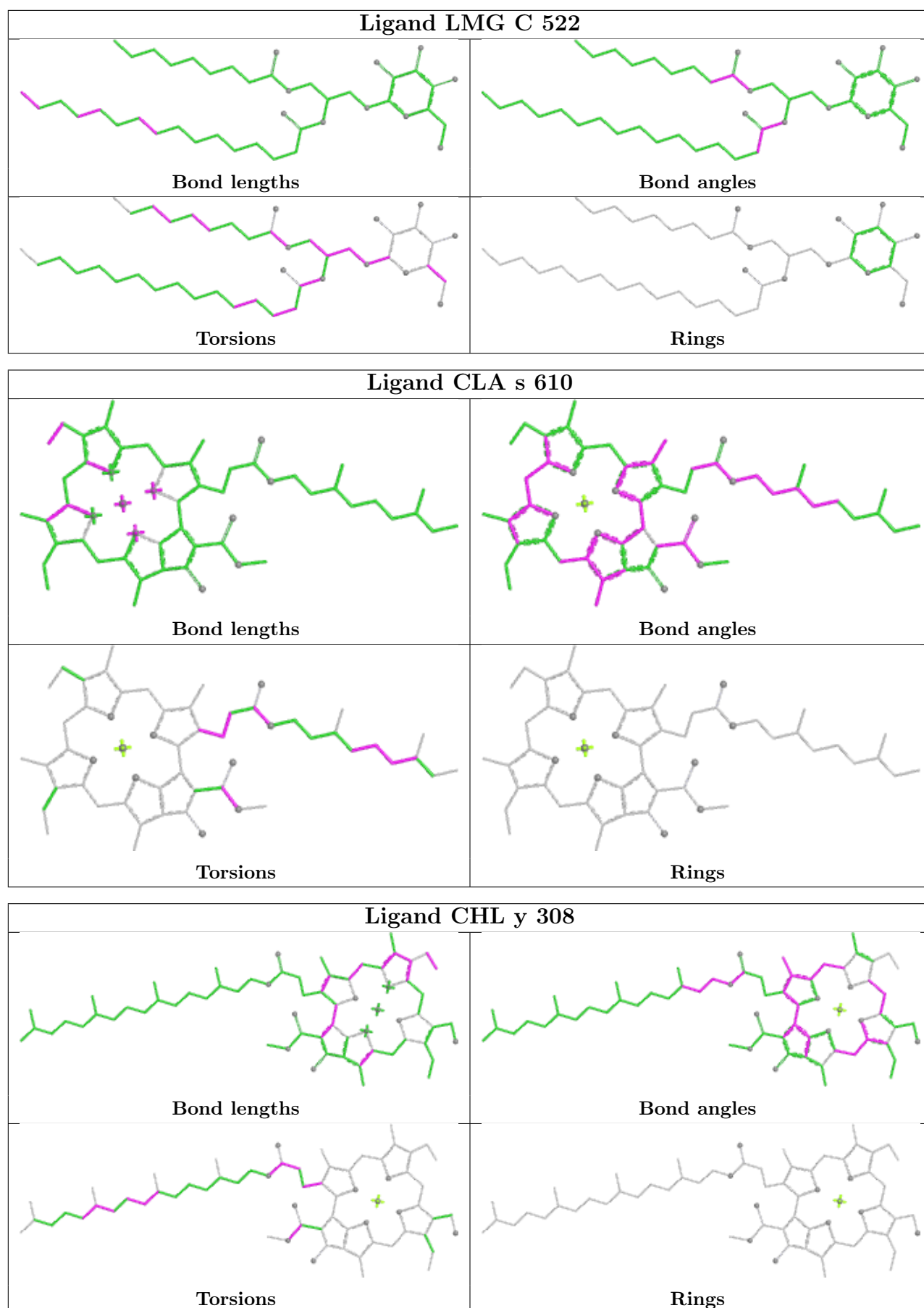




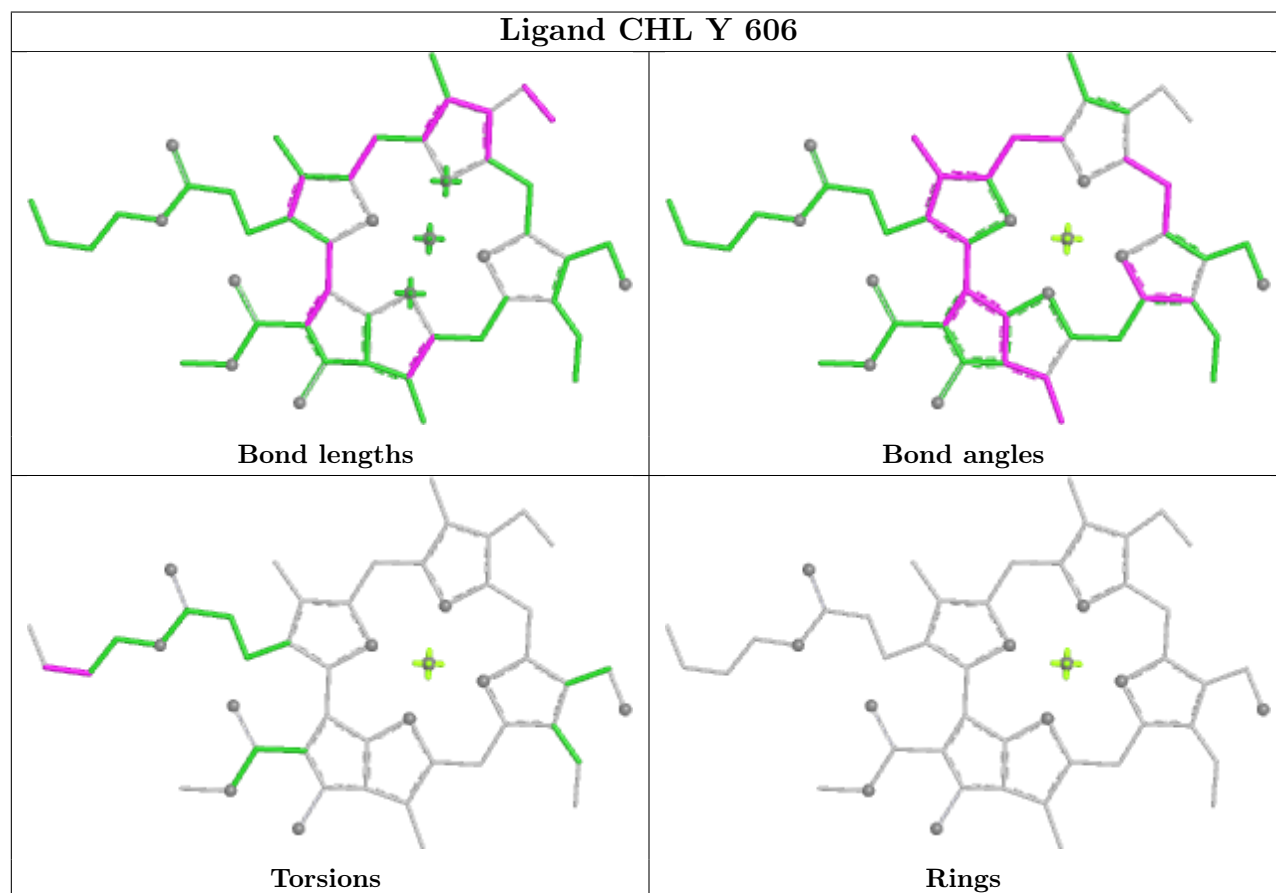
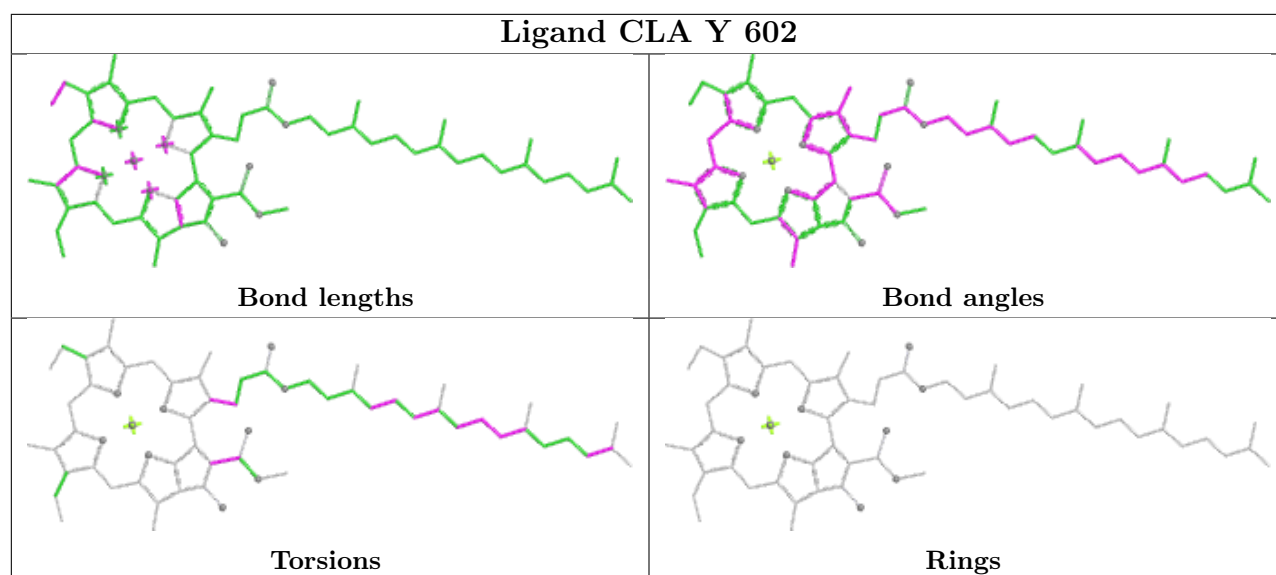


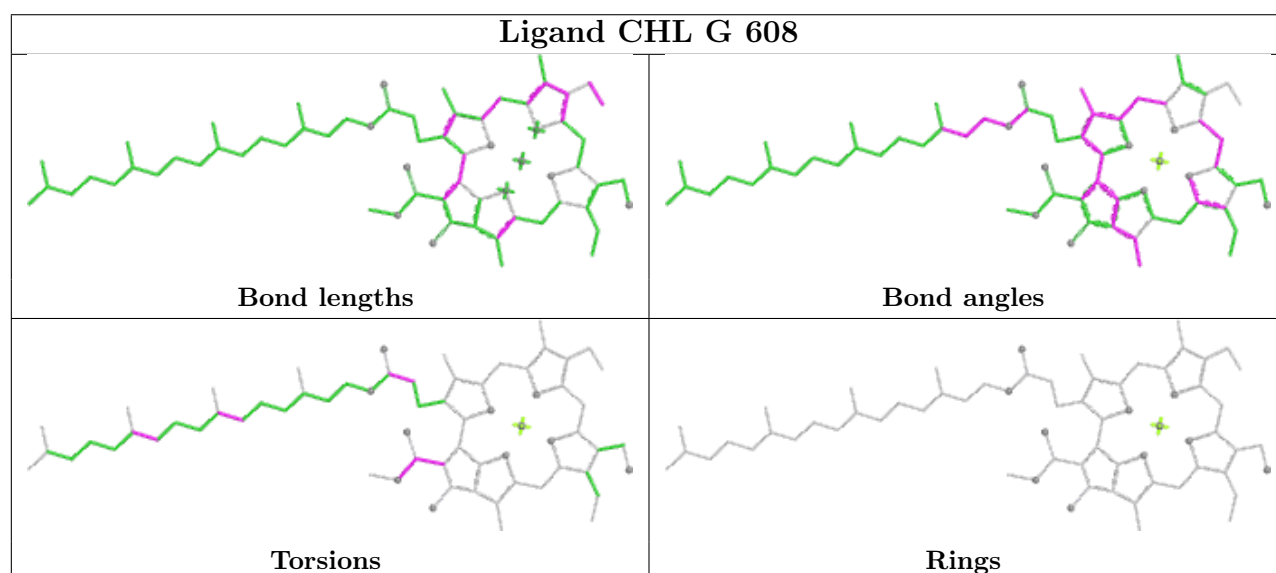
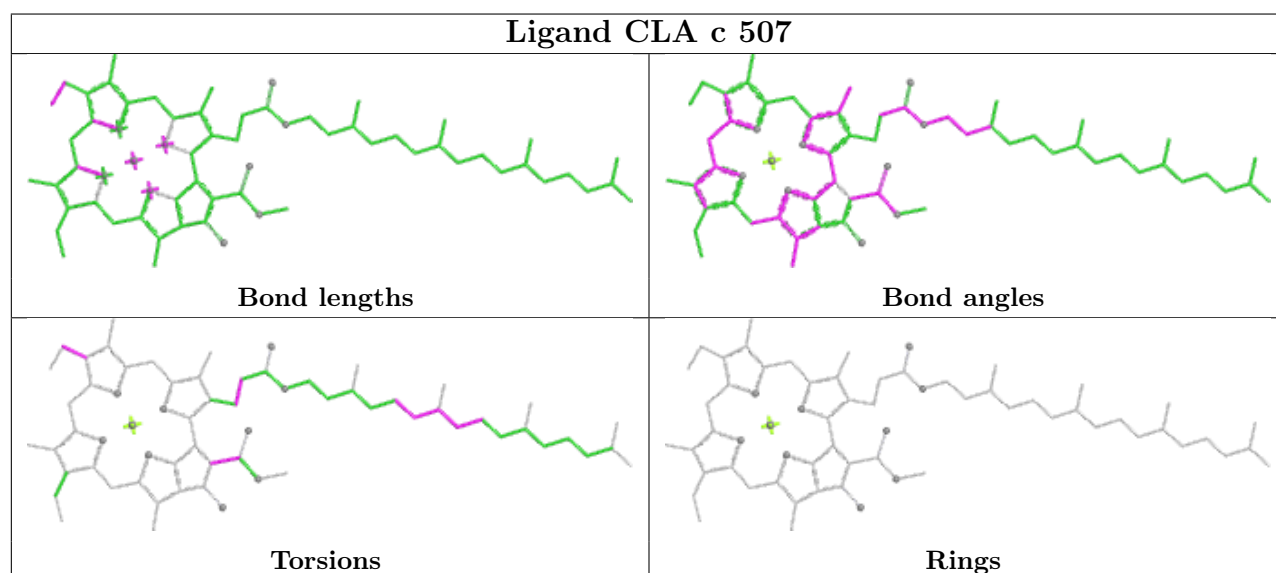
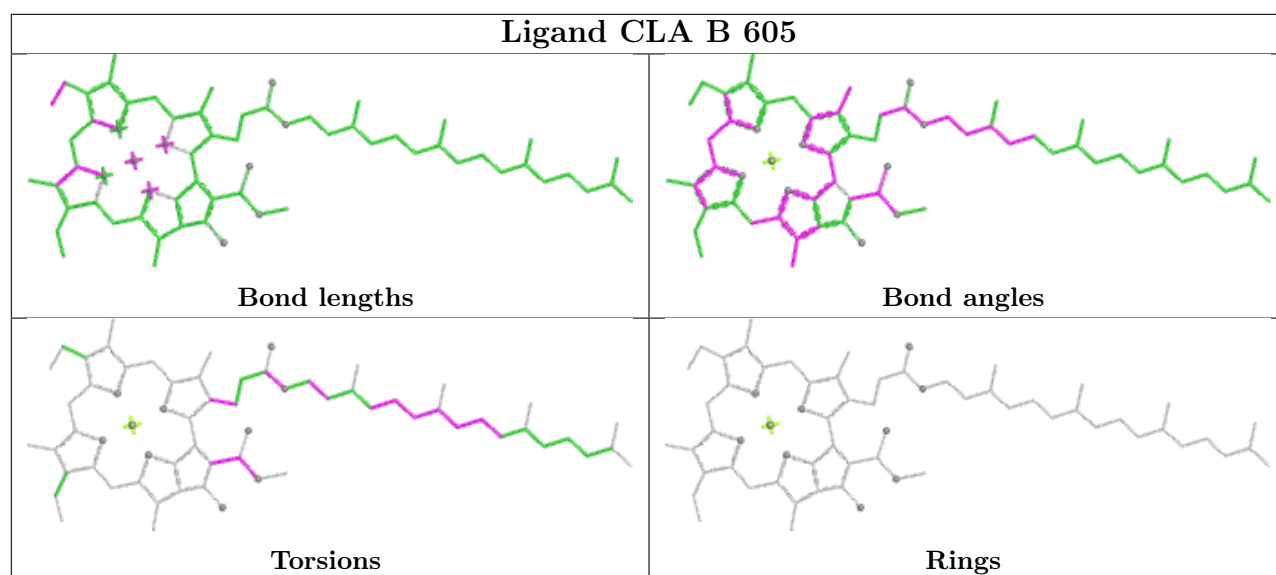


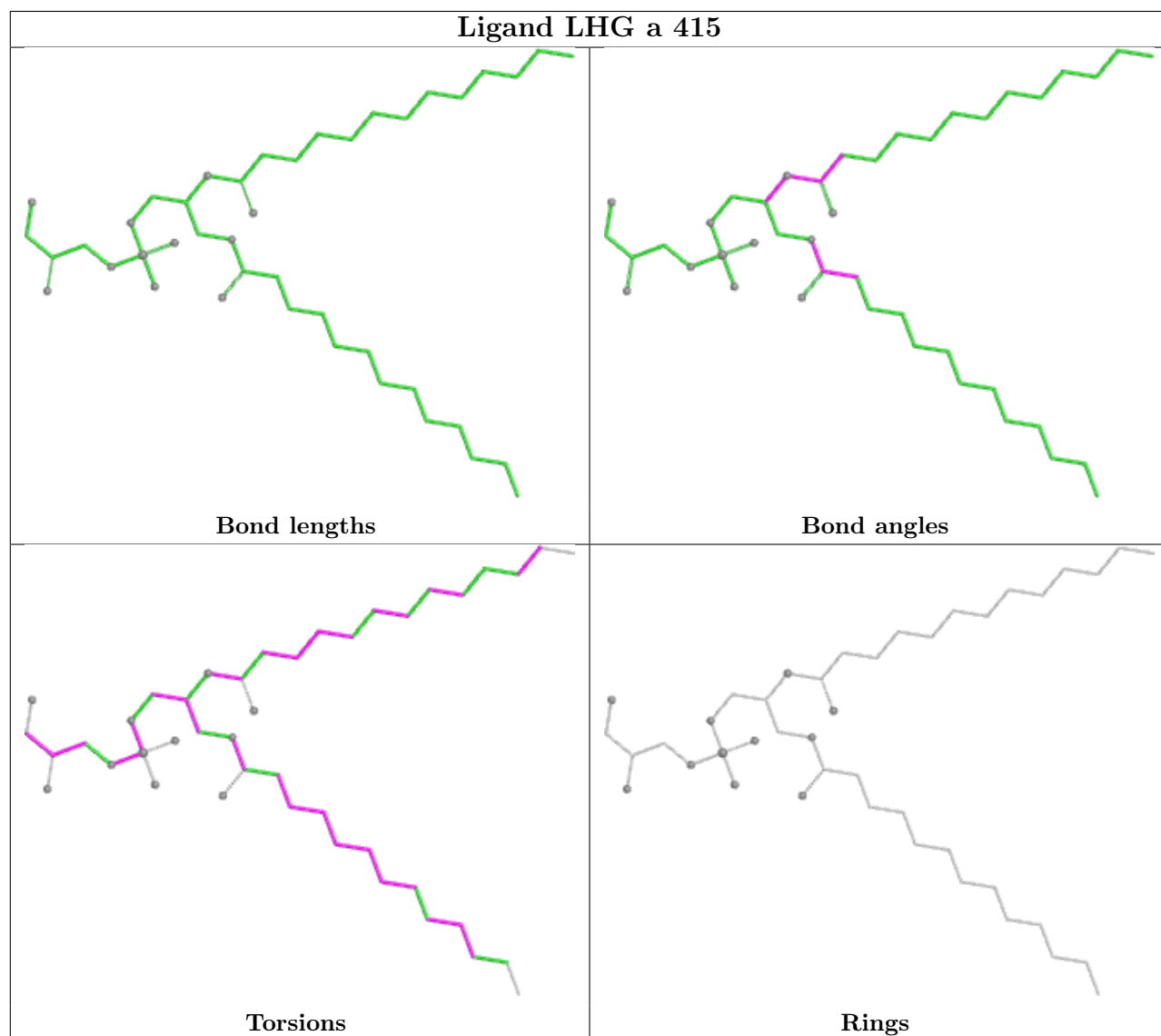
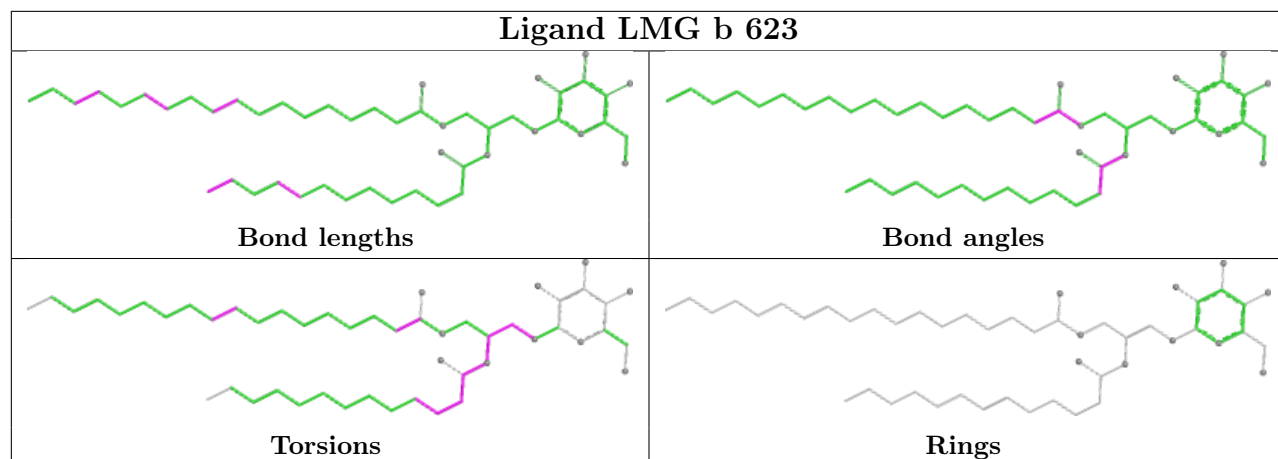


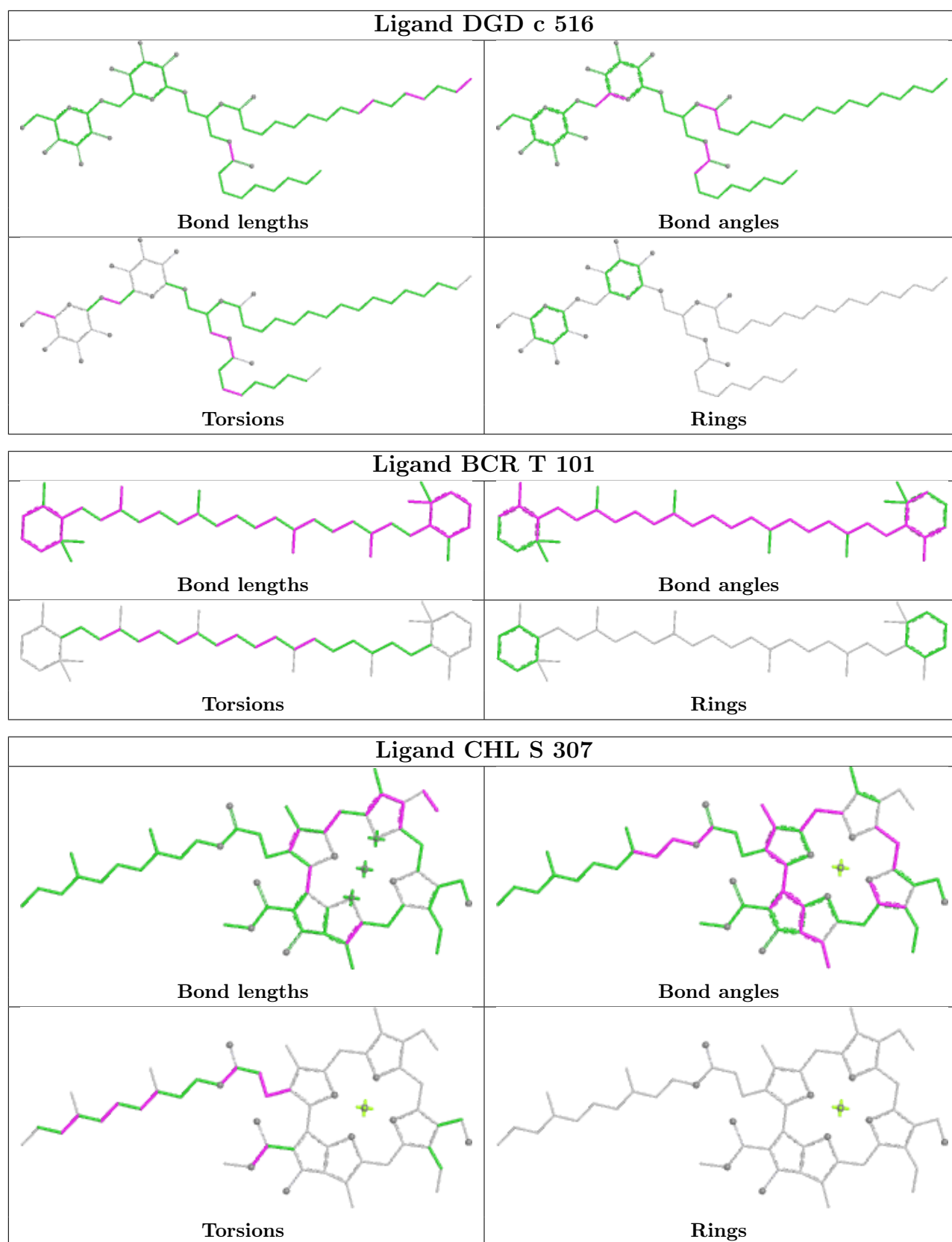


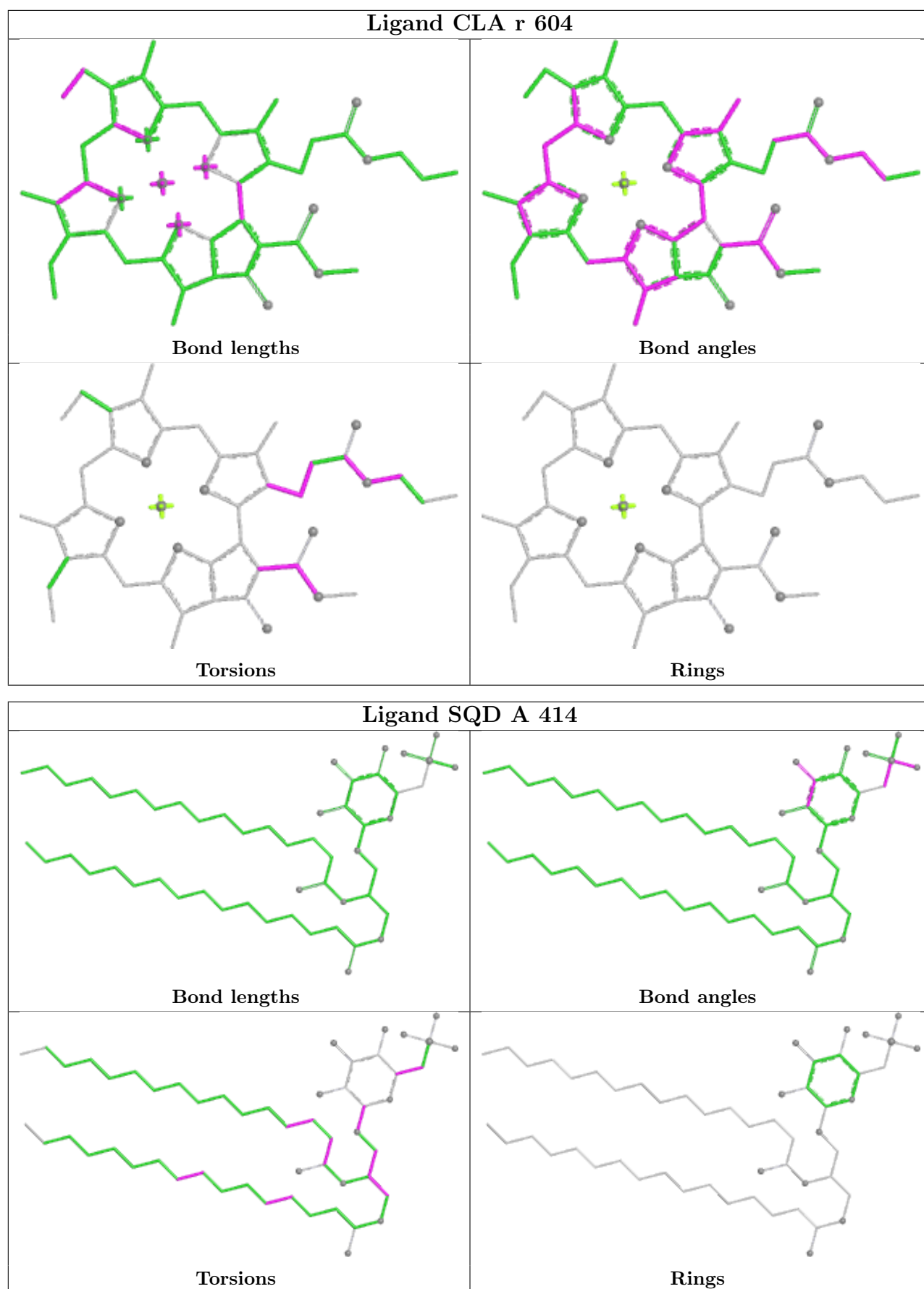


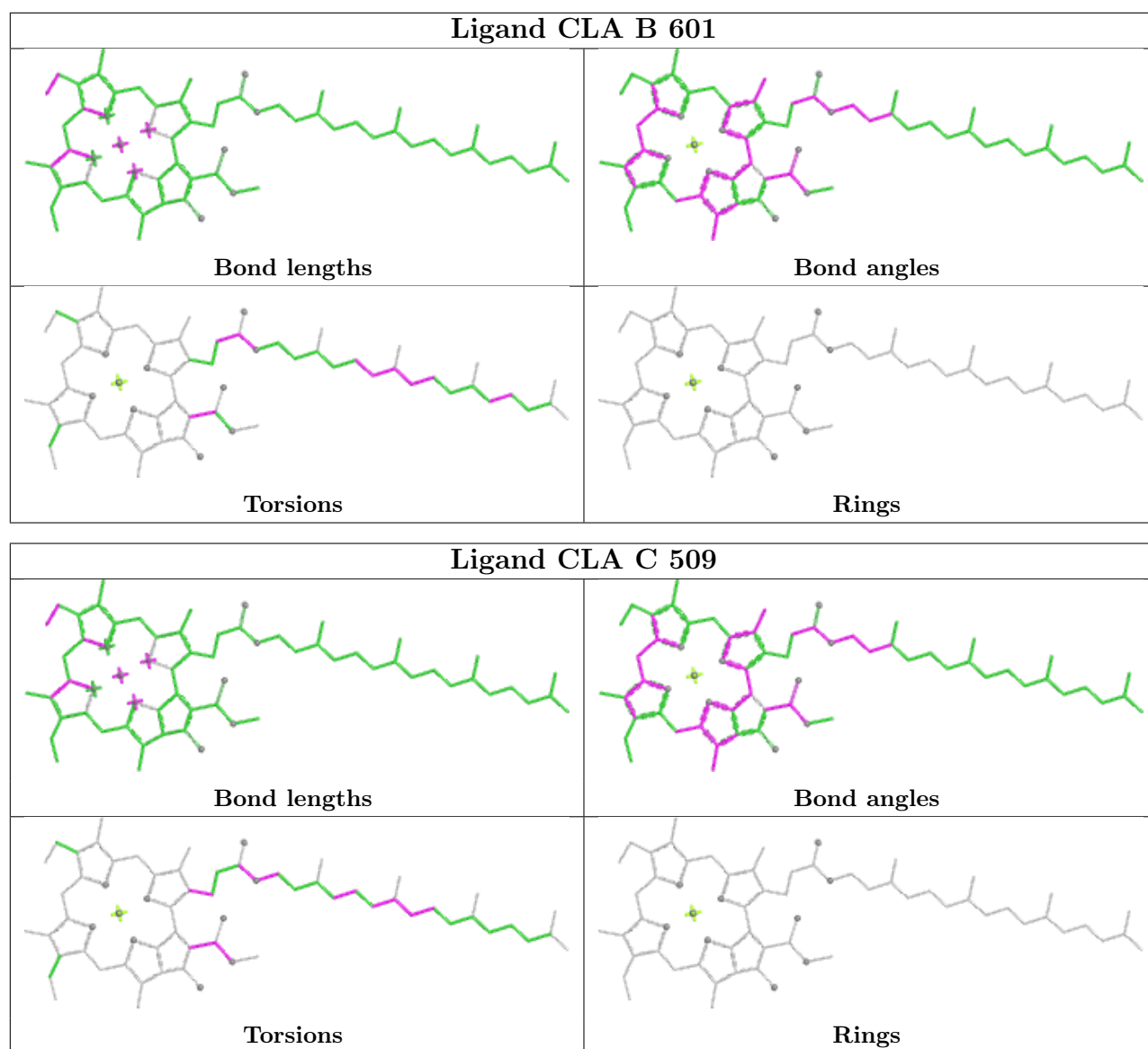


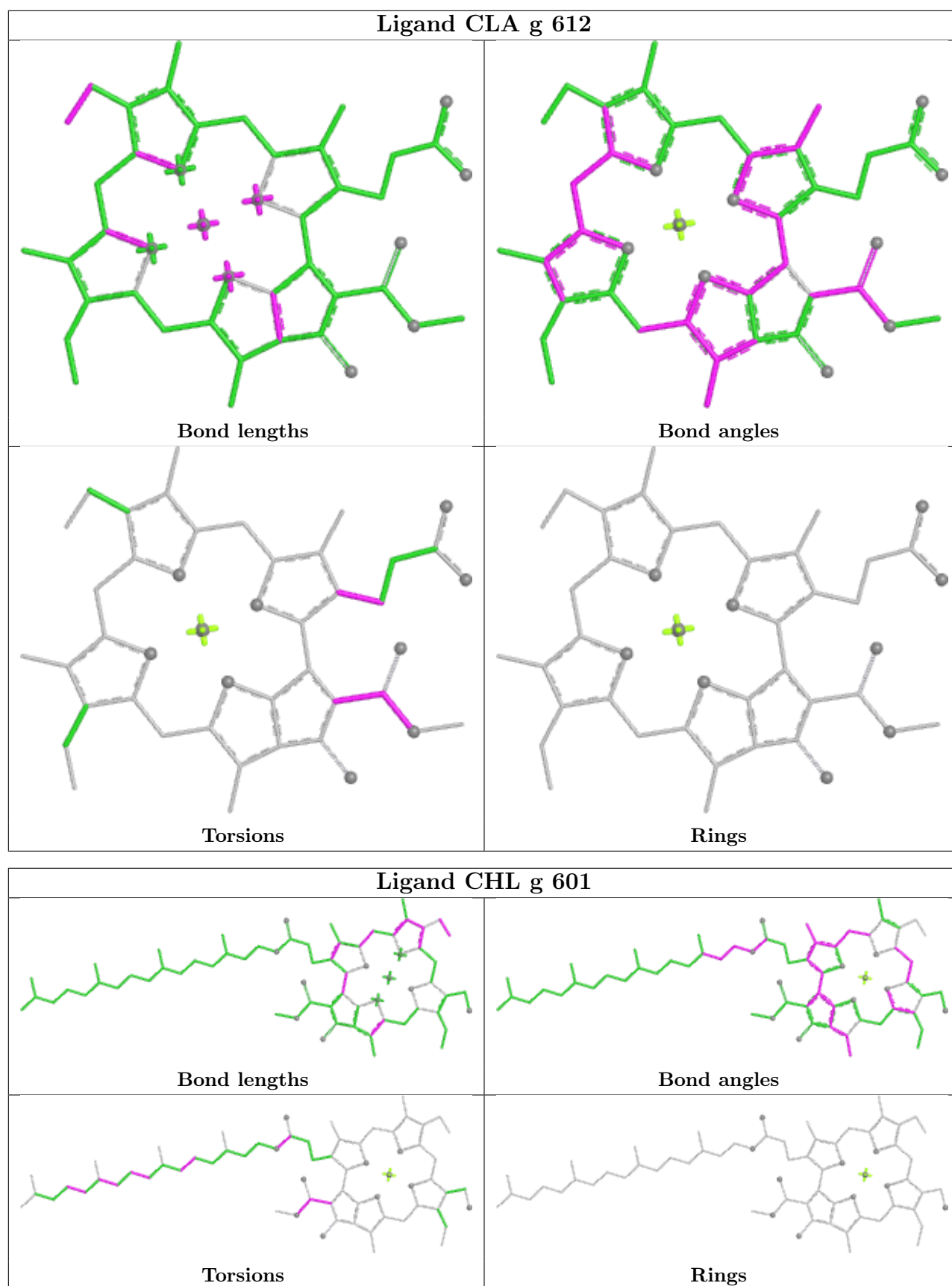


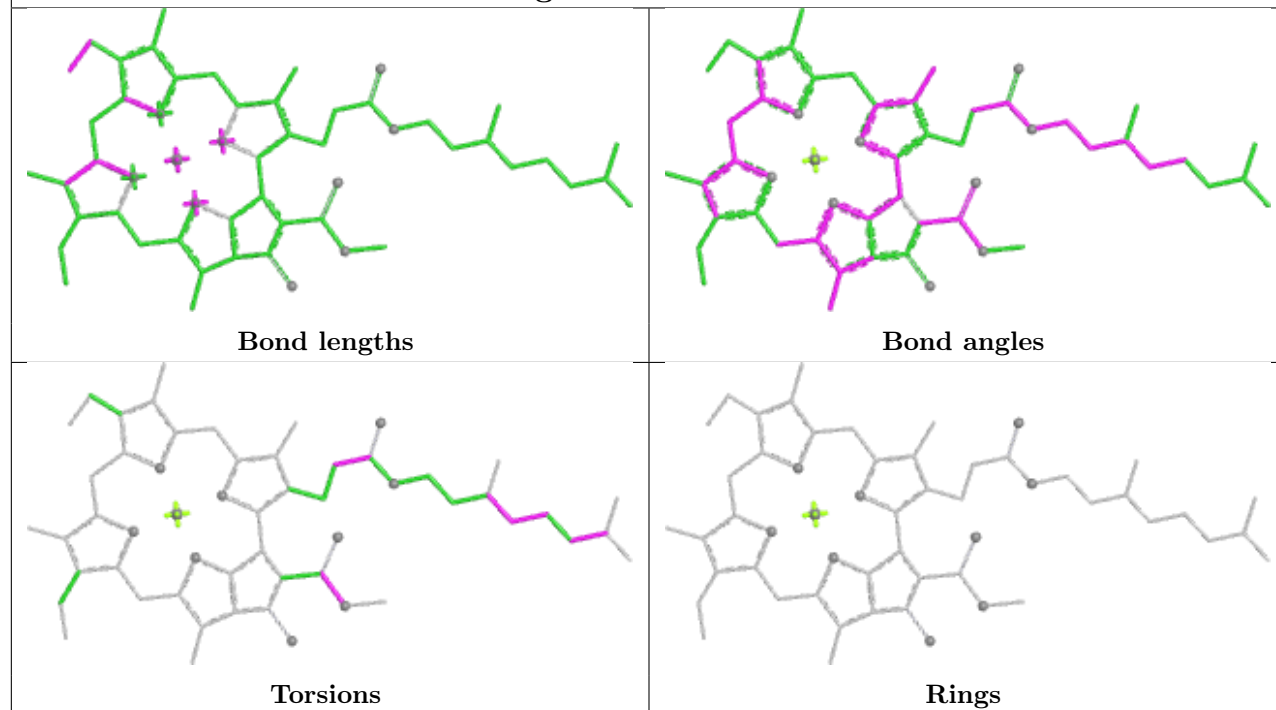
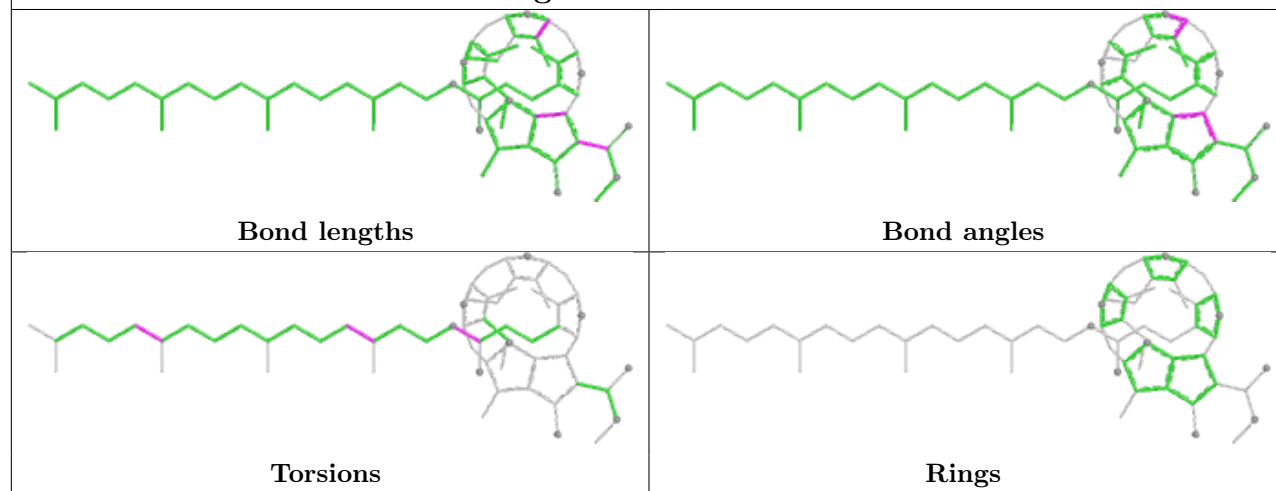




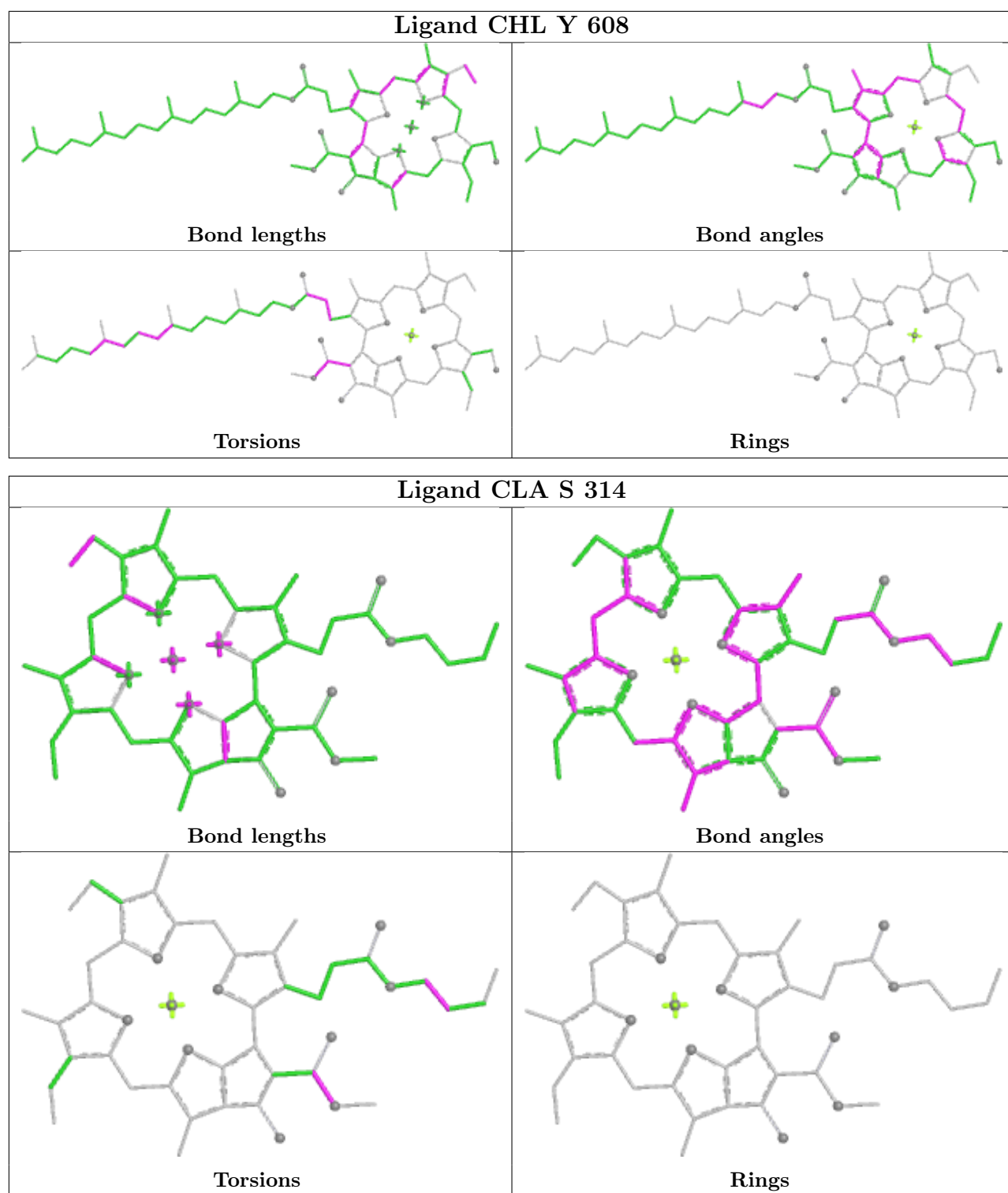


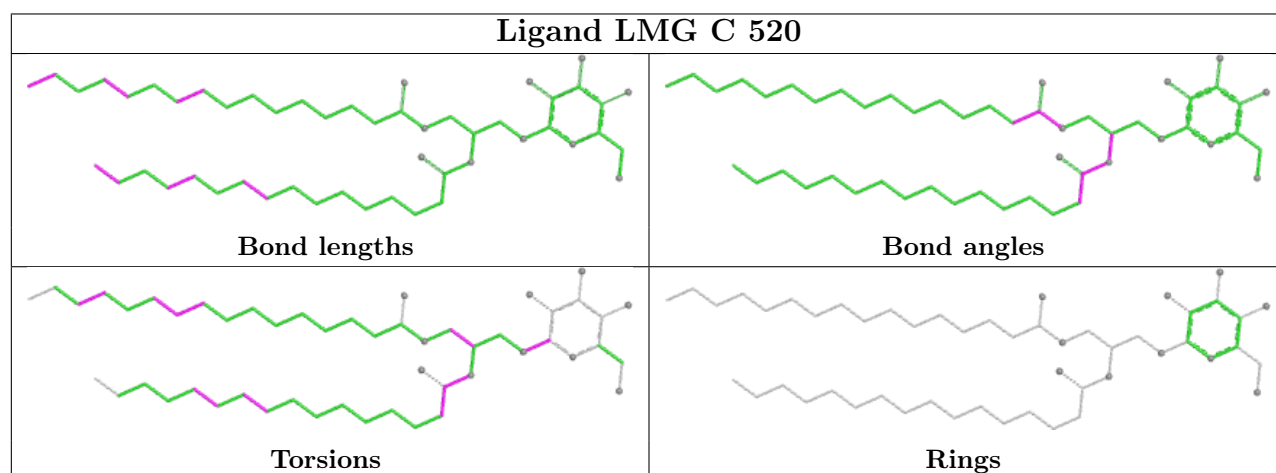
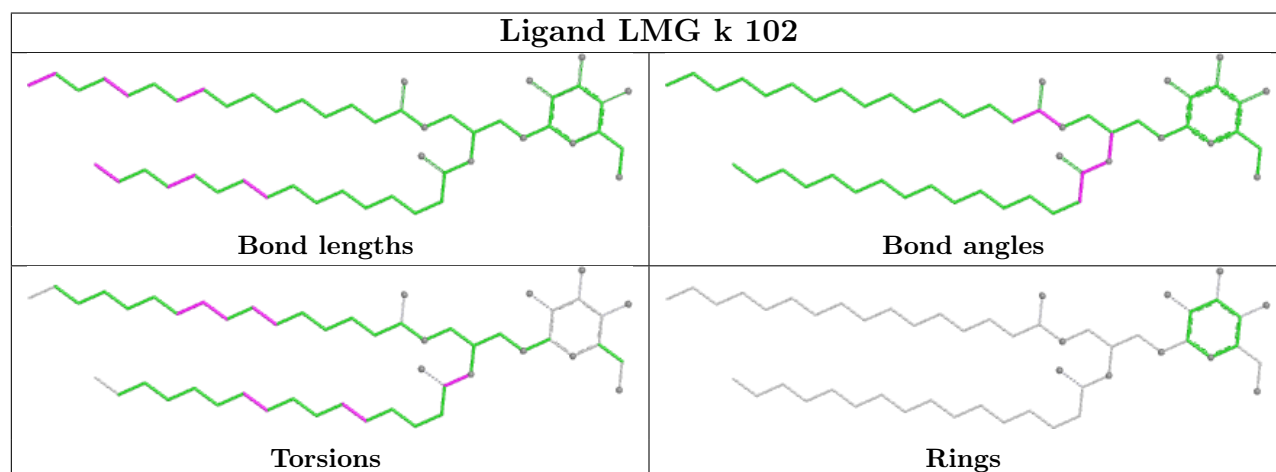
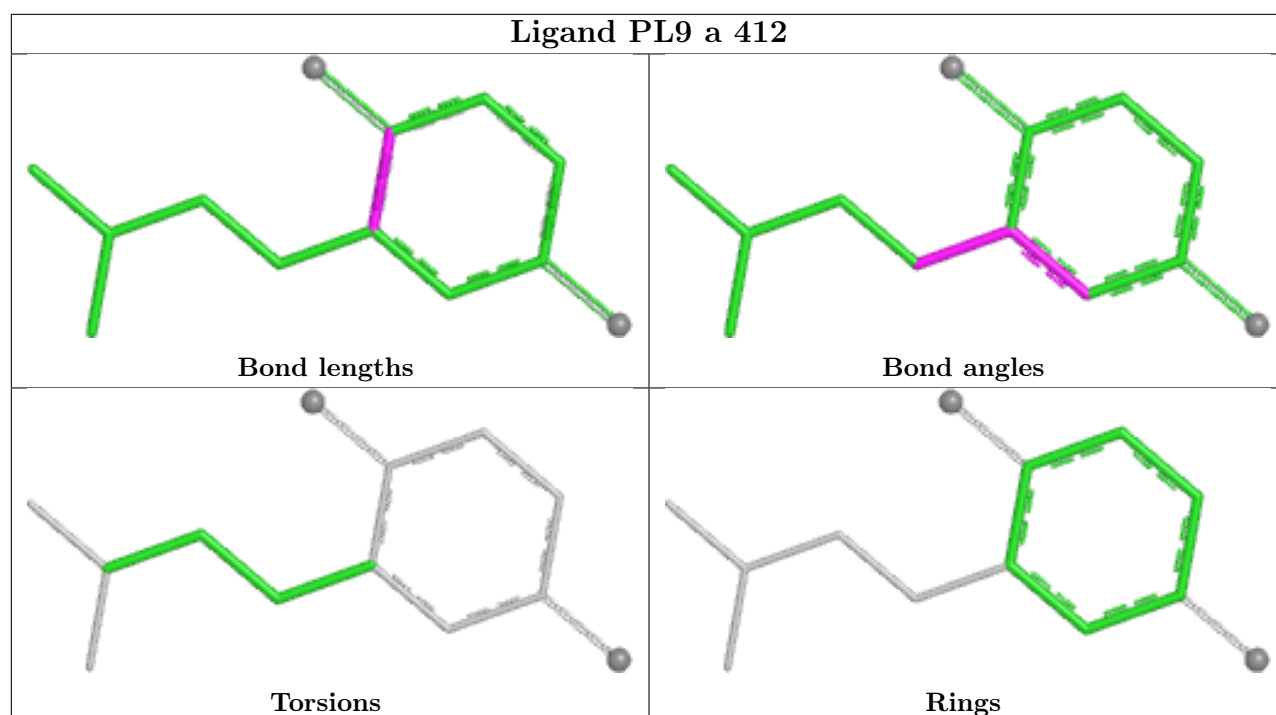


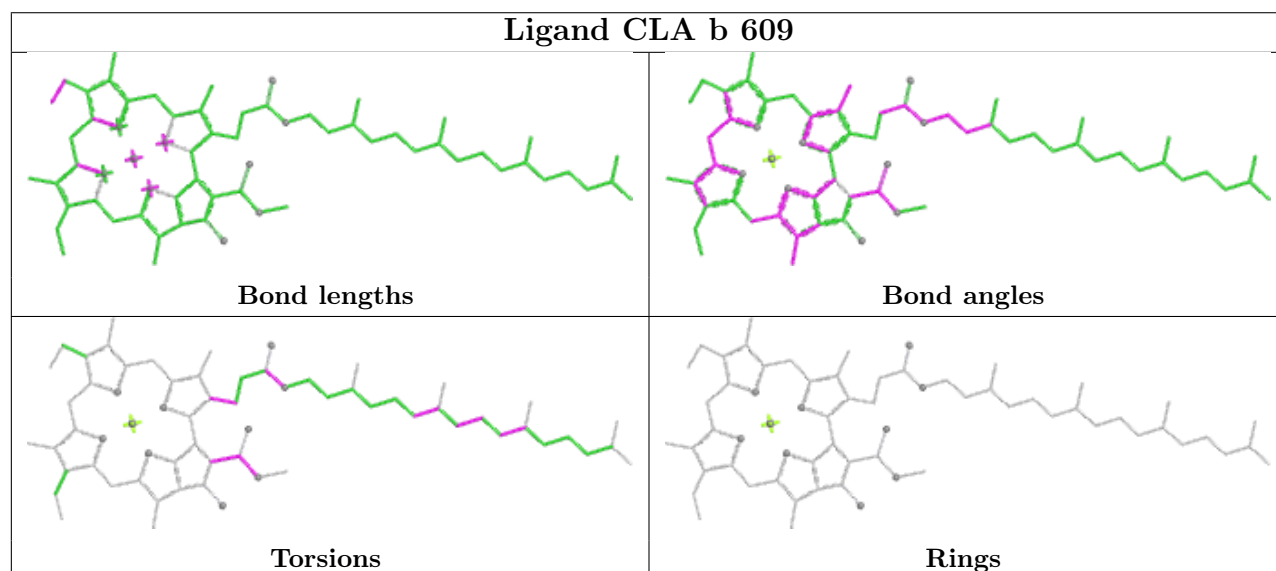
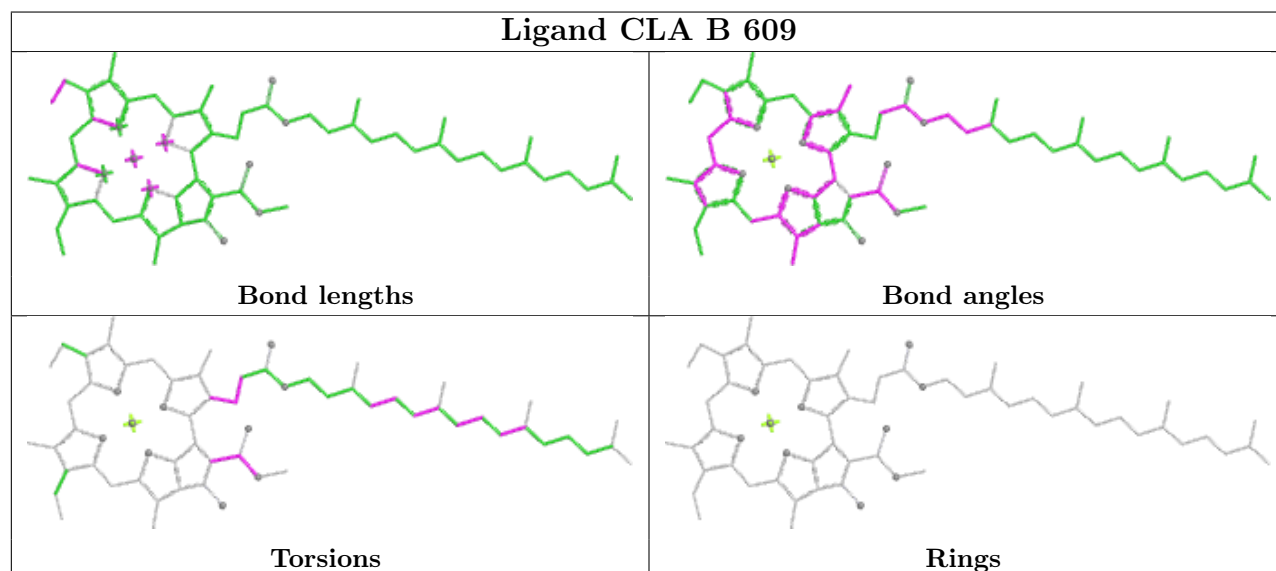
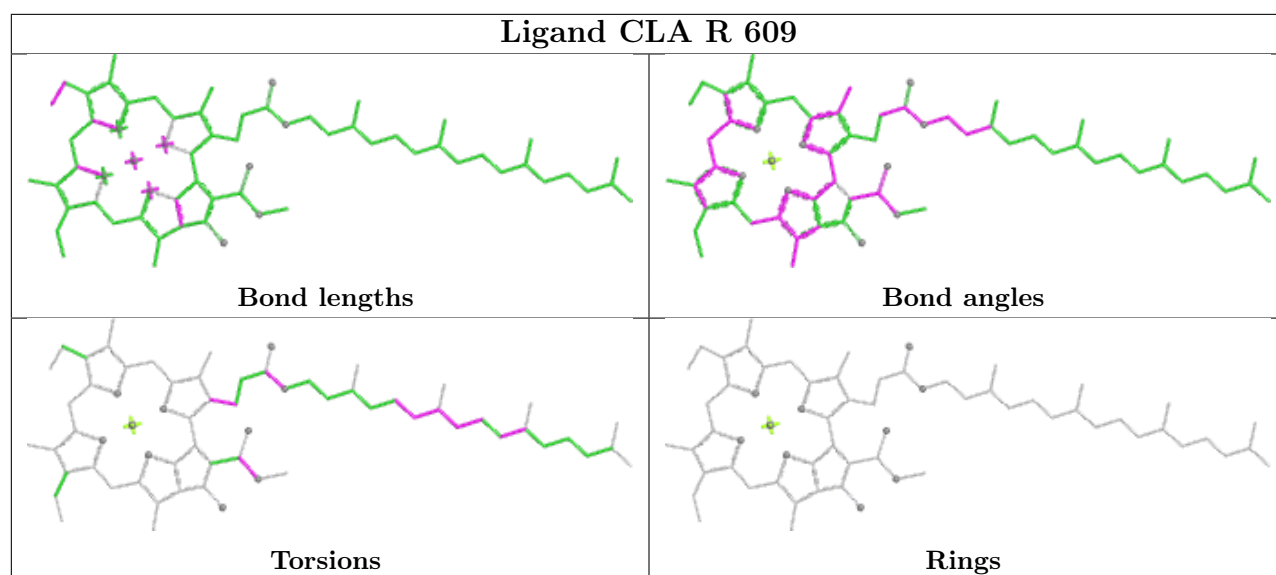


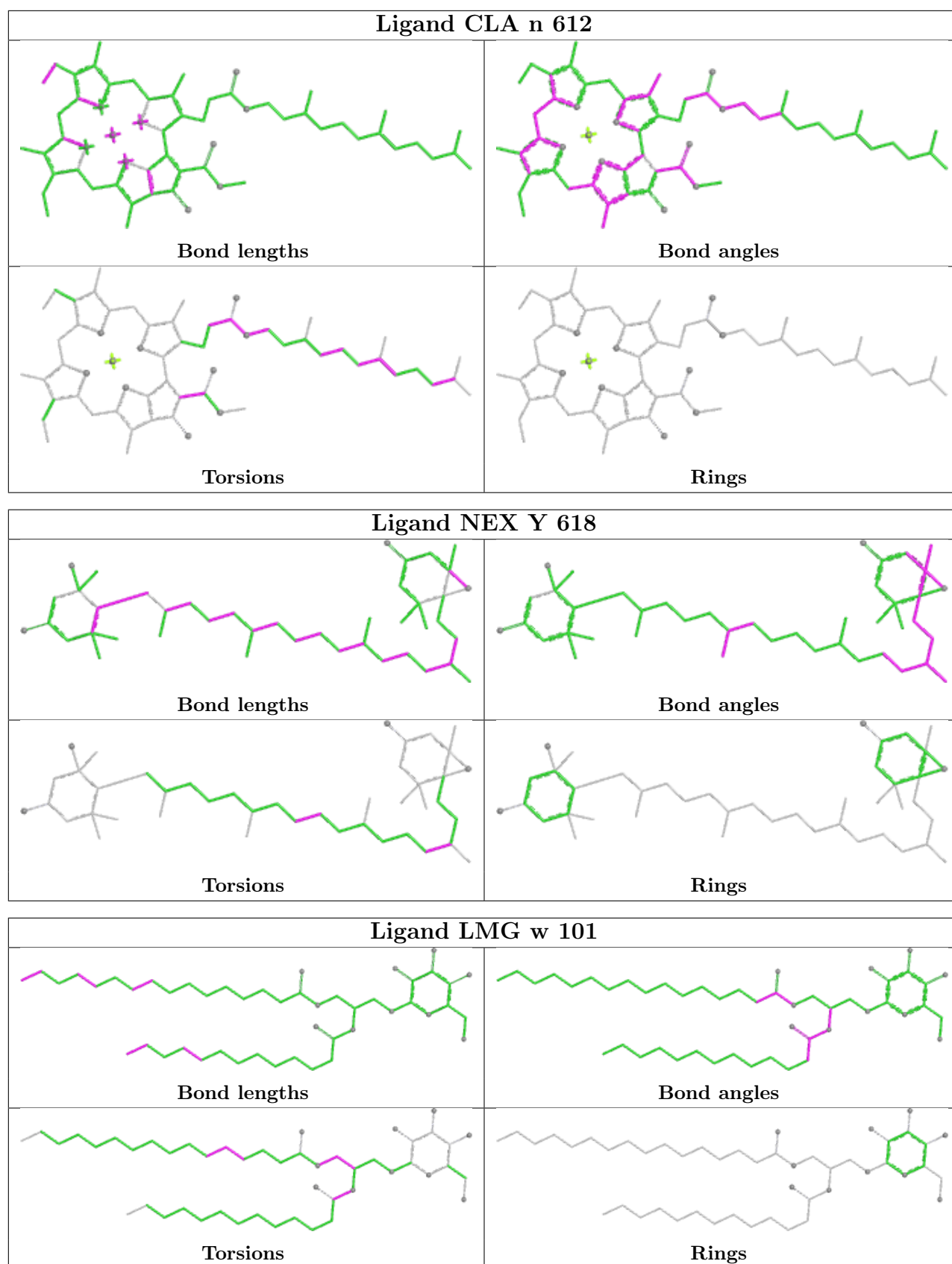
**Ligand CLA S 313****Ligand PHO a 408**

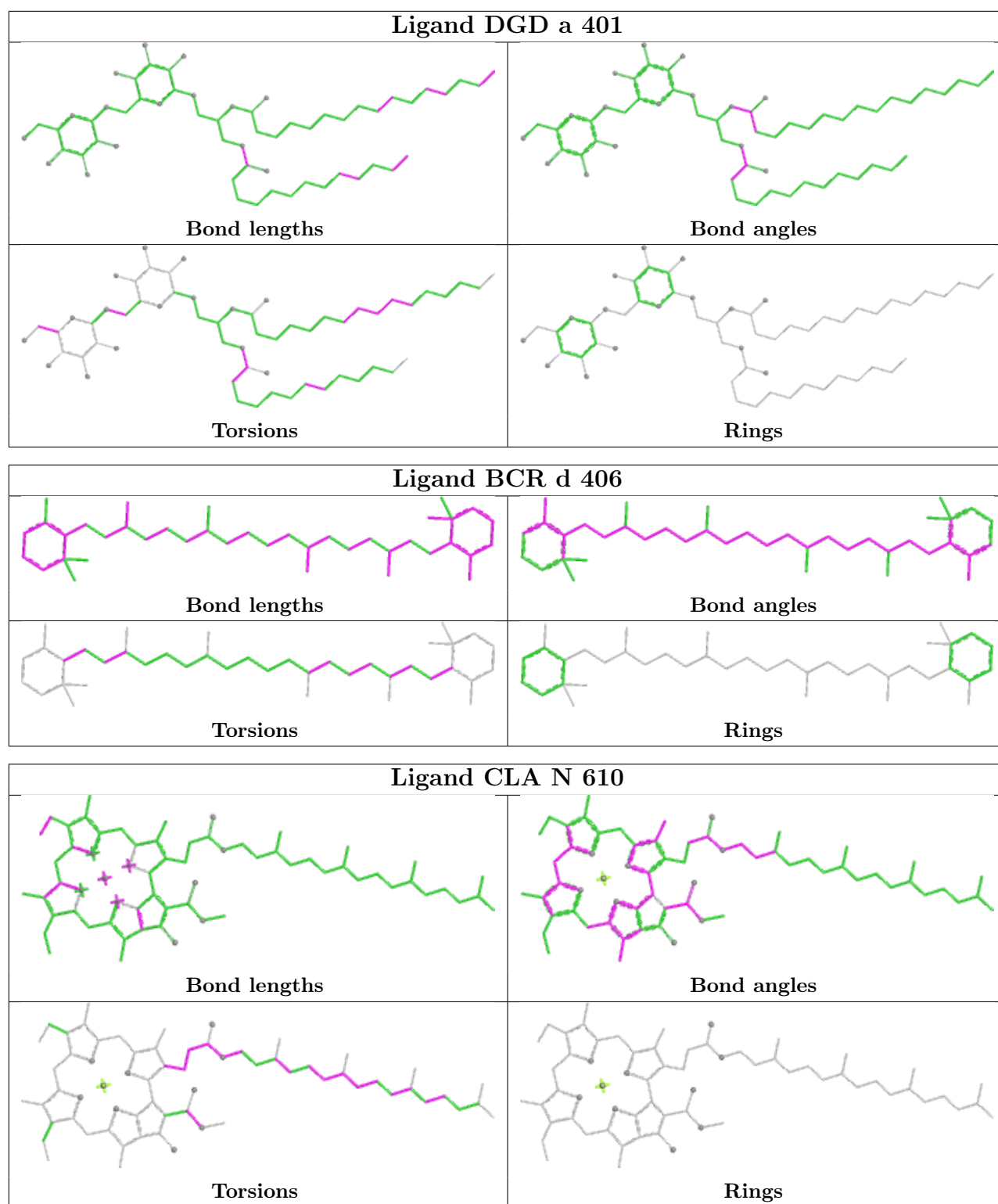


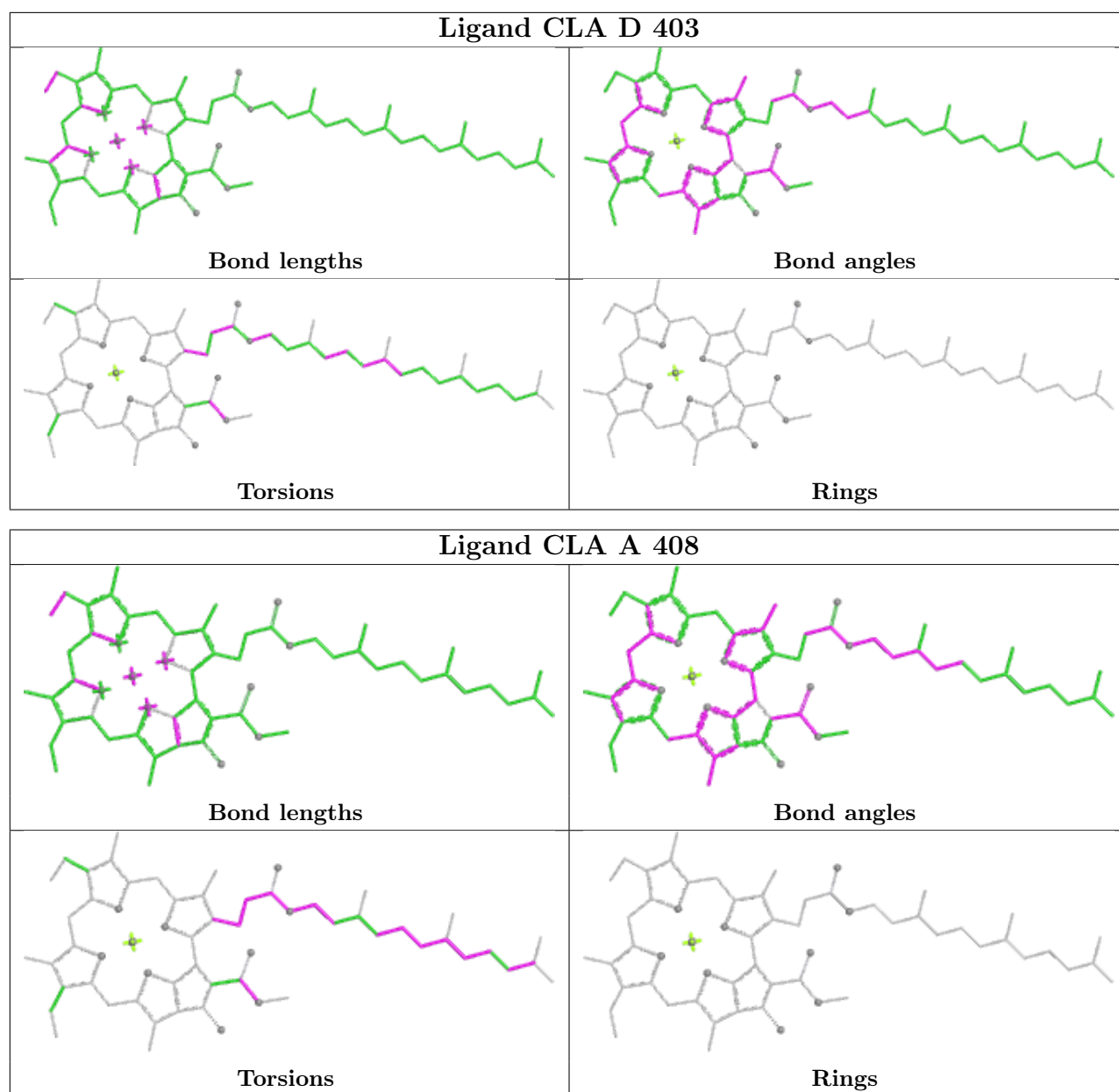


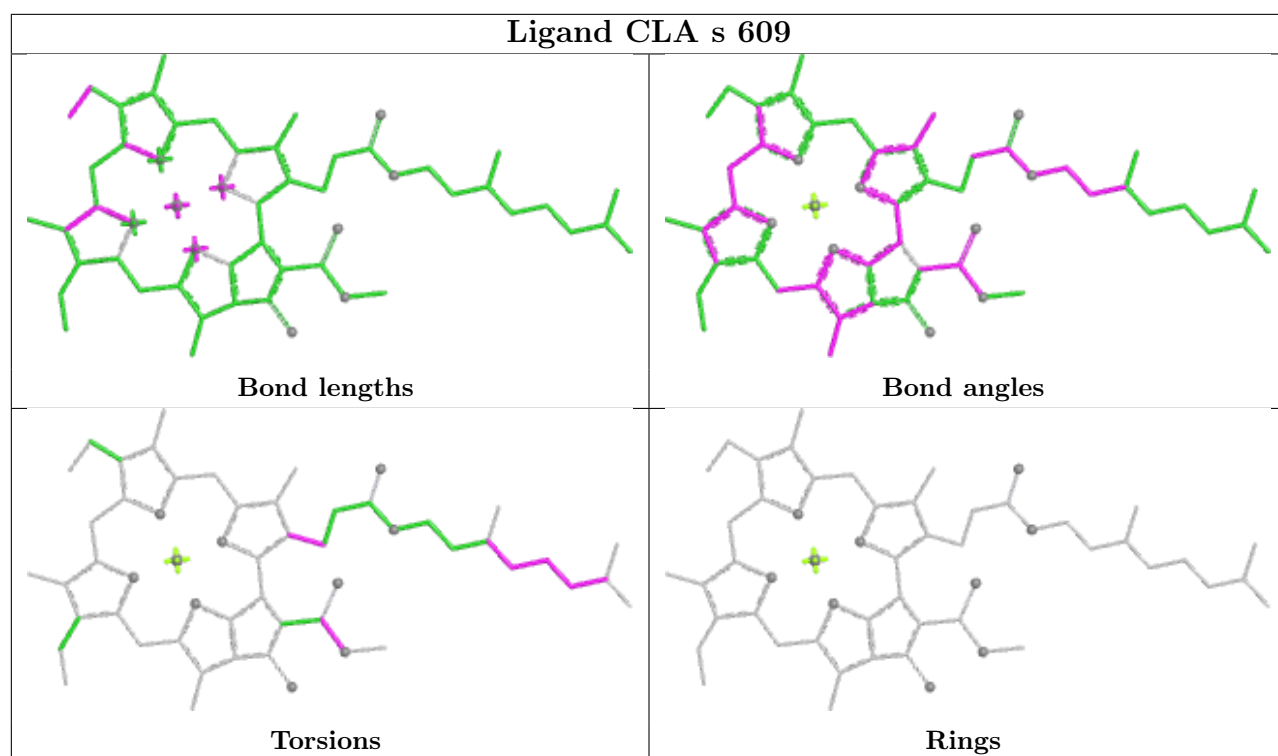


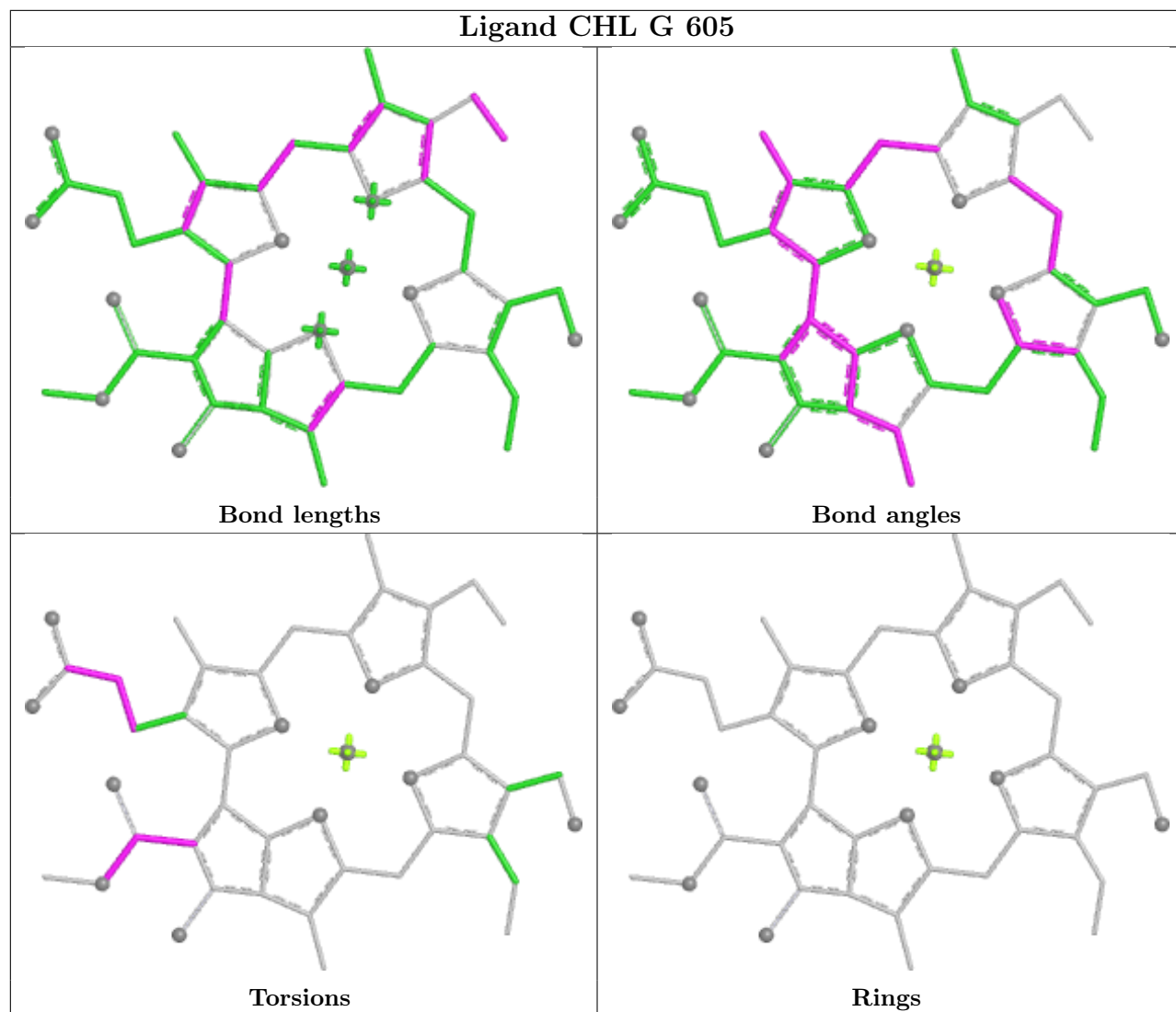




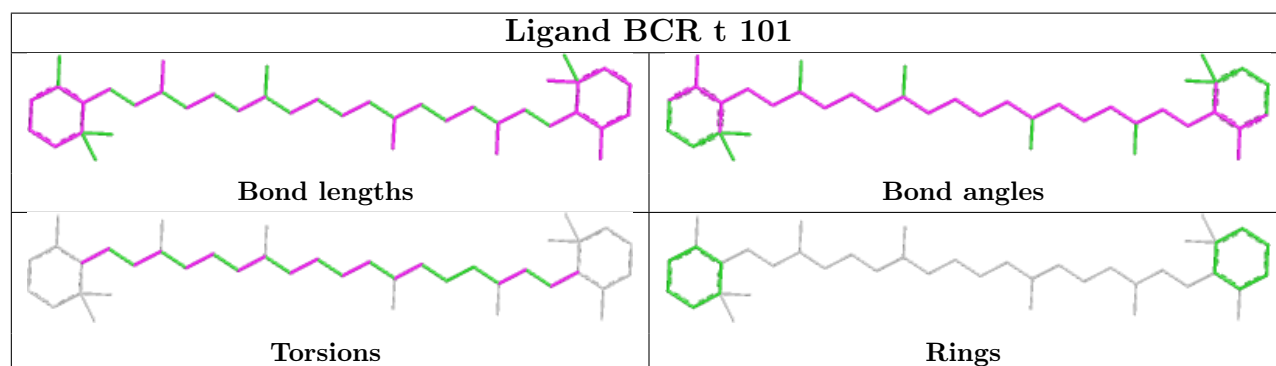
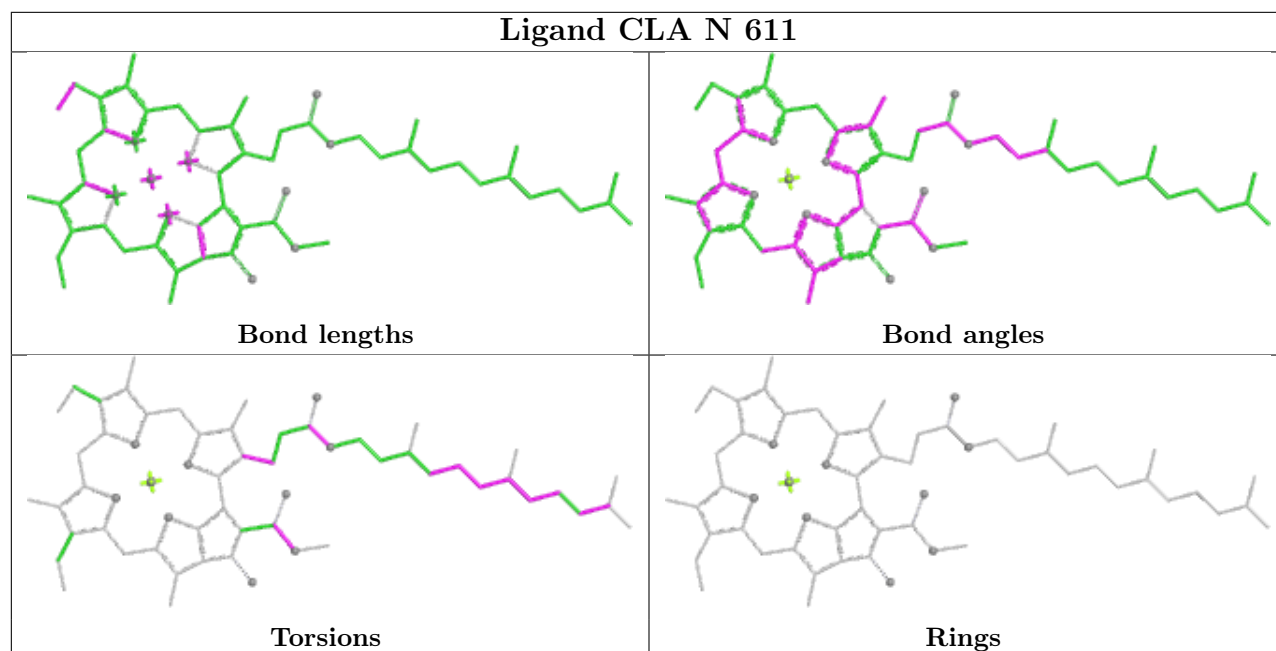
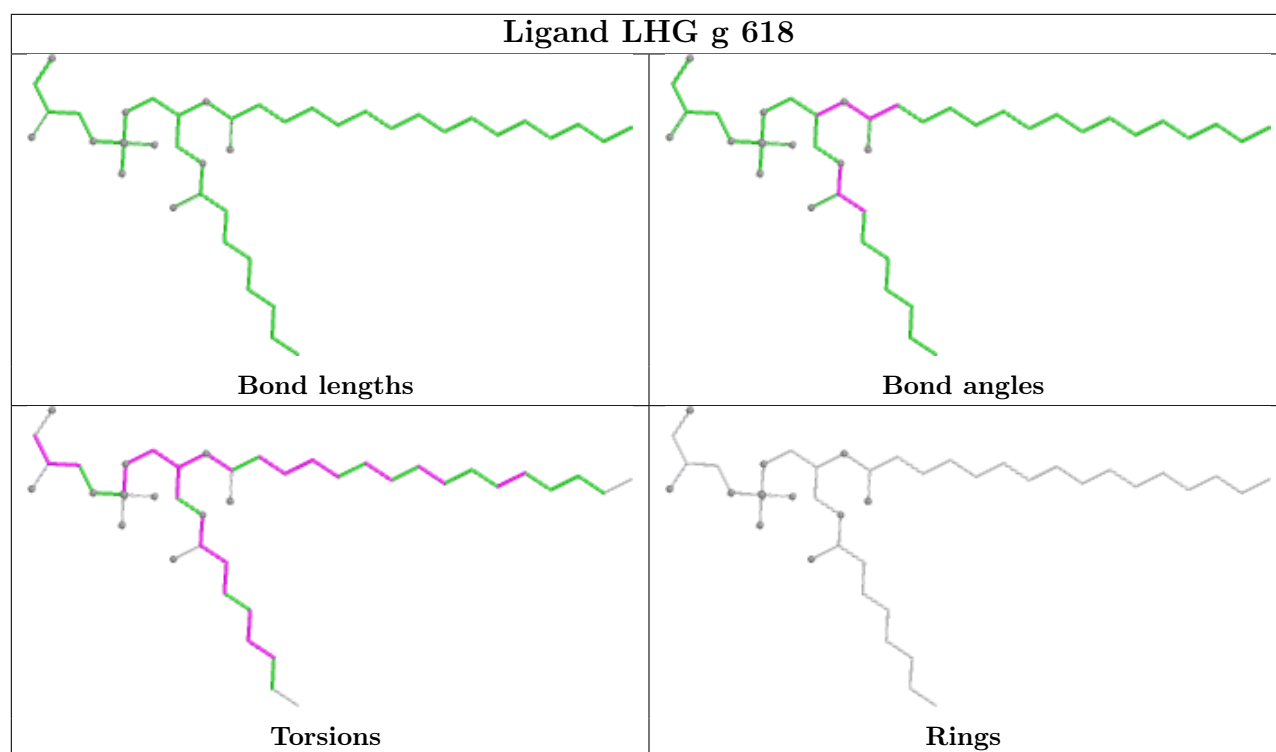


