



## wwPDB EM Validation Summary Report ⓘ

Dec 22, 2022 – 06:33 pm GMT

PDB ID : 7PI0  
EMDB ID : EMD-13429  
Title : Unstacked compact Dunaliella PSII  
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.  
Deposited on : 2021-08-19  
Resolution : 2.43 Å(reported)  
Based on initial model : 6KAC

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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

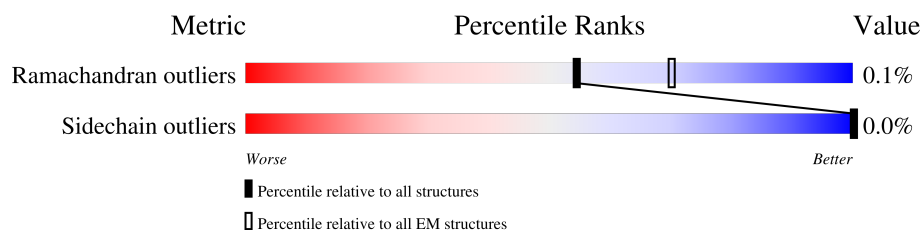
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.43 Å.

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


















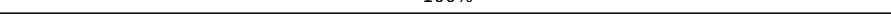
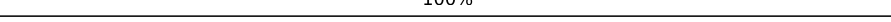
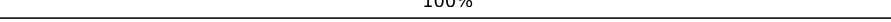

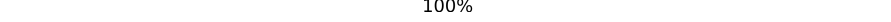
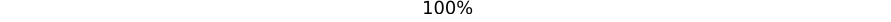
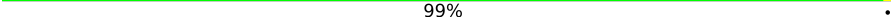
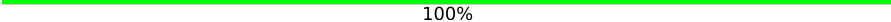


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	336	
1	a	336	
2	B	484	
2	b	484	
3	V	32	
3	v	32	
4	C	449	
4	c	449	
5	D	348	

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Mol	Chain	Length	Quality of chain
5	d	348	 100%
6	E	76	 100%
6	e	76	 100%
7	F	31	 100%
7	f	31	 100%
8	H	67	 100%
8	h	67	 100%
9	I	35	 100%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 100%
12	l	38	 100%
13	M	31	 100%
13	m	31	 100%
14	O	238	 100%
14	o	238	 100%
15	P	187	 21% 100%
15	p	187	 8% 99%
16	T	30	 100%
16	t	30	 100%
17	W	44	 100%
17	w	44	 100%

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Mol	Chain	Length	Quality of chain
18	X	30	 100%
18	x	30	 100%
19	Z	61	 100%
19	z	61	 100%
20	N	222	 100%
20	n	222	 100%
21	G	221	 100%
21	g	221	 100%
22	R	196	 99%
22	r	196	 99%
23	S	243	 100%
23	s	243	 100%
24	Y	222	 99%
24	y	222	 100%
25	U	27	 100%
25	u	27	 100%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	S	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	c	512	X	-	-	-
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-
29	CLA	r	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
44	RRX	H	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	RRX	h	101	X	-	-	-
45	CHL	G	601	X	-	-	-
45	CHL	G	605	X	-	-	-
45	CHL	G	606	X	-	-	-
45	CHL	G	607	X	-	-	-
45	CHL	G	608	X	-	-	-
45	CHL	G	609	X	-	-	-
45	CHL	N	601	X	-	-	-
45	CHL	N	605	X	-	-	-
45	CHL	N	606	X	-	-	-
45	CHL	N	607	X	-	-	-
45	CHL	N	608	X	-	-	-
45	CHL	N	609	X	-	-	-
45	CHL	R	606	X	-	-	-
45	CHL	R	607	X	-	-	-
45	CHL	S	601	X	-	-	-
45	CHL	S	606	X	-	-	-
45	CHL	S	607	X	-	-	-
45	CHL	S	608	X	-	-	-
45	CHL	Y	601	X	-	-	-
45	CHL	Y	605	X	-	-	-
45	CHL	Y	606	X	-	-	-
45	CHL	Y	607	X	-	-	-
45	CHL	Y	609	X	-	-	-
45	CHL	g	601	X	-	-	-
45	CHL	g	605	X	-	-	-
45	CHL	g	606	X	-	-	-
45	CHL	g	607	X	-	-	-
45	CHL	g	608	X	-	-	-
45	CHL	g	609	X	-	-	-
45	CHL	n	601	X	-	-	-
45	CHL	n	605	X	-	-	-
45	CHL	n	606	X	-	-	-
45	CHL	n	607	X	-	-	-
45	CHL	n	608	X	-	-	-
45	CHL	n	609	X	-	-	-
45	CHL	r	606	X	-	-	-
45	CHL	r	607	X	-	-	-
45	CHL	s	601	X	-	-	-
45	CHL	s	606	X	-	-	-
45	CHL	s	607	X	-	-	-
45	CHL	s	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CHL	y	601	X	-	-	-
45	CHL	y	605	X	-	-	-
45	CHL	y	606	X	-	-	-
45	CHL	y	607	X	-	-	-
45	CHL	y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-
48	XAT	R	621	X	-	-	-
48	XAT	Y	622	X	-	-	-
48	XAT	g	622	X	-	-	-
48	XAT	n	622	X	-	-	-
48	XAT	r	621	X	-	-	-
48	XAT	y	622	X	-	-	-

## 2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 77465 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	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		
1	a	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- 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	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		



- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	30	Total	C	N	O	S	0	0
			201	132	32	37			
18	x	30	Total	C	N	O	S	0	0
			201	132	32	37			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
20	n	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		
22	r	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

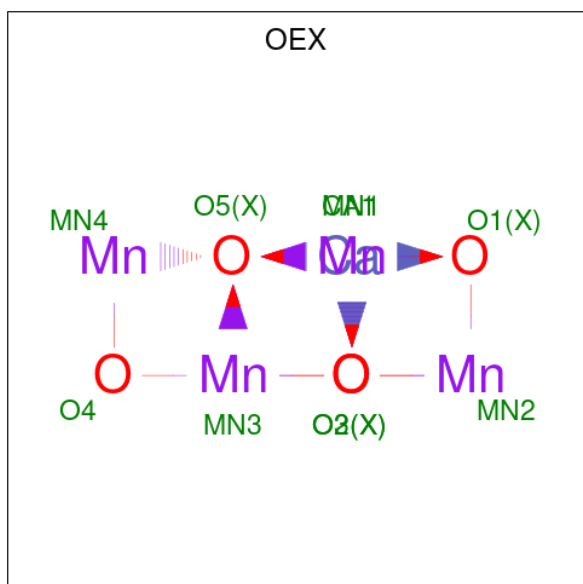
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

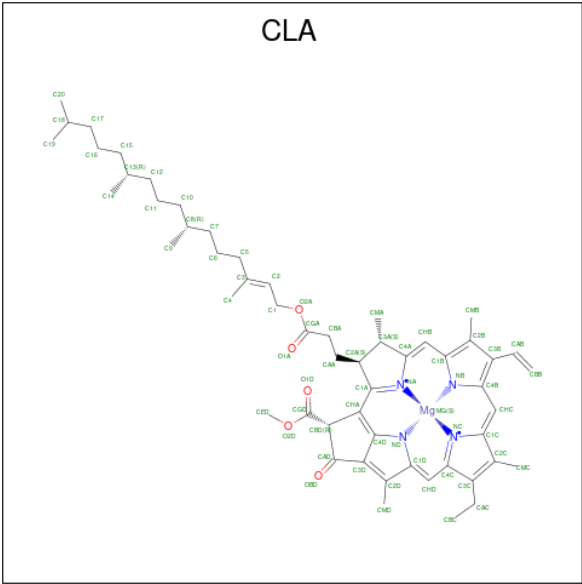
- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1030	870	16	64	80	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			830	700	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 830	C 700	Mg 13	N 52	O 65	0
29	C	1	Total 830	C 700	Mg 13	N 52	O 65	0
29	D	1	Total 125	C 105	Mg 2	N 8	O 10	0
29	D	1	Total 125	C 105	Mg 2	N 8	O 10	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	R	1	Total 385	C 315	Mg 7	N 28	O 35	0

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	
29	R	1	Total	C	Mg	N	O	0
			385	315	7	28	35	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			620	510	11	44	55	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0
29	b	1	Total 1032	C 872	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1032	872	16	64	80	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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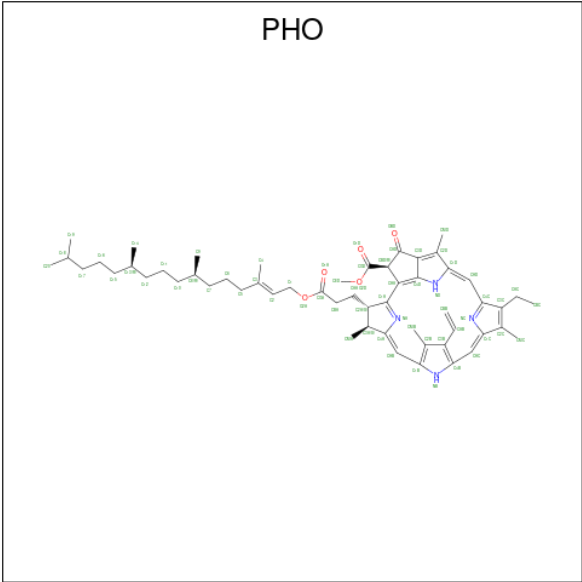
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0
29	r	1	Total 400	C 330	Mg 7	N 28	O 35	0

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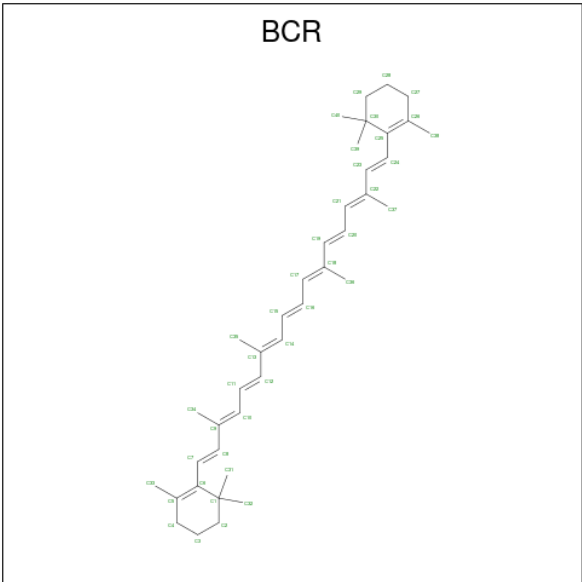
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0

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



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	

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

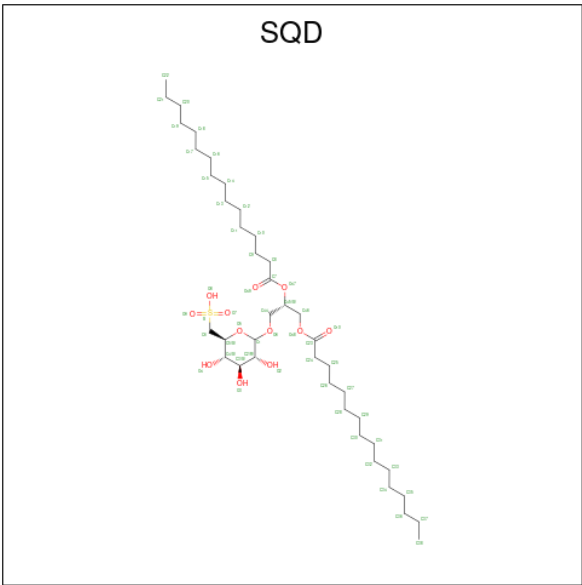


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 80 80	0
31	B	1	Total C 80 80	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 80 80	0
31	b	1	Total C 80 80	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0

- Molecule 32 is SODIUM ION (three-letter code: NA) (formula: Na).

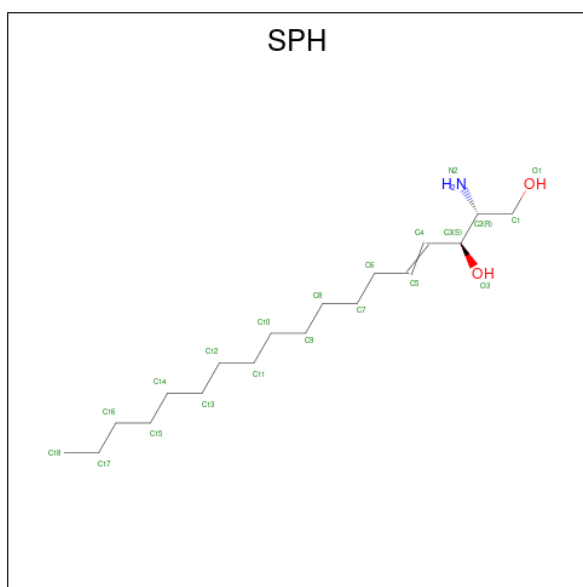
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Na 1 1	0
32	a	1	Total Na 1 1	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



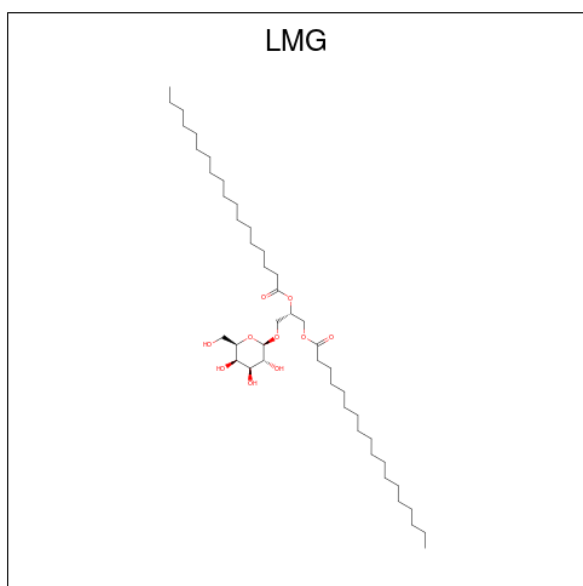
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			42	29	12	1	
33	B	1	Total	C	O	S	0
			96	70	24	2	
33	B	1	Total	C	O	S	0
			96	70	24	2	
33	C	1	Total	C	O	S	0
			36	23	12	1	
33	M	1	Total	C	O	S	0
			42	29	12	1	
33	a	1	Total	C	O	S	0
			51	38	12	1	
33	b	1	Total	C	O	S	0
			96	70	24	2	
33	b	1	Total	C	O	S	0
			96	70	24	2	
33	c	1	Total	C	O	S	0
			54	41	12	1	
33	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 34 is SPHINGOSINE (three-letter code: SPH) (formula: C<sub>18</sub>H<sub>37</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			21	18	1	2	
34	Y	1	Total	C	N	O	0
			21	18	1	2	
34	a	1	Total	C	N	O	0
			21	18	1	2	
34	y	1	Total	C	N	O	0
			21	18	1	2	

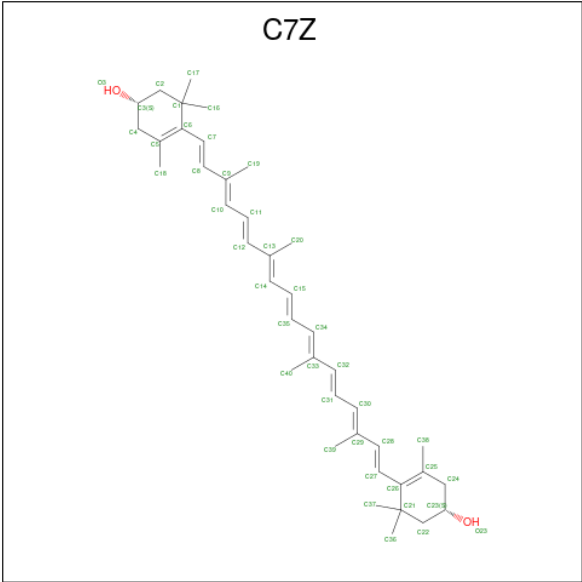
- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total 40	C 30	O 10	0
35	B	1	Total 44	C 34	O 10	0
35	C	1	Total 144	C 114	O 30	0
35	C	1	Total 144	C 114	O 30	0
35	C	1	Total 144	C 114	O 30	0
35	D	1	Total 42	C 32	O 10	0
35	H	1	Total 48	C 38	O 10	0
35	W	1	Total 39	C 29	O 10	0
35	a	1	Total 48	C 38	O 10	0
35	b	1	Total 44	C 34	O 10	0
35	c	1	Total 106	C 86	O 20	0
35	c	1	Total 106	C 86	O 20	0
35	d	1	Total 46	C 36	O 10	0
35	h	1	Total 48	C 38	O 10	0
35	w	1	Total 39	C 29	O 10	0

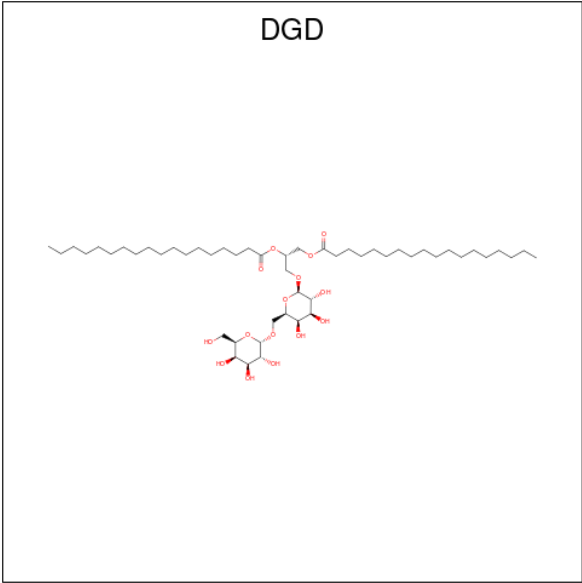
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



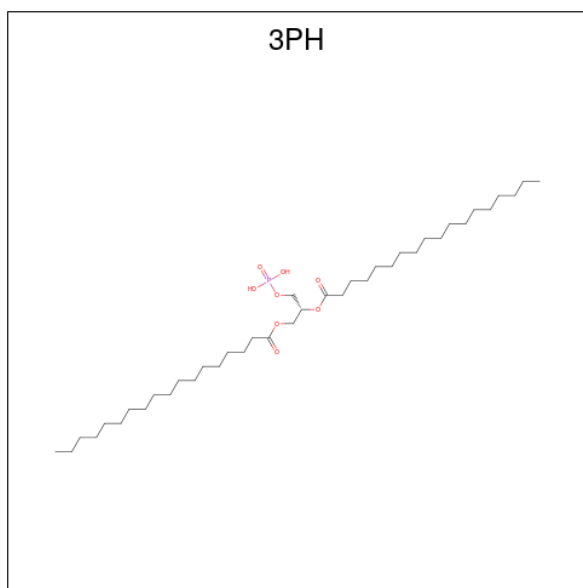
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			43	28	15	

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Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			157	112	45	
37	C	1	Total	C	O	0
			157	112	45	
37	C	1	Total	C	O	0
			157	112	45	
37	b	1	Total	C	O	0
			43	28	15	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



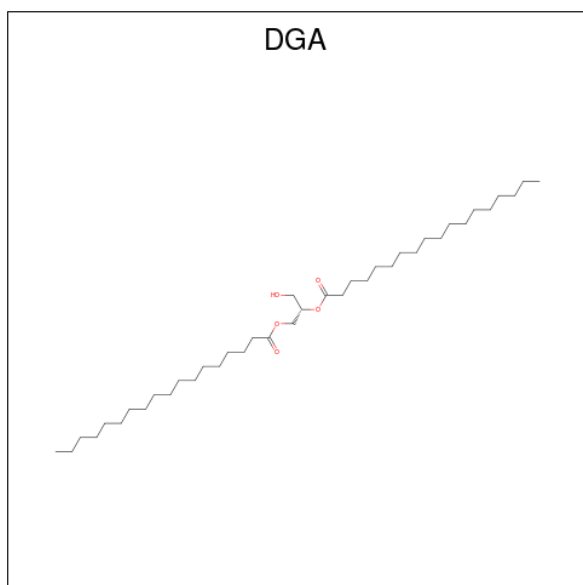
Mol	Chain	Residues	Atoms				AltConf
38	B	1	Total	C	O	P	0
			48	39	8	1	
38	T	1	Total	C	O	P	0
			48	39	8	1	
38	S	1	Total	C	O	P	0
			30	21	8	1	
38	b	1	Total	C	O	P	0
			39	30	8	1	

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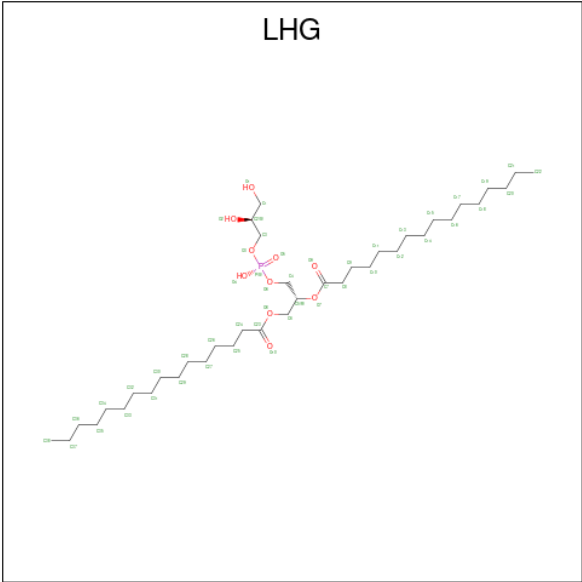
Mol	Chain	Residues	Atoms				AltConf
38	t	1	Total	C	O	P	0
			48	39	8	1	
38	s	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 39 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
39	B	1	Total	C	O		0
			37	32	5		
39	C	1	Total	C	O		0
			44	39	5		
39	J	1	Total	C	O		0
			29	24	5		
39	b	1	Total	C	O		0
			44	39	5		
39	c	1	Total	C	O		0
			44	39	5		
39	j	1	Total	C	O		0
			29	24	5		

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



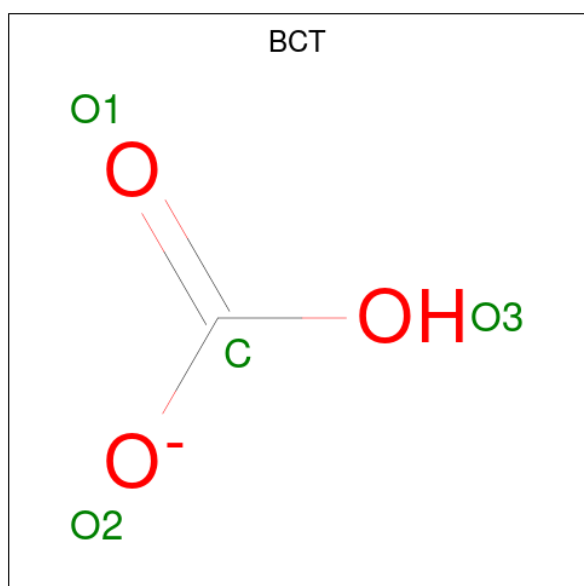
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	O	P	0
			35	24	10	1	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	L	1	Total	C	O	P	0
			49	38	10	1	
40	N	1	Total	C	O	P	0
			49	38	10	1	
40	G	1	Total	C	O	P	0
			49	38	10	1	
40	S	1	Total	C	O	P	0
			45	34	10	1	
40	Y	1	Total	C	O	P	0
			49	38	10	1	
40	c	1	Total	C	O	P	0
			85	63	20	2	
40	c	1	Total	C	O	P	0
			85	63	20	2	
40	d	1	Total	C	O	P	0
			132	99	30	3	
40	d	1	Total	C	O	P	0
			132	99	30	3	
40	d	1	Total	C	O	P	0
			132	99	30	3	

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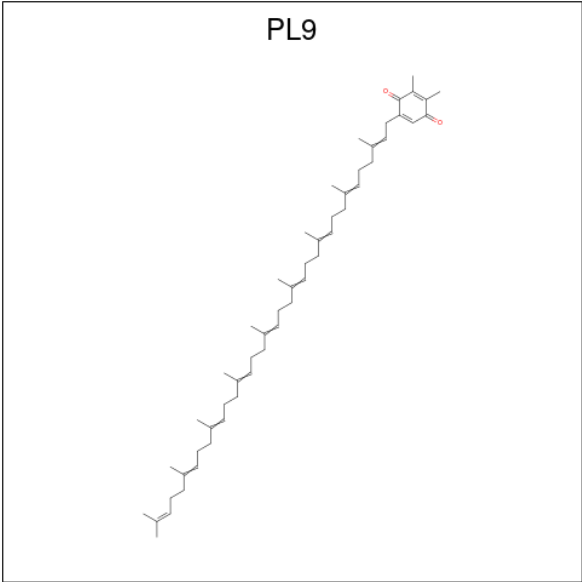
Mol	Chain	Residues	Atoms				AltConf
40	l	1	Total	C	O	P	0
			49	38	10	1	
40	n	1	Total	C	O	P	0
			42	31	10	1	
40	g	1	Total	C	O	P	0
			49	38	10	1	
40	s	1	Total	C	O	P	0
			45	34	10	1	
40	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



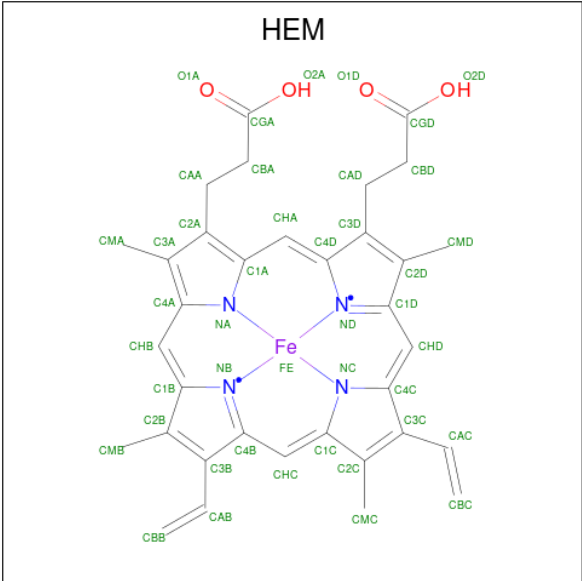
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			4	1	3	
41	d	1	Total	C	O	0
			4	1	3	

- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



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

- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



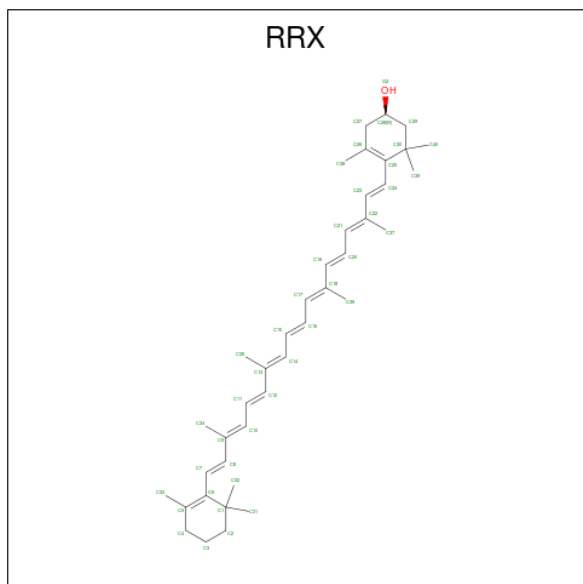
Mol	Chain	Residues	Atoms					AltConf
43	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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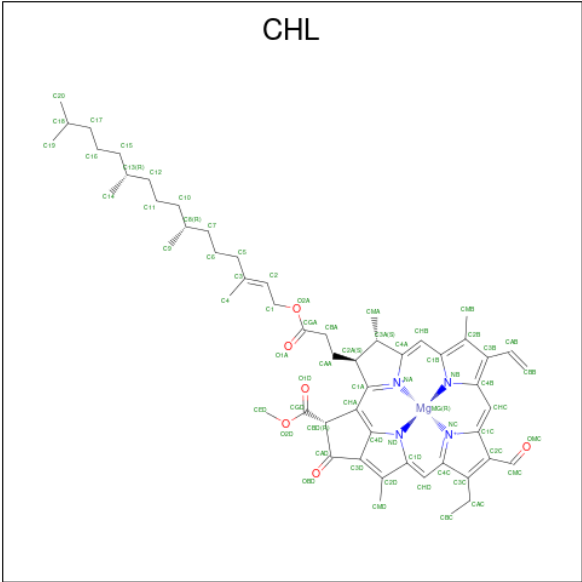
Mol	Chain	Residues	Atoms					AltConf
43	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).



Mol	Chain	Residues	Atoms			AltConf
44	H	1	Total	C	O	0
			41	40	1	
44	h	1	Total	C	O	0
			41	40	1	

- Molecule 45 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	G	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	R	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	R	1	Total	C	Mg	N	O	0
			94	74	2	8	10	

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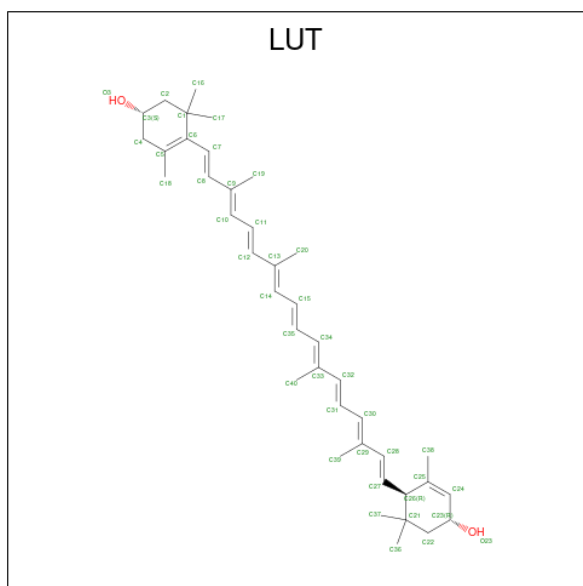
Mol	Chain	Residues	Atoms					AltConf
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	S	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	Y	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	n	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
45	g	1	Total	C	Mg	N	O	0
			340	276	6	24	34	

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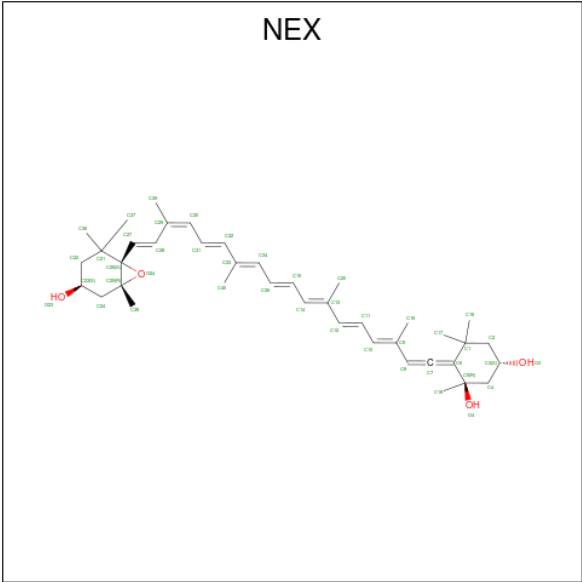
Mol	Chain	Residues	Atoms					AltConf
45	r	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	r	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	s	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	
45	y	1	Total	C	Mg	N	O	0
			295	240	5	20	30	

- Molecule 46 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



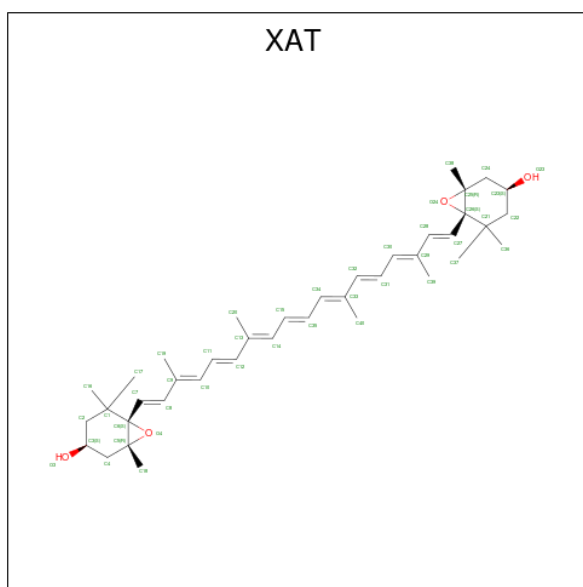
Mol	Chain	Residues	Atoms			AltConf
46	N	1	Total	C	O	0
			84	80	4	
46	N	1	Total	C	O	0
			84	80	4	
46	G	1	Total	C	O	0
			84	80	4	
46	G	1	Total	C	O	0
			84	80	4	
46	R	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			84	80	4	
46	S	1	Total	C	O	0
			84	80	4	
46	Y	1	Total	C	O	0
			84	80	4	
46	Y	1	Total	C	O	0
			84	80	4	
46	n	1	Total	C	O	0
			84	80	4	
46	n	1	Total	C	O	0
			84	80	4	
46	g	1	Total	C	O	0
			84	80	4	
46	g	1	Total	C	O	0
			84	80	4	
46	r	1	Total	C	O	0
			42	40	2	
46	s	1	Total	C	O	0
			84	80	4	
46	s	1	Total	C	O	0
			84	80	4	
46	y	1	Total	C	O	0
			84	80	4	
46	y	1	Total	C	O	0
			84	80	4	

- Molecule 47 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



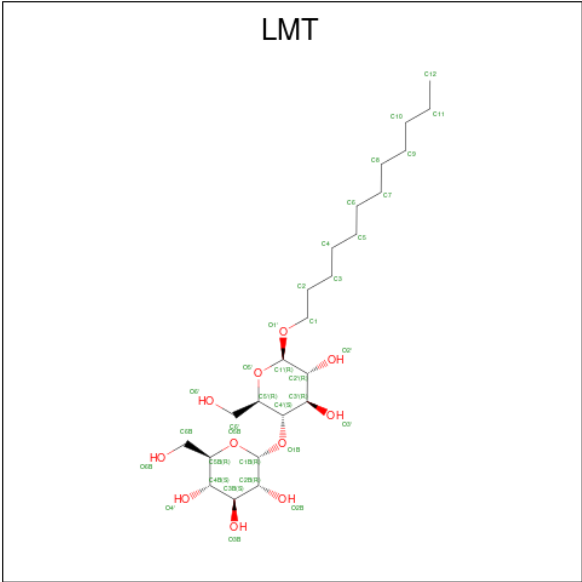
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			44	40	4	
47	G	1	Total	C	O	0
			44	40	4	
47	R	1	Total	C	O	0
			27	25	2	
47	S	1	Total	C	O	0
			44	40	4	
47	Y	1	Total	C	O	0
			44	40	4	
47	n	1	Total	C	O	0
			44	40	4	
47	g	1	Total	C	O	0
			44	40	4	
47	r	1	Total	C	O	0
			27	25	2	
47	s	1	Total	C	O	0
			44	40	4	
47	y	1	Total	C	O	0
			44	40	4	

- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



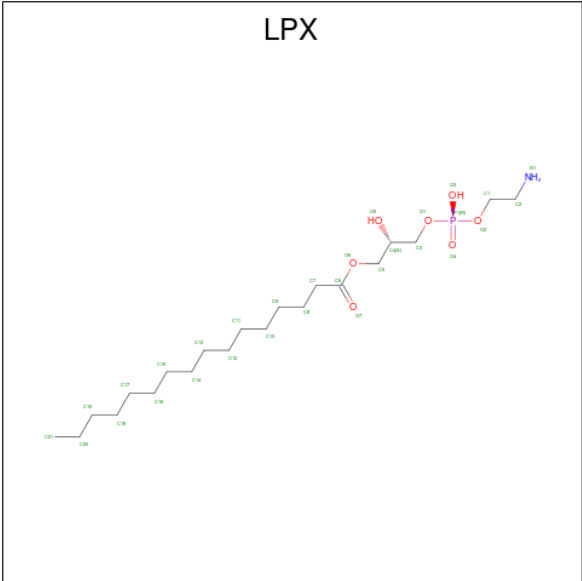
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
49	R	1	Total	C	O	0
			35	24	11	
49	r	1	Total	C	O	0
			35	24	11	

- Molecule 50 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



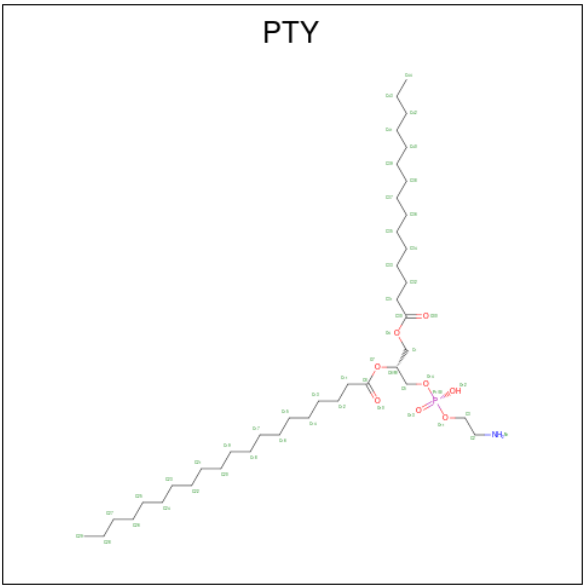
Mol	Chain	Residues	Atoms					AltConf
50	S	1	Total	C	N	O	P	0
			20	11	1	7	1	

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Mol	Chain	Residues	Atoms					AltConf
50	s	1	Total	C	N	O	P	0
			19	10	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
51	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
51	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
51	y	1	Total	C	N	O	P	0
			69	49	2	16	2	
51	y	1	Total	C	N	O	P	0
			69	49	2	16	2	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	27	Total	O	0
			93	93	
52	A	7	Total	O	0
			93	93	
52	A	7	Total	O	0
			93	93	
52	A	22	Total	O	0
			93	93	

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Mol	Chain	Residues	Atoms		AltConf
52	A	10	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	2	Total 93	O 93	0
52	A	2	Total 93	O 93	0
52	A	4	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	A	1	Total 93	O 93	0
52	B	6	Total 125	O 125	0
52	B	11	Total 125	O 125	0
52	B	12	Total 125	O 125	0
52	B	4	Total 125	O 125	0
52	B	1	Total 125	O 125	0

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Mol	Chain	Residues	Atoms		AltConf
52	B	40	Total 125	O 125	0
52	B	16	Total 125	O 125	0
52	B	2	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	9	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	4	Total 125	O 125	0
52	B	2	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	5	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	B	1	Total 125	O 125	0
52	V	5	Total 6	O 6	0

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Mol	Chain	Residues	Atoms	AltConf
52	V	1	Total O 6 6	0
52	C	3	Total O 113 113	0
52	C	3	Total O 113 113	0
52	C	15	Total O 113 113	0
52	C	56	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	3	Total O 113 113	0
52	C	2	Total O 113 113	0
52	C	12	Total O 113 113	0
52	C	3	Total O 113 113	0
52	C	3	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0
52	C	1	Total O 113 113	0

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Mol	Chain	Residues	Atoms		AltConf
52	C	1	Total 113	O 113	0
52	C	1	Total 113	O 113	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	3	Total 77	O 77	0
52	D	6	Total 77	O 77	0
52	D	8	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	3	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	11	Total 77	O 77	0
52	D	12	Total 77	O 77	0
52	D	9	Total 77	O 77	0

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Mol	Chain	Residues	Atoms		AltConf
52	D	5	Total 77	O 77	0
52	D	2	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	D	1	Total 77	O 77	0
52	E	1	Total 18	O 18	0
52	E	1	Total 18	O 18	0
52	E	15	Total 18	O 18	0
52	E	1	Total 18	O 18	0
52	F	1	Total 1	O 1	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	1	Total 19	O 19	0
52	H	13	Total 19	O 19	0
52	I	1	Total 6	O 6	0
52	I	2	Total 6	O 6	0
52	I	3	Total 6	O 6	0

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Mol	Chain	Residues	Atoms		AltConf
52	J	3	Total 4	O 4	0
52	J	1	Total 4	O 4	0
52	K	1	Total 10	O 10	0
52	K	9	Total 10	O 10	0
52	L	6	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	L	1	Total 11	O 11	0
52	M	1	Total 8	O 8	0
52	M	1	Total 8	O 8	0
52	M	1	Total 8	O 8	0
52	M	3	Total 8	O 8	0
52	M	2	Total 8	O 8	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	2	Total 79	O 79	0
52	O	1	Total 79	O 79	0

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Mol	Chain	Residues	Atoms		AltConf
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	1	Total 79	O 79	0
52	O	18	Total 79	O 79	0
52	O	5	Total 79	O 79	0
52	O	18	Total 79	O 79	0
52	O	10	Total 79	O 79	0
52	O	9	Total 79	O 79	0
52	O	6	Total 79	O 79	0
52	O	2	Total 79	O 79	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	1	Total 25	O 25	0
52	P	13	Total 25	O 25	0
52	P	7	Total 25	O 25	0
52	T	1	Total 5	O 5	0
52	T	2	Total 5	O 5	0
52	T	2	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
52	W	1	Total 8	O 8	0
52	W	1	Total 8	O 8	0
52	W	2	Total 8	O 8	0
52	W	4	Total 8	O 8	0
52	X	3	Total 3	O 3	0
52	Z	1	Total 4	O 4	0
52	Z	3	Total 4	O 4	0
52	N	27	Total 61	O 61	0
52	N	11	Total 61	O 61	0
52	N	10	Total 61	O 61	0
52	N	6	Total 61	O 61	0
52	N	5	Total 61	O 61	0
52	N	1	Total 61	O 61	0
52	N	1	Total 61	O 61	0
52	G	1	Total 60	O 60	0
52	G	1	Total 60	O 60	0
52	G	7	Total 60	O 60	0
52	G	37	Total 60	O 60	0
52	G	14	Total 60	O 60	0
52	R	1	Total 35	O 35	0
52	R	29	Total 35	O 35	0

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Mol	Chain	Residues	Atoms		AltConf
52	R	4	Total 35	O 35	0
52	R	1	Total 35	O 35	0
52	S	1	Total 33	O 33	0
52	S	29	Total 33	O 33	0
52	S	3	Total 33	O 33	0
52	Y	1	Total 56	O 56	0
52	Y	1	Total 56	O 56	0
52	Y	1	Total 56	O 56	0
52	Y	21	Total 56	O 56	0
52	Y	21	Total 56	O 56	0
52	Y	11	Total 56	O 56	0
52	U	1	Total 8	O 8	0
52	U	7	Total 8	O 8	0
52	a	15	Total 91	O 91	0
52	a	5	Total 91	O 91	0
52	a	20	Total 91	O 91	0
52	a	9	Total 91	O 91	0
52	a	2	Total 91	O 91	0
52	a	6	Total 91	O 91	0
52	a	9	Total 91	O 91	0
52	a	4	Total 91	O 91	0

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Mol	Chain	Residues	Atoms		AltConf
52	a	5	Total 91	O 91	0
52	a	6	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	1	Total 91	O 91	0
52	a	2	Total 91	O 91	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	48	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	21	Total 115	O 115	0
52	b	2	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	8	Total 115	O 115	0
52	b	2	Total 115	O 115	0
52	b	1	Total 115	O 115	0

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Mol	Chain	Residues	Atoms		AltConf
52	b	6	Total 115	O 115	0
52	b	7	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	11	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	b	1	Total 115	O 115	0
52	v	1	Total 2	O 2	0
52	v	1	Total 2	O 2	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	16	Total 101	O 101	0
52	c	14	Total 101	O 101	0
52	c	20	Total 101	O 101	0
52	c	2	Total 101	O 101	0
52	c	21	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	2	Total 101	O 101	0

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Mol	Chain	Residues	Atoms		AltConf
52	c	16	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	c	1	Total 101	O 101	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	3	Total 65	O 65	0
52	d	28	Total 65	O 65	0
52	d	11	Total 65	O 65	0
52	d	12	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	5	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	d	1	Total 65	O 65	0
52	e	1	Total 20	O 20	0
52	e	6	Total 20	O 20	0
52	e	11	Total 20	O 20	0
52	e	2	Total 20	O 20	0

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Mol	Chain	Residues	Atoms		AltConf
52	f	3	Total 3	O 3	0
52	h	1	Total 20	O 20	0
52	h	2	Total 20	O 20	0
52	h	1	Total 20	O 20	0
52	h	1	Total 20	O 20	0
52	h	9	Total 20	O 20	0
52	h	4	Total 20	O 20	0
52	h	2	Total 20	O 20	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	i	9	Total 14	O 14	0
52	i	1	Total 14	O 14	0
52	j	3	Total 3	O 3	0
52	k	5	Total 8	O 8	0
52	k	3	Total 8	O 8	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0
52	l	1	Total 10	O 10	0

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Mol	Chain	Residues	Atoms		AltConf
52	l	1	Total 10	O 10	0
52	l	5	Total 10	O 10	0
52	m	1	Total 7	O 7	0
52	m	1	Total 7	O 7	0
52	m	2	Total 7	O 7	0
52	m	3	Total 7	O 7	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	29	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	o	15	Total 81	O 81	0
52	o	7	Total 81	O 81	0
52	o	8	Total 81	O 81	0
52	o	13	Total 81	O 81	0
52	o	1	Total 81	O 81	0
52	p	1	Total 68	O 68	0

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Mol	Chain	Residues	Atoms		AltConf
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	1	Total 68	O 68	0
52	p	13	Total 68	O 68	0
52	p	34	Total 68	O 68	0
52	p	13	Total 68	O 68	0
52	t	2	Total 2	O 2	0
52	w	1	Total 10	O 10	0
52	w	1	Total 10	O 10	0
52	w	4	Total 10	O 10	0
52	w	2	Total 10	O 10	0
52	w	2	Total 10	O 10	0
52	x	9	Total 9	O 9	0
52	z	1	Total 8	O 8	0
52	z	6	Total 8	O 8	0
52	z	1	Total 8	O 8	0
52	n	1	Total 36	O 36	0

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Mol	Chain	Residues	Atoms		AltConf
52	n	19	Total 36	O 36	0
52	n	7	Total 36	O 36	0
52	n	6	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	n	1	Total 36	O 36	0
52	g	2	Total 31	O 31	0
52	g	24	Total 31	O 31	0
52	g	5	Total 31	O 31	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	1	Total 38	O 38	0
52	r	11	Total 38	O 38	0
52	r	21	Total 38	O 38	0
52	s	1	Total 39	O 39	0
52	s	24	Total 39	O 39	0
52	s	10	Total 39	O 39	0
52	s	4	Total 39	O 39	0

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Mol	Chain	Residues	Atoms		AltConf
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	1	Total 63	O 63	0
52	y	29	Total 63	O 63	0
52	y	26	Total 63	O 63	0
52	y	4	Total 63	O 63	0
52	u	1	Total 7	O 7	0
52	u	1	Total 7	O 7	0
52	u	5	Total 7	O 7	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0
52	Q	1	Total 5	O 5	0

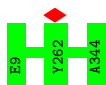


### 3 Residue-property plots

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.

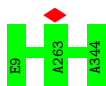
- Molecule 1: Photosystem II protein D1

Chain A:  100%



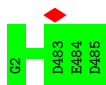
- Molecule 1: Photosystem II protein D1

Chain a:  100%



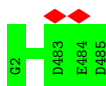
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  100%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%

There are no outlier residues recorded for this chain.

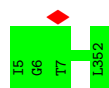
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Photosystem II D2 protein

Chain D:  100%



- Molecule 5: Photosystem II D2 protein

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

Chain I:  100%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain J:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: PsbM

Chain M:  100%

There are no outlier residues recorded for this chain.

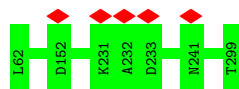
- Molecule 13: PsbM

Chain m:  100%

There are no outlier residues recorded for this chain.

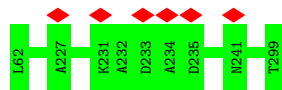
- Molecule 14: PsbO

Chain O:  100%



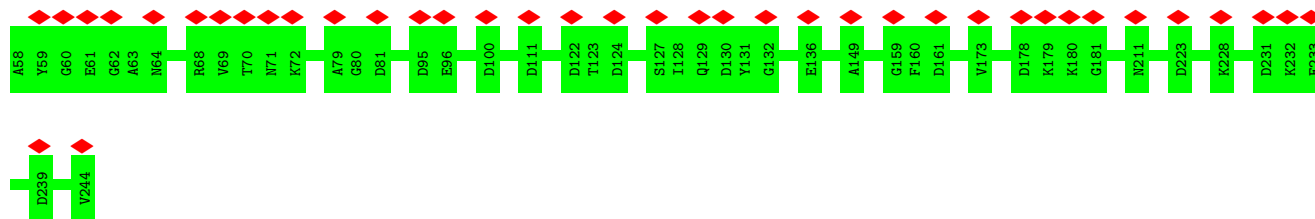
- Molecule 14: PsbO

Chain o:  100%



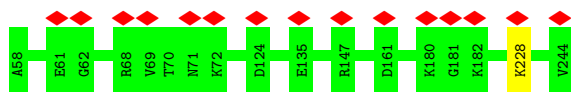
- Molecule 15: PsbP

Chain P:  21% 100%



- Molecule 15: PsbP

Chain p:  8% 99%



- Molecule 16: Photosystem II reaction center protein T

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: Photosystem II reaction center protein T

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: PsbW

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: PsbW

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: PsbX

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: PsbX

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: LHCII M3

Chain N:  100%



- Molecule 20: LHCII M3

Chain n: 100%



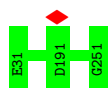
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G: 100%

There are no outlier residues recorded for this chain.

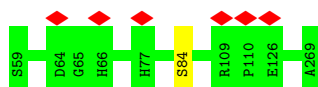
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain g: 100%



- Molecule 22: CP29

Chain R: 99%



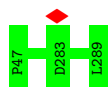
- Molecule 22: CP29

Chain r: 99%



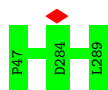
- Molecule 23: CP26

Chain S: 100%



- Molecule 23: CP26

Chain s: 100%



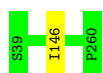
- Molecule 24: LHCII M1

Chain Y:  99%



- Molecule 24: LHCII M1

Chain y:  100%



- Molecule 25: PsbU

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: PsbU

Chain u:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-16.255	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.5	Depositor
Map size ( $\text{\AA}$ )	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.896, 0.896, 0.896	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SEP, PL9, NA, PTY, LUT, C7Z, DGA, XAT, BCT, BCR, SPH, NEX, CLA, RRX, PHO, LMT, CSD, 3PH, OEX, SQD, LPX, DGD, CHL, LMG, CL, FE2, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.32	0/2717	0.50	0/3707
1	a	0.33	0/2717	0.50	0/3707
2	B	0.31	0/3906	0.50	0/5319
2	b	0.31	0/3906	0.50	0/5319
3	V	0.25	0/228	0.46	0/311
3	v	0.24	0/228	0.47	0/311
4	C	0.30	0/3602	0.49	0/4913
4	c	0.31	0/3602	0.49	0/4913
5	D	0.30	0/2860	0.49	0/3899
5	d	0.32	0/2860	0.49	0/3899
6	E	0.29	0/639	0.53	0/870
6	e	0.29	0/639	0.52	0/870
7	F	0.27	0/259	0.49	0/351
7	f	0.26	0/259	0.48	0/351
8	H	0.28	0/513	0.50	0/703
8	h	0.29	0/513	0.48	0/703
9	I	0.32	0/287	0.48	0/386
9	i	0.32	0/287	0.48	0/386
10	J	0.25	0/272	0.43	0/369
10	j	0.26	0/272	0.48	0/369
11	K	0.33	0/308	0.50	0/423
11	k	0.34	0/308	0.53	0/423
12	L	0.31	0/321	0.47	0/435
12	l	0.33	0/321	0.46	0/435
13	M	0.31	0/237	0.49	0/323
13	m	0.30	0/237	0.49	0/323
14	O	0.29	0/1855	0.54	0/2505
14	o	0.29	0/1855	0.55	0/2505
15	P	0.27	0/1473	0.53	0/1988
15	p	0.28	0/1473	0.52	0/1988
16	T	0.34	0/254	0.47	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	t	0.33	0/254	0.46	0/342
17	W	0.27	0/339	0.50	0/460
17	w	0.29	0/339	0.49	0/460
18	X	0.28	0/202	0.43	0/276
18	x	0.27	0/202	0.41	0/276
19	Z	0.26	0/469	0.40	0/641
19	z	0.26	0/469	0.42	0/641
20	N	0.29	0/1751	0.47	0/2386
20	n	0.29	0/1751	0.45	0/2386
21	G	0.27	0/1725	0.47	0/2348
21	g	0.28	0/1725	0.47	0/2348
22	R	0.27	0/1506	0.49	0/2035
22	r	0.27	0/1506	0.48	0/2035
23	S	0.28	0/1903	0.49	0/2590
23	s	0.29	0/1903	0.49	0/2590
24	Y	0.28	0/1715	0.48	1/2338 (0.0%)
24	y	0.29	0/1715	0.46	0/2338
25	U	0.27	0/224	0.58	0/298
25	u	0.35	0/224	0.75	0/298
All	All	0.30	0/59130	0.49	1/80432 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
24	Y	78	ALA	C-N-CA	-5.42	108.14	121.70

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
1	a	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	B	481/484 (99%)	470 (98%)	11 (2%)	0	100	100
2	b	481/484 (99%)	468 (97%)	13 (3%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
4	c	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
5	D	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	d	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
6	E	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h	65/67 (97%)	65 (100%)	0	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
14	o	236/238 (99%)	218 (92%)	18 (8%)	0	100	100
15	P	185/187 (99%)	175 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
16	t	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	34
20	n	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	34
21	G	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
21	g	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	R	191/196 (97%)	178 (93%)	13 (7%)	0	100	100
22	r	191/196 (97%)	174 (91%)	16 (8%)	1 (0%)	29	34
23	S	241/243 (99%)	228 (95%)	13 (5%)	0	100	100
23	s	241/243 (99%)	220 (91%)	21 (9%)	0	100	100
24	Y	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	29	34
24	y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	34
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	7334/7442 (98%)	7065 (96%)	264 (4%)	5 (0%)	54	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	r	176	LEU
24	y	146	ILE
24	Y	146	ILE
20	n	145	ILE
20	N	145	ILE

### 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	275/275 (100%)	275 (100%)	0	100	100
1	a	275/275 (100%)	275 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	150 (99%)	1 (1%)	84	90
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5934/5934 (100%)	5933 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	p	228	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
20	N	148	GLN
2	b	394	GLN
15	p	71	ASN
19	z	6	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
2	CSD	b	218	2	3,7,8	0.88	0	1,8,10	0.59	0
22	SEP	R	84	22	8,9,10	1.50	1 (12%)	8,12,14	1.64	2 (25%)
2	CSD	B	218	2	3,7,8	0.83	0	1,8,10	0.58	0
22	SEP	r	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.53	2 (25%)

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
2	CSD	b	218	2	-	1/2/6/8	-
22	SEP	R	84	22	-	1/5/8/10	-
2	CSD	B	218	2	-	1/2/6/8	-
22	SEP	r	84	22	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.35	1.61	1.50
22	r	84	SEP	P-O1P	3.33	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	84	SEP	P-OG-CB	-3.02	109.98	118.30
22	r	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	R	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	r	84	SEP	P-OG-CB	-2.25	112.11	118.30

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	r	84	SEP	N-CA-CB-OG
22	r	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P
22	r	84	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 8 are monoatomic - leaving 346 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
41	BCT	D	401	-	2,3,3	1.32	0	2,3,3	2.60	2 (100%)
46	LUT	n	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.89	12 (23%)
47	NEX	N	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.61	11 (22%)
38	3PH	T	101	-	47,47,47	0.84	3 (6%)	51,52,52	1.12	2 (3%)
45	CHL	n	606	-	66,74,74	0.95	3 (4%)	73,114,114	1.12	7 (9%)
29	CLA	r	608	-	60,68,73	1.06	4 (6%)	70,107,113	1.10	4 (5%)
29	CLA	s	610	23	65,73,73	1.01	4 (6%)	76,113,113	1.12	5 (6%)
29	CLA	S	610	23	65,73,73	1.02	3 (4%)	76,113,113	1.05	3 (3%)
29	CLA	S	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.02	3 (3%)
45	CHL	N	605	20	66,74,74	0.86	3 (4%)	73,114,114	1.21	7 (9%)
45	CHL	N	609	20	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	r	602	22	60,68,73	1.05	3 (5%)	70,107,113	1.11	4 (5%)
29	CLA	Y	608	52	50,58,73	1.15	3 (6%)	58,95,113	1.09	3 (5%)
33	SQD	B	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
29	CLA	B	606	-	65,73,73	1.00	3 (4%)	76,113,113	1.13	3 (3%)
46	LUT	s	621	-	42,43,43	2.29	1 (2%)	51,60,60	1.92	12 (23%)
34	SPH	A	414	-	19,20,20	0.64	0	18,21,21	1.07	1 (5%)
39	DGA	J	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.24	2 (6%)
29	CLA	n	613	20	65,73,73	1.01	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	a	405	-	65,73,73	1.03	3 (4%)	76,113,113	1.18	5 (6%)
45	CHL	S	601	23	46,54,74	1.06	4 (8%)	49,90,114	1.41	7 (14%)
31	BCR	a	411	-	41,41,41	1.83	5 (12%)	56,56,56	4.25	15 (26%)
29	CLA	B	614	-	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
40	LHG	l	101	-	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
31	BCR	c	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	20 (35%)
29	CLA	b	613	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	2 (2%)
35	LMG	C	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.04	2 (3%)
29	CLA	g	602	21	65,73,73	1.03	3 (4%)	76,113,113	0.99	3 (3%)
29	CLA	n	610	20	65,73,73	1.03	4 (6%)	76,113,113	1.16	6 (7%)
29	CLA	a	406	52	65,73,73	1.01	3 (4%)	76,113,113	1.08	6 (7%)
33	SQD	b	626	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
29	CLA	C	501	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
46	LUT	S	621	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
29	CLA	n	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.07	5 (6%)
46	LUT	R	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.01	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	c	503	-	65,73,73	1.03	3 (4%)	76,113,113	0.95	4 (5%)
29	CLA	N	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.89	3 (3%)
29	CLA	D	402	-	65,73,73	1.01	3 (4%)	76,113,113	1.02	2 (2%)
45	CHL	g	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.38	10 (19%)
29	CLA	b	610	-	65,73,73	1.02	3 (4%)	76,113,113	1.07	4 (5%)
29	CLA	s	612	23	45,53,73	1.23	3 (6%)	52,89,113	1.12	3 (5%)
46	LUT	G	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	13 (25%)
45	CHL	G	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.26	10 (13%)
45	CHL	n	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.25	9 (12%)
31	BCR	B	618	-	41,41,41	1.86	5 (12%)	56,56,56	4.22	19 (33%)
29	CLA	r	603	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	7 (10%)
29	CLA	c	501	-	65,73,73	1.02	3 (4%)	76,113,113	1.02	5 (6%)
29	CLA	R	602	22	60,68,73	1.06	3 (5%)	70,107,113	1.09	4 (5%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
29	CLA	b	609	-	65,73,73	0.99	3 (4%)	76,113,113	0.98	1 (1%)
45	CHL	y	601	24	66,74,74	0.89	3 (4%)	73,114,114	1.19	10 (13%)
45	CHL	y	607	-	66,74,74	0.79	2 (3%)	73,114,114	1.27	11 (15%)
45	CHL	y	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	8 (16%)
29	CLA	C	507	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	3 (3%)
29	CLA	s	617	23	50,58,73	1.16	3 (6%)	58,95,113	1.21	6 (10%)
38	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.10	2 (3%)
26	OEX	a	401	52,1,4	0,15,15	-	-	-	-	-
35	LMG	A	413	-	40,40,55	0.76	2 (5%)	48,48,63	1.15	4 (8%)
29	CLA	d	402	-	65,73,73	1.01	4 (6%)	76,113,113	1.03	2 (2%)
50	LPX	s	625	-	18,18,29	1.23	2 (11%)	20,22,33	1.03	1 (5%)
29	CLA	Y	614	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	3 (3%)
29	CLA	B	610	-	65,73,73	1.02	4 (6%)	76,113,113	1.05	3 (3%)
45	CHL	n	605	20	66,74,74	0.91	4 (6%)	73,114,114	1.25	12 (16%)
29	CLA	S	609	23	60,68,73	1.06	3 (5%)	70,107,113	1.08	3 (4%)
29	CLA	b	606	-	65,73,73	1.01	3 (4%)	76,113,113	1.14	4 (5%)
29	CLA	b	614	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	2 (2%)
35	LMG	c	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.11	3 (5%)
45	CHL	G	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.26	11 (15%)
51	PTY	y	627	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
33	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	CHL	Y	606	-	66,74,74	0.94	4 (6%)	73,114,114	1.15	9 (12%)
29	CLA	n	612	20	45,53,73	1.23	3 (6%)	52,89,113	1.10	4 (7%)
29	CLA	G	611	-	65,73,73	1.02	3 (4%)	76,113,113	1.06	3 (3%)
29	CLA	Y	602	24	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
47	NEX	n	623	-	38,46,46	3.36	9 (23%)	50,70,70	1.60	10 (20%)
48	XAT	G	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	B	602	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
43	HEM	f	101	7,6	41,50,50	1.44	4 (9%)	45,82,82	1.30	4 (8%)
29	CLA	R	608	-	60,68,73	1.06	4 (6%)	70,107,113	1.04	3 (4%)
45	CHL	y	606	52	51,59,74	0.97	3 (5%)	55,96,114	1.39	11 (20%)
29	CLA	y	611	40	65,73,73	1.02	3 (4%)	76,113,113	0.96	3 (3%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	13 (23%)
29	CLA	Y	612	24	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
46	LUT	r	620	-	42,43,43	2.42	2 (4%)	51,60,60	1.94	14 (27%)
34	SPH	a	414	-	19,20,20	0.65	0	18,21,21	1.08	1 (5%)
45	CHL	N	601	20	66,74,74	0.82	3 (4%)	73,114,114	1.23	10 (13%)
47	NEX	Y	623	-	38,46,46	3.31	9 (23%)	50,70,70	1.84	11 (22%)
45	CHL	r	606	-	44,52,74	1.07	3 (6%)	46,87,114	1.35	8 (17%)
29	CLA	A	410	-	60,68,73	1.04	3 (5%)	70,107,113	1.10	4 (5%)
48	XAT	R	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.87	13 (24%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.02	2 (4%)
30	PHO	a	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.25	5 (10%)
31	BCR	c	515	-	41,41,41	1.82	5 (12%)	56,56,56	4.17	19 (33%)
29	CLA	B	617	-	55,63,73	1.10	4 (7%)	64,101,113	1.08	3 (4%)
29	CLA	B	605	-	65,73,73	1.01	3 (4%)	76,113,113	1.21	6 (7%)
48	XAT	N	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.00	14 (25%)
36	C7Z	b	620	-	43,43,43	5.29	27 (62%)	58,60,60	2.41	24 (41%)
35	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.08	3 (5%)
29	CLA	R	612	-	50,58,73	1.17	3 (6%)	58,95,113	1.08	4 (6%)
29	CLA	y	602	24	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	s	609	-	60,68,73	1.05	3 (5%)	70,107,113	1.08	3 (4%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.04	2 (4%)
33	SQD	b	621	-	41,42,54	0.87	0	50,53,65	0.96	3 (6%)
29	CLA	N	604	-	65,73,73	1.01	3 (4%)	76,113,113	1.02	4 (5%)
29	CLA	S	604	-	55,63,73	1.11	3 (5%)	64,101,113	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	c	520	-	60,60,67	1.06	6 (10%)	74,74,81	0.95	2 (2%)
46	LUT	g	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.96	13 (25%)
33	SQD	m	101	-	41,42,54	0.88	0	50,53,65	0.96	3 (6%)
45	CHL	Y	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.22	10 (13%)
29	CLA	R	603	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	5 (7%)
37	DGD	c	519	-	63,63,67	1.11	7 (11%)	77,77,81	0.94	3 (3%)
29	CLA	Y	603	-	65,73,73	1.02	3 (4%)	76,113,113	0.93	2 (2%)
29	CLA	C	511	4	65,73,73	1.04	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	b	616	-	65,73,73	1.01	3 (4%)	76,113,113	0.91	2 (2%)
40	LHG	d	410	-	38,38,48	0.41	0	41,44,54	1.09	2 (4%)
35	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
46	LUT	N	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	12 (23%)
40	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.05	2 (4%)
45	CHL	N	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.14	9 (12%)
29	CLA	b	602	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	4 (5%)
45	CHL	g	605	21	48,56,74	1.00	3 (6%)	51,92,114	1.31	9 (17%)
29	CLA	B	607	-	65,73,73	1.02	3 (4%)	76,113,113	1.05	4 (5%)
45	CHL	s	608	-	61,69,74	0.88	3 (4%)	67,108,114	1.26	10 (14%)
49	LMT	R	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.18	5 (10%)
29	CLA	c	511	4	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
29	CLA	b	617	-	65,73,73	1.01	4 (6%)	76,113,113	0.98	3 (3%)
29	CLA	B	603	-	65,73,73	1.00	3 (4%)	76,113,113	1.06	2 (2%)
29	CLA	g	610	21	65,73,73	1.01	4 (6%)	76,113,113	1.25	5 (6%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.08	1 (5%)
29	CLA	C	510	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	3 (3%)
45	CHL	S	607	-	43,51,74	1.03	3 (6%)	45,86,114	1.47	9 (20%)
29	CLA	B	608	52	65,73,73	0.99	3 (4%)	76,113,113	1.01	3 (3%)
51	PTY	Y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.45	2 (9%)
45	CHL	Y	609	24	66,74,74	0.84	3 (4%)	73,114,114	1.27	11 (15%)
46	LUT	Y	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	15 (29%)
46	LUT	g	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	12 (23%)
31	BCR	A	411	-	41,41,41	1.84	5 (12%)	56,56,56	4.27	15 (26%)
29	CLA	C	509	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
33	SQD	C	526	-	35,36,54	0.94	0	44,47,65	1.04	2 (4%)
29	CLA	C	504	52	55,63,73	1.08	3 (5%)	64,101,113	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	S	602	23	60,68,73	1.06	3 (5%)	70,107,113	0.99	4 (5%)
29	CLA	r	612	-	51,59,73	1.17	3 (5%)	59,96,113	1.24	5 (8%)
35	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.07	3 (5%)
40	LHG	g	624	29	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
40	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
29	CLA	b	612	-	65,73,73	1.03	3 (4%)	76,113,113	1.08	4 (5%)
40	LHG	n	624	-	41,41,48	0.41	0	44,47,54	1.15	4 (9%)
40	LHG	c	497	-	37,37,48	0.44	0	40,43,54	1.16	3 (7%)
45	CHL	g	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.36	14 (19%)
47	NEX	S	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.80	13 (26%)
29	CLA	A	406	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	d	403	-	65,73,73	1.02	3 (4%)	76,113,113	1.09	5 (6%)
29	CLA	a	407	52	49,57,73	1.15	3 (6%)	55,93,113	1.18	4 (7%)
48	XAT	r	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.89	11 (20%)
29	CLA	g	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.00	2 (2%)
29	CLA	r	609	22	60,68,73	1.08	3 (5%)	70,107,113	1.04	4 (5%)
29	CLA	c	509	-	65,73,73	1.03	3 (4%)	76,113,113	1.06	4 (5%)
36	C7Z	B	620	-	43,43,43	5.30	27 (62%)	58,60,60	2.46	23 (39%)
29	CLA	c	510	-	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)
29	CLA	G	602	21	65,73,73	1.04	3 (4%)	76,113,113	0.96	3 (3%)
50	LPX	S	625	-	19,19,29	1.20	2 (10%)	21,23,33	1.04	1 (4%)
51	PTY	y	626	-	49,49,49	0.88	4 (8%)	52,54,54	1.05	2 (3%)
34	SPH	y	625	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
45	CHL	g	608	-	44,52,74	1.06	3 (6%)	46,87,114	1.46	10 (21%)
45	CHL	G	609	21	66,74,74	0.86	3 (4%)	73,114,114	1.24	12 (16%)
37	DGD	C	520	-	54,54,67	0.93	4 (7%)	68,68,81	0.90	2 (2%)
29	CLA	s	605	23	50,58,73	1.14	3 (6%)	58,95,113	1.24	6 (10%)
45	CHL	n	608	-	50,58,74	0.93	2 (4%)	52,94,114	1.44	11 (21%)
29	CLA	s	604	-	55,63,73	1.10	3 (5%)	64,101,113	1.20	3 (4%)
45	CHL	y	609	24	66,74,74	0.86	3 (4%)	73,114,114	1.35	12 (16%)
29	CLA	b	608	52	65,73,73	0.99	3 (4%)	76,113,113	1.09	2 (2%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	1.23	3 (5%)
29	CLA	C	502	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
29	CLA	s	611	40	65,73,73	1.02	3 (4%)	76,113,113	1.06	4 (5%)
51	PTY	Y	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	h	102	-	48,48,55	0.99	4 (8%)	56,56,63	1.11	2 (3%)
44	RRX	h	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.50	23 (40%)
31	BCR	C	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
30	PHO	A	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.20	4 (8%)
31	BCR	D	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.13	14 (25%)
29	CLA	b	615	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
29	CLA	c	505	-	65,73,73	1.02	4 (6%)	76,113,113	1.08	3 (3%)
29	CLA	G	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.91	1 (1%)
46	LUT	S	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.85	10 (19%)
29	CLA	y	608	-	50,58,73	1.16	3 (6%)	58,95,113	1.08	3 (5%)
40	LHG	y	624	29	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
30	PHO	A	408	-	51,69,69	0.98	4 (7%)	47,99,99	1.20	5 (10%)
45	CHL	S	606	-	44,52,74	1.08	3 (6%)	46,87,114	1.34	7 (15%)
29	CLA	A	407	-	50,58,73	1.15	3 (6%)	58,95,113	1.09	4 (6%)
29	CLA	a	410	-	60,68,73	1.03	3 (5%)	70,107,113	1.11	5 (7%)
45	CHL	G	606	-	50,58,74	1.03	4 (8%)	52,94,114	1.41	9 (17%)
29	CLA	C	508	-	65,73,73	1.01	3 (4%)	76,113,113	1.08	5 (6%)
45	CHL	Y	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	9 (18%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
47	NEX	g	623	-	38,46,46	3.29	9 (23%)	50,70,70	1.87	13 (26%)
29	CLA	g	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.09	4 (7%)
35	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.16	3 (6%)
29	CLA	N	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.00	5 (6%)
47	NEX	y	623	-	38,46,46	3.31	11 (28%)	50,70,70	1.82	13 (26%)
29	CLA	B	613	-	65,73,73	1.00	3 (4%)	76,113,113	1.05	2 (2%)
29	CLA	y	614	-	65,73,73	1.03	3 (4%)	76,113,113	1.02	5 (6%)
29	CLA	g	603	-	65,73,73	1.01	3 (4%)	76,113,113	0.98	3 (3%)
44	RRX	H	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.58	22 (38%)
40	LHG	s	624	29	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
40	LHG	G	624	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
29	CLA	y	603	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	2 (2%)
33	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	c	504	-	65,73,73	0.98	3 (4%)	76,113,113	1.05	3 (3%)
35	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.12	4 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	G	612	21	43,51,73	1.22	3 (6%)	49,86,113	1.06	3 (6%)
35	LMG	C	527	-	42,42,55	0.78	2 (4%)	50,50,63	1.17	4 (8%)
45	CHL	N	607	-	66,74,74	0.89	3 (4%)	73,114,114	1.25	12 (16%)
49	LMT	r	625	-	36,36,36	1.24	6 (16%)	47,47,47	1.16	4 (8%)
29	CLA	b	604	-	65,73,73	1.00	3 (4%)	76,113,113	1.12	3 (3%)
29	CLA	g	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
47	NEX	G	623	-	38,46,46	3.31	9 (23%)	50,70,70	1.83	15 (30%)
29	CLA	C	512	-	65,73,73	1.02	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	c	508	-	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
35	LMG	w	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
29	CLA	G	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.94	3 (3%)
37	DGD	b	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.19	5 (8%)
45	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.44	10 (19%)
45	CHL	s	607	-	43,51,74	1.09	3 (6%)	45,86,114	1.45	7 (15%)
46	LUT	y	620	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	13 (25%)
29	CLA	C	506	-	65,73,73	1.01	3 (4%)	76,113,113	0.94	3 (3%)
40	LHG	C	525	-	34,34,48	0.44	0	37,40,54	1.17	2 (5%)
29	CLA	N	612	20	45,53,73	1.22	3 (6%)	52,89,113	1.03	4 (7%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	18 (32%)
29	CLA	G	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.02	2 (3%)
29	CLA	N	613	20	65,73,73	1.03	3 (4%)	76,113,113	0.96	2 (2%)
47	NEX	R	622	-	24,28,46	3.24	6 (25%)	32,42,70	1.76	7 (21%)
45	CHL	s	601	23	46,54,74	1.05	4 (8%)	49,90,114	1.41	9 (18%)
29	CLA	B	609	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	2 (2%)
37	DGD	C	518	-	52,52,67	1.02	4 (7%)	66,66,81	0.93	2 (3%)
39	DGA	B	625	-	36,36,43	1.19	2 (5%)	38,38,45	1.30	3 (7%)
31	BCR	B	619	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
29	CLA	C	513	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	2 (2%)
29	CLA	C	503	-	65,73,73	1.03	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	g	604	-	49,57,73	1.16	3 (6%)	55,93,113	1.11	3 (5%)
29	CLA	D	403	-	60,68,73	1.07	3 (5%)	70,107,113	1.14	4 (5%)
31	BCR	C	514	-	41,41,41	1.82	4 (9%)	56,56,56	4.21	14 (25%)
29	CLA	N	611	40	49,57,73	1.17	3 (6%)	55,93,113	1.09	3 (5%)
29	CLA	y	613	24	65,73,73	1.00	3 (4%)	76,113,113	0.89	1 (1%)
29	CLA	s	602	23	60,68,73	1.05	3 (5%)	70,107,113	1.14	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	d	404	-	41,41,41	1.82	4 (9%)	56,56,56	4.27	17 (30%)
40	LHG	S	624	29	44,44,48	0.41	0	47,50,54	1.04	3 (6%)
45	CHL	n	609	20	66,74,74	0.82	2 (3%)	73,114,114	1.31	12 (16%)
29	CLA	N	614	-	49,57,73	1.16	3 (6%)	55,93,113	1.05	4 (7%)
29	CLA	c	507	52	65,73,73	1.03	4 (6%)	76,113,113	1.10	4 (5%)
45	CHL	S	608	-	61,69,74	0.90	3 (4%)	67,108,114	1.36	12 (17%)
45	CHL	n	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.26	12 (16%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.94	2 (2%)
39	DGA	c	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	A	405	-	65,73,73	1.01	3 (4%)	76,113,113	1.05	4 (5%)
48	XAT	n	622	-	39,47,47	0.73	1 (2%)	54,74,74	2.03	13 (24%)
29	CLA	B	615	-	65,73,73	1.04	3 (4%)	76,113,113	1.08	3 (3%)
41	BCT	d	401	27	2,3,3	1.15	0	2,3,3	4.30	2 (100%)
29	CLA	B	612	-	65,73,73	1.02	3 (4%)	76,113,113	1.11	5 (6%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.18	2 (3%)
29	CLA	b	607	-	57,65,73	1.07	3 (5%)	66,103,113	1.08	3 (4%)
29	CLA	S	612	23	45,53,73	1.23	3 (6%)	52,89,113	1.03	4 (7%)
45	CHL	Y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.23	10 (13%)
45	CHL	g	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
29	CLA	c	502	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	4 (5%)
29	CLA	n	604	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	3 (3%)
29	CLA	N	610	-	65,73,73	1.01	3 (4%)	76,113,113	1.11	3 (3%)
29	CLA	G	610	21	65,73,73	1.02	3 (4%)	76,113,113	1.21	5 (6%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
48	XAT	g	622	-	39,47,47	0.73	1 (2%)	54,74,74	1.99	13 (24%)
40	LHG	Y	624	29	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
29	CLA	n	611	-	49,57,73	1.16	3 (6%)	55,93,113	1.04	3 (5%)
38	3PH	S	626	-	29,29,47	1.09	4 (13%)	33,34,52	1.24	2 (6%)
29	CLA	y	610	24	65,73,73	1.00	4 (6%)	76,113,113	1.11	4 (5%)
47	NEX	s	623	-	38,46,46	3.36	9 (23%)	50,70,70	1.67	10 (20%)
29	CLA	s	614	-	55,63,73	1.10	3 (5%)	64,101,113	1.03	3 (4%)
33	SQD	M	101	-	41,42,54	0.89	0	50,53,65	0.96	3 (6%)
46	LUT	n	621	-	42,43,43	2.32	1 (2%)	51,60,60	1.81	12 (23%)
29	CLA	r	604	-	49,57,73	1.15	3 (6%)	55,93,113	1.03	2 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	G	604	-	49,57,73	1.19	3 (6%)	55,93,113	1.07	4 (7%)
33	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.93	2 (3%)
29	CLA	s	603	-	65,73,73	1.02	4 (6%)	76,113,113	1.17	5 (6%)
29	CLA	c	513	-	65,73,73	1.01	3 (4%)	76,113,113	1.04	3 (3%)
30	PHO	a	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.22	5 (10%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	R	604	-	49,57,73	1.16	3 (6%)	55,93,113	1.03	1 (1%)
39	DGA	C	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.49	3 (6%)
35	LMG	H	102	-	48,48,55	0.99	4 (8%)	56,56,63	1.08	2 (3%)
31	BCR	b	619	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
29	CLA	S	605	23	50,58,73	1.15	3 (6%)	58,95,113	1.32	3 (5%)
45	CHL	R	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.39	9 (17%)
29	CLA	b	603	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	3 (3%)
29	CLA	y	612	24	65,73,73	1.01	3 (4%)	76,113,113	1.02	3 (3%)
46	LUT	N	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.88	13 (25%)
29	CLA	r	610	22	60,68,73	1.07	3 (5%)	70,107,113	1.17	5 (7%)
29	CLA	c	512	-	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
29	CLA	b	611	52	65,73,73	1.01	3 (4%)	76,113,113	0.92	1 (1%)
35	LMG	D	411	-	42,42,55	0.76	2 (4%)	50,50,63	0.97	2 (4%)
46	LUT	Y	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
29	CLA	Y	613	24	65,73,73	1.01	3 (4%)	76,113,113	0.88	1 (1%)
46	LUT	G	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.93	11 (21%)
48	XAT	Y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.75	20 (37%)
42	PL9	D	405	-	55,55,55	1.34	6 (10%)	68,69,69	1.47	11 (16%)
35	LMG	d	411	-	46,46,55	0.91	3 (6%)	54,54,63	1.05	2 (3%)
33	SQD	A	412	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
45	CHL	G	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.39	8 (15%)
29	CLA	S	603	-	65,73,73	1.03	4 (6%)	76,113,113	1.18	7 (9%)
45	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.40	8 (17%)
47	NEX	r	622	-	24,28,46	3.23	6 (25%)	32,42,70	1.83	7 (21%)
29	CLA	S	617	23	50,58,73	1.18	3 (6%)	58,95,113	1.27	6 (10%)
29	CLA	Y	604	52	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)
29	CLA	b	605	-	65,73,73	1.02	4 (6%)	76,113,113	1.22	5 (6%)
29	CLA	B	604	-	65,73,73	0.99	3 (4%)	76,113,113	1.12	5 (6%)
29	CLA	S	614	-	50,58,73	1.16	3 (6%)	58,95,113	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	s	613	23	55,63,73	1.11	3 (5%)	64,101,113	1.10	3 (4%)
29	CLA	S	613	23	55,63,73	1.12	3 (5%)	64,101,113	1.14	3 (4%)
29	CLA	Y	611	40	65,73,73	1.01	3 (4%)	76,113,113	1.01	6 (7%)
29	CLA	g	612	21	43,51,73	1.20	3 (6%)	49,86,113	1.11	2 (4%)
29	CLA	y	604	52	65,73,73	1.00	3 (4%)	76,113,113	1.11	5 (6%)
42	PL9	d	405	-	55,55,55	1.28	5 (9%)	68,69,69	1.51	11 (16%)
29	CLA	c	506	-	60,68,73	1.05	3 (5%)	70,107,113	1.10	5 (7%)
29	CLA	B	616	-	65,73,73	1.00	3 (4%)	76,113,113	0.89	2 (2%)
46	LUT	s	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.99	15 (29%)
29	CLA	R	609	22	46,54,73	1.19	3 (6%)	53,90,113	1.19	4 (7%)
29	CLA	B	611	52	65,73,73	1.01	3 (4%)	76,113,113	0.93	2 (2%)
37	DGD	C	519	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	3 (4%)
38	3PH	b	624	-	38,38,47	0.96	4 (10%)	42,43,52	1.17	2 (4%)
45	CHL	g	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
45	CHL	s	606	-	44,52,74	0.98	2 (4%)	46,87,114	1.45	8 (17%)
31	BCR	b	618	-	41,41,41	1.85	4 (9%)	56,56,56	4.22	15 (26%)
37	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
29	CLA	n	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.20	3 (5%)
43	HEM	F	101	7,6	41,50,50	1.45	3 (7%)	45,82,82	1.36	5 (11%)
46	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	13 (25%)
48	XAT	y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
26	OEX	A	401	52,1,4	0,15,15	-	-	-	-	-
29	CLA	Y	610	24	65,73,73	1.01	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	n	603	-	65,73,73	1.01	3 (4%)	76,113,113	1.00	4 (5%)
29	CLA	C	505	-	60,68,73	1.07	4 (6%)	70,107,113	1.04	2 (2%)
31	BCR	c	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	19 (33%)
40	LHG	N	624	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)
35	LMG	b	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.07	2 (3%)
29	CLA	R	610	22	60,68,73	1.06	3 (5%)	70,107,113	1.08	4 (5%)
45	CHL	r	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.44	8 (15%)
45	CHL	R	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	8 (17%)

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
46	LUT	n	620	-	-	4/29/67/67	0/2/2/2
47	NEX	N	623	-	-	2/27/83/83	1/3/3/3
38	3PH	T	101	-	-	27/49/49/49	-
45	CHL	n	606	-	4/4/20/26	9/39/137/137	-
29	CLA	r	608	-	1/1/14/20	13/31/109/115	-
29	CLA	s	610	23	1/1/15/20	11/37/115/115	-
29	CLA	S	610	23	1/1/15/20	10/37/115/115	-
29	CLA	S	611	40	1/1/15/20	17/37/115/115	-
45	CHL	N	605	20	4/4/20/26	15/39/137/137	-
45	CHL	N	609	20	4/4/20/26	6/39/137/137	-
29	CLA	r	602	22	1/1/14/20	7/31/109/115	-
29	CLA	Y	608	52	1/1/12/20	8/19/97/115	-
33	SQD	B	626	-	-	14/49/69/69	0/1/1/1
29	CLA	B	606	-	1/1/15/20	8/37/115/115	-
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
34	SPH	A	414	-	-	10/21/21/21	-
39	DGA	J	101	-	-	14/30/30/45	-
29	CLA	n	613	20	-	14/37/115/115	-
29	CLA	a	405	-	1/1/15/20	12/37/115/115	-
45	CHL	S	601	23	3/3/16/26	3/15/113/137	-
31	BCR	a	411	-	-	9/29/63/63	0/2/2/2
29	CLA	B	614	-	1/1/15/20	11/37/115/115	-
40	LHG	l	101	-	-	31/53/53/53	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	b	613	-	1/1/15/20	10/37/115/115	-
35	LMG	C	523	-	-	21/50/70/70	0/1/1/1
29	CLA	g	602	21	1/1/15/20	16/37/115/115	-
29	CLA	n	610	20	1/1/15/20	11/37/115/115	-
29	CLA	a	406	52	1/1/15/20	15/37/115/115	-
33	SQD	b	626	-	-	19/49/69/69	0/1/1/1
29	CLA	C	501	-	-	13/37/115/115	-
46	LUT	S	621	-	-	3/29/67/67	0/2/2/2
29	CLA	n	602	20	1/1/15/20	11/37/115/115	-
46	LUT	R	620	-	-	5/29/67/67	0/2/2/2
29	CLA	c	503	-	-	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	603	-	1/1/15/20	21/37/115/115	-
29	CLA	D	402	-	1/1/15/20	6/37/115/115	-
45	CHL	g	606	-	3/3/16/26	3/20/118/137	-
29	CLA	b	610	-	1/1/15/20	5/37/115/115	-
29	CLA	s	612	23	1/1/11/20	2/13/91/115	-
46	LUT	G	620	-	-	0/29/67/67	0/2/2/2
45	CHL	G	601	21	4/4/20/26	11/39/137/137	-
45	CHL	n	601	20	4/4/20/26	12/39/137/137	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
29	CLA	r	603	-	-	12/31/109/115	-
29	CLA	c	501	-	-	13/37/115/115	-
29	CLA	R	602	22	1/1/14/20	6/31/109/115	-
39	DGA	j	101	-	-	16/30/30/45	-
29	CLA	b	609	-	-	4/37/115/115	-
45	CHL	y	601	24	4/4/20/26	8/39/137/137	-
45	CHL	y	607	-	4/4/20/26	12/39/137/137	-
45	CHL	y	605	24	3/3/16/26	4/15/113/137	-
29	CLA	C	507	52	1/1/15/20	12/37/115/115	-
29	CLA	s	617	23	1/1/12/20	5/19/97/115	-
38	3PH	s	626	-	-	23/49/49/49	-
35	LMG	A	413	-	-	10/35/55/70	0/1/1/1
29	CLA	d	402	-	1/1/15/20	5/37/115/115	-
50	LPX	s	625	-	-	10/20/20/31	-
29	CLA	Y	614	-	1/1/15/20	13/37/115/115	-
29	CLA	B	610	-	1/1/15/20	12/37/115/115	-
45	CHL	n	605	20	4/4/20/26	11/39/137/137	-
29	CLA	S	609	23	1/1/14/20	9/31/109/115	-
29	CLA	b	606	-	1/1/15/20	9/37/115/115	-
29	CLA	b	614	-	1/1/15/20	11/37/115/115	-
45	CHL	G	607	-	4/4/20/26	13/39/137/137	-
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
51	PTY	y	627	-	-	14/20/20/53	-
33	SQD	B	621	-	-	14/37/57/69	0/1/1/1
45	CHL	Y	606	-	4/4/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	n	612	20	1/1/11/20	6/13/91/115	-
29	CLA	G	611	-	1/1/15/20	11/37/115/115	-
29	CLA	Y	602	24	1/1/15/20	12/37/115/115	-
48	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
47	NEX	n	623	-	-	2/27/83/83	1/3/3/3
29	CLA	B	602	-	1/1/15/20	18/37/115/115	-
43	HEM	f	101	7,6	-	1/12/54/54	-
29	CLA	R	608	-	1/1/14/20	11/31/109/115	-
45	CHL	y	606	52	3/3/17/26	2/21/119/137	-
29	CLA	y	611	40	1/1/15/20	6/37/115/115	-
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
29	CLA	Y	612	24	1/1/15/20	13/37/115/115	-
46	LUT	r	620	-	-	5/29/67/67	0/2/2/2
34	SPH	a	414	-	-	11/21/21/21	-
45	CHL	N	601	20	4/4/20/26	9/39/137/137	-
47	NEX	Y	623	-	-	8/27/83/83	0/3/3/3
45	CHL	r	606	-	3/3/15/26	4/13/111/137	-
48	XAT	R	621	-	2/2/12/26	0/31/93/93	0/4/4/4
29	CLA	A	410	-	-	8/31/109/115	-
40	LHG	D	408	-	-	16/48/48/53	-
30	PHO	a	409	-	-	6/37/103/103	0/5/6/6
31	BCR	c	515	-	-	13/29/63/63	0/2/2/2
29	CLA	B	617	-	1/1/13/20	11/25/103/115	-
29	CLA	B	605	-	1/1/15/20	16/37/115/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
36	C7Z	b	620	-	1/1/12/26	7/29/67/67	0/2/2/2
35	LMG	B	622	-	-	13/39/59/70	0/1/1/1
29	CLA	R	612	-	1/1/12/20	9/19/97/115	-
29	CLA	y	602	24	1/1/15/20	6/37/115/115	-
29	CLA	s	609	-	1/1/14/20	17/31/109/115	-
40	LHG	D	410	-	-	18/43/43/53	-
33	SQD	b	621	-	-	13/37/57/69	0/1/1/1
29	CLA	N	604	-	1/1/15/20	8/37/115/115	-
29	CLA	S	604	-	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	c	520	-	-	8/48/88/95	0/2/2/2
46	LUT	g	620	-	-	2/29/67/67	0/2/2/2
33	SQD	m	101	-	-	21/37/57/69	0/1/1/1
45	CHL	Y	601	24	4/4/20/26	5/39/137/137	-
29	CLA	R	603	-	-	11/31/109/115	-
37	DGD	c	519	-	-	17/51/91/95	0/2/2/2
29	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
29	CLA	C	511	4	1/1/15/20	5/37/115/115	-
29	CLA	b	616	-	1/1/15/20	12/37/115/115	-
40	LHG	d	410	-	-	21/43/43/53	-
35	LMG	c	523	-	-	13/50/70/70	0/1/1/1
46	LUT	N	621	-	-	3/29/67/67	0/2/2/2
40	LHG	d	408	-	-	22/48/48/53	-
45	CHL	N	606	-	4/4/20/26	9/39/137/137	-
29	CLA	b	602	-	1/1/15/20	22/37/115/115	-
45	CHL	g	605	21	3/3/16/26	4/18/116/137	-
29	CLA	B	607	-	1/1/15/20	14/37/115/115	-
45	CHL	s	608	-	4/4/19/26	5/33/131/137	-
49	LMT	R	625	-	-	2/21/61/61	0/2/2/2
29	CLA	c	511	4	-	12/37/115/115	-
29	CLA	b	617	-	1/1/15/20	15/37/115/115	-
29	CLA	B	603	-	1/1/15/20	4/37/115/115	-
29	CLA	g	610	21	1/1/15/20	5/37/115/115	-
34	SPH	Y	625	-	-	11/21/21/21	-
29	CLA	C	510	-	1/1/15/20	14/37/115/115	-
45	CHL	S	607	-	3/3/15/26	0/12/110/137	-
29	CLA	B	608	52	1/1/15/20	23/37/115/115	-
51	PTY	Y	627	-	-	12/20/20/53	-
45	CHL	Y	609	24	4/4/20/26	6/39/137/137	-
46	LUT	Y	620	-	-	2/29/67/67	0/2/2/2
46	LUT	g	621	-	-	1/29/67/67	0/2/2/2
31	BCR	A	411	-	-	9/29/63/63	0/2/2/2
29	CLA	C	509	-	1/1/15/20	16/37/115/115	-
33	SQD	C	526	-	-	12/31/51/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	504	52	1/1/13/20	8/25/103/115	-
29	CLA	S	602	23	1/1/14/20	10/31/109/115	-
29	CLA	r	612	-	1/1/12/20	9/21/99/115	-
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
40	LHG	g	624	29	-	30/53/53/53	-
40	LHG	d	409	-	-	22/53/53/53	-
29	CLA	b	612	-	-	12/37/115/115	-
40	LHG	n	624	-	-	30/46/46/53	-
40	LHG	c	497	-	-	19/42/42/53	-
45	CHL	g	607	-	4/4/20/26	10/39/137/137	-
47	NEX	S	623	-	-	2/27/83/83	0/3/3/3
29	CLA	A	406	52	1/1/15/20	16/37/115/115	-
29	CLA	d	403	-	1/1/15/20	10/37/115/115	-
48	XAT	r	621	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	a	407	52	-	5/18/96/115	-
29	CLA	g	611	40	1/1/15/20	8/37/115/115	-
29	CLA	r	609	22	1/1/14/20	13/31/109/115	-
29	CLA	c	509	-	1/1/15/20	14/37/115/115	-
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	c	510	-	1/1/15/20	9/37/115/115	-
29	CLA	G	602	21	1/1/15/20	14/37/115/115	-
50	LPX	S	625	-	-	7/21/21/31	-
51	PTY	y	626	-	-	28/53/53/53	-
34	SPH	y	625	-	-	3/21/21/21	-
45	CHL	g	608	-	3/3/15/26	0/13/111/137	-
45	CHL	G	609	21	4/4/20/26	11/39/137/137	-
37	DGD	C	520	-	-	5/42/82/95	0/2/2/2
29	CLA	s	605	23	-	6/19/97/115	-
45	CHL	n	608	-	3/3/16/26	3/20/118/137	-
29	CLA	s	604	-	1/1/13/20	11/25/103/115	-
45	CHL	y	609	24	4/4/20/26	6/39/137/137	-
29	CLA	b	608	52	1/1/15/20	7/37/115/115	-
40	LHG	L	101	-	-	33/53/53/53	-
29	CLA	C	502	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	611	40	1/1/15/20	14/37/115/115	-
51	PTY	Y	626	-	-	18/53/53/53	-
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
44	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
31	BCR	C	515	-	-	10/29/63/63	0/2/2/2
30	PHO	A	409	-	-	4/37/103/103	0/5/6/6
31	BCR	D	404	-	-	12/29/63/63	0/2/2/2
29	CLA	b	615	-	1/1/15/20	13/37/115/115	-
29	CLA	c	505	-	1/1/15/20	18/37/115/115	-
29	CLA	G	613	21	1/1/15/20	10/37/115/115	-
46	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	y	608	-	1/1/12/20	8/19/97/115	-
40	LHG	y	624	29	-	28/53/53/53	-
40	LHG	c	525	-	-	30/51/51/53	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
45	CHL	S	606	-	3/3/15/26	1/13/111/137	-
29	CLA	A	407	-	1/1/12/20	8/19/97/115	-
45	CHL	G	606	-	3/3/16/26	5/20/118/137	-
29	CLA	a	410	-	-	8/31/109/115	-
29	CLA	C	508	-	1/1/15/20	7/37/115/115	-
45	CHL	Y	605	24	3/3/16/26	5/15/113/137	-
38	3PH	B	624	-	-	20/49/49/49	-
47	NEX	g	623	-	-	5/27/83/83	0/3/3/3
29	CLA	g	614	-	1/1/11/20	9/18/96/115	-
35	LMG	W	201	-	-	16/34/54/70	0/1/1/1
29	CLA	N	602	20	1/1/15/20	14/37/115/115	-
47	NEX	y	623	-	-	8/27/83/83	0/3/3/3
29	CLA	B	613	-	1/1/15/20	9/37/115/115	-
29	CLA	y	614	-	1/1/15/20	14/37/115/115	-
29	CLA	g	603	-	1/1/15/20	20/37/115/115	-
44	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
40	LHG	s	624	29	-	22/49/49/53	-
40	LHG	G	624	-	-	29/53/53/53	-
29	CLA	y	603	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SQD	c	526	-	-	15/49/69/69	0/1/1/1
29	CLA	c	504	-	1/1/15/20	12/37/115/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
29	CLA	G	612	21	1/1/10/20	3/11/89/115	-
35	LMG	C	527	-	-	19/37/57/70	0/1/1/1
45	CHL	N	607	-	4/4/20/26	12/39/137/137	-
49	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	b	604	-	1/1/15/20	8/37/115/115	-
29	CLA	g	613	21	-	21/37/115/115	-
47	NEX	G	623	-	-	4/27/83/83	0/3/3/3
29	CLA	C	512	-	1/1/15/20	17/37/115/115	-
29	CLA	c	508	-	1/1/15/20	6/37/115/115	-
35	LMG	w	201	-	-	17/34/54/70	0/1/1/1
29	CLA	G	603	-	1/1/15/20	10/37/115/115	-
37	DGD	b	623	-	-	8/32/72/95	0/2/2/2
45	CHL	N	608	-	3/3/16/26	5/20/118/137	-
45	CHL	s	607	-	3/3/15/26	0/12/110/137	-
46	LUT	y	620	-	-	2/29/67/67	0/2/2/2
29	CLA	C	506	-	-	8/37/115/115	-
40	LHG	C	525	-	-	23/39/39/53	-
29	CLA	N	612	20	1/1/11/20	4/13/91/115	-
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2
29	CLA	G	614	-	1/1/11/20	7/18/96/115	-
29	CLA	N	613	20	1/1/15/20	13/37/115/115	-
47	NEX	R	622	-	-	9/19/50/83	0/2/2/3
45	CHL	s	601	23	3/3/16/26	4/15/113/137	-
29	CLA	B	609	-	1/1/15/20	7/37/115/115	-
37	DGD	C	518	-	-	8/40/80/95	0/2/2/2
39	DGA	B	625	-	-	19/38/38/45	-
31	BCR	B	619	-	-	13/29/63/63	0/2/2/2
29	CLA	g	604	-	1/1/11/20	8/18/96/115	-
29	CLA	C	503	-	-	11/37/115/115	-
29	CLA	C	513	-	-	13/37/115/115	-
29	CLA	D	403	-	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	514	-	-	13/29/63/63	0/2/2/2
29	CLA	N	611	40	1/1/11/20	4/18/96/115	-
29	CLA	y	613	24	-	8/37/115/115	-
29	CLA	s	602	23	1/1/14/20	6/31/109/115	-
31	BCR	d	404	-	-	11/29/63/63	0/2/2/2
40	LHG	S	624	29	-	15/49/49/53	-
45	CHL	n	609	20	4/4/20/26	7/39/137/137	-
29	CLA	N	614	-	1/1/11/20	8/18/96/115	-
29	CLA	c	507	52	1/1/15/20	13/37/115/115	-
45	CHL	S	608	-	4/4/19/26	7/33/131/137	-
45	CHL	n	607	-	4/4/20/26	11/39/137/137	-
40	LHG	D	409	-	-	18/53/53/53	-
37	DGD	c	518	-	-	10/44/84/95	0/2/2/2
39	DGA	c	524	-	-	27/45/45/45	-
29	CLA	A	405	-	1/1/15/20	12/37/115/115	-
48	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	B	615	-	1/1/15/20	11/37/115/115	-
29	CLA	B	612	-	-	11/37/115/115	-
38	3PH	t	101	-	-	25/49/49/49	-
29	CLA	b	607	-	1/1/13/20	11/28/106/115	-
29	CLA	S	612	23	1/1/11/20	3/13/91/115	-
45	CHL	Y	607	-	4/4/20/26	11/39/137/137	-
45	CHL	g	609	21	4/4/20/26	8/39/137/137	-
29	CLA	c	502	-	1/1/15/20	11/37/115/115	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
29	CLA	N	610	-	1/1/15/20	13/37/115/115	-
29	CLA	G	610	21	1/1/15/20	5/37/115/115	-
31	BCR	C	516	-	-	11/29/63/63	0/2/2/2
48	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
40	LHG	Y	624	29	-	28/53/53/53	-
29	CLA	n	611	-	1/1/11/20	5/18/96/115	-
38	3PH	S	626	-	-	7/31/31/49	-
29	CLA	y	610	24	1/1/15/20	6/37/115/115	-
47	NEX	s	623	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	614	-	1/1/13/20	6/25/103/115	-
33	SQD	M	101	-	-	20/37/57/69	0/1/1/1
46	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	r	604	-	1/1/11/20	9/18/96/115	-
29	CLA	G	604	-	1/1/11/20	9/18/96/115	-
33	SQD	a	412	-	-	17/46/66/69	0/1/1/1
29	CLA	s	603	-	-	14/37/115/115	-
29	CLA	c	513	-	-	12/37/115/115	-
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
39	DGA	b	625	-	-	19/45/45/45	-
29	CLA	R	604	-	1/1/11/20	6/18/96/115	-
39	DGA	C	524	-	-	23/45/45/45	-
35	LMG	H	102	-	-	17/43/63/70	0/1/1/1
31	BCR	b	619	-	-	12/29/63/63	0/2/2/2
29	CLA	S	605	23	1/1/12/20	7/19/97/115	-
45	CHL	R	607	-	3/3/16/26	6/20/118/137	-
29	CLA	b	603	-	1/1/15/20	8/37/115/115	-
29	CLA	y	612	24	1/1/15/20	12/37/115/115	-
46	LUT	N	620	-	-	3/29/67/67	0/2/2/2
29	CLA	r	610	22	1/1/14/20	7/31/109/115	-
29	CLA	c	512	-	1/1/15/20	15/37/115/115	-
29	CLA	b	611	52	1/1/15/20	6/37/115/115	-
35	LMG	D	411	-	-	3/37/57/70	0/1/1/1
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	Y	613	24	1/1/15/20	18/37/115/115	-
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
48	XAT	Y	622	-	1/1/12/26	0/31/93/93	0/4/4/4
42	PL9	D	405	-	-	10/53/73/73	0/1/1/1
35	LMG	d	411	-	-	7/41/61/70	0/1/1/1
33	SQD	A	412	-	-	9/37/57/69	0/1/1/1
45	CHL	G	605	21	3/3/16/26	6/18/116/137	-
29	CLA	S	603	-	1/1/15/20	17/37/115/115	-
45	CHL	G	608	-	3/3/15/26	1/13/111/137	-
47	NEX	r	622	-	-	5/19/50/83	0/2/2/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	617	23	1/1/12/20	6/19/97/115	-
29	CLA	Y	604	52	1/1/15/20	15/37/115/115	-
29	CLA	b	605	-	1/1/15/20	12/37/115/115	-
29	CLA	B	604	-	1/1/15/20	10/37/115/115	-
29	CLA	S	614	-	1/1/12/20	8/19/97/115	-
29	CLA	s	613	23	1/1/13/20	11/25/103/115	-
29	CLA	S	613	23	1/1/13/20	11/25/103/115	-
29	CLA	Y	611	40	1/1/15/20	9/37/115/115	-
29	CLA	g	612	21	-	2/11/89/115	-
29	CLA	y	604	52	1/1/15/20	15/37/115/115	-
42	PL9	d	405	-	-	11/53/73/73	0/1/1/1
29	CLA	c	506	-	-	9/31/109/115	-
29	CLA	B	616	-	1/1/15/20	9/37/115/115	-
46	LUT	s	620	-	-	4/29/67/67	0/2/2/2
29	CLA	R	609	22	1/1/11/20	8/15/93/115	-
29	CLA	B	611	52	1/1/15/20	7/37/115/115	-
37	DGD	C	519	-	-	11/42/82/95	0/2/2/2
45	CHL	g	601	21	4/4/20/26	10/39/137/137	-
38	3PH	b	624	-	-	28/40/40/49	-
45	CHL	s	606	-	3/3/15/26	1/13/111/137	-
31	BCR	b	618	-	-	11/29/63/63	0/2/2/2
37	DGD	B	623	-	-	13/32/72/95	0/2/2/2
29	CLA	n	614	-	1/1/11/20	3/18/96/115	-
43	HEM	F	101	7,6	-	1/12/54/54	-
46	LUT	y	621	-	-	1/29/67/67	0/2/2/2
48	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	Y	610	24	1/1/15/20	4/37/115/115	-
29	CLA	n	603	-	1/1/15/20	12/37/115/115	-
29	CLA	C	505	-	1/1/14/20	14/31/109/115	-
31	BCR	c	516	-	-	12/29/63/63	0/2/2/2
40	LHG	N	624	29	-	30/53/53/53	-
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1
29	CLA	R	610	22	1/1/14/20	11/31/109/115	-
45	CHL	r	607	-	3/3/16/26	5/20/118/137	-
45	CHL	R	606	-	3/3/15/26	4/13/111/137	-

The worst 5 of 1090 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	H	101	RRX	C26-C25	15.61	1.61	1.34
44	h	101	RRX	C26-C25	15.51	1.61	1.34
36	B	620	C7Z	C25-C26	15.39	1.61	1.34
36	b	620	C7Z	C25-C26	15.36	1.61	1.34
36	B	620	C7Z	C5-C6	14.83	1.60	1.34

The worst 5 of 2038 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	404	BCR	C10-C11-C12	17.66	178.32	123.22
31	C	517	BCR	C10-C11-C12	17.51	177.86	123.22
31	c	517	BCR	C10-C11-C12	17.44	177.64	123.22
31	b	618	BCR	C10-C11-C12	17.38	177.47	123.22
31	b	619	BCR	C10-C11-C12	17.35	177.38	123.22

5 of 311 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	B	602	CLA	ND
29	B	603	CLA	ND

5 of 3579 torsion outliers are listed below:

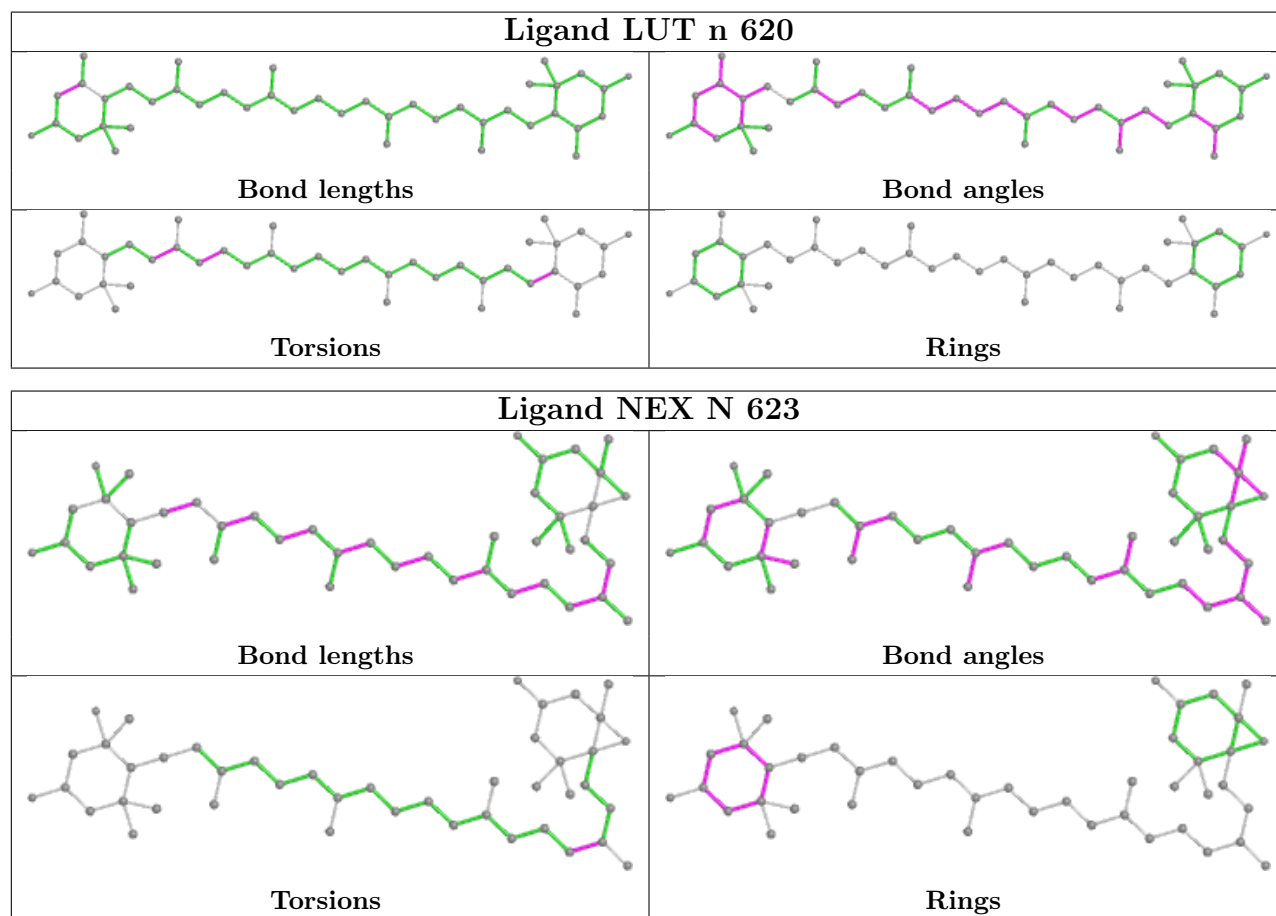
Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA

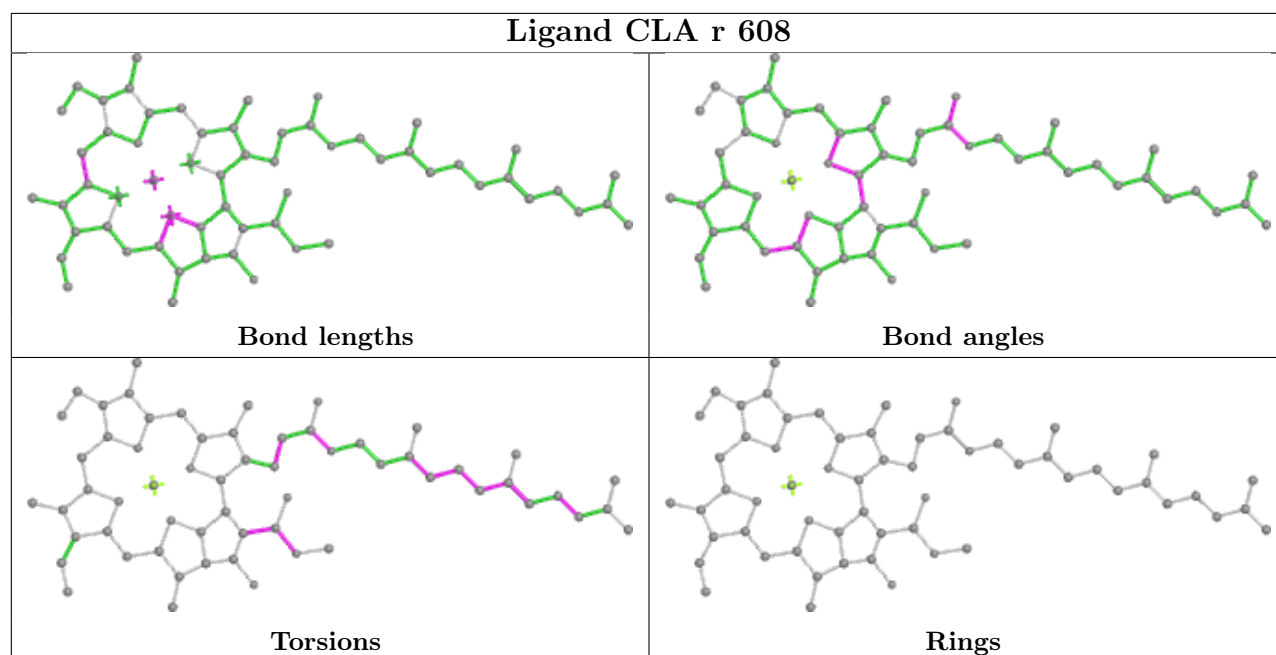
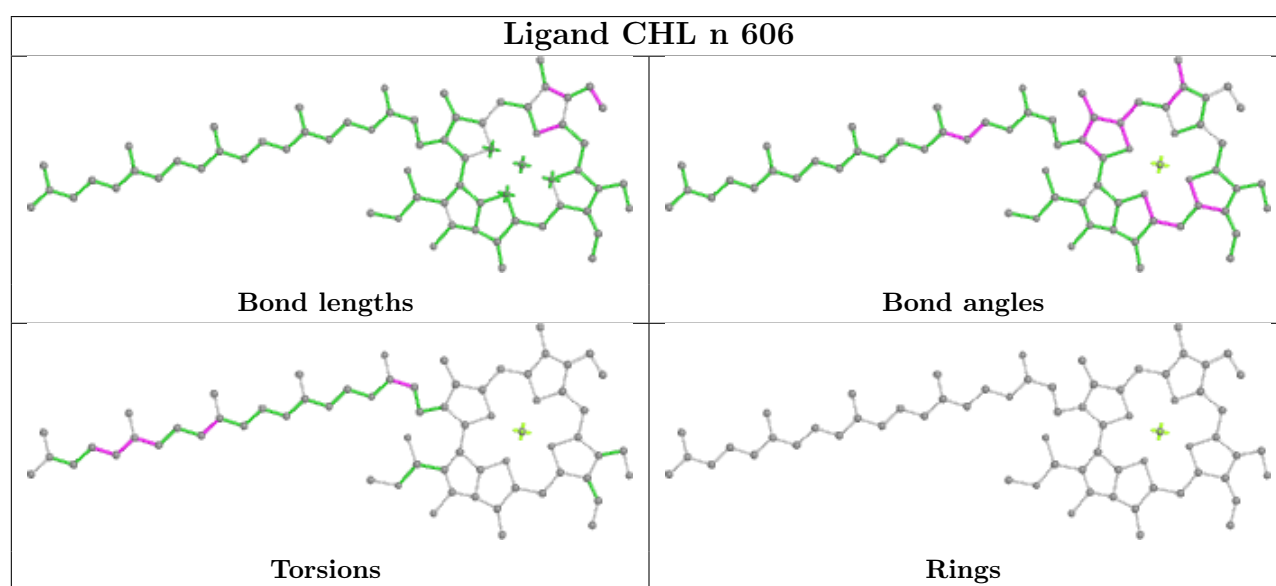
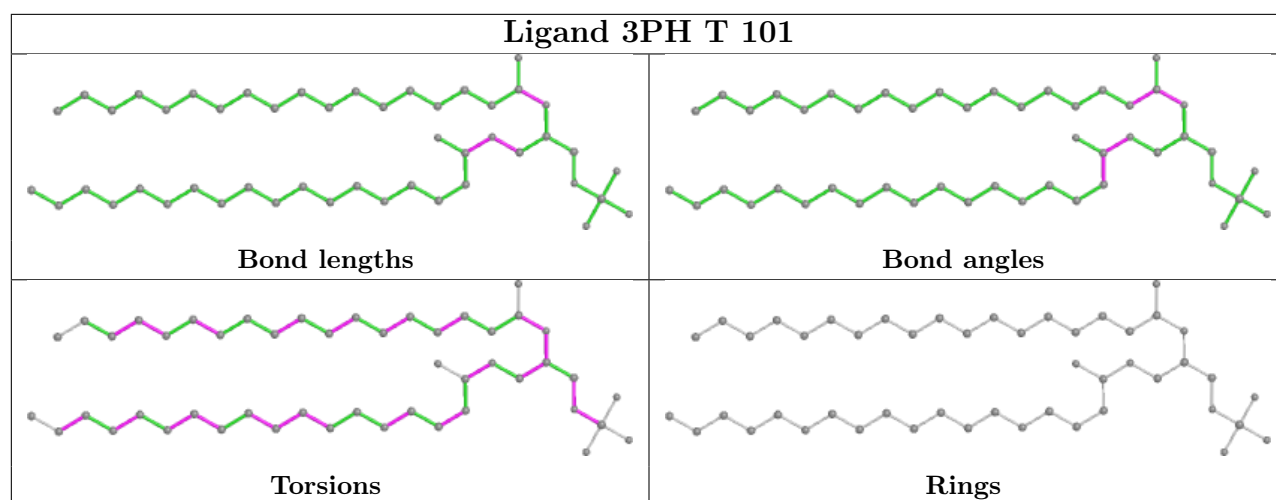
All (2) ring outliers are listed below:

