



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 01:26 PM JST

PDB ID : 3JCU  
EMDB ID : EMD-6617  
Title : Cryo-EM structure of spinach PSII-LHCII supercomplex at 3.2 Angstrom resolution  
Authors : Wei, X.P.; Zhang, X.Z.; Su, X.D.; Cao, P.; Liu, X.Y.; Li, M.; Chang, W.R.; Liu, Z.F.  
Deposited on : 2016-03-10  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

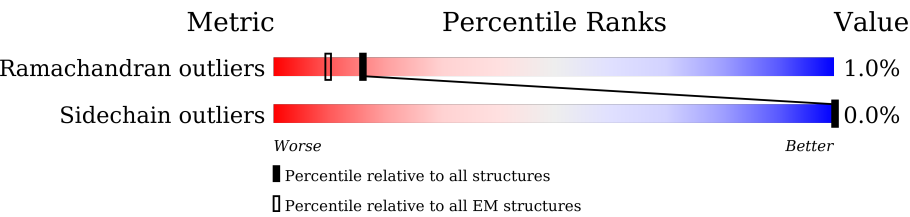
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	344	<div><div>9%</div><div>97%</div><div>.</div></div>
1	a	344	<div><div>9%</div><div>97%</div><div>.</div></div>
2	B	508	<div><div>8%</div><div>95%</div><div>..</div></div>
2	b	508	<div><div>8%</div><div>95%</div><div>..</div></div>
3	C	473	<div><div>10%</div><div>95%</div><div>5%</div></div>
3	c	473	<div><div>10%</div><div>95%</div><div>5%</div></div>
4	D	353	<div><div>9%</div><div>96%</div><div>.</div></div>
4	d	353	<div><div>10%</div><div>96%</div><div>.</div></div>
5	E	83	<div><div>28%</div><div>95%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	Y	267	
7	g	267	
7	n	267	
7	y	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	59	
11	k	59	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	
14	o	332	
15	P	267	
15	p	267	

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Mol	Chain	Length	Quality of chain
16	Q	232	
16	q	232	
17	R	243	
17	r	243	
18	S	295	
18	s	295	
19	T	33	
19	t	33	
20	U	99	
20	u	99	
21	W	137	
21	w	137	
22	X	117	
22	x	117	
23	Z	62	
23	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	405	X	-	-	-
27	CLA	A	406	X	-	-	-
27	CLA	A	407	X	-	-	-
27	CLA	A	410	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	616	X	-	-	-
27	CLA	B	617	X	-	-	-
27	CLA	C	501	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	403	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	G	612	X	-	-	-
27	CLA	G	613	X	-	-	-
27	CLA	G	614	X	-	-	-
27	CLA	N	602	X	-	-	-
27	CLA	N	603	X	-	-	-
27	CLA	N	604	X	-	-	-
27	CLA	N	610	X	-	-	-
27	CLA	N	611	X	-	-	-
27	CLA	N	612	X	-	-	-
27	CLA	N	613	X	-	-	-
27	CLA	N	614	X	-	-	-
27	CLA	R	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	R	602	X	-	-	-
27	CLA	R	603	X	-	-	-
27	CLA	R	604	X	-	-	-
27	CLA	R	609	X	-	-	-
27	CLA	R	610	X	-	-	-
27	CLA	R	611	X	-	-	-
27	CLA	R	612	X	-	-	-
27	CLA	R	613	X	-	-	-
27	CLA	R	616	X	-	-	-
27	CLA	S	602	X	-	-	-
27	CLA	S	604	X	-	-	-
27	CLA	S	609	X	-	-	-
27	CLA	S	610	X	-	-	-
27	CLA	S	611	X	-	-	-
27	CLA	S	612	X	-	-	-
27	CLA	S	613	X	-	-	-
27	CLA	S	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-
27	CLA	a	405	X	-	-	-
27	CLA	a	406	X	-	-	-
27	CLA	a	407	X	-	-	-
27	CLA	a	410	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-
27	CLA	b	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	615	X	-	-	-
27	CLA	b	616	X	-	-	-
27	CLA	b	617	X	-	-	-
27	CLA	c	501	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	403	X	-	-	-
27	CLA	g	602	X	-	-	-
27	CLA	g	603	X	-	-	-
27	CLA	g	604	X	-	-	-
27	CLA	g	610	X	-	-	-
27	CLA	g	611	X	-	-	-
27	CLA	g	612	X	-	-	-
27	CLA	g	613	X	-	-	-
27	CLA	g	614	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	611	X	-	-	-
27	CLA	n	612	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	n	614	X	-	-	-
27	CLA	r	601	X	-	-	-
27	CLA	r	602	X	-	-	-
27	CLA	r	603	X	-	-	-
27	CLA	r	604	X	-	-	-
27	CLA	r	609	X	-	-	-
27	CLA	r	610	X	-	-	-
27	CLA	r	611	X	-	-	-
27	CLA	r	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	r	613	X	-	-	-
27	CLA	r	616	X	-	-	-
27	CLA	s	602	X	-	-	-
27	CLA	s	604	X	-	-	-
27	CLA	s	609	X	-	-	-
27	CLA	s	610	X	-	-	-
27	CLA	s	611	X	-	-	-
27	CLA	s	612	X	-	-	-
27	CLA	s	613	X	-	-	-
27	CLA	s	614	X	-	-	-
27	CLA	y	602	X	-	-	-
27	CLA	y	603	X	-	-	-
27	CLA	y	604	X	-	-	-
27	CLA	y	610	X	-	-	-
27	CLA	y	611	X	-	-	-
27	CLA	y	612	X	-	-	-
27	CLA	y	613	X	-	-	-
27	CLA	y	614	X	-	-	-
37	CHL	G	601	X	-	-	-
37	CHL	G	605	X	-	-	-
37	CHL	G	606	X	-	-	-
37	CHL	G	607	X	-	-	-
37	CHL	G	608	X	-	-	-
37	CHL	G	609	X	-	-	-
37	CHL	N	601	X	-	-	-
37	CHL	N	605	X	-	-	-
37	CHL	N	606	X	-	-	-
37	CHL	N	607	X	-	-	-
37	CHL	N	608	X	-	-	-
37	CHL	N	609	X	-	-	-
37	CHL	R	606	X	-	-	-
37	CHL	R	607	X	-	-	-
37	CHL	R	608	X	-	-	-
37	CHL	S	601	X	-	-	-
37	CHL	S	606	X	-	-	-
37	CHL	S	607	X	-	-	-
37	CHL	S	608	X	-	-	-
37	CHL	Y	601	X	-	-	-
37	CHL	Y	605	X	-	-	-
37	CHL	Y	606	X	-	-	-
37	CHL	Y	607	X	-	-	-
37	CHL	Y	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	Y	609	X	-	-	-
37	CHL	g	601	X	-	-	-
37	CHL	g	605	X	-	-	-
37	CHL	g	606	X	-	-	-
37	CHL	g	607	X	-	-	-
37	CHL	g	608	X	-	-	-
37	CHL	g	609	X	-	-	-
37	CHL	n	601	X	-	-	-
37	CHL	n	605	X	-	-	-
37	CHL	n	606	X	-	-	-
37	CHL	n	607	X	-	-	-
37	CHL	n	608	X	-	-	-
37	CHL	n	609	X	-	-	-
37	CHL	r	606	X	-	-	-
37	CHL	r	607	X	-	-	-
37	CHL	r	608	X	-	-	-
37	CHL	s	601	X	-	-	-
37	CHL	s	606	X	-	-	-
37	CHL	s	607	X	-	-	-
37	CHL	s	608	X	-	-	-
37	CHL	y	601	X	-	-	-
37	CHL	y	605	X	-	-	-
37	CHL	y	606	X	-	-	-
37	CHL	y	607	X	-	-	-
37	CHL	y	608	X	-	-	-
37	CHL	y	609	X	-	-	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 75994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		
1	a	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		
2	b	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		
3	c	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		
4	d	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total	C	N	O	0	0
			636	412	104	120		
5	e	79	Total	C	N	O	0	0
			636	412	104	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			257	174	43	39	1		
6	f	32	Total	C	N	O	S	0	0
			257	174	43	39	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	g	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	n	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			434	288	65	78	3		
8	h	59	Total	C	N	O	S	0	0
			434	288	65	78	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	34	Total	C	N	O		0	0
			247	168	38	41			
10	j	34	Total	C	N	O		0	0
			247	168	38	41			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			307	217	43	46	1		
11	k	37	Total	C	N	O	S	0	0
			307	217	43	46	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	33	Total	C	N	O		0	0
			258	176	37	45			
13	m	33	Total	C	N	O		0	0
			258	176	37	45			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		
14	o	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		



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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		
15	p	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O		0	0
			1162	736	202	224			
16	q	148	Total	C	N	O		0	0
			1162	736	202	224			

- Molecule 17 is a protein called Chlorophyll A-B Binding protein 29 kD (CP29).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		
17	r	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		

- Molecule 18 is a protein called Chlorophyll A-B Binding protein 26 kD (CP26).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		
18	s	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		

- Molecule 19 is a protein called Photosystem II Reaction Center protein Tc.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			245	171	34	39	1		
19	t	30	Total	C	N	O	S	0	0
			245	171	34	39	1		

- Molecule 20 is a protein called Photosystem II Reaction Center Tn protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	276	61	81	1		
21	w	54	Total	C	N	O	S	0	0
			419	276	61	81	1		

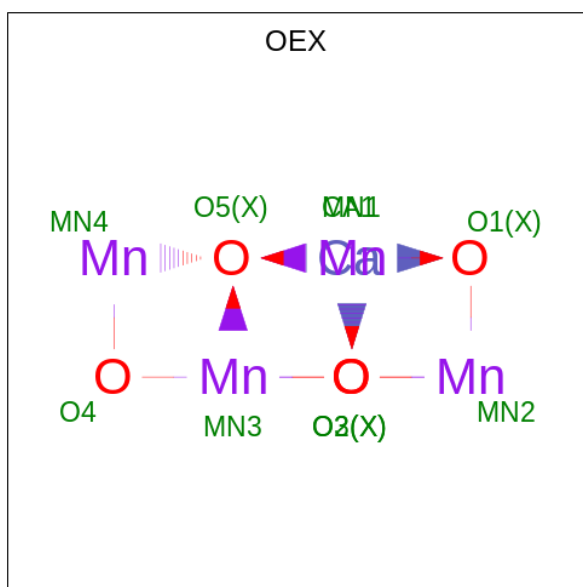
- Molecule 22 is a protein called Photosystem II Reaction Center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	35	Total	C	N	O	0	0
			246	163	38	45		
22	x	35	Total	C	N	O	0	0
			246	163	38	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	61	Total	C	N	O	0	0
			454	306	68	80		
23	z	61	Total	C	N	O	0	0
			454	306	68	80		

- Molecule 24 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

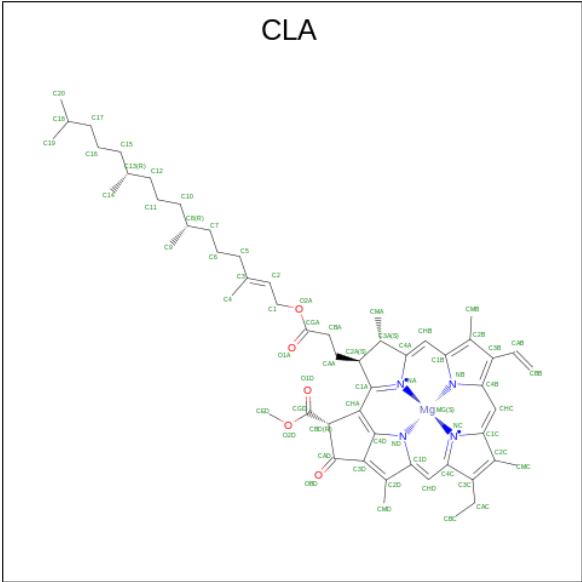
- Molecule 25 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 27 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
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0

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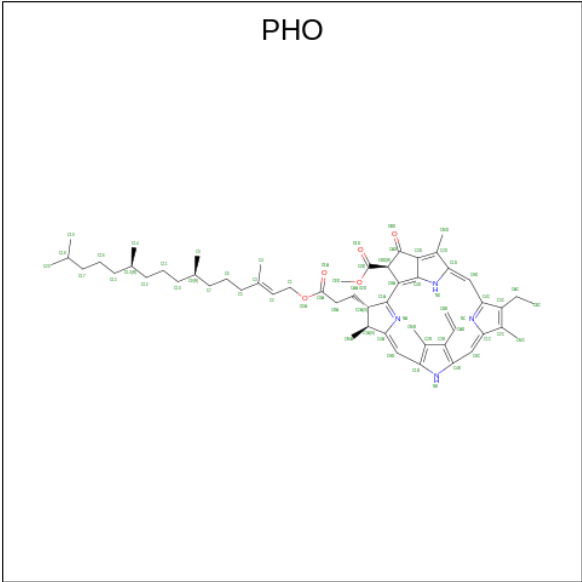
Mol	Chain	Residues	Atoms					AltConf
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0

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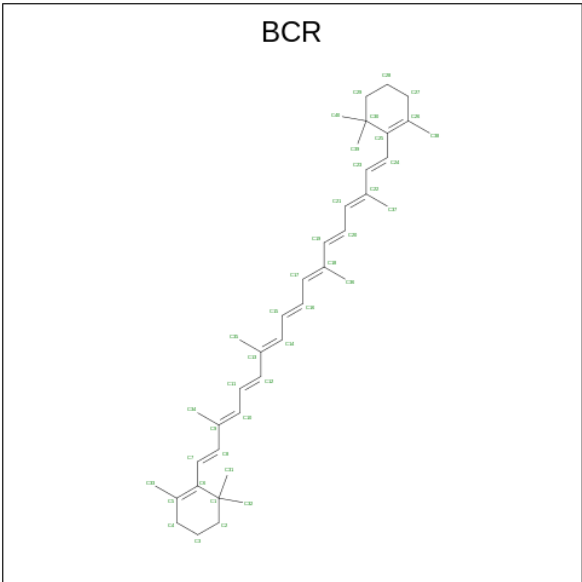
Mol	Chain	Residues	Atoms					AltConf
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	y	1	Total 49	C 39	Mg 1	N 4	O 5	0

- Molecule 28 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



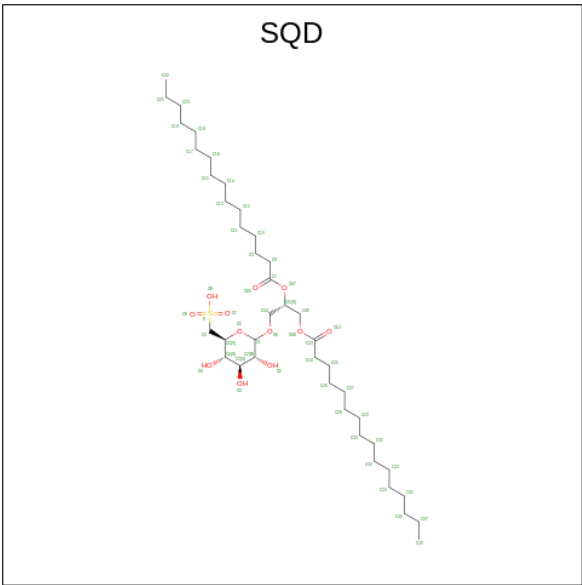
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			64	55	4	5	
28	A	1	Total	C	N	O	0
			64	55	4	5	
28	a	1	Total	C	N	O	0
			64	55	4	5	
28	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



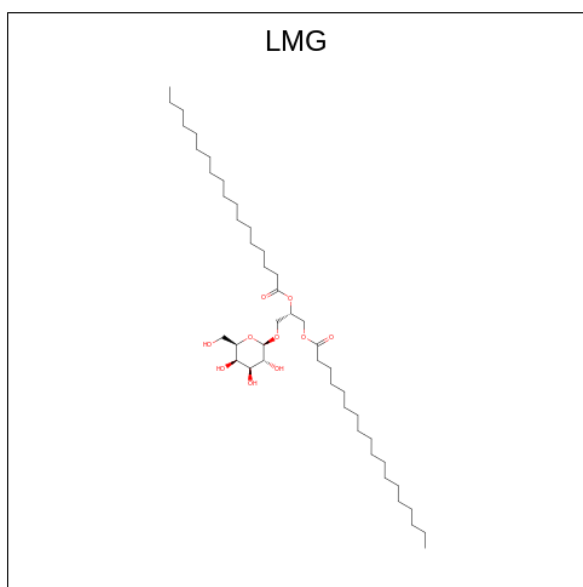
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	C	1	Total C 40 40	0
29	D	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	b	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	c	1	Total C 40 40	0
29	d	1	Total C 40 40	0
29	h	1	Total C 40 40	0

- Molecule 30 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).



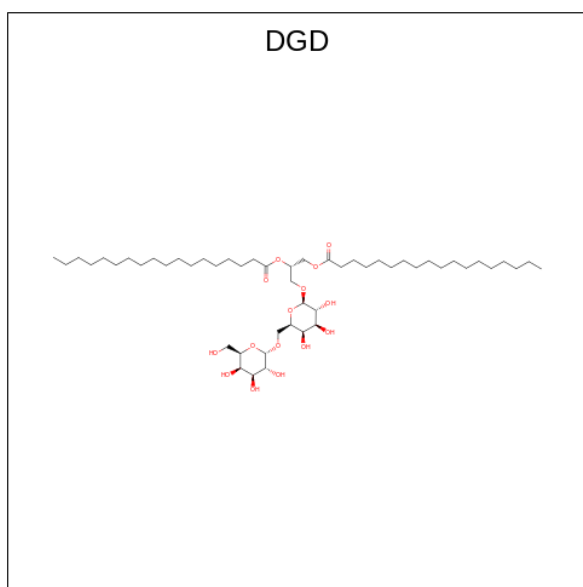
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			48	38	10	
31	B	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	D	1	Total	C	O	0
			46	36	10	
31	Z	1	Total	C	O	0
			51	41	10	
31	a	1	Total	C	O	0
			48	38	10	
31	b	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	d	1	Total	C	O	0
			46	36	10	
31	z	1	Total	C	O	0
			51	41	10	

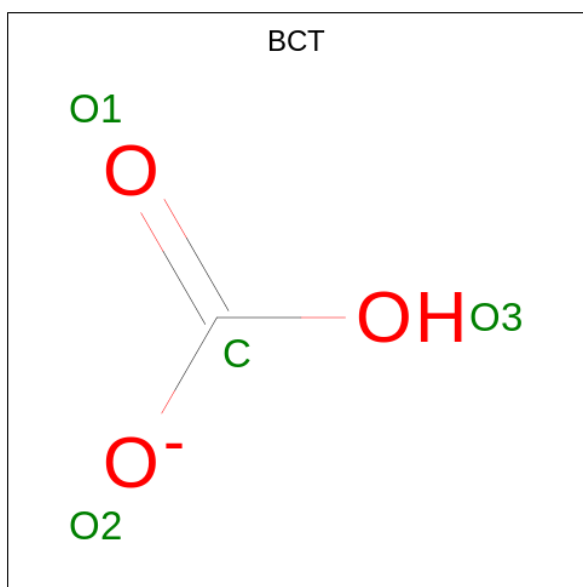
- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			55	40	15	
32	C	1	Total	C	O	0
			62	47	15	
32	C	1	Total	C	O	0
			62	47	15	
32	H	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			55	40	15	
32	c	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			62	47	15	
32	h	1	Total	C	O	0
			62	47	15	

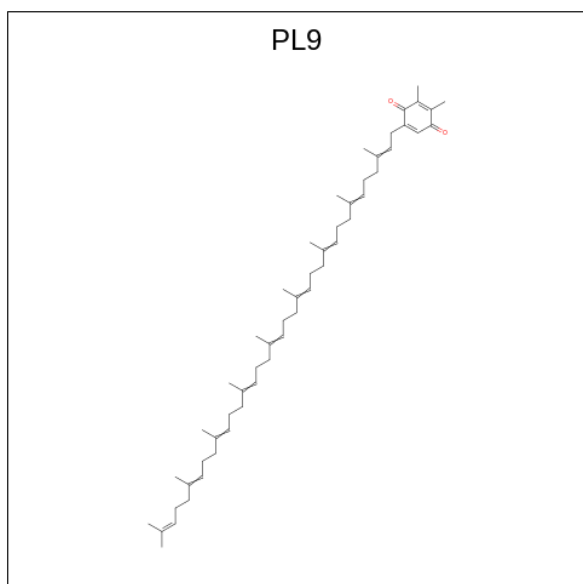
- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).





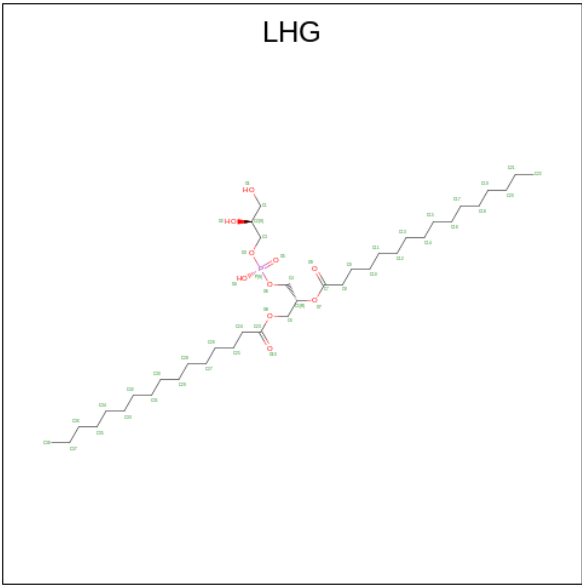
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

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



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

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
35	D	1	Total	C	O	P	0
			43	32	10	1	
35	D	1	Total	C	O	P	0
			49	38	10	1	
35	D	1	Total	C	O	P	0
			37	26	10	1	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			49	38	10	1	
35	R	1	Total	C	O	P	0
			49	38	10	1	
35	S	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	

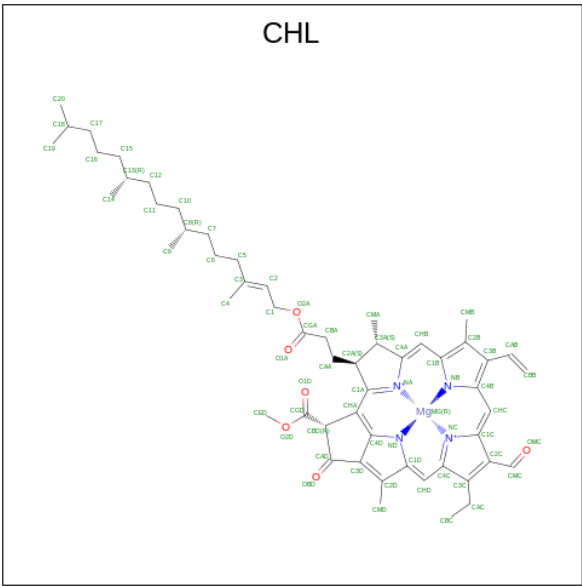
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Mol	Chain	Residues	Atoms				AltConf
35	d	1	Total 43	C 32	O 10	P 1	0
35	d	1	Total 49	C 38	O 10	P 1	0
35	d	1	Total 37	C 26	O 10	P 1	0
35	g	1	Total 49	C 38	O 10	P 1	0
35	l	1	Total 49	C 38	O 10	P 1	0
35	n	1	Total 49	C 38	O 10	P 1	0
35	r	1	Total 49	C 38	O 10	P 1	0
35	s	1	Total 49	C 38	O 10	P 1	0
35	y	1	Total 49	C 38	O 10	P 1	0

- # HEM

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

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
37	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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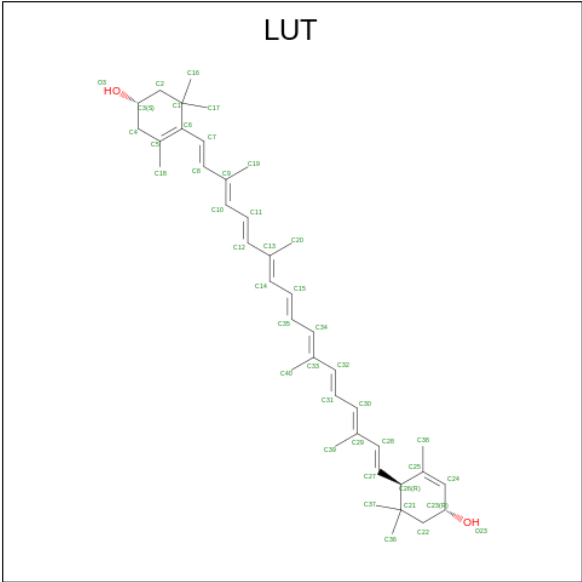
Mol	Chain	Residues	Atoms					AltConf
37	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
37	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
37	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
37	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	n	1	Total 50	C 39	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
37	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
37	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 38 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>).



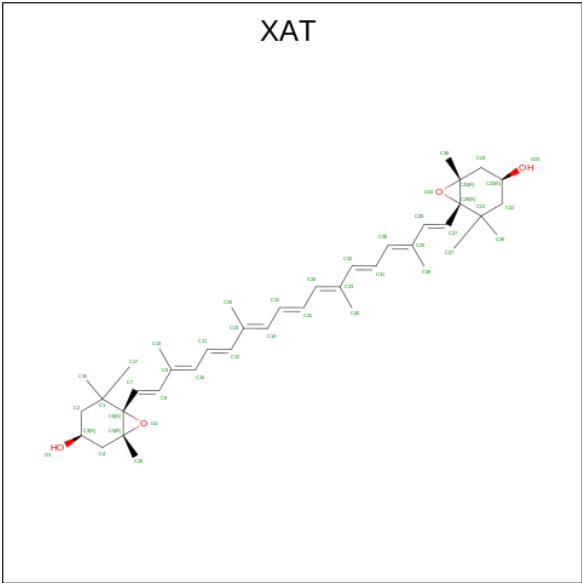
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			42	40	2	
38	G	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	N	1	Total	C	O	0
			42	40	2	
38	R	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			42	40	2	
38	Y	1	Total	C	O	0
			42	40	2	
38	Y	1	Total	C	O	0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

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

- Molecule 39 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
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	R	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	g	1	Total	C	O	0
			44	40	4	
39	n	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

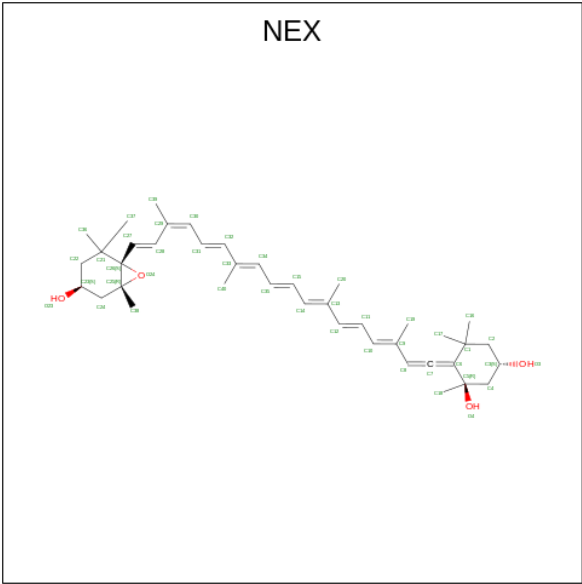
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	y	1	44	40	4	0

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-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
			Total	C	O	
40	G	1	44	40	4	0
40	N	1	44	40	4	0
40	R	1	44	40	4	0
40	S	1	44	40	4	0
40	Y	1	44	40	4	0
40	g	1	44	40	4	0
40	n	1	44	40	4	0
40	r	1	44	40	4	0
40	s	1	44	40	4	0

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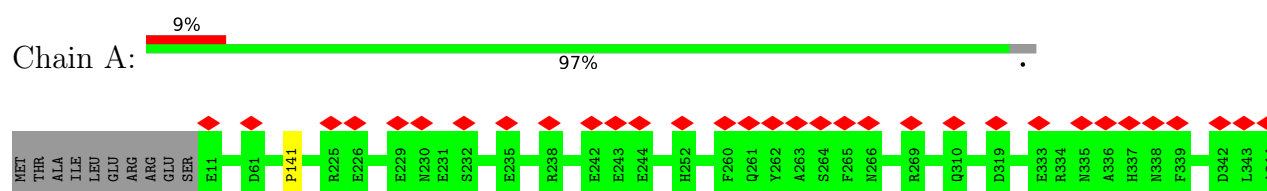
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	y	1	44	40	4	0

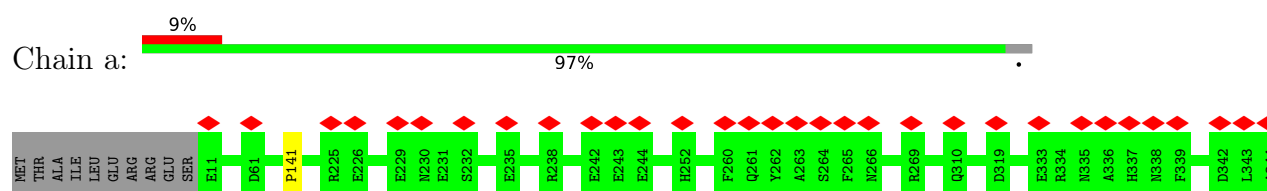
### 3 Residue-property plots [i](#)

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

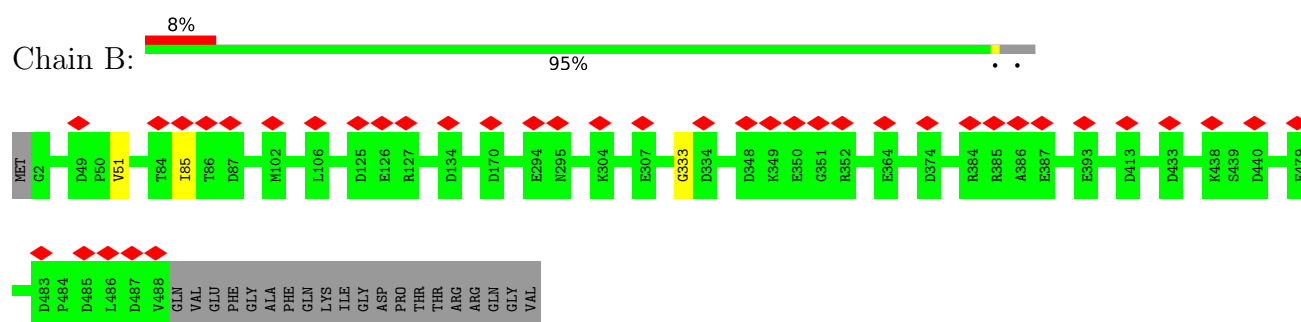
- Molecule 1: Photosystem II protein D1



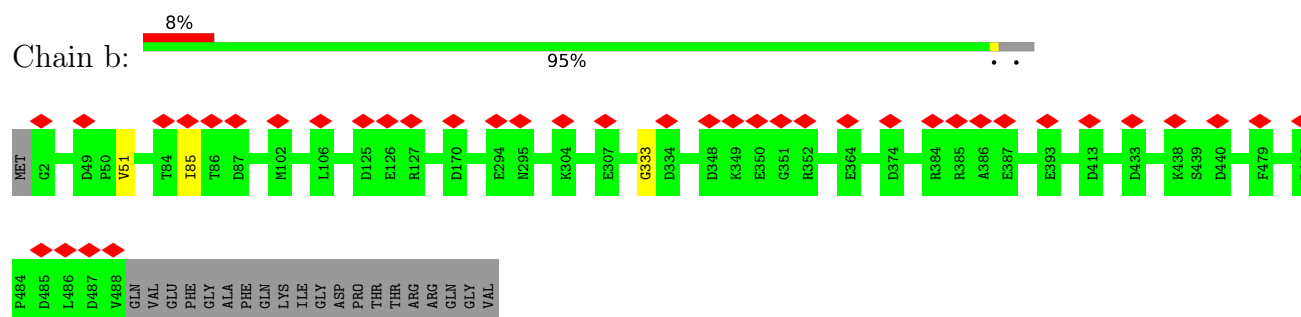
- Molecule 1: Photosystem II protein D1



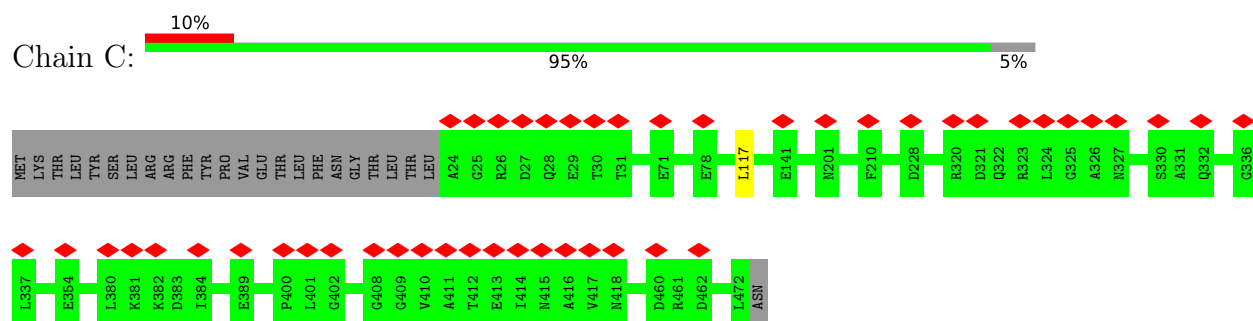
- Molecule 2: Photosystem II CP47 reaction center protein



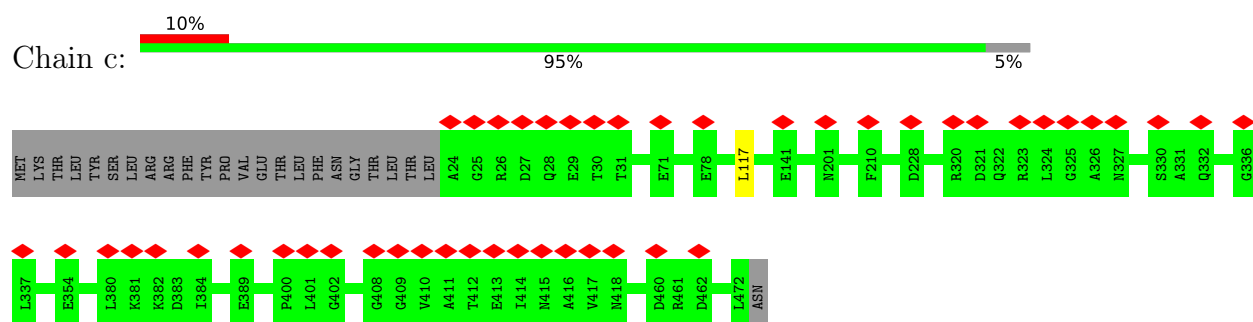
- Molecule 2: Photosystem II CP47 reaction center protein



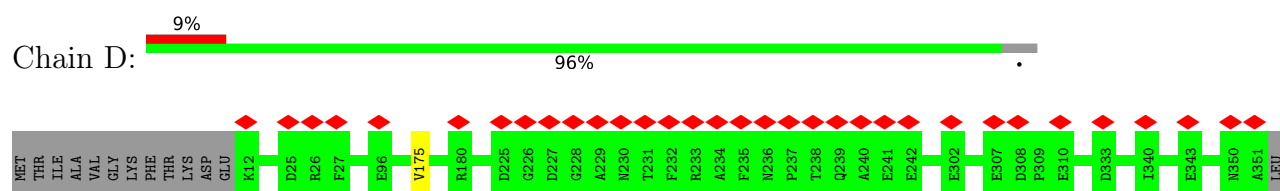
- Molecule 3: Photosystem II CP43 reaction center protein



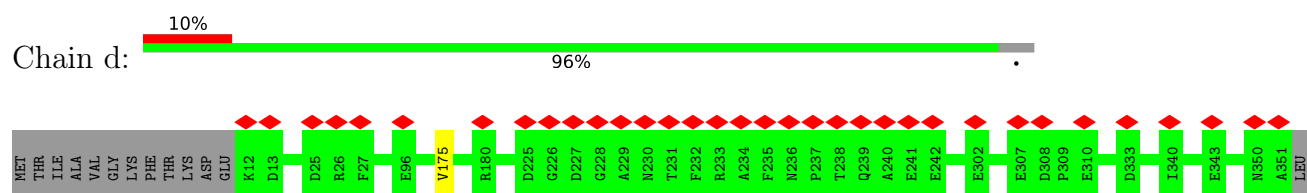
- Molecule 3: Photosystem II CP43 reaction center protein



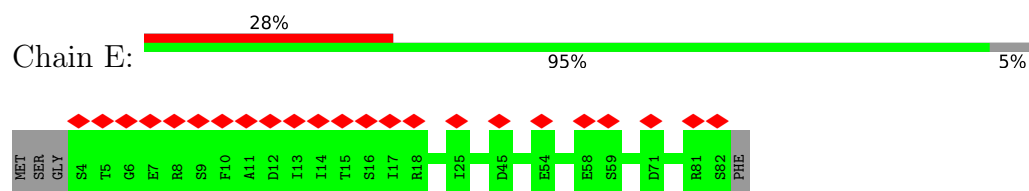
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein

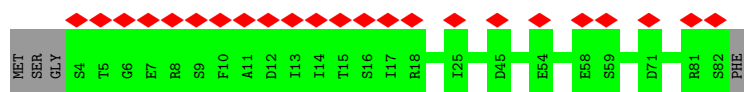


- Molecule 5: Cytochrome b559 subunit alpha

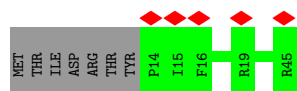
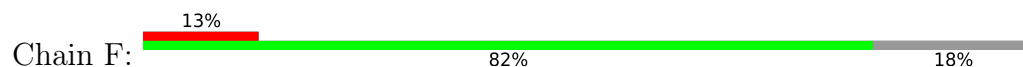


- Molecule 5: Cytochrome b559 subunit alpha

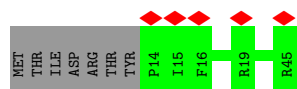
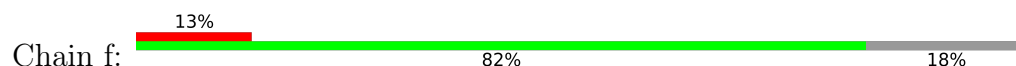




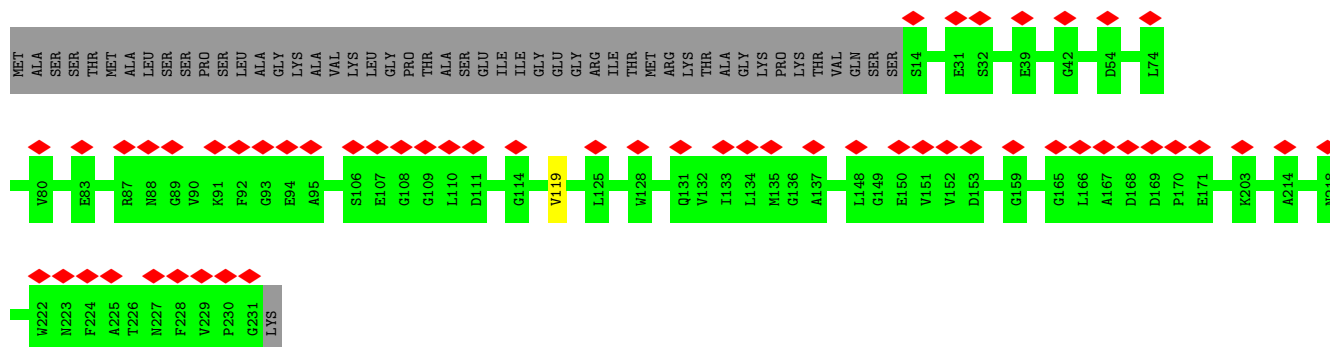
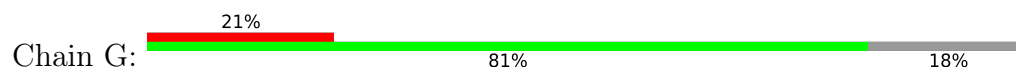
- Molecule 6: Cytochrome b559 subunit beta



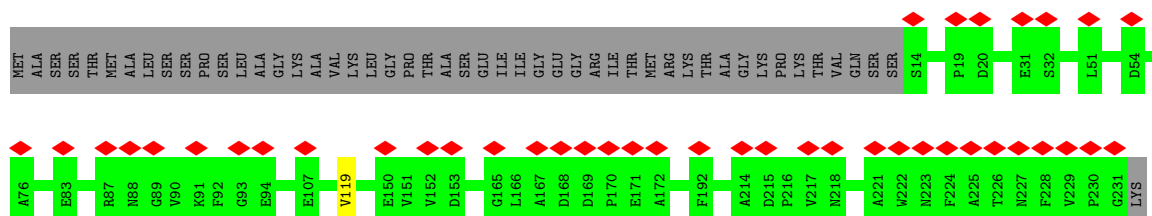
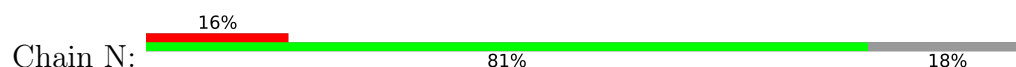
- Molecule 6: Cytochrome b559 subunit beta



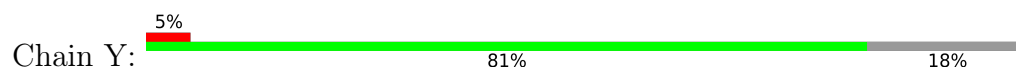
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

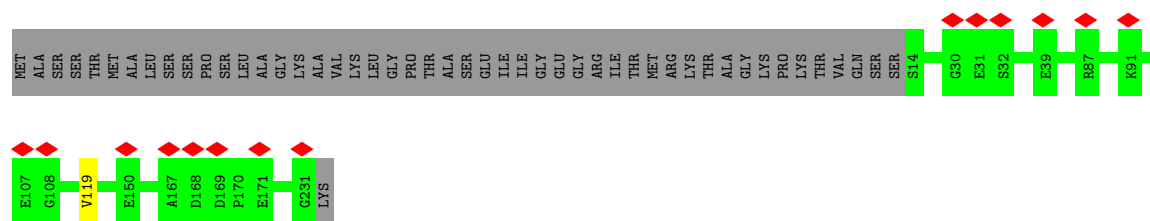


- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



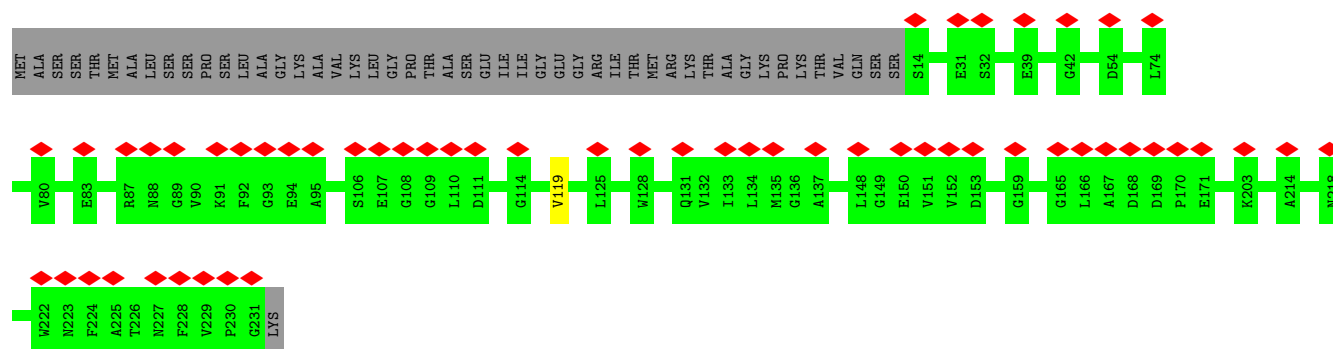
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic





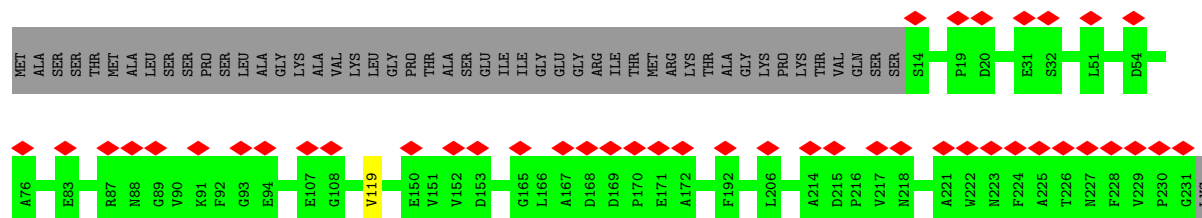
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain g: 21% 81% 18%



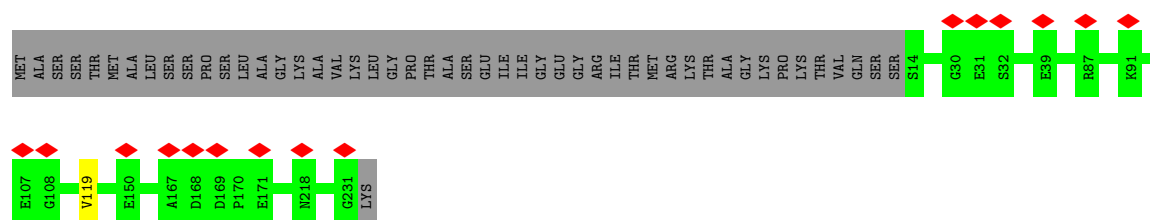
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain n: 16% 81% 18%



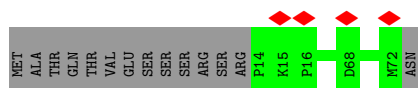
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain y: 6% 81% 18%

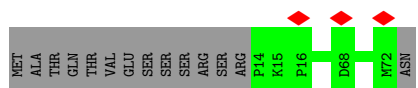
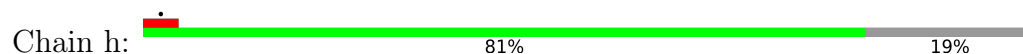


- Molecule 8: Photosystem II reaction center protein H

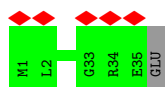
Chain H: 5% 81% 19%



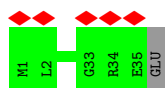
- Molecule 8: Photosystem II reaction center protein H



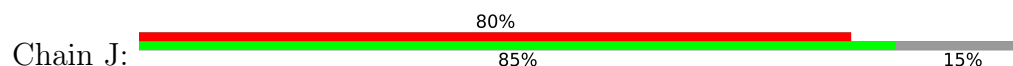
- Molecule 9: Protein Photosystem II reaction center protein I



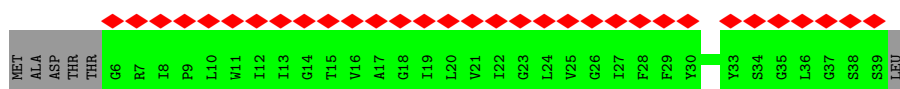
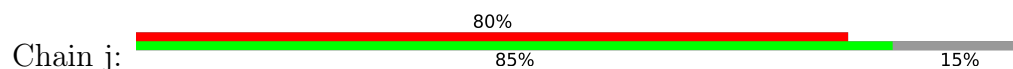
- Molecule 9: Protein Photosystem II reaction center protein I



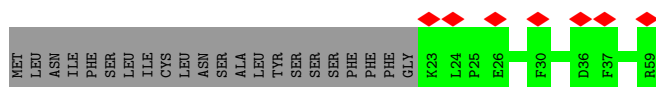
- Molecule 10: Photosystem II reaction center protein J



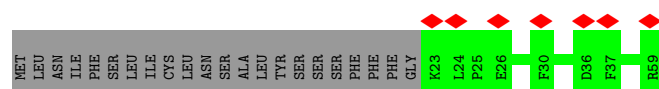
- Molecule 10: Photosystem II reaction center protein J



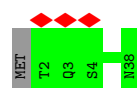
- Molecule 11: Photosystem II reaction center protein K



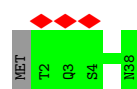
- Molecule 11: Photosystem II reaction center protein K



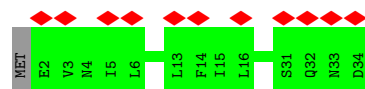
- Molecule 12: Protein Photosystem II reaction center protein L



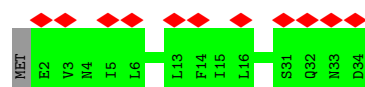
- Molecule 12: Protein Photosystem II reaction center protein L



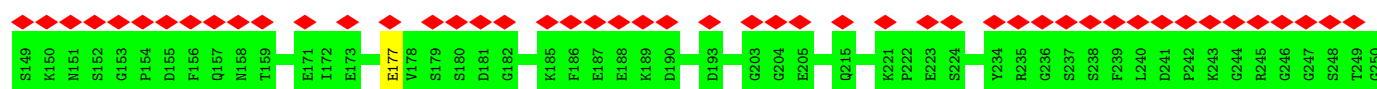
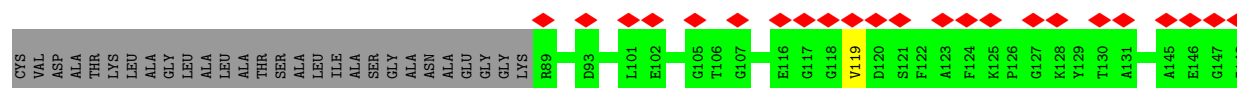
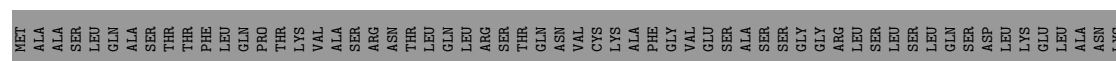
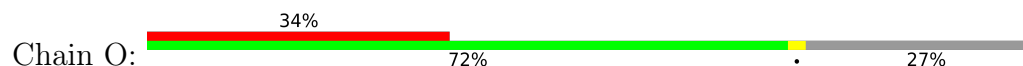
- Molecule 13: Photosystem II reaction center protein M



- Molecule 13: Photosystem II reaction center protein M



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

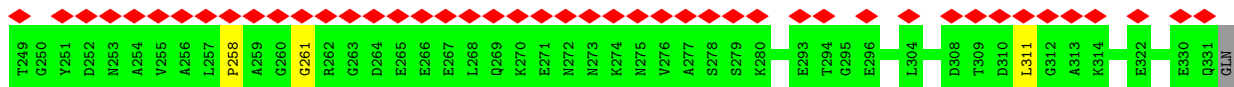
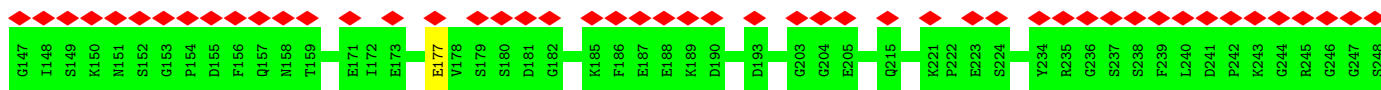
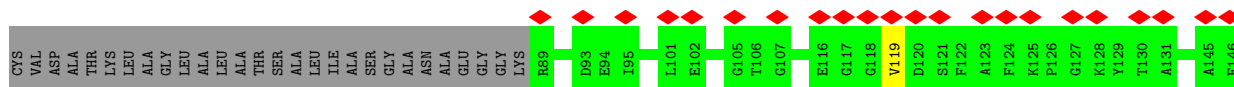
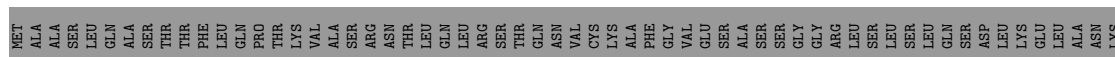






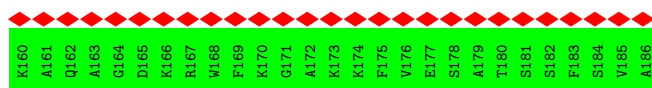
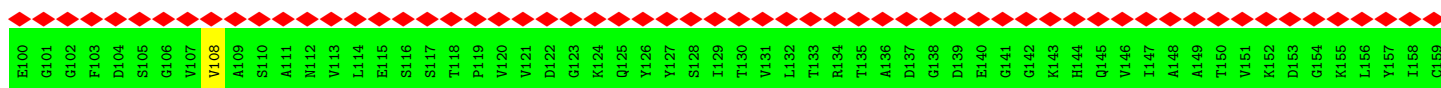
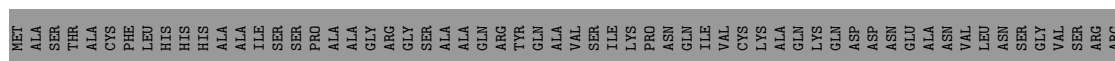
• Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 35% 72% 27%



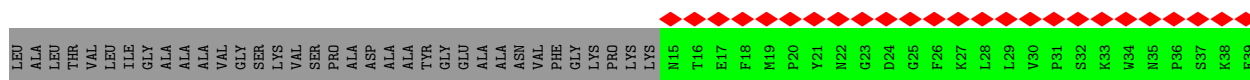
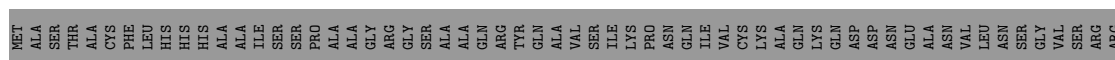
• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

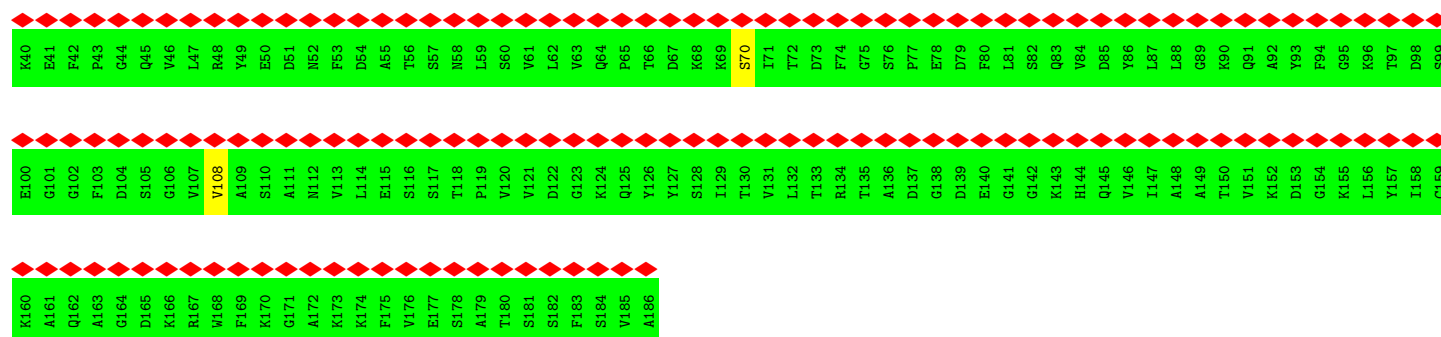
Chain P: 64% 64% 36%



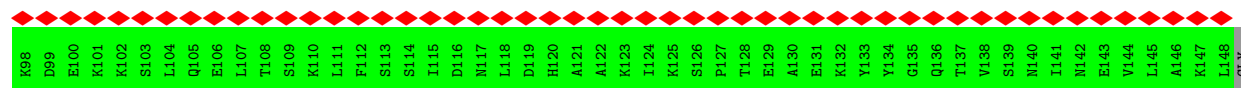
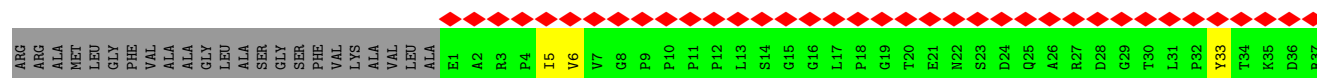
• Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p: 64% 64% 36%

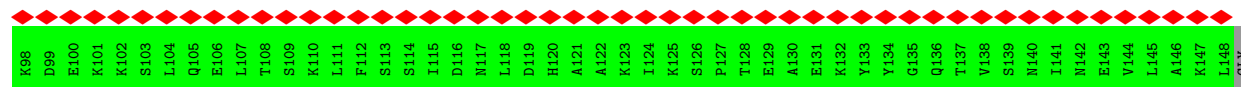
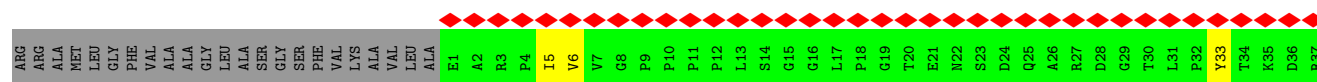




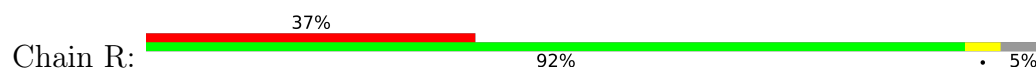
• Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

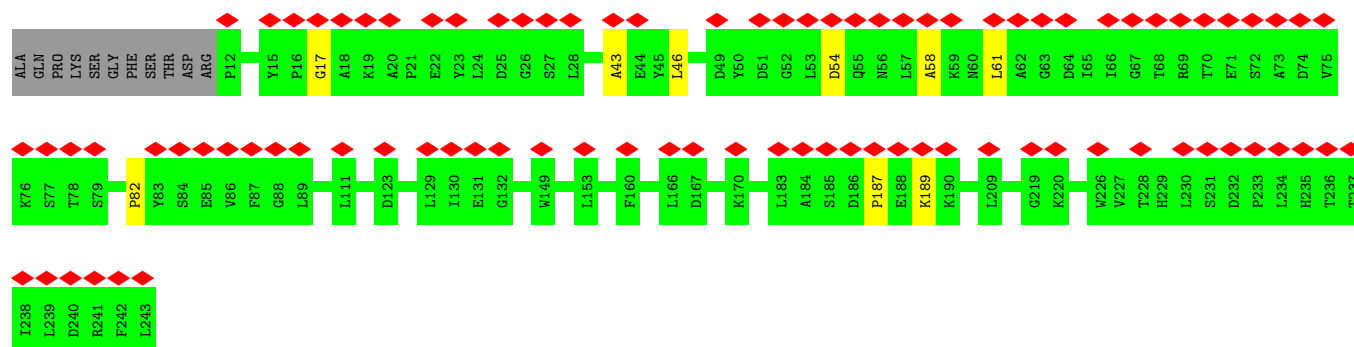


• Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic



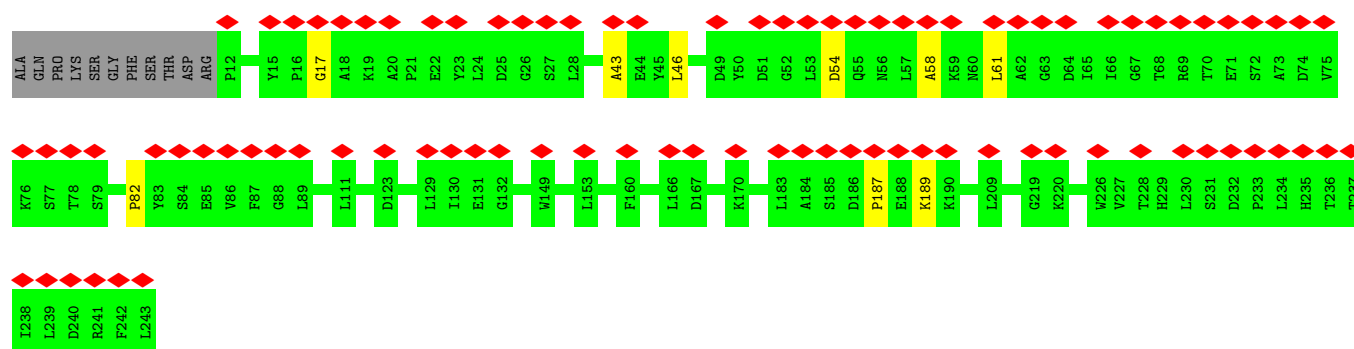
• Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)





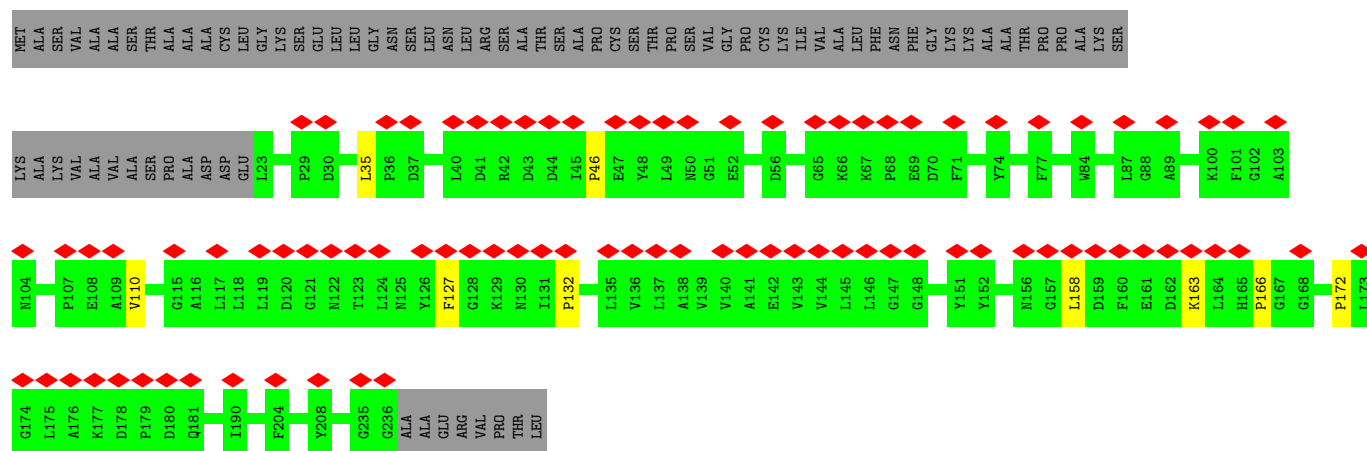
• Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

Chain r: 37% 92% 5%



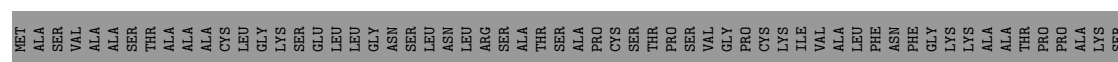
• Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

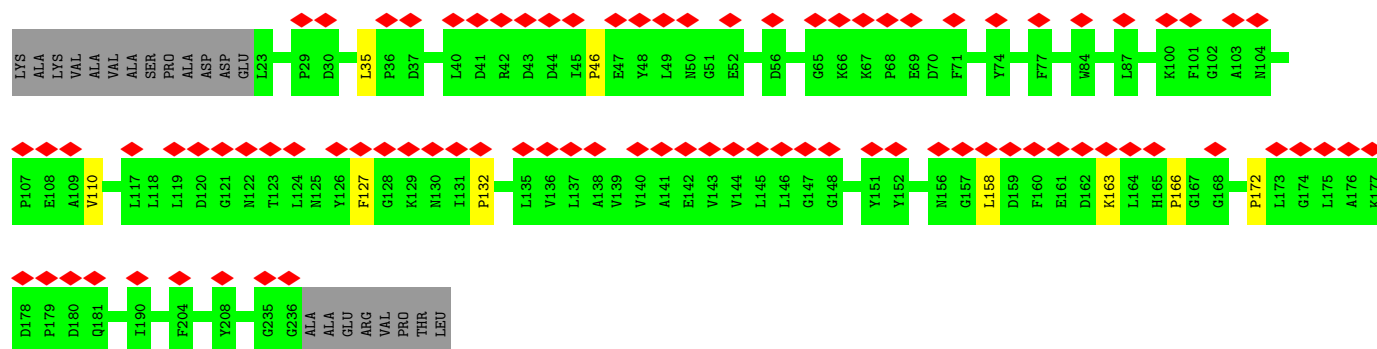
Chain S: 30% 69% 27%



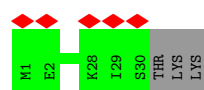
• Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

Chain s: 29% 69% 27%

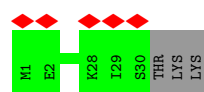




• Molecule 19: Photosystem II Reaction Center protein Tc



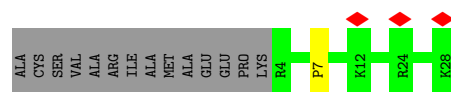
• Molecule 19: Photosystem II Reaction Center protein Tc



• Molecule 20: Photosystem II Reaction Center Tn protein

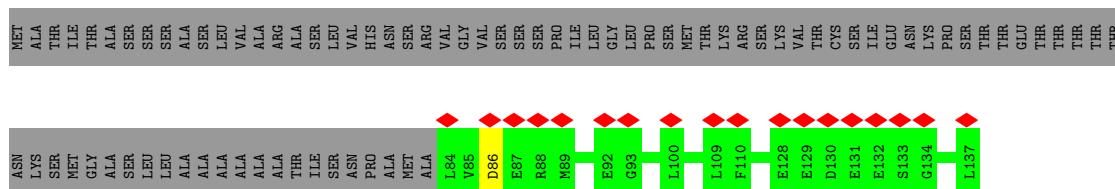


• Molecule 20: Photosystem II Reaction Center Tn protein

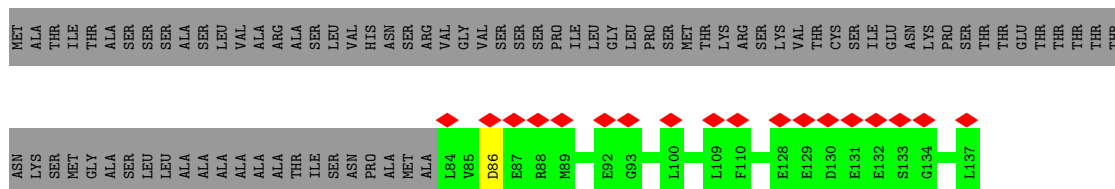


• Molecule 21: Photosystem II reaction center W protein, chloroplastic

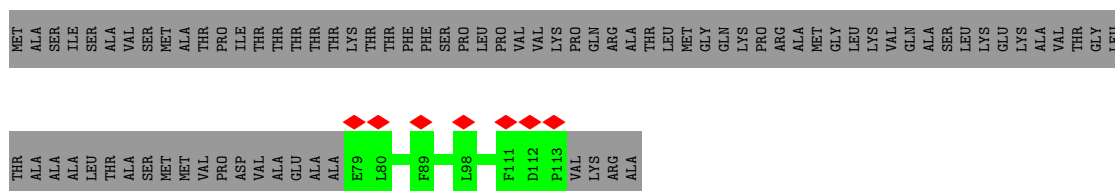




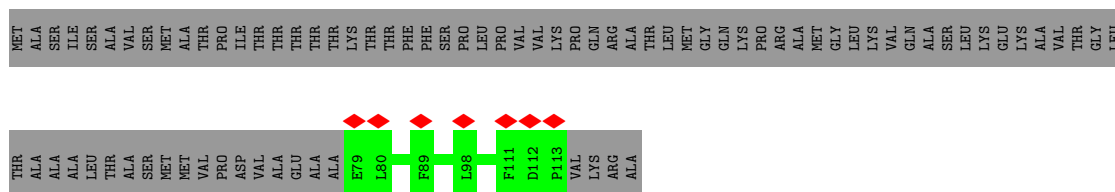
- Molecule 21: Photosystem II reaction center W protein, chloroplasic



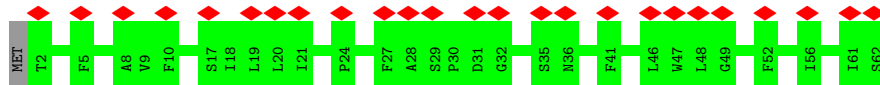
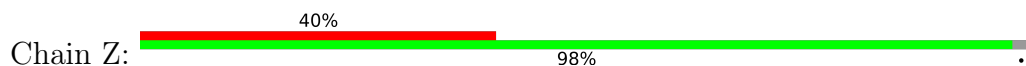
- Molecule 22: Photosystem II Reaction Center X protein



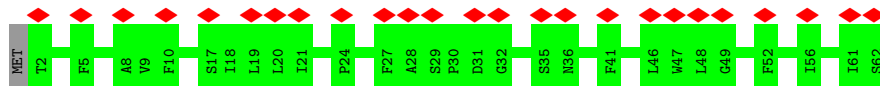
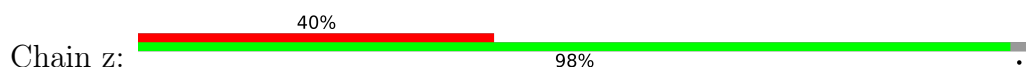
- Molecule 22: Photosystem II Reaction Center X protein



- Molecule 23: Photosystem II reaction center protein Z



- Molecule 23: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	109042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	337.5, 337.5, 216.0	wwPDB
Map dimensions	250, 250, 160	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.35, 1.35, 1.35	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.60	0/2695	0.59	0/3674
1	a	0.60	0/2695	0.59	0/3674
2	B	0.59	0/3951	0.55	0/5379
2	b	0.59	0/3951	0.55	0/5379
3	C	0.56	0/3589	0.55	0/4891
3	c	0.56	0/3589	0.55	0/4891
4	D	0.62	0/2796	0.56	0/3811
4	d	0.62	0/2796	0.56	0/3811
5	E	0.42	0/654	0.48	0/889
5	e	0.42	0/654	0.48	0/889
6	F	0.42	0/265	0.48	0/358
6	f	0.43	0/265	0.48	0/358
7	G	0.42	0/1713	0.49	0/2333
7	N	0.42	0/1713	0.49	0/2333
7	Y	0.51	0/1713	0.51	0/2333
7	g	0.42	0/1713	0.49	0/2333
7	n	0.41	0/1713	0.49	0/2333
7	y	0.51	0/1713	0.51	0/2333
8	H	0.49	0/444	0.53	0/605
8	h	0.49	0/444	0.53	0/605
9	I	0.62	0/294	0.57	0/397
9	i	0.62	0/294	0.58	0/397
10	J	0.28	0/253	0.45	0/343
10	j	0.29	0/253	0.45	0/343
11	K	0.49	0/320	0.49	0/436
11	k	0.49	0/320	0.49	0/436
12	L	0.60	0/319	0.49	0/434
12	l	0.60	0/319	0.49	0/434
13	M	0.52	0/262	0.55	0/359
13	m	0.52	0/262	0.55	0/359
14	O	0.39	0/1880	0.51	0/2541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	o	0.39	0/1880	0.51	0/2541
15	P	0.28	0/1353	0.49	0/1828
15	p	0.28	0/1353	0.49	0/1828
16	Q	0.28	0/1186	0.57	2/1609 (0.1%)
16	q	0.28	0/1186	0.57	2/1609 (0.1%)
17	R	0.41	0/1853	0.55	0/2522
17	r	0.41	0/1853	0.55	0/2522
18	S	0.39	0/1700	0.62	0/2310
18	s	0.39	0/1700	0.62	0/2310
19	T	0.56	0/252	0.55	0/341
19	t	0.56	0/252	0.55	0/341
20	U	0.44	0/197	0.55	0/264
20	u	0.44	0/197	0.55	0/264
21	W	0.49	0/429	0.60	0/582
21	w	0.49	0/429	0.60	0/582
22	X	0.42	0/250	0.50	0/342
22	x	0.43	0/250	0.50	0/342
23	Z	0.38	0/464	0.53	0/636
23	z	0.38	0/464	0.53	0/636
All	All	0.50	0/61090	0.54	4/83100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
18	S	0	1
18	s	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	42	PRO	CA-C-N	5.67	129.68	117.20
16	Q	42	PRO	CA-C-N	5.67	129.67	117.20
16	Q	42	PRO	C-N-CA	5.03	134.26	121.70
16	q	42	PRO	C-N-CA	5.01	134.22	121.70



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
18	S	35	LEU	Peptide
1	a	141	PRO	Peptide
18	s	35	LEU	Peptide

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

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

## 5.3 Torsion angles [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	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
2	B	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	22	57
2	b	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	22	57
3	C	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
3	c	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
4	D	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	37	69
4	d	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	37	69
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	30/39 (77%)	30 (100%)	0	0	100	100
6	f	30/39 (77%)	30 (100%)	0	0	100	100
7	G	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	25	60
7	Y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	25	60
7	g	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	25	60
7	n	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	25	60
7	y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	25	60
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
9	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
9	i	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
10	J	32/40 (80%)	32 (100%)	0	0	100	100
10	j	32/40 (80%)	32 (100%)	0	0	100	100
11	K	35/59 (59%)	35 (100%)	0	0	100	100
11	k	35/59 (59%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
13	m	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
14	O	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	5	31
14	o	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	5	31
15	P	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	11	43
15	p	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	11	43
16	Q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	4	26
16	q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	4	26
17	R	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	2	18
17	r	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	2	18
18	S	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	2	18
18	s	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	2	18
19	T	28/33 (85%)	28 (100%)	0	0	100	100
19	t	28/33 (85%)	28 (100%)	0	0	100	100
20	U	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	16
20	u	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	W	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	6	34
21	w	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	6	34
22	X	33/117 (28%)	33 (100%)	0	0	100	100
22	x	33/117 (28%)	33 (100%)	0	0	100	100
23	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
23	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
All	All	7548/9396 (80%)	7100 (94%)	374 (5%)	74 (1%)	16	47

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
14	O	258	PRO
14	O	311	LEU
15	P	108	VAL
18	S	110	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	270 (100%)	0	100	100
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	389/406 (96%)	389 (100%)	0	100	100
2	b	389/406 (96%)	389 (100%)	0	100	100
3	C	351/374 (94%)	350 (100%)	1 (0%)	91	96
3	c	351/374 (94%)	350 (100%)	1 (0%)	91	96
4	D	272/283 (96%)	272 (100%)	0	100	100
4	d	272/283 (96%)	272 (100%)	0	100	100
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	27/34 (79%)	27 (100%)	0	100	100
6	f	27/34 (79%)	27 (100%)	0	100	100
7	G	168/206 (82%)	168 (100%)	0	100	100
7	N	168/206 (82%)	168 (100%)	0	100	100
7	Y	168/206 (82%)	168 (100%)	0	100	100
7	g	168/206 (82%)	168 (100%)	0	100	100
7	n	168/206 (82%)	168 (100%)	0	100	100
7	y	168/206 (82%)	168 (100%)	0	100	100
8	H	48/61 (79%)	48 (100%)	0	100	100
8	h	48/61 (79%)	48 (100%)	0	100	100
9	I	32/33 (97%)	32 (100%)	0	100	100
9	i	32/33 (97%)	32 (100%)	0	100	100
10	J	25/30 (83%)	25 (100%)	0	100	100
10	j	25/30 (83%)	25 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	35 (100%)	0	100	100
13	M	29/30 (97%)	29 (100%)	0	100	100
13	m	29/30 (97%)	29 (100%)	0	100	100
14	O	202/269 (75%)	202 (100%)	0	100	100
14	o	202/269 (75%)	202 (100%)	0	100	100
15	P	144/212 (68%)	144 (100%)	0	100	100
15	p	144/212 (68%)	144 (100%)	0	100	100
16	Q	129/187 (69%)	129 (100%)	0	100	100
16	q	129/187 (69%)	129 (100%)	0	100	100
17	R	189/198 (96%)	189 (100%)	0	100	100
17	r	189/198 (96%)	189 (100%)	0	100	100
18	S	167/226 (74%)	167 (100%)	0	100	100
18	s	167/226 (74%)	167 (100%)	0	100	100
19	T	27/30 (90%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	t	27/30 (90%)	27 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/110 (40%)	44 (100%)	0	100	100
21	w	44/110 (40%)	44 (100%)	0	100	100
22	X	26/90 (29%)	26 (100%)	0	100	100
22	x	26/90 (29%)	26 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
23	z	52/53 (98%)	52 (100%)	0	100	100
All	All	6170/7528 (82%)	6168 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	117	LEU
3	c	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
13	m	32	GLN
7	y	103	GLN
7	n	208	ASN
17	r	55	GLN
14	O	331	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 322 ligands modelled in this entry, 6 are monoatomic - leaving 316 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$
40	NEX	g	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.59	16 (32%)
27	CLA	r	610	17	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
27	CLA	B	605	-	65,73,73	1.45	12 (18%)	76,113,113	1.60	9 (11%)
27	CLA	c	508	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	8 (10%)
27	CLA	b	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	8 (10%)
38	LUT	n	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.77	15 (29%)
27	CLA	c	510	-	65,73,73	1.42	9 (13%)	76,113,113	1.46	7 (9%)
40	NEX	y	1623	-	38,46,46	1.09	2 (5%)	50,70,70	2.50	16 (32%)
29	BCR	B	620	-	41,41,41	0.96	2 (4%)	56,56,56	2.12	17 (30%)
39	XAT	R	622	-	39,47,47	0.98	1 (2%)	54,74,74	2.85	22 (40%)
37	CHL	Y	608	-	50,58,74	2.11	13 (26%)	52,94,114	2.77	19 (36%)
27	CLA	B	615	-	65,73,73	1.42	10 (15%)	76,113,113	1.38	7 (9%)
28	PHO	A	409	-	51,69,69	1.14	7 (13%)	47,99,99	1.37	6 (12%)
33	BCT	D	401	-	2,3,3	0.69	0	2,3,3	1.05	0
27	CLA	b	604	-	65,73,73	1.45	10 (15%)	76,113,113	1.37	6 (7%)
27	CLA	b	608	-	65,73,73	1.43	10 (15%)	76,113,113	1.46	9 (11%)
27	CLA	y	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.54	6 (10%)
27	CLA	c	513	-	49,57,73	1.64	10 (20%)	55,93,113	1.70	7 (12%)
37	CHL	G	606	-	50,58,74	2.19	14 (28%)	52,94,114	2.81	20 (38%)
33	BCT	d	401	-	2,3,3	0.69	0	2,3,3	1.05	0
37	CHL	r	608	-	50,58,74	2.16	16 (32%)	52,94,114	2.89	18 (34%)
27	CLA	N	610	7	65,73,73	1.44	9 (13%)	76,113,113	1.45	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	BCR	C	516	-	41,41,41	0.79	0	56,56,56	2.30	18 (32%)
29	BCR	h	101	-	41,41,41	0.87	1 (2%)	56,56,56	2.00	19 (33%)
29	BCR	b	618	-	41,41,41	0.92	3 (7%)	56,56,56	2.20	18 (32%)
35	LHG	r	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
31	LMG	D	411	-	46,46,55	0.84	4 (8%)	54,54,63	1.41	6 (11%)
38	LUT	r	620	-	42,43,43	0.82	1 (2%)	51,60,60	1.66	15 (29%)
27	CLA	c	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	8 (10%)
31	LMG	c	521	-	51,51,55	0.74	0	59,59,63	1.39	7 (11%)
37	CHL	y	609	7	66,74,74	1.84	13 (19%)	73,114,114	2.45	24 (32%)
27	CLA	y	612	7	65,73,73	1.43	10 (15%)	76,113,113	1.37	8 (10%)
35	LHG	l	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
28	PHO	a	409	-	51,69,69	1.14	7 (13%)	47,99,99	1.38	6 (12%)
37	CHL	G	601	7	66,74,74	1.86	14 (21%)	73,114,114	2.44	24 (32%)
38	LUT	Y	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.83	18 (35%)
37	CHL	S	607	-	50,58,74	2.26	16 (32%)	52,94,114	2.74	22 (42%)
27	CLA	g	612	7	49,57,73	1.69	10 (20%)	55,93,113	1.56	7 (12%)
27	CLA	B	604	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	6 (7%)
27	CLA	G	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.52	6 (10%)
37	CHL	Y	605	7	48,56,74	2.15	13 (27%)	51,92,114	2.84	19 (37%)
27	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.55	8 (10%)
27	CLA	B	608	-	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
38	LUT	g	1620	-	42,43,43	0.85	1 (2%)	51,60,60	1.79	15 (29%)
24	OEX	a	401	3,1	0,15,15	-	-	-	-	-
38	LUT	S	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.76	17 (33%)
27	CLA	b	603	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	7 (9%)
35	LHG	D	409	-	48,48,48	0.76	1 (2%)	51,54,54	1.36	8 (15%)
37	CHL	n	608	-	50,58,74	2.09	14 (28%)	52,94,114	2.87	20 (38%)
35	LHG	y	2630	27	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
27	CLA	B	607	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	11 (14%)
27	CLA	g	614	-	49,57,73	1.67	6 (12%)	55,93,113	1.57	7 (12%)
27	CLA	a	407	-	49,57,73	1.64	10 (20%)	55,93,113	1.63	8 (14%)
36	HEM	f	101	6,5	41,50,50	1.91	5 (12%)	45,82,82	1.42	5 (11%)
27	CLA	n	614	-	49,57,73	1.64	6 (12%)	55,93,113	1.61	7 (12%)
27	CLA	y	611	35	65,73,73	1.44	9 (13%)	76,113,113	1.39	7 (9%)
35	LHG	L	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	CHL	s	608	-	49,57,74	2.34	15 (30%)	52,93,114	2.65	20 (38%)
38	LUT	y	1621	-	42,43,43	1.01	3 (7%)	51,60,60	1.94	18 (35%)
37	CHL	g	606	-	50,58,74	2.18	15 (30%)	52,94,114	2.81	20 (38%)
37	CHL	n	607	-	66,74,74	1.86	14 (21%)	73,114,114	2.44	22 (30%)
27	CLA	r	603	-	49,57,73	1.67	9 (18%)	55,93,113	1.55	7 (12%)
30	SQD	b	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
27	CLA	b	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.55	8 (10%)
27	CLA	c	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.39	8 (10%)
40	NEX	s	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.43	14 (28%)
27	CLA	n	613	7	49,57,73	1.64	9 (18%)	55,93,113	1.59	6 (10%)
27	CLA	c	512	-	65,73,73	1.41	10 (15%)	76,113,113	1.43	7 (9%)
37	CHL	y	601	7	66,74,74	1.87	14 (21%)	73,114,114	2.42	23 (31%)
27	CLA	c	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.35	8 (10%)
27	CLA	B	617	-	65,73,73	1.47	9 (13%)	76,113,113	1.43	7 (9%)
27	CLA	b	611	-	65,73,73	1.44	10 (15%)	76,113,113	1.45	8 (10%)
27	CLA	y	610	7	65,73,73	1.45	9 (13%)	76,113,113	1.46	8 (10%)
32	DGD	H	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
27	CLA	S	614	-	49,57,73	1.65	10 (20%)	55,93,113	1.54	7 (12%)
27	CLA	G	603	-	49,57,73	1.67	8 (16%)	55,93,113	1.59	7 (12%)
37	CHL	s	606	-	50,58,74	2.22	16 (32%)	52,94,114	2.74	20 (38%)
37	CHL	S	608	-	49,57,74	2.34	15 (30%)	52,93,114	2.65	21 (40%)
37	CHL	R	608	-	50,58,74	2.16	16 (32%)	52,94,114	2.88	19 (36%)
27	CLA	s	609	18	49,57,73	1.70	6 (12%)	55,93,113	1.54	7 (12%)
32	DGD	C	518	-	56,56,67	1.14	8 (14%)	70,70,81	1.71	16 (22%)
37	CHL	N	608	-	50,58,74	2.09	14 (28%)	52,94,114	2.87	20 (38%)
27	CLA	d	403	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	8 (10%)
27	CLA	C	512	-	65,73,73	1.41	10 (15%)	76,113,113	1.43	7 (9%)
27	CLA	r	609	17	49,57,73	1.65	7 (14%)	55,93,113	1.57	7 (12%)
27	CLA	A	405	-	65,73,73	1.46	10 (15%)	76,113,113	1.50	8 (10%)
38	LUT	n	1620	-	42,43,43	0.83	1 (2%)	51,60,60	1.84	16 (31%)
27	CLA	R	611	35	49,57,73	1.66	6 (12%)	55,93,113	1.53	7 (12%)
27	CLA	b	606	-	65,73,73	1.50	10 (15%)	76,113,113	1.37	9 (11%)
29	BCR	a	411	-	41,41,41	0.91	2 (4%)	56,56,56	2.09	17 (30%)
29	BCR	c	517	-	41,41,41	0.96	3 (7%)	56,56,56	2.33	16 (28%)
28	PHO	A	408	-	51,69,69	1.14	6 (11%)	47,99,99	1.26	5 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	BCR	d	404	-	41,41,41	0.81	0	56,56,56	2.20	14 (25%)
37	CHL	s	607	-	50,58,74	2.27	16 (32%)	52,94,114	2.74	22 (42%)
27	CLA	N	611	35	49,57,73	1.65	7 (14%)	55,93,113	1.63	8 (14%)
31	LMG	z	101	-	51,51,55	0.72	0	59,59,63	1.35	6 (10%)
32	DGD	C	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.51	14 (18%)
30	SQD	a	418	-	53,54,54	0.98	5 (9%)	62,65,65	1.48	10 (16%)
27	CLA	B	611	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
29	BCR	C	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
40	NEX	Y	1623	-	38,46,46	1.10	2 (5%)	50,70,70	2.50	16 (32%)
31	LMG	a	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
37	CHL	R	607	-	50,58,74	2.16	15 (30%)	52,94,114	2.80	21 (40%)
27	CLA	c	504	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	6 (7%)
27	CLA	a	406	-	65,73,73	1.42	10 (15%)	76,113,113	1.52	8 (10%)
27	CLA	y	614	-	49,57,73	1.61	8 (16%)	55,93,113	1.58	7 (12%)
37	CHL	N	609	7	50,58,74	2.15	13 (26%)	52,94,114	2.81	22 (42%)
29	BCR	B	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.19	18 (32%)
37	CHL	N	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.92	20 (38%)
27	CLA	D	402	-	65,73,73	1.46	10 (15%)	76,113,113	1.49	8 (10%)
27	CLA	s	613	18	49,57,73	1.64	9 (18%)	55,93,113	1.58	6 (10%)
32	DGD	C	520	-	63,63,67	0.97	4 (6%)	77,77,81	1.51	11 (14%)
35	LHG	N	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
27	CLA	n	602	7	65,73,73	1.48	8 (12%)	76,113,113	1.38	6 (7%)
34	PL9	D	405	-	55,55,55	1.88	12 (21%)	68,69,69	1.57	15 (22%)
37	CHL	y	607	-	50,58,74	2.09	15 (30%)	52,94,114	2.77	21 (40%)
37	CHL	y	605	7	48,56,74	2.14	13 (27%)	51,92,114	2.84	19 (37%)
27	CLA	S	612	18	49,57,73	1.64	9 (18%)	55,93,113	1.53	7 (12%)
31	LMG	d	411	-	46,46,55	0.84	4 (8%)	54,54,63	1.41	7 (12%)
31	LMG	Z	101	-	51,51,55	0.72	0	59,59,63	1.35	6 (10%)
27	CLA	b	617	-	65,73,73	1.47	9 (13%)	76,113,113	1.43	7 (9%)
37	CHL	Y	609	7	66,74,74	1.85	13 (19%)	73,114,114	2.46	24 (32%)
37	CHL	R	606	-	50,58,74	2.09	14 (28%)	52,94,114	2.85	20 (38%)
39	XAT	y	1622	-	39,47,47	0.90	0	54,74,74	3.05	21 (38%)
27	CLA	g	611	35	49,57,73	1.68	9 (18%)	55,93,113	1.61	9 (16%)
38	LUT	S	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.89	15 (29%)
37	CHL	g	609	7	50,58,74	2.20	15 (30%)	52,94,114	2.80	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	c	501	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)
37	CHL	N	601	7	50,58,74	2.23	15 (30%)	52,94,114	2.78	21 (40%)
39	XAT	G	1622	-	39,47,47	0.97	2 (5%)	54,74,74	2.99	18 (33%)
27	CLA	R	604	-	49,57,73	1.65	8 (16%)	55,93,113	1.65	7 (12%)
37	CHL	g	607	-	50,58,74	2.12	14 (28%)	52,94,114	2.78	19 (36%)
38	LUT	g	1621	-	42,43,43	0.91	1 (2%)	51,60,60	1.87	17 (33%)
27	CLA	C	508	-	65,73,73	1.47	11 (16%)	76,113,113	1.57	8 (10%)
27	CLA	C	501	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)
27	CLA	S	613	18	49,57,73	1.63	9 (18%)	55,93,113	1.58	6 (10%)
35	LHG	d	409	-	48,48,48	0.76	1 (2%)	51,54,54	1.36	9 (17%)
27	CLA	N	614	-	49,57,73	1.63	7 (14%)	55,93,113	1.62	7 (12%)
27	CLA	Y	610	7	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)
29	BCR	D	404	-	41,41,41	0.80	0	56,56,56	2.20	14 (25%)
40	NEX	R	623	-	38,46,46	1.09	2 (5%)	50,70,70	2.41	21 (42%)
37	CHL	y	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.82	20 (38%)
27	CLA	r	604	-	49,57,73	1.63	8 (16%)	55,93,113	1.64	7 (12%)
30	SQD	B	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.56	10 (16%)
27	CLA	g	610	7	65,73,73	1.45	7 (10%)	76,113,113	1.45	9 (11%)
27	CLA	B	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.55	8 (10%)
27	CLA	n	610	7	65,73,73	1.45	10 (15%)	76,113,113	1.44	9 (11%)
27	CLA	r	601	17	49,57,73	1.66	6 (12%)	55,93,113	1.62	9 (16%)
27	CLA	g	613	7	49,57,73	1.68	10 (20%)	55,93,113	1.57	7 (12%)
27	CLA	N	604	-	49,57,73	1.64	9 (18%)	55,93,113	1.63	6 (10%)
35	LHG	D	408	-	42,42,48	0.77	1 (2%)	45,48,54	1.28	5 (11%)
35	LHG	S	2630	27	48,48,48	0.64	1 (2%)	51,54,54	1.28	6 (11%)
27	CLA	R	601	17	49,57,73	1.66	7 (14%)	55,93,113	1.63	9 (16%)
27	CLA	B	612	-	65,73,73	1.47	10 (15%)	76,113,113	1.52	9 (11%)
27	CLA	Y	604	-	49,57,73	1.67	10 (20%)	55,93,113	1.64	7 (12%)
27	CLA	Y	613	7	65,73,73	1.45	10 (15%)	76,113,113	1.40	7 (9%)
27	CLA	R	616	17	49,57,73	1.67	7 (14%)	55,93,113	1.60	9 (16%)
37	CHL	N	605	7	48,56,74	2.24	15 (31%)	51,92,114	2.82	21 (41%)
27	CLA	S	610	18	49,57,73	1.63	7 (14%)	55,93,113	1.63	7 (12%)
37	CHL	G	607	-	50,58,74	2.12	14 (28%)	52,94,114	2.78	19 (36%)
27	CLA	R	609	17	49,57,73	1.64	7 (14%)	55,93,113	1.57	7 (12%)
40	NEX	n	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.50	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.45	9 (14%)
35	LHG	Y	2630	27	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
27	CLA	r	613	17	49,57,73	1.64	8 (16%)	55,93,113	1.63	7 (12%)
27	CLA	n	603	-	49,57,73	1.67	9 (18%)	55,93,113	1.60	6 (10%)
27	CLA	c	509	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
40	NEX	N	1623	-	38,46,46	1.03	2 (5%)	50,70,70	2.51	15 (30%)
37	CHL	g	608	-	50,58,74	2.17	15 (30%)	52,94,114	2.73	19 (36%)
27	CLA	Y	611	35	65,73,73	1.44	9 (13%)	76,113,113	1.39	7 (9%)
27	CLA	Y	612	7	65,73,73	1.43	10 (15%)	76,113,113	1.38	8 (10%)
38	LUT	N	1621	-	42,43,43	0.91	2 (4%)	51,60,60	1.76	15 (29%)
27	CLA	g	603	-	49,57,73	1.67	8 (16%)	55,93,113	1.59	7 (12%)
31	LMG	B	622	-	51,51,55	0.80	2 (3%)	59,59,63	1.45	8 (13%)
27	CLA	C	504	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	6 (7%)
32	DGD	c	518	-	56,56,67	1.14	9 (16%)	70,70,81	1.71	16 (22%)
35	LHG	D	410	-	36,36,48	0.70	0	39,42,54	1.27	4 (10%)
27	CLA	B	609	-	65,73,73	1.41	9 (13%)	76,113,113	1.44	9 (11%)
27	CLA	R	602	17	65,73,73	1.44	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	B	602	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
35	LHG	g	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.29	7 (13%)
27	CLA	r	616	17	49,57,73	1.67	7 (14%)	55,93,113	1.59	9 (16%)
36	HEM	F	101	6,5	41,50,50	1.92	5 (12%)	45,82,82	1.43	5 (11%)
27	CLA	B	614	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	8 (10%)
27	CLA	Y	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.53	6 (10%)
27	CLA	N	602	7	65,73,73	1.46	8 (12%)	76,113,113	1.39	6 (7%)
38	LUT	s	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.76	17 (33%)
27	CLA	s	611	35	49,57,73	1.65	10 (20%)	55,93,113	1.58	8 (14%)
27	CLA	Y	602	7	65,73,73	1.44	10 (15%)	76,113,113	1.48	8 (10%)
27	CLA	Y	614	-	49,57,73	1.60	8 (16%)	55,93,113	1.56	7 (12%)
31	LMG	A	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
27	CLA	C	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.38	8 (10%)
27	CLA	b	605	-	65,73,73	1.45	12 (18%)	76,113,113	1.60	10 (13%)
27	CLA	s	602	18	49,57,73	1.68	7 (14%)	55,93,113	1.59	8 (14%)
37	CHL	n	609	7	50,58,74	2.16	14 (28%)	52,94,114	2.81	22 (42%)
27	CLA	C	502	-	65,73,73	1.42	10 (15%)	76,113,113	1.45	7 (9%)
27	CLA	n	612	7	49,57,73	1.66	7 (14%)	55,93,113	1.59	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	s	614	-	49,57,73	1.65	10 (20%)	55,93,113	1.53	7 (12%)
27	CLA	n	604	-	49,57,73	1.63	9 (18%)	55,93,113	1.63	6 (10%)
27	CLA	A	407	-	49,57,73	1.63	9 (18%)	55,93,113	1.63	8 (14%)
27	CLA	S	602	18	49,57,73	1.68	7 (14%)	55,93,113	1.60	7 (12%)
27	CLA	g	602	7	65,73,73	1.44	9 (13%)	76,113,113	1.43	6 (7%)
27	CLA	a	410	-	60,68,73	1.47	11 (18%)	70,107,113	1.57	8 (11%)
37	CHL	G	608	-	50,58,74	2.16	14 (28%)	52,94,114	2.73	19 (36%)
27	CLA	S	603	-	49,57,73	1.64	7 (14%)	55,93,113	1.56	6 (10%)
27	CLA	R	612	-	49,57,73	1.65	6 (12%)	55,93,113	1.50	7 (12%)
29	BCR	c	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	18 (32%)
27	CLA	G	613	7	49,57,73	1.68	10 (20%)	55,93,113	1.57	7 (12%)
27	CLA	s	603	-	49,57,73	1.64	7 (14%)	55,93,113	1.56	6 (10%)
37	CHL	y	608	-	50,58,74	2.11	13 (26%)	52,94,114	2.77	18 (34%)
37	CHL	n	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.92	20 (38%)
27	CLA	R	603	-	49,57,73	1.66	9 (18%)	55,93,113	1.53	7 (12%)
35	LHG	G	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	7 (13%)
27	CLA	G	612	7	49,57,73	1.70	10 (20%)	55,93,113	1.55	7 (12%)
37	CHL	g	601	7	66,74,74	1.86	13 (19%)	73,114,114	2.44	22 (30%)
35	LHG	d	408	-	42,42,48	0.77	1 (2%)	45,48,54	1.28	5 (11%)
27	CLA	c	511	3	65,73,73	1.45	10 (15%)	76,113,113	1.53	7 (9%)
27	CLA	D	403	-	65,73,73	1.41	8 (12%)	76,113,113	1.47	8 (10%)
38	LUT	G	1621	-	42,43,43	0.92	1 (2%)	51,60,60	1.86	17 (33%)
37	CHL	G	605	7	48,56,74	2.28	16 (33%)	51,92,114	2.75	19 (37%)
39	XAT	N	1622	-	39,47,47	1.00	1 (2%)	54,74,74	3.06	23 (42%)
27	CLA	G	611	35	49,57,73	1.67	9 (18%)	55,93,113	1.60	9 (16%)
27	CLA	r	612	-	49,57,73	1.67	7 (14%)	55,93,113	1.50	7 (12%)
37	CHL	Y	601	7	66,74,74	1.87	14 (21%)	73,114,114	2.43	23 (31%)
29	BCR	C	517	-	41,41,41	0.96	4 (9%)	56,56,56	2.33	16 (28%)
27	CLA	B	606	-	65,73,73	1.51	10 (15%)	76,113,113	1.36	9 (11%)
27	CLA	S	609	18	49,57,73	1.71	6 (12%)	55,93,113	1.54	7 (12%)
37	CHL	S	601	18	52,60,74	2.11	14 (26%)	56,97,114	2.76	24 (42%)
37	CHL	r	606	-	50,58,74	2.09	14 (28%)	52,94,114	2.85	20 (38%)
39	XAT	Y	1622	-	39,47,47	0.90	0	54,74,74	3.05	20 (37%)
32	DGD	h	102	-	63,63,67	0.99	4 (6%)	77,77,81	1.48	8 (10%)
29	BCR	B	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.08	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	s	610	18	49,57,73	1.63	7 (14%)	55,93,113	1.63	7 (12%)
35	LHG	n	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
27	CLA	s	612	18	49,57,73	1.65	9 (18%)	55,93,113	1.53	7 (12%)
30	SQD	A	418	-	53,54,54	0.98	5 (9%)	62,65,65	1.49	10 (16%)
28	PHO	a	408	-	51,69,69	1.14	6 (11%)	47,99,99	1.26	5 (10%)
29	BCR	b	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.09	17 (30%)
27	CLA	n	611	35	49,57,73	1.64	8 (16%)	55,93,113	1.63	8 (14%)
30	SQD	A	412	-	53,54,54	0.98	5 (9%)	62,65,65	1.44	10 (16%)
35	LHG	s	2630	27	48,48,48	0.64	1 (2%)	51,54,54	1.28	6 (11%)
29	BCR	c	516	-	41,41,41	0.78	0	56,56,56	2.30	18 (32%)
27	CLA	R	610	17	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
38	LUT	y	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.83	18 (35%)
27	CLA	b	614	-	65,73,73	1.46	10 (15%)	76,113,113	1.36	9 (11%)
37	CHL	S	606	-	50,58,74	2.22	16 (32%)	52,94,114	2.74	19 (36%)
27	CLA	y	613	7	65,73,73	1.44	10 (15%)	76,113,113	1.41	8 (10%)
27	CLA	G	614	-	49,57,73	1.68	6 (12%)	55,93,113	1.57	7 (12%)
37	CHL	g	605	7	48,56,74	2.28	16 (33%)	51,92,114	2.74	19 (37%)
27	CLA	d	402	-	65,73,73	1.46	10 (15%)	76,113,113	1.49	8 (10%)
27	CLA	B	616	-	65,73,73	1.44	9 (13%)	76,113,113	1.38	6 (7%)
27	CLA	S	611	35	49,57,73	1.66	10 (20%)	55,93,113	1.57	7 (12%)
27	CLA	b	616	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	6 (7%)
31	LMG	b	622	-	51,51,55	0.80	2 (3%)	59,59,63	1.45	8 (13%)
34	PL9	d	405	-	55,55,55	1.88	12 (21%)	68,69,69	1.57	15 (22%)
27	CLA	C	513	-	49,57,73	1.63	10 (20%)	55,93,113	1.69	7 (12%)
38	LUT	s	1620	-	42,43,43	0.86	1 (2%)	51,60,60	1.89	15 (29%)
27	CLA	c	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.55	8 (10%)
27	CLA	y	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.64	7 (12%)
27	CLA	y	602	7	65,73,73	1.44	10 (15%)	76,113,113	1.48	7 (9%)
38	LUT	G	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.78	15 (29%)
27	CLA	b	602	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
27	CLA	c	502	-	65,73,73	1.41	10 (15%)	76,113,113	1.45	7 (9%)
37	CHL	N	607	-	66,74,74	1.86	13 (19%)	73,114,114	2.43	23 (31%)
27	CLA	r	602	17	65,73,73	1.43	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	C	510	-	65,73,73	1.41	9 (13%)	76,113,113	1.46	7 (9%)
35	LHG	R	2630	27	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	B	610	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	8 (10%)
31	LMG	C	521	-	51,51,55	0.74	0	59,59,63	1.39	8 (13%)
27	CLA	G	610	7	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
37	CHL	Y	606	-	50,58,74	2.11	14 (28%)	52,94,114	2.82	20 (38%)
38	LUT	R	620	-	42,43,43	0.82	1 (2%)	51,60,60	1.65	15 (29%)
35	LHG	d	410	-	36,36,48	0.70	0	39,42,54	1.27	4 (10%)
40	NEX	S	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.42	14 (28%)
40	NEX	G	1623	-	38,46,46	1.01	2 (5%)	50,70,70	2.60	16 (32%)
27	CLA	A	406	-	65,73,73	1.41	9 (13%)	76,113,113	1.53	8 (10%)
24	OEX	A	401	3,1	0,15,15	-	-	-	-	-
39	XAT	r	622	-	39,47,47	0.99	1 (2%)	54,74,74	2.84	21 (38%)
27	CLA	G	602	7	65,73,73	1.44	9 (13%)	76,113,113	1.43	6 (7%)
27	CLA	C	509	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	12 (15%)
27	CLA	C	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.36	8 (10%)
39	XAT	g	1622	-	39,47,47	0.96	2 (5%)	54,74,74	2.99	19 (35%)
27	CLA	R	613	17	49,57,73	1.64	8 (16%)	55,93,113	1.61	7 (12%)
37	CHL	Y	607	-	50,58,74	2.09	15 (30%)	52,94,114	2.77	20 (38%)
27	CLA	b	609	-	65,73,73	1.41	10 (15%)	76,113,113	1.44	9 (11%)
27	CLA	N	603	-	49,57,73	1.68	9 (18%)	55,93,113	1.59	6 (10%)
27	CLA	C	506	-	65,73,73	1.46	10 (15%)	76,113,113	1.47	8 (10%)
39	XAT	n	1622	-	39,47,47	1.00	1 (2%)	54,74,74	3.05	23 (42%)
27	CLA	b	607	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	11 (14%)
37	CHL	s	601	18	52,60,74	2.12	15 (28%)	56,97,114	2.75	24 (42%)
29	BCR	c	514	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	18 (32%)
38	LUT	Y	1621	-	42,43,43	1.01	3 (7%)	51,60,60	1.93	18 (35%)
32	DGD	c	519	-	63,63,67	0.98	4 (6%)	77,77,81	1.51	13 (16%)
27	CLA	C	511	3	65,73,73	1.46	10 (15%)	76,113,113	1.54	7 (9%)
27	CLA	A	410	-	60,68,73	1.46	11 (18%)	70,107,113	1.57	8 (11%)
27	CLA	r	611	35	49,57,73	1.66	6 (12%)	55,93,113	1.53	8 (14%)
27	CLA	s	604	-	49,57,73	1.62	9 (18%)	55,93,113	1.68	7 (12%)
27	CLA	b	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	9 (11%)
37	CHL	n	605	7	48,56,74	2.25	15 (31%)	51,92,114	2.82	21 (41%)
27	CLA	B	603	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	S	604	-	49,57,73	1.62	8 (16%)	55,93,113	1.69	7 (12%)
27	CLA	g	604	-	49,57,73	1.65	10 (20%)	55,93,113	1.52	6 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	LUT	N	1620	-	42,43,43	0.85	1 (2%)	51,60,60	1.83	16 (31%)
37	CHL	n	601	7	50,58,74	2.23	15 (30%)	52,94,114	2.77	21 (40%)
29	BCR	A	411	-	41,41,41	0.92	2 (4%)	56,56,56	2.09	17 (30%)
29	BCR	b	620	-	41,41,41	0.96	3 (7%)	56,56,56	2.12	17 (30%)
27	CLA	b	615	-	65,73,73	1.43	10 (15%)	76,113,113	1.38	7 (9%)
27	CLA	N	613	7	49,57,73	1.64	9 (18%)	55,93,113	1.59	6 (10%)
32	DGD	c	520	-	63,63,67	0.97	4 (6%)	77,77,81	1.51	11 (14%)
27	CLA	N	612	7	49,57,73	1.66	9 (18%)	55,93,113	1.60	8 (14%)
27	CLA	a	405	-	65,73,73	1.46	9 (13%)	76,113,113	1.51	8 (10%)
29	BCR	C	514	-	41,41,41	0.91	1 (2%)	56,56,56	2.02	18 (32%)
40	NEX	r	623	-	38,46,46	1.09	1 (2%)	50,70,70	2.41	21 (42%)
37	CHL	G	609	7	50,58,74	2.20	15 (30%)	52,94,114	2.80	19 (36%)
37	CHL	r	607	-	50,58,74	2.16	15 (30%)	52,94,114	2.80	21 (40%)
29	BCR	H	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.01	18 (32%)

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
40	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	r	610	17	1/1/15/20	15/37/115/115	-
27	CLA	B	605	-	1/1/15/20	17/37/115/115	-
27	CLA	c	508	-	1/1/15/20	11/37/115/115	-
27	CLA	b	610	-	1/1/15/20	13/37/115/115	-
38	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	c	510	-	1/1/15/20	18/37/115/115	-
40	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
29	BCR	B	620	-	-	6/29/63/63	0/2/2/2
39	XAT	R	622	-	-	2/31/93/93	0/4/4/4
37	CHL	Y	608	-	3/3/16/26	9/20/118/137	-
27	CLA	B	615	-	1/1/15/20	14/37/115/115	-
28	PHO	A	409	-	-	17/37/103/103	0/5/6/6
27	CLA	b	604	-	1/1/15/20	13/37/115/115	-
27	CLA	b	608	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	y	603	-	1/1/11/20	4/18/96/115	-
27	CLA	c	513	-	1/1/11/20	6/18/96/115	-
37	CHL	G	606	-	3/3/16/26	3/20/118/137	-
37	CHL	r	608	-	3/3/16/26	12/20/118/137	-
27	CLA	N	610	7	1/1/15/20	10/37/115/115	-
29	BCR	C	516	-	-	7/29/63/63	0/2/2/2
29	BCR	h	101	-	-	4/29/63/63	0/2/2/2
29	BCR	b	618	-	-	4/29/63/63	0/2/2/2
35	LHG	r	2630	27	-	13/53/53/53	-
31	LMG	D	411	-	-	13/41/61/70	0/1/1/1
38	LUT	r	620	-	-	2/29/67/67	0/2/2/2
27	CLA	c	506	-	1/1/15/20	18/37/115/115	-
31	LMG	c	521	-	-	20/46/66/70	0/1/1/1
37	CHL	y	609	7	4/4/20/26	19/39/137/137	-
27	CLA	y	612	7	1/1/15/20	10/37/115/115	-
35	LHG	l	101	-	-	27/53/53/53	-
28	PHO	a	409	-	-	17/37/103/103	0/5/6/6
37	CHL	G	601	7	4/4/20/26	20/39/137/137	-
38	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
37	CHL	S	607	-	3/3/16/26	9/20/118/137	-
27	CLA	g	612	7	1/1/11/20	6/18/96/115	-
27	CLA	B	604	-	1/1/15/20	13/37/115/115	-
27	CLA	G	604	-	1/1/11/20	9/18/96/115	-
37	CHL	Y	605	7	3/3/16/26	8/18/116/137	-
27	CLA	C	505	-	1/1/15/20	10/37/115/115	-
27	CLA	B	608	-	1/1/15/20	8/37/115/115	-
38	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
38	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	b	603	-	1/1/15/20	16/37/115/115	-
35	LHG	D	409	-	-	15/53/53/53	-
37	CHL	n	608	-	3/3/16/26	7/20/118/137	-
35	LHG	y	2630	27	-	20/53/53/53	-
27	CLA	B	607	-	1/1/15/20	5/37/115/115	-
27	CLA	g	614	-	1/1/11/20	7/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	407	-	1/1/11/20	6/18/96/115	-
36	HEM	f	101	6,5	-	0/12/54/54	-
27	CLA	n	614	-	1/1/11/20	10/18/96/115	-
27	CLA	y	611	35	1/1/15/20	9/37/115/115	-
37	CHL	s	608	-	3/3/16/26	5/19/117/137	-
35	LHG	L	101	-	-	27/53/53/53	-
38	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
37	CHL	g	606	-	3/3/16/26	3/20/118/137	-
37	CHL	n	607	-	4/4/20/26	16/39/137/137	-
27	CLA	r	603	-	1/1/11/20	6/18/96/115	-
30	SQD	b	621	-	-	24/49/69/69	0/1/1/1
27	CLA	b	613	-	1/1/15/20	17/37/115/115	-
27	CLA	c	503	-	1/1/15/20	12/37/115/115	-
40	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	n	613	7	1/1/11/20	7/18/96/115	-
27	CLA	c	512	-	1/1/15/20	17/37/115/115	-
37	CHL	y	601	7	4/4/20/26	17/39/137/137	-
27	CLA	c	507	-	1/1/15/20	15/37/115/115	-
27	CLA	B	617	-	1/1/15/20	15/37/115/115	-
27	CLA	b	611	-	1/1/15/20	10/37/115/115	-
27	CLA	y	610	7	1/1/15/20	15/37/115/115	-
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
27	CLA	S	614	-	1/1/11/20	7/18/96/115	-
27	CLA	G	603	-	1/1/11/20	6/18/96/115	-
37	CHL	s	606	-	3/3/16/26	10/20/118/137	-
37	CHL	S	608	-	3/3/16/26	5/19/117/137	-
37	CHL	R	608	-	3/3/16/26	12/20/118/137	-
27	CLA	s	609	18	1/1/11/20	8/18/96/115	-
37	CHL	N	608	-	3/3/16/26	7/20/118/137	-
32	DGD	C	518	-	-	17/44/84/95	0/2/2/2
27	CLA	d	403	-	1/1/15/20	12/37/115/115	-
27	CLA	C	512	-	1/1/15/20	17/37/115/115	-
27	CLA	r	609	17	1/1/11/20	8/18/96/115	-
27	CLA	A	405	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	R	611	35	1/1/11/20	9/18/96/115	-
27	CLA	b	606	-	1/1/15/20	14/37/115/115	-
29	BCR	a	411	-	-	0/29/63/63	0/2/2/2
29	BCR	c	517	-	-	1/29/63/63	0/2/2/2
28	PHO	A	408	-	-	10/37/103/103	0/5/6/6
29	BCR	d	404	-	-	9/29/63/63	0/2/2/2
37	CHL	s	607	-	3/3/16/26	9/20/118/137	-
27	CLA	N	611	35	1/1/11/20	6/18/96/115	-
31	LMG	z	101	-	-	22/46/66/70	0/1/1/1
32	DGD	C	519	-	-	23/51/91/95	0/2/2/2
30	SQD	a	418	-	-	20/49/69/69	0/1/1/1
27	CLA	B	611	-	1/1/15/20	10/37/115/115	-
29	BCR	C	515	-	-	0/29/63/63	0/2/2/2
40	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
31	LMG	a	413	-	-	15/43/63/70	0/1/1/1
37	CHL	R	607	-	3/3/16/26	9/20/118/137	-
27	CLA	c	504	-	1/1/15/20	14/37/115/115	-
27	CLA	a	406	-	1/1/15/20	12/37/115/115	-
27	CLA	y	614	-	1/1/11/20	8/18/96/115	-
37	CHL	N	609	7	3/3/16/26	7/20/118/137	-
37	CHL	N	606	-	3/3/16/26	4/20/118/137	-
29	BCR	B	618	-	-	4/29/63/63	0/2/2/2
27	CLA	D	402	-	1/1/15/20	10/37/115/115	-
27	CLA	s	613	18	1/1/11/20	6/18/96/115	-
32	DGD	C	520	-	-	14/51/91/95	0/2/2/2
35	LHG	N	2630	27	-	24/53/53/53	-
27	CLA	n	602	7	1/1/15/20	10/37/115/115	-
34	PL9	D	405	-	-	14/53/73/73	0/1/1/1
37	CHL	y	607	-	3/3/16/26	8/20/118/137	-
37	CHL	y	605	7	3/3/16/26	8/18/116/137	-
27	CLA	S	612	18	1/1/11/20	5/18/96/115	-
31	LMG	d	411	-	-	13/41/61/70	0/1/1/1
31	LMG	Z	101	-	-	22/46/66/70	0/1/1/1
27	CLA	b	617	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	Y	609	7	4/4/20/26	19/39/137/137	-
37	CHL	R	606	-	3/3/16/26	10/20/118/137	-
39	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	g	611	35	1/1/11/20	6/18/96/115	-
38	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
37	CHL	g	609	7	3/3/16/26	11/20/118/137	-
27	CLA	c	501	-	1/1/15/20	12/37/115/115	-
37	CHL	N	601	7	3/3/16/26	6/20/118/137	-
39	XAT	G	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	R	604	-	1/1/11/20	9/18/96/115	-
37	CHL	g	607	-	3/3/16/26	9/20/118/137	-
38	LUT	g	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	C	508	-	1/1/15/20	11/37/115/115	-
27	CLA	C	501	-	1/1/15/20	12/37/115/115	-
27	CLA	S	613	18	1/1/11/20	6/18/96/115	-
35	LHG	d	409	-	-	15/53/53/53	-
27	CLA	N	614	-	1/1/11/20	11/18/96/115	-
27	CLA	Y	610	7	1/1/15/20	15/37/115/115	-
29	BCR	D	404	-	-	9/29/63/63	0/2/2/2
40	NEX	R	623	-	-	3/27/83/83	0/3/3/3
37	CHL	y	606	-	3/3/16/26	6/20/118/137	-
27	CLA	r	604	-	1/1/11/20	9/18/96/115	-
30	SQD	B	621	-	-	24/49/69/69	0/1/1/1
27	CLA	g	610	7	1/1/15/20	15/37/115/115	-
27	CLA	B	613	-	1/1/15/20	17/37/115/115	-
27	CLA	n	610	7	1/1/15/20	10/37/115/115	-
27	CLA	r	601	17	1/1/11/20	13/18/96/115	-
27	CLA	g	613	7	1/1/11/20	6/18/96/115	-
27	CLA	N	604	-	1/1/11/20	4/18/96/115	-
35	LHG	D	408	-	-	20/47/47/53	-
35	LHG	S	2630	27	-	23/53/53/53	-
27	CLA	R	601	17	1/1/11/20	13/18/96/115	-
27	CLA	B	612	-	1/1/15/20	15/37/115/115	-
27	CLA	Y	604	-	1/1/11/20	6/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	Y	613	7	1/1/15/20	14/37/115/115	-
27	CLA	R	616	17	1/1/11/20	9/18/96/115	-
37	CHL	N	605	7	3/3/16/26	9/18/116/137	-
27	CLA	S	610	18	1/1/11/20	5/18/96/115	-
37	CHL	G	607	-	3/3/16/26	9/20/118/137	-
27	CLA	R	609	17	1/1/11/20	8/18/96/115	-
40	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
30	SQD	a	412	-	-	28/49/69/69	0/1/1/1
35	LHG	Y	2630	27	-	20/53/53/53	-
27	CLA	r	613	17	1/1/11/20	7/18/96/115	-
27	CLA	n	603	-	1/1/11/20	11/18/96/115	-
27	CLA	c	509	-	1/1/15/20	9/37/115/115	-
40	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
37	CHL	g	608	-	3/3/16/26	10/20/118/137	-
27	CLA	Y	611	35	1/1/15/20	9/37/115/115	-
27	CLA	Y	612	7	1/1/15/20	10/37/115/115	-
38	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	g	603	-	1/1/11/20	6/18/96/115	-
31	LMG	B	622	-	-	23/46/66/70	0/1/1/1
27	CLA	C	504	-	1/1/15/20	14/37/115/115	-
32	DGD	c	518	-	-	17/44/84/95	0/2/2/2
35	LHG	D	410	-	-	21/41/41/53	-
27	CLA	B	609	-	1/1/15/20	16/37/115/115	-
27	CLA	R	602	17	1/1/15/20	15/37/115/115	-
27	CLA	B	602	-	1/1/15/20	19/37/115/115	-
35	LHG	g	2630	27	-	30/53/53/53	-
27	CLA	r	616	17	1/1/11/20	9/18/96/115	-
36	HEM	F	101	6,5	-	0/12/54/54	-
27	CLA	B	614	-	1/1/15/20	9/37/115/115	-
27	CLA	Y	603	-	1/1/11/20	4/18/96/115	-
27	CLA	N	602	7	1/1/15/20	10/37/115/115	-
38	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
27	CLA	s	611	35	1/1/11/20	7/18/96/115	-
27	CLA	Y	602	7	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	Y	614	-	1/1/11/20	8/18/96/115	-
31	LMG	A	413	-	-	15/43/63/70	0/1/1/1
27	CLA	C	503	-	1/1/15/20	12/37/115/115	-
27	CLA	b	605	-	1/1/15/20	17/37/115/115	-
27	CLA	s	602	18	1/1/11/20	7/18/96/115	-
37	CHL	n	609	7	3/3/16/26	7/20/118/137	-
27	CLA	C	502	-	1/1/15/20	14/37/115/115	-
27	CLA	n	612	7	1/1/11/20	9/18/96/115	-
27	CLA	s	614	-	1/1/11/20	7/18/96/115	-
27	CLA	n	604	-	1/1/11/20	4/18/96/115	-
27	CLA	A	407	-	1/1/11/20	6/18/96/115	-
27	CLA	S	602	18	1/1/11/20	7/18/96/115	-
27	CLA	g	602	7	1/1/15/20	15/37/115/115	-
27	CLA	a	410	-	1/1/14/20	11/31/109/115	-
37	CHL	G	608	-	3/3/16/26	10/20/118/137	-
27	CLA	S	603	-	-	11/18/96/115	-
27	CLA	R	612	-	1/1/11/20	4/18/96/115	-
29	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	CLA	G	613	7	1/1/11/20	6/18/96/115	-
27	CLA	s	603	-	-	11/18/96/115	-
37	CHL	y	608	-	3/3/16/26	9/20/118/137	-
37	CHL	n	606	-	3/3/16/26	4/20/118/137	-
27	CLA	R	603	-	1/1/11/20	6/18/96/115	-
37	CHL	g	601	7	4/4/20/26	20/39/137/137	-
27	CLA	G	612	7	1/1/11/20	6/18/96/115	-
35	LHG	G	2630	27	-	30/53/53/53	-
35	LHG	d	408	-	-	20/47/47/53	-
27	CLA	c	511	3	1/1/15/20	9/37/115/115	-
27	CLA	D	403	-	1/1/15/20	12/37/115/115	-
38	LUT	G	1621	-	-	1/29/67/67	0/2/2/2
37	CHL	G	605	7	3/3/16/26	5/18/116/137	-
39	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	G	611	35	1/1/11/20	6/18/96/115	-
27	CLA	r	612	-	1/1/11/20	4/18/96/115	-
37	CHL	Y	601	7	4/4/20/26	17/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	C	517	-	-	1/29/63/63	0/2/2/2
27	CLA	B	606	-	1/1/15/20	14/37/115/115	-
27	CLA	S	609	18	1/1/11/20	8/18/96/115	-
37	CHL	S	601	18	3/3/17/26	9/23/121/137	-
37	CHL	r	606	-	3/3/16/26	10/20/118/137	-
39	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
32	DGD	h	102	-	-	19/51/91/95	0/2/2/2
29	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	CLA	s	610	18	1/1/11/20	5/18/96/115	-
35	LHG	n	2630	27	-	24/53/53/53	-
27	CLA	s	612	18	1/1/11/20	5/18/96/115	-
30	SQD	A	418	-	-	20/49/69/69	0/1/1/1
28	PHO	a	408	-	-	10/37/103/103	0/5/6/6
29	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	CLA	n	611	35	1/1/11/20	6/18/96/115	-
30	SQD	A	412	-	-	28/49/69/69	0/1/1/1
35	LHG	s	2630	27	-	23/53/53/53	-
29	BCR	c	516	-	-	7/29/63/63	0/2/2/2
27	CLA	R	610	17	1/1/15/20	15/37/115/115	-
38	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	b	614	-	1/1/15/20	9/37/115/115	-
37	CHL	S	606	-	3/3/16/26	10/20/118/137	-
27	CLA	y	613	7	1/1/15/20	14/37/115/115	-
27	CLA	G	614	-	1/1/11/20	7/18/96/115	-
37	CHL	g	605	7	3/3/16/26	5/18/116/137	-
27	CLA	d	402	-	1/1/15/20	10/37/115/115	-
27	CLA	B	616	-	1/1/15/20	11/37/115/115	-
27	CLA	S	611	35	1/1/11/20	7/18/96/115	-
27	CLA	b	616	-	1/1/15/20	11/37/115/115	-
31	LMG	b	622	-	-	23/46/66/70	0/1/1/1
34	PL9	d	405	-	-	14/53/73/73	0/1/1/1
27	CLA	C	513	-	1/1/11/20	6/18/96/115	-
38	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	c	505	-	1/1/15/20	10/37/115/115	-
27	CLA	y	604	-	1/1/11/20	6/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	y	602	7	1/1/15/20	12/37/115/115	-
38	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	b	602	-	1/1/15/20	19/37/115/115	-
27	CLA	c	502	-	1/1/15/20	14/37/115/115	-
37	CHL	N	607	-	4/4/20/26	16/39/137/137	-
27	CLA	r	602	17	1/1/15/20	15/37/115/115	-
27	CLA	C	510	-	1/1/15/20	18/37/115/115	-
35	LHG	R	2630	27	-	13/53/53/53	-
27	CLA	B	610	-	1/1/15/20	13/37/115/115	-
31	LMG	C	521	-	-	20/46/66/70	0/1/1/1
27	CLA	G	610	7	1/1/15/20	15/37/115/115	-
37	CHL	Y	606	-	3/3/16/26	6/20/118/137	-
38	LUT	R	620	-	-	2/29/67/67	0/2/2/2
35	LHG	d	410	-	-	21/41/41/53	-
40	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
40	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	A	406	-	1/1/15/20	12/37/115/115	-
39	XAT	r	622	-	-	2/31/93/93	0/4/4/4
27	CLA	G	602	7	1/1/15/20	15/37/115/115	-
27	CLA	C	509	-	1/1/15/20	10/37/115/115	-
27	CLA	C	507	-	1/1/15/20	15/37/115/115	-
39	XAT	g	1622	-	-	3/31/93/93	0/4/4/4
27	CLA	R	613	17	1/1/11/20	7/18/96/115	-
37	CHL	Y	607	-	3/3/16/26	8/20/118/137	-
27	CLA	b	609	-	1/1/15/20	16/37/115/115	-
27	CLA	N	603	-	1/1/11/20	11/18/96/115	-
27	CLA	C	506	-	1/1/15/20	18/37/115/115	-
39	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	b	607	-	1/1/15/20	4/37/115/115	-
37	CHL	s	601	18	3/3/17/26	9/23/121/137	-
29	BCR	c	514	-	-	4/29/63/63	0/2/2/2
38	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
32	DGD	c	519	-	-	23/51/91/95	0/2/2/2
27	CLA	C	511	3	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	410	-	1/1/14/20	11/31/109/115	-
27	CLA	r	611	35	1/1/11/20	9/18/96/115	-
27	CLA	s	604	-	1/1/11/20	11/18/96/115	-
27	CLA	b	612	-	1/1/15/20	15/37/115/115	-
37	CHL	n	605	7	3/3/16/26	9/18/116/137	-
27	CLA	B	603	-	1/1/15/20	15/37/115/115	-
27	CLA	S	604	-	1/1/11/20	11/18/96/115	-
27	CLA	g	604	-	1/1/11/20	9/18/96/115	-
38	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
37	CHL	n	601	7	3/3/16/26	6/20/118/137	-
29	BCR	A	411	-	-	0/29/63/63	0/2/2/2
29	BCR	b	620	-	-	6/29/63/63	0/2/2/2
27	CLA	b	615	-	1/1/15/20	14/37/115/115	-
27	CLA	N	613	7	1/1/11/20	7/18/96/115	-
32	DGD	c	520	-	-	14/51/91/95	0/2/2/2
27	CLA	N	612	7	1/1/11/20	9/18/96/115	-
27	CLA	a	405	-	1/1/15/20	14/37/115/115	-
29	BCR	C	514	-	-	4/29/63/63	0/2/2/2
40	NEX	r	623	-	-	3/27/83/83	0/3/3/3
37	CHL	G	609	7	3/3/16/26	11/20/118/137	-
37	CHL	r	607	-	3/3/16/26	9/20/118/137	-
29	BCR	H	101	-	-	4/29/63/63	0/2/2/2

