



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:14 AM UTC

PDB ID : 6KAC / pdb_00006kac
EMDB ID : EMD-9955
Title : Cryo-EM structure of the C2S2-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Sheng, X.; Li, A.J.; Song, D.F.; Liu, Z.F.
Deposited on : 2019-06-21
Resolution : 2.70 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

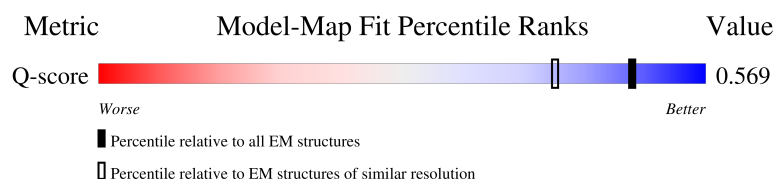
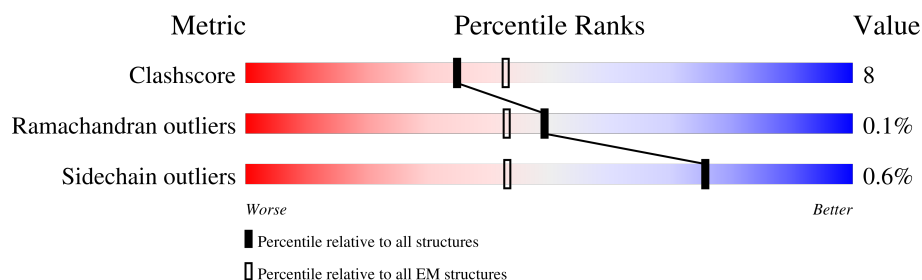
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



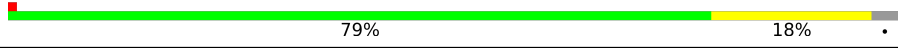
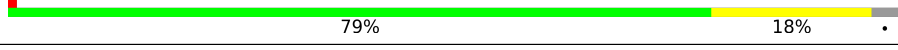
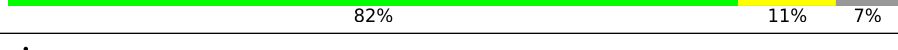
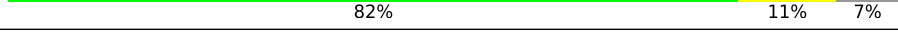
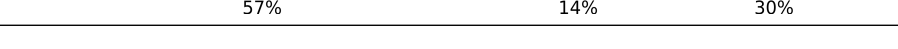
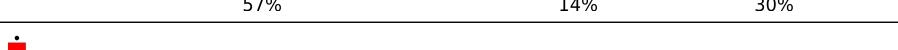
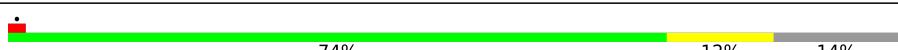
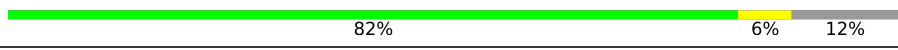
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	352	
1	a	352	
2	B	508	
2	b	508	

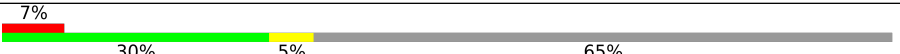
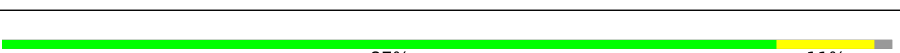
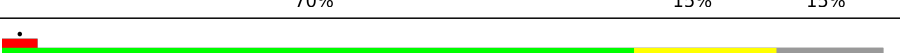
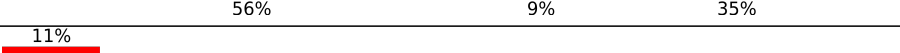
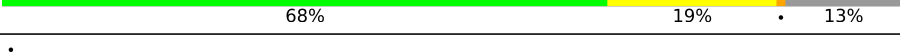
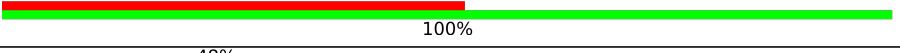
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	V	33	
3	v	33	
4	C	461	
4	c	461	
5	D	352	
5	d	352	
6	E	82	
6	e	82	
7	F	44	
7	f	44	
8	H	88	
8	h	88	
9	I	37	
9	i	37	
10	J	42	
10	j	42	
11	K	46	
11	k	46	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	291	
14	o	291	
15	P	245	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	p	245	
16	Q	199	
16	q	199	
17	T	31	
17	t	31	
18	W	115	
18	w	115	
19	X	101	
19	x	101	
20	Z	62	
20	z	62	
21	N	257	
21	n	257	
22	G	249	
22	g	249	
23	R	280	
23	r	280	
24	S	289	
24	s	289	
25	Y	256	
25	y	256	
26	U	178	
26	u	178	
27	0	25	
27	1	25	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	3	25	64% 100%
28	4	25	60% 92% 8%