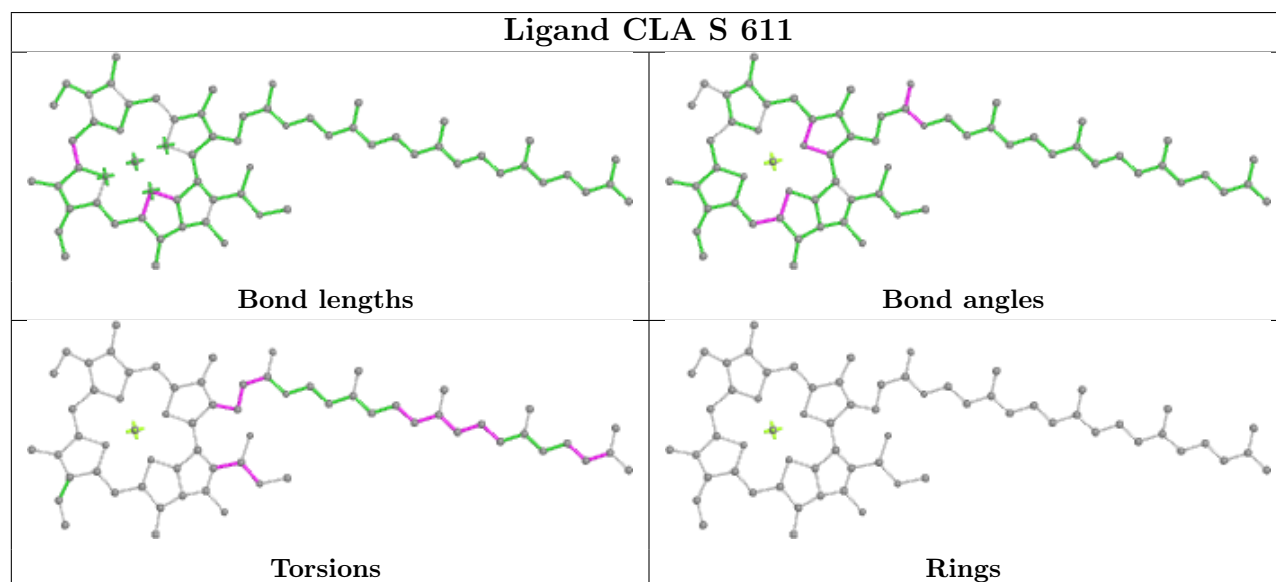
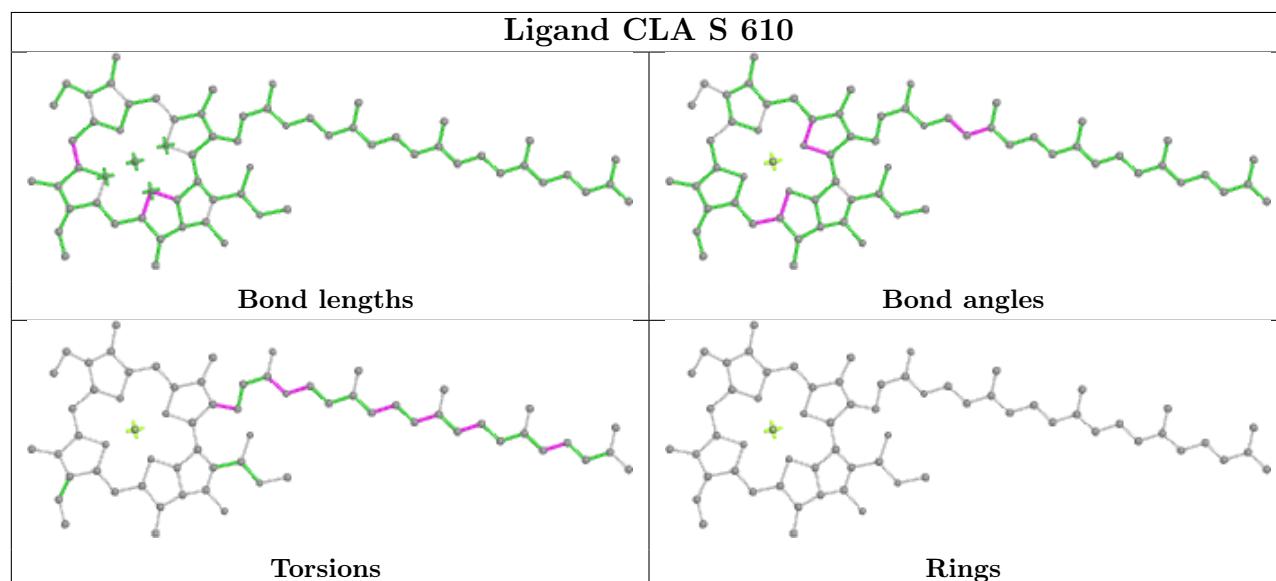
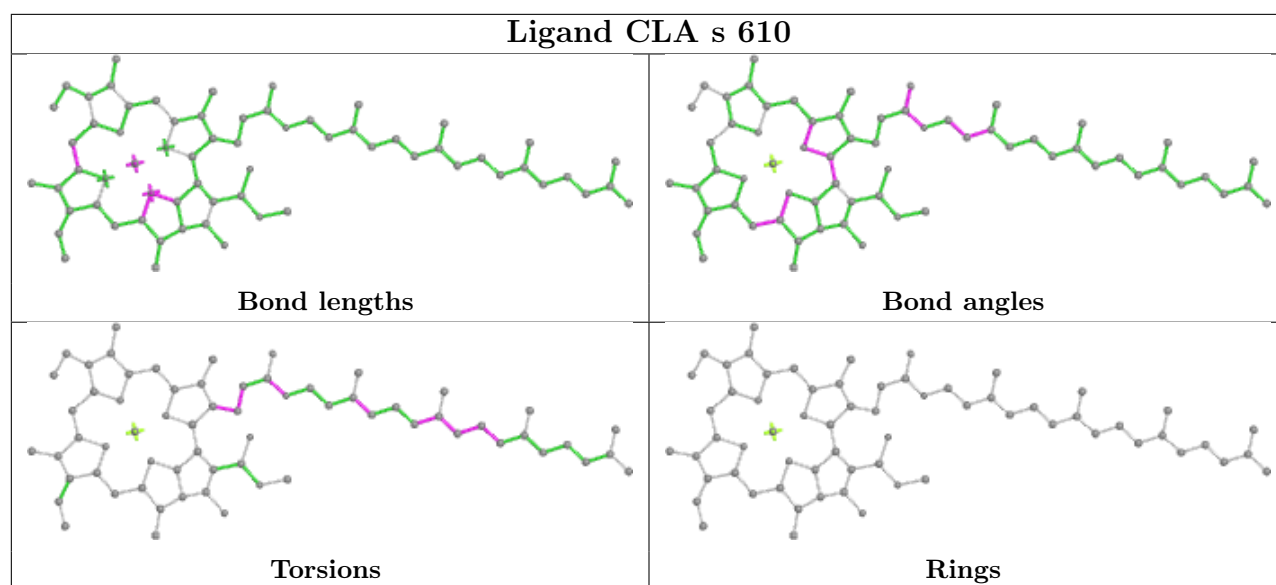
Mol	Chain	Res	Type	Atoms
47	n	623	NEX	C1-C2-C3-C4-C5-C6
47	N	623	NEX	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

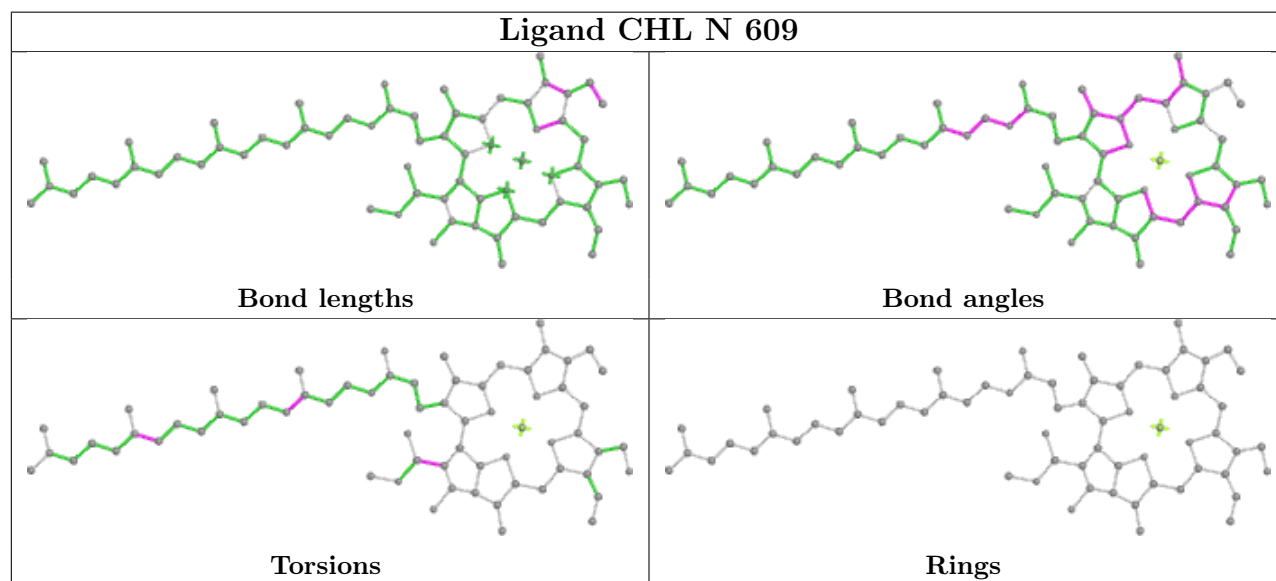
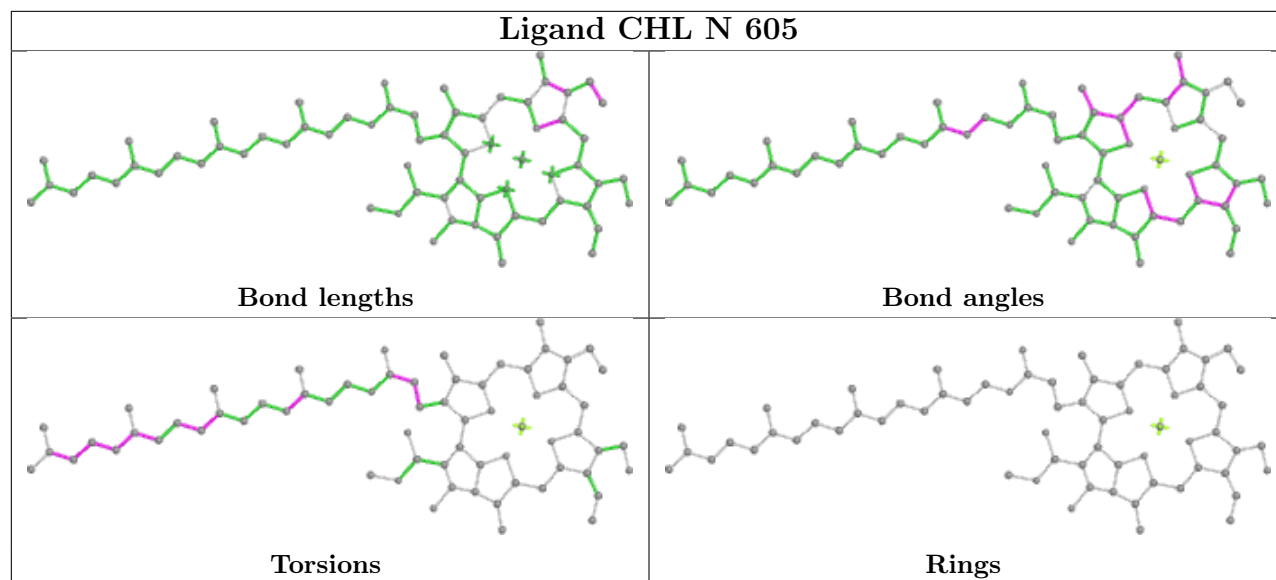
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



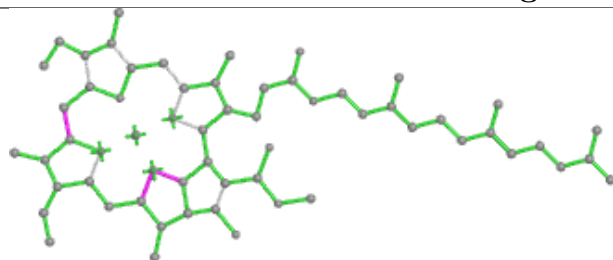




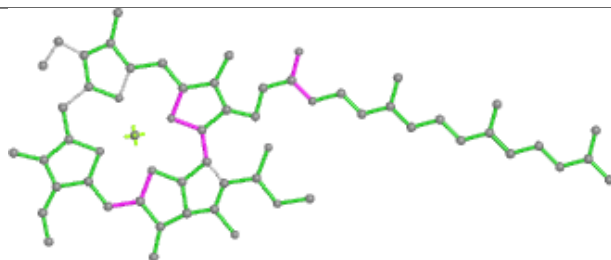




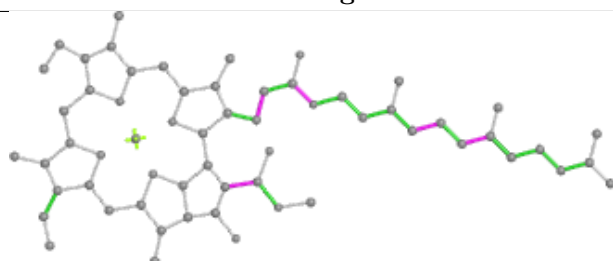
## Ligand CLA r 602



Bond lengths



Bond angles

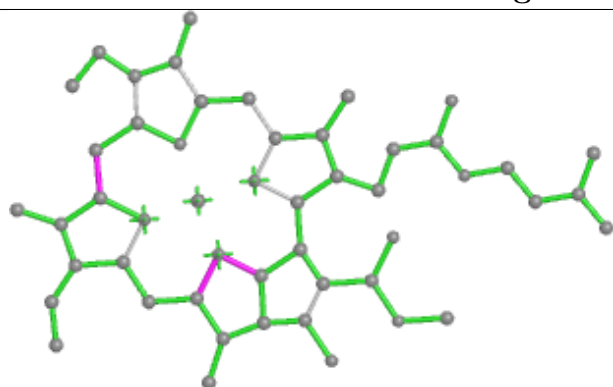


Torsions

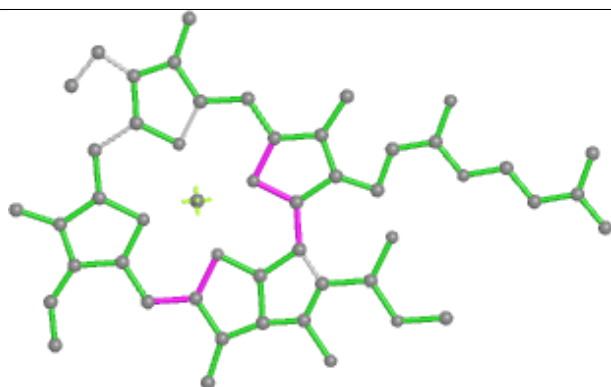


Rings

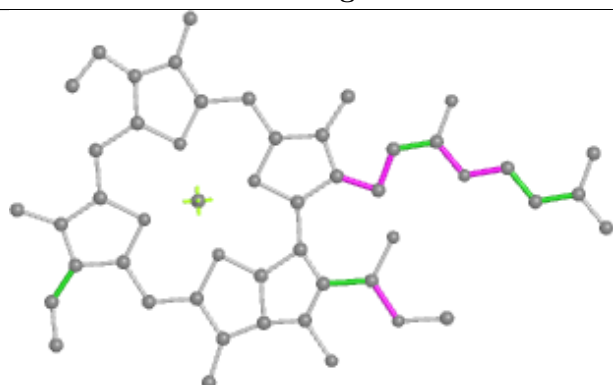
## Ligand CLA Y 608



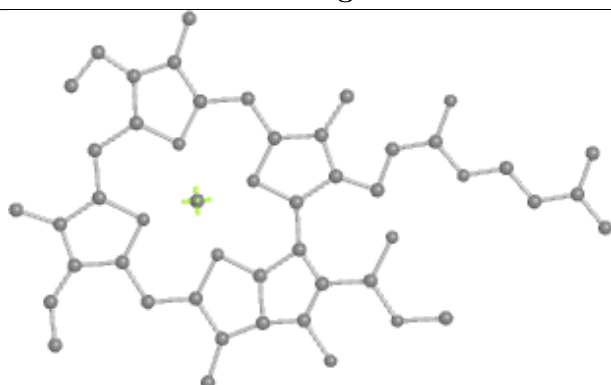
Bond lengths



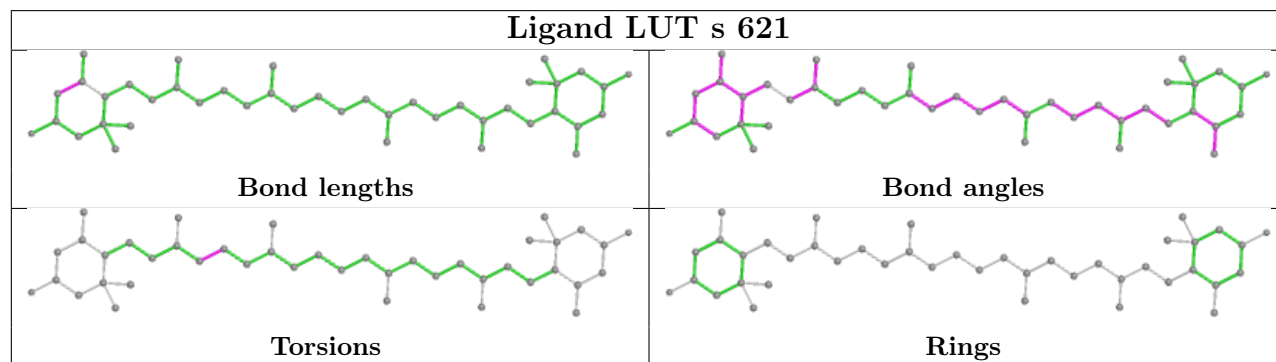
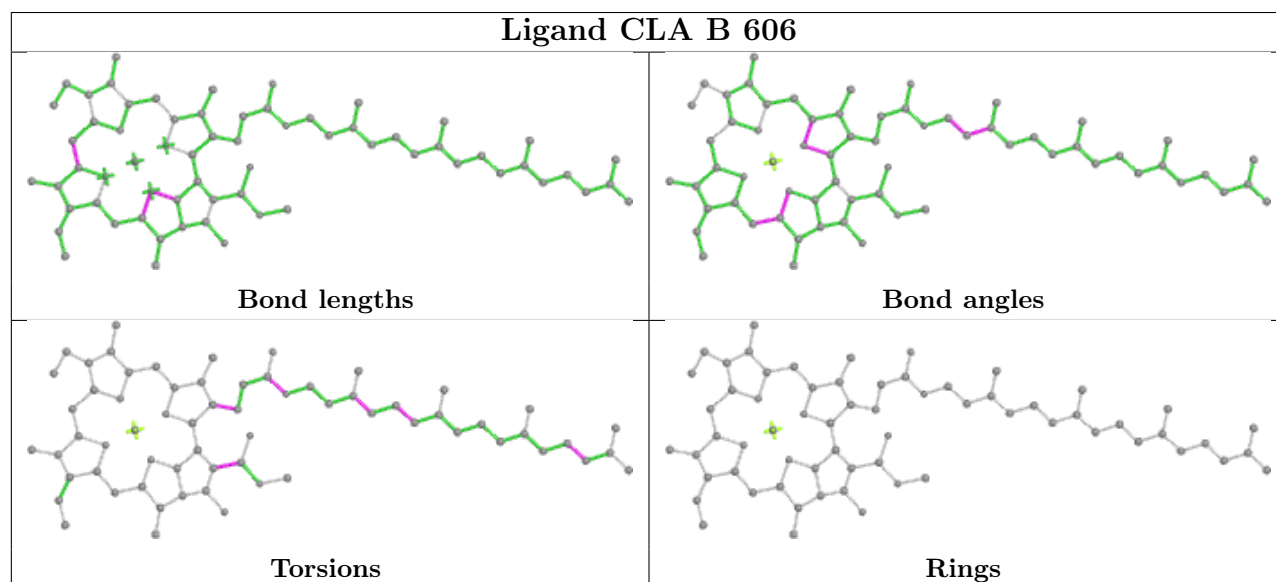
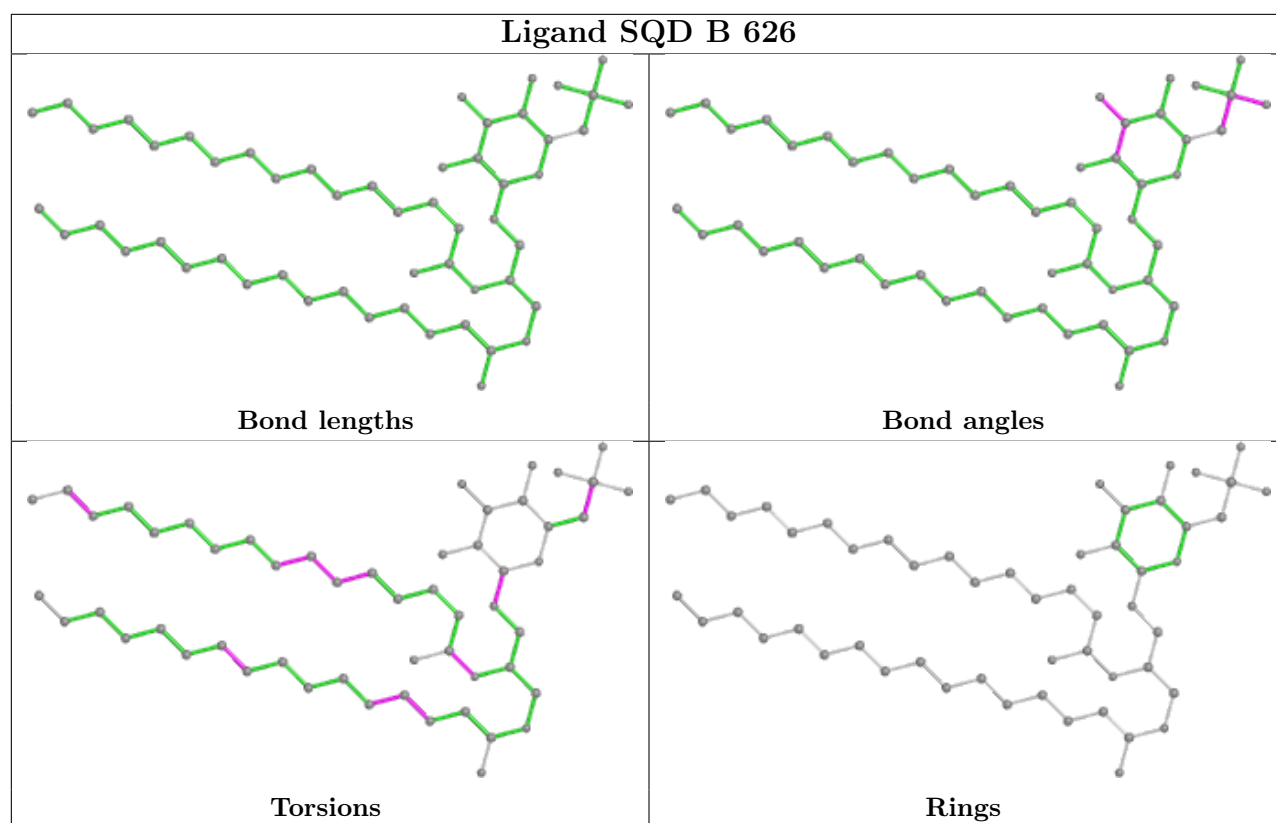
Bond angles

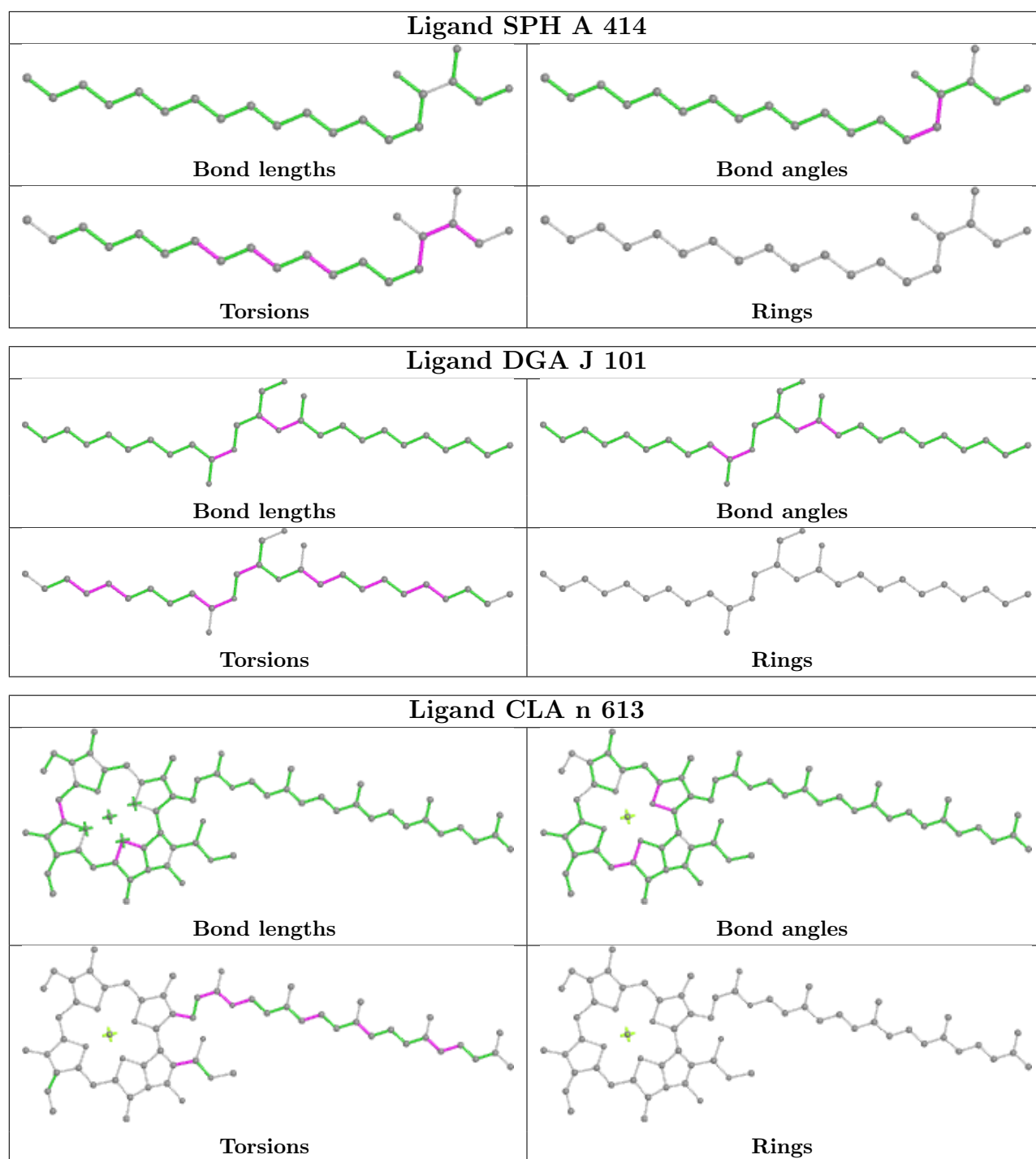


Torsions

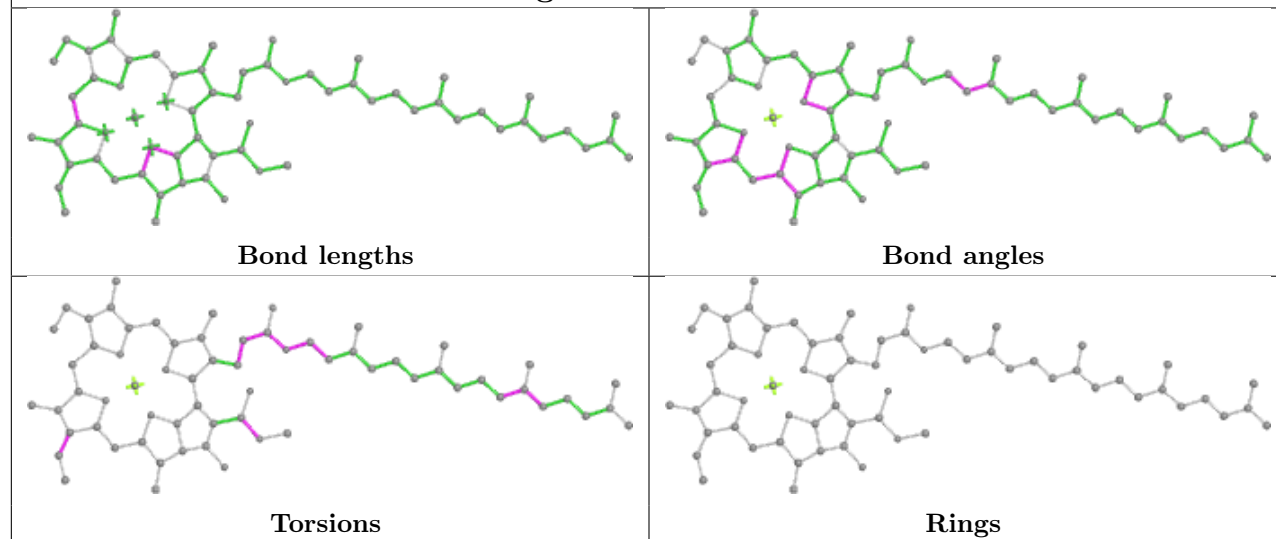


Rings

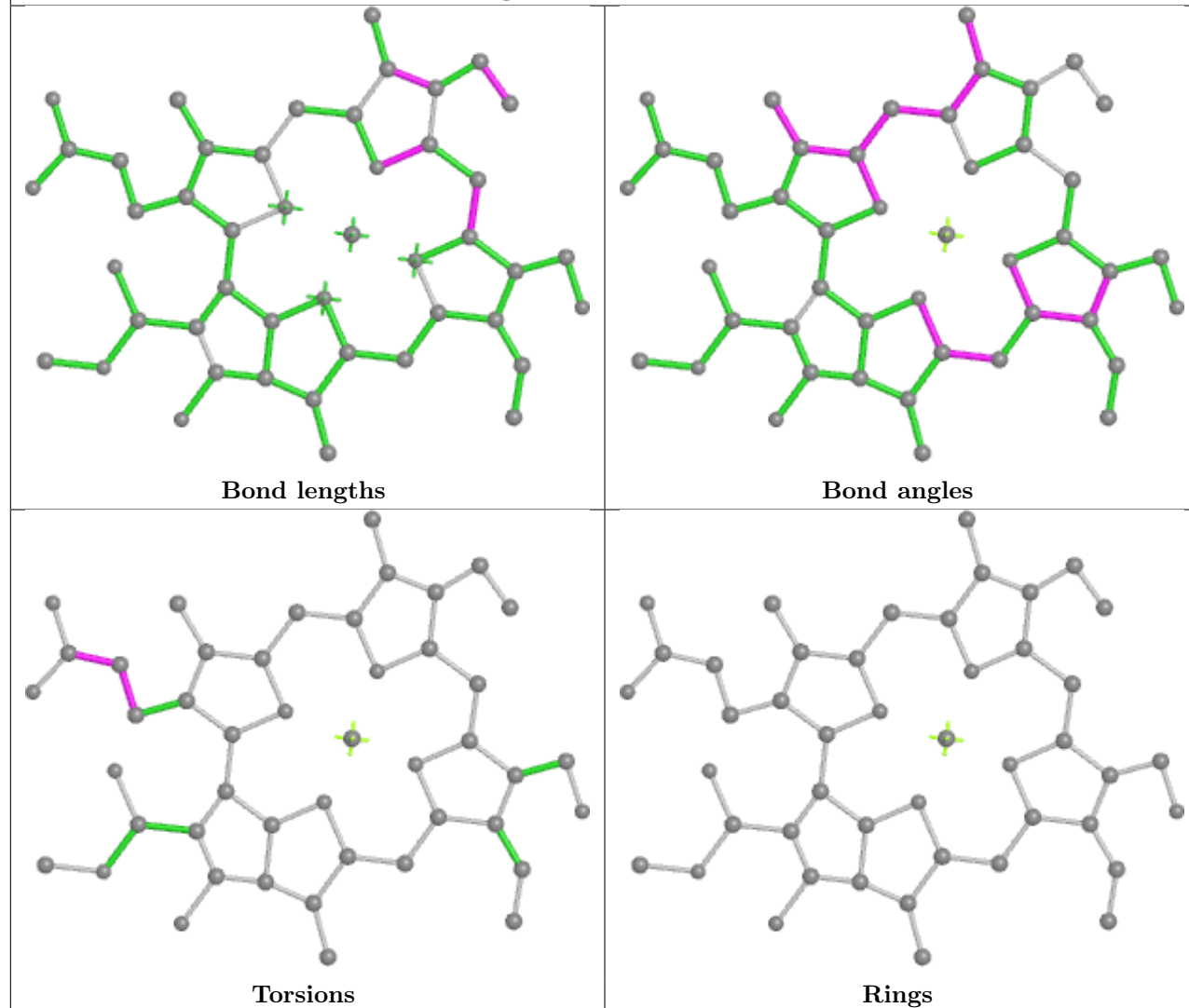


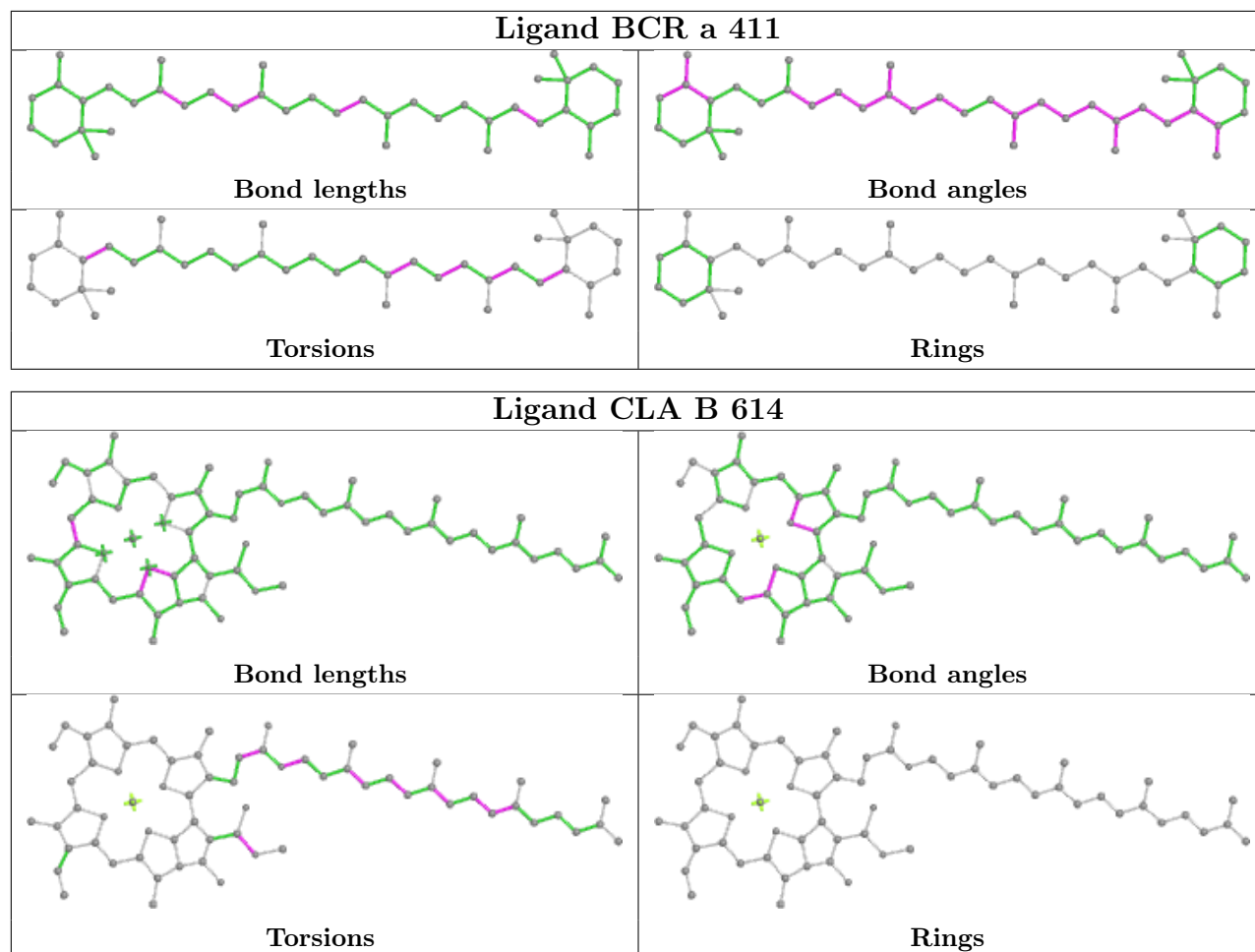


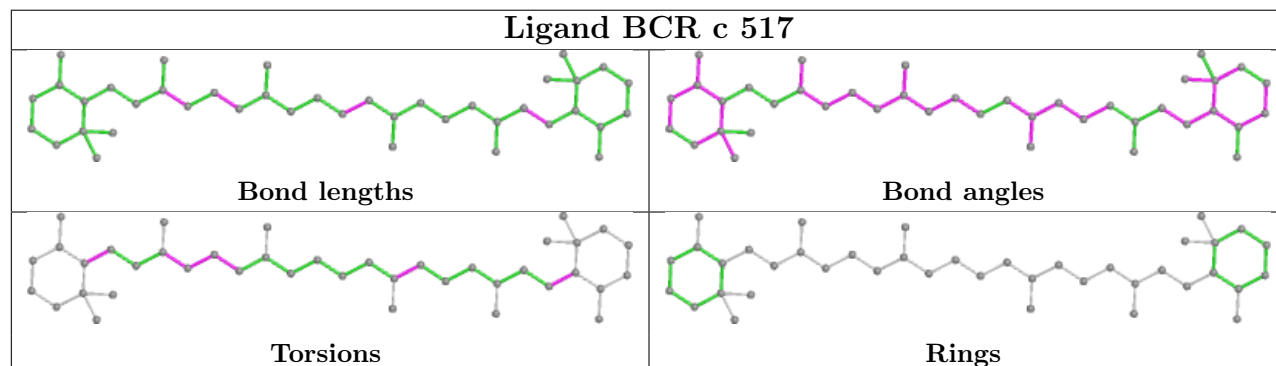
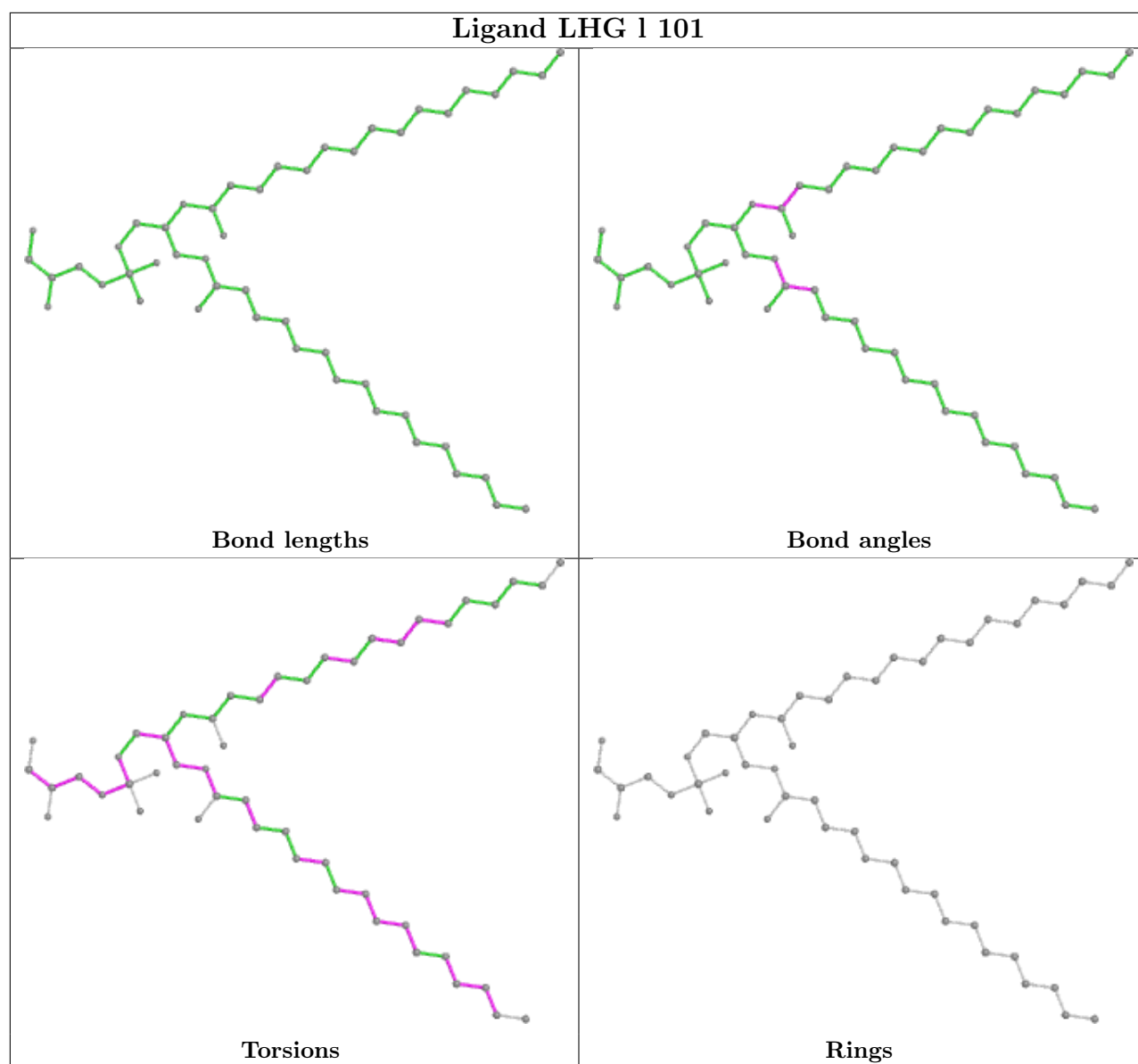
## Ligand CLA a 405

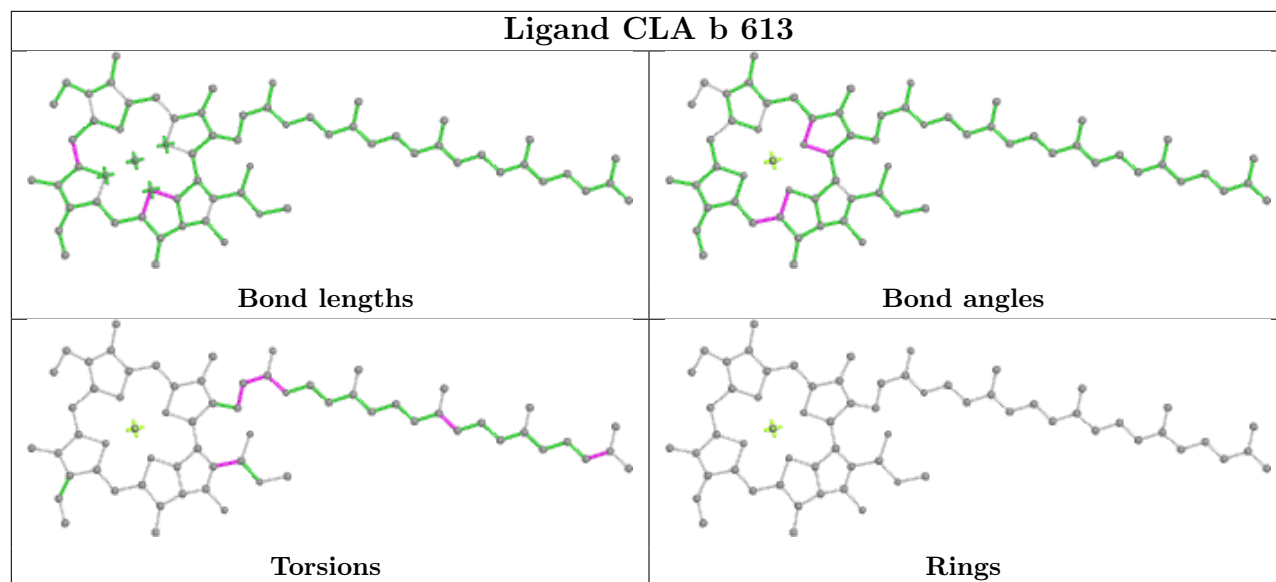
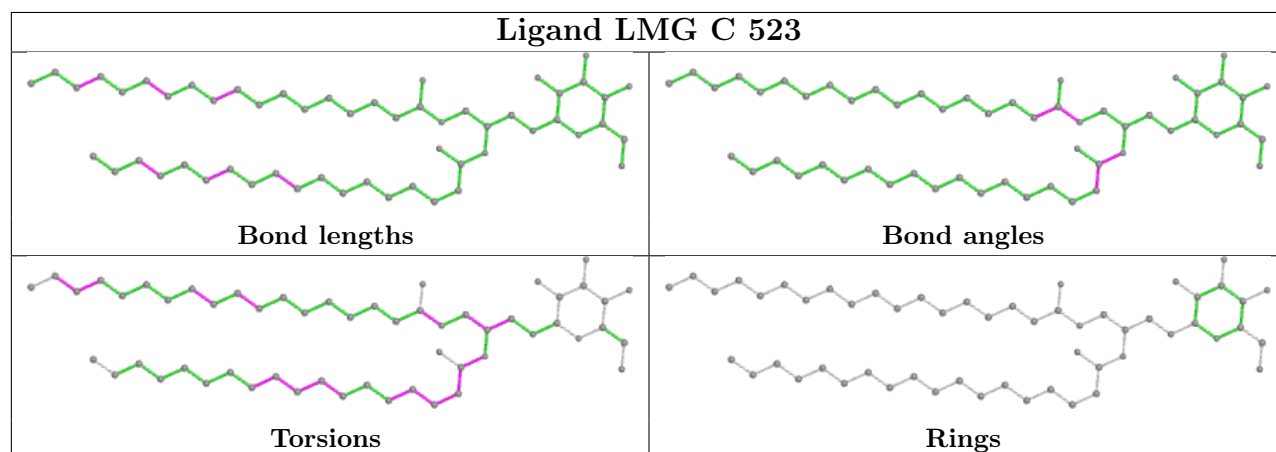
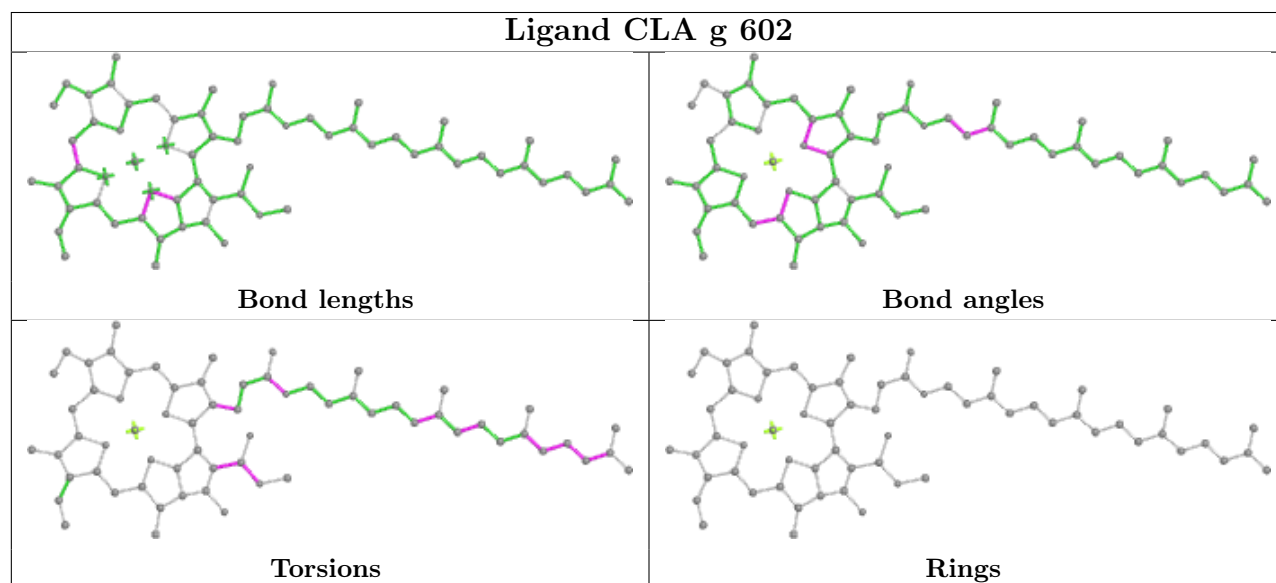


## Ligand CHL S 601

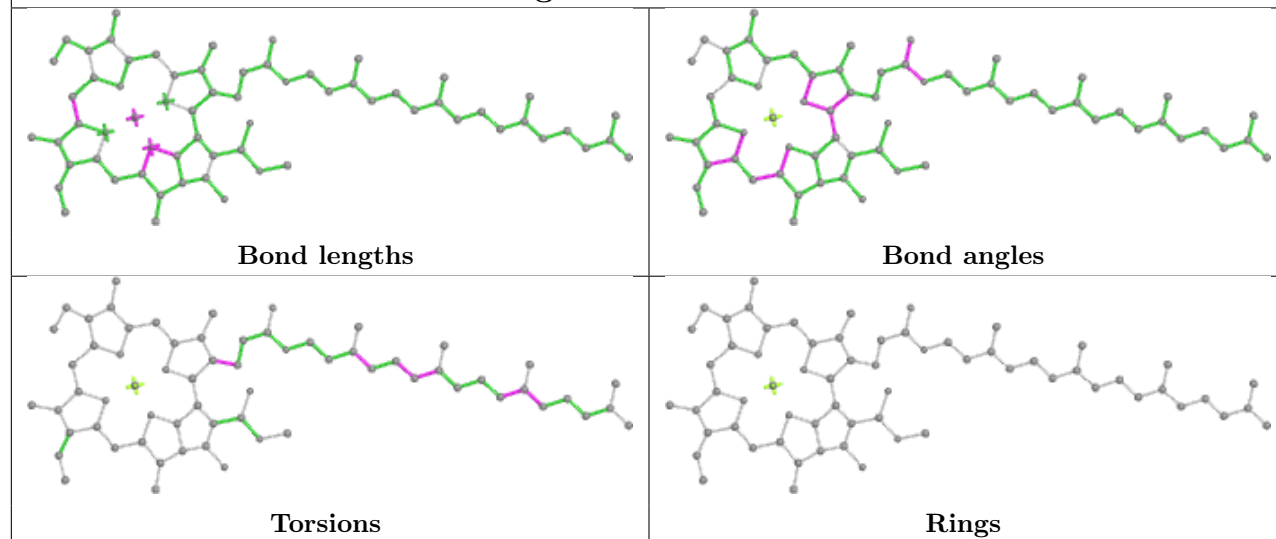
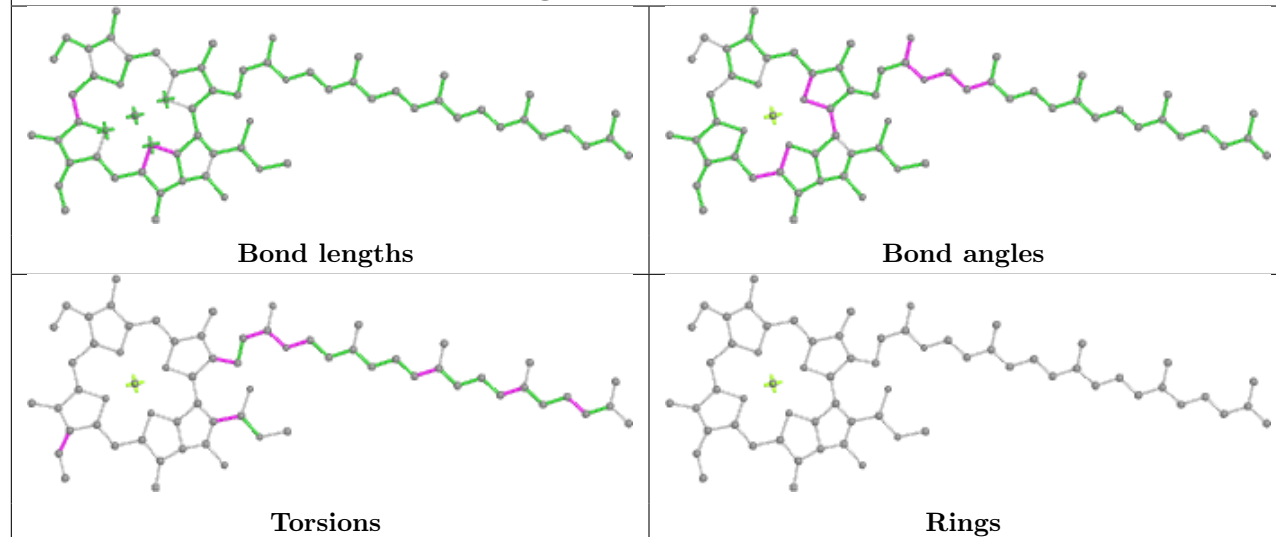


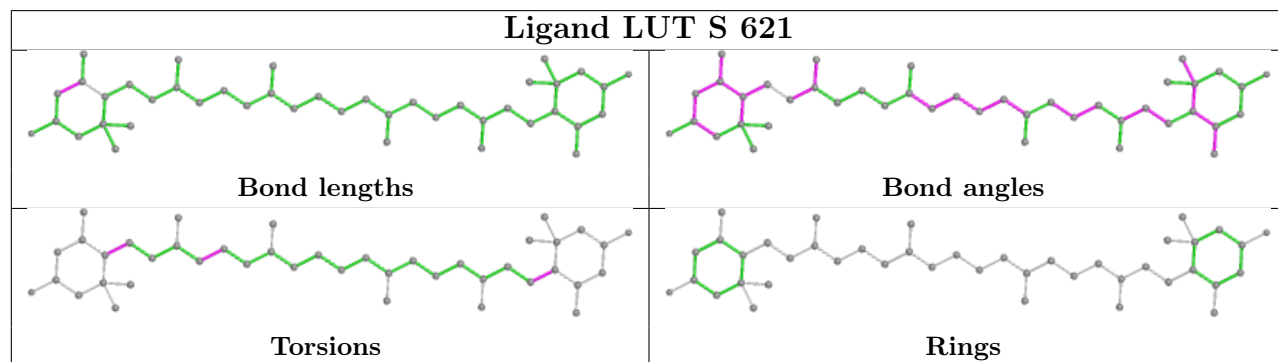
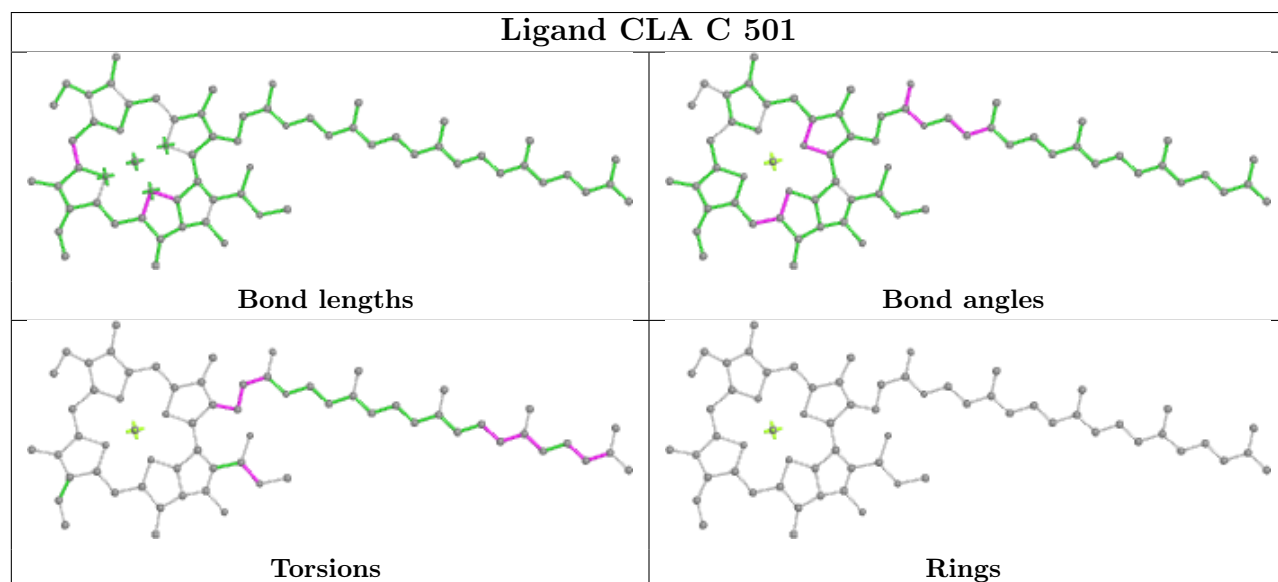
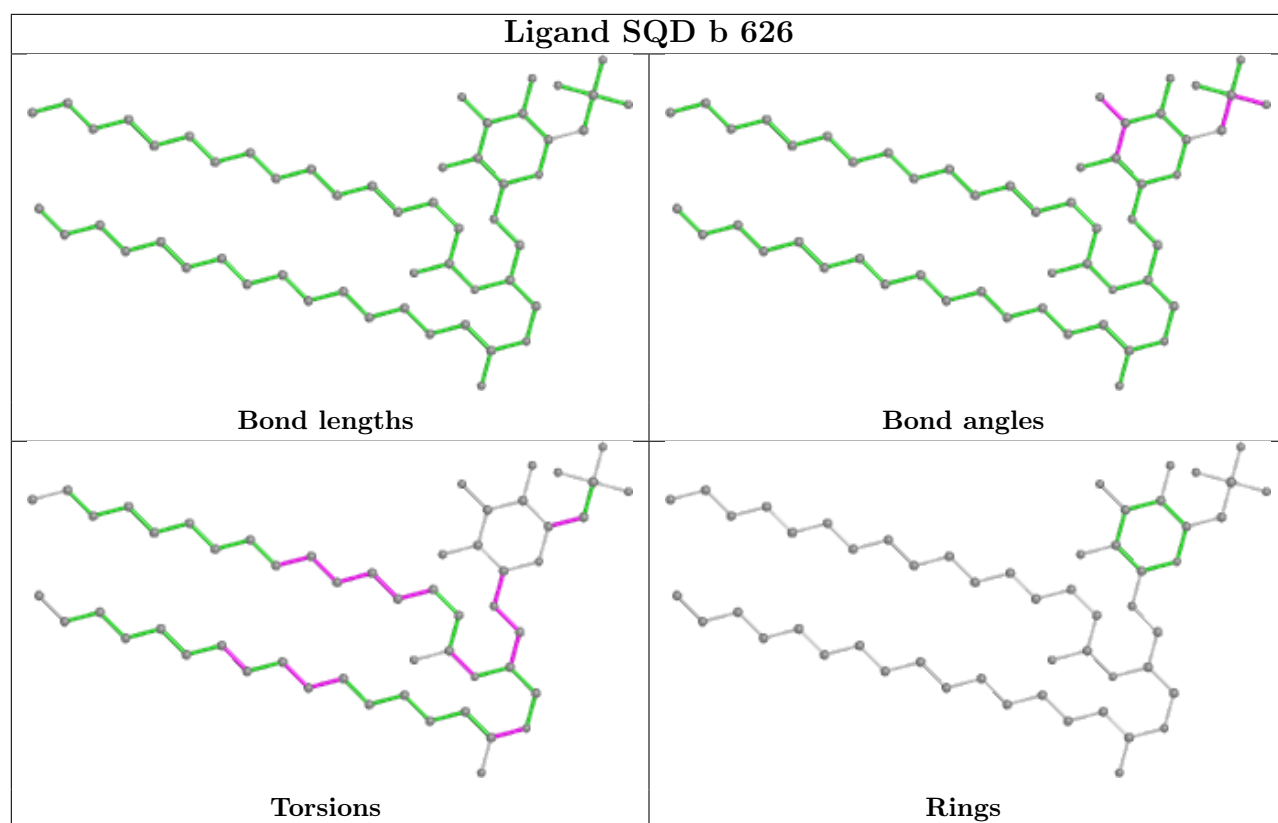


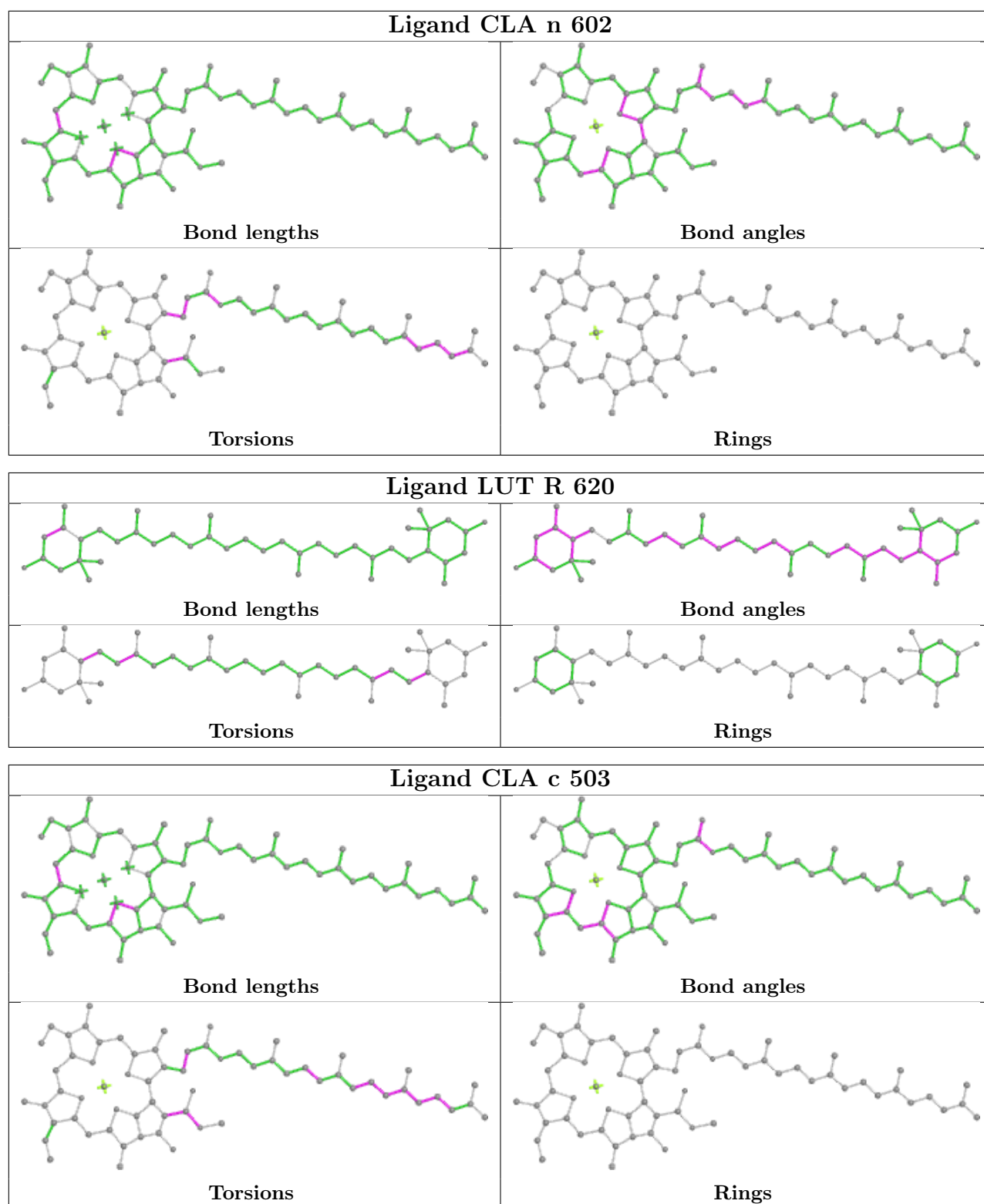


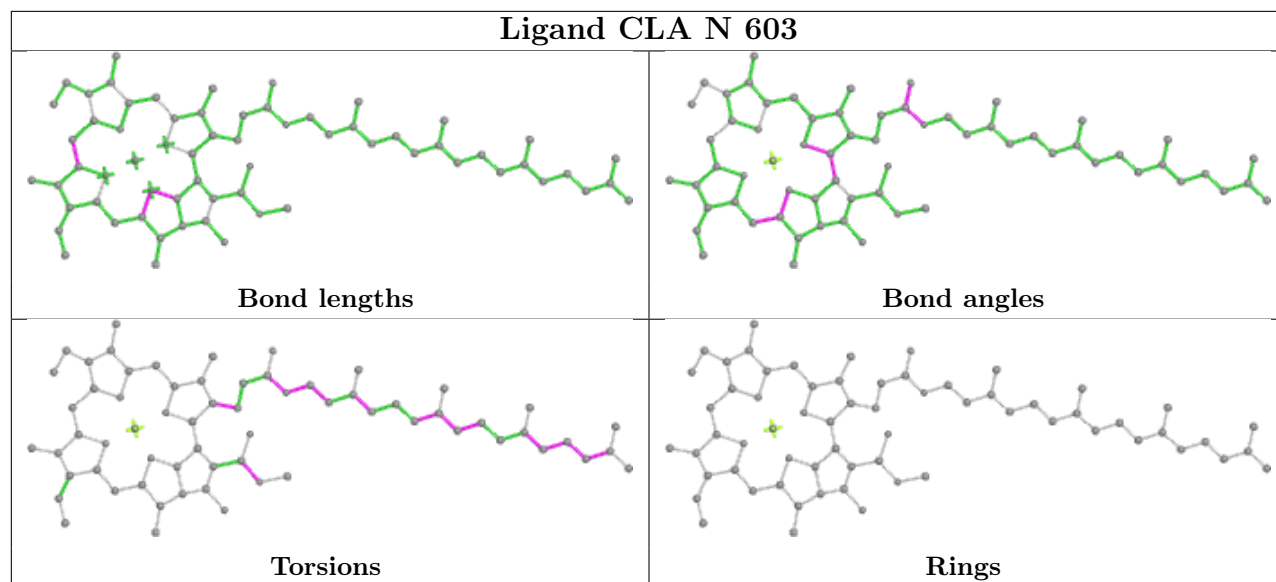
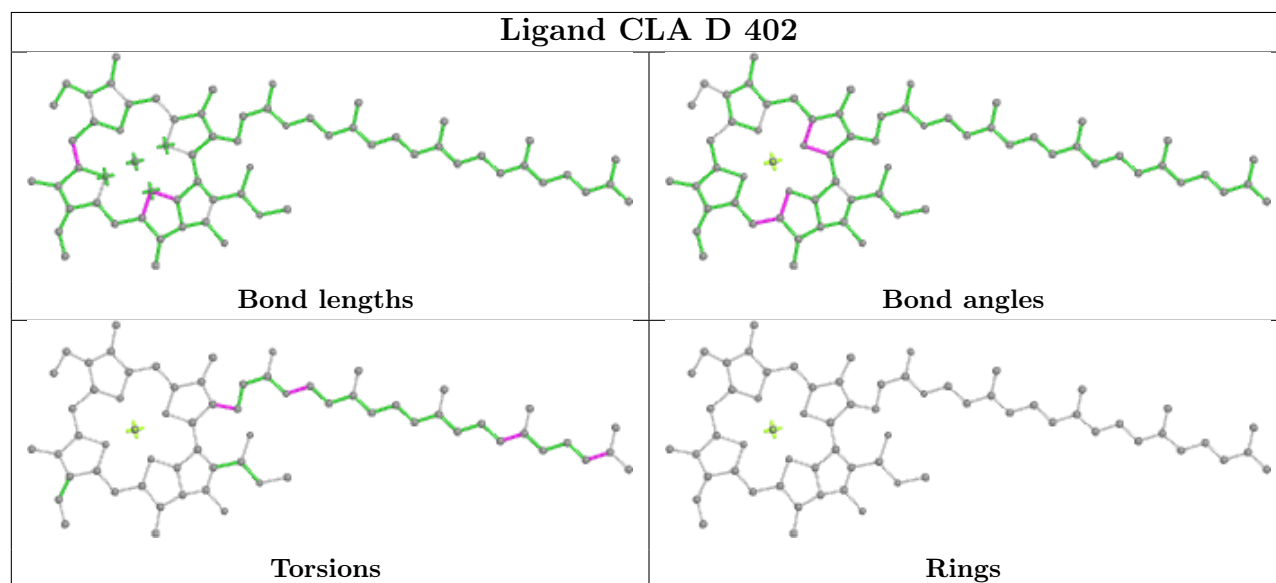
**Ligand CLA b 613****Ligand LMG C 523****Ligand CLA g 602**

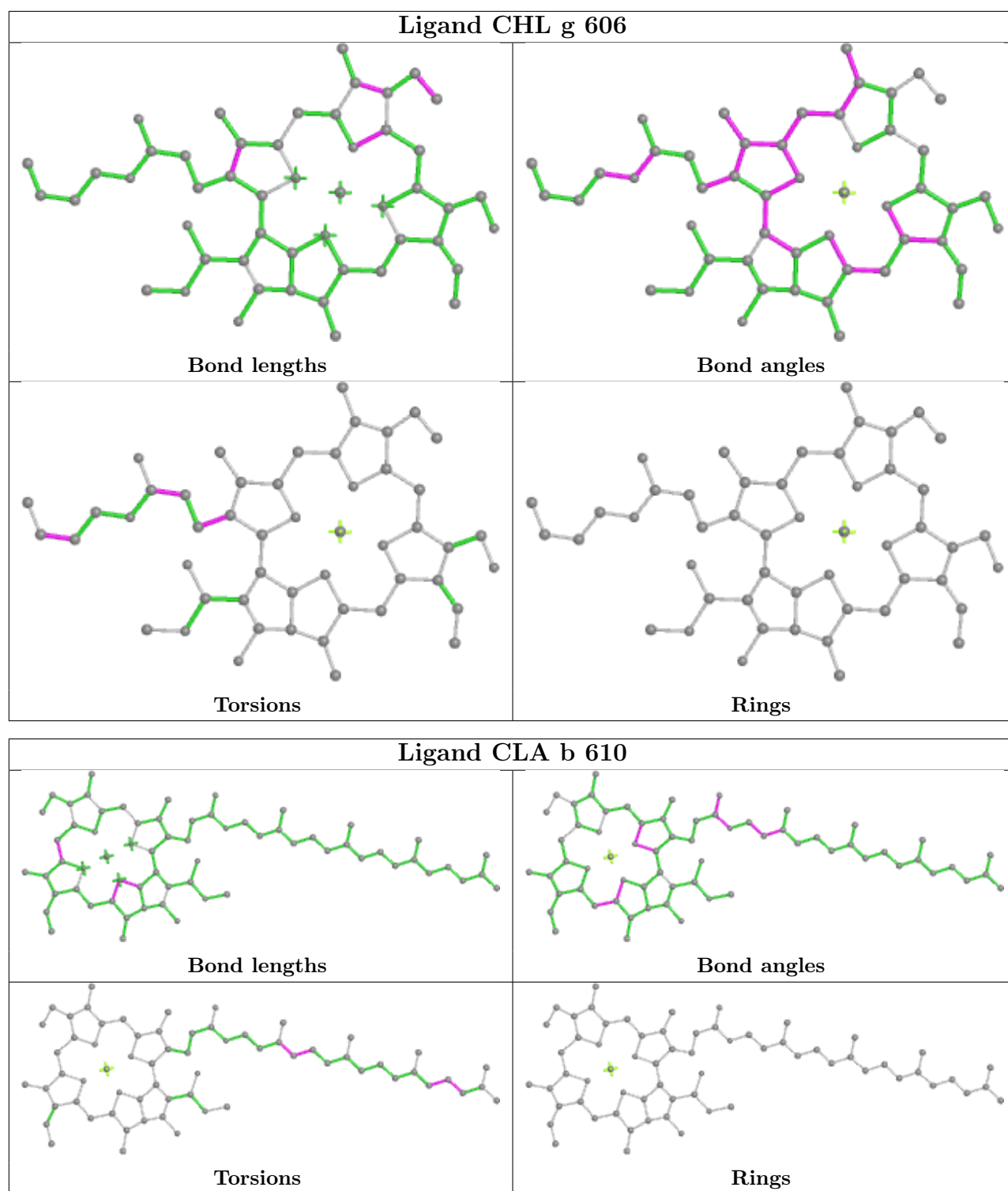


**Ligand CLA n 610****Ligand CLA a 406**

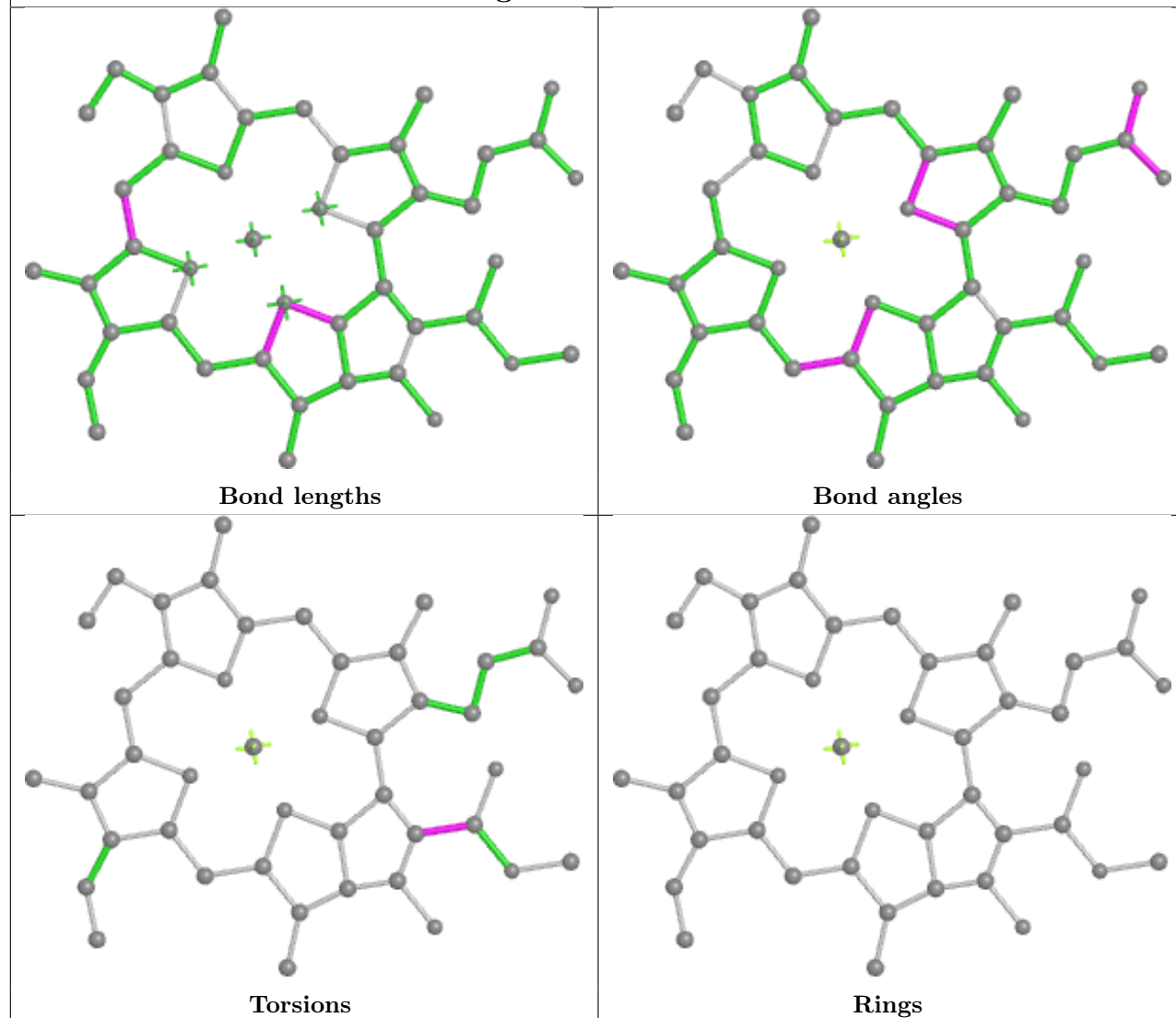




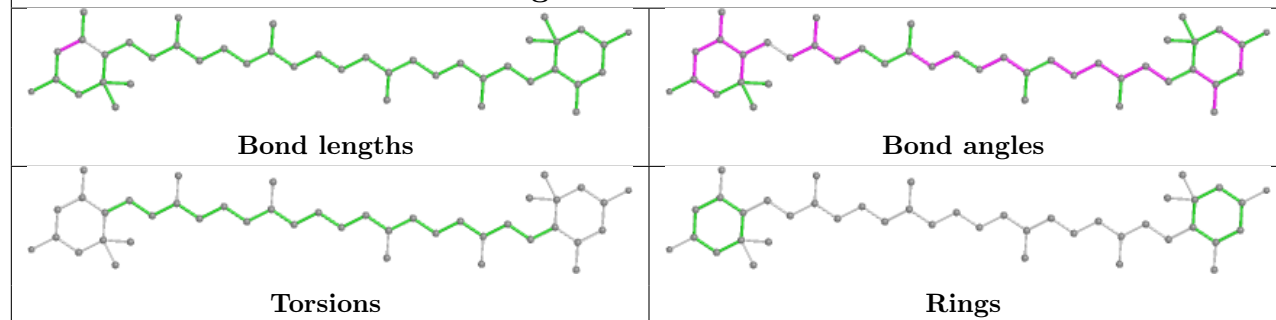
**Ligand CLA N 603****Ligand CLA D 402**

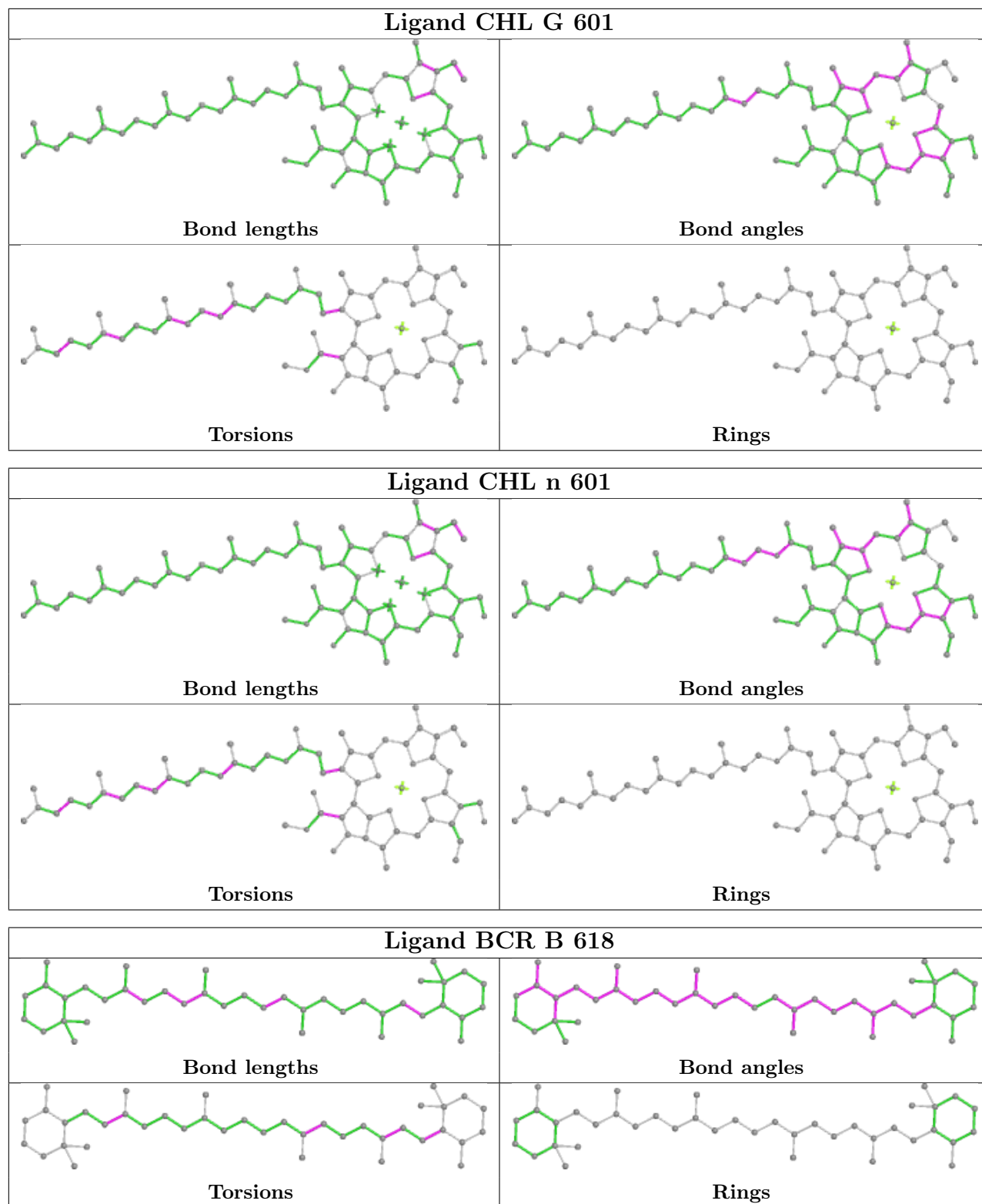


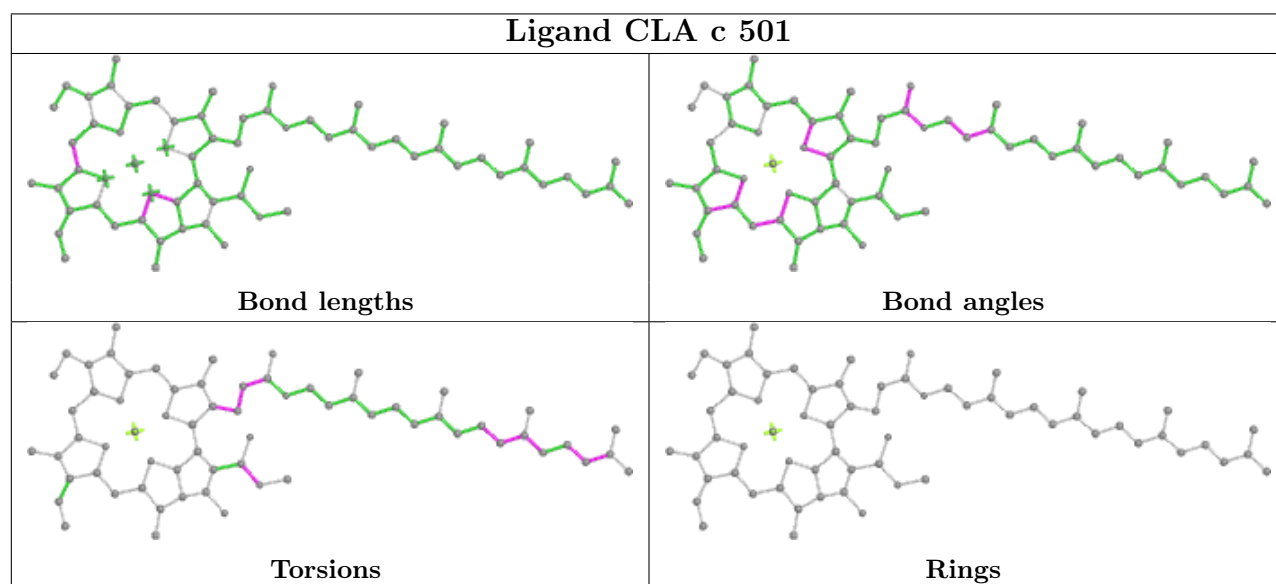
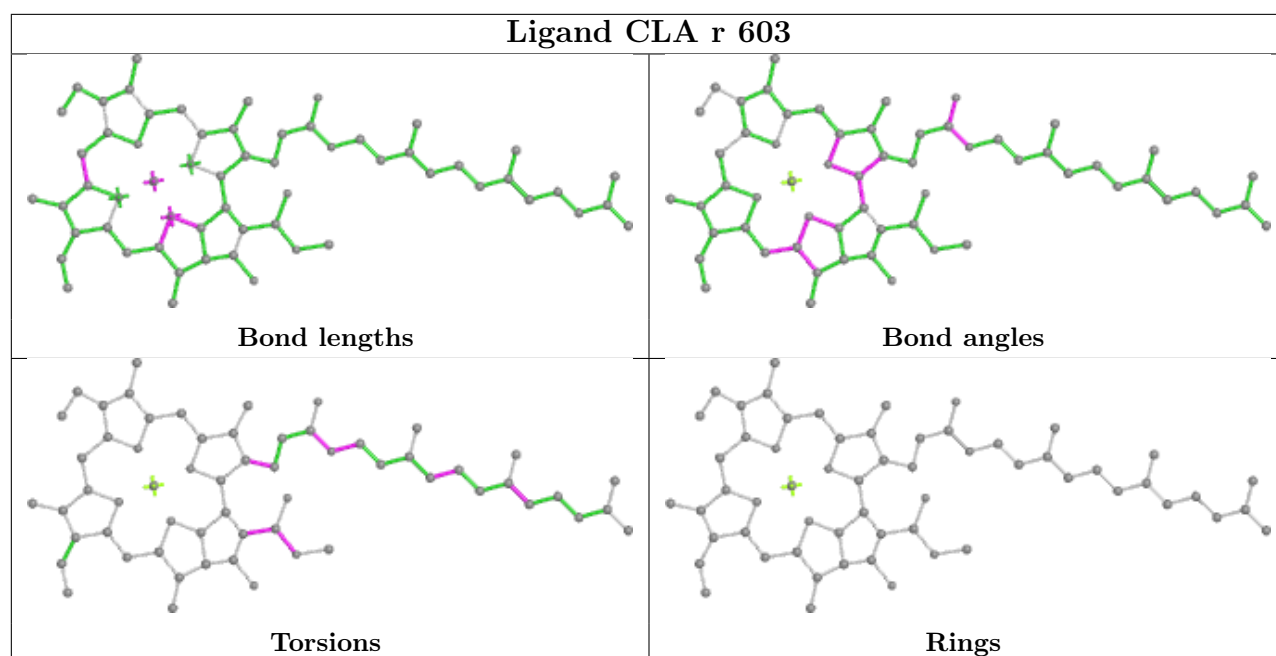
## Ligand CLA s 612



## Ligand LUT G 620

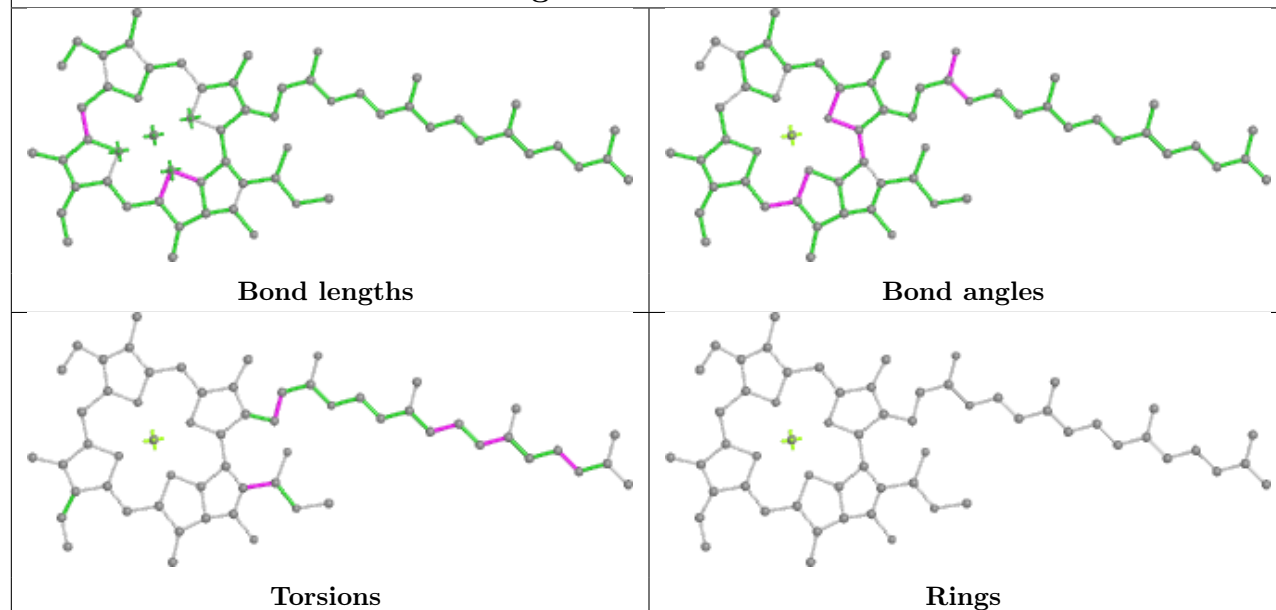




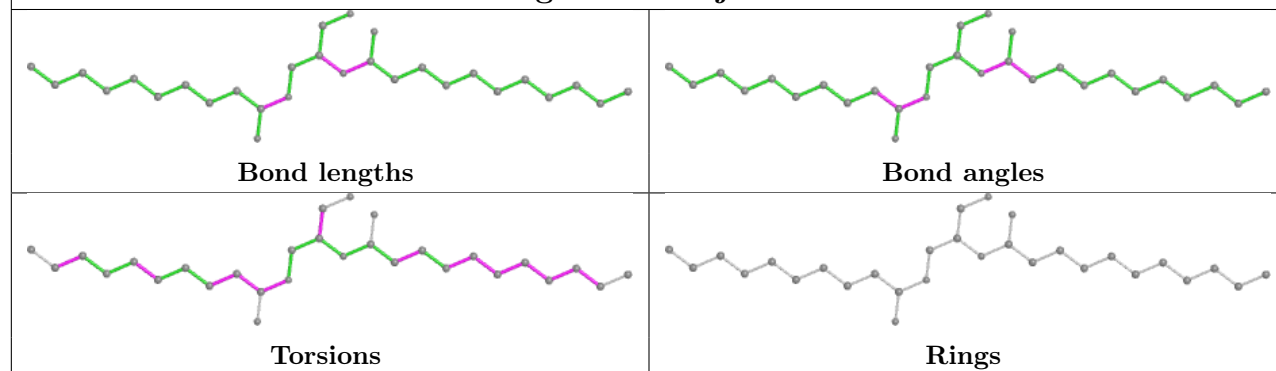




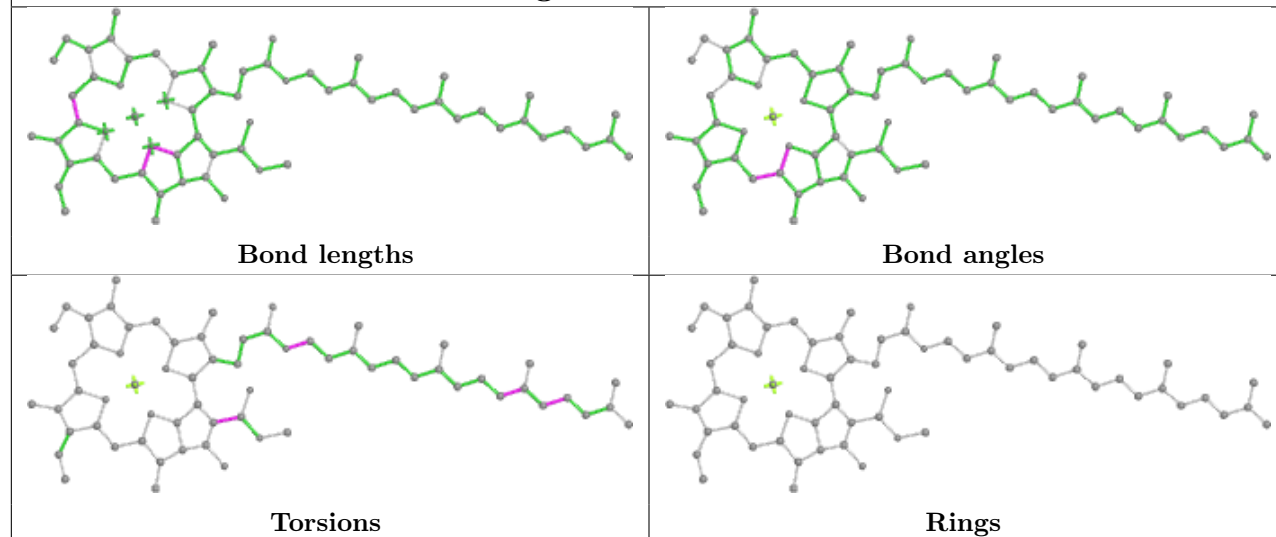
## Ligand CLA R 602

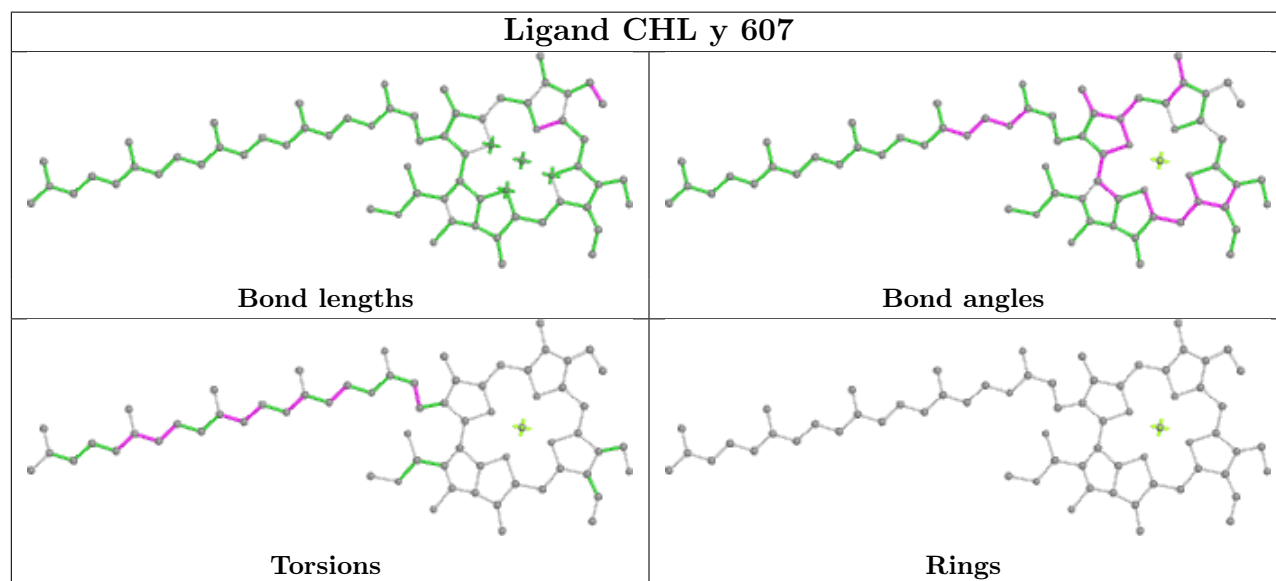
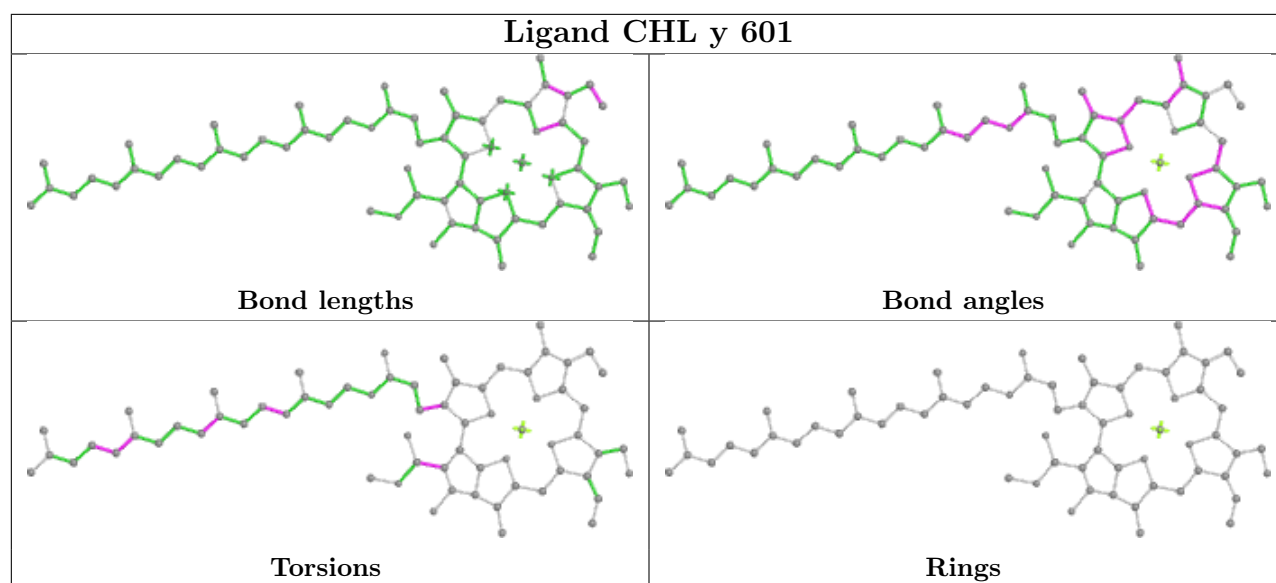


## Ligand DGA j 101

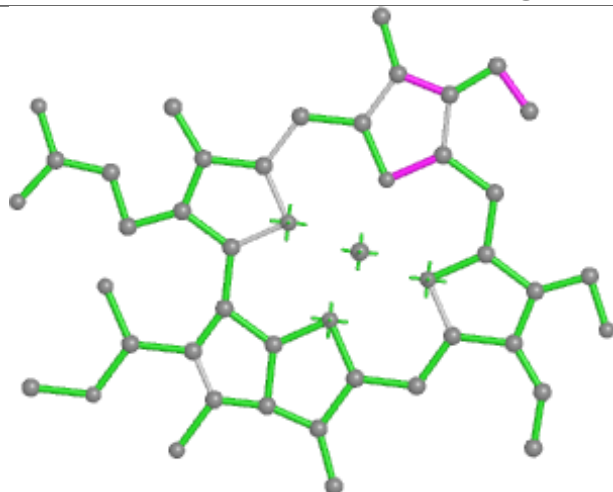


## Ligand CLA b 609

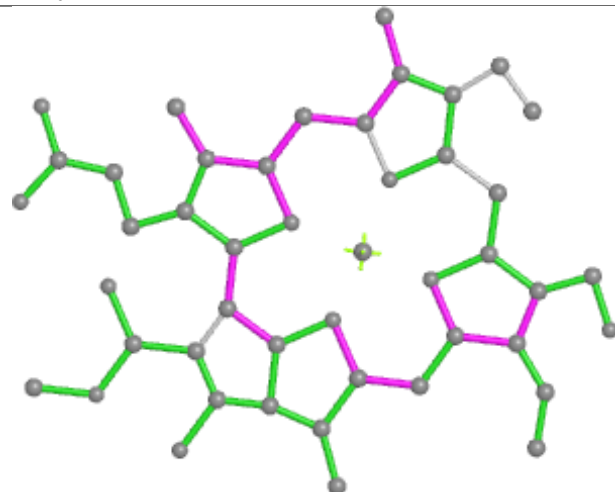




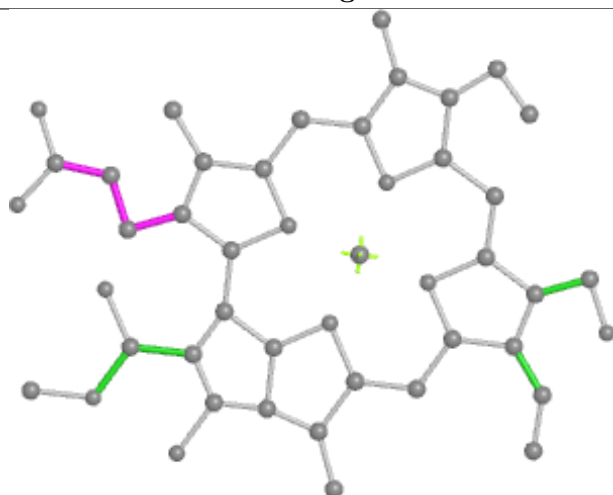
## Ligand CHL y 605



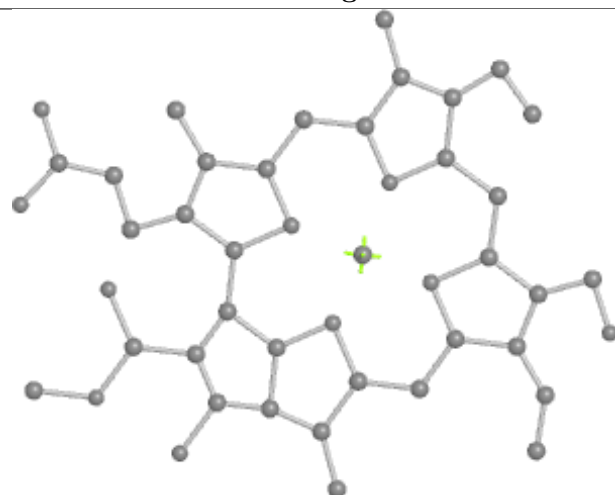
Bond lengths



Bond angles

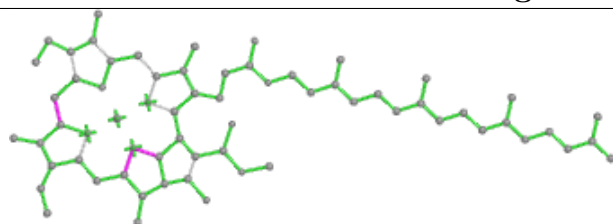


Torsions

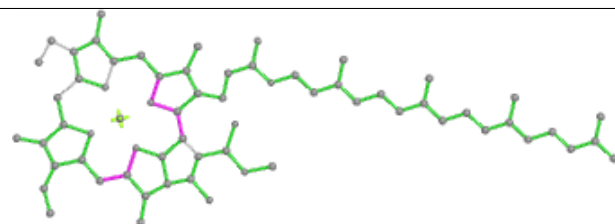


Rings

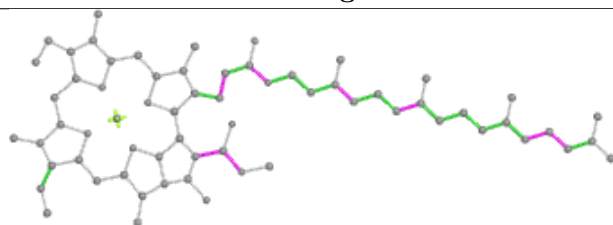
## Ligand CLA C 507



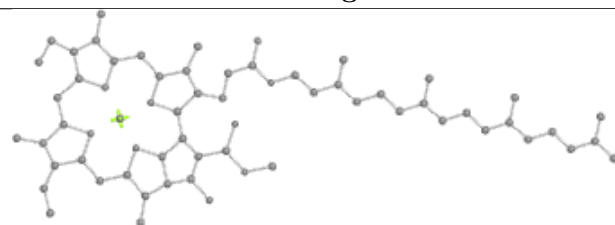
Bond lengths



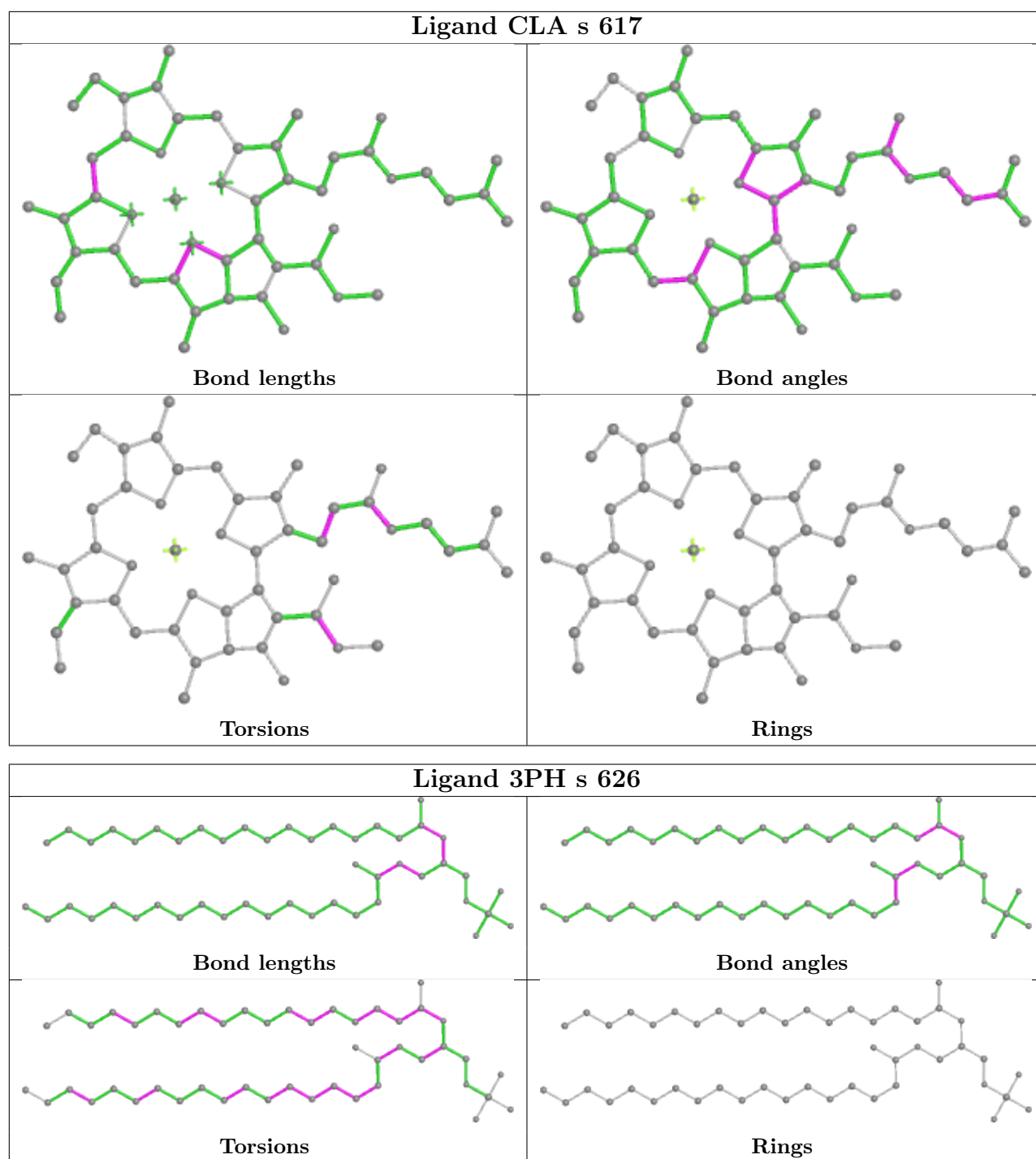
Bond angles

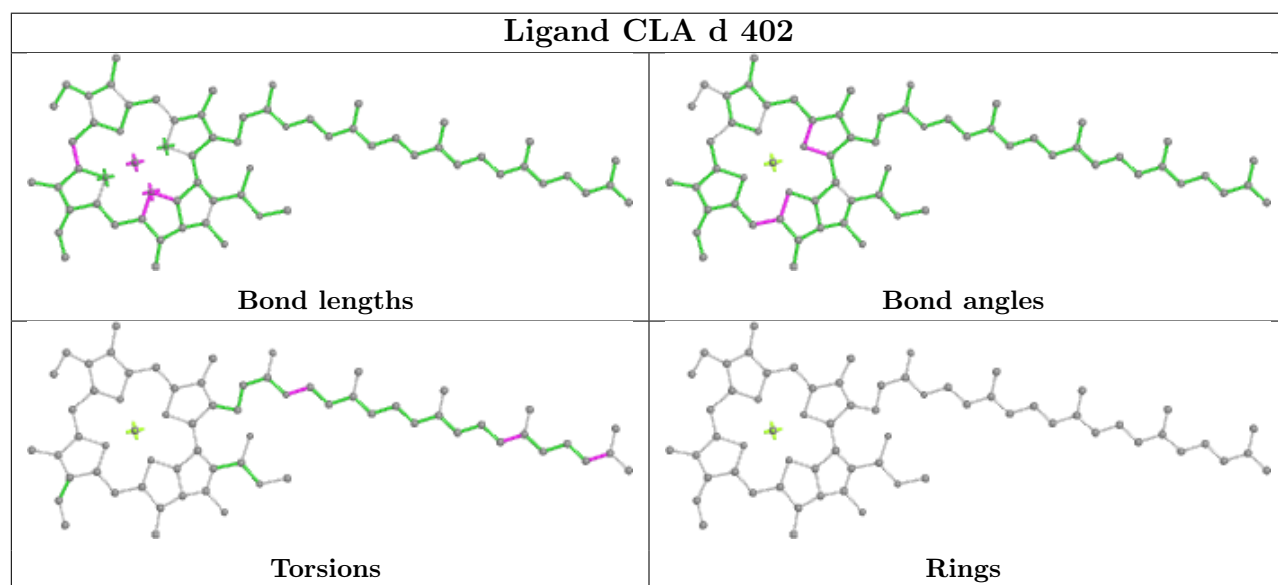
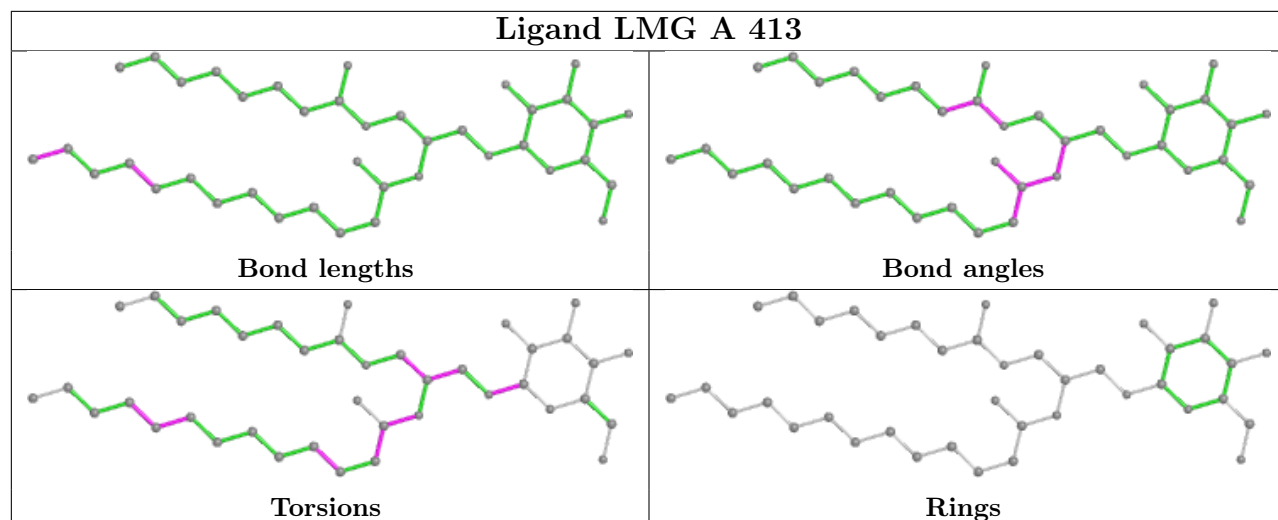