The worst 5 of 2376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	101	HEM	C3D-C2D	7.74	1.53	1.36
36	f	101	HEM	C3D-C2D	7.73	1.53	1.36
27	S	609	CLA	C4B-NB	7.39	1.41	1.35
27	s	609	CLA	C4B-NB	7.33	1.41	1.35
27	R	601	CLA	C4B-NB	7.11	1.41	1.35

The worst 5 of 3583 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	Y	1622	XAT	O4-C5-C4	11.88	122.31	113.38
39	y	1622	XAT	O4-C5-C4	11.85	122.28	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	1622	XAT	O4-C5-C4	10.80	121.50	113.38
39	g	1622	XAT	O4-C5-C4	10.77	121.47	113.38
40	G	1623	NEX	O24-C25-C24	9.46	120.49	113.38

5 of 312 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	A	405	CLA	ND
27	A	406	CLA	ND
27	A	407	CLA	ND
27	A	410	CLA	ND
27	B	602	CLA	ND

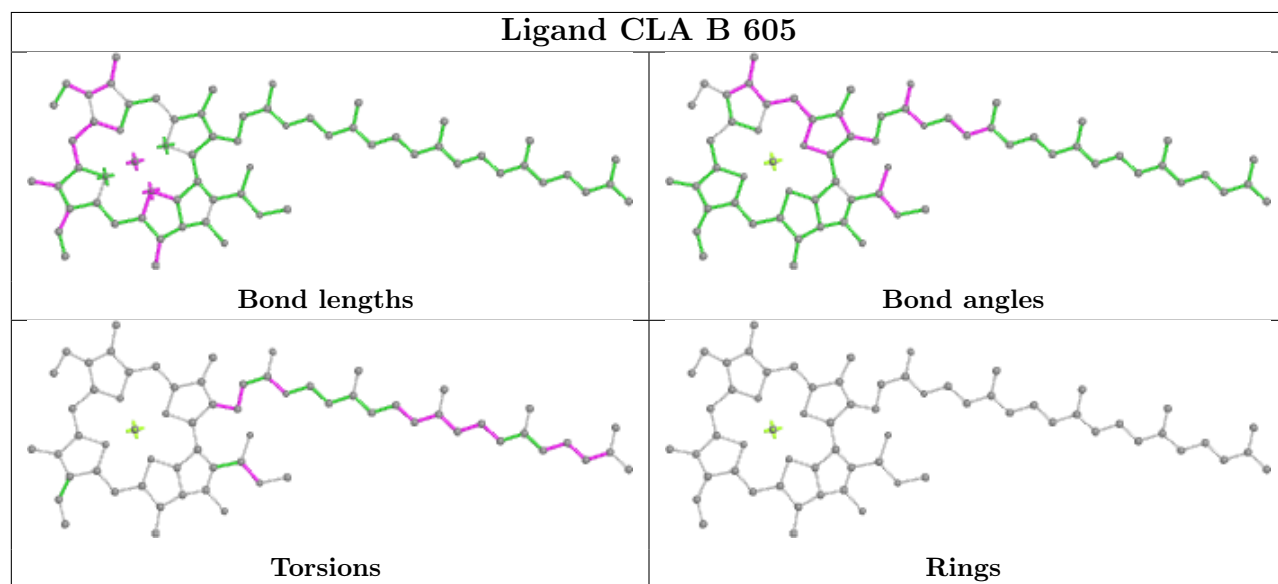
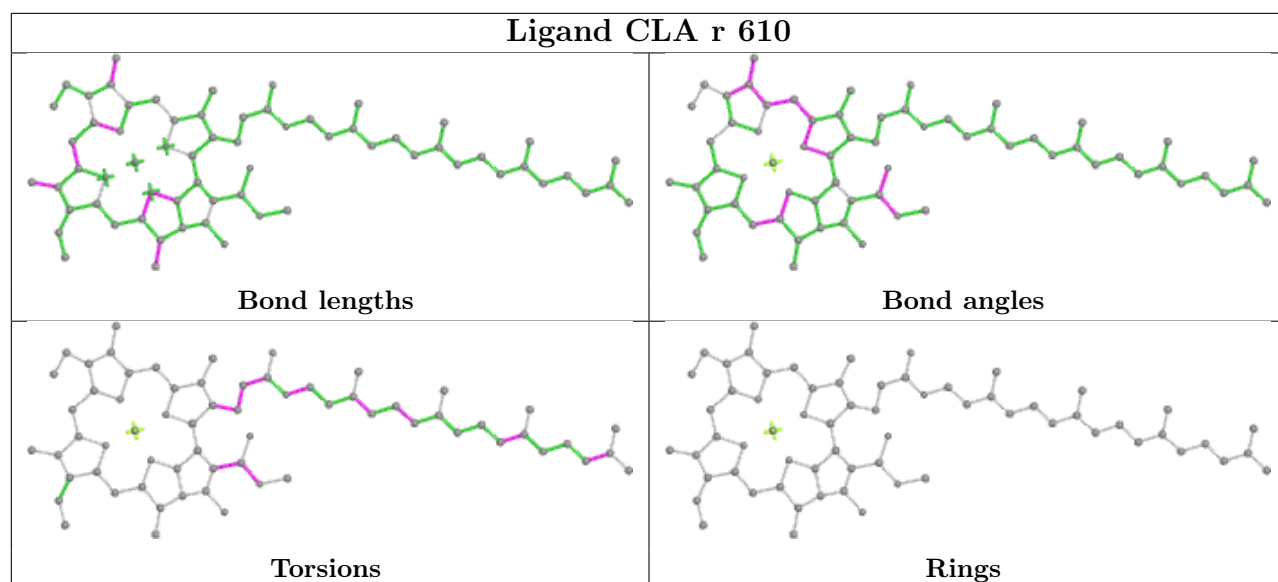
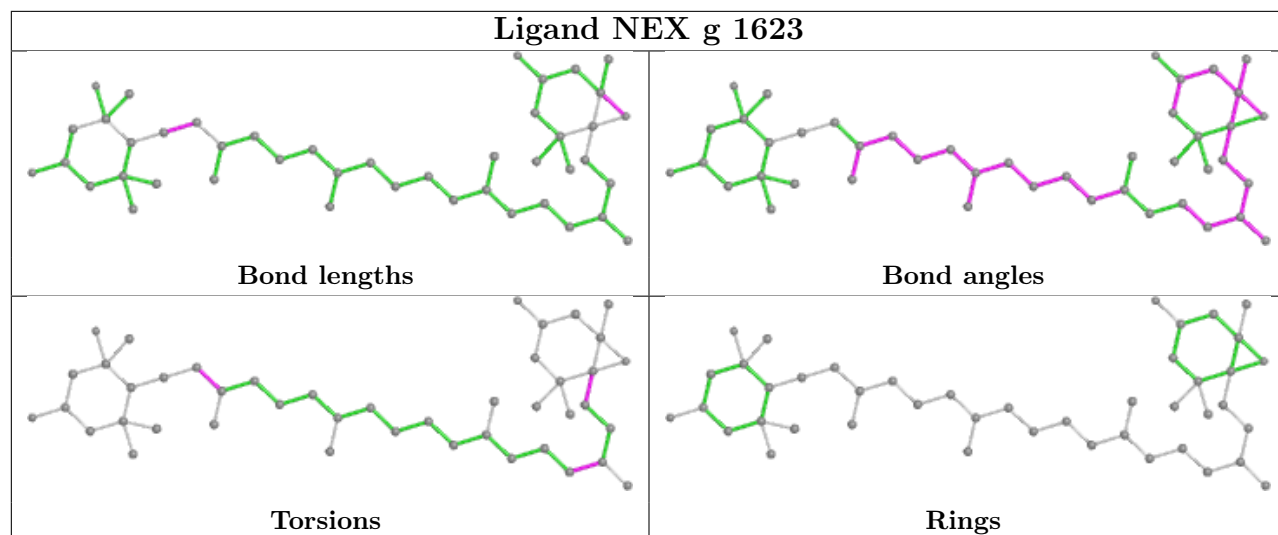
5 of 3220 torsion outliers are listed below:

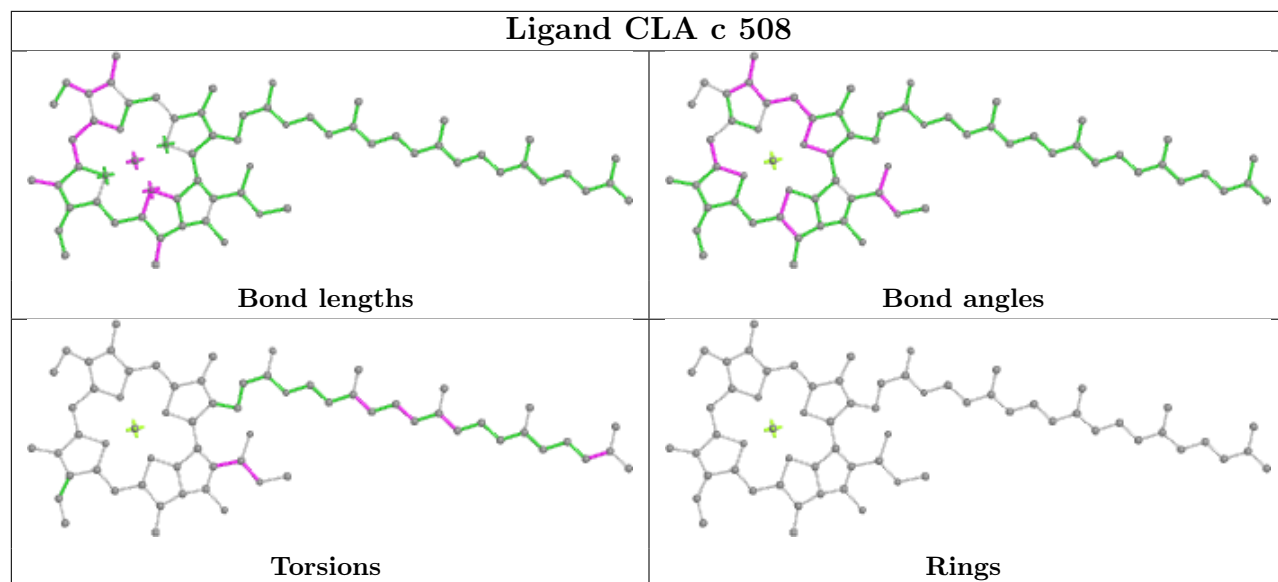
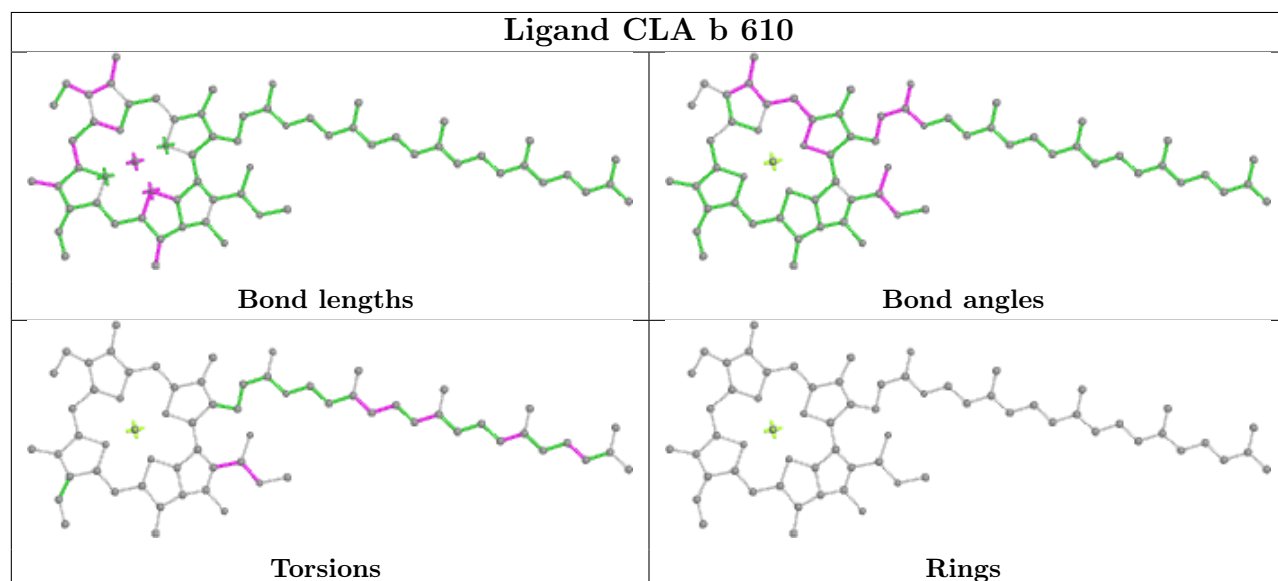
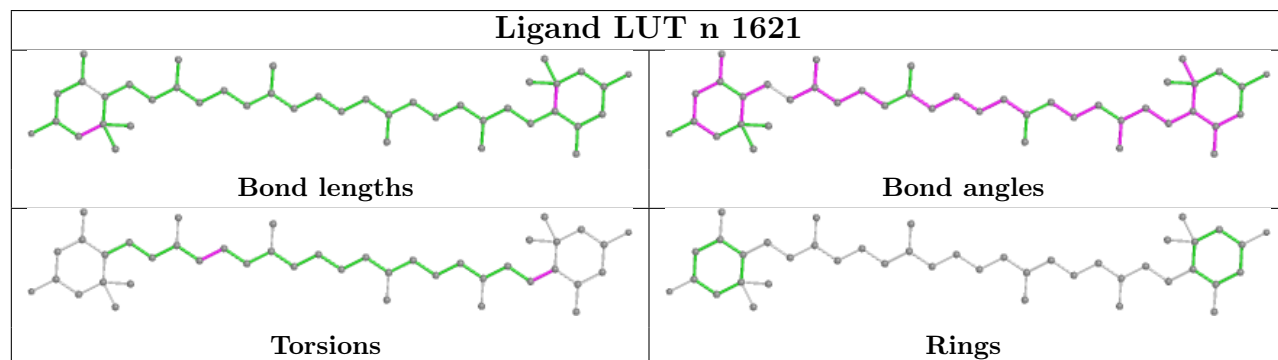
Mol	Chain	Res	Type	Atoms
27	A	405	CLA	CBD-CGD-O2D-CED
27	A	406	CLA	CHA-CBD-CGD-O1D
27	A	406	CLA	CHA-CBD-CGD-O2D
27	A	407	CLA	CBD-CGD-O2D-CED
27	B	602	CLA	C1A-C2A-CAA-CBA

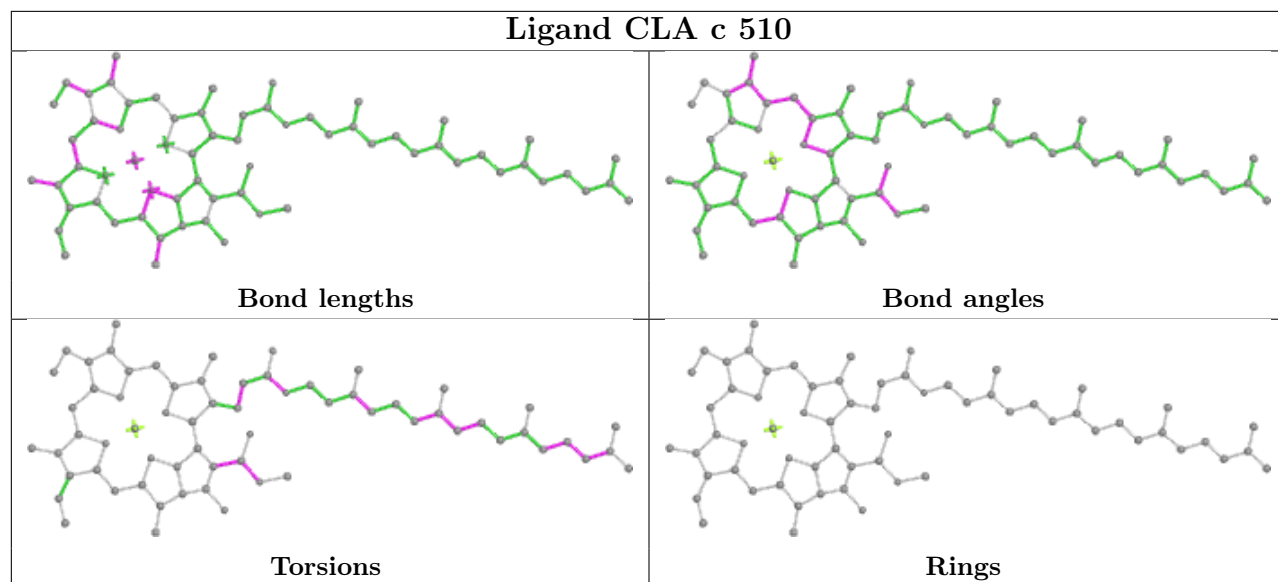
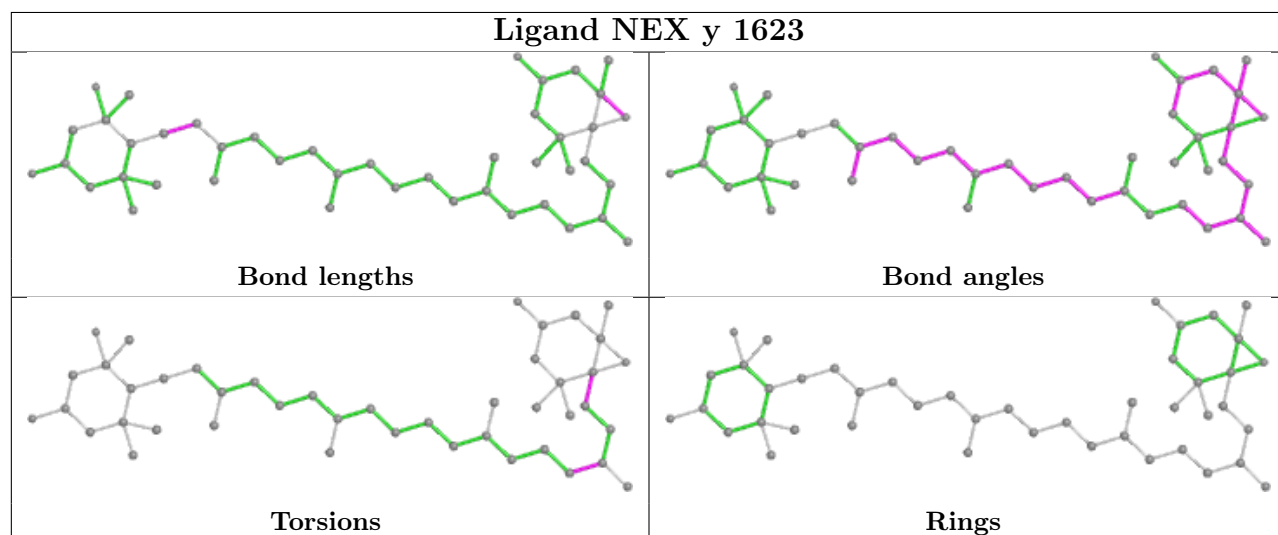
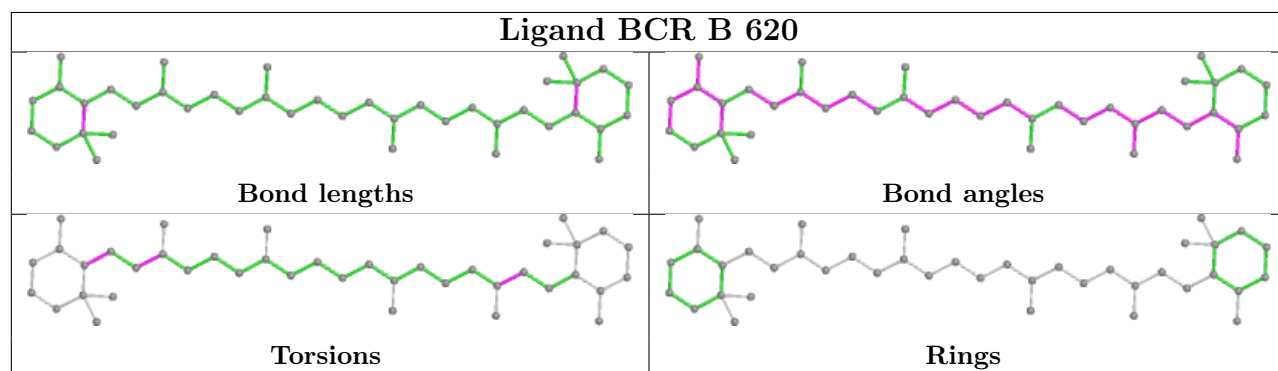
There are no ring outliers.

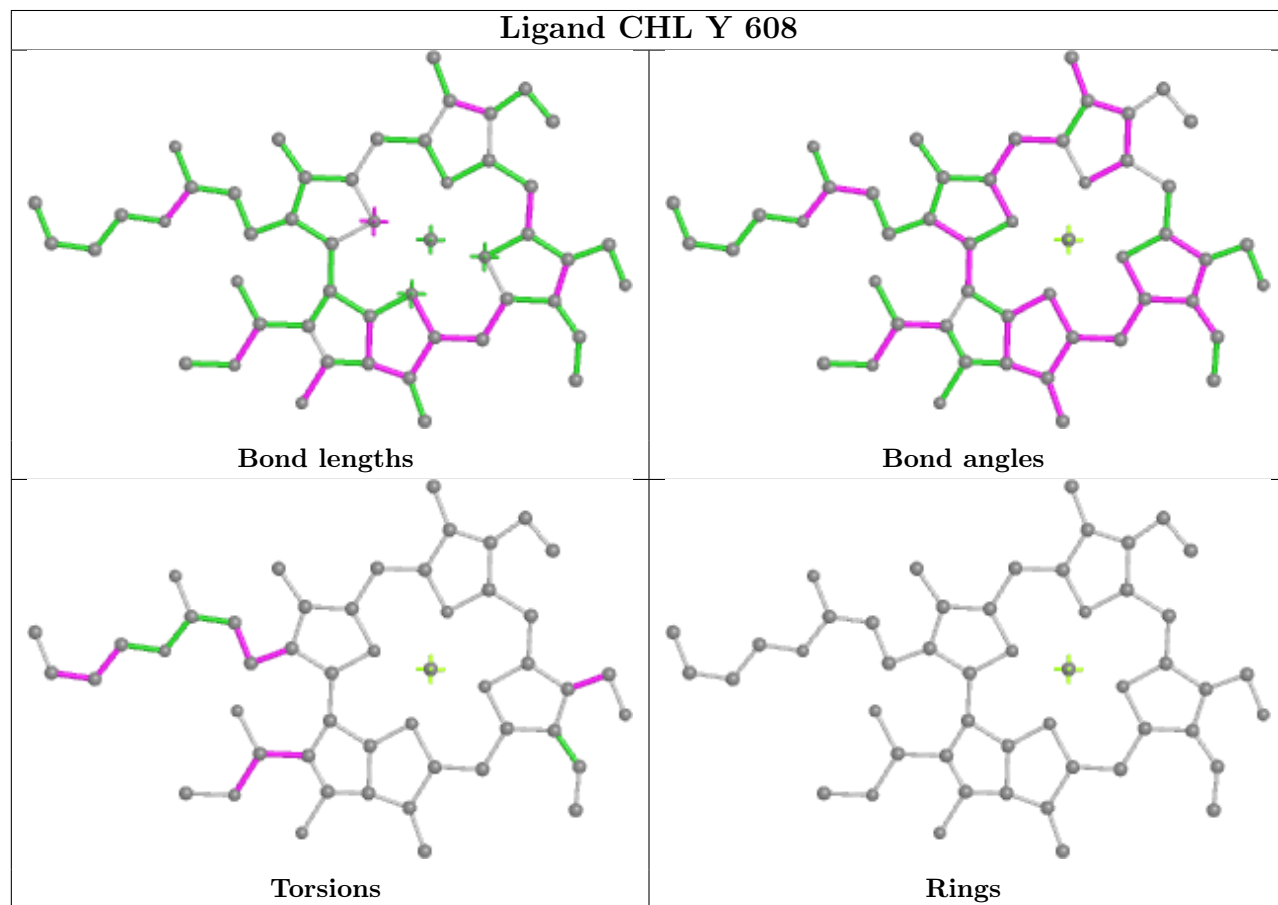
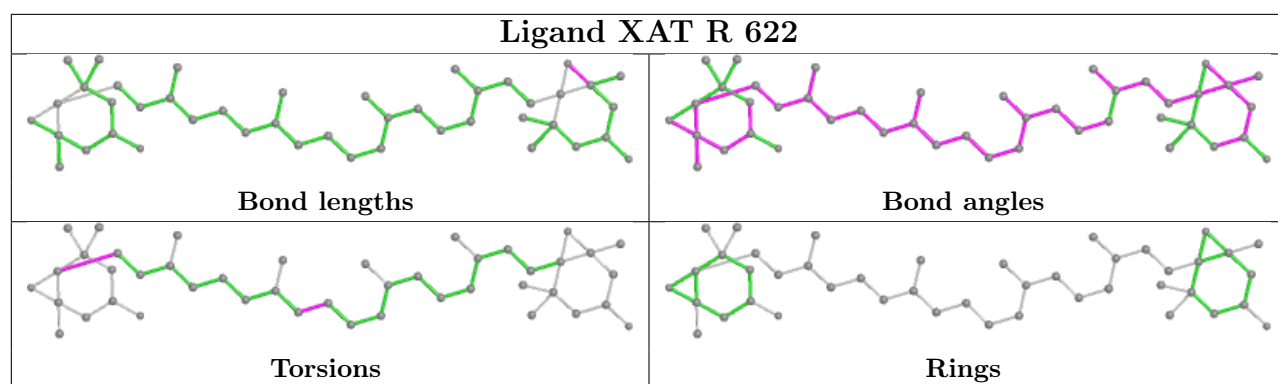
No monomer is involved in short contacts.

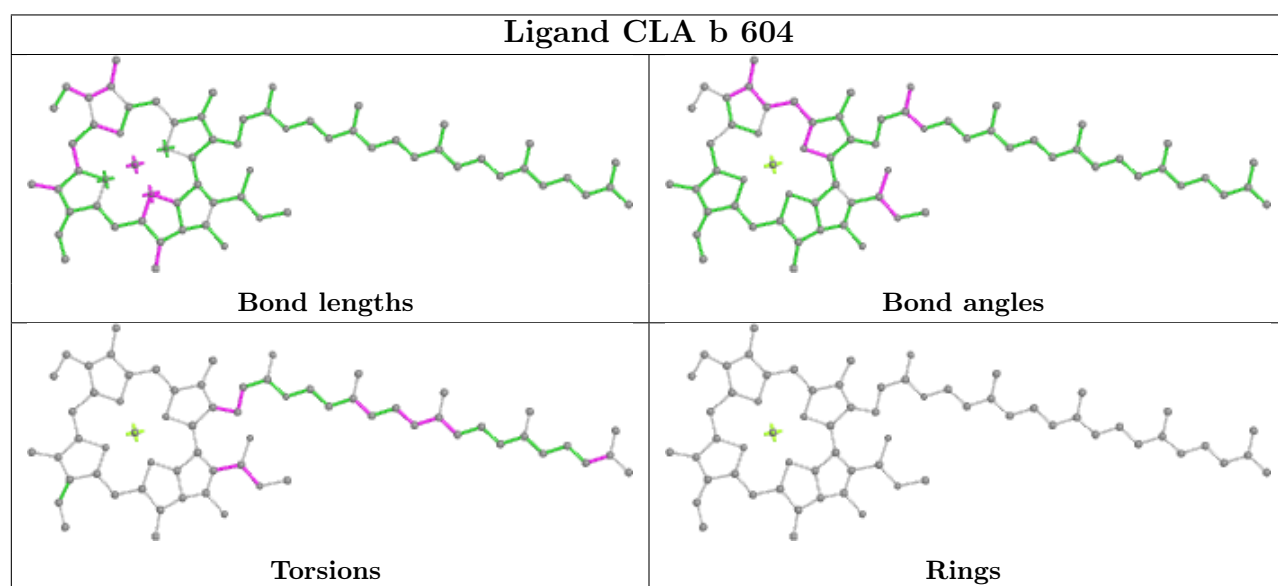
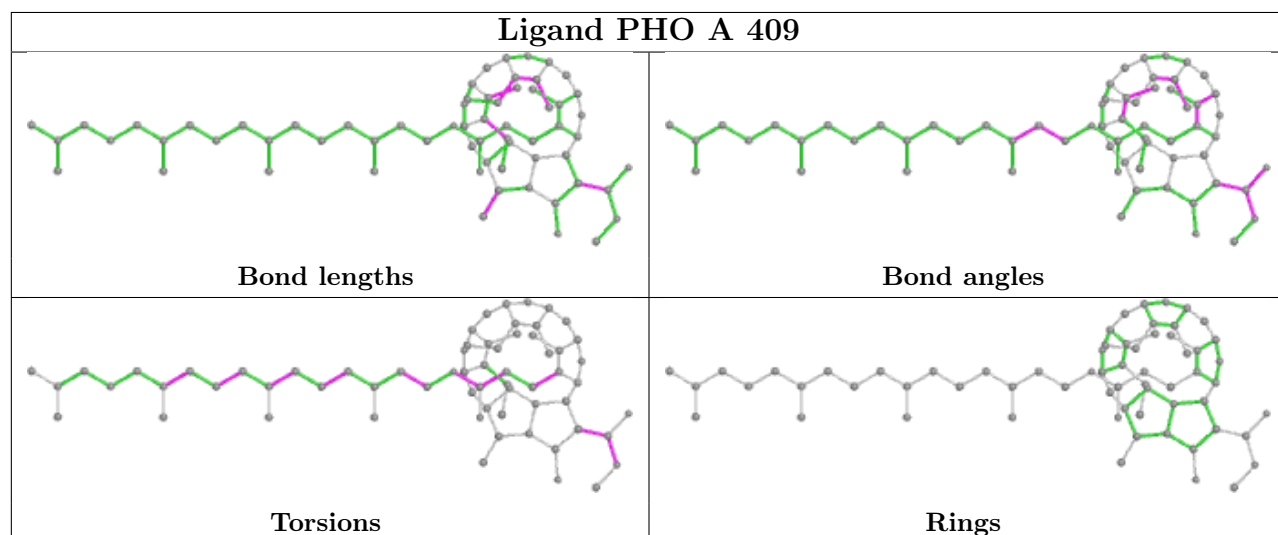
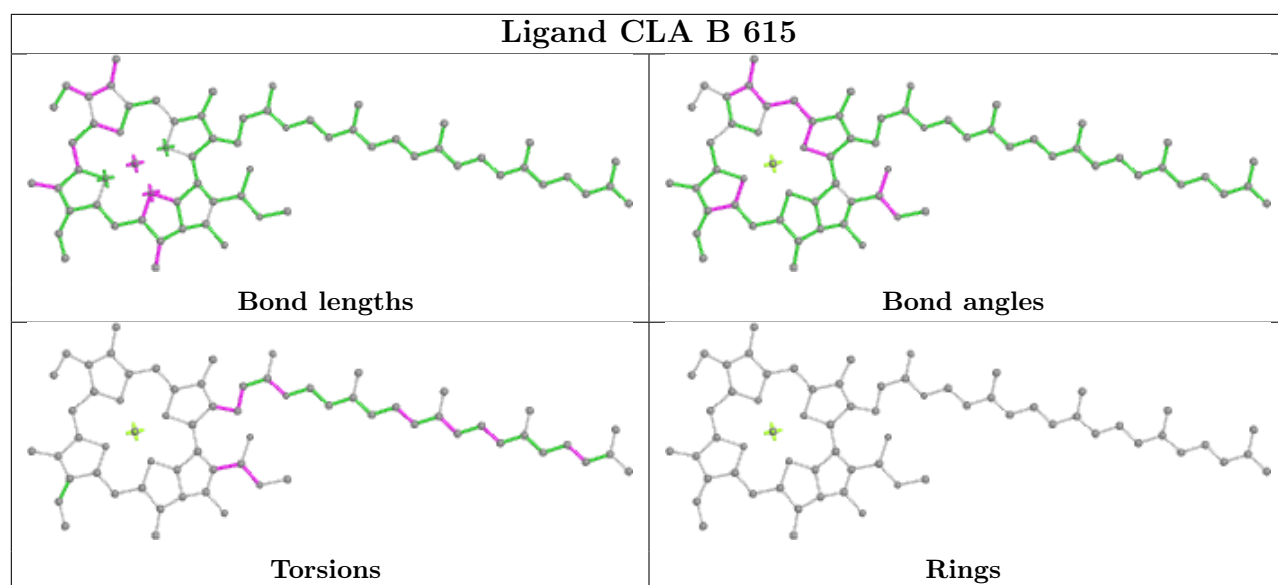
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



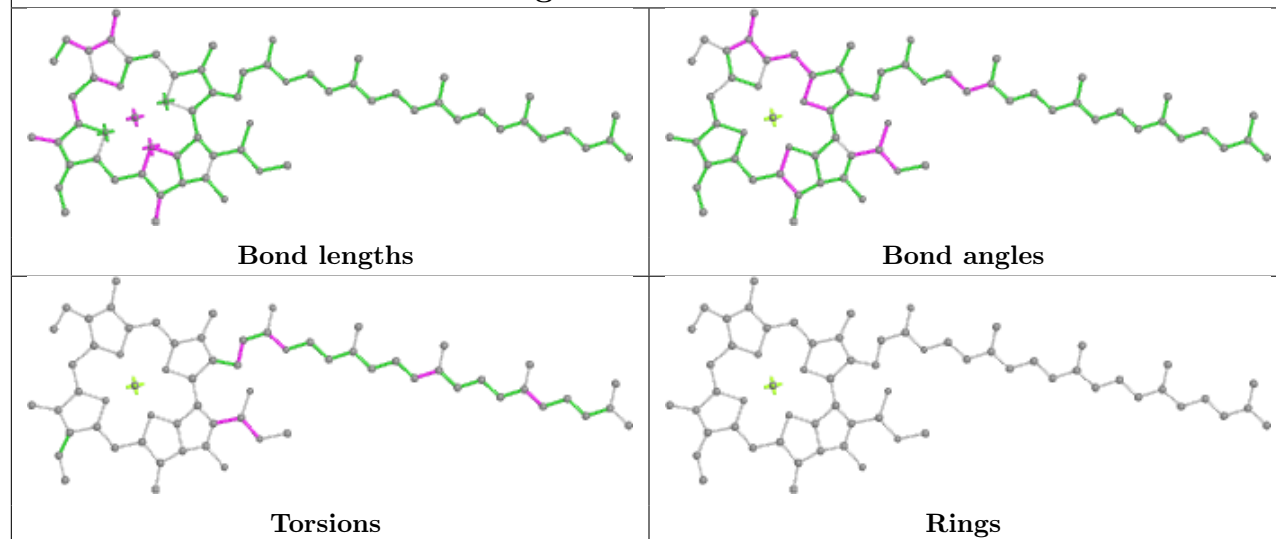
**Ligand CLA c 508****Ligand CLA b 610****Ligand LUT n 1621**

**Ligand CLA c 510****Ligand NEX y 1623****Ligand BCR B 620**

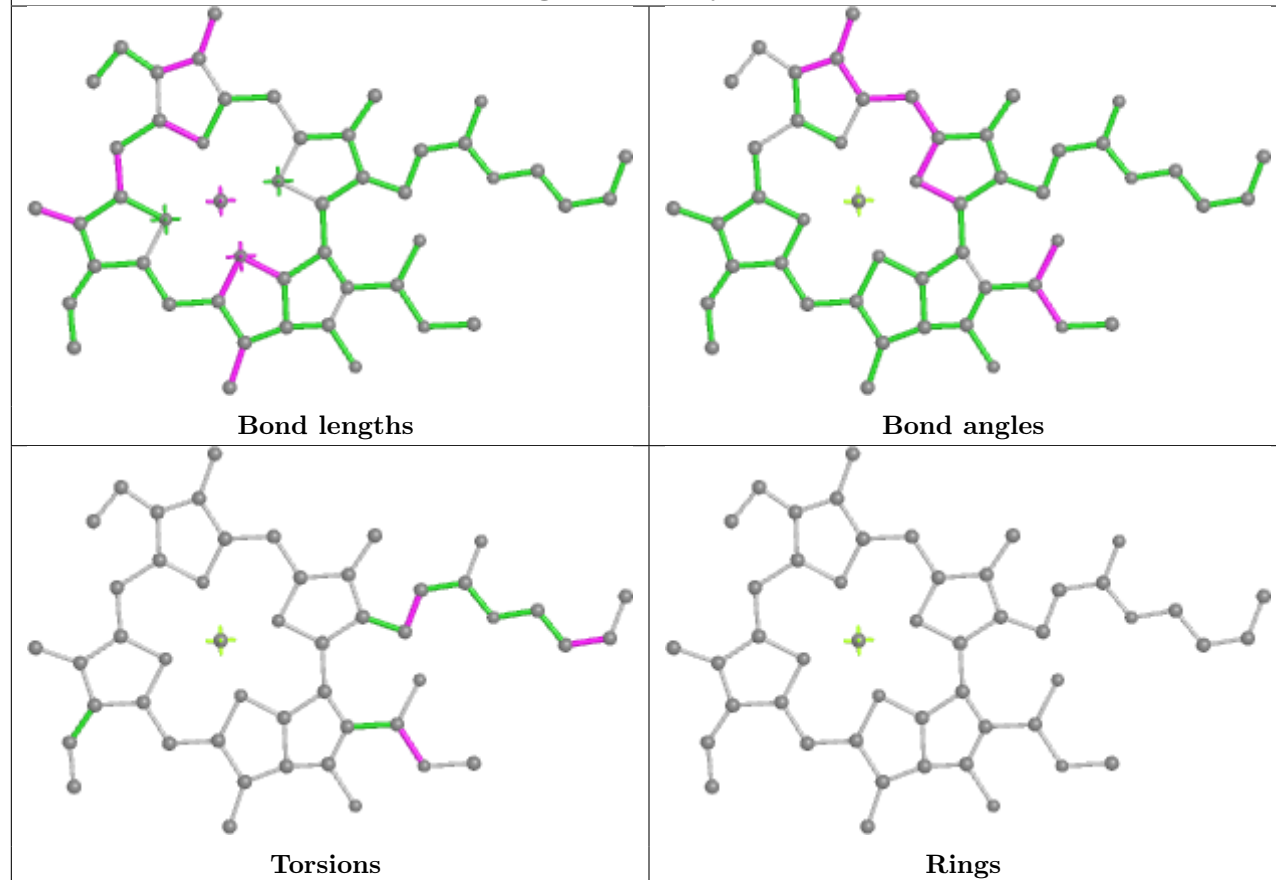




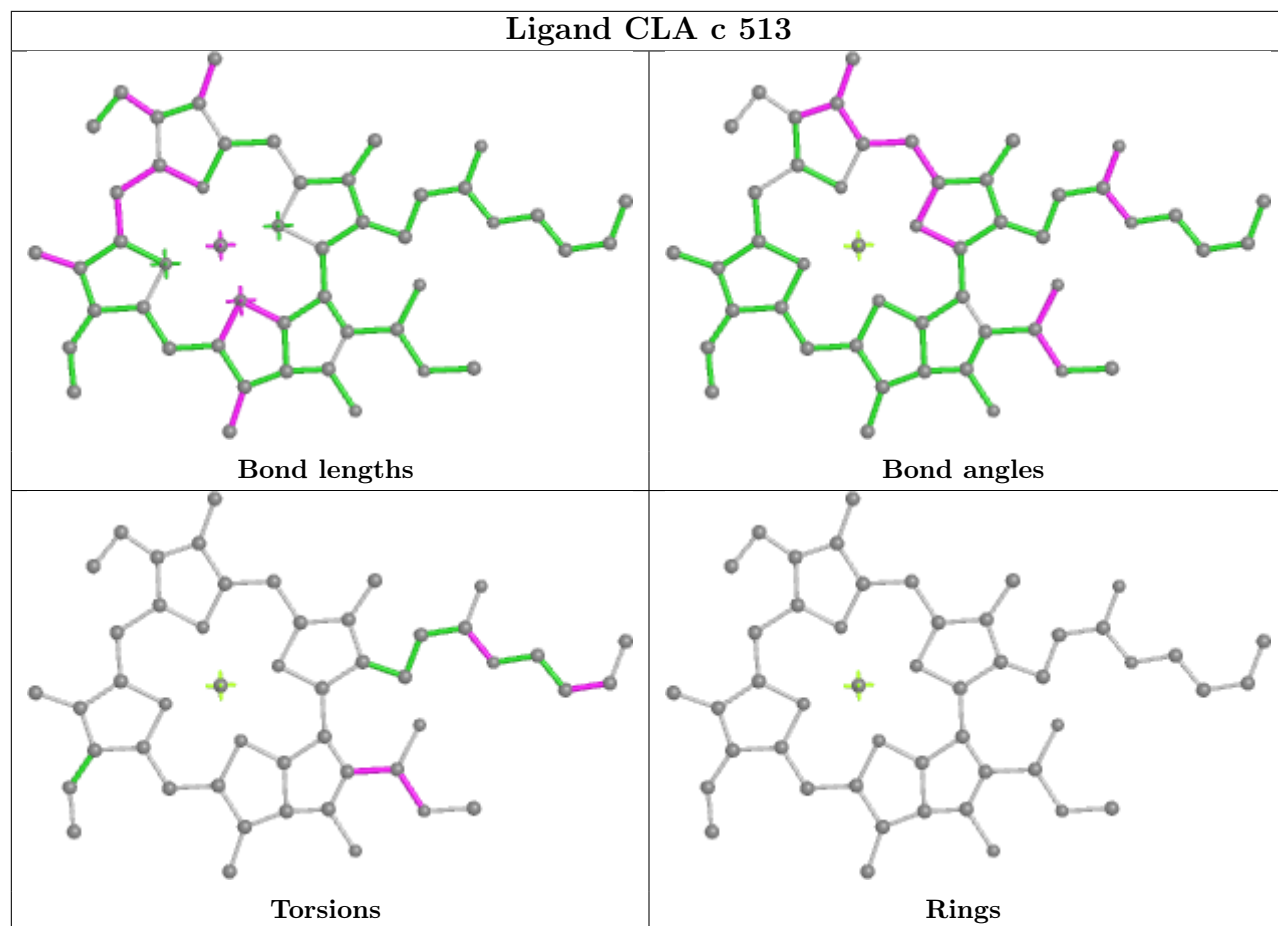
## Ligand CLA b 608



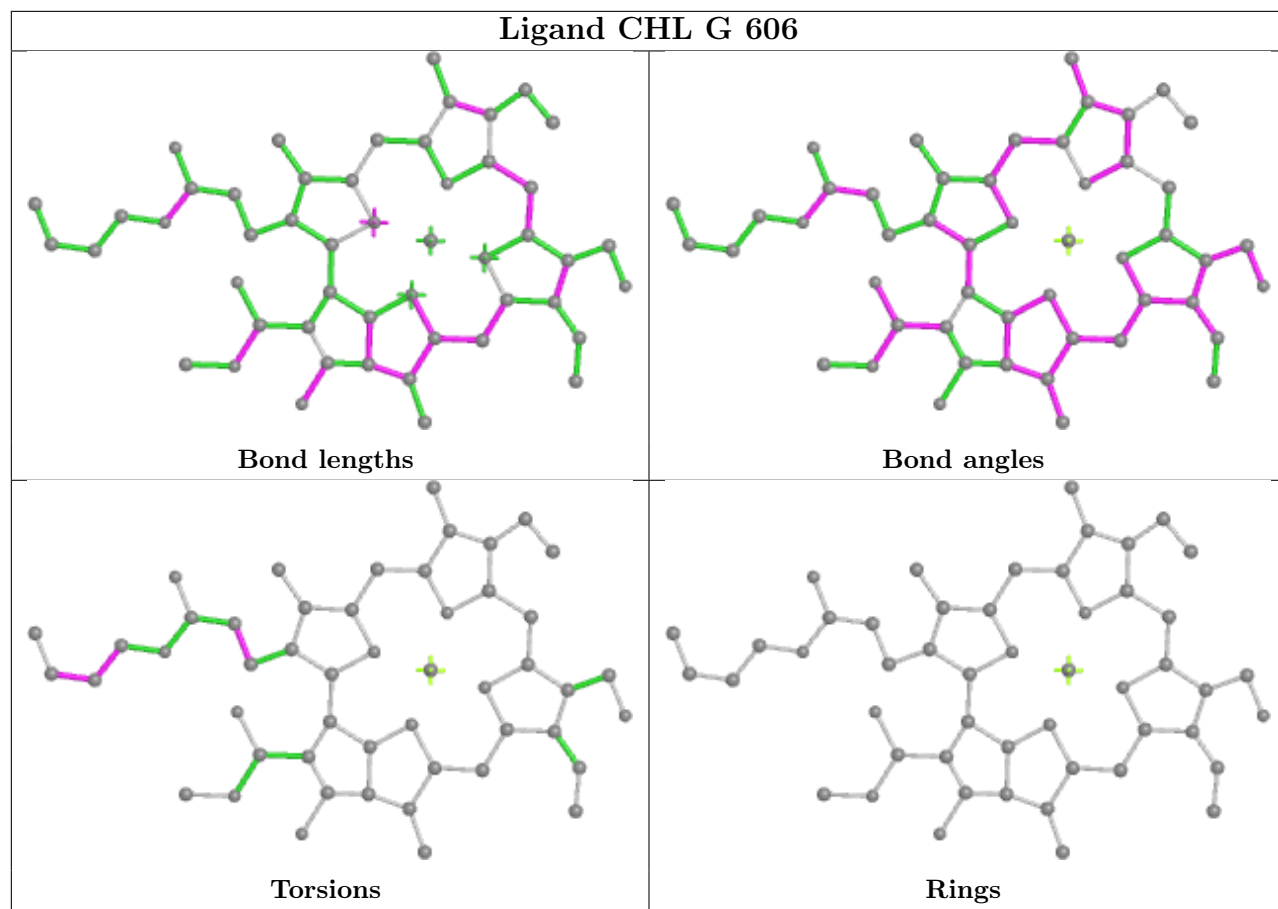
## Ligand CLA y 603



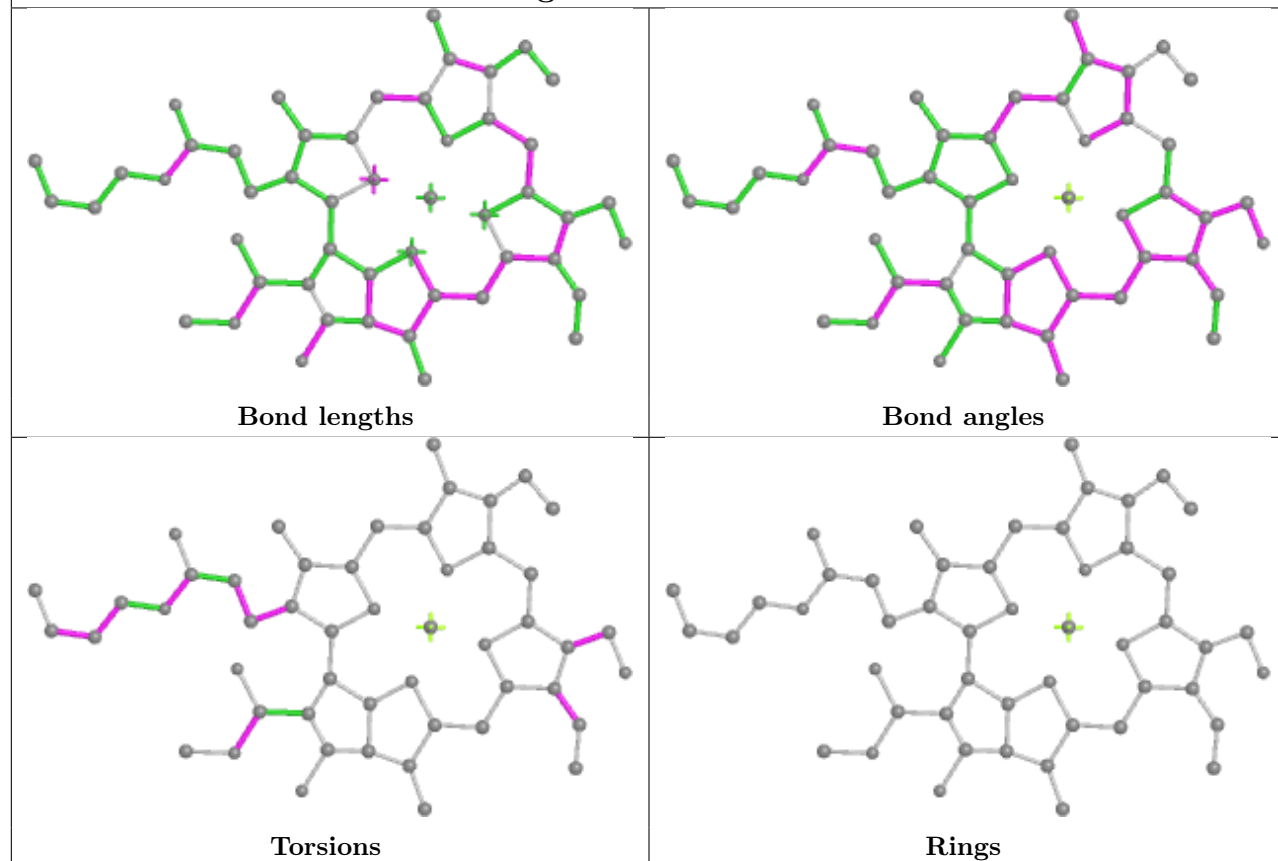
## Ligand CLA c 513



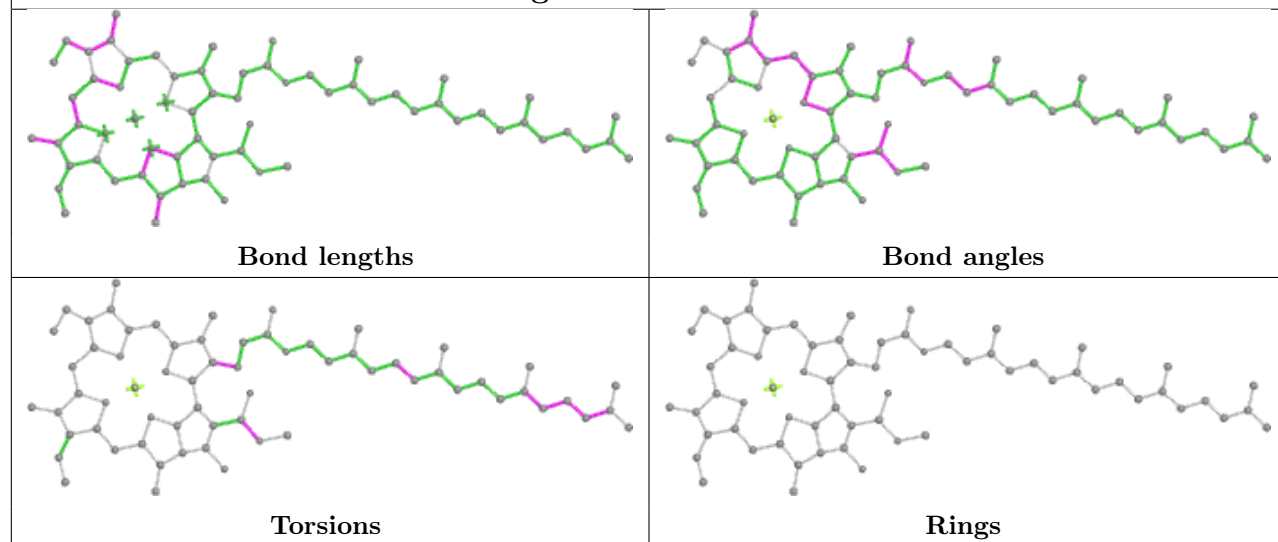


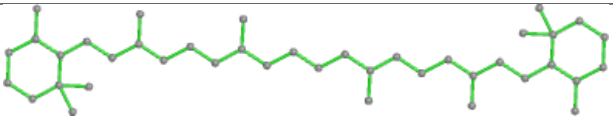
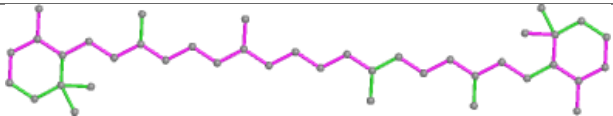
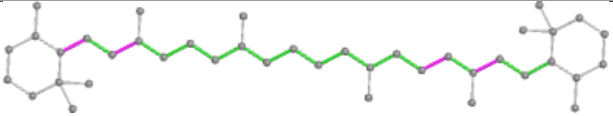
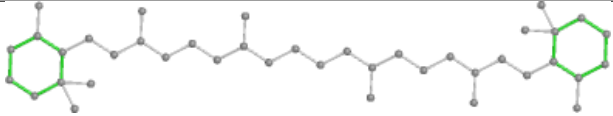


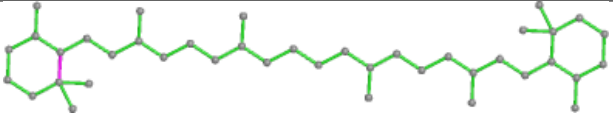
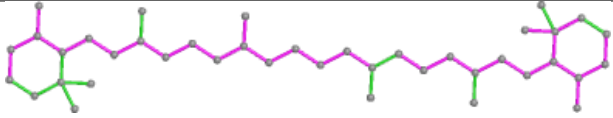
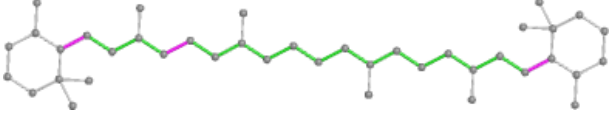
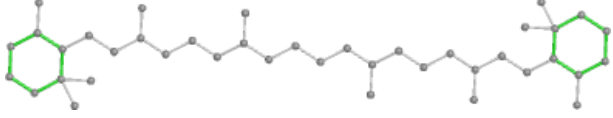
## Ligand CHL r 608

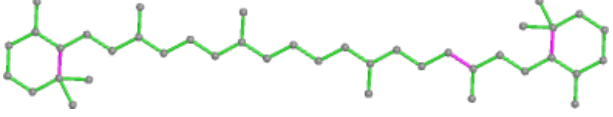
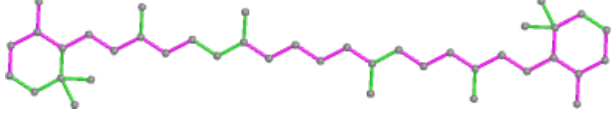
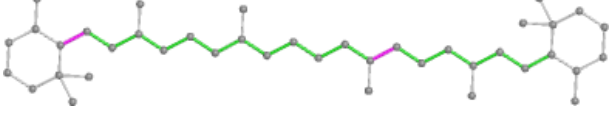
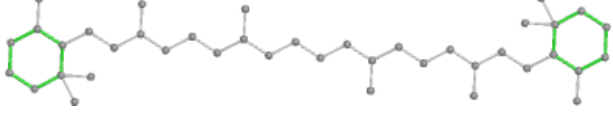


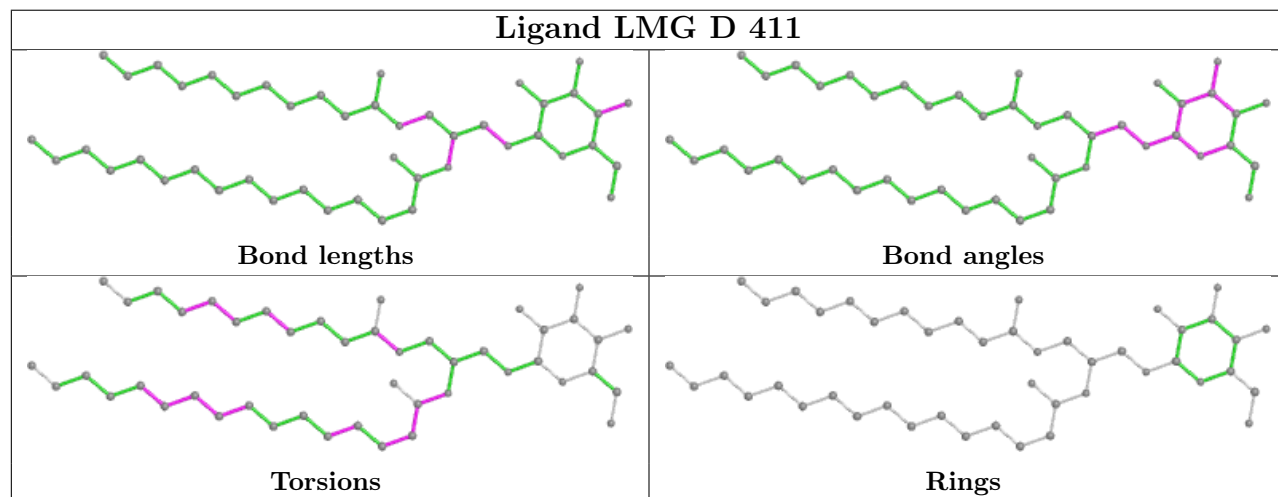
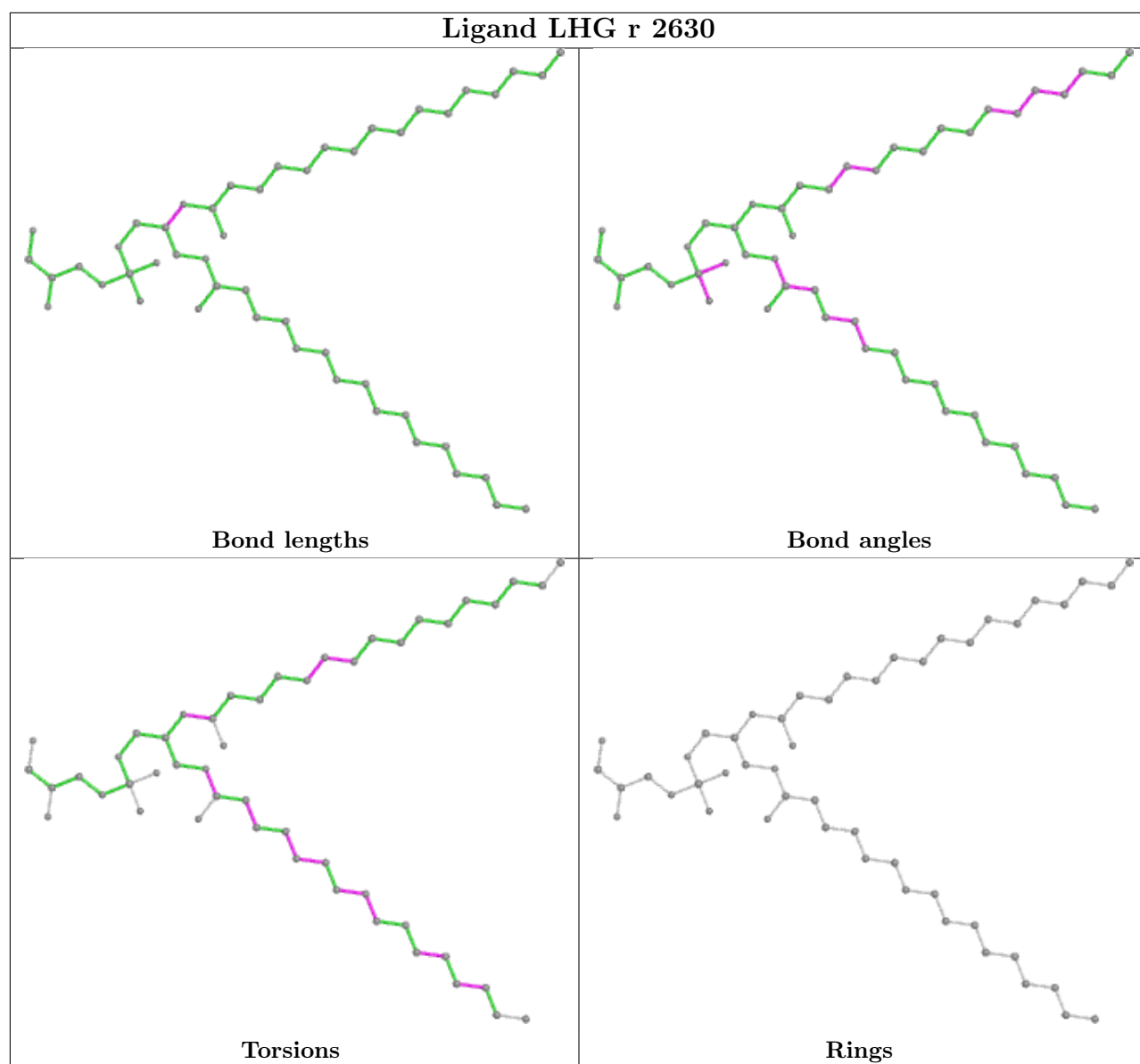
## Ligand CLA N 610

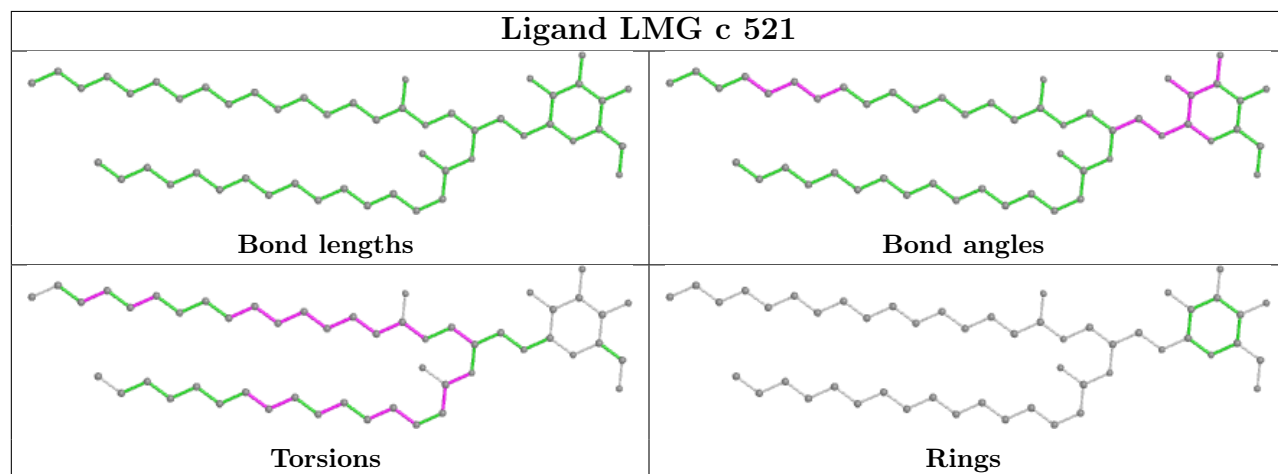
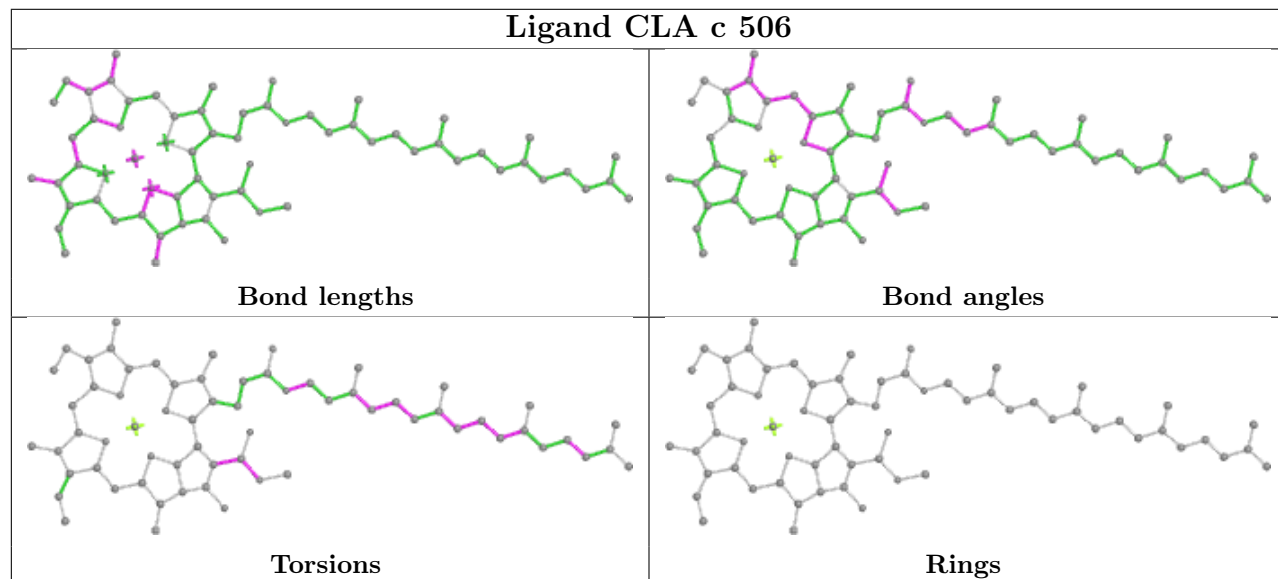
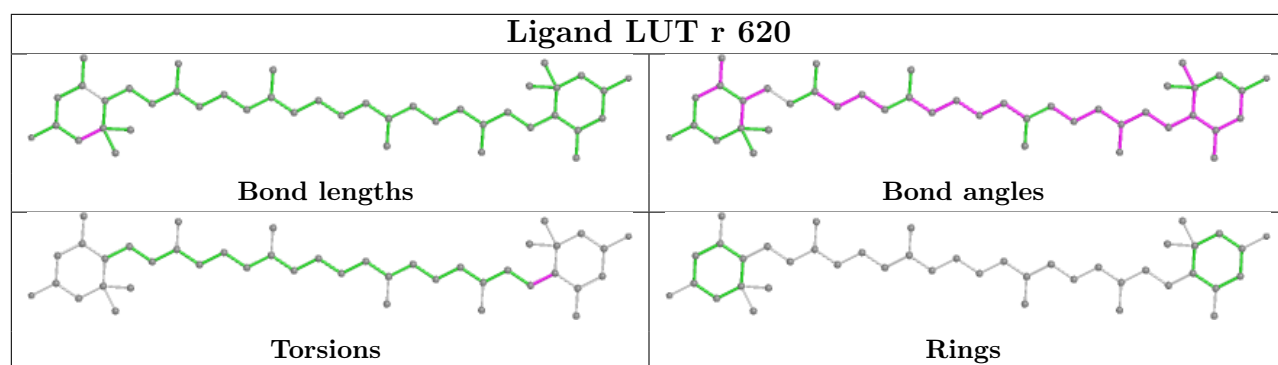


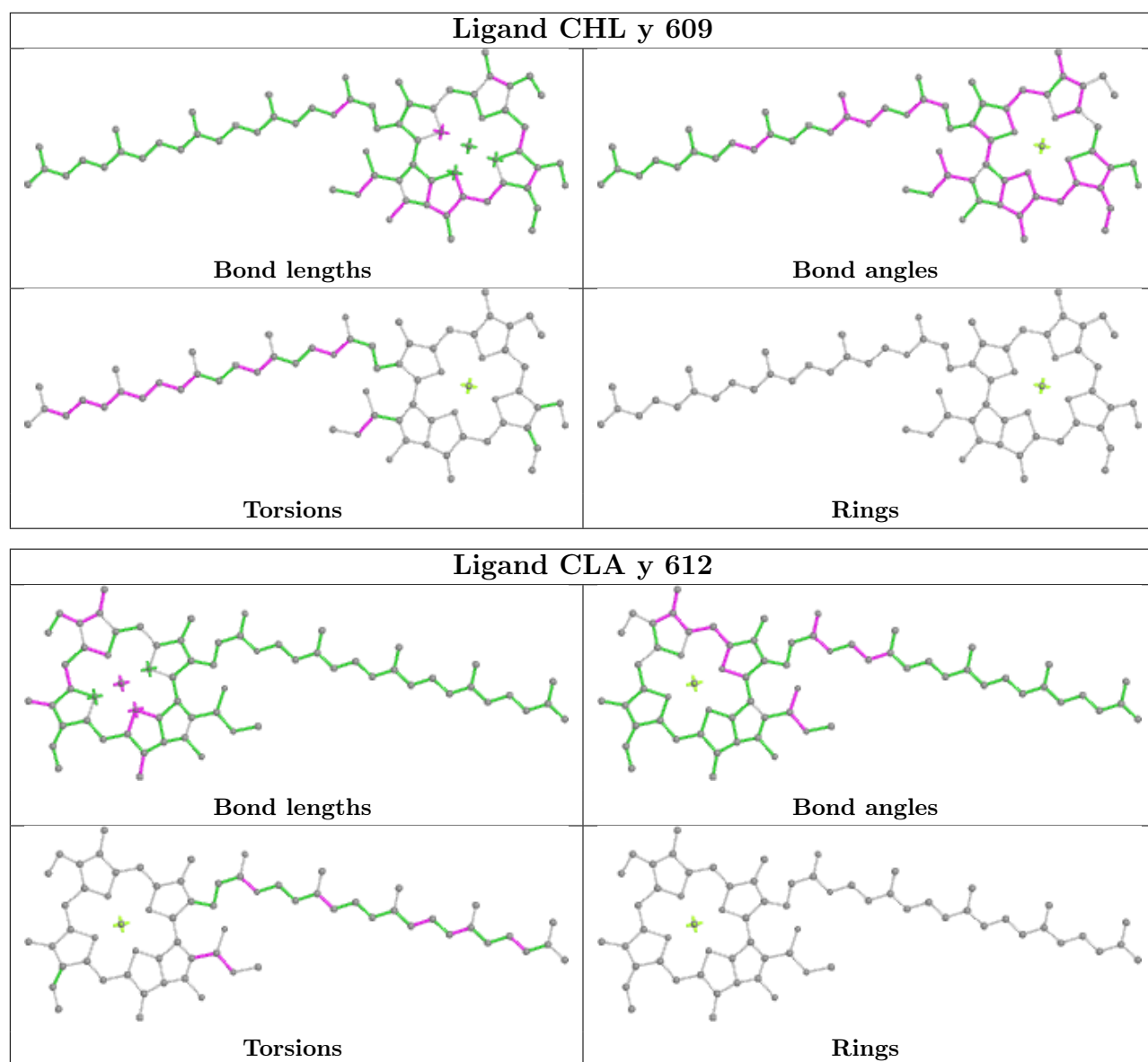
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

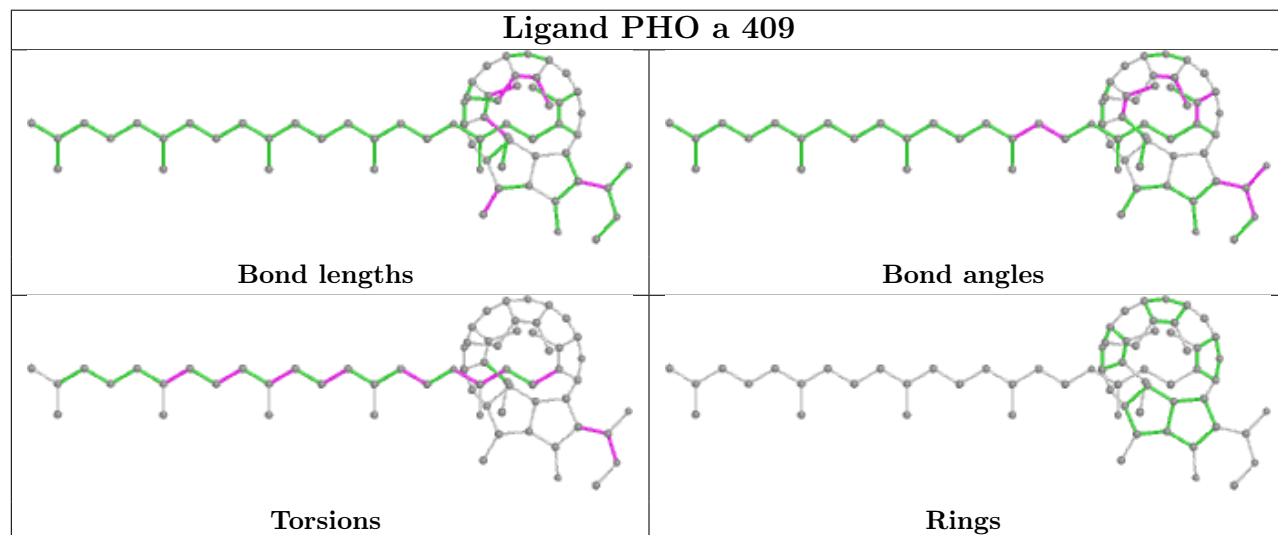
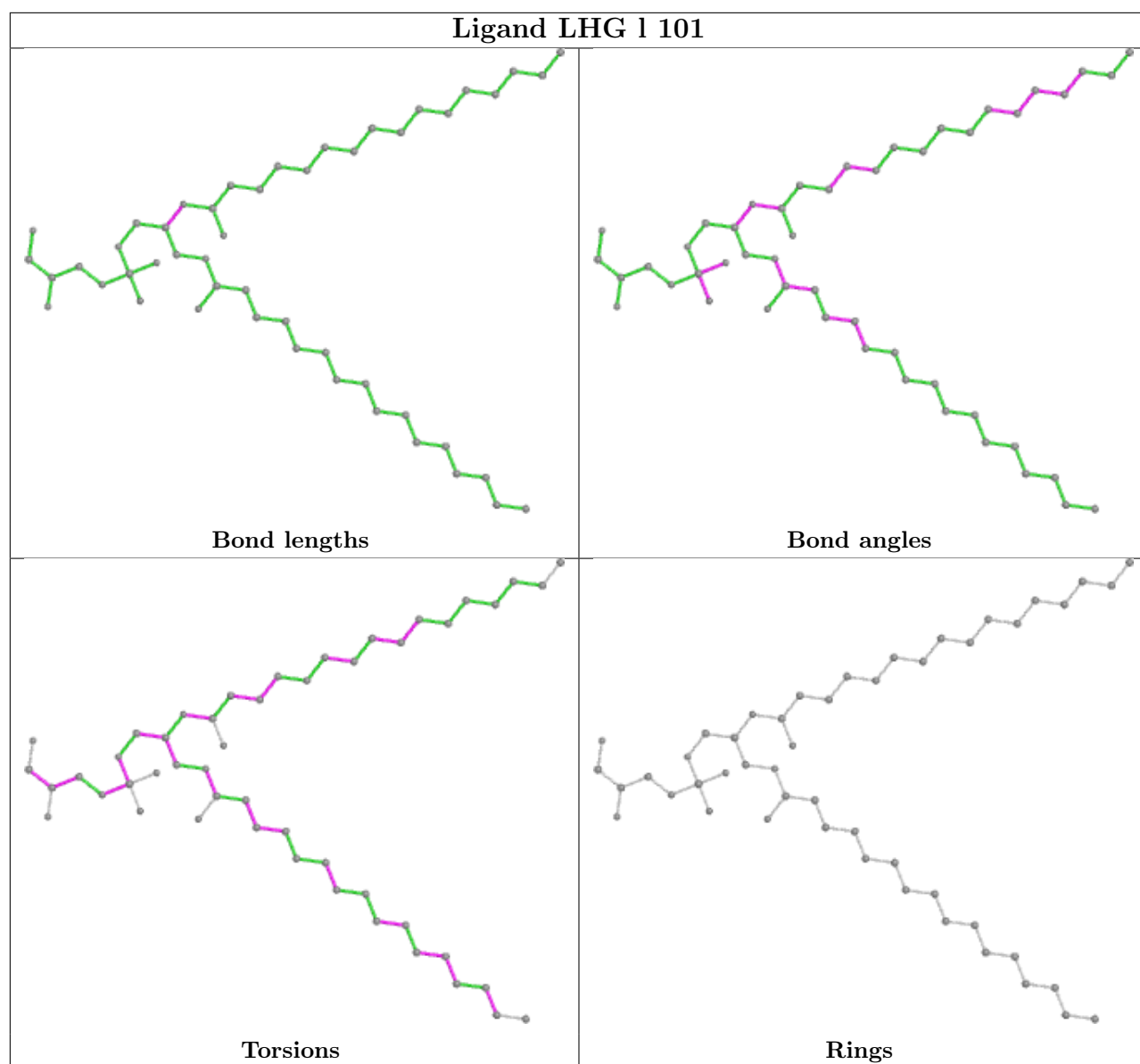
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

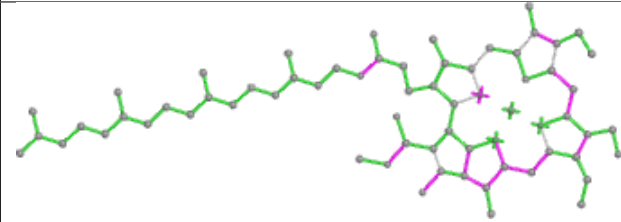
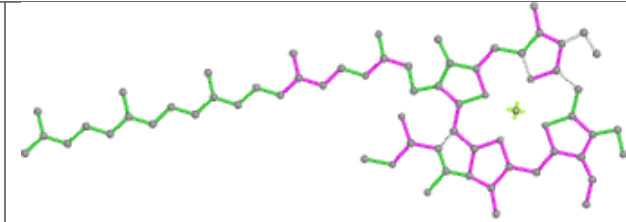
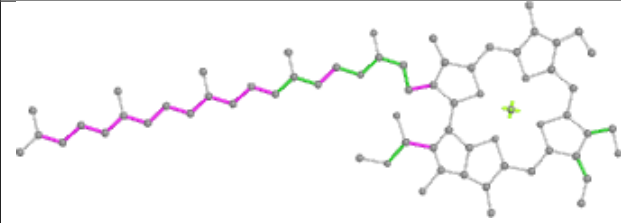
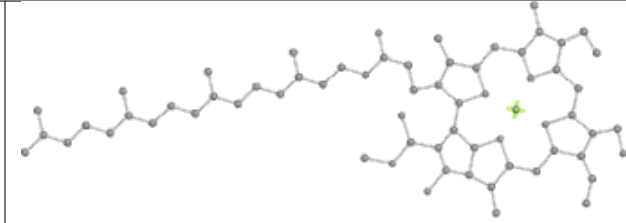
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

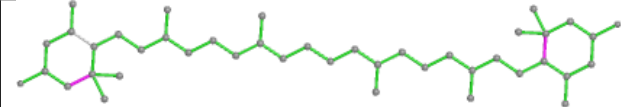
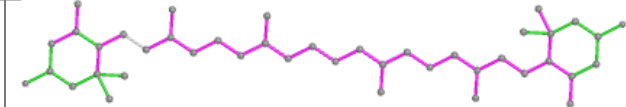
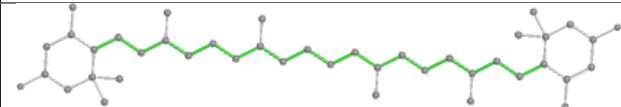
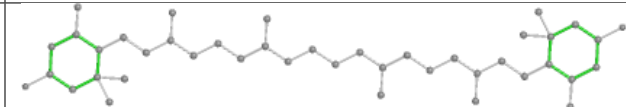






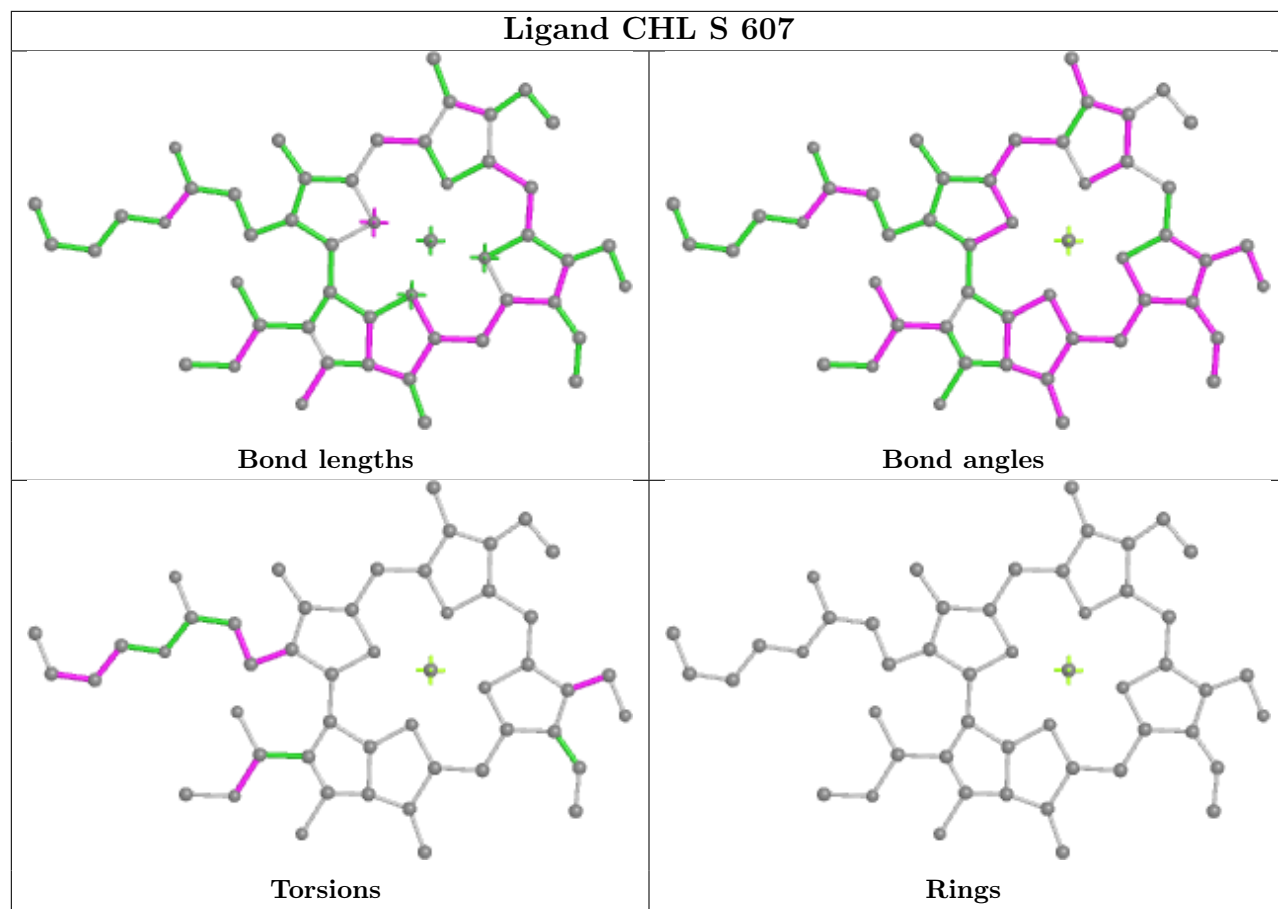


Ligand CHL G 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

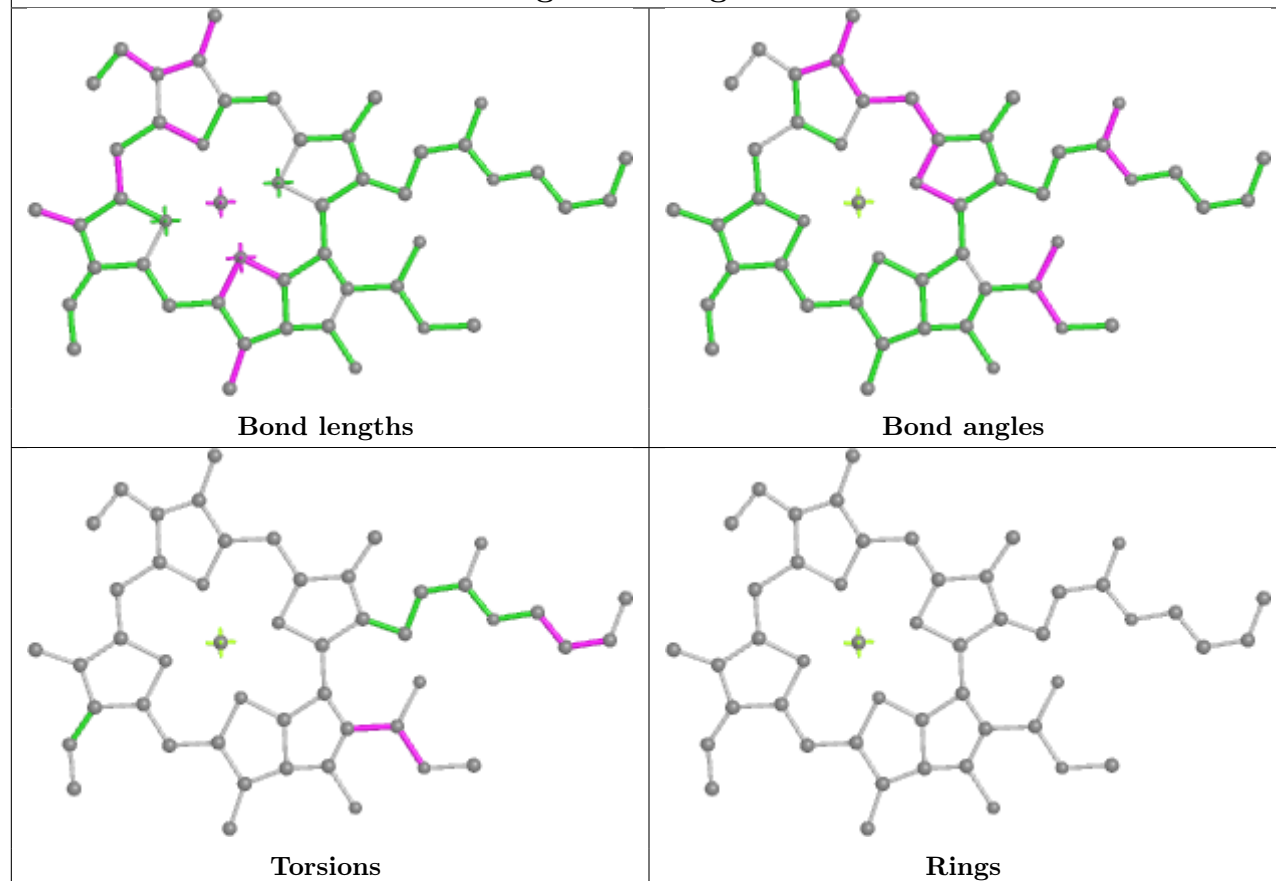
Ligand LUT Y 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings



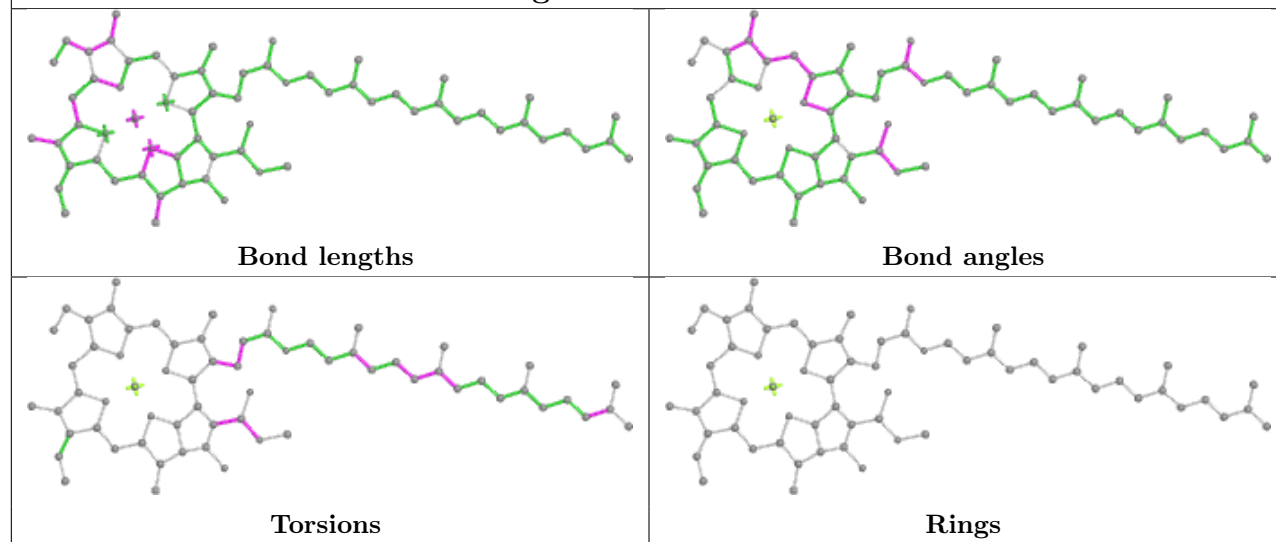
## Ligand CHL S 607

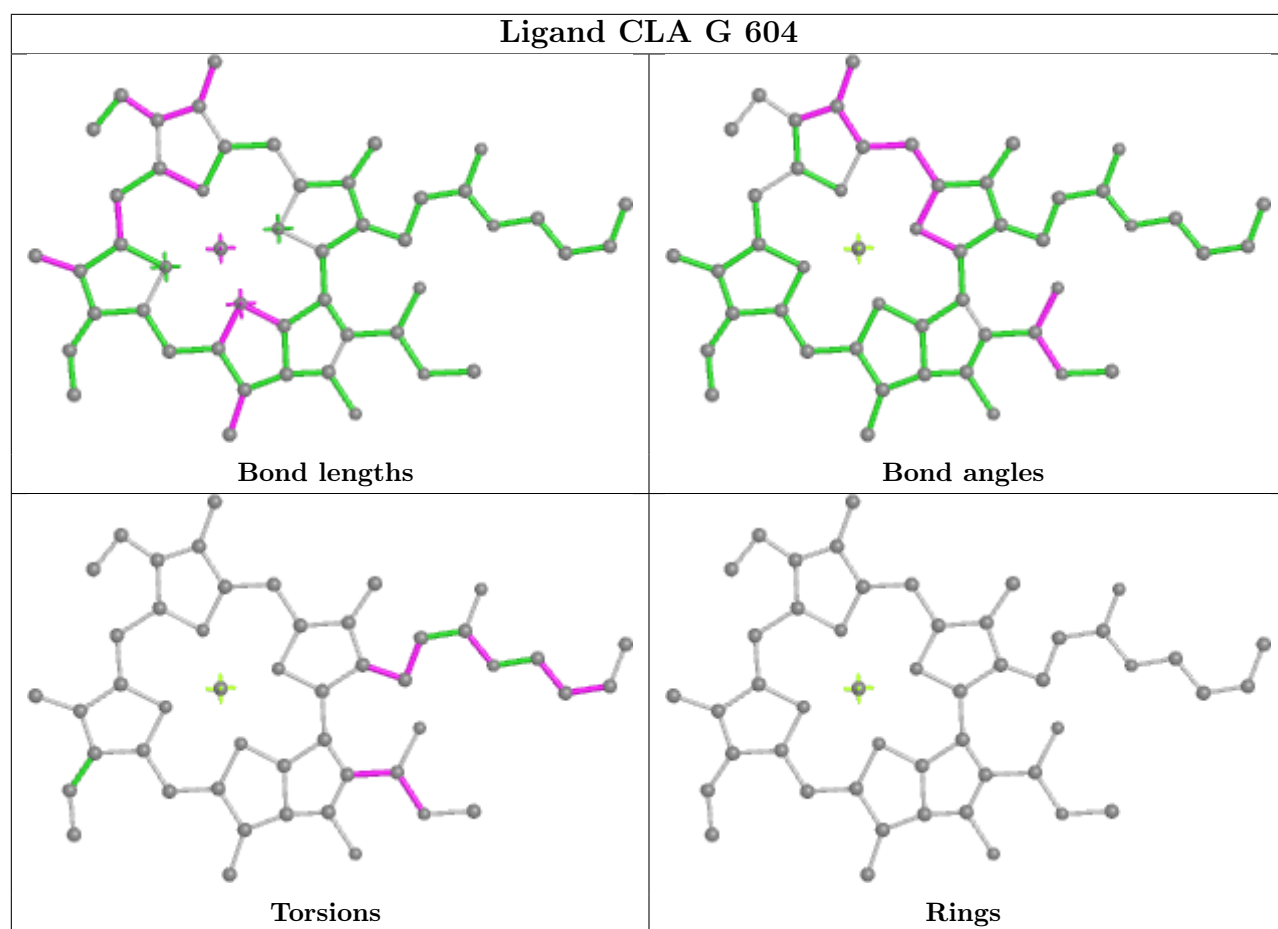


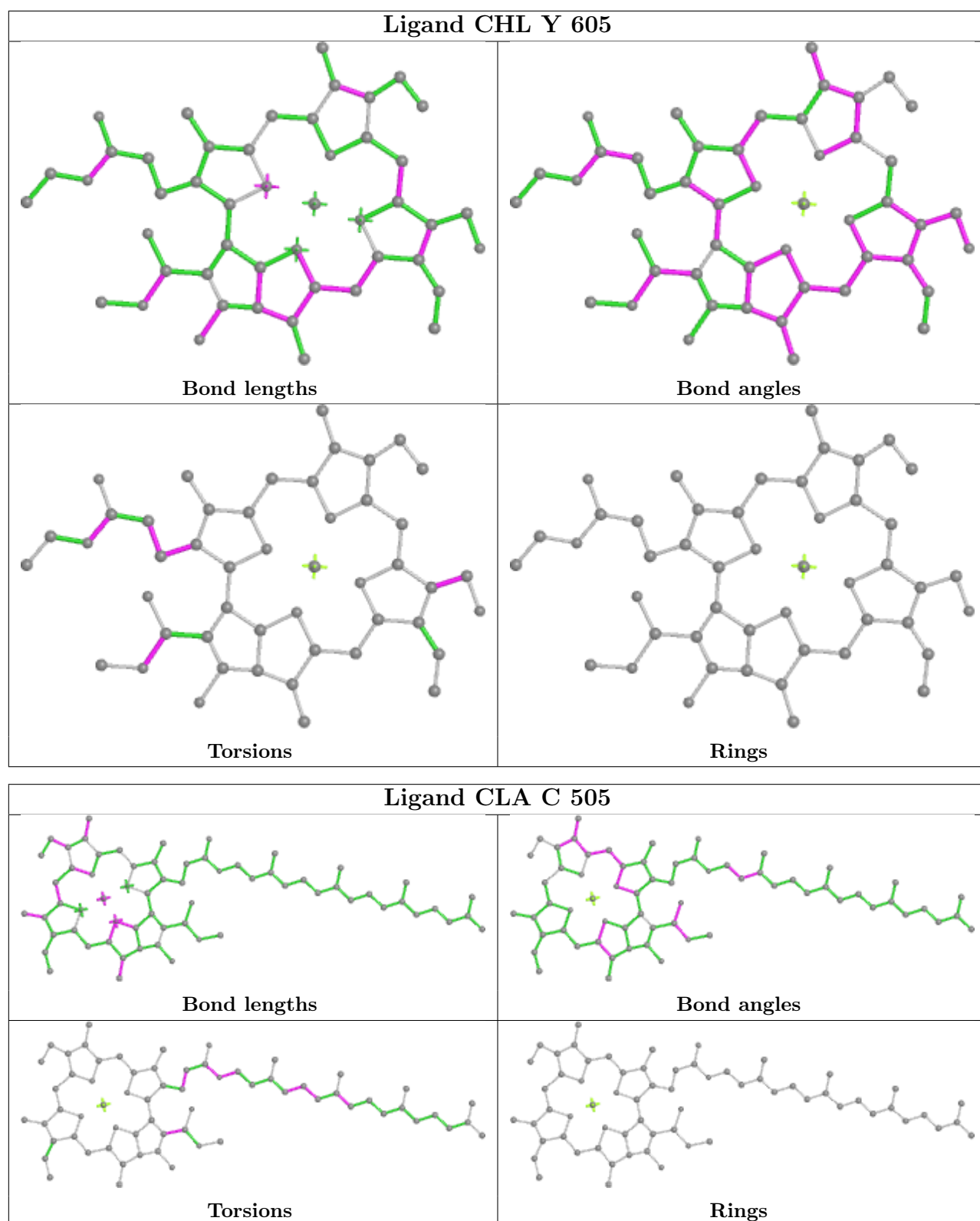
## Ligand CLA g 612

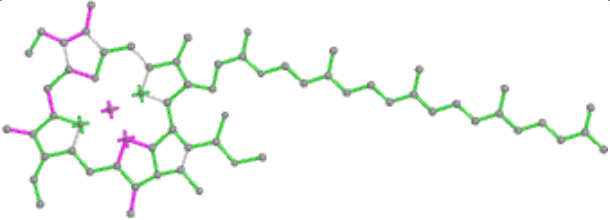
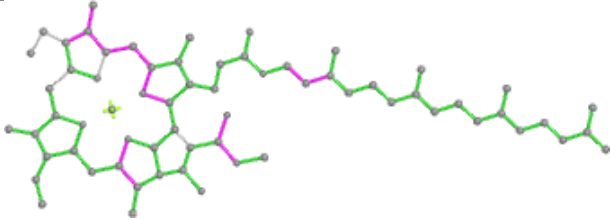
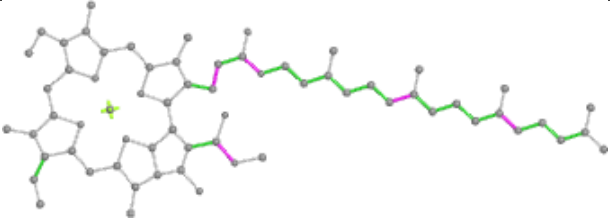
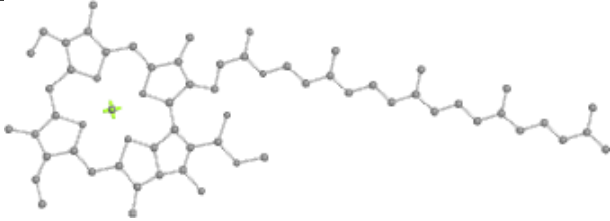
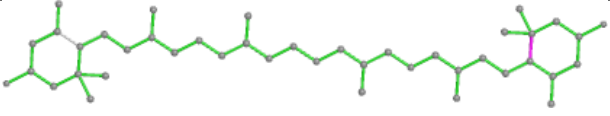
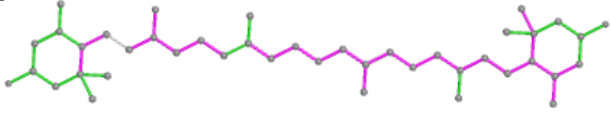
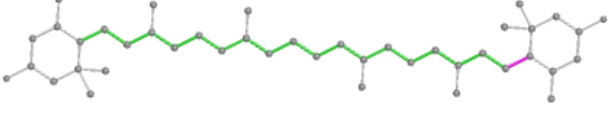
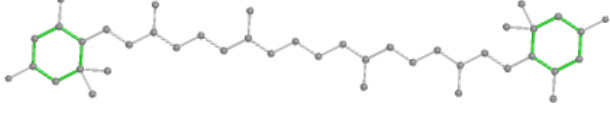
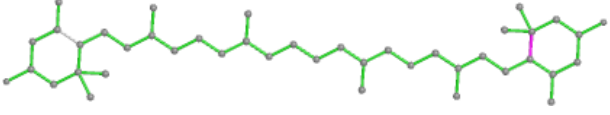
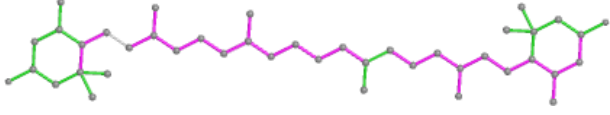
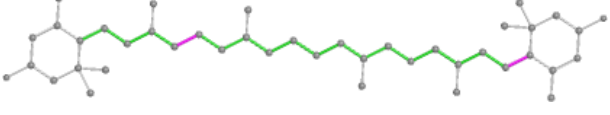
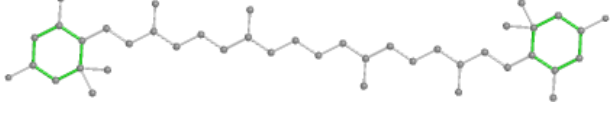


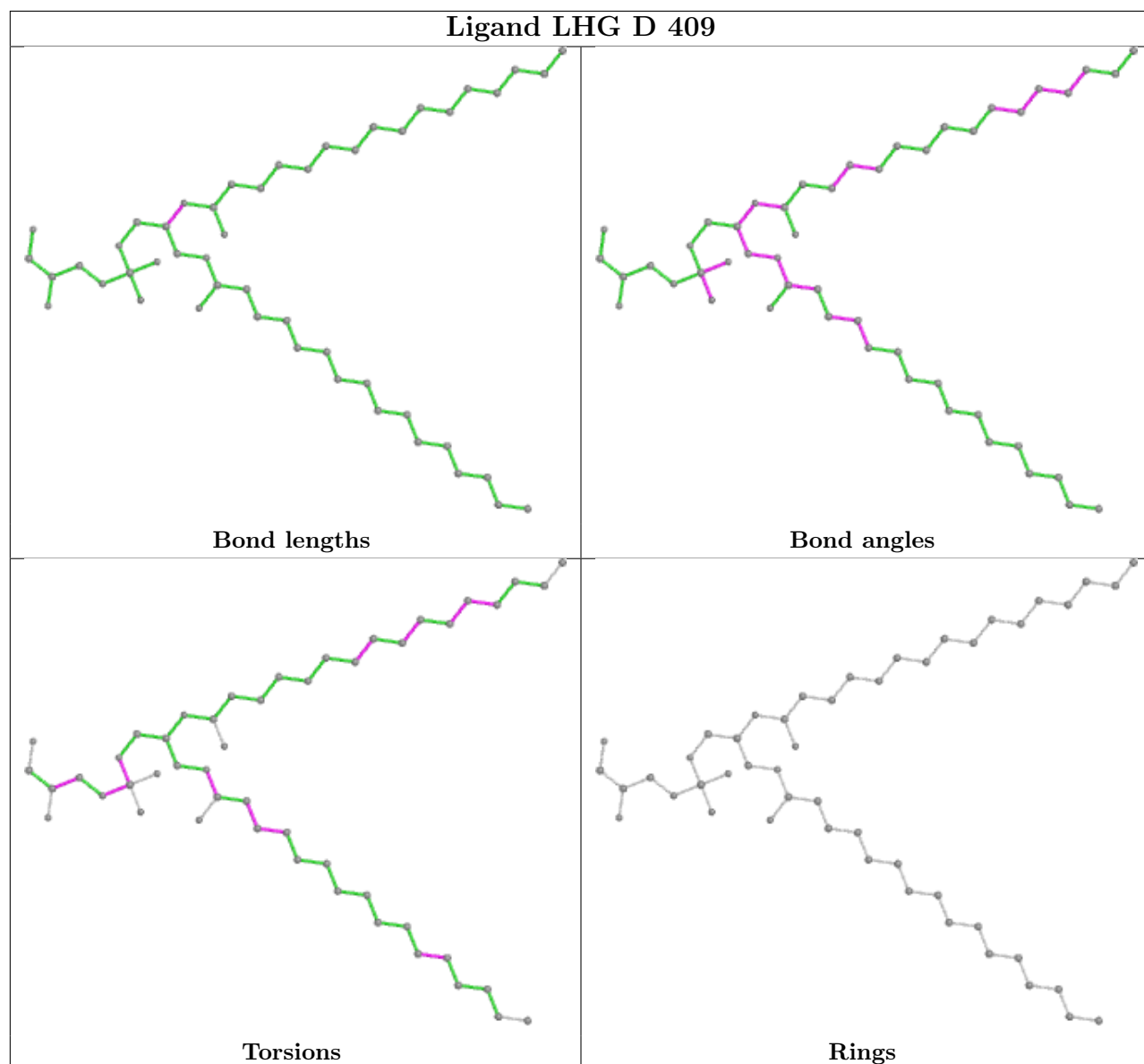
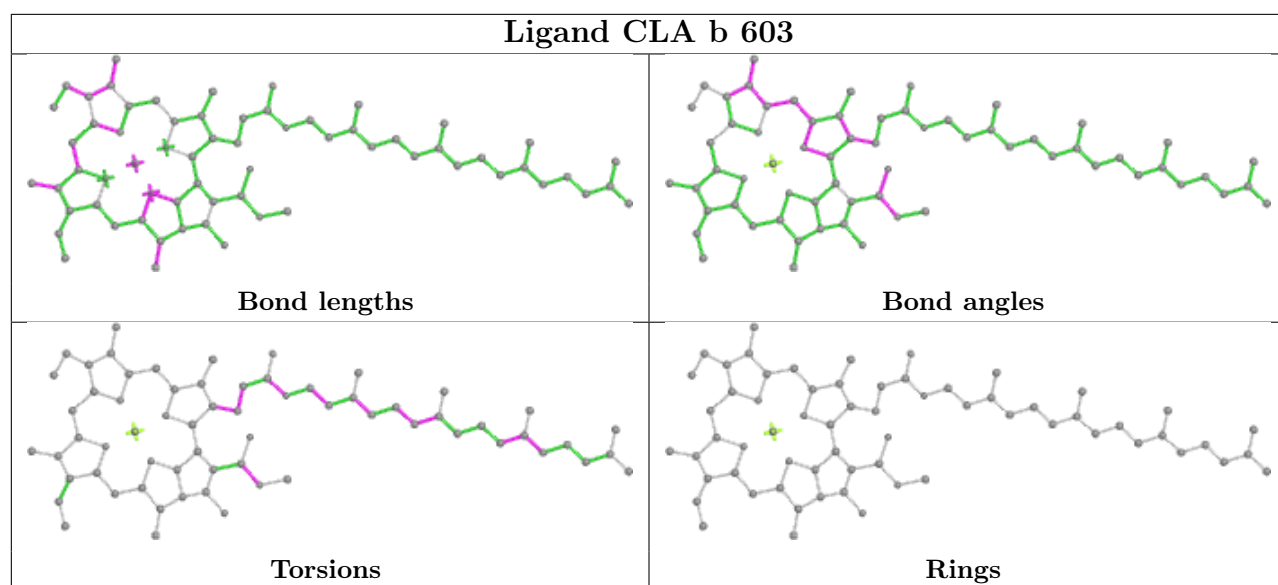
## Ligand CLA B 604



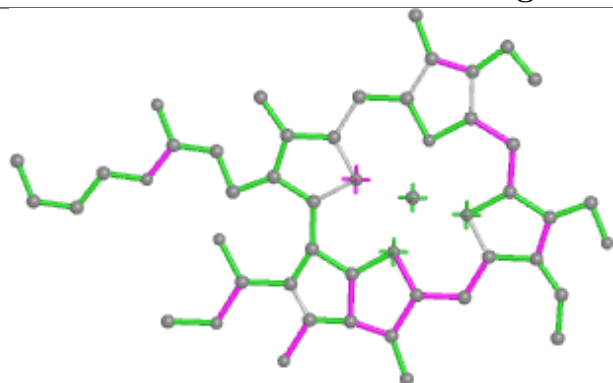




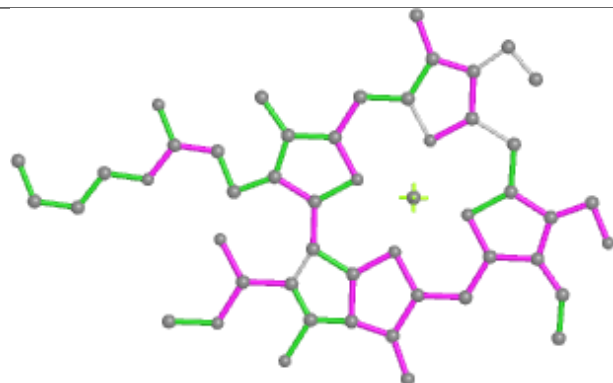
Ligand CLA B 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT g 1620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S 1621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



