



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2025 – 12:45 AM JST

PDB ID : 9LK4 / pdb_00009lk4
EMDB ID : EMD-63167
Title : Cryo-EM structure of Lhcb4.1-C2S2 PSII-LHCII supercomplex from *Arabidopsis thaliana*
Authors : Zhou, Q.; Caferri, R.; Shan, J.Y.; Amelii, A.; Bassi, R.; Liu, Z.F.
Deposited on : 2025-01-16
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

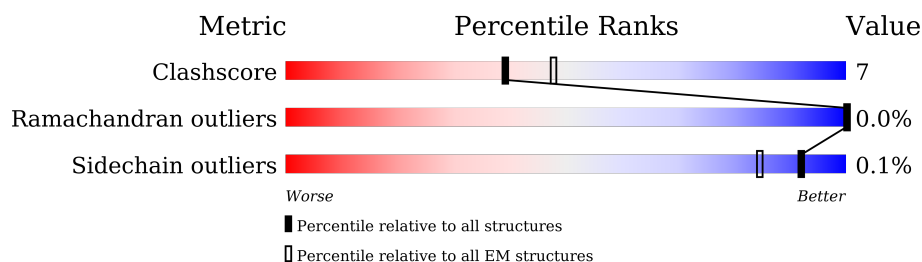
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



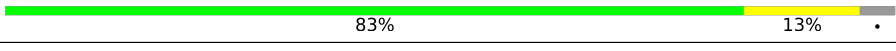

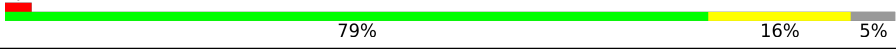



The reported resolution of this entry is 3.10 Å.

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









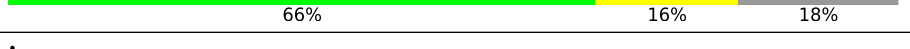
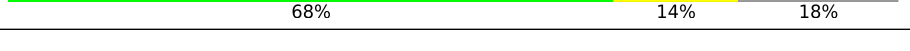
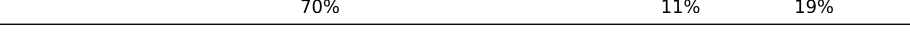
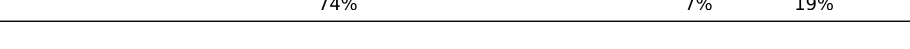
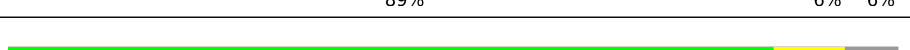

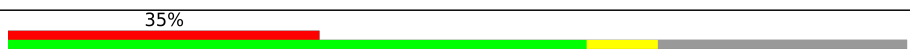
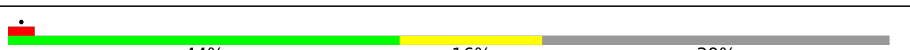
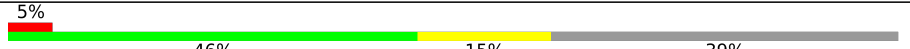
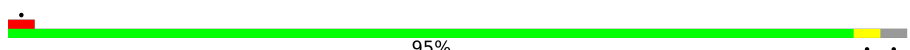





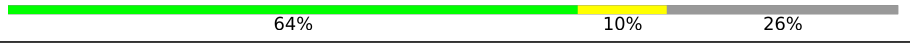



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	353	
1	a	353	
2	B	508	
2	b	508	
3	C	473	
3	c	473	
4	D	353	
4	d	353	

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Mol	Chain	Length	Quality of chain
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	g	267	
7	n	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	61	
11	k	61	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	
14	o	332	
15	R	300	
15	r	300	
16	T	33	

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Mol	Chain	Length	Quality of chain
16	t	33	
17	U	103	
17	u	103	
18	W	133	
18	w	133	
19	X	116	
19	x	116	
20	Y	265	
20	y	265	
21	Z	62	
21	z	62	
22	S	280	
22	s	280	

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
23	CLA	A	401	X	-	-	-
23	CLA	A	402	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	G	602	X	-	-	-
23	CLA	G	603	X	-	-	-
23	CLA	G	604	X	-	-	-
23	CLA	G	610	X	-	-	-
23	CLA	G	611	X	-	-	-
23	CLA	G	612	X	-	-	-
23	CLA	G	613	X	-	-	-
23	CLA	G	614	X	-	-	-
23	CLA	N	303	X	-	-	-
23	CLA	N	304	X	-	-	-
23	CLA	N	305	X	-	-	-
23	CLA	N	311	X	-	-	-
23	CLA	N	312	X	-	-	-
23	CLA	N	313	X	-	-	-
23	CLA	N	314	X	-	-	-
23	CLA	N	315	X	-	-	-
23	CLA	R	601	X	-	-	-
23	CLA	R	602	X	-	-	-
23	CLA	R	603	X	-	-	-
23	CLA	R	604	X	-	-	-
23	CLA	R	608	X	-	-	-
23	CLA	R	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	R	610	X	-	-	-
23	CLA	R	611	X	-	-	-
23	CLA	R	612	X	-	-	-
23	CLA	R	614	X	-	-	-
23	CLA	S	602	X	-	-	-
23	CLA	S	603	X	-	-	-
23	CLA	S	604	X	-	-	-
23	CLA	S	608	X	-	-	-
23	CLA	S	609	X	-	-	-
23	CLA	S	610	X	-	-	-
23	CLA	S	611	X	-	-	-
23	CLA	S	612	X	-	-	-
23	CLA	S	613	X	-	-	-
23	CLA	Y	303	X	-	-	-
23	CLA	Y	304	X	-	-	-
23	CLA	Y	305	X	-	-	-
23	CLA	Y	310	X	-	-	-
23	CLA	Y	311	X	-	-	-
23	CLA	Y	312	X	-	-	-
23	CLA	Y	313	X	-	-	-
23	CLA	Y	314	X	-	-	-
23	CLA	a	401	X	-	-	-
23	CLA	a	402	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-
23	CLA	g	602	X	-	-	-
23	CLA	g	603	X	-	-	-
23	CLA	g	604	X	-	-	-
23	CLA	g	610	X	-	-	-
23	CLA	g	611	X	-	-	-
23	CLA	g	612	X	-	-	-
23	CLA	g	613	X	-	-	-
23	CLA	g	614	X	-	-	-
23	CLA	n	303	X	-	-	-
23	CLA	n	304	X	-	-	-
23	CLA	n	305	X	-	-	-
23	CLA	n	311	X	-	-	-
23	CLA	n	312	X	-	-	-
23	CLA	n	313	X	-	-	-
23	CLA	n	314	X	-	-	-
23	CLA	n	315	X	-	-	-
23	CLA	r	601	X	-	-	-
23	CLA	r	602	X	-	-	-
23	CLA	r	603	X	-	-	-
23	CLA	r	604	X	-	-	-
23	CLA	r	608	X	-	-	-
23	CLA	r	609	X	-	-	-
23	CLA	r	610	X	-	-	-
23	CLA	r	611	X	-	-	-
23	CLA	r	612	X	-	-	-
23	CLA	r	614	X	-	-	-
23	CLA	s	602	X	-	-	-
23	CLA	s	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	s	604	X	-	-	-
23	CLA	s	608	X	-	-	-
23	CLA	s	609	X	-	-	-
23	CLA	s	610	X	-	-	-
23	CLA	s	611	X	-	-	-
23	CLA	s	612	X	-	-	-
23	CLA	s	613	X	-	-	-
23	CLA	y	303	X	-	-	-
23	CLA	y	304	X	-	-	-
23	CLA	y	305	X	-	-	-
23	CLA	y	310	X	-	-	-
23	CLA	y	311	X	-	-	-
23	CLA	y	312	X	-	-	-
23	CLA	y	313	X	-	-	-
23	CLA	y	314	X	-	-	-
31	BCT	D	403	-	-	X	-
31	BCT	d	403	-	-	X	-
34	CHL	G	601	X	-	-	-
34	CHL	G	605	X	-	-	-
34	CHL	G	606	X	-	-	-
34	CHL	G	607	X	-	-	-
34	CHL	G	608	X	-	-	-
34	CHL	G	609	X	-	-	-
34	CHL	G	619	X	-	-	-
34	CHL	N	302	X	-	-	-
34	CHL	N	306	X	-	-	-
34	CHL	N	307	X	-	-	-
34	CHL	N	308	X	-	-	-
34	CHL	N	309	X	-	-	-
34	CHL	N	310	X	-	-	-
34	CHL	R	605	X	-	-	-
34	CHL	R	606	X	-	-	-
34	CHL	R	607	X	-	-	-
34	CHL	R	613	X	-	-	-
34	CHL	S	601	X	-	-	-
34	CHL	S	605	X	-	-	-
34	CHL	S	606	X	-	-	-
34	CHL	S	607	X	-	-	-
34	CHL	Y	302	X	-	-	-
34	CHL	Y	306	X	-	-	-
34	CHL	Y	307	X	-	-	-
34	CHL	Y	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	CHL	Y	309	X	-	-	-
34	CHL	g	601	X	-	-	-
34	CHL	g	605	X	-	-	-
34	CHL	g	606	X	-	-	-
34	CHL	g	607	X	-	-	-
34	CHL	g	608	X	-	-	-
34	CHL	g	609	X	-	-	-
34	CHL	g	619	X	-	-	-
34	CHL	n	302	X	-	-	-
34	CHL	n	306	X	-	-	-
34	CHL	n	307	X	-	-	-
34	CHL	n	308	X	-	-	-
34	CHL	n	309	X	-	-	-
34	CHL	n	310	X	-	-	-
34	CHL	r	605	X	-	-	-
34	CHL	r	606	X	-	-	-
34	CHL	r	607	X	-	-	-
34	CHL	r	613	X	-	-	-
34	CHL	s	601	X	-	-	-
34	CHL	s	605	X	-	-	-
34	CHL	s	606	X	-	-	-
34	CHL	s	607	X	-	-	-
34	CHL	y	302	X	-	-	-
34	CHL	y	306	X	-	-	-
34	CHL	y	307	X	-	-	-
34	CHL	y	308	X	-	-	-
34	CHL	y	309	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 70366 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	332	Total	C	N	O	S	0	0
			2599	1696	428	462	13		
1	a	332	Total	C	N	O	S	0	0
			2599	1696	428	462	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		
2	b	489	Total	C	N	O	S	0	0
			3829	2506	647	664	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
			3480	2285	582	602	11		
3	c	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		
4	d	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	66	Total	C	N	O	0	0
			540	354	88	98		
5	e	66	Total	C	N	O	0	0
			540	354	88	98		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			224	150	37	36	1		
6	f	29	Total	C	N	O	S	0	0
			224	150	37	36	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
7	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

- 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
			438	289	68	79	2		
8	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			277	190	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	29	Total	C	N	O	0	0
			219	152	33	34		
10	j	29	Total	C	N	O	0	0
			219	152	33	34		

- 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
			301	211	44	45	1		
11	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			309	204	48	57		
12	l	37	Total	C	N	O	0	0
			309	204	48	57		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			250	172	36	42		
13	m	32	Total	C	N	O	0	0
			250	172	36	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		
14	o	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	222	Total	C	N	O	S	0	0
			1724	1118	283	320	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	222	Total	C	N	O	S	0	0
			1724	1118	283	320	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	291	GLY	-	expression tag	UNP Q07473
R	292	GLY	-	expression tag	UNP Q07473
R	293	GLY	-	expression tag	UNP Q07473
R	294	GLY	-	expression tag	UNP Q07473
R	295	HIS	-	expression tag	UNP Q07473
R	296	HIS	-	expression tag	UNP Q07473
R	297	HIS	-	expression tag	UNP Q07473
R	298	HIS	-	expression tag	UNP Q07473
R	299	HIS	-	expression tag	UNP Q07473
R	300	HIS	-	expression tag	UNP Q07473
r	291	GLY	-	expression tag	UNP Q07473
r	292	GLY	-	expression tag	UNP Q07473
r	293	GLY	-	expression tag	UNP Q07473
r	294	GLY	-	expression tag	UNP Q07473
r	295	HIS	-	expression tag	UNP Q07473
r	296	HIS	-	expression tag	UNP Q07473
r	297	HIS	-	expression tag	UNP Q07473
r	298	HIS	-	expression tag	UNP Q07473
r	299	HIS	-	expression tag	UNP Q07473
r	300	HIS	-	expression tag	UNP Q07473

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	23	Total	C	N	O	S	0	0
			179	114	31	31	3		
17	u	23	Total	C	N	O	S	0	0
			179	114	31	31	3		

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
18	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 19 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total	C	N	O		0	0
			267	176	42	49			
19	x	38	Total	C	N	O		0	0
			267	176	42	49			

- Molecule 20 is a protein called Chlorophyll a-b binding protein 2.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		
20	y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		

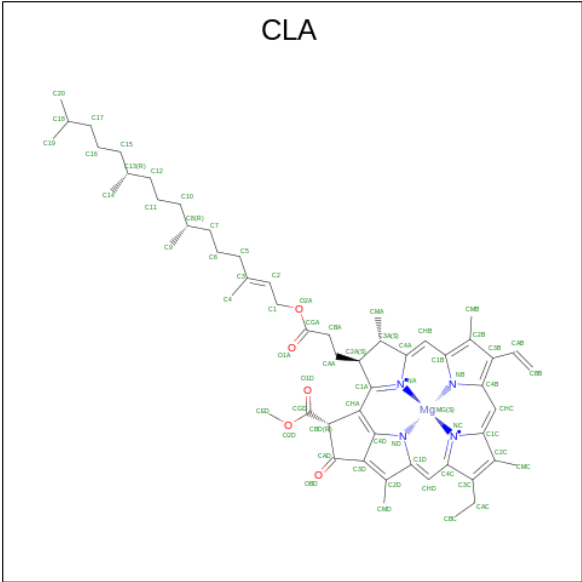
- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
21	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

- Molecule 22 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		
22	s	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	C	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	N	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	R	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	Y	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	c	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	g	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	n	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	n	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	n	1	Total 60	C 50	Mg 1	N 4	O 5	0

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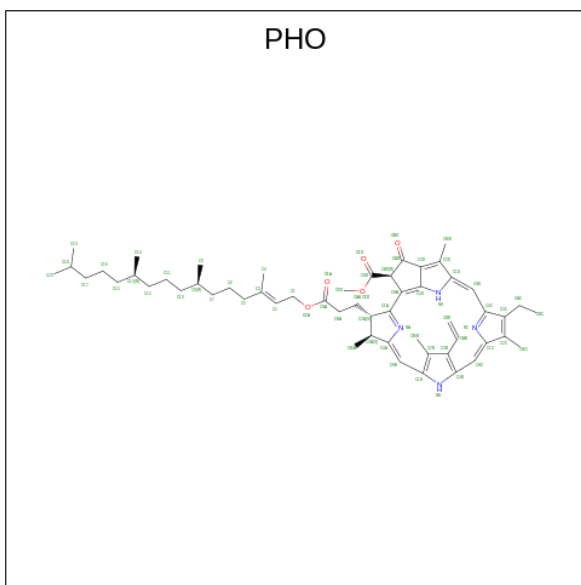
Mol	Chain	Residues	Atoms					AltConf
23	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	r	1	Total 48	C 38	Mg 1	N 4	O 5	0
23	r	1	Total 58	C 48	Mg 1	N 4	O 5	0
23	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	r	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	y	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	S	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

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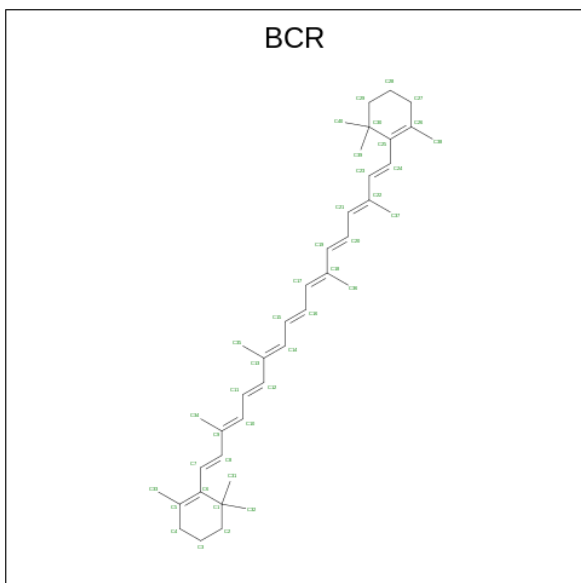
Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



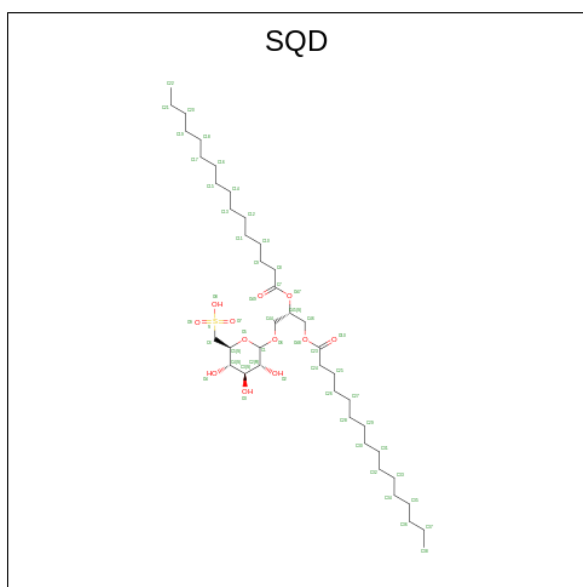
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



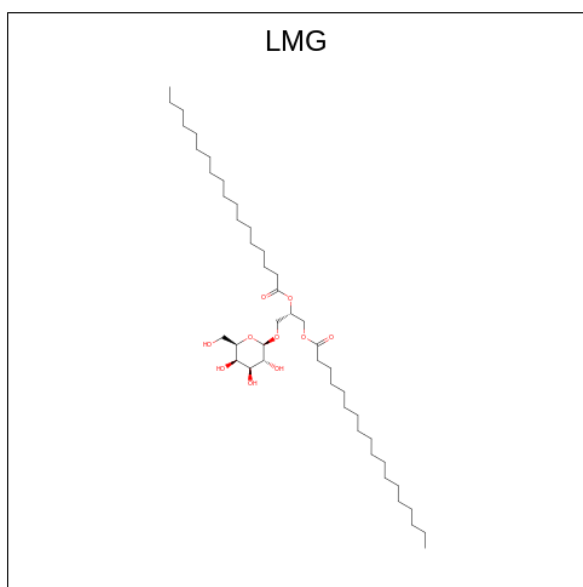
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	Z	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



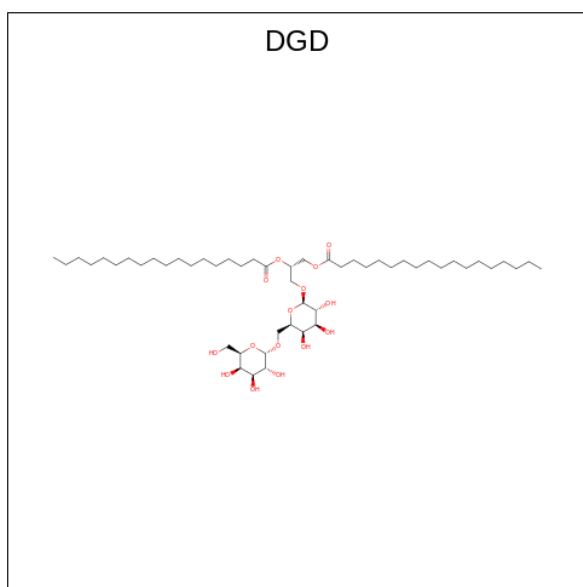
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	M	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			54	41	12	1	
26	d	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			40	30	10	
27	B	1	Total	C	O	0
			51	41	10	
27	B	1	Total	C	O	0
			40	30	10	
27	C	1	Total	C	O	0
			48	38	10	
27	D	1	Total	C	O	0
			46	36	10	
27	a	1	Total	C	O	0
			48	38	10	
27	b	1	Total	C	O	0
			51	41	10	
27	d	1	Total	C	O	0
			46	36	10	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

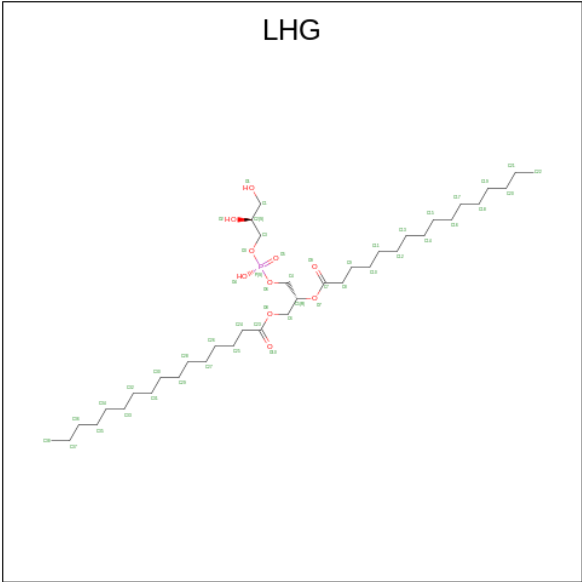


Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			59	44	15	
28	C	1	Total	C	O	0
			55	40	15	
28	H	1	Total	C	O	0
			62	47	15	
28	a	1	Total	C	O	0
			59	44	15	
28	c	1	Total	C	O	0
			55	40	15	
28	d	1	Total	C	O	0
			62	47	15	

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



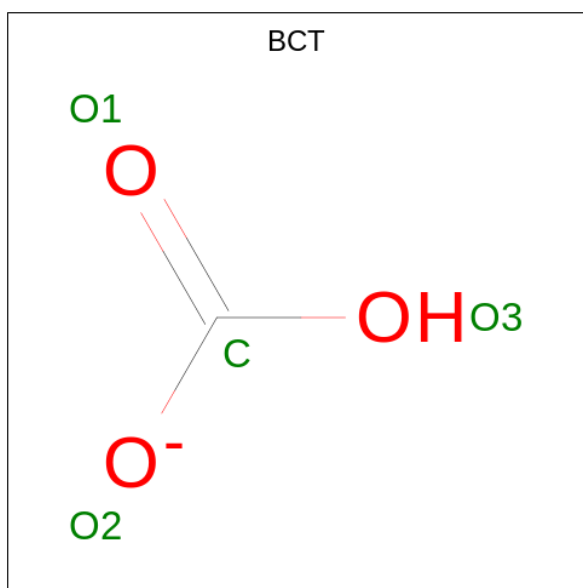
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			46	35	10	1	
30	A	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	C	1	Total	C	O	P	0
			49	38	10	1	
30	G	1	Total	C	O	P	0
			46	35	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	T	1	Total	C	O	P	0
			49	38	10	1	
30	W	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	a	1	Total	C	O	P	0
			46	35	10	1	

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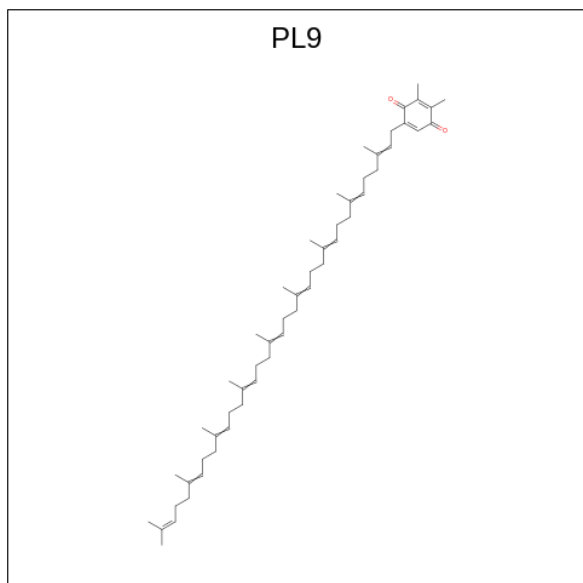
Mol	Chain	Residues	Atoms				AltConf
30	a	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	b	1	Total	C	O	P	0
			49	38	10	1	
30	c	1	Total	C	O	P	0
			49	38	10	1	
30	d	1	Total	C	O	P	0
			49	38	10	1	
30	g	1	Total	C	O	P	0
			46	35	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	w	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



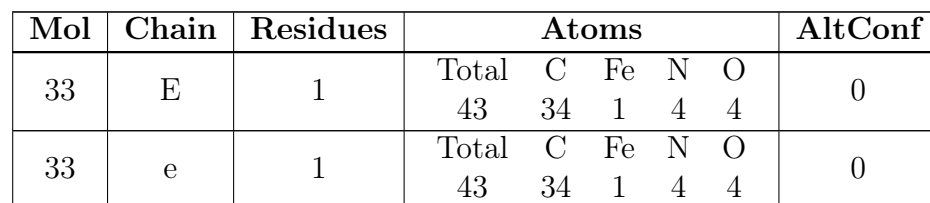
Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	0
			4	1	3	
31	d	1	Total	C	O	0
			4	1	3	

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



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # CHL

Mol	Chain	Residues	Atoms					AltConf
34	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
34	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	G	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
34	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	Y	1	Total 51	C 40	Mg 1	N 4	O 6	0
34	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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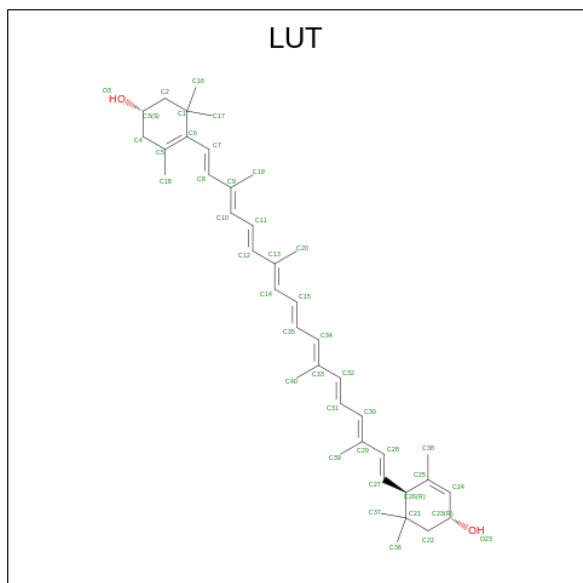
Mol	Chain	Residues	Atoms					AltConf
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	g	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	g	1	Total 43	C 34	Mg 1	N 4	O 4	0
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	g	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
34	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
34	r	1	Total 61	C 50	Mg 1	N 4	O 6	0
34	r	1	Total 42	C 33	Mg 1	N 4	O 4	0
34	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
34	y	1	Total 51	C 40	Mg 1	N 4	O 6	0
34	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
34	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
34	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
34	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
34	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
34	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
34	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
34	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
34	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
34	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
34	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



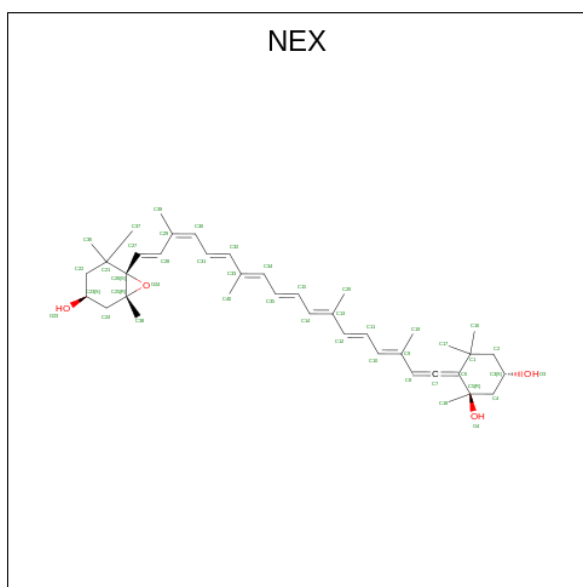
Mol	Chain	Residues	Atoms				AltConf
35	G	1	Total	C	O		0
			42	40	2		

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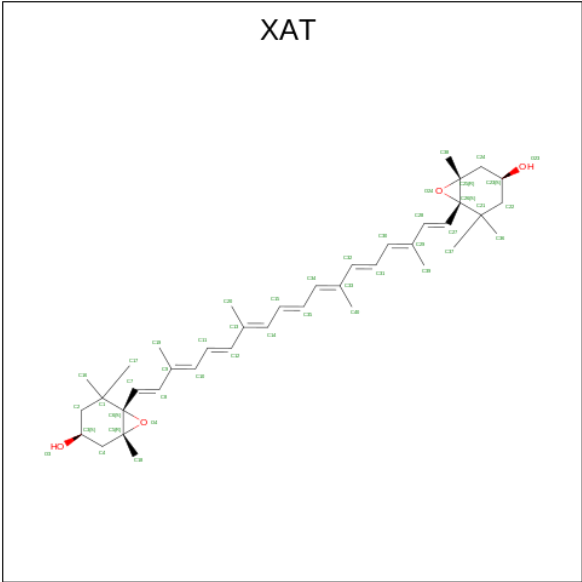
Mol	Chain	Residues	Atoms			AltConf
35	G	1	Total	C	O	0
			42	40	2	
35	N	1	Total	C	O	0
			42	40	2	
35	N	1	Total	C	O	0
			42	40	2	
35	R	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	g	1	Total	C	O	0
			42	40	2	
35	g	1	Total	C	O	0
			42	40	2	
35	n	1	Total	C	O	0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

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 37 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

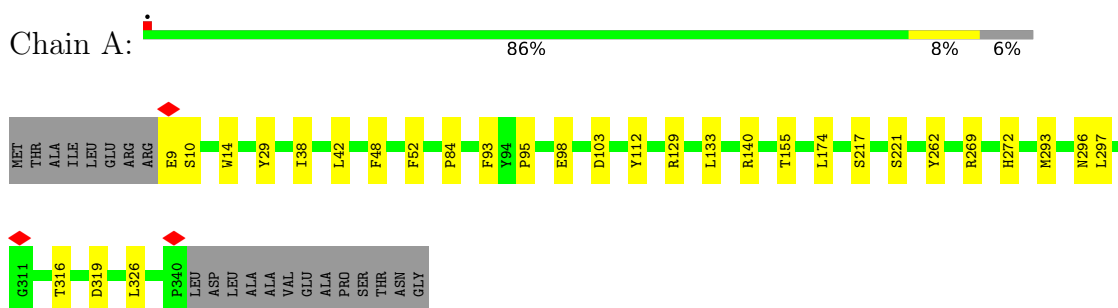


Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	40	4	
37	N	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	
37	Y	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	n	1	Total	C	O	0
			44	40	4	
37	r	1	Total	C	O	0
			44	40	4	
37	y	1	Total	C	O	0
			44	40	4	

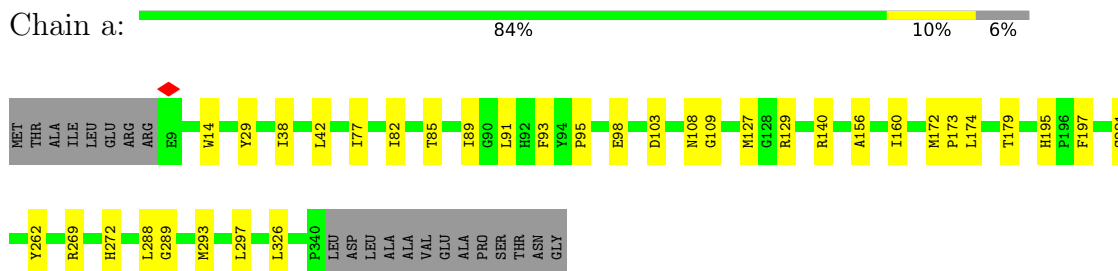
3 Residue-property plots [i](#)

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.

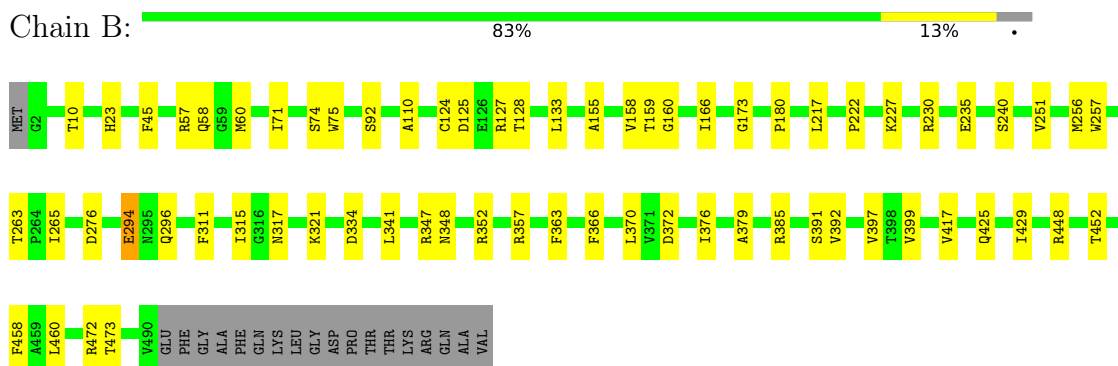
- Molecule 1: Photosystem II protein D1




- Molecule 1: Photosystem II protein D1

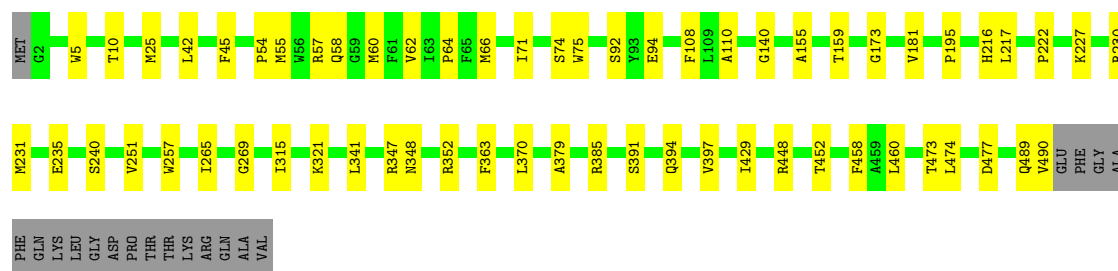


- Molecule 2: Photosystem II CP47 reaction center protein




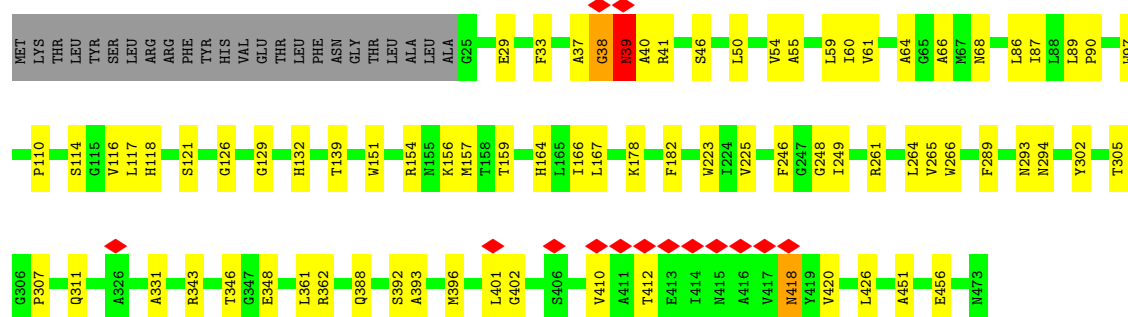
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  84% 12% .




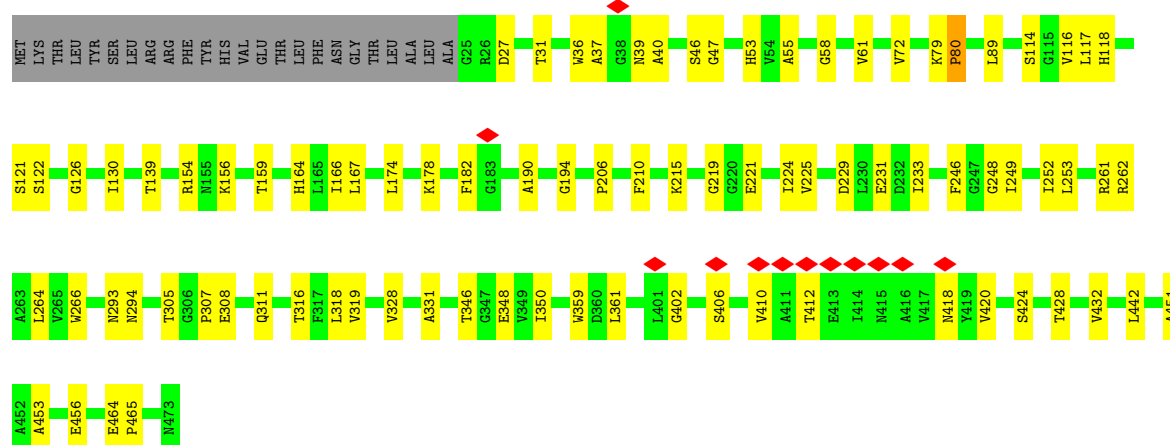
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  79% 16% 5%




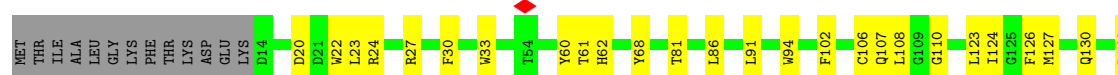
• Molecule 3: Photosystem II CP43 reaction center protein

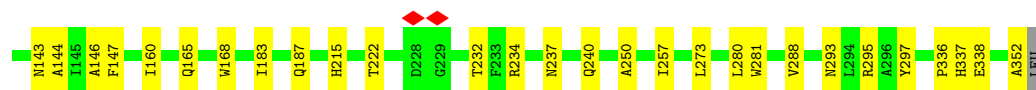
Chain c:  77% 18% 5%



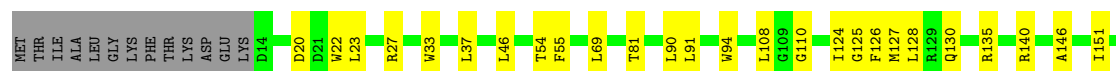
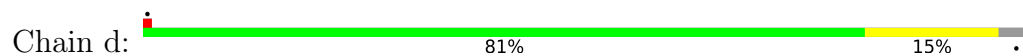
• Molecule 4: Photosystem II D2 protein

Chain D:  81% 15% .





• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha



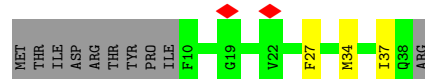
• Molecule 5: Cytochrome b559 subunit alpha



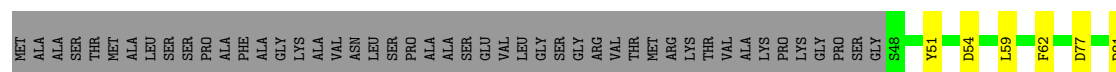
• Molecule 6: Cytochrome b559 subunit beta

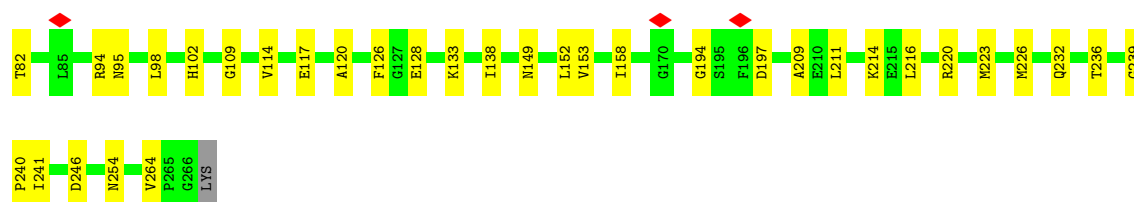


• Molecule 6: Cytochrome b559 subunit beta



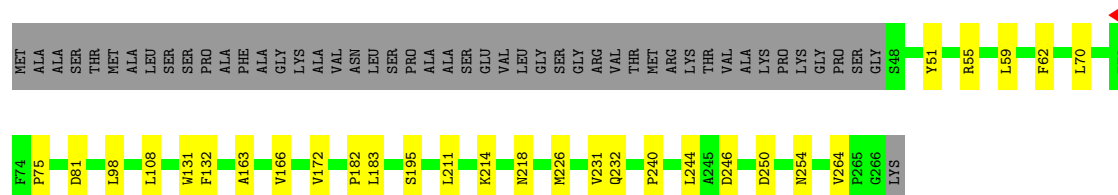
• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic





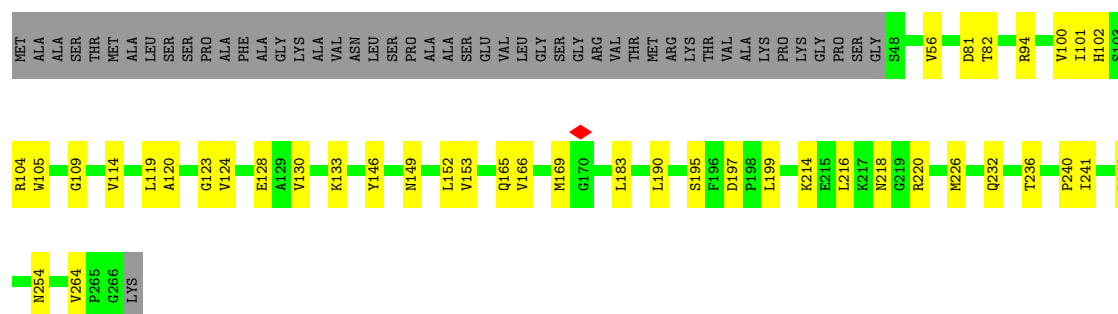
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain N: 71% 11% 18%



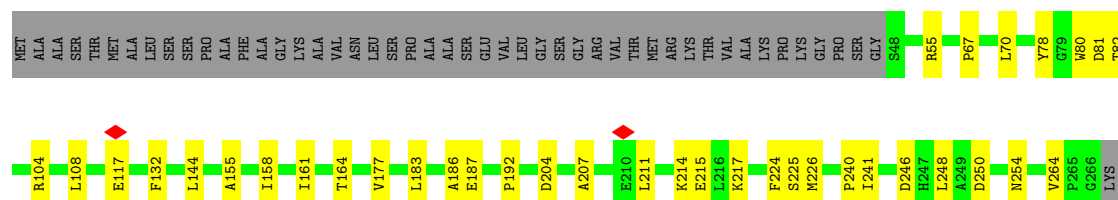
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain g: 66% 16% 18%



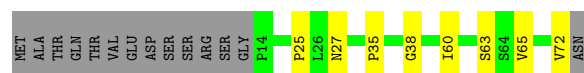
- Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain n: 68% 14% 18%



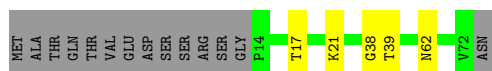
- Molecule 8: Photosystem II reaction center protein H

Chain H: 70% 11% 19%




- Molecule 8: Photosystem II reaction center protein H

Chain h:  74% 7% 19%




• Molecule 9: Photosystem II reaction center protein I

Chain I:  89% 6% 6%




• Molecule 9: Photosystem II reaction center protein I

Chain i:  86% 8% 6%



• Molecule 10: Photosystem II reaction center protein J

Chain J:  40% 68% 5% 28%



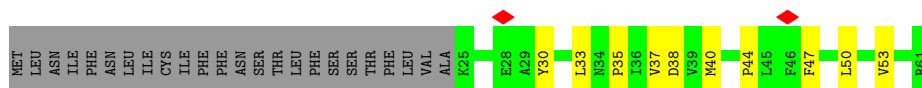
• Molecule 10: Photosystem II reaction center protein J

Chain j:  35% 65% 8% 28%



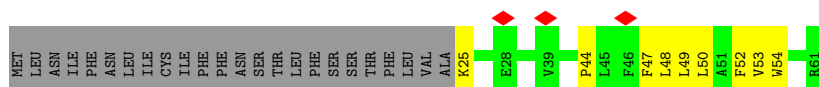
• Molecule 11: Photosystem II reaction center protein K

Chain K:  44% 16% 39%



• Molecule 11: Photosystem II reaction center protein K

Chain k:  5% 46% 15% 39%




- Molecule 12: Photosystem II reaction center protein L

Chain L:  95%




- Molecule 12: Photosystem II reaction center protein L

Chain l:  84% 13%




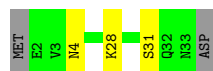
- Molecule 13: Photosystem II reaction center protein M

Chain M:  82% 12% 6%



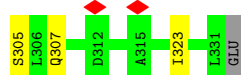
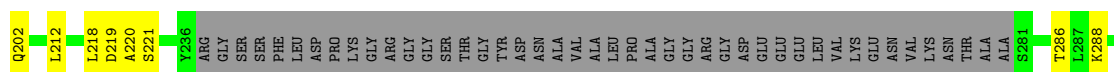
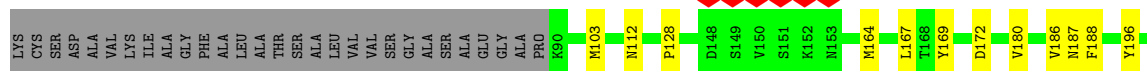
- Molecule 13: Photosystem II reaction center protein M

Chain m:  85% 9% 6%



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

Chain O:  53% 7% 40%

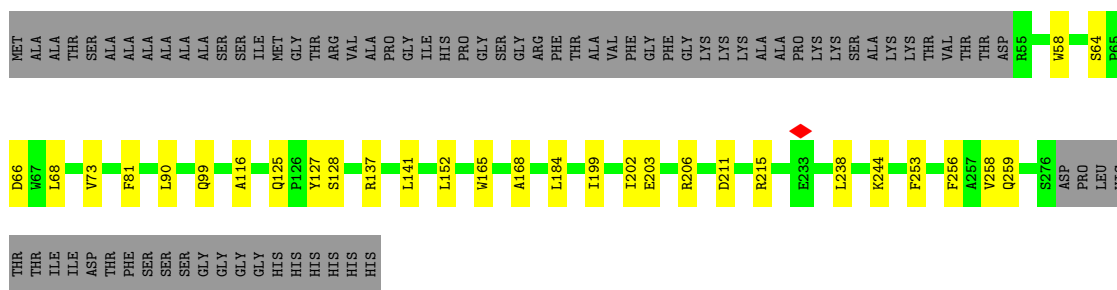


- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

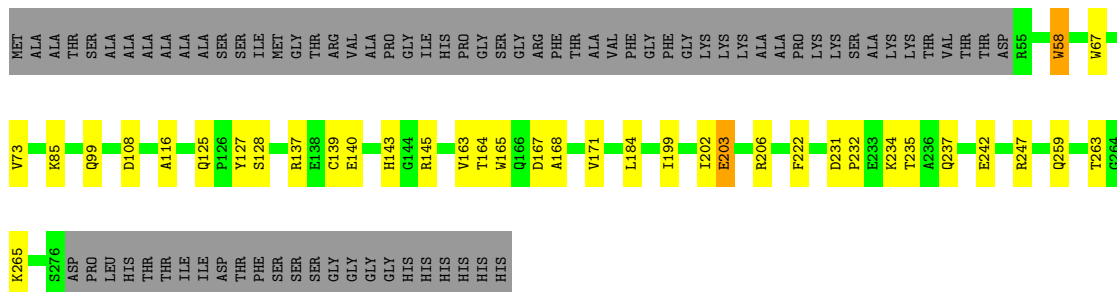
Chain o:  53% 7% 40%



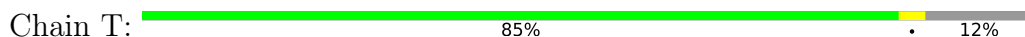
- Molecule 15: Chlorophyll a-b binding protein CP29.1, chloroplastic



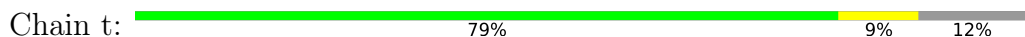
- Molecule 15: Chlorophyll a-b binding protein CP29.1, chloroplastic

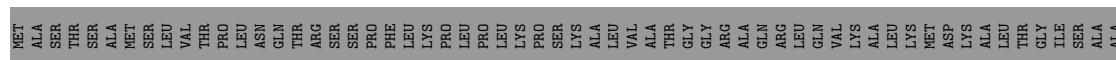


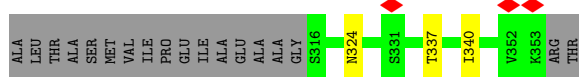
- Molecule 16: Photosystem II reaction center protein T



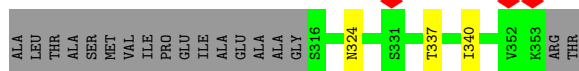
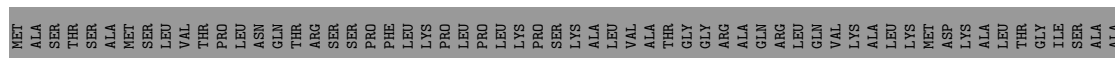
- Molecule 16: Photosystem II reaction center protein T



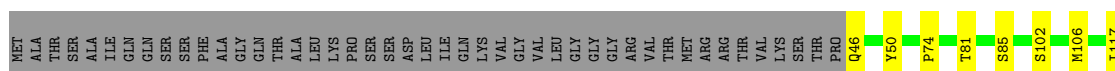




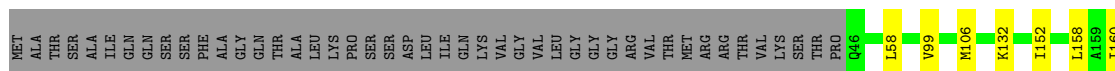
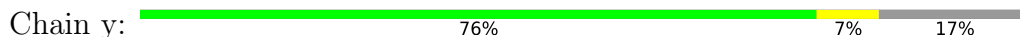
- Molecule 19: (thale cress) hypothetical protein



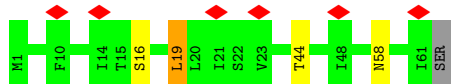
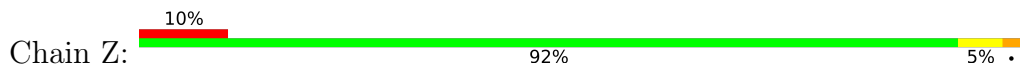
- Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic



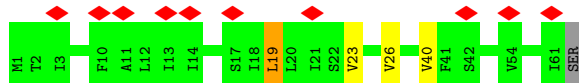
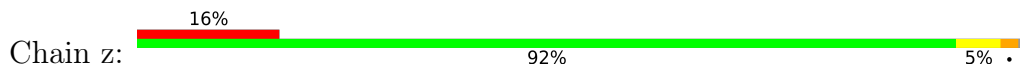
- Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic



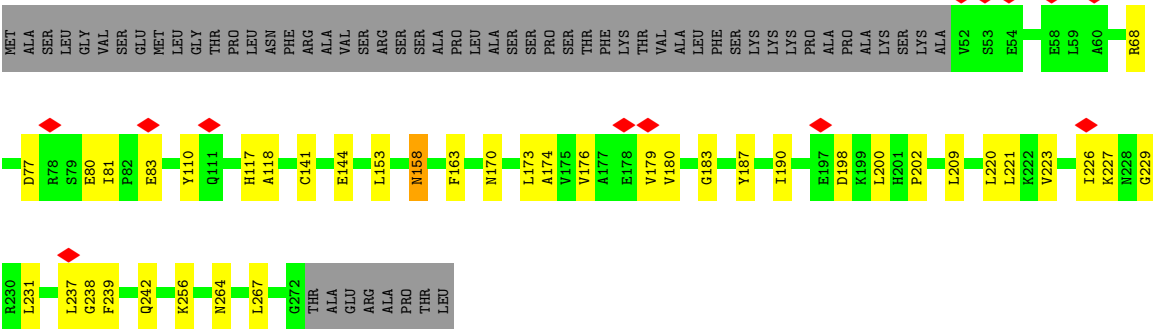
- Molecule 21: Photosystem II reaction center protein Z



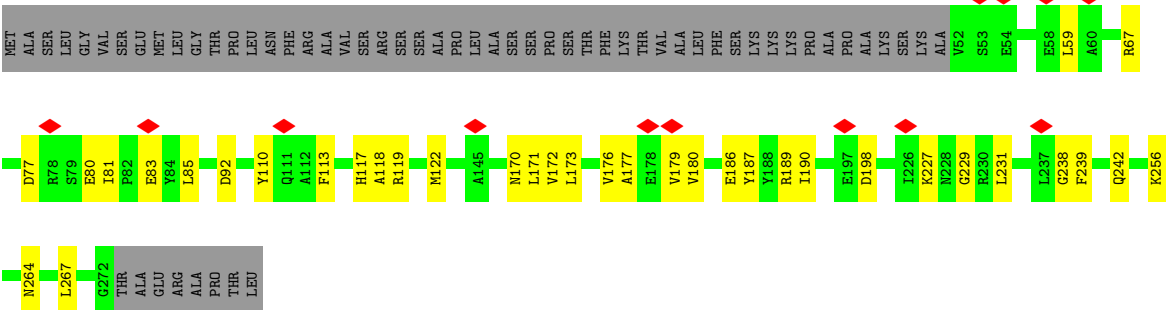
- Molecule 21: Photosystem II reaction center protein Z



- Molecule 22: Chlorophyll a-b binding protein CP26, chloroplastic



● Molecule 22: Chlorophyll a-b binding protein CP26, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67864	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	37.376	Depositor
Minimum map value	-22.323	Depositor
Average map value	0.013	Depositor
Map value standard deviation	1.095	Depositor
Recommended contour level	3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.36	0/2680	0.65	0/3654
1	a	0.38	0/2680	0.69	1/3654 (0.0%)
2	B	0.35	0/3959	0.58	2/5394 (0.0%)
2	b	0.33	0/3959	0.57	0/5394
3	C	0.35	0/3595	0.73	2/4899 (0.0%)
3	c	0.34	0/3595	0.71	1/4899 (0.0%)
4	D	0.35	0/2789	0.61	0/3803
4	d	0.35	0/2789	0.64	0/3803
5	E	0.37	1/557 (0.2%)	0.71	0/758
5	e	0.38	1/557 (0.2%)	0.75	0/758
6	F	0.31	0/230	0.68	0/313
6	f	0.29	0/230	0.66	0/313
7	G	0.32	0/1716	0.64	0/2336
7	N	0.33	0/1716	0.70	1/2336 (0.0%)
7	g	0.33	0/1716	0.67	0/2336
7	n	0.33	0/1716	0.67	0/2336
8	H	0.34	0/447	0.67	0/608
8	h	0.33	0/447	0.60	0/608
9	I	0.38	0/285	0.74	0/385
9	i	0.38	0/285	0.80	0/385
10	J	0.26	0/225	0.48	0/306
10	j	0.32	0/225	0.58	0/306
11	K	0.40	0/312	0.87	0/428
11	k	0.37	0/312	0.84	0/428
12	L	0.31	0/317	0.55	0/431
12	l	0.28	0/317	0.53	0/431
13	M	0.30	0/254	0.61	0/348
13	m	0.30	0/254	0.65	0/348
14	O	0.26	0/1556	0.63	2/2104 (0.1%)
14	o	0.27	0/1556	0.63	0/2104
15	R	0.29	0/1772	0.60	0/2414
15	r	0.27	0/1772	0.65	1/2414 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	T	0.28	0/246	0.59	0/333
16	t	0.28	0/246	0.58	0/333
17	U	0.22	0/181	0.57	0/242
17	u	0.18	0/181	0.45	0/242
18	W	0.28	0/438	0.57	0/594
18	w	0.28	0/438	0.55	0/594
19	X	0.28	0/270	0.63	0/367
19	x	0.28	0/270	0.59	0/367
20	Y	0.31	0/1753	0.64	2/2385 (0.1%)
20	y	0.29	0/1753	0.59	0/2385
21	Z	0.28	0/468	0.67	2/641 (0.3%)
21	z	0.31	0/468	0.70	2/641 (0.3%)
22	S	0.35	0/1750	0.77	2/2376 (0.1%)
22	s	0.32	0/1750	0.73	3/2376 (0.1%)
All	All	0.33	2/55032 (0.0%)	0.66	21/74910 (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
3	C	0	1
3	c	0	1
15	R	0	1
15	r	0	1
22	S	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	27	ILE	C-N	6.30	1.40	1.34
5	E	27	ILE	C-N	5.79	1.39	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	r	203	GLU	CA-CB-CG	6.87	127.83	114.10
7	N	232	GLN	CA-CB-CG	6.59	127.28	114.10
3	c	224	ILE	N-CA-C	-6.57	106.72	113.10
1	a	179	THR	CA-CB-OG1	6.47	119.31	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	38	GLY	CA-C-N	-6.32	111.69	122.56

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	39	ASN	Peptide
15	R	58	TRP	Peptide
22	S	200	LEU	Peptide
3	c	80	PRO	Peptide
15	r	58	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2599	0	2501	30	0
1	a	2599	0	2501	30	0
2	B	3829	0	3707	45	0
2	b	3829	0	3707	41	0
3	C	3480	0	3409	62	0
3	c	3480	0	3409	65	0
4	D	2696	0	2585	42	0
4	d	2696	0	2585	44	0
5	E	540	0	521	7	0
5	e	540	0	521	10	0
6	F	224	0	229	5	0
6	f	224	0	229	5	0
7	G	1666	0	1593	31	0
7	N	1666	0	1593	26	0
7	g	1666	0	1593	35	0
7	n	1666	0	1593	27	0
8	H	438	0	465	7	0
8	h	438	0	465	4	0
9	I	277	0	289	2	0
9	i	277	0	289	3	0
10	J	219	0	231	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	j	219	0	231	2	0
11	K	301	0	313	6	0
11	k	301	0	313	6	0
12	L	309	0	298	1	0
12	l	309	0	298	4	0
13	M	250	0	273	4	0
13	m	250	0	273	3	0
14	O	1523	0	1504	16	0
14	o	1523	0	1504	15	0
15	R	1724	0	1684	25	0
15	r	1724	0	1684	30	0
16	T	239	0	255	1	0
16	t	239	0	255	3	0
17	U	179	0	190	4	0
17	u	179	0	190	2	0
18	W	427	0	405	8	0
18	w	427	0	405	7	0
19	X	267	0	292	2	0
19	x	267	0	292	2	0
20	Y	1699	0	1630	21	0
20	y	1699	0	1630	14	0
21	Z	458	0	490	3	0
21	z	458	0	490	2	0
22	S	1705	0	1681	28	0
22	s	1705	0	1681	24	0
23	A	175	0	169	7	0
23	B	1040	0	1152	27	0
23	C	810	0	854	24	0
23	D	195	0	216	9	0
23	G	448	0	429	11	0
23	N	435	0	396	7	0
23	R	530	0	466	10	0
23	S	414	0	313	9	0
23	Y	466	0	454	6	0
23	a	240	0	242	8	0
23	b	1040	0	1152	29	0
23	c	810	0	854	29	0
23	d	130	0	144	9	0
23	g	448	0	429	12	0
23	n	435	0	396	6	0
23	r	530	0	466	14	0
23	s	414	0	313	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	y	466	0	454	6	0
24	A	64	0	74	2	0
24	D	64	0	74	7	0
24	a	64	0	74	1	0
24	d	64	0	74	4	0
25	A	40	0	56	4	0
25	B	120	0	168	6	0
25	C	80	0	112	9	0
25	F	40	0	56	2	0
25	H	40	0	56	4	0
25	K	40	0	56	2	0
25	Z	40	0	56	3	0
25	a	40	0	56	2	0
25	b	120	0	168	8	0
25	c	120	0	168	15	0
25	d	40	0	56	2	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
26	A	104	0	145	1	0
26	L	54	0	78	4	0
26	M	54	0	78	3	0
26	a	54	0	78	1	0
26	d	50	0	67	2	0
27	A	40	0	50	0	0
27	B	91	0	122	5	0
27	C	48	0	66	2	0
27	D	46	0	62	2	0
27	a	48	0	66	2	0
27	b	51	0	72	4	0
27	d	46	0	62	0	0
28	A	59	0	76	4	0
28	C	55	0	68	4	0
28	H	62	0	82	4	0
28	a	59	0	76	3	0
28	c	55	0	68	2	0
28	d	62	0	82	4	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	A	95	0	139	4	0
30	B	98	0	148	2	0
30	C	49	0	74	3	0
30	G	46	0	65	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	L	98	0	148	5	0
30	N	49	0	74	2	0
30	R	42	0	57	2	0
30	S	49	0	74	3	0
30	T	49	0	74	2	0
30	W	49	0	74	1	0
30	Y	49	0	74	1	0
30	a	95	0	139	4	0
30	b	98	0	148	2	0
30	c	49	0	74	2	0
30	d	49	0	74	6	0
30	g	46	0	65	3	0
30	n	49	0	74	1	0
30	r	42	0	57	2	0
30	s	49	0	74	2	0
30	w	49	0	74	1	0
30	y	49	0	74	1	0
31	D	4	0	0	2	0
31	d	4	0	0	3	0
32	D	55	0	80	2	0
32	d	55	0	80	3	0
33	E	43	0	30	1	0
33	e	43	0	30	0	0
34	G	391	0	356	12	0
34	N	338	0	305	8	0
34	R	195	0	146	4	0
34	S	184	0	125	5	0
34	Y	299	0	284	10	0
34	g	391	0	356	19	0
34	n	338	0	305	7	0
34	r	195	0	146	4	0
34	s	184	0	125	2	0
34	y	299	0	284	8	0
35	G	84	0	112	8	0
35	N	84	0	112	7	0
35	R	42	0	56	2	0
35	S	84	0	112	8	0
35	Y	84	0	112	6	0
35	g	84	0	112	13	0
35	n	84	0	112	4	0
35	r	42	0	56	3	0
35	s	84	0	112	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	y	84	0	112	5	0
36	G	44	0	56	3	0
36	N	44	0	56	2	0
36	R	44	0	56	2	0
36	S	44	0	56	0	0
36	Y	44	0	56	0	0
36	g	44	0	56	3	0
36	n	44	0	56	3	0
36	r	44	0	56	2	0
36	s	44	0	56	2	0
36	y	44	0	56	0	0
37	G	44	0	56	6	0
37	N	44	0	56	0	0
37	R	44	0	56	1	0
37	Y	44	0	56	5	0
37	g	44	0	56	3	0
37	n	44	0	56	2	0
37	r	44	0	56	0	0
37	y	44	0	56	4	0
All	All	70366	0	70511	980	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 980 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ALA:O	3:C:40:ALA:HB3	1.77	0.84
22:s:242:GLN:OE1	23:s:612:CLA:NA	2.15	0.79
34:g:606:CHL:HBB2	35:g:616:LUT:H7	1.68	0.74
7:N:226:MET:HG2	35:N:317:LUT:H12	1.69	0.74
5:e:43:ALA:O	5:e:47:PHE:HB2	1.88	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/353 (94%)	314 (95%)	16 (5%)	0	100	100
1	a	330/353 (94%)	313 (95%)	17 (5%)	0	100	100
2	B	487/508 (96%)	465 (96%)	22 (4%)	0	100	100
2	b	487/508 (96%)	468 (96%)	19 (4%)	0	100	100
3	C	447/473 (94%)	415 (93%)	32 (7%)	0	100	100
3	c	447/473 (94%)	416 (93%)	31 (7%)	0	100	100
4	D	337/353 (96%)	321 (95%)	16 (5%)	0	100	100
4	d	337/353 (96%)	320 (95%)	17 (5%)	0	100	100
5	E	64/83 (77%)	64 (100%)	0	0	100	100
5	e	64/83 (77%)	61 (95%)	3 (5%)	0	100	100
6	F	27/39 (69%)	26 (96%)	1 (4%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	G	217/267 (81%)	209 (96%)	7 (3%)	1 (0%)	25	58
7	N	217/267 (81%)	198 (91%)	19 (9%)	0	100	100
7	g	217/267 (81%)	204 (94%)	13 (6%)	0	100	100
7	n	217/267 (81%)	201 (93%)	16 (7%)	0	100	100
8	H	57/73 (78%)	54 (95%)	3 (5%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
9	i	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
10	J	27/40 (68%)	26 (96%)	1 (4%)	0	100	100
10	j	27/40 (68%)	27 (100%)	0	0	100	100
11	K	35/61 (57%)	34 (97%)	1 (3%)	0	100	100
11	k	35/61 (57%)	33 (94%)	2 (6%)	0	100	100
12	L	35/38 (92%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	35/38 (92%)	35 (100%)	0	0	100	100
13	M	30/34 (88%)	28 (93%)	2 (7%)	0	100	100
13	m	30/34 (88%)	28 (93%)	2 (7%)	0	100	100
14	O	194/332 (58%)	182 (94%)	12 (6%)	0	100	100
14	o	194/332 (58%)	183 (94%)	11 (6%)	0	100	100
15	R	220/300 (73%)	211 (96%)	9 (4%)	0	100	100
15	r	220/300 (73%)	209 (95%)	11 (5%)	0	100	100
16	T	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
16	t	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
17	U	21/103 (20%)	20 (95%)	1 (5%)	0	100	100
17	u	21/103 (20%)	20 (95%)	1 (5%)	0	100	100
18	W	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
18	w	52/133 (39%)	50 (96%)	2 (4%)	0	100	100
19	X	36/116 (31%)	36 (100%)	0	0	100	100
19	x	36/116 (31%)	36 (100%)	0	0	100	100
20	Y	218/265 (82%)	203 (93%)	14 (6%)	1 (0%)	25	58
20	y	218/265 (82%)	208 (95%)	9 (4%)	1 (0%)	25	58
21	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
21	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
22	S	219/280 (78%)	202 (92%)	17 (8%)	0	100	100
22	s	219/280 (78%)	206 (94%)	13 (6%)	0	100	100
All	All	6776/8498 (80%)	6419 (95%)	354 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	Y	152	ILE
20	y	152	ILE
7	G	153	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	269/285 (94%)	269 (100%)	0	100	100
1	a	269/285 (94%)	269 (100%)	0	100	100
2	B	387/402 (96%)	387 (100%)	0	100	100
2	b	387/402 (96%)	387 (100%)	0	100	100
3	C	352/373 (94%)	350 (99%)	2 (1%)	84	91
3	c	352/373 (94%)	352 (100%)	0	100	100
4	D	271/283 (96%)	271 (100%)	0	100	100
4	d	271/283 (96%)	271 (100%)	0	100	100
5	E	59/73 (81%)	59 (100%)	0	100	100
5	e	59/73 (81%)	59 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (100%)	0	100	100
7	G	167/201 (83%)	167 (100%)	0	100	100
7	N	167/201 (83%)	167 (100%)	0	100	100
7	g	167/201 (83%)	167 (100%)	0	100	100
7	n	167/201 (83%)	167 (100%)	0	100	100
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	31/33 (94%)	31 (100%)	0	100	100
9	i	31/33 (94%)	31 (100%)	0	100	100
10	J	22/30 (73%)	22 (100%)	0	100	100
10	j	22/30 (73%)	22 (100%)	0	100	100
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	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	28/30 (93%)	28 (100%)	0	100	100
13	m	28/30 (93%)	28 (100%)	0	100	100
14	O	170/268 (63%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	o	170/268 (63%)	170 (100%)	0	100	100
15	R	176/231 (76%)	176 (100%)	0	100	100
15	r	176/231 (76%)	176 (100%)	0	100	100
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	U	19/82 (23%)	19 (100%)	0	100	100
17	u	19/82 (23%)	19 (100%)	0	100	100
18	W	47/102 (46%)	47 (100%)	0	100	100
18	w	47/102 (46%)	47 (100%)	0	100	100
19	X	32/92 (35%)	32 (100%)	0	100	100
19	x	32/92 (35%)	32 (100%)	0	100	100
20	Y	173/209 (83%)	173 (100%)	0	100	100
20	y	173/209 (83%)	173 (100%)	0	100	100
21	Z	53/54 (98%)	53 (100%)	0	100	100
21	z	53/54 (98%)	53 (100%)	0	100	100
22	S	172/219 (78%)	171 (99%)	1 (1%)	84	91
22	s	172/219 (78%)	172 (100%)	0	100	100
All	All	5522/6768 (82%)	5519 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	39	ASN
3	C	418	ASN
22	S	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	108	ASN
4	d	293	ASN
20	y	252	ASN
1	a	303	ASN
3	c	311	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 322 ligands modelled in this entry, 2 are monoatomic - leaving 320 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$
23	CLA	y	311	30	60,68,73	1.58	10 (16%)	70,107,113	1.48	9 (12%)
23	CLA	S	610	30	42,50,73	1.78	6 (14%)	48,85,113	1.57	9 (18%)
23	CLA	D	401	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	D	404	4	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
33	HEM	e	101	6,5	41,50,50	1.51	4 (9%)	45,82,82	1.62	11 (24%)
23	CLA	B	604	2	65,73,73	1.50	8 (12%)	76,113,113	1.49	8 (10%)
23	CLA	B	607	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	7 (9%)
35	LUT	G	615	-	42,43,43	0.87	2 (4%)	51,60,60	1.74	14 (27%)
23	CLA	r	612	15	47,55,73	1.70	6 (12%)	54,91,113	1.64	9 (16%)
23	CLA	g	612	7	45,53,73	1.81	9 (20%)	52,89,113	1.60	10 (19%)
23	CLA	B	602	2	65,73,73	1.44	7 (10%)	76,113,113	1.33	7 (9%)
36	NEX	r	617	-	38,46,46	0.93	2 (5%)	50,70,70	2.52	16 (32%)
23	CLA	G	611	30	60,68,73	1.60	9 (15%)	70,107,113	1.35	6 (8%)
28	DGD	d	410	-	63,63,67	0.88	2 (3%)	77,77,81	1.09	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	r	614	15	45,53,73	1.77	6 (13%)	52,89,113	1.67	7 (13%)
25	BCR	d	406	-	41,41,41	0.69	0	56,56,56	1.72	15 (26%)
34	CHL	n	302	7	66,74,74	1.40	7 (10%)	73,114,114	1.55	10 (13%)
23	CLA	S	612	22	55,63,73	1.69	7 (12%)	64,101,113	1.69	8 (12%)
23	CLA	s	609	22	45,53,73	1.81	8 (17%)	52,89,113	1.54	8 (15%)
35	LUT	y	316	-	42,43,43	0.80	1 (2%)	51,60,60	1.51	10 (19%)
23	CLA	b	605	2	65,73,73	1.46	10 (15%)	76,113,113	1.58	14 (18%)
35	LUT	g	615	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	14 (27%)
34	CHL	y	309	20	66,74,74	1.48	8 (12%)	73,114,114	1.38	7 (9%)
35	LUT	s	614	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
23	CLA	G	602	7	65,73,73	1.53	8 (12%)	76,113,113	1.34	8 (10%)
35	LUT	N	316	-	42,43,43	0.73	0	51,60,60	1.60	9 (17%)
23	CLA	y	310	20	60,68,73	1.52	7 (11%)	70,107,113	1.40	8 (11%)
23	CLA	D	405	4	65,73,73	1.49	9 (13%)	76,113,113	1.50	8 (10%)
23	CLA	g	604	36	49,57,73	1.67	10 (20%)	55,93,113	1.56	6 (10%)
23	CLA	y	304	20	65,73,73	1.50	11 (16%)	76,113,113	1.50	11 (14%)
23	CLA	A	402	-	50,58,73	1.71	7 (14%)	58,95,113	1.54	9 (15%)
34	CHL	R	607	-	61,69,74	1.51	7 (11%)	67,108,114	1.38	8 (11%)
23	CLA	c	503	3	65,73,73	1.48	8 (12%)	76,113,113	1.33	4 (5%)
23	CLA	B	610	-	65,73,73	1.39	9 (13%)	76,113,113	1.56	8 (10%)
35	LUT	S	614	-	42,43,43	0.78	0	51,60,60	1.70	16 (31%)
23	CLA	c	504	-	60,68,73	1.59	7 (11%)	70,107,113	1.32	6 (8%)
23	CLA	B	614	2	65,73,73	1.46	8 (12%)	76,113,113	1.40	10 (13%)
23	CLA	R	611	15	49,57,73	1.71	7 (14%)	55,93,113	1.44	9 (16%)
23	CLA	S	604	-	50,58,73	1.74	7 (14%)	58,95,113	1.62	8 (13%)
23	CLA	r	608	15	58,66,73	1.64	9 (15%)	67,104,113	1.34	8 (11%)
23	CLA	a	402	1	65,73,73	1.53	11 (16%)	76,113,113	1.47	12 (15%)
36	NEX	n	318	-	38,46,46	0.96	2 (5%)	50,70,70	2.27	16 (32%)
34	CHL	R	606	-	46,54,74	1.75	6 (13%)	49,90,114	1.57	8 (16%)
34	CHL	Y	308	-	66,74,74	1.42	7 (10%)	73,114,114	1.30	8 (10%)
34	CHL	G	609	7	61,69,74	1.54	9 (14%)	67,108,114	1.98	17 (25%)
23	CLA	a	403	-	50,58,73	1.73	8 (16%)	58,95,113	1.52	9 (15%)
35	LUT	G	616	-	42,43,43	0.79	0	51,60,60	1.47	7 (13%)
23	CLA	C	508	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	11 (14%)
23	CLA	c	506	3	51,59,73	1.67	8 (15%)	59,96,113	1.59	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	n	313	7	45,53,73	1.75	6 (13%)	52,89,113	1.69	9 (17%)
23	CLA	C	514	3	65,73,73	1.49	6 (9%)	76,113,113	1.29	9 (11%)
34	CHL	G	601	7	66,74,74	1.45	9 (13%)	73,114,114	1.62	15 (20%)
23	CLA	n	303	7	61,69,73	1.52	9 (14%)	71,108,113	1.40	9 (12%)
34	CHL	g	605	7	46,54,74	1.76	6 (13%)	49,90,114	1.61	10 (20%)
34	CHL	s	601	22	46,54,74	1.70	6 (13%)	49,90,114	1.76	8 (16%)
34	CHL	N	309	-	66,74,74	1.41	7 (10%)	73,114,114	1.41	11 (15%)
35	LUT	s	615	-	42,43,43	0.73	0	51,60,60	1.59	11 (21%)
23	CLA	C	510	3	65,73,73	1.45	7 (10%)	76,113,113	1.68	13 (17%)
30	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	3 (5%)
37	XAT	r	616	-	39,47,47	0.96	1 (2%)	54,74,74	2.62	18 (33%)
30	LHG	Y	318	23	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
34	CHL	N	310	7	66,74,74	1.47	9 (13%)	73,114,114	1.92	12 (16%)
23	CLA	G	603	7	65,73,73	1.50	11 (16%)	76,113,113	1.41	10 (13%)
23	CLA	Y	310	20	60,68,73	1.54	7 (11%)	70,107,113	1.38	7 (10%)
23	CLA	n	315	7	41,49,73	1.84	5 (12%)	47,84,113	1.61	9 (19%)
34	CHL	S	607	-	49,57,74	1.72	6 (12%)	52,93,114	1.64	14 (26%)
30	LHG	r	618	-	41,41,48	1.03	2 (4%)	44,47,54	1.22	4 (9%)
25	BCR	a	406	-	41,41,41	0.73	0	56,56,56	1.73	15 (26%)
24	PHO	d	401	-	51,69,69	0.75	1 (1%)	47,99,99	1.10	3 (6%)
23	CLA	n	305	-	50,58,73	1.60	8 (16%)	58,95,113	1.69	9 (15%)
23	CLA	s	612	22	55,63,73	1.70	7 (12%)	64,101,113	1.68	9 (14%)
23	CLA	C	512	3	65,73,73	1.53	9 (13%)	76,113,113	1.36	9 (11%)
30	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	2 (3%)
30	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	2 (3%)
34	CHL	n	307	-	46,54,74	1.75	9 (19%)	49,90,114	1.90	11 (22%)
23	CLA	y	313	20	65,73,73	1.52	10 (15%)	76,113,113	1.59	11 (14%)
23	CLA	N	314	7	60,68,73	1.56	8 (13%)	70,107,113	1.75	14 (20%)
23	CLA	R	603	15	60,68,73	1.53	8 (13%)	70,107,113	1.42	9 (12%)
23	CLA	c	511	3	65,73,73	1.50	8 (12%)	76,113,113	1.42	9 (11%)
23	CLA	S	611	22	45,53,73	1.80	9 (20%)	52,89,113	1.57	10 (19%)
23	CLA	r	602	15	60,68,73	1.53	9 (15%)	70,107,113	1.30	7 (10%)
35	LUT	Y	315	-	42,43,43	0.75	0	51,60,60	1.44	8 (15%)
23	CLA	B	616	2	65,73,73	1.49	8 (12%)	76,113,113	1.34	10 (13%)
23	CLA	Y	304	20	65,73,73	1.49	10 (15%)	76,113,113	1.52	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	513	3	65,73,73	1.50	9 (13%)	76,113,113	1.32	11 (14%)
34	CHL	n	308	-	46,54,74	1.70	9 (19%)	49,90,114	1.76	11 (22%)
23	CLA	r	611	15	49,57,73	1.69	6 (12%)	55,93,113	1.47	9 (16%)
36	NEX	s	616	-	38,46,46	0.87	2 (5%)	50,70,70	2.52	13 (26%)
30	LHG	C	518	-	48,48,48	0.92	2 (4%)	51,54,54	0.90	2 (3%)
34	CHL	y	302	20	66,74,74	1.38	7 (10%)	73,114,114	1.52	8 (10%)
30	LHG	w	201	-	48,48,48	0.94	2 (4%)	51,54,54	1.17	3 (5%)
23	CLA	Y	313	20	65,73,73	1.51	10 (15%)	76,113,113	1.45	9 (11%)
23	CLA	N	312	30	60,68,73	1.54	8 (13%)	70,107,113	1.44	8 (11%)
30	LHG	T	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
30	LHG	b	621	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
23	CLA	C	509	3	65,73,73	1.41	8 (12%)	76,113,113	1.49	7 (9%)
36	NEX	S	616	-	38,46,46	0.96	2 (5%)	50,70,70	2.52	14 (28%)
23	CLA	N	315	7	41,49,73	1.81	5 (12%)	47,84,113	1.67	10 (21%)
27	LMG	a	407	-	48,48,55	0.95	2 (4%)	56,56,63	1.30	6 (10%)
34	CHL	y	306	20	51,59,74	1.62	8 (15%)	55,96,114	1.76	12 (21%)
25	BCR	A	405	-	41,41,41	0.73	0	56,56,56	1.71	13 (23%)
34	CHL	N	302	7	66,74,74	1.40	7 (10%)	73,114,114	1.41	10 (13%)
23	CLA	R	609	15	65,73,73	1.47	8 (12%)	76,113,113	1.31	8 (10%)
23	CLA	s	608	22	45,53,73	1.79	6 (13%)	52,89,113	1.63	10 (19%)
28	DGD	a	408	-	60,60,67	0.91	2 (3%)	74,74,81	1.03	2 (2%)
34	CHL	Y	307	-	50,58,74	1.56	7 (14%)	52,94,114	1.52	6 (11%)
23	CLA	y	303	20	61,69,73	1.55	8 (13%)	71,108,113	1.46	9 (12%)
25	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.89	14 (25%)
34	CHL	G	619	-	66,74,74	1.41	7 (10%)	73,114,114	1.52	10 (13%)
25	BCR	b	619	-	41,41,41	0.71	0	56,56,56	1.87	14 (25%)
23	CLA	R	614	15,23	45,53,73	1.78	9 (20%)	52,89,113	1.59	7 (13%)
37	XAT	g	620	-	39,47,47	0.93	1 (2%)	54,74,74	2.53	17 (31%)
23	CLA	r	610	-	49,57,73	1.73	6 (12%)	55,93,113	1.49	7 (12%)
34	CHL	y	308	-	66,74,74	1.42	7 (10%)	73,114,114	1.29	7 (9%)
28	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.11	3 (3%)
23	CLA	A	404	1	60,68,73	1.46	8 (13%)	70,107,113	1.56	7 (10%)
23	CLA	B	601	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	8 (10%)
23	CLA	N	311	7	59,67,73	1.52	8 (13%)	68,105,113	1.40	7 (10%)
23	CLA	a	405	1	60,68,73	1.47	8 (13%)	70,107,113	1.53	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	615	2	65,73,73	1.49	8 (12%)	76,113,113	1.39	9 (11%)
36	NEX	N	318	-	38,46,46	0.92	2 (5%)	50,70,70	2.38	20 (40%)
23	CLA	c	510	3	65,73,73	1.47	8 (12%)	76,113,113	1.52	9 (11%)
25	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.84	13 (23%)
26	SQD	d	402	-	49,50,54	1.23	4 (8%)	58,61,65	1.13	4 (6%)
23	CLA	d	405	4	65,73,73	1.50	8 (12%)	76,113,113	1.45	7 (9%)
23	CLA	n	312	30	60,68,73	1.55	9 (15%)	70,107,113	1.47	8 (11%)
23	CLA	R	612	15	47,55,73	1.74	6 (12%)	54,91,113	1.63	7 (12%)
23	CLA	c	507	-	65,73,73	1.49	10 (15%)	76,113,113	1.47	12 (15%)
34	CHL	N	306	7	48,56,74	1.64	6 (12%)	51,92,114	1.48	7 (13%)
23	CLA	B	613	2	65,73,73	1.47	9 (13%)	76,113,113	1.50	8 (10%)
23	CLA	s	603	22	45,53,73	1.82	10 (22%)	52,89,113	1.74	9 (17%)
34	CHL	n	309	-	66,74,74	1.42	9 (13%)	73,114,114	1.45	8 (10%)
23	CLA	N	303	7	61,69,73	1.53	9 (14%)	71,108,113	1.44	10 (14%)
23	CLA	N	304	7	59,67,73	1.56	9 (15%)	68,105,113	1.59	11 (16%)
37	XAT	Y	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.51	20 (37%)
24	PHO	D	402	-	51,69,69	0.76	2 (3%)	47,99,99	1.15	2 (4%)
23	CLA	b	608	2	65,73,73	1.51	10 (15%)	76,113,113	1.61	11 (14%)
23	CLA	B	606	2	65,73,73	1.52	8 (12%)	76,113,113	1.30	7 (9%)
23	CLA	C	505	-	60,68,73	1.58	6 (10%)	70,107,113	1.37	7 (10%)
34	CHL	G	606	-	43,51,74	1.74	9 (20%)	45,86,114	1.51	8 (17%)
27	LMG	d	409	-	46,46,55	1.00	2 (4%)	54,54,63	1.01	2 (3%)
34	CHL	Y	306	20	51,59,74	1.63	8 (15%)	55,96,114	1.86	12 (21%)
23	CLA	y	305	-	50,58,73	1.67	9 (18%)	58,95,113	1.57	8 (13%)
34	CHL	s	607	-	49,57,74	1.66	6 (12%)	52,93,114	1.64	10 (19%)
23	CLA	R	604	-	48,56,73	1.66	7 (14%)	55,92,113	1.79	9 (16%)
23	CLA	Y	311	30	60,68,73	1.56	10 (16%)	70,107,113	1.49	9 (12%)
23	CLA	c	505	3	58,66,73	1.52	8 (13%)	67,104,113	1.55	11 (16%)
30	LHG	A	411	-	45,45,48	0.95	2 (4%)	48,51,54	1.02	2 (4%)
37	XAT	R	616	-	39,47,47	0.96	2 (5%)	54,74,74	2.62	19 (35%)
23	CLA	c	508	3	65,73,73	1.39	8 (12%)	76,113,113	1.56	10 (13%)
25	BCR	c	515	-	41,41,41	0.76	0	56,56,56	1.82	15 (26%)
28	DGD	C	517	-	56,56,67	0.88	2 (3%)	70,70,81	1.15	7 (10%)
34	CHL	G	608	-	66,74,74	1.45	7 (10%)	73,114,114	1.36	10 (13%)
23	CLA	s	602	22	46,54,73	1.72	10 (21%)	53,90,113	1.55	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HEM	E	101	6,5	41,50,50	1.47	3 (7%)	45,82,82	1.64	9 (20%)
34	CHL	R	605	-	46,54,74	1.76	7 (15%)	49,90,114	1.61	8 (16%)
26	SQD	A	406	-	49,50,54	1.23	4 (8%)	58,61,65	1.18	4 (6%)
28	DGD	A	408	-	60,60,67	0.90	2 (3%)	74,74,81	1.02	2 (2%)
35	LUT	r	615	-	42,43,43	0.74	0	51,60,60	1.72	10 (19%)
25	BCR	c	518	-	41,41,41	0.68	0	56,56,56	1.82	14 (25%)
23	CLA	Y	303	20	61,69,73	1.50	8 (13%)	71,108,113	1.41	9 (12%)
23	CLA	c	509	3	65,73,73	1.59	8 (12%)	76,113,113	1.36	10 (13%)
23	CLA	c	512	3	56,64,73	1.63	9 (16%)	65,102,113	1.67	17 (26%)
23	CLA	b	601	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	8 (10%)
34	CHL	r	605	-	46,54,74	1.74	7 (15%)	49,90,114	1.52	8 (16%)
35	LUT	y	315	-	42,43,43	0.76	0	51,60,60	1.46	7 (13%)
23	CLA	Y	314	20	45,53,73	1.69	6 (13%)	52,89,113	1.82	9 (17%)
34	CHL	N	307	-	46,54,74	1.74	9 (19%)	49,90,114	1.84	11 (22%)
23	CLA	y	314	20	45,53,73	1.69	6 (13%)	52,89,113	1.81	8 (15%)
27	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	3 (5%)
23	CLA	r	601	15	49,57,73	1.76	7 (14%)	55,93,113	1.66	12 (21%)
30	LHG	a	412	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	3 (5%)
34	CHL	r	607	-	61,69,74	1.47	5 (8%)	67,108,114	1.35	7 (10%)
32	PL9	D	406	-	55,55,55	4.24	20 (36%)	68,69,69	3.79	34 (50%)
30	LHG	S	617	23	48,48,48	0.92	2 (4%)	51,54,54	1.04	2 (3%)
25	BCR	F	101	-	41,41,41	0.69	0	56,56,56	1.65	15 (26%)
23	CLA	b	603	2	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
35	LUT	g	616	-	42,43,43	0.81	0	51,60,60	1.56	13 (25%)
28	DGD	c	516	-	56,56,67	0.88	2 (3%)	70,70,81	1.14	7 (10%)
23	CLA	s	610	30	42,50,73	1.80	6 (14%)	48,85,113	1.54	8 (16%)
23	CLA	G	613	7	58,66,73	1.57	9 (15%)	67,104,113	1.55	9 (13%)
24	PHO	a	404	-	51,69,69	0.74	0	47,99,99	0.97	2 (4%)
34	CHL	R	613	15	42,50,74	1.82	6 (14%)	44,85,114	1.64	9 (20%)
23	CLA	c	501	3	65,73,73	1.49	9 (13%)	76,113,113	1.35	7 (9%)
23	CLA	c	502	3	65,73,73	1.50	11 (16%)	76,113,113	1.71	10 (13%)
23	CLA	R	608	15,23	58,66,73	1.60	7 (12%)	67,104,113	1.36	6 (8%)
27	LMG	D	407	-	46,46,55	1.01	2 (4%)	54,54,63	1.00	2 (3%)
25	BCR	Z	101	-	41,41,41	0.69	0	56,56,56	1.78	15 (26%)
30	LHG	a	411	-	45,45,48	0.94	2 (4%)	48,51,54	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	CHL	g	608	-	66,74,74	1.48	7 (10%)	73,114,114	1.29	10 (13%)
23	CLA	N	313	7	45,53,73	1.82	8 (17%)	52,89,113	1.61	8 (15%)
37	XAT	G	620	-	39,47,47	0.94	1 (2%)	54,74,74	2.55	17 (31%)
31	BCT	D	403	29	2,3,3	0.88	0	2,3,3	3.02	2 (100%)
23	CLA	b	609	2	65,73,73	1.50	9 (13%)	76,113,113	1.36	8 (10%)
30	LHG	c	517	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
27	LMG	B	622	-	40,40,55	1.09	2 (5%)	48,48,63	1.10	2 (4%)
24	PHO	A	403	-	51,69,69	0.74	1 (1%)	47,99,99	0.95	2 (4%)
23	CLA	y	312	20	60,68,73	1.50	7 (11%)	70,107,113	1.58	11 (15%)
35	LUT	R	615	-	42,43,43	0.73	0	51,60,60	1.72	12 (23%)
23	CLA	a	401	1	65,73,73	1.41	8 (12%)	76,113,113	1.80	19 (25%)
23	CLA	B	609	2	65,73,73	1.54	11 (16%)	76,113,113	1.31	8 (10%)
25	BCR	k	101	-	41,41,41	0.70	0	56,56,56	1.78	13 (23%)
23	CLA	B	603	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
23	CLA	g	614	7	42,50,73	1.82	6 (14%)	48,85,113	1.54	7 (14%)
23	CLA	G	610	7	64,72,73	1.49	6 (9%)	74,111,113	1.42	7 (9%)
36	NEX	G	617	-	38,46,46	1.00	2 (5%)	50,70,70	2.81	16 (32%)
23	CLA	C	502	3	65,73,73	1.49	8 (12%)	76,113,113	1.34	9 (11%)
37	XAT	n	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.56	16 (29%)
35	LUT	n	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.34	7 (13%)
30	LHG	A	412	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
34	CHL	G	607	-	43,51,74	1.79	6 (13%)	45,86,114	1.86	11 (24%)
25	BCR	K	101	-	41,41,41	0.68	0	56,56,56	1.72	10 (17%)
30	LHG	W	201	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
36	NEX	R	617	-	38,46,46	0.94	2 (5%)	50,70,70	2.50	18 (36%)
23	CLA	C	511	3	65,73,73	1.48	8 (12%)	76,113,113	1.50	11 (14%)
23	CLA	Y	312	20	60,68,73	1.50	7 (11%)	70,107,113	1.62	12 (17%)
34	CHL	N	308	-	46,54,74	1.69	8 (17%)	49,90,114	1.78	12 (24%)
25	BCR	B	619	-	41,41,41	0.72	0	56,56,56	1.91	14 (25%)
23	CLA	C	513	3	56,64,73	1.63	10 (17%)	65,102,113	1.56	15 (23%)
34	CHL	y	307	-	50,58,74	1.55	6 (12%)	52,94,114	1.59	9 (17%)
27	LMG	A	407	-	40,40,55	1.07	2 (5%)	48,48,63	1.13	3 (6%)
23	CLA	R	601	15	49,57,73	1.78	8 (16%)	55,93,113	1.56	10 (18%)
23	CLA	b	613	2	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
34	CHL	Y	302	20	66,74,74	1.38	7 (10%)	73,114,114	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	617	-	41,41,41	0.75	0	56,56,56	1.75	11 (19%)
34	CHL	s	605	-	46,54,74	1.78	6 (13%)	49,90,114	1.50	8 (16%)
32	PL9	d	407	-	55,55,55	4.23	20 (36%)	68,69,69	3.80	33 (48%)
23	CLA	S	613	22	41,49,73	1.92	7 (17%)	47,84,113	1.51	8 (17%)
30	LHG	y	318	23	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
34	CHL	n	310	7	66,74,74	1.45	9 (13%)	73,114,114	1.82	10 (13%)
30	LHG	B	621	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	4 (7%)
23	CLA	b	610	-	65,73,73	1.40	8 (12%)	76,113,113	1.54	8 (10%)
23	CLA	R	610	30	49,57,73	1.73	6 (12%)	55,93,113	1.55	8 (14%)
23	CLA	B	615	2	65,73,73	1.48	8 (12%)	76,113,113	1.39	11 (14%)
23	CLA	r	604	-	48,56,73	1.66	7 (14%)	55,92,113	1.83	9 (16%)
36	NEX	g	617	23	38,46,46	0.97	2 (5%)	50,70,70	2.62	10 (20%)
26	SQD	a	409	-	53,54,54	1.19	4 (7%)	62,65,65	3.64	8 (12%)
23	CLA	S	608	22	45,53,73	1.77	6 (13%)	52,89,113	1.64	10 (19%)
27	LMG	C	501	-	48,48,55	0.96	2 (4%)	56,56,63	1.23	6 (10%)
25	BCR	b	618	-	41,41,41	0.78	0	56,56,56	1.87	18 (32%)
30	LHG	R	618	23	41,41,48	1.04	2 (4%)	44,47,54	1.10	2 (4%)
26	SQD	M	101	-	53,54,54	1.15	4 (7%)	62,65,65	1.16	4 (6%)
35	LUT	N	317	-	42,43,43	0.93	1 (2%)	51,60,60	1.42	7 (13%)
34	CHL	g	601	7	66,74,74	1.44	10 (15%)	73,114,114	1.62	16 (21%)
23	CLA	n	314	7	60,68,73	1.56	11 (18%)	70,107,113	1.62	11 (15%)
34	CHL	S	601	22	46,54,74	1.71	6 (13%)	49,90,114	1.72	9 (18%)
35	LUT	S	615	-	42,43,43	0.74	0	51,60,60	1.64	10 (19%)
23	CLA	n	311	7	59,67,73	1.53	7 (11%)	68,105,113	1.48	8 (11%)
23	CLA	b	604	2	65,73,73	1.51	8 (12%)	76,113,113	1.50	9 (11%)
23	CLA	n	304	7	59,67,73	1.57	8 (13%)	68,105,113	1.53	9 (13%)
36	NEX	Y	317	-	38,46,46	1.16	3 (7%)	50,70,70	4.24	20 (40%)
23	CLA	G	612	7	45,53,73	1.80	9 (20%)	52,89,113	1.76	11 (21%)
23	CLA	g	610	7	64,72,73	1.49	6 (9%)	74,111,113	1.43	8 (10%)
30	LHG	n	319	23	48,48,48	0.94	2 (4%)	51,54,54	1.04	2 (3%)
30	LHG	s	617	23	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
34	CHL	g	619	-	66,74,74	1.40	7 (10%)	73,114,114	1.51	10 (13%)
34	CHL	G	605	7	46,54,74	1.79	6 (13%)	49,90,114	1.60	10 (20%)
23	CLA	C	503	3	65,73,73	1.50	10 (15%)	76,113,113	1.60	11 (14%)
23	CLA	b	616	2	65,73,73	1.50	8 (12%)	76,113,113	1.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	608	2	65,73,73	1.47	9 (13%)	76,113,113	1.56	9 (11%)
25	BCR	b	617	-	41,41,41	0.75	0	56,56,56	1.76	12 (21%)
26	SQD	L	103	-	53,54,54	1.16	4 (7%)	62,65,65	1.16	5 (8%)
30	LHG	g	618	23	45,45,48	0.95	2 (4%)	48,51,54	1.13	3 (6%)
31	BCT	d	403	29	2,3,3	0.88	0	2,3,3	3.06	2 (100%)
30	LHG	b	622	-	48,48,48	0.88	2 (4%)	51,54,54	1.10	4 (7%)
30	LHG	G	618	23	45,45,48	0.96	2 (4%)	48,51,54	1.15	3 (6%)
23	CLA	N	305	-	50,58,73	1.64	10 (20%)	58,95,113	1.62	8 (13%)
25	BCR	B	618	-	41,41,41	0.78	0	56,56,56	1.89	17 (30%)
23	CLA	A	401	1	65,73,73	1.43	8 (12%)	76,113,113	1.78	16 (21%)
34	CHL	s	606	-	43,51,74	1.81	6 (13%)	45,86,114	1.83	9 (20%)
23	CLA	C	507	3	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
23	CLA	G	604	-	49,57,73	1.66	10 (20%)	55,93,113	1.56	7 (12%)
35	LUT	Y	316	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	9 (17%)
23	CLA	R	602	15	60,68,73	1.53	8 (13%)	70,107,113	1.45	7 (10%)
23	CLA	r	609	15	65,73,73	1.47	9 (13%)	76,113,113	1.23	9 (11%)
23	CLA	g	613	7	58,66,73	1.56	10 (17%)	67,104,113	1.55	9 (13%)
23	CLA	r	603	15	60,68,73	1.54	10 (16%)	70,107,113	1.44	8 (11%)
23	CLA	g	603	7	65,73,73	1.51	11 (16%)	76,113,113	1.40	10 (13%)
25	BCR	H	101	-	41,41,41	0.75	0	56,56,56	1.67	10 (17%)
36	NEX	y	317	-	38,46,46	1.40	4 (10%)	50,70,70	4.19	20 (40%)
23	CLA	C	504	3	65,73,73	1.48	8 (12%)	76,113,113	1.42	8 (10%)
30	LHG	B	623	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
23	CLA	Y	305	-	50,58,73	1.63	8 (16%)	58,95,113	1.58	7 (12%)
23	CLA	s	613	22	41,49,73	1.94	7 (17%)	47,84,113	1.58	8 (17%)
23	CLA	g	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.40	8 (11%)
23	CLA	S	603	22	45,53,73	1.78	8 (17%)	52,89,113	1.76	10 (19%)
25	BCR	h	101	-	41,41,41	0.73	0	56,56,56	1.59	10 (17%)
26	SQD	A	409	-	53,54,54	1.18	4 (7%)	62,65,65	3.65	9 (14%)
23	CLA	b	611	2	65,73,73	1.46	8 (12%)	76,113,113	1.39	6 (7%)
35	LUT	n	316	-	42,43,43	0.71	0	51,60,60	1.67	11 (21%)
34	CHL	g	606	-	43,51,74	1.74	7 (16%)	45,86,114	1.73	12 (26%)
27	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	3 (5%)
23	CLA	C	506	3	58,66,73	1.53	8 (13%)	67,104,113	1.64	12 (17%)
23	CLA	b	602	2	65,73,73	1.41	7 (10%)	76,113,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	XAT	N	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.55	19 (35%)
23	CLA	b	607	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	6 (7%)
34	CHL	S	605	-	46,54,74	1.80	11 (23%)	49,90,114	1.81	16 (32%)
25	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.78	16 (28%)
34	CHL	Y	309	20	66,74,74	1.53	9 (13%)	73,114,114	1.46	9 (12%)
23	CLA	G	614	7	42,50,73	1.83	7 (16%)	48,85,113	1.55	7 (14%)
34	CHL	S	606	-	43,51,74	1.81	6 (13%)	45,86,114	2.00	11 (24%)
34	CHL	r	613	15	42,50,74	1.82	6 (14%)	44,85,114	1.68	9 (20%)
34	CHL	g	607	-	43,51,74	1.80	7 (16%)	45,86,114	1.98	12 (26%)
34	CHL	n	306	7	48,56,74	1.66	7 (14%)	51,92,114	1.49	8 (15%)
23	CLA	s	604	-	50,58,73	1.72	8 (16%)	58,95,113	1.59	10 (17%)
23	CLA	g	602	7	65,73,73	1.52	8 (12%)	76,113,113	1.36	8 (10%)
30	LHG	N	319	23	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
23	CLA	S	609	22	45,53,73	1.83	9 (20%)	52,89,113	1.52	10 (19%)
23	CLA	B	612	2	65,73,73	1.41	8 (12%)	76,113,113	1.58	6 (7%)
37	XAT	y	301	-	39,47,47	0.90	1 (2%)	54,74,74	2.54	20 (37%)
34	CHL	r	606	-	46,54,74	1.77	6 (13%)	49,90,114	1.55	8 (16%)
23	CLA	B	611	2	65,73,73	1.46	9 (13%)	76,113,113	1.40	7 (9%)
34	CHL	g	609	7	61,69,74	1.55	9 (14%)	67,108,114	1.87	14 (20%)
23	CLA	B	605	2	65,73,73	1.47	10 (15%)	76,113,113	1.53	14 (18%)
23	CLA	d	404	4	65,73,73	1.46	8 (12%)	76,113,113	1.44	8 (10%)
23	CLA	s	611	22	45,53,73	1.79	9 (20%)	52,89,113	1.58	9 (17%)
23	CLA	S	602	22	46,54,73	1.74	9 (19%)	53,90,113	1.55	9 (16%)
23	CLA	b	612	2	65,73,73	1.41	8 (12%)	76,113,113	1.60	8 (10%)
23	CLA	b	614	2	65,73,73	1.46	8 (12%)	76,113,113	1.40	10 (13%)
23	CLA	b	606	2	65,73,73	1.52	8 (12%)	76,113,113	1.28	7 (9%)

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
23	CLA	y	311	30	1/1/14/20	12/31/109/115	-
23	CLA	S	610	30	1/1/10/20	4/10/88/115	-
23	CLA	D	401	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	404	4	1/1/15/20	10/37/115/115	-
33	HEM	e	101	6,5	-	4/12/54/54	-
23	CLA	B	604	2	1/1/15/20	14/37/115/115	-
23	CLA	B	607	-	1/1/15/20	14/37/115/115	-
35	LUT	G	615	-	-	2/29/67/67	0/2/2/2
23	CLA	r	612	15	1/1/11/20	7/16/94/115	-
23	CLA	g	612	7	1/1/11/20	6/13/91/115	-
23	CLA	B	602	2	1/1/15/20	7/37/115/115	-
36	NEX	r	617	-	-	3/27/83/83	0/3/3/3
23	CLA	G	611	30	1/1/14/20	9/31/109/115	-
28	DGD	d	410	-	-	10/51/91/95	0/2/2/2
23	CLA	r	614	15	1/1/11/20	8/13/91/115	-
34	CHL	n	302	7	3/3/20/26	13/39/137/137	-
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
23	CLA	S	612	22	1/1/13/20	12/25/103/115	-
23	CLA	s	609	22	1/1/11/20	8/13/91/115	-
35	LUT	y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	b	605	2	1/1/15/20	10/37/115/115	-
35	LUT	g	615	-	-	2/29/67/67	0/2/2/2
34	CHL	y	309	20	3/3/20/26	25/39/137/137	-
35	LUT	s	614	-	-	2/29/67/67	0/2/2/2
23	CLA	G	602	7	1/1/15/20	13/37/115/115	-
35	LUT	N	316	-	-	3/29/67/67	0/2/2/2
23	CLA	y	310	20	1/1/14/20	8/31/109/115	-
23	CLA	D	405	4	1/1/15/20	12/37/115/115	-
23	CLA	g	604	36	1/1/11/20	5/18/96/115	-
23	CLA	y	304	20	1/1/15/20	13/37/115/115	-
23	CLA	A	402	-	1/1/12/20	9/19/97/115	-
34	CHL	R	607	-	3/3/19/26	10/33/131/137	-
23	CLA	c	503	3	1/1/15/20	18/37/115/115	-
23	CLA	B	610	-	1/1/15/20	14/37/115/115	-
35	LUT	S	614	-	-	2/29/67/67	0/2/2/2
23	CLA	c	504	-	1/1/14/20	13/31/109/115	-
23	CLA	B	614	2	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	R	611	15	1/1/11/20	3/18/96/115	-
23	CLA	S	604	-	1/1/12/20	4/19/97/115	-
23	CLA	r	608	15	1/1/13/20	9/29/107/115	-
23	CLA	a	402	1	1/1/15/20	16/37/115/115	-
36	NEX	n	318	-	-	4/27/83/83	0/3/3/3
34	CHL	R	606	-	3/3/16/26	7/15/113/137	-
34	CHL	Y	308	-	3/3/20/26	14/39/137/137	-
34	CHL	G	609	7	3/3/19/26	13/33/131/137	-
23	CLA	a	403	-	1/1/12/20	9/19/97/115	-
35	LUT	G	616	-	-	2/29/67/67	0/2/2/2
23	CLA	C	508	-	1/1/15/20	11/37/115/115	-
23	CLA	c	506	3	1/1/12/20	9/21/99/115	-
23	CLA	n	313	7	1/1/11/20	8/13/91/115	-
23	CLA	C	514	3	1/1/15/20	10/37/115/115	-
34	CHL	G	601	7	3/3/20/26	11/39/137/137	-
23	CLA	n	303	7	1/1/14/20	9/33/111/115	-
34	CHL	g	605	7	3/3/16/26	8/15/113/137	-
34	CHL	s	601	22	3/3/16/26	9/15/113/137	-
34	CHL	N	309	-	3/3/20/26	14/39/137/137	-
35	LUT	s	615	-	-	6/29/67/67	0/2/2/2
23	CLA	C	510	3	1/1/15/20	16/37/115/115	-
30	LHG	L	102	-	-	10/53/53/53	-
37	XAT	r	616	-	-	2/31/93/93	0/4/4/4
30	LHG	Y	318	23	-	12/53/53/53	-
34	CHL	N	310	7	3/3/20/26	16/39/137/137	-
23	CLA	G	603	7	1/1/15/20	7/37/115/115	-
23	CLA	Y	310	20	1/1/14/20	8/31/109/115	-
23	CLA	n	315	7	1/1/10/20	2/8/86/115	-
34	CHL	S	607	-	3/3/16/26	13/19/117/137	-
30	LHG	r	618	-	-	11/46/46/53	-
25	BCR	a	406	-	-	2/29/63/63	0/2/2/2
24	PHO	d	401	-	-	12/37/103/103	0/5/6/6
23	CLA	n	305	-	1/1/12/20	9/19/97/115	-
23	CLA	s	612	22	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	512	3	1/1/15/20	17/37/115/115	-
30	LHG	L	101	-	-	11/53/53/53	-
30	LHG	d	408	-	-	8/53/53/53	-
34	CHL	n	307	-	3/3/16/26	8/15/113/137	-
23	CLA	y	313	20	1/1/15/20	15/37/115/115	-
23	CLA	N	314	7	1/1/14/20	12/31/109/115	-
23	CLA	R	603	15	1/1/14/20	5/31/109/115	-
23	CLA	c	511	3	1/1/15/20	14/37/115/115	-
23	CLA	S	611	22	1/1/11/20	8/13/91/115	-
23	CLA	r	602	15	1/1/14/20	9/31/109/115	-
35	LUT	Y	315	-	-	5/29/67/67	0/2/2/2
23	CLA	B	616	2	1/1/15/20	11/37/115/115	-
23	CLA	Y	304	20	1/1/15/20	13/37/115/115	-
23	CLA	c	513	3	1/1/15/20	13/37/115/115	-
34	CHL	n	308	-	3/3/16/26	11/15/113/137	-
23	CLA	r	611	15	1/1/11/20	6/18/96/115	-
36	NEX	s	616	-	-	2/27/83/83	0/3/3/3
30	LHG	C	518	-	-	11/53/53/53	-
34	CHL	y	302	20	3/3/20/26	18/39/137/137	-
30	LHG	w	201	-	-	19/53/53/53	-
23	CLA	Y	313	20	1/1/15/20	15/37/115/115	-
23	CLA	N	312	30	1/1/14/20	7/31/109/115	-
30	LHG	T	101	-	-	10/53/53/53	-
30	LHG	b	621	-	-	11/53/53/53	-
23	CLA	C	509	3	1/1/15/20	10/37/115/115	-
36	NEX	S	616	-	-	3/27/83/83	0/3/3/3
23	CLA	N	315	7	1/1/10/20	2/8/86/115	-
27	LMG	a	407	-	-	7/43/63/70	0/1/1/1
34	CHL	y	306	20	3/3/17/26	9/21/119/137	-
25	BCR	A	405	-	-	2/29/63/63	0/2/2/2
34	CHL	N	302	7	3/3/20/26	14/39/137/137	-
23	CLA	R	609	15	1/1/15/20	11/37/115/115	-
23	CLA	s	608	22	1/1/11/20	7/13/91/115	-
28	DGD	a	408	-	-	10/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	CHL	Y	307	-	3/3/16/26	10/20/118/137	-
23	CLA	y	303	20	1/1/14/20	17/33/111/115	-
25	BCR	c	514	-	-	5/29/63/63	0/2/2/2
34	CHL	G	619	-	3/3/20/26	23/39/137/137	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	R	614	15,23	1/1/11/20	7/13/91/115	-
37	XAT	g	620	-	-	1/31/93/93	0/4/4/4
23	CLA	r	610	-	1/1/11/20	7/18/96/115	-
34	CHL	y	308	-	3/3/20/26	17/39/137/137	-
28	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	A	404	1	1/1/14/20	11/31/109/115	-
23	CLA	B	601	-	1/1/15/20	14/37/115/115	-
23	CLA	N	311	7	1/1/13/20	10/30/108/115	-
23	CLA	a	405	1	1/1/14/20	14/31/109/115	-
23	CLA	b	615	2	1/1/15/20	11/37/115/115	-
36	NEX	N	318	-	-	3/27/83/83	0/3/3/3
23	CLA	c	510	3	1/1/15/20	18/37/115/115	-
25	BCR	C	516	-	-	4/29/63/63	0/2/2/2
26	SQD	d	402	-	-	11/45/65/69	0/1/1/1
23	CLA	d	405	4	1/1/15/20	13/37/115/115	-
23	CLA	n	312	30	1/1/14/20	9/31/109/115	-
23	CLA	R	612	15	1/1/11/20	8/16/94/115	-
23	CLA	c	507	-	1/1/15/20	10/37/115/115	-
34	CHL	N	306	7	3/3/16/26	9/18/116/137	-
23	CLA	B	613	2	1/1/15/20	11/37/115/115	-
23	CLA	s	603	22	1/1/11/20	7/13/91/115	-
34	CHL	n	309	-	3/3/20/26	14/39/137/137	-
23	CLA	N	303	7	1/1/14/20	11/33/111/115	-
23	CLA	N	304	7	1/1/13/20	10/30/108/115	-
37	XAT	Y	301	-	-	2/31/93/93	0/4/4/4
24	PHO	D	402	-	-	13/37/103/103	0/5/6/6
23	CLA	b	608	2	1/1/15/20	14/37/115/115	-
23	CLA	B	606	2	1/1/15/20	7/37/115/115	-
23	CLA	C	505	-	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	CHL	G	606	-	3/3/15/26	8/12/110/137	-
27	LMG	d	409	-	-	6/41/61/70	0/1/1/1
34	CHL	Y	306	20	3/3/17/26	11/21/119/137	-
23	CLA	y	305	-	1/1/12/20	7/19/97/115	-
34	CHL	s	607	-	3/3/16/26	14/19/117/137	-
23	CLA	R	604	-	1/1/11/20	7/17/95/115	-
23	CLA	Y	311	30	1/1/14/20	11/31/109/115	-
23	CLA	c	505	3	1/1/13/20	14/29/107/115	-
30	LHG	A	411	-	-	10/50/50/53	-
37	XAT	R	616	-	-	2/31/93/93	0/4/4/4
23	CLA	c	508	3	1/1/15/20	11/37/115/115	-
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2
28	DGD	C	517	-	-	6/44/84/95	0/2/2/2
34	CHL	G	608	-	3/3/20/26	19/39/137/137	-
23	CLA	s	602	22	1/1/11/20	7/15/93/115	-
33	HEM	E	101	6,5	-	5/12/54/54	-
34	CHL	R	605	-	3/3/16/26	1/15/113/137	-
26	SQD	A	406	-	-	11/45/65/69	0/1/1/1
28	DGD	A	408	-	-	10/48/88/95	0/2/2/2
35	LUT	r	615	-	-	3/29/67/67	0/2/2/2
25	BCR	c	518	-	-	6/29/63/63	0/2/2/2
23	CLA	Y	303	20	1/1/14/20	17/33/111/115	-
23	CLA	c	509	3	1/1/15/20	14/37/115/115	-
23	CLA	c	512	3	1/1/13/20	9/27/105/115	-
23	CLA	b	601	-	1/1/15/20	14/37/115/115	-
34	CHL	r	605	-	3/3/16/26	2/15/113/137	-
35	LUT	y	315	-	-	5/29/67/67	0/2/2/2
23	CLA	Y	314	20	1/1/11/20	4/13/91/115	-
34	CHL	N	307	-	3/3/16/26	10/15/113/137	-
23	CLA	y	314	20	1/1/11/20	4/13/91/115	-
27	LMG	b	620	-	-	8/46/66/70	0/1/1/1
23	CLA	r	601	15	1/1/11/20	8/18/96/115	-
34	CHL	r	607	-	3/3/19/26	12/33/131/137	-
30	LHG	a	412	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PL9	D	406	-	-	24/53/73/73	0/1/1/1
30	LHG	S	617	23	-	10/53/53/53	-
25	BCR	F	101	-	-	5/29/63/63	0/2/2/2
23	CLA	b	603	2	1/1/15/20	16/37/115/115	-
35	LUT	g	616	-	-	5/29/67/67	0/2/2/2
28	DGD	c	516	-	-	10/44/84/95	0/2/2/2
23	CLA	s	610	30	1/1/10/20	6/10/88/115	-
23	CLA	G	613	7	1/1/13/20	7/29/107/115	-
24	PHO	a	404	-	-	13/37/103/103	0/5/6/6
34	CHL	R	613	15	3/3/15/26	7/10/108/137	-
23	CLA	c	501	3	1/1/15/20	9/37/115/115	-
23	CLA	c	502	3	1/1/15/20	20/37/115/115	-
23	CLA	R	608	15,23	1/1/13/20	6/29/107/115	-
27	LMG	D	407	-	-	5/41/61/70	0/1/1/1
25	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
30	LHG	a	411	-	-	13/50/50/53	-
34	CHL	g	608	-	3/3/20/26	19/39/137/137	-
23	CLA	N	313	7	1/1/11/20	5/13/91/115	-
37	XAT	G	620	-	-	0/31/93/93	0/4/4/4
23	CLA	b	609	2	1/1/15/20	13/37/115/115	-
30	LHG	c	517	-	-	11/53/53/53	-
27	LMG	B	622	-	-	5/35/55/70	0/1/1/1
24	PHO	A	403	-	-	12/37/103/103	0/5/6/6
23	CLA	y	312	20	1/1/14/20	10/31/109/115	-
35	LUT	R	615	-	-	3/29/67/67	0/2/2/2
23	CLA	a	401	1	1/1/15/20	15/37/115/115	-
23	CLA	B	609	2	1/1/15/20	13/37/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	603	2	1/1/15/20	15/37/115/115	-
23	CLA	g	614	7	1/1/10/20	2/10/88/115	-
23	CLA	G	610	7	1/1/14/20	12/36/114/115	-
36	NEX	G	617	-	-	2/27/83/83	0/3/3/3
23	CLA	C	502	3	1/1/15/20	13/37/115/115	-
37	XAT	n	301	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LUT	n	317	-	-	5/29/67/67	0/2/2/2
34	CHL	G	607	-	3/3/15/26	7/12/110/137	-
30	LHG	A	412	-	-	15/53/53/53	-
25	BCR	K	101	-	-	6/29/63/63	0/2/2/2
30	LHG	W	201	-	-	18/53/53/53	-
36	NEX	R	617	-	-	3/27/83/83	0/3/3/3
23	CLA	C	511	3	1/1/15/20	16/37/115/115	-
23	CLA	Y	312	20	1/1/14/20	9/31/109/115	-
34	CHL	N	308	-	3/3/16/26	11/15/113/137	-
25	BCR	B	619	-	-	6/29/63/63	0/2/2/2
23	CLA	C	513	3	1/1/13/20	8/27/105/115	-
34	CHL	y	307	-	3/3/16/26	11/20/118/137	-
27	LMG	A	407	-	-	6/35/55/70	0/1/1/1
23	CLA	R	601	15	1/1/11/20	5/18/96/115	-
23	CLA	b	613	2	1/1/15/20	11/37/115/115	-
34	CHL	Y	302	20	3/3/20/26	14/39/137/137	-
34	CHL	s	605	-	3/3/16/26	9/15/113/137	-
25	BCR	B	617	-	-	6/29/63/63	0/2/2/2
32	PL9	d	407	-	-	25/53/73/73	0/1/1/1
23	CLA	S	613	22	1/1/10/20	5/8/86/115	-
30	LHG	y	318	23	-	10/53/53/53	-
34	CHL	n	310	7	3/3/20/26	18/39/137/137	-
30	LHG	B	621	-	-	12/53/53/53	-
23	CLA	b	610	-	1/1/15/20	11/37/115/115	-
23	CLA	R	610	30	1/1/11/20	7/18/96/115	-
23	CLA	B	615	2	1/1/15/20	12/37/115/115	-
23	CLA	r	604	-	1/1/11/20	9/17/95/115	-
36	NEX	g	617	23	-	4/27/83/83	0/3/3/3
26	SQD	a	409	-	-	16/49/69/69	0/1/1/1
23	CLA	S	608	22	1/1/11/20	4/13/91/115	-
27	LMG	C	501	-	-	7/43/63/70	0/1/1/1
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
30	LHG	R	618	23	-	11/46/46/53	-
26	SQD	M	101	-	-	16/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LUT	N	317	-	-	3/29/67/67	0/2/2/2
34	CHL	g	601	7	3/3/20/26	10/39/137/137	-
23	CLA	n	314	7	1/1/14/20	13/31/109/115	-
34	CHL	S	601	22	3/3/16/26	7/15/113/137	-
35	LUT	S	615	-	-	6/29/67/67	0/2/2/2
23	CLA	n	311	7	1/1/13/20	10/30/108/115	-
23	CLA	b	604	2	1/1/15/20	13/37/115/115	-
23	CLA	n	304	7	1/1/13/20	9/30/108/115	-
36	NEX	Y	317	-	-	3/27/83/83	0/3/3/3
23	CLA	G	612	7	1/1/11/20	6/13/91/115	-
23	CLA	g	610	7	1/1/14/20	11/36/114/115	-
30	LHG	n	319	23	-	15/53/53/53	-
30	LHG	s	617	23	-	10/53/53/53	-
34	CHL	g	619	-	3/3/20/26	25/39/137/137	-
34	CHL	G	605	7	3/3/16/26	11/15/113/137	-
23	CLA	C	503	3	1/1/15/20	22/37/115/115	-
23	CLA	b	616	2	1/1/15/20	12/37/115/115	-
23	CLA	B	608	2	1/1/15/20	16/37/115/115	-
25	BCR	b	617	-	-	6/29/63/63	0/2/2/2
26	SQD	L	103	-	-	17/49/69/69	0/1/1/1
30	LHG	g	618	23	-	11/50/50/53	-
30	LHG	b	622	-	-	8/53/53/53	-
30	LHG	G	618	23	-	15/50/50/53	-
23	CLA	N	305	-	1/1/12/20	9/19/97/115	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
23	CLA	A	401	1	1/1/15/20	15/37/115/115	-
34	CHL	s	606	-	3/3/15/26	6/12/110/137	-
23	CLA	C	507	3	1/1/12/20	9/21/99/115	-
23	CLA	G	604	-	1/1/11/20	9/18/96/115	-
35	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	R	602	15	1/1/14/20	8/31/109/115	-
23	CLA	r	609	15	1/1/15/20	10/37/115/115	-
23	CLA	g	613	7	1/1/13/20	5/29/107/115	-
23	CLA	r	603	15	1/1/14/20	7/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	g	603	7	1/1/15/20	8/37/115/115	-
25	BCR	H	101	-	-	5/29/63/63	0/2/2/2
36	NEX	y	317	-	-	4/27/83/83	0/3/3/3
23	CLA	C	504	3	1/1/15/20	17/37/115/115	-
30	LHG	B	623	-	-	10/53/53/53	-
23	CLA	Y	305	-	1/1/12/20	8/19/97/115	-
23	CLA	s	613	22	1/1/10/20	5/8/86/115	-
23	CLA	g	611	30	1/1/14/20	10/31/109/115	-
23	CLA	S	603	22	1/1/11/20	7/13/91/115	-
25	BCR	h	101	-	-	7/29/63/63	0/2/2/2
26	SQD	A	409	-	-	14/49/69/69	0/1/1/1
23	CLA	b	611	2	1/1/15/20	8/37/115/115	-
35	LUT	n	316	-	-	2/29/67/67	0/2/2/2
34	CHL	g	606	-	3/3/15/26	9/12/110/137	-
27	LMG	B	620	-	-	9/46/66/70	0/1/1/1
23	CLA	C	506	3	1/1/13/20	13/29/107/115	-
23	CLA	b	602	2	1/1/15/20	8/37/115/115	-
37	XAT	N	301	-	-	1/31/93/93	0/4/4/4
23	CLA	b	607	-	1/1/15/20	14/37/115/115	-
34	CHL	S	605	-	3/3/16/26	11/15/113/137	-
25	BCR	C	515	-	-	5/29/63/63	0/2/2/2
34	CHL	Y	309	20	3/3/20/26	23/39/137/137	-
23	CLA	G	614	7	1/1/10/20	0/10/88/115	-
34	CHL	S	606	-	3/3/15/26	9/12/110/137	-
34	CHL	r	613	15	3/3/15/26	7/10/108/137	-
34	CHL	g	607	-	3/3/15/26	8/12/110/137	-
34	CHL	n	306	7	3/3/16/26	9/18/116/137	-
23	CLA	s	604	-	1/1/12/20	5/19/97/115	-
30	LHG	N	319	23	-	11/53/53/53	-
23	CLA	g	602	7	1/1/15/20	19/37/115/115	-
23	CLA	S	609	22	1/1/11/20	8/13/91/115	-
23	CLA	B	612	2	1/1/15/20	15/37/115/115	-
37	XAT	y	301	-	-	2/31/93/93	0/4/4/4
34	CHL	r	606	-	3/3/16/26	8/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	2	1/1/15/20	7/37/115/115	-
34	CHL	g	609	7	3/3/19/26	8/33/131/137	-
23	CLA	B	605	2	1/1/15/20	11/37/115/115	-
23	CLA	d	404	4	1/1/15/20	9/37/115/115	-
23	CLA	s	611	22	1/1/11/20	6/13/91/115	-
23	CLA	S	602	22	1/1/11/20	8/15/93/115	-
23	CLA	b	612	2	1/1/15/20	15/37/115/115	-
23	CLA	b	614	2	1/1/15/20	21/37/115/115	-
23	CLA	b	606	2	1/1/15/20	6/37/115/115	-