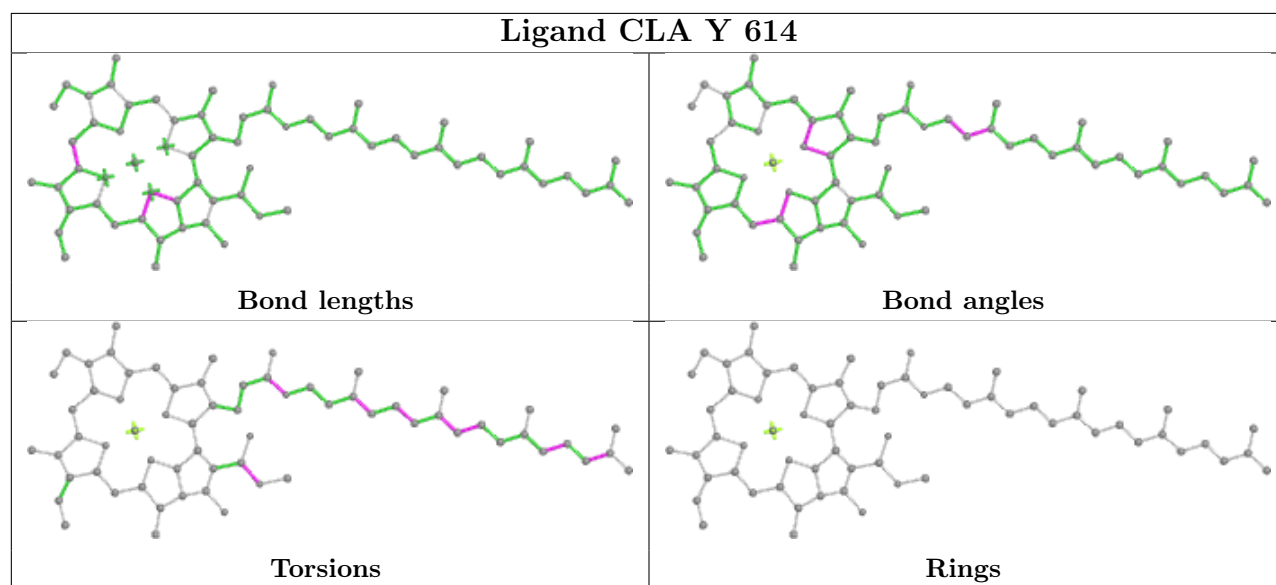
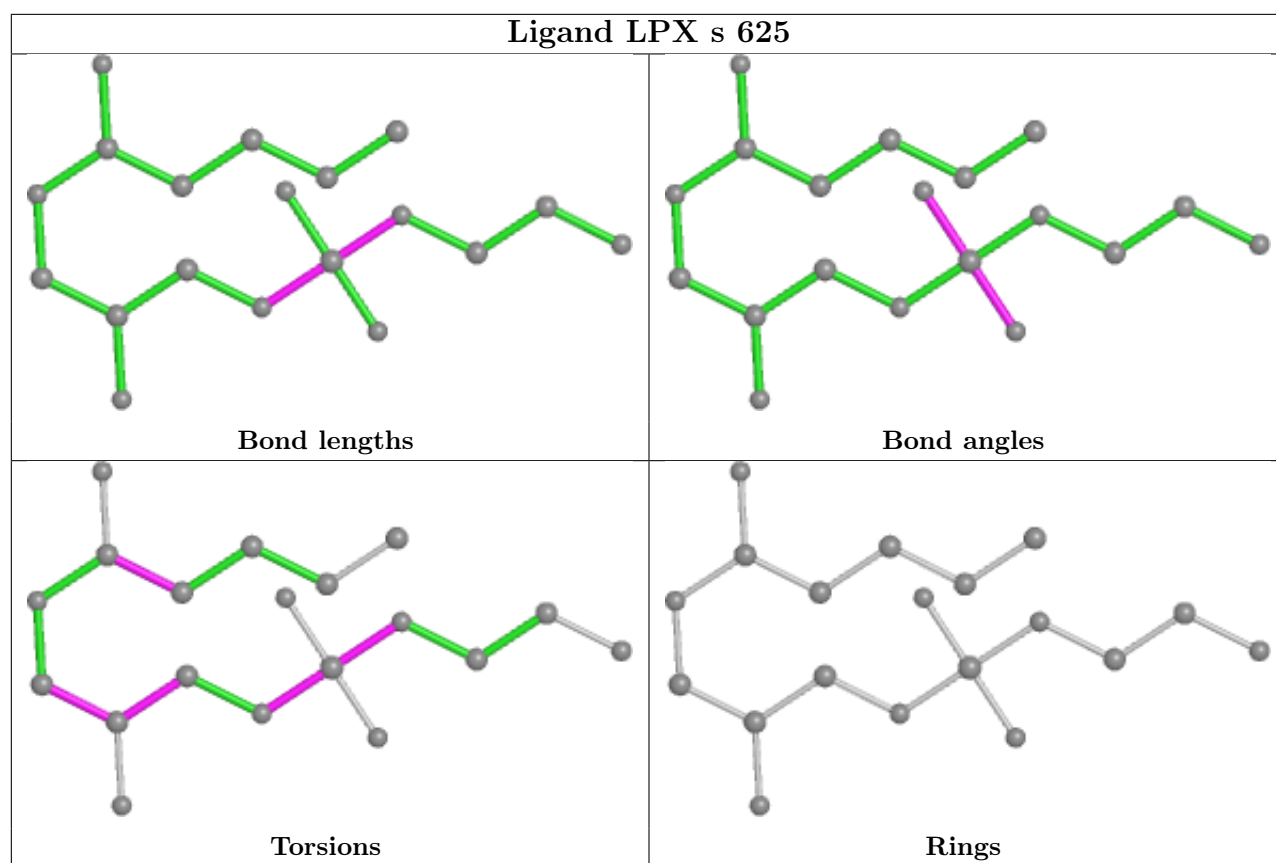
Torsions

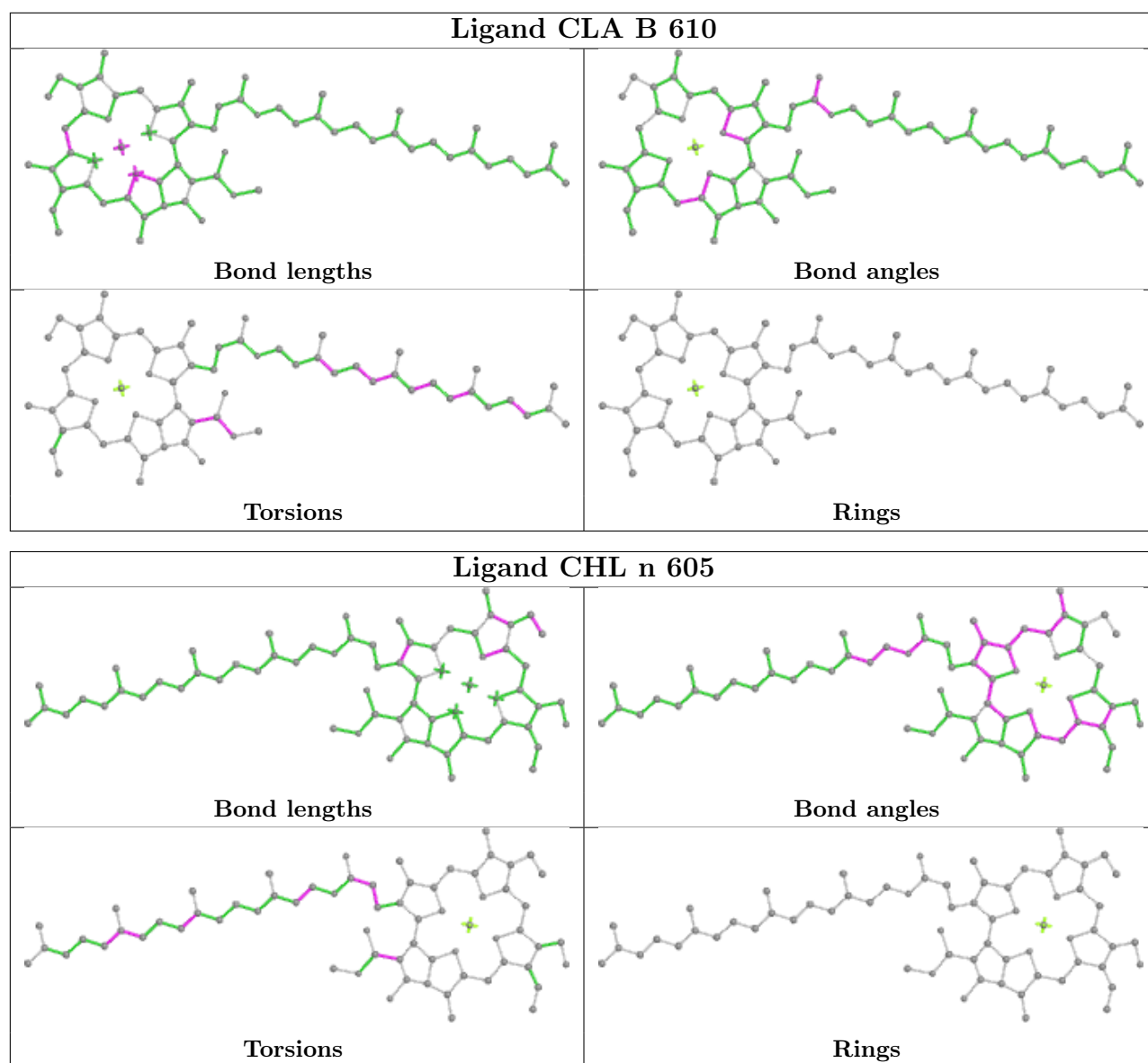


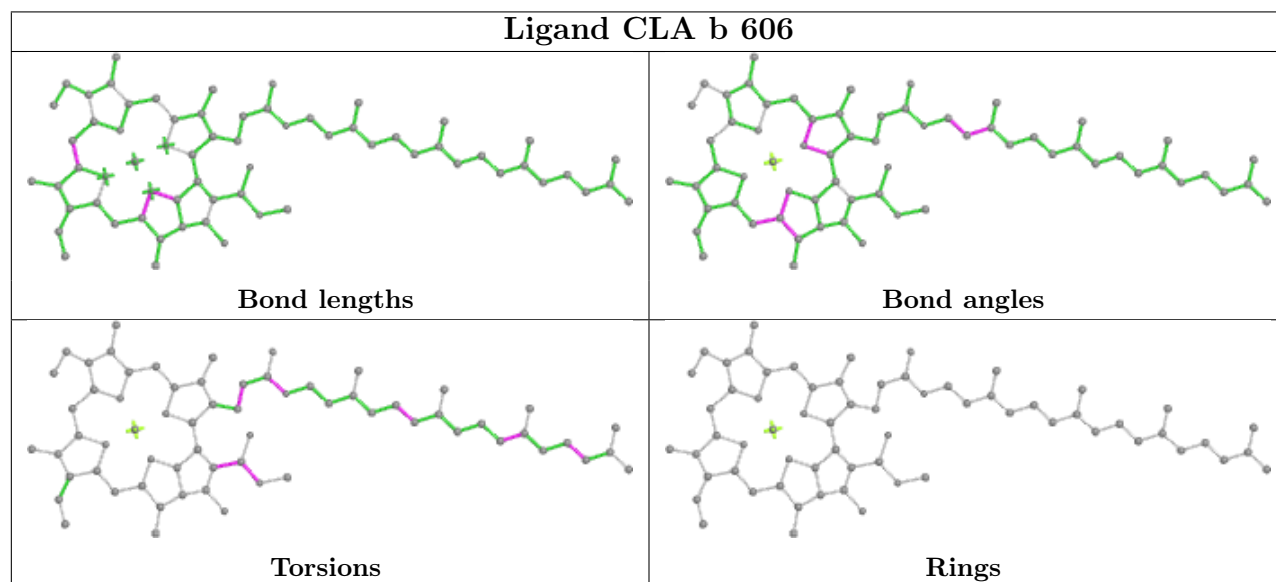
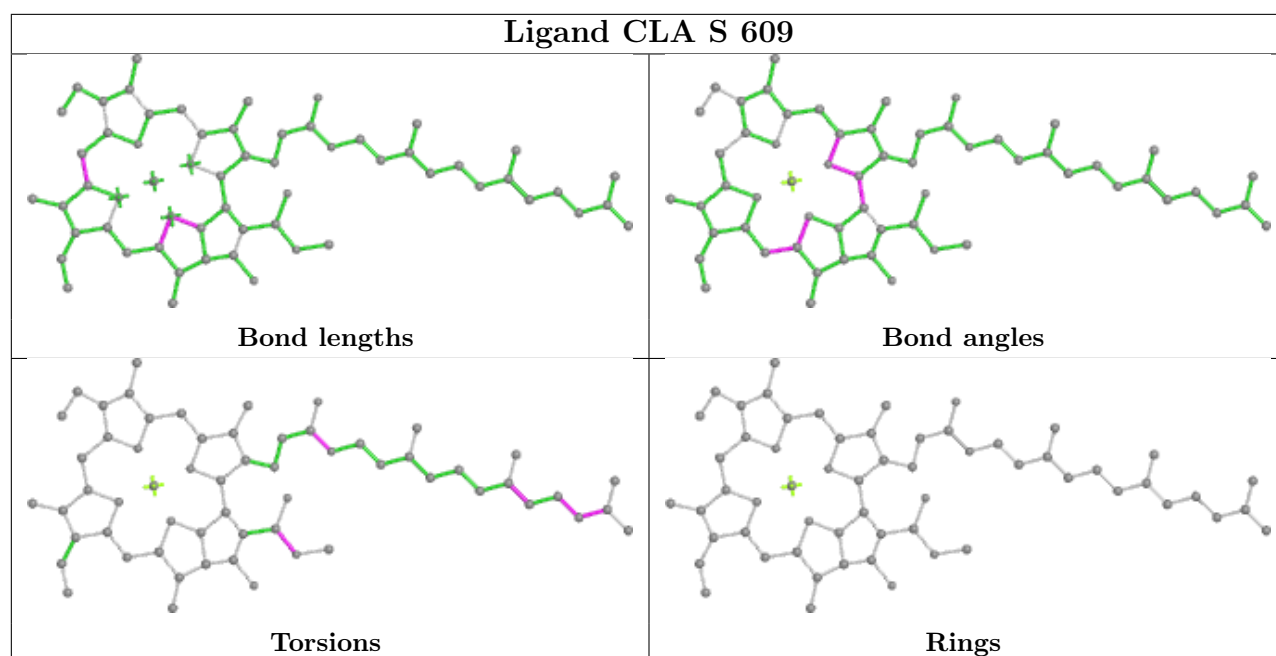
Rings



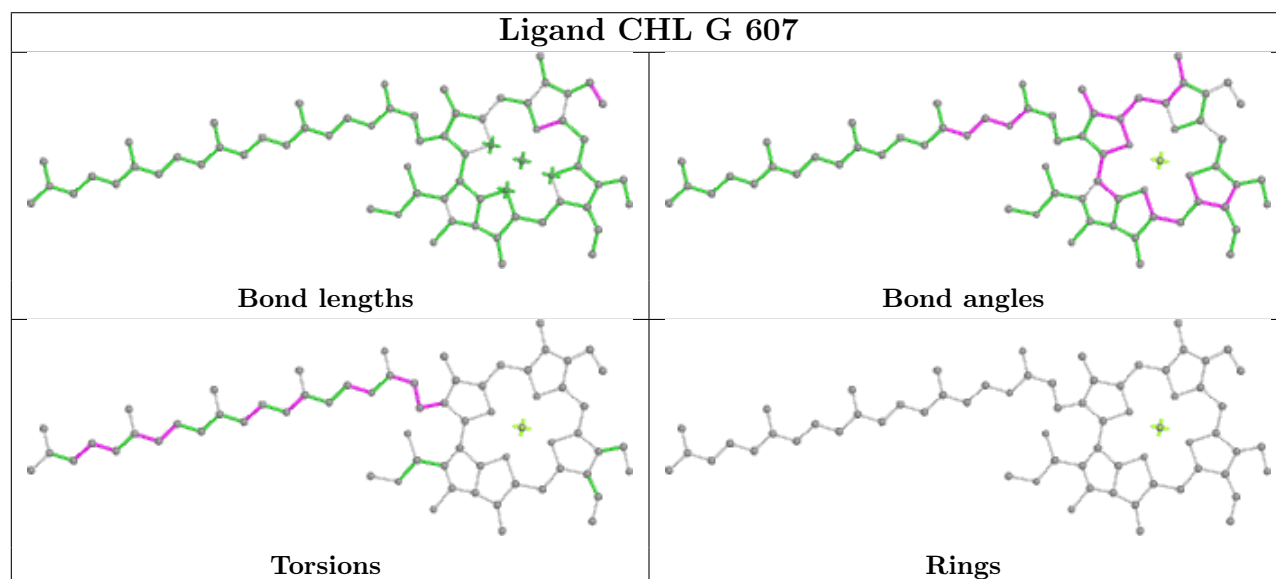
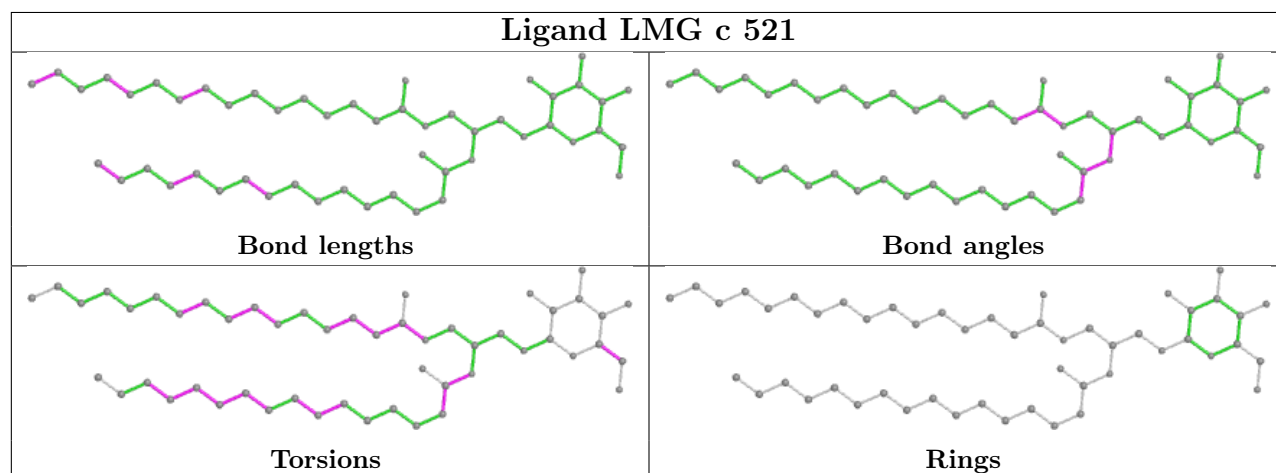
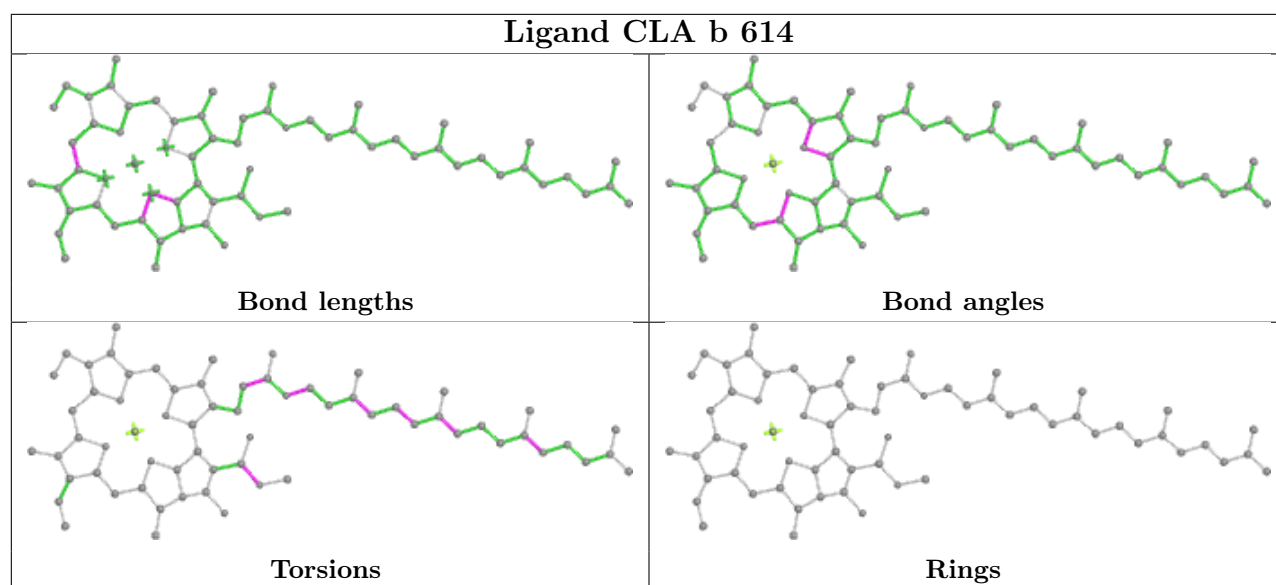


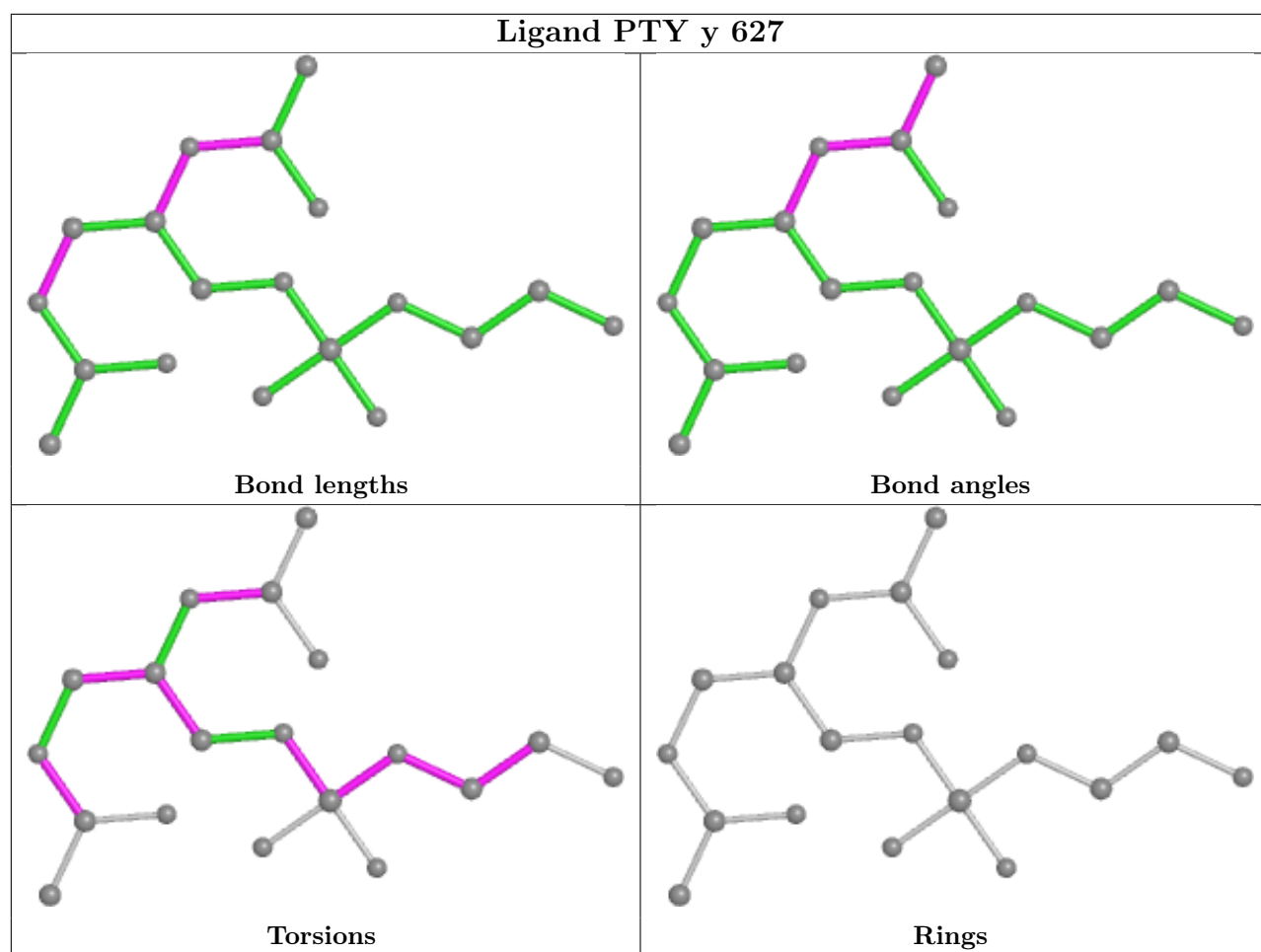


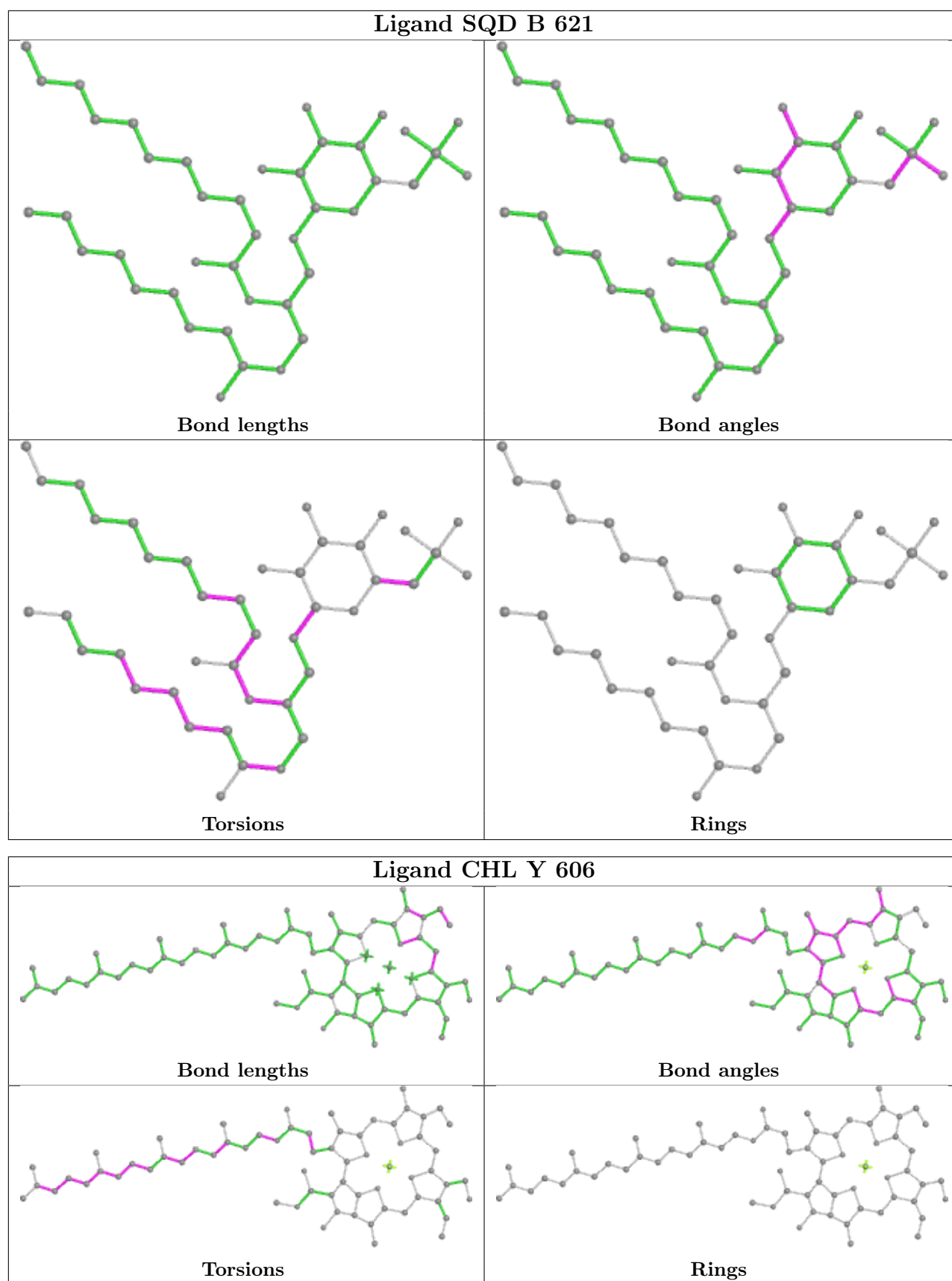




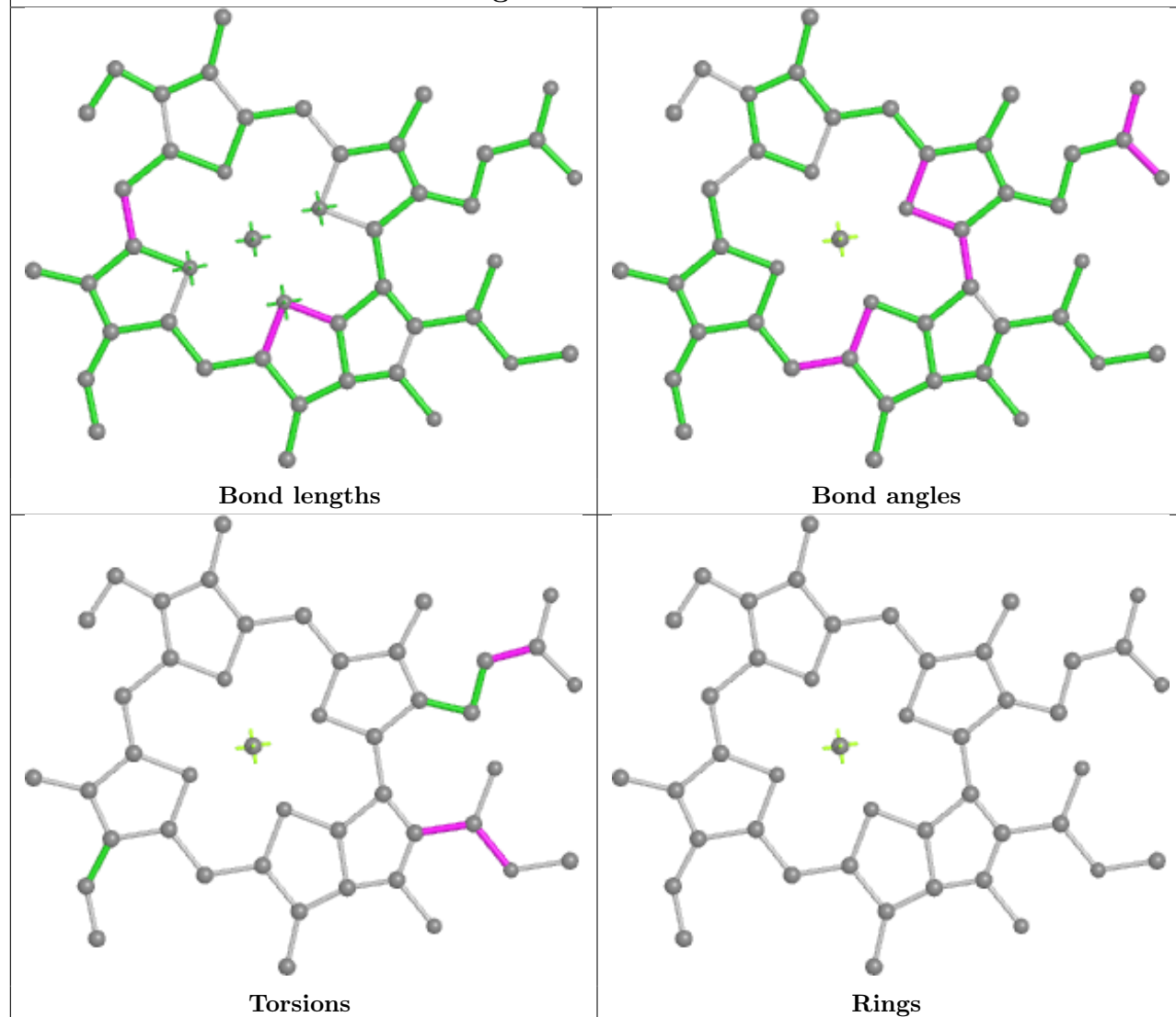




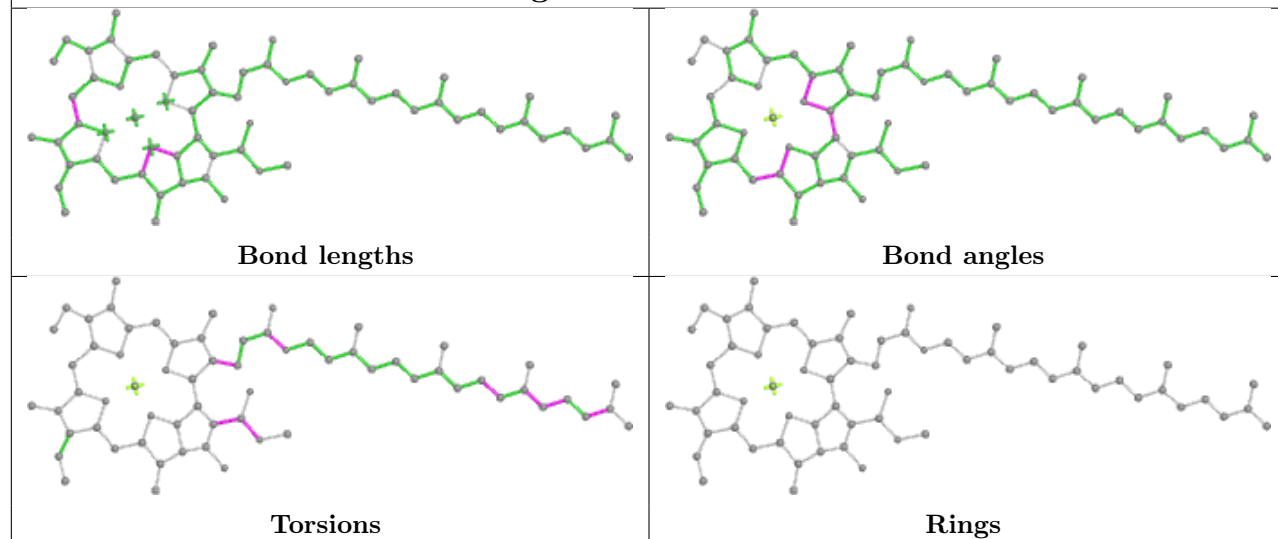


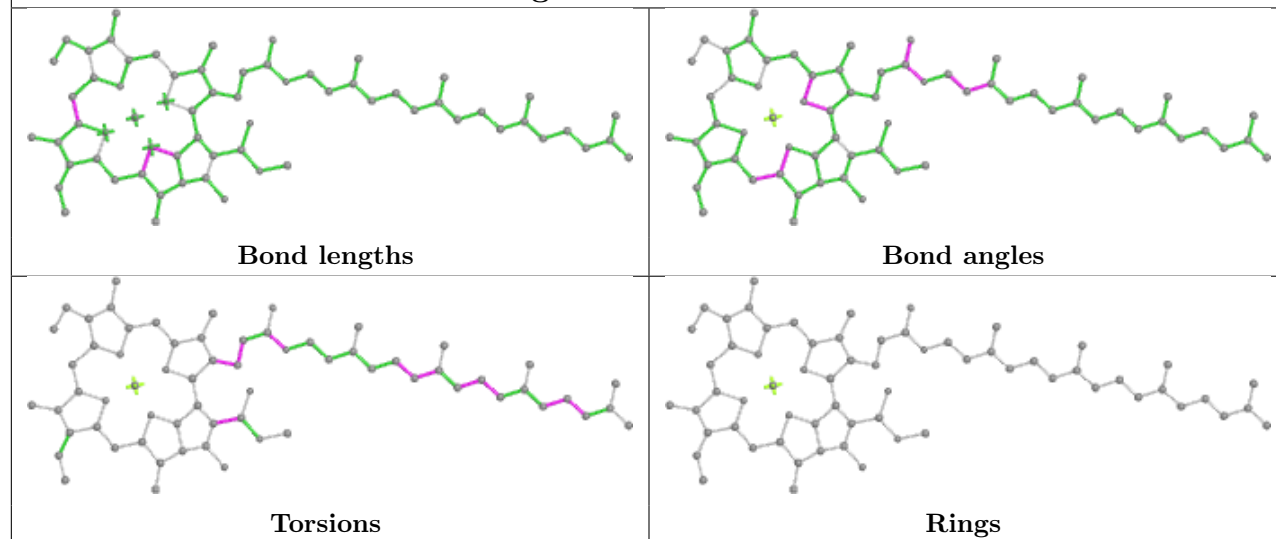
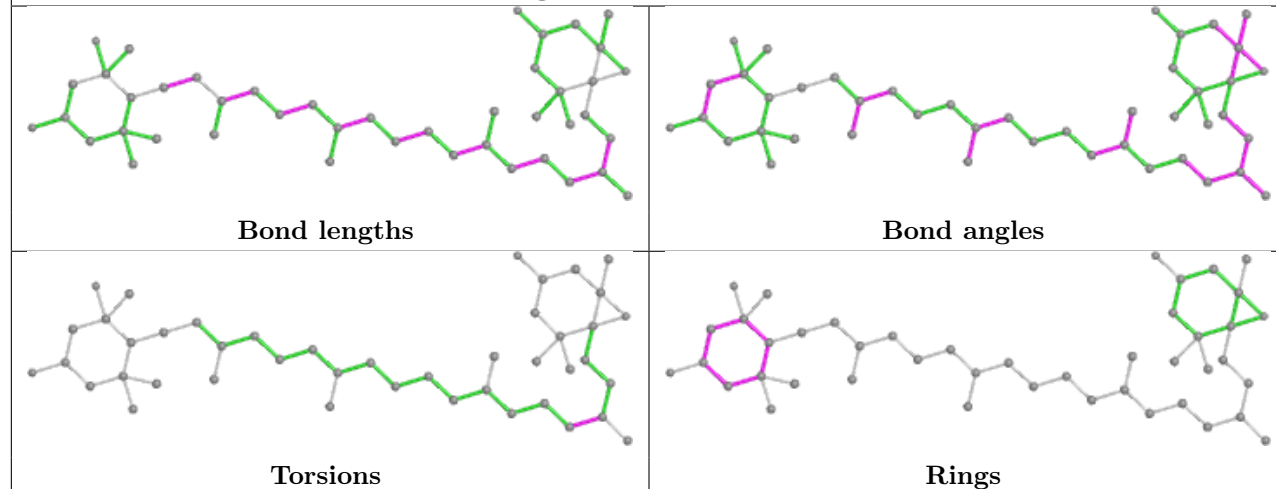
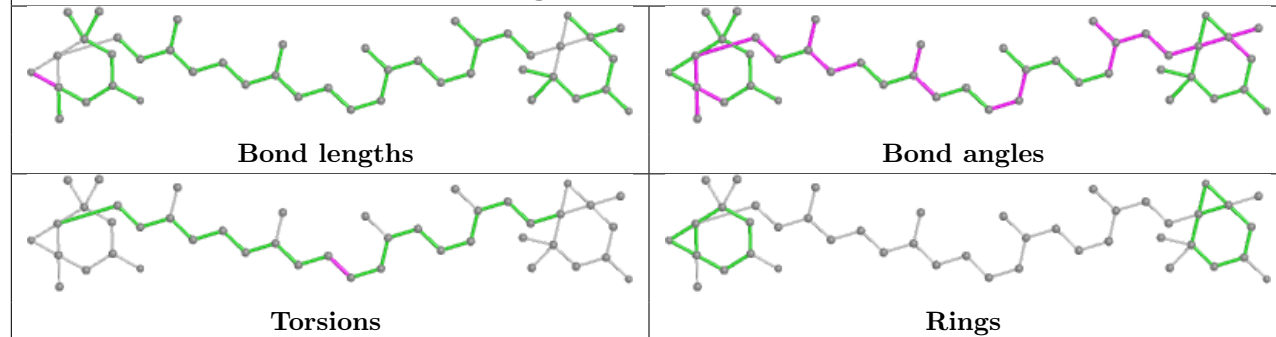


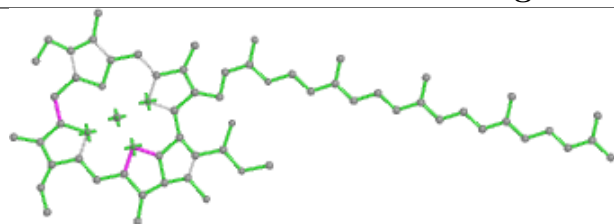
## Ligand CLA n 612



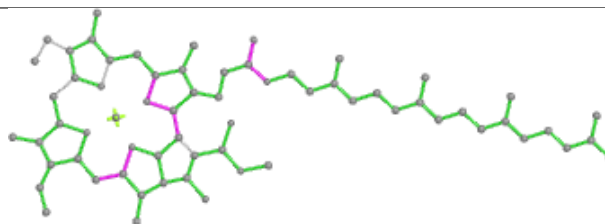
## Ligand CLA G 611



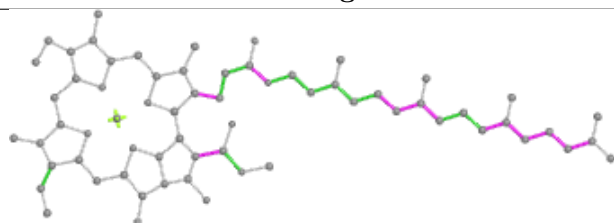
**Ligand CLA Y 602****Ligand NEX n 623****Ligand XAT G 622**

**Ligand CLA B 602**

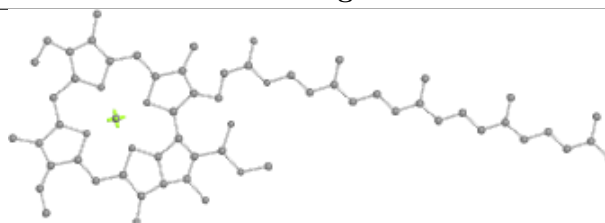
Bond lengths



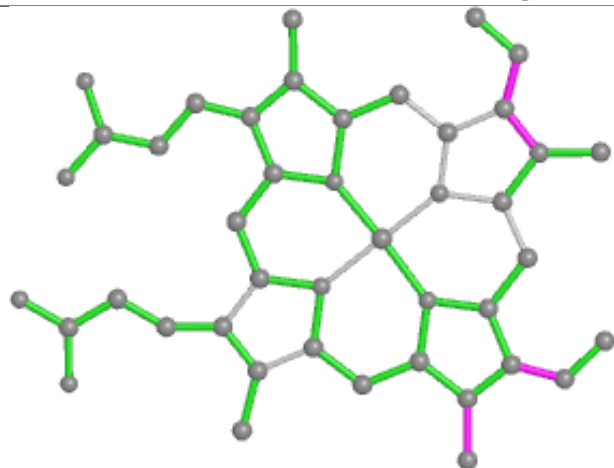
Bond angles



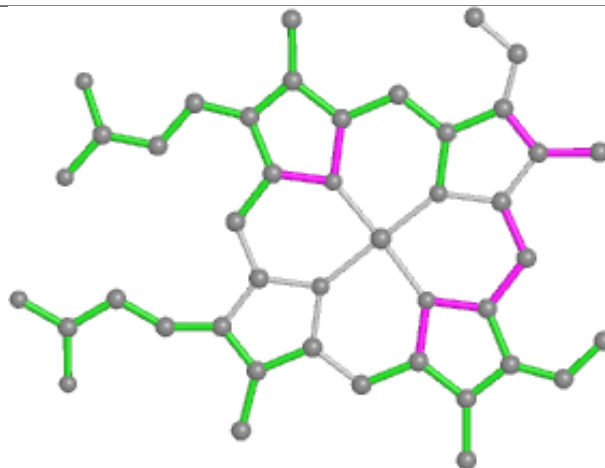
Torsions



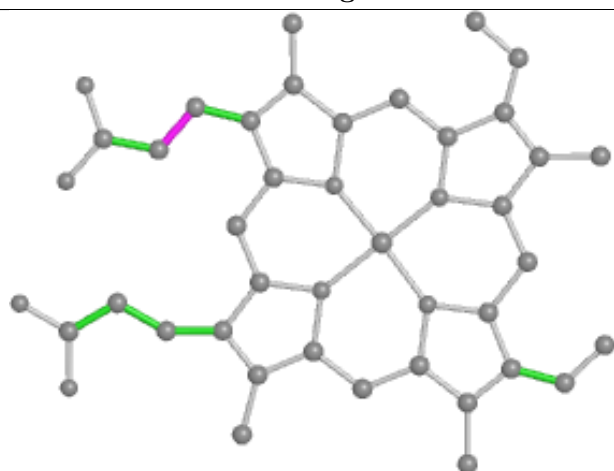
Rings

**Ligand HEM f 101**

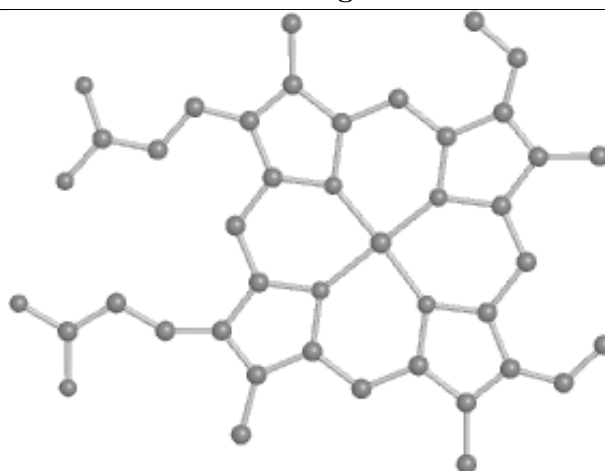
Bond lengths



Bond angles

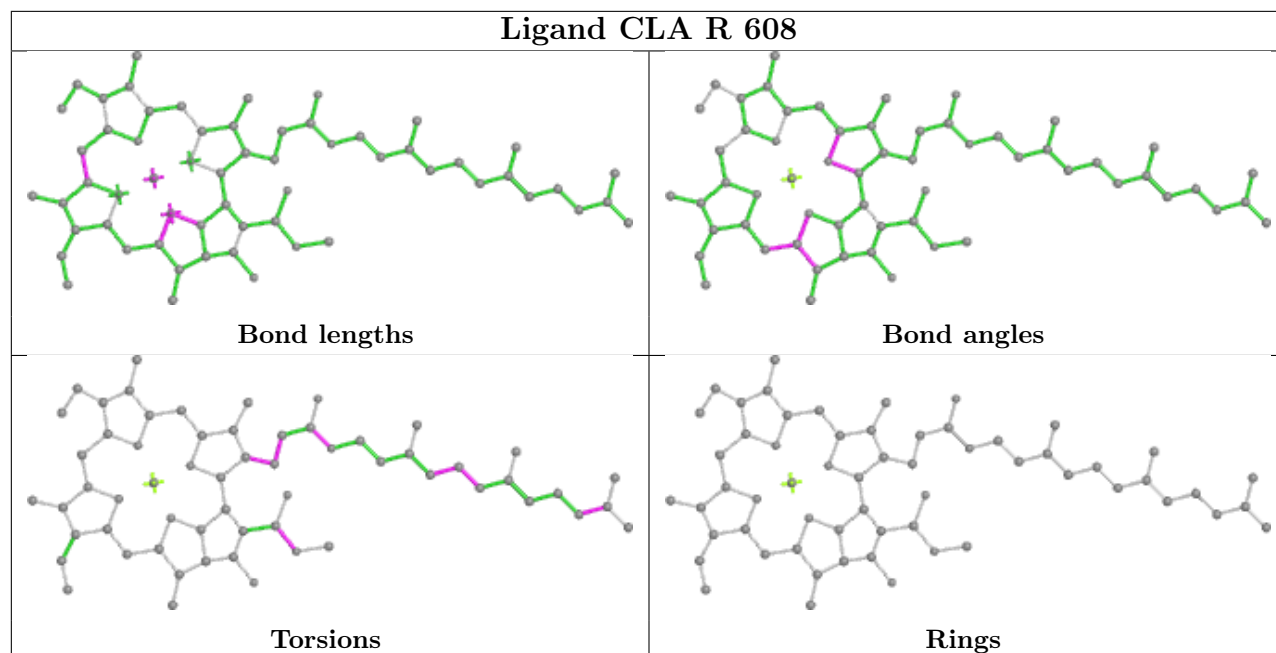


Torsions

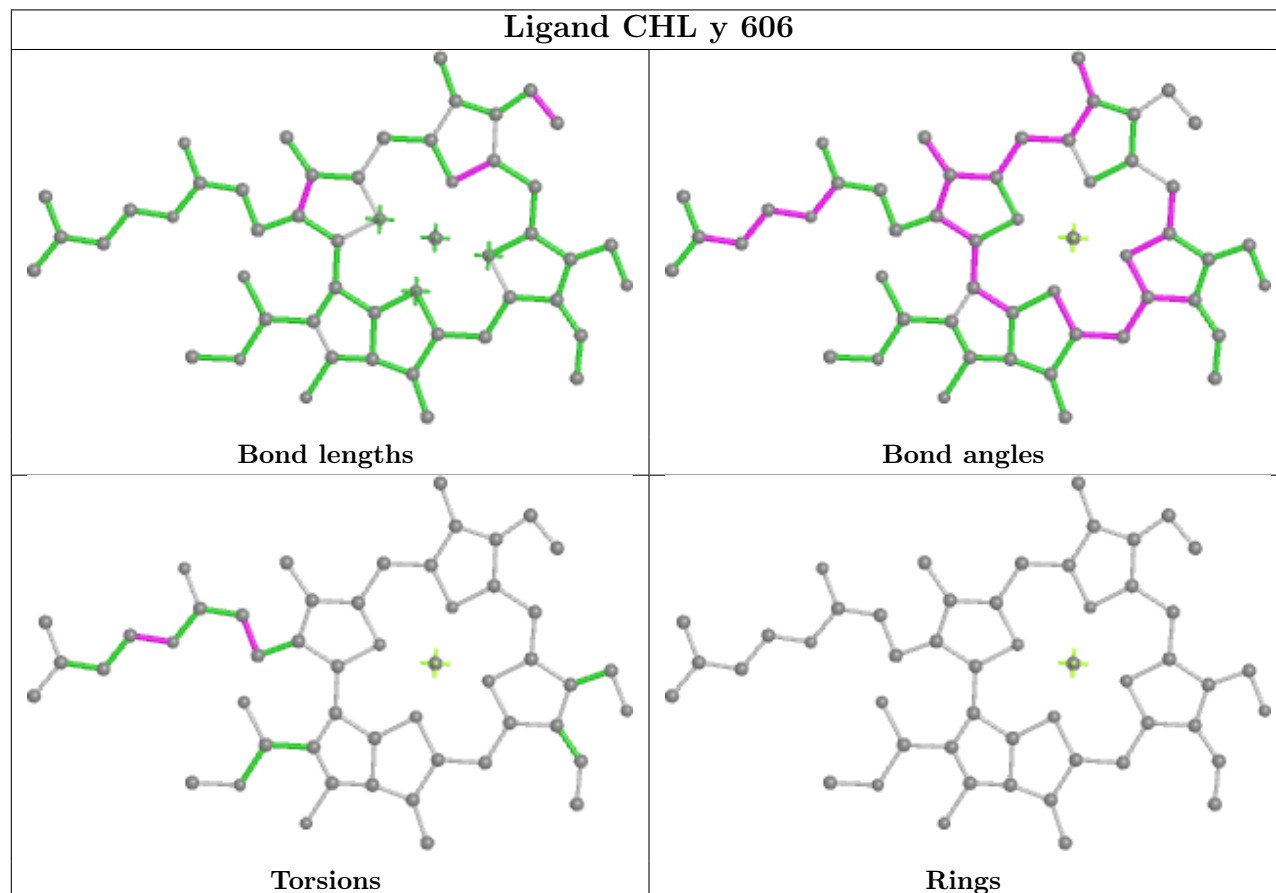


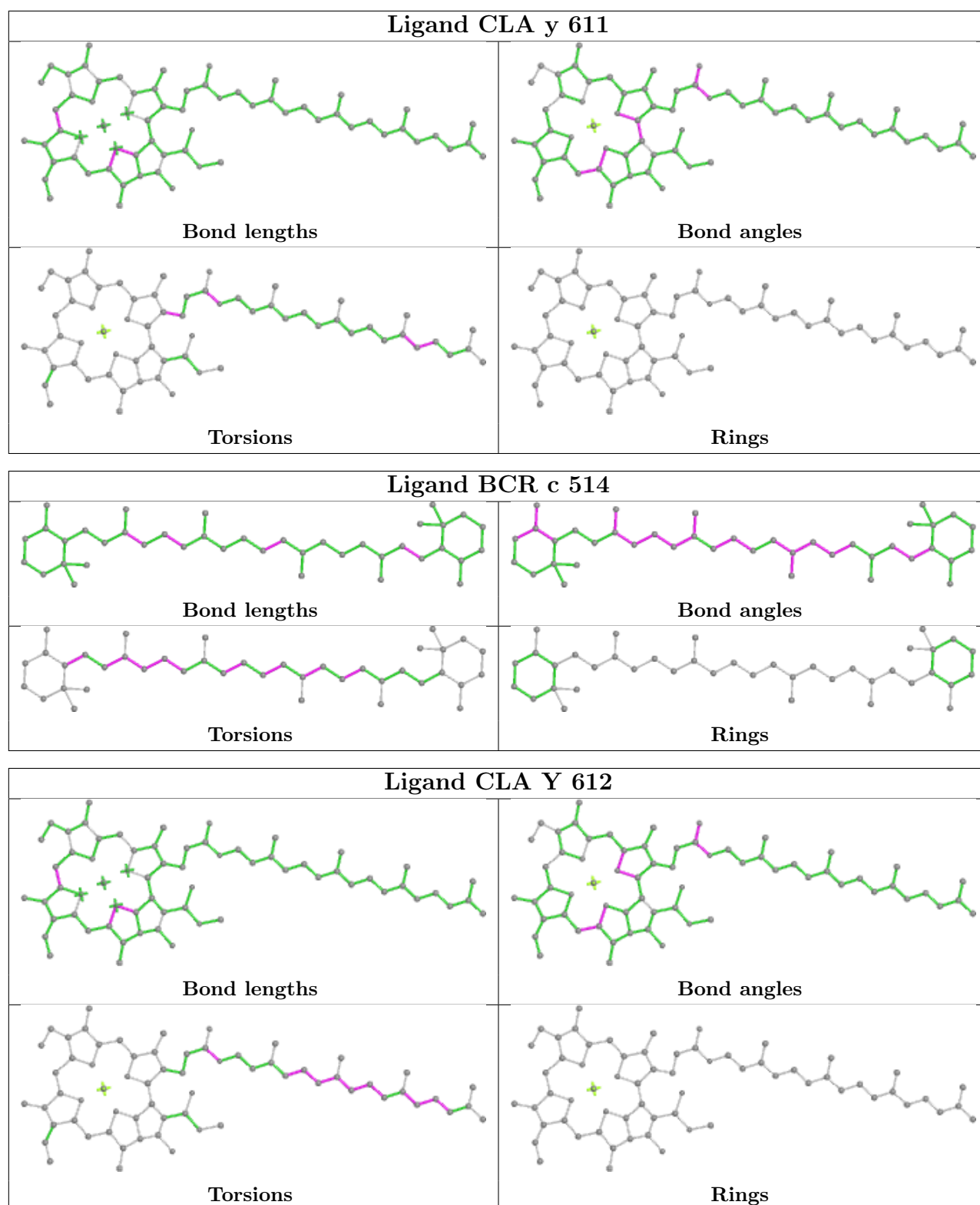
Rings

## Ligand CLA R 608

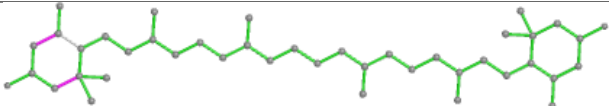
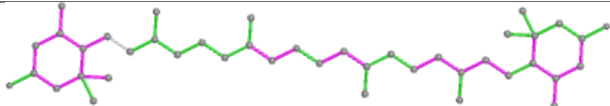
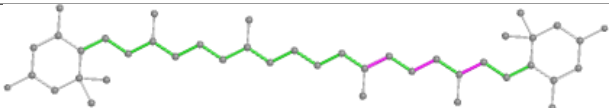
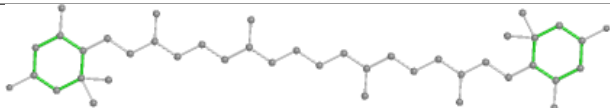


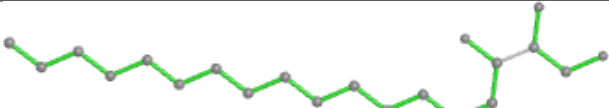
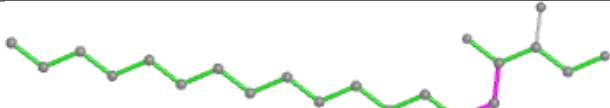
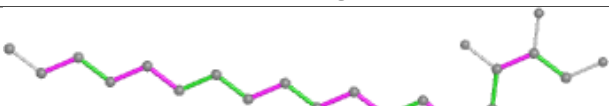
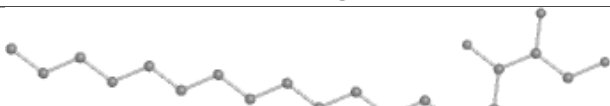
## Ligand CHL y 606

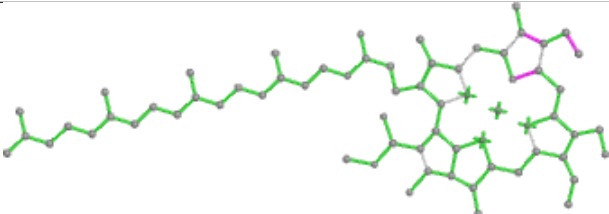
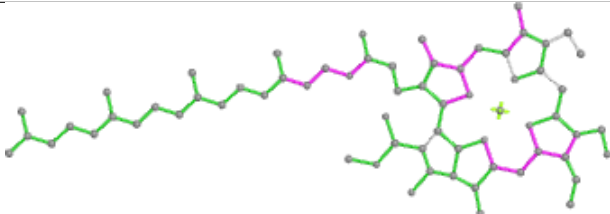
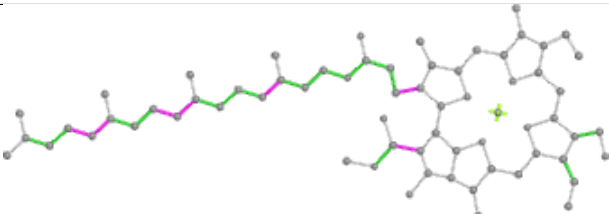
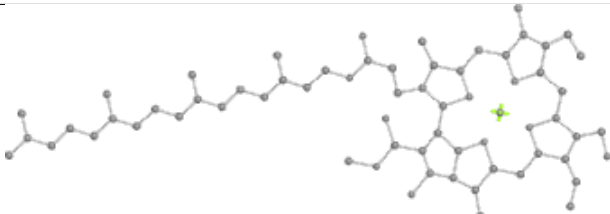


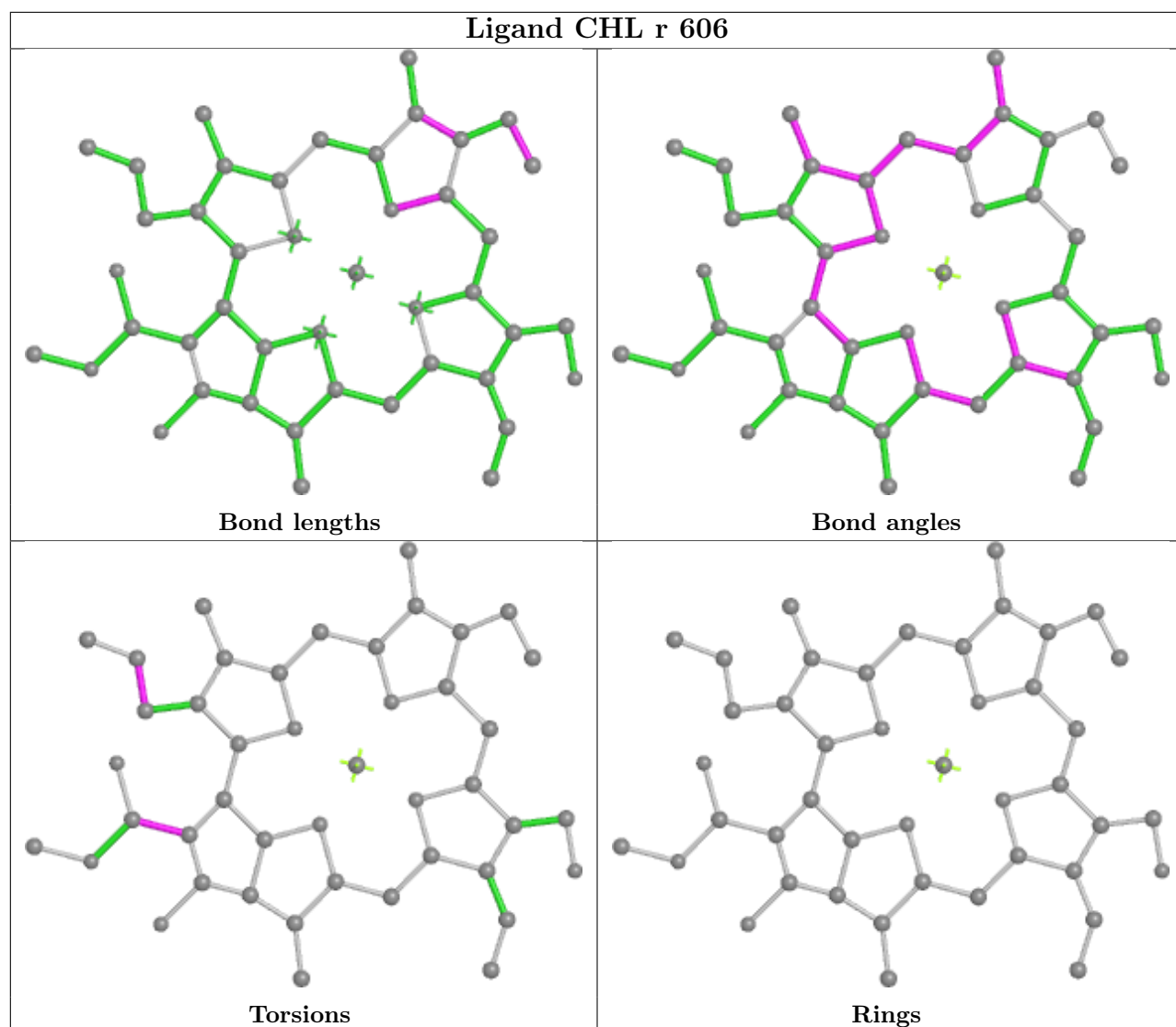
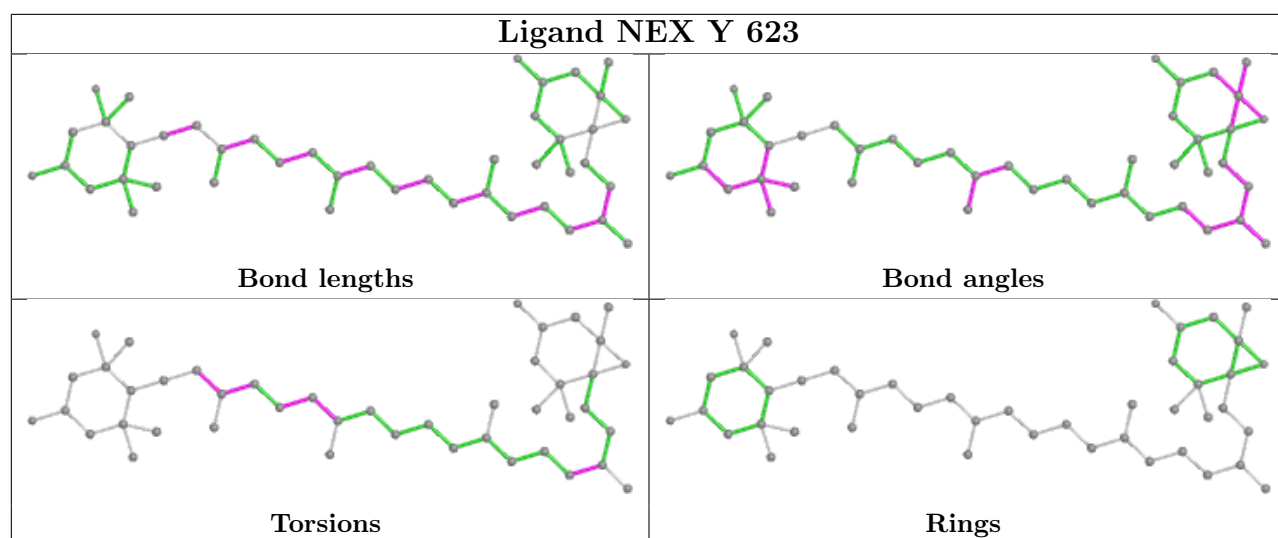


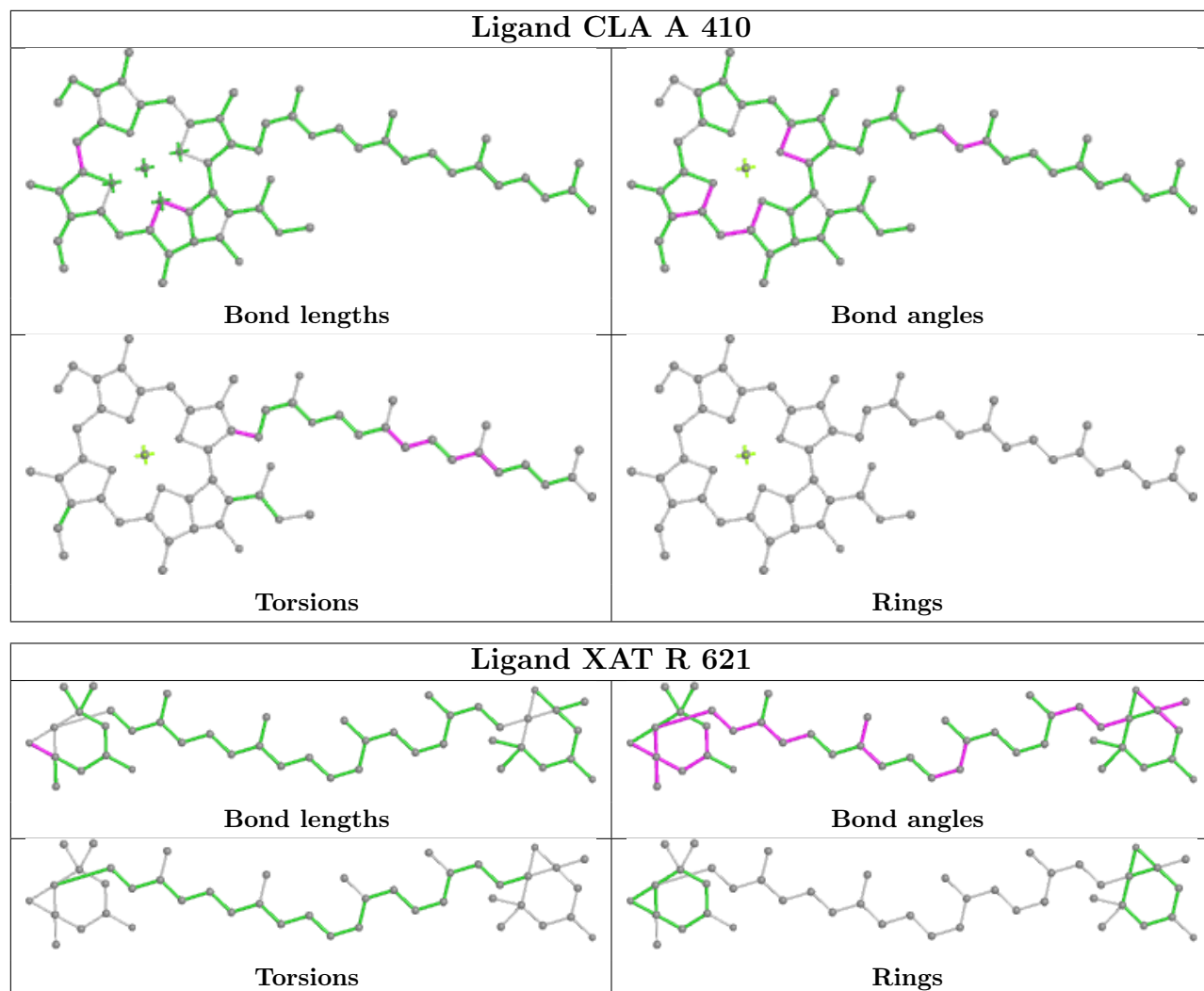


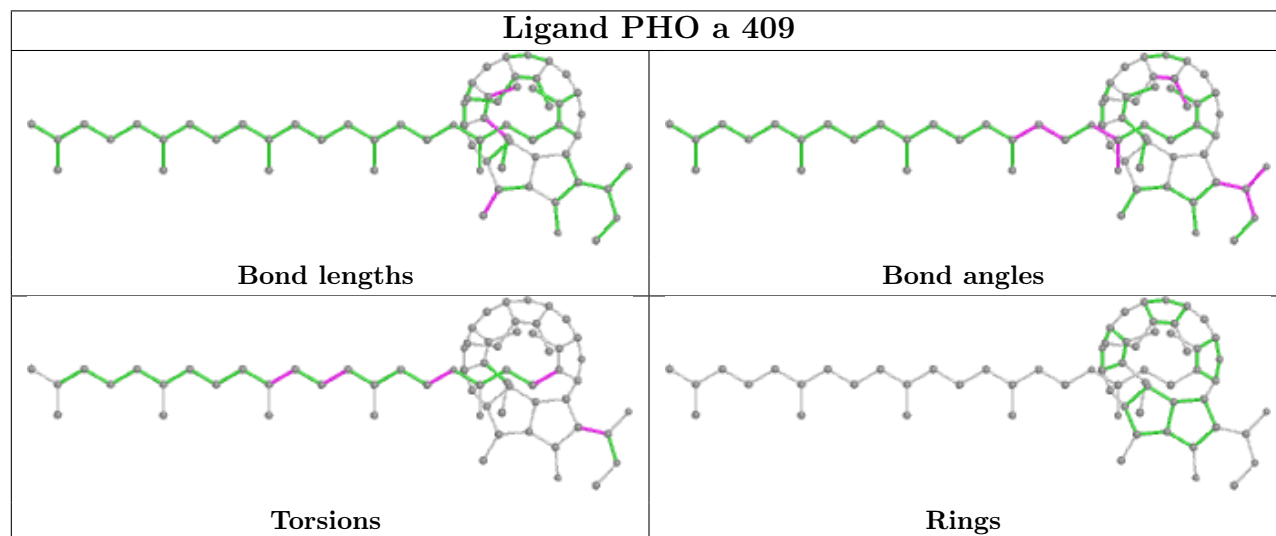
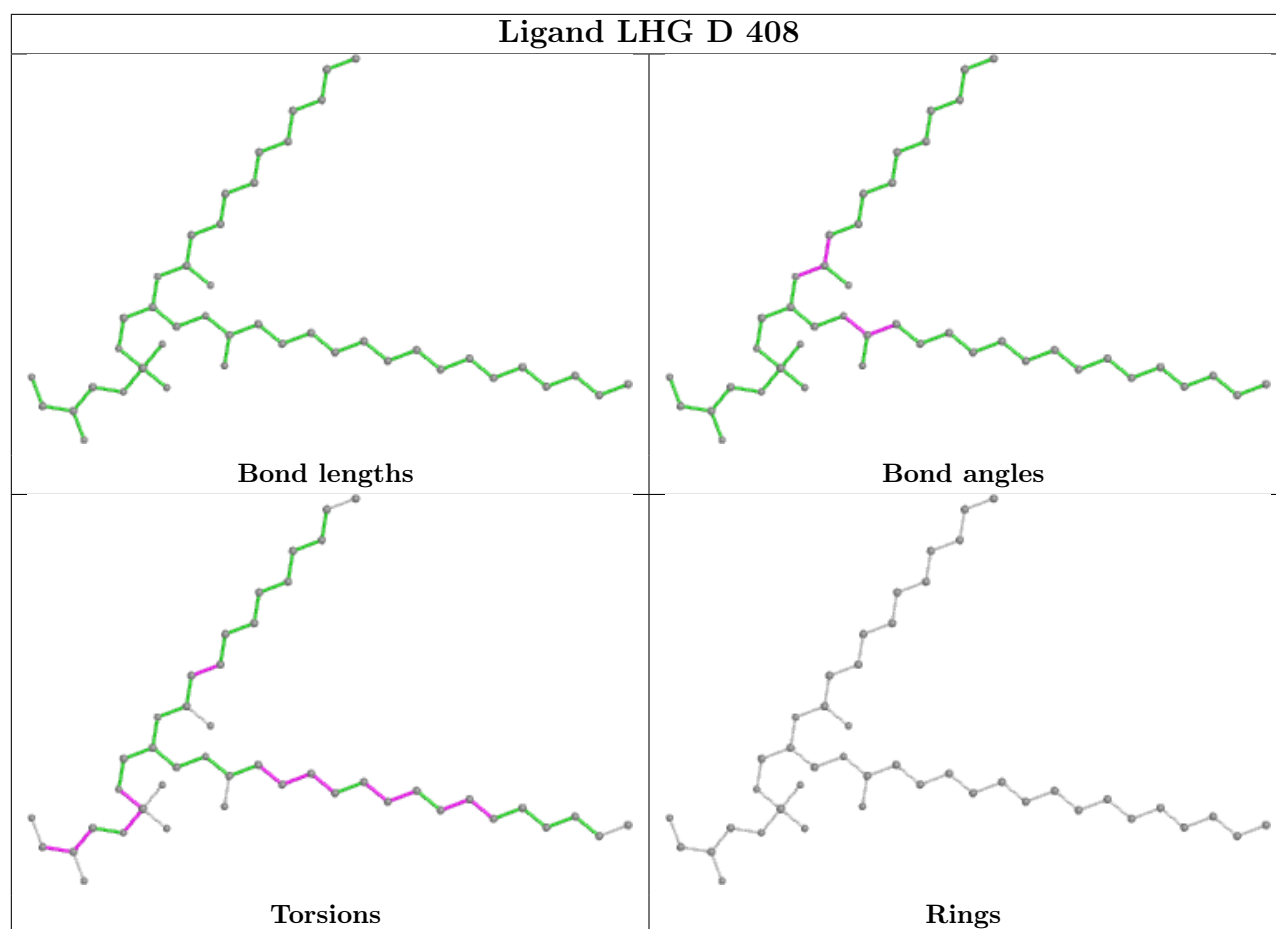
Ligand LUT r 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

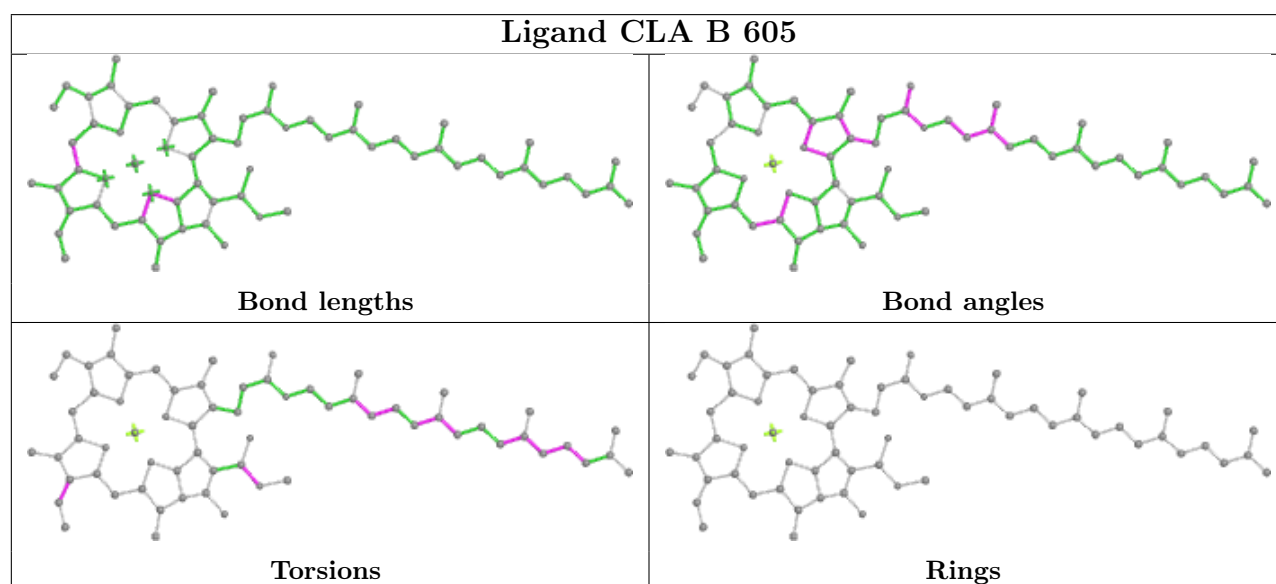
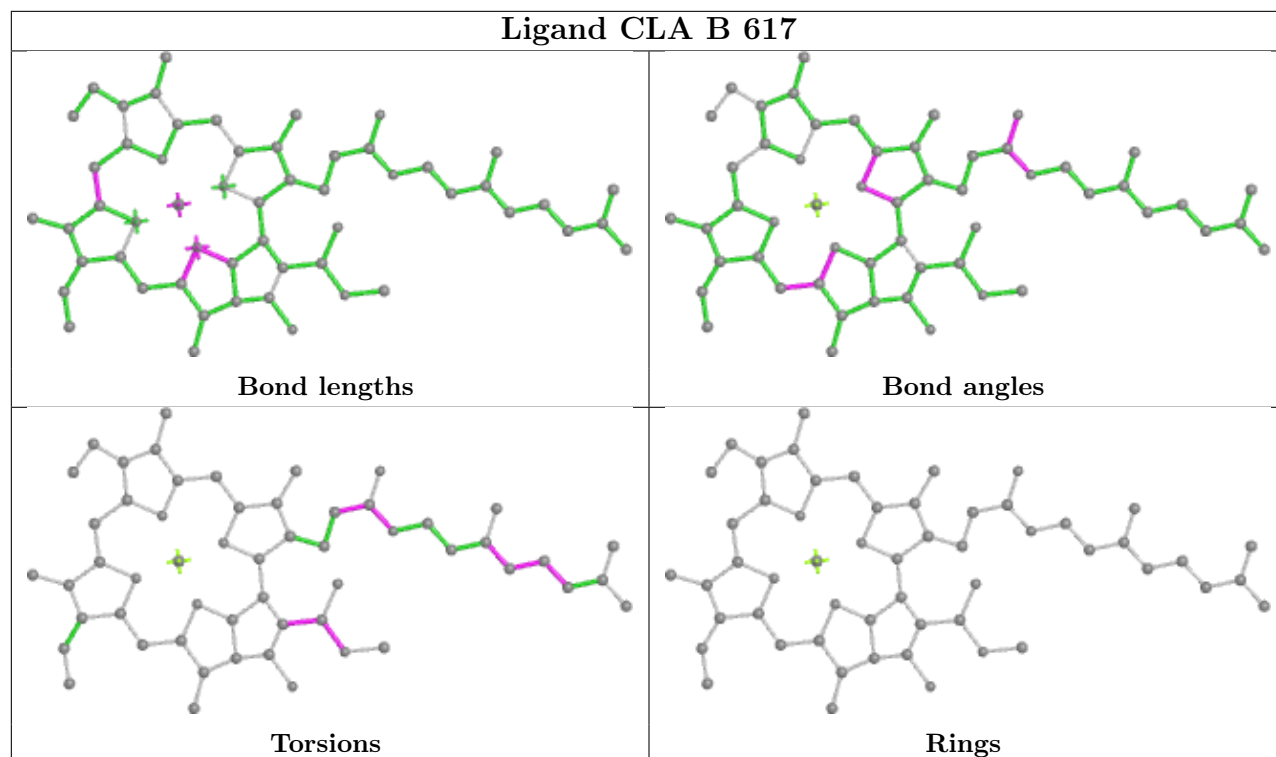
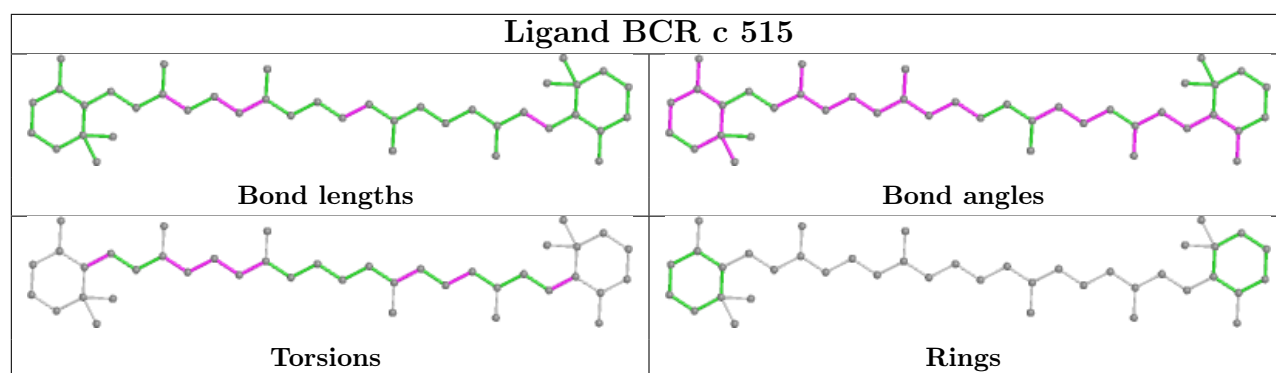
Ligand SPH a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

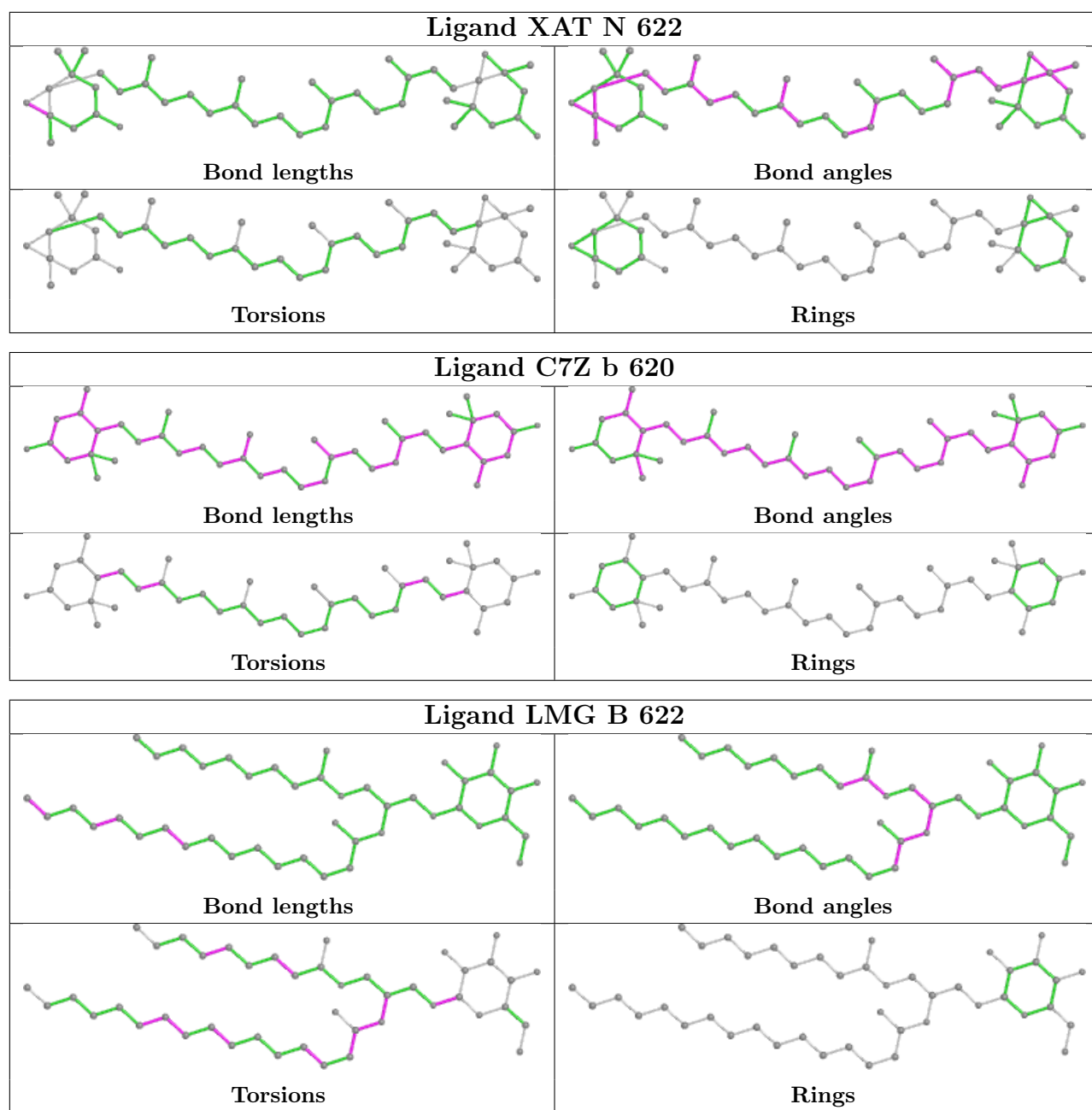
Ligand CHL N 601	
	
Bond lengths	Bond angles
	
Torsions	Rings



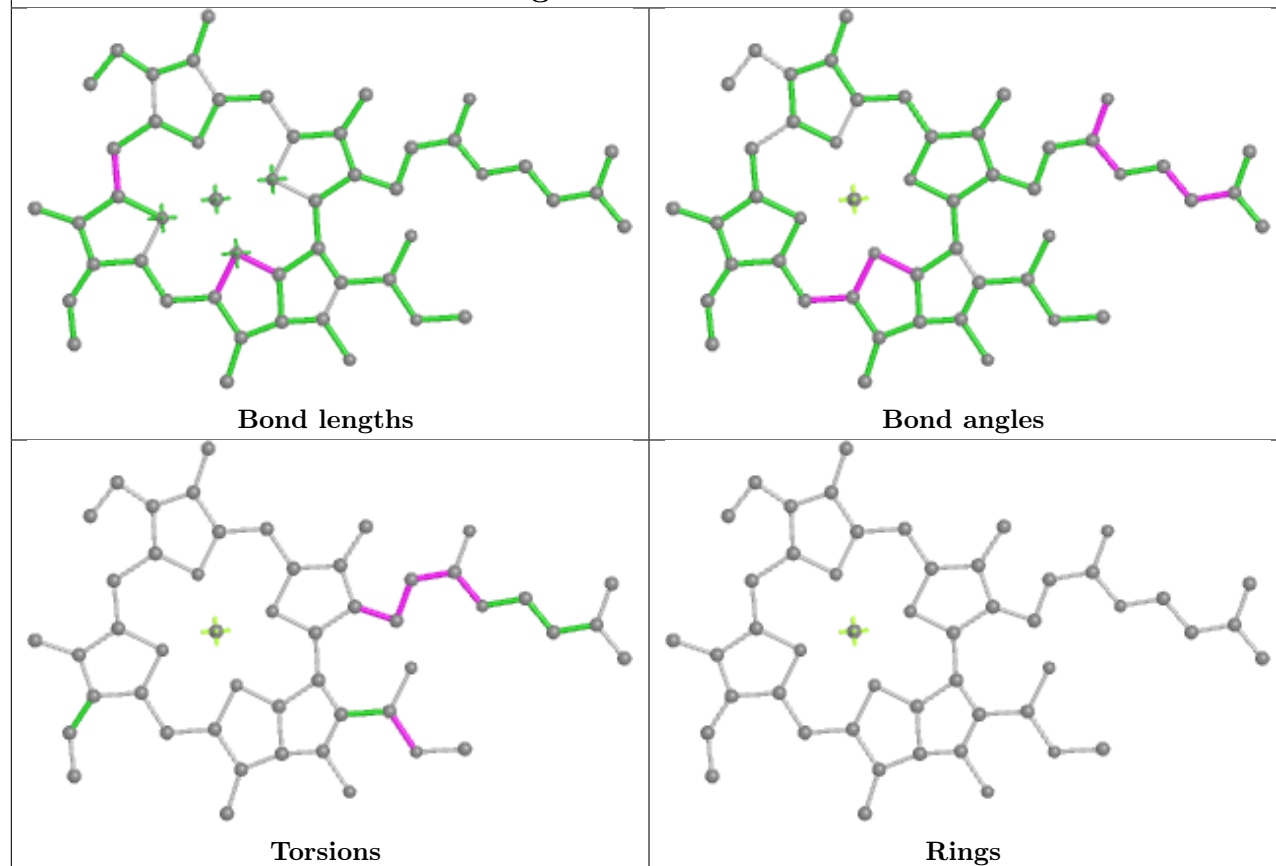




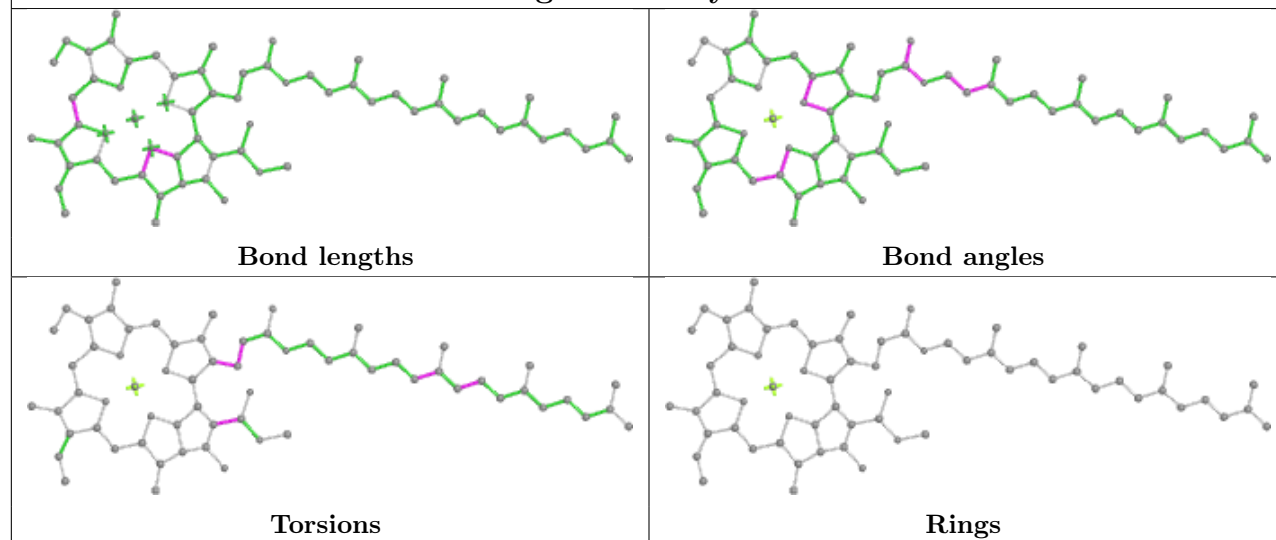


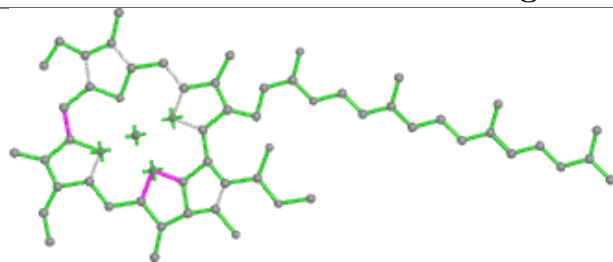
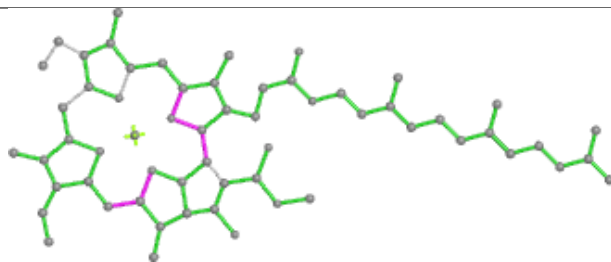
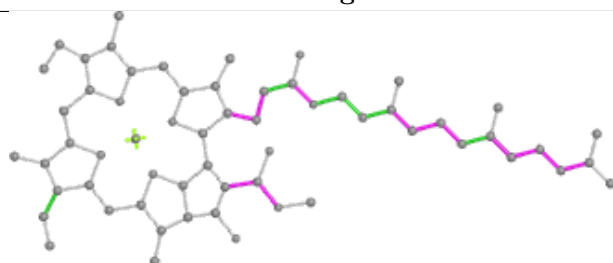
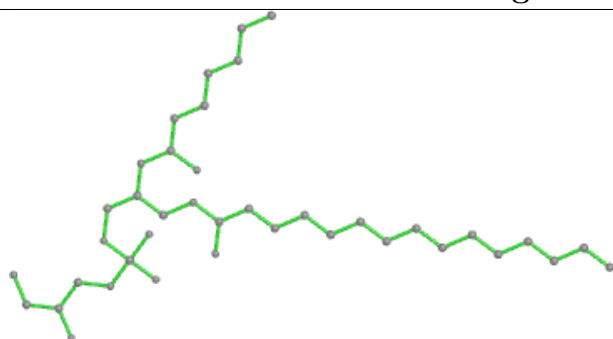
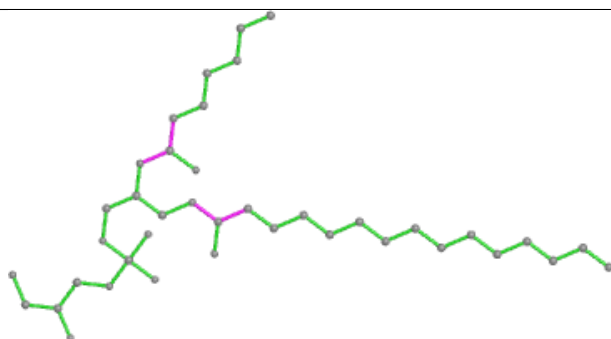
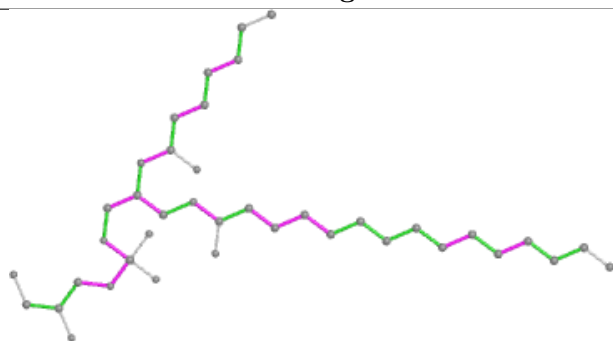
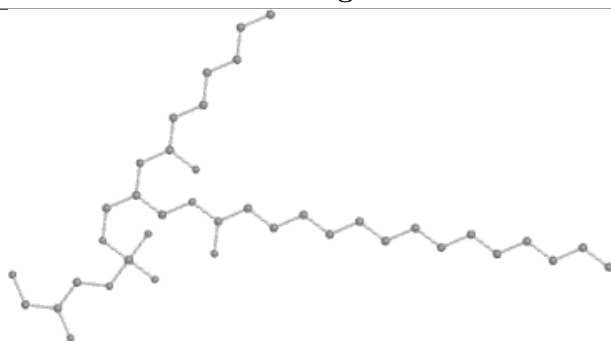


## Ligand CLA R 612

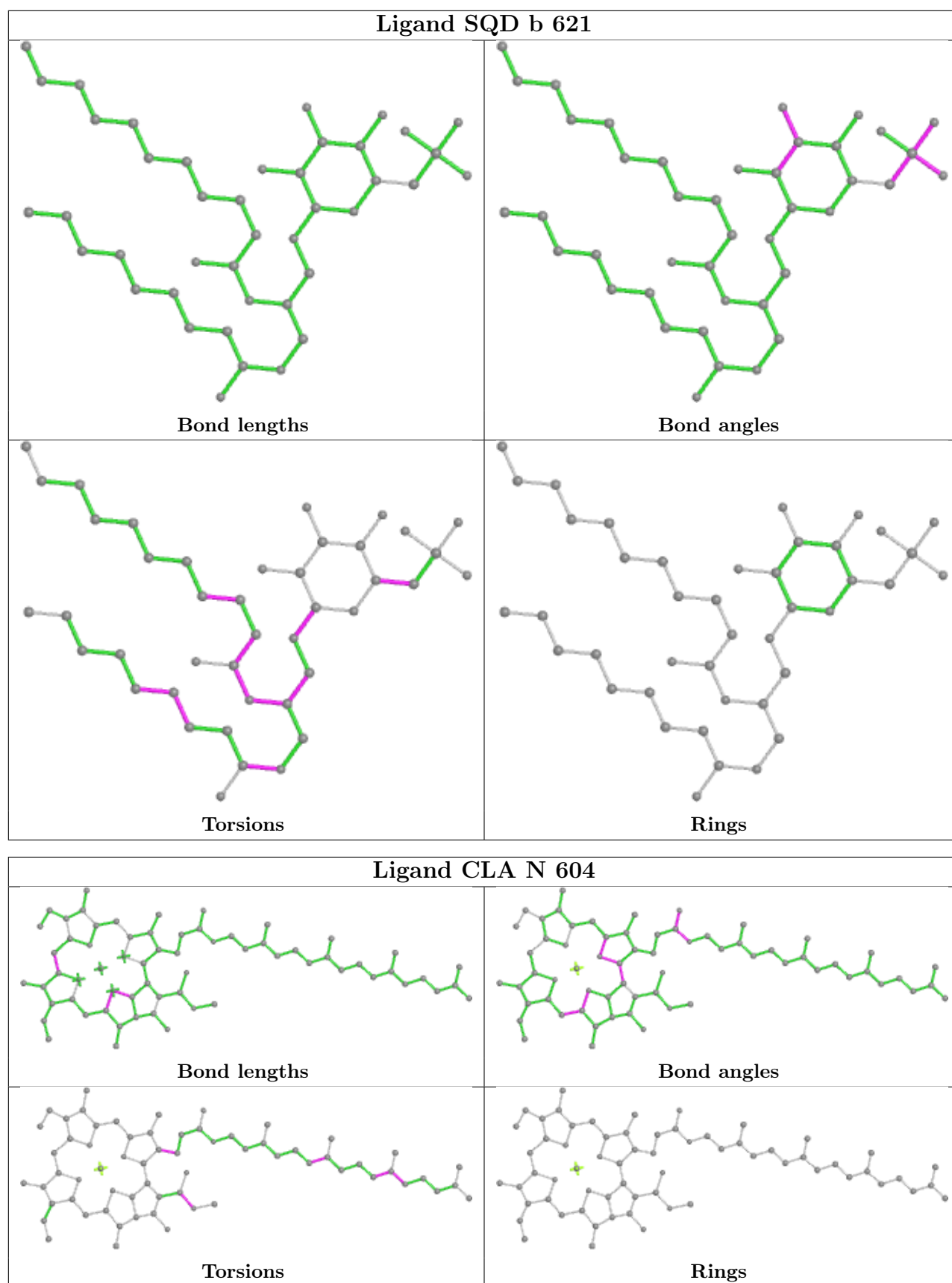


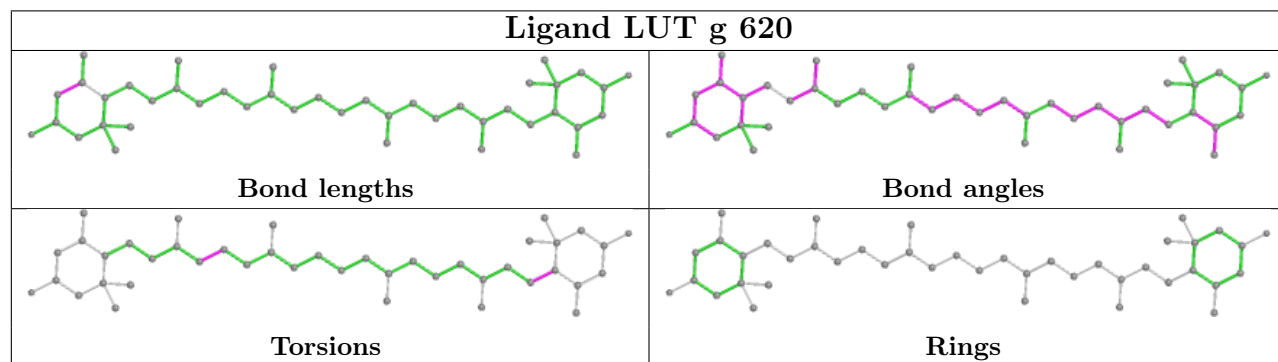
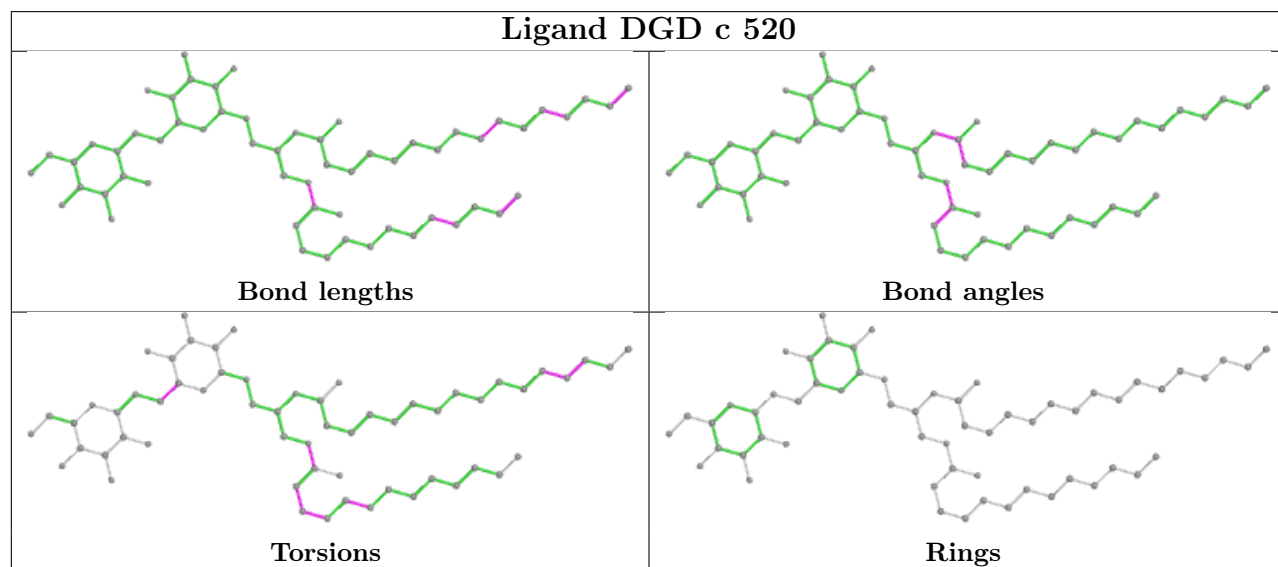
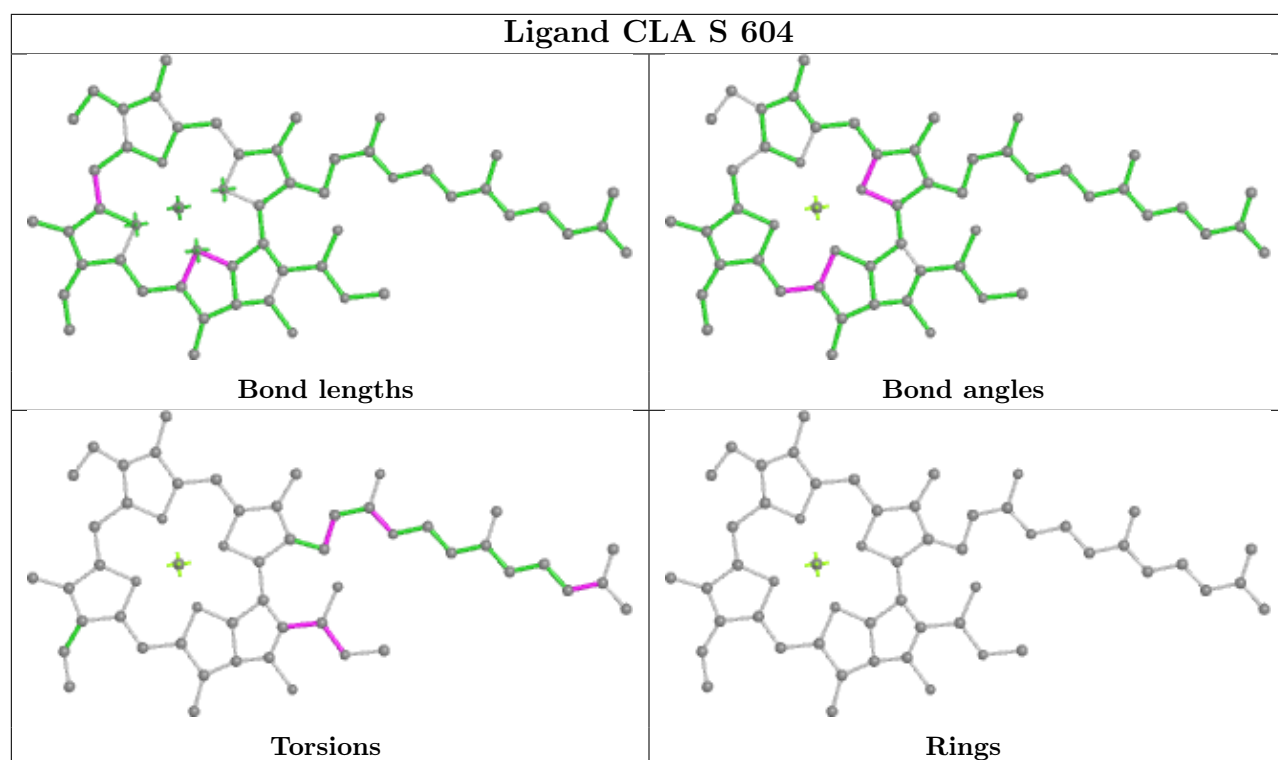
## Ligand CLA y 602

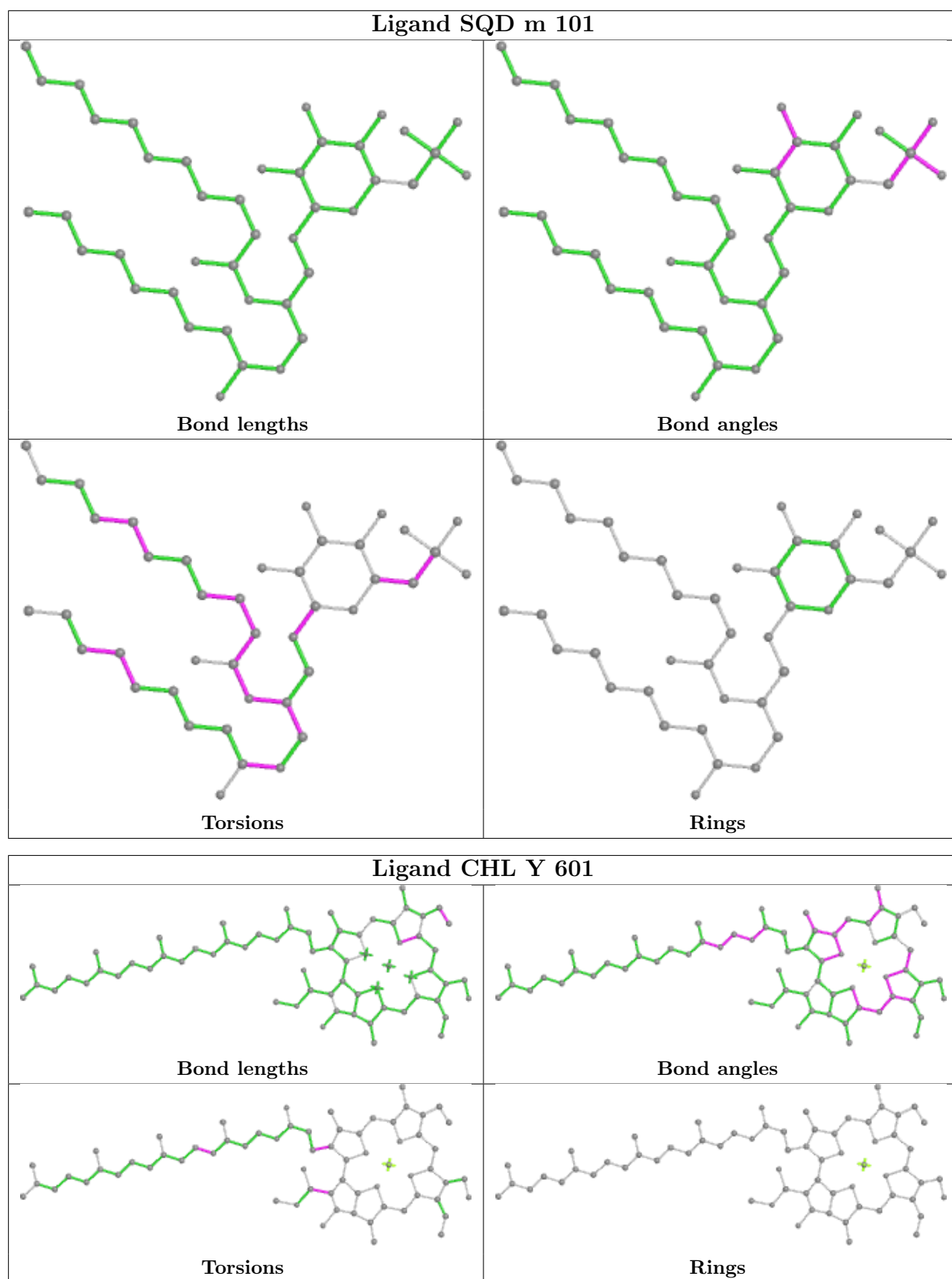


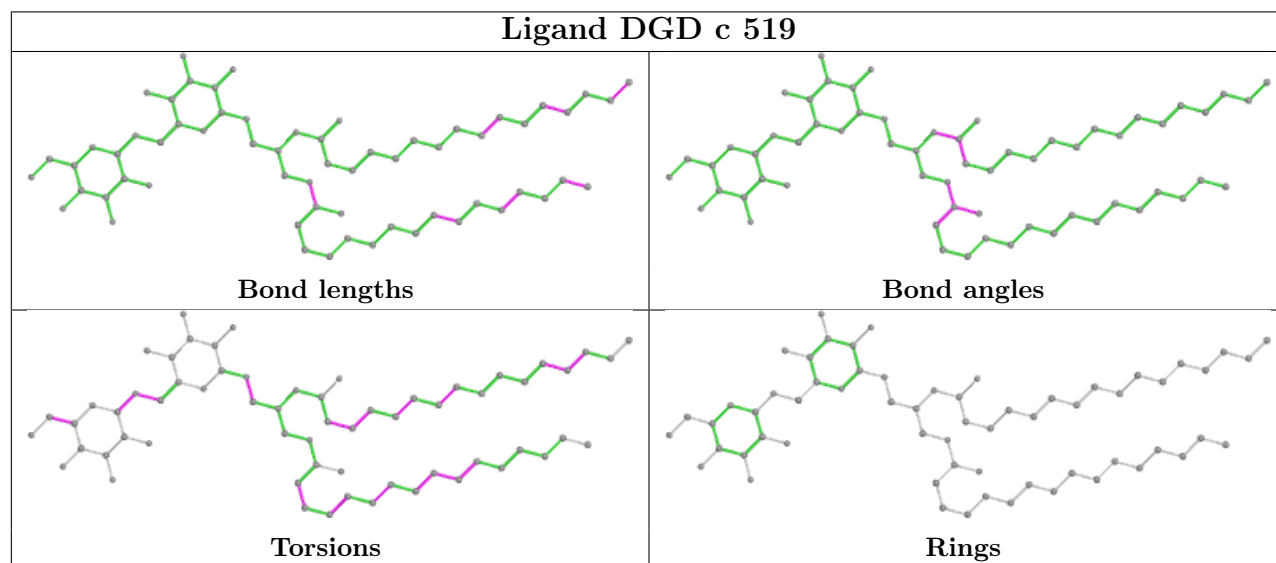
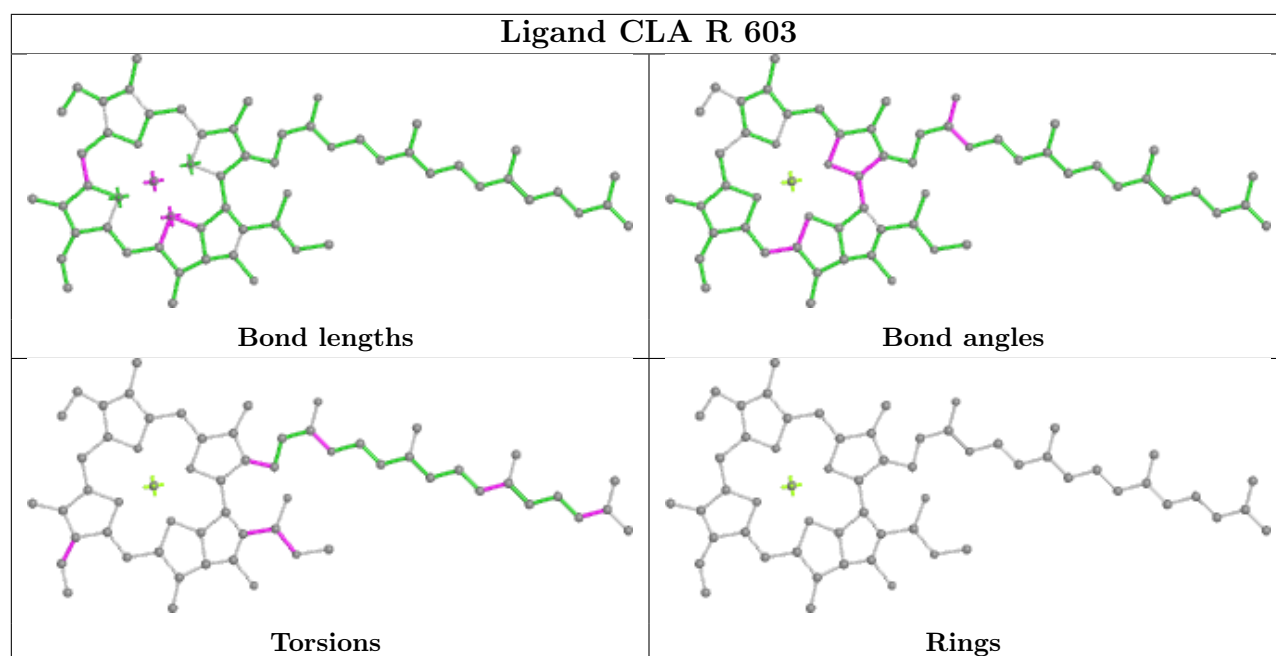
**Ligand CLA s 609****Bond lengths****Bond angles****Torsions****Rings****Ligand LHG D 410****Bond lengths****Bond angles****Torsions****Rings**