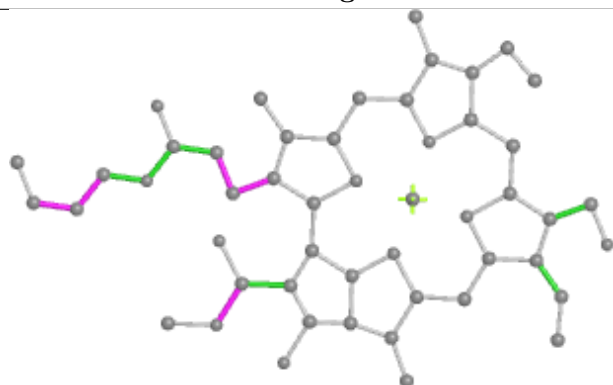
## Ligand CHL n 608



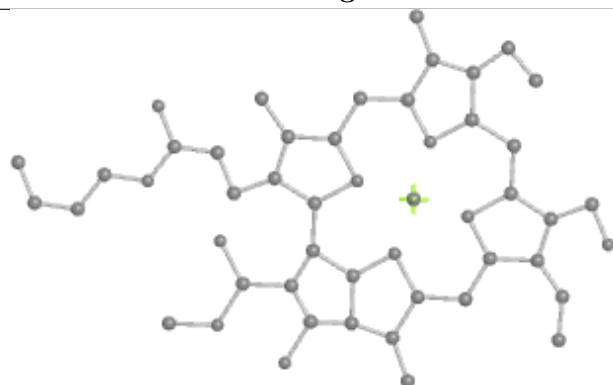
Bond lengths



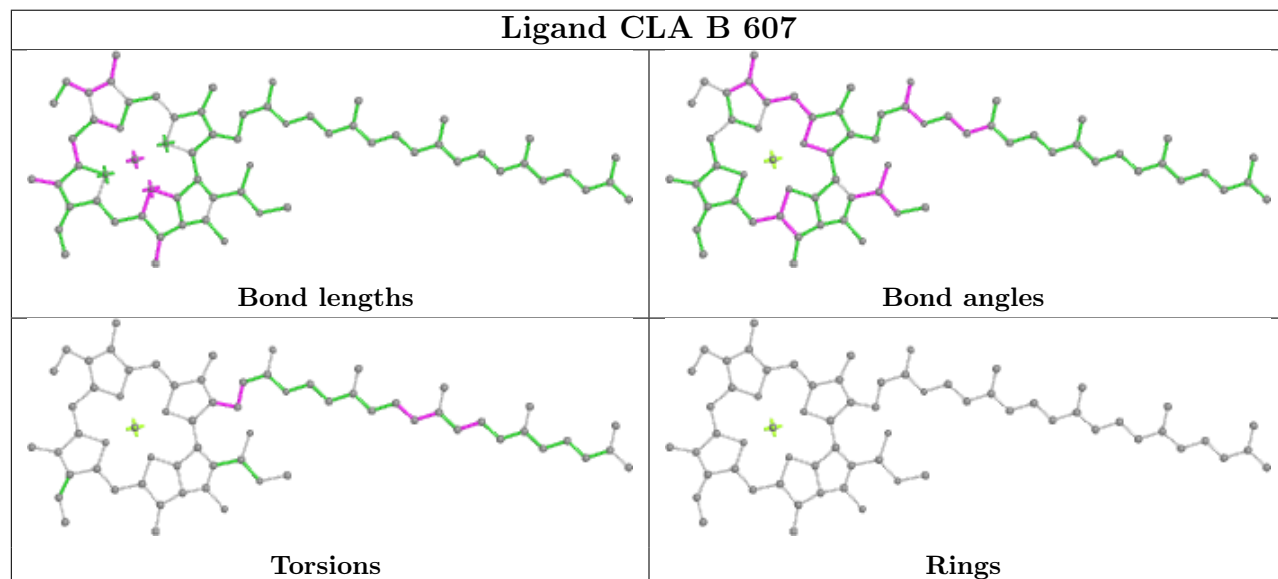
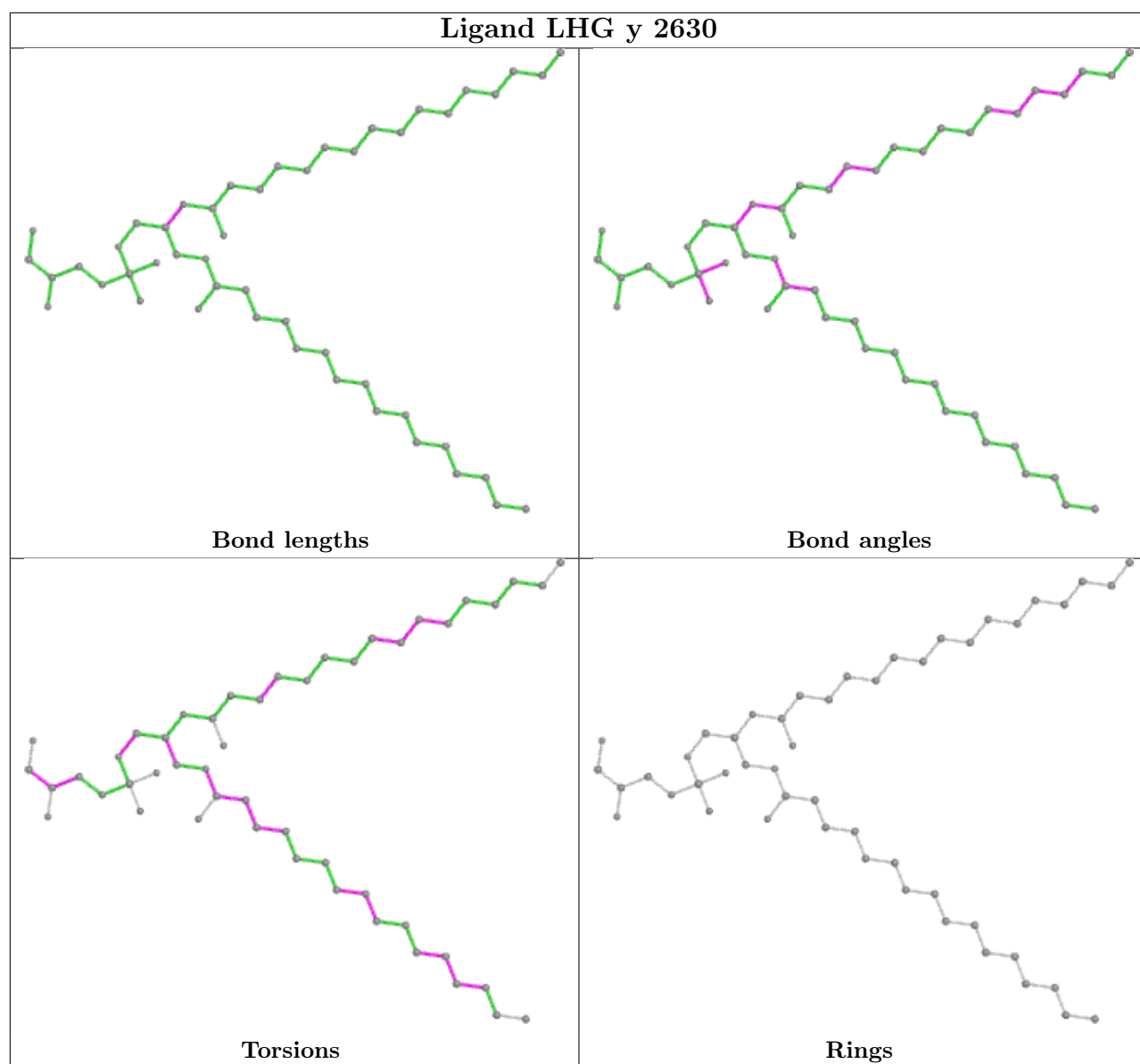
Bond angles



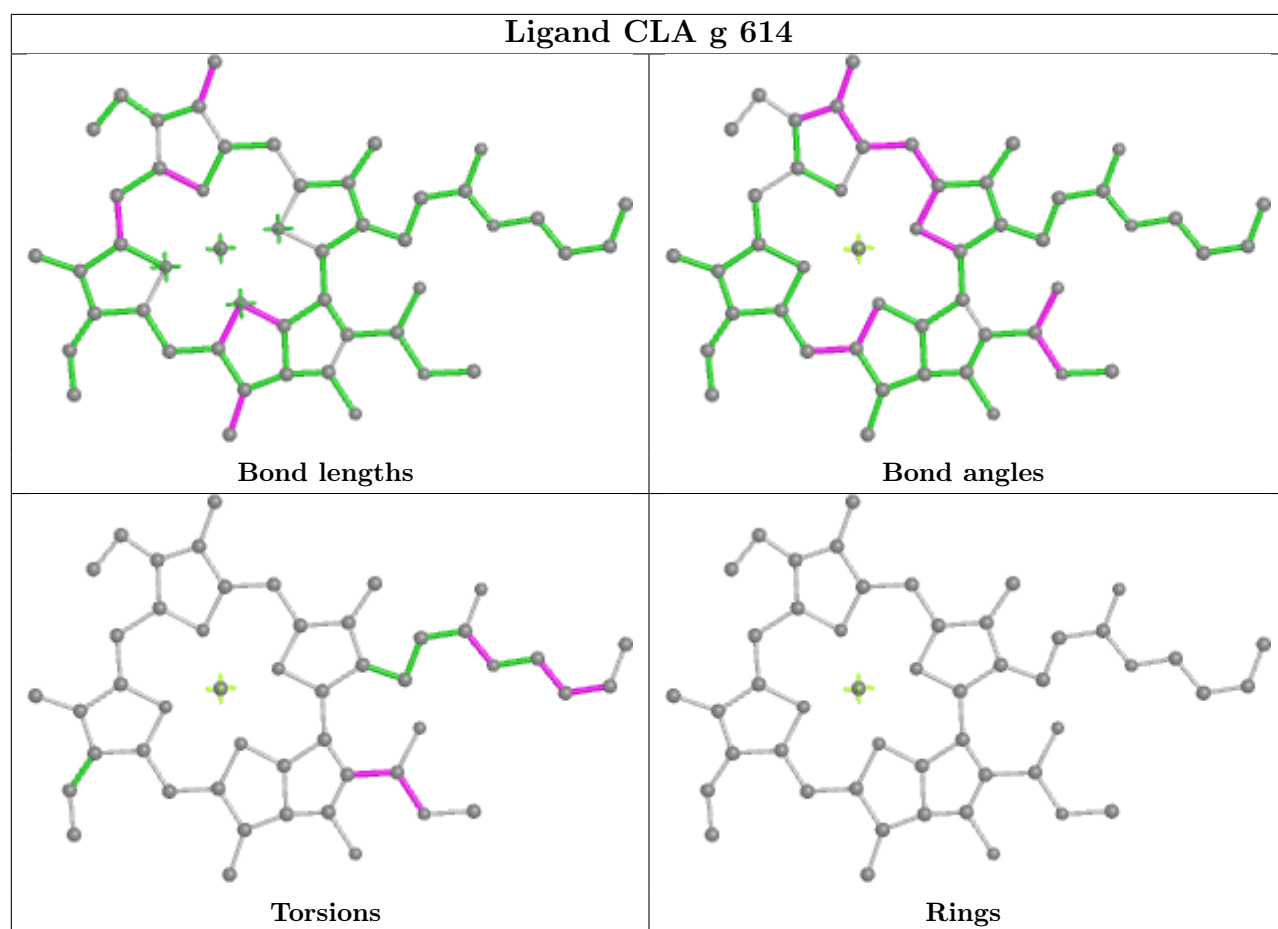
Torsions



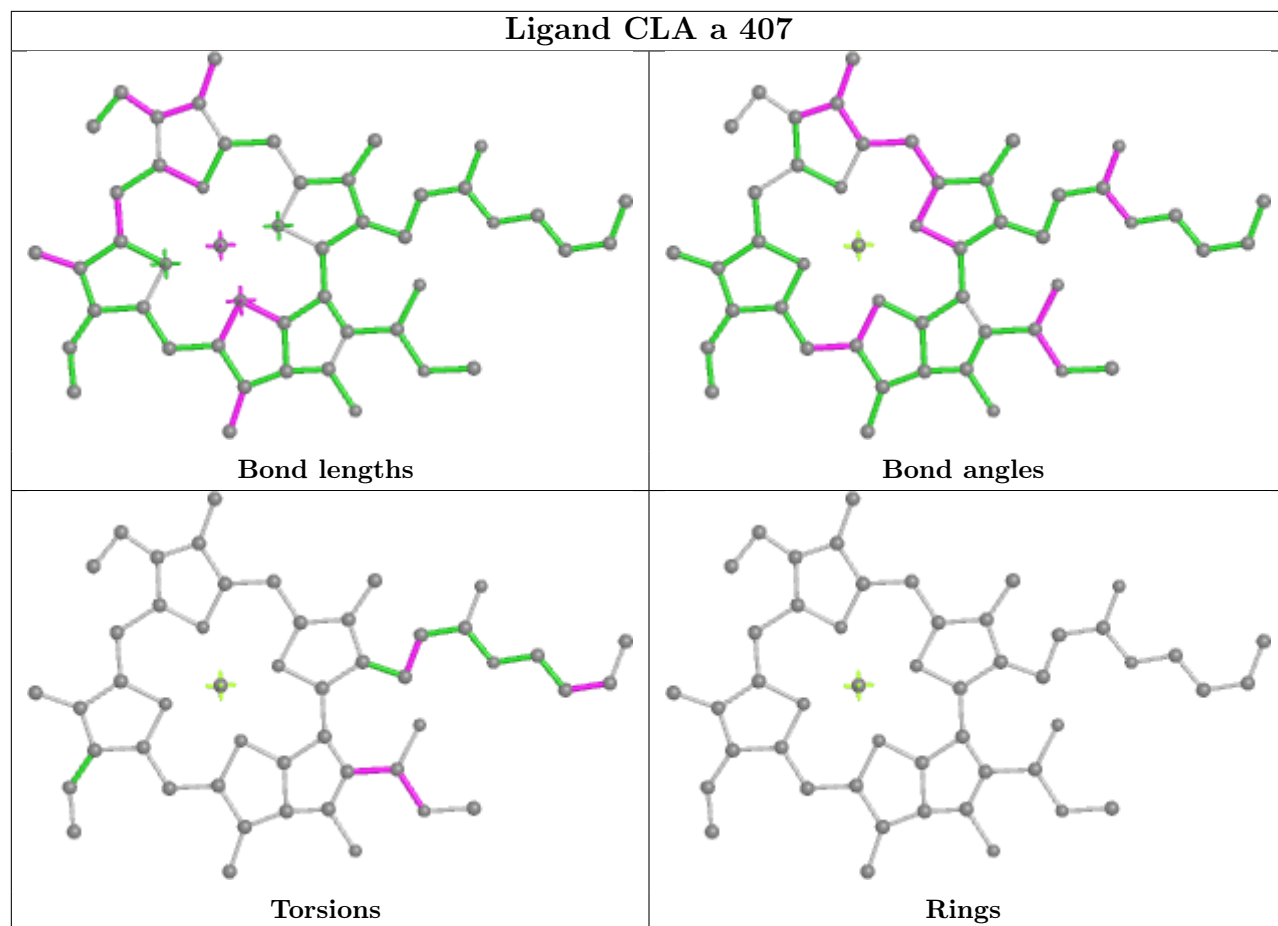
Rings

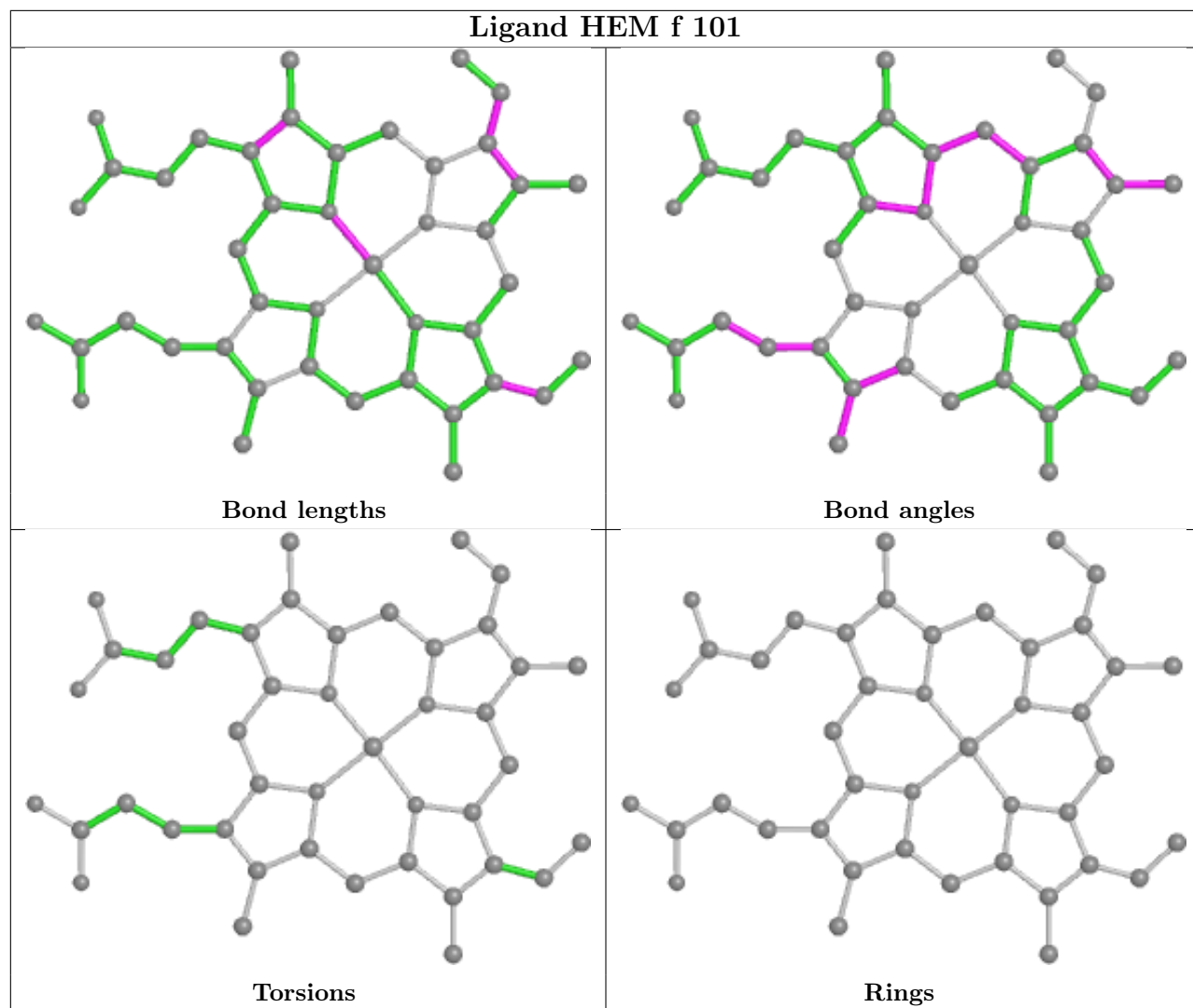




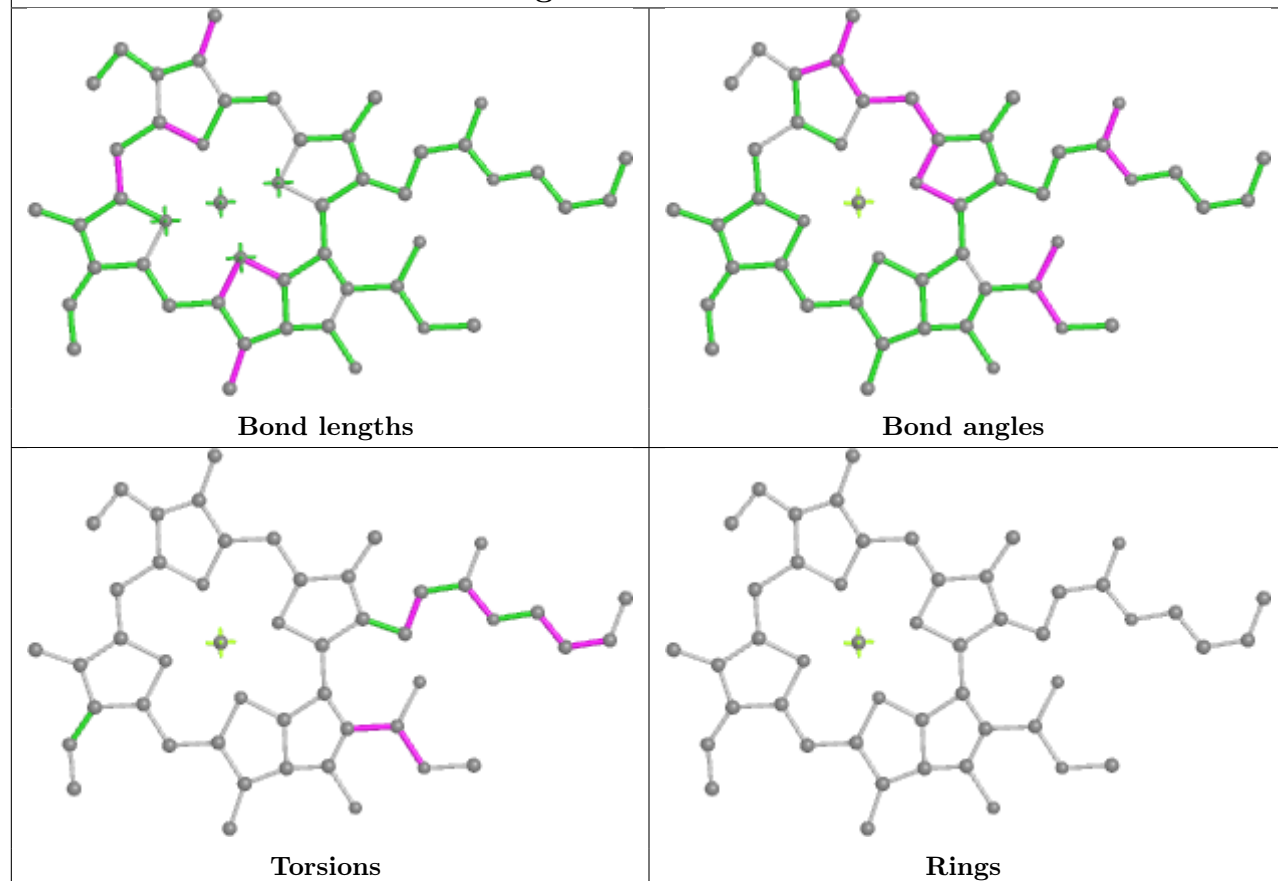


## Ligand CLA a 407

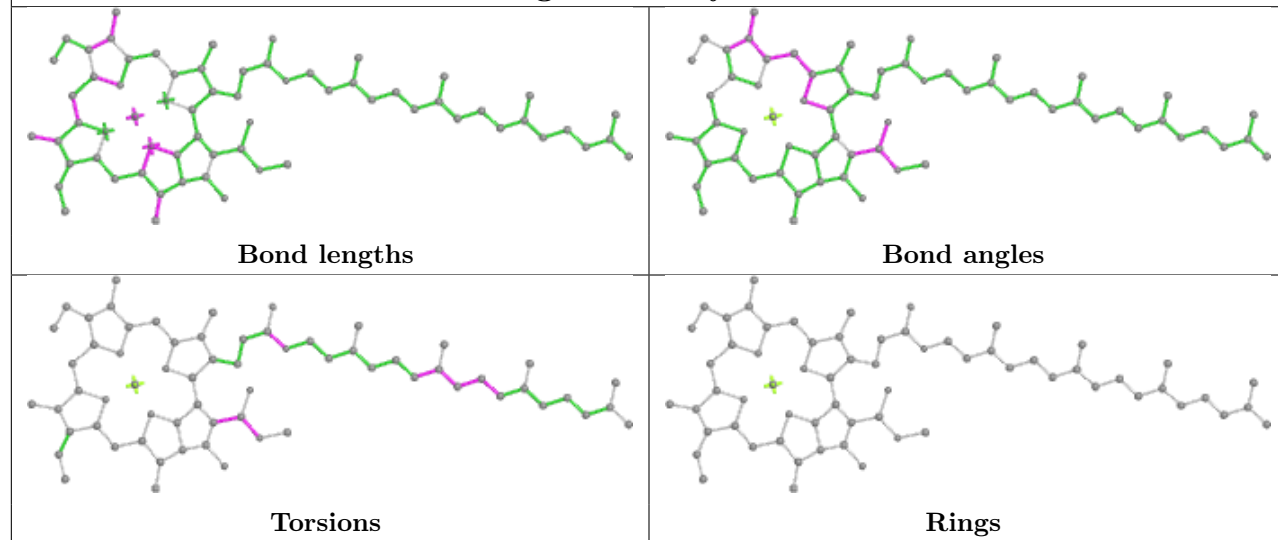


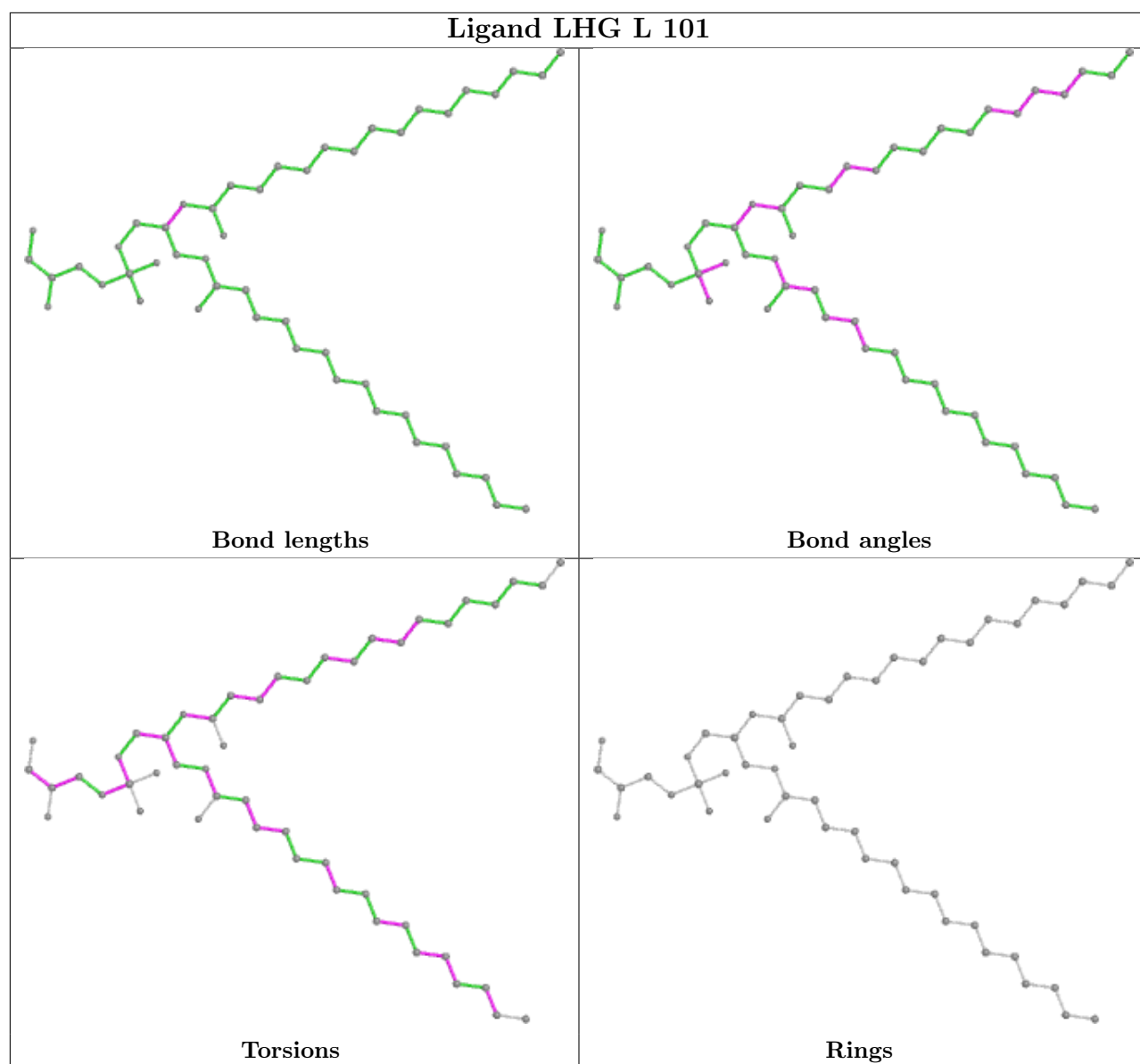


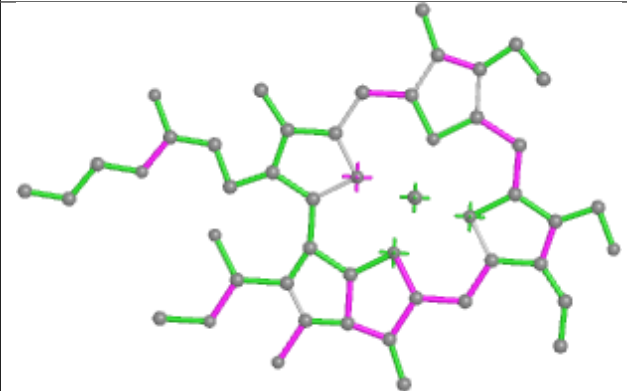
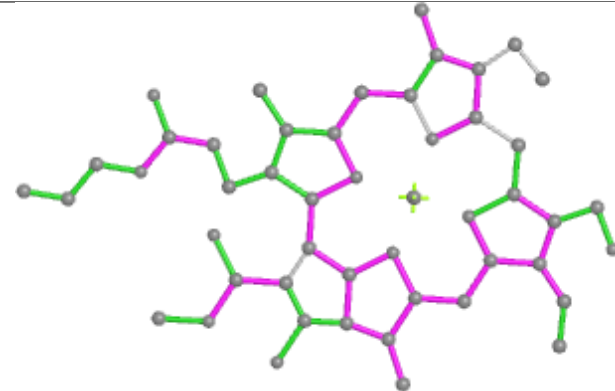
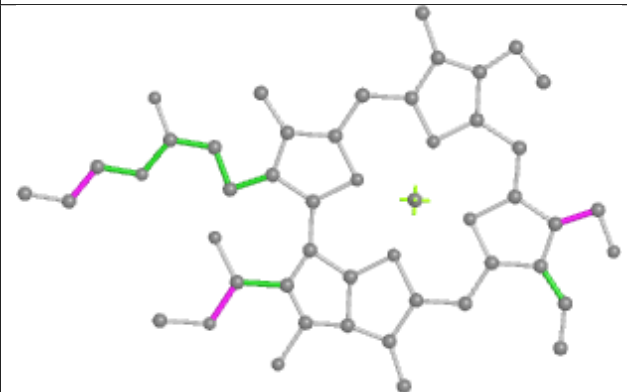
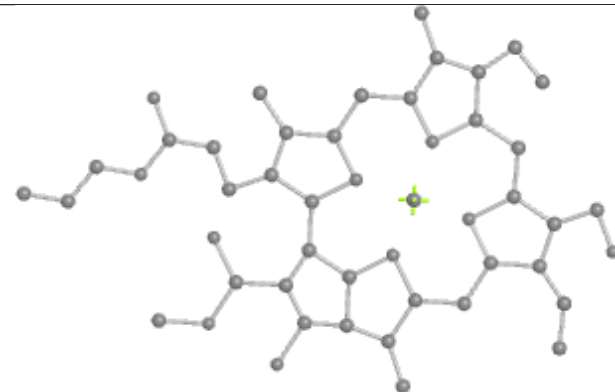
## Ligand CLA n 614

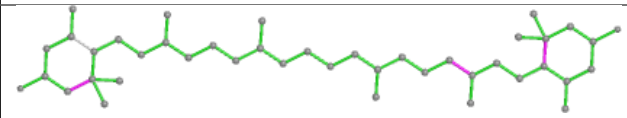
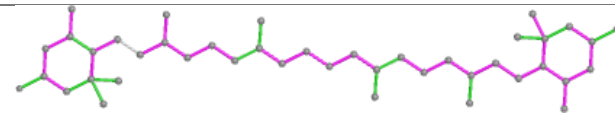
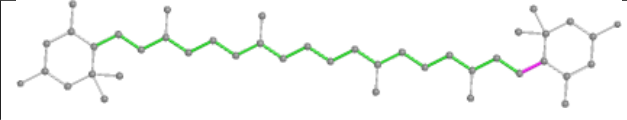
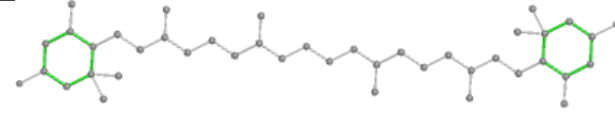


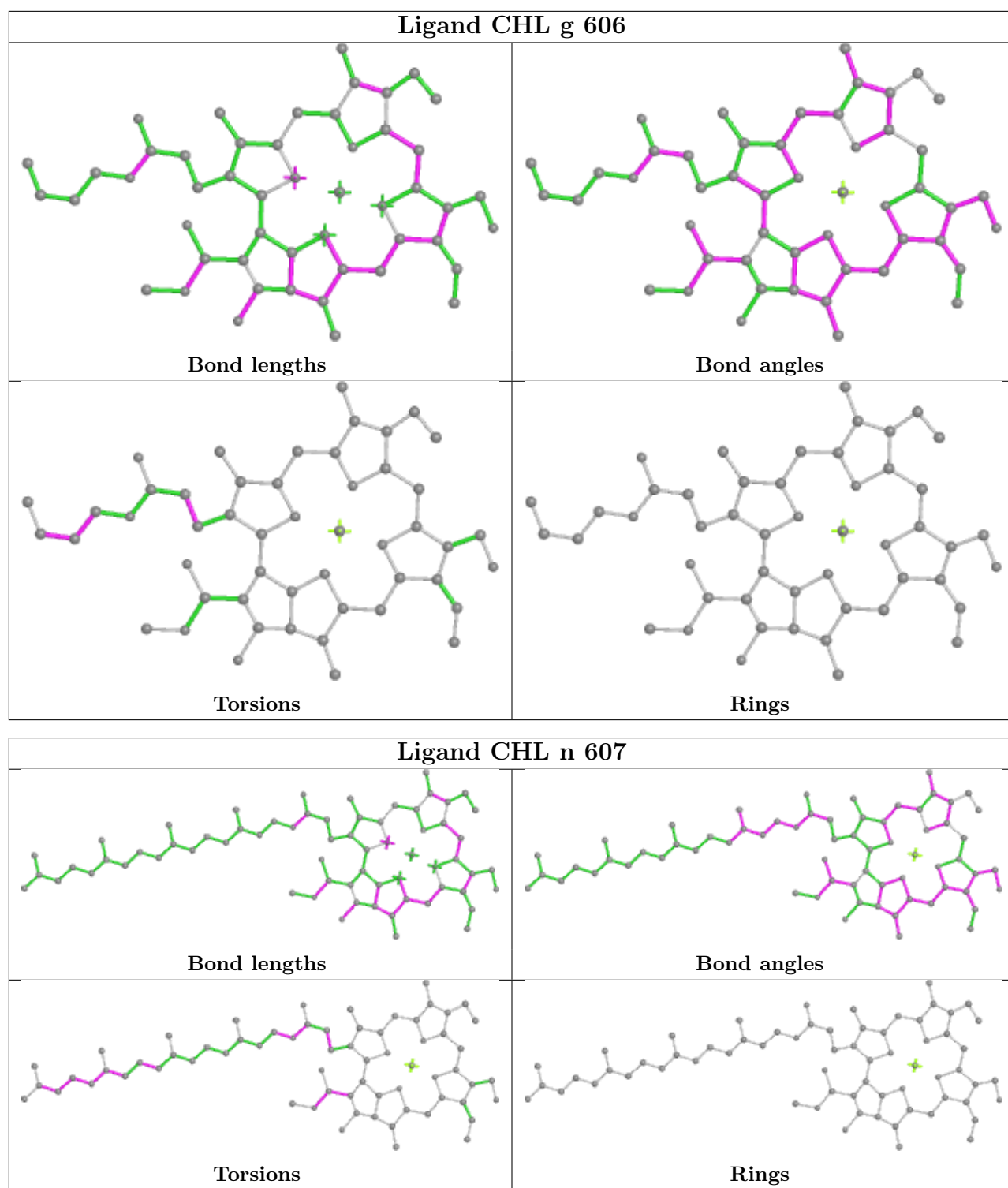
## Ligand CLA y 611



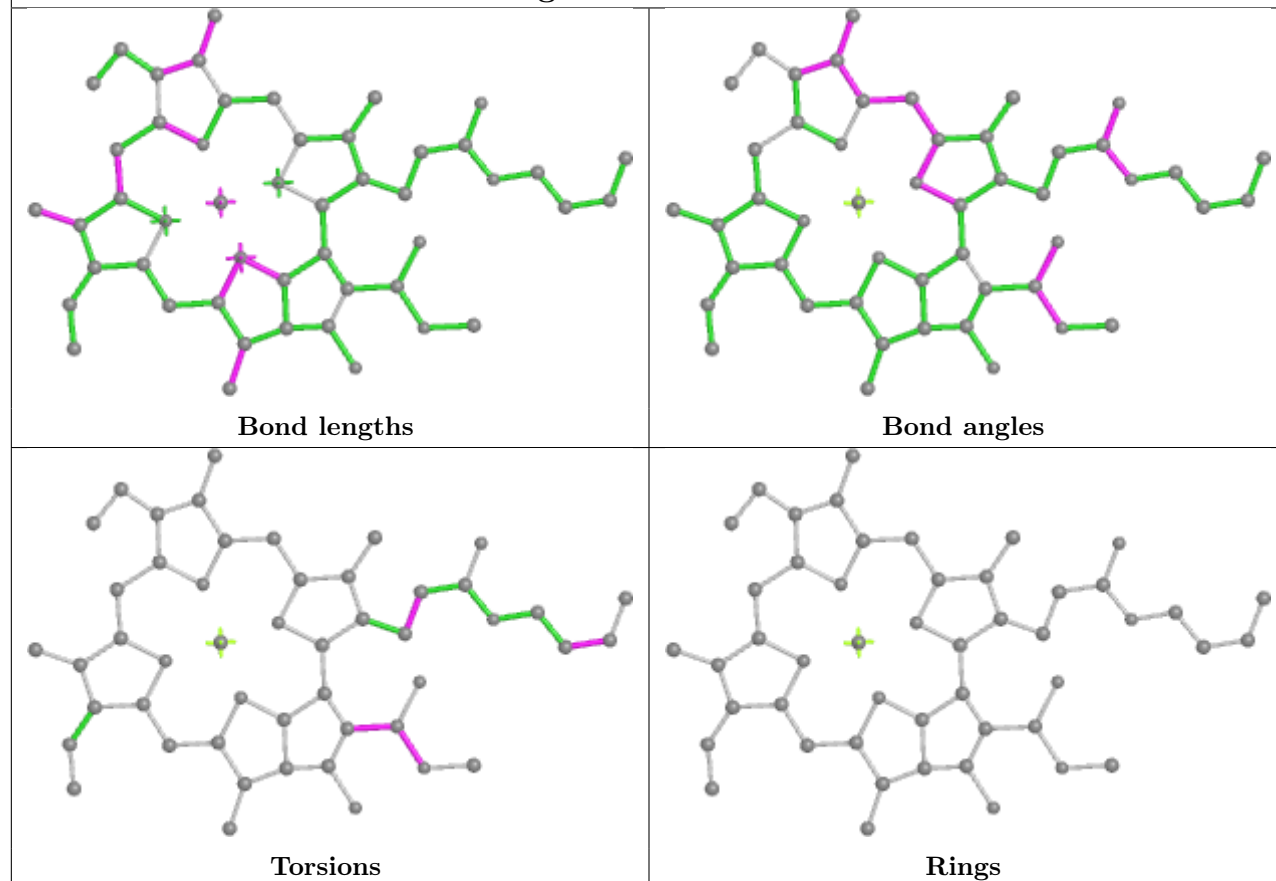


Ligand CHL s 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

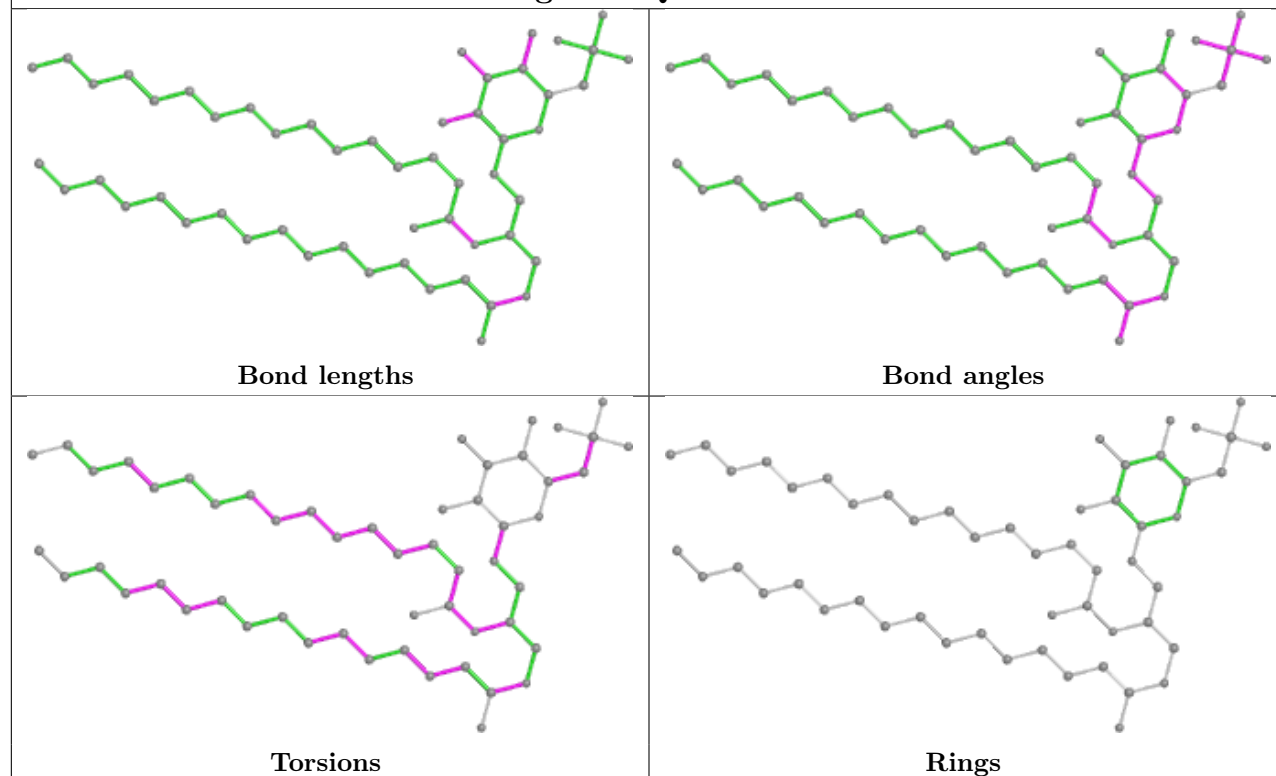
Ligand LUT y 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings



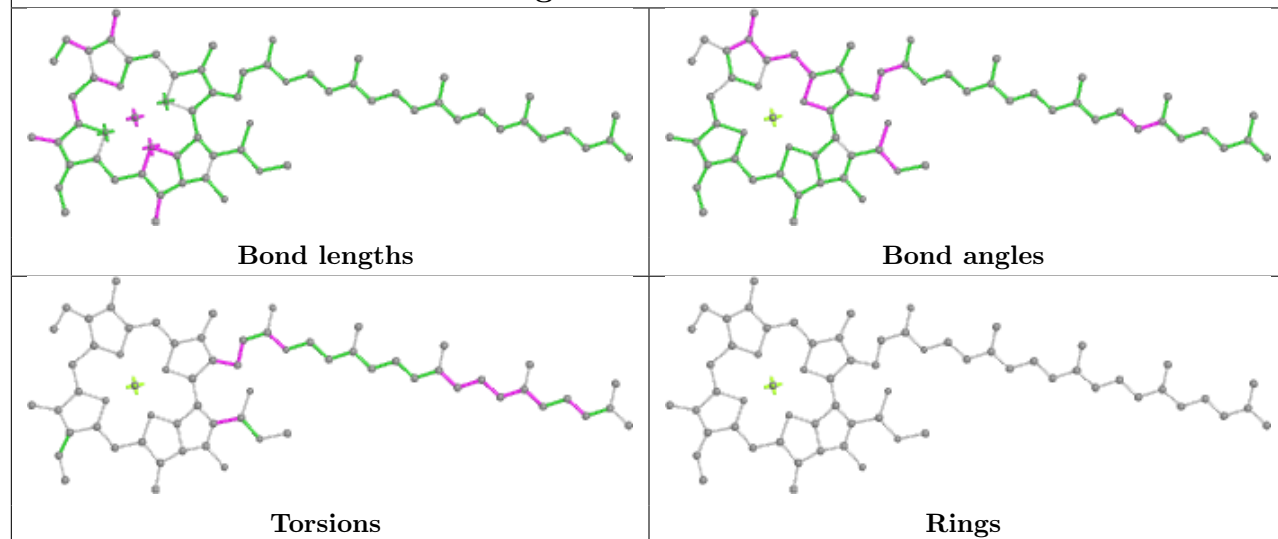
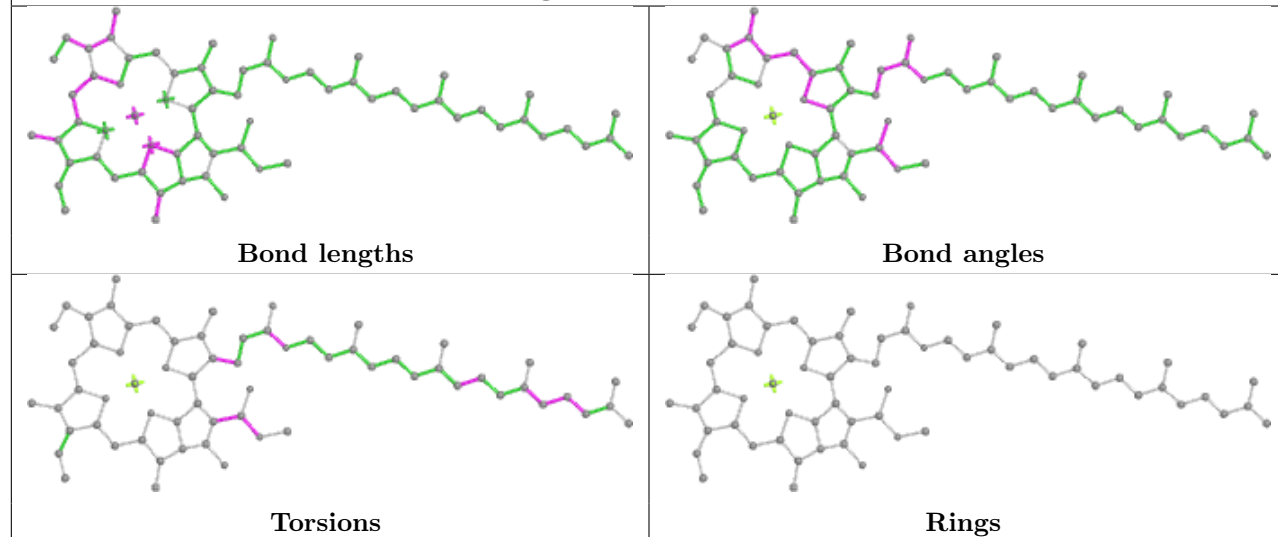
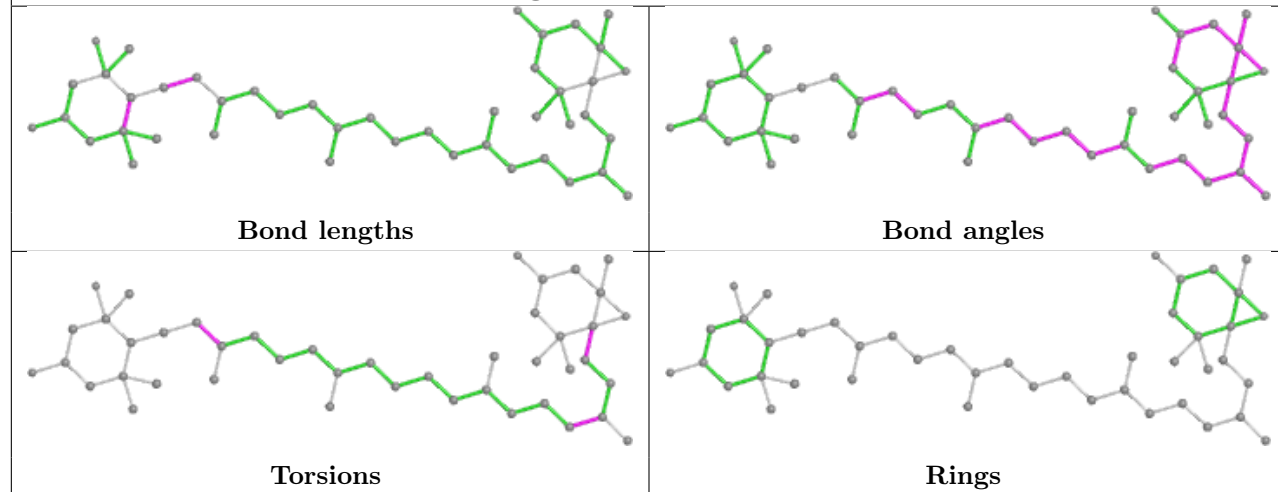
## Ligand CLA r 603



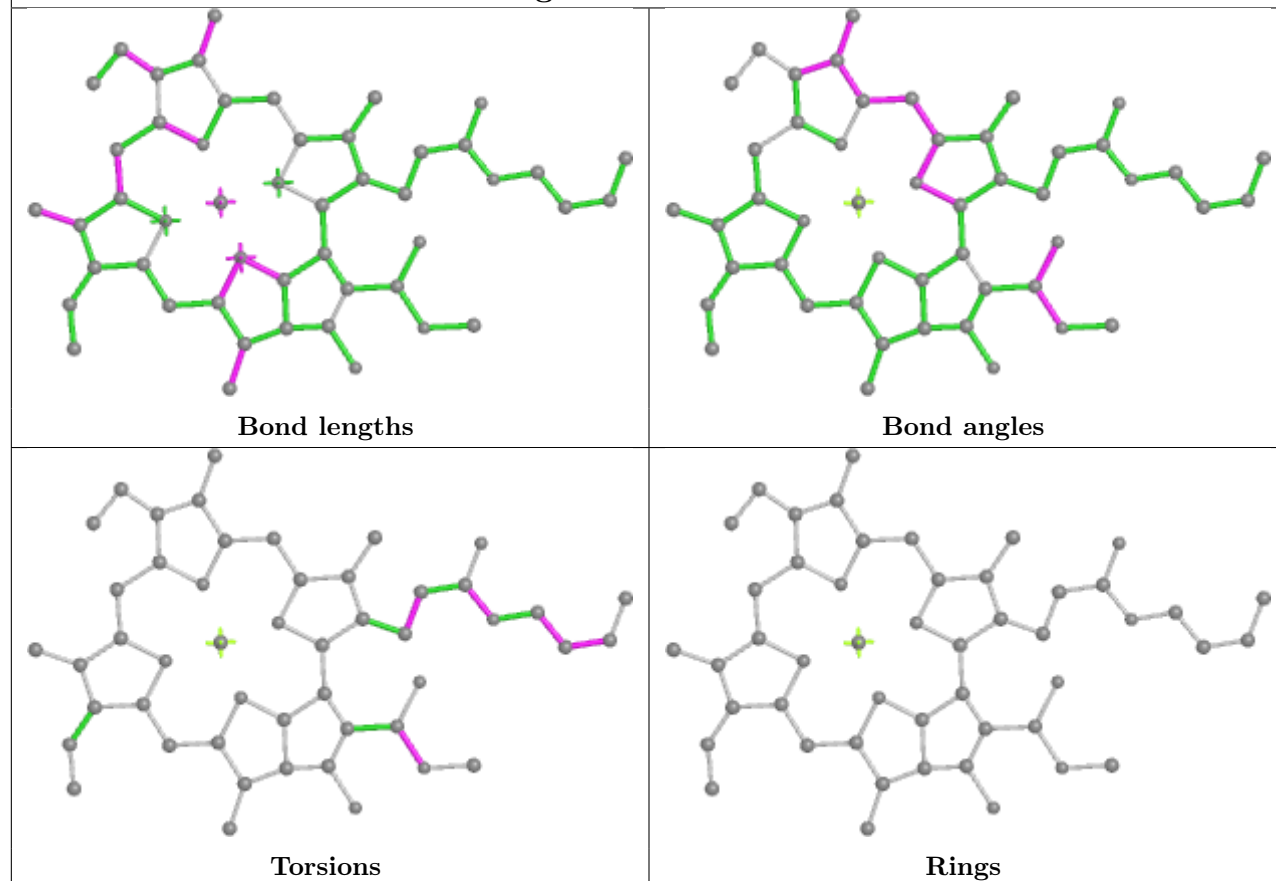
## Ligand SQD b 621



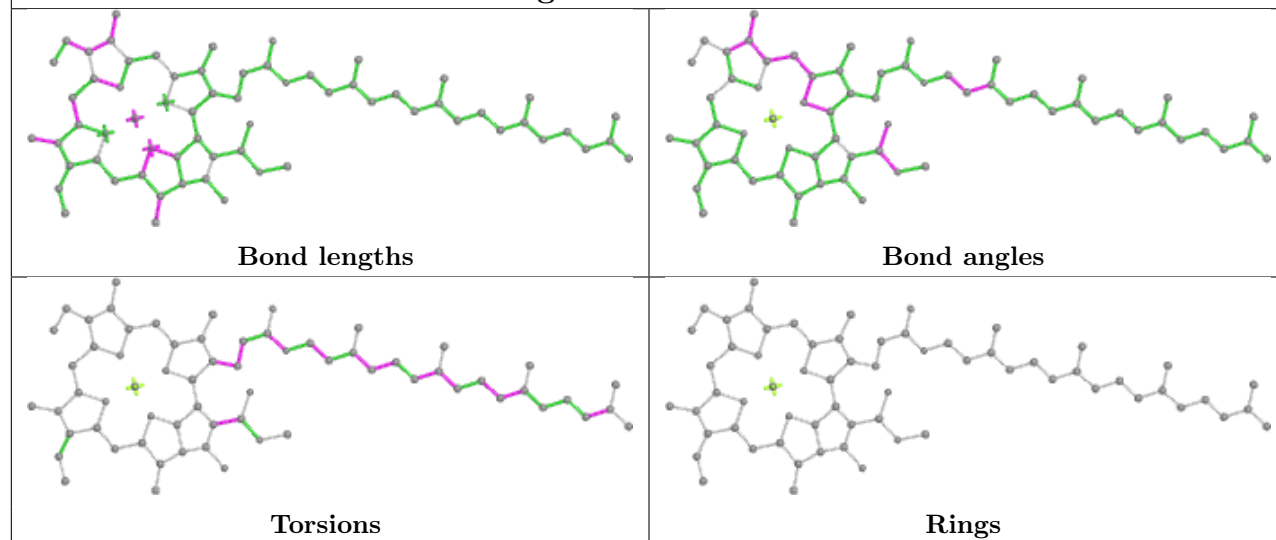


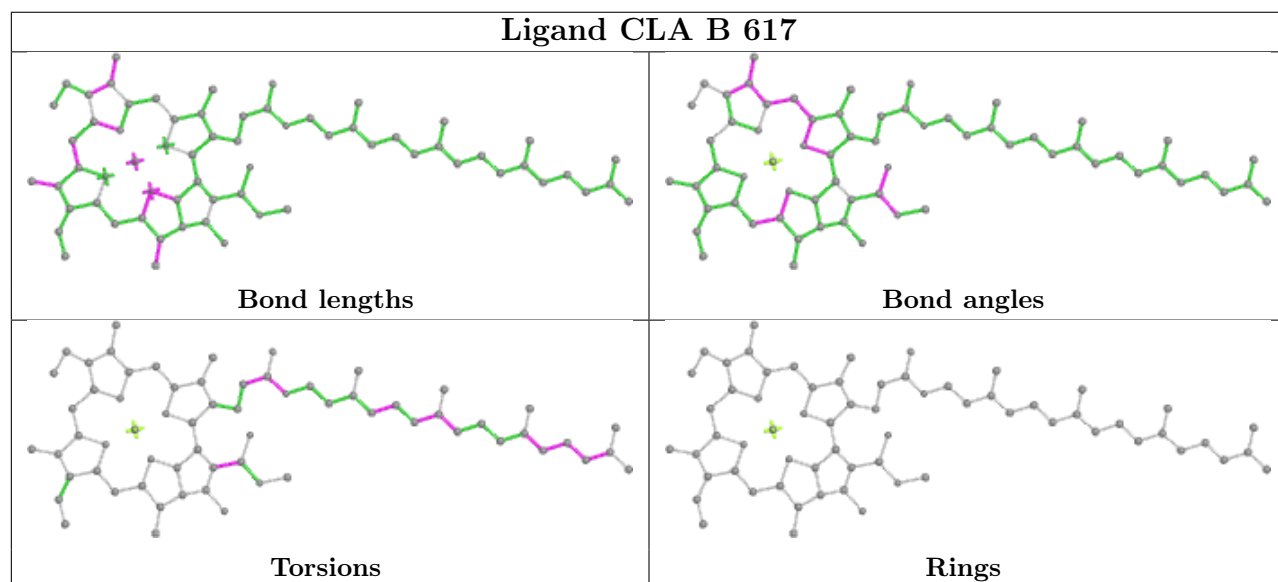
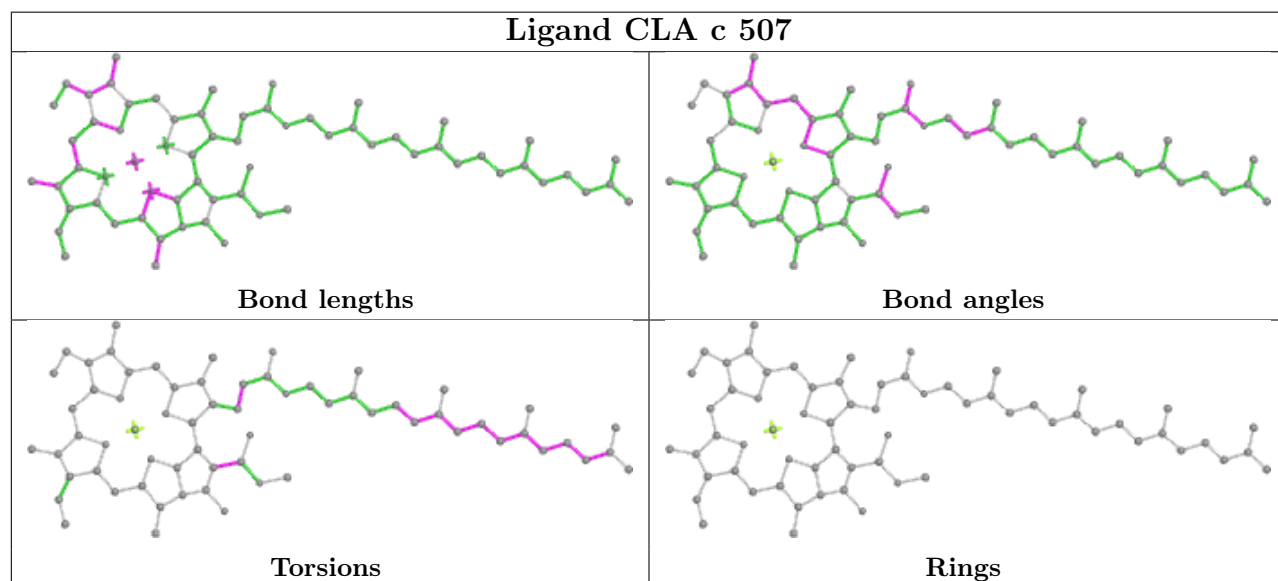
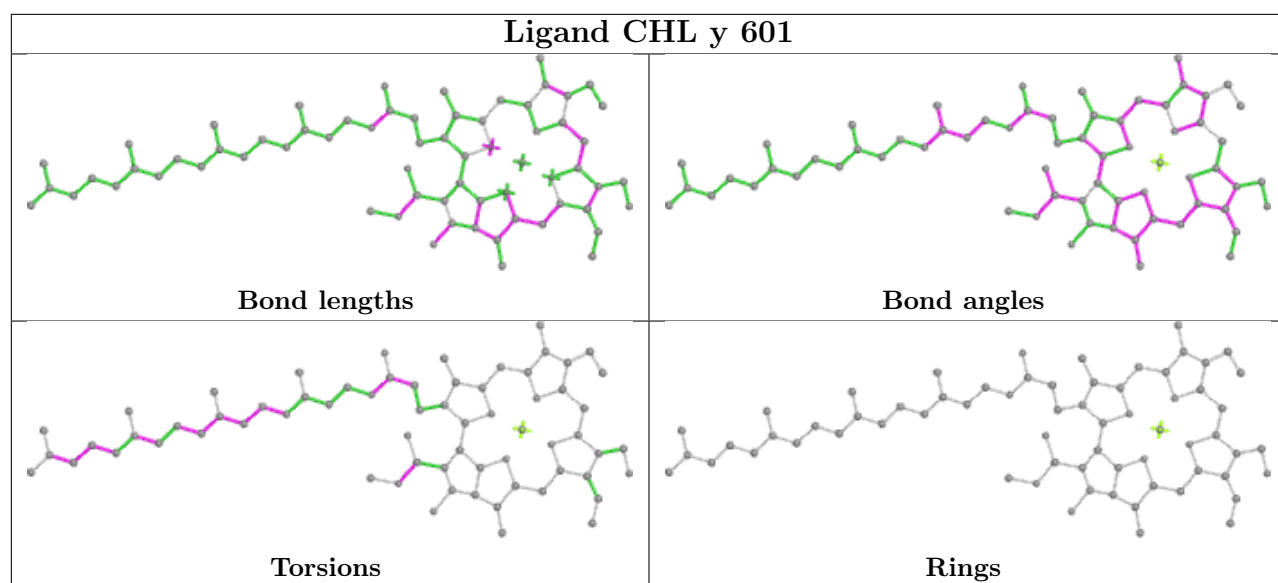
**Ligand CLA b 613****Ligand CLA c 503****Ligand NEX s 1623**

## Ligand CLA n 613

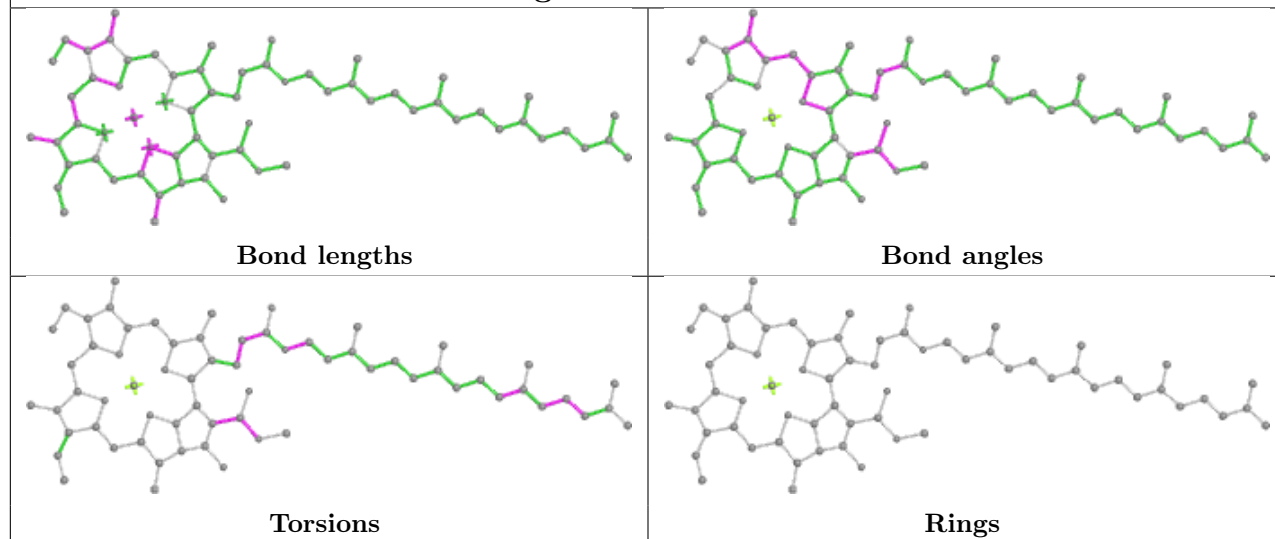


## Ligand CLA c 512

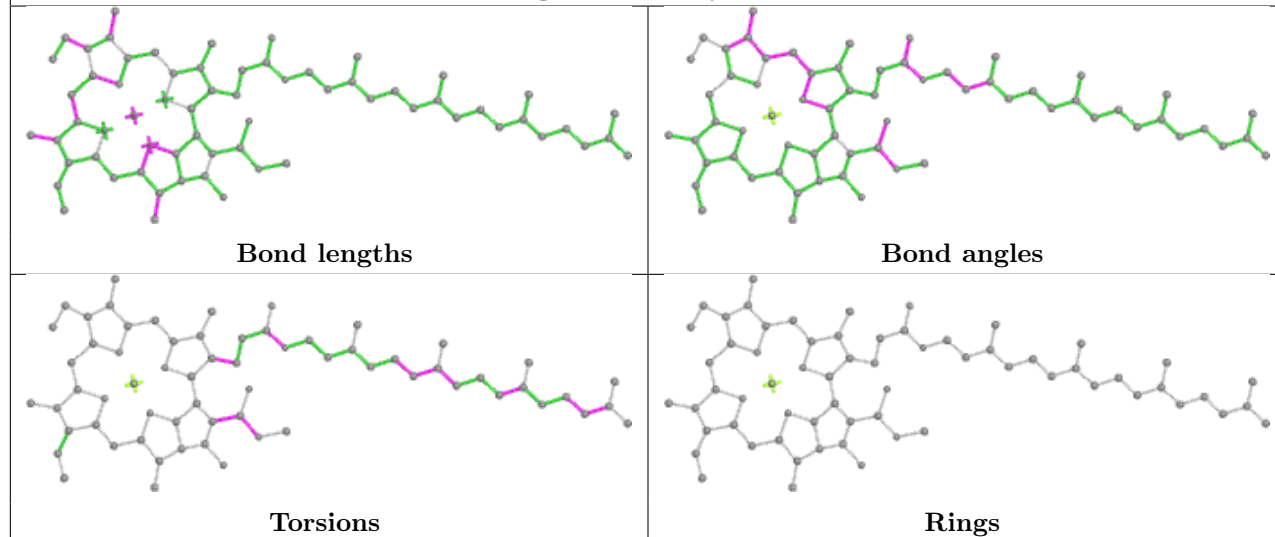




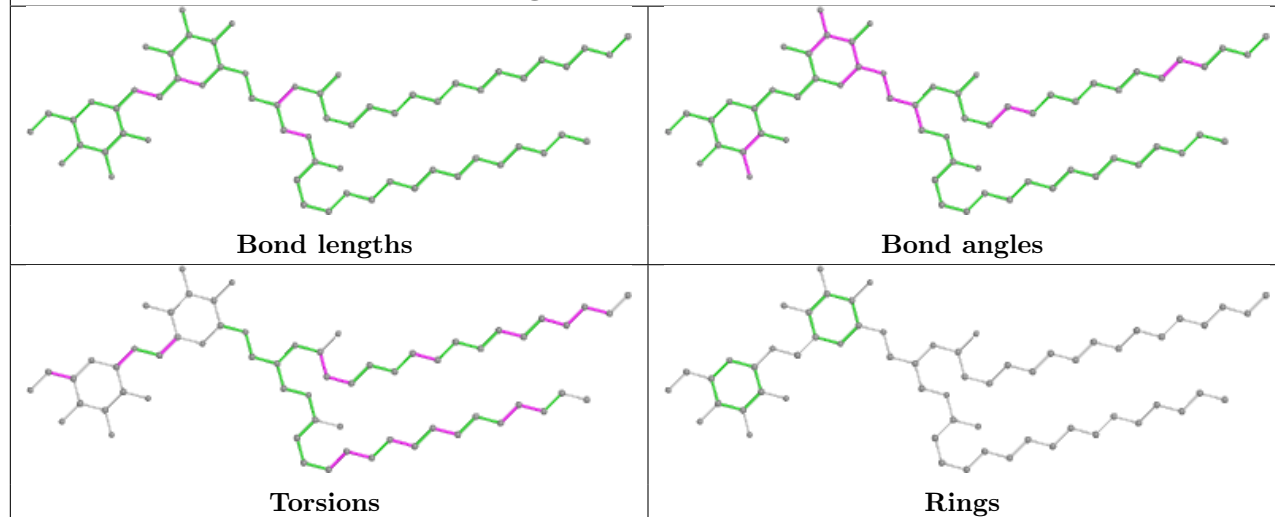
## Ligand CLA b 611



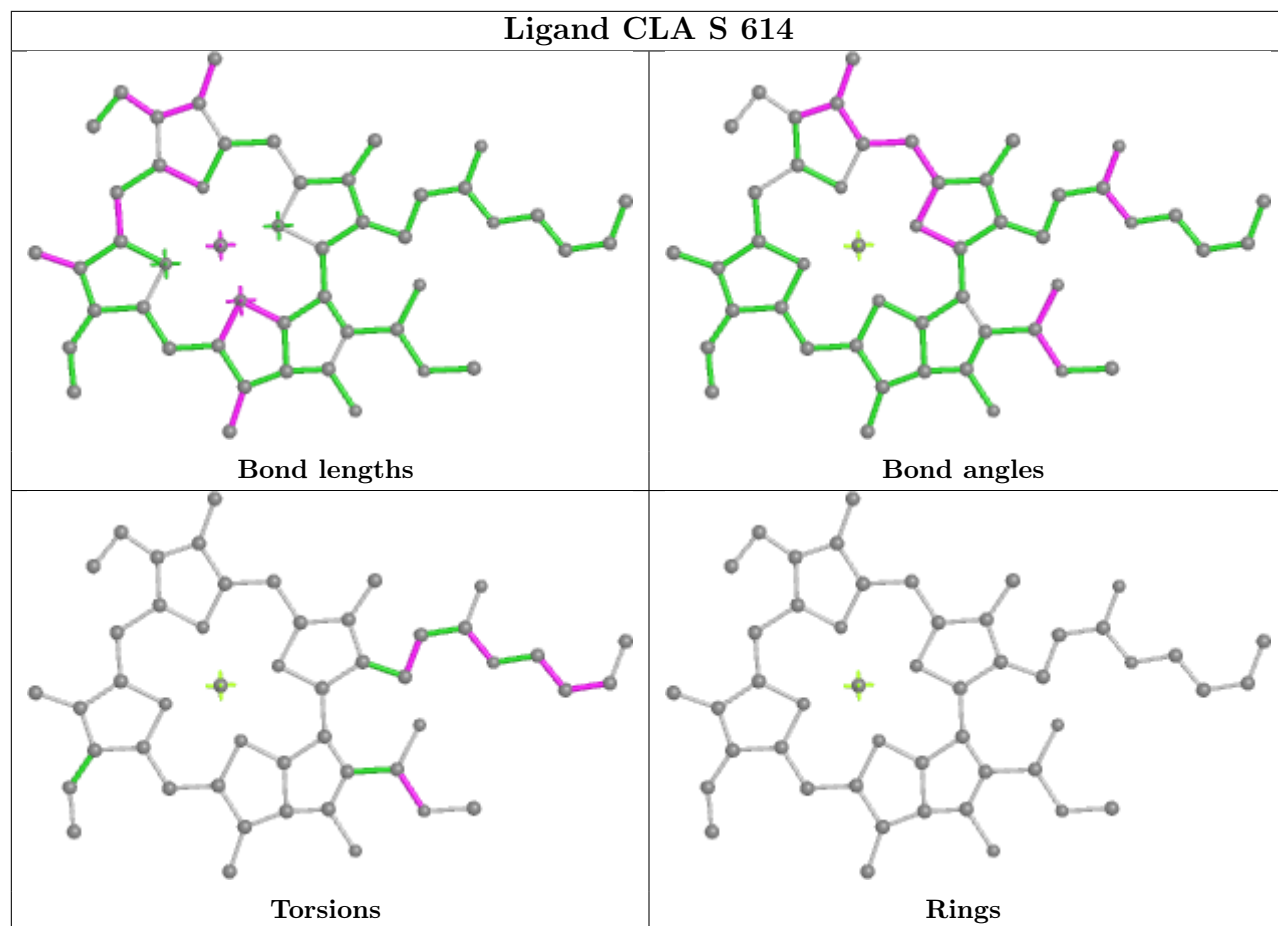
## Ligand CLA y 610

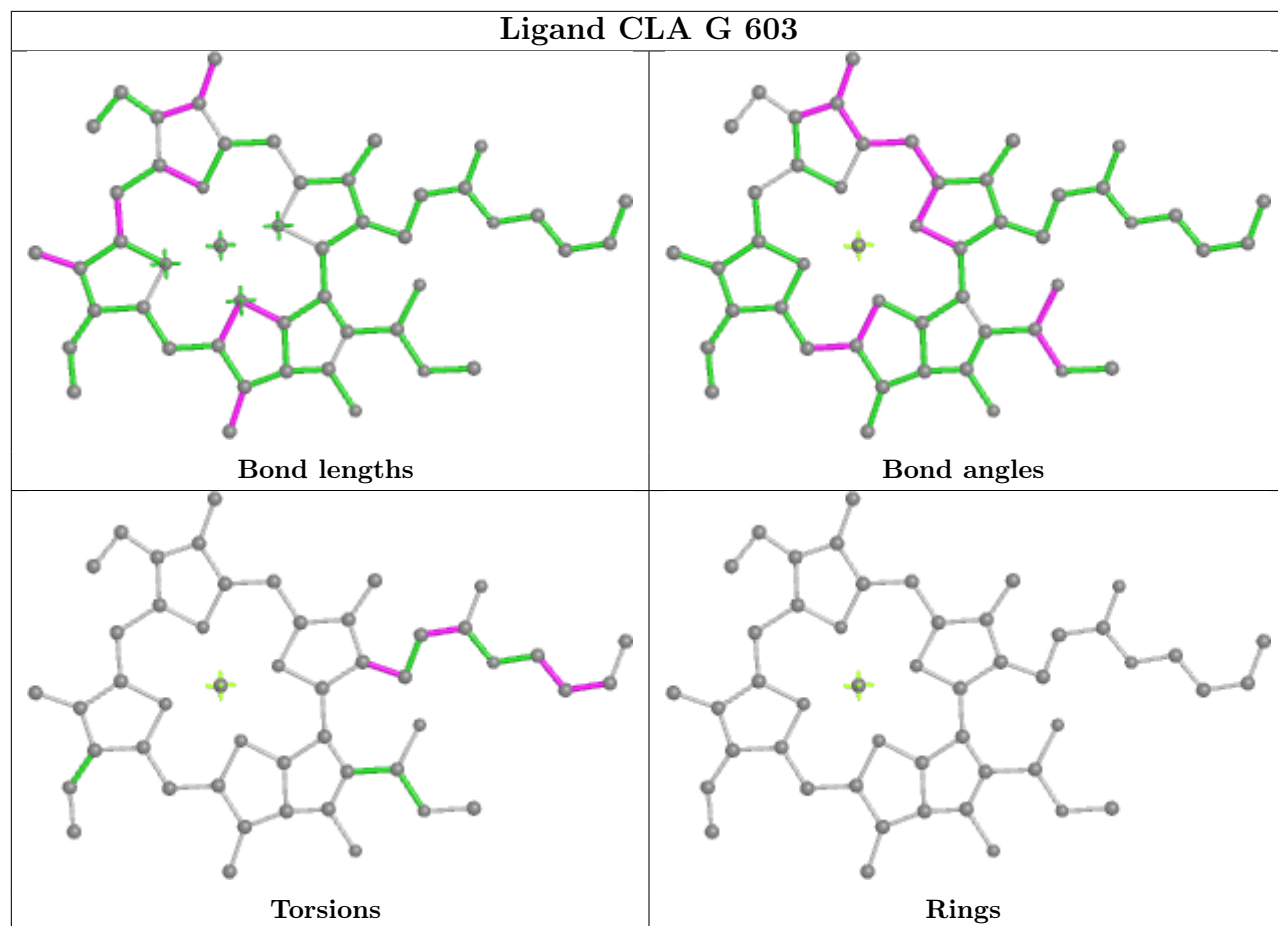


## Ligand DGD H 102

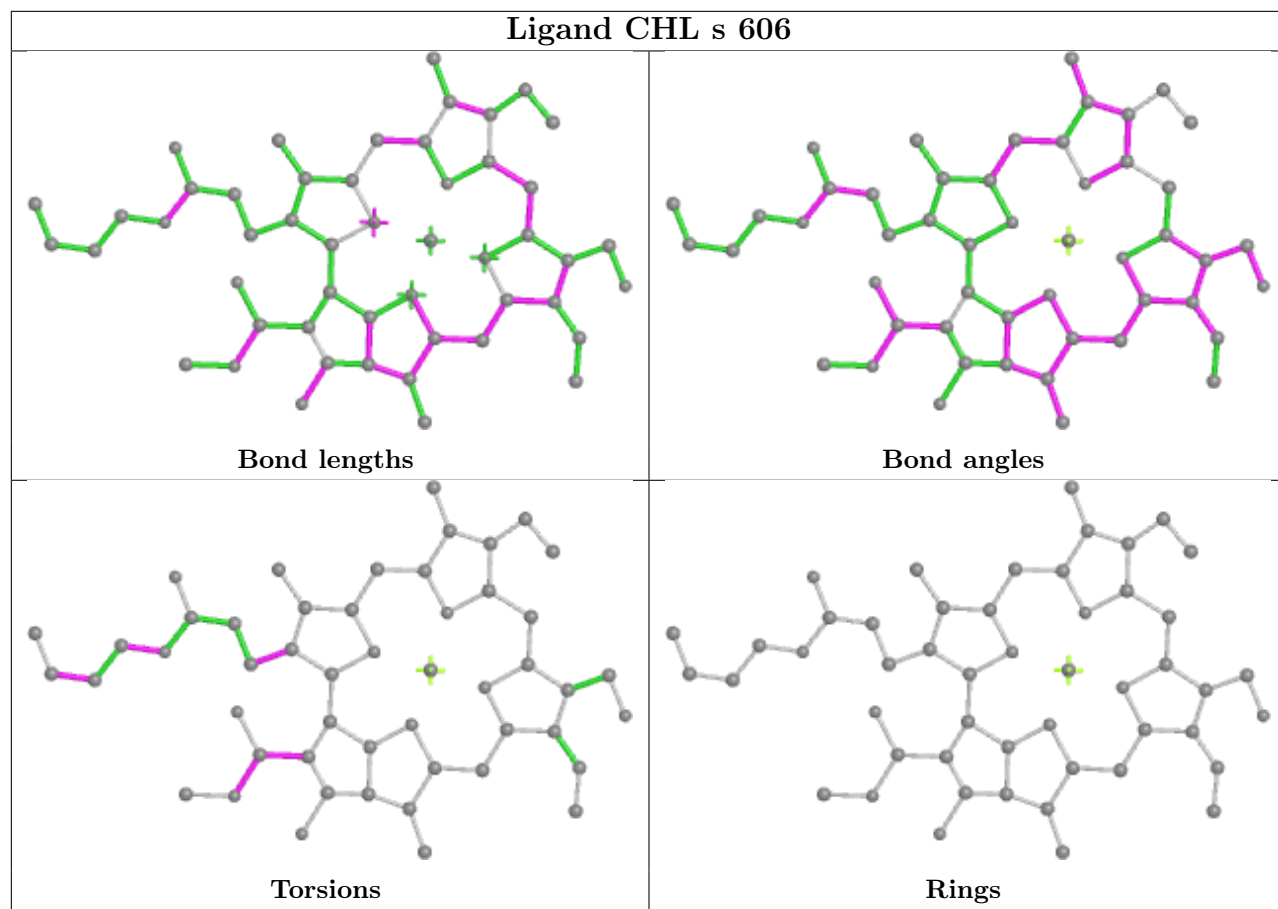


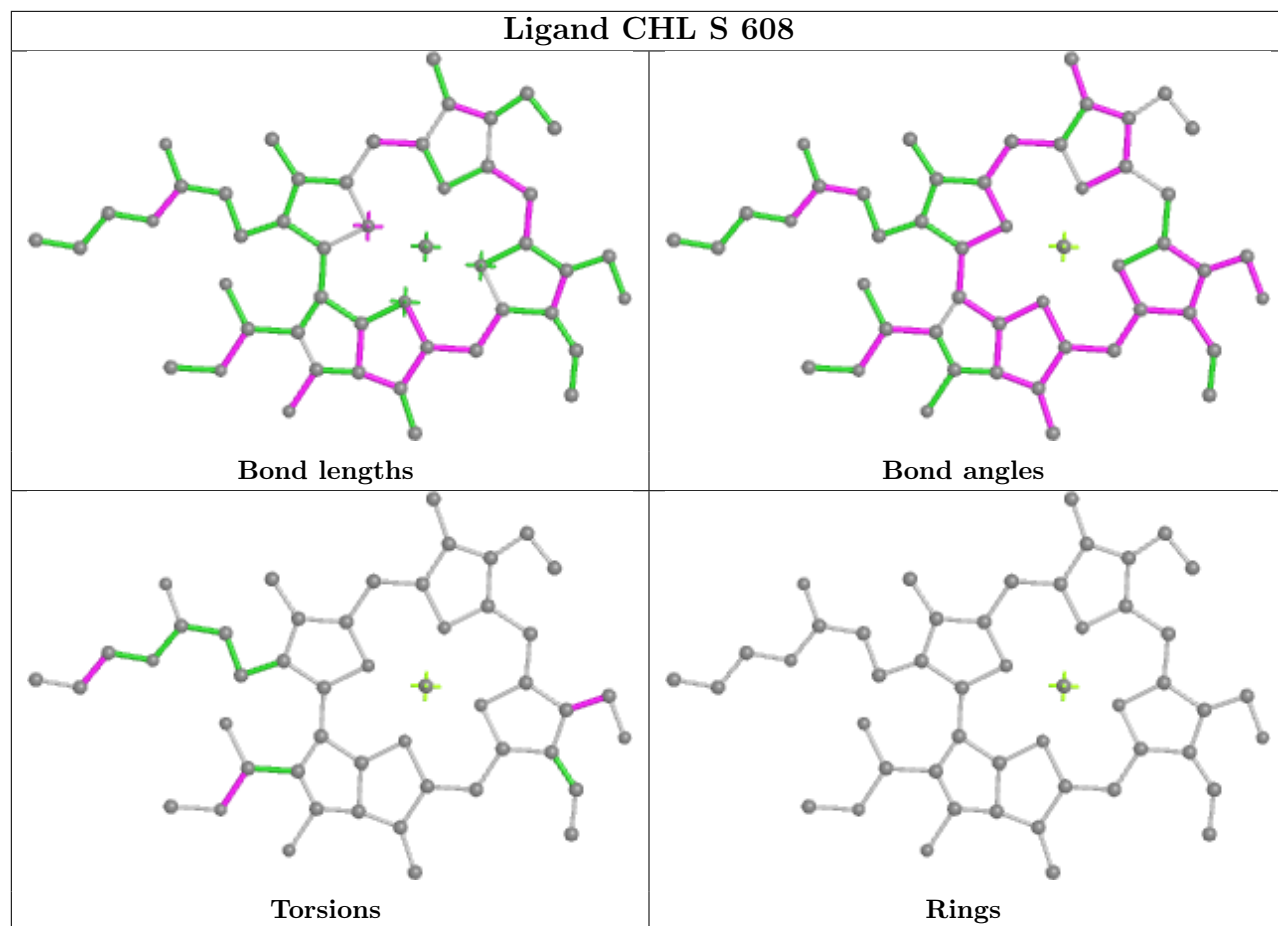
## Ligand CLA S 614





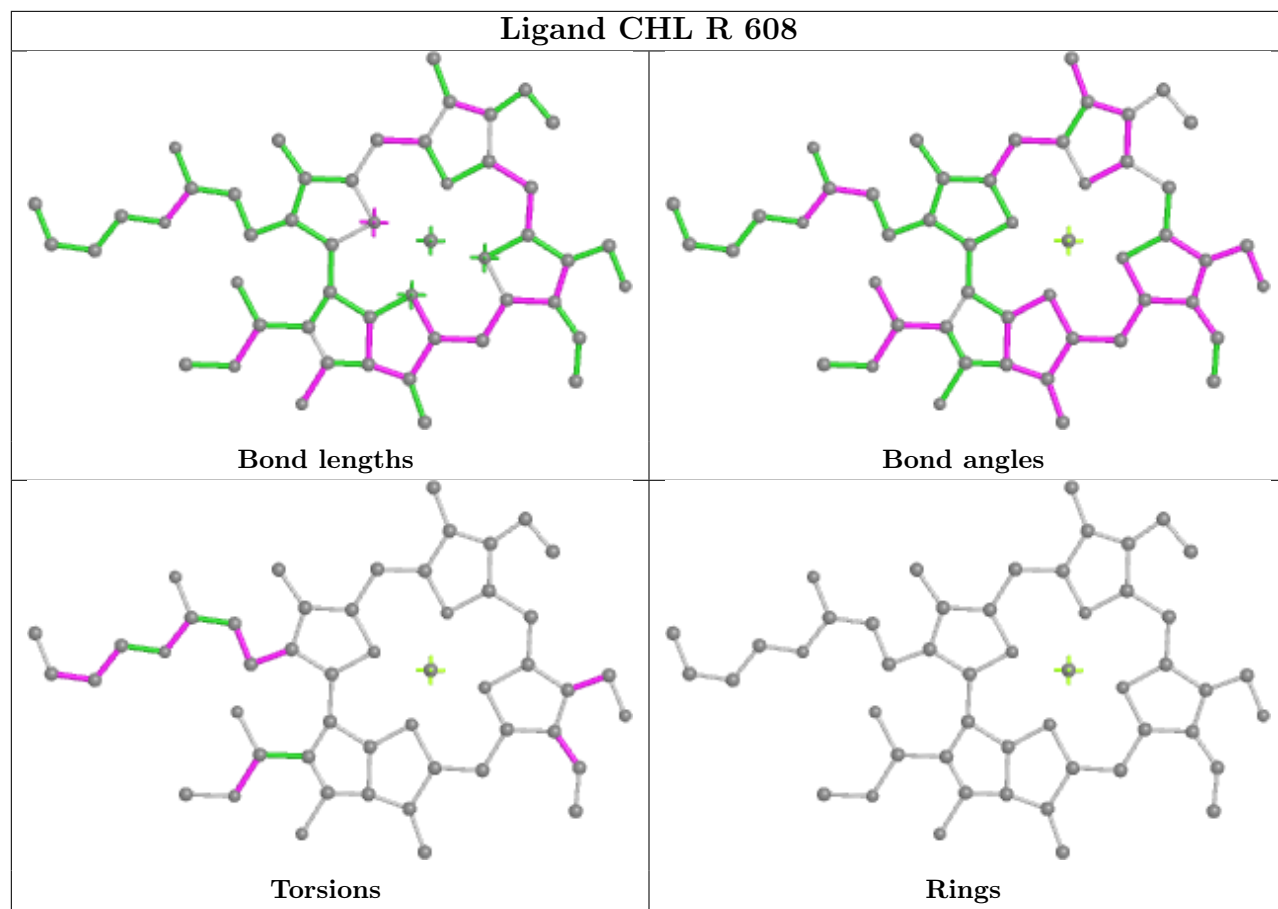
## Ligand CHL s 606



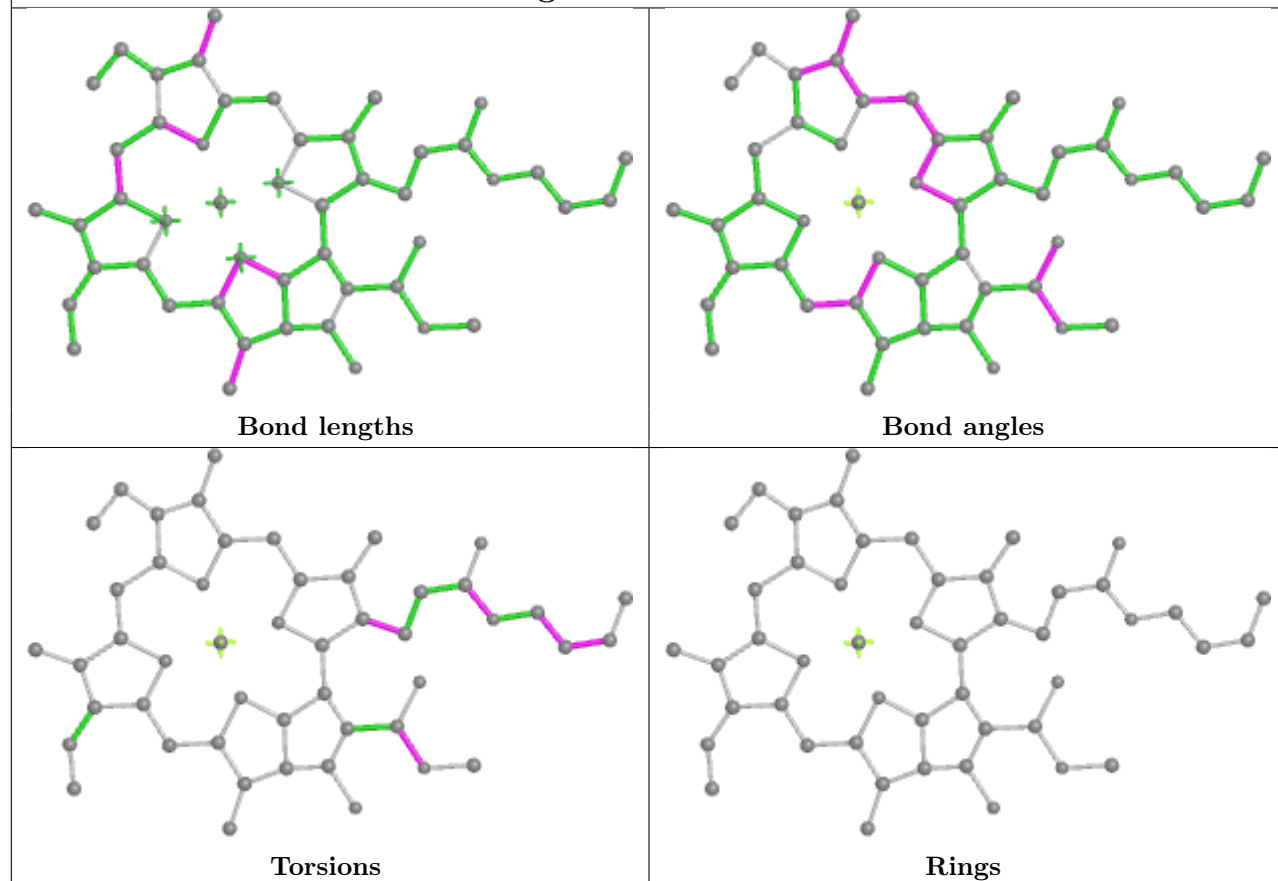




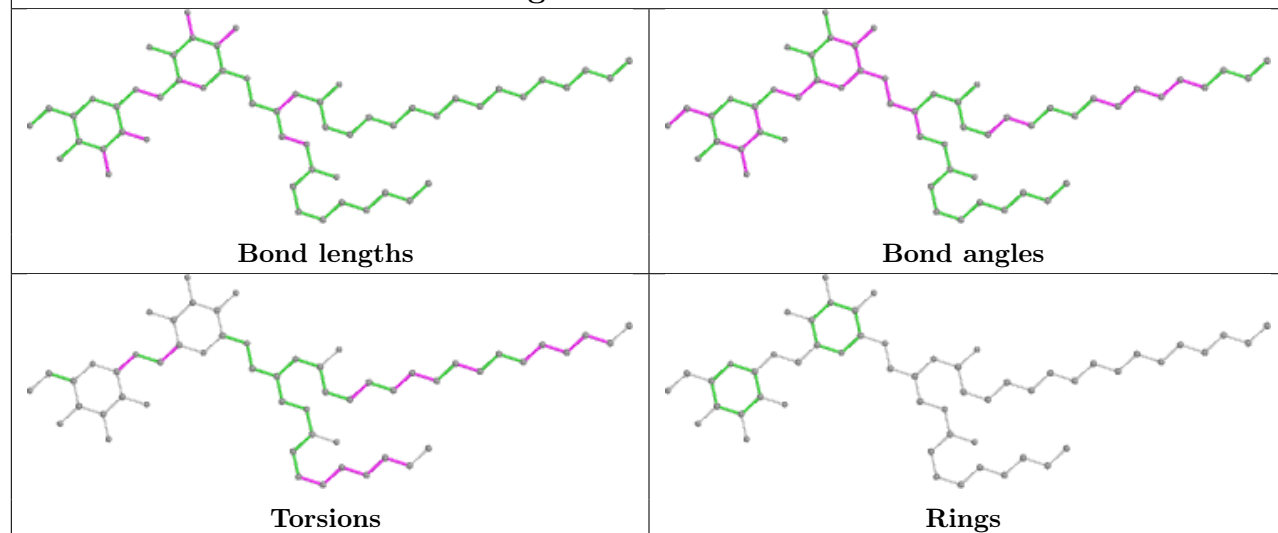
## Ligand CHL R 608

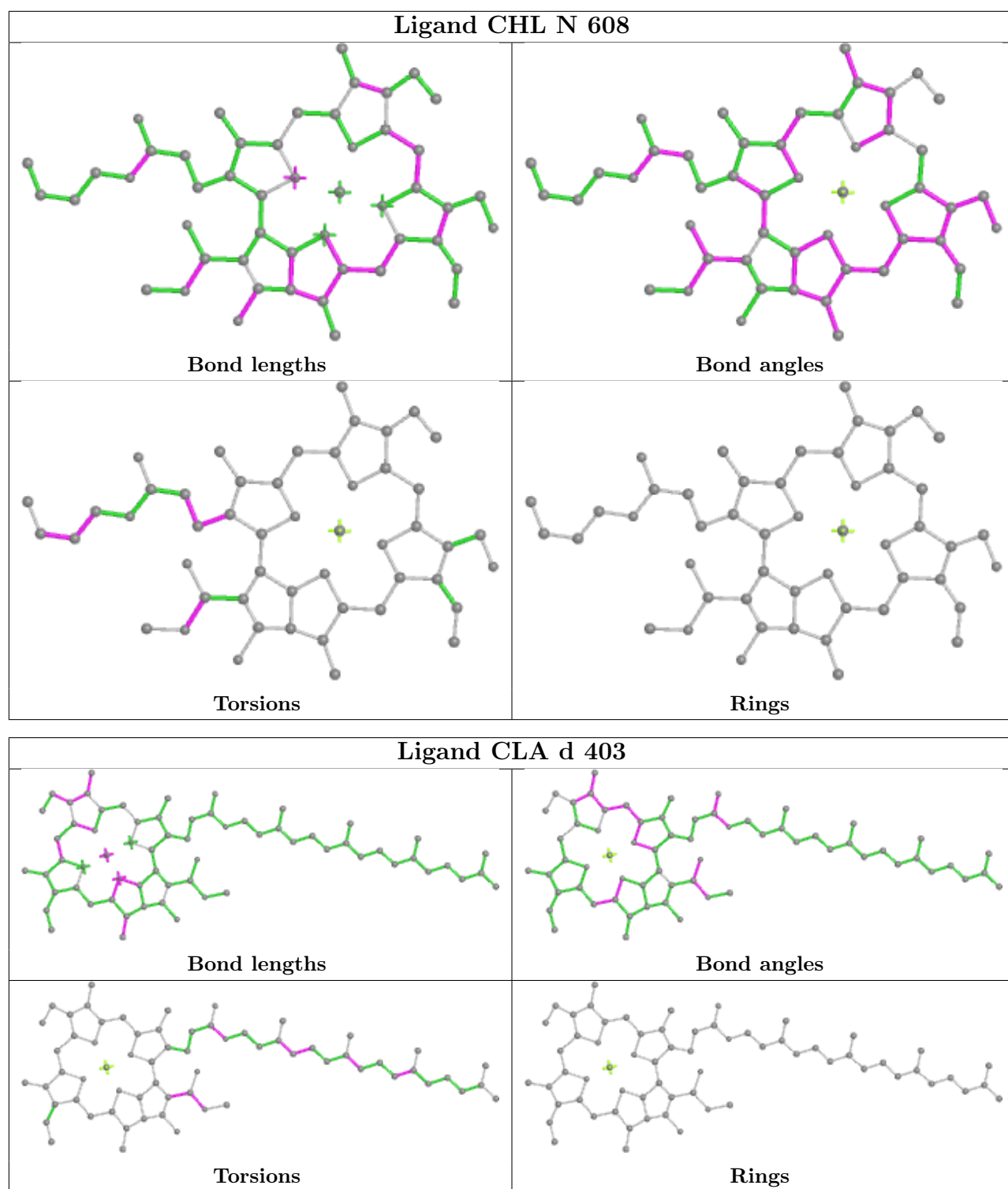


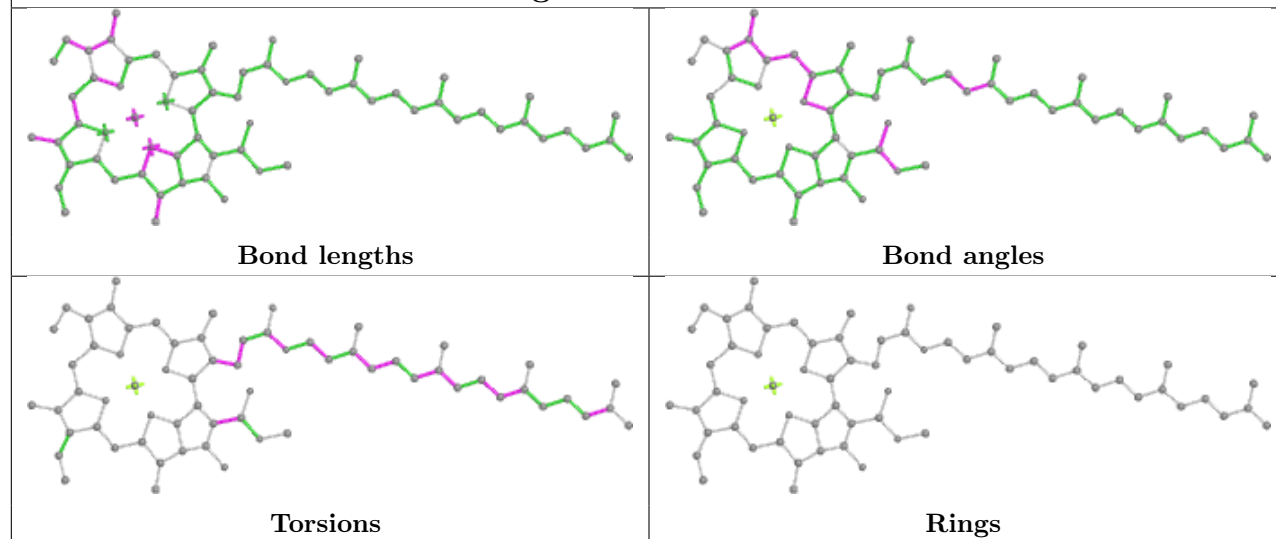
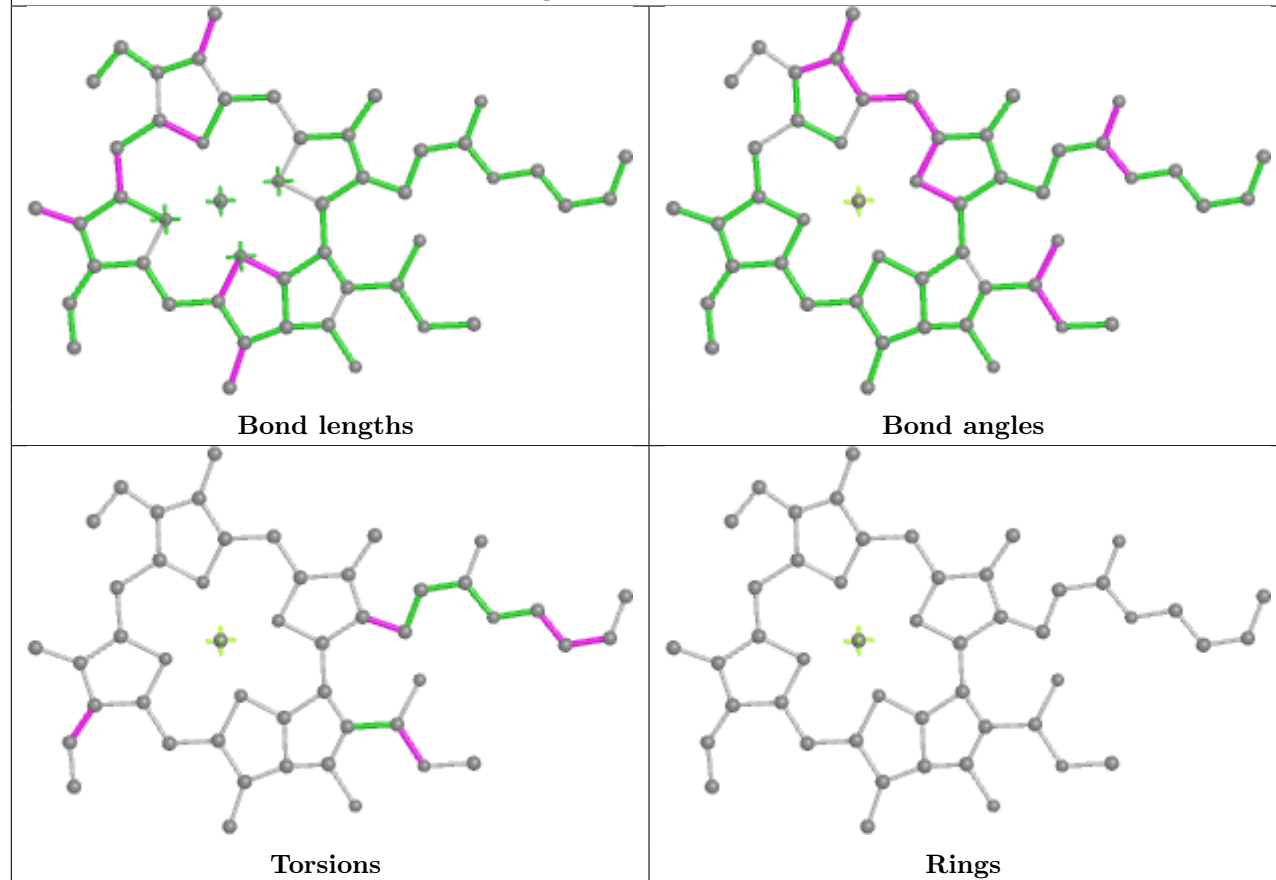
## Ligand CLA s 609

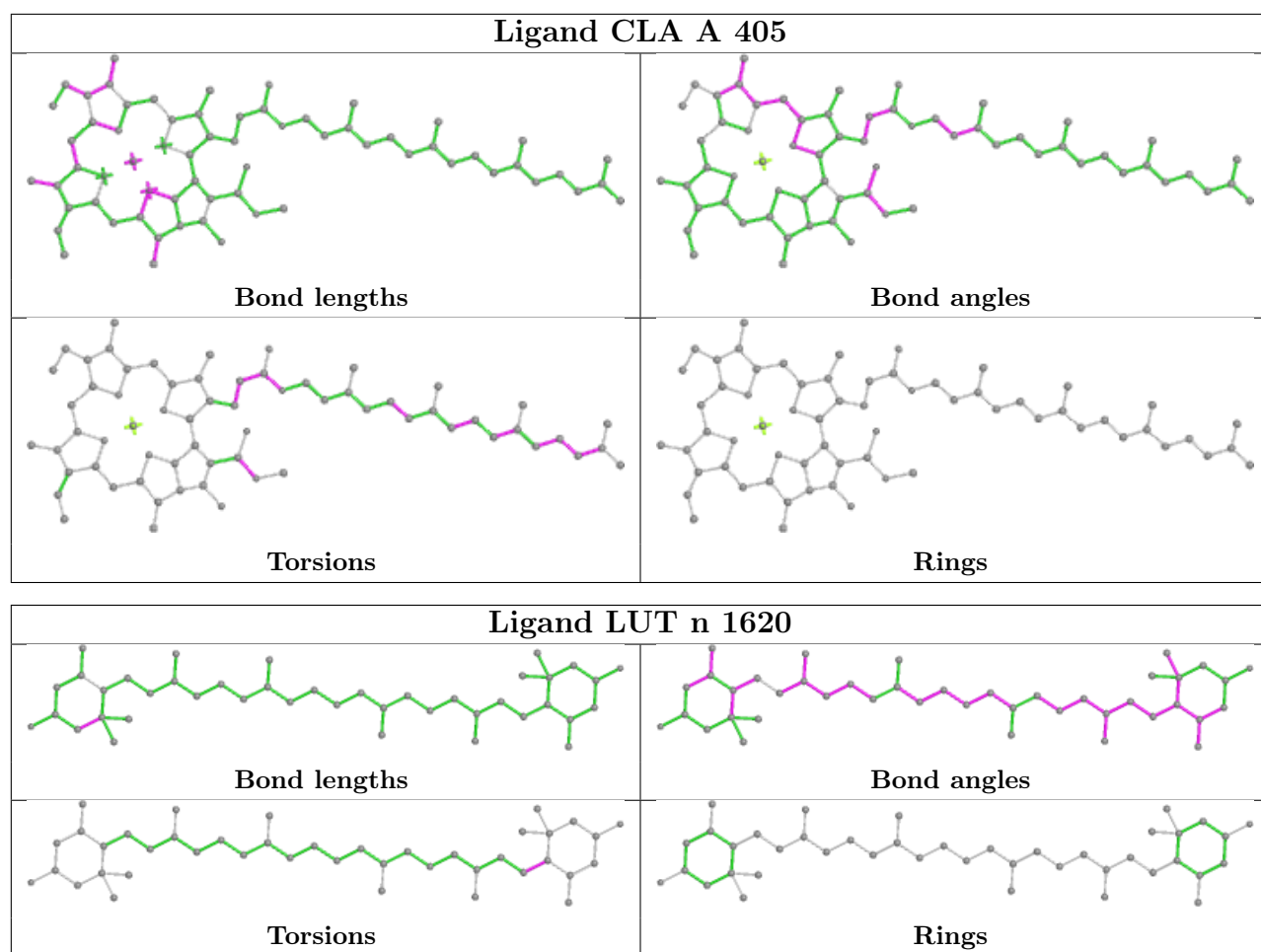


## Ligand DGD C 518

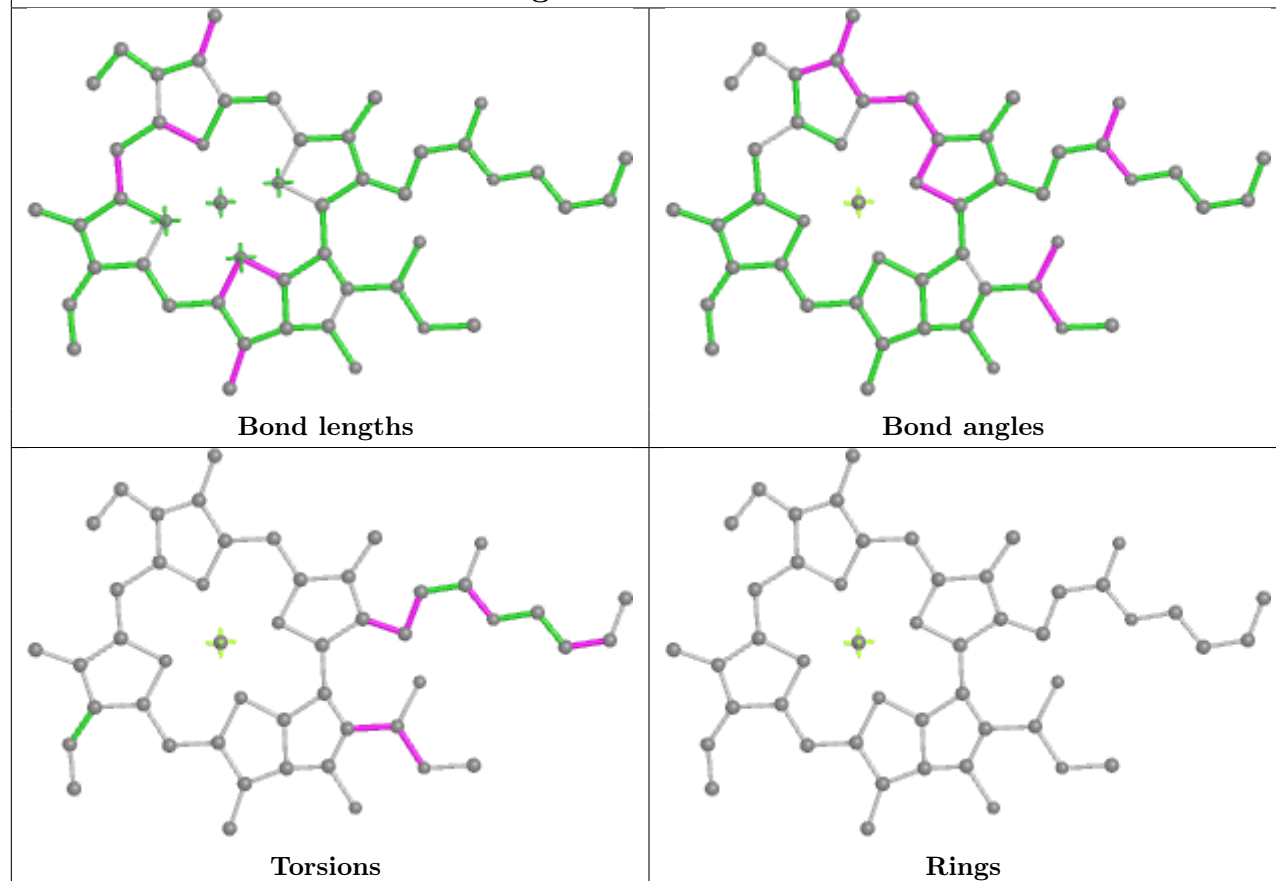




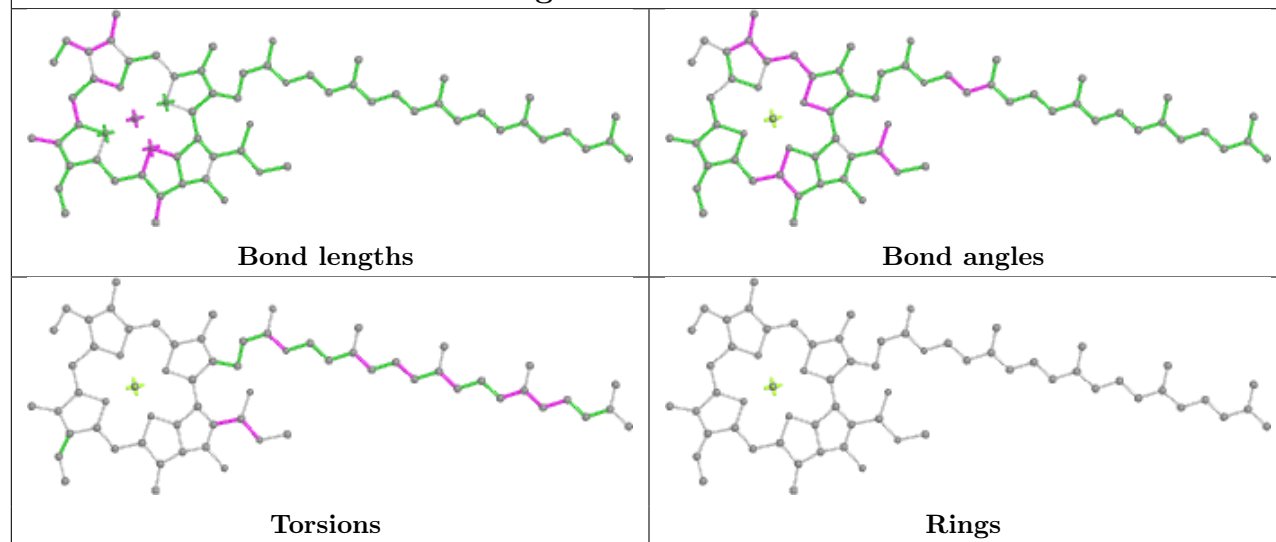
**Ligand CLA C 512****Ligand CLA r 609**

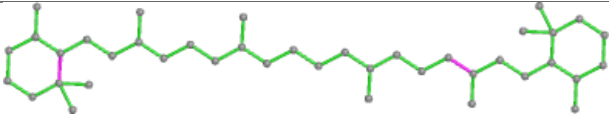
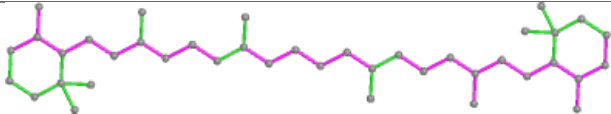
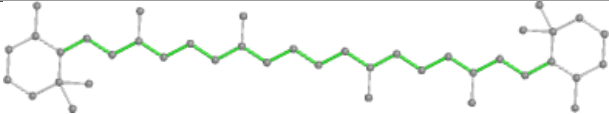
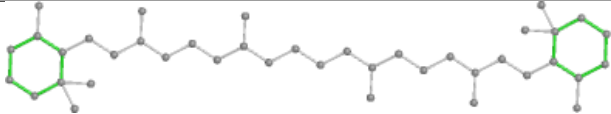
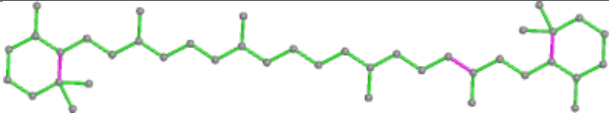
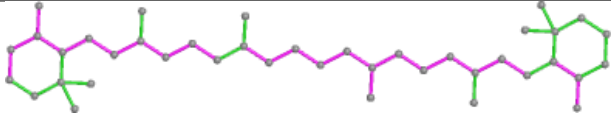
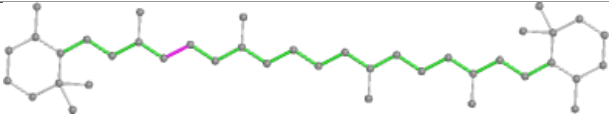
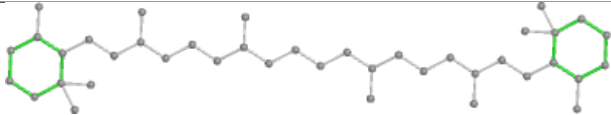
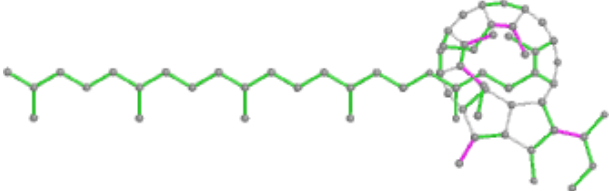
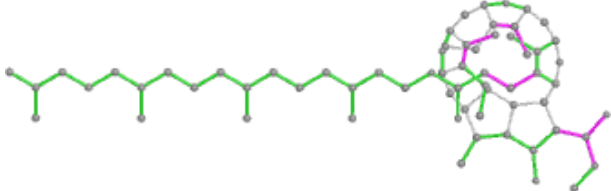
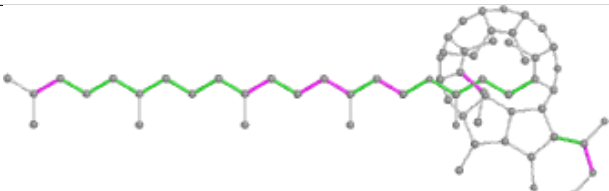
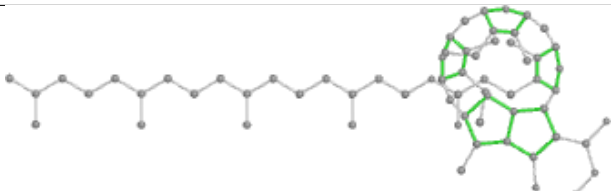
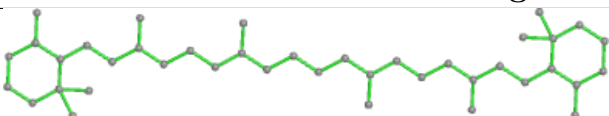
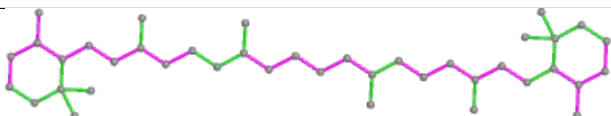
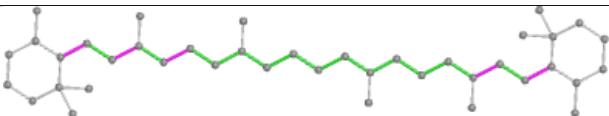
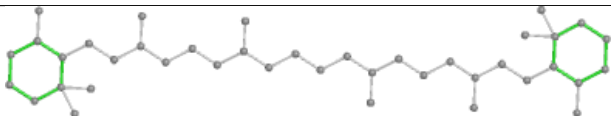