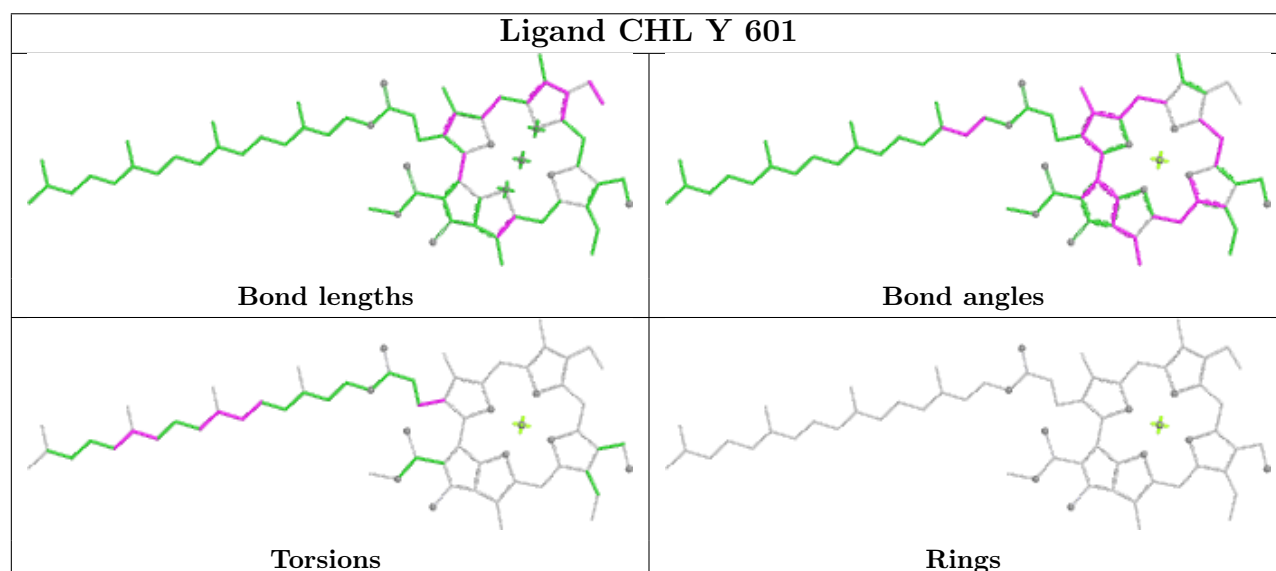
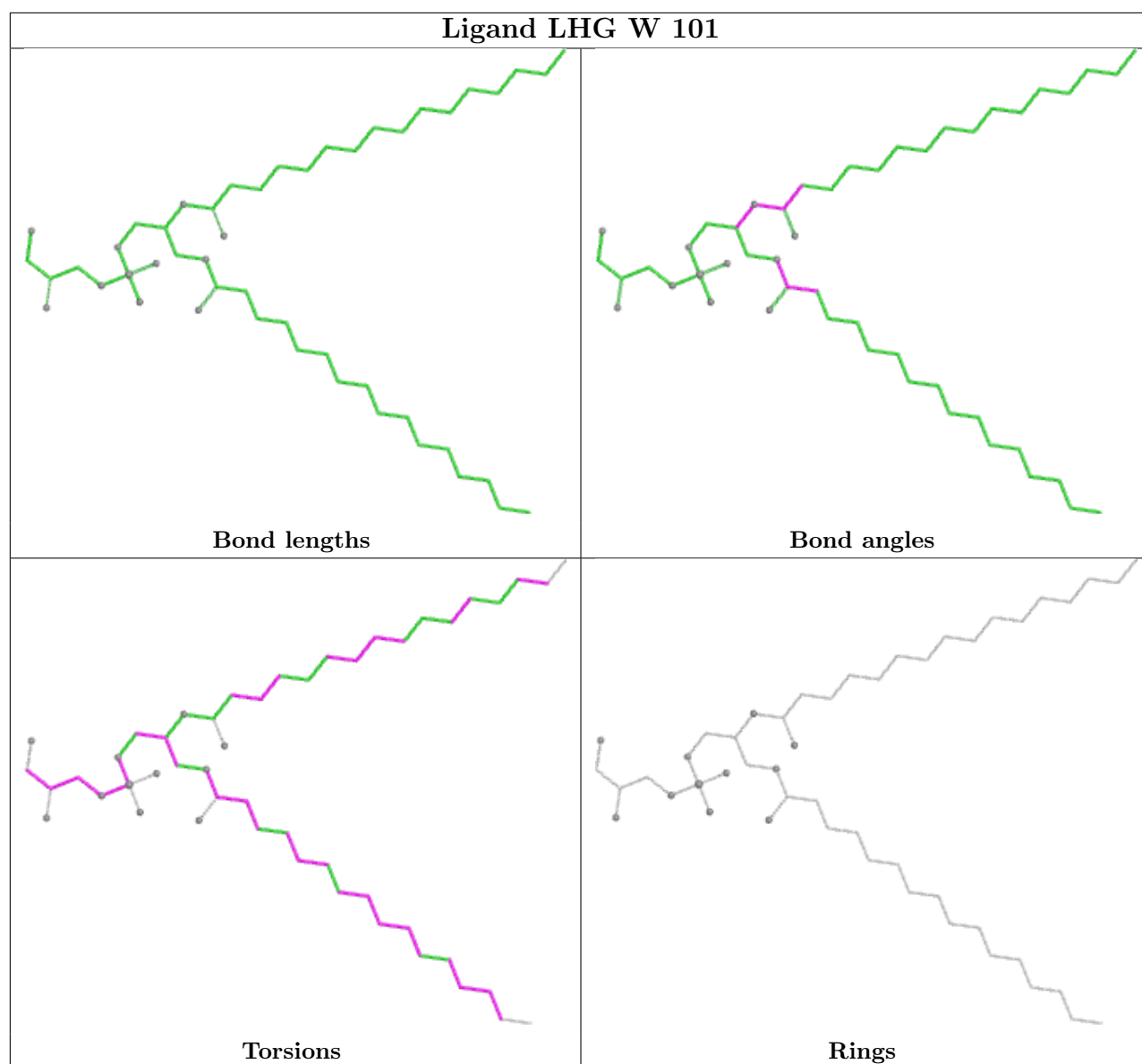


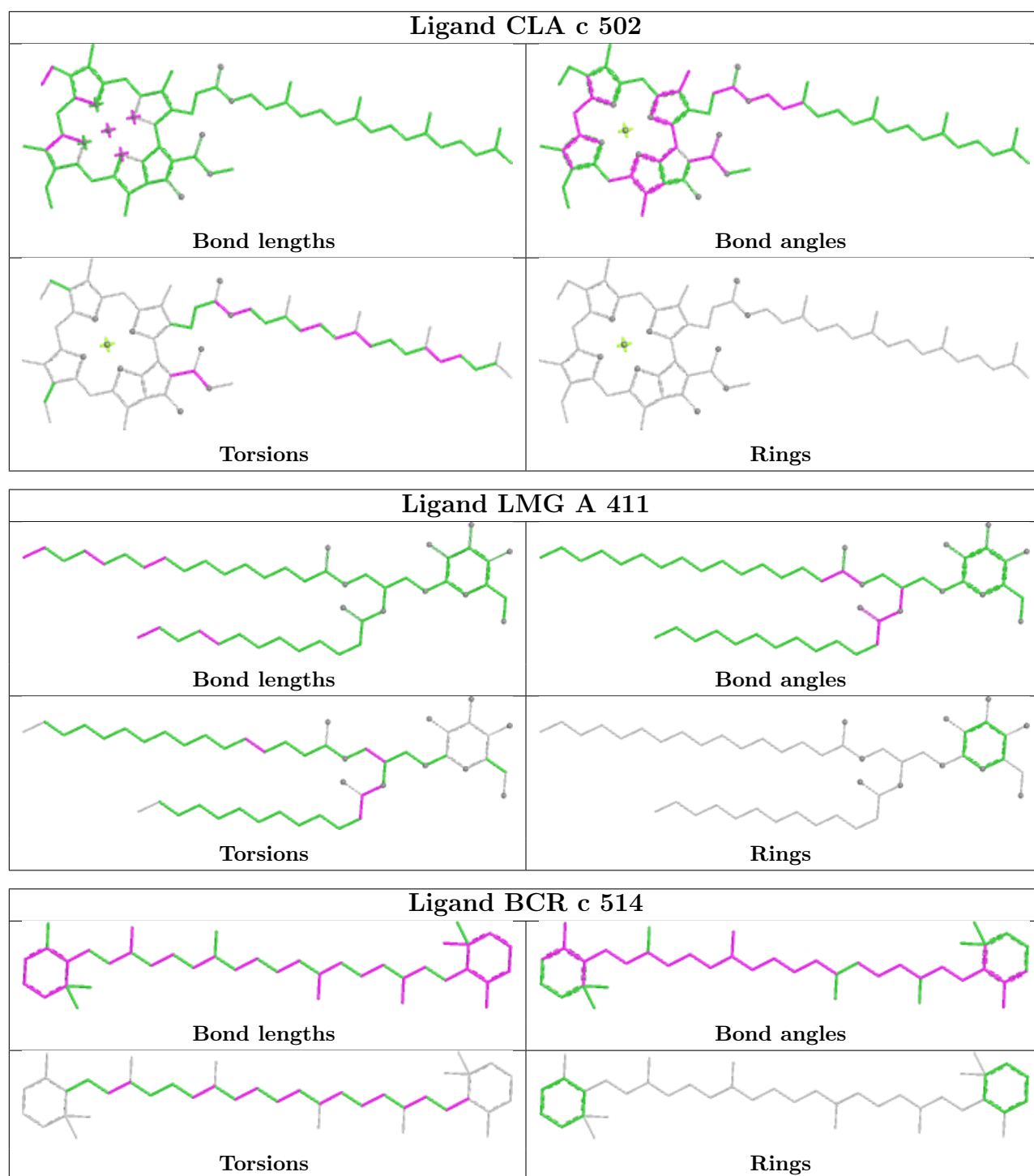


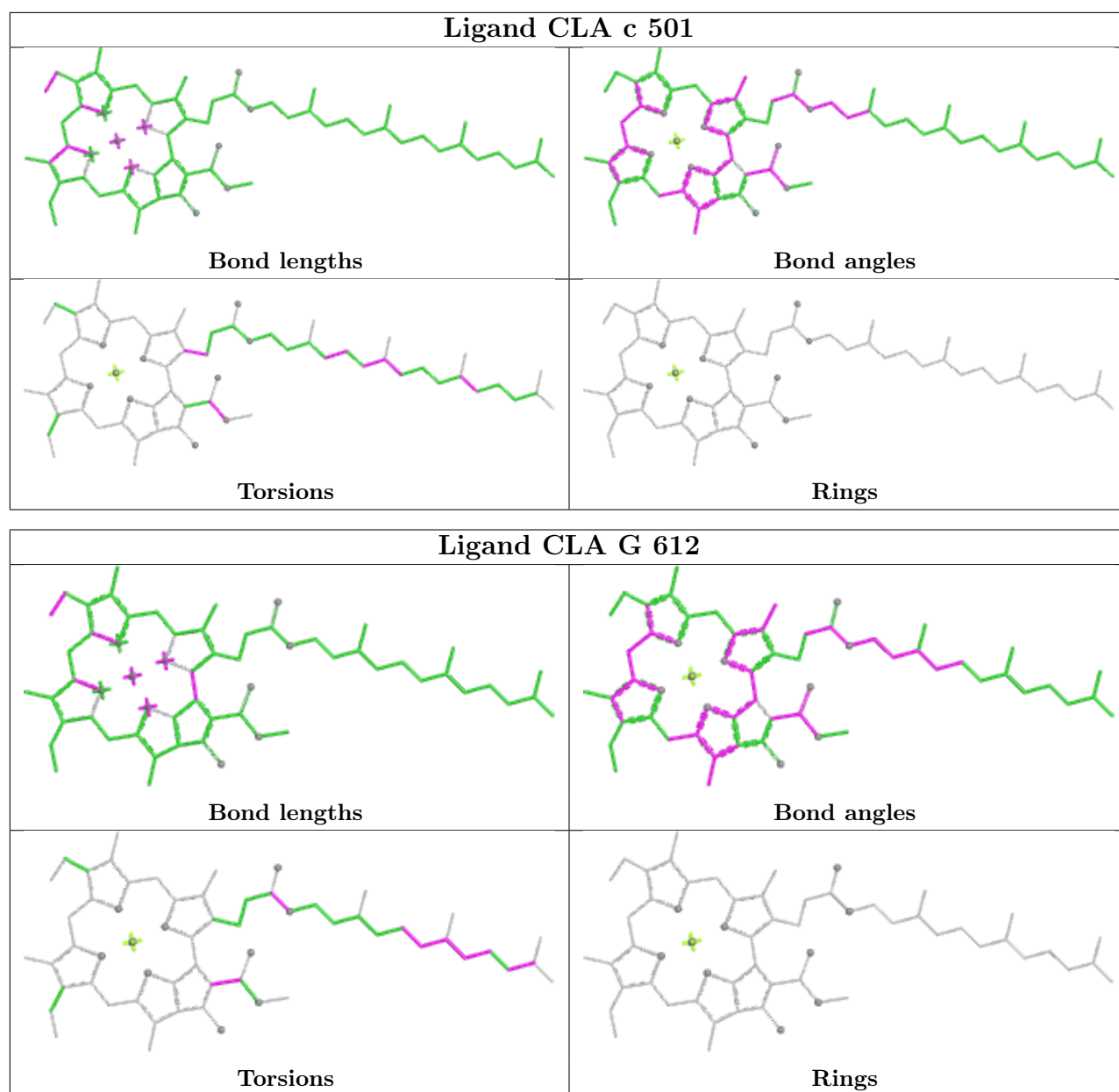




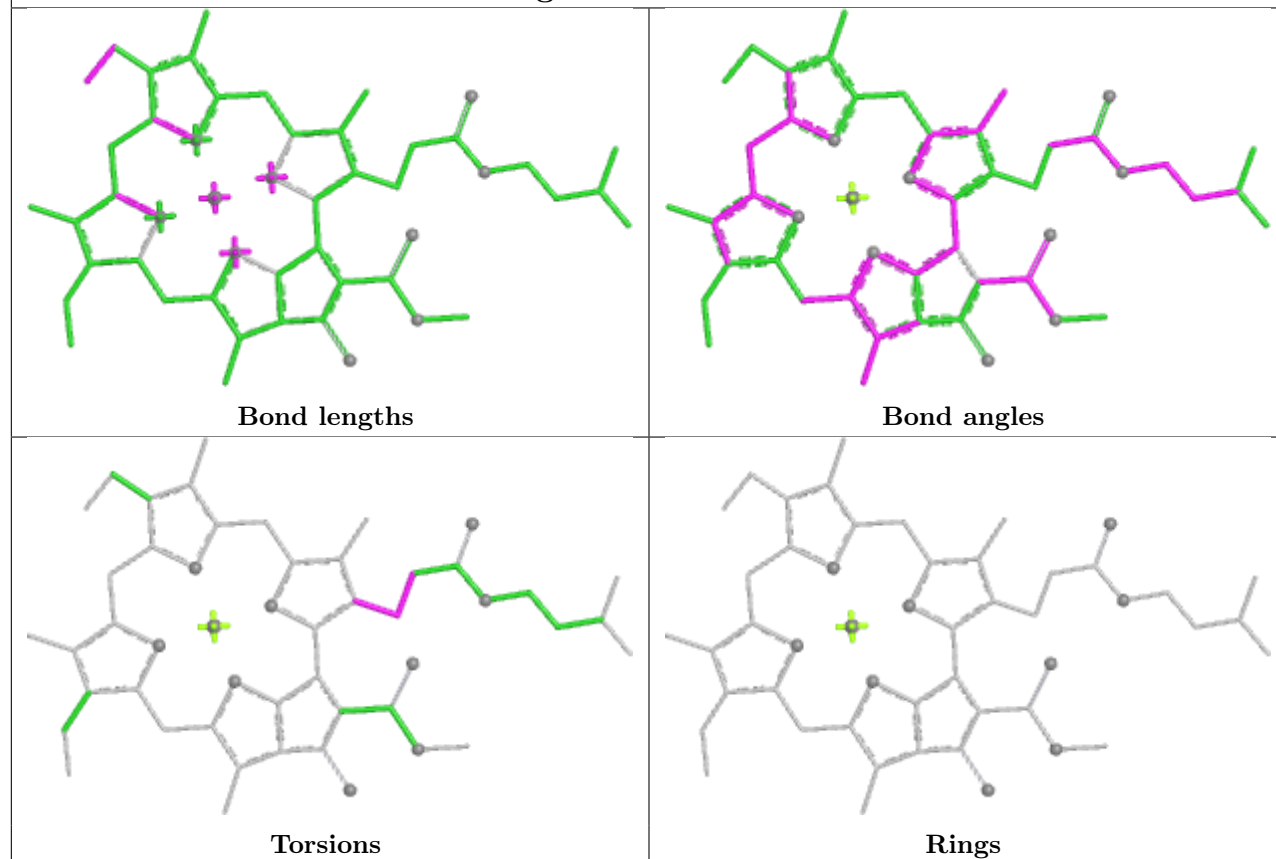




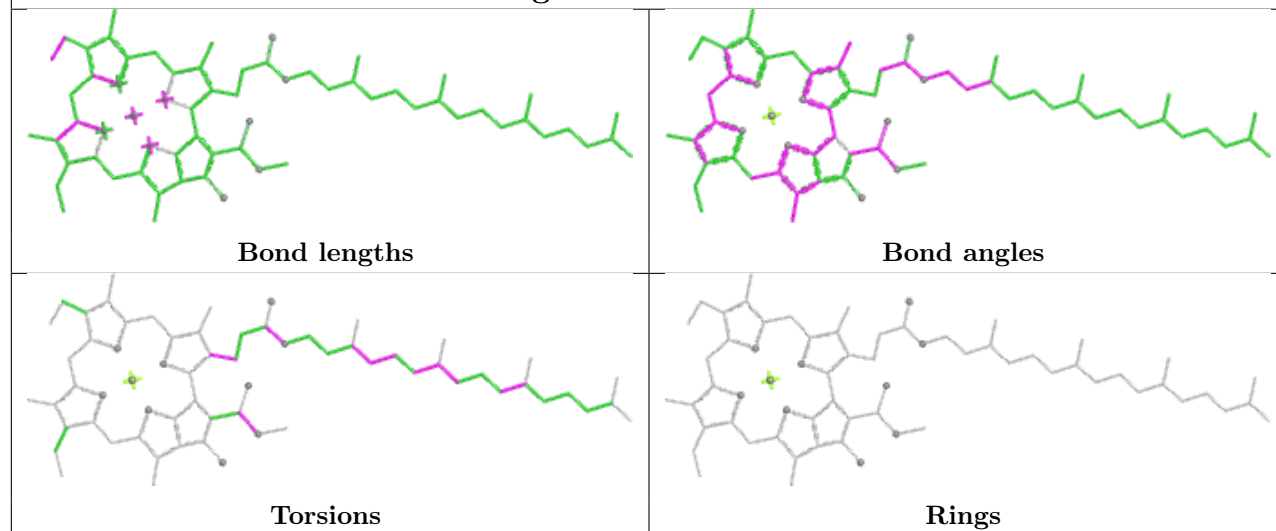


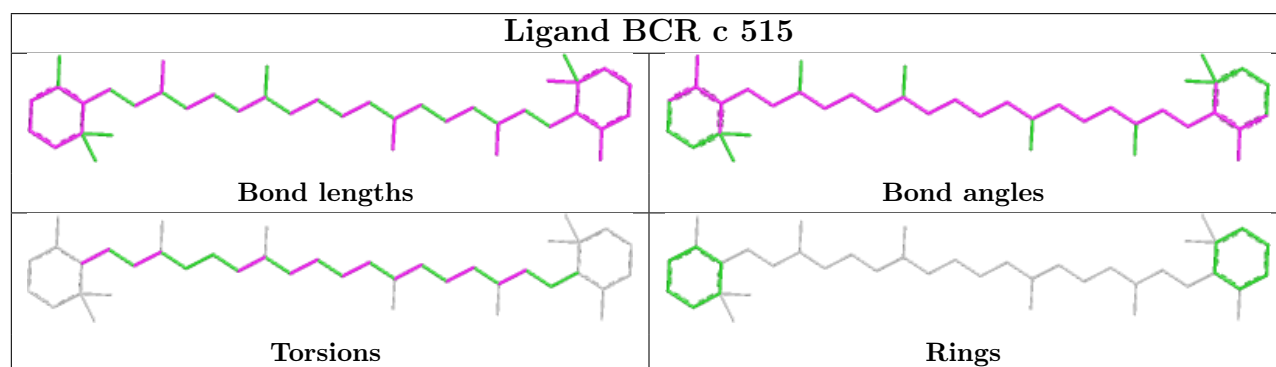
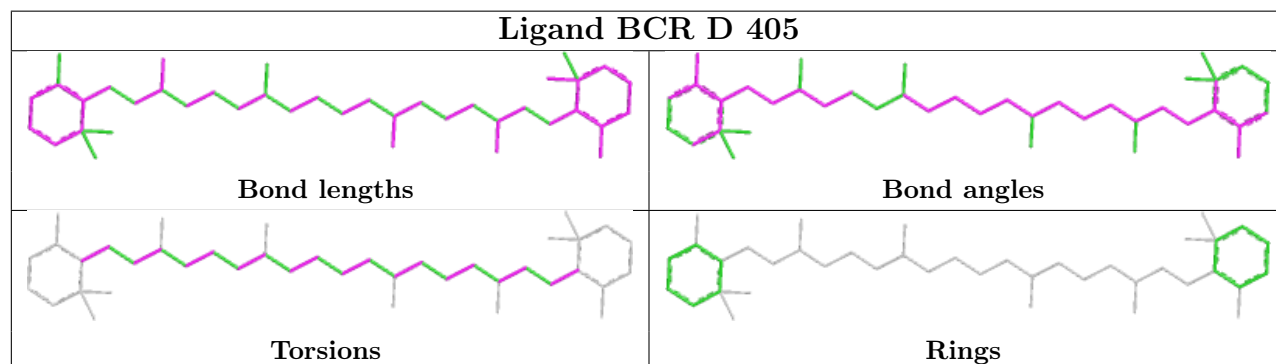
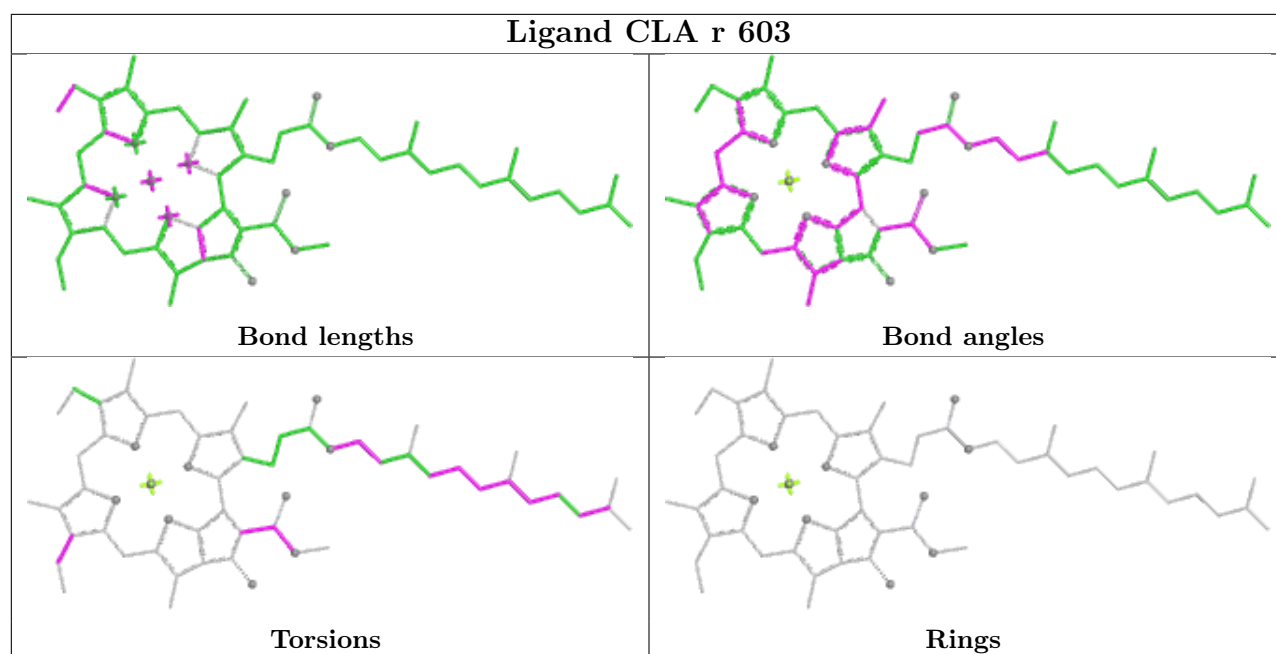


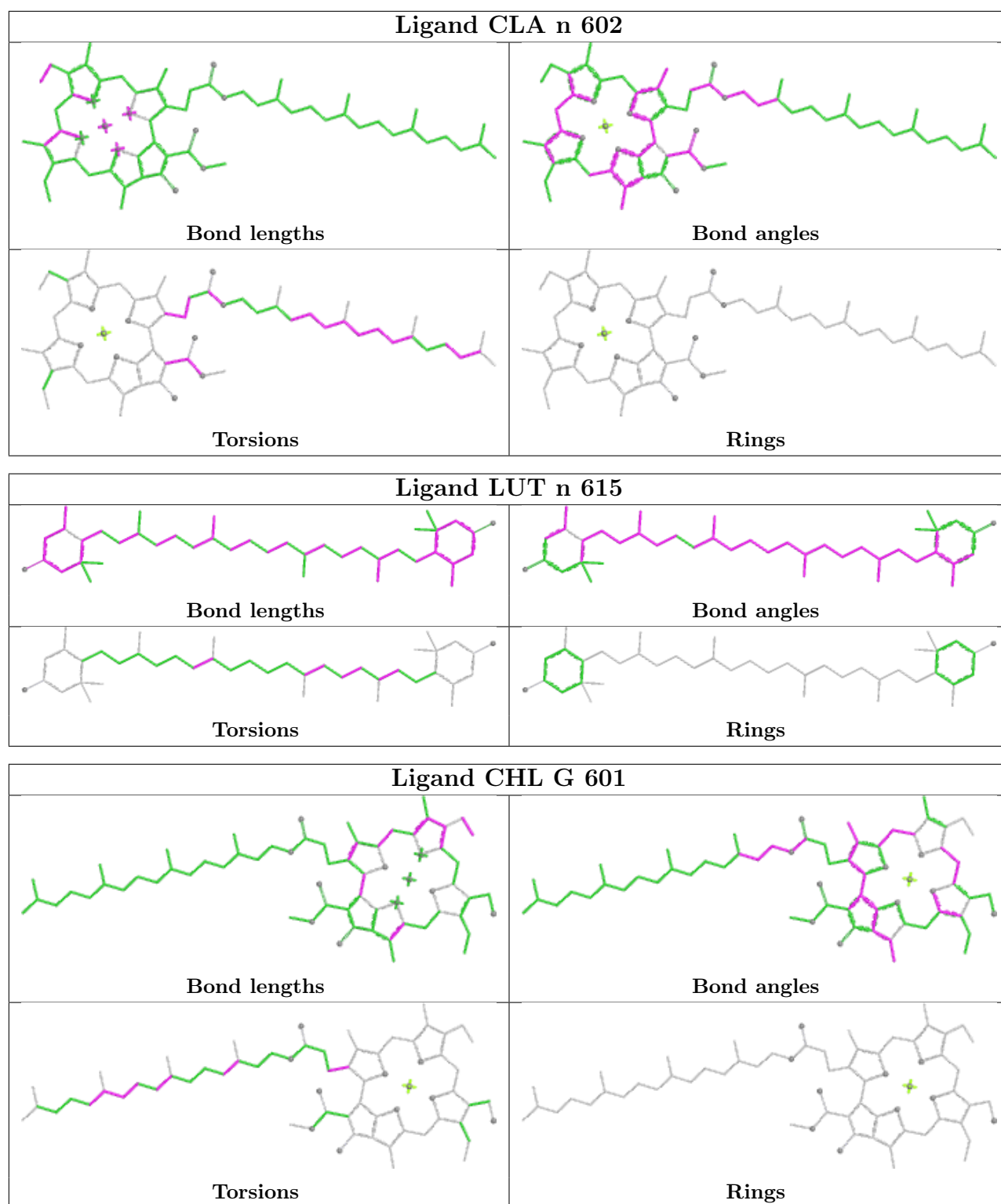
## Ligand CLA a 407

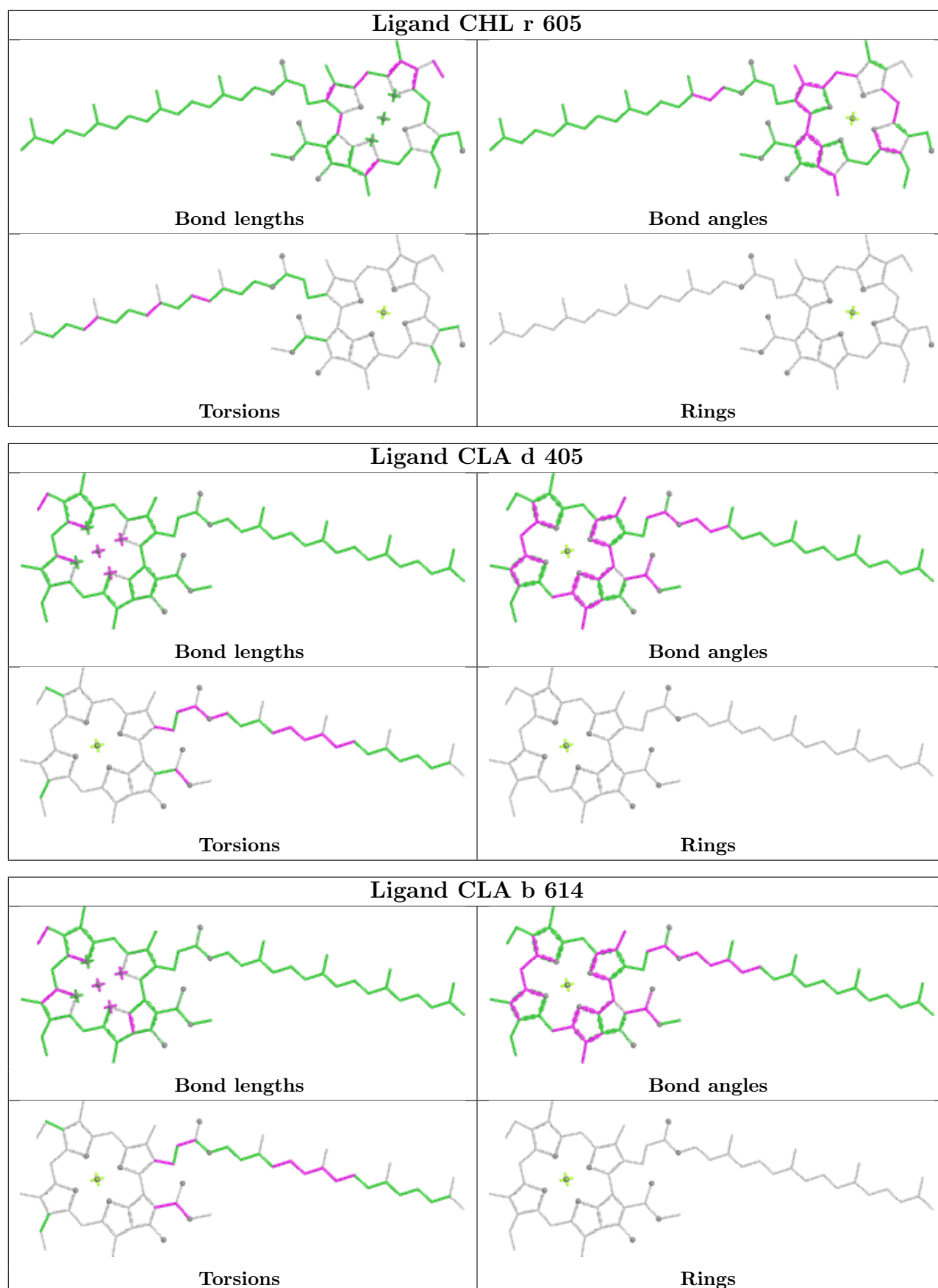


## Ligand CLA B 603

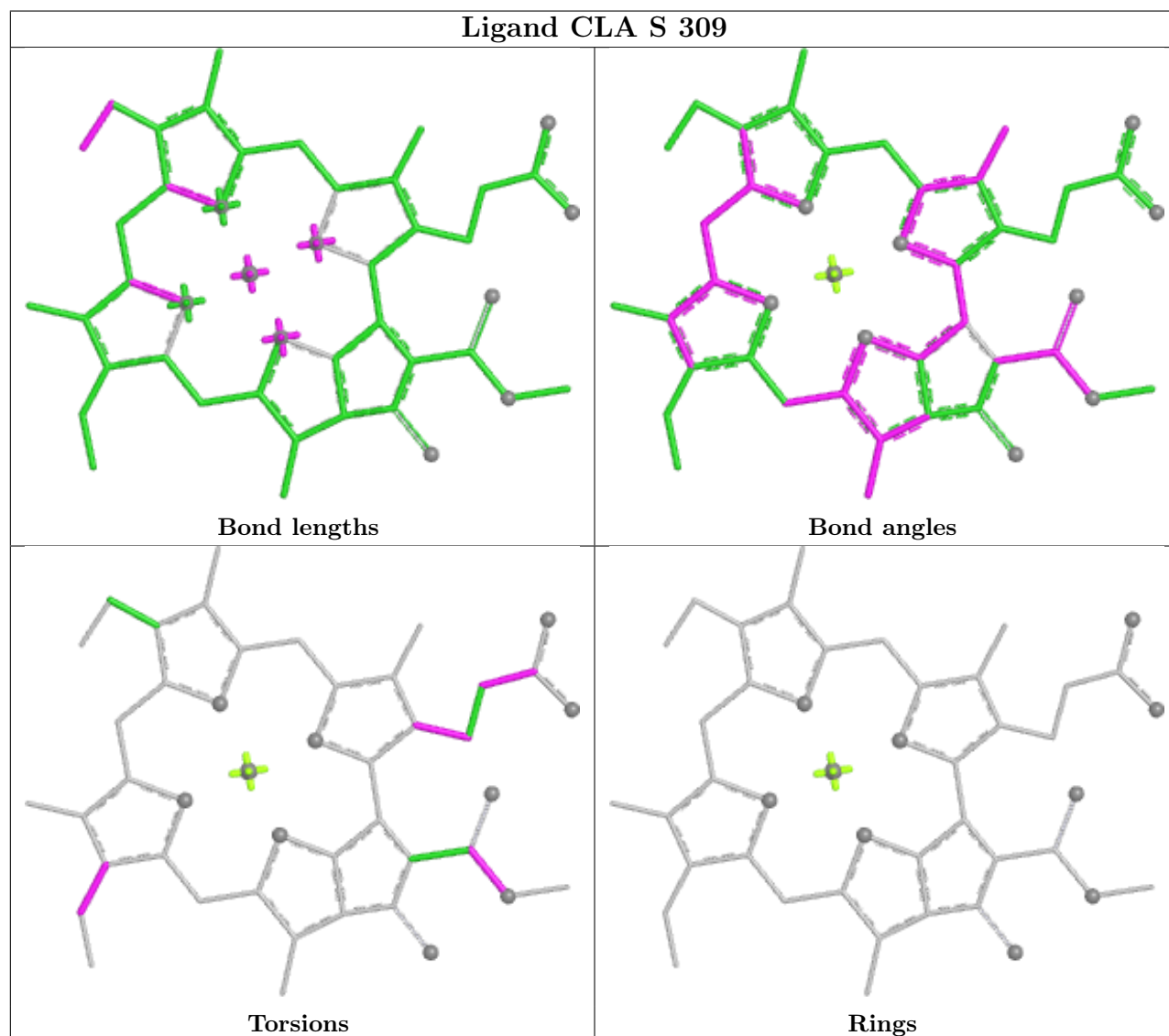
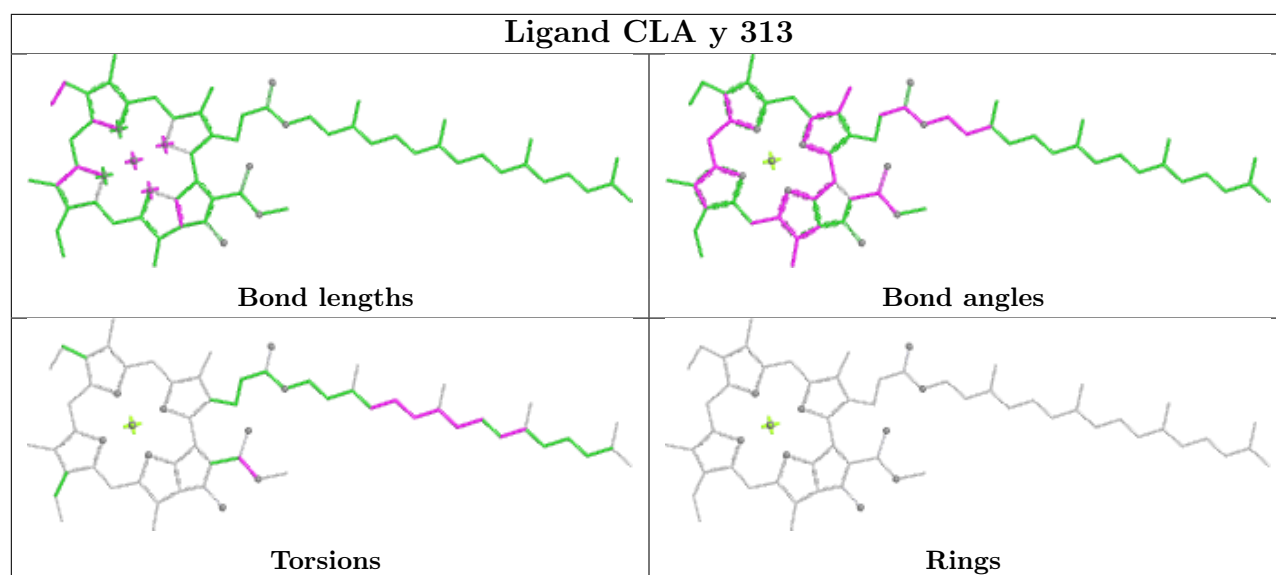


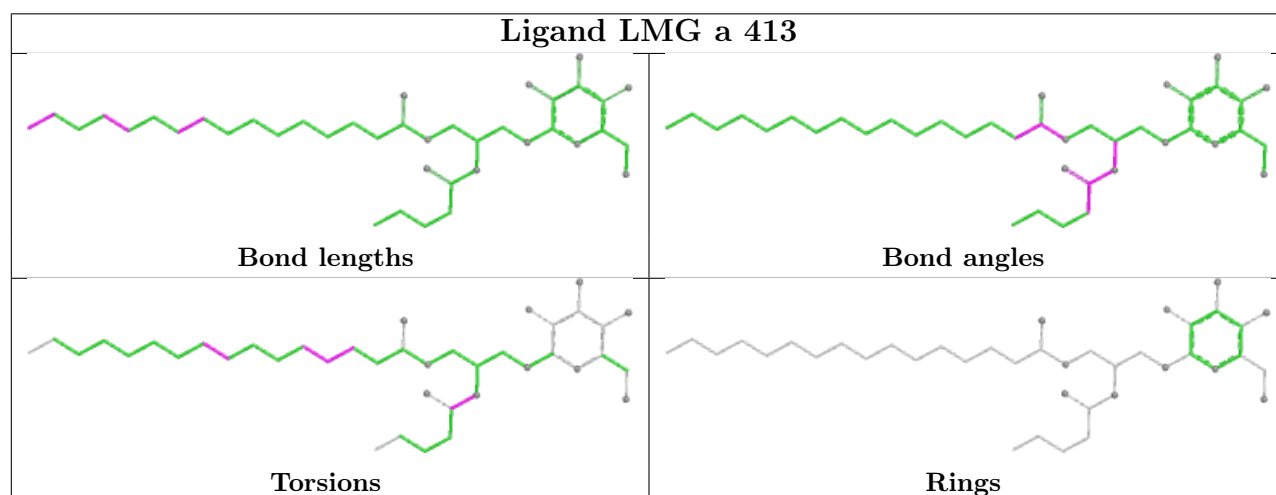
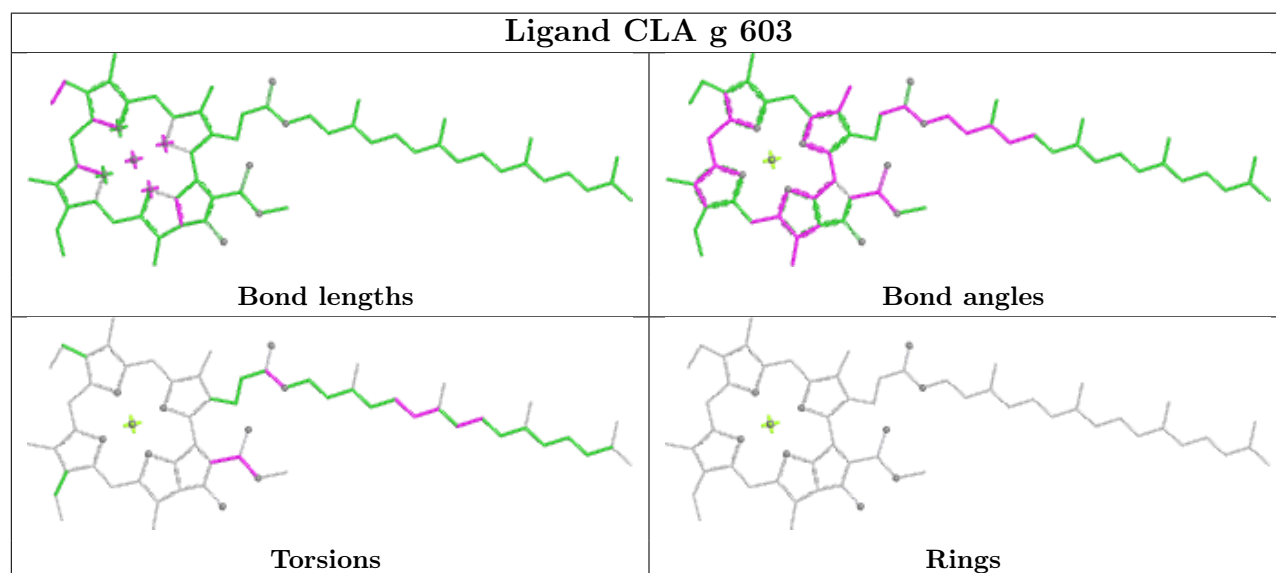
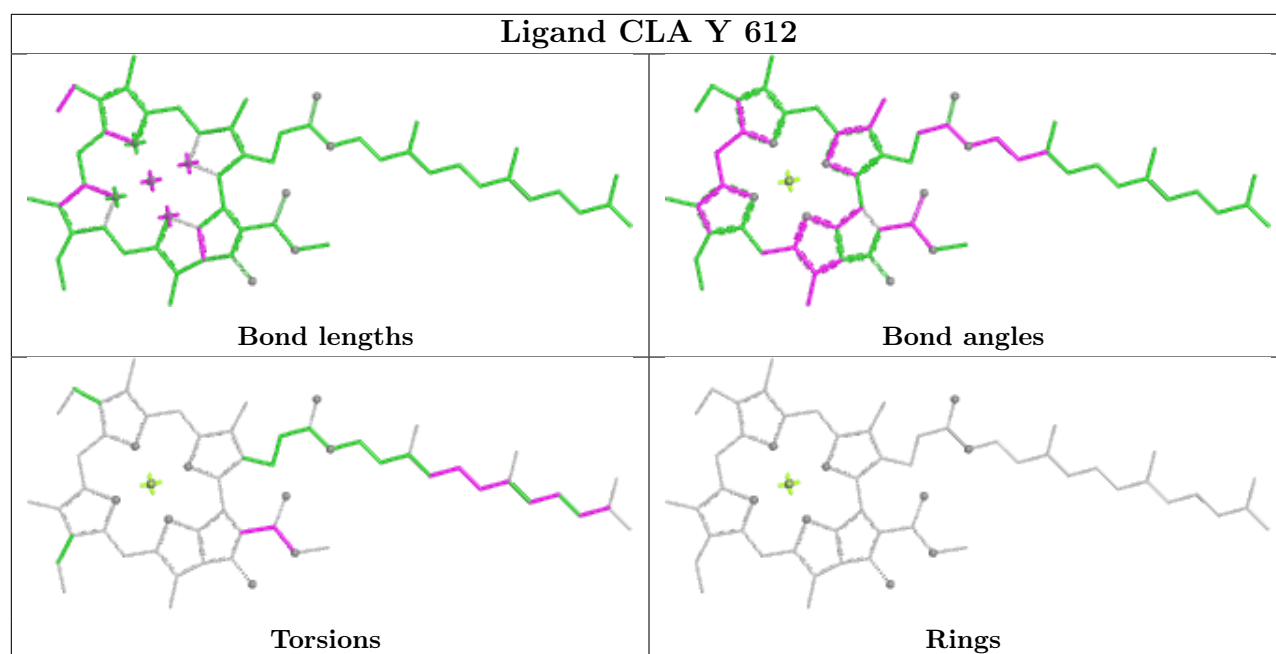


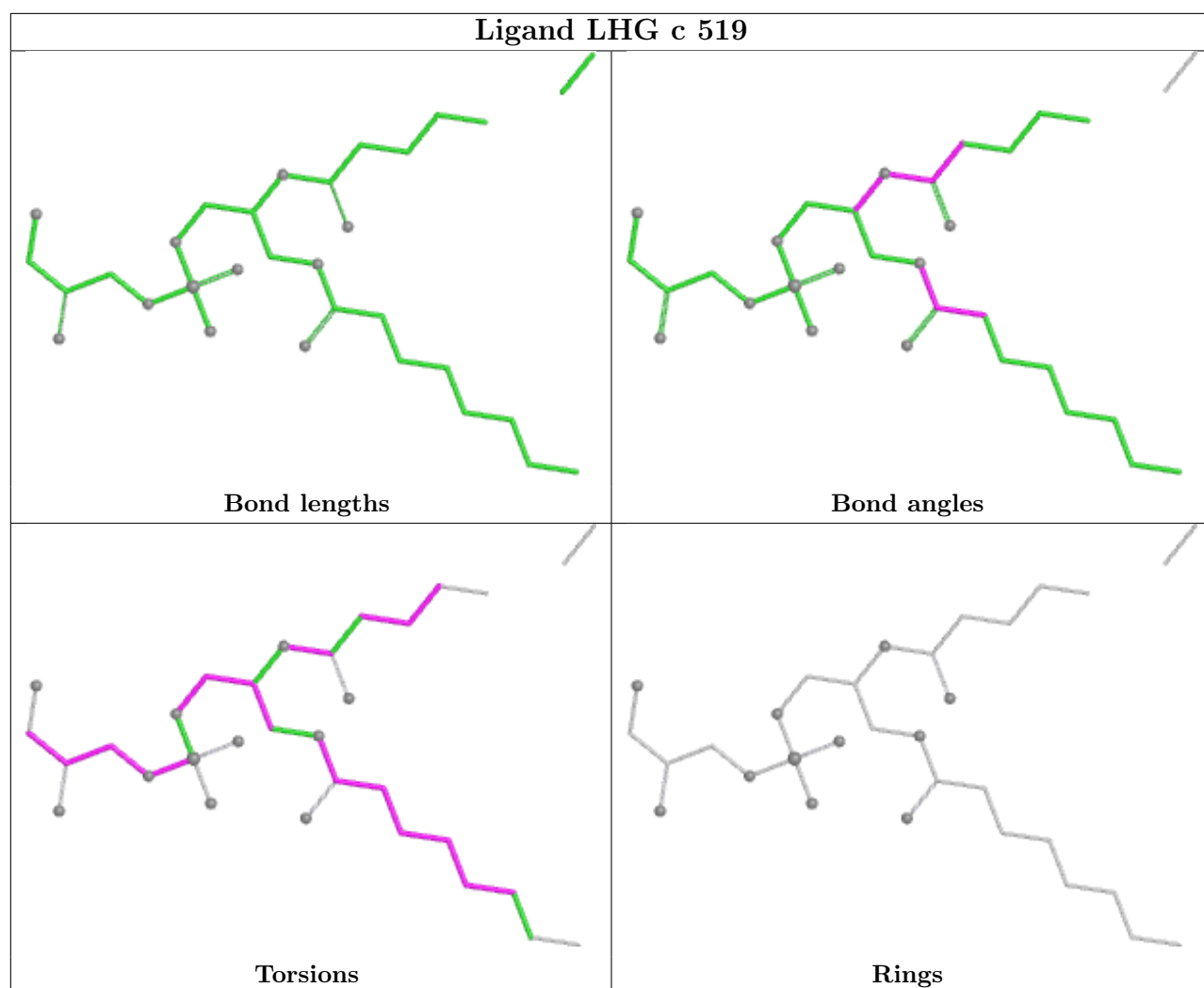


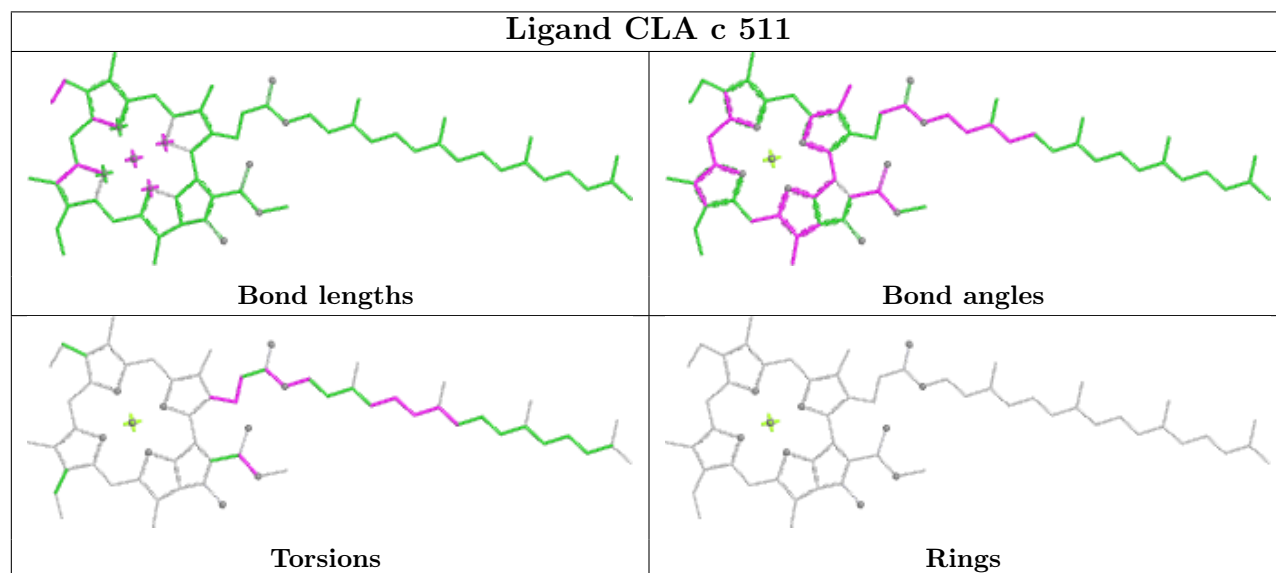
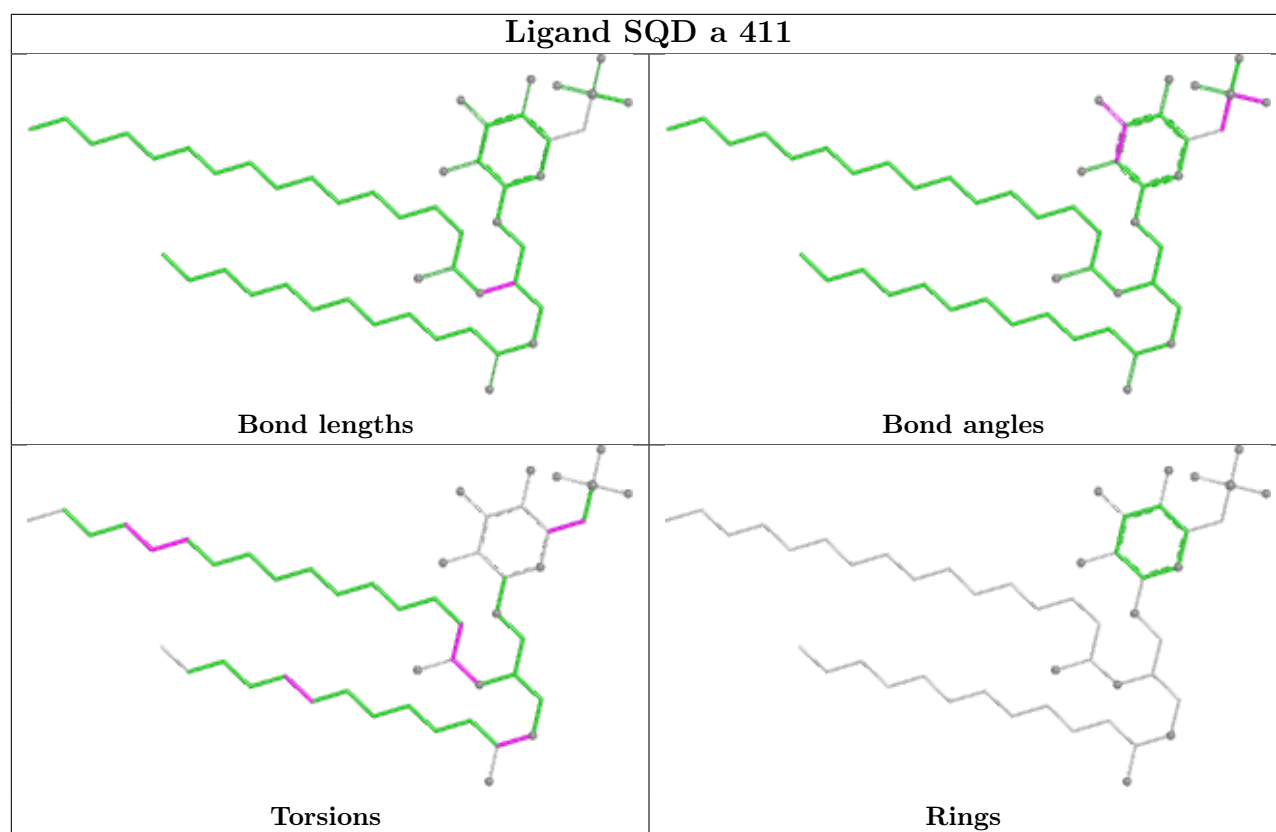




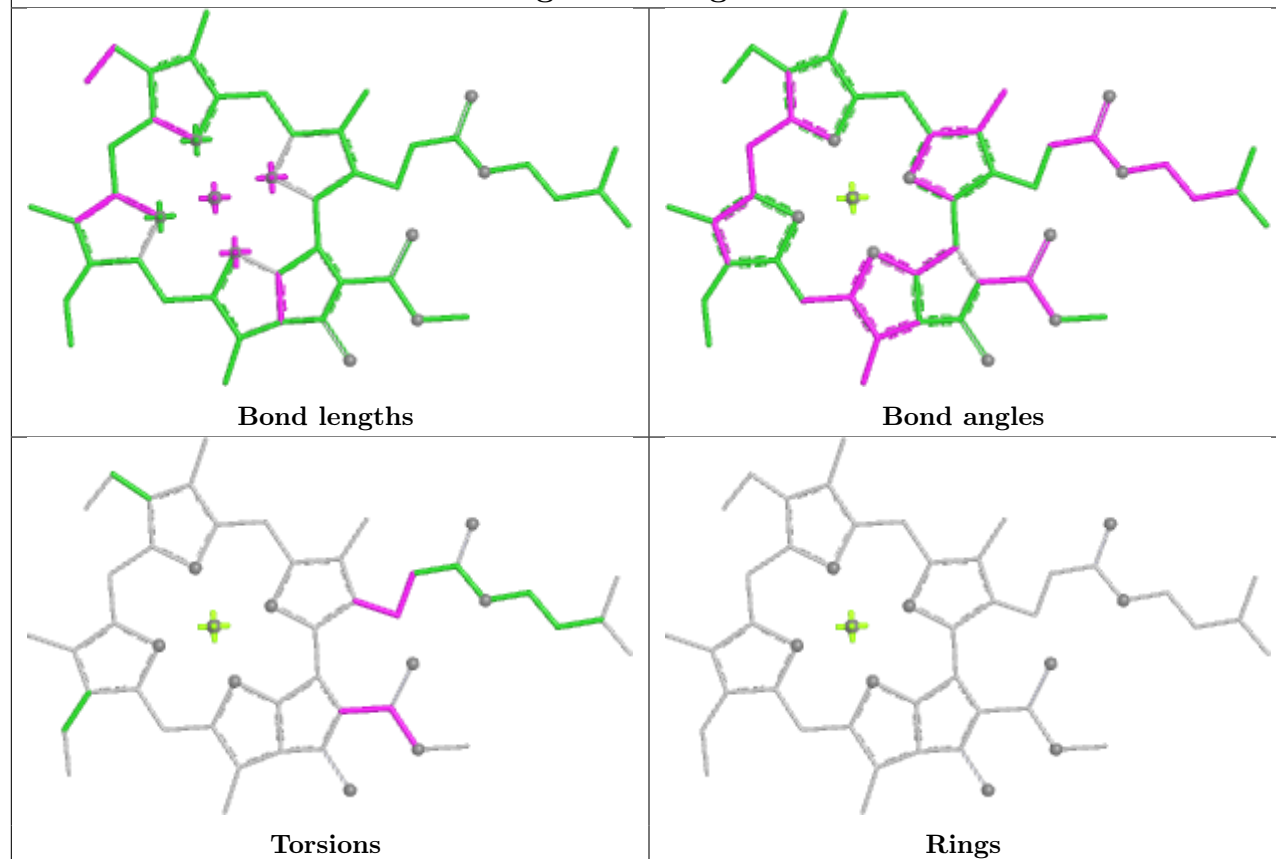




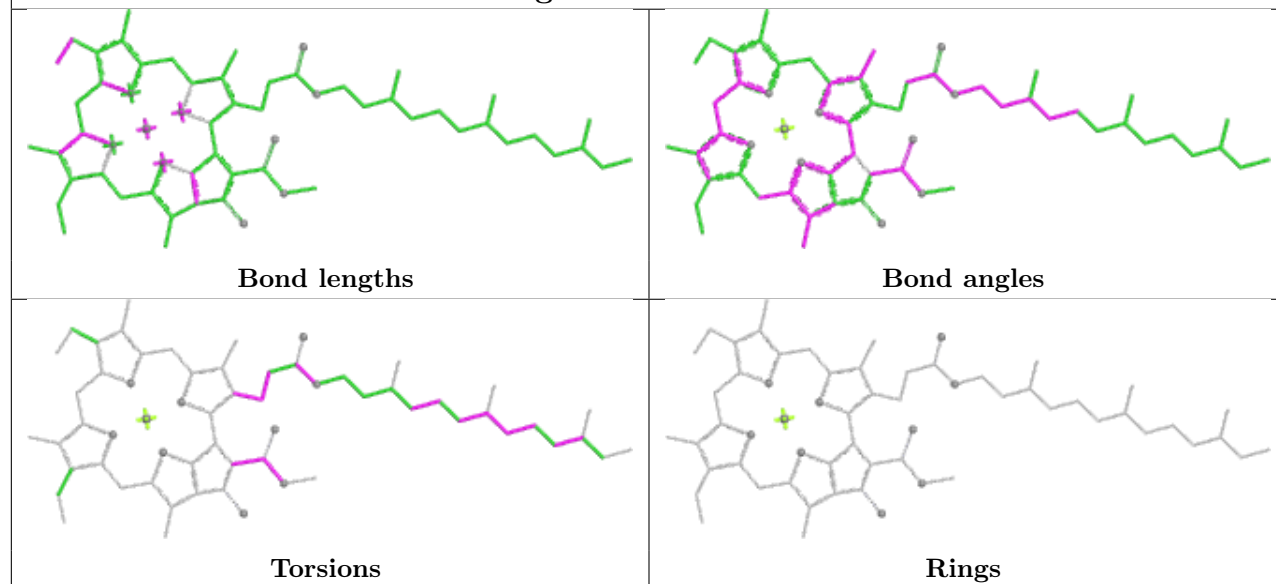


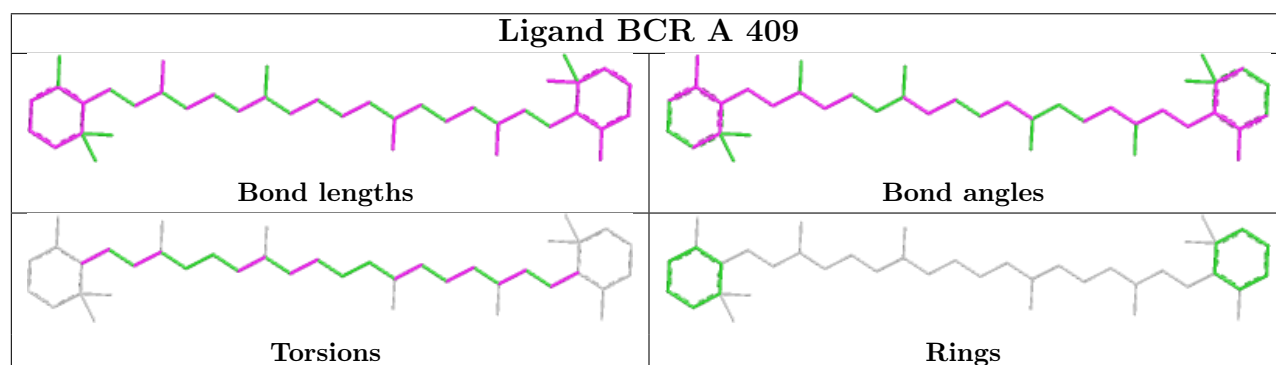
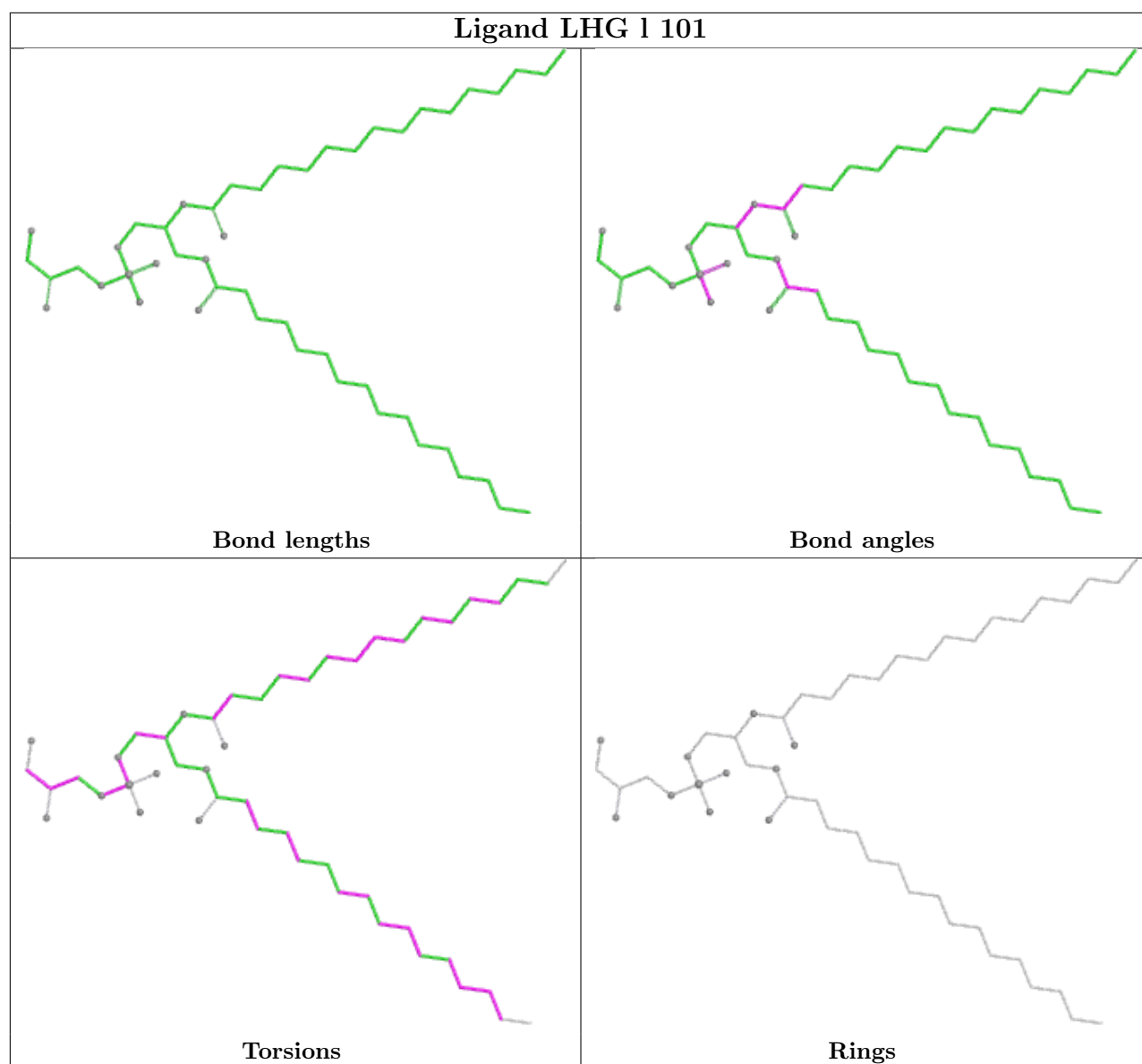