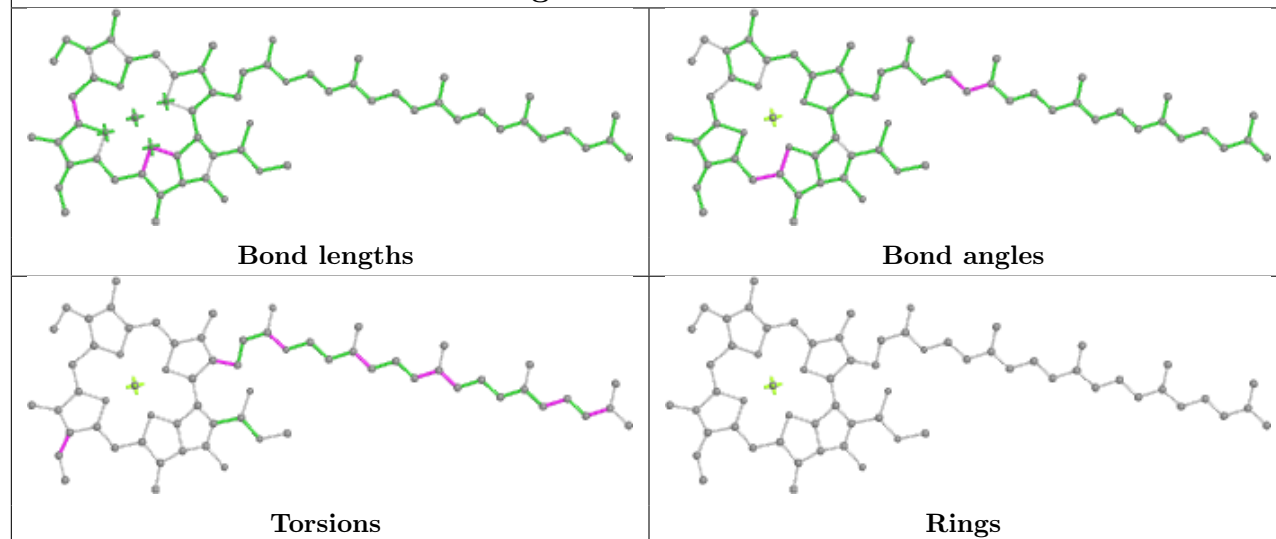
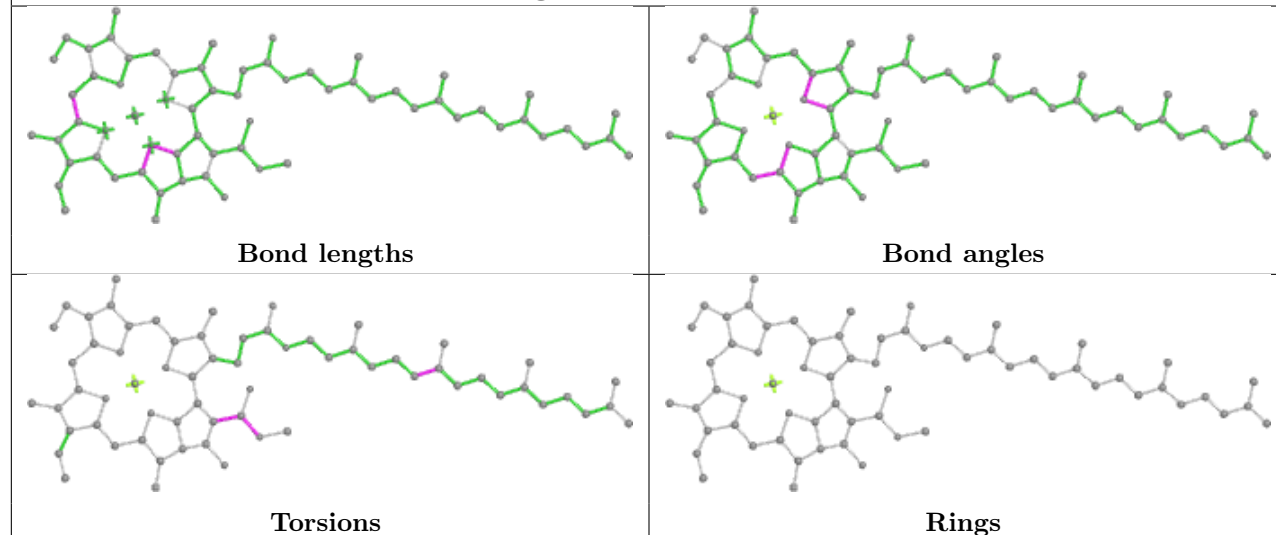
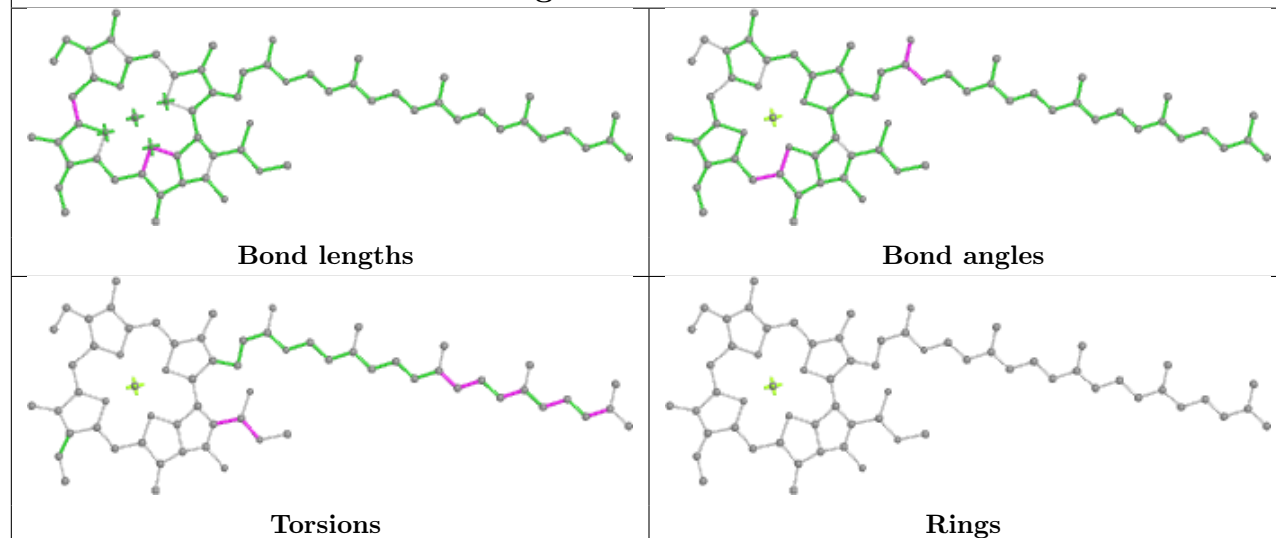


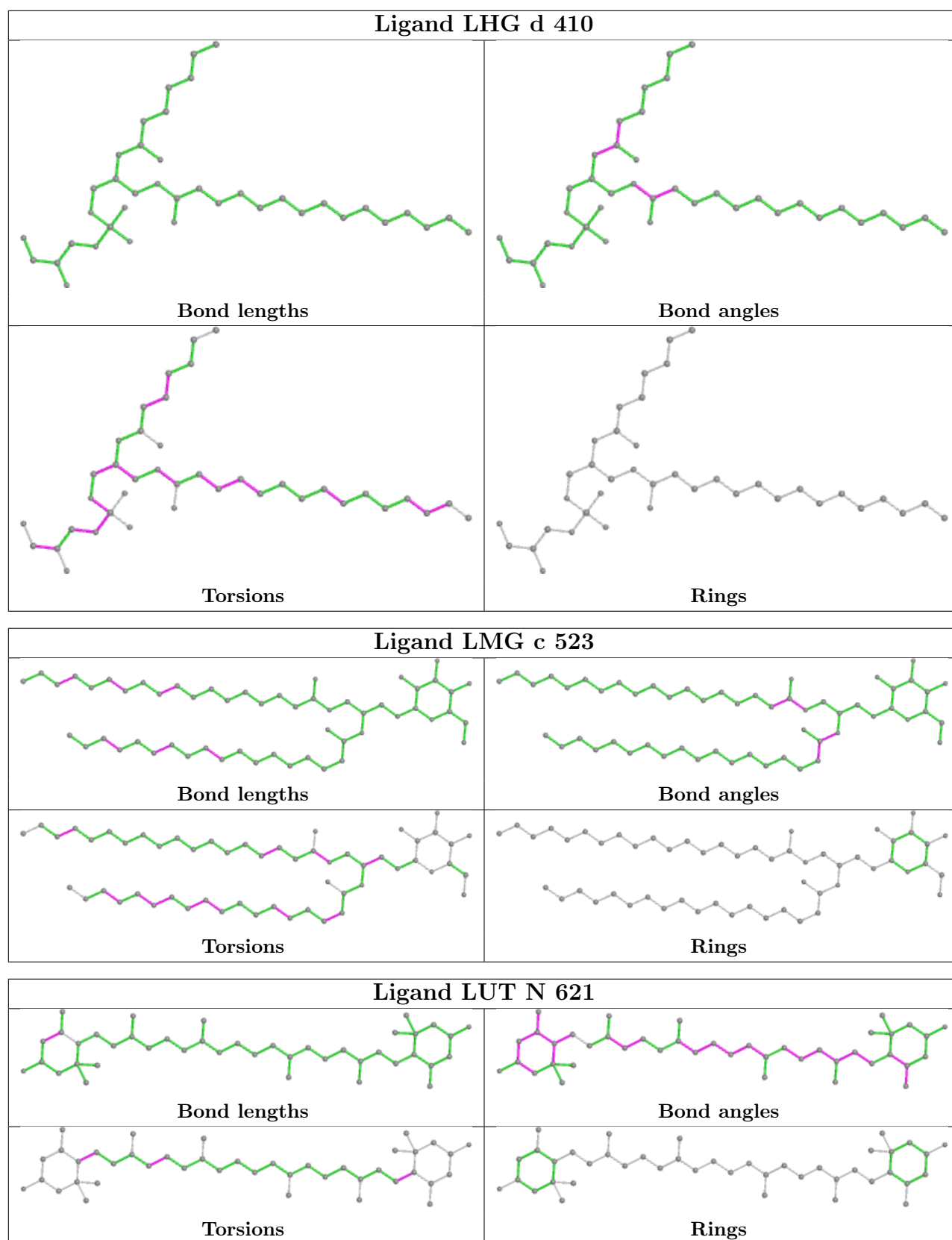




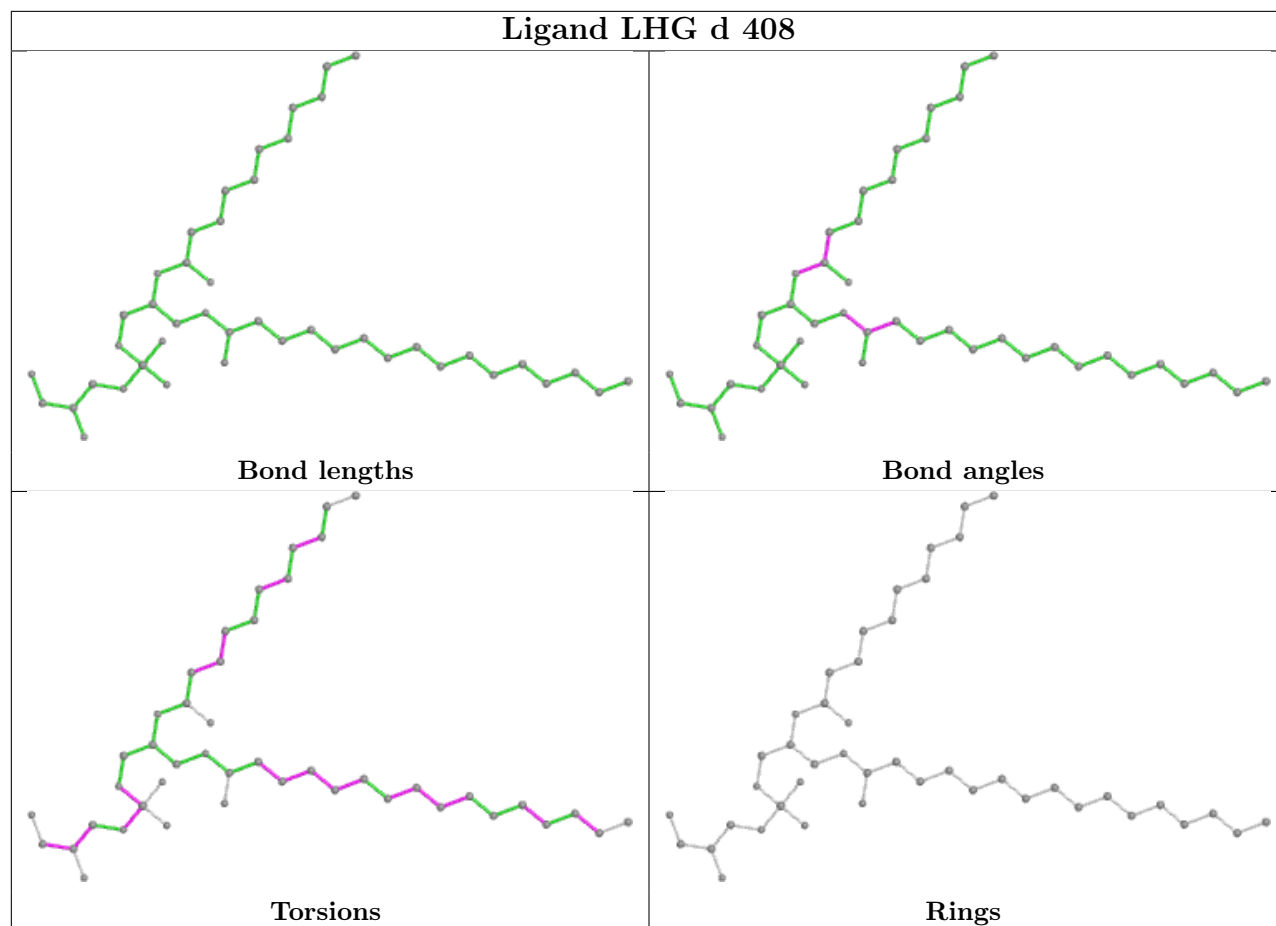




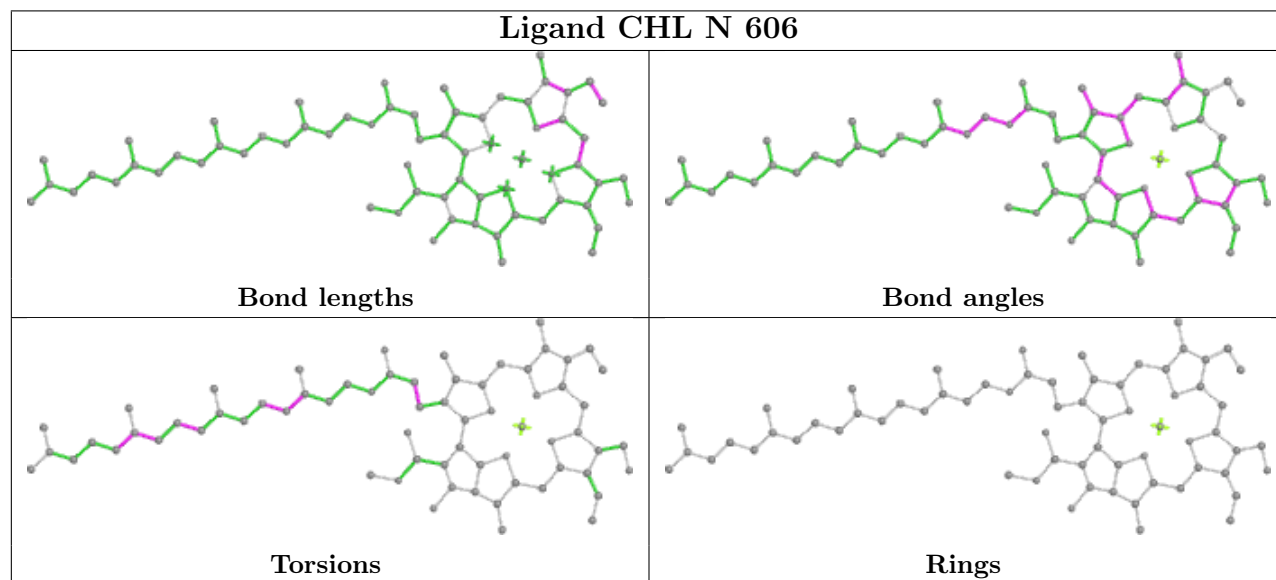
**Ligand CLA Y 603****Ligand CLA C 511****Ligand CLA b 616**



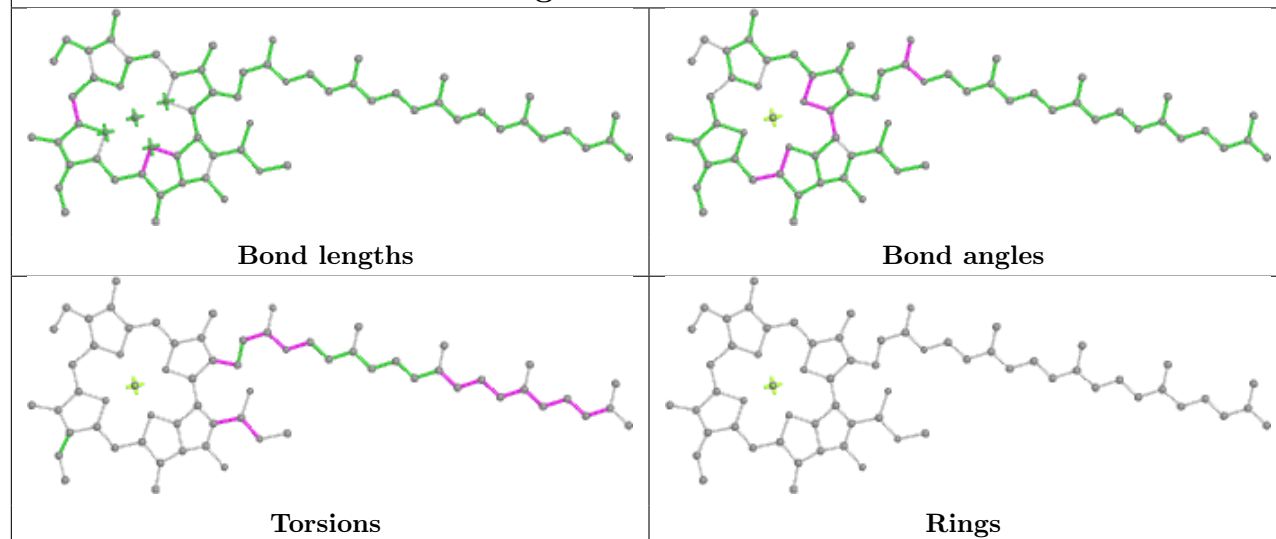
## Ligand LHG d 408



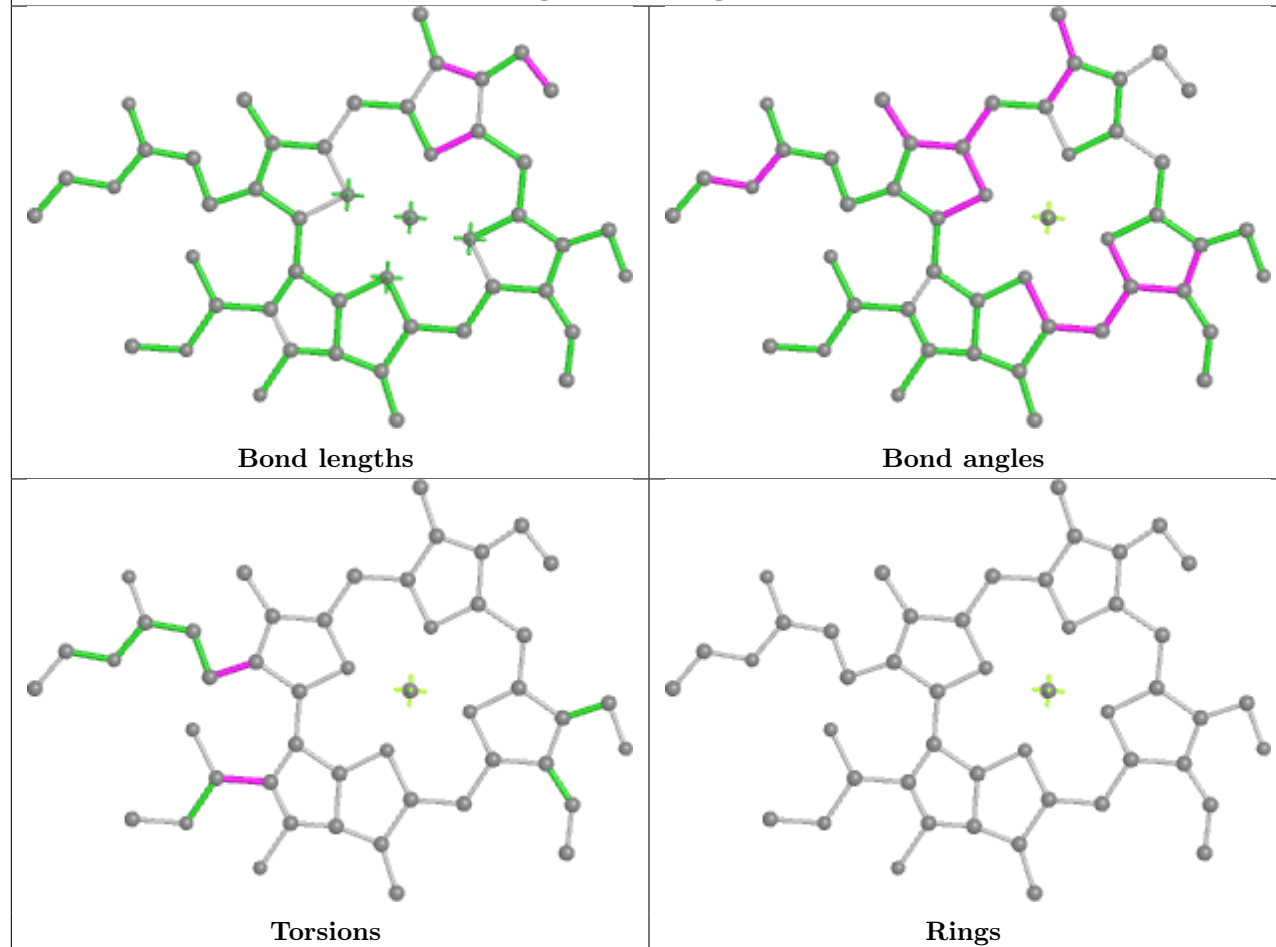
## Ligand CHL N 606



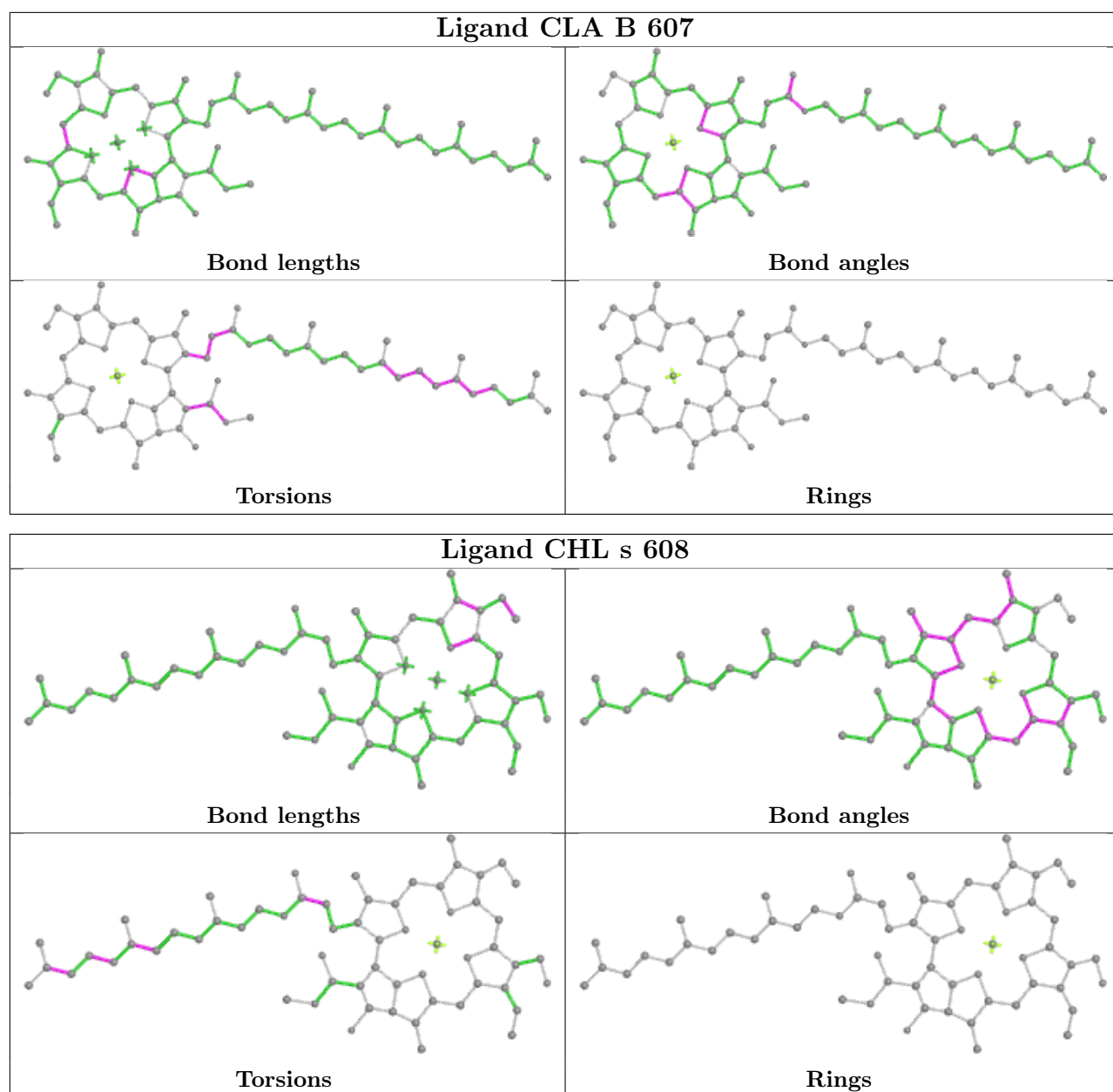
## Ligand CLA b 602

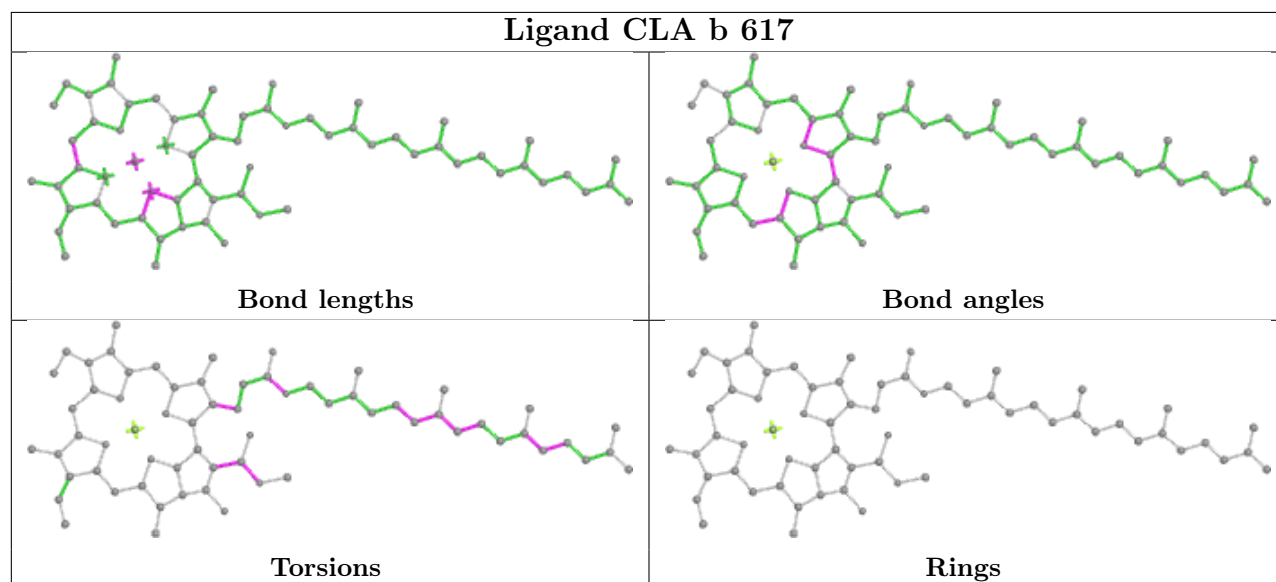
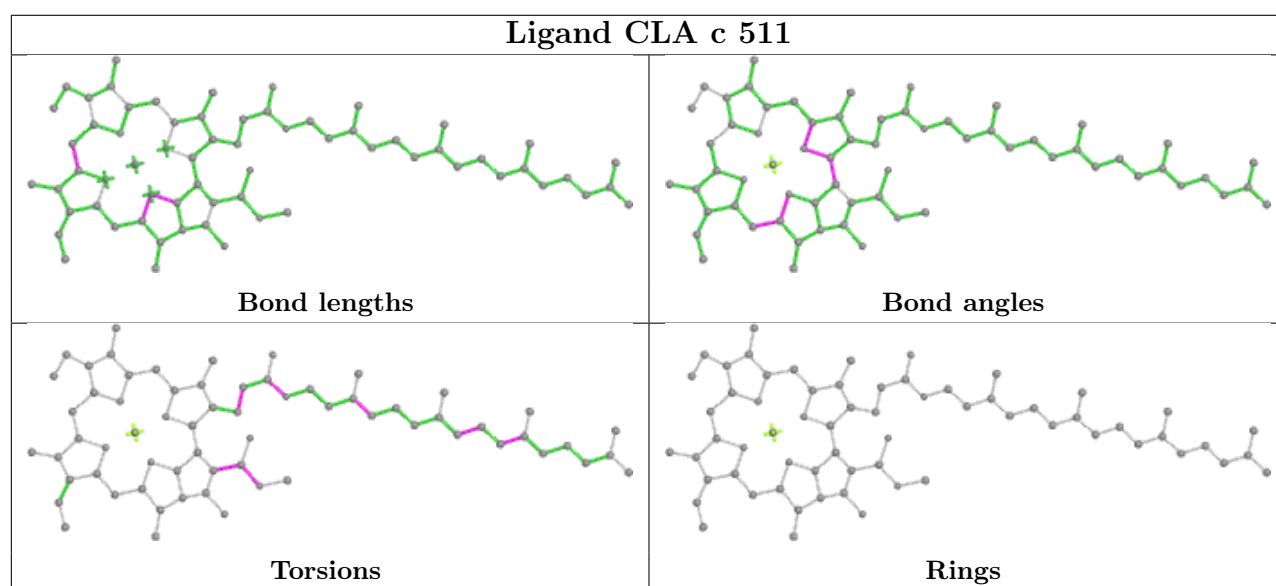
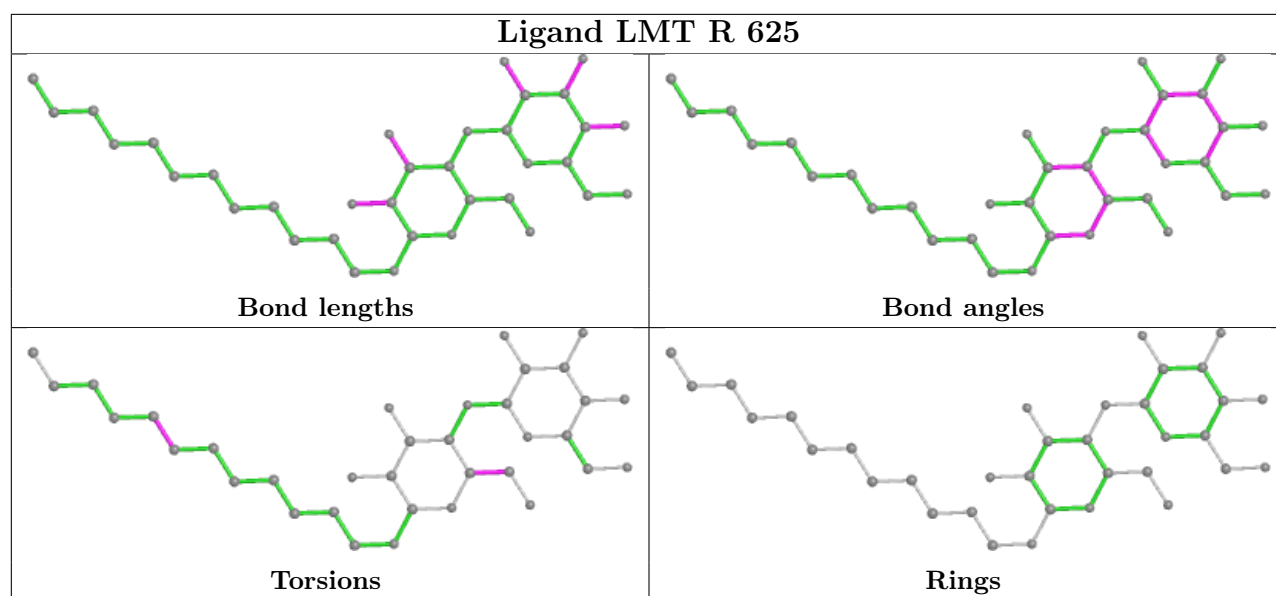


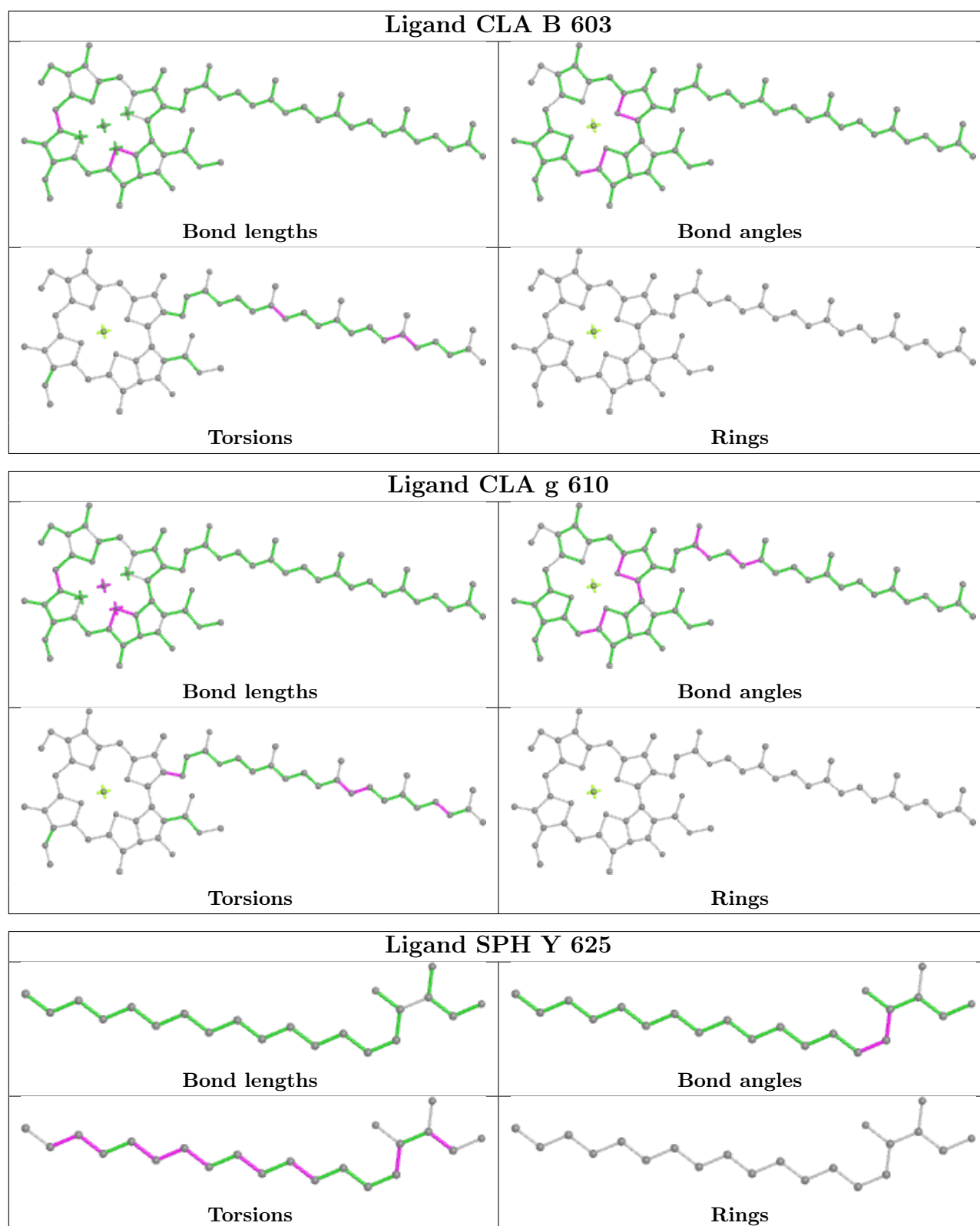
## Ligand CHL g 605



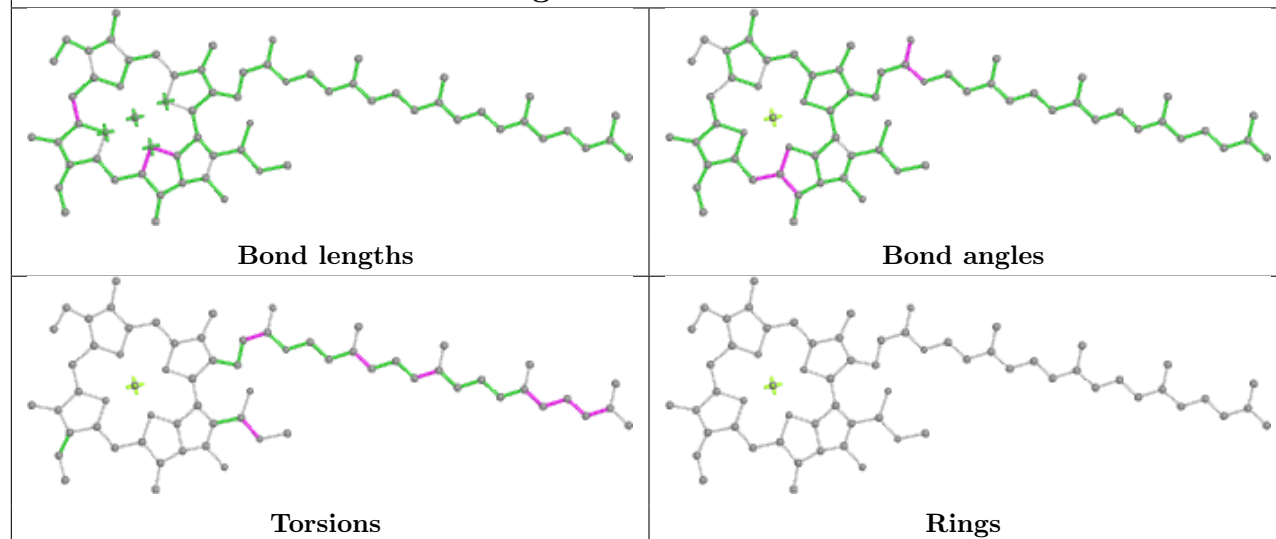




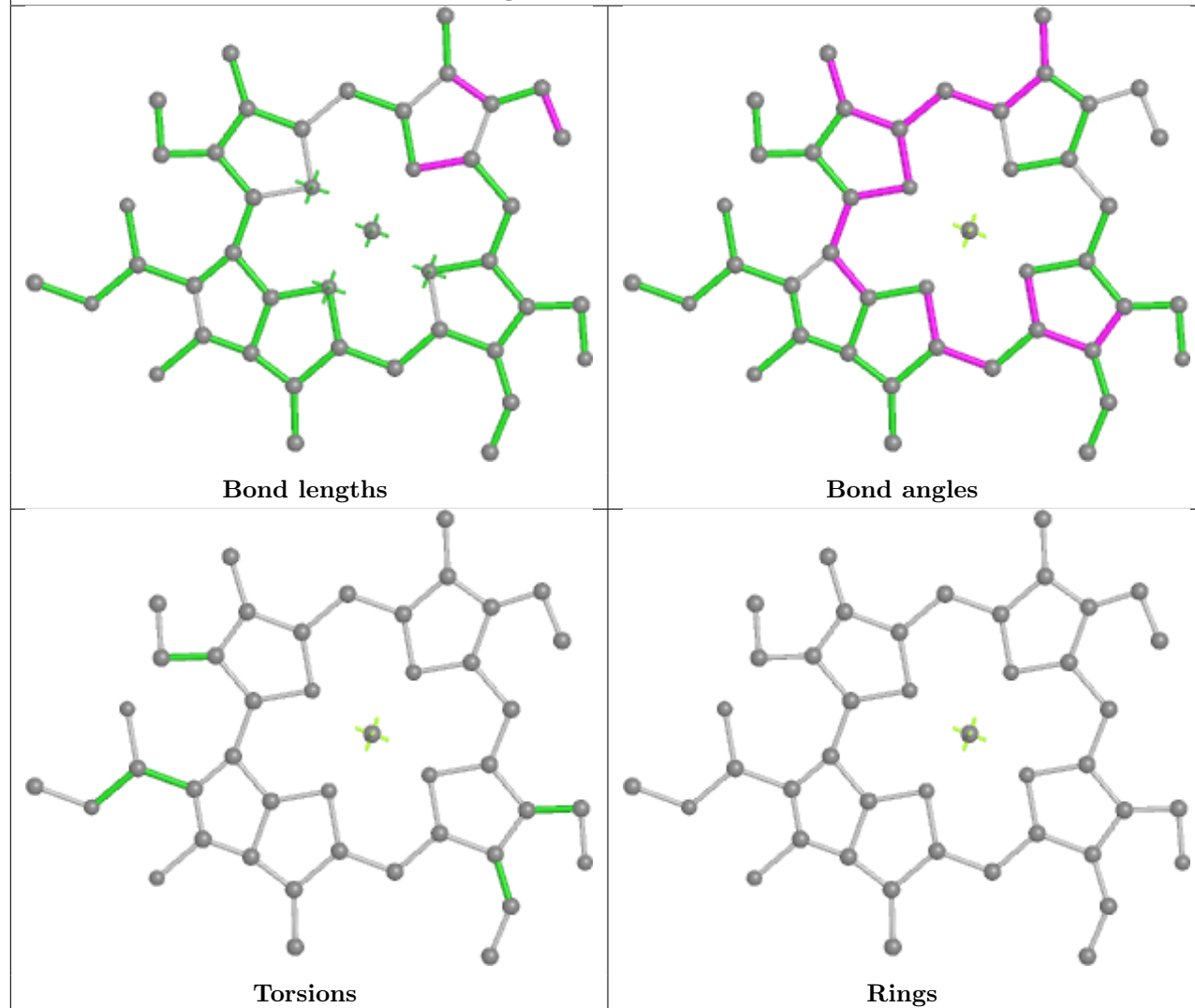


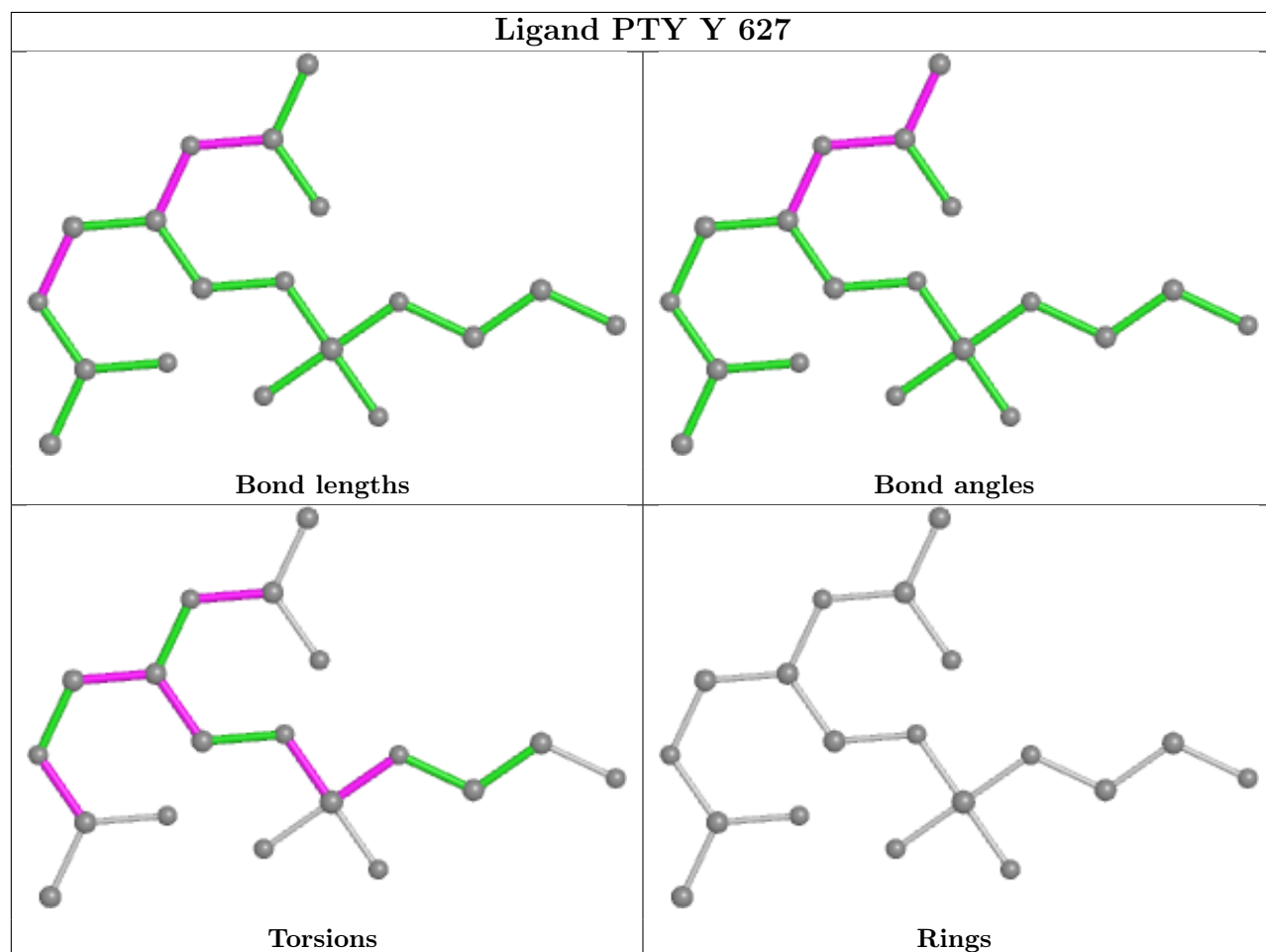
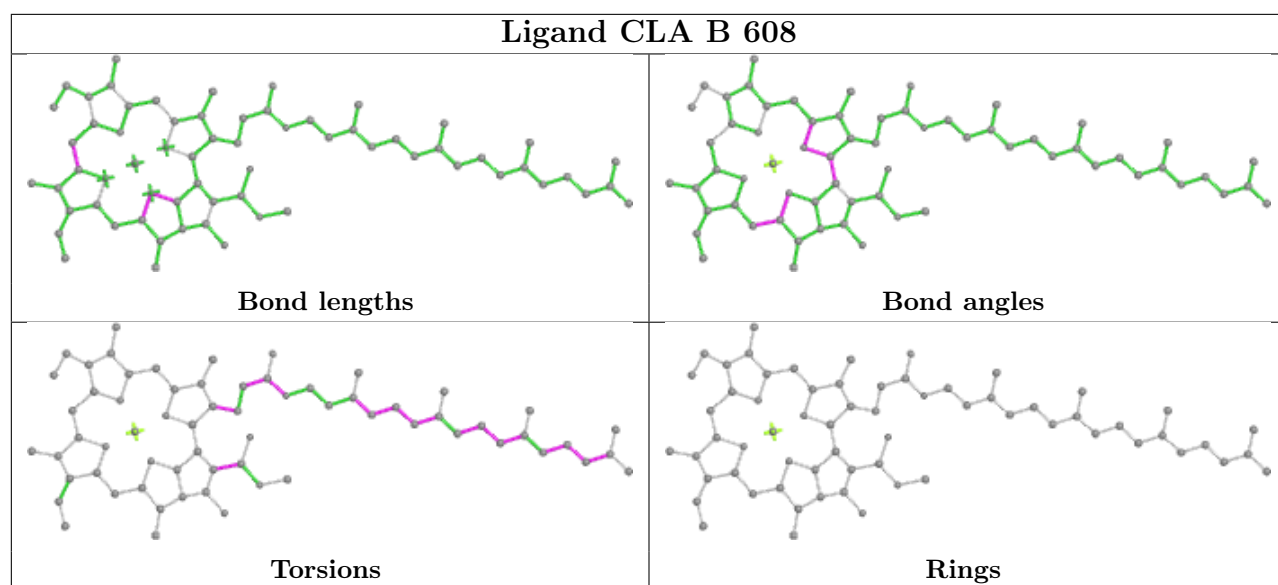


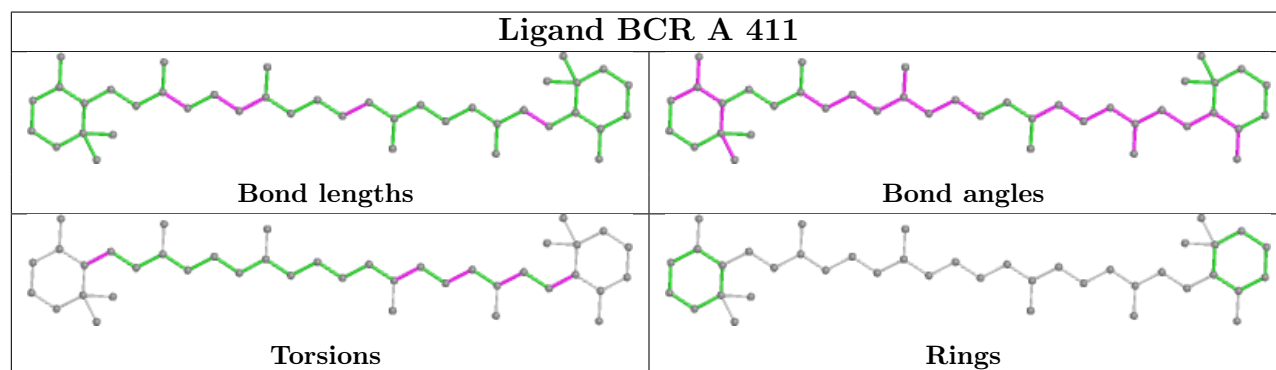
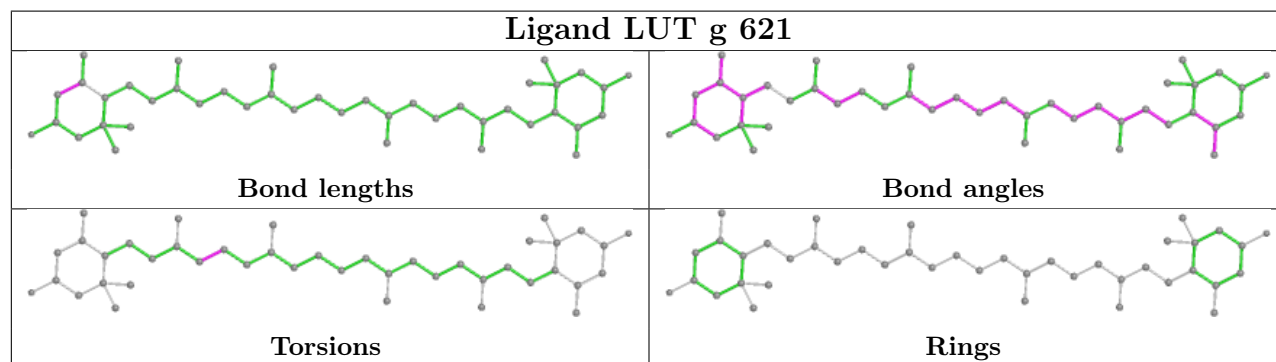
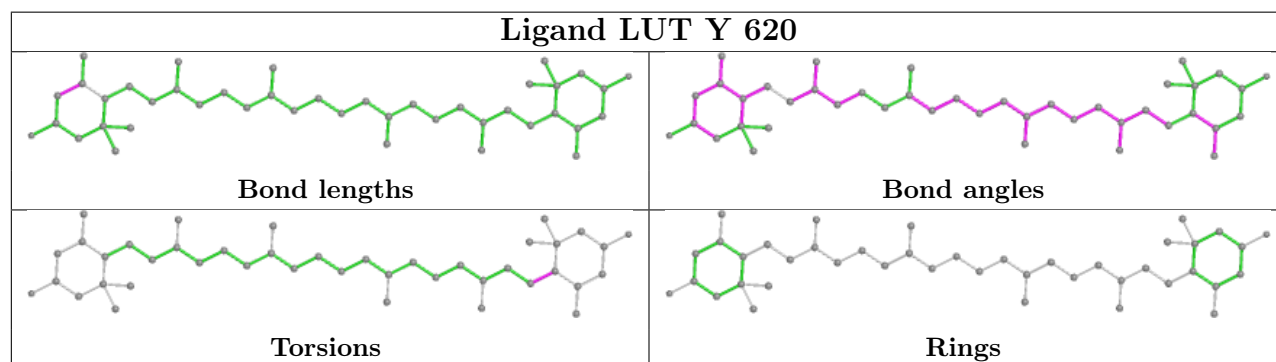
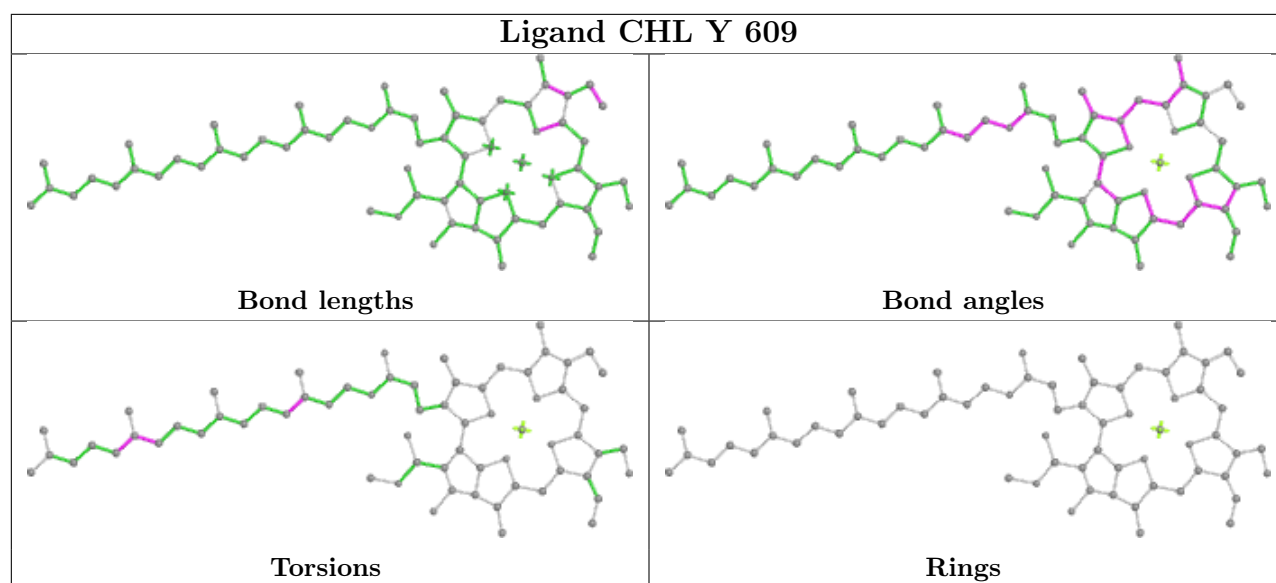
## Ligand CLA C 510



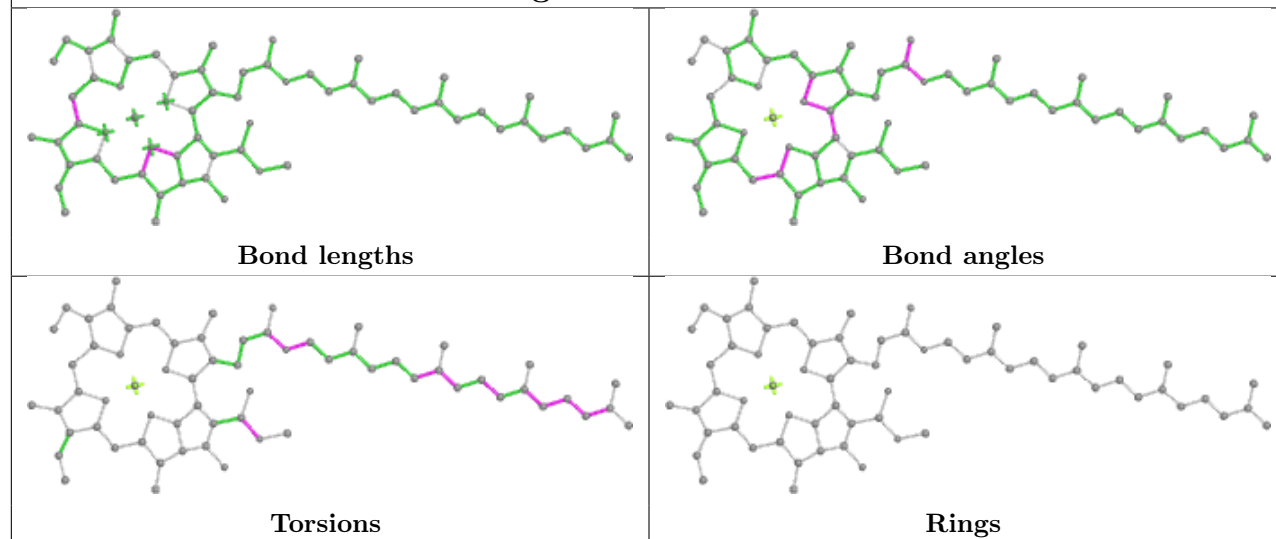
## Ligand CHL S 607



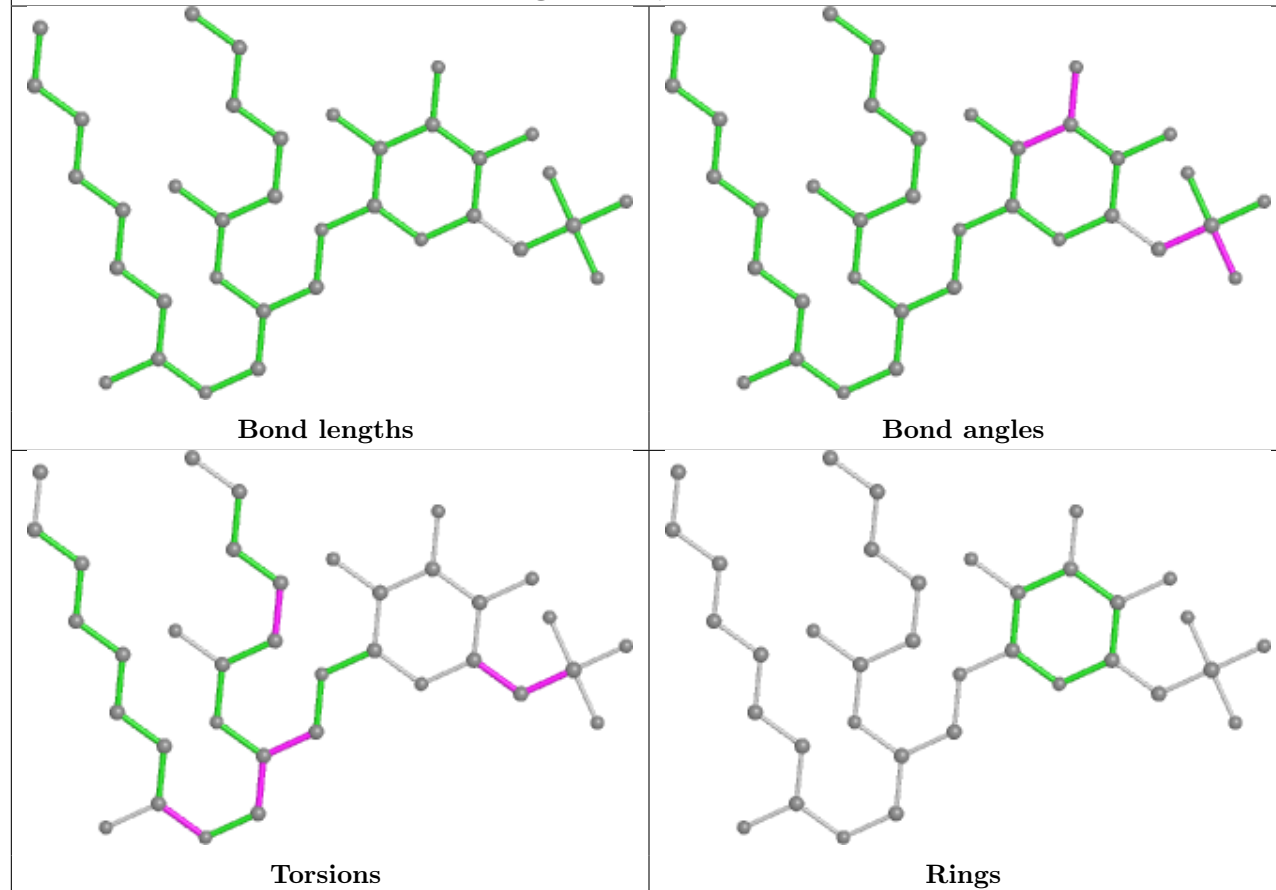




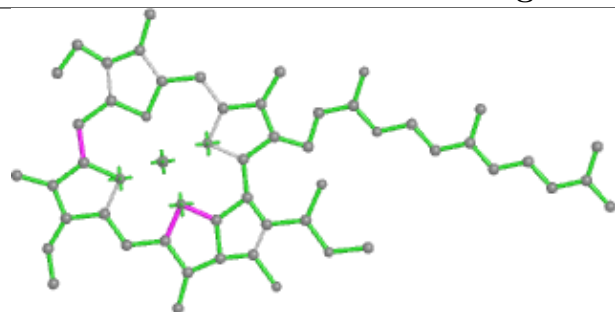
## Ligand CLA C 509



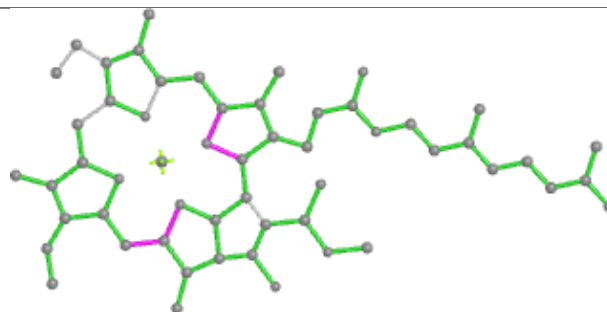
## Ligand SQD C 526



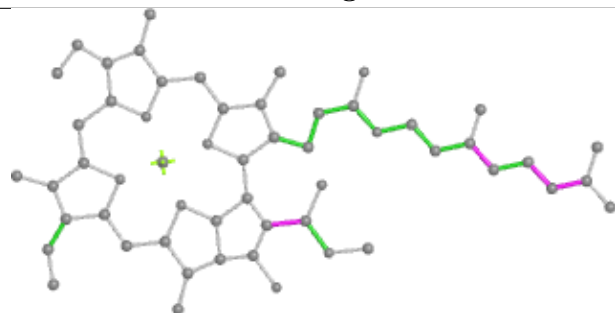
## Ligand CLA C 504



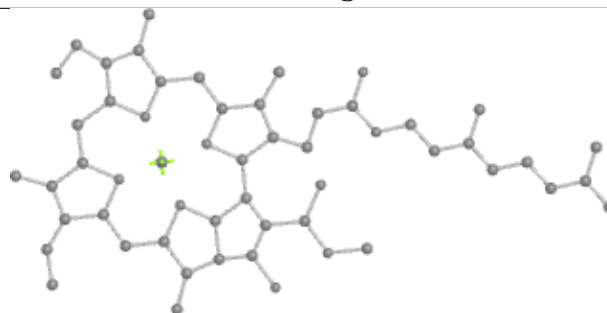
Bond lengths



Bond angles

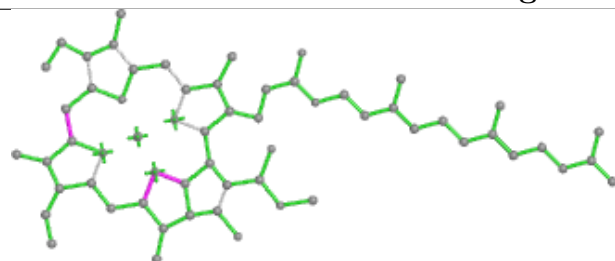


Torsions

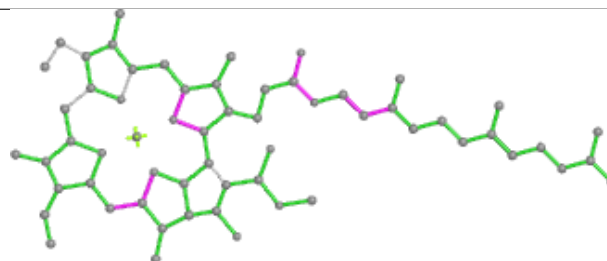


Rings

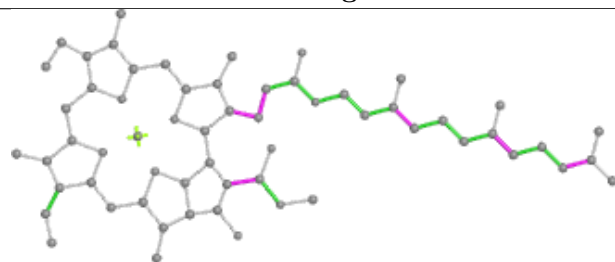
## Ligand CLA S 602



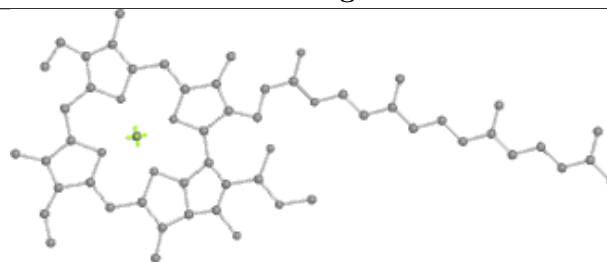
Bond lengths



Bond angles



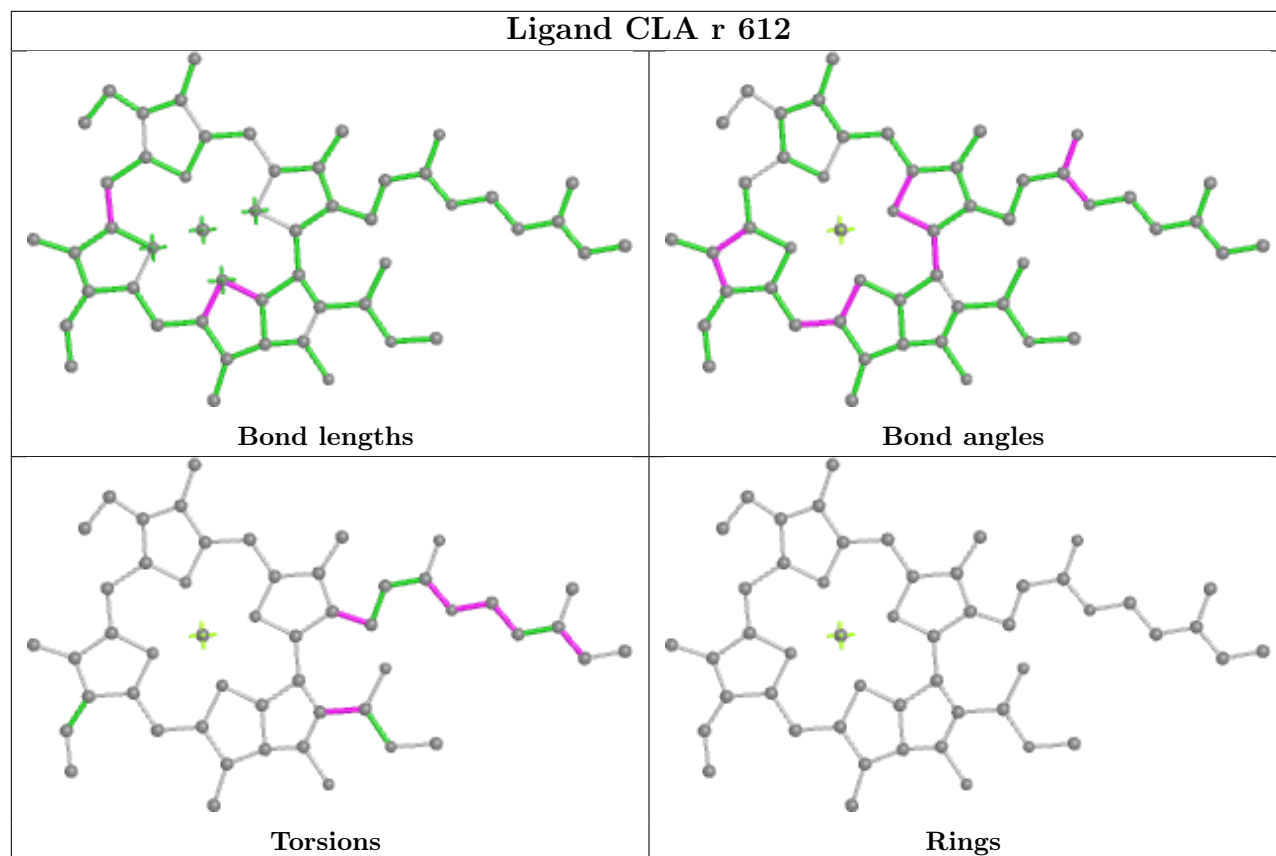
Torsions



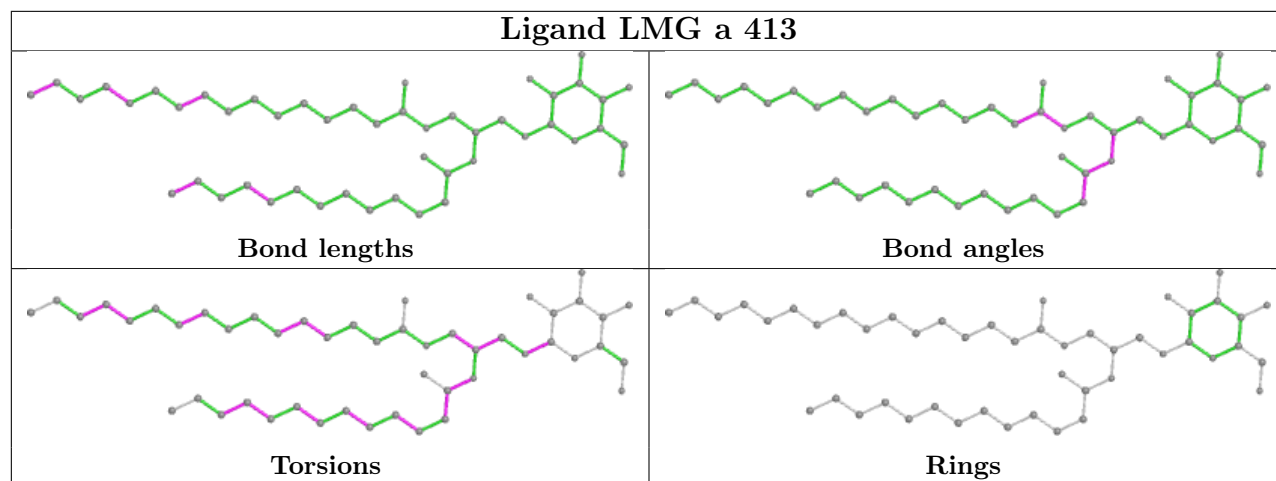
Rings

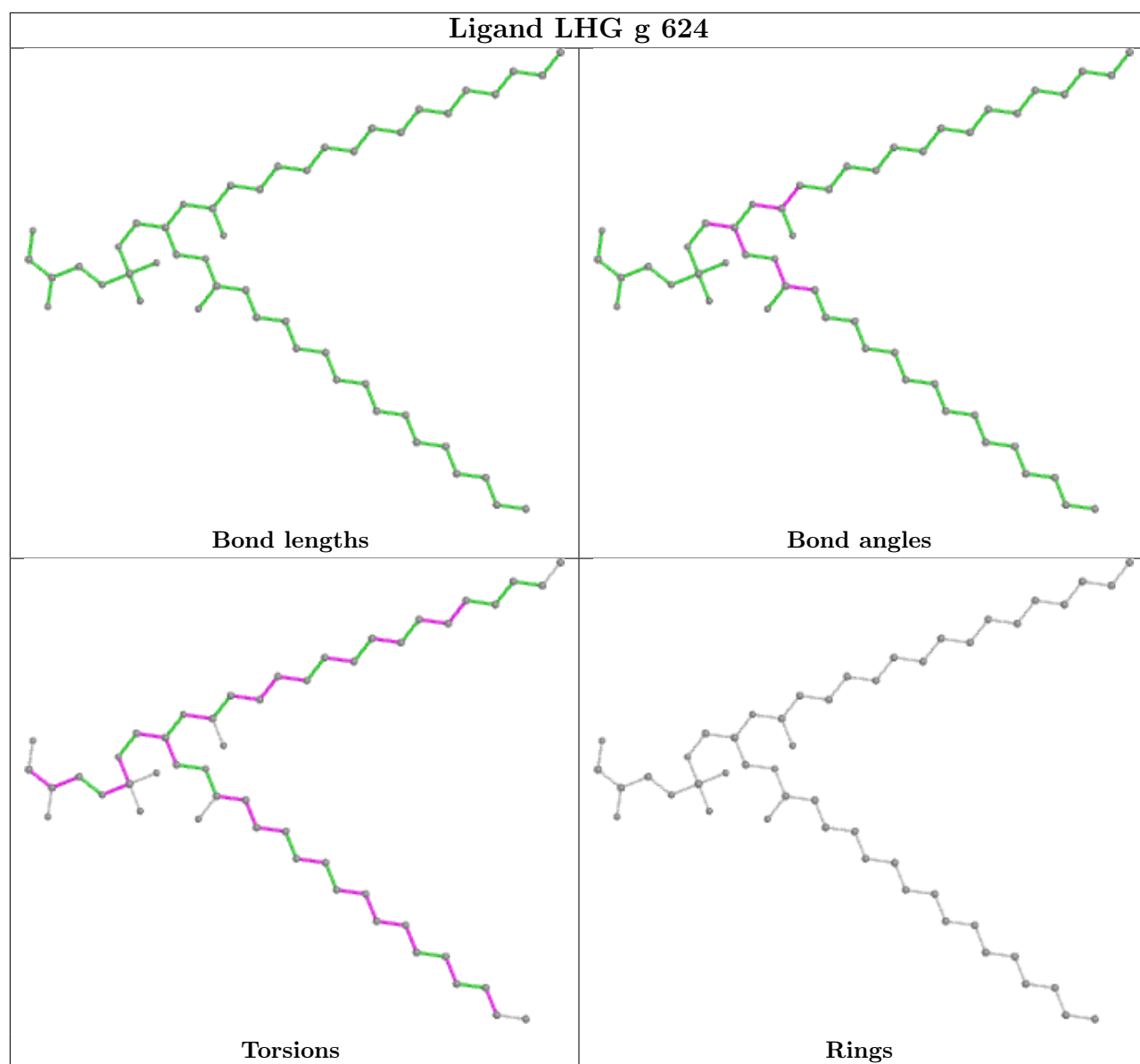


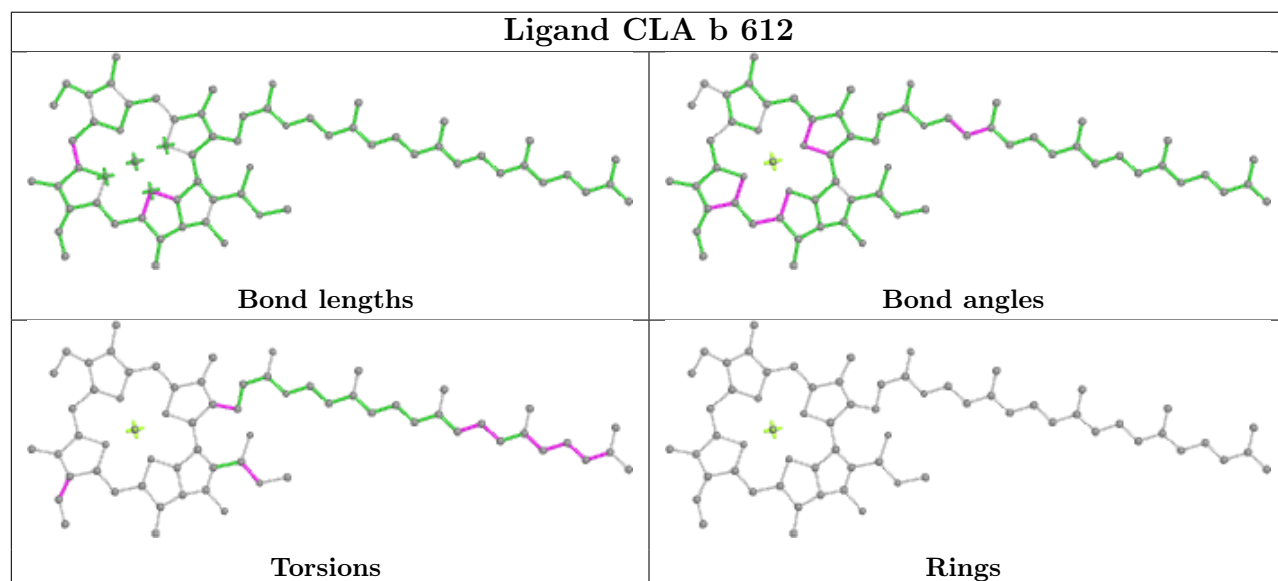
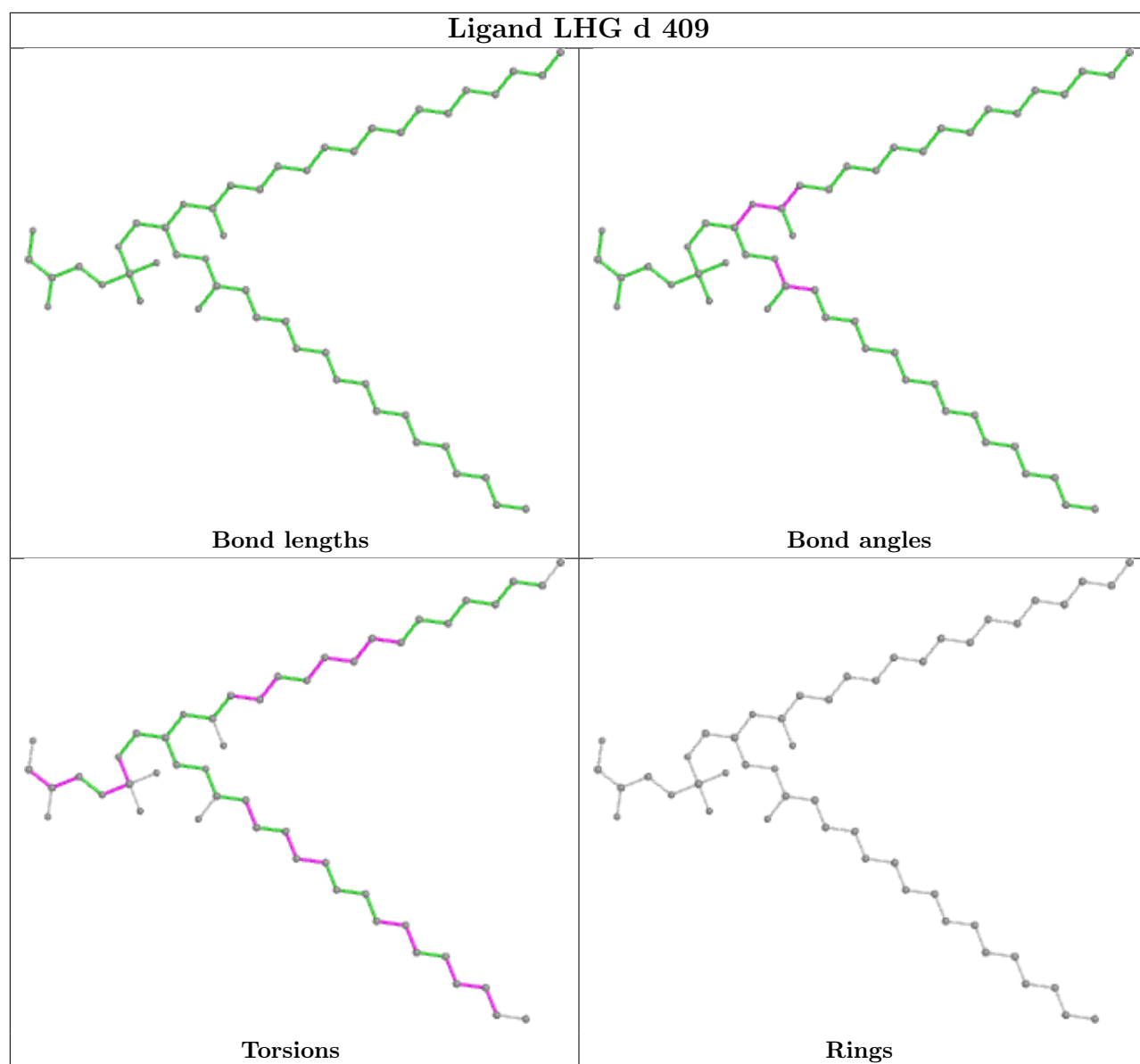
## Ligand CLA r 612

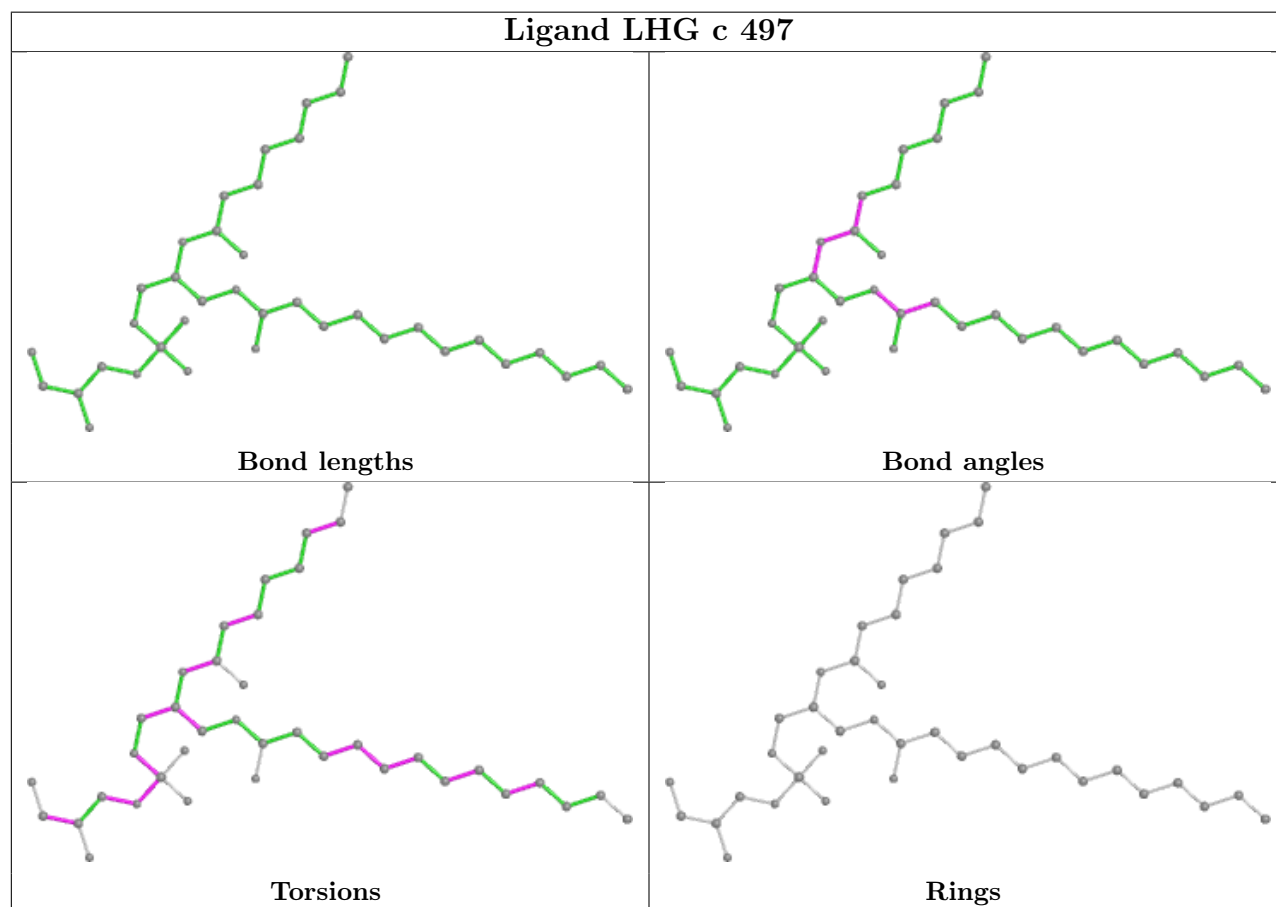
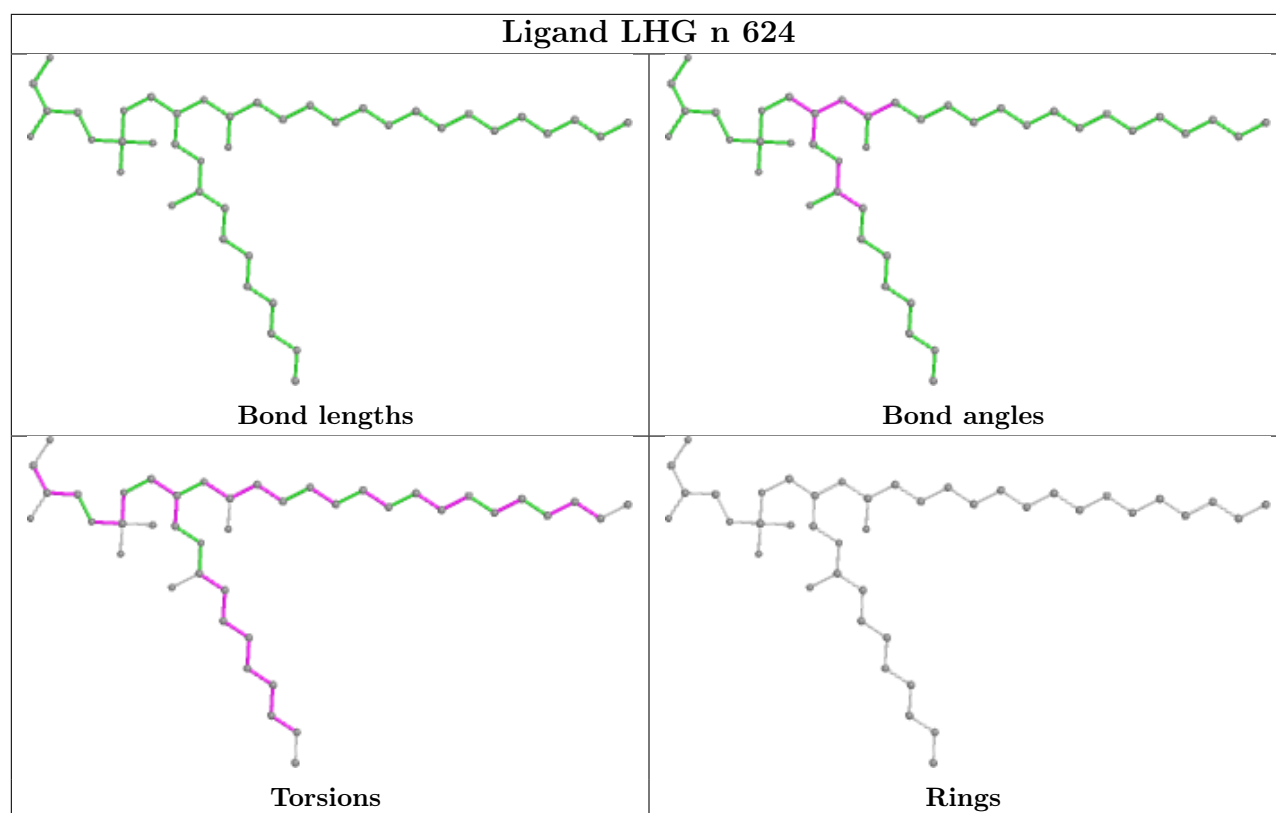


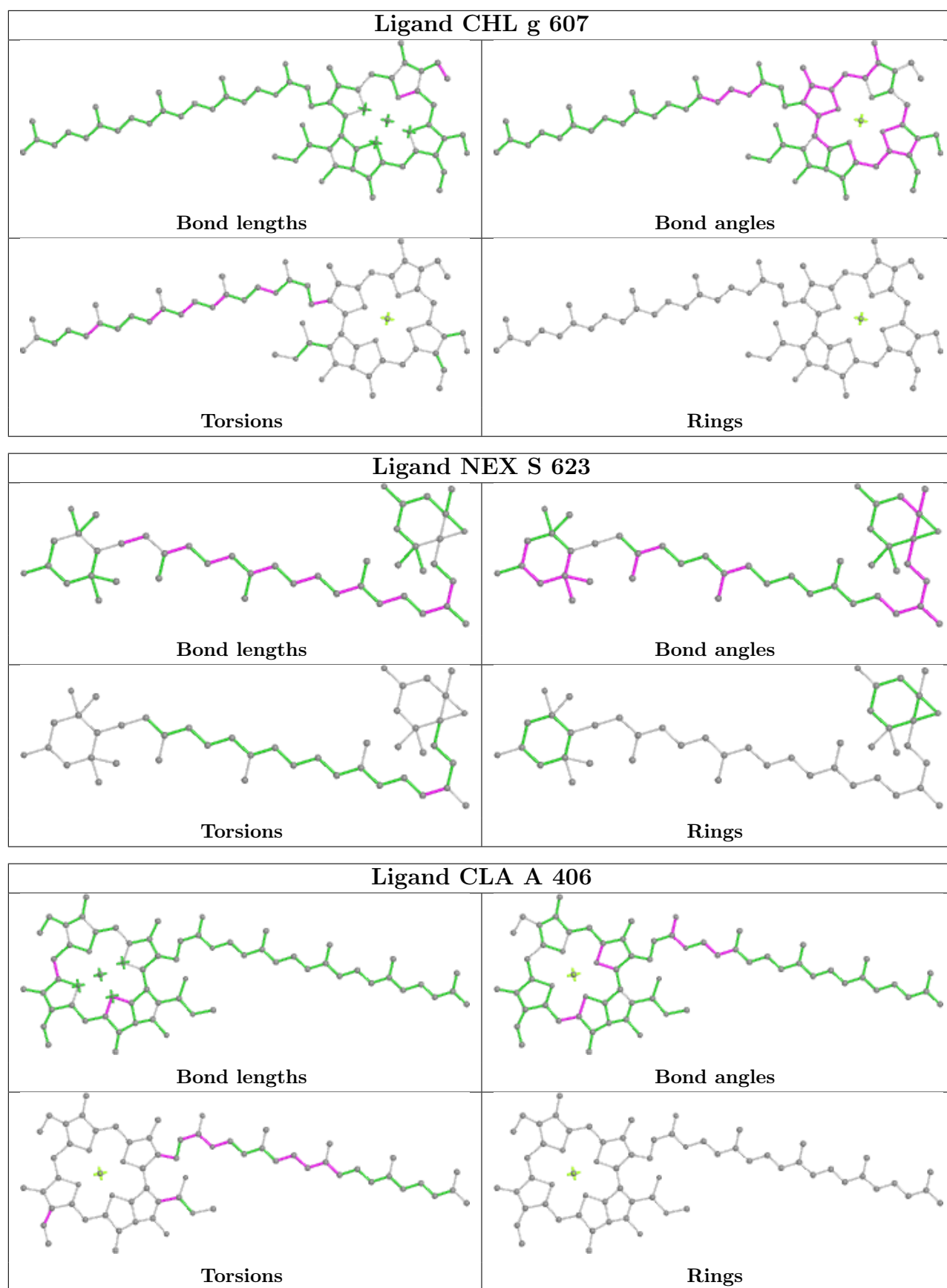
## Ligand LMG a 413



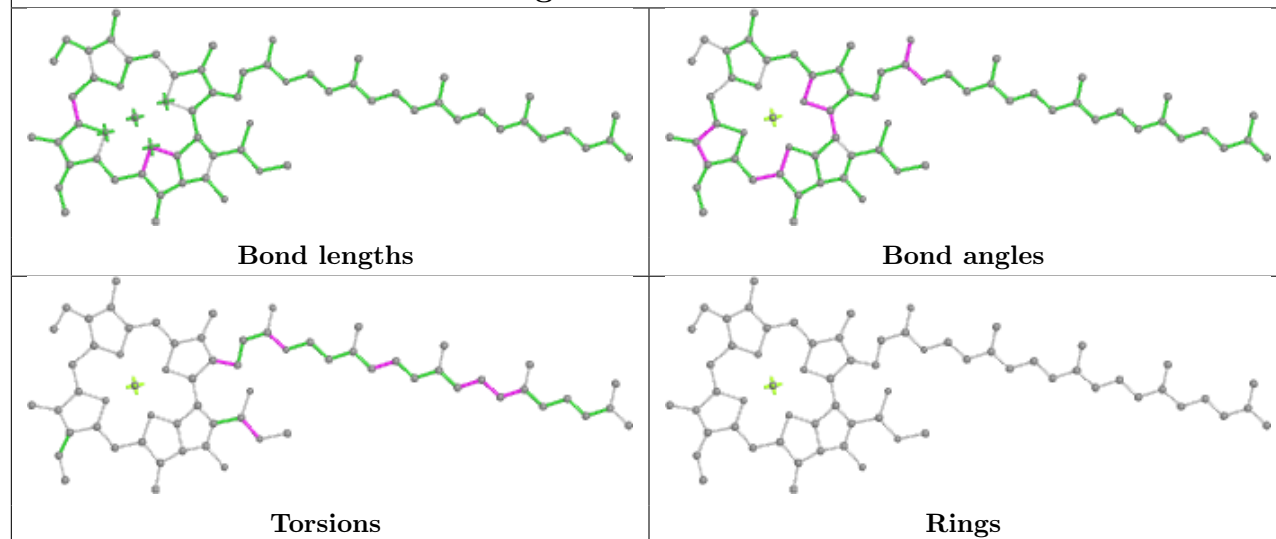




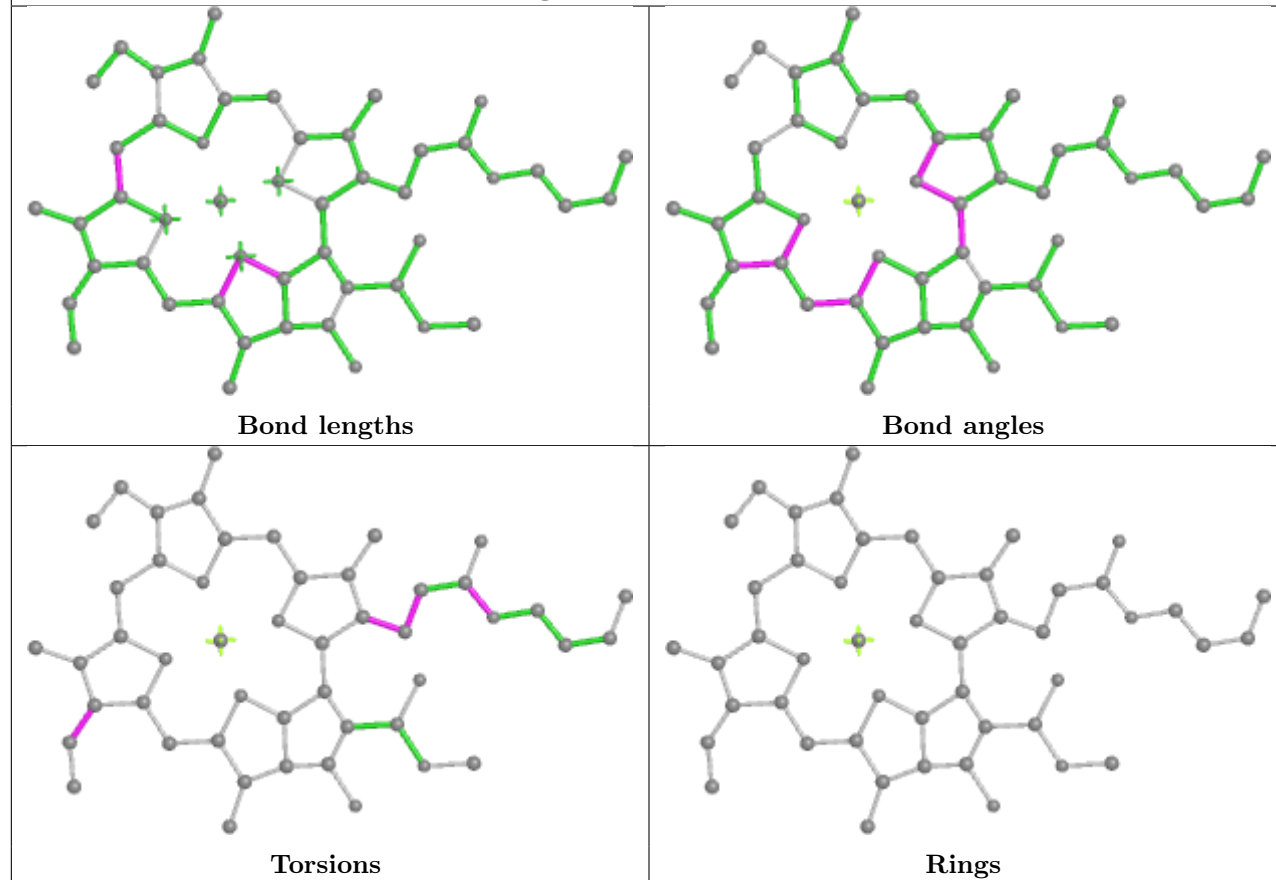


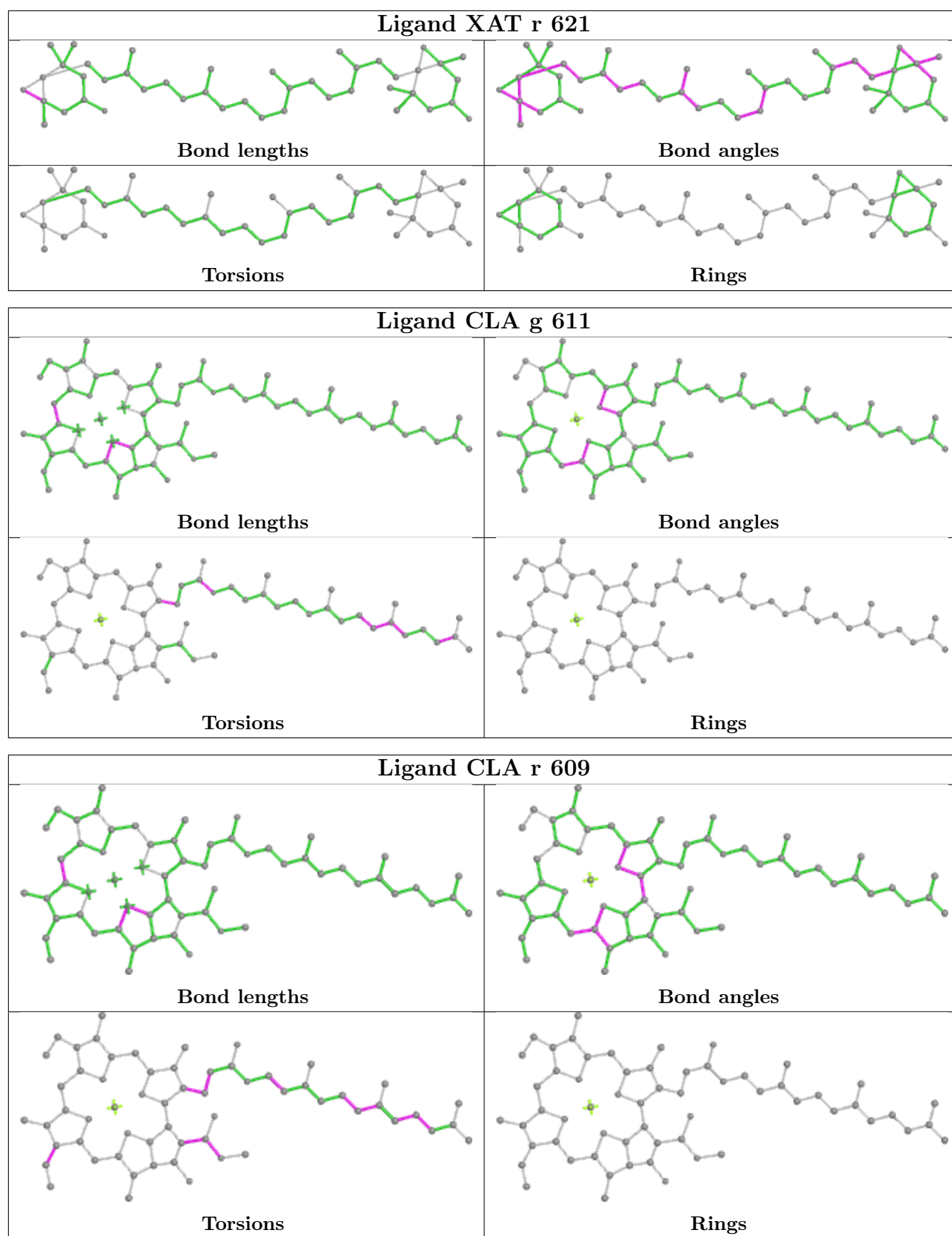


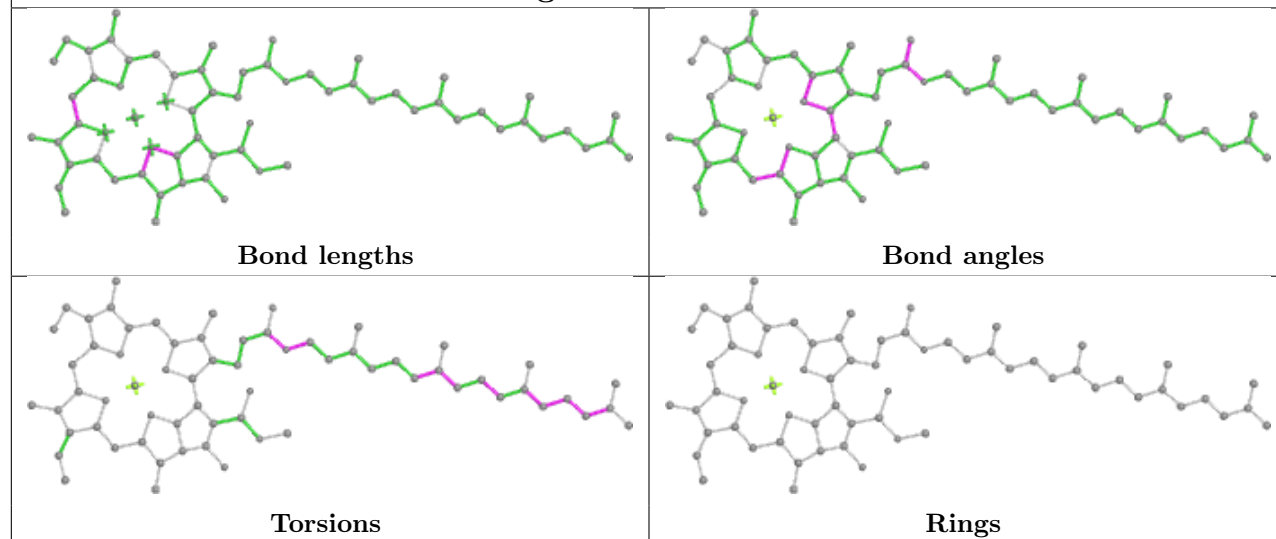
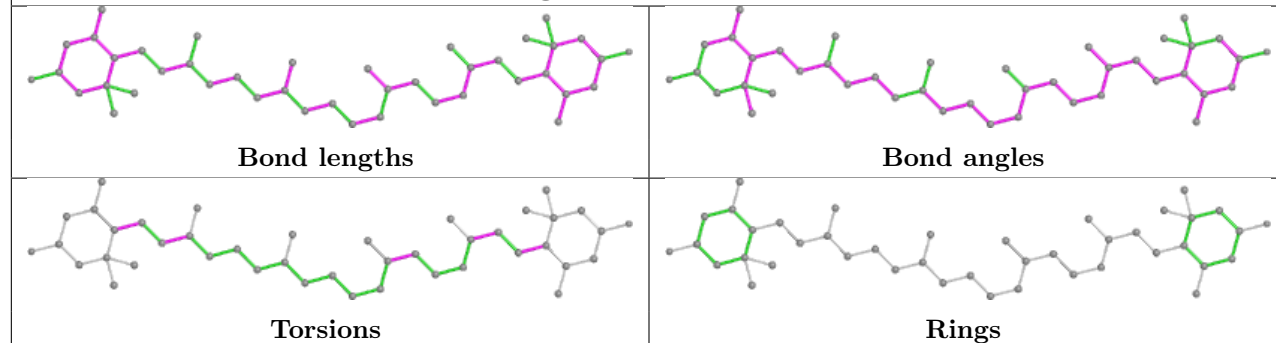
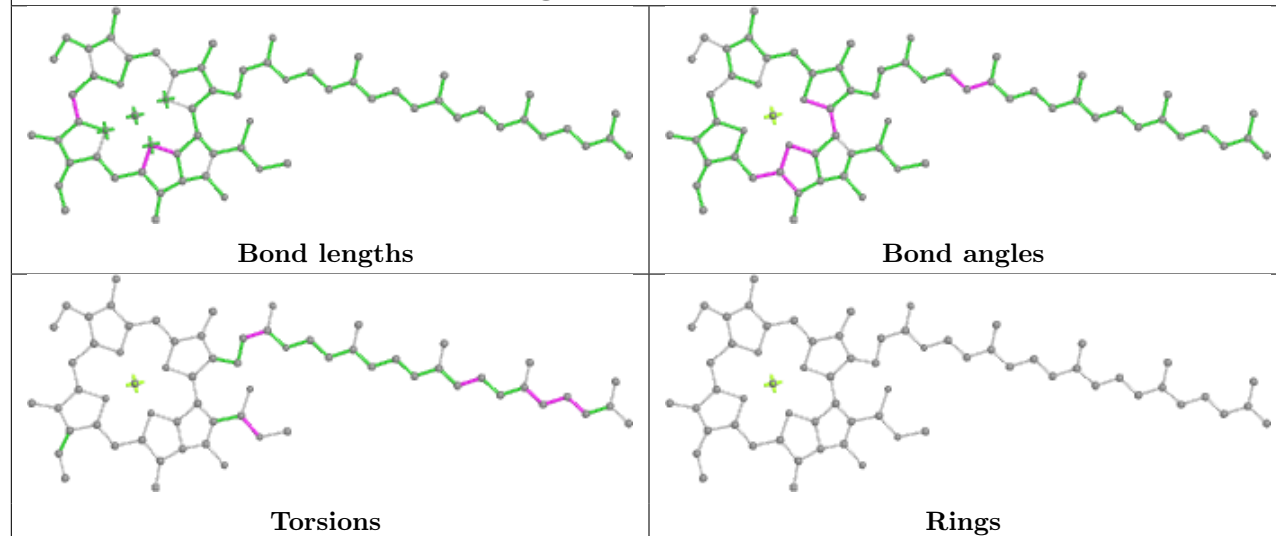
## Ligand CLA d 403