## Ligand CLA R 611

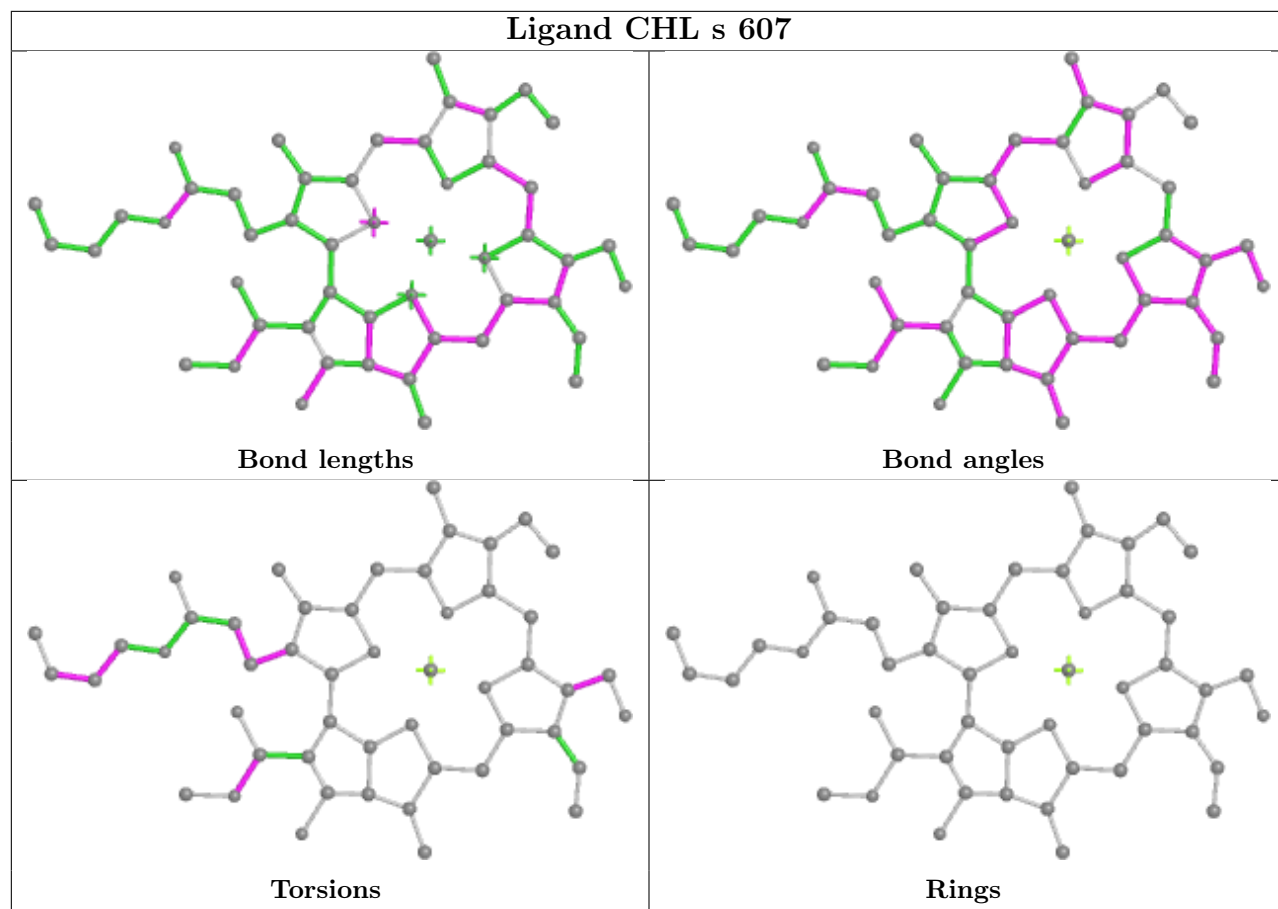


## Ligand CLA b 606

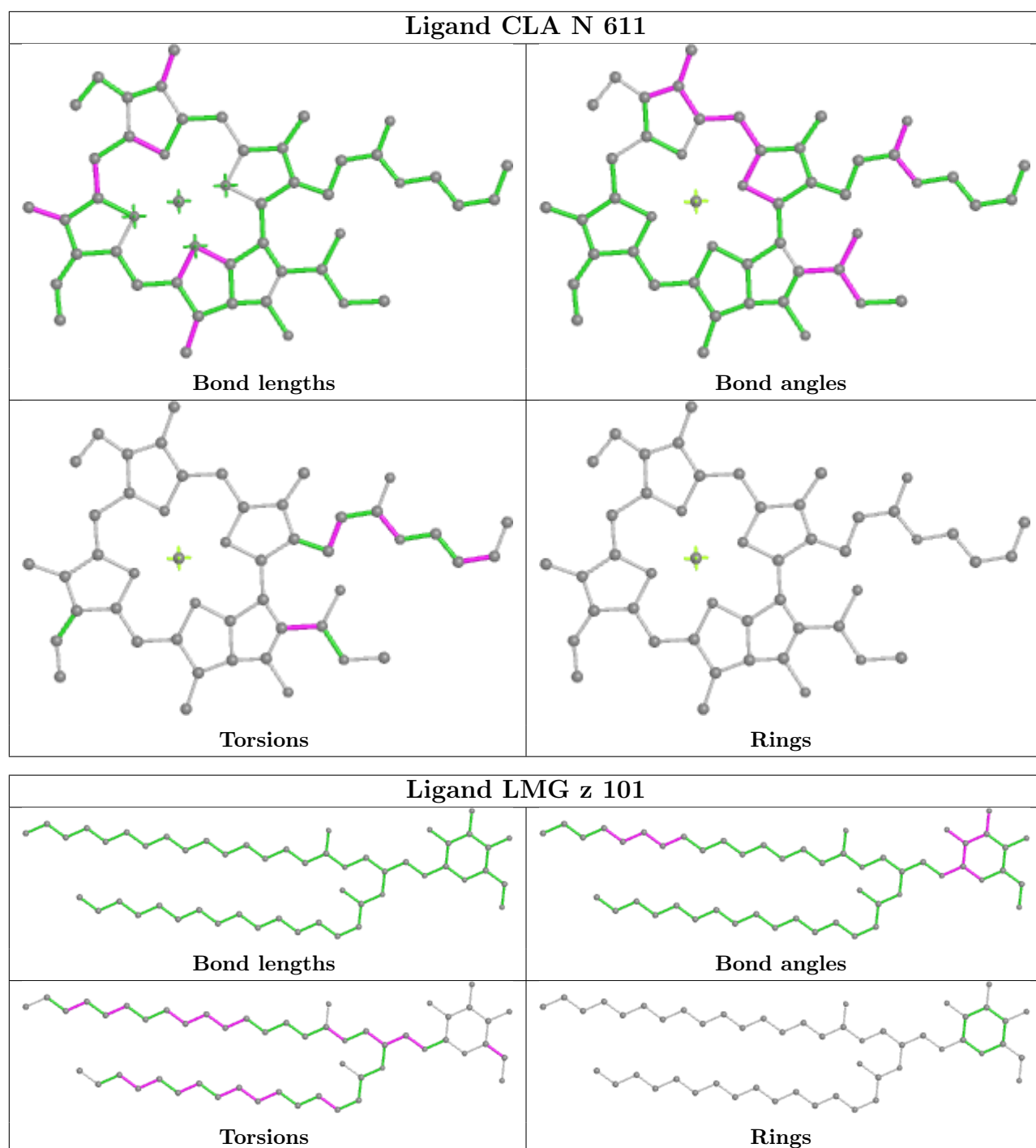


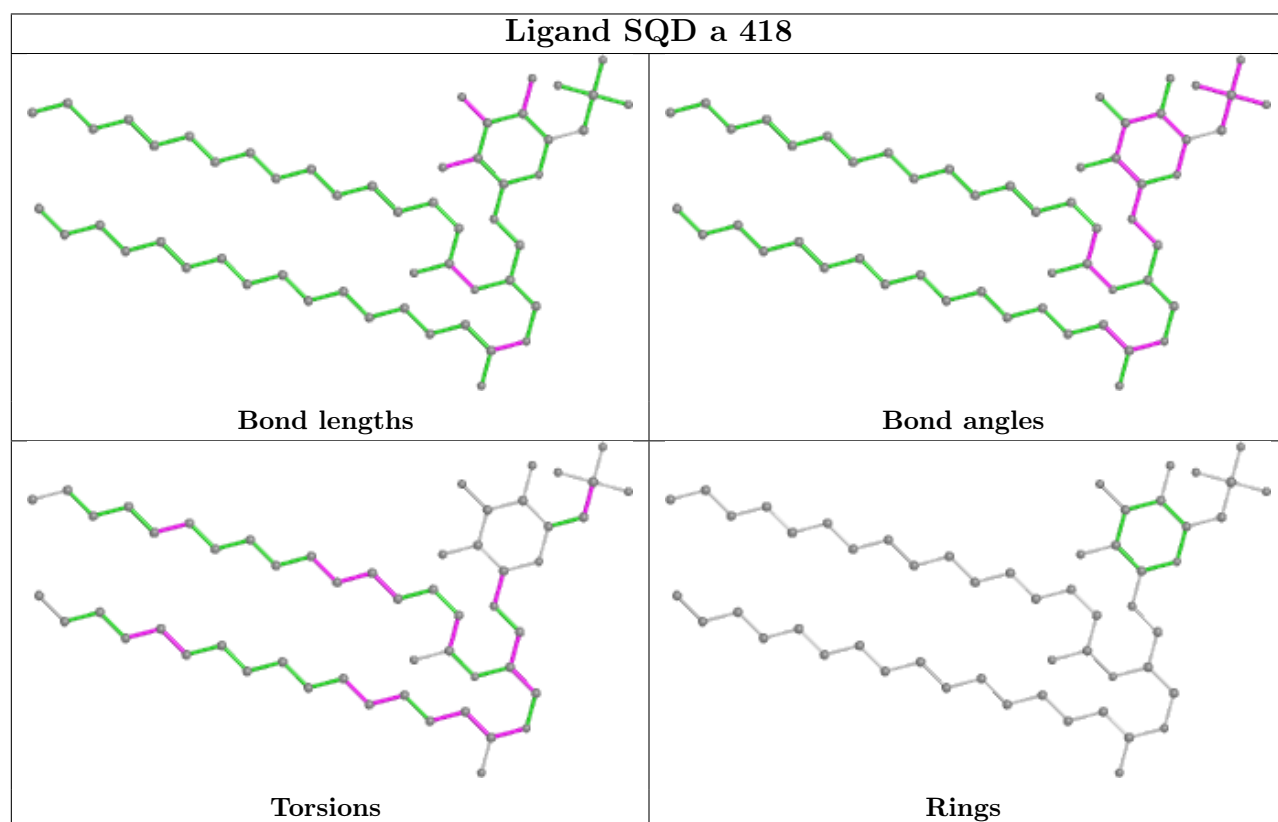
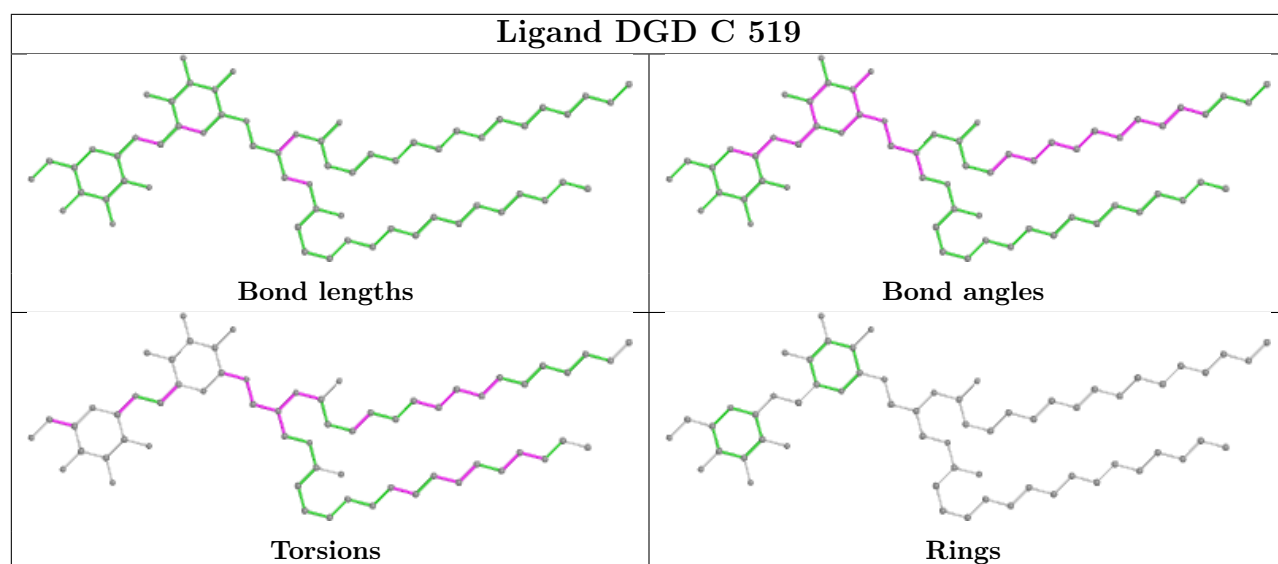
Ligand BCR a 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c 517	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PHO A 408	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR d 404	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

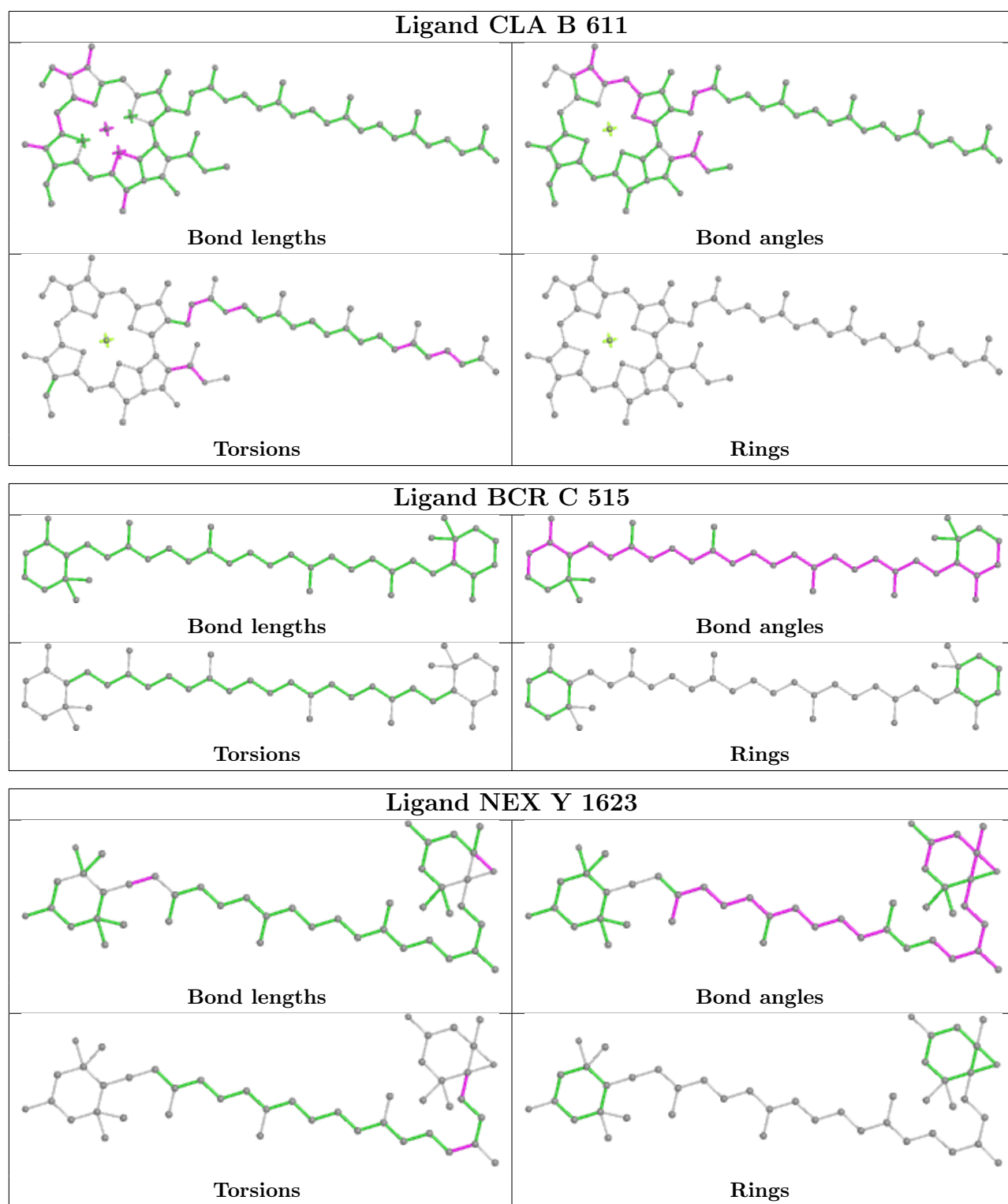
## Ligand CHL s 607

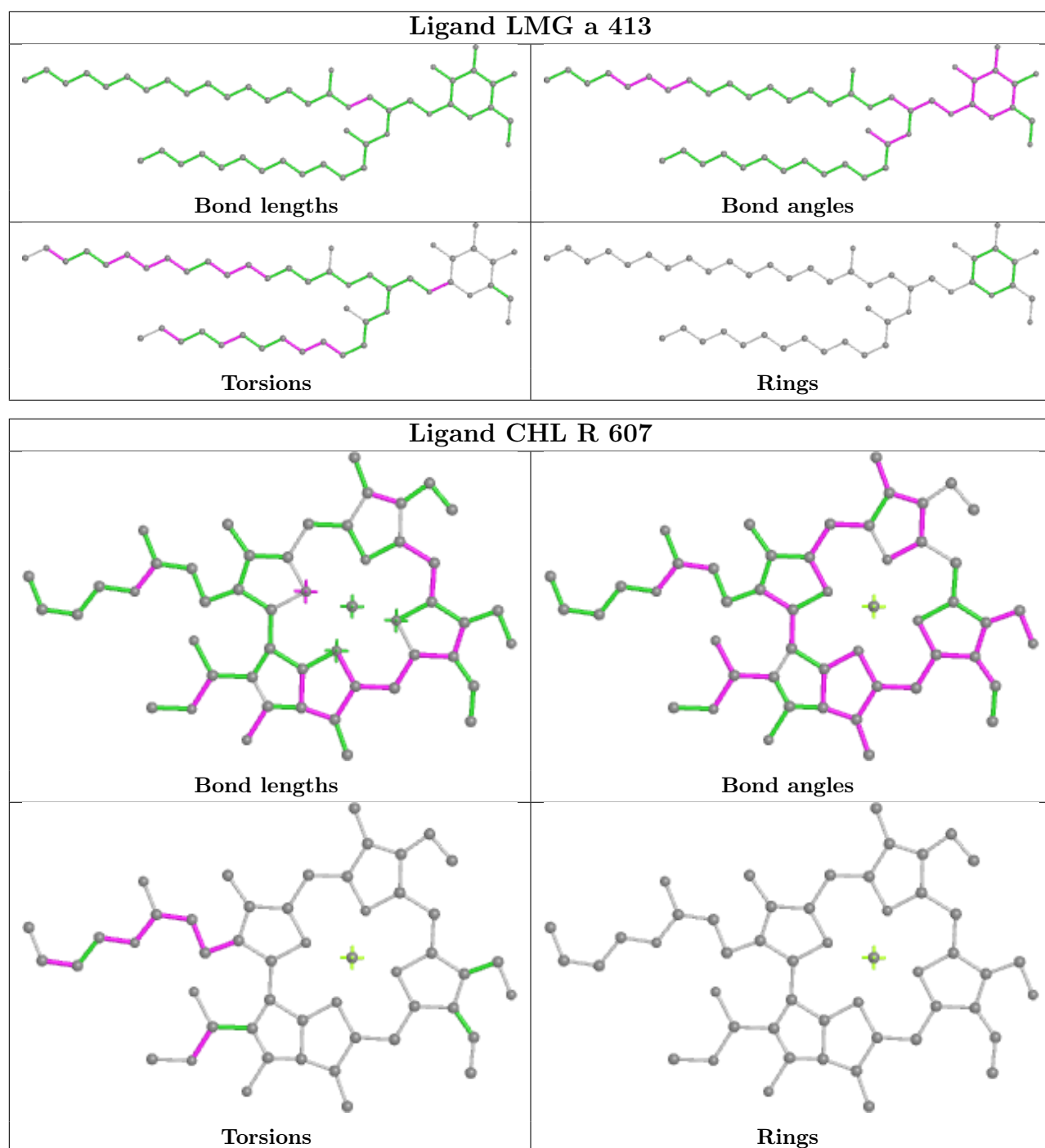


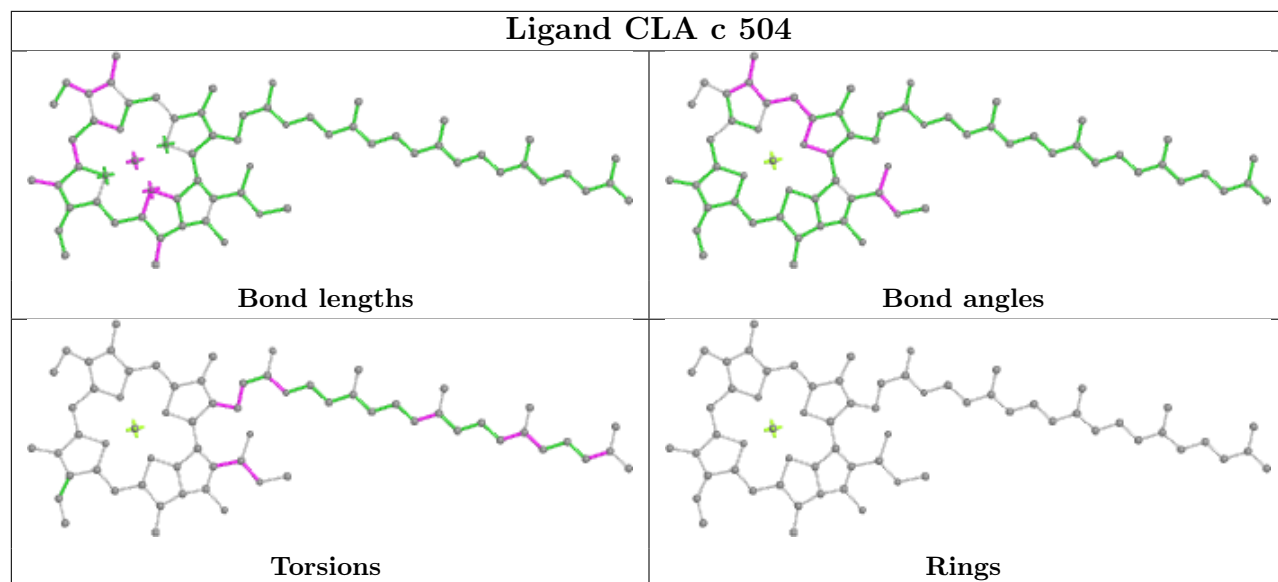
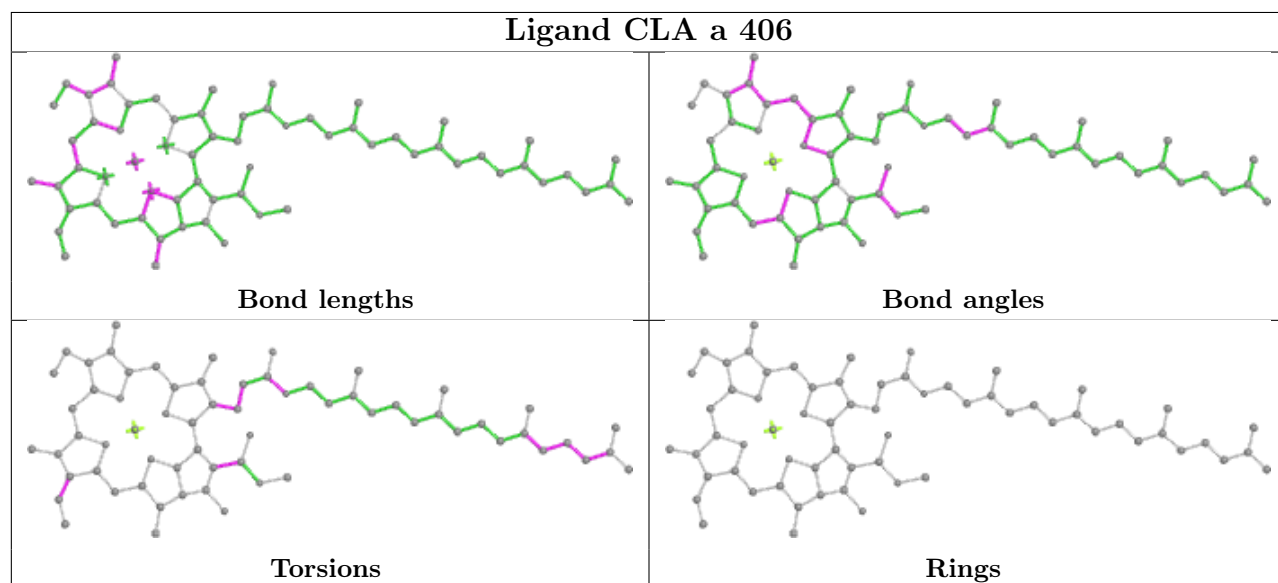




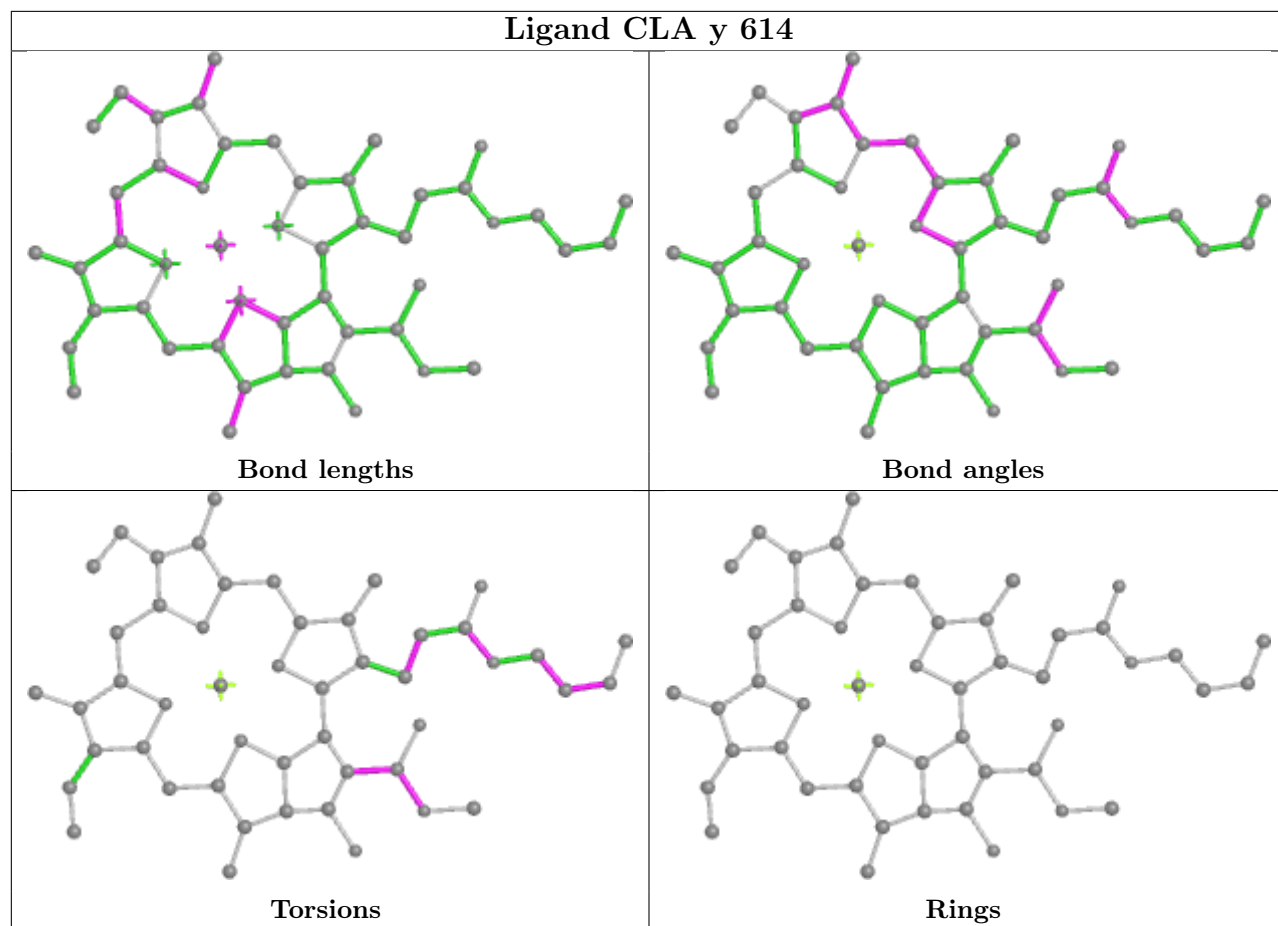


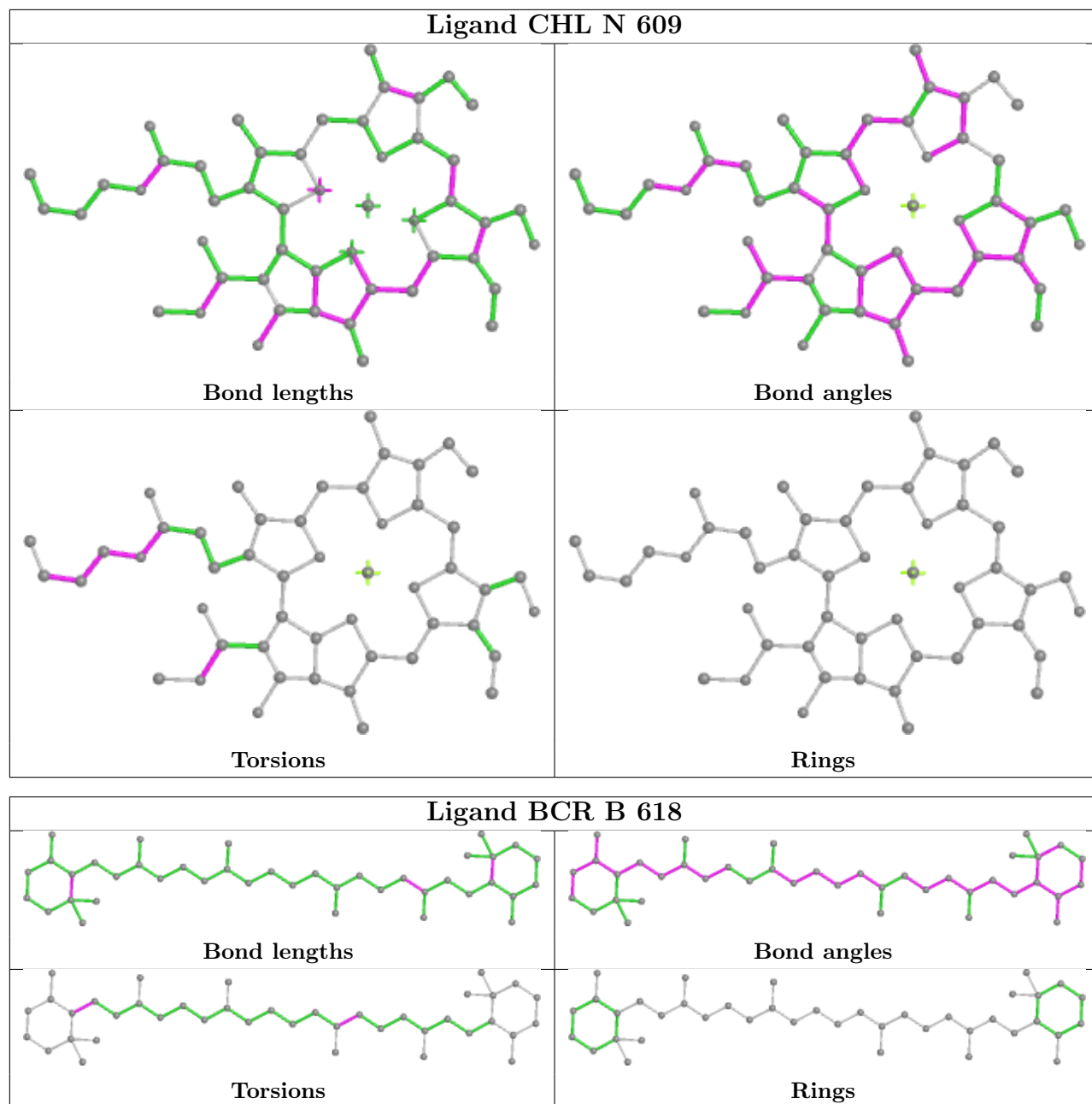


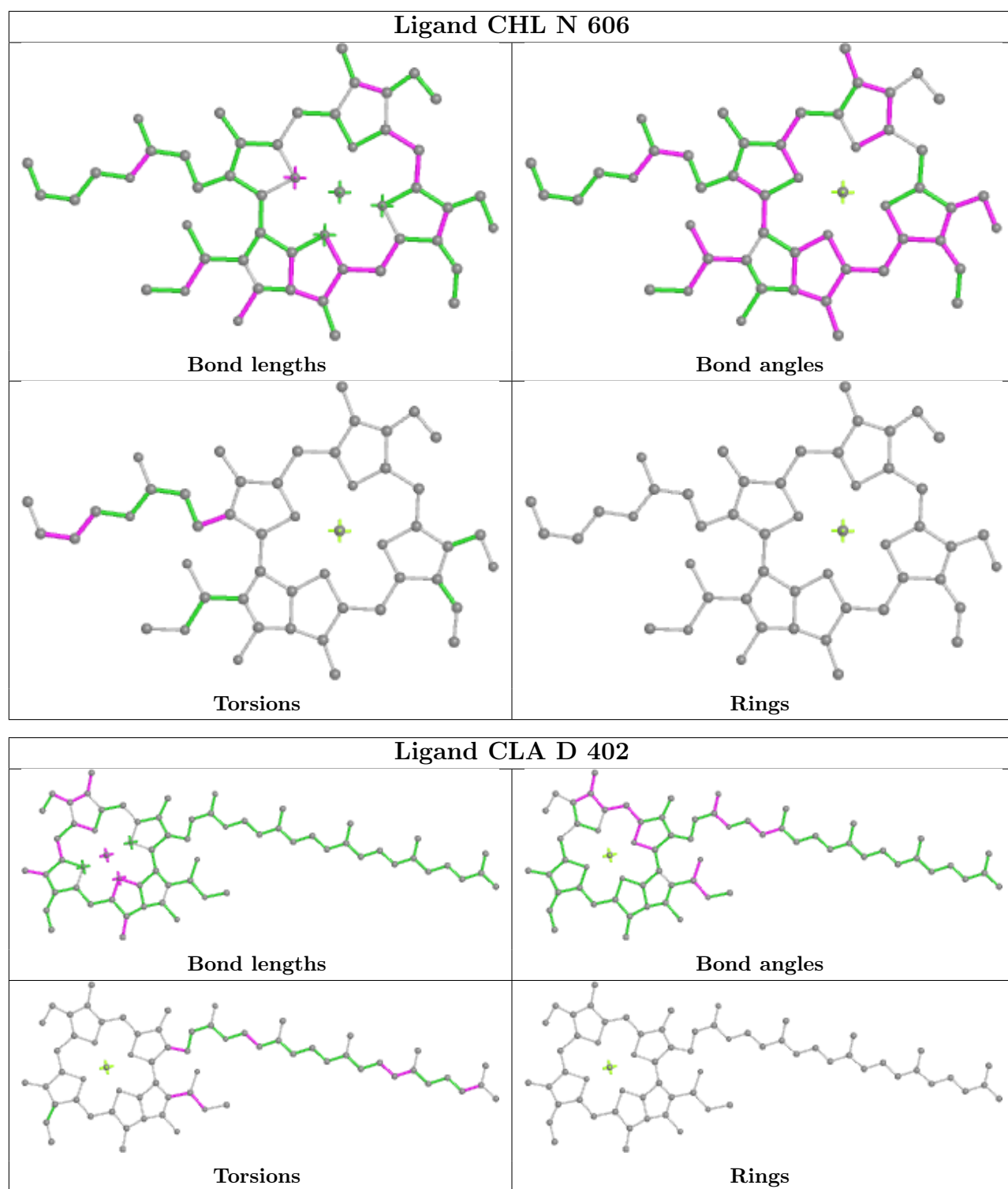


**Ligand CLA c 504****Ligand CLA a 406**

## Ligand CLA y 614

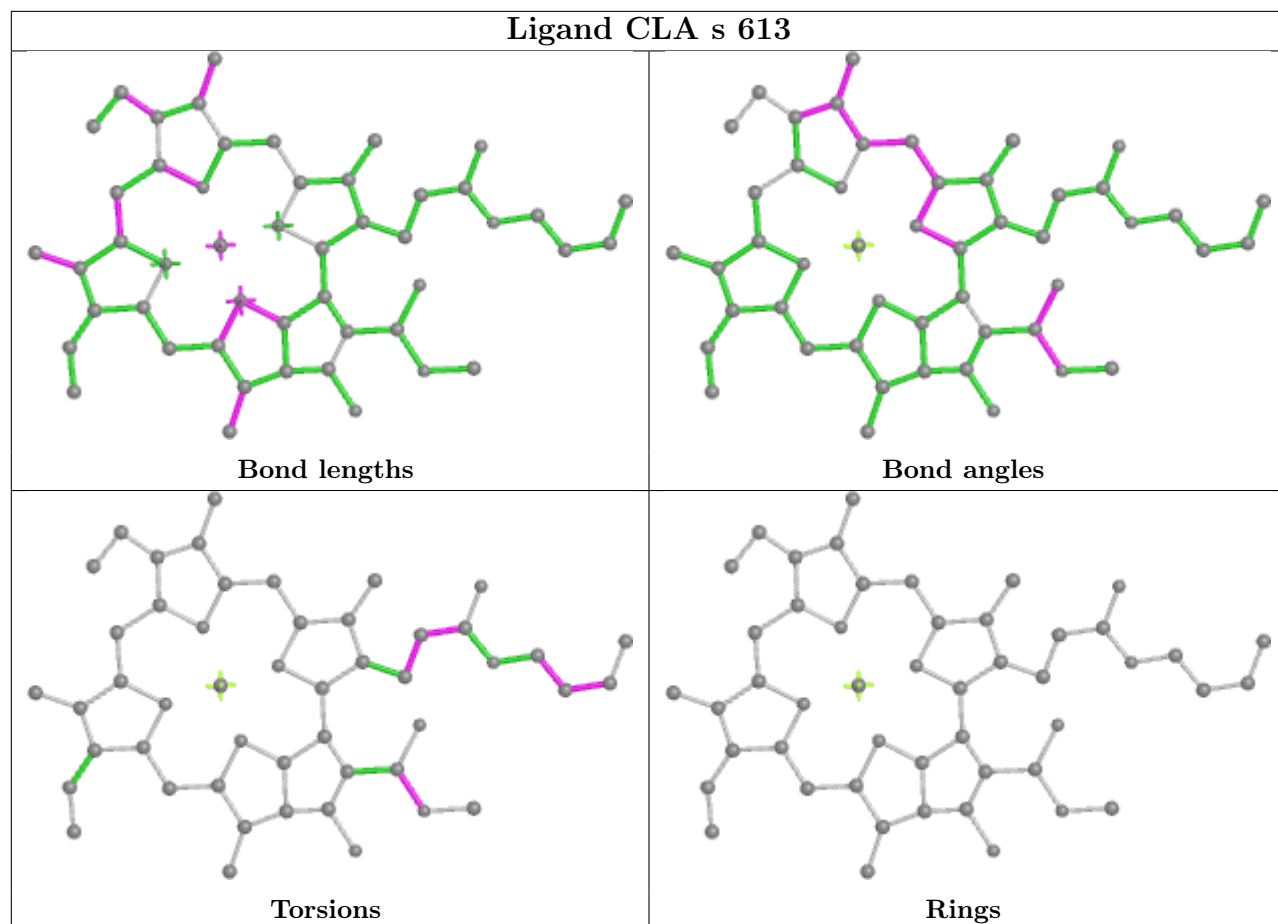




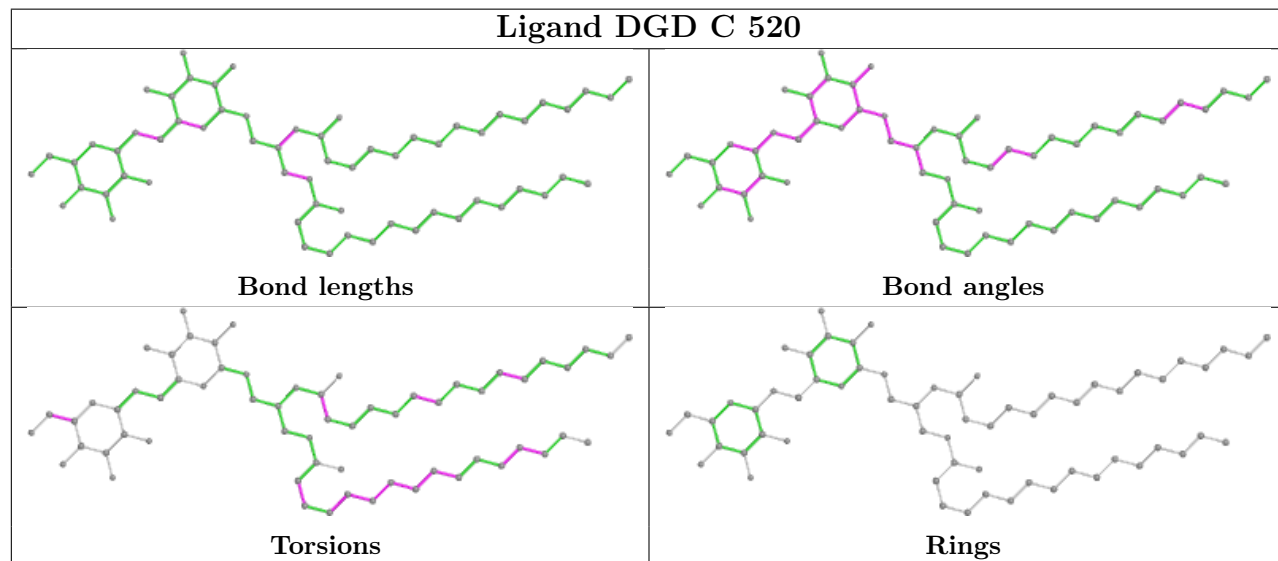


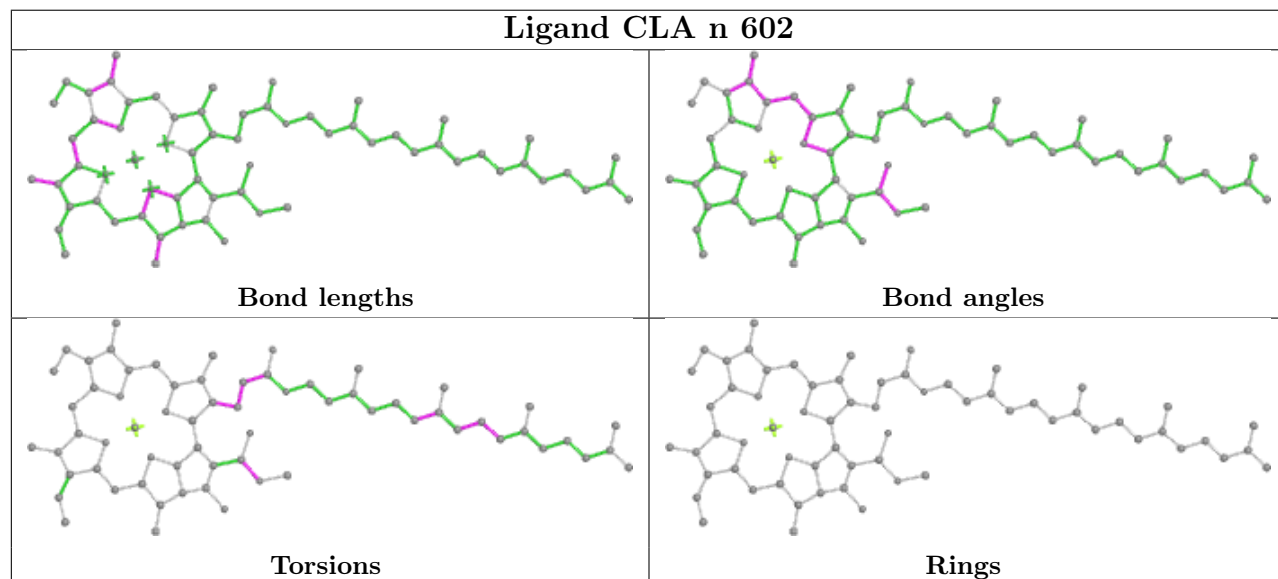
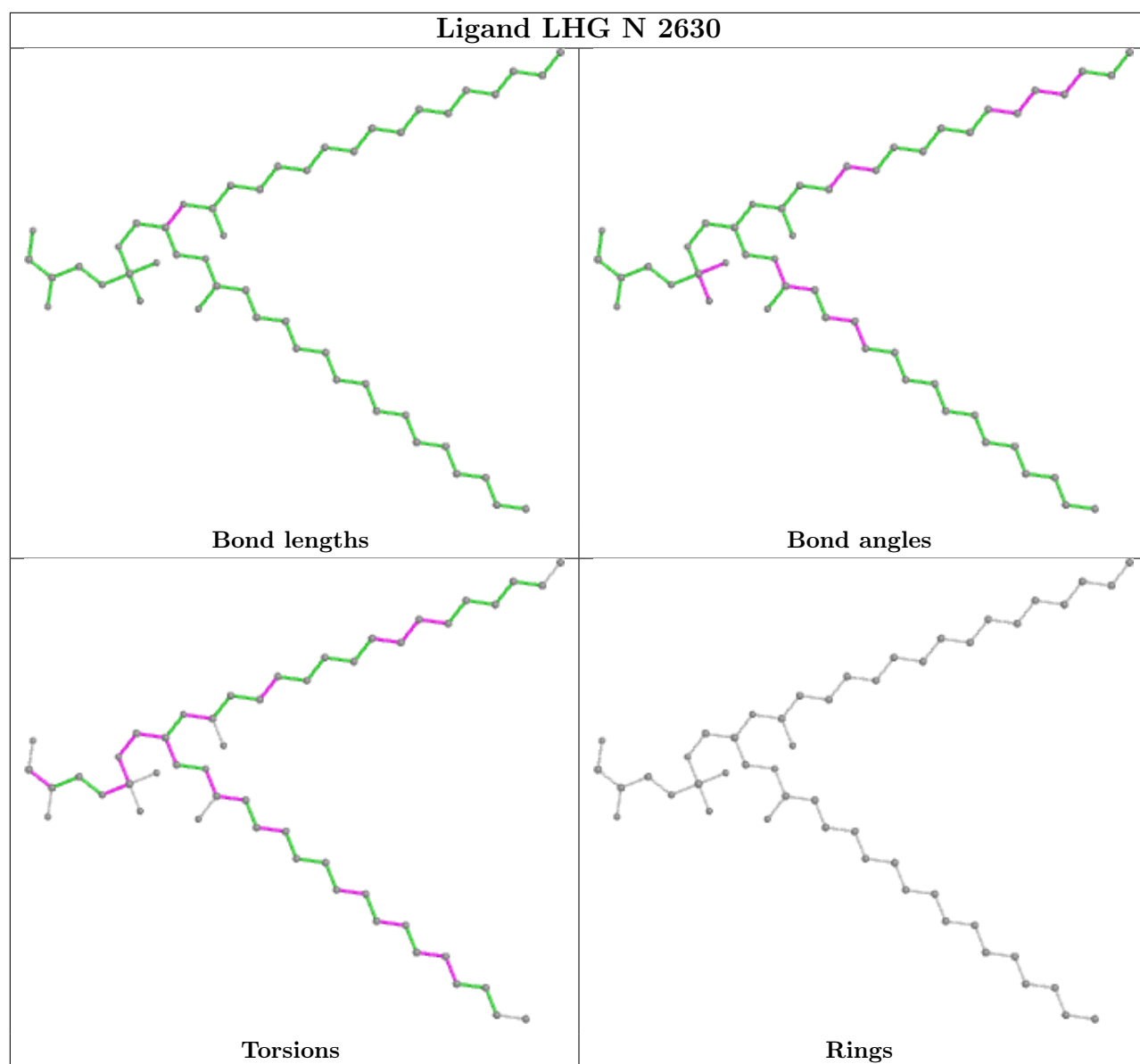


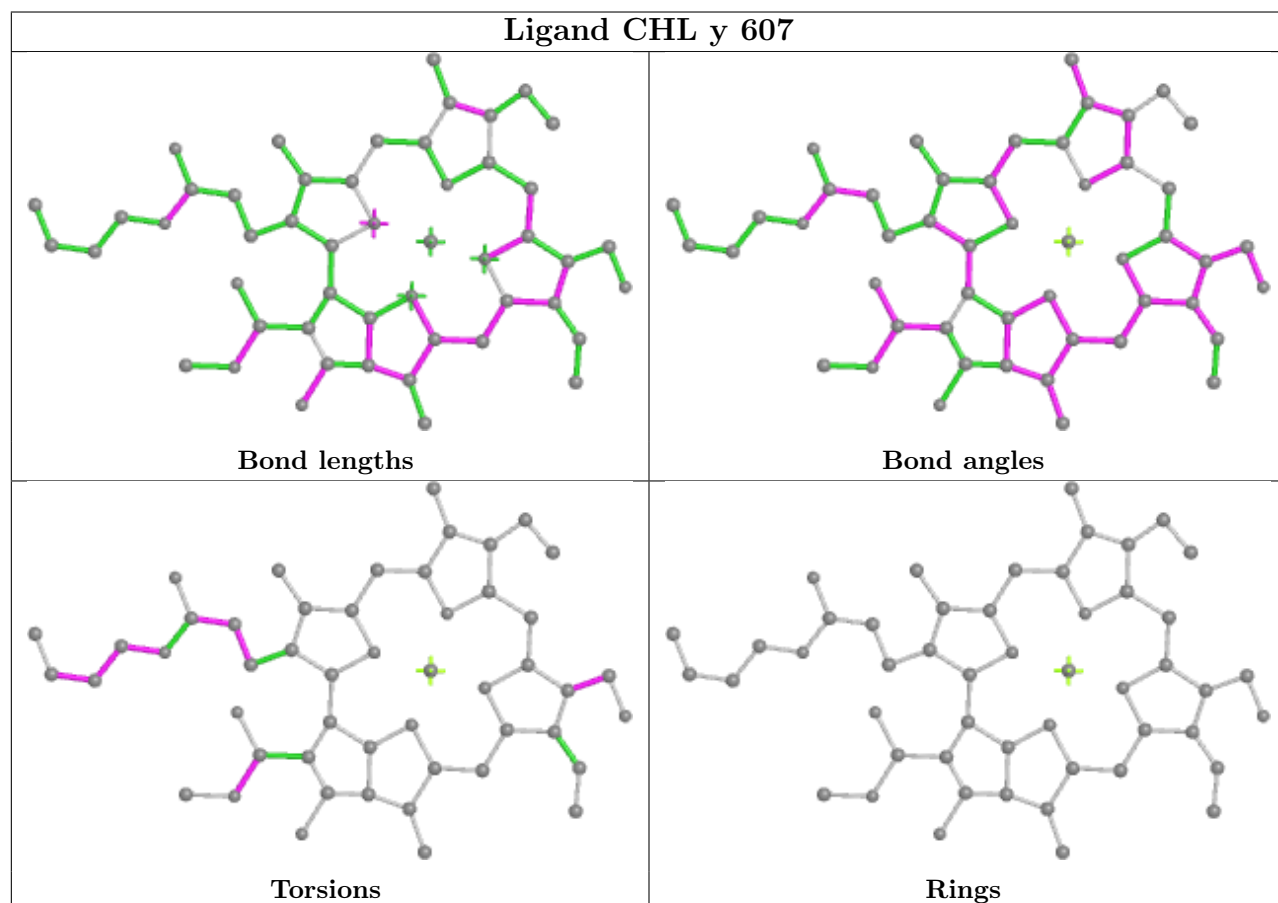
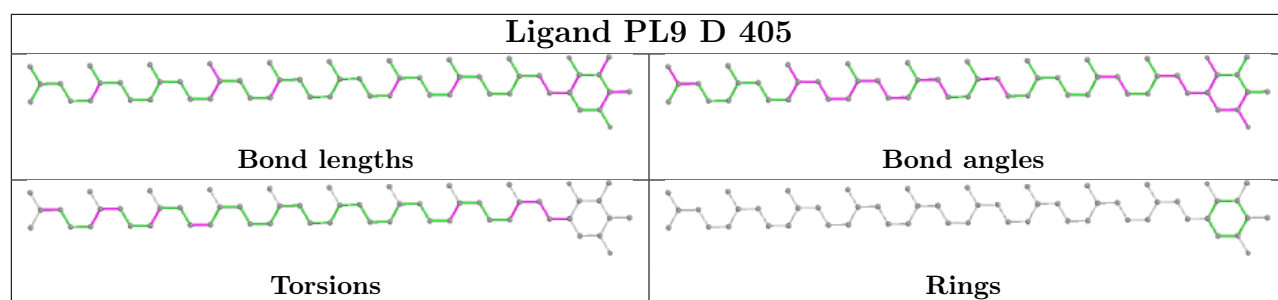
## Ligand CLA s 613

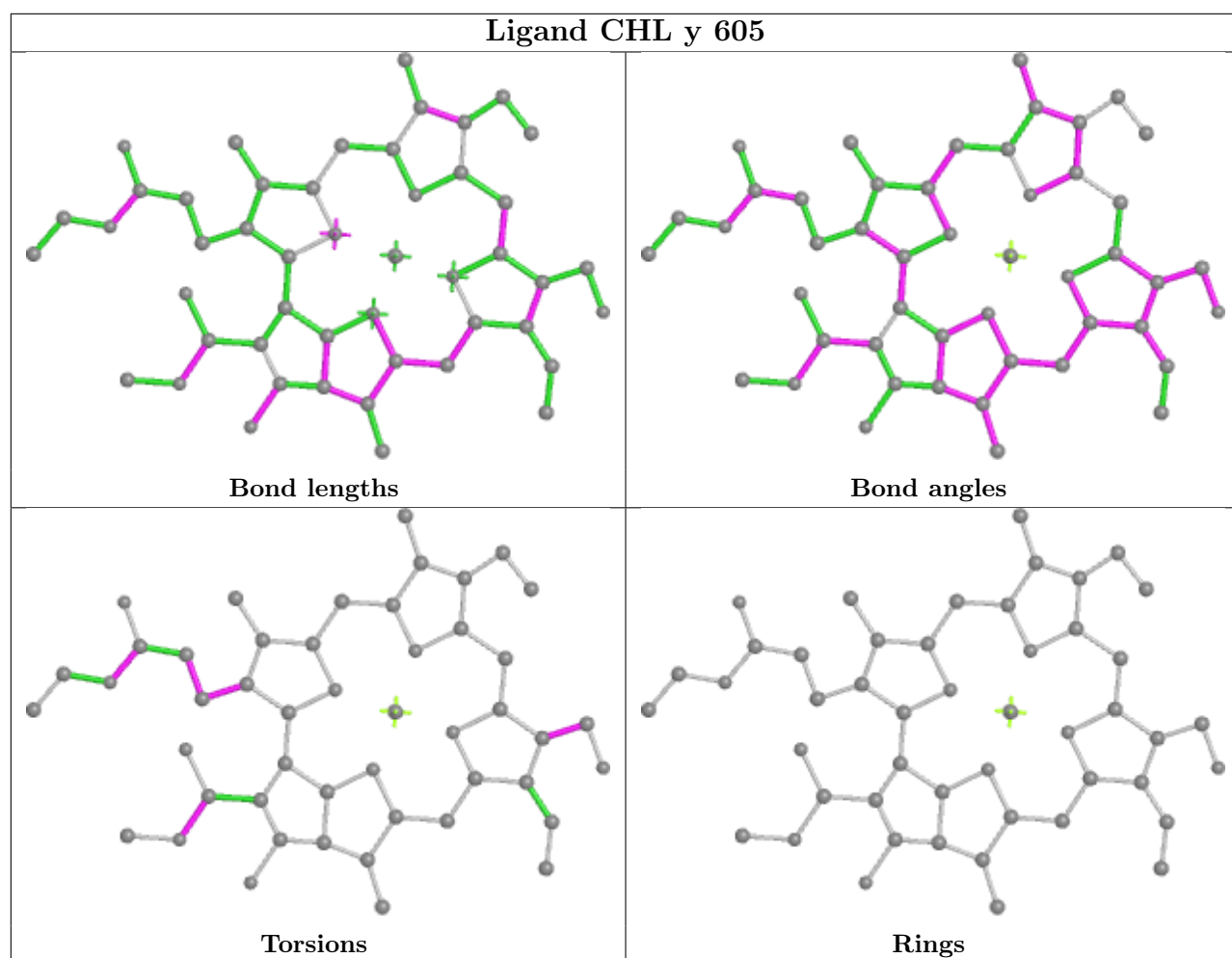


## Ligand DGD C 520

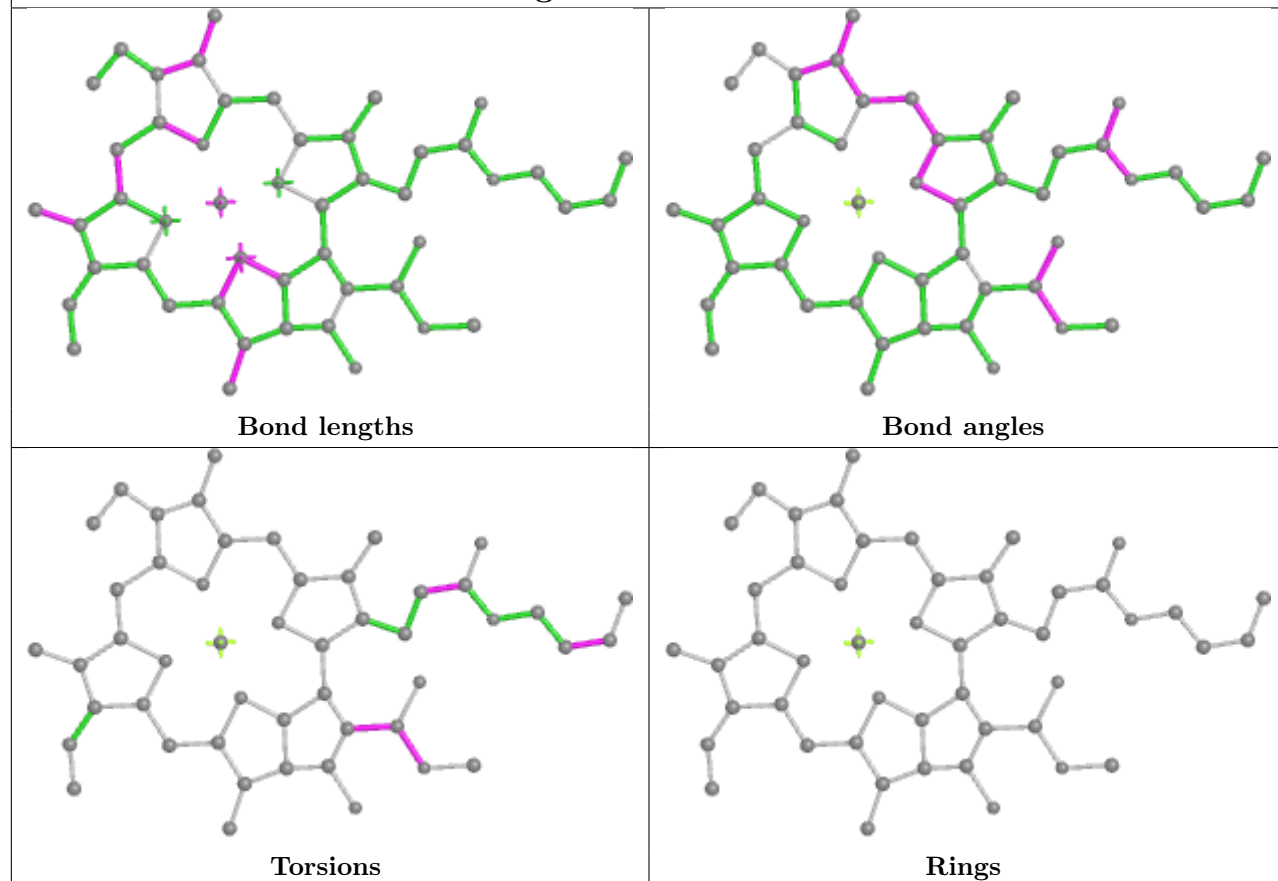




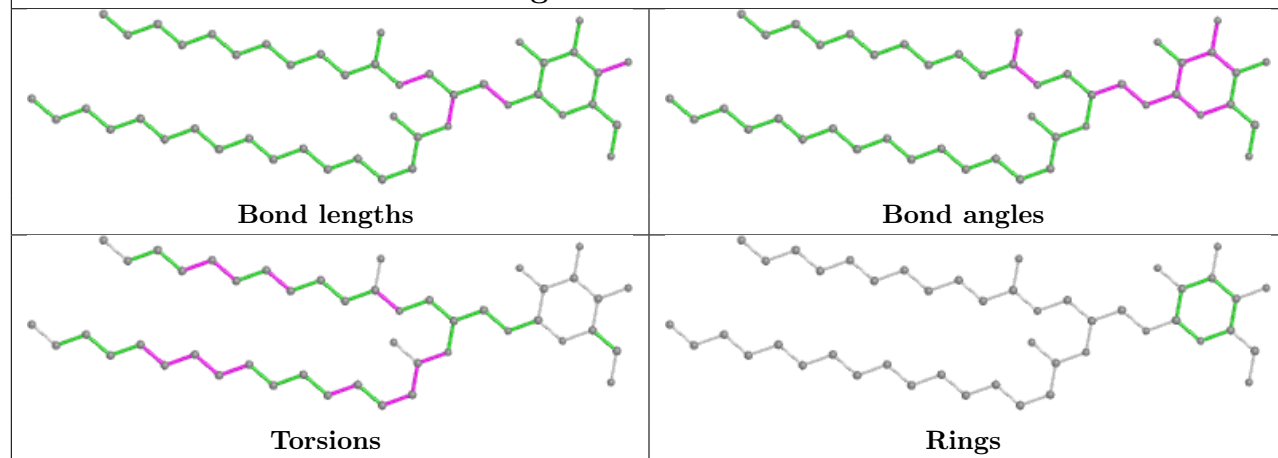


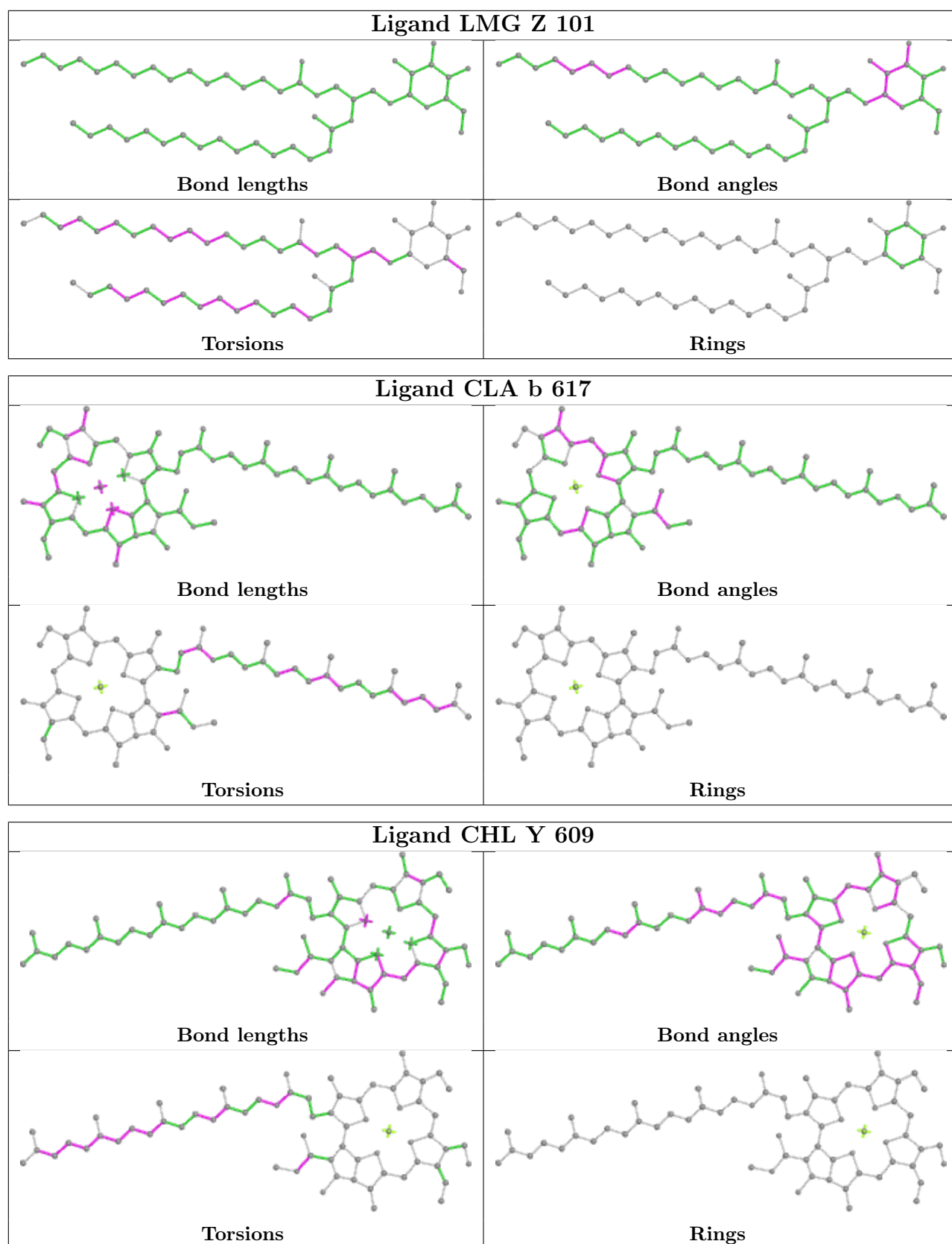


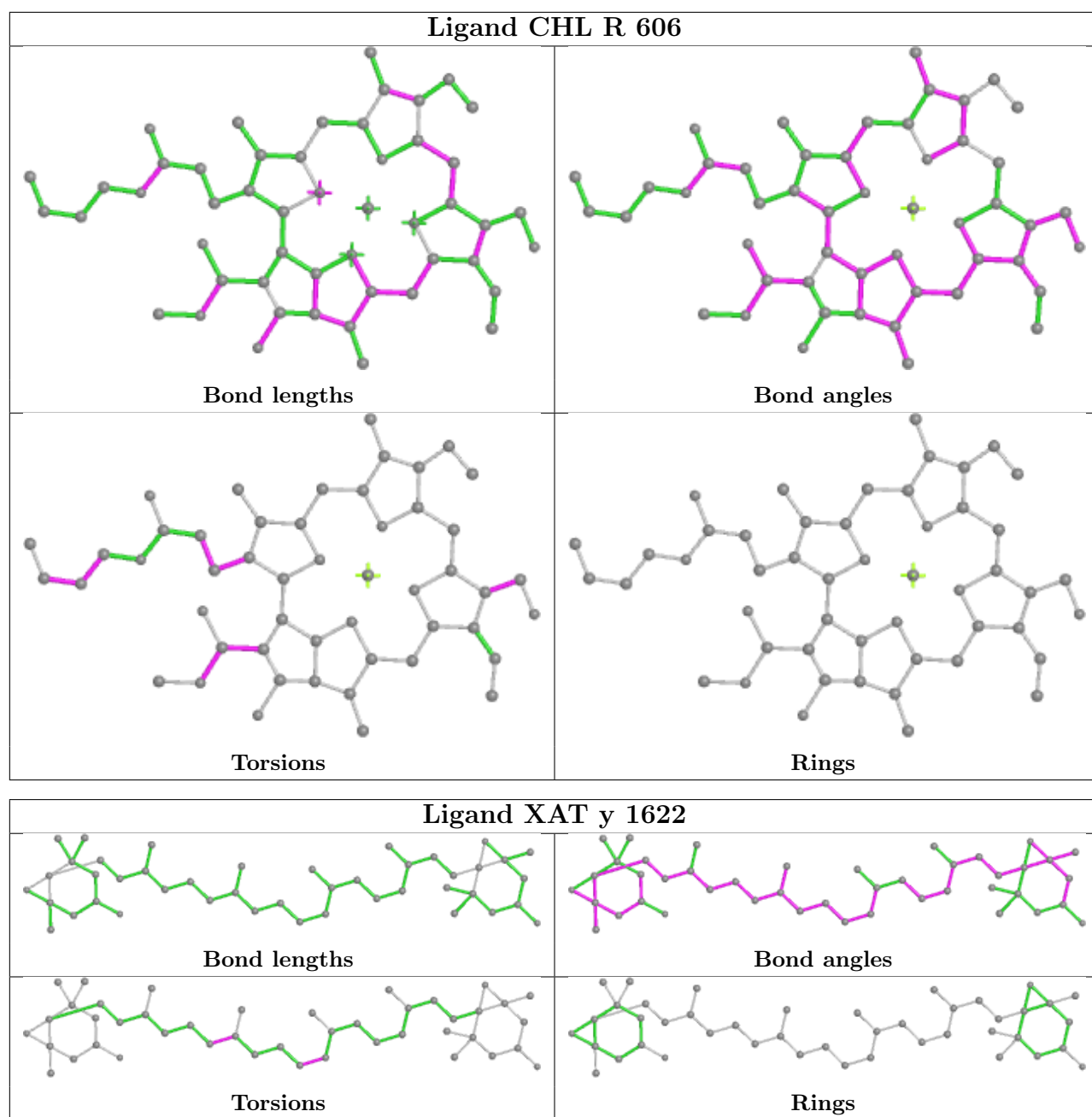
## Ligand CLA S 612



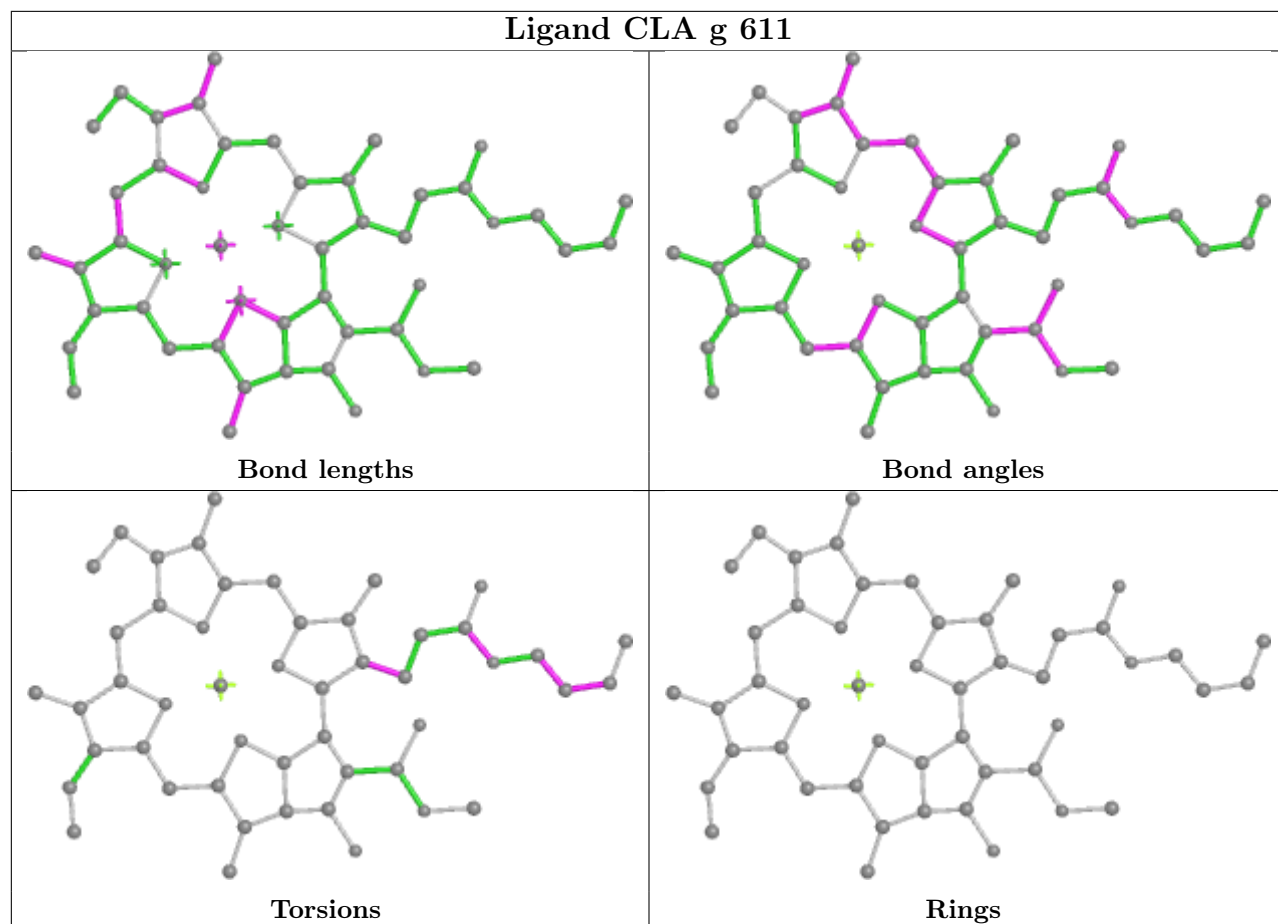
## Ligand LMG d 411



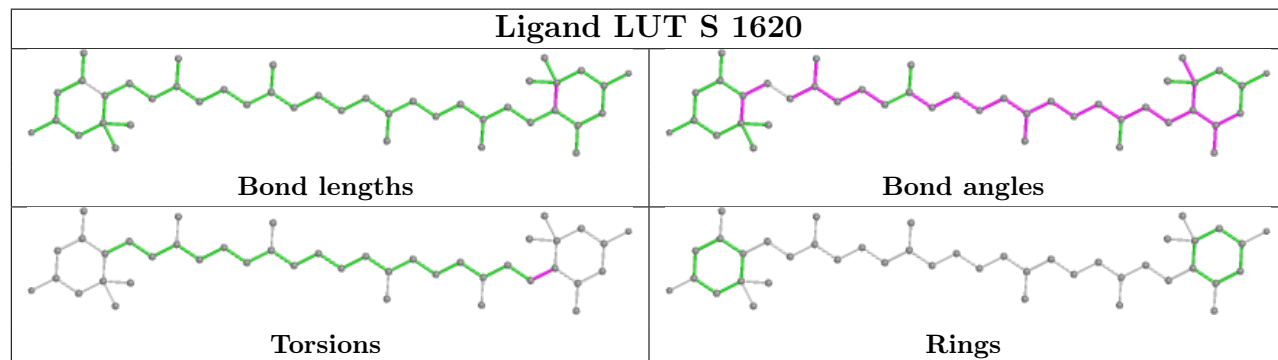




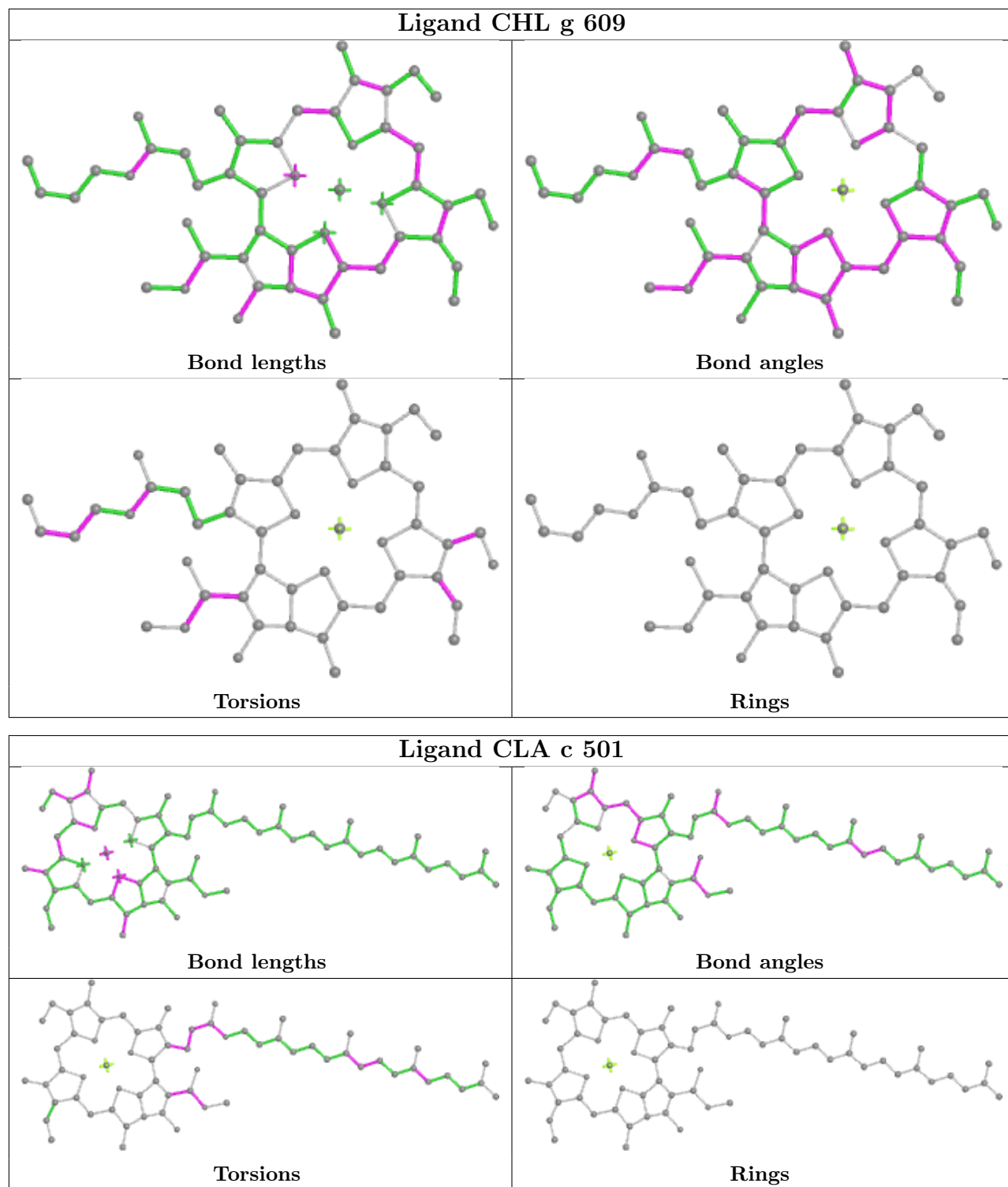
## Ligand CLA g 611

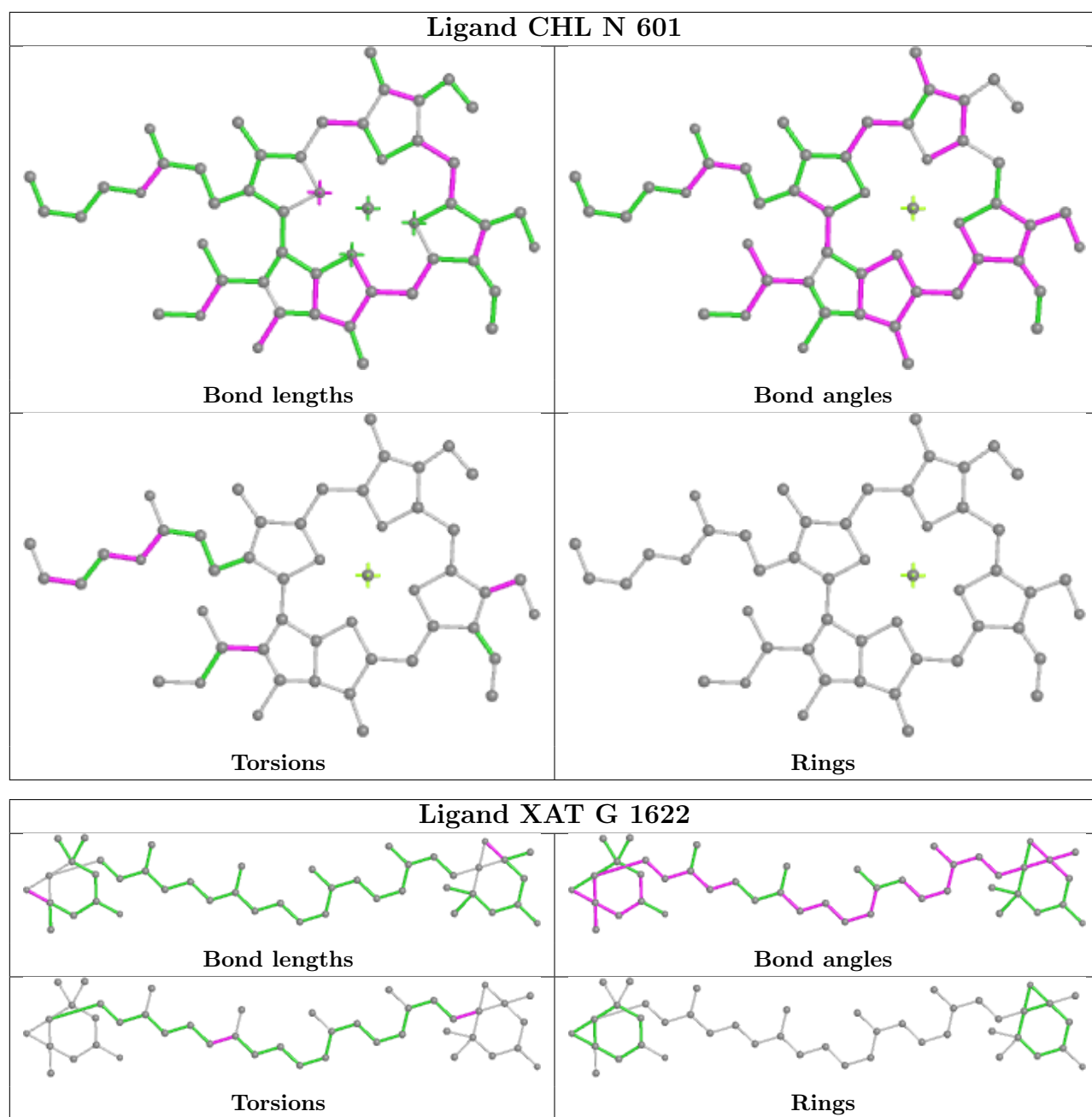


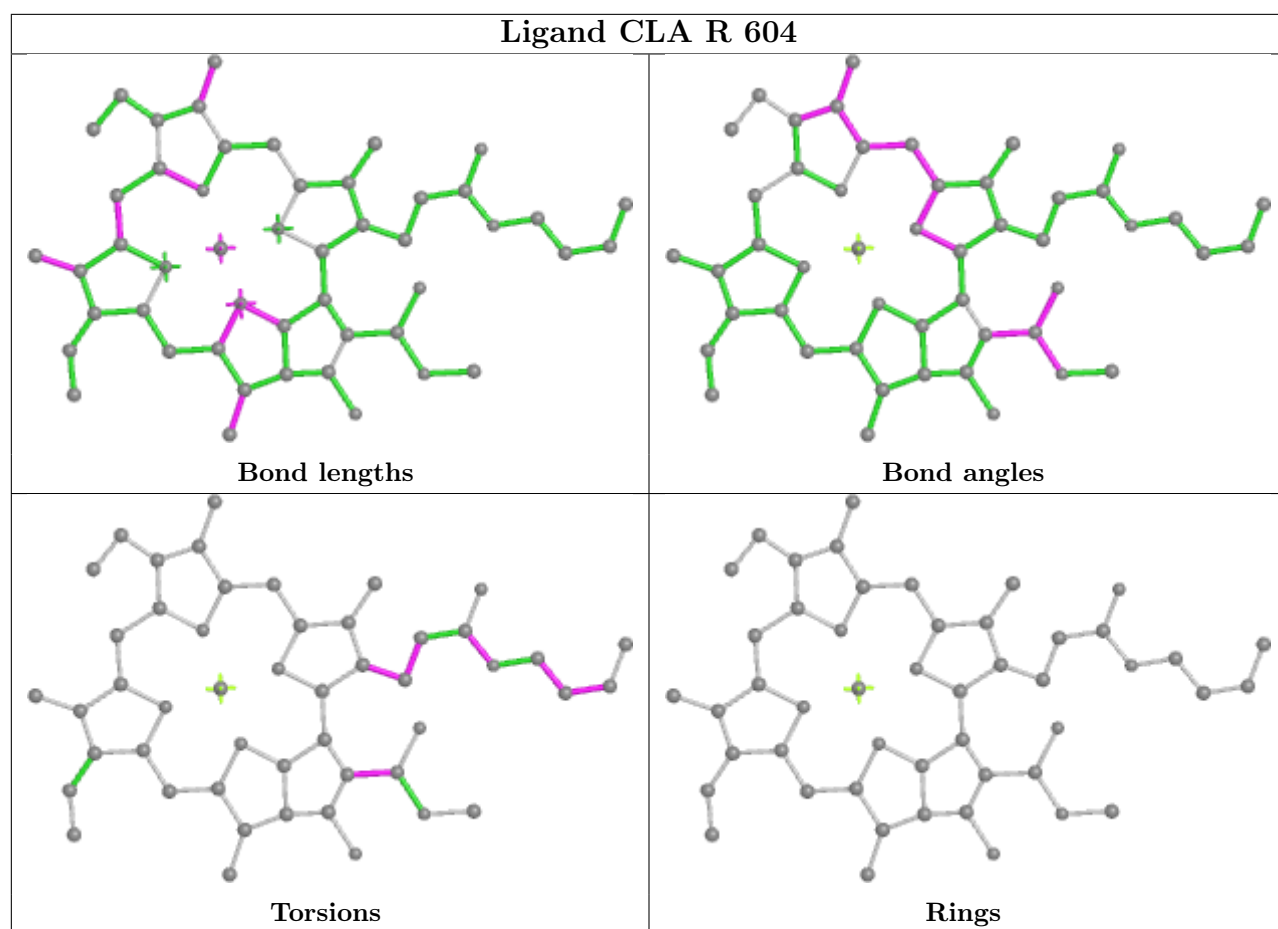
## Ligand LUT S 1620

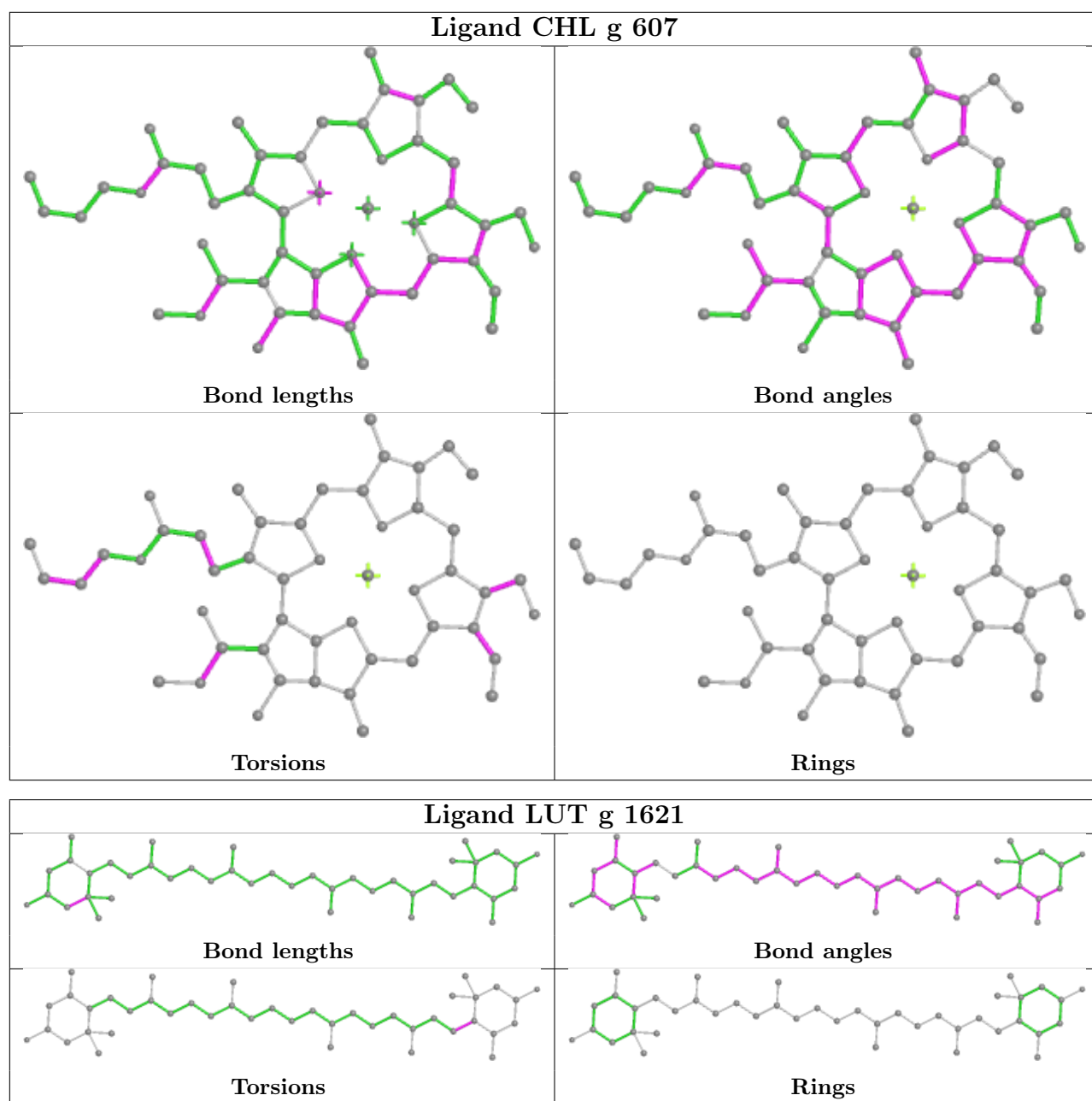


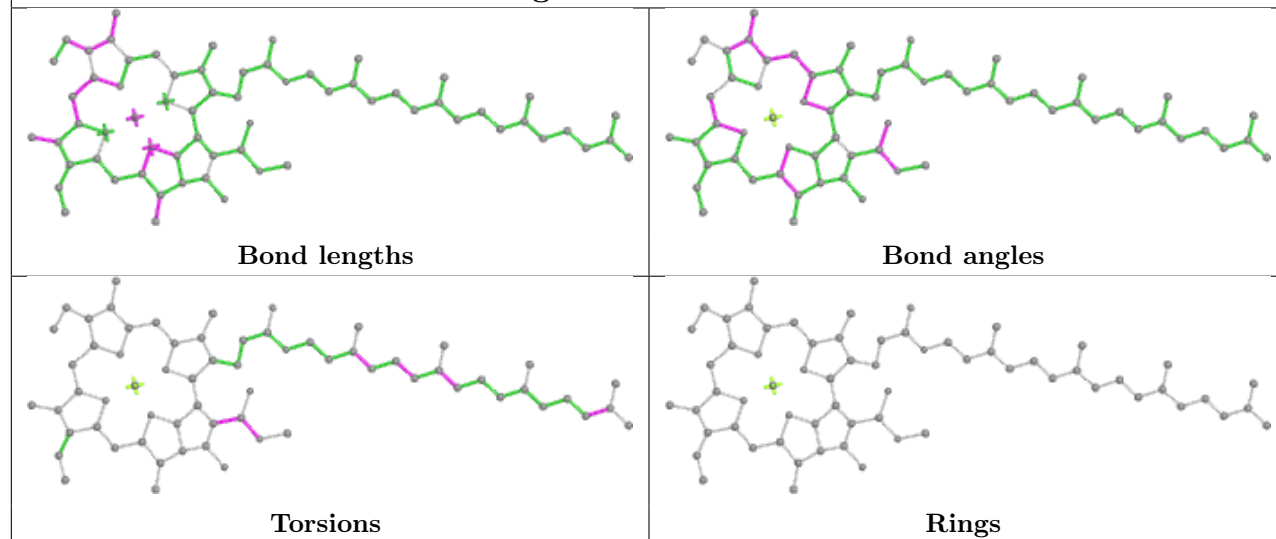
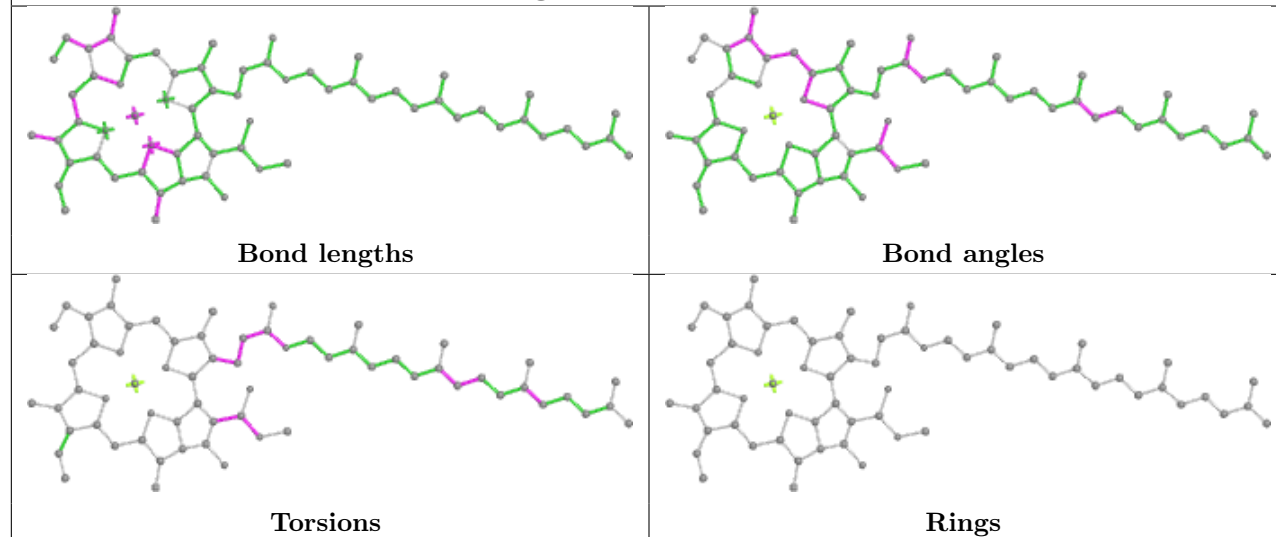




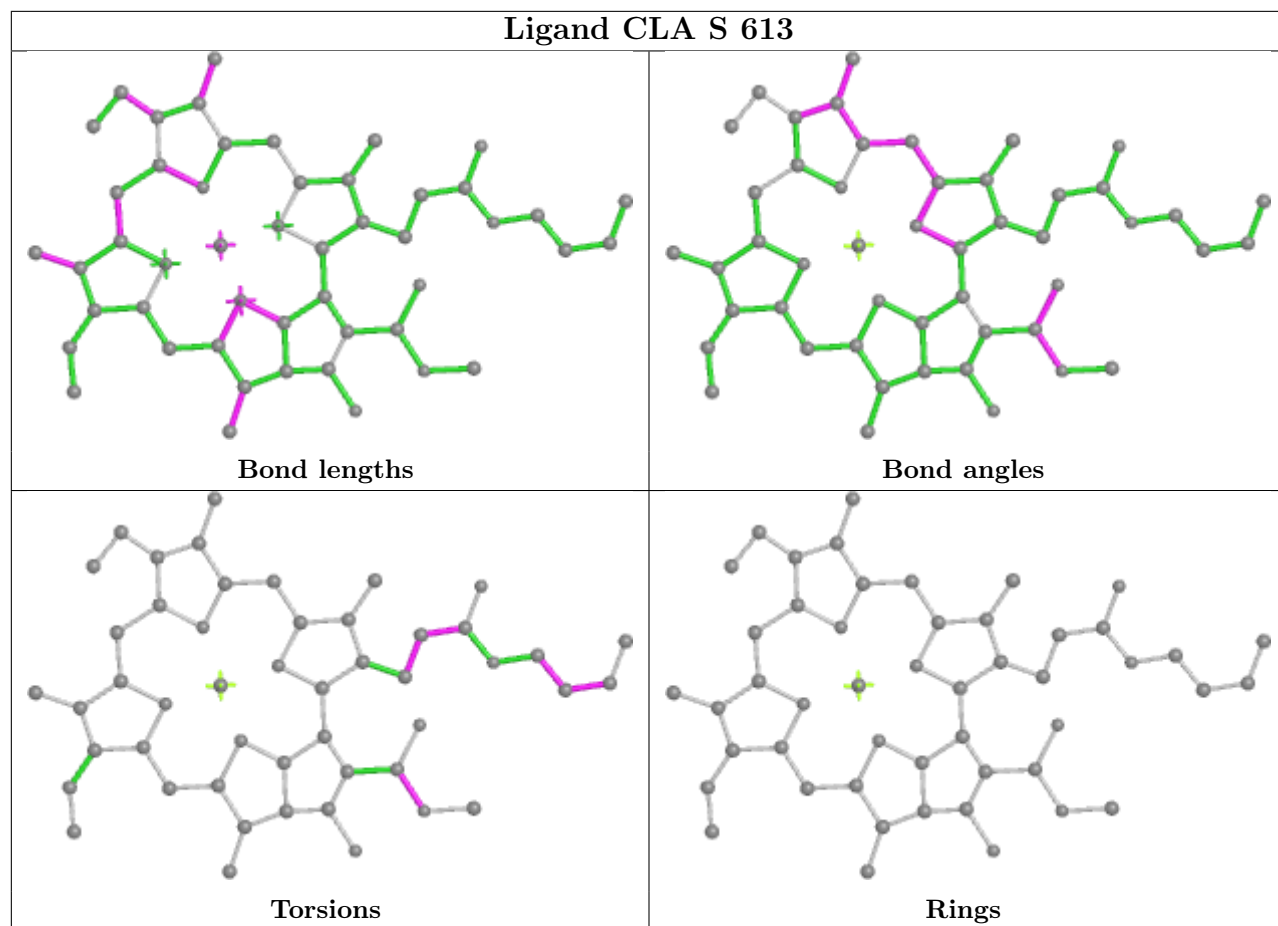


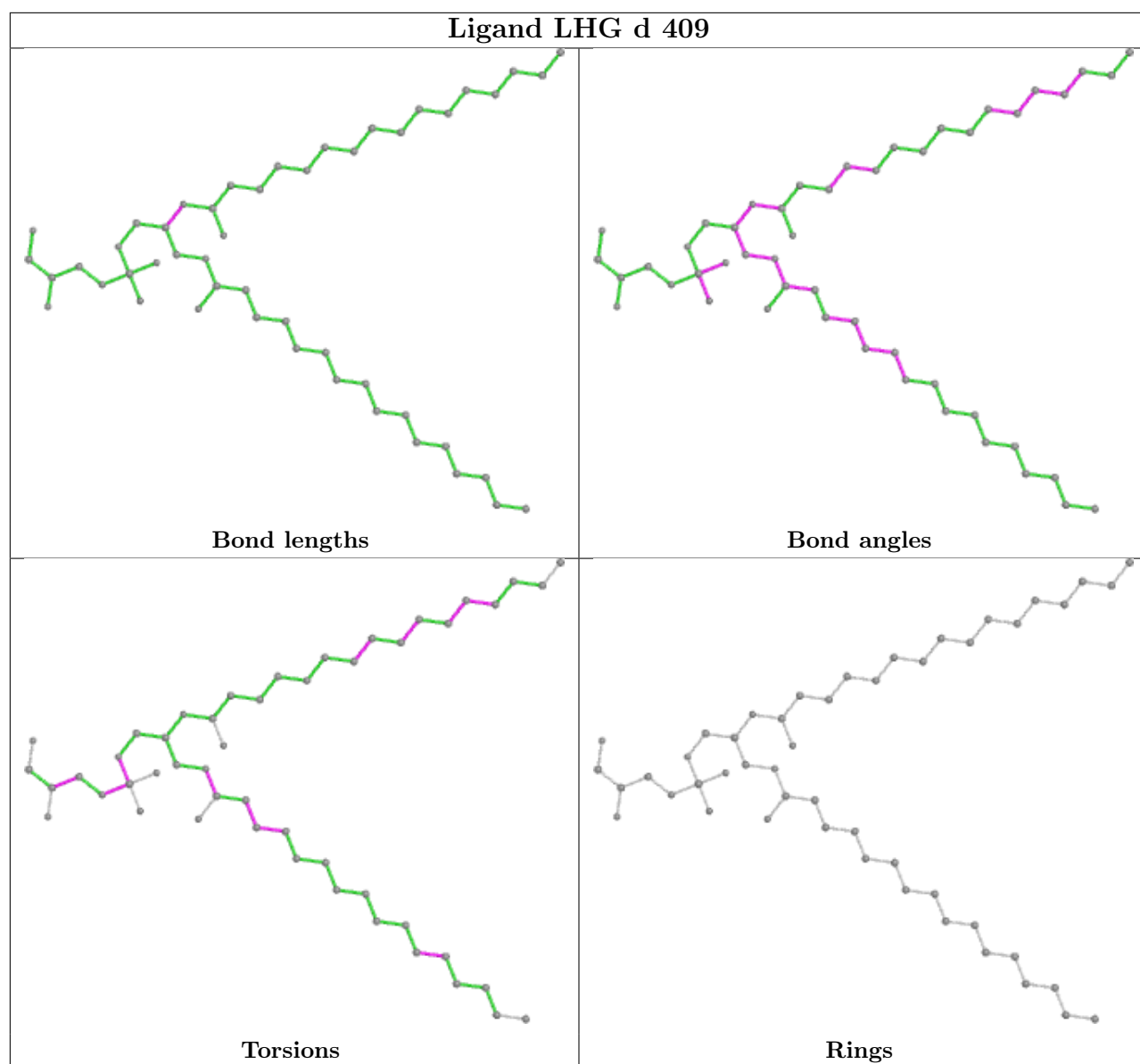


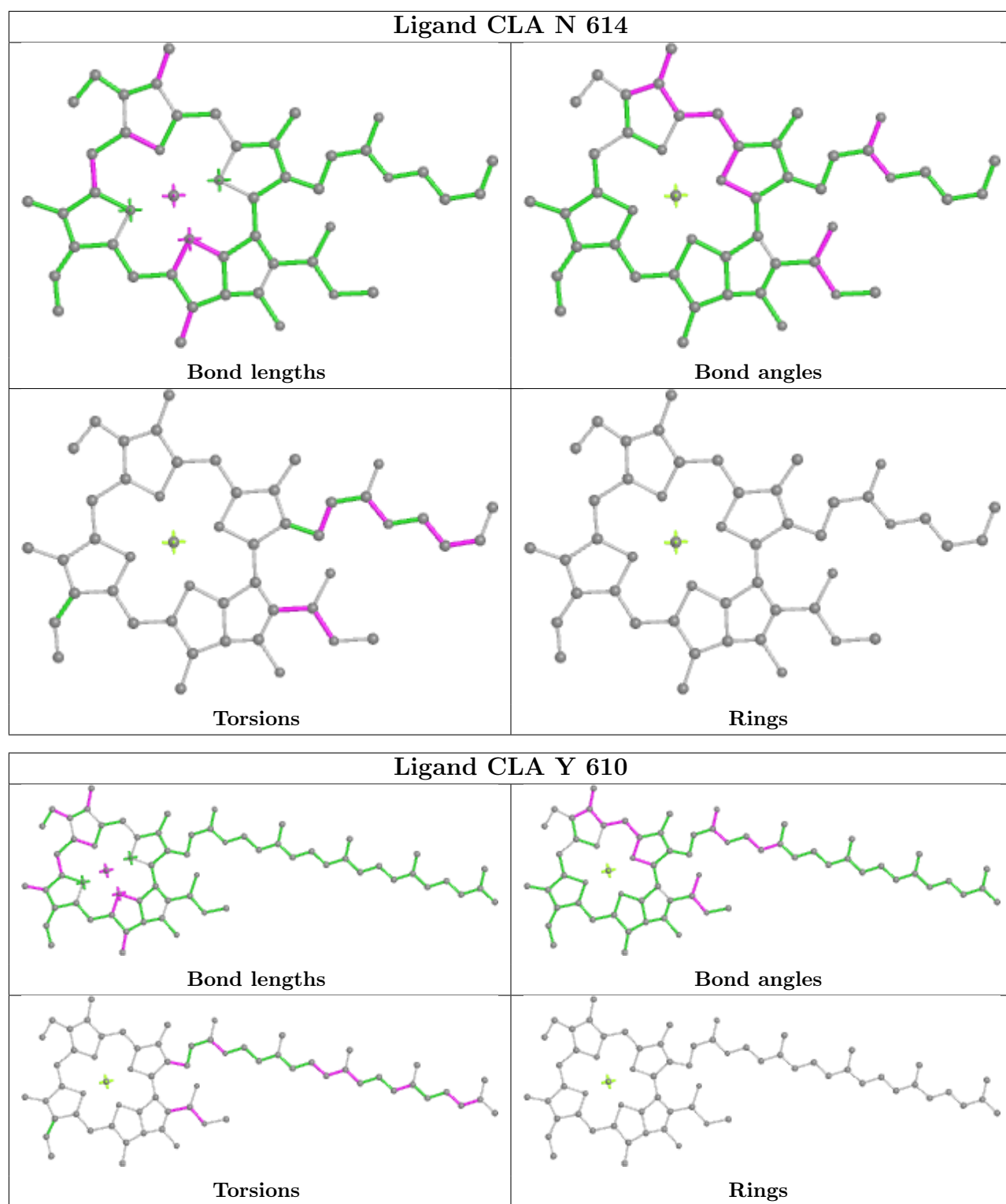


**Ligand CLA C 508****Ligand CLA C 501**

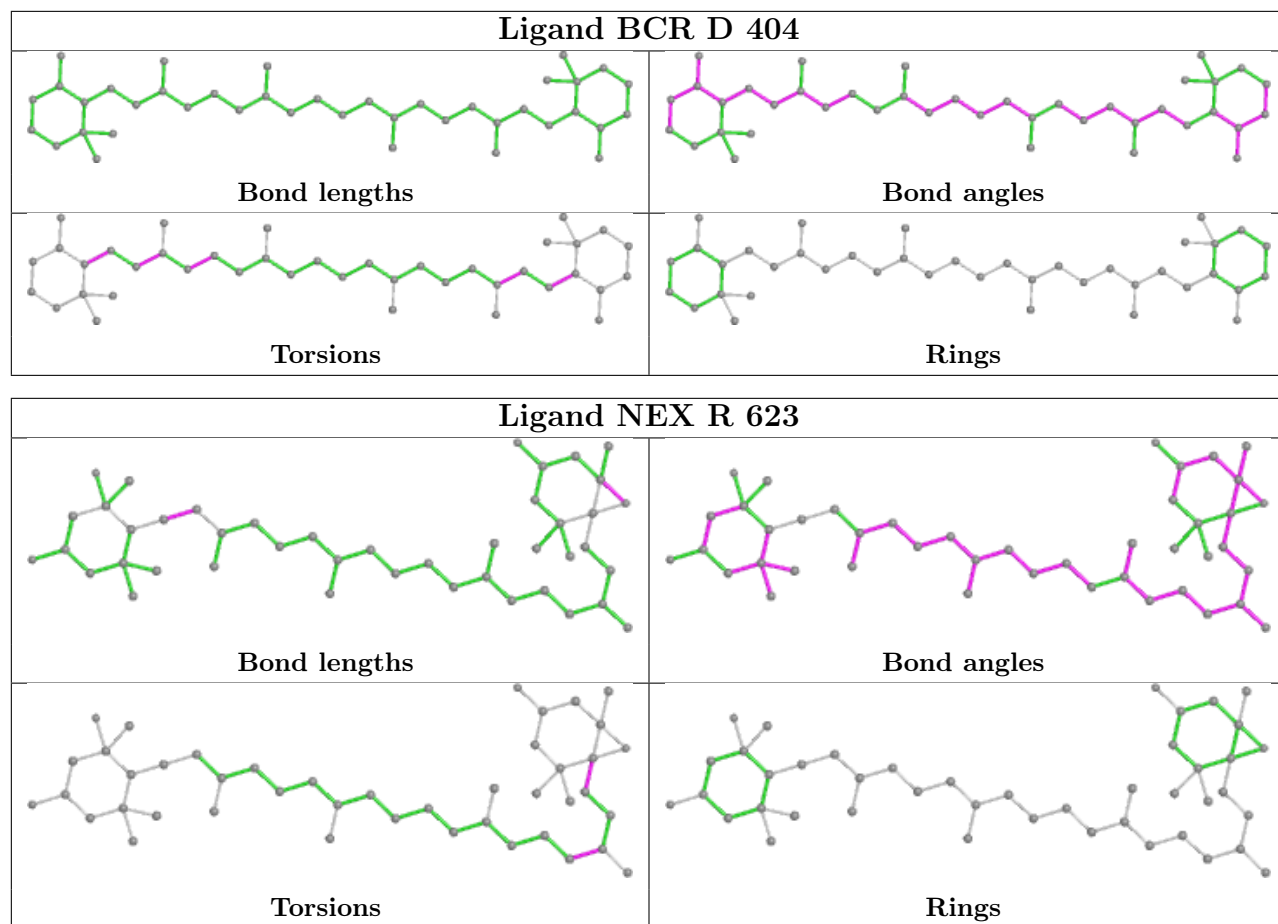
## Ligand CLA S 613

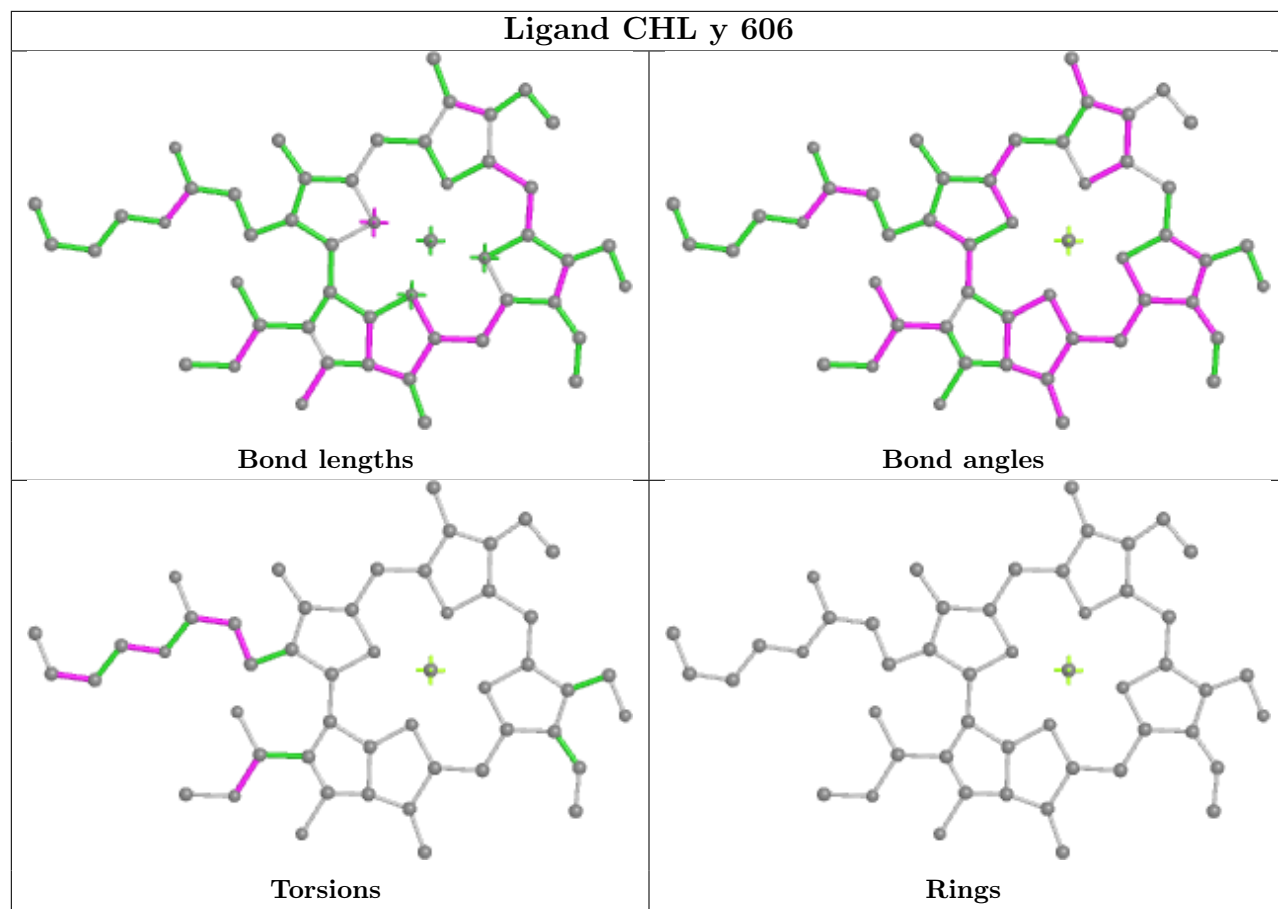




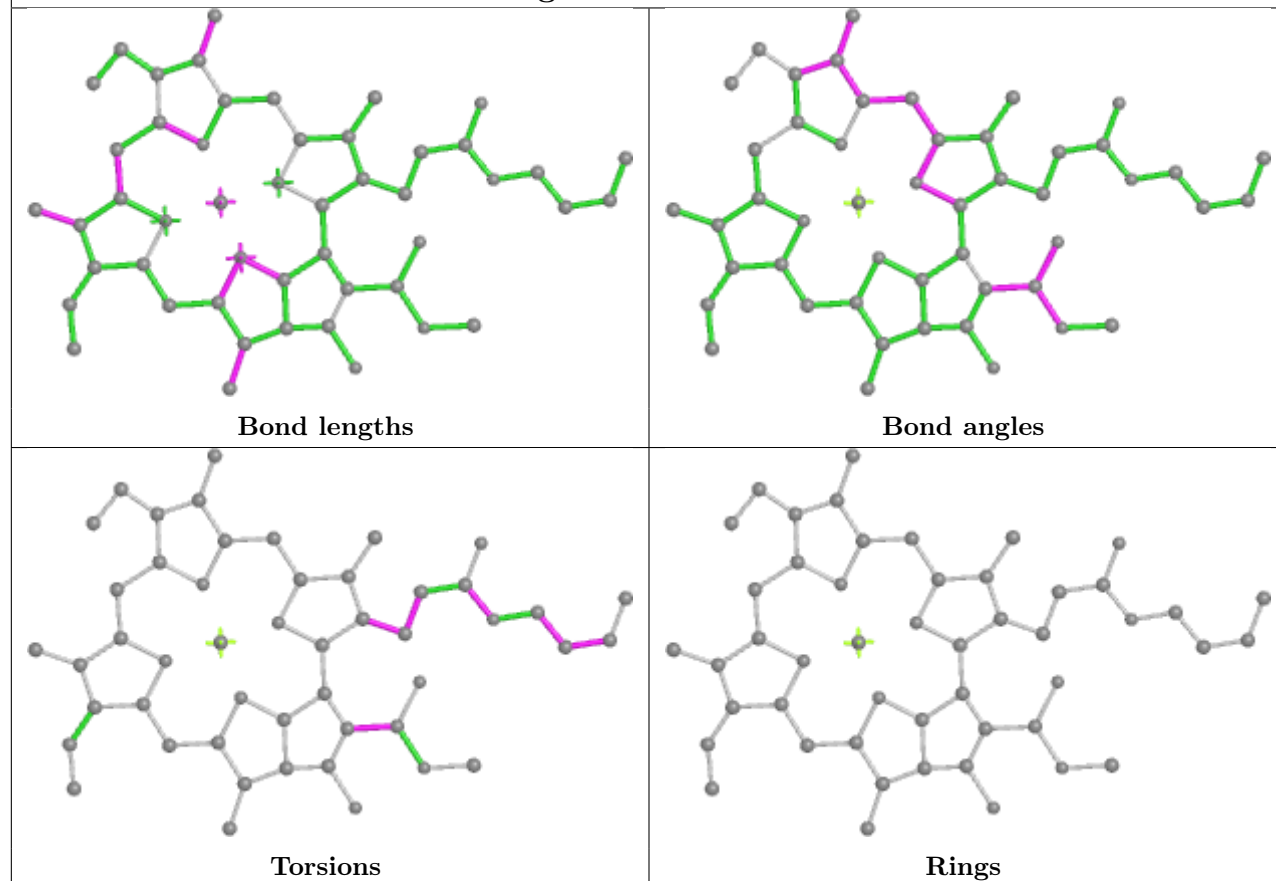




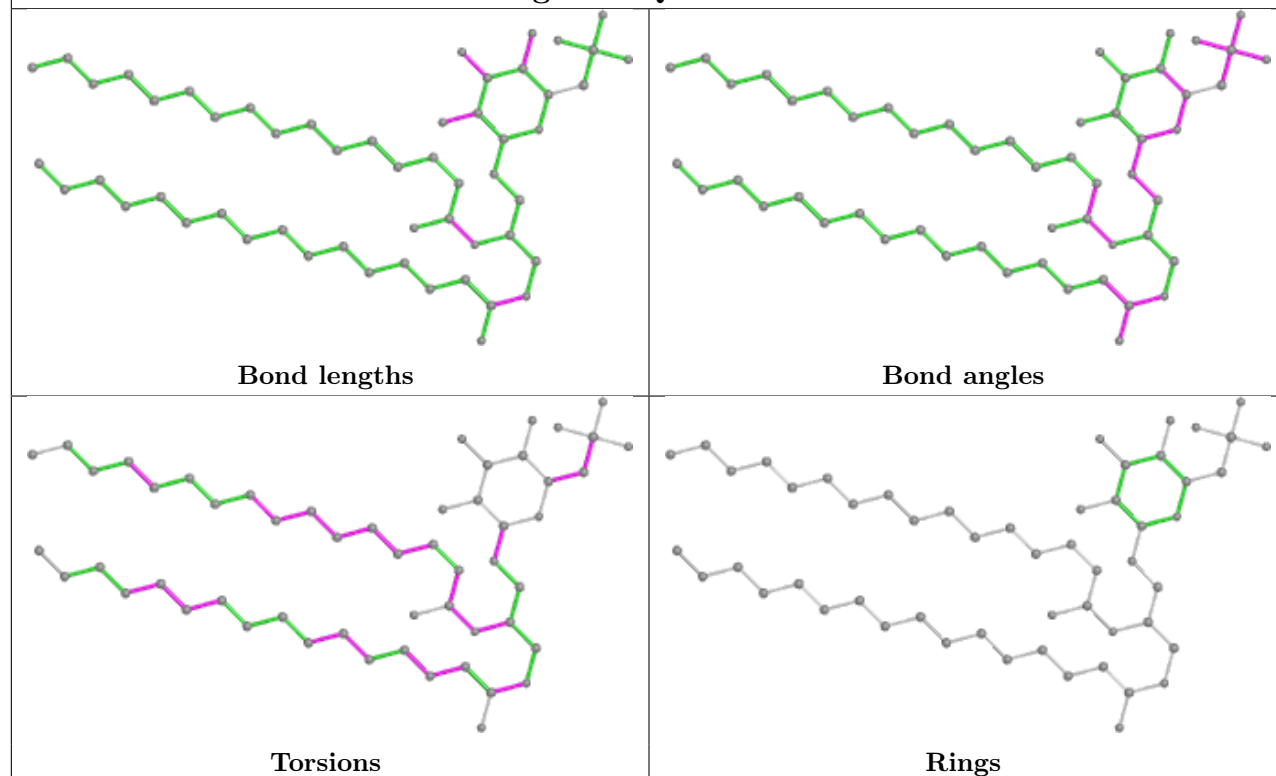


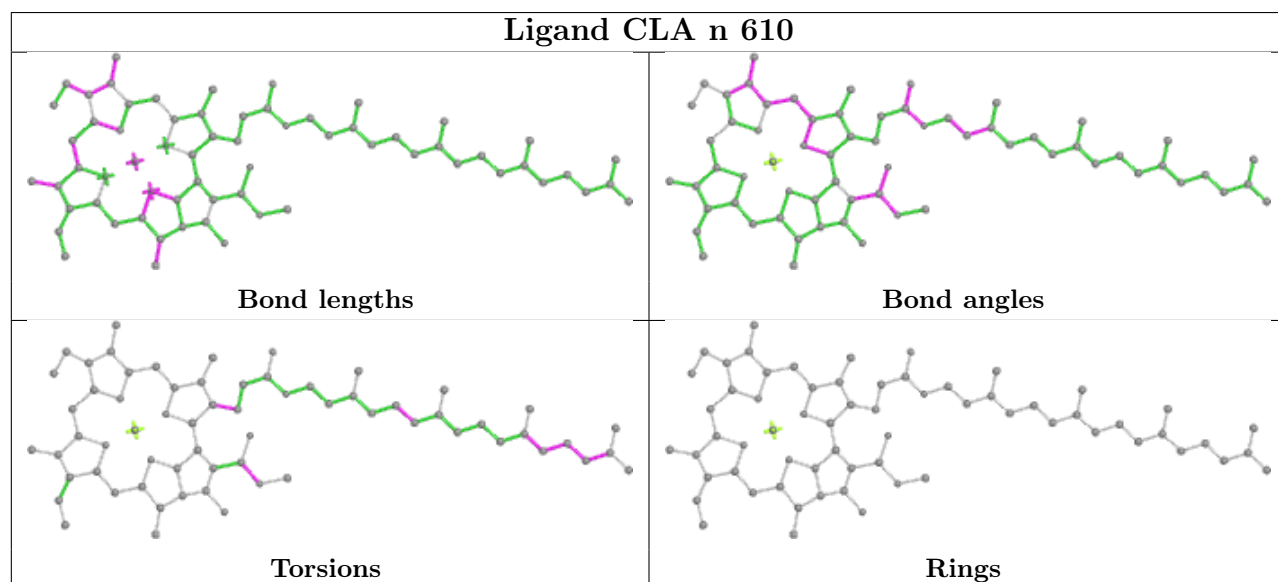
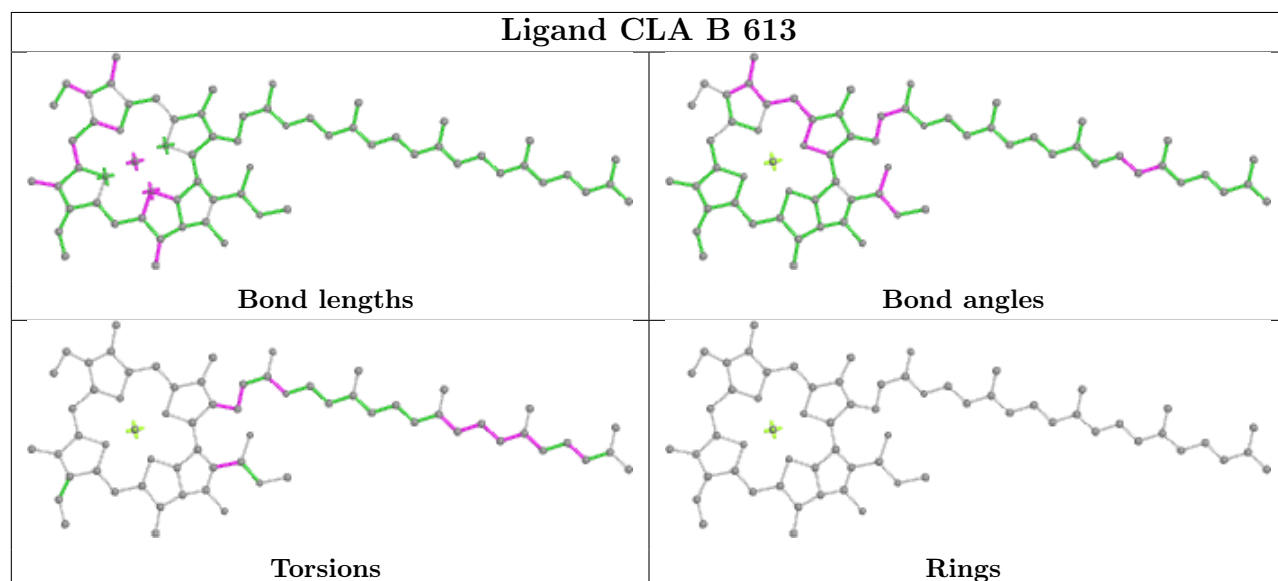
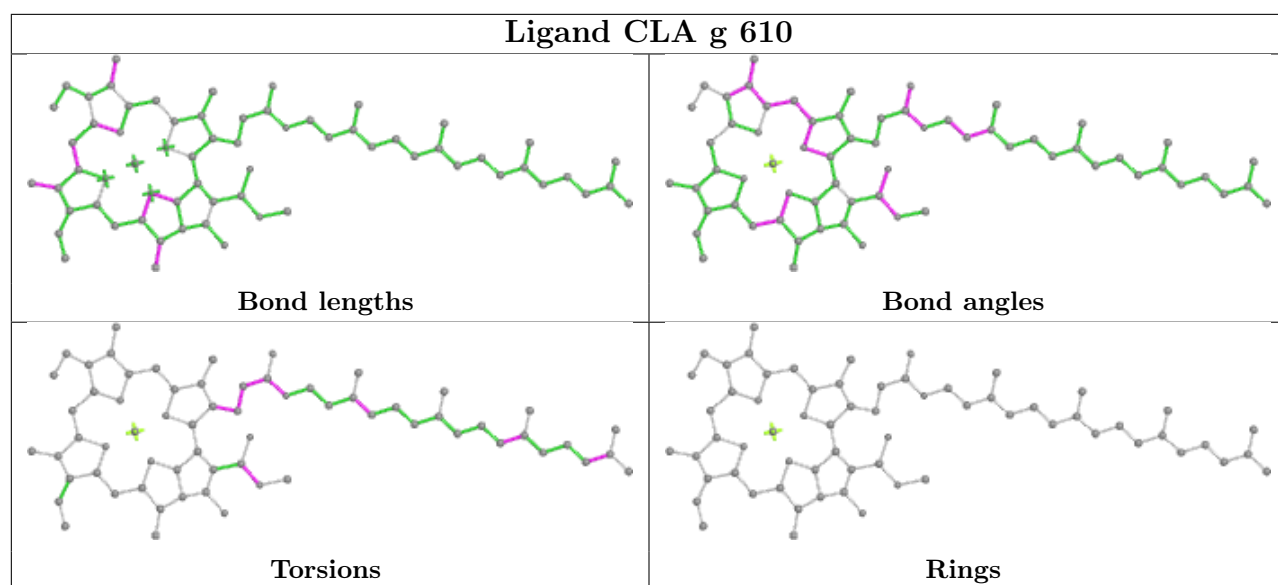