The worst 5 of 1846 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	407	PL9	C23-C24	10.19	1.57	1.33
32	D	406	PL9	C23-C24	10.15	1.57	1.33
32	D	406	PL9	C38-C39	9.99	1.56	1.33
32	d	407	PL9	C38-C39	9.88	1.56	1.33
32	d	407	PL9	C18-C19	9.44	1.55	1.33

The worst 5 of 2943 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	SQD	O9-S-C6	-19.33	83.97	106.94
26	a	409	SQD	O9-S-C6	-19.29	84.01	106.94
36	Y	317	NEX	C17-C1-C6	-19.09	93.39	110.47
36	y	317	NEX	C17-C1-C6	-17.33	94.96	110.47
36	G	617	NEX	O24-C25-C24	13.28	123.36	113.38

5 of 312 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	401	CLA	ND
23	A	402	CLA	ND
23	A	404	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

5 of 3010 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	401	CLA	C2-C3-C5-C6
23	A	401	CLA	C4-C3-C5-C6
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	402	CLA	C3A-C2A-CAA-CBA
23	A	402	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

252 monomers are involved in 515 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	y	311	CLA	1	0
23	S	610	CLA	1	0
23	D	401	CLA	3	0
23	D	404	CLA	6	0
23	B	604	CLA	1	0
23	B	607	CLA	1	0
35	G	615	LUT	3	0
23	g	612	CLA	1	0
23	B	602	CLA	2	0
36	r	617	NEX	2	0
28	d	410	DGD	4	0
23	r	614	CLA	2	0
25	d	406	BCR	2	0
34	n	302	CHL	1	0
23	S	612	CLA	3	0
23	s	609	CLA	1	0
35	y	316	LUT	2	0
23	b	605	CLA	4	0
35	g	615	LUT	4	0
34	y	309	CHL	3	0
35	s	614	LUT	4	0
23	G	602	CLA	4	0
35	N	316	LUT	3	0
23	y	310	CLA	1	0
23	g	604	CLA	2	0
23	A	402	CLA	2	0
34	R	607	CHL	3	0
23	c	503	CLA	5	0
23	B	610	CLA	4	0
35	S	614	LUT	5	0
23	B	614	CLA	1	0
23	r	608	CLA	2	0
23	a	402	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	n	318	NEX	3	0
34	R	606	CHL	1	0
34	G	609	CHL	2	0
23	a	403	CLA	2	0
35	G	616	LUT	5	0
23	c	506	CLA	1	0
23	C	514	CLA	3	0
34	G	601	CHL	4	0
34	g	605	CHL	1	0
34	N	309	CHL	4	0
23	C	510	CLA	3	0
30	L	102	LHG	1	0
30	Y	318	LHG	1	0
34	N	310	CHL	3	0
23	G	603	CLA	3	0
23	Y	310	CLA	1	0
23	n	315	CLA	1	0
34	S	607	CHL	1	0
30	r	618	LHG	2	0
25	a	406	BCR	2	0
24	d	401	PHO	4	0
23	n	305	CLA	1	0
23	s	612	CLA	5	0
23	C	512	CLA	2	0
30	L	101	LHG	4	0
30	d	408	LHG	6	0
34	n	307	CHL	2	0
23	y	313	CLA	1	0
23	N	314	CLA	3	0
23	c	511	CLA	7	0
23	r	602	CLA	1	0
35	Y	315	LUT	4	0
23	B	616	CLA	2	0
23	c	513	CLA	2	0
34	n	308	CHL	2	0
23	r	611	CLA	2	0
36	s	616	NEX	2	0
30	C	518	LHG	3	0
34	y	302	CHL	3	0
30	w	201	LHG	1	0
23	Y	313	CLA	1	0
23	N	312	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	T	101	LHG	2	0
23	C	509	CLA	1	0
27	a	407	LMG	2	0
34	y	306	CHL	2	0
25	A	405	BCR	4	0
23	R	609	CLA	2	0
28	a	408	DGD	3	0
23	y	303	CLA	2	0
25	c	514	BCR	7	0
34	G	619	CHL	3	0
25	b	619	BCR	3	0
23	R	614	CLA	2	0
37	g	620	XAT	3	0
23	r	610	CLA	1	0
28	H	102	DGD	4	0
23	A	404	CLA	2	0
23	B	601	CLA	2	0
23	N	311	CLA	2	0
23	a	405	CLA	1	0
36	N	318	NEX	2	0
23	c	510	CLA	5	0
25	C	516	BCR	4	0
26	d	402	SQD	2	0
23	d	405	CLA	2	0
23	R	612	CLA	2	0
23	B	613	CLA	2	0
34	n	309	CHL	3	0
37	Y	301	XAT	5	0
24	D	402	PHO	7	0
23	b	608	CLA	6	0
23	B	606	CLA	2	0
23	C	505	CLA	1	0
34	G	606	CHL	1	0
34	Y	306	CHL	2	0
34	s	607	CHL	1	0
23	R	604	CLA	3	0
23	Y	311	CLA	2	0
23	c	505	CLA	1	0
37	R	616	XAT	1	0
23	c	508	CLA	3	0
25	c	515	BCR	5	0
28	C	517	DGD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	G	608	CHL	1	0
23	s	602	CLA	2	0
33	E	101	HEM	1	0
34	R	605	CHL	1	0
28	A	408	DGD	4	0
35	r	615	LUT	3	0
25	c	518	BCR	3	0
23	Y	303	CLA	2	0
23	c	509	CLA	2	0
23	c	512	CLA	2	0
23	b	601	CLA	3	0
34	r	605	CHL	1	0
35	y	315	LUT	3	0
34	N	307	CHL	1	0
27	b	620	LMG	4	0
23	r	601	CLA	2	0
30	a	412	LHG	4	0
34	r	607	CHL	3	0
32	D	406	PL9	2	0
30	S	617	LHG	3	0
25	F	101	BCR	2	0
23	b	603	CLA	7	0
35	g	616	LUT	9	0
28	c	516	DGD	2	0
23	s	610	CLA	1	0
24	a	404	PHO	1	0
23	c	501	CLA	1	0
23	c	502	CLA	4	0
27	D	407	LMG	2	0
25	Z	101	BCR	3	0
34	g	608	CHL	2	0
37	G	620	XAT	6	0
31	D	403	BCT	2	0
23	b	609	CLA	3	0
30	c	517	LHG	2	0
24	A	403	PHO	2	0
23	y	312	CLA	1	0
35	R	615	LUT	2	0
23	a	401	CLA	3	0
25	k	101	BCR	2	0
23	B	603	CLA	5	0
23	g	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	610	CLA	2	0
36	G	617	NEX	3	0
23	C	502	CLA	1	0
37	n	301	XAT	2	0
35	n	317	LUT	2	0
30	A	412	LHG	4	0
34	G	607	CHL	1	0
25	K	101	BCR	2	0
30	W	201	LHG	1	0
36	R	617	NEX	2	0
23	C	511	CLA	3	0
34	N	308	CHL	1	0
25	B	619	BCR	2	0
23	C	513	CLA	4	0
23	b	613	CLA	1	0
34	Y	302	CHL	4	0
25	B	617	BCR	2	0
34	s	605	CHL	1	0
32	d	407	PL9	3	0
23	S	613	CLA	3	0
30	y	318	LHG	1	0
34	n	310	CHL	1	0
23	b	610	CLA	4	0
23	B	615	CLA	4	0
23	r	604	CLA	1	0
36	g	617	NEX	3	0
26	a	409	SQD	1	0
27	C	501	LMG	2	0
25	b	618	BCR	3	0
30	R	618	LHG	2	0
26	M	101	SQD	3	0
35	N	317	LUT	4	0
34	g	601	CHL	6	0
23	n	314	CLA	2	0
34	S	601	CHL	1	0
35	S	615	LUT	3	0
23	n	311	CLA	2	0
23	b	604	CLA	1	0
23	G	612	CLA	1	0
23	g	610	CLA	2	0
30	n	319	LHG	1	0
30	s	617	LHG	2	0

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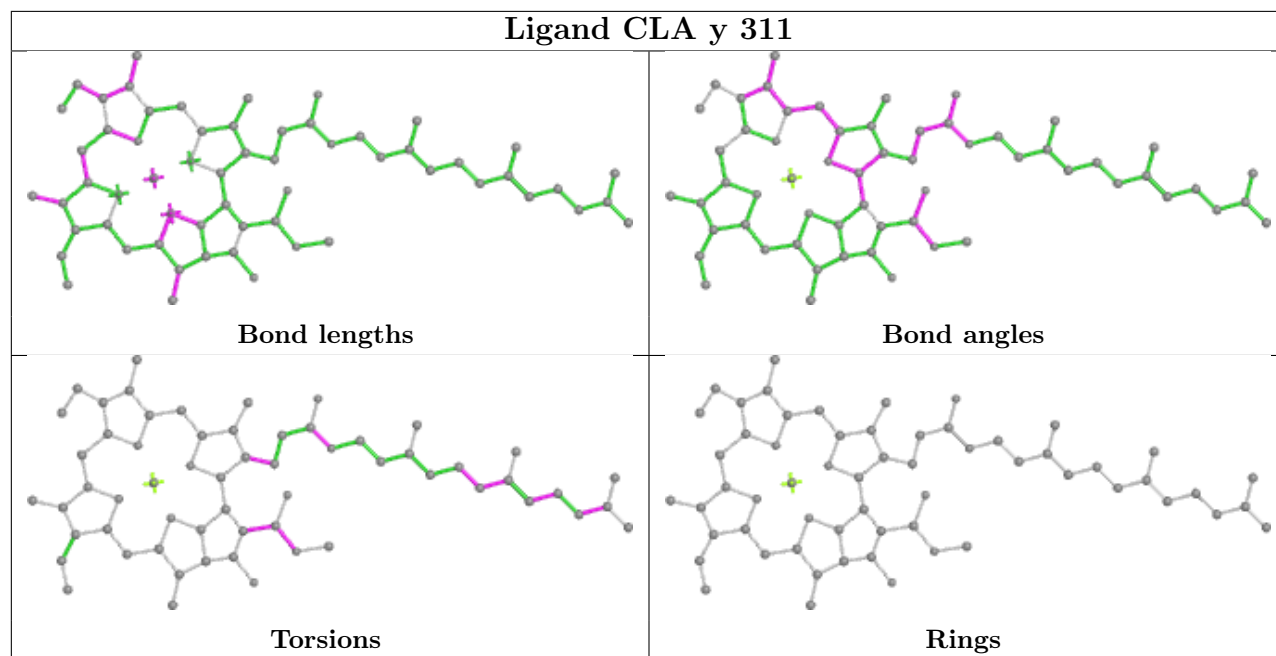
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	g	619	CHL	4	0
23	C	503	CLA	4	0
23	B	608	CLA	3	0
25	b	617	BCR	2	0
26	L	103	SQD	4	0
30	g	618	LHG	3	0
31	d	403	BCT	3	0
30	b	622	LHG	2	0
30	G	618	LHG	3	0
23	N	305	CLA	1	0
25	B	618	BCR	2	0
23	A	401	CLA	3	0
23	C	507	CLA	1	0
23	G	604	CLA	1	0
35	Y	316	LUT	2	0
23	R	602	CLA	1	0
23	r	609	CLA	4	0
23	g	603	CLA	2	0
25	H	101	BCR	4	0
23	C	504	CLA	4	0
30	B	623	LHG	2	0
23	s	613	CLA	4	0
23	g	611	CLA	2	0
23	S	603	CLA	1	0
25	h	101	BCR	5	0
26	A	409	SQD	1	0
23	b	611	CLA	1	0
35	n	316	LUT	2	0
34	g	606	CHL	3	0
27	B	620	LMG	5	0
23	C	506	CLA	1	0
23	b	602	CLA	1	0
23	b	607	CLA	1	0
34	S	605	CHL	2	0
25	C	515	BCR	5	0
34	Y	309	CHL	4	0
34	S	606	CHL	2	0
34	g	607	CHL	2	0
23	g	602	CLA	2	0
30	N	319	LHG	2	0
23	S	609	CLA	1	0
23	B	612	CLA	3	0

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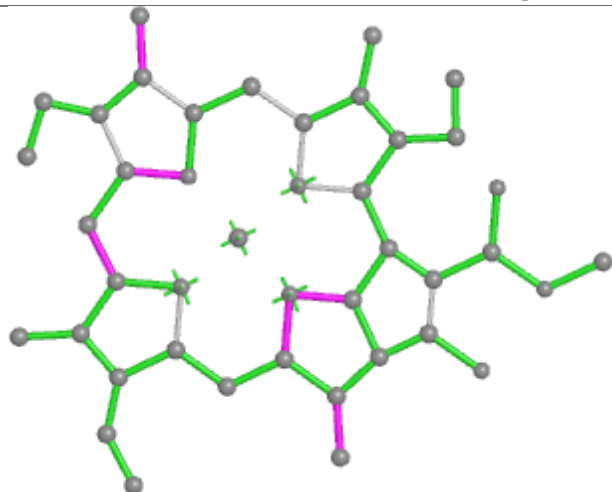
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	y	301	XAT	4	0
34	r	606	CHL	1	0
34	g	609	CHL	1	0
23	B	605	CLA	3	0
23	d	404	CLA	7	0
23	S	602	CLA	2	0
23	b	612	CLA	1	0
23	b	614	CLA	1	0
23	b	606	CLA	2	0

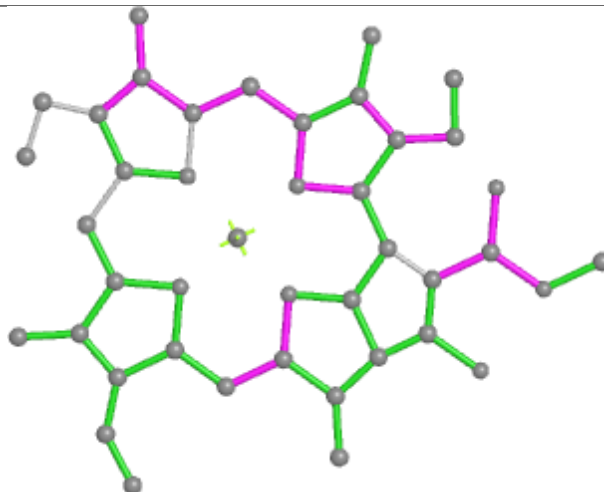
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



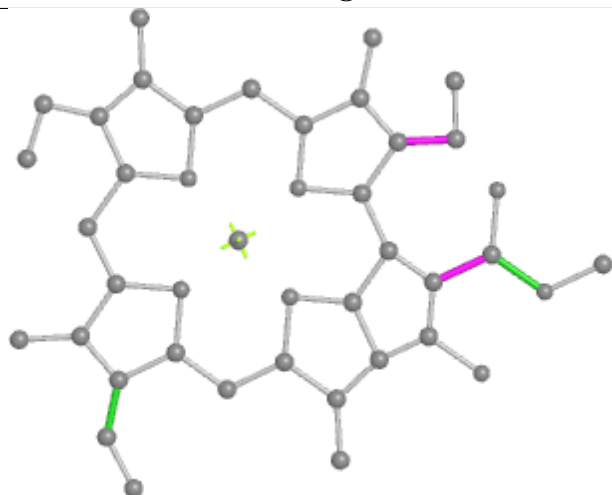
Ligand CLA S 610



Bond lengths



Bond angles

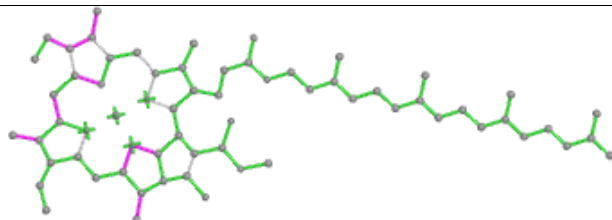


Torsions

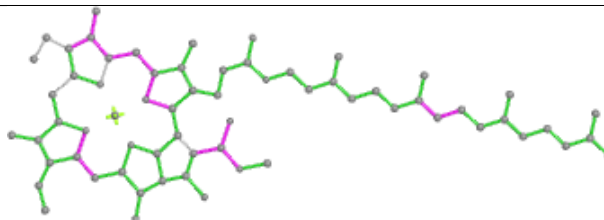


Rings

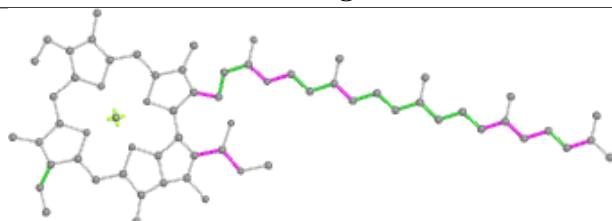
Ligand CLA D 401



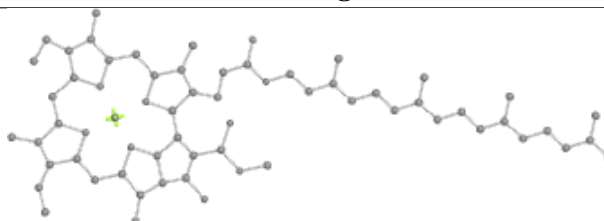
Bond lengths



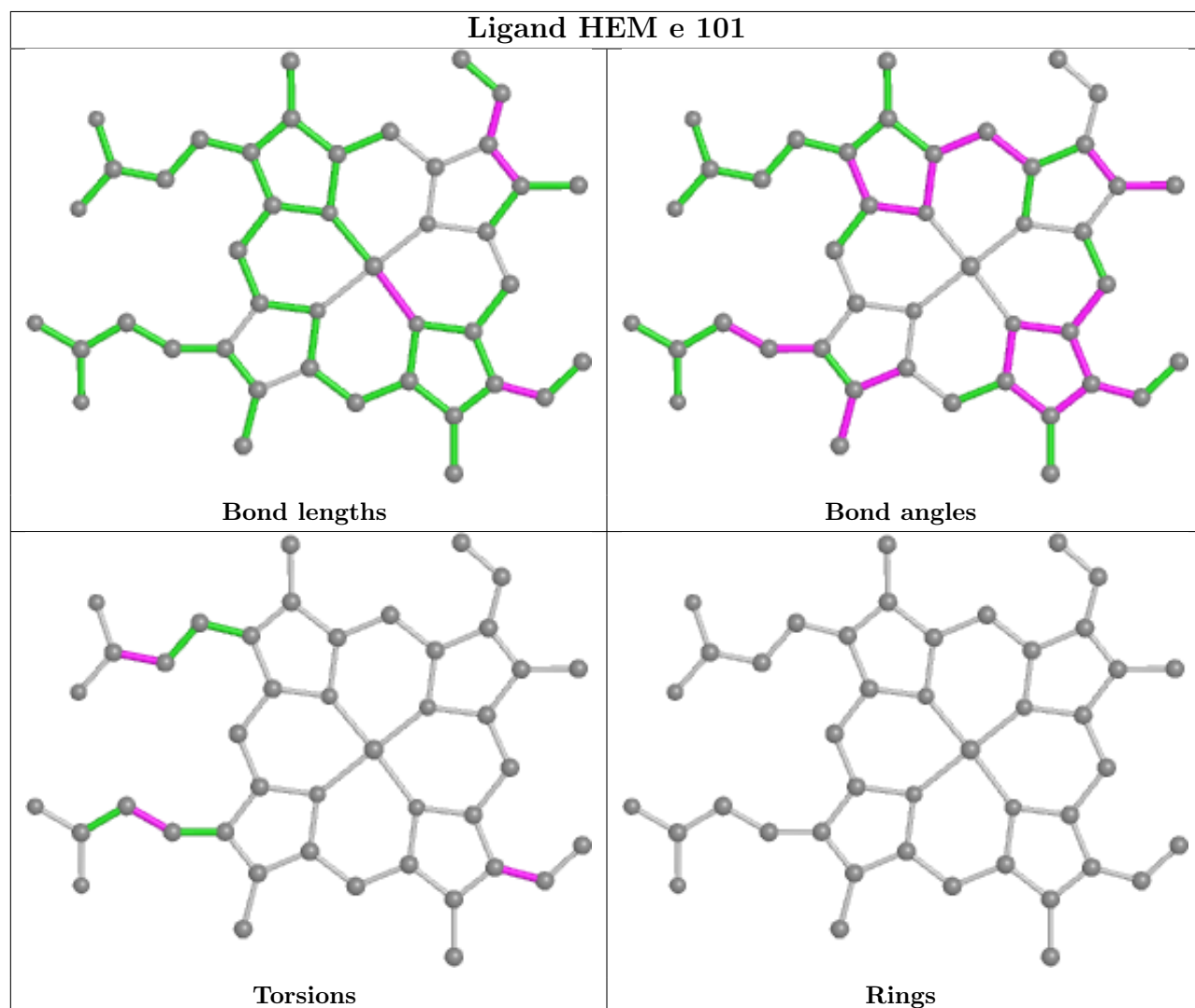
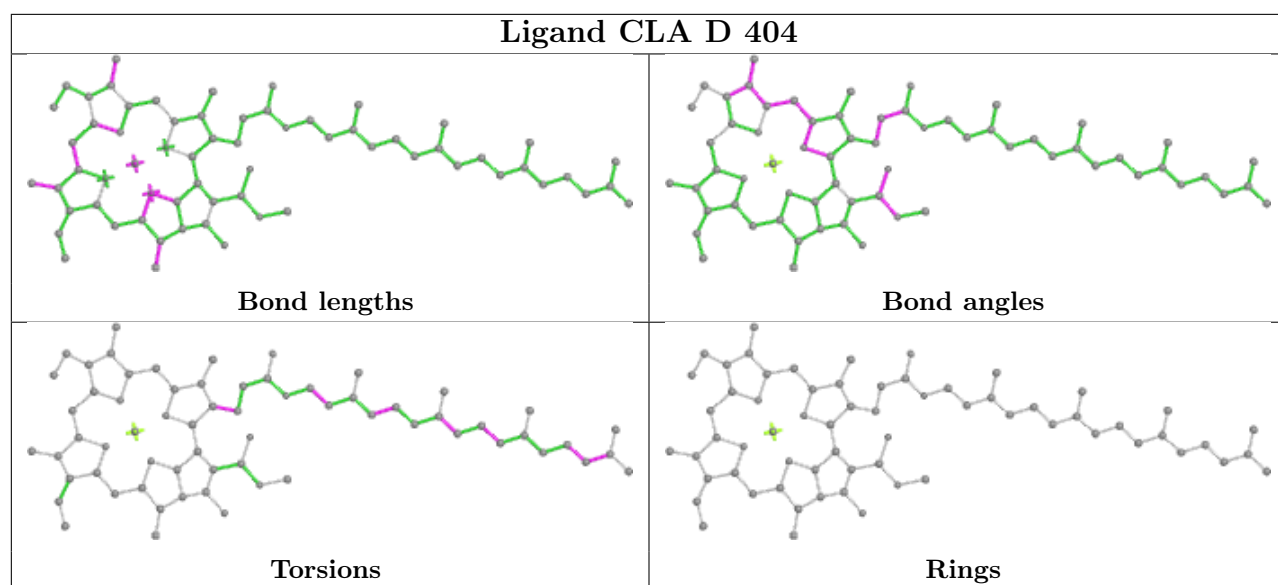
Bond angles

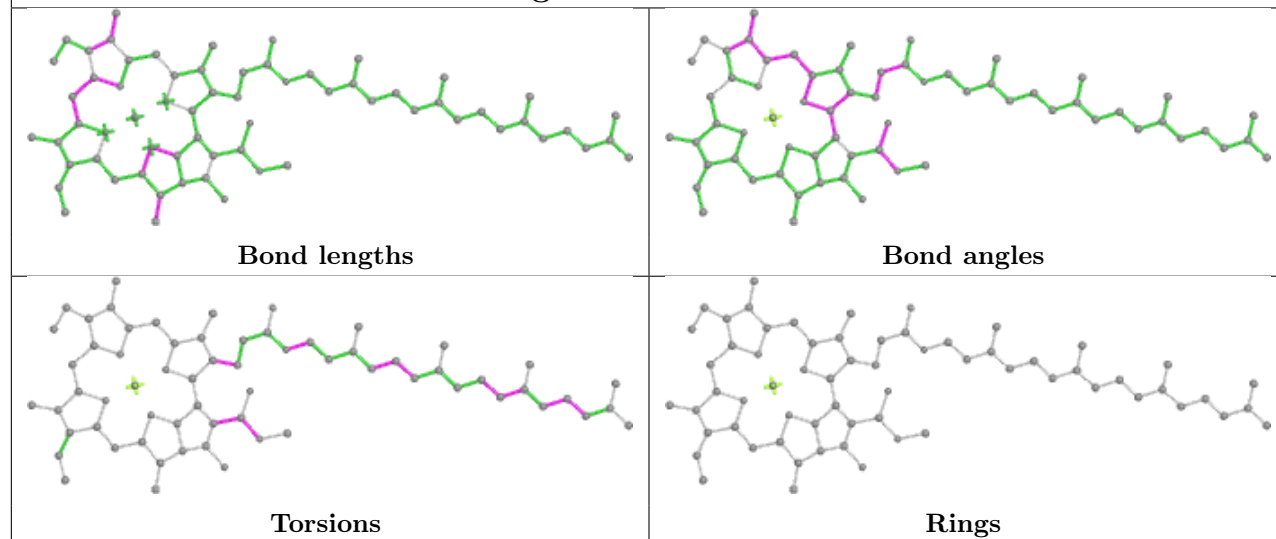
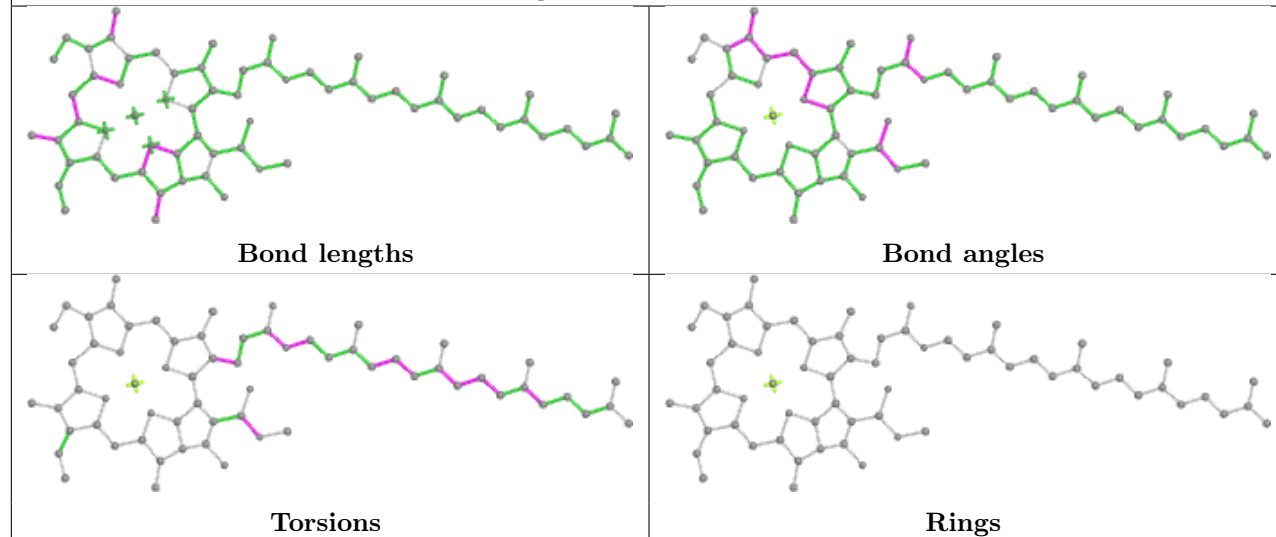
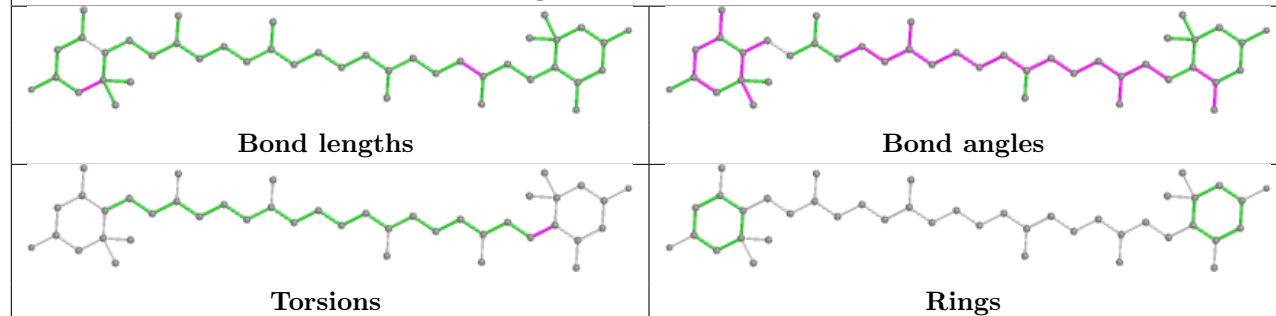


Torsions

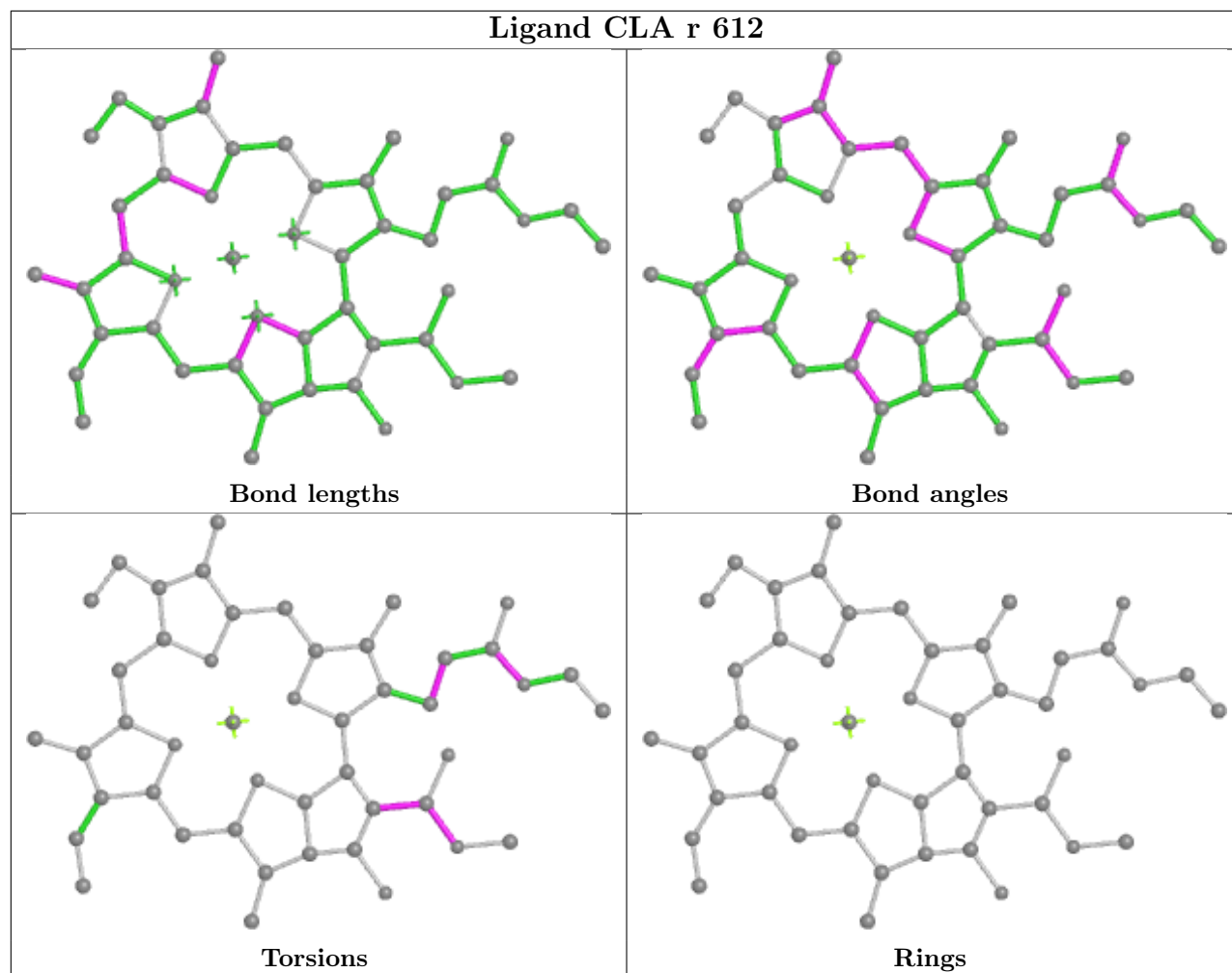


Rings

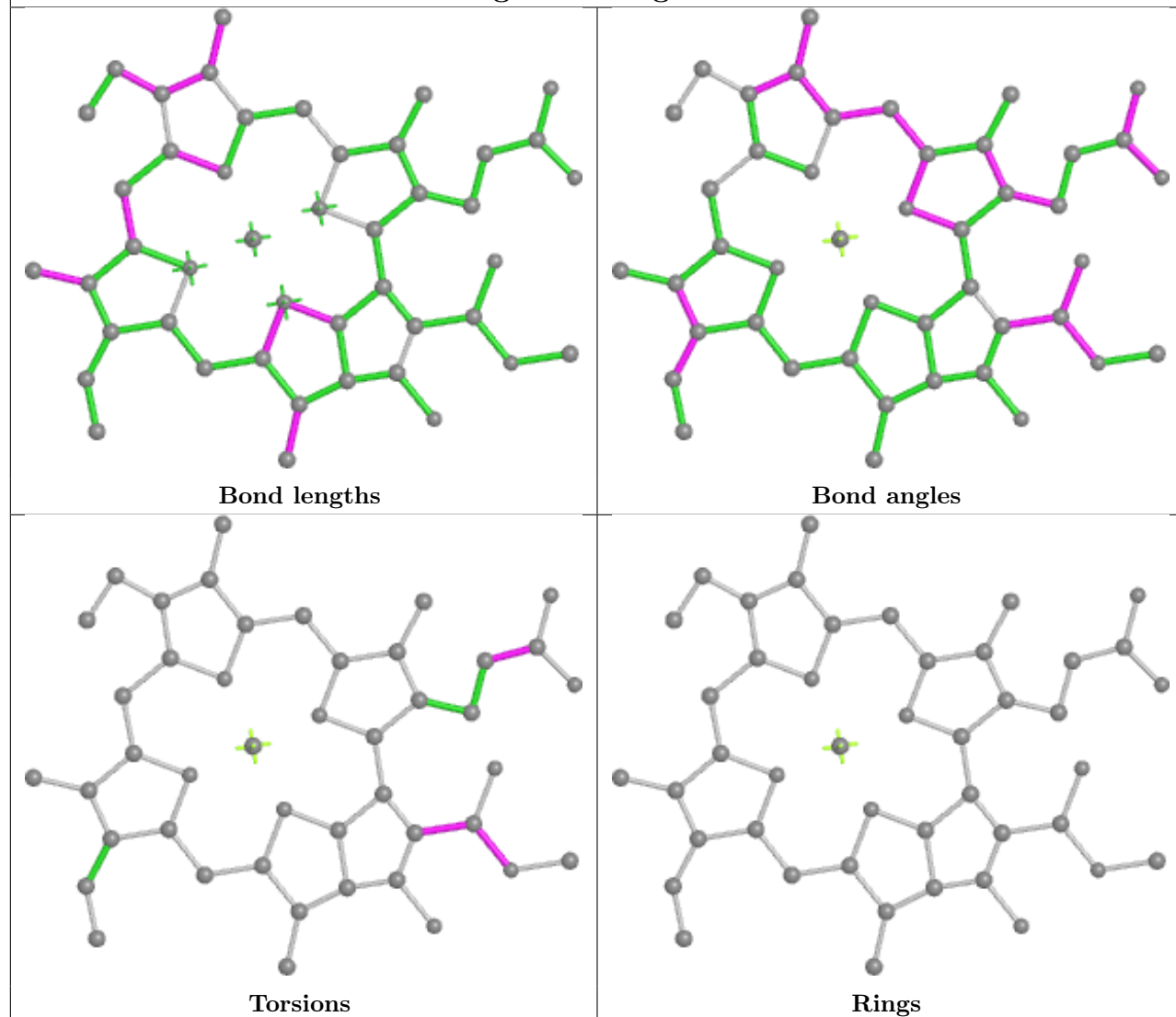


Ligand CLA B 604**Ligand CLA B 607****Ligand LUT G 615**

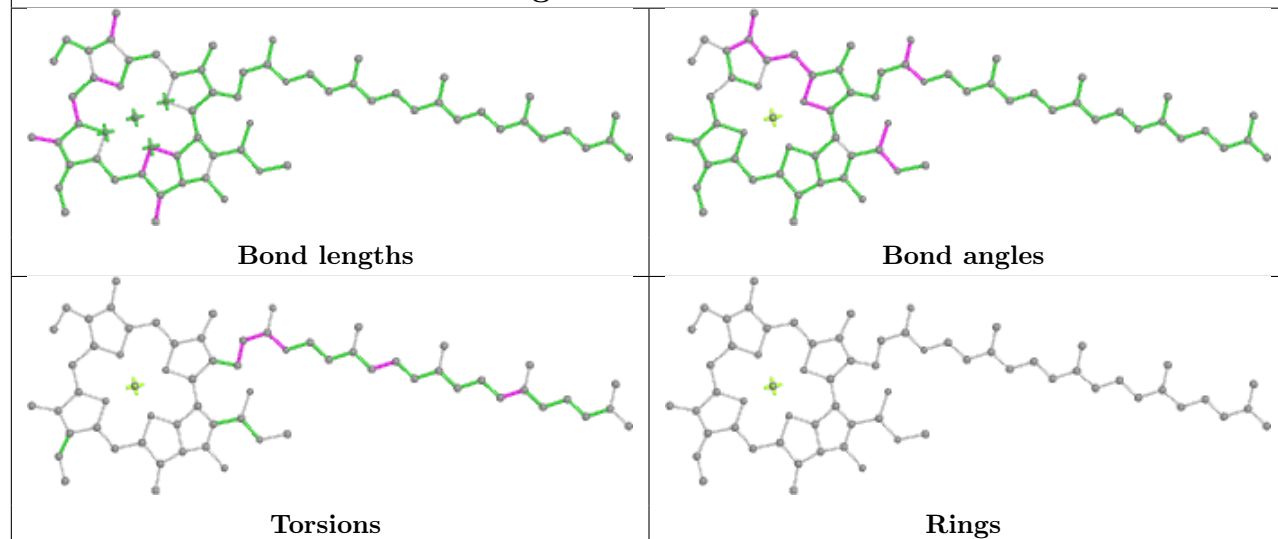
Ligand CLA r 612

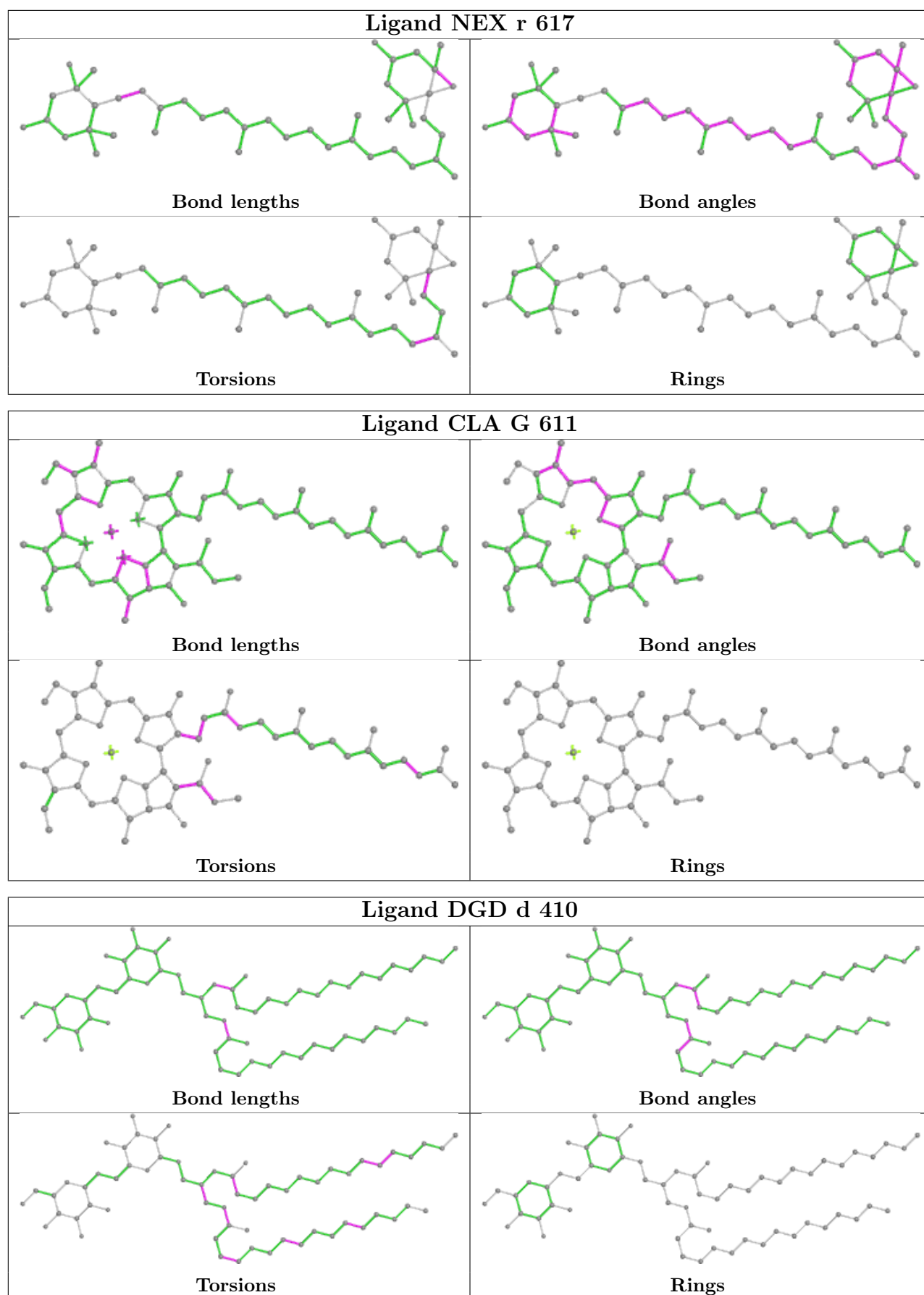


Ligand CLA g 612

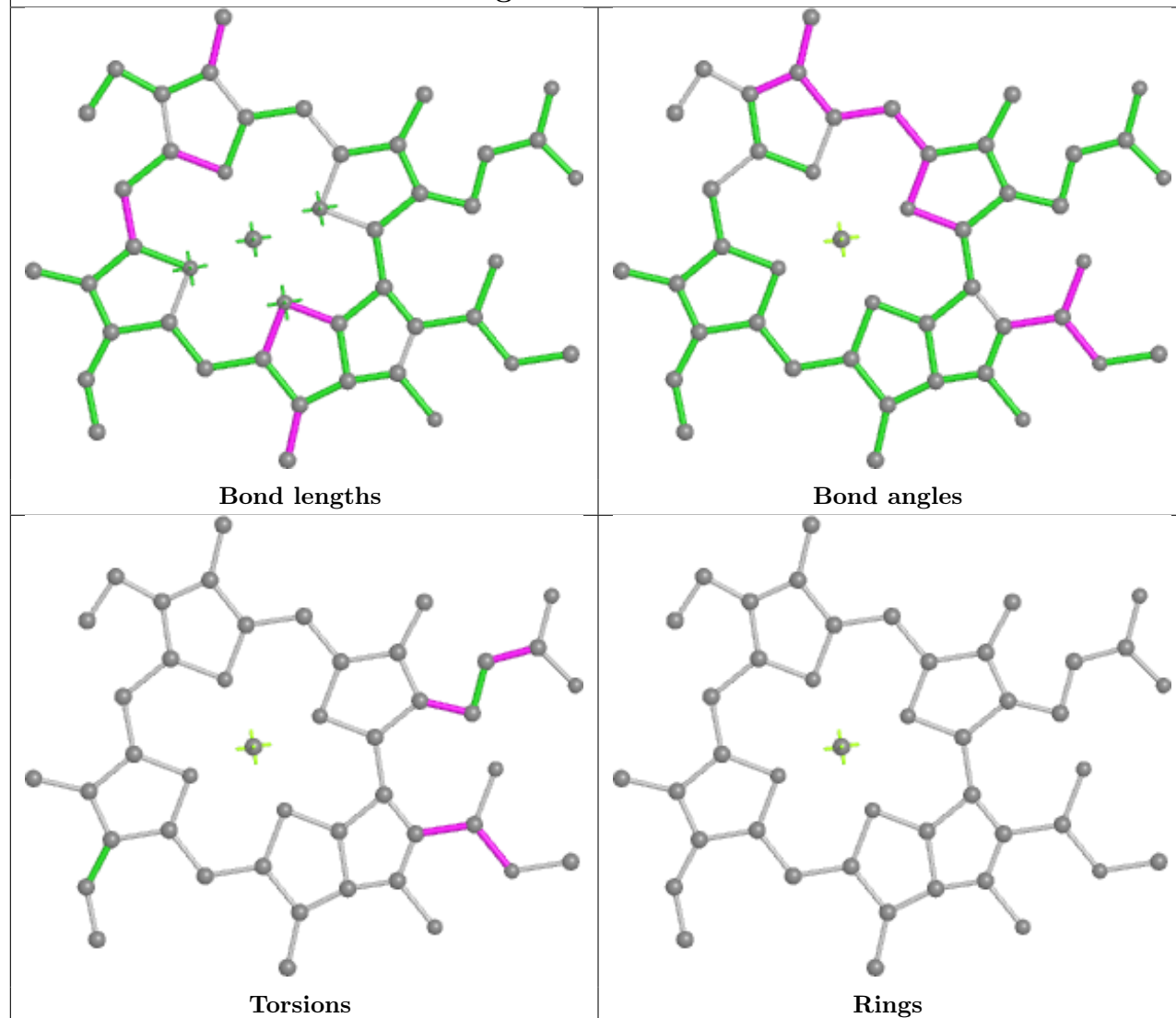


Ligand CLA B 602

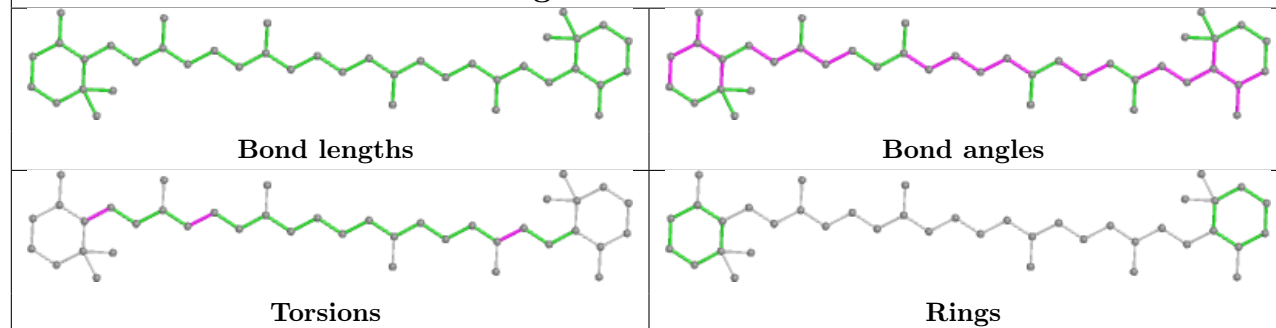


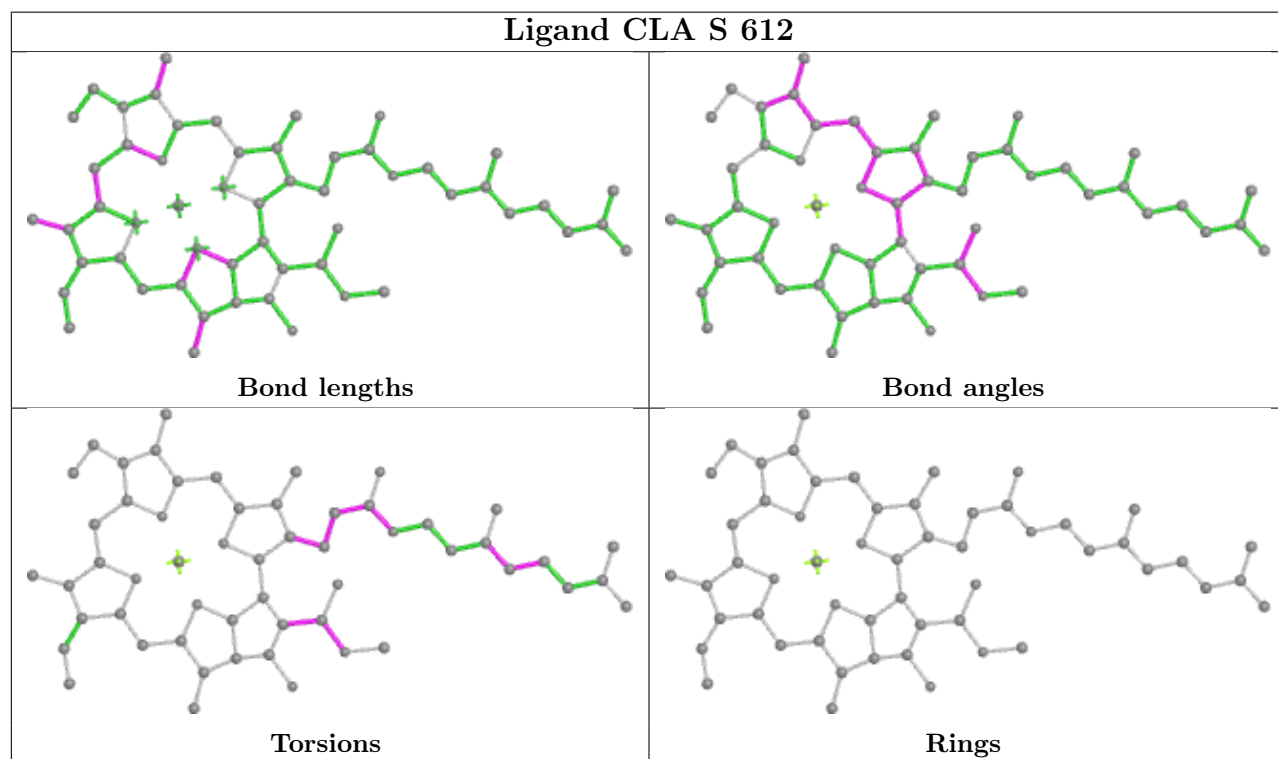
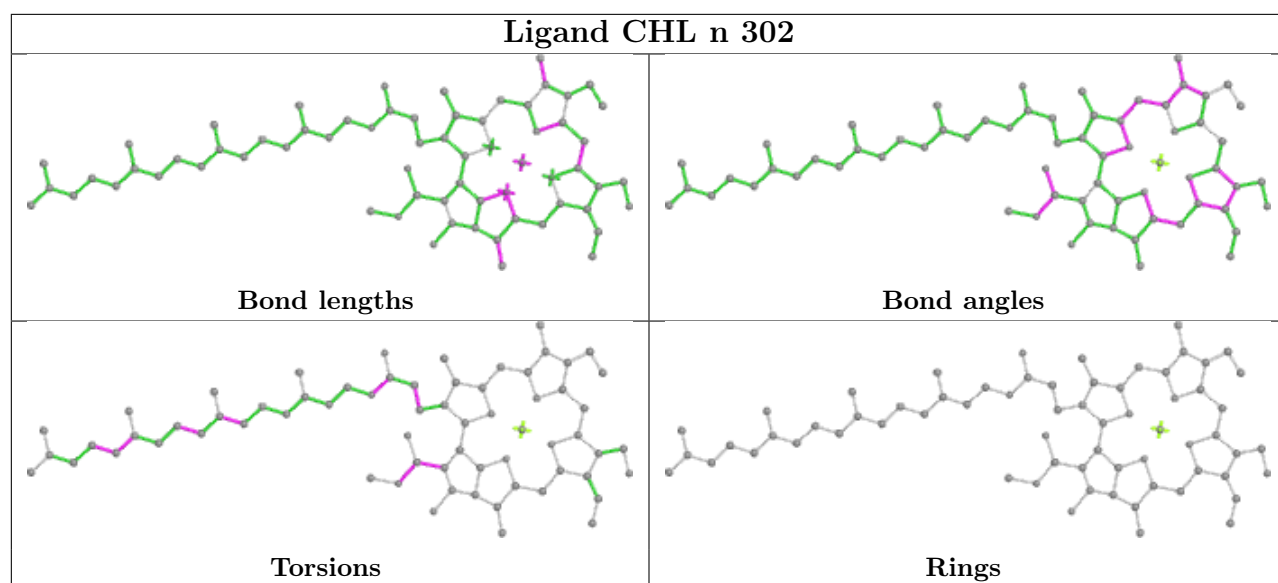


Ligand CLA r 614

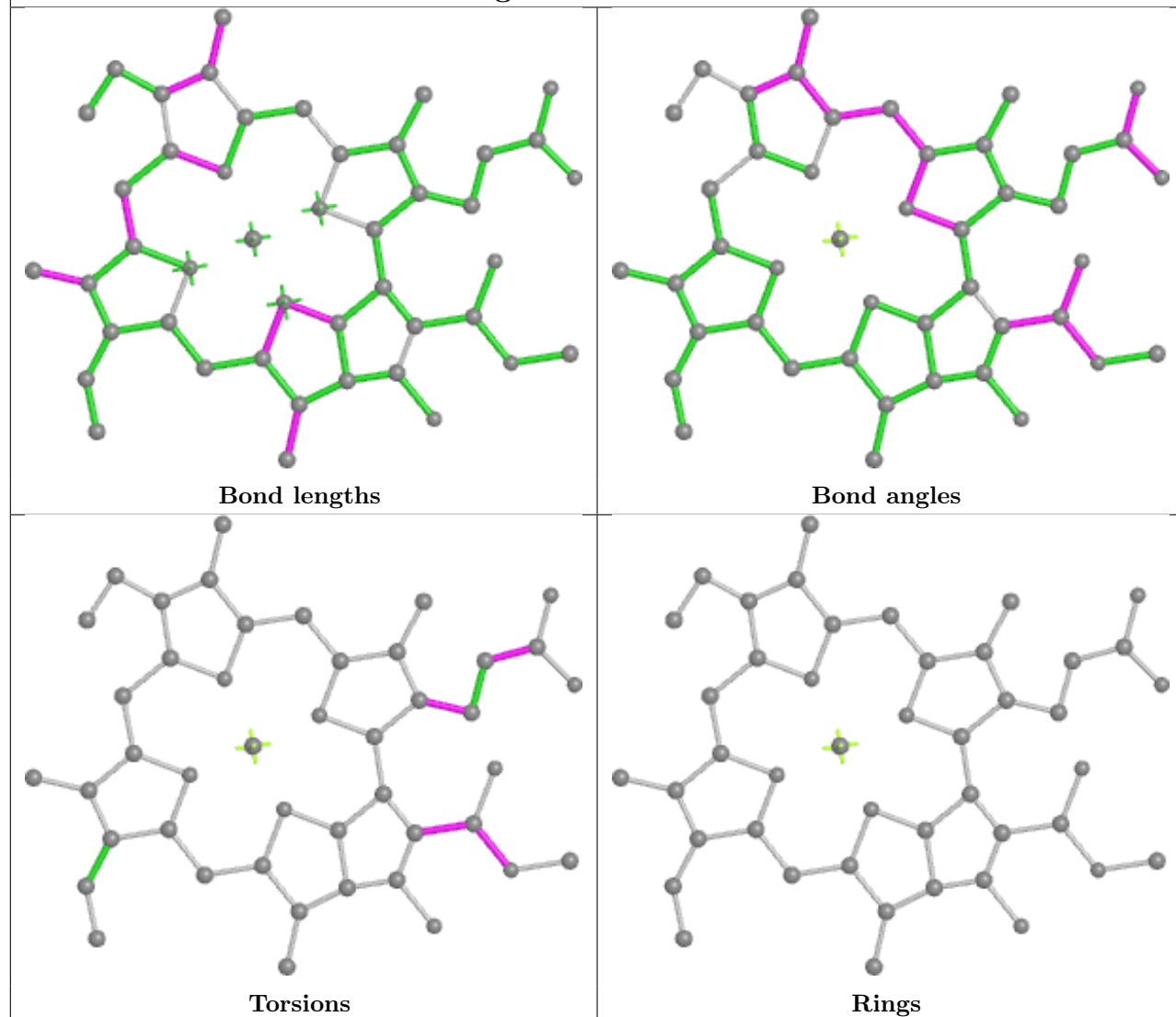


Ligand BCR d 406

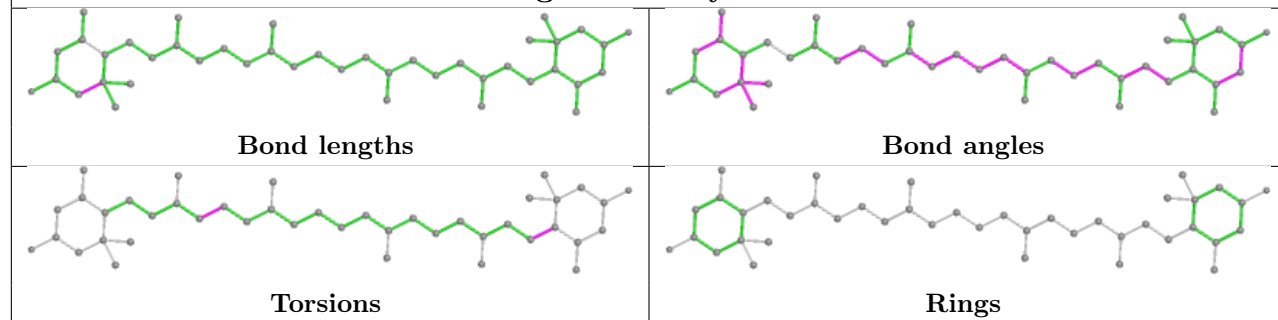


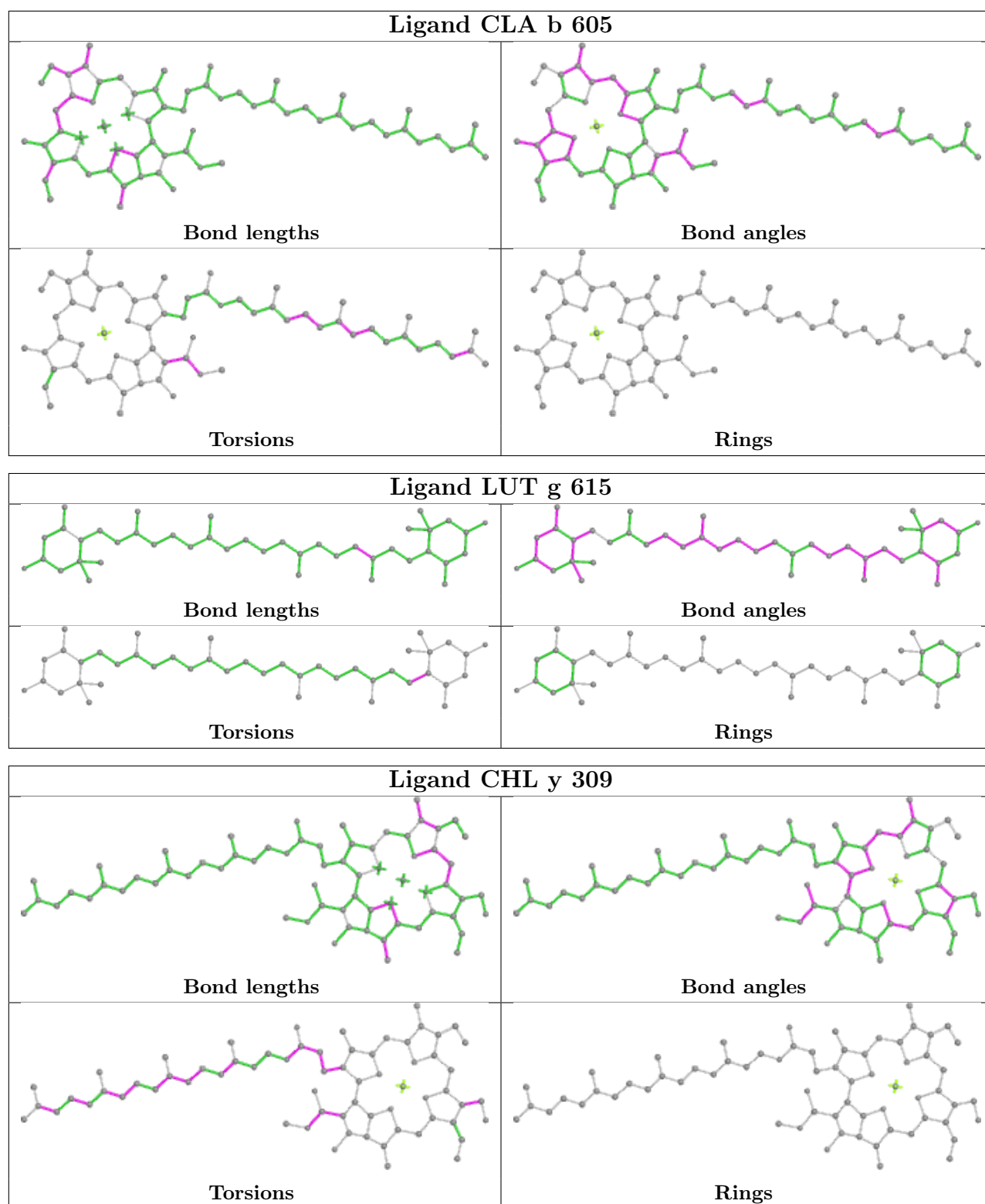


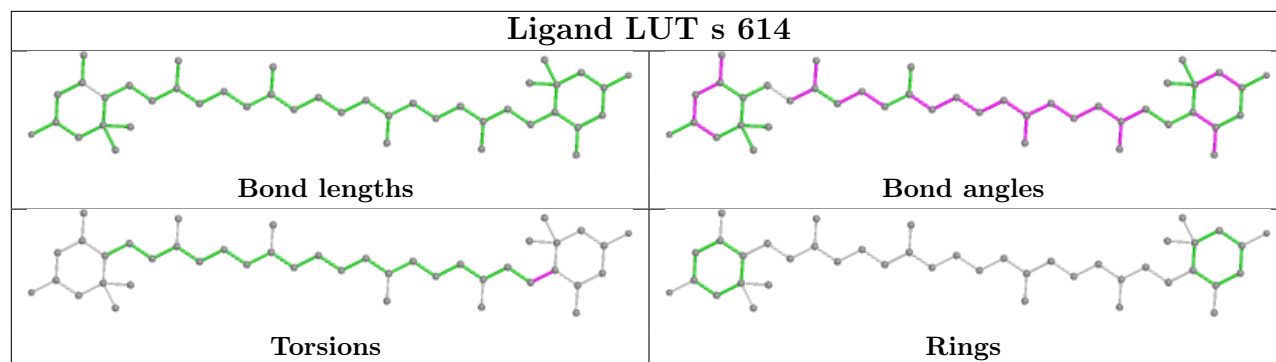
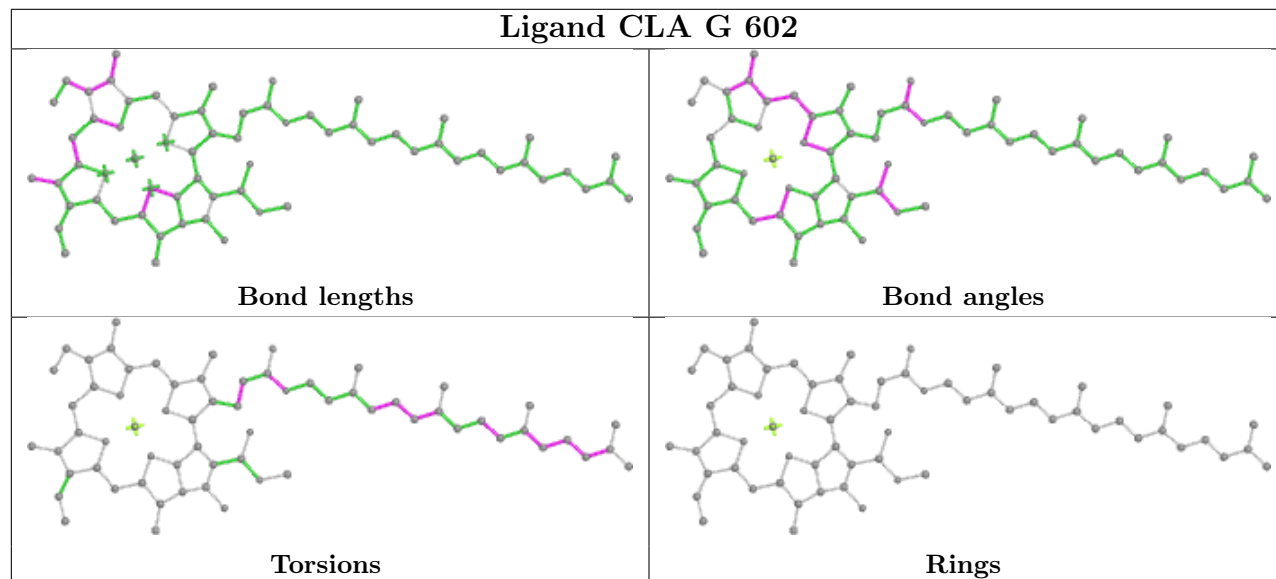
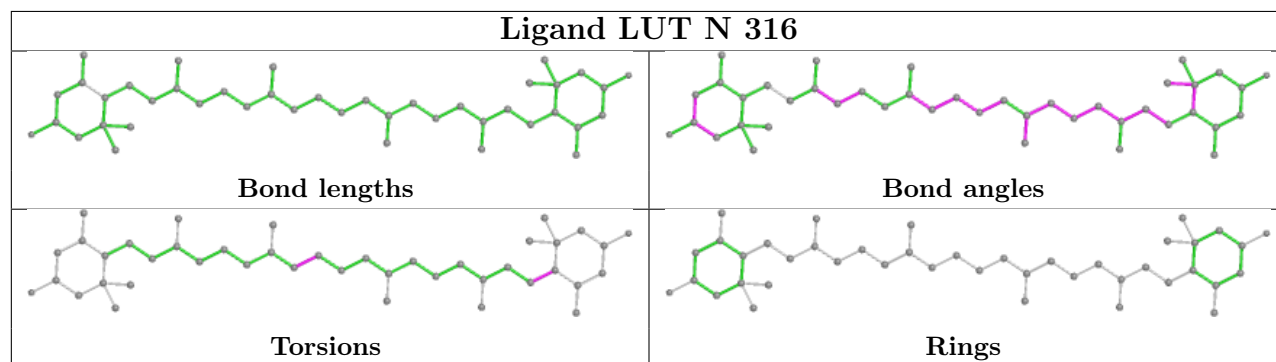
Ligand CLA s 609

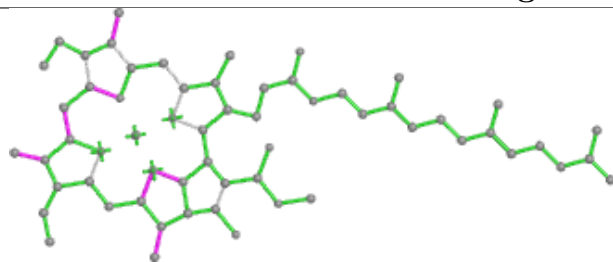


Ligand LUT y 316

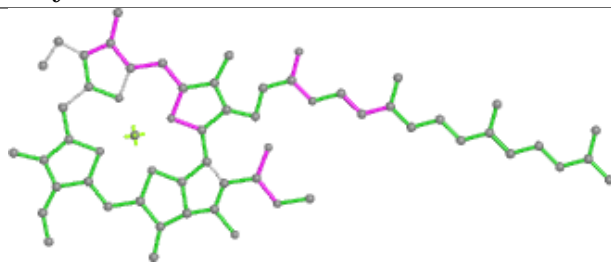




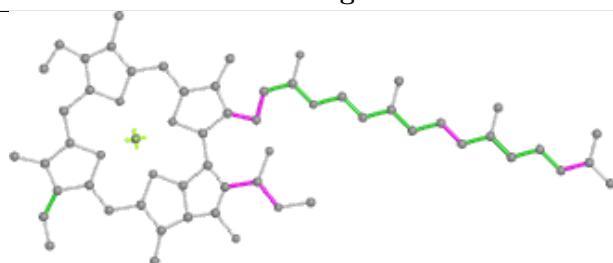
Ligand LUT s 614**Ligand CLA G 602****Ligand LUT N 316**

Ligand CLA y 310

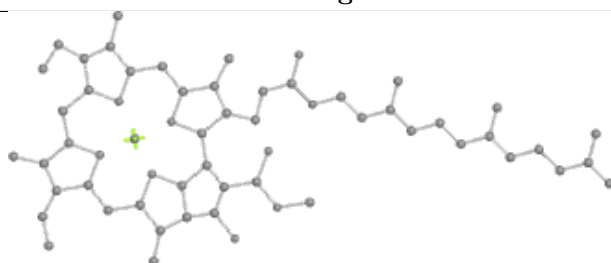
Bond lengths



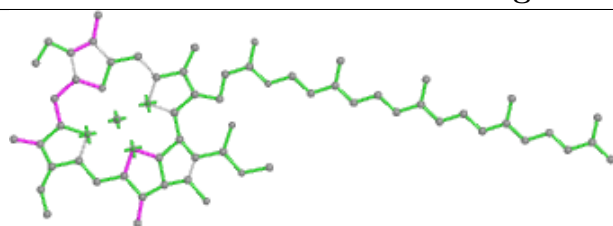
Bond angles



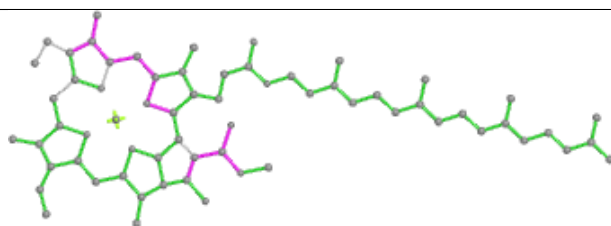
Torsions



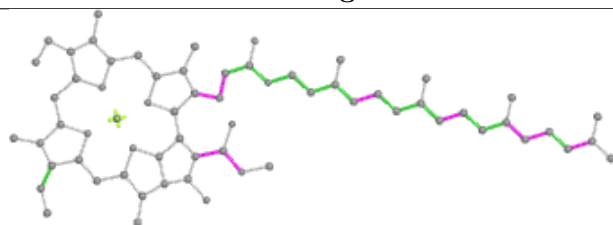
Rings

Ligand CLA D 405

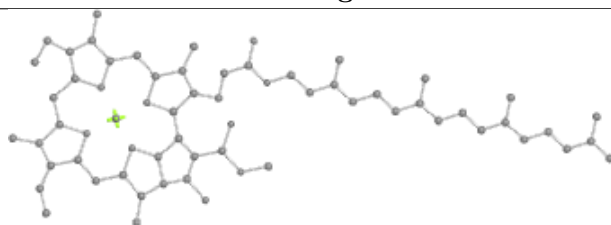
Bond lengths



Bond angles

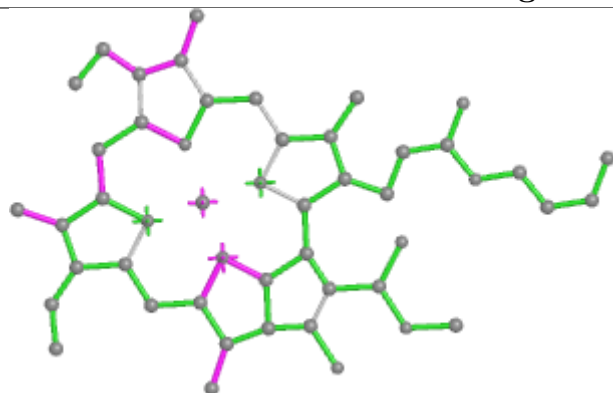


Torsions

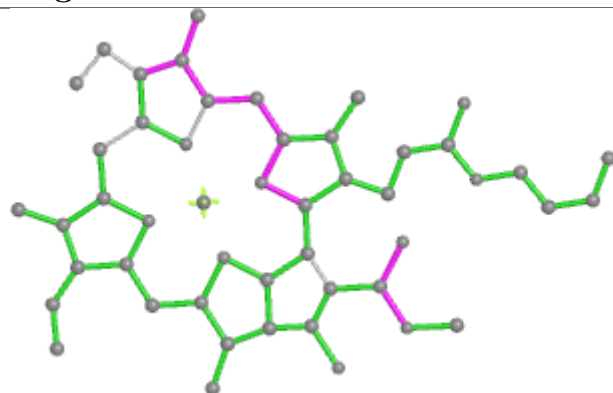


Rings

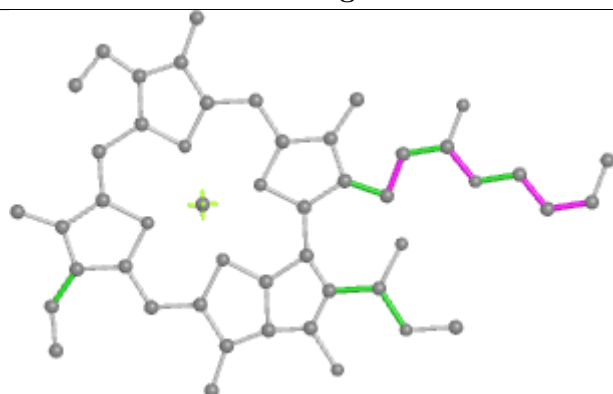
Ligand CLA g 604



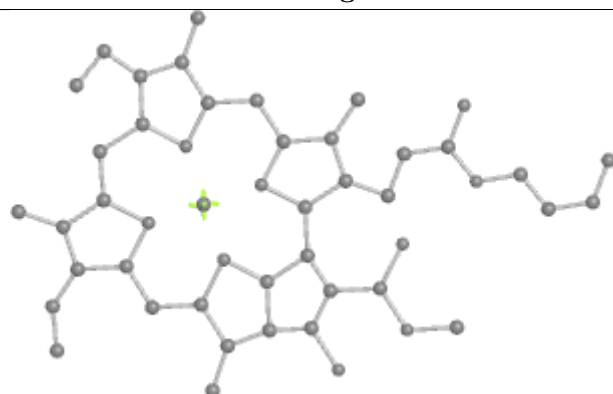
Bond lengths



Bond angles

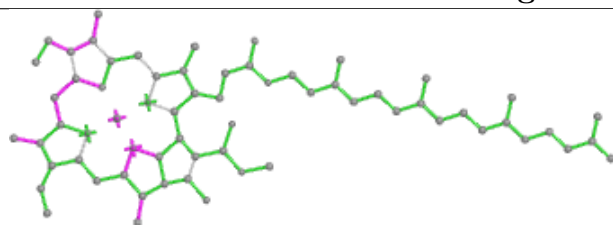


Torsions

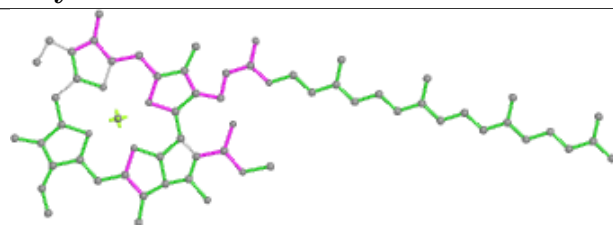


Rings

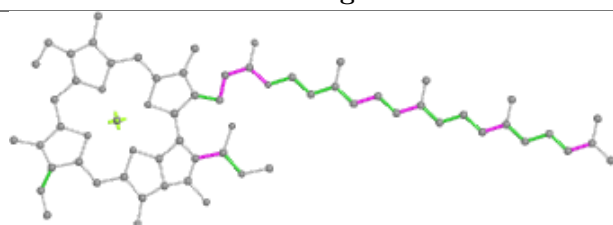
Ligand CLA y 304



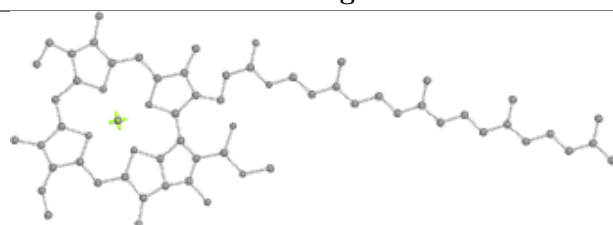
Bond lengths



Bond angles

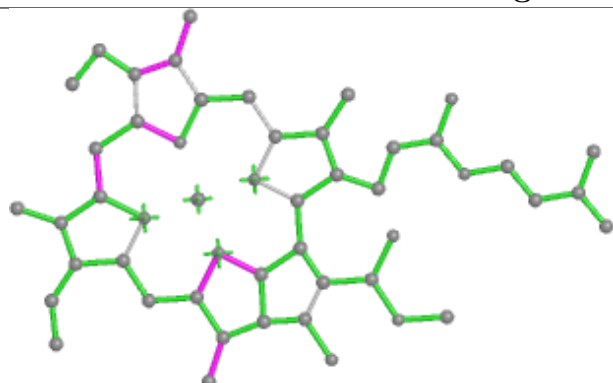


Torsions

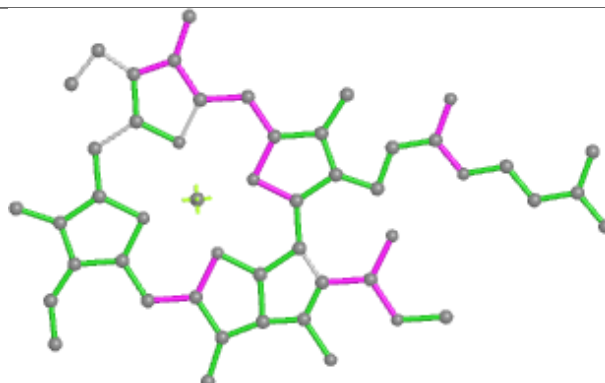


Rings

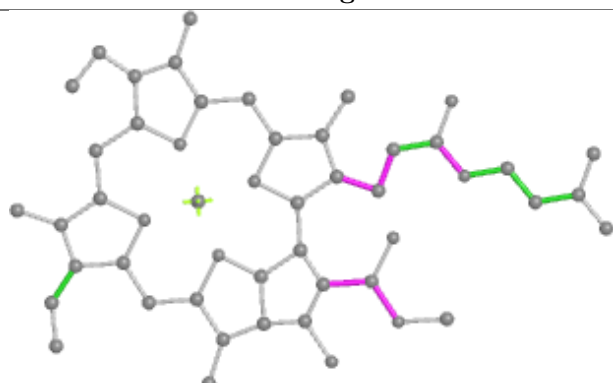
Ligand CLA A 402



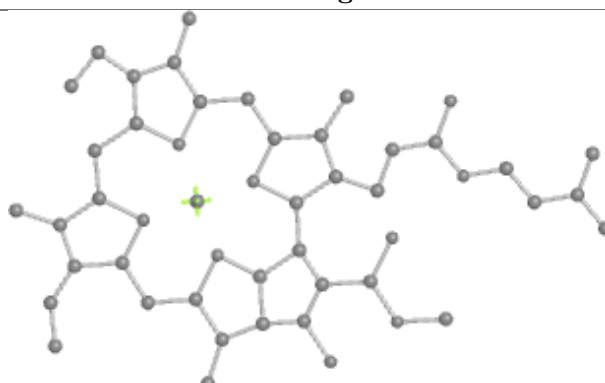
Bond lengths



Bond angles

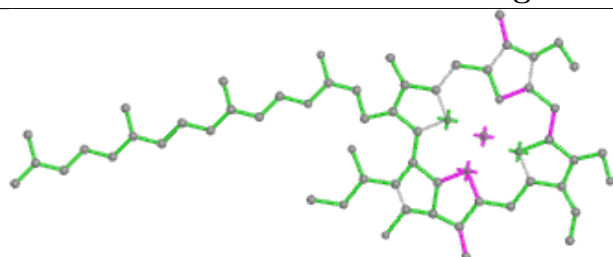


Torsions

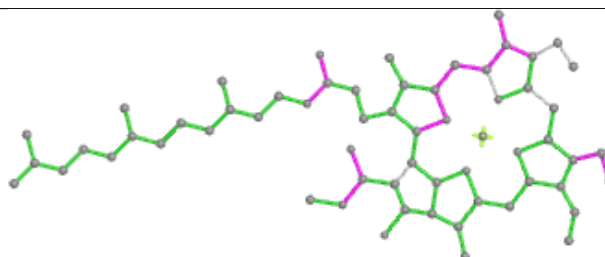


Rings

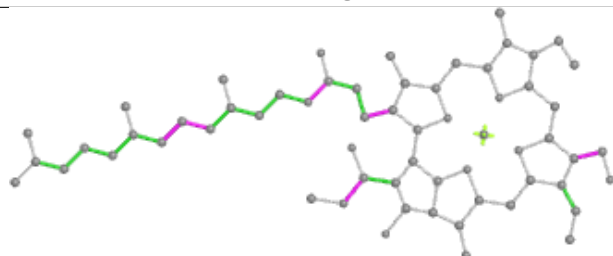
Ligand CHL R 607



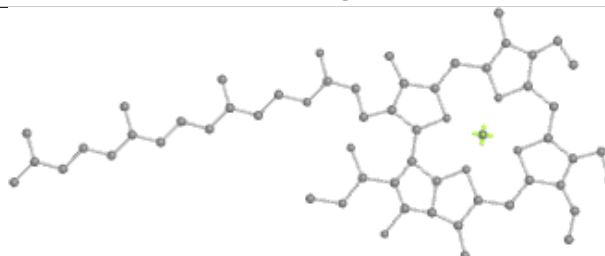
Bond lengths



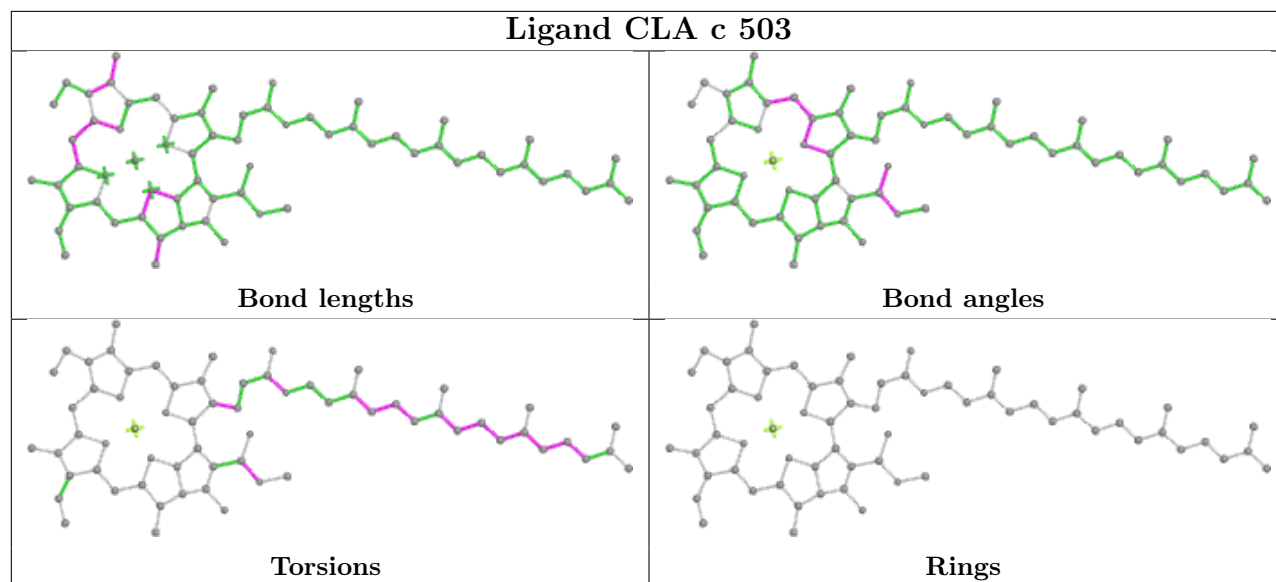
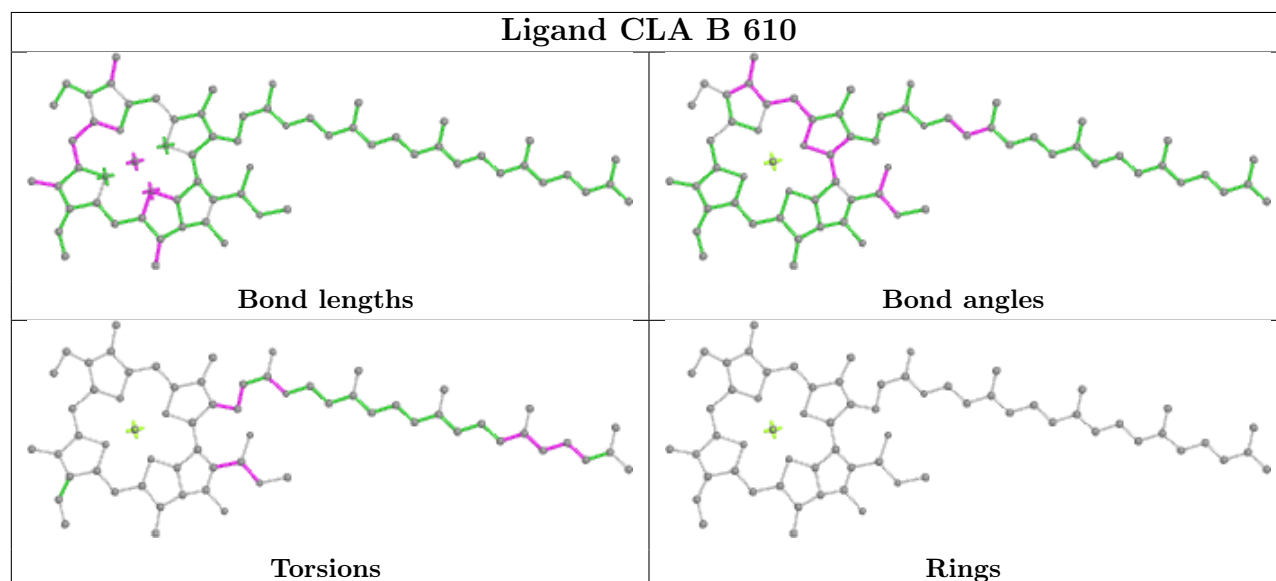
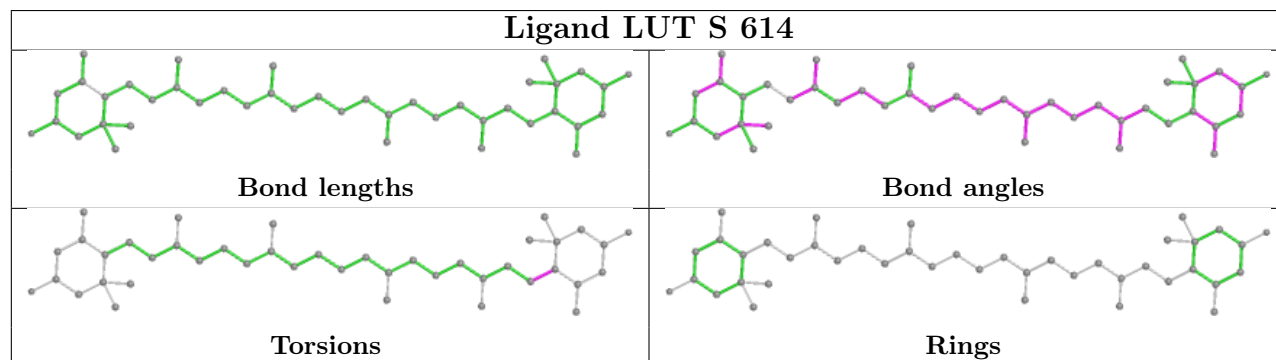
Bond angles



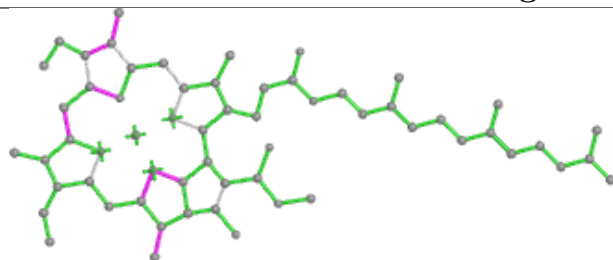
Torsions



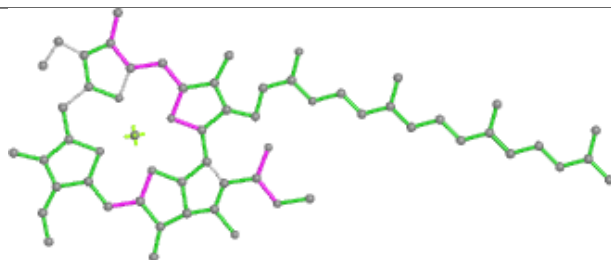
Rings

Ligand CLA c 503**Ligand CLA B 610****Ligand LUT S 614**

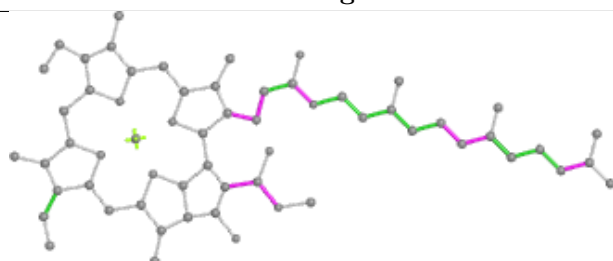
Ligand CLA c 504



Bond lengths



Bond angles

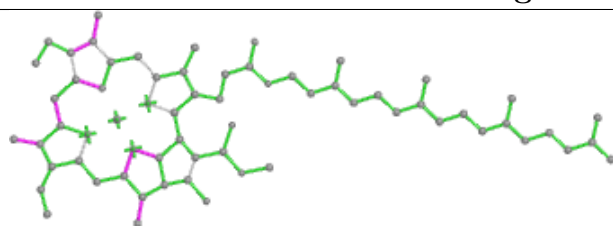


Torsions

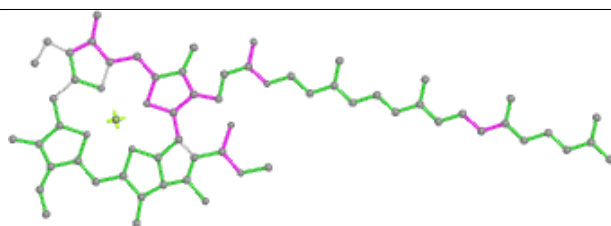


Rings

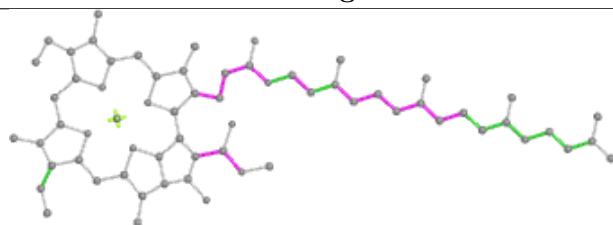
Ligand CLA B 614



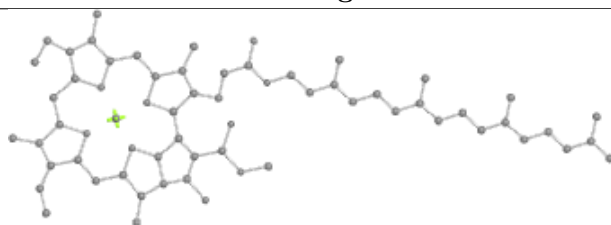
Bond lengths



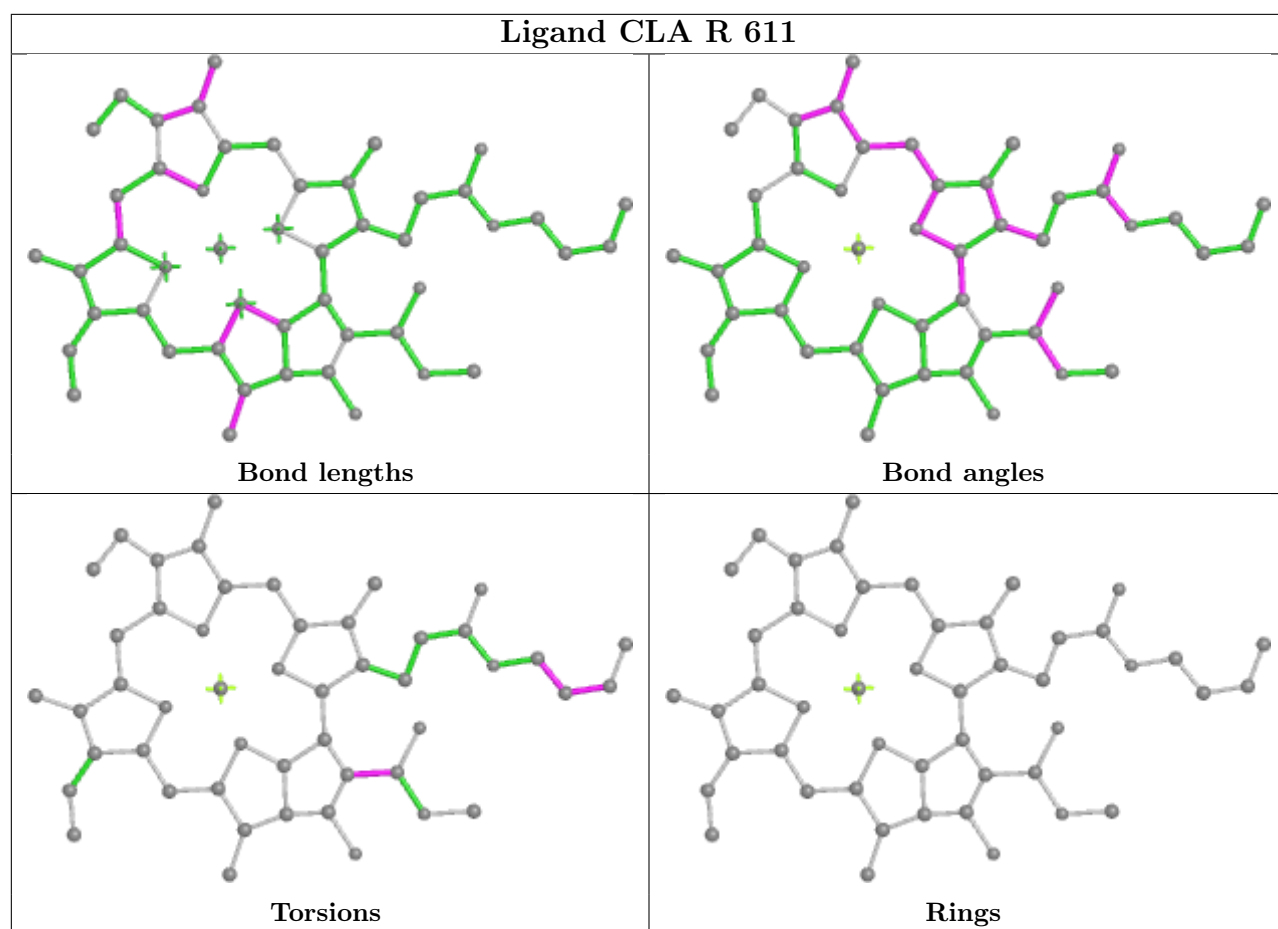
Bond angles



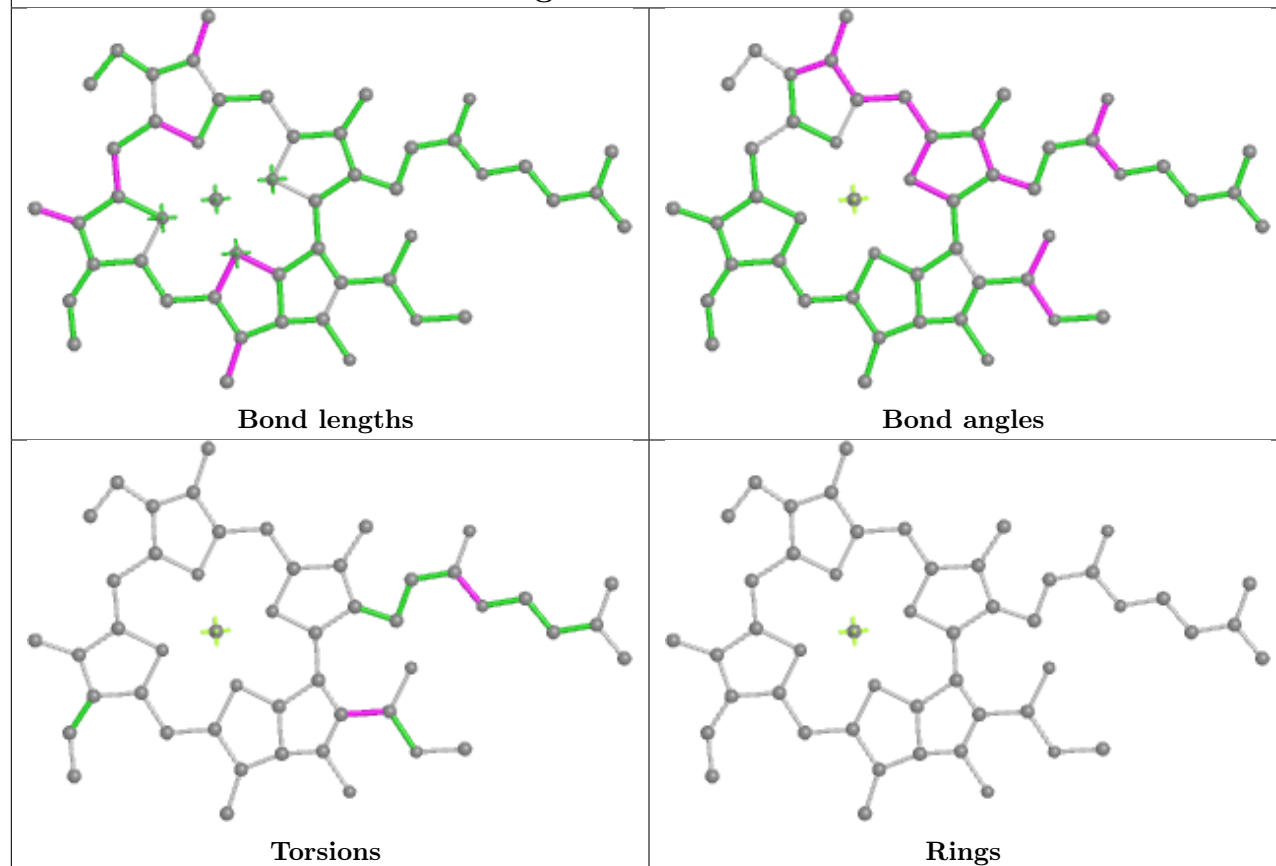
Torsions



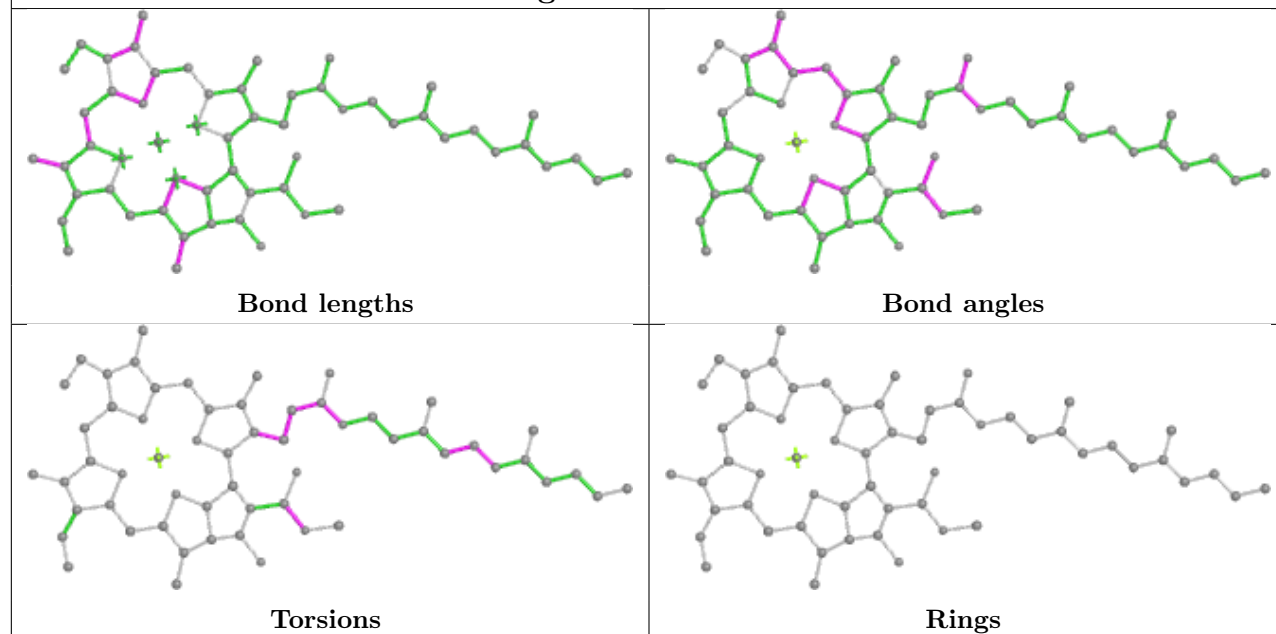
Rings

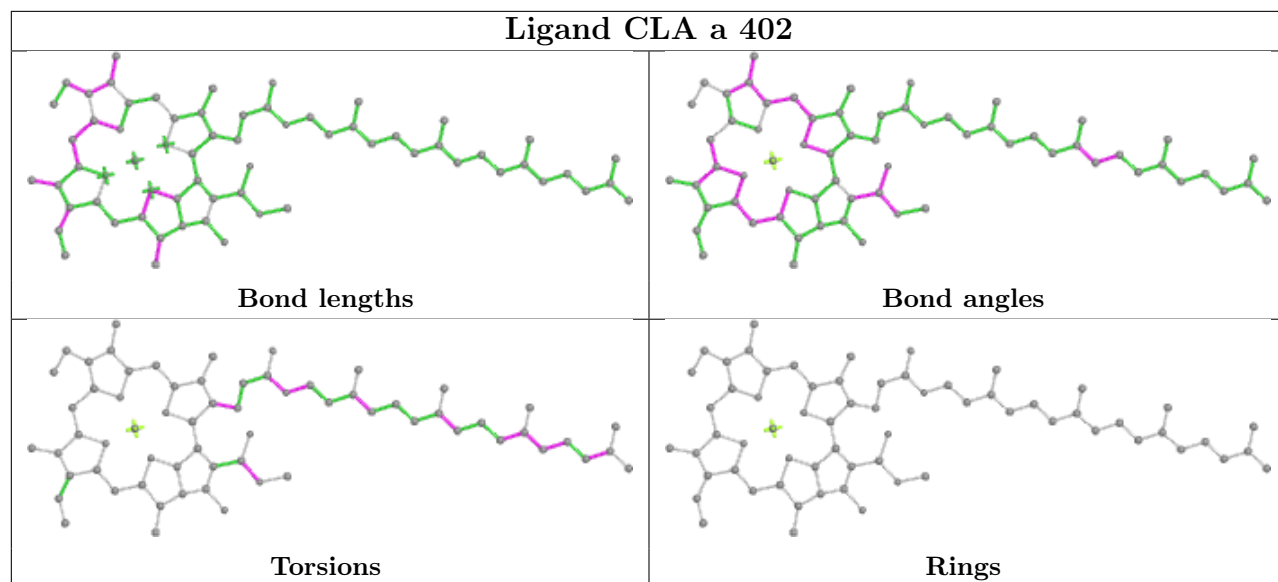
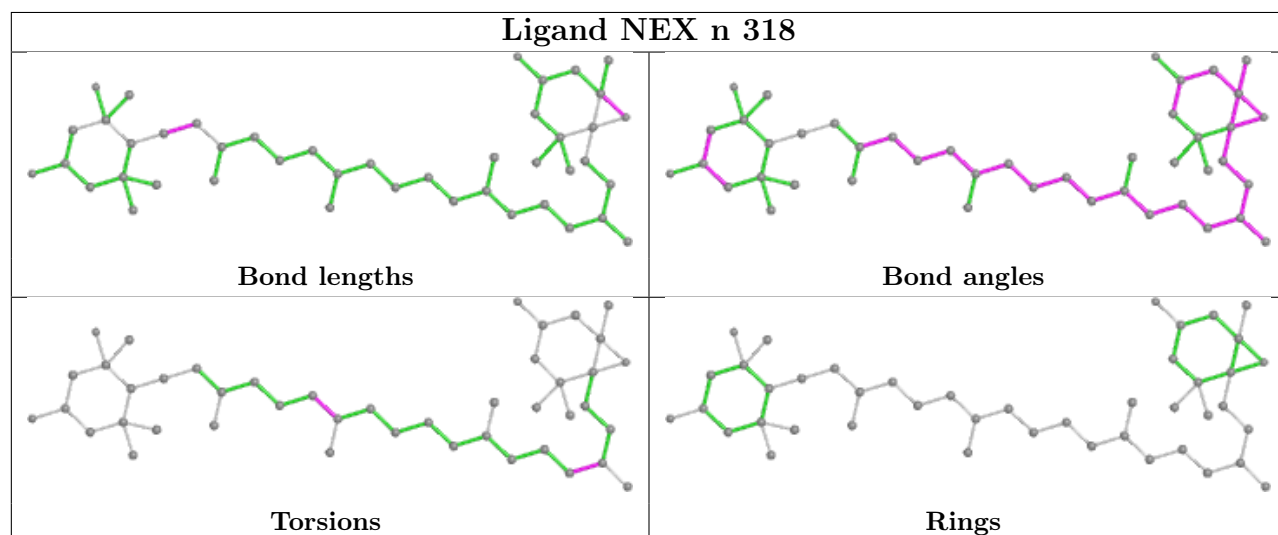


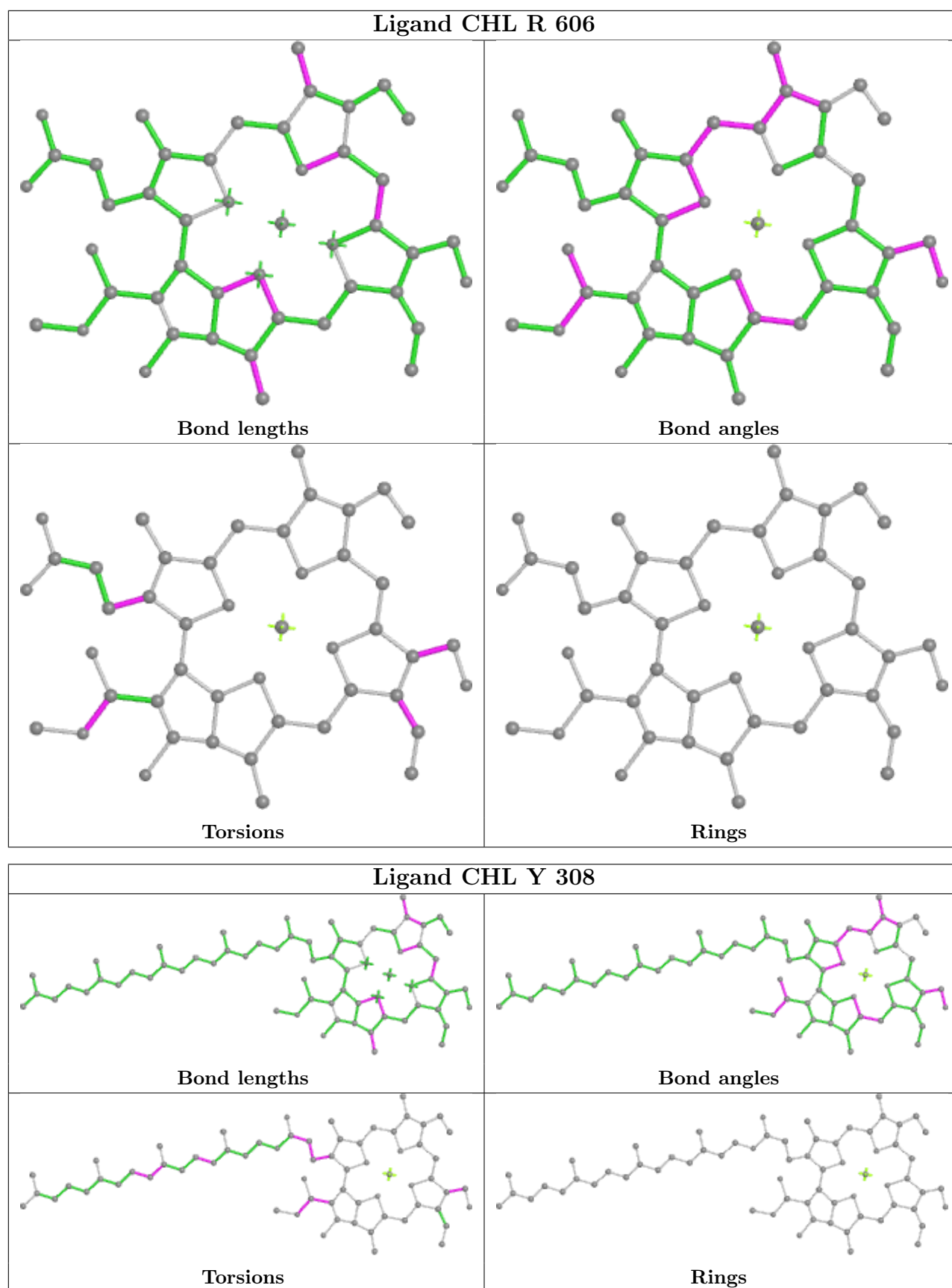
Ligand CLA S 604

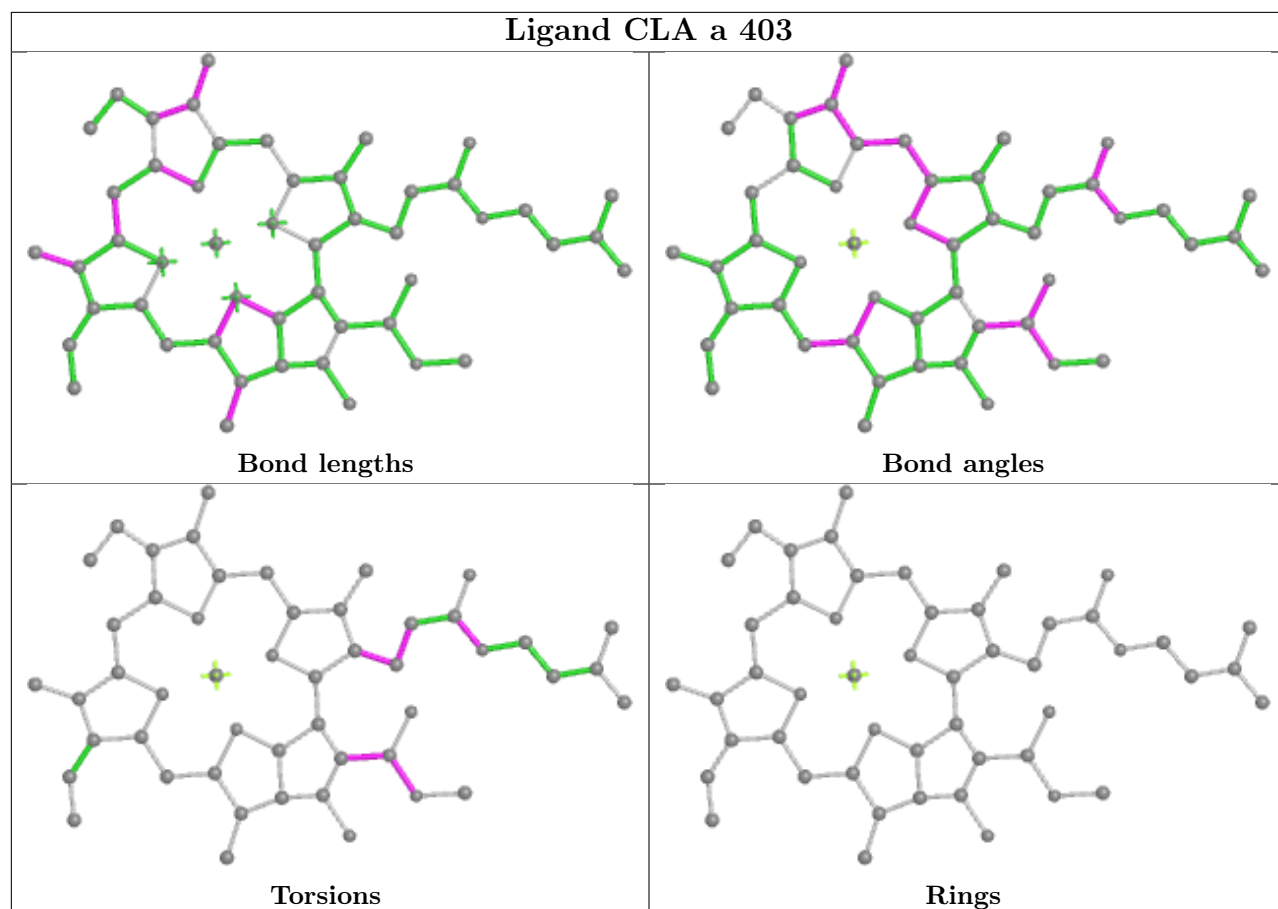
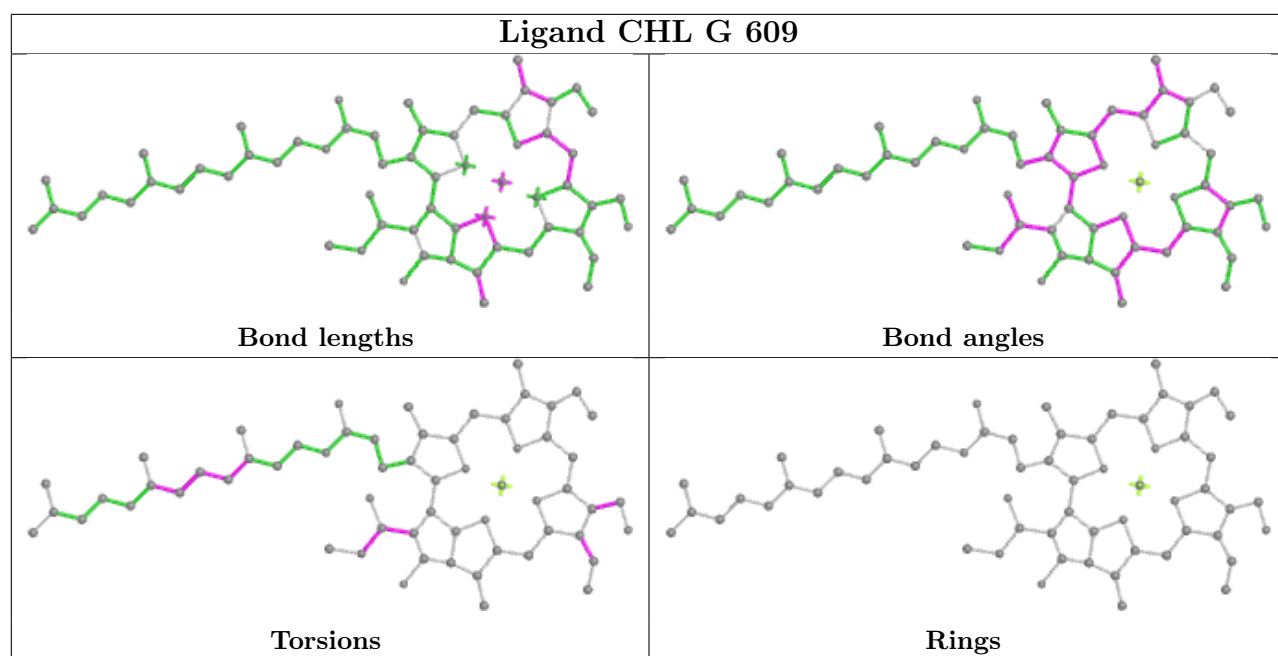