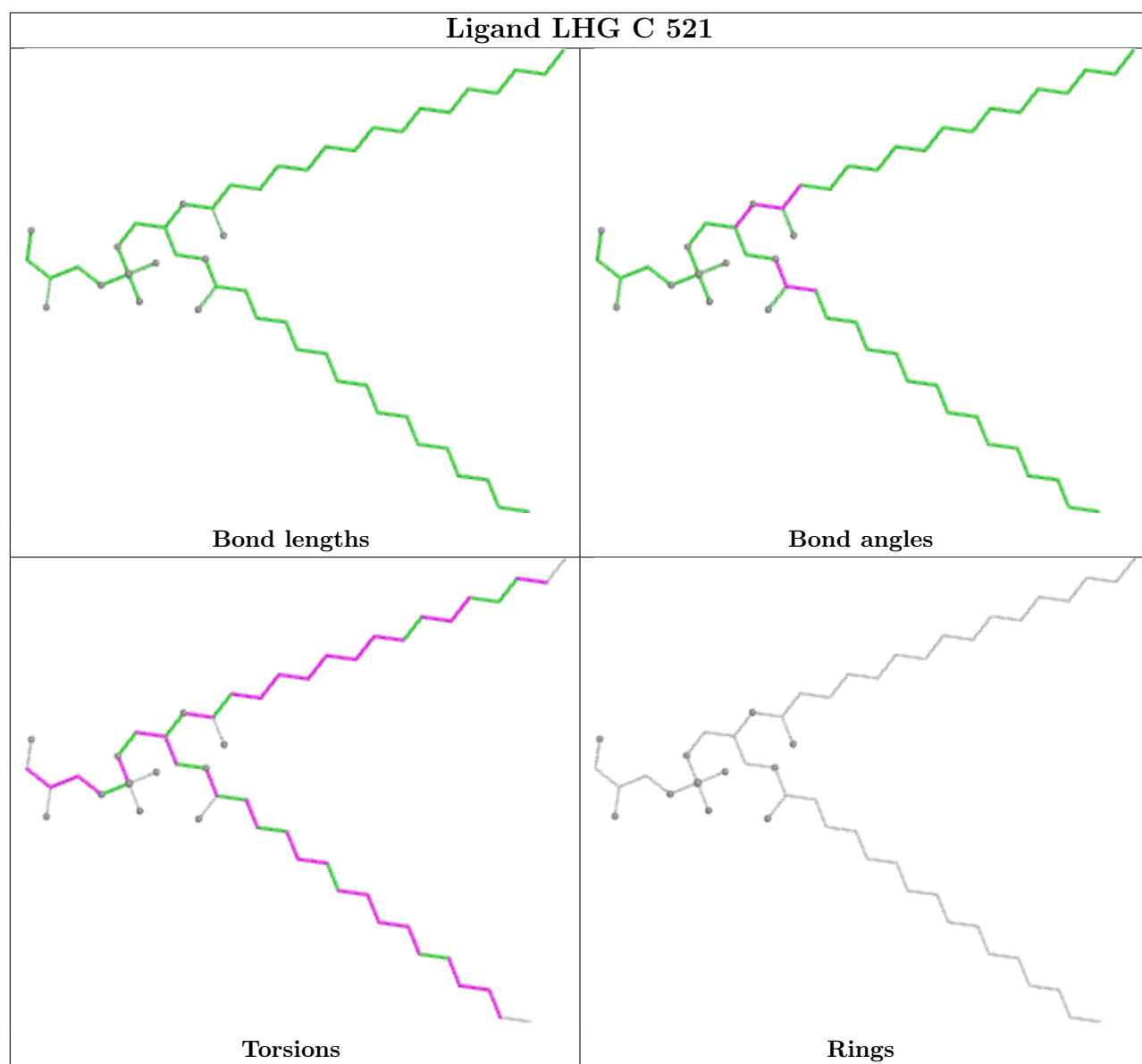
## Ligand CLA g 604



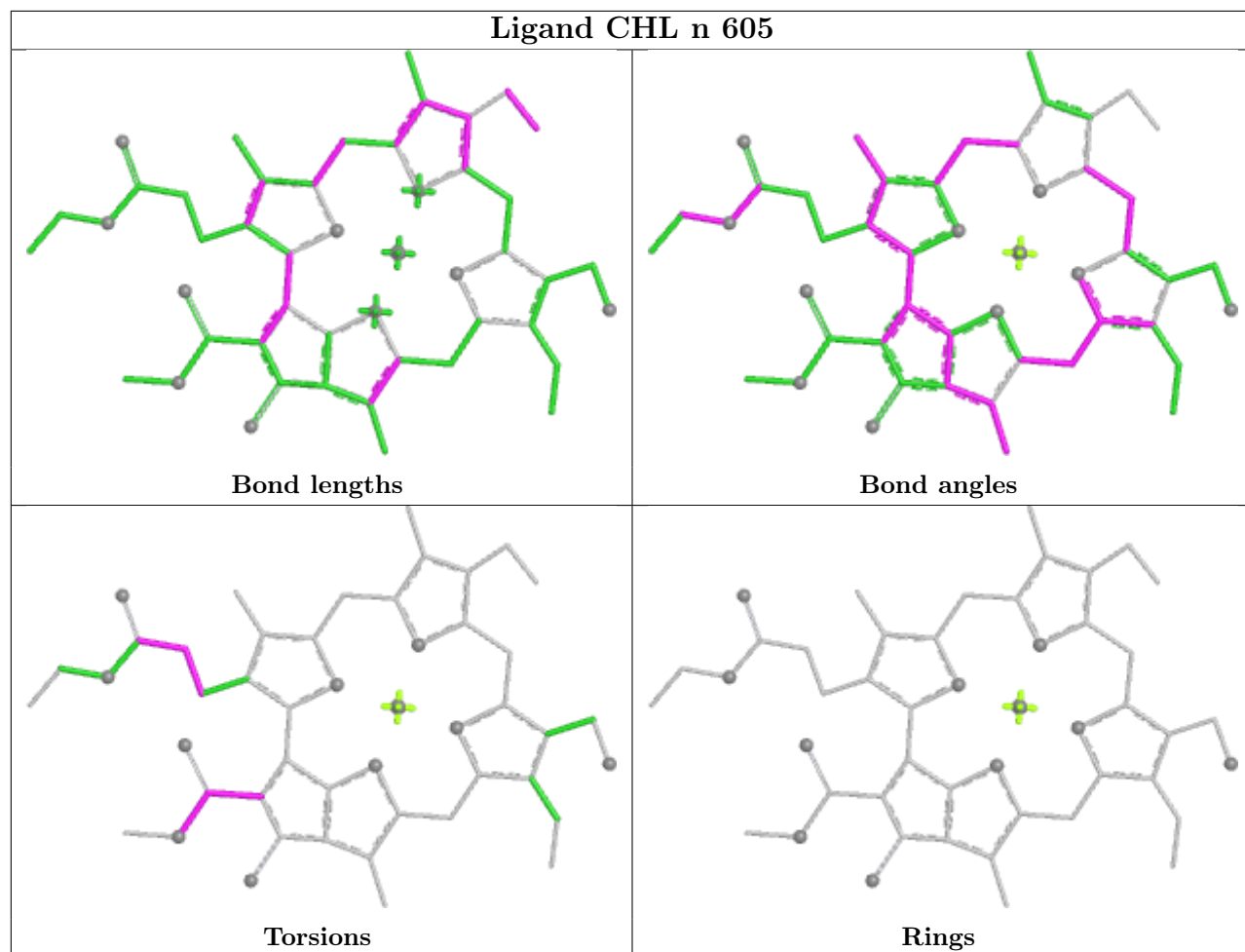
## Ligand CLA S 303



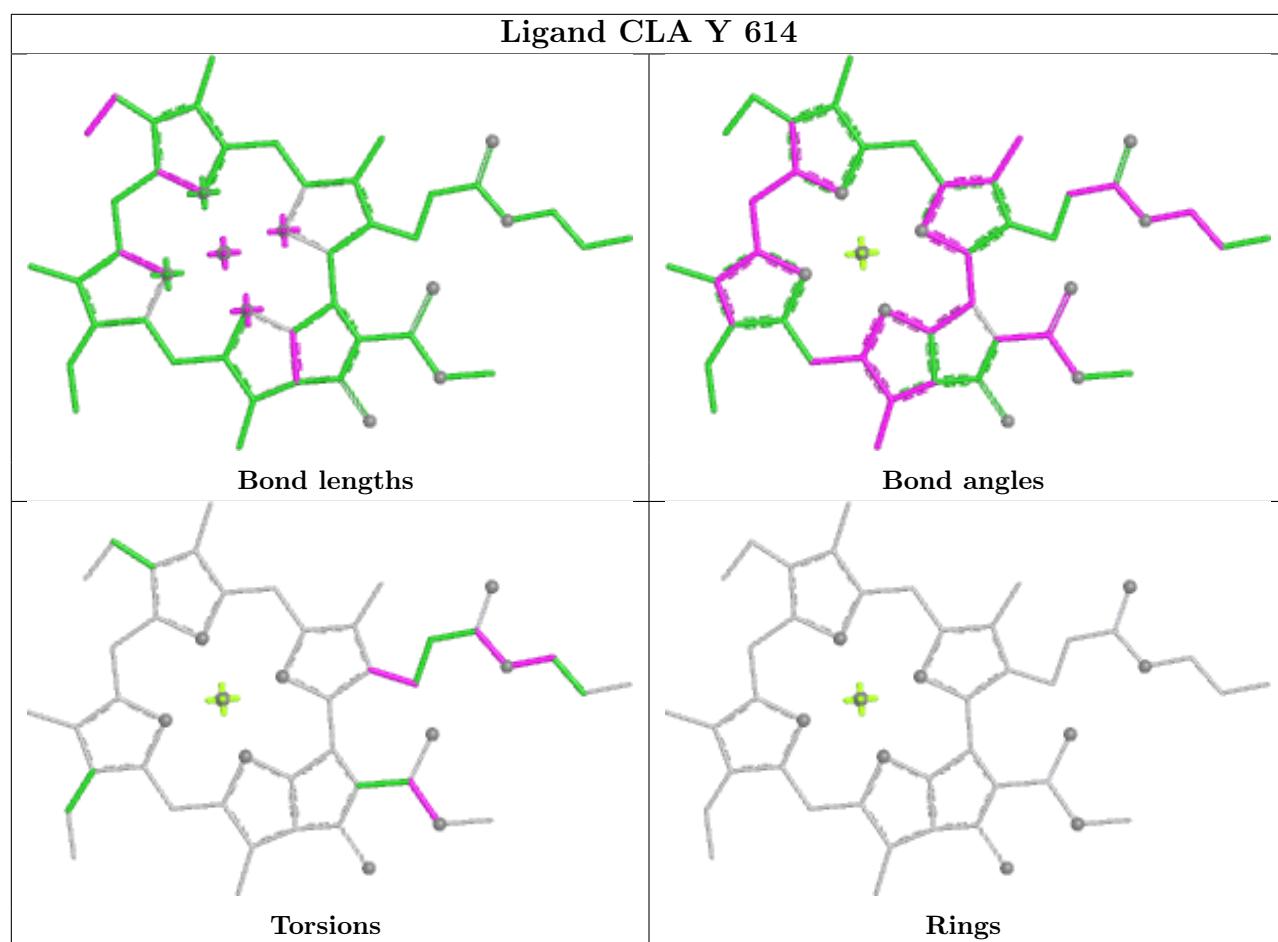




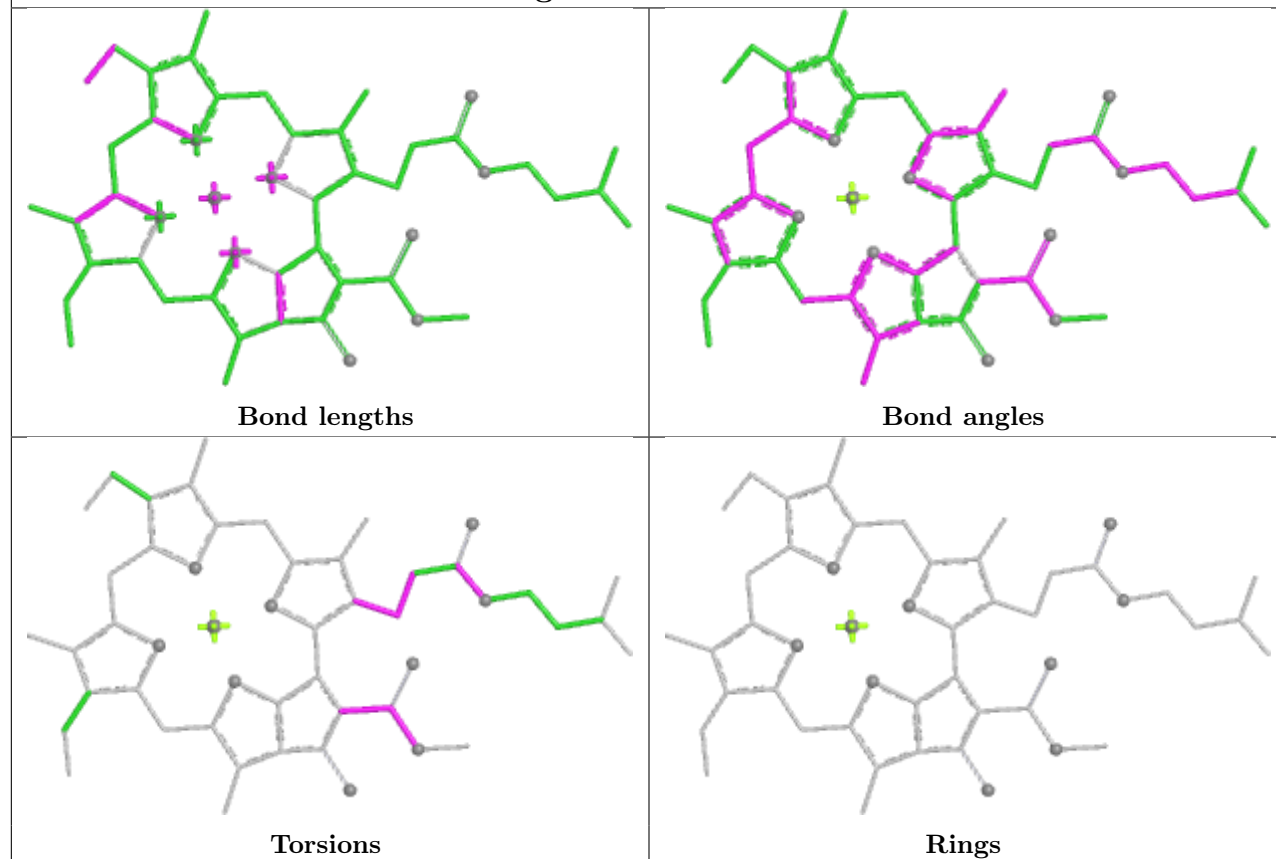
## Ligand CHL n 605



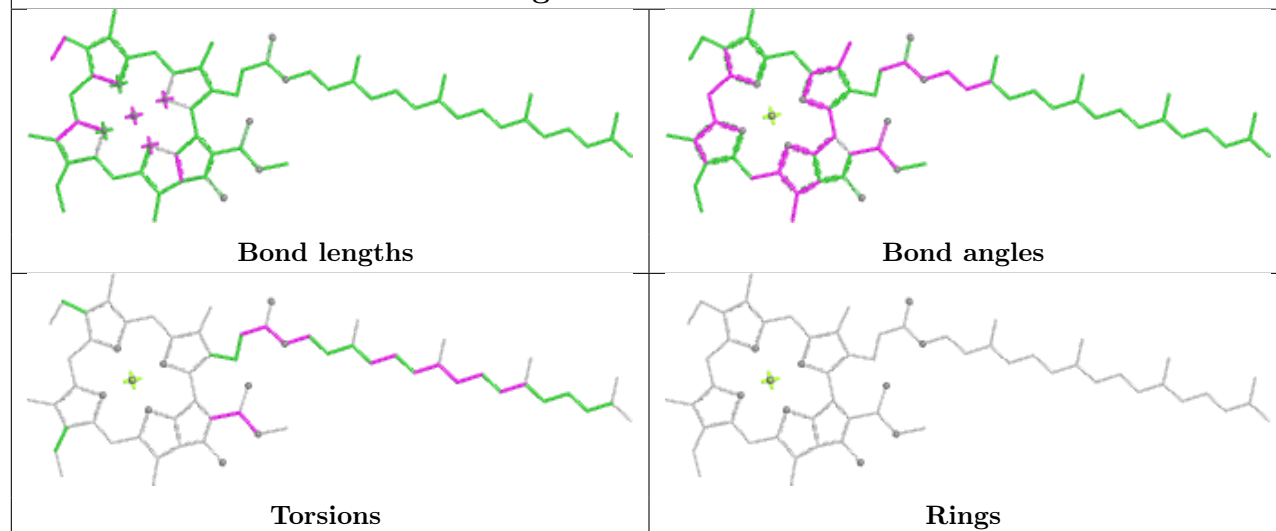


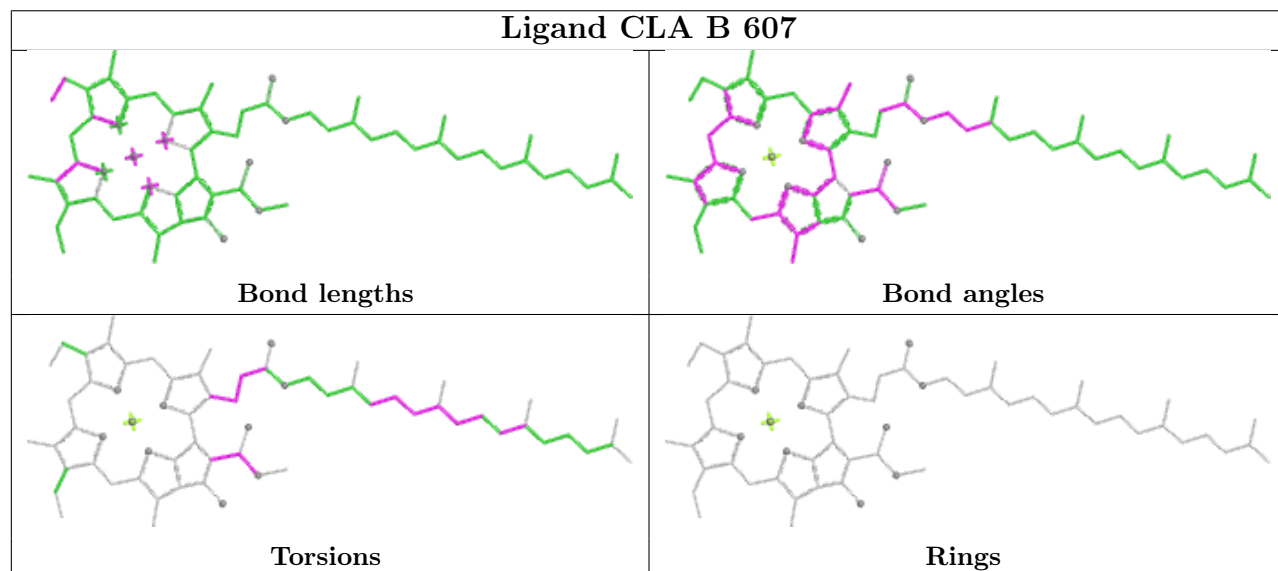
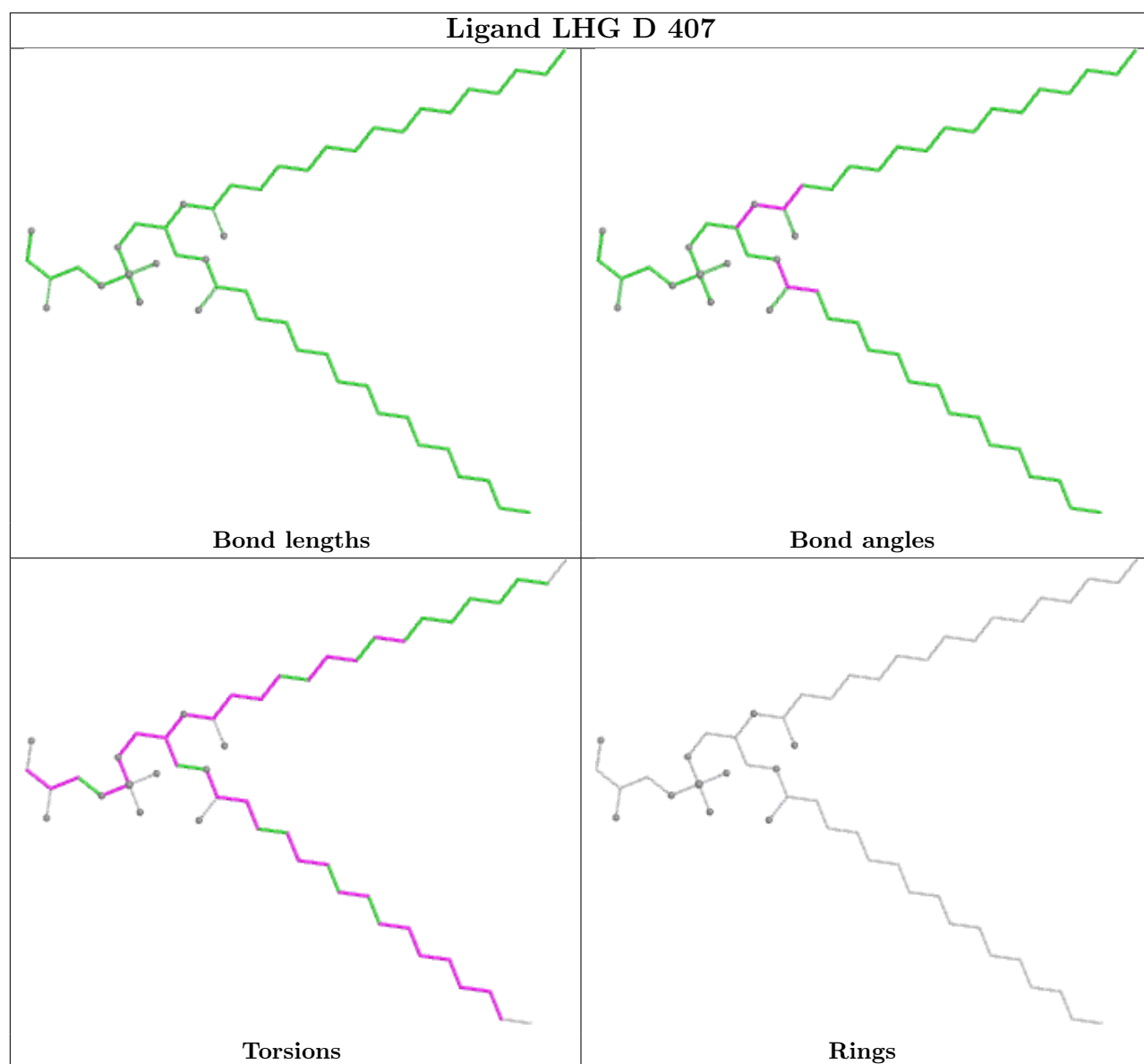


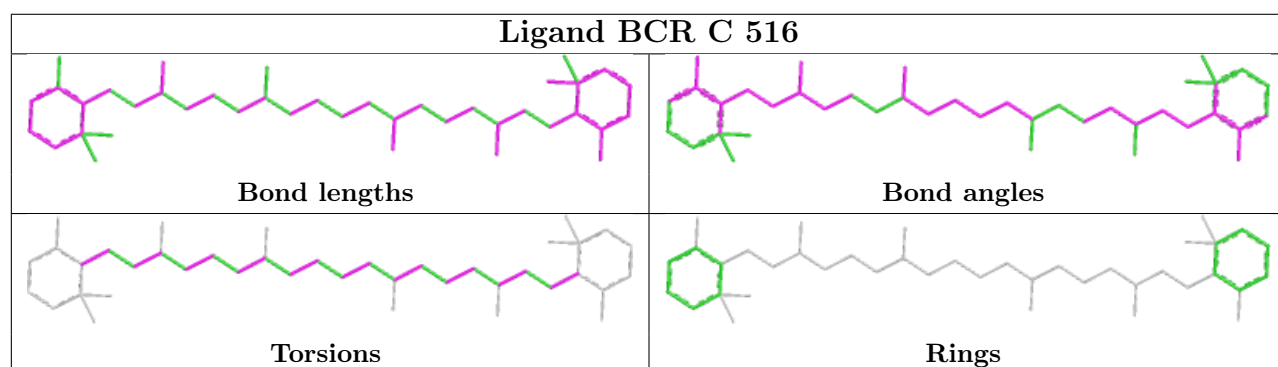
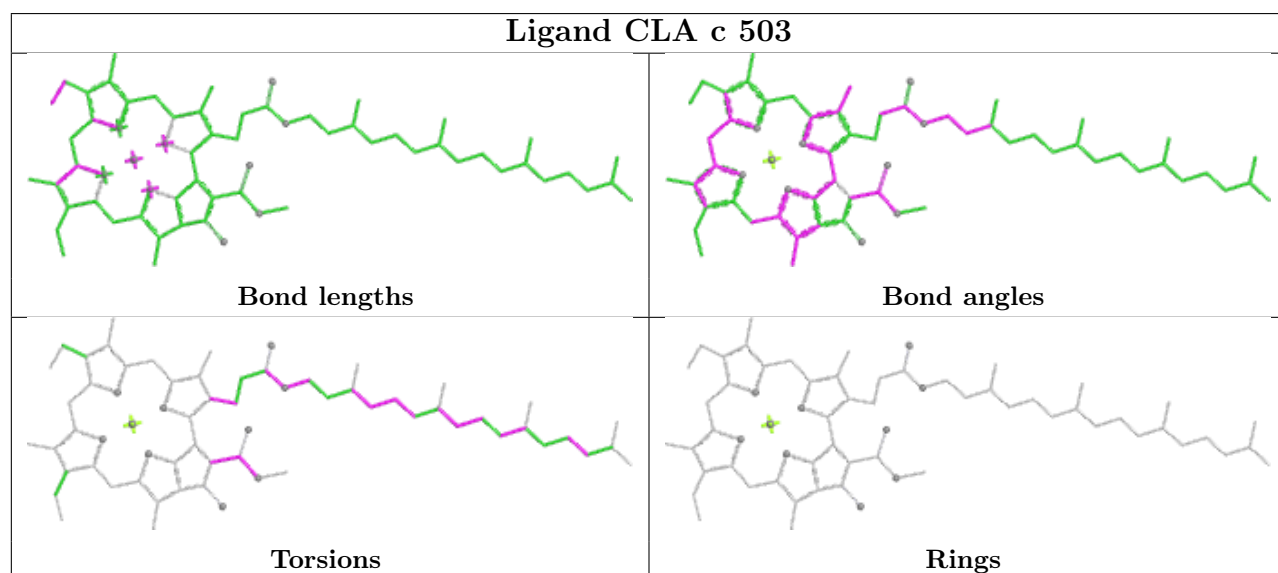
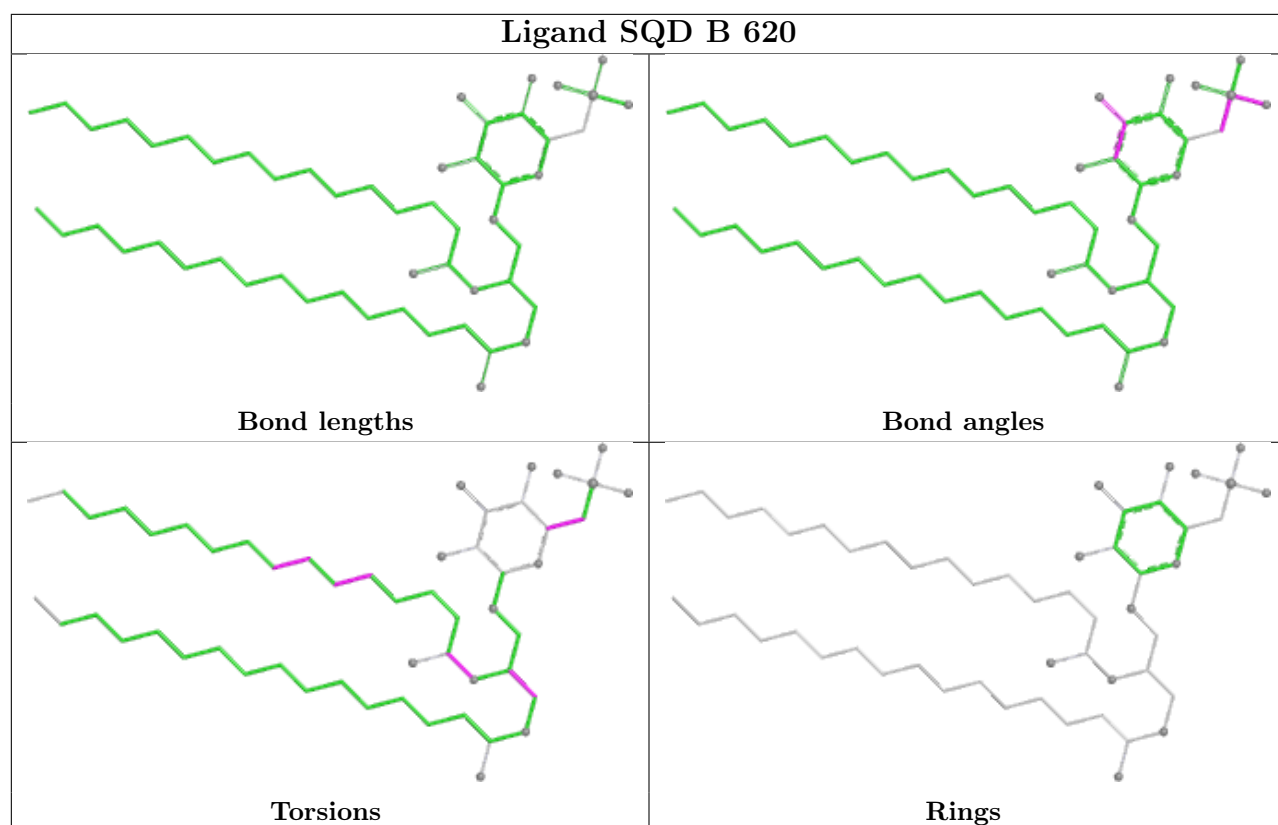
## Ligand CLA n 604

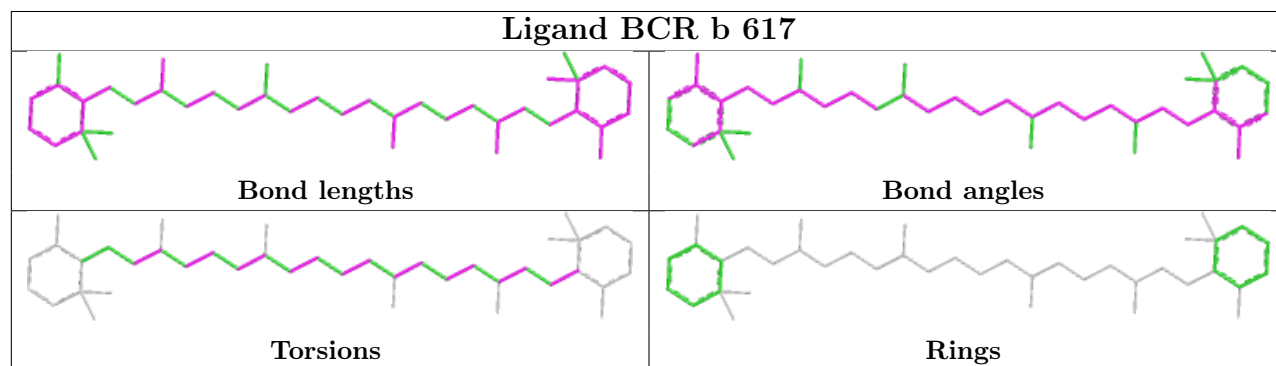
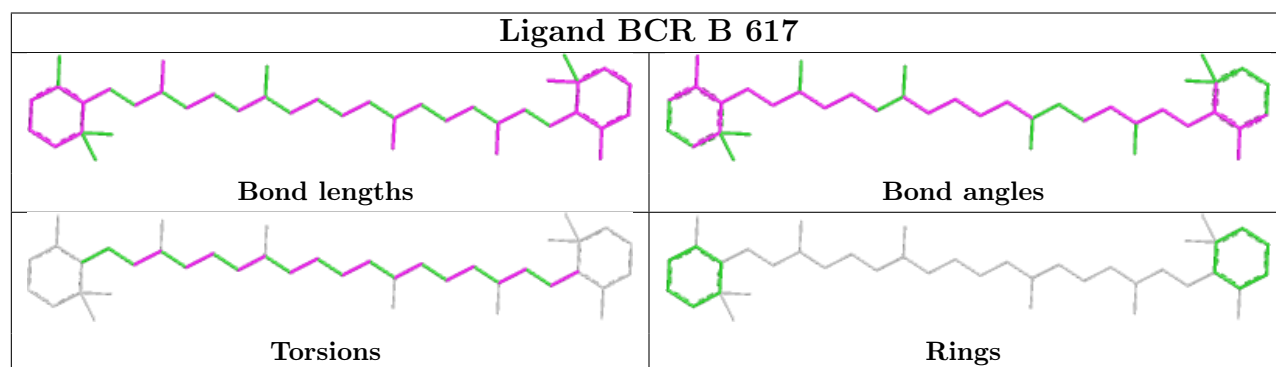
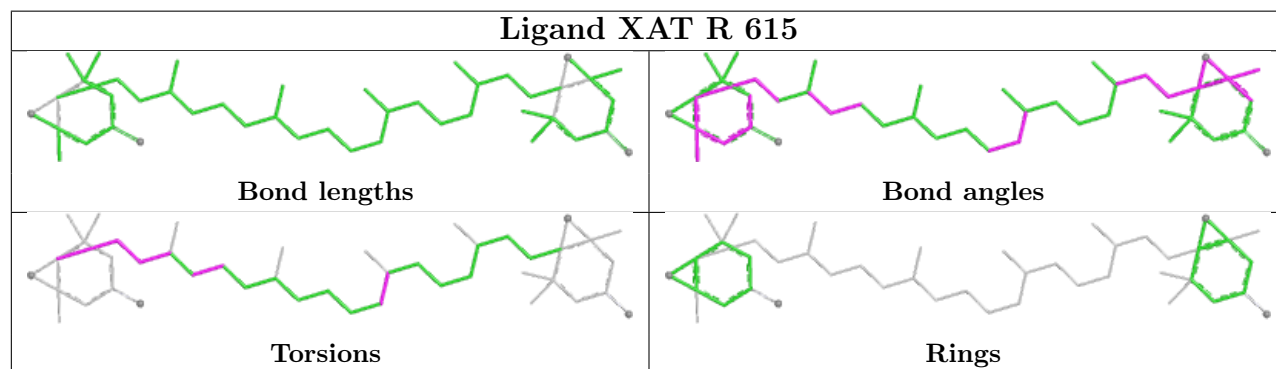
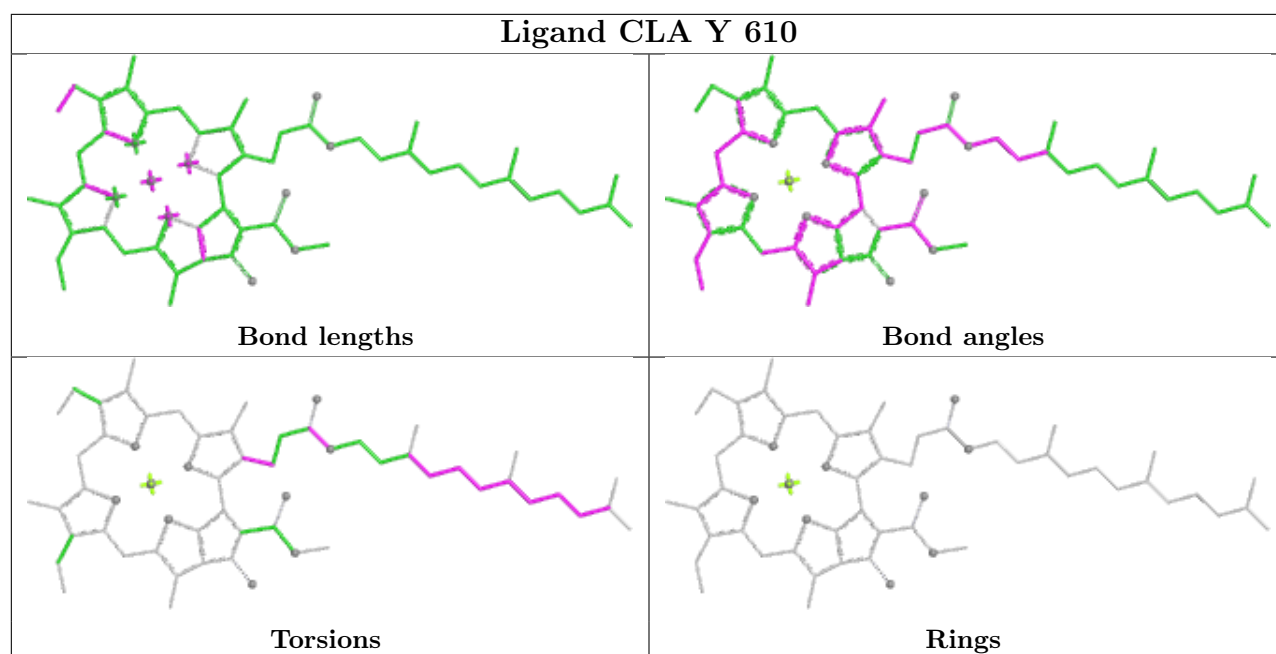


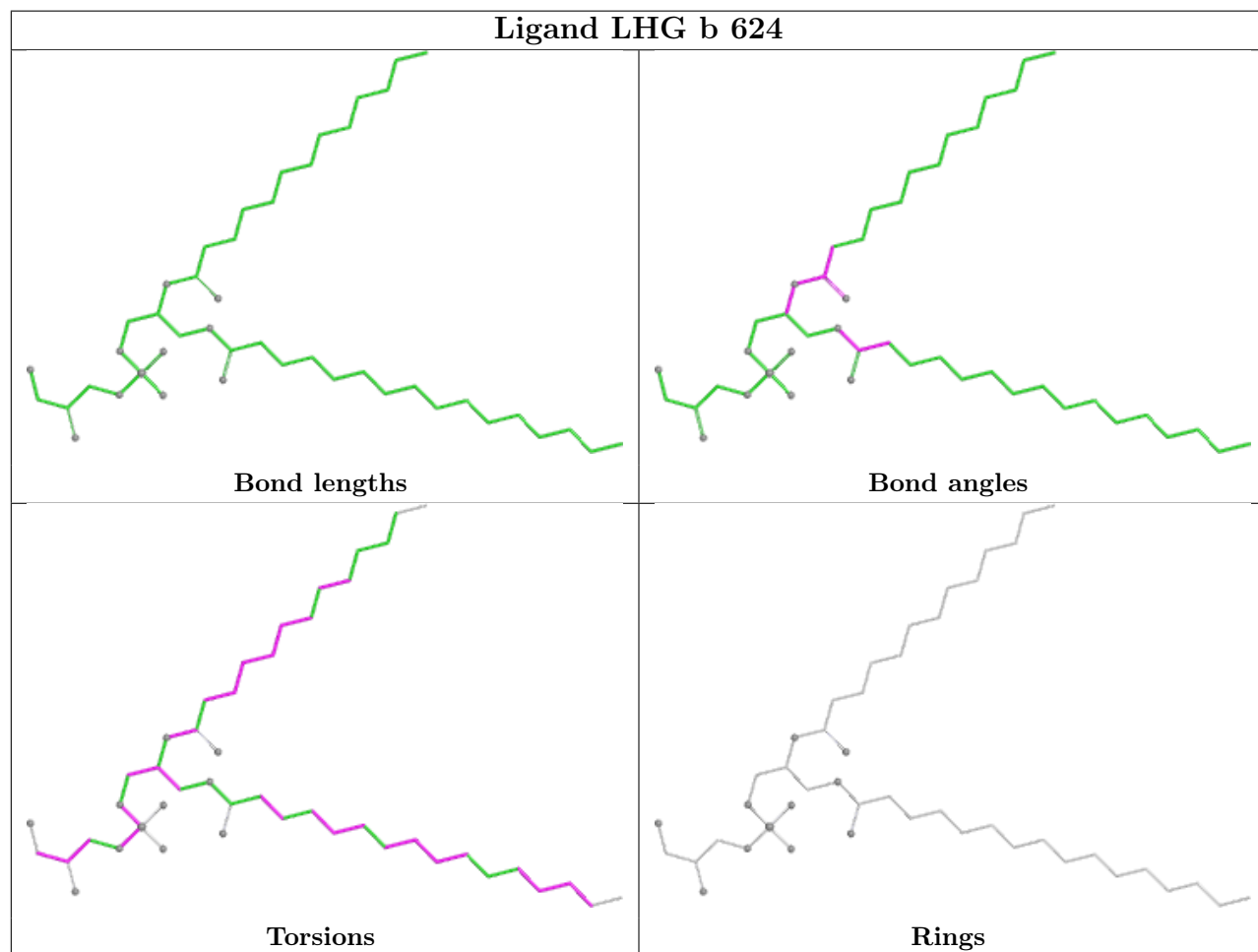
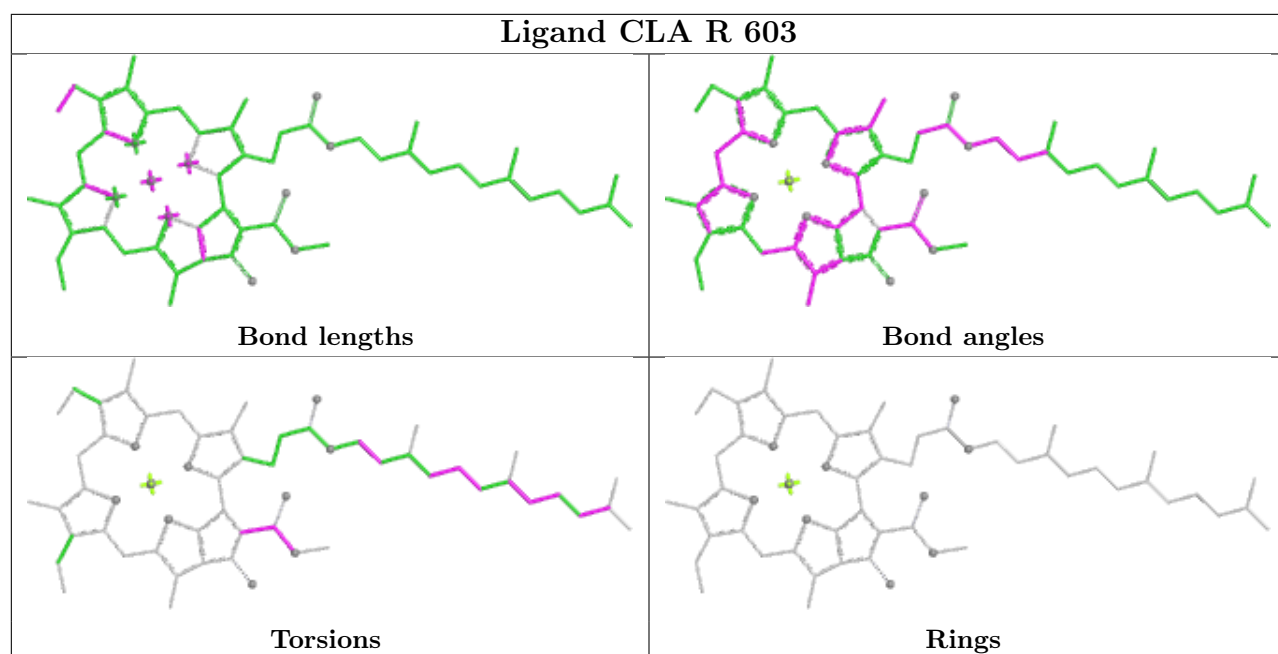
## Ligand CLA C 510

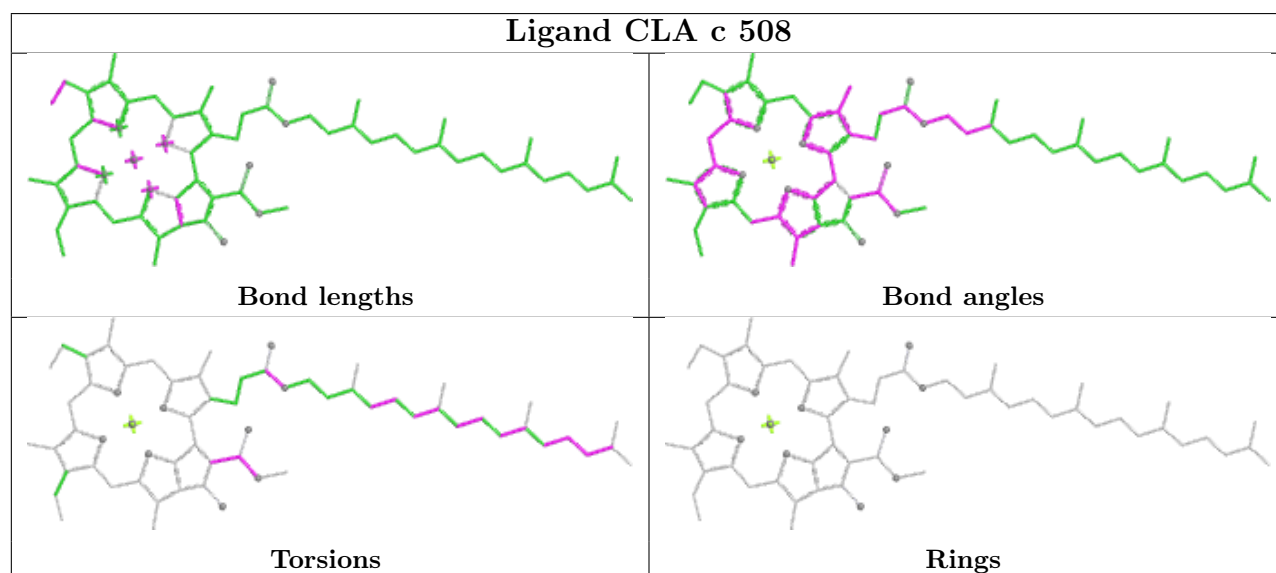
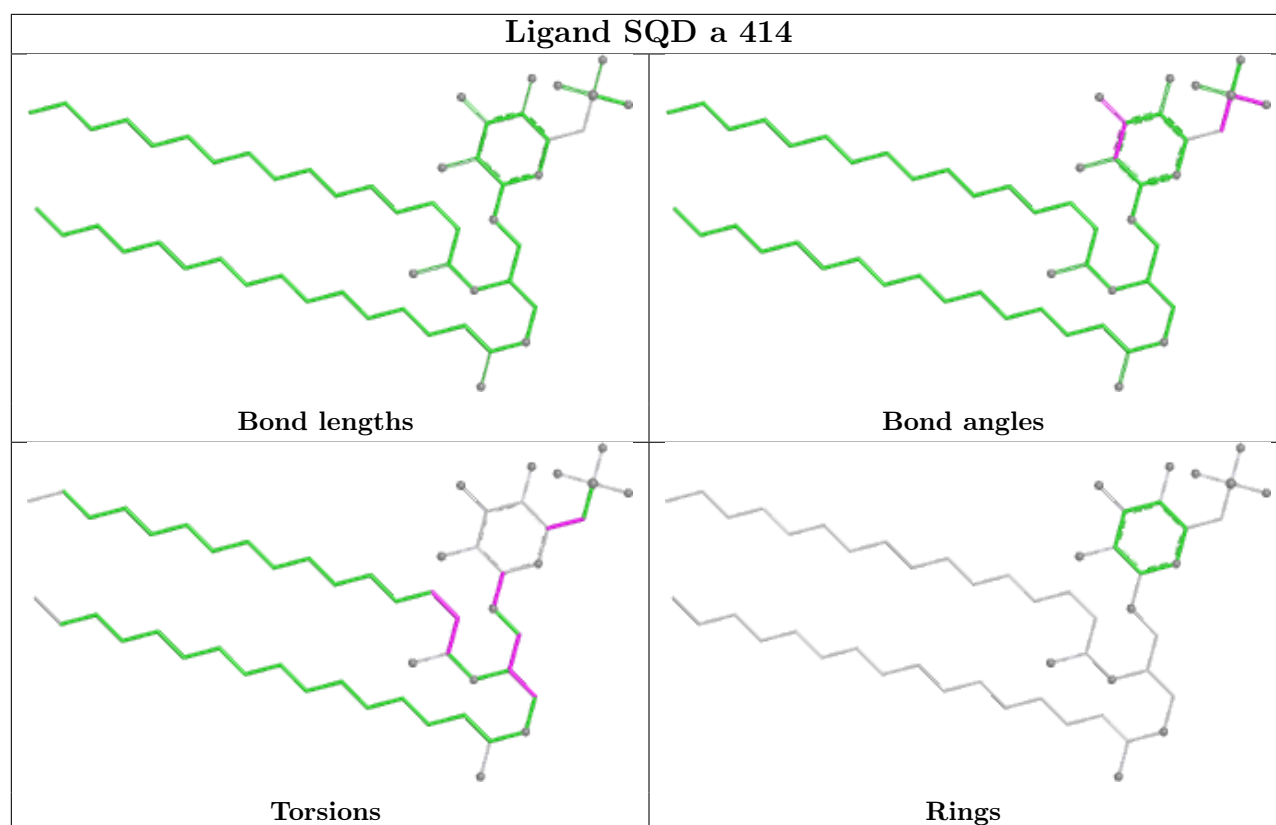




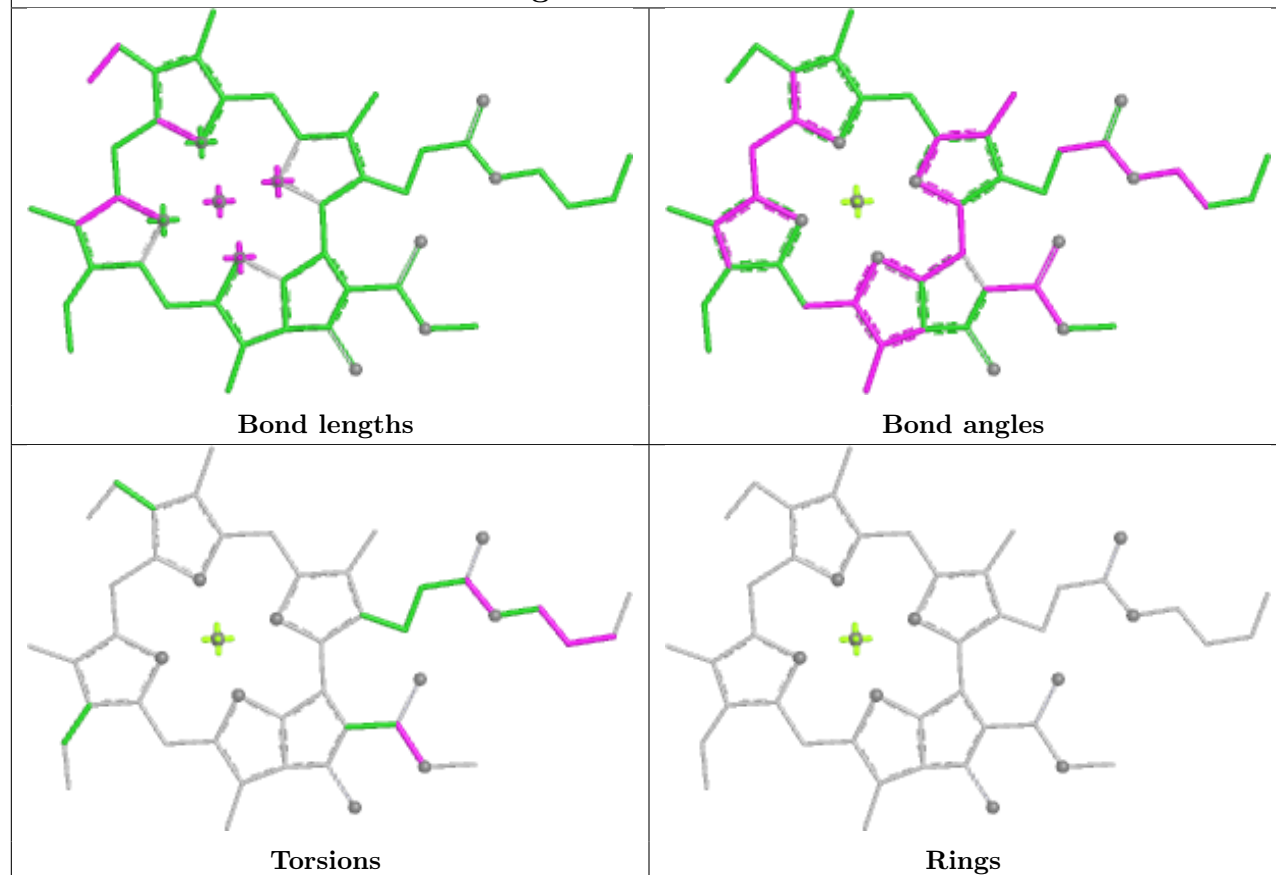




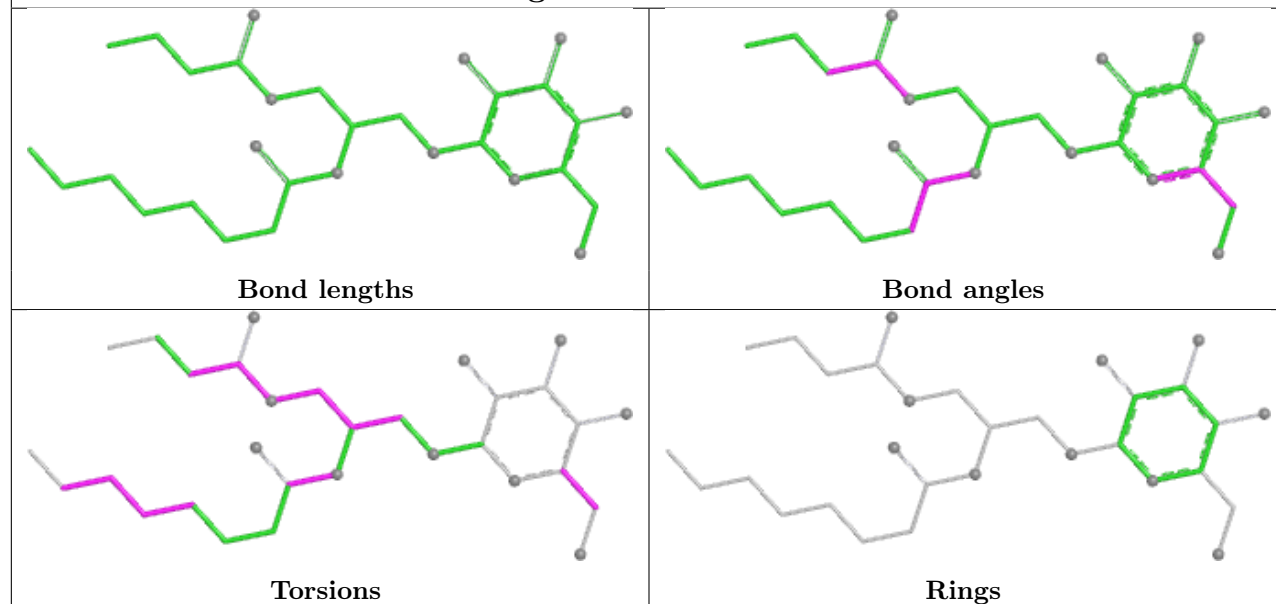




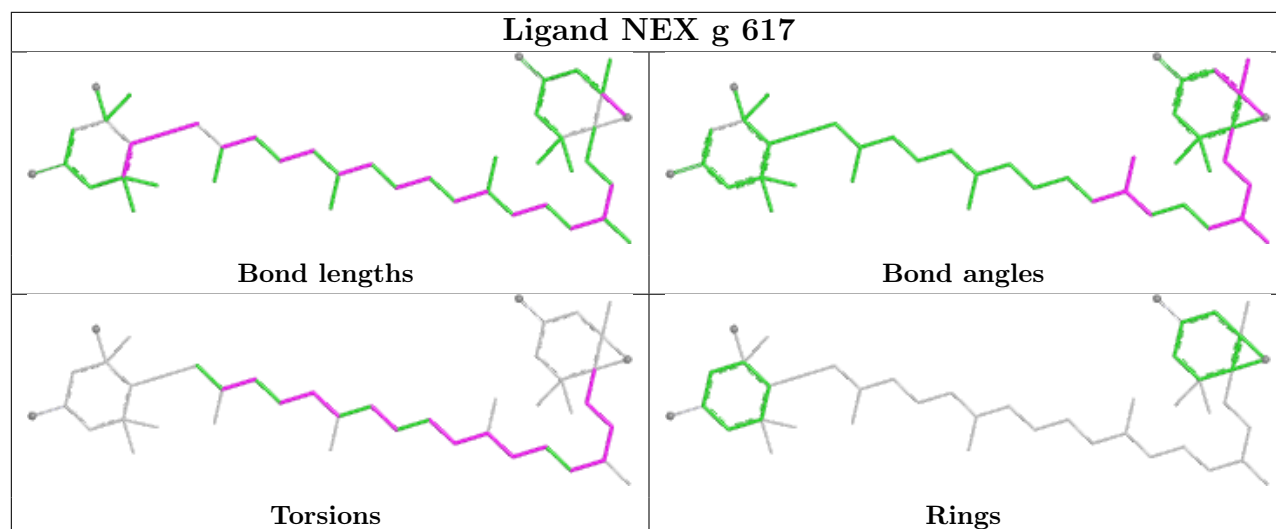
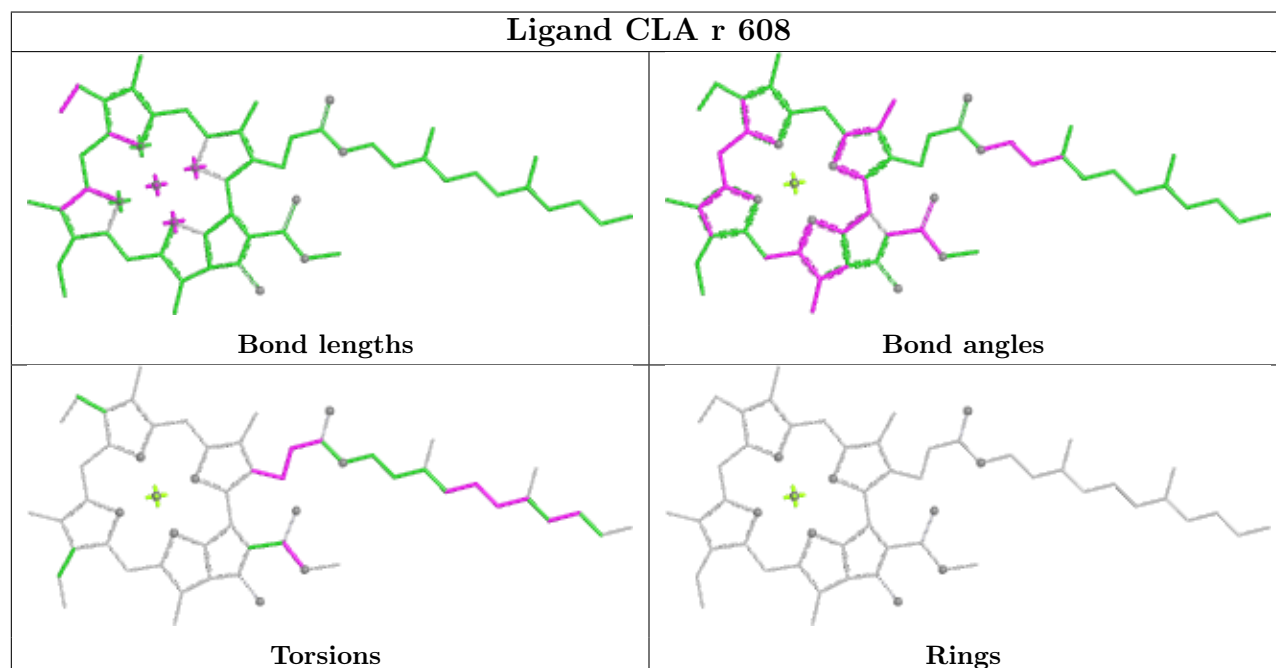
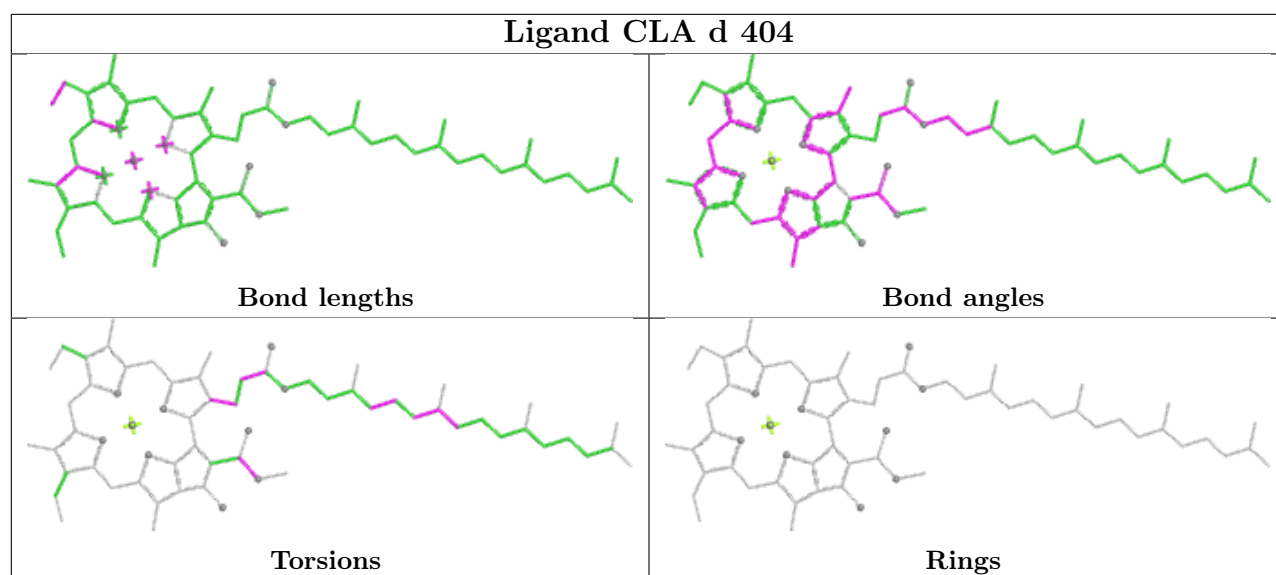
## Ligand CLA R 611



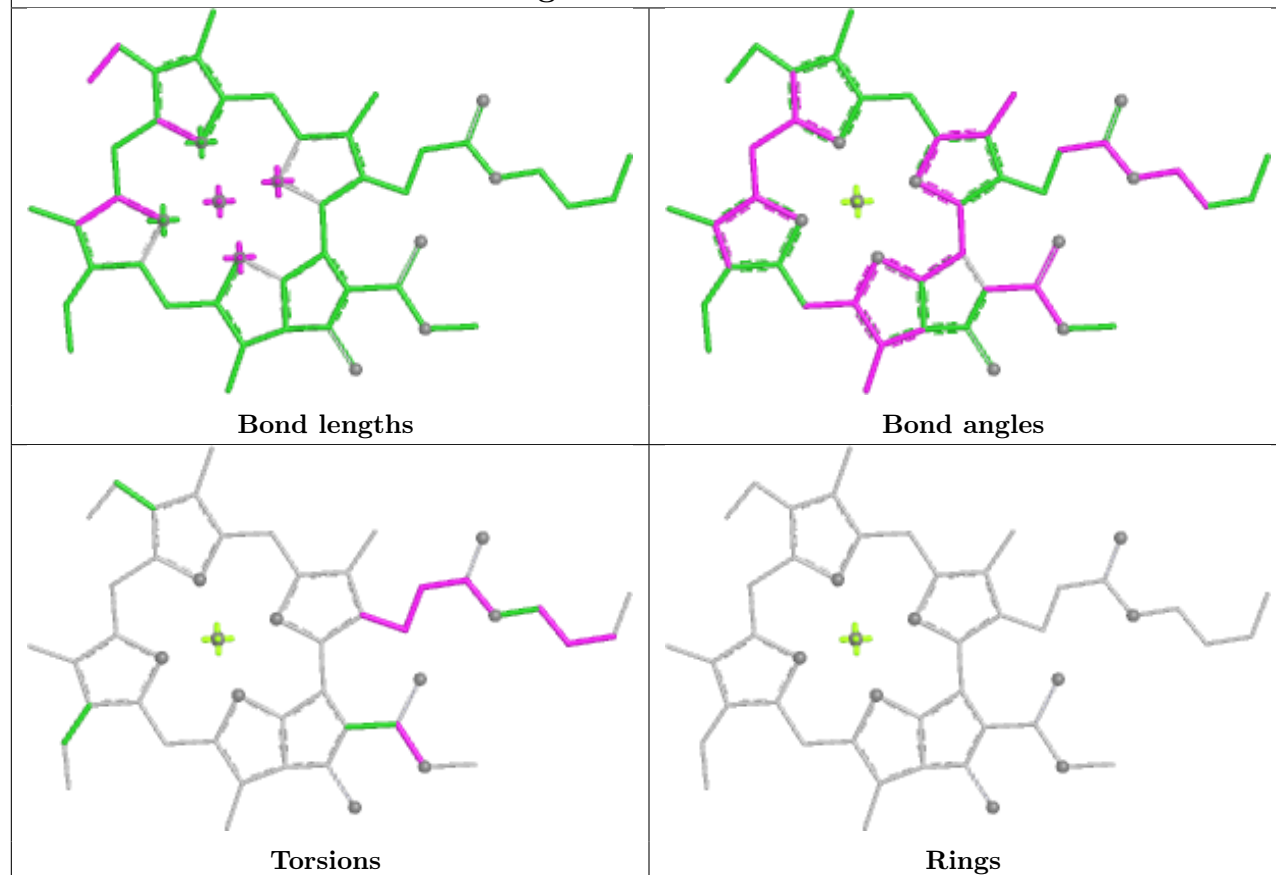
## Ligand LMG B 624



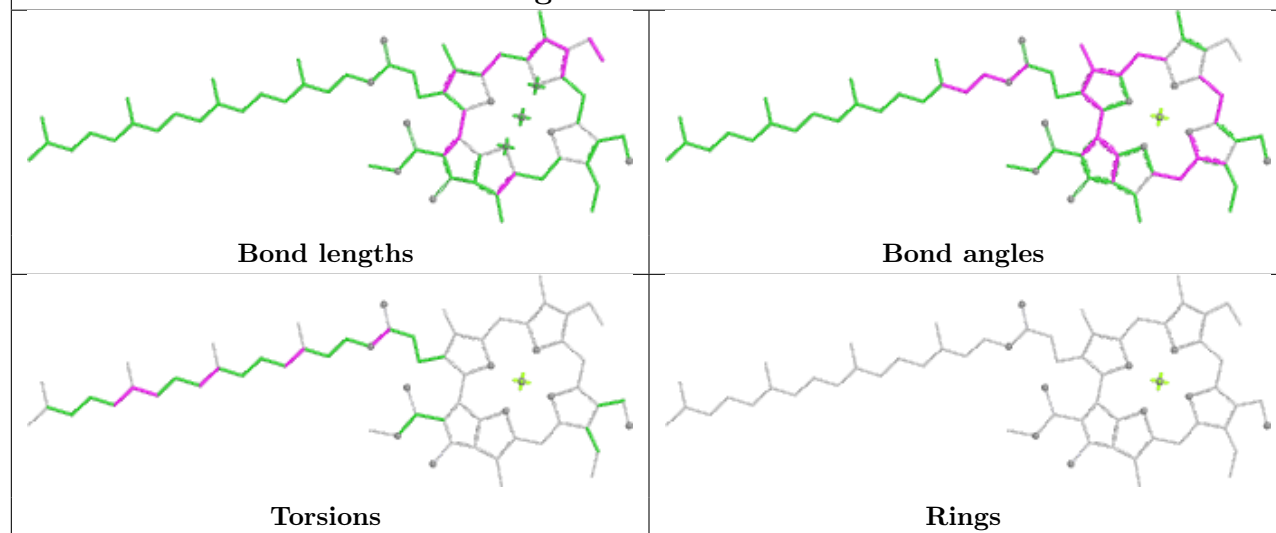


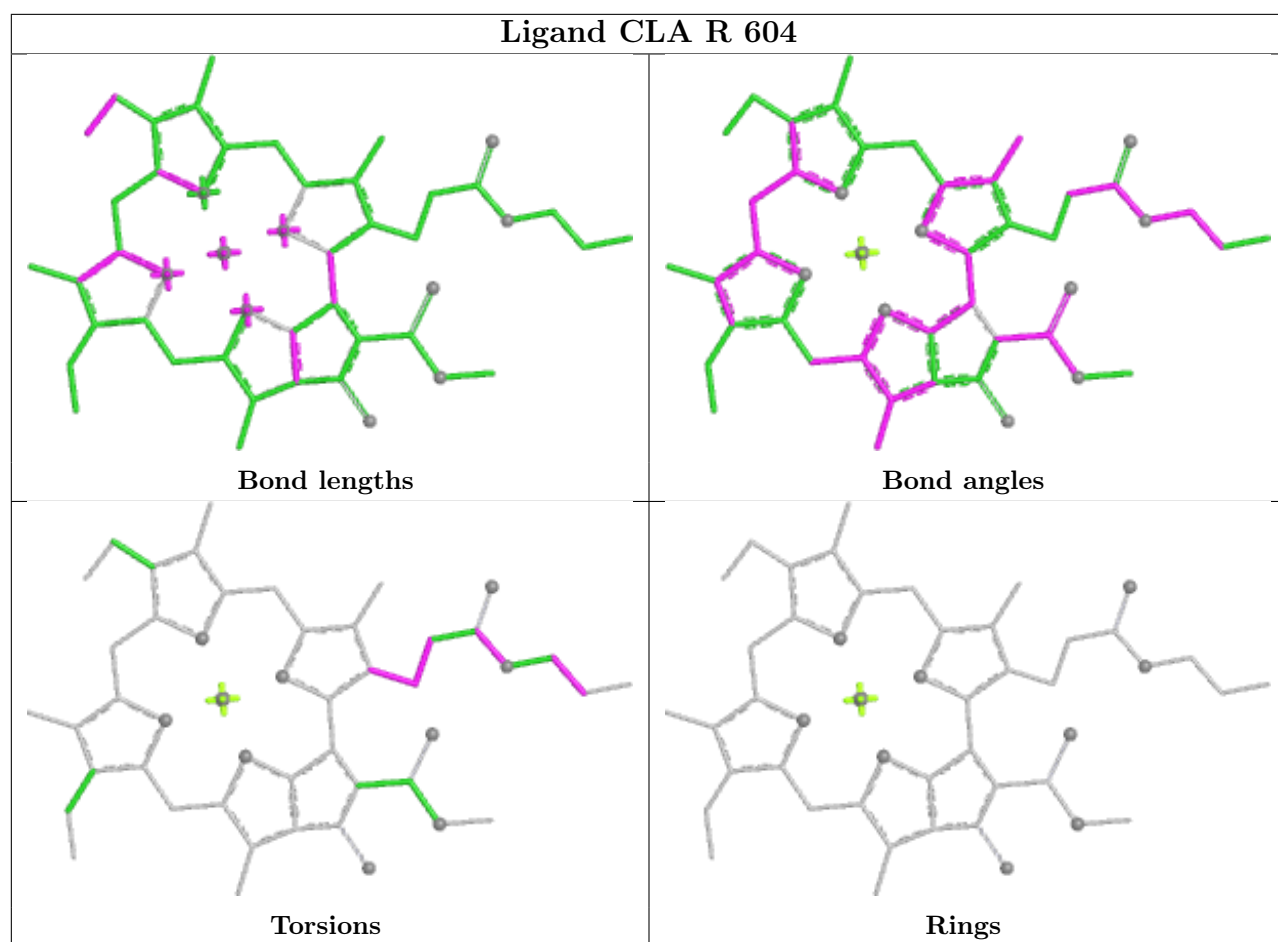


## Ligand CLA r 610

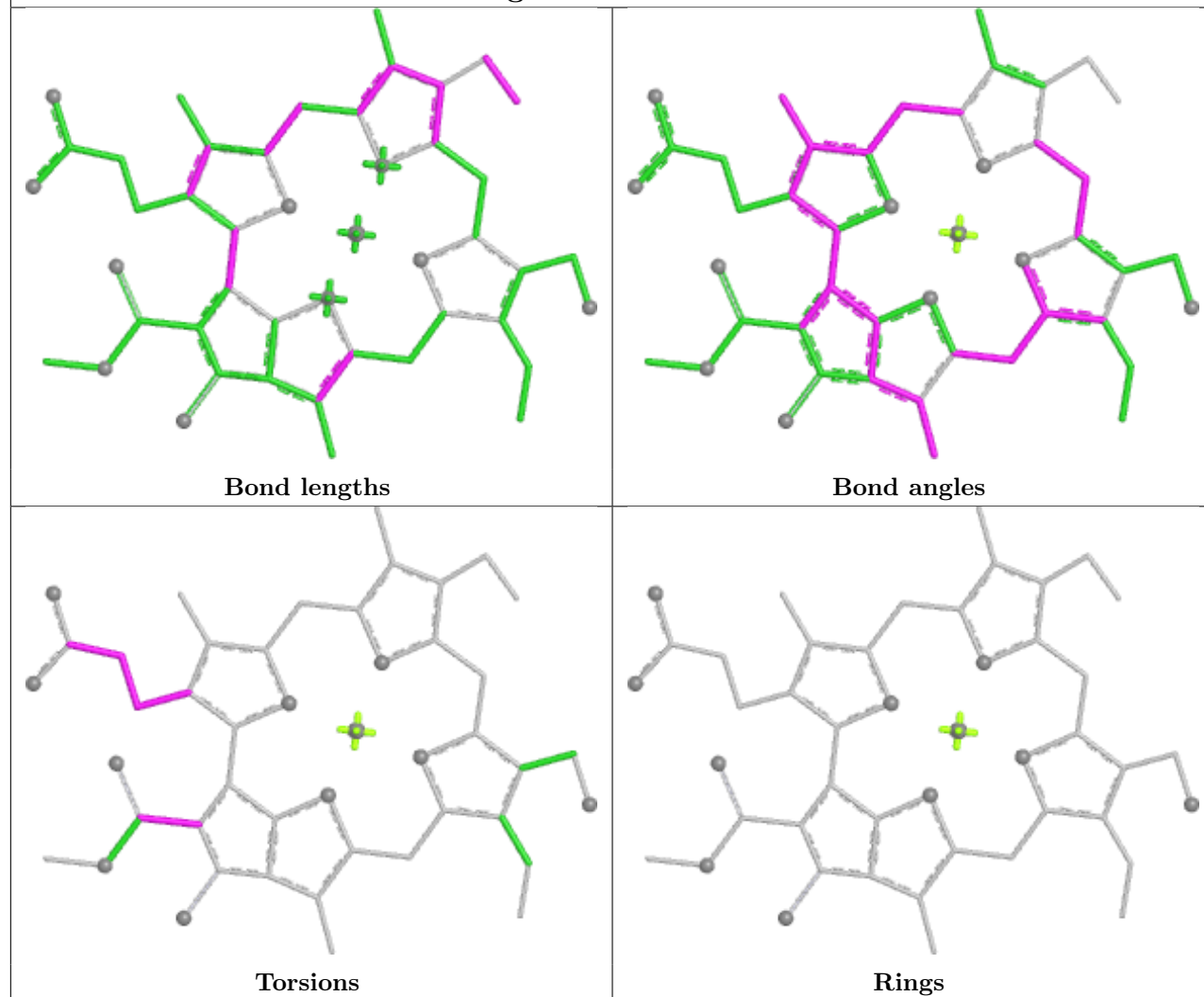


## Ligand CHL n 609

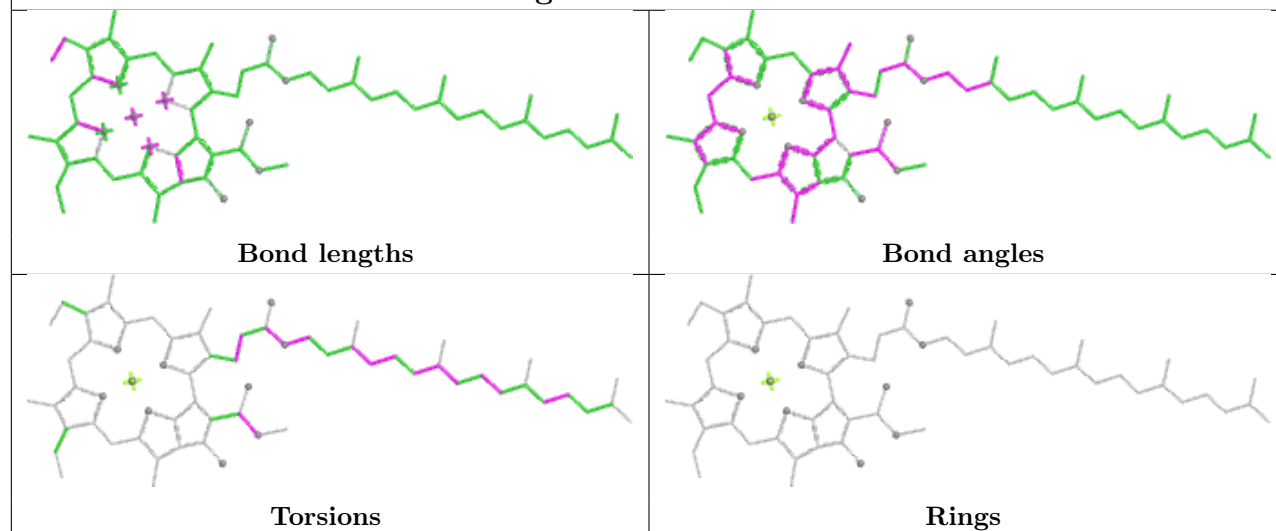


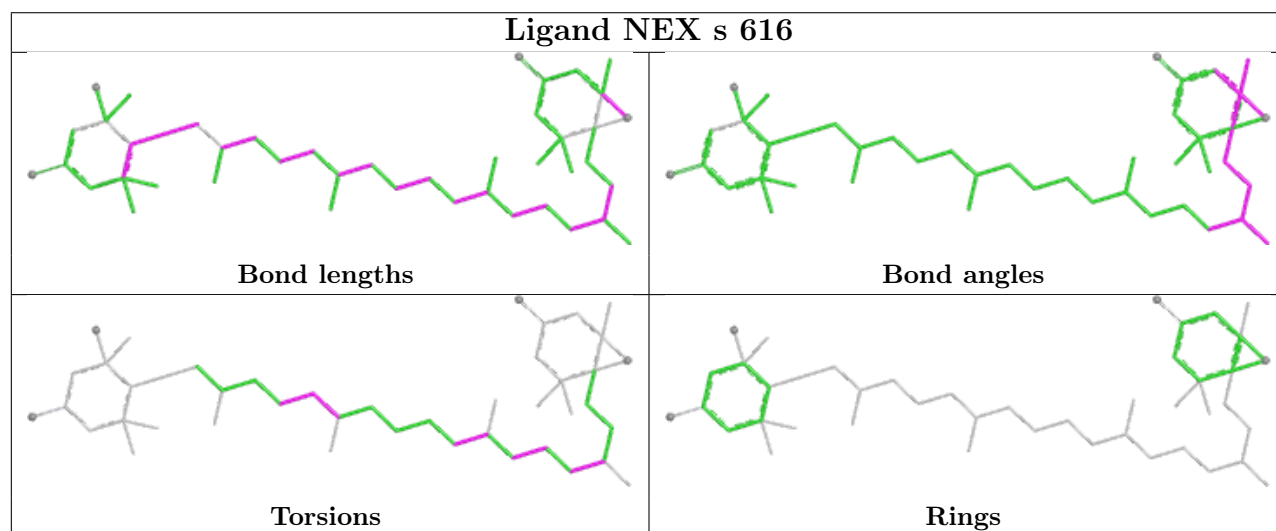
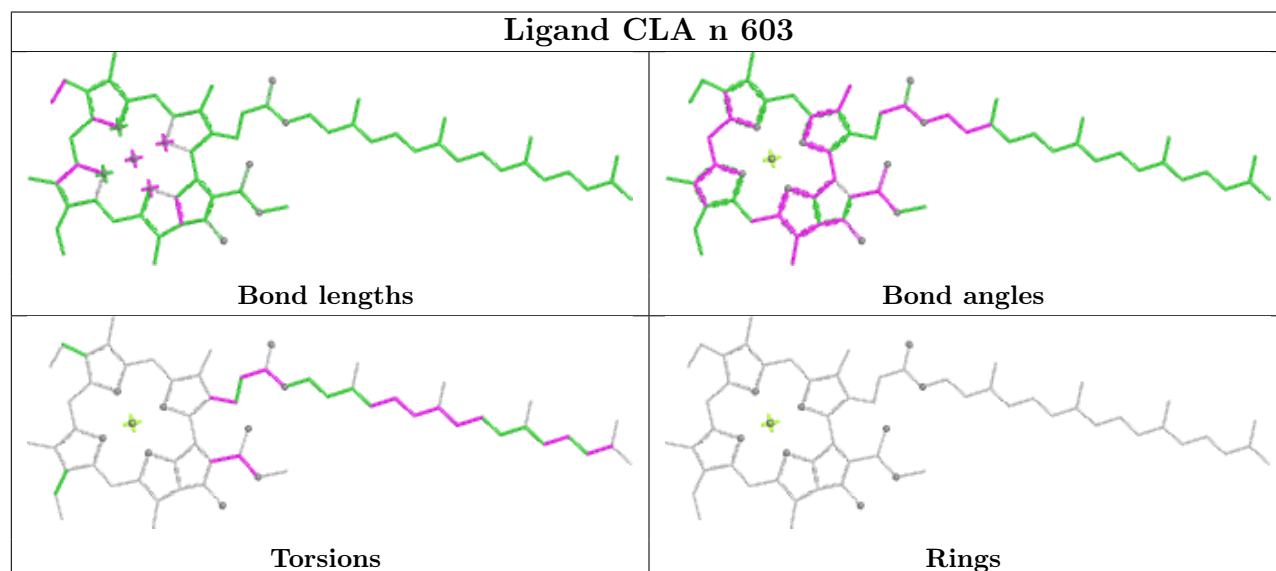
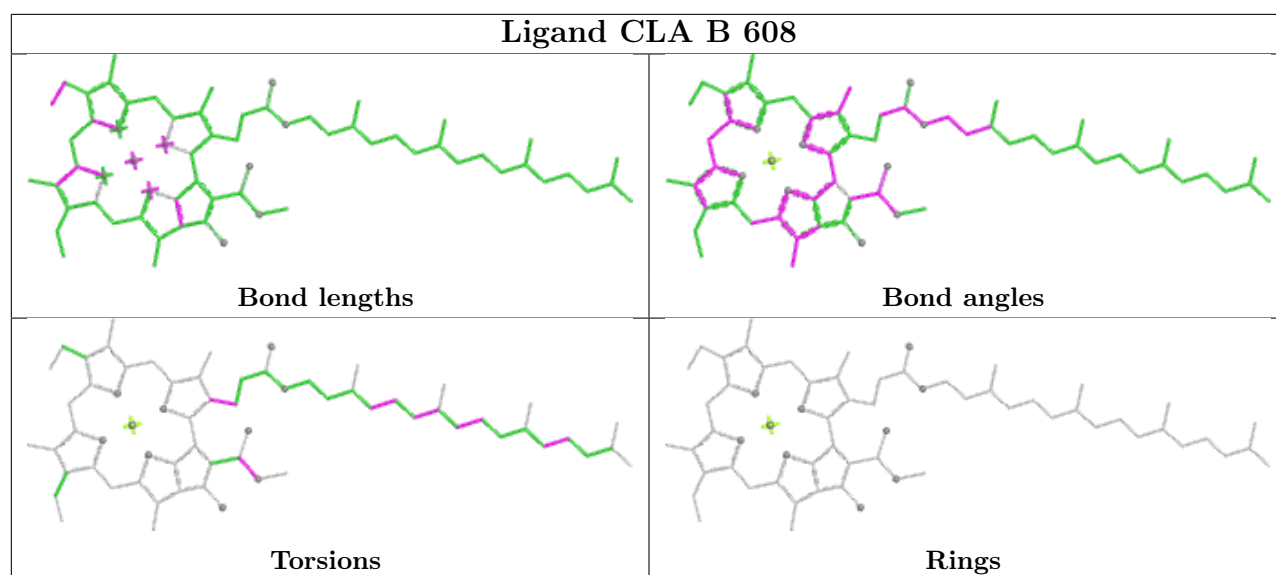