## Ligand CLA a 407

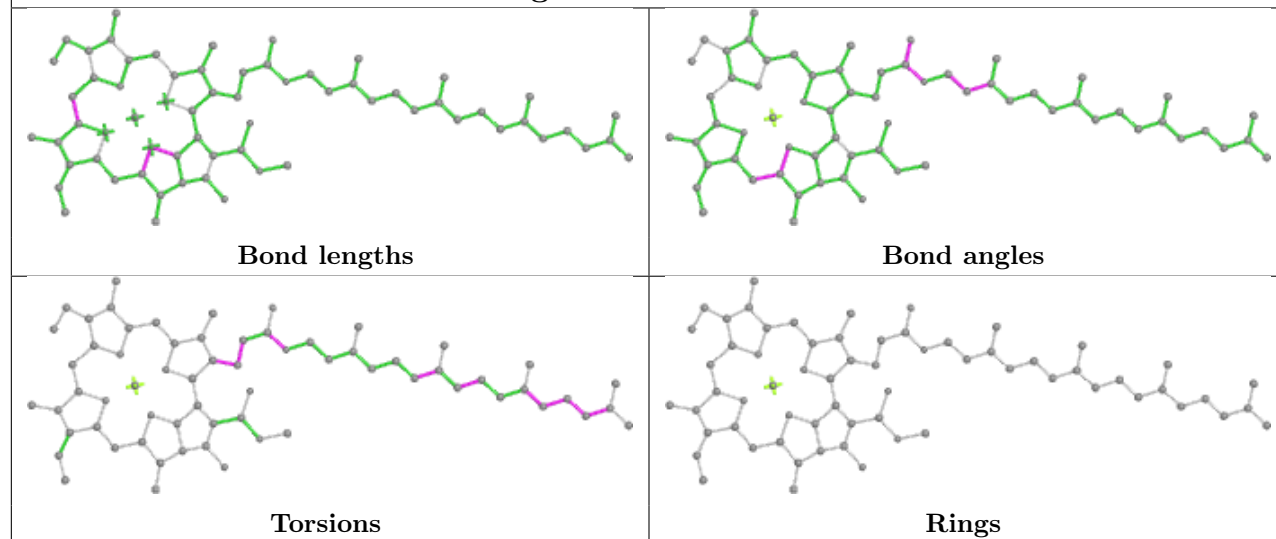




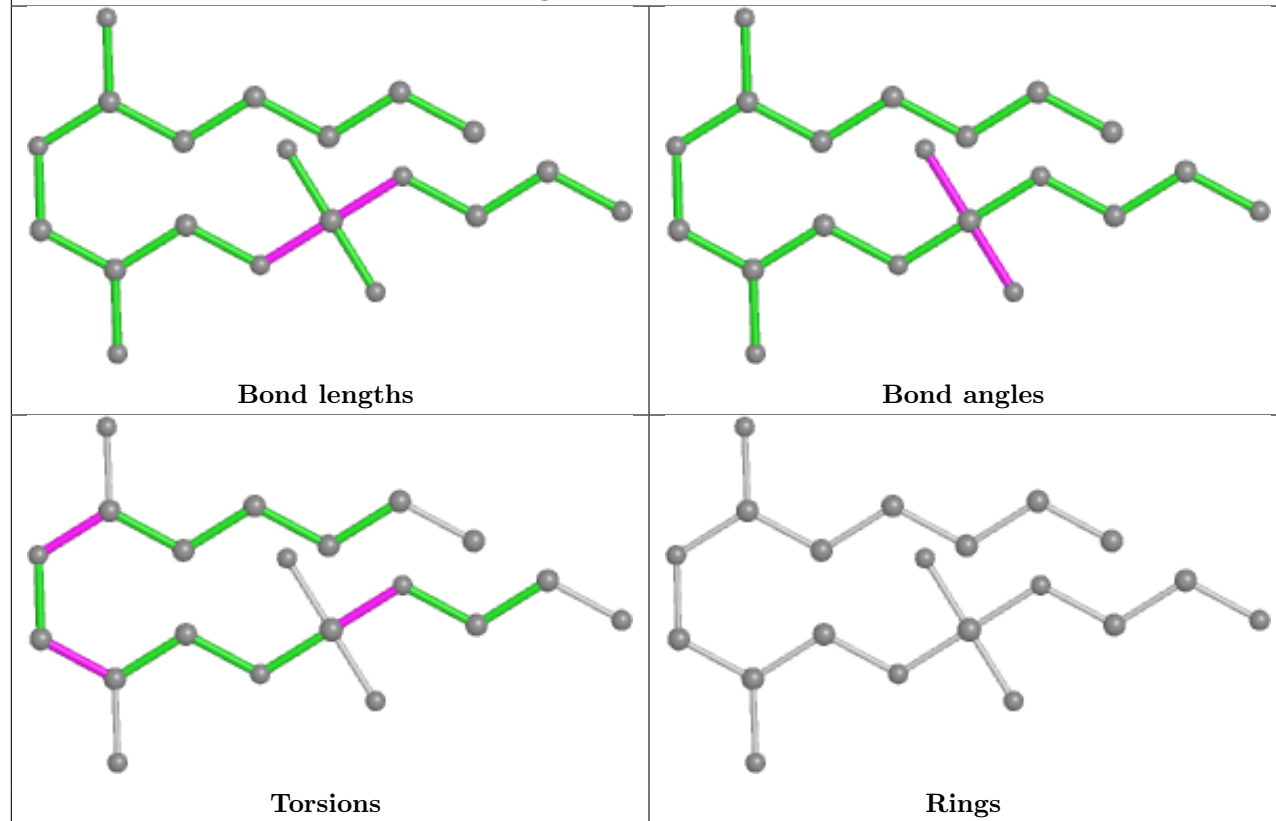
**Ligand CLA c 509****Ligand C7Z B 620****Ligand CLA c 510**

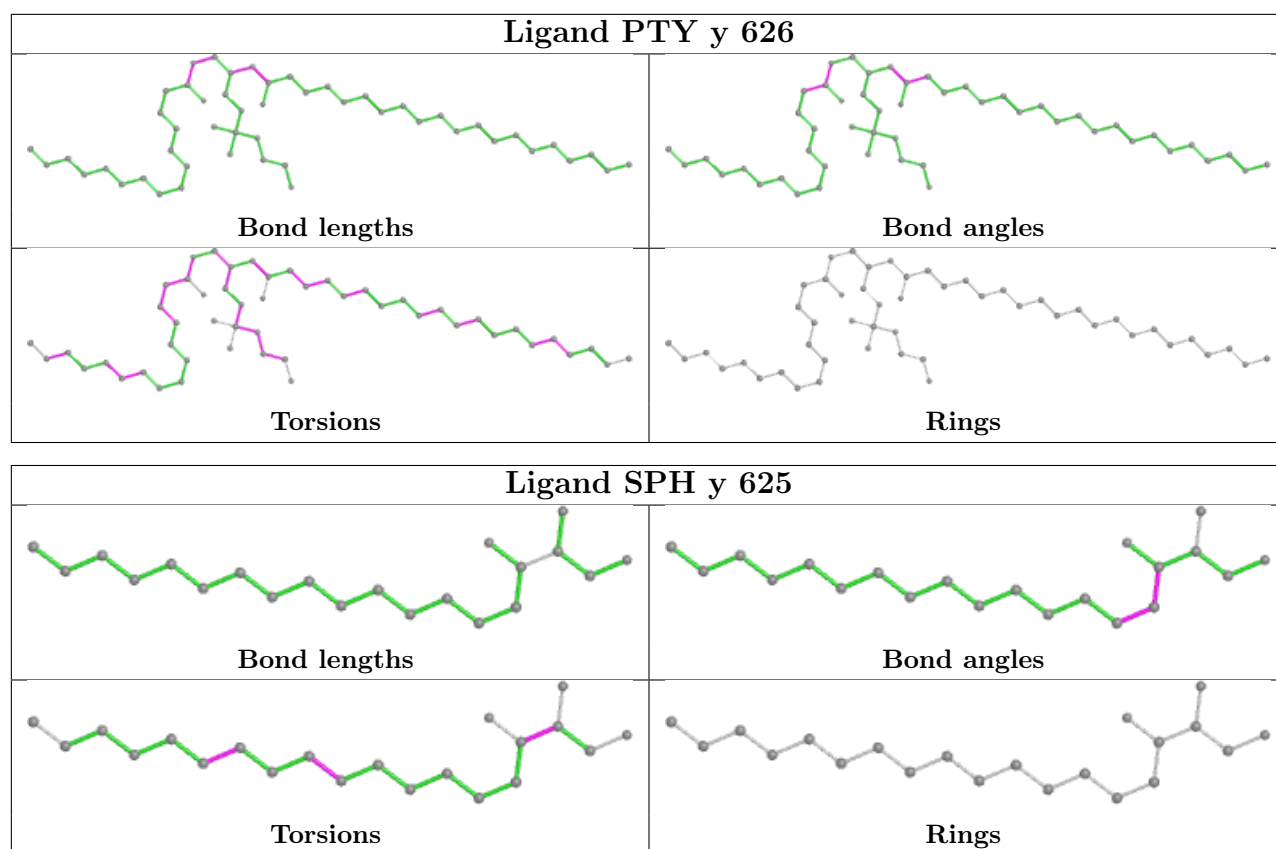


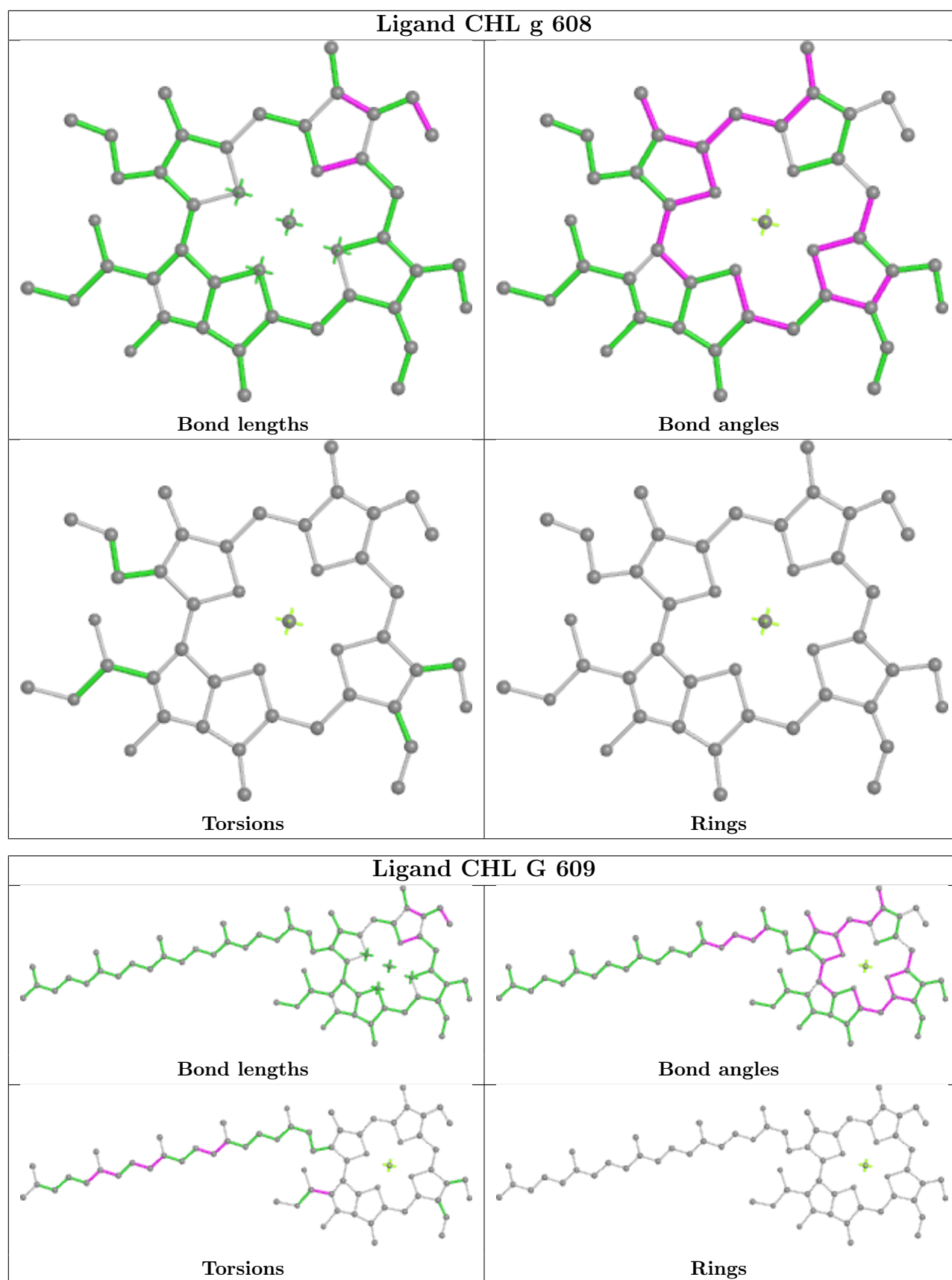
## Ligand CLA G 602

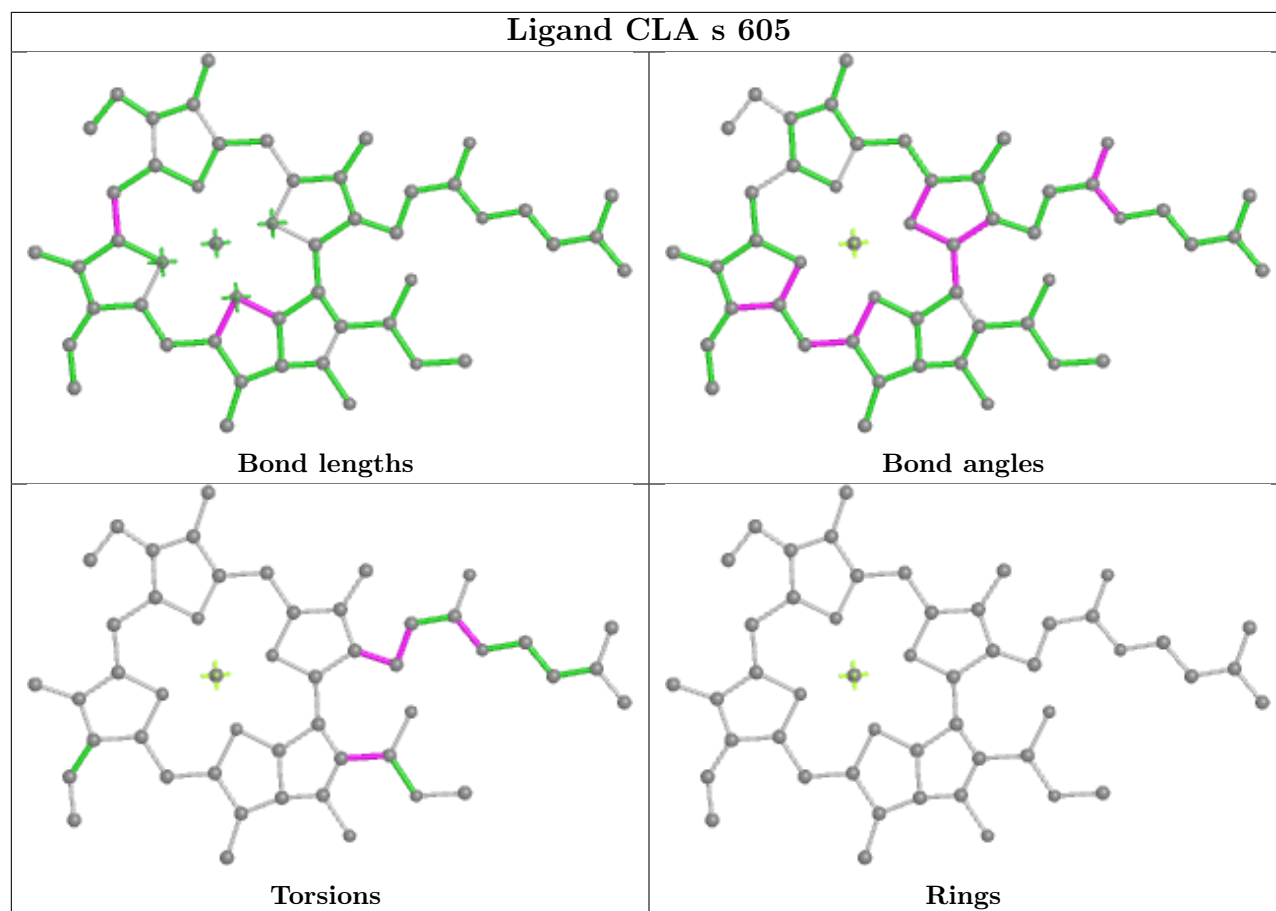
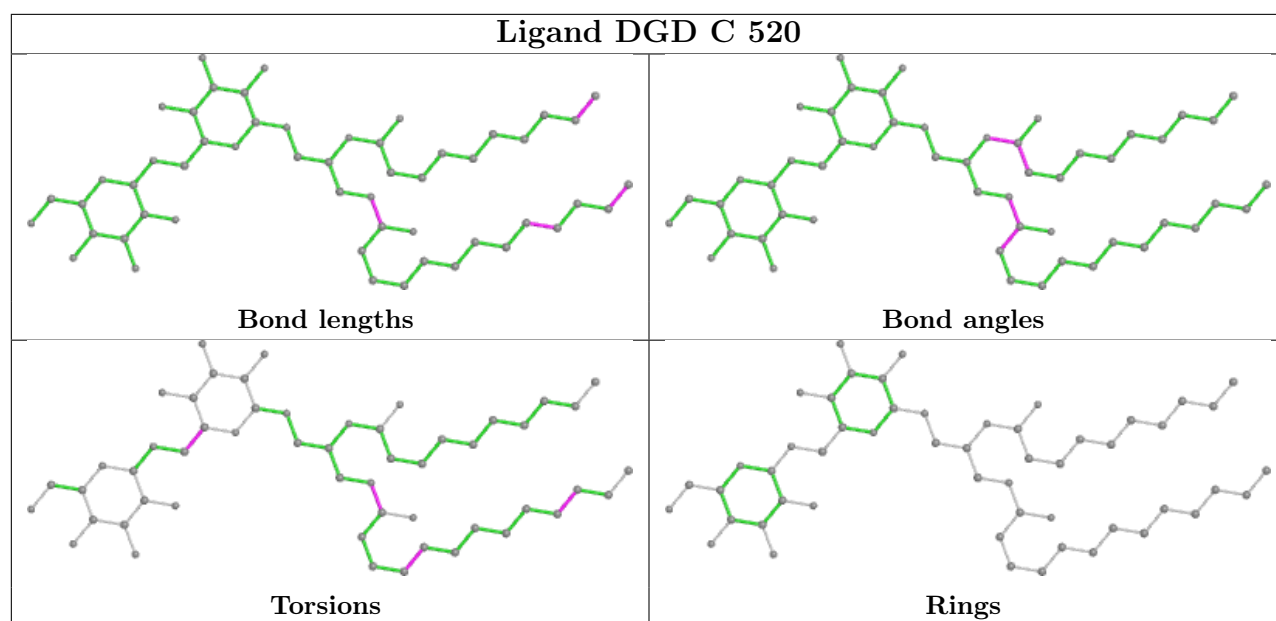


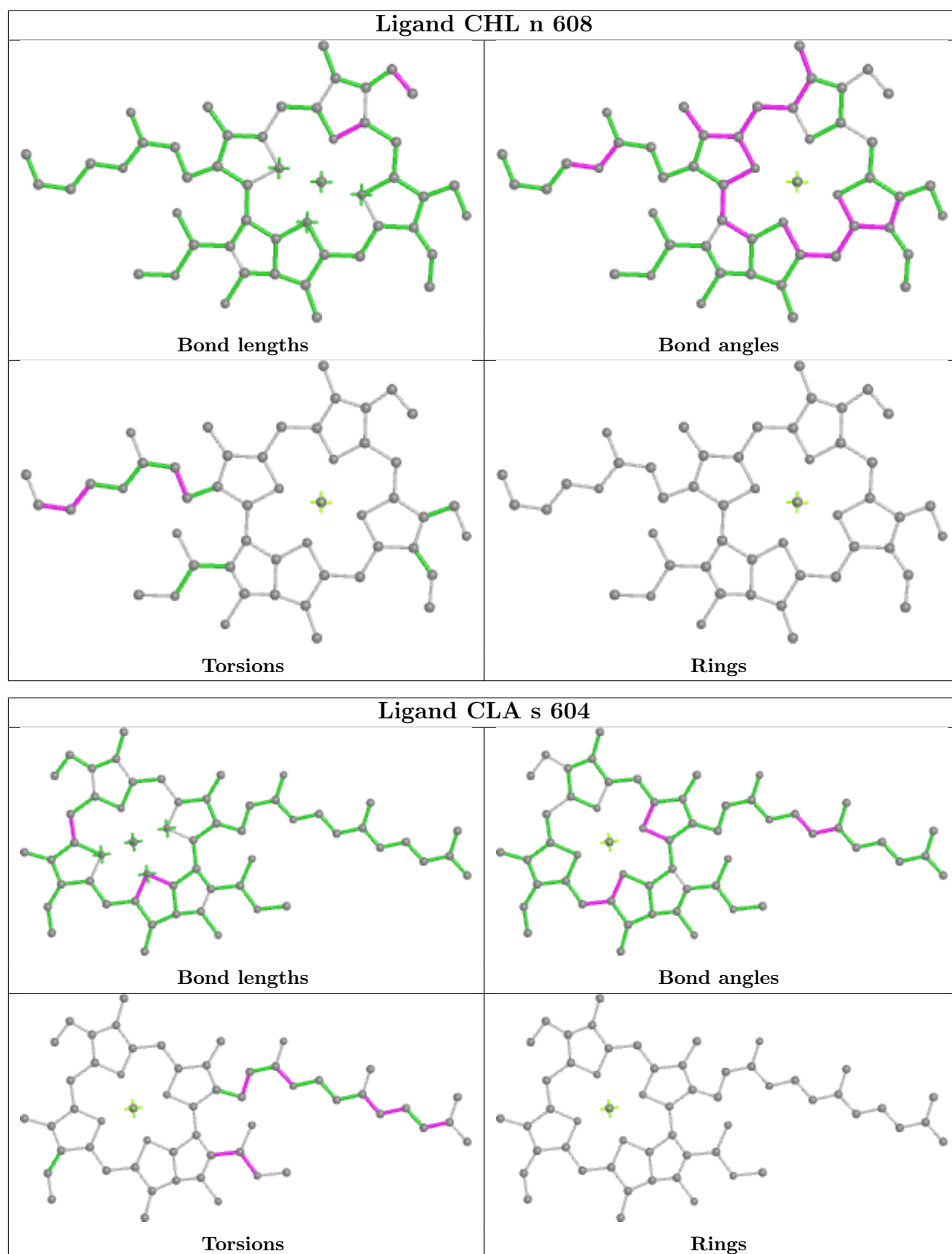
## Ligand LPX S 625

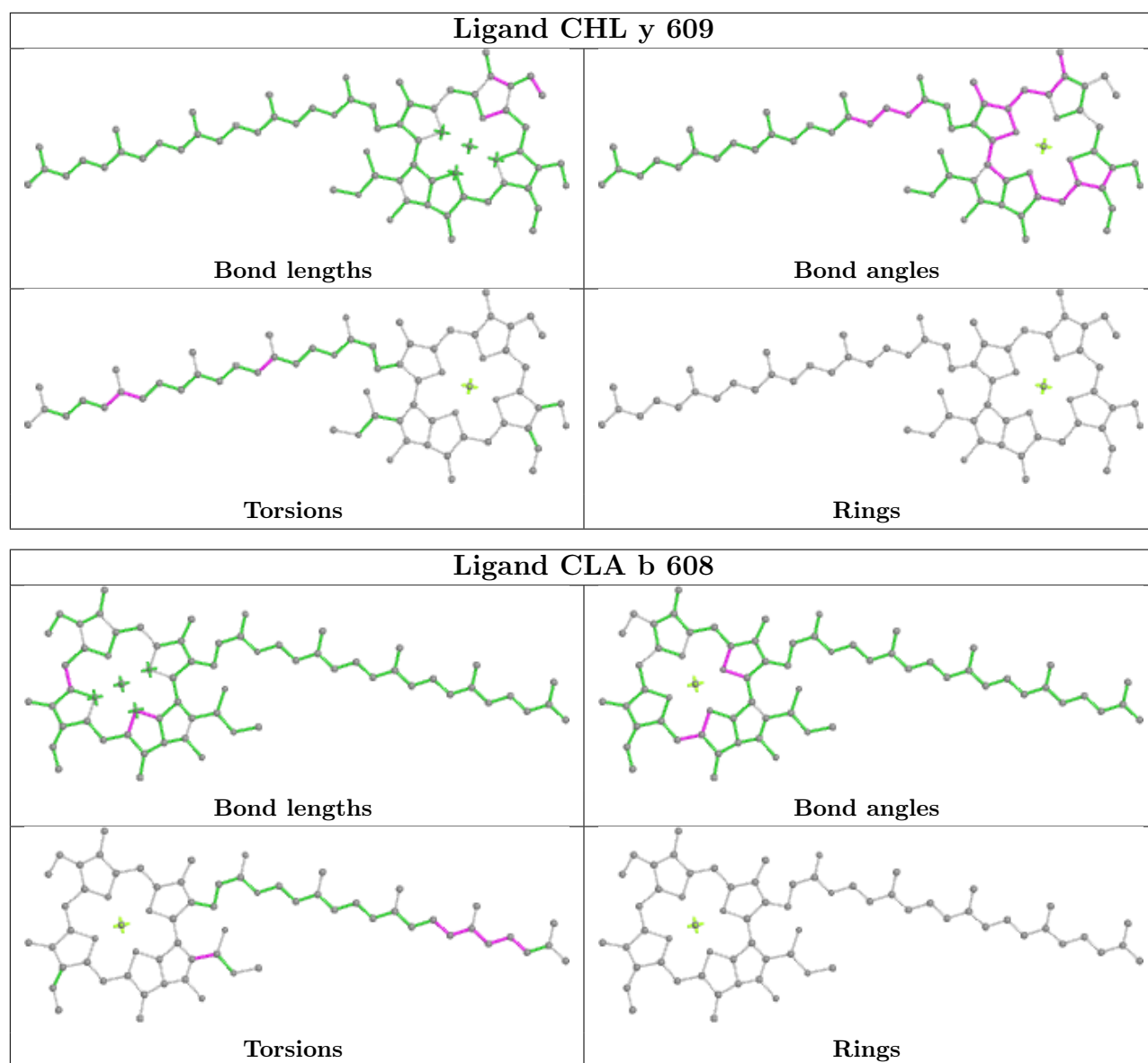


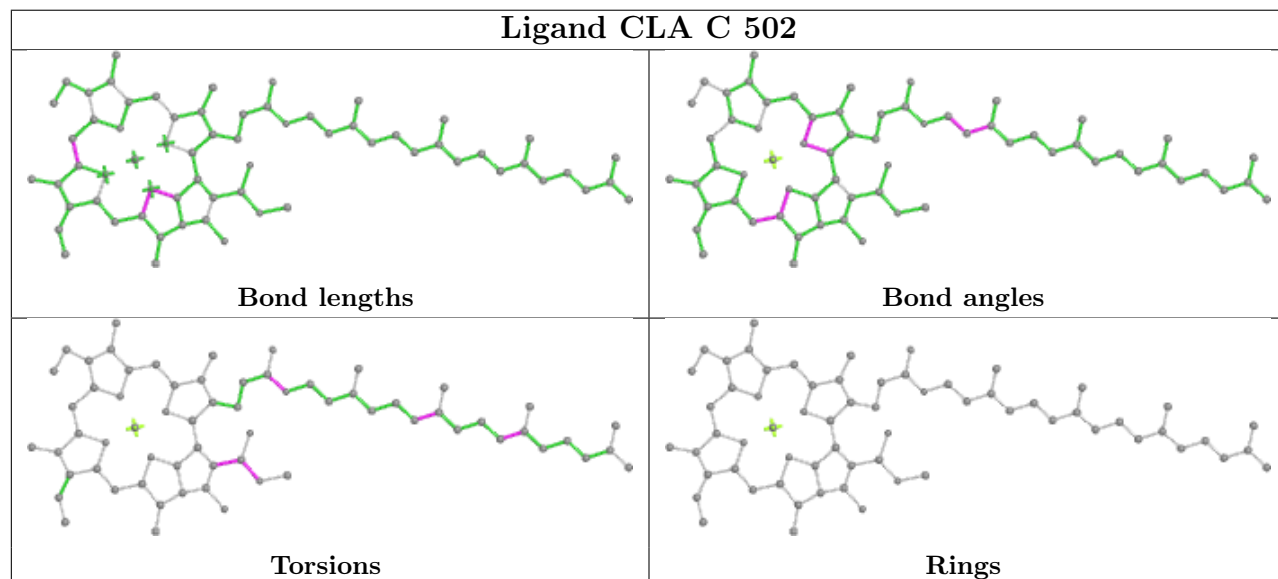
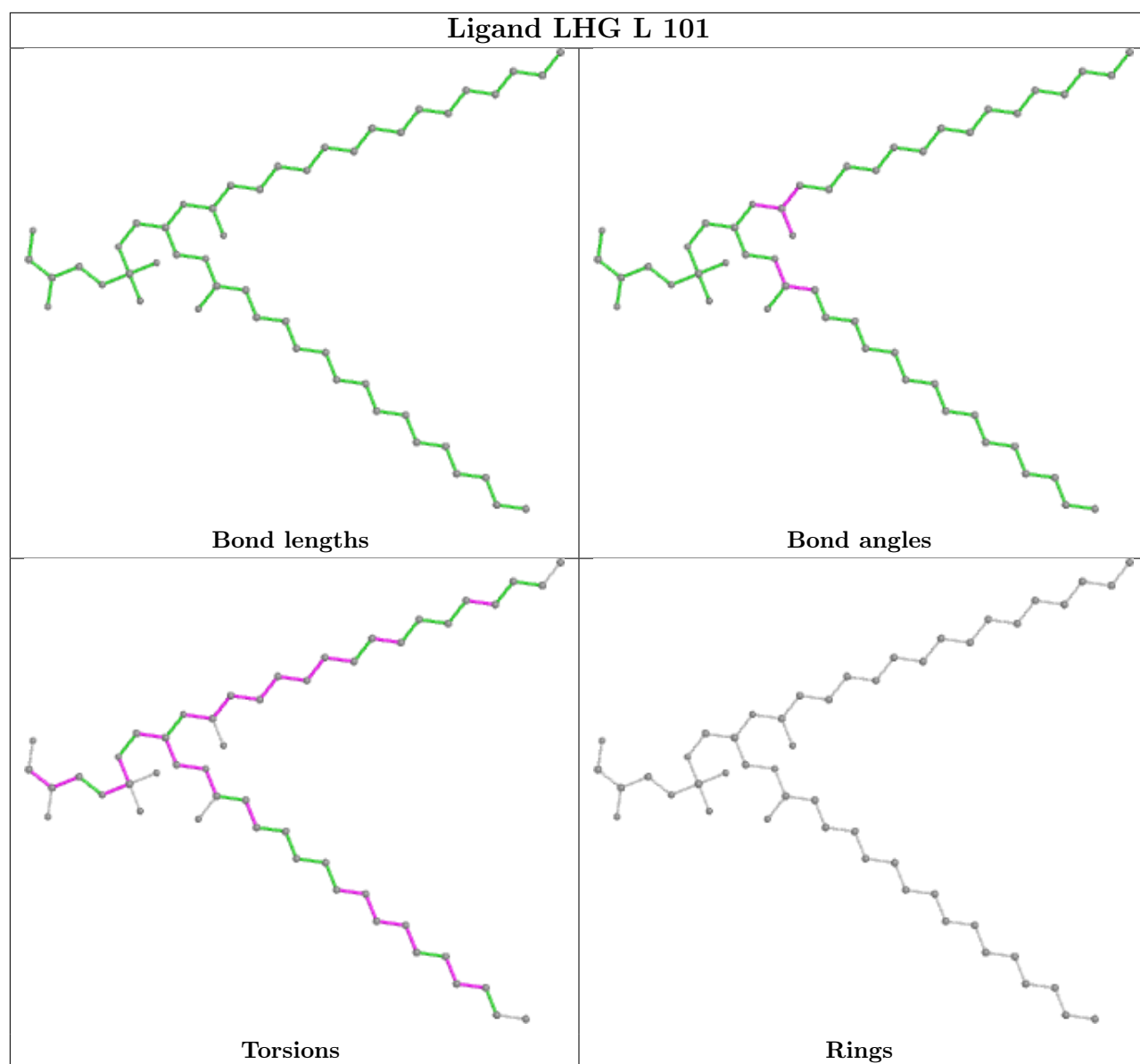


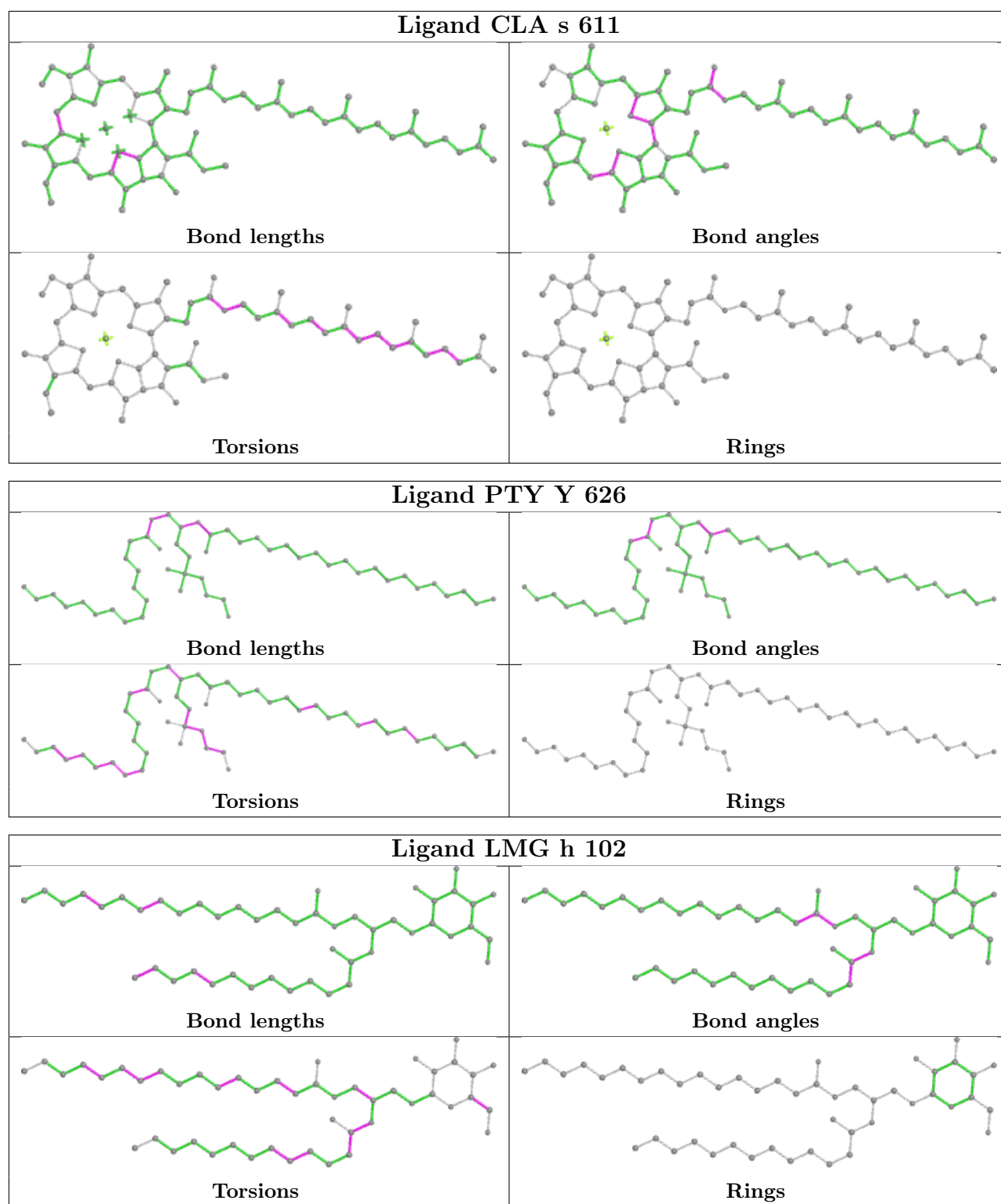




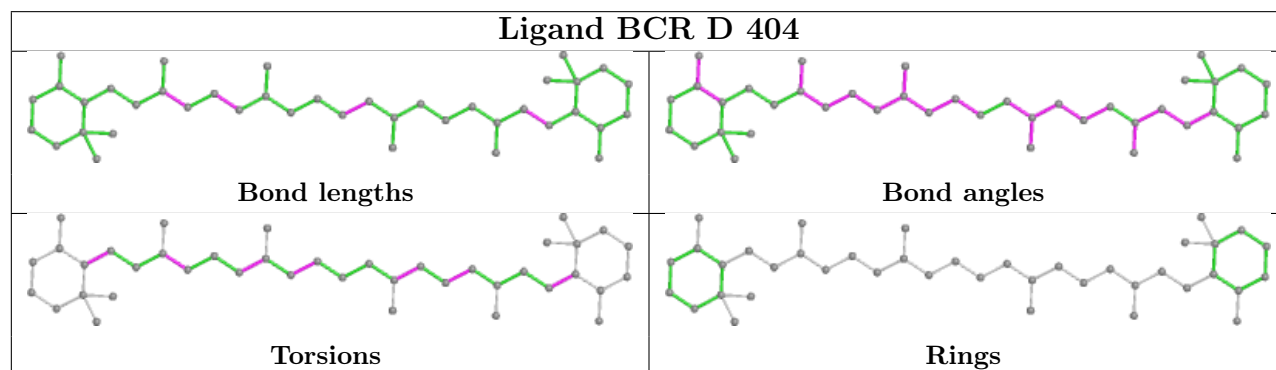
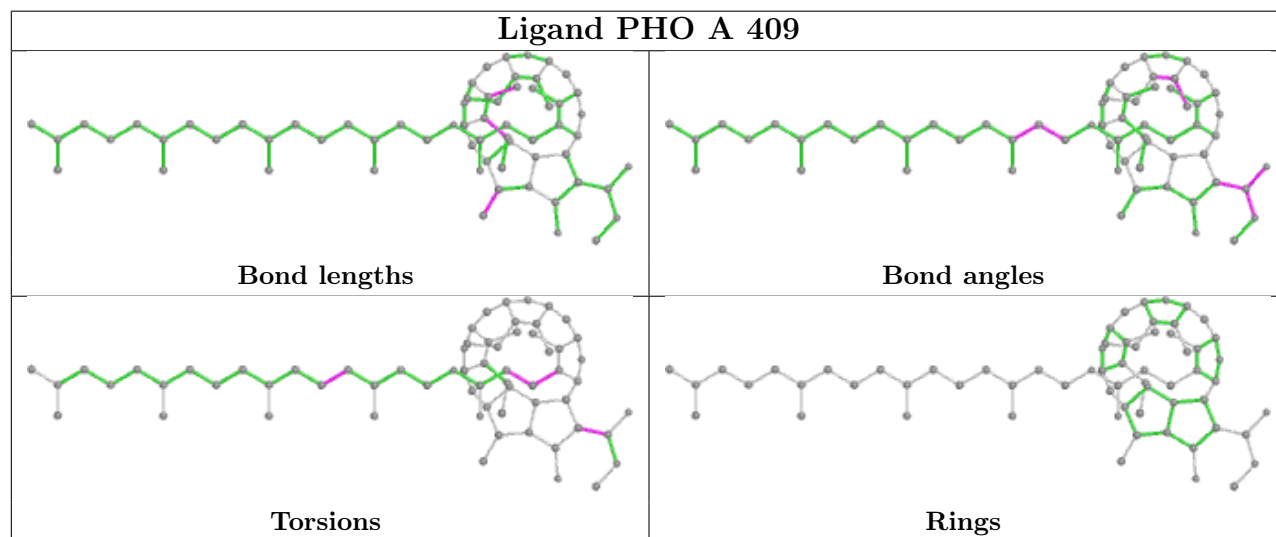
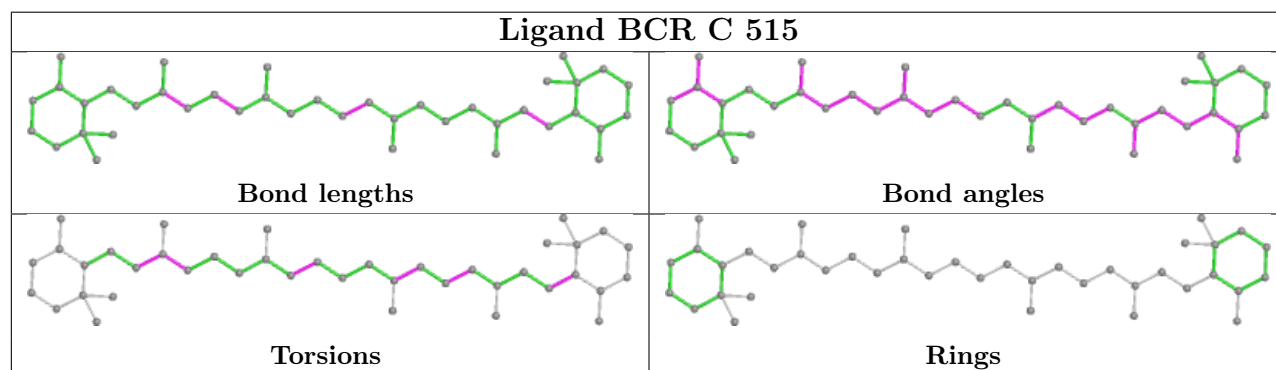
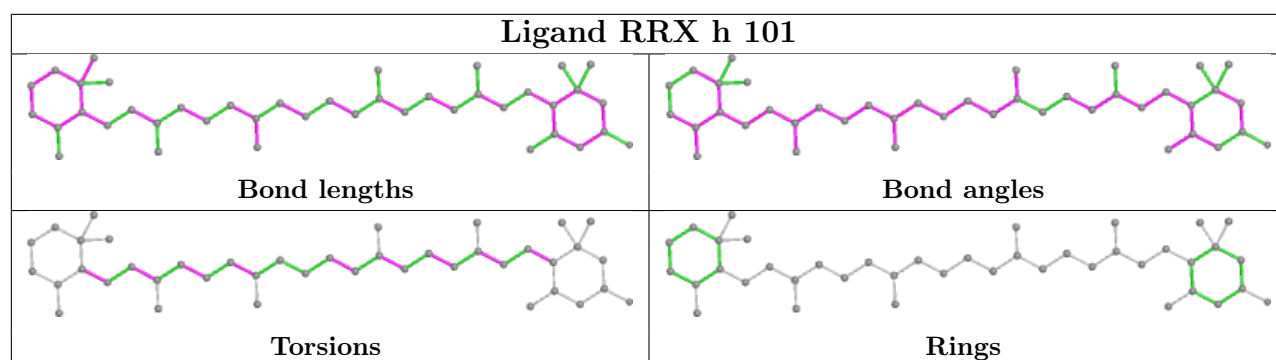


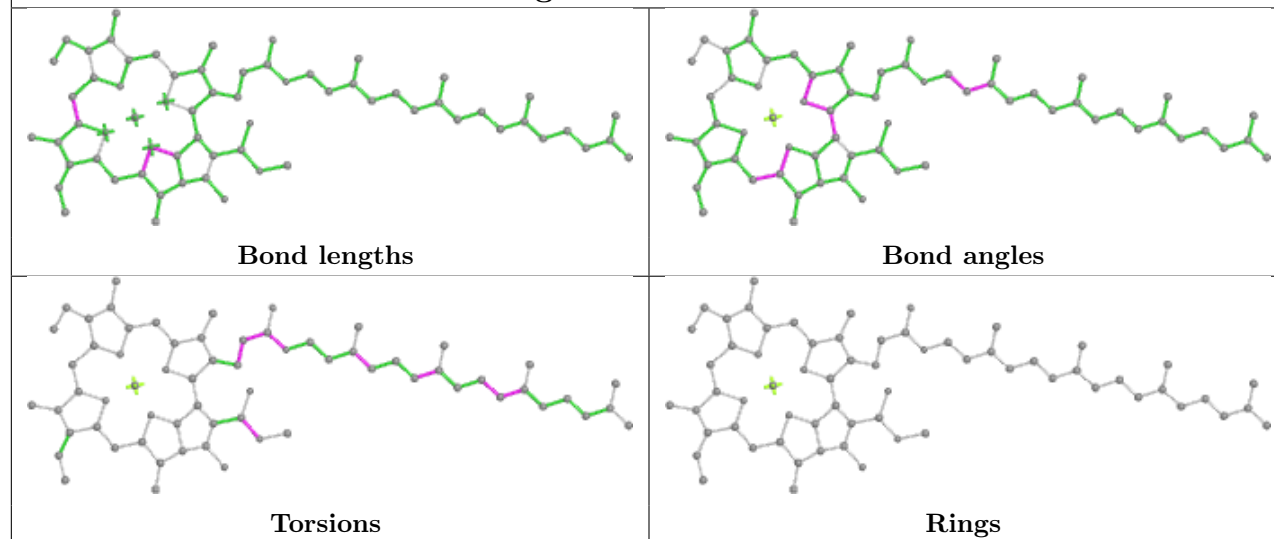
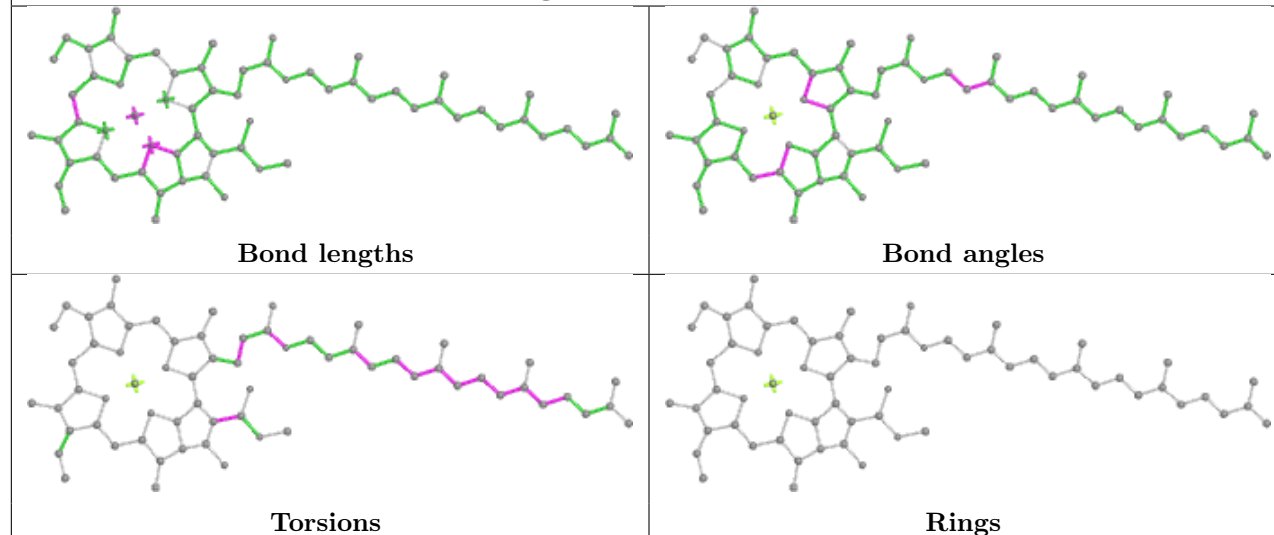
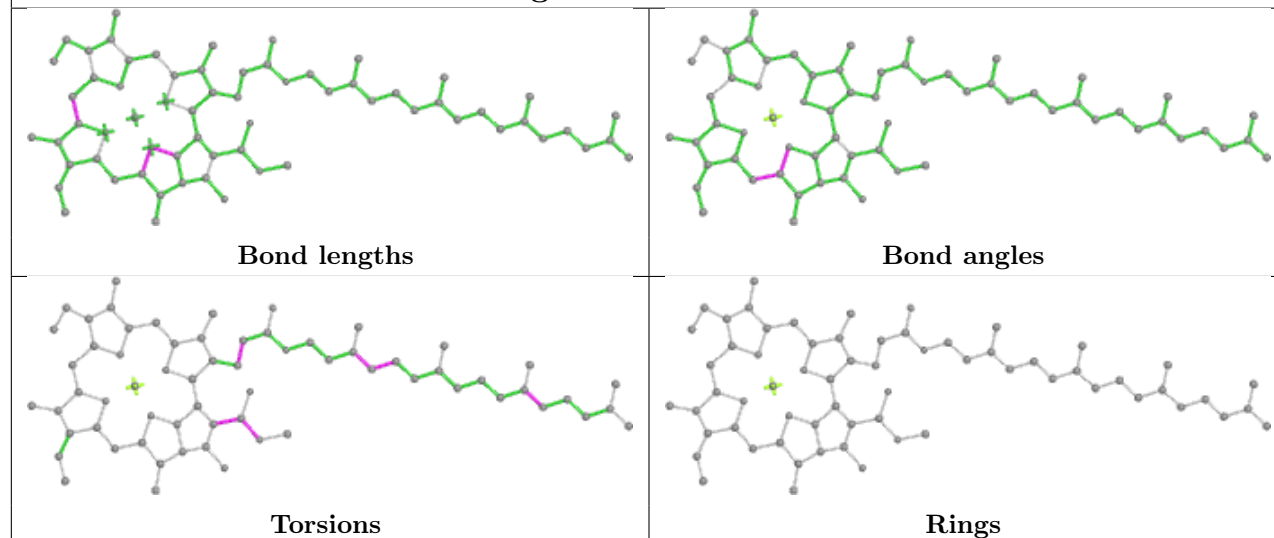


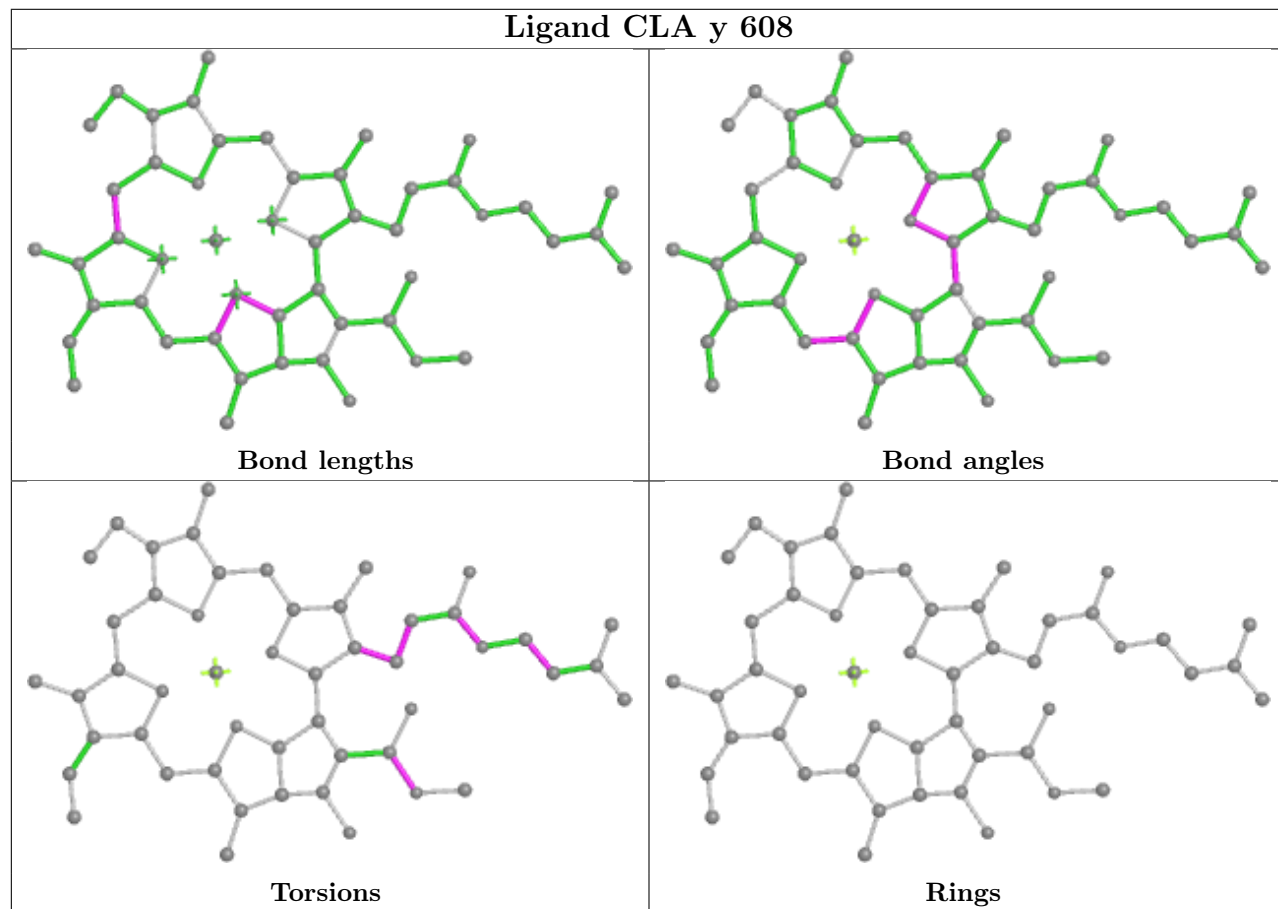
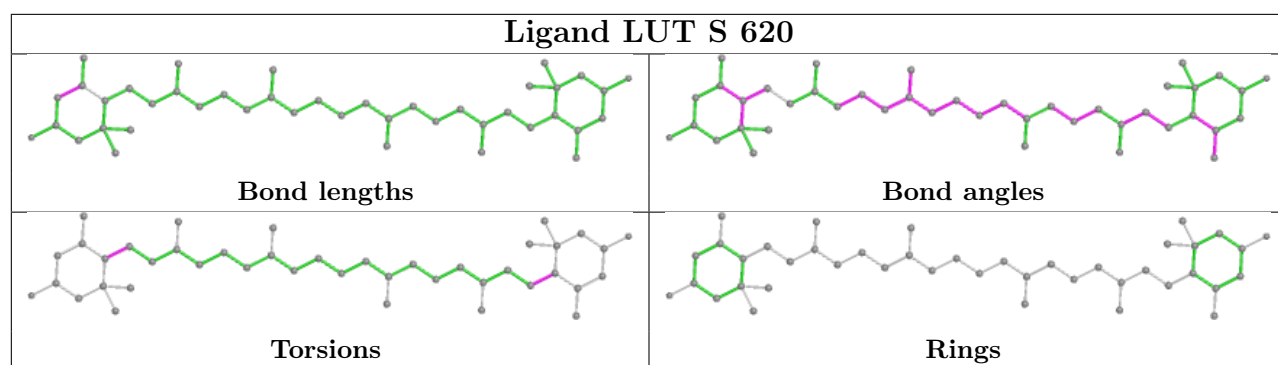


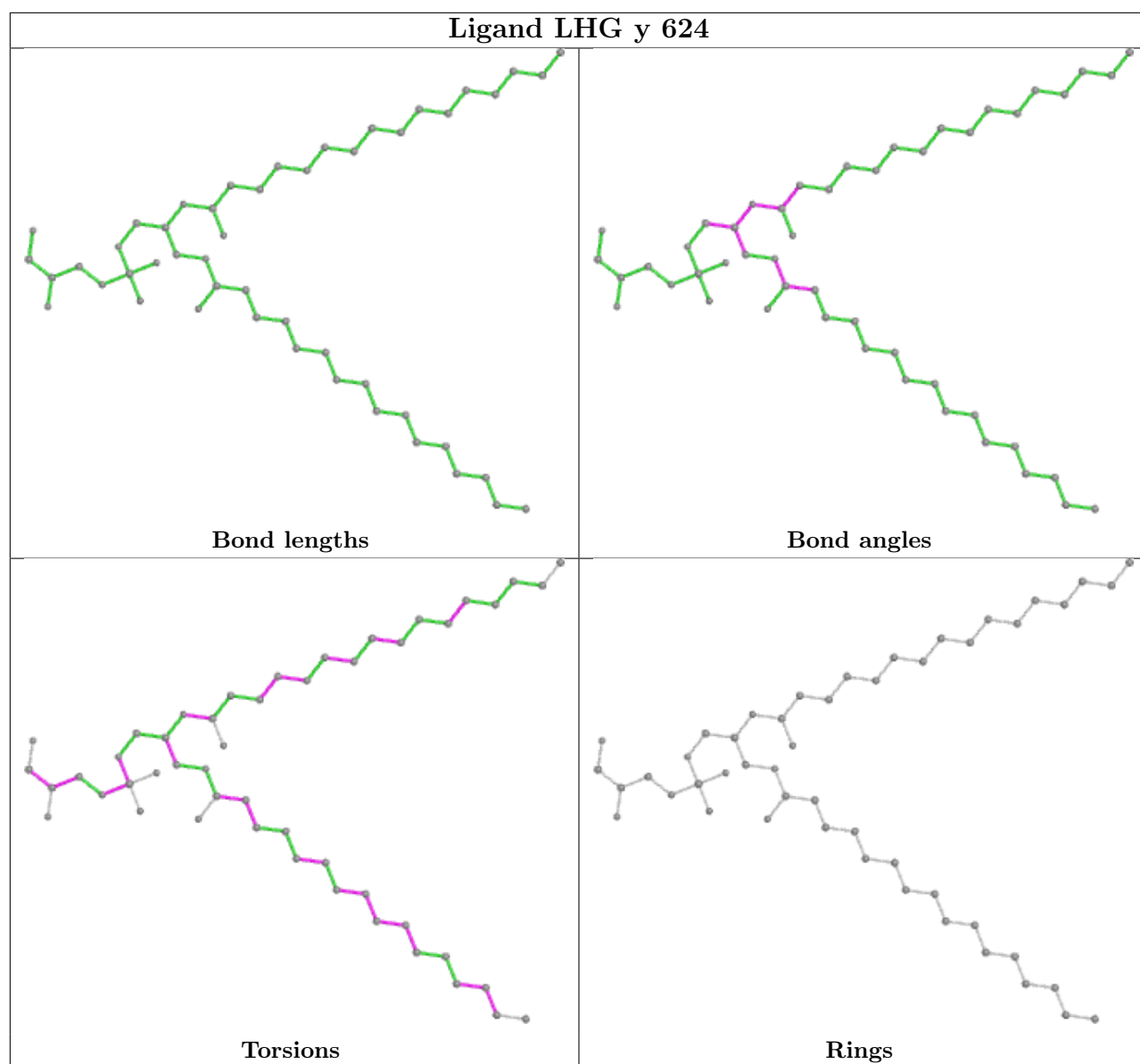


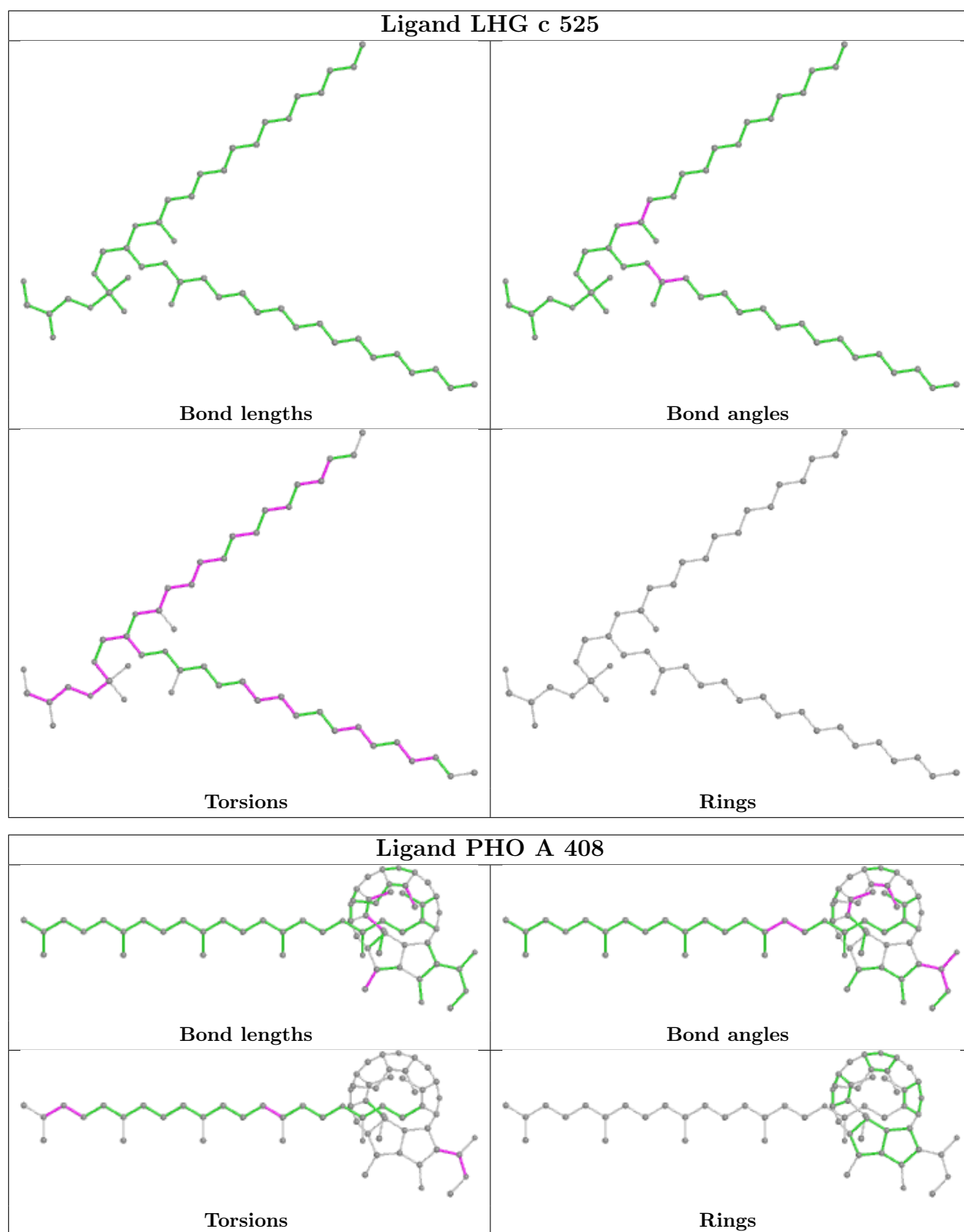




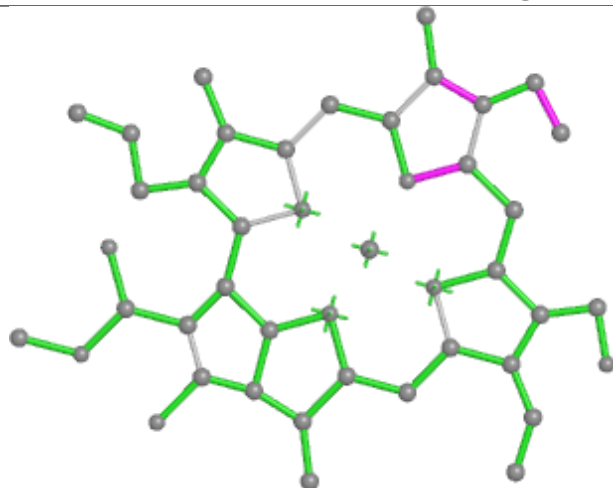
**Ligand CLA b 615****Ligand CLA c 505****Ligand CLA G 613**



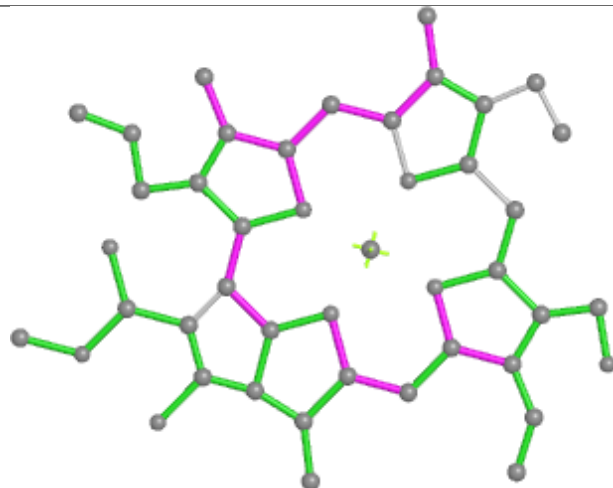




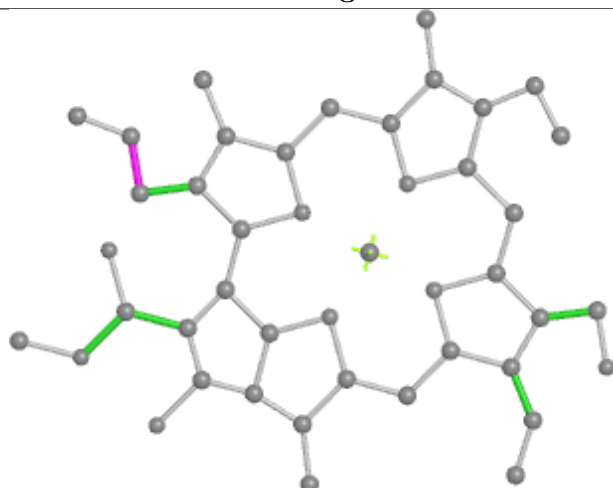
## Ligand CHL S 606



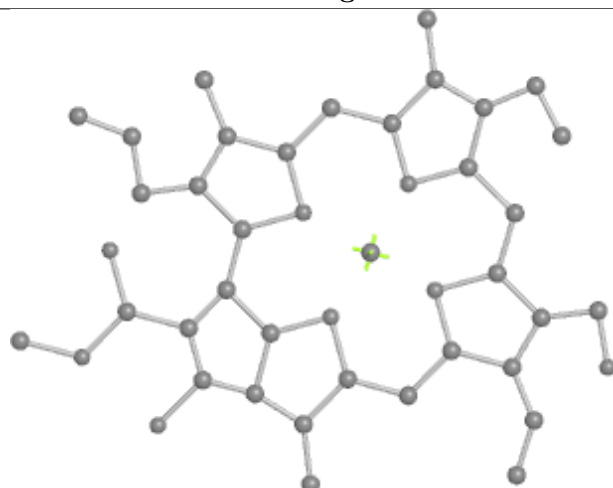
Bond lengths



Bond angles

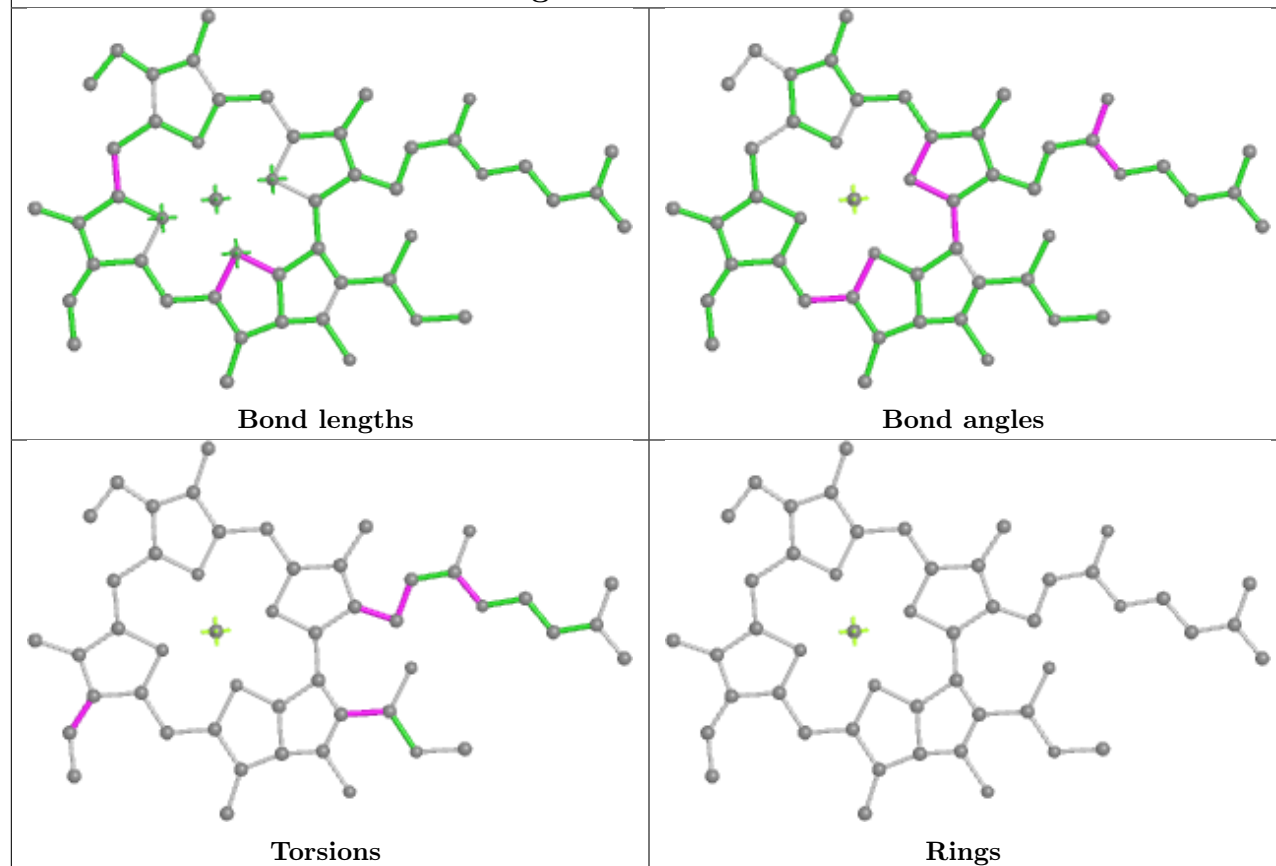


Torsions

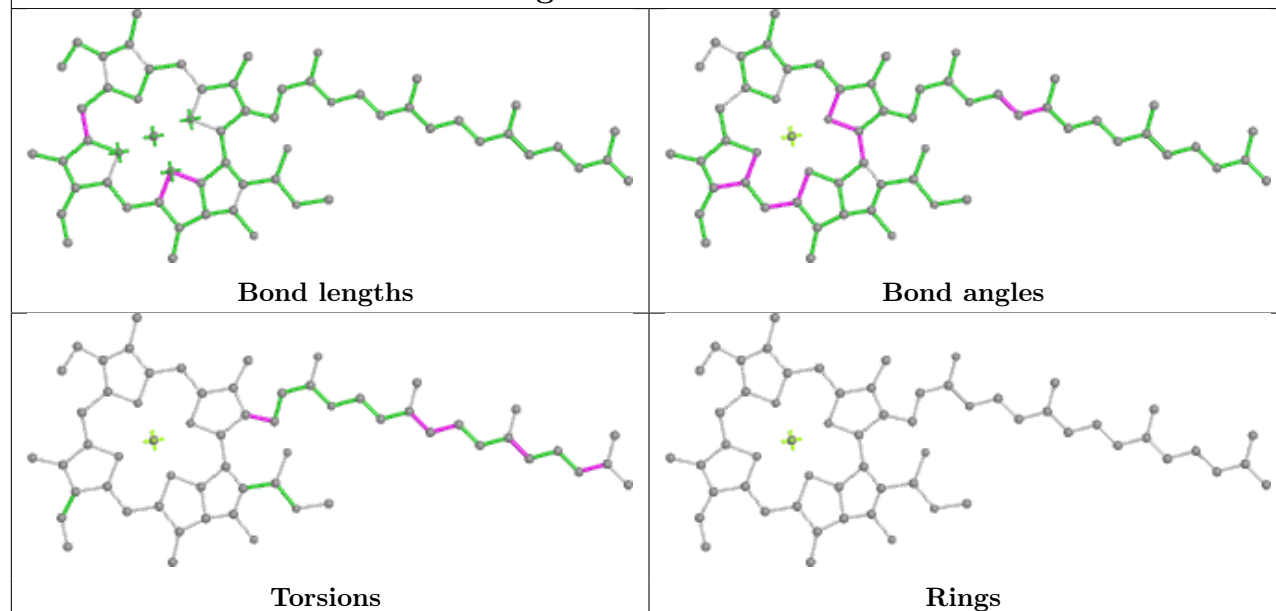


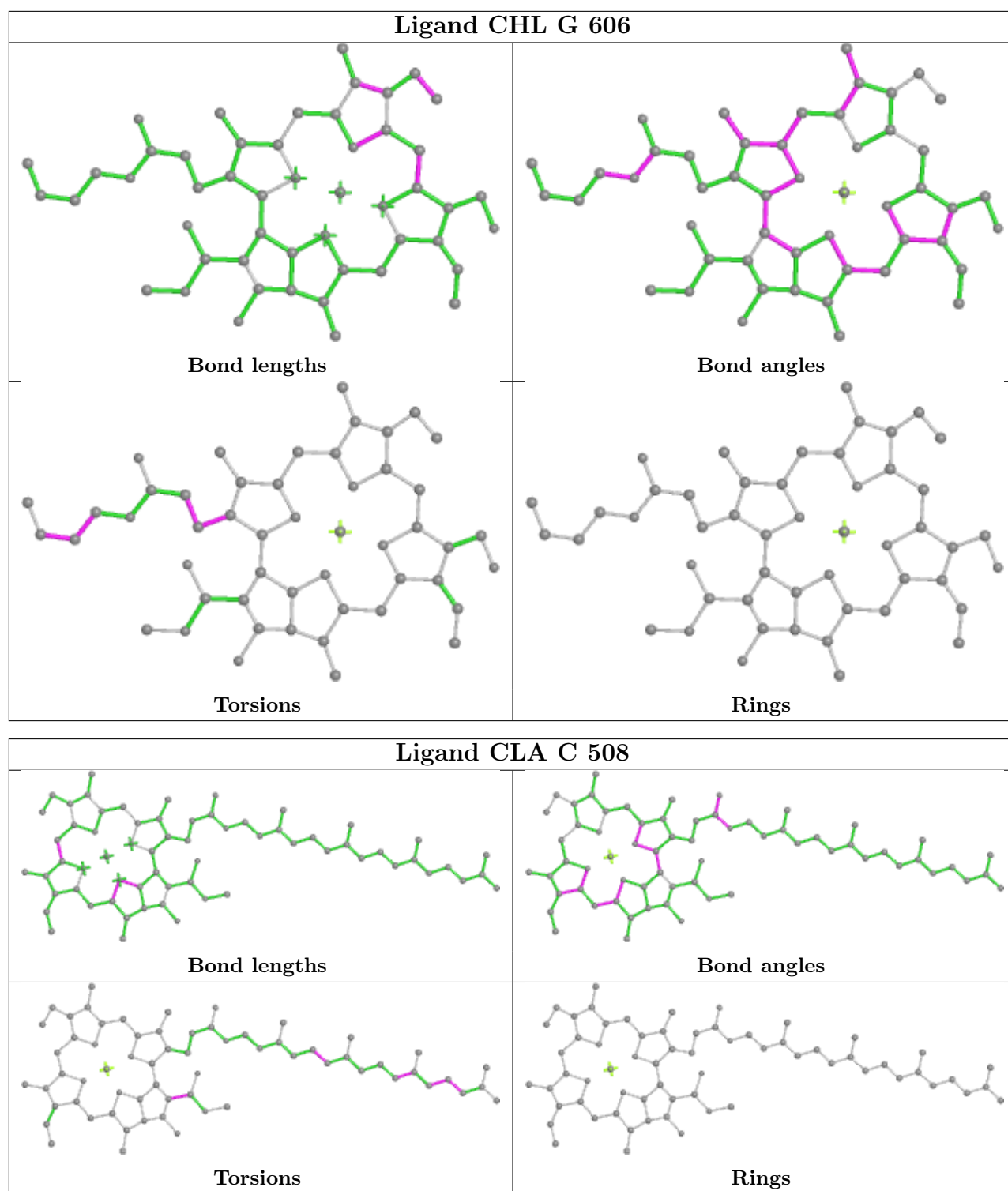
Rings

## Ligand CLA A 407

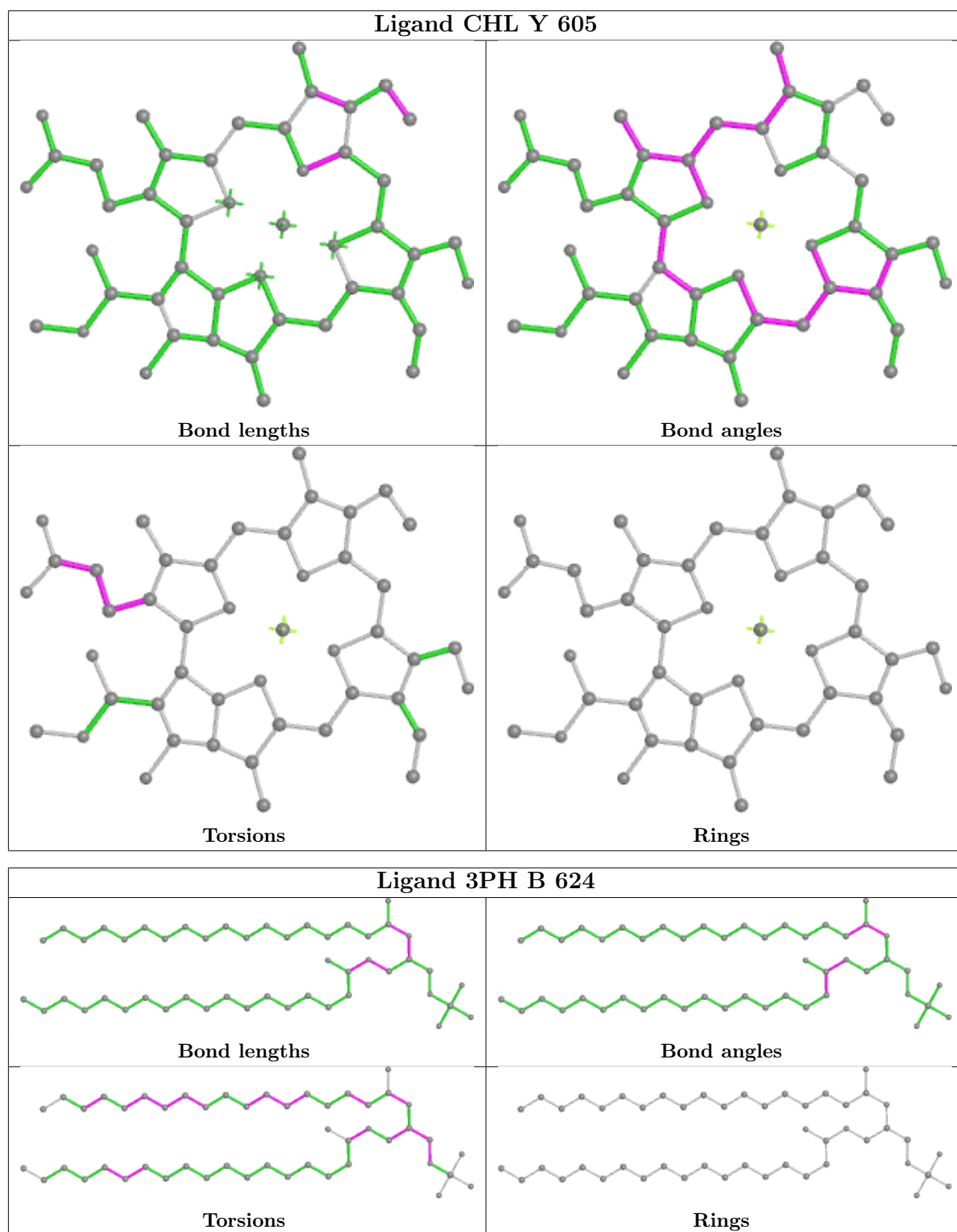


## Ligand CLA a 410

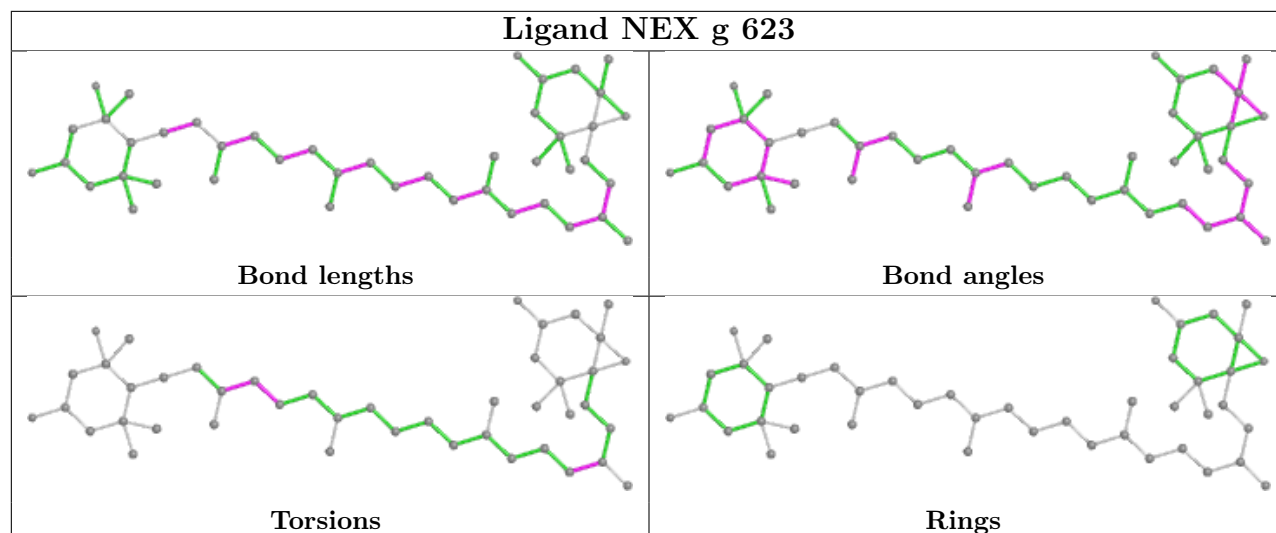




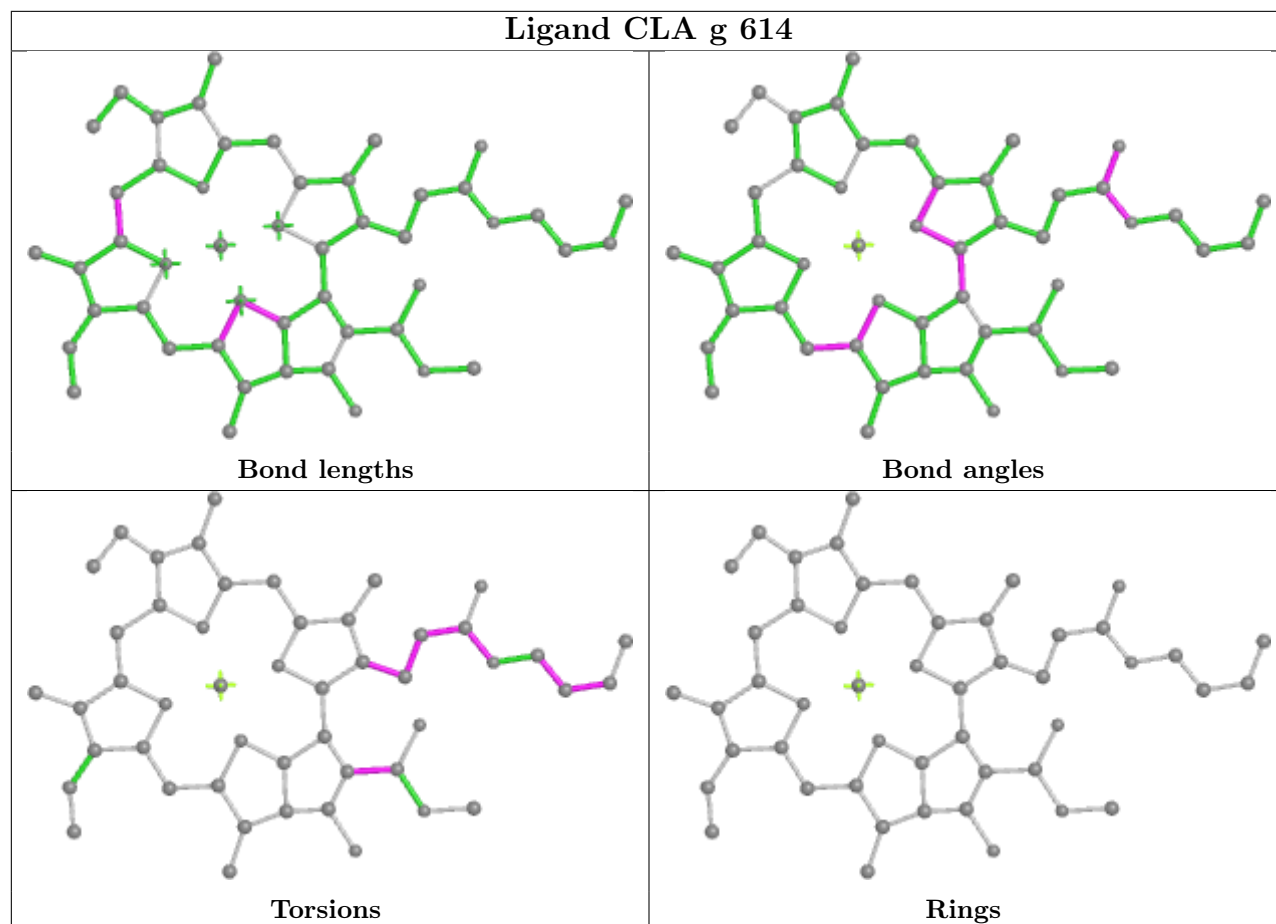


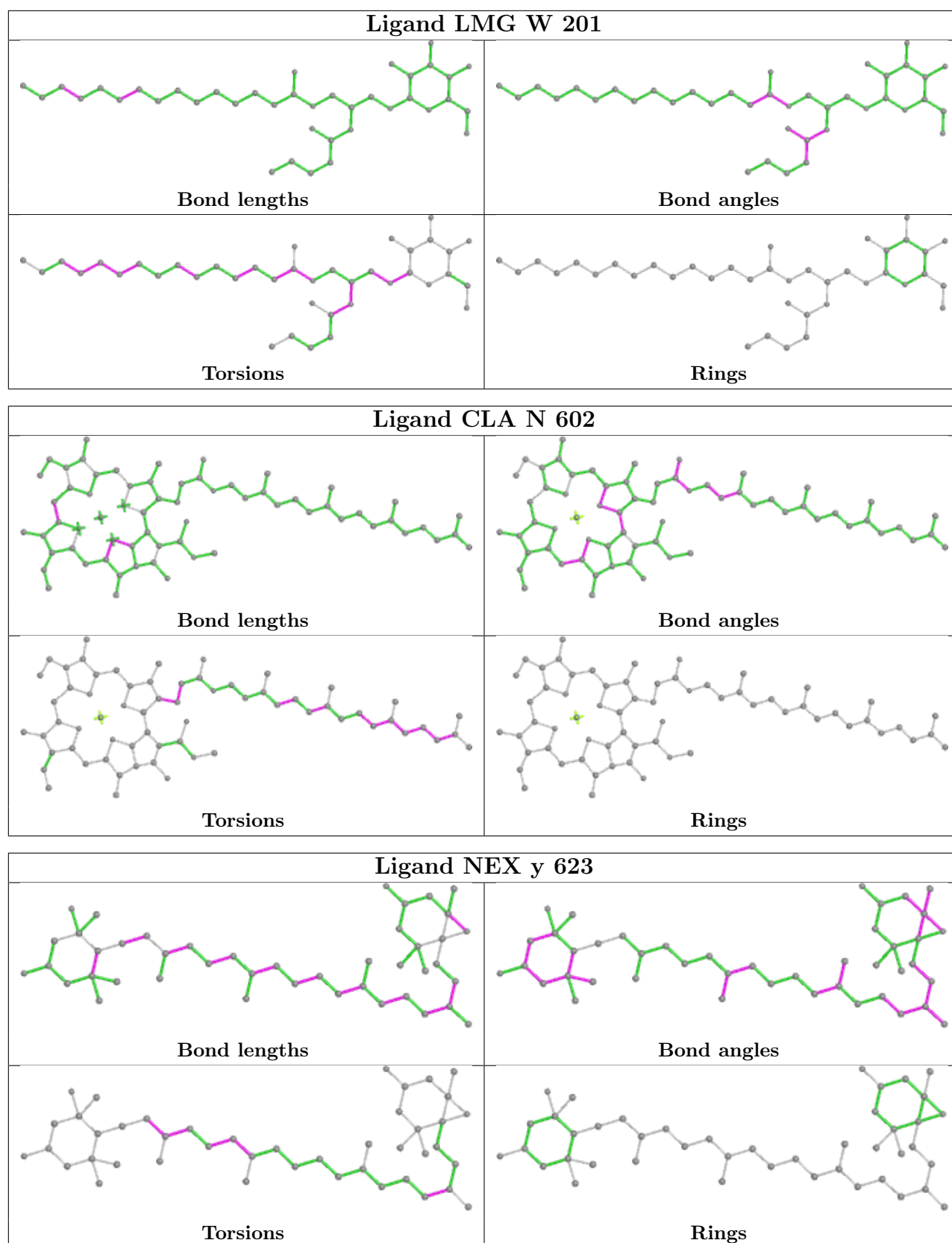


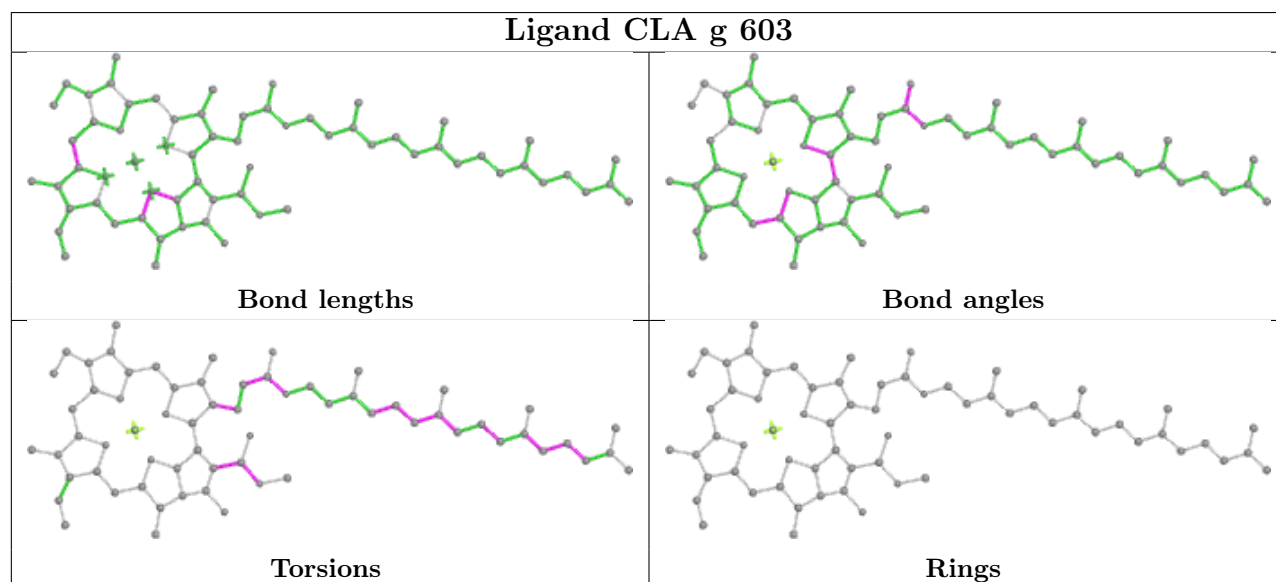
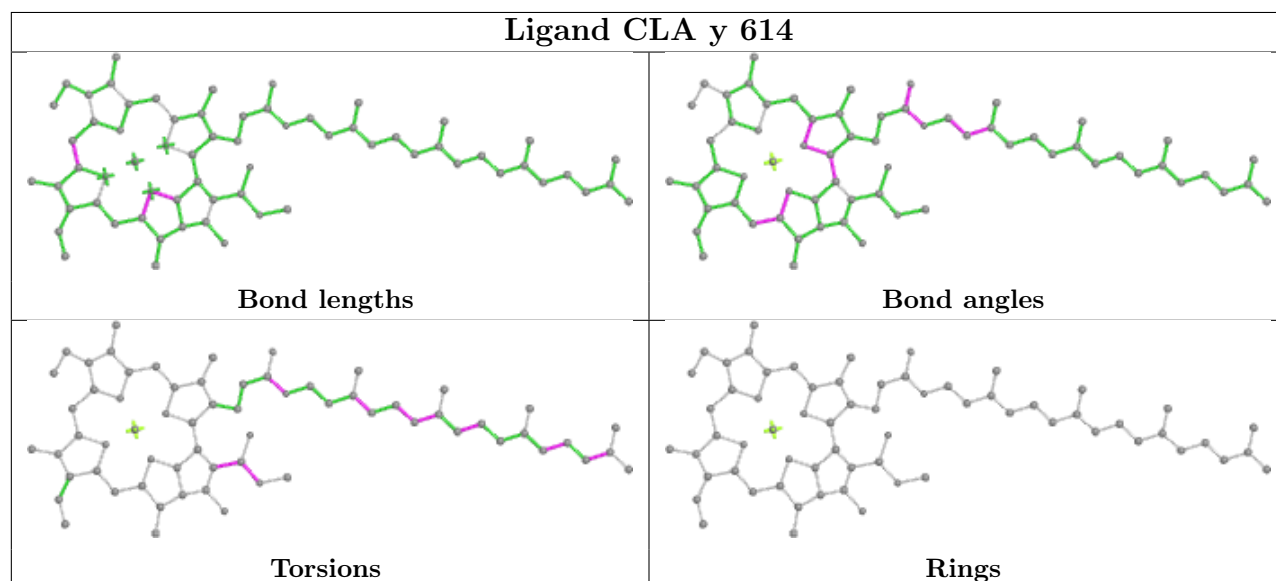
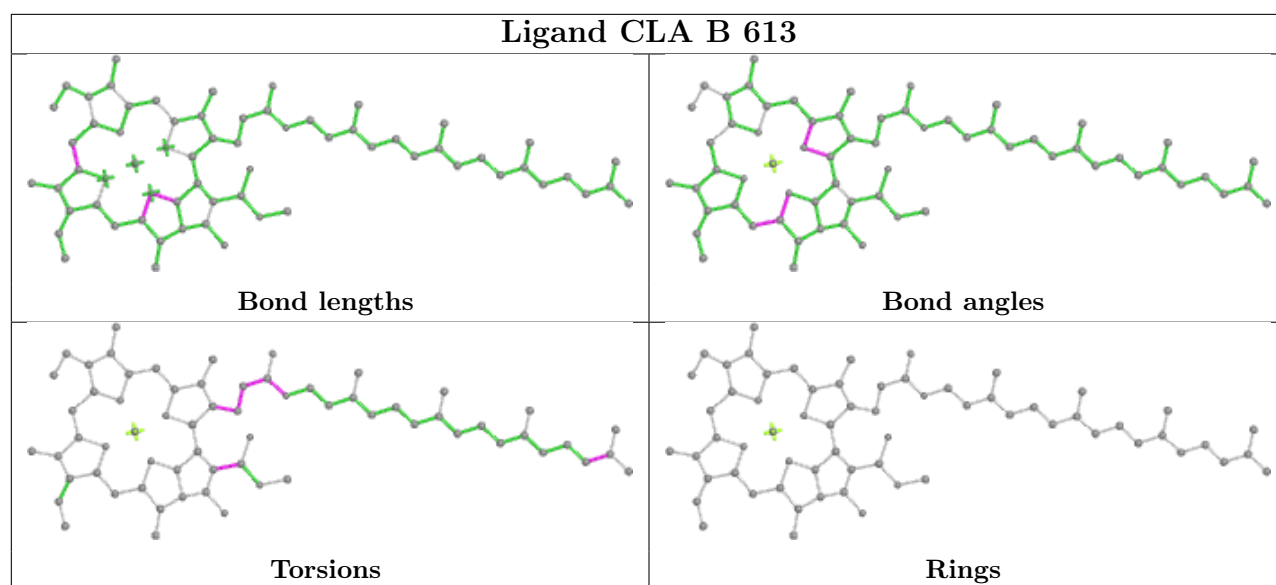
## Ligand NEX g 623

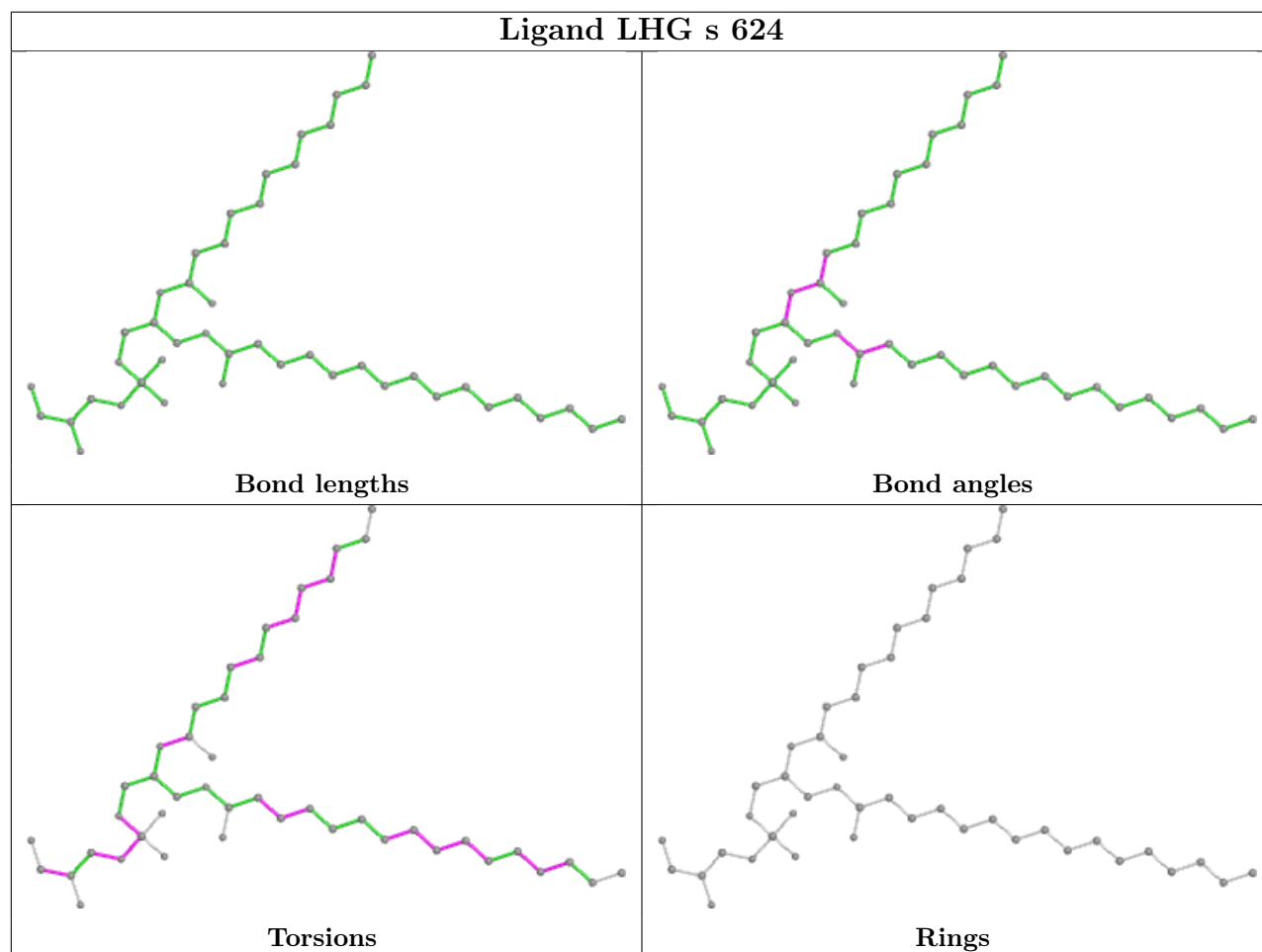
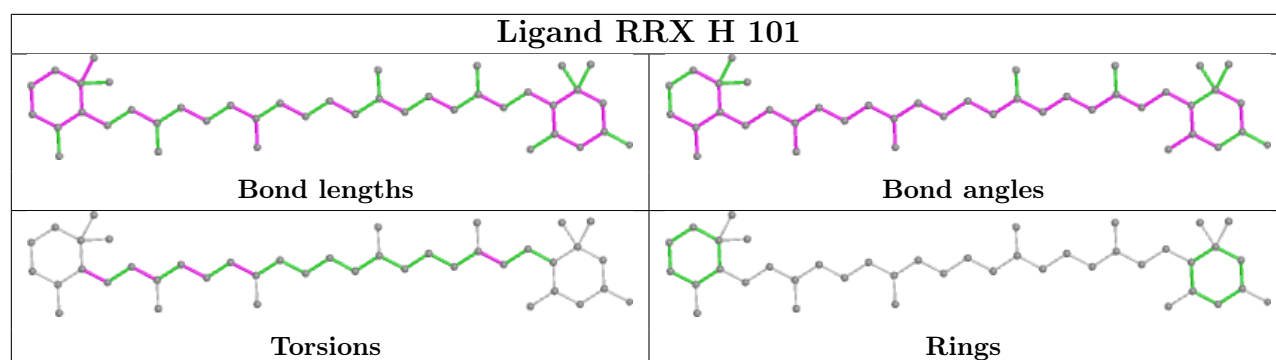


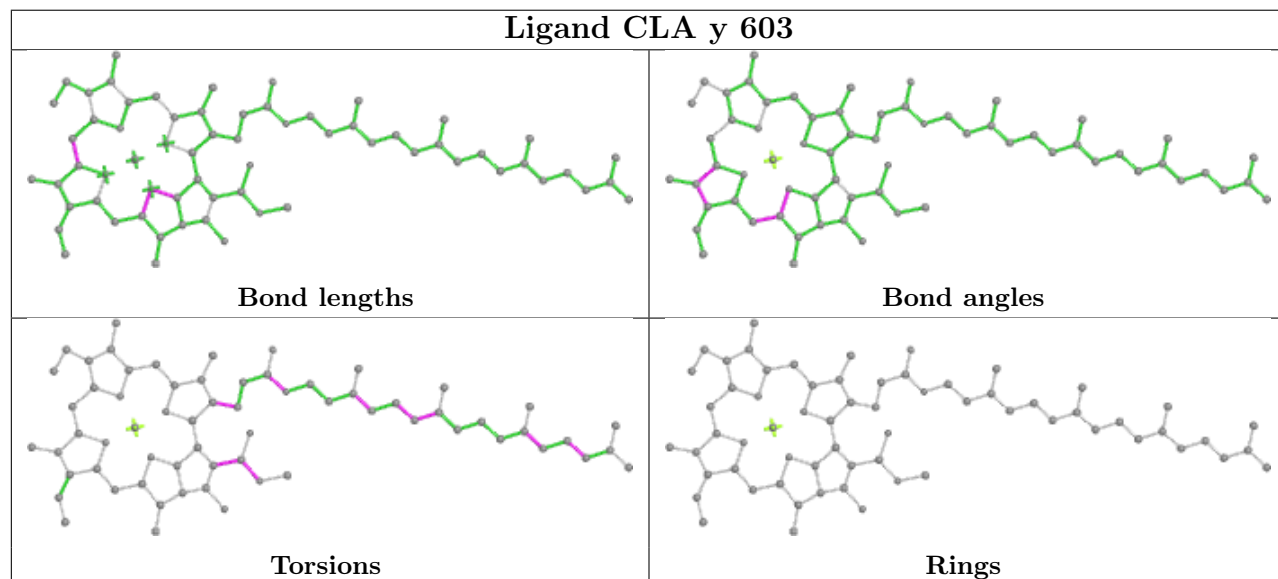
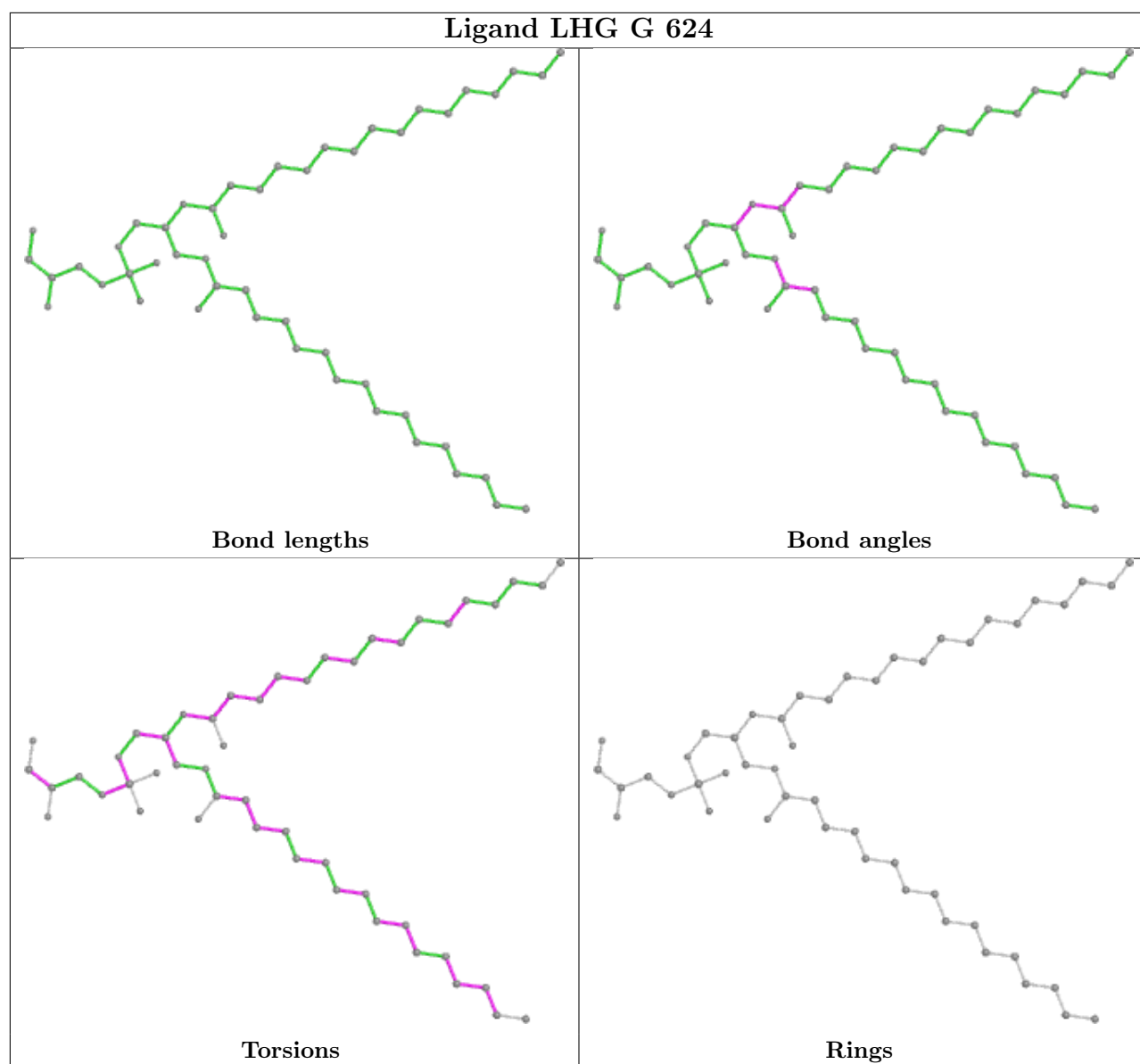
## Ligand CLA g 614

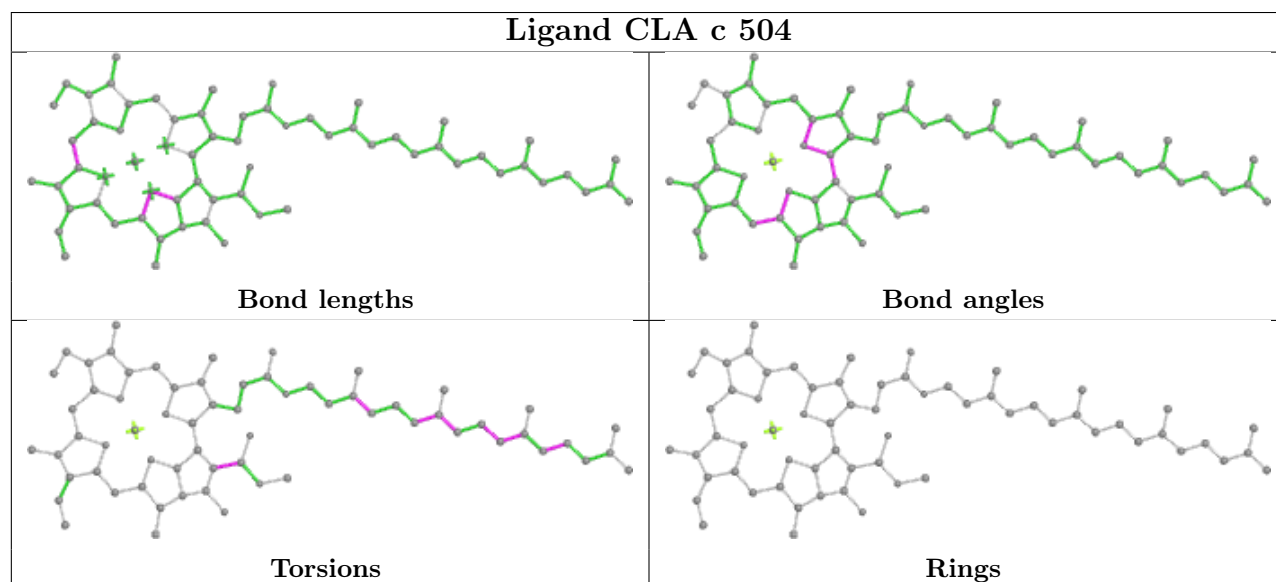
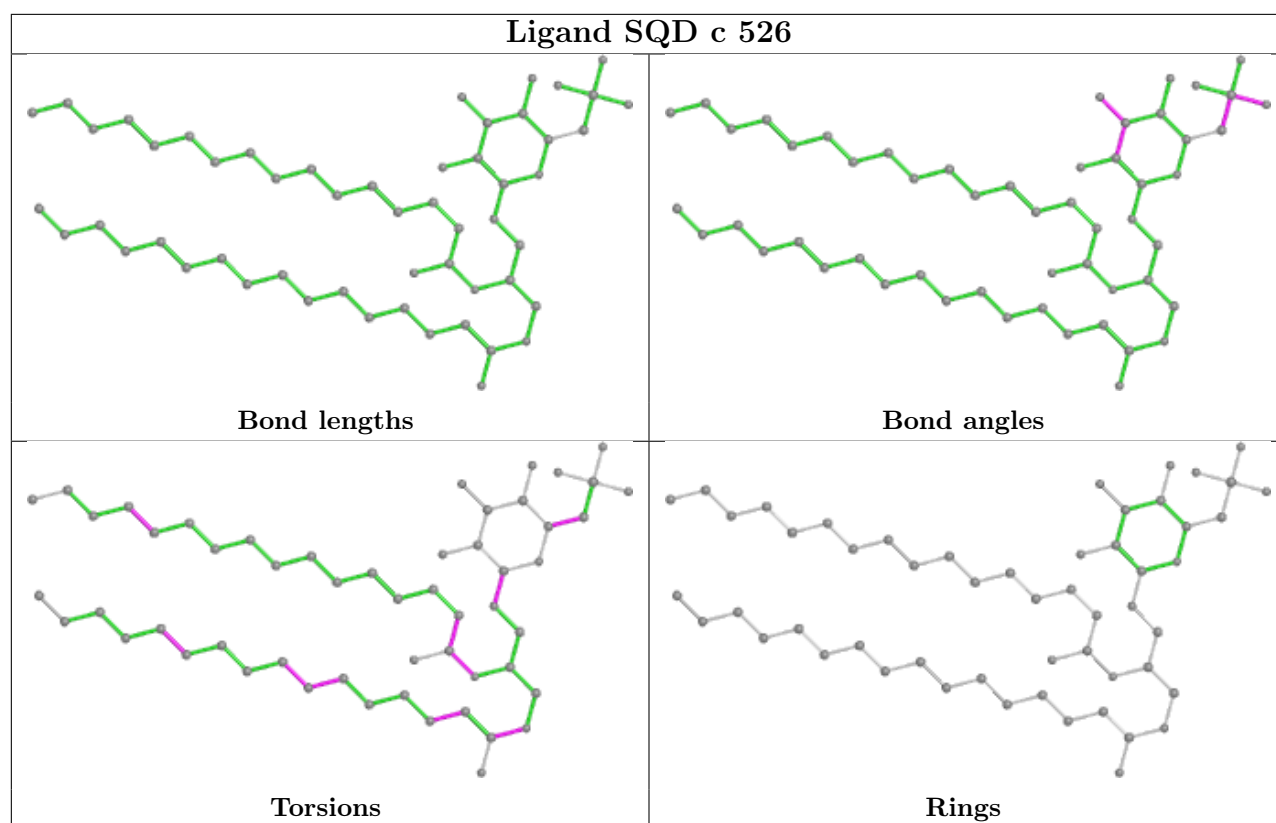