## Ligand CLA r 604

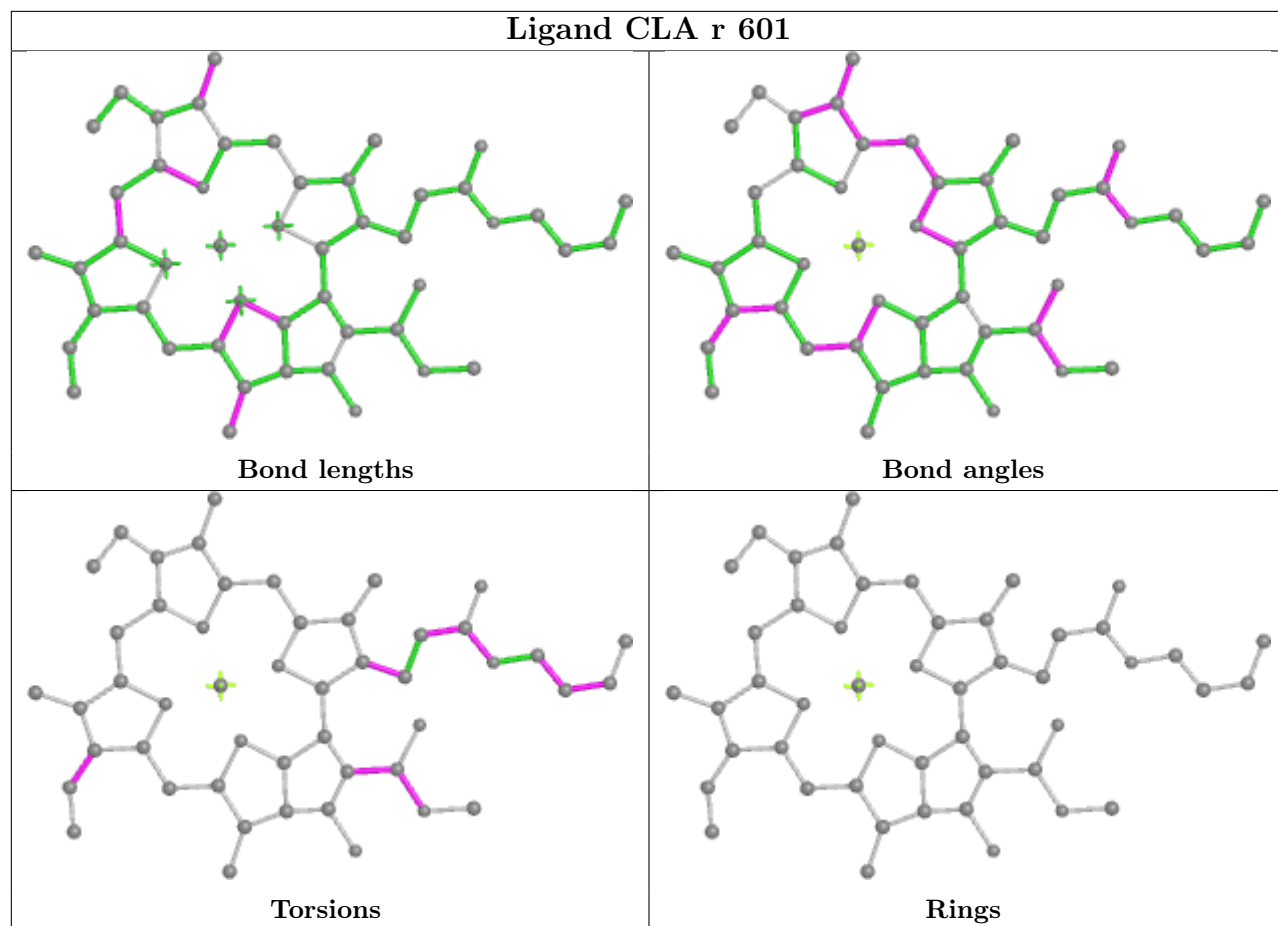


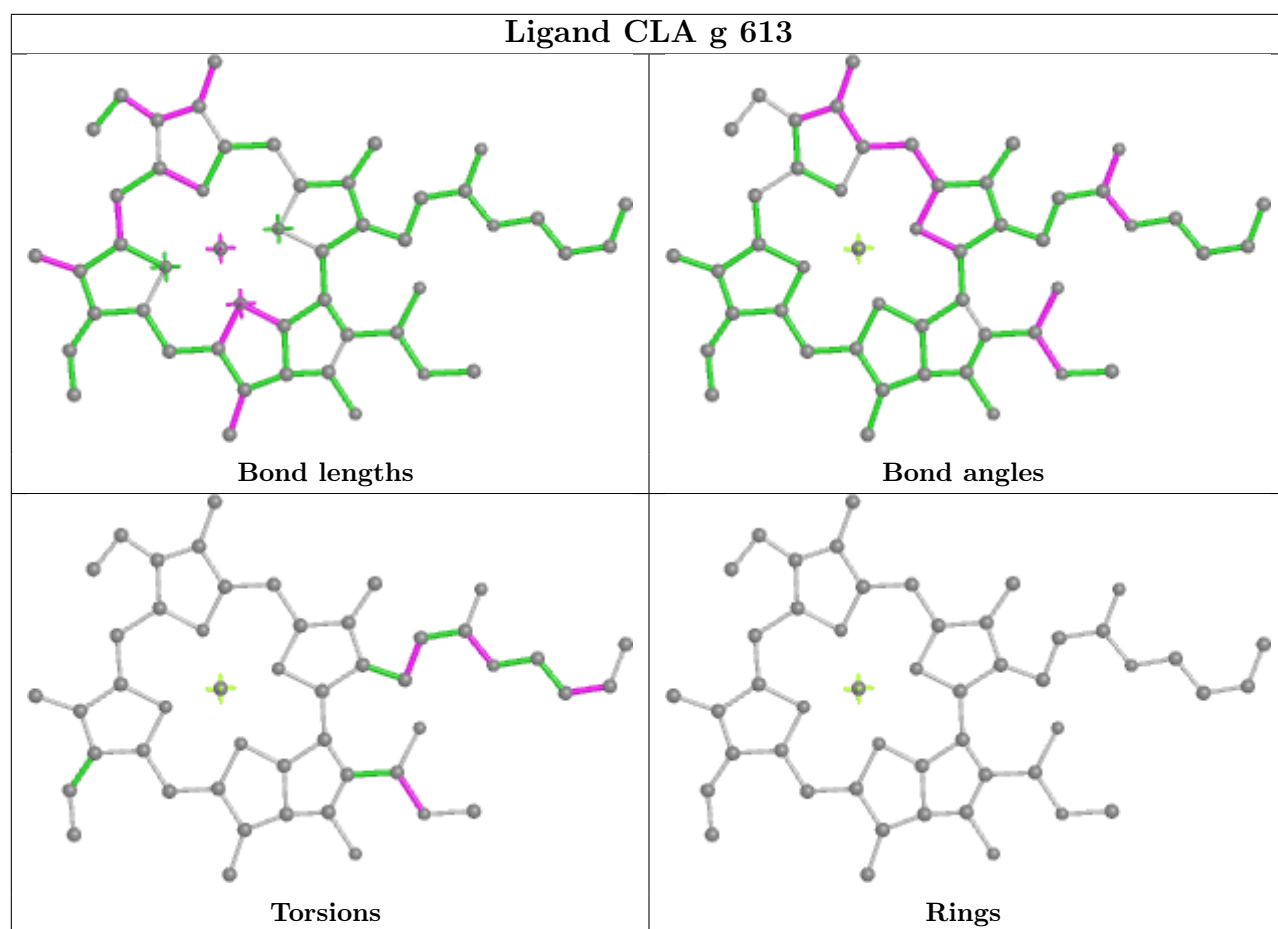
## Ligand SQD B 621

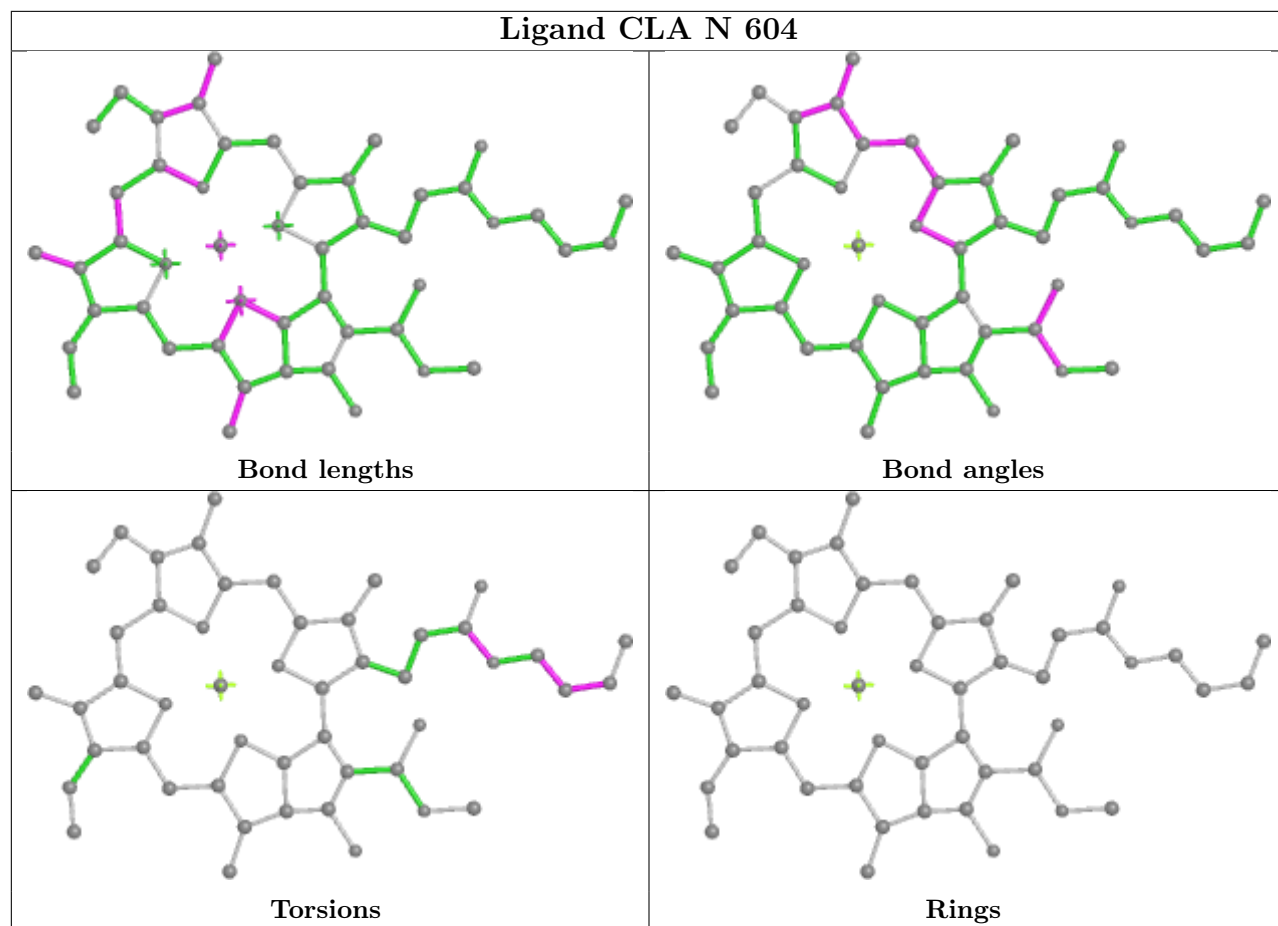


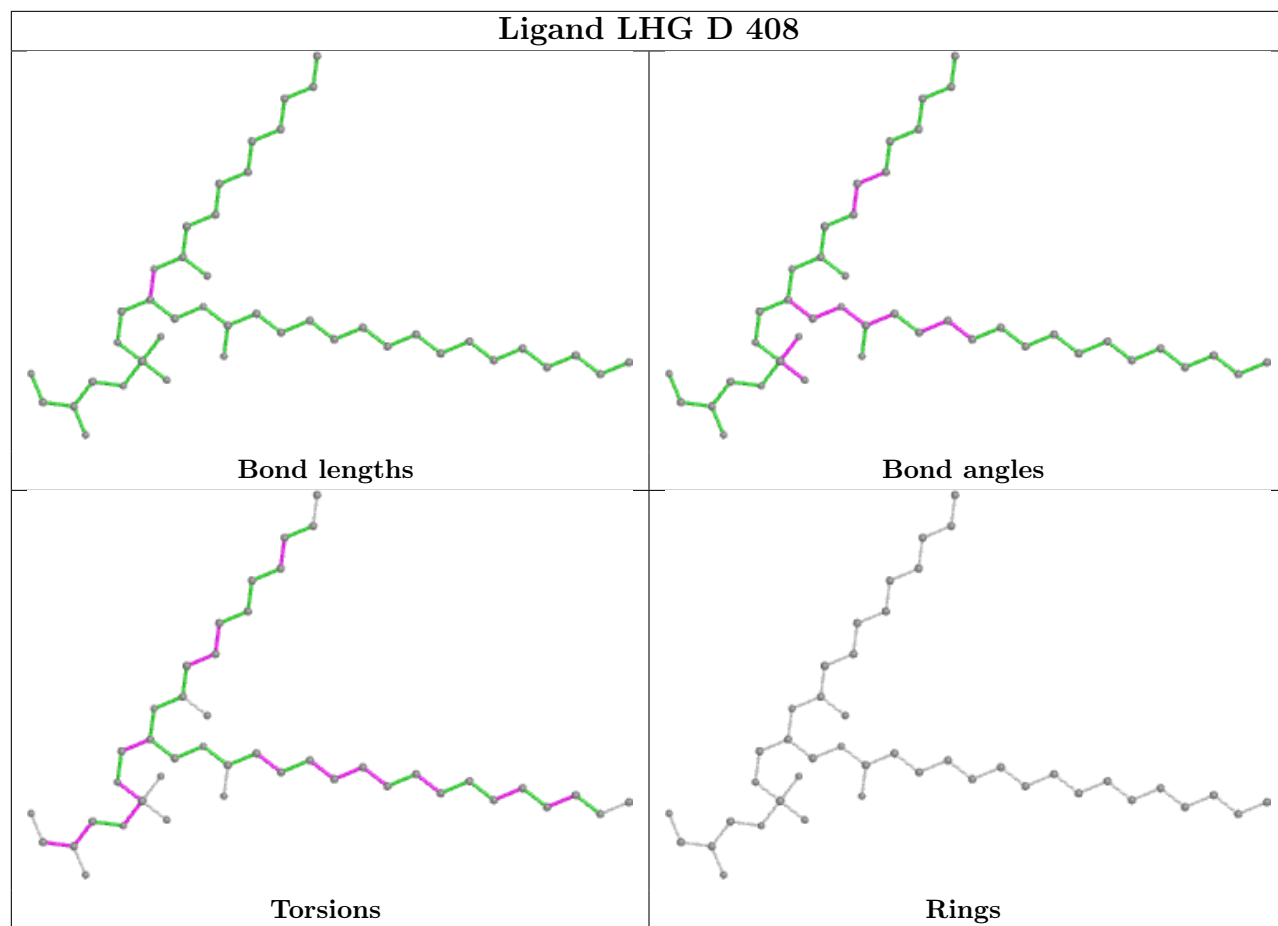


## Ligand CLA r 601

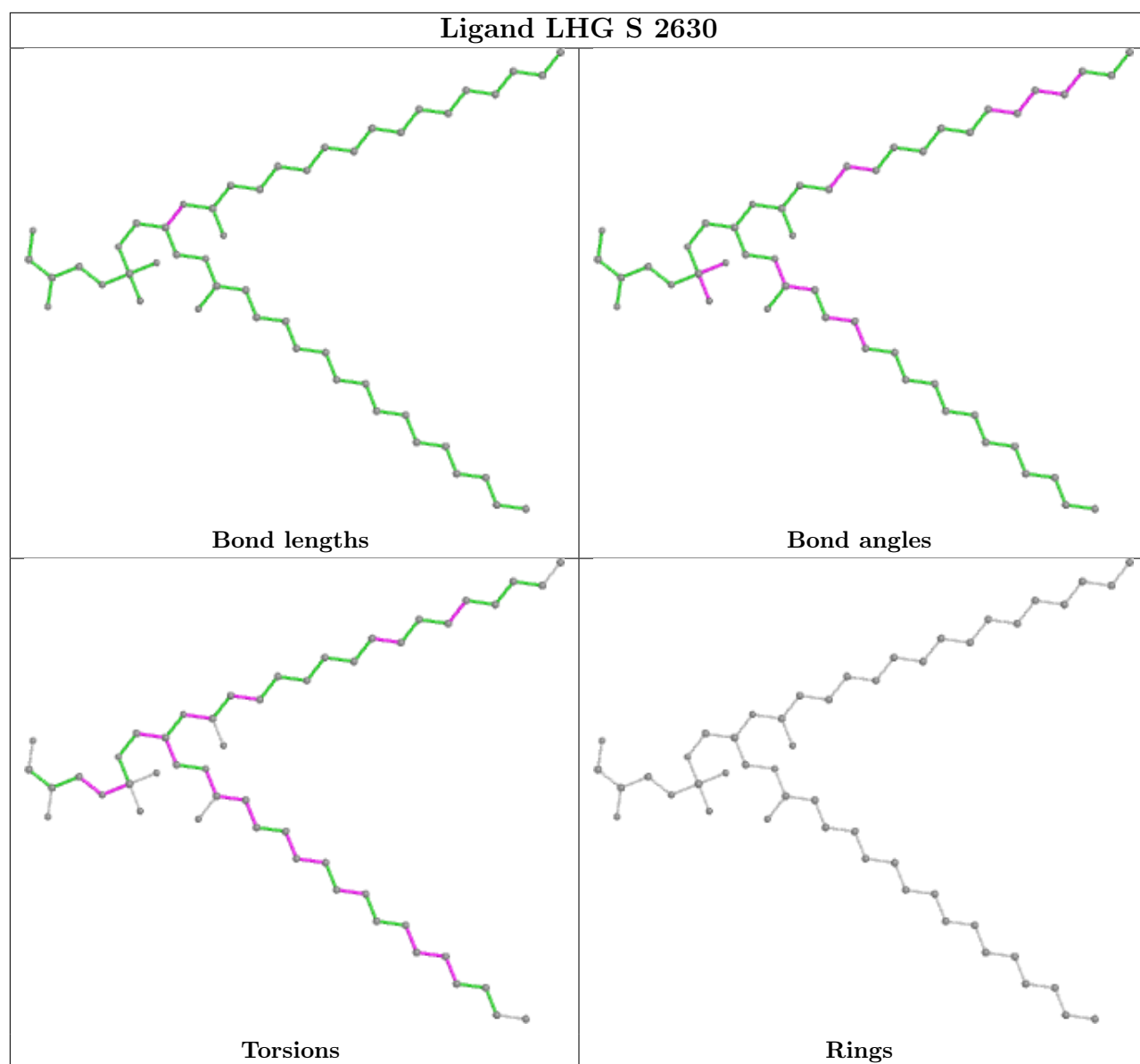




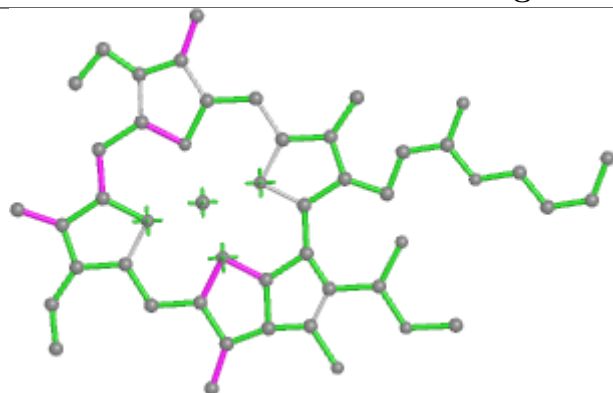




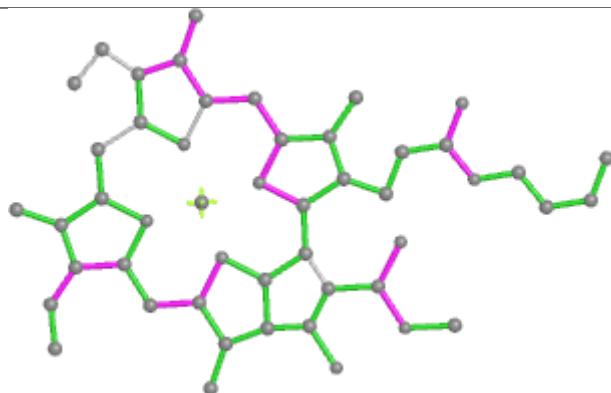




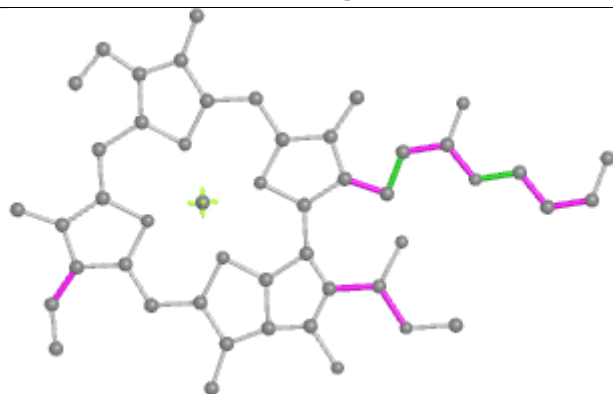
## Ligand CLA R 601



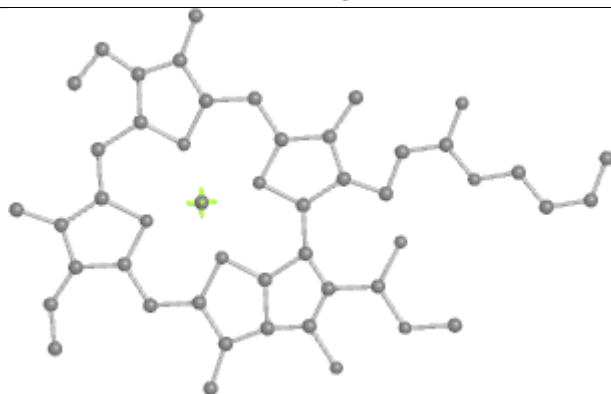
Bond lengths



Bond angles

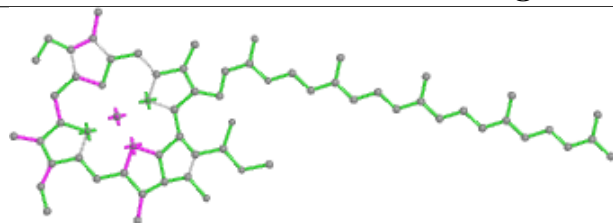


Torsions

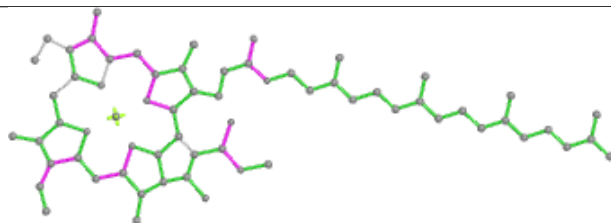


Rings

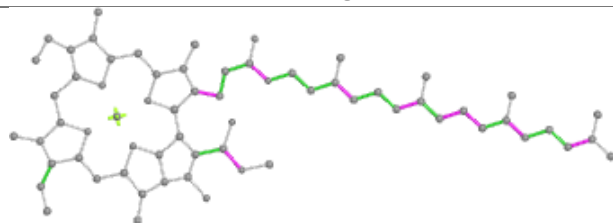
## Ligand CLA B 612



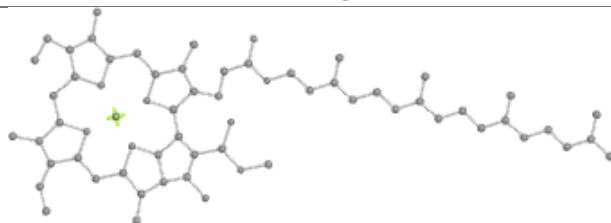
Bond lengths



Bond angles

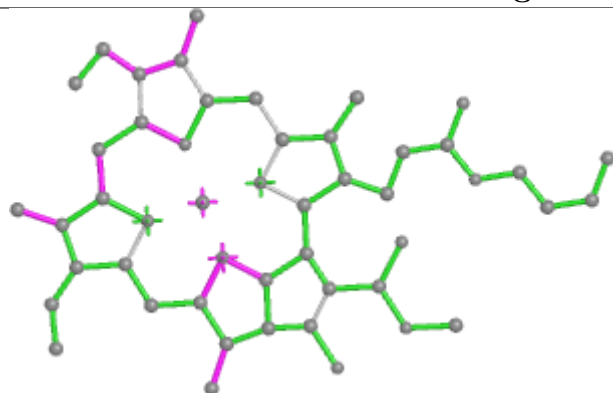


Torsions

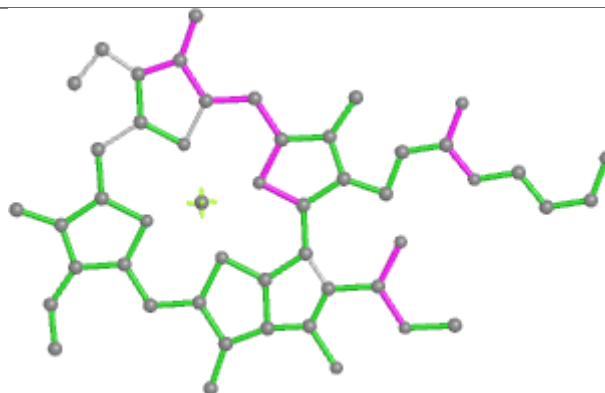


Rings

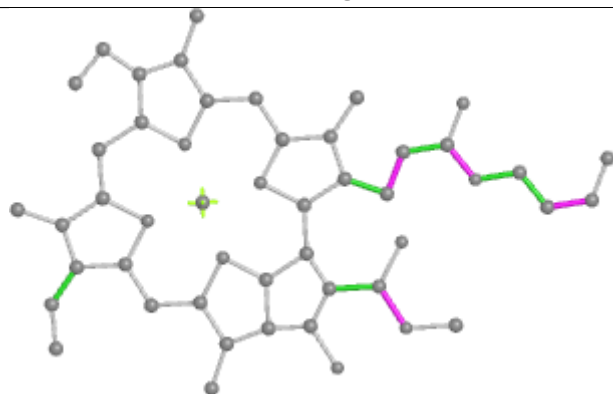
## Ligand CLA Y 604



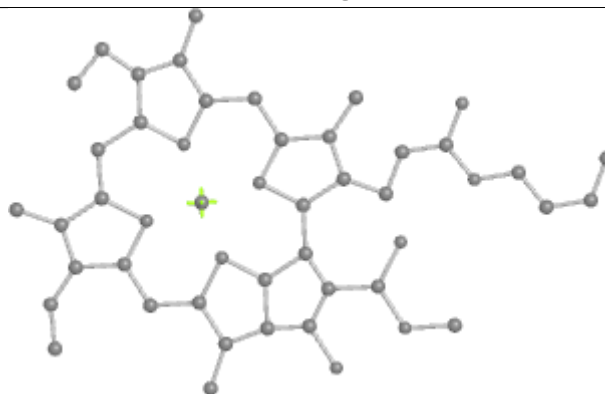
Bond lengths



Bond angles

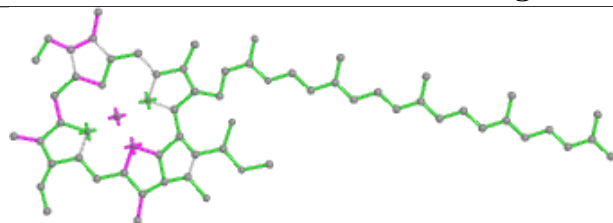


Torsions

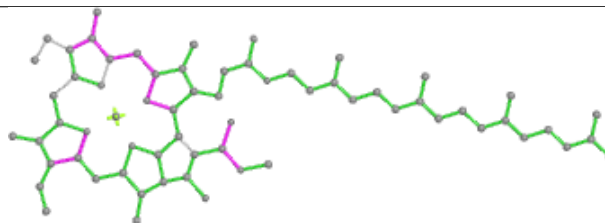


Rings

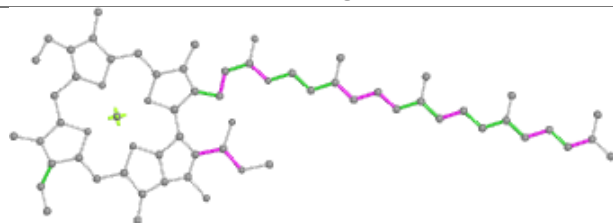
## Ligand CLA Y 613



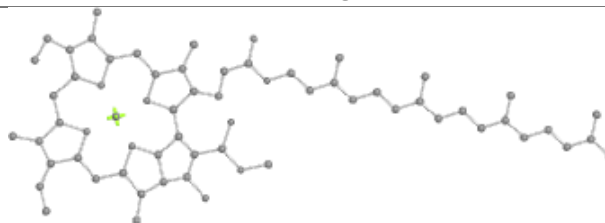
Bond lengths



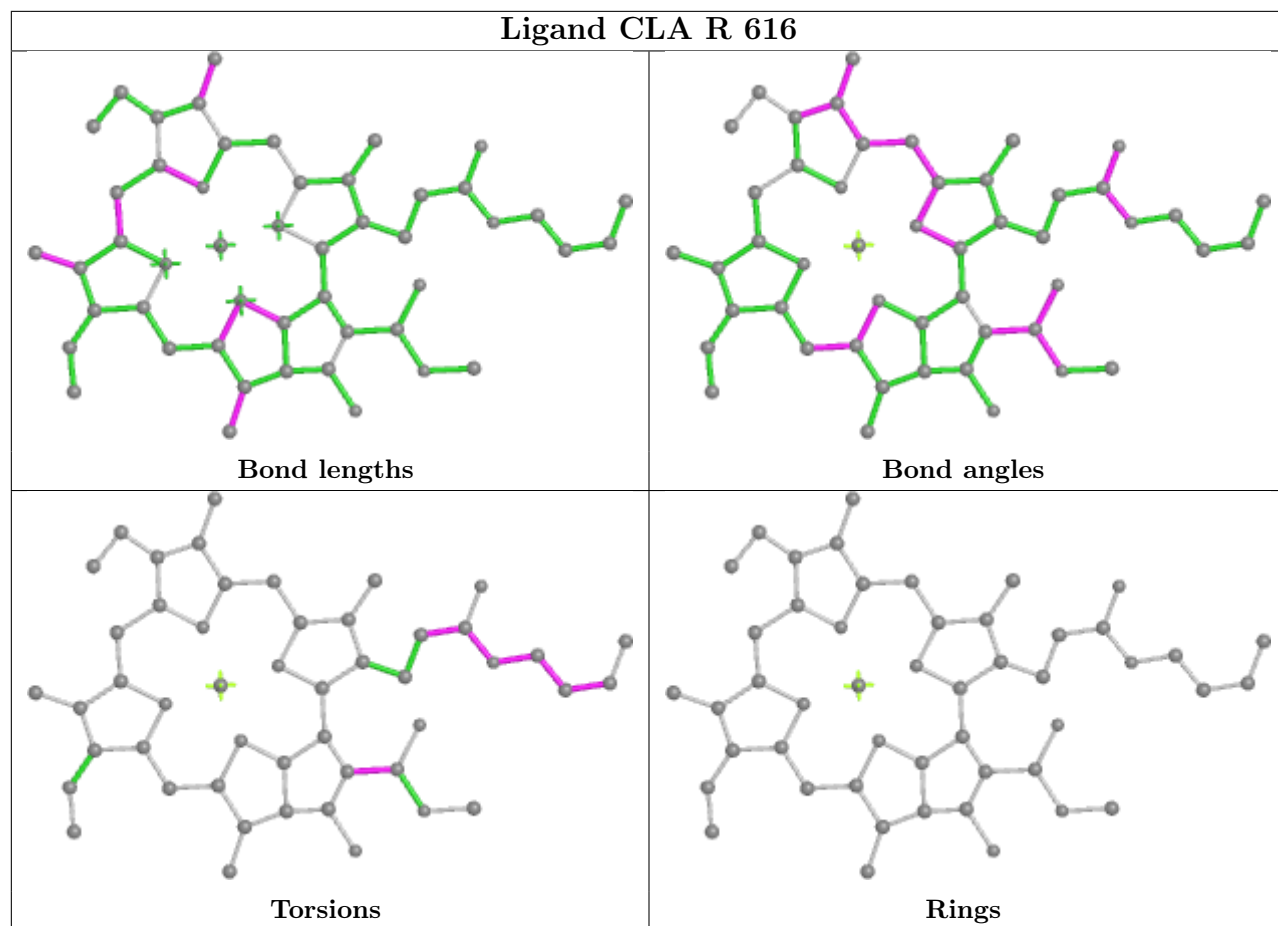
Bond angles

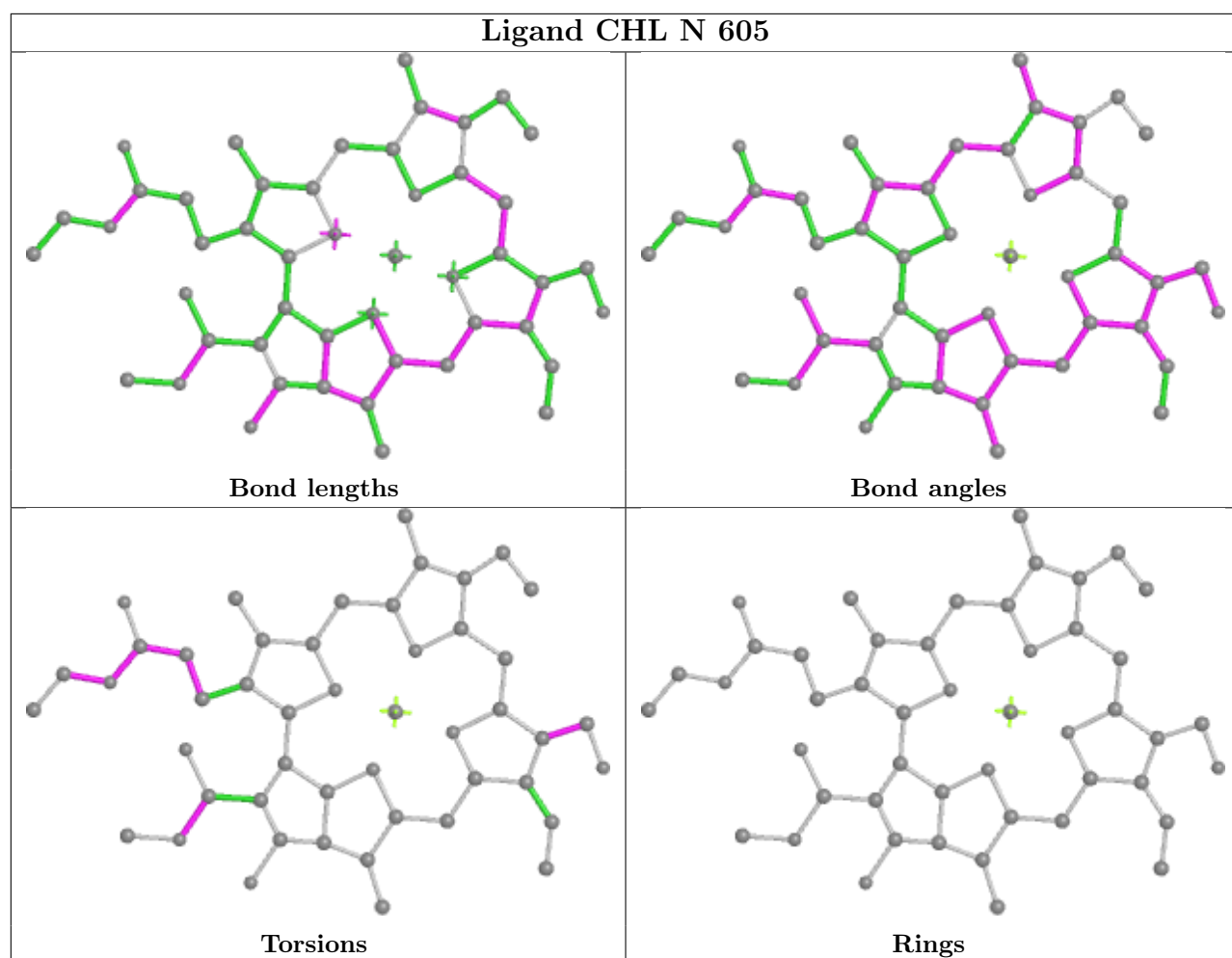


Torsions

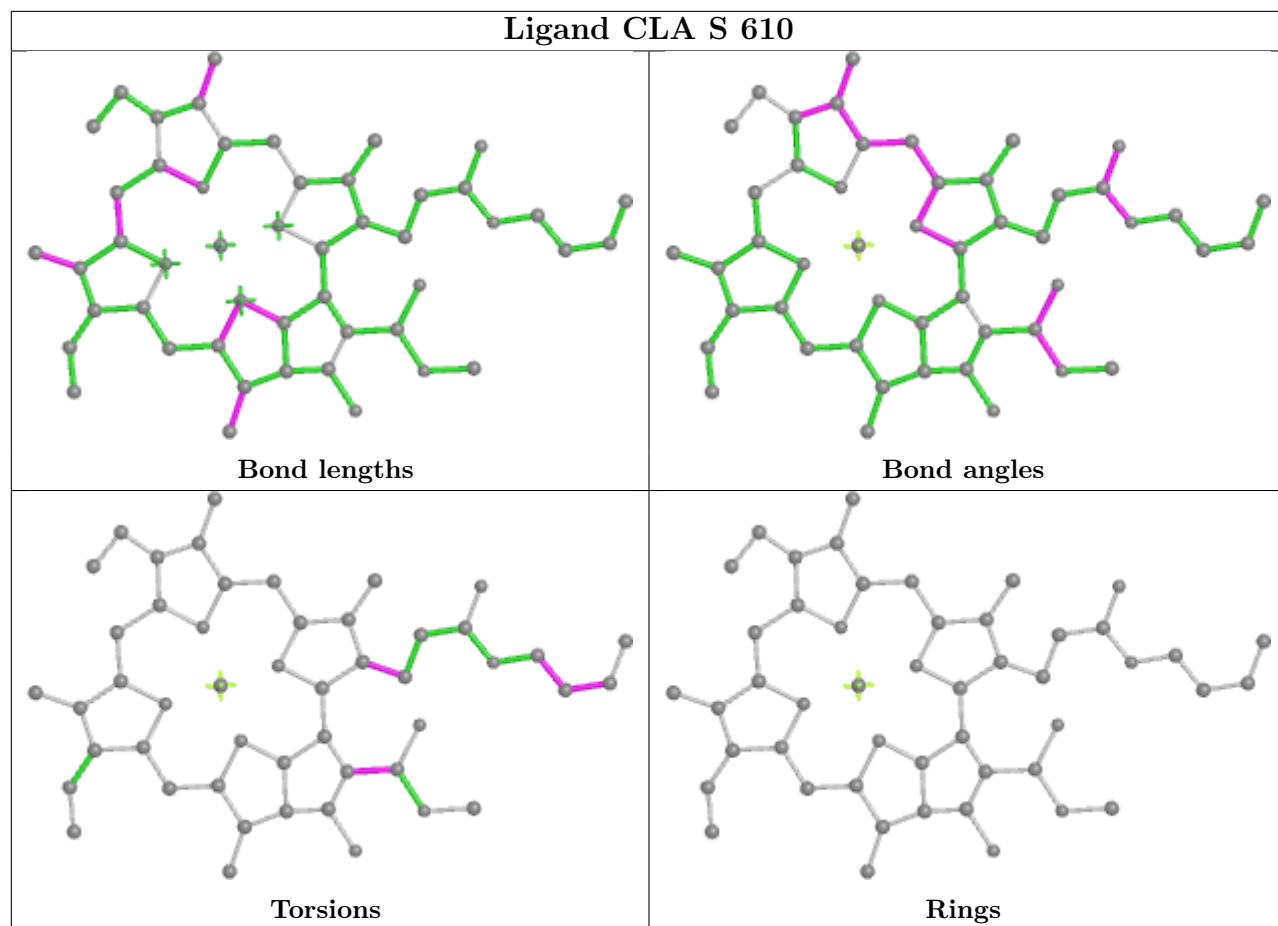


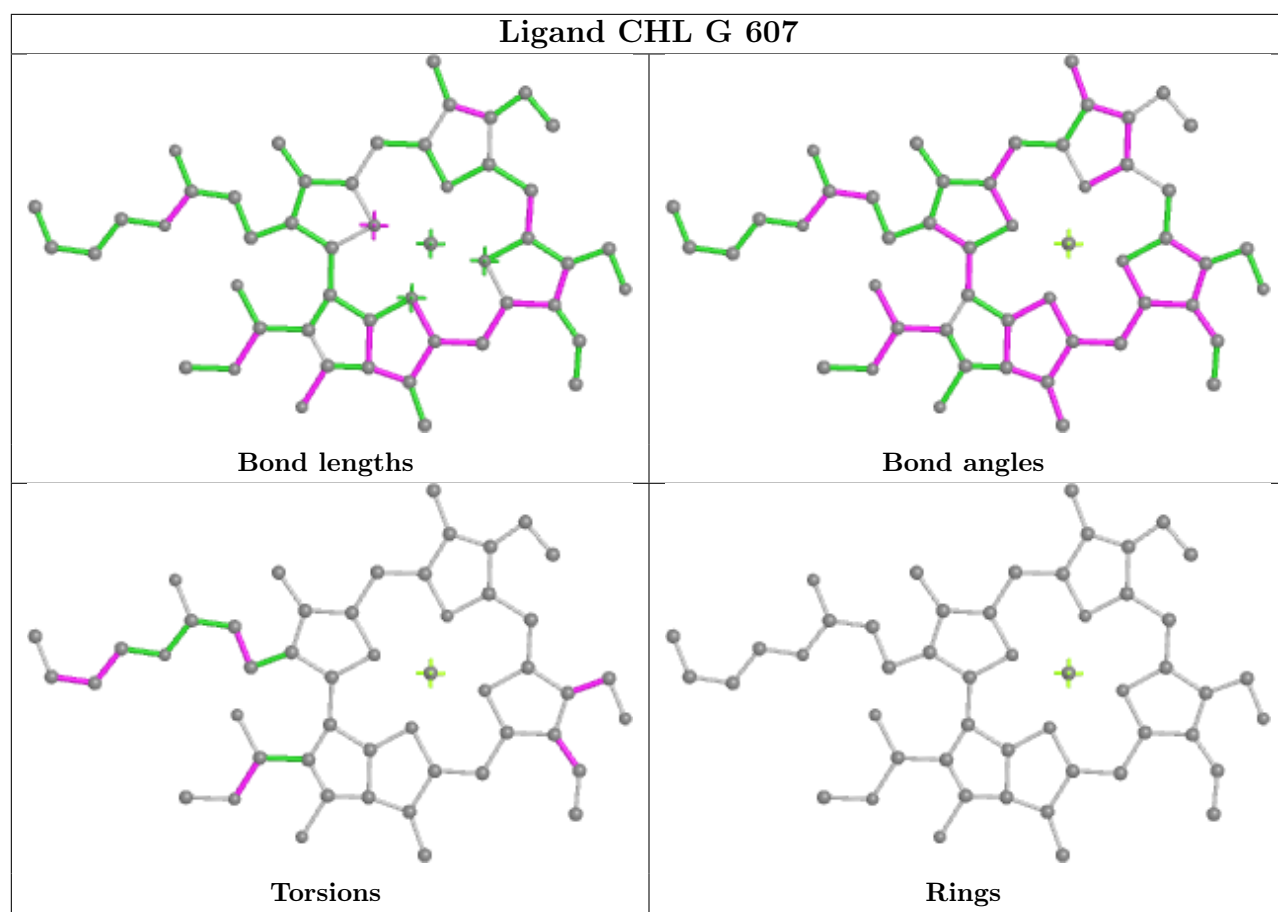
Rings



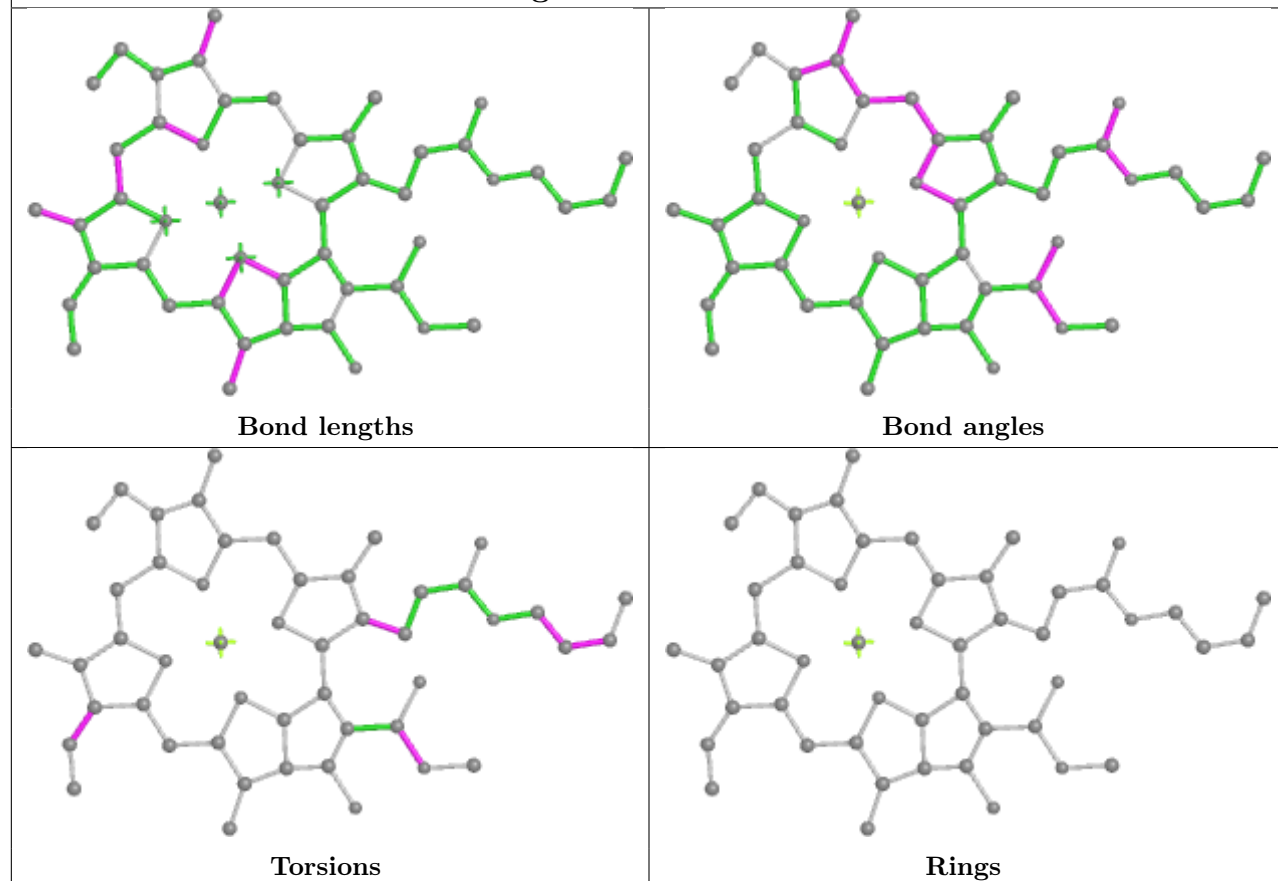


## Ligand CLA S 610

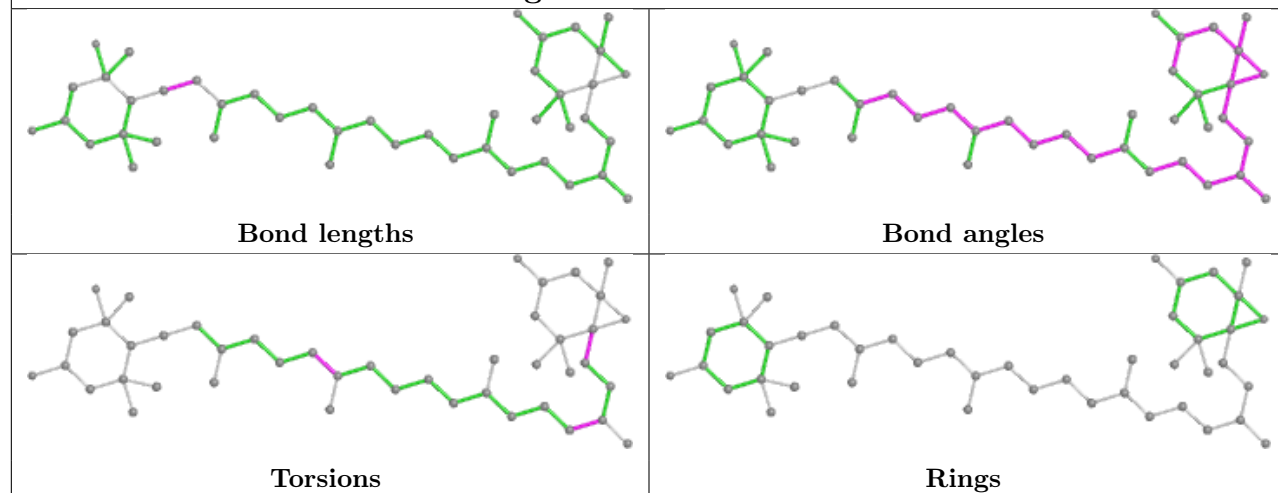




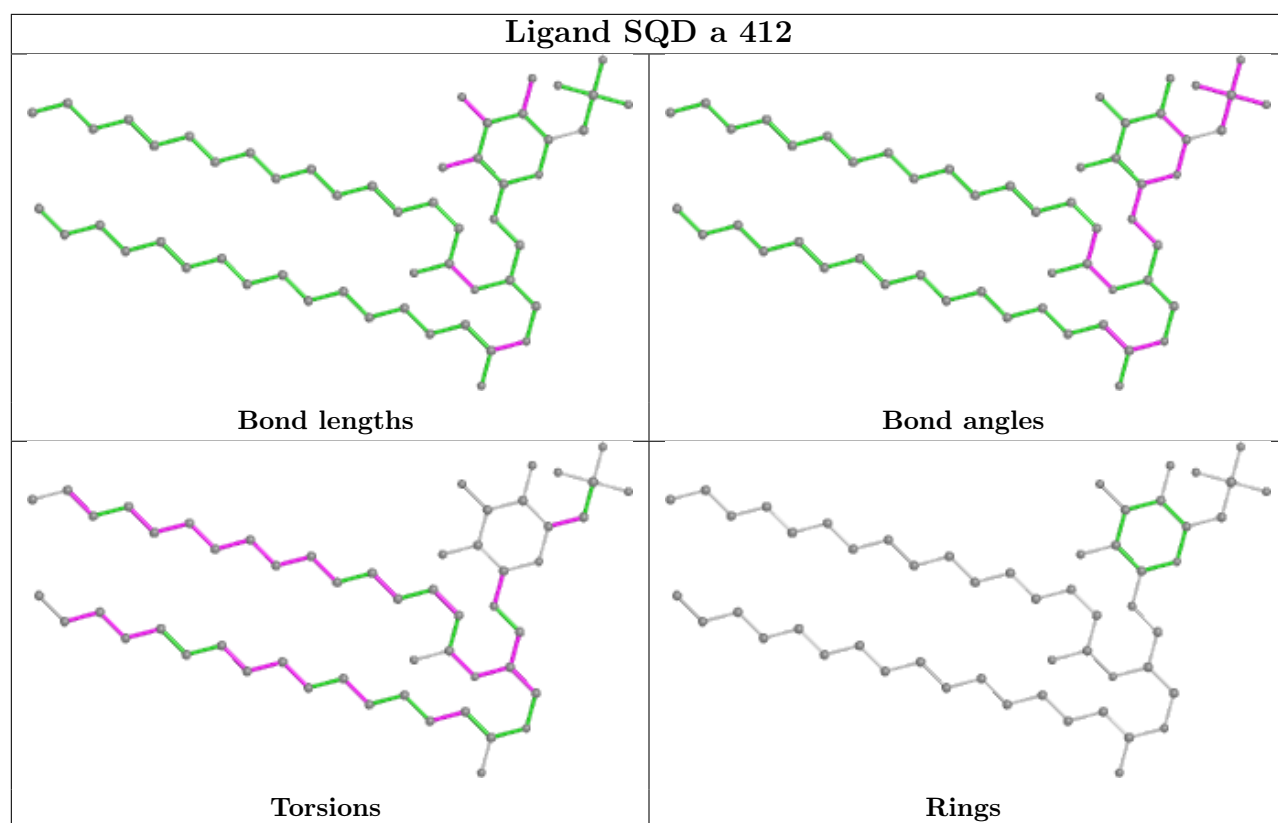
## Ligand CLA R 609

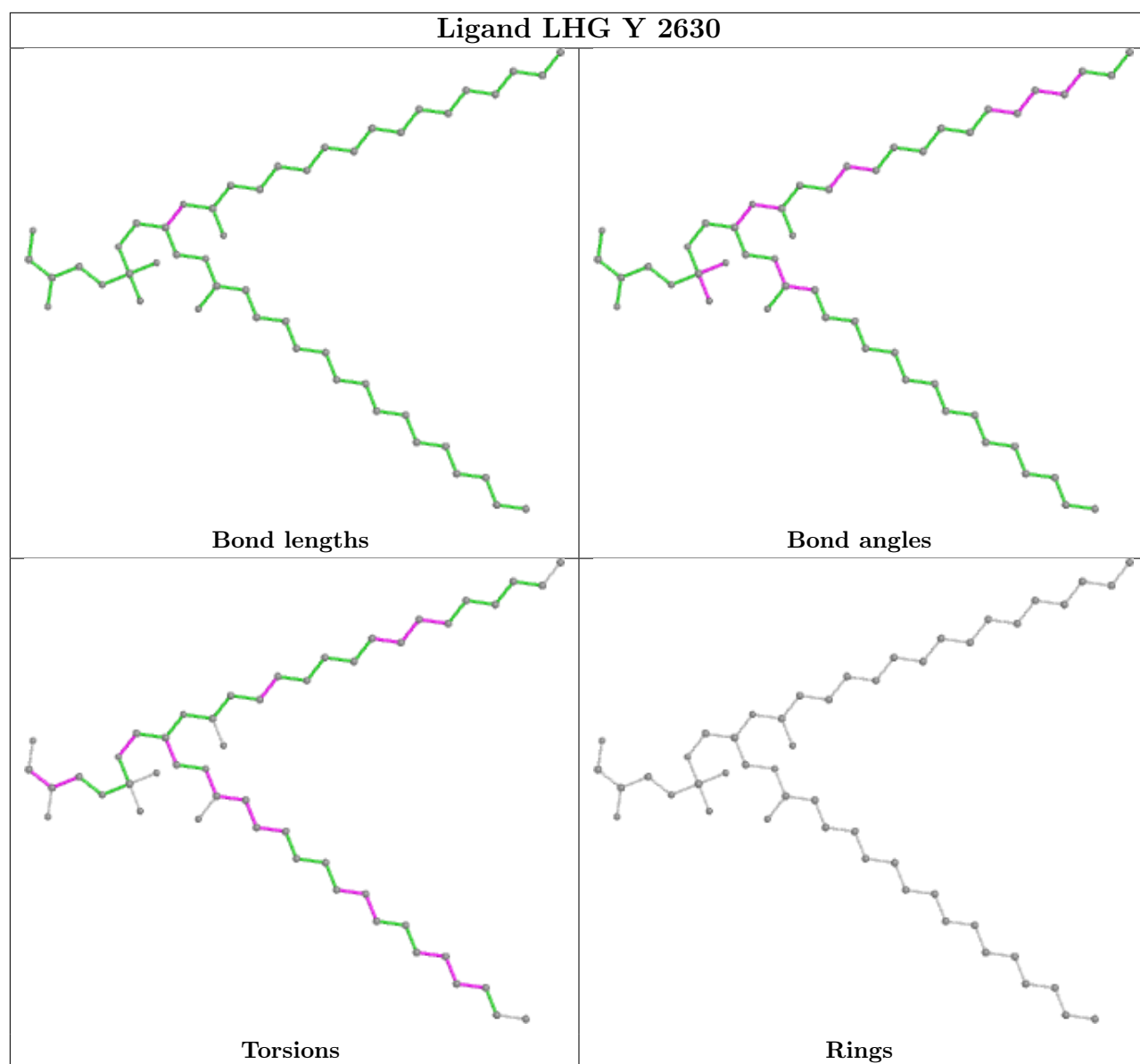


## Ligand NEX n 1623

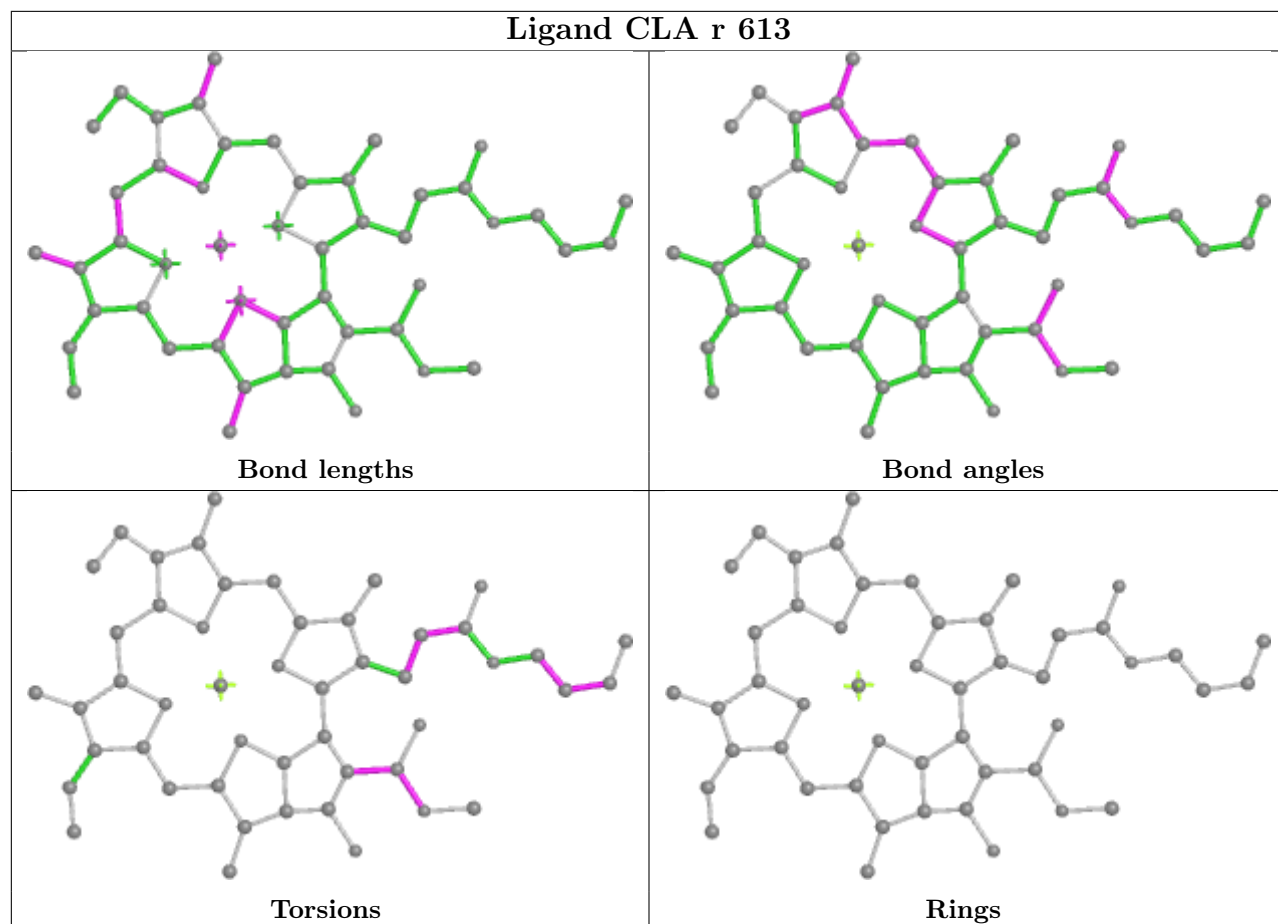




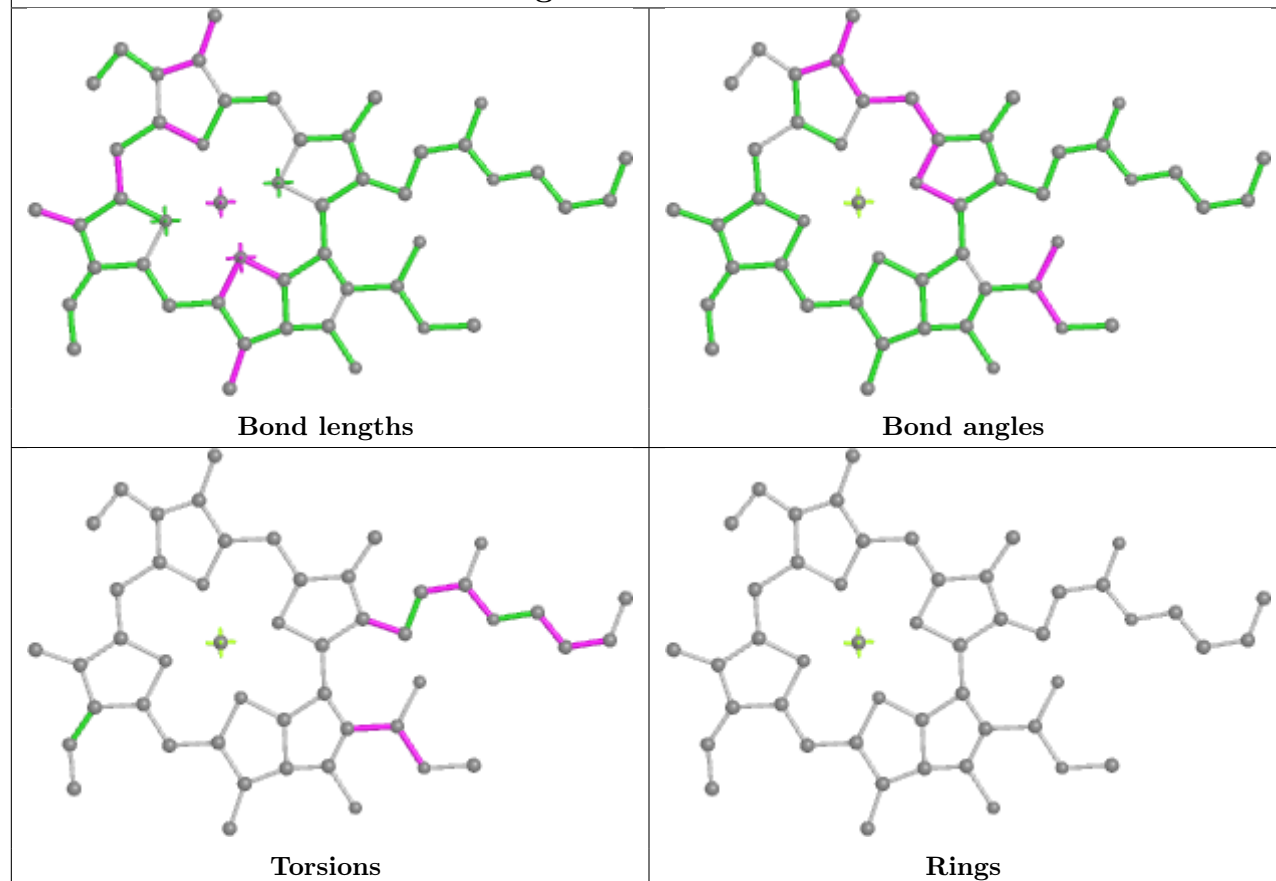




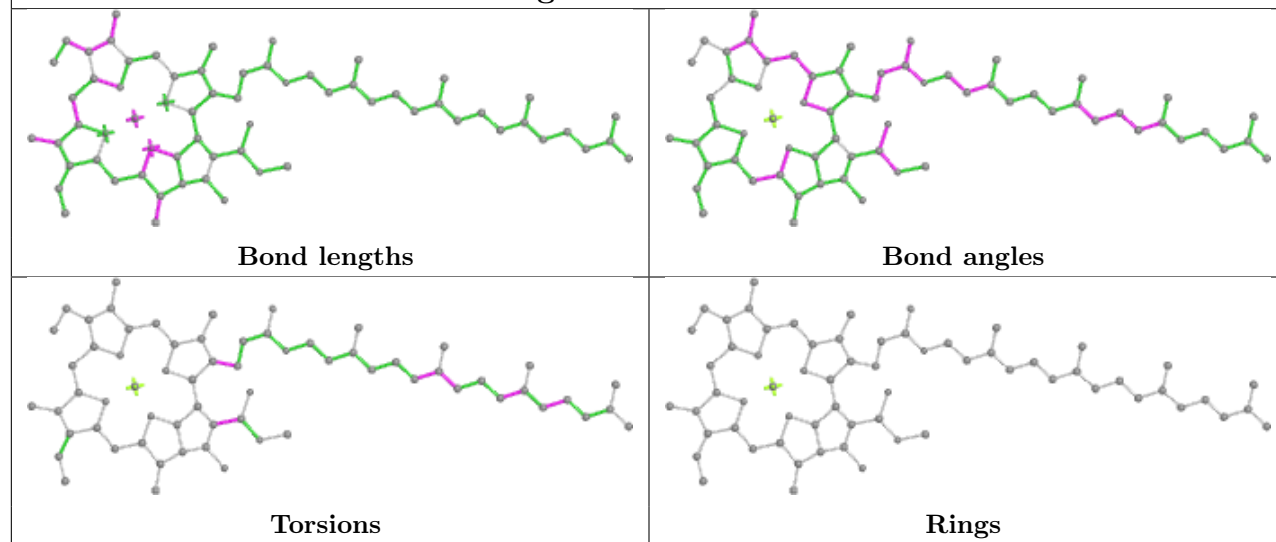
## Ligand CLA r 613

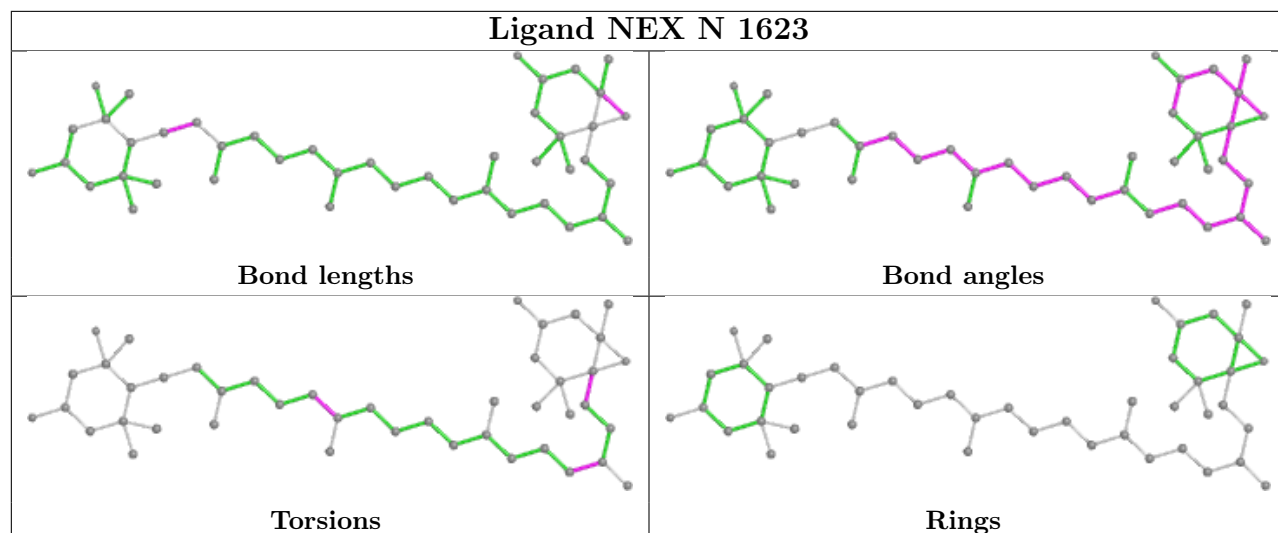
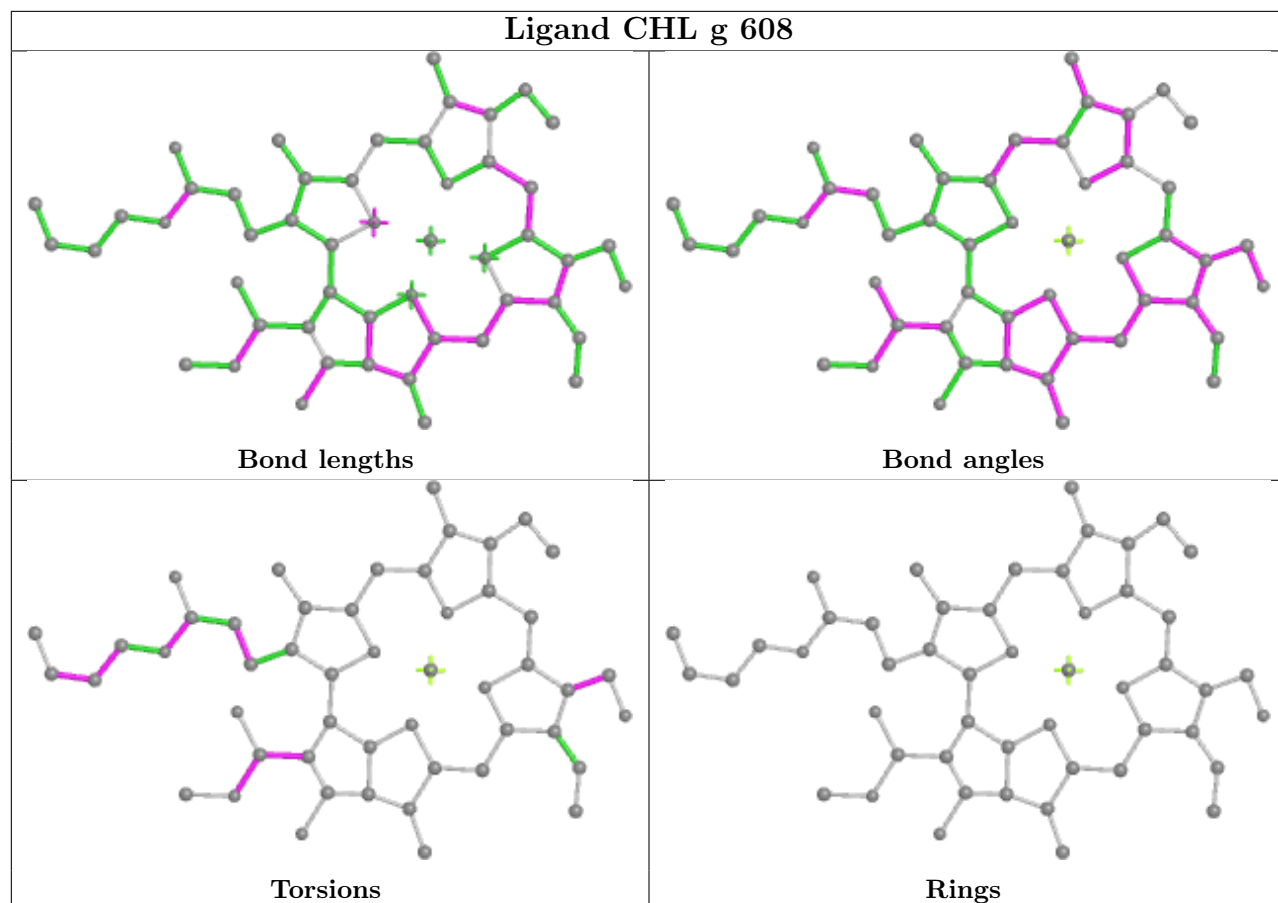


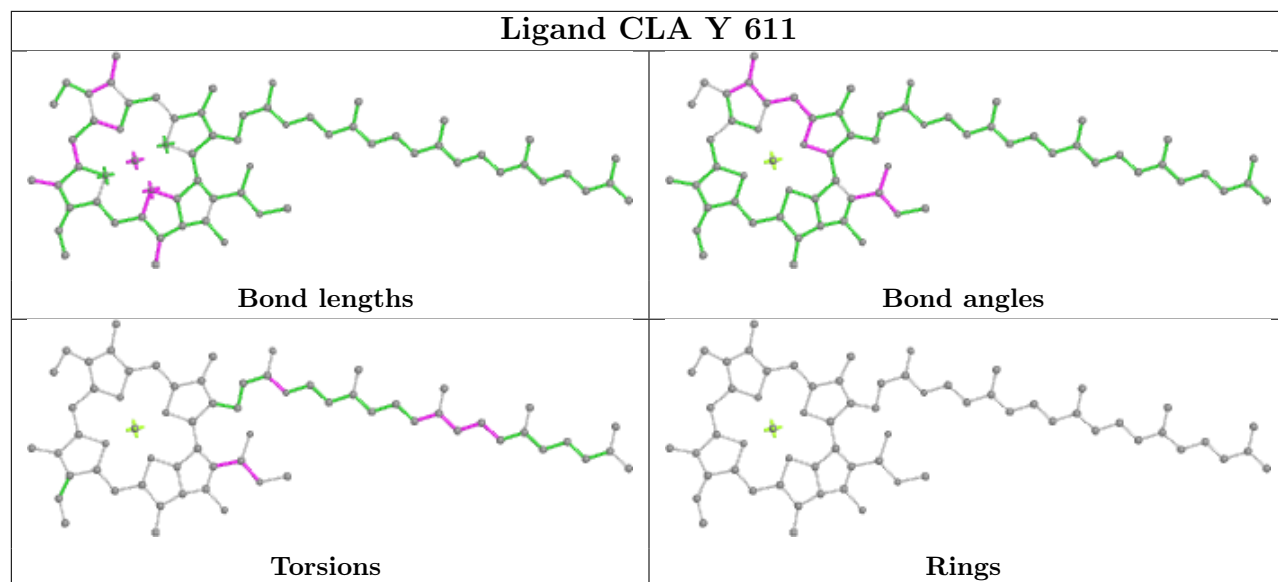
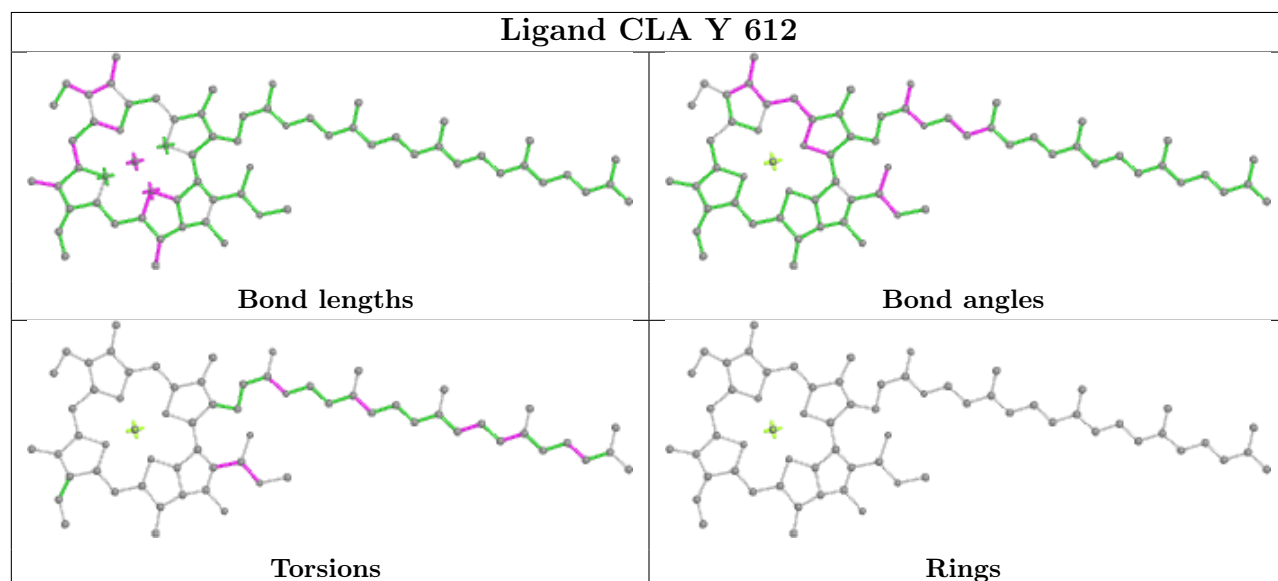
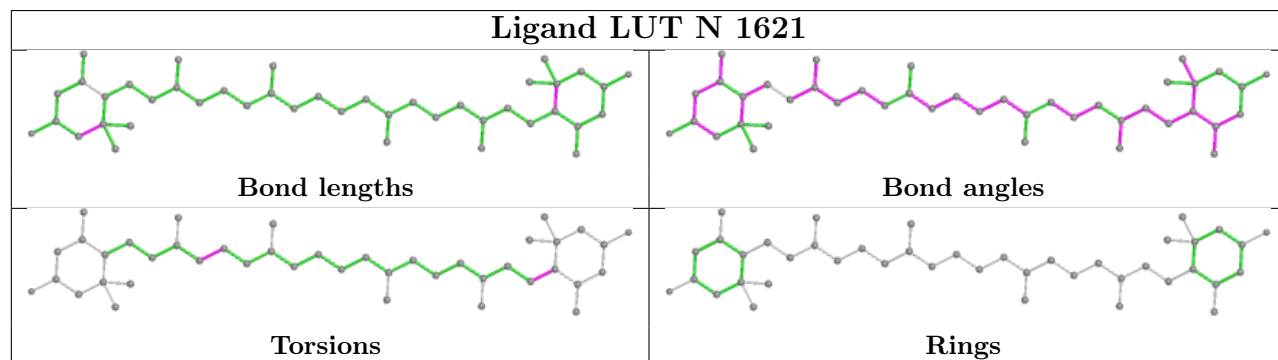
## Ligand CLA n 603



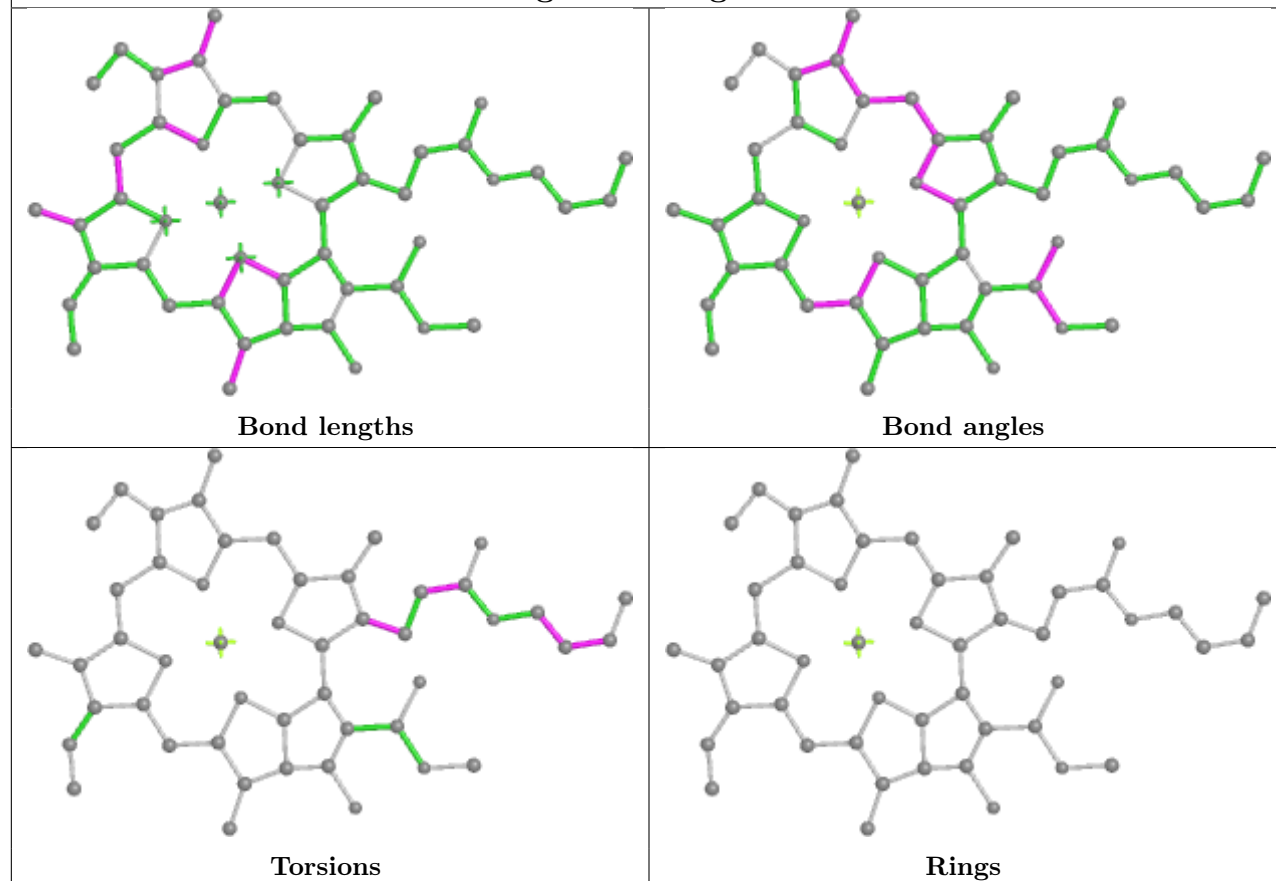
## Ligand CLA c 509



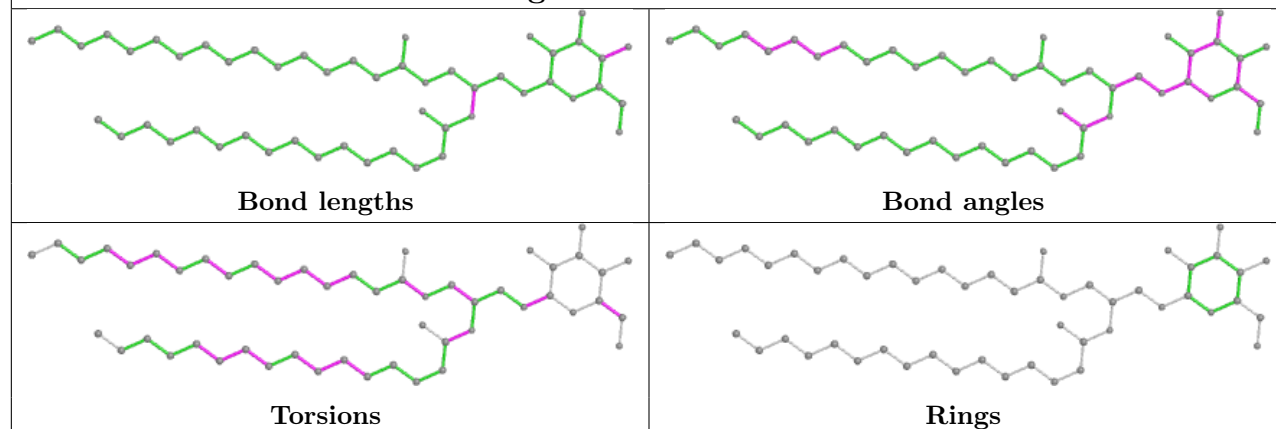
**Ligand NEX N 1623****Ligand CHL g 608**

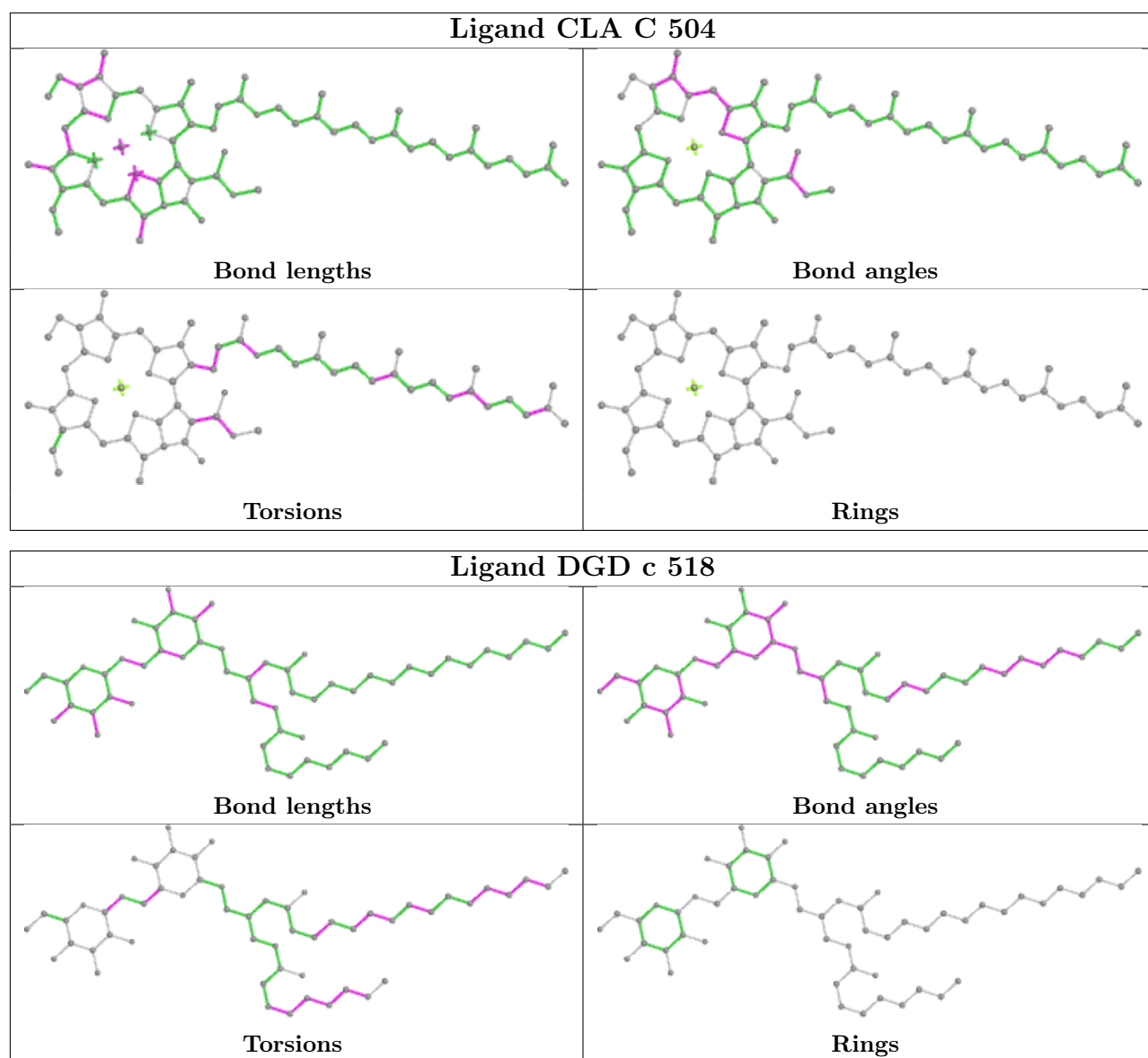
**Ligand CLA Y 611****Ligand CLA Y 612****Ligand LUT N 1621**

## Ligand CLA g 603

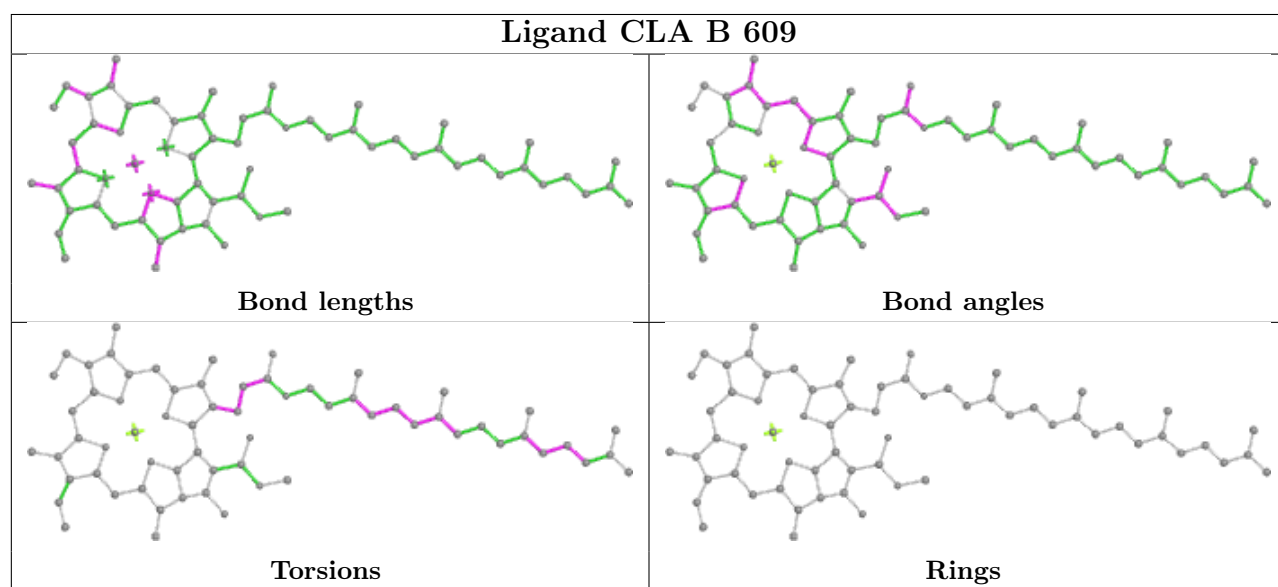
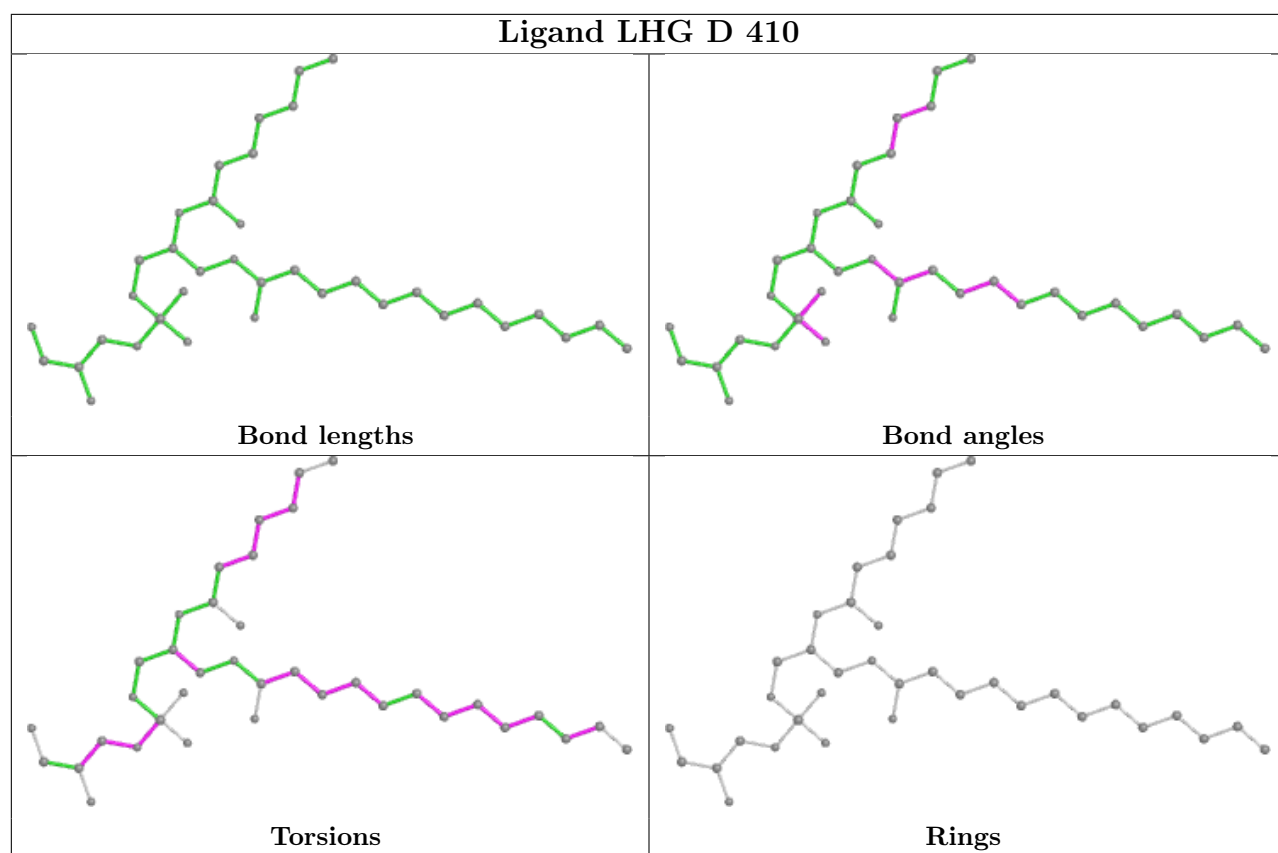


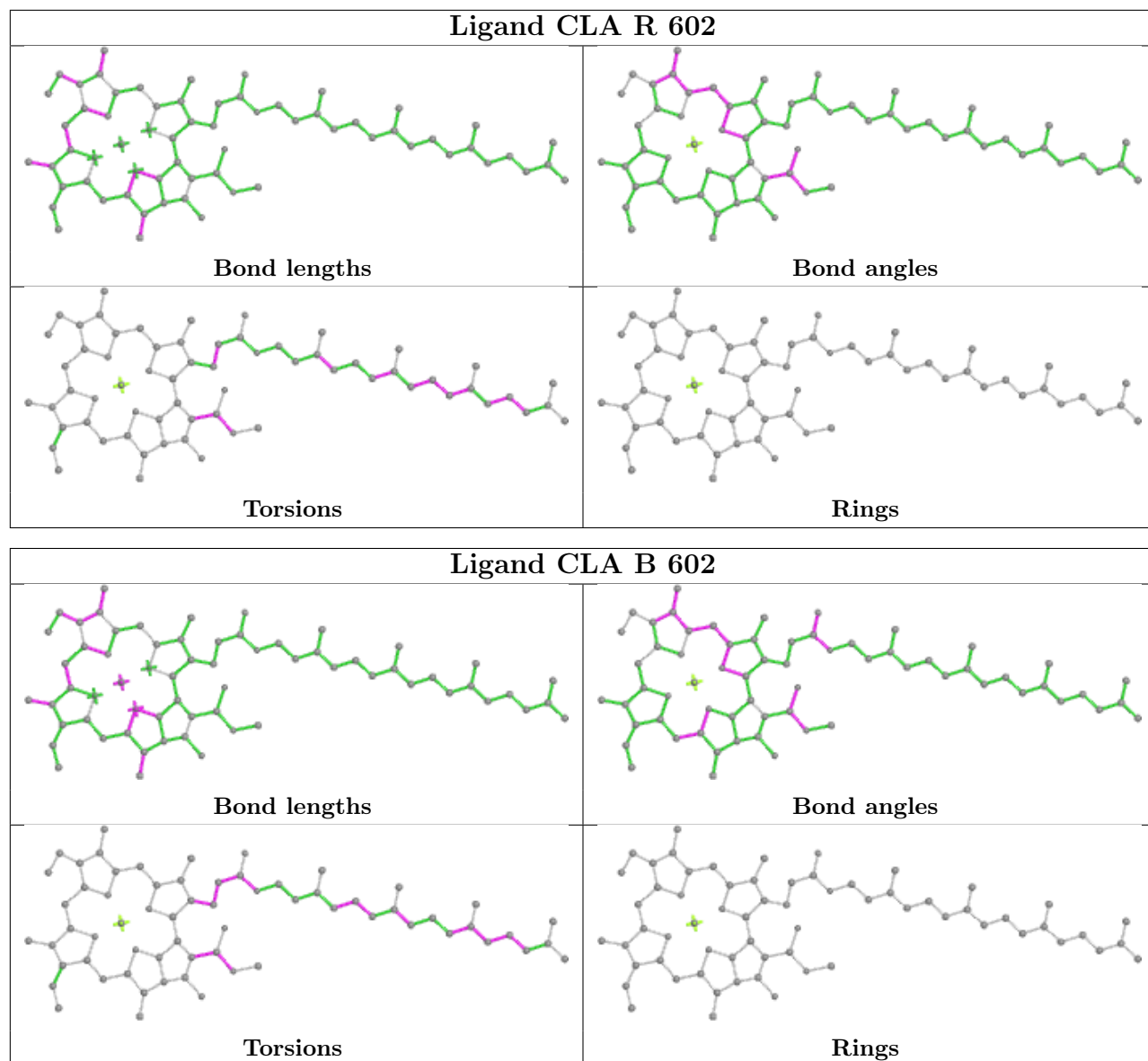
## Ligand LMG B 622

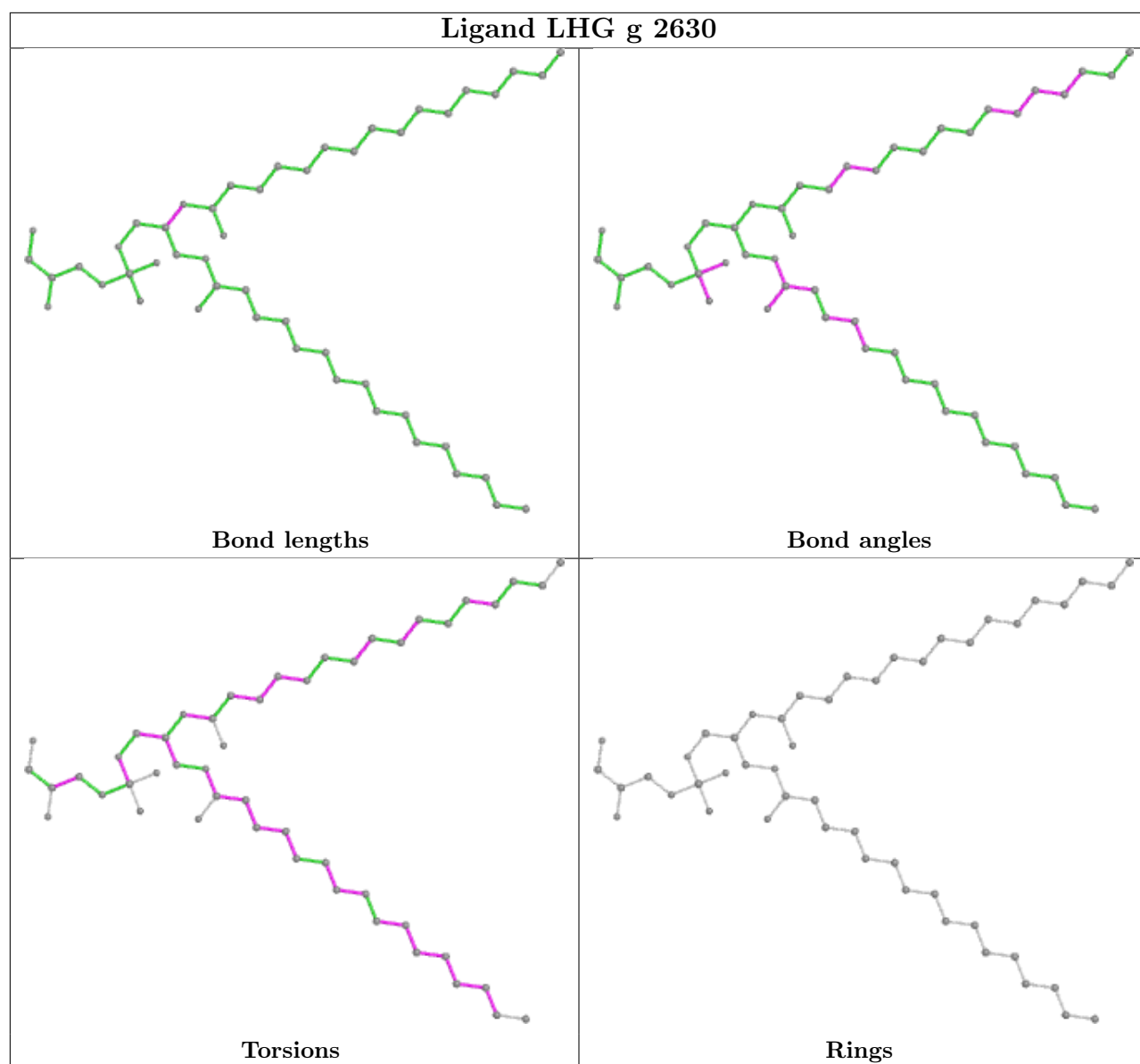




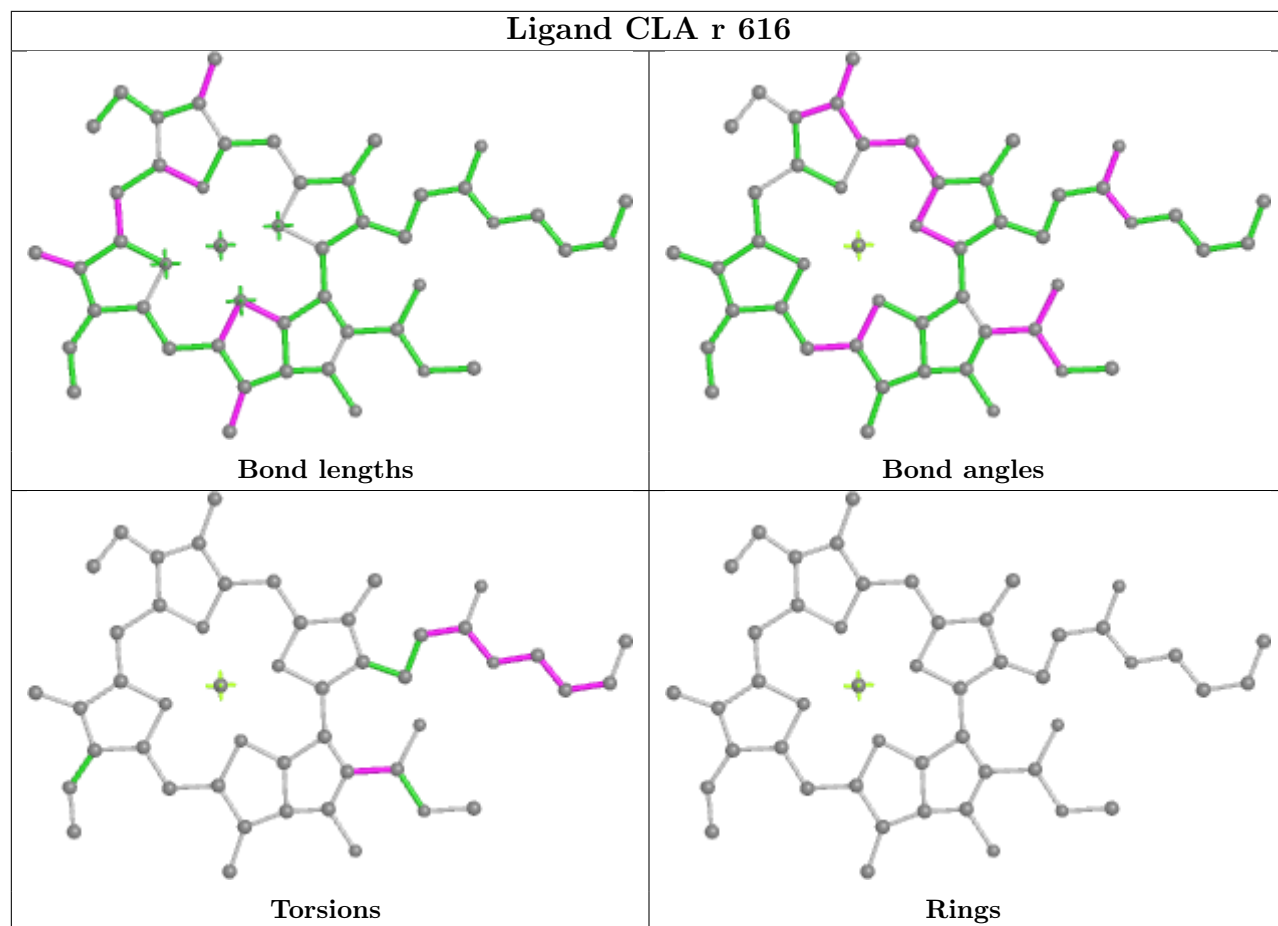


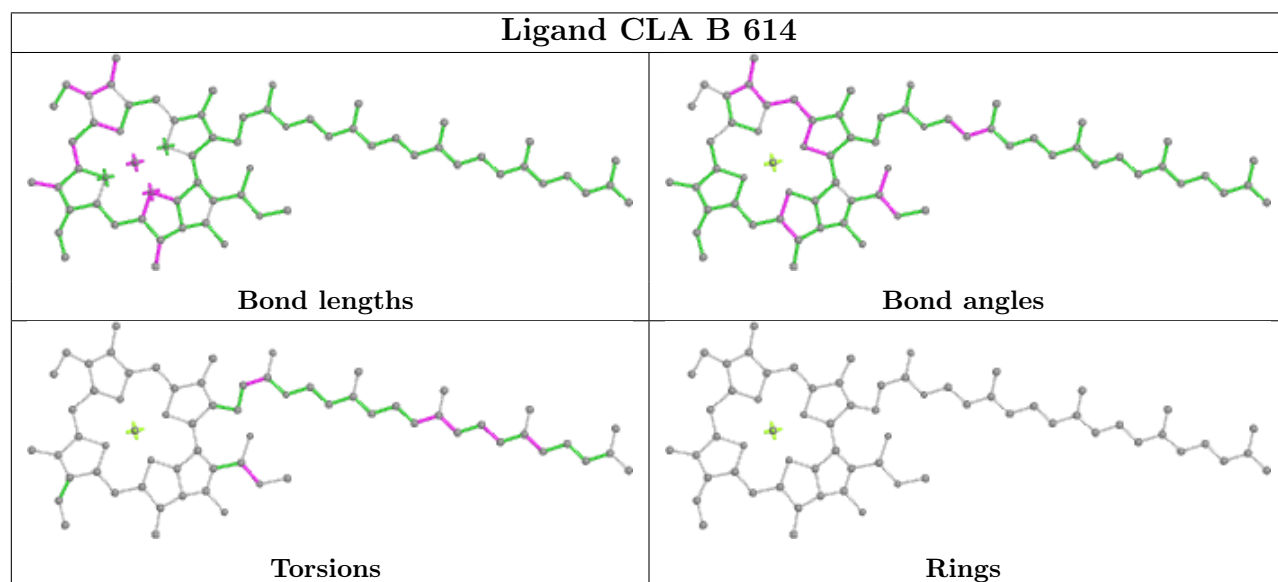
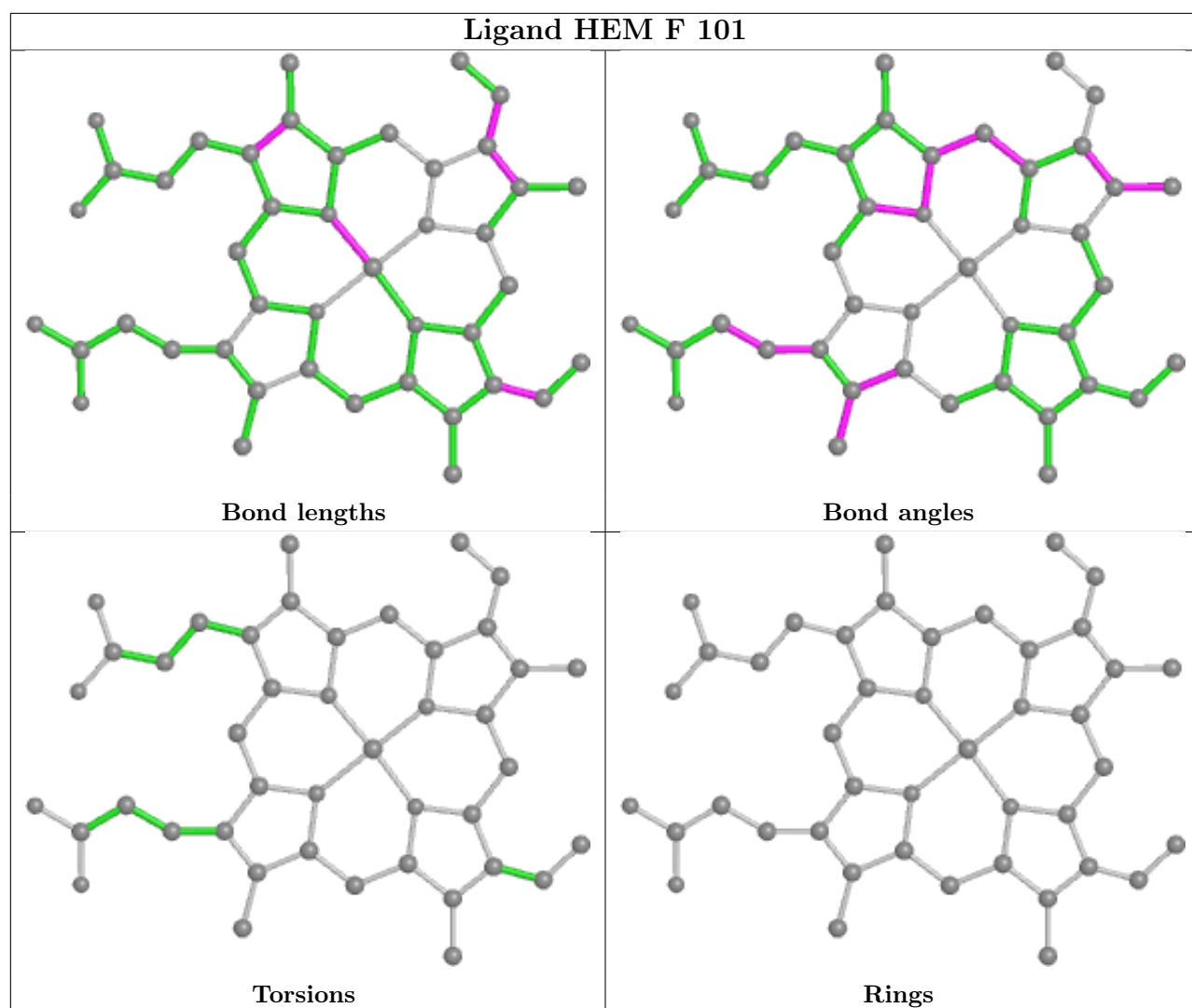