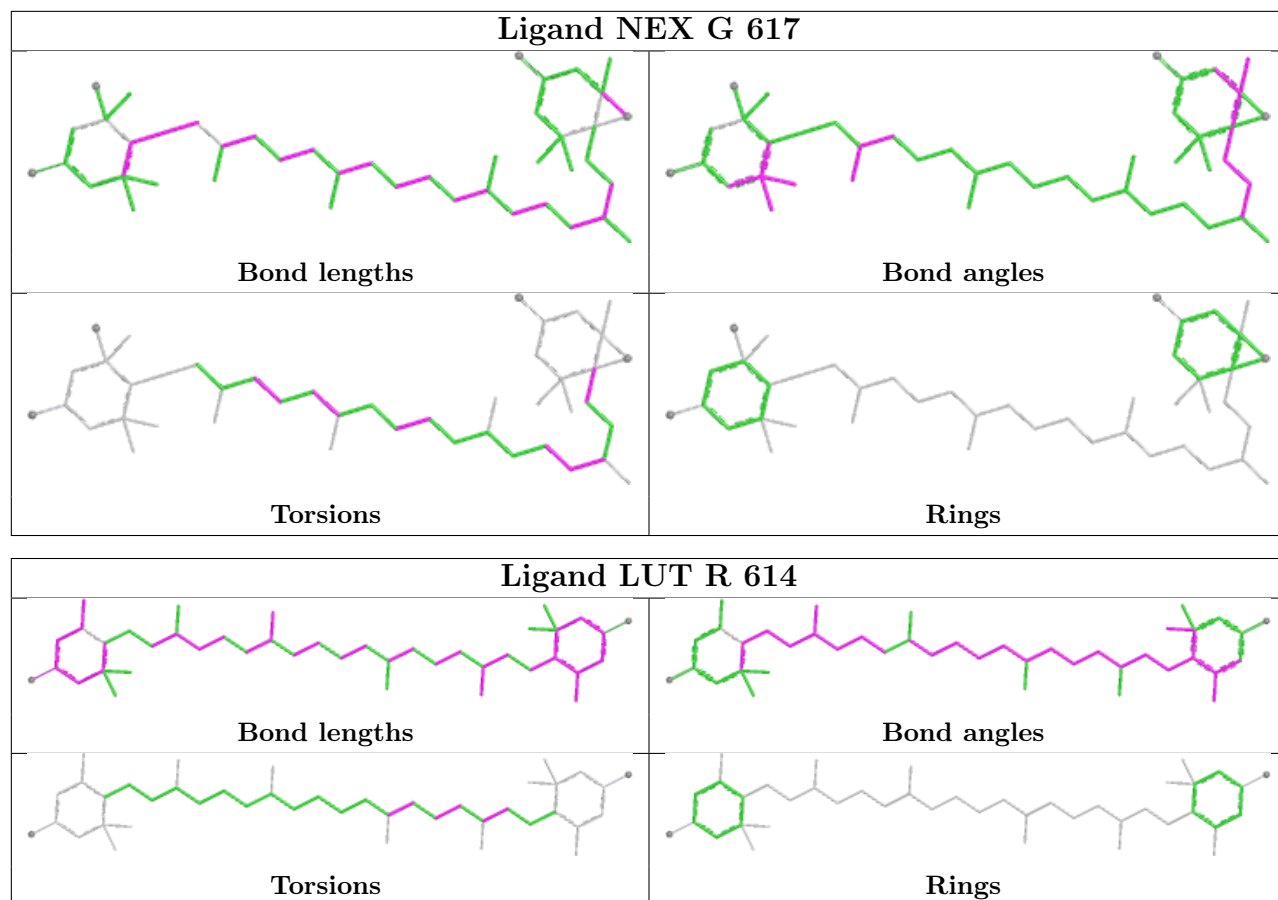
## Ligand CHL s 601



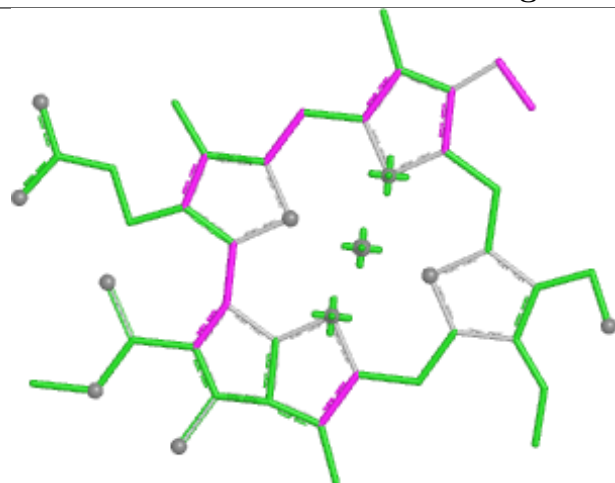
## Ligand CLA b 606



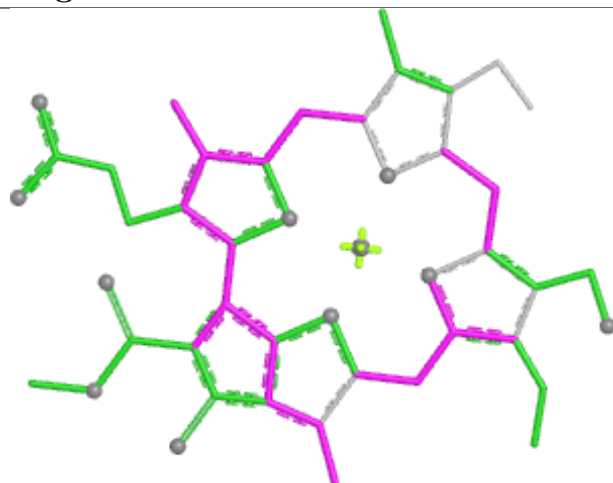




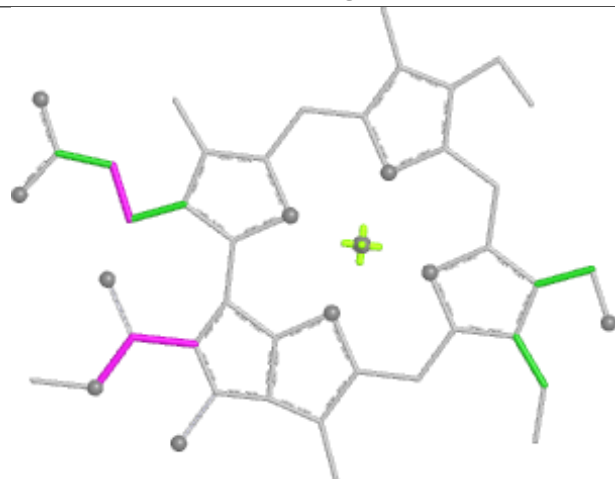
## Ligand CHL g 605



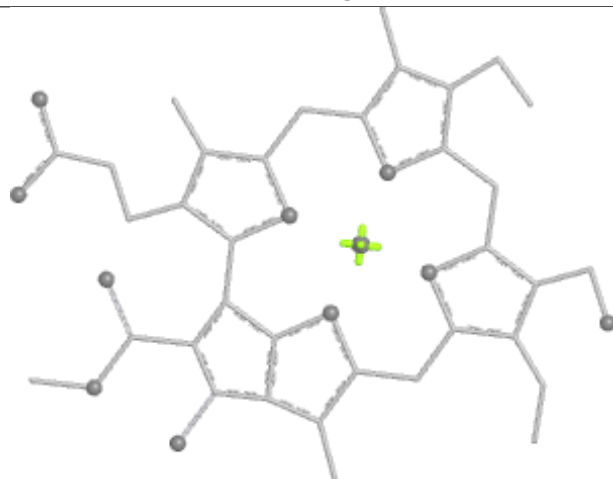
Bond lengths



Bond angles

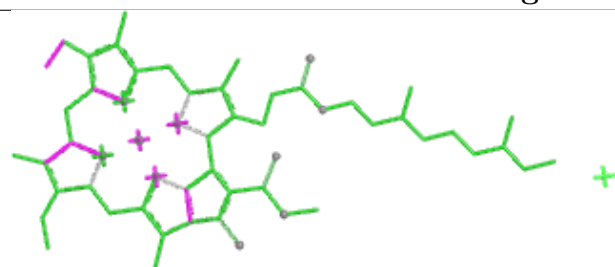


Torsions

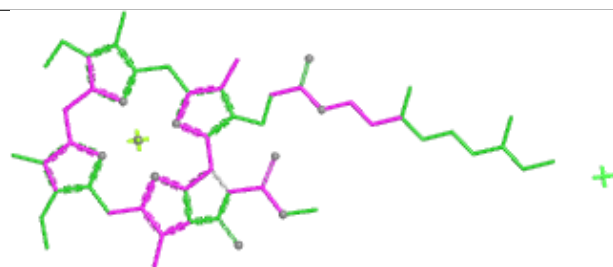


Rings

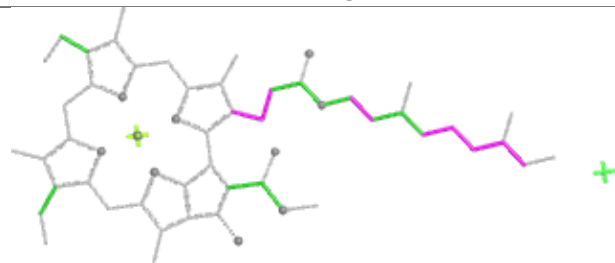
## Ligand CLA c 506



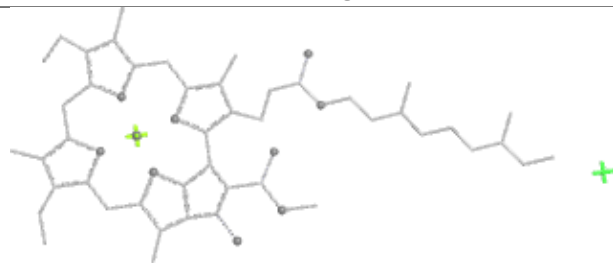
Bond lengths



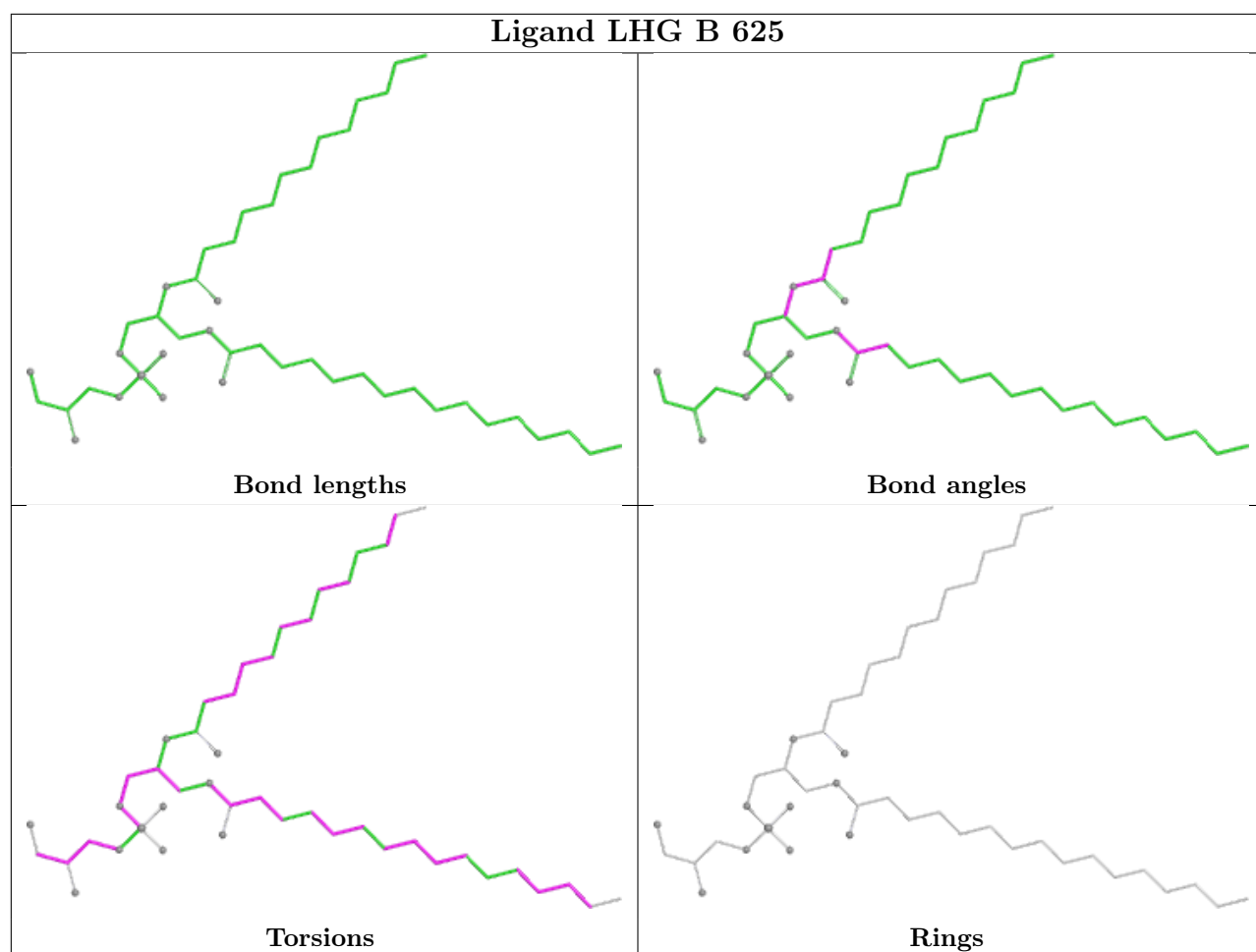
Bond angles



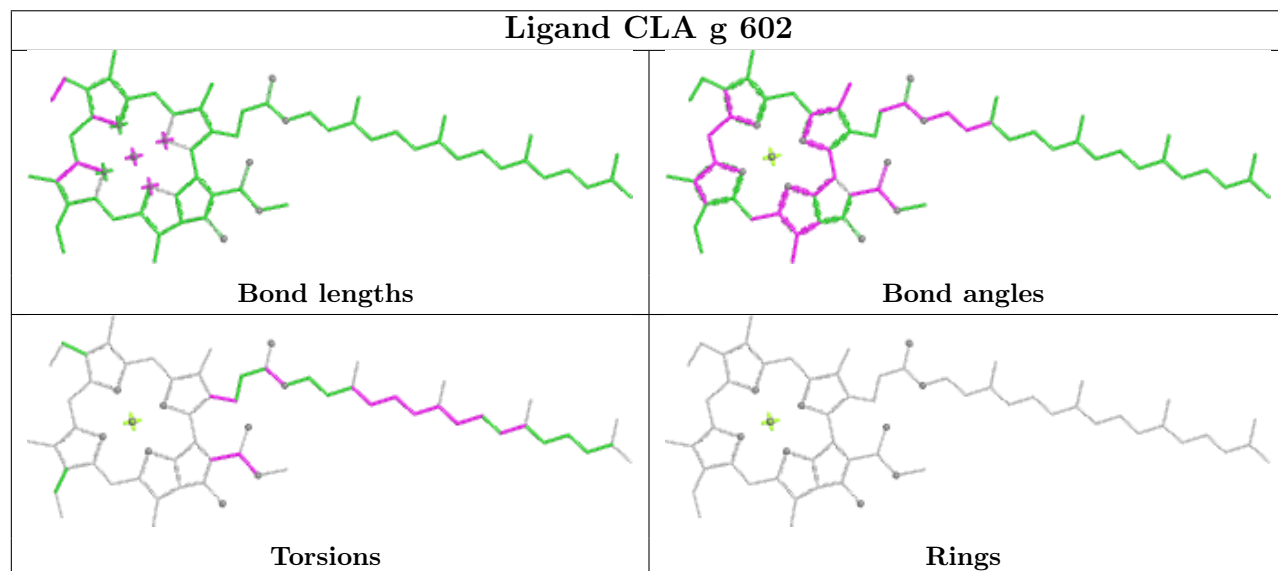
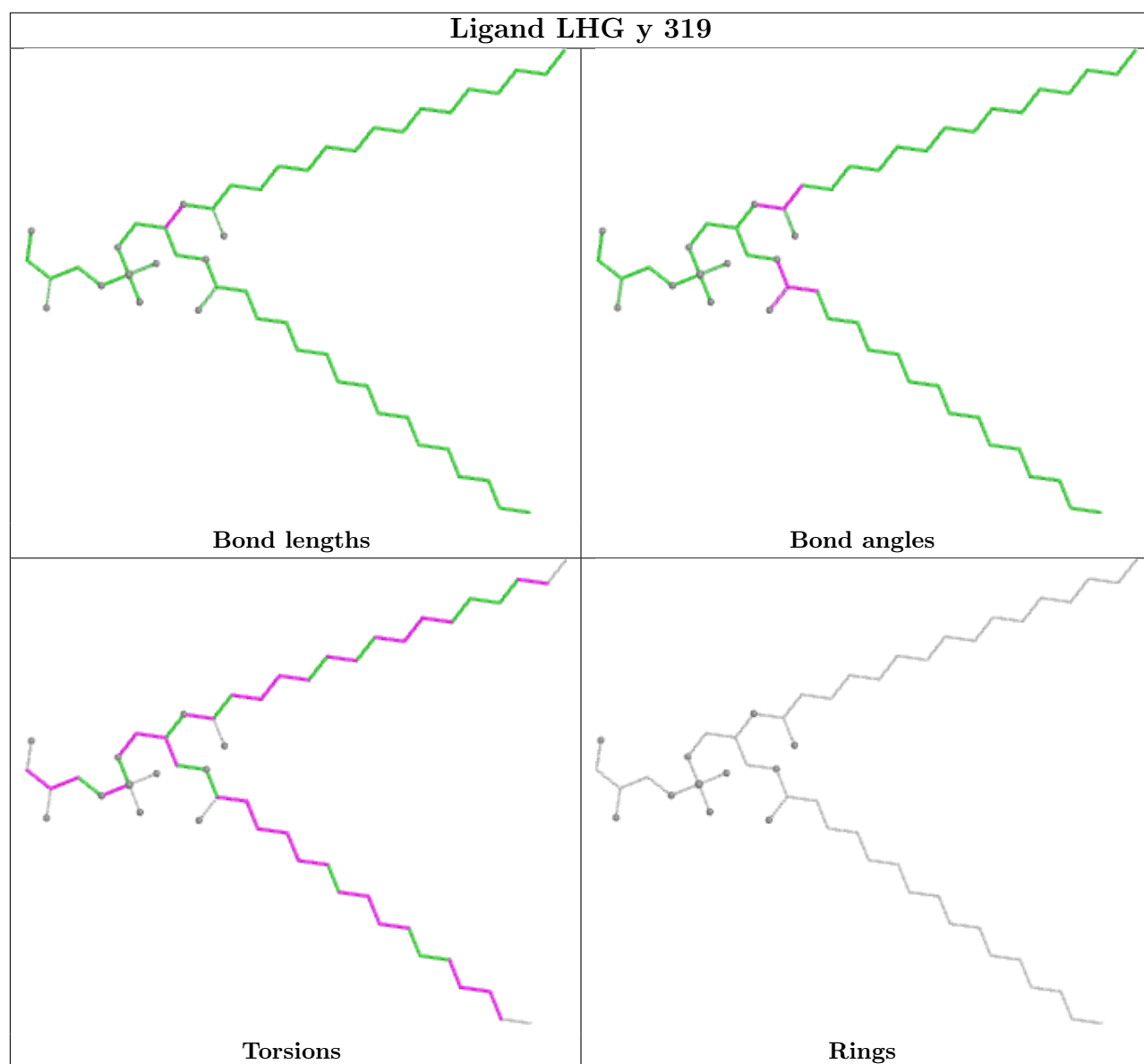
Torsions

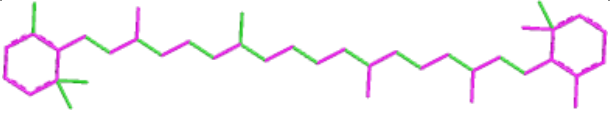

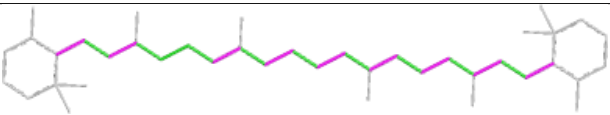
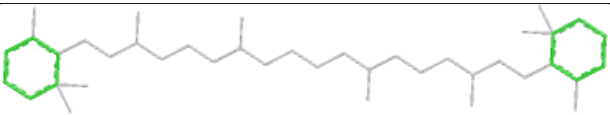
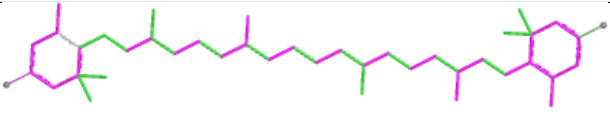
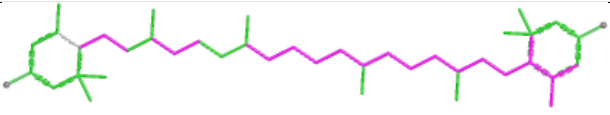
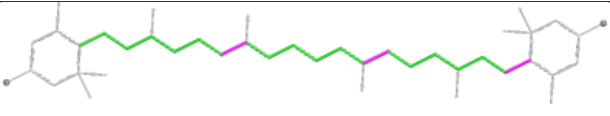
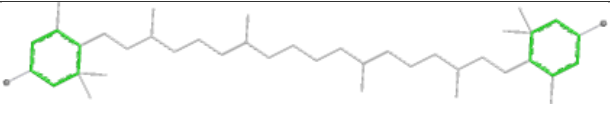
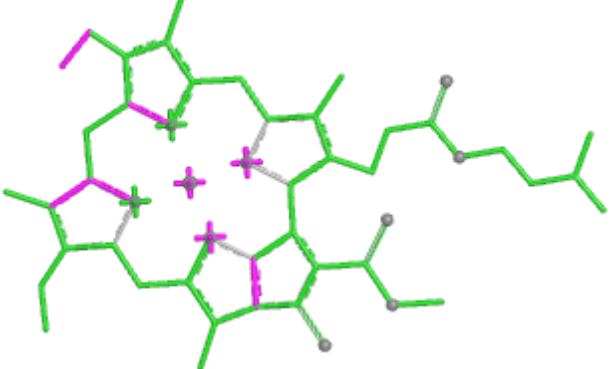
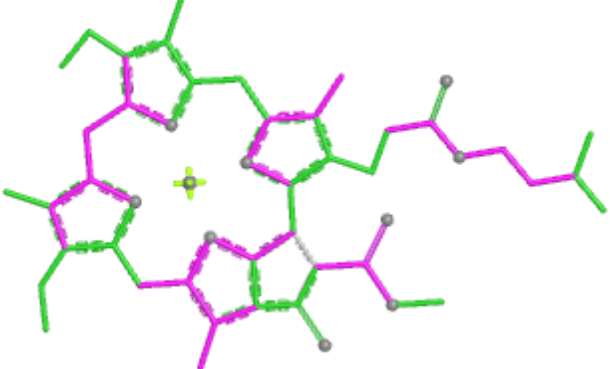
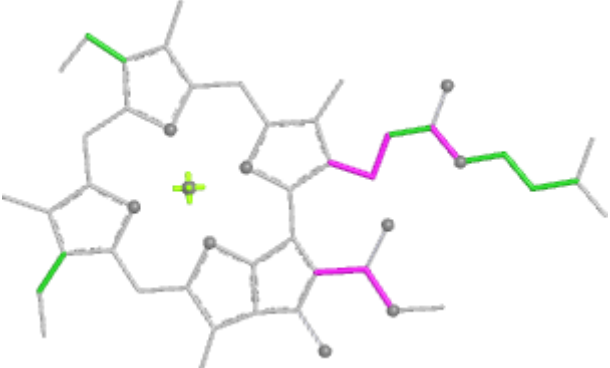
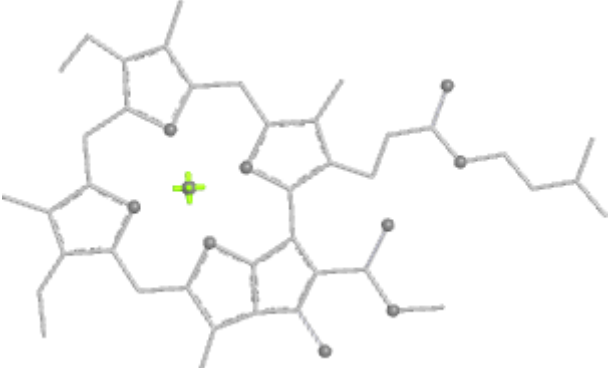


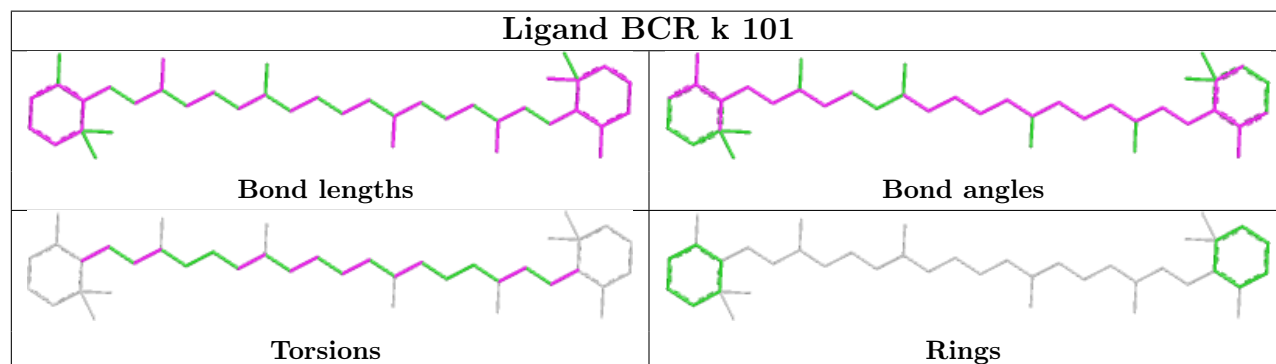
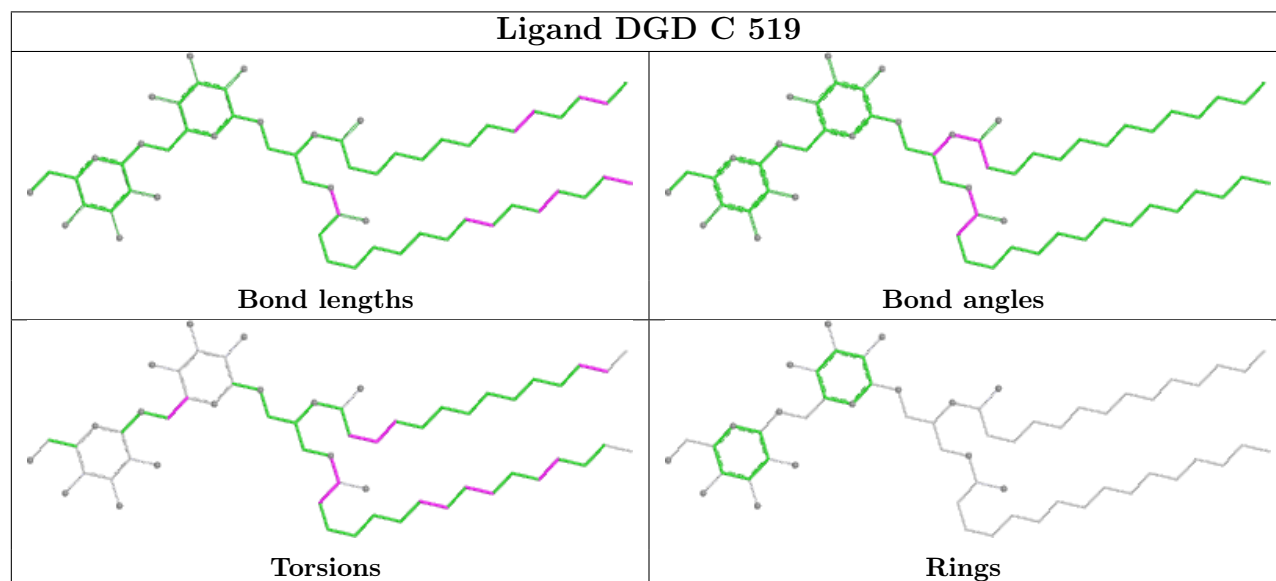
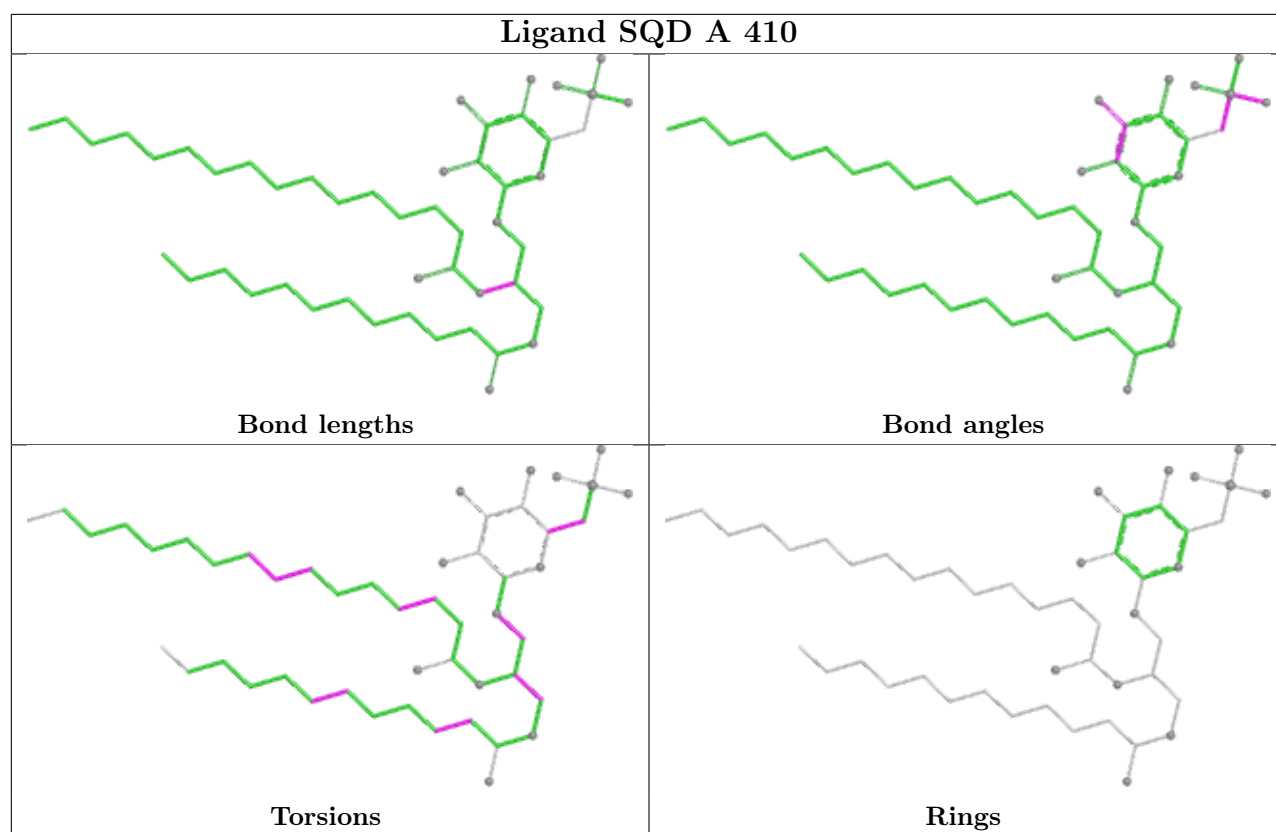
Rings

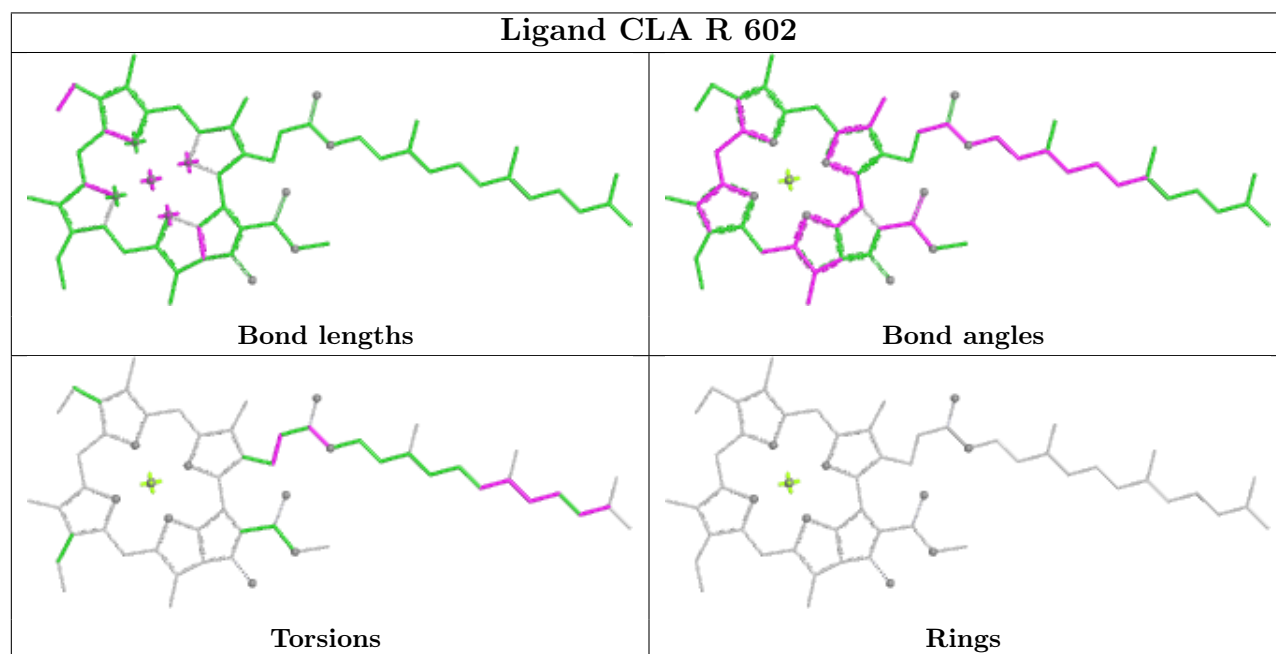
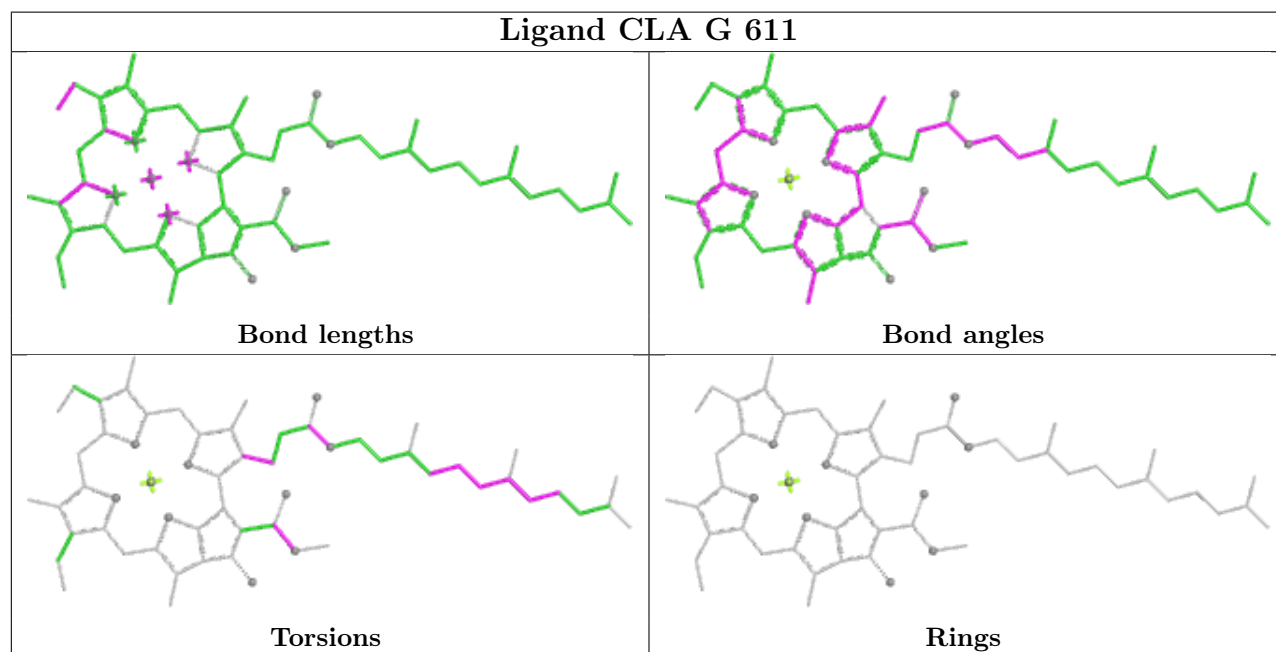
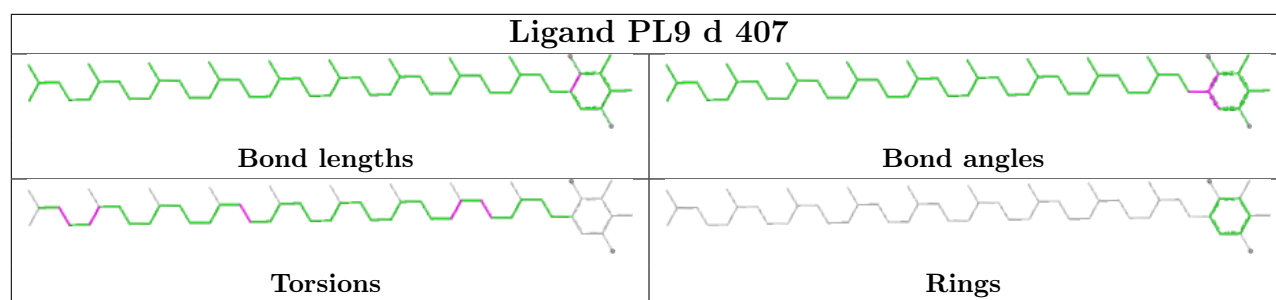


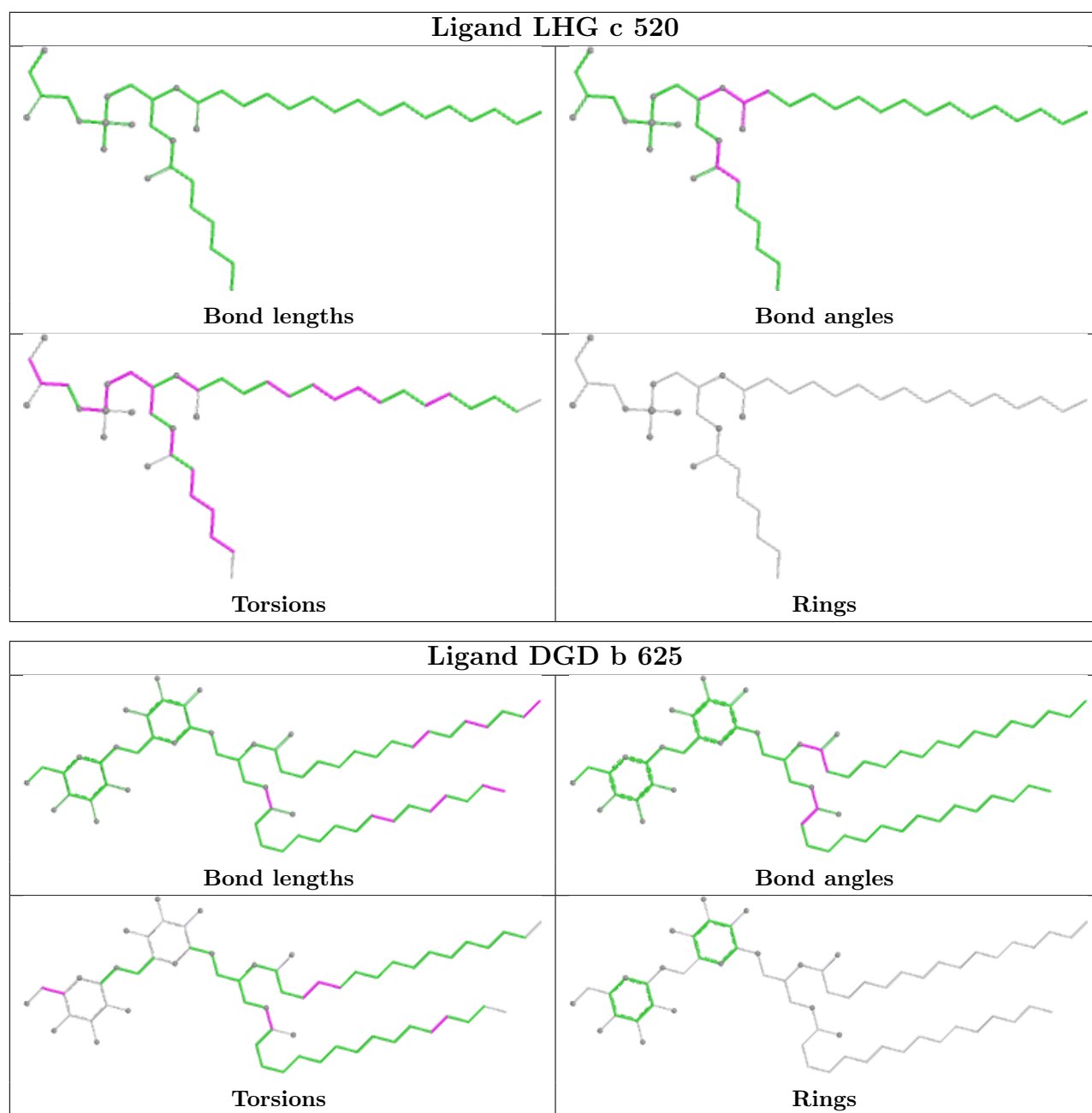




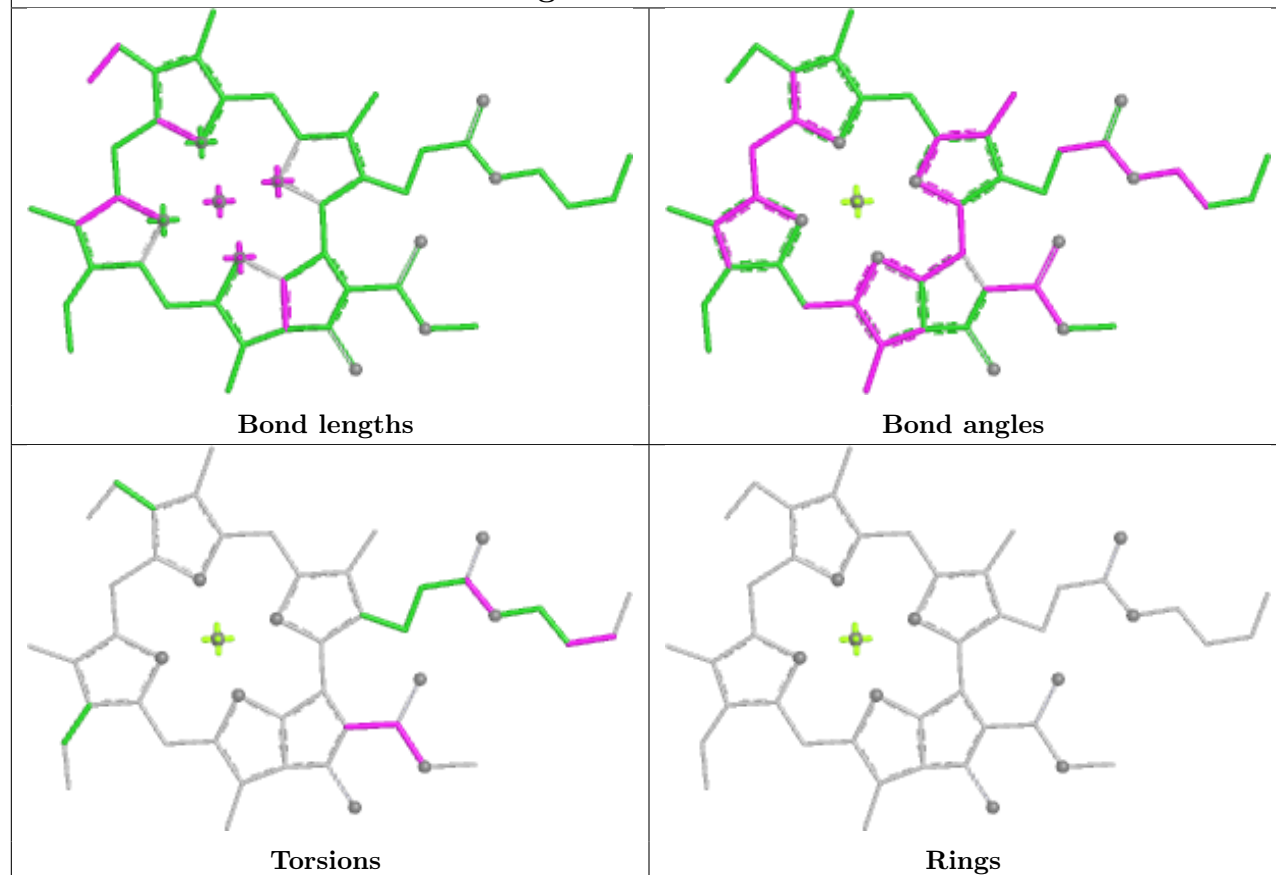
Ligand BCR B 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT g 615	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA Y 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



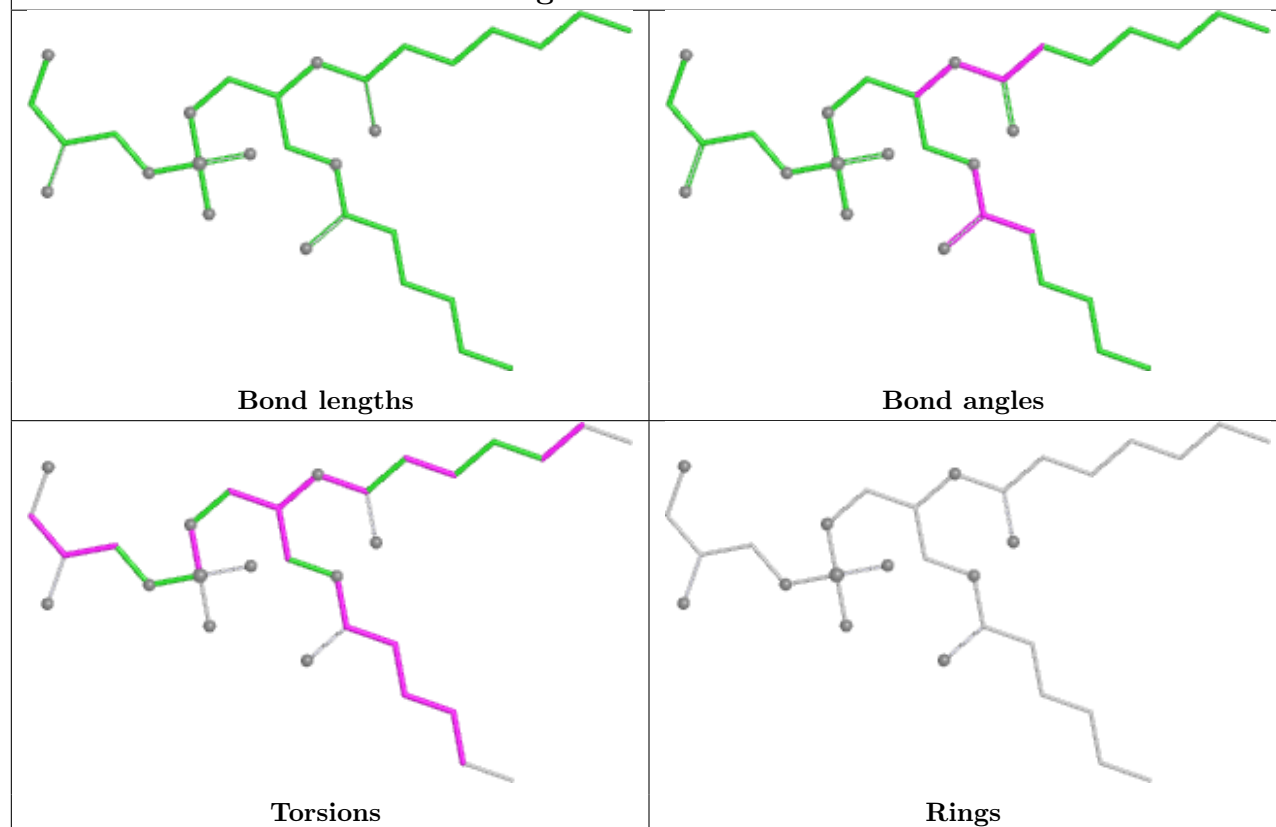




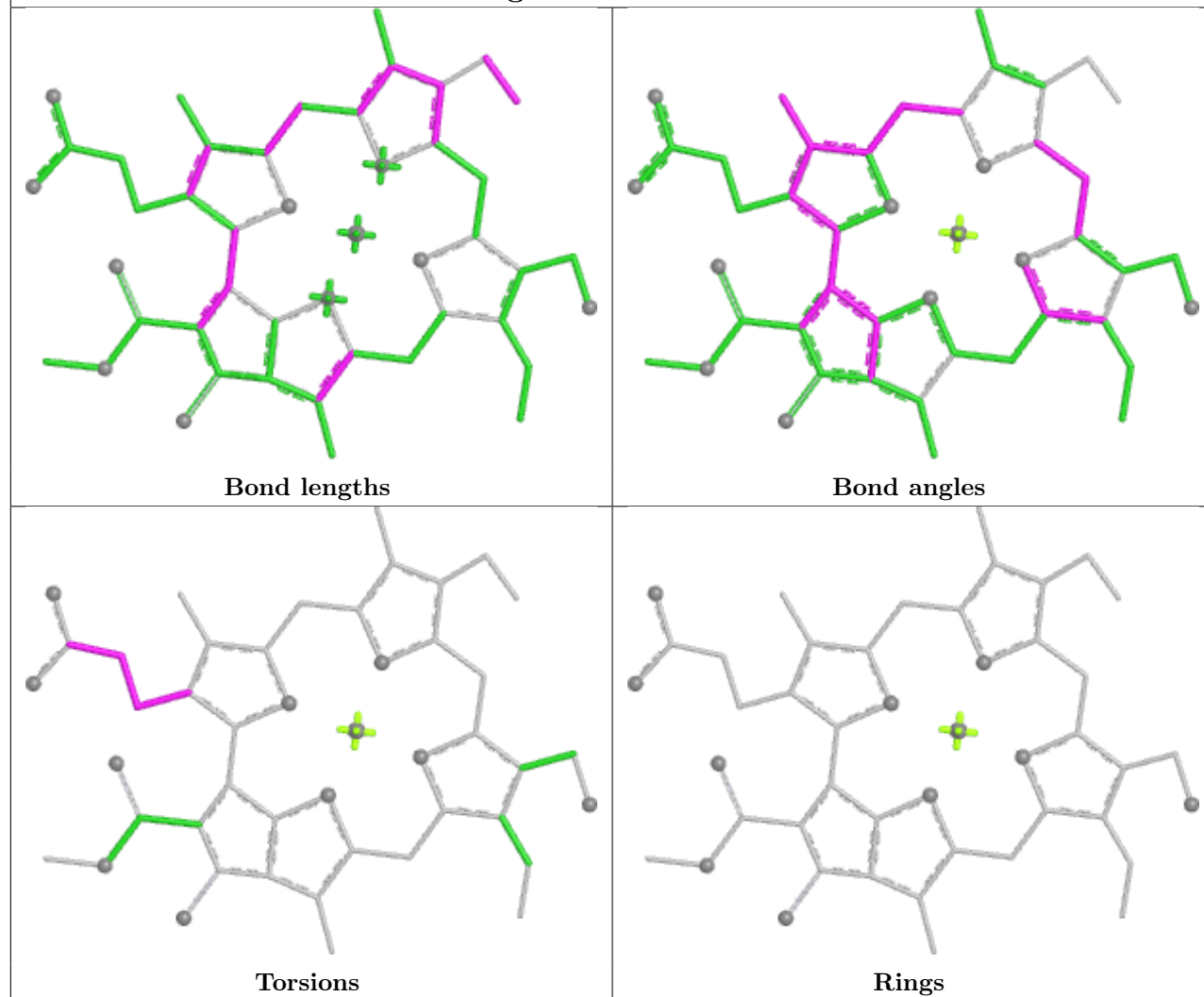
## Ligand CLA s 611



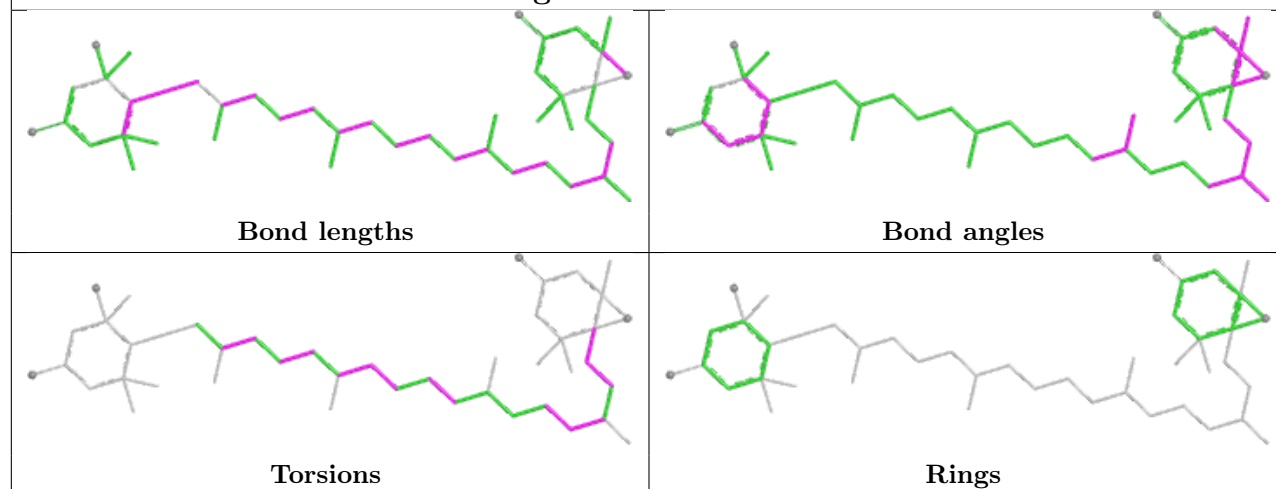
## Ligand LHG r 617

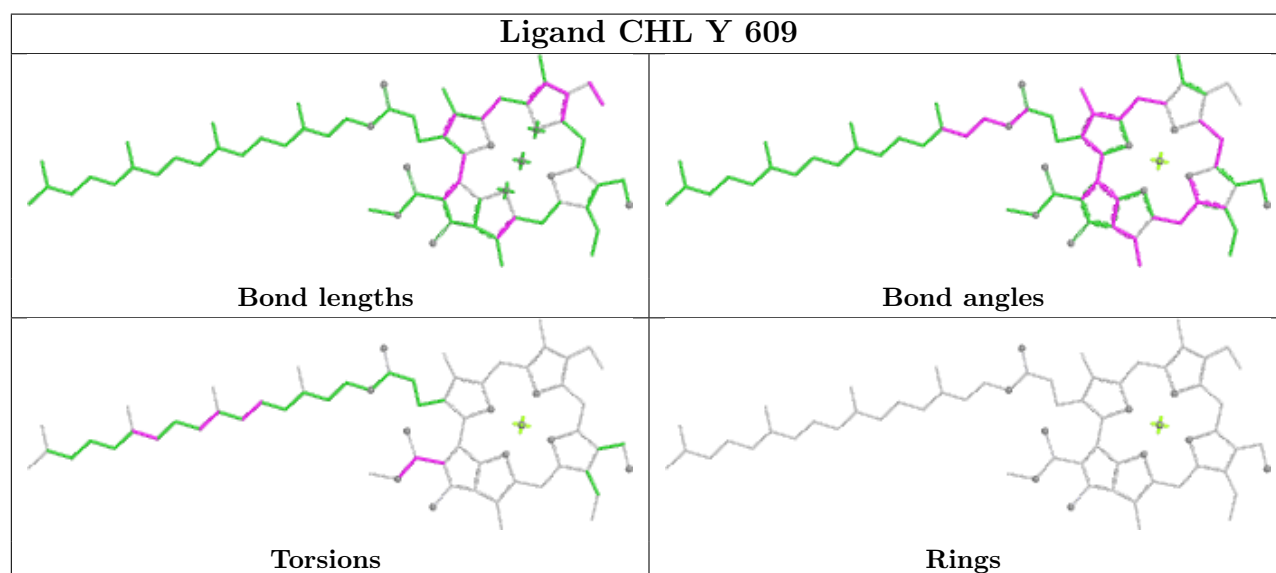
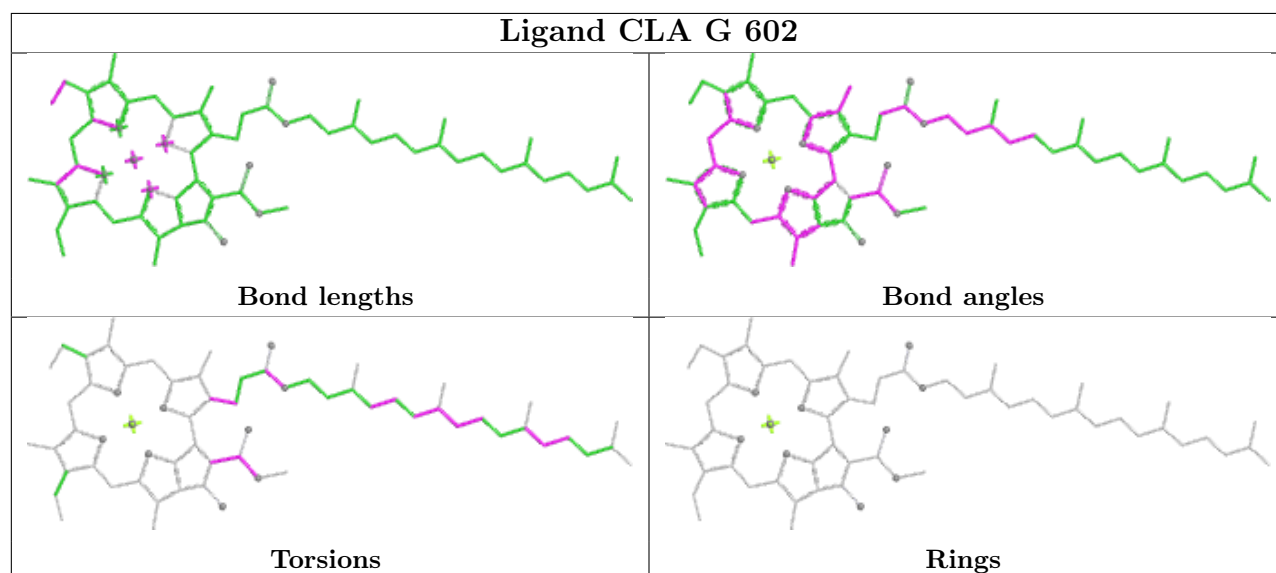
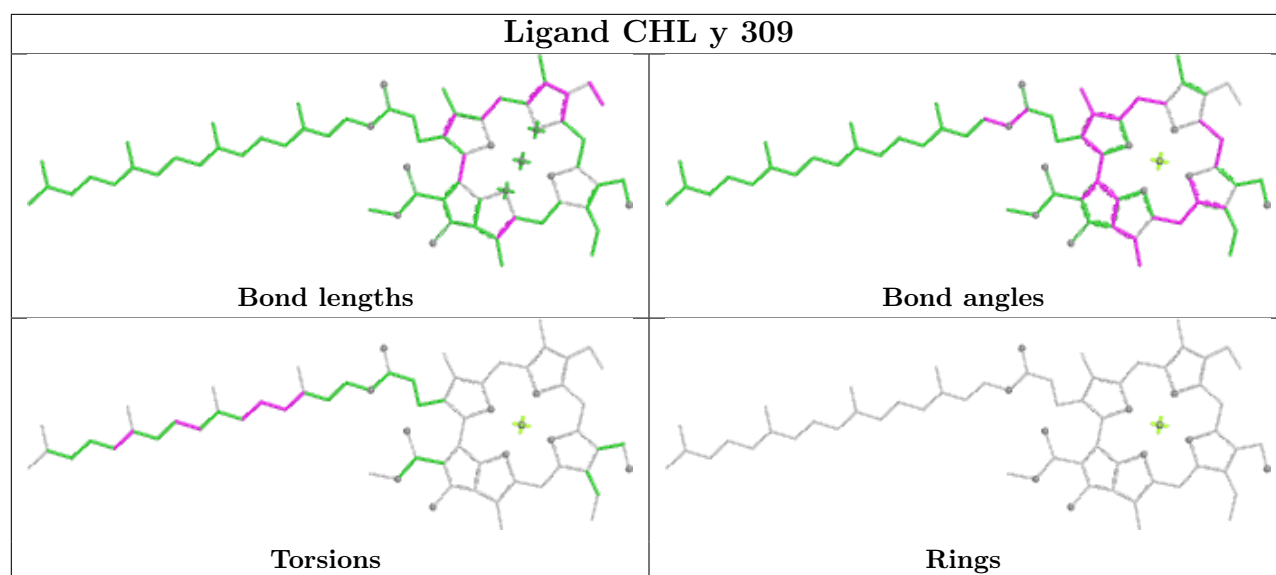


## Ligand CHL s 607

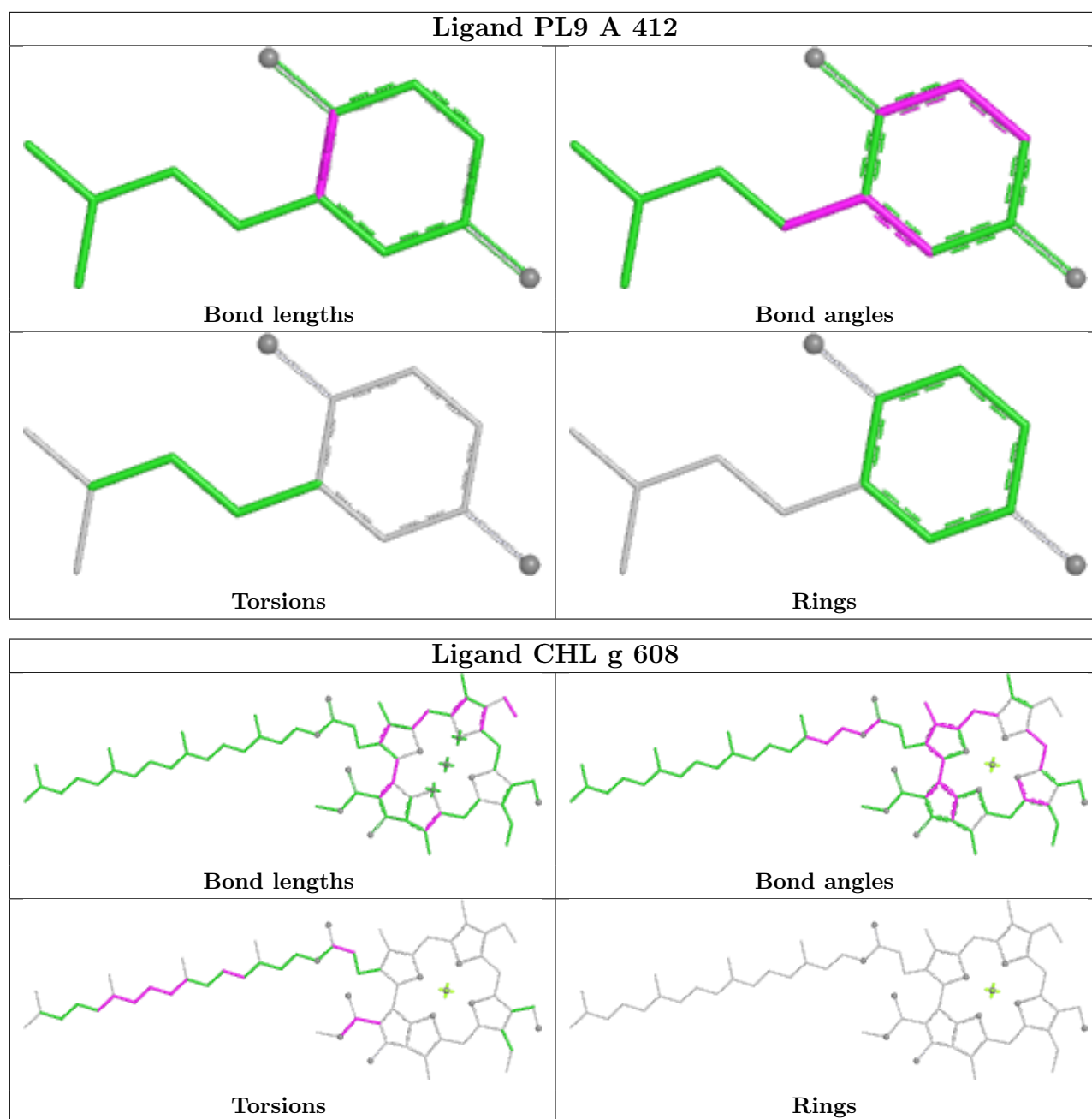


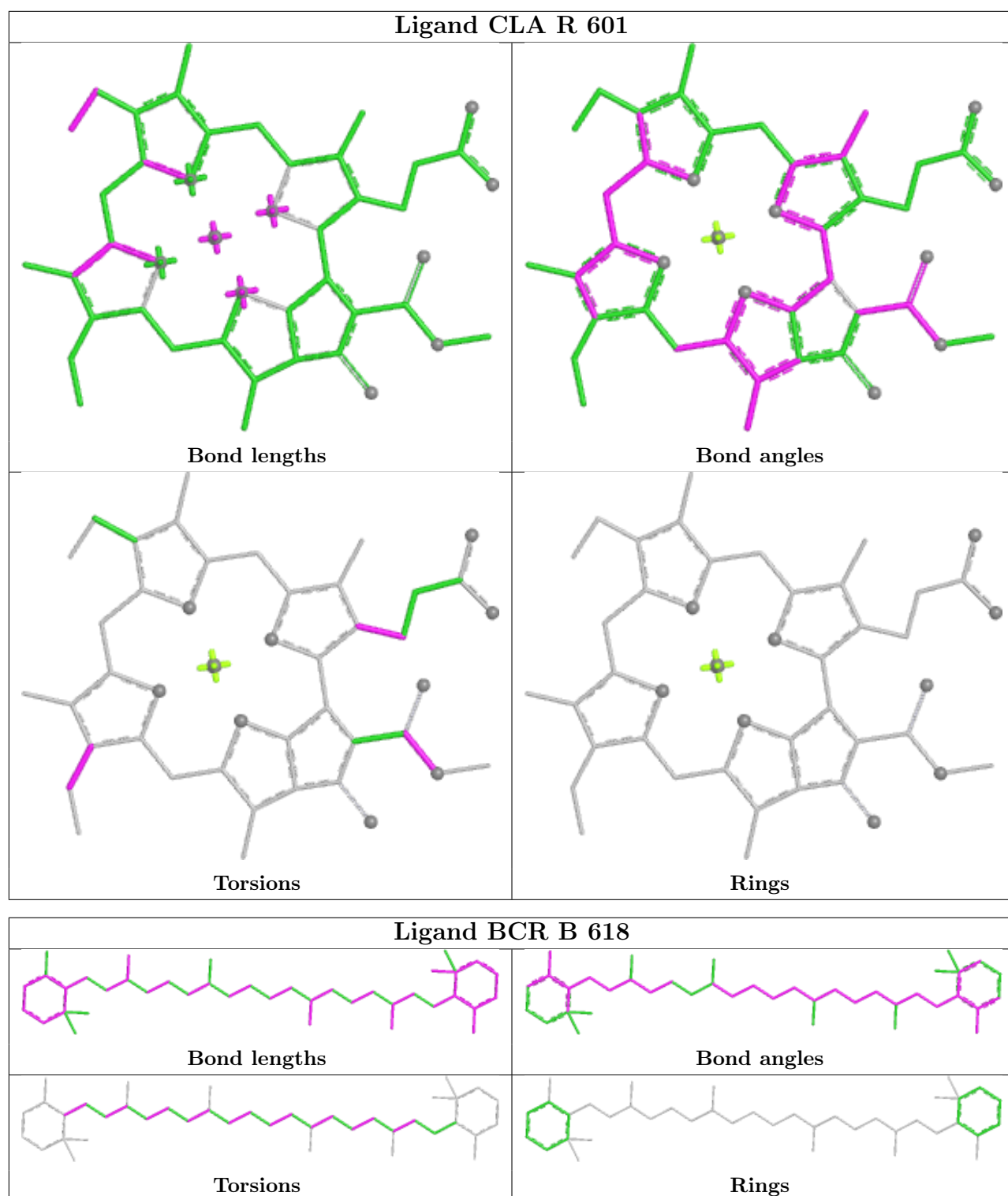
## Ligand NEX n 617

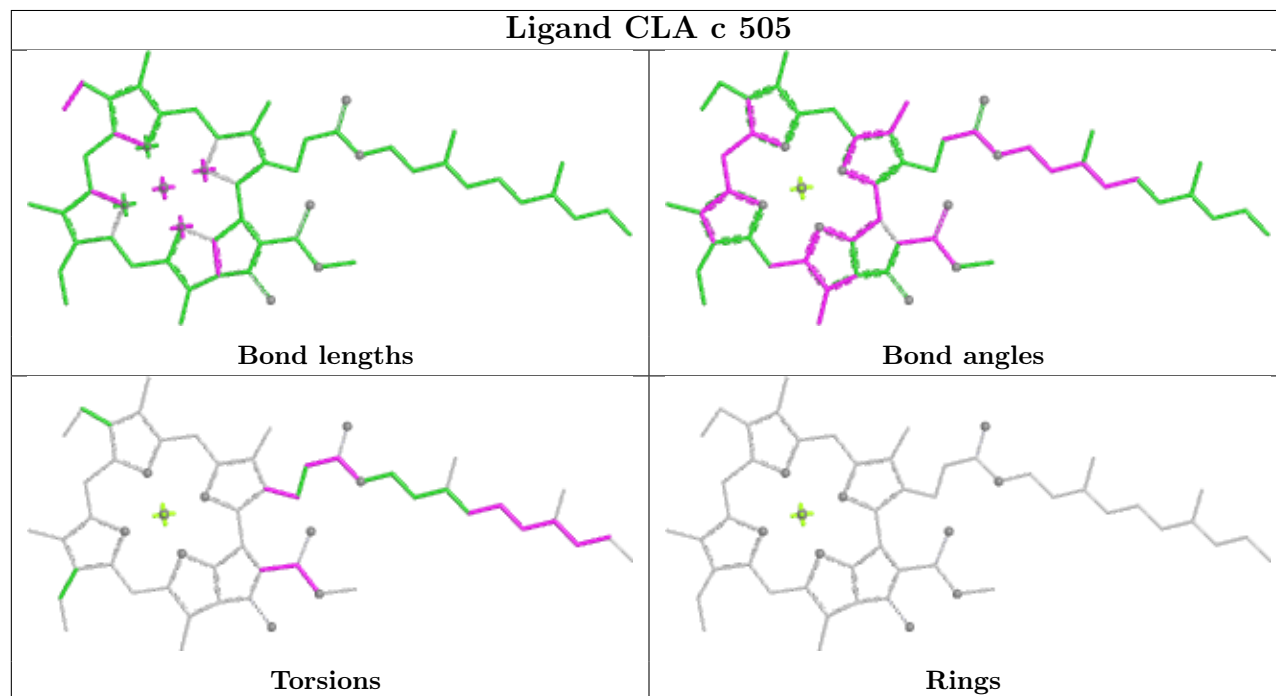
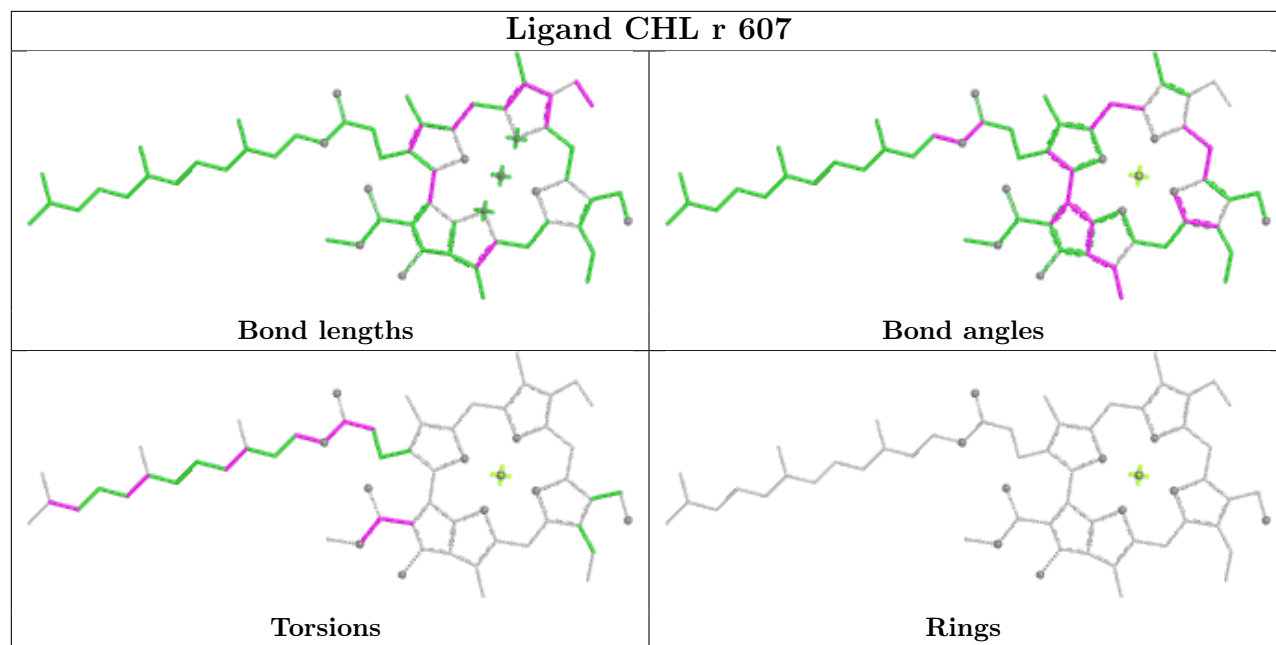