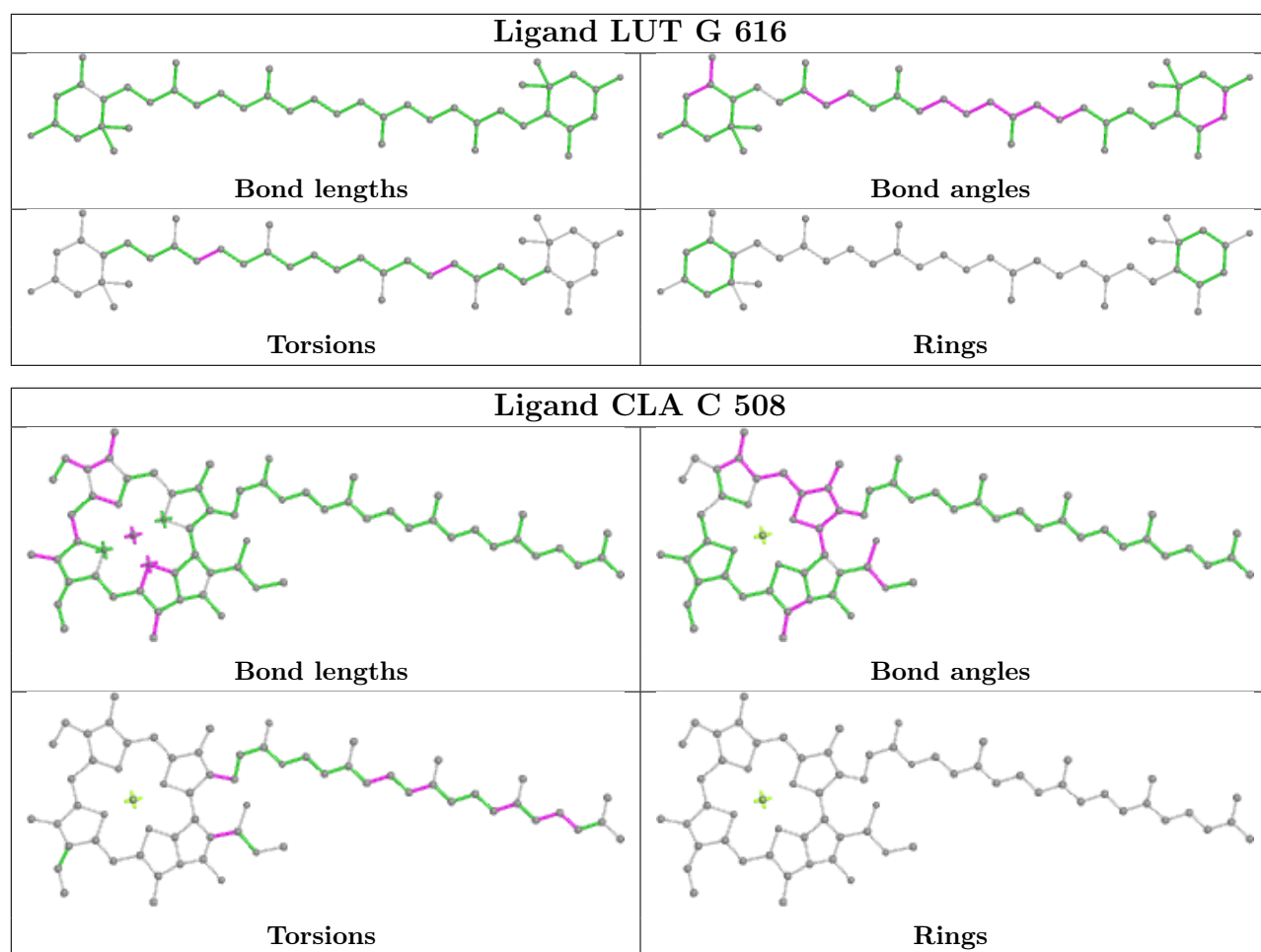
Ligand CLA r 608

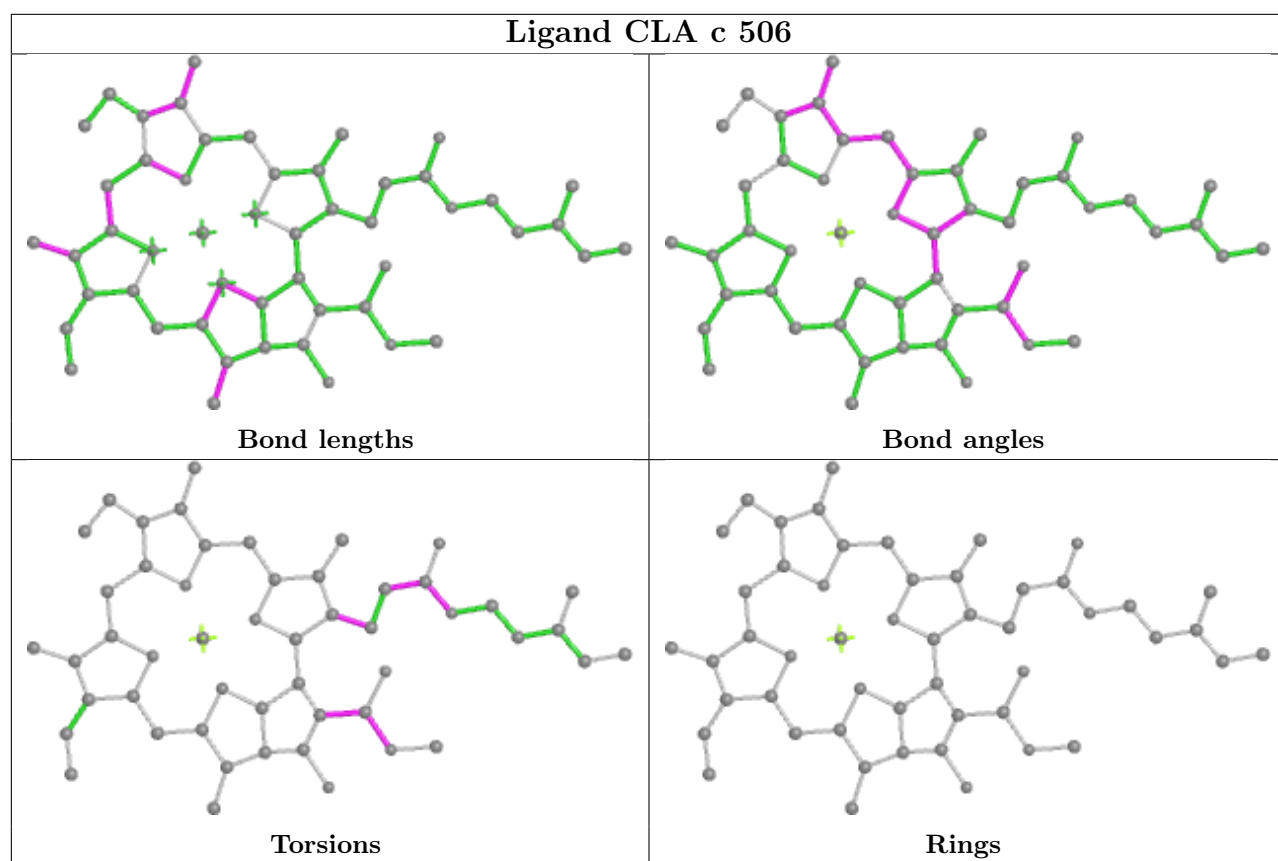


Ligand CLA a 402**Ligand NEX n 318**

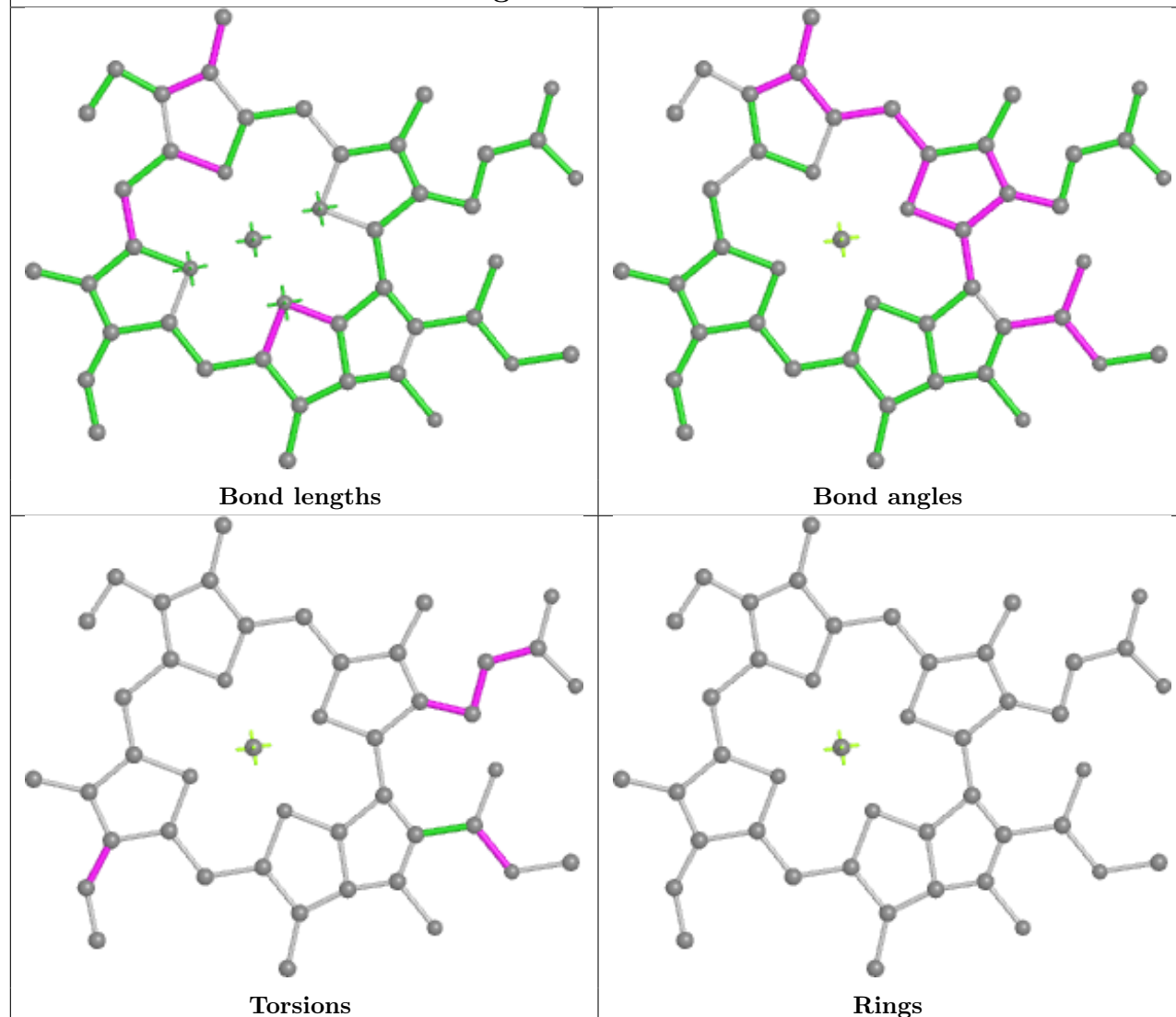




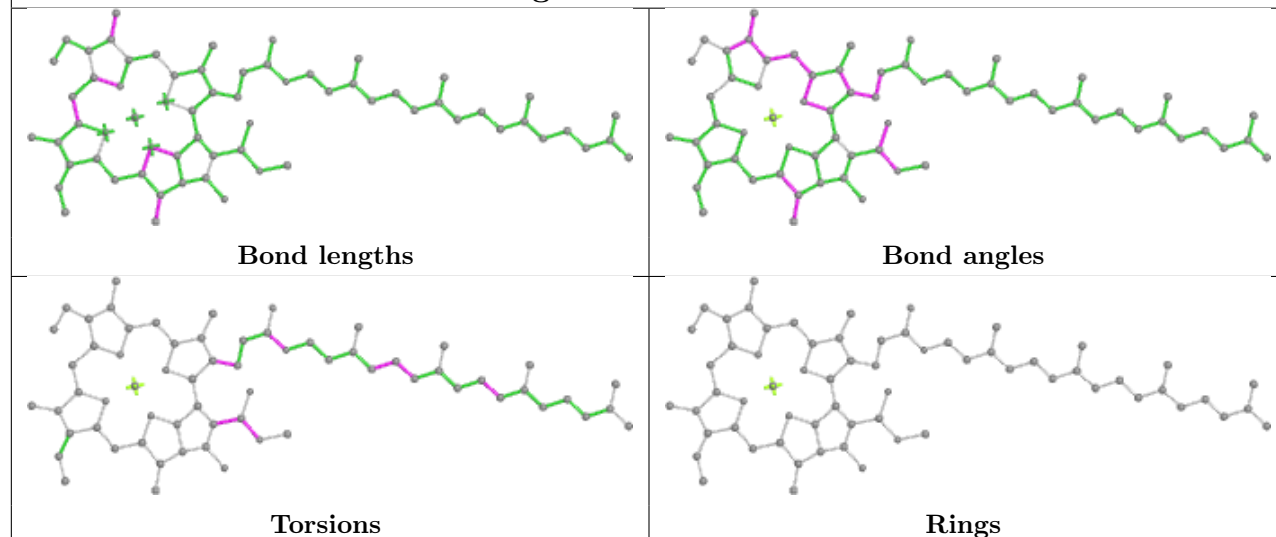


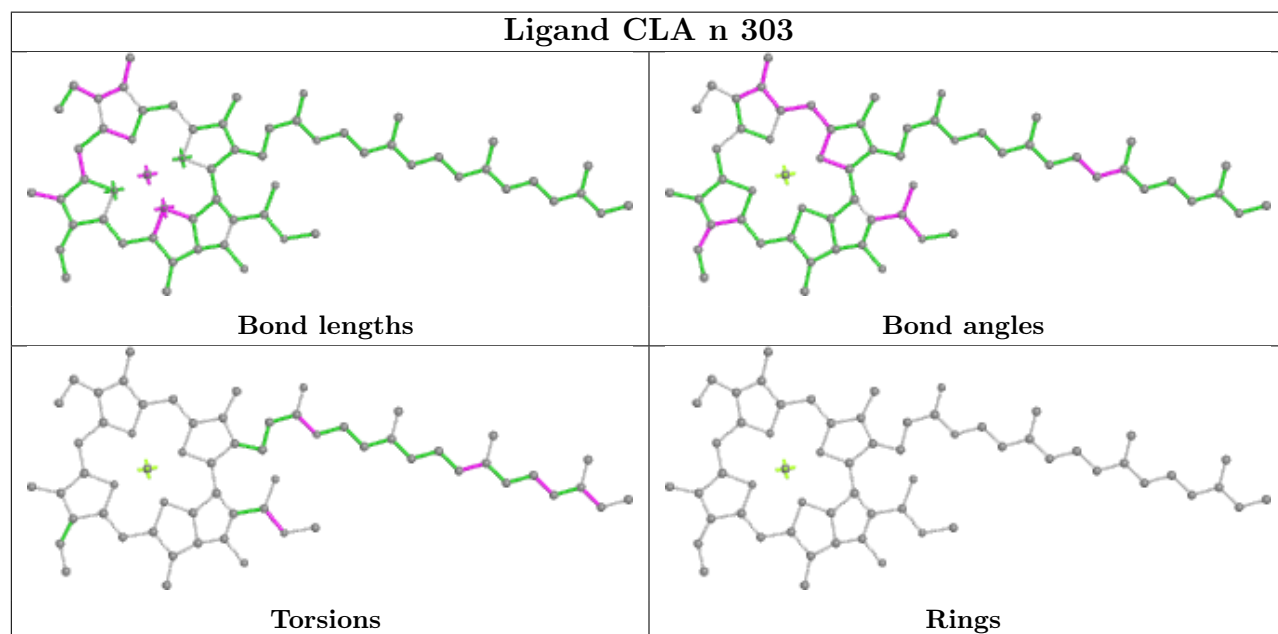
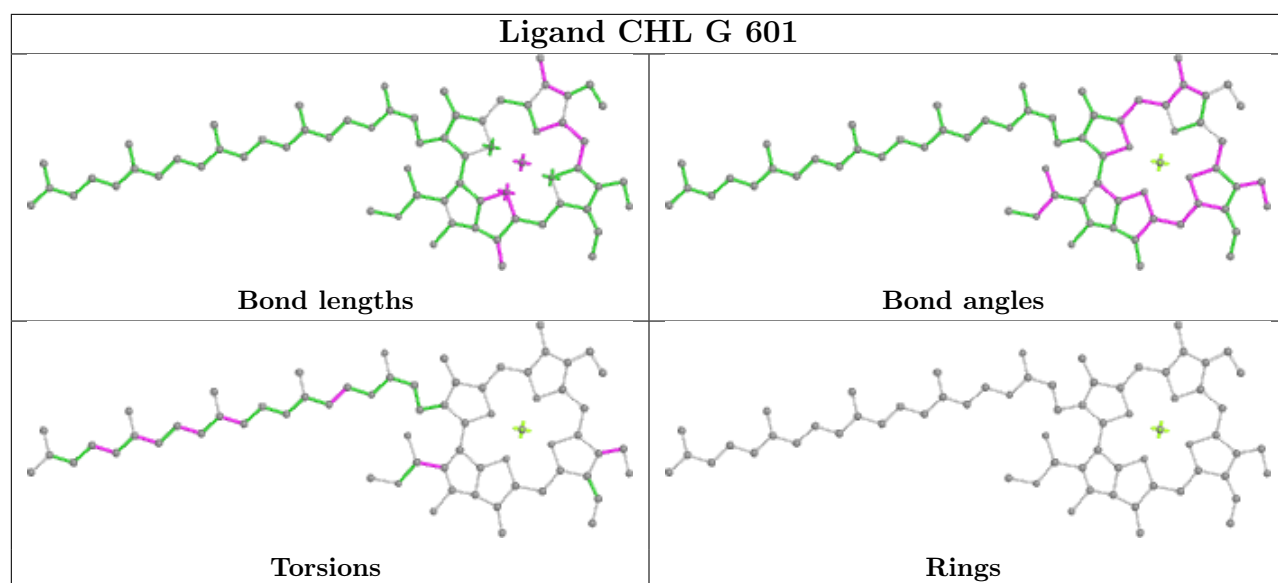


Ligand CLA n 313

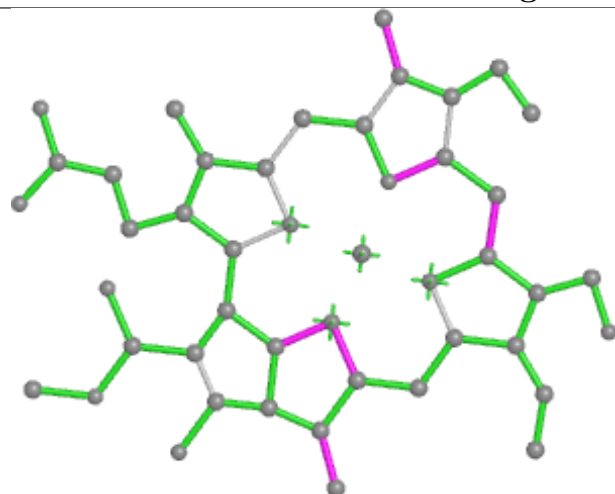


Ligand CLA C 514

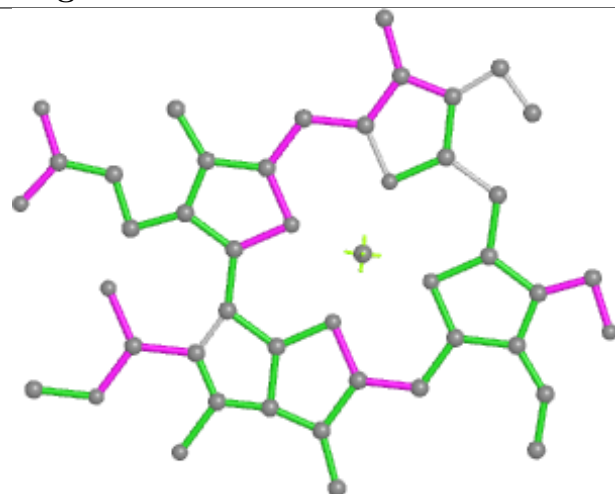




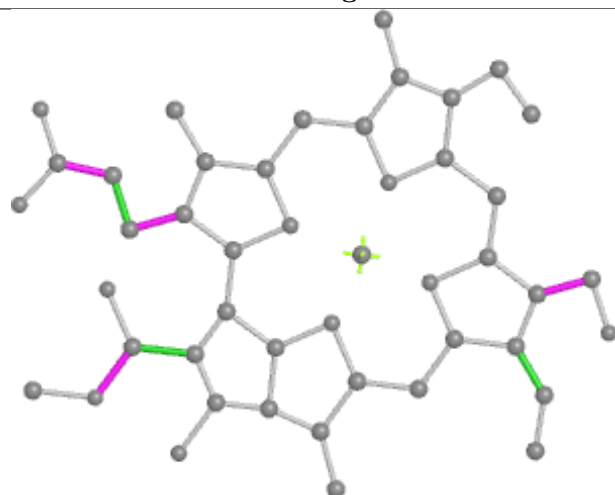
Ligand CHL g 605



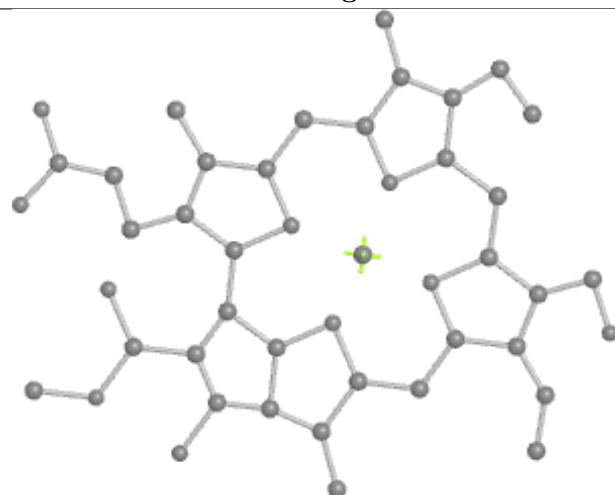
Bond lengths



Bond angles

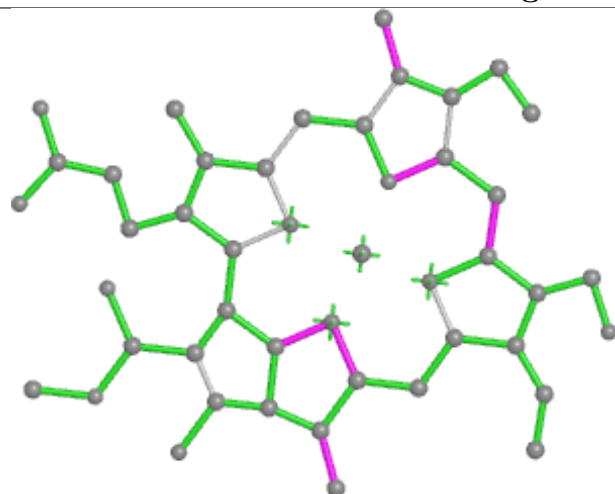


Torsions

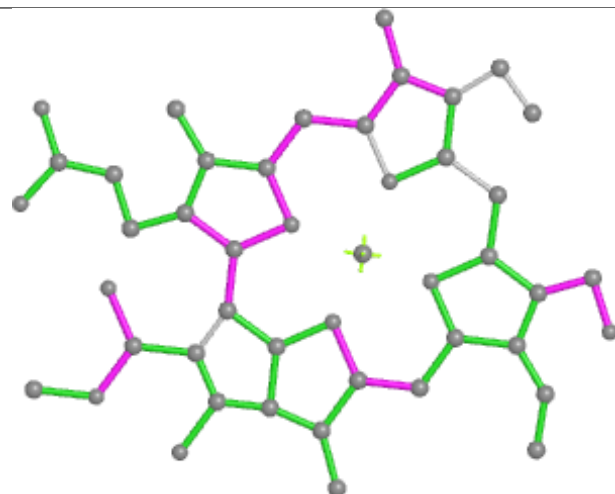


Rings

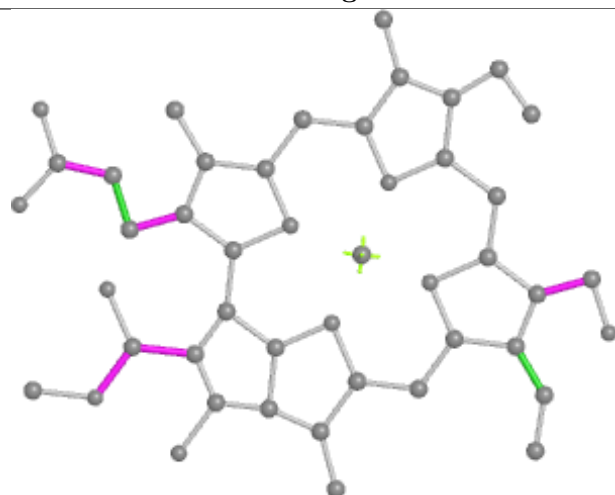
Ligand CHL s 601



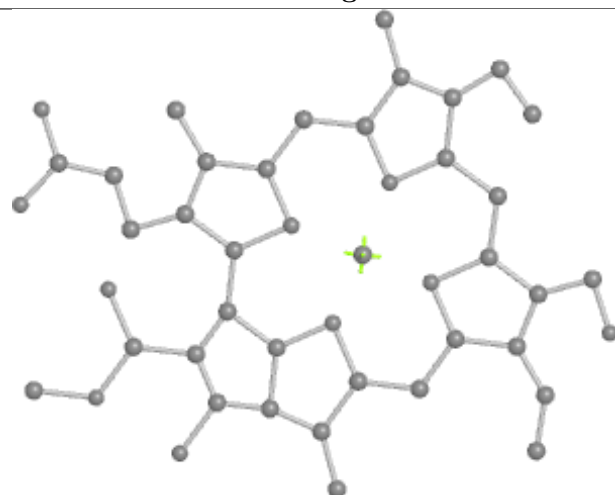
Bond lengths



Bond angles

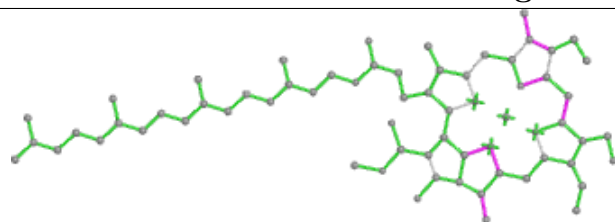


Torsions

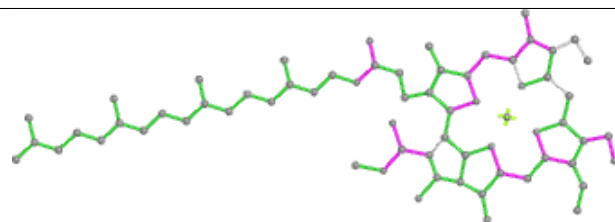


Rings

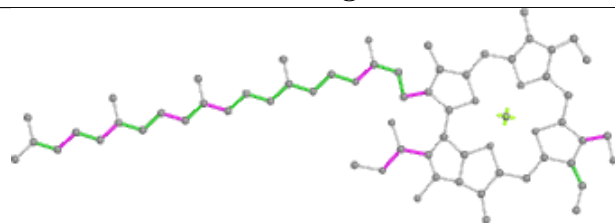
Ligand CHL N 309



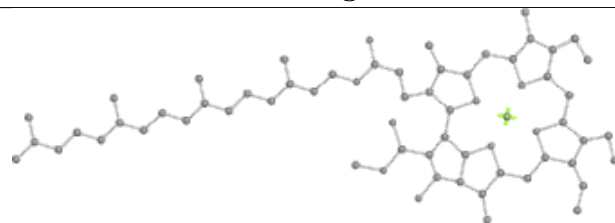
Bond lengths



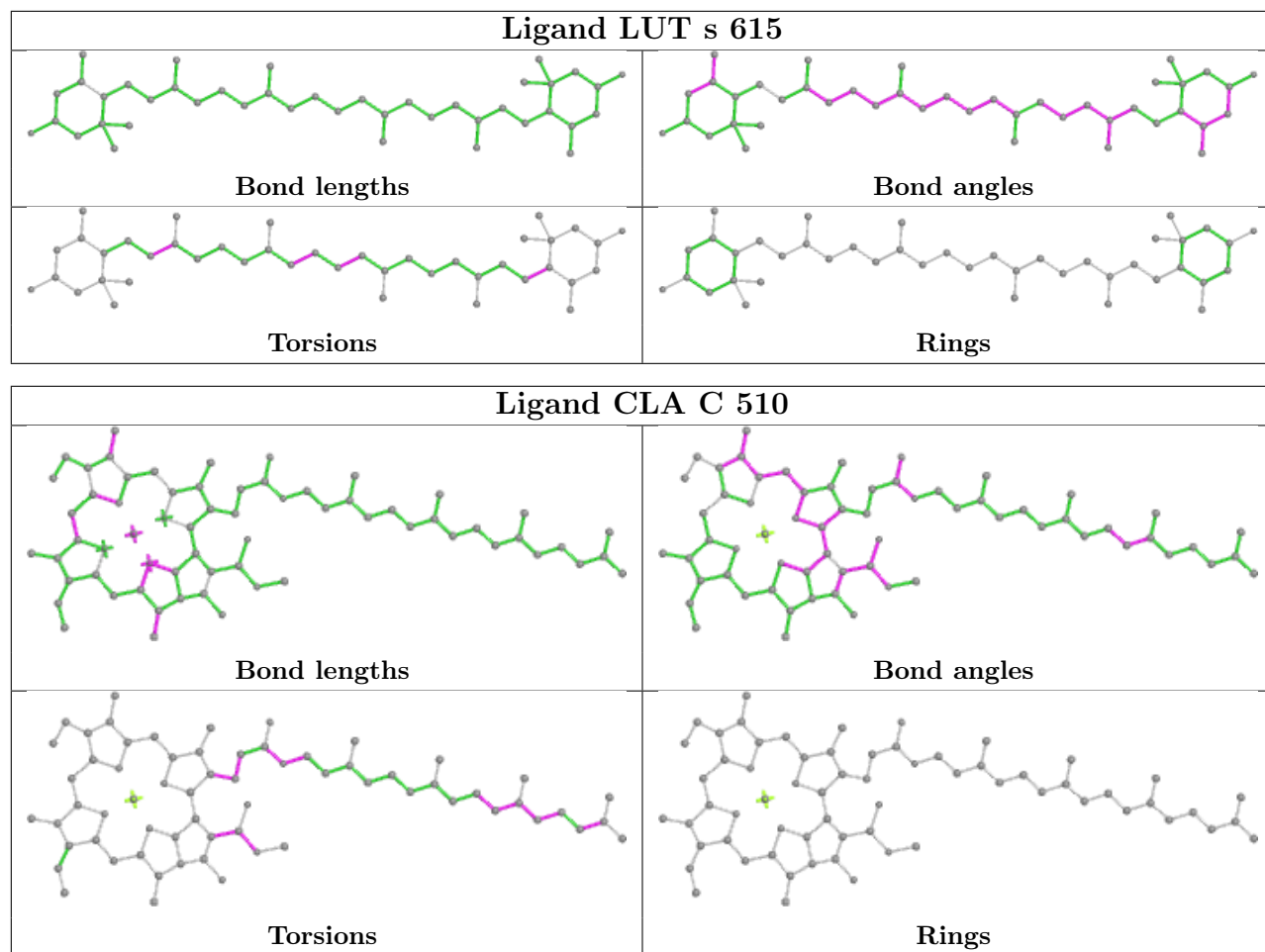
Bond angles

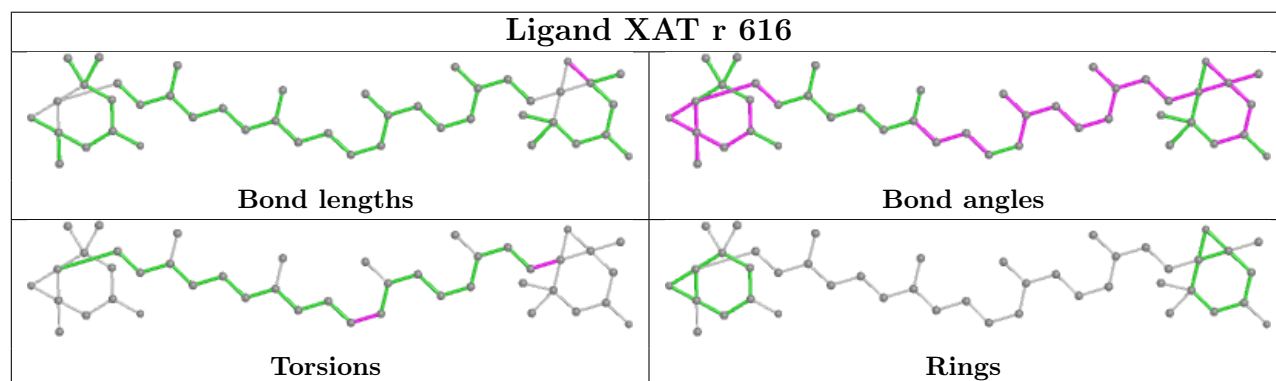
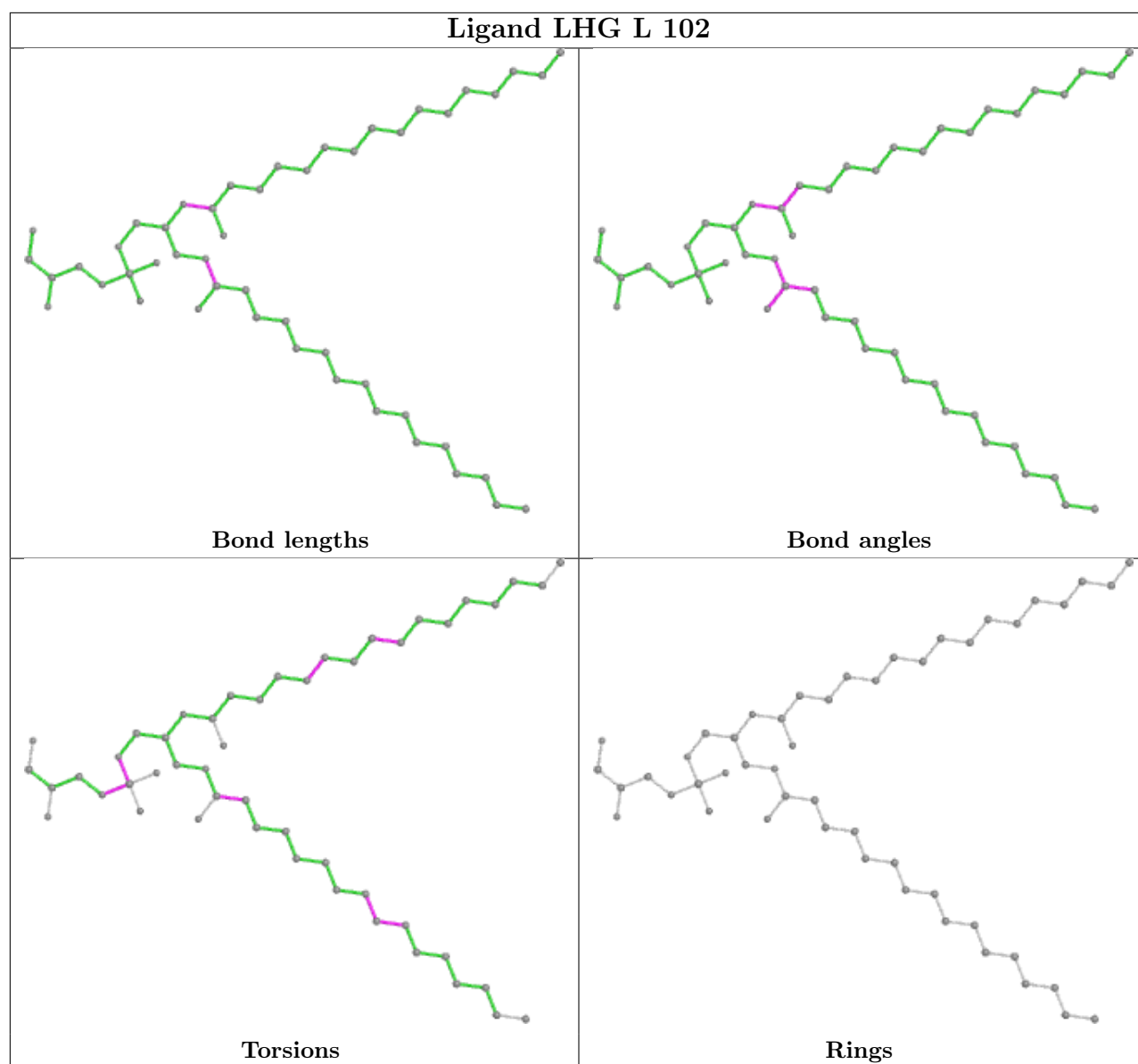


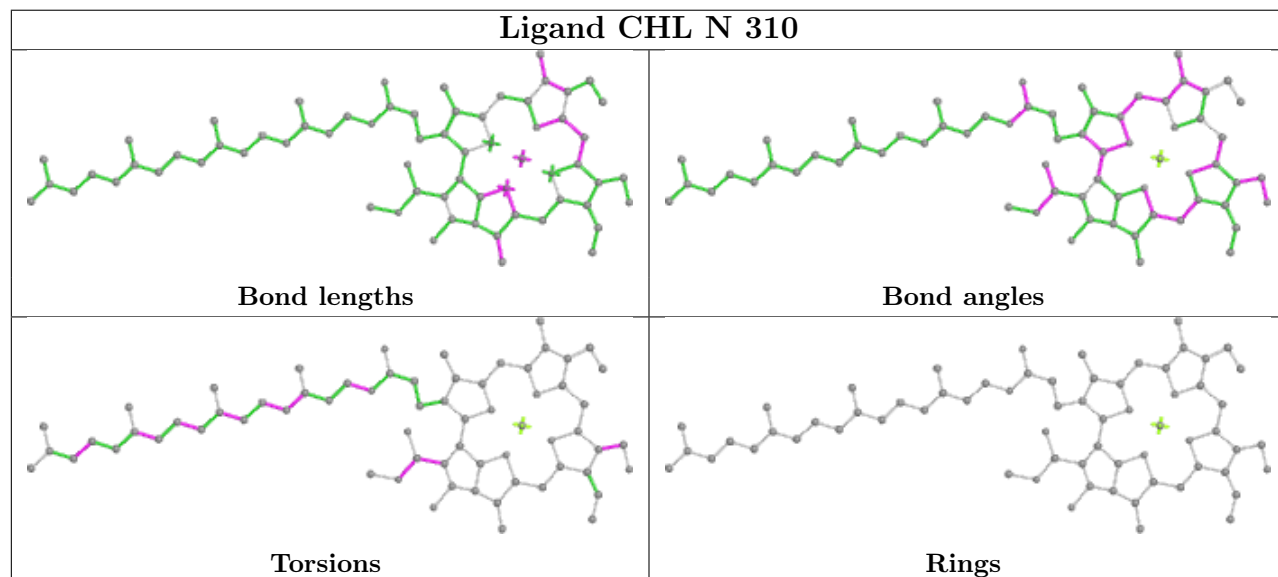
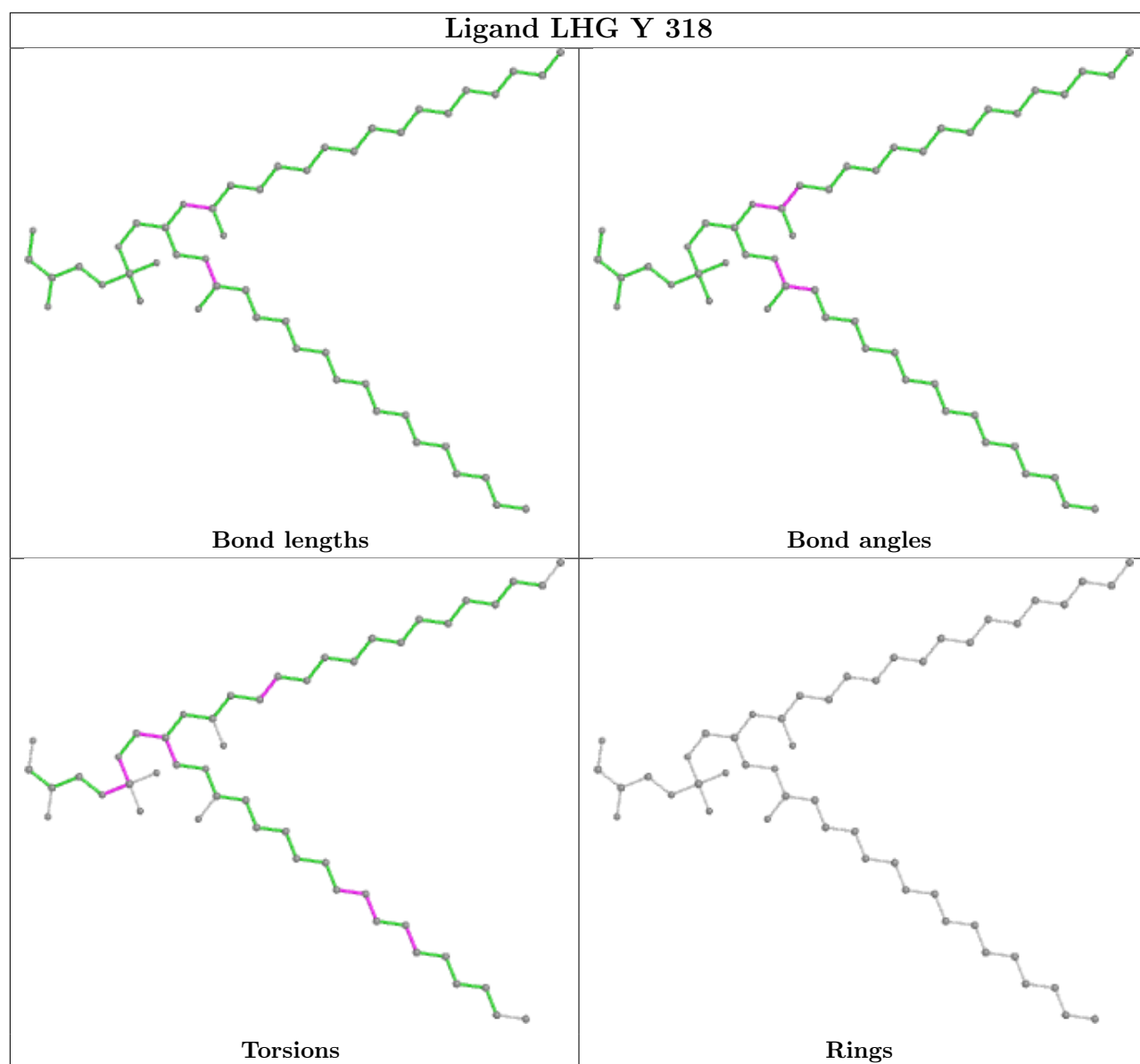
Torsions

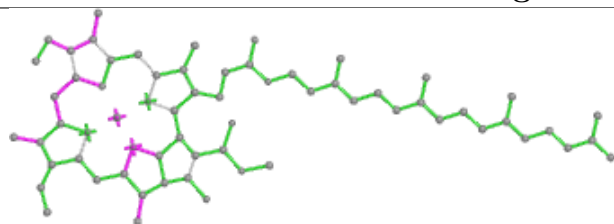
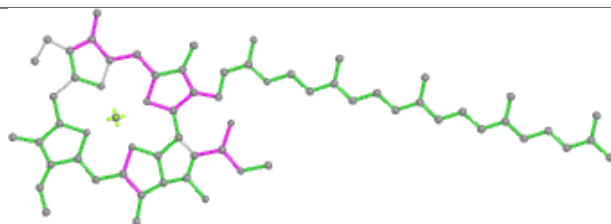
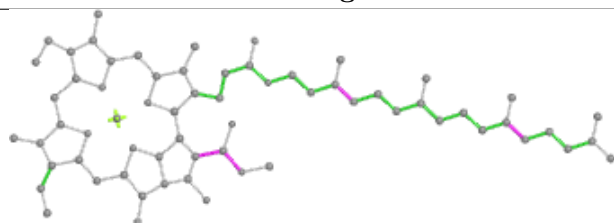
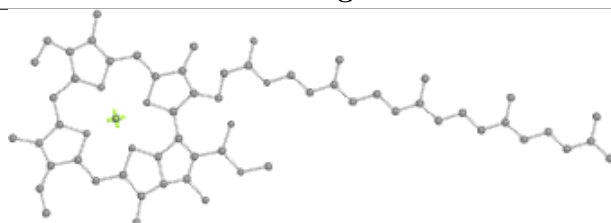
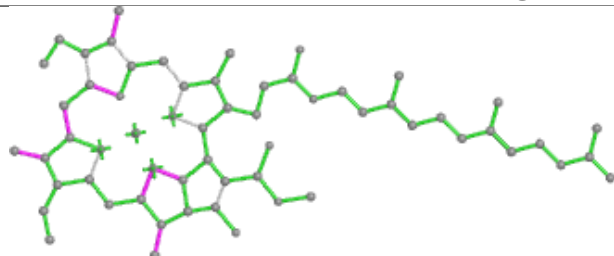
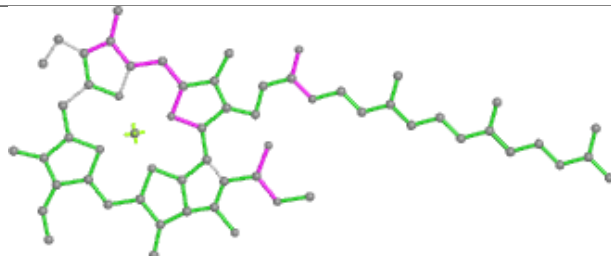
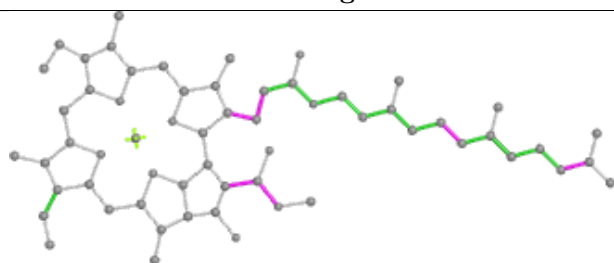
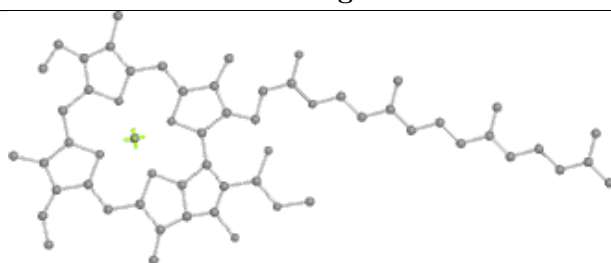


Rings

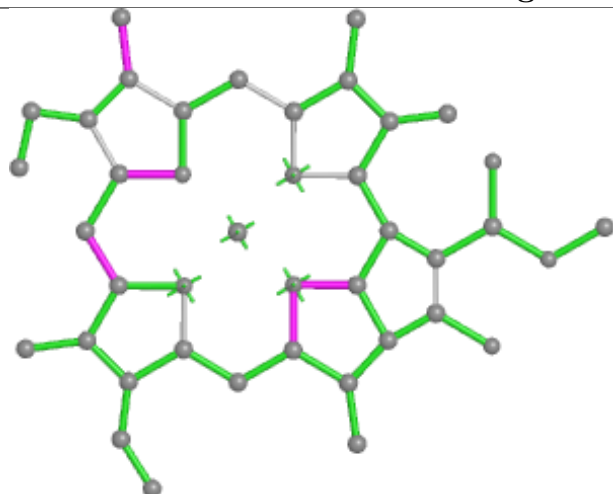




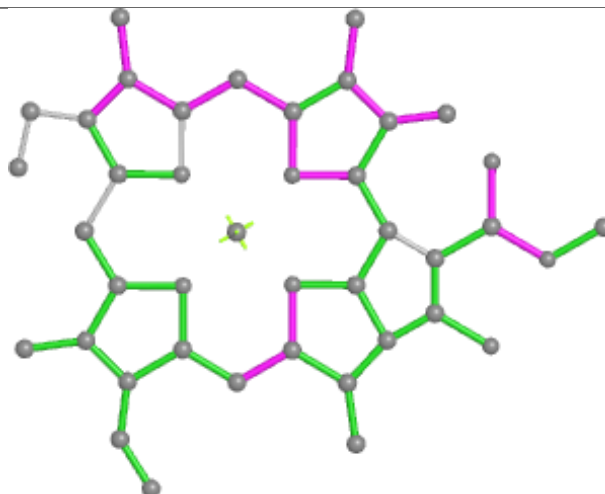


Ligand CLA G 603**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA Y 310****Bond lengths****Bond angles****Torsions****Rings**

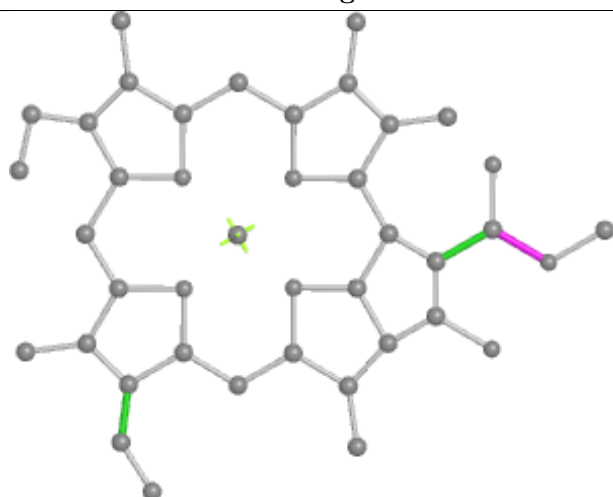
Ligand CLA n 315



Bond lengths



Bond angles

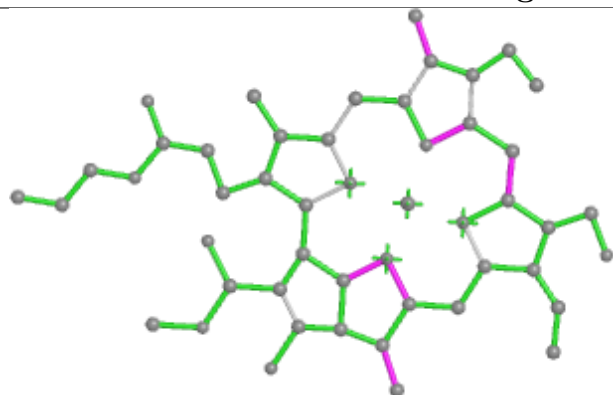


Torsions

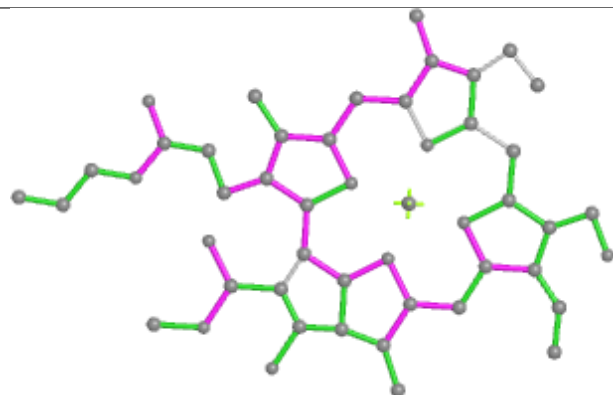


Rings

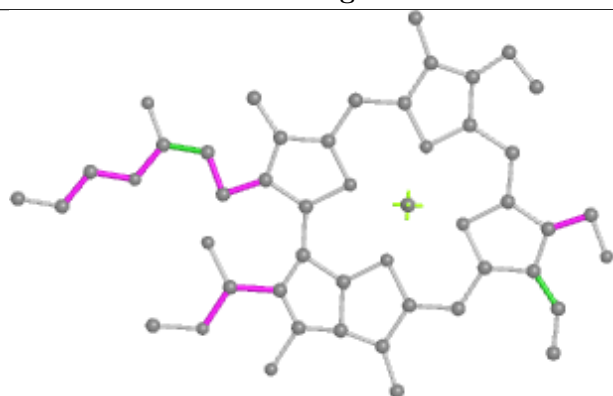
Ligand CHL S 607



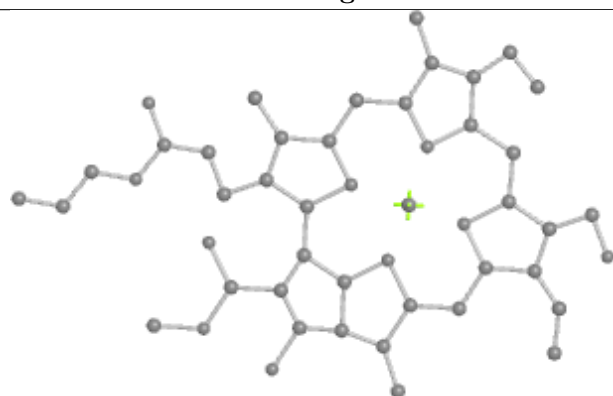
Bond lengths



Bond angles

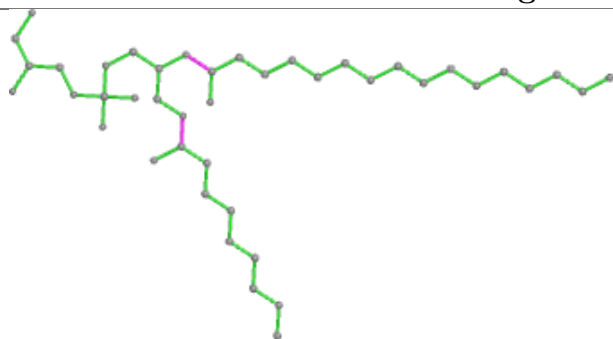


Torsions

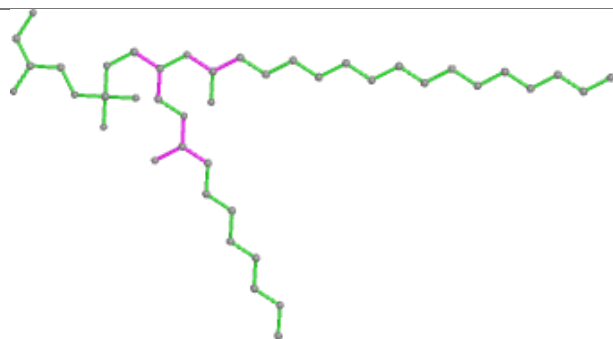


Rings

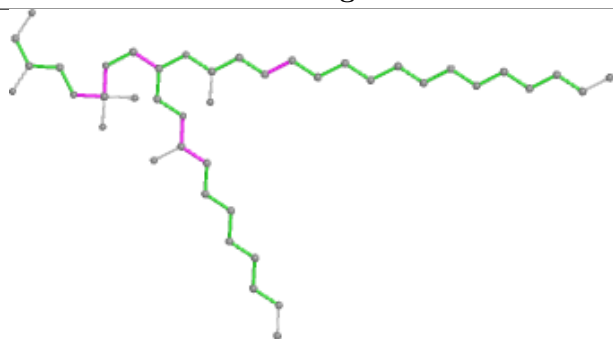
Ligand LHG r 618



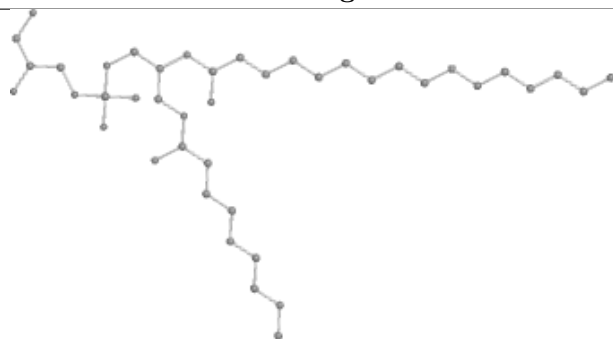
Bond lengths



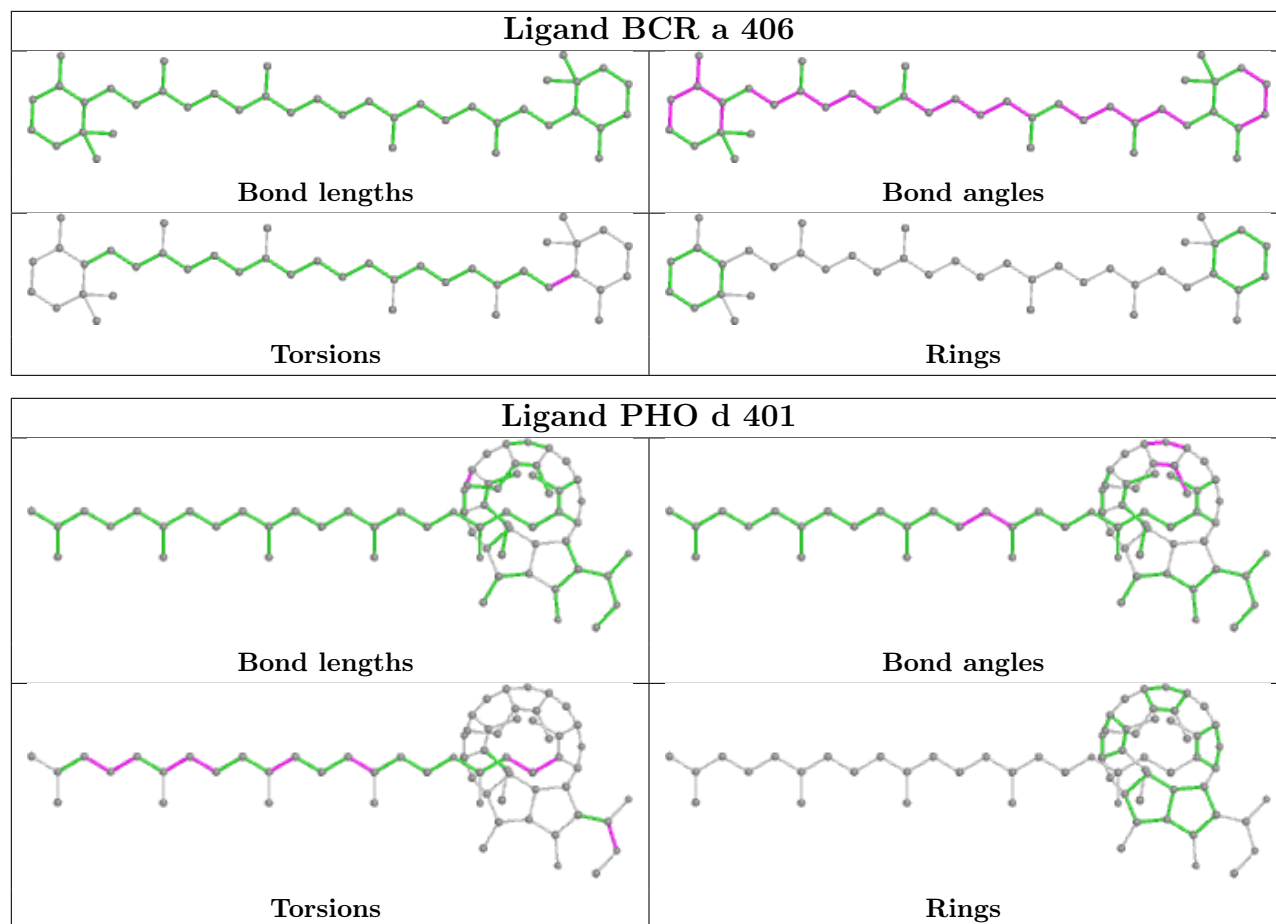
Bond angles



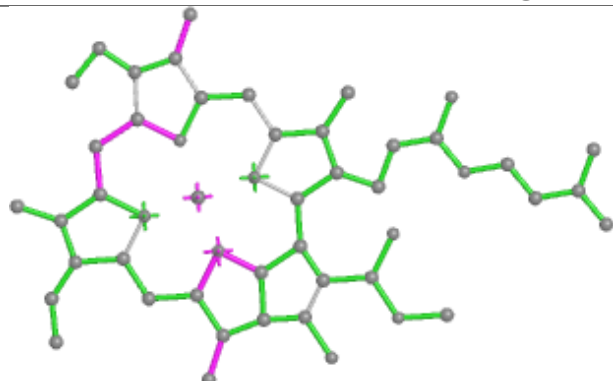
Torsions



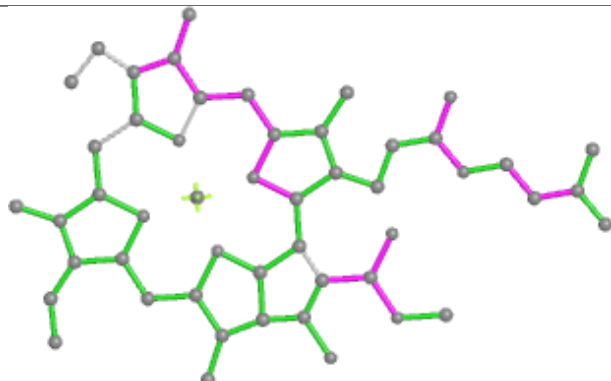
Rings



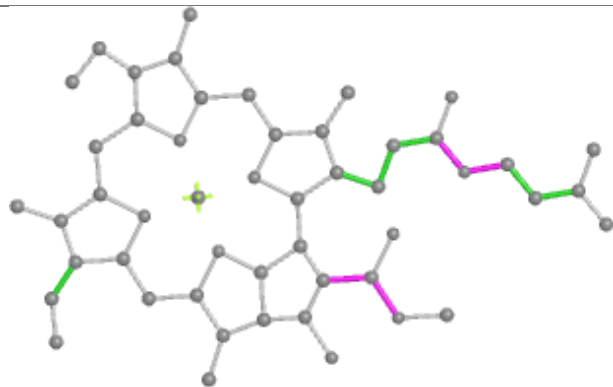
Ligand CLA n 305



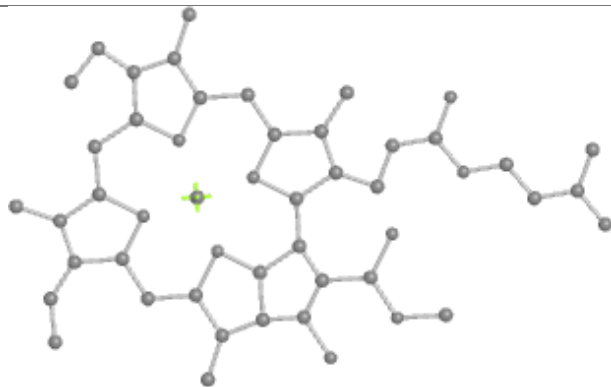
Bond lengths



Bond angles

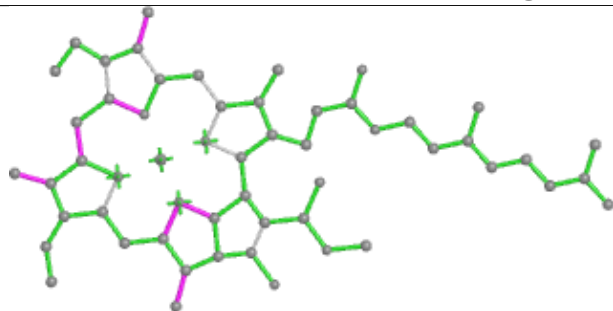


Torsions

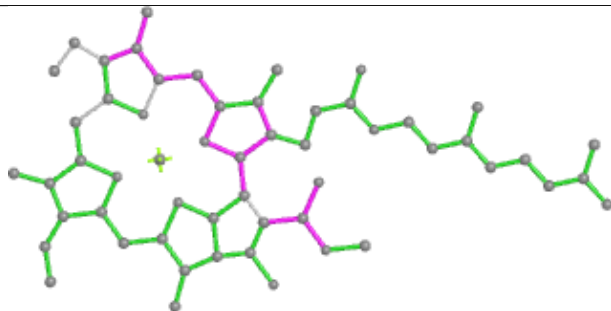


Rings

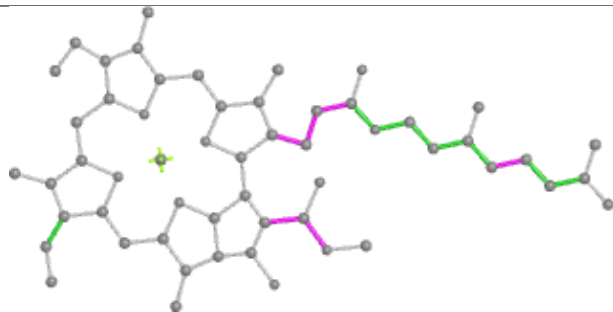
Ligand CLA s 612



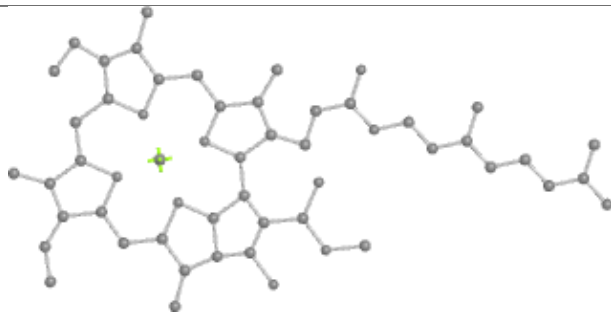
Bond lengths



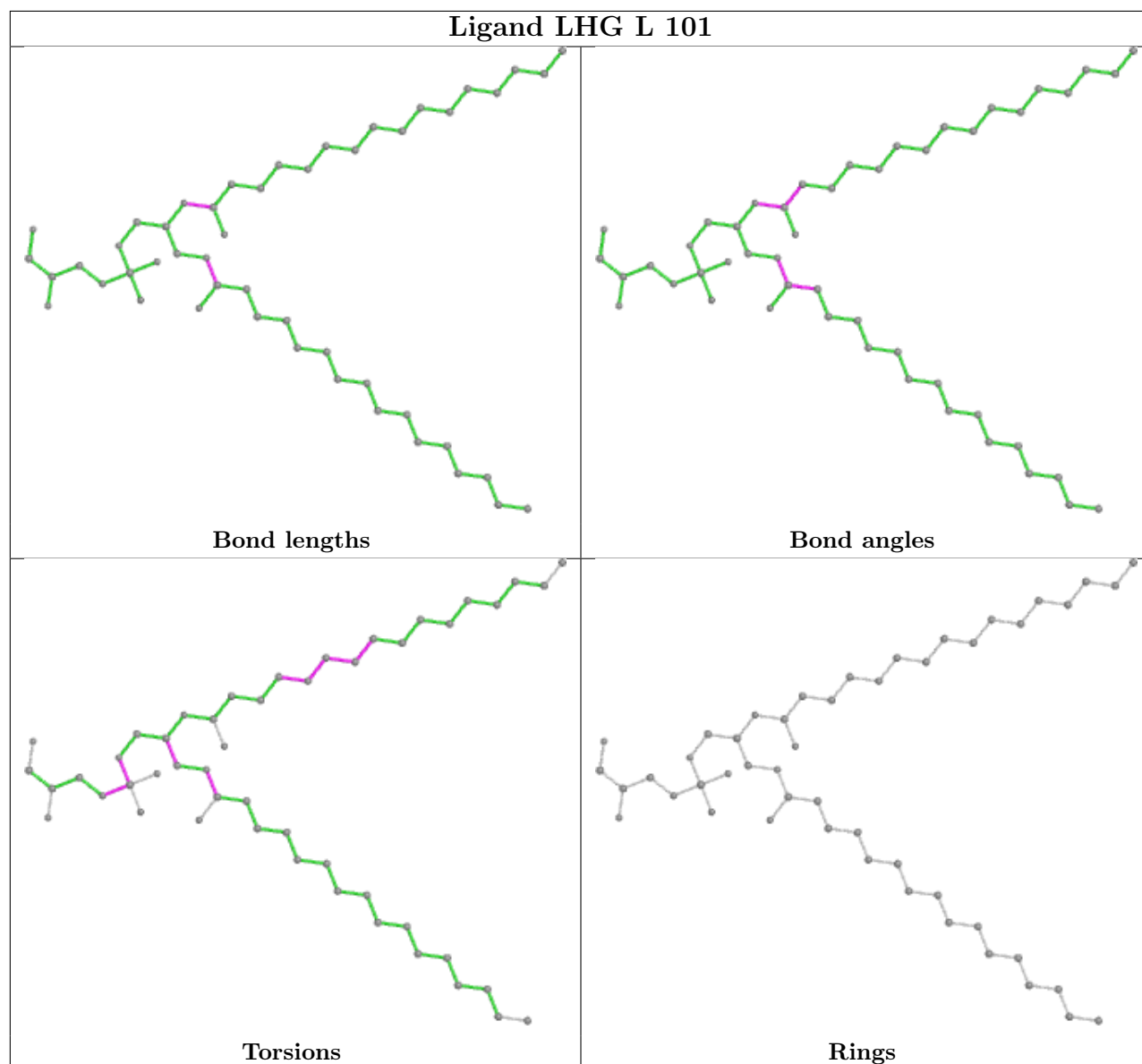
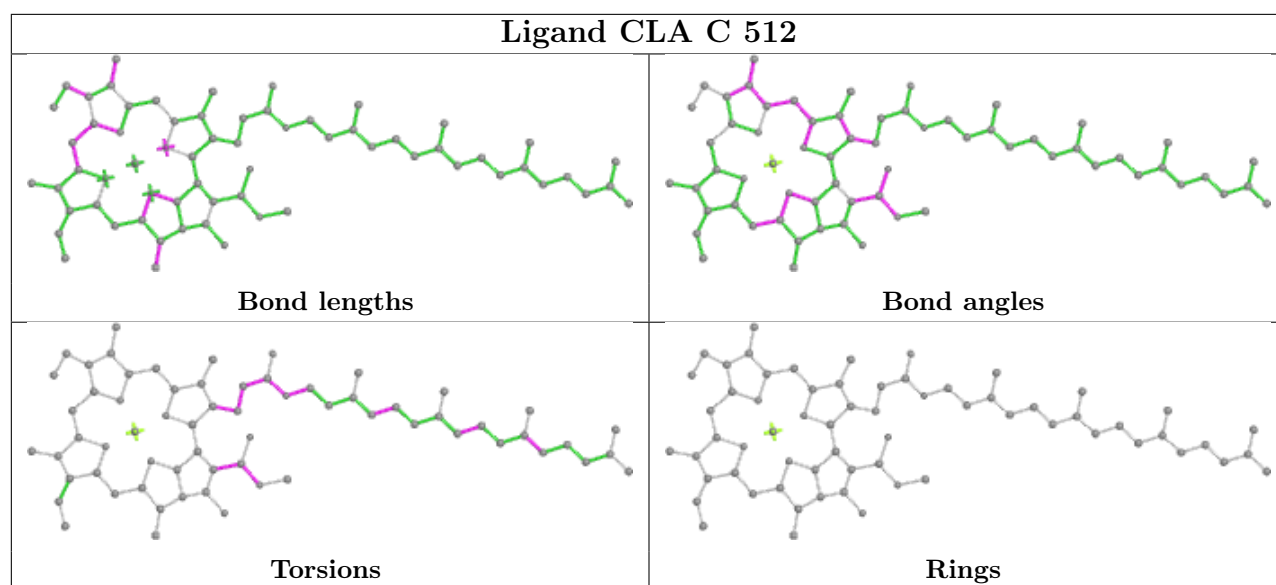
Bond angles

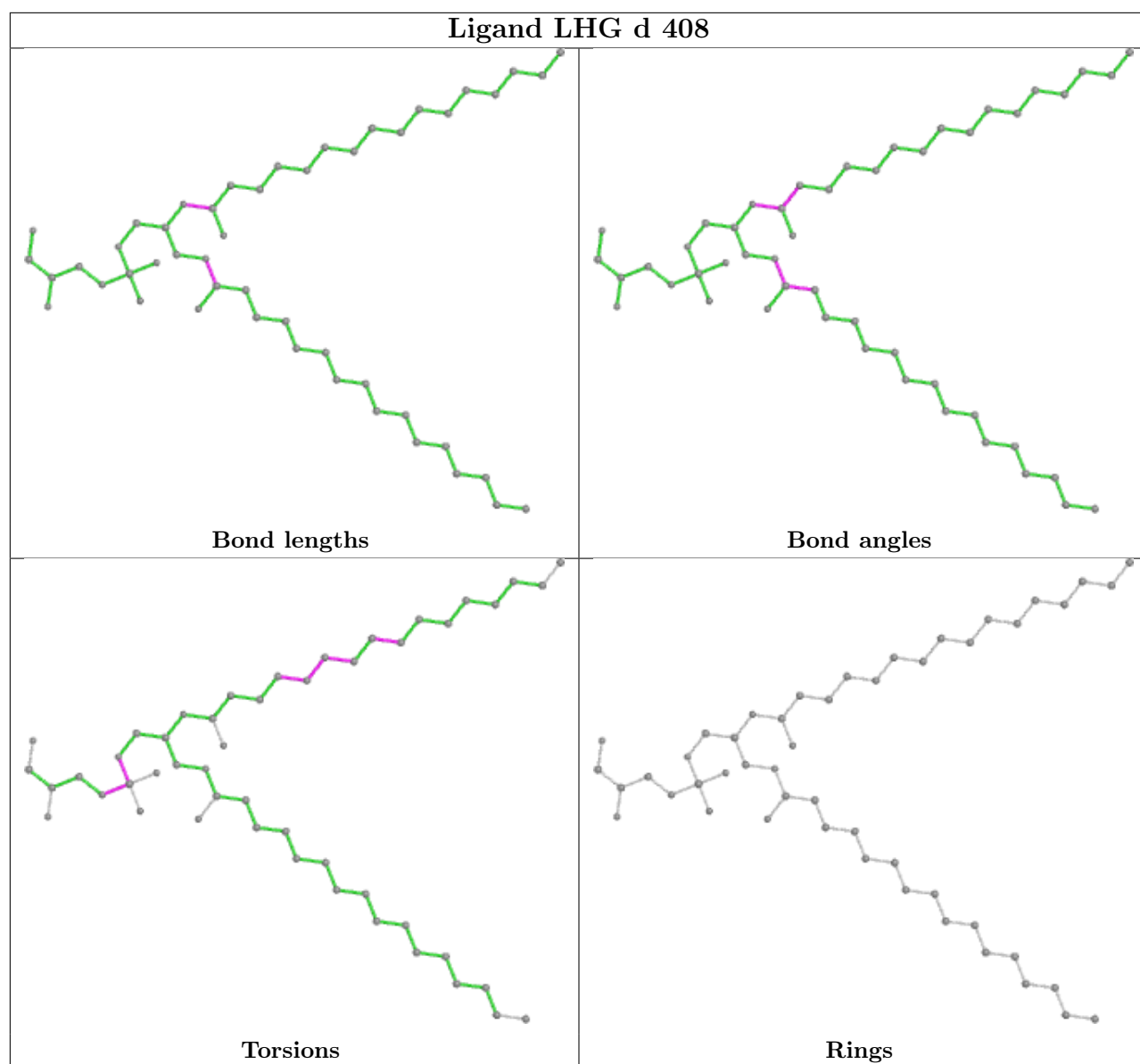


Torsions

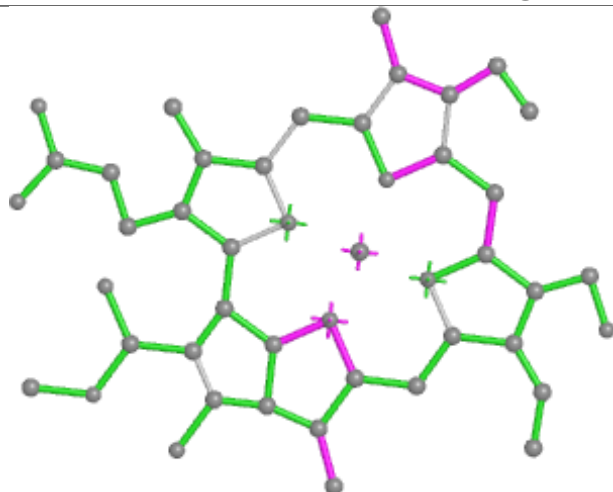


Rings

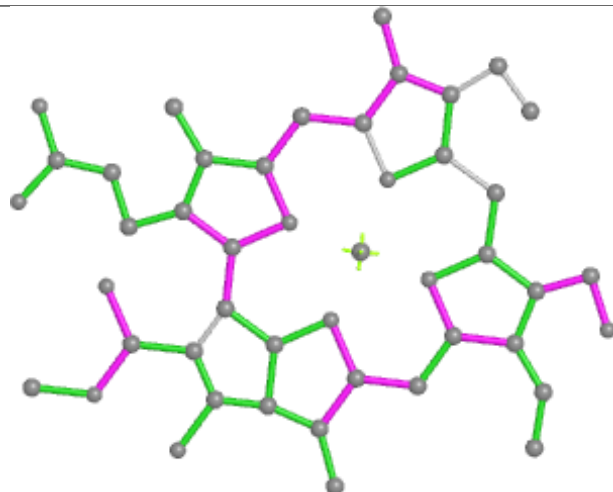




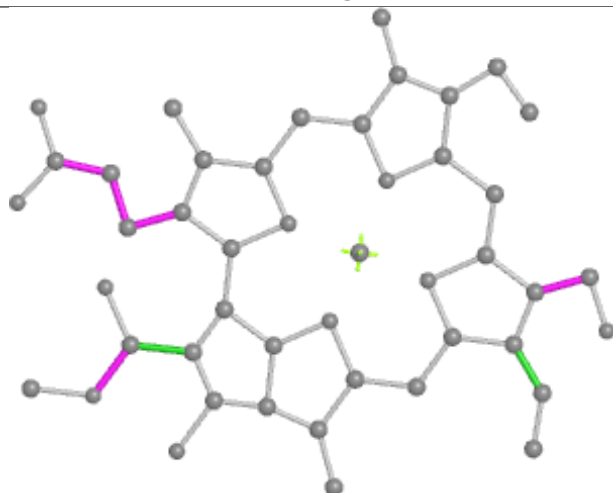
Ligand CHL n 307



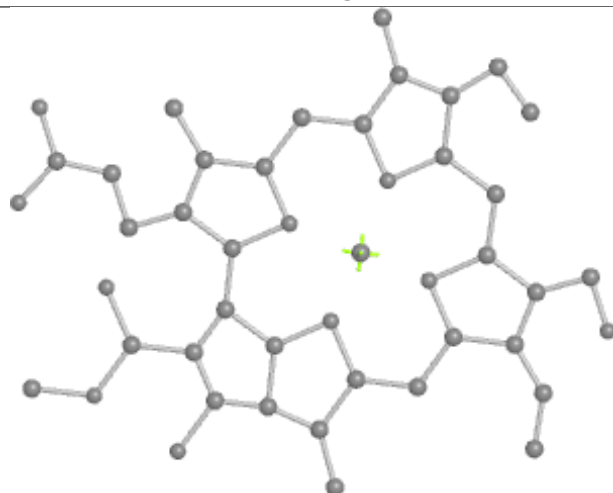
Bond lengths



Bond angles

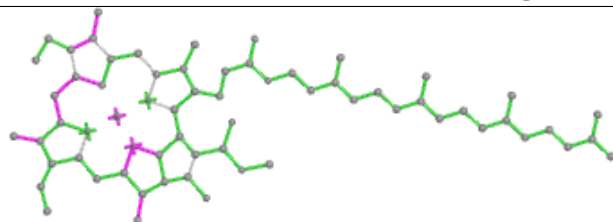


Torsions

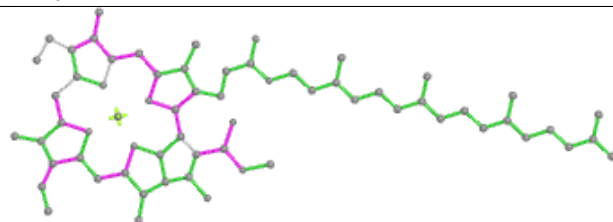


Rings

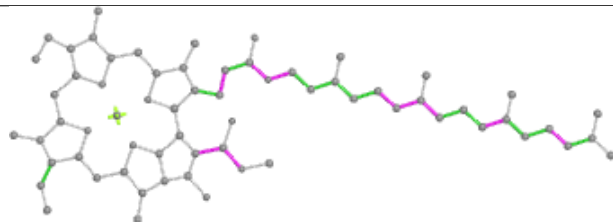
Ligand CLA y 313



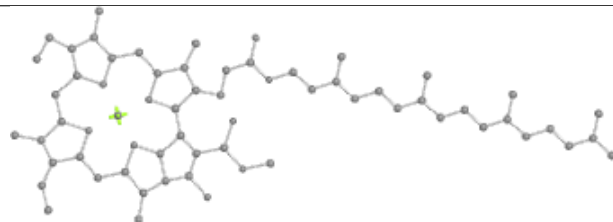
Bond lengths



Bond angles

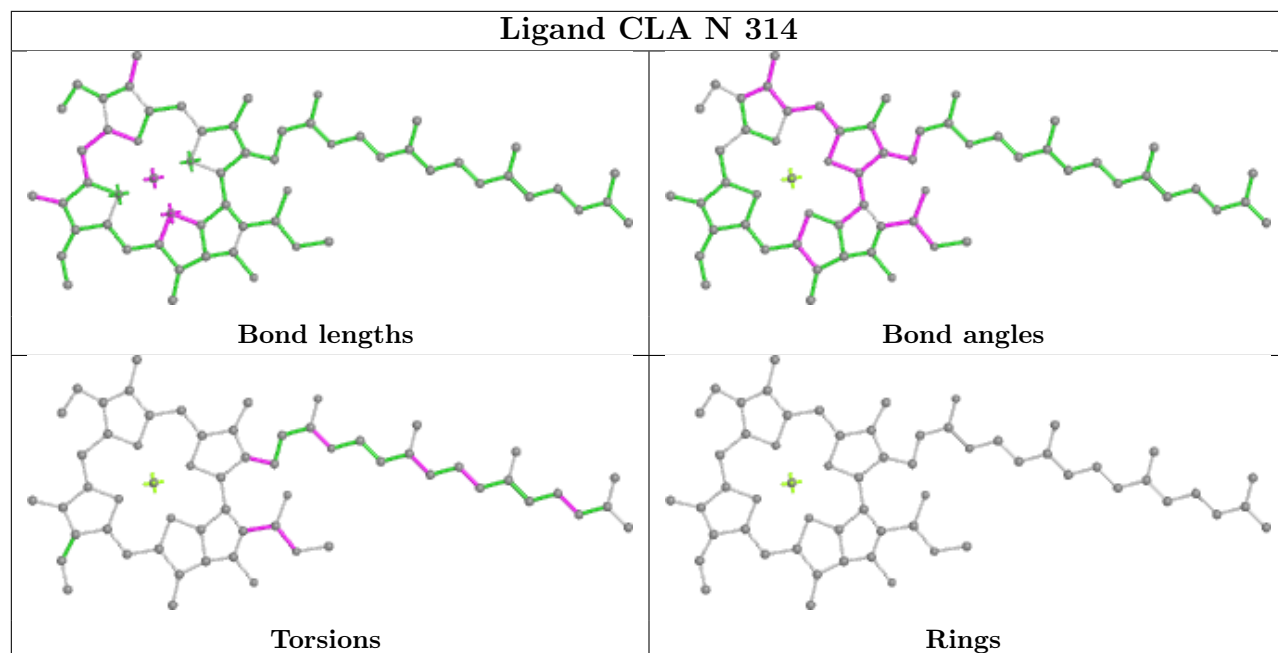


Torsions

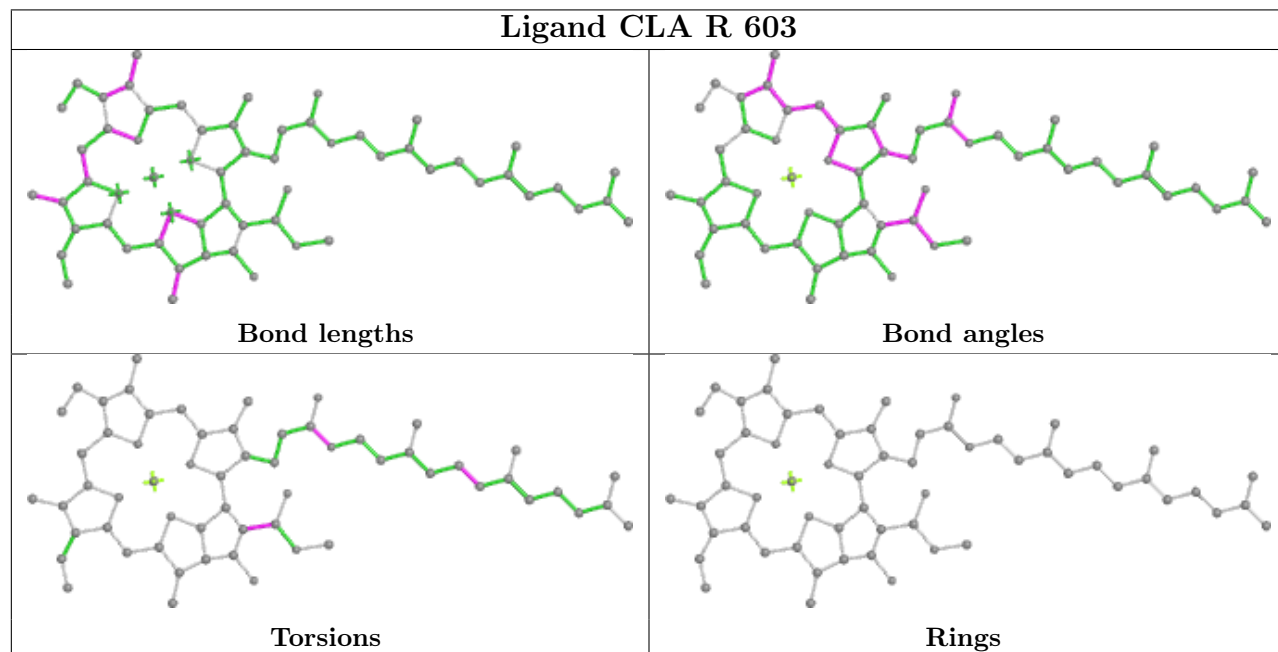


Rings

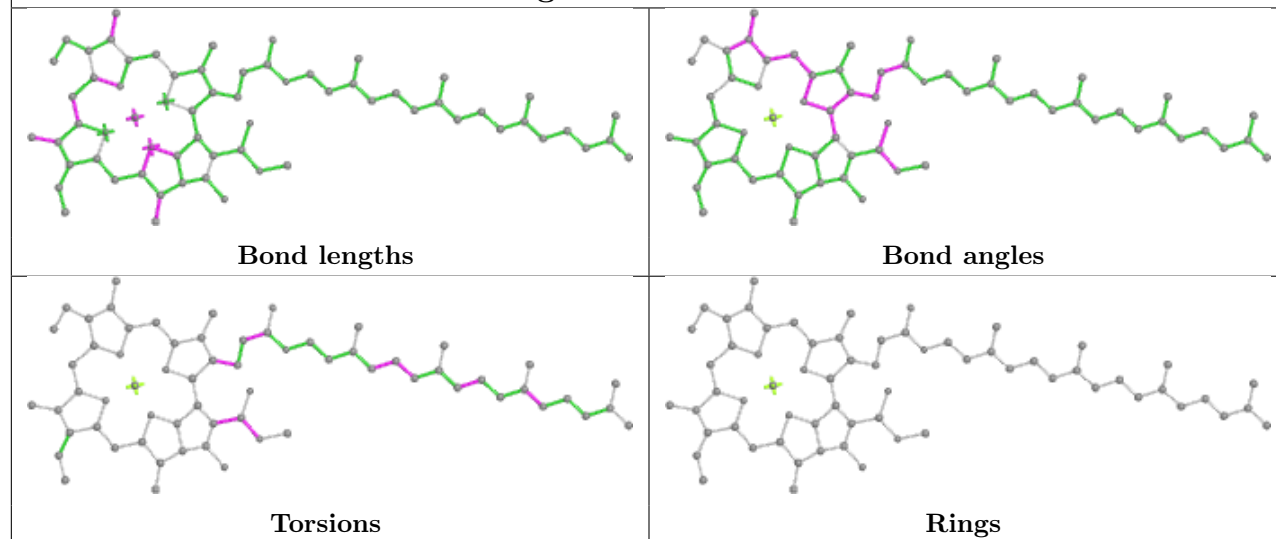
Ligand CLA N 314



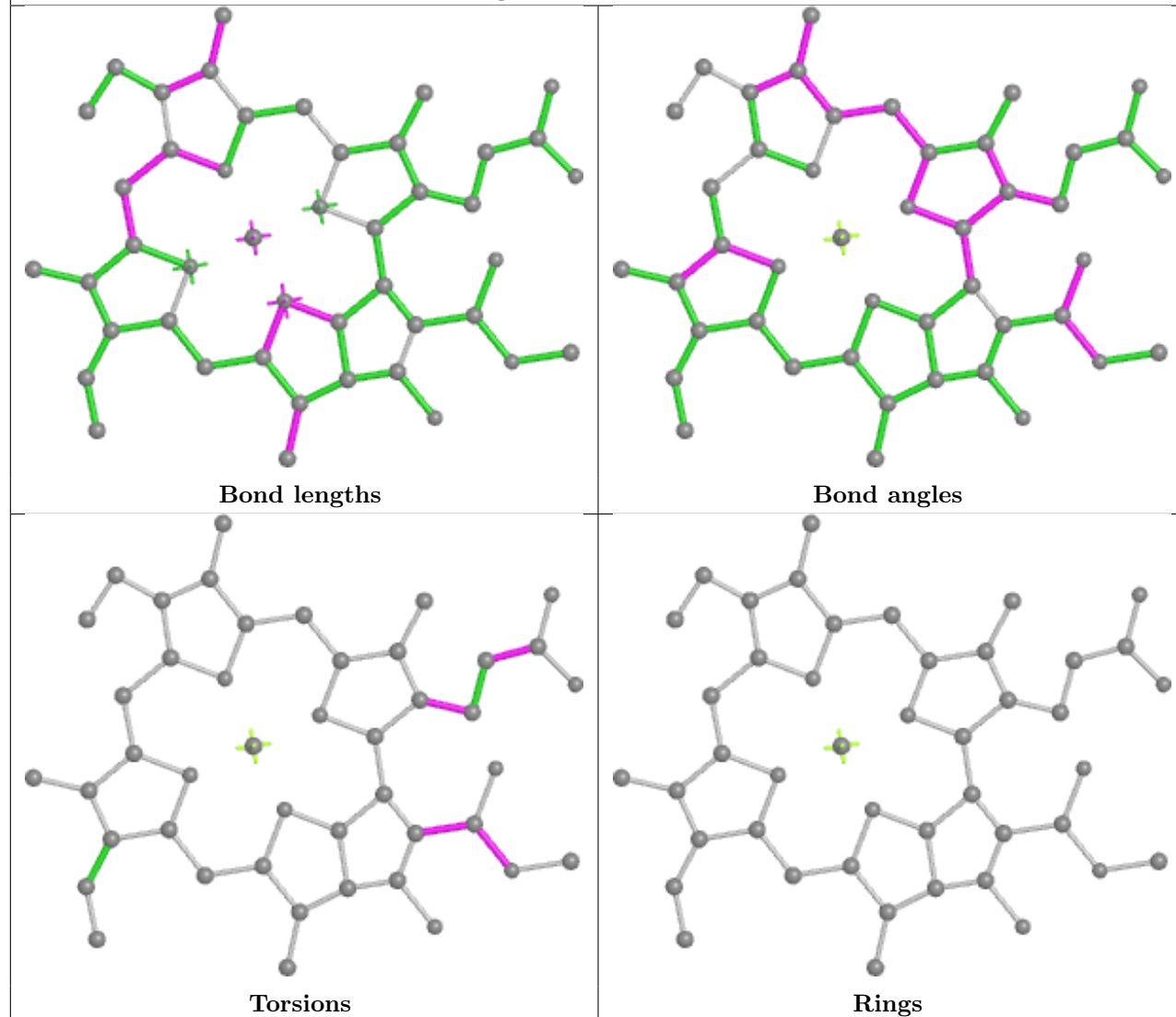
Ligand CLA R 603

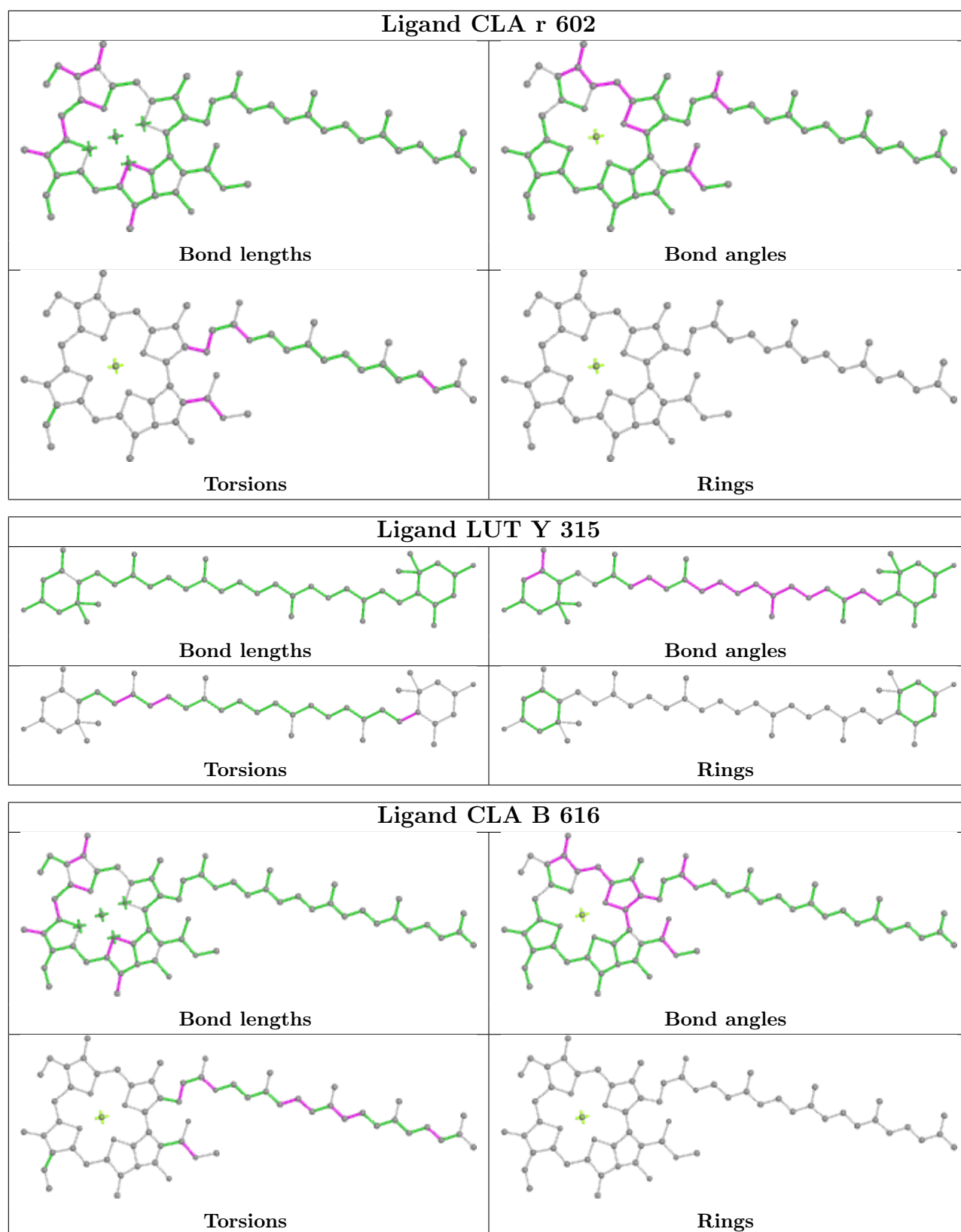


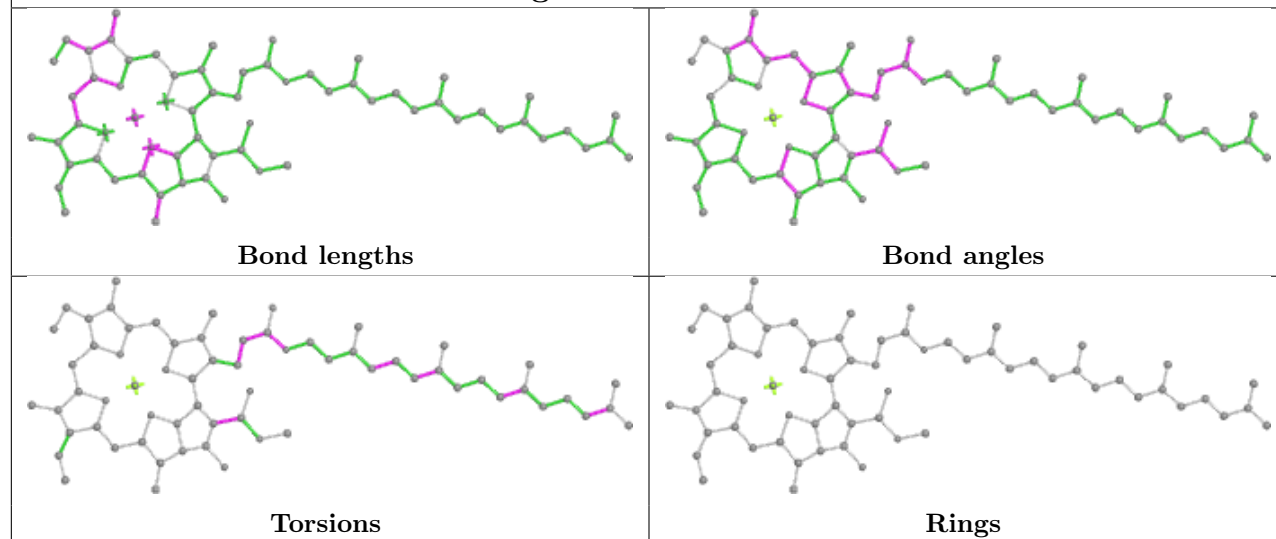
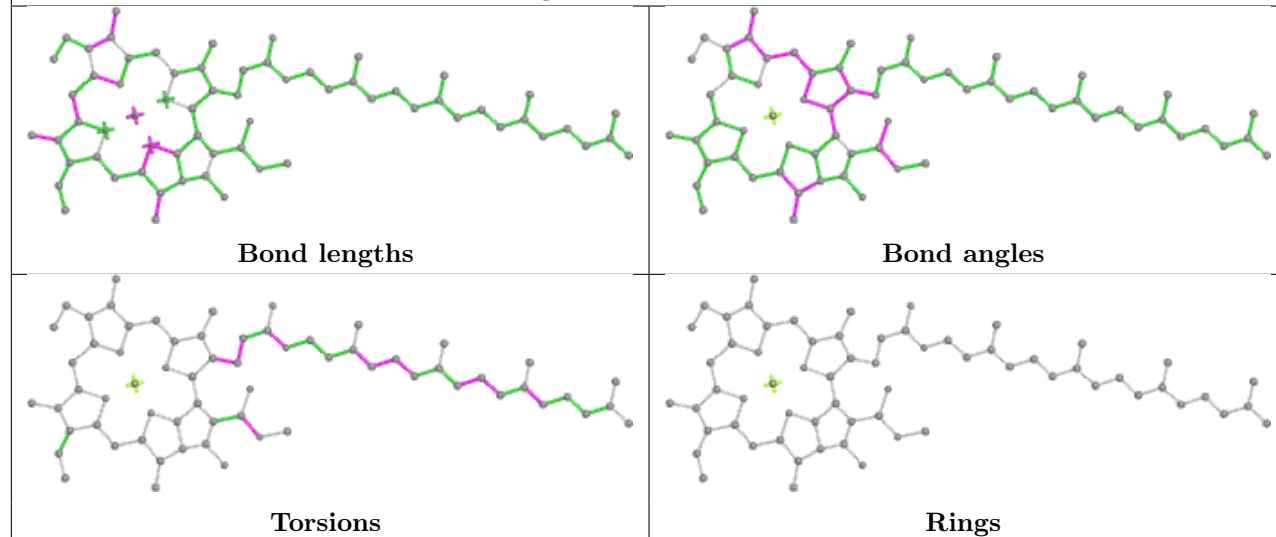
Ligand CLA c 511



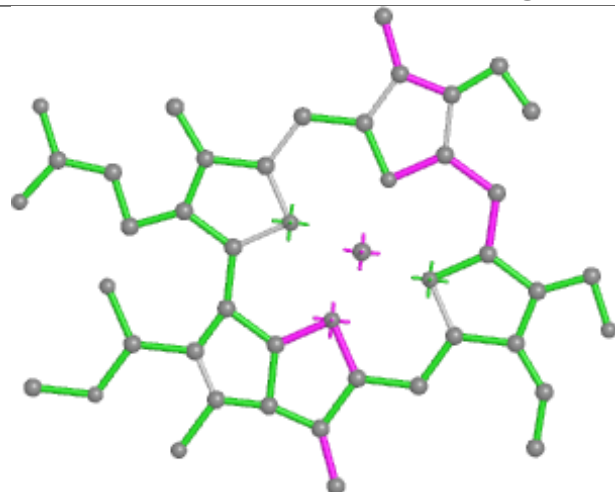
Ligand CLA S 611



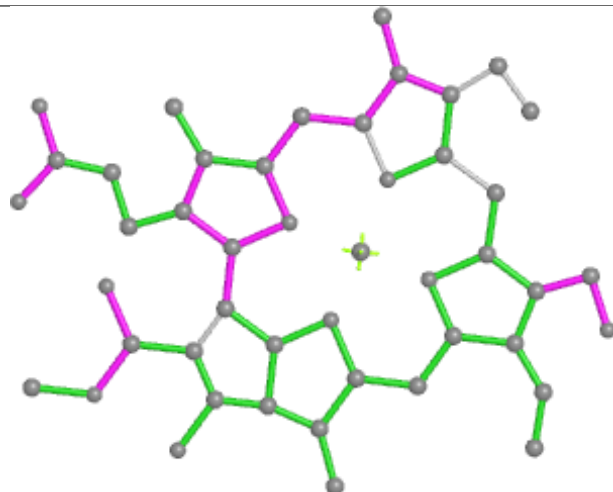


Ligand CLA Y 304**Ligand CLA c 513**

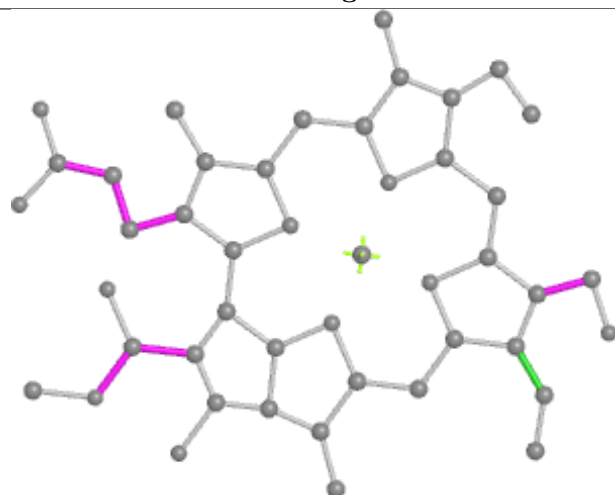
Ligand CHL n 308



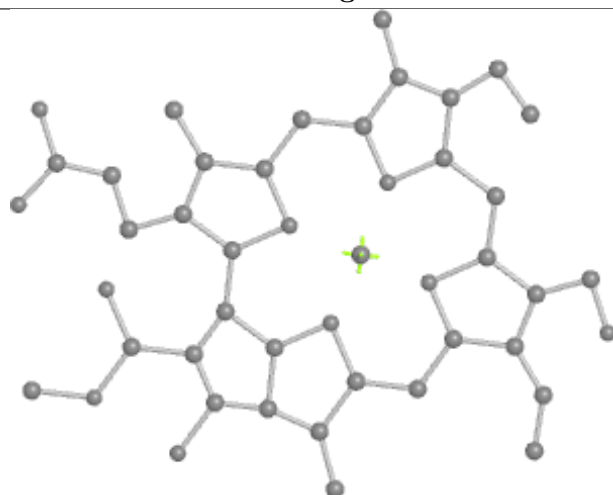
Bond lengths



Bond angles

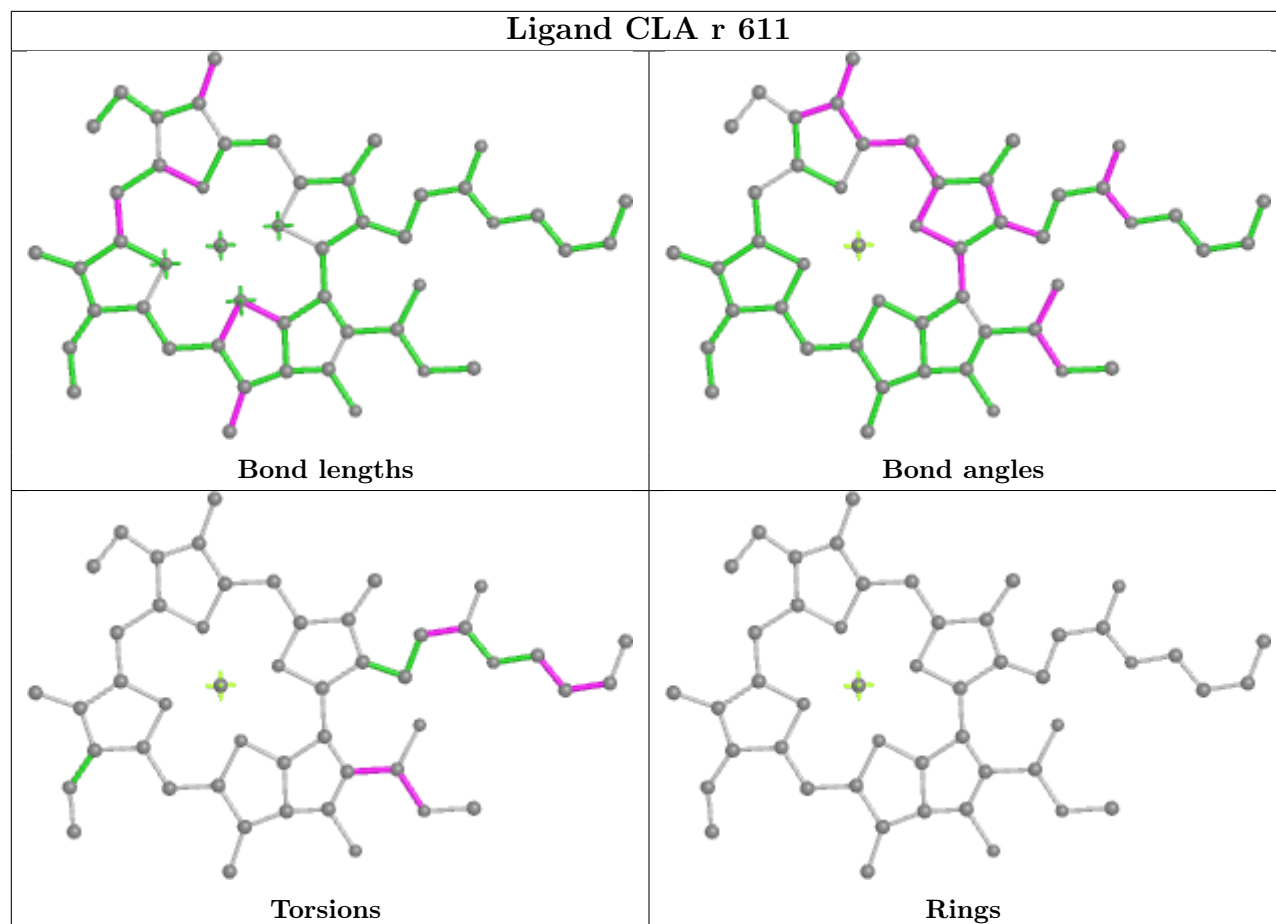


Torsions

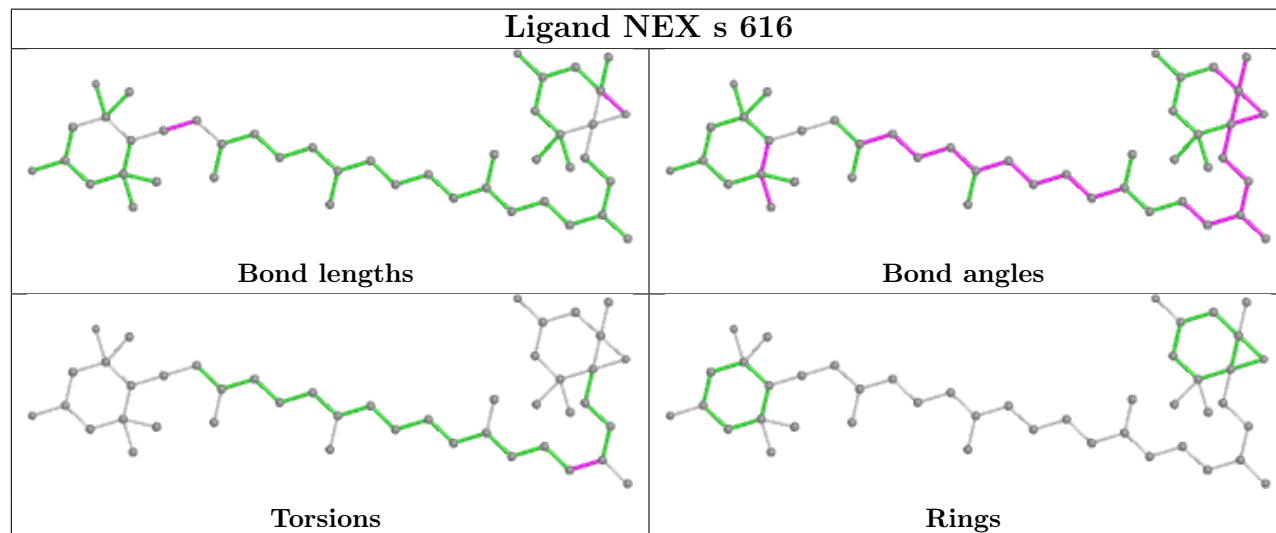


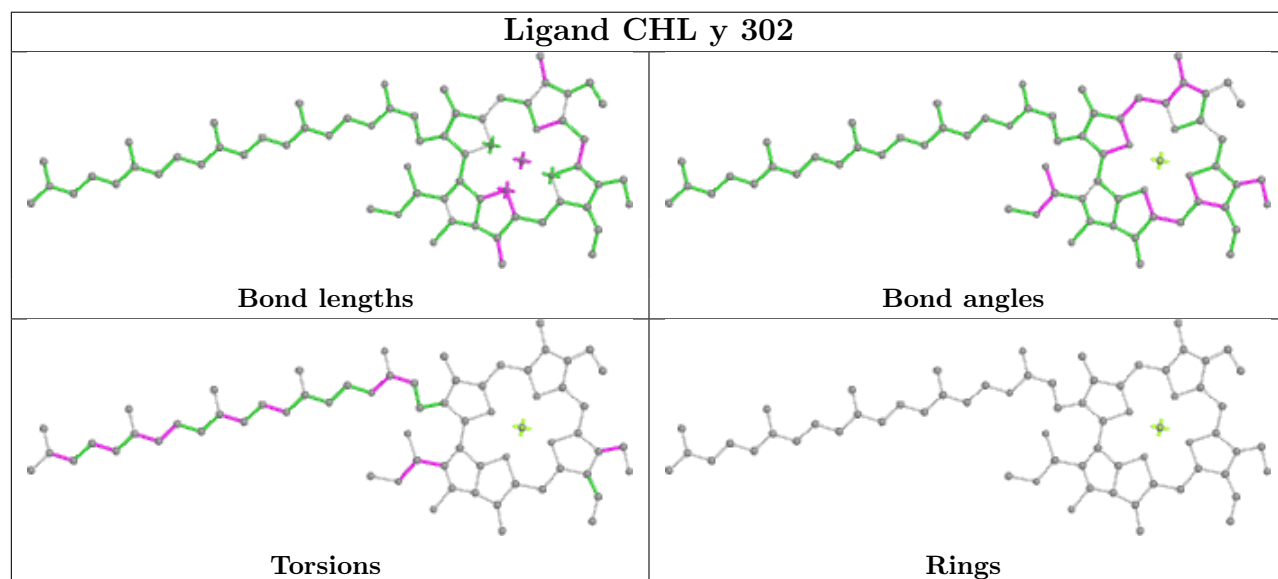
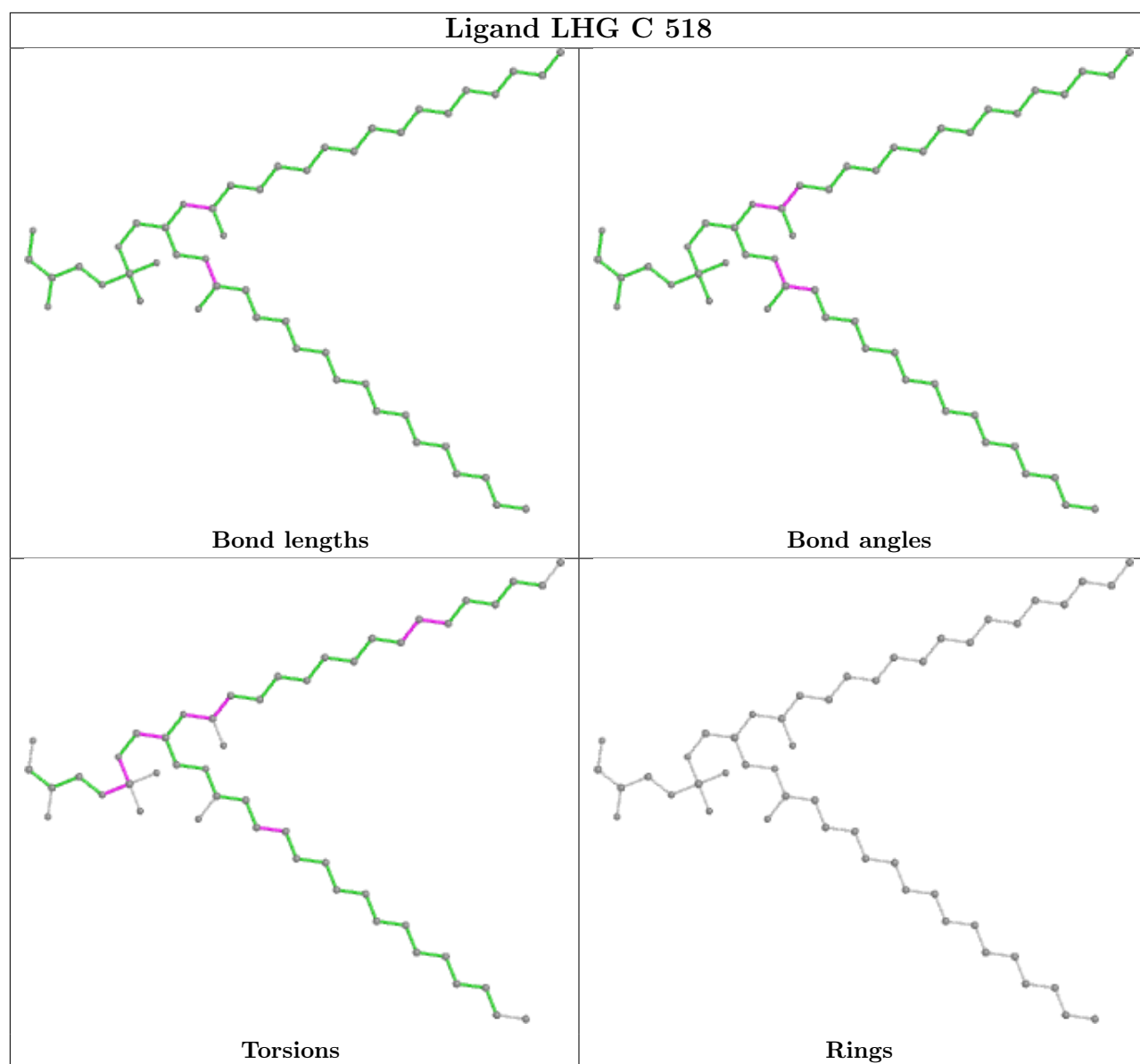
Rings

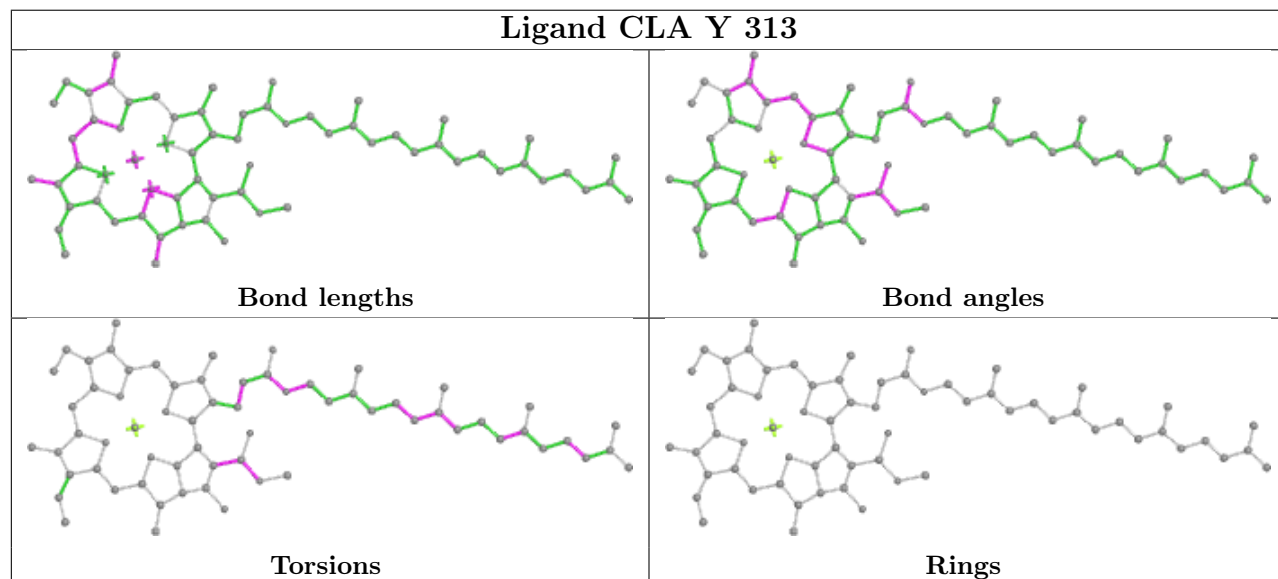
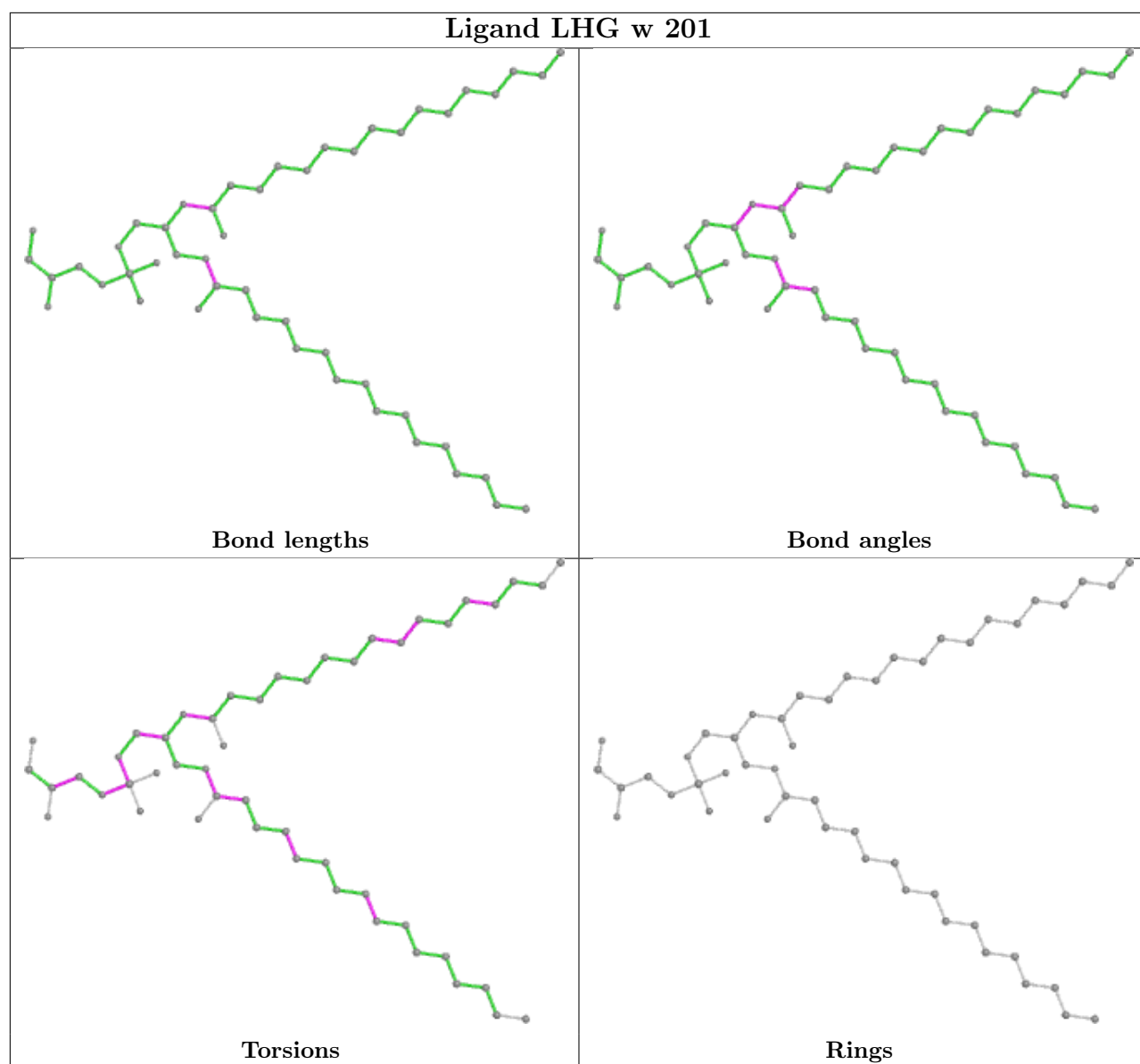
Ligand CLA r 611