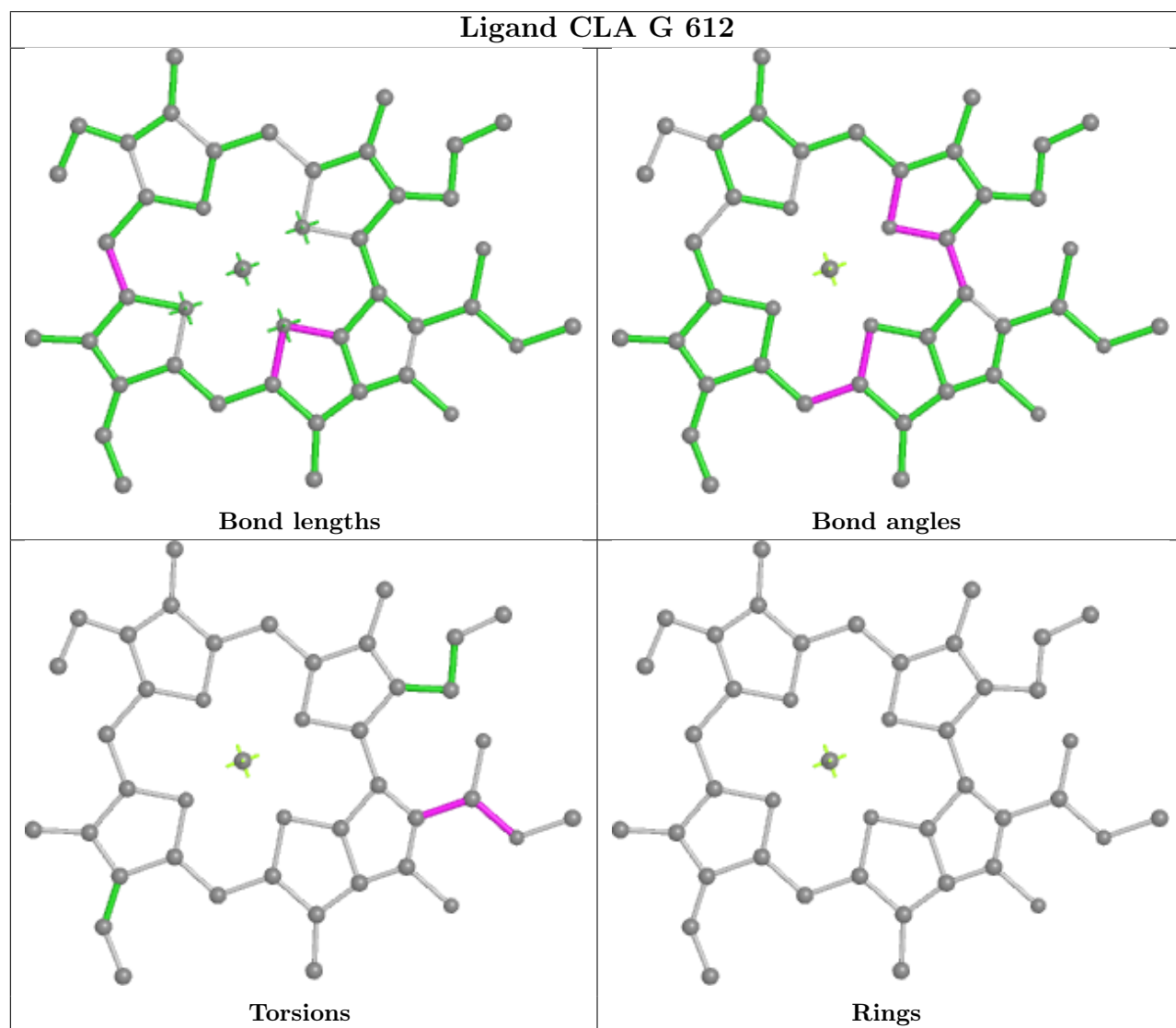
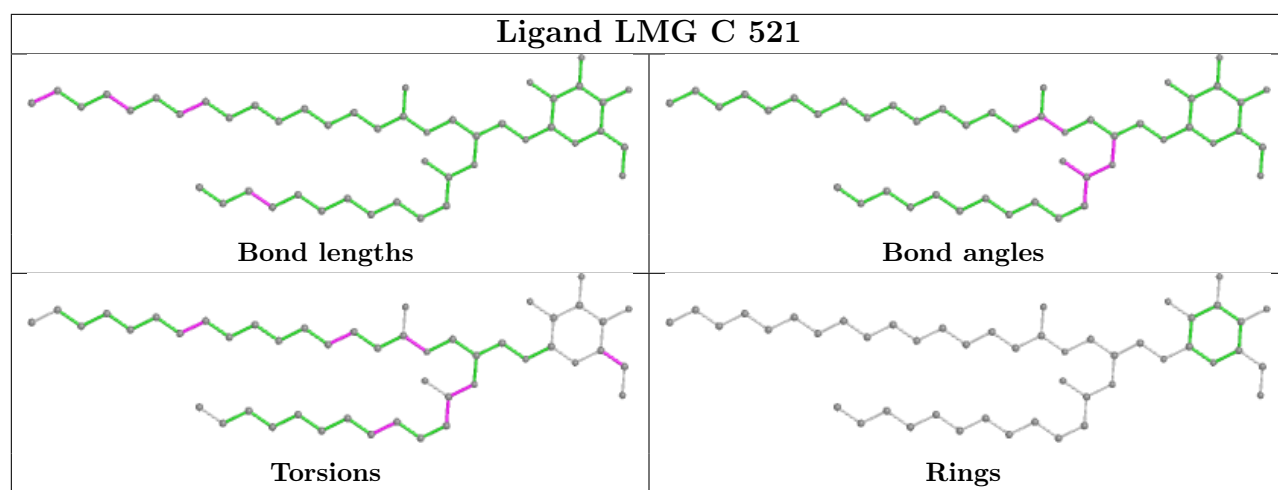




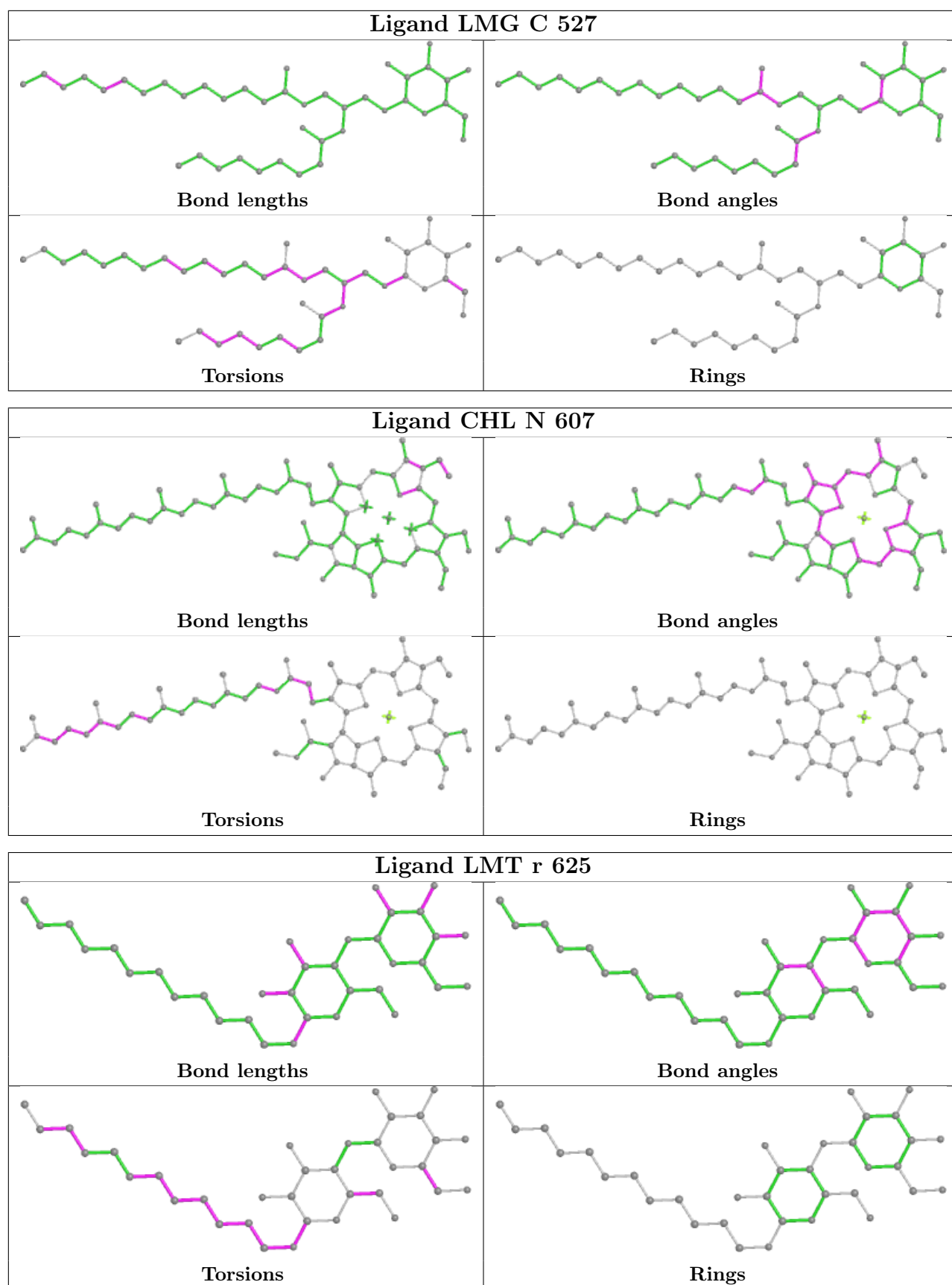




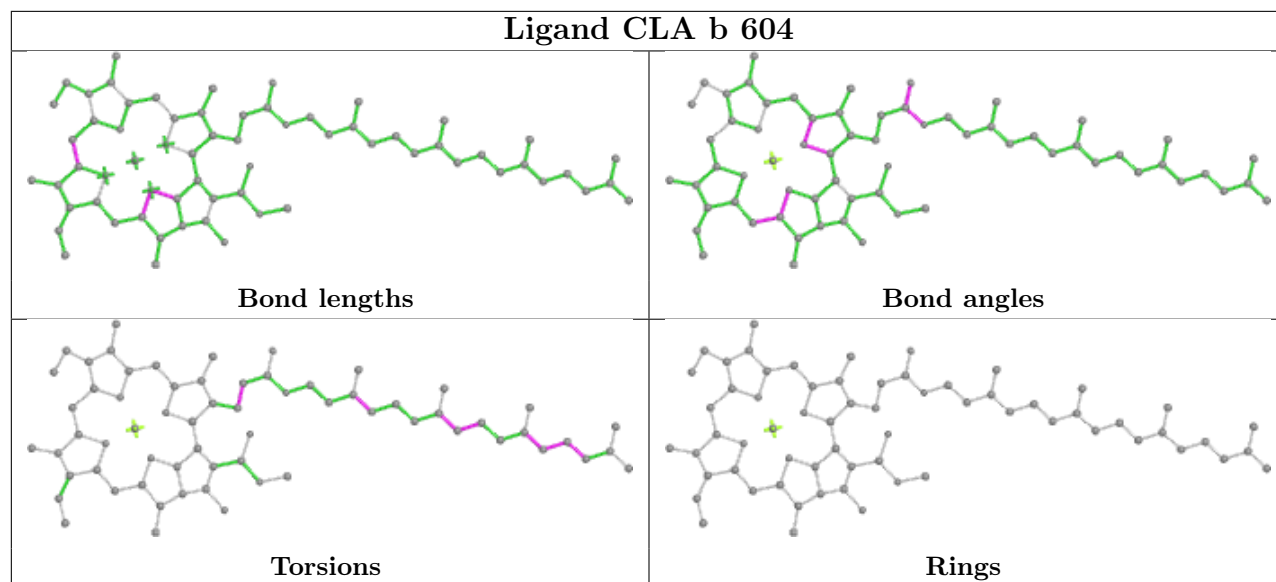




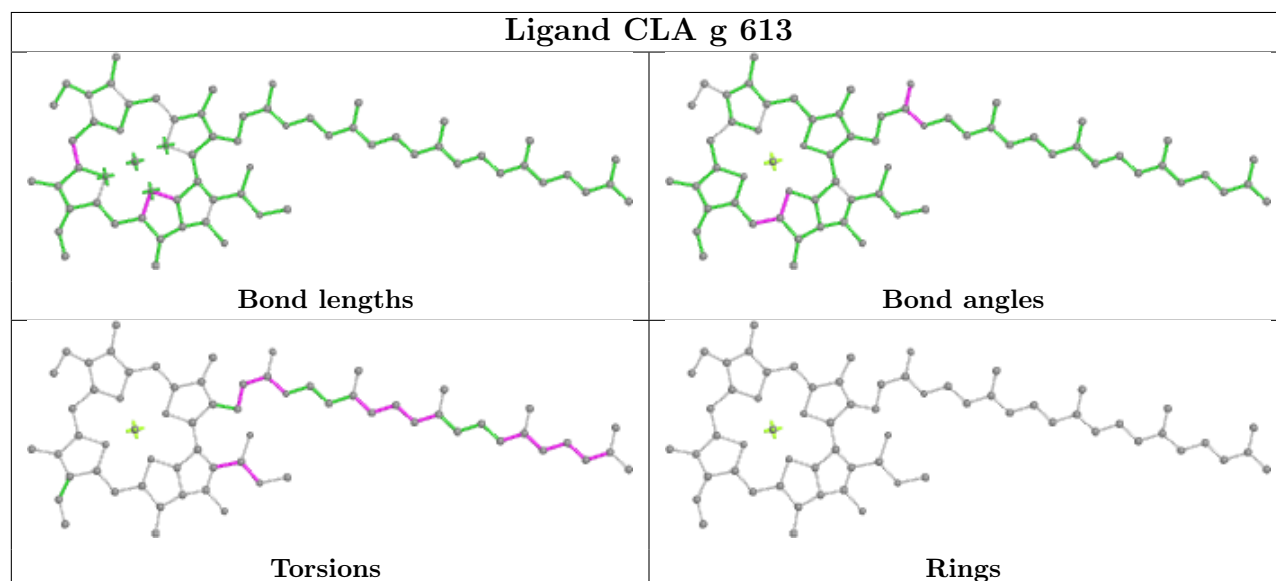




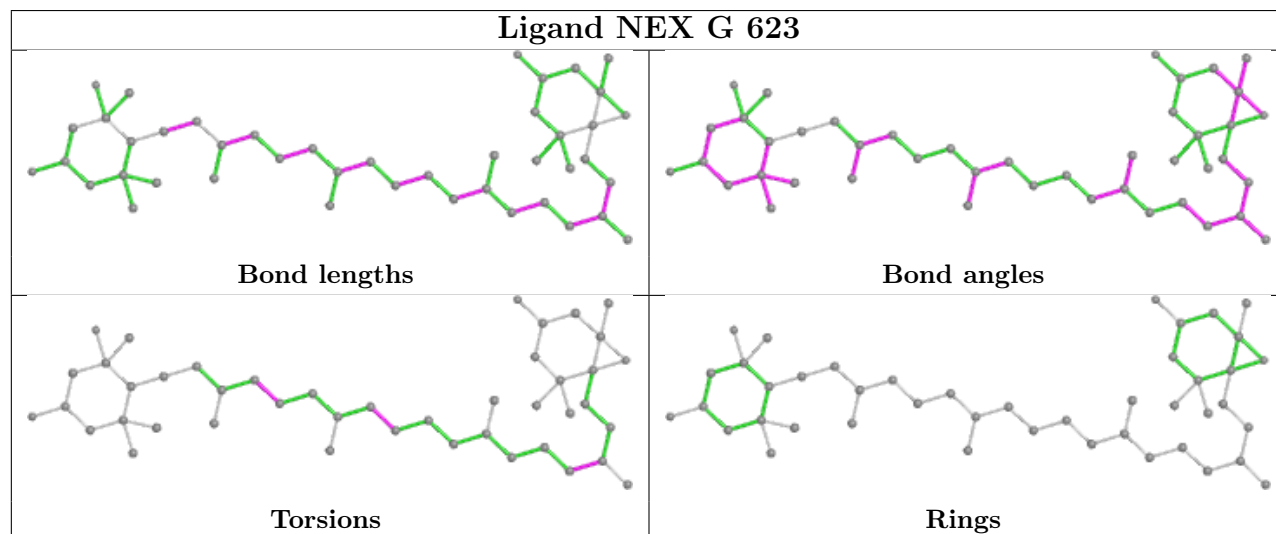
## Ligand CLA b 604

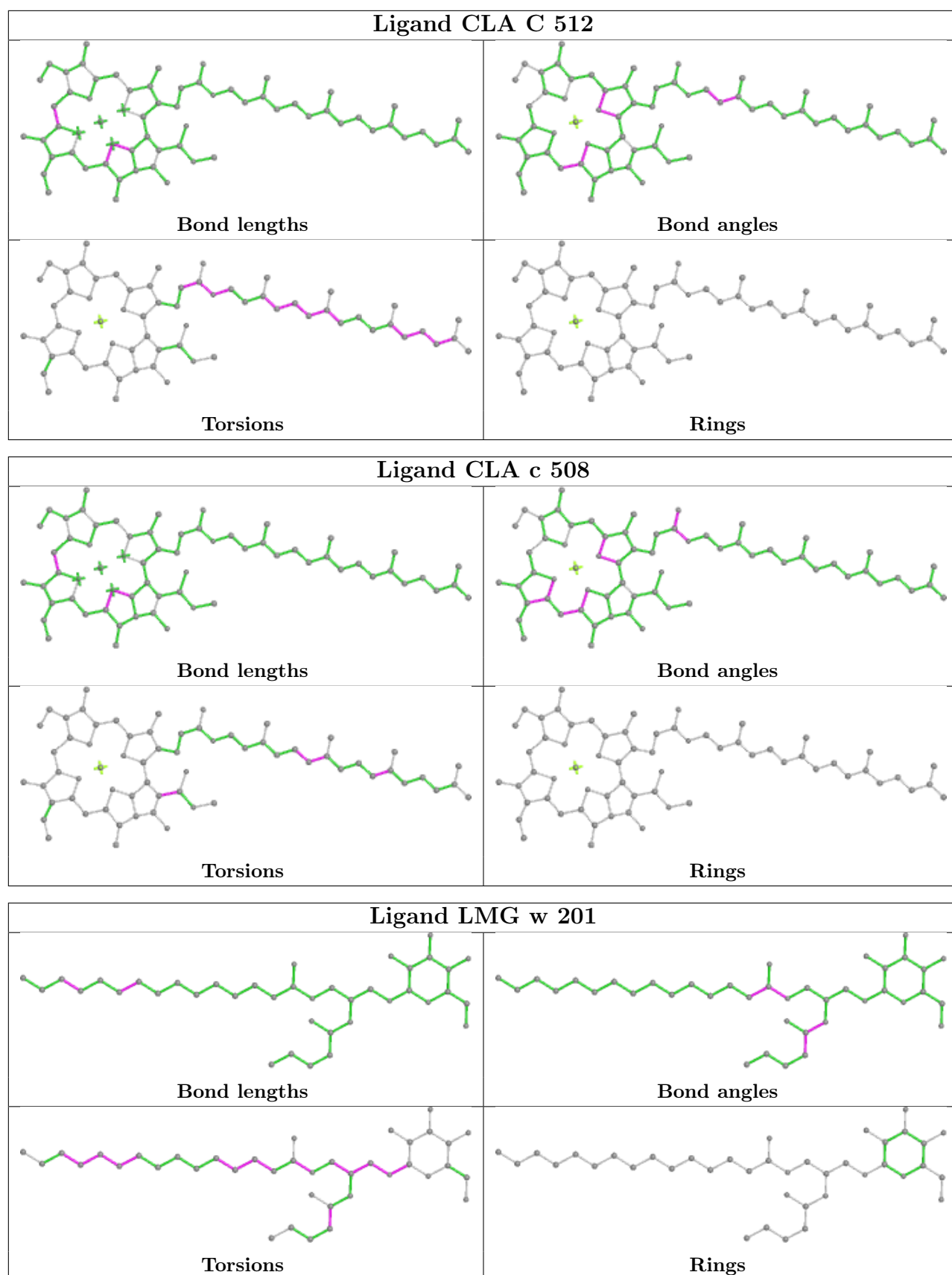


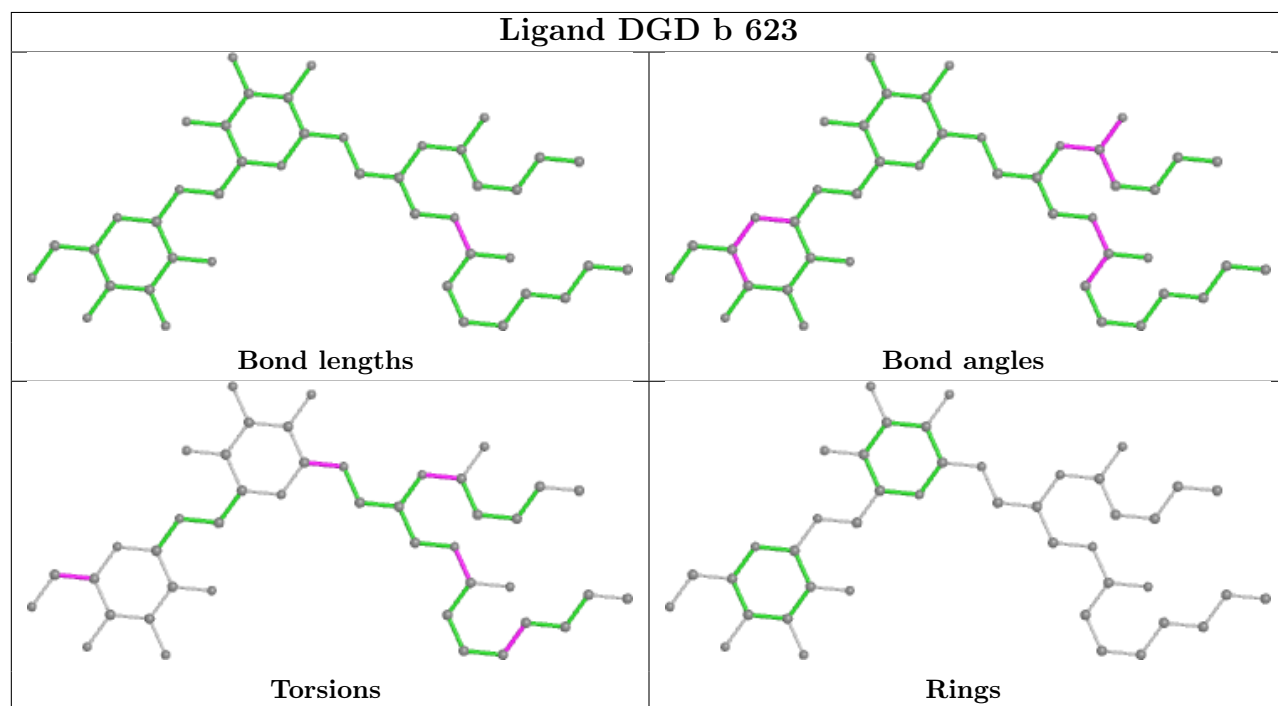
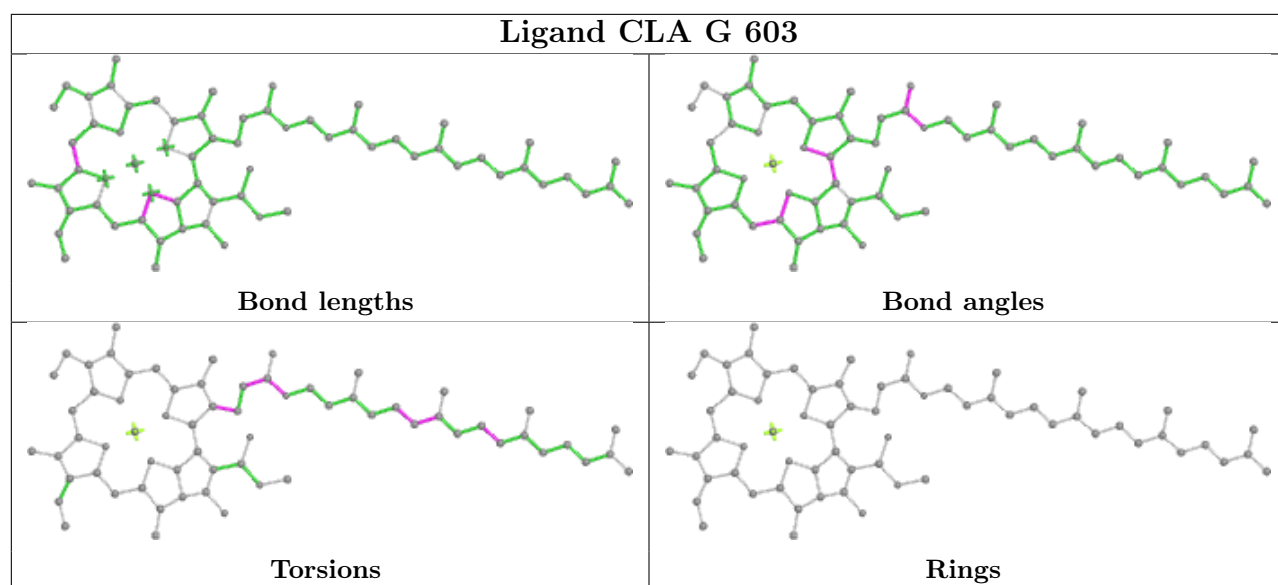
## Ligand CLA g 613

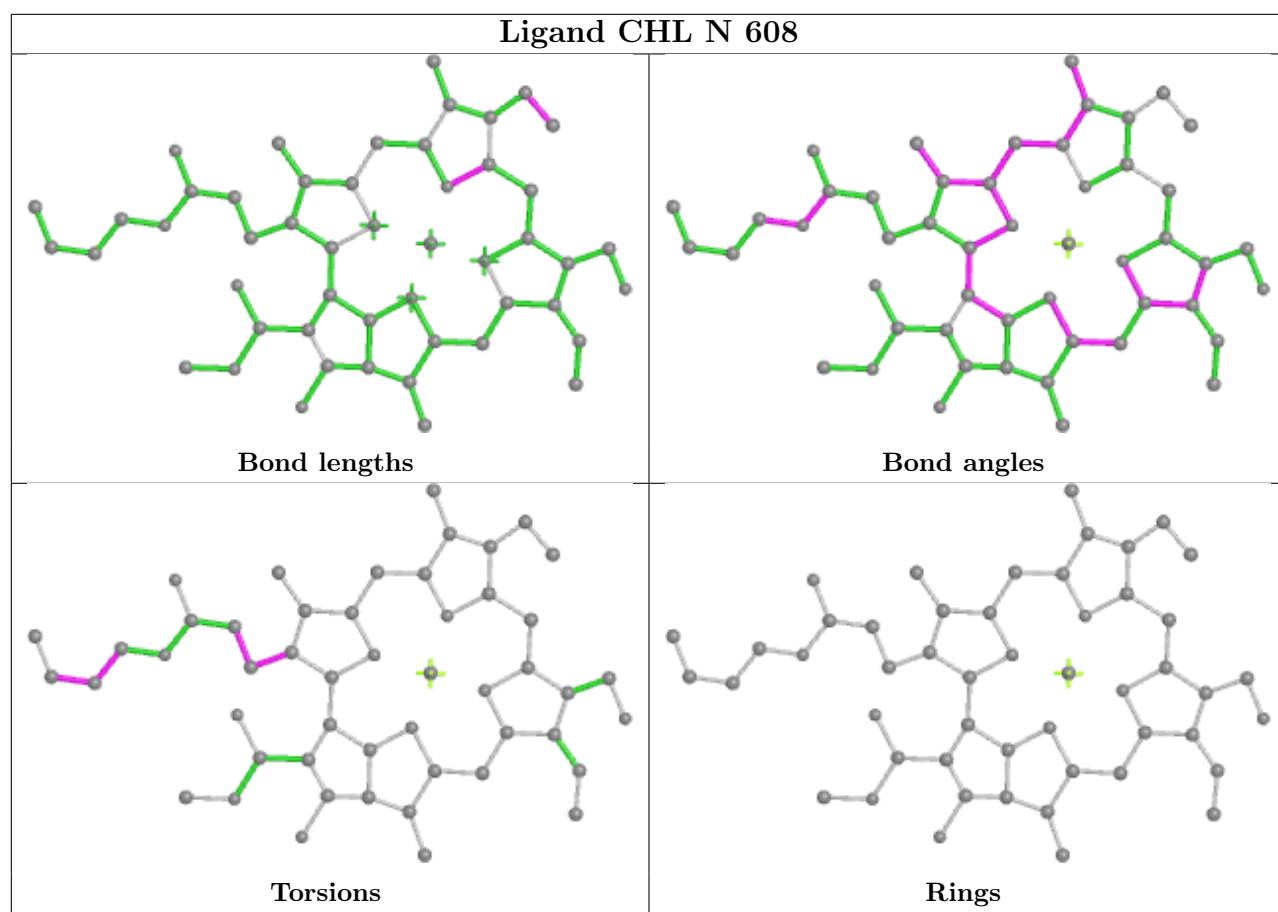


## Ligand NEX G 623

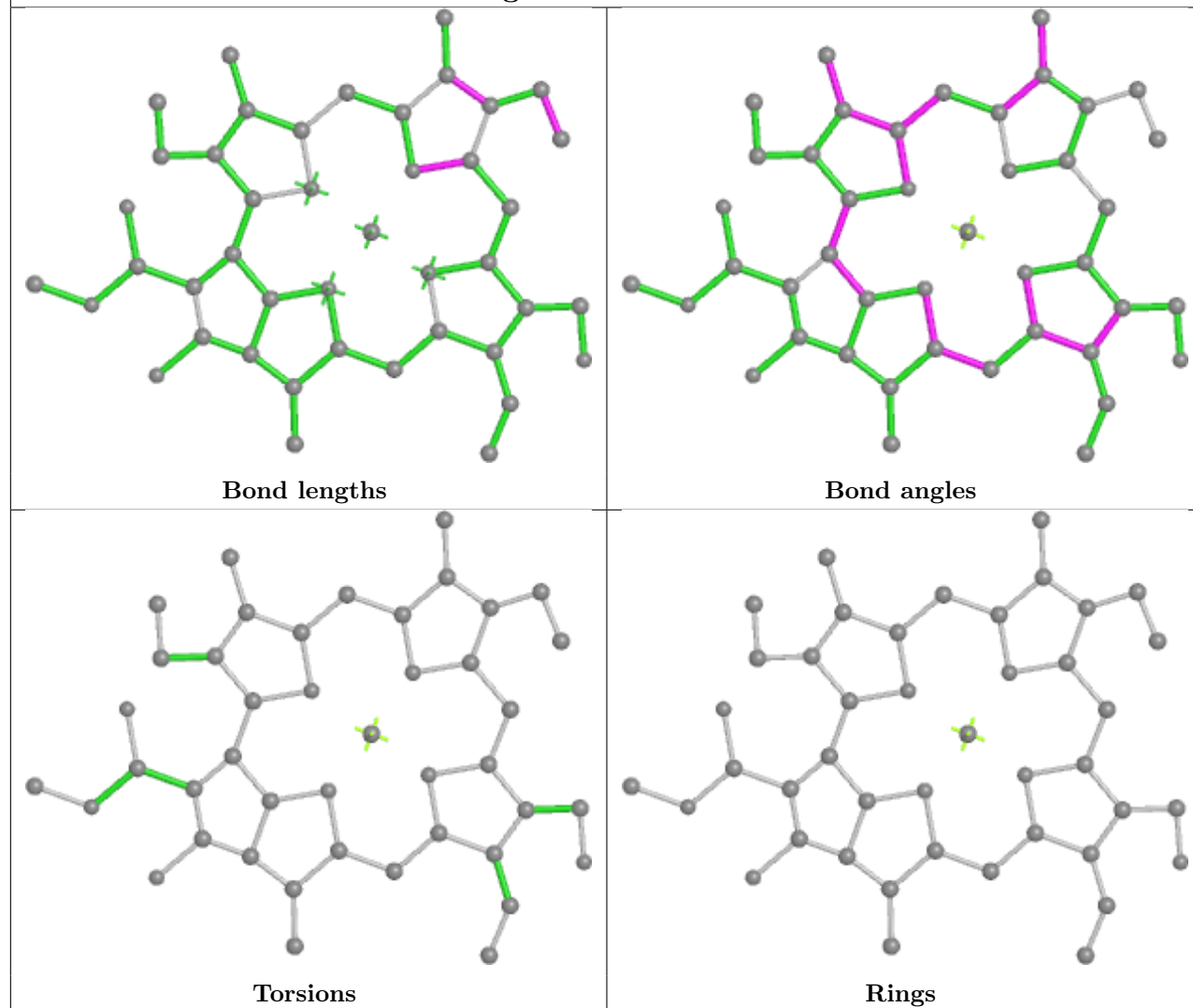




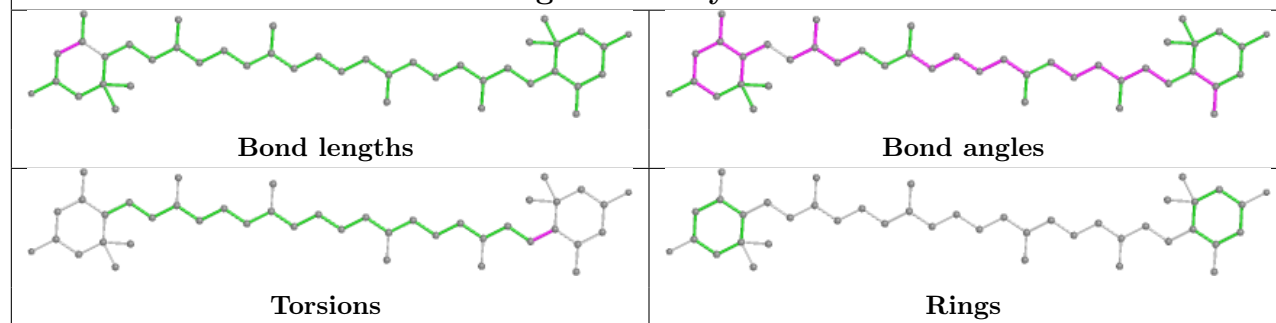


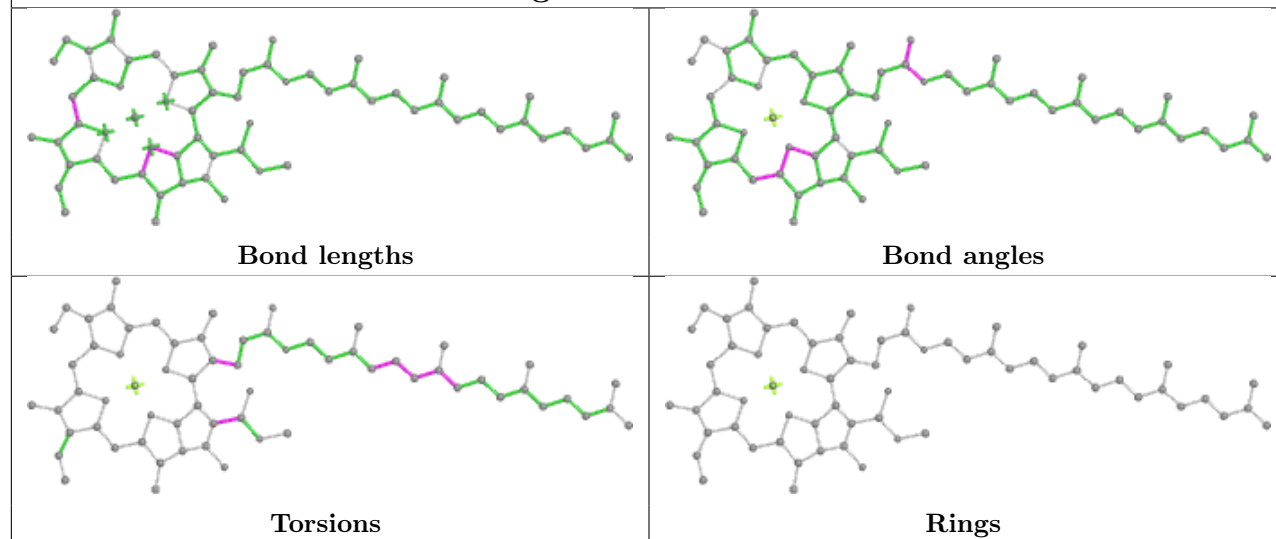
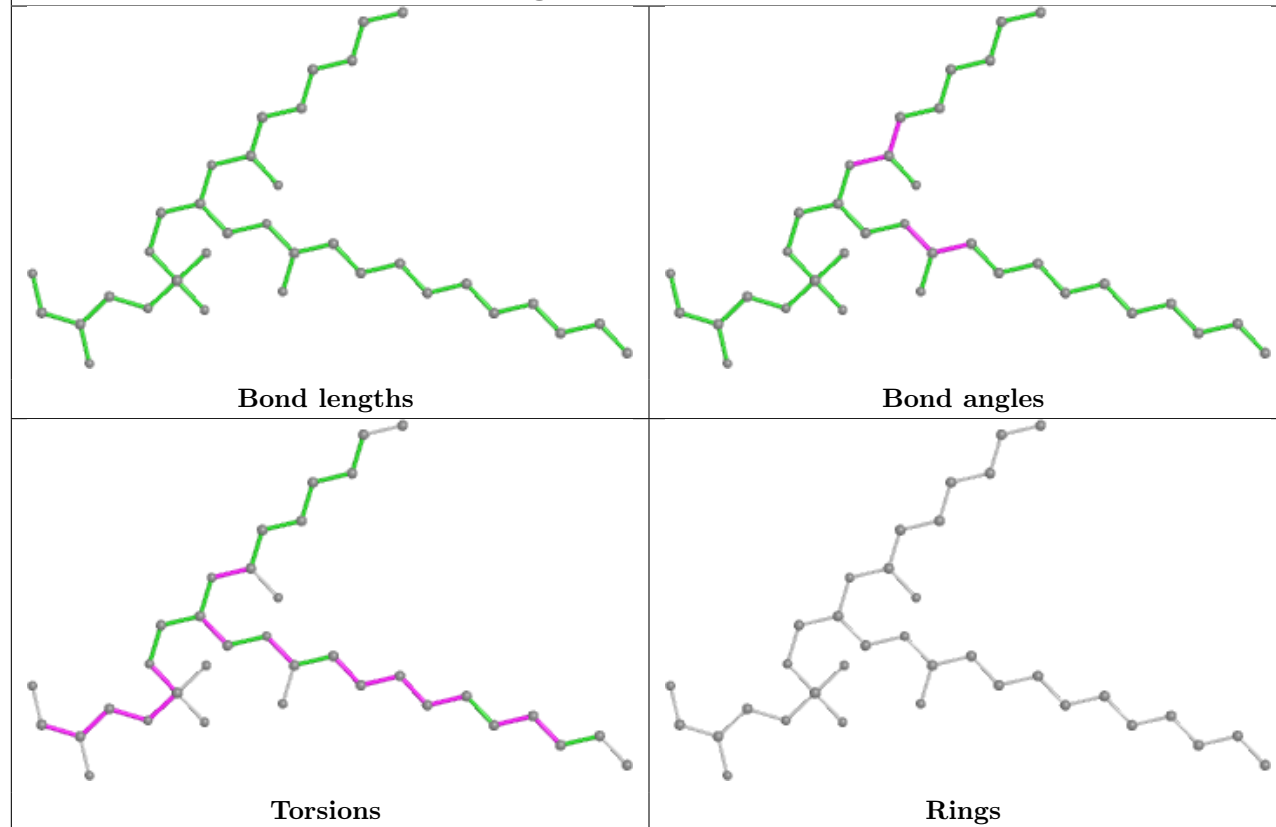


## Ligand CHL s 607

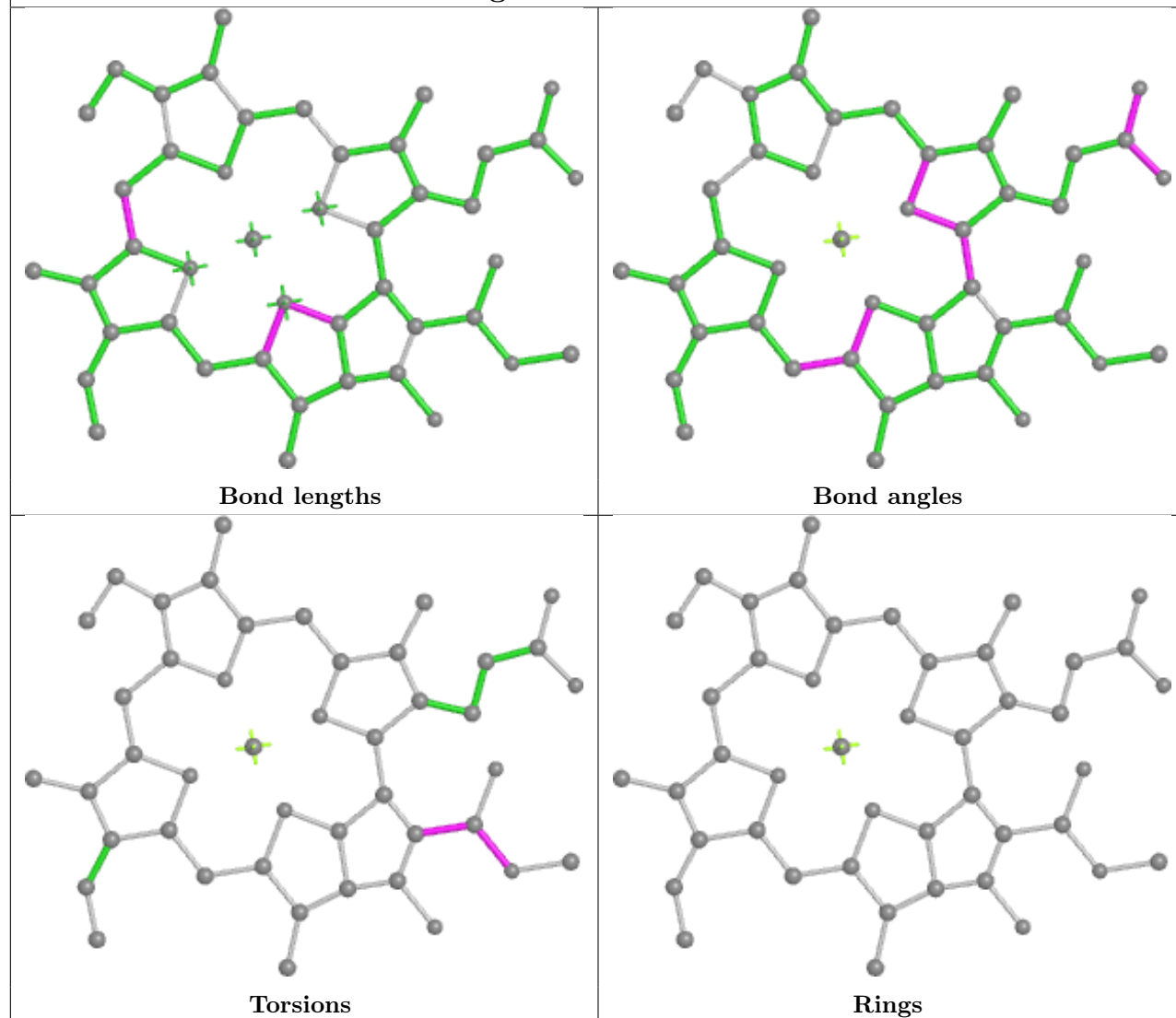


## Ligand LUT y 620

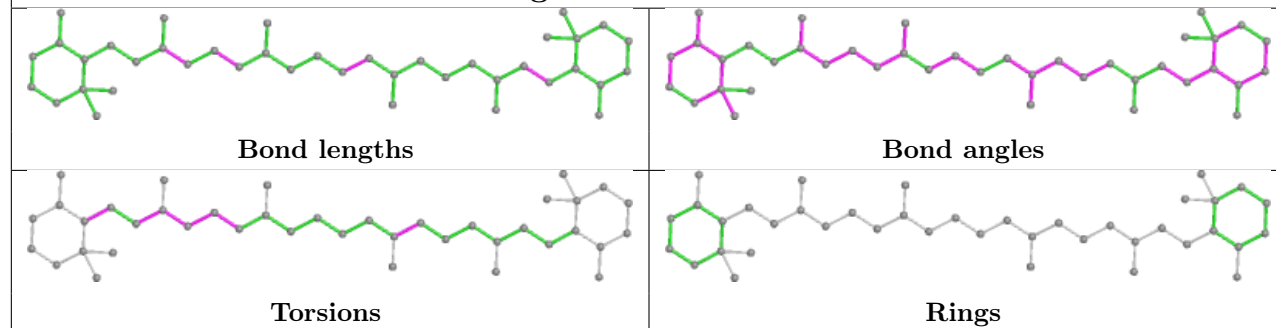


**Ligand CLA C 506****Ligand LHG C 525**

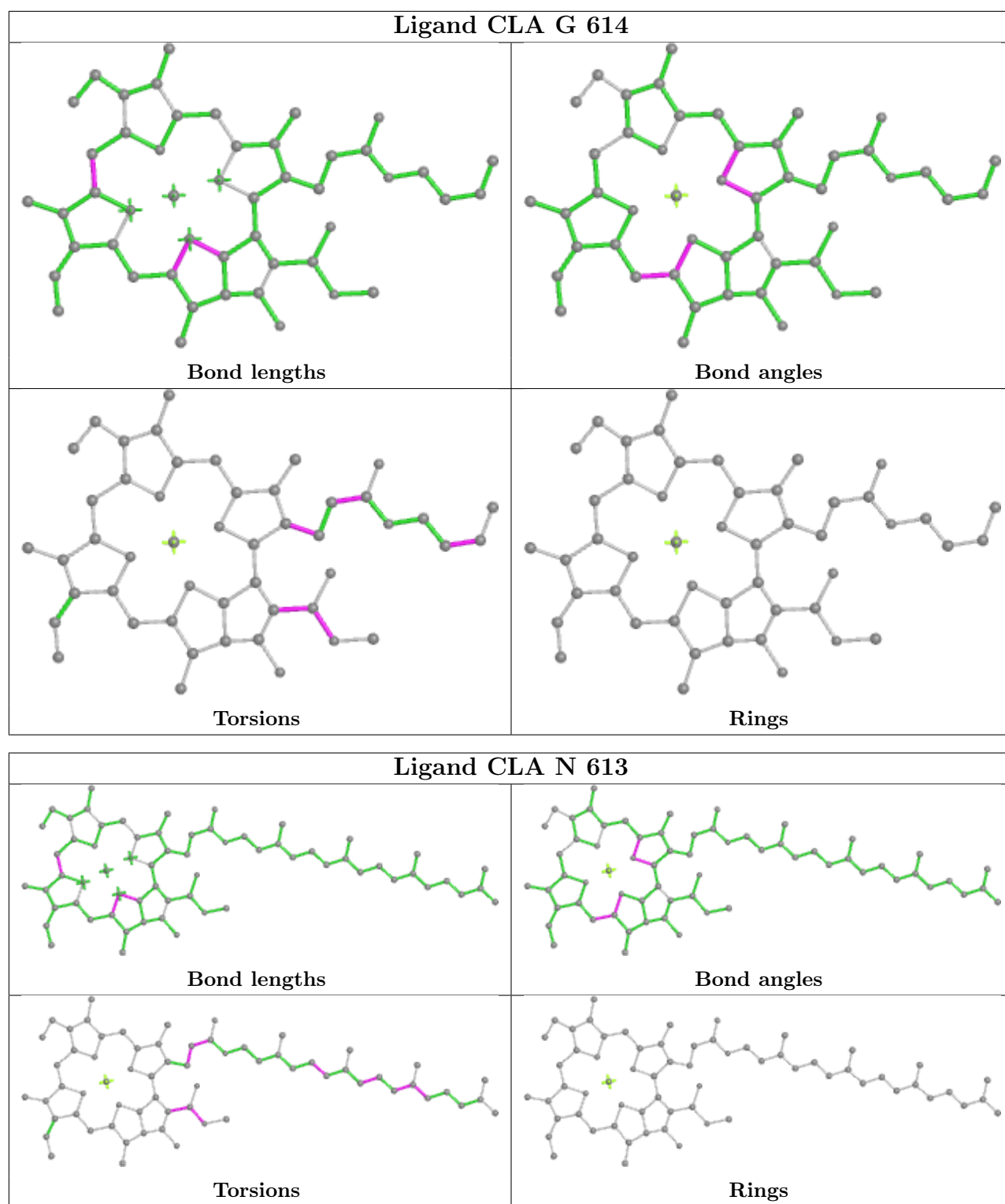
## Ligand CLA N 612

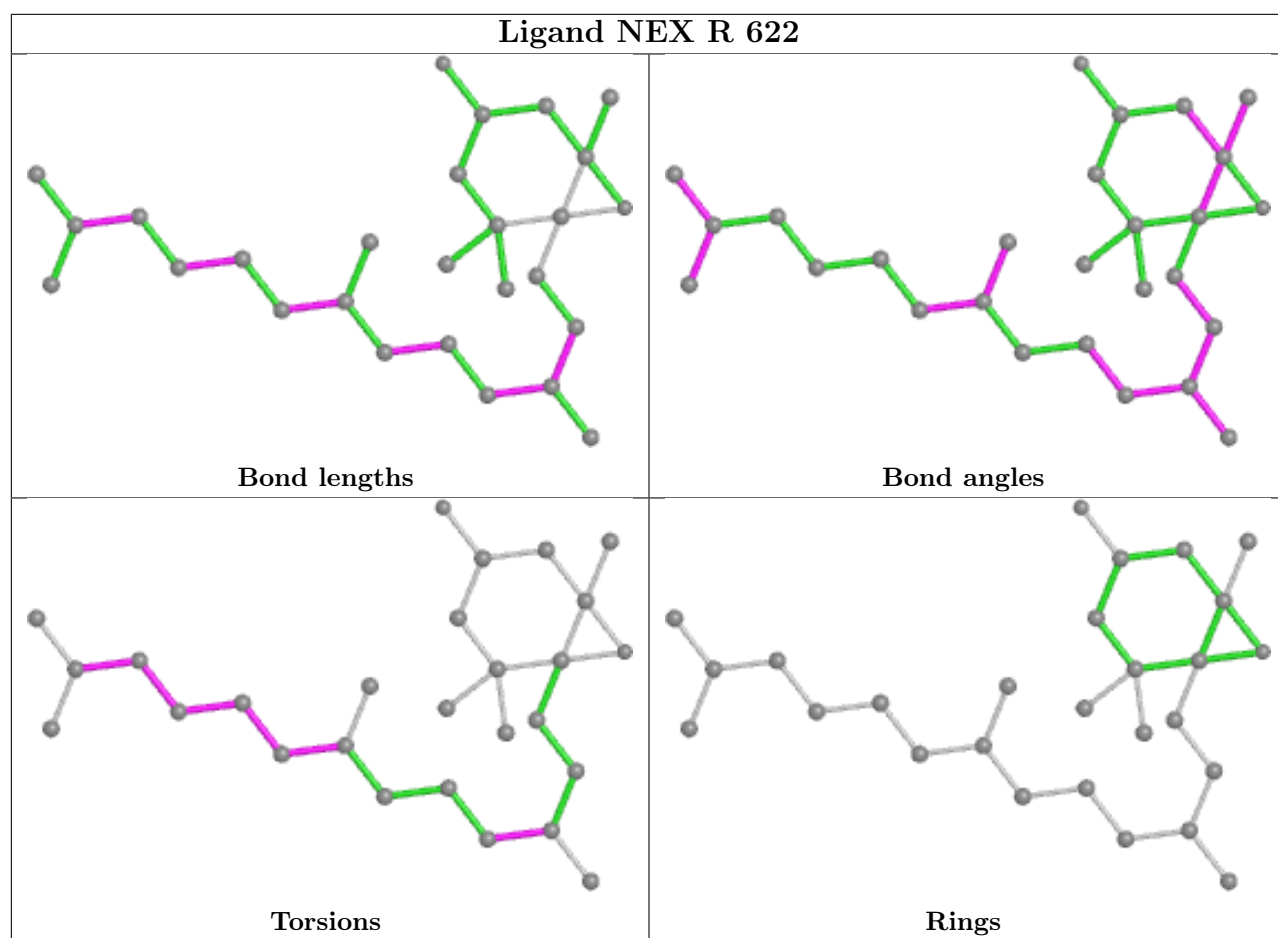


## Ligand BCR C 517

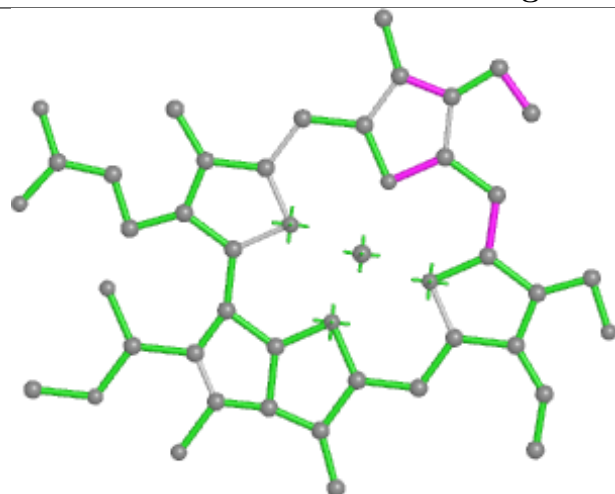




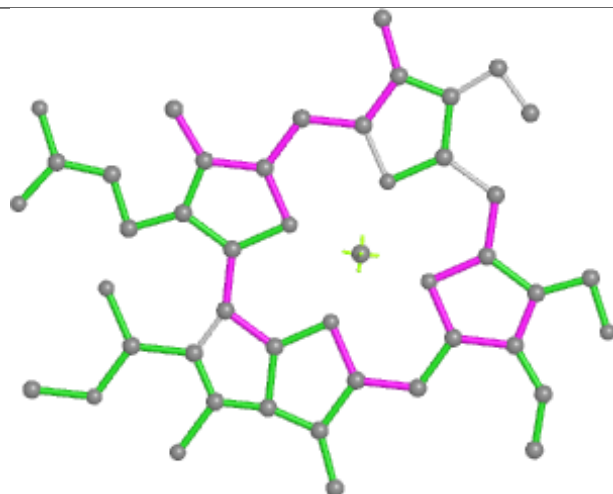




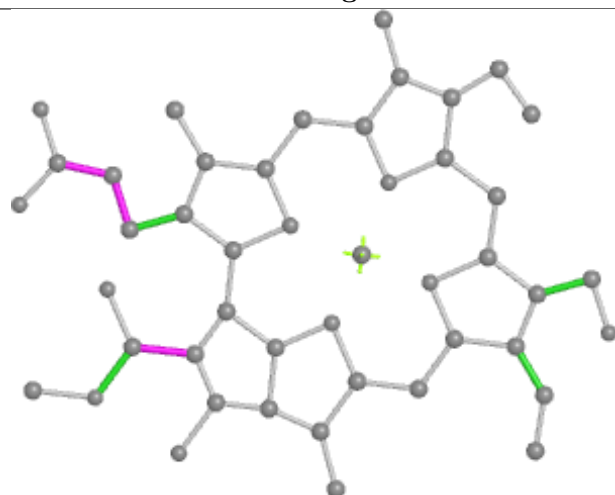
## Ligand CHL s 601



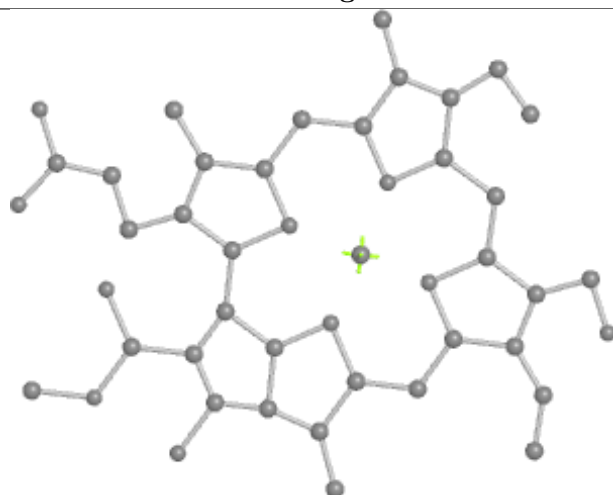
Bond lengths



Bond angles

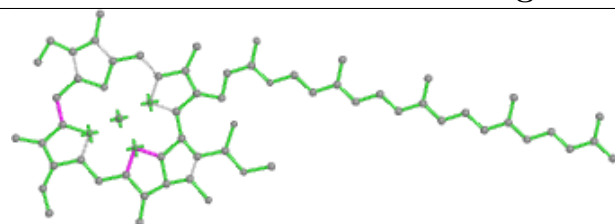


Torsions

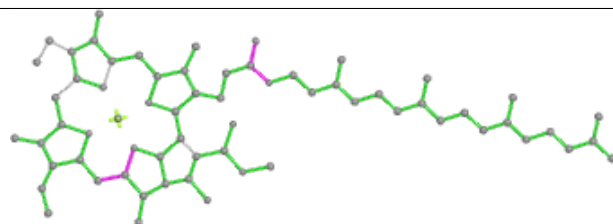


Rings

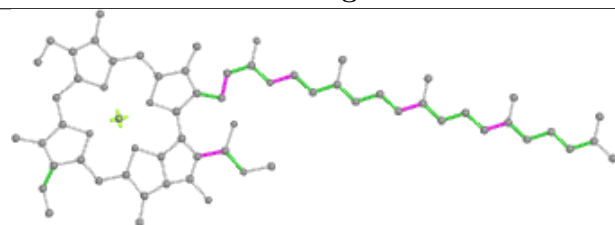
## Ligand CLA B 609



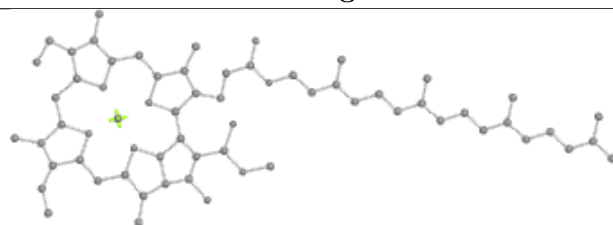
Bond lengths



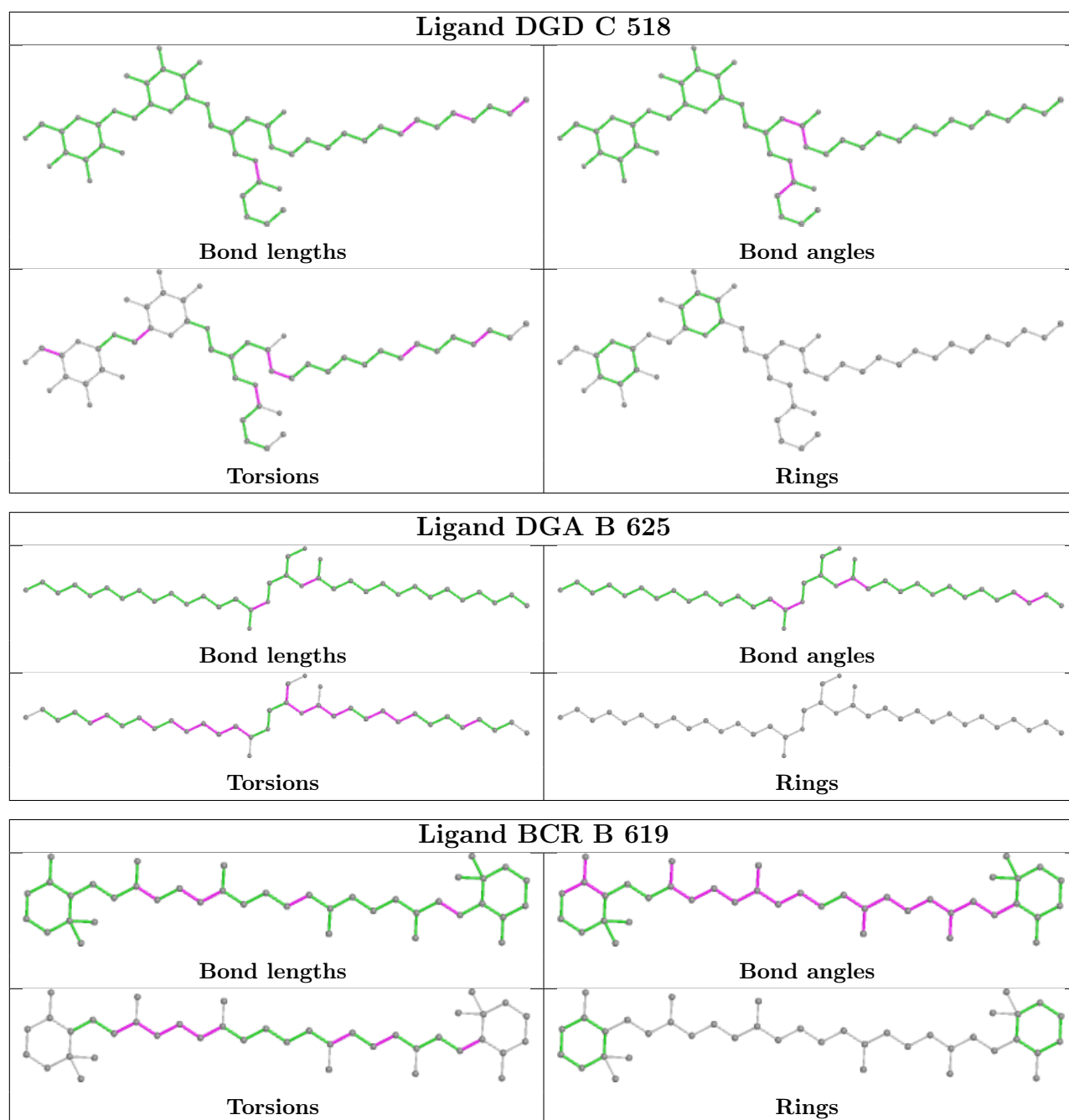
Bond angles

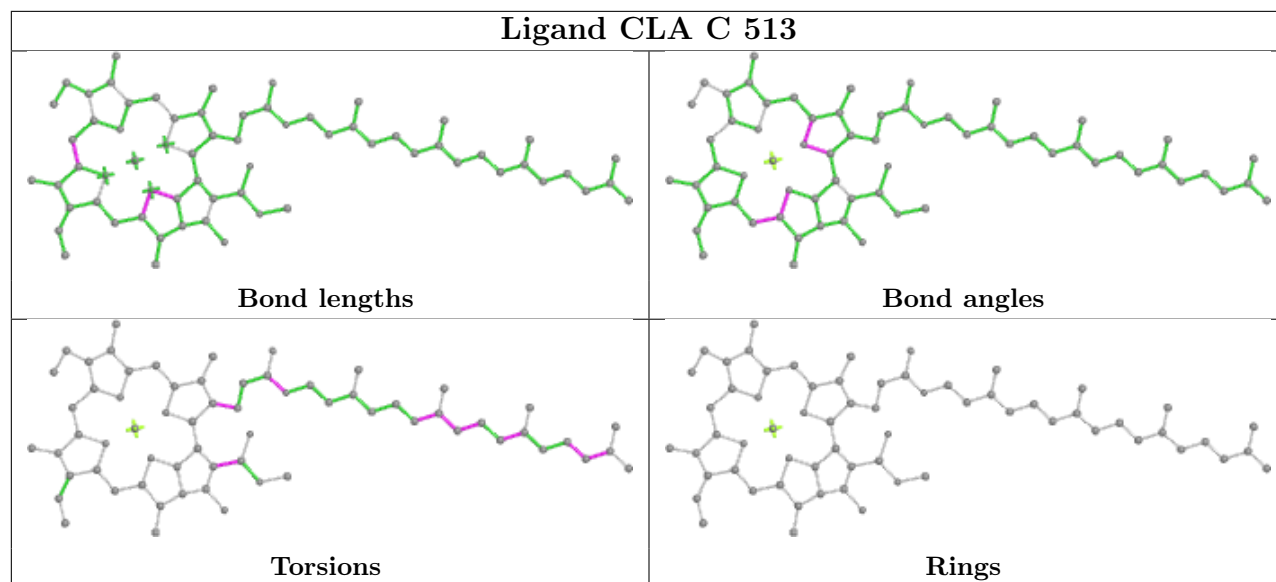
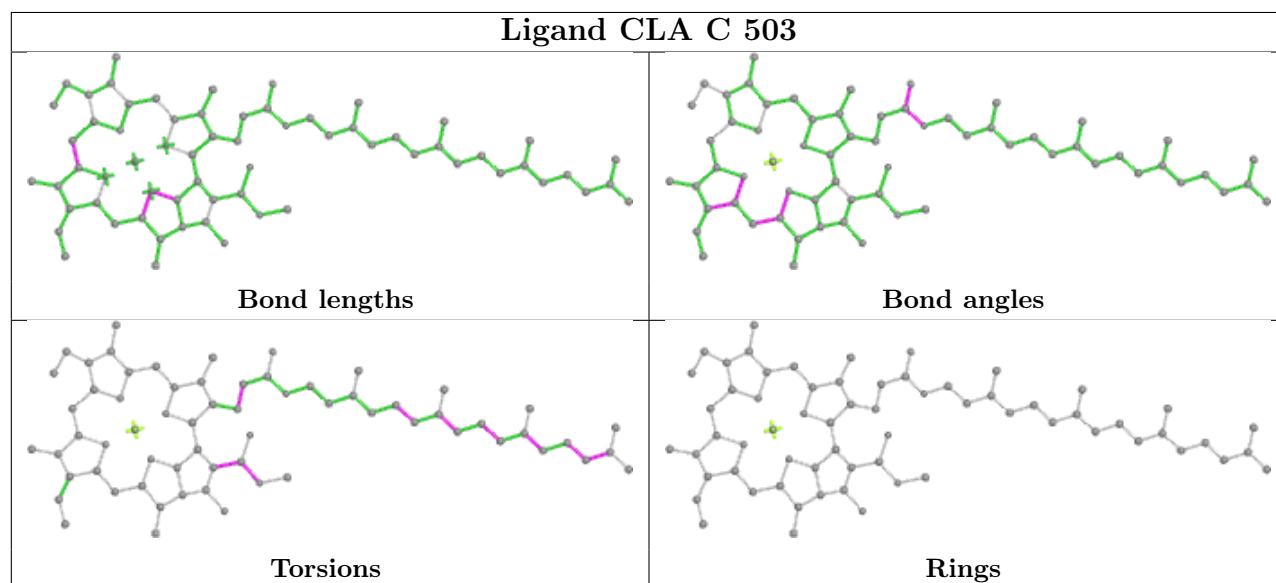


Torsions

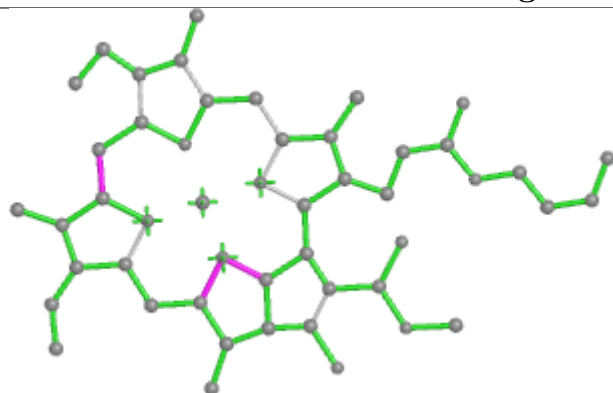


Rings

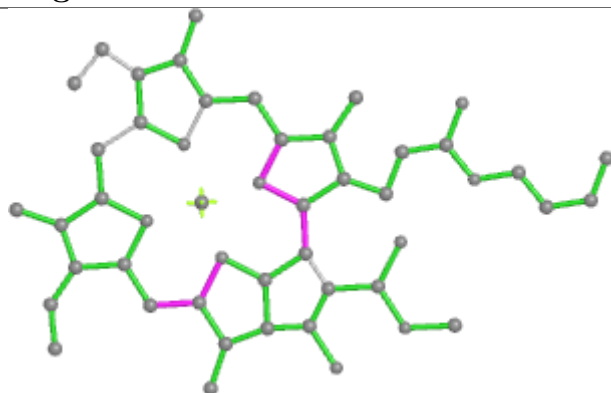


**Ligand CLA C 513****Ligand CLA C 503**

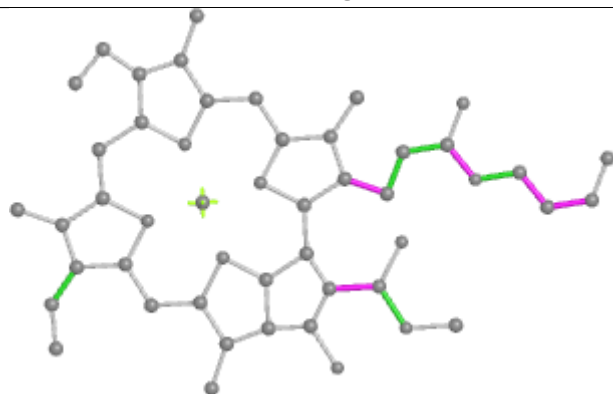
## Ligand CLA g 604



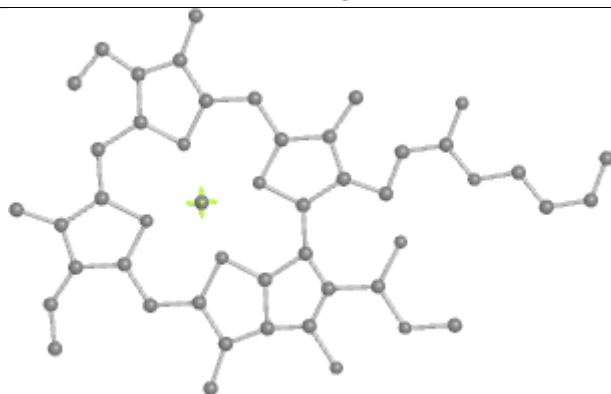
Bond lengths



Bond angles

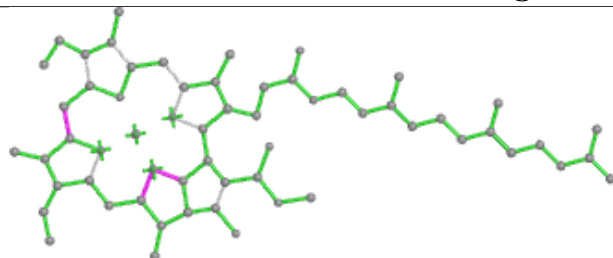


Torsions

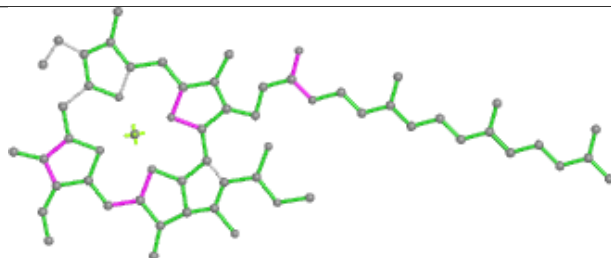


Rings

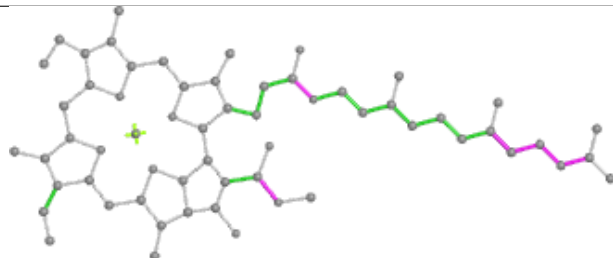
## Ligand CLA D 403



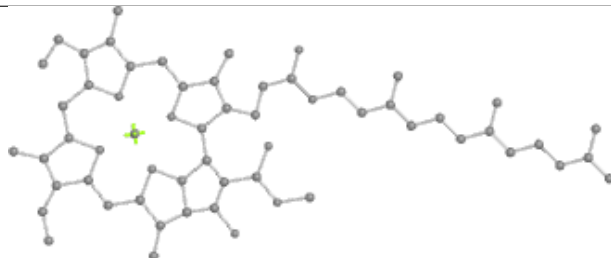
Bond lengths



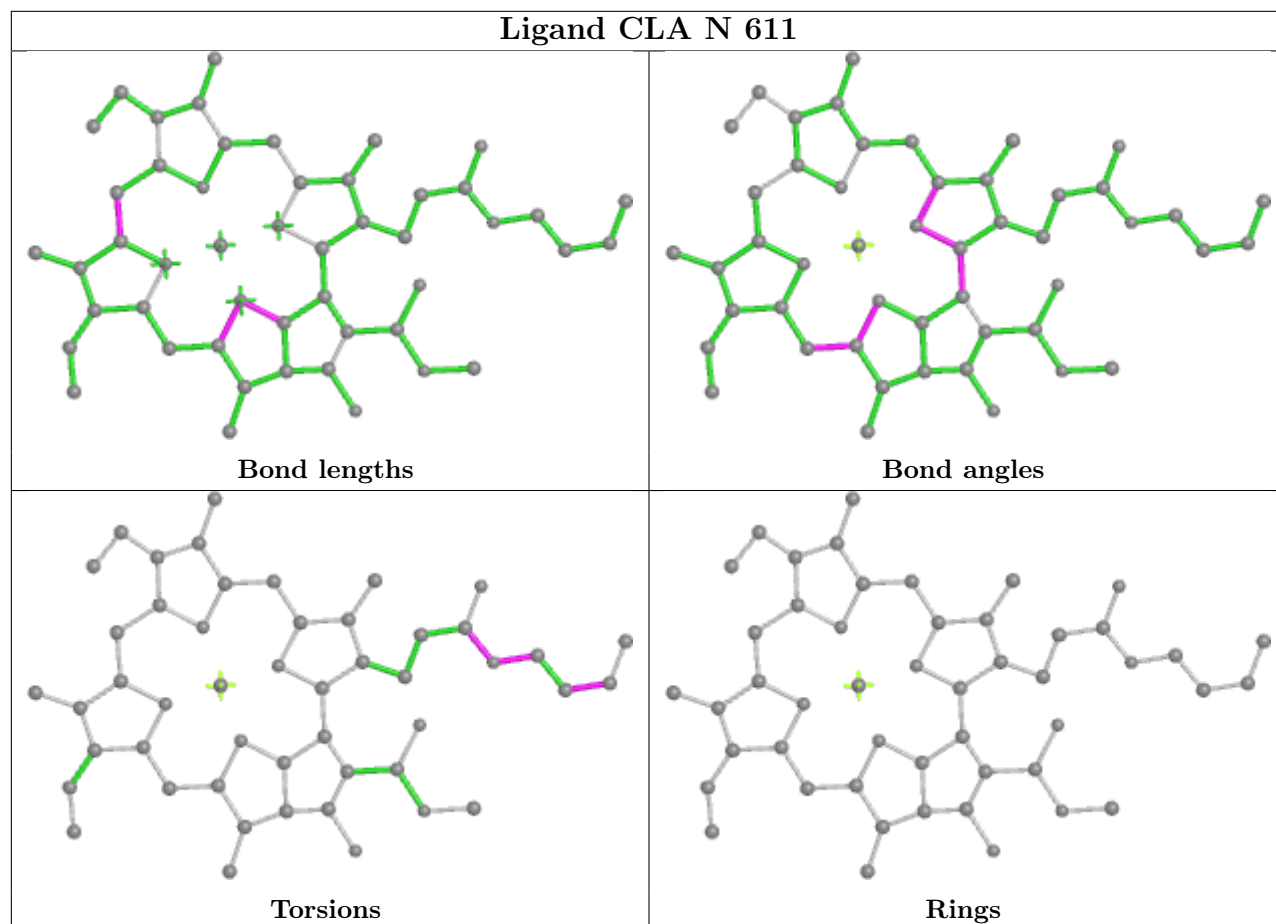
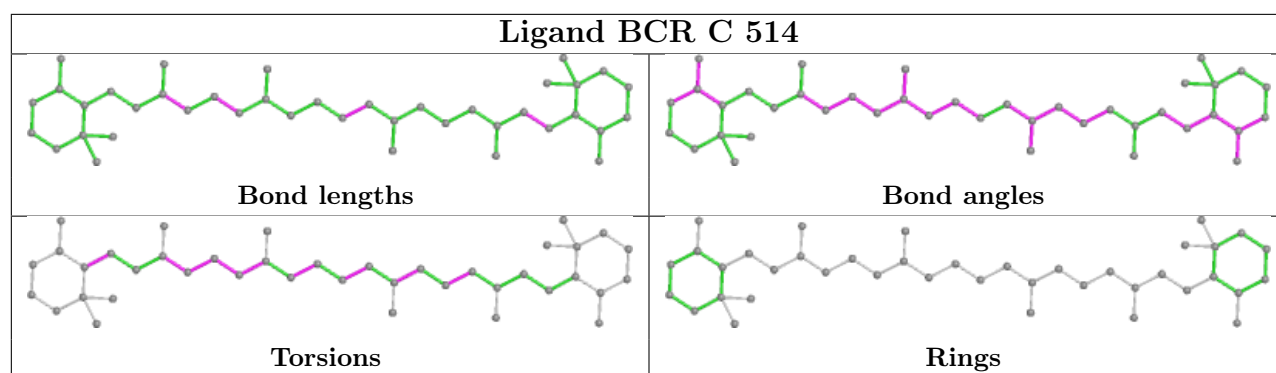
Bond angles

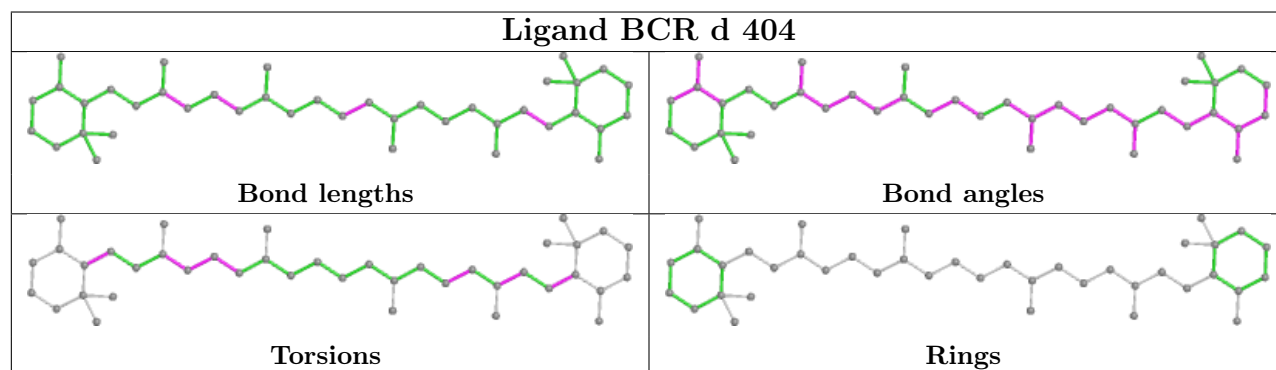
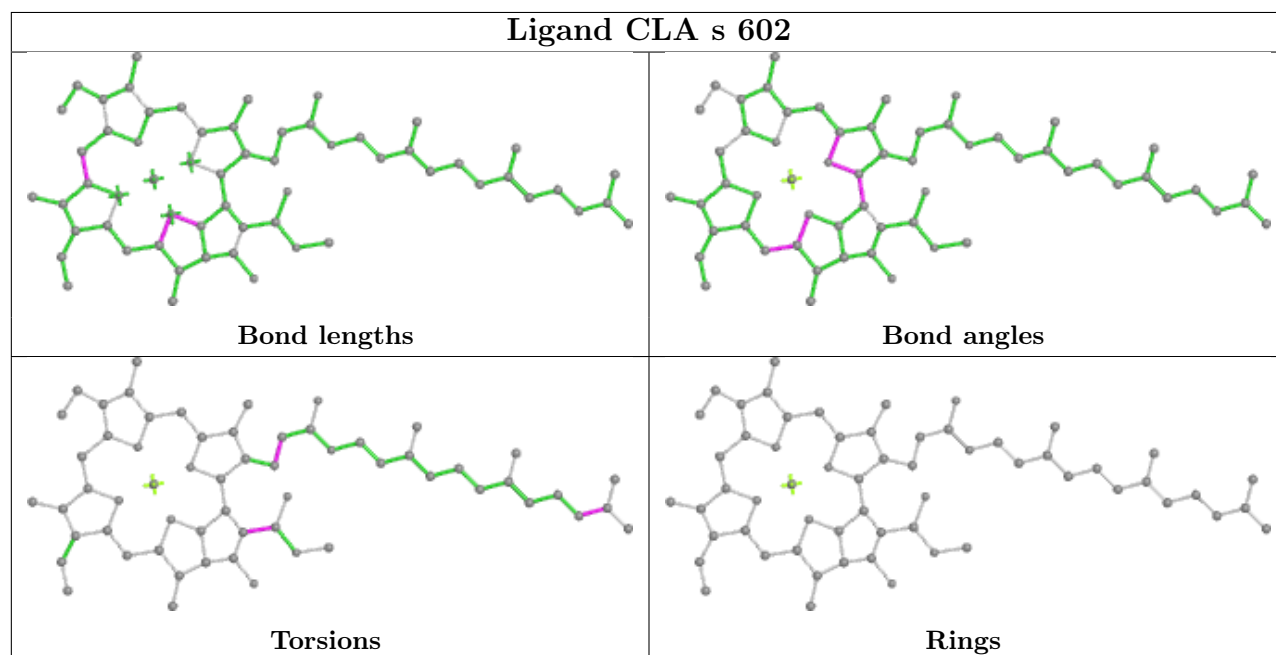
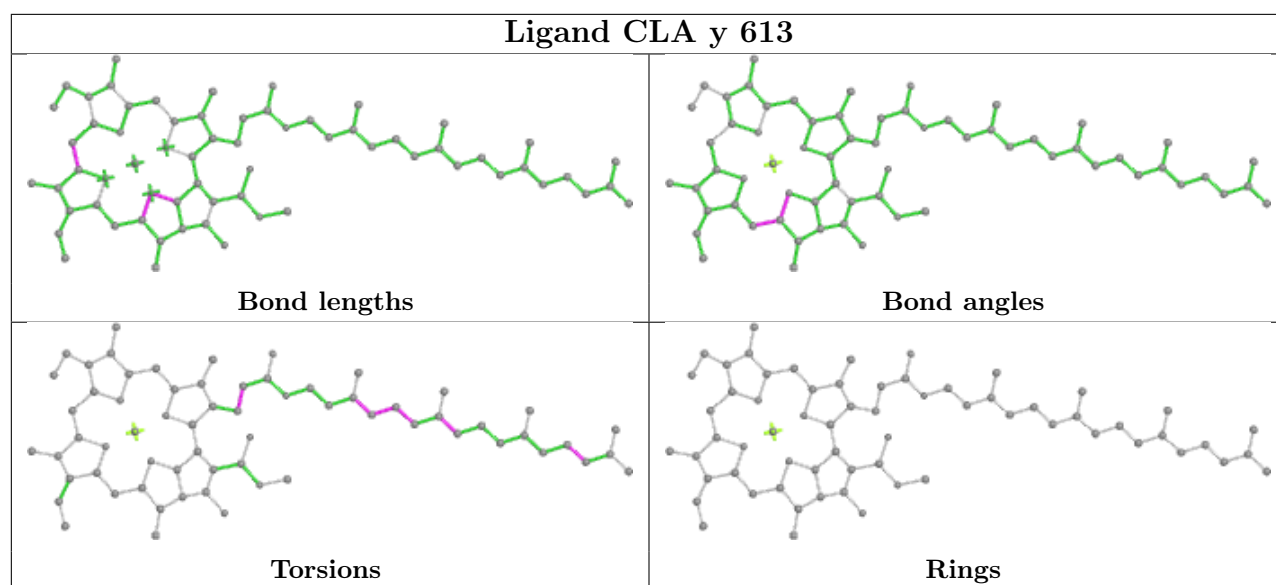


Torsions



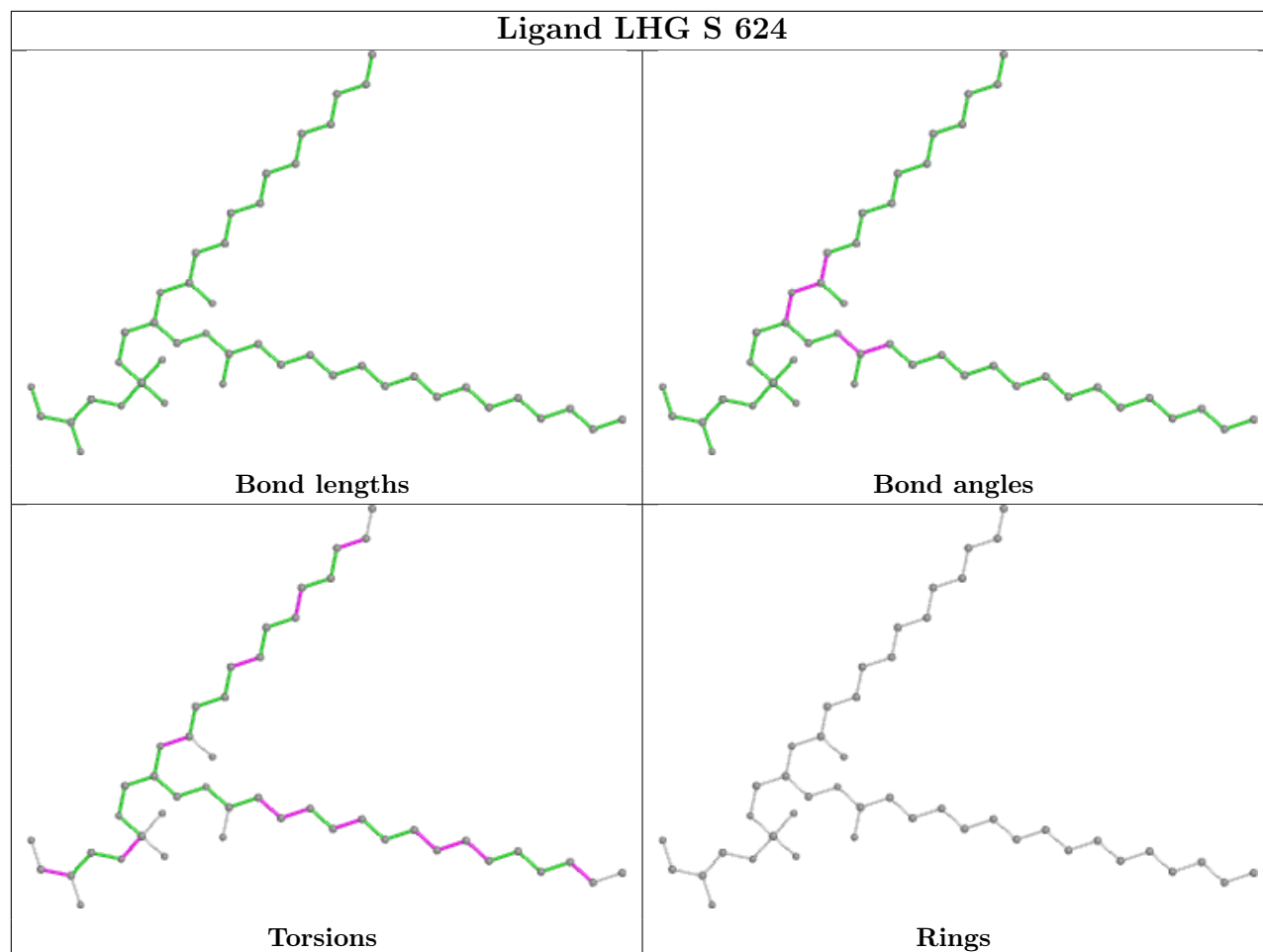
Rings



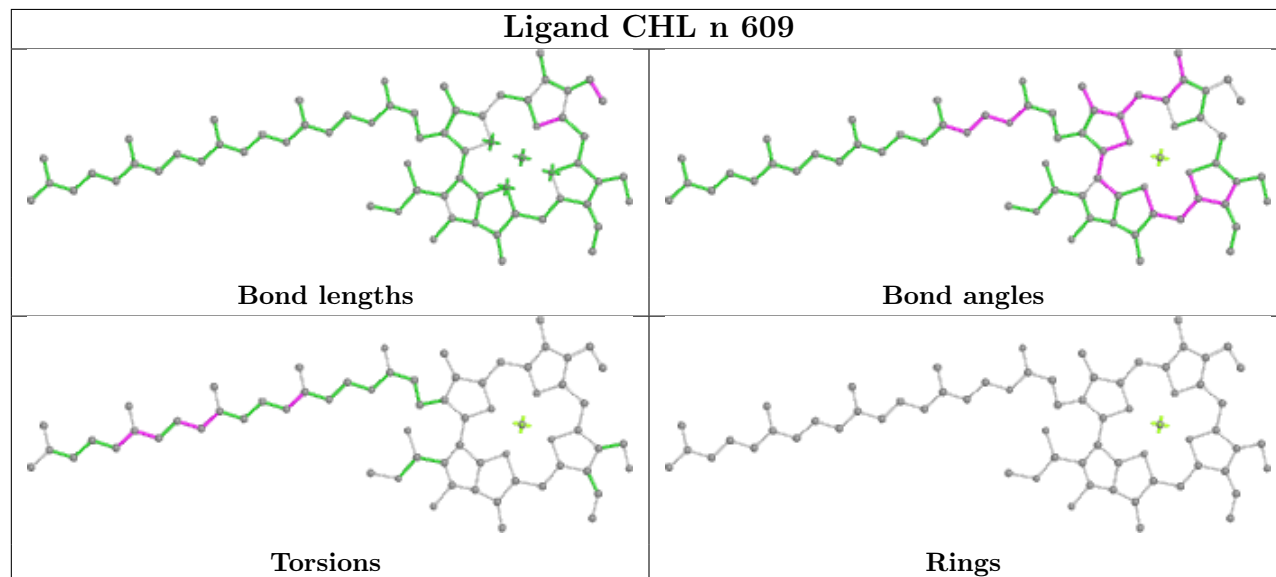




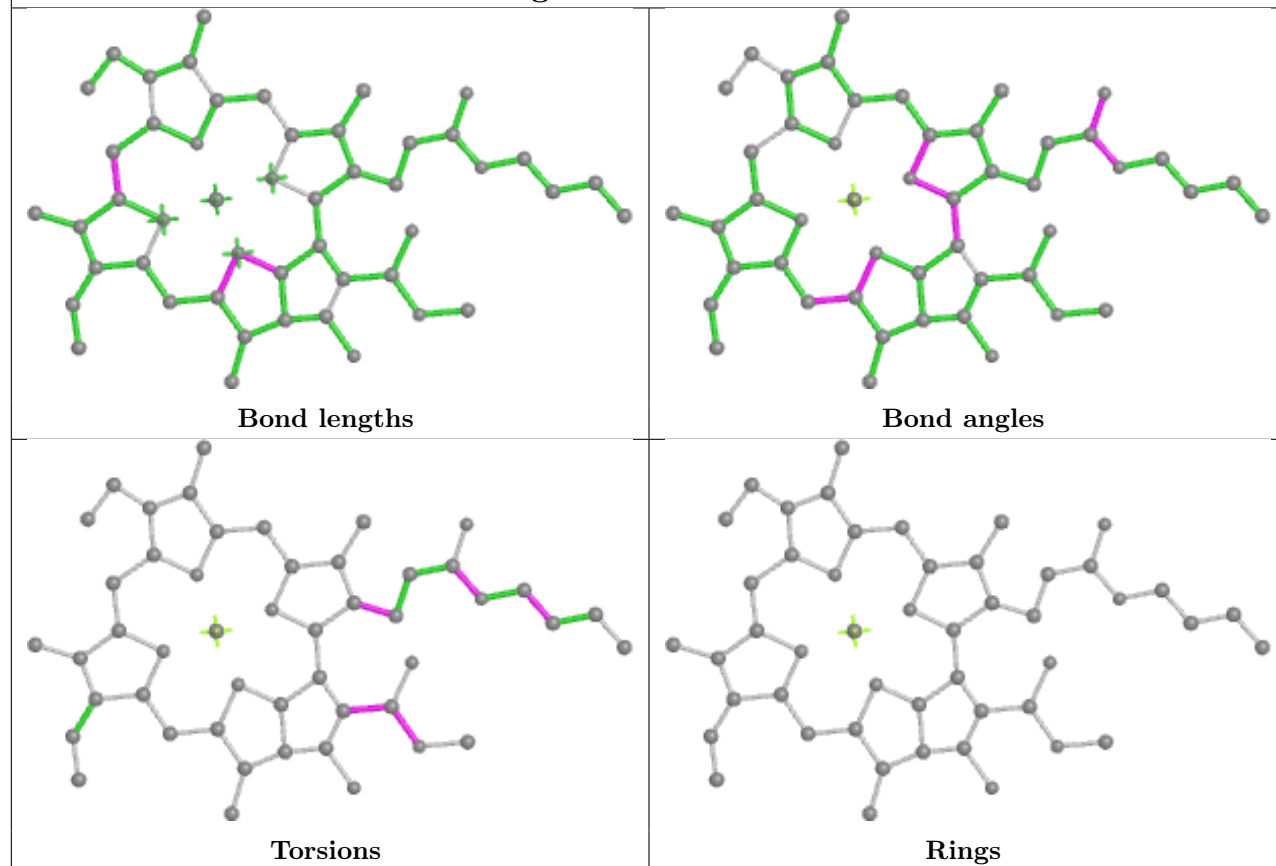
## Ligand LHG S 624



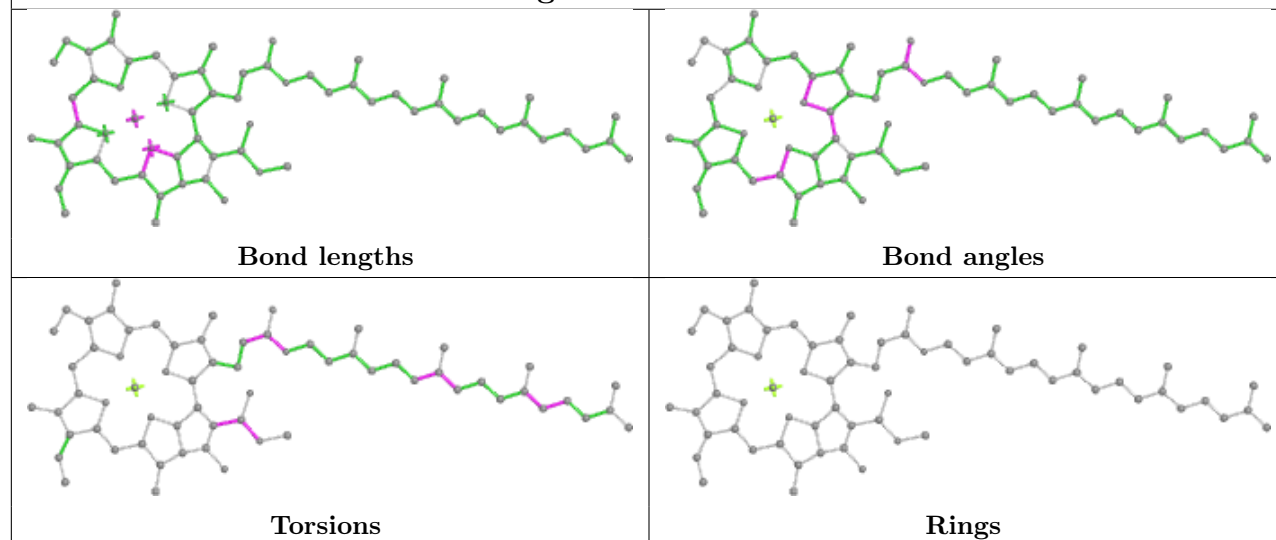
## Ligand CHL n 609

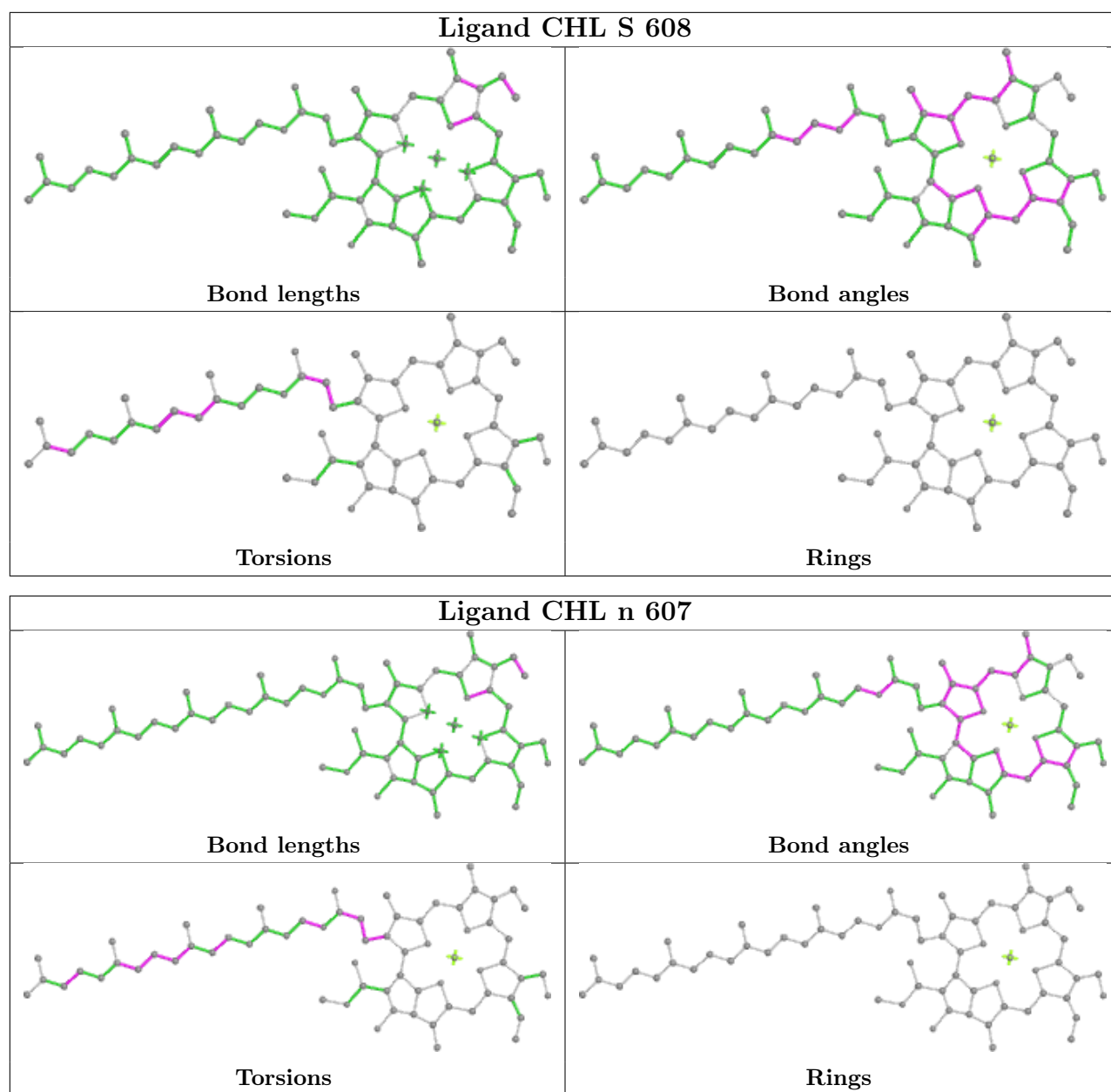


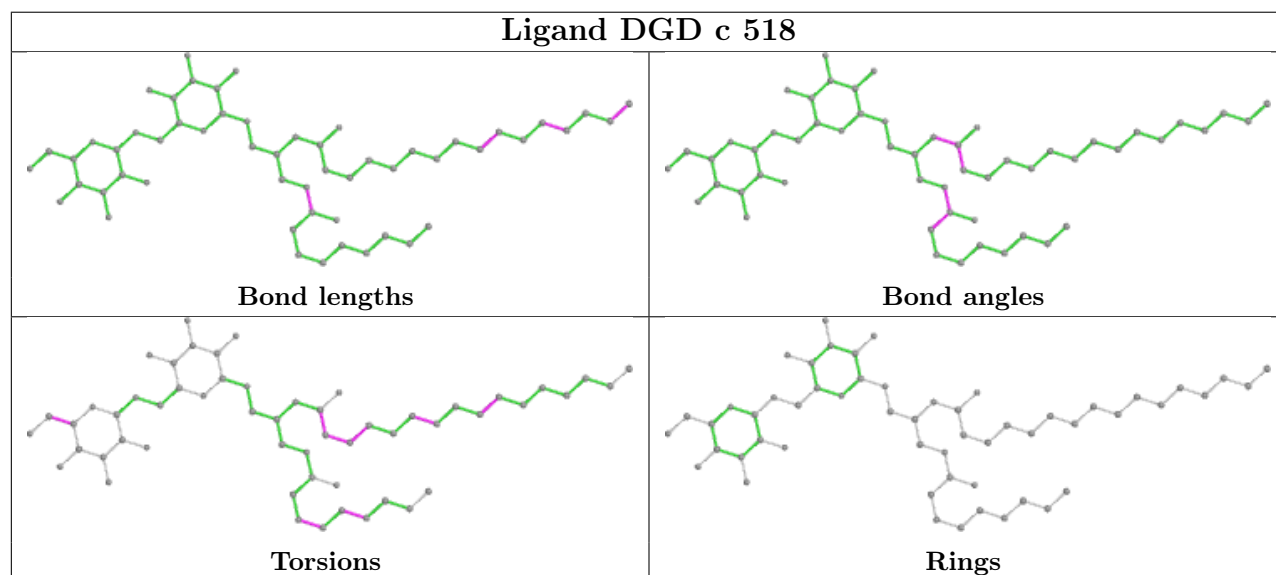
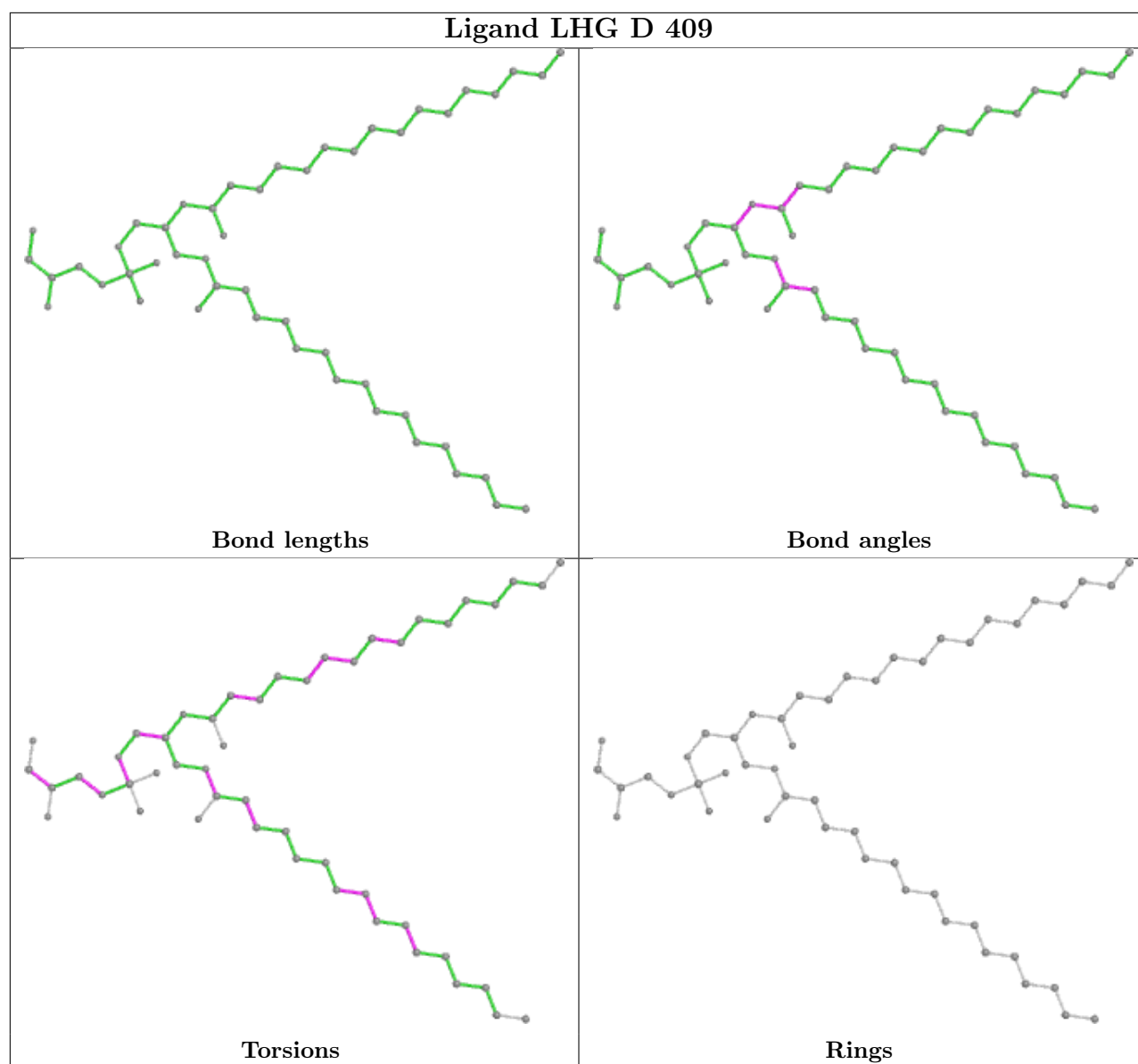
## Ligand CLA N 614

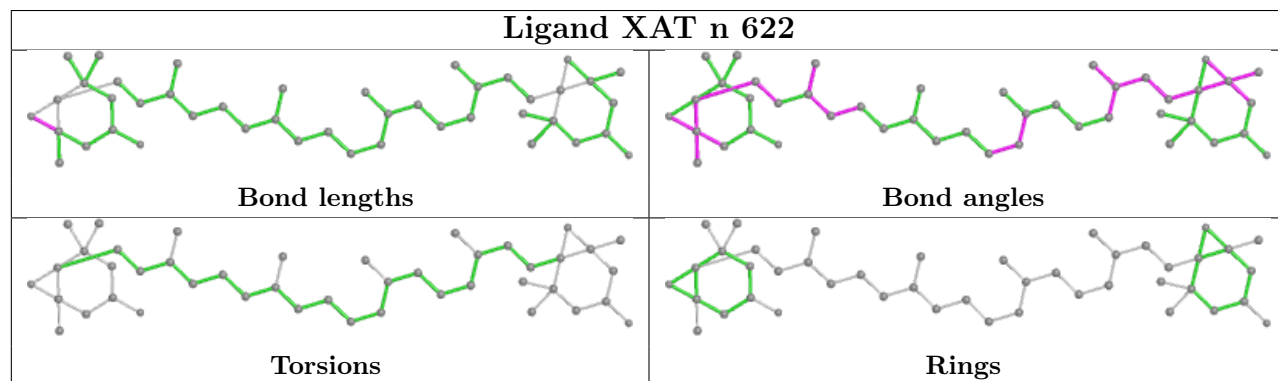
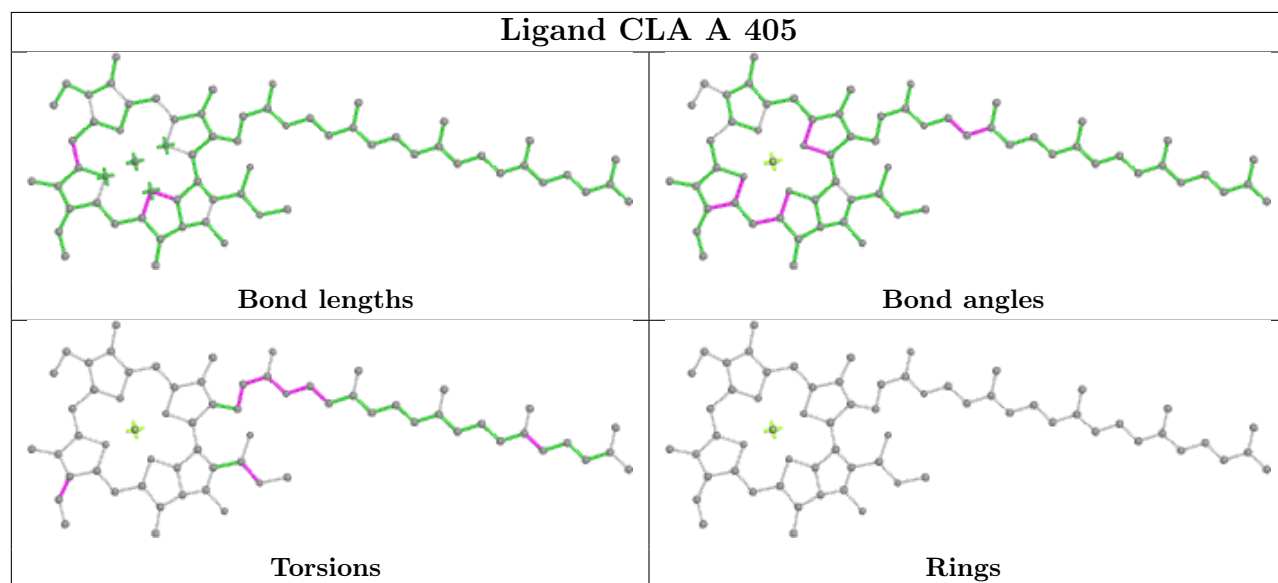
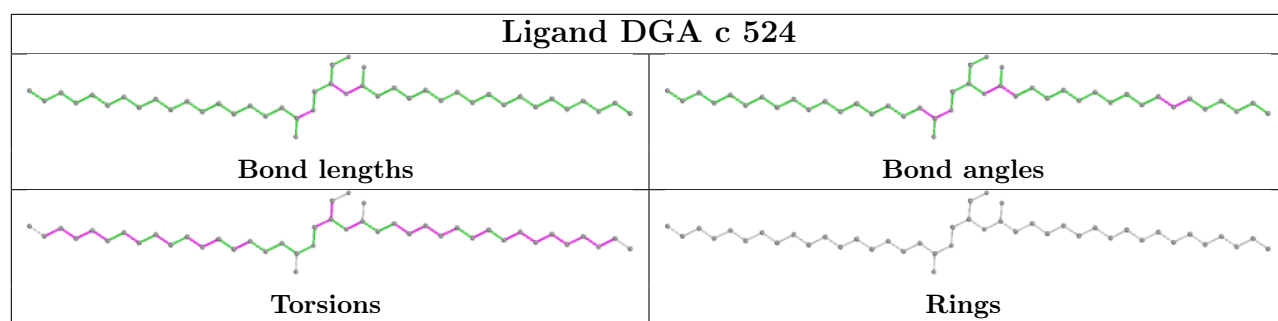


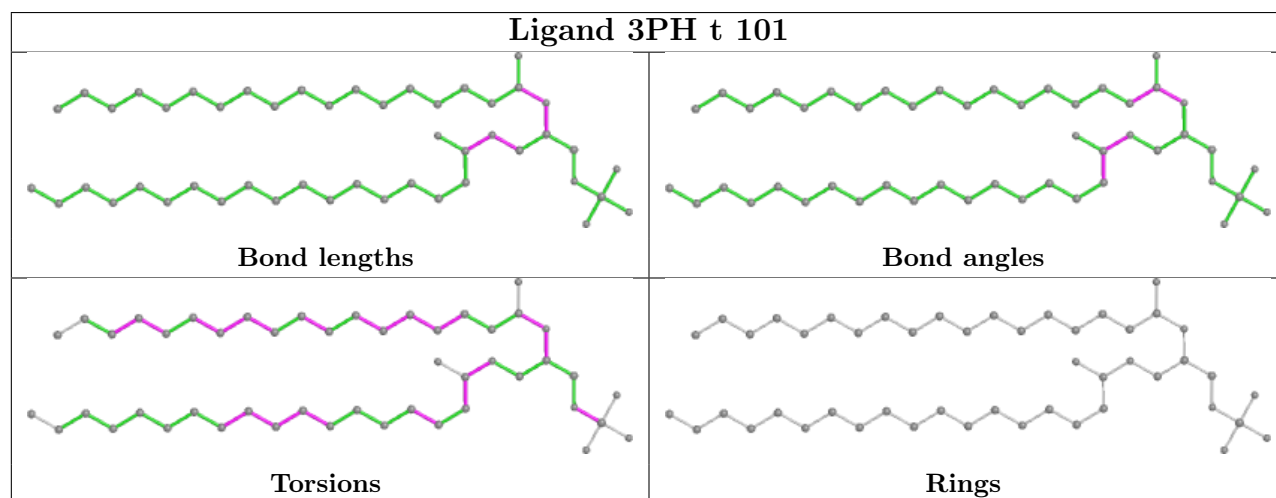
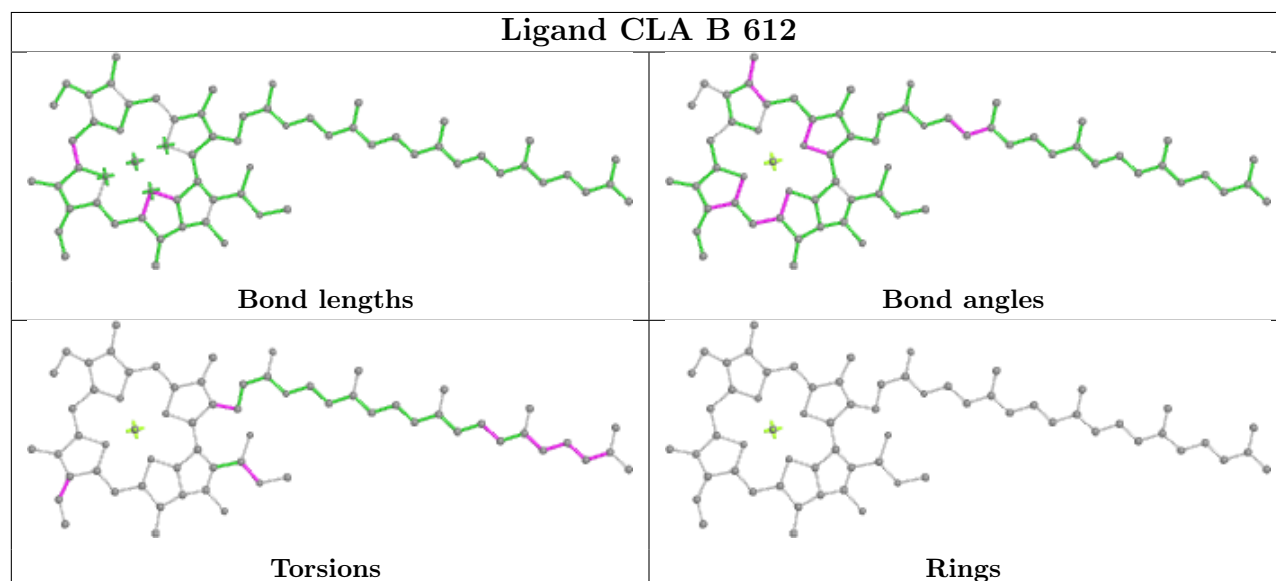
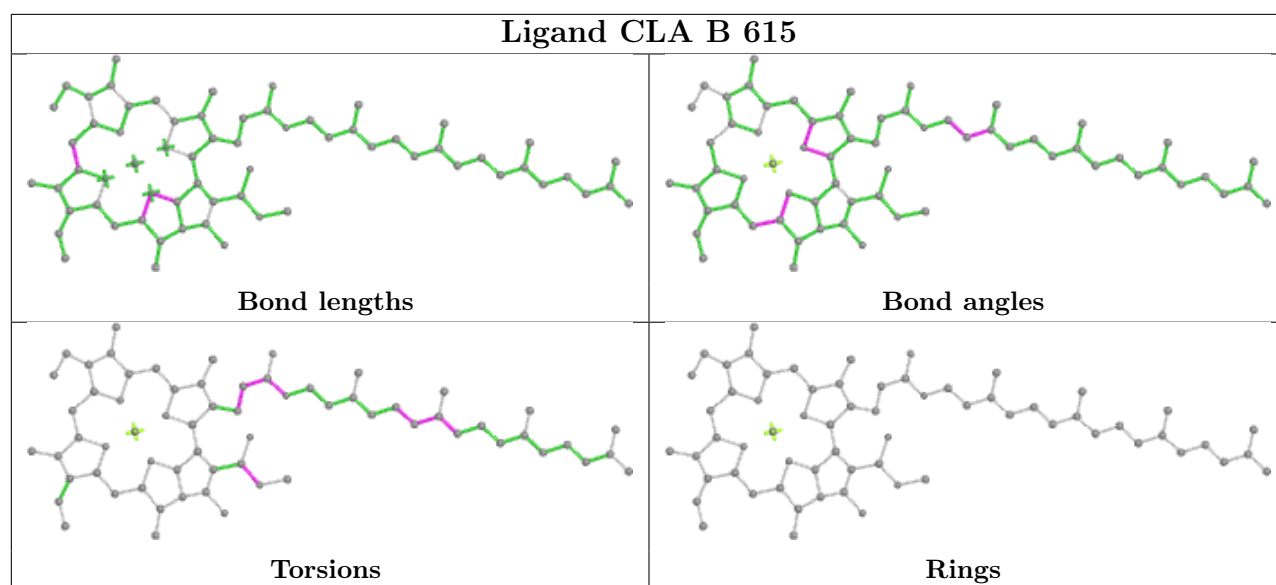
## Ligand CLA c 507