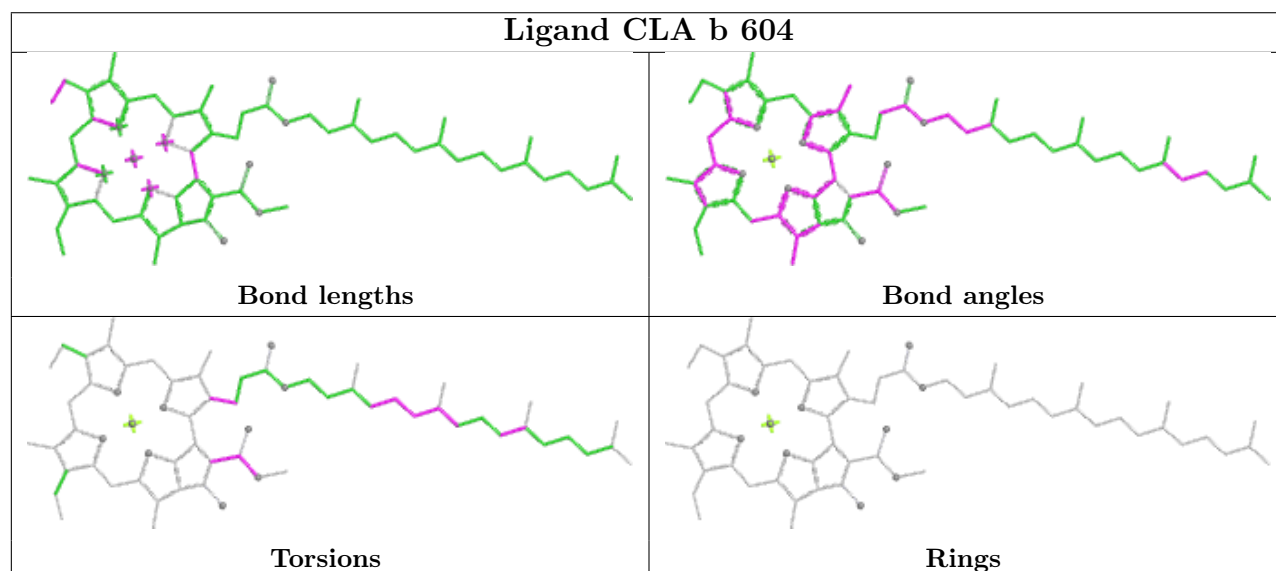
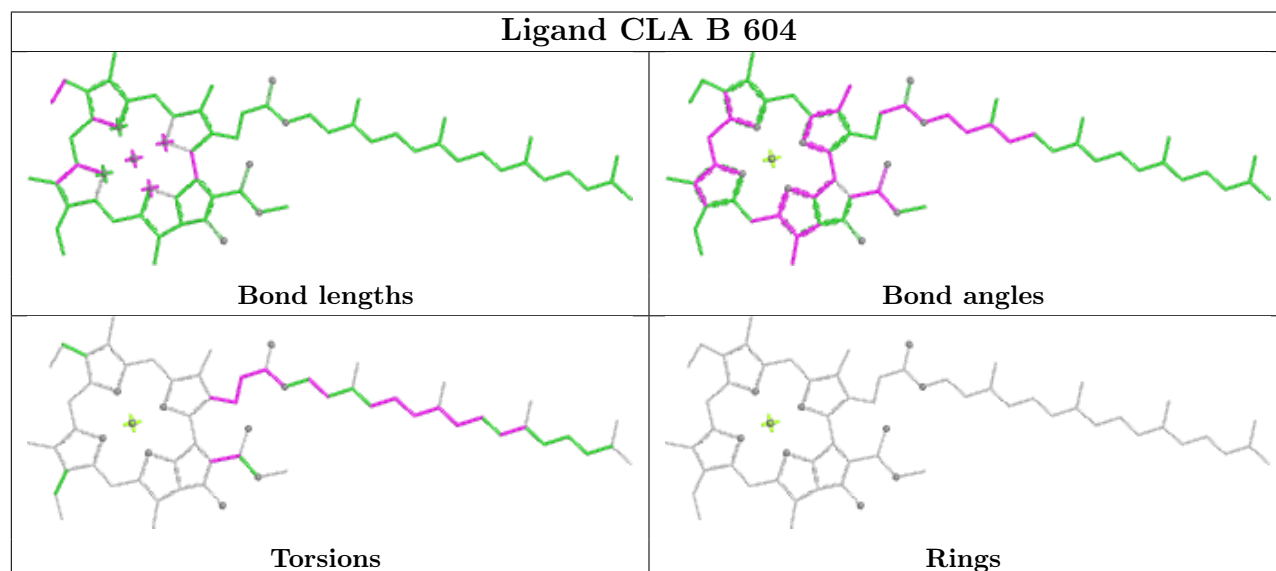
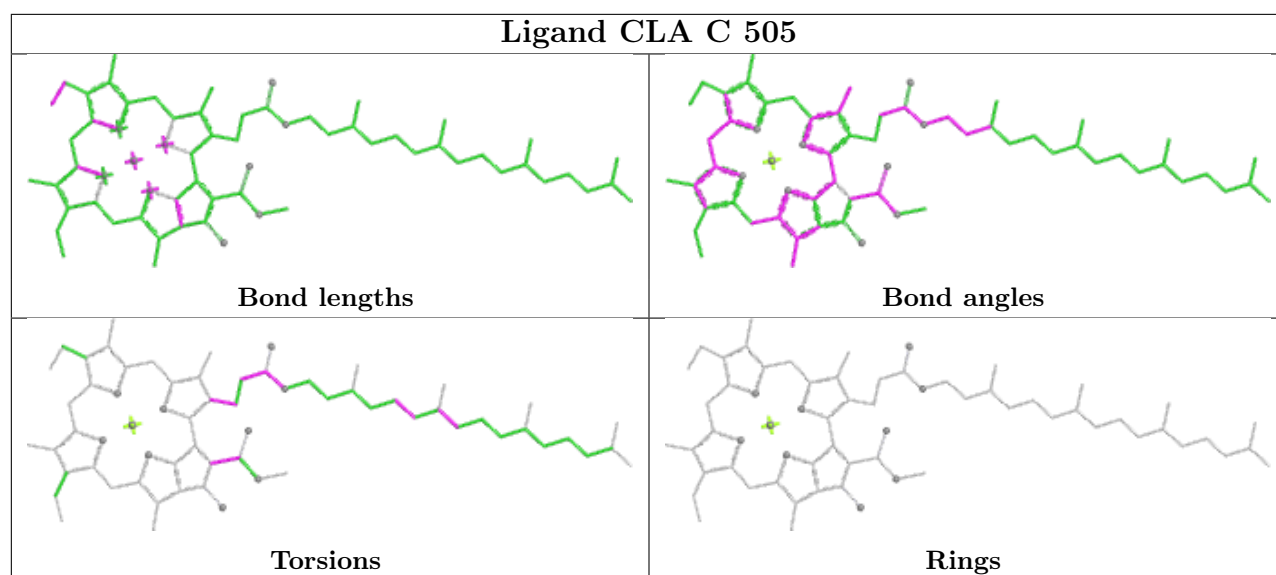




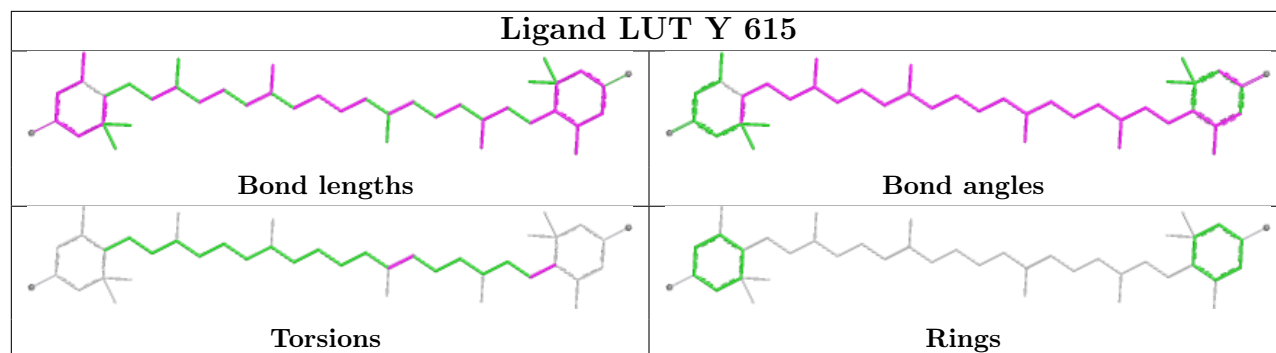




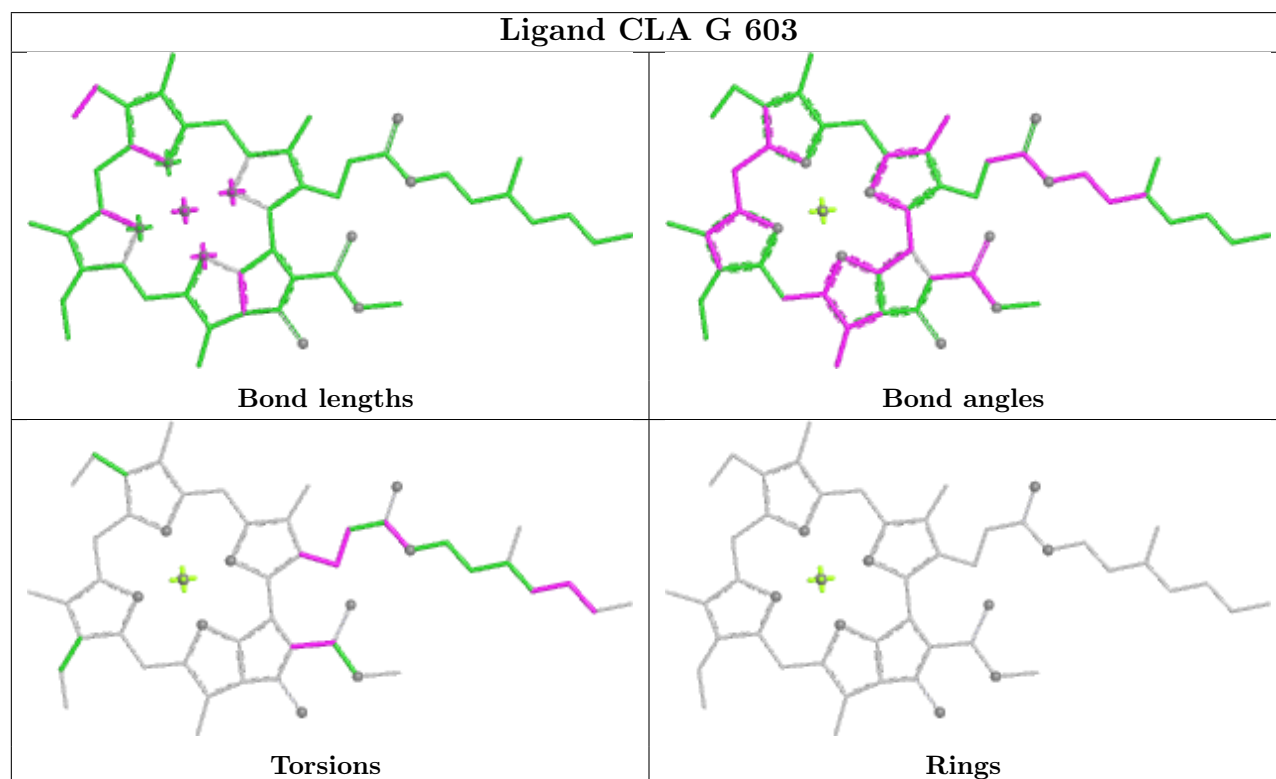




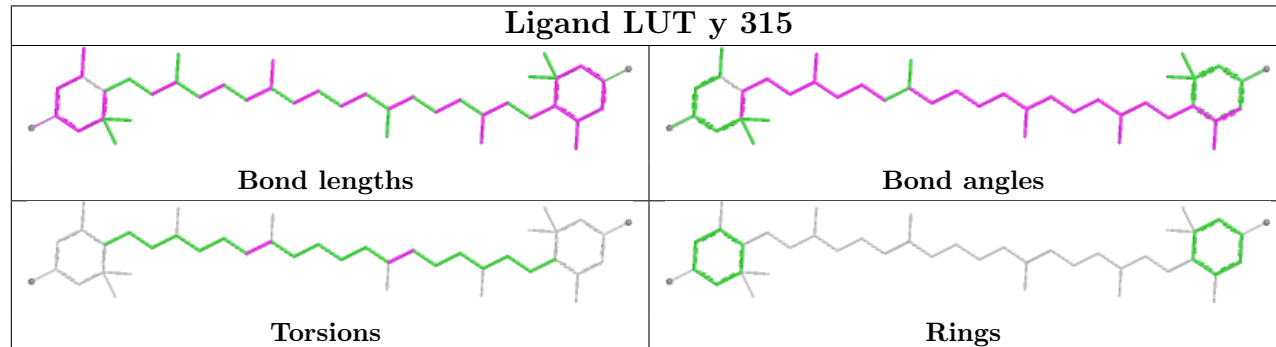
## Ligand LUT Y 615

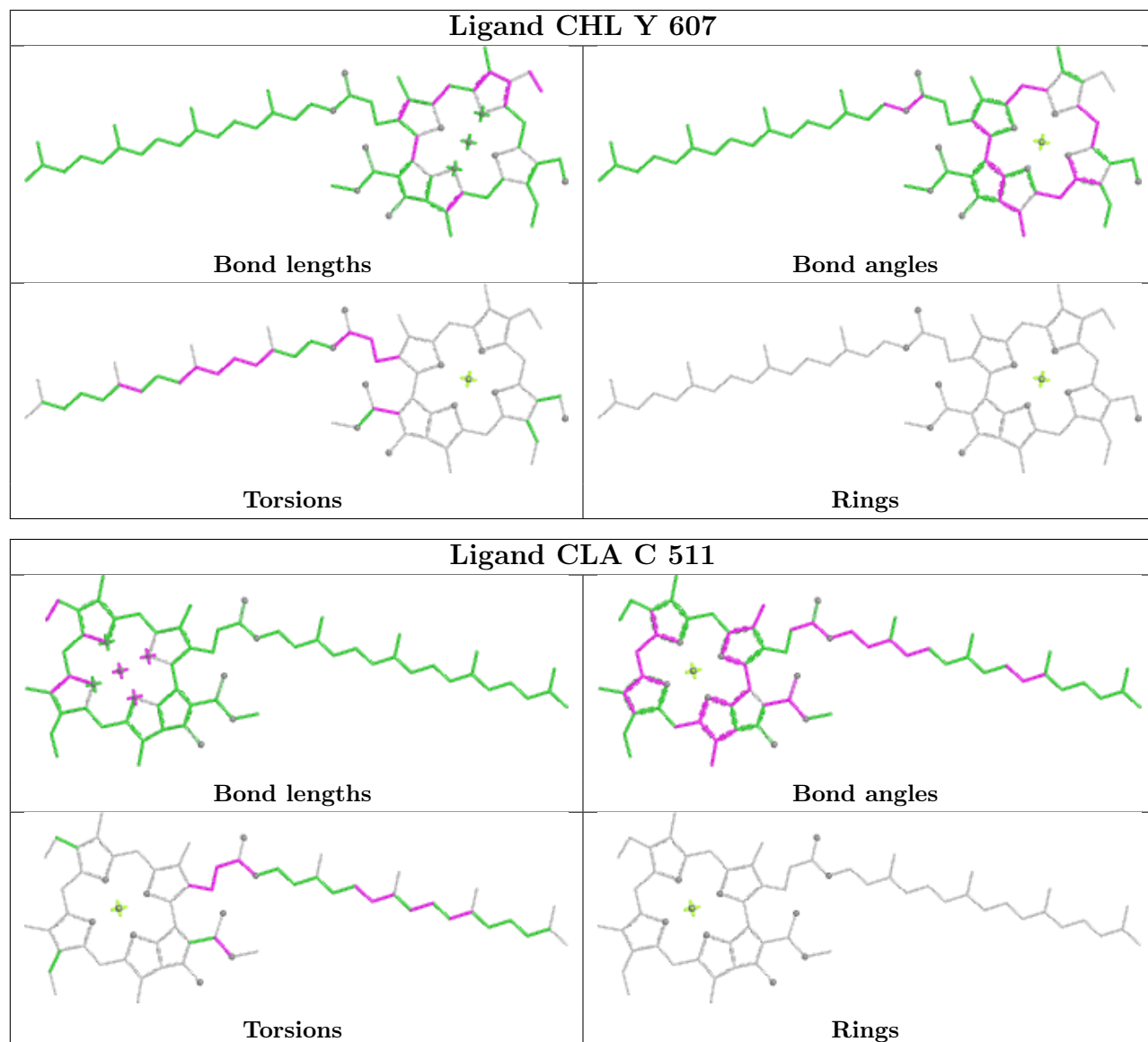


## Ligand CLA G 603

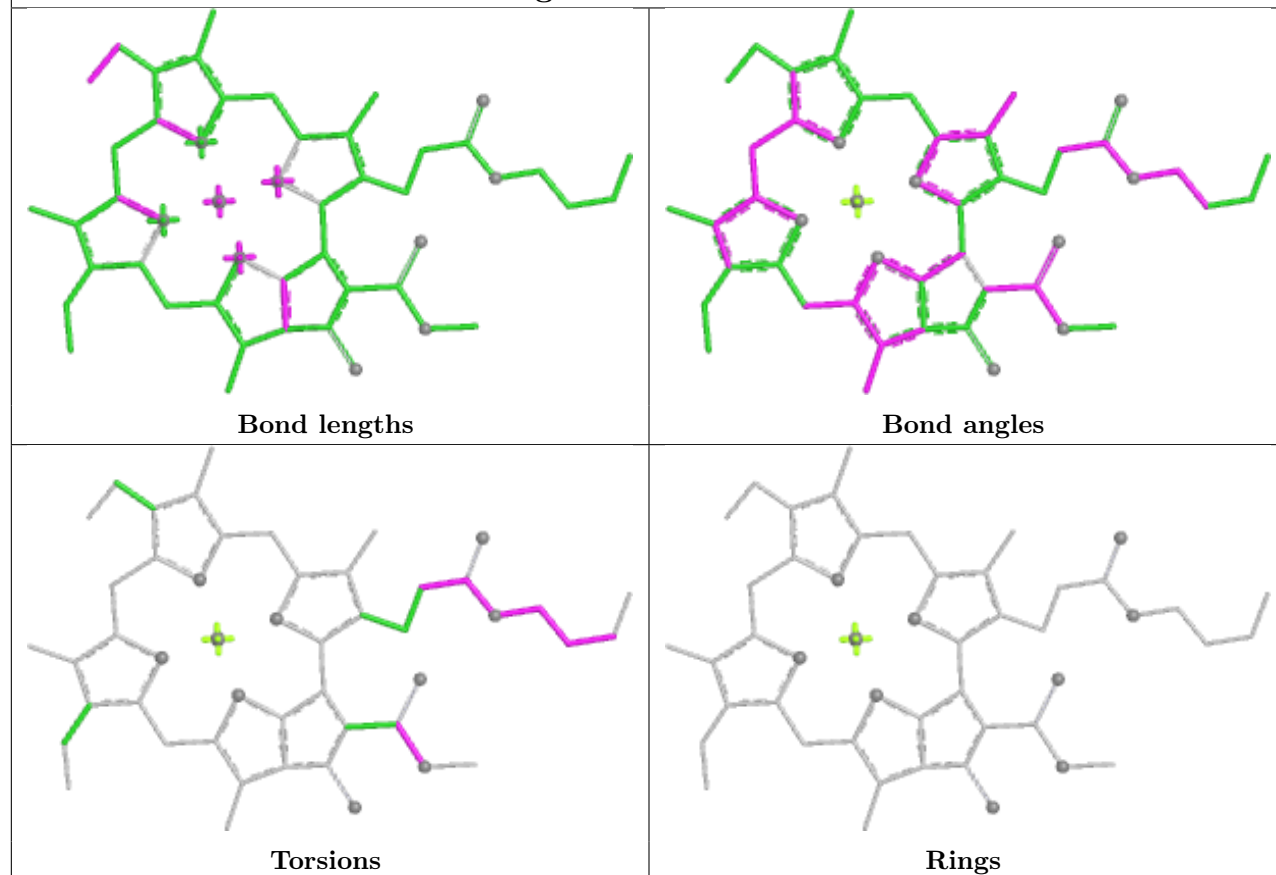


## Ligand LUT y 315

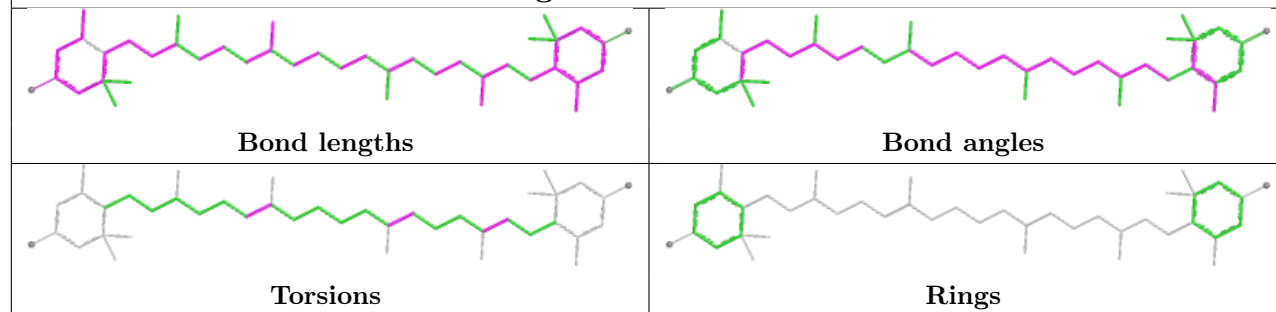


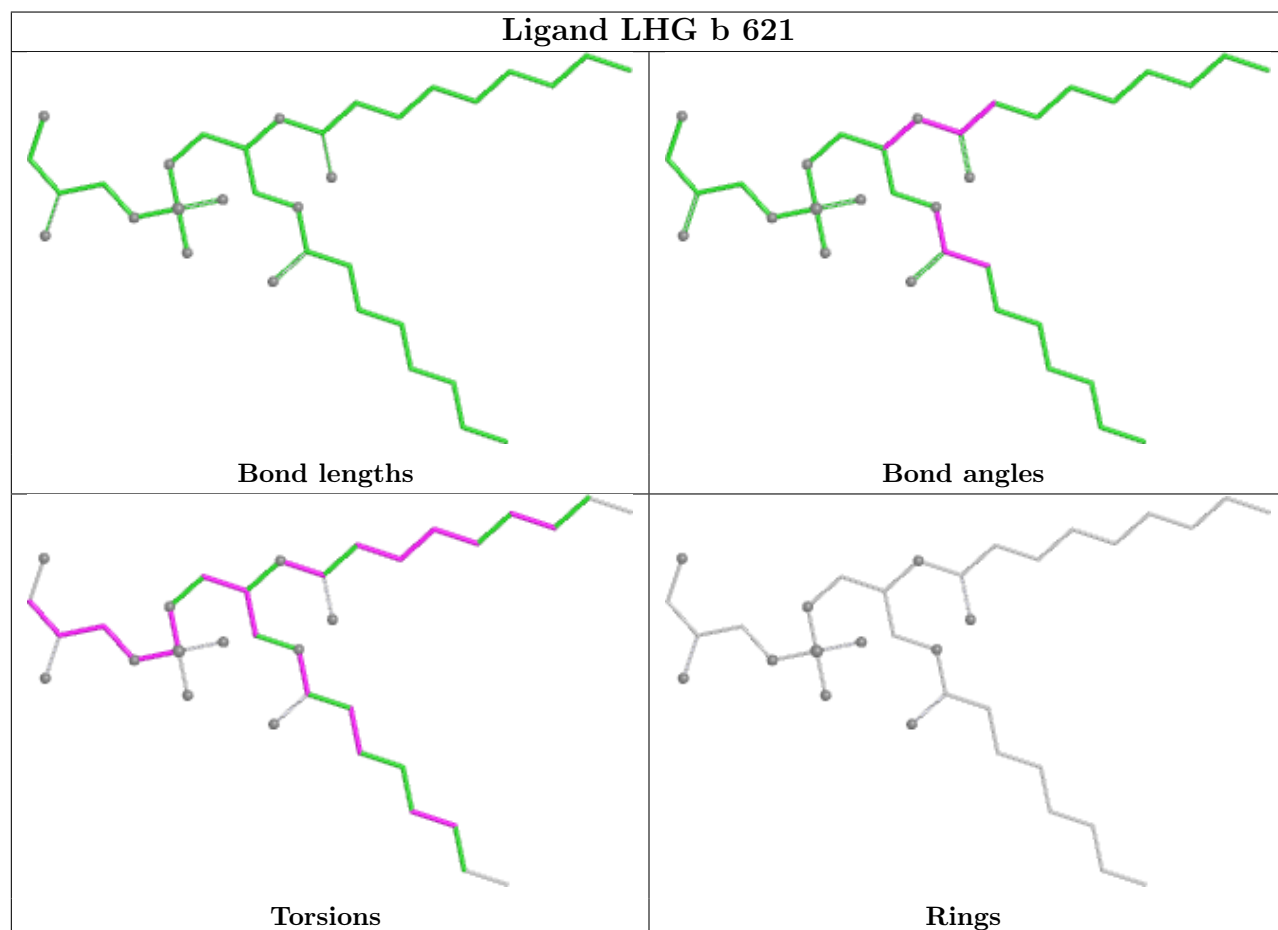
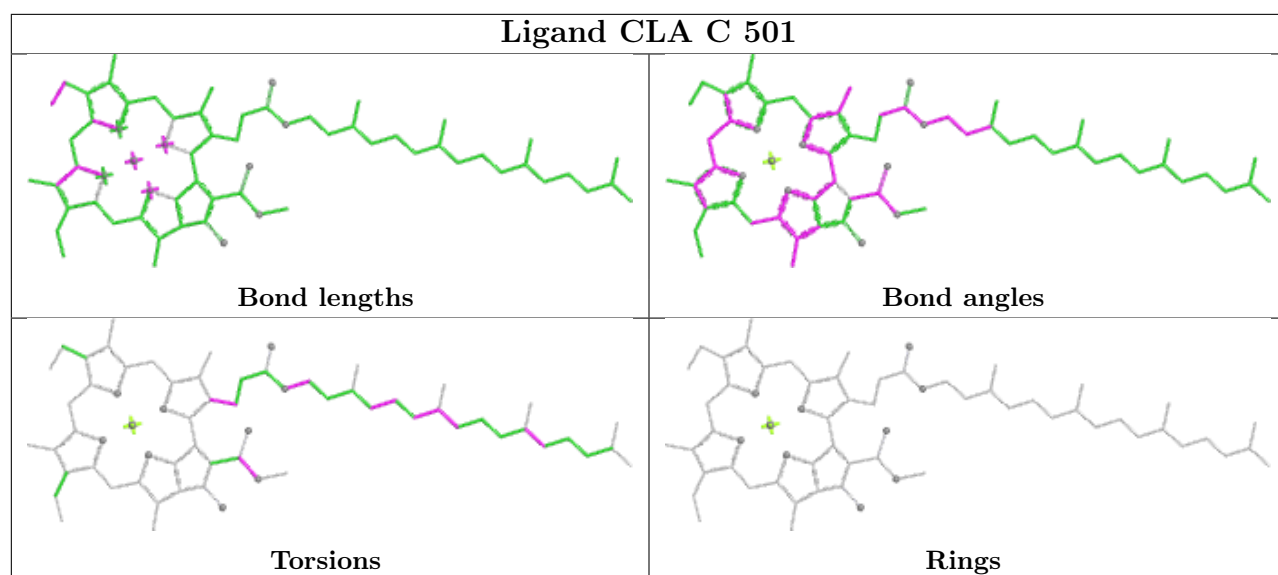


## Ligand CLA S 312



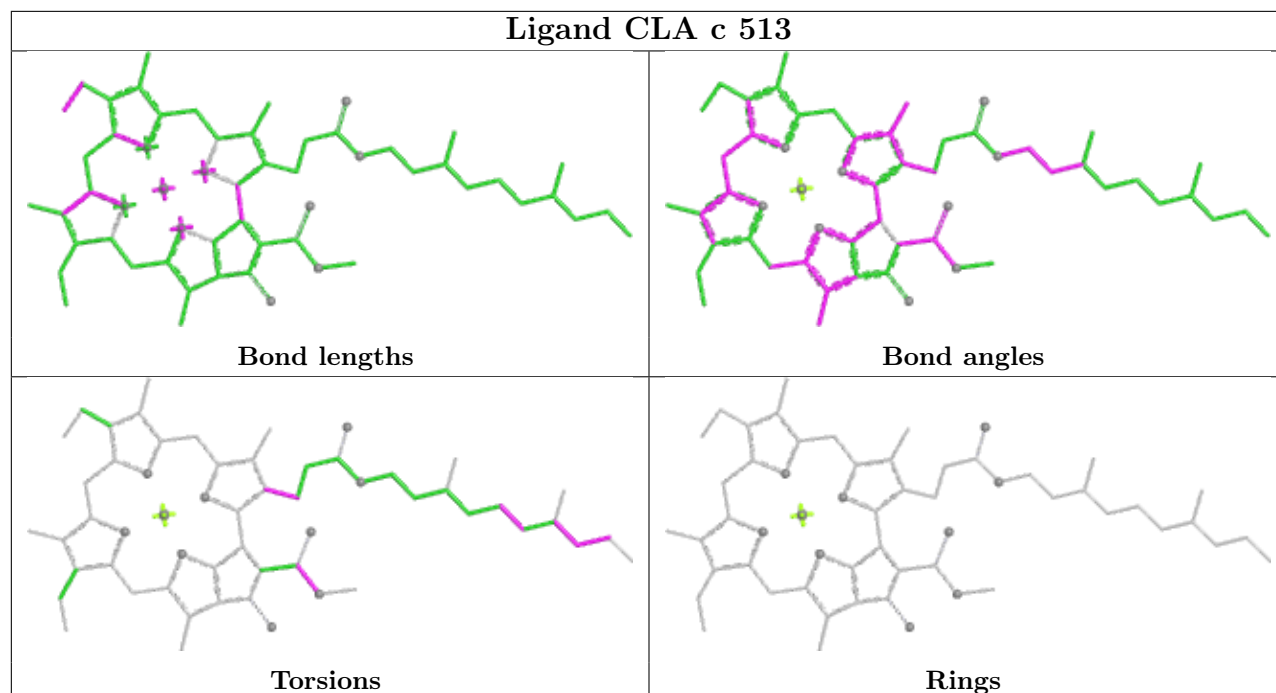
## Ligand LUT S 316



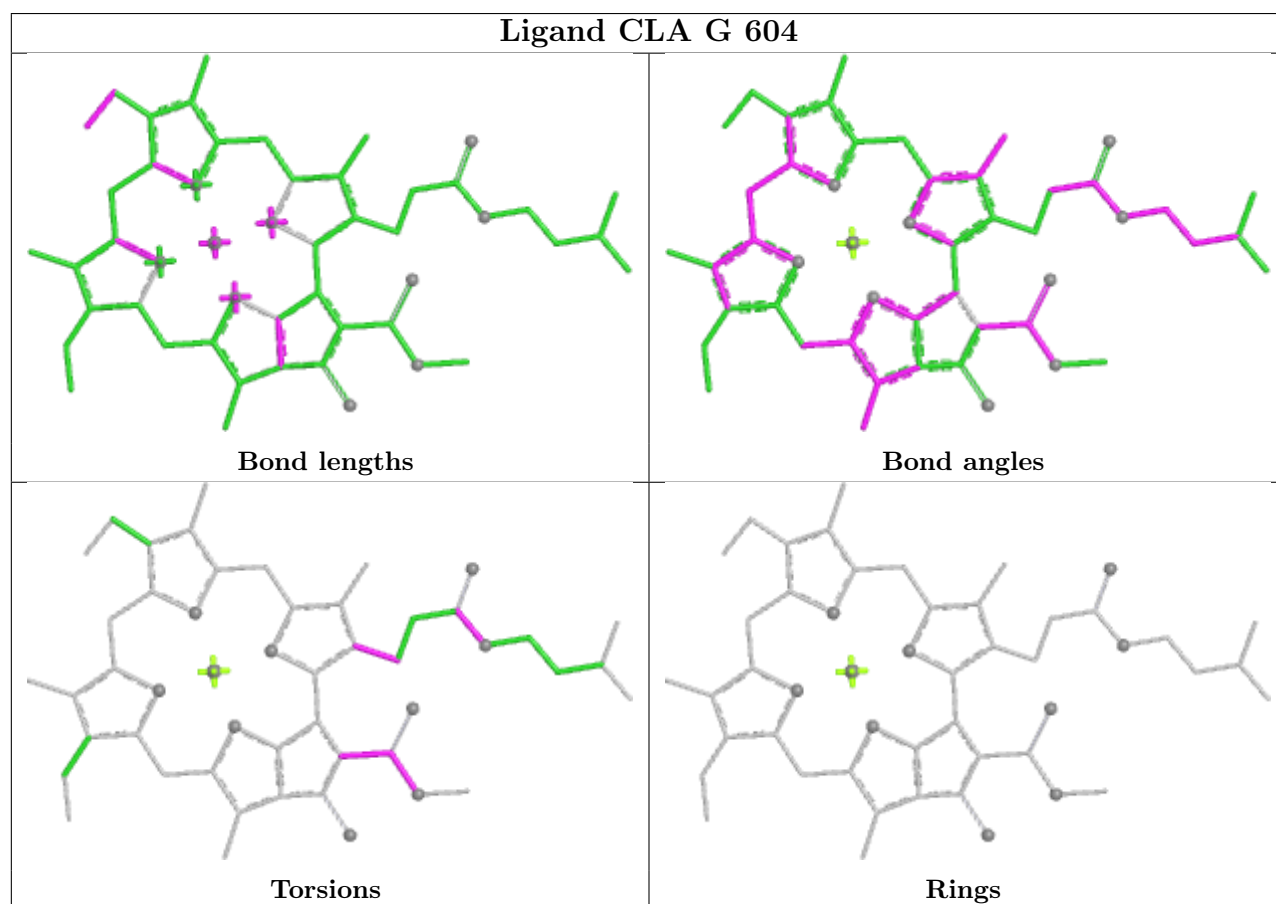


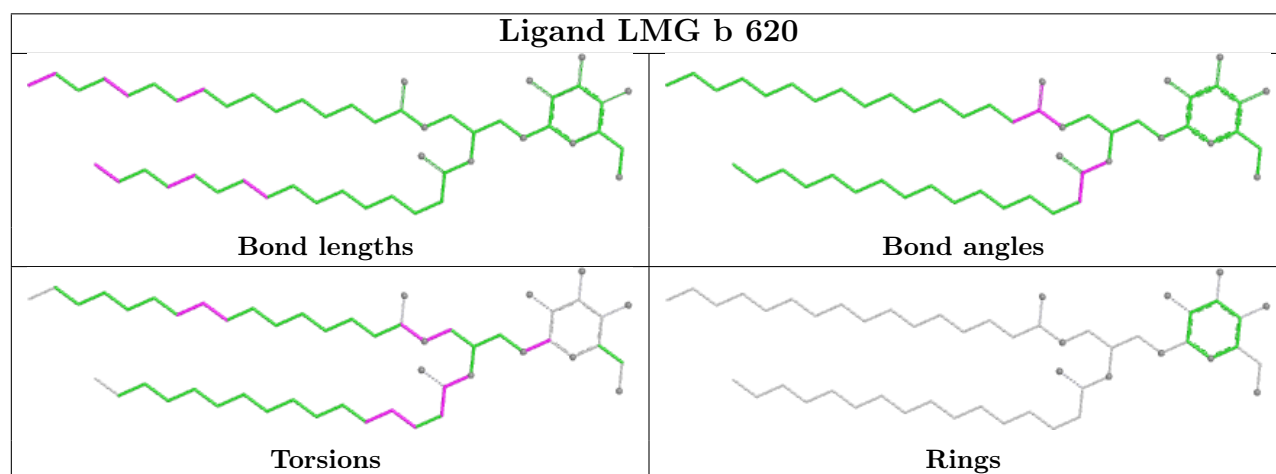
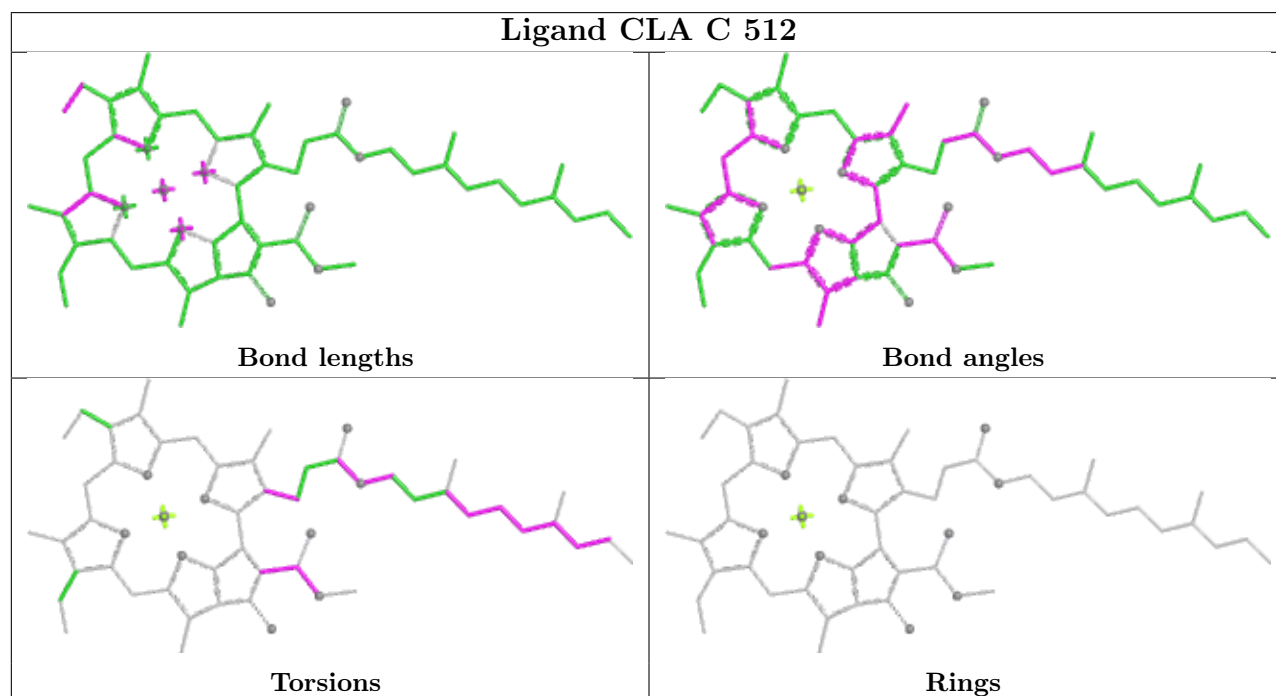
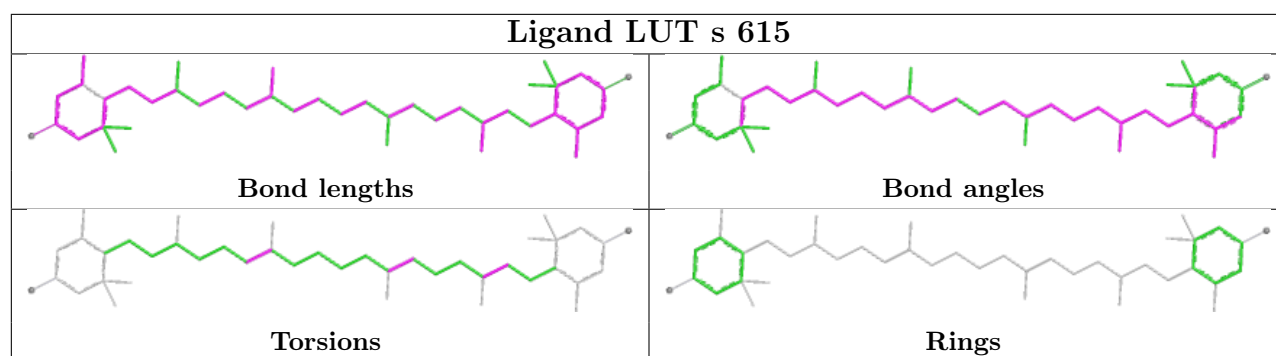


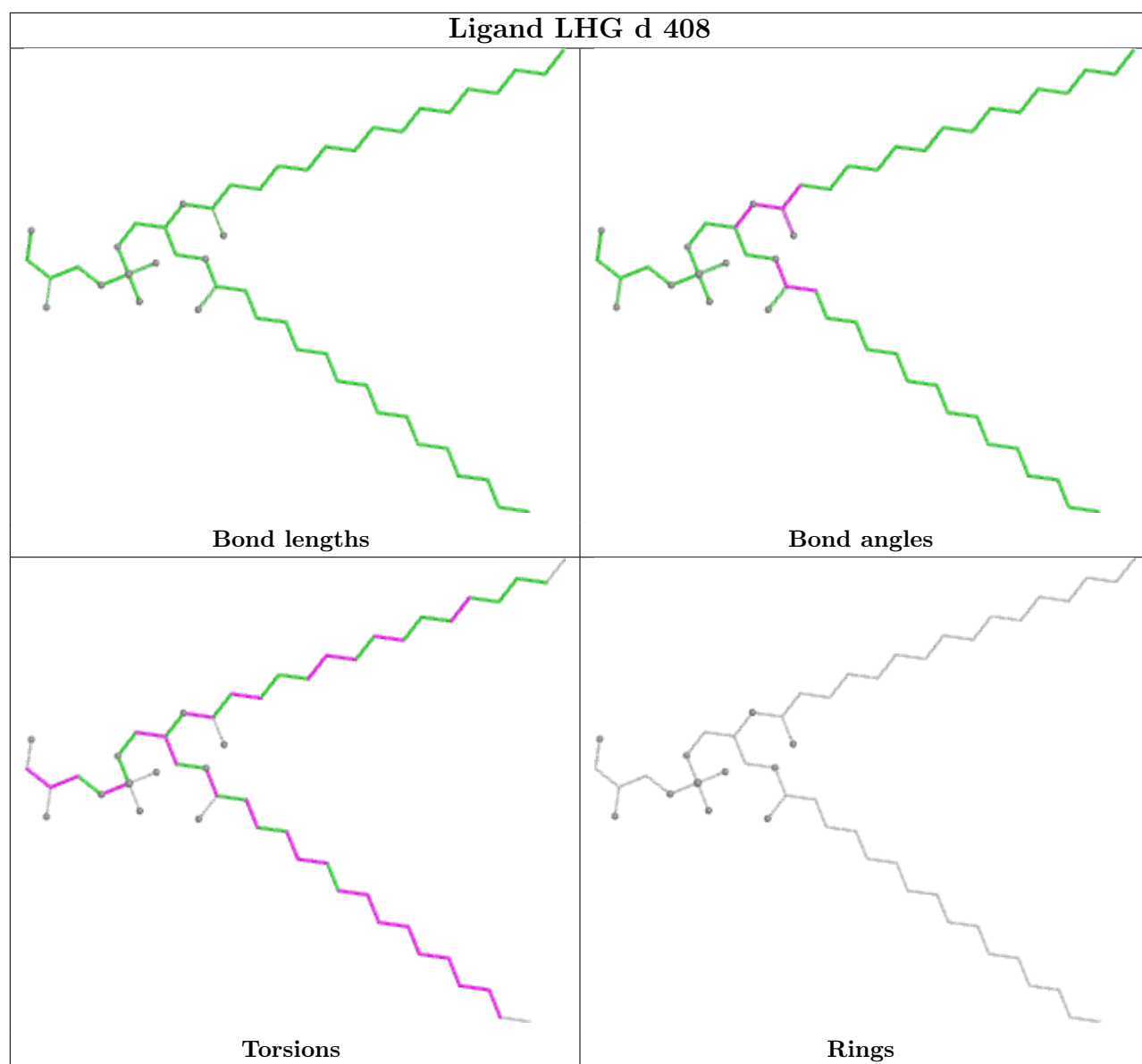
## Ligand CLA c 513

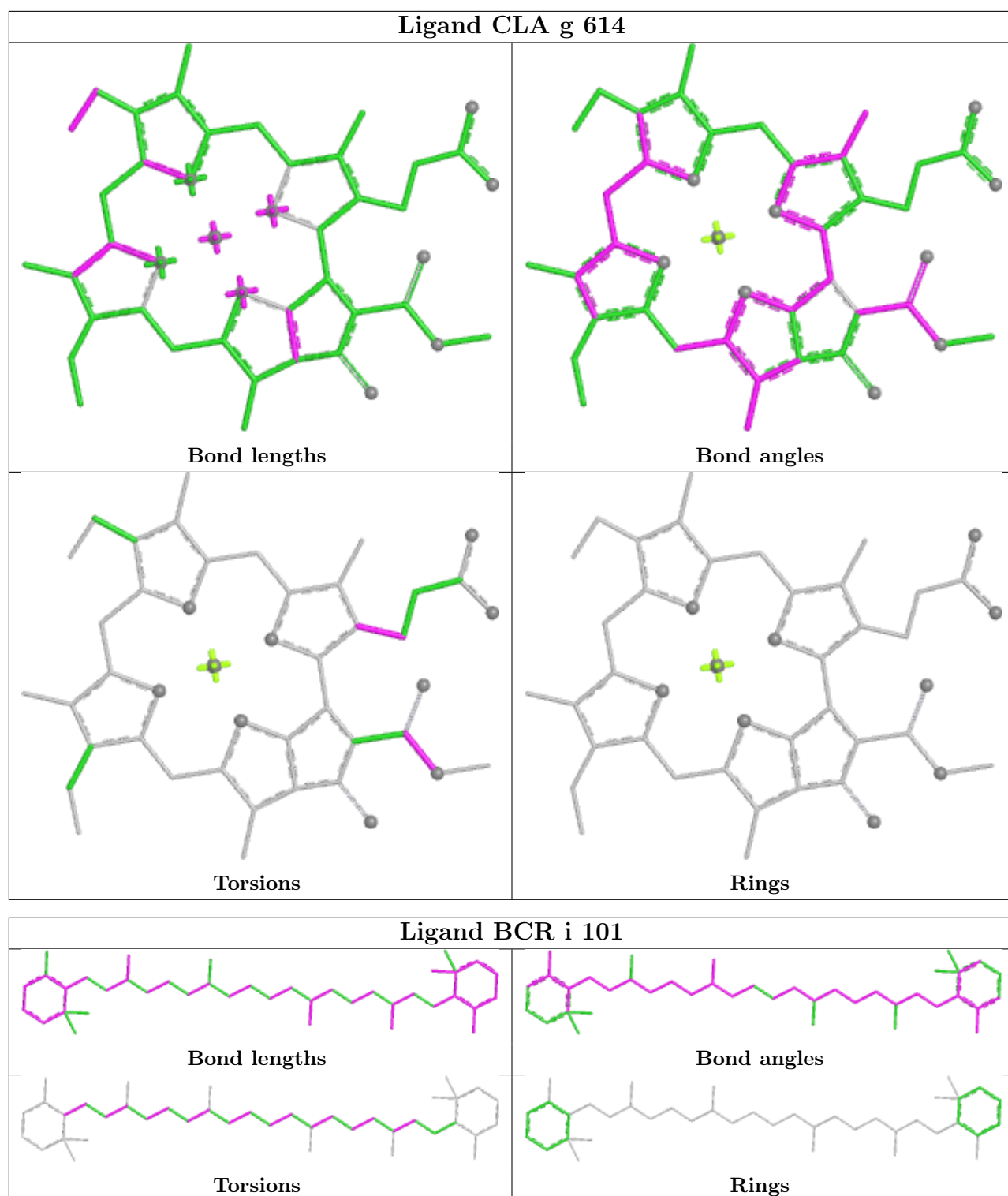


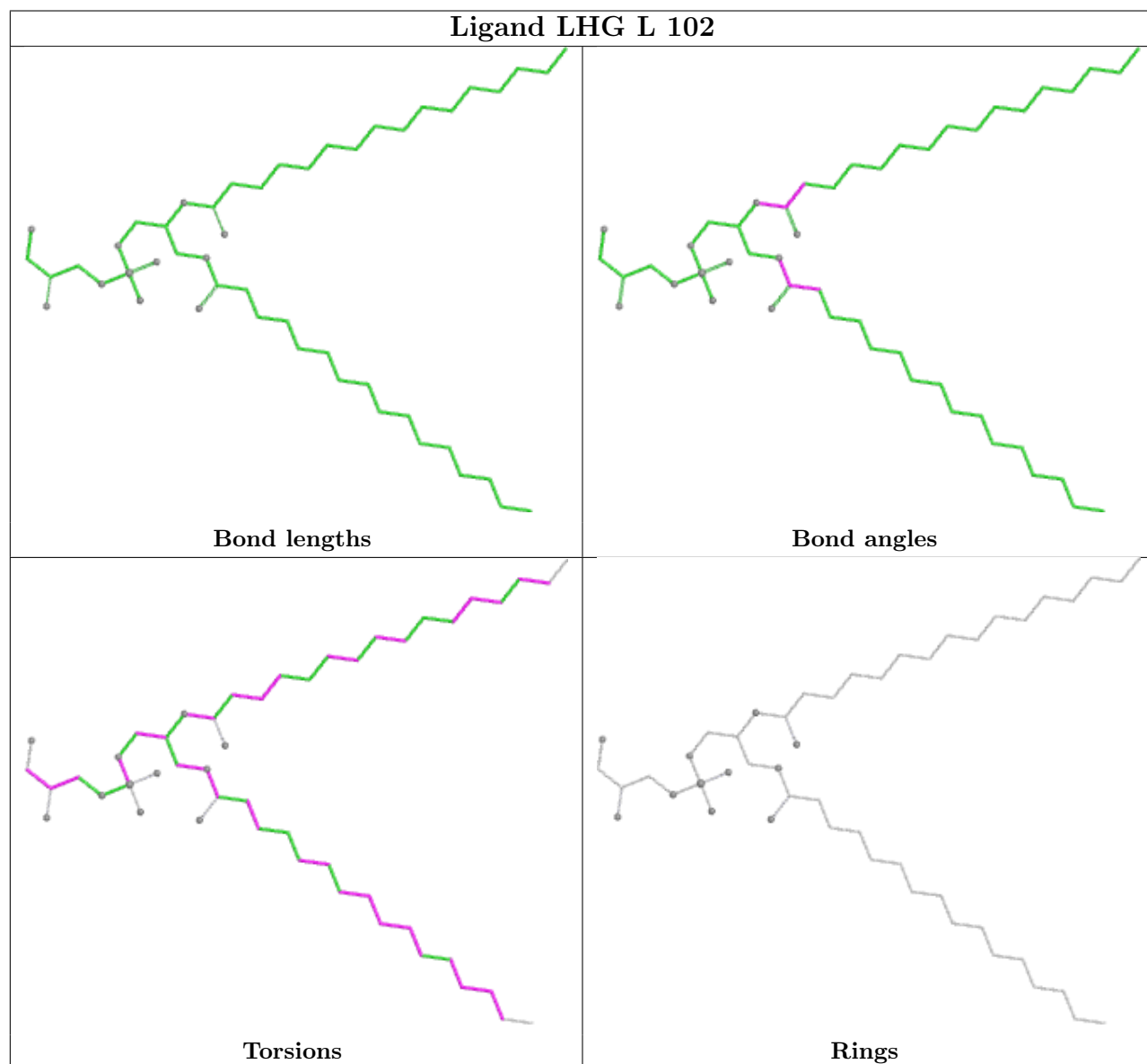
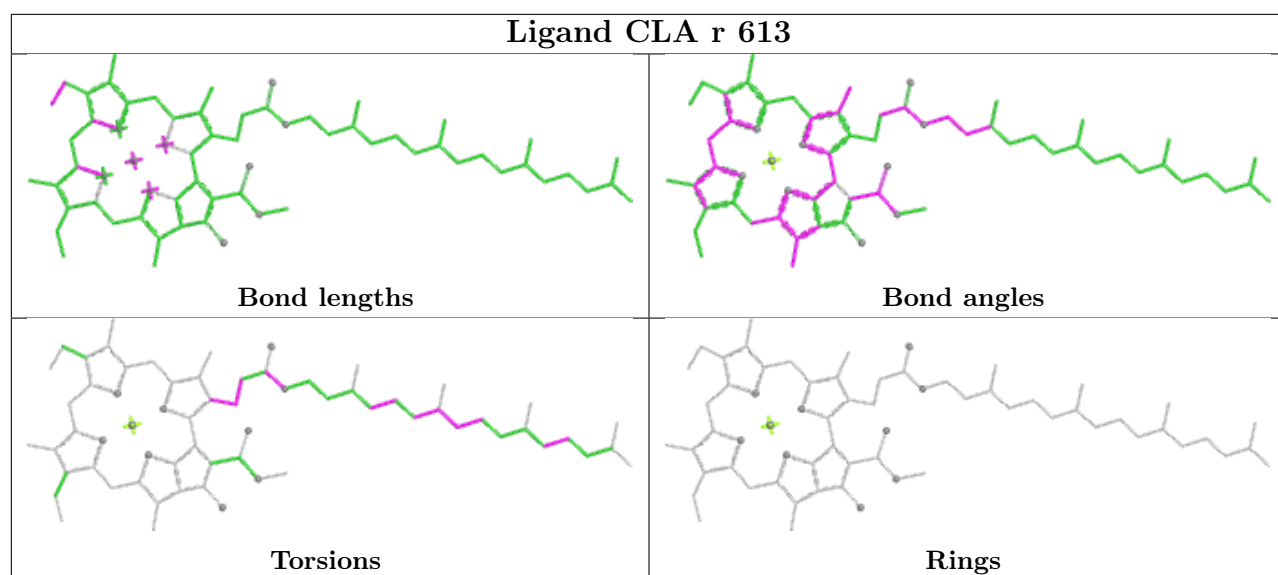
## Ligand CLA G 604



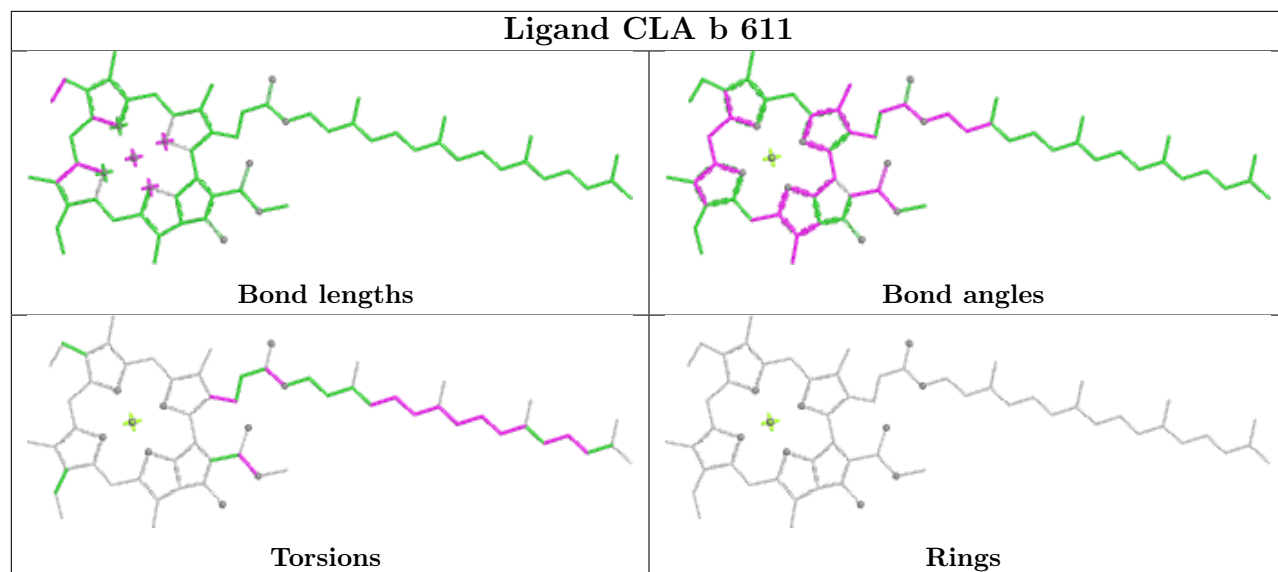




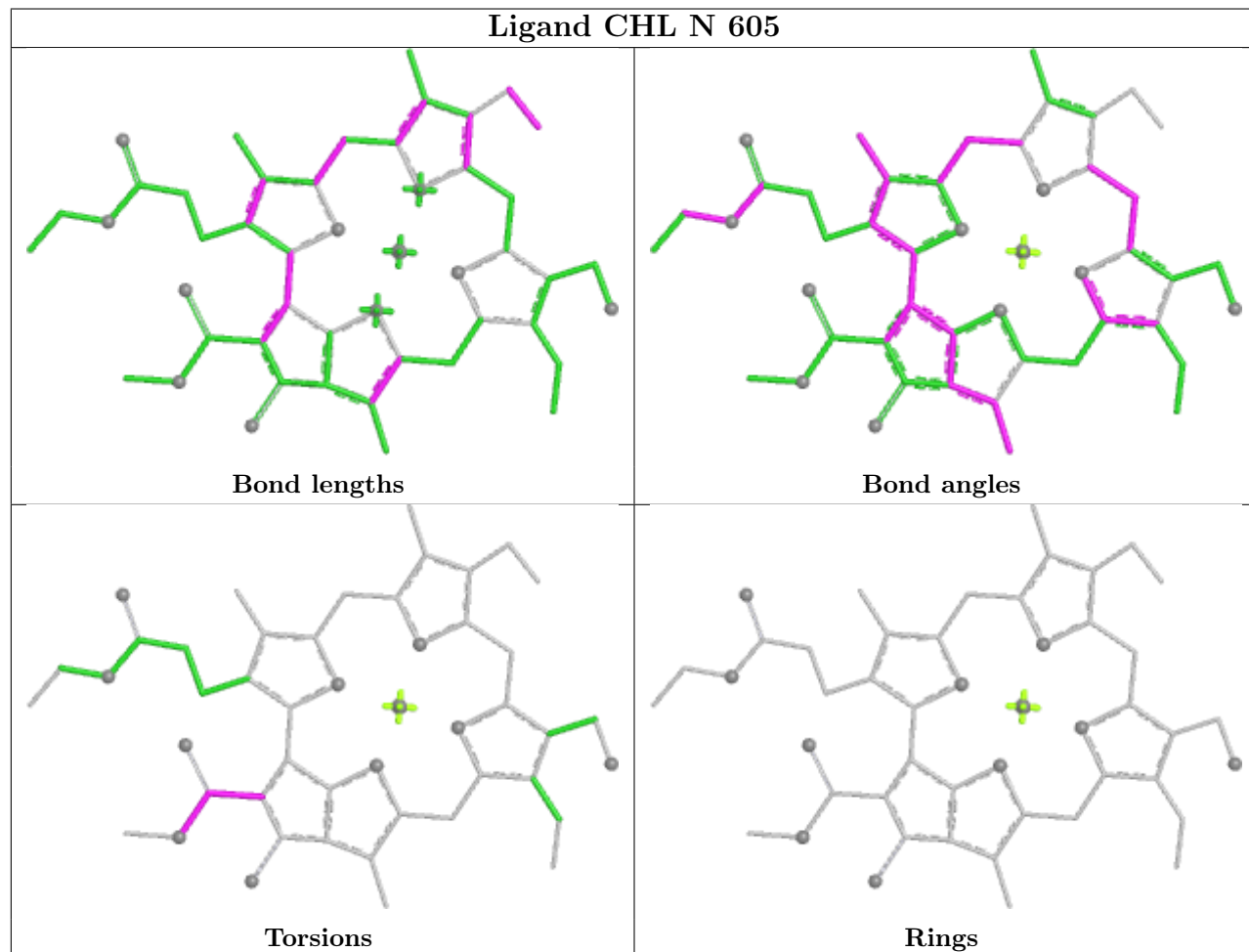


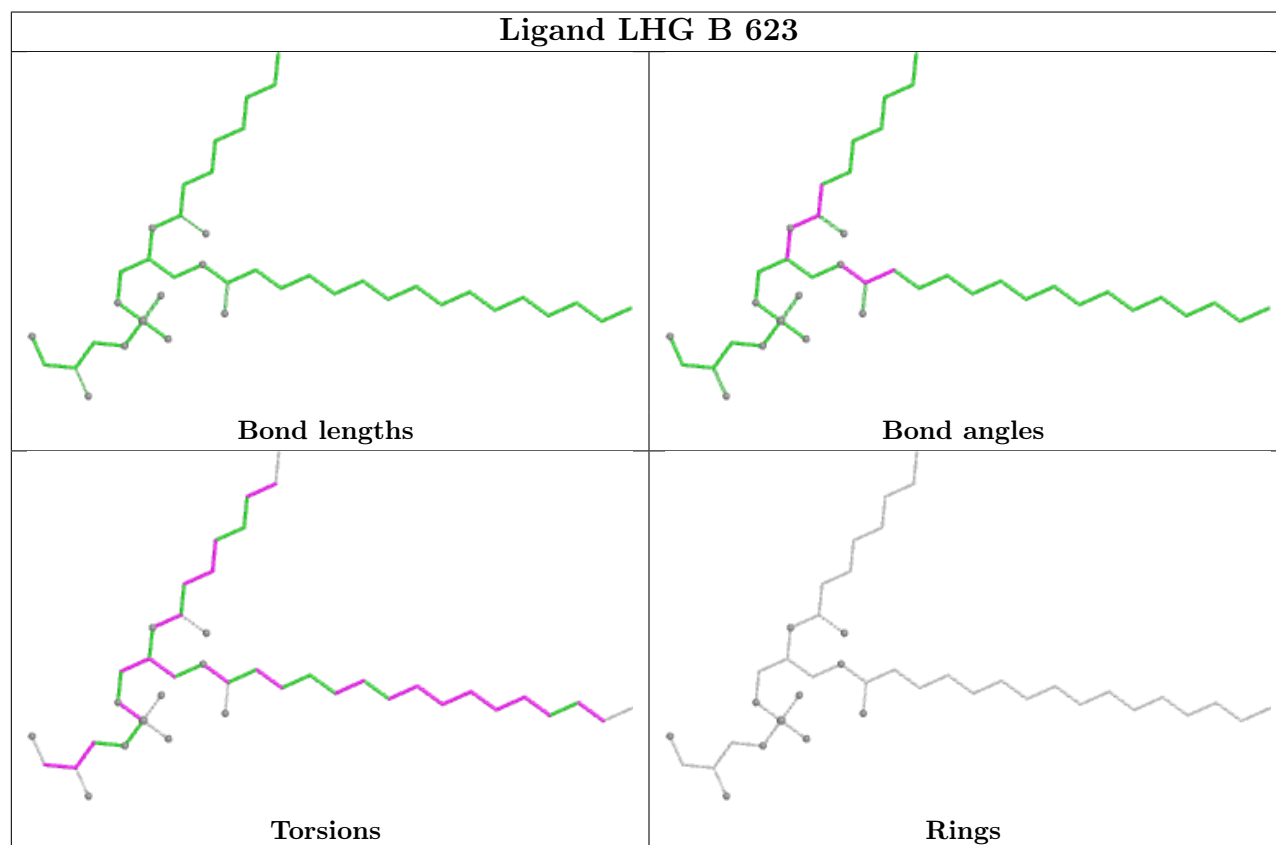
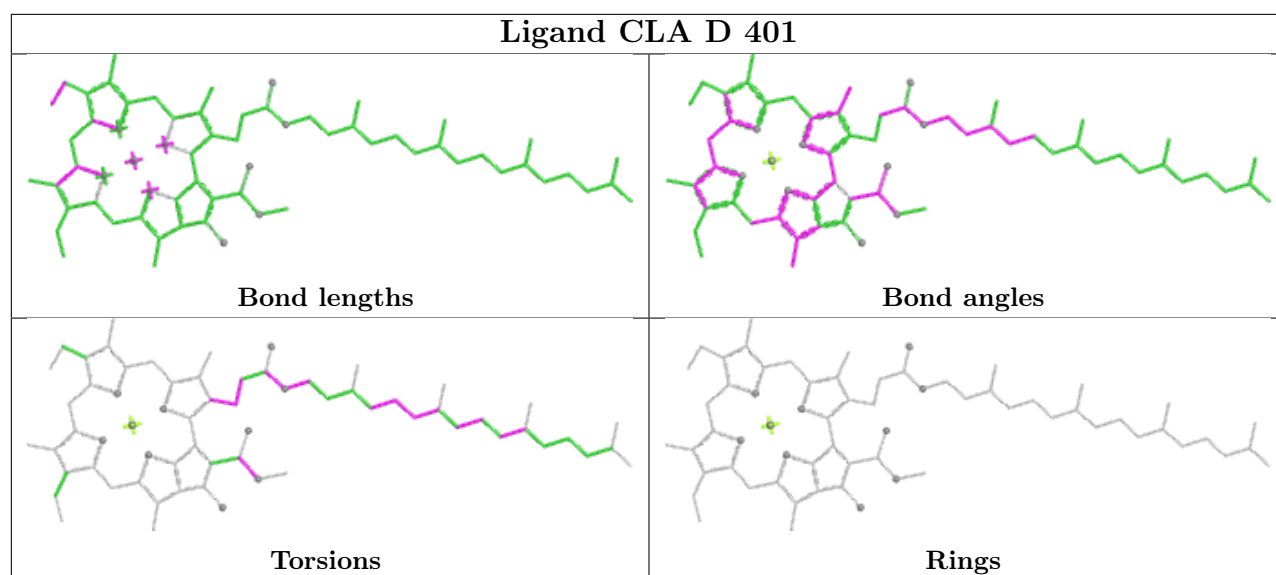


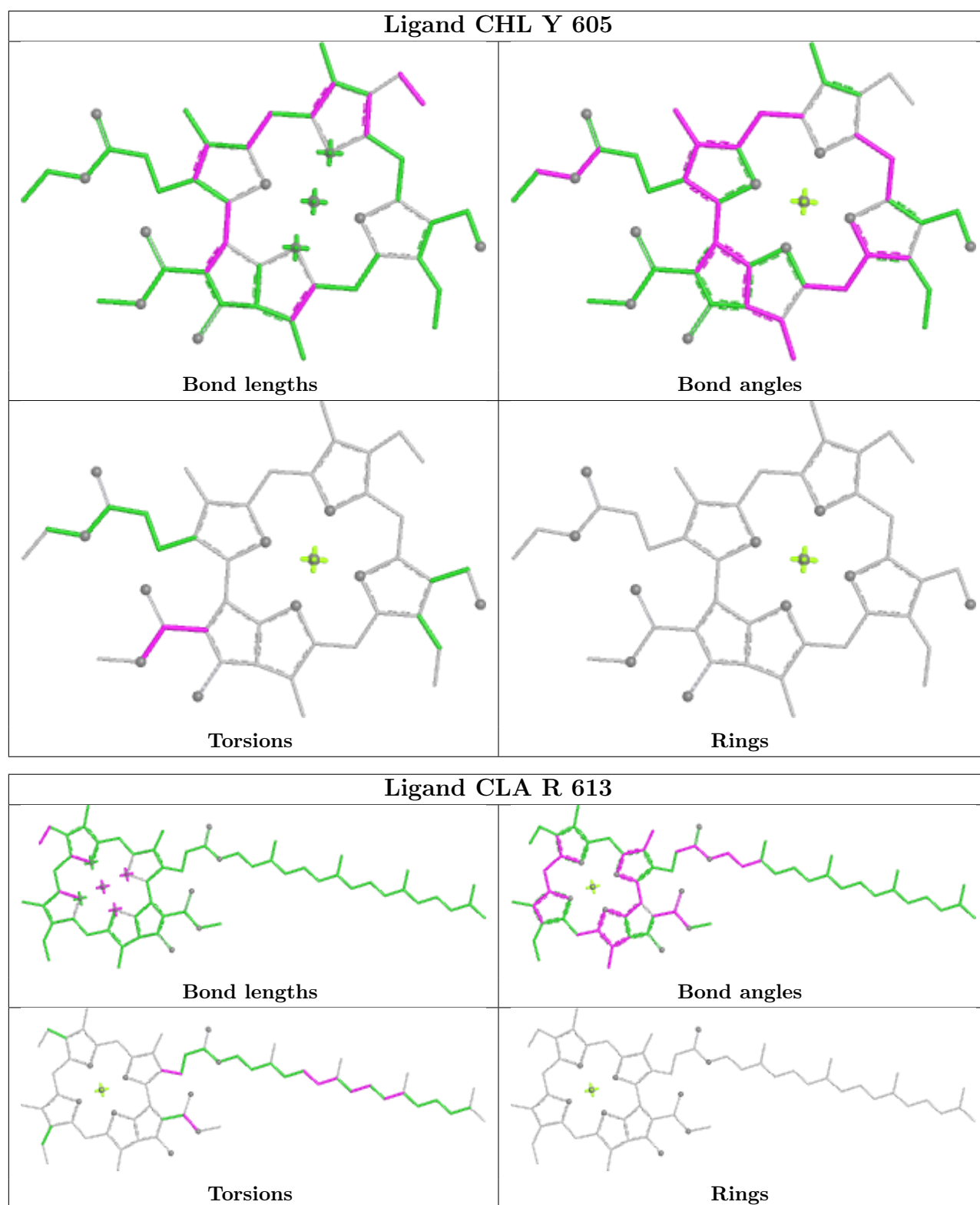
## Ligand CLA b 611



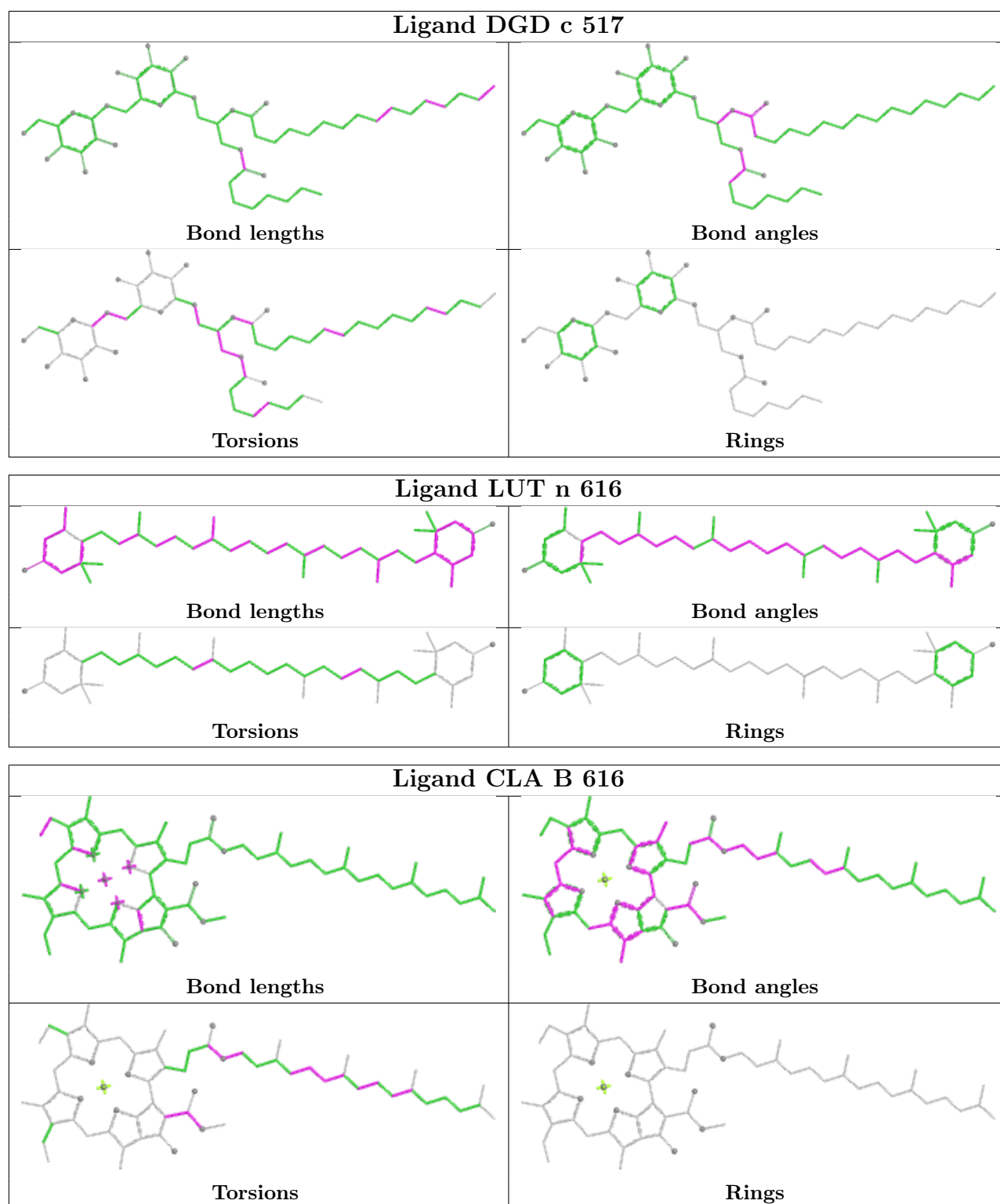
## Ligand CHL N 605

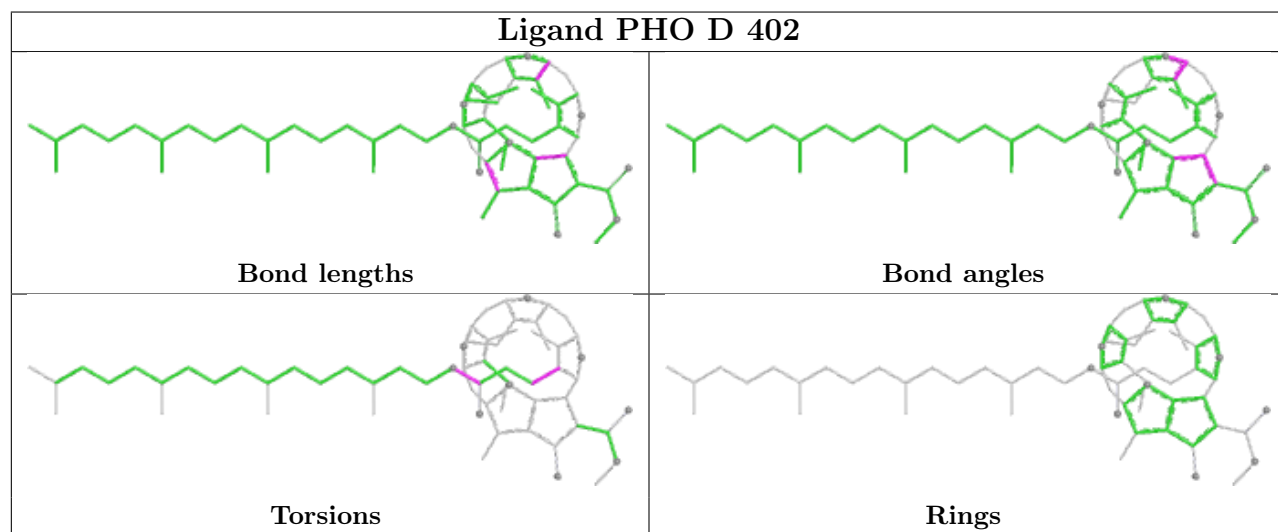
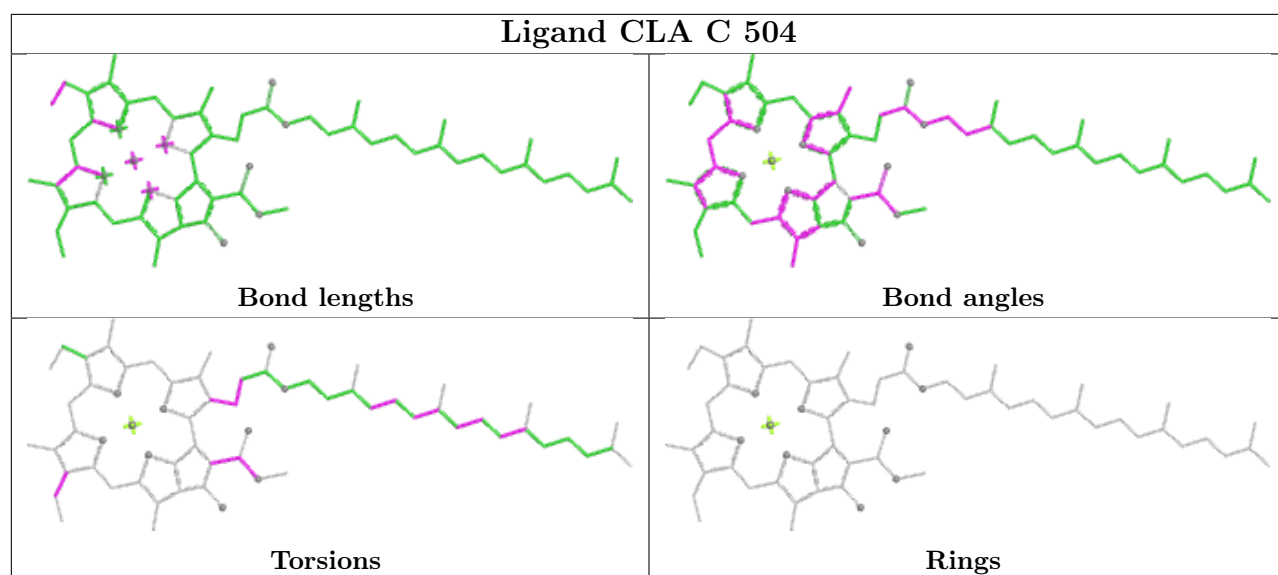