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
32	CLA	A	405	X	-	-	-
32	CLA	A	407	X	-	-	-
32	CLA	B	602	X	-	-	-
32	CLA	B	603	X	-	-	-
32	CLA	B	605	X	-	-	-
32	CLA	B	606	X	-	-	-
32	CLA	B	607	X	-	-	-
32	CLA	B	608	X	-	-	-
32	CLA	B	609	X	-	-	-
32	CLA	B	611	X	-	-	-
32	CLA	B	612	X	-	-	-
32	CLA	B	613	X	-	-	-
32	CLA	B	614	X	-	-	-
32	CLA	B	615	X	-	-	-
32	CLA	B	616	X	-	-	-
32	CLA	B	617	X	-	-	-
32	CLA	C	501	X	-	-	-
32	CLA	C	503	X	-	-	-
32	CLA	C	504	X	-	-	-
32	CLA	C	507	X	-	-	-
32	CLA	C	508	X	-	-	-
32	CLA	C	509	X	-	-	-
32	CLA	C	510	X	-	-	-
32	CLA	C	512	X	-	-	-
32	CLA	C	513	X	-	-	-
32	CLA	D	402	X	-	-	-
32	CLA	G	602	X	-	-	-
32	CLA	G	603	X	-	-	-
32	CLA	G	604	X	-	-	-
32	CLA	G	610	X	-	-	-
32	CLA	G	611	X	-	-	-
32	CLA	G	612	X	-	-	-
32	CLA	G	614	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	N	602	X	-	-	-
32	CLA	N	603	X	-	-	-
32	CLA	N	604	X	-	-	-
32	CLA	N	610	X	-	-	-
32	CLA	N	611	X	-	-	-
32	CLA	N	612	X	-	-	-
32	CLA	N	614	X	-	-	-
32	CLA	R	602	X	-	-	-
32	CLA	R	603	X	-	-	-
32	CLA	R	604	X	-	-	-
32	CLA	R	609	X	-	-	-
32	CLA	R	610	X	-	-	-
32	CLA	S	602	X	-	-	-
32	CLA	S	603	X	-	-	-
32	CLA	S	604	X	-	-	-
32	CLA	S	605	X	-	-	-
32	CLA	S	609	X	-	-	-
32	CLA	S	610	X	-	-	-
32	CLA	S	611	X	-	-	-
32	CLA	S	612	X	-	-	-
32	CLA	S	614	X	-	-	-
32	CLA	Y	602	X	-	-	-
32	CLA	Y	603	X	-	-	-
32	CLA	Y	604	X	-	-	-
32	CLA	Y	610	X	-	-	-
32	CLA	Y	611	X	-	-	-
32	CLA	Y	612	X	-	-	-
32	CLA	Y	614	X	-	-	-
32	CLA	a	405	X	-	-	-
32	CLA	a	407	X	-	-	-
32	CLA	b	602	X	-	-	-
32	CLA	b	603	X	-	-	-
32	CLA	b	605	X	-	-	-
32	CLA	b	606	X	-	-	-
32	CLA	b	607	X	-	-	-
32	CLA	b	608	X	-	-	-
32	CLA	b	609	X	-	-	-
32	CLA	b	611	X	-	-	-
32	CLA	b	612	X	-	-	-
32	CLA	b	613	X	-	-	-
32	CLA	b	614	X	-	-	-
32	CLA	b	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	b	616	X	-	-	-
32	CLA	b	617	X	-	-	-
32	CLA	c	501	X	-	-	-
32	CLA	c	503	X	-	-	-
32	CLA	c	504	X	-	-	-
32	CLA	c	507	X	-	-	-
32	CLA	c	508	X	-	-	-
32	CLA	c	509	X	-	-	-
32	CLA	c	510	X	-	-	-
32	CLA	c	512	X	-	-	-
32	CLA	c	513	X	-	-	-
32	CLA	d	402	X	-	-	-
32	CLA	g	602	X	-	-	-
32	CLA	g	603	X	-	-	-
32	CLA	g	604	X	-	-	-
32	CLA	g	610	X	-	-	-
32	CLA	g	611	X	-	-	-
32	CLA	g	612	X	-	-	-
32	CLA	g	614	X	-	-	-
32	CLA	n	602	X	-	-	-
32	CLA	n	603	X	-	-	-
32	CLA	n	604	X	-	-	-
32	CLA	n	610	X	-	-	-
32	CLA	n	611	X	-	-	-
32	CLA	n	612	X	-	-	-
32	CLA	n	614	X	-	-	-
32	CLA	r	602	X	-	-	-
32	CLA	r	603	X	-	-	-
32	CLA	r	604	X	-	-	-
32	CLA	r	609	X	-	-	-
32	CLA	r	610	X	-	-	-
32	CLA	s	602	X	-	-	-
32	CLA	s	603	X	-	-	-
32	CLA	s	604	X	-	-	-
32	CLA	s	605	X	-	-	-
32	CLA	s	609	X	-	-	-
32	CLA	s	610	X	-	-	-
32	CLA	s	611	X	-	-	-
32	CLA	s	612	X	-	-	-
32	CLA	s	614	X	-	-	-
32	CLA	y	602	X	-	-	-
32	CLA	y	603	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	y	604	X	-	-	-
32	CLA	y	610	X	-	-	-
32	CLA	y	611	X	-	-	-
32	CLA	y	612	X	-	-	-
32	CLA	y	614	X	-	-	-
43	CHL	G	601	X	-	-	-
43	CHL	G	605	X	-	-	-
43	CHL	G	606	X	-	-	-
43	CHL	G	607	X	-	-	-
43	CHL	G	608	X	-	-	-
43	CHL	G	609	X	-	-	-
43	CHL	N	601	X	-	-	-
43	CHL	N	605	X	-	-	-
43	CHL	N	606	X	-	-	-
43	CHL	N	607	X	-	-	-
43	CHL	N	608	X	-	-	-
43	CHL	N	609	X	-	-	-
43	CHL	R	606	X	-	-	-
43	CHL	R	607	X	-	-	-
43	CHL	R	608	X	-	-	-
43	CHL	S	601	X	-	-	-
43	CHL	S	606	X	-	-	-
43	CHL	S	607	X	-	-	-
43	CHL	S	608	X	-	-	-
43	CHL	Y	601	X	-	-	-
43	CHL	Y	605	X	-	-	-
43	CHL	Y	606	X	-	-	-
43	CHL	Y	607	X	-	-	-
43	CHL	Y	608	X	-	-	-
43	CHL	Y	609	X	-	-	-
43	CHL	g	601	X	-	-	-
43	CHL	g	605	X	-	-	-
43	CHL	g	606	X	-	-	-
43	CHL	g	607	X	-	-	-
43	CHL	g	608	X	-	-	-
43	CHL	g	609	X	-	-	-
43	CHL	n	601	X	-	-	-
43	CHL	n	605	X	-	-	-
43	CHL	n	606	X	-	-	-
43	CHL	n	607	X	-	-	-
43	CHL	n	608	X	-	-	-
43	CHL	n	609	X	-	-	-

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 77947 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		
1	a	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		
2	b	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			224	147	37	40		
3	v	32	Total	C	N	O	0	0
			224	147	37	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		
4	c	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		
5	d	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			619	404	102	113			
6	e	76	Total	C	N	O	S	0	0
			619	404	102	113			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	68	Total	C	N	O	S	0	0
			519	347	77	93	2		
8	h	68	Total	C	N	O	S	0	0
			519	347	77	93	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		
9	i	35	Total	C	N	O	S	0	0
			283	193	43	45	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			262	178	40	44		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			262	178	40	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		
11	k	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		
12	l	35	Total	C	N	O	0	0
			290	196	45	49		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	30	Total	C	N	O	0	0
			230	158	32	40		
13	m	30	Total	C	N	O	0	0
			230	158	32	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		
14	o	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		
15	p	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	148	Total	C	N	O	0	0
			1192	746	214	232		
16	q	148	Total	C	N	O	0	0
			1192	746	214	232		

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
17	t	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		
18	w	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

- Molecule 19 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	35	Total	C	N	O	0	0
			242	159	39	44		
19	x	35	Total	C	N	O	0	0
			242	159	39	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
20	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
21	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
22	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		
23	r	183	Total	C	N	O	S	0	0
			1400	891	239	265	5		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		
24	s	252	Total	C	N	O	S	0	0
			1914	1236	315	359	4		

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
25	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

- Molecule 26 is a protein called Predicted protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	24	Total	C	N	O	0	0
			184	113	32	39		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
26	u	24	Total	C	N	O	0	0
			184	113	32	39		

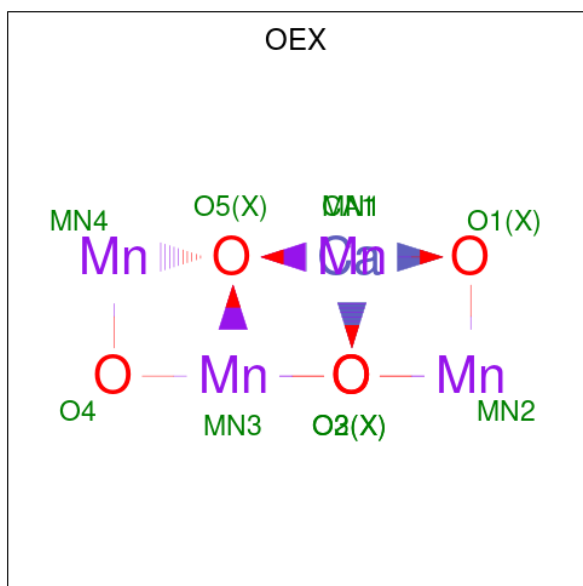
- Molecule 27 is a protein called 10 kDa photosystem II polypeptide PsbR (potential).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	25	Total	C	N	O	0	0
			121	71	25	25		
27	0	25	Total	C	N	O	0	0
			121	71	25	25		

- Molecule 28 is a protein called Unidentified Stromal Protein (USP).