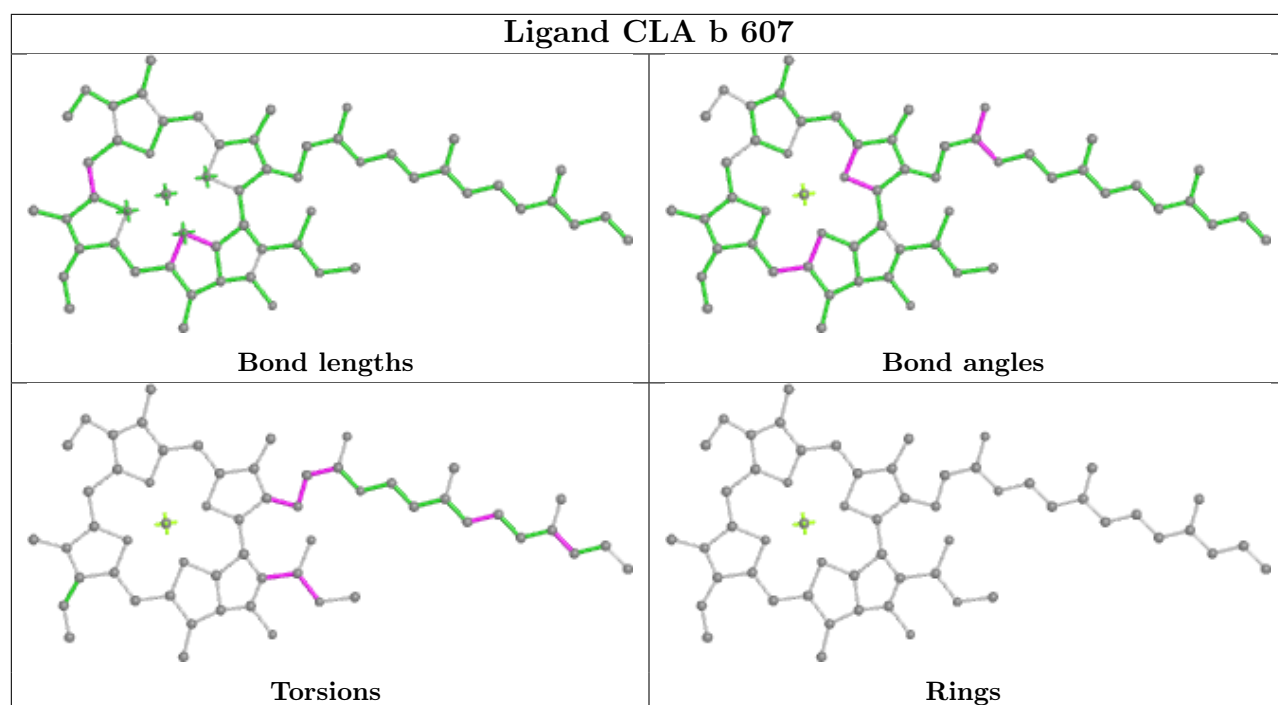




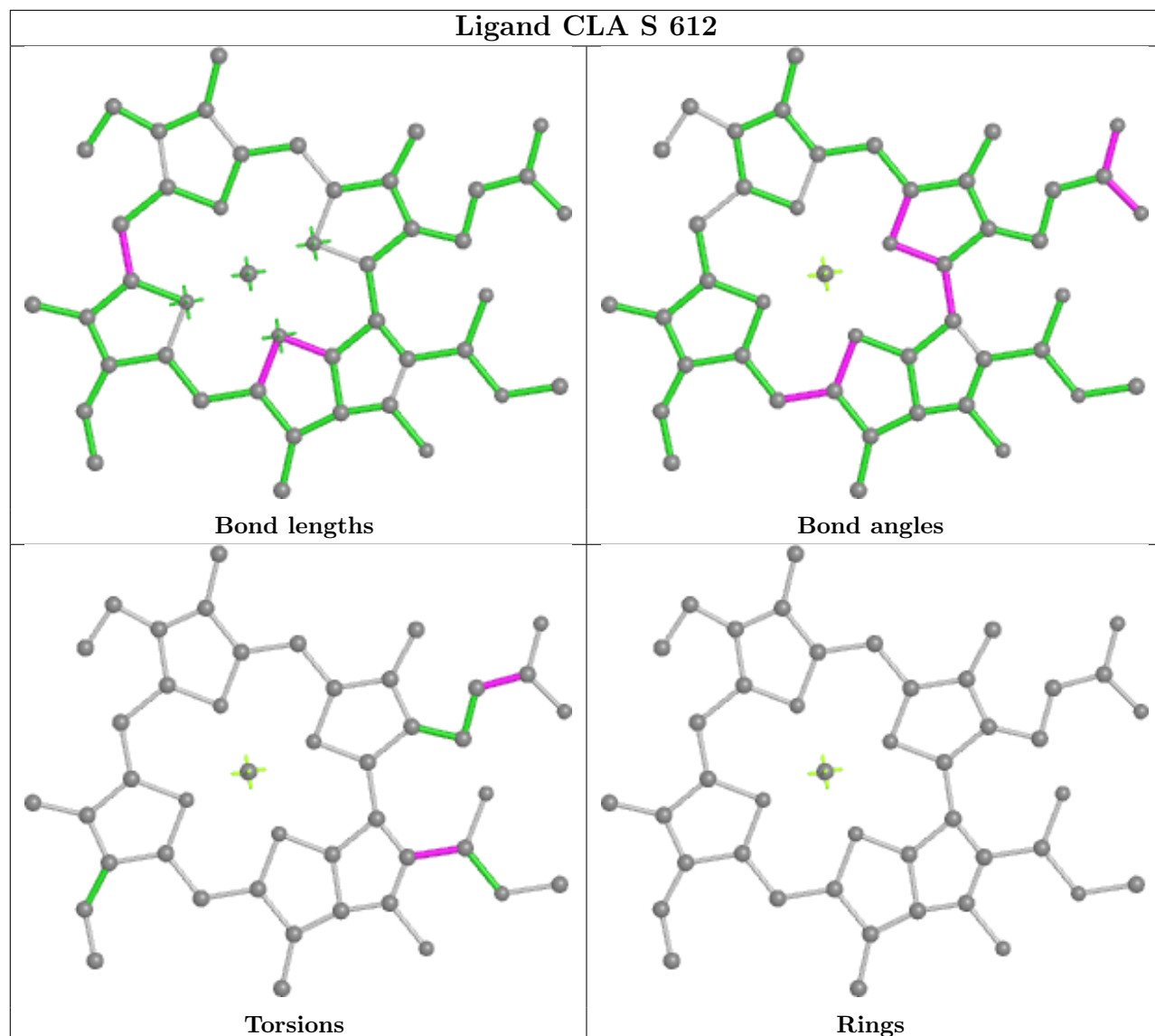




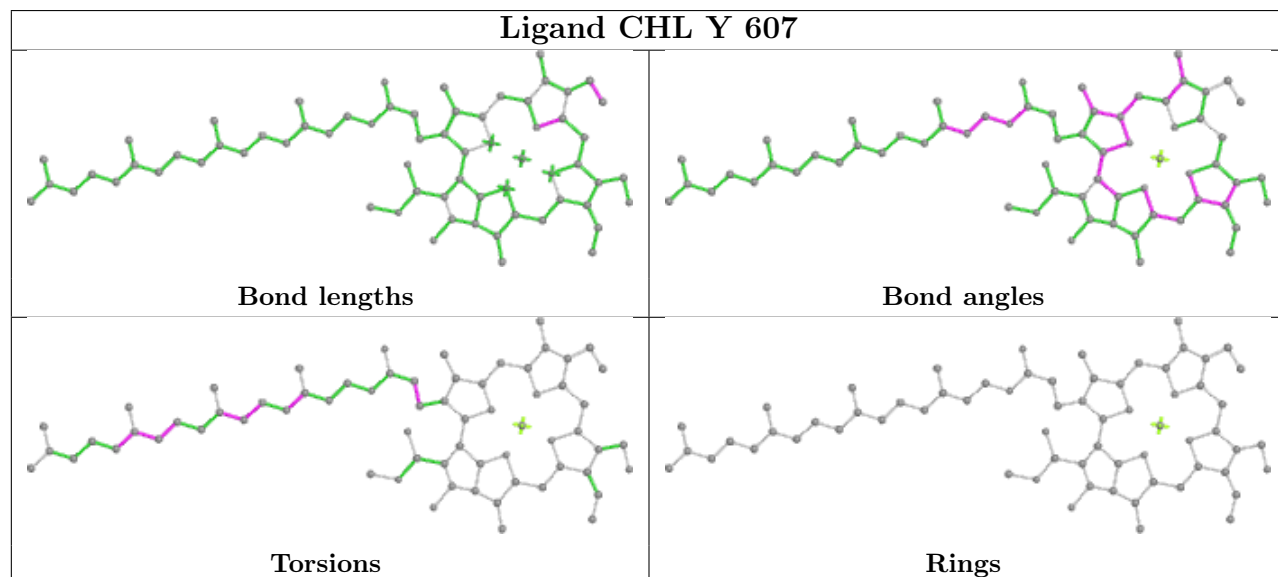




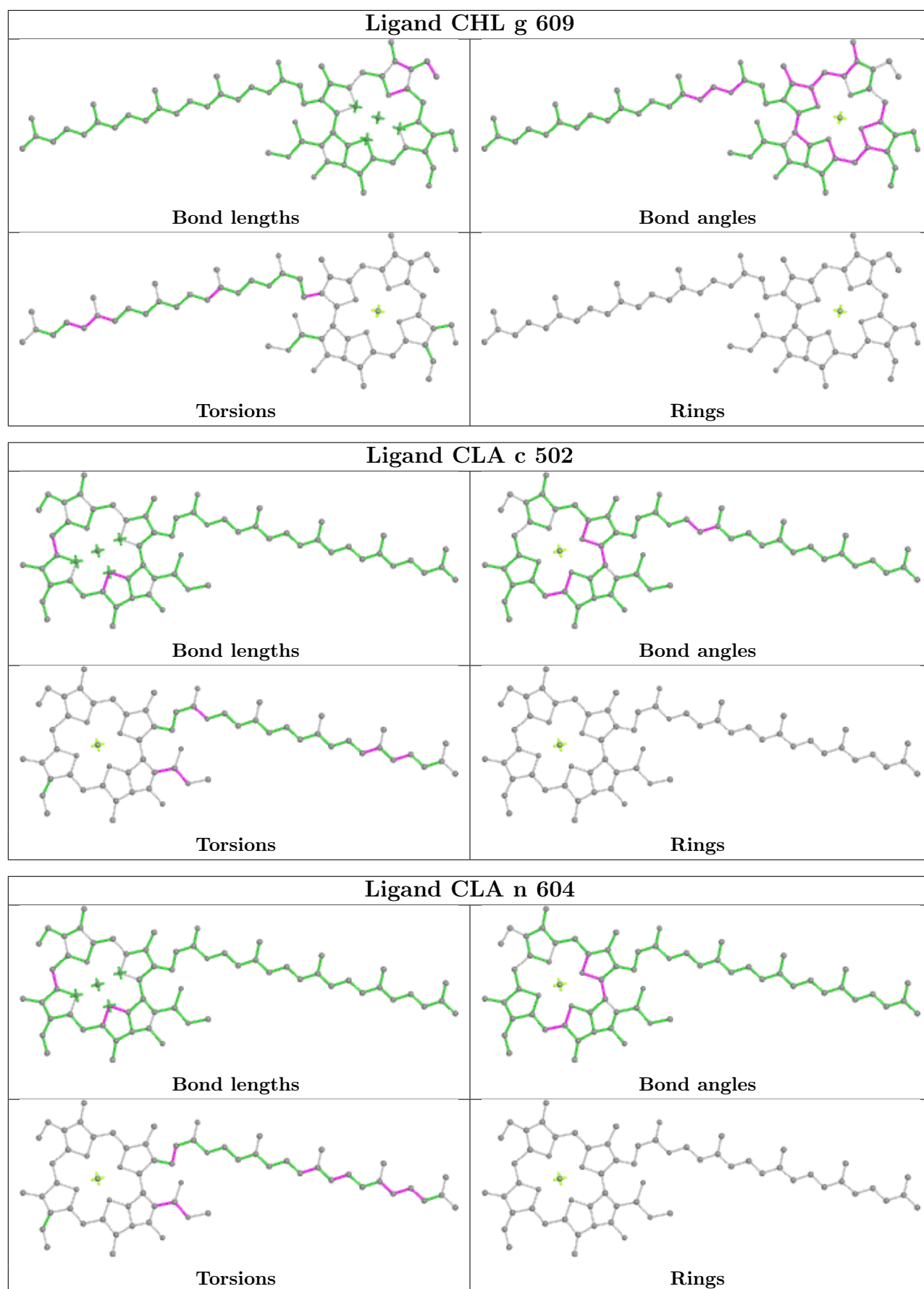
## Ligand CLA S 612

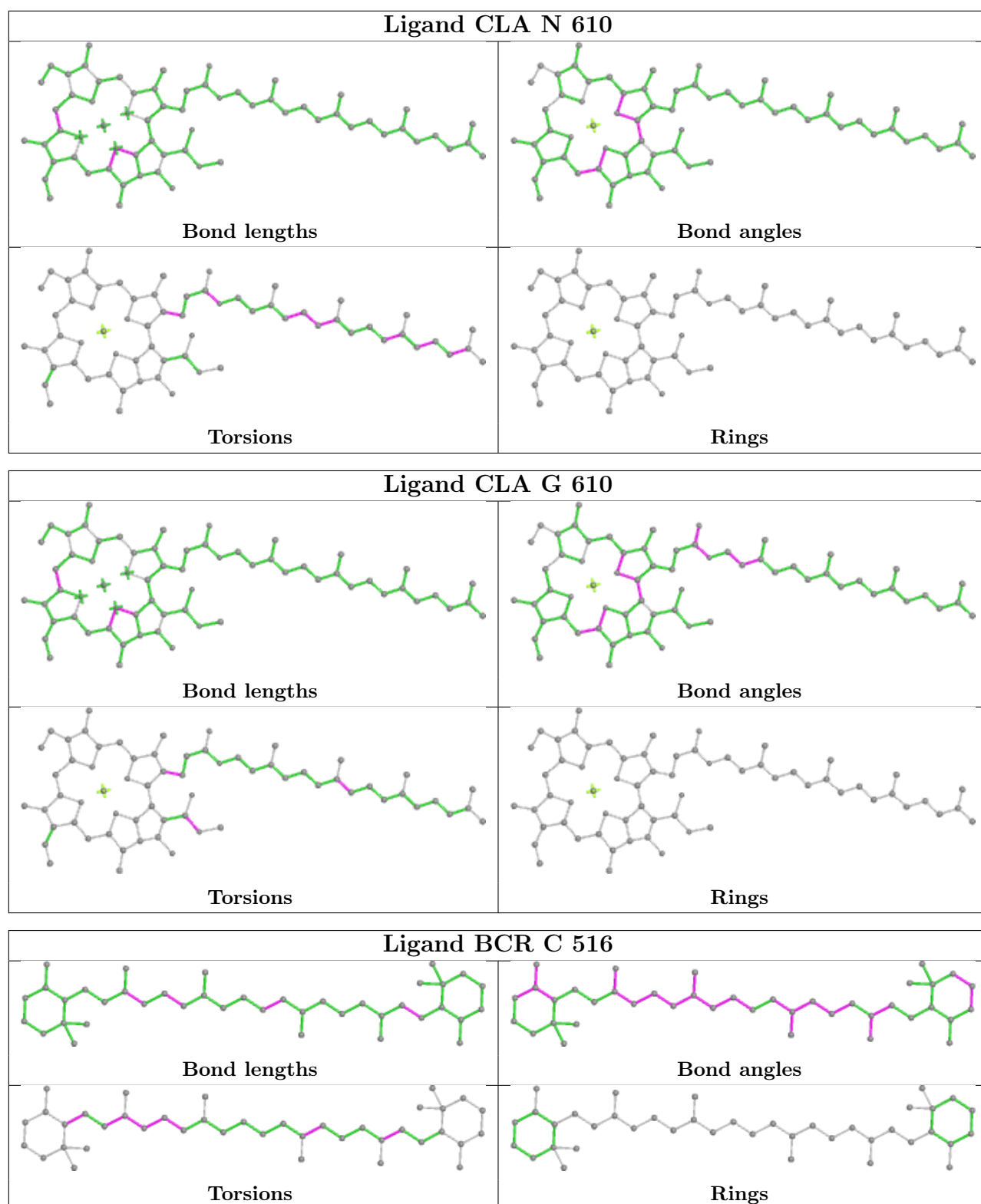


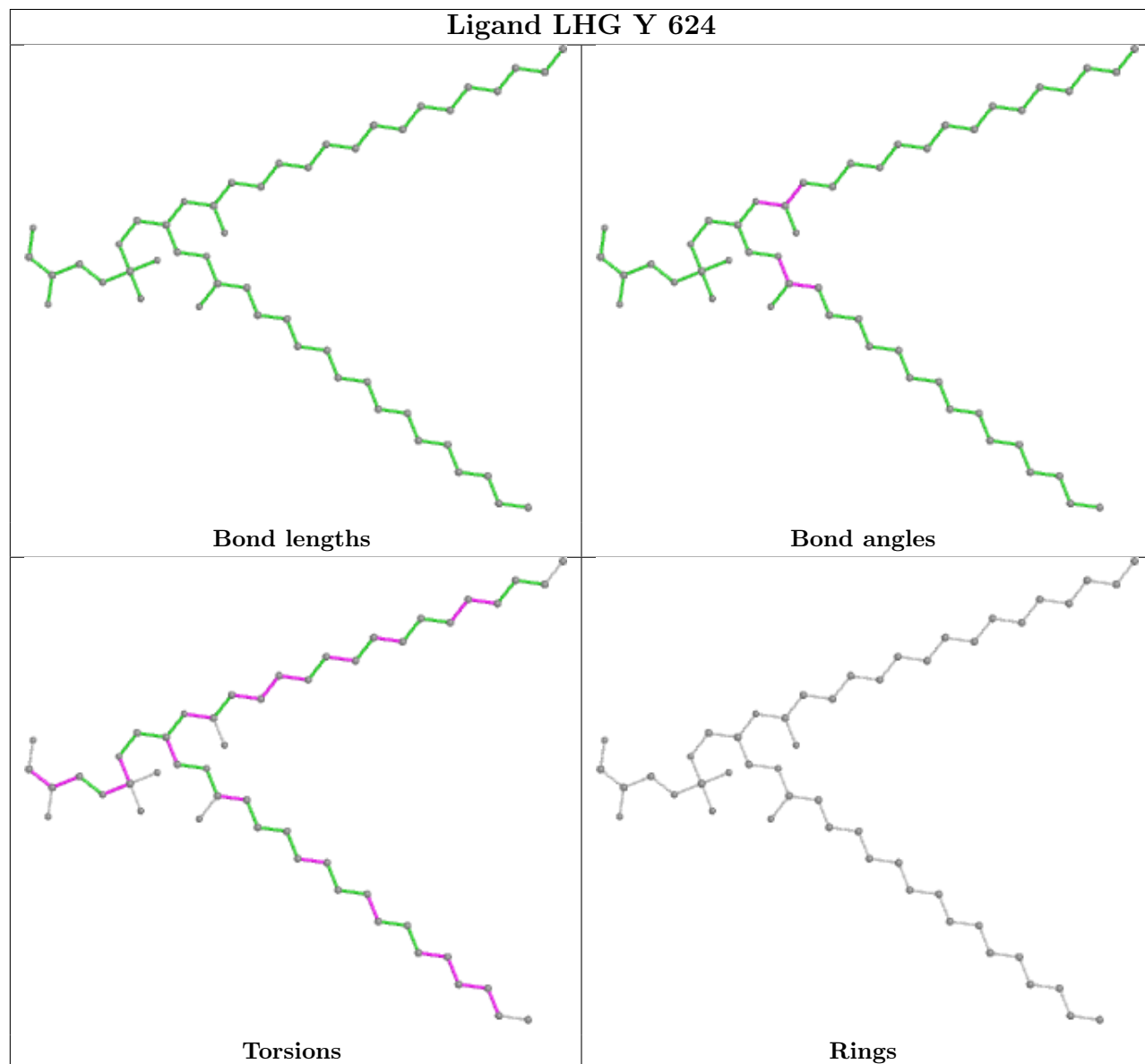
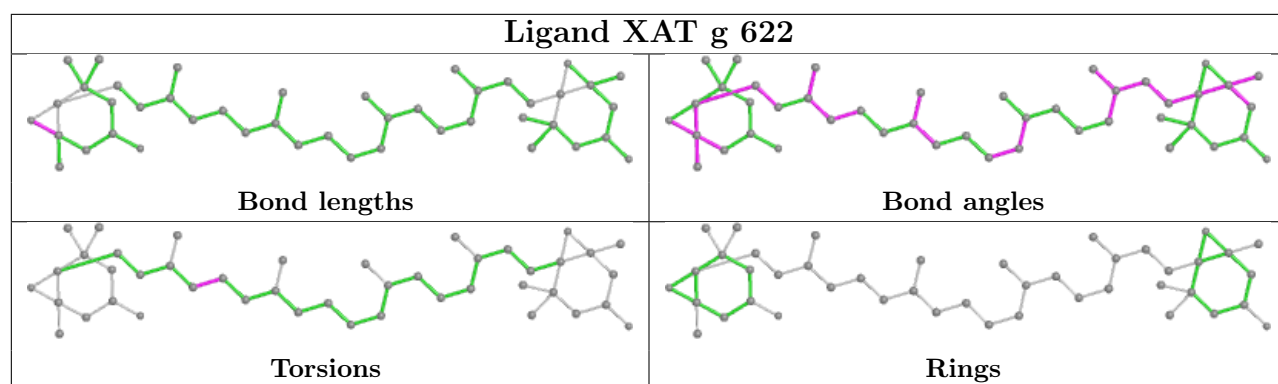
## Ligand CHL Y 607



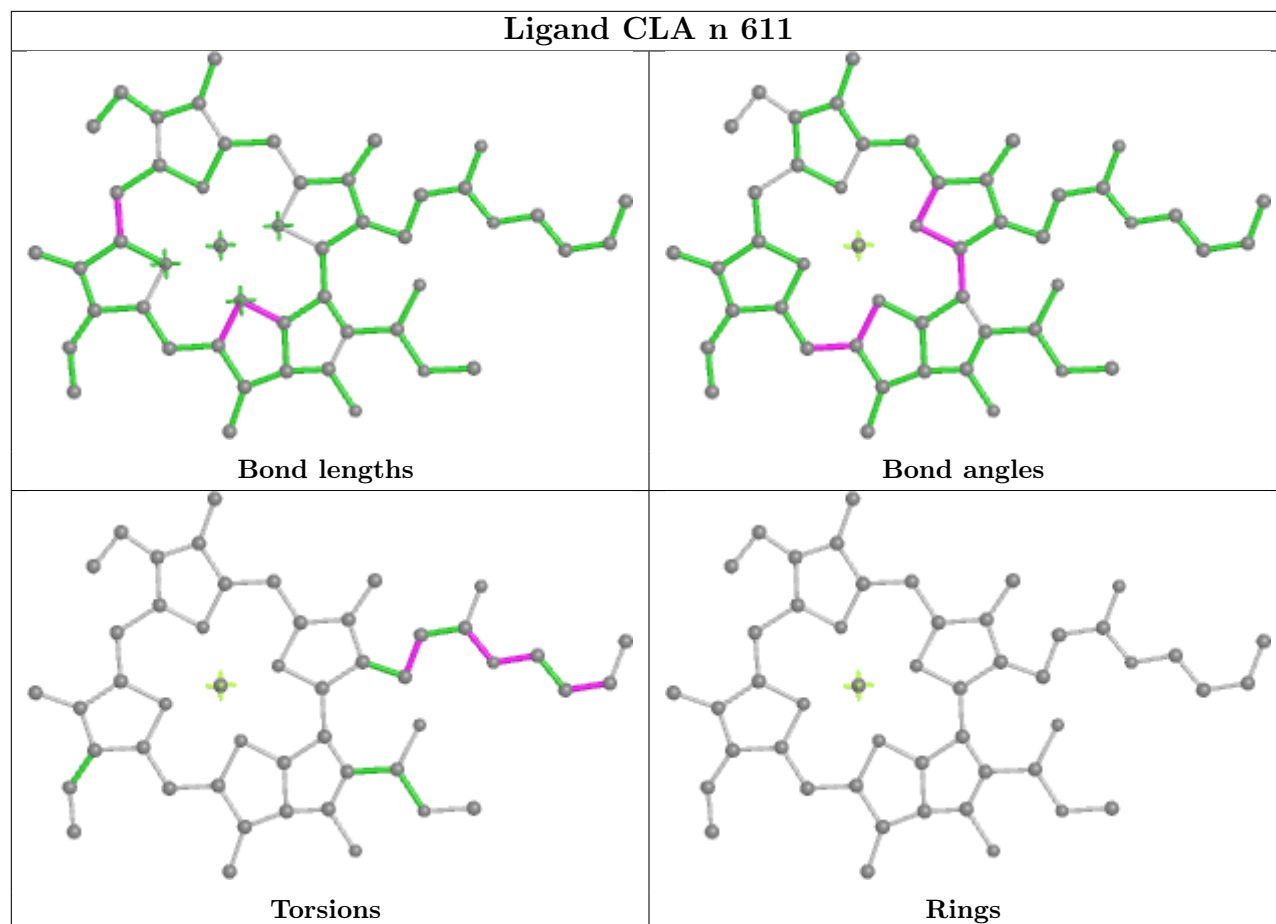




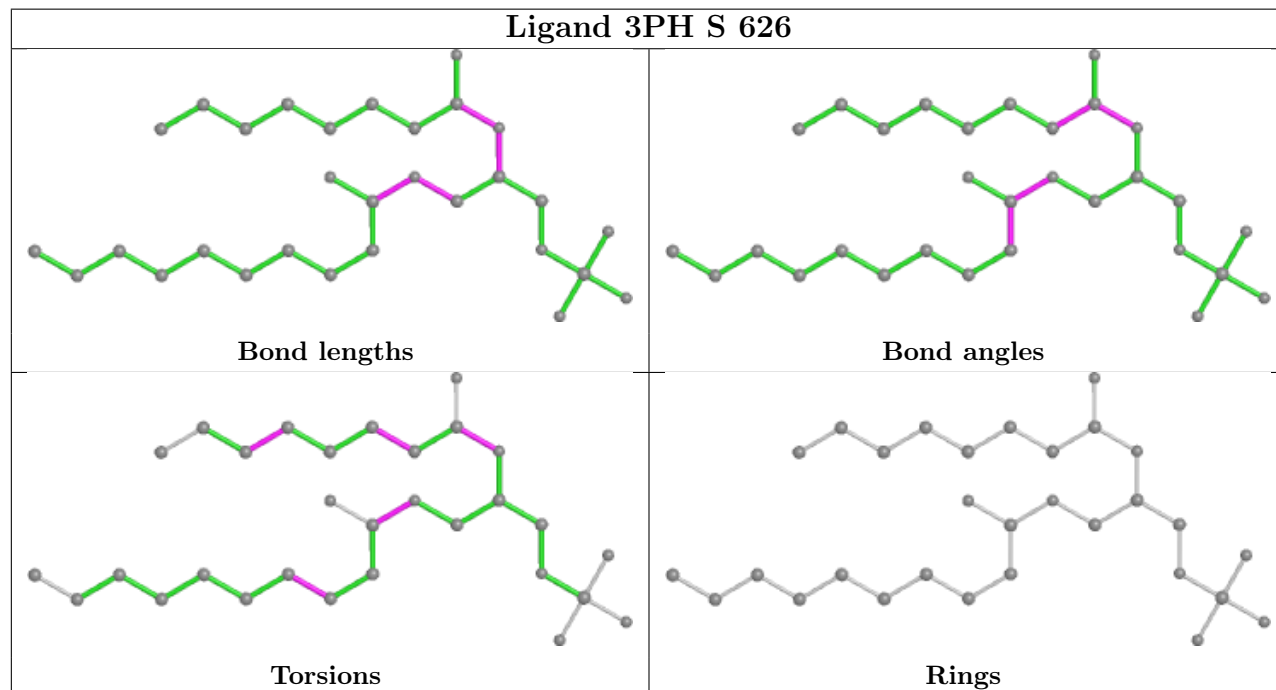


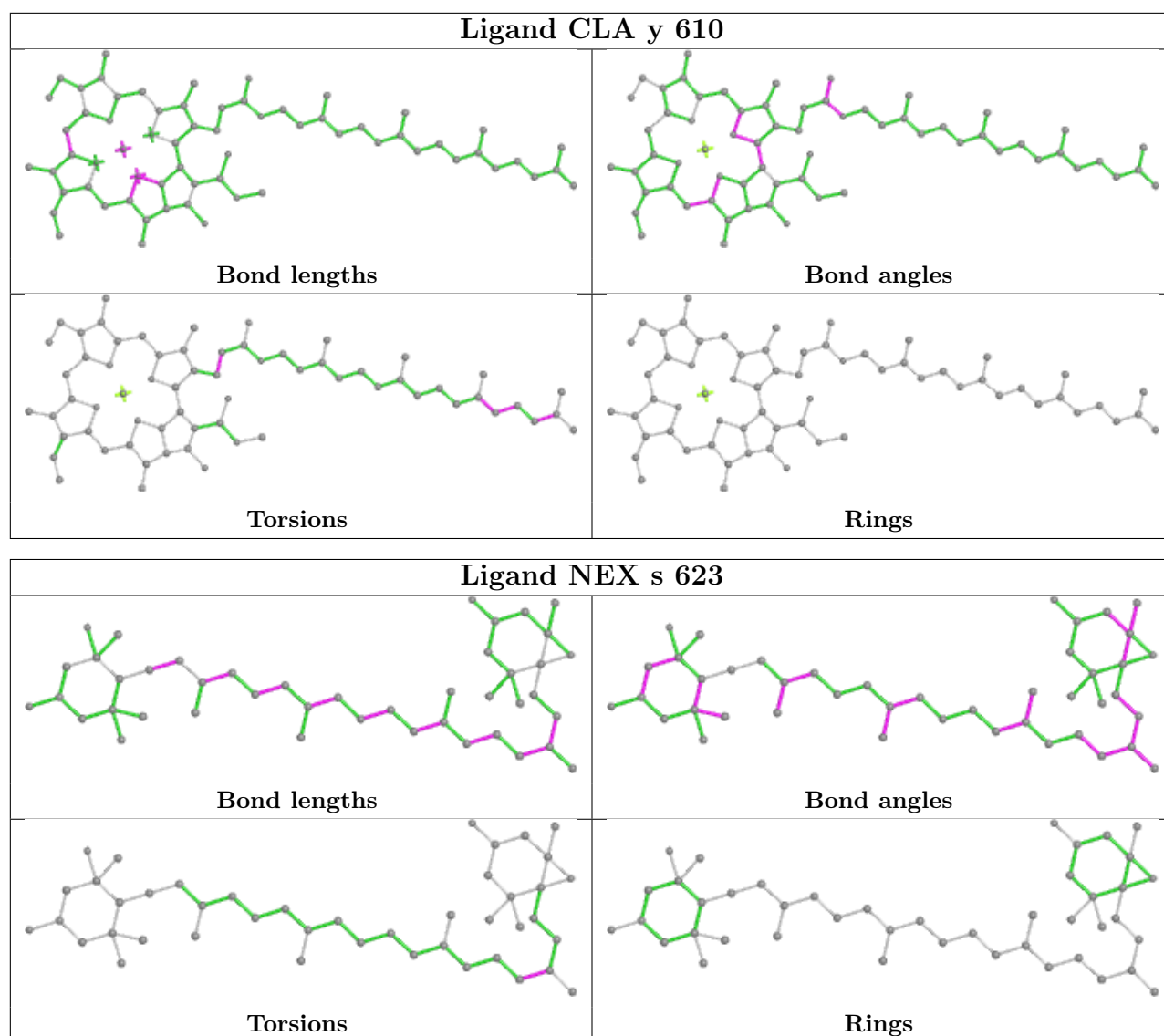


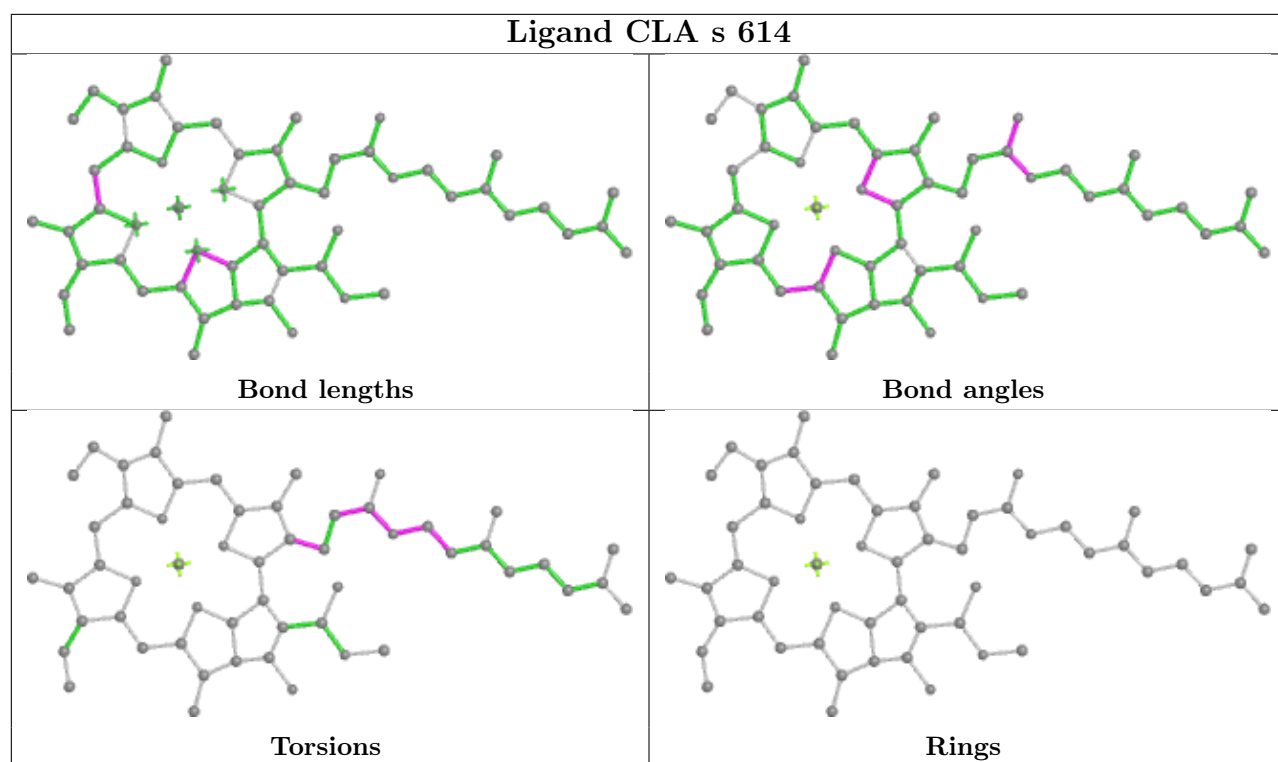
## Ligand CLA n 611

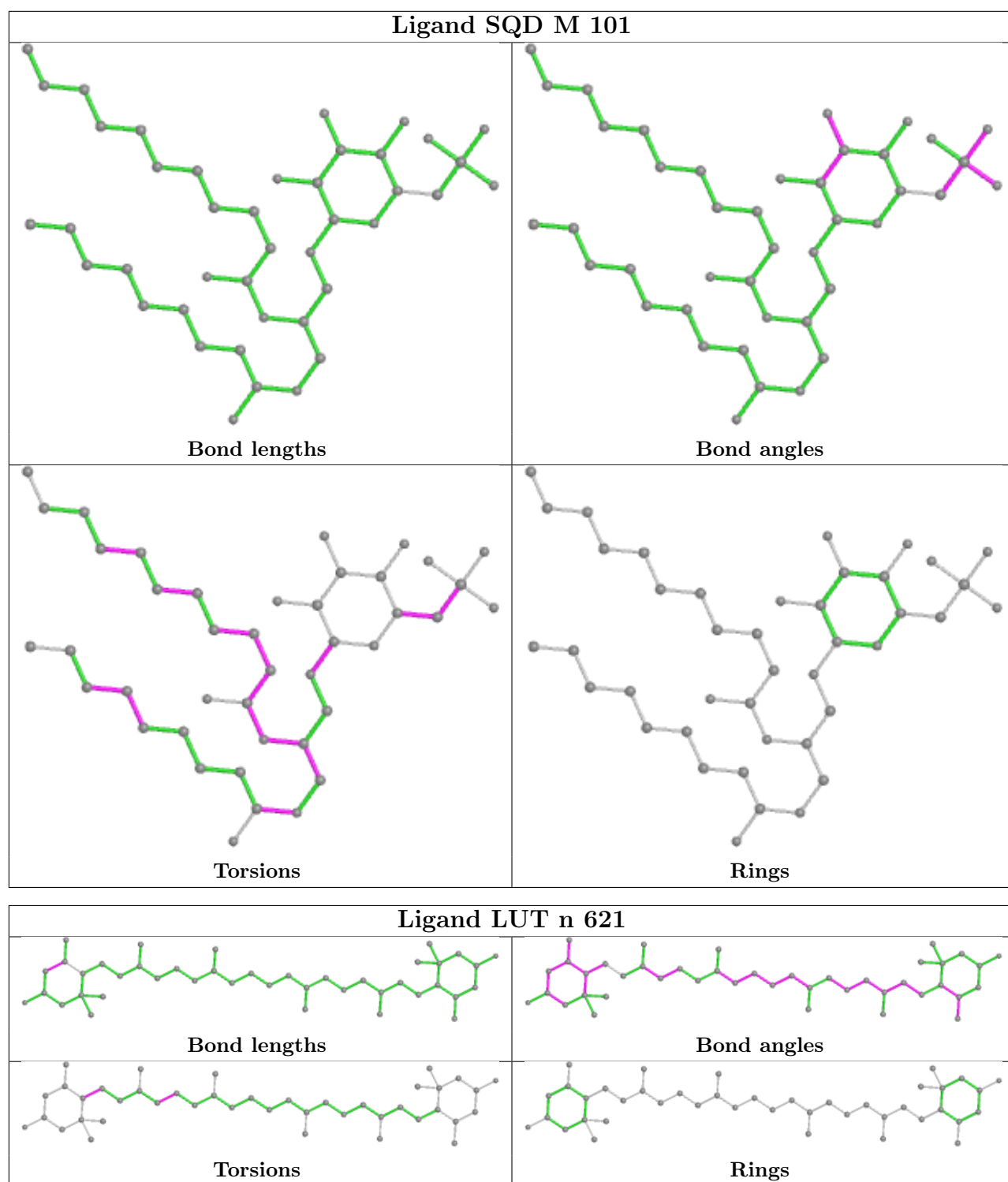


## Ligand 3PH S 626

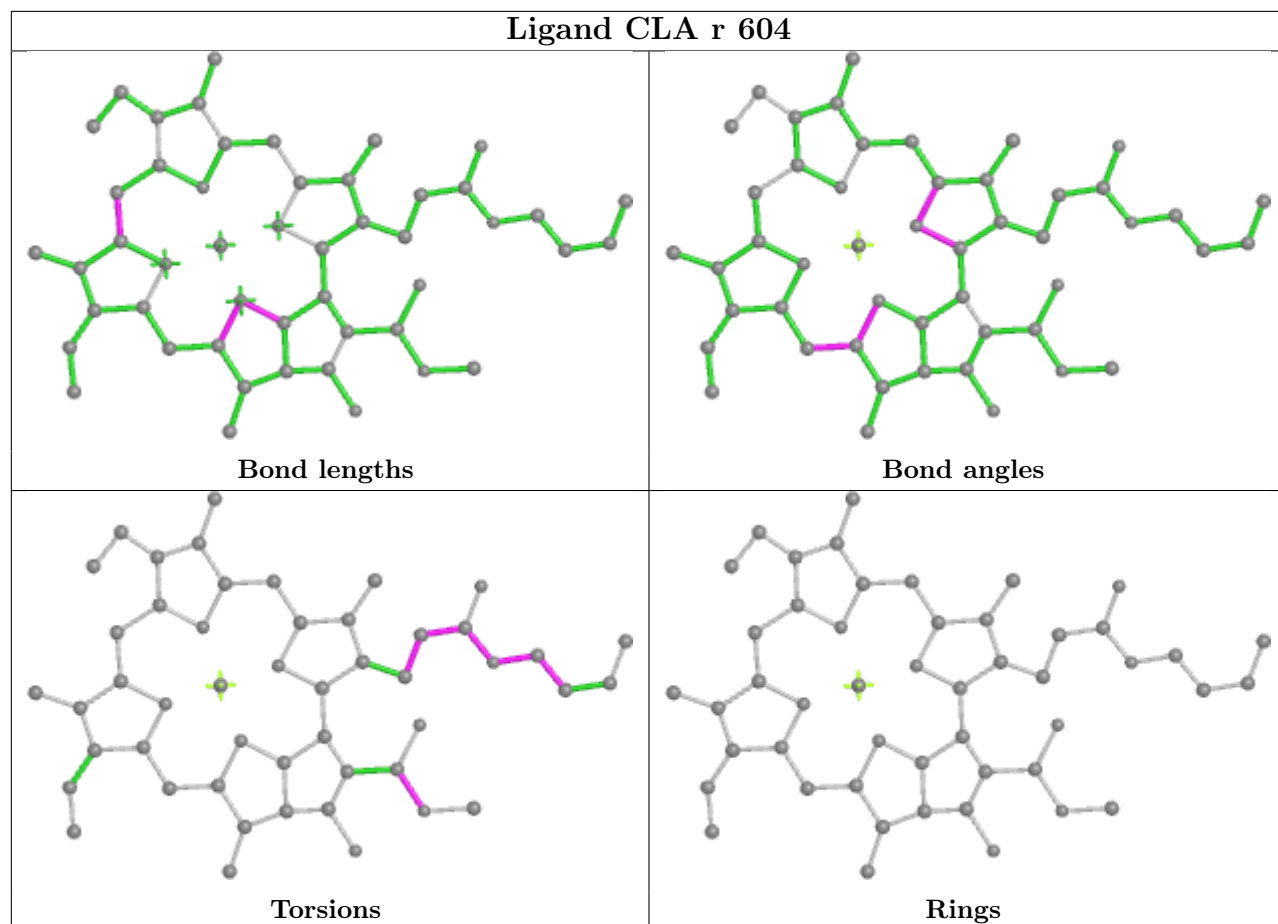




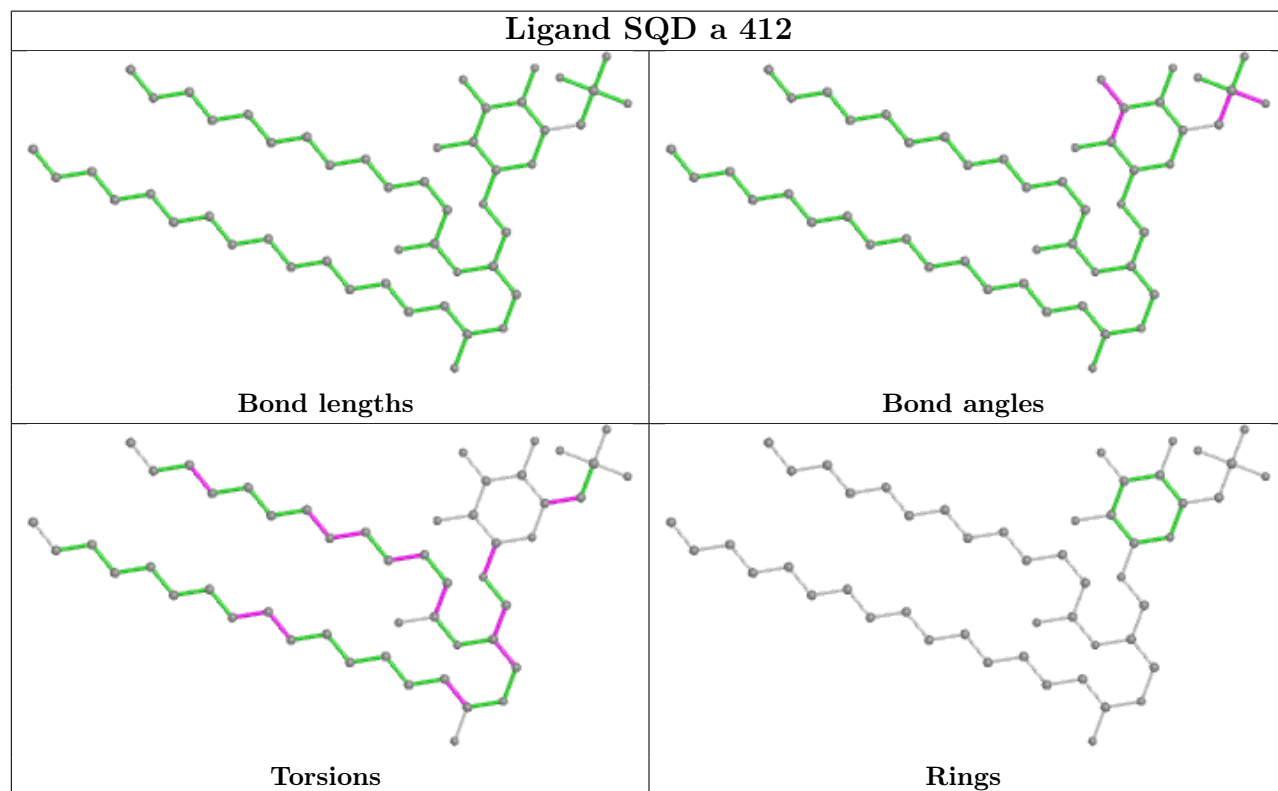
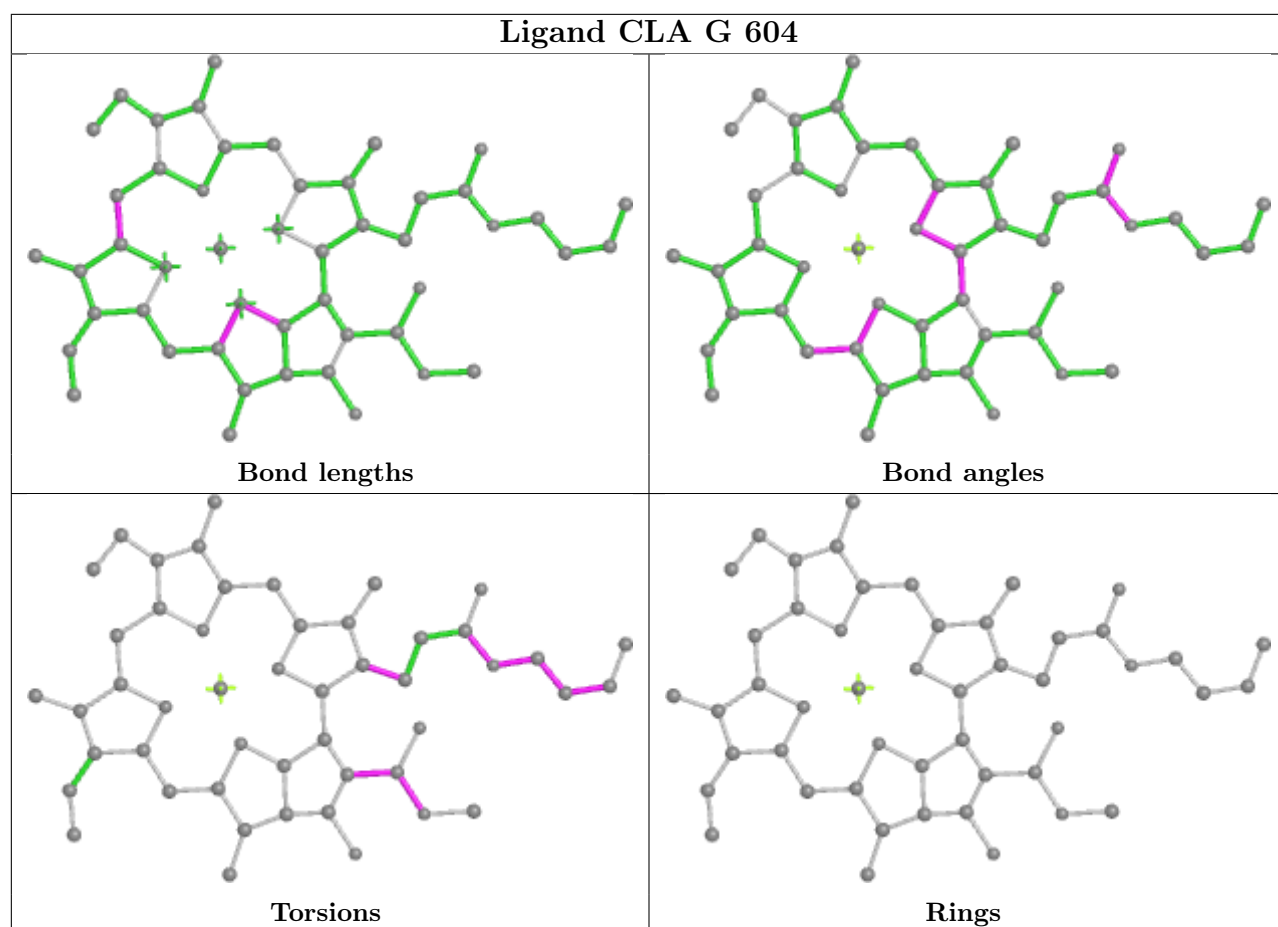


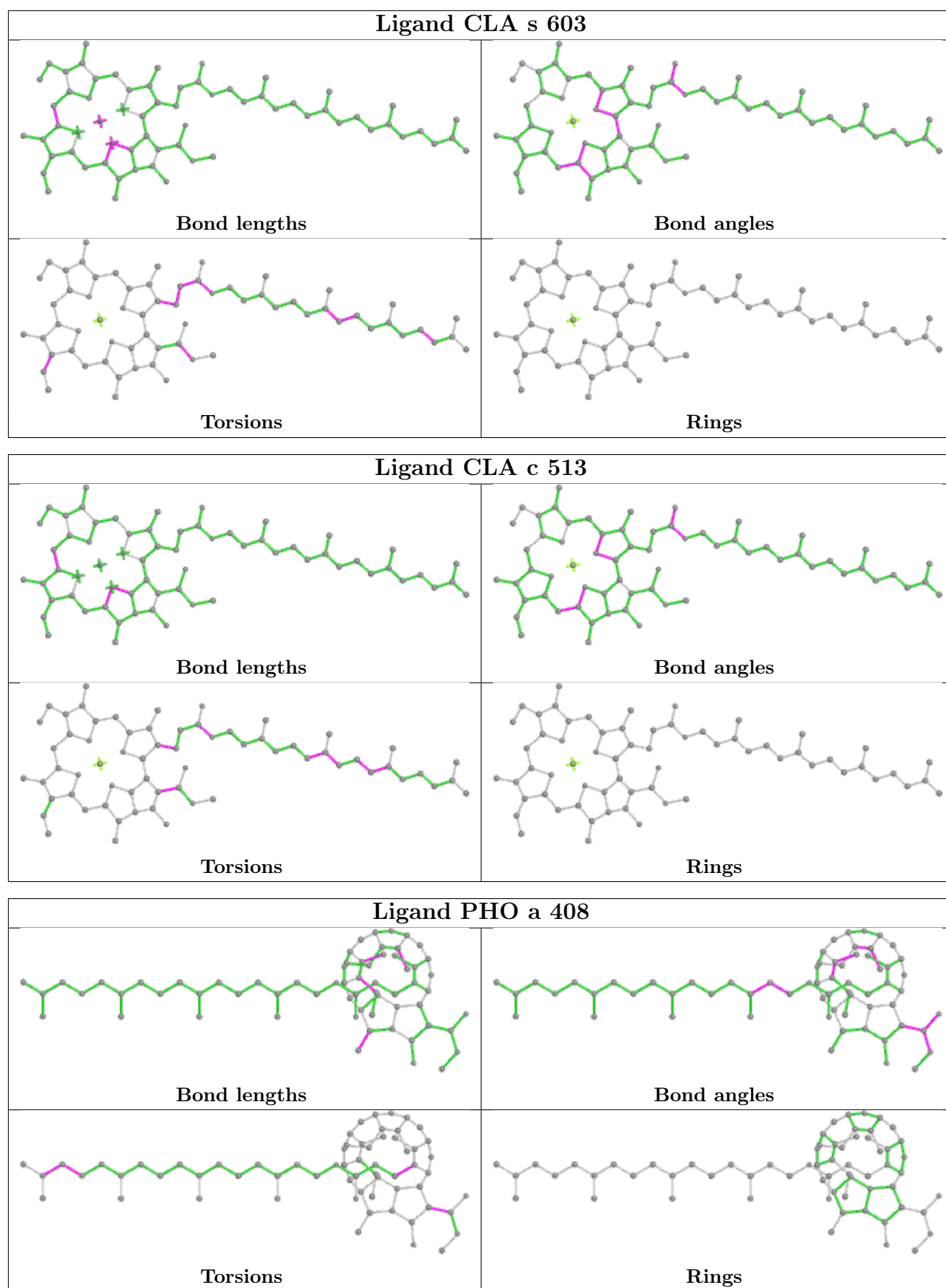


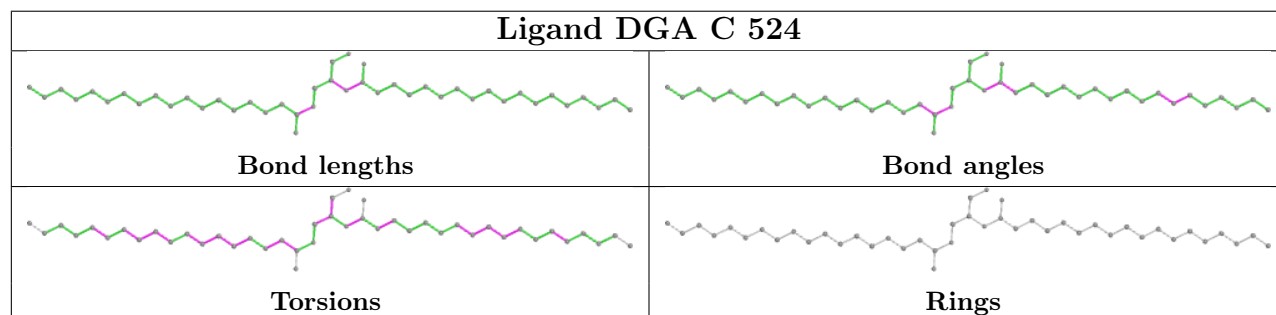
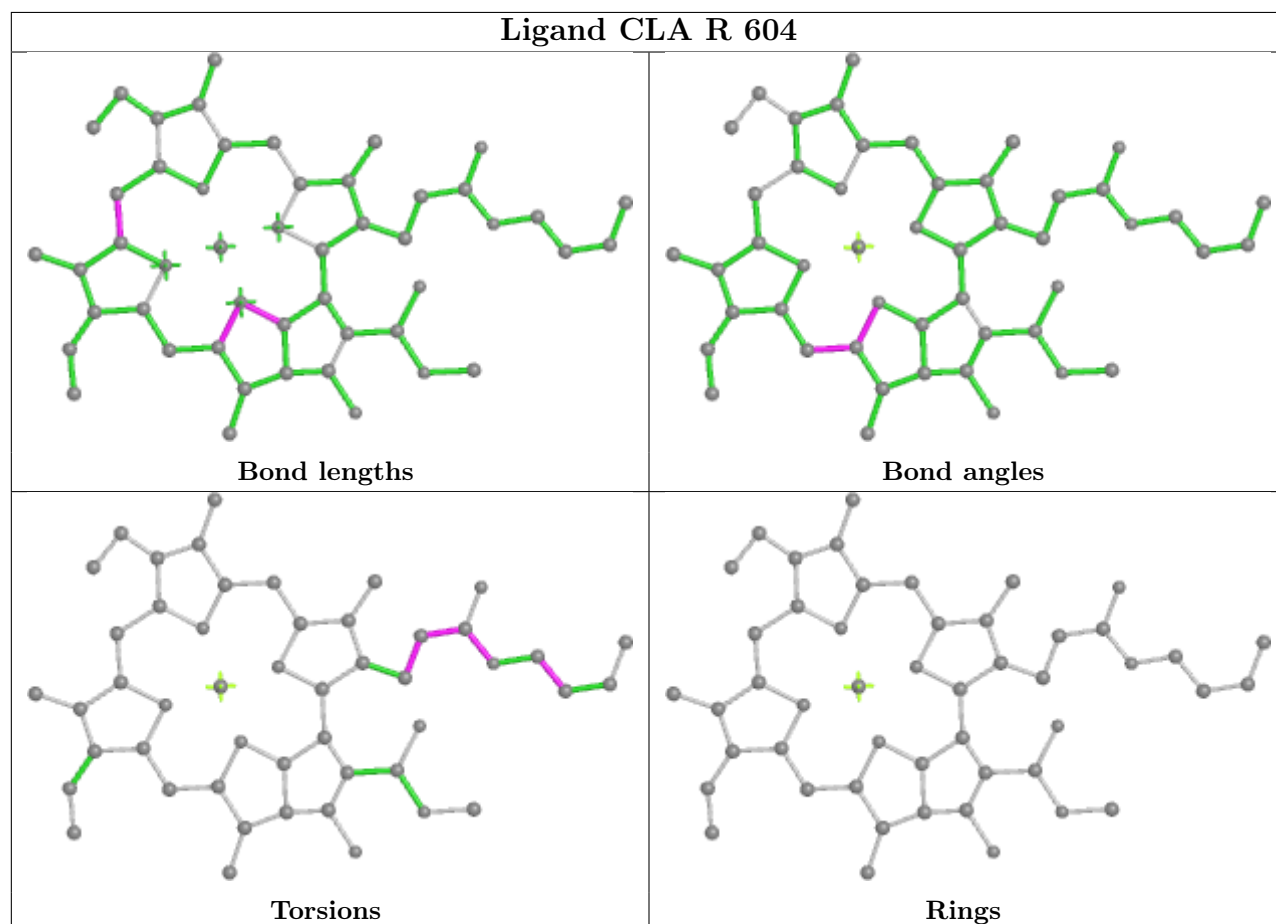
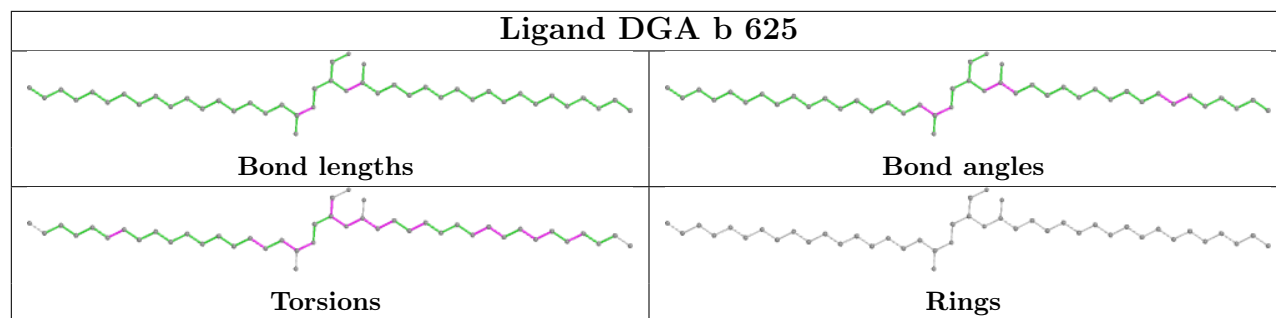
## Ligand CLA r 604

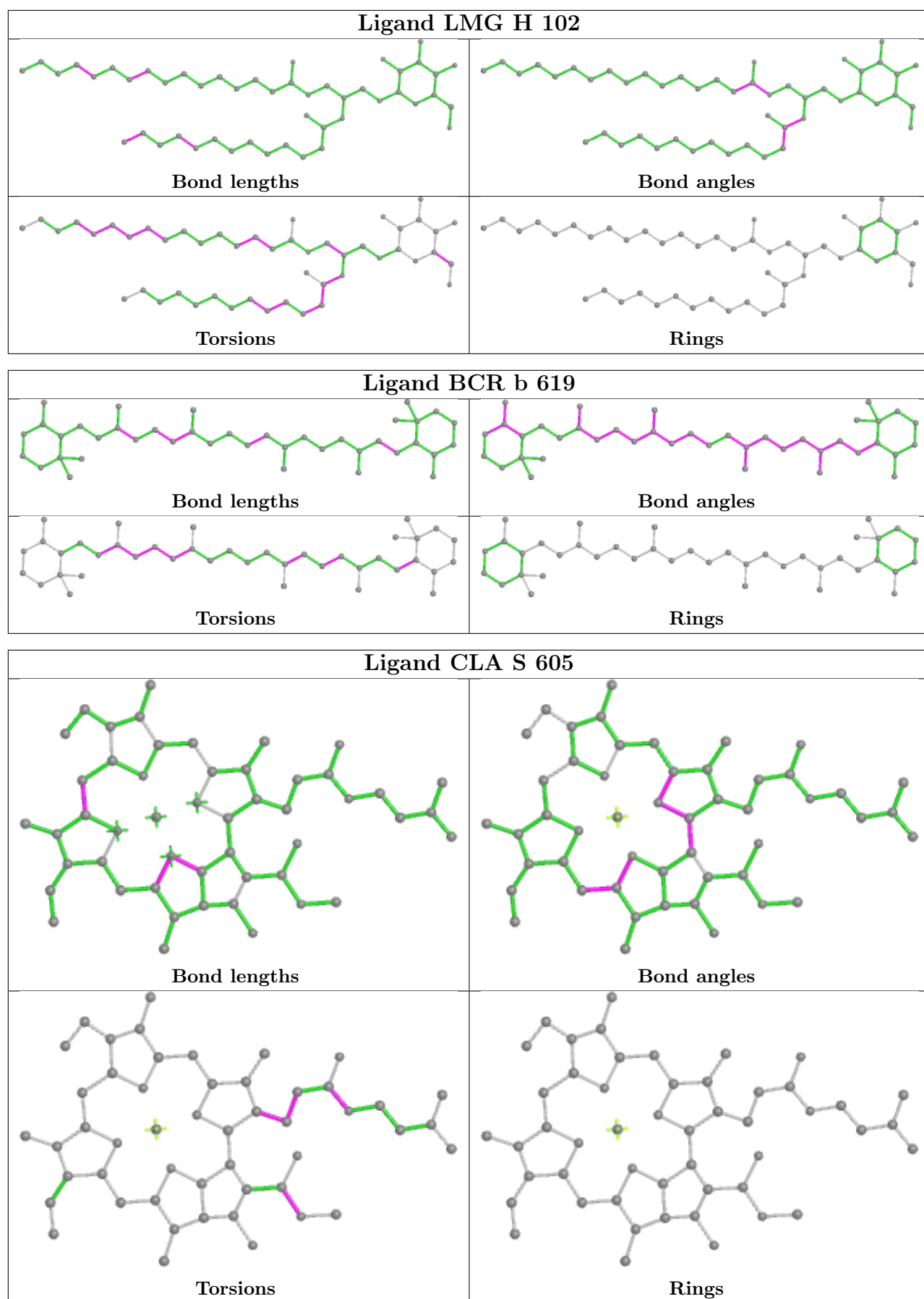




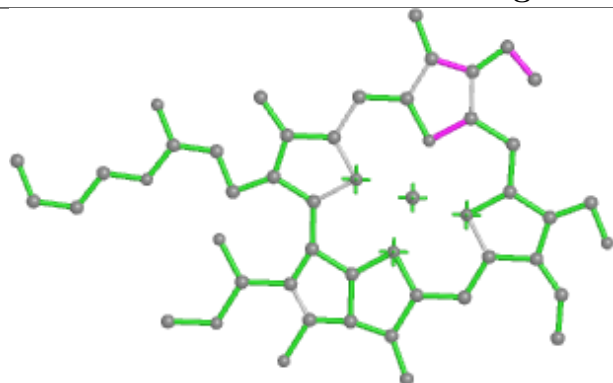




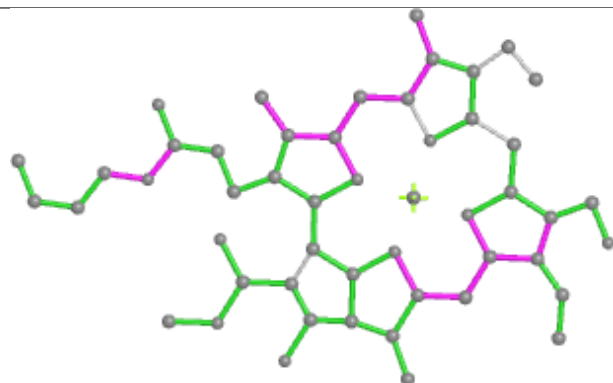




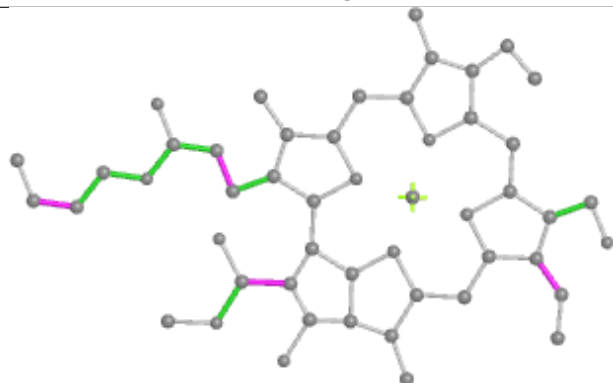
## Ligand CHL R 607



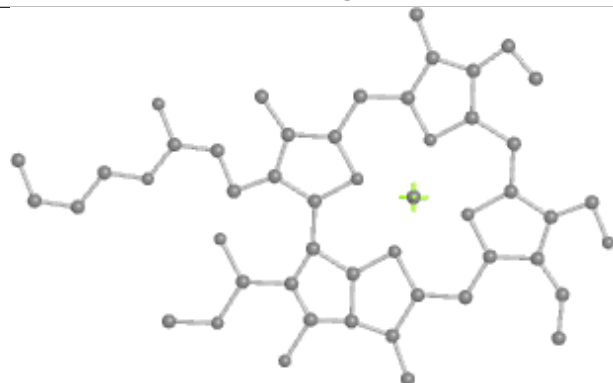
Bond lengths



Bond angles

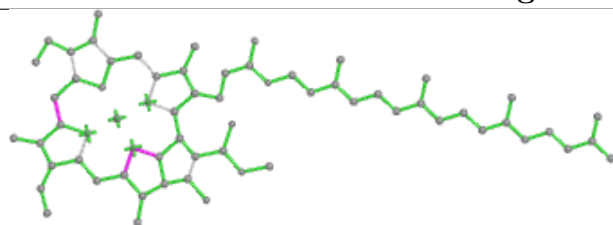


Torsions

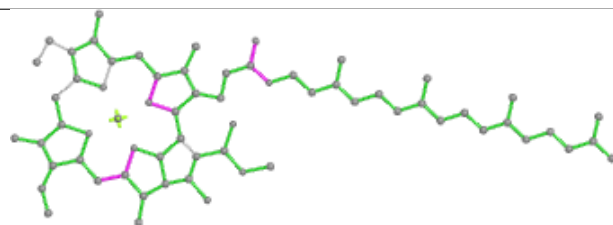


Rings

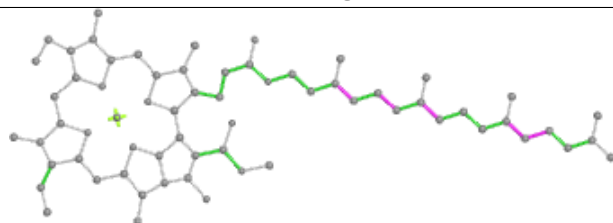
## Ligand CLA b 603



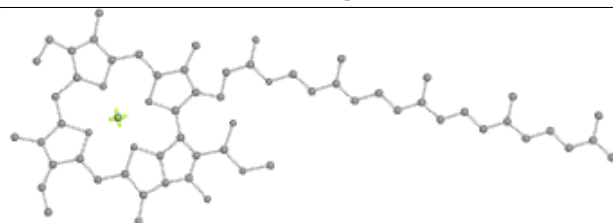
Bond lengths



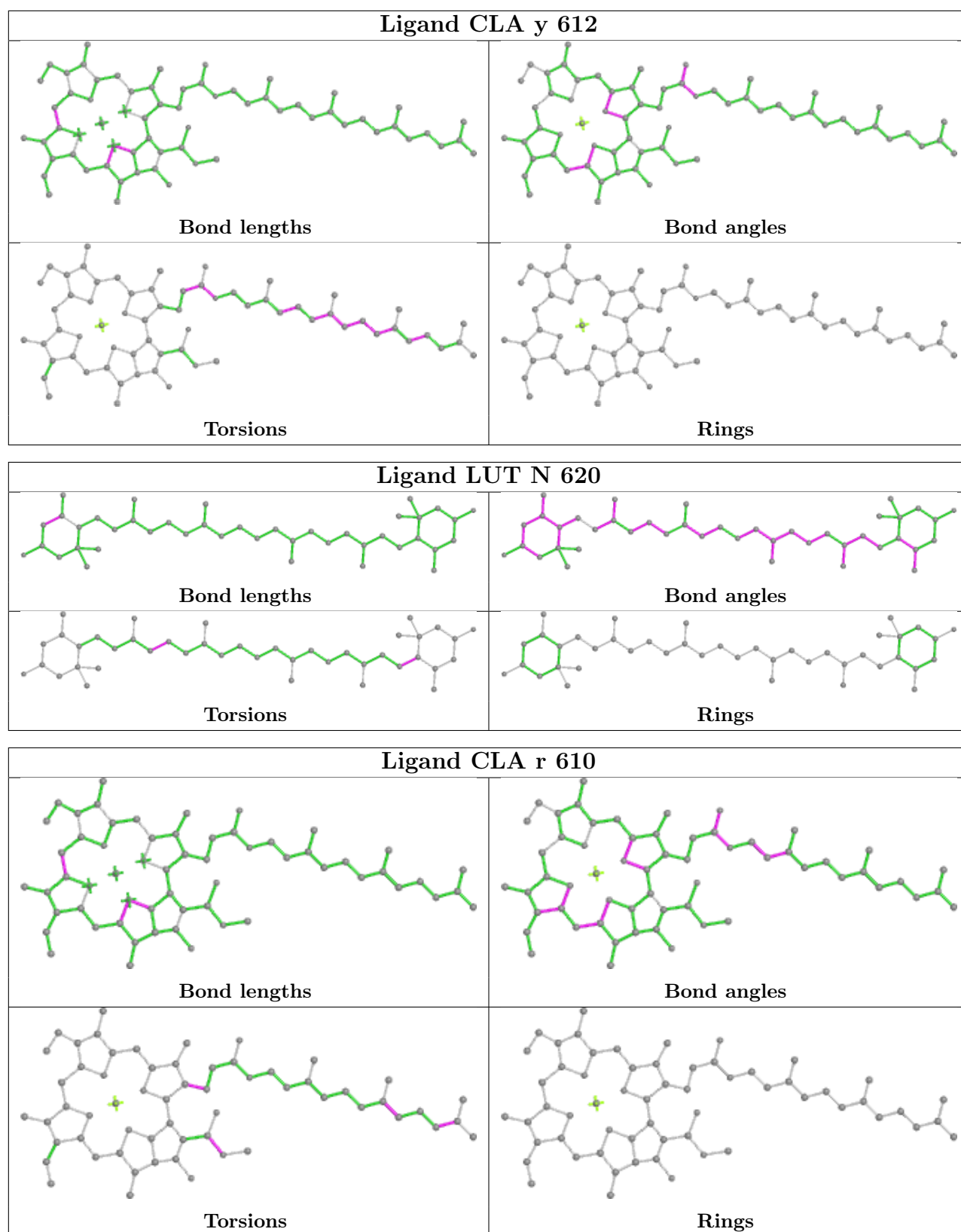
Bond angles

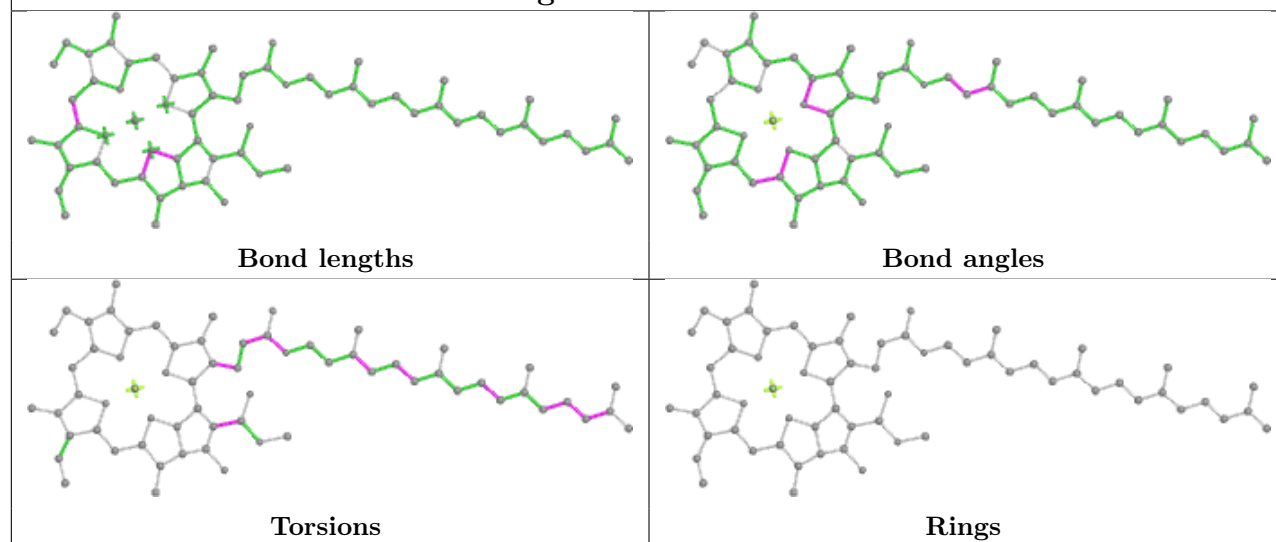
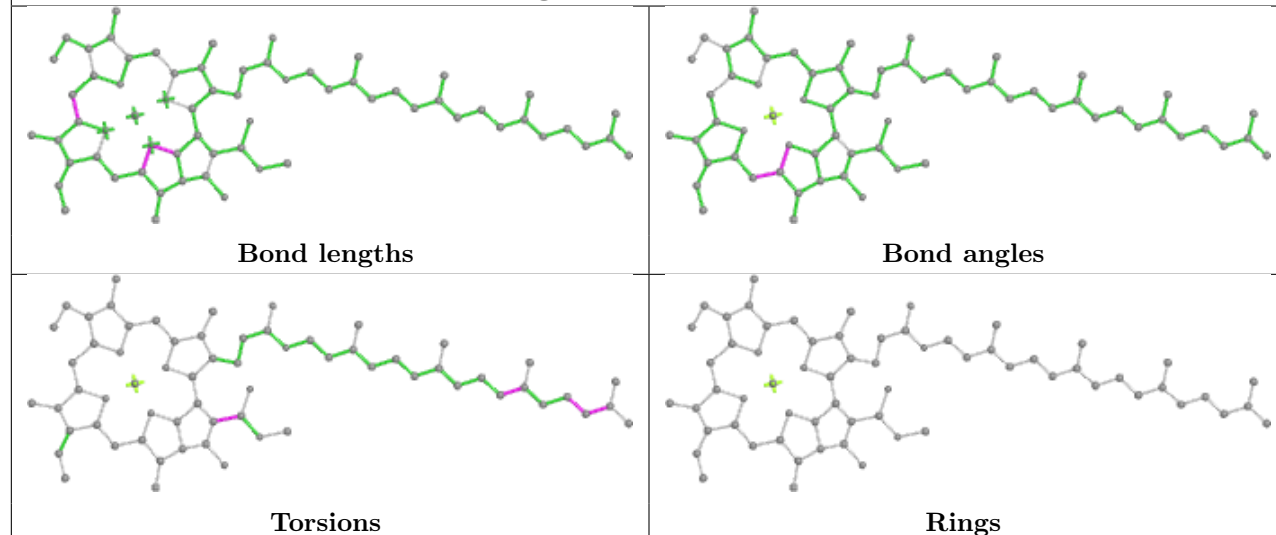
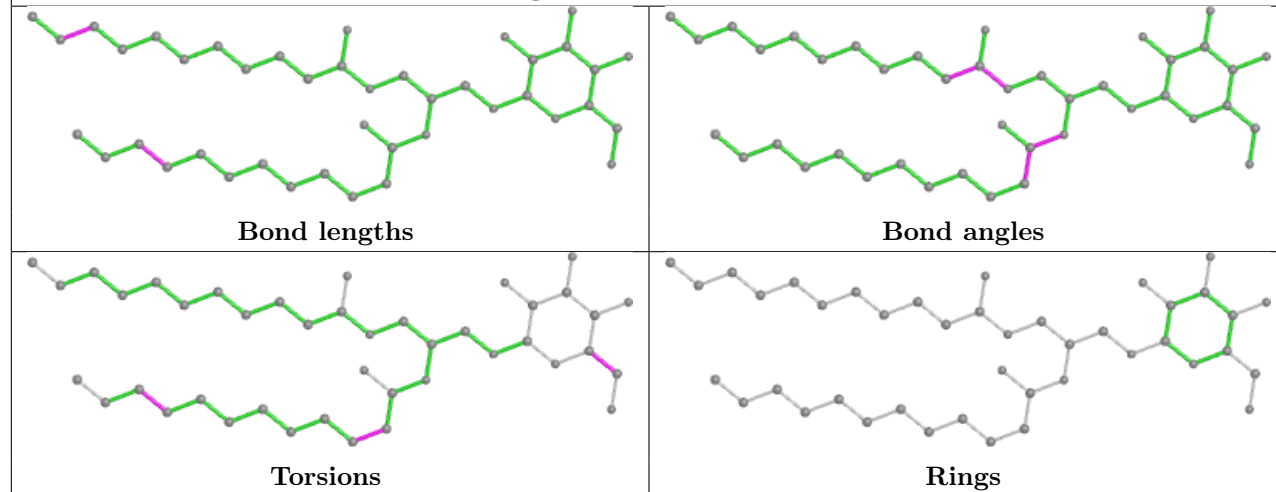


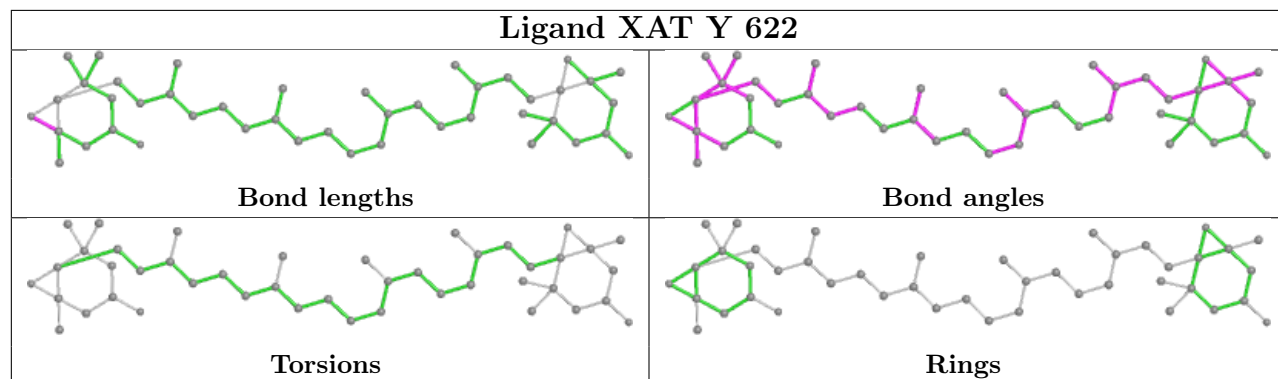
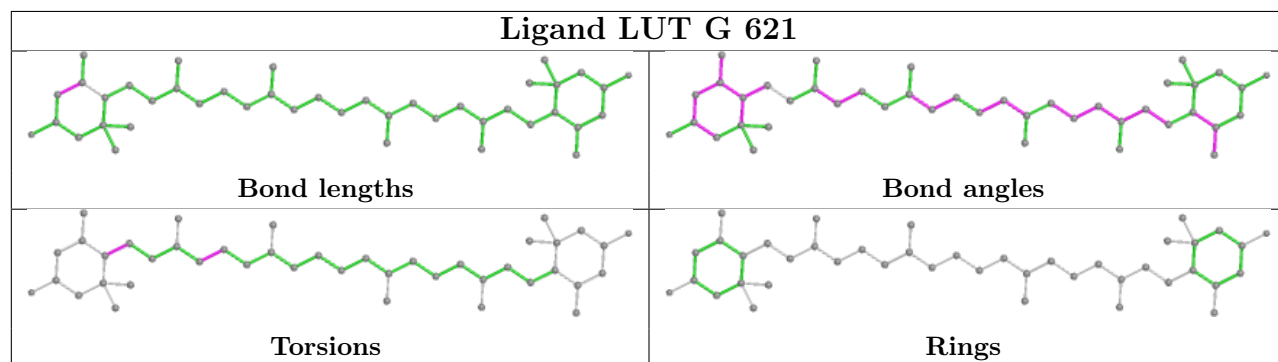
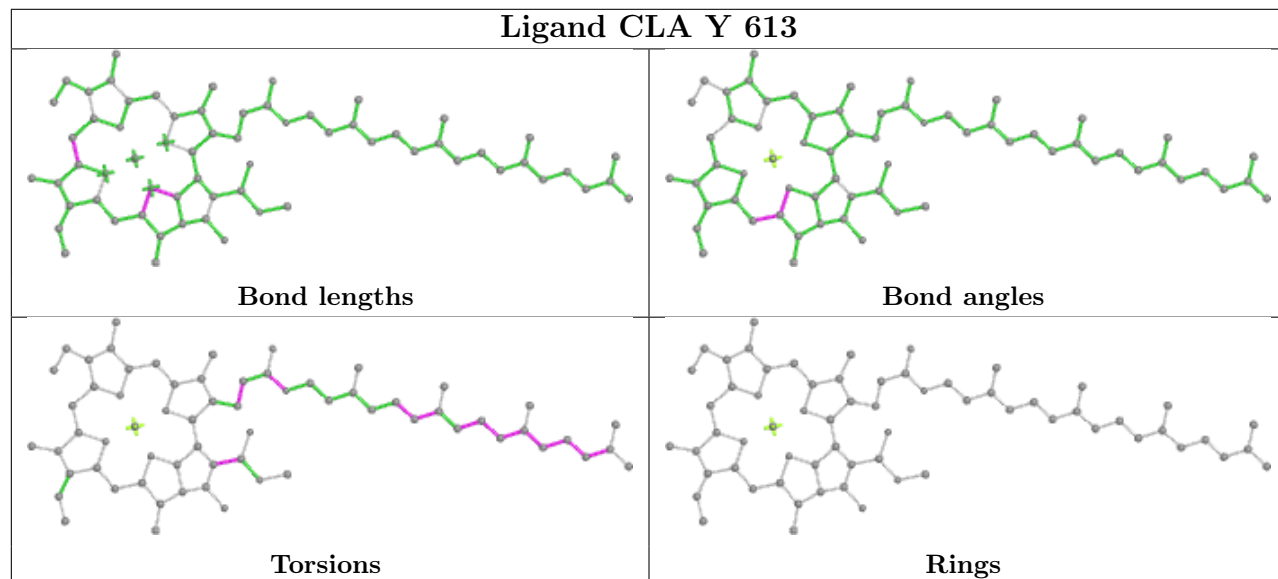
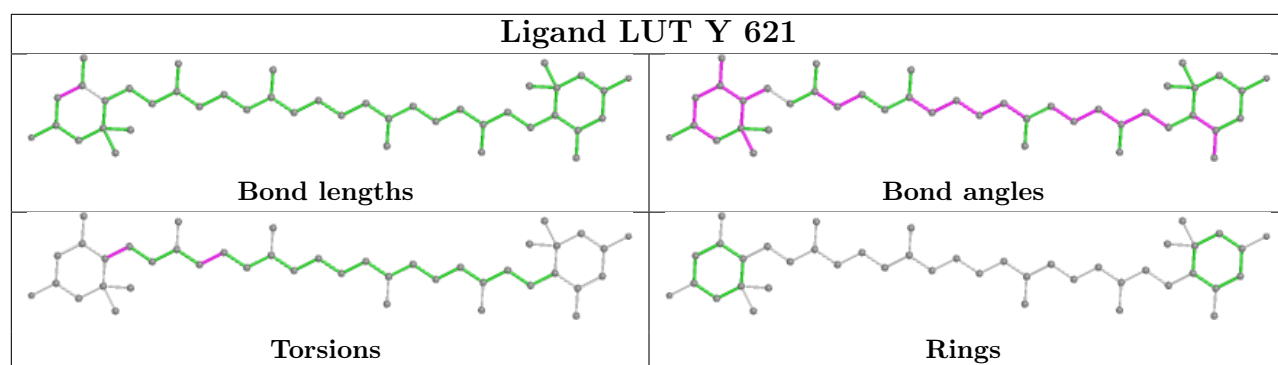
Torsions



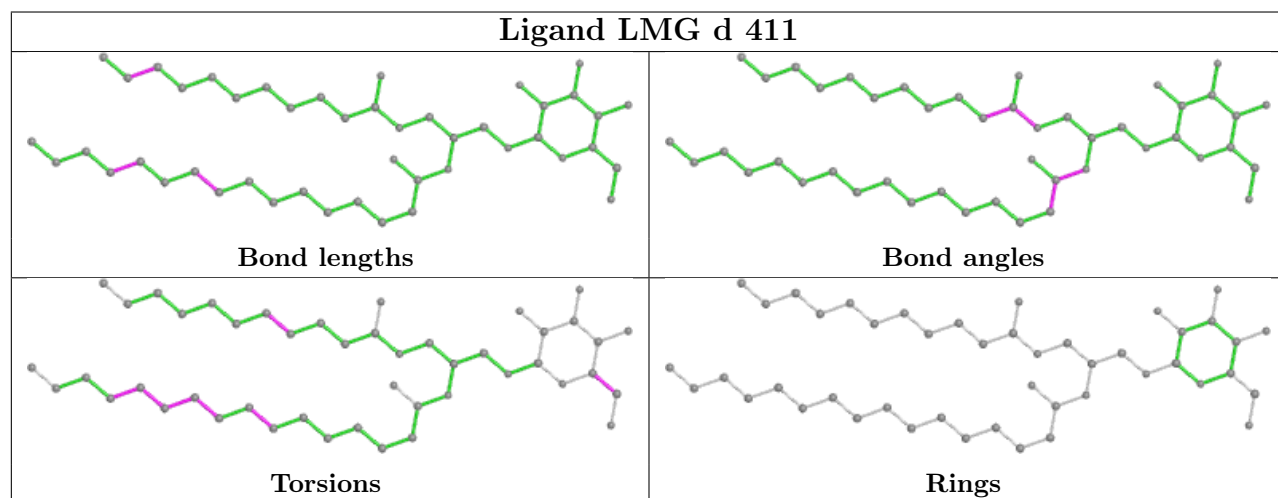
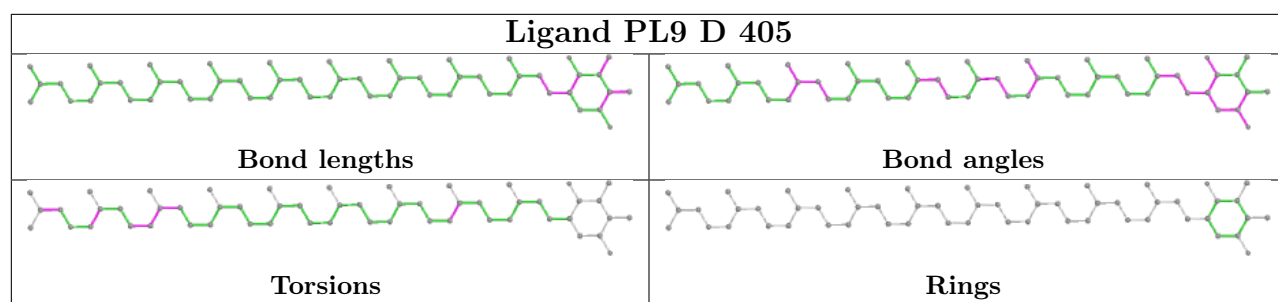
Rings

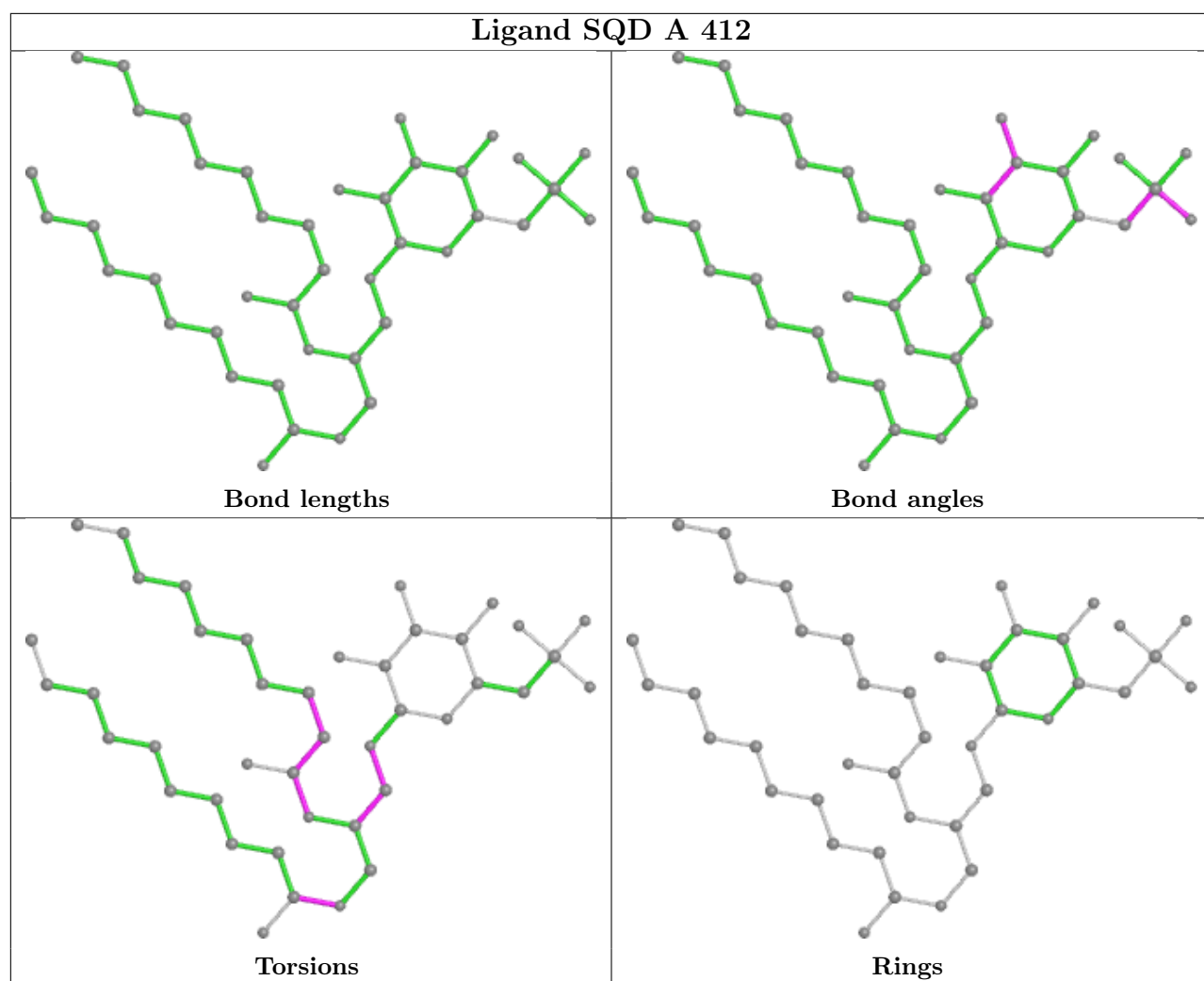


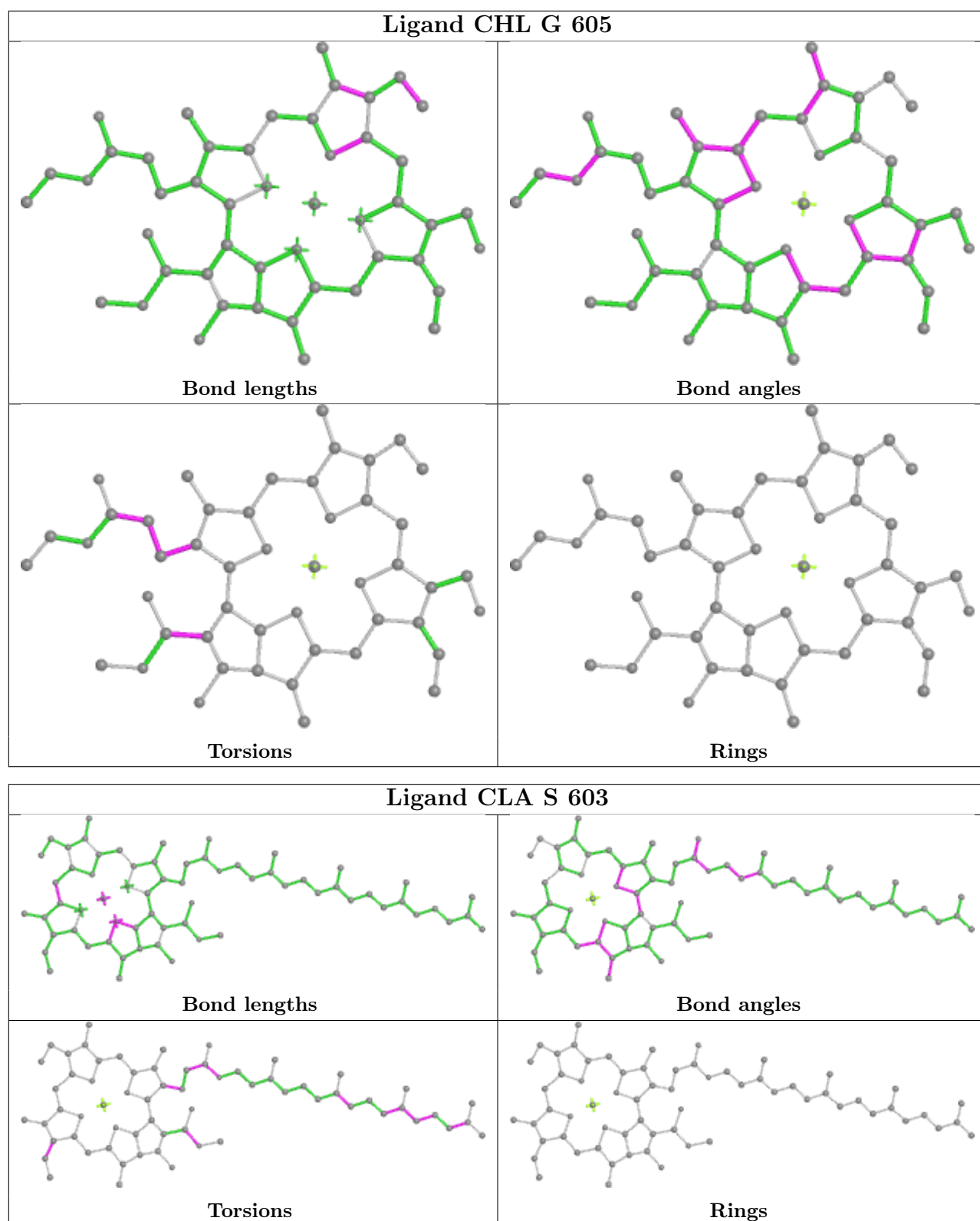
**Ligand CLA c 512****Ligand CLA b 611****Ligand LMG D 411**

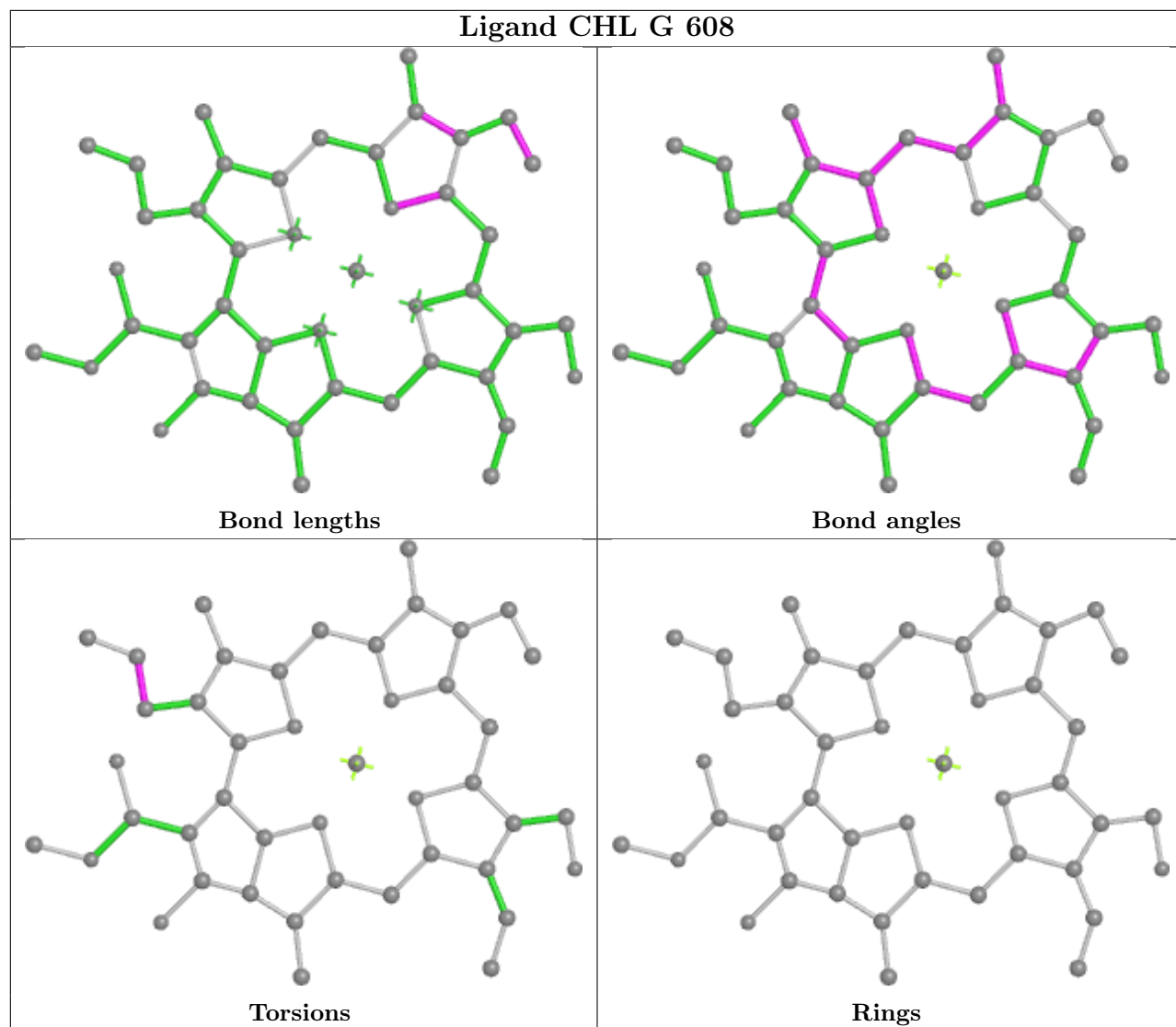


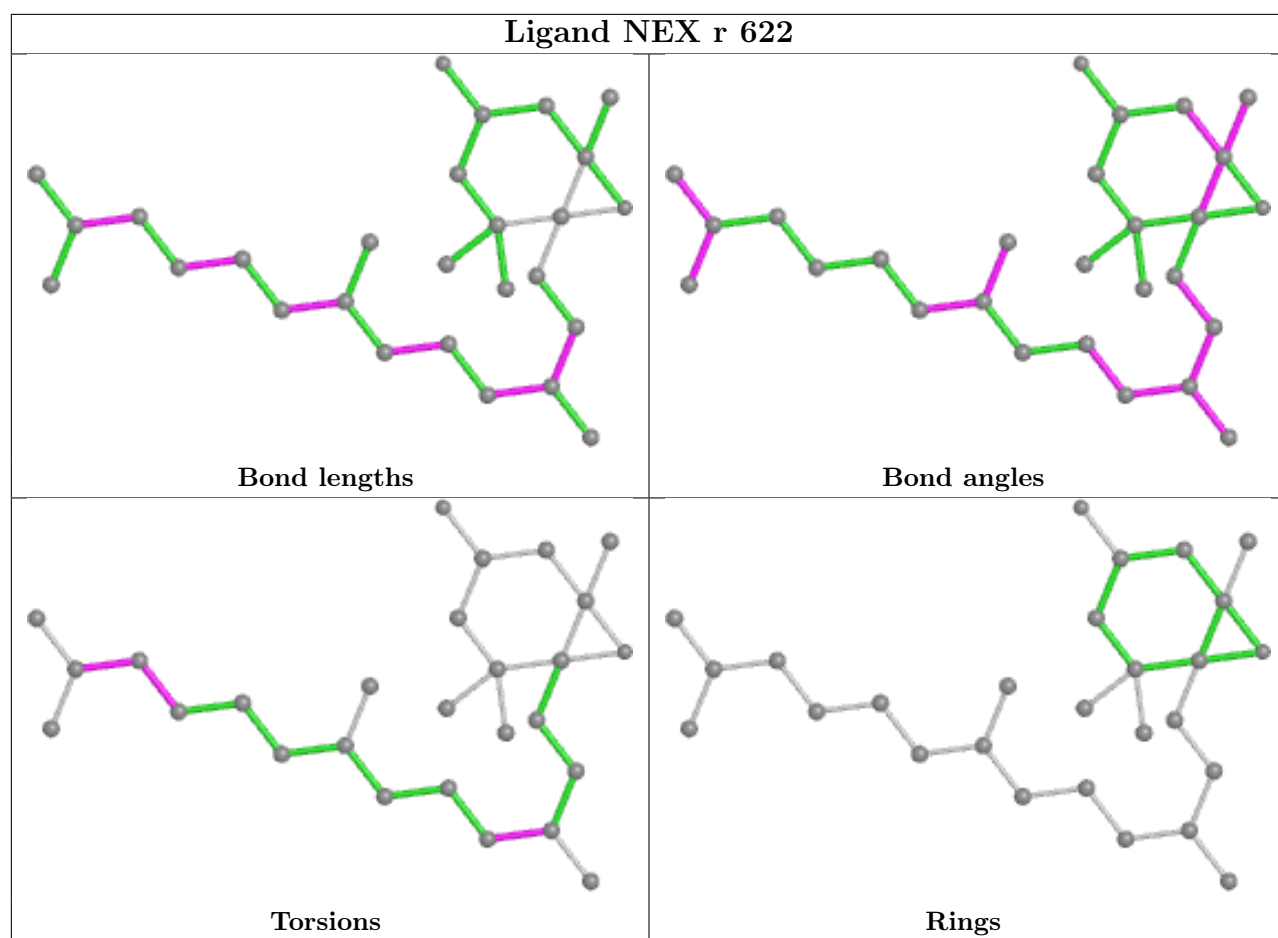




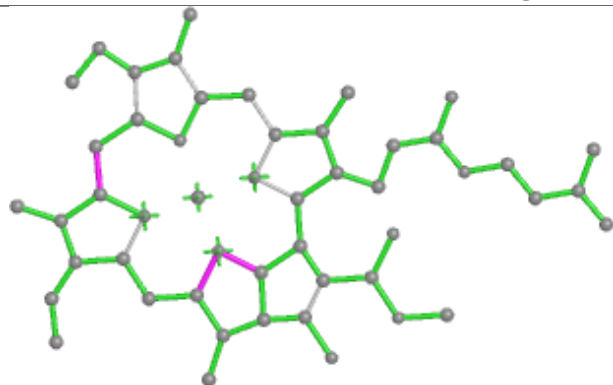




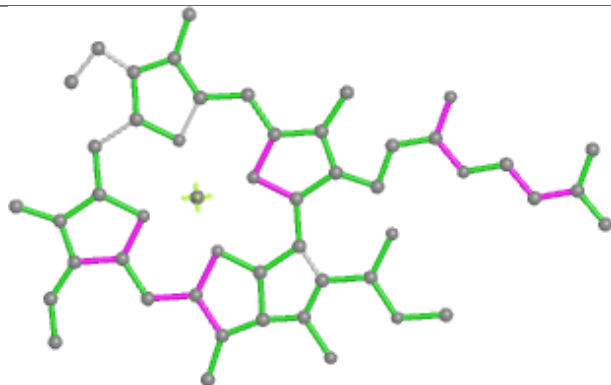




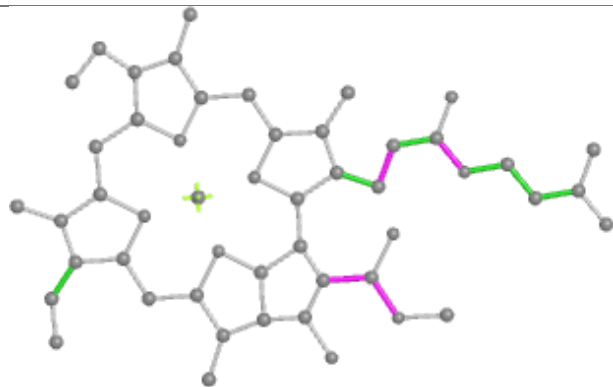
## Ligand CLA S 617



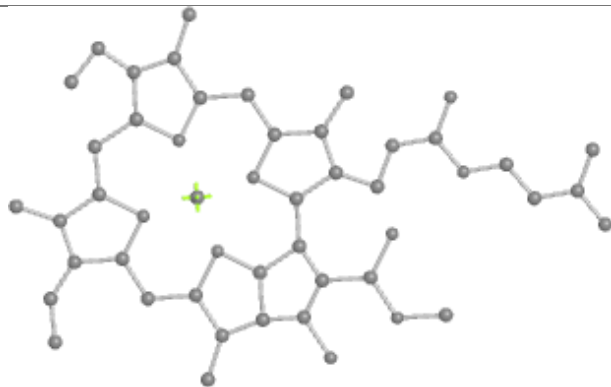
Bond lengths



Bond angles

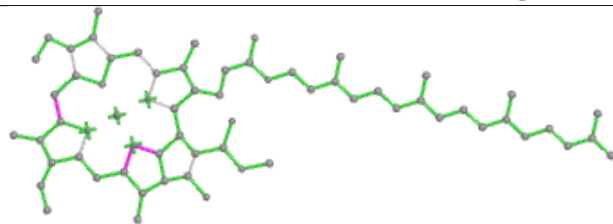


Torsions

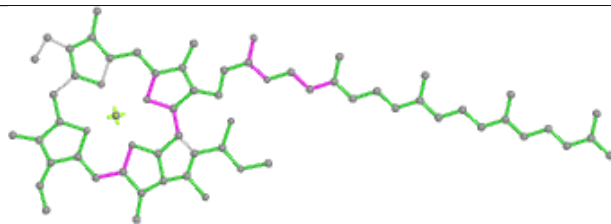


Rings

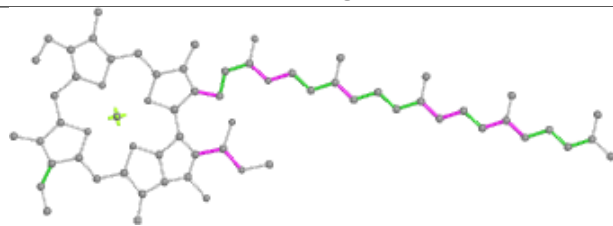
## Ligand CLA Y 604



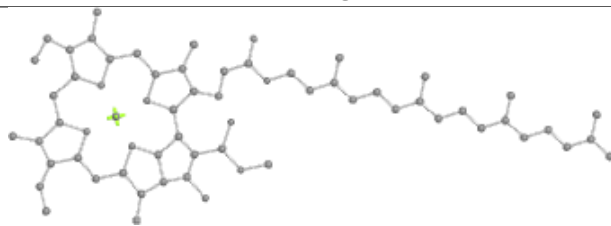
Bond lengths



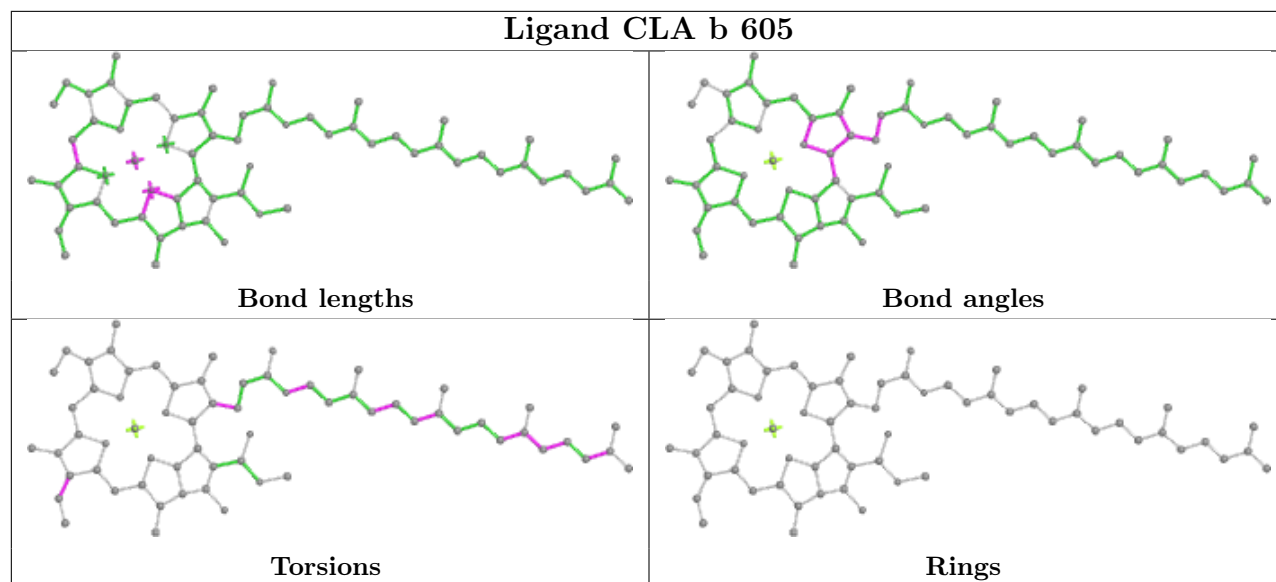
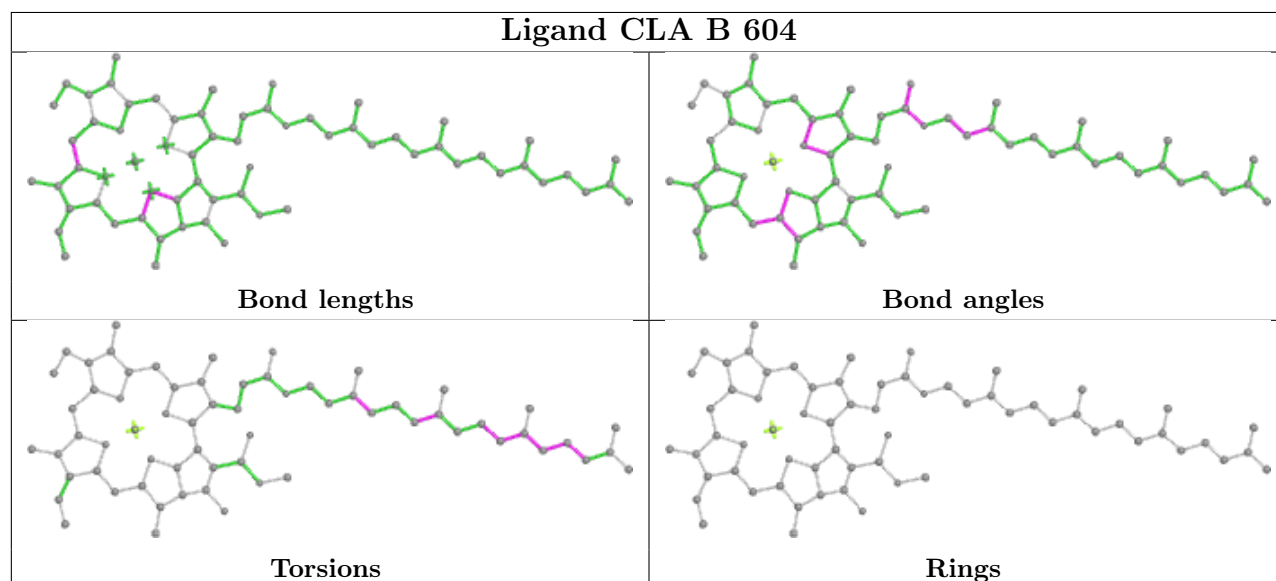
Bond angles