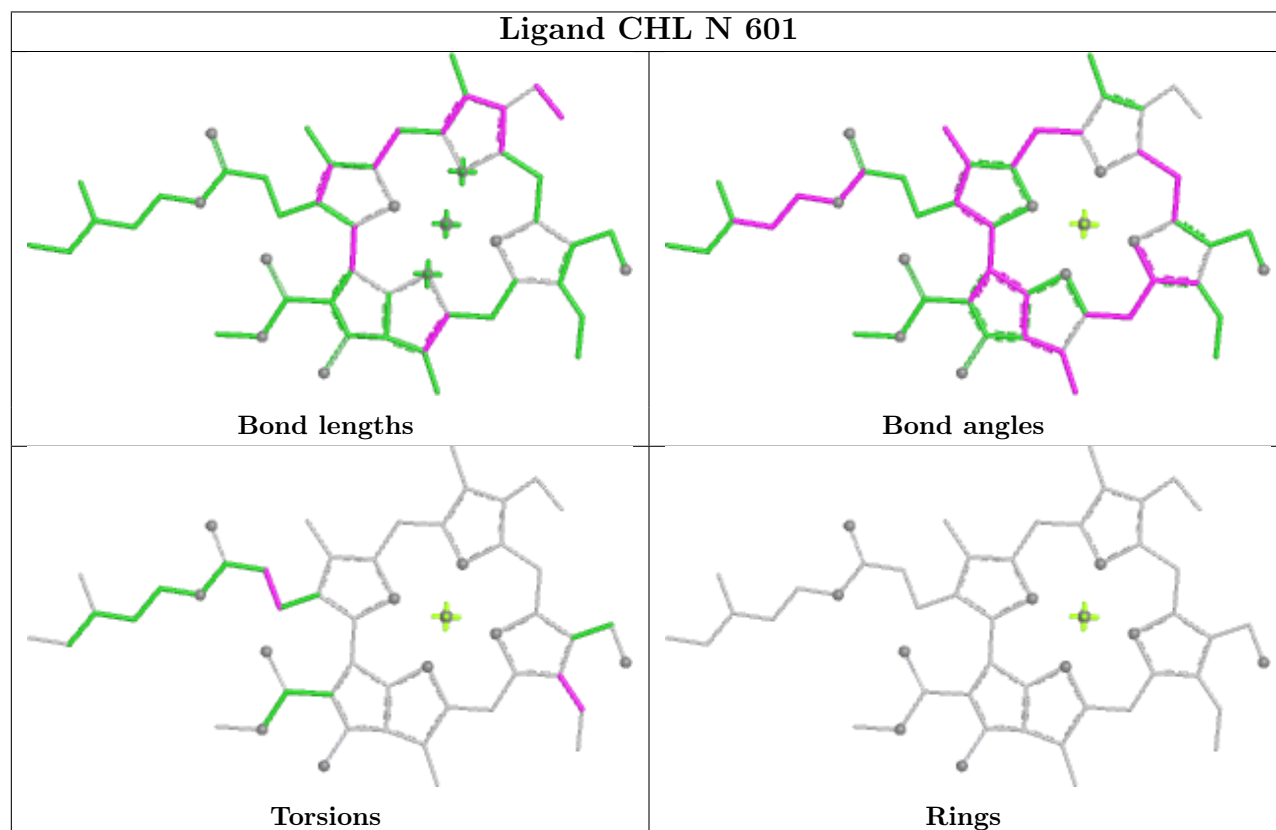
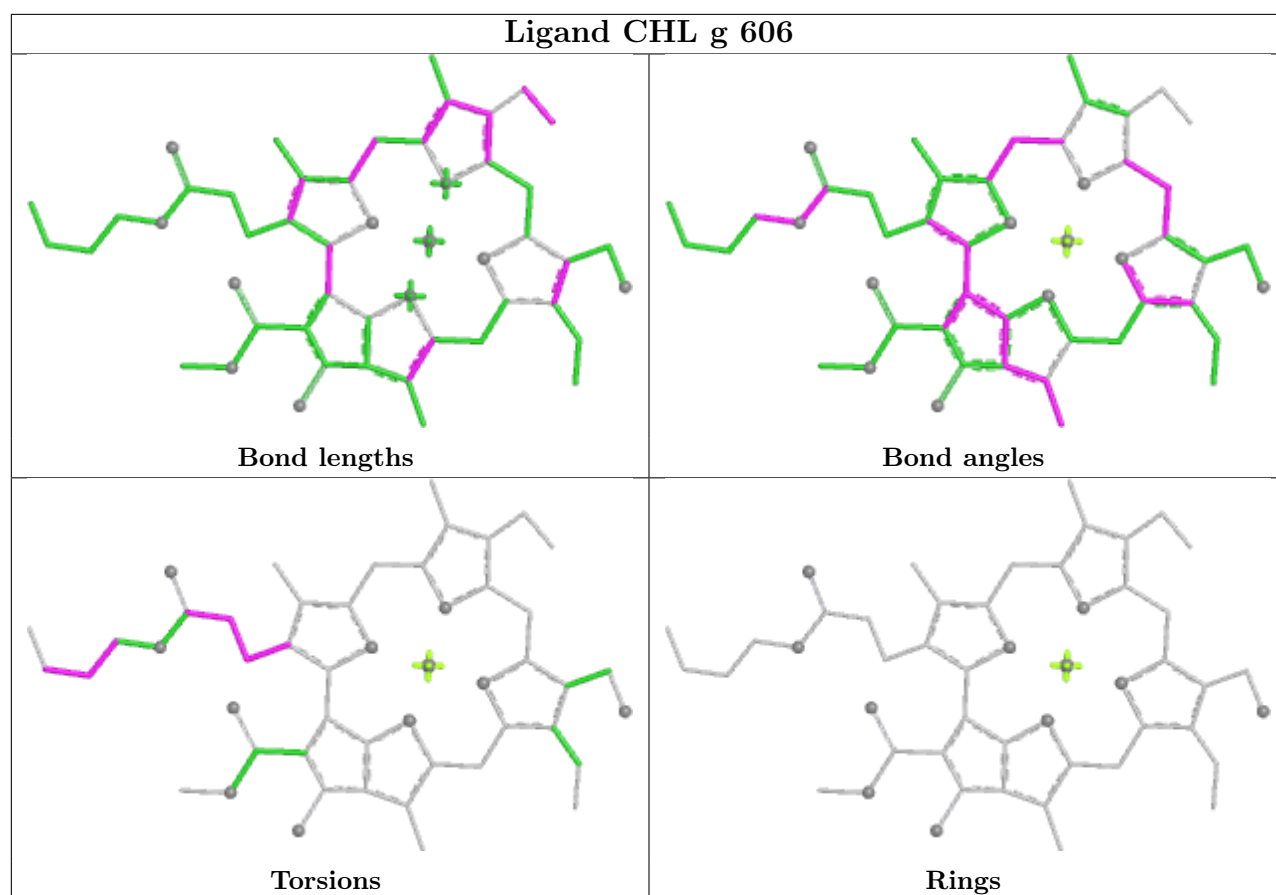


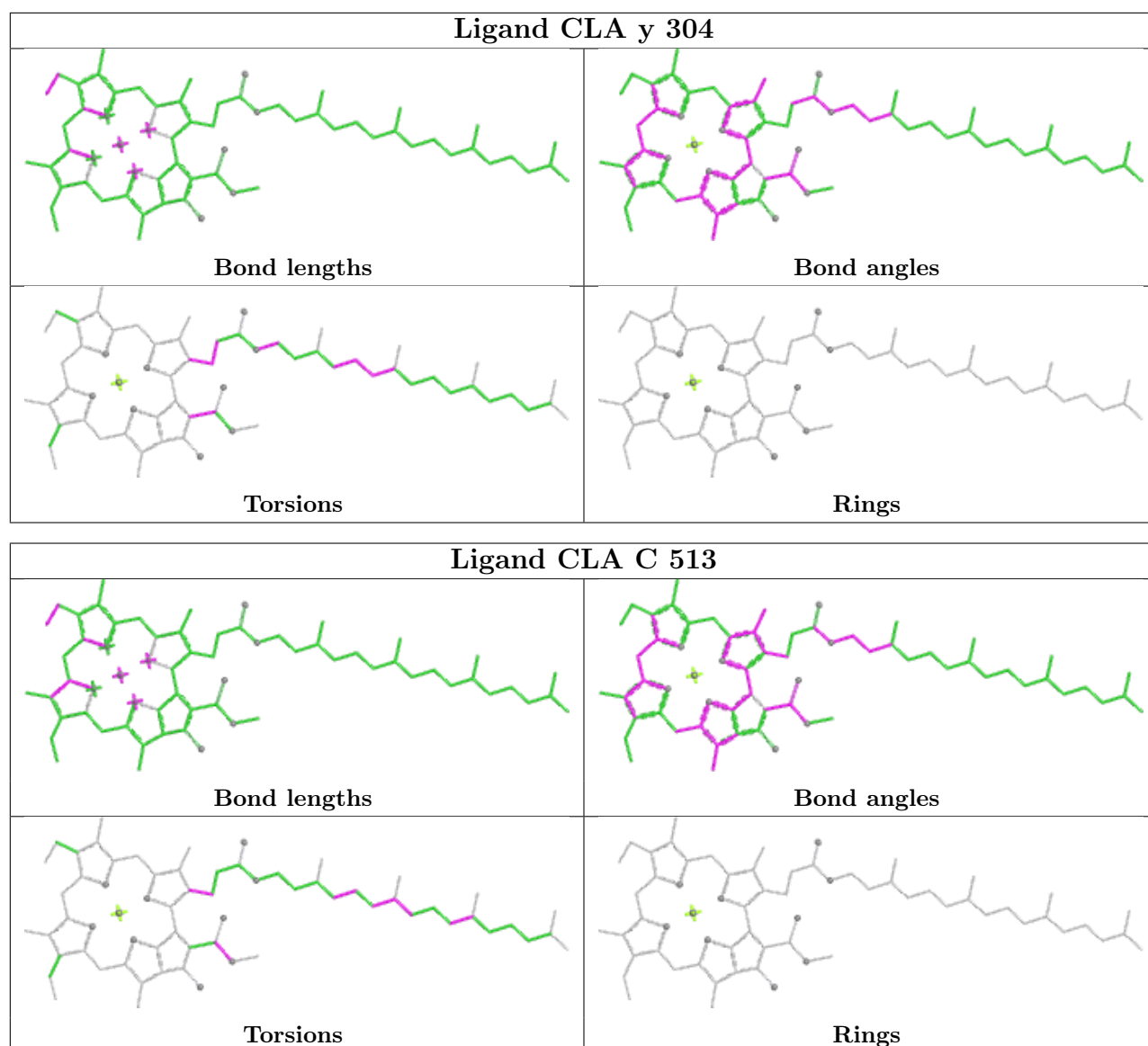




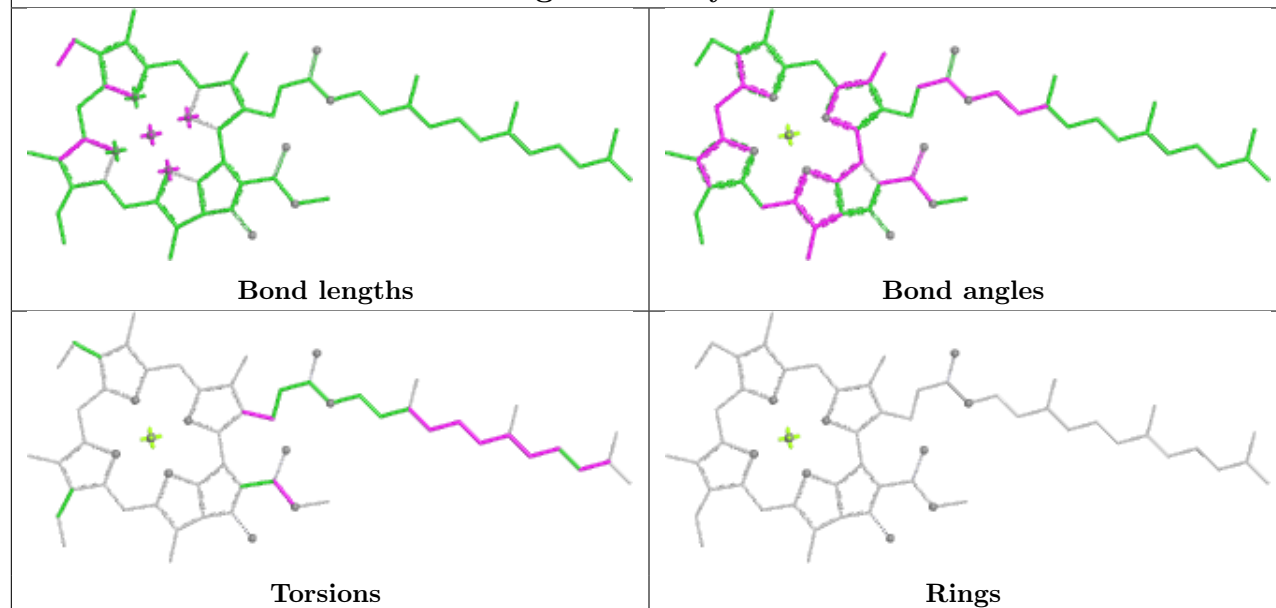




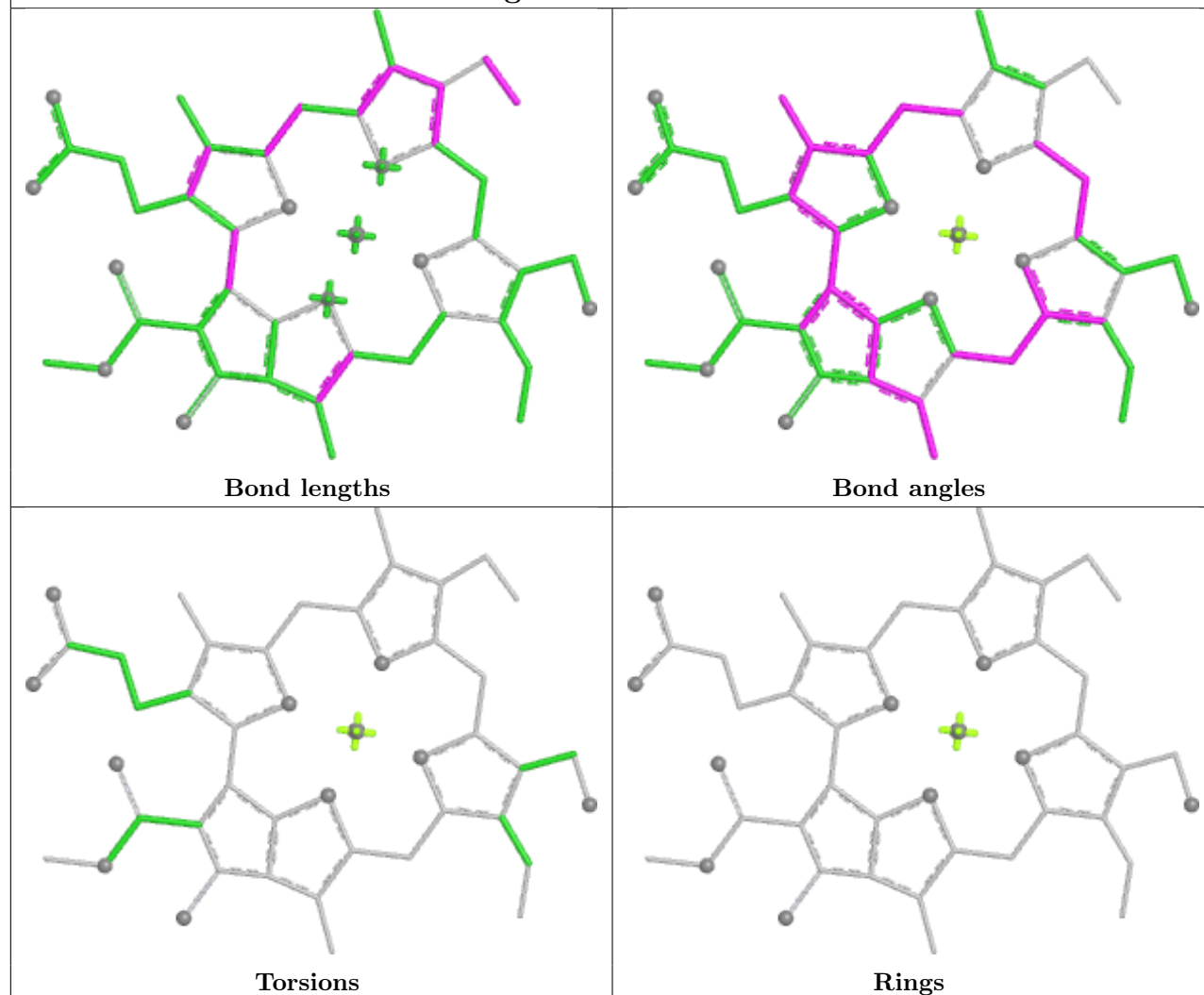




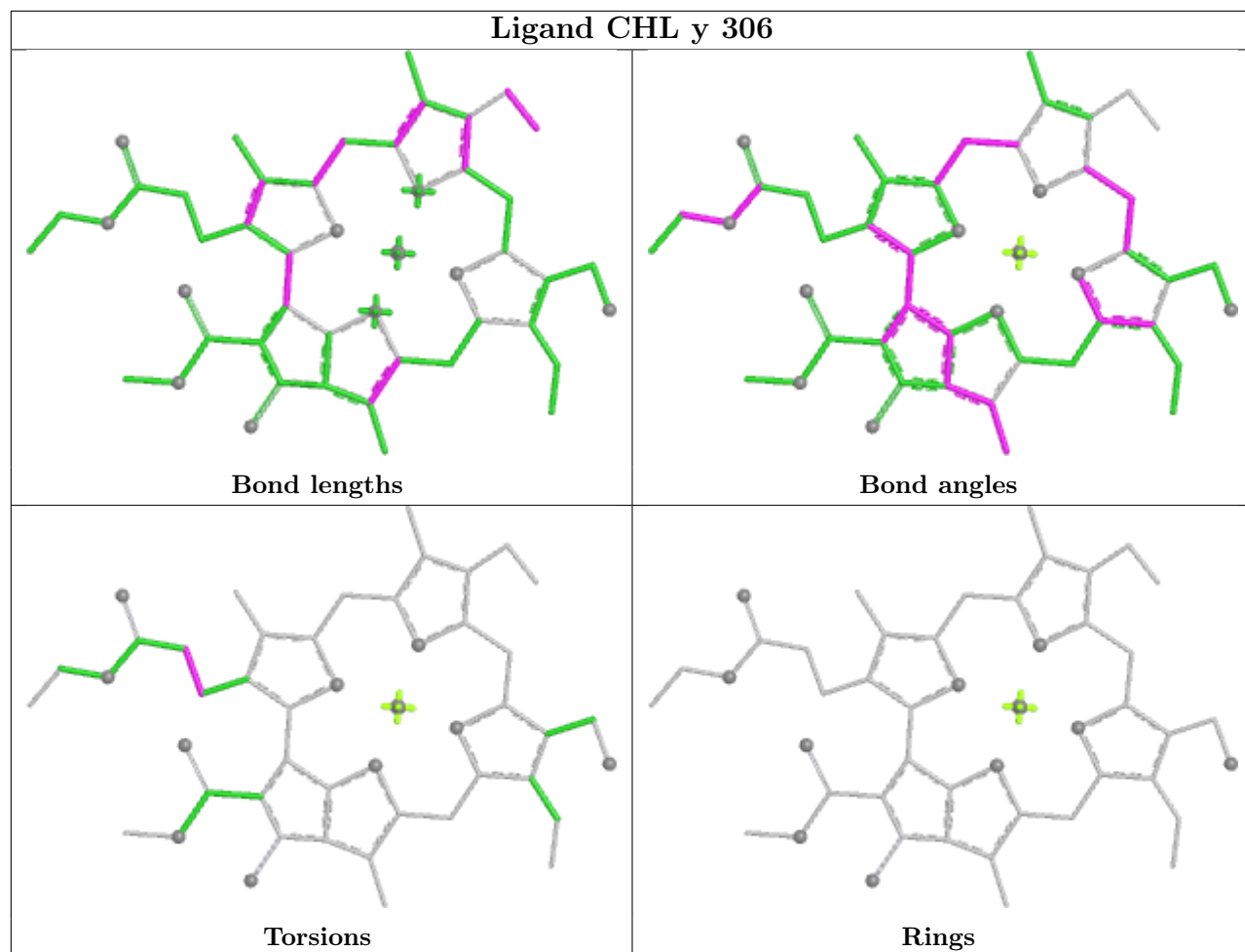
## Ligand CLA y 310

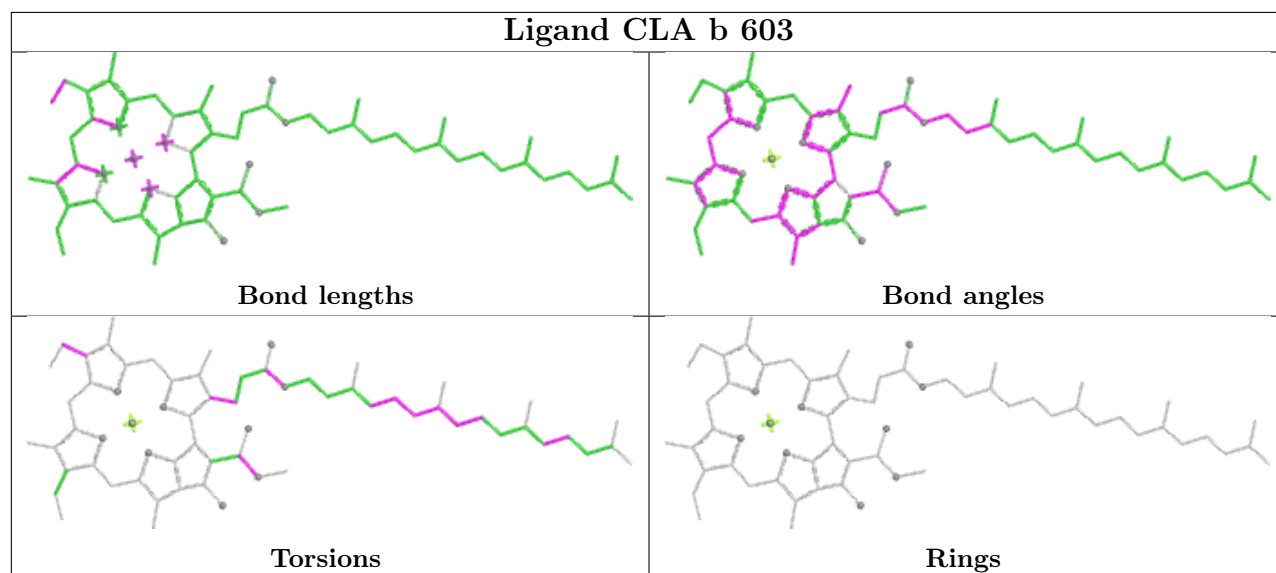
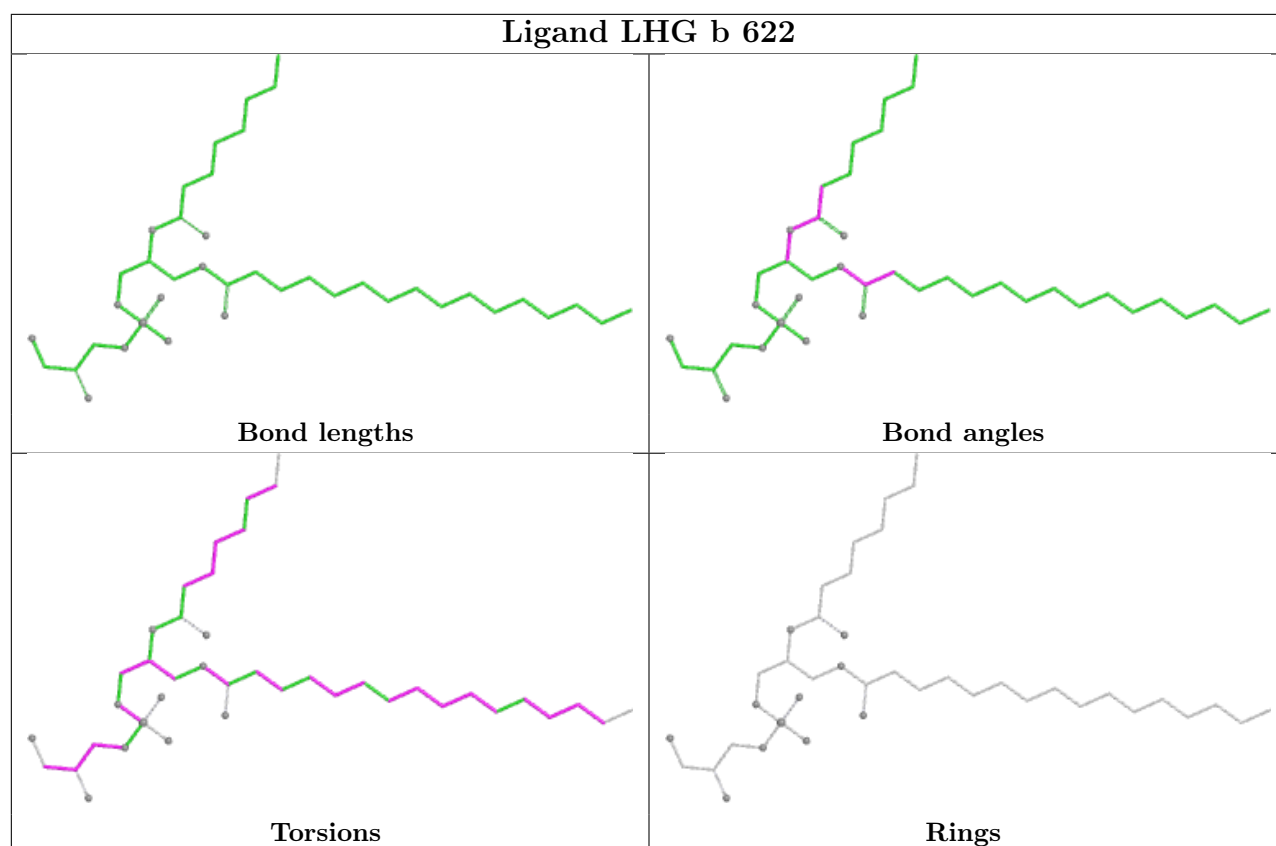


## Ligand CHL S 302

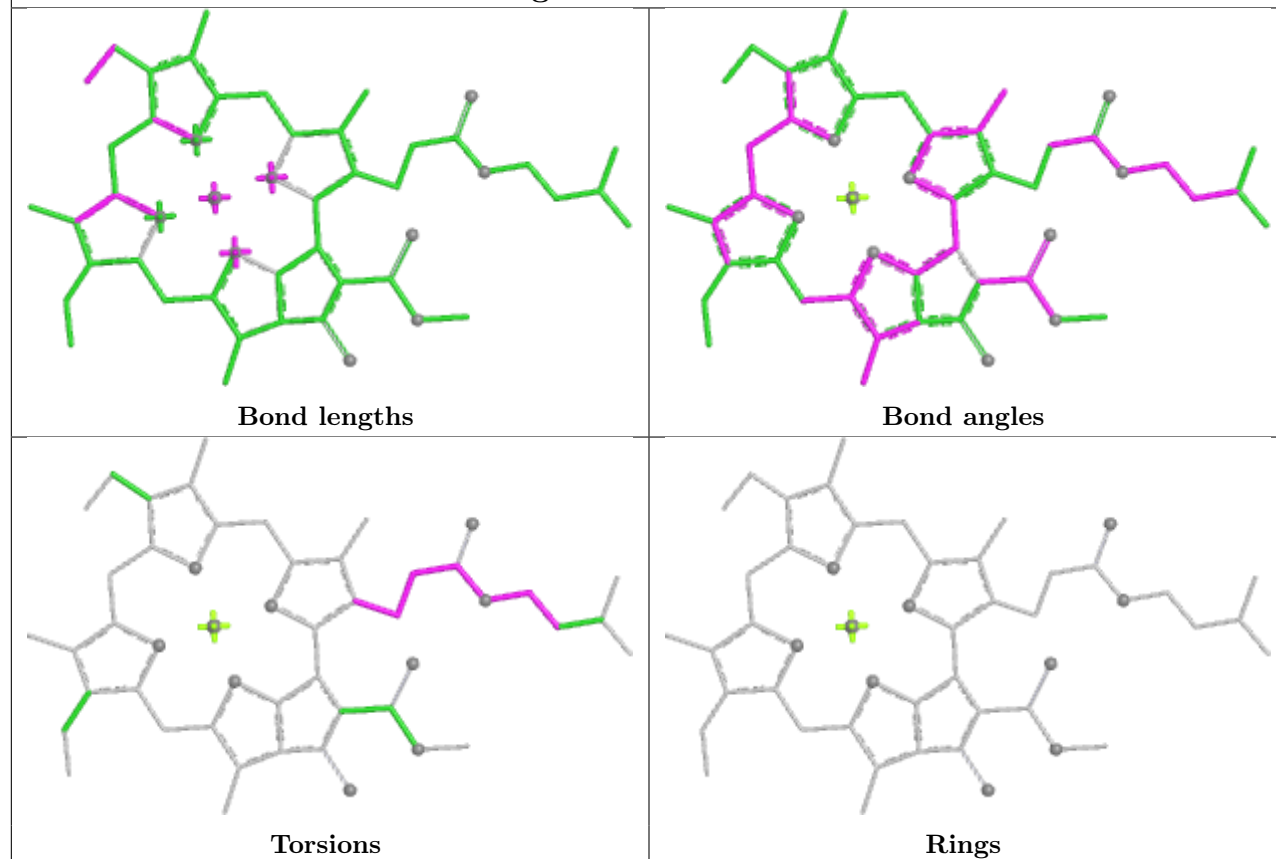


## Ligand CHL y 306

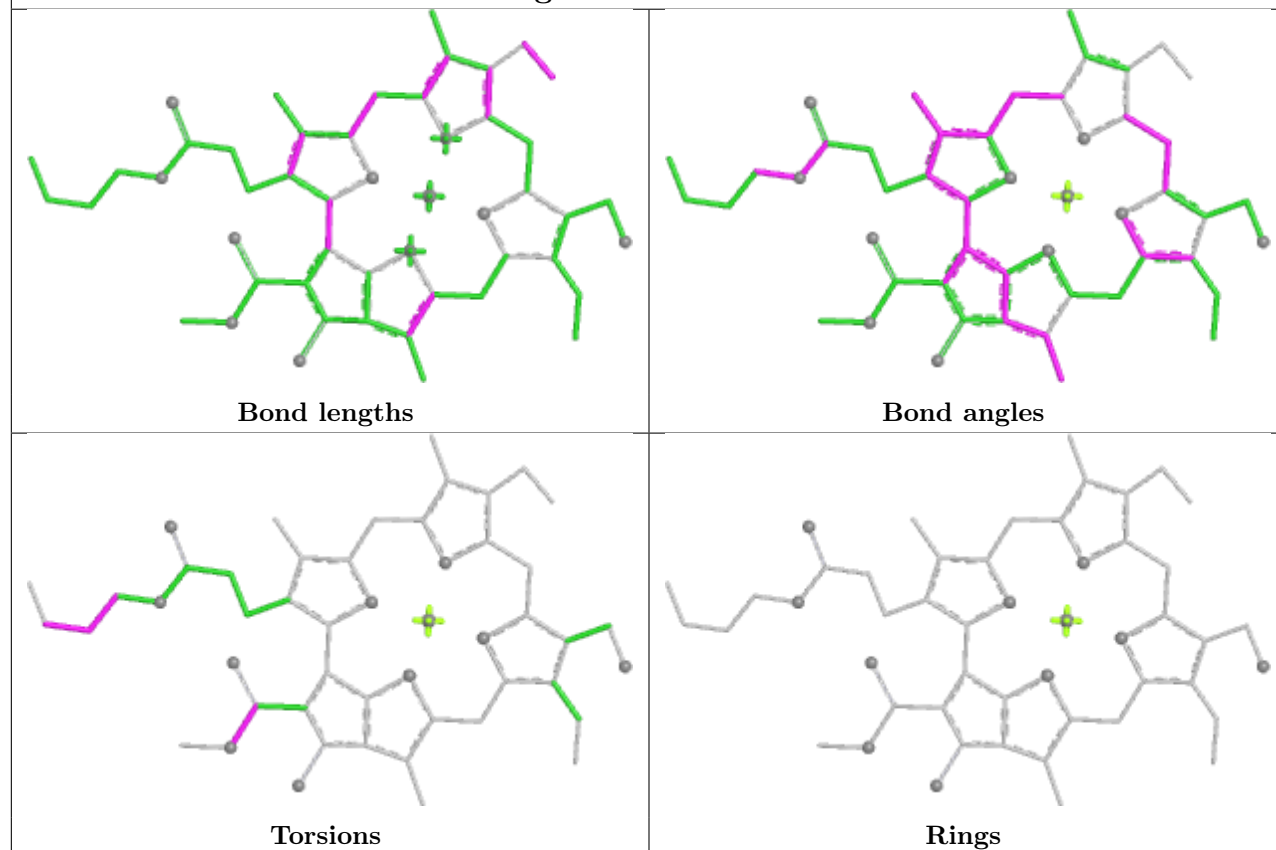




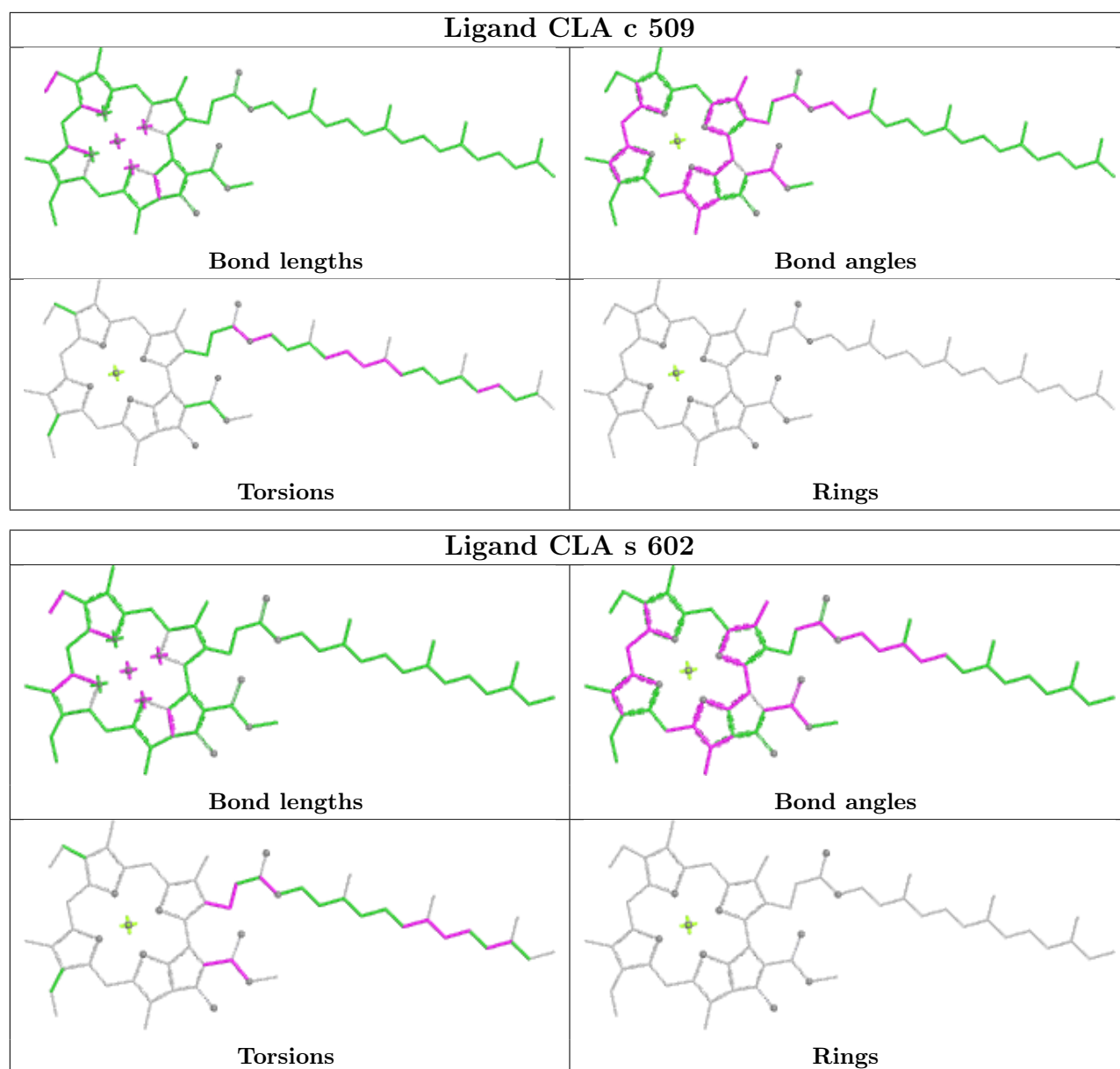
## Ligand CLA A 406



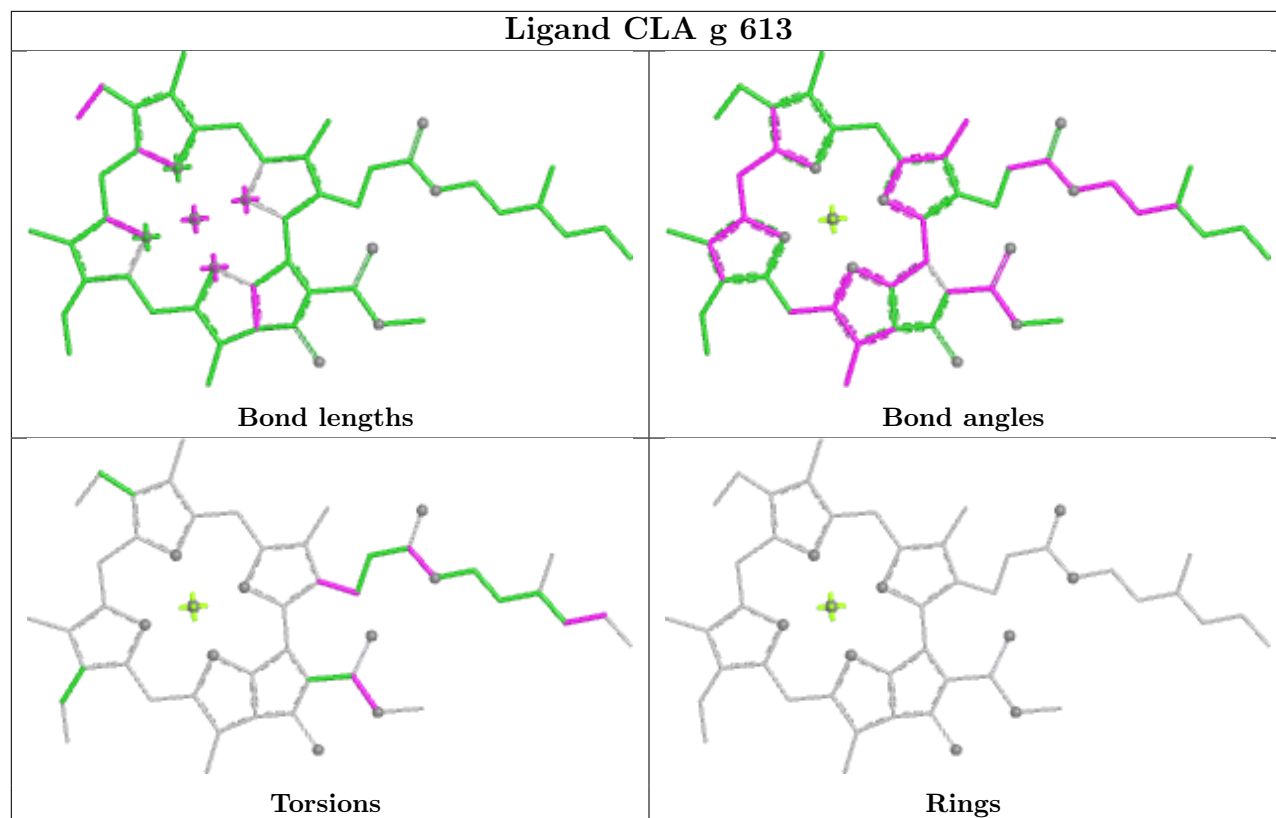
## Ligand CHL n 606



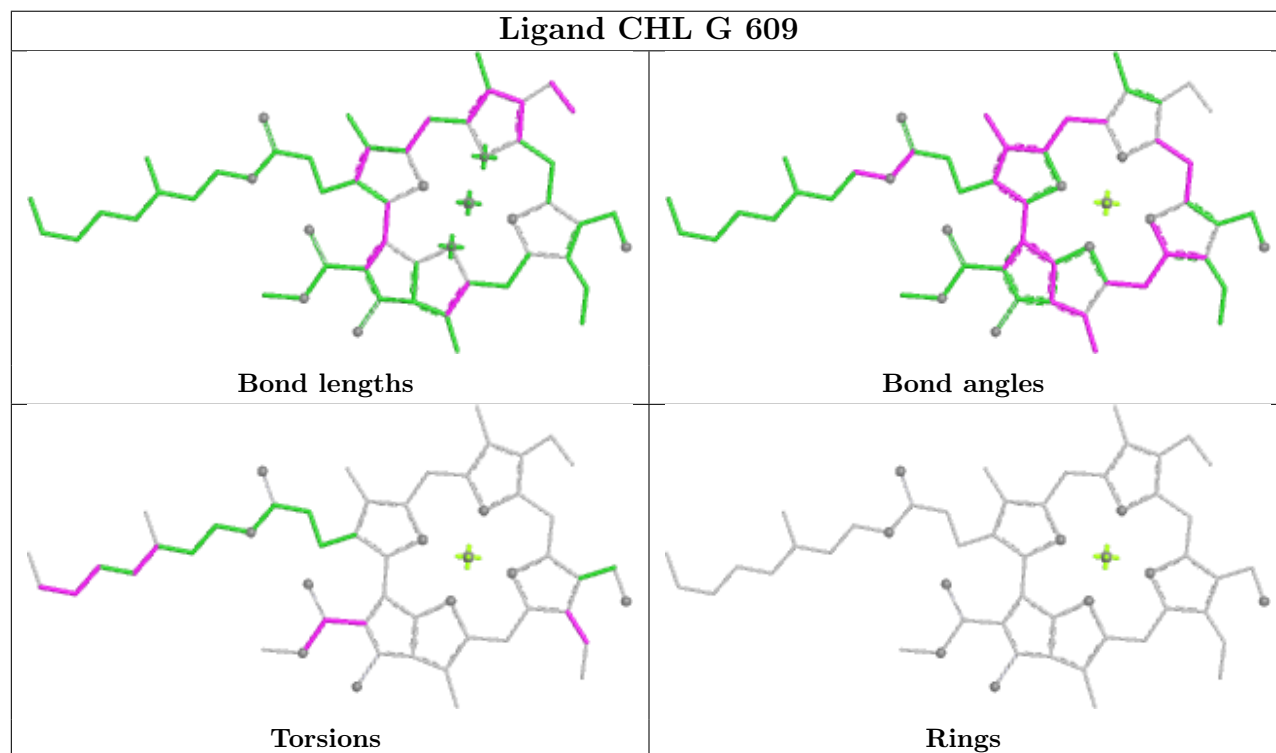


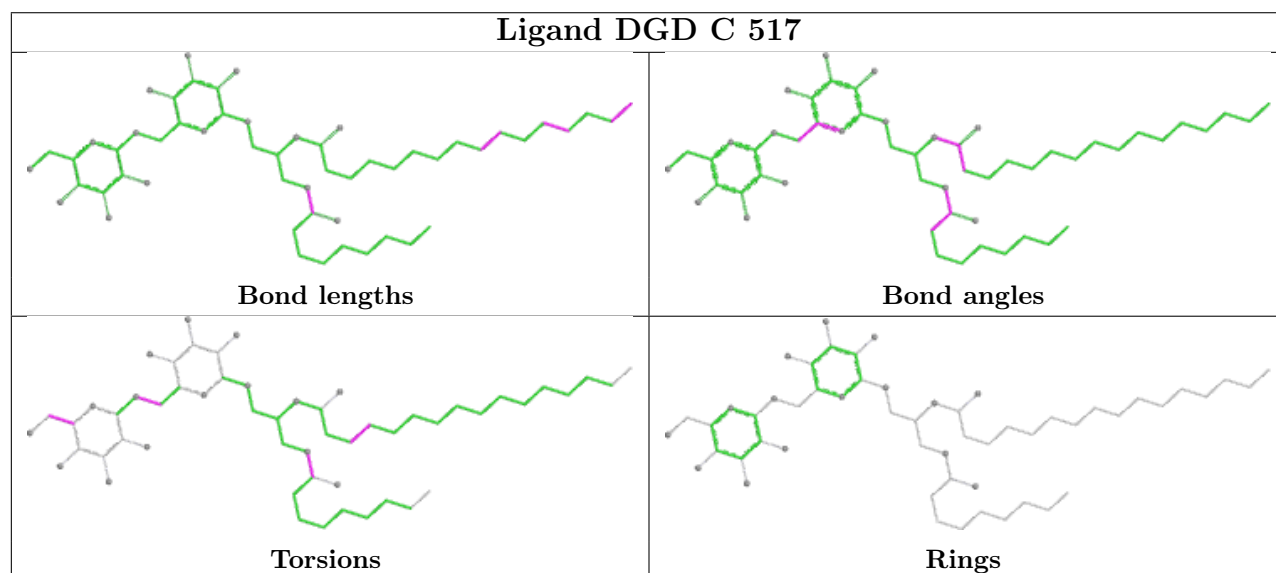
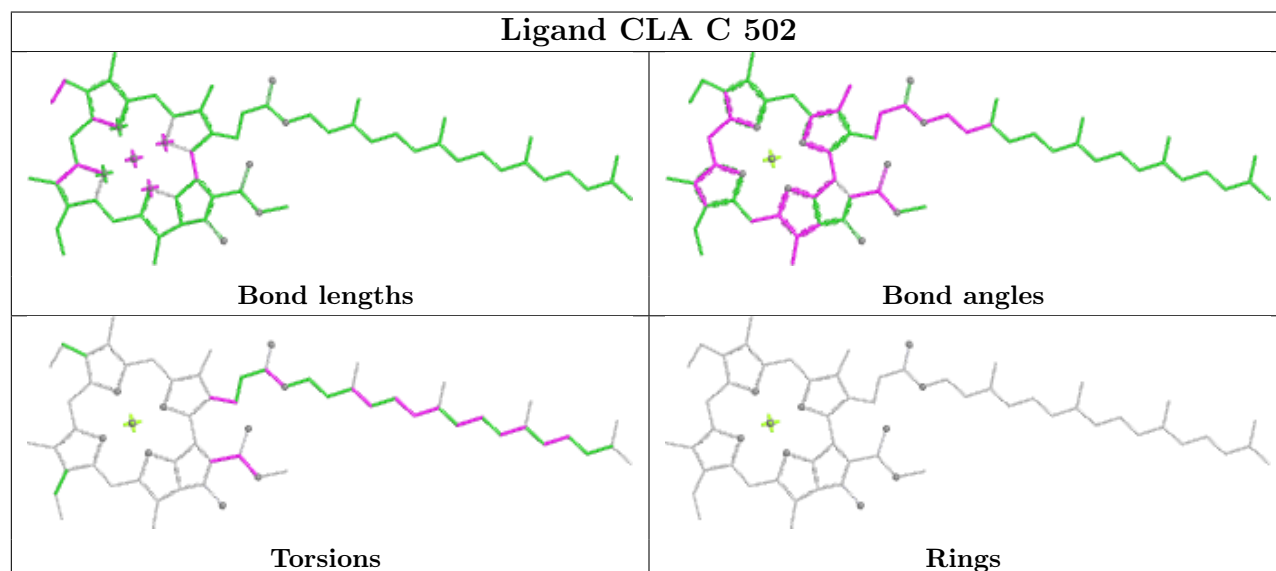
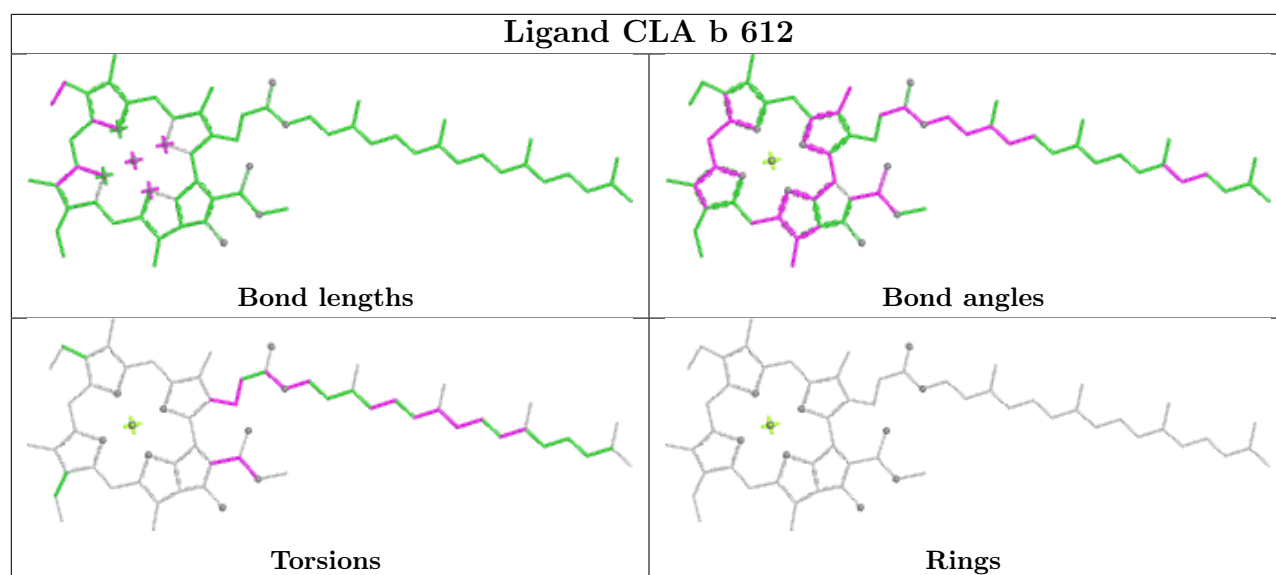


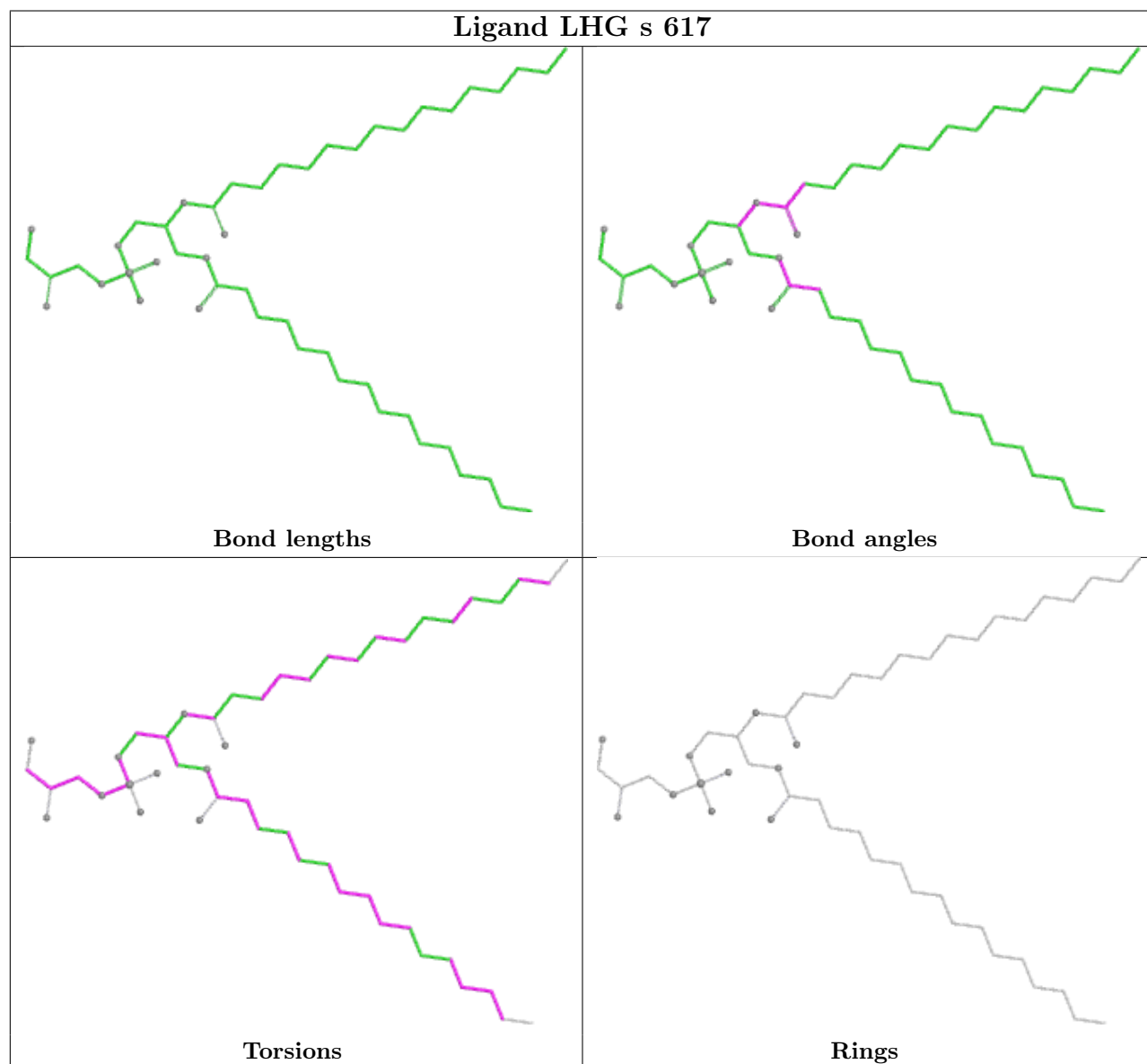
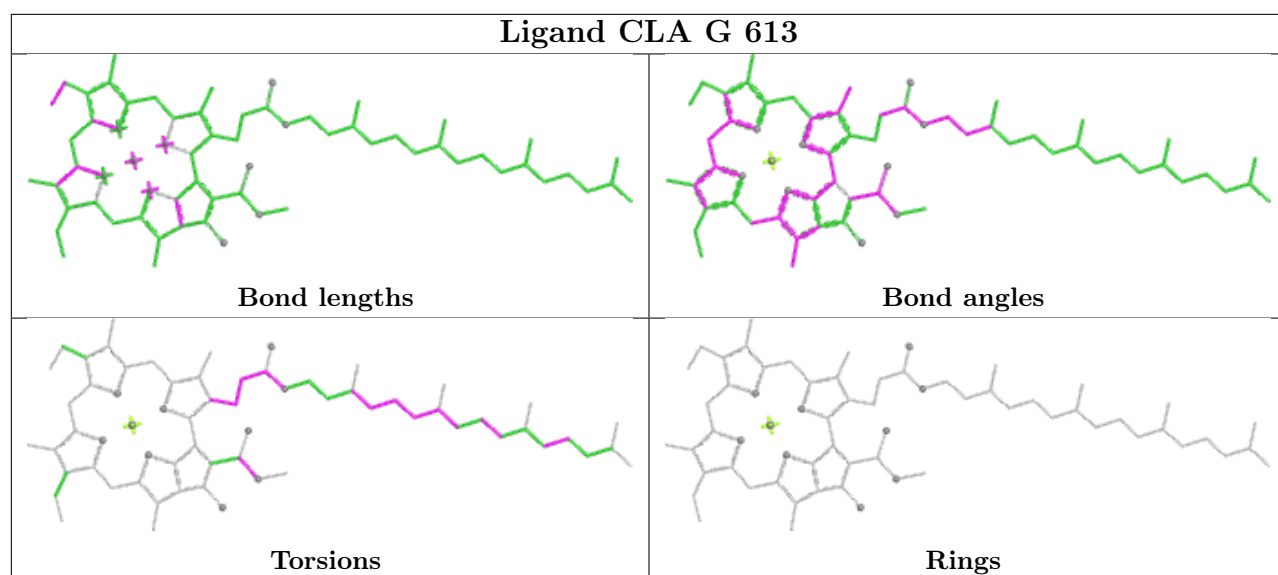
## Ligand CLA g 613

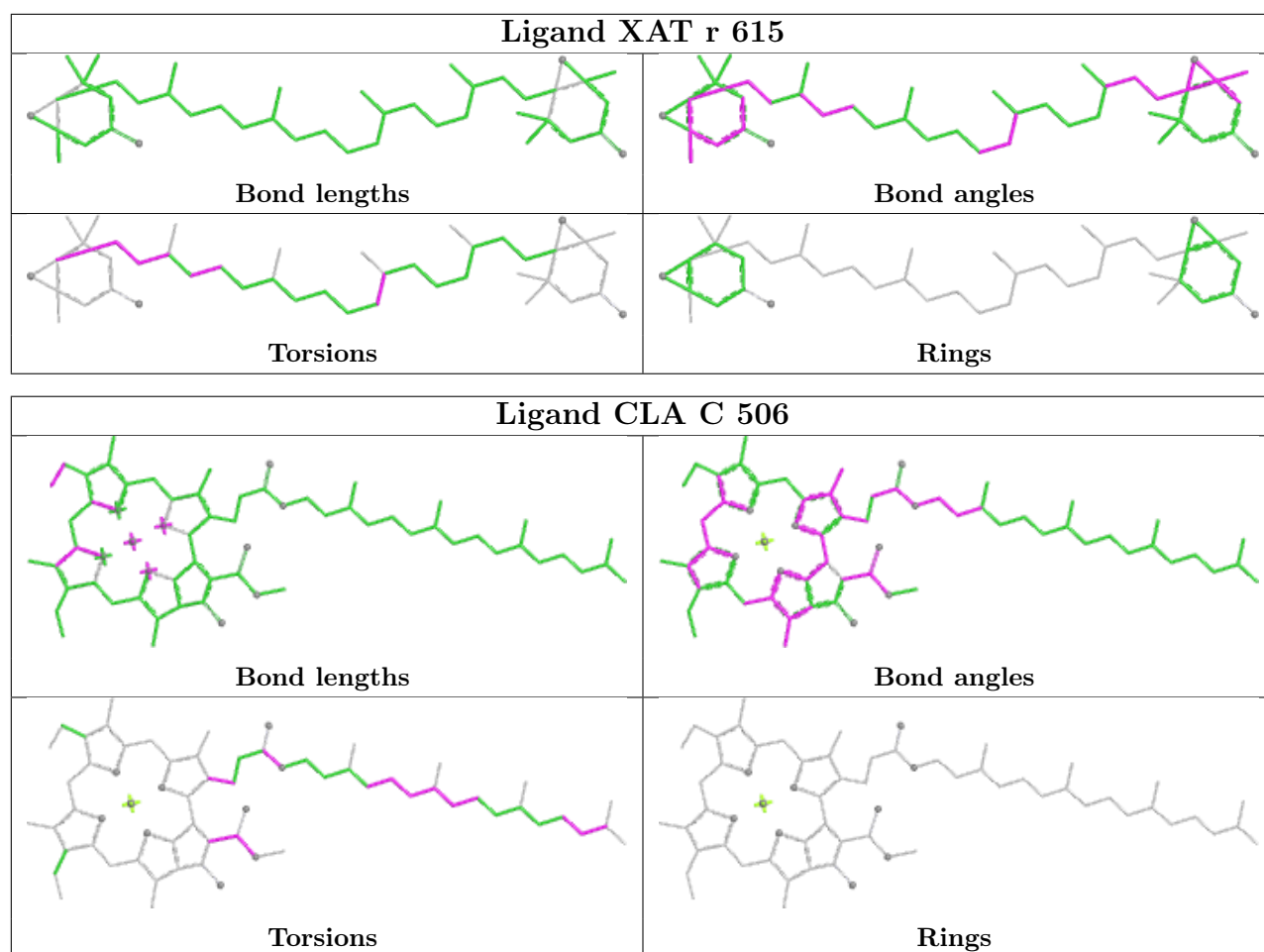


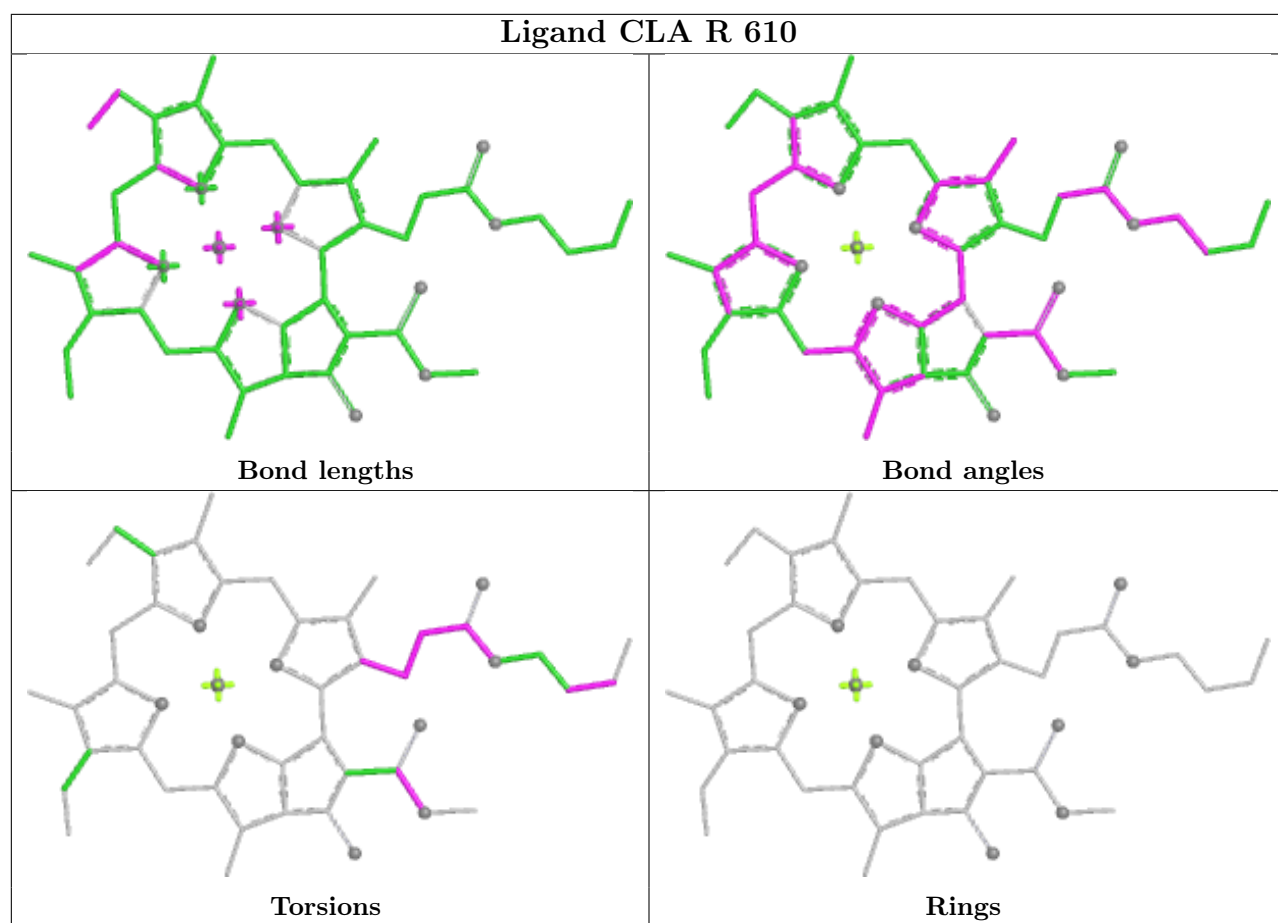
## Ligand CHL G 609



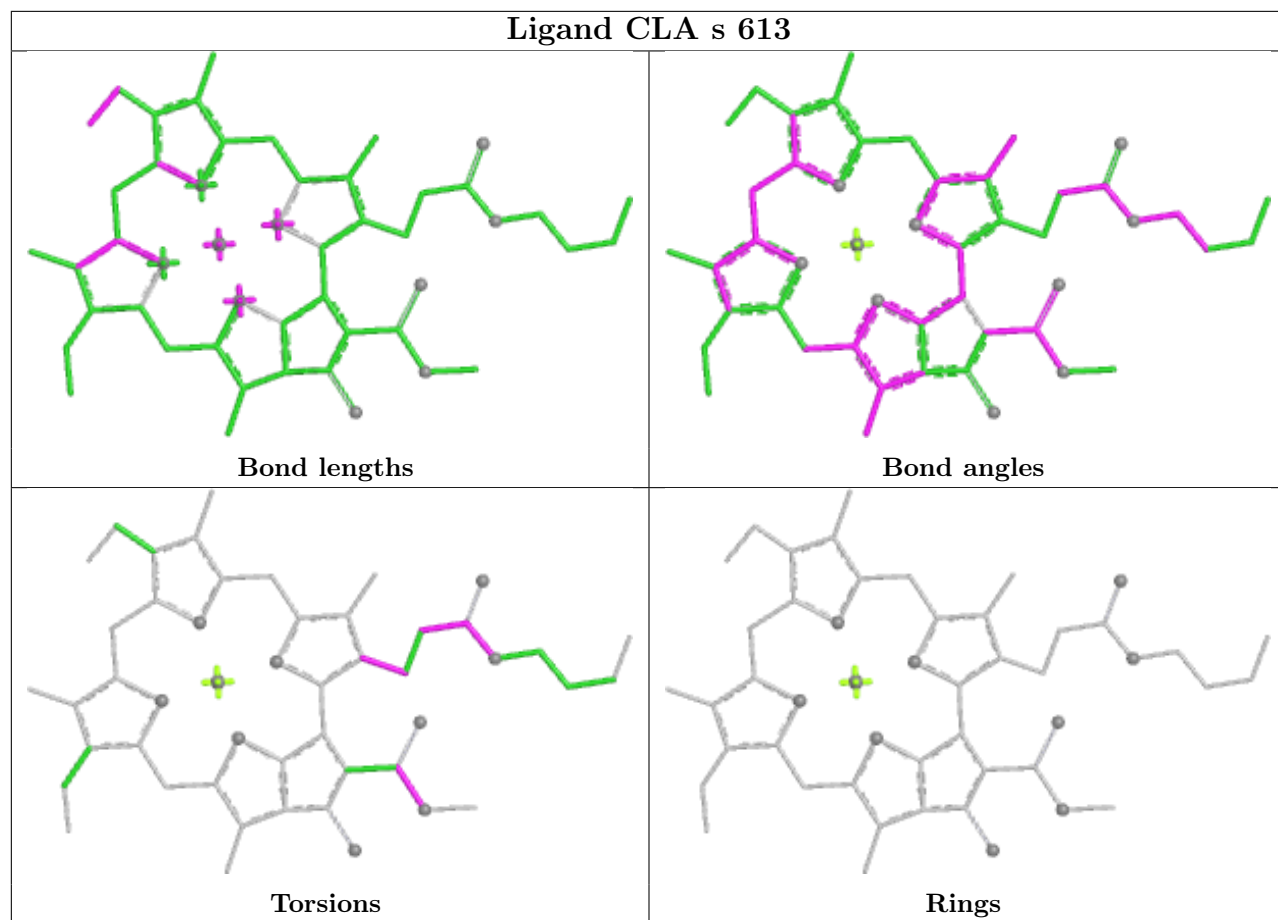




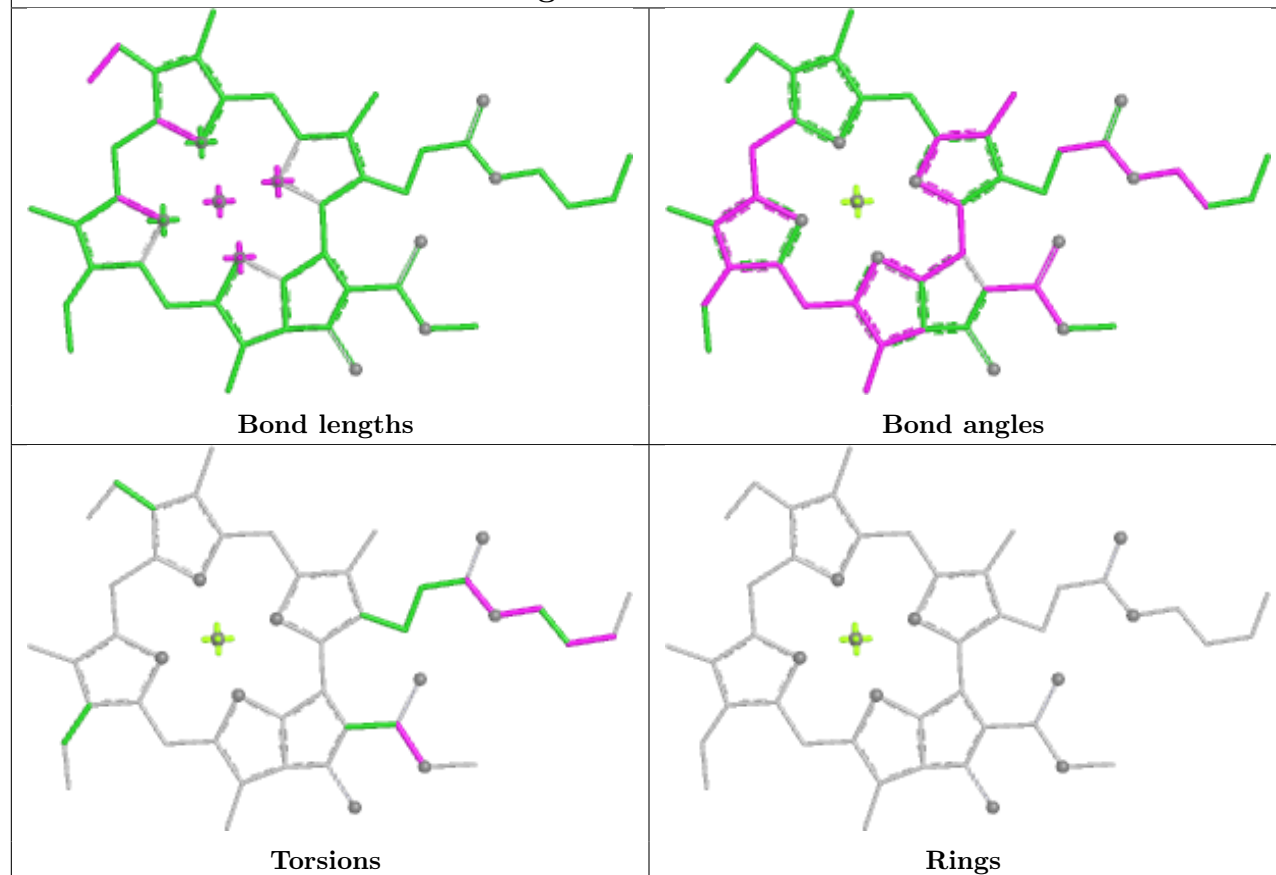




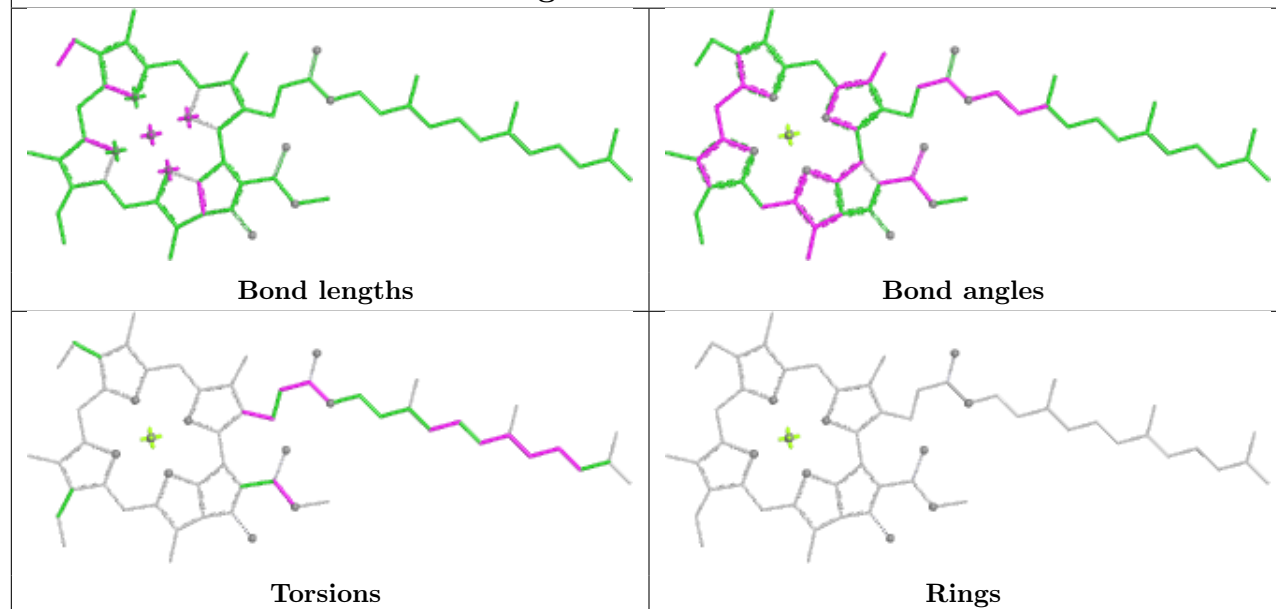
## Ligand CLA s 613



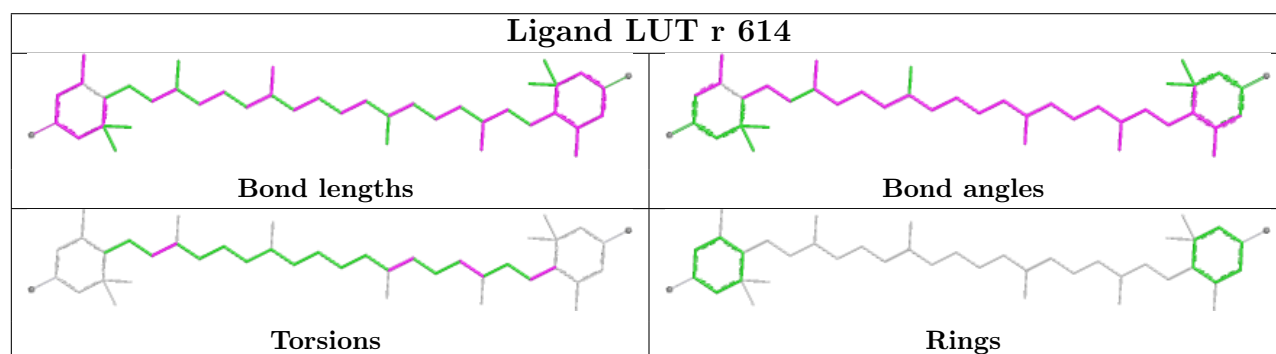
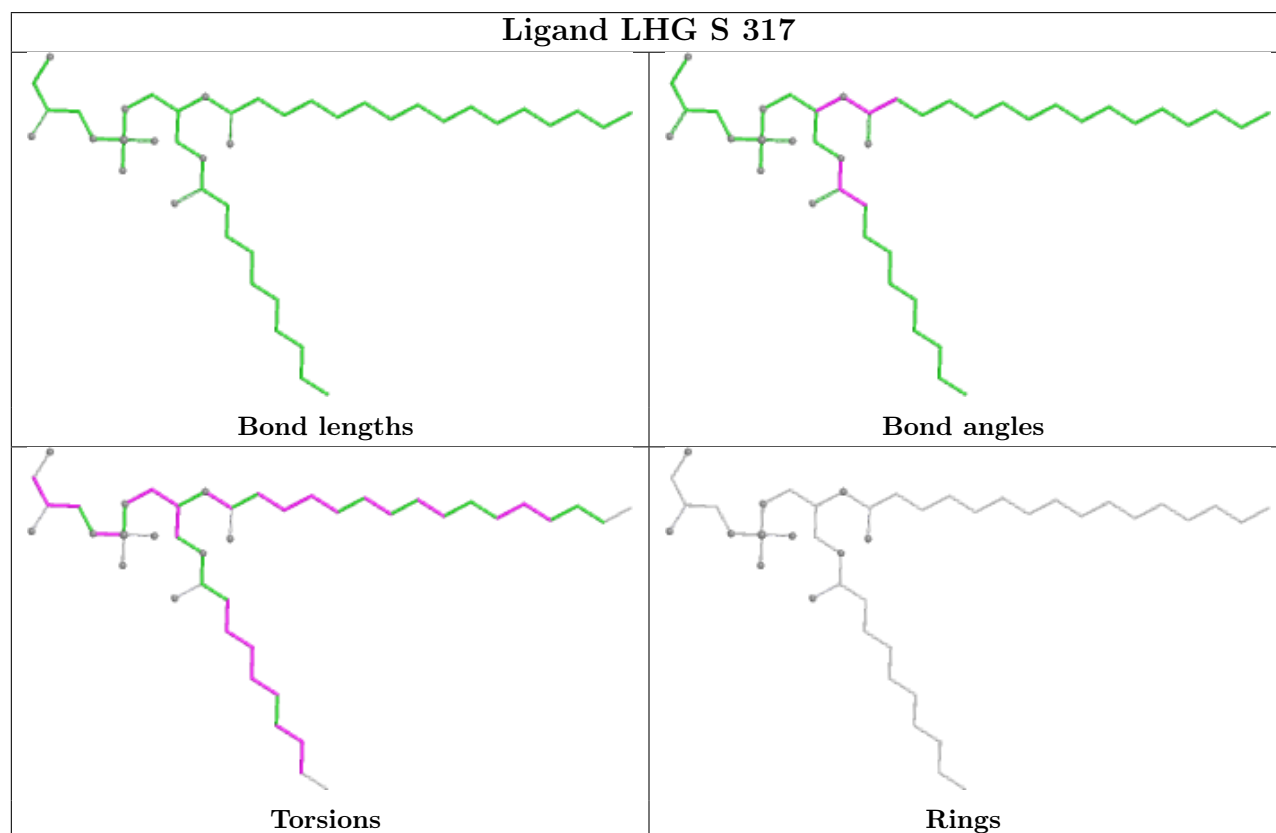
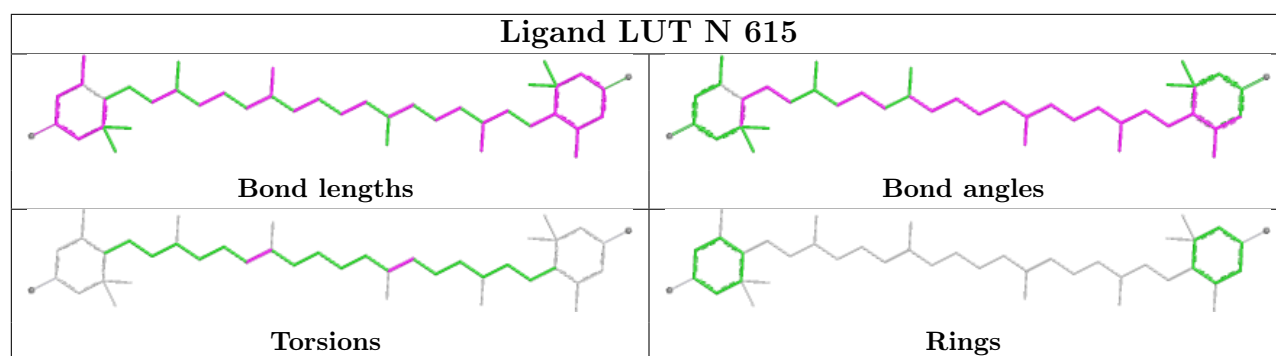
## Ligand CLA r 611