Mol	Chain	Residues	Atoms				AltConf	Trace
28	4	25	Total	C	N	O	0	0
			169	109	29	31		
28	3	25	Total	C	N	O	0	0
			169	109	29	31		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

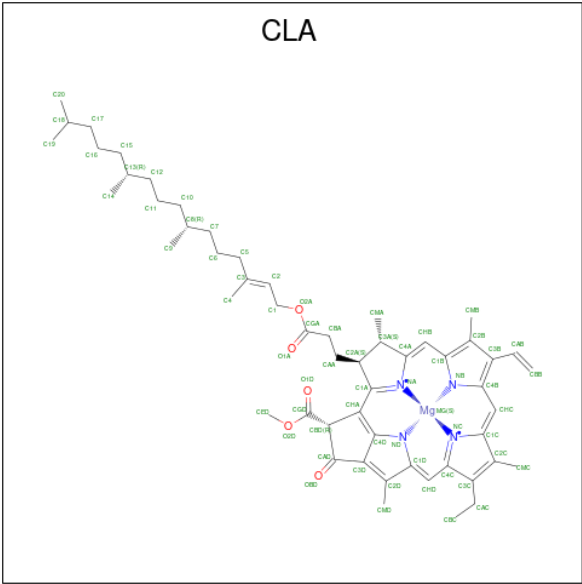
- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

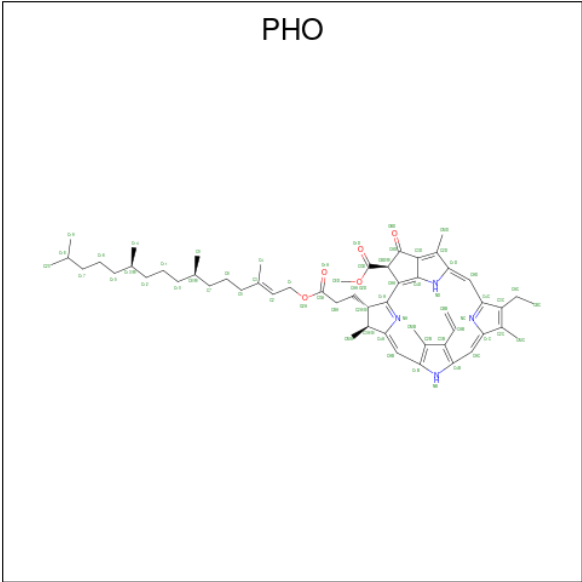
Mol	Chain	Residues	Atoms					AltConf
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	r	1	Total 41	C 33	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

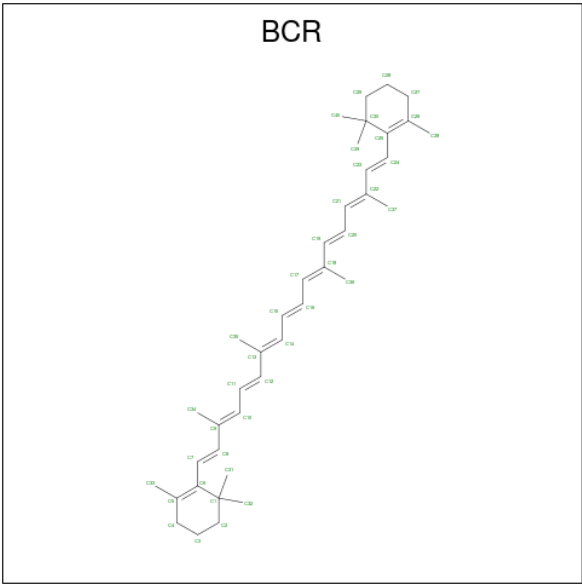
Mol	Chain	Residues	Atoms					AltConf
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



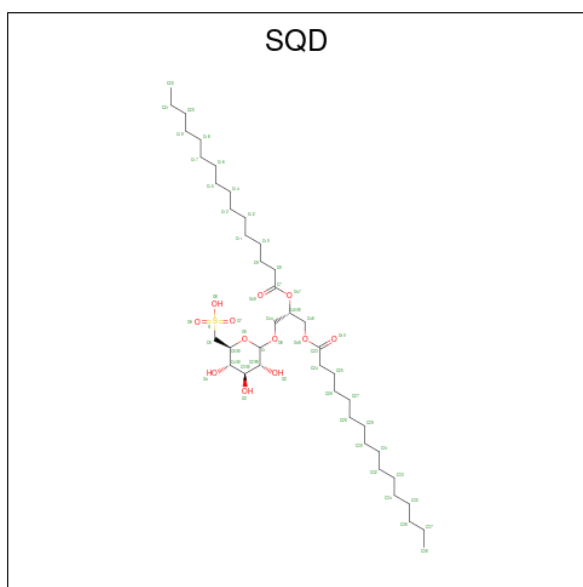
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	A	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	
33	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



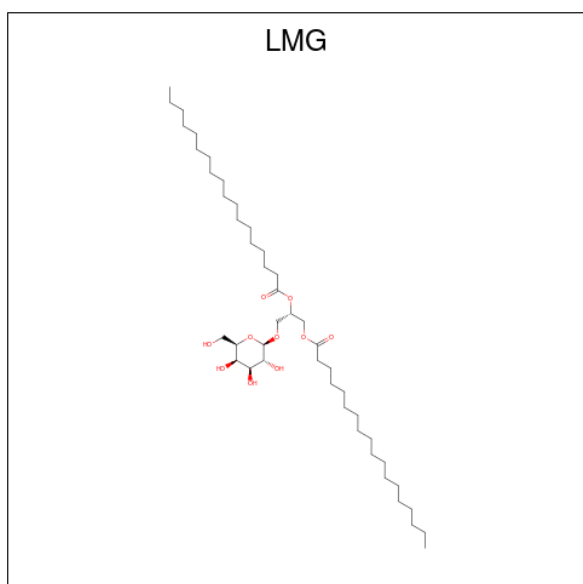
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	B	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	C	1	Total C 40 40	0
34	D	1	Total C 40 40	0
34	H	1	Total C 40 40	0
34	a	1	Total C 40 40	0
34	b	1	Total C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

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



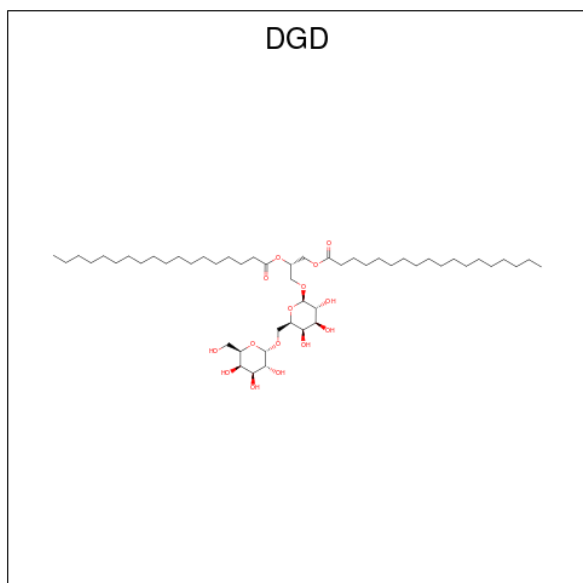
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			54	41	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	
35	b	1	Total	C	O	S	0
			54	41	12	1	

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



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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