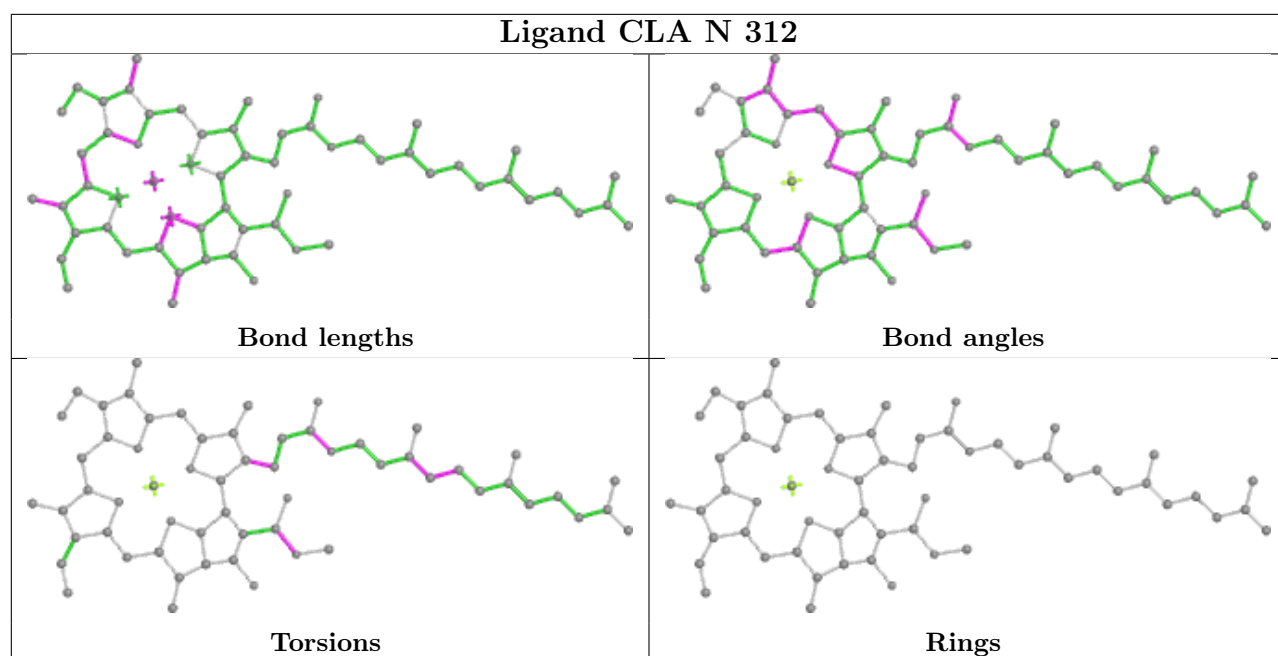


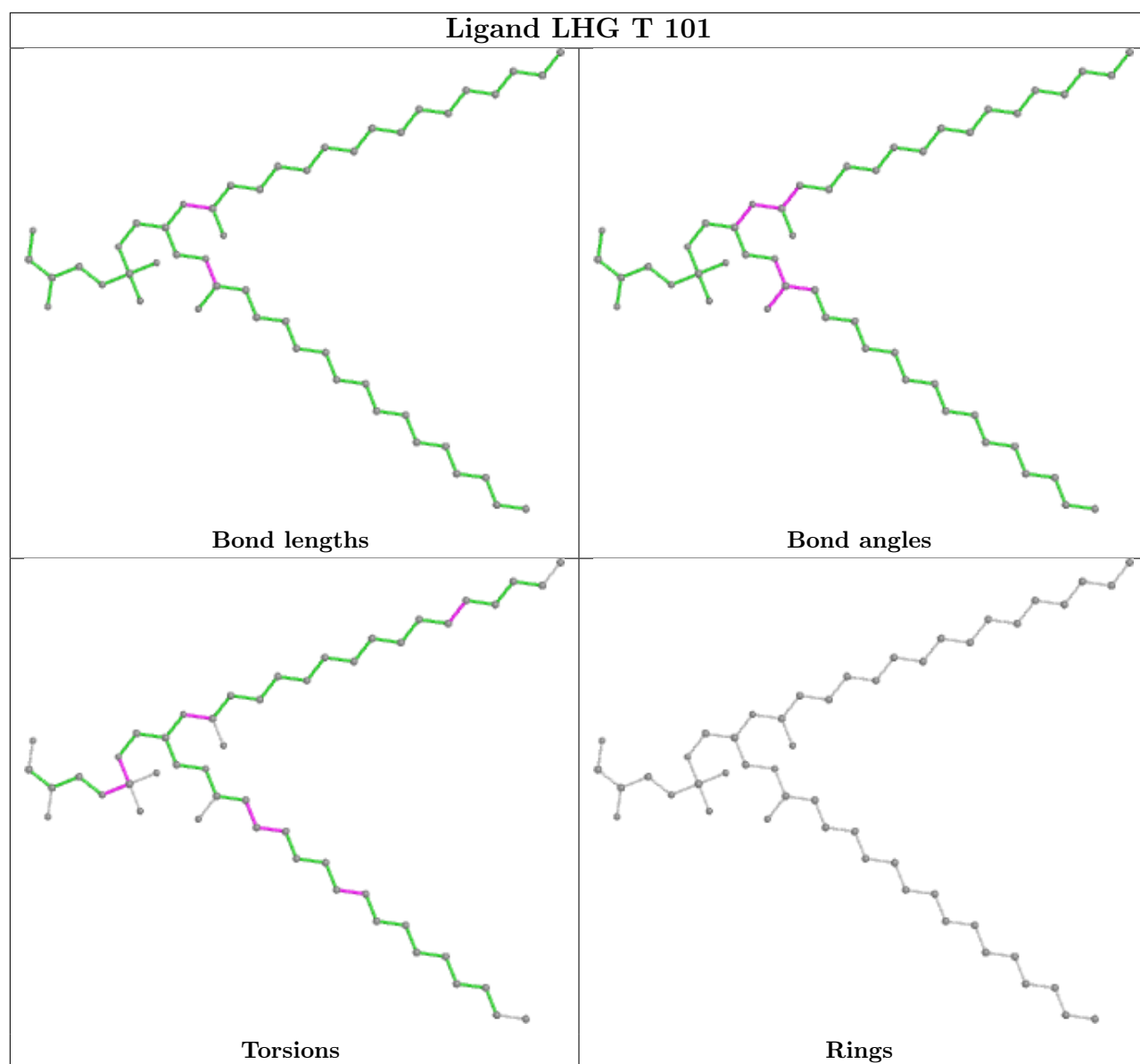
Ligand NEX s 616

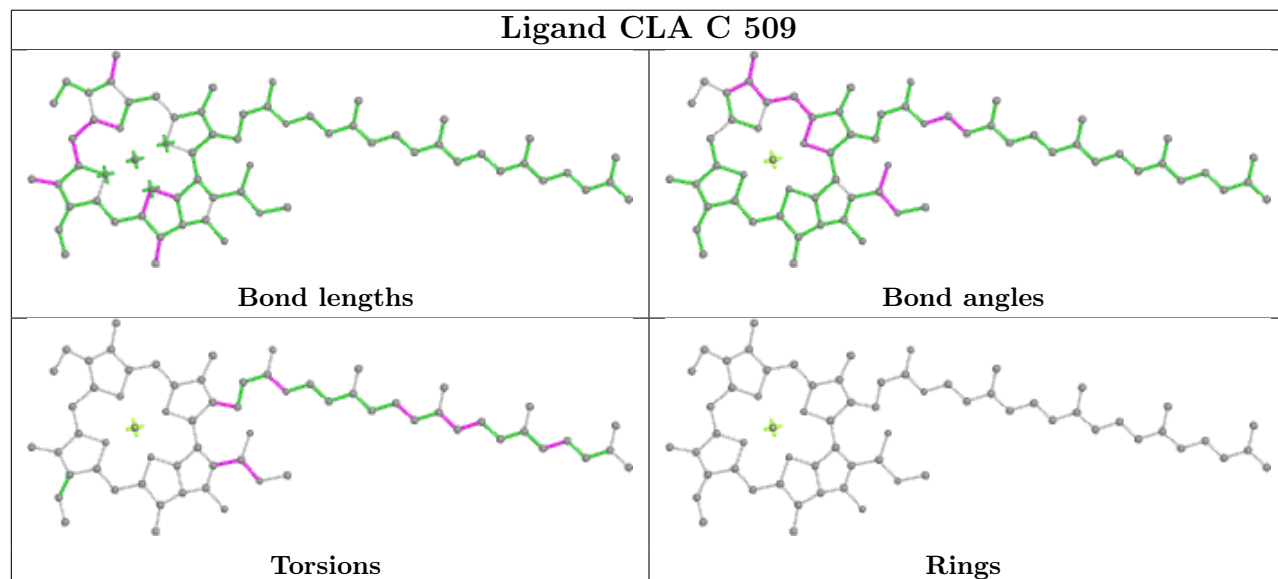
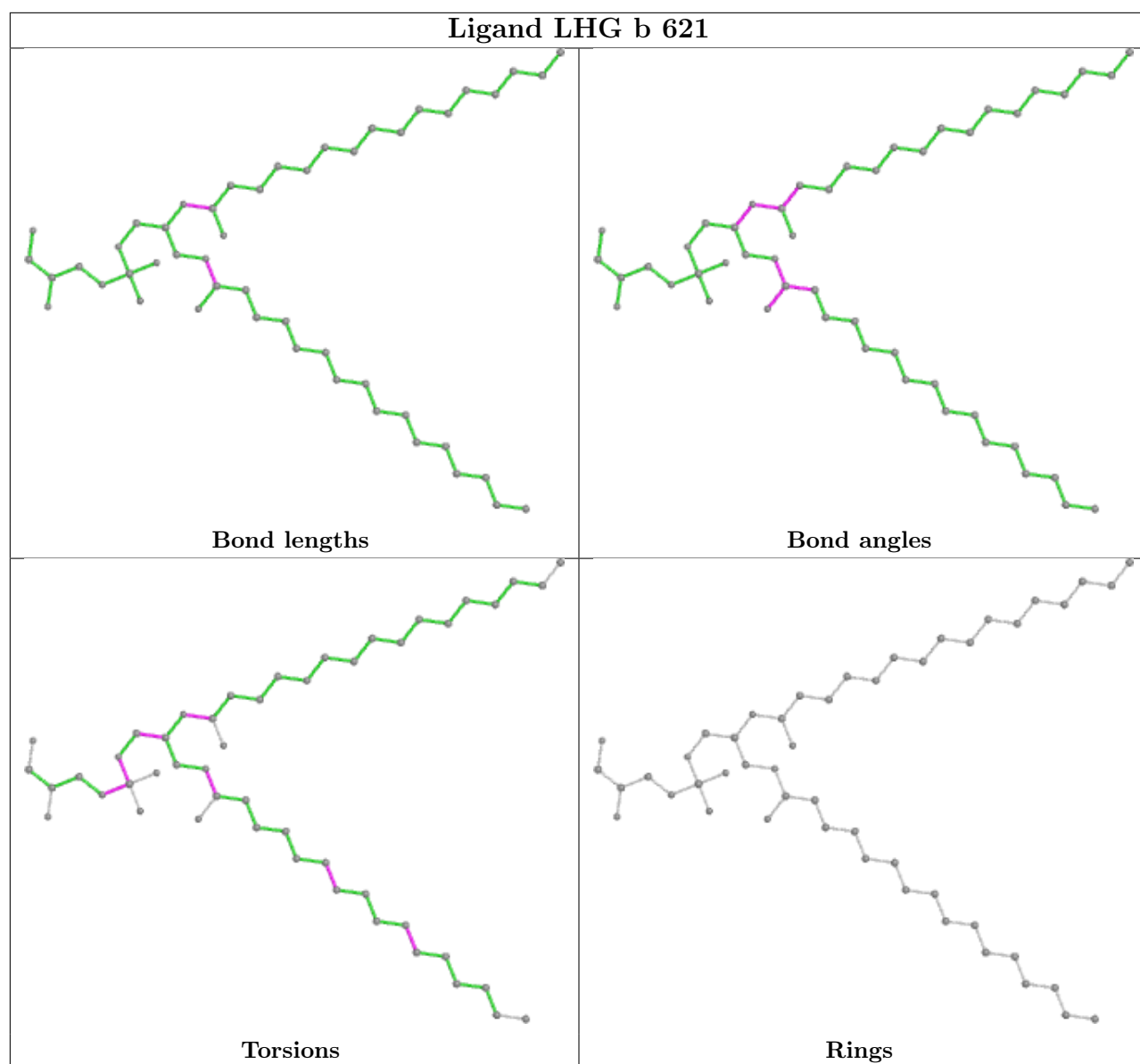




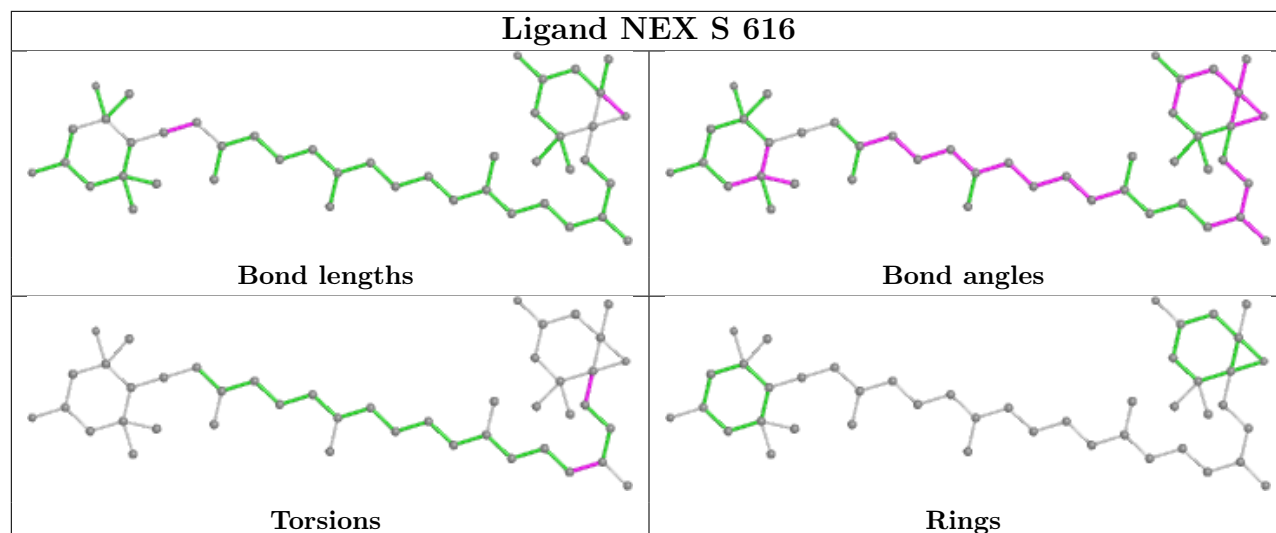




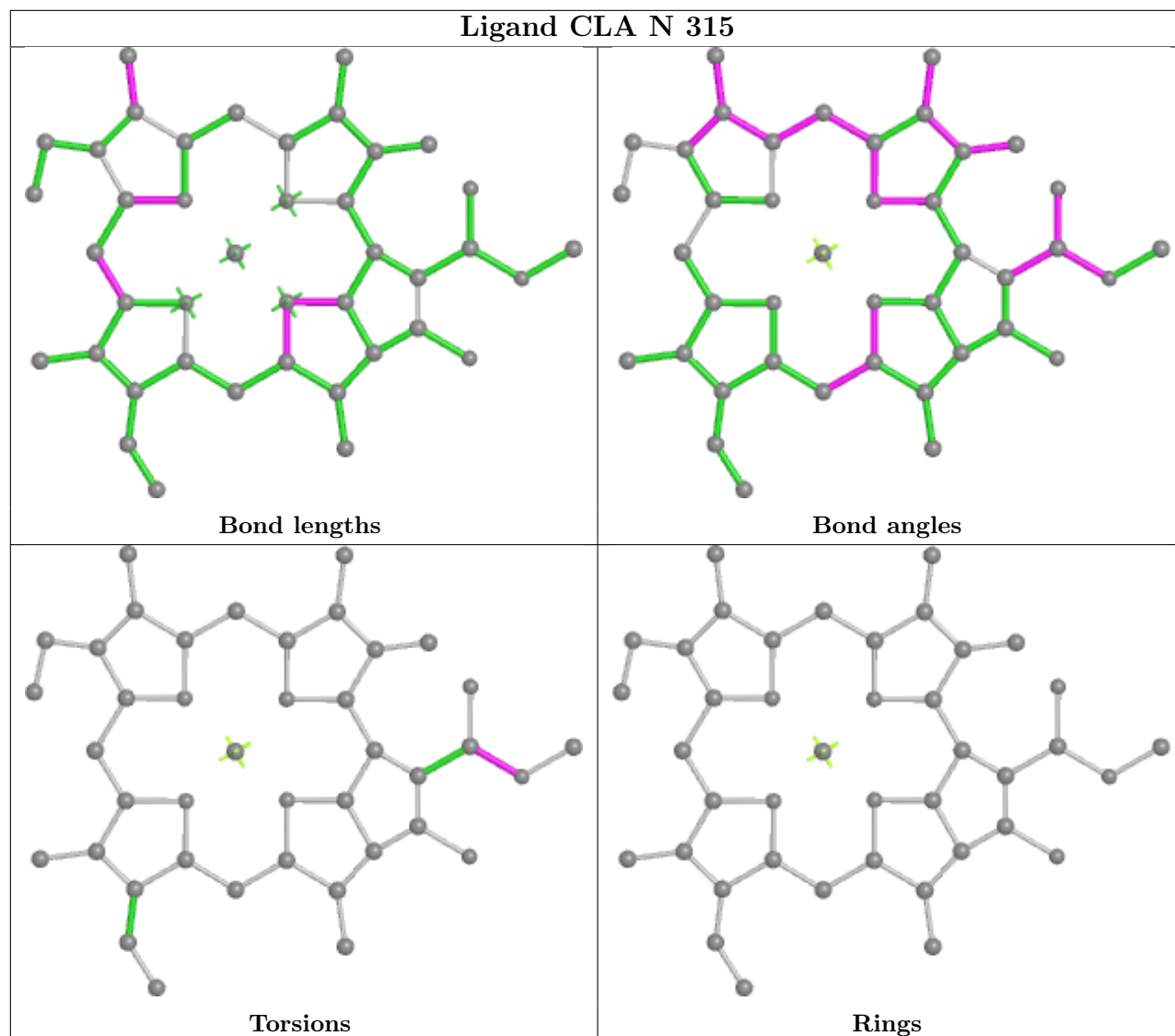


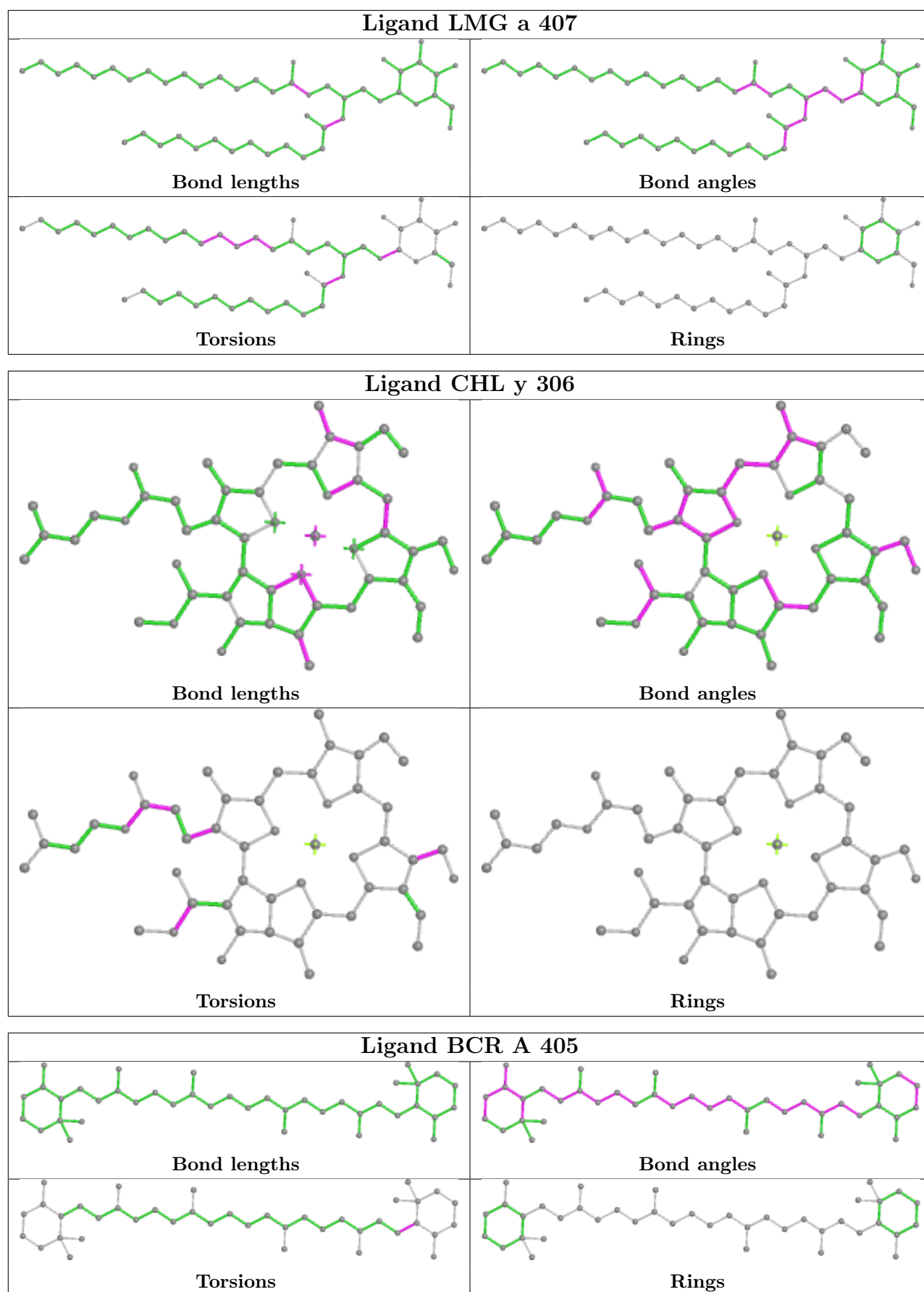


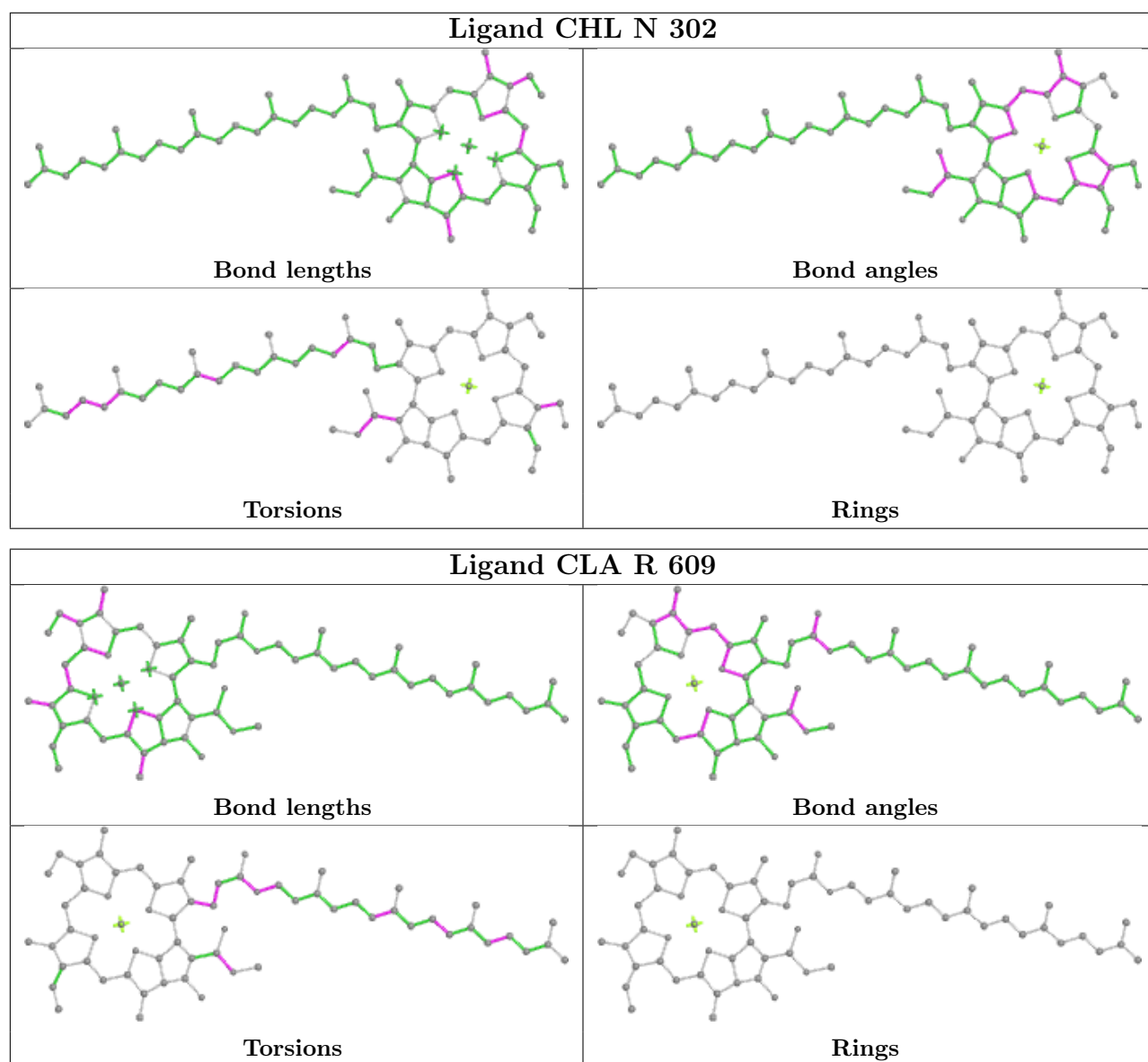
Ligand NEX S 616



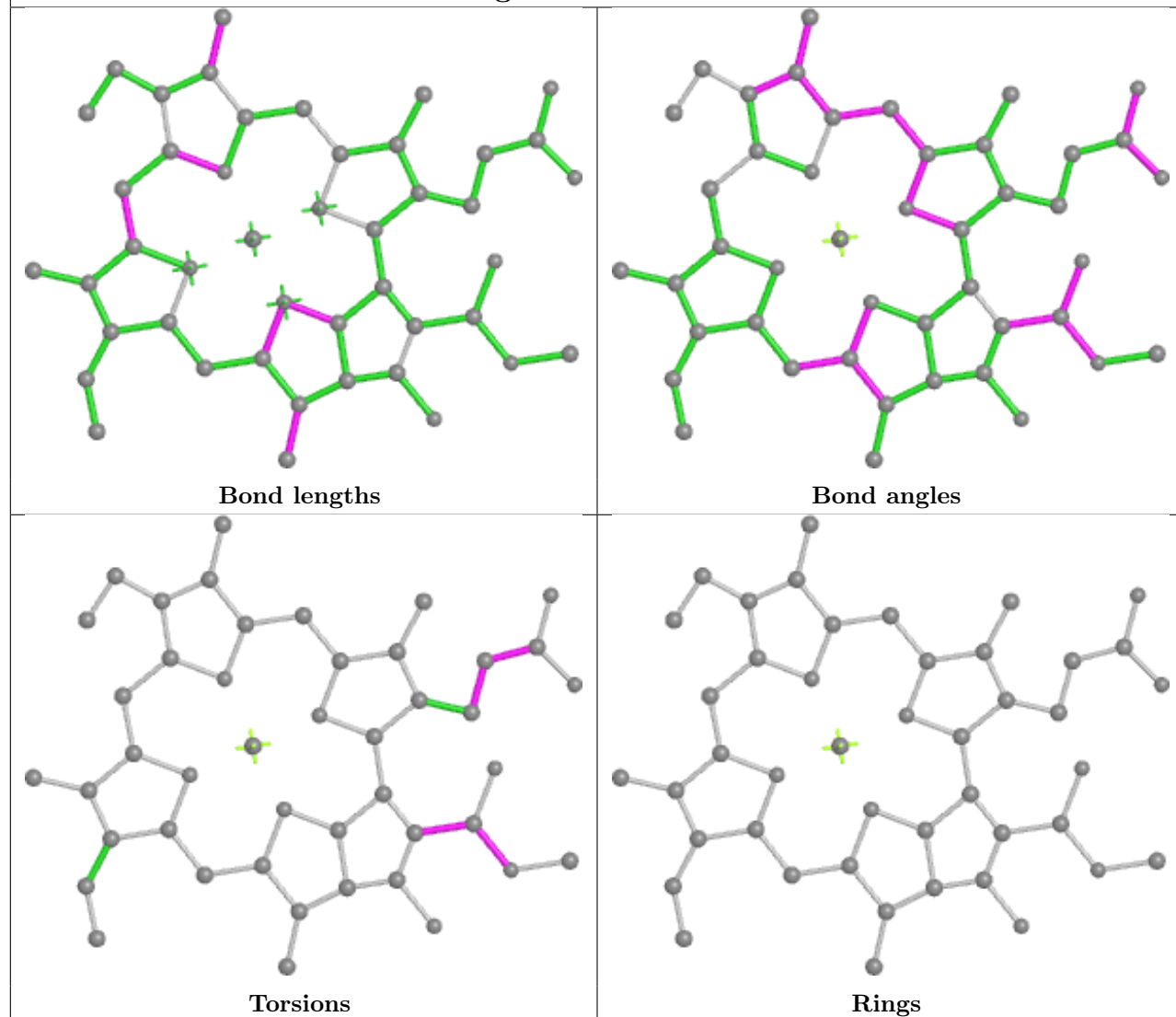
Ligand CLA N 315



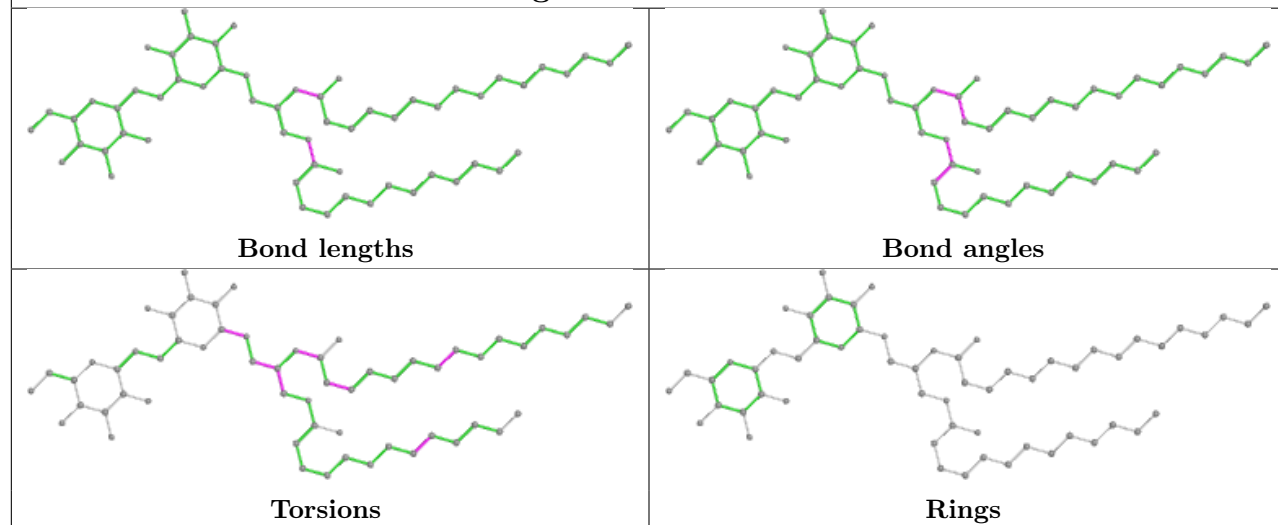




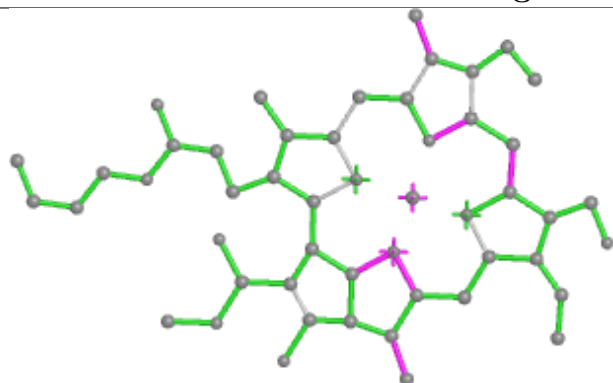
Ligand CLA s 608



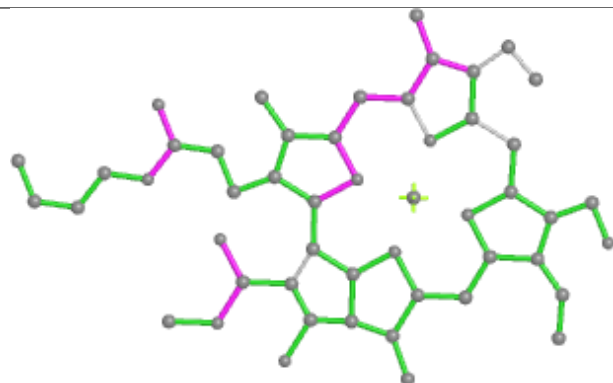
Ligand DGD a 408



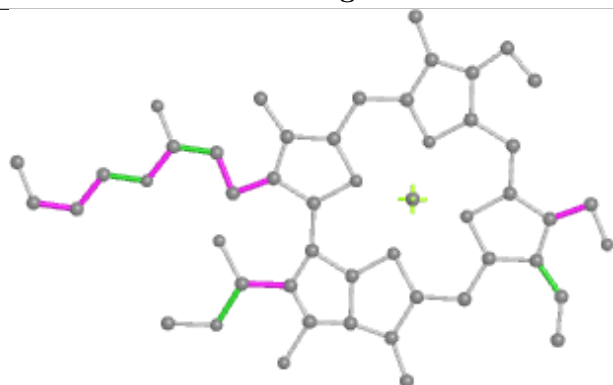
Ligand CHL Y 307



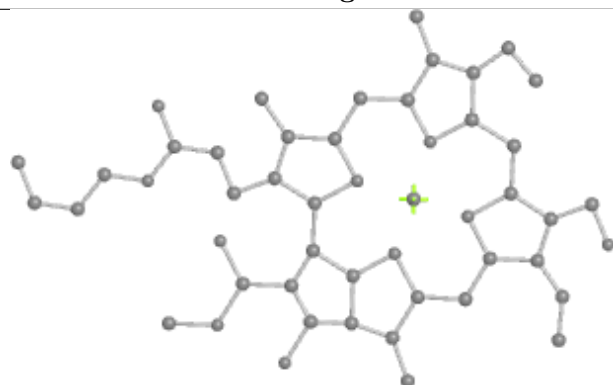
Bond lengths



Bond angles

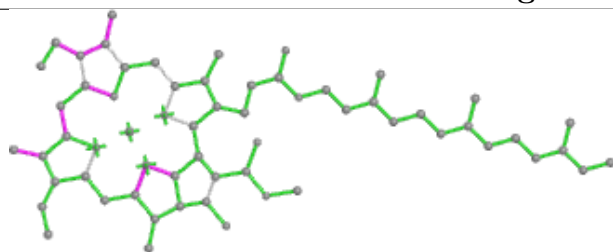


Torsions

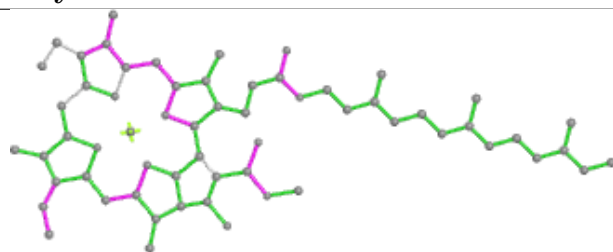


Rings

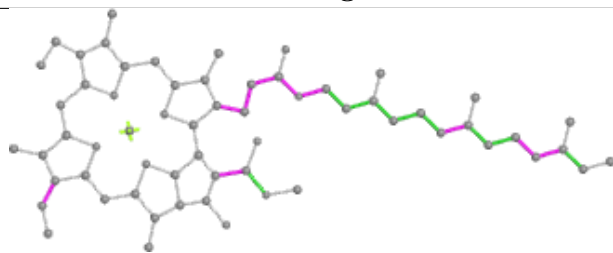
Ligand CLA y 303



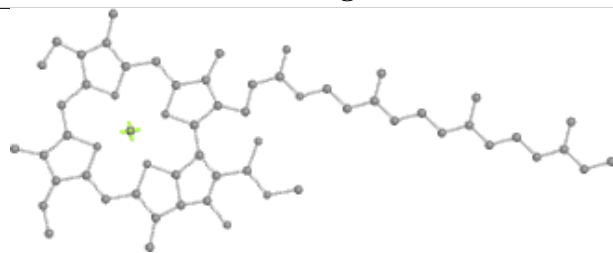
Bond lengths



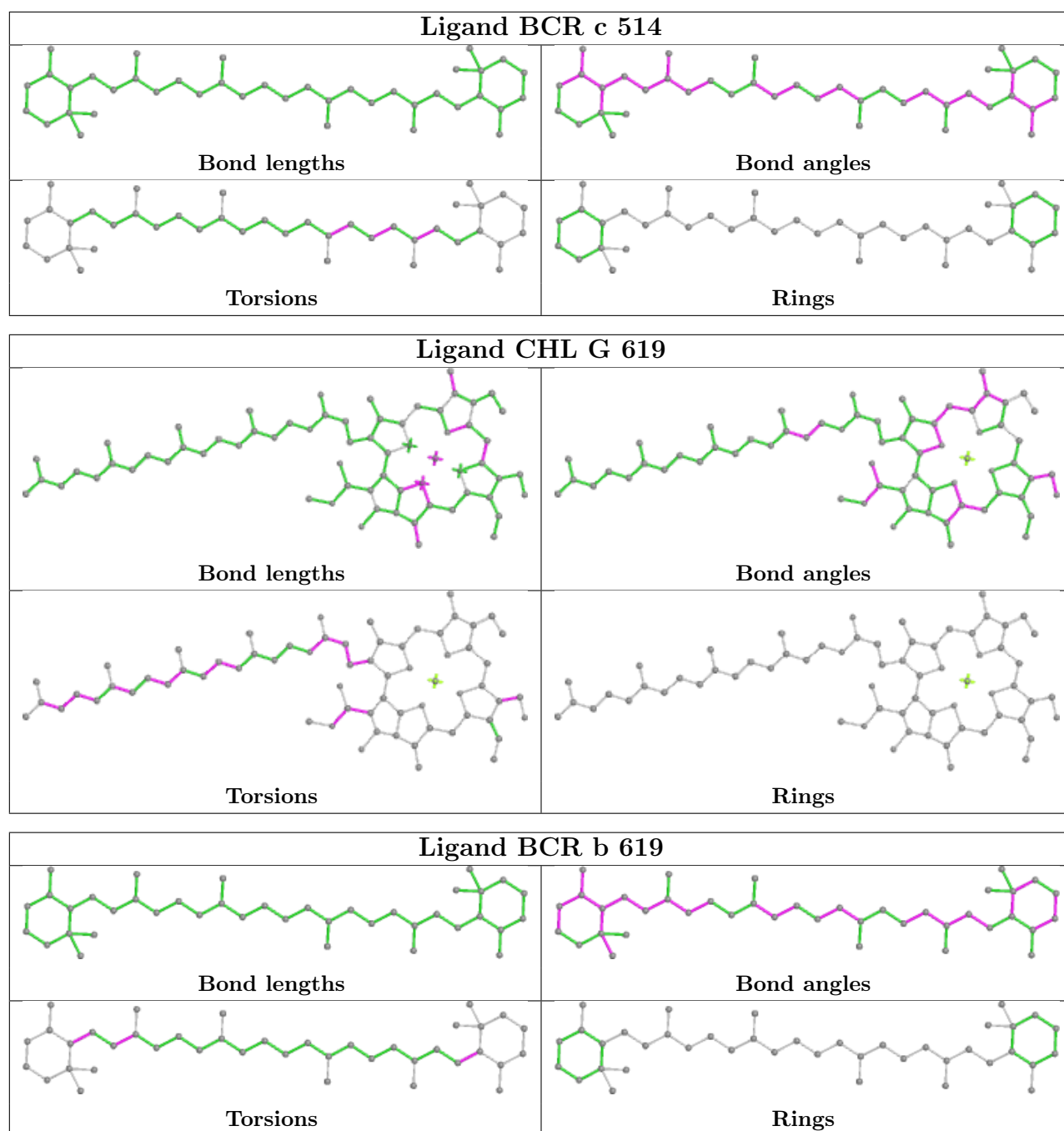
Bond angles



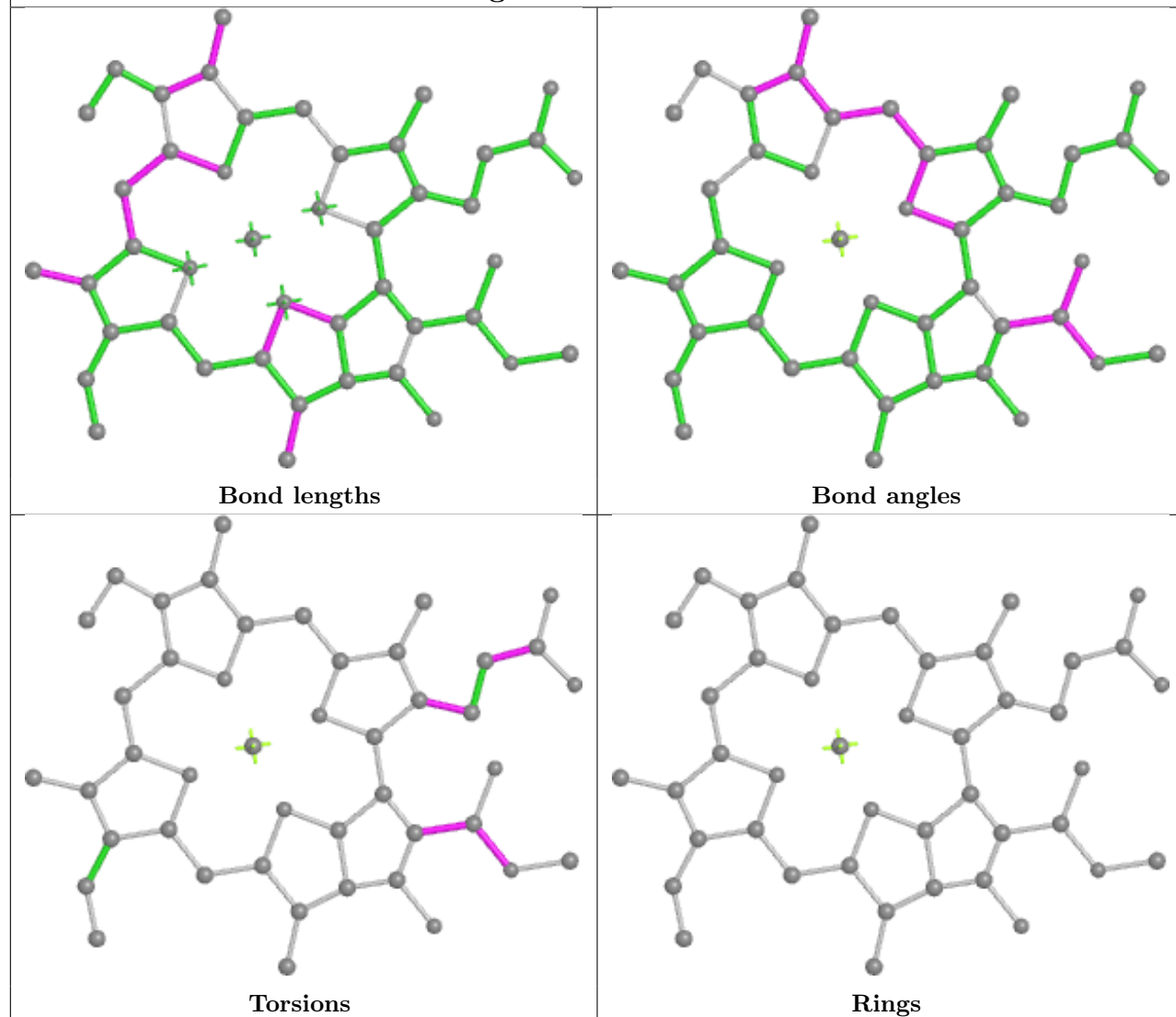
Torsions



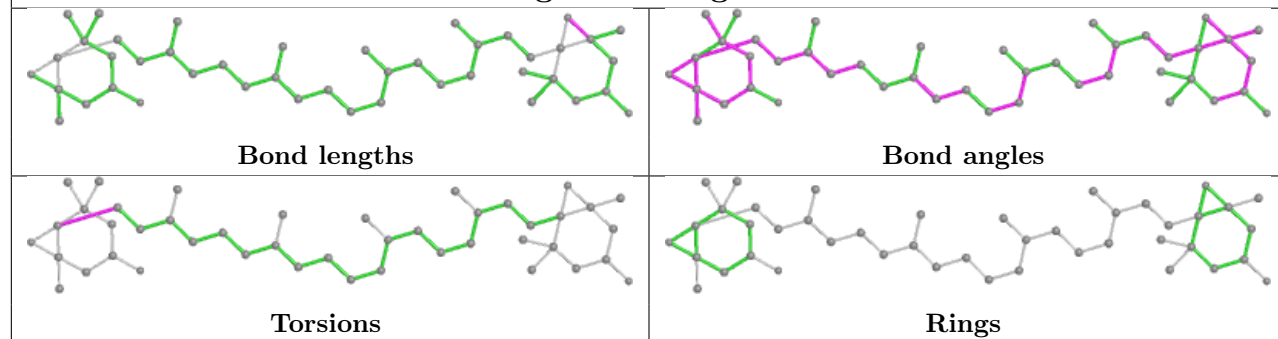
Rings



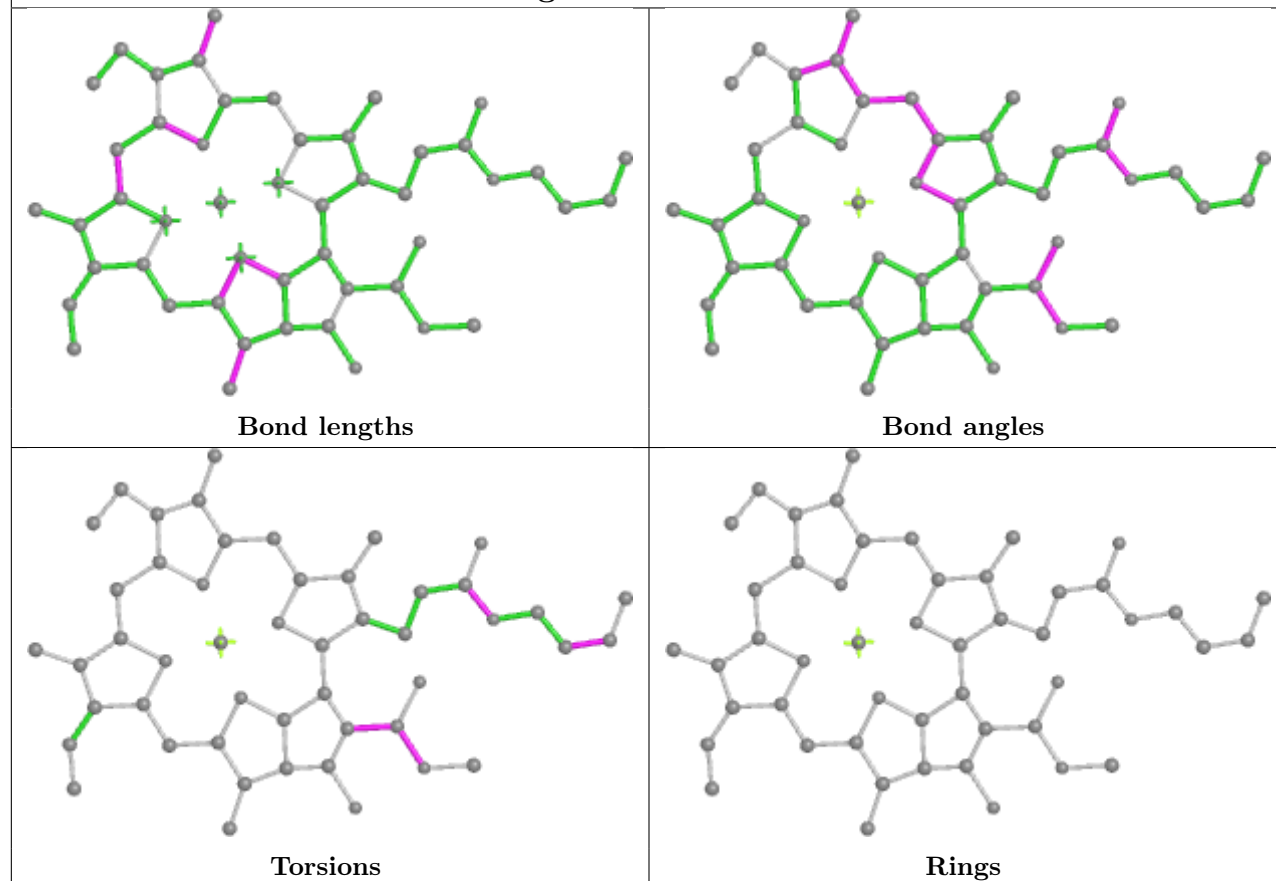
Ligand CLA R 614



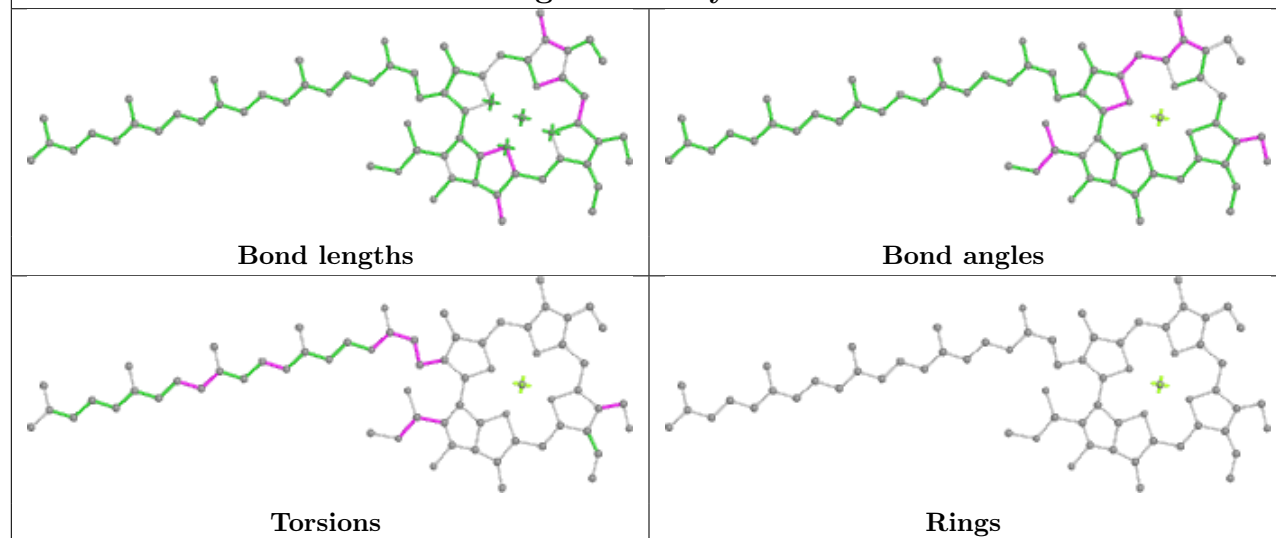
Ligand XAT g 620

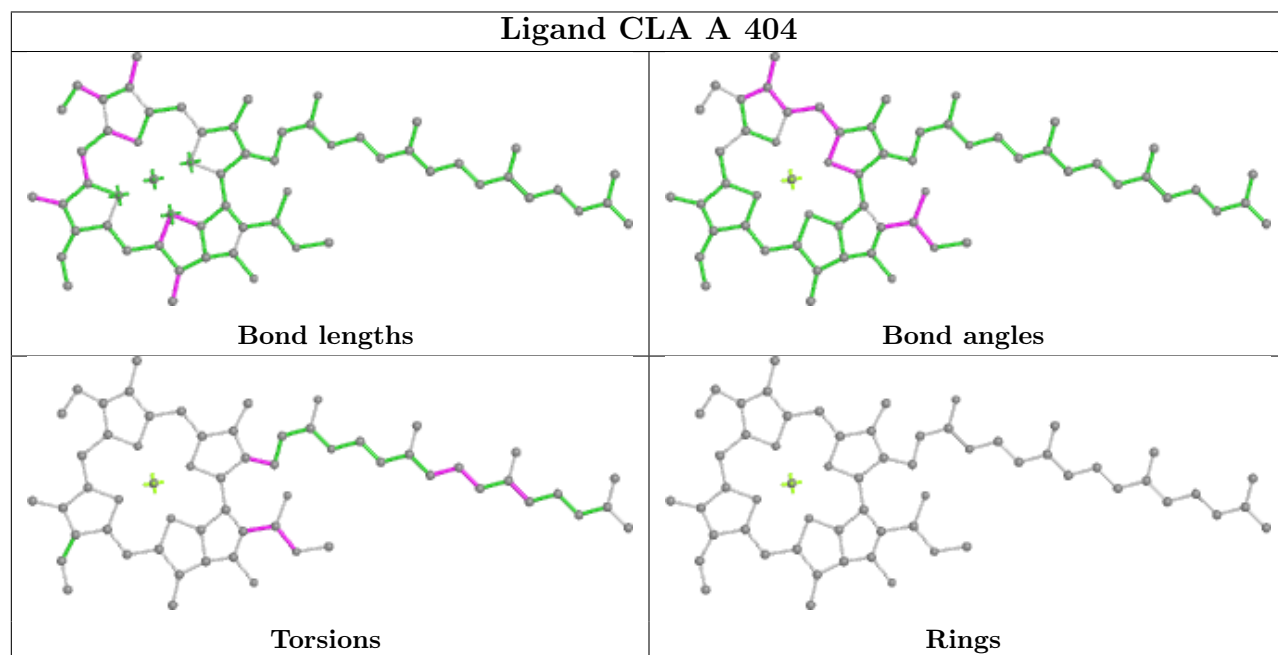
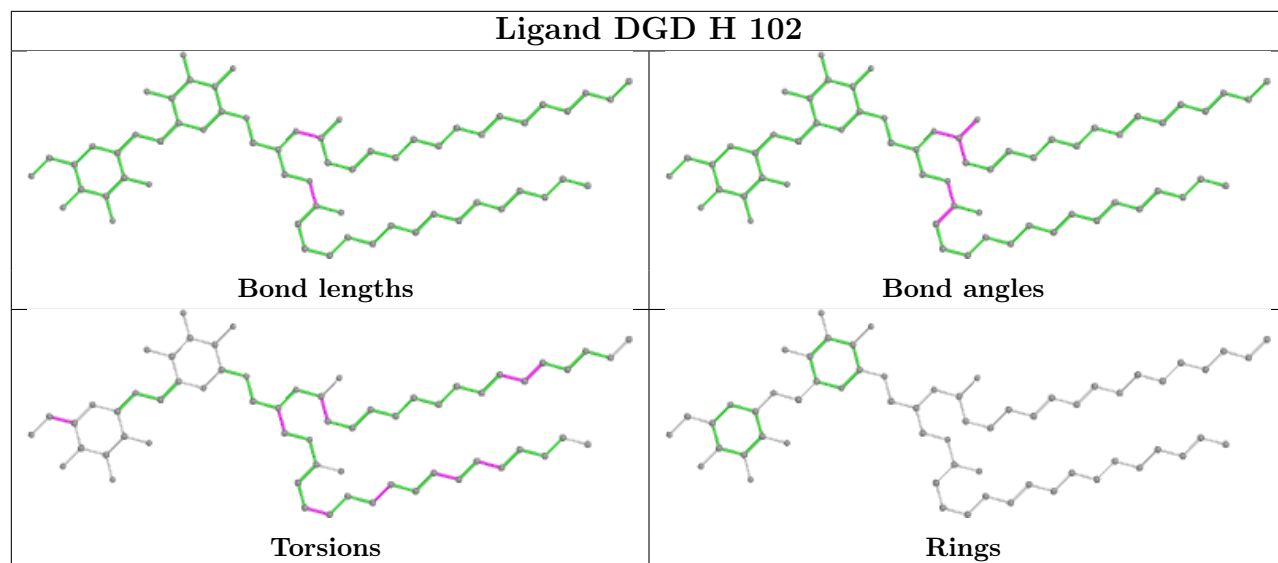


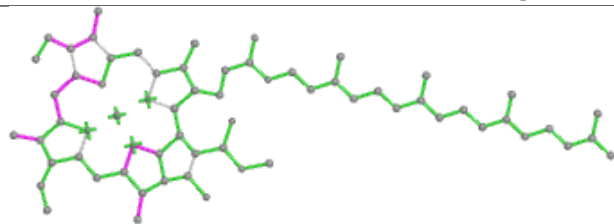
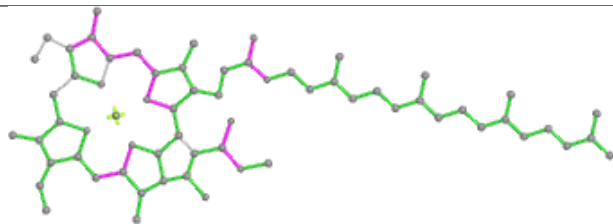
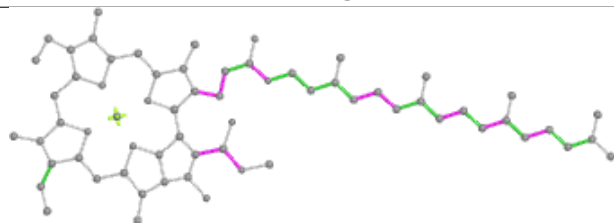
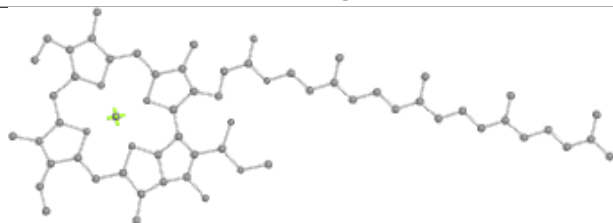
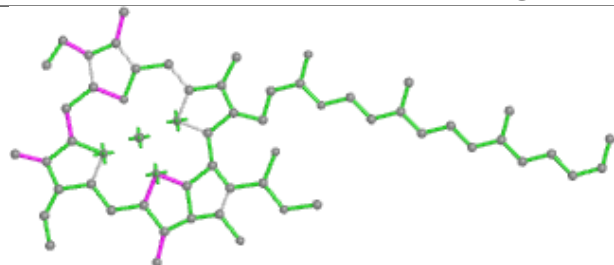
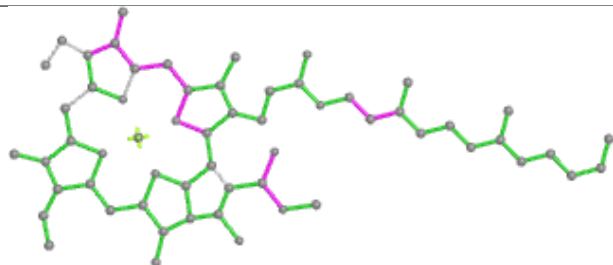
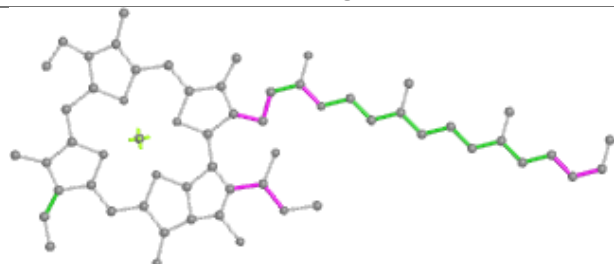
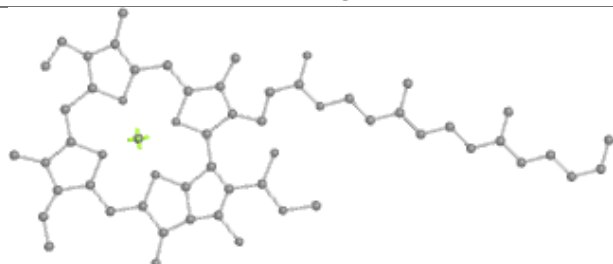
Ligand CLA r 610

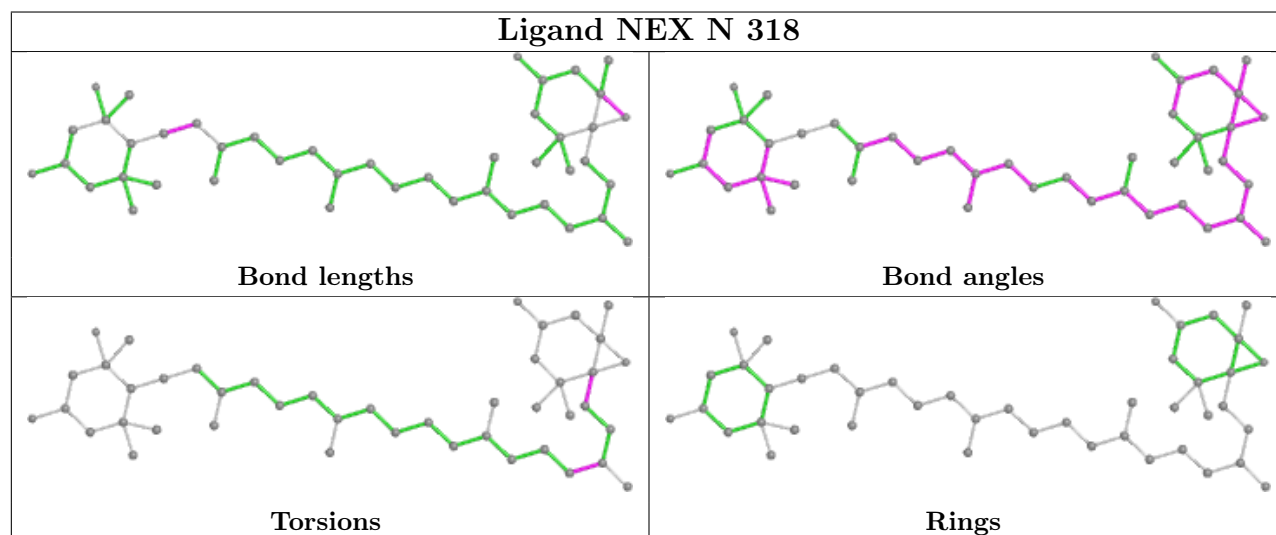
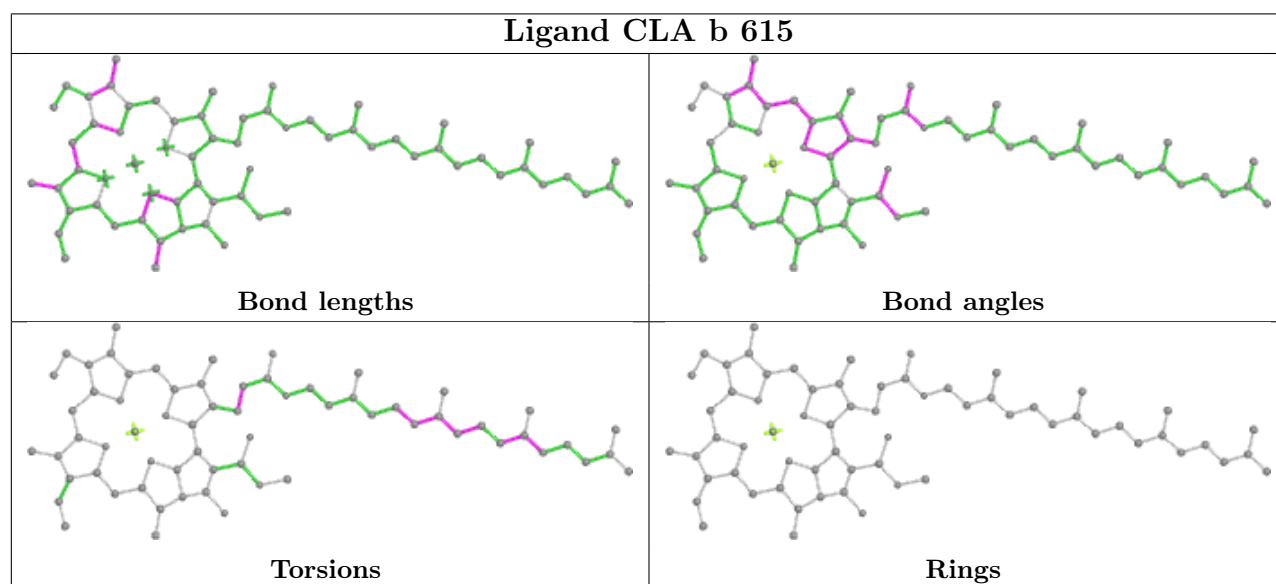
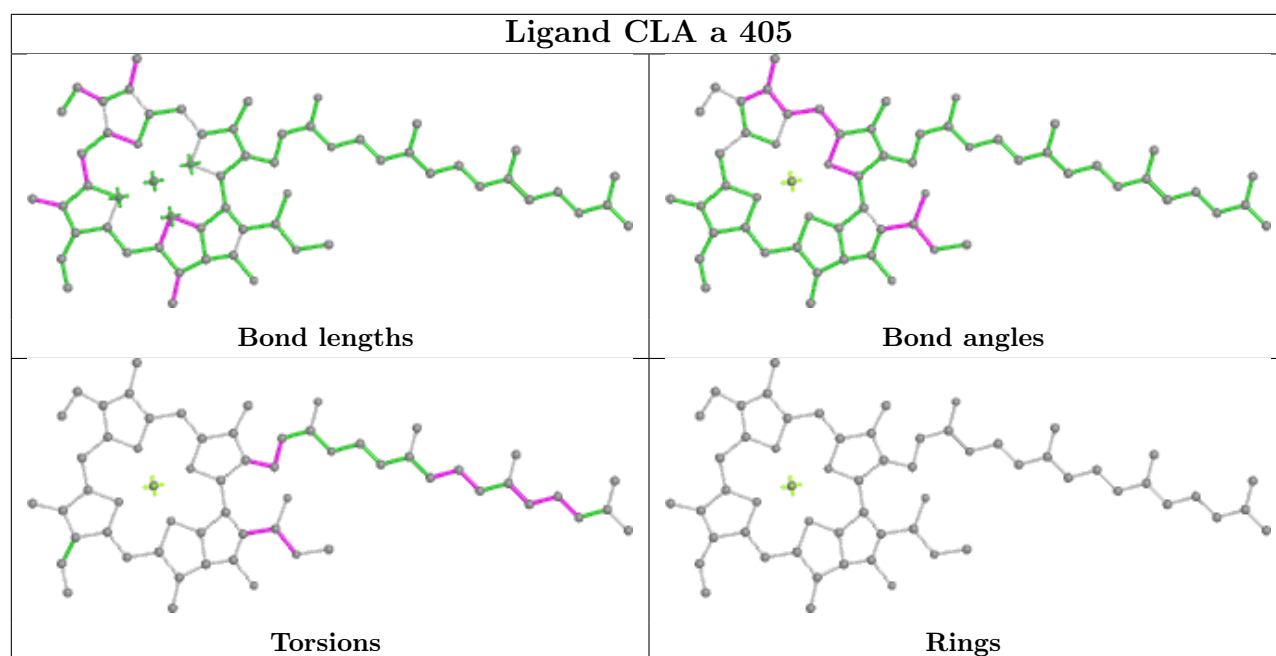


Ligand CHL y 308

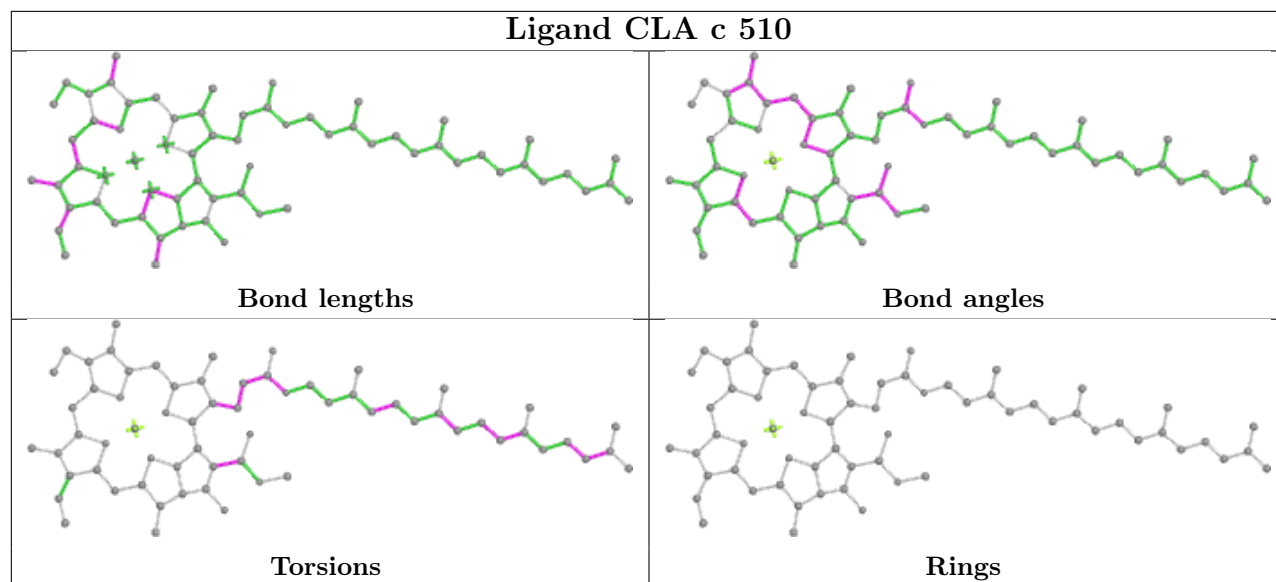




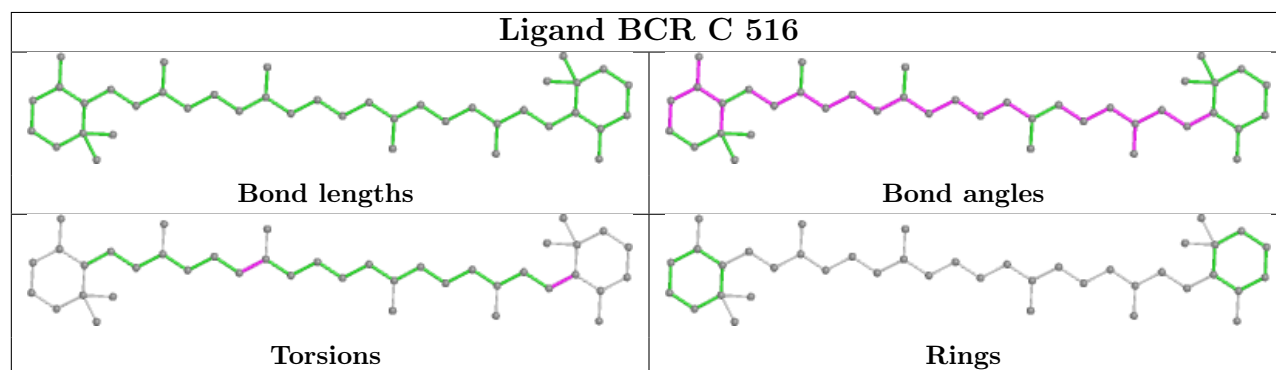
Ligand CLA B 601**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA N 311****Bond lengths****Bond angles****Torsions****Rings**



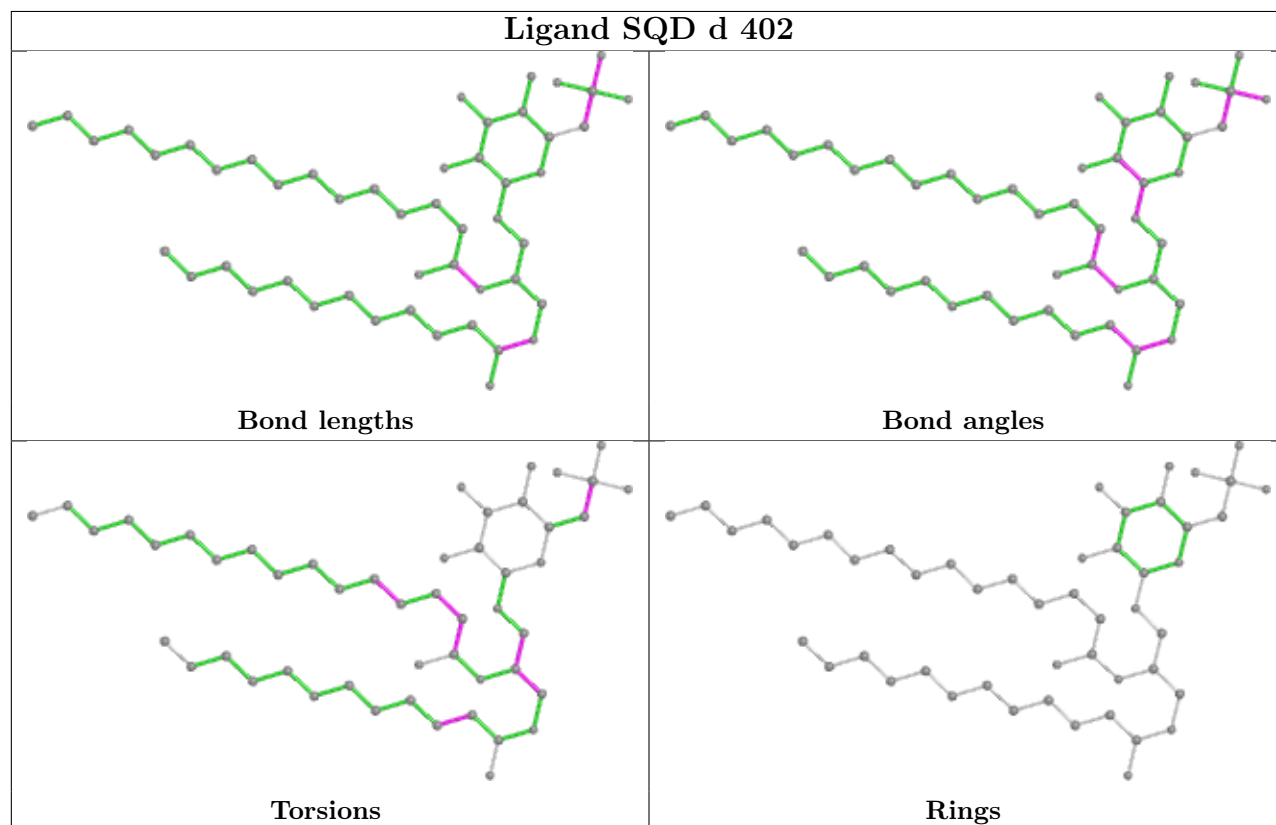
Ligand CLA c 510

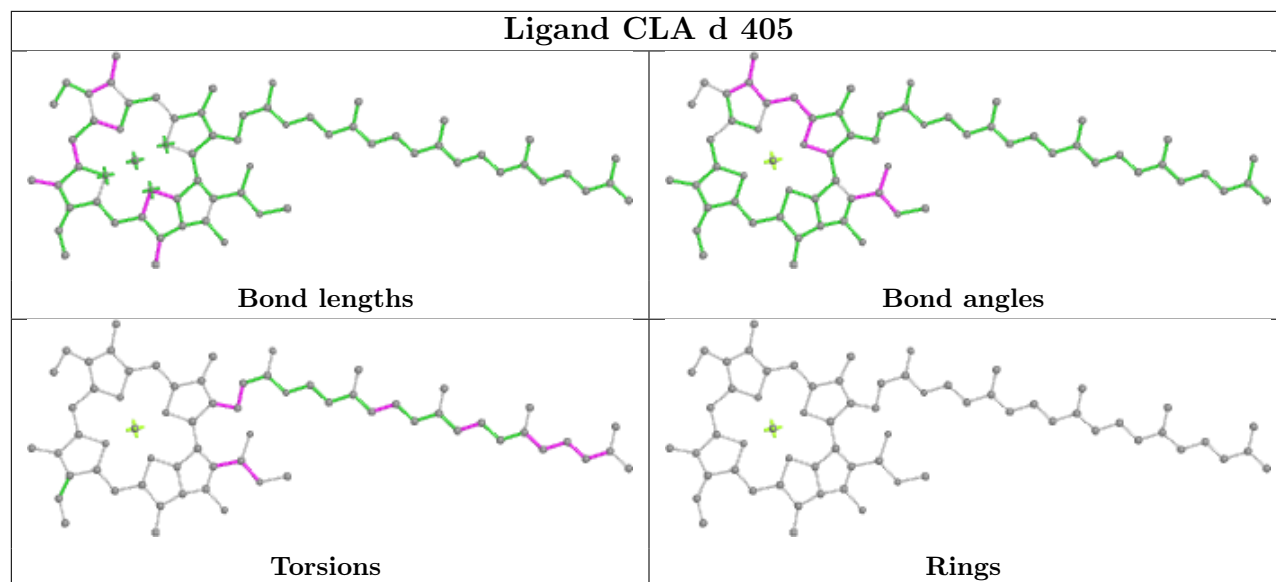
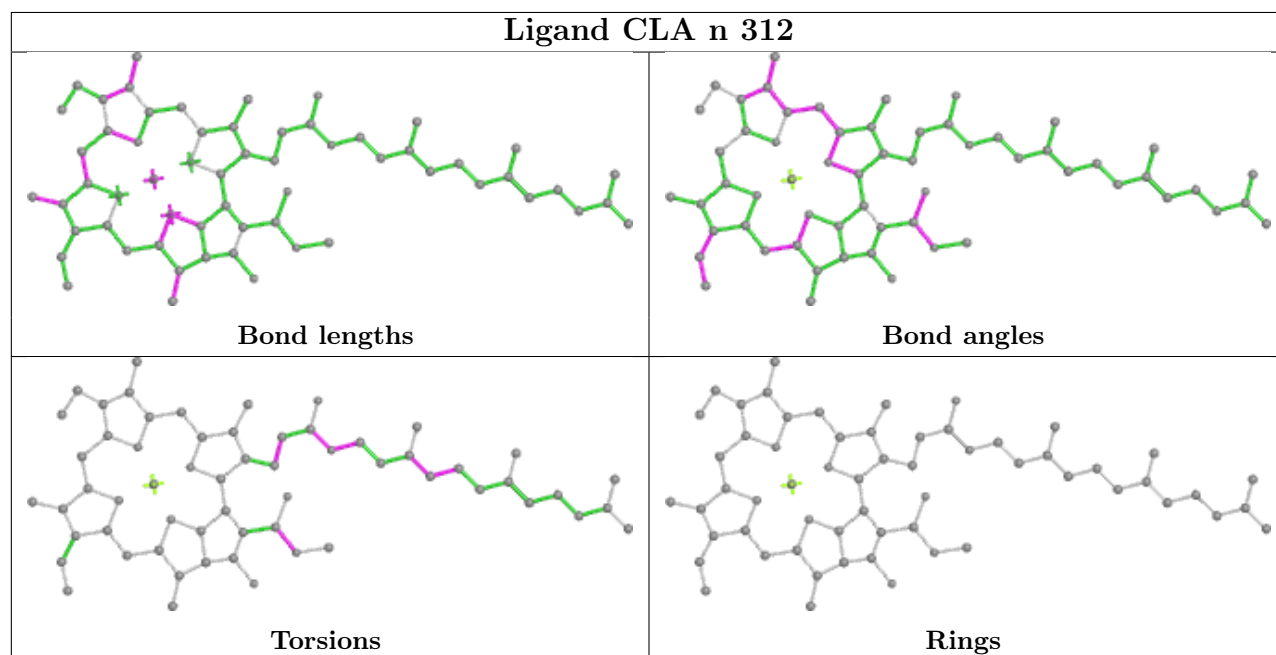


Ligand BCR C 516

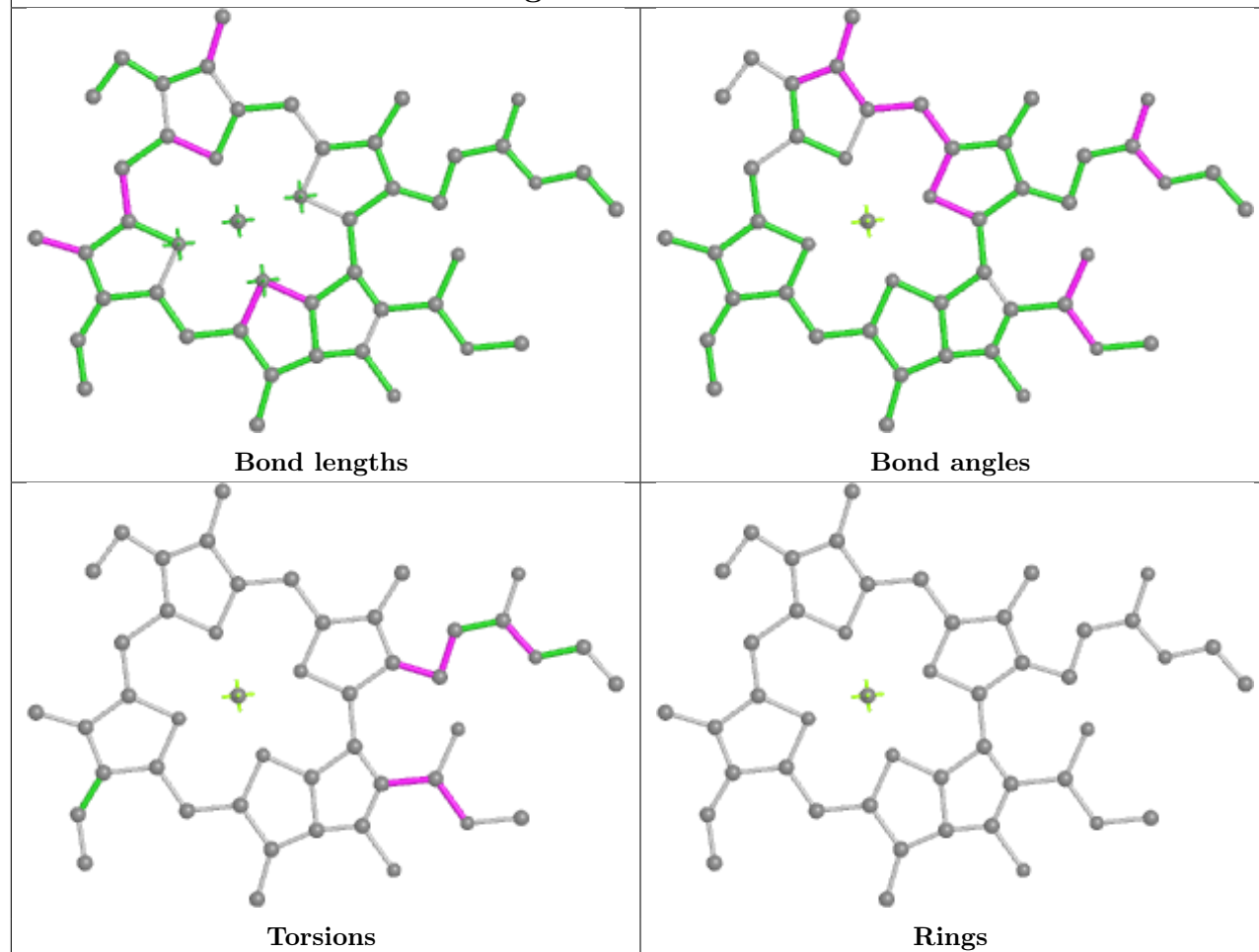


Ligand SQD d 402

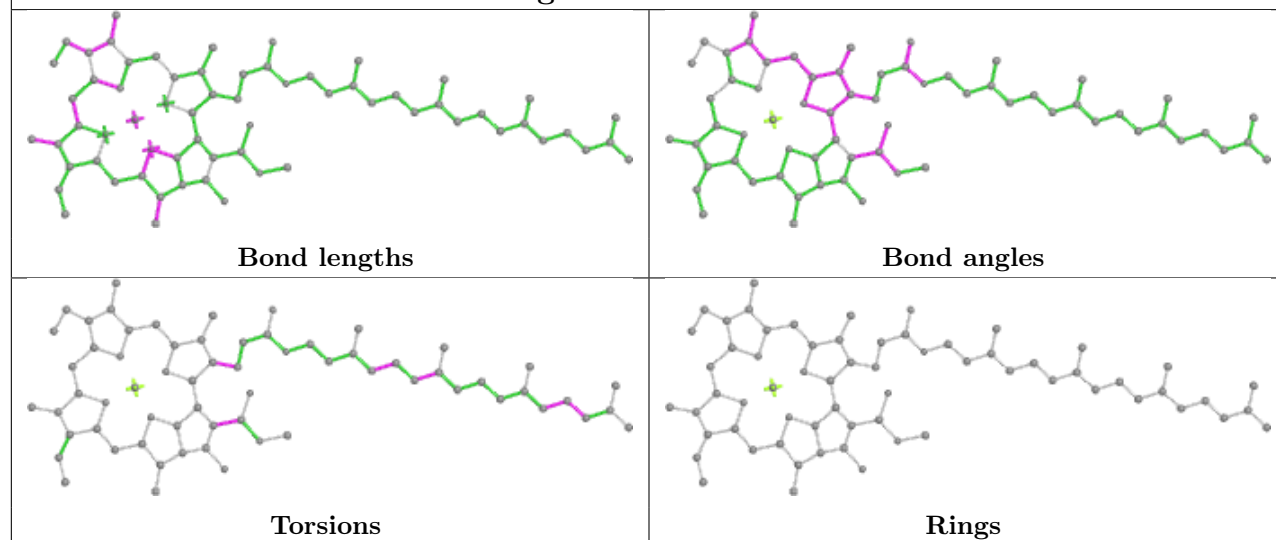


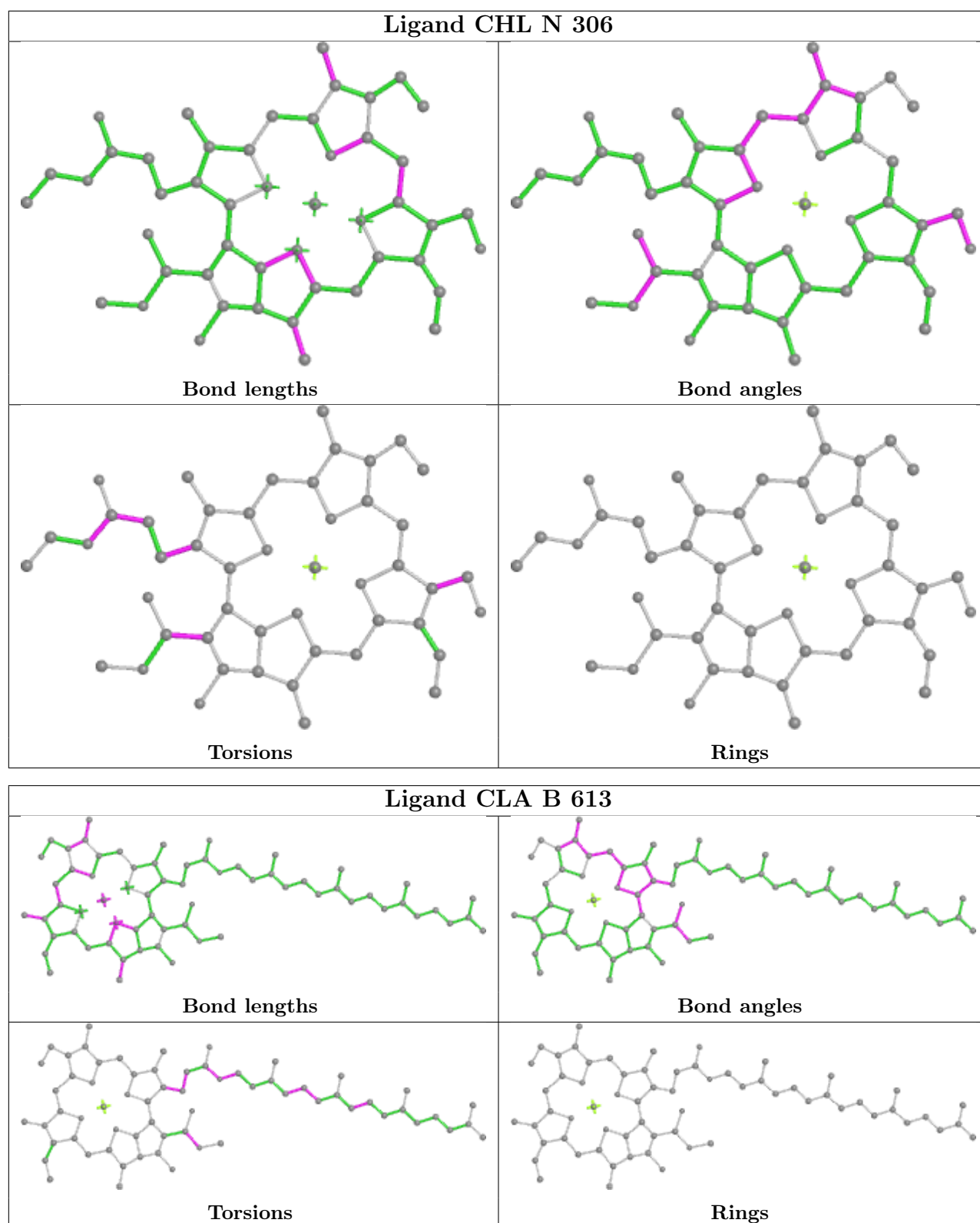
Ligand CLA d 405**Ligand CLA n 312**

Ligand CLA R 612

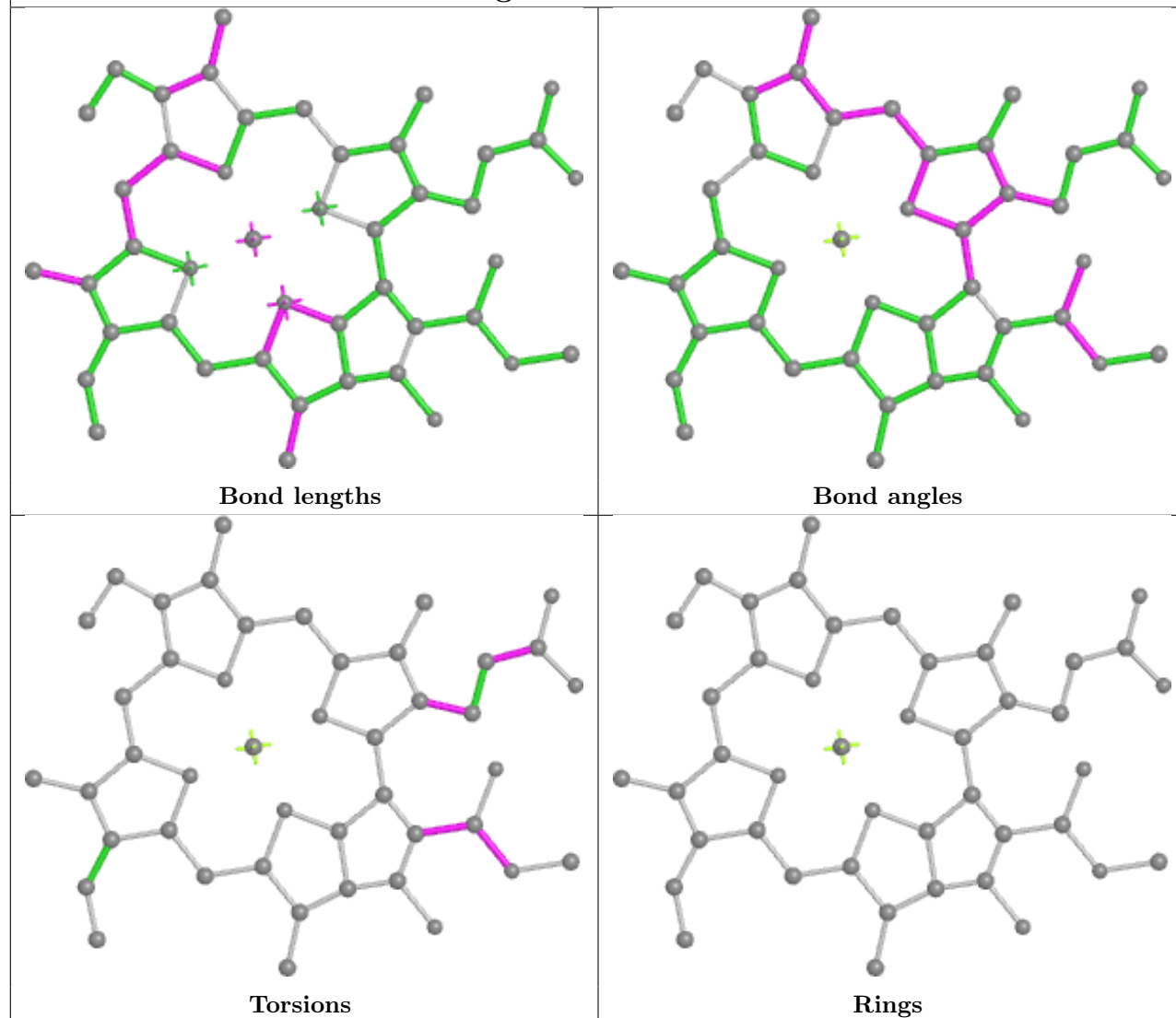


Ligand CLA c 507

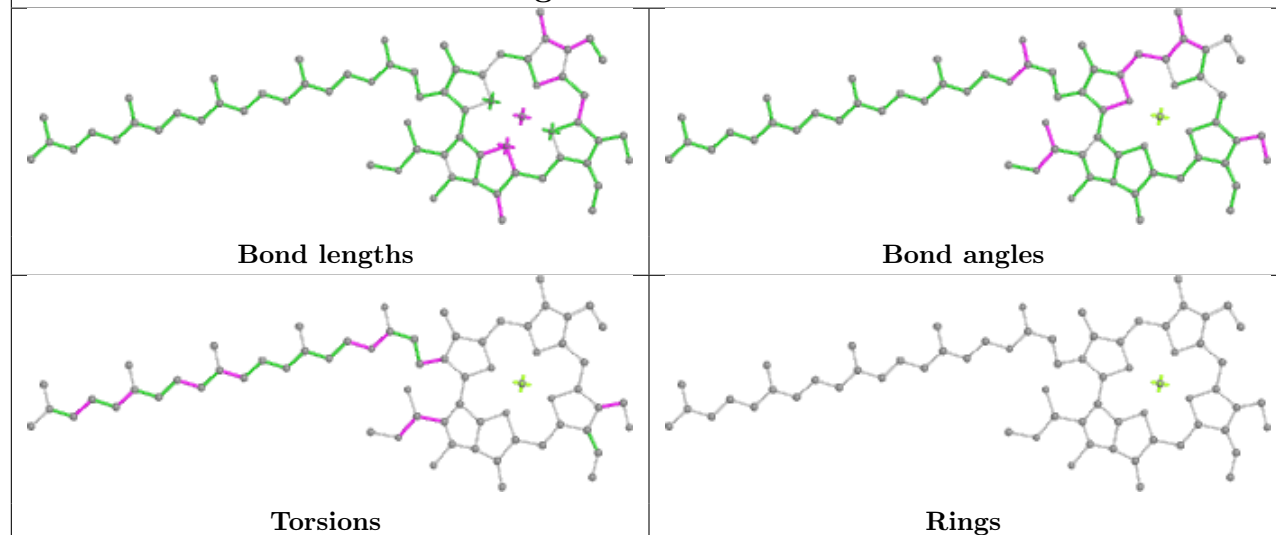


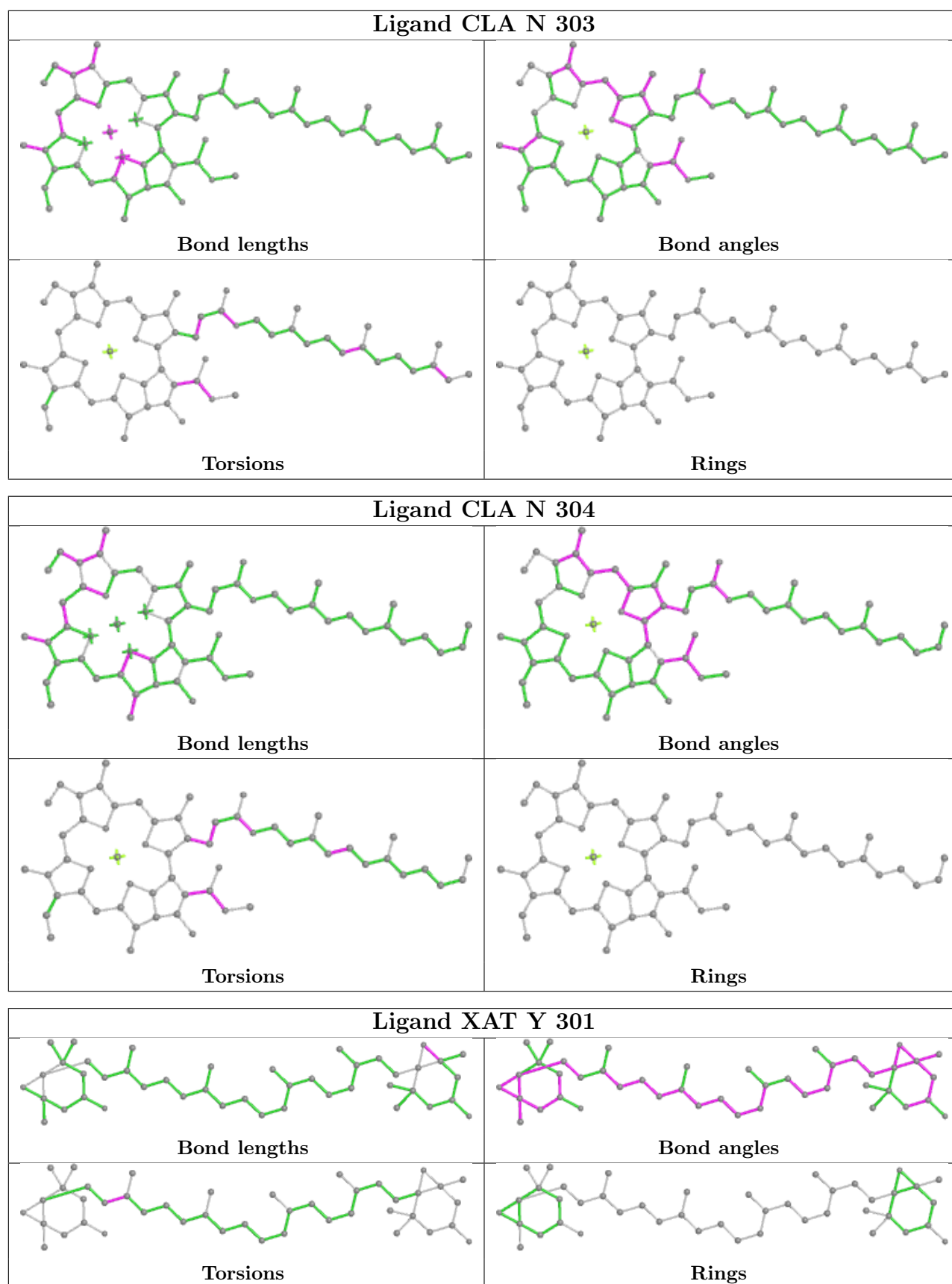


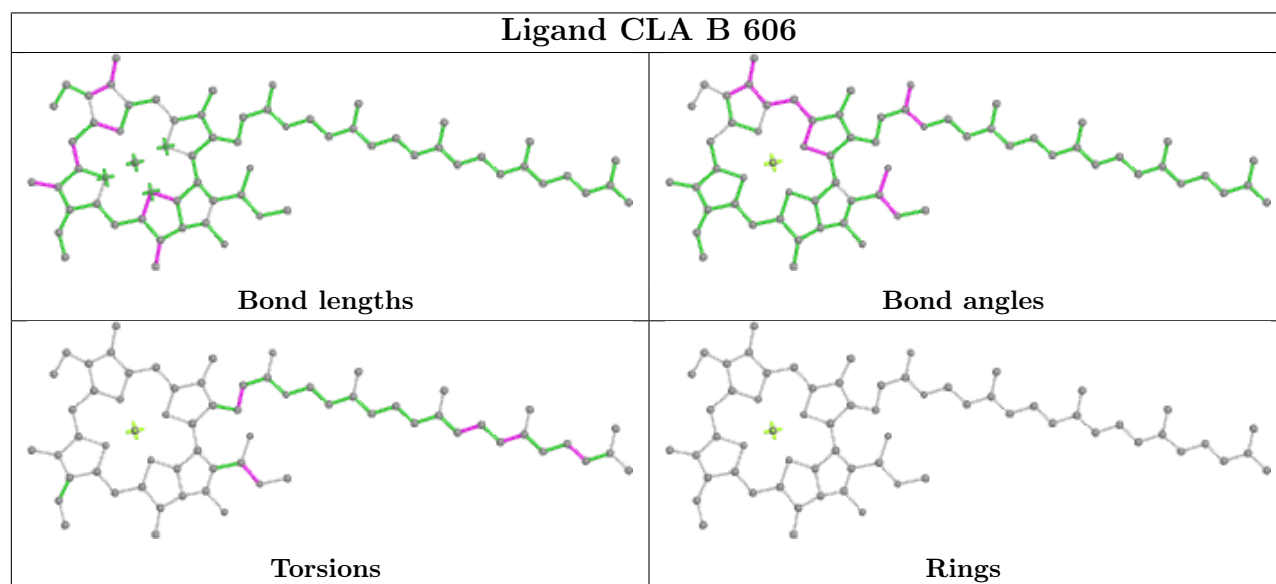
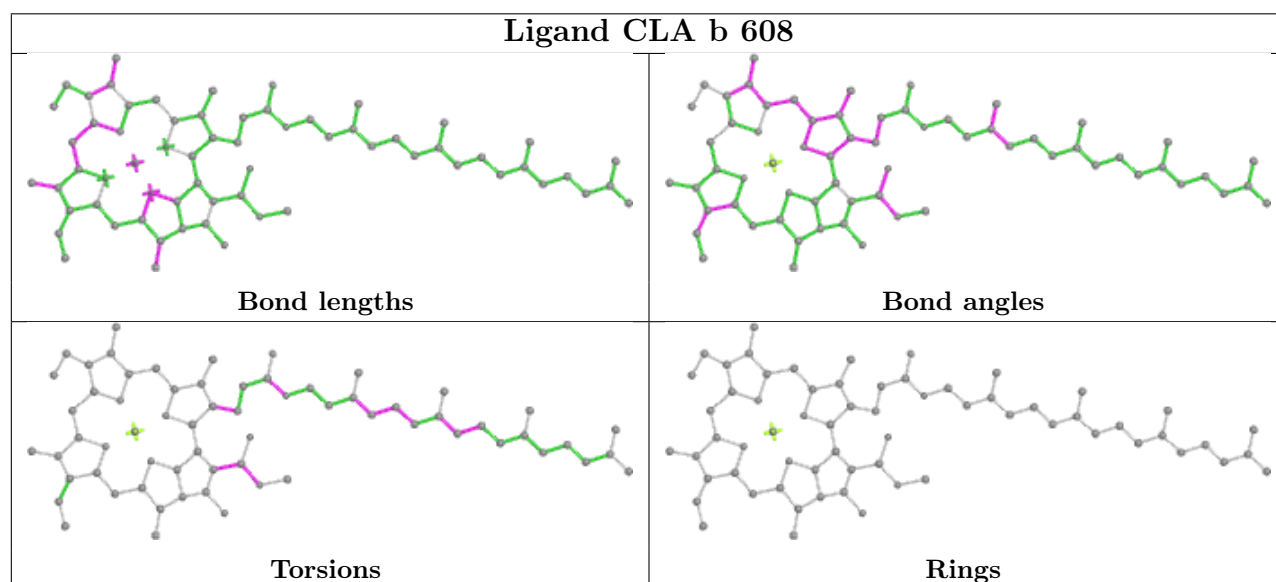
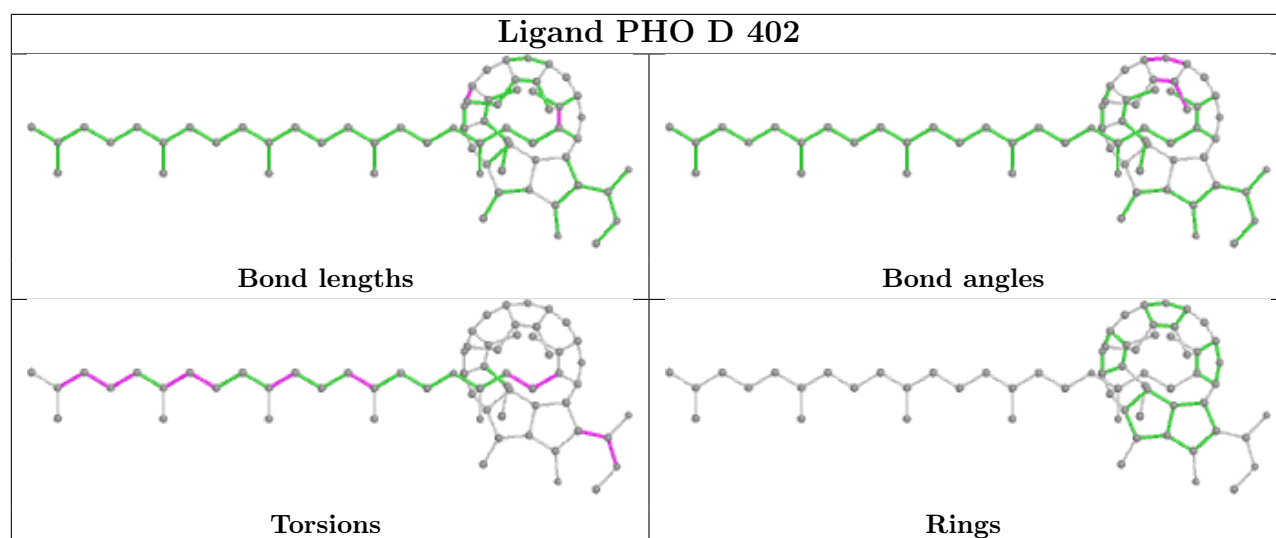
Ligand CLA s 603



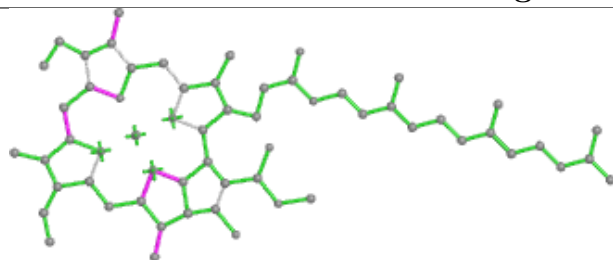
Ligand CHL n 309



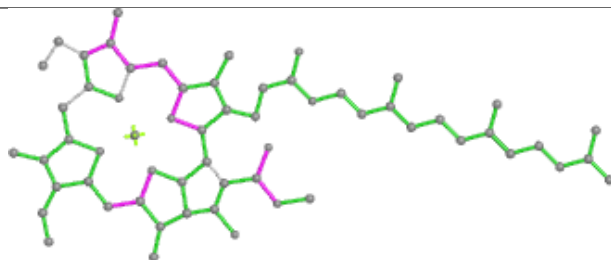




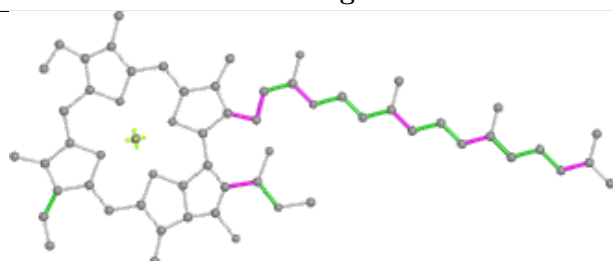
Ligand CLA C 505



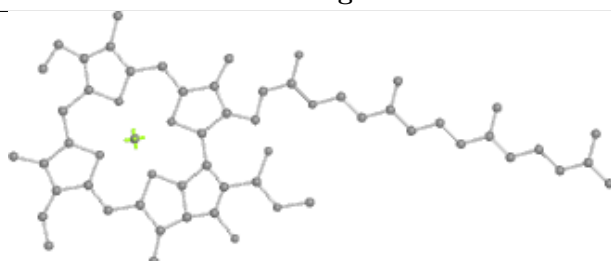
Bond lengths



Bond angles

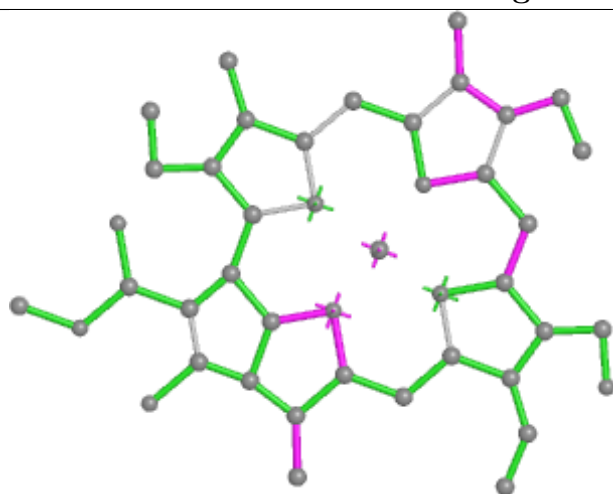


Torsions

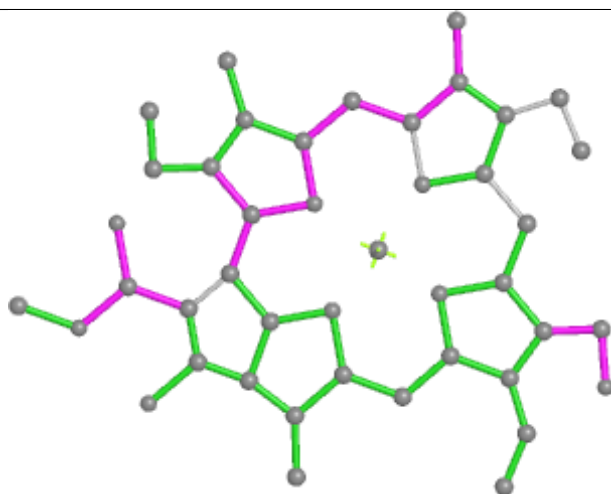


Rings

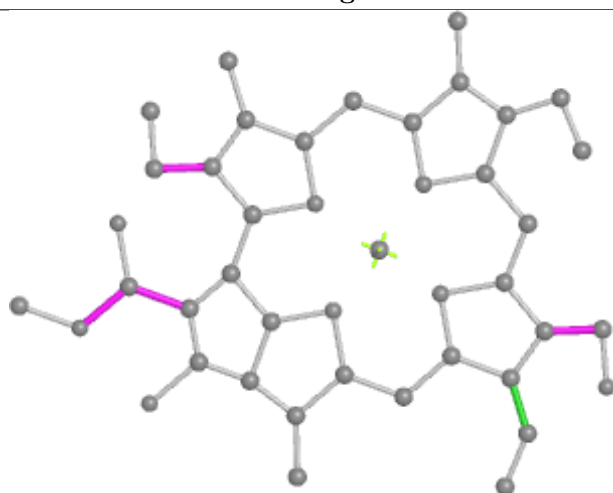
Ligand CHL G 606



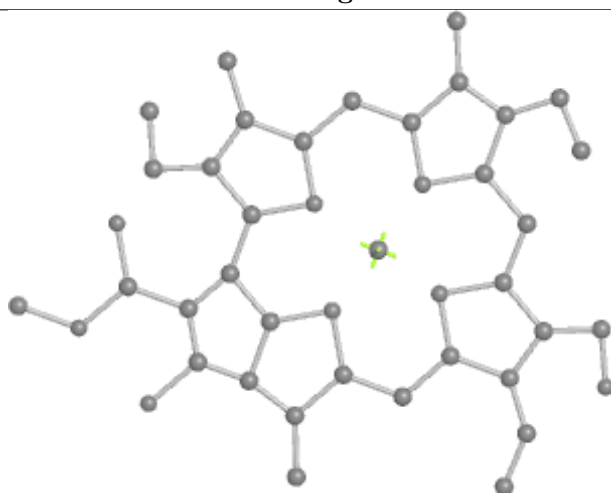
Bond lengths



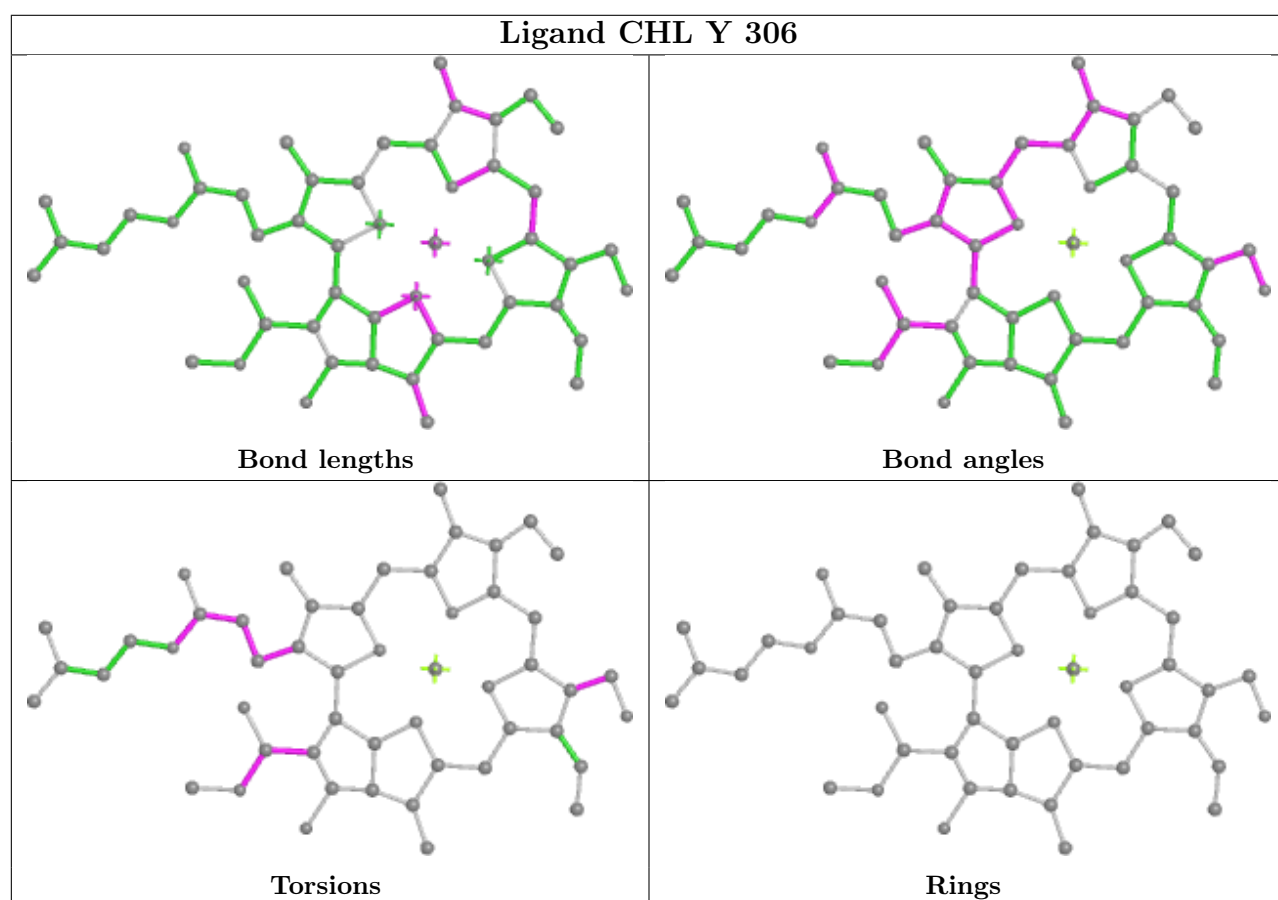
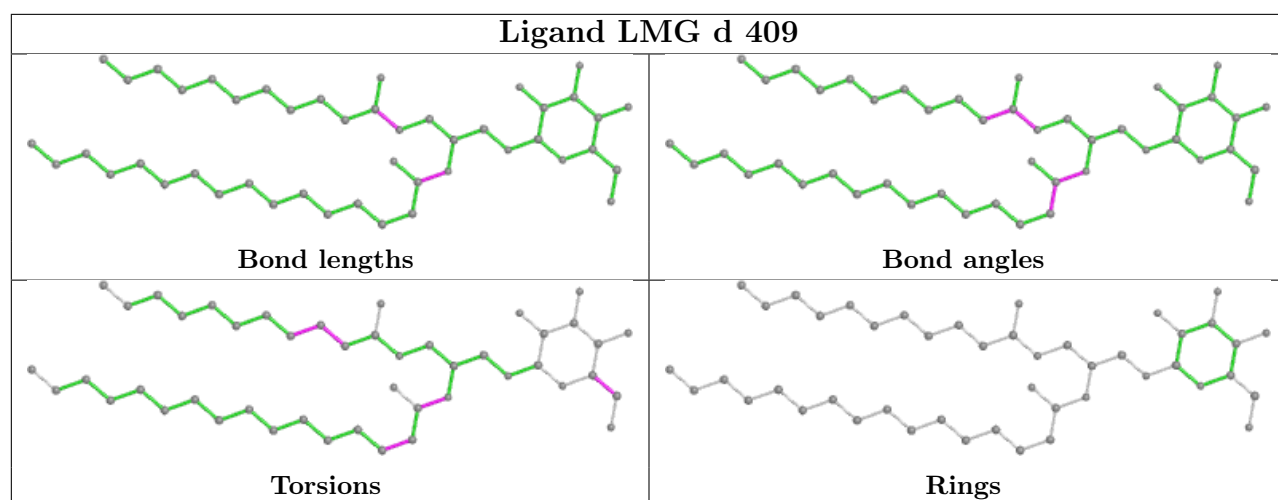
Bond angles