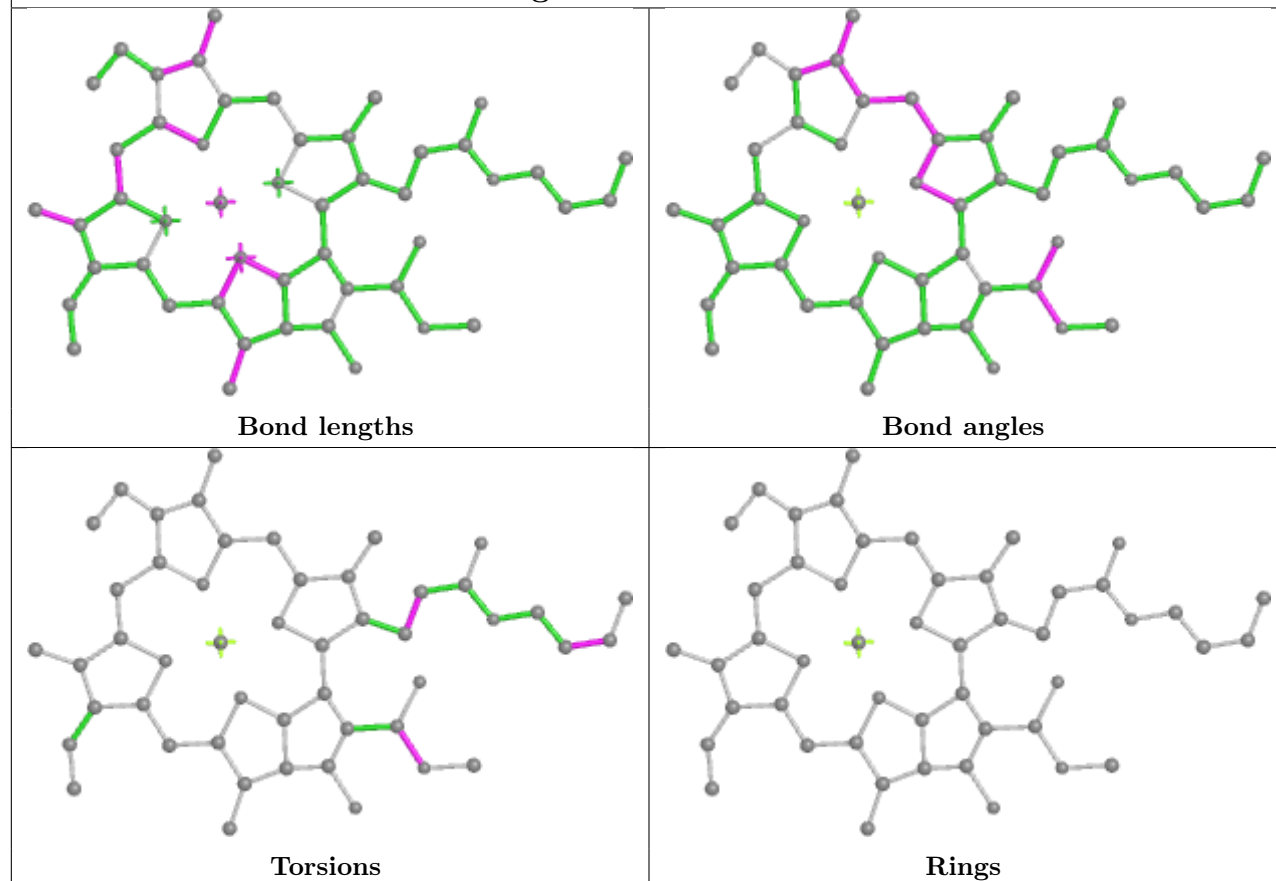


## Ligand CLA r 616

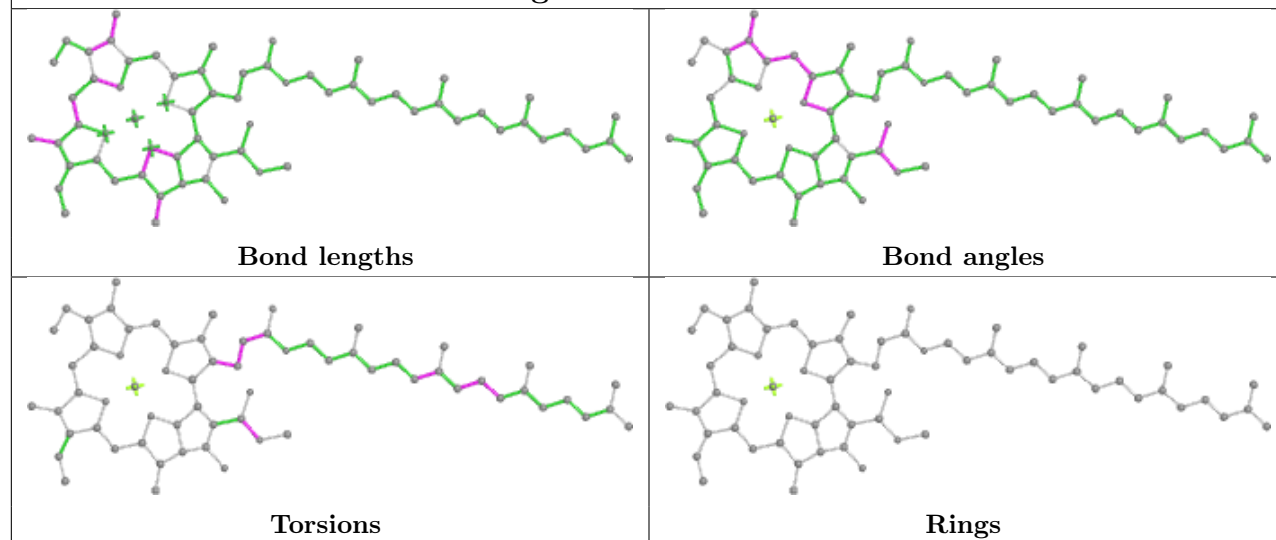


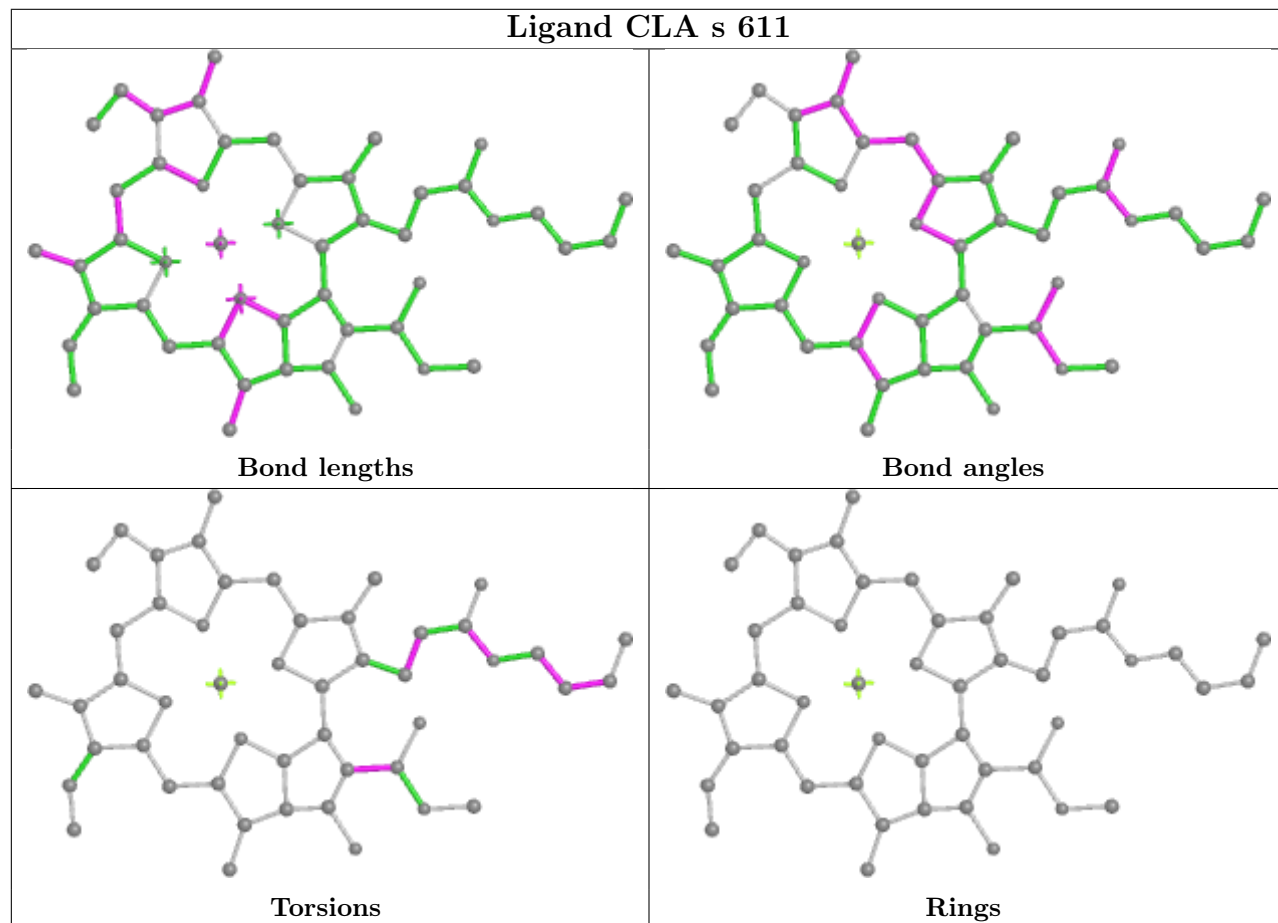
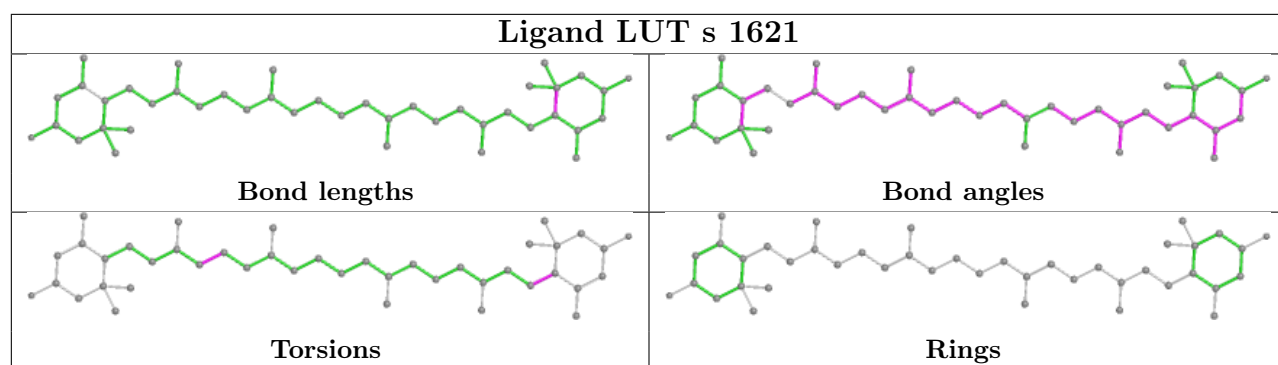