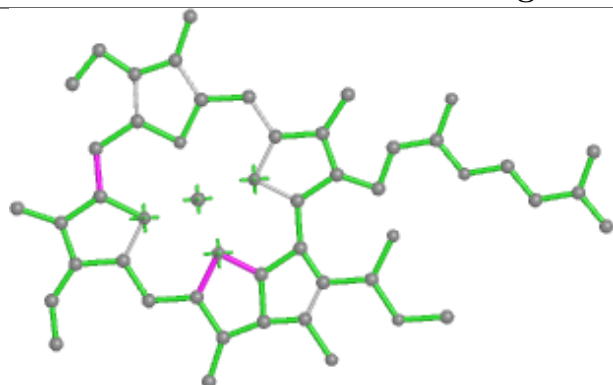
Torsions



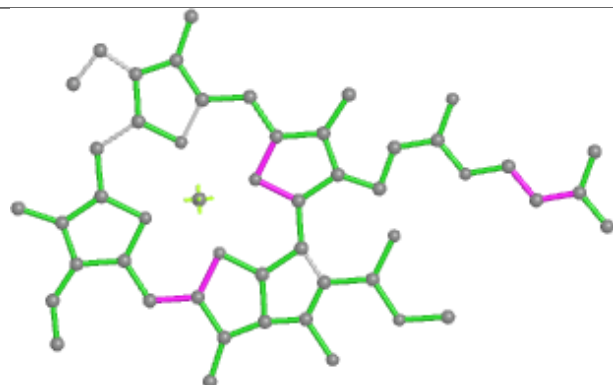
Rings

**Ligand CLA b 605****Ligand CLA B 604**

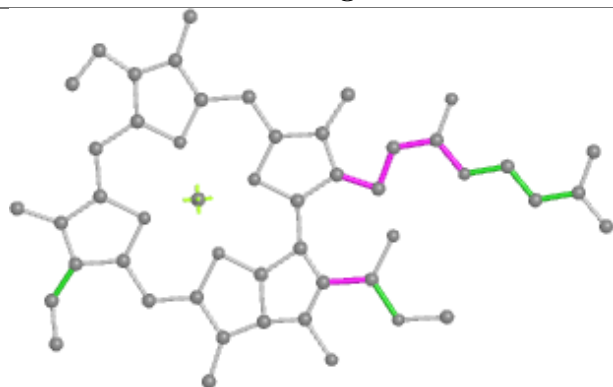
## Ligand CLA S 614



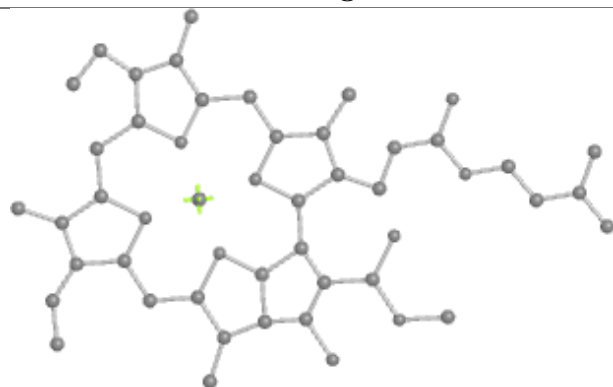
Bond lengths



Bond angles

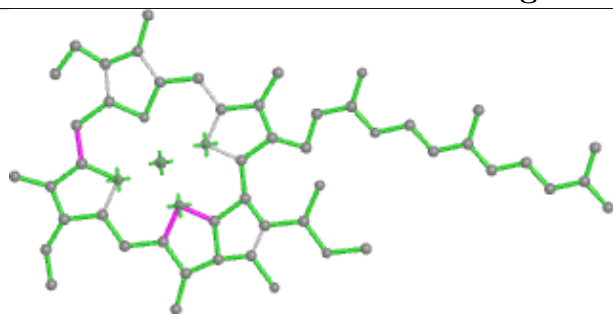


Torsions

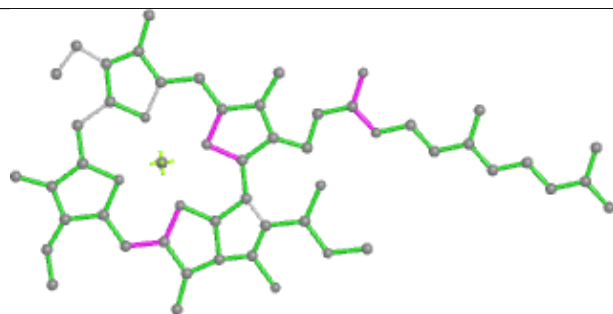


Rings

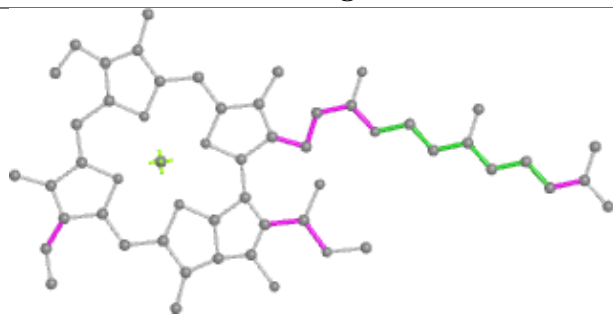
## Ligand CLA s 613



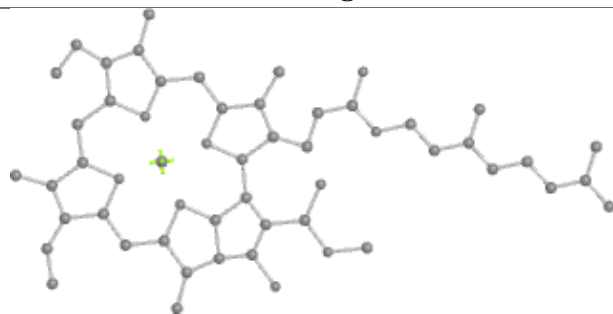
Bond lengths



Bond angles

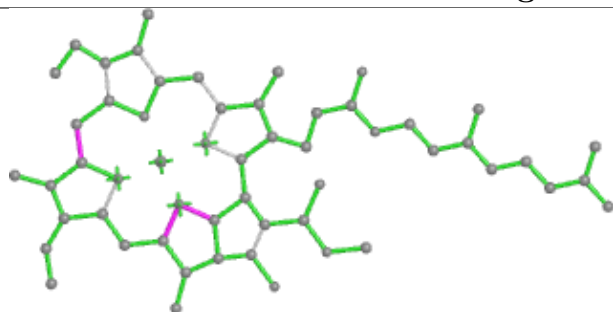


Torsions

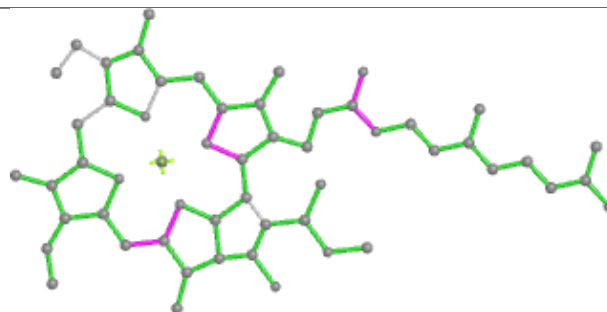


Rings

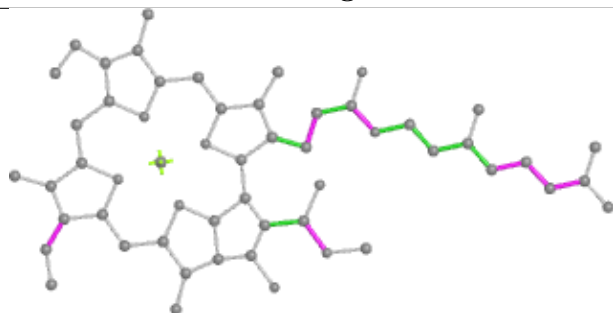


**Ligand CLA S 613**

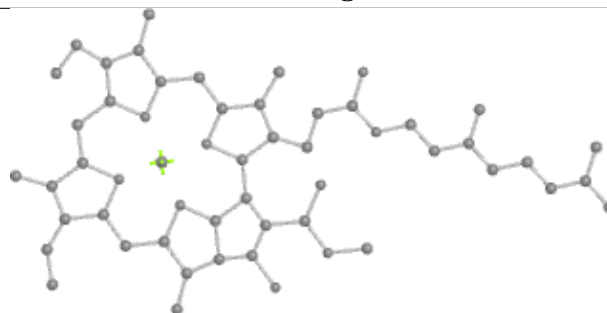
Bond lengths



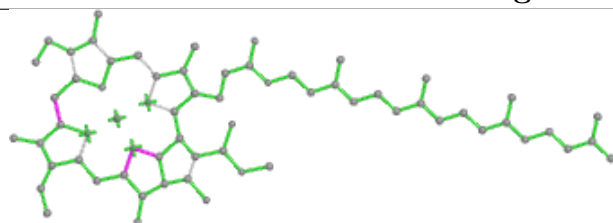
Bond angles



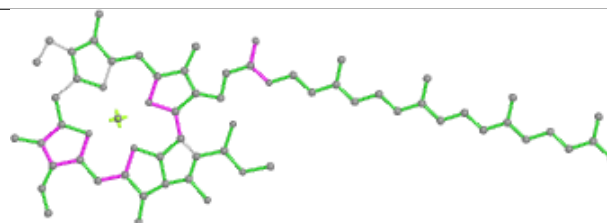
Torsions



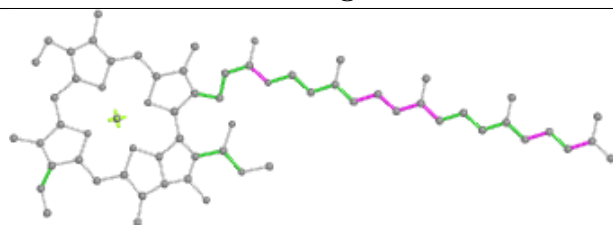
Rings

**Ligand CLA Y 611**

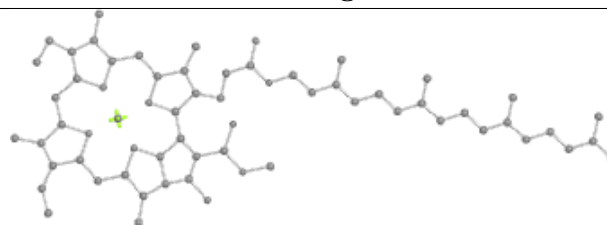
Bond lengths



Bond angles

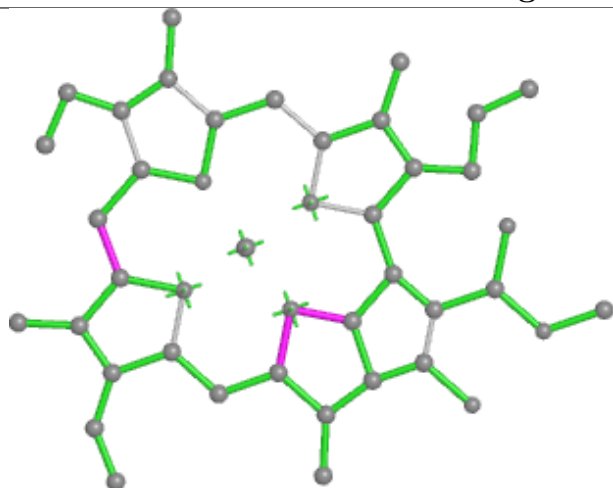


Torsions

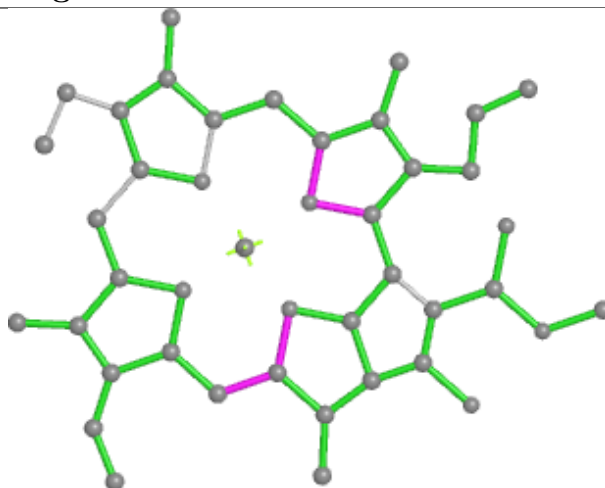


Rings

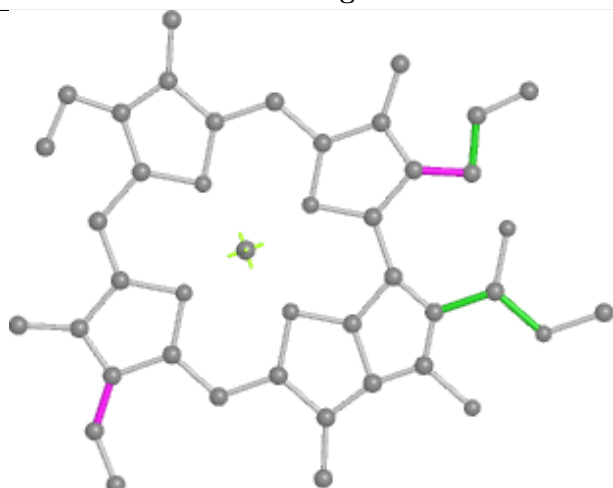
## Ligand CLA g 612



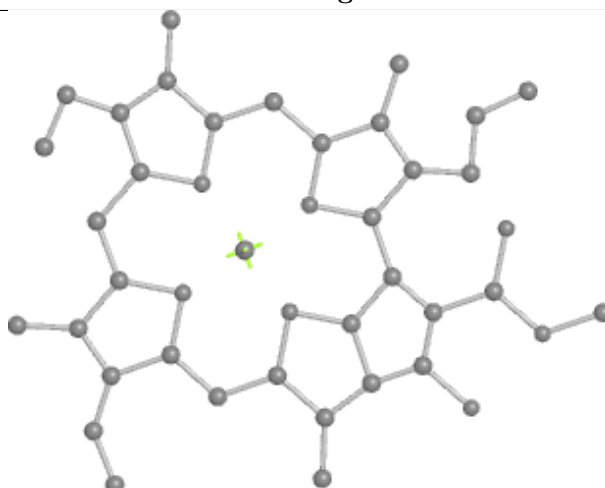
Bond lengths



Bond angles

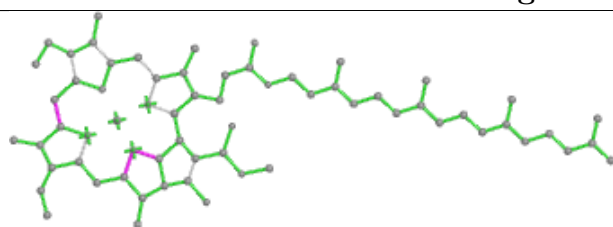


Torsions

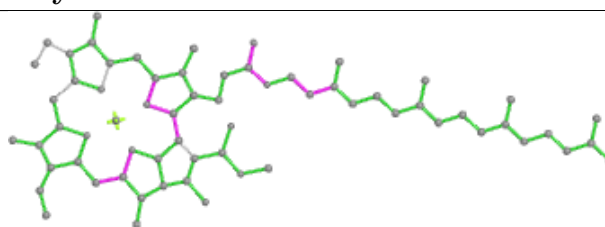


Rings

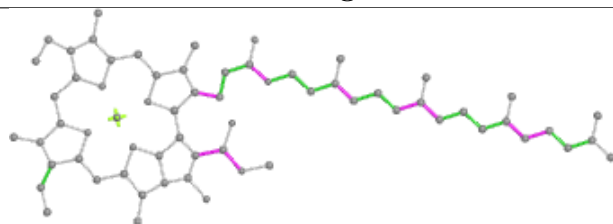
## Ligand CLA y 604



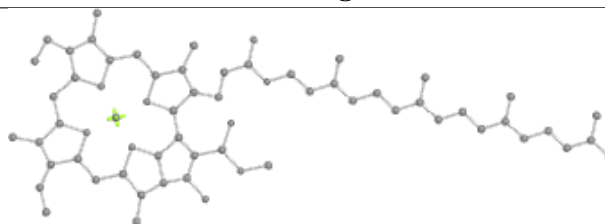
Bond lengths



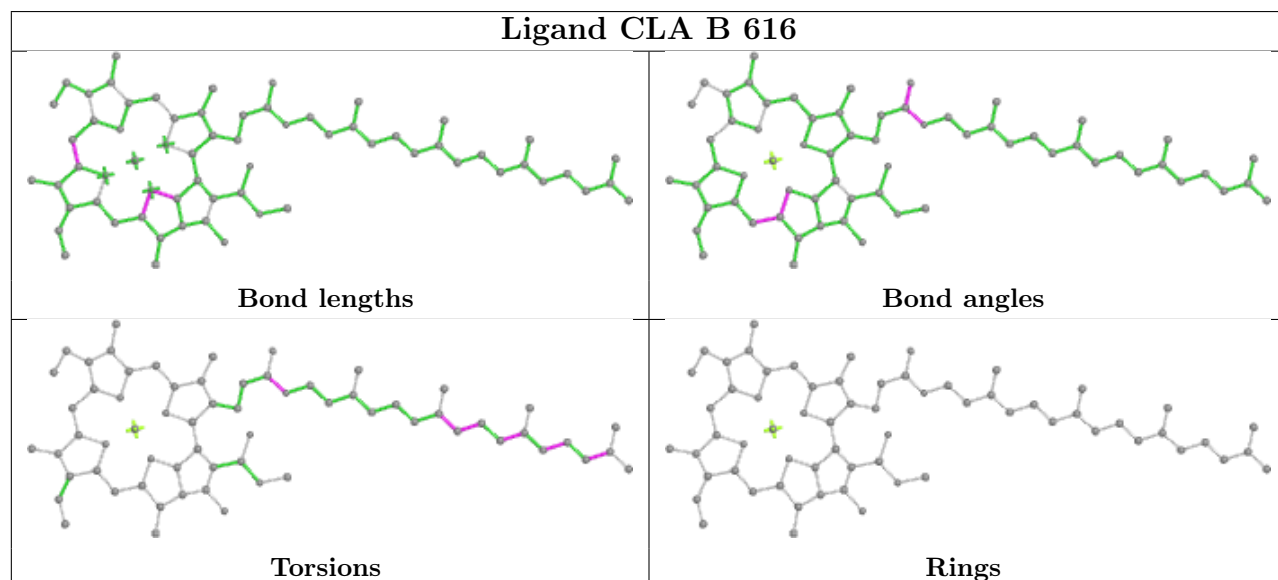
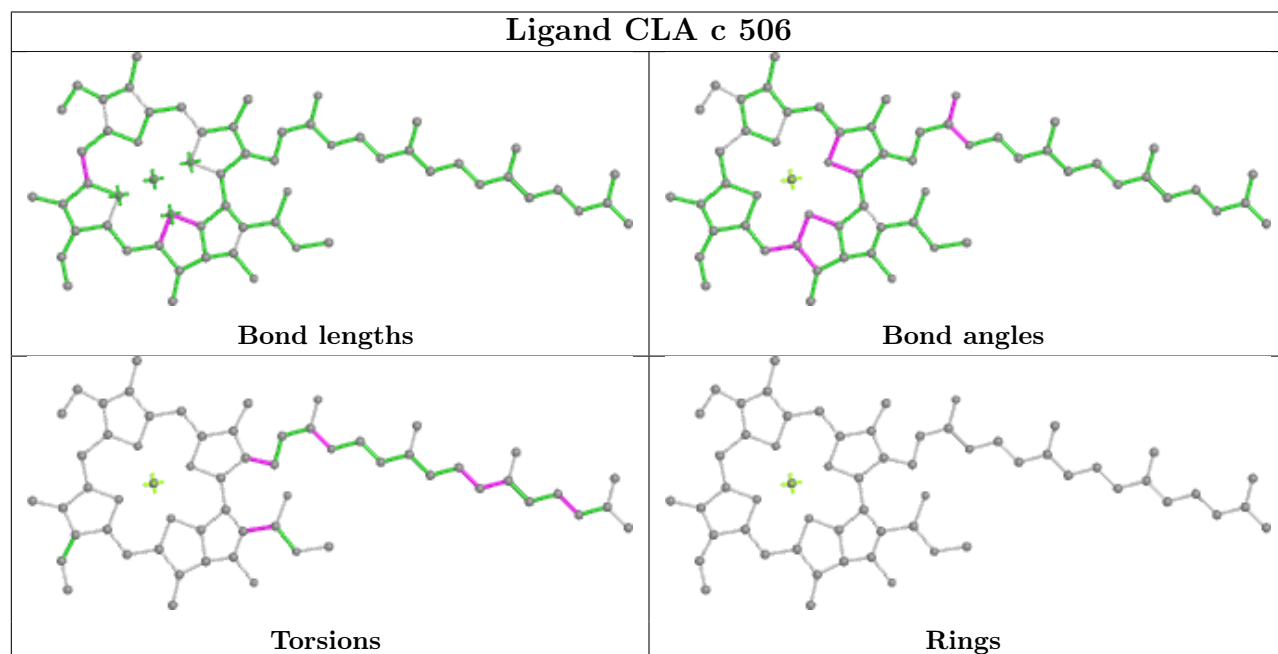
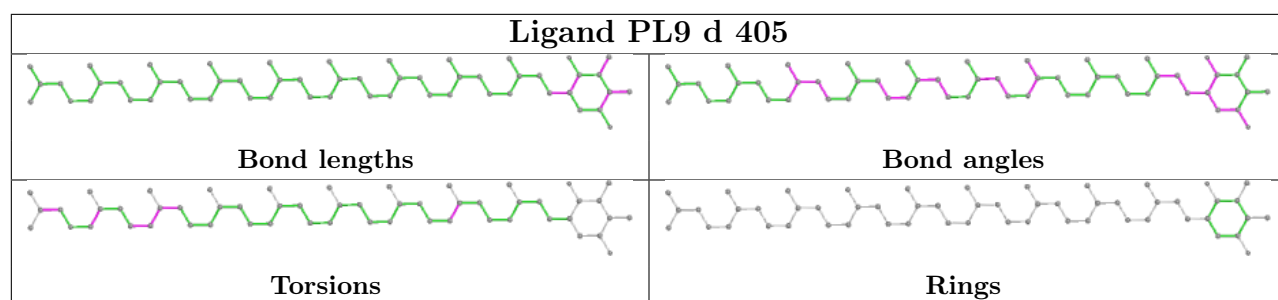
Bond angles



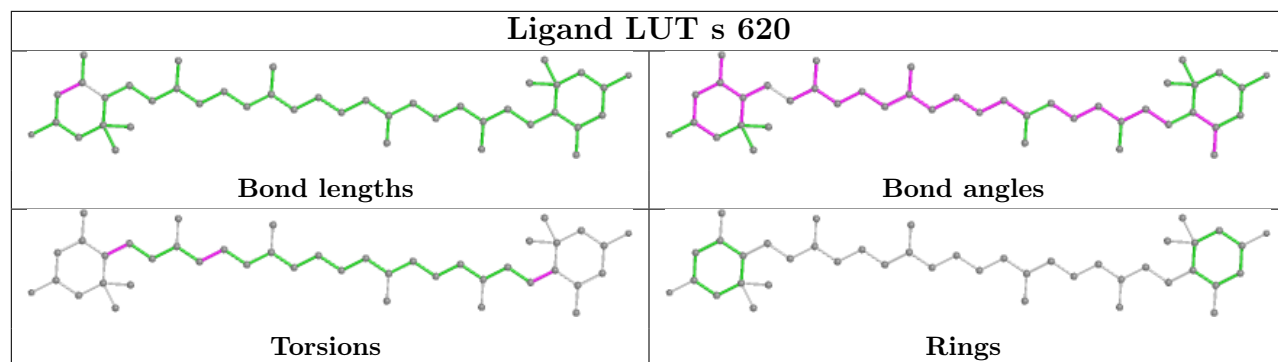
Torsions



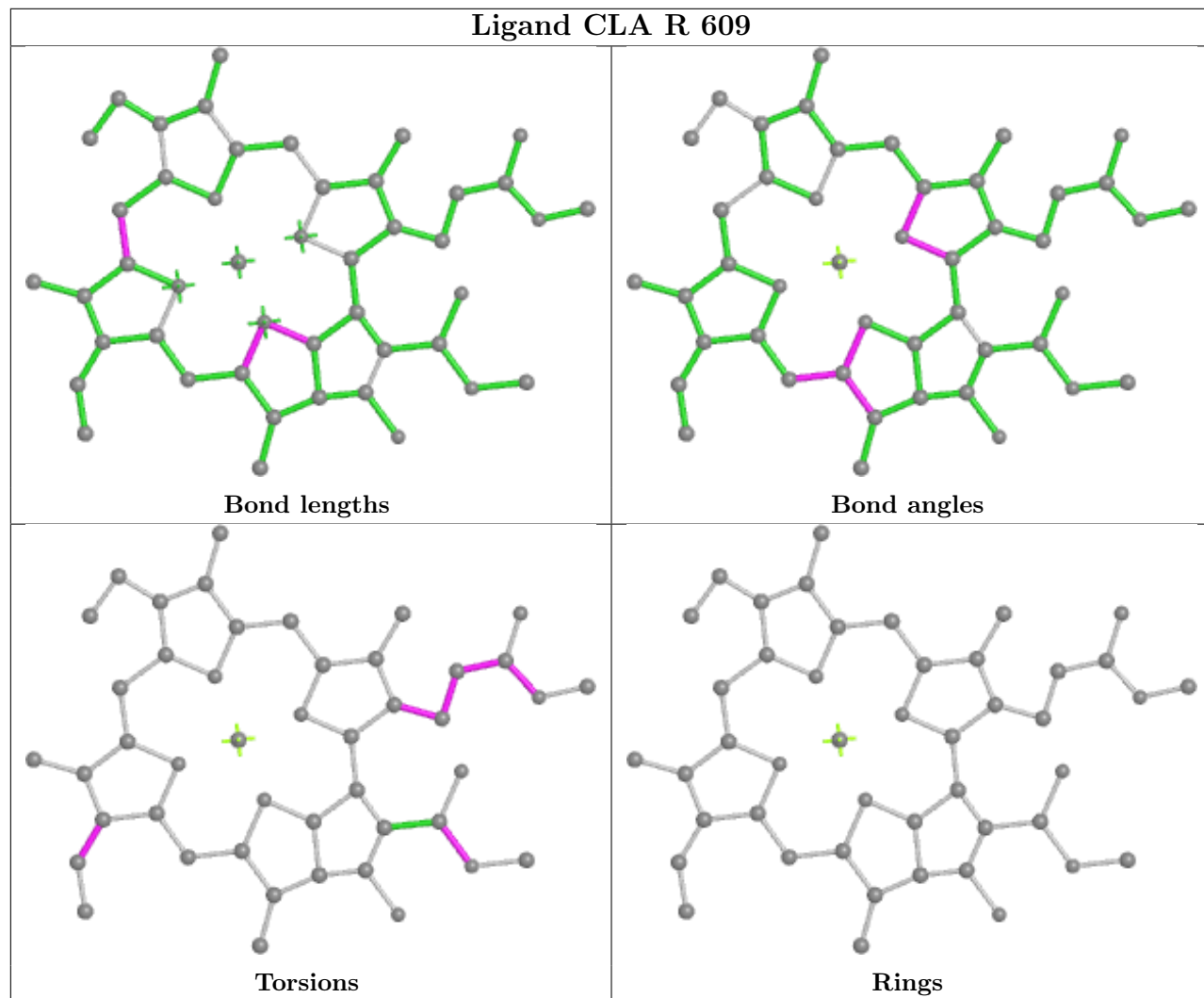
Rings

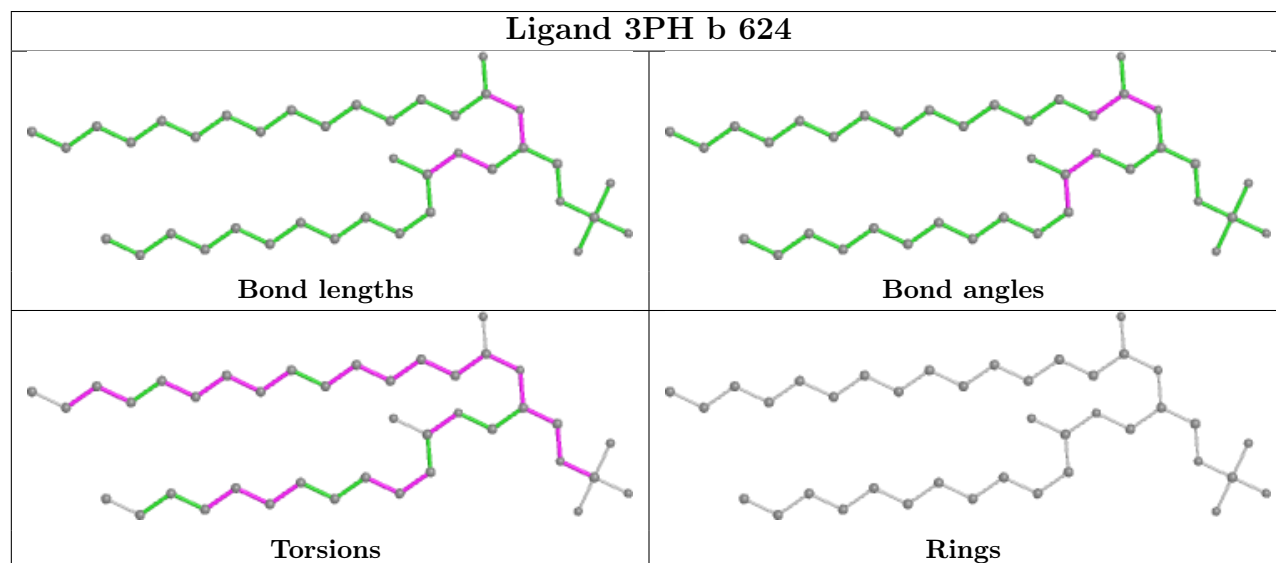
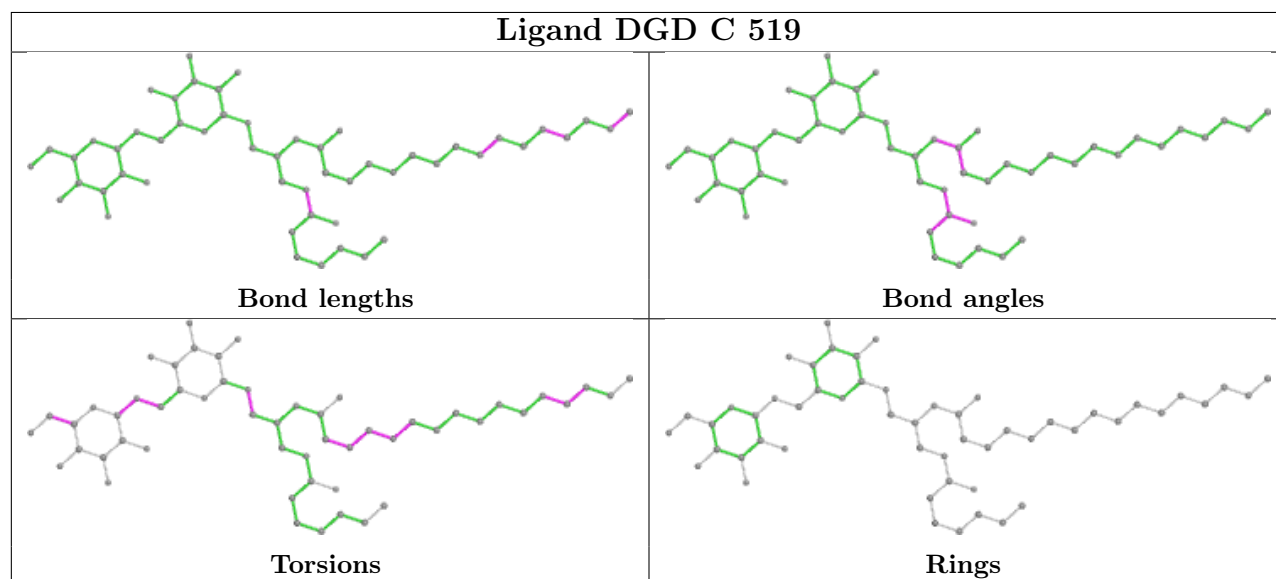
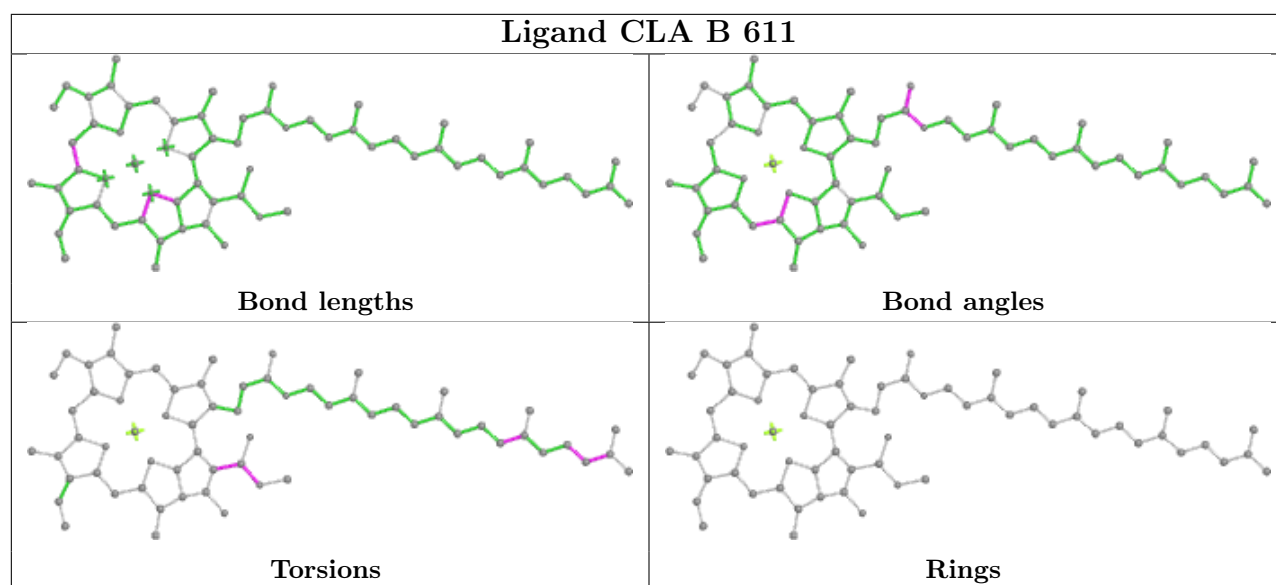


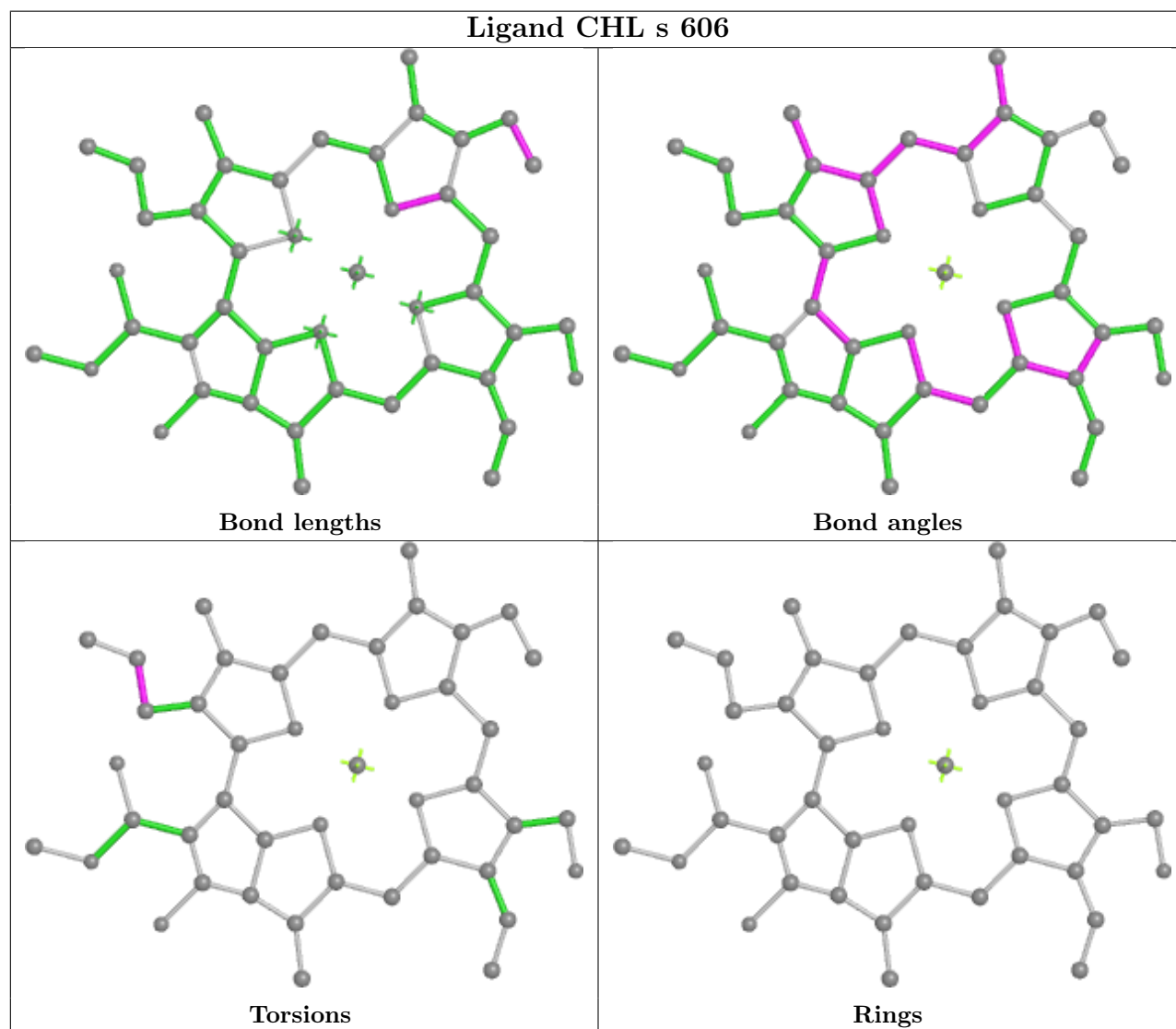
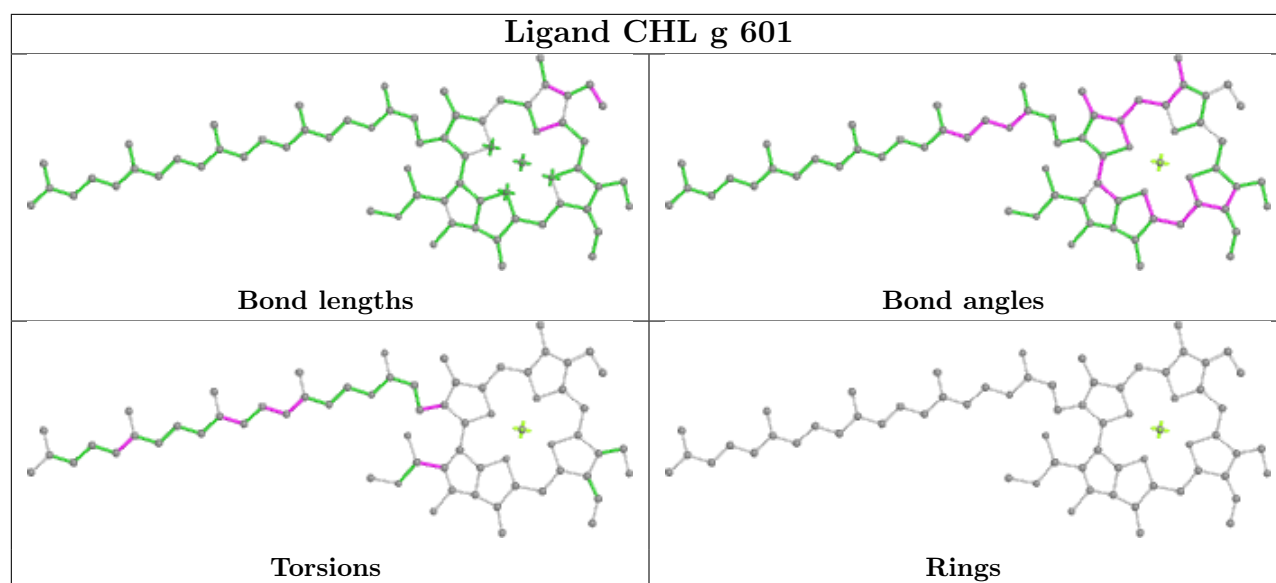
## Ligand LUT s 620

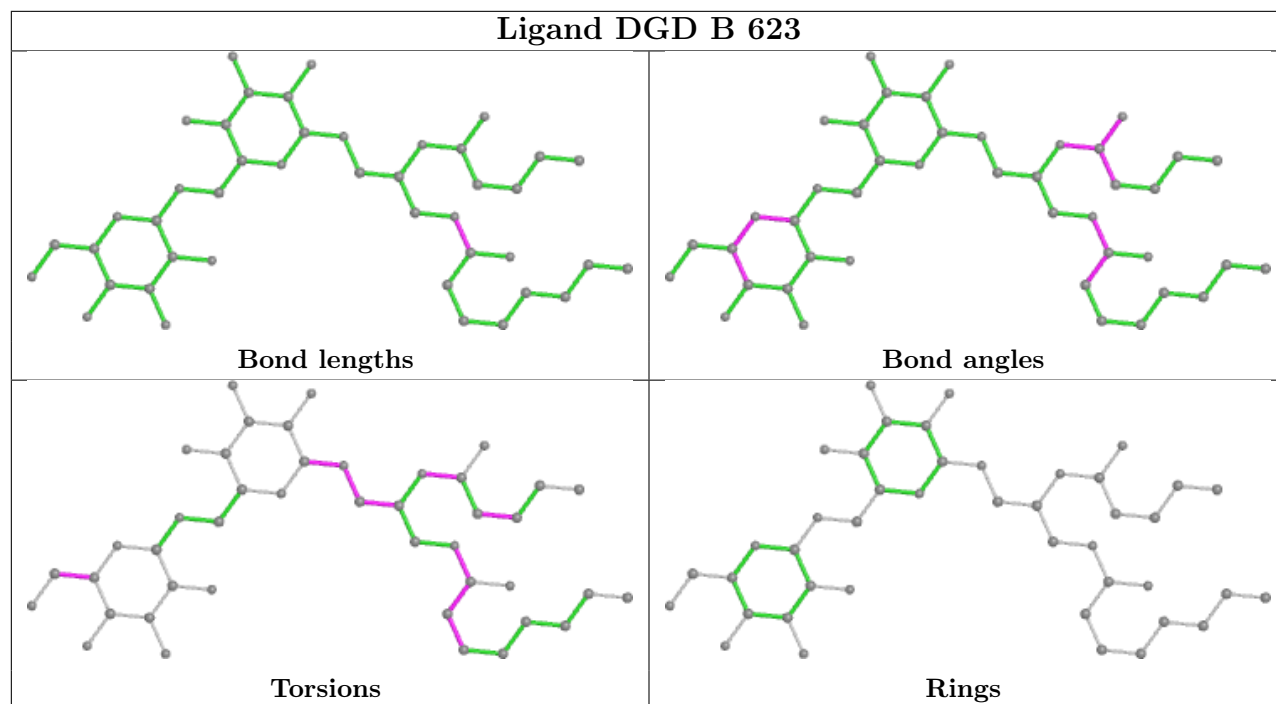
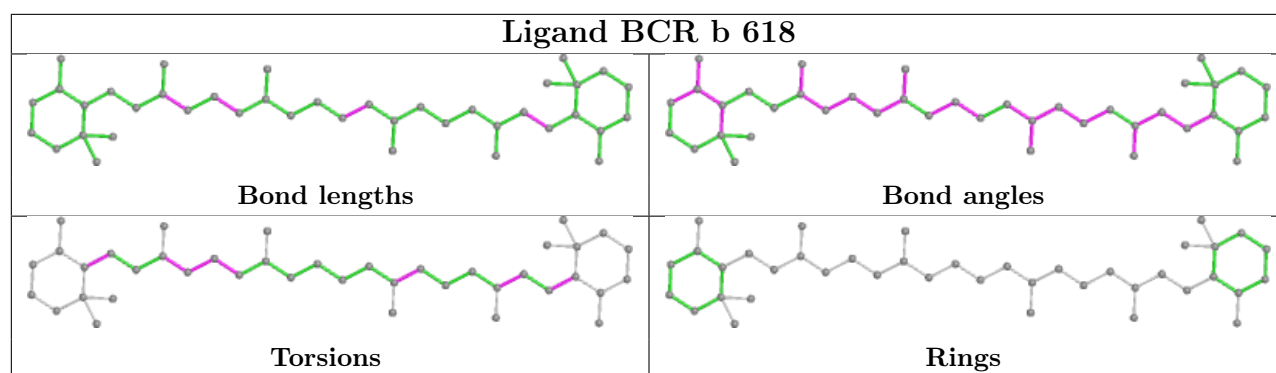


## Ligand CLA R 609

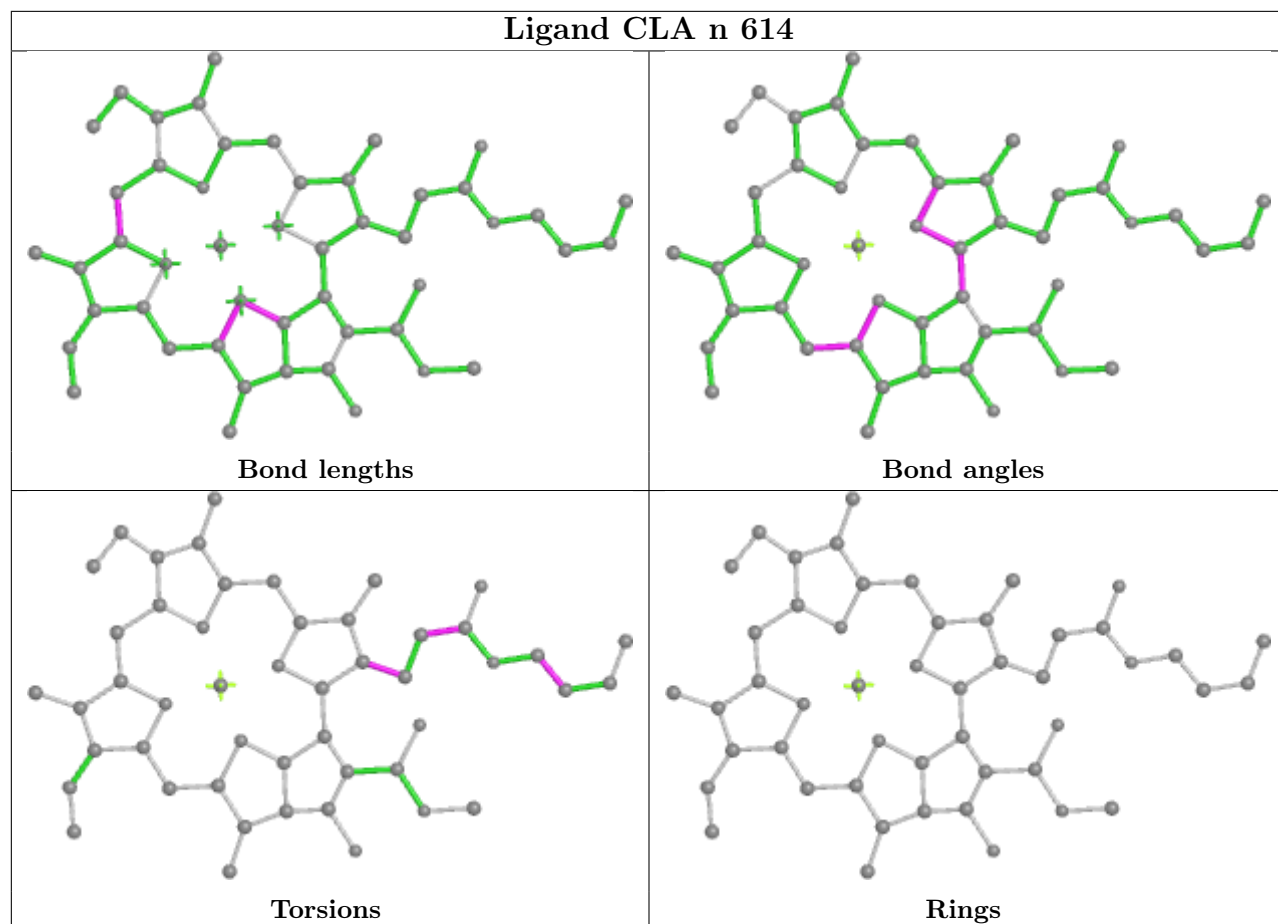




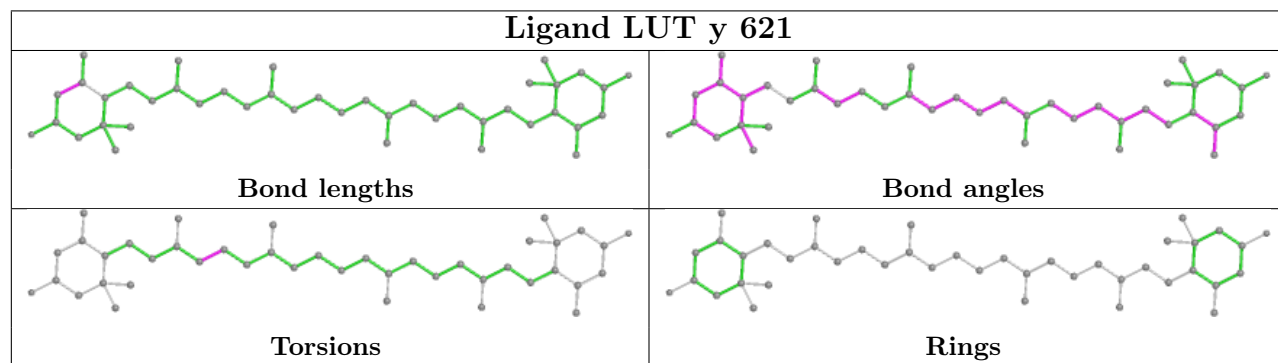
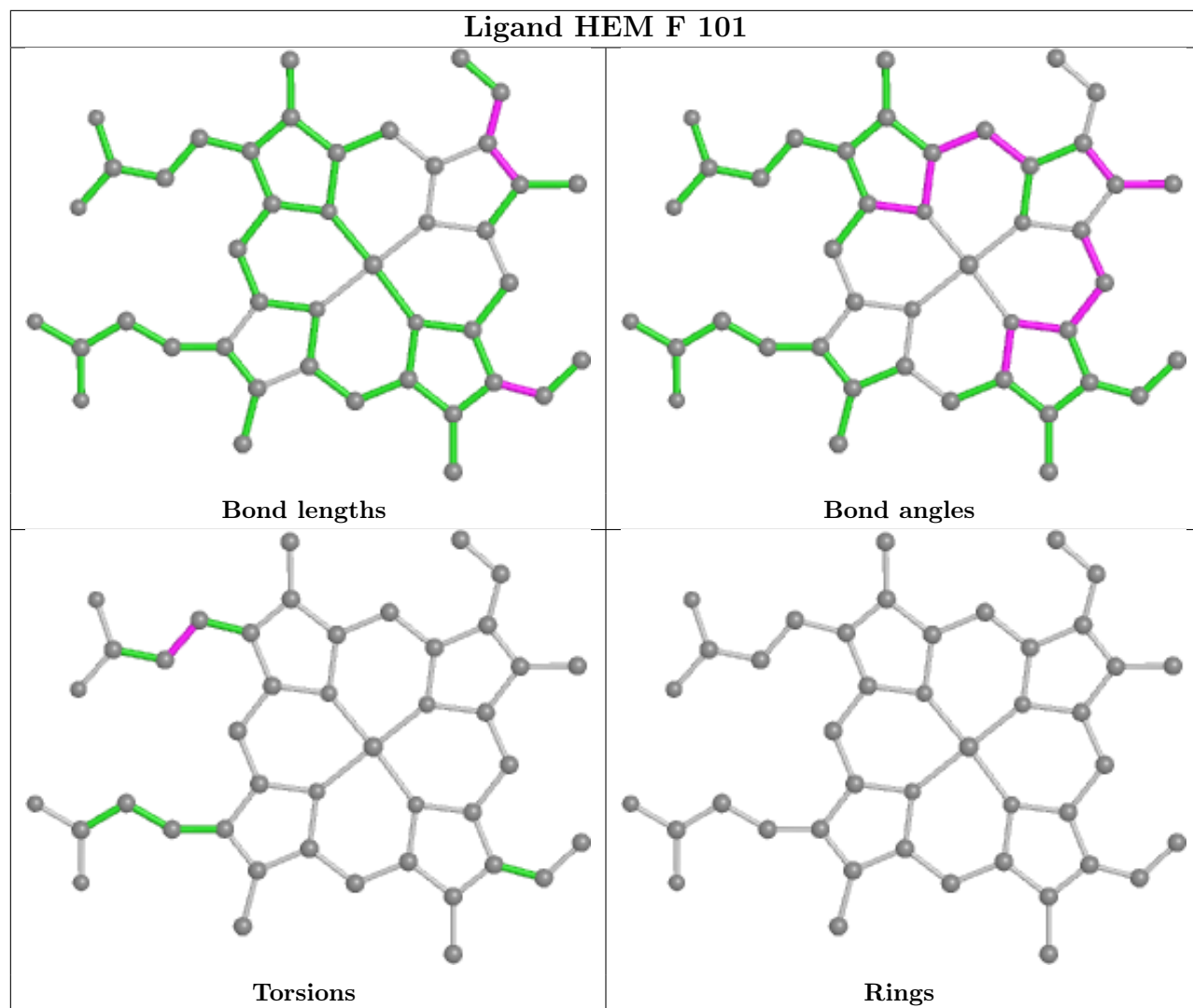


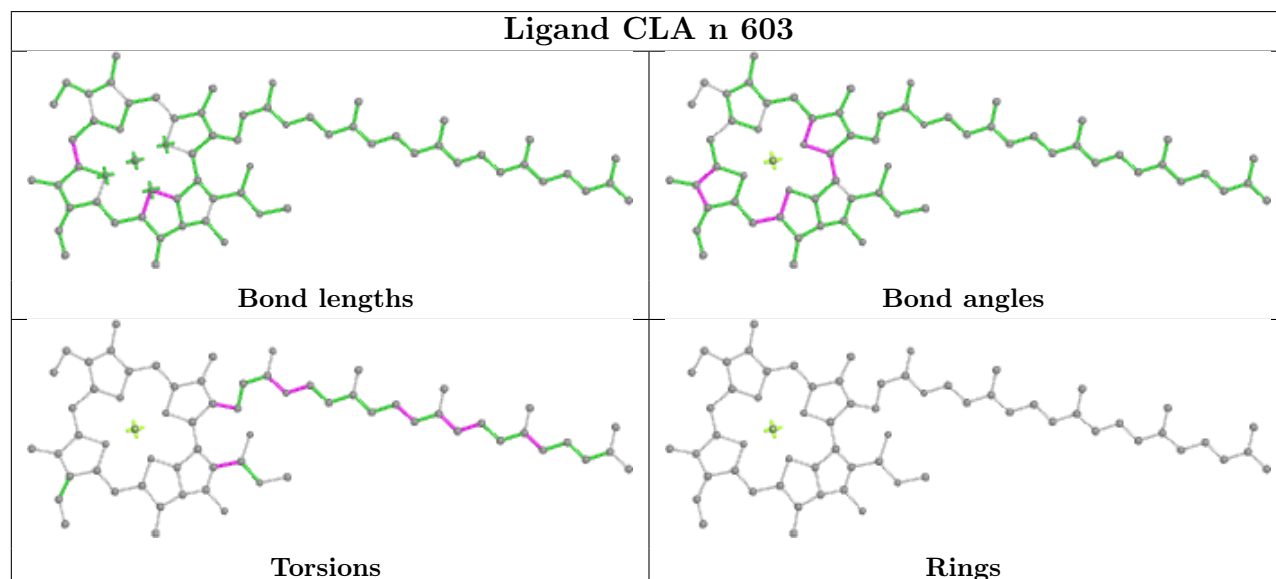
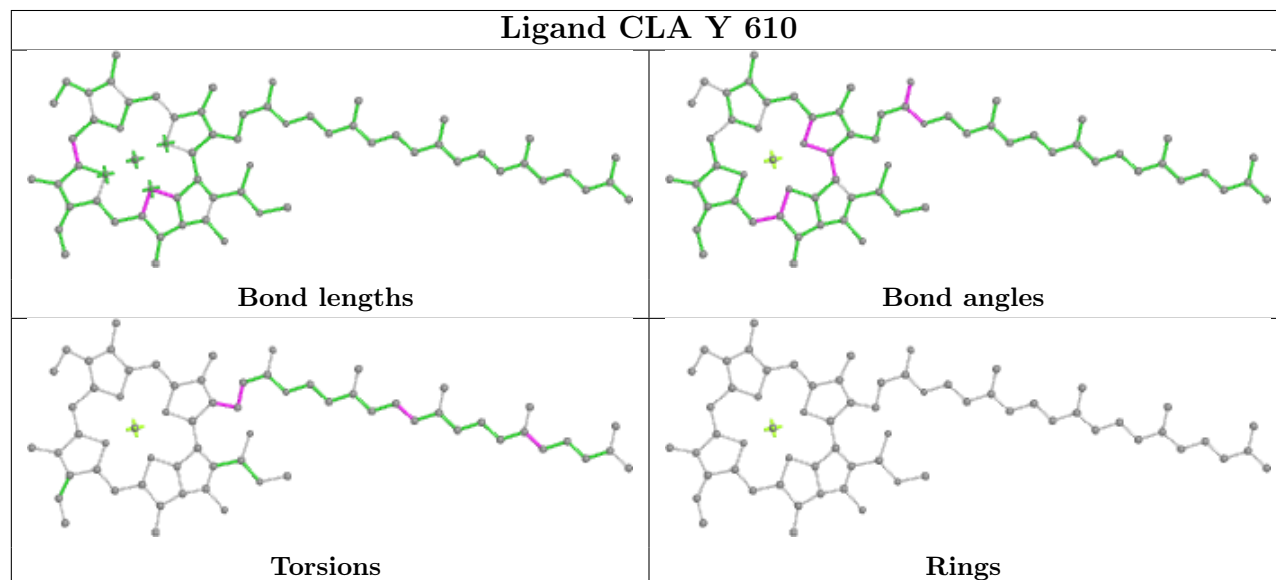
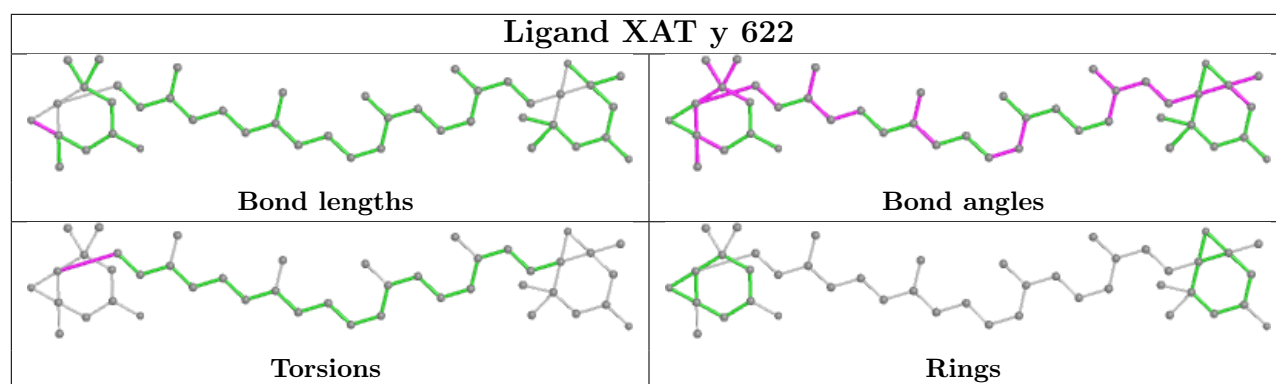


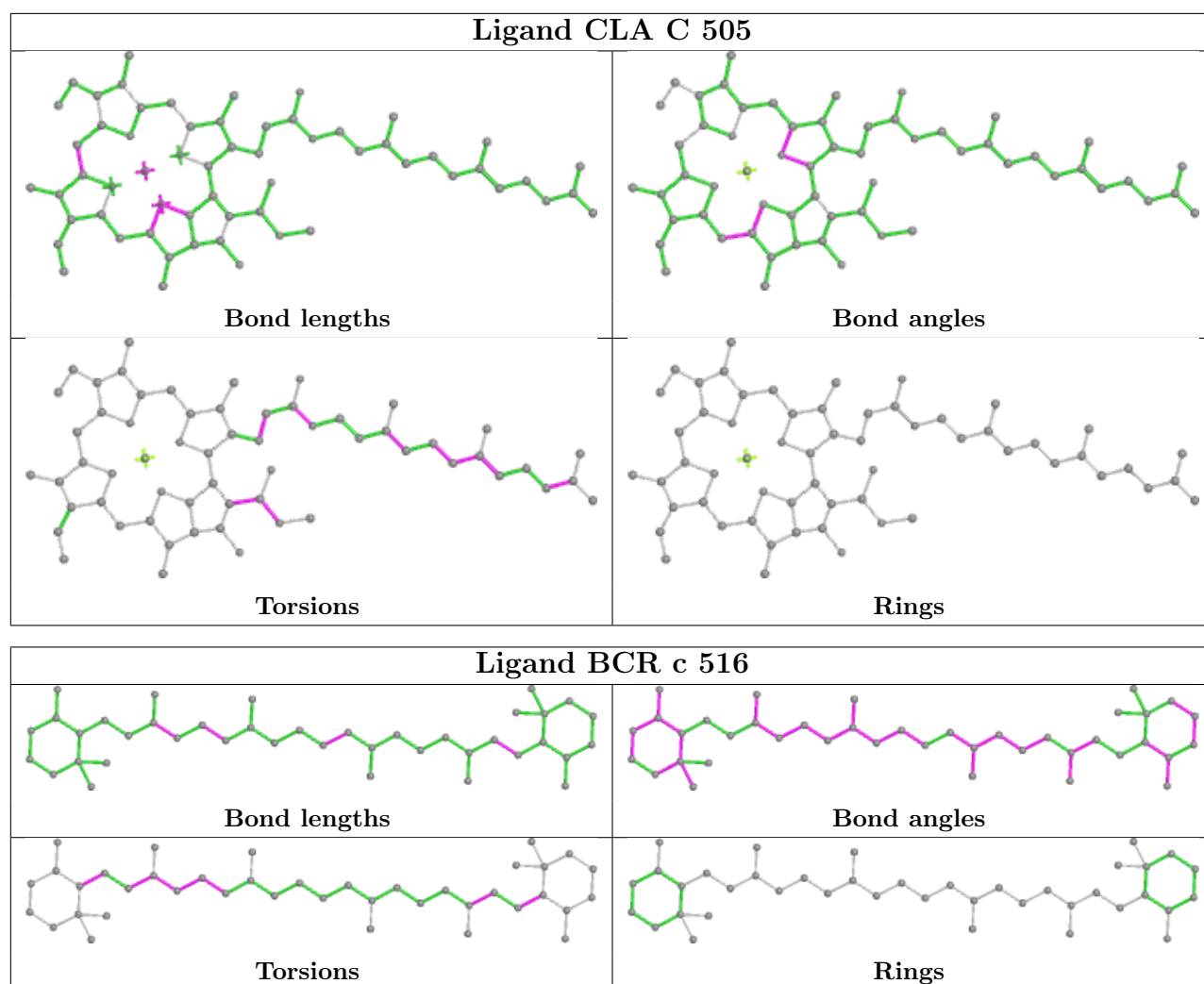
## Ligand CLA n 614

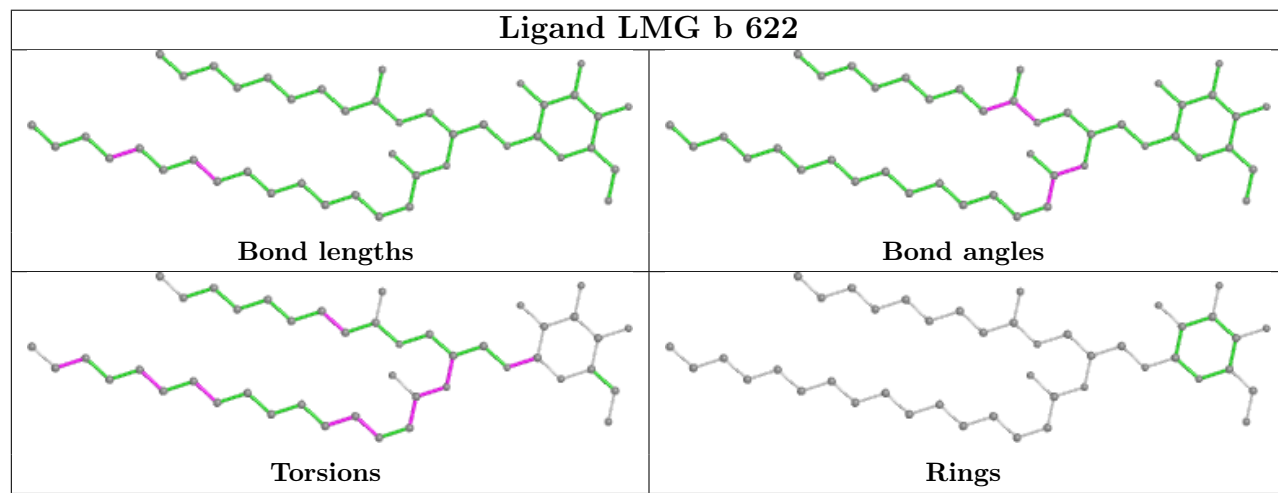
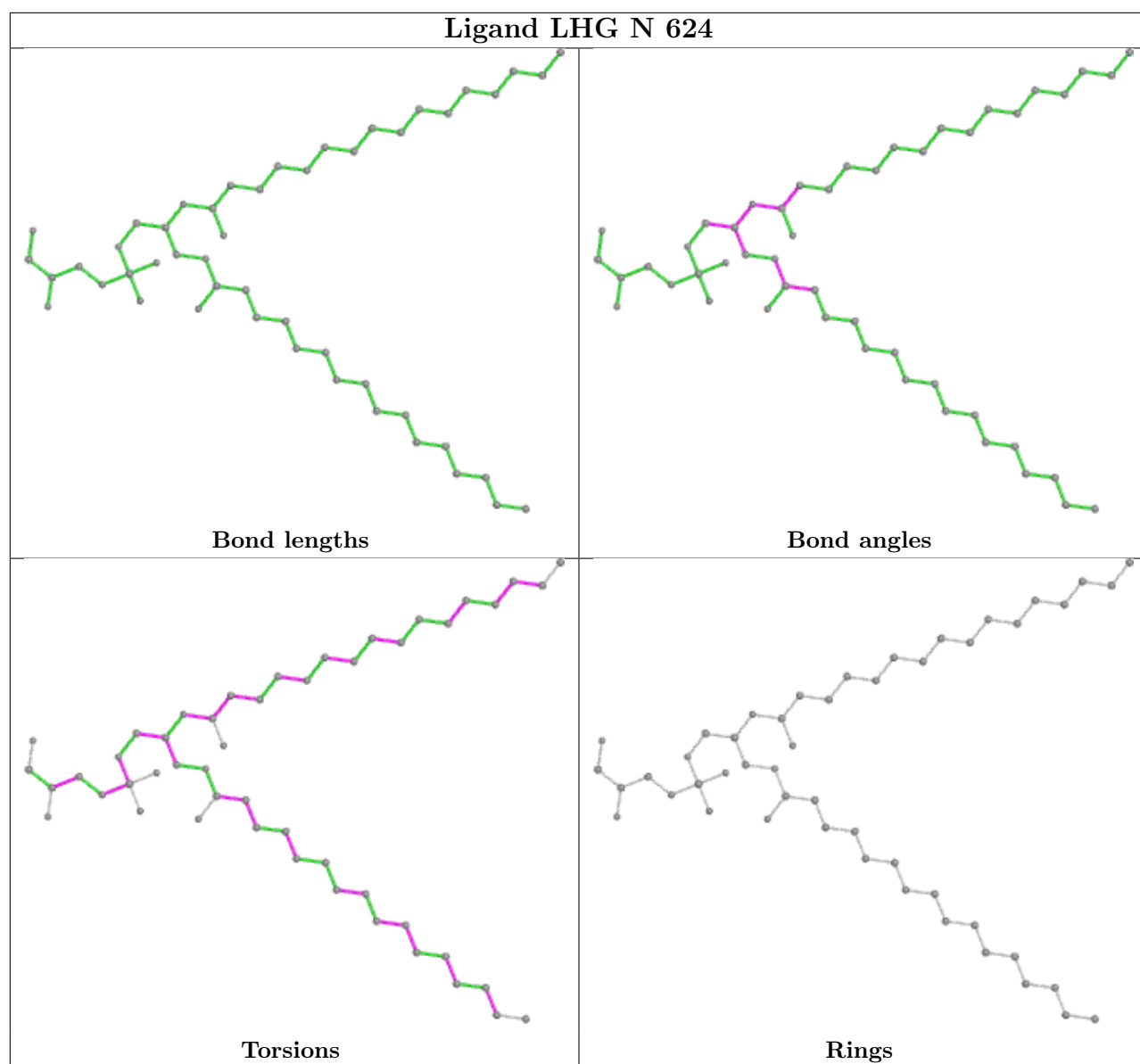




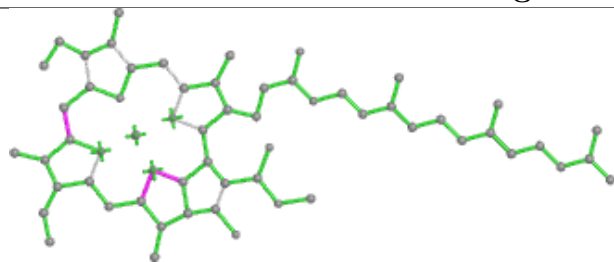




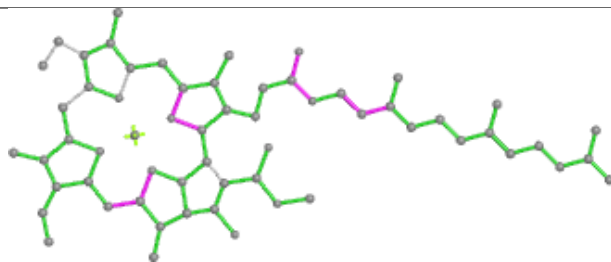




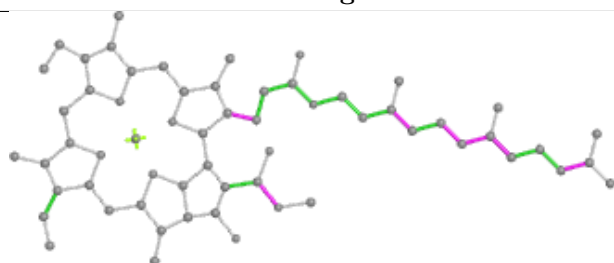
## Ligand CLA R 610



Bond lengths



Bond angles

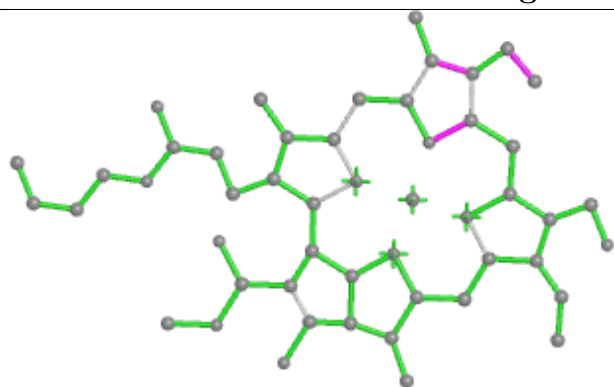


Torsions

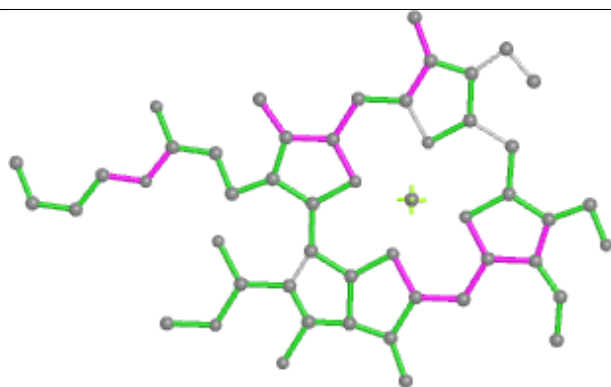


Rings

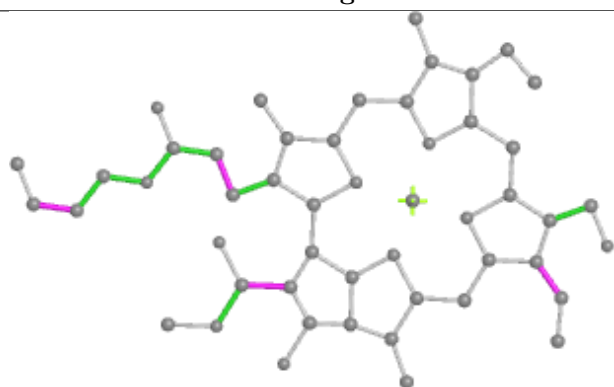
## Ligand CHL r 607



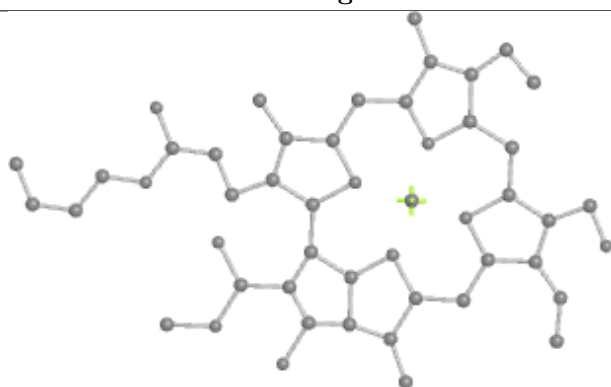
Bond lengths



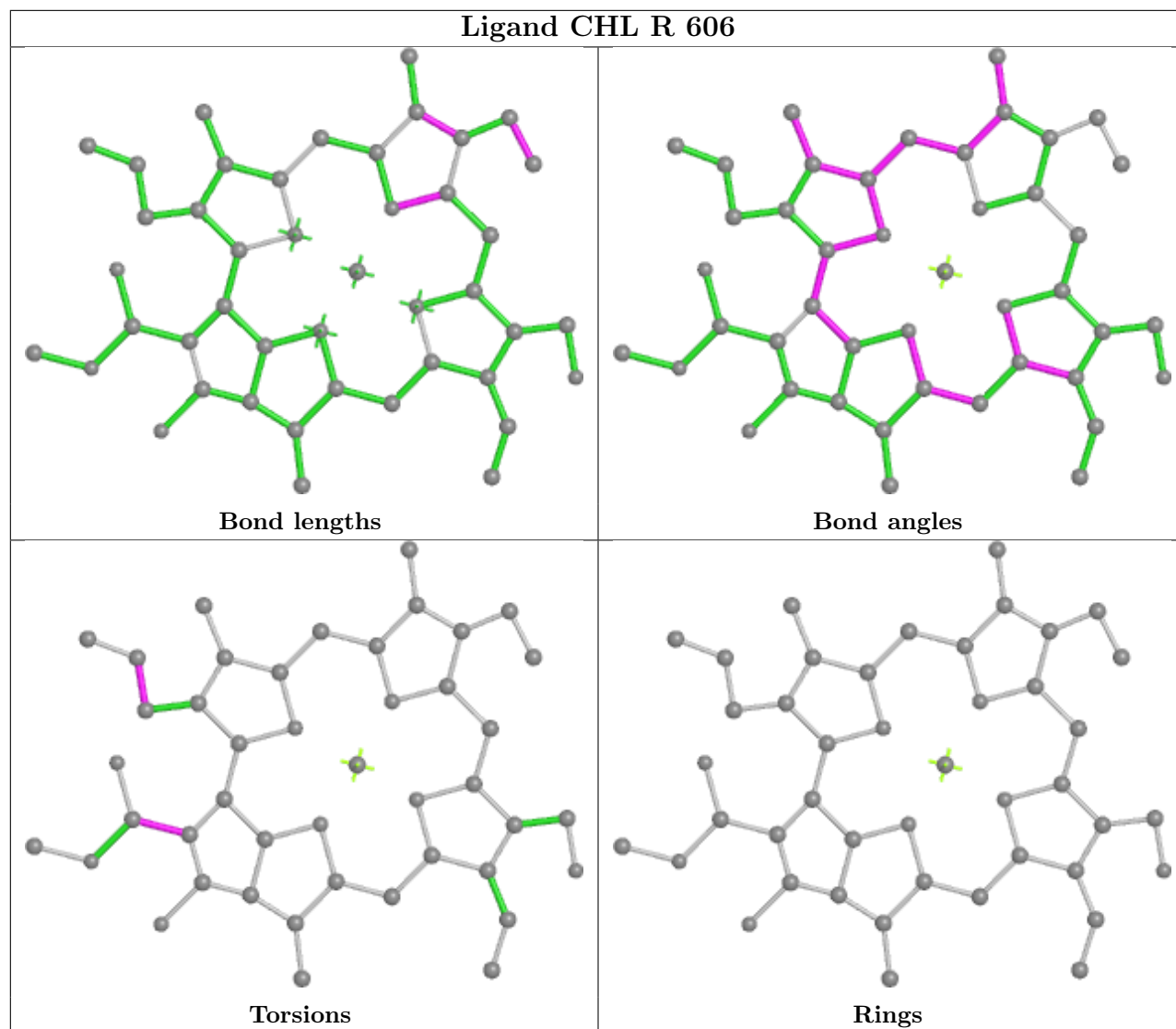
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.60
1	R	110:PRO	C	126:GLU	N	12.92

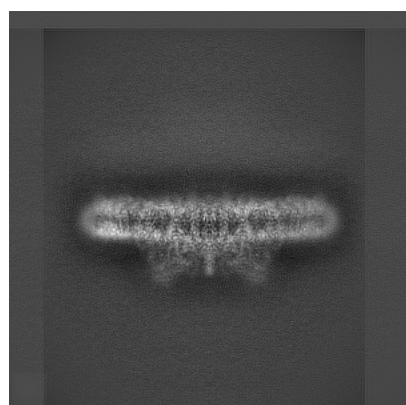
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13429. These allow visual inspection of the internal detail of the map and identification of artifacts.

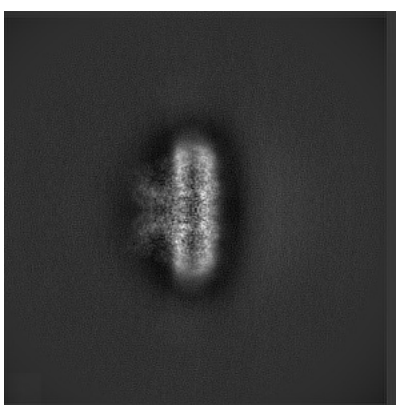
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

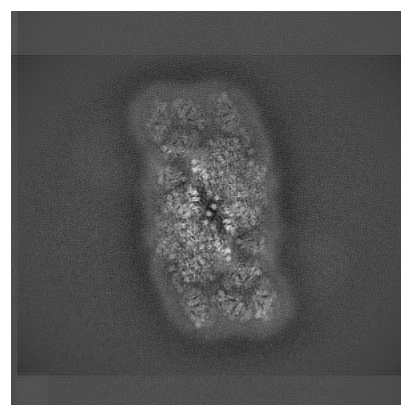
#### 6.1.1 Primary map



X



Y

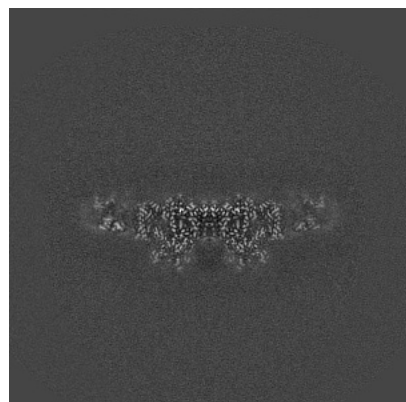


Z

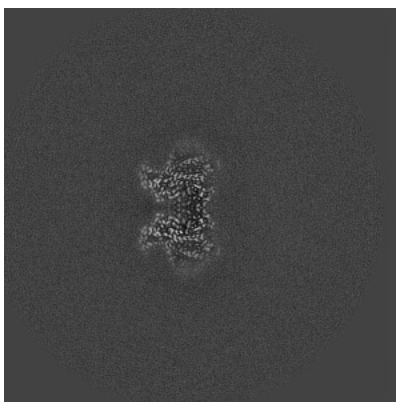
The images above show the map projected in three orthogonal directions.

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

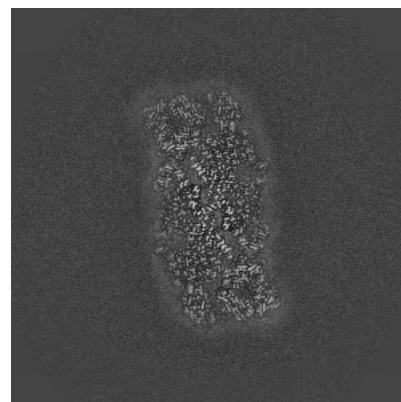
#### 6.2.1 Primary map



X Index: 250



Y Index: 250



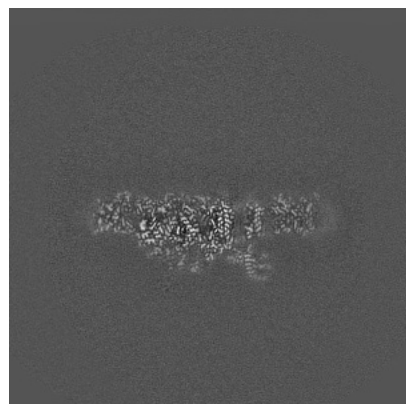
Z Index: 250



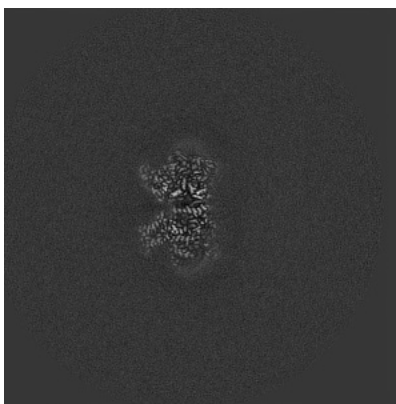
The images above show central slices of the map in three orthogonal directions.

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

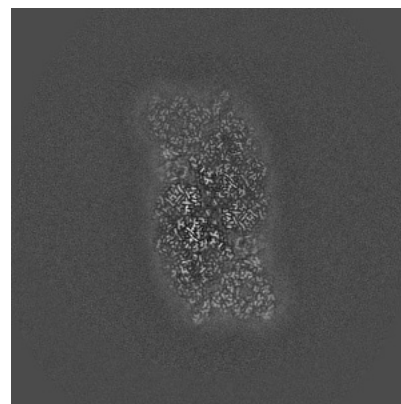
### 6.3.1 Primary map



X Index: 229



Y Index: 247



Z Index: 221

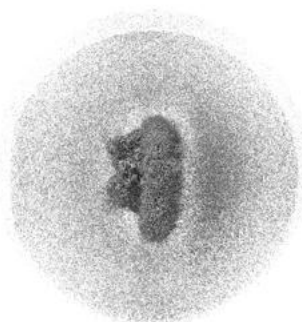
The images above show the largest variance slices of the map in three orthogonal directions.

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

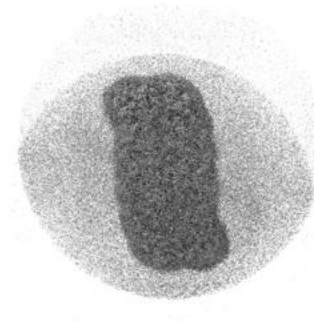
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

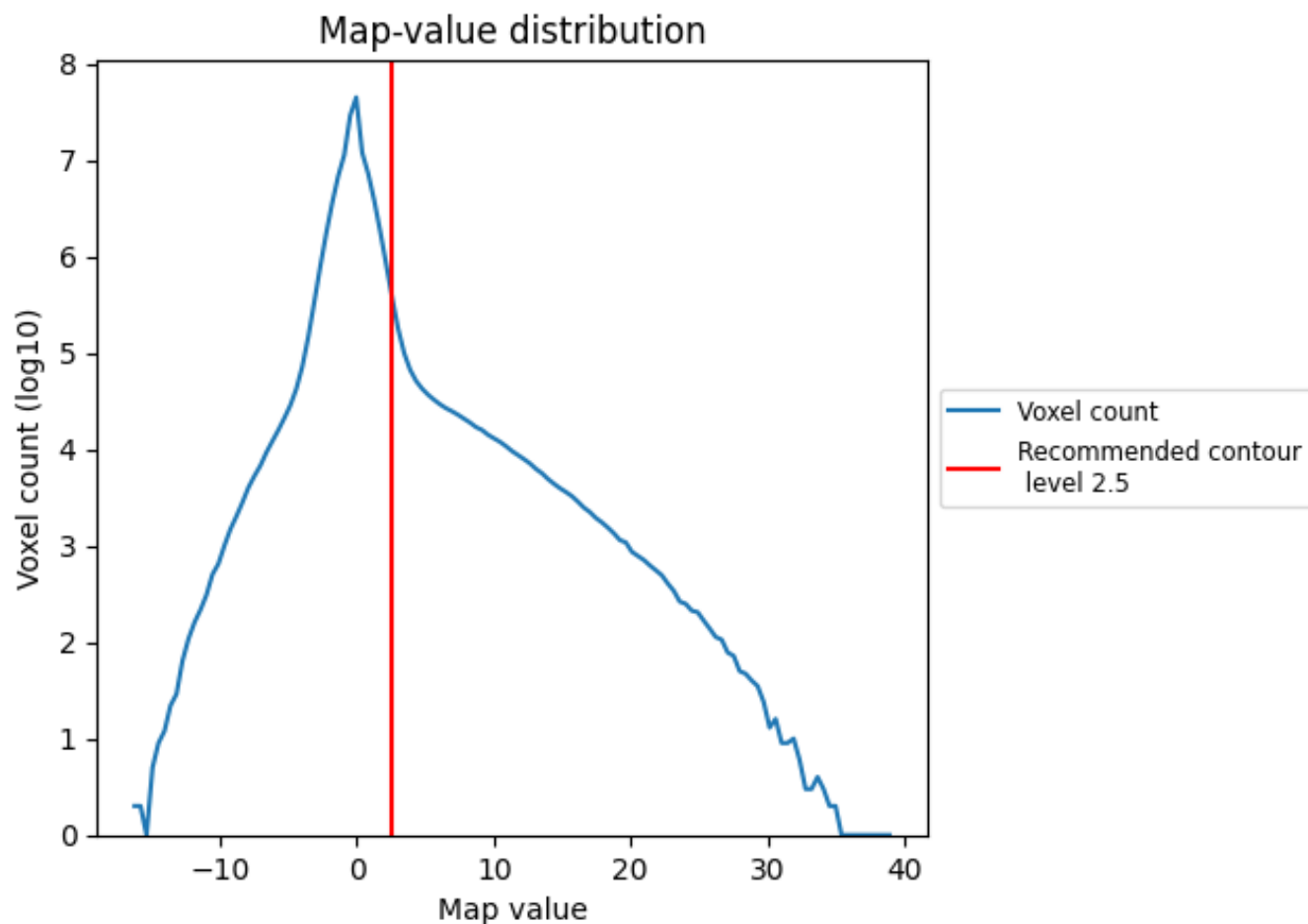
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

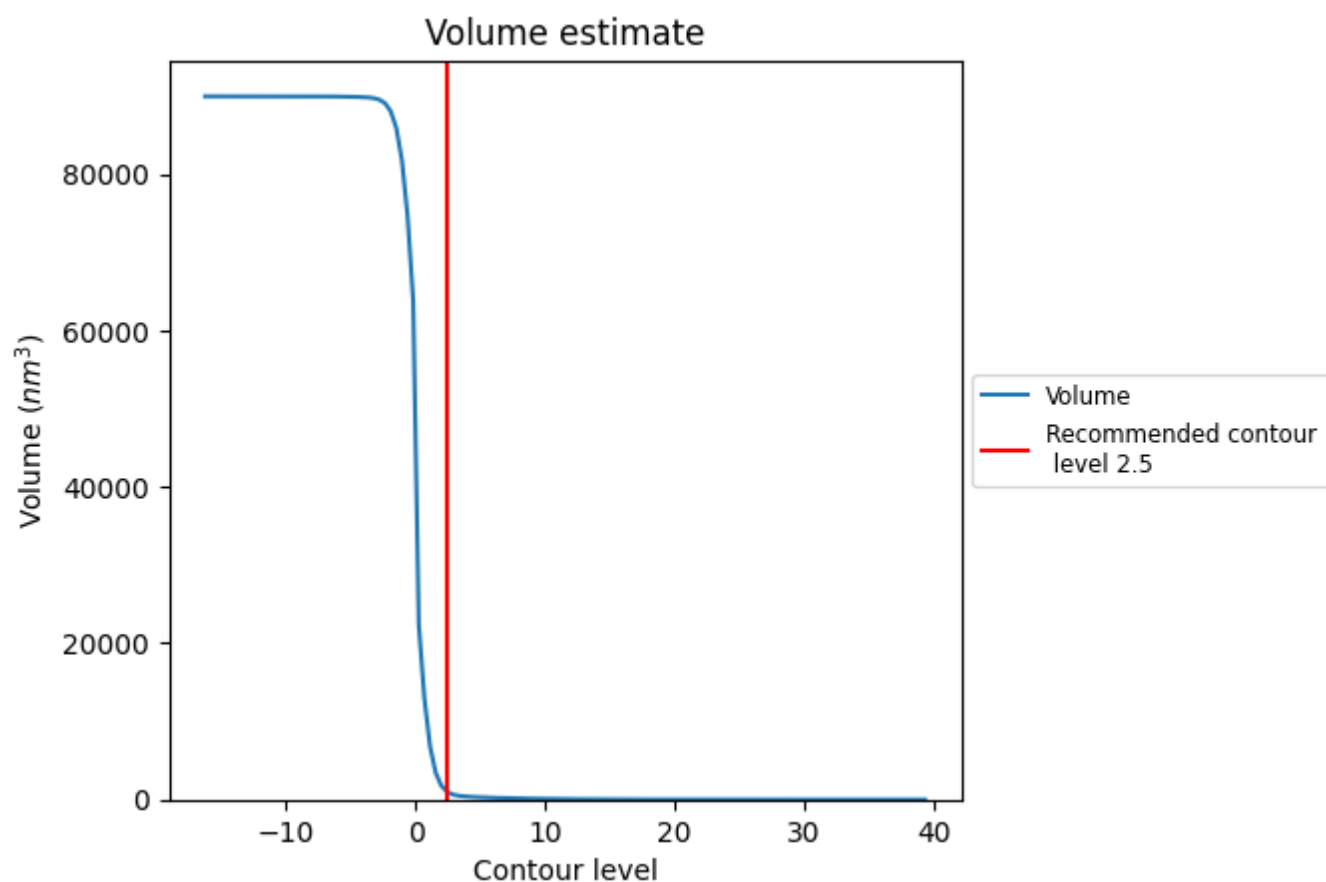
This section contains the results of statistical analysis of the map.

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



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

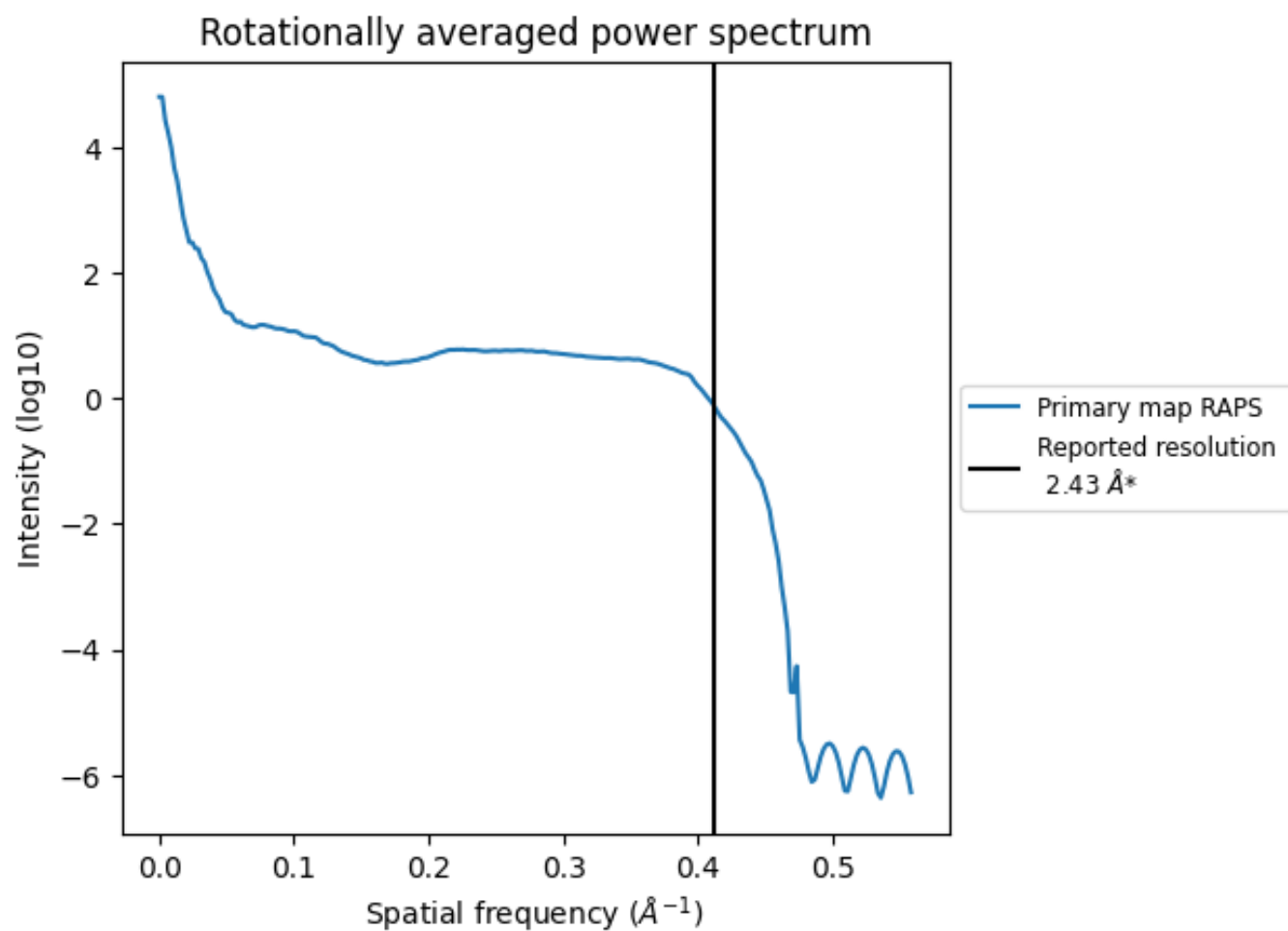
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948  $\text{nm}^3$ ; this corresponds to an approximate mass of 856 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 ⓘ

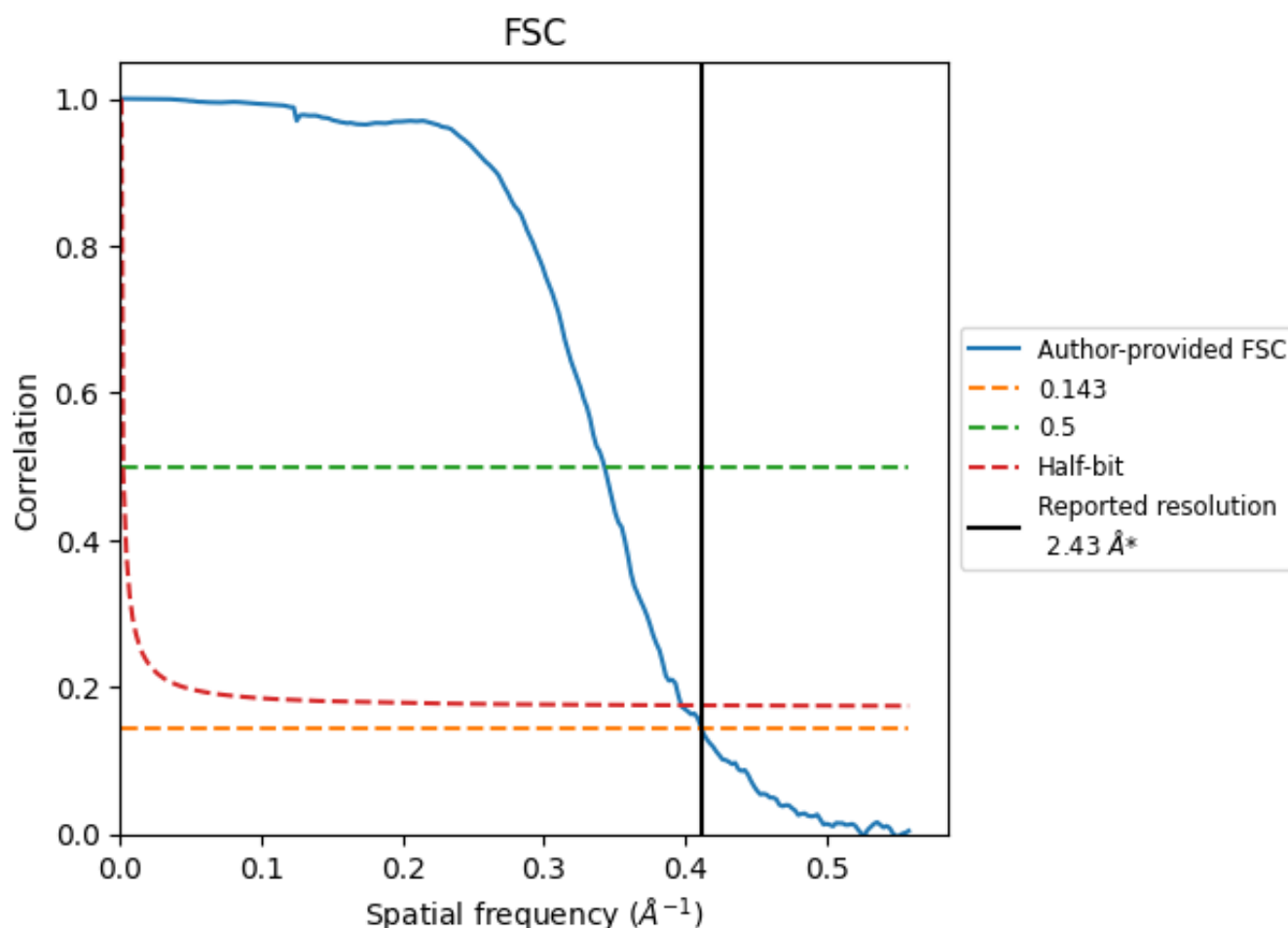


\*Reported resolution corresponds to spatial frequency of 0.412 Å<sup>-1</sup>

## 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 0.412 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

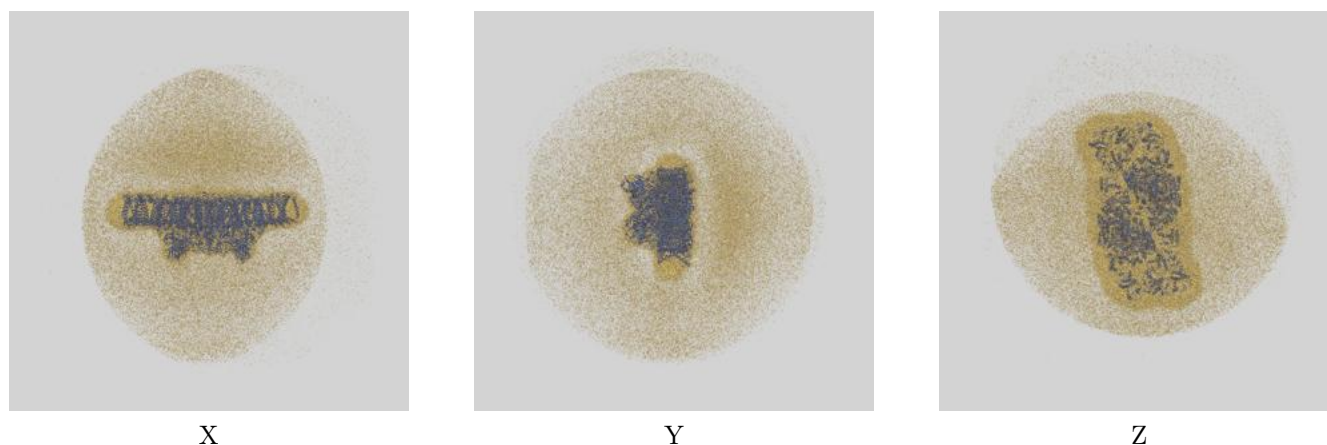
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

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

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

This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in [section 3](#) on [page 61](#).

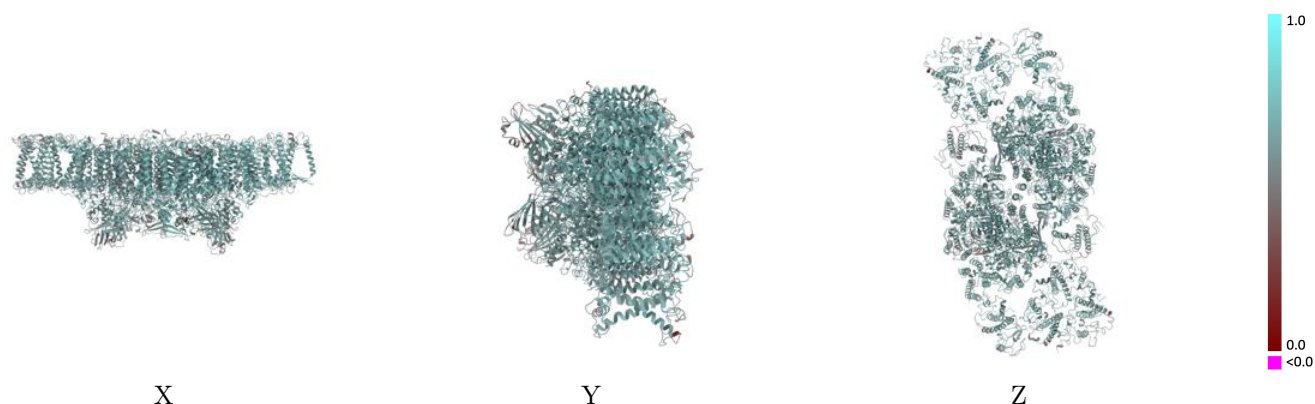
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

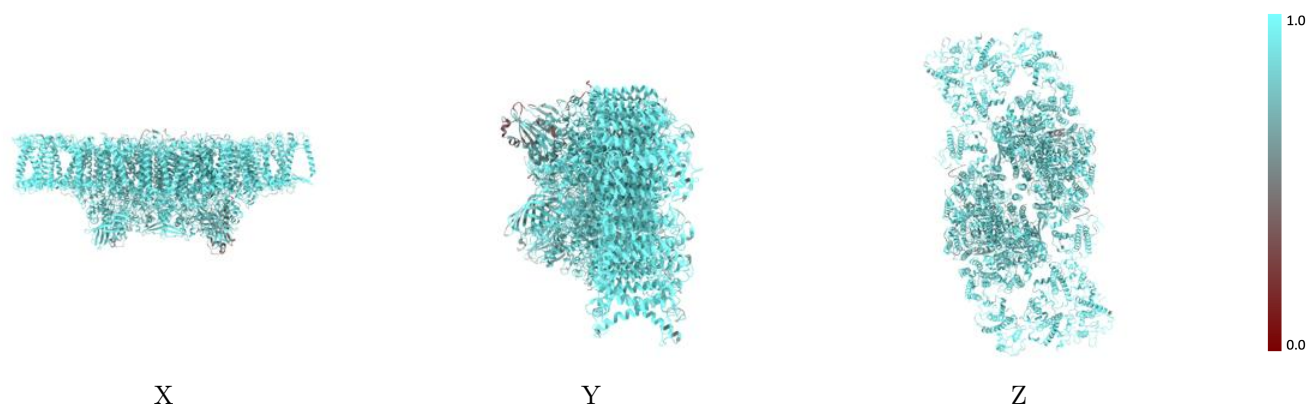


## 9.2 Q-score mapped to coordinate model [i](#)



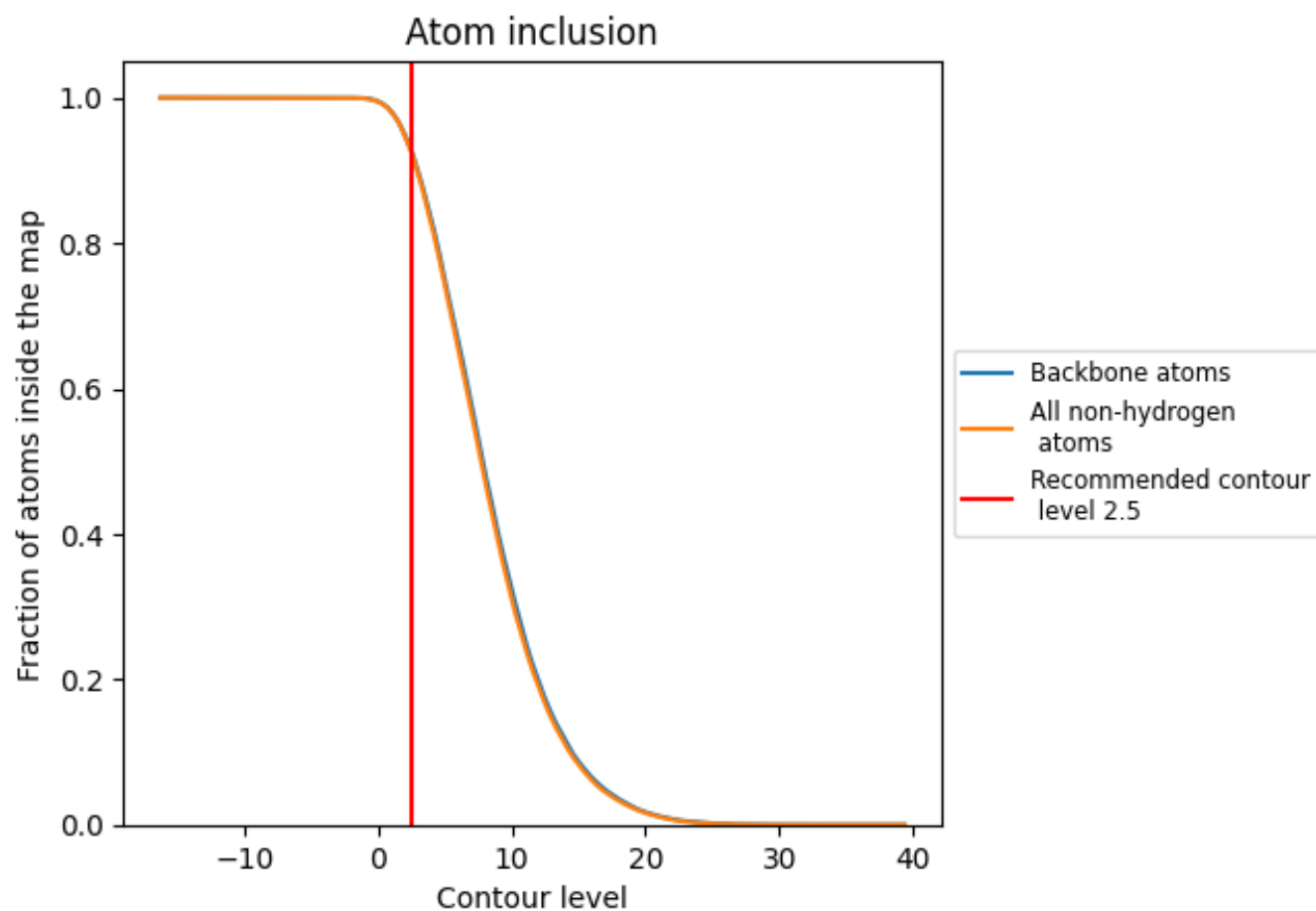
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6230
A	 0.9692	 0.6720
B	 0.9579	 0.6590
C	 0.9473	 0.6640
D	 0.9646	 0.6740
E	 0.9439	 0.6310
F	 0.9476	 0.6320
G	 0.8999	 0.6030
H	 0.9574	 0.6470
I	 0.9601	 0.6560
J	 0.9207	 0.6230
K	 0.9522	 0.6600
L	 0.9521	 0.6430
M	 0.9382	 0.6120
N	 0.9127	 0.6210
O	 0.8919	 0.5830
P	 0.6077	 0.5280
R	 0.8975	 0.5670
S	 0.9138	 0.6190
T	 0.9062	 0.6210
U	 0.8303	 0.5380
V	 0.9289	 0.6250
W	 0.9208	 0.5970
X	 0.8955	 0.5910
Y	 0.9183	 0.6310
Z	 0.9582	 0.6380
a	 0.9604	 0.6570
b	 0.9562	 0.6440
c	 0.9403	 0.6430
d	 0.9560	 0.6510
e	 0.9389	 0.5970
f	 0.9196	 0.5960
g	 0.9365	 0.5760
h	 0.9574	 0.6240
i	 0.9601	 0.6560



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Chain	Atom inclusion	Q-score
j	 0.9069	 0.6080
k	 0.9556	 0.6300
l	 0.9662	 0.6480
m	 0.9491	 0.6110
n	 0.9434	 0.6050
o	 0.8975	 0.5620
p	 0.7120	 0.5100
r	 0.9079	 0.5520
s	 0.9204	 0.5880
t	 0.9097	 0.6220
u	 0.7936	 0.5120
v	 0.9156	 0.5980
w	 0.9071	 0.5810
x	 0.8856	 0.5720
y	 0.9345	 0.6200
z	 0.9538	 0.6090