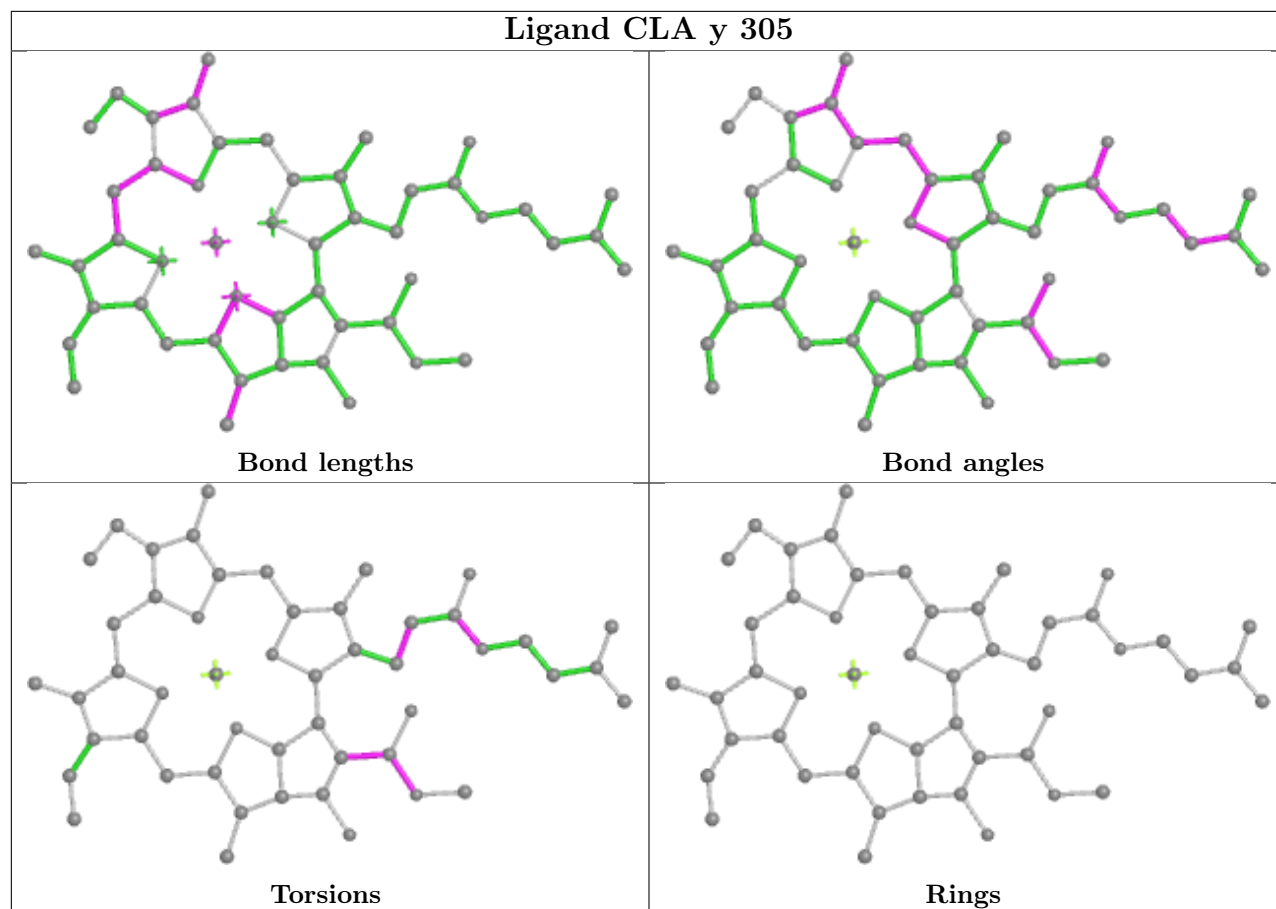
Torsions



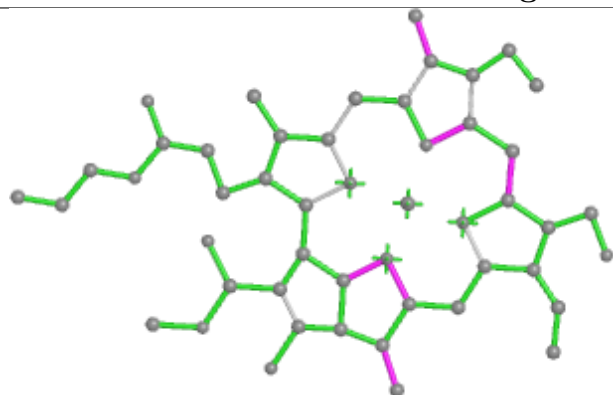
Rings



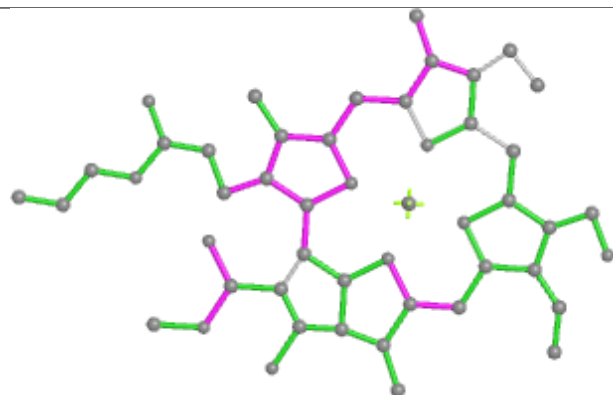
Ligand CLA y 305



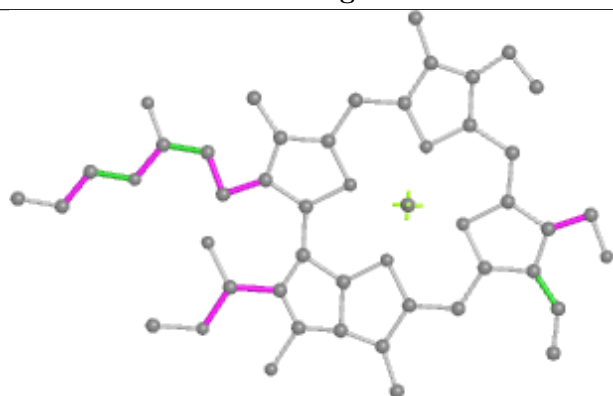
Ligand CHL s 607



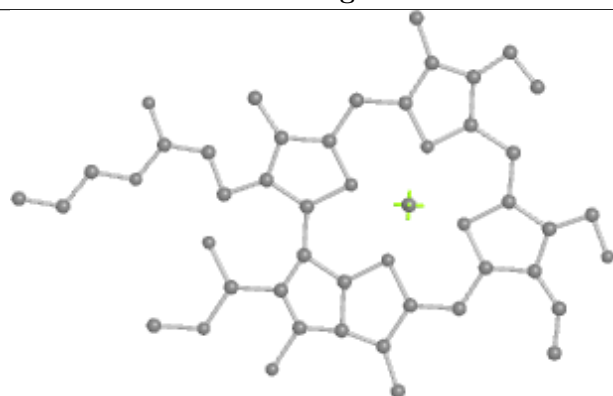
Bond lengths



Bond angles

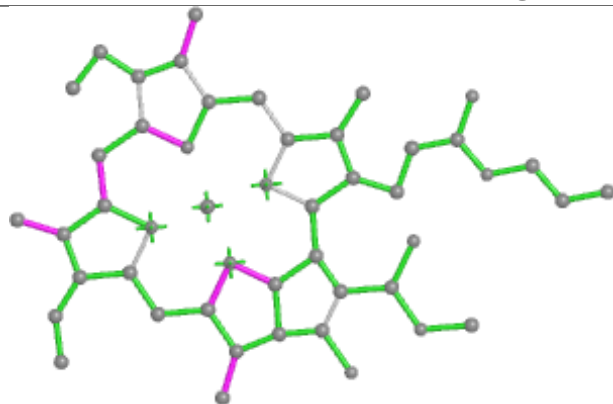


Torsions

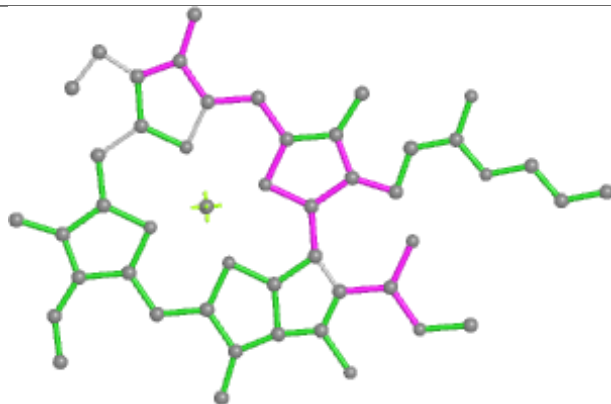


Rings

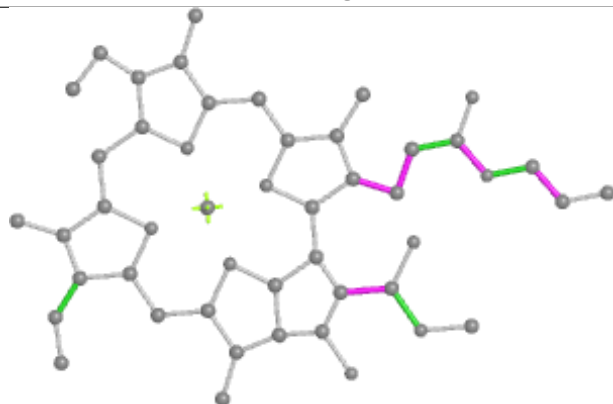
Ligand CLA R 604



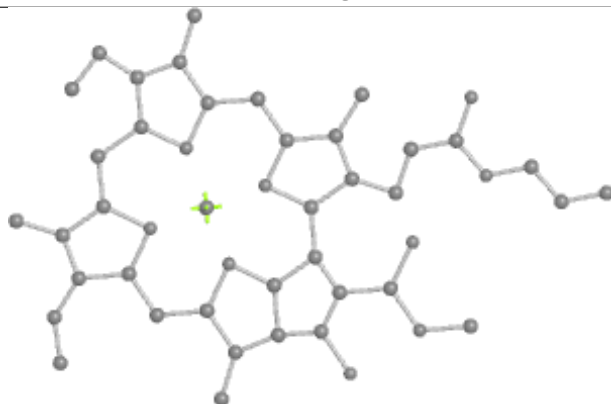
Bond lengths



Bond angles

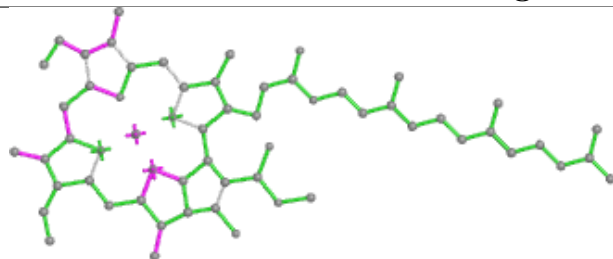


Torsions

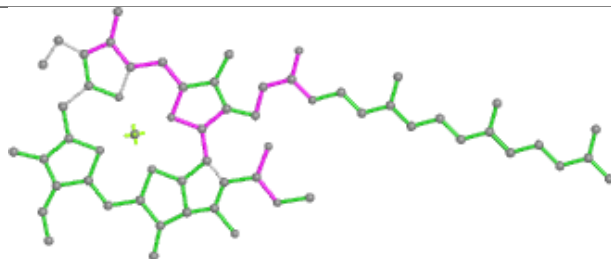


Rings

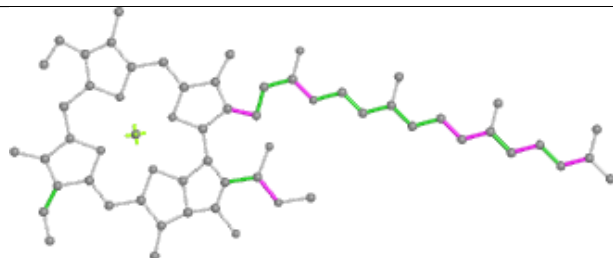
Ligand CLA Y 311



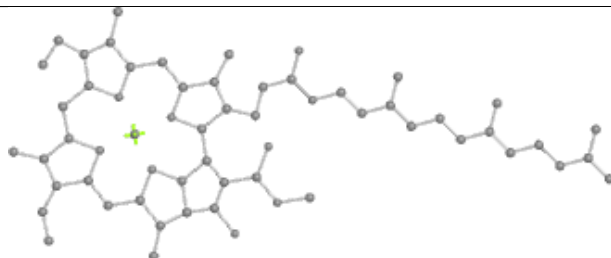
Bond lengths



Bond angles

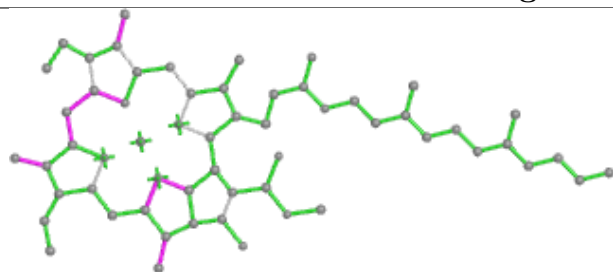


Torsions

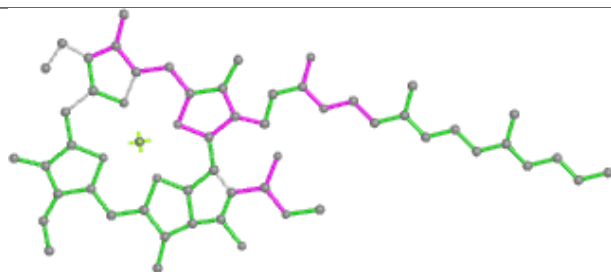


Rings

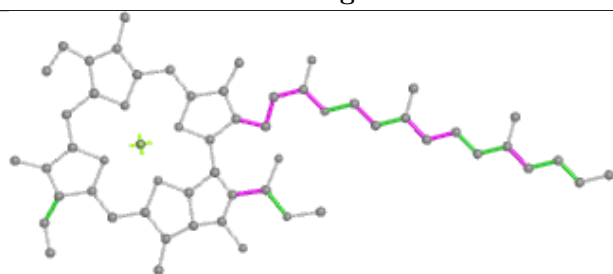
Ligand CLA c 505



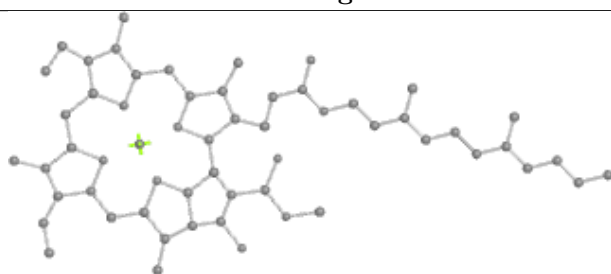
Bond lengths



Bond angles

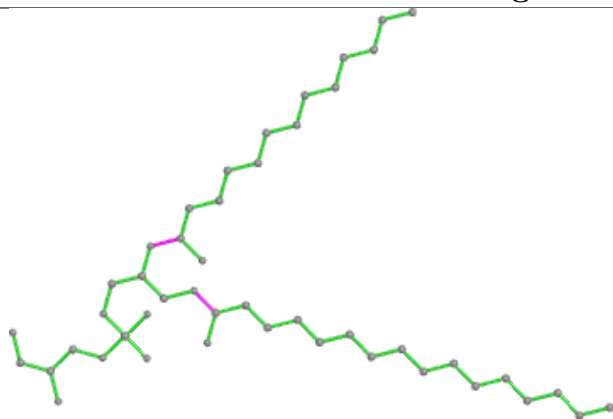


Torsions

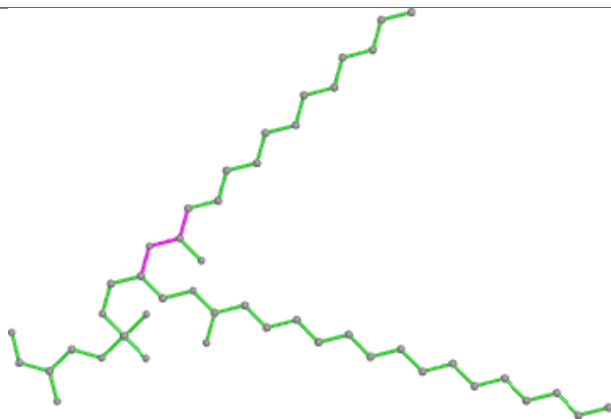


Rings

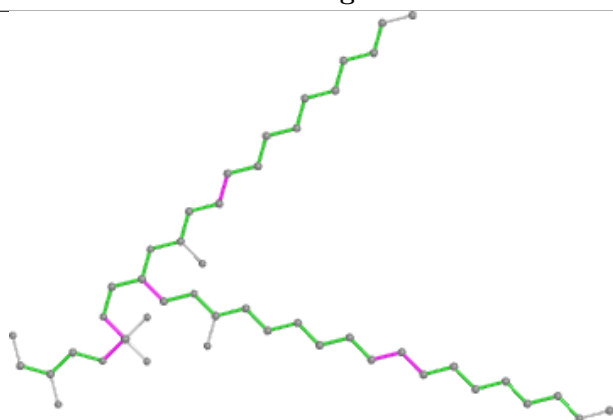
Ligand LHG A 411



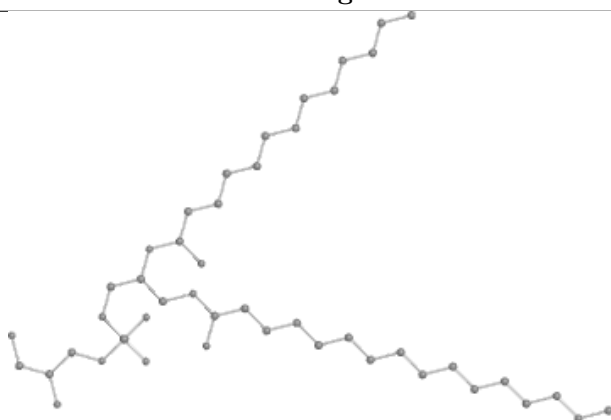
Bond lengths



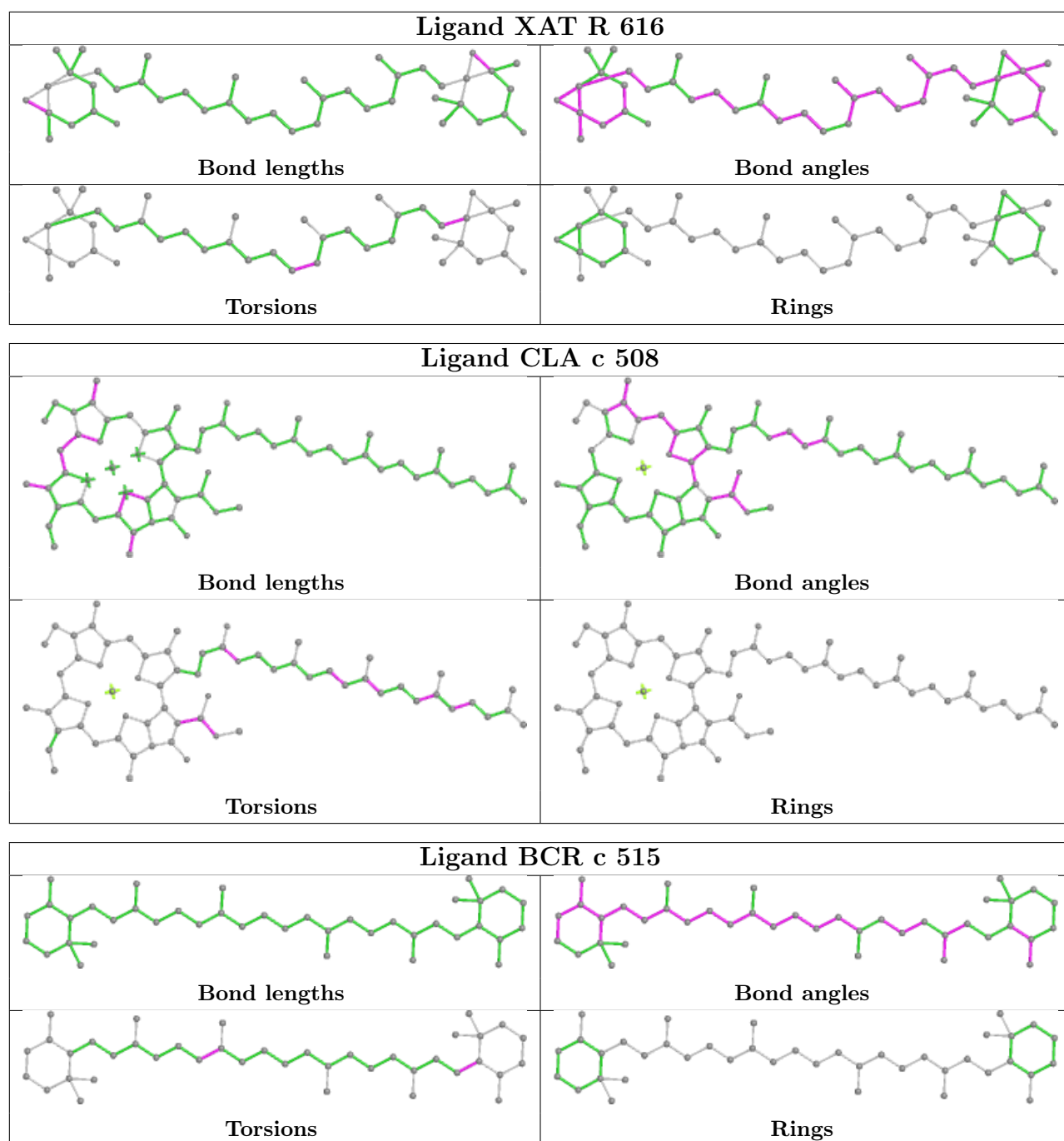
Bond angles

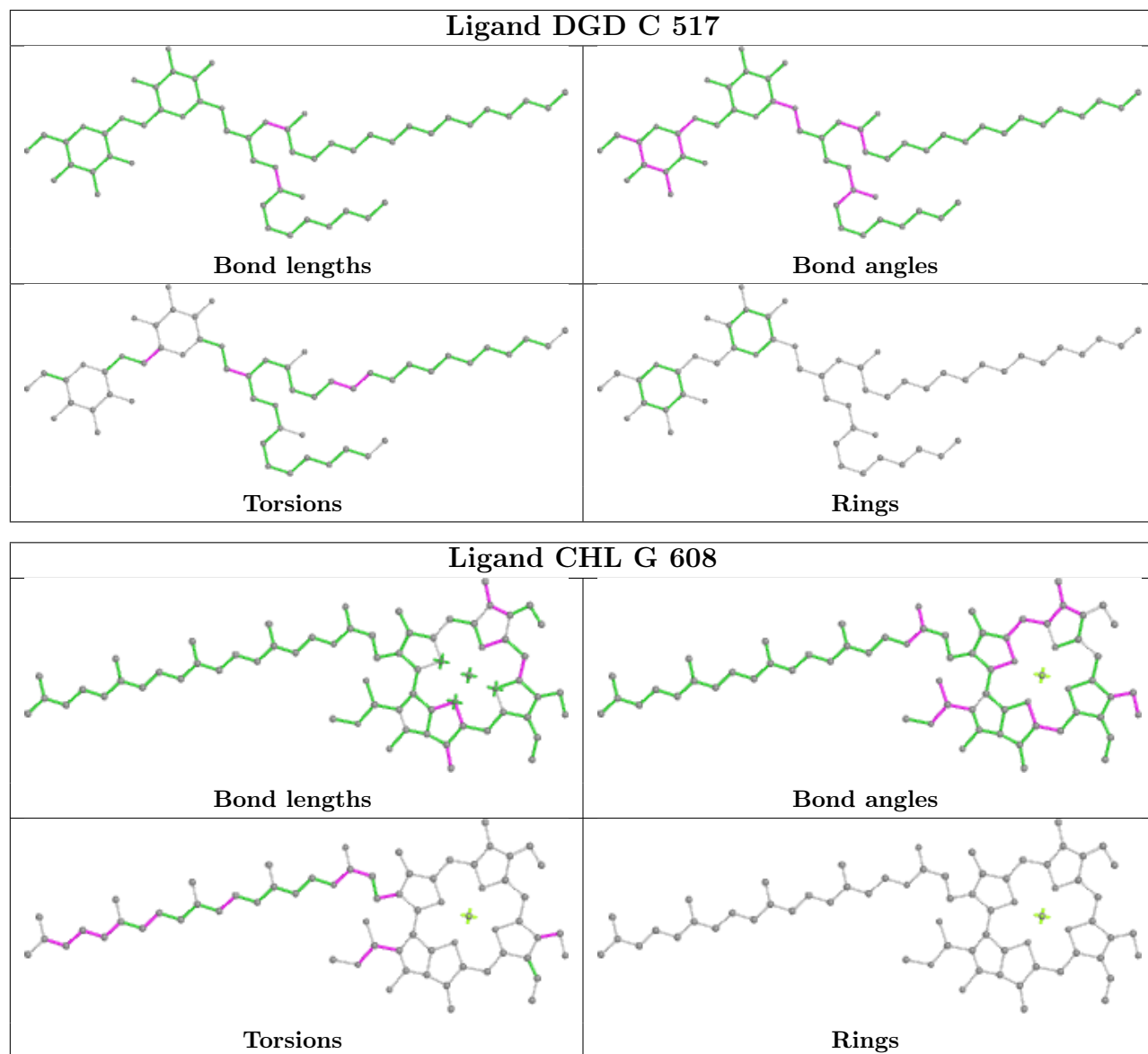


Torsions

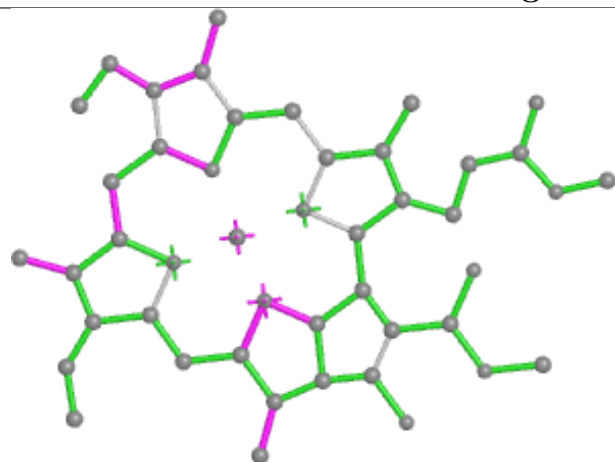


Rings

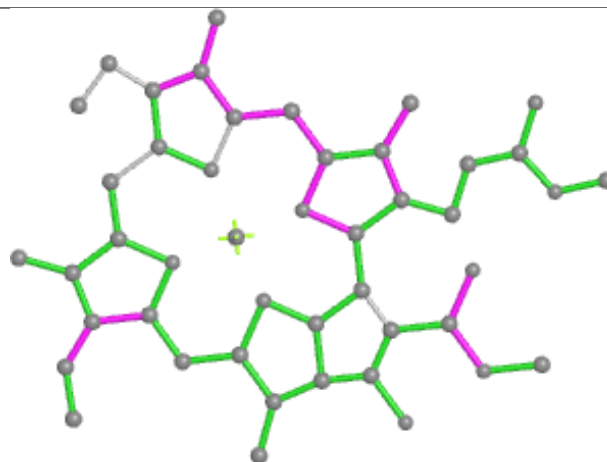




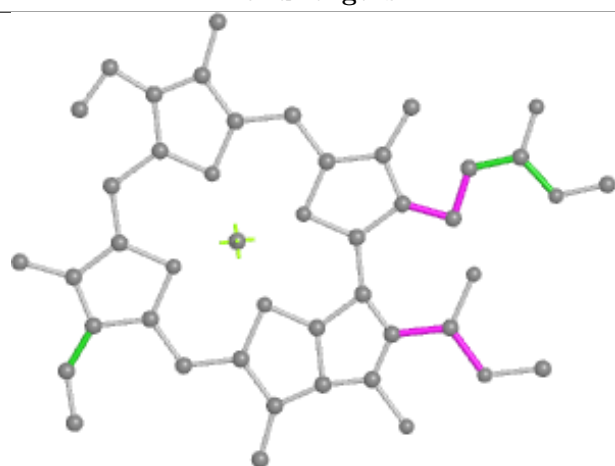
Ligand CLA s 602



Bond lengths



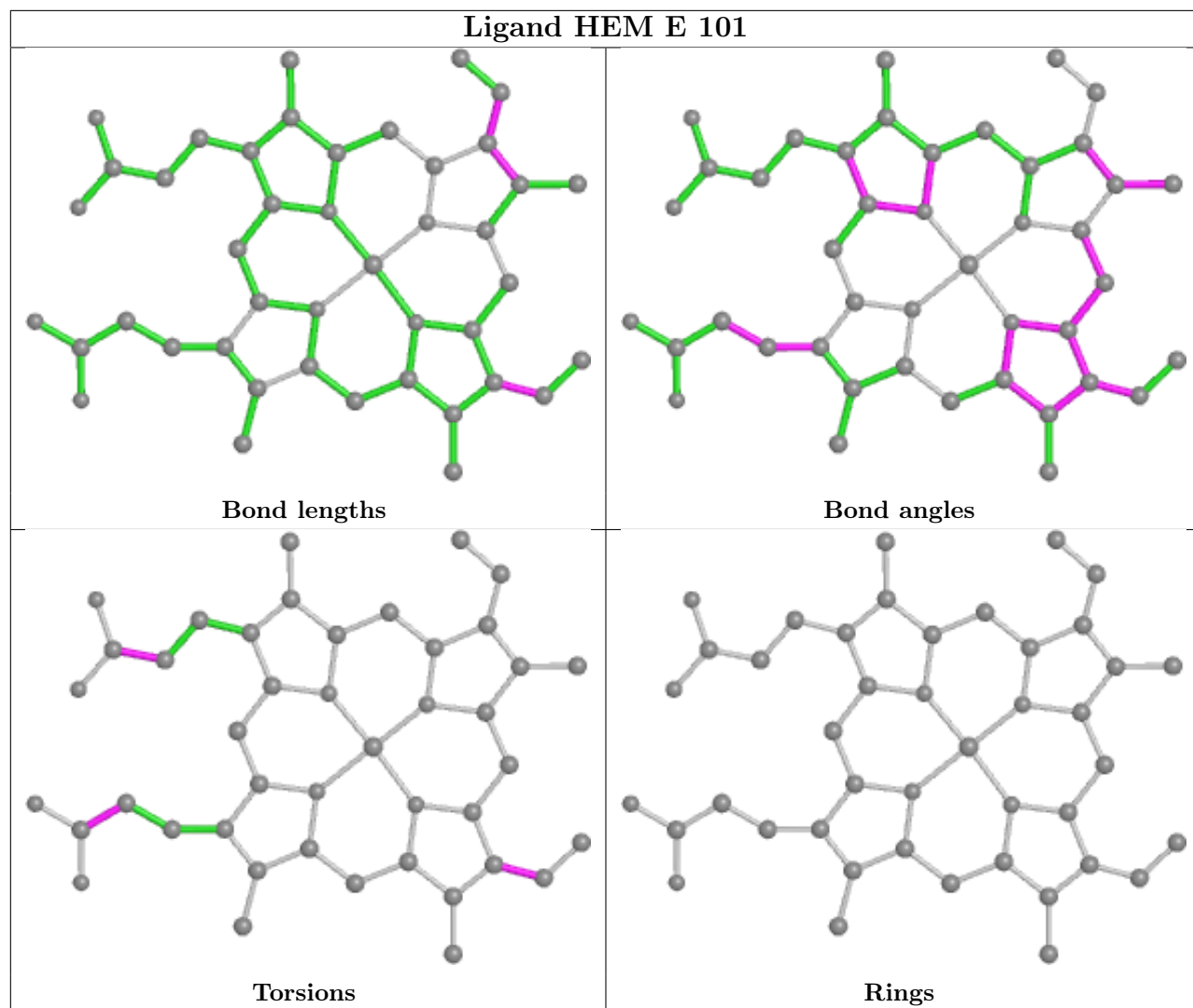
Bond angles



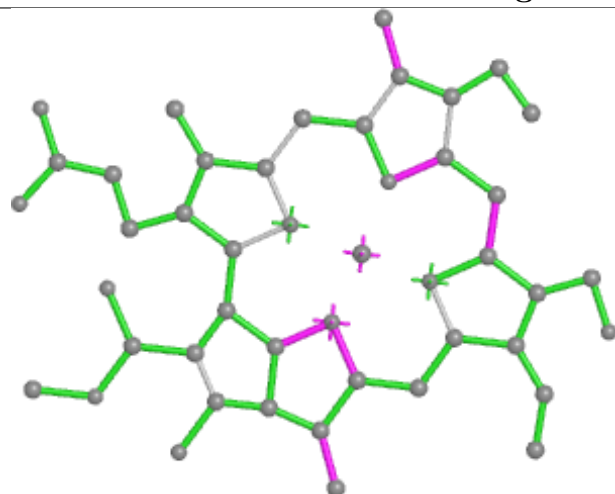
Torsions



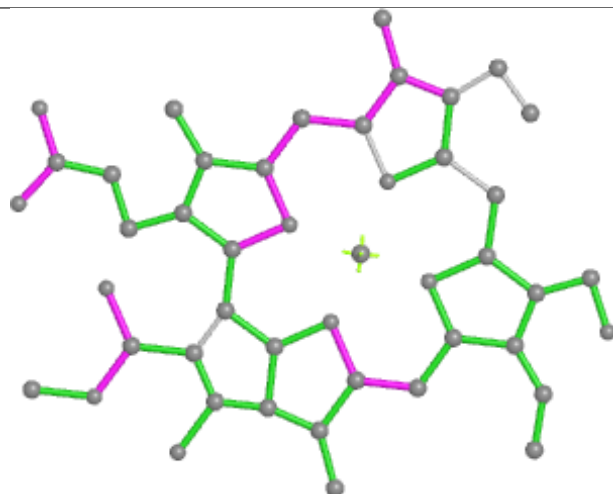
Rings



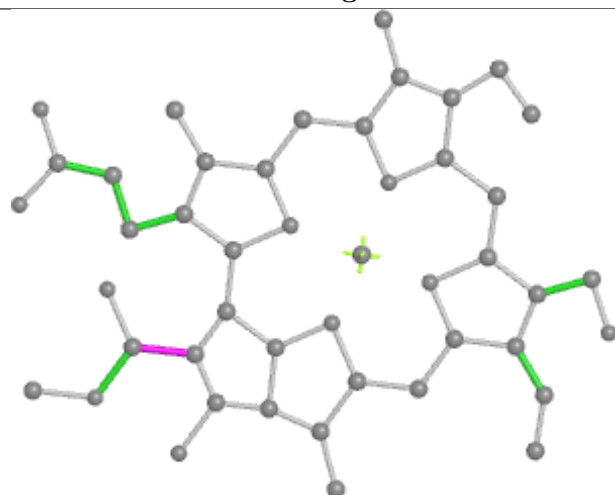
Ligand CHL R 605



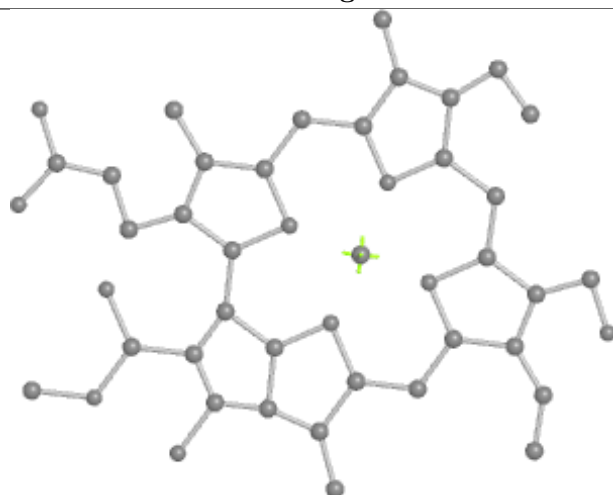
Bond lengths



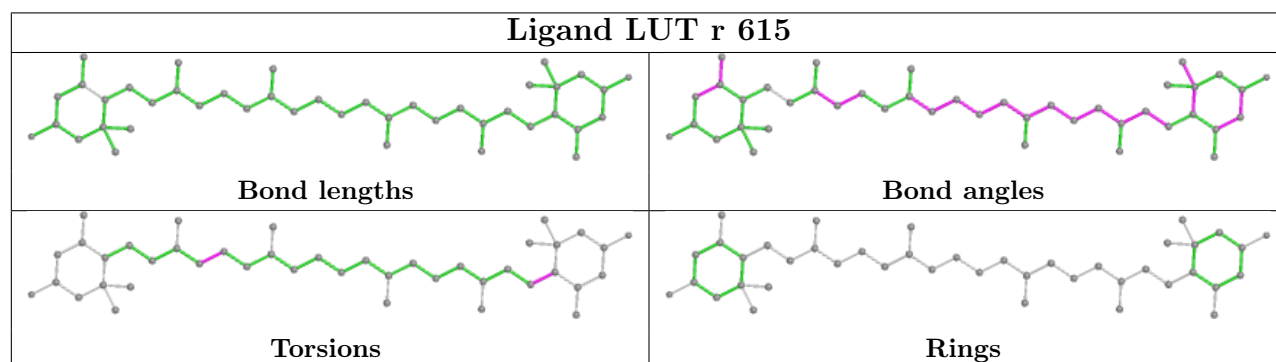
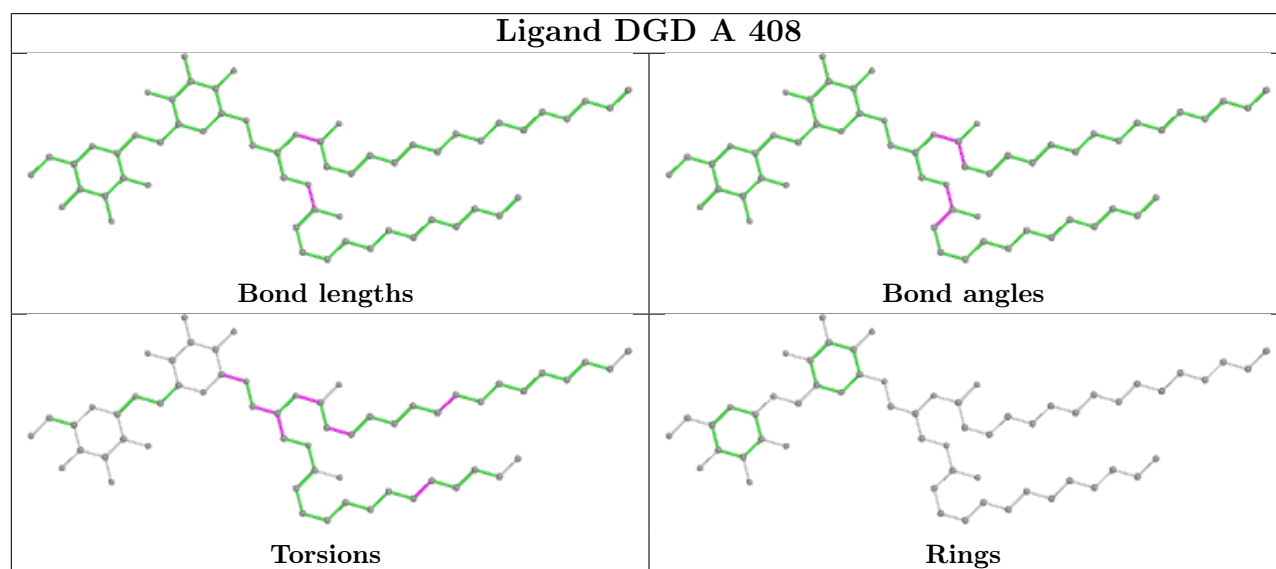
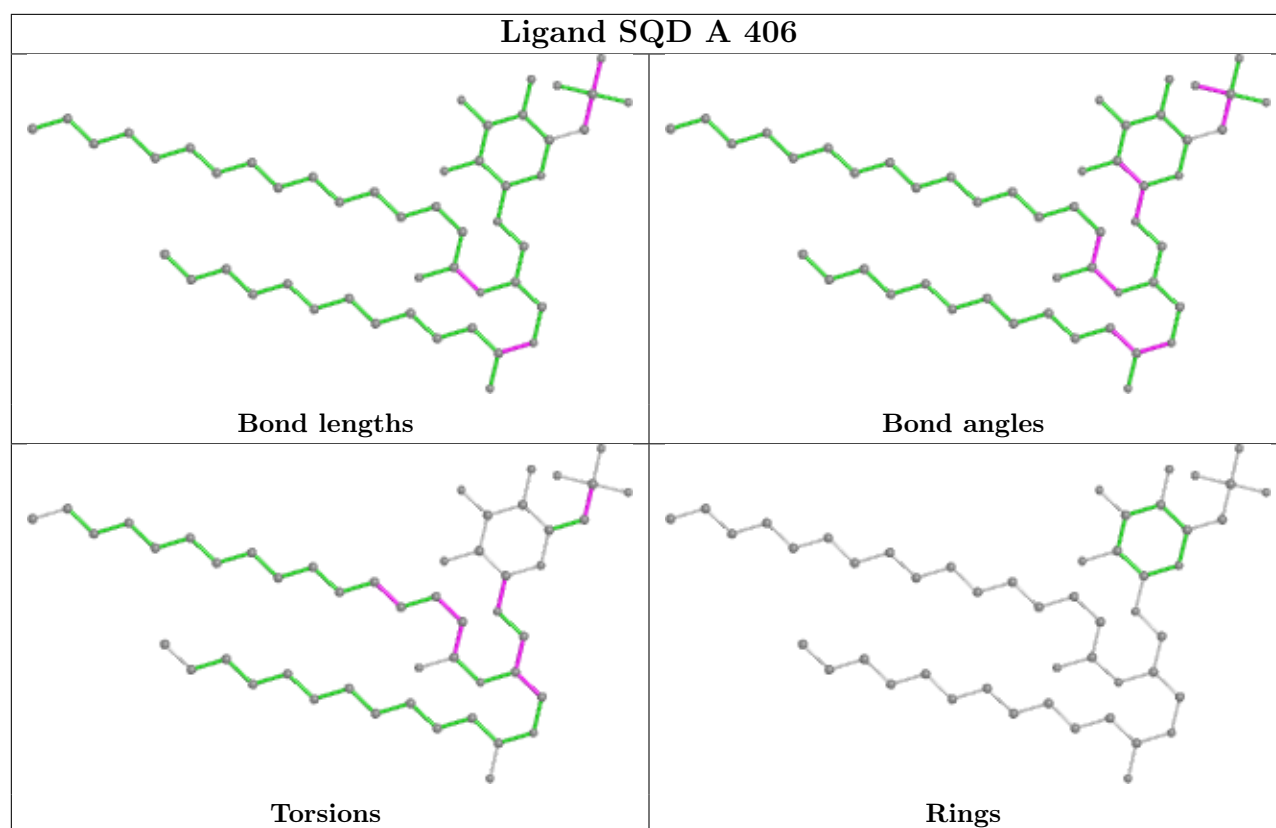
Bond angles

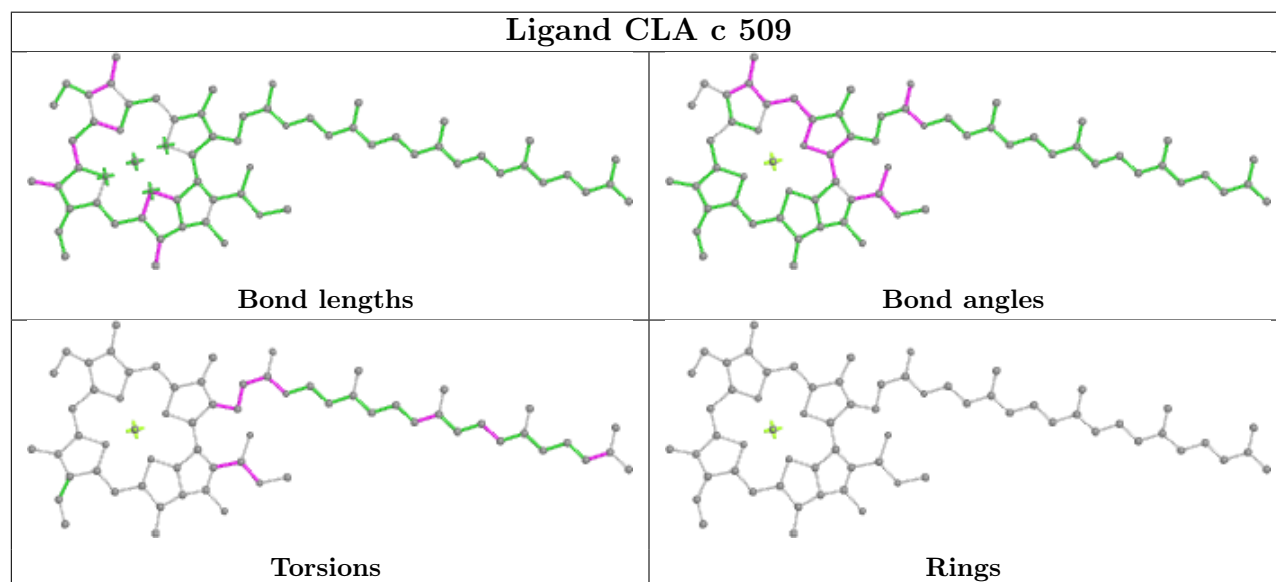
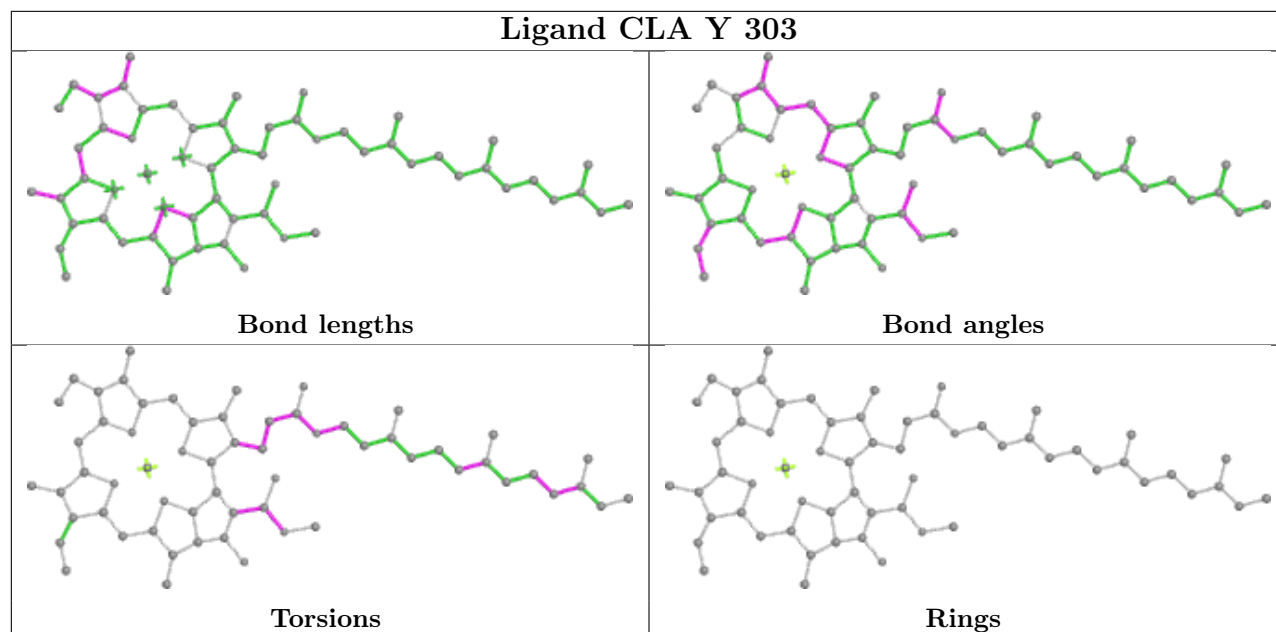
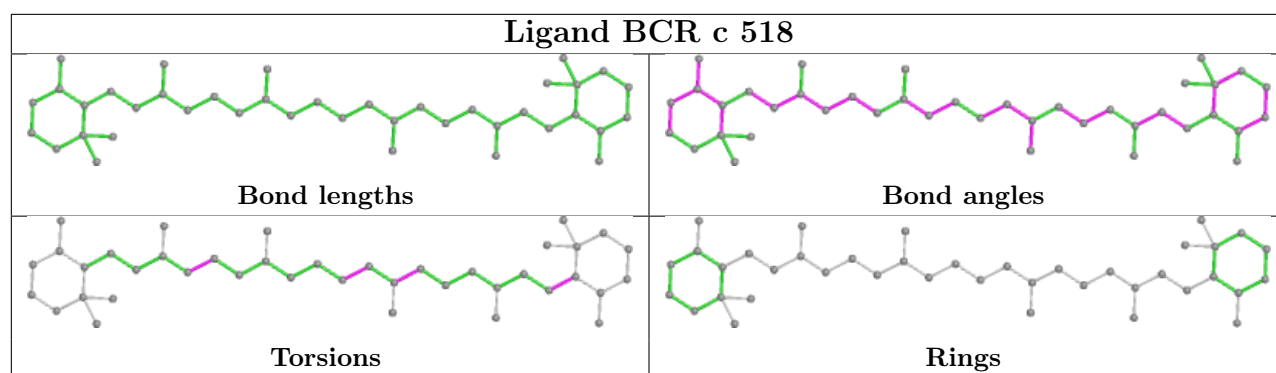


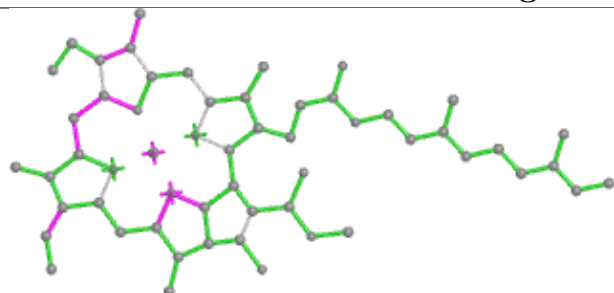
Torsions



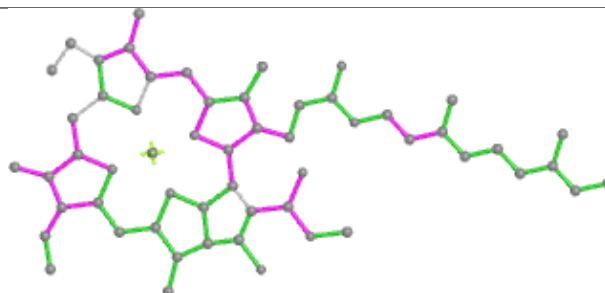
Rings



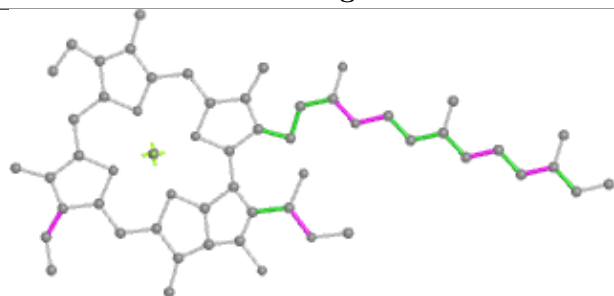


Ligand CLA c 512

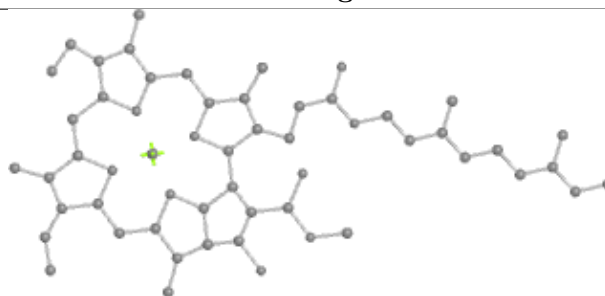
Bond lengths



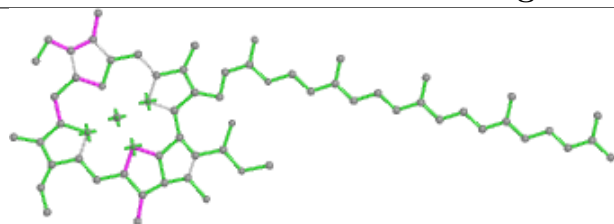
Bond angles



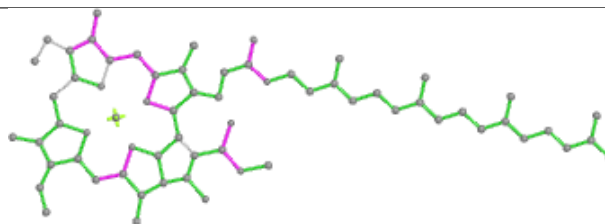
Torsions



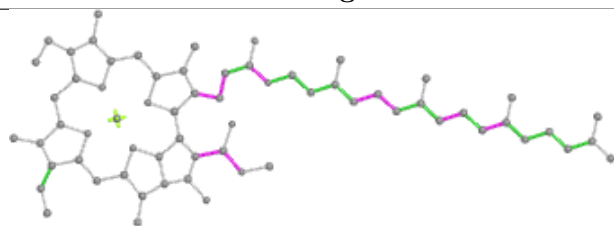
Rings

Ligand CLA b 601

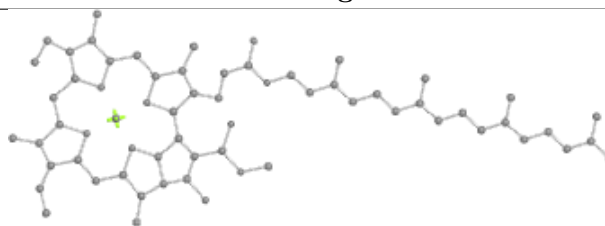
Bond lengths



Bond angles

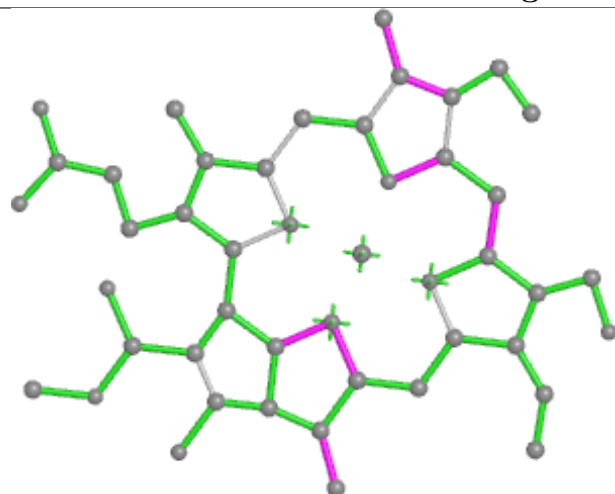


Torsions

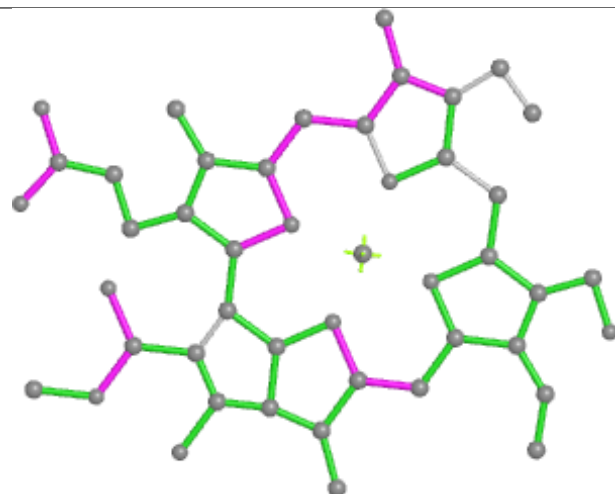


Rings

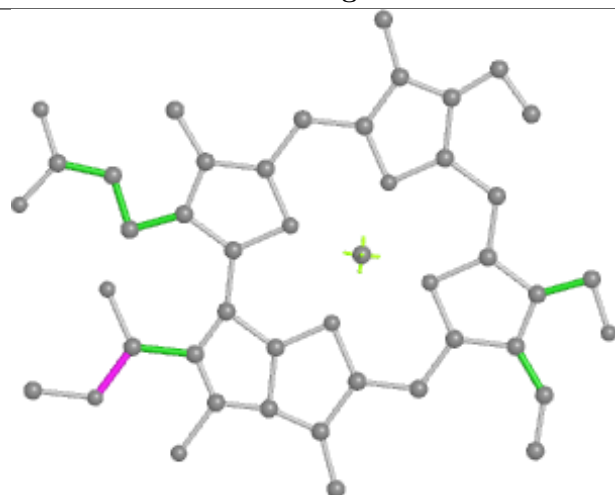
Ligand CHL r 605



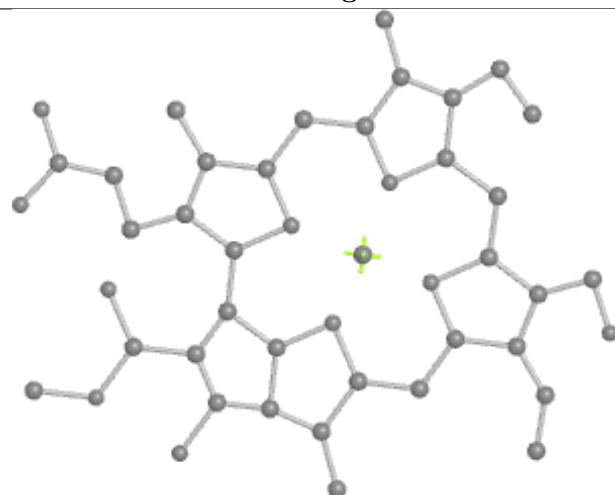
Bond lengths



Bond angles

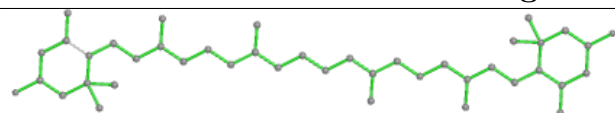


Torsions

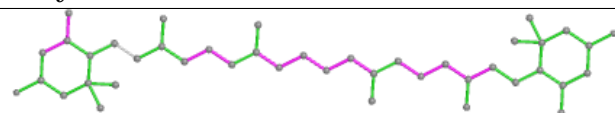


Rings

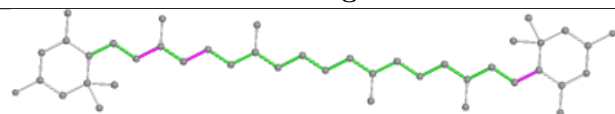
Ligand LUT y 315



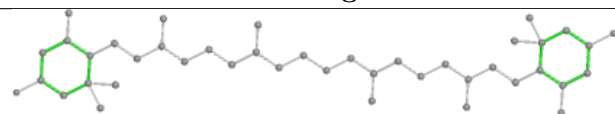
Bond lengths



Bond angles

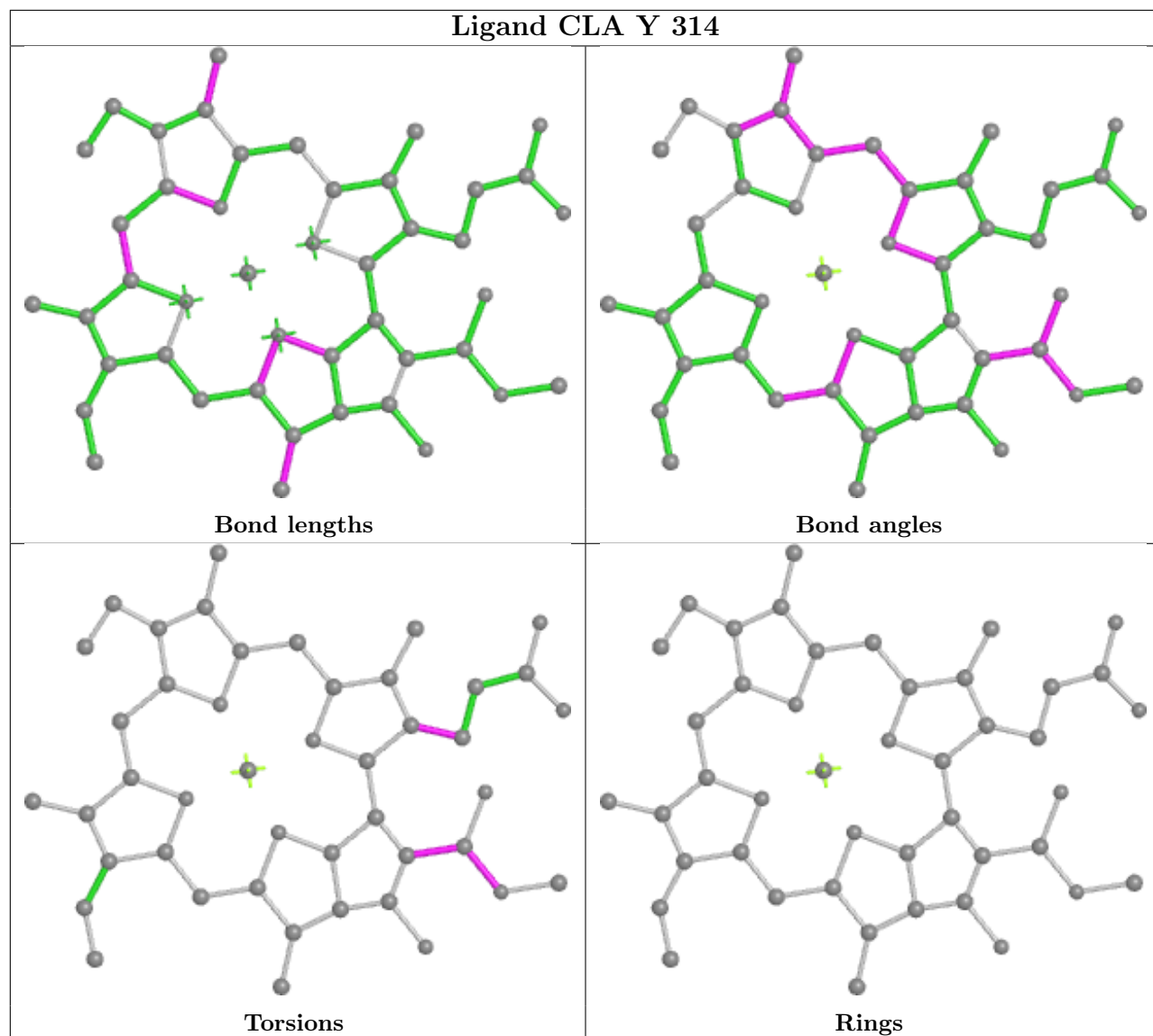


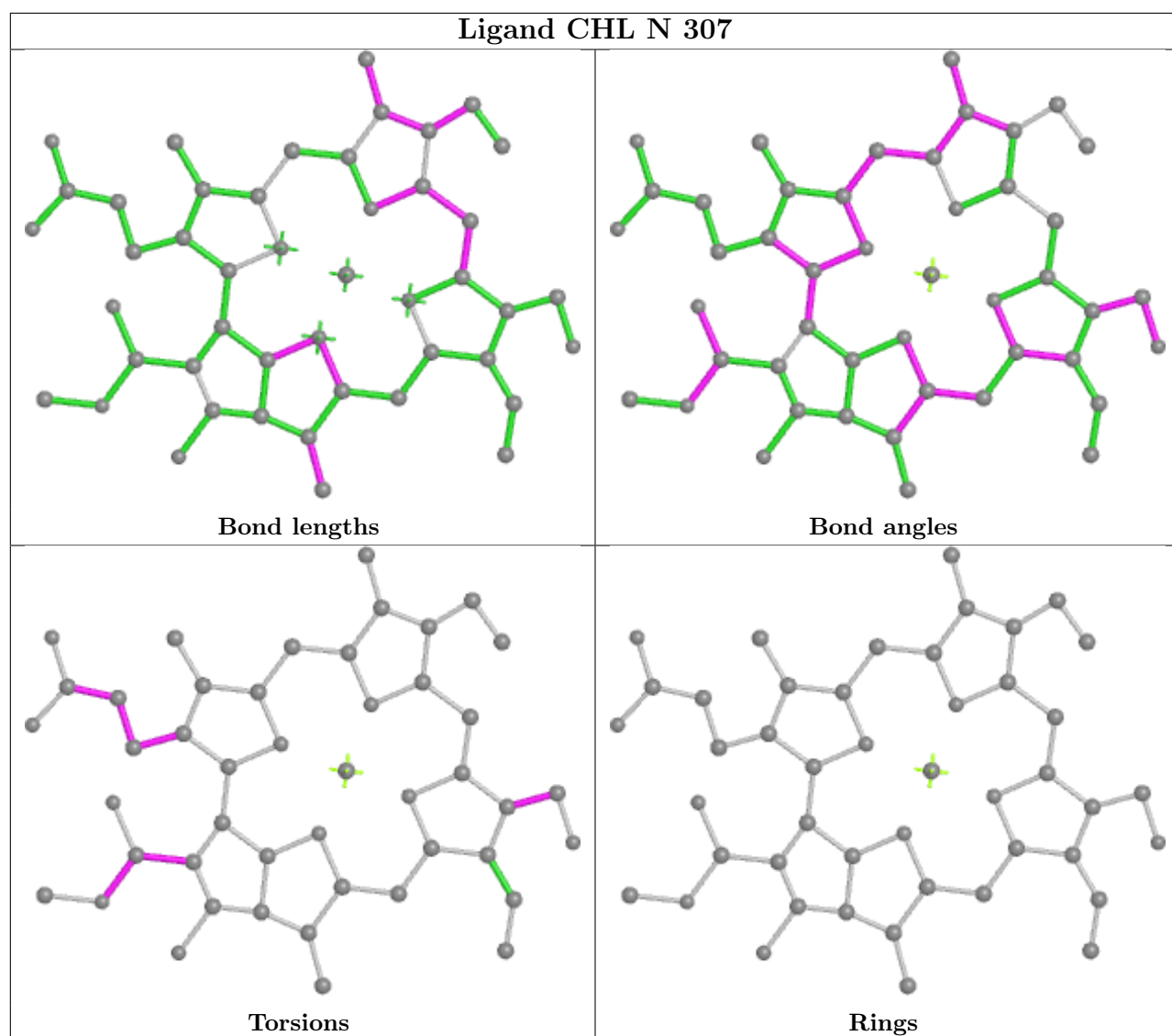
Torsions



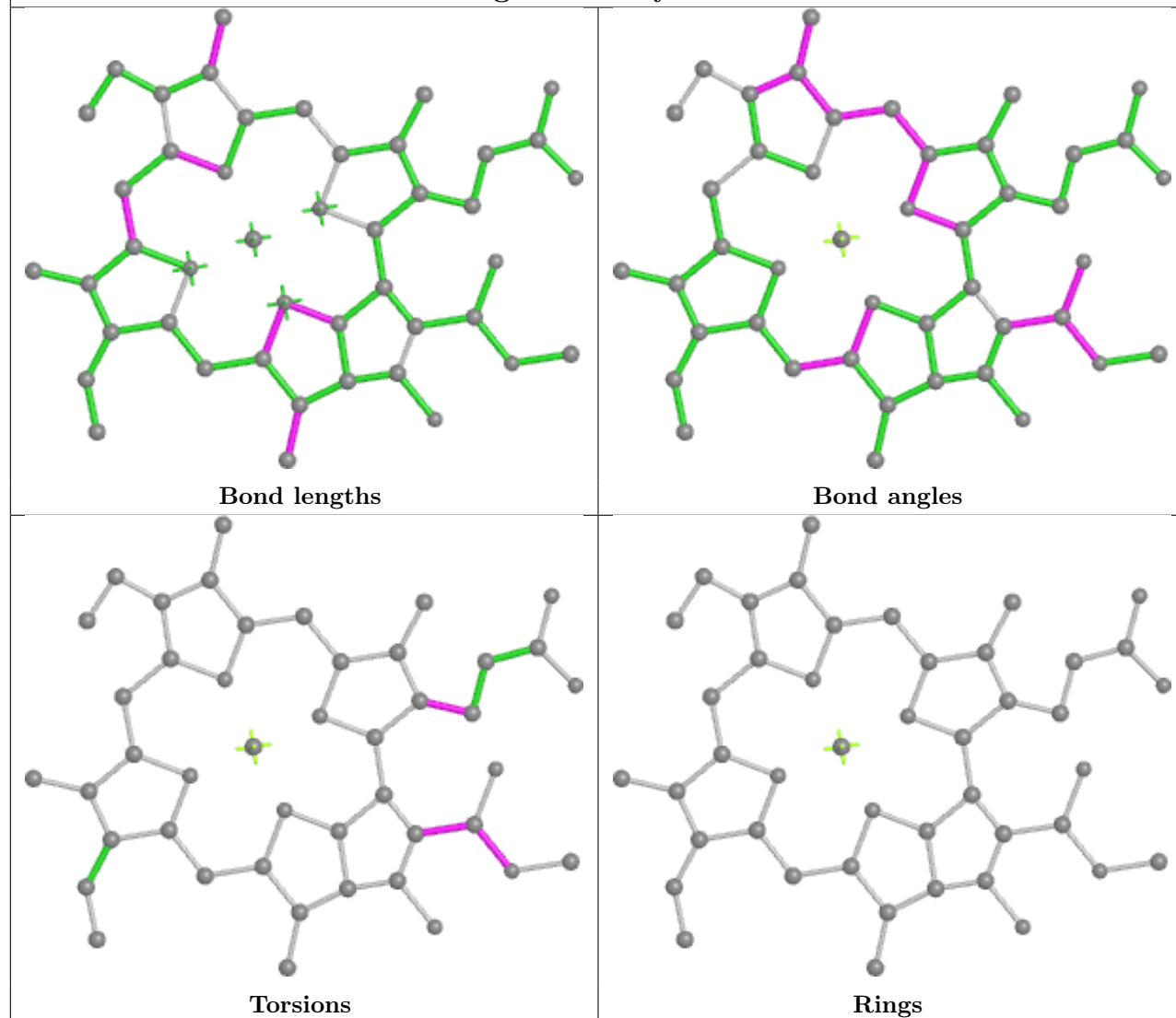
Rings

Ligand CLA Y 314

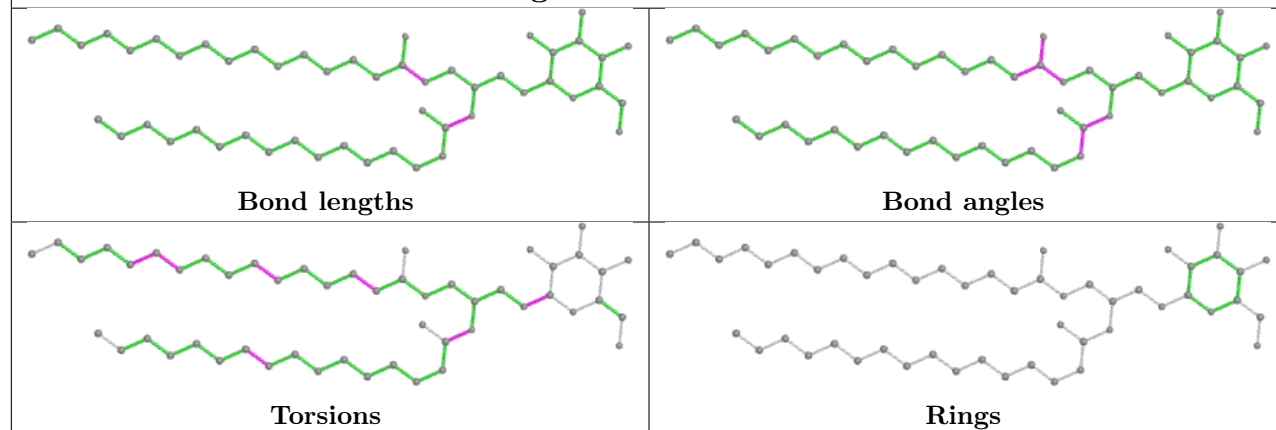




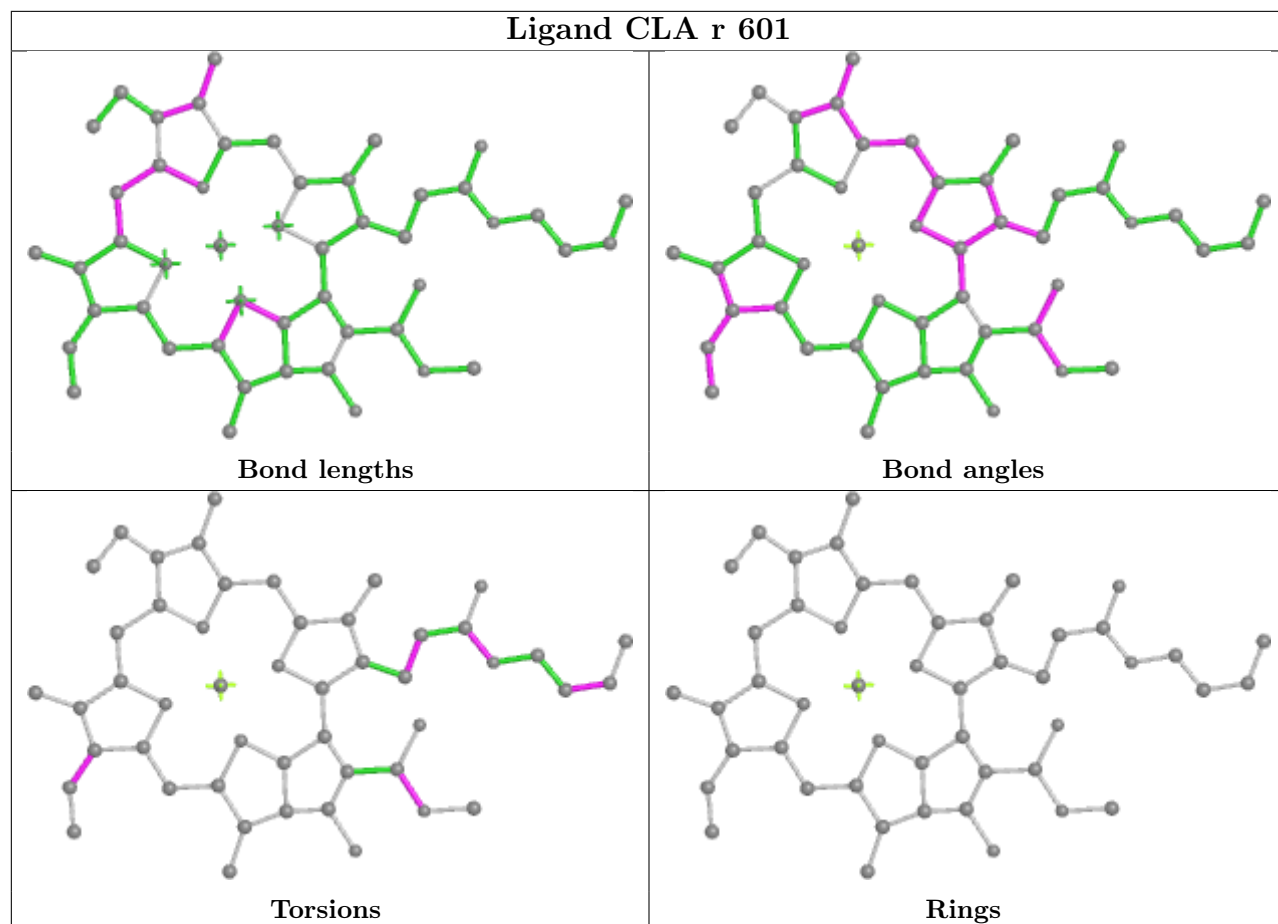
Ligand CLA y 314

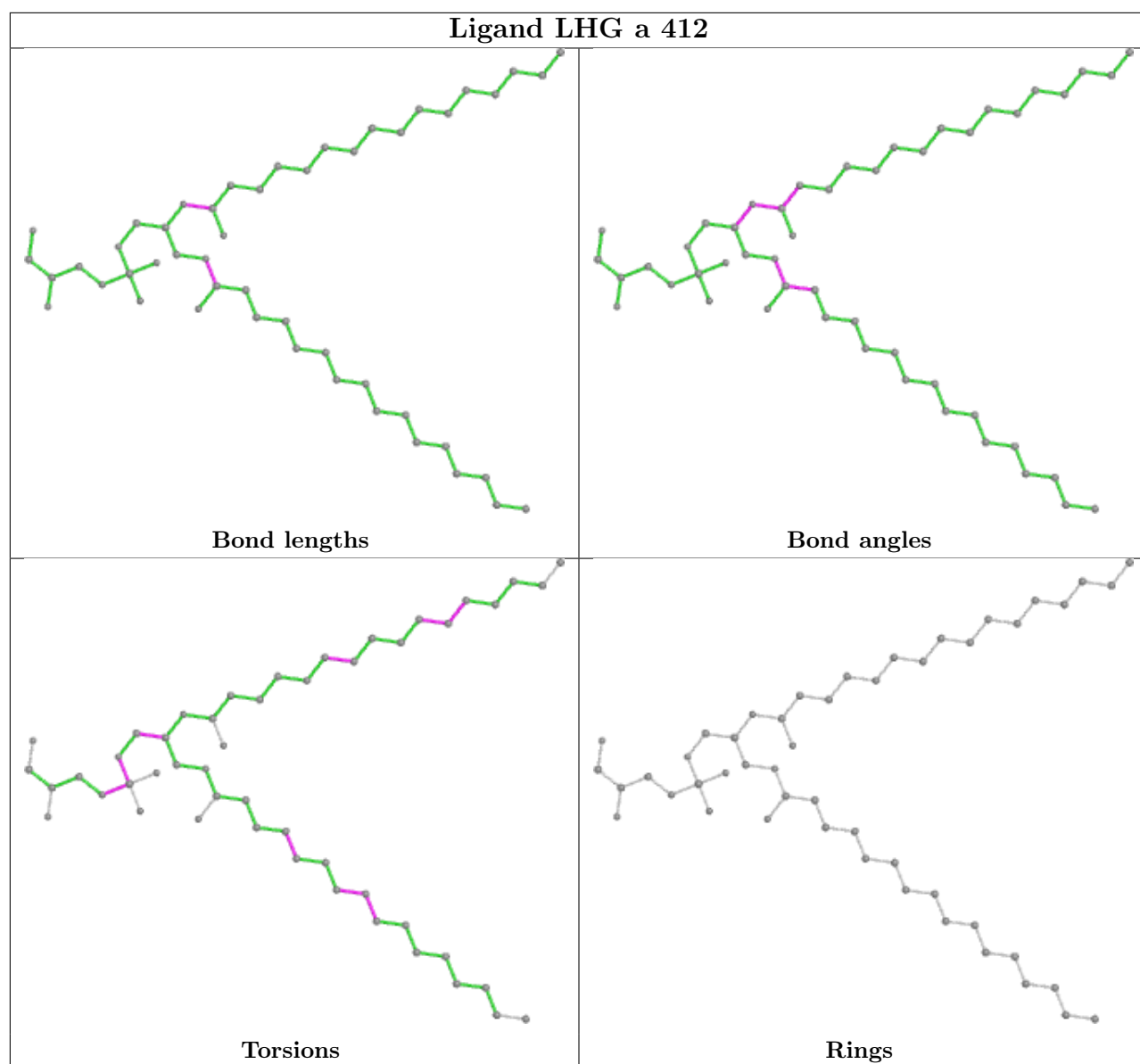


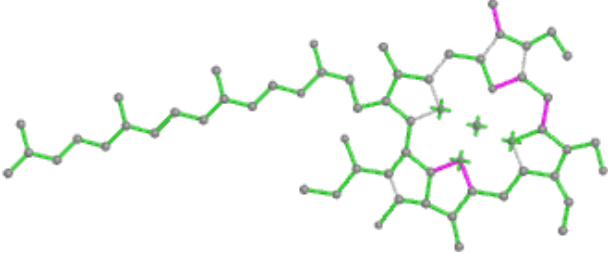
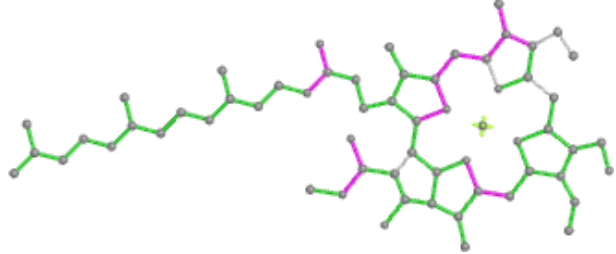
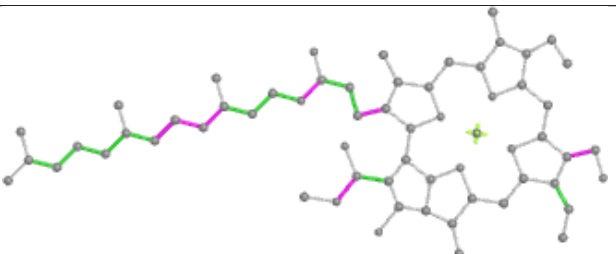
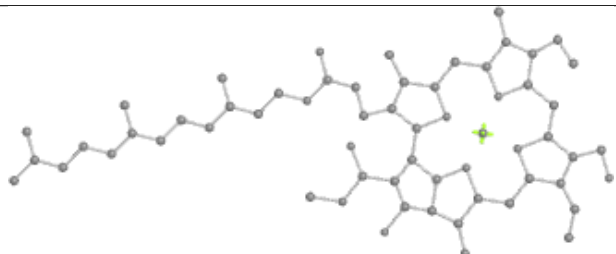
Ligand LMG b 620

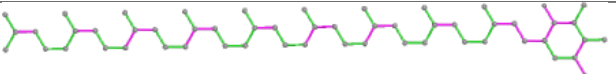
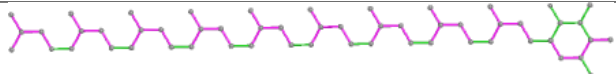
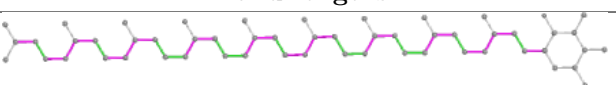
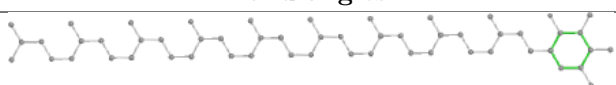


Ligand CLA r 601

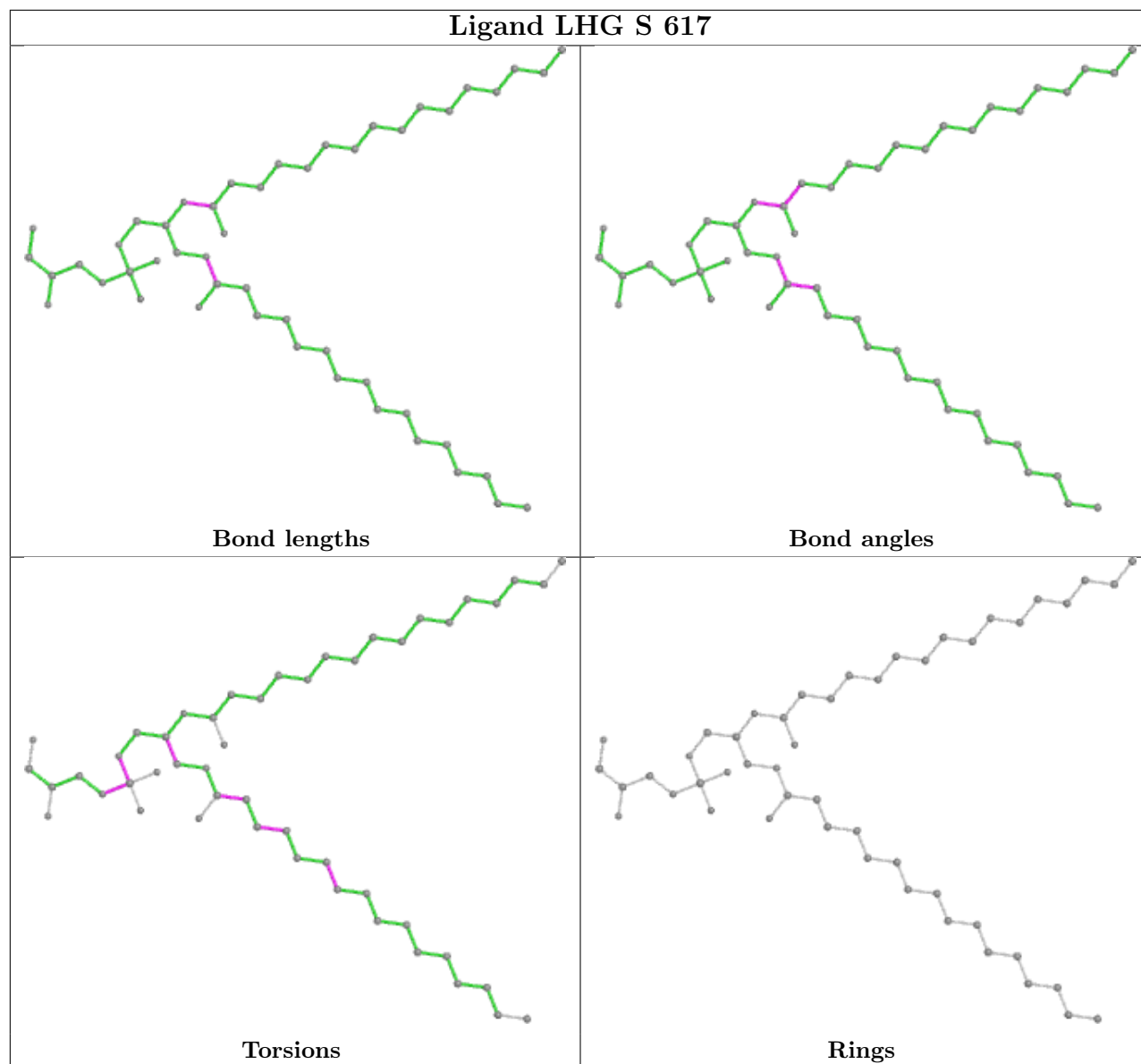




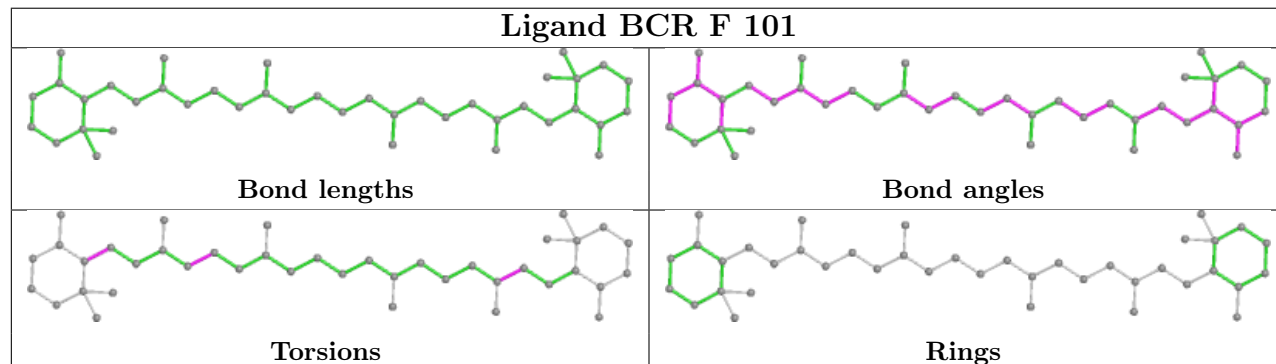
Ligand CHL r 607			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

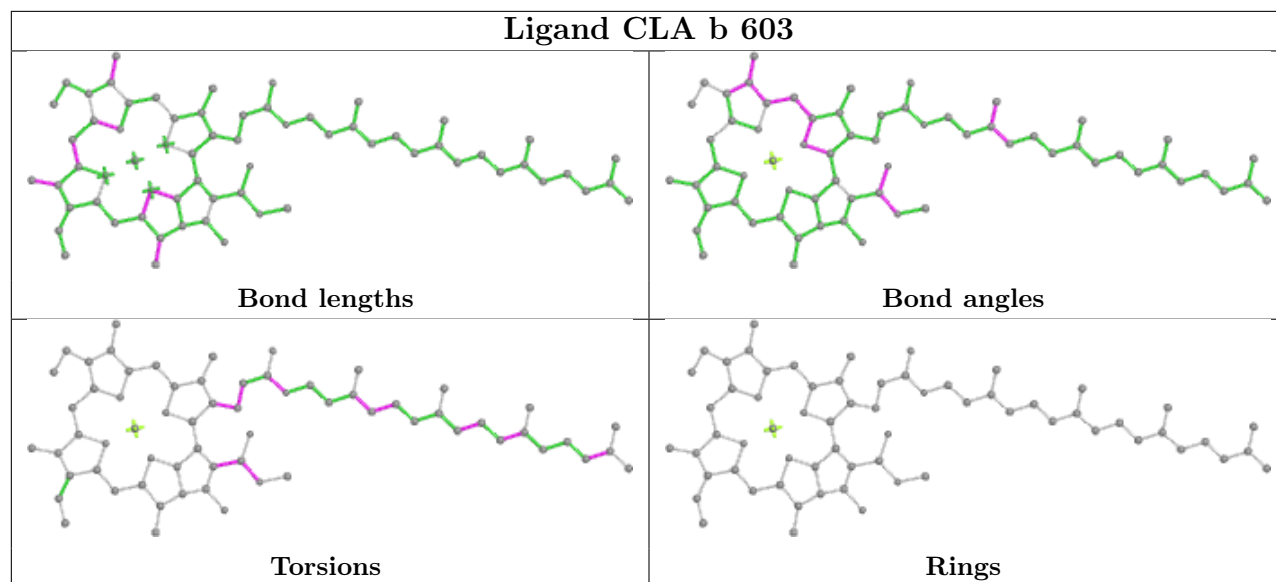
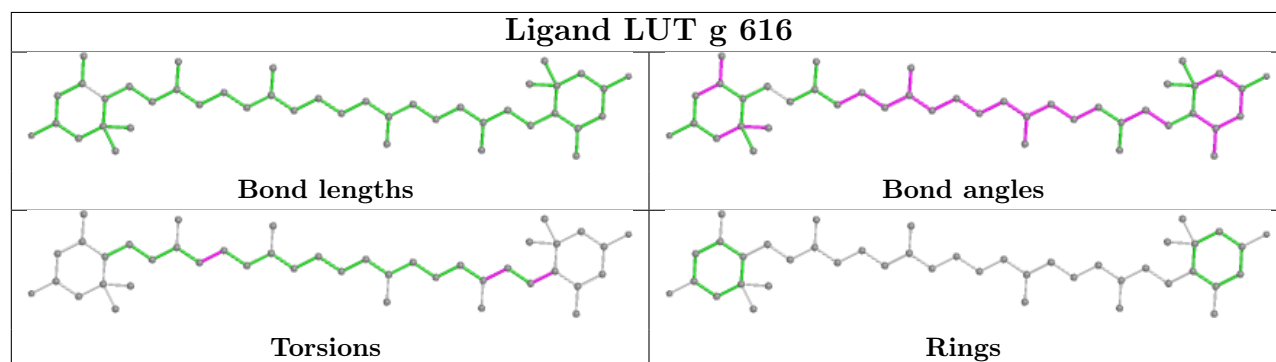
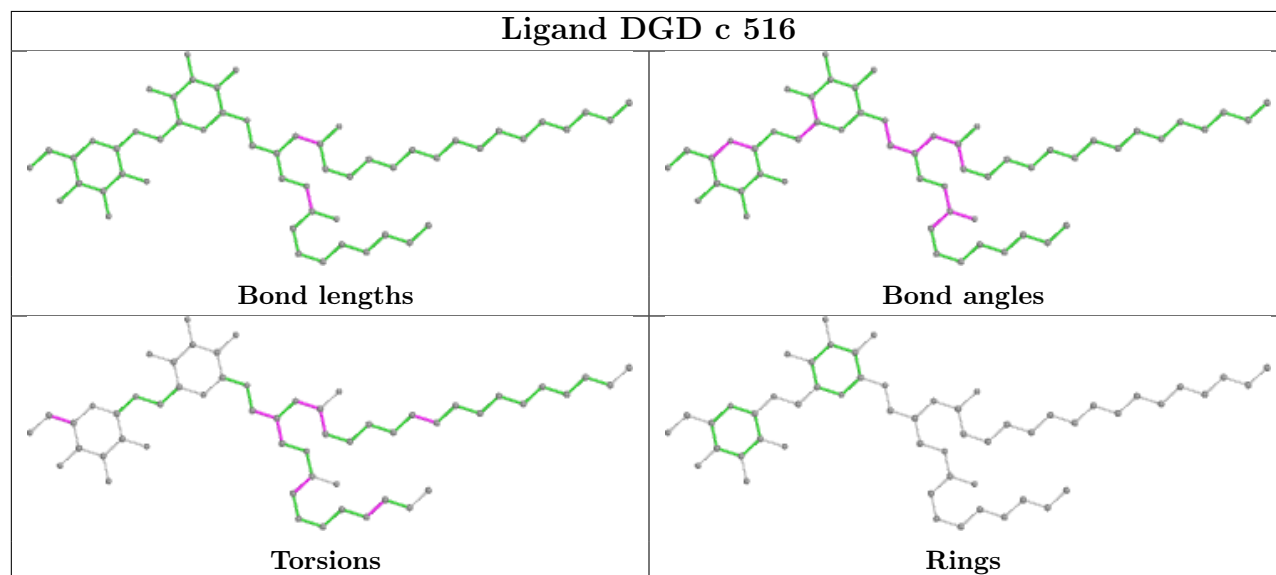
Ligand PL9 D 406			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand LHG S 617

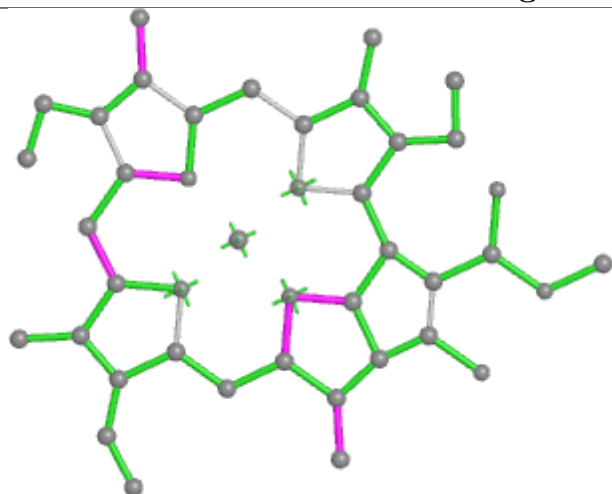


Ligand BCR F 101

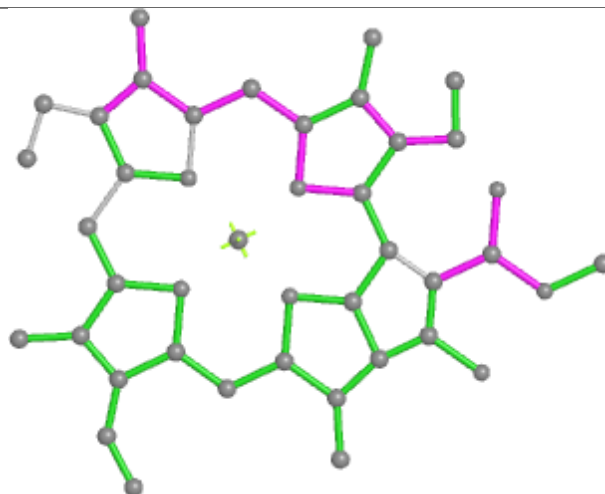


Ligand CLA b 603**Ligand LUT g 616****Ligand DGD c 516**

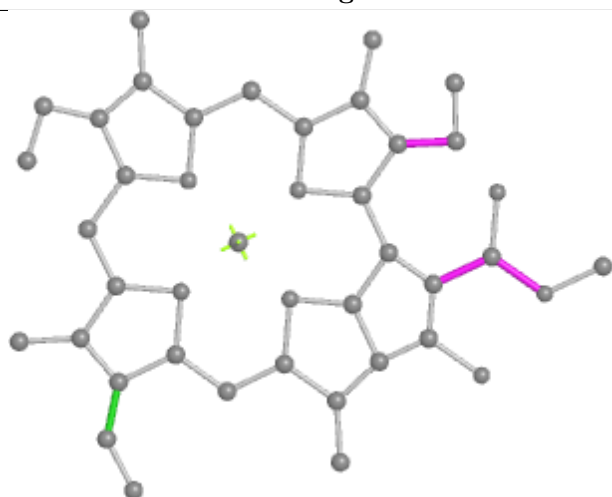
Ligand CLA s 610



Bond lengths



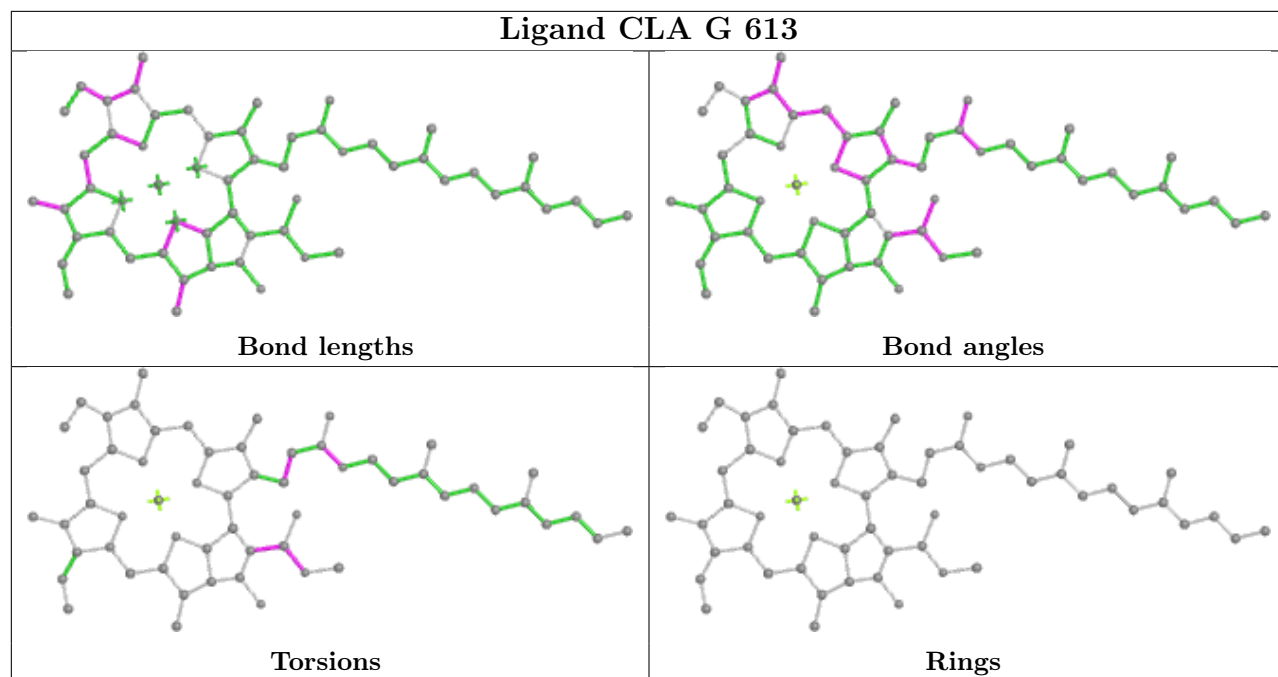
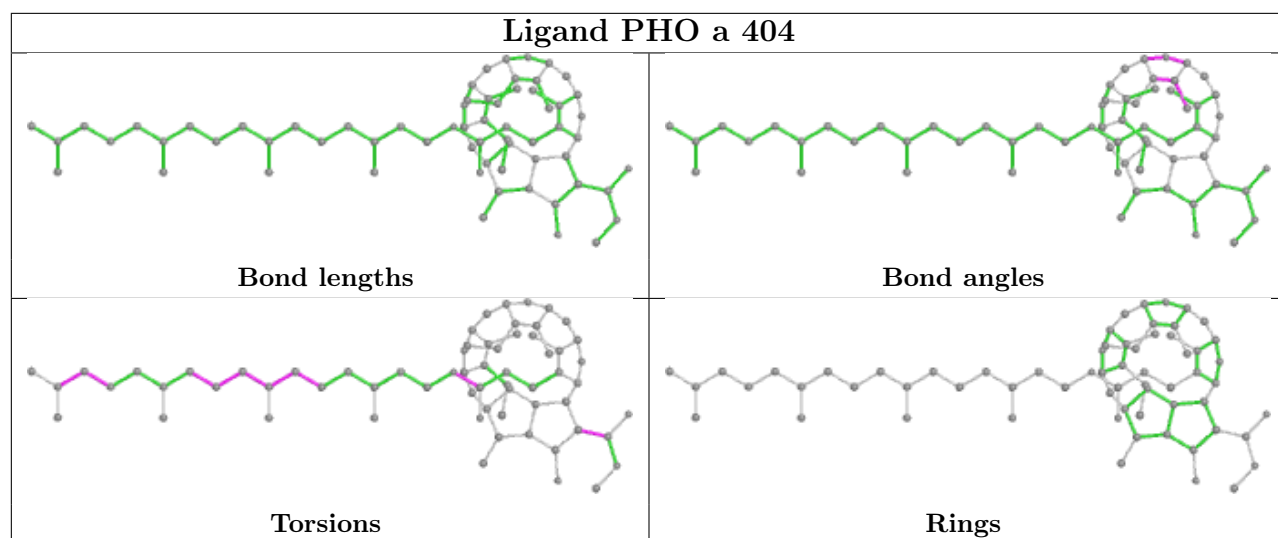
Bond angles

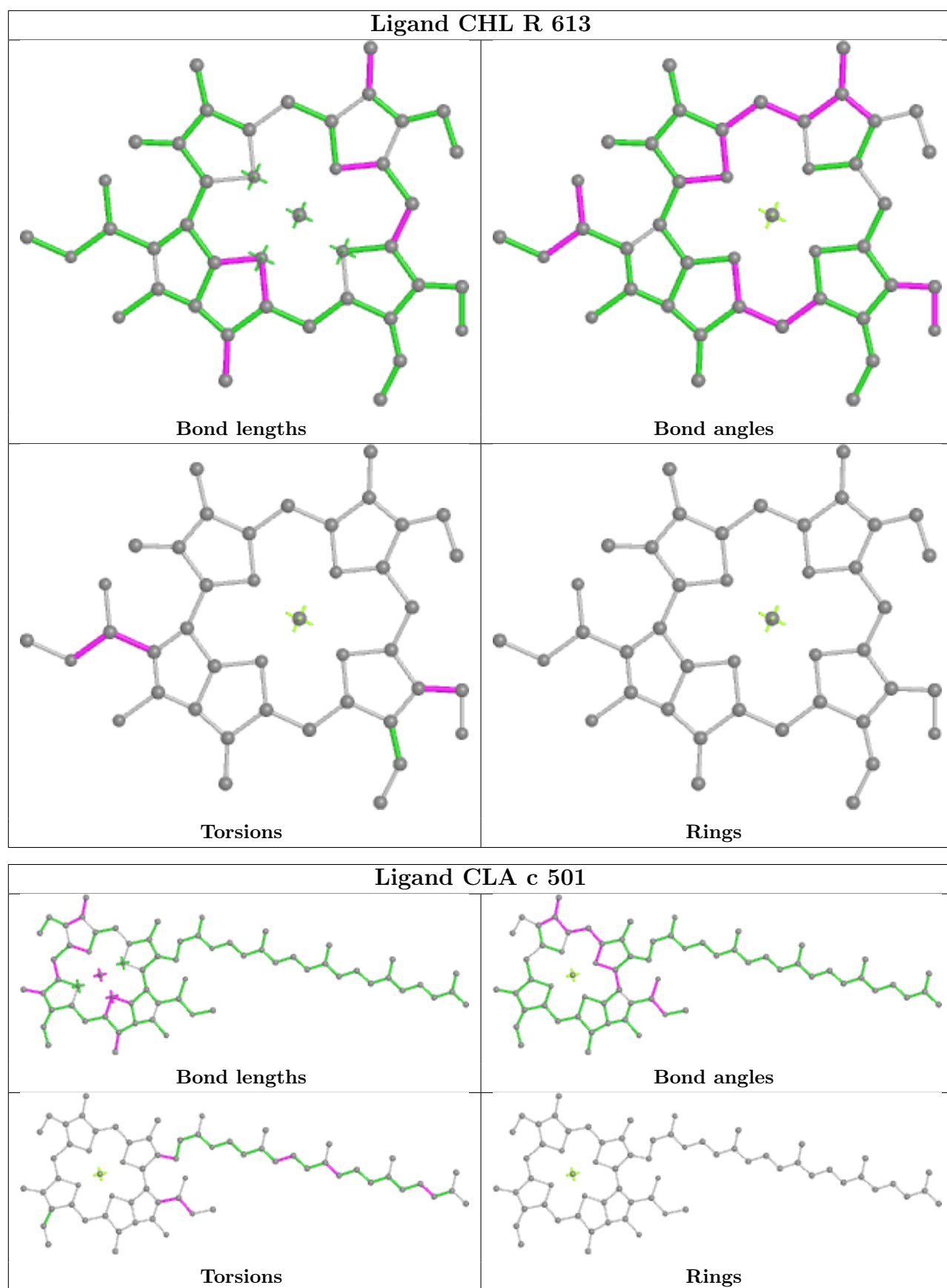


Torsions

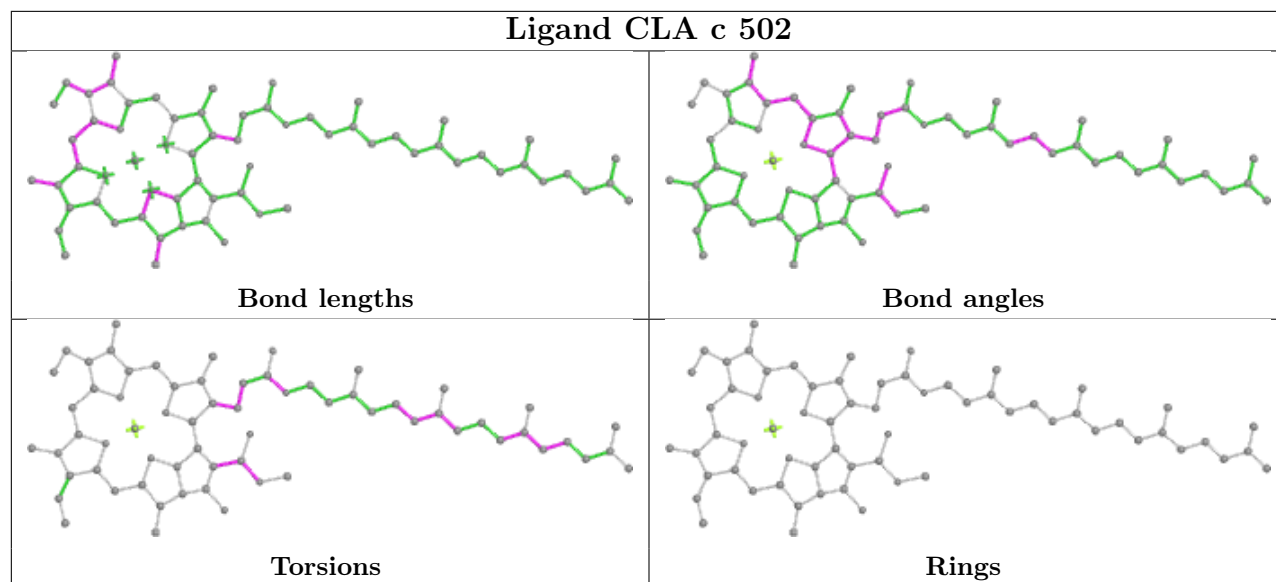


Rings

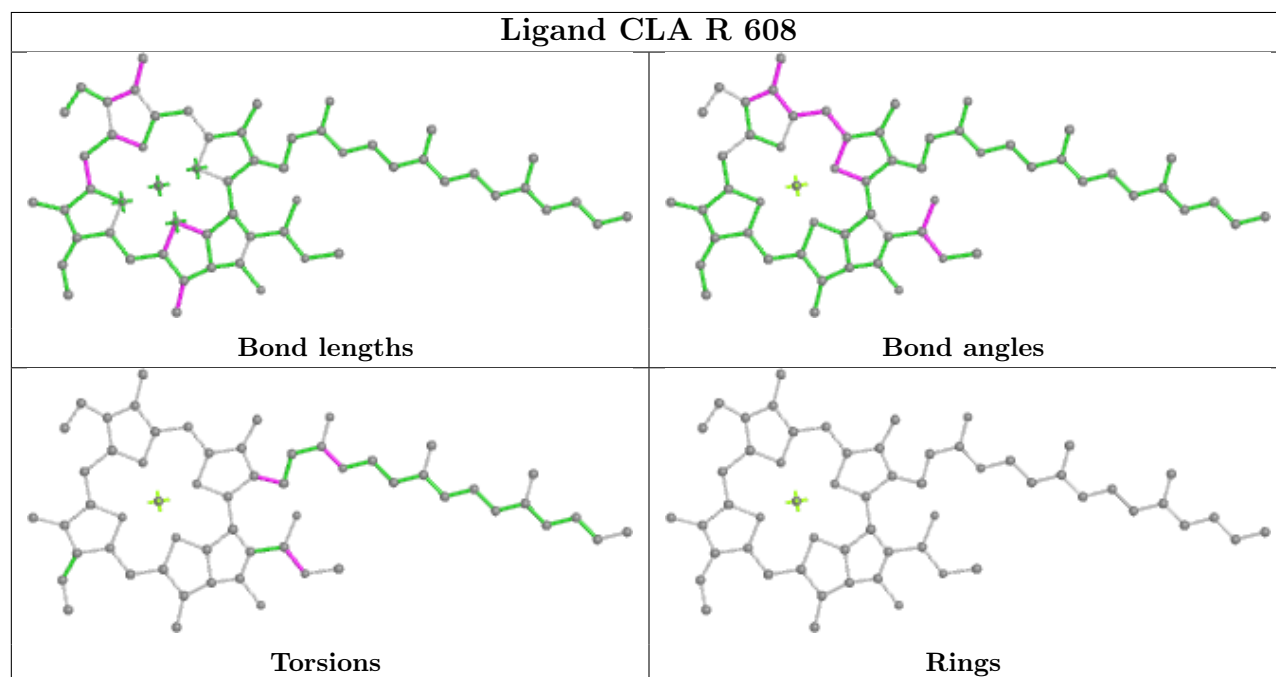
Ligand CLA G 613**Ligand PHO a 404**



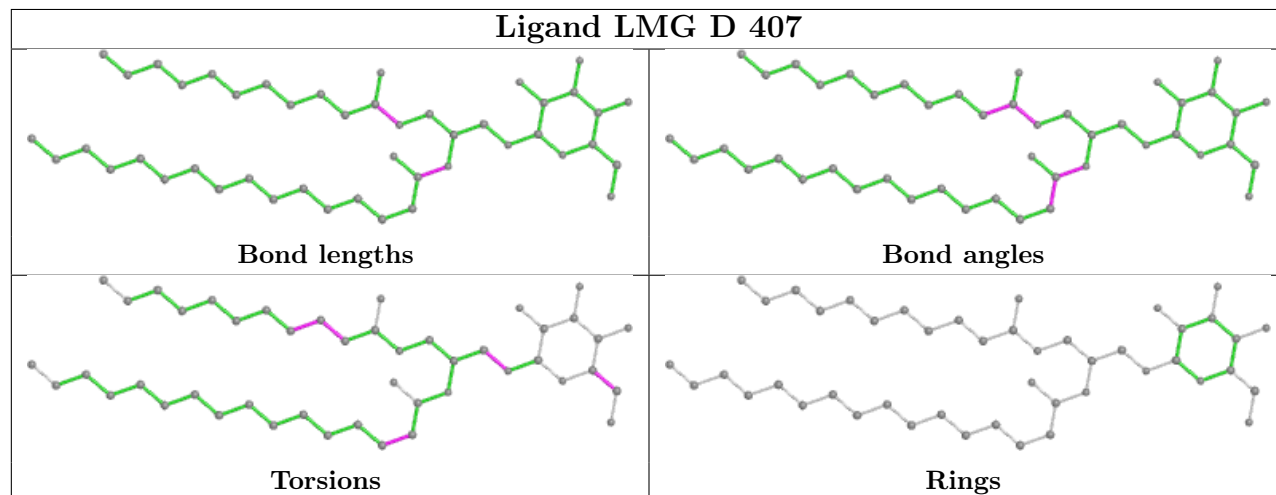
Ligand CLA c 502

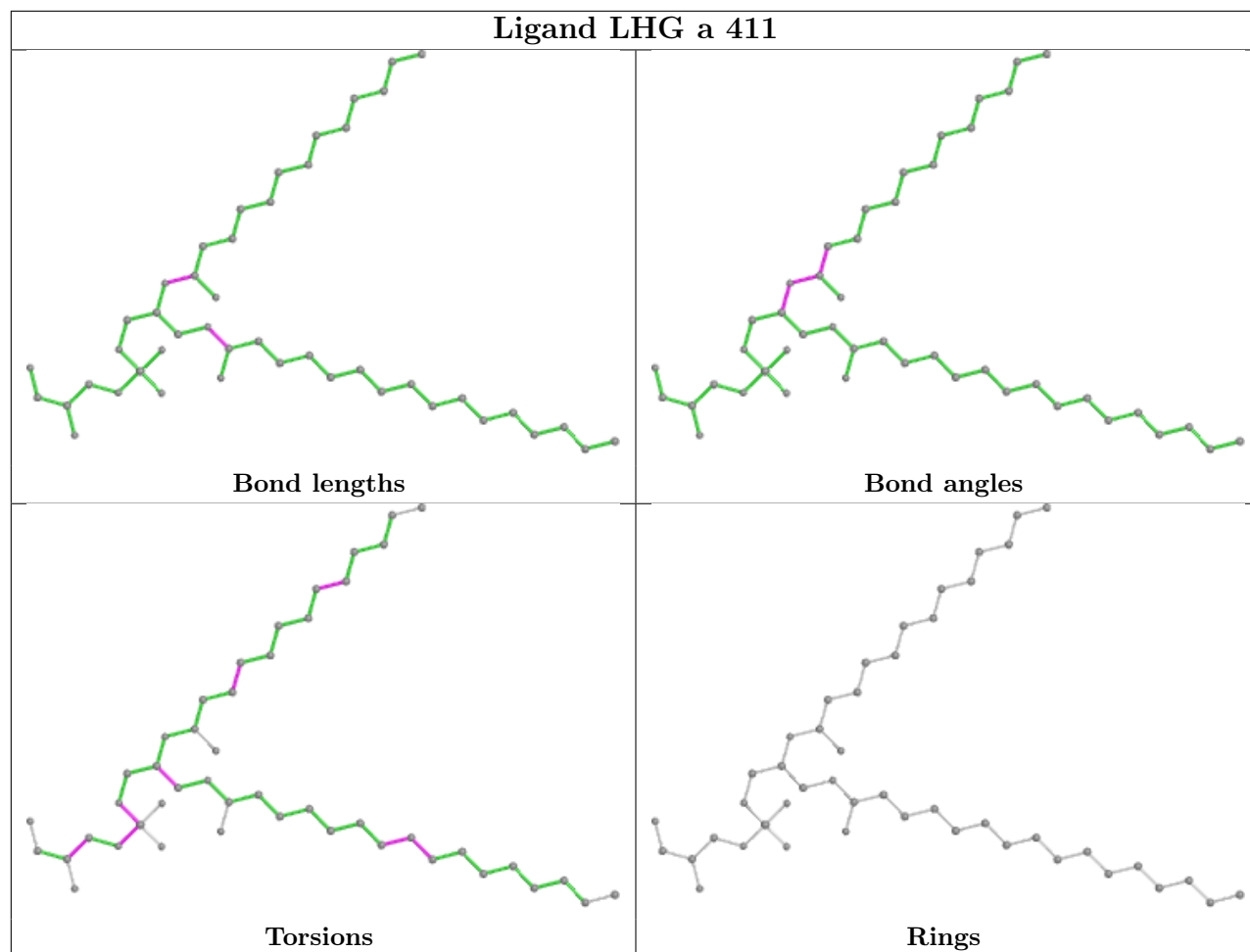
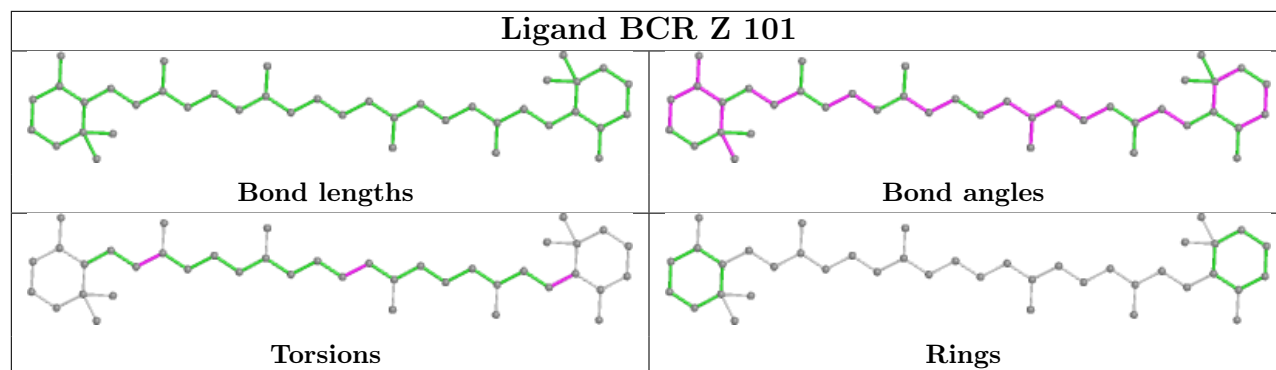