## Ligand CLA Y 603

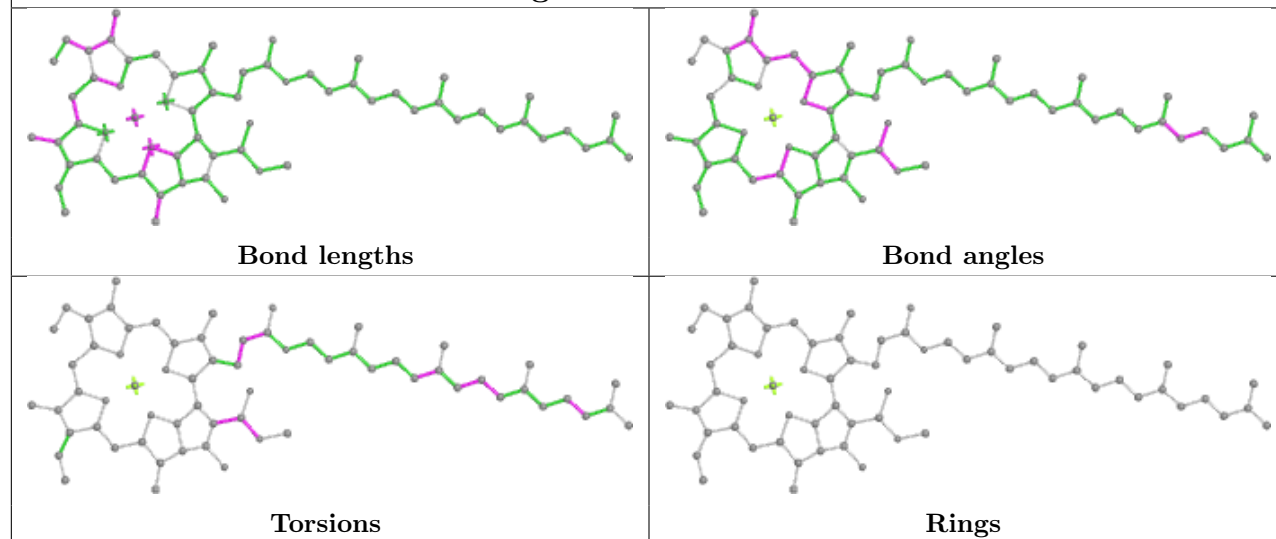


## Ligand CLA N 602

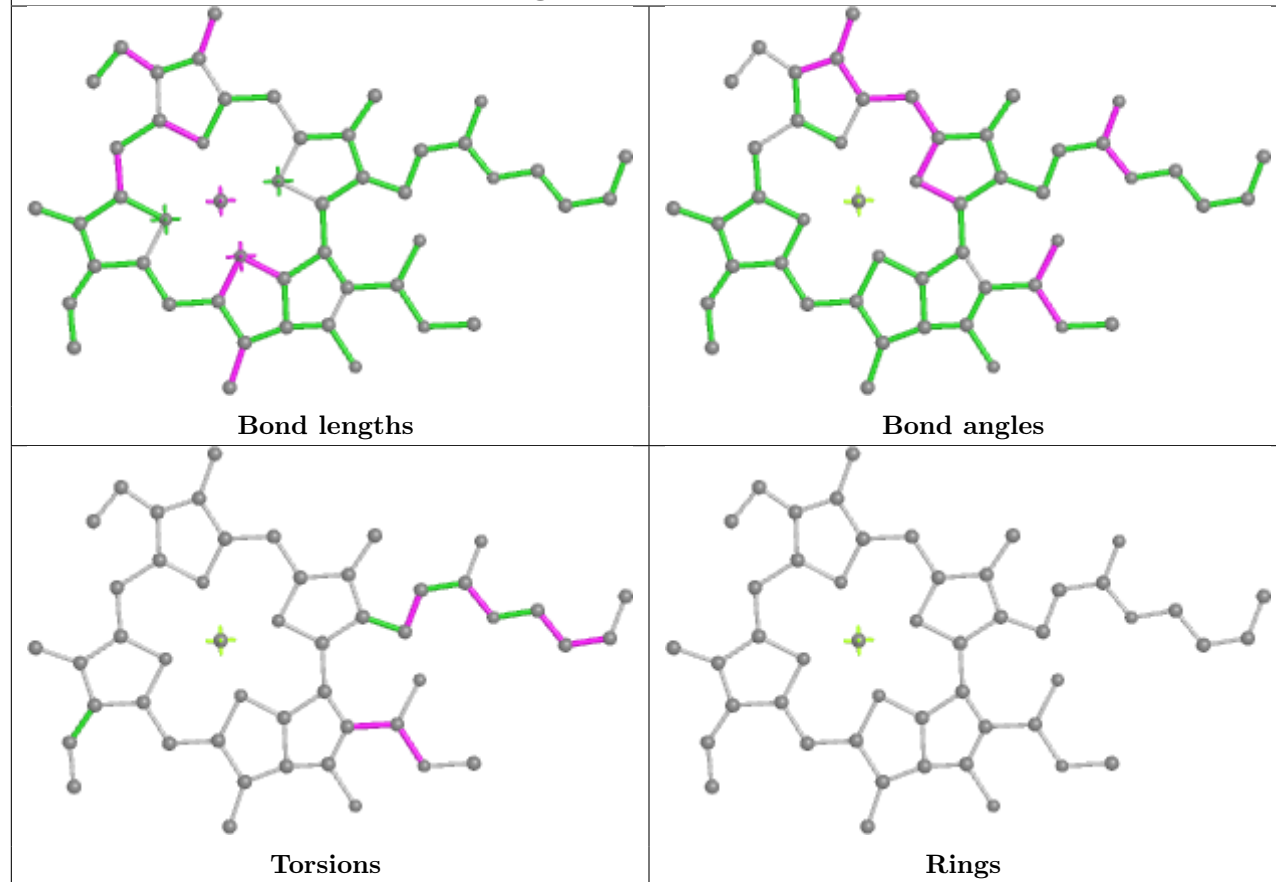




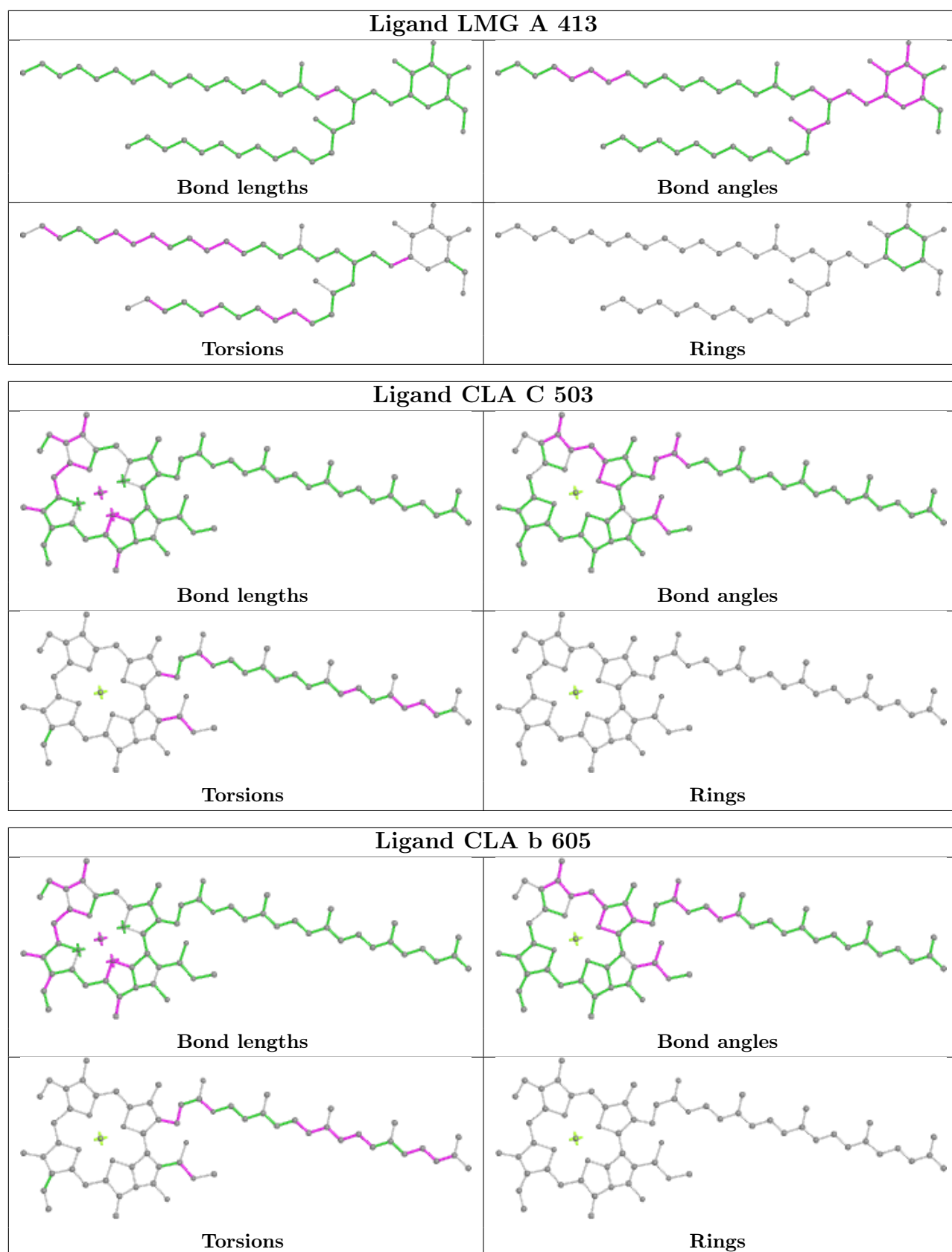
## Ligand CLA Y 602

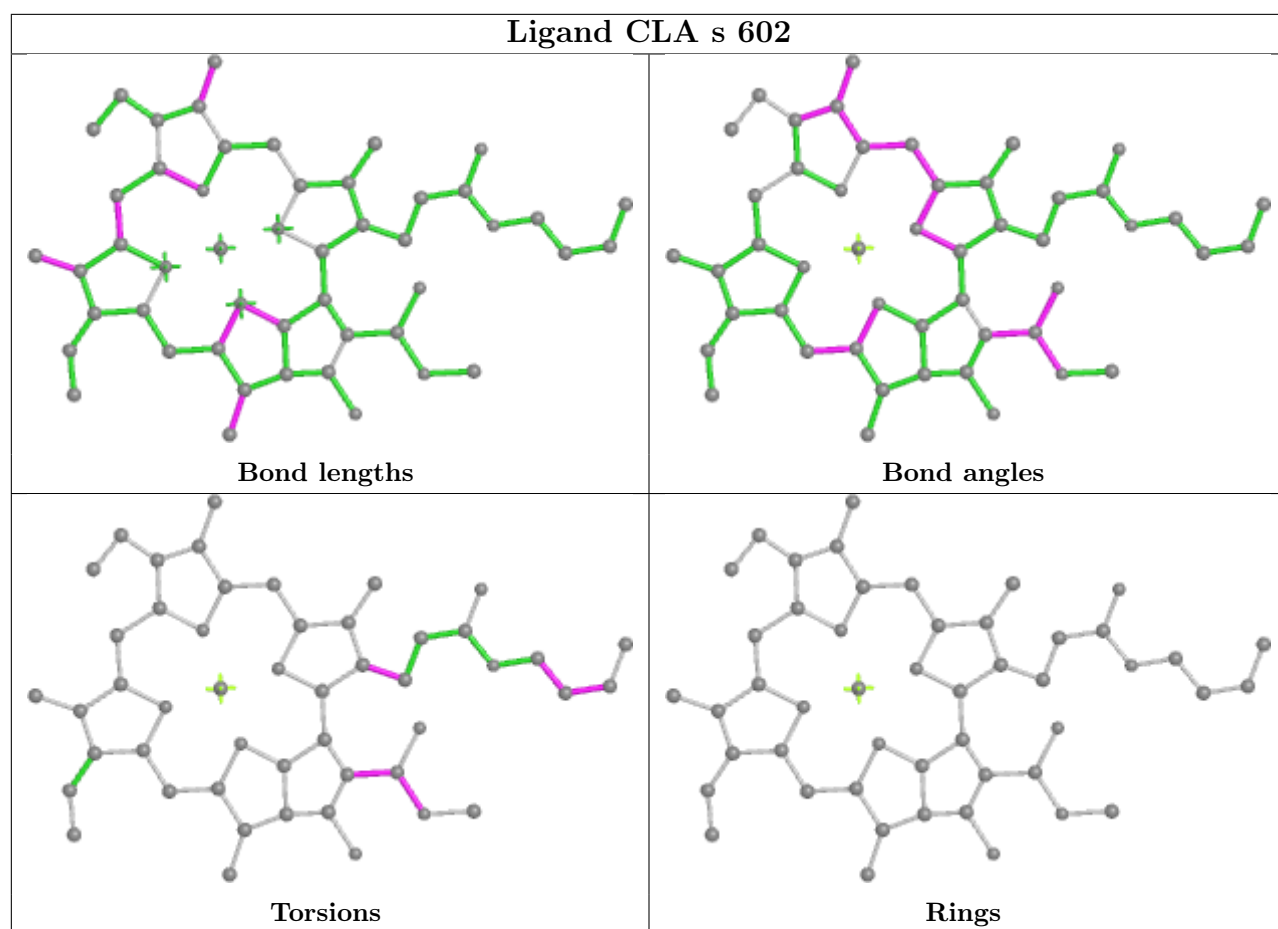


## Ligand CLA Y 614

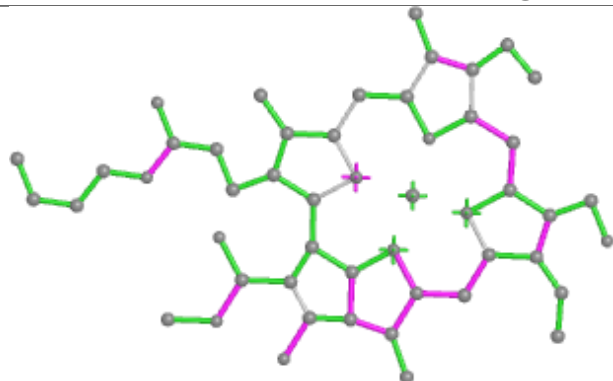




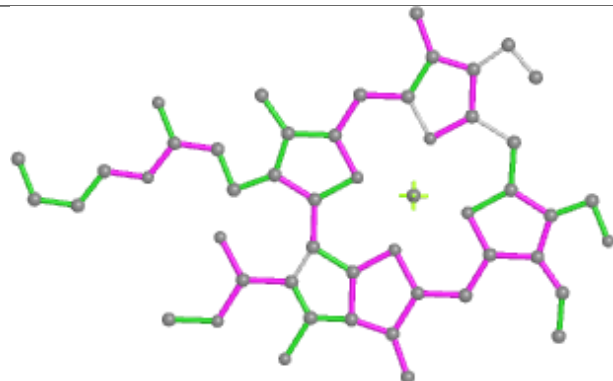




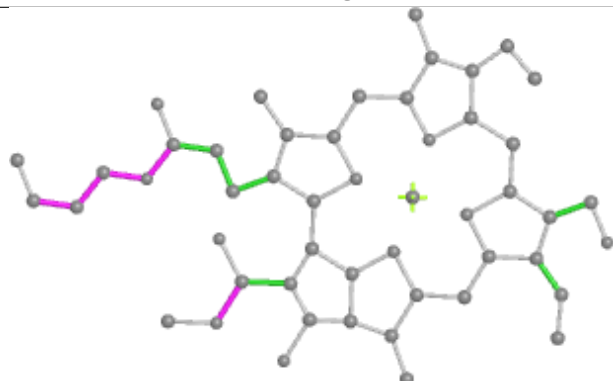
## Ligand CHL n 609



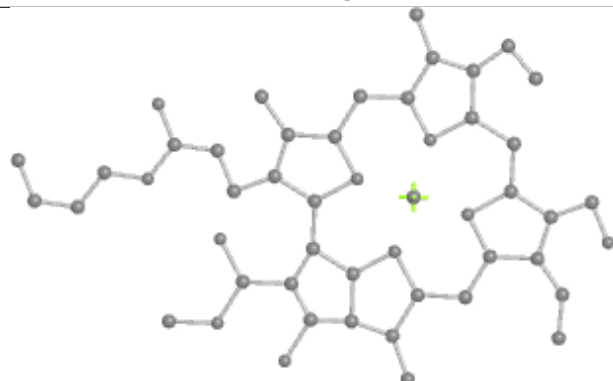
Bond lengths



Bond angles

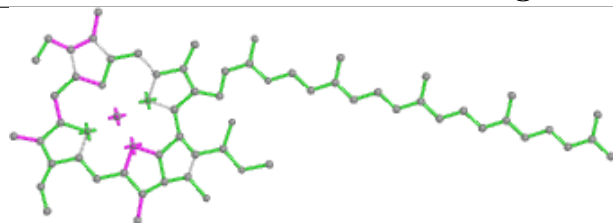


Torsions

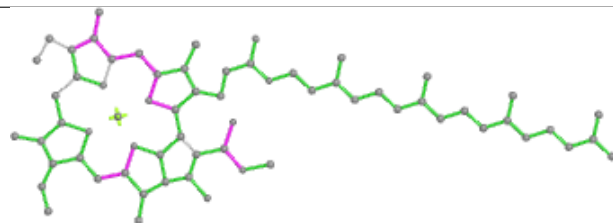


Rings

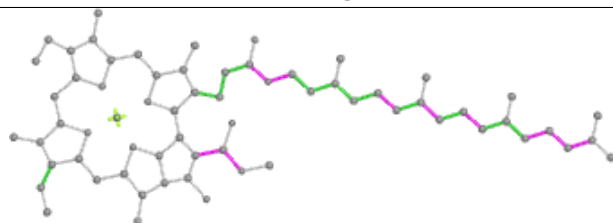
## Ligand CLA C 502



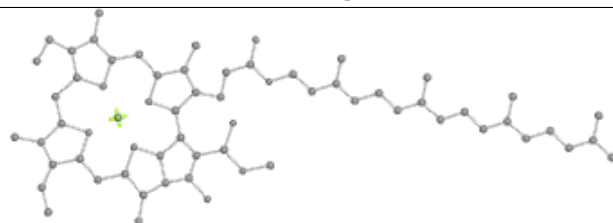
Bond lengths



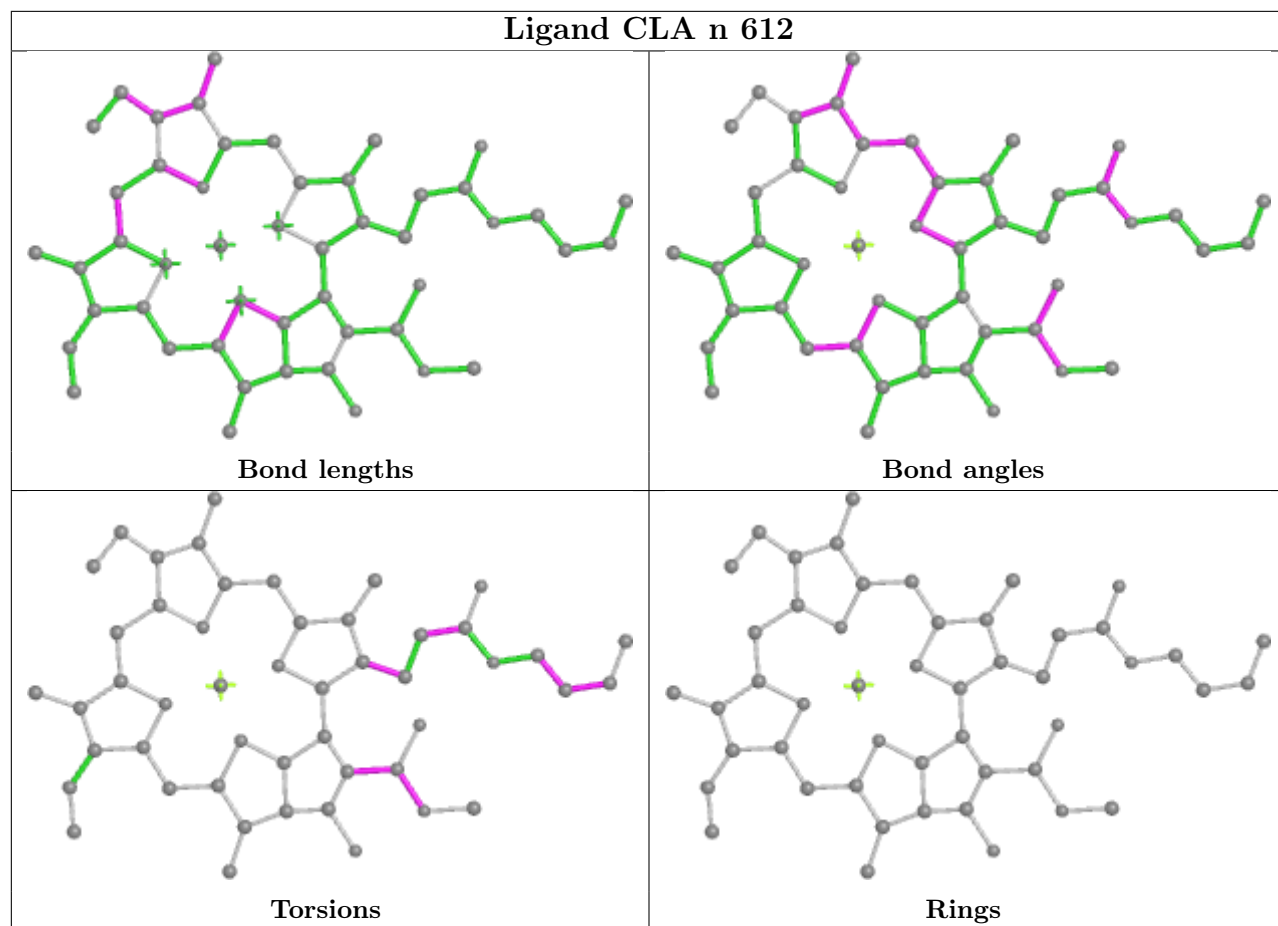
Bond angles

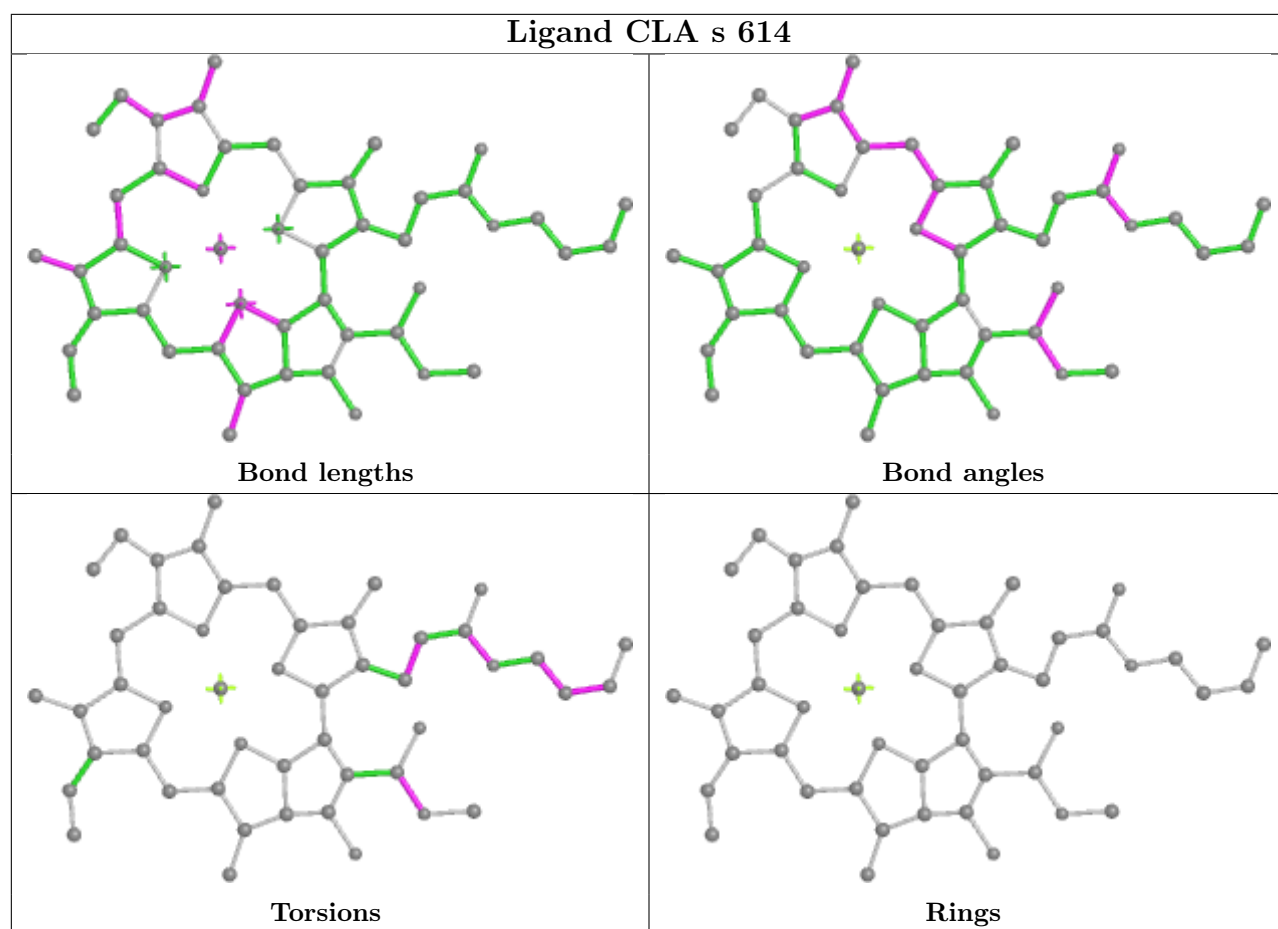


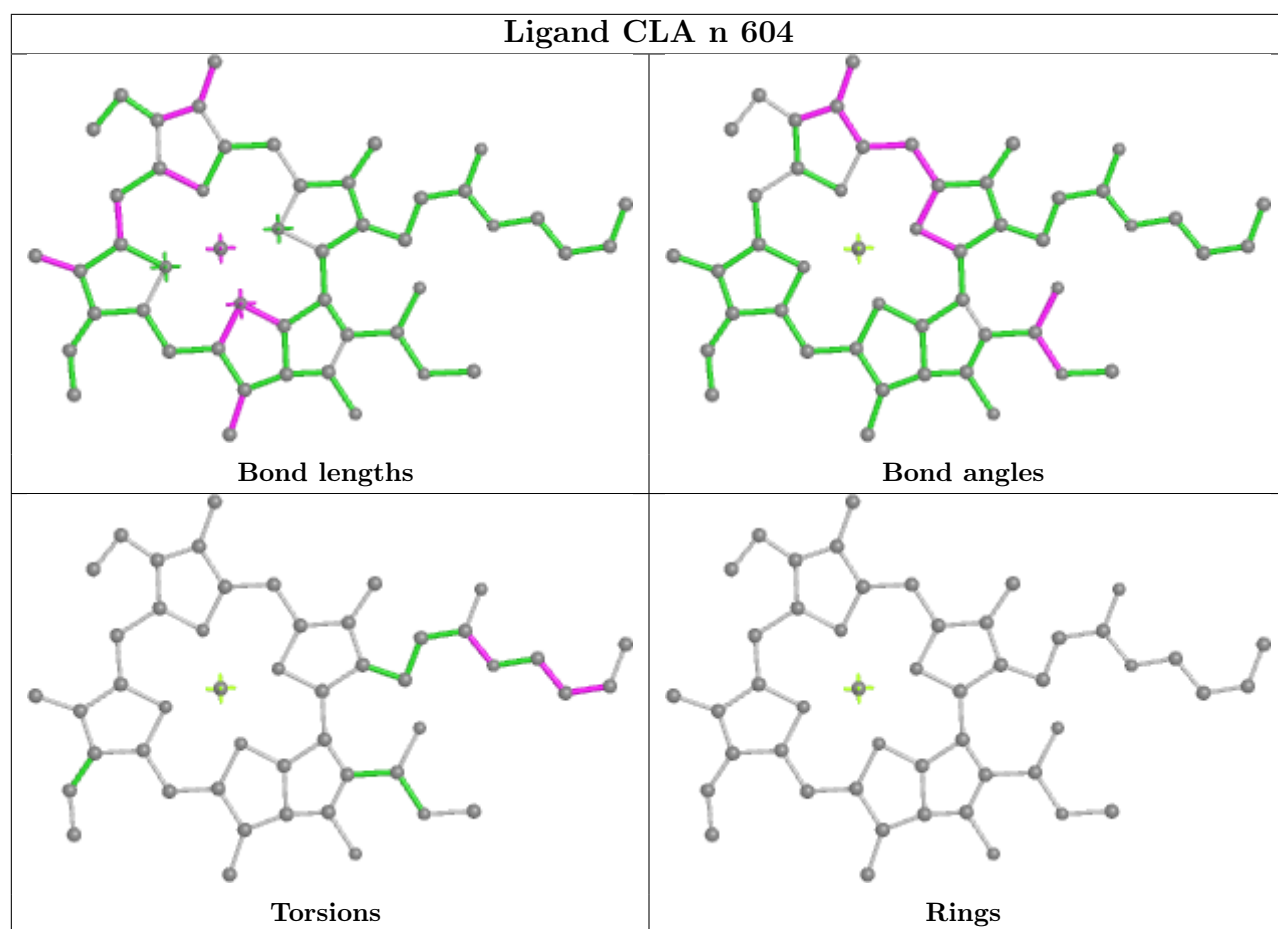
Torsions

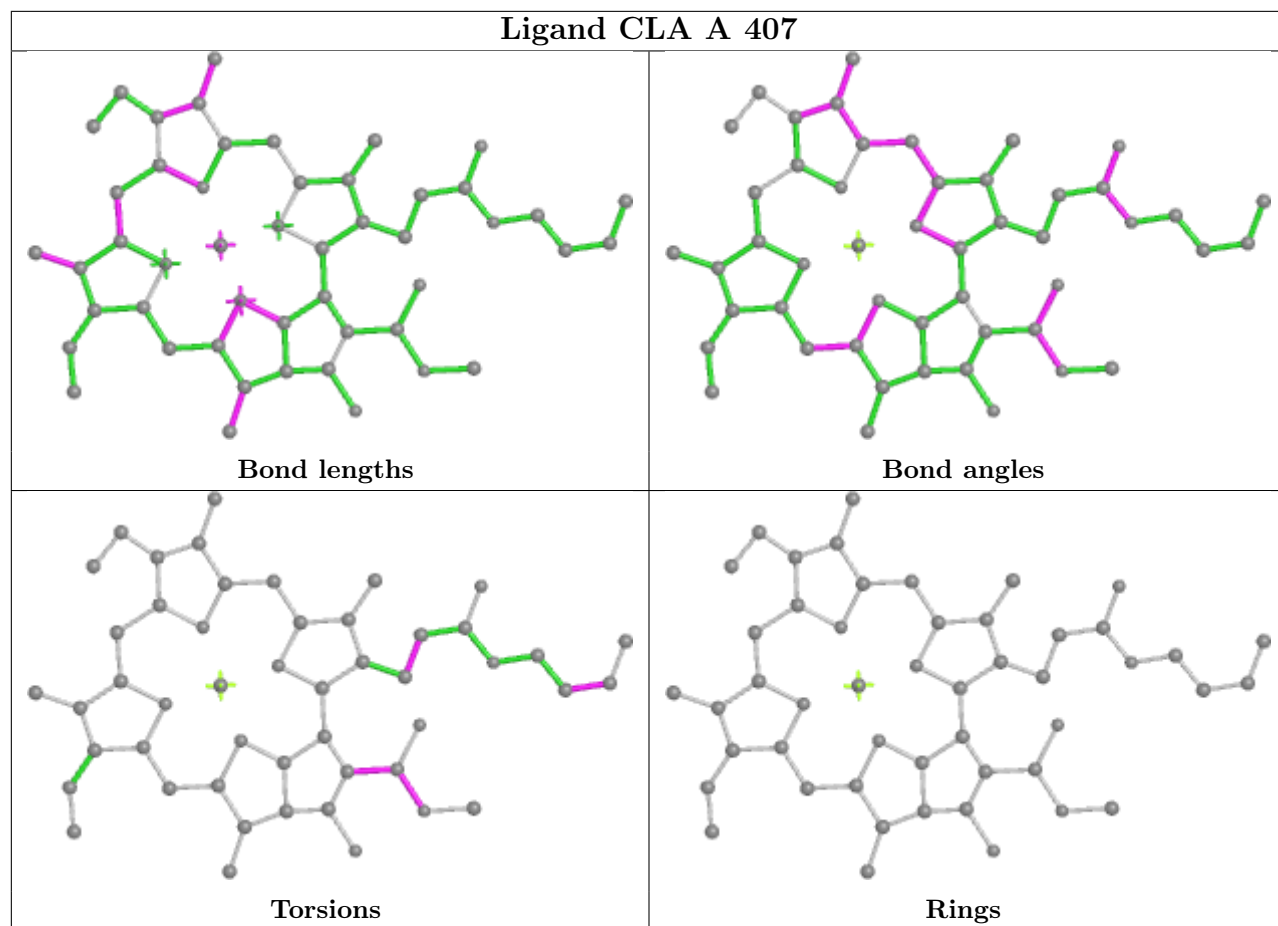


Rings

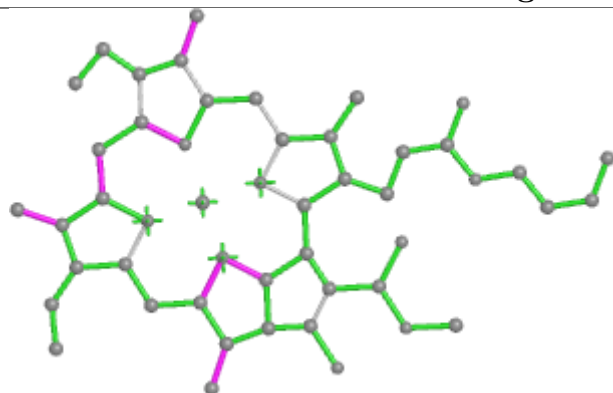




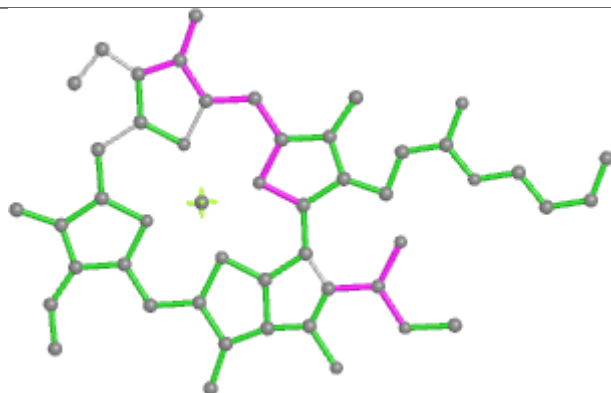




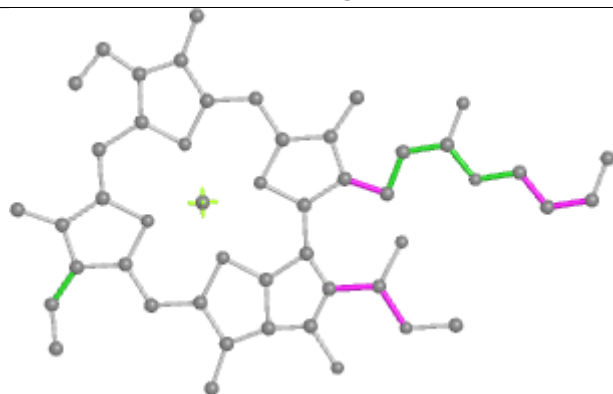
## Ligand CLA S 602



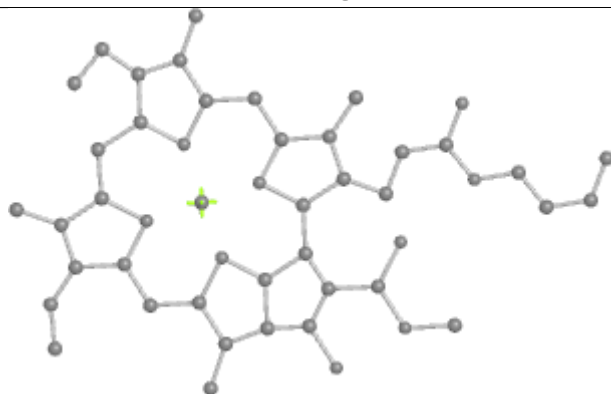
Bond lengths



Bond angles

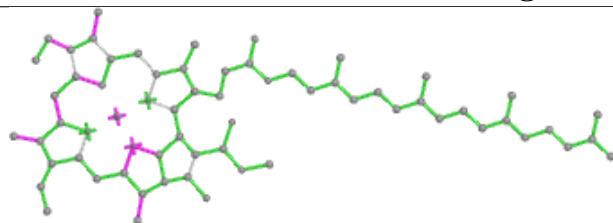


Torsions

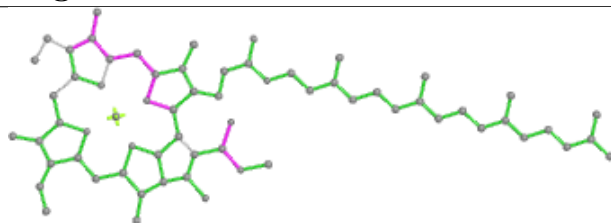


Rings

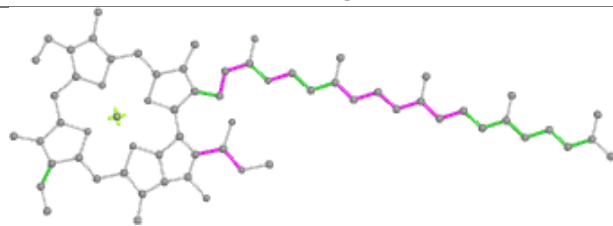
## Ligand CLA g 602



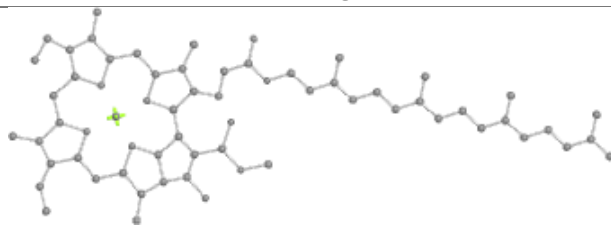
Bond lengths



Bond angles



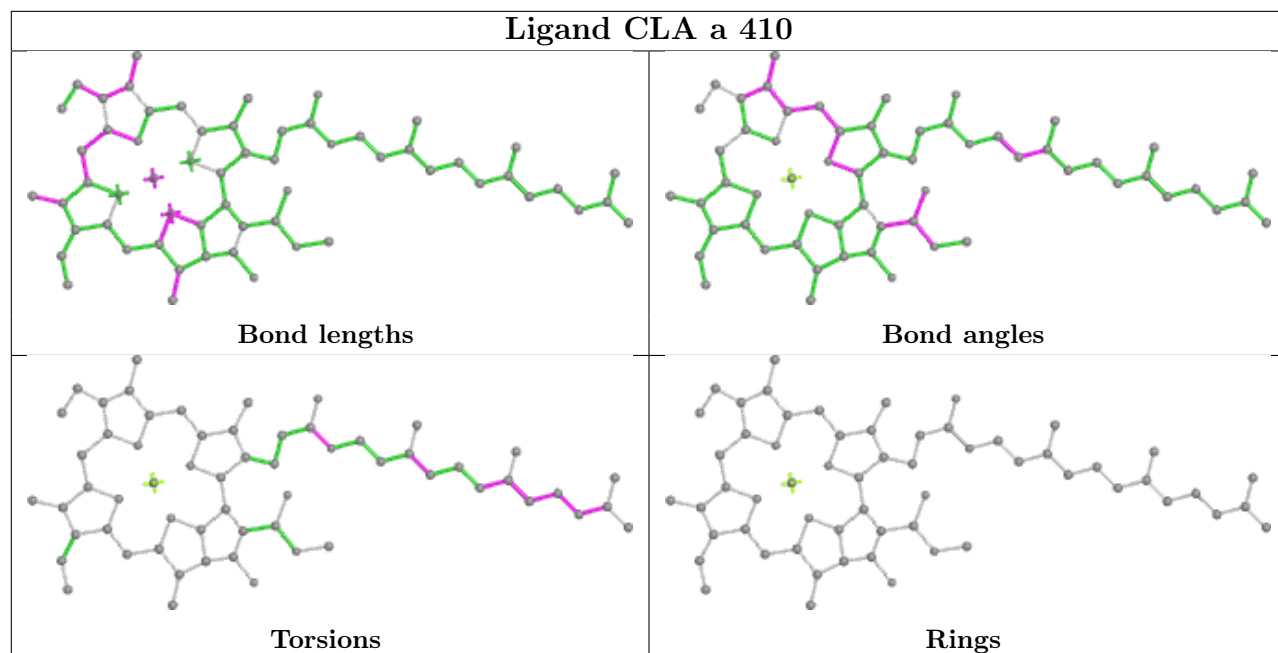
Torsions



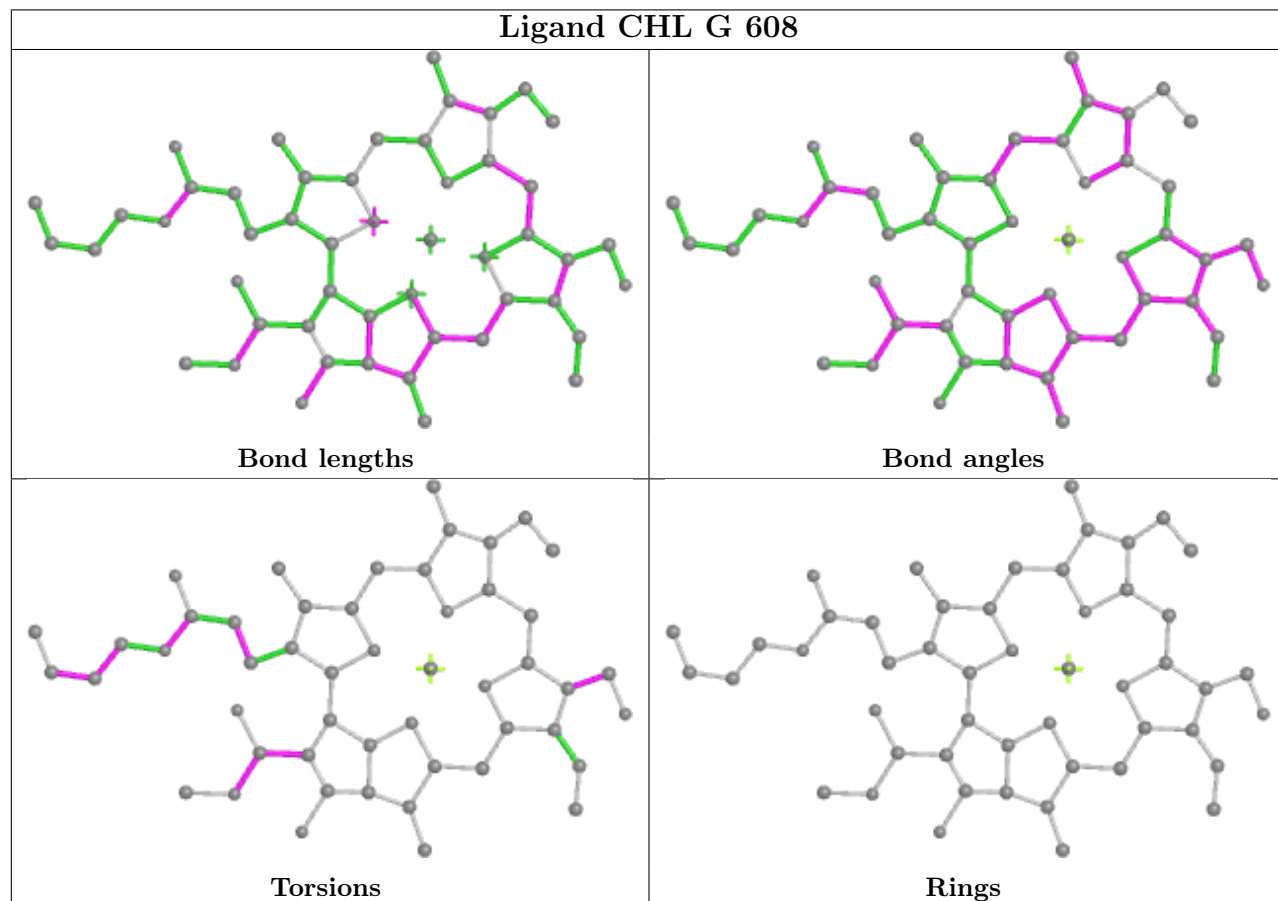
Rings



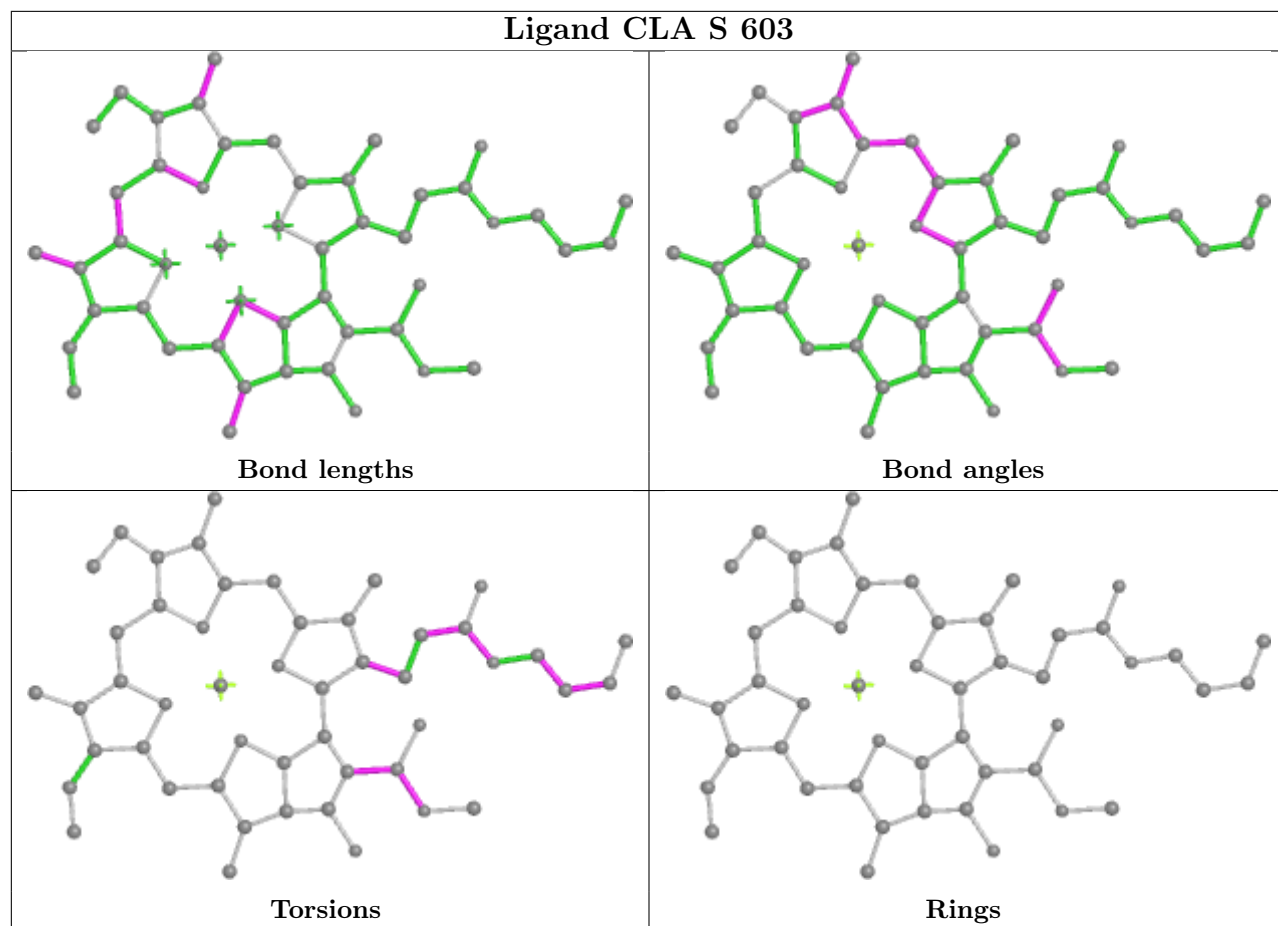
## Ligand CLA a 410



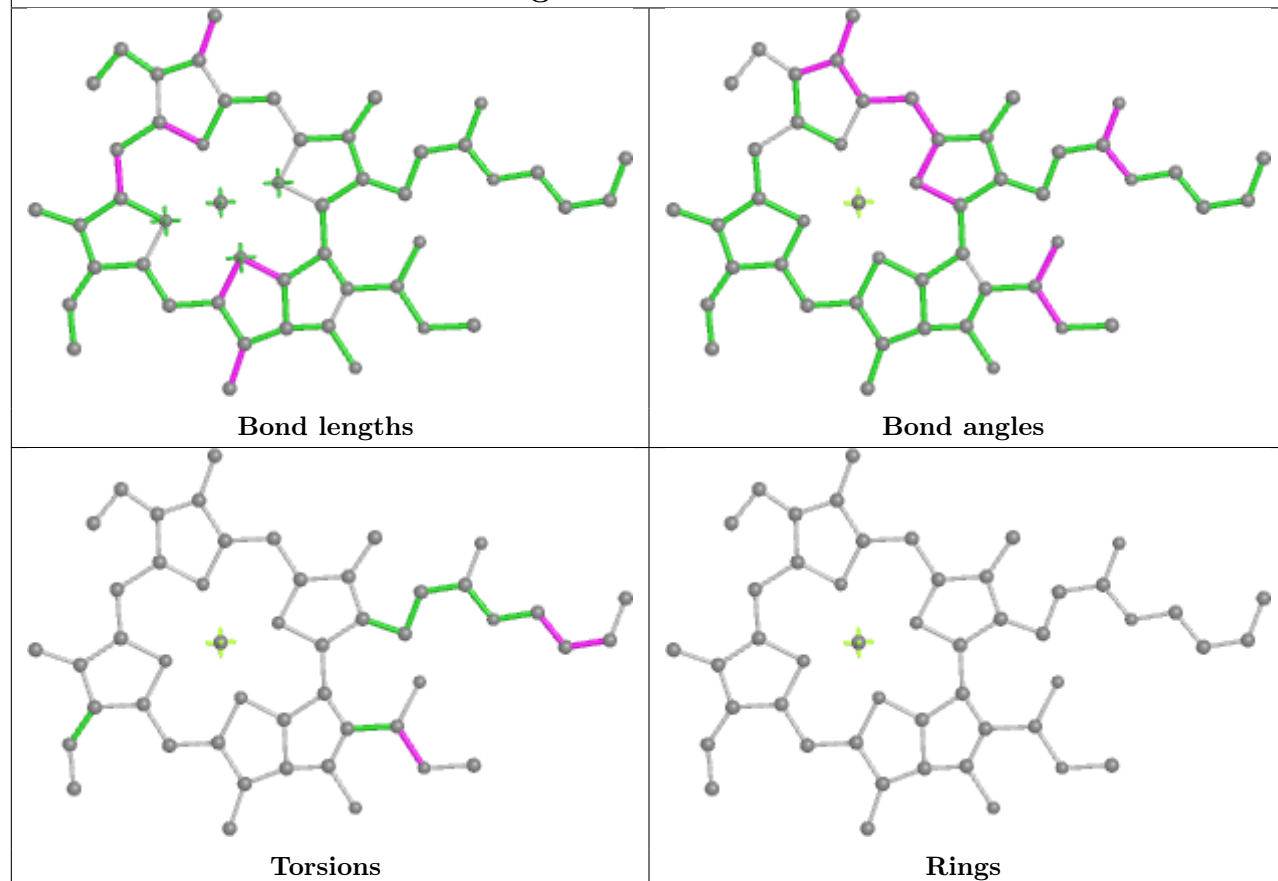
## Ligand CHL G 608



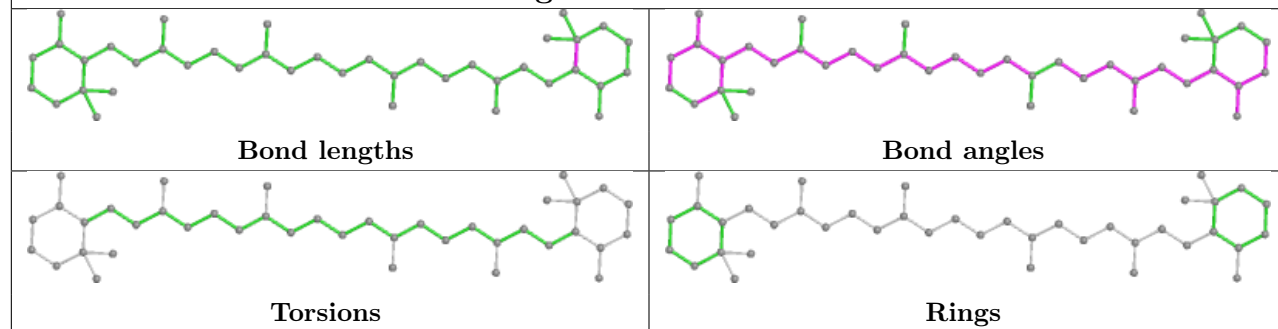
## Ligand CLA S 603

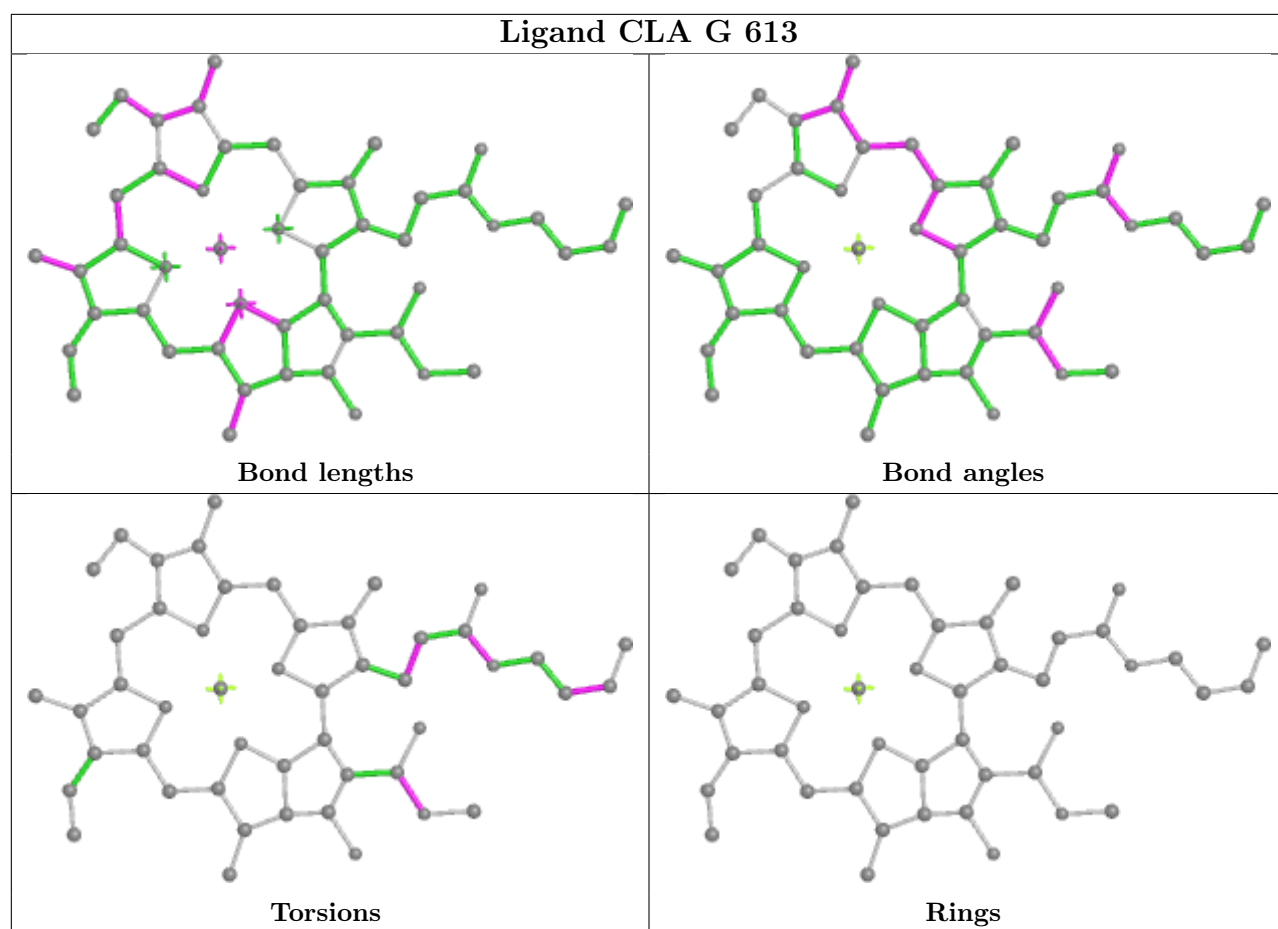


## Ligand CLA R 612

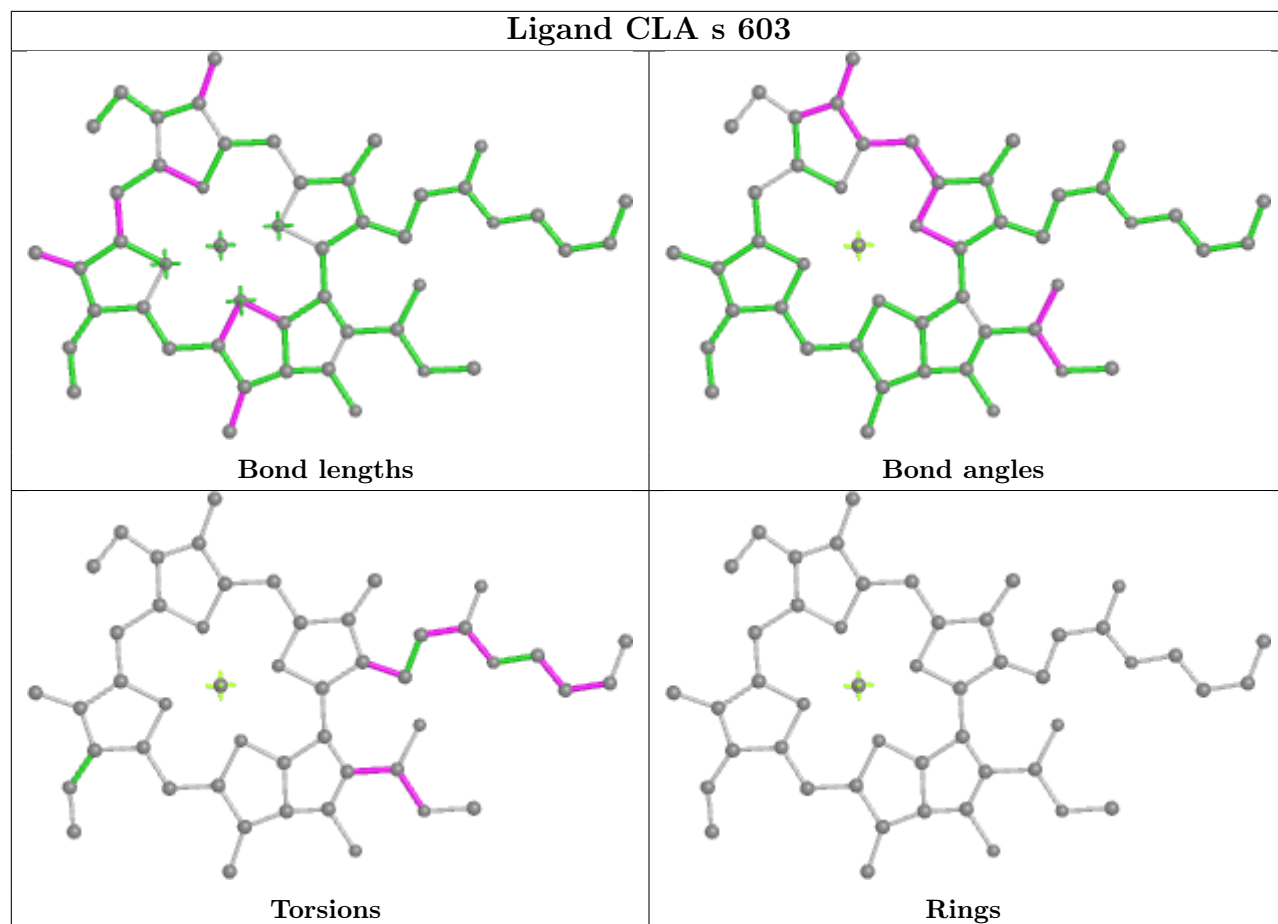


## Ligand BCR c 515

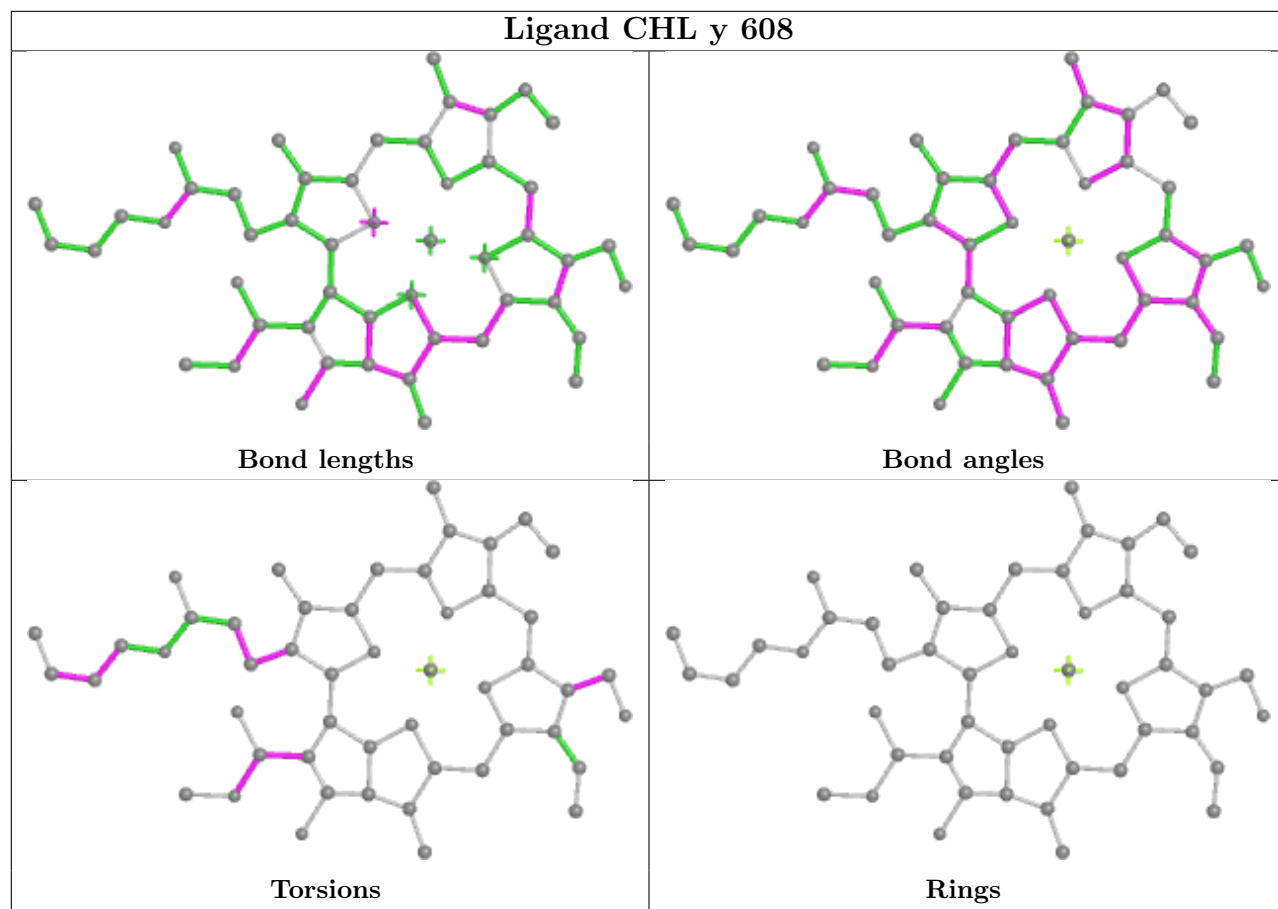




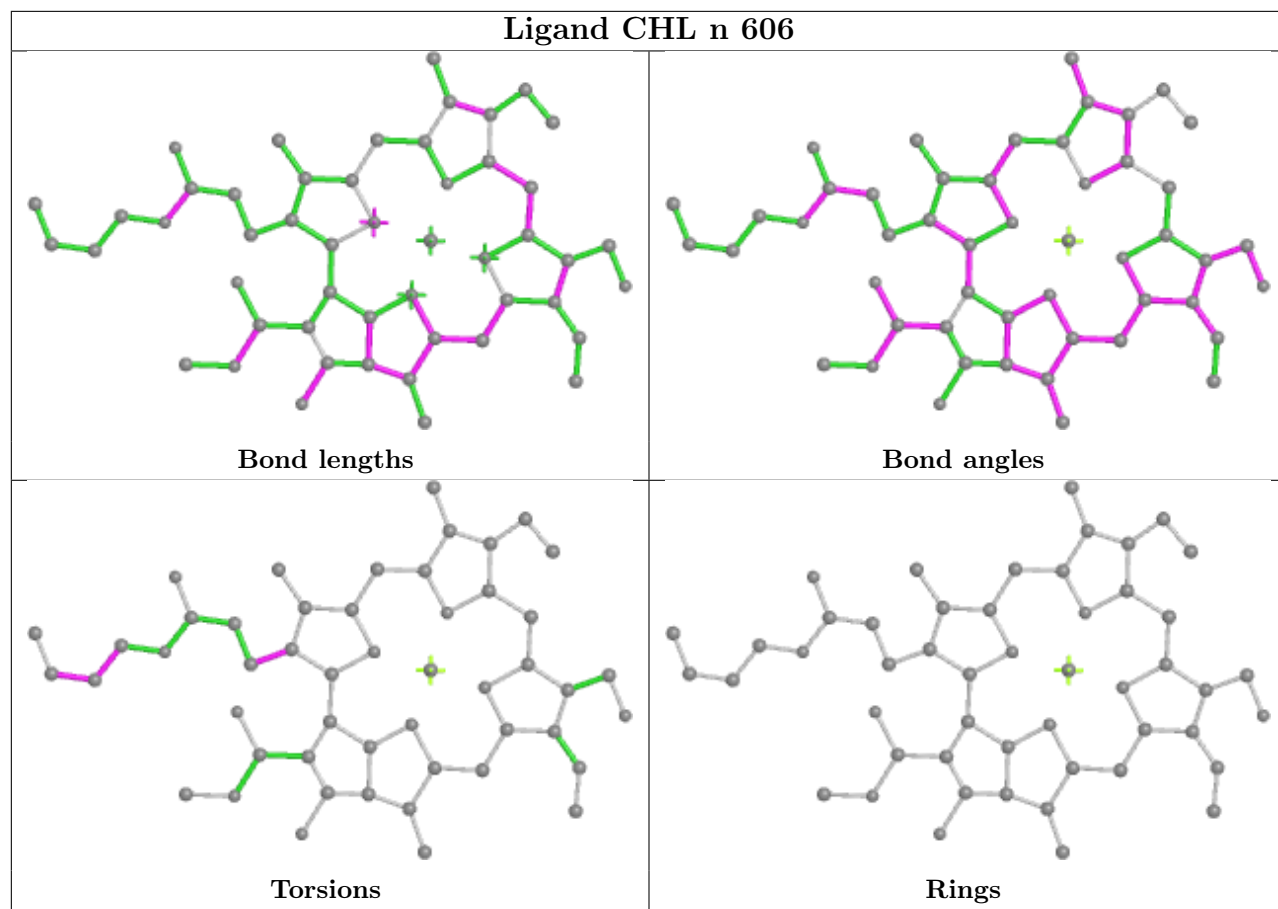
## Ligand CLA s 603

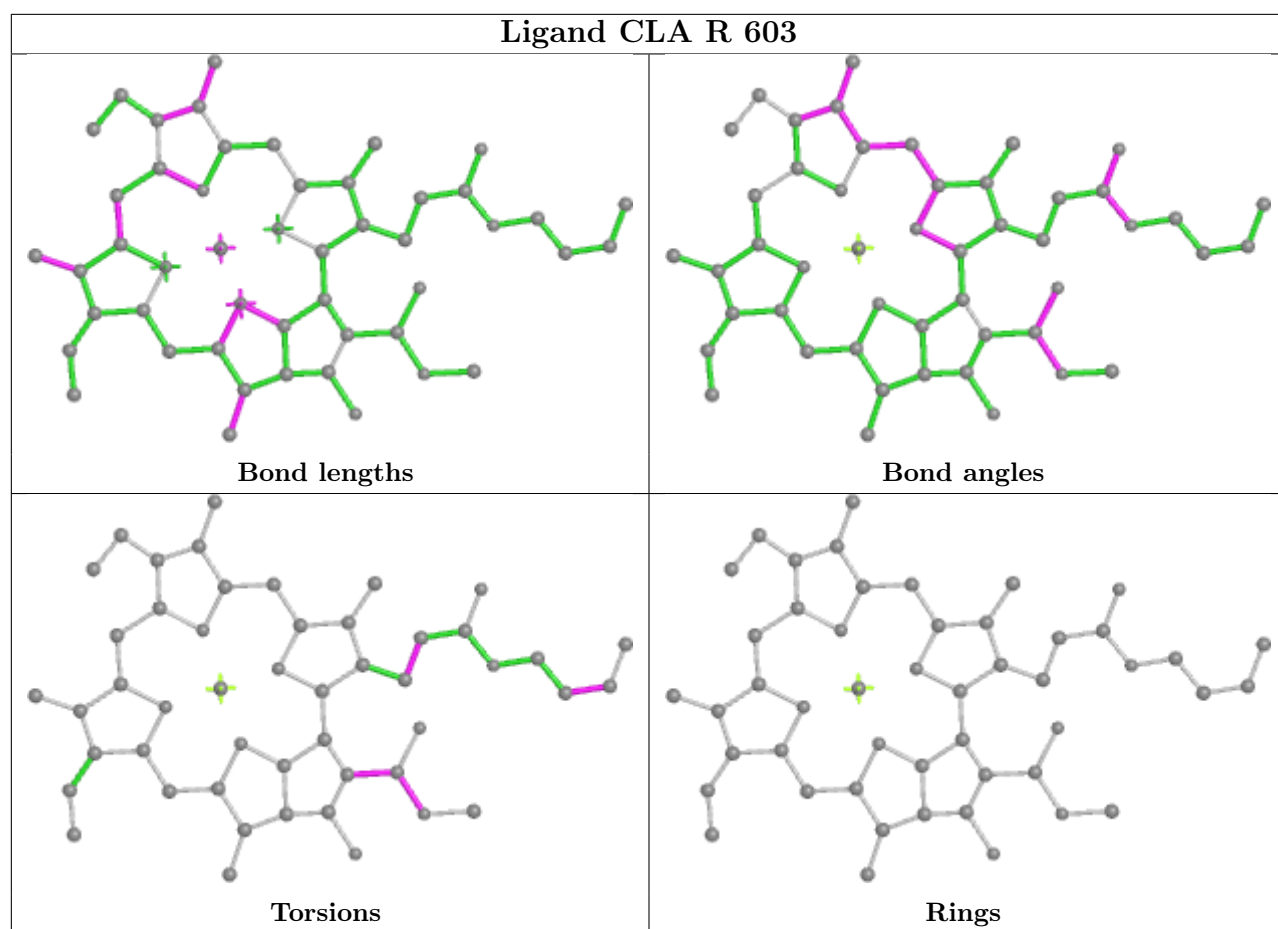


## Ligand CHL y 608

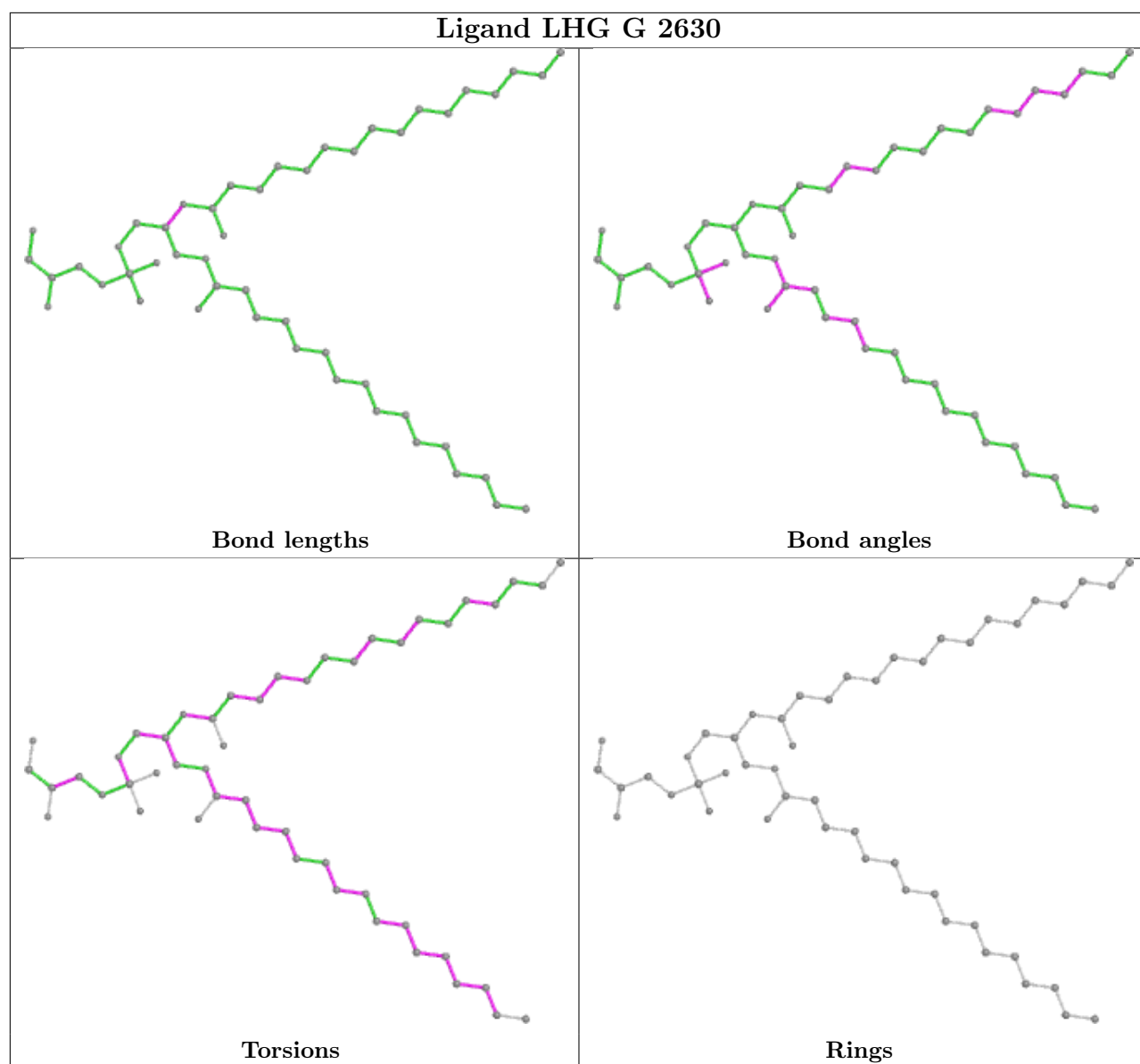


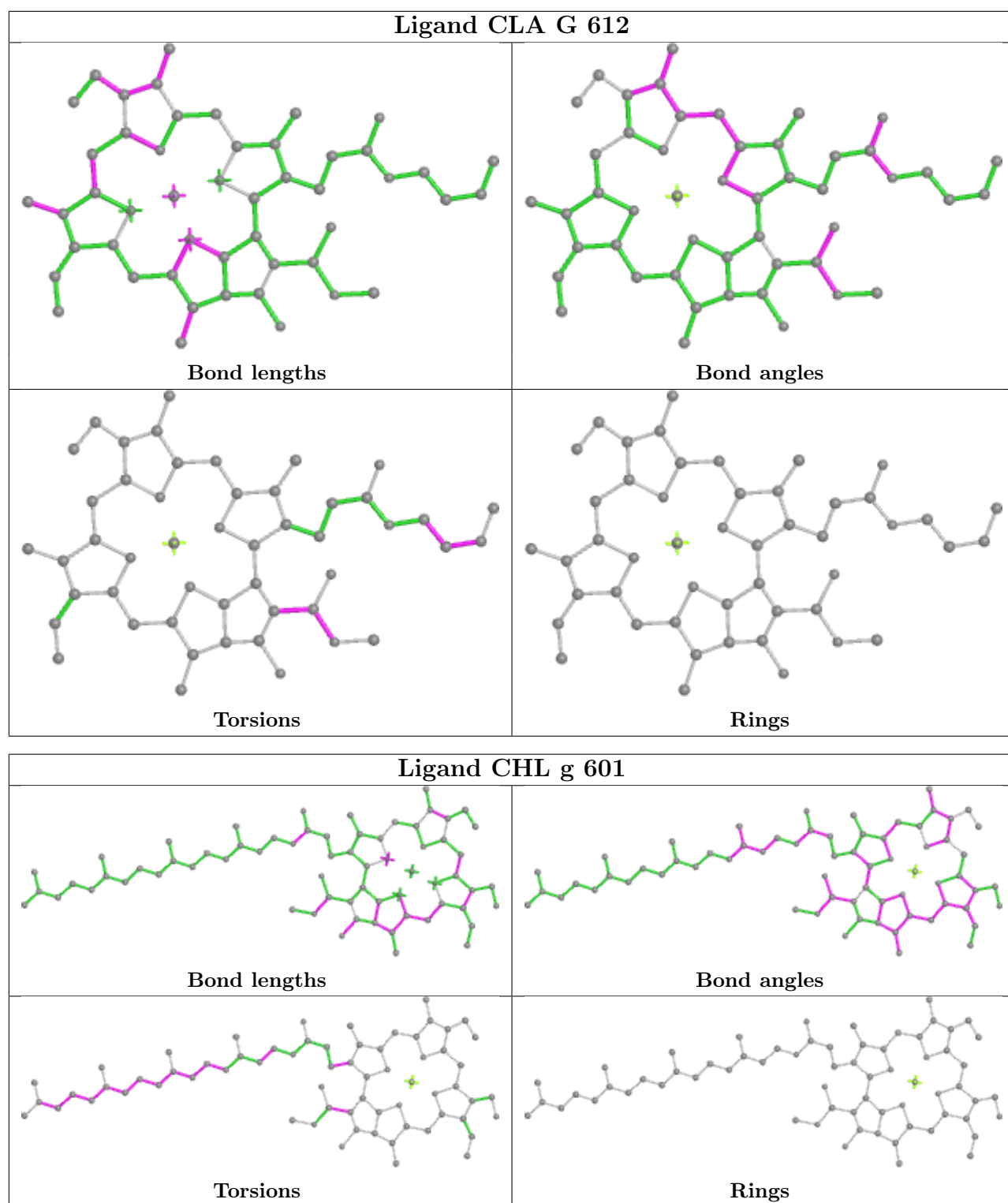
## Ligand CHL n 606



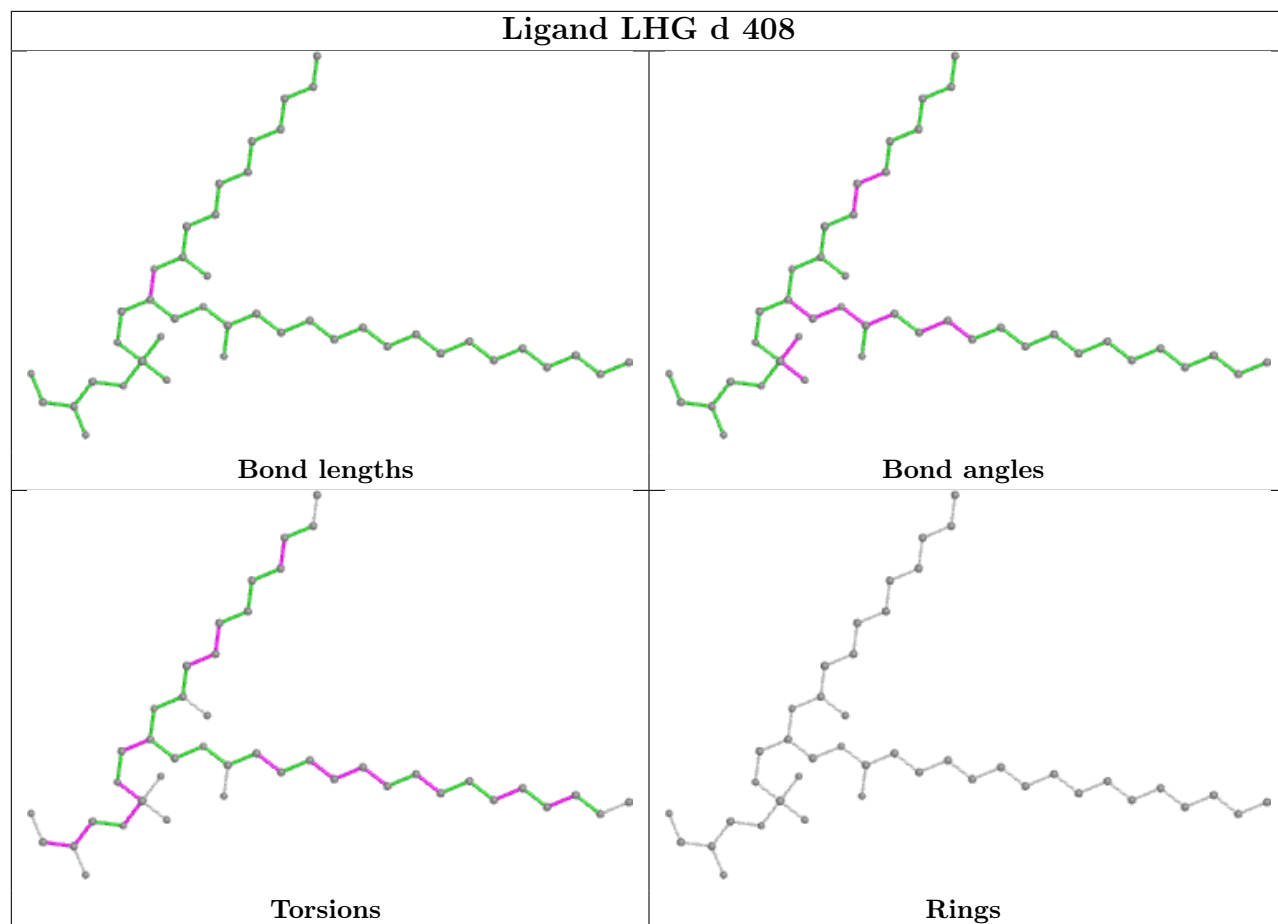




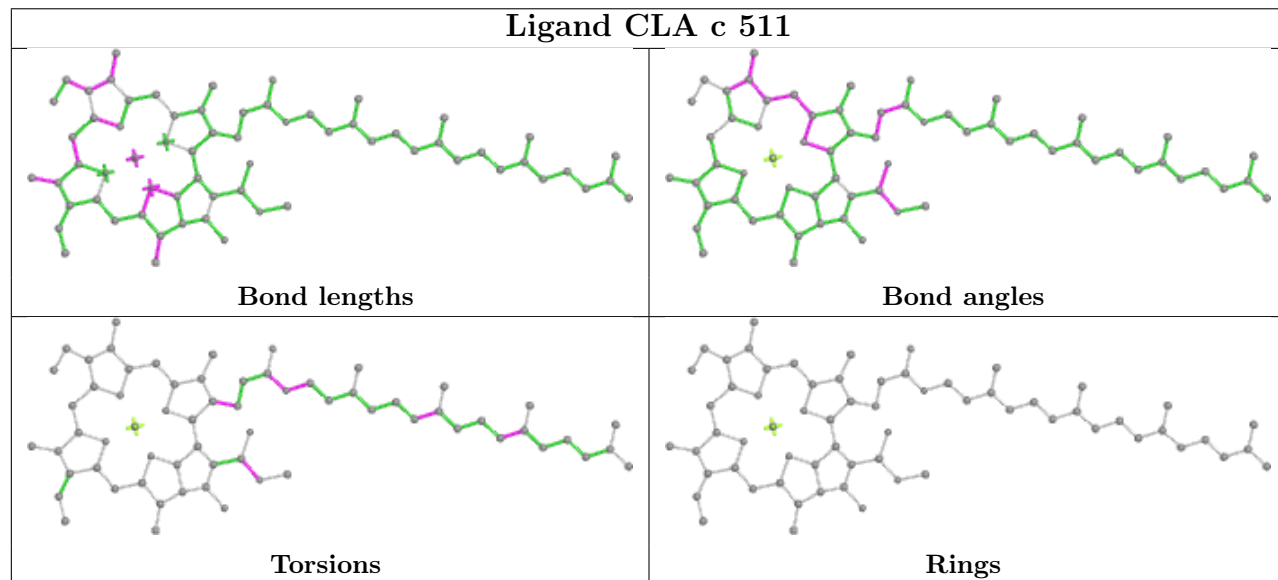


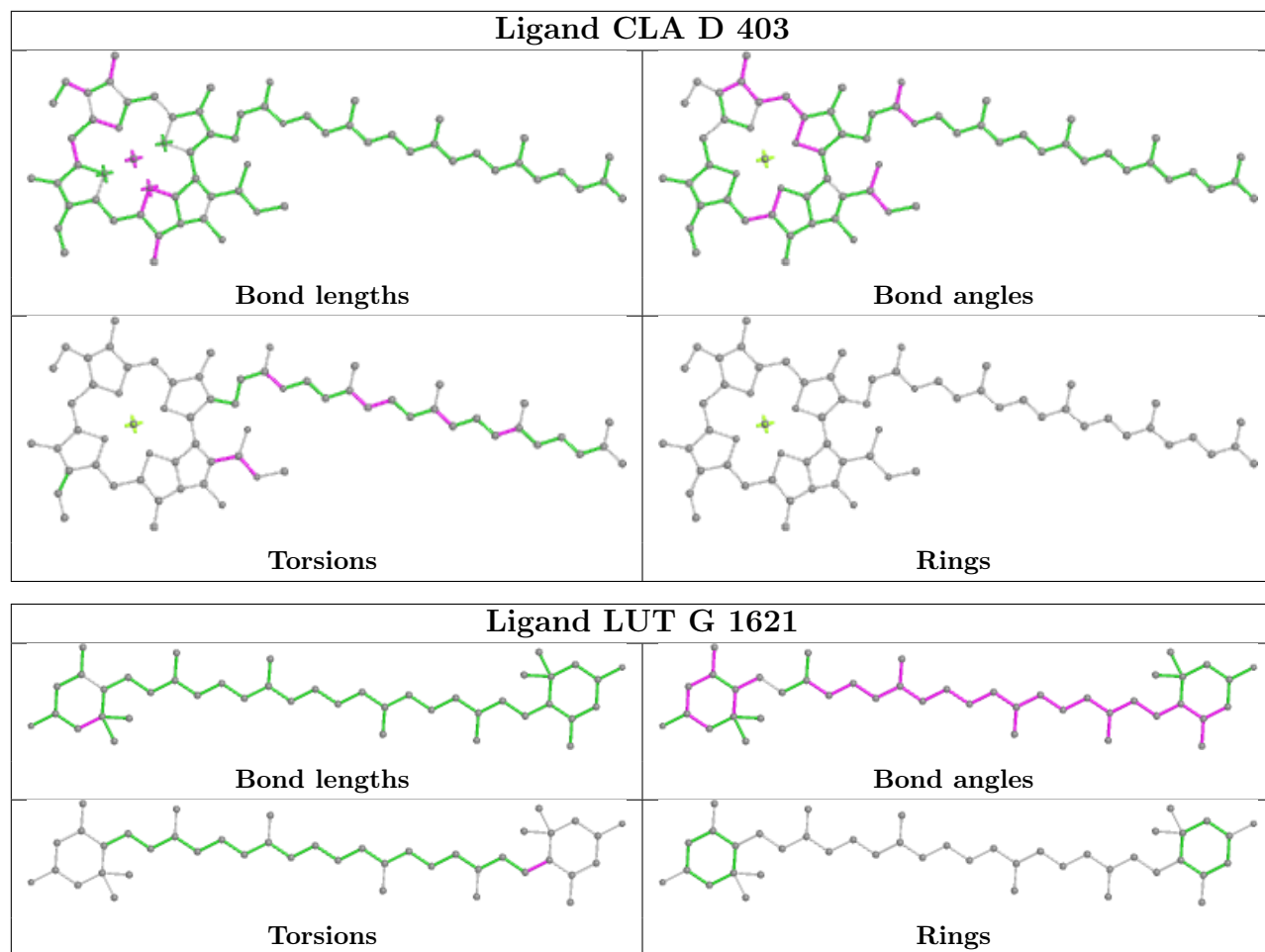


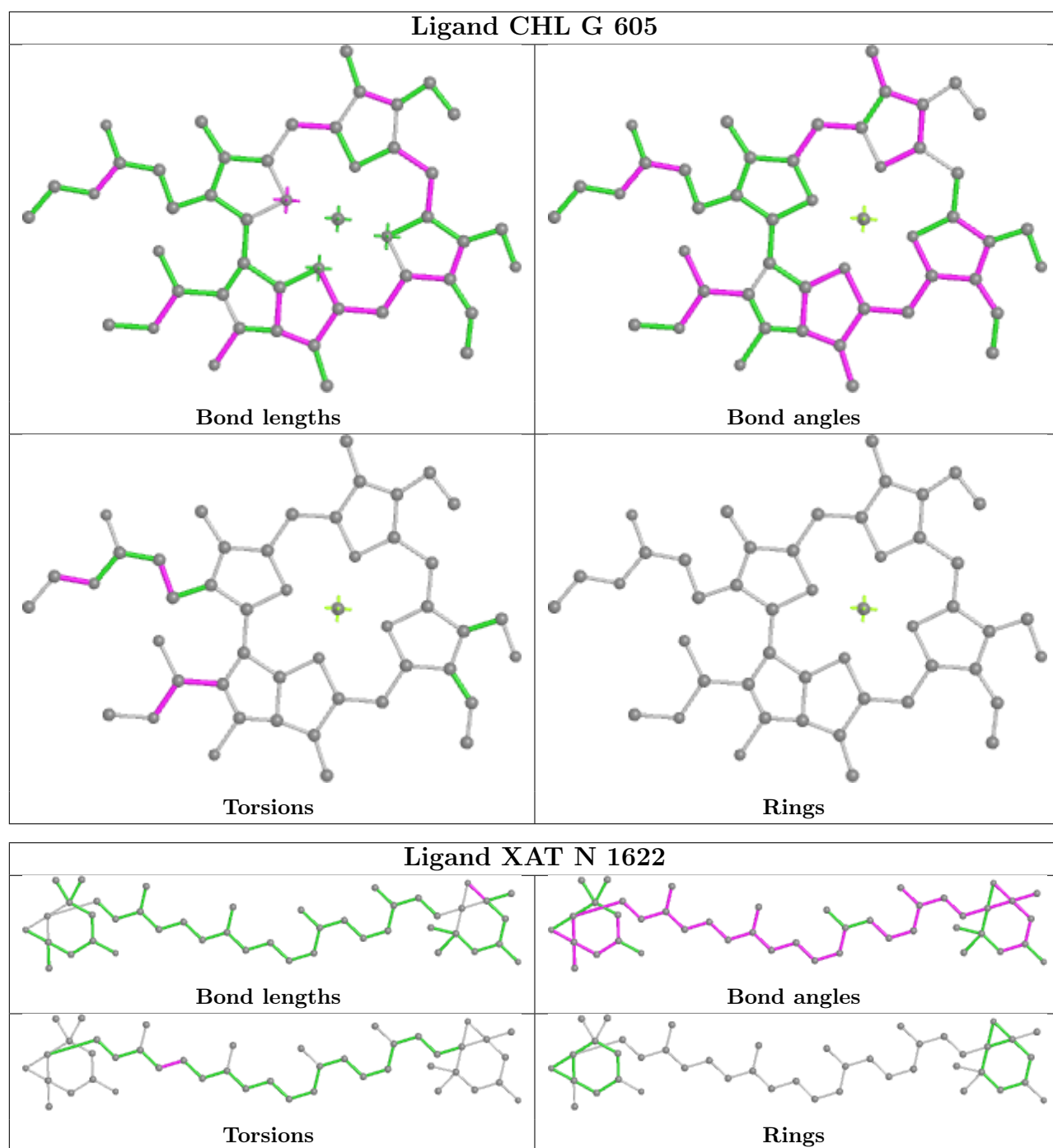
## Ligand LHG d 408

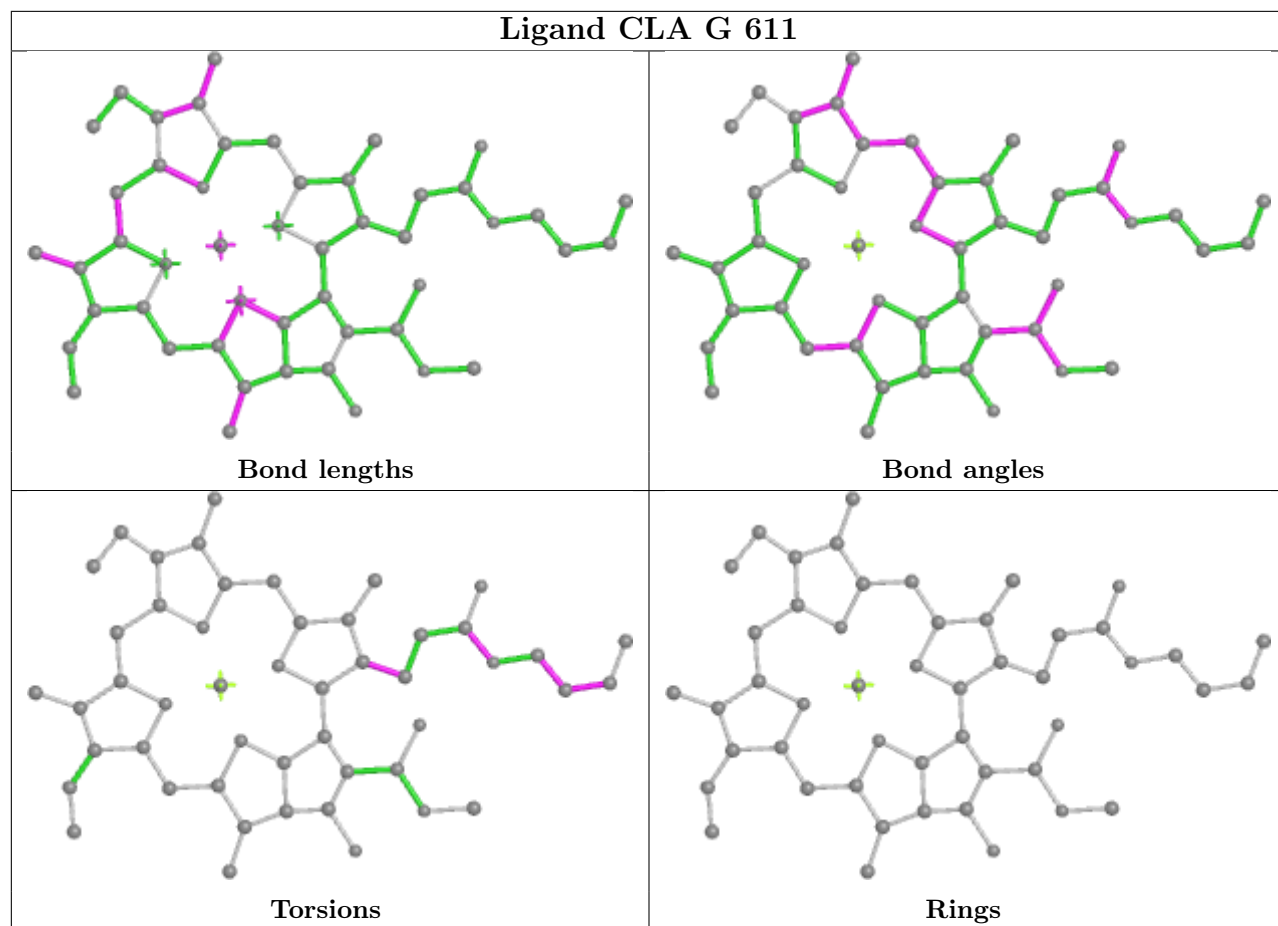


## Ligand CLA c 511

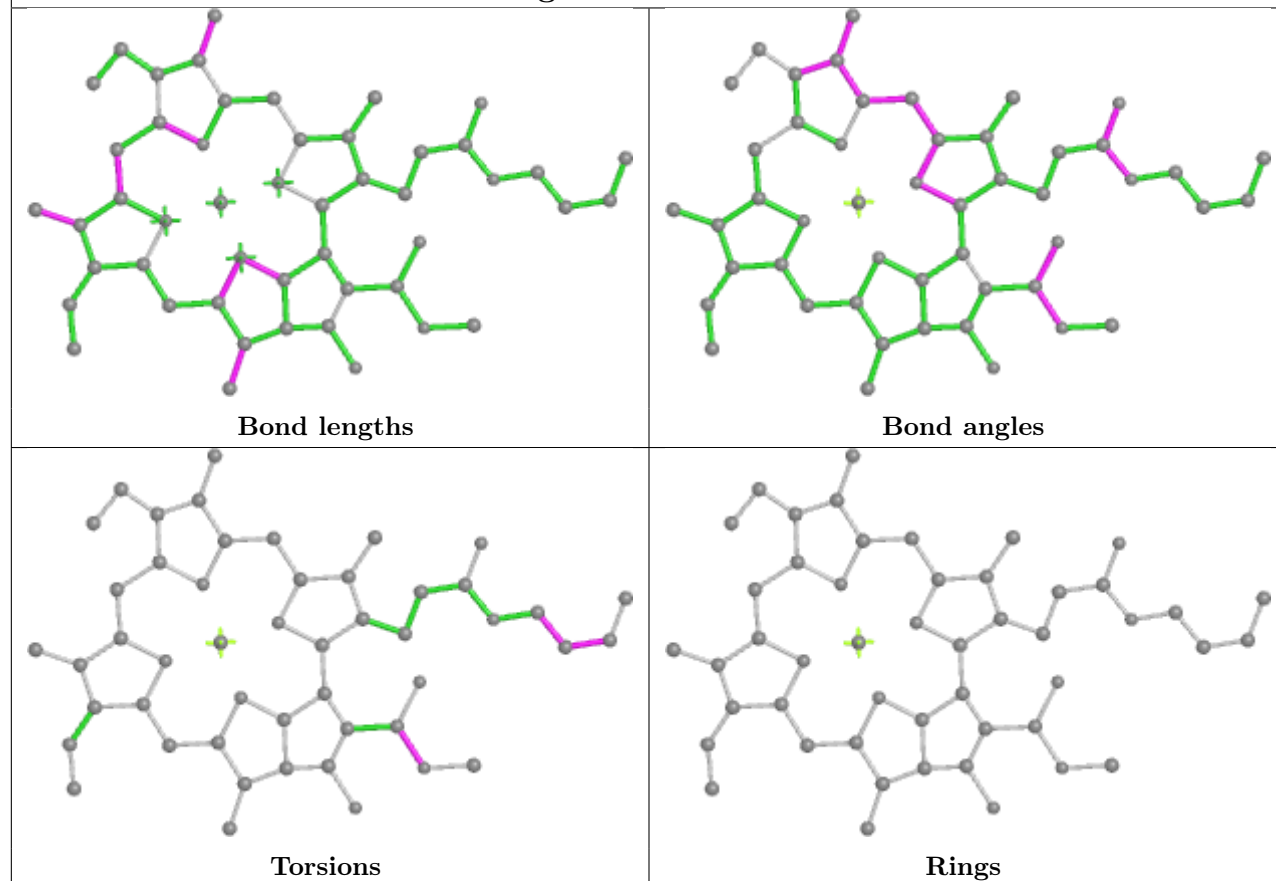




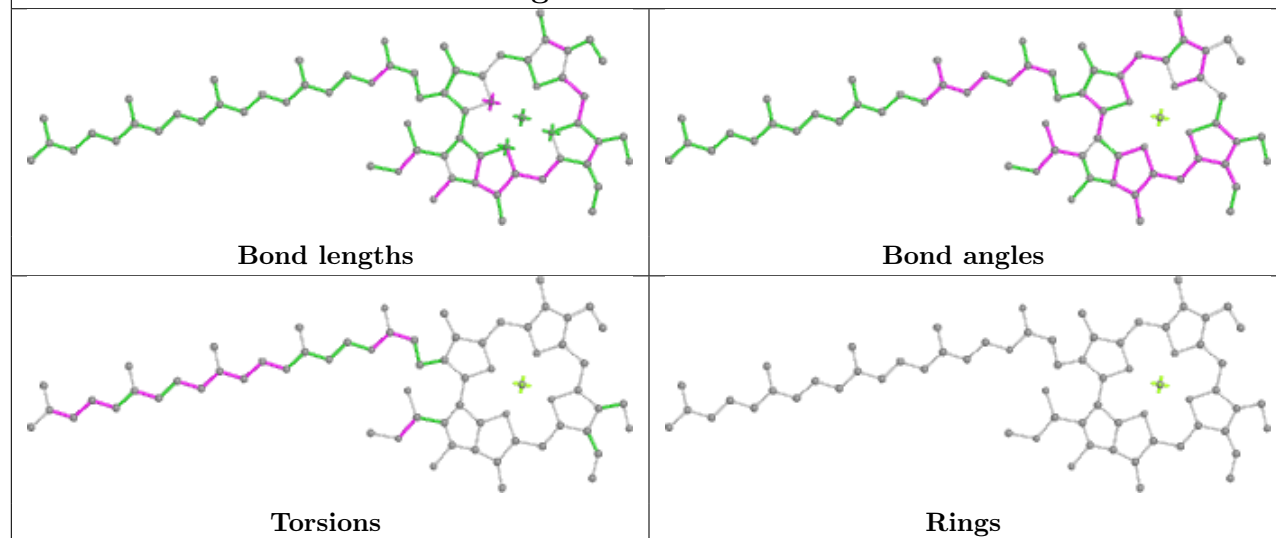


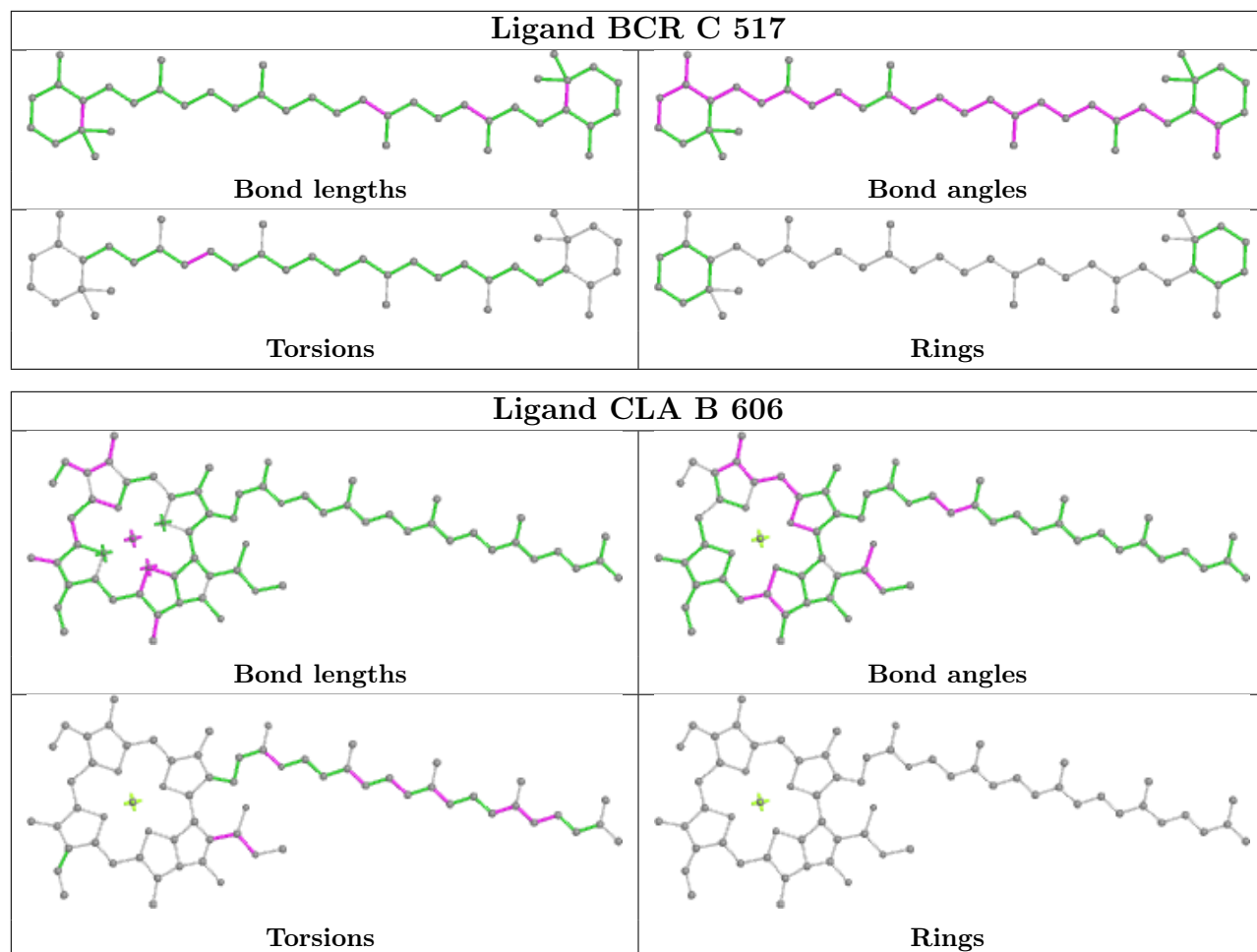


## Ligand CLA r 612



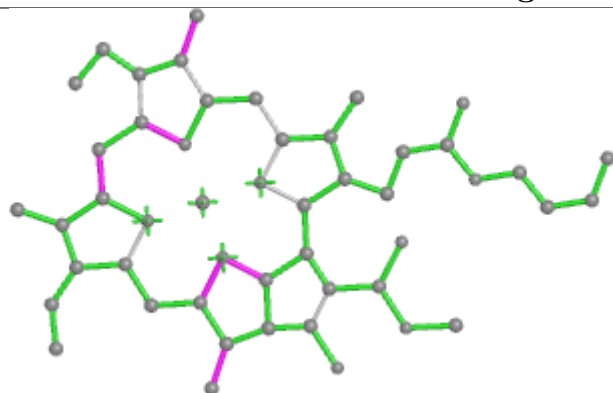
## Ligand CHL Y 601



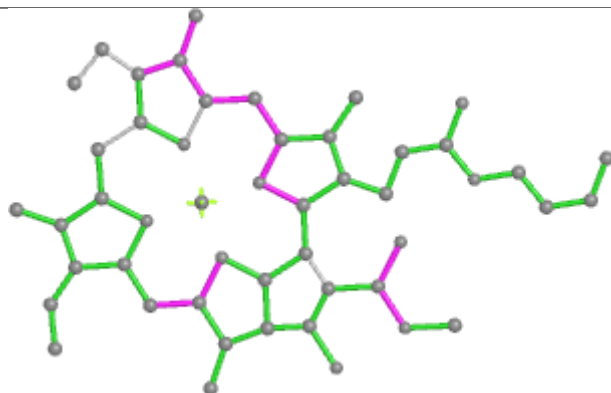




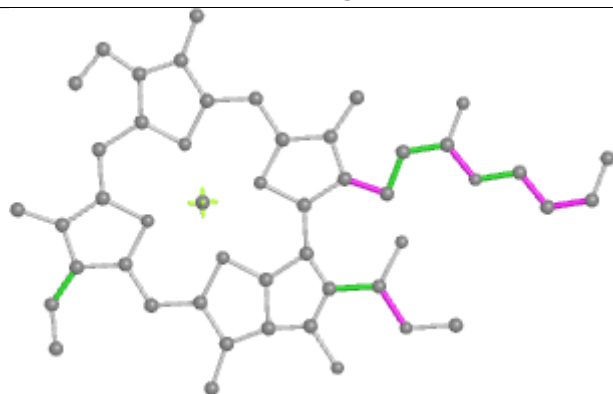
## Ligand CLA S 609



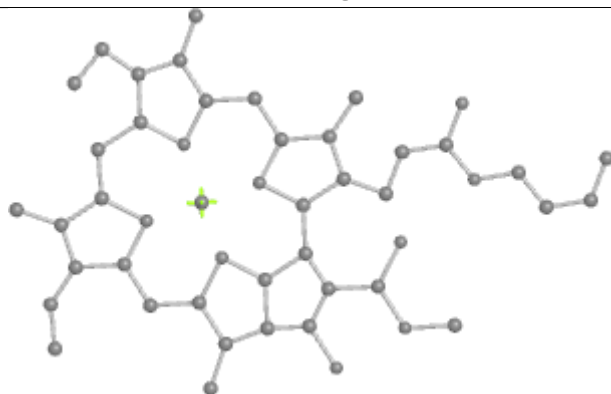
Bond lengths



Bond angles

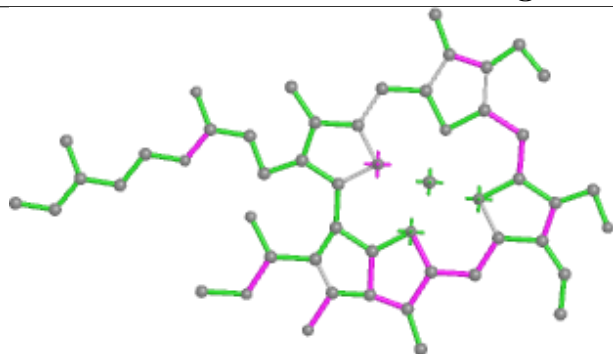


Torsions

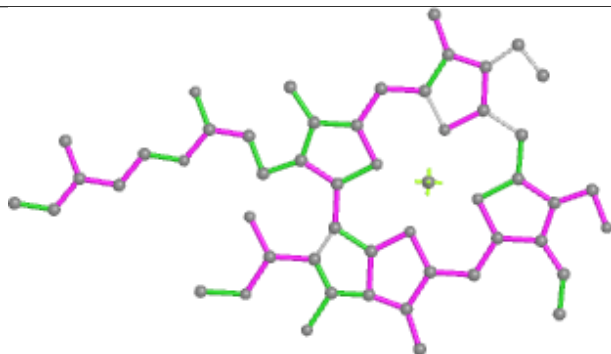


Rings

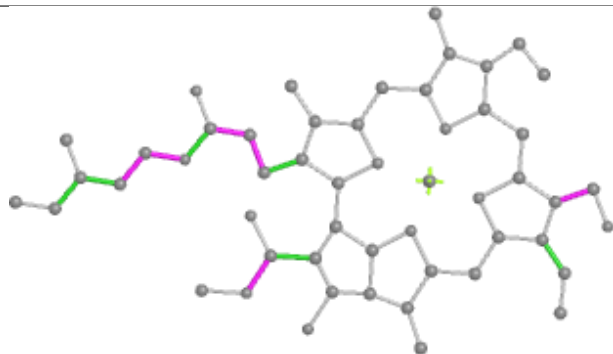
## Ligand CHL S 601



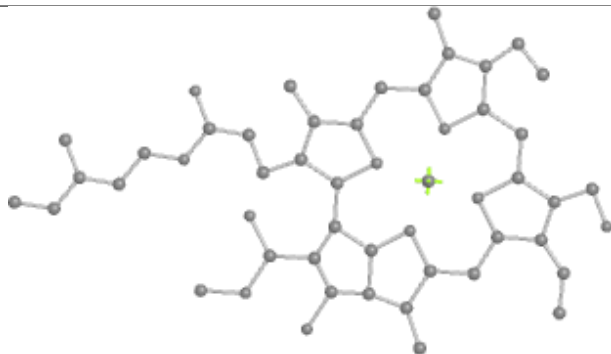
Bond lengths



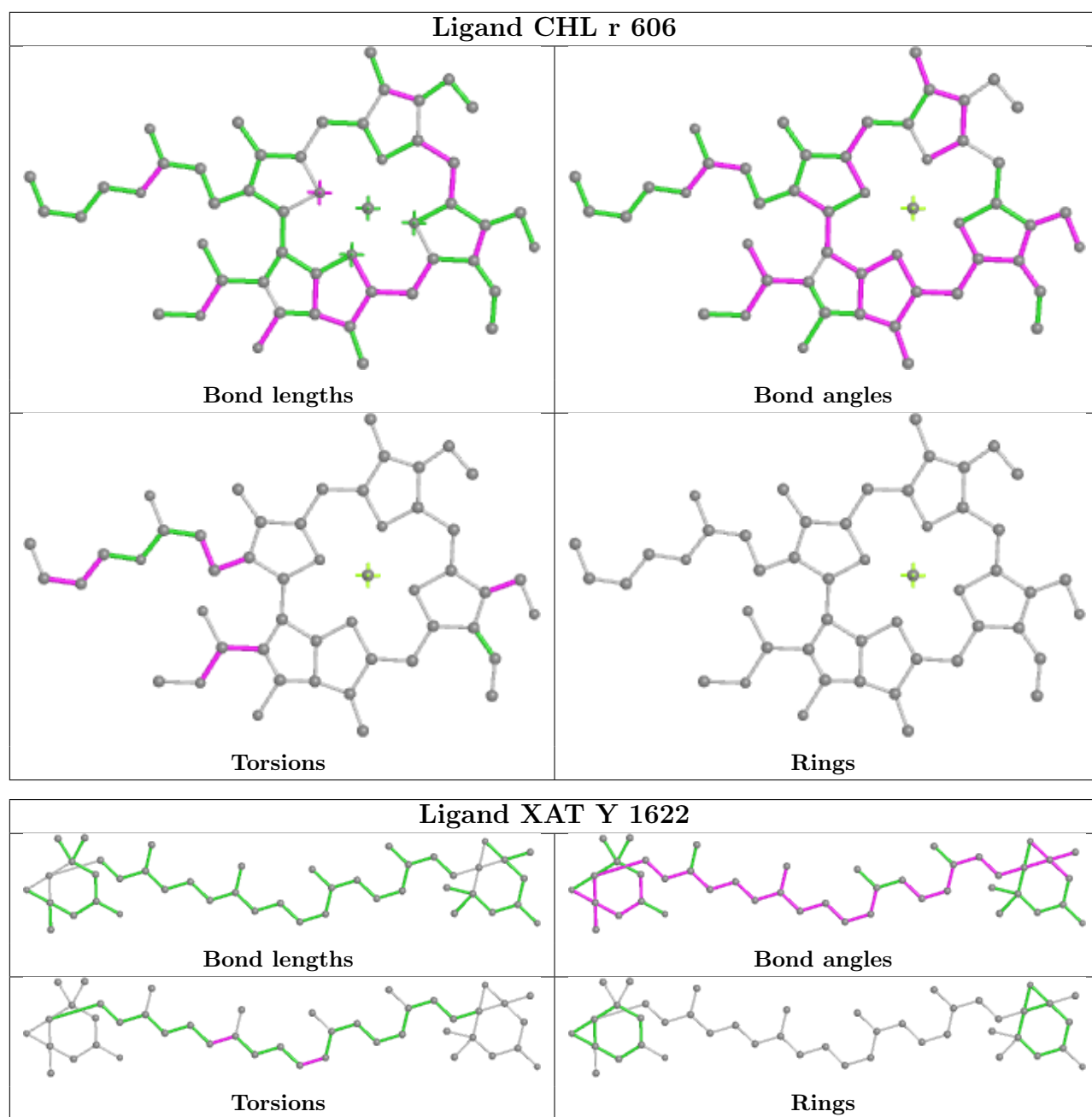
Bond angles

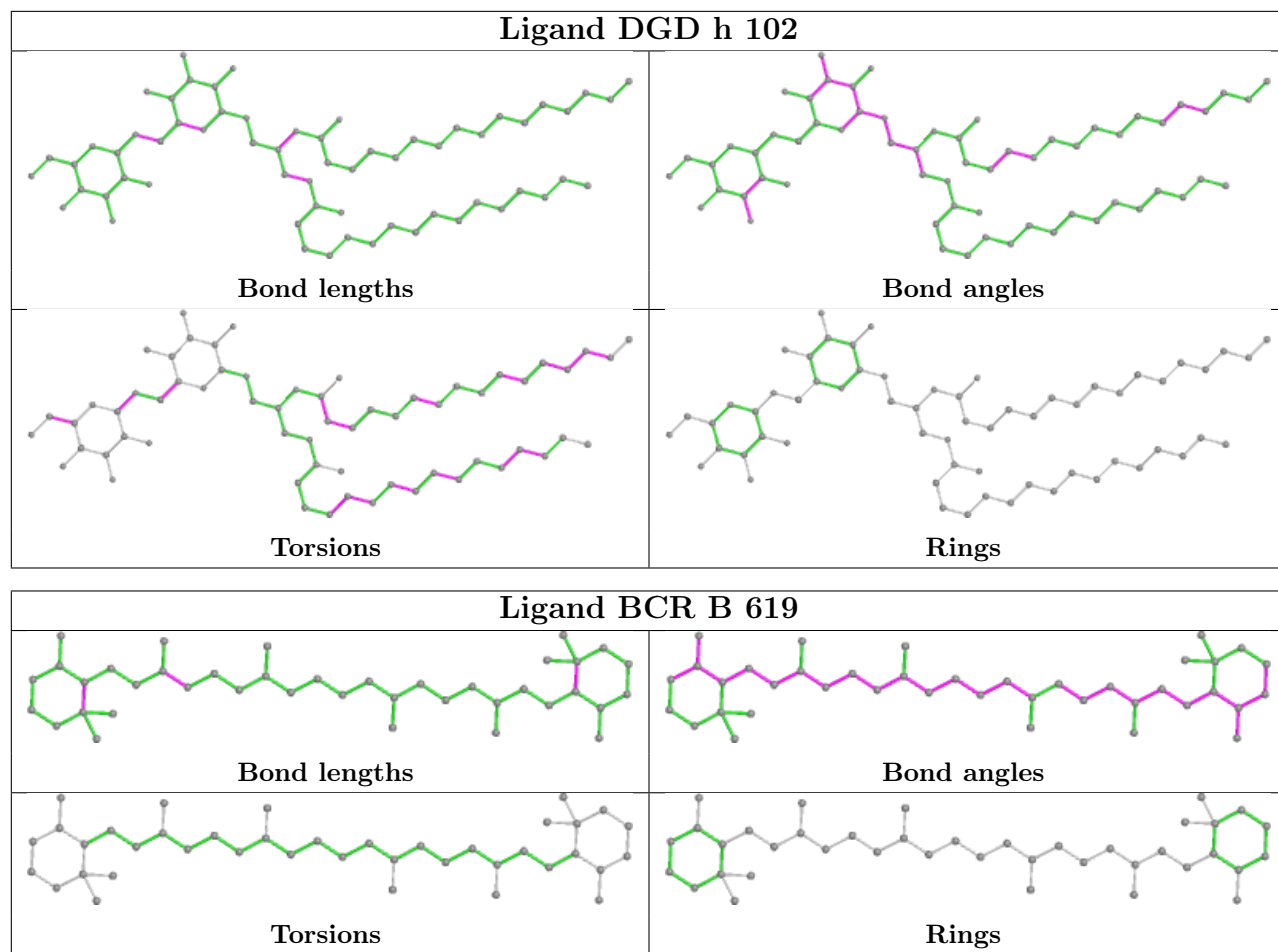


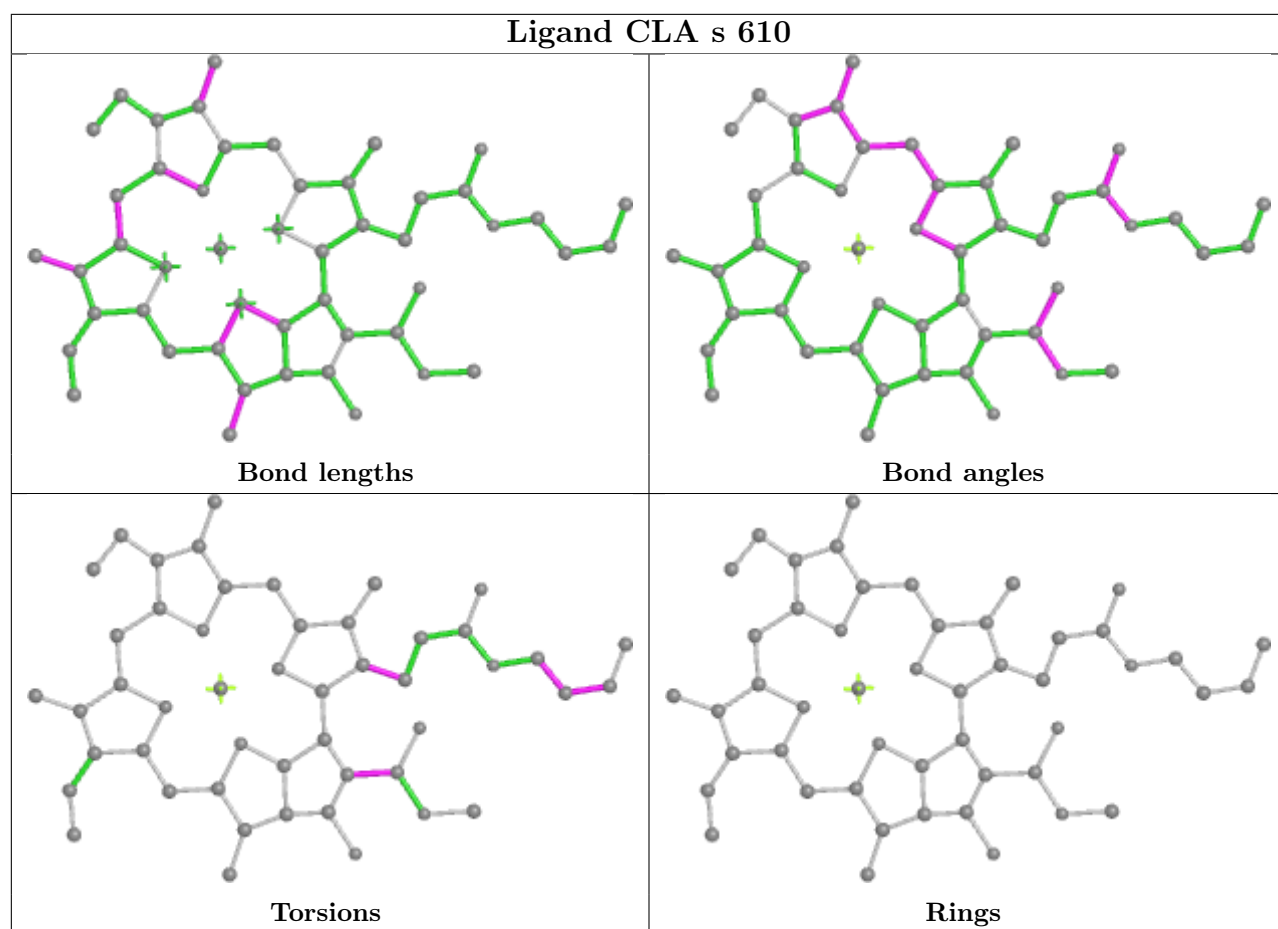
Torsions

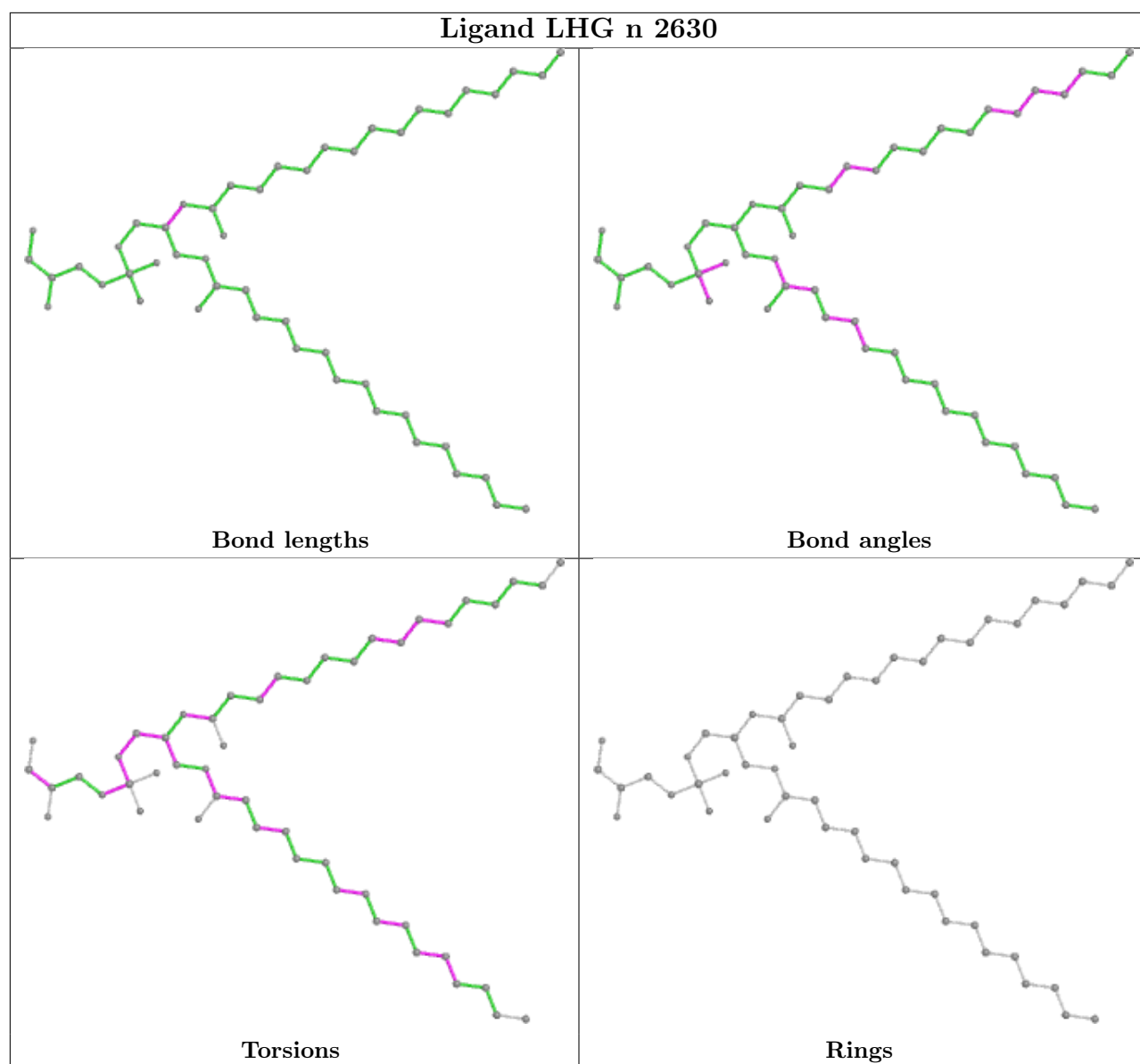


Rings

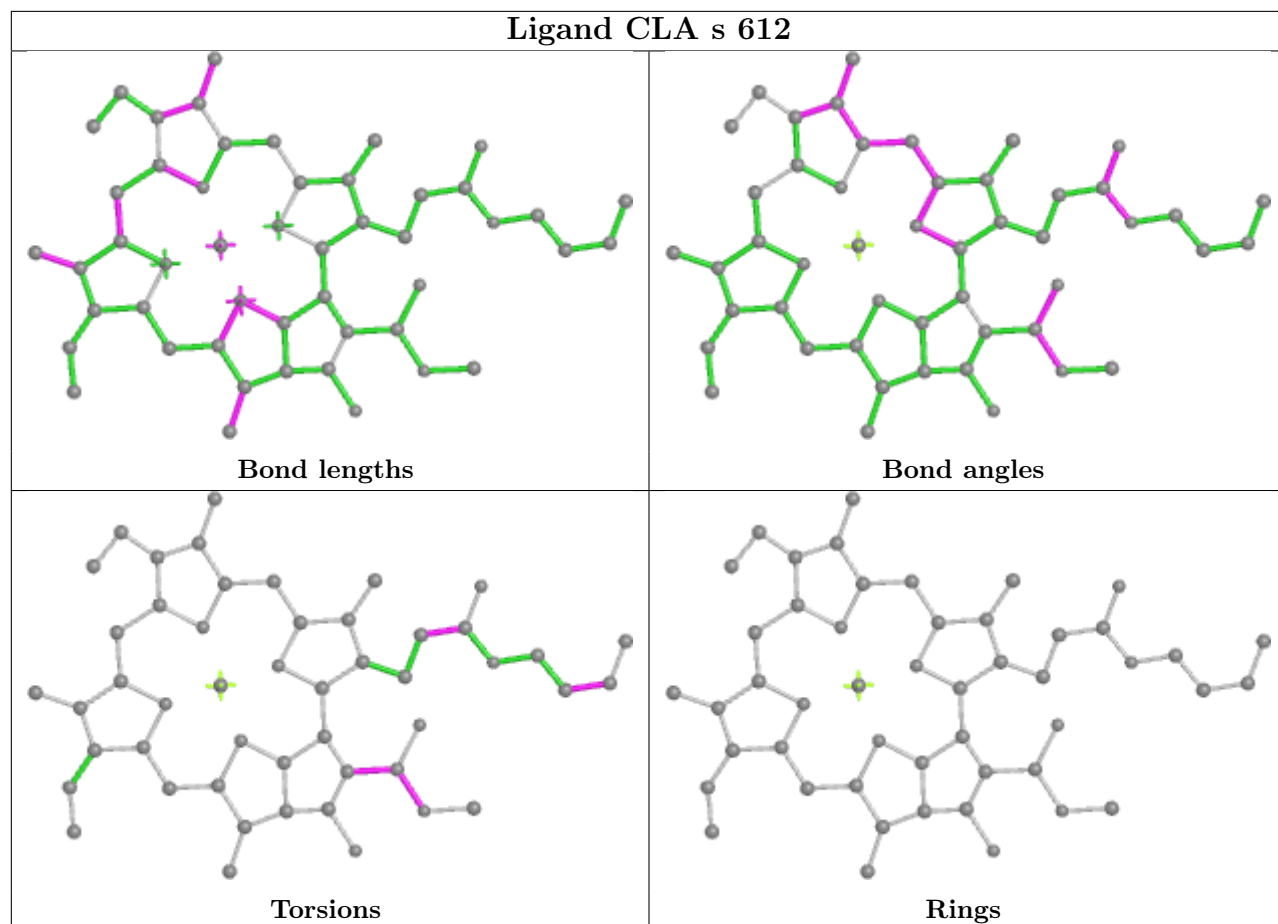




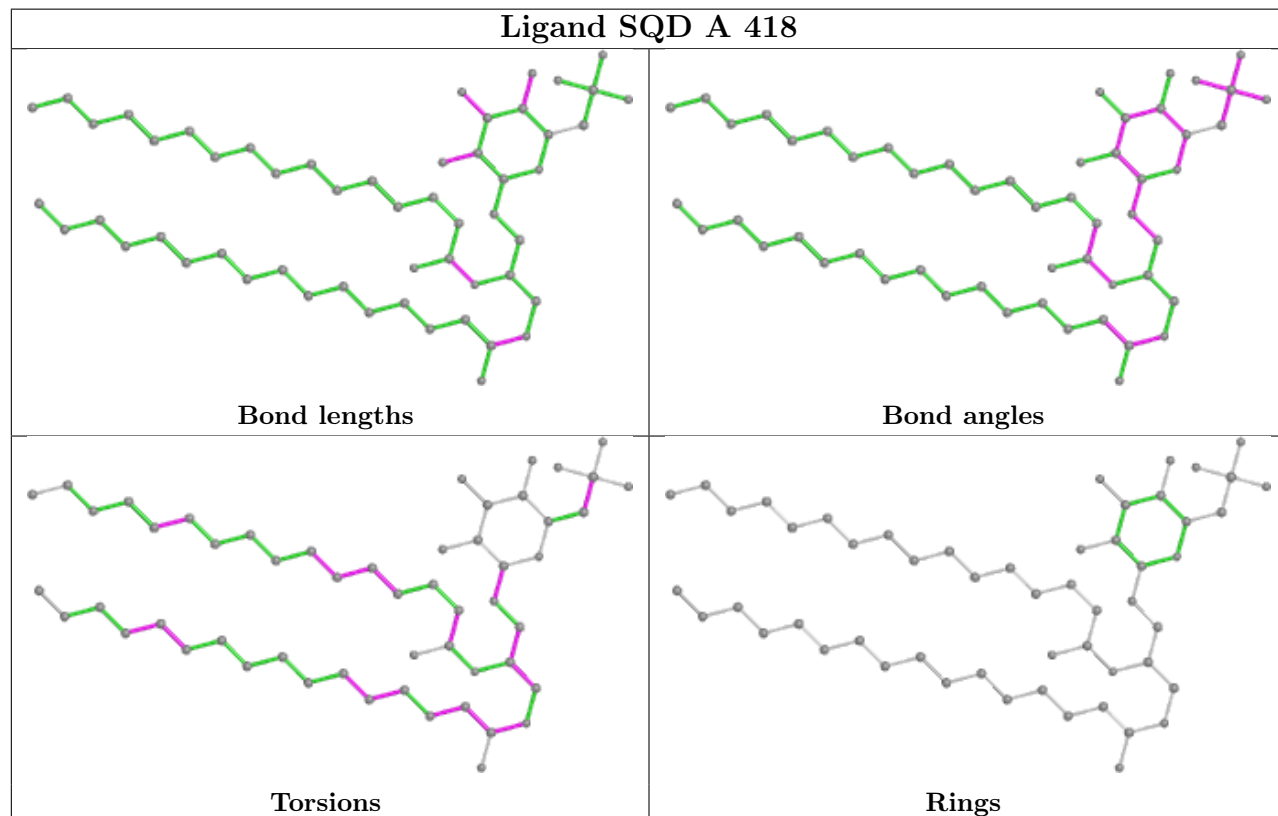


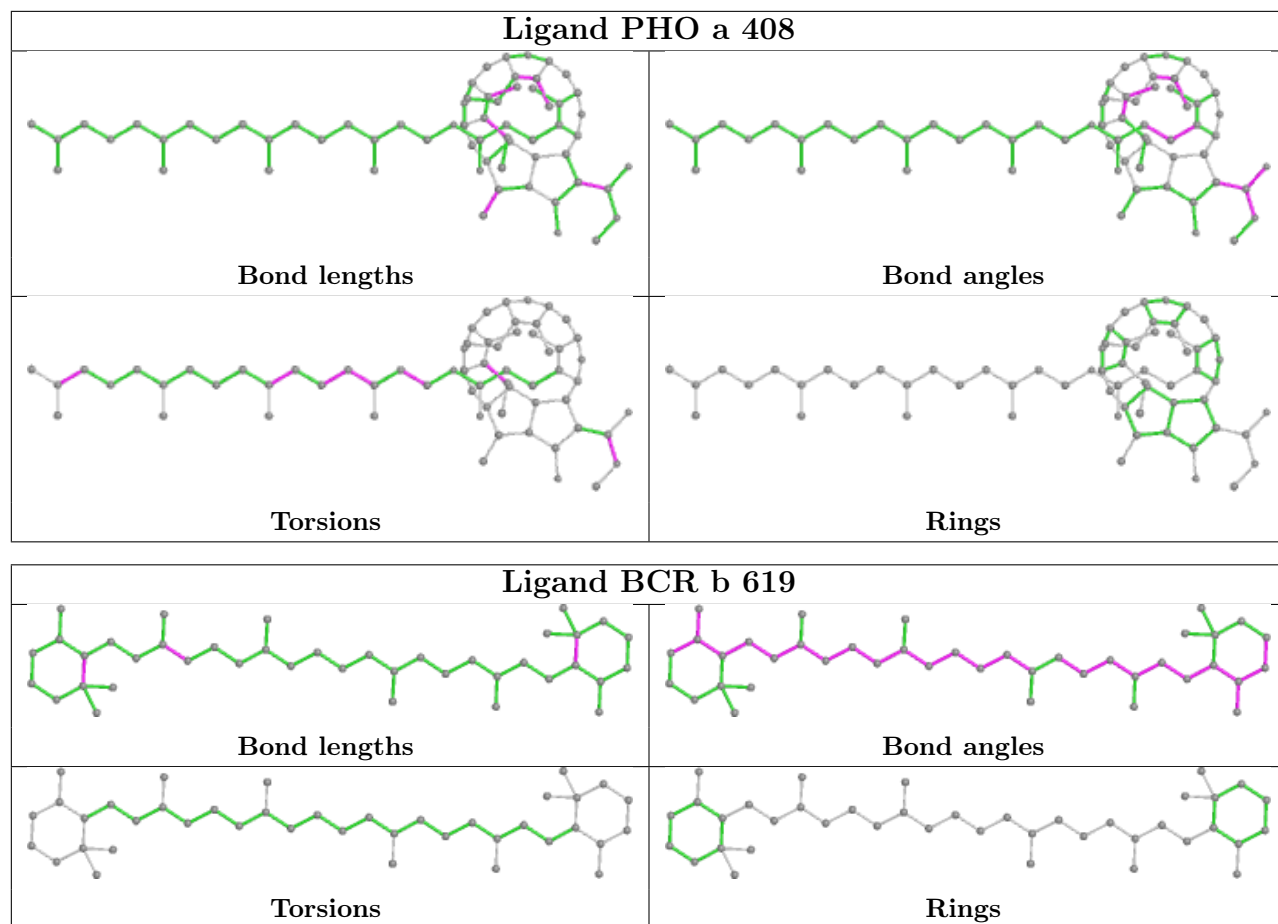


## Ligand CLA s 612

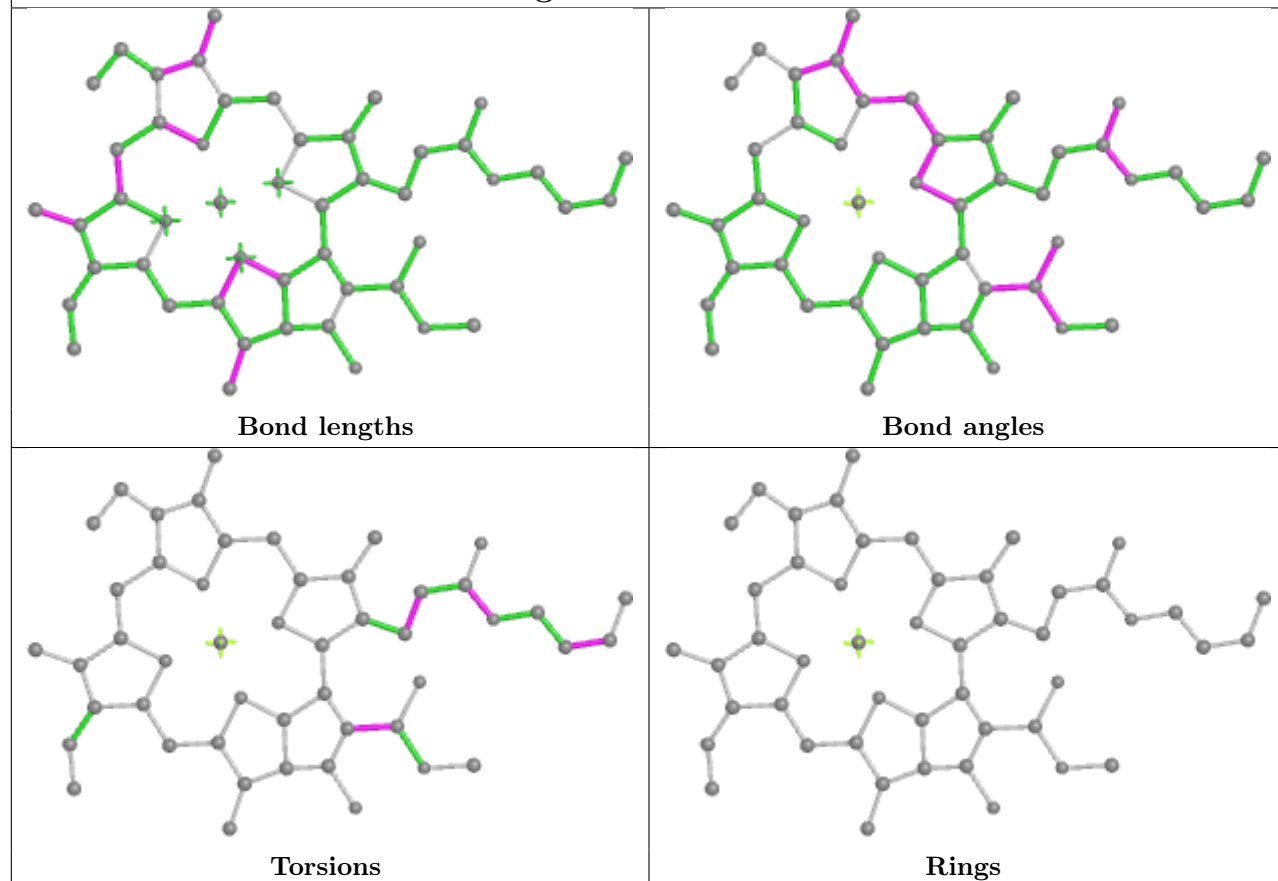


## Ligand SQD A 418

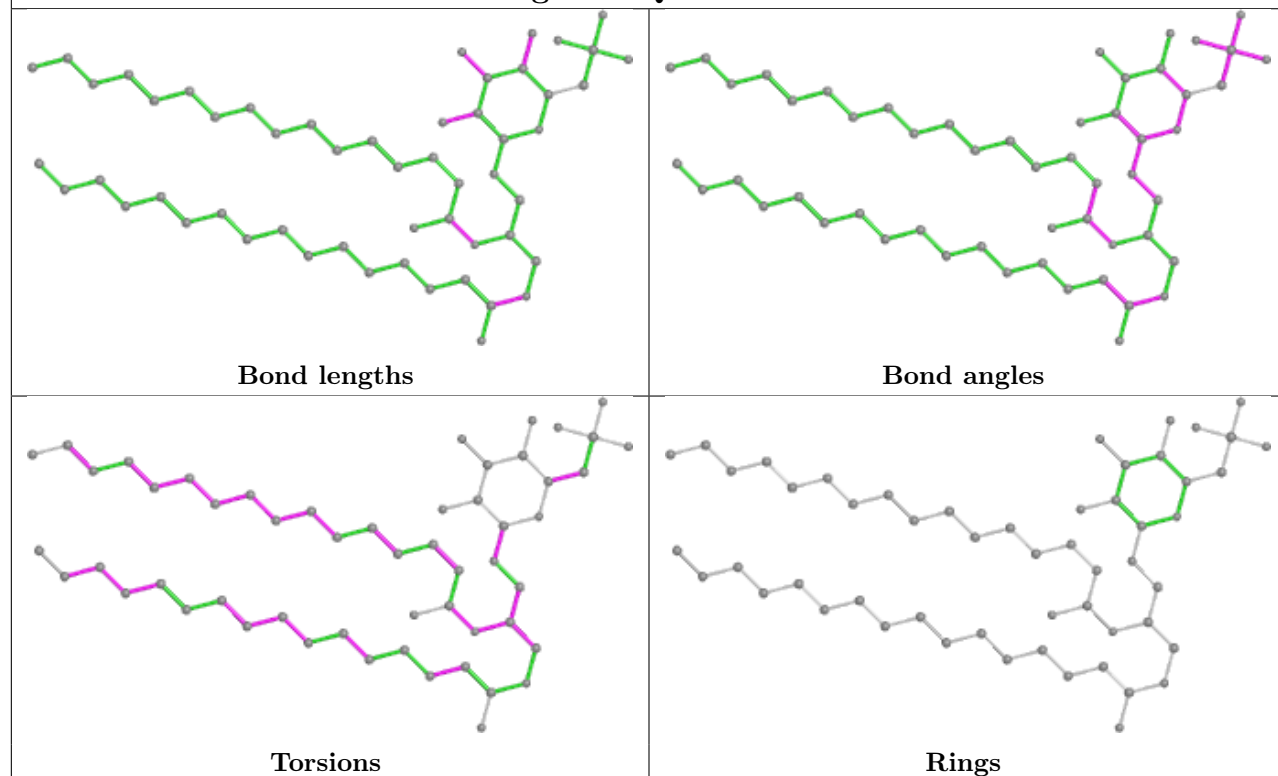




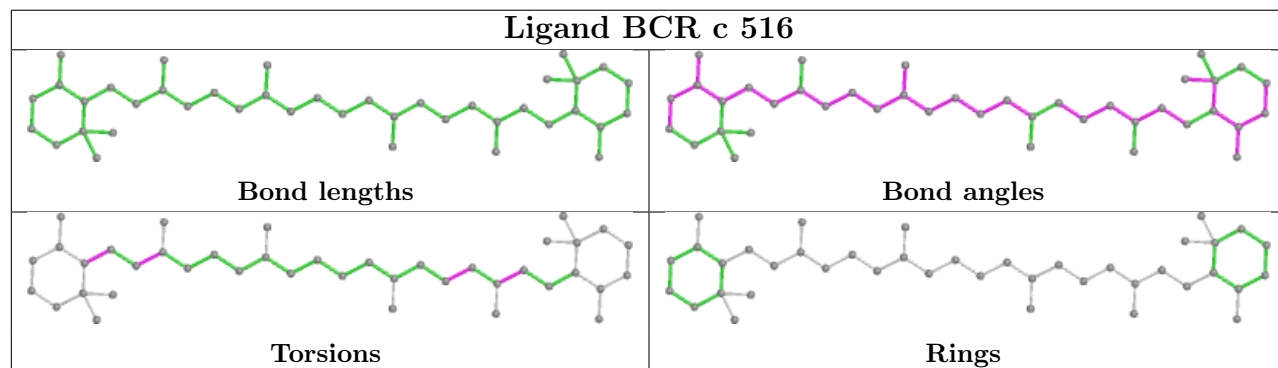
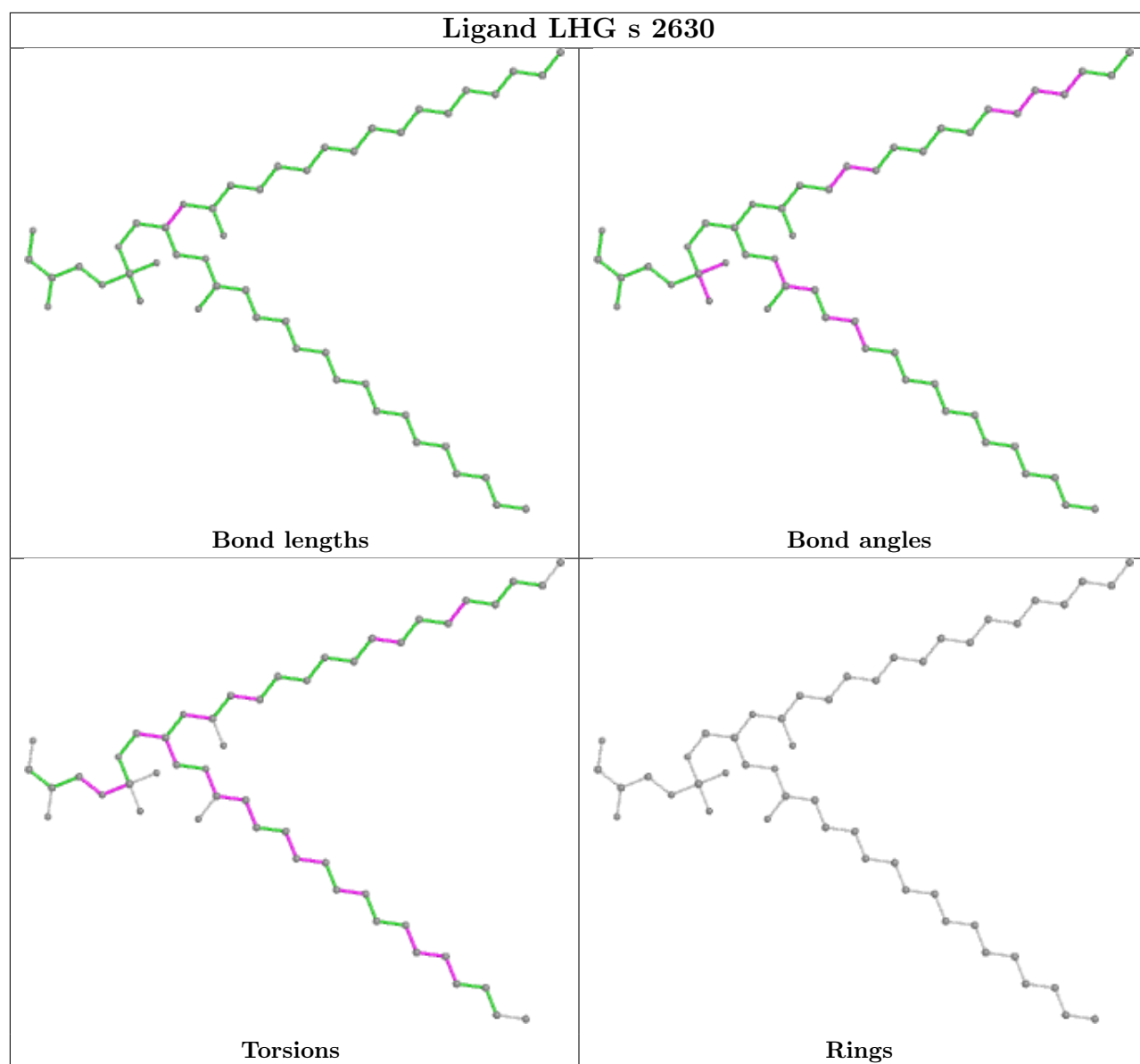
## Ligand CLA n 611

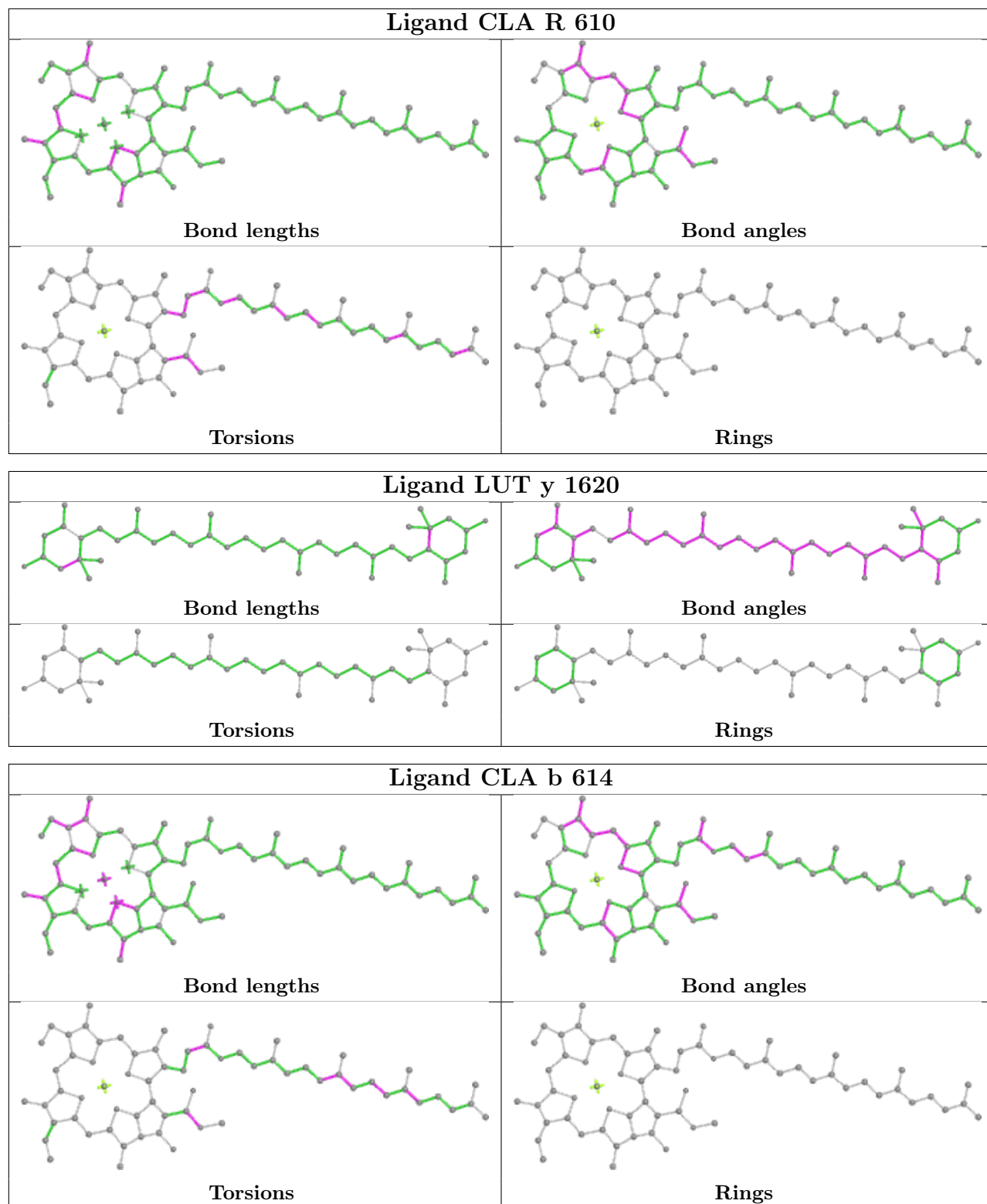


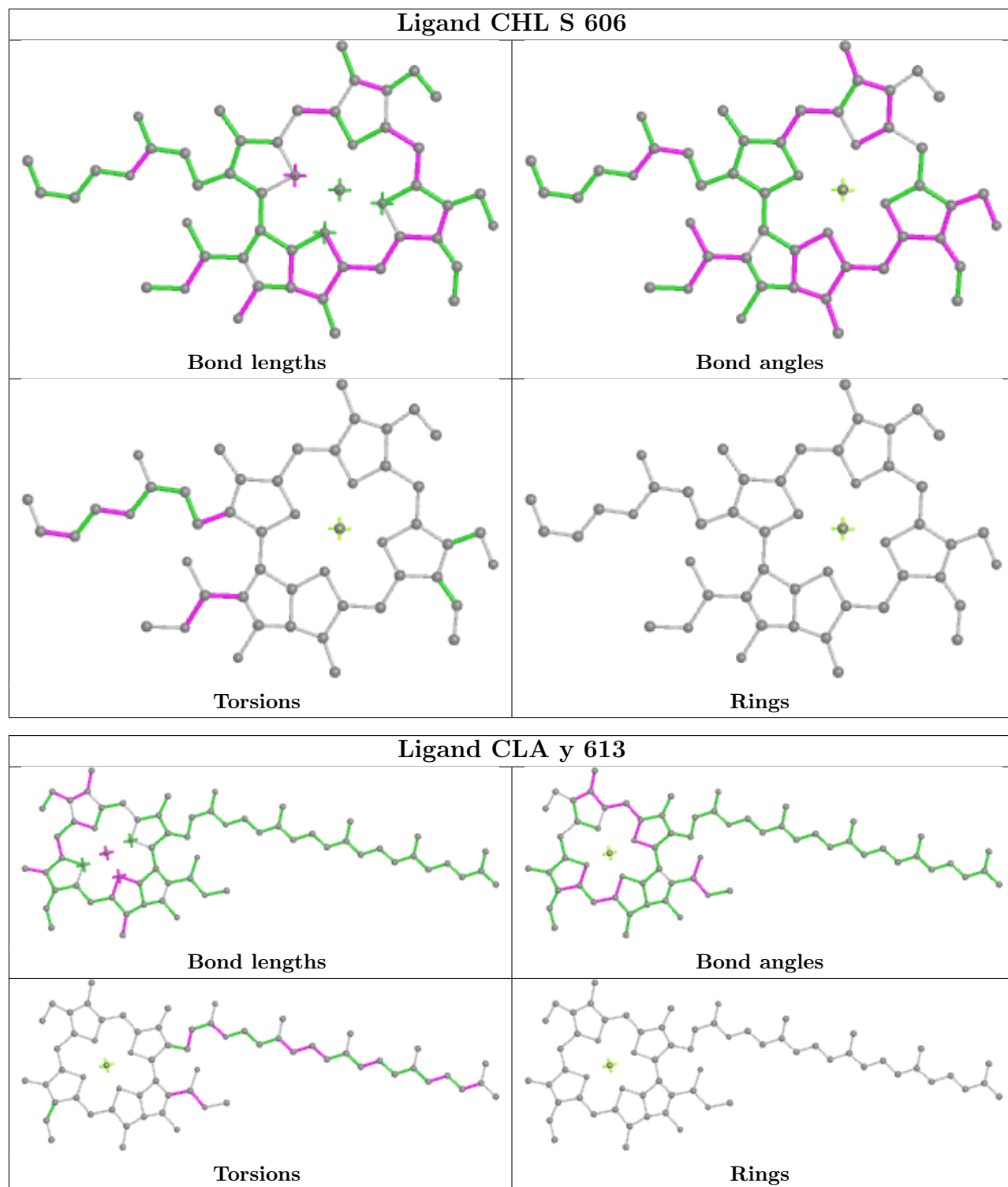
## Ligand SQD A 412

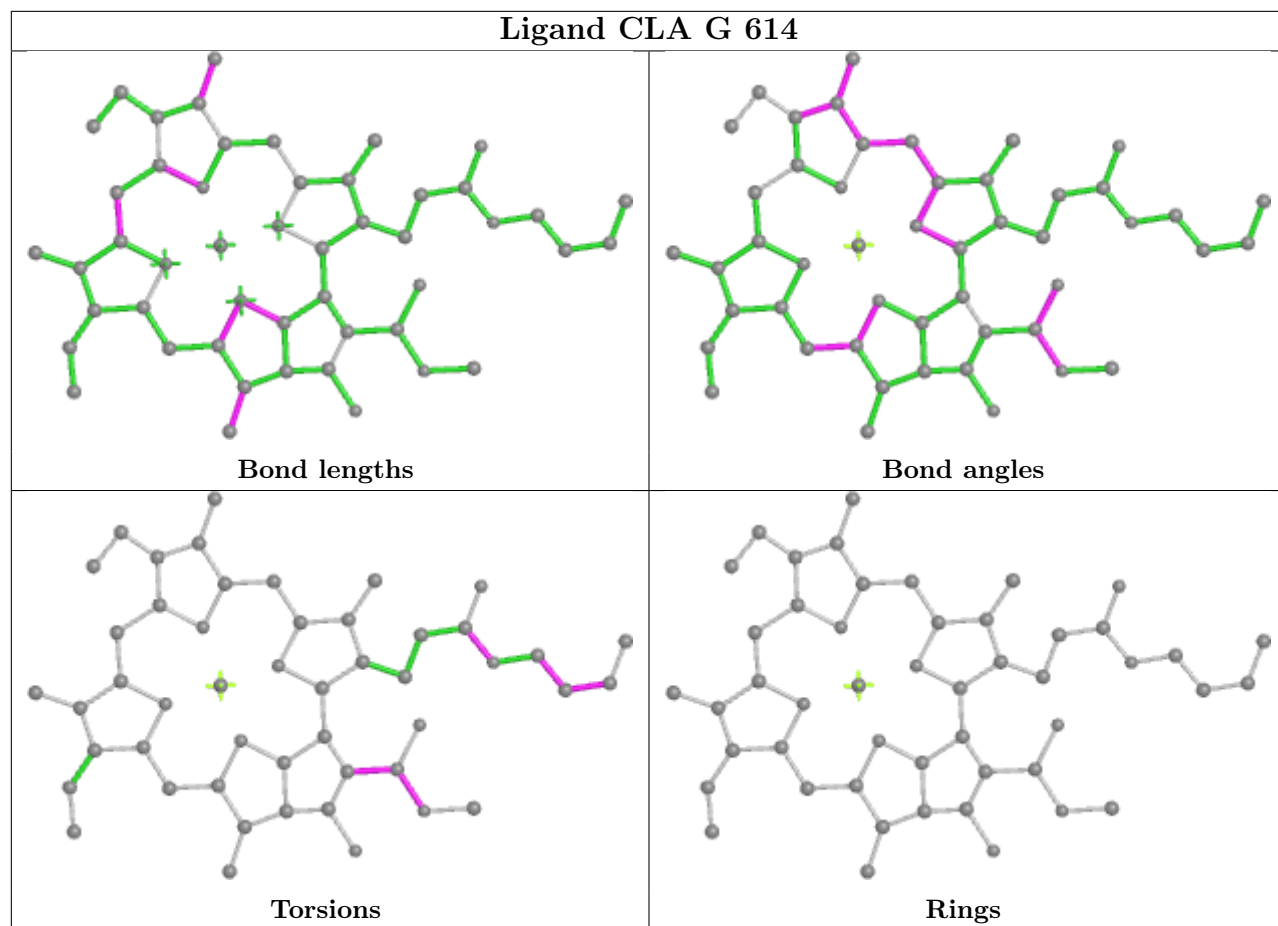


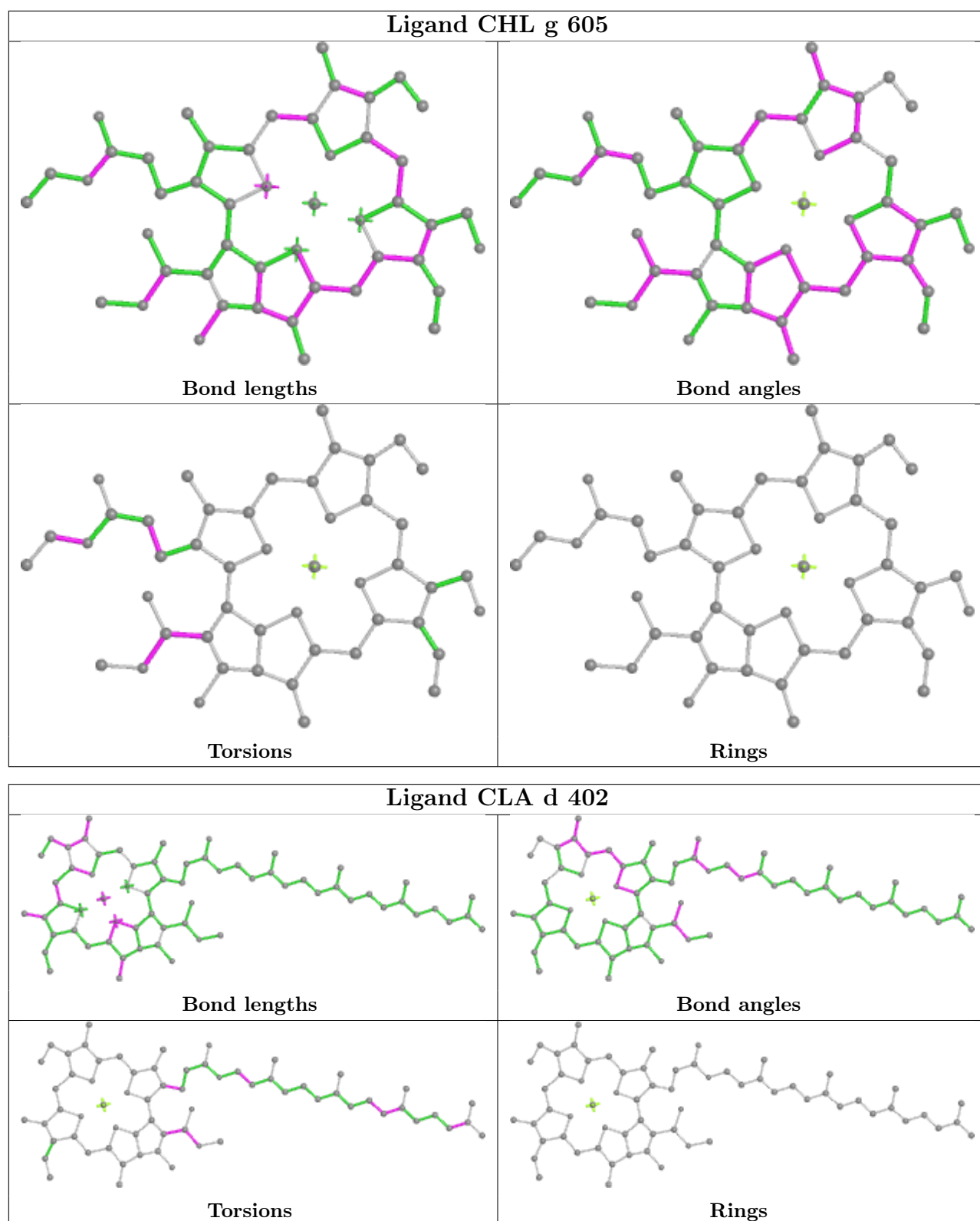




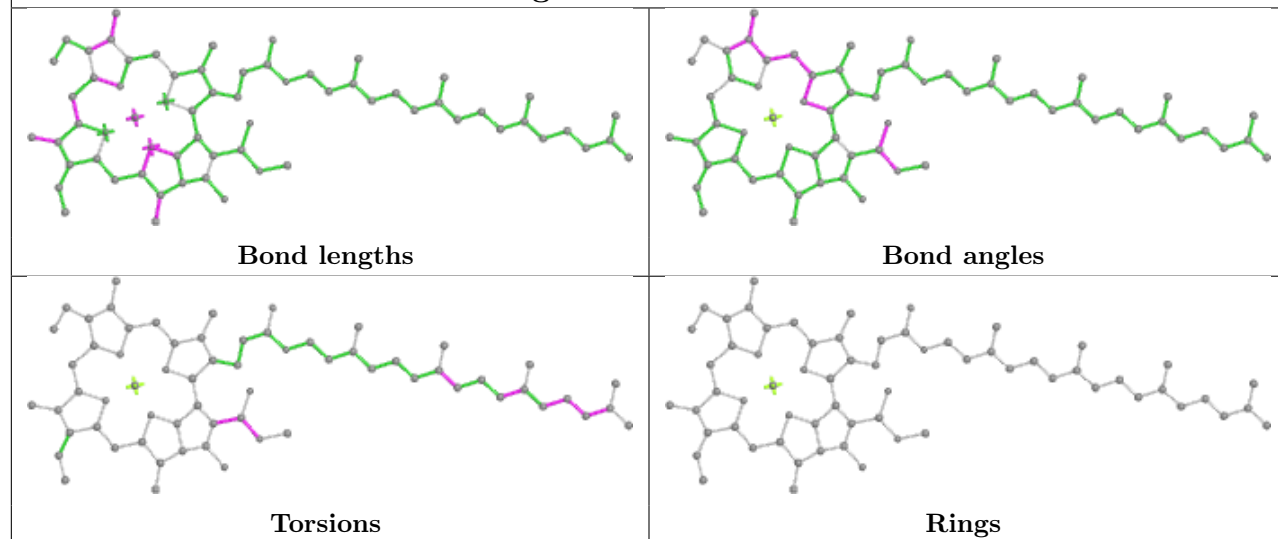




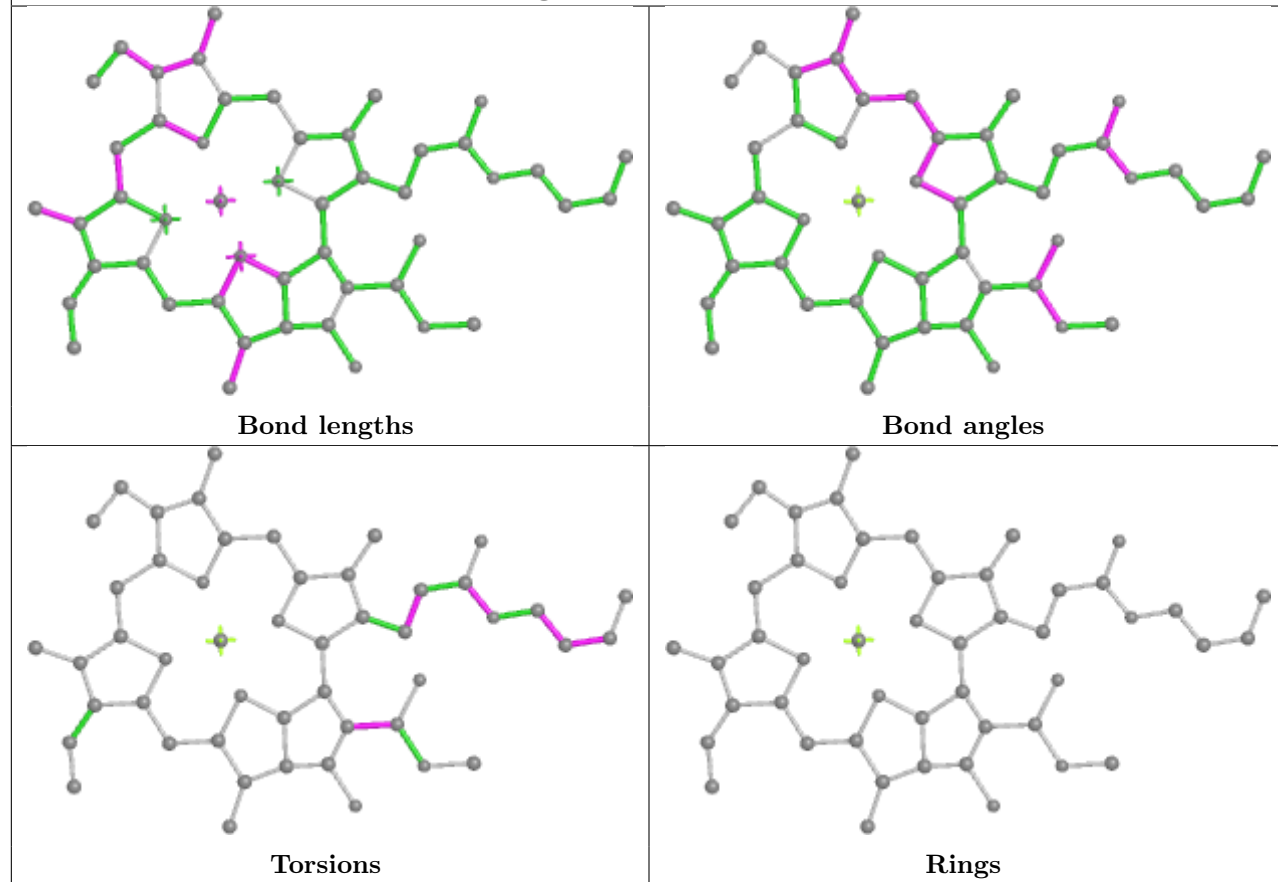


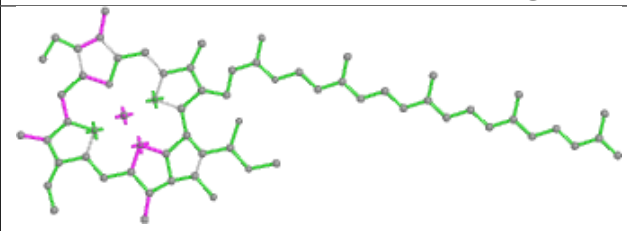
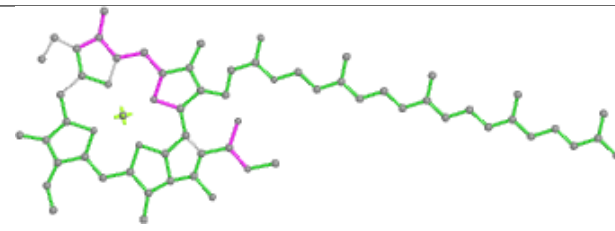
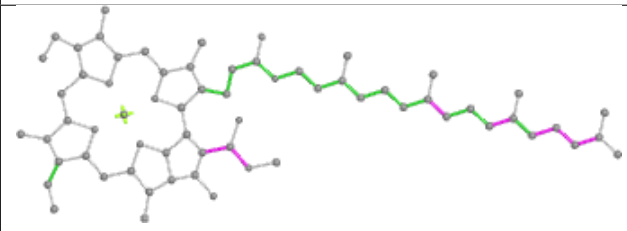
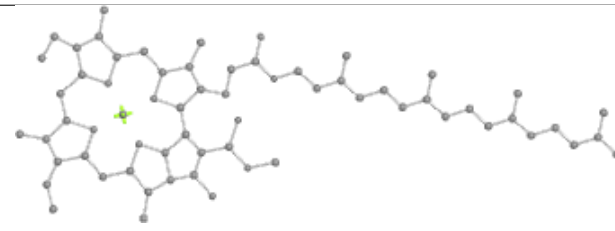


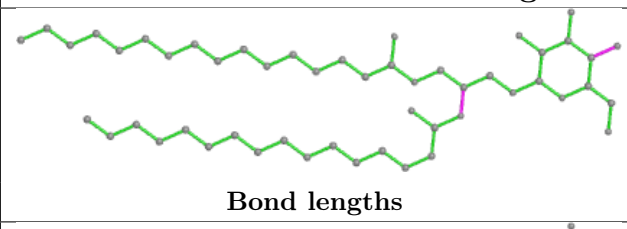
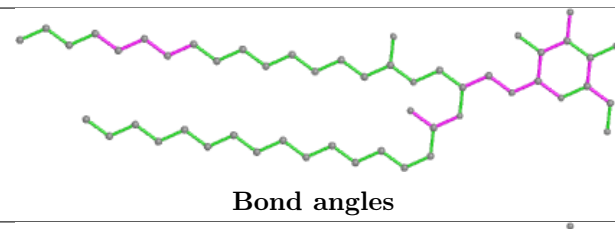
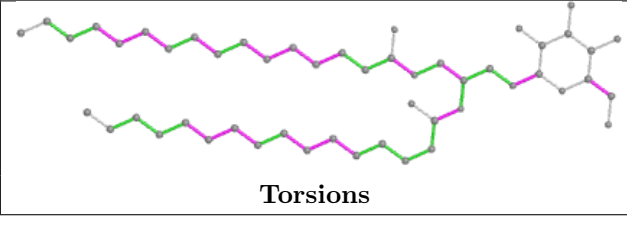
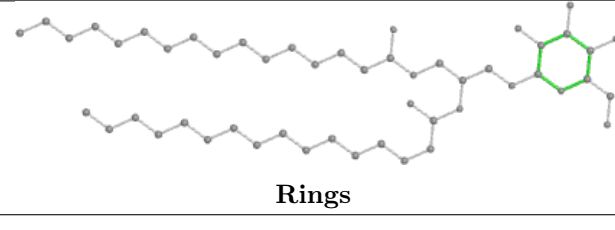
## Ligand CLA B 616

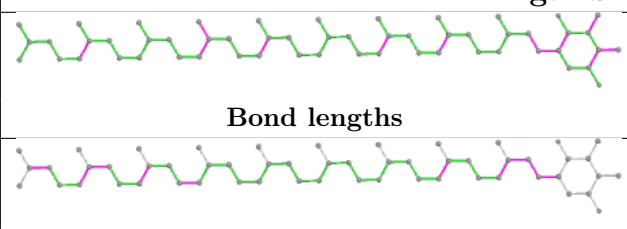
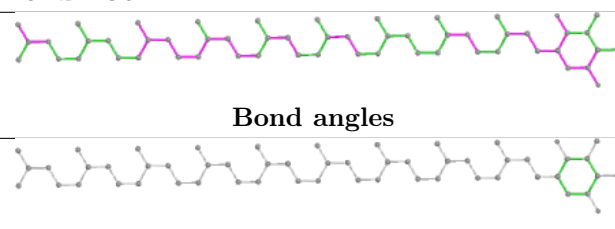
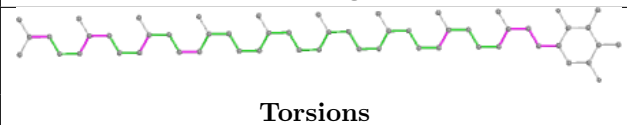
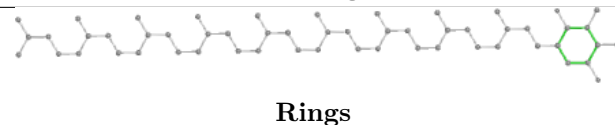


## Ligand CLA S 611

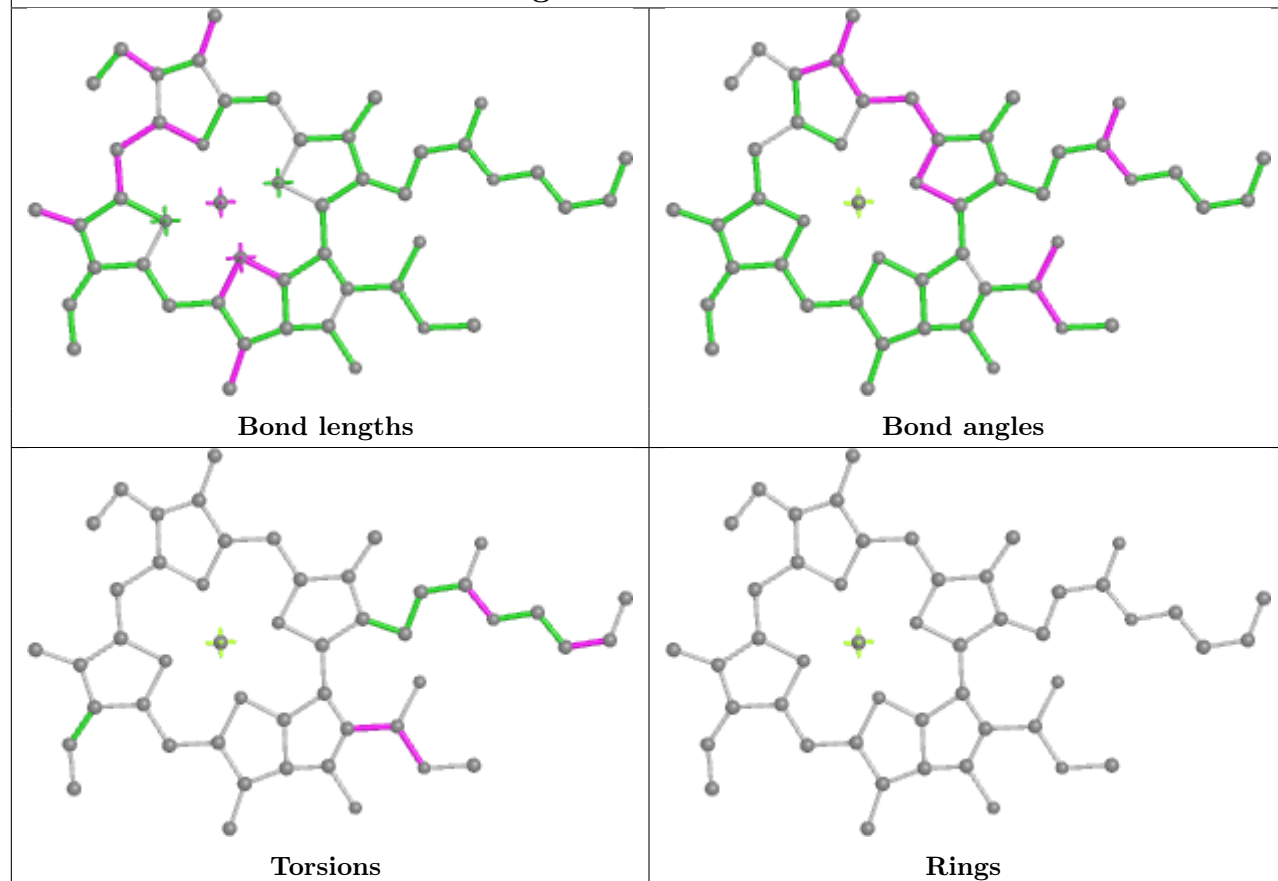


Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

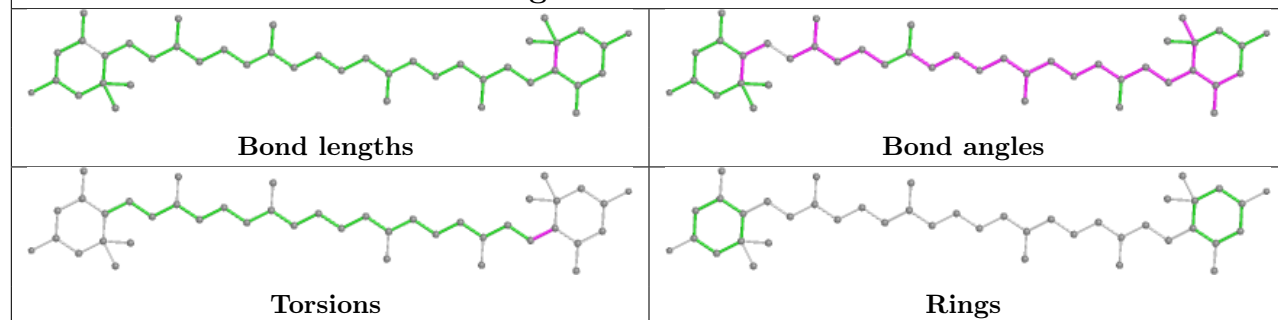
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

## Ligand CLA C 513

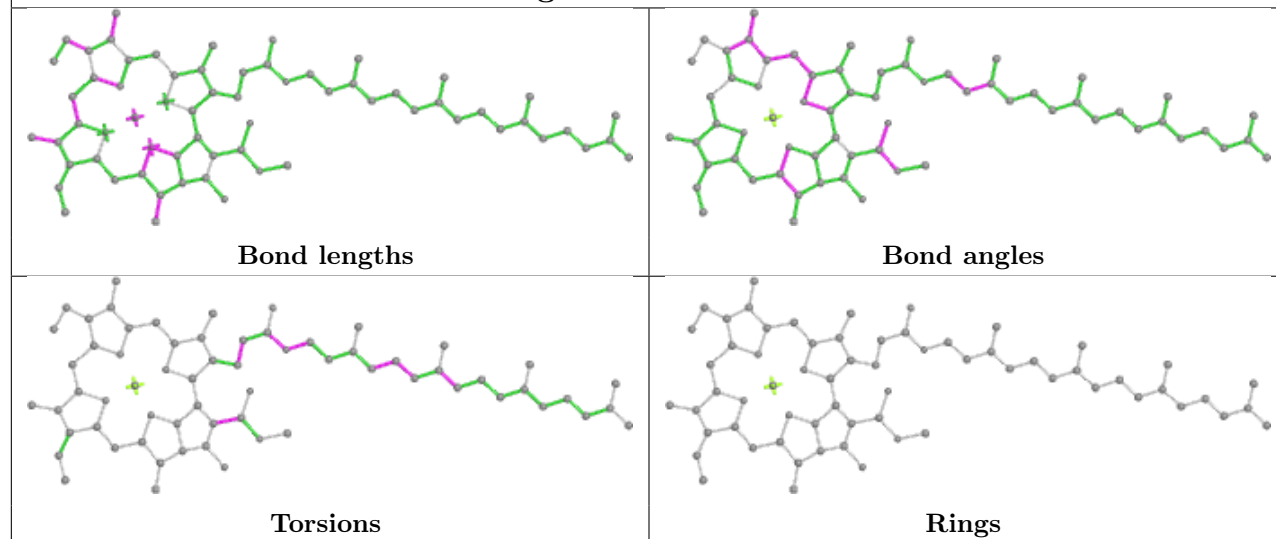


## Ligand LUT s 1620

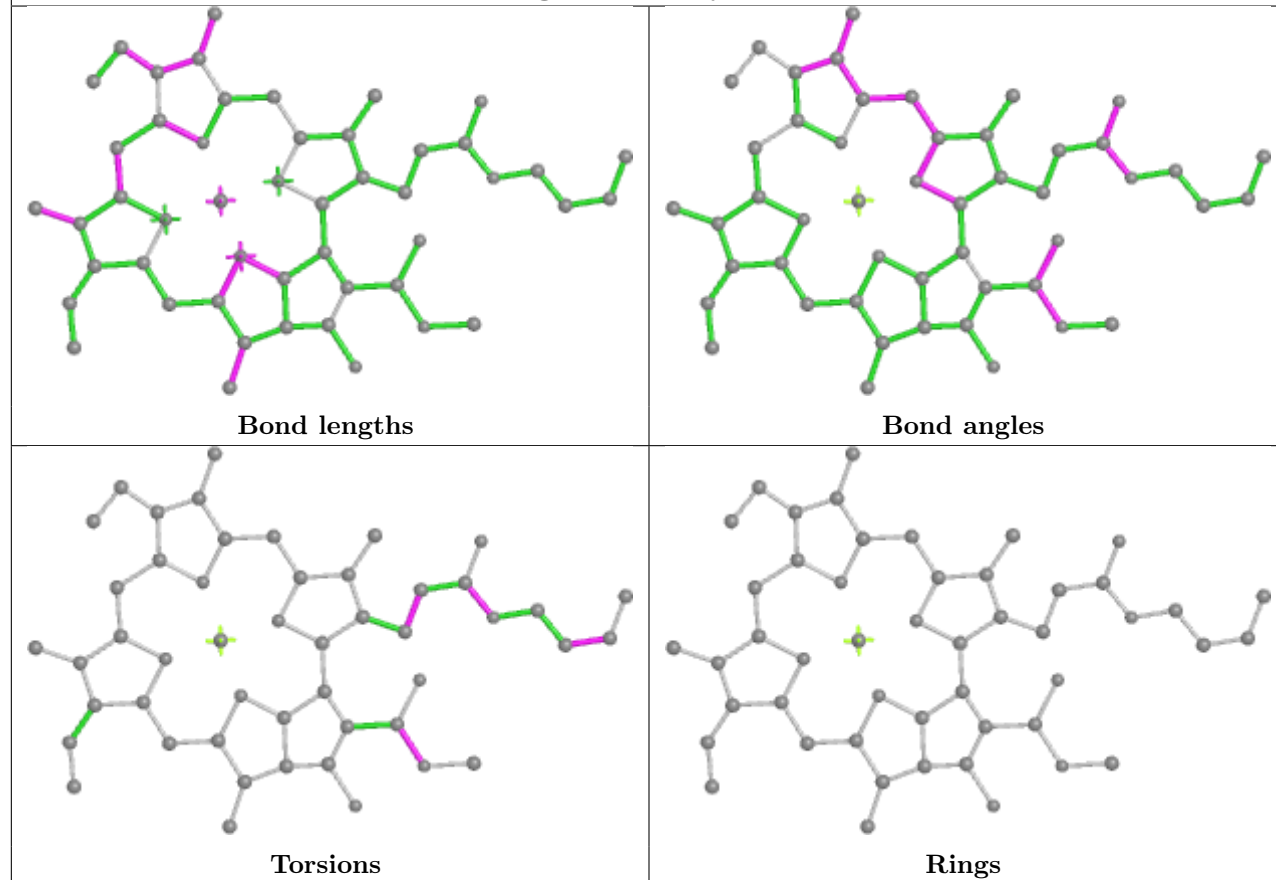


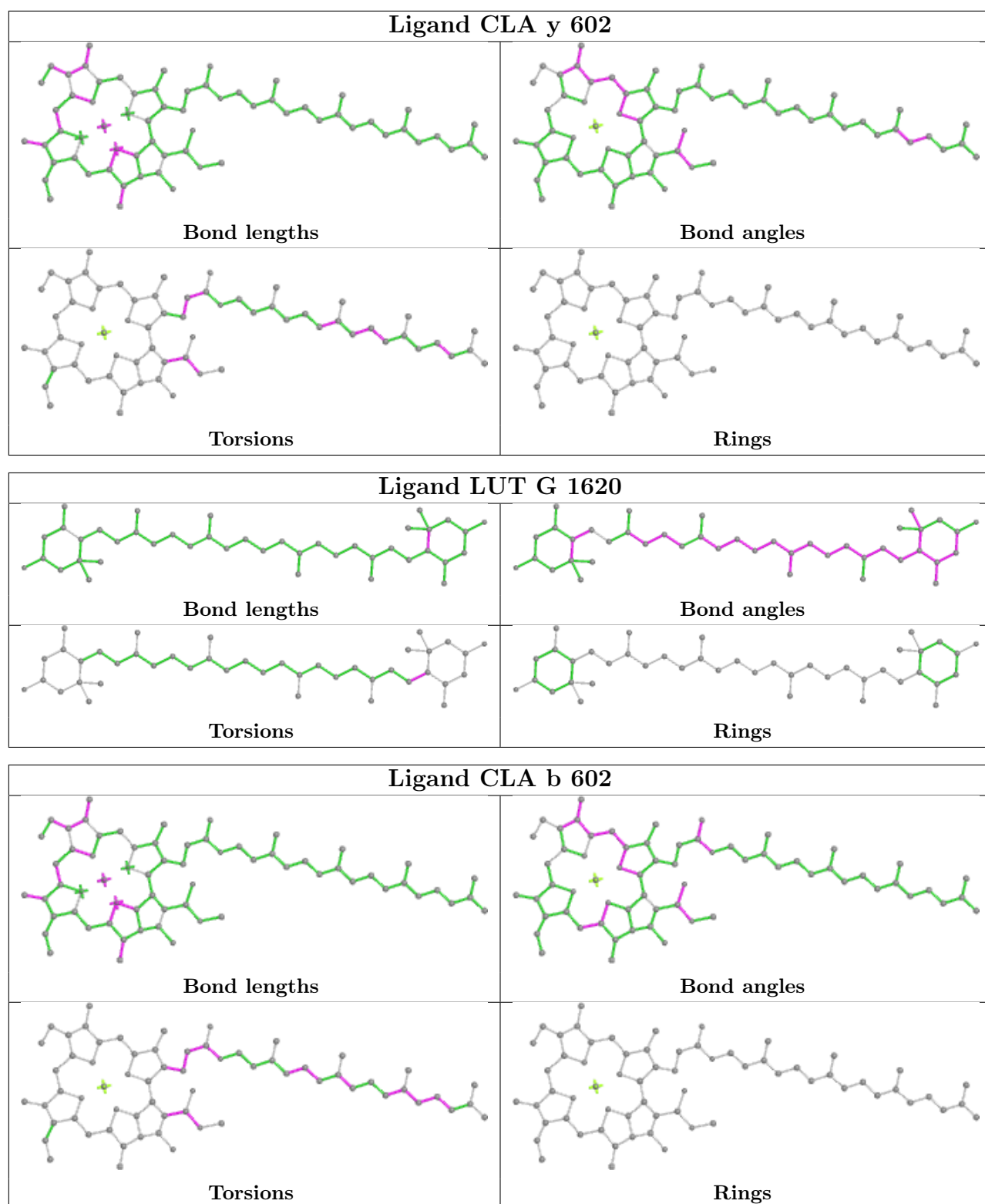


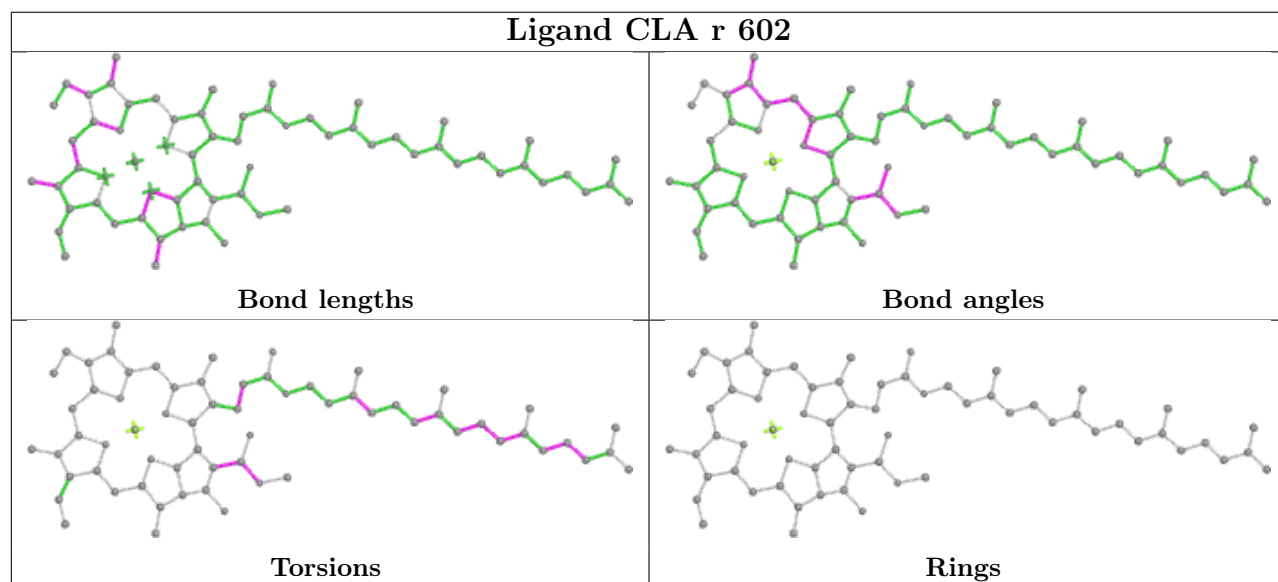
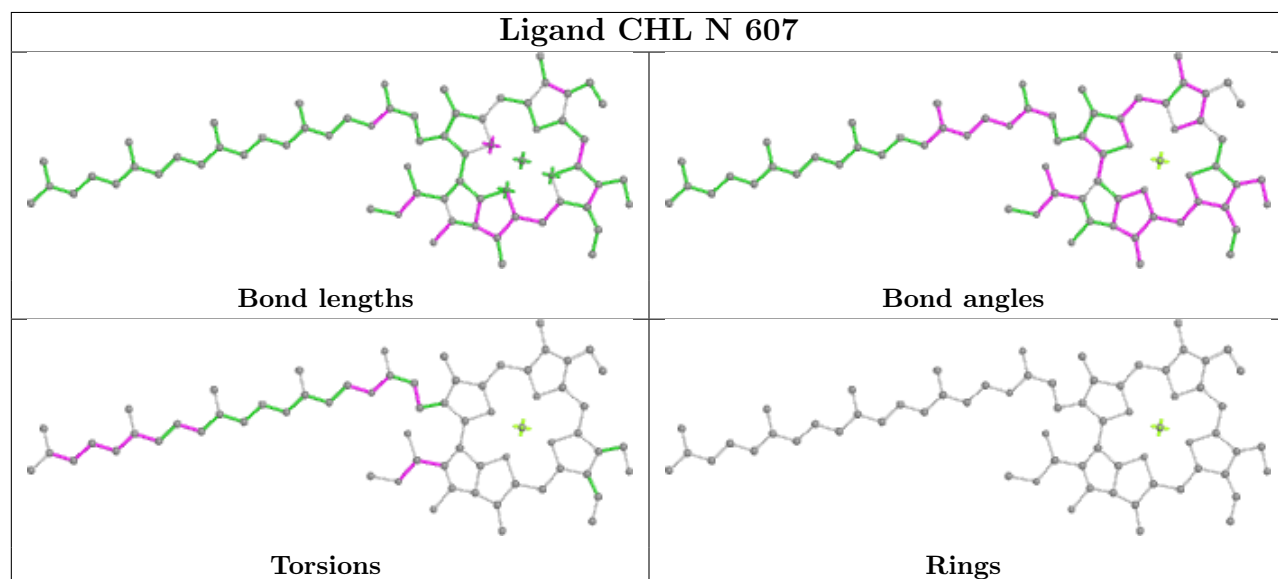
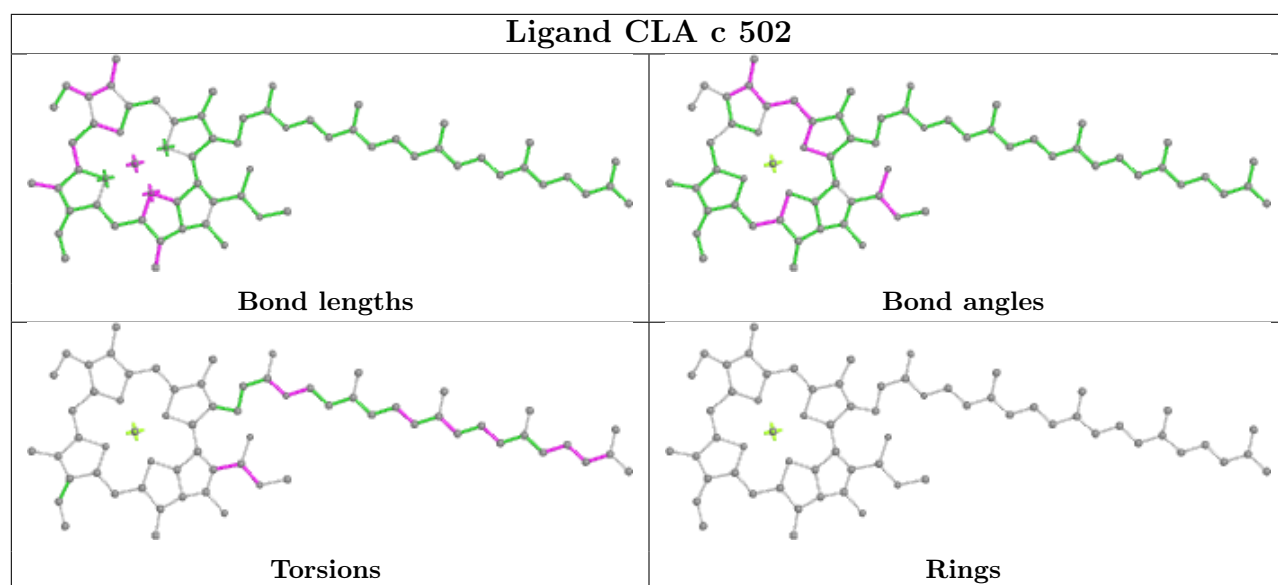
## Ligand CLA c 505

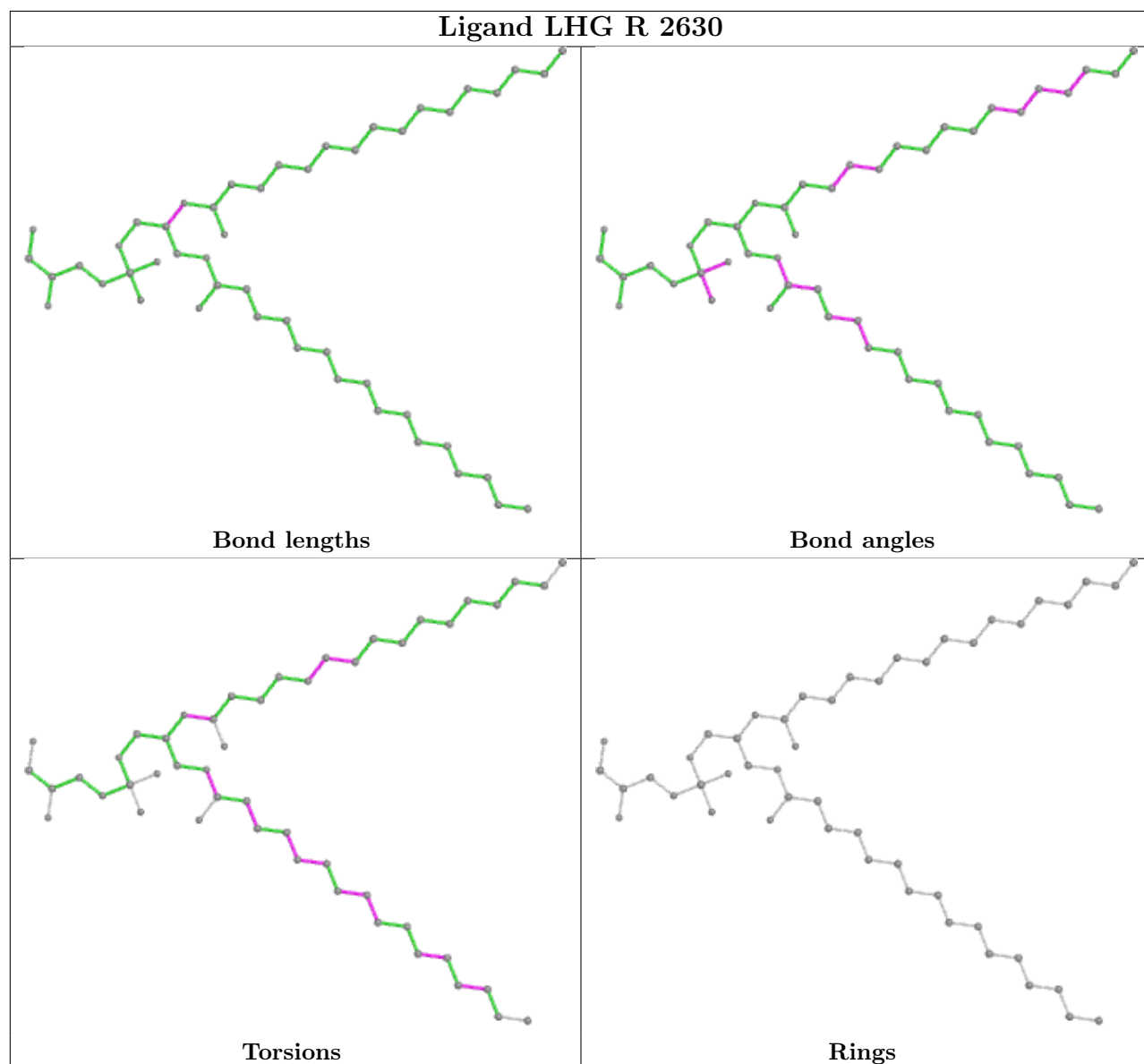
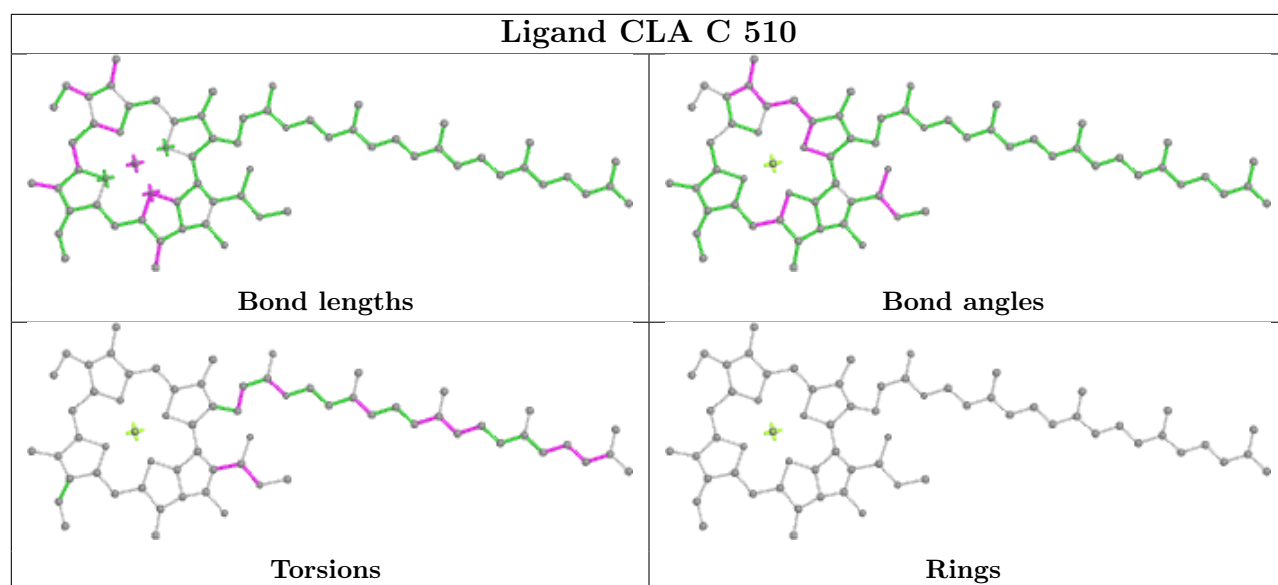


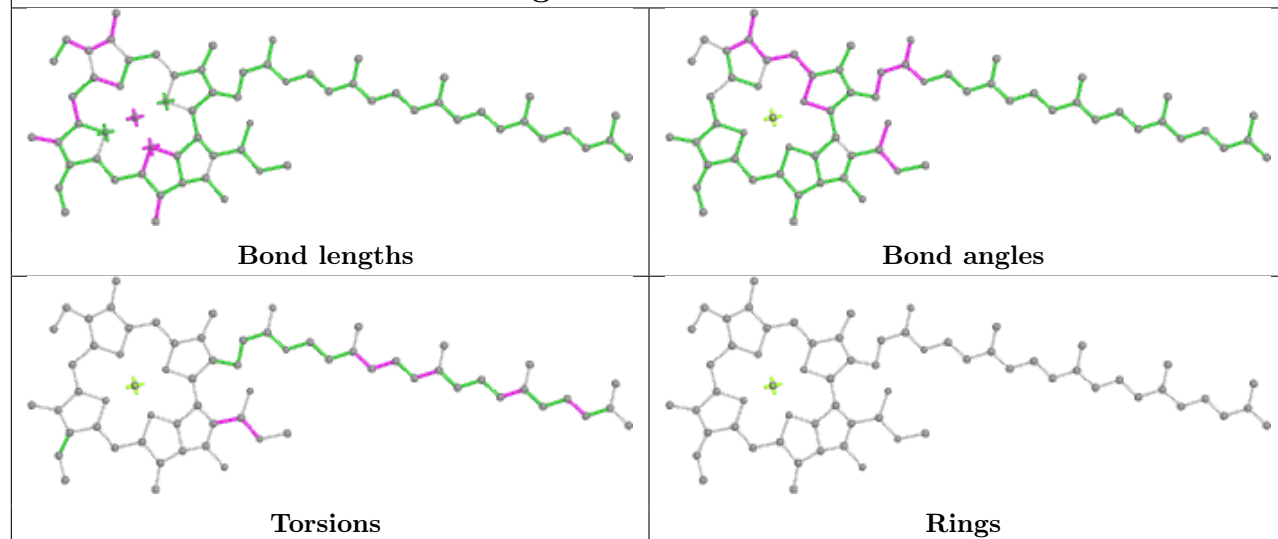
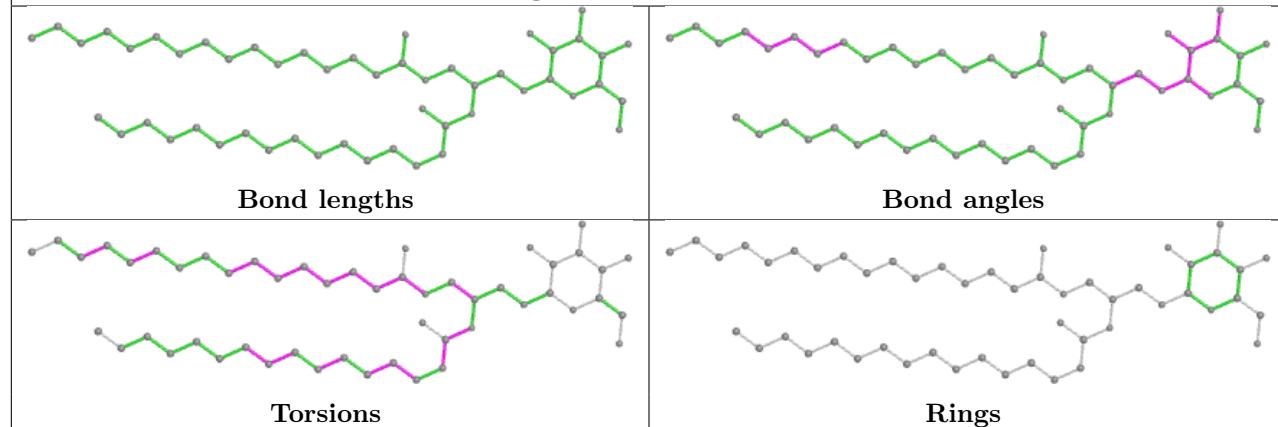
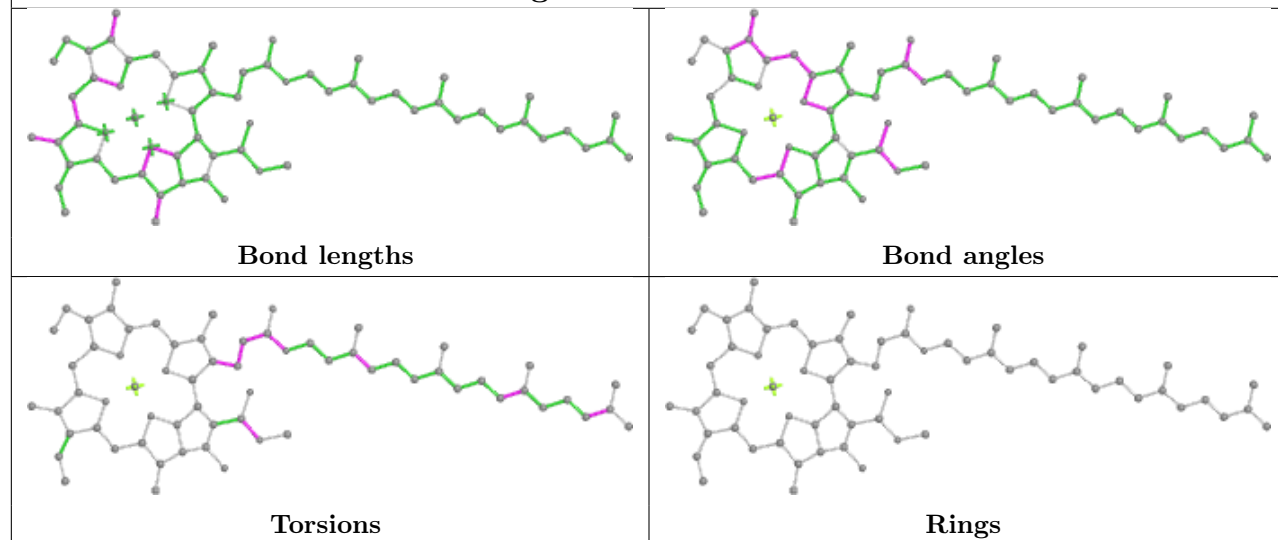
## Ligand CLA y 604

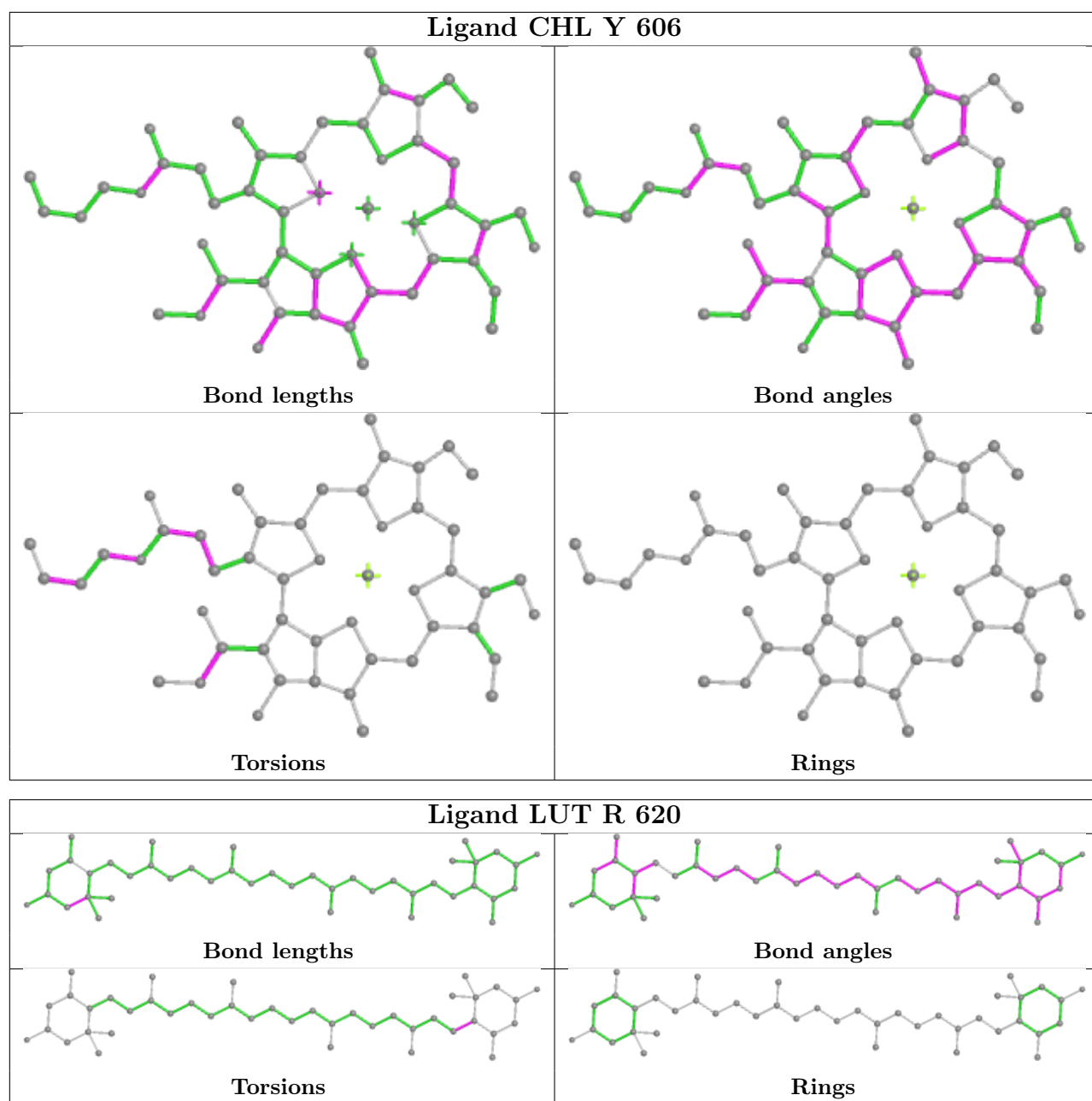


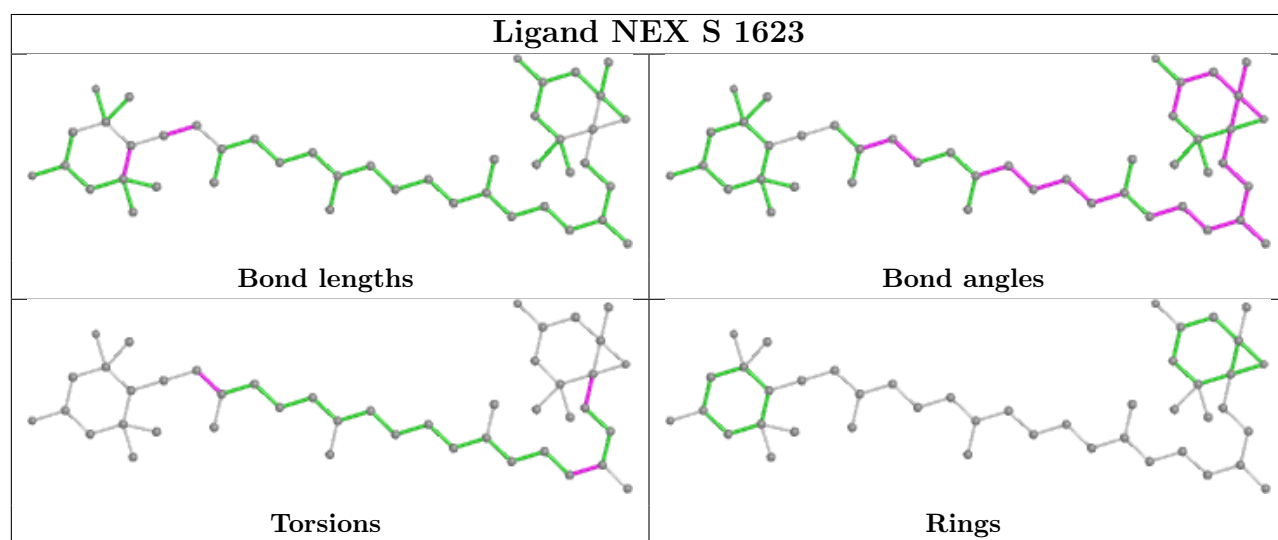
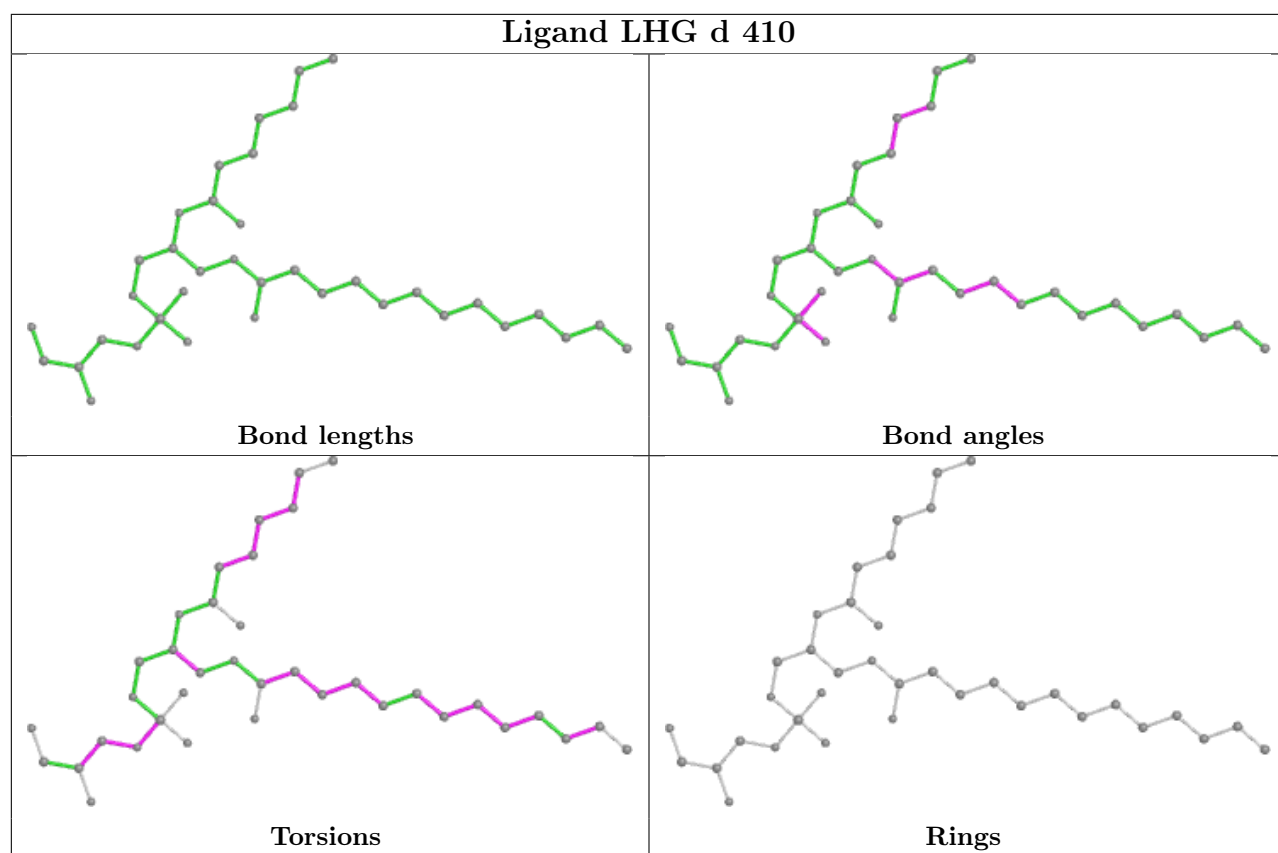