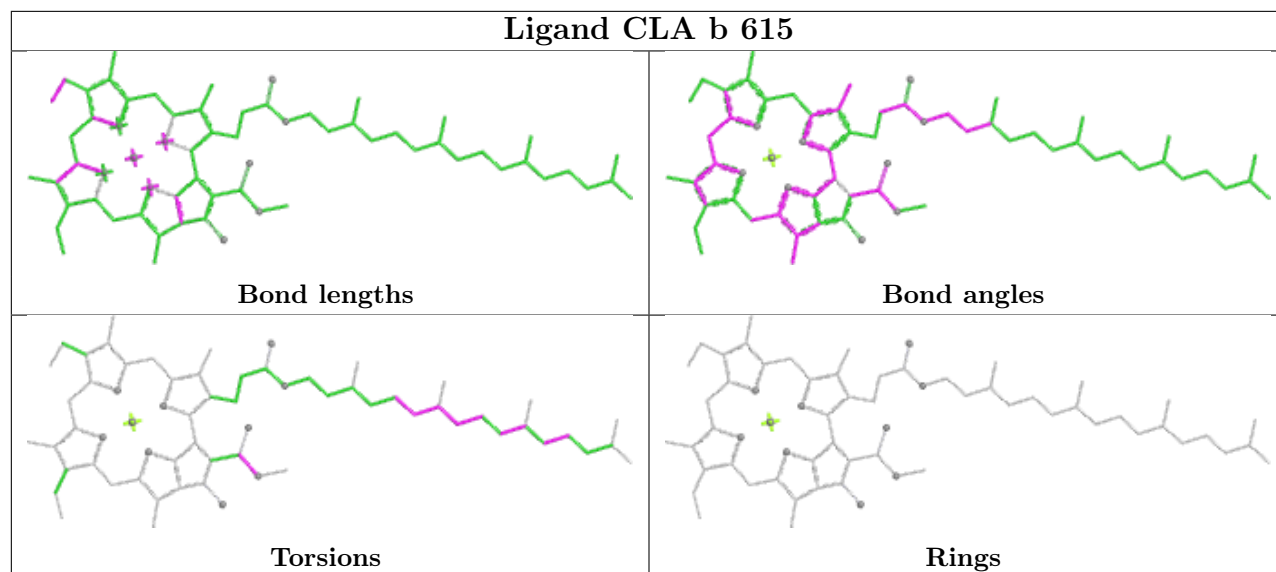
## Ligand CLA r 612



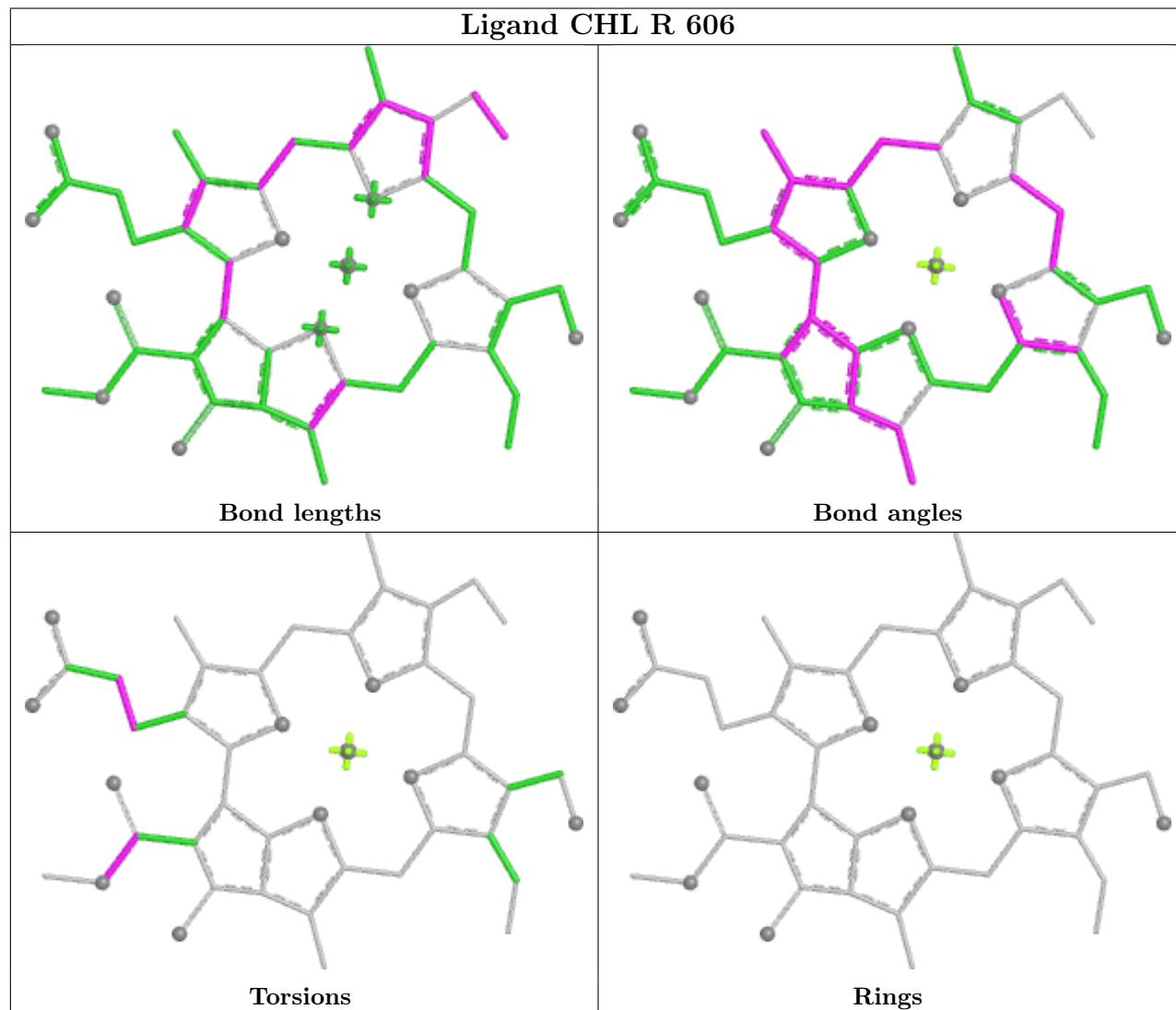


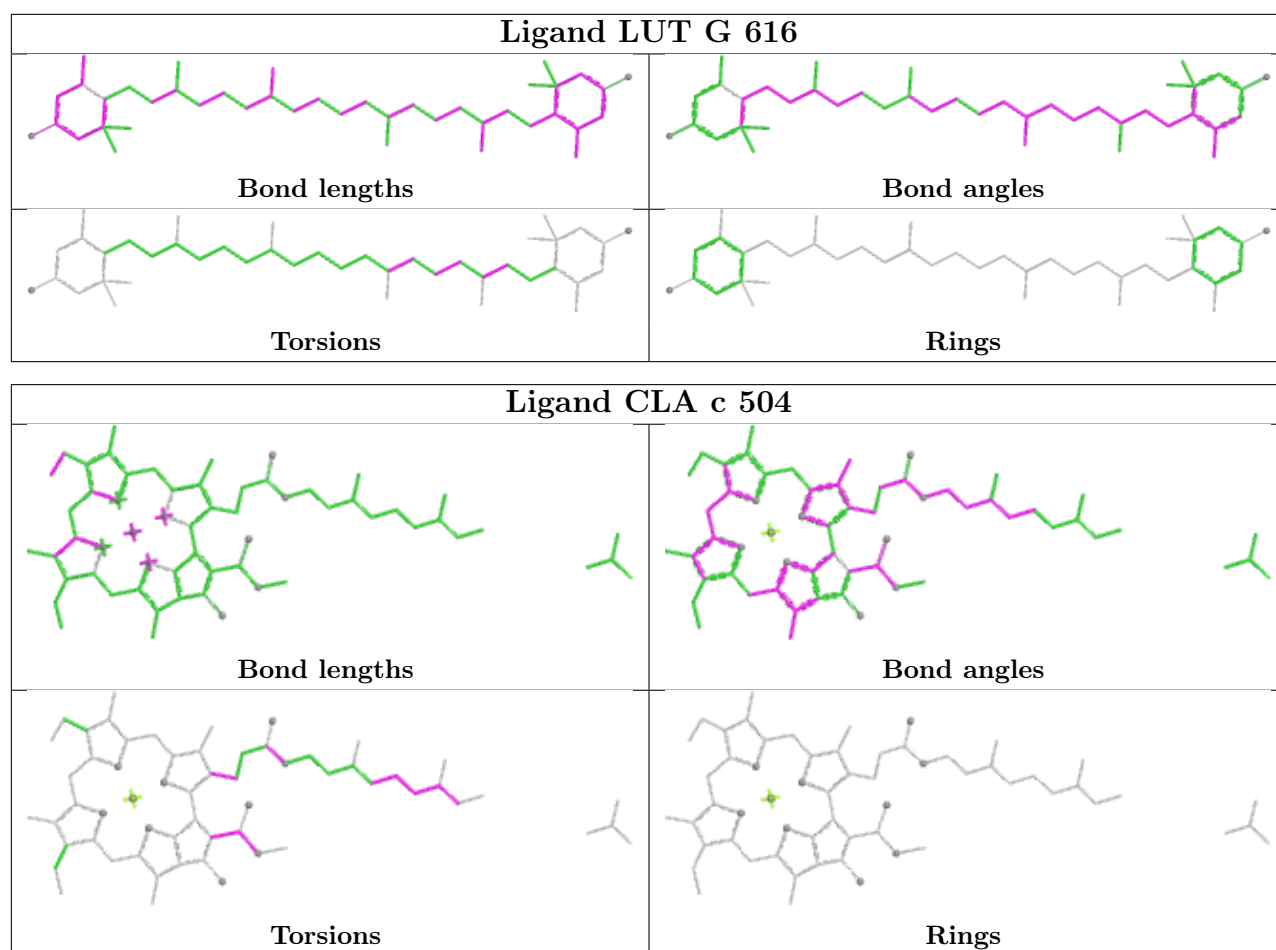


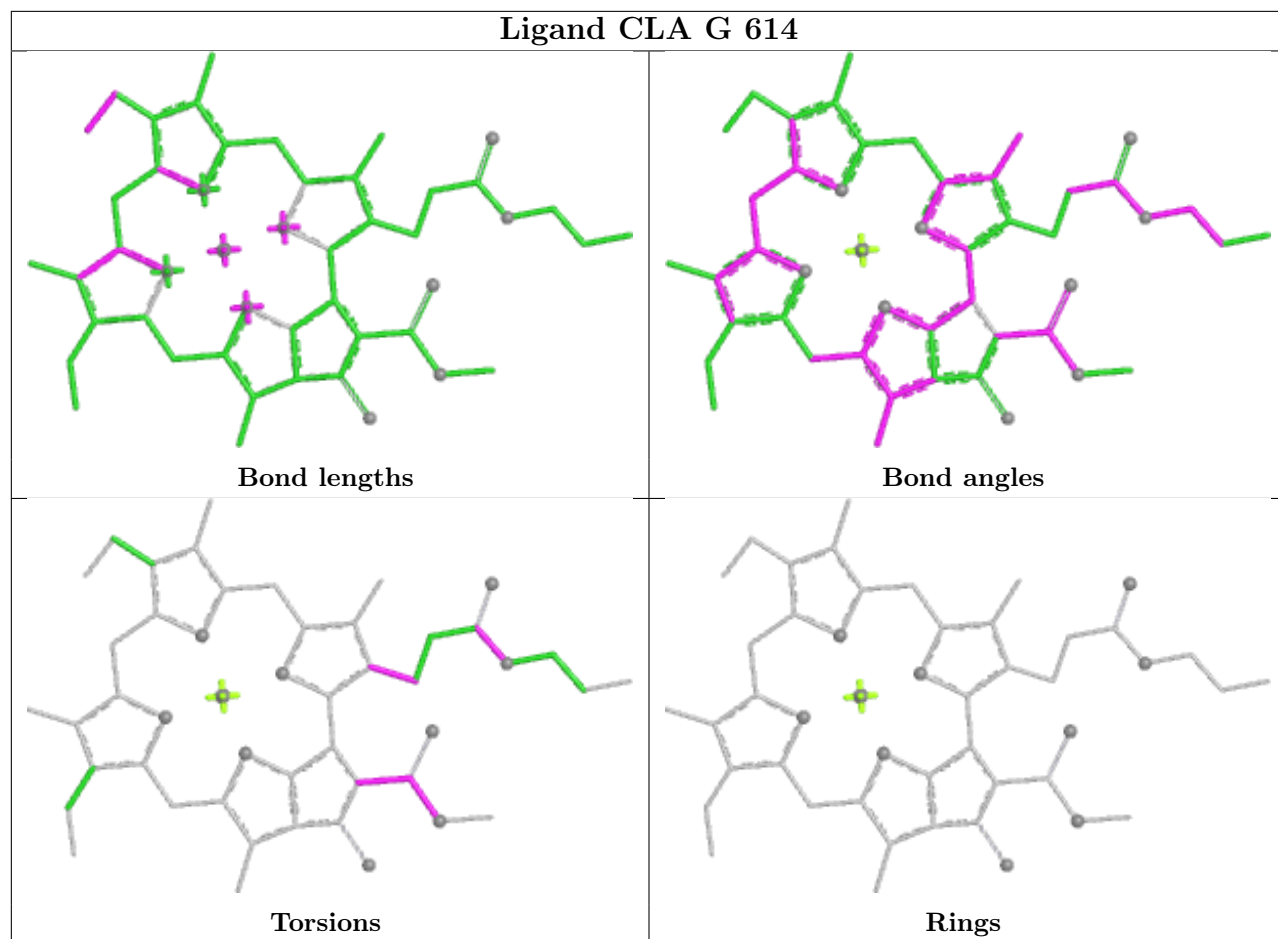
## Ligand CLA b 615

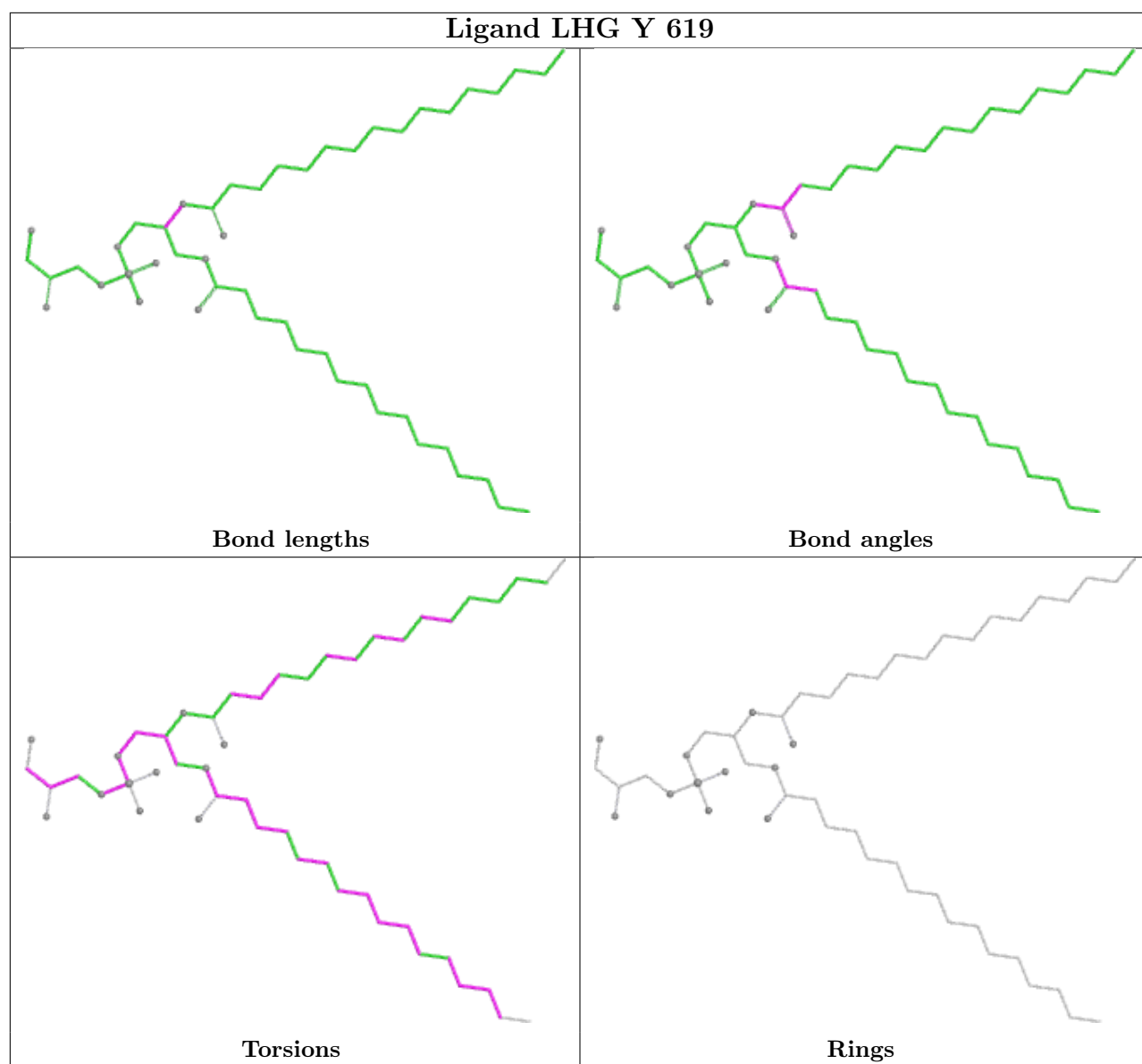


## Ligand CHL R 606

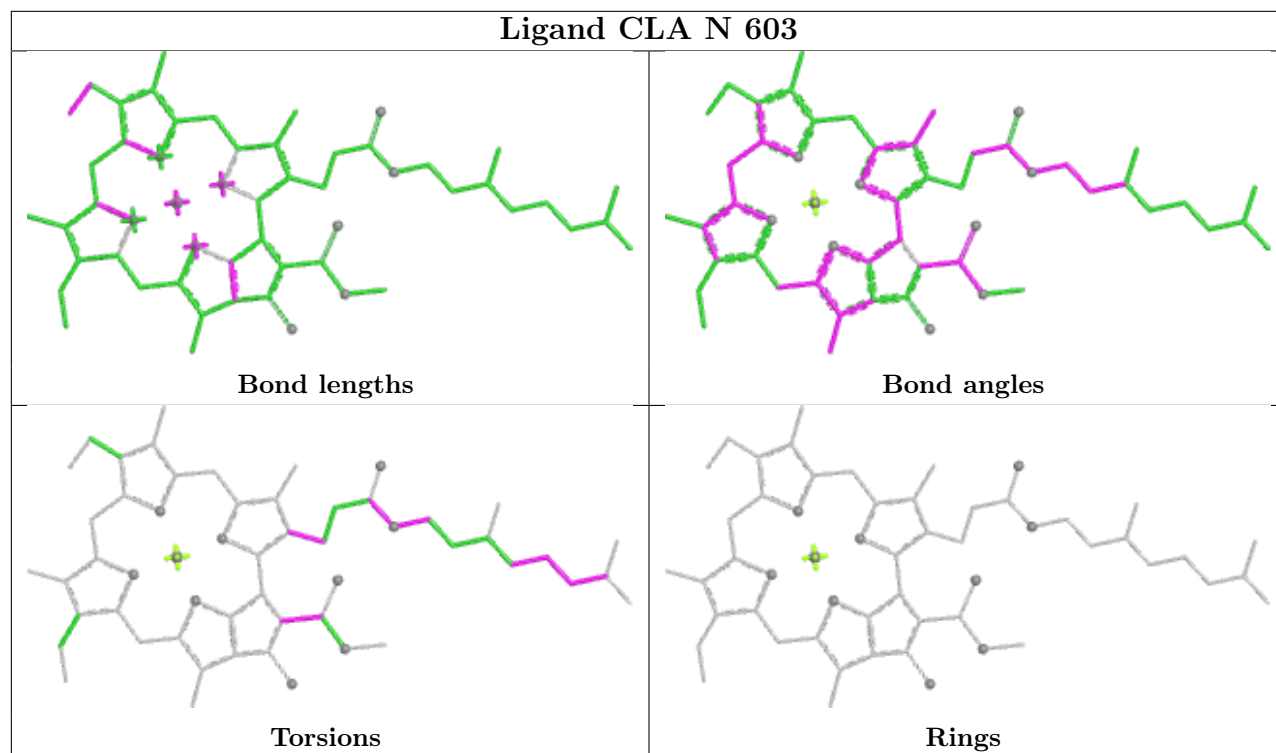




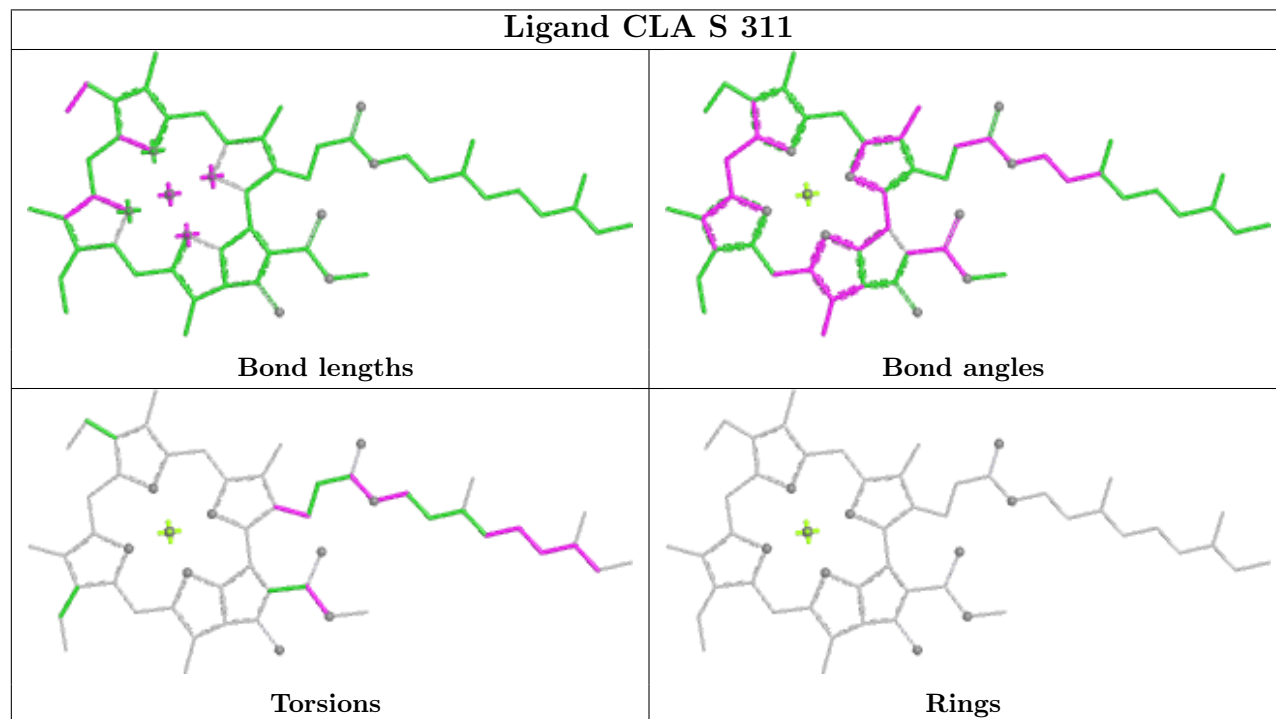


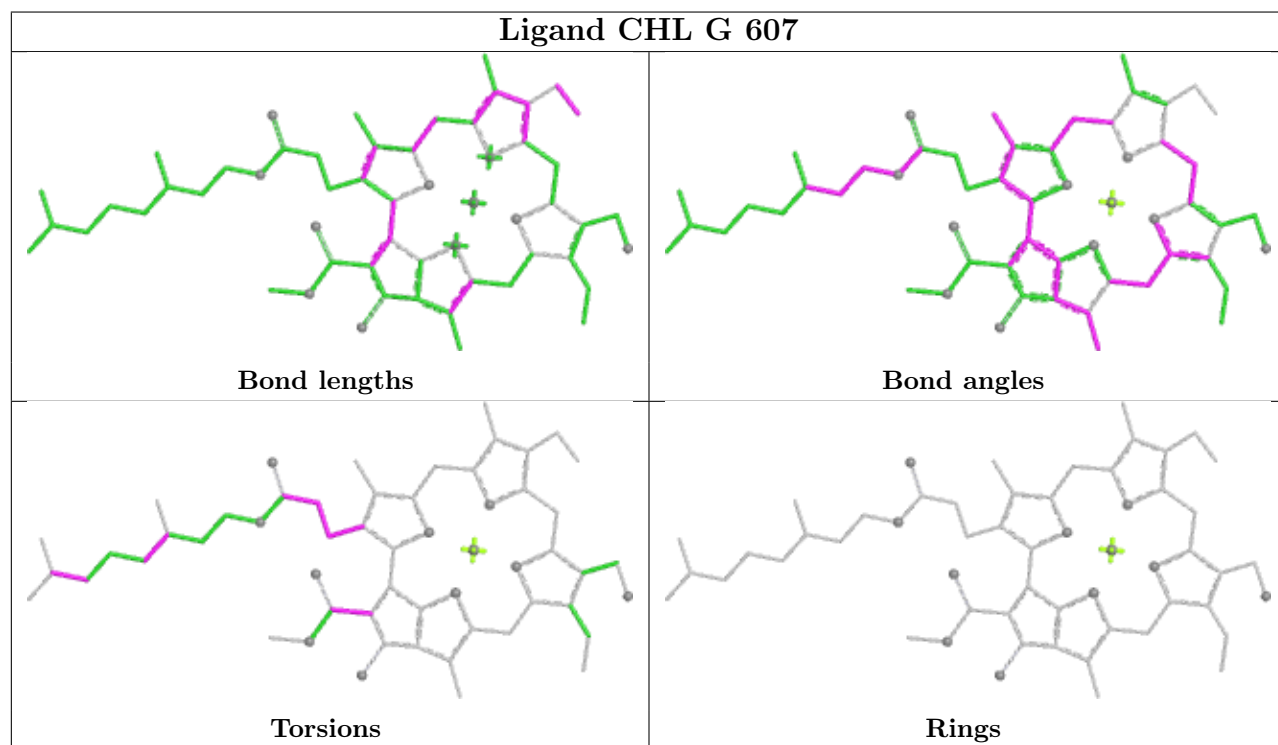
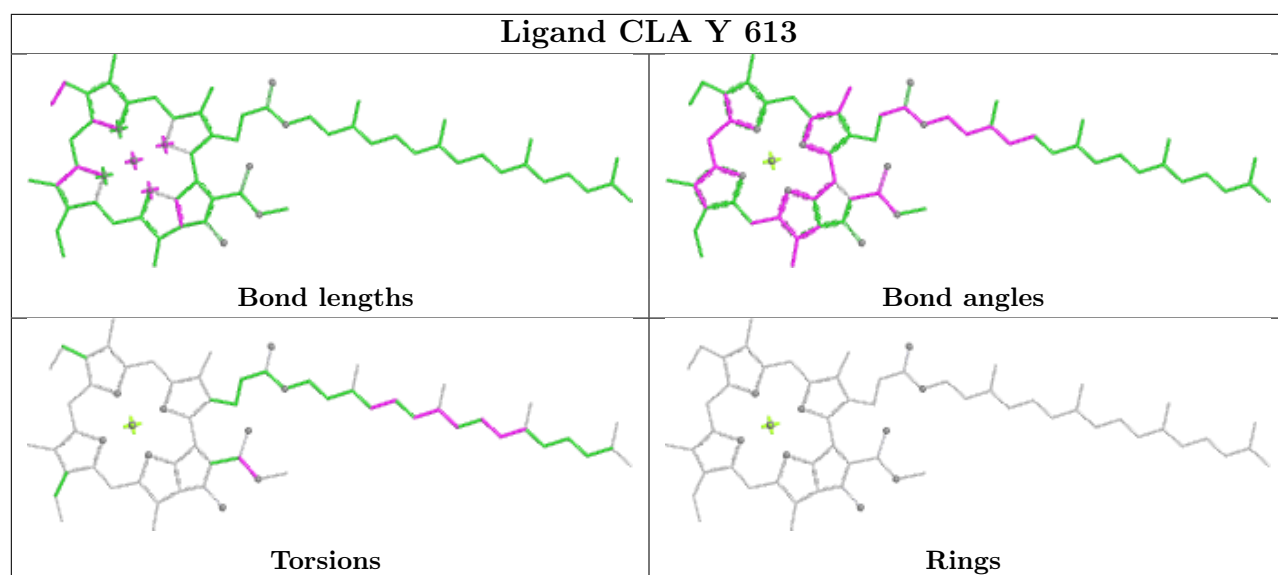


## Ligand CLA N 603

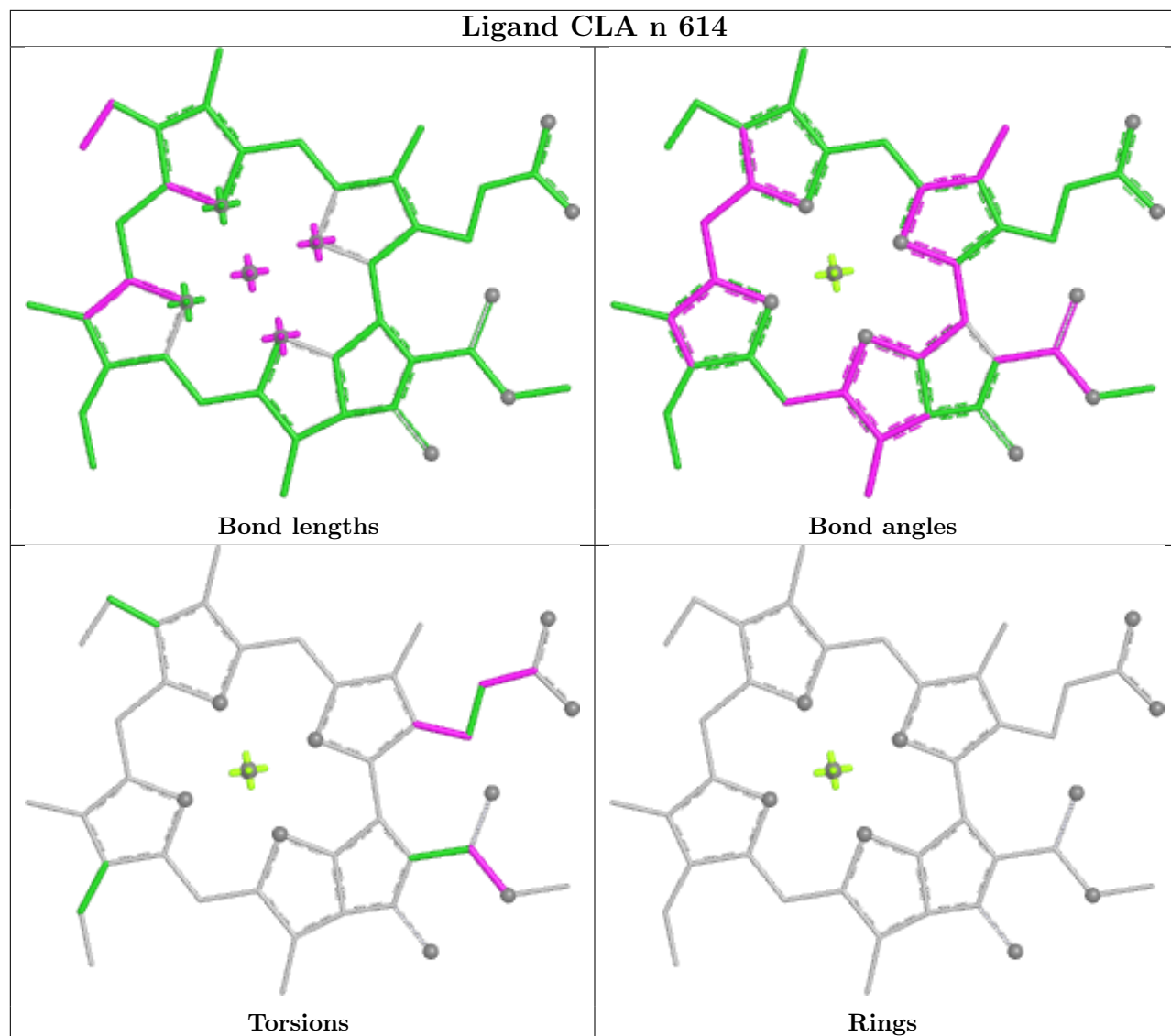


## Ligand CLA S 311

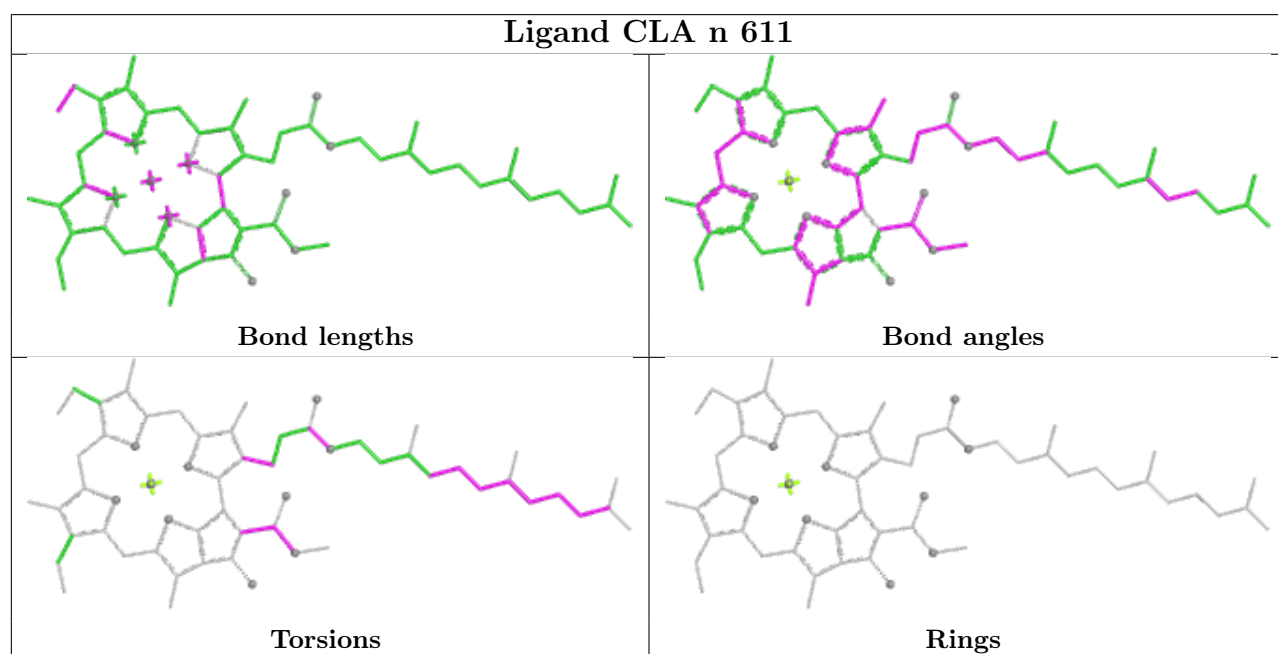
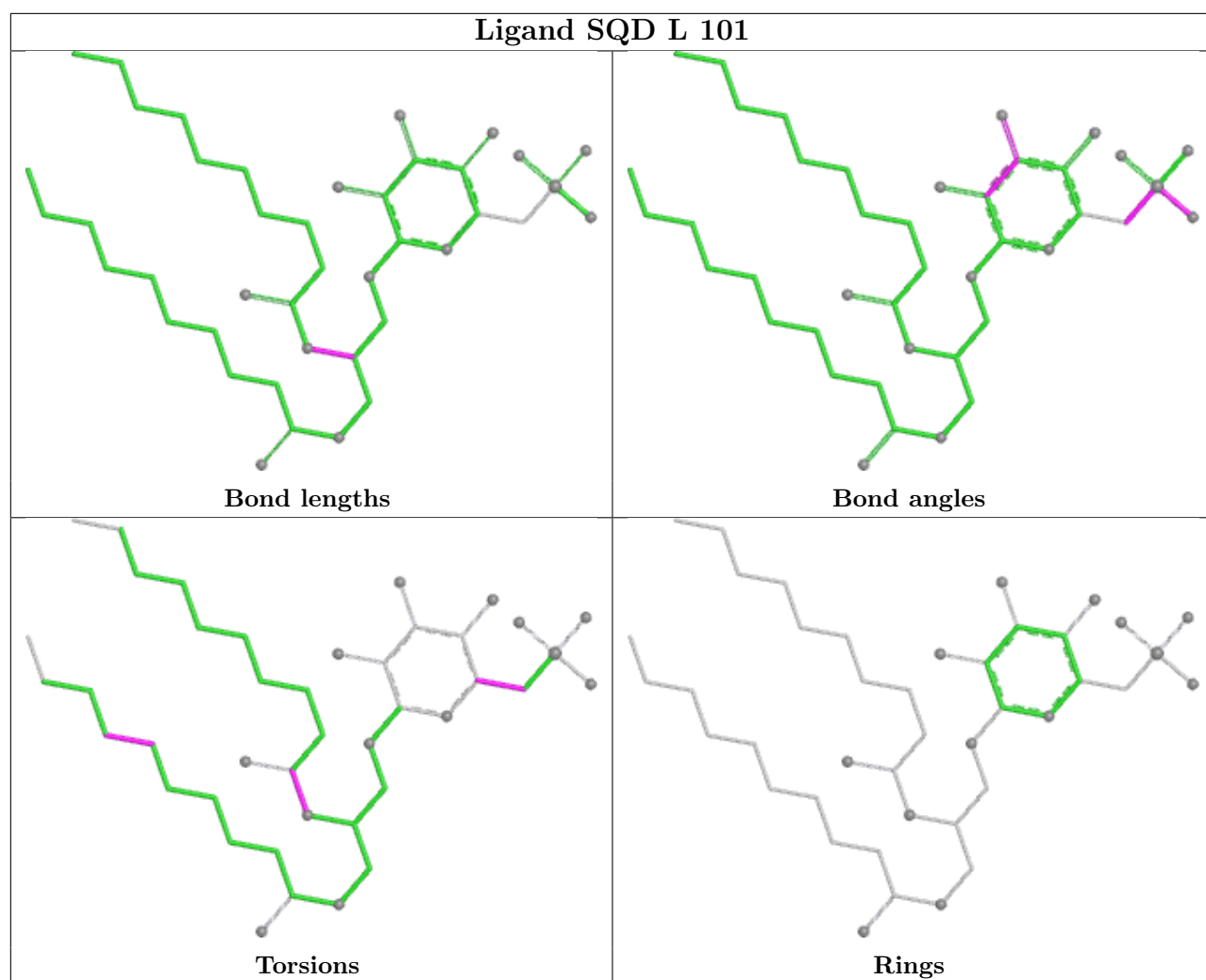


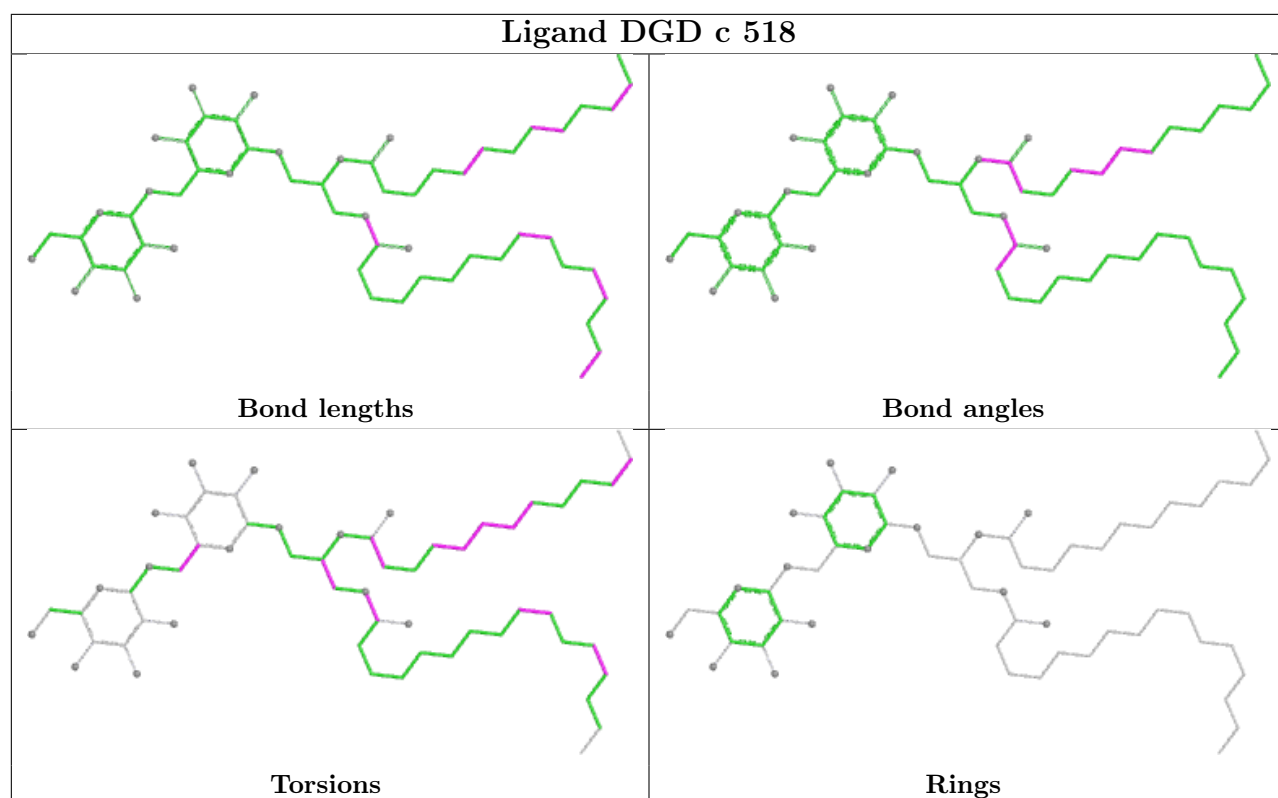


## Ligand CLA n 614

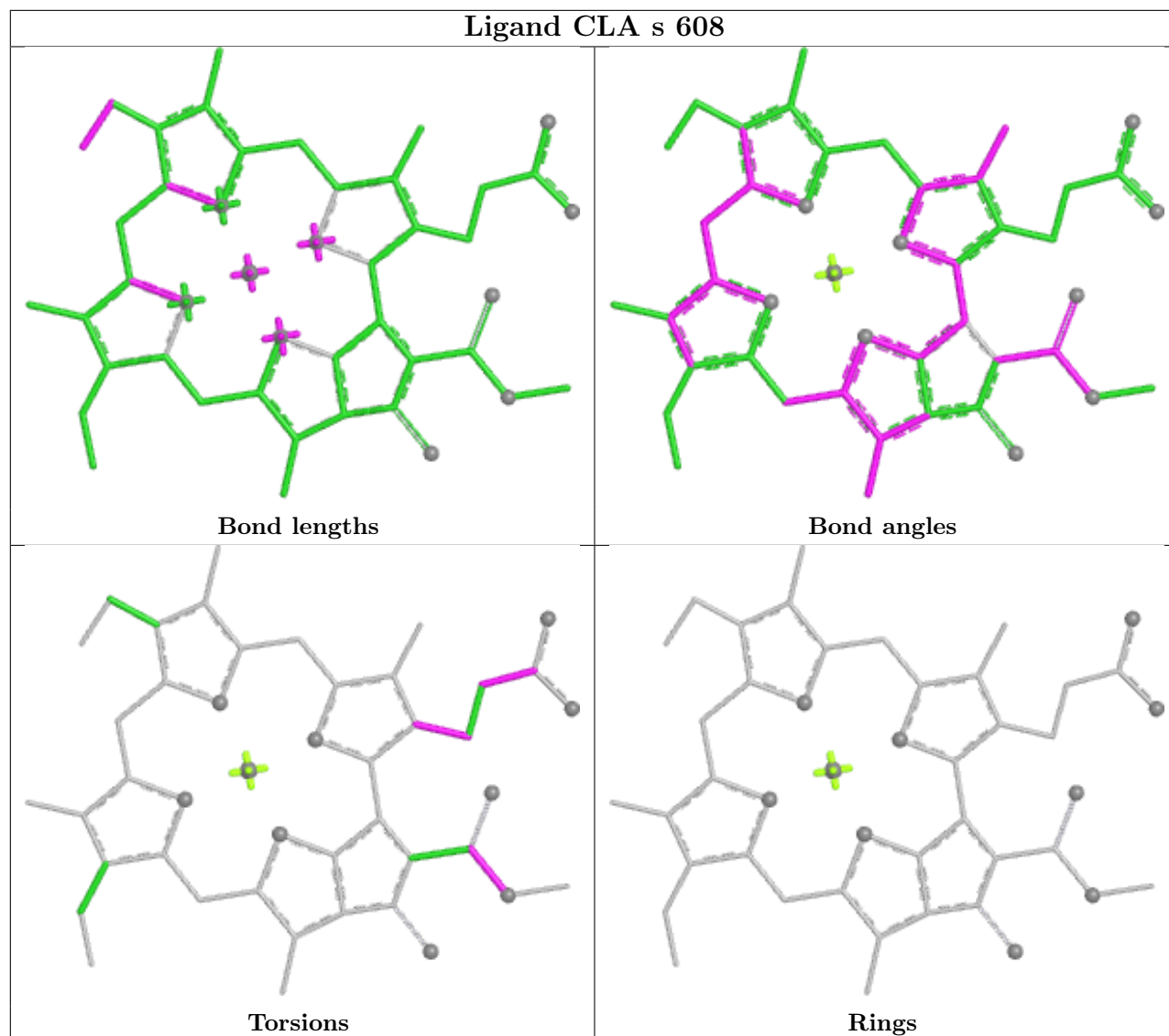




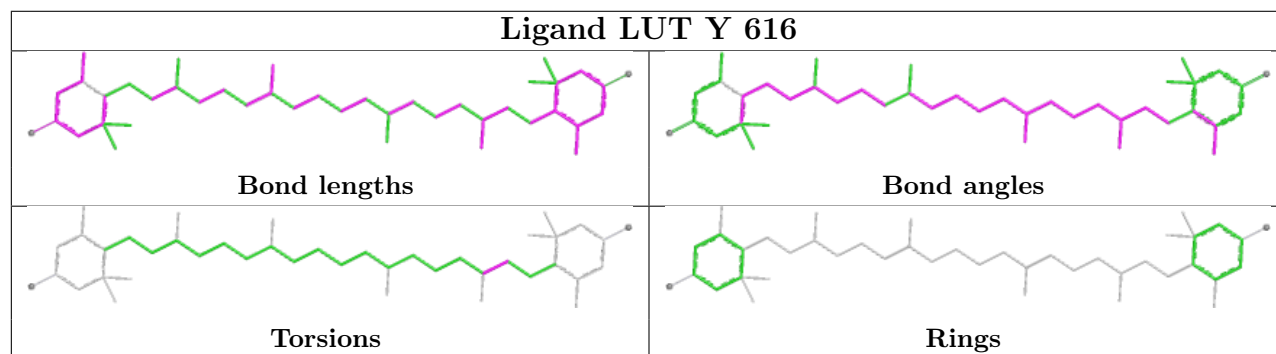


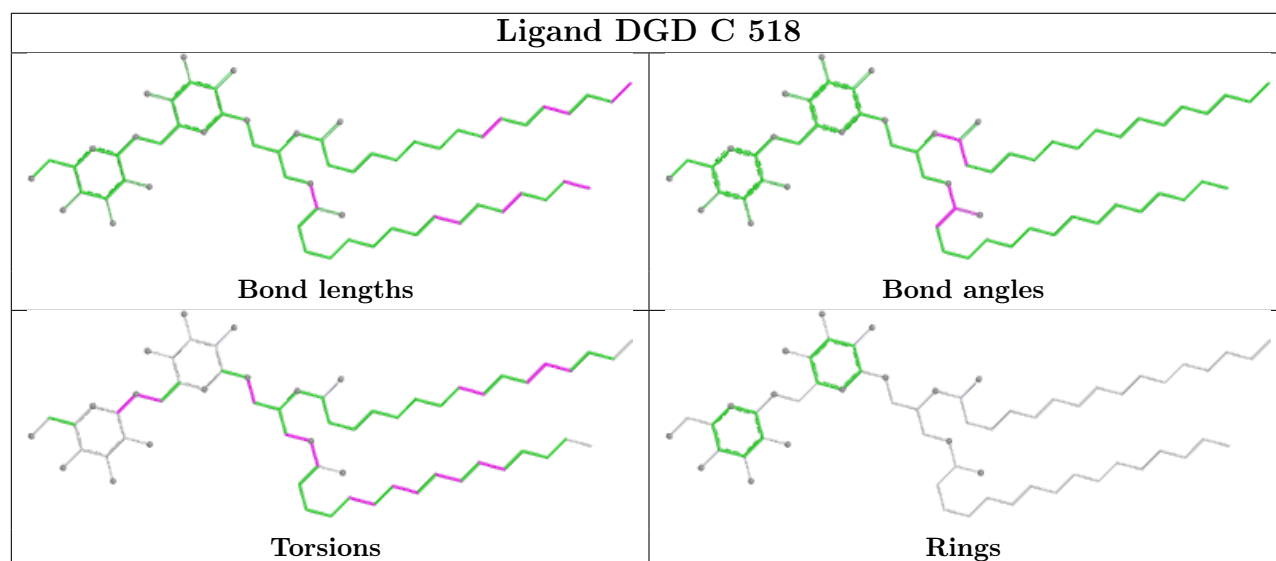
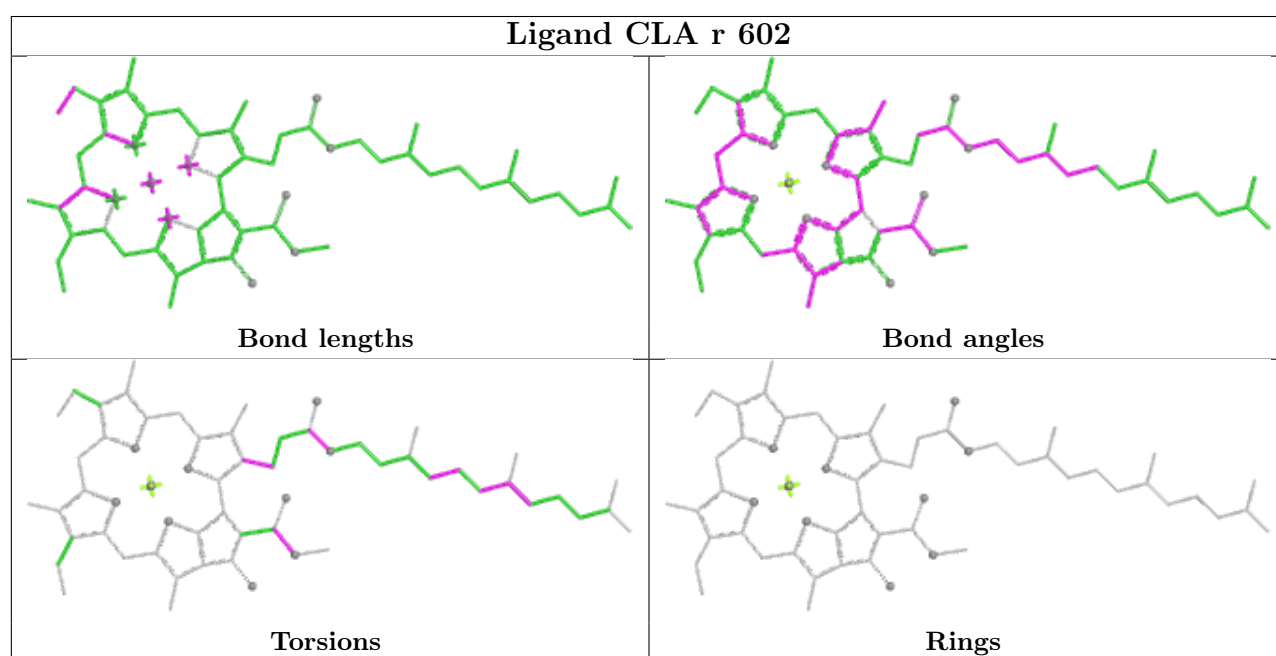
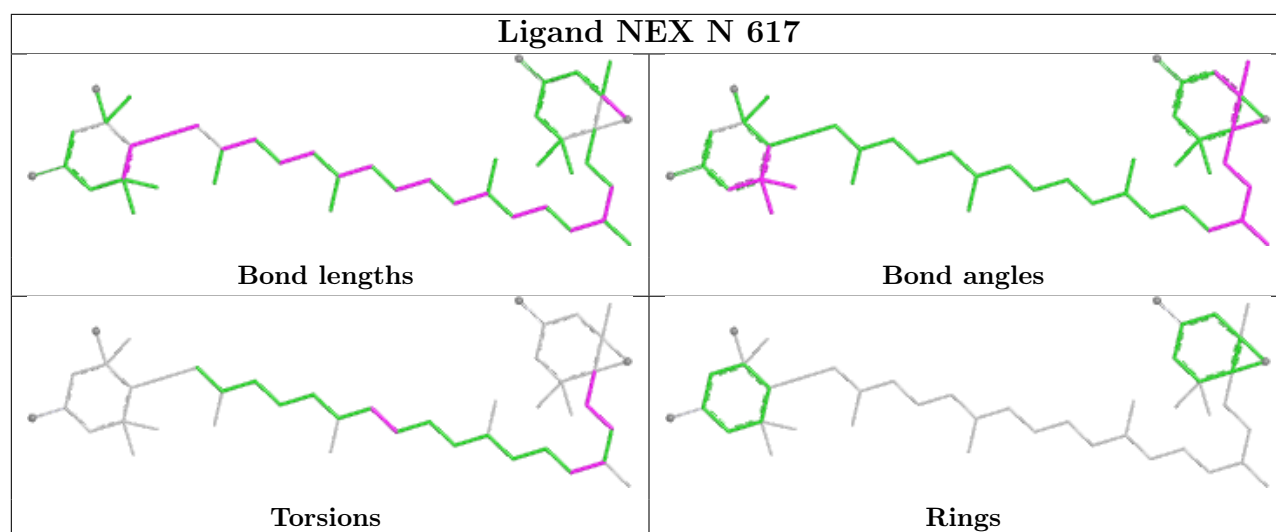


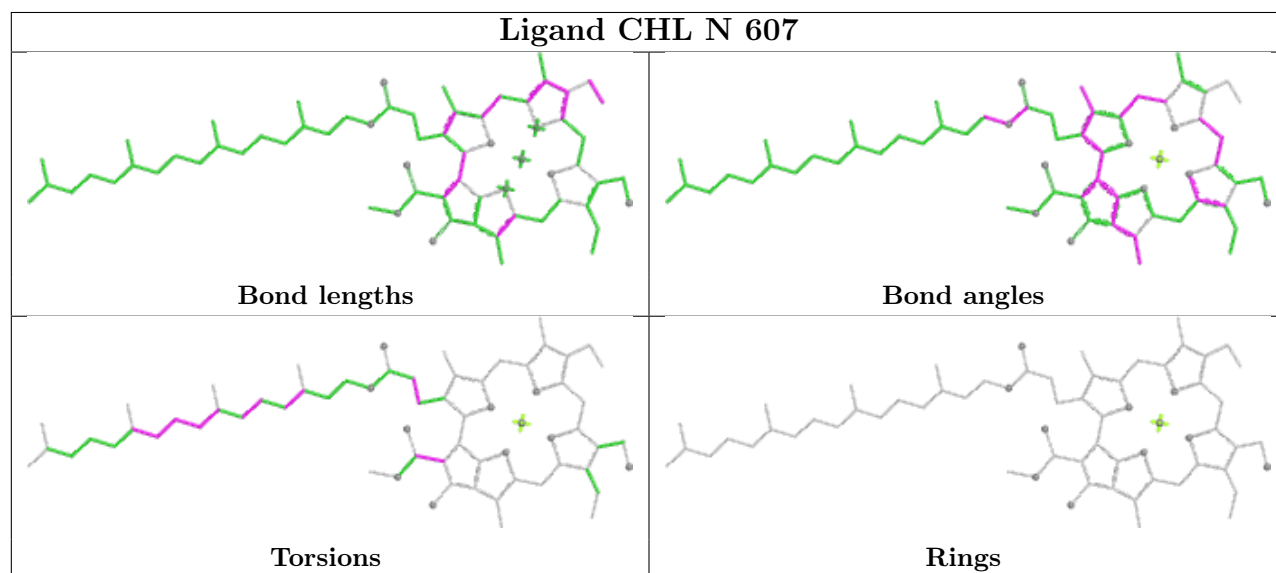
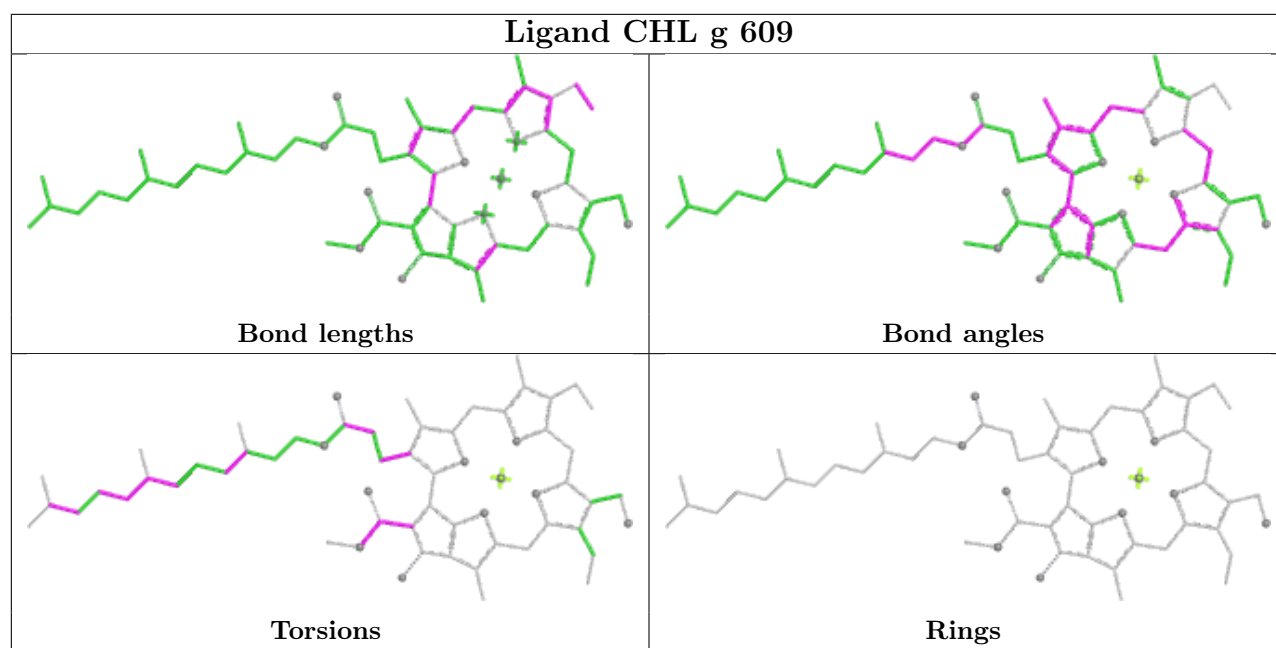
## Ligand CLA s 608

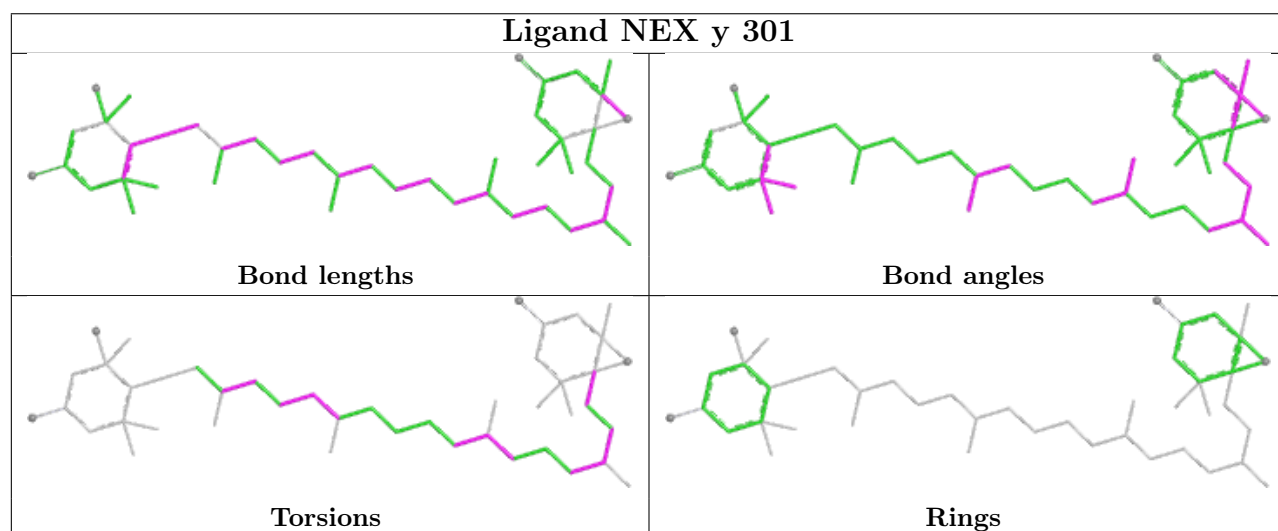
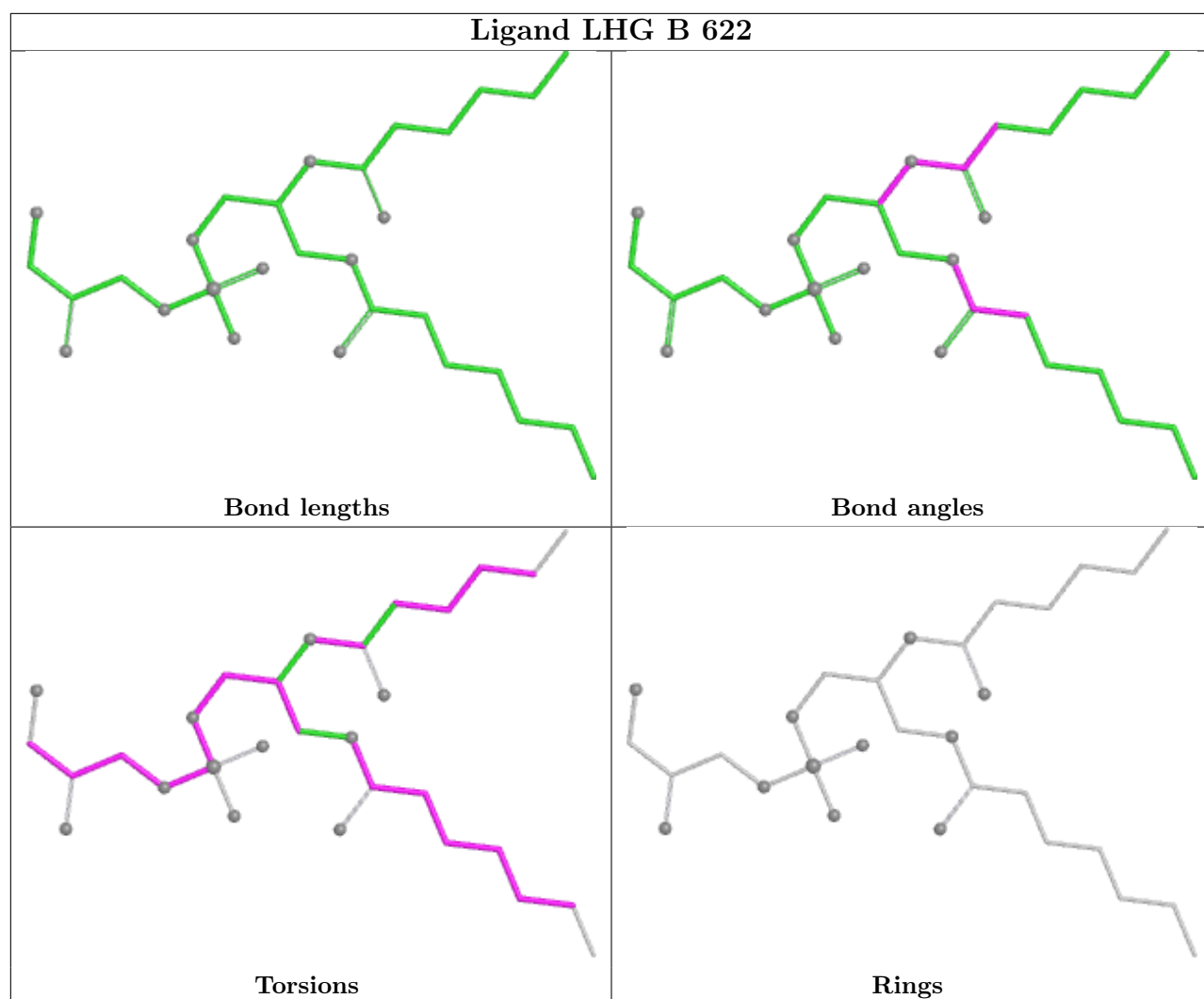


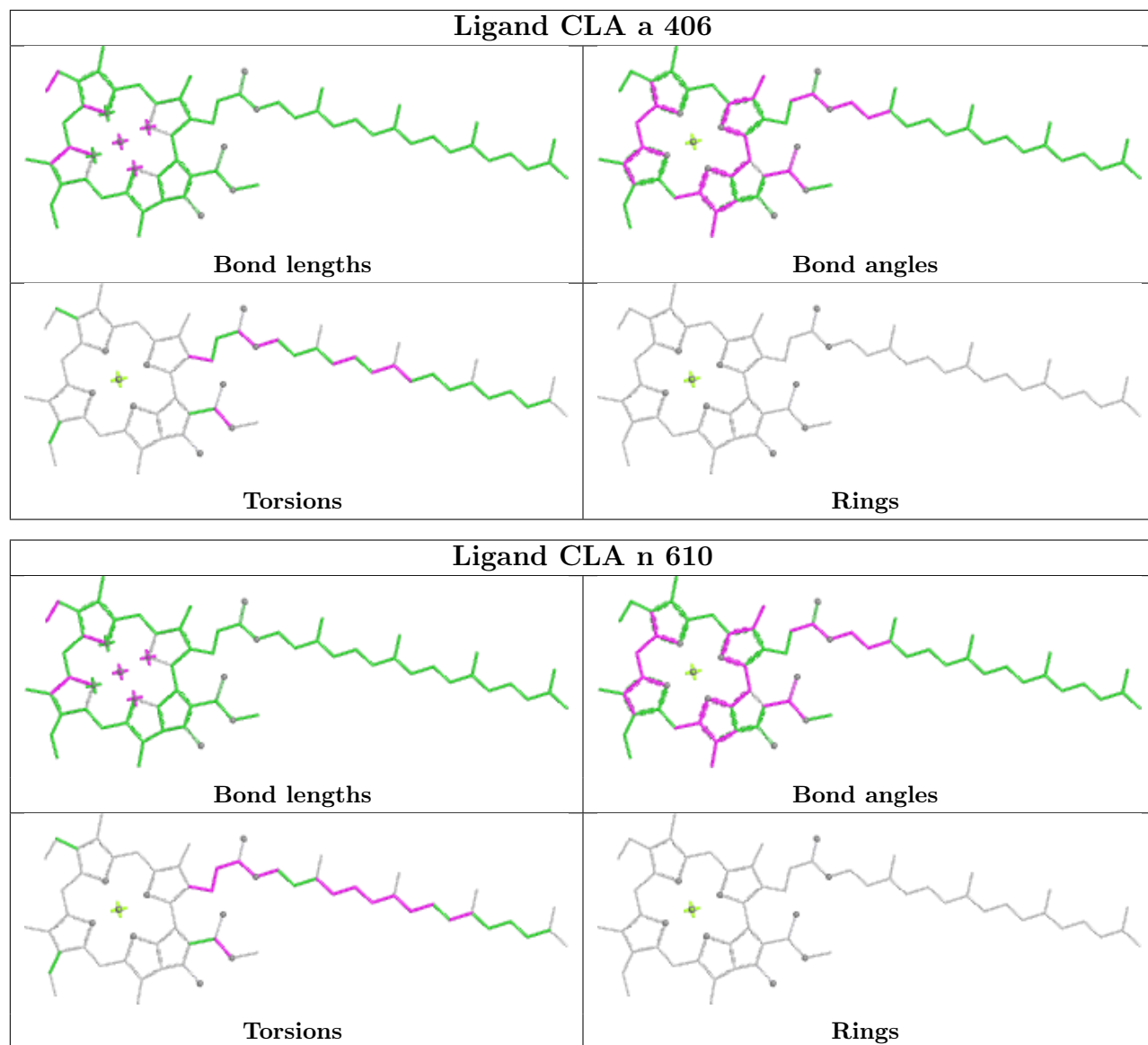
## Ligand LUT Y 616

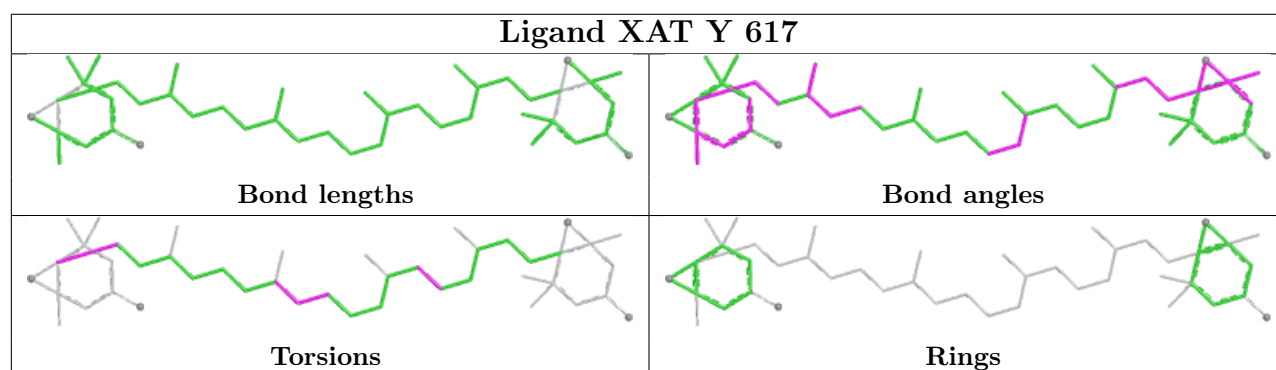
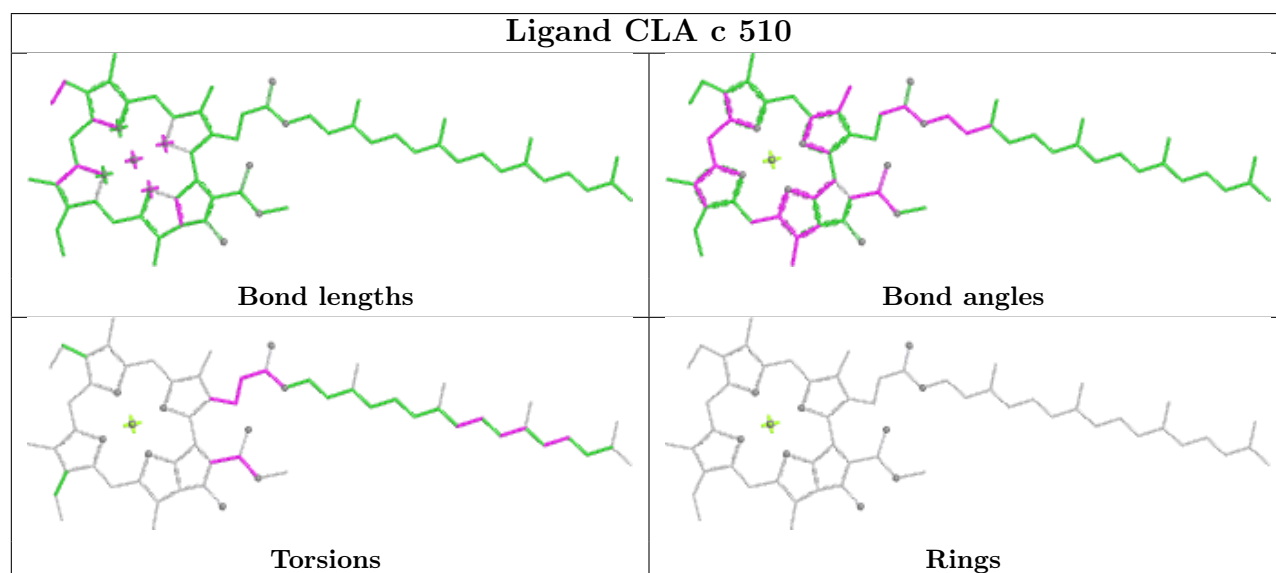
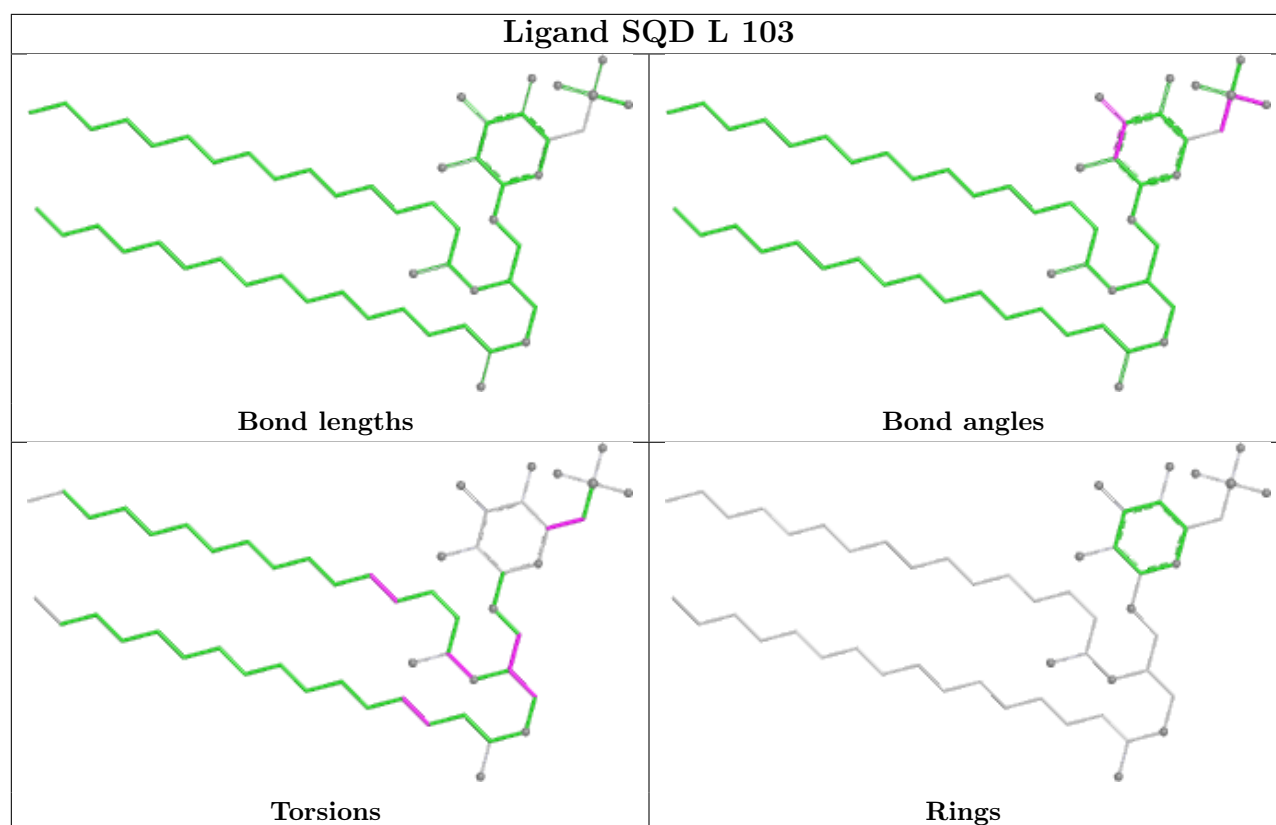