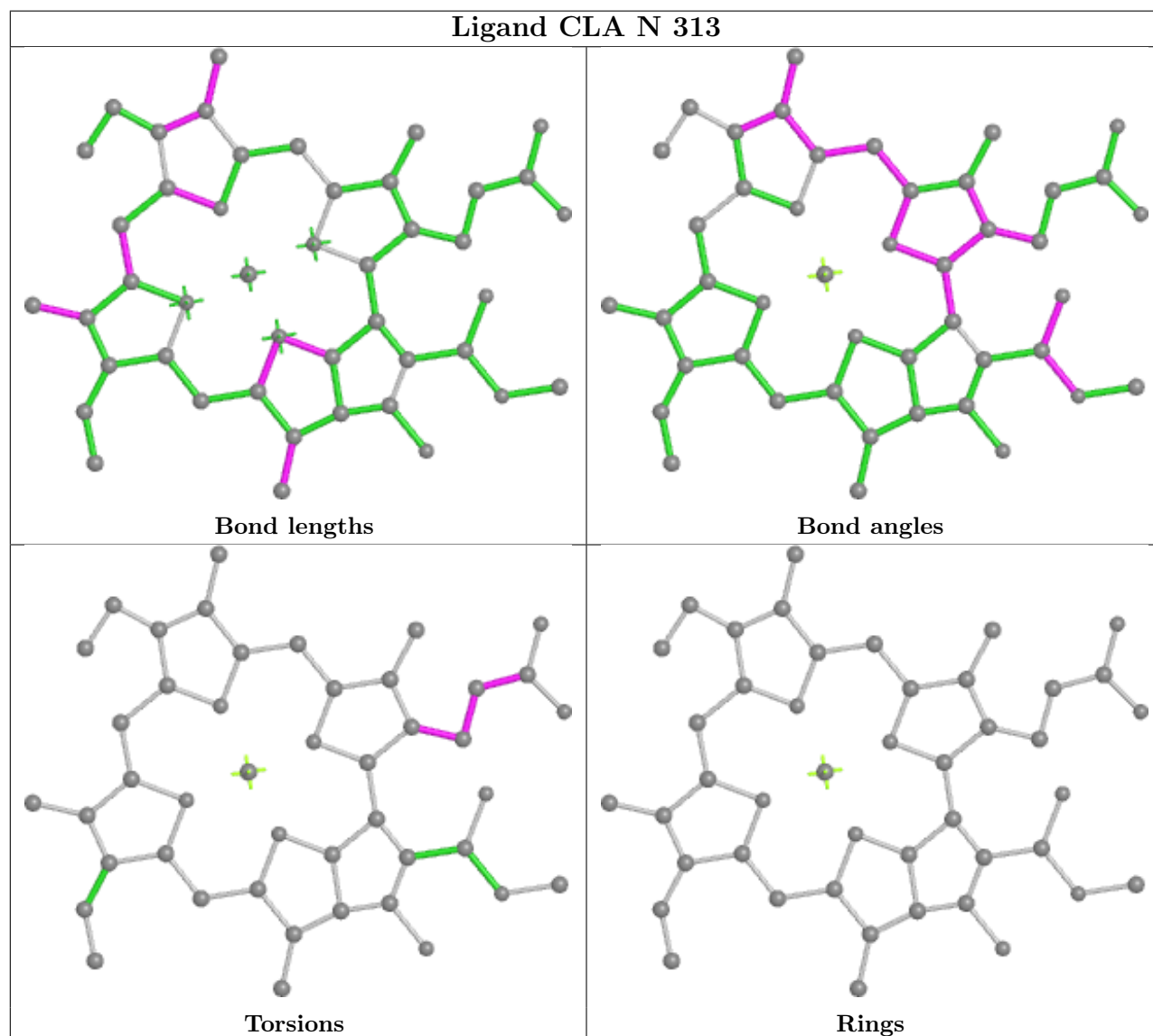
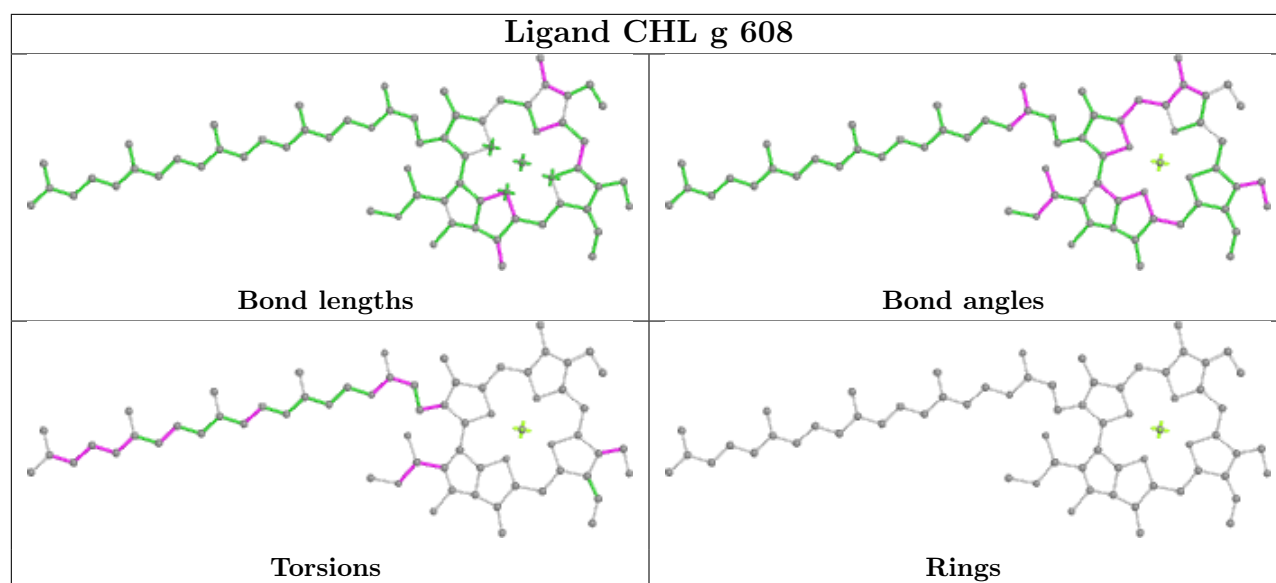
Ligand CLA R 608

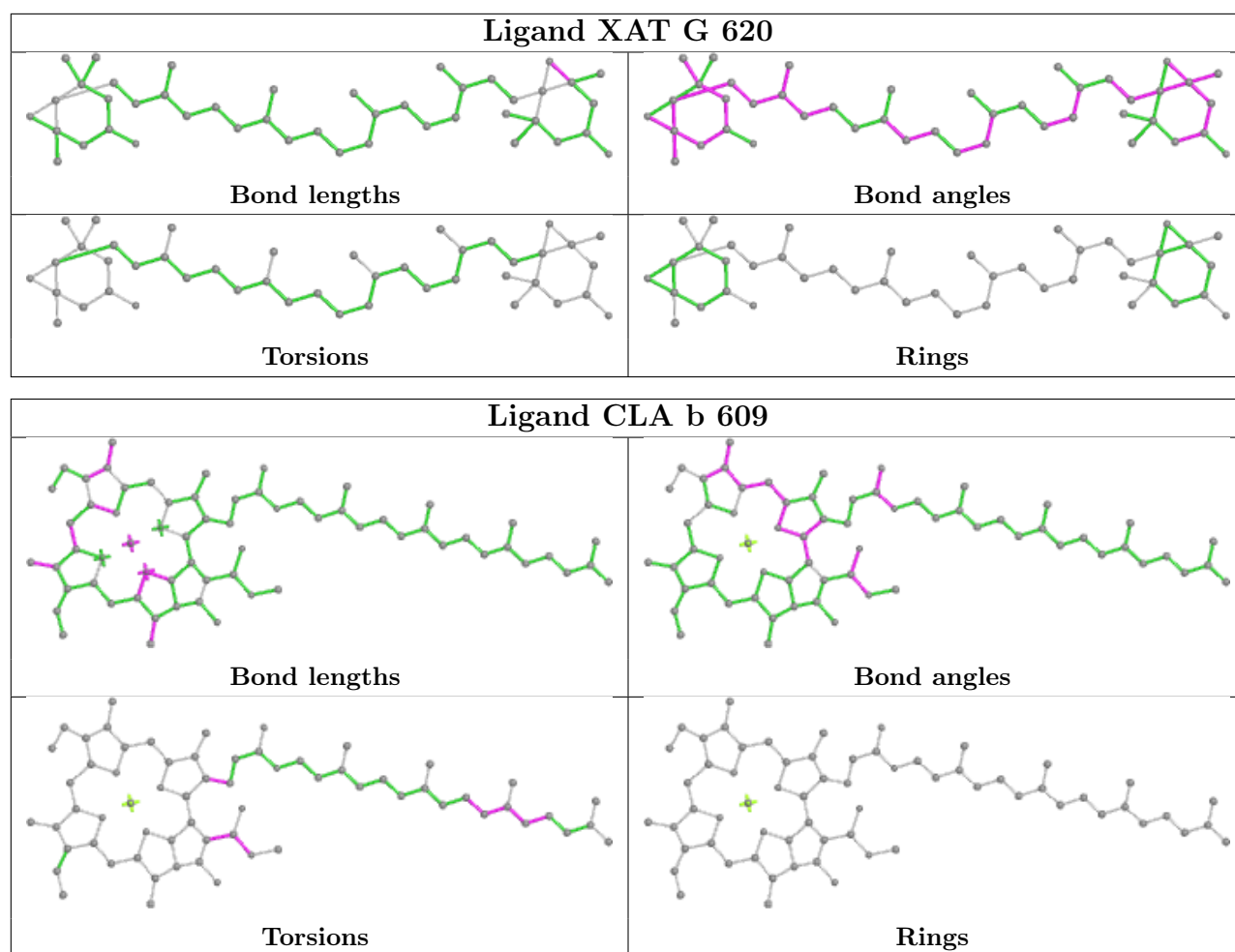


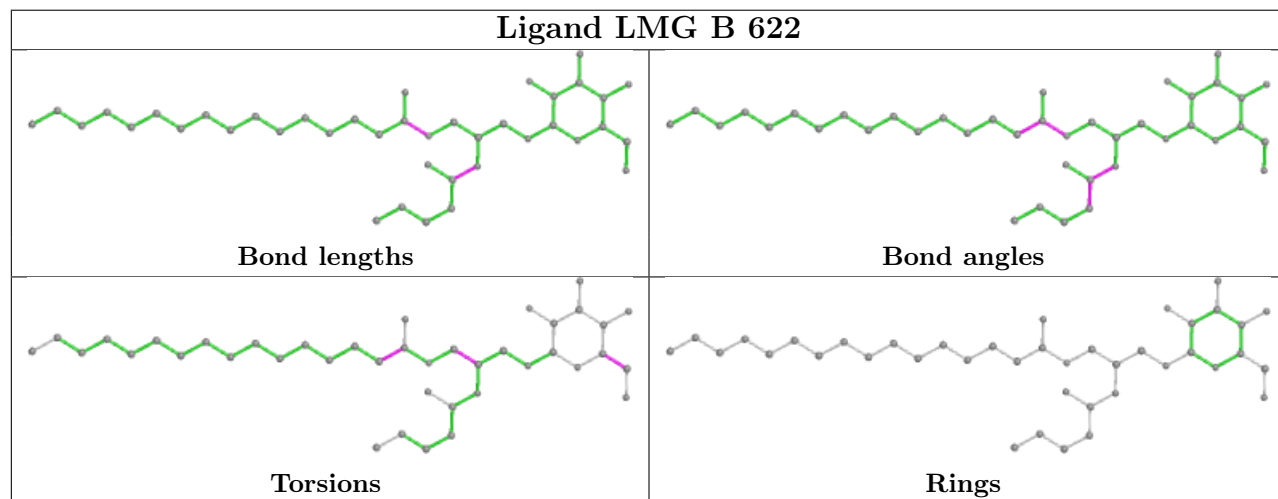
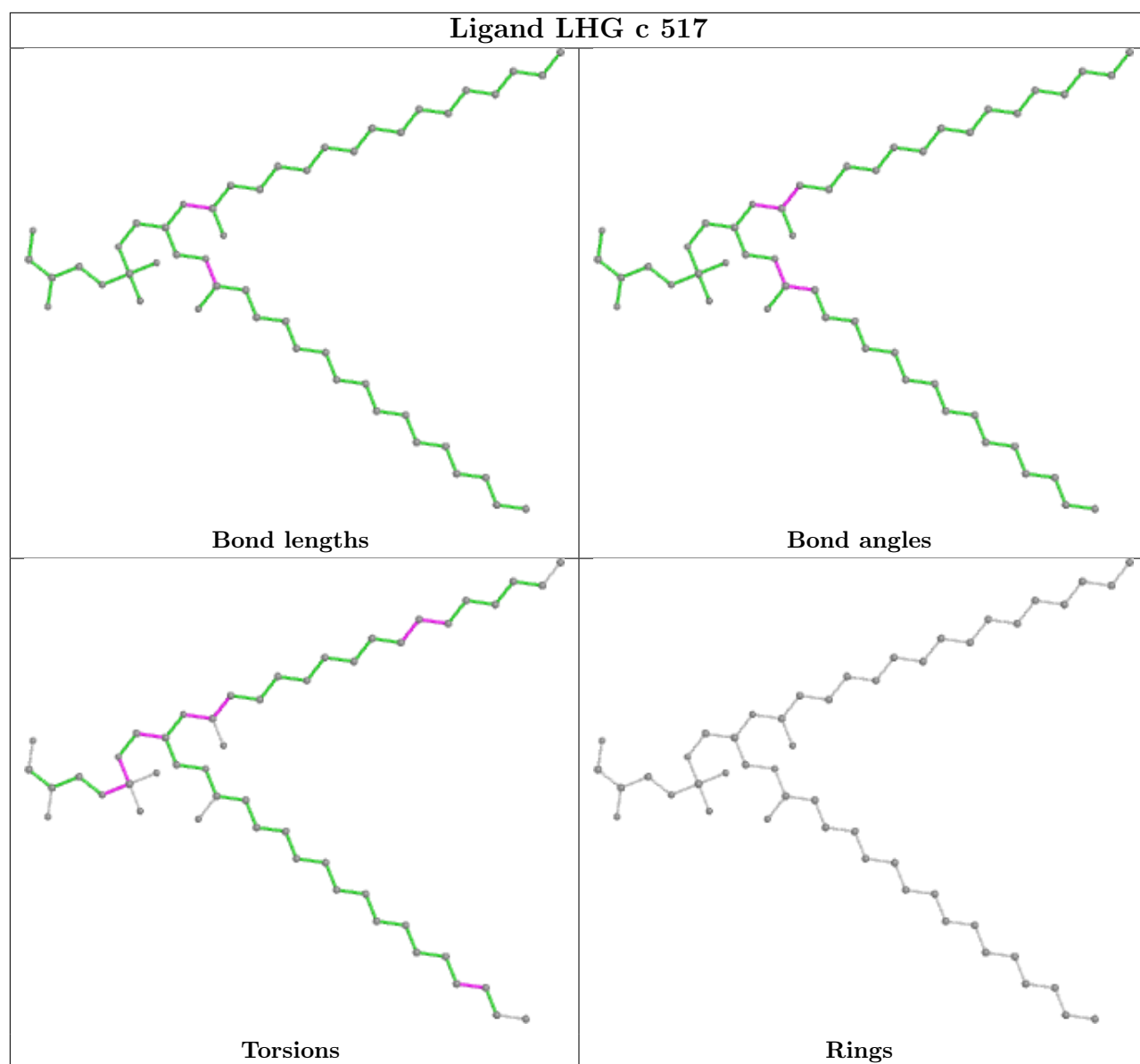
Ligand LMG D 407

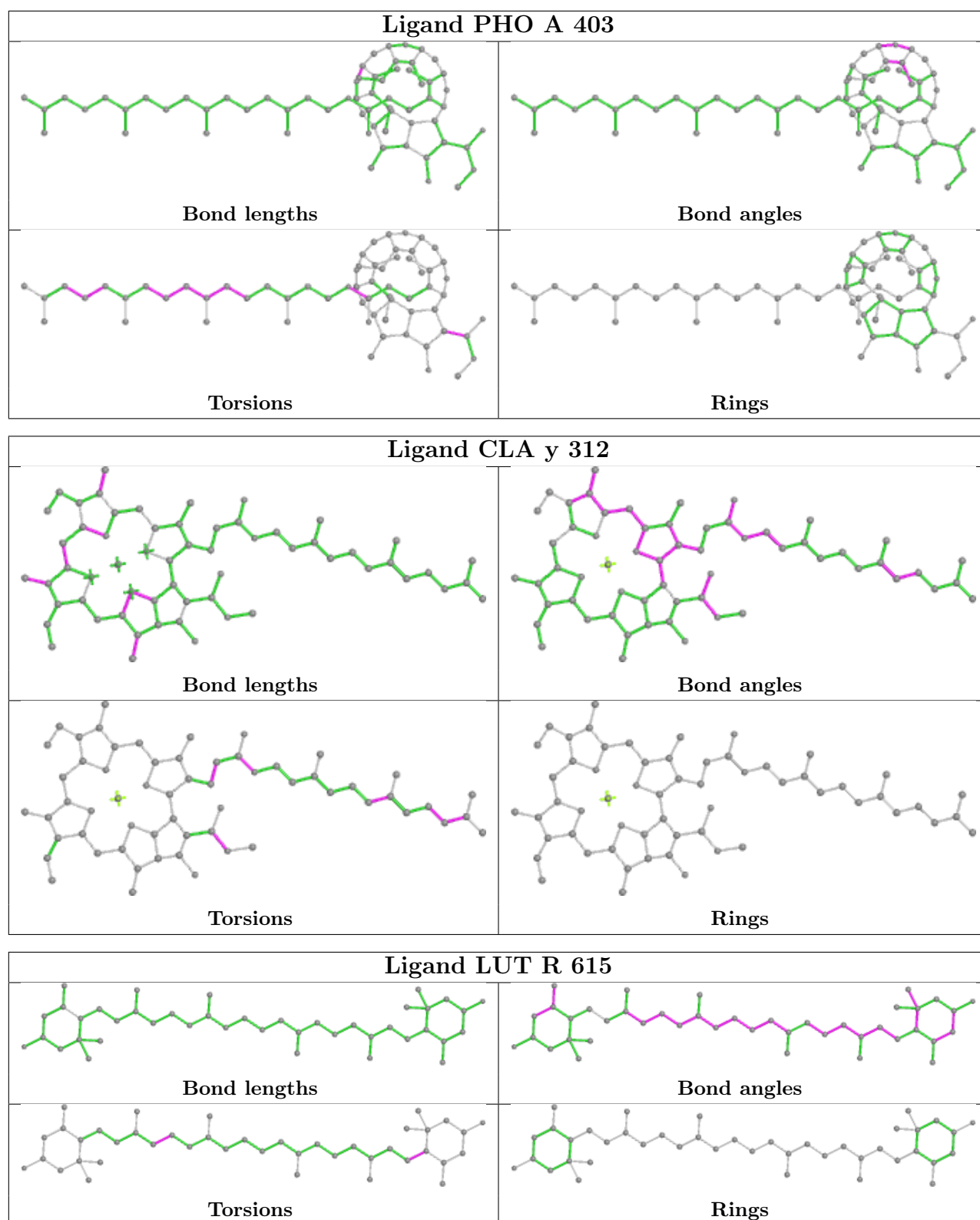


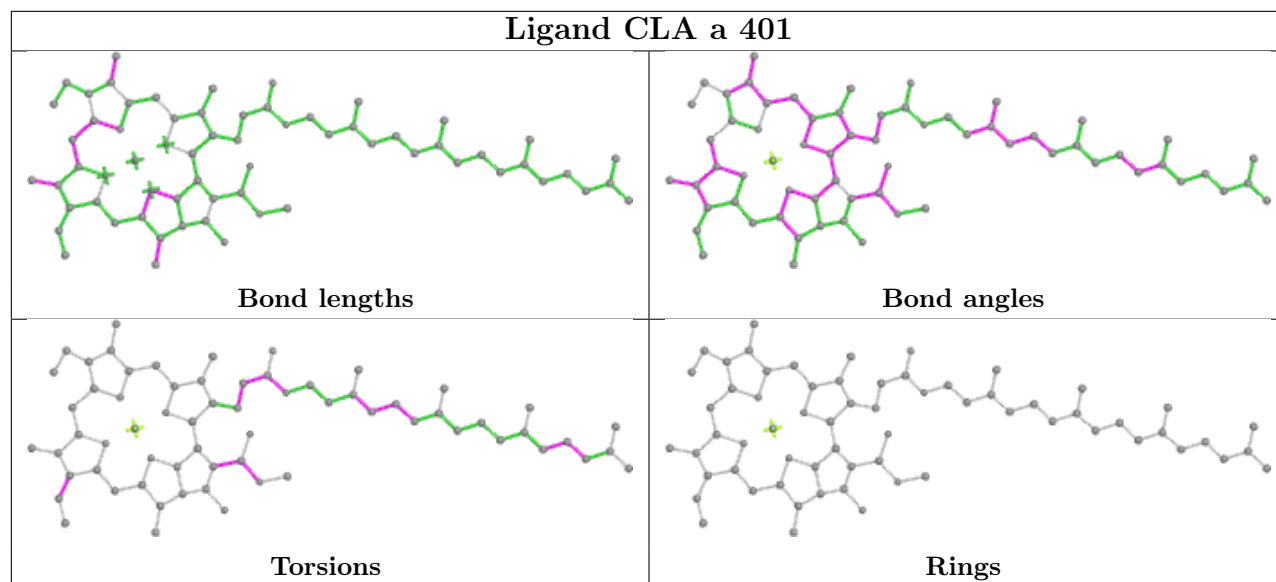
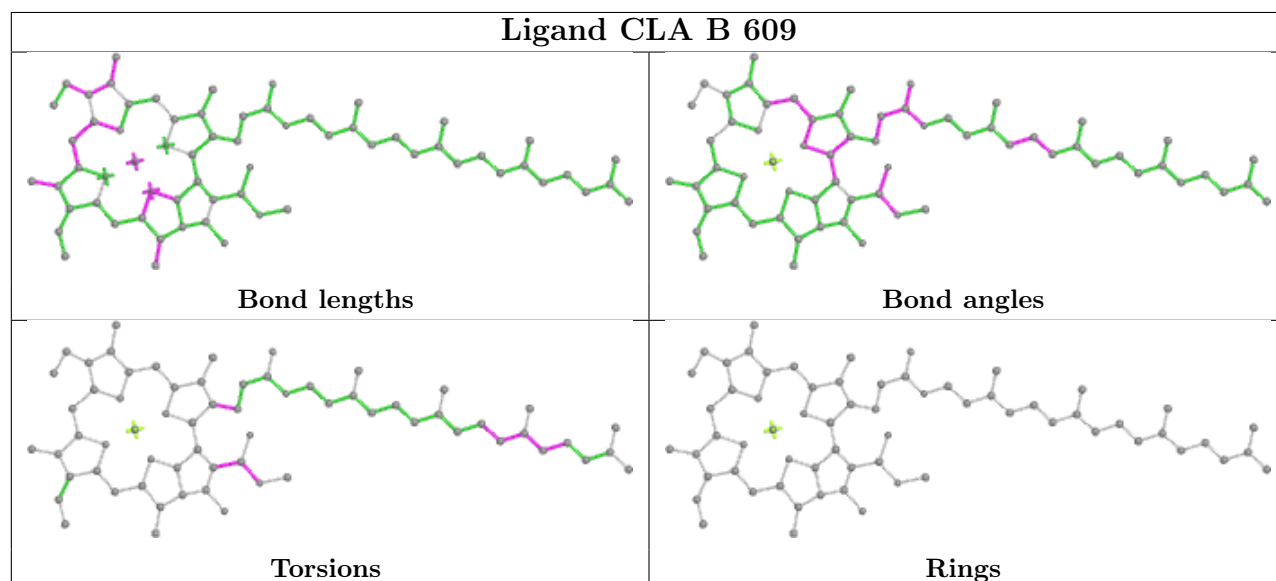
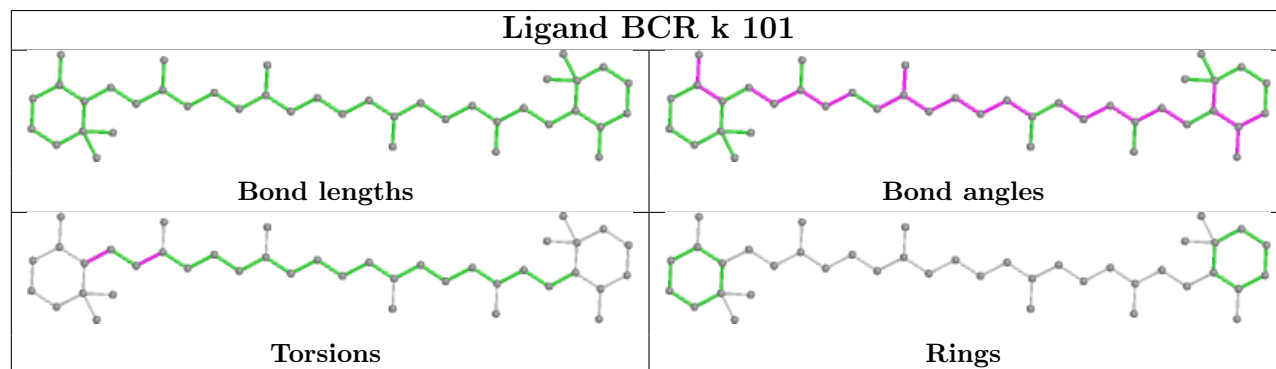




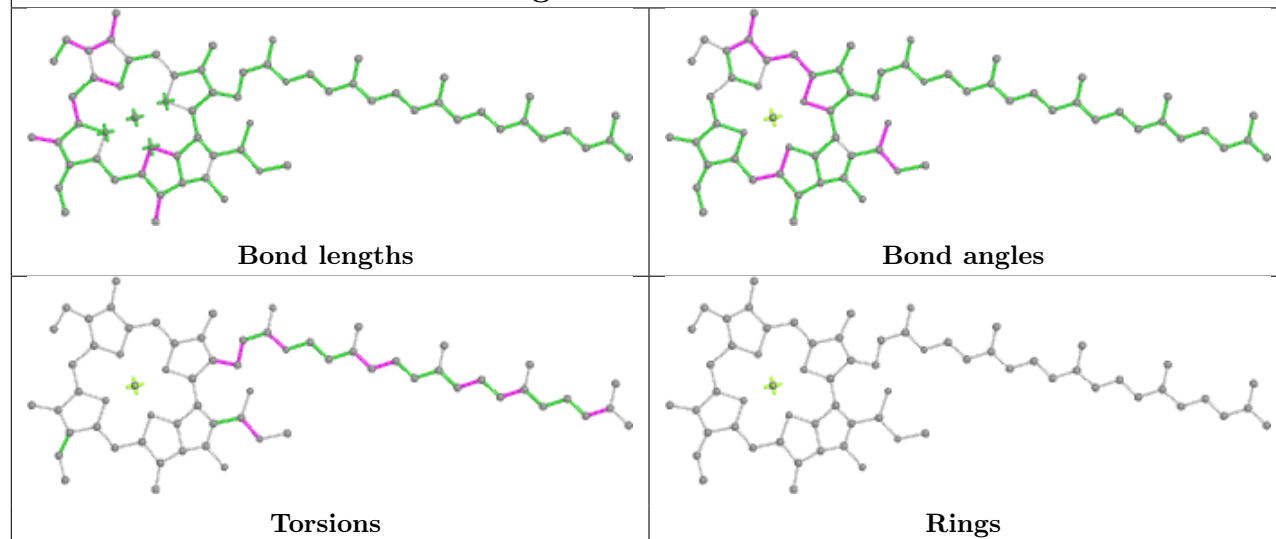




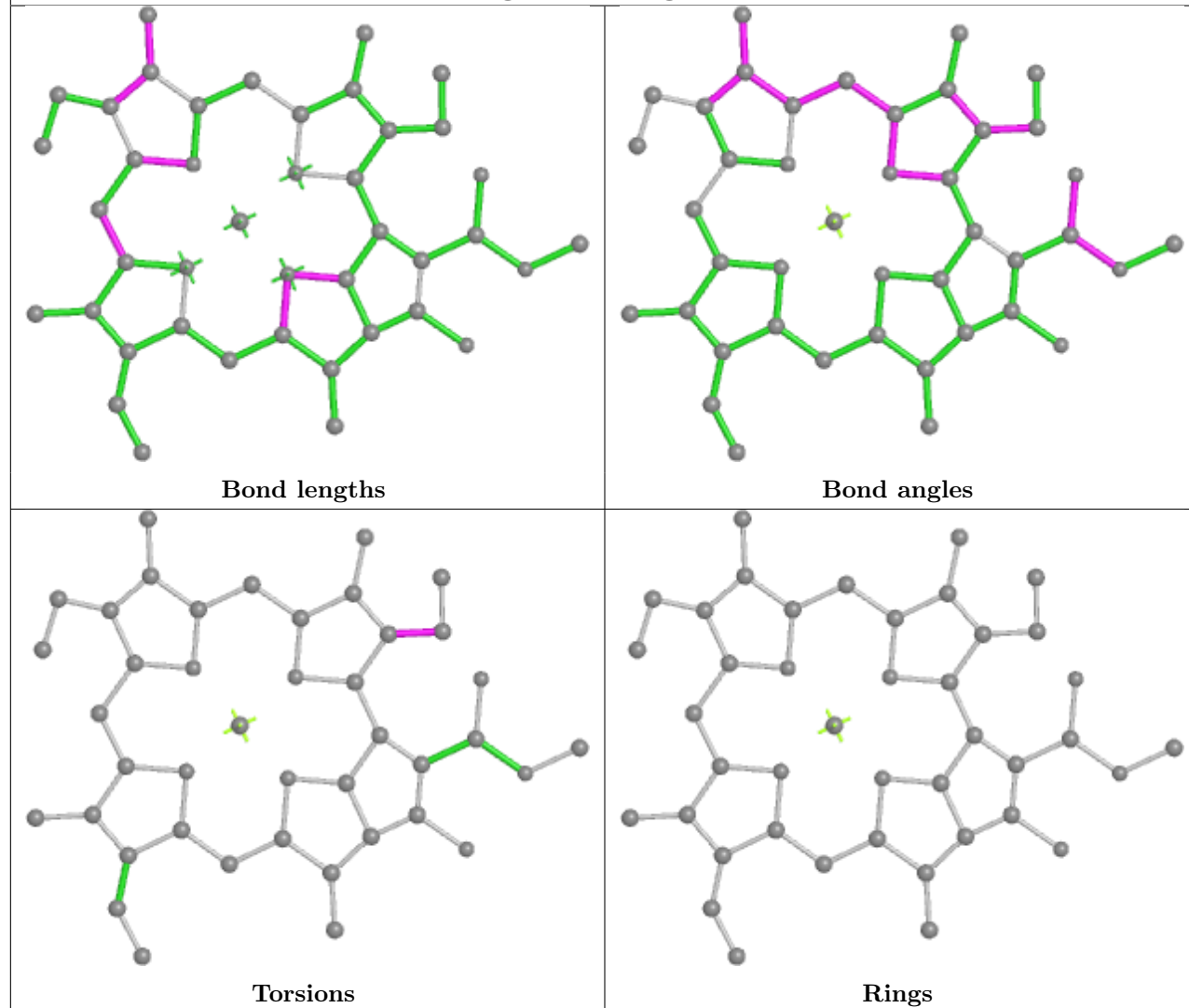


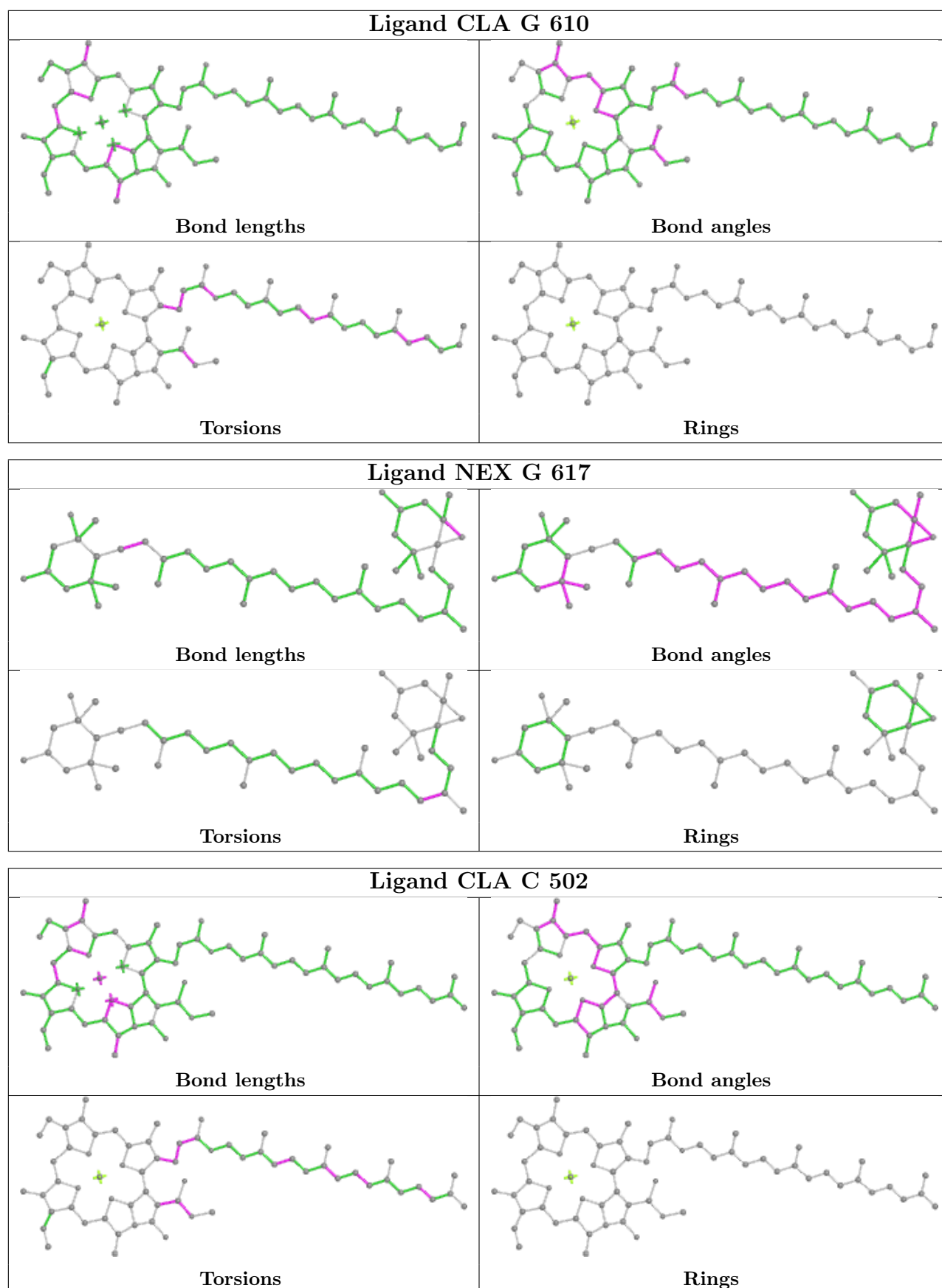
Ligand CLA a 401**Ligand CLA B 609****Ligand BCR k 101**

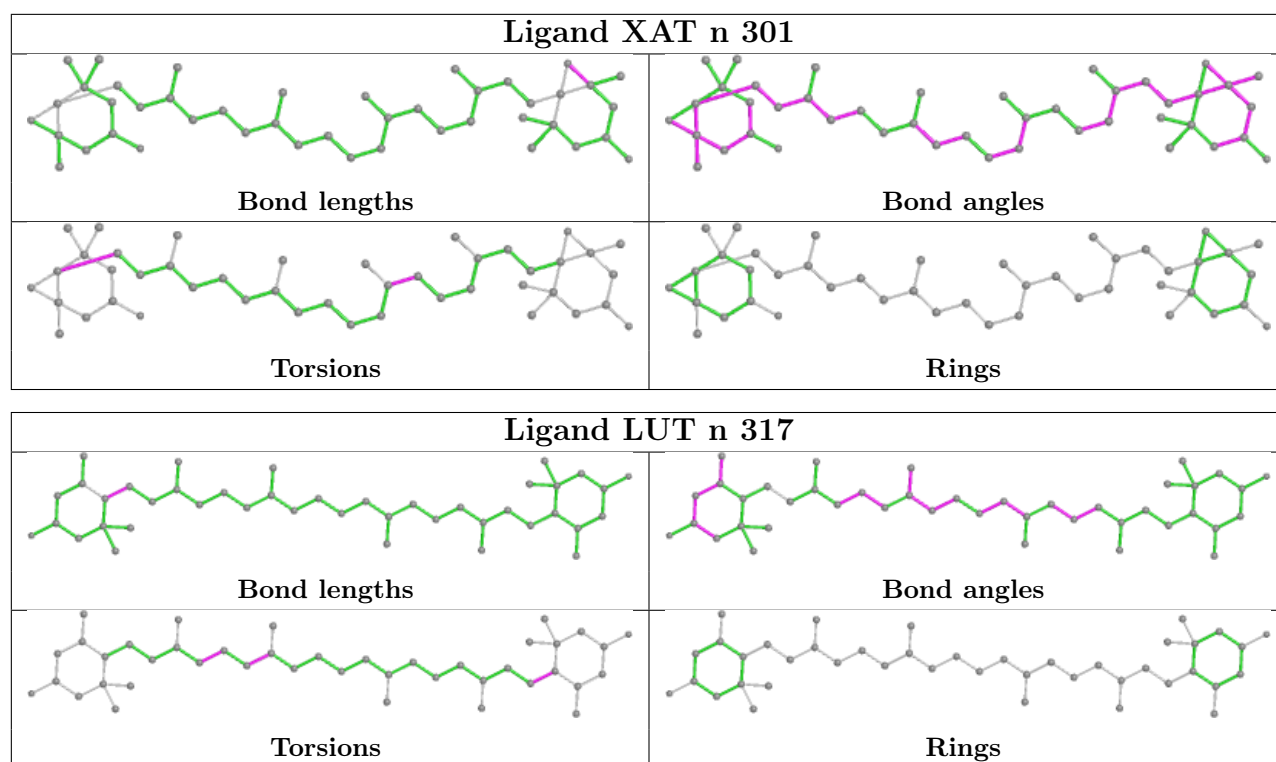
Ligand CLA B 603

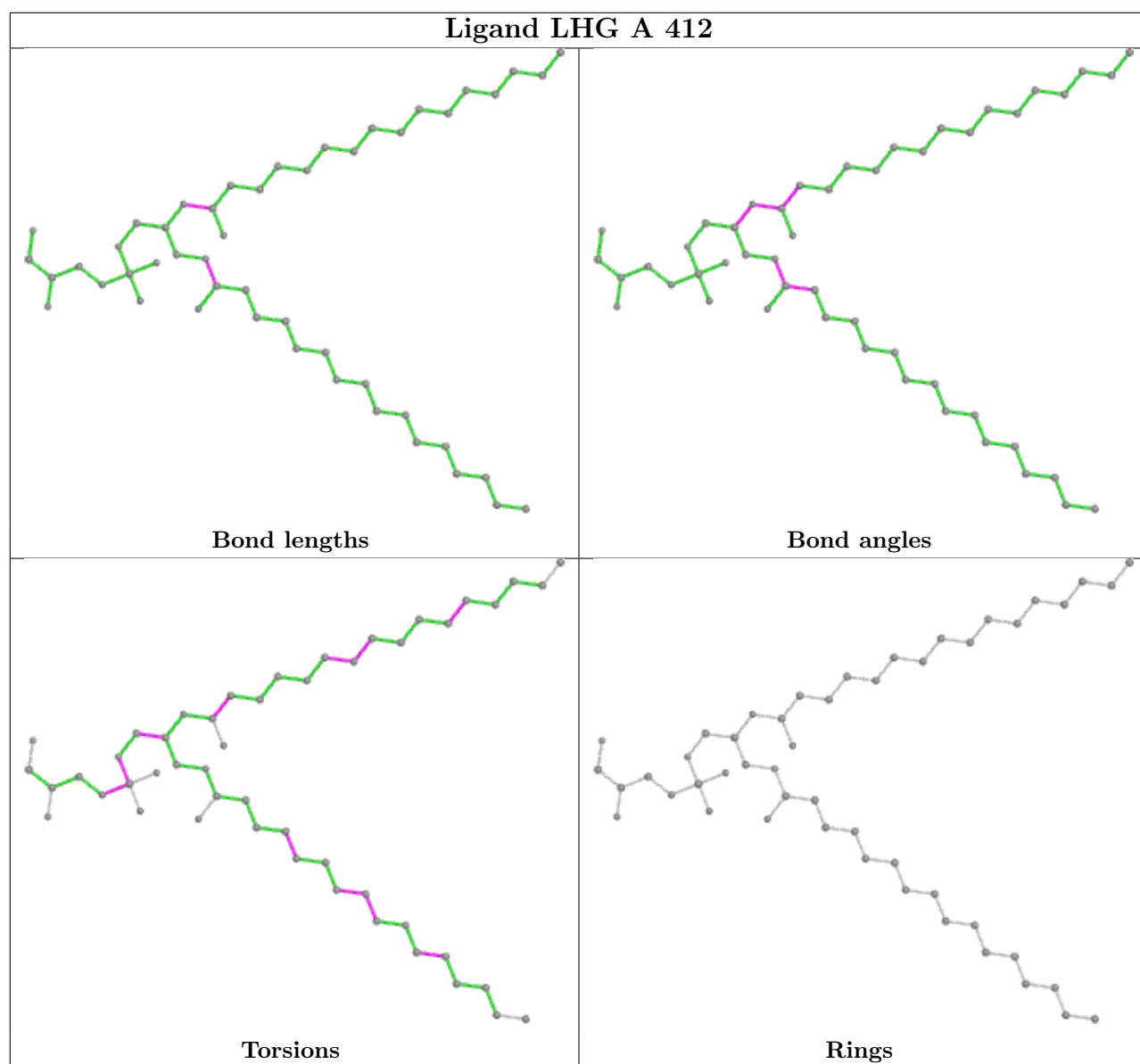


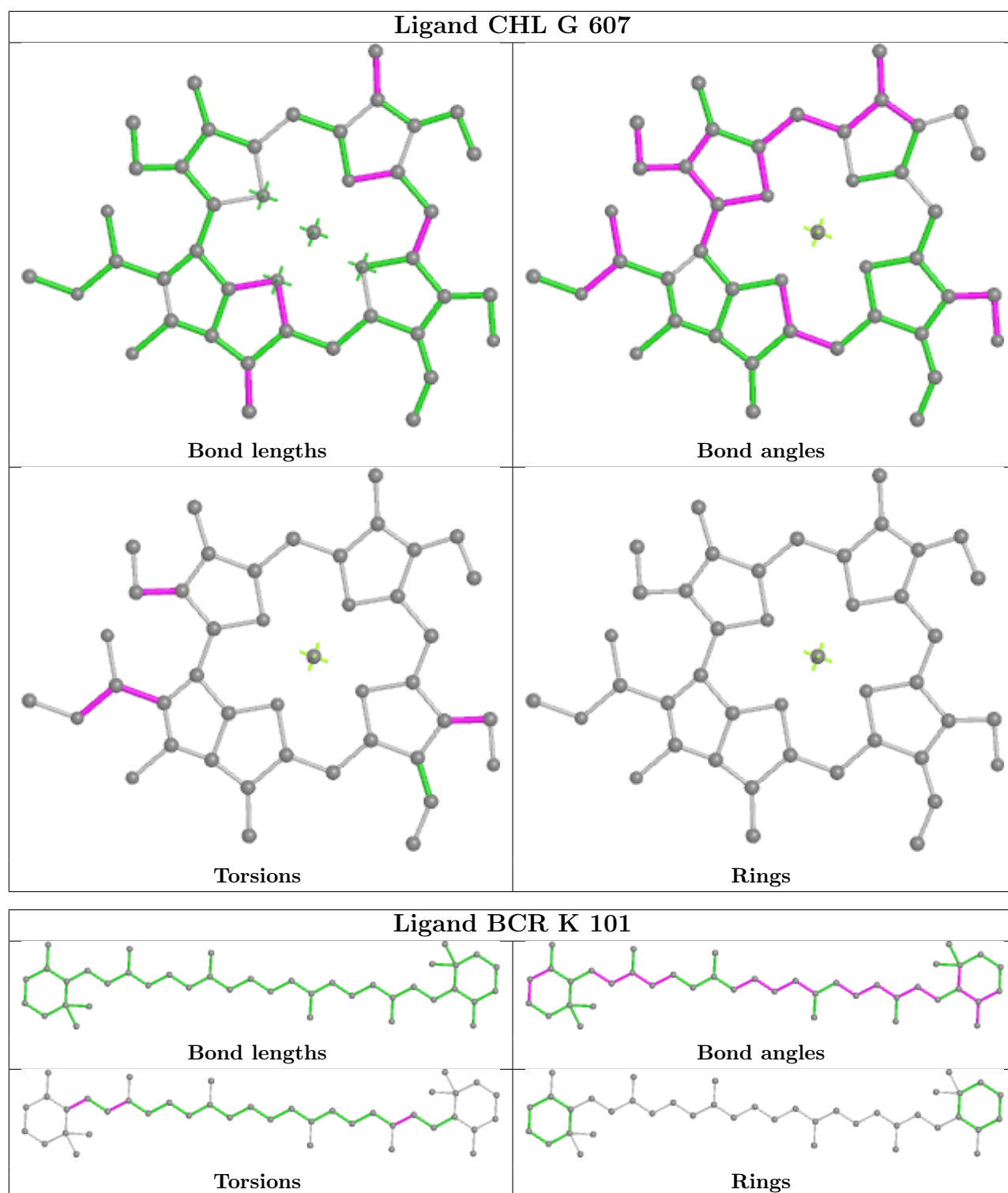
Ligand CLA g 614

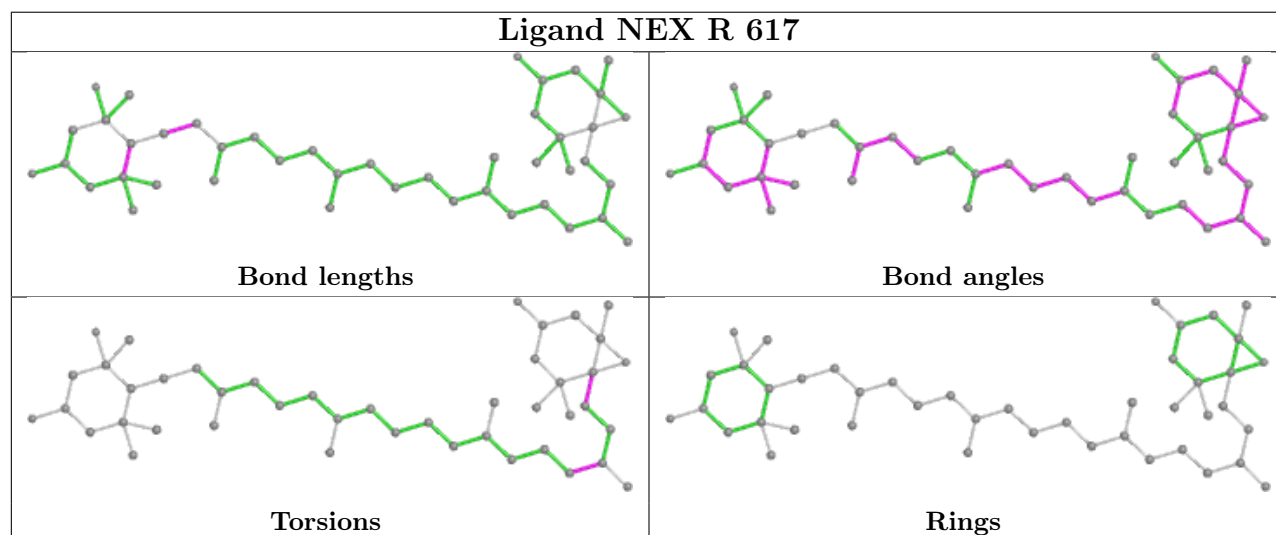
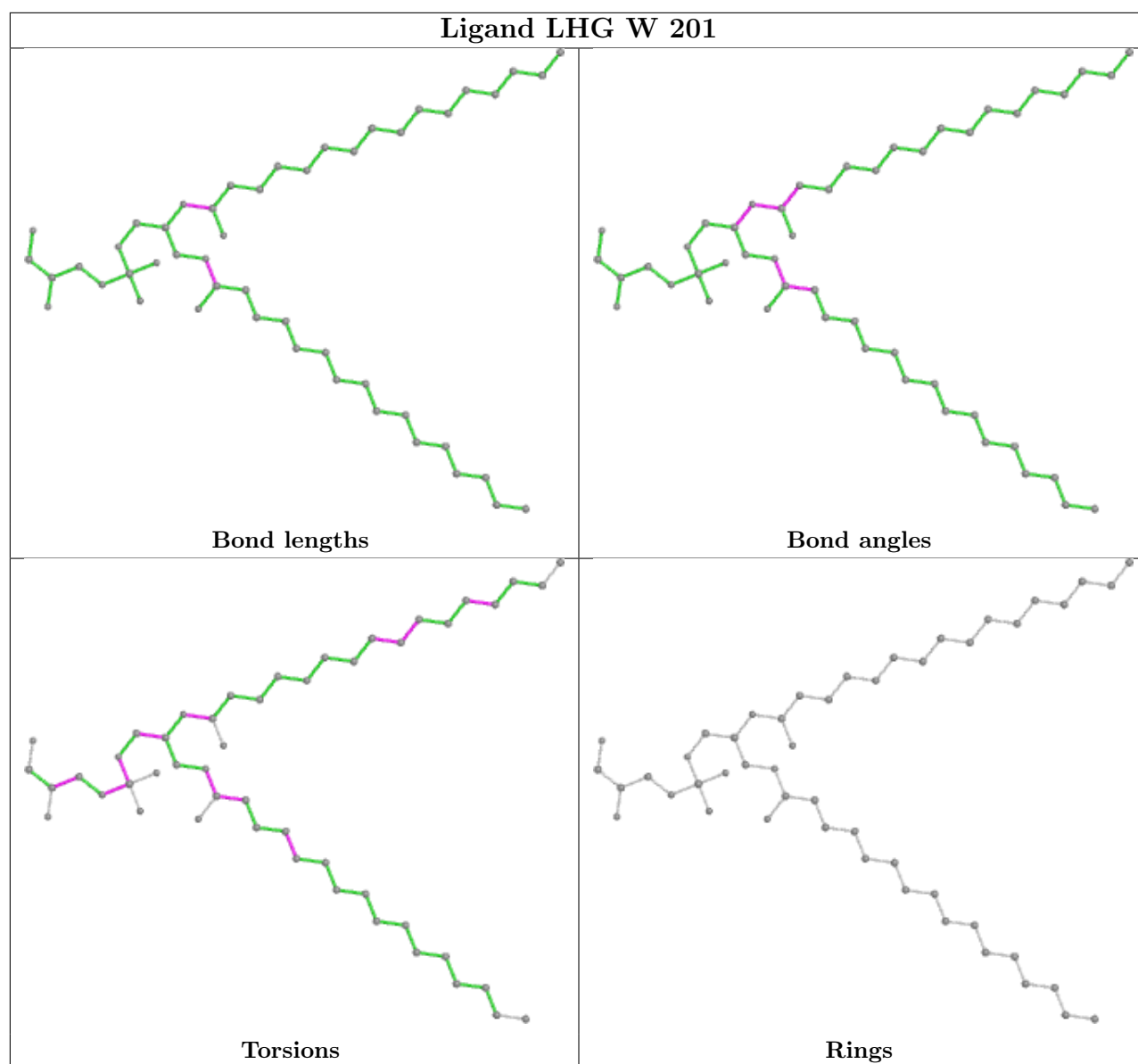




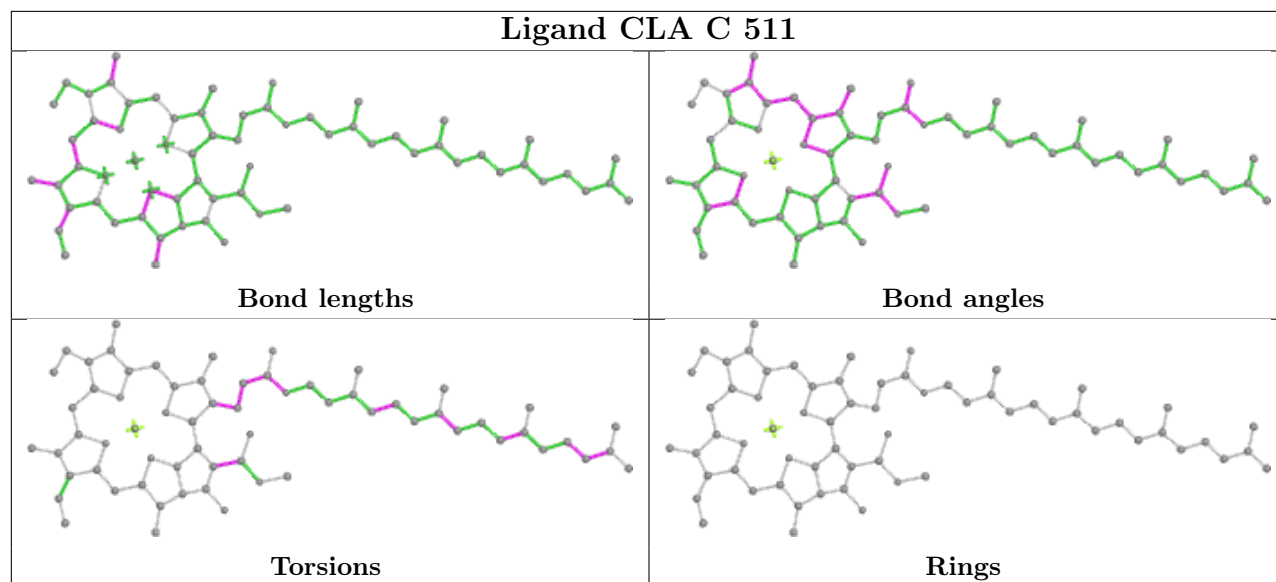




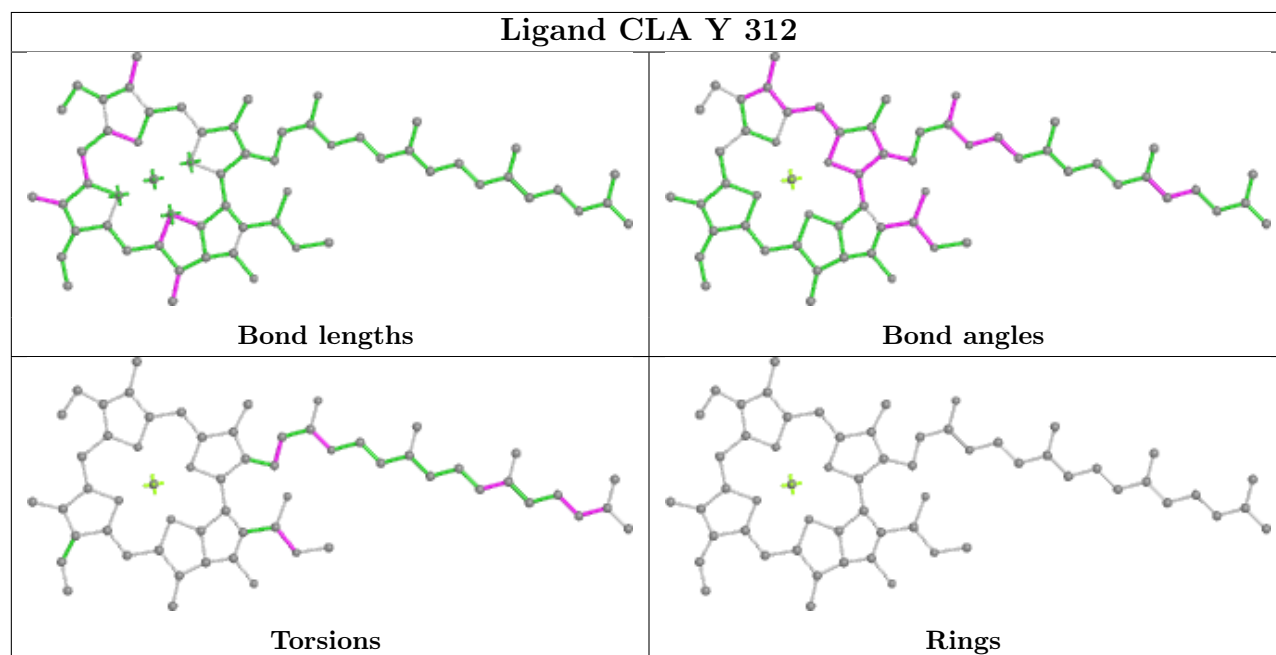




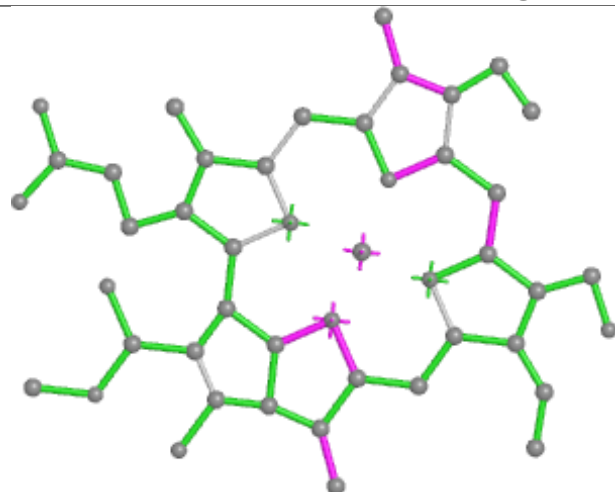
Ligand CLA C 511



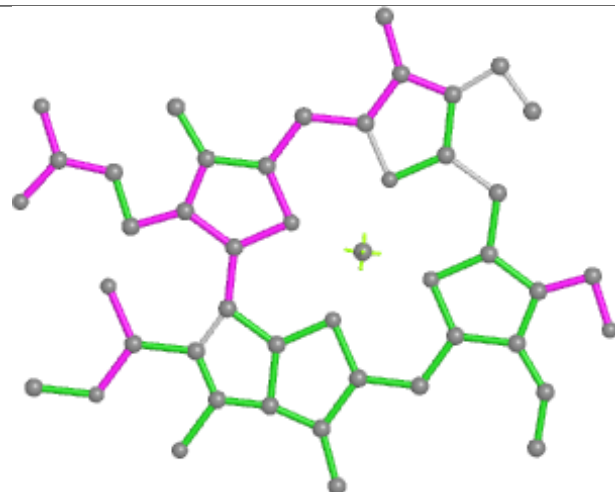
Ligand CLA Y 312



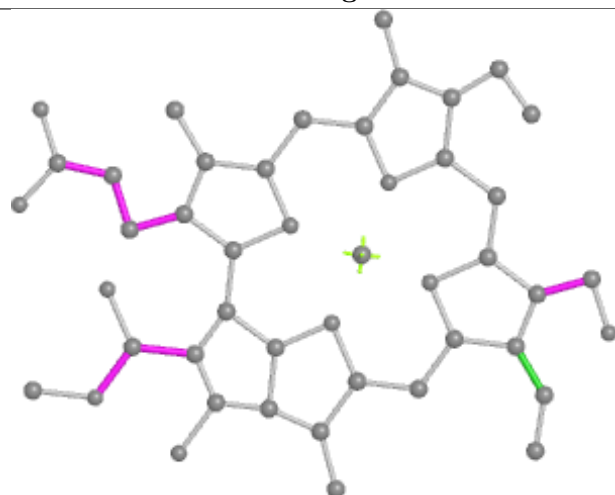
Ligand CHL N 308



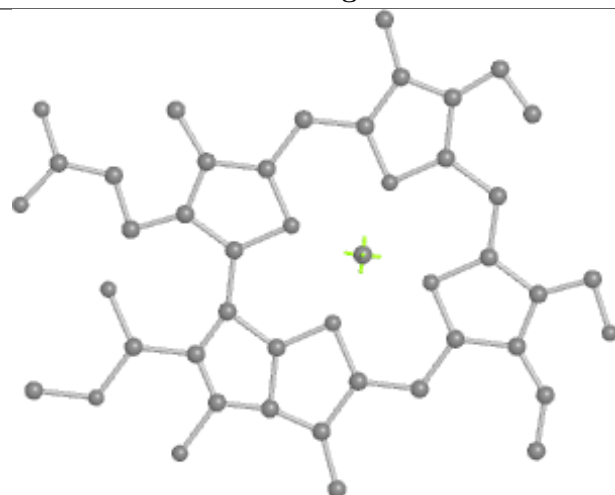
Bond lengths



Bond angles

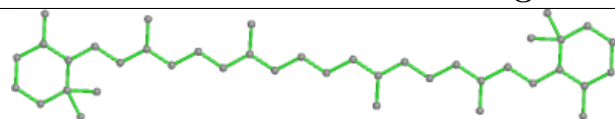


Torsions

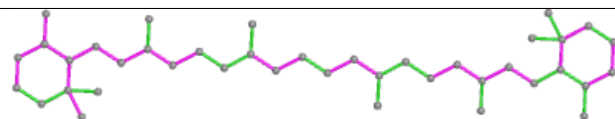


Rings

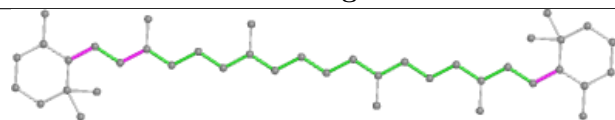
Ligand BCR B 619



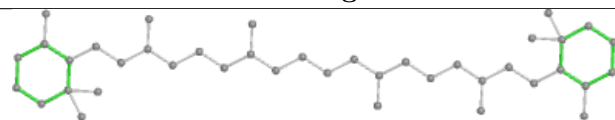
Bond lengths



Bond angles

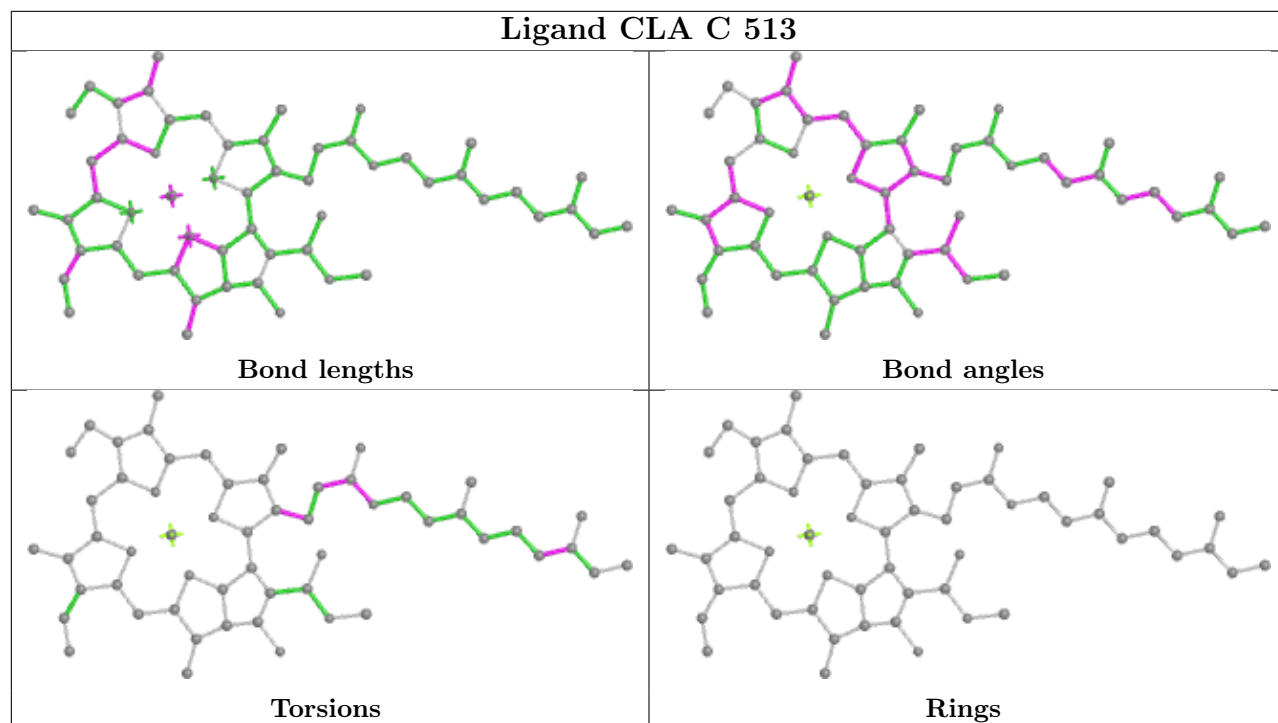


Torsions

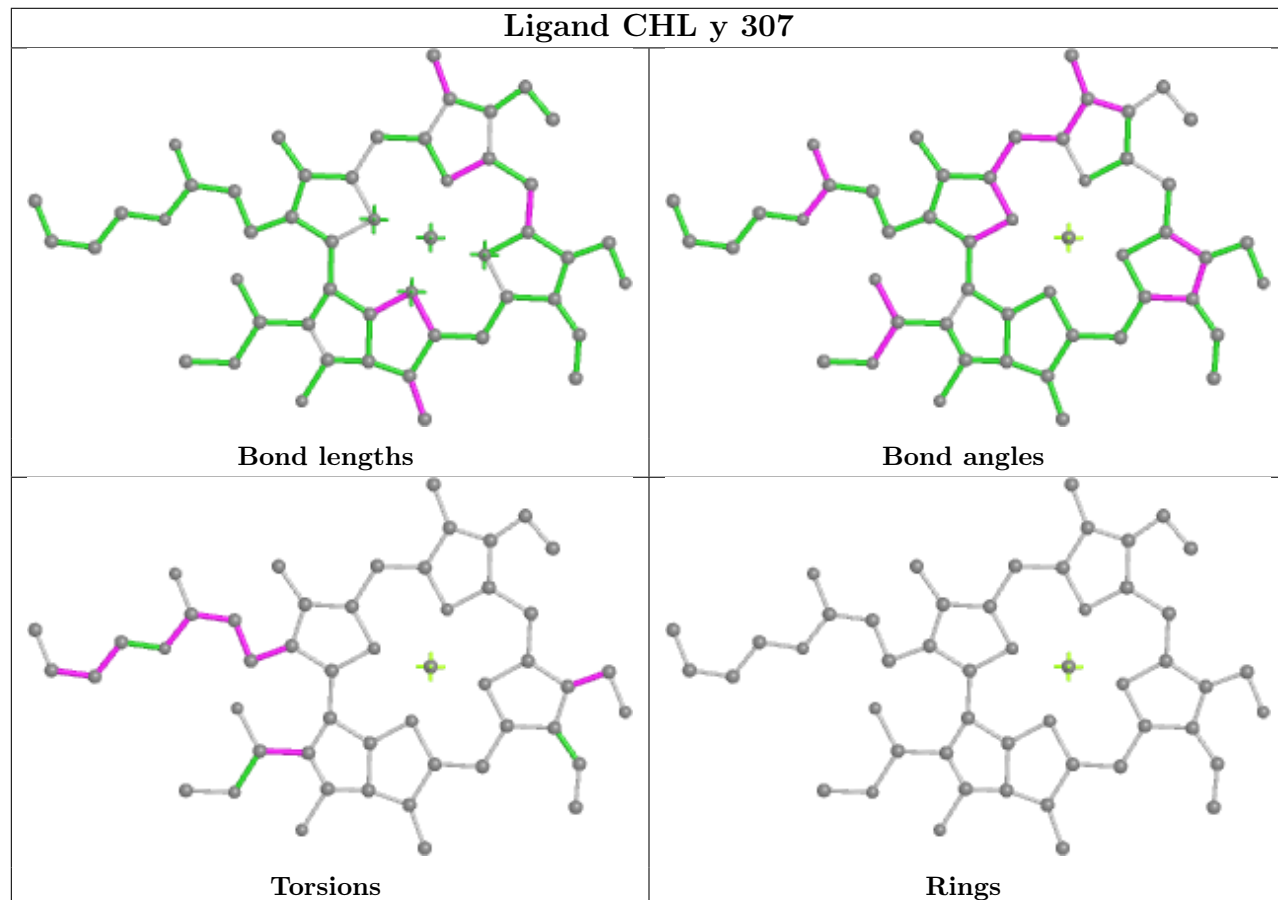


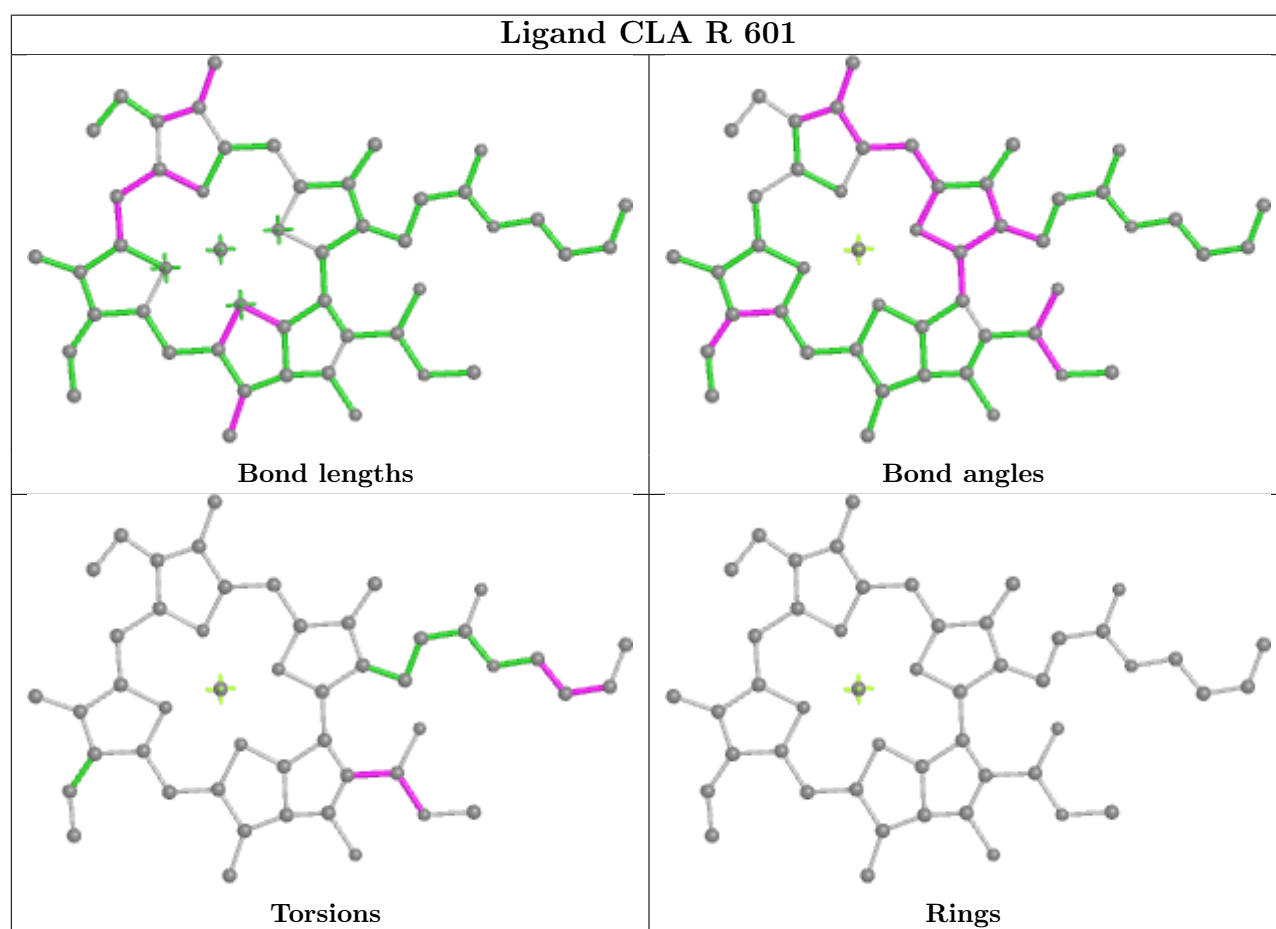
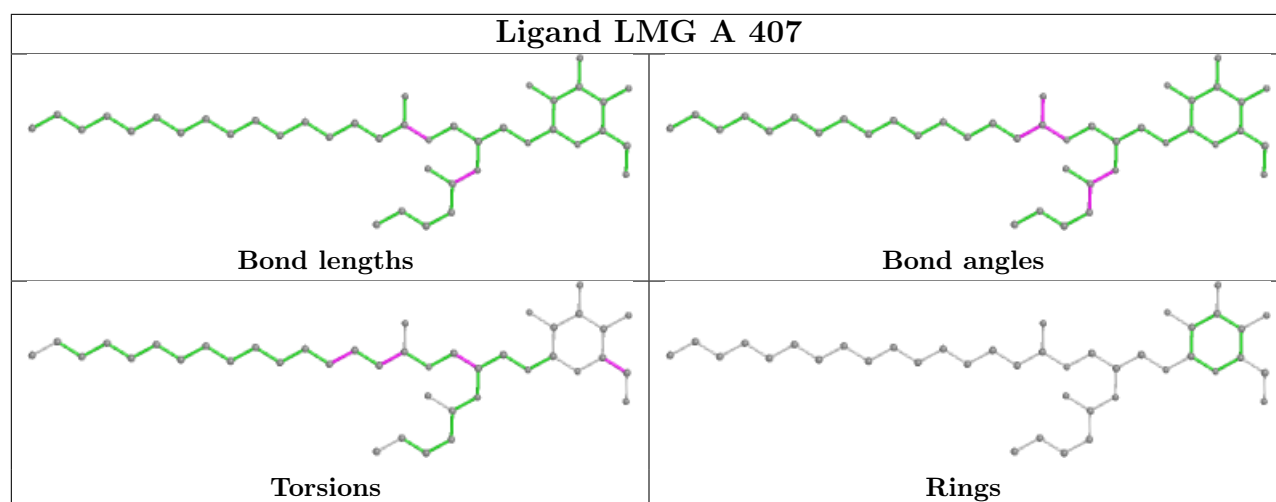
Rings

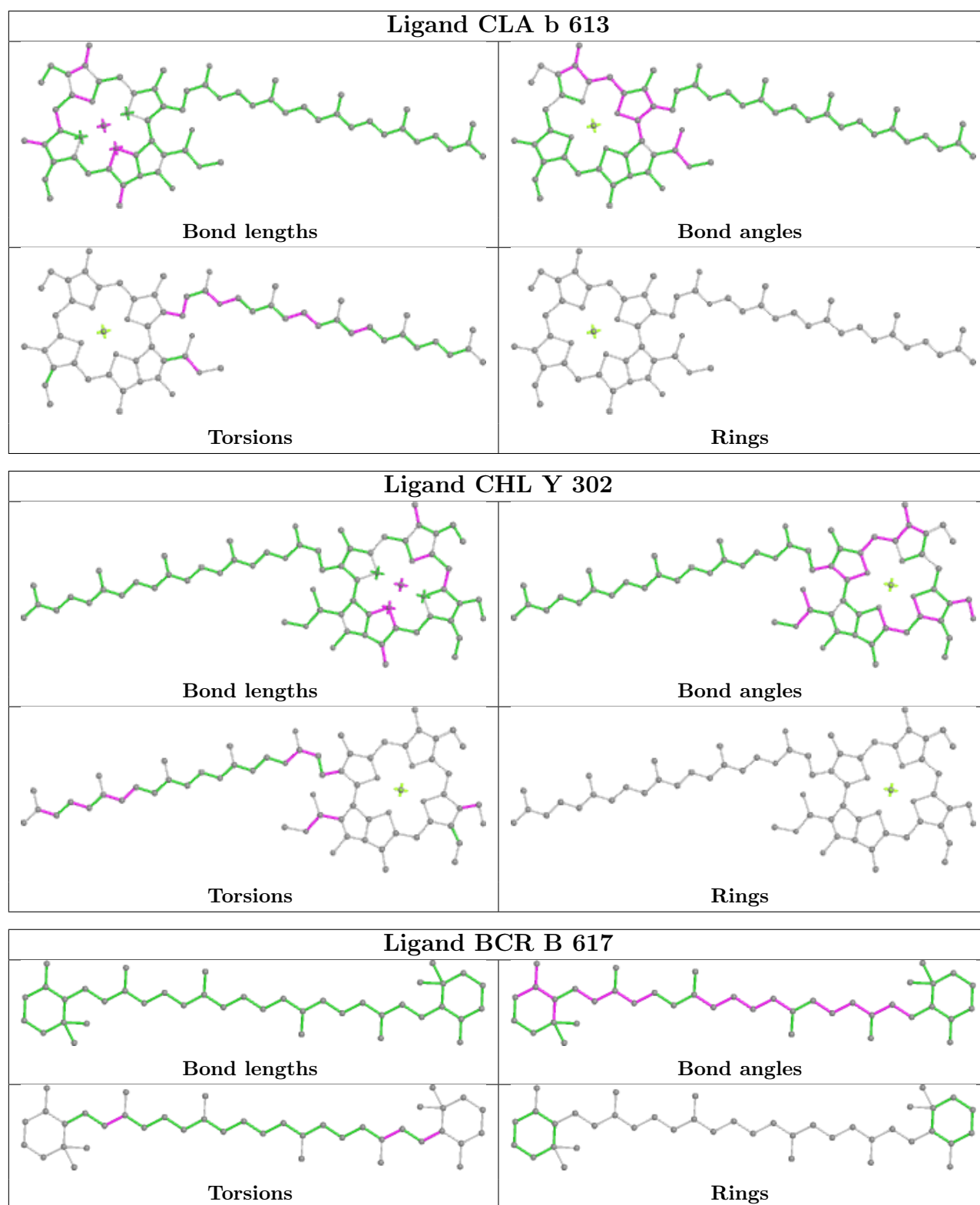
Ligand CLA C 513

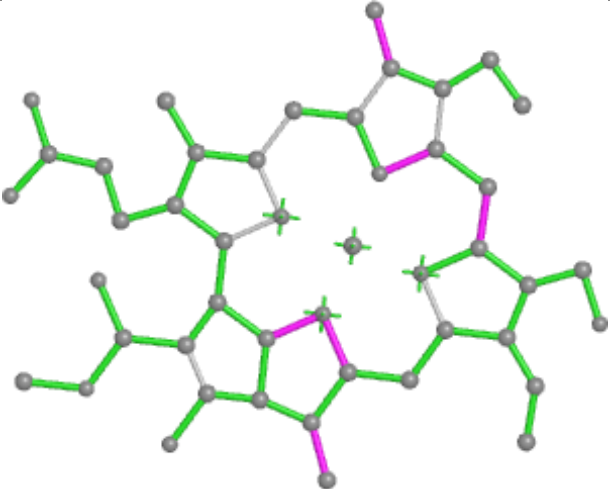
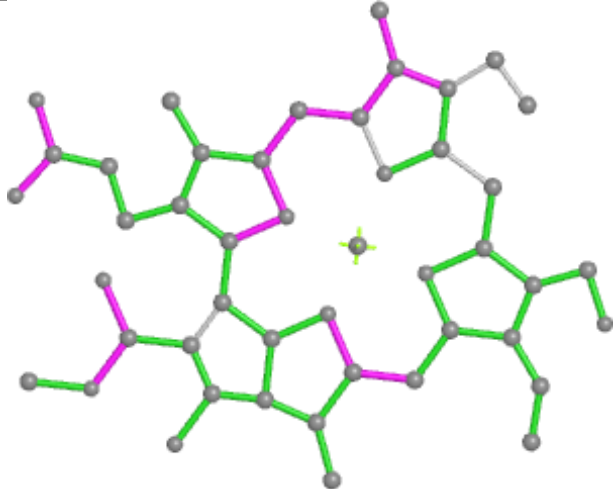
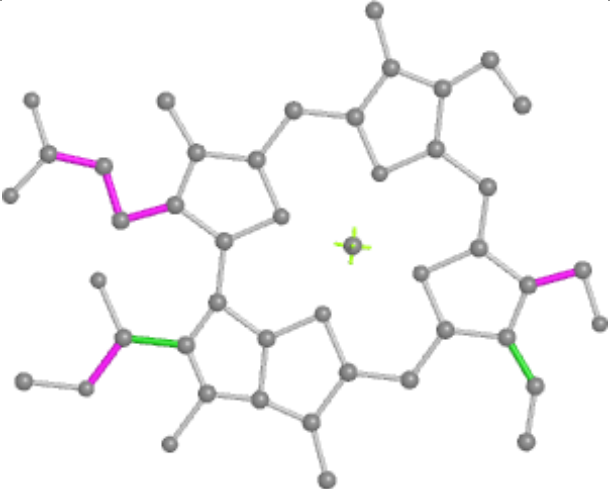
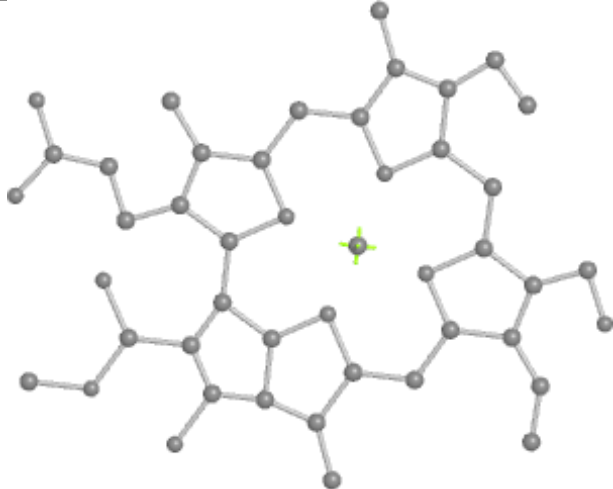


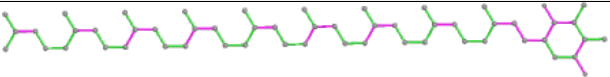
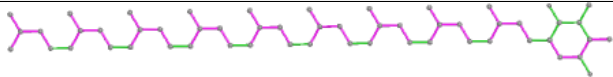
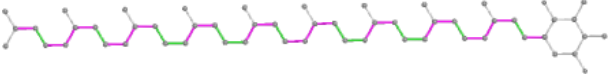
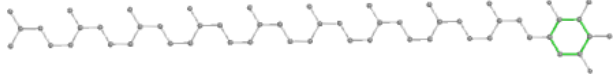
Ligand CHL y 307



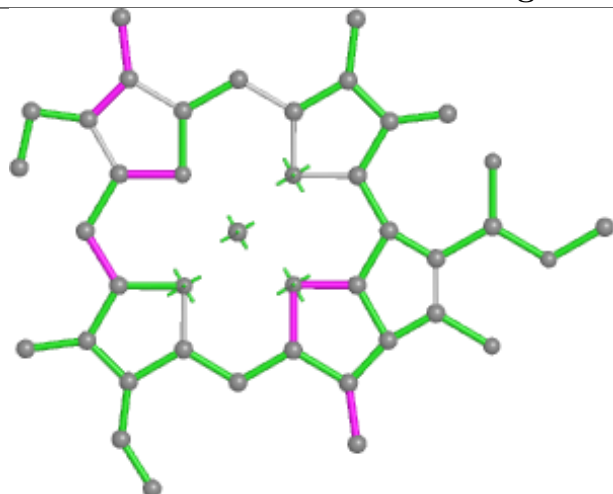




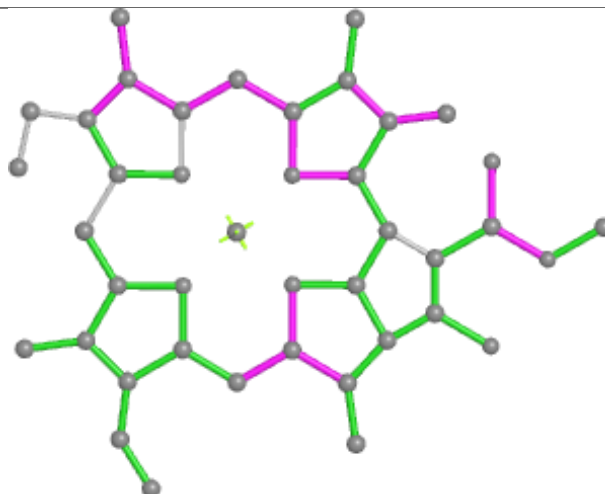
Ligand CHL s 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 613



Bond lengths



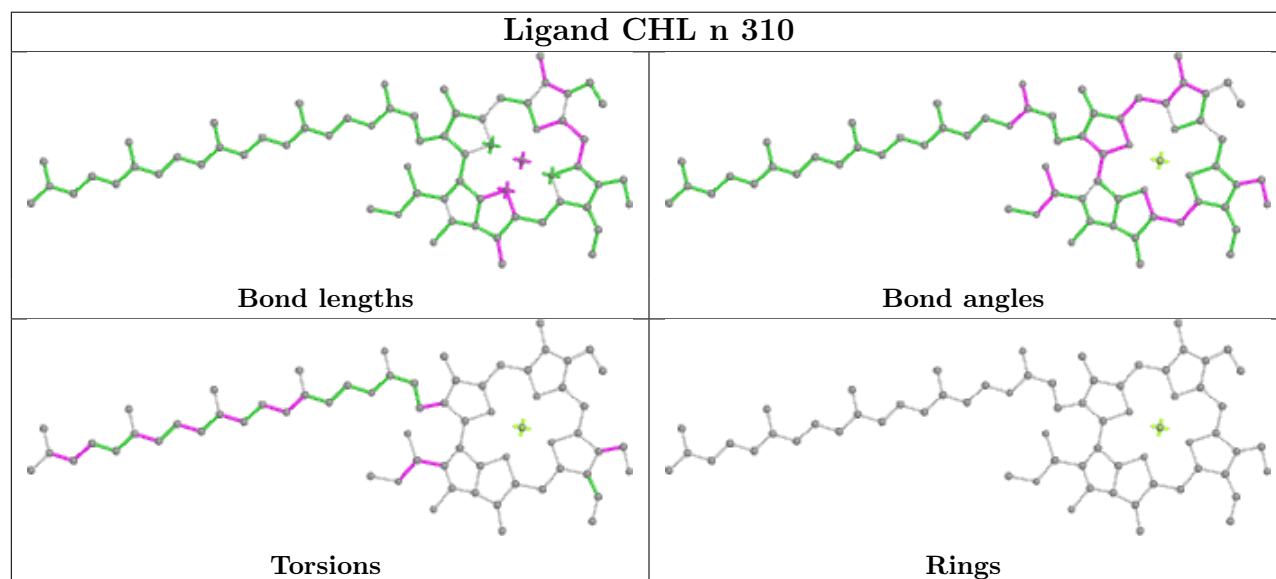
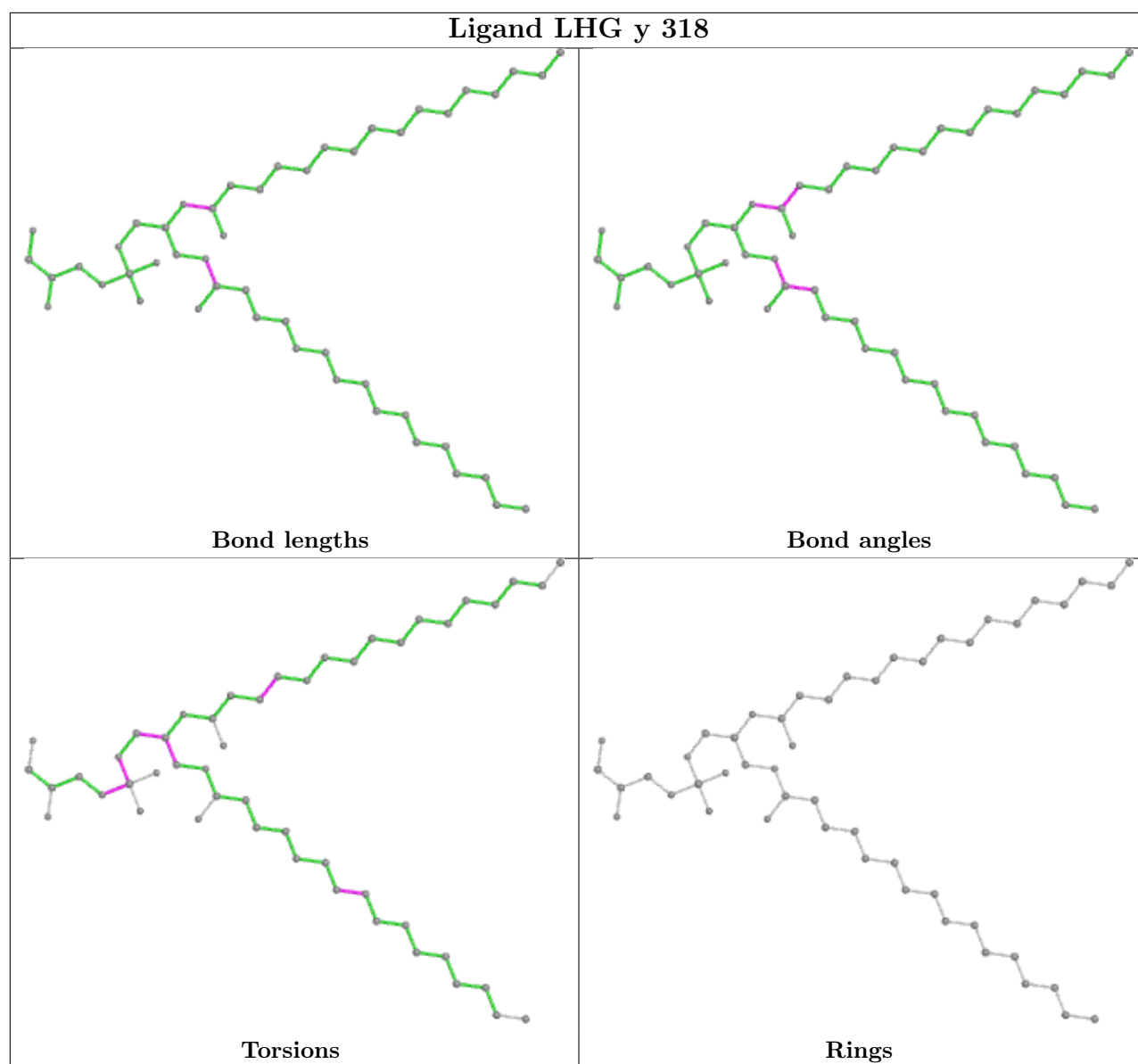
Bond angles

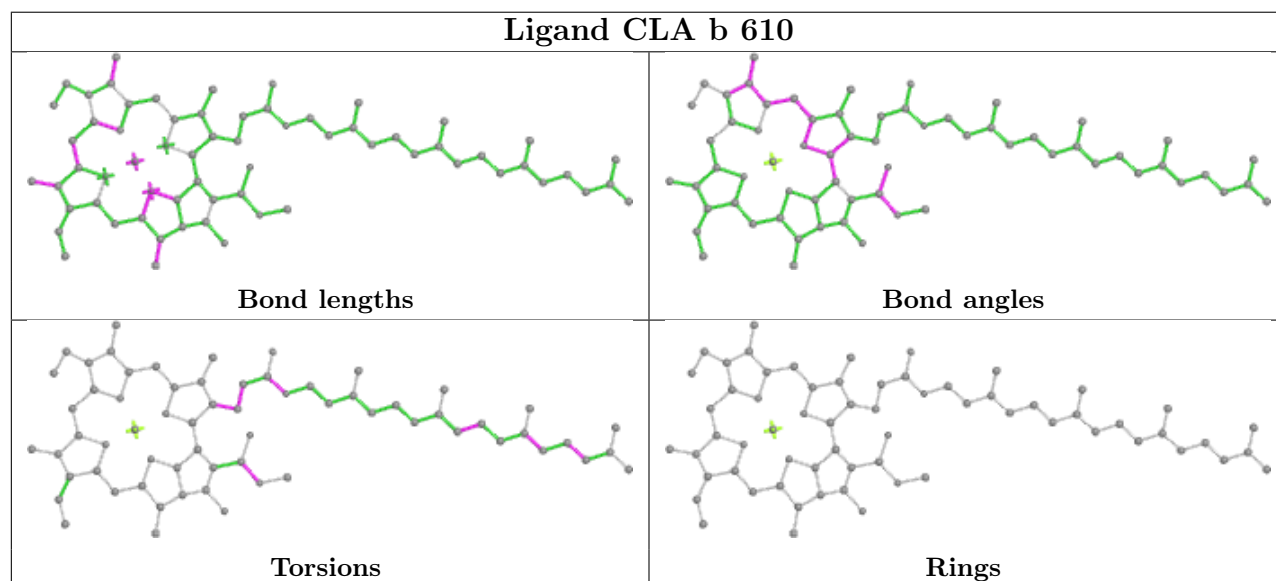
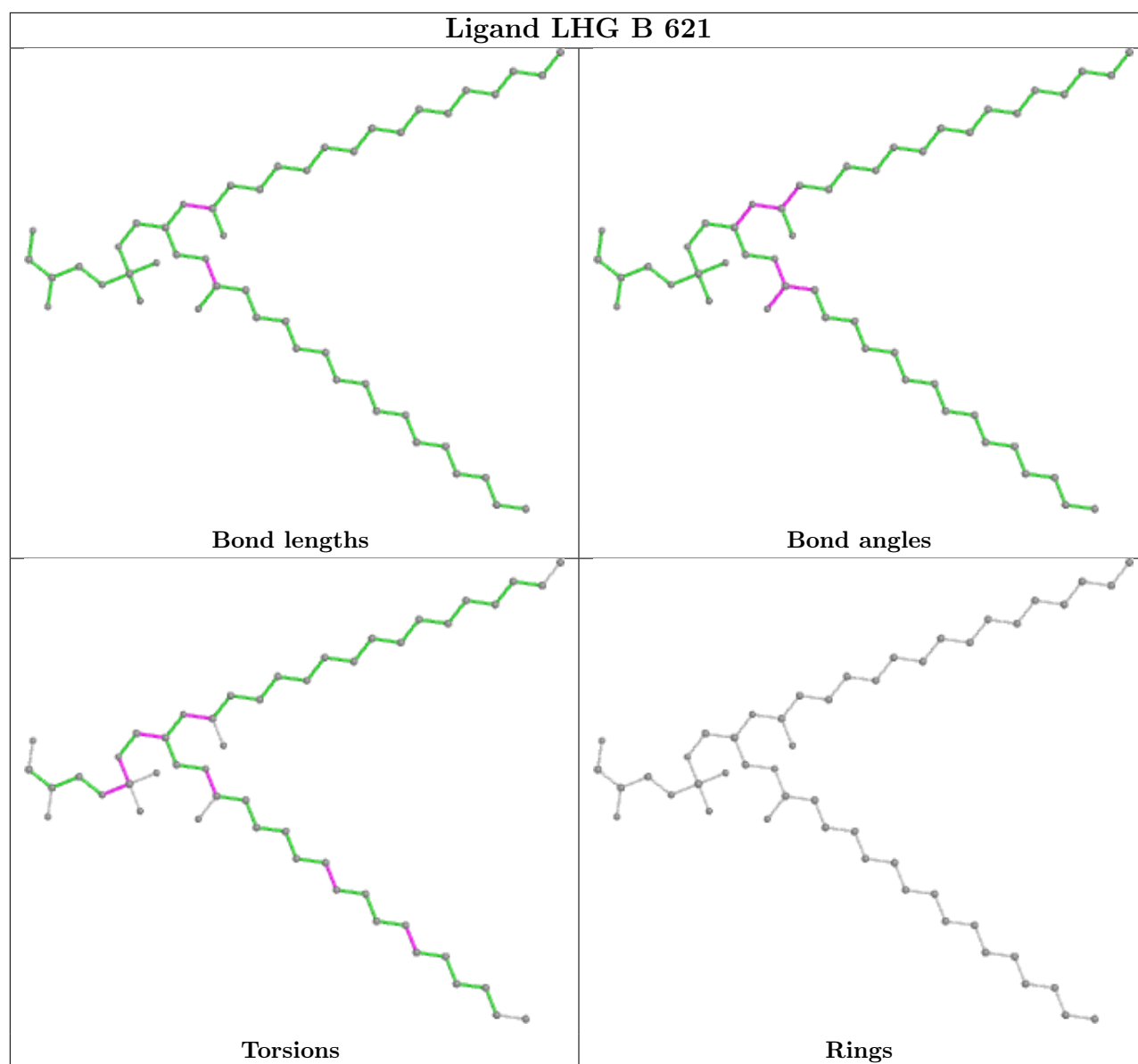


Torsions

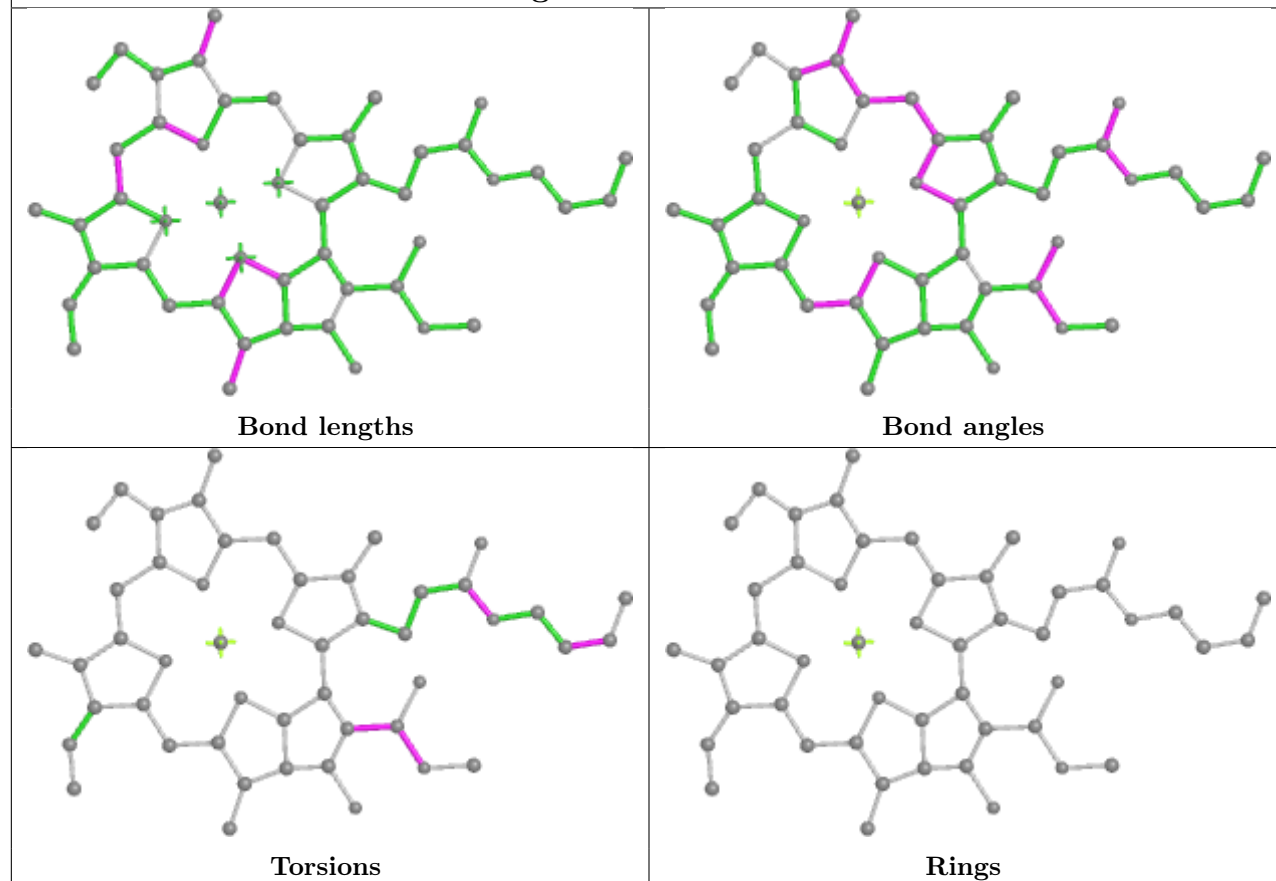


Rings

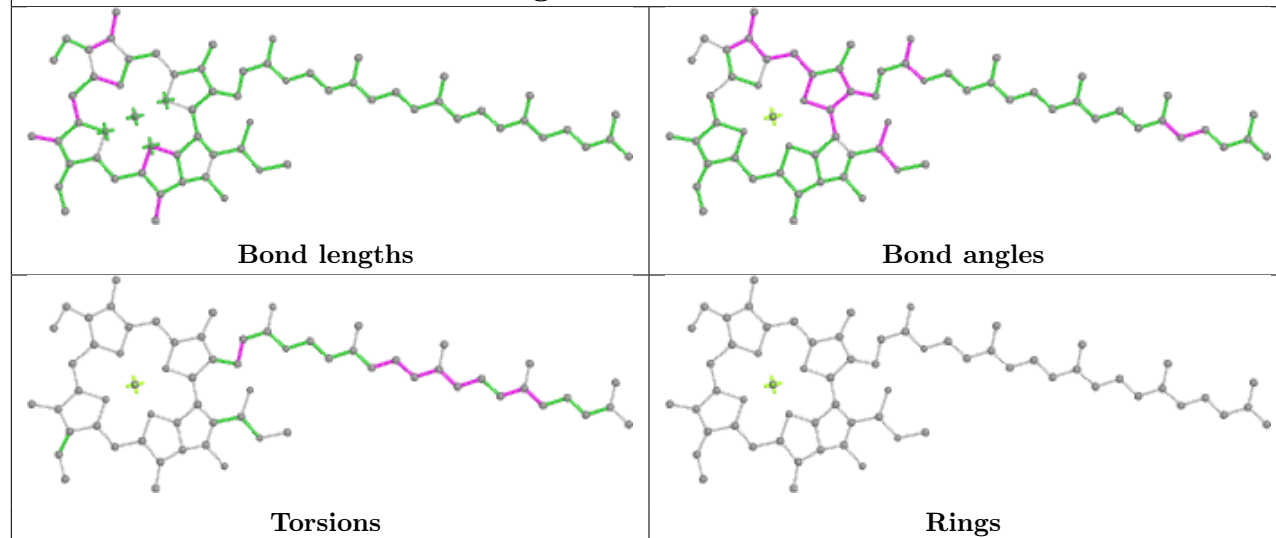




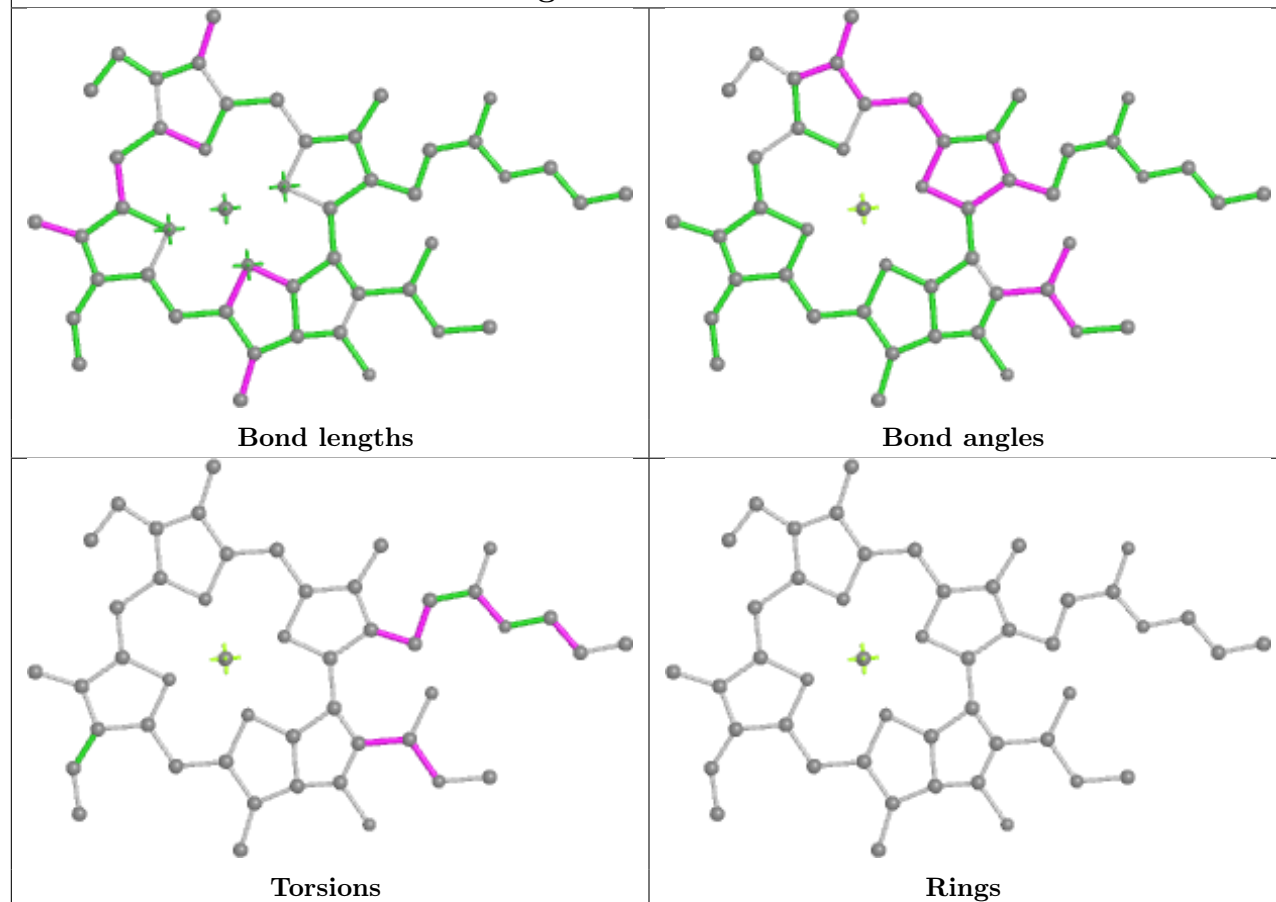
Ligand CLA R 610



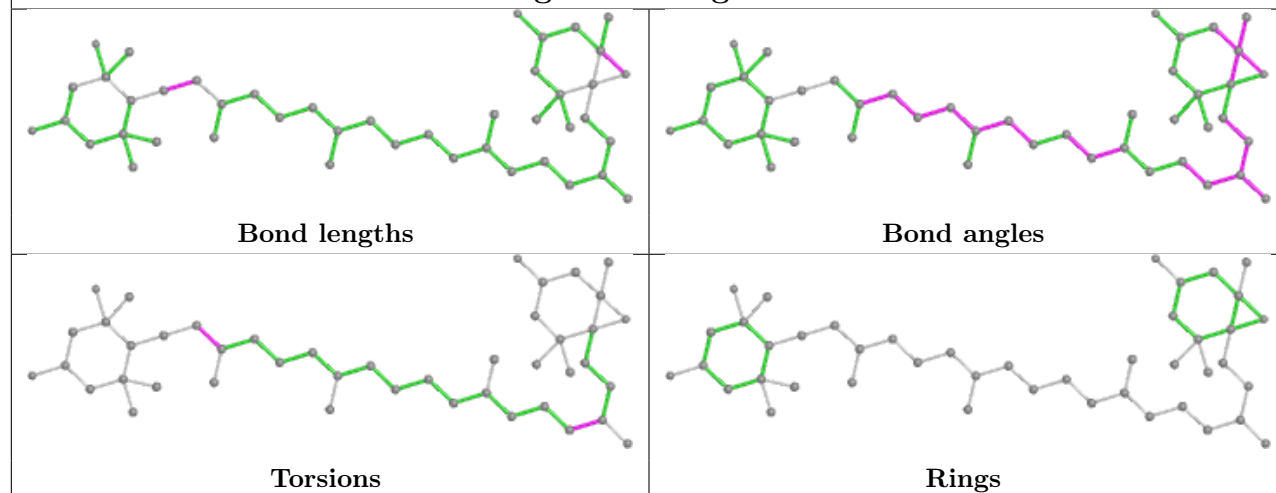
Ligand CLA B 615

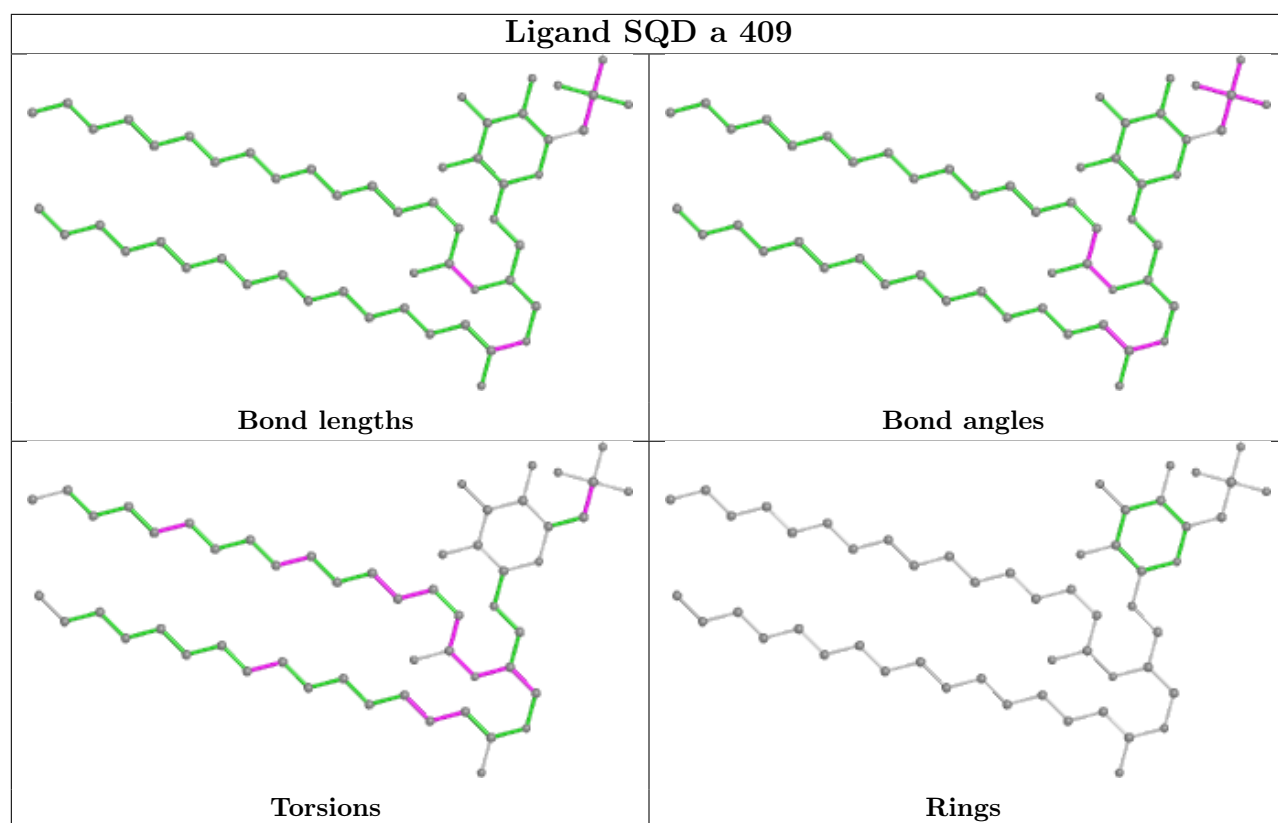


Ligand CLA r 604

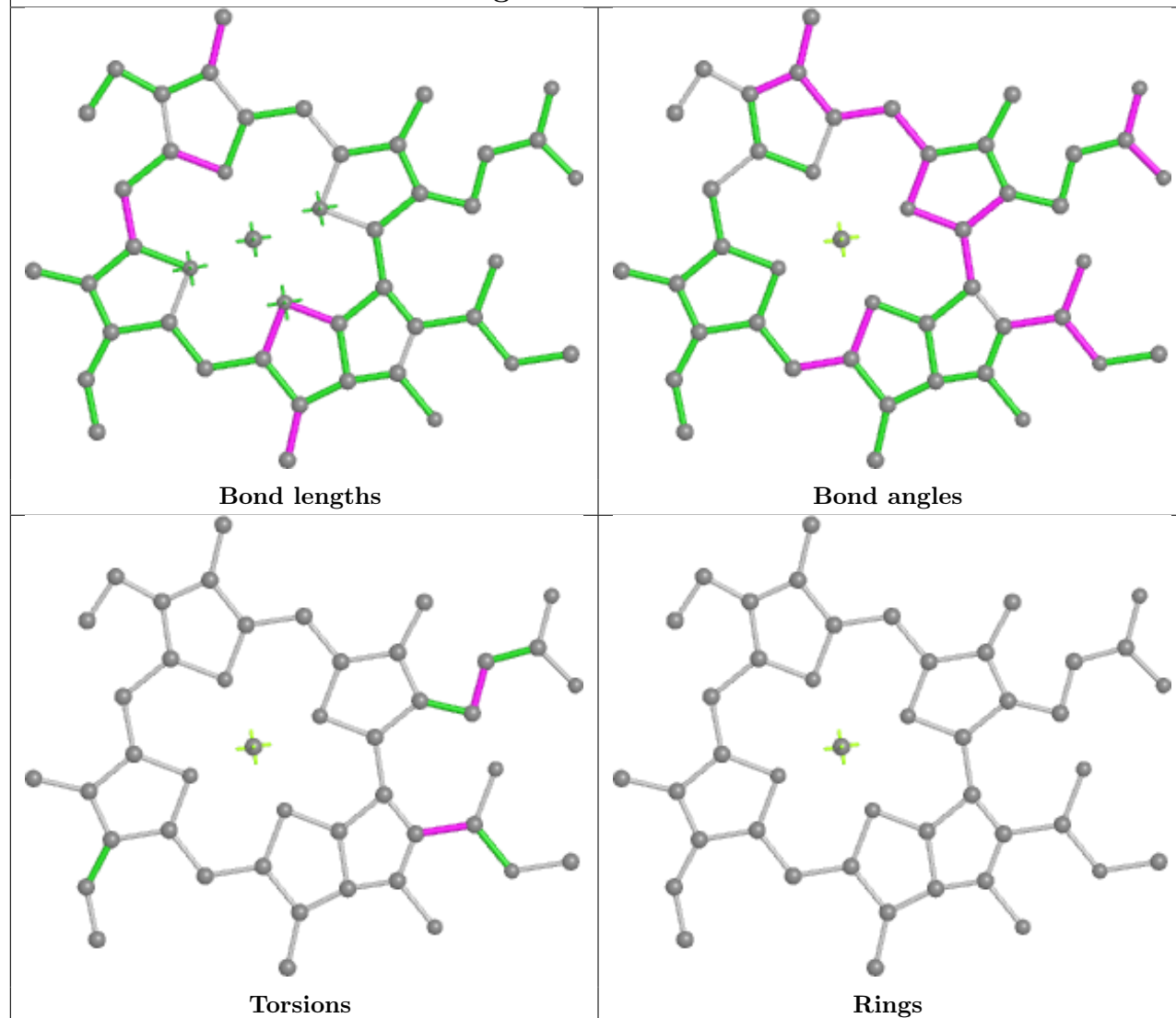


Ligand NEX g 617

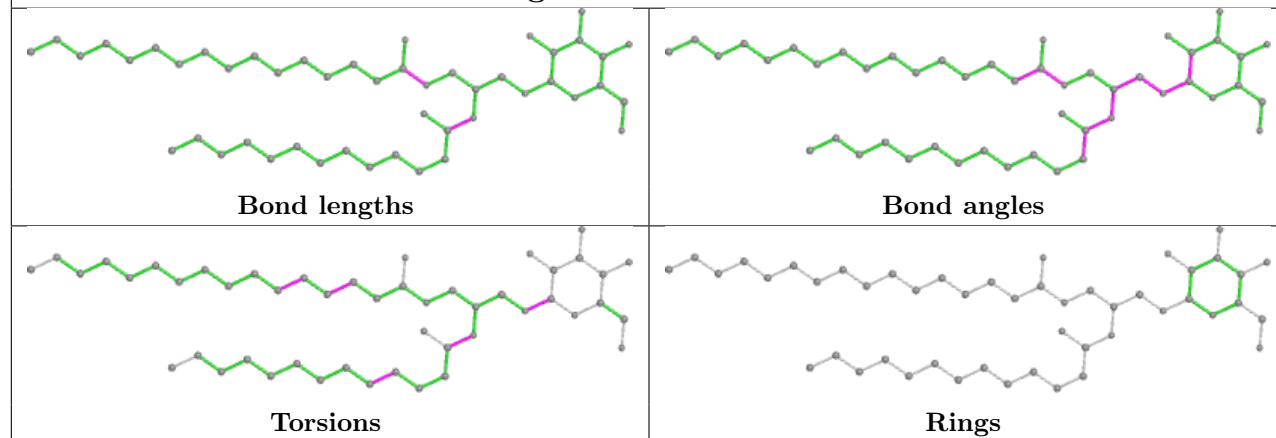


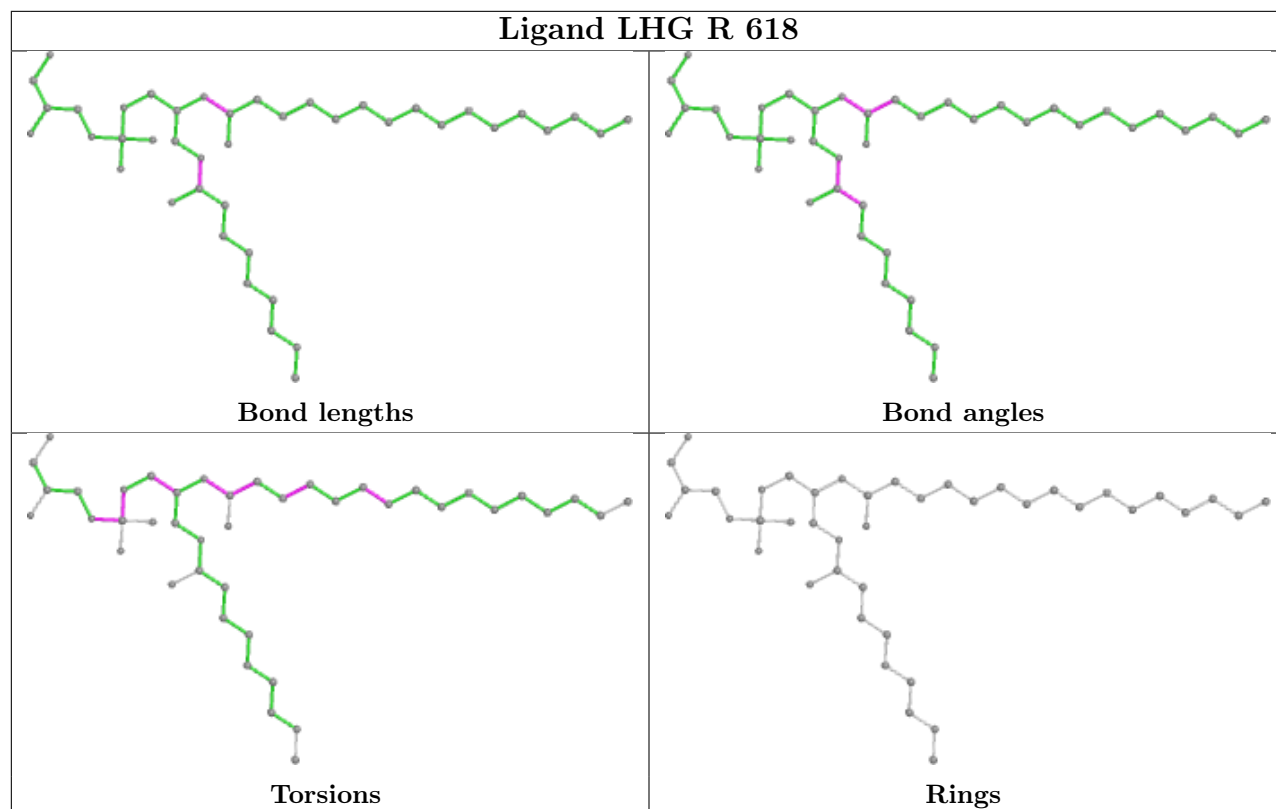
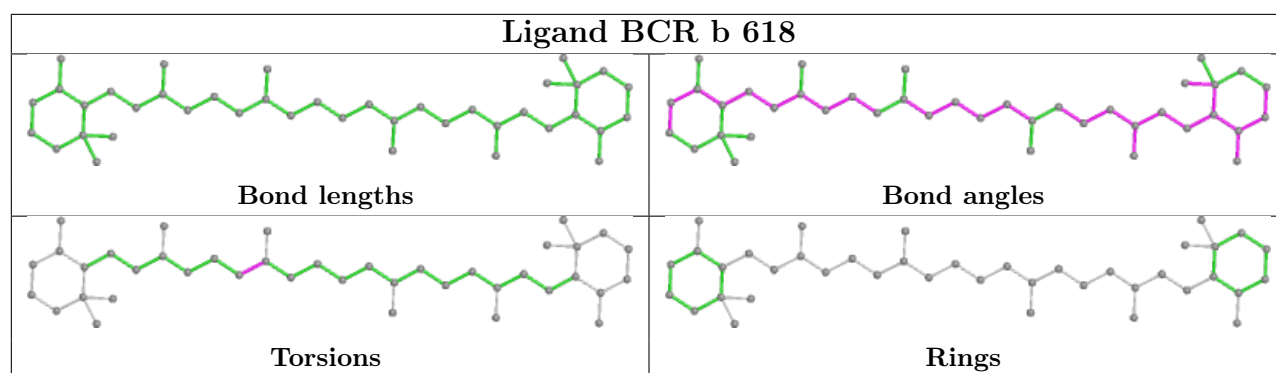