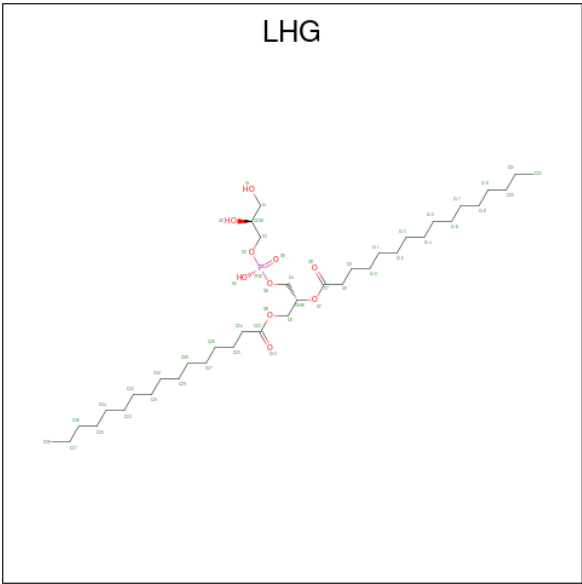
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			55	40	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			62	47	15	
37	C	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			66	51	15	
37	C	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			55	40	15	
37	c	1	Total	C	O	0
			62	47	15	
37	c	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			66	51	15	
37	c	1	Total	C	O	0
			66	51	15	

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



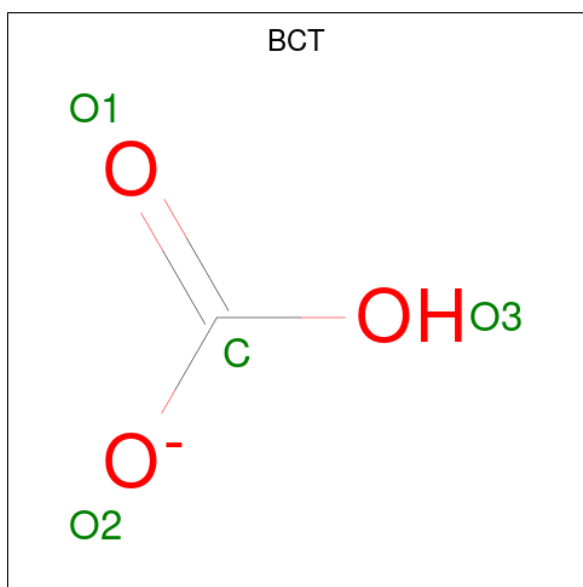
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	

Continued on next page...

Continued from previous page...

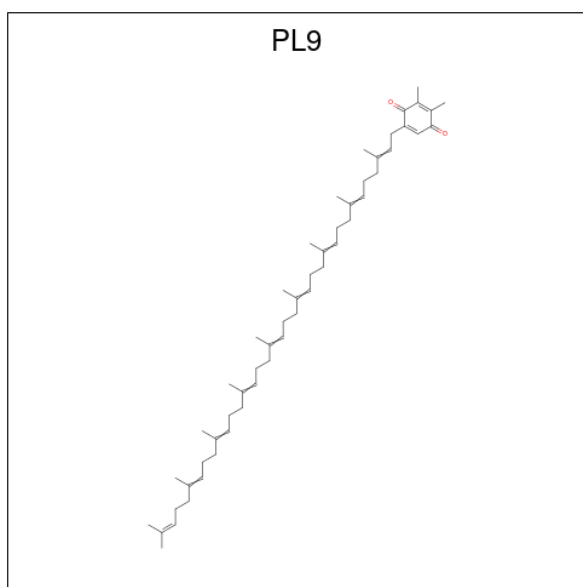
Mol	Chain	Residues	Atoms				AltConf
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			44	33	10	1	
38	d	1	Total	C	O	P	0
			49	38	10	1	
38	d	1	Total	C	O	P	0
			39	28	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	
38	n	1	Total	C	O	P	0
			49	38	10	1	
38	g	1	Total	C	O	P	0
			49	38	10	1	
38	s	1	Total	C	O	P	0
			45	34	10	1	
38	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 40 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
40	D	1	Total	C	O	0
			55	53	2	

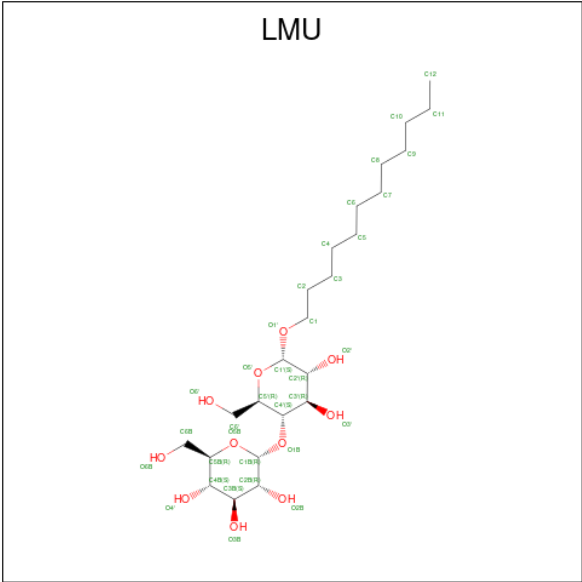
Continued on next page...

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

- # HEM

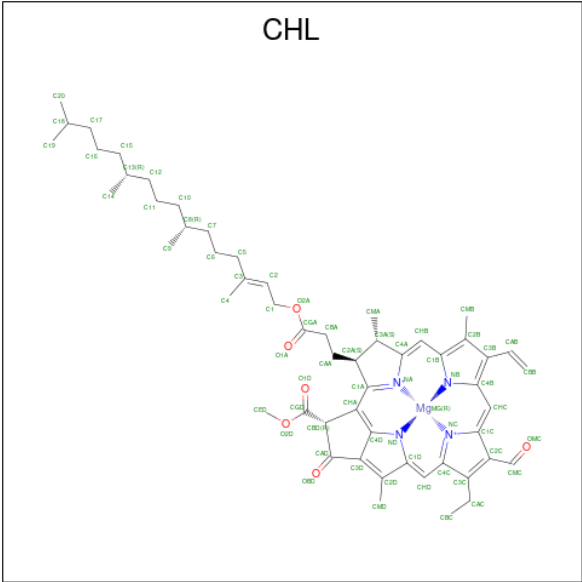
Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- 



Mol	Chain	Residues	Atoms			AltConf
42	Z	1	Total	C	O	0
			35	24	11	
42	Z	1	Total	C	O	0
			35	24	11	
42	Y	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	z	1	Total	C	O	0
			35	24	11	
42	y	1	Total	C	O	0
			35	24	11	

- Molecule 43 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	N	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			50	39	1	4	6		
43	G	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	G	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
43	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
43	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

Continued on next page...

Continued from previous page...