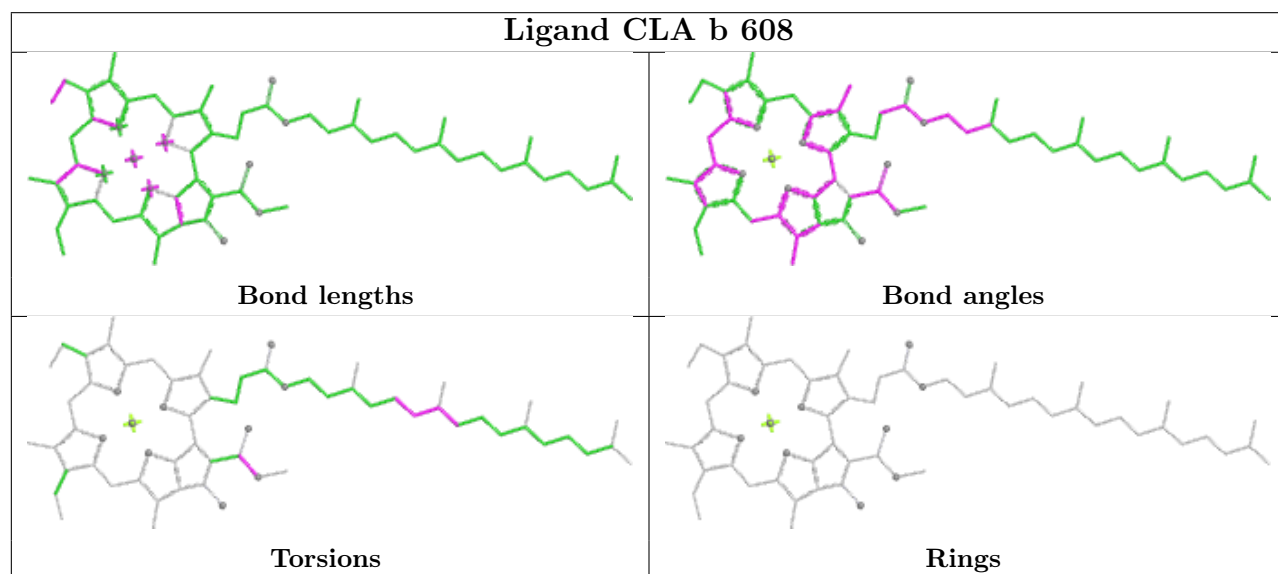
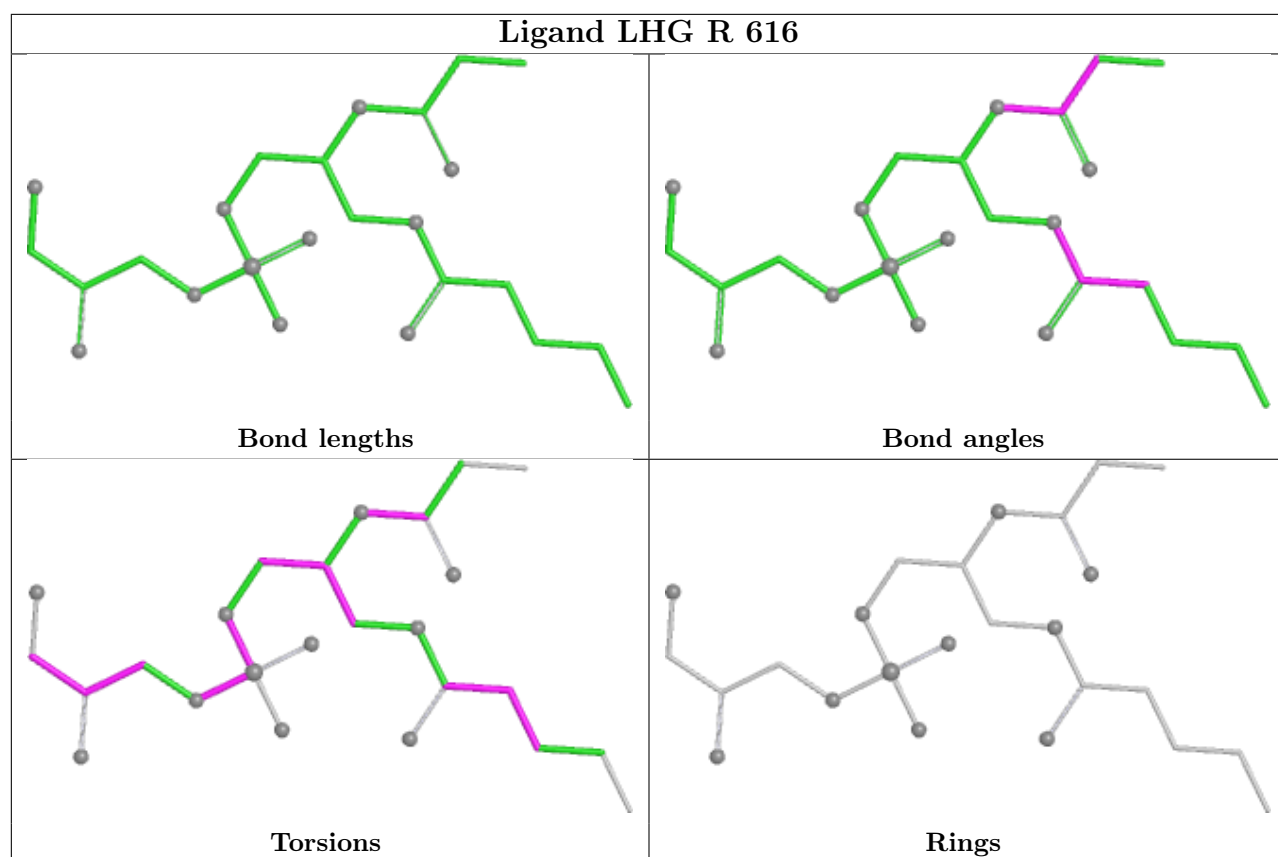


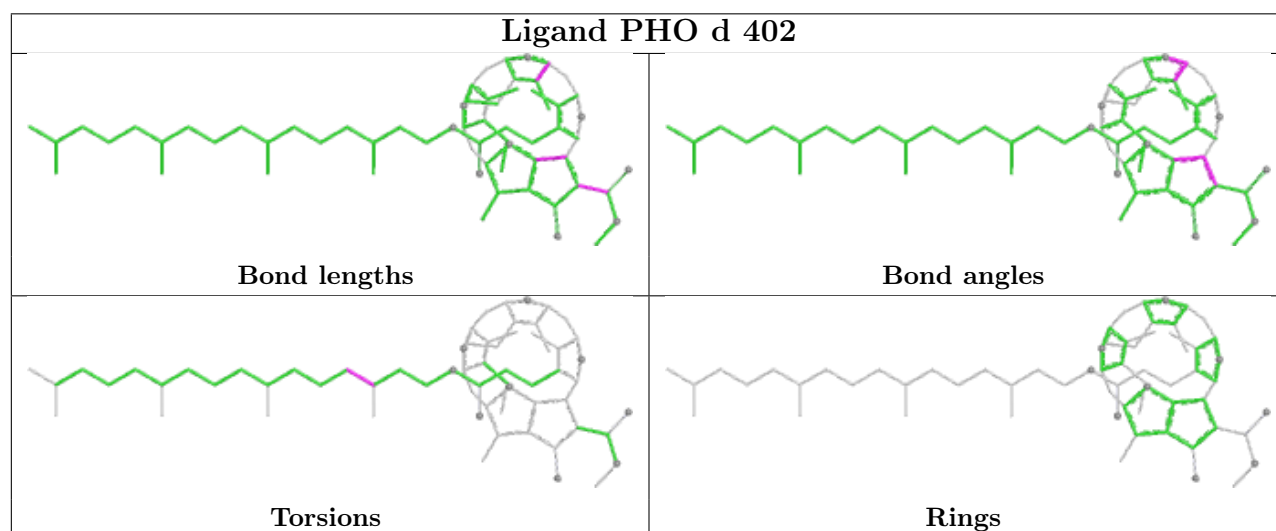
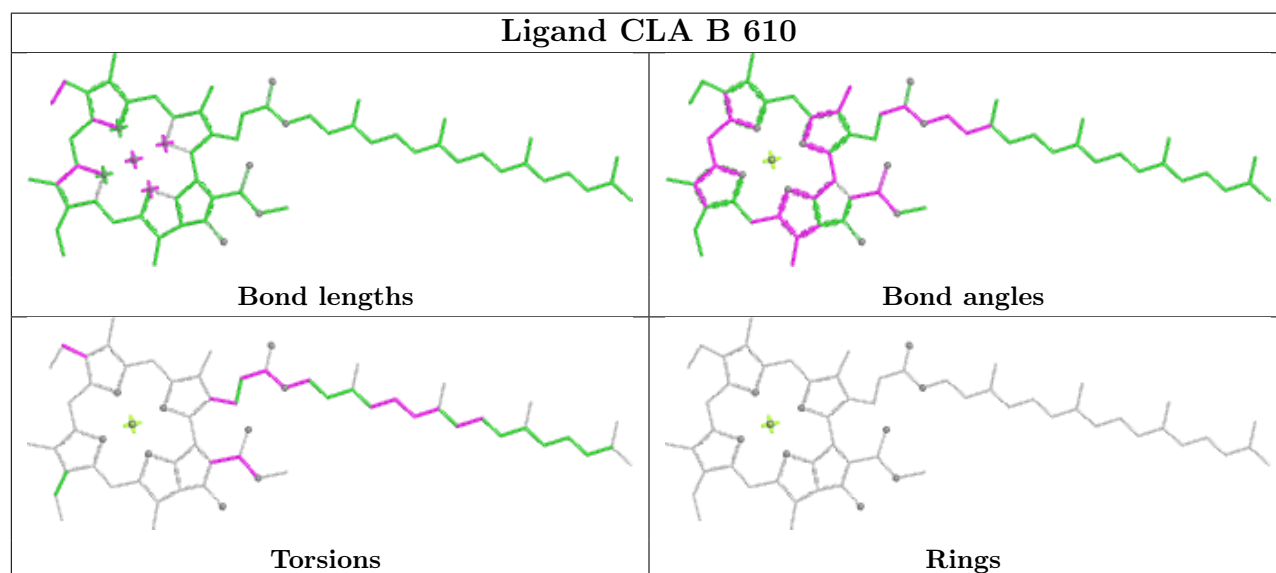
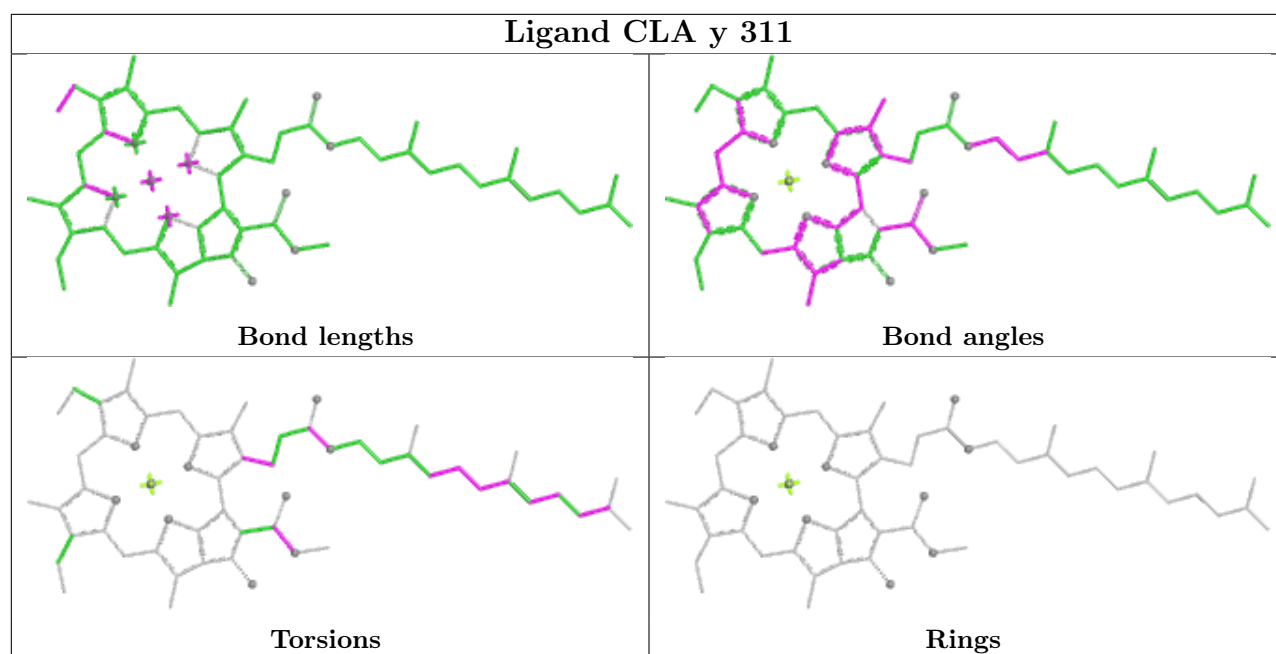




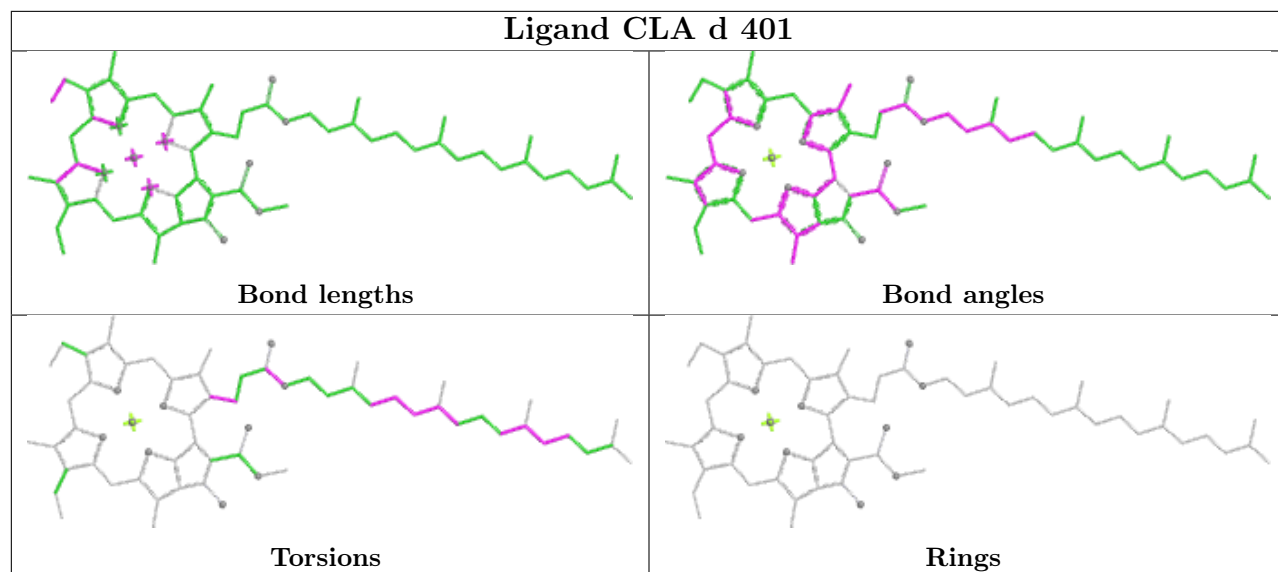




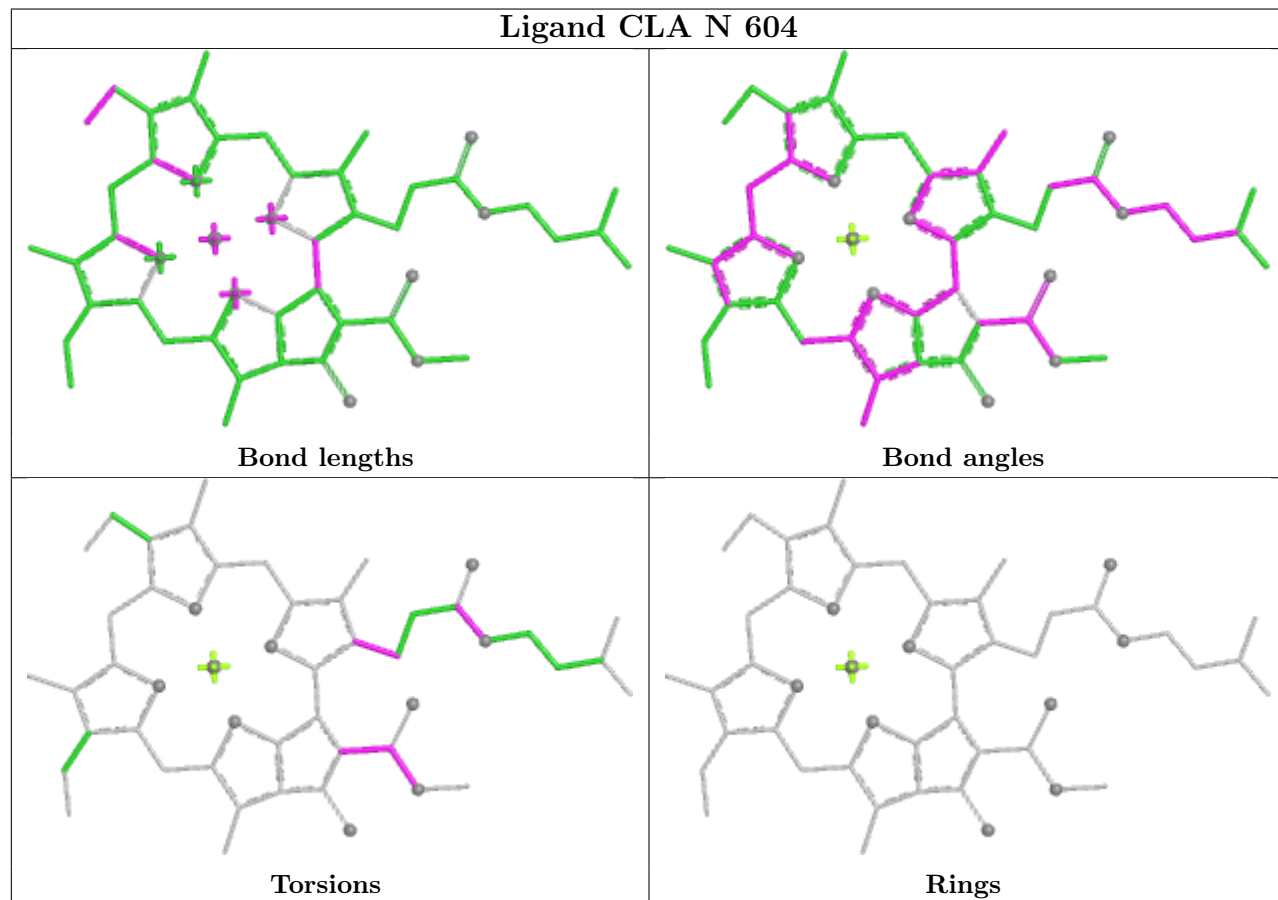


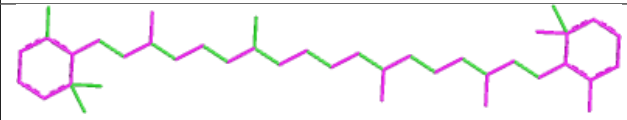
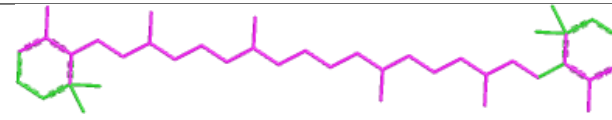
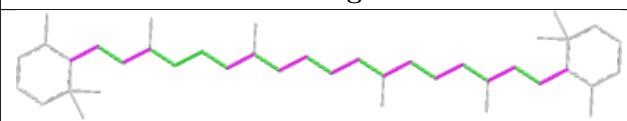
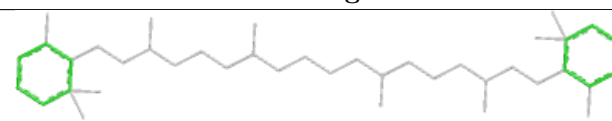


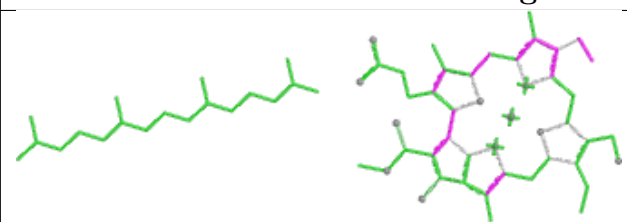
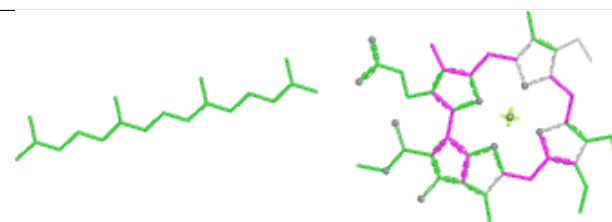
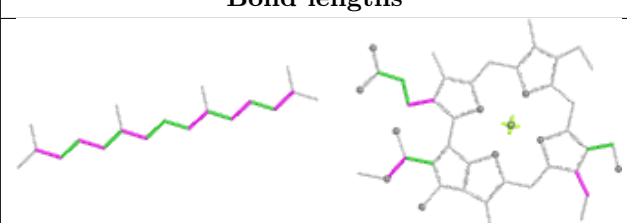
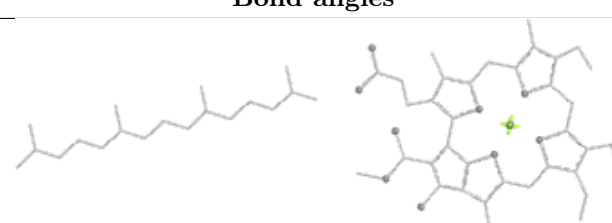
## Ligand CLA d 401

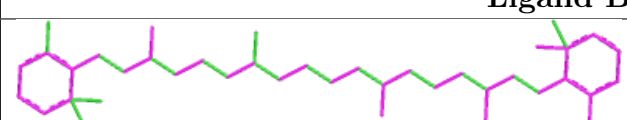
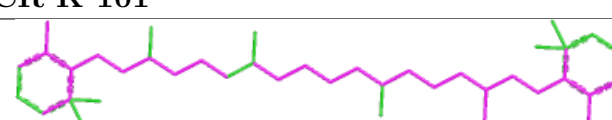
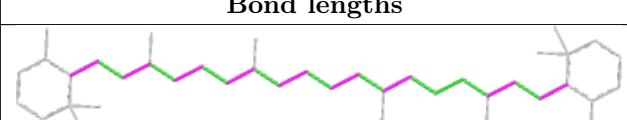
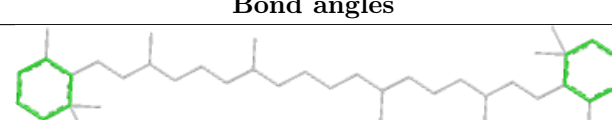




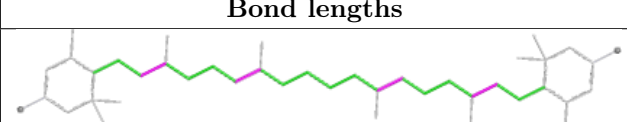
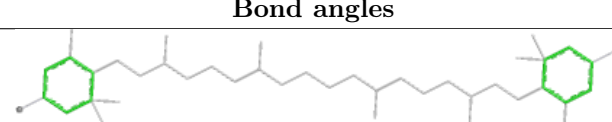
## Ligand CLA N 604

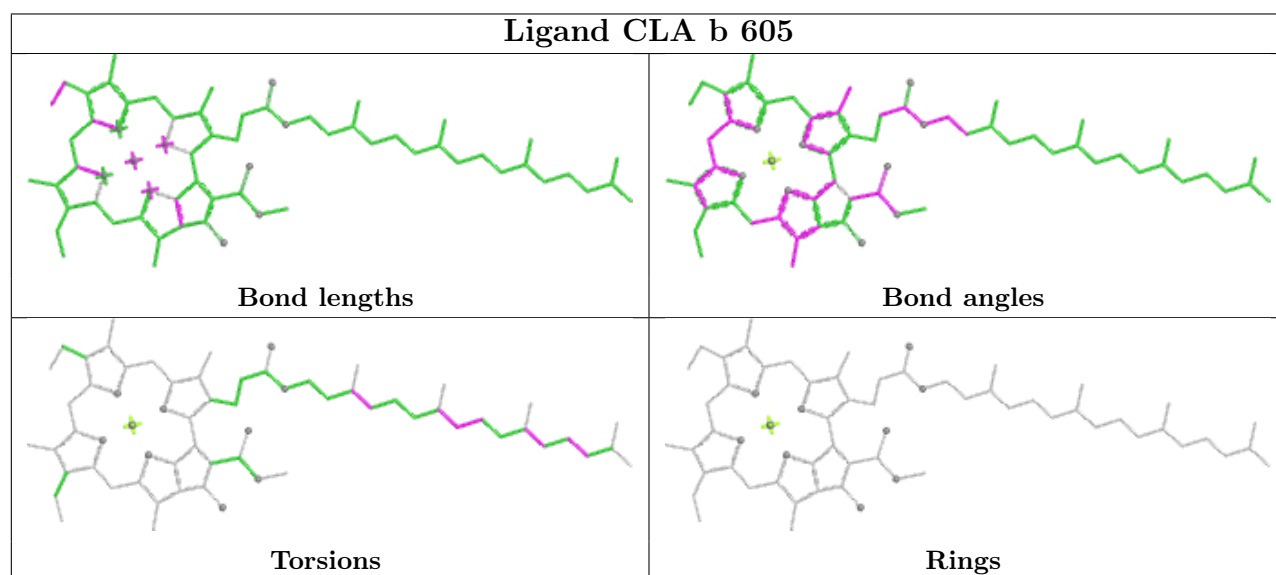
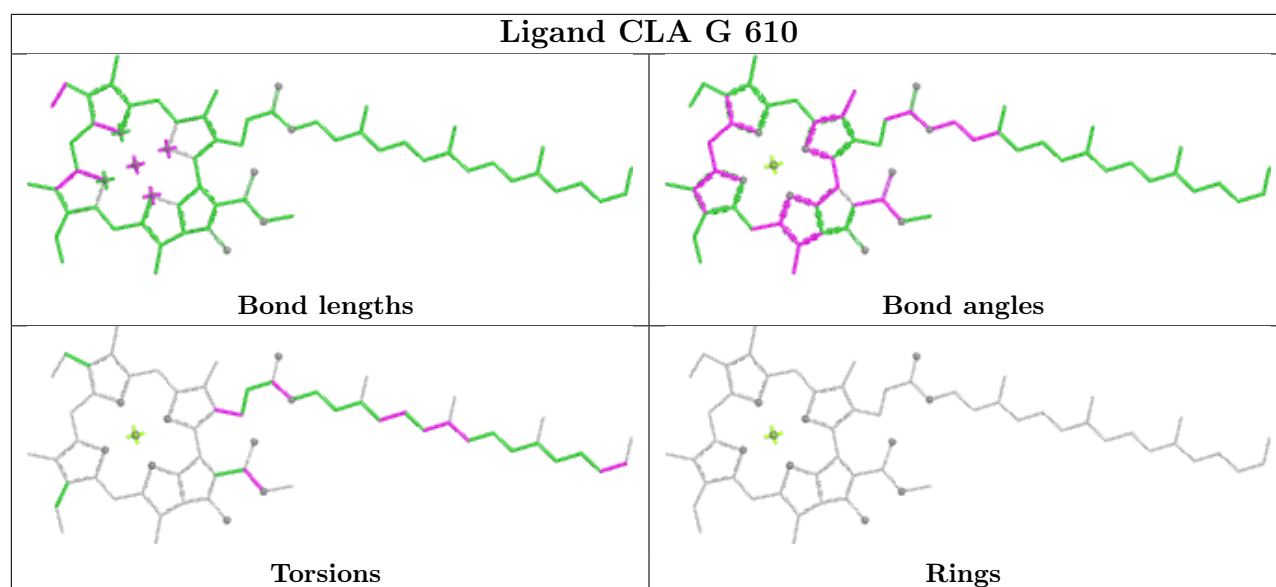


Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

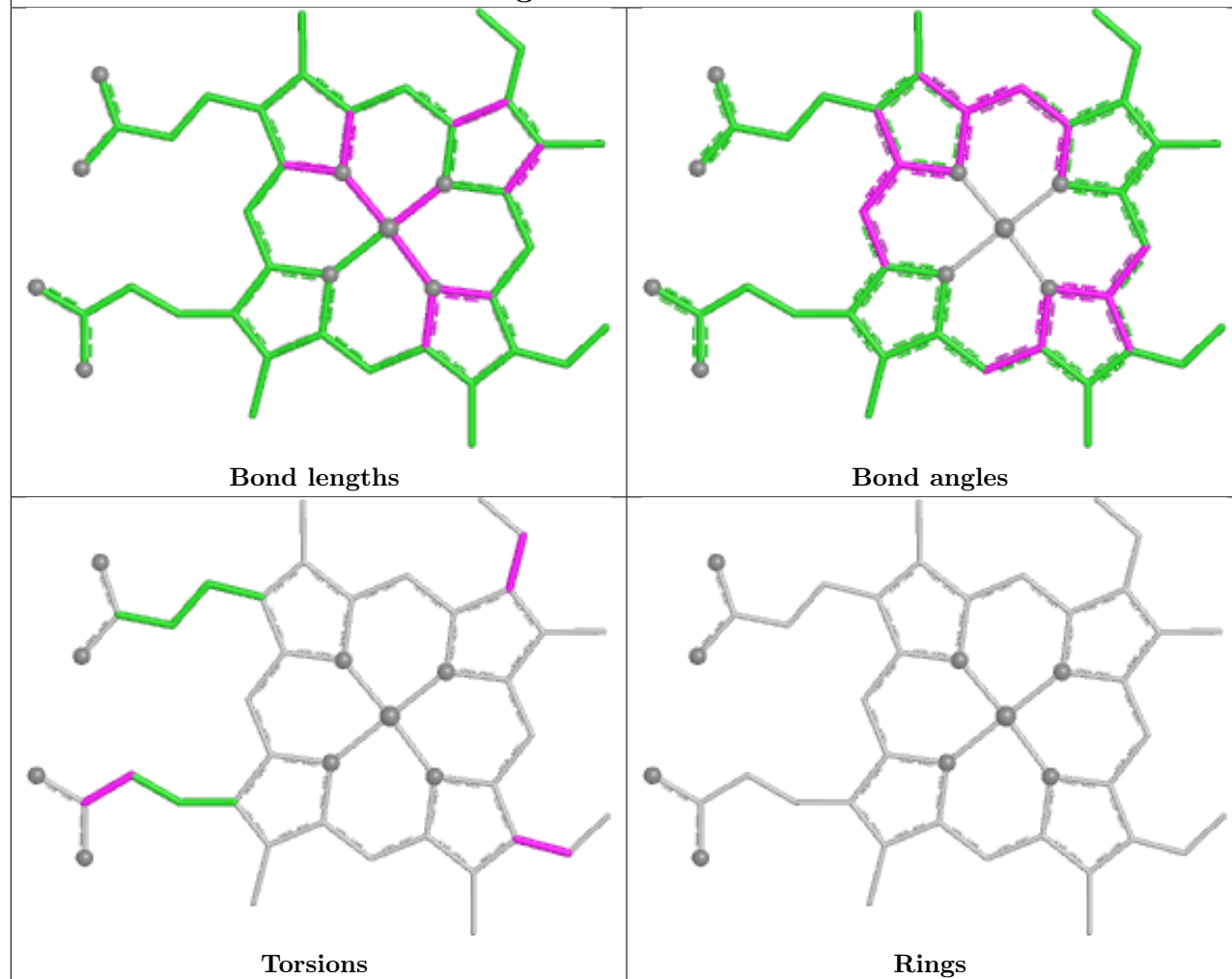
Ligand CHL N 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

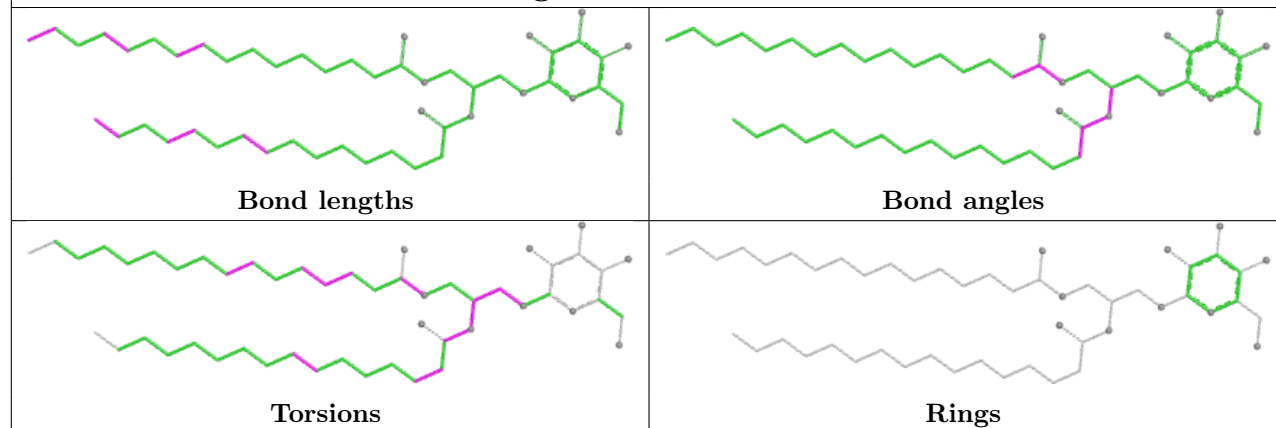
Ligand LUT s 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

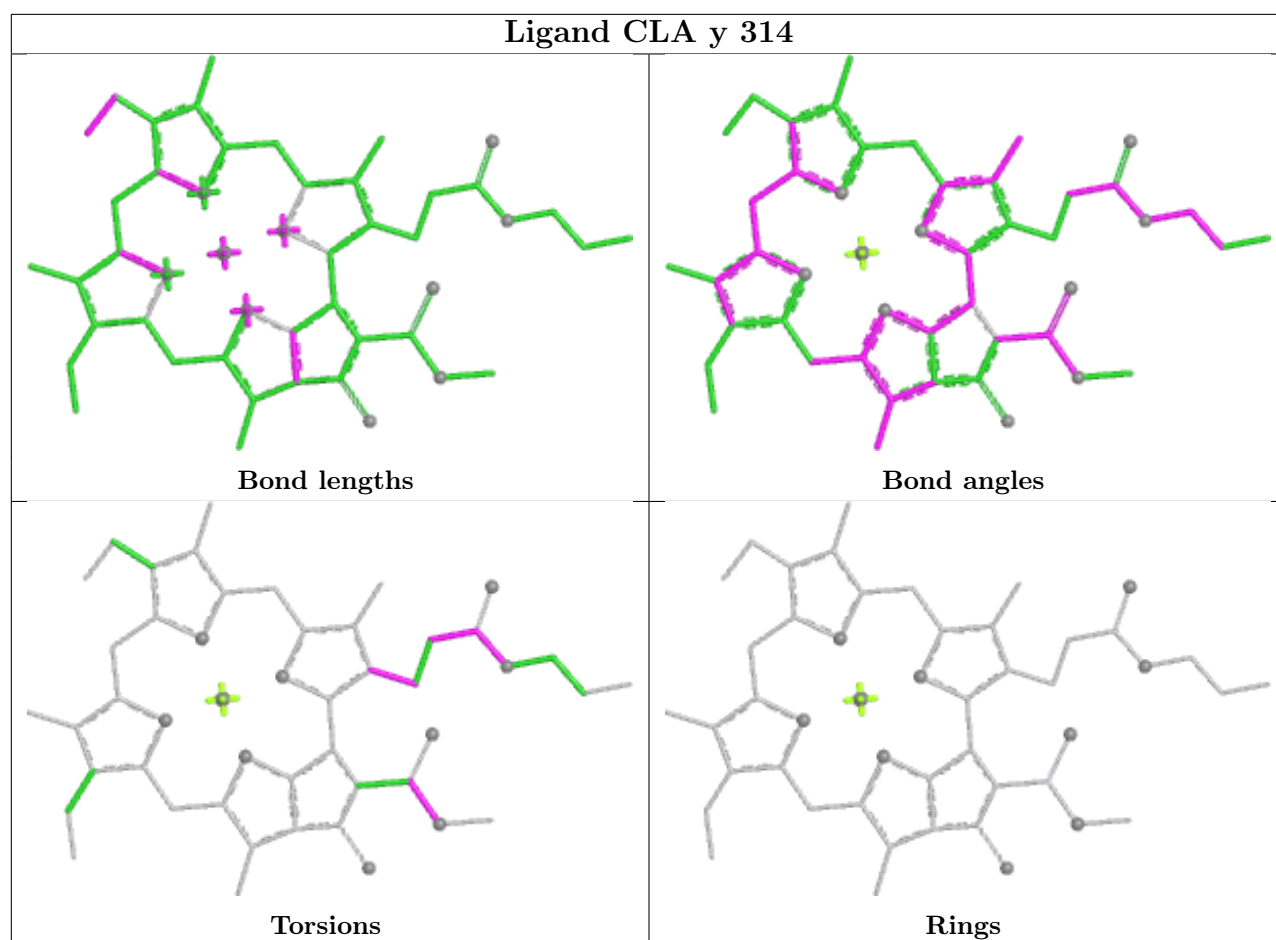


## Ligand HEM f 101



## Ligand LMG c 521





## 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.

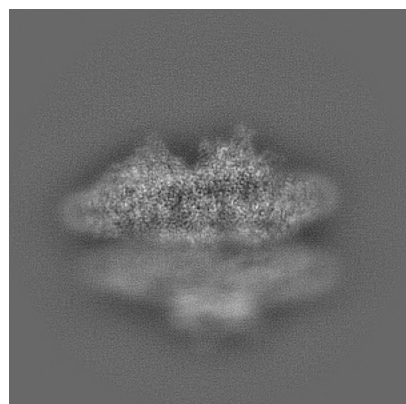
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52846. These allow visual inspection of the internal detail of the map and identification of artifacts.

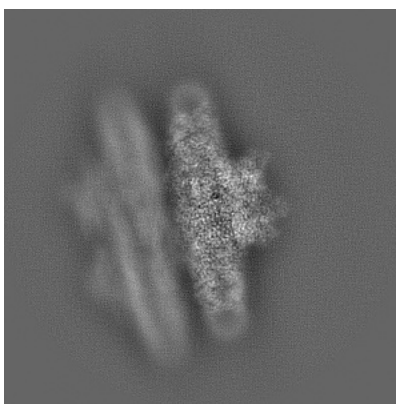
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

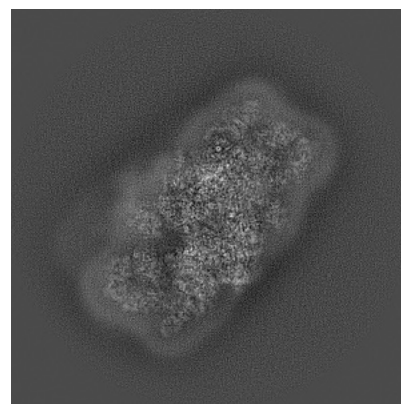
#### 6.1.1 Primary map



X

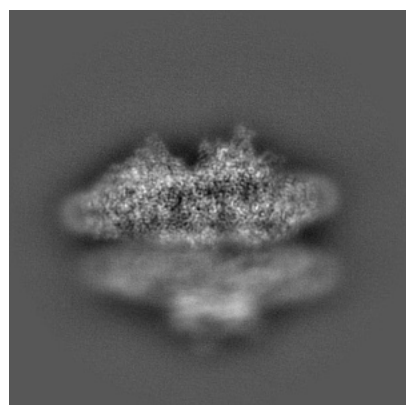


Y

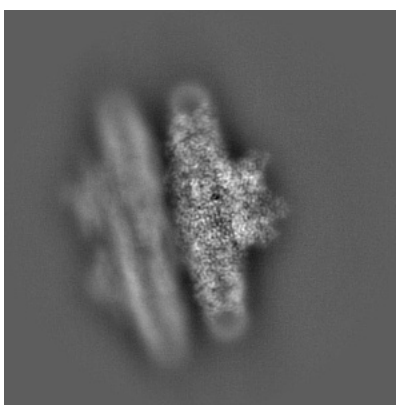


Z

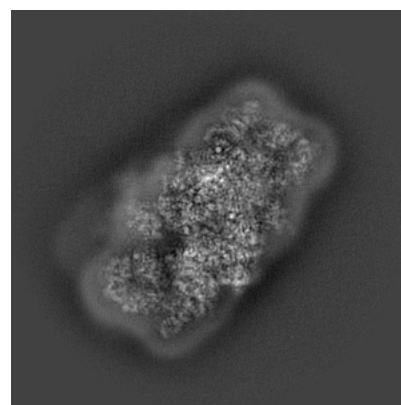
#### 6.1.2 Raw map



X



Y



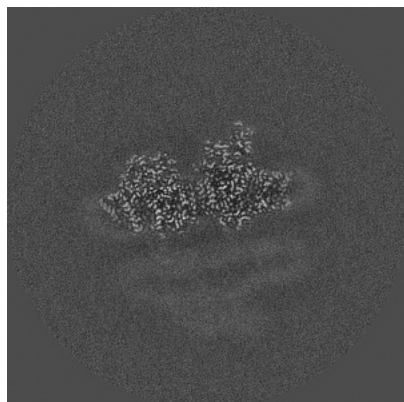
Z

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

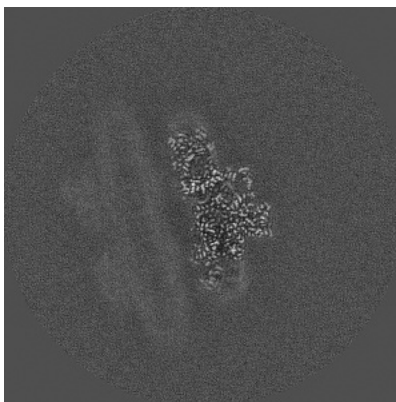


## 6.2 Central slices [i](#)

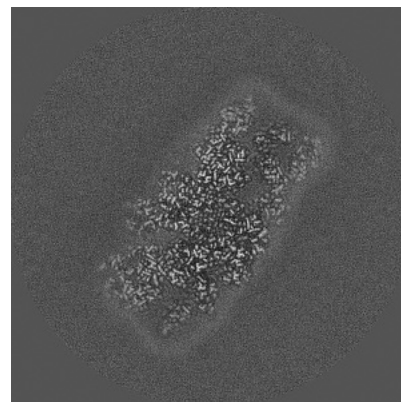
### 6.2.1 Primary map



X Index: 250

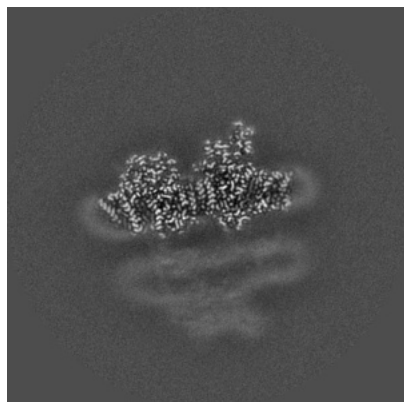


Y Index: 250

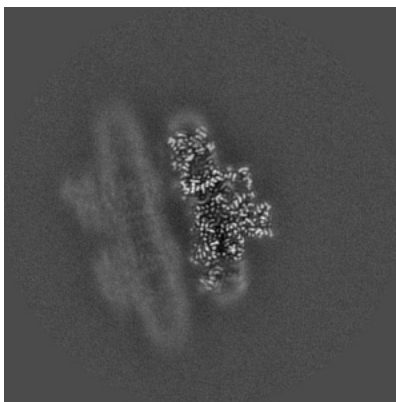


Z Index: 250

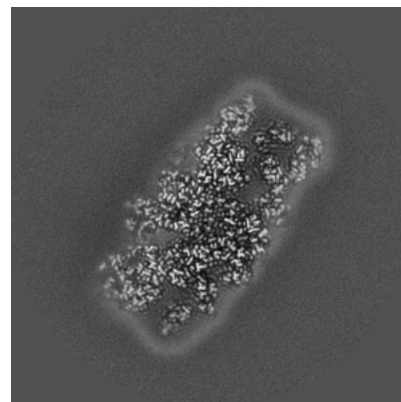
### 6.2.2 Raw map



X Index: 250



Y Index: 250

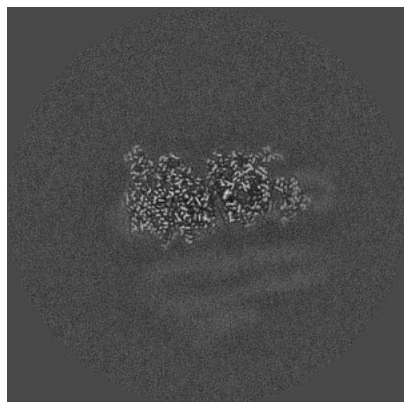


Z Index: 250

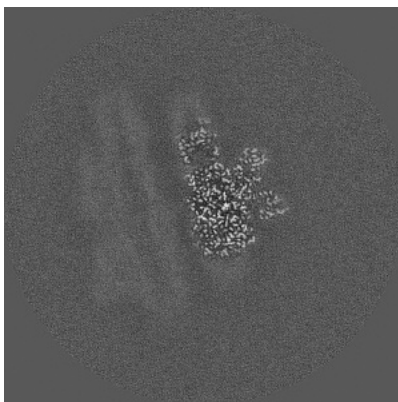
The images above show central slices of the map in three orthogonal directions.

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

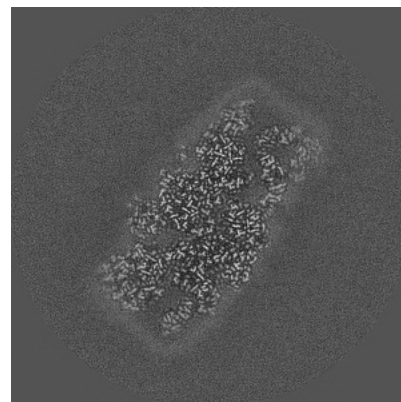
### 6.3.1 Primary map



X Index: 283

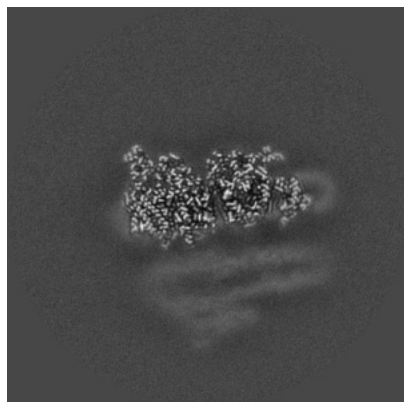


Y Index: 282

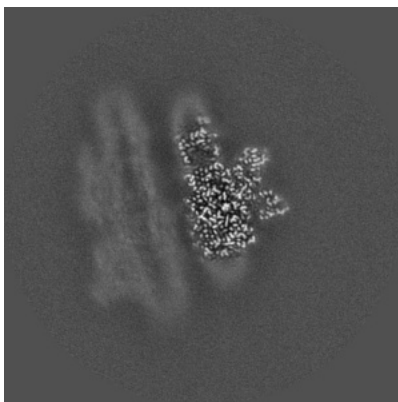


Z Index: 254

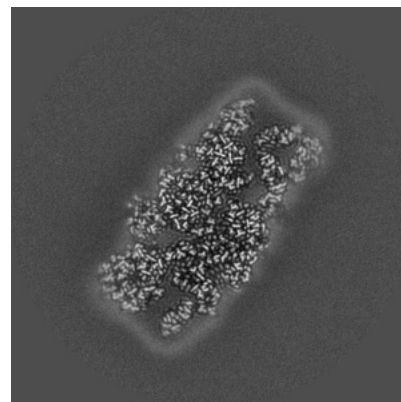
### 6.3.2 Raw map



X Index: 283



Y Index: 282

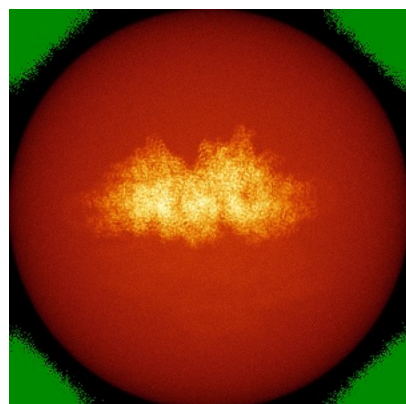


Z Index: 254

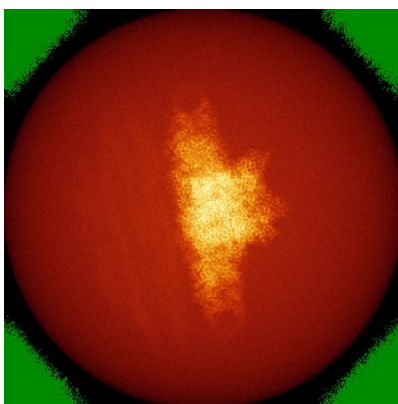
The images above show the largest variance slices of the map in three orthogonal directions.

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

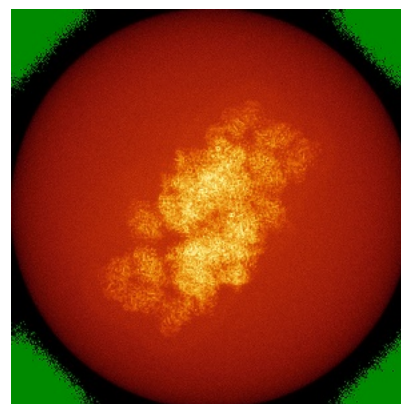
### 6.4.1 Primary map



X

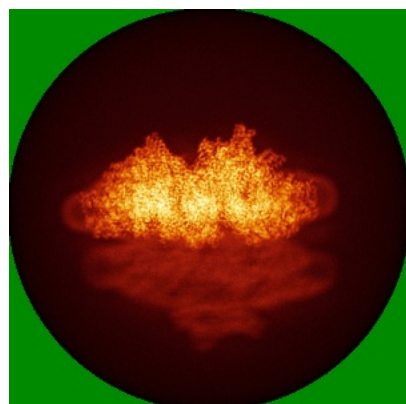


Y

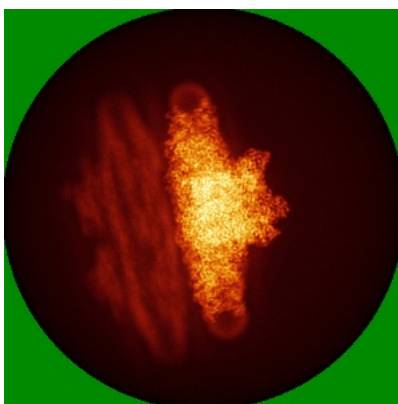


Z

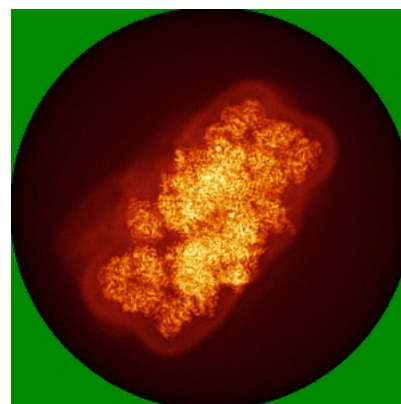
### 6.4.2 Raw map



X



Y

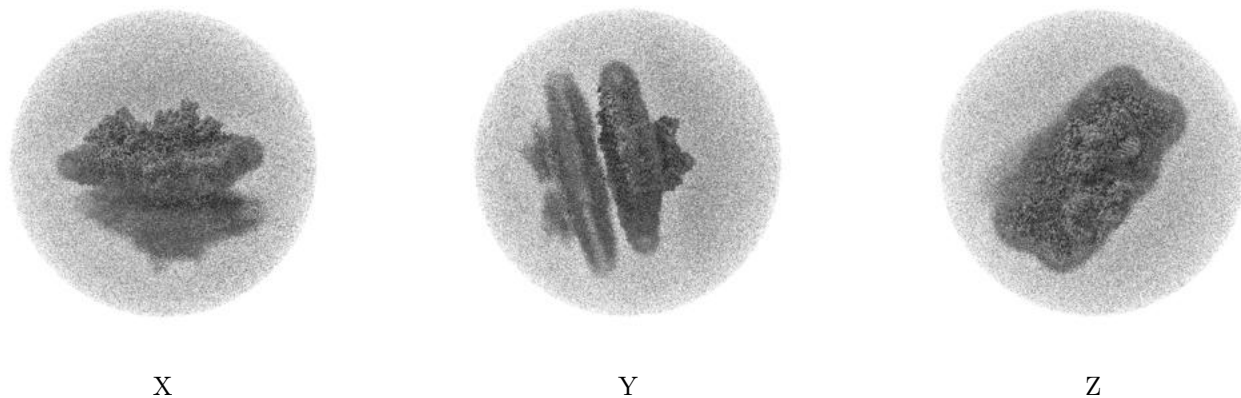


Z

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

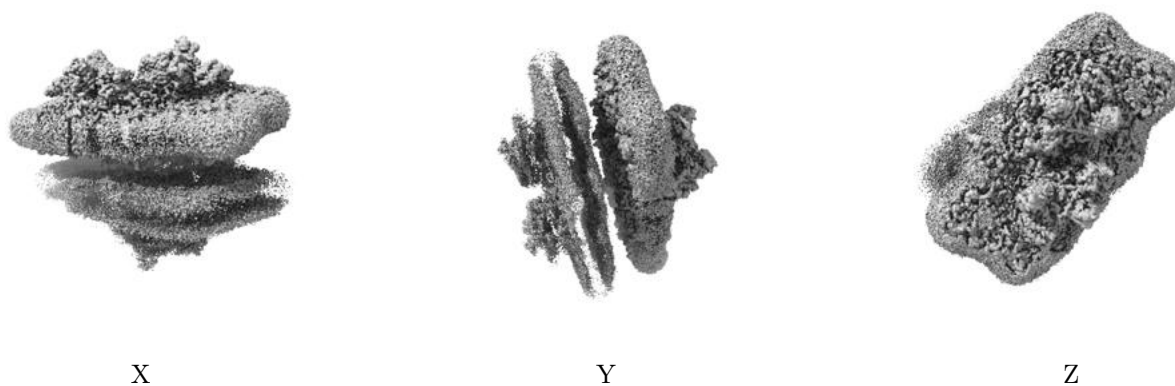
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

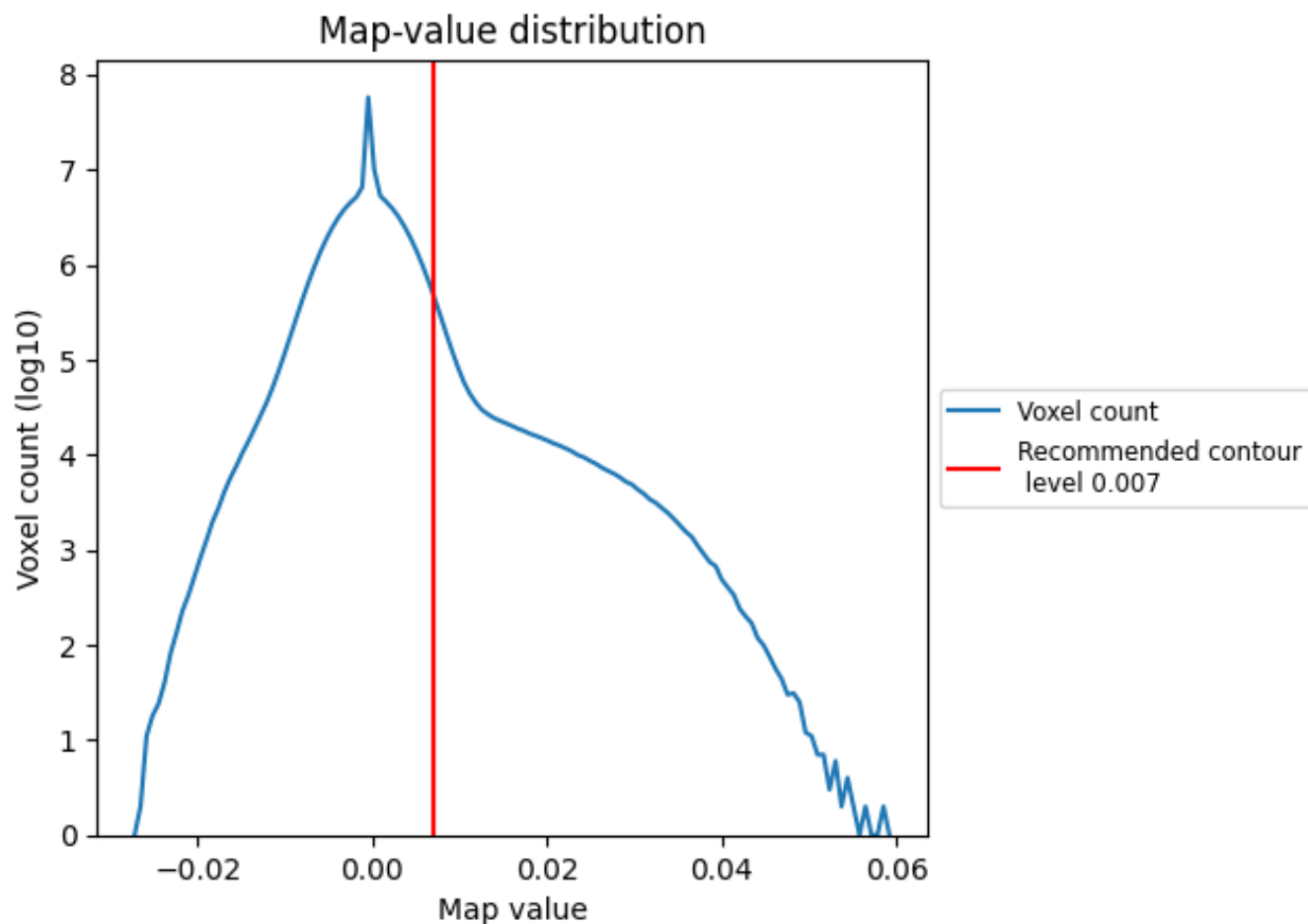
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

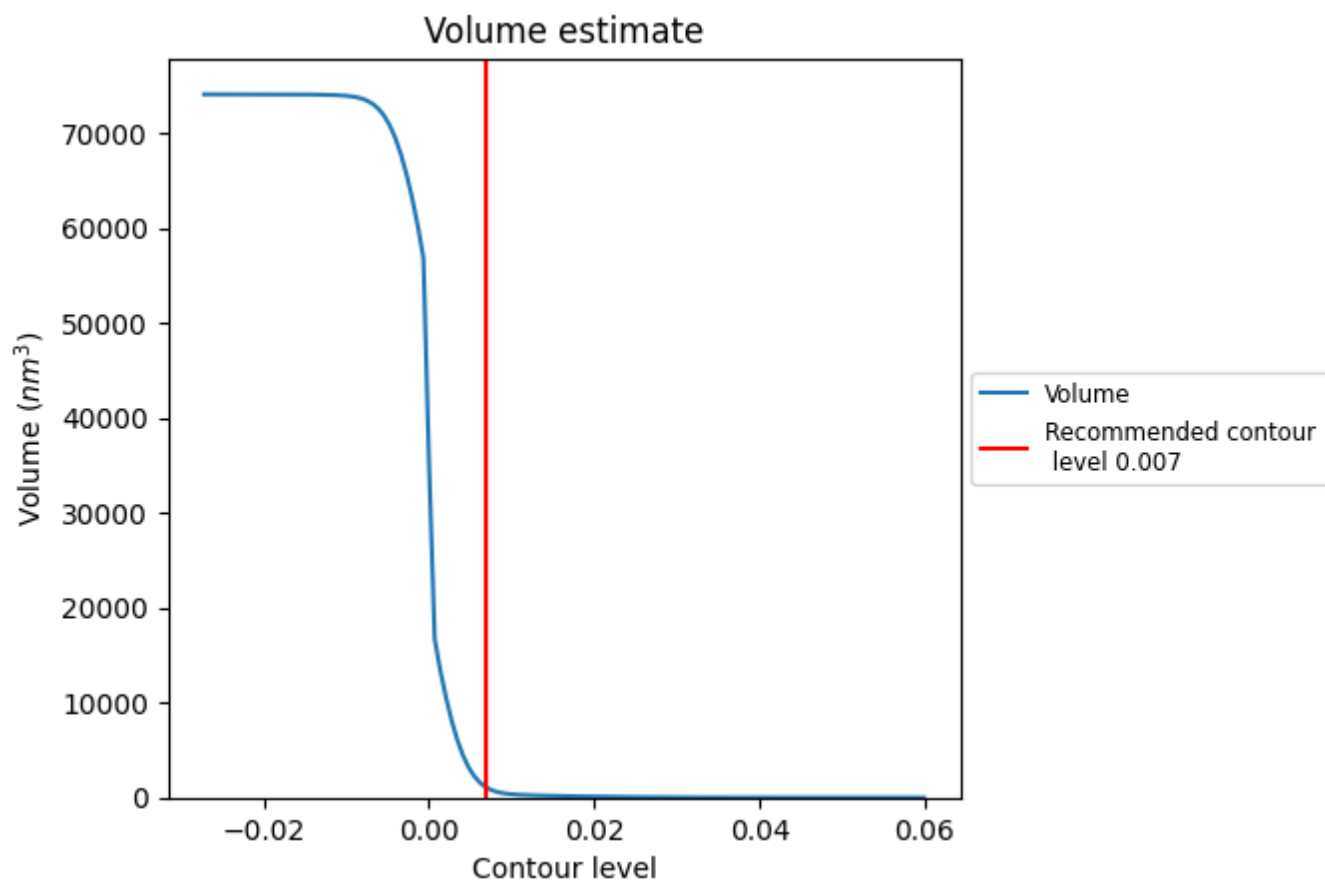
This section contains the results of statistical analysis of the map.

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



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

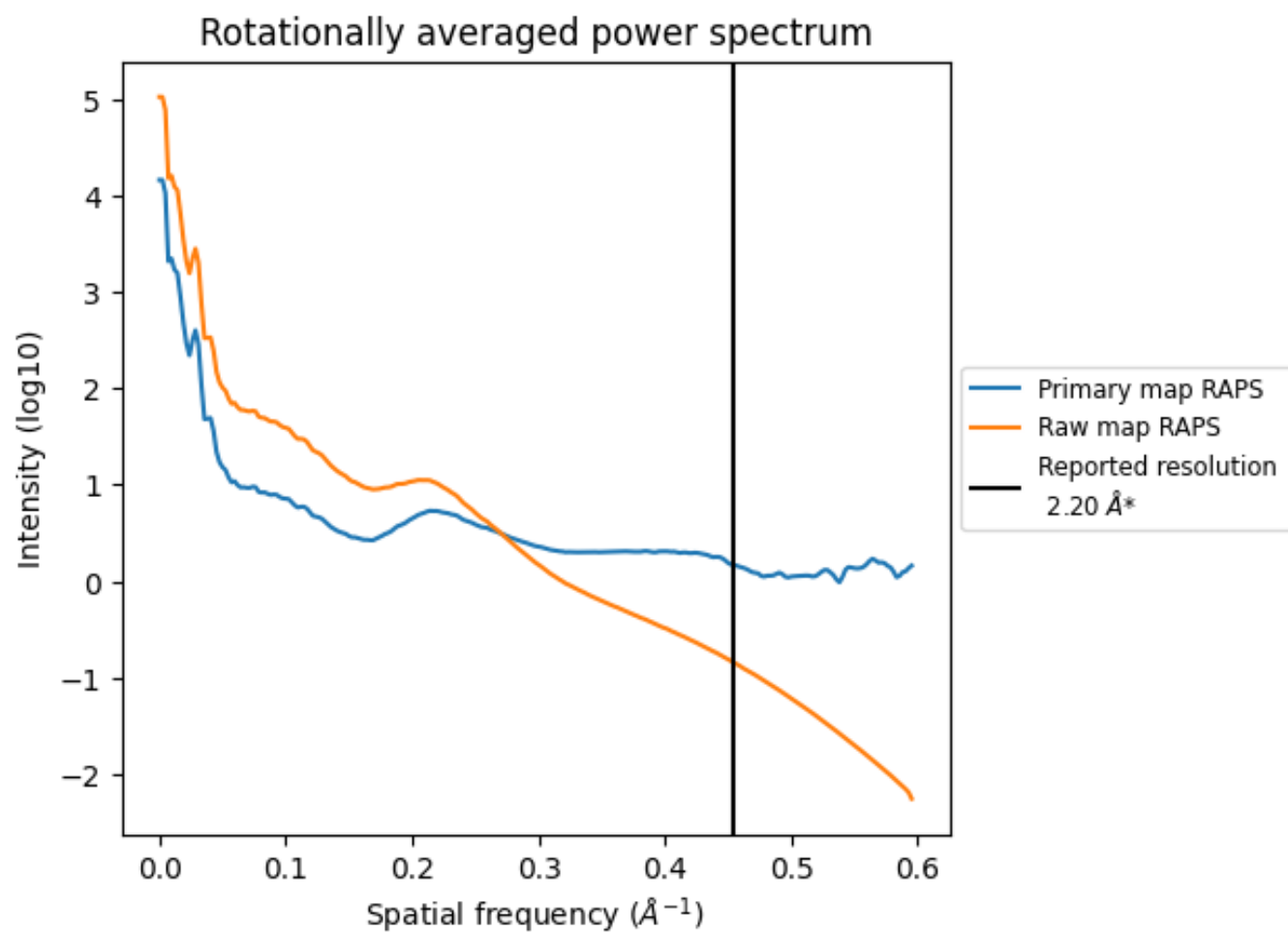
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10520 nm<sup>3</sup>; this corresponds to an approximate mass of 950 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 ⓘ

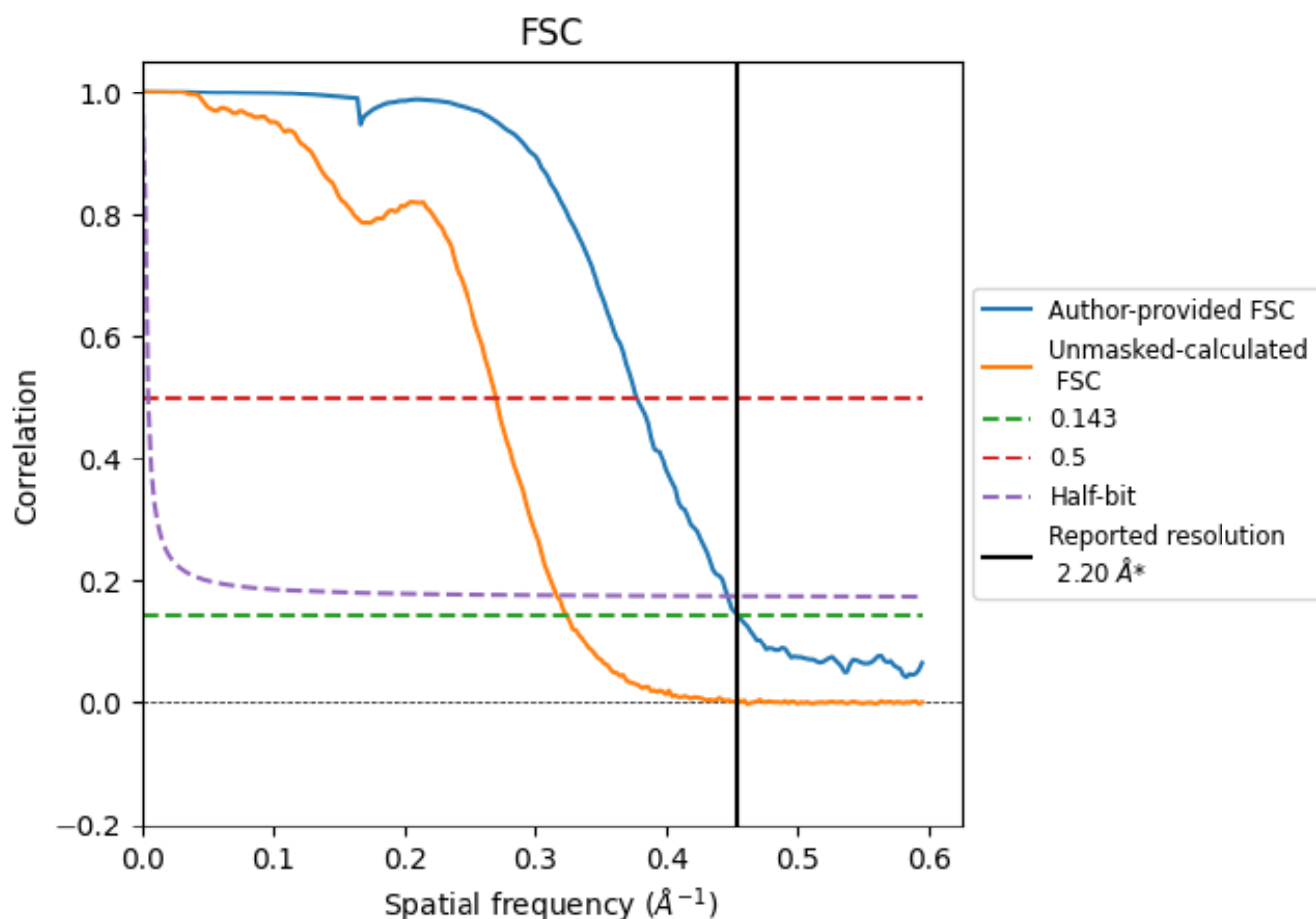


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.455 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

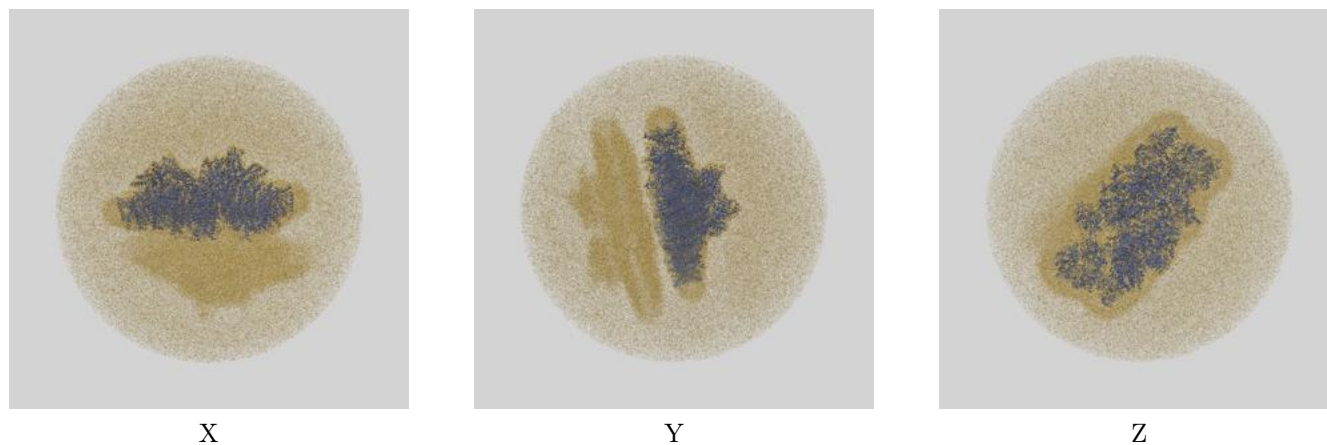
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.65	2.24
Unmasked-calculated*	3.09	3.70	3.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.2 by more than 10 %

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

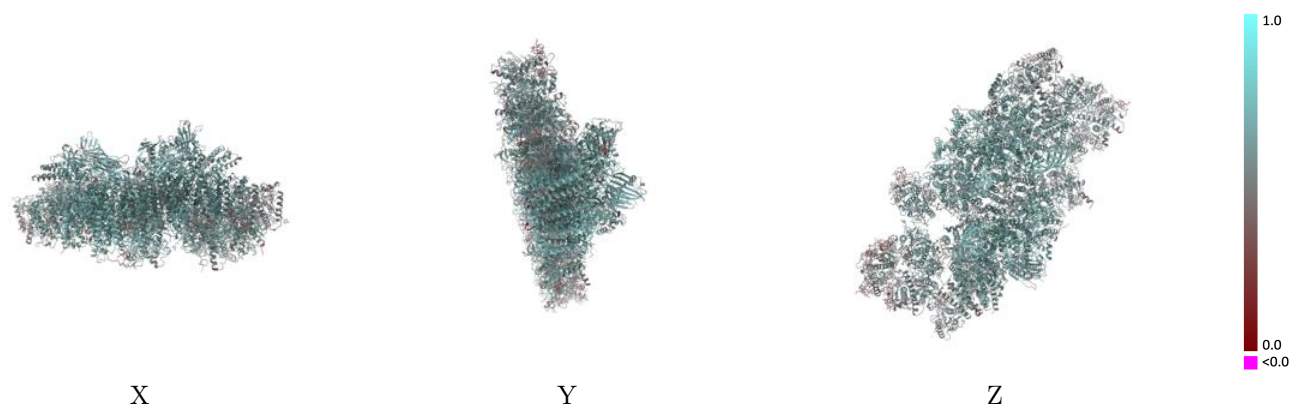
This section contains information regarding the fit between EMDB map EMD-52846 and PDB model 9IFM. Per-residue inclusion information can be found in [section 3](#) on [page 43](#).

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



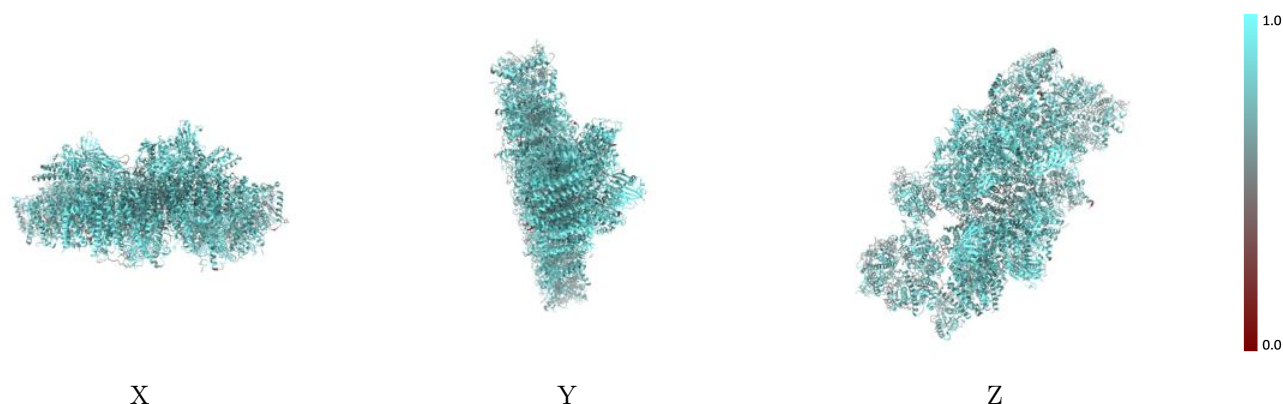
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



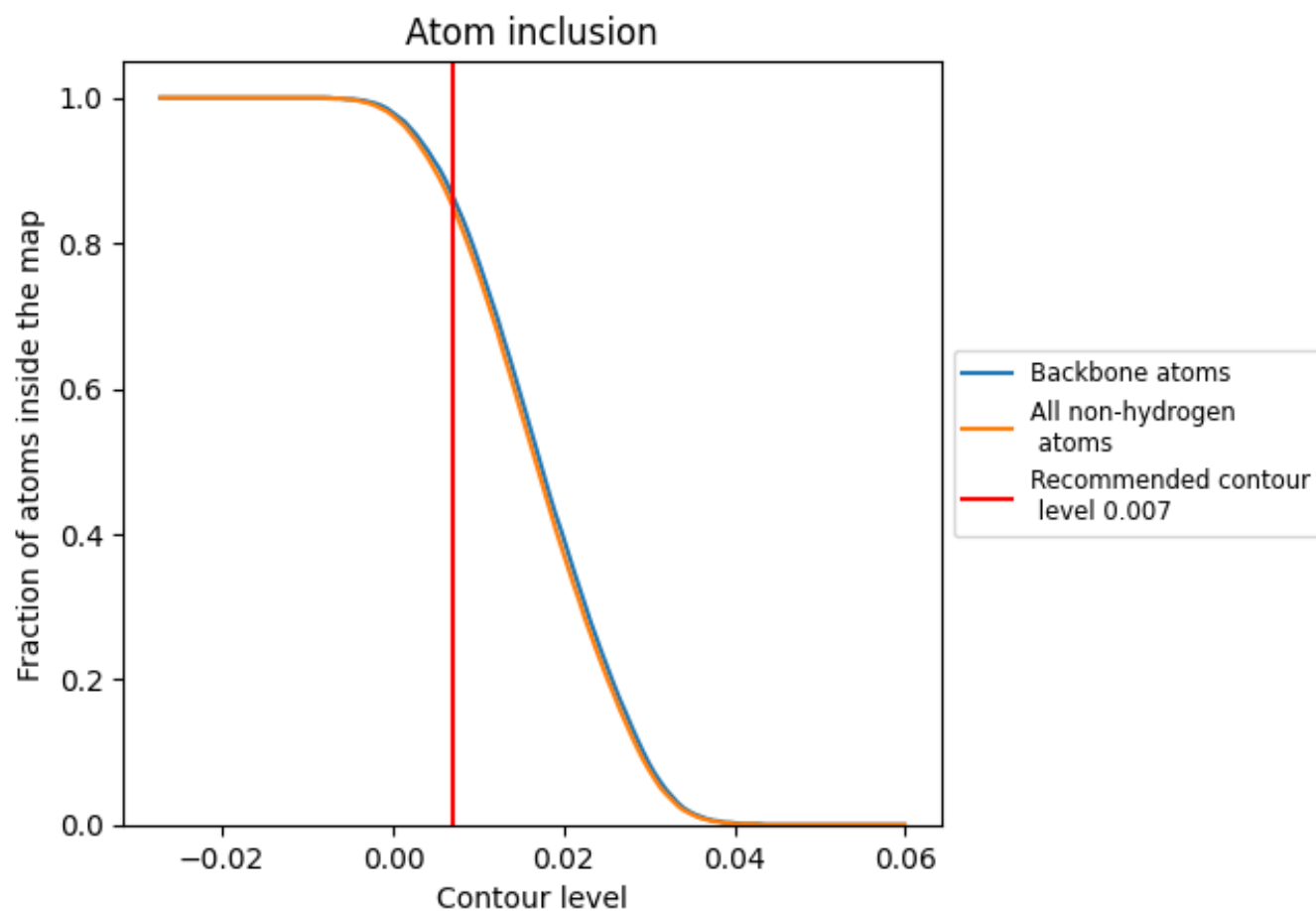
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.5990
A	 0.9000	 0.6540
B	 0.8850	 0.6340
C	 0.8900	 0.6310
D	 0.9200	 0.6580
E	 0.8960	 0.6110
F	 0.9150	 0.6340
G	 0.7160	 0.4780
H	 0.9220	 0.6500
I	 0.9340	 0.6660
J	 0.8370	 0.6090
K	 0.8300	 0.6090
L	 0.7790	 0.6010
M	 0.7140	 0.5630
N	 0.7700	 0.5190
O	 0.8690	 0.6070
P	 0.8720	 0.6040
Q	 0.8090	 0.5690
R	 0.8240	 0.5660
S	 0.7490	 0.4950
T	 0.8480	 0.6410
U	 0.7800	 0.5290
W	 0.7900	 0.5670
X	 0.8390	 0.5890
Y	 0.8580	 0.5970
Z	 0.7800	 0.5590
a	 0.9030	 0.6500
b	 0.9000	 0.6400
c	 0.9070	 0.6470
d	 0.9200	 0.6610
e	 0.9090	 0.6080
f	 0.8980	 0.6340
g	 0.7540	 0.5090
h	 0.9260	 0.6400
i	 0.9390	 0.6610



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Chain	Atom inclusion	Q-score
j	 0.8490	 0.6150
k	 0.7760	 0.5710
l	 0.9170	 0.6630
m	 0.7800	 0.6070
n	 0.7870	 0.5420
o	 0.8690	 0.6110
p	 0.8870	 0.6100
q	 0.8160	 0.5660
r	 0.8070	 0.5620
s	 0.7410	 0.4970
t	 0.8300	 0.6340
u	 0.7710	 0.5200
w	 0.8060	 0.5830
x	 0.8290	 0.5910
y	 0.8670	 0.6060
z	 0.7520	 0.5530