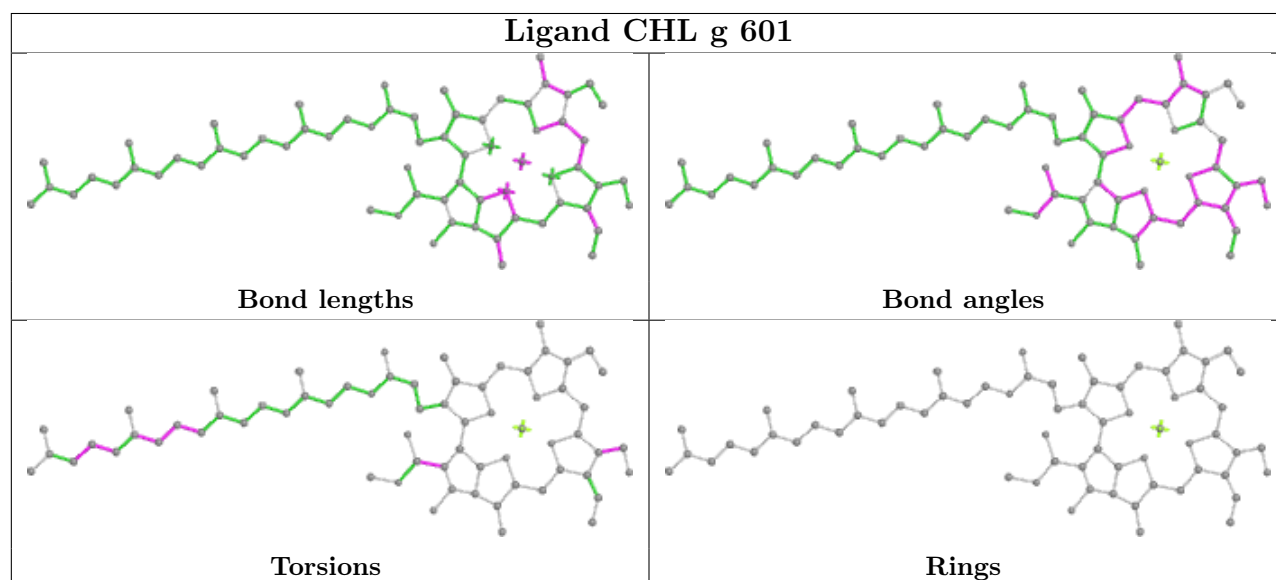
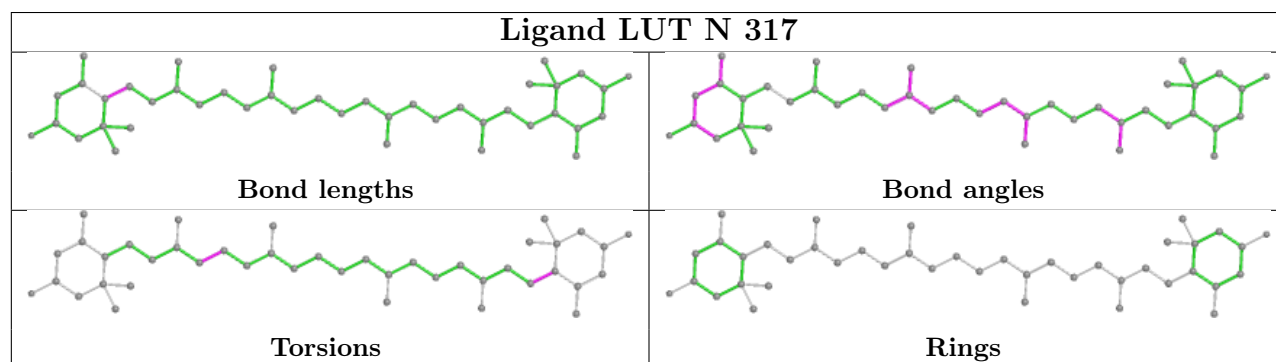
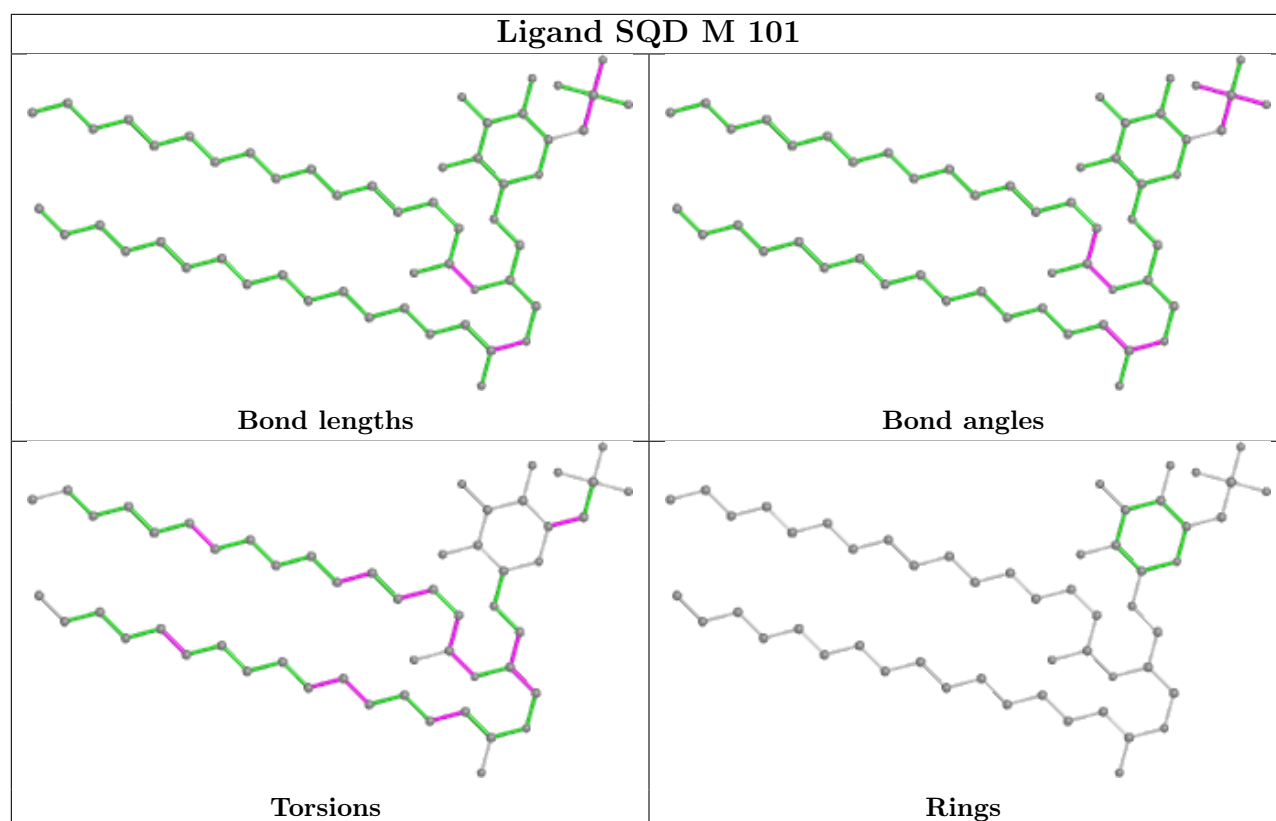
Ligand CLA S 608



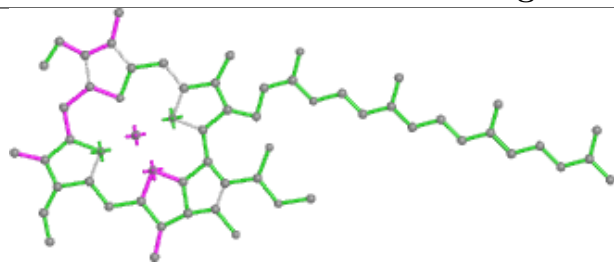
Ligand LMG C 501



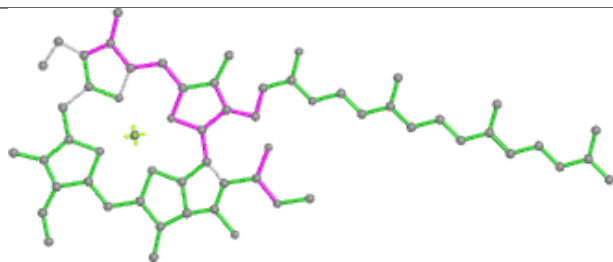




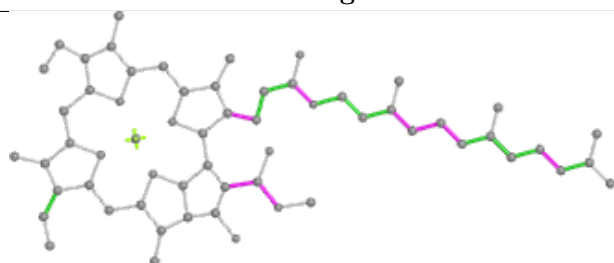
Ligand CLA n 314



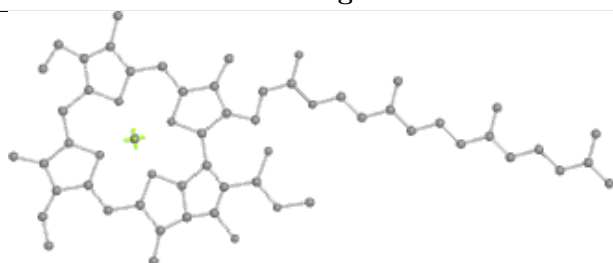
Bond lengths



Bond angles

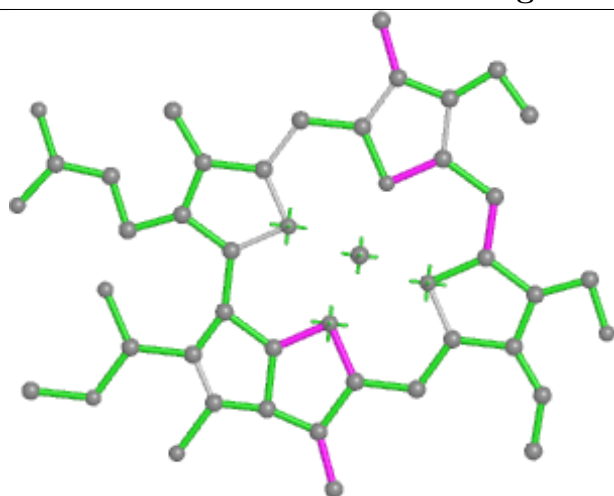


Torsions

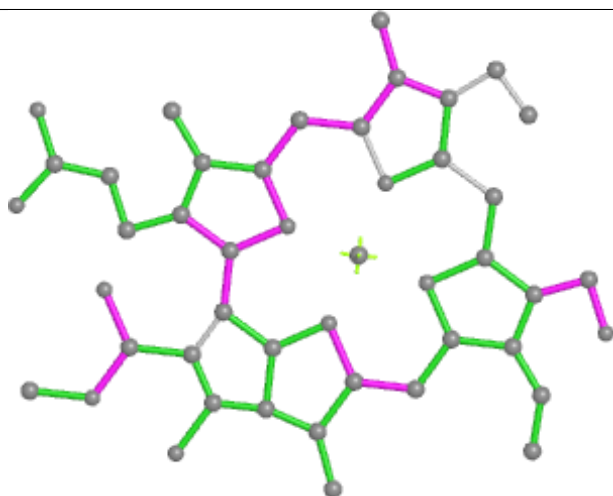


Rings

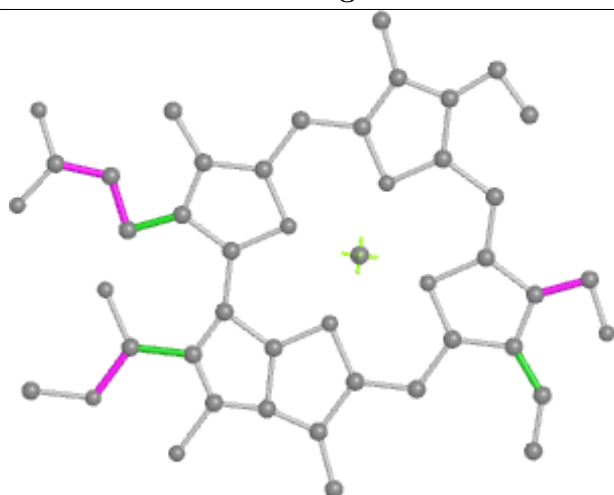
Ligand CHL S 601



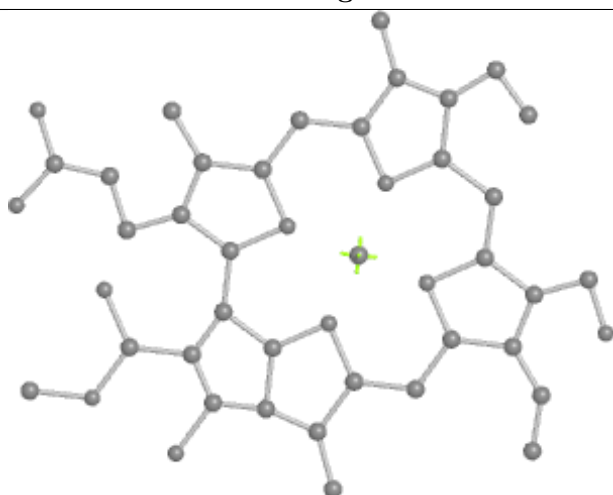
Bond lengths



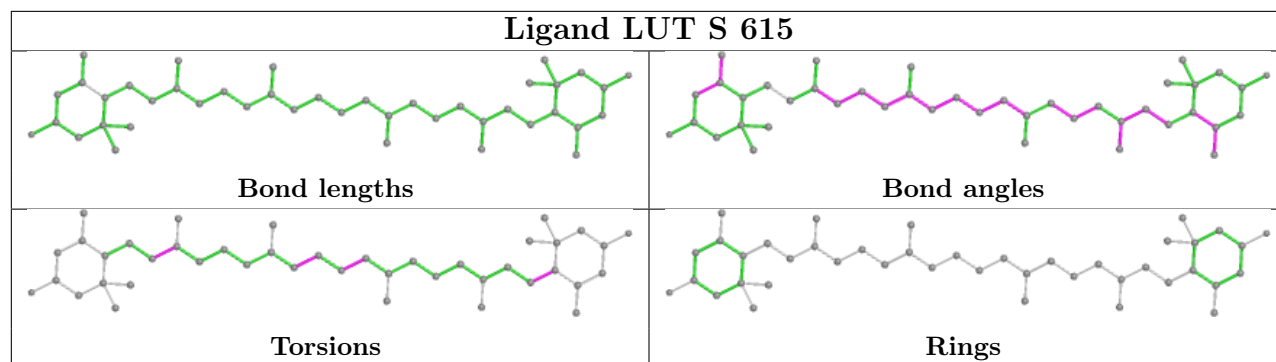
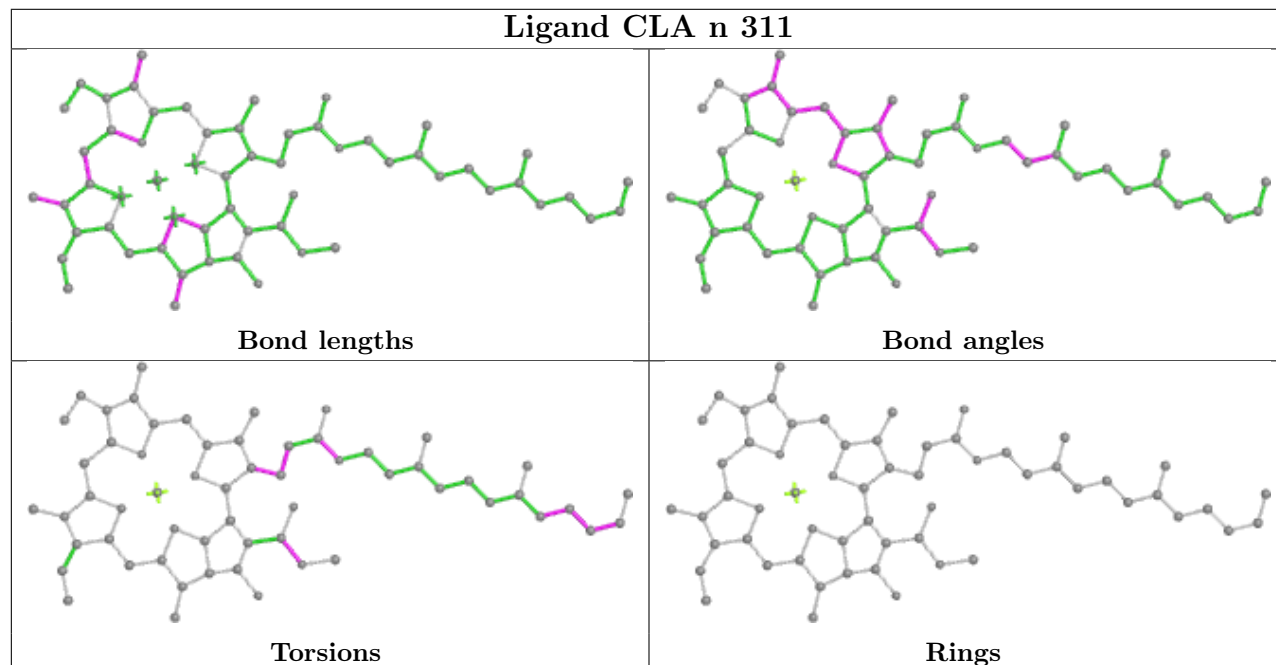
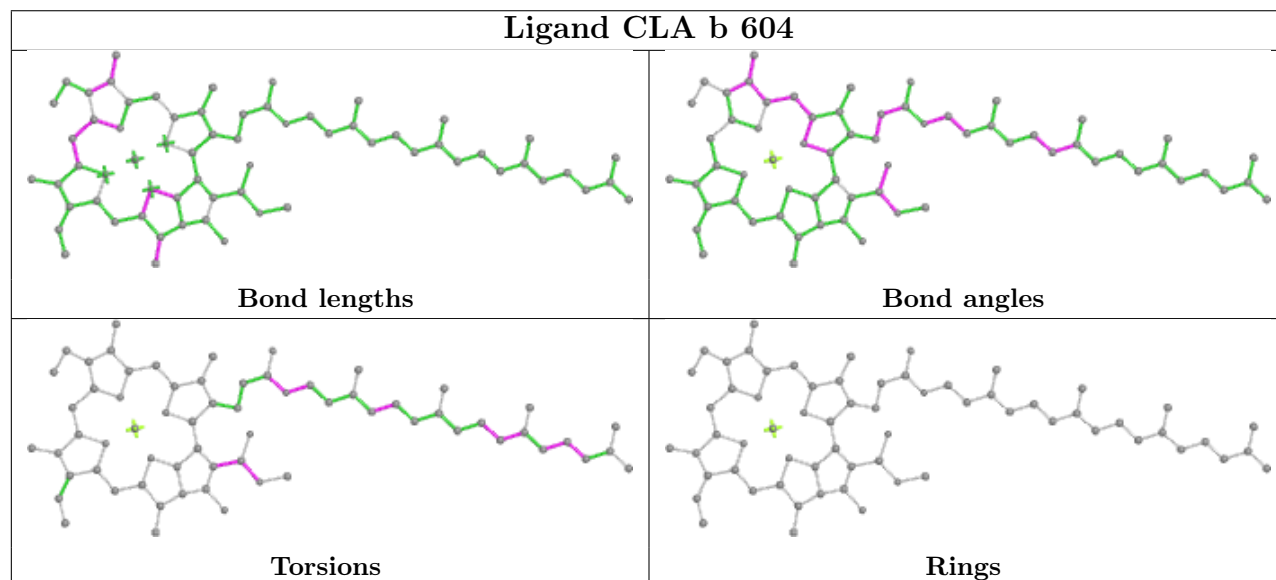
Bond angles



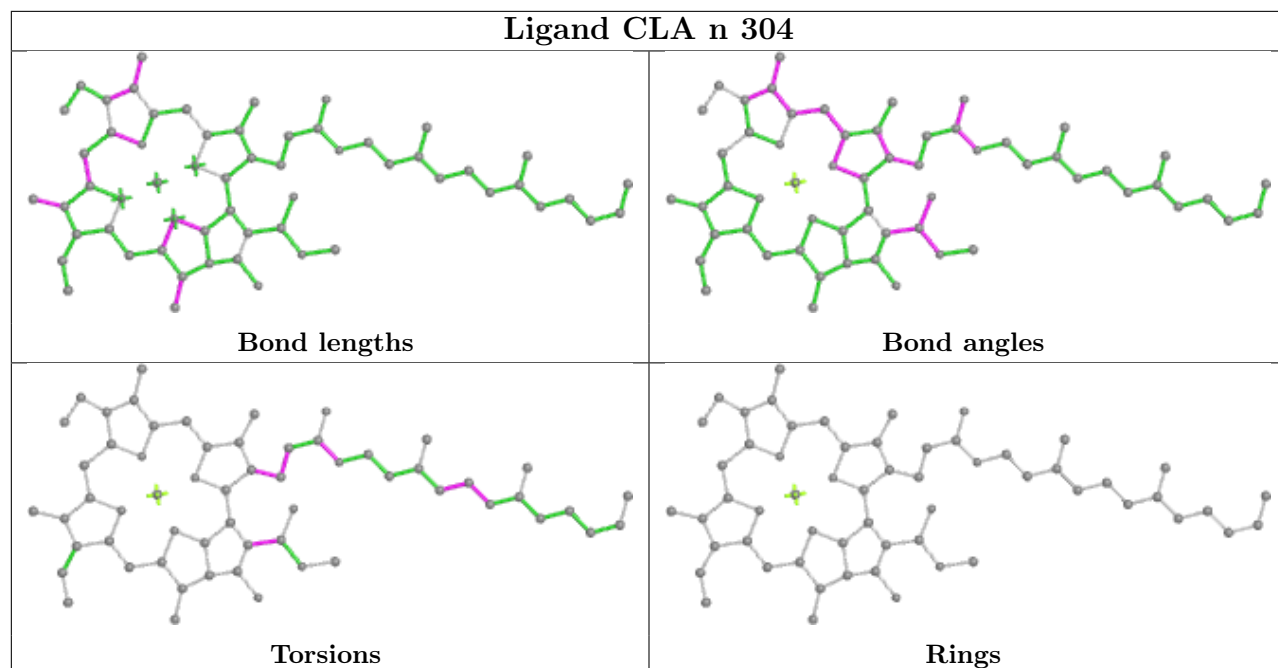
Torsions



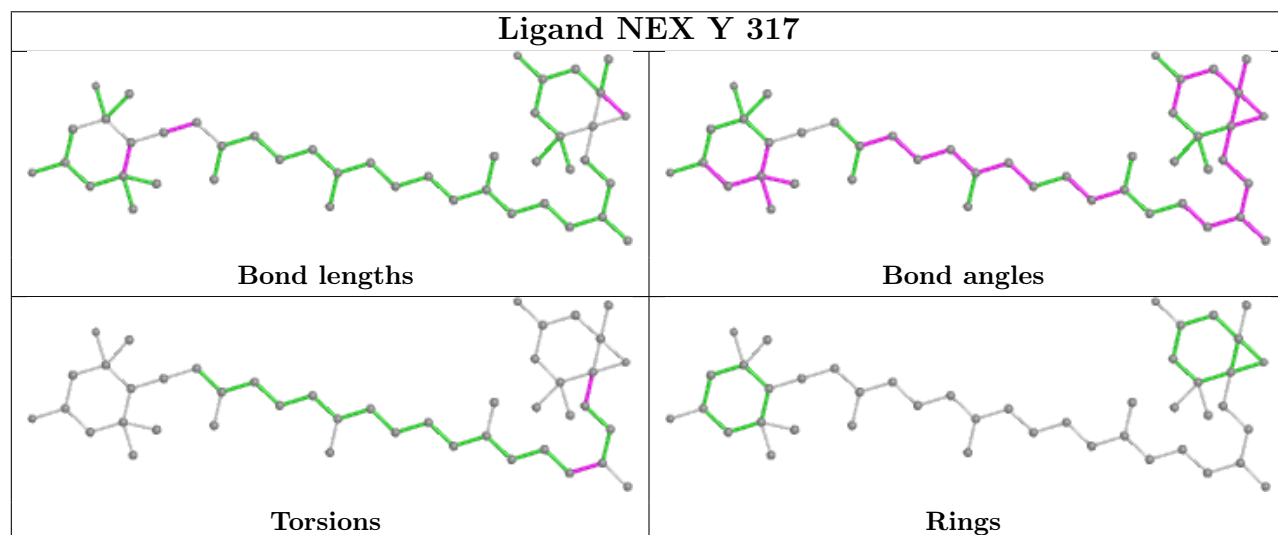
Rings

Ligand LUT S 615**Ligand CLA n 311****Ligand CLA b 604**

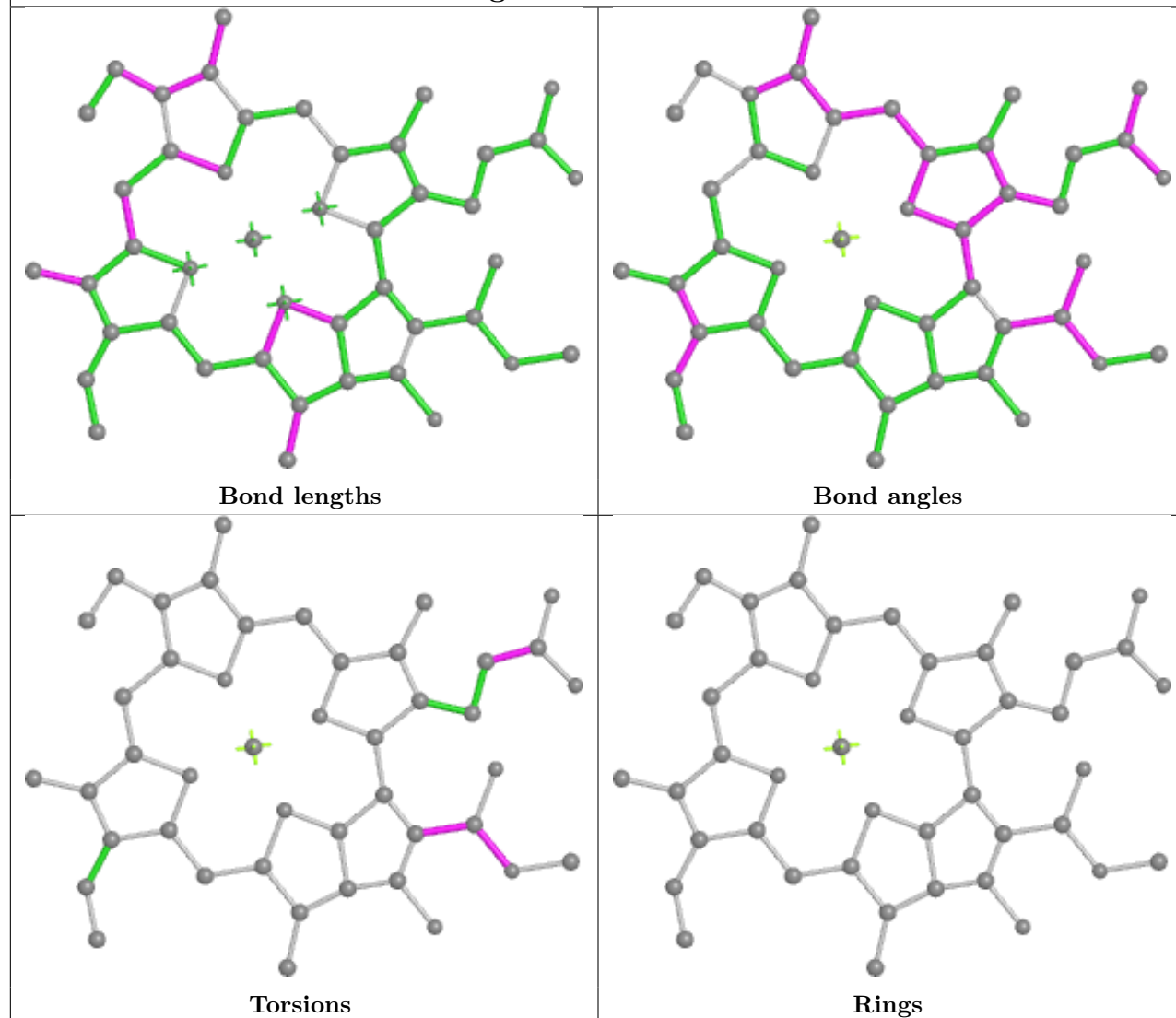
Ligand CLA n 304



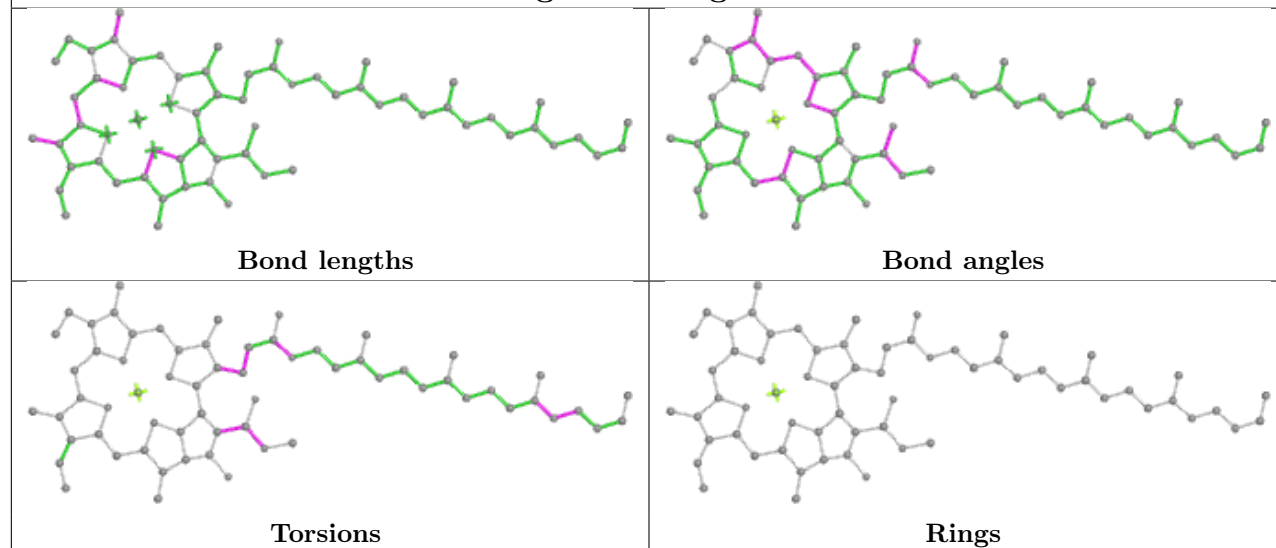
Ligand NEX Y 317

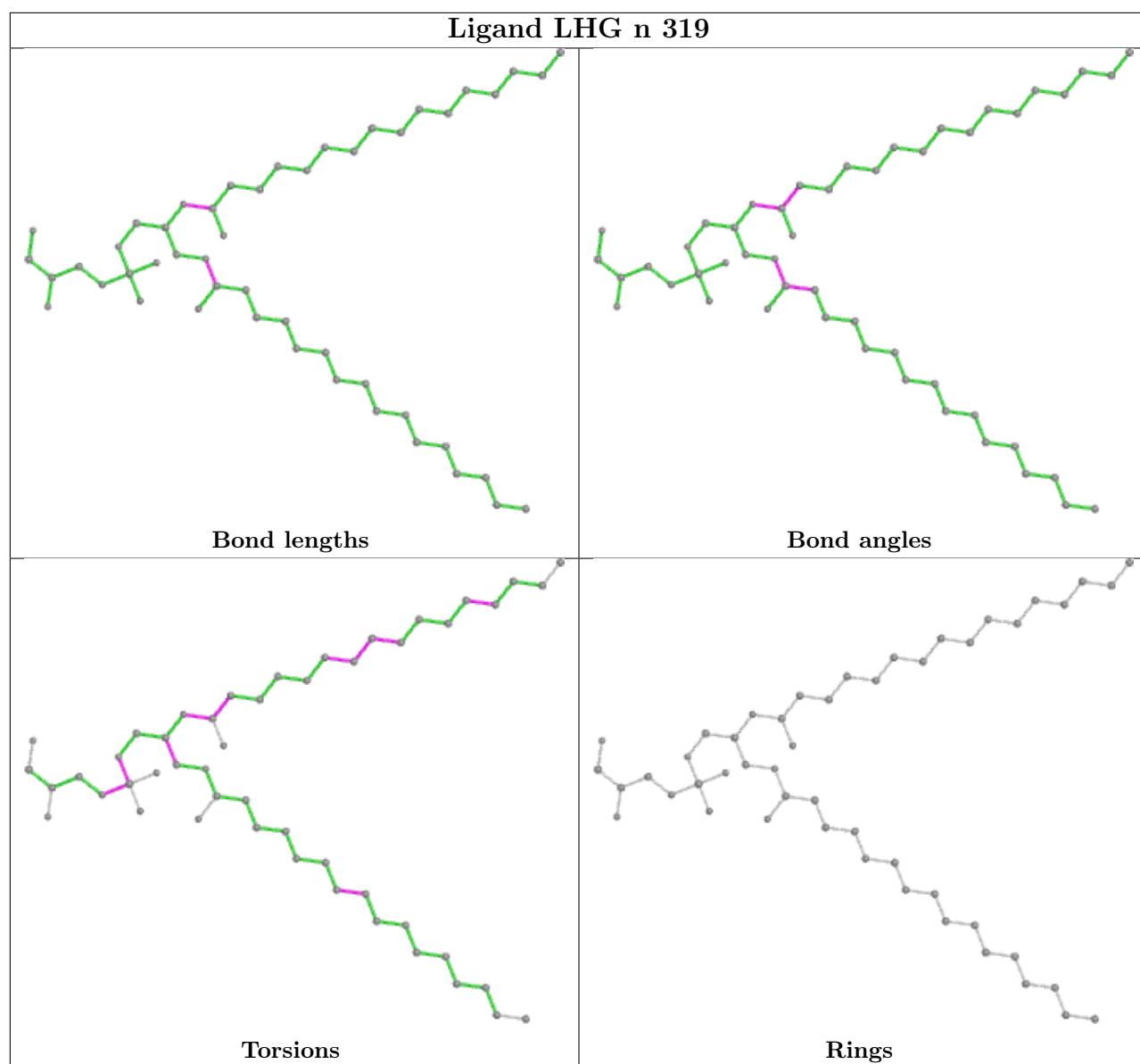


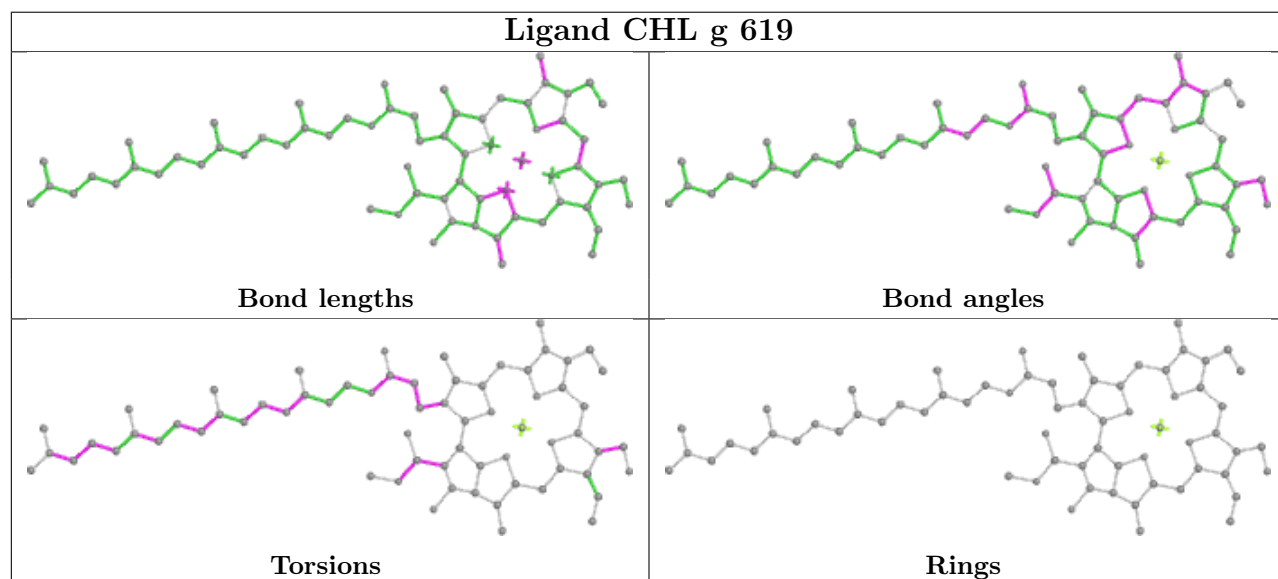
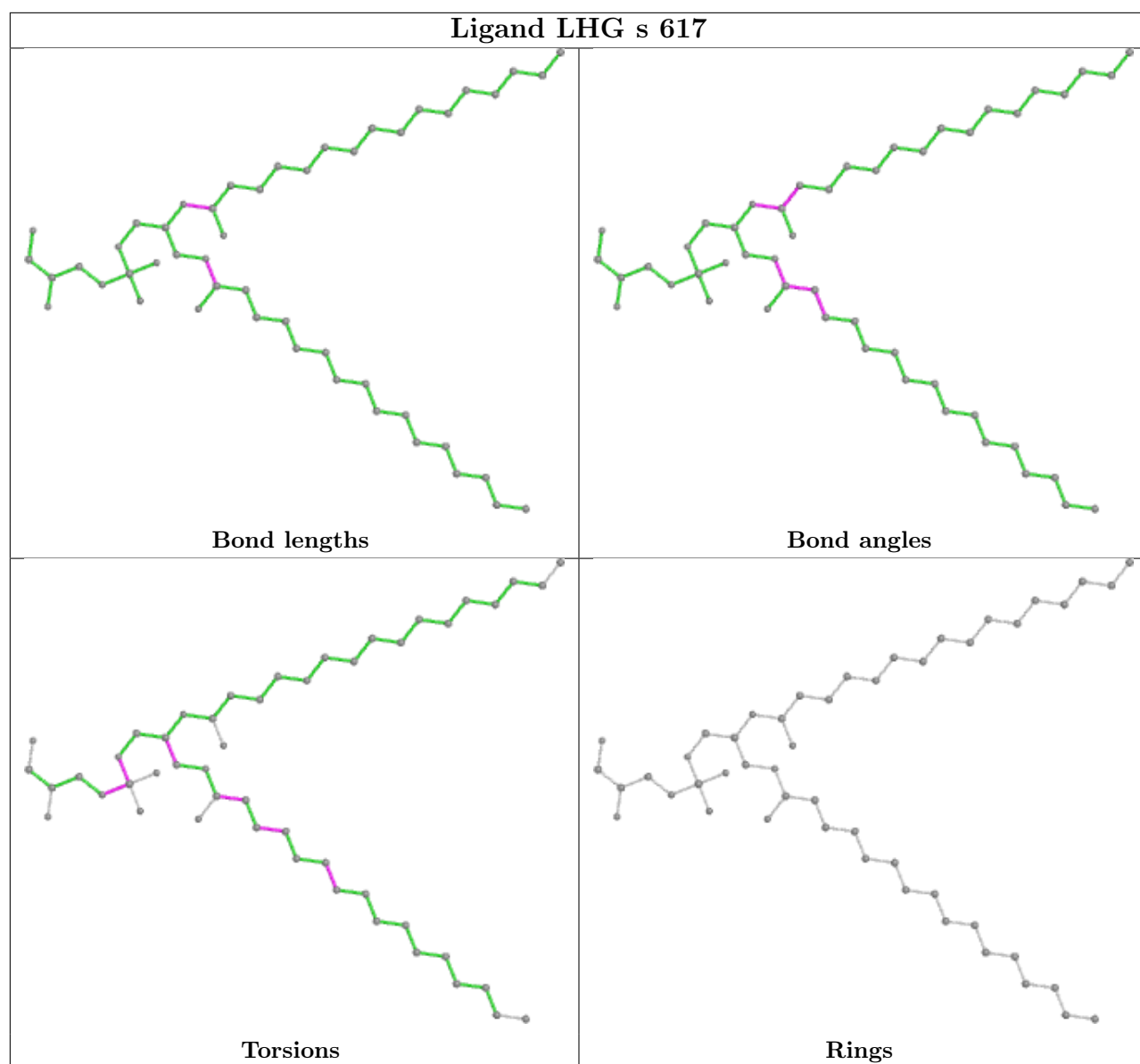
Ligand CLA G 612

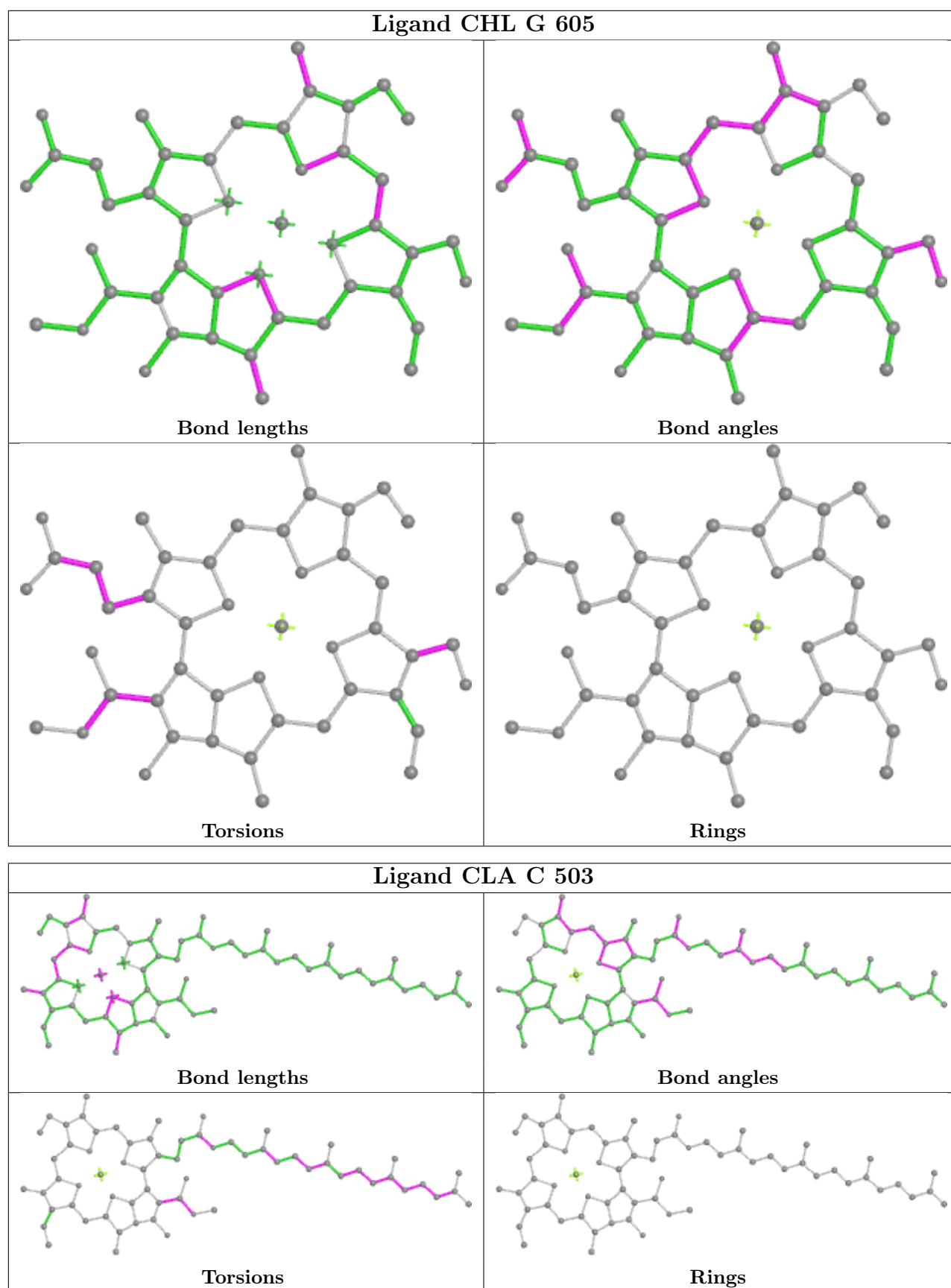


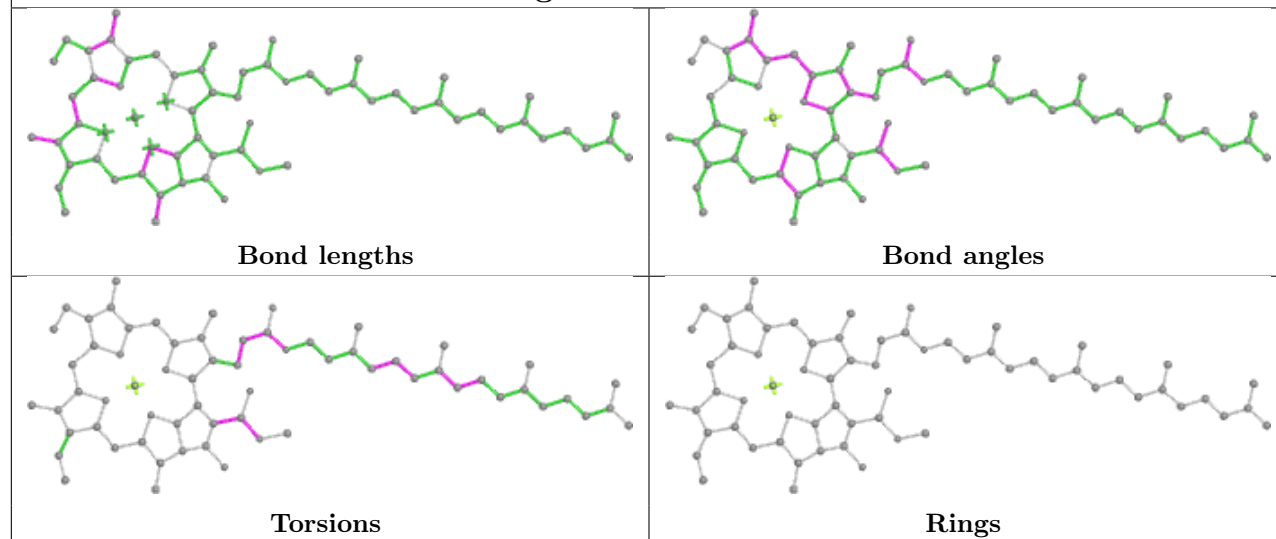
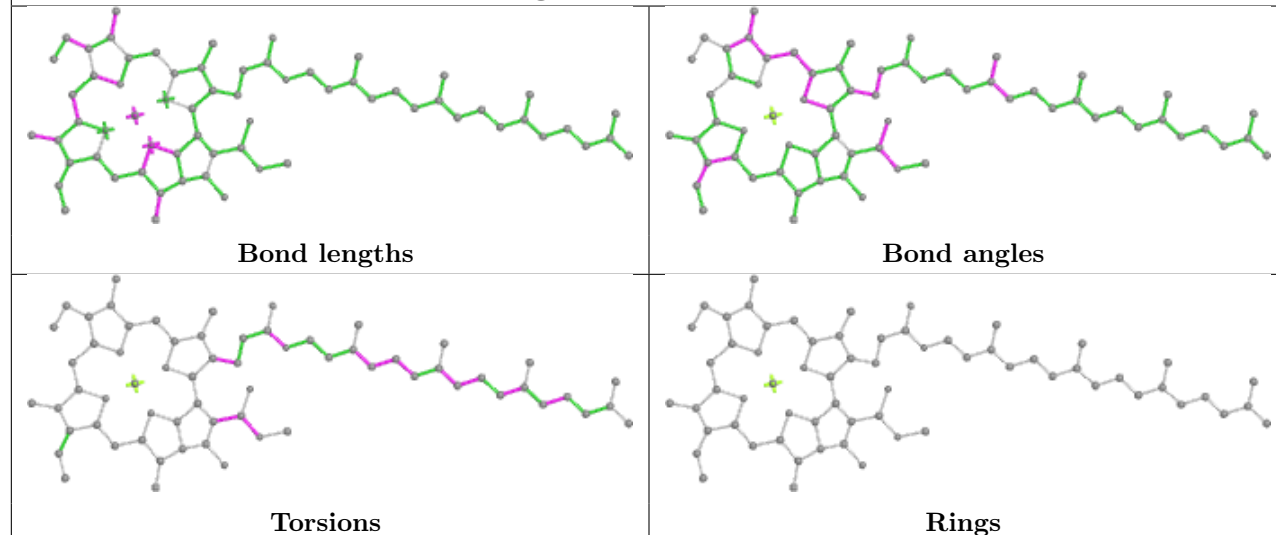
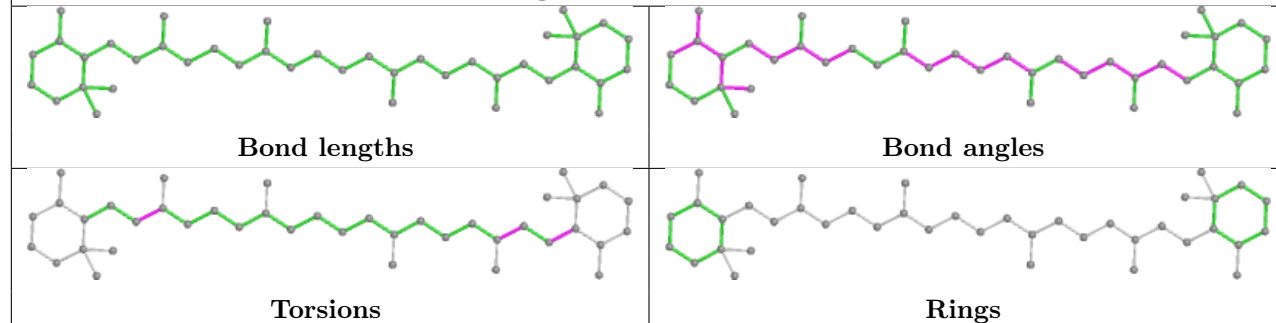
Ligand CLA g 610

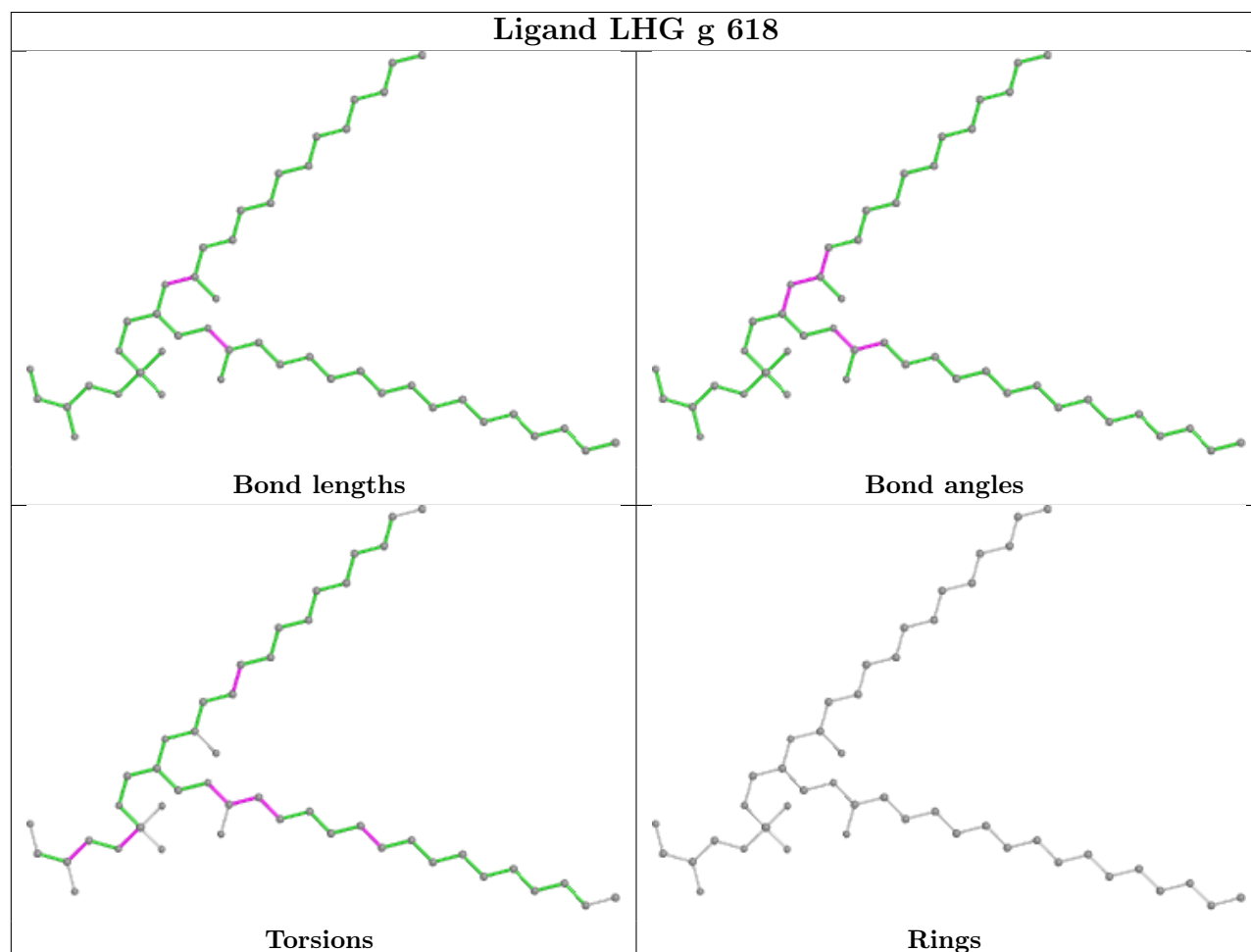
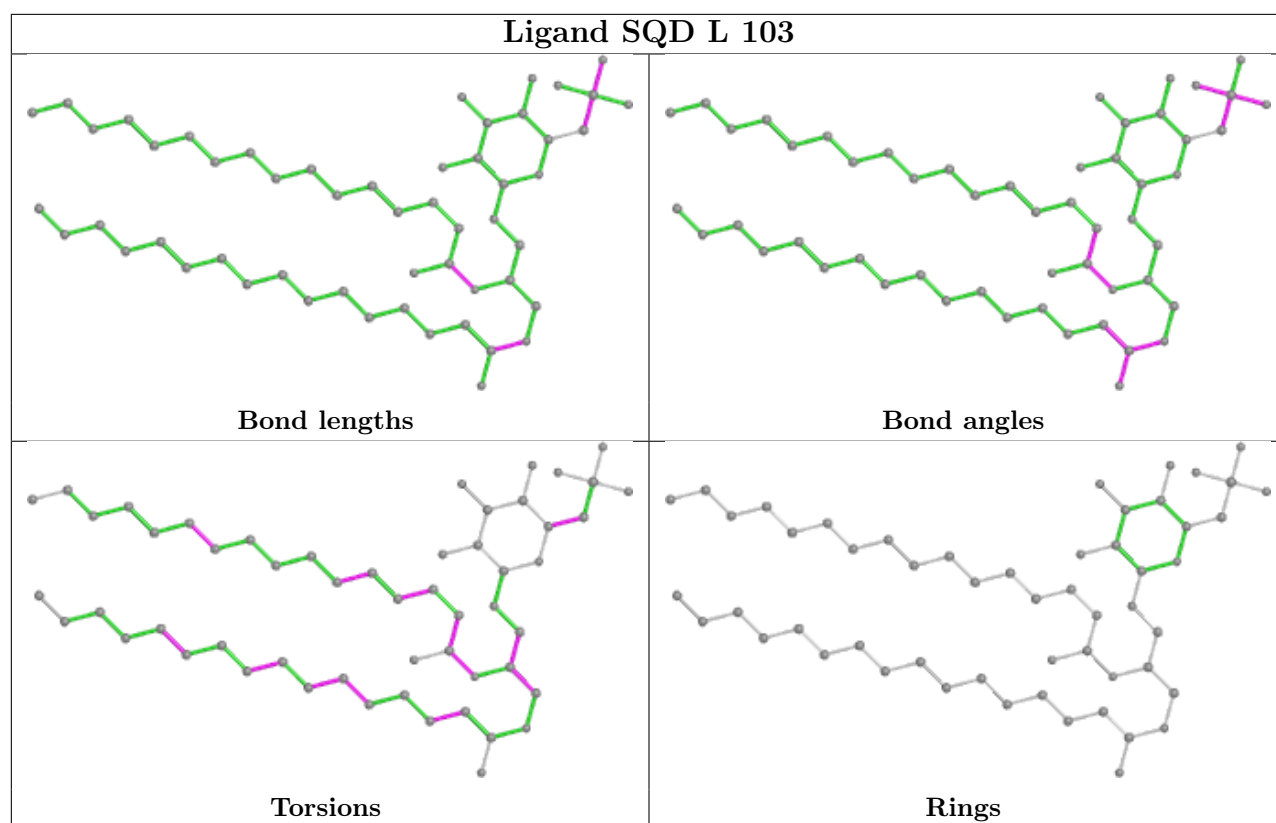


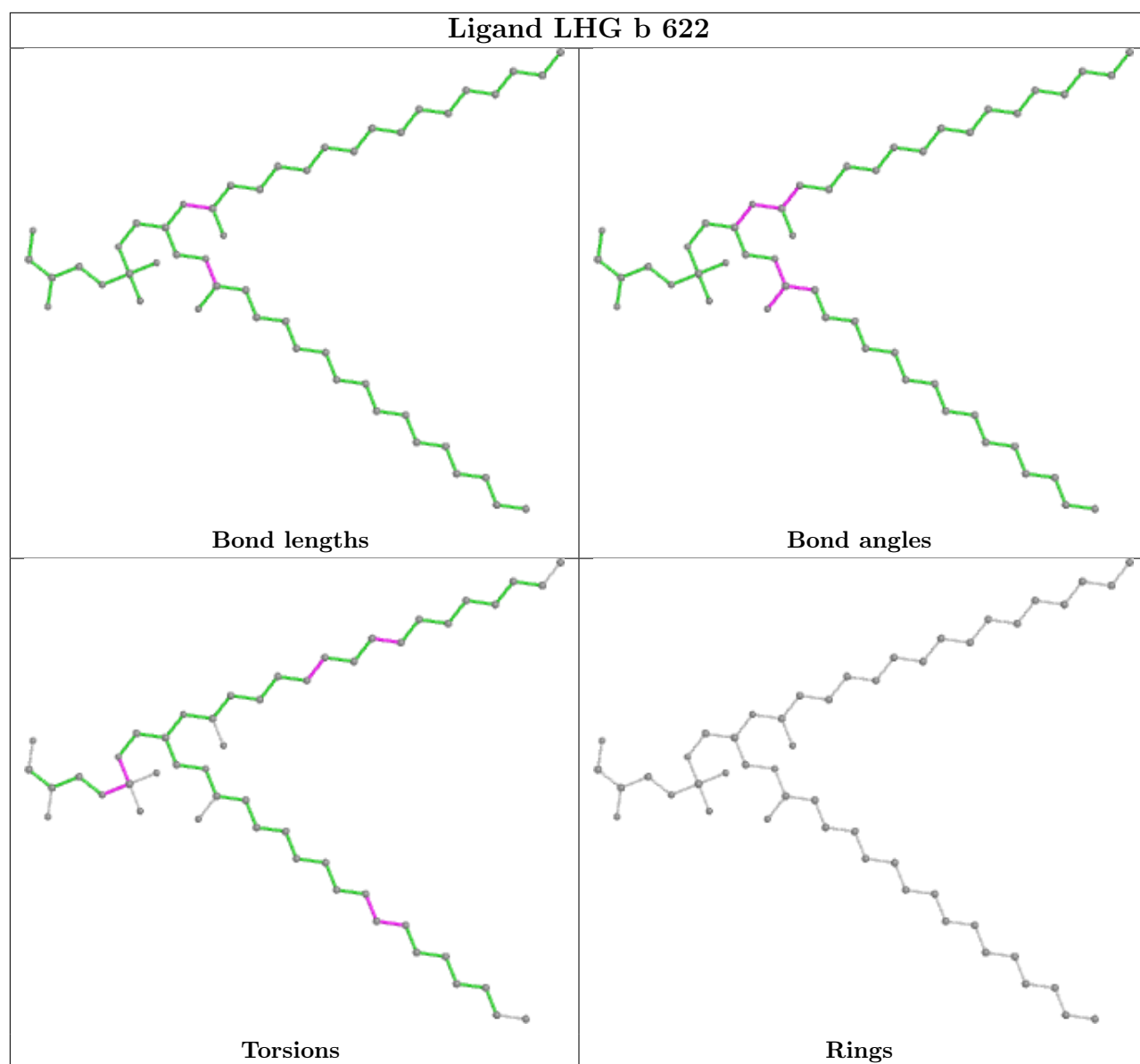


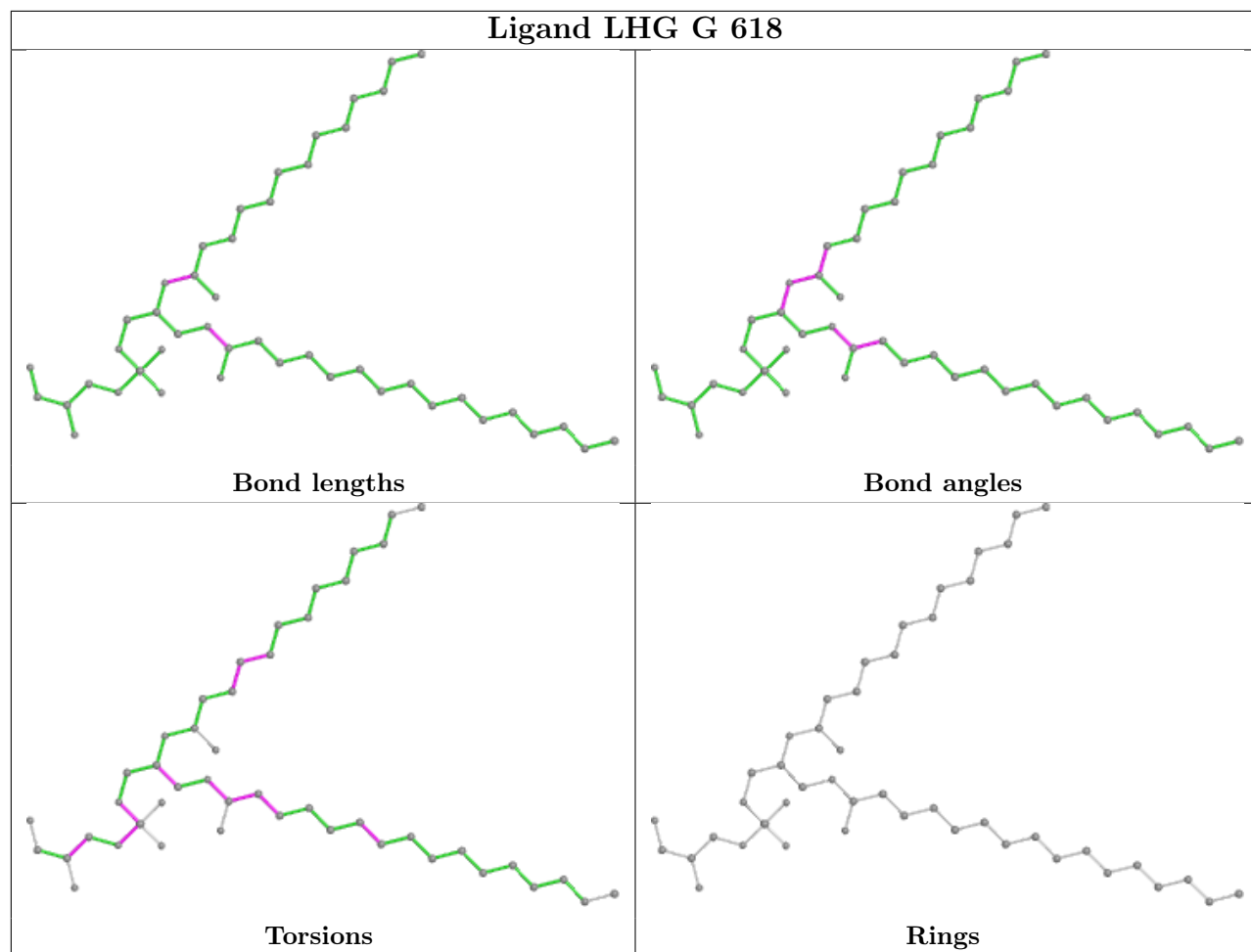


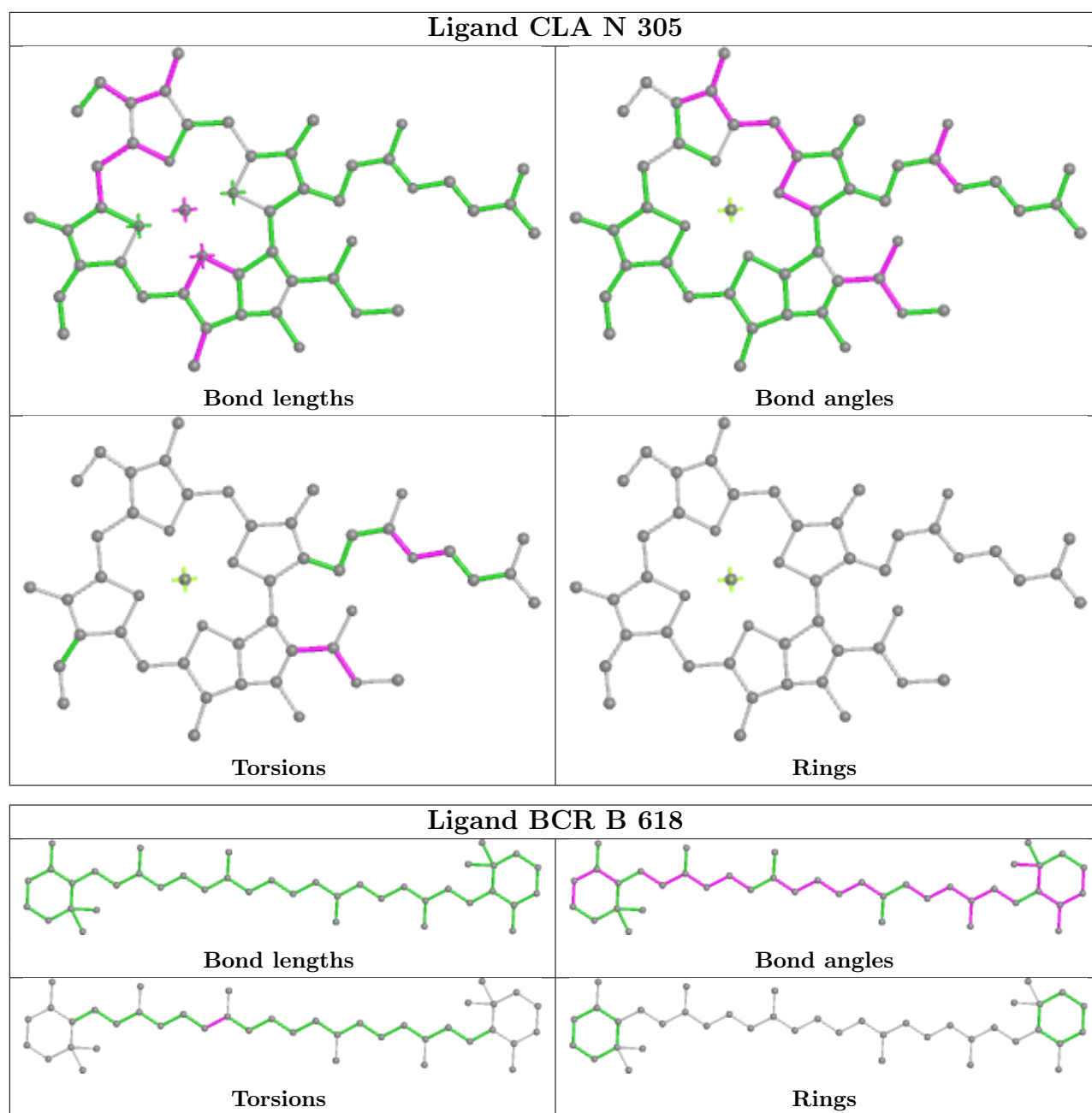


Ligand CLA b 616**Ligand CLA B 608****Ligand BCR b 617**

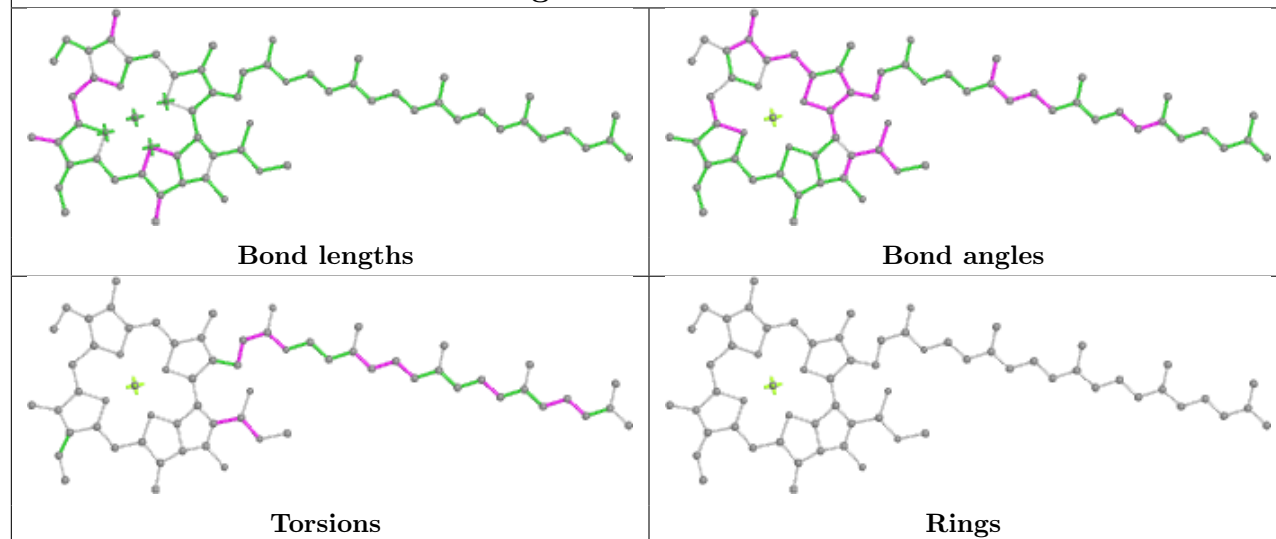




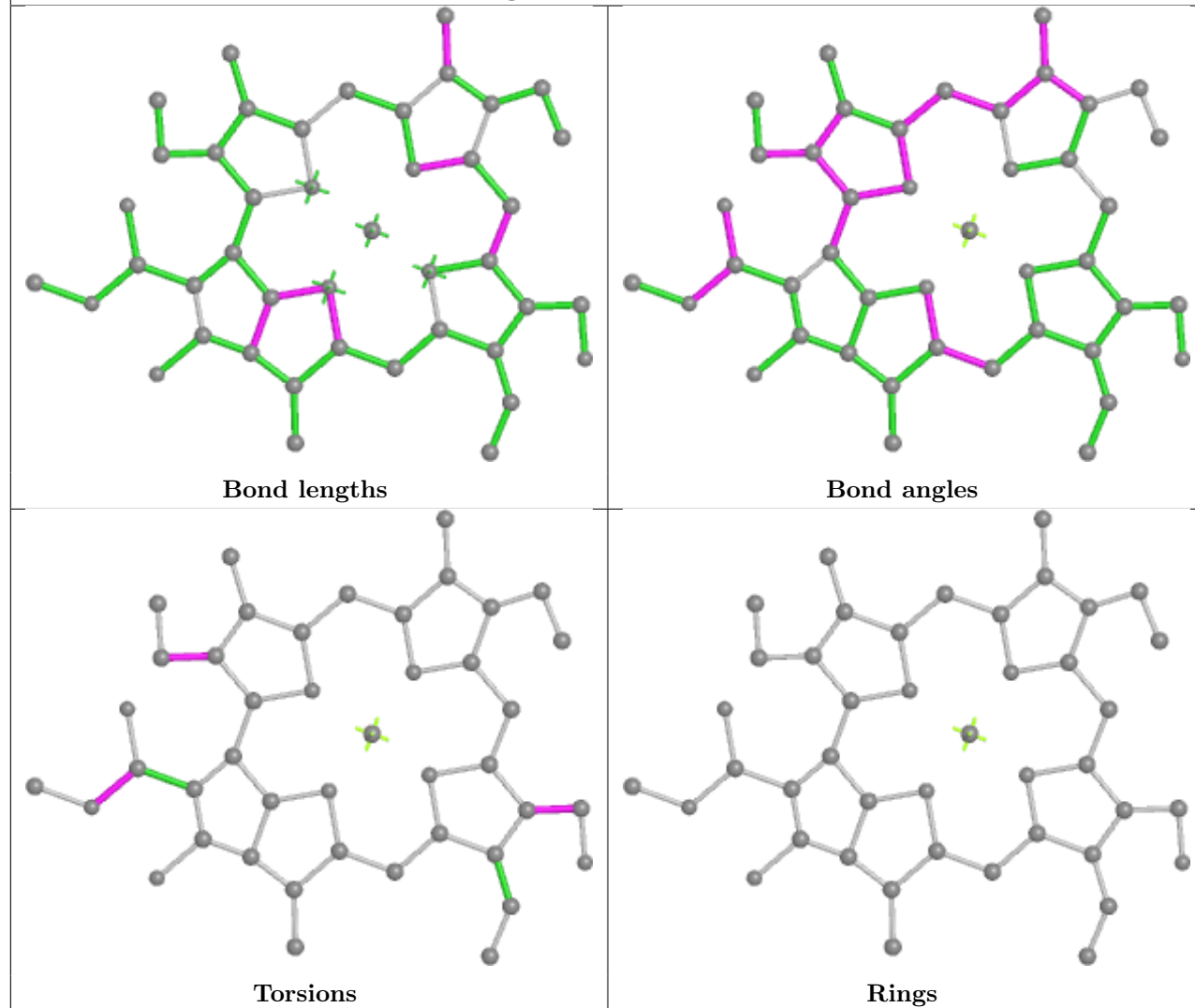




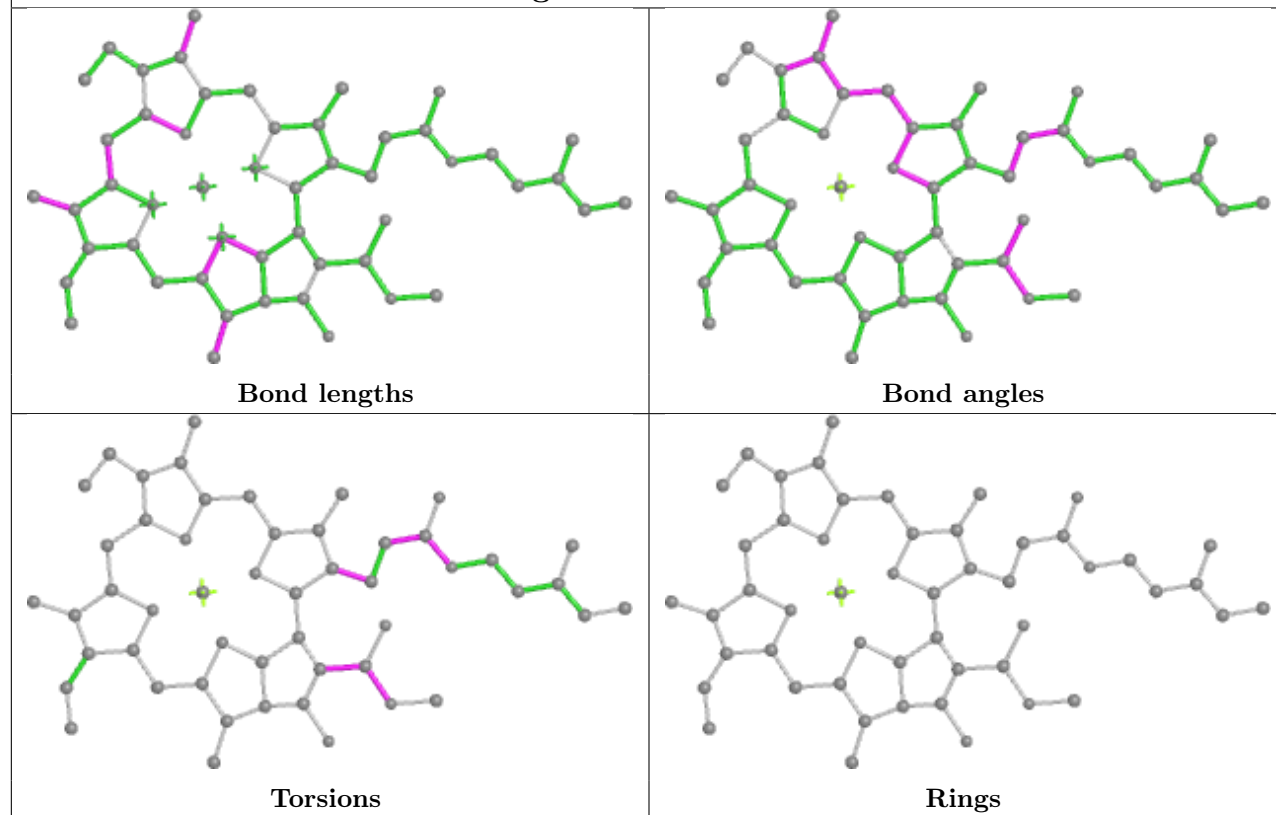
Ligand CLA A 401



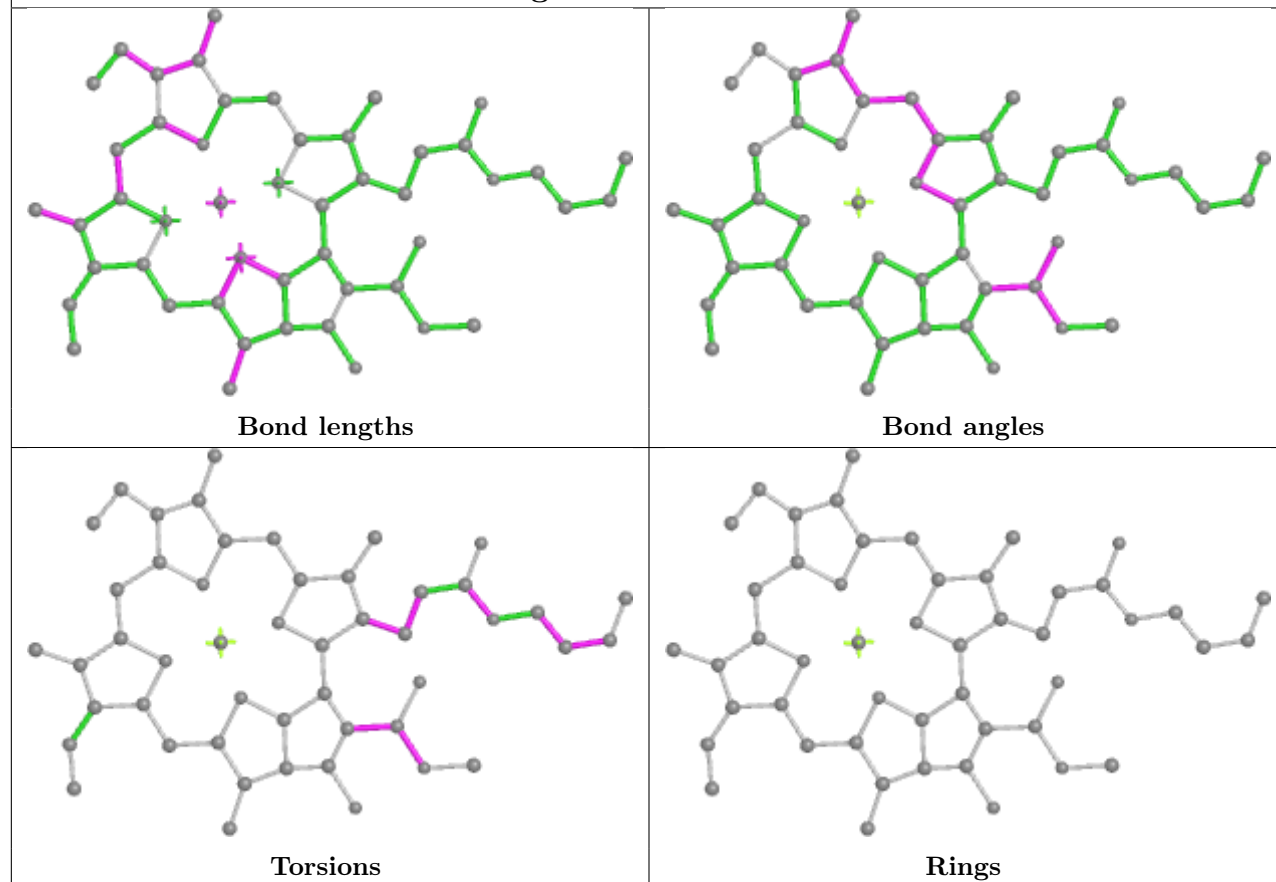
Ligand CHL s 606

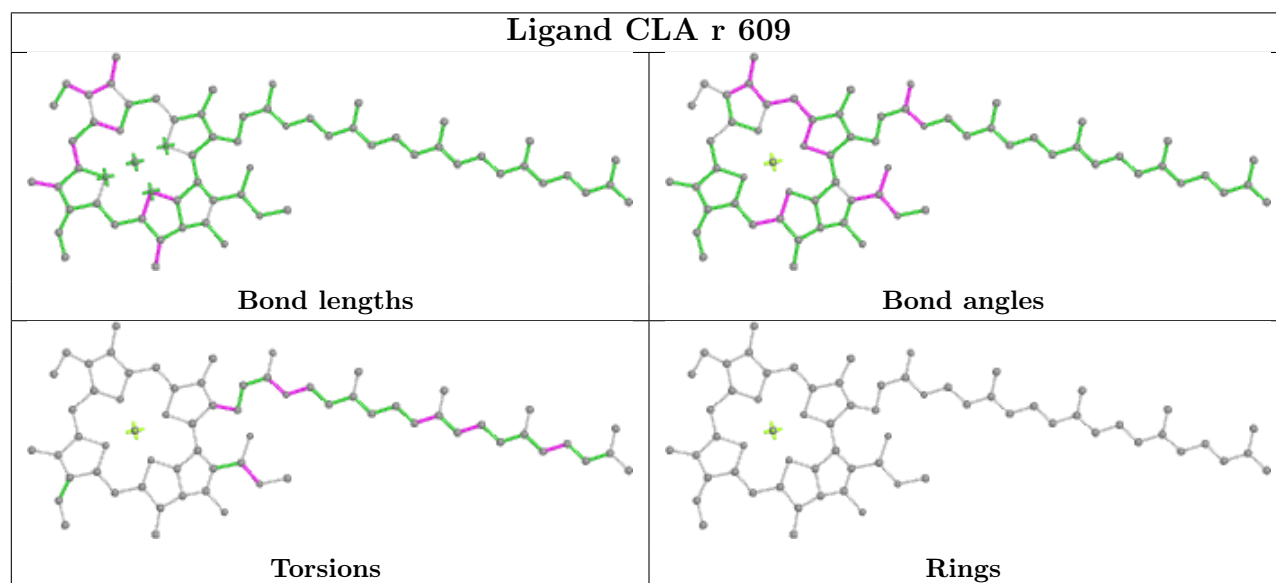
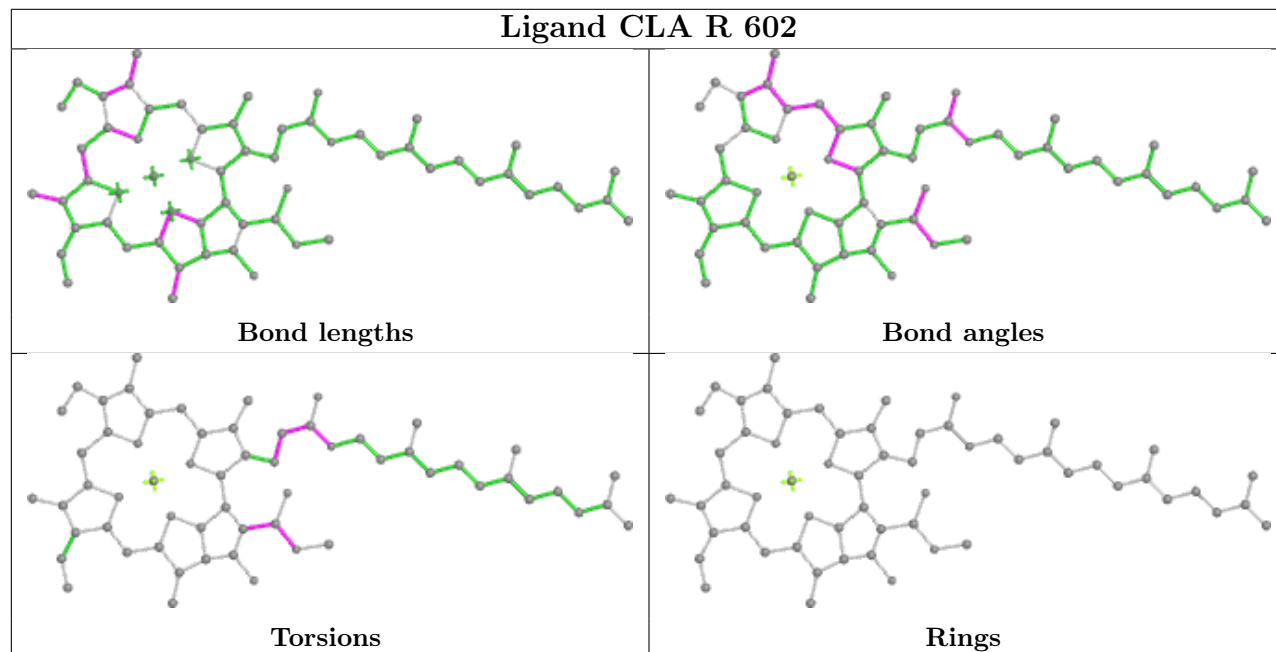
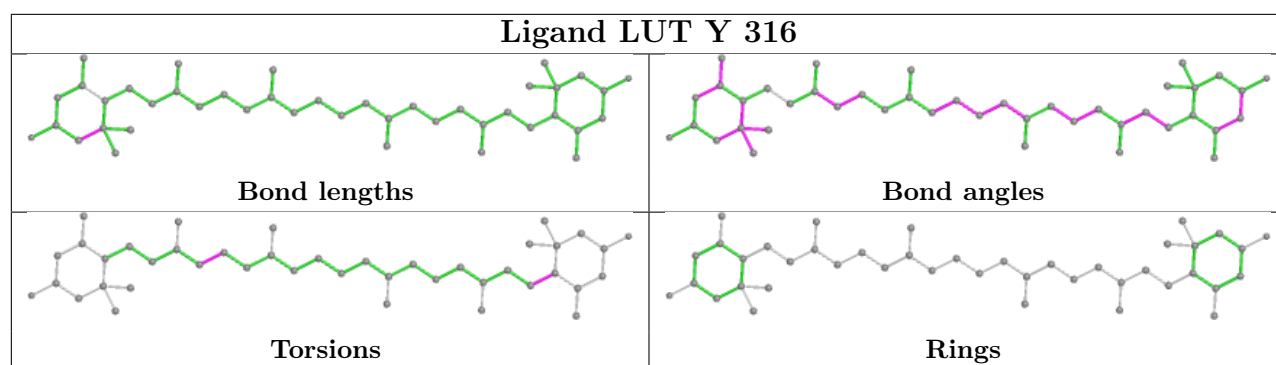


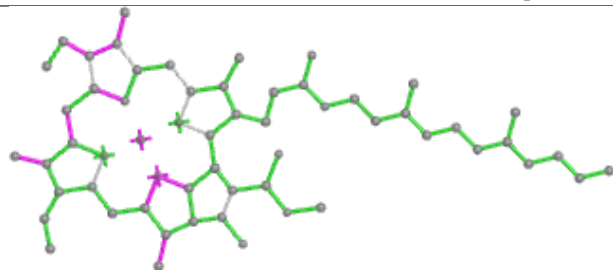
Ligand CLA C 507



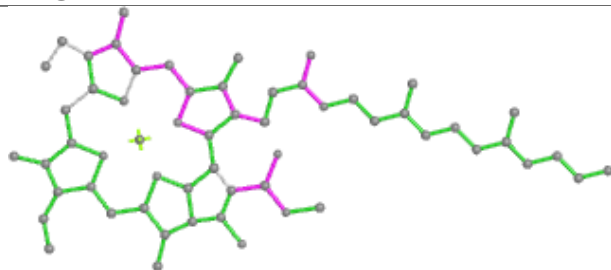
Ligand CLA G 604



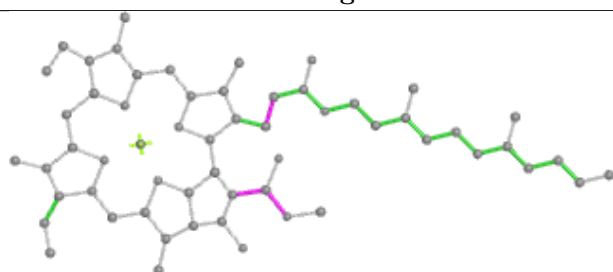


Ligand CLA g 613

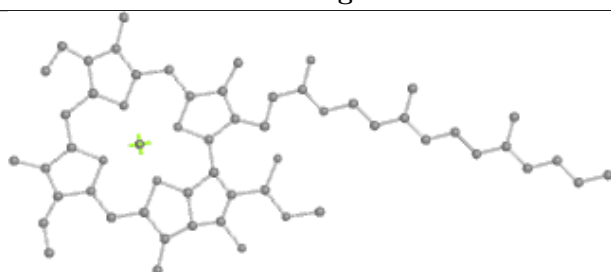
Bond lengths



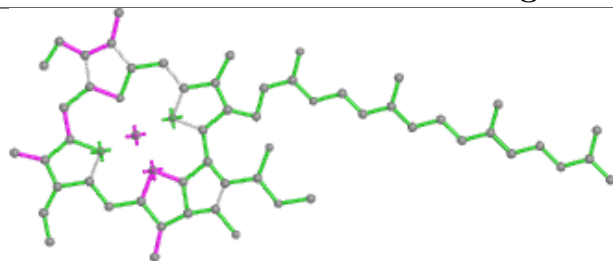
Bond angles



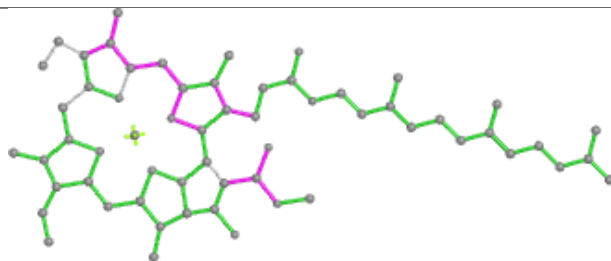
Torsions



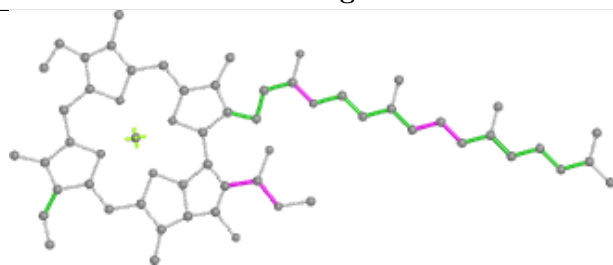
Rings

Ligand CLA r 603

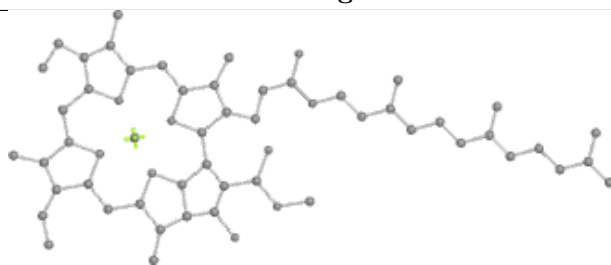
Bond lengths



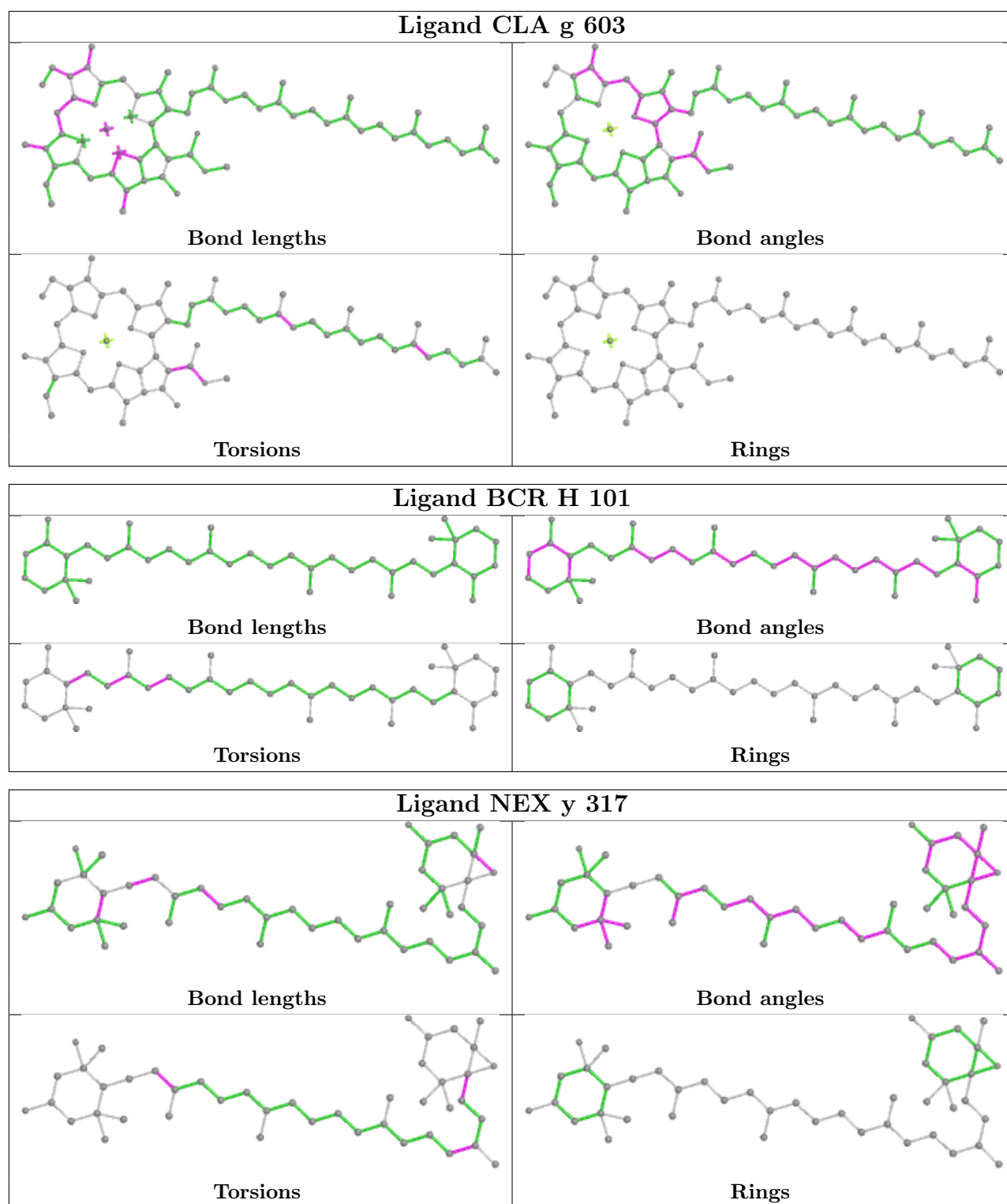
Bond angles

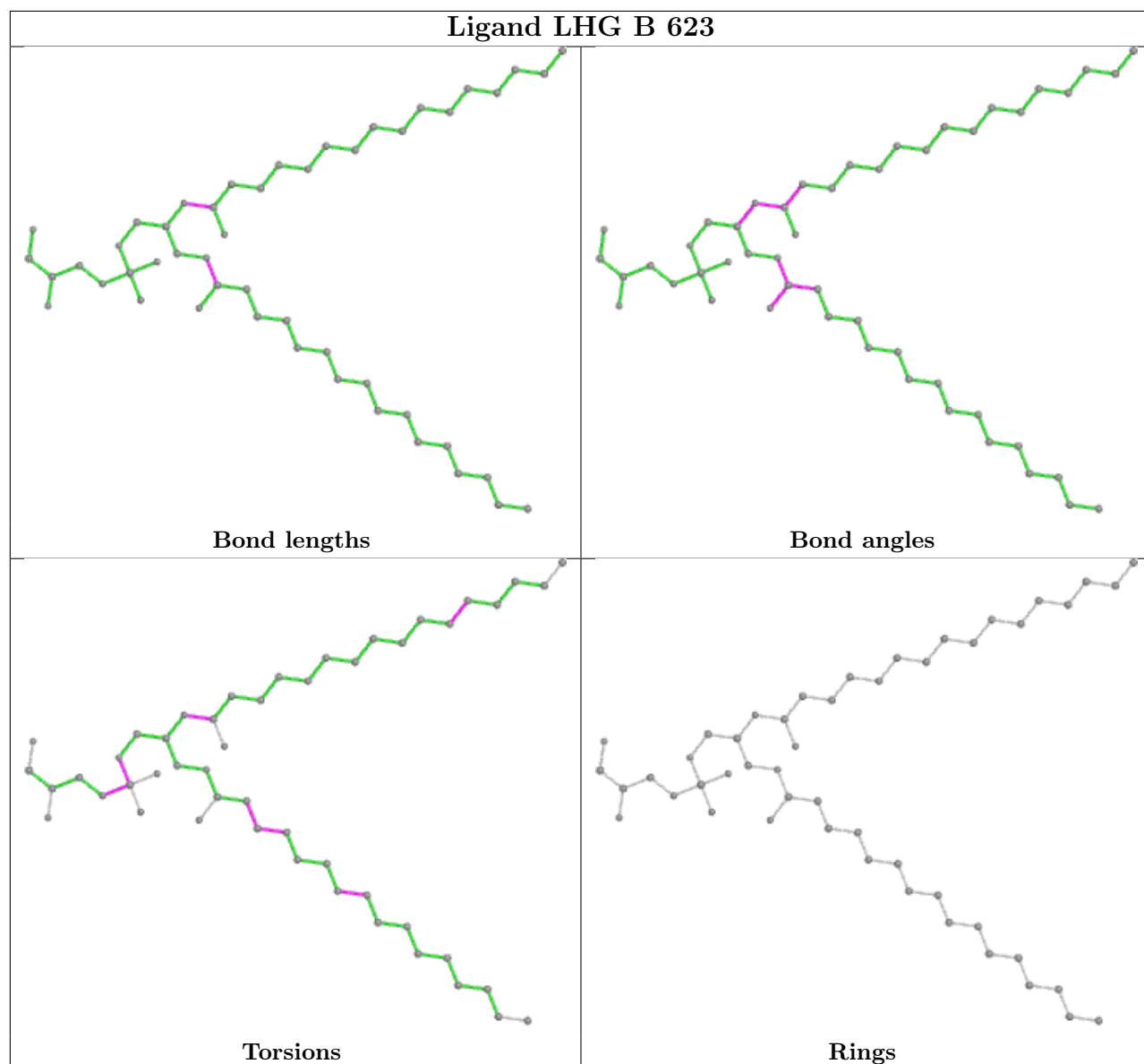
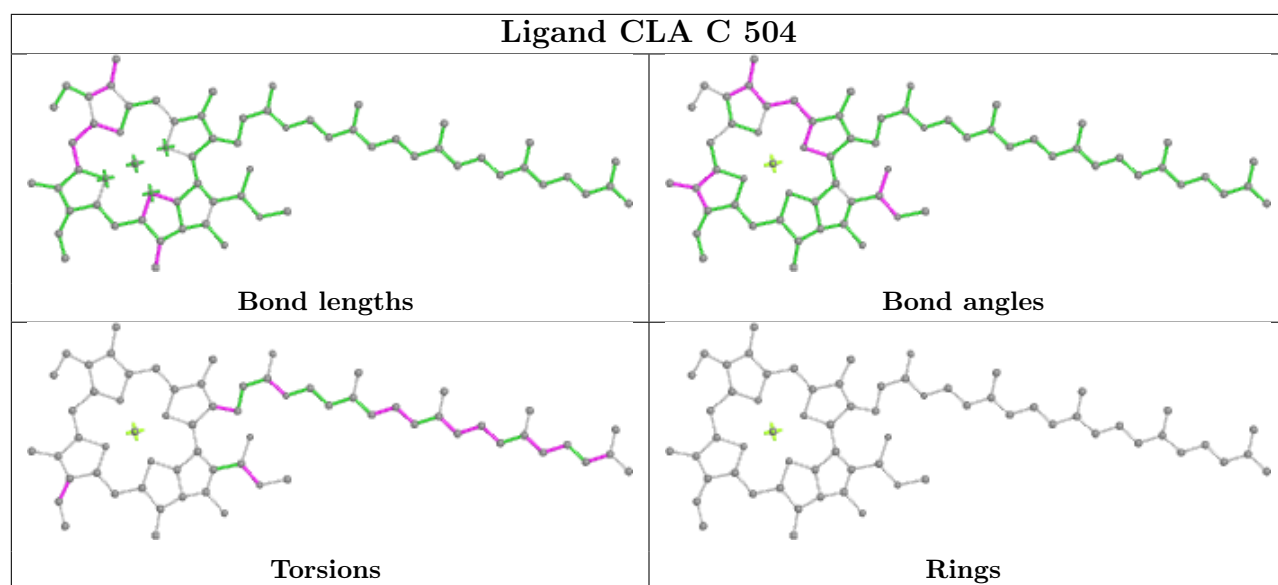


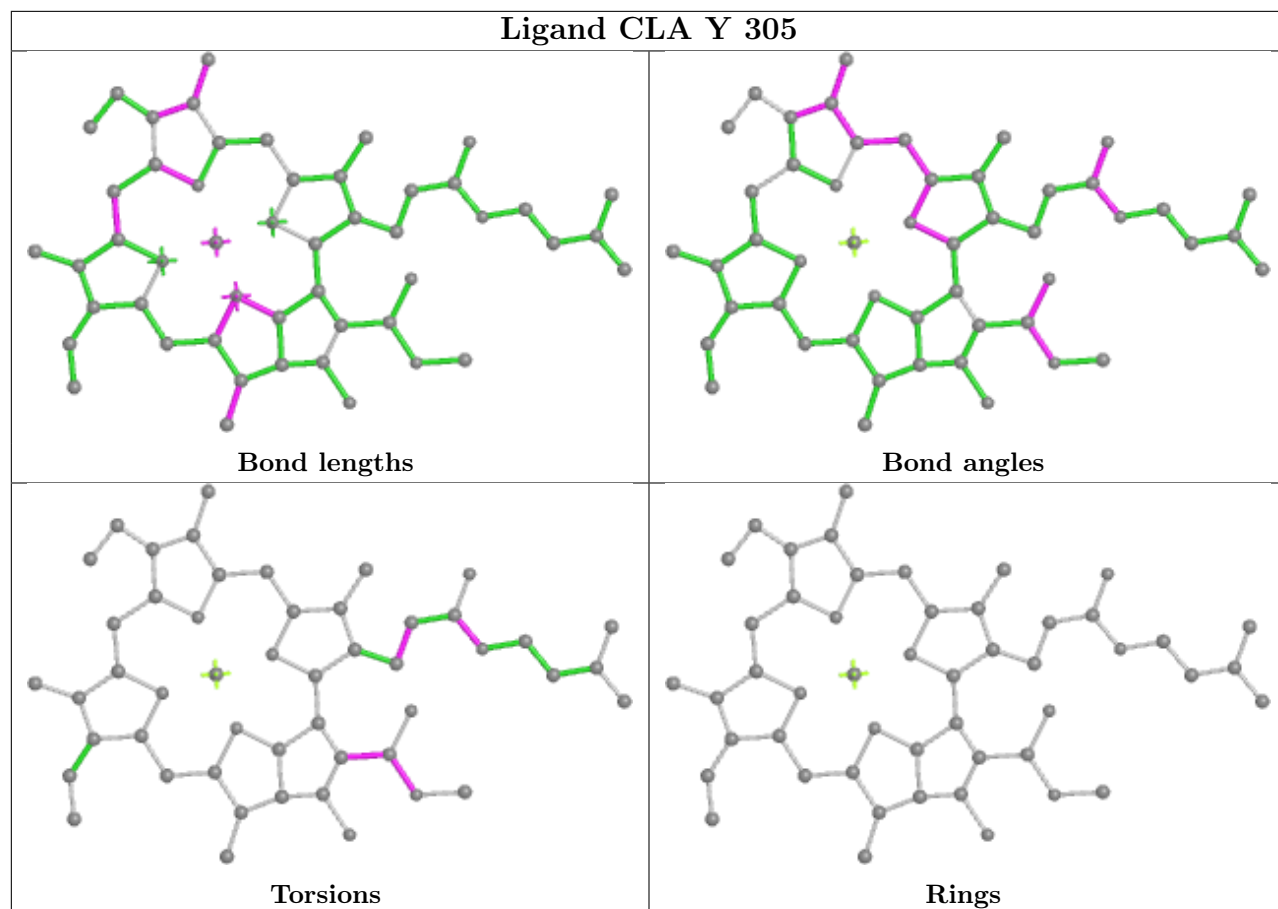
Torsions



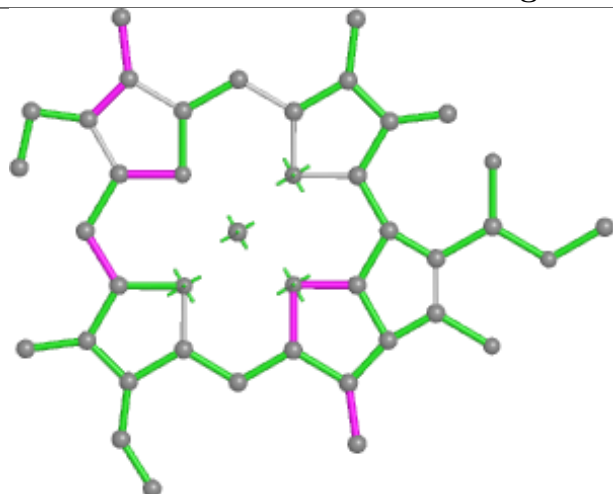
Rings



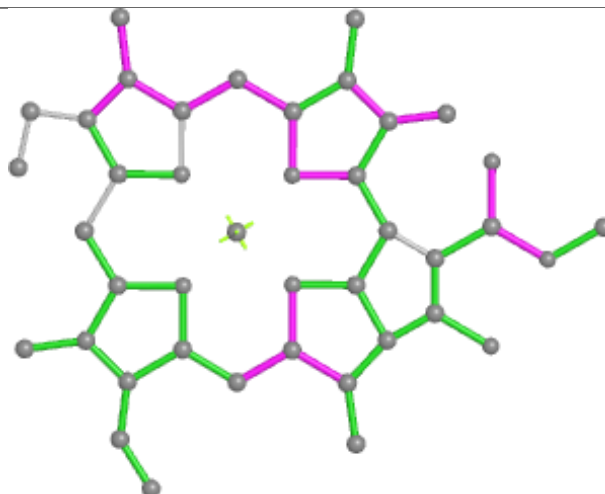




Ligand CLA s 613



Bond lengths



Bond angles

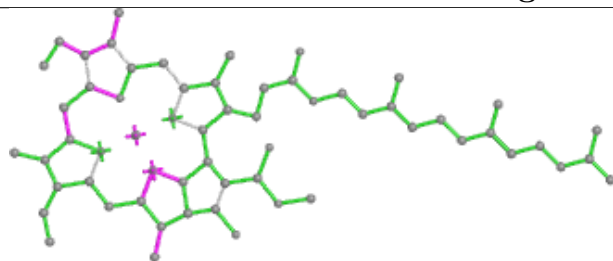


Torsions

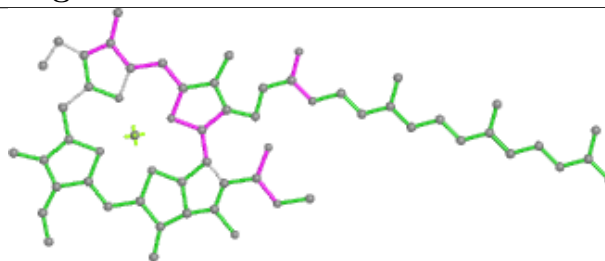


Rings

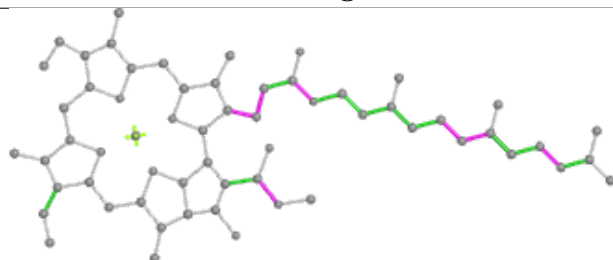
Ligand CLA g 611



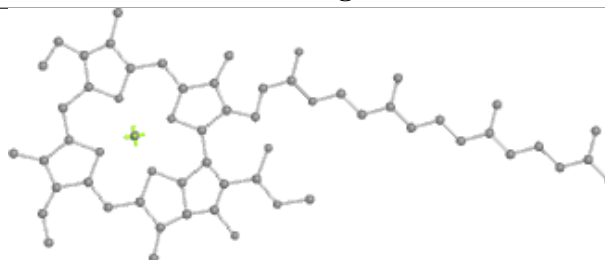
Bond lengths



Bond angles

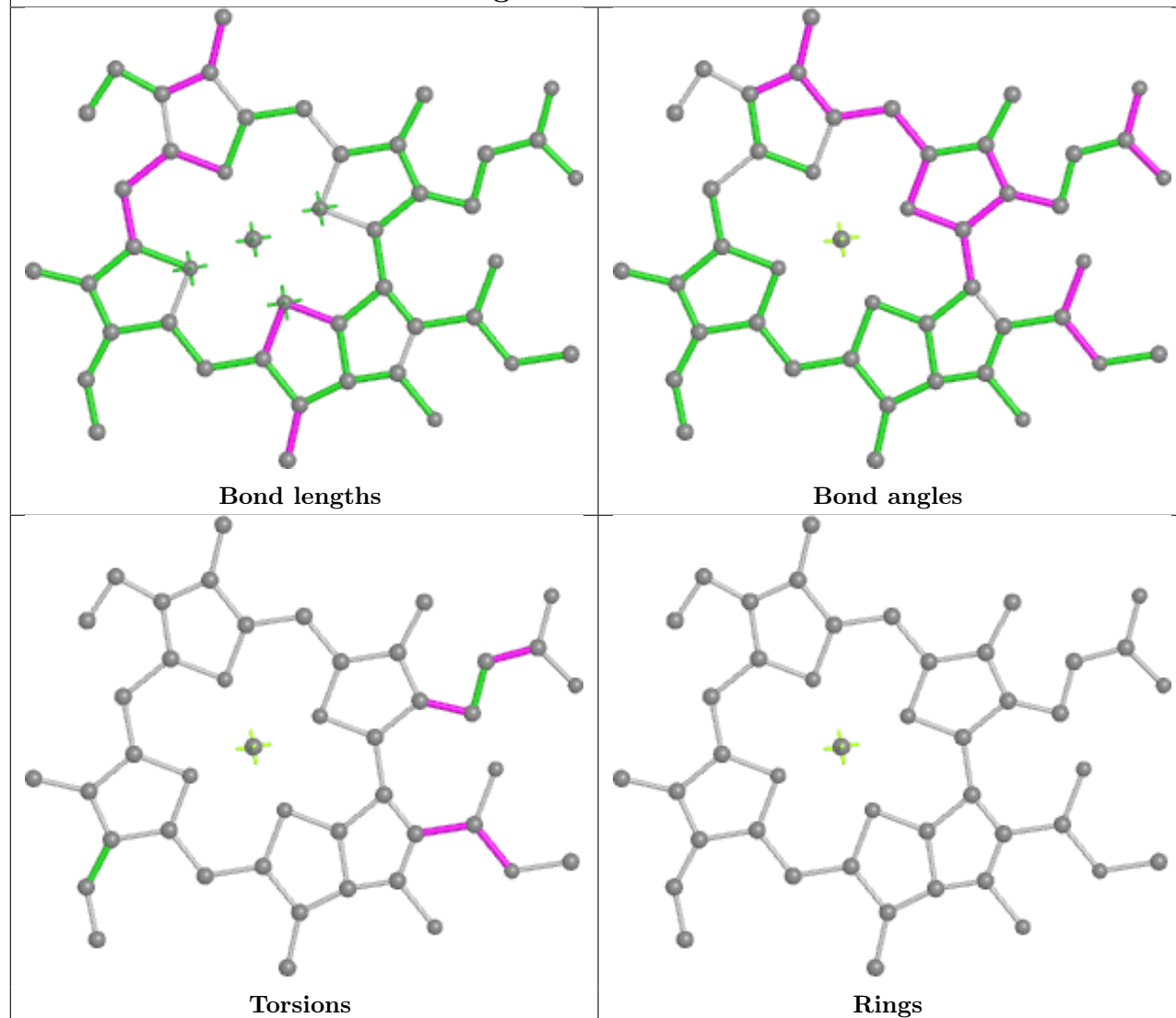


Torsions

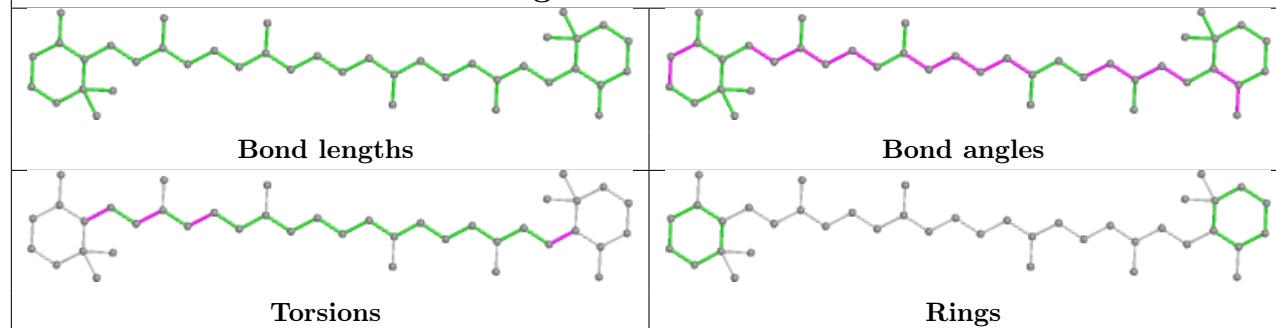


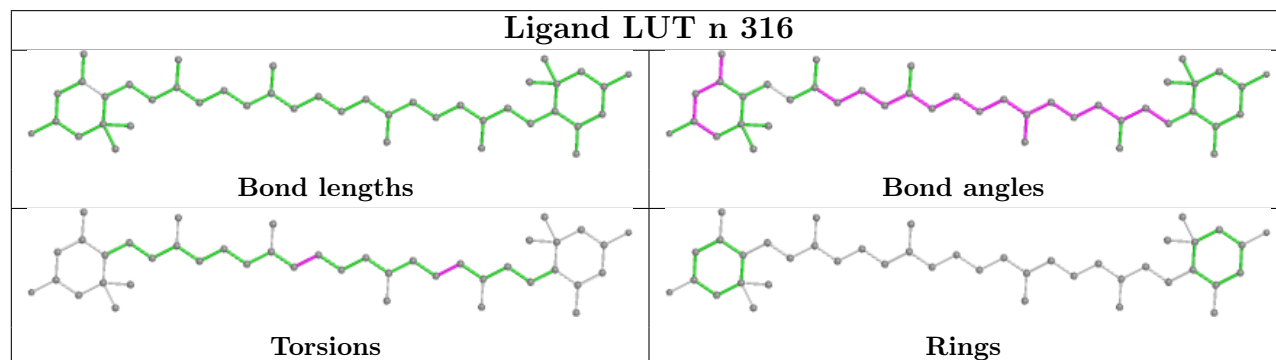
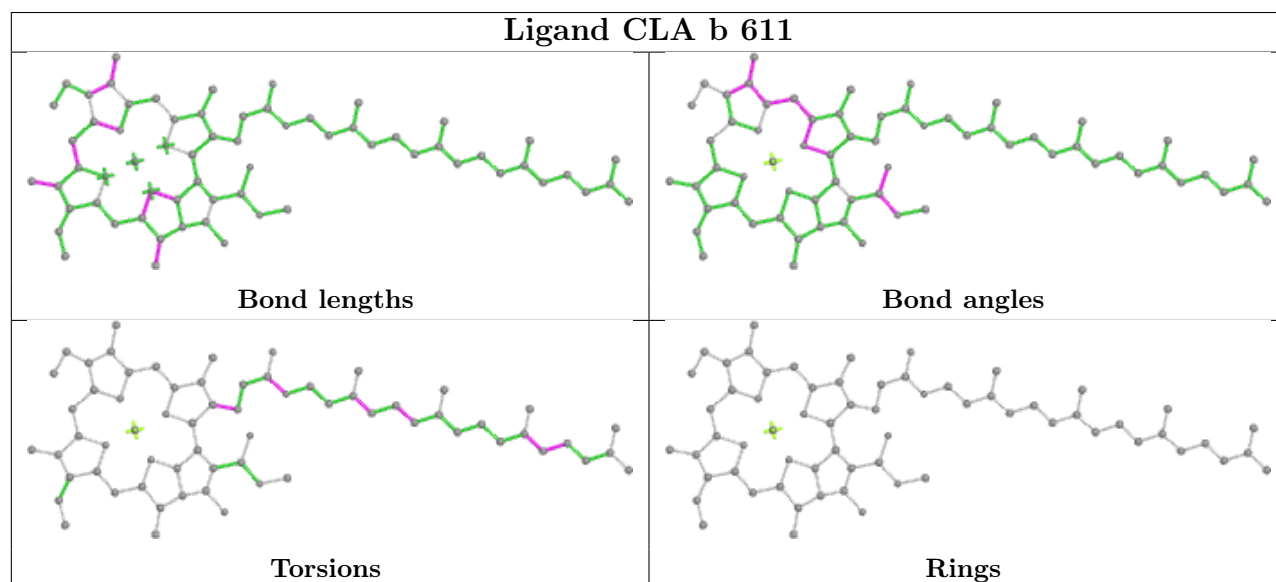
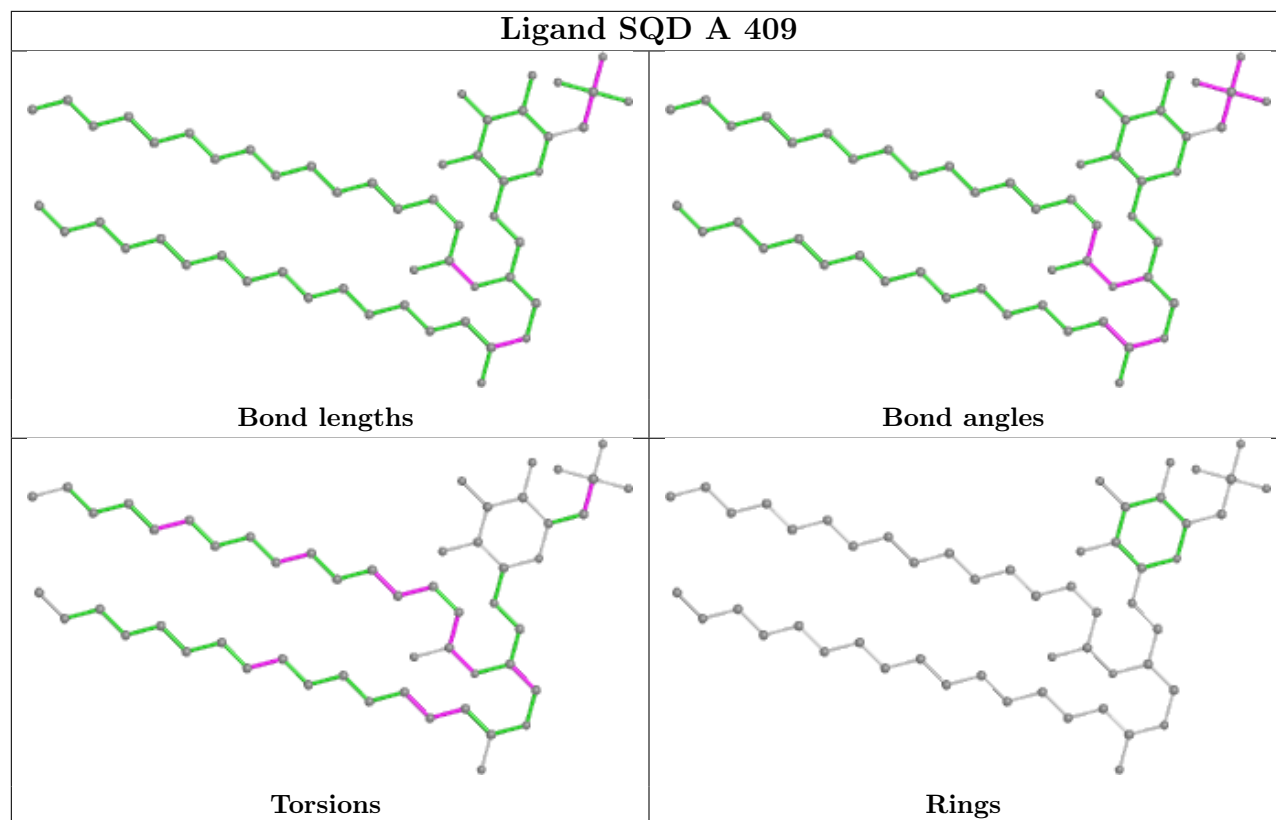
Rings