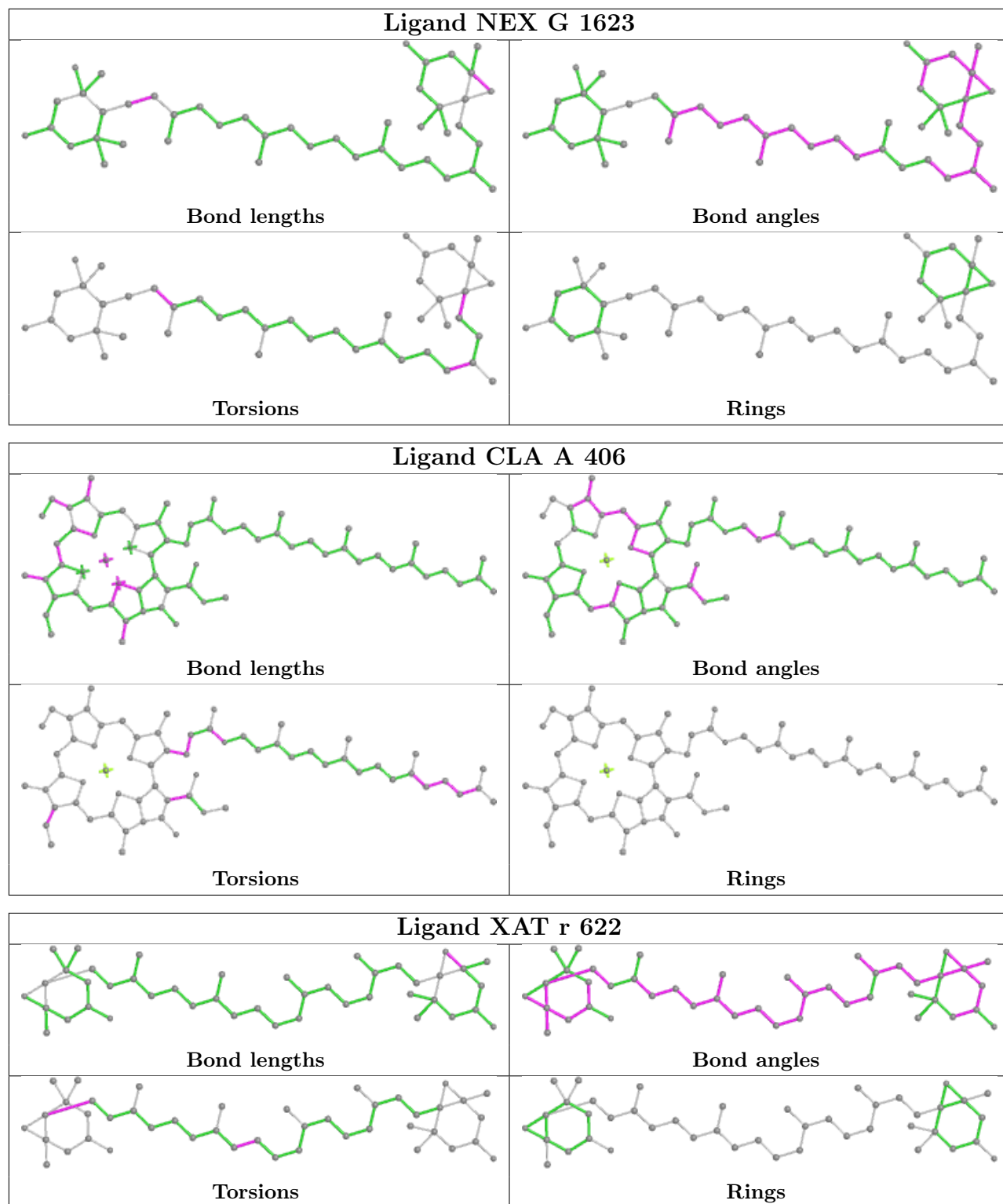




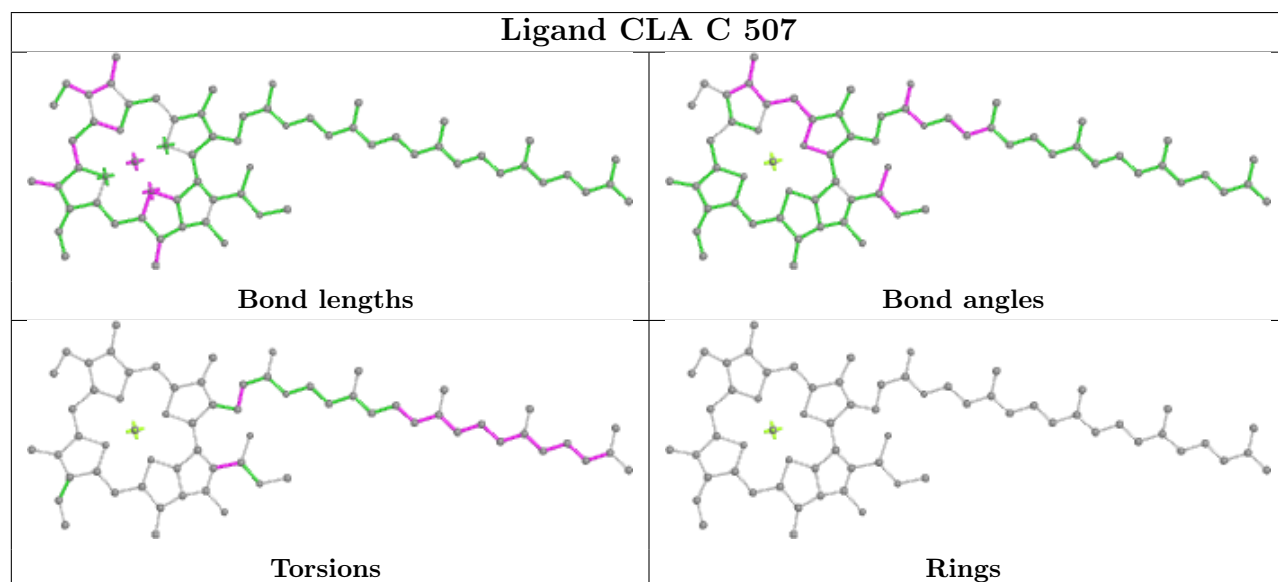
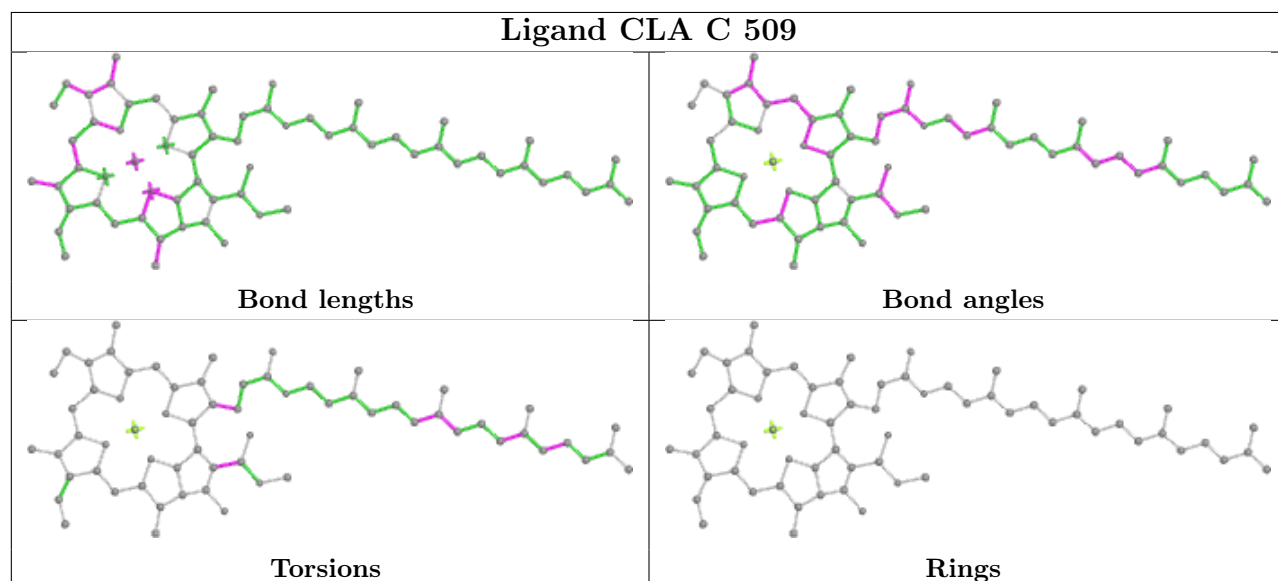
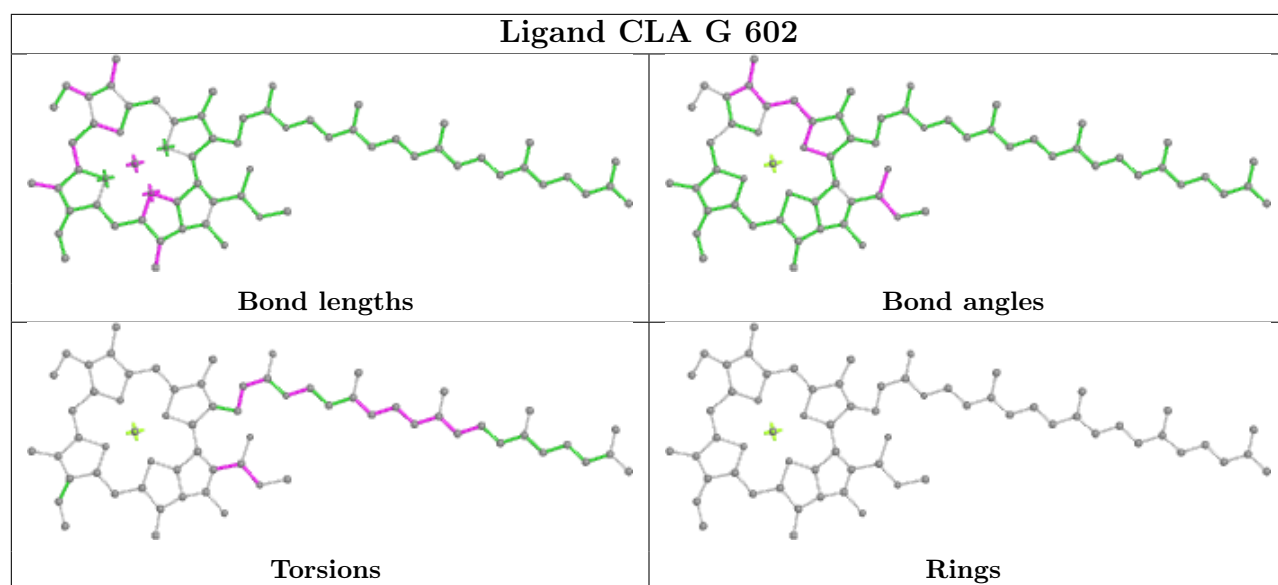
**Ligand CLA B 610****Ligand LMG C 521****Ligand CLA G 610**

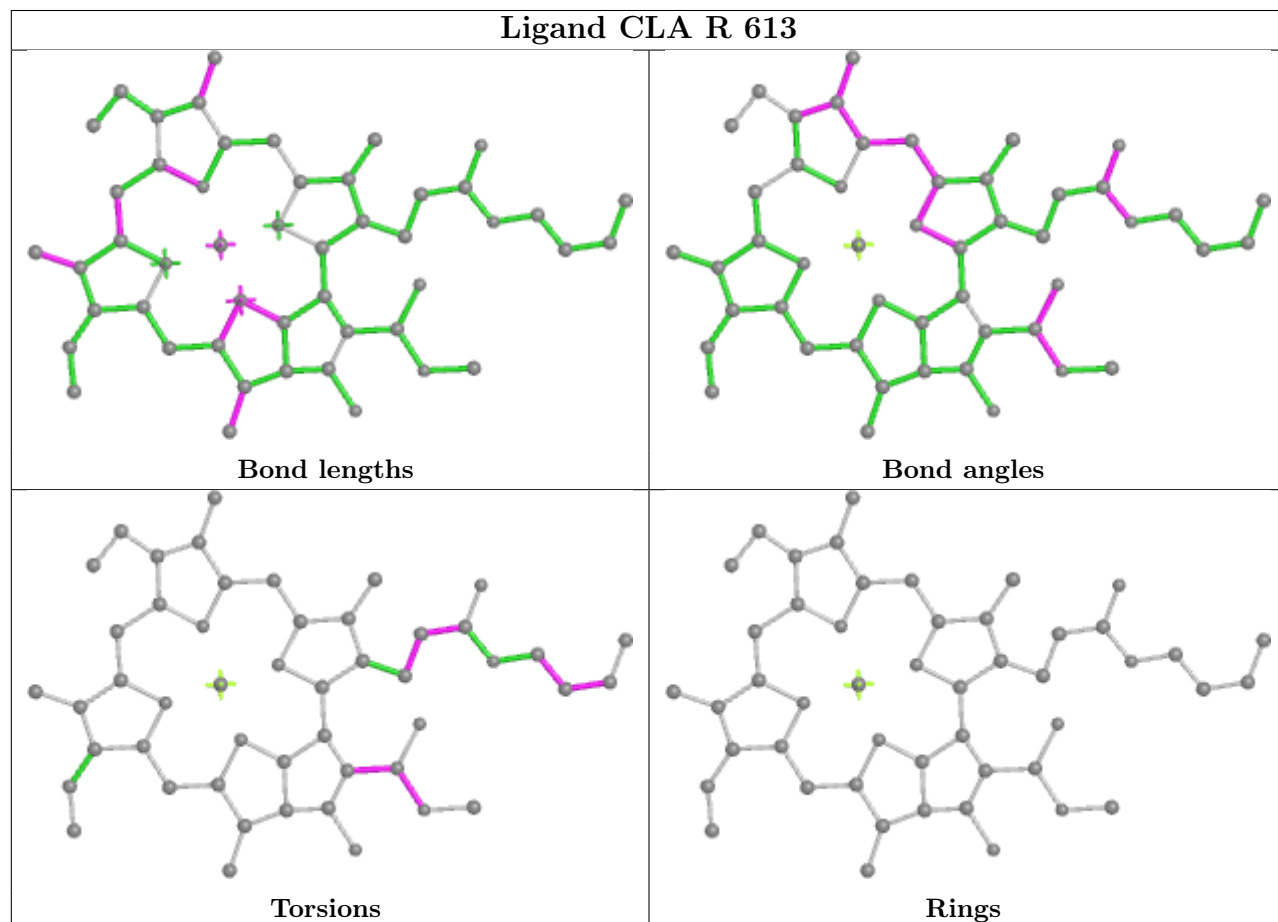
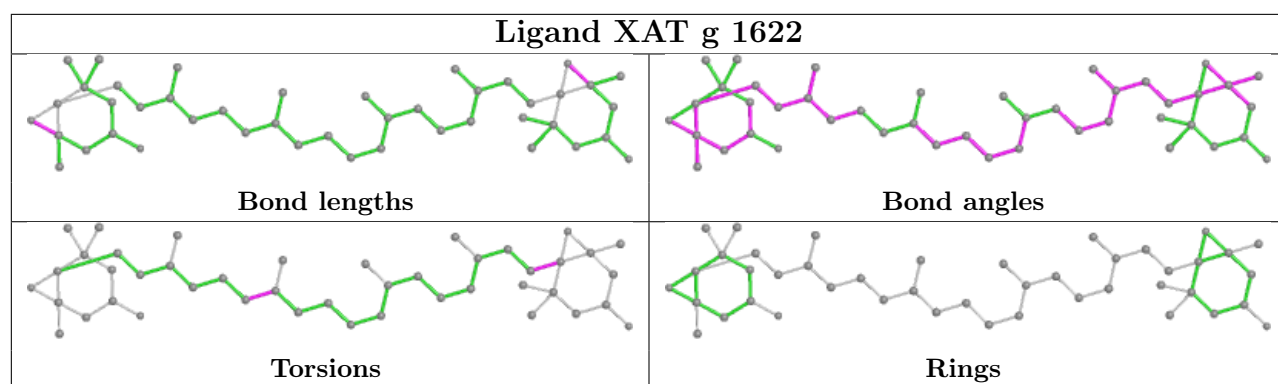


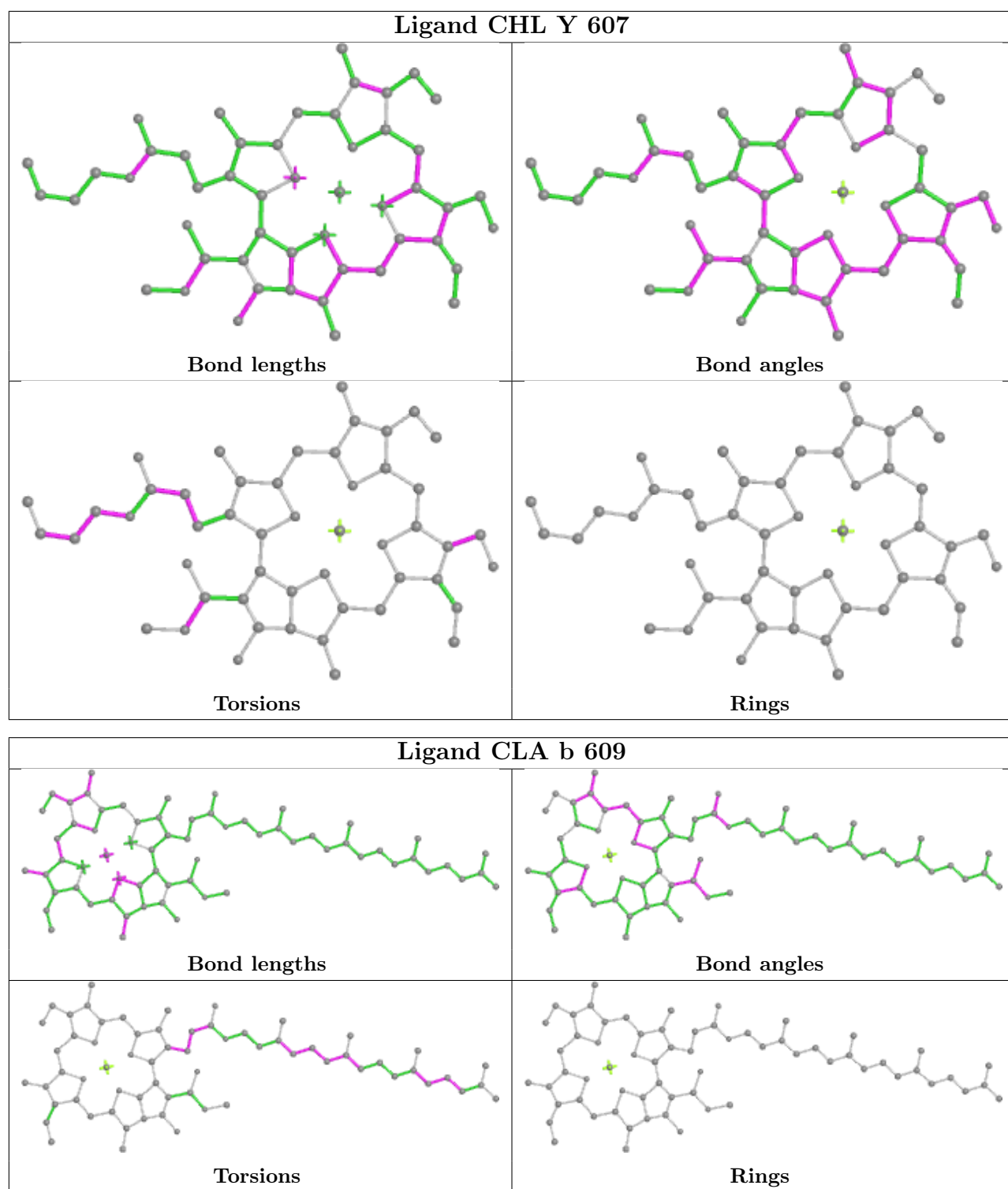




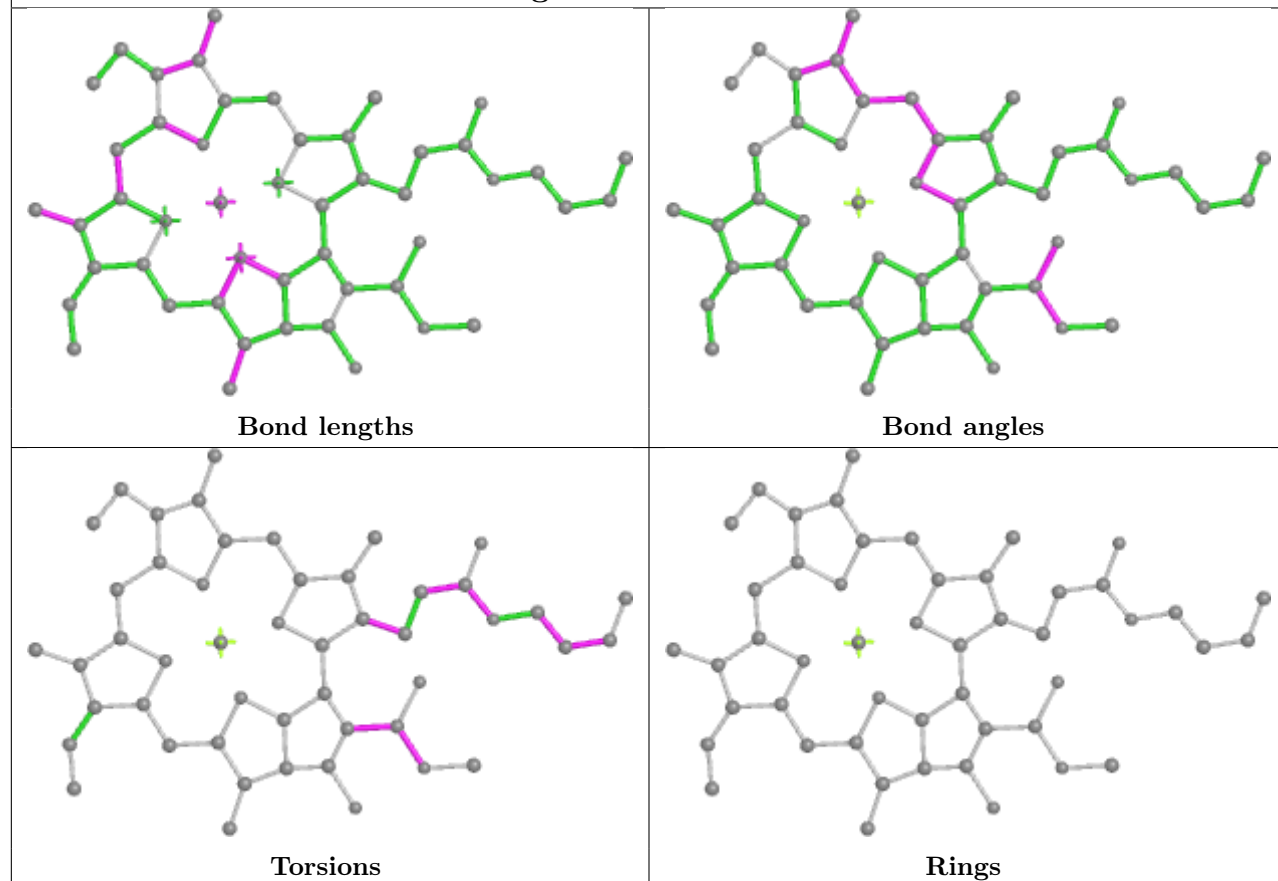




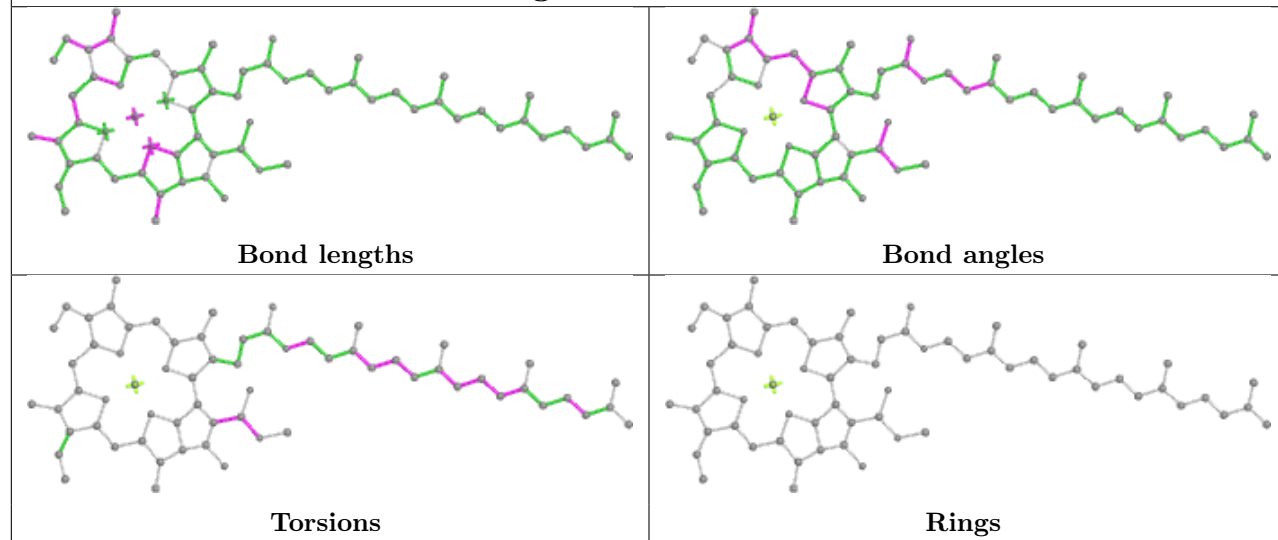


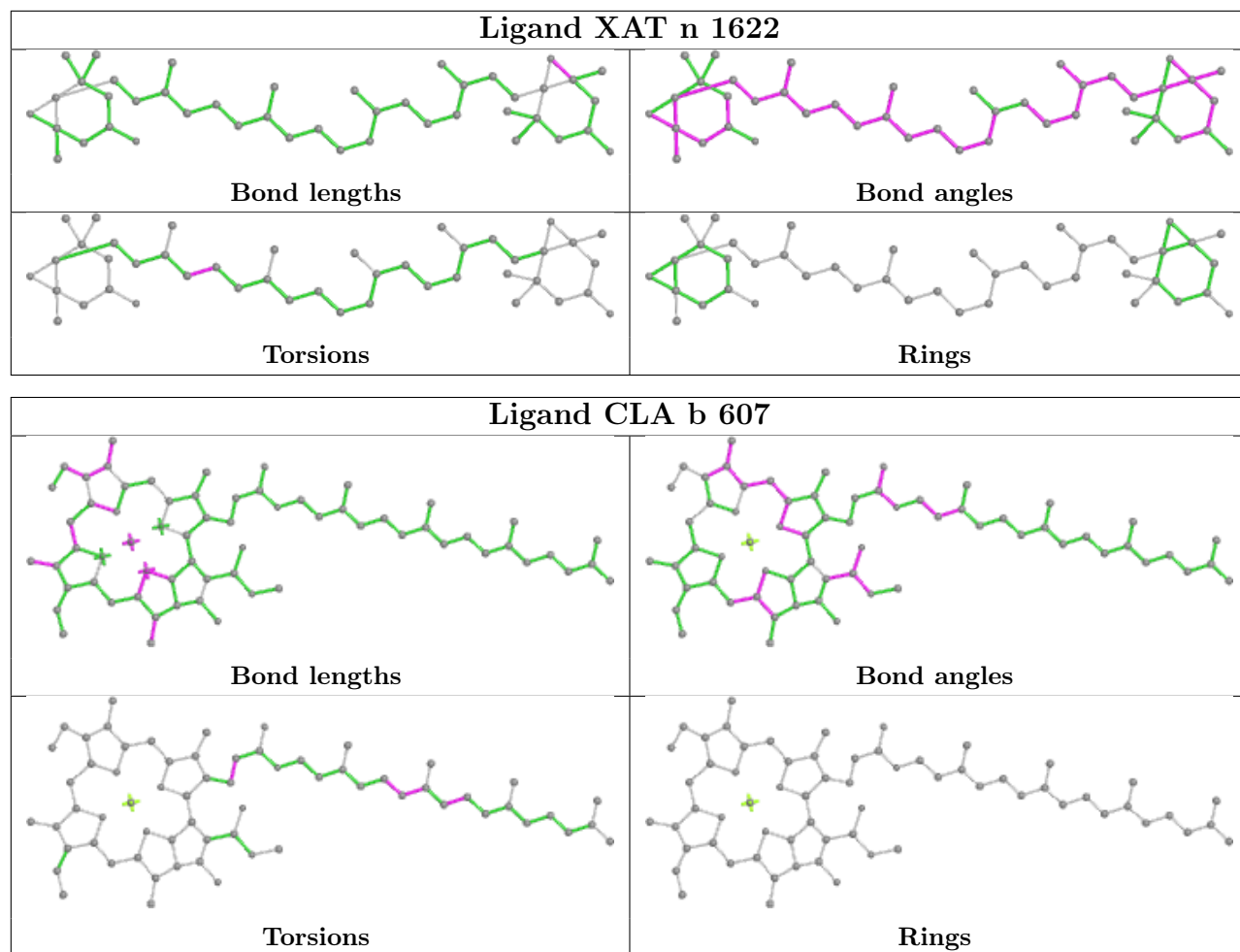


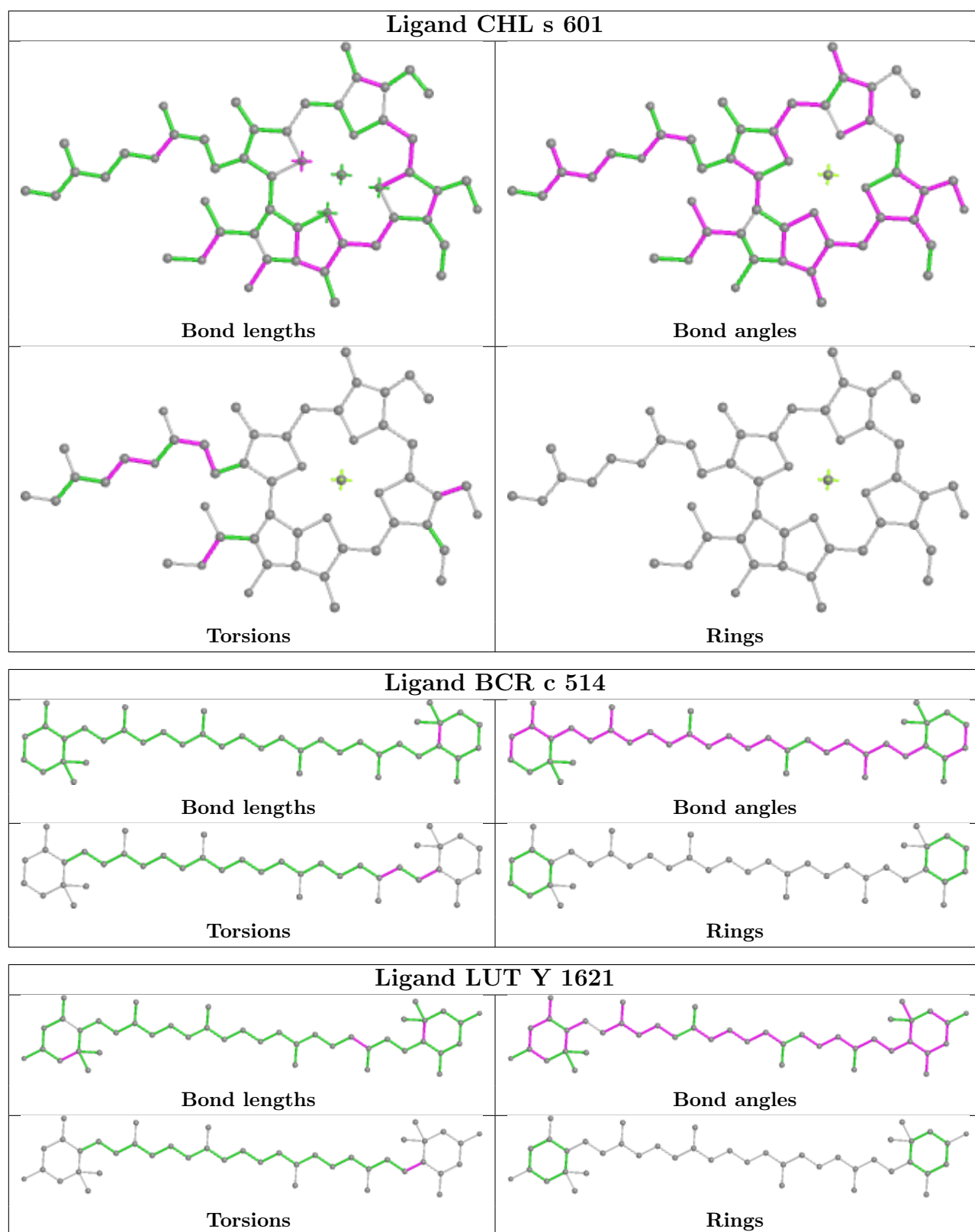
## Ligand CLA N 603

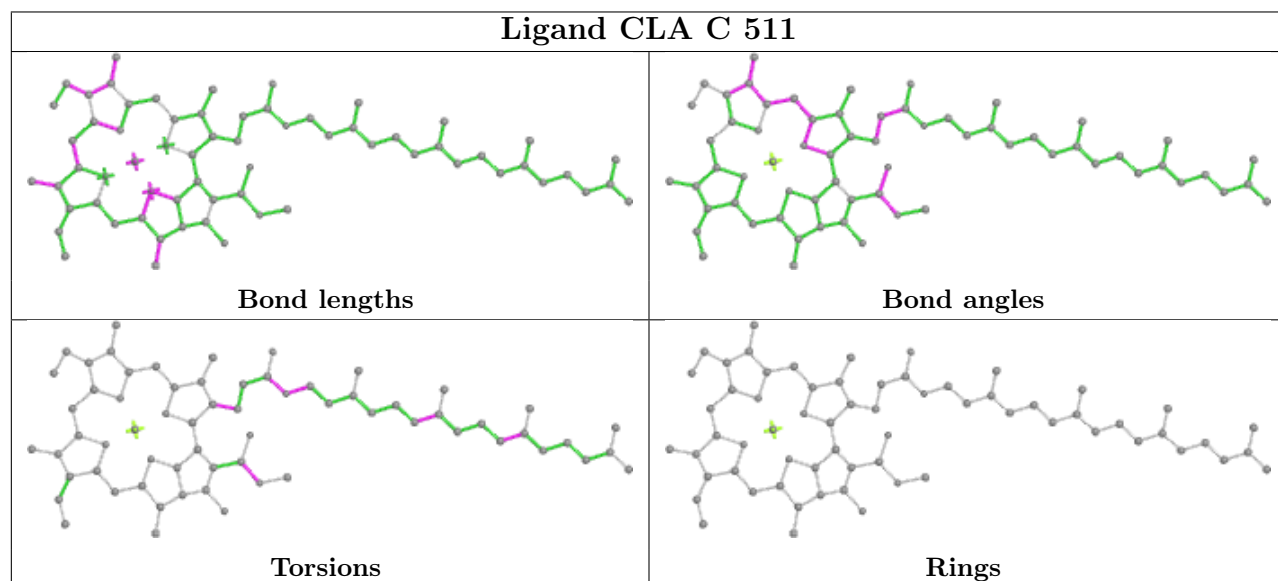
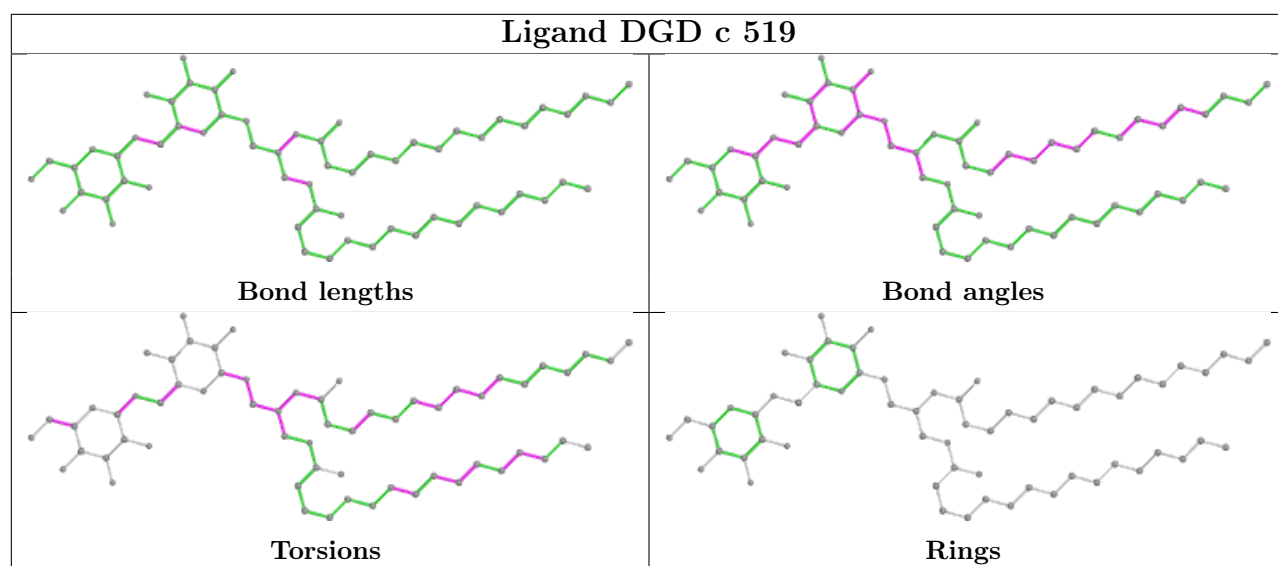


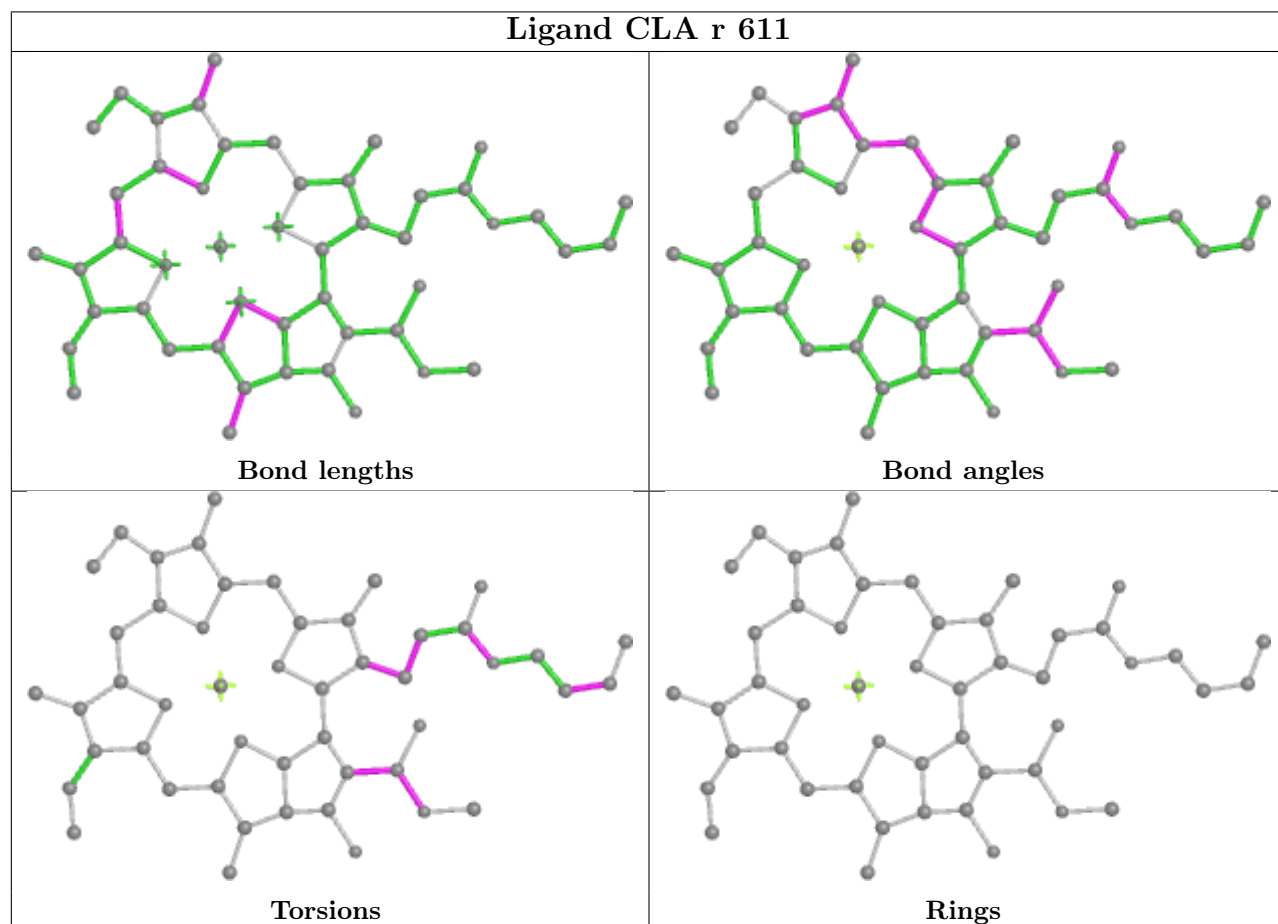
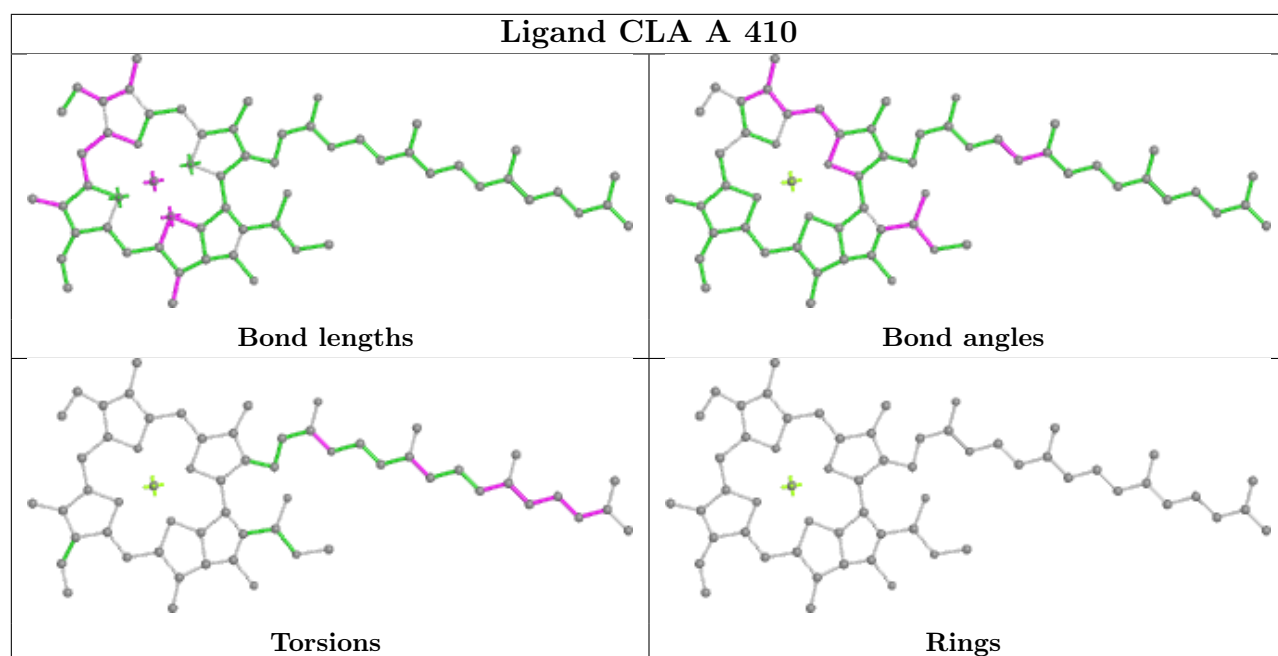
## Ligand CLA C 506





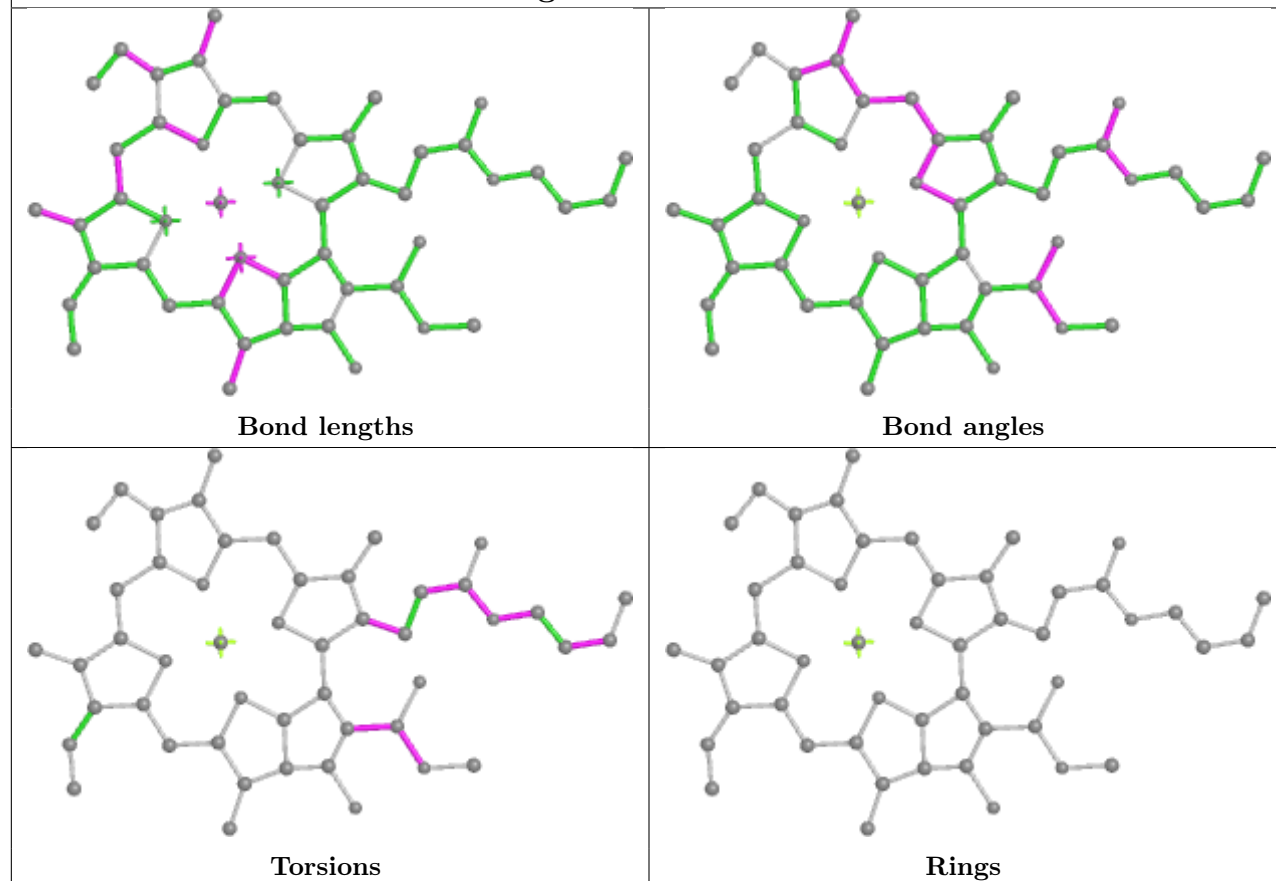




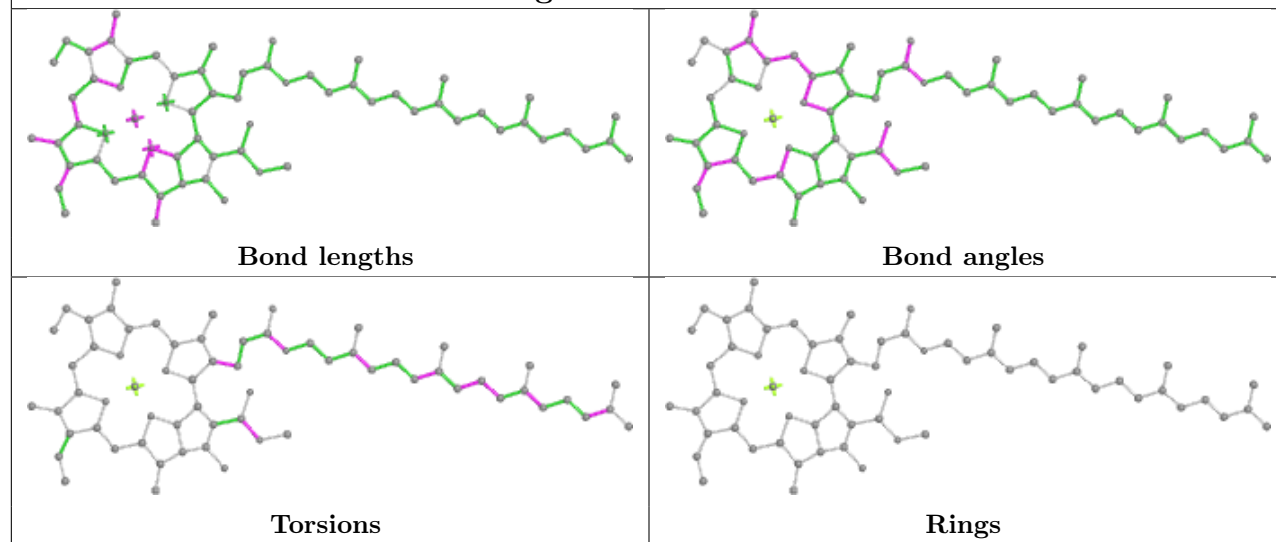




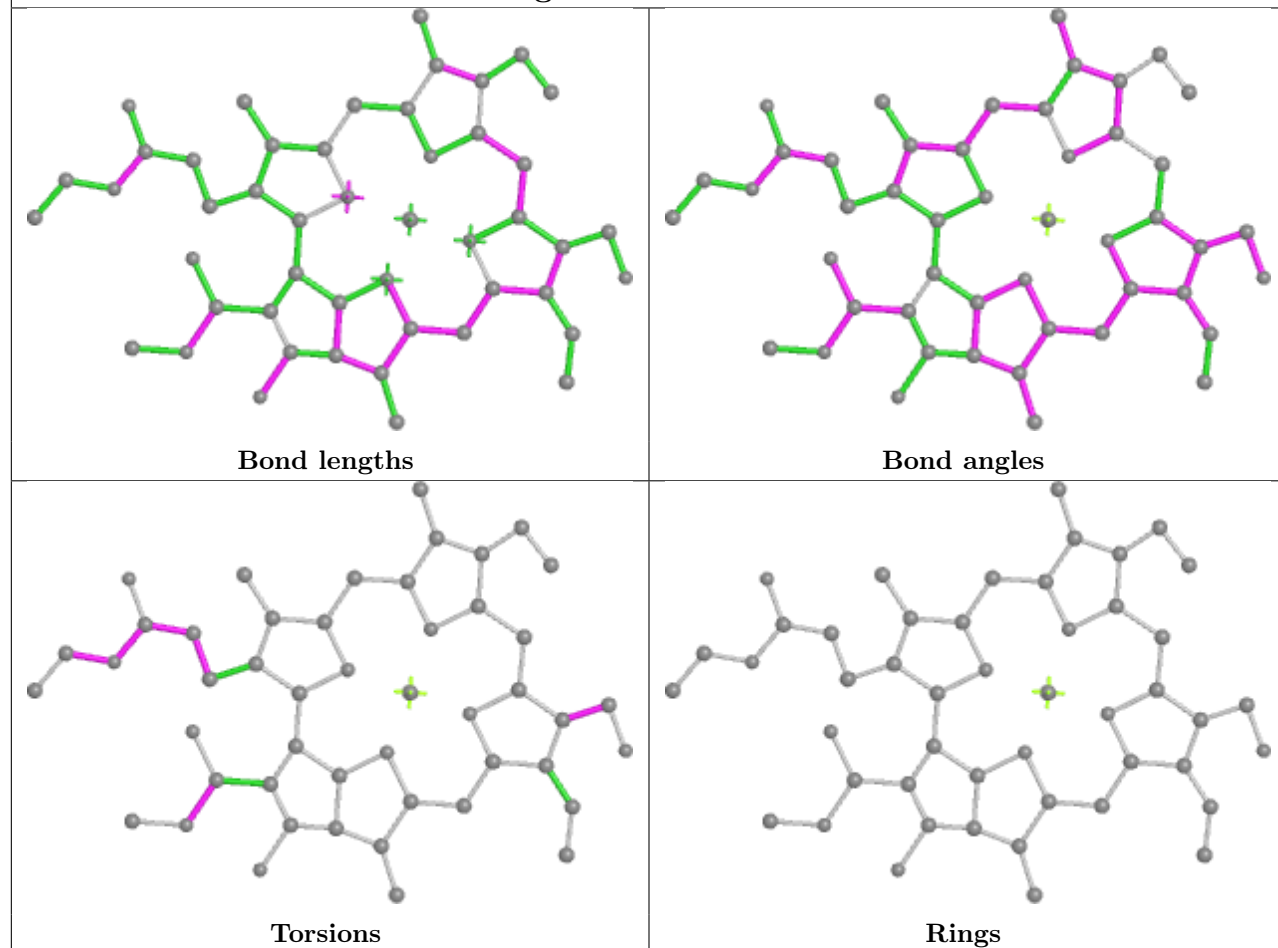
## Ligand CLA s 604



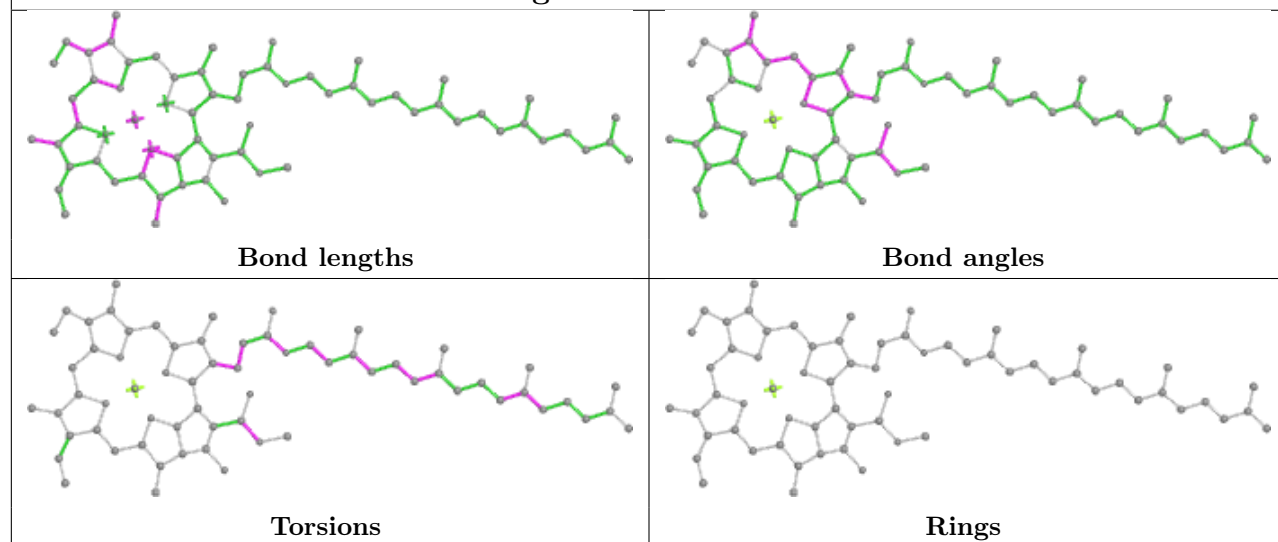
## Ligand CLA b 612



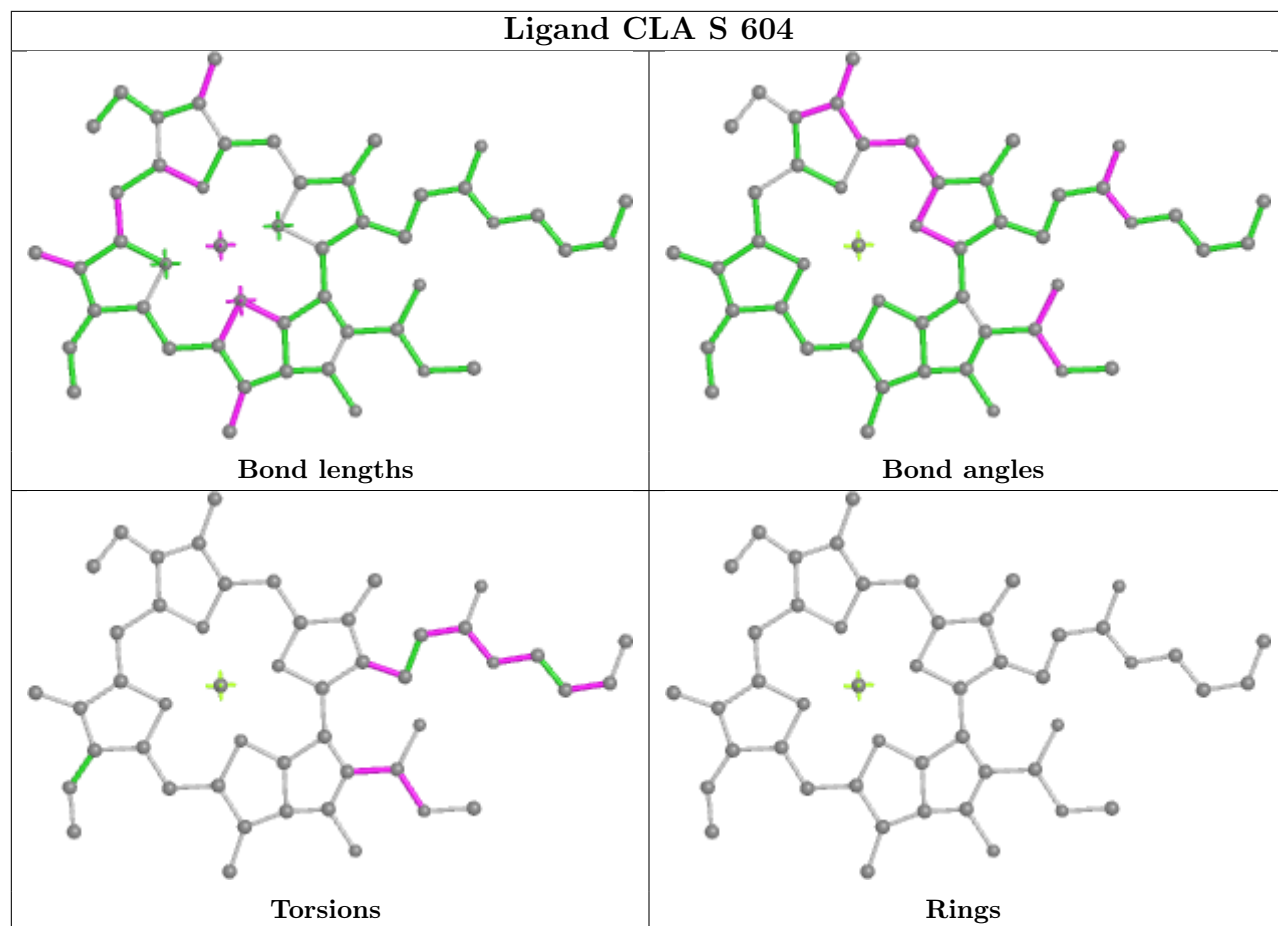
## Ligand CHL n 605



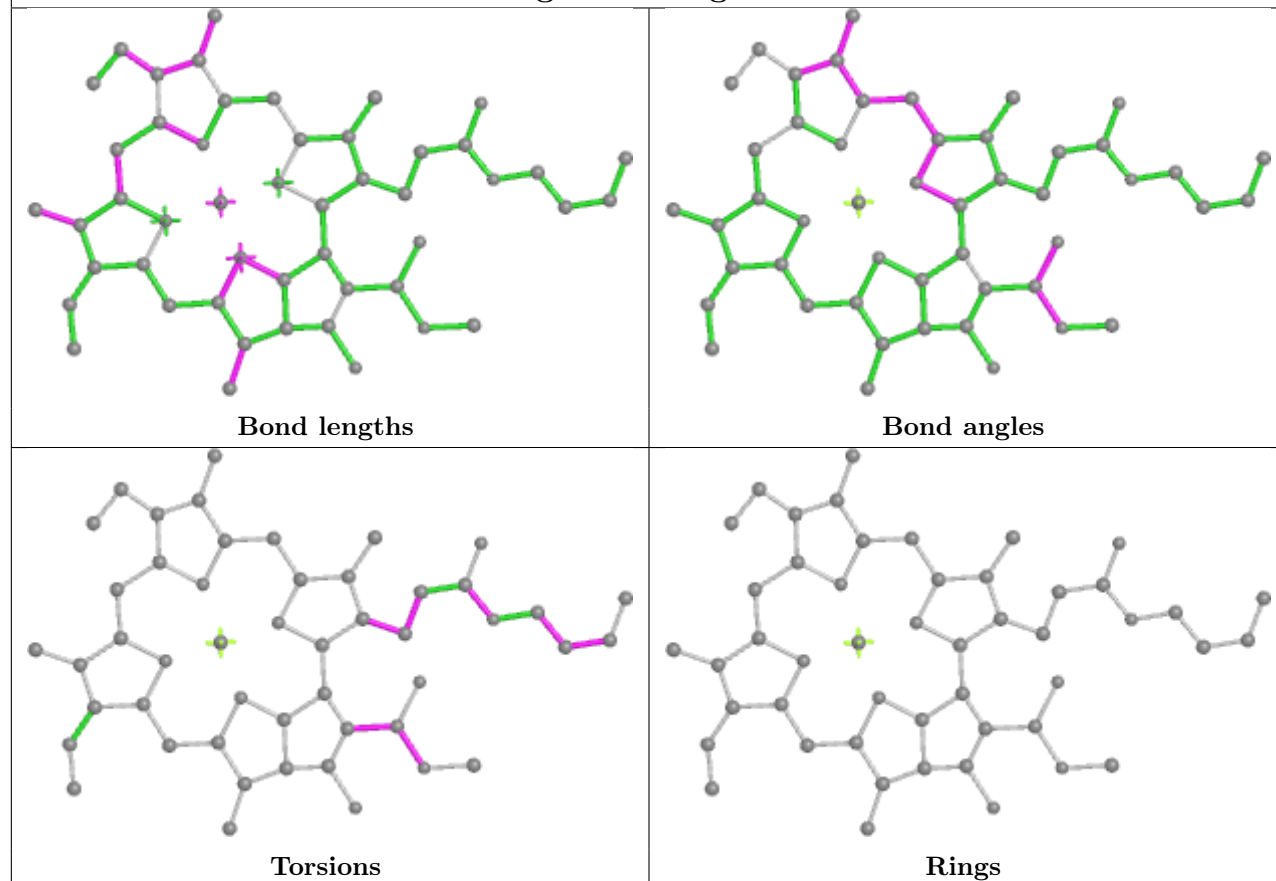
## Ligand CLA B 603



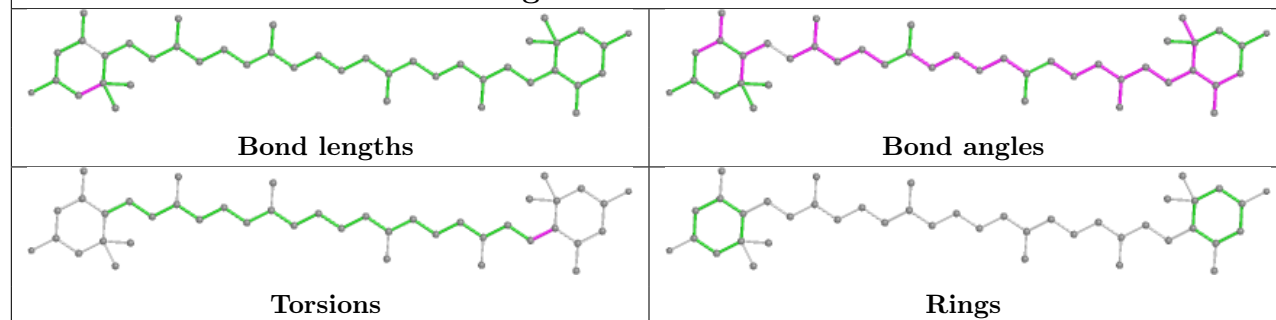
## Ligand CLA S 604

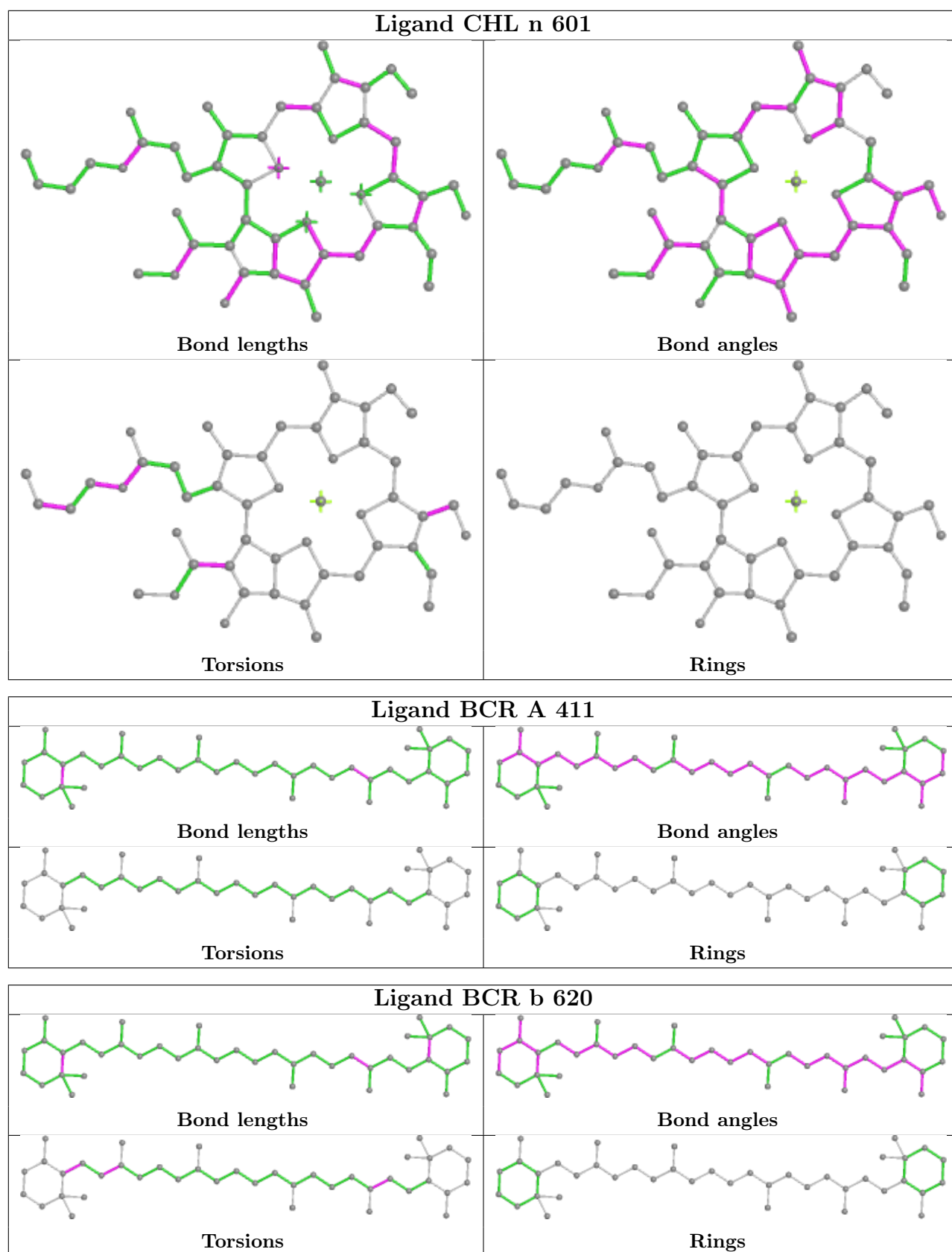


## Ligand CLA g 604

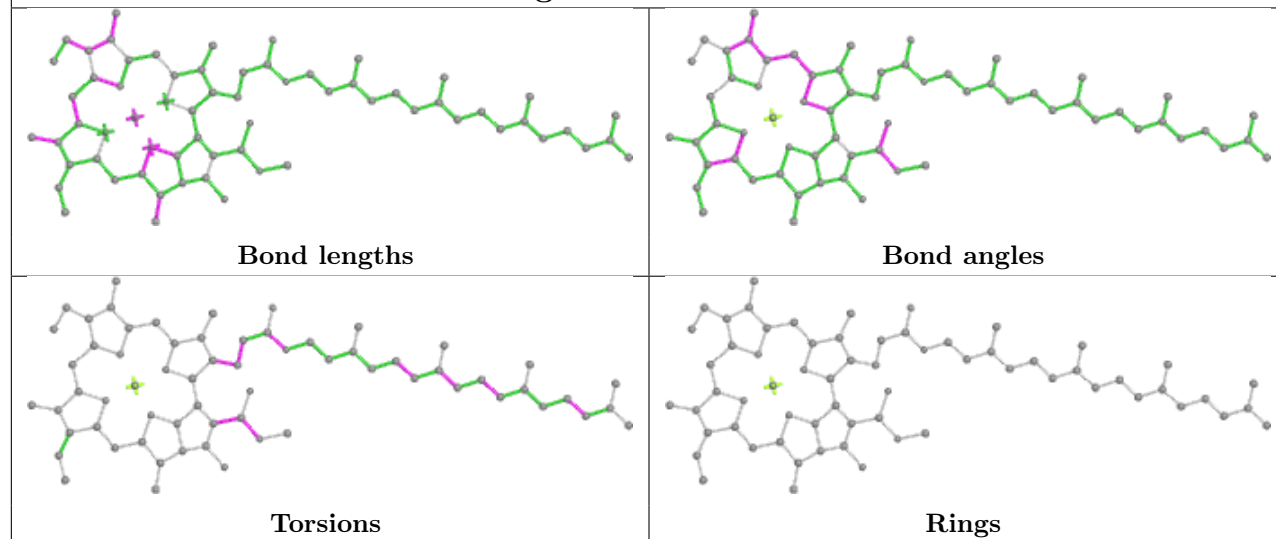


## Ligand LUT N 1620

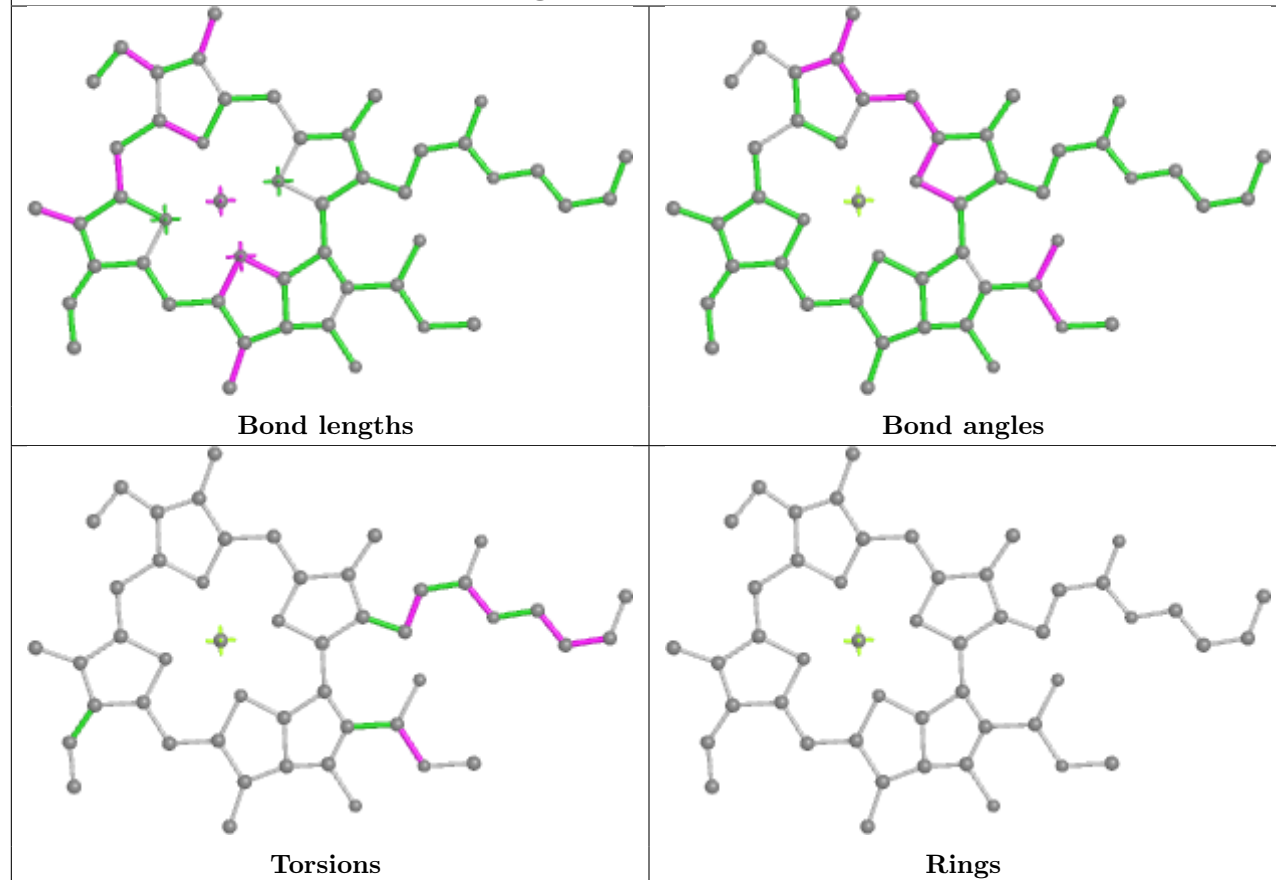


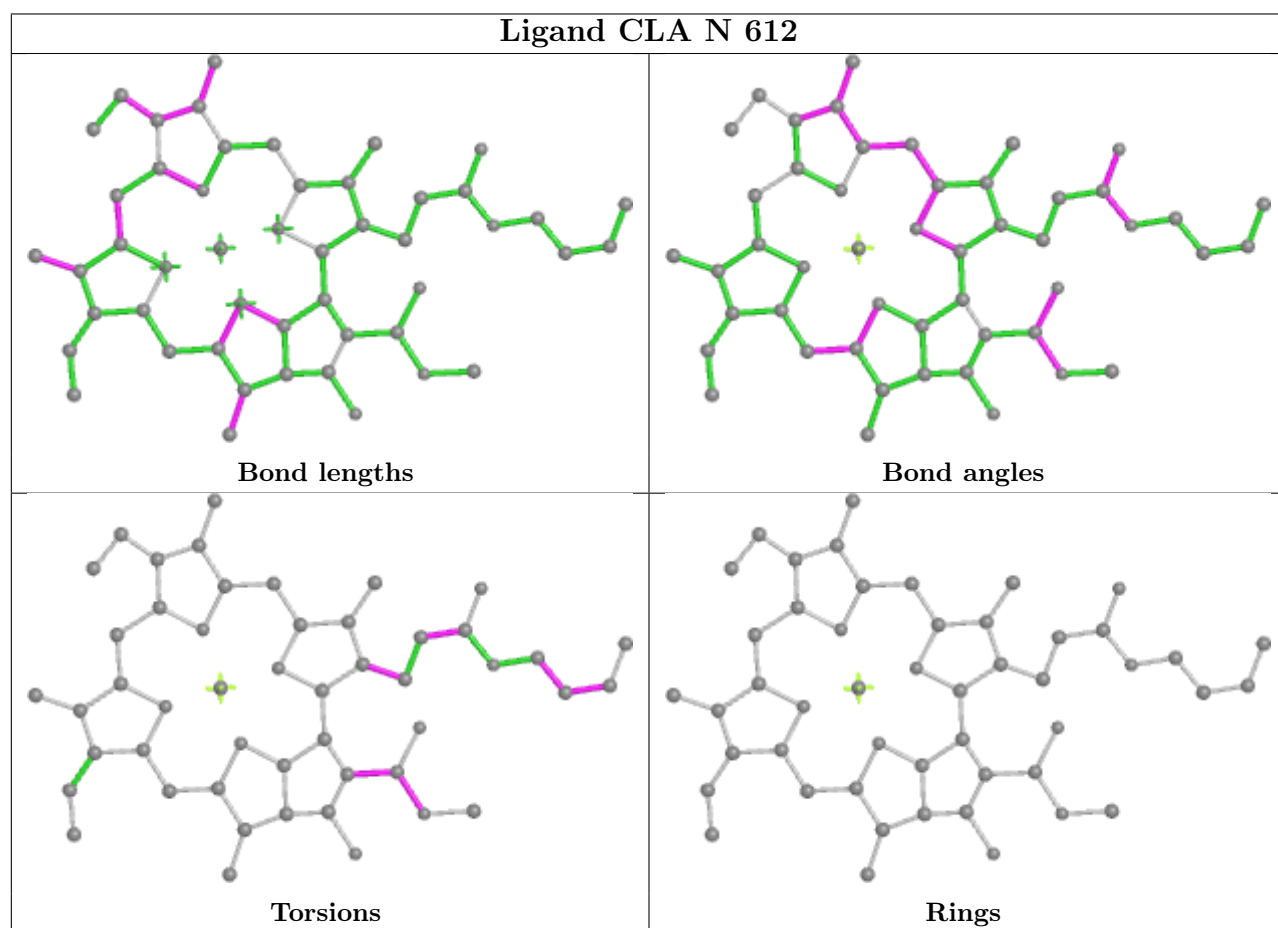
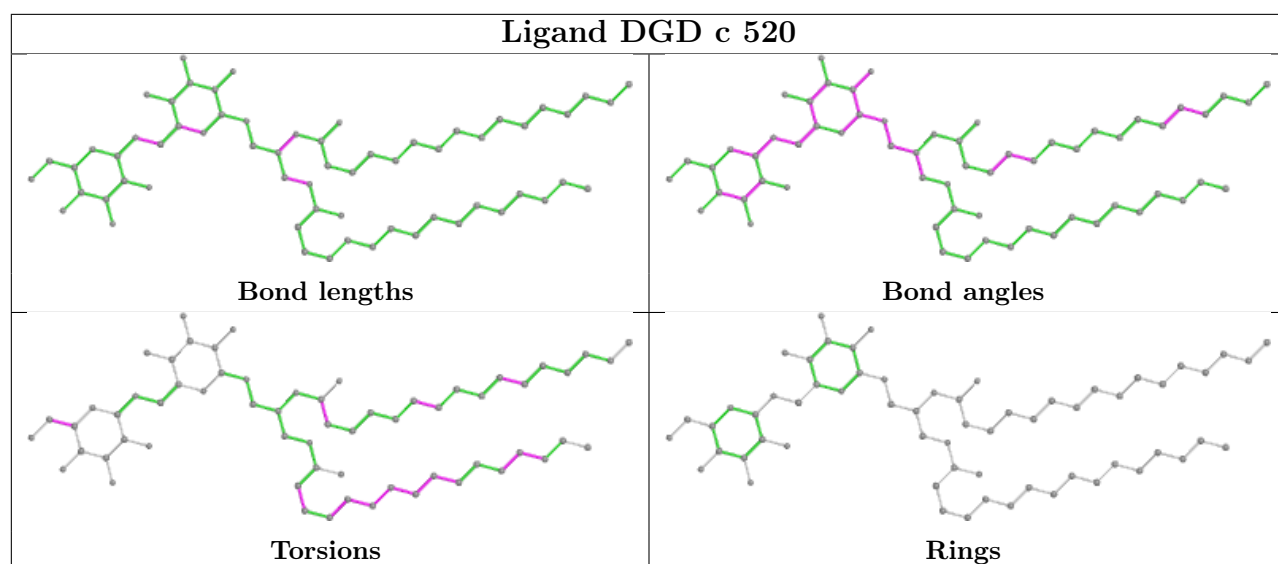


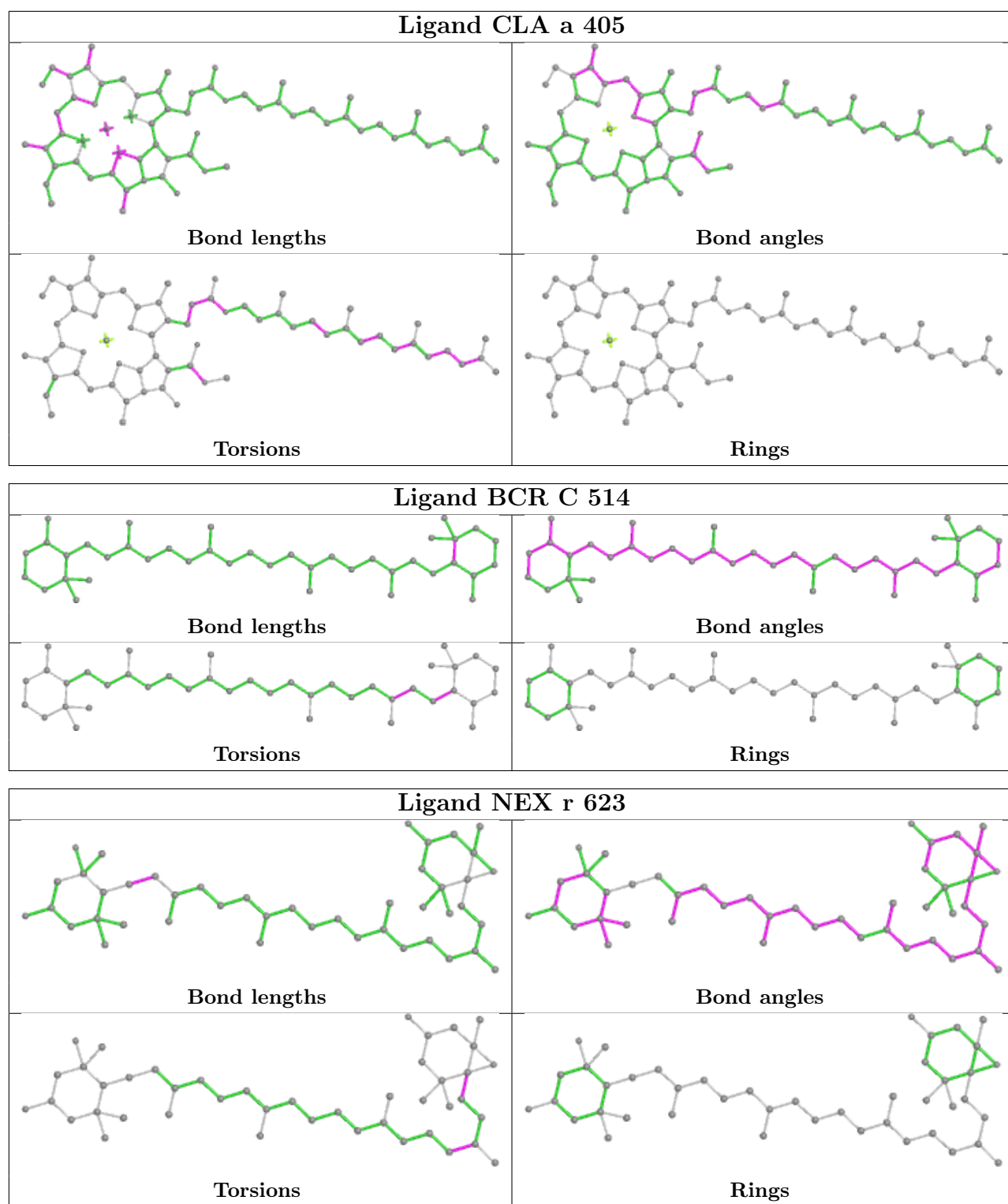
## Ligand CLA b 615



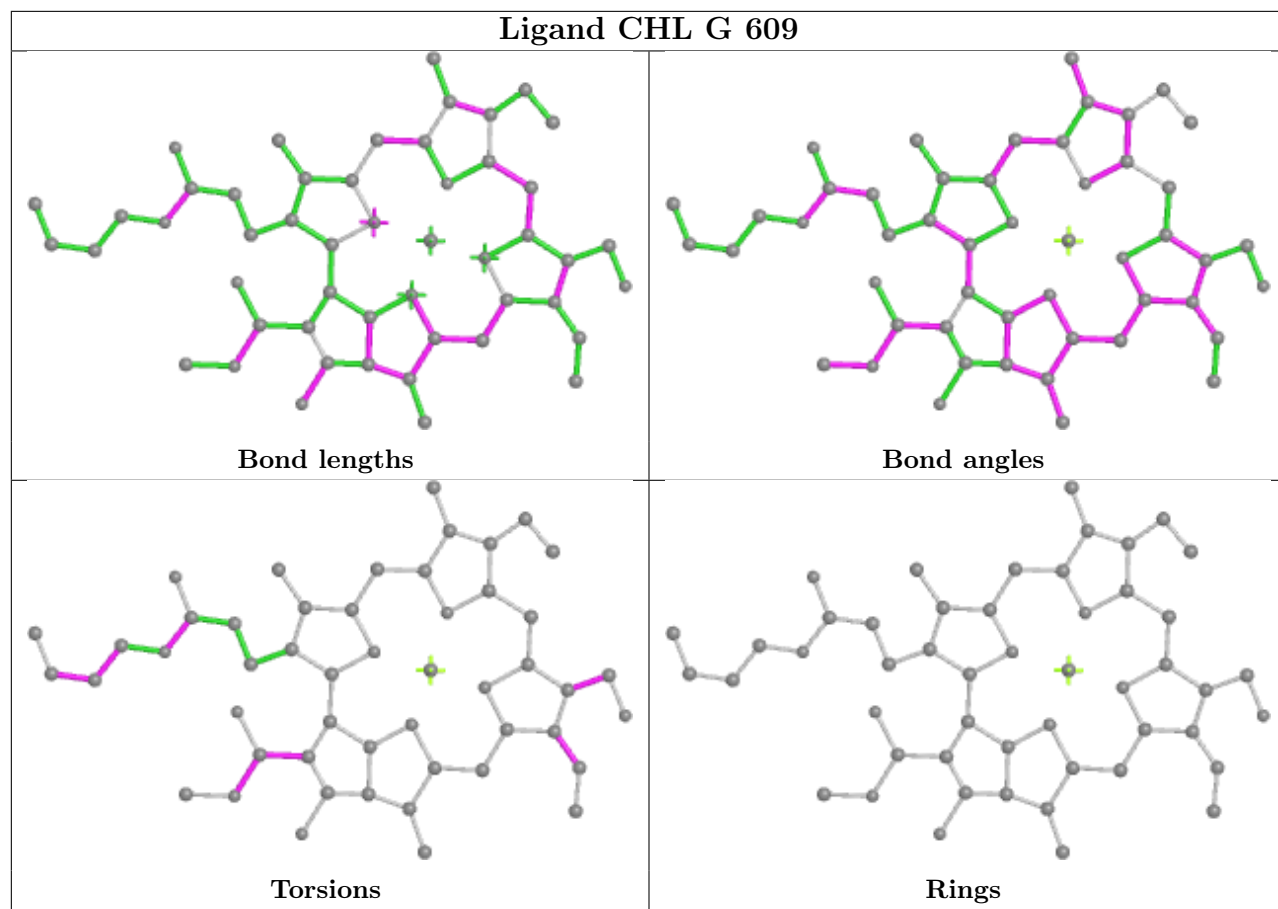
## Ligand CLA N 613

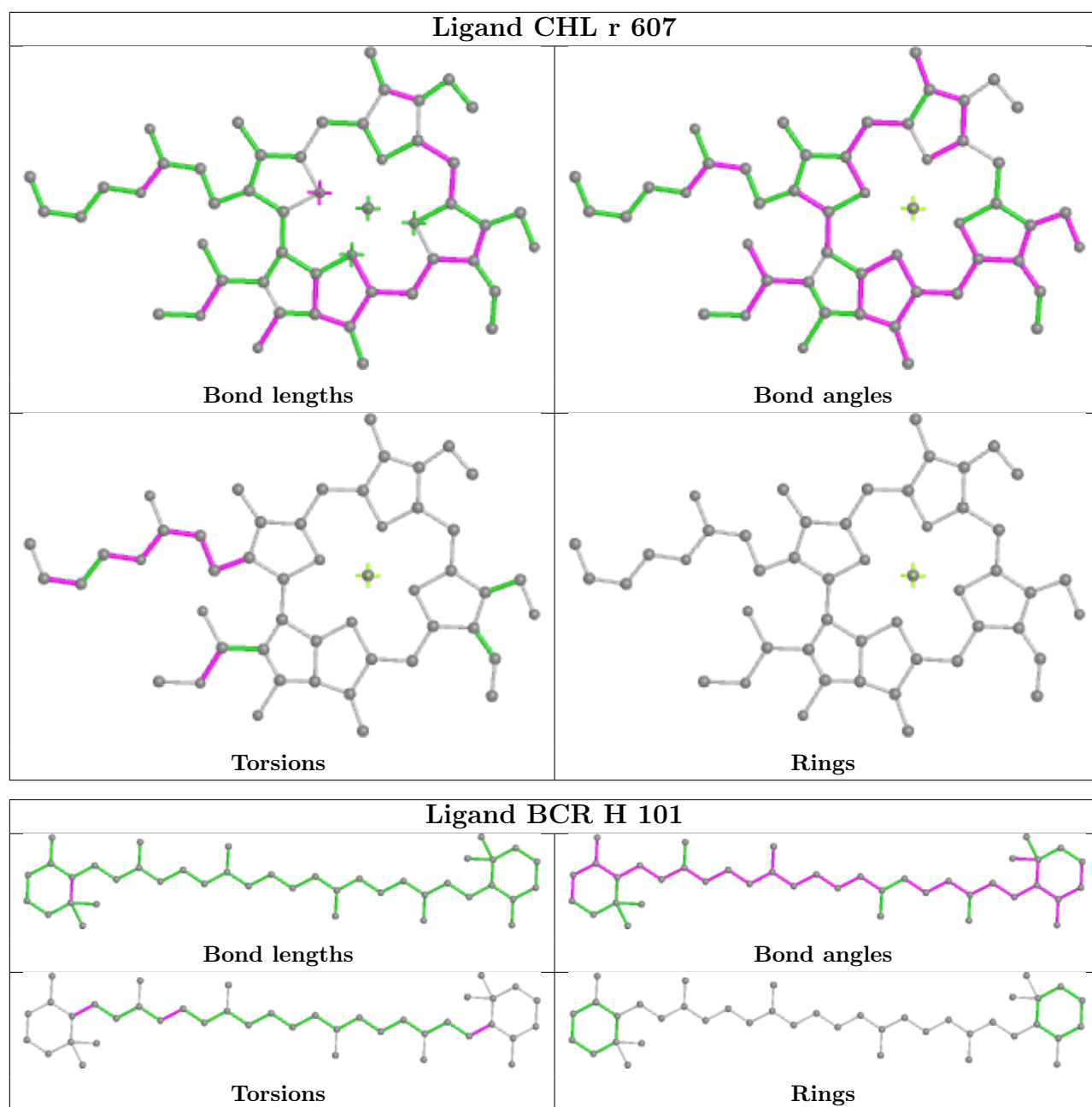












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

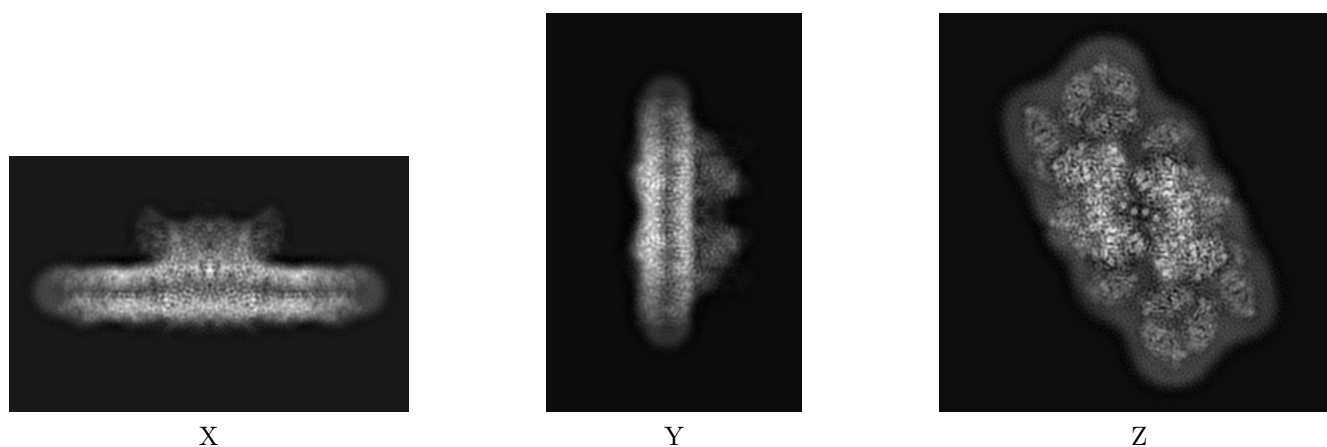
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6617. 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](#)

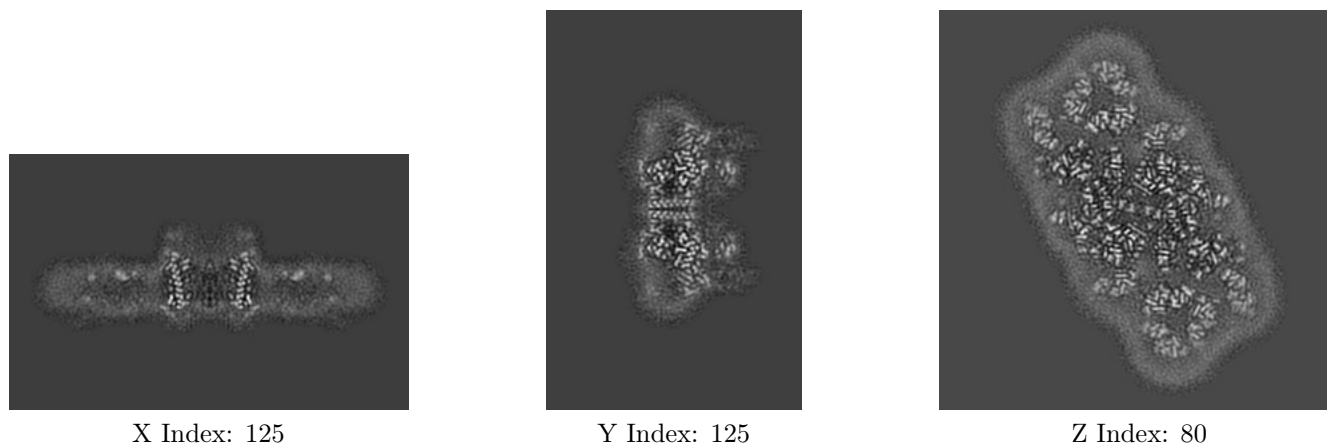
#### 6.1.1 Primary map



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

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

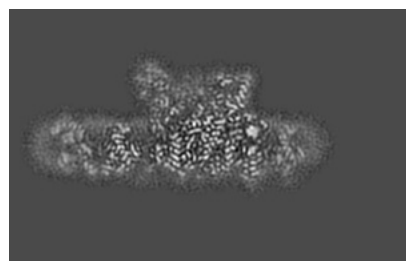
#### 6.2.1 Primary map



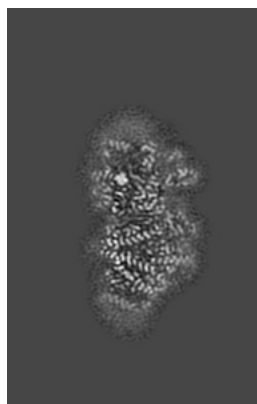
The images above show central slices of the map in three orthogonal directions.

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

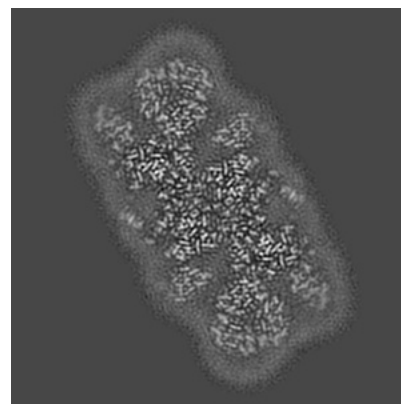
### 6.3.1 Primary map



X Index: 146



Y Index: 147

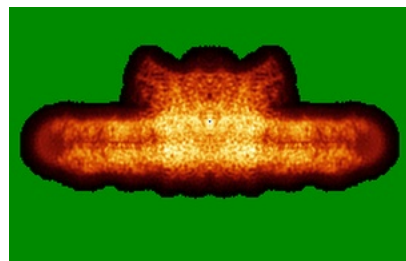


Z Index: 69

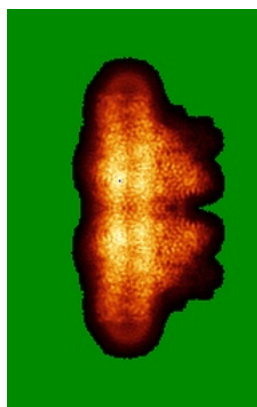
The images above show the largest variance slices of the map in three orthogonal directions.

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

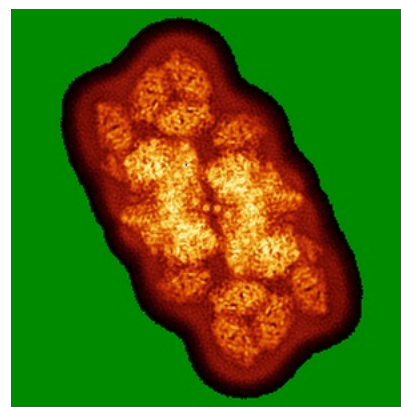
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

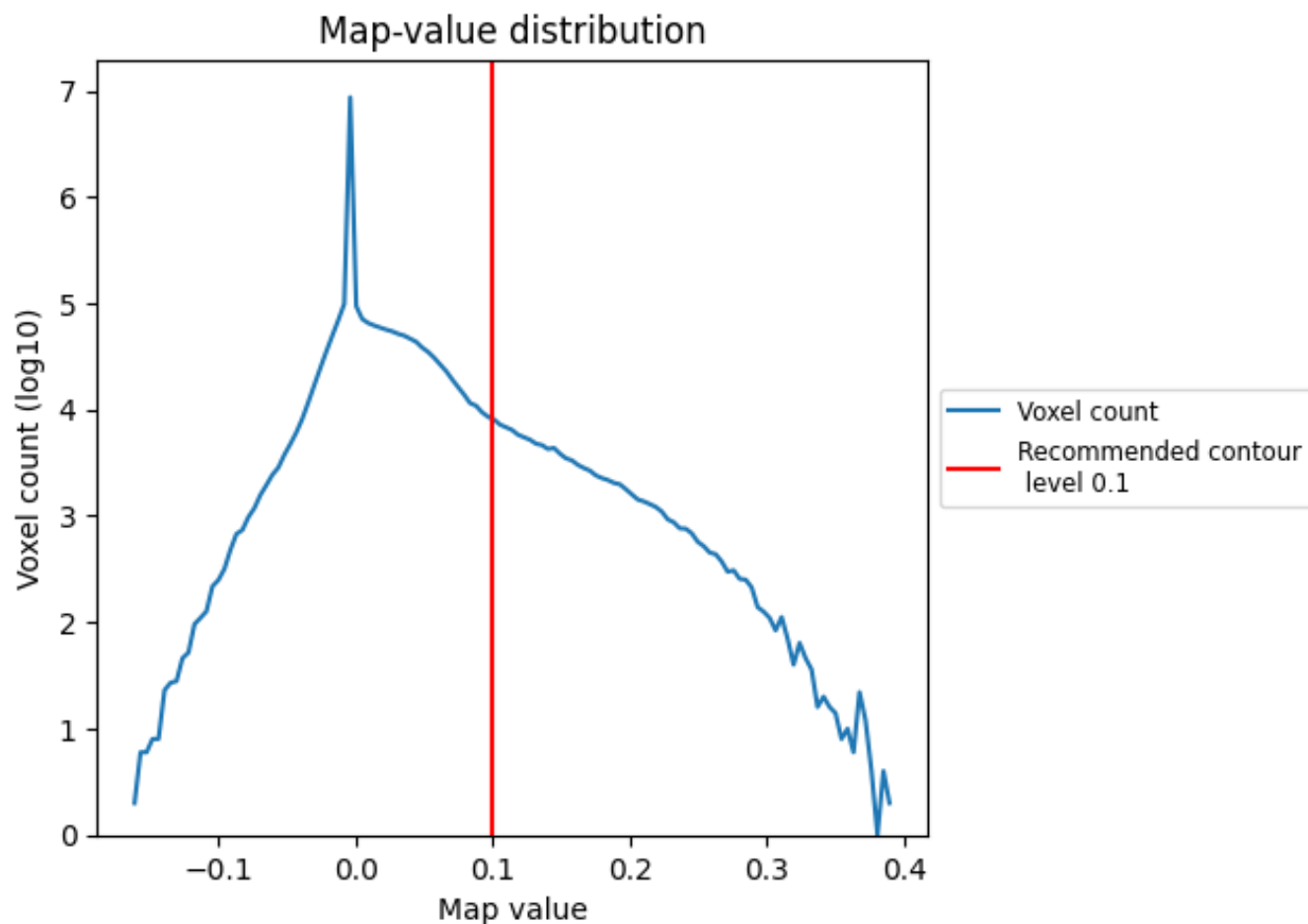
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

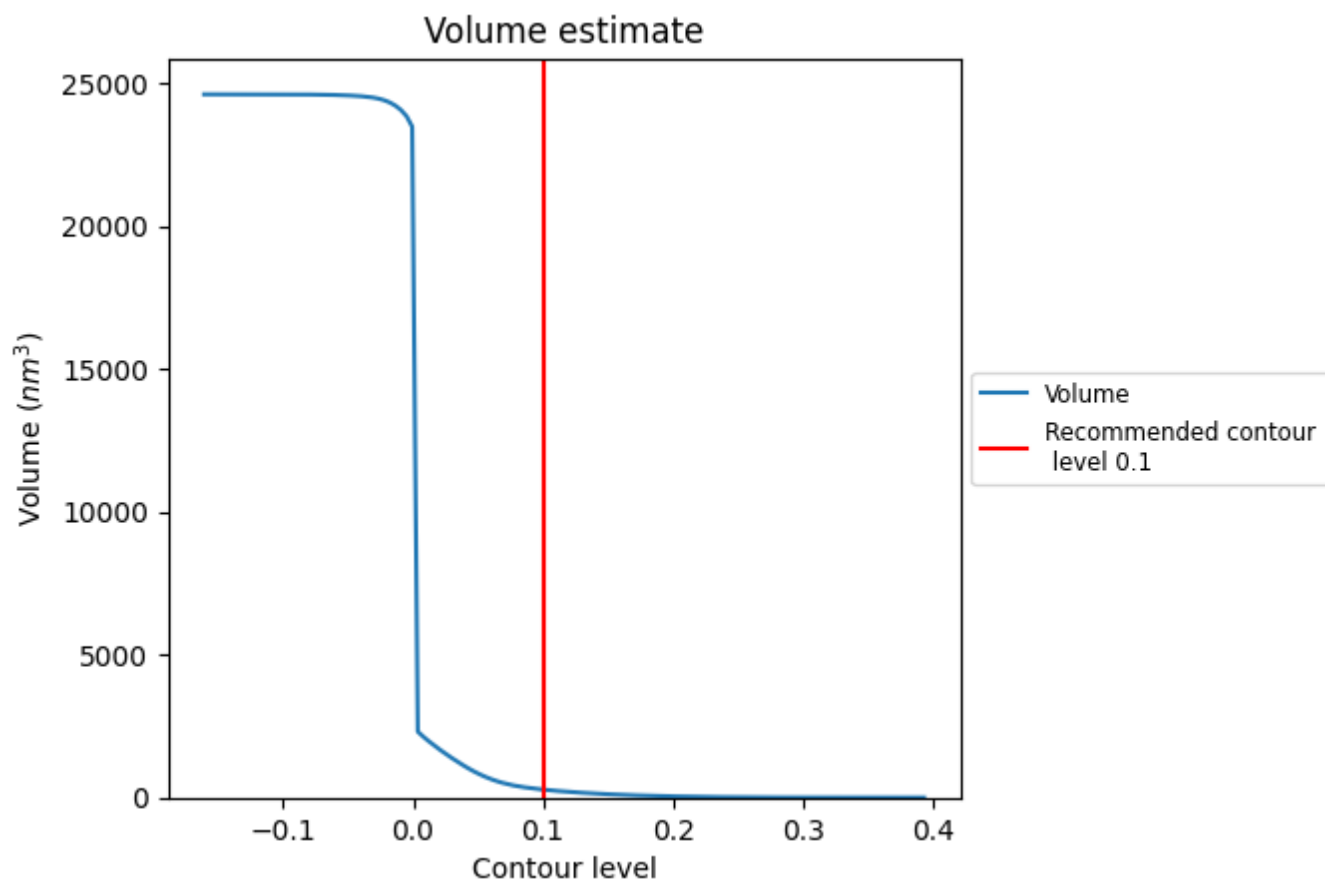
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm<sup>3</sup>; this corresponds to an approximate mass of 252 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation

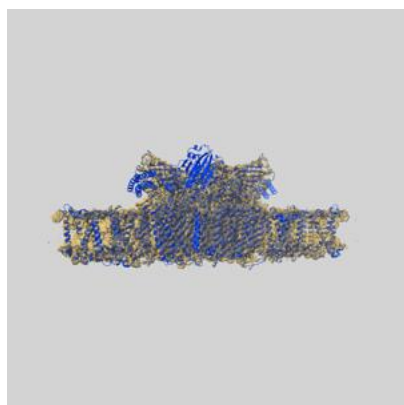
This section was not generated. No FSC curve or half-maps provided.



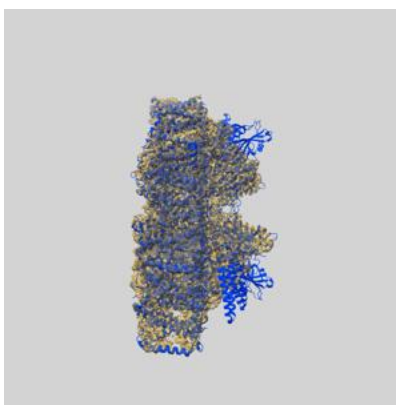
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6617 and PDB model 3JCU. Per-residue inclusion information can be found in section [3](#) on page [39](#).

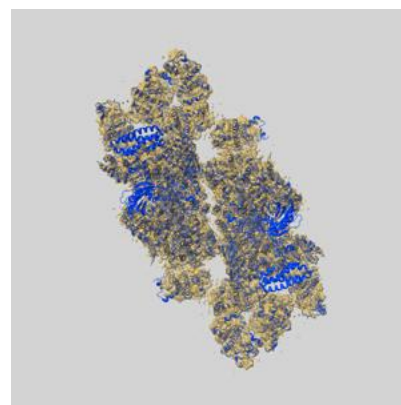
### 9.1 Map-model overlay [i](#)



X



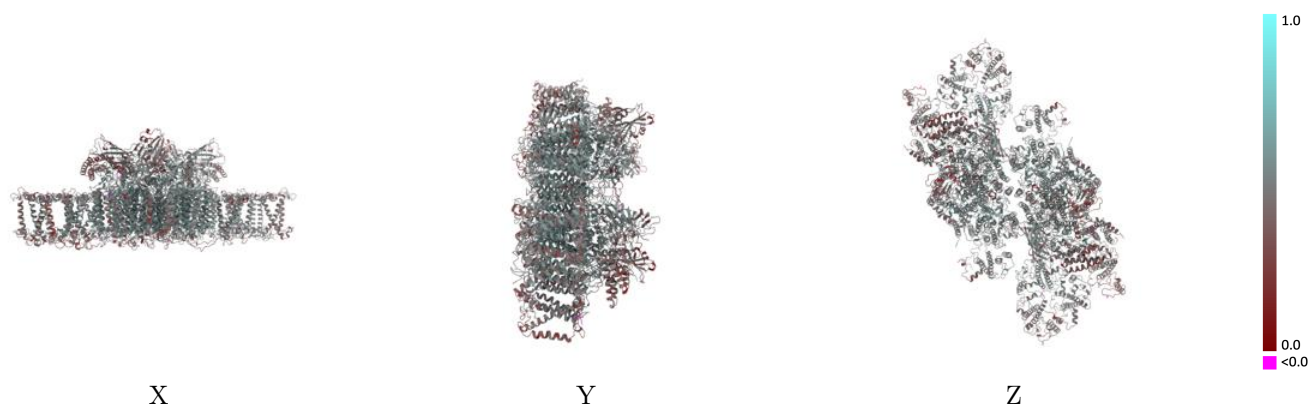
Y



Z

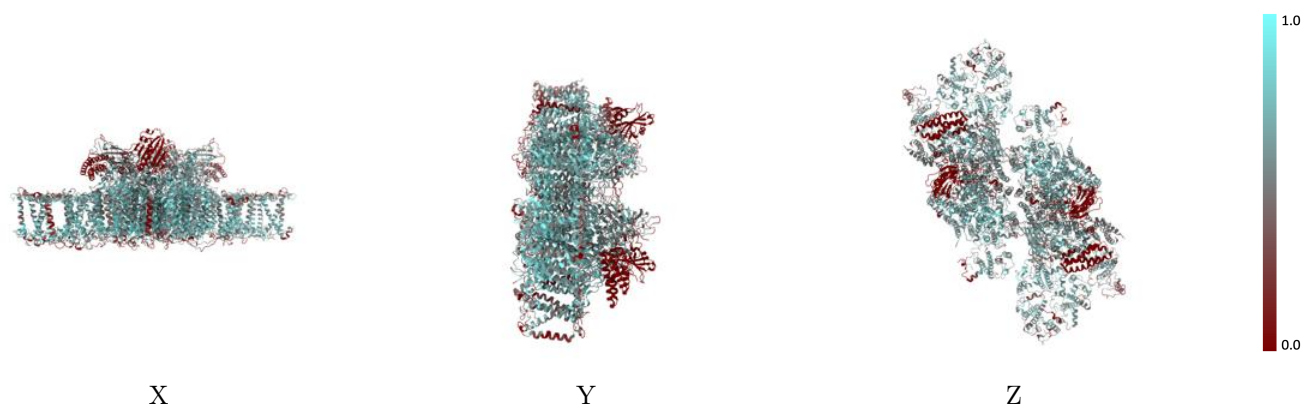
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



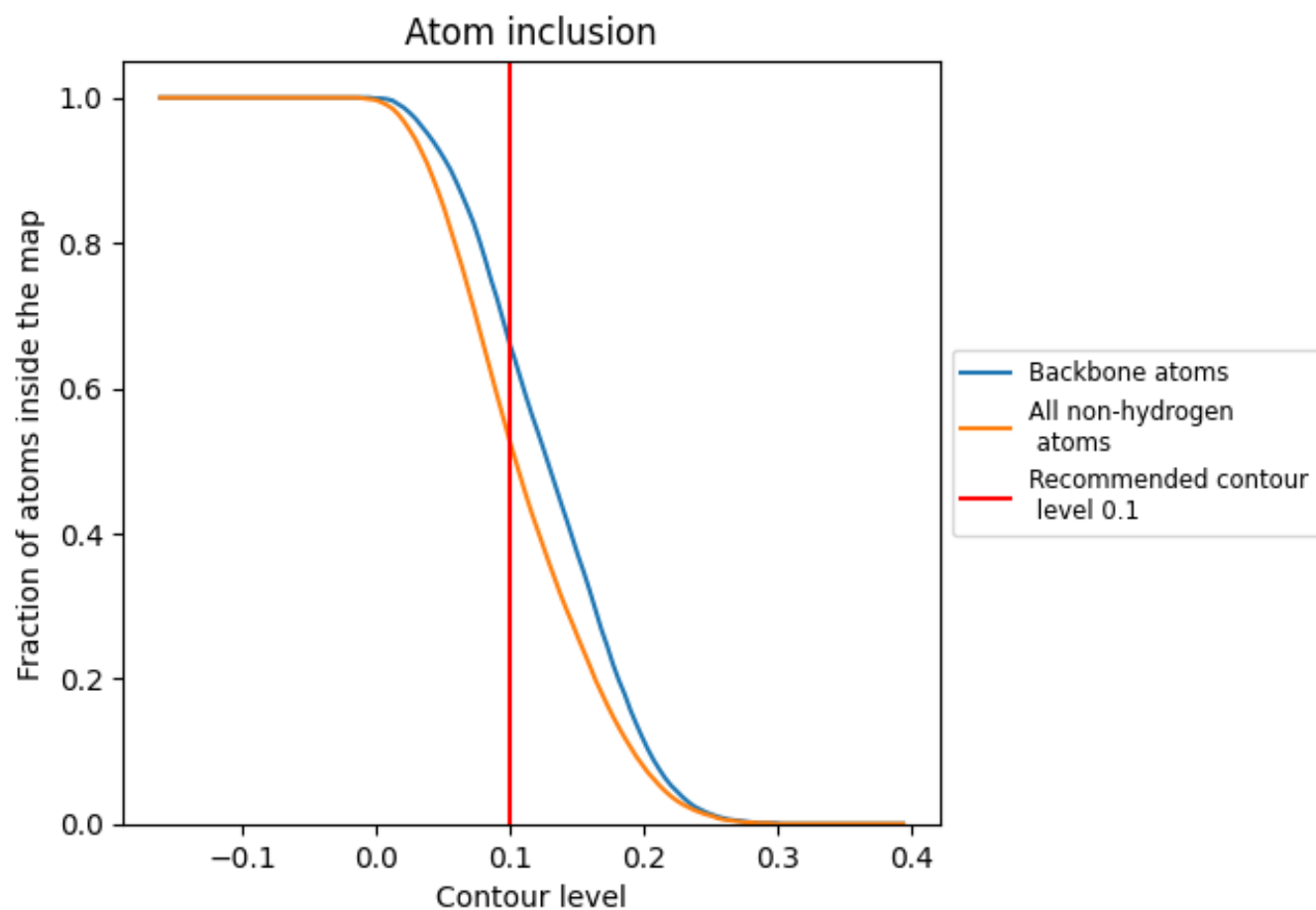
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

































The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.4830
A	 0.6230	 0.5310
B	 0.6540	 0.5350
C	 0.6200	 0.5220
D	 0.6450	 0.5370
E	 0.5350	 0.4210
F	 0.5600	 0.4540
G	 0.5190	 0.4420
H	 0.5950	 0.5320
I	 0.6190	 0.5090
J	 0.1120	 0.3960
K	 0.5580	 0.4630
L	 0.5750	 0.5270
M	 0.4670	 0.4960
N	 0.5450	 0.4720
O	 0.3670	 0.4340
P	 0.0020	 0.3960
Q	 0.0040	 0.3390
R	 0.4520	 0.4510
S	 0.4440	 0.3950
T	 0.5580	 0.5170
U	 0.6310	 0.4660
W	 0.4910	 0.4880
X	 0.4960	 0.4600
Y	 0.6290	 0.5190
Z	 0.3900	 0.4340
a	 0.6240	 0.5310
b	 0.6540	 0.5350
c	 0.6190	 0.5210
d	 0.6450	 0.5360
e	 0.5360	 0.4210
f	 0.5600	 0.4530
g	 0.5170	 0.4440
h	 0.5950	 0.5310
i	 0.6190	 0.5140



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Chain	Atom inclusion	Q-score
j	 0.1120	 0.3980
k	 0.5610	 0.4620
l	 0.5750	 0.5280
m	 0.4670	 0.4950
n	 0.5430	 0.4720
o	 0.3660	 0.4350
p	 0.0020	 0.3950
q	 0.0040	 0.3370
r	 0.4520	 0.4510
s	 0.4440	 0.3940
t	 0.5580	 0.5200
u	 0.6310	 0.4680
w	 0.4940	 0.4870
x	 0.4960	 0.4640
y	 0.6300	 0.5180
z	 0.3900	 0.4340