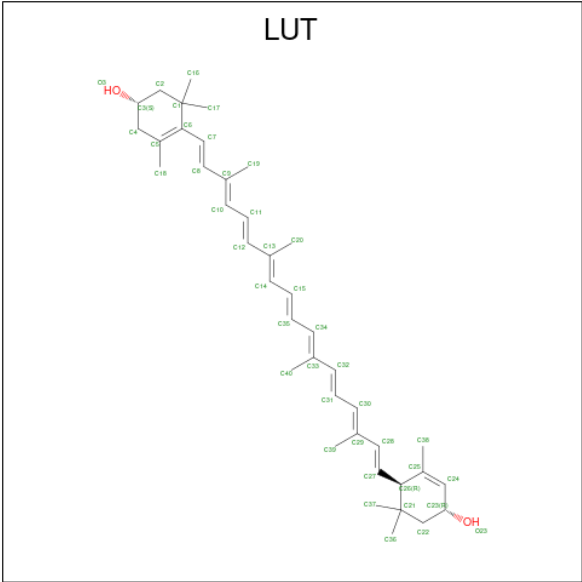
Mol	Chain	Residues	Atoms					AltConf
43	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
43	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	g	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
43	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	r	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
43	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
43	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
43	y	1	Total 50	C 39	Mg 1	N 4	O 6	0
43	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 44 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



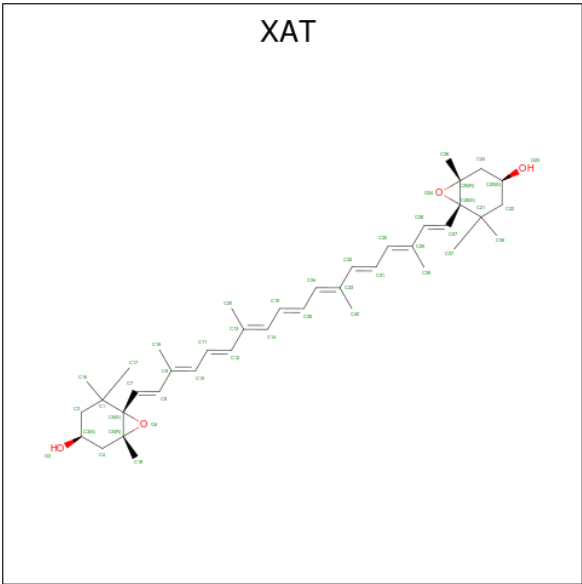
Mol	Chain	Residues	Atoms			AltConf
44	N	1	Total	C	O	0
			42	40	2	
44	N	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	G	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	S	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	Y	1	Total	C	O	0
			42	40	2	
44	n	1	Total	C	O	0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

Continued on next page...

Continued from previous page...

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

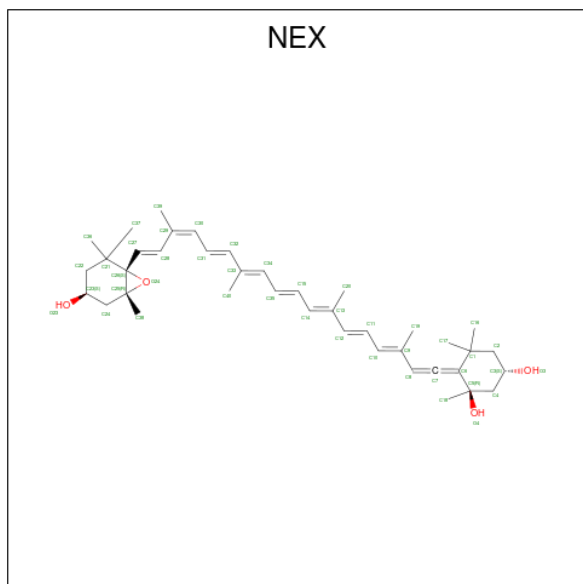
- Molecule 45 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



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

- Molecule 46 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2

,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA
DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,
3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



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

- Molecule 47 is water.

Mol	Chain	Residues	Atoms		AltConf
47	A	40	Total 40	O 40	0
47	B	57	Total 57	O 57	0
47	V	6	Total 6	O 6	0
47	C	28	Total 28	O 28	0
47	D	28	Total 28	O 28	0
47	E	6	Total 6	O 6	0
47	F	3	Total 3	O 3	0
47	H	7	Total 7	O 7	0
47	I	5	Total 5	O 5	0
47	J	1	Total 1	O 1	0
47	L	1	Total 1	O 1	0
47	M	3	Total 3	O 3	0
47	O	43	Total 43	O 43	0
47	P	23	Total 23	O 23	0
47	Q	20	Total 20	O 20	0
47	T	3	Total 3	O 3	0
47	W	3	Total 3	O 3	0
47	X	1	Total 1	O 1	0
47	Z	3	Total 3	O 3	0
47	N	3	Total 3	O 3	0
47	G	6	Total 6	O 6	0
47	Y	8	Total 8	O 8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	a	40	Total 40	O 40	0
47	b	57	Total 57	O 57	0
47	v	6	Total 6	O 6	0
47	c	28	Total 28	O 28	0
47	d	28	Total 28	O 28	0
47	e	6	Total 6	O 6	0
47	f	3	Total 3	O 3	0
47	h	7	Total 7	O 7	0
47	i	5	Total 5	O 5	0
47	j	1	Total 1	O 1	0
47	l	1	Total 1	O 1	0
47	m	2	Total 2	O 2	0
47	o	43	Total 43	O 43	0
47	p	23	Total 23	O 23	0
47	q	20	Total 20	O 20	0
47	t	3	Total 3	O 3	0
47	w	3	Total 3	O 3	0
47	x	1	Total 1	O 1	0
47	z	3	Total 3	O 3	0
47	n	3	Total 3	O 3	0
47	g	6	Total 6	O 6	0

Continued on next page...

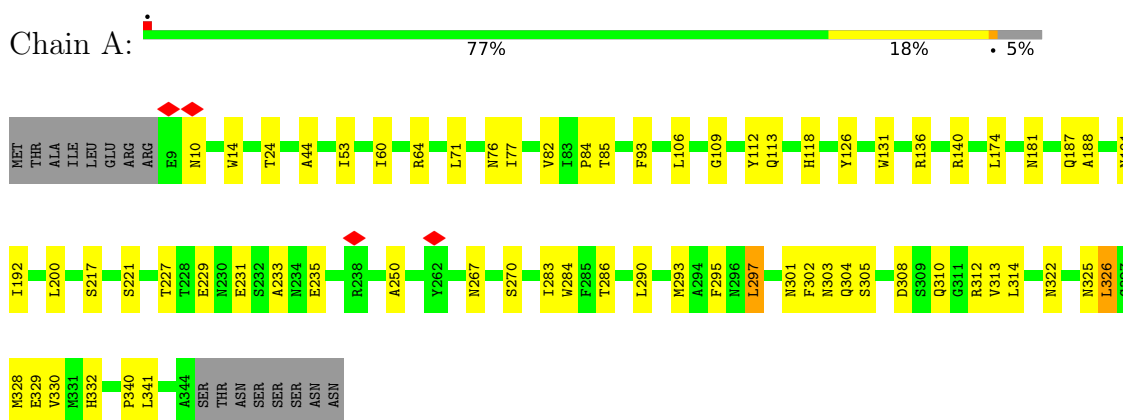
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	y	8	Total	O	0
			8	8	

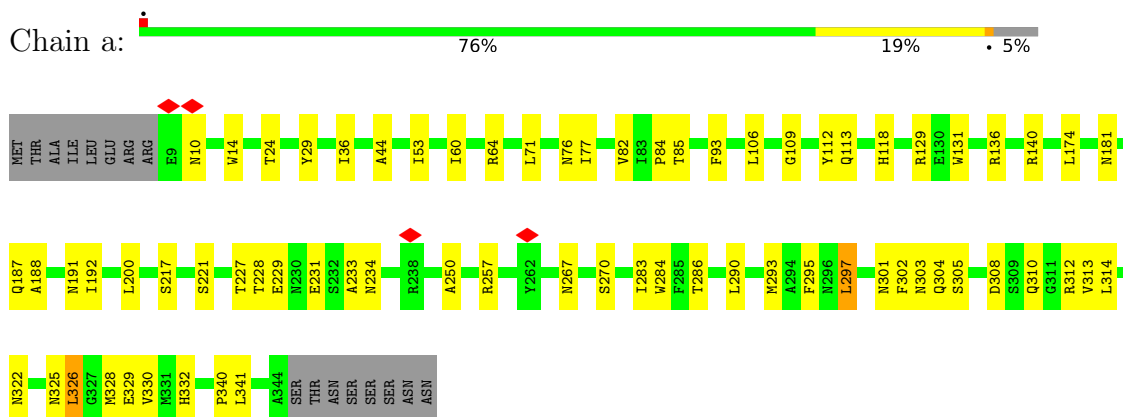
3 Residue-property plots

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

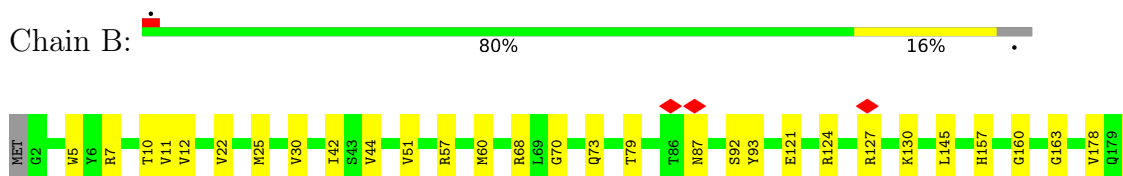
- Molecule 1: Photosystem II protein D1

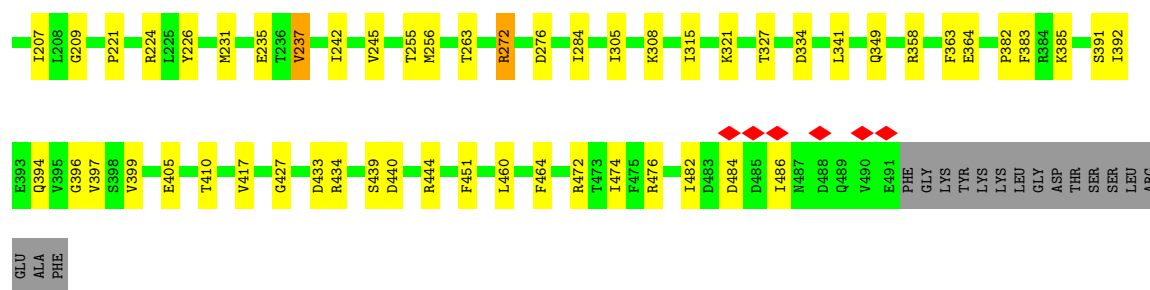


- Molecule 1: Photosystem II protein D1



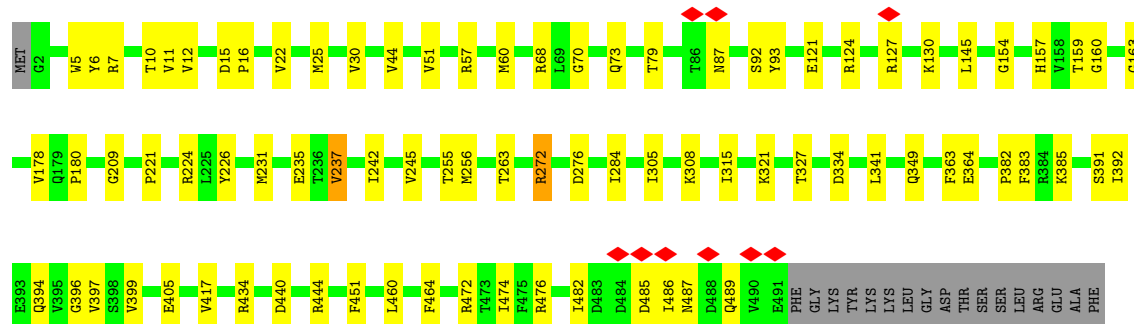
- Molecule 2: Photosystem II CP47 reaction center protein





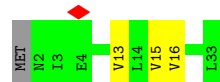
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 16%



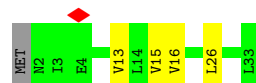
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V: 88% 9%



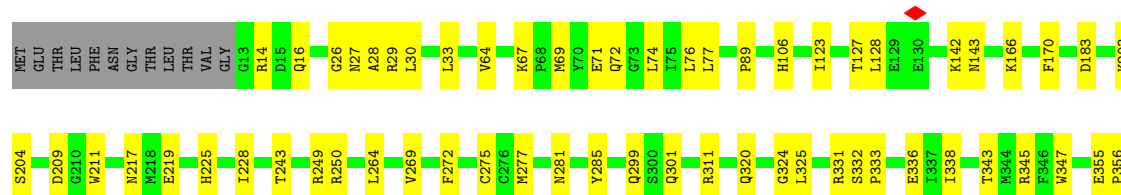
• Molecule 3: Photosystem II reaction center protein Ycf12

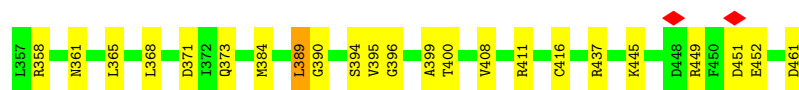
Chain v: 85% 12%



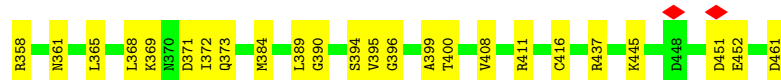
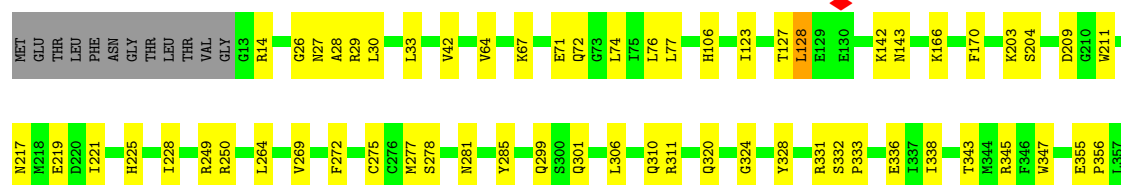
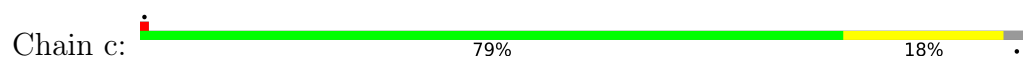
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 79% 18%

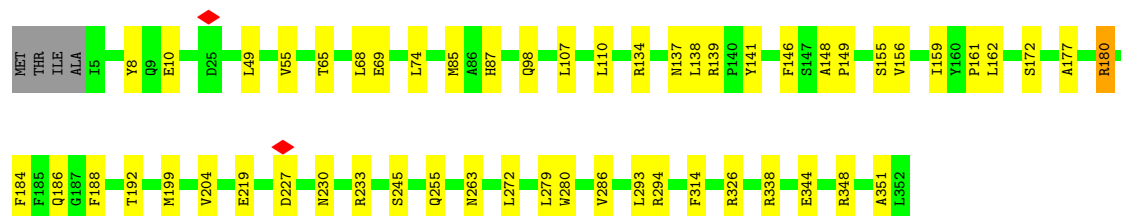
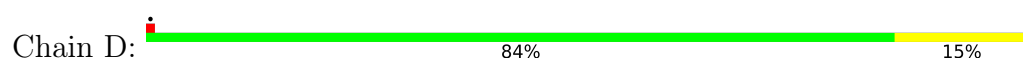




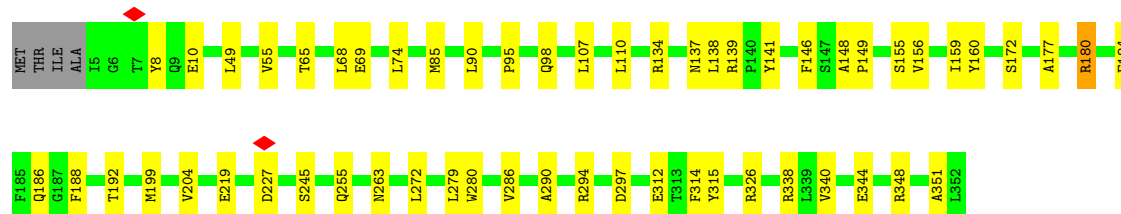
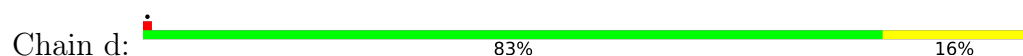
- Molecule 4: Photosystem II CP43 reaction center protein



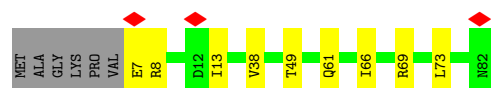
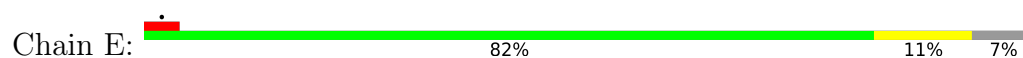
- Molecule 5: Photosystem II D2 protein



- Molecule 5: Photosystem II D2 protein

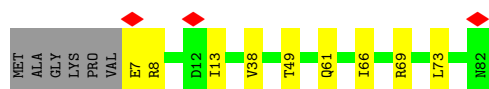


- Molecule 6: Cytochrome b559 subunit alpha



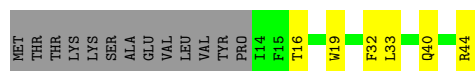
- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  82% 11% 7%



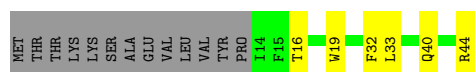
- Molecule 7: Cytochrome b559 subunit beta

Chain F:  57% 14% 30%



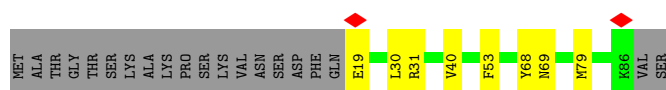
- Molecule 7: Cytochrome b559 subunit beta

Chain f:  57% 14% 30%



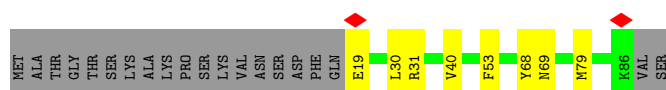
- Molecule 8: Photosystem II reaction center protein H

Chain H:  68% 9% 23%



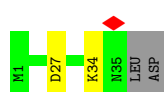
- Molecule 8: Photosystem II reaction center protein H

Chain h:  68% 9% 23%



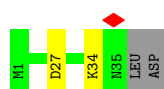
- Molecule 9: Photosystem II reaction center protein I

Chain I:  89% 5% 5%

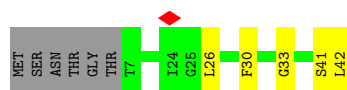
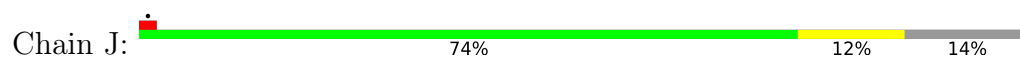


- Molecule 9: Photosystem II reaction center protein I

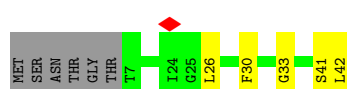
Chain i:  89% 5% 5%



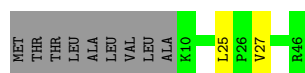
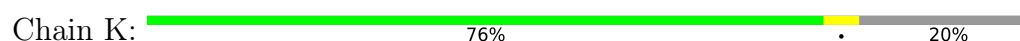
- Molecule 10: Photosystem II reaction center protein J



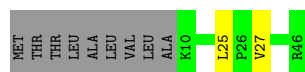
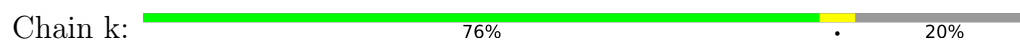
- Molecule 10: Photosystem II reaction center protein J



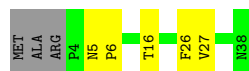
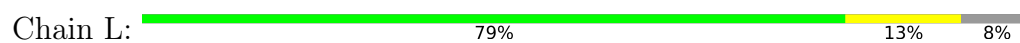
- Molecule 11: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein K



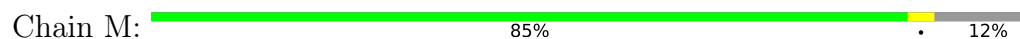
- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein M



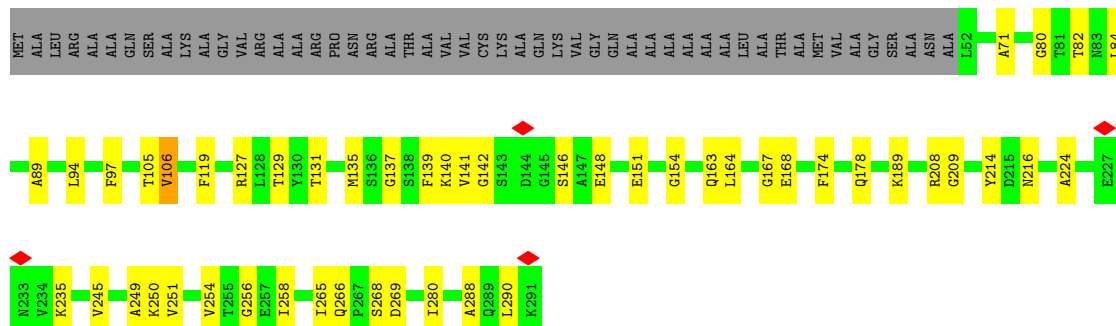
- Molecule 13: Photosystem II reaction center protein M

Chain m:  82% 6% 12%



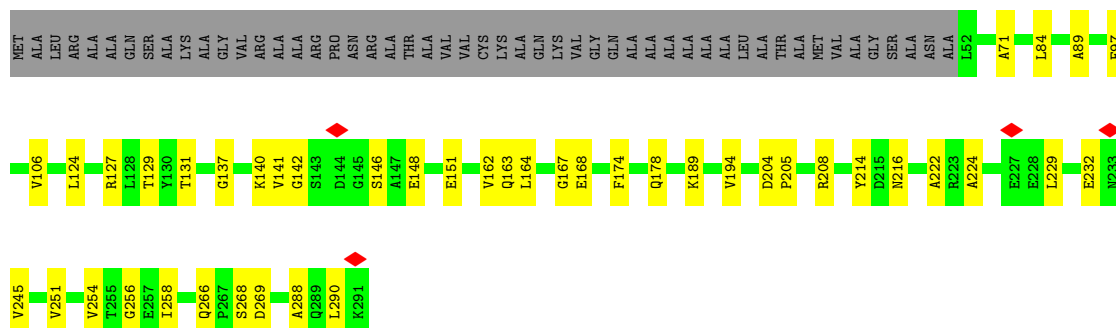
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplactic

Chain O:  65% 17% 18%



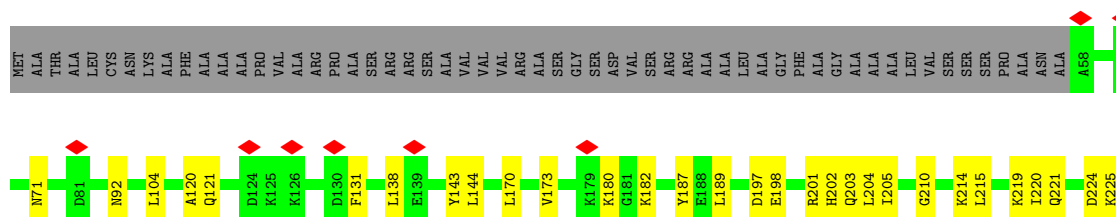
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplactic

Chain o:  67% 15% 18%



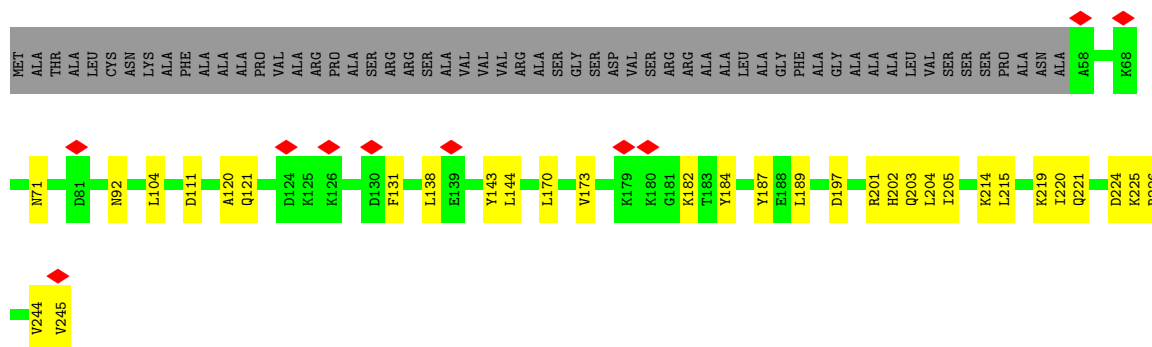
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplactic

Chain P:  64% 13% 23%

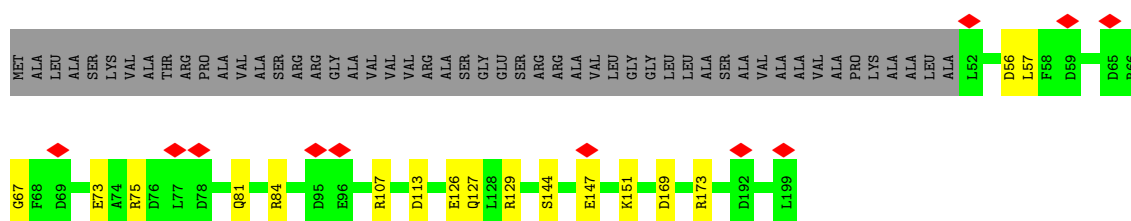


- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplactic

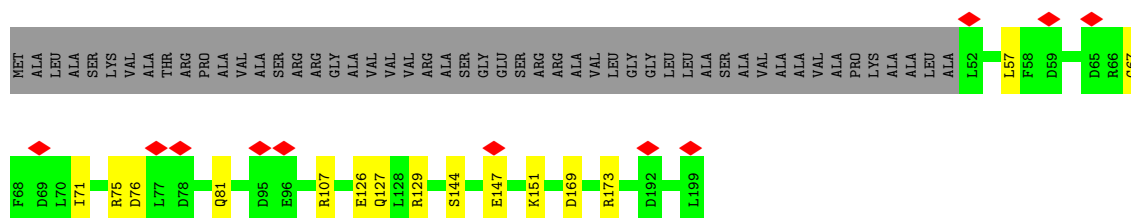
Chain p:  64% 13% 23%



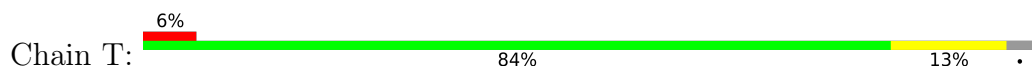
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic



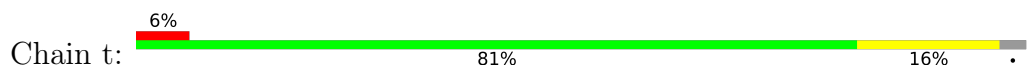
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic



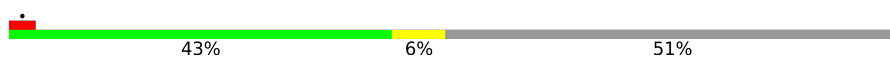
- Molecule 17: Photosystem II reaction center protein T



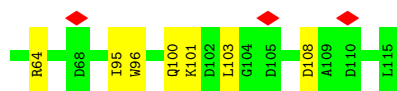
- Molecule 17: Photosystem II reaction center protein T



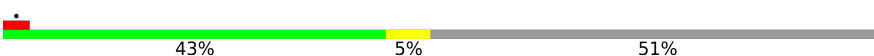
- Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain W: 

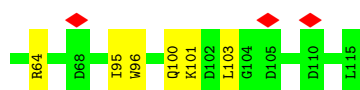
MET GLN ALA LEU SER ARG ALA PRO ARG VAL ALA LYS PRO VAL SER ARG SER GLY ALA ARG SER SER VAL THR VAL VAL CYS LYS THR THR VAL ARG SER SER GLU VAL ALA LYS LYS VAL ALA MET LEU THR THR PRO ALA THR ALA ALA HIS PRO ALA PHE ALA L60



- Molecule 18: Photosystem II reaction center W protein, chloroplastic

Chain w: 

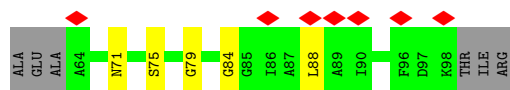
MET GLN ALA LEU SER ARG ALA PRO ARG VAL ALA LYS PRO VAL SER ARG SER GLY ALA ARG SER SER VAL THR VAL VAL CYS LYS THR THR VAL ARG SER SER GLU VAL ALA LYS LYS VAL ALA MET LEU THR THR PRO ALA THR ALA ALA HIS PRO ALA PHE ALA L60



- Molecule 19: 4.1 kDa photosystem II subunit

Chain X: 

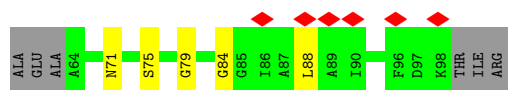
MET ALA ALA VAL CYS VAL SER SER LYS VAL ALA VAL VAL ARG PRO THR THR VAL ALA SER ARG PRO THR VAL ALA ALA ARG MET VAL VAL ARG ALA SER ALA LYS PRO PRO GLN TLE SER GLU LYS LYS TLE ALA ALA GLY VAL SER ALA ALA ALA ALA SER LEU LEU ALA PRO TLE



- Molecule 19: 4.1 kDa photosystem II subunit

Chain x: 

MET ALA ALA VAL CYS VAL SER SER LYS VAL ALA VAL VAL ARG PRO THR THR VAL ALA SER ARG PRO THR VAL ALA ALA ARG MET VAL VAL ARG ALA SER ALA LYS PRO PRO GLN TLE SER GLU LYS LYS TLE ALA ALA GLY VAL SER ALA ALA ALA ALA SER LEU LEU ALA PRO TLE



- Molecule 20: Photosystem II reaction center protein Z