Ligand CLA S 603

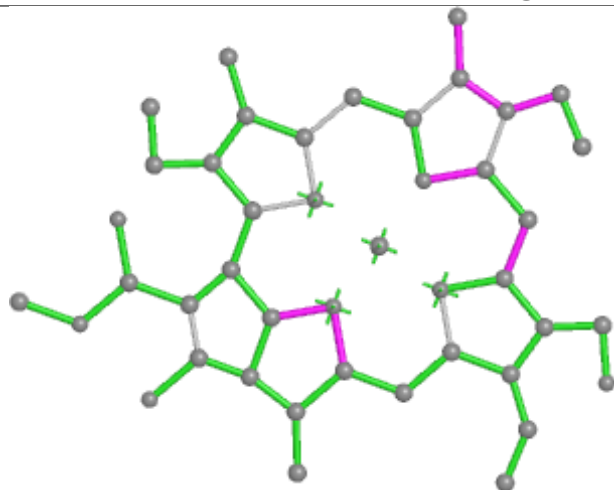


Ligand BCR h 101

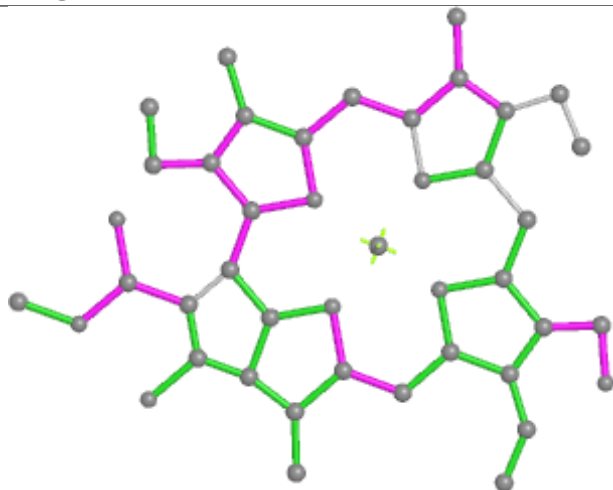




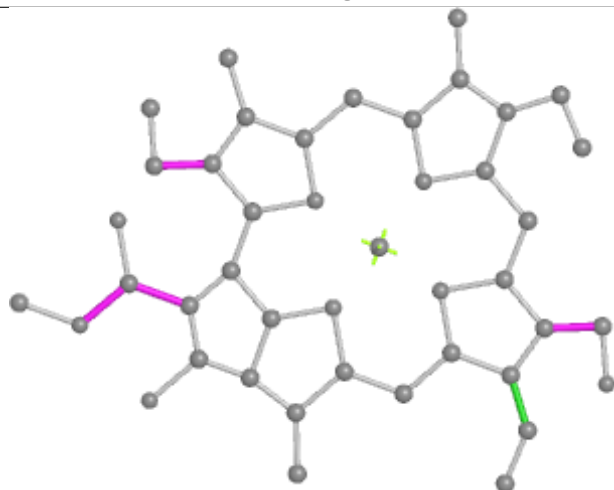
Ligand CHL g 606



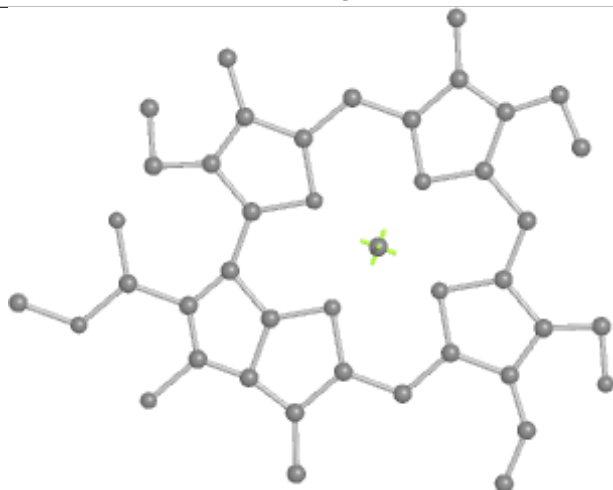
Bond lengths



Bond angles

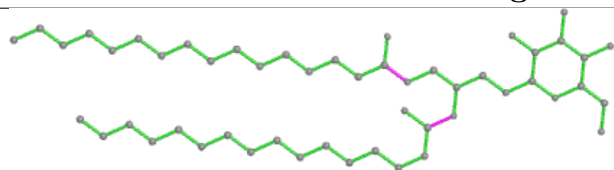


Torsions

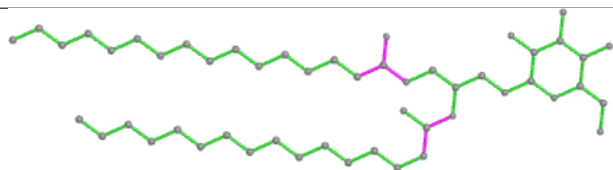


Rings

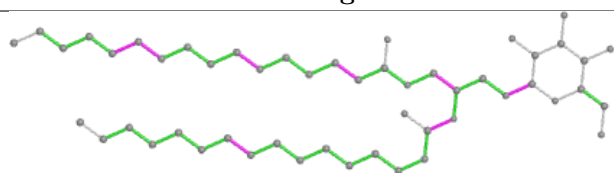
Ligand LMG B 620



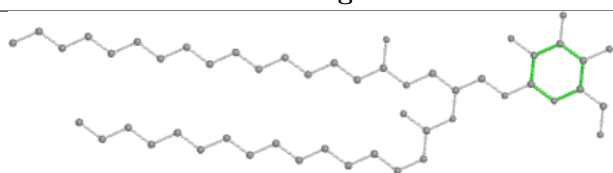
Bond lengths



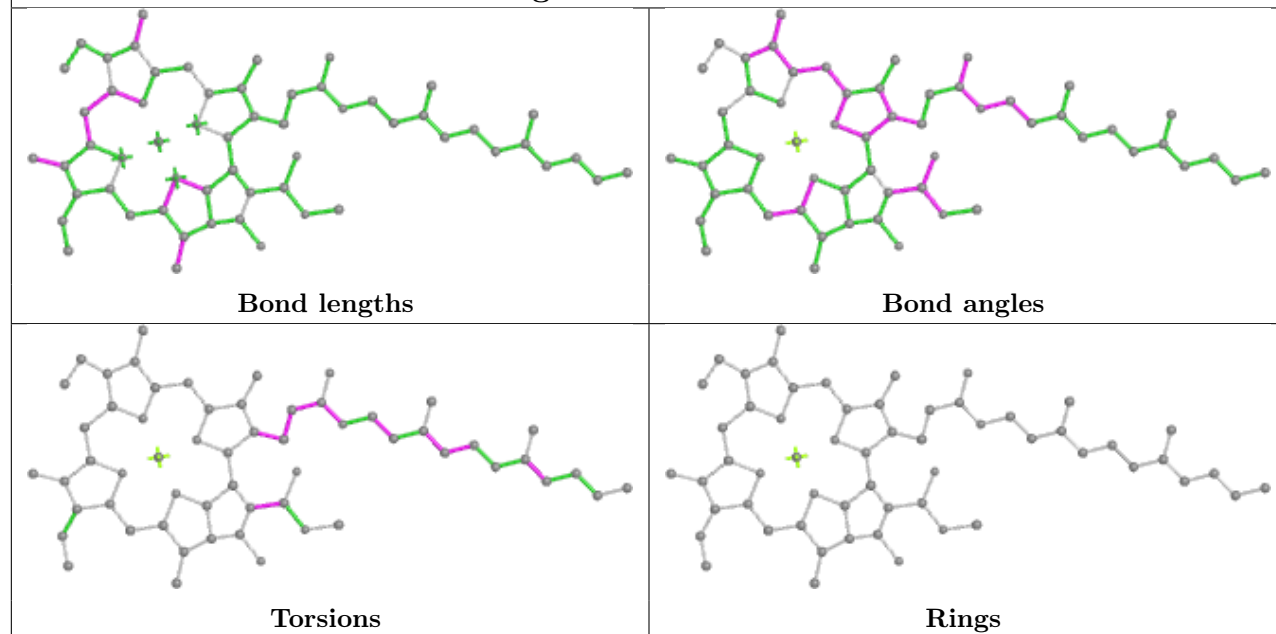
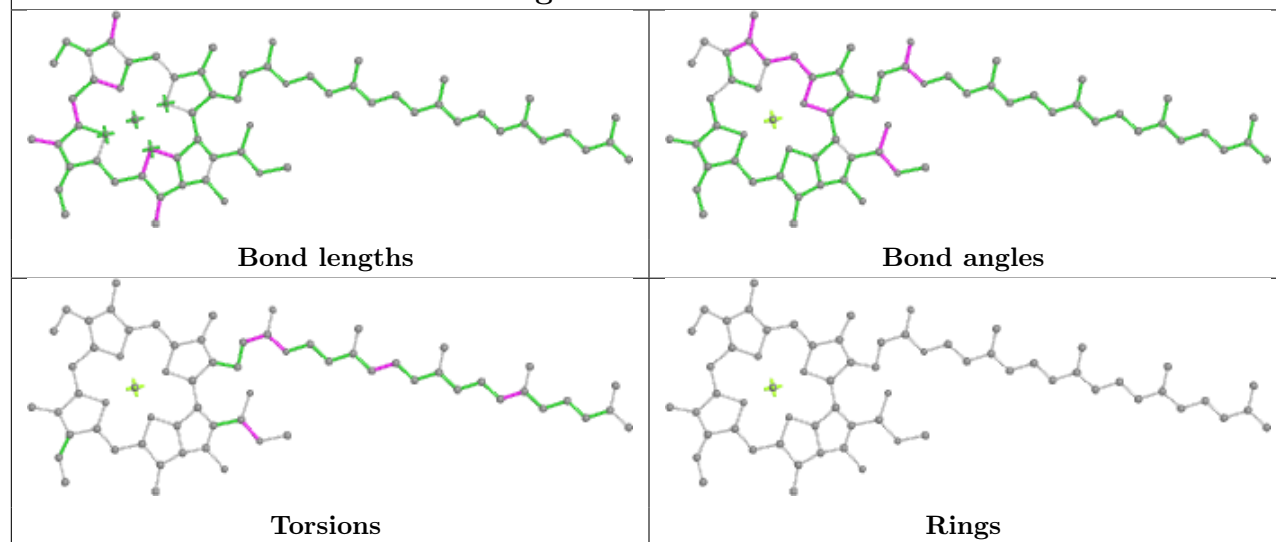
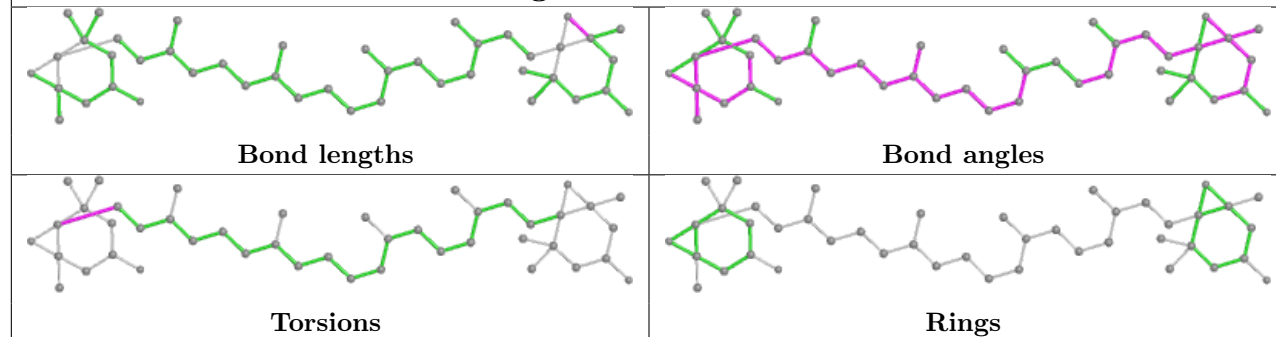
Bond angles



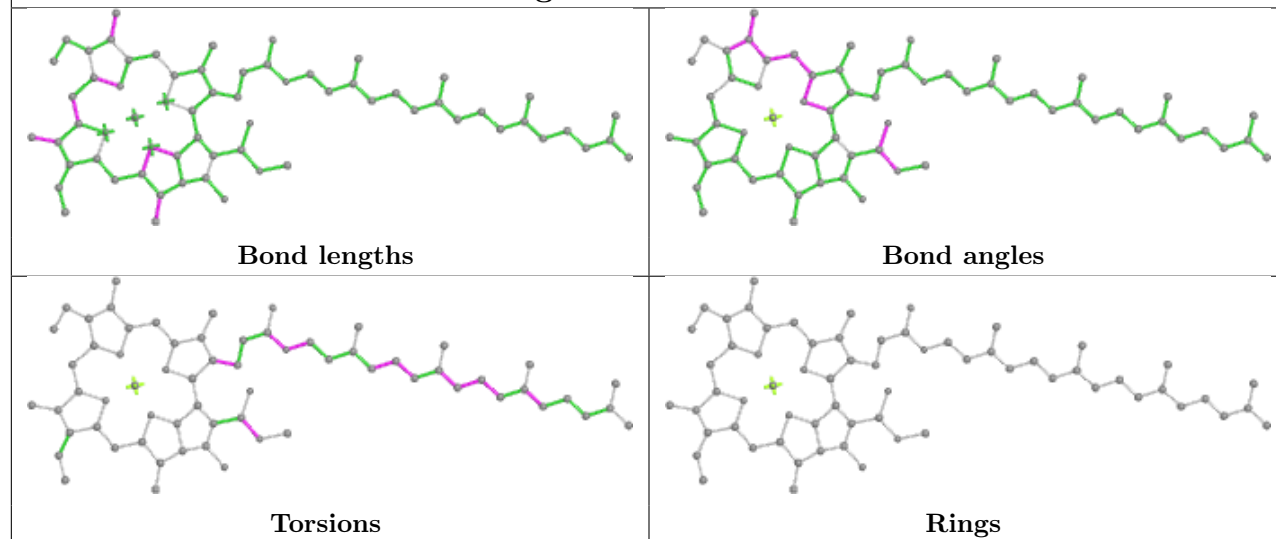
Torsions



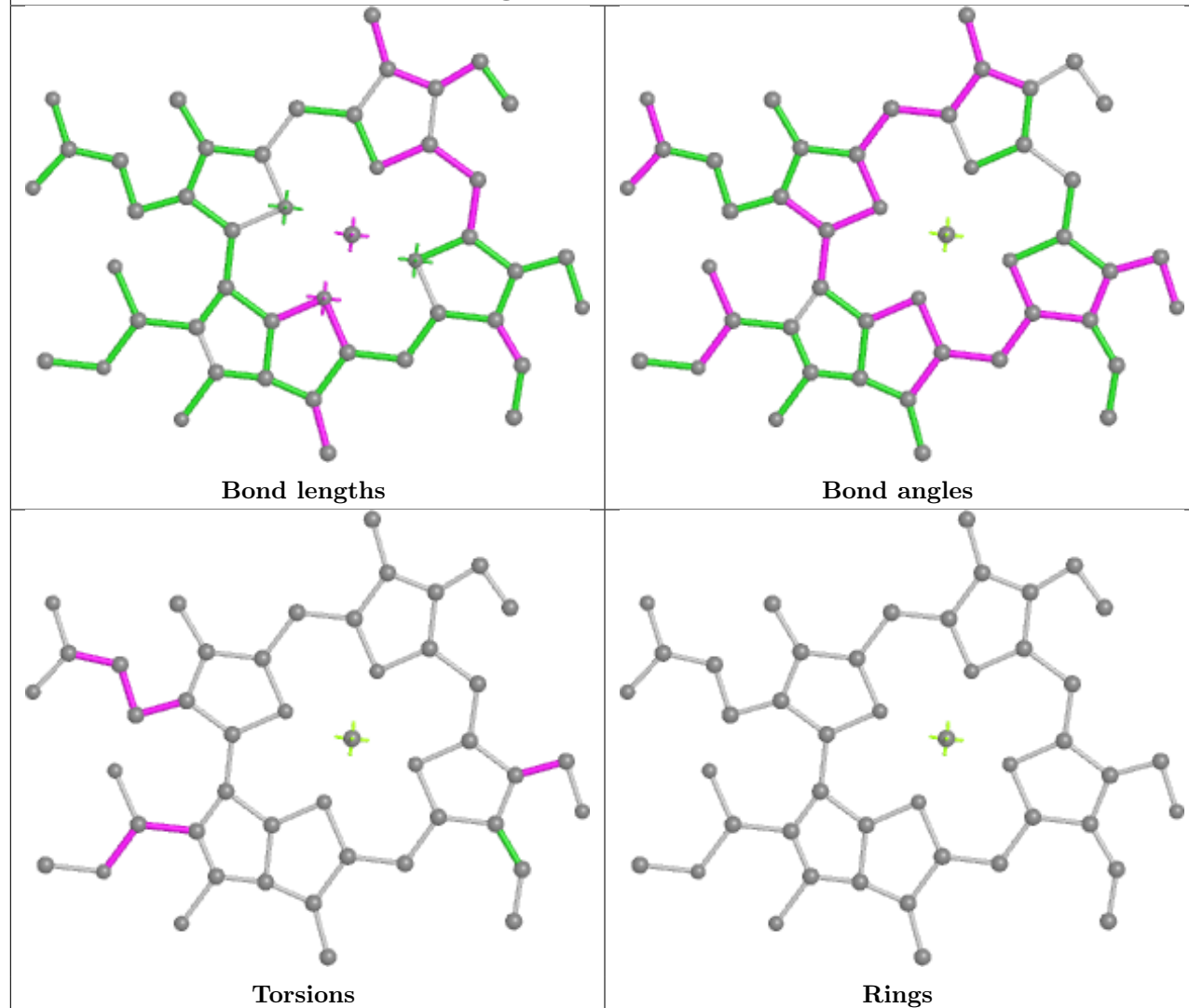
Rings

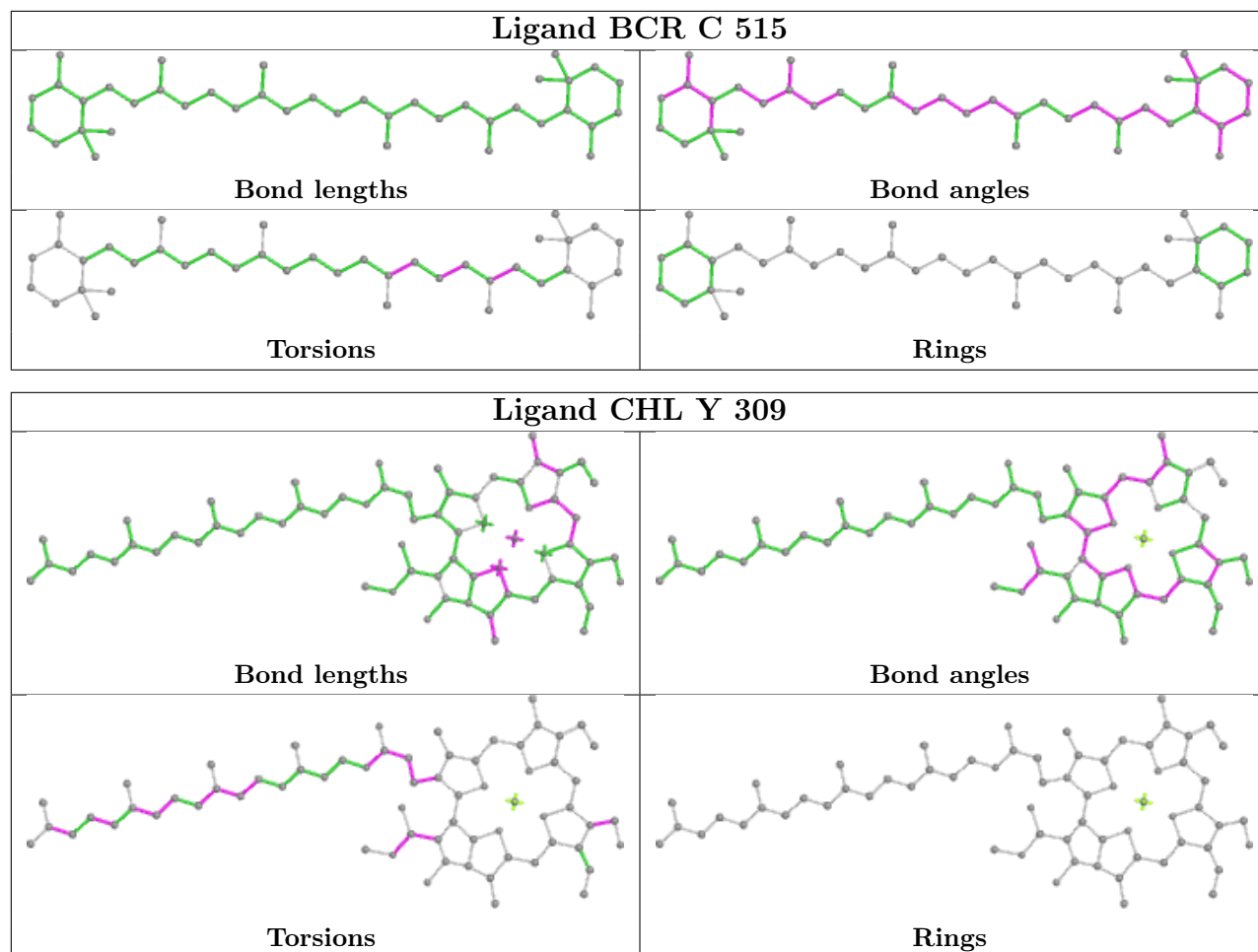
Ligand CLA C 506**Ligand CLA b 602****Ligand XAT N 301**

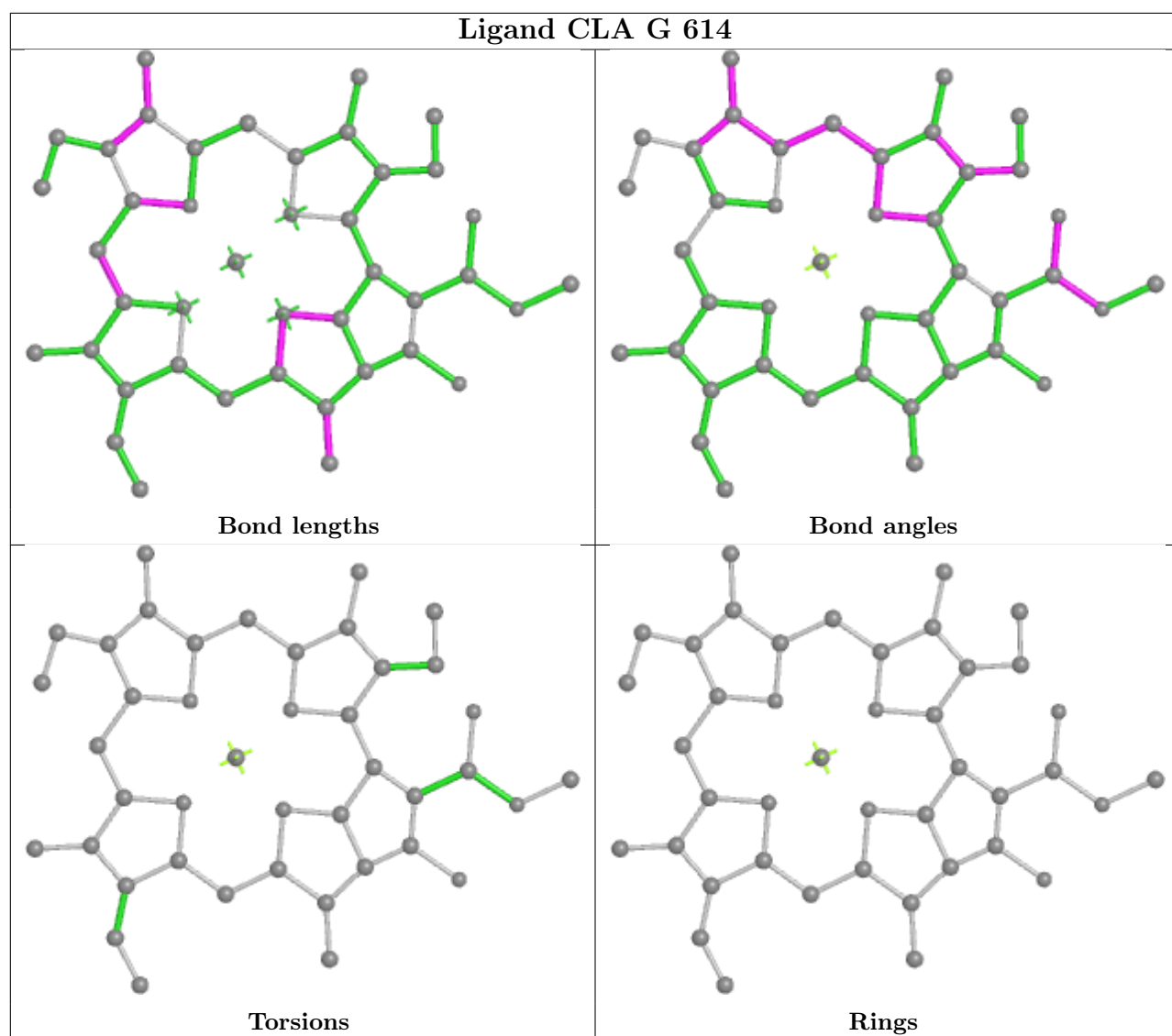
Ligand CLA b 607



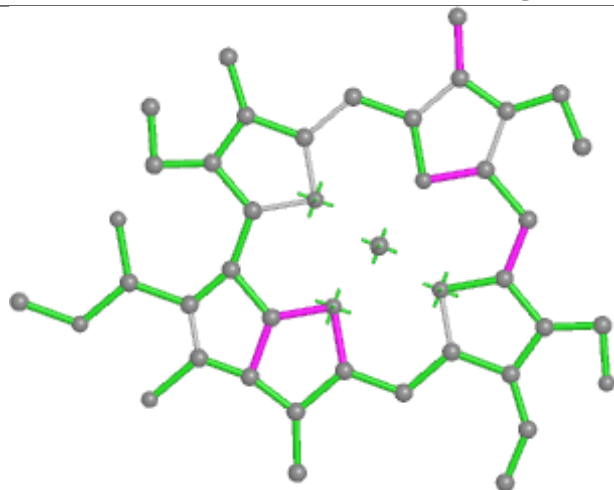
Ligand CHL S 605



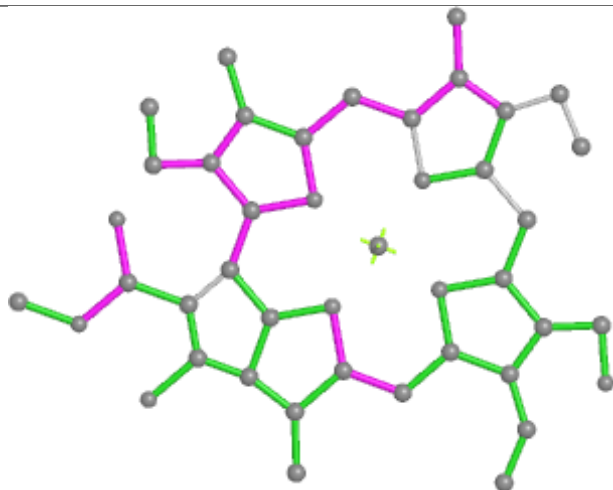




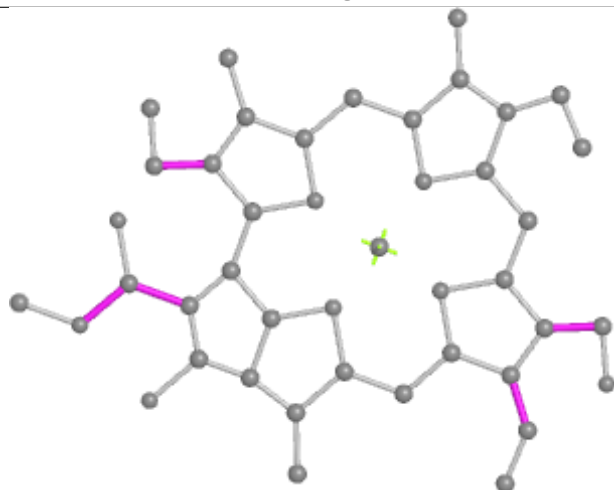
Ligand CHL S 606



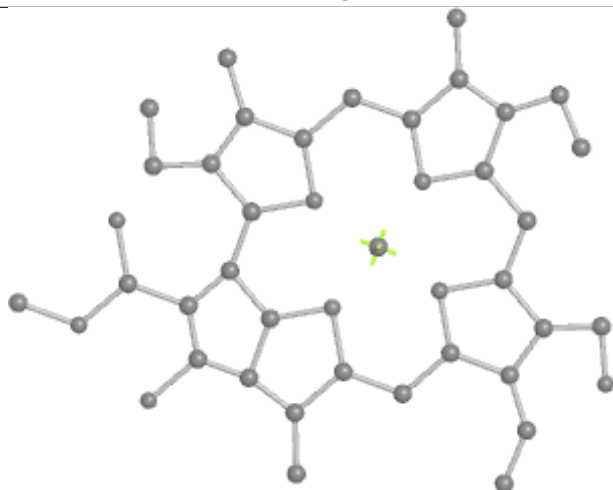
Bond lengths



Bond angles

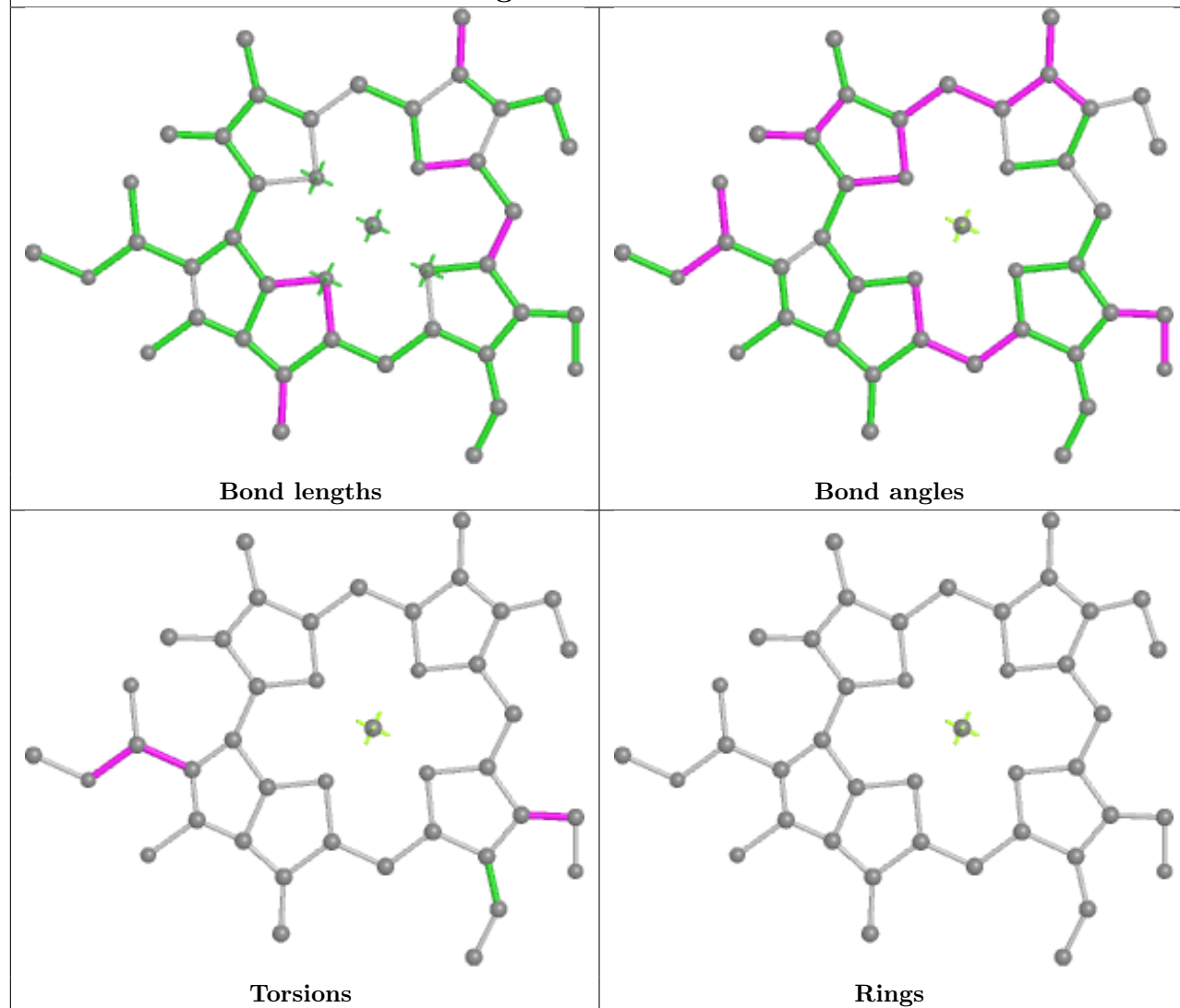


Torsions

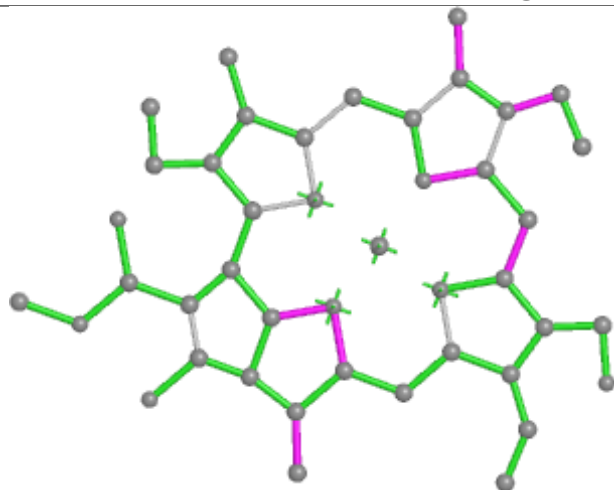


Rings

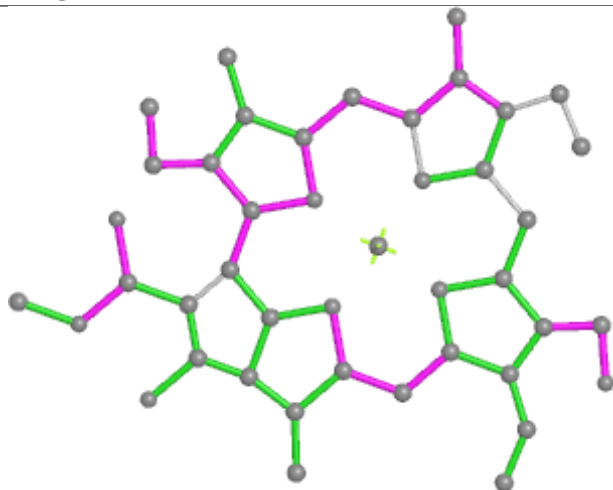
Ligand CHL r 613



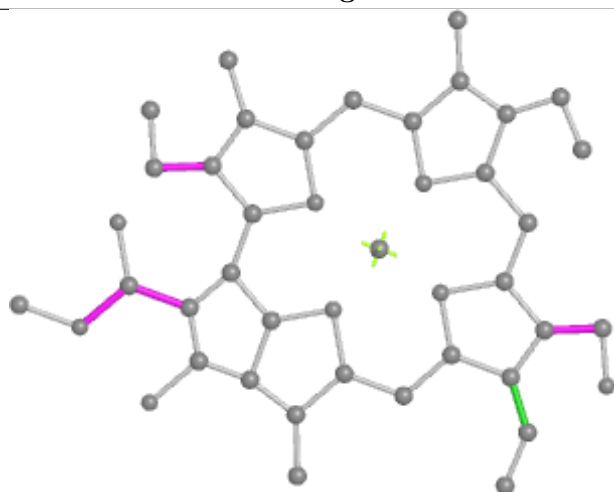
Ligand CHL g 607



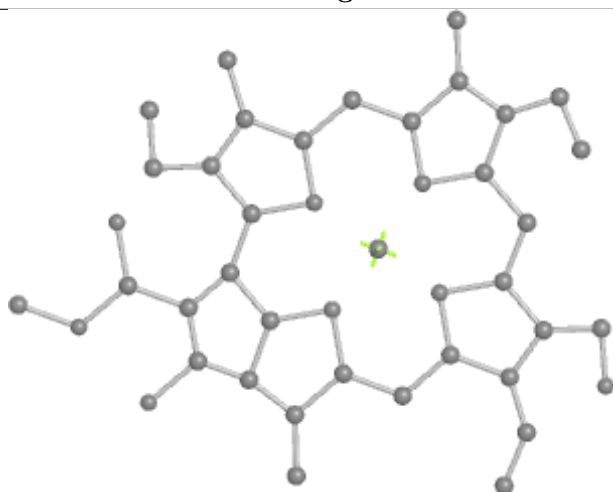
Bond lengths



Bond angles

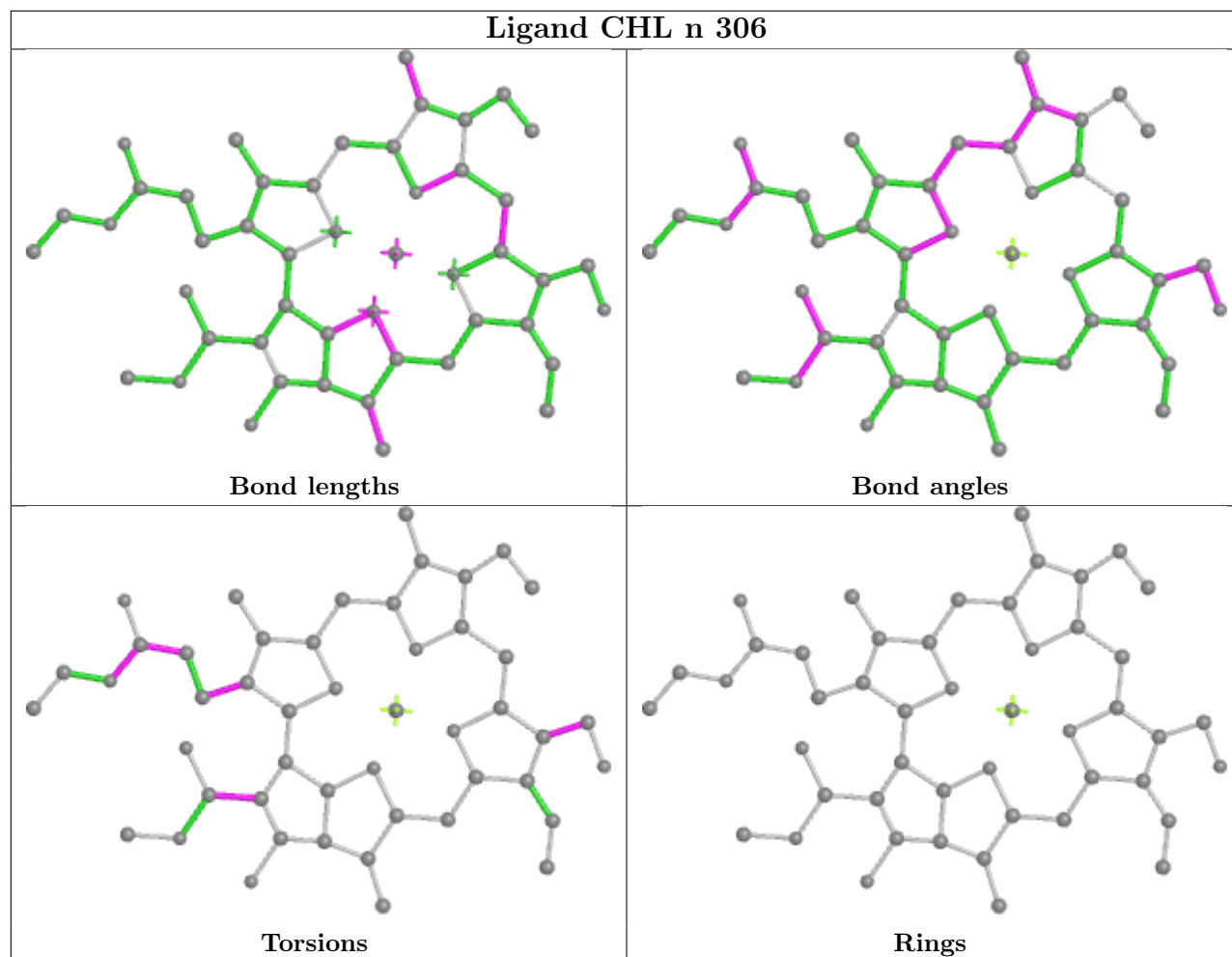


Torsions

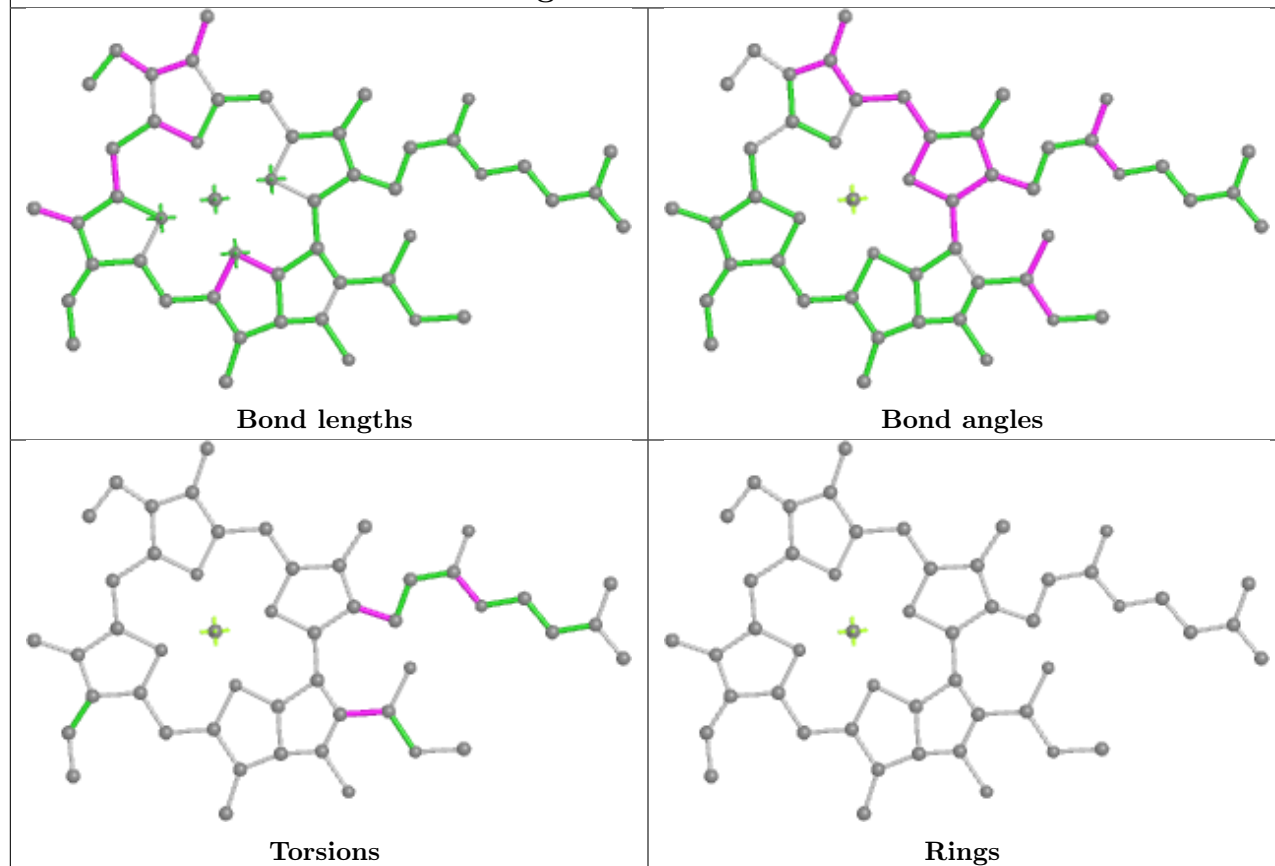


Rings

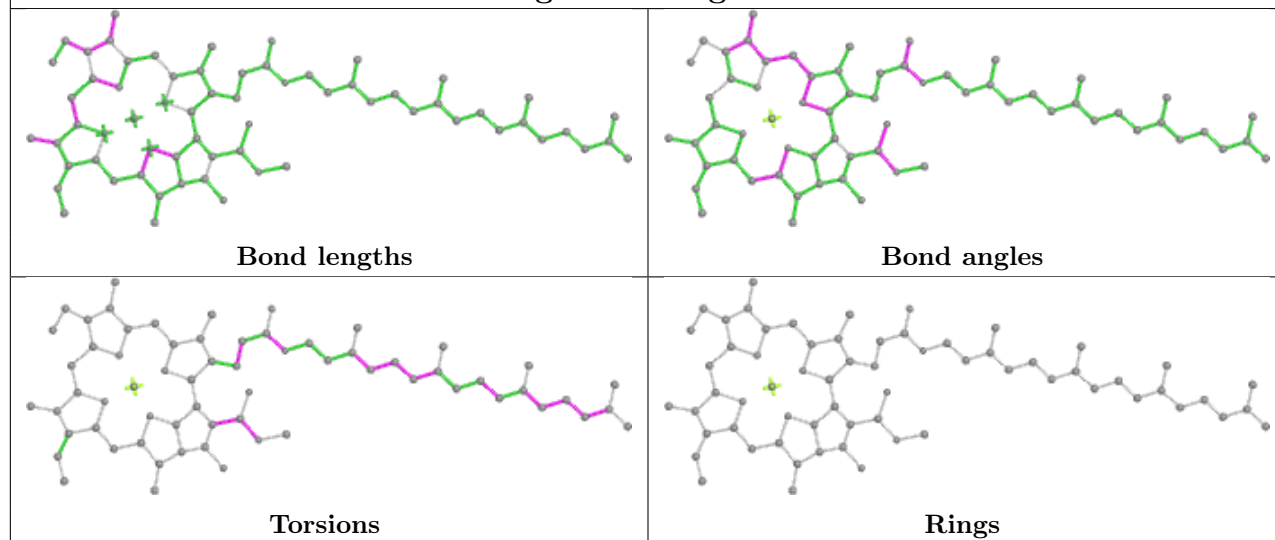
Ligand CHL n 306

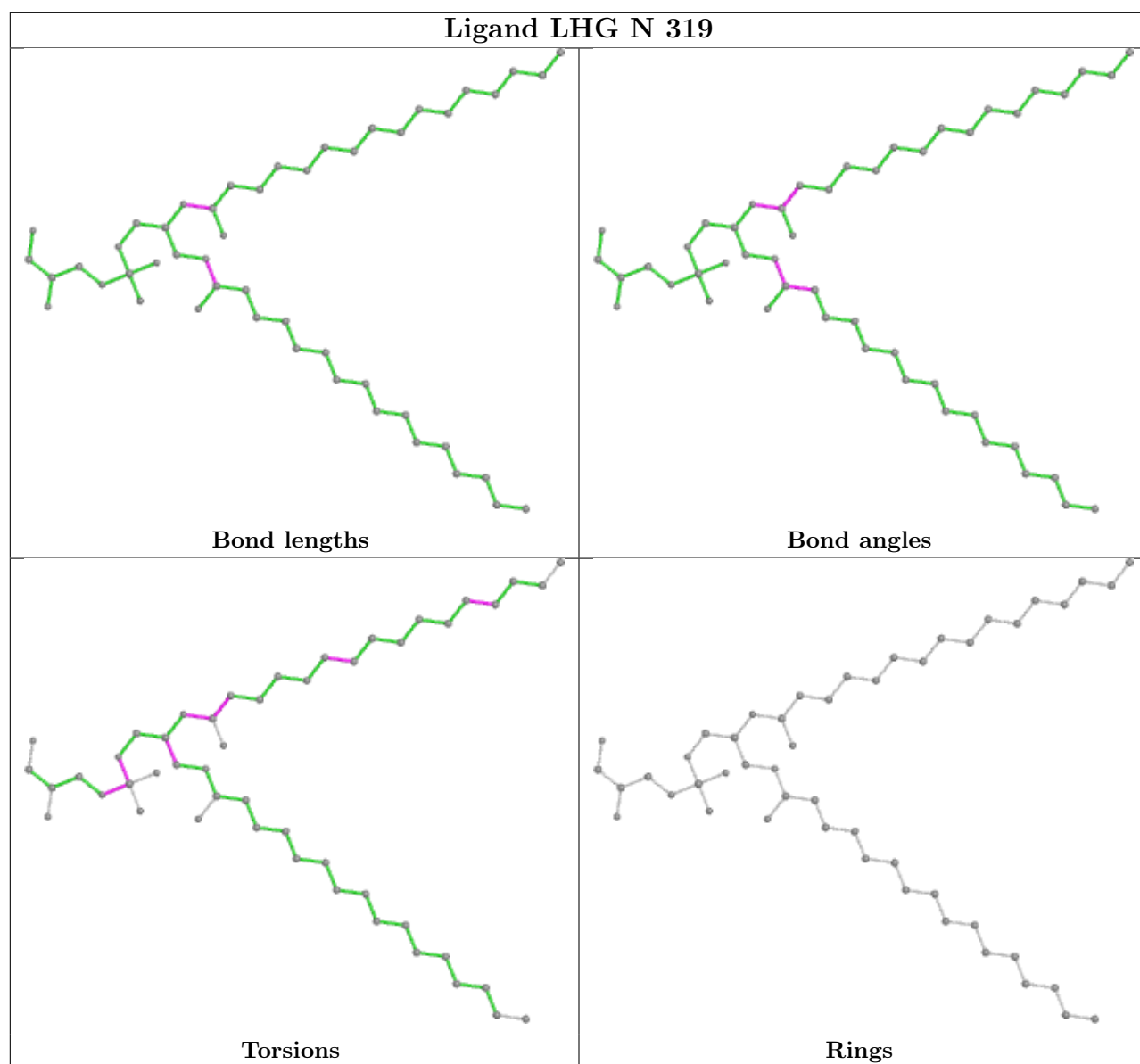


Ligand CLA s 604

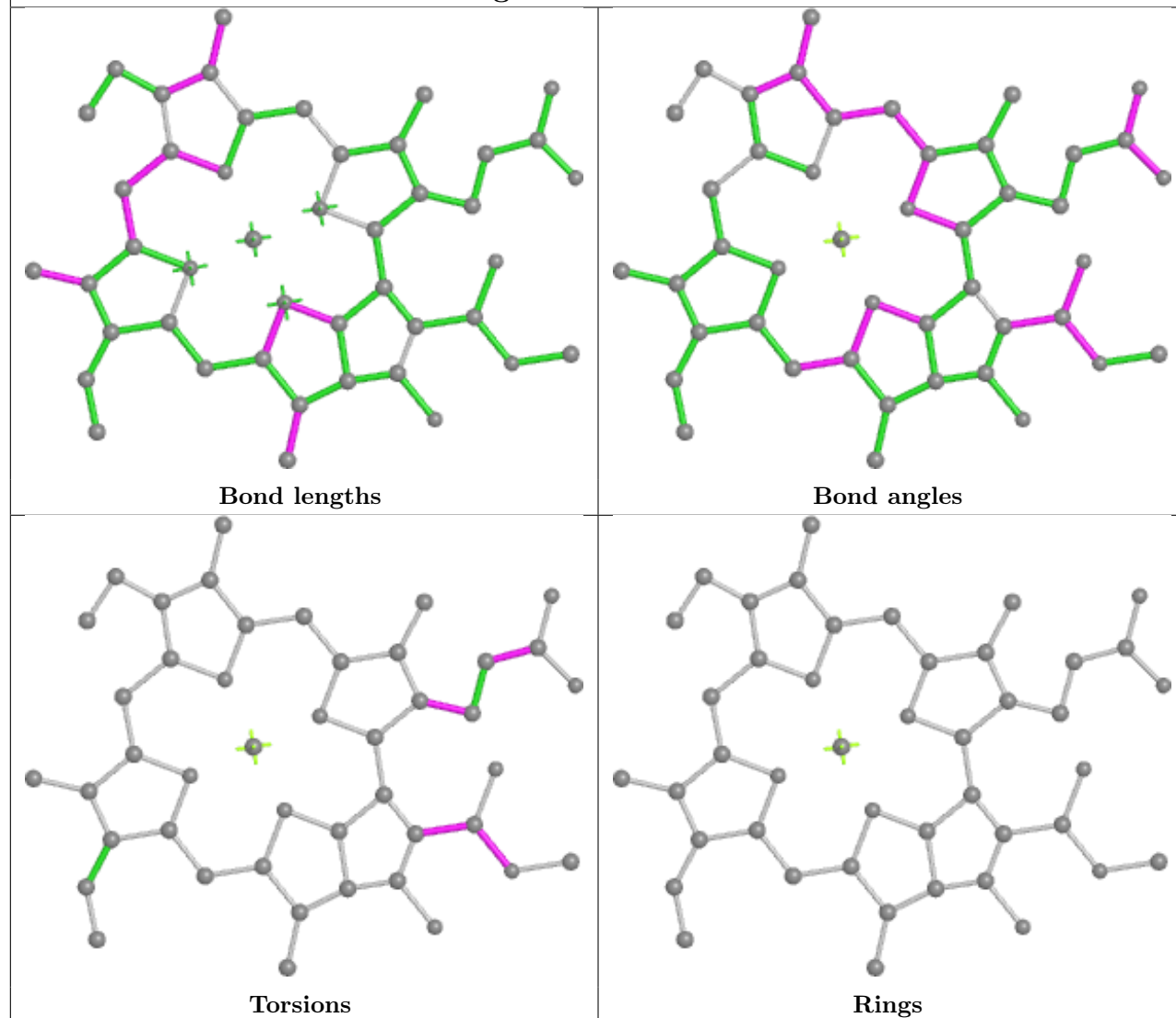


Ligand CLA g 602

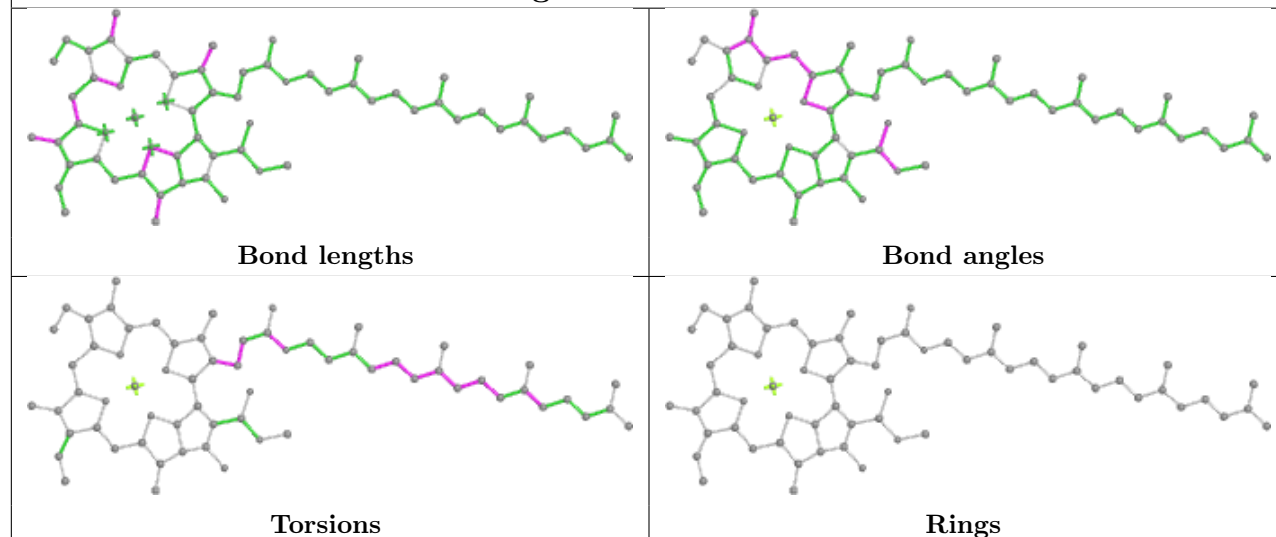


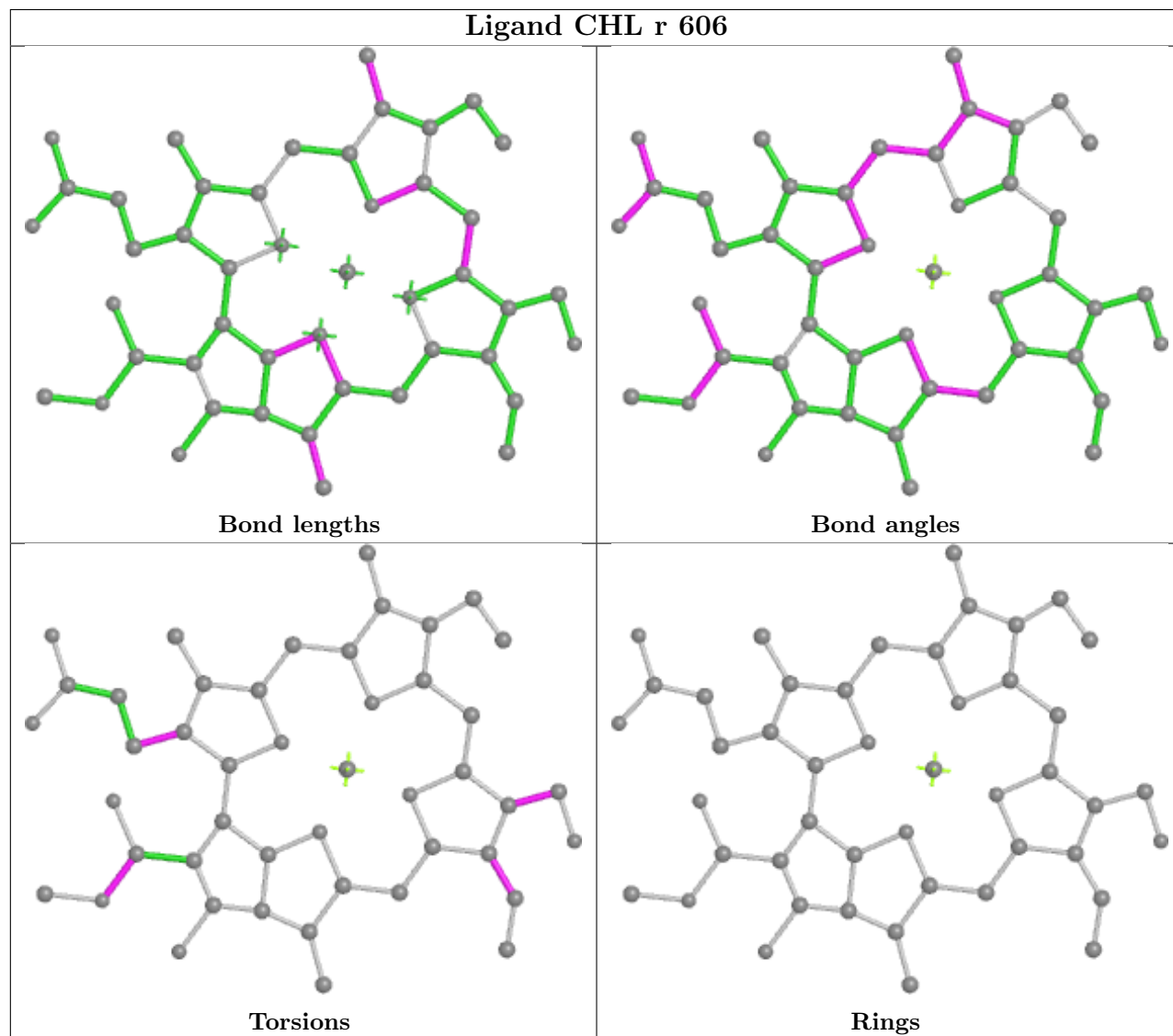
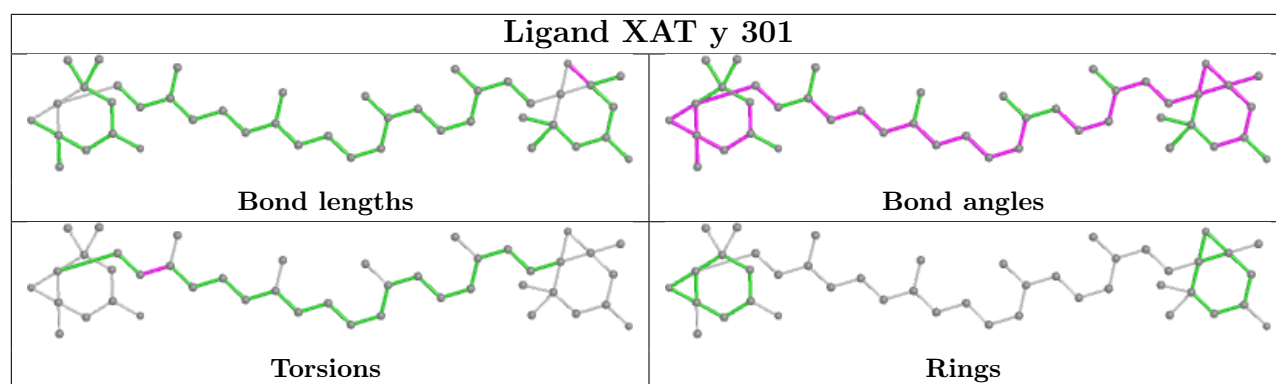


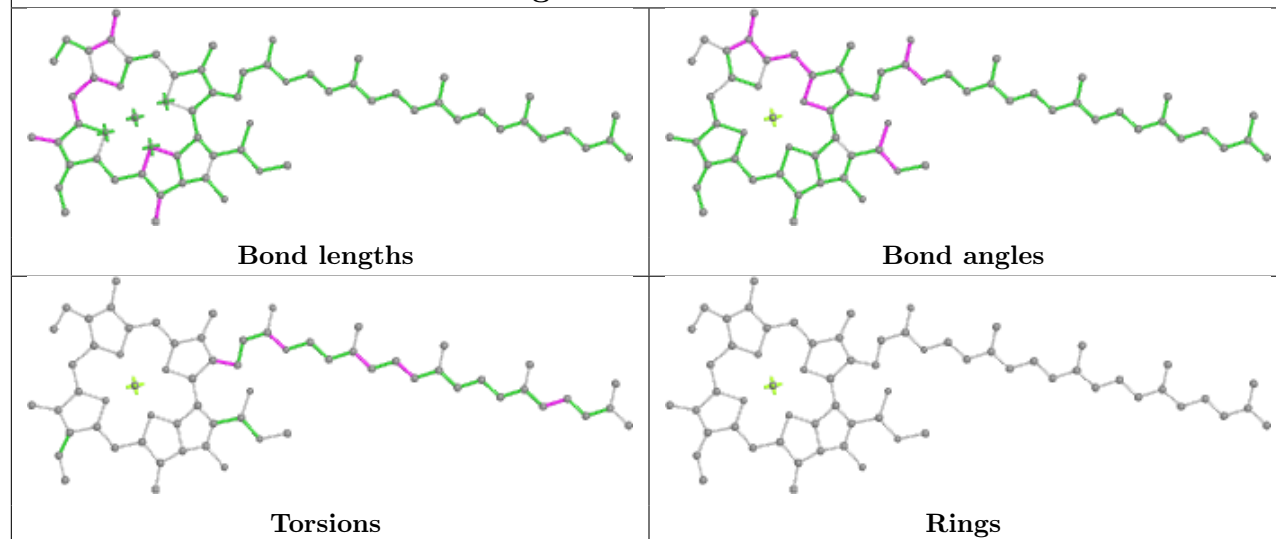
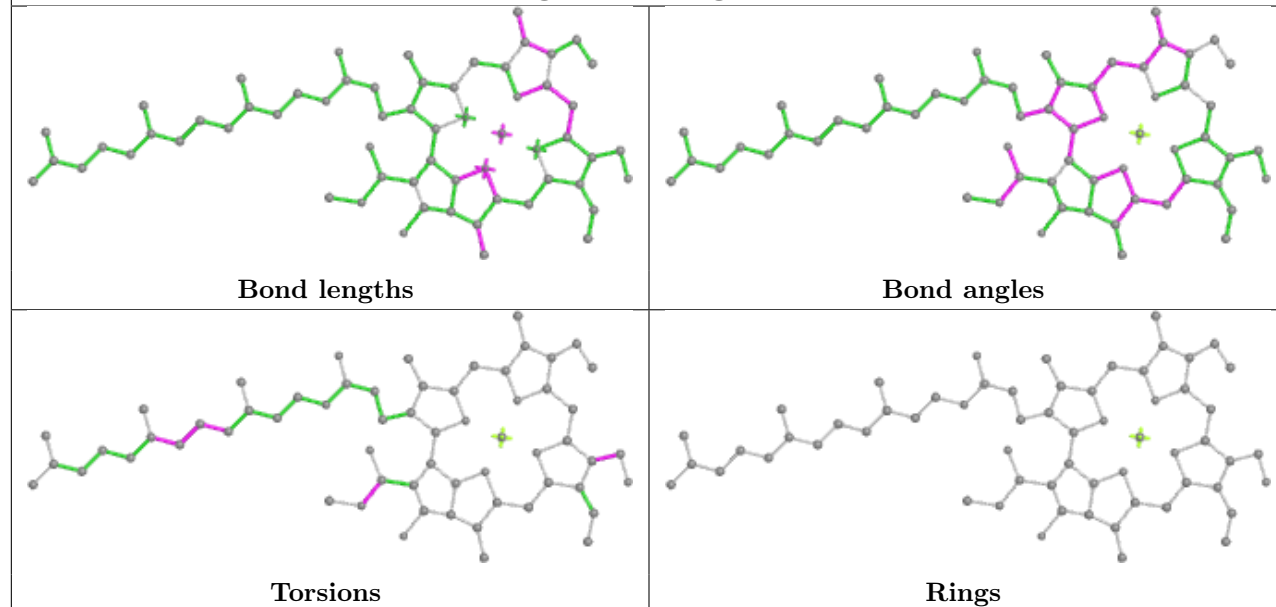
Ligand CLA S 609

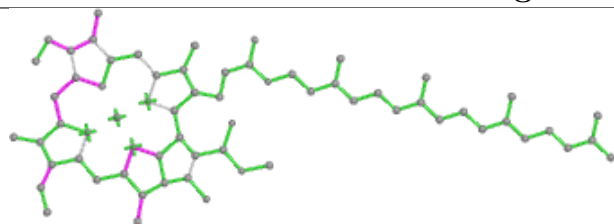
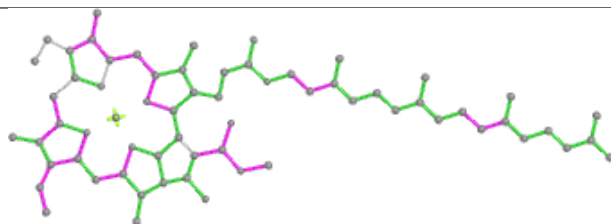
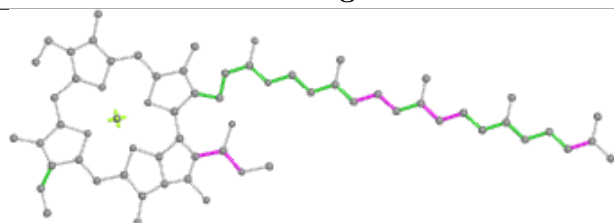
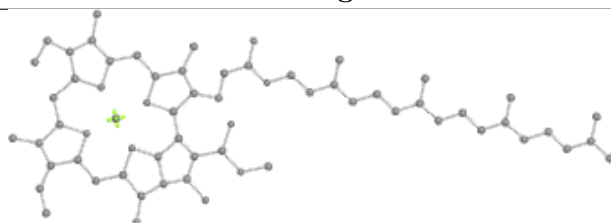
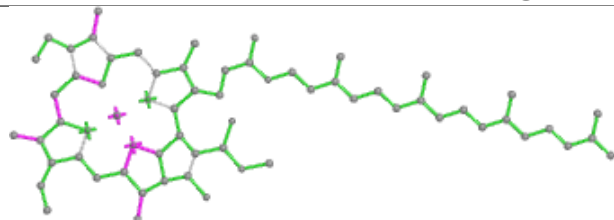
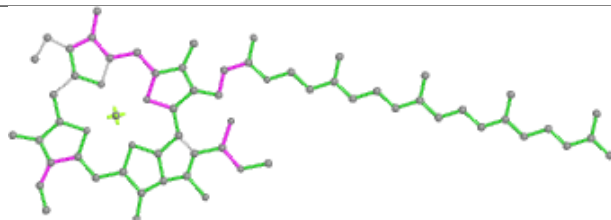
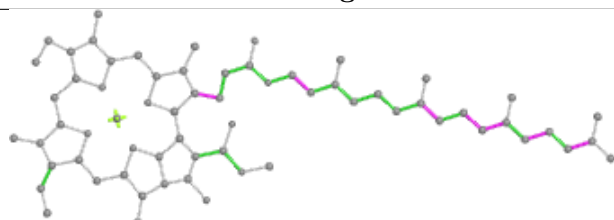
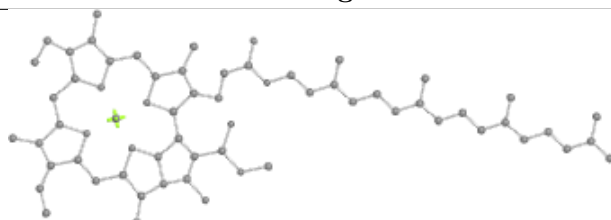


Ligand CLA B 612

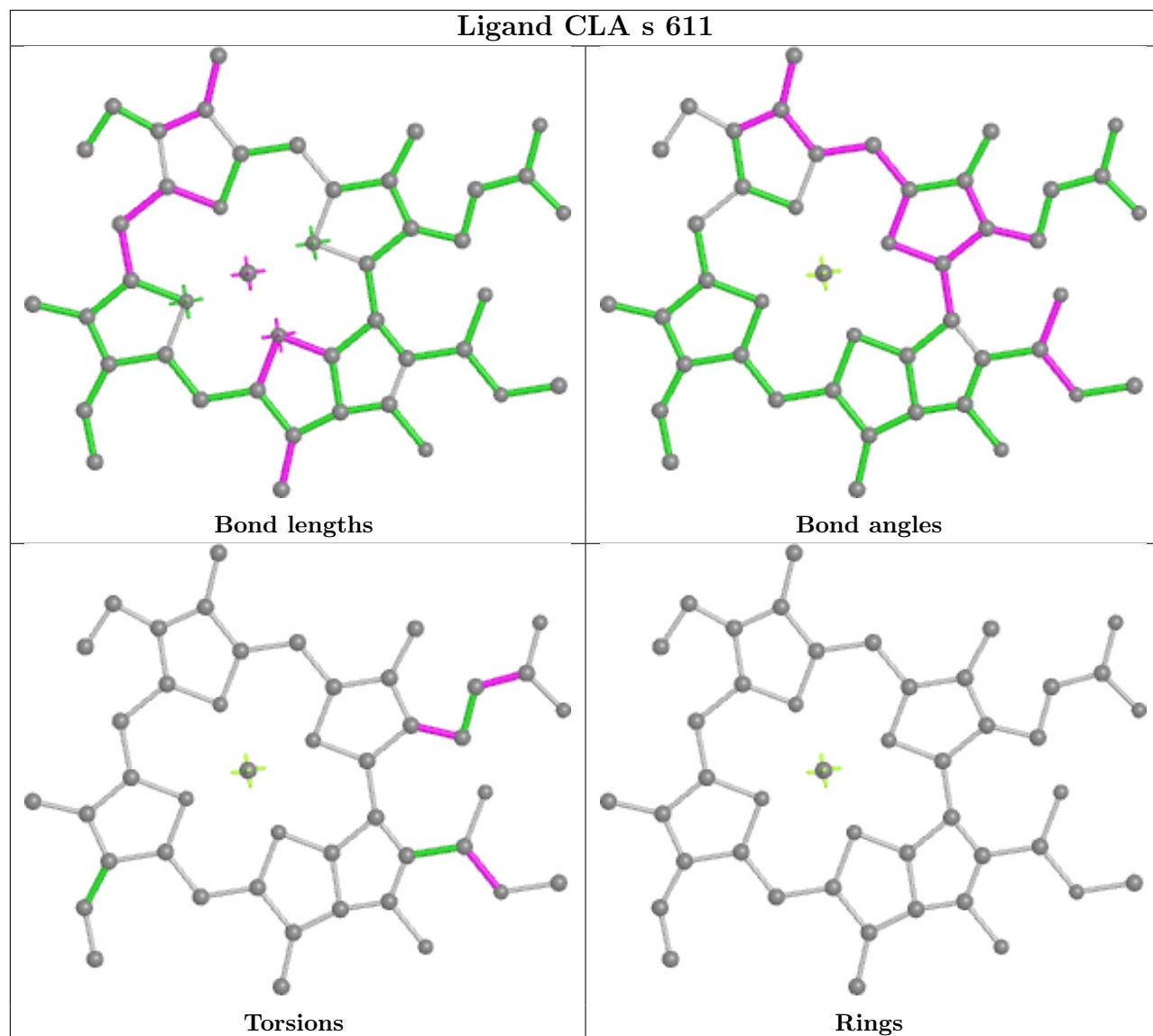




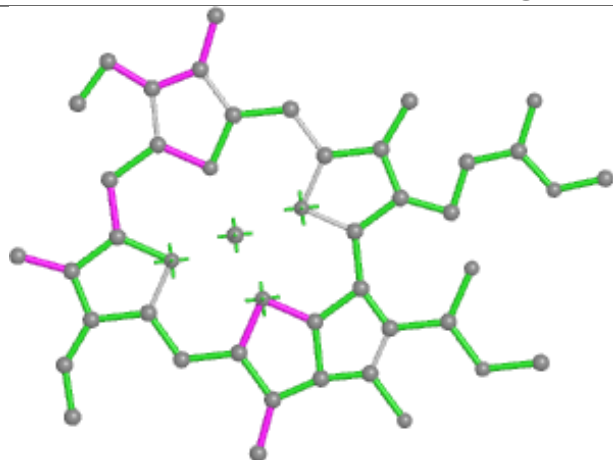
Ligand CLA B 611**Ligand CHL g 609**

Ligand CLA B 605**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA d 404****Bond lengths****Bond angles****Torsions****Rings**

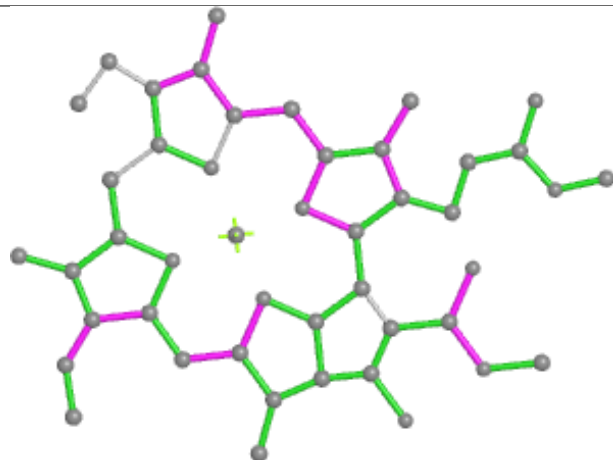
Ligand CLA s 611



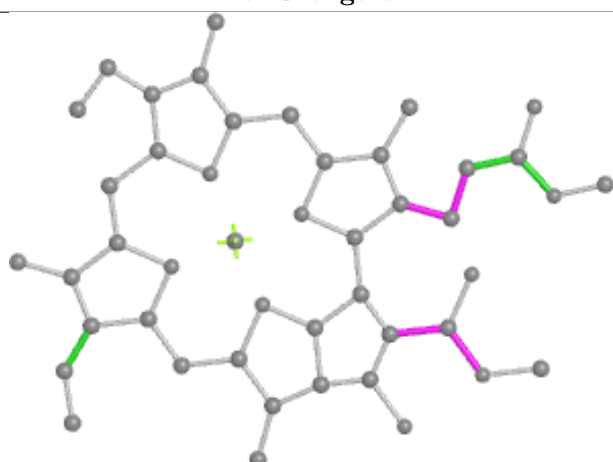
Ligand CLA S 602



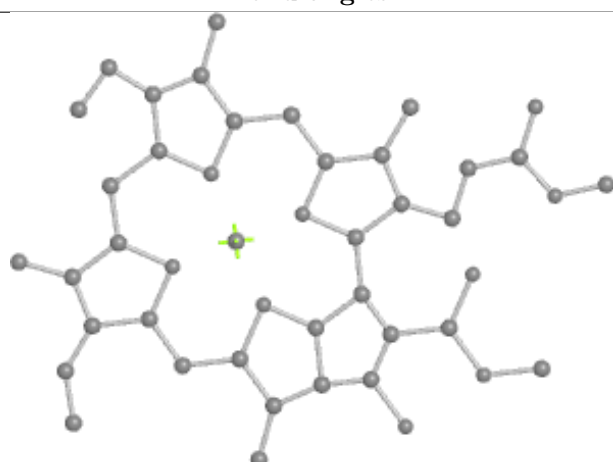
Bond lengths



Bond angles

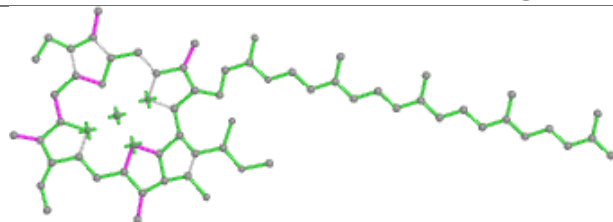


Torsions

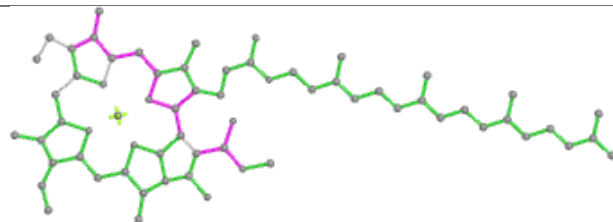


Rings

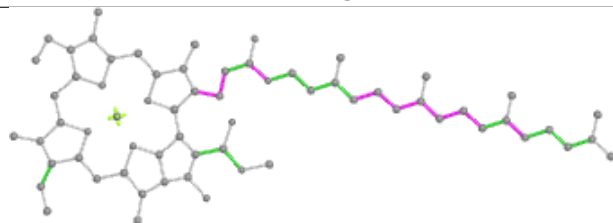
Ligand CLA b 612



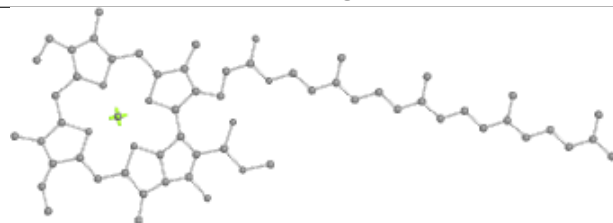
Bond lengths



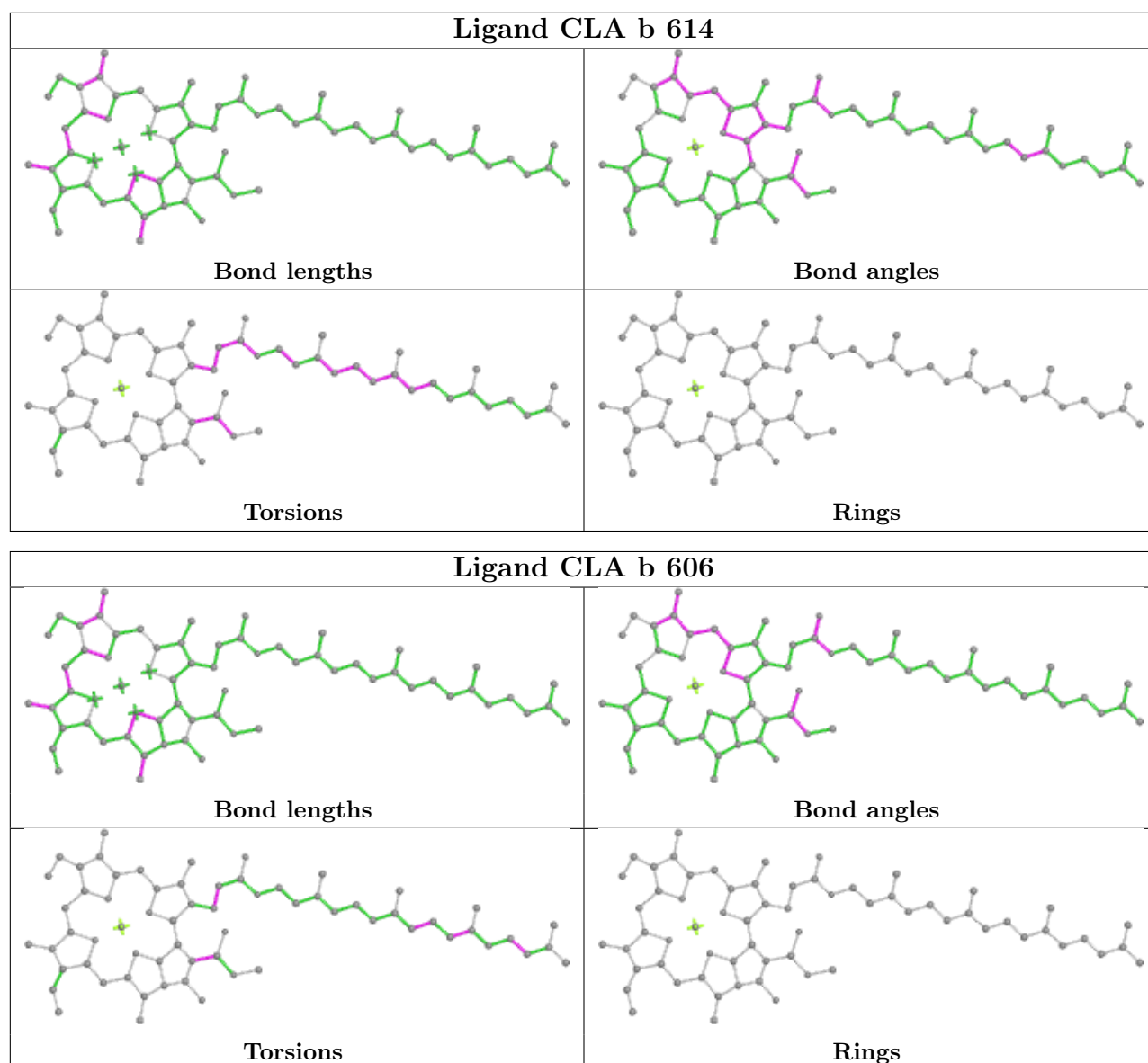
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

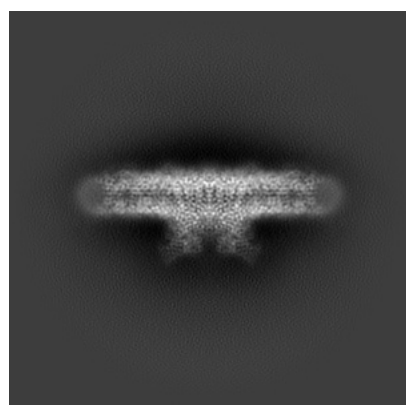
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63167. These allow visual inspection of the internal detail of the map and identification of artifacts.

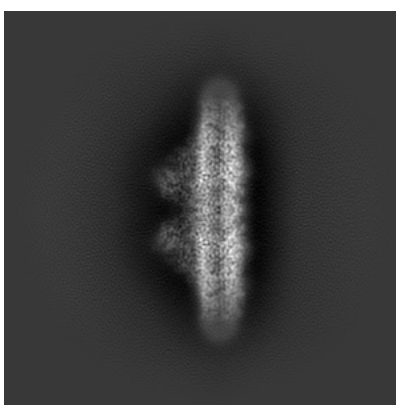
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

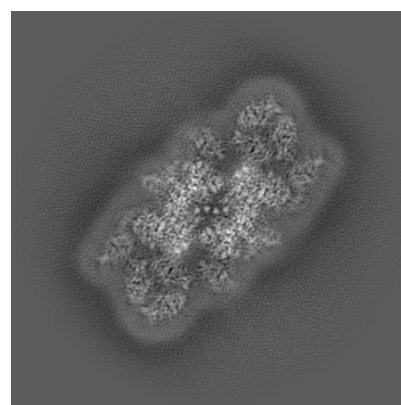
6.1.1 Primary map



X



Y

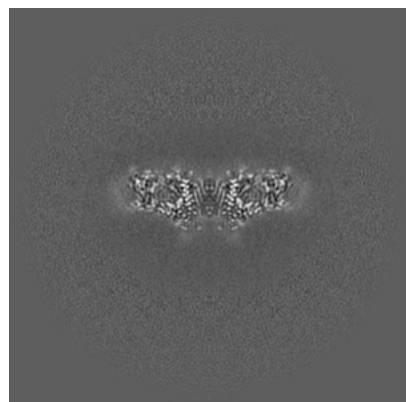


Z

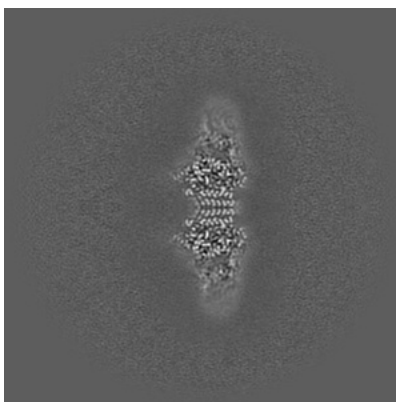
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

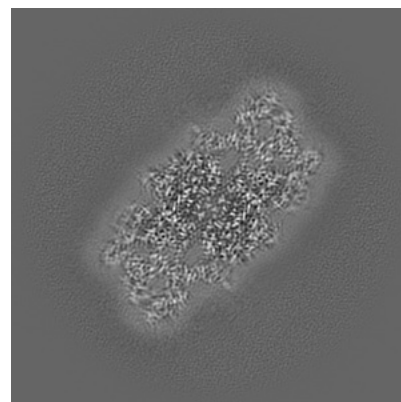
6.2.1 Primary map



X Index: 200



Y Index: 200

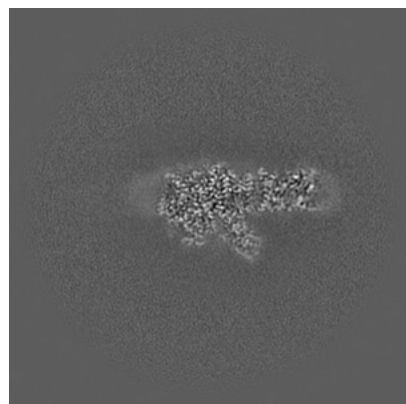


Z Index: 200

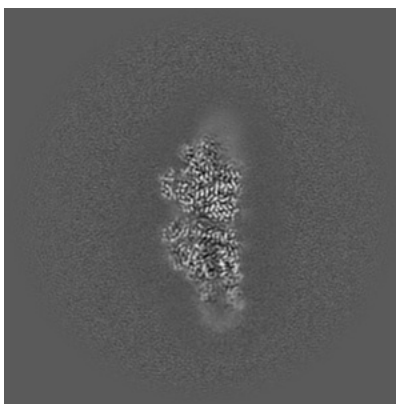
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

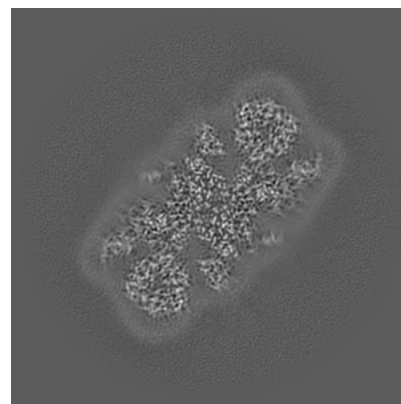
6.3.1 Primary map



X Index: 236



Y Index: 177

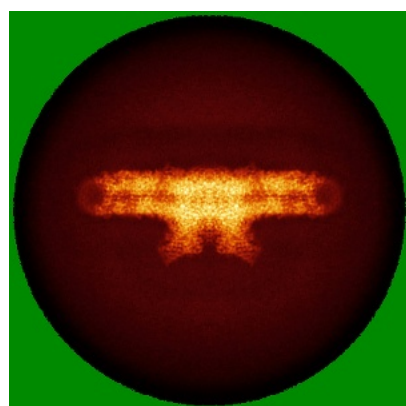


Z Index: 222

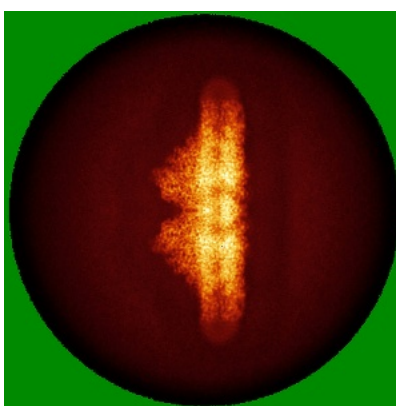
The images above show the largest variance slices of the map in three orthogonal directions.

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

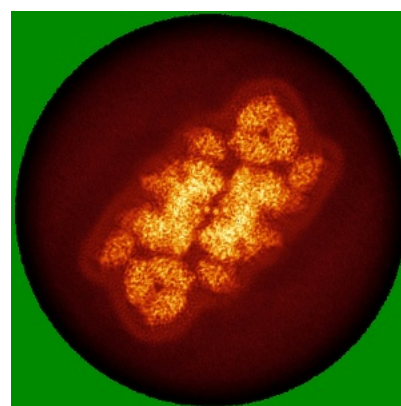
6.4.1 Primary map



X



Y

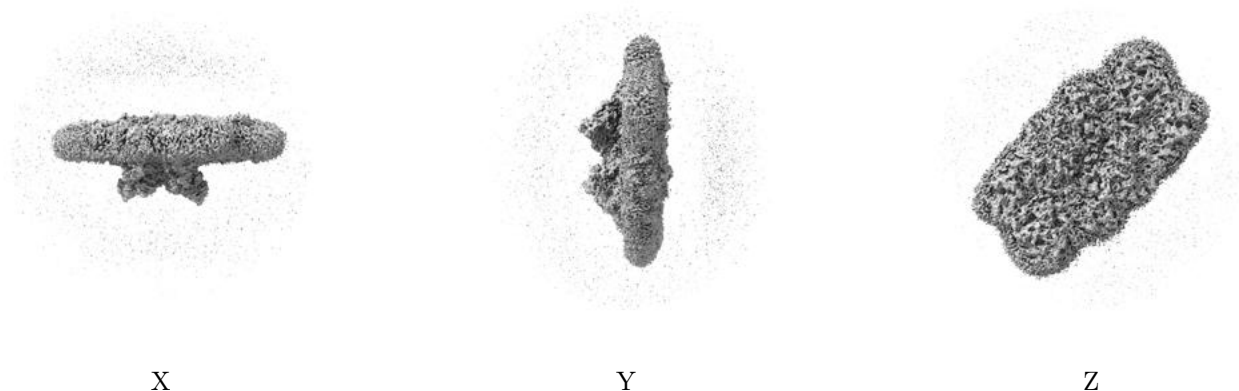


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

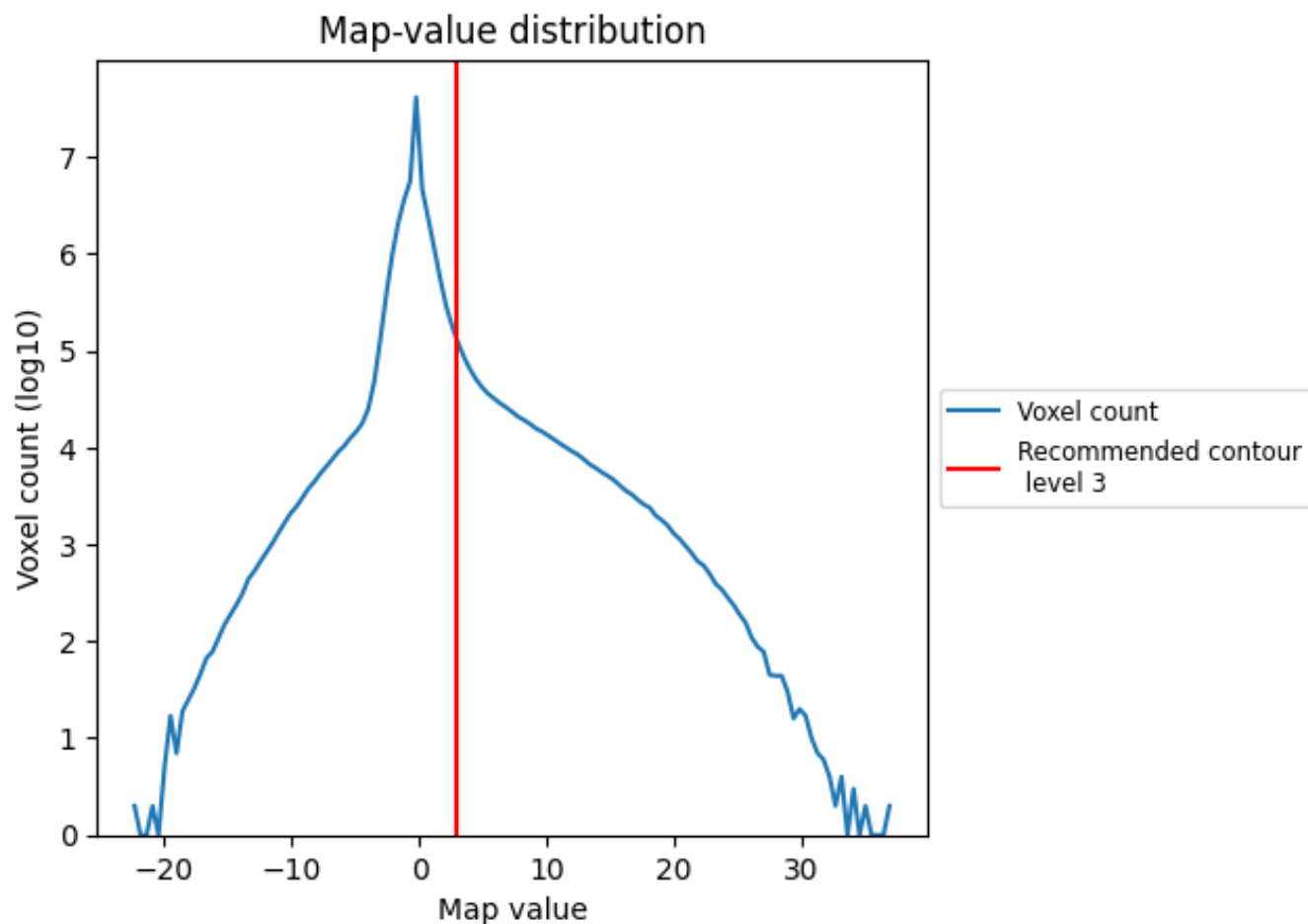
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

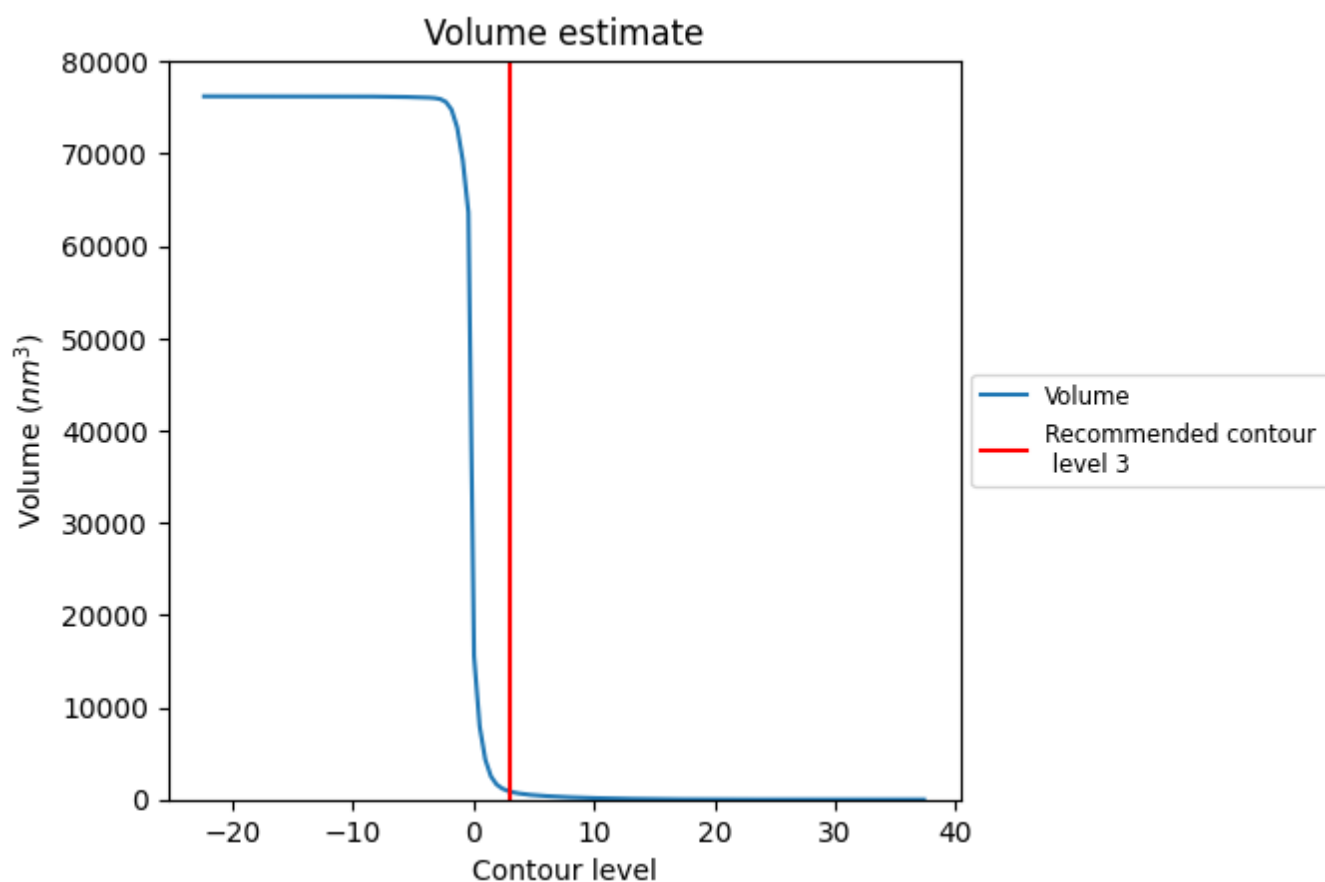
This section contains the results of statistical analysis of the map.

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.

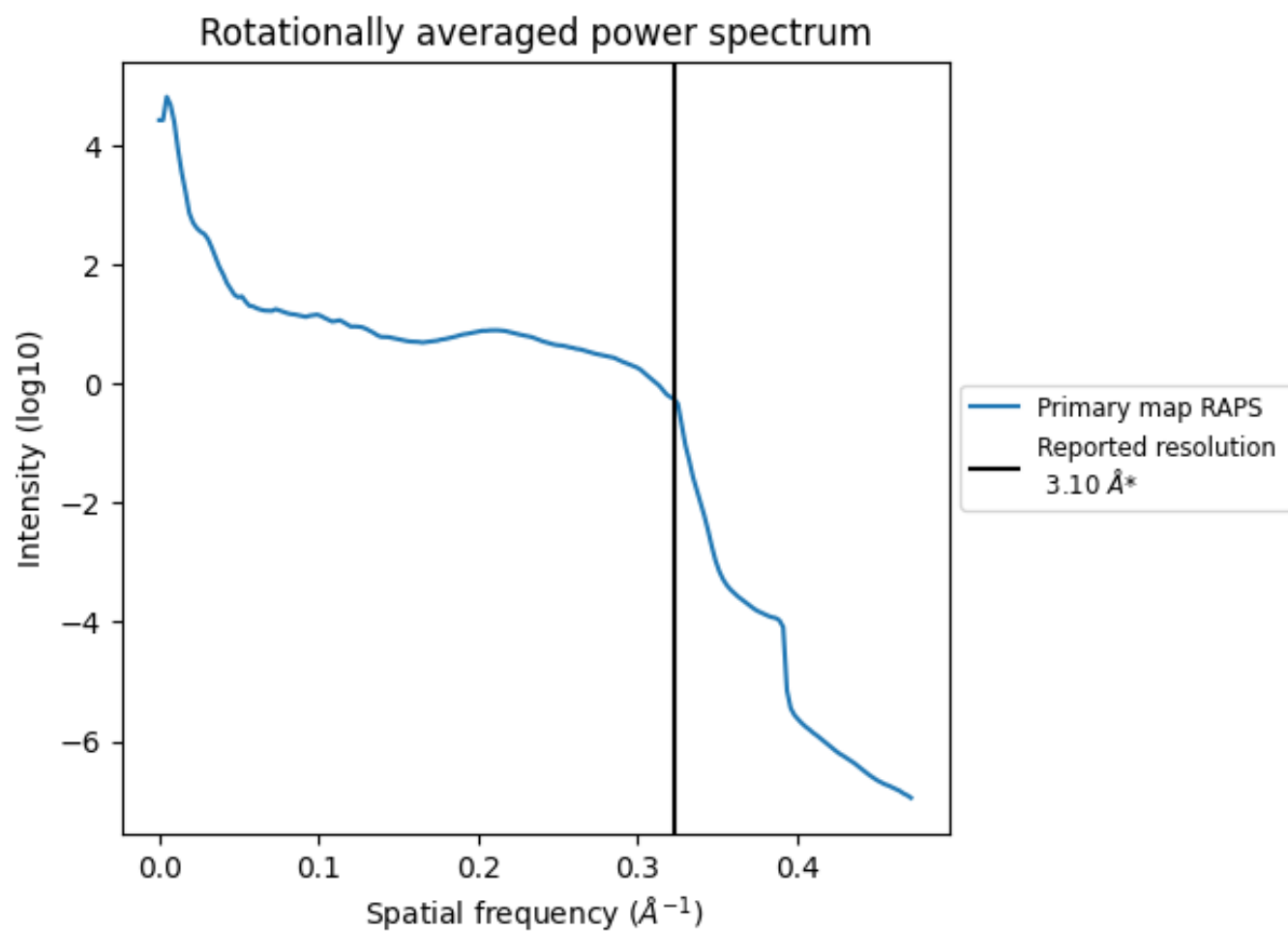
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 896 nm³; this corresponds to an approximate mass of 809 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

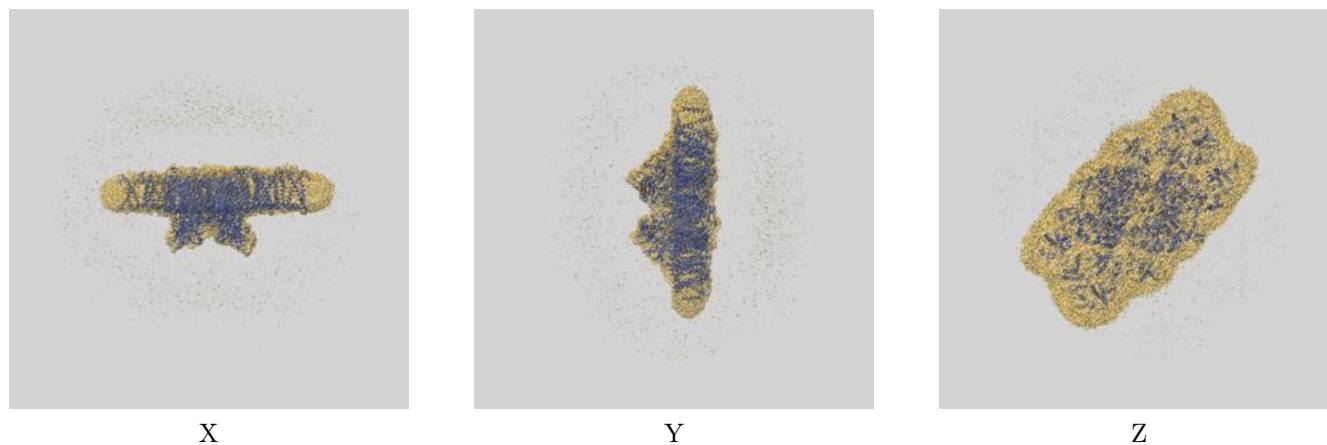
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

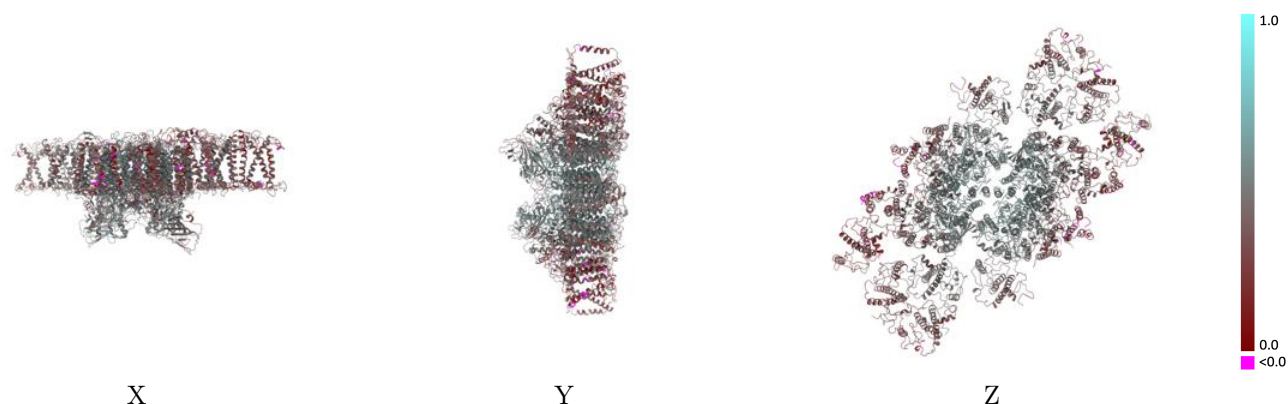
This section contains information regarding the fit between EMDB map EMD-63167 and PDB model 9LK4. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



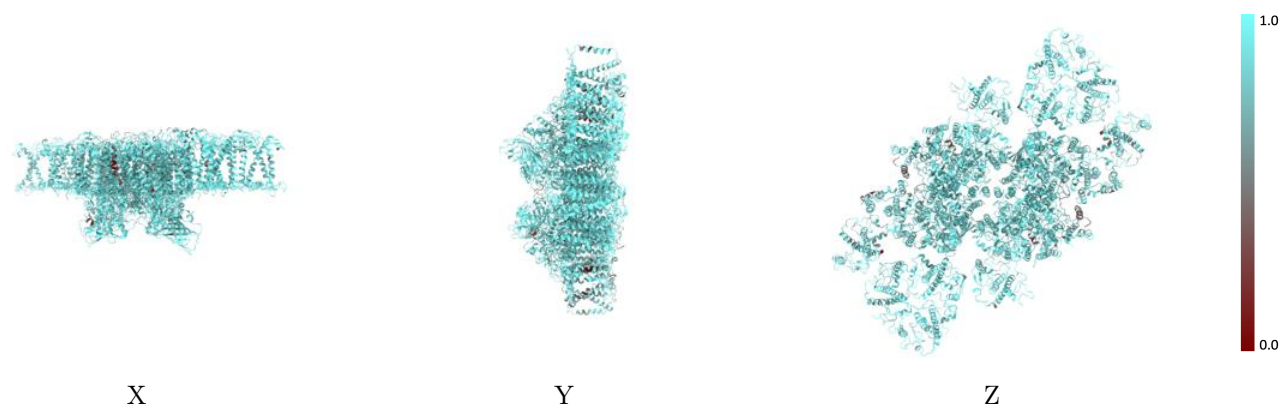
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



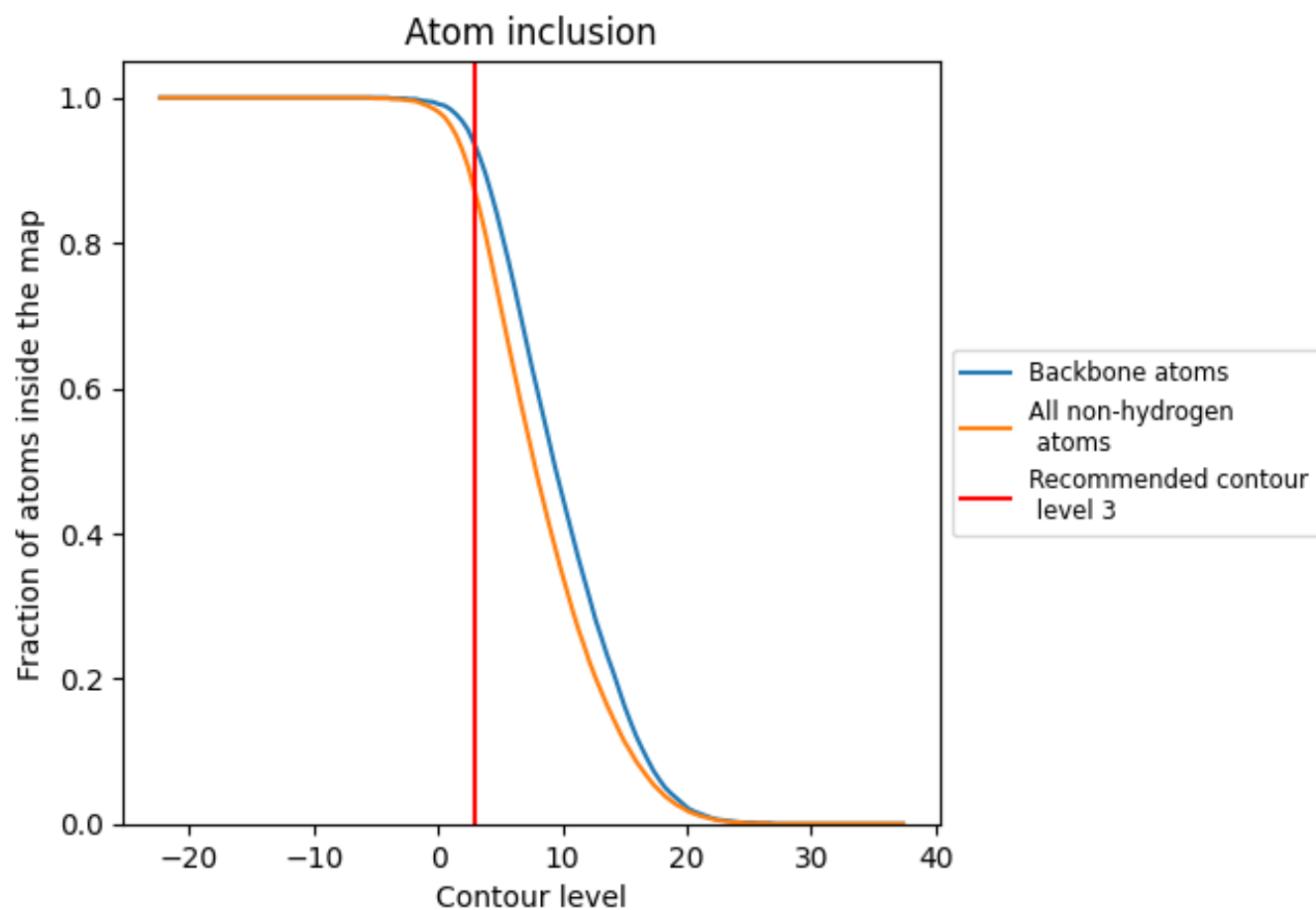
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.4220
A	 0.9160	 0.4940
B	 0.9350	 0.5310
C	 0.8450	 0.3820
D	 0.9130	 0.4760
E	 0.8370	 0.2940
F	 0.8050	 0.2910
G	 0.8560	 0.3620
H	 0.9180	 0.4740
I	 0.9260	 0.5020
J	 0.4020	 0.1440
K	 0.7800	 0.3440
L	 0.9250	 0.5530
M	 0.8810	 0.5120
N	 0.8230	 0.3550
O	 0.8600	 0.4430
R	 0.8590	 0.4150
S	 0.7930	 0.2840
T	 0.9260	 0.5410
U	 0.5770	 0.4010
W	 0.8340	 0.4490
X	 0.7830	 0.3340
Y	 0.8870	 0.4450
Z	 0.7420	 0.2760
a	 0.9270	 0.5010
b	 0.9380	 0.5300
c	 0.8470	 0.3790
d	 0.9030	 0.4730
e	 0.8400	 0.3080
f	 0.8640	 0.2750
g	 0.8540	 0.3540
h	 0.9260	 0.4690
i	 0.9340	 0.5030
j	 0.4530	 0.1240
k	 0.7680	 0.3350



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Chain	Atom inclusion	Q-score
l	 0.9310	 0.5420
m	 0.9120	 0.5190
n	 0.8240	 0.3470
o	 0.8660	 0.4500
r	 0.8560	 0.4050
s	 0.7940	 0.2790
t	 0.9410	 0.5460
u	 0.5600	 0.3730
w	 0.8300	 0.4500
x	 0.8090	 0.3340
y	 0.8930	 0.4490
z	 0.6970	 0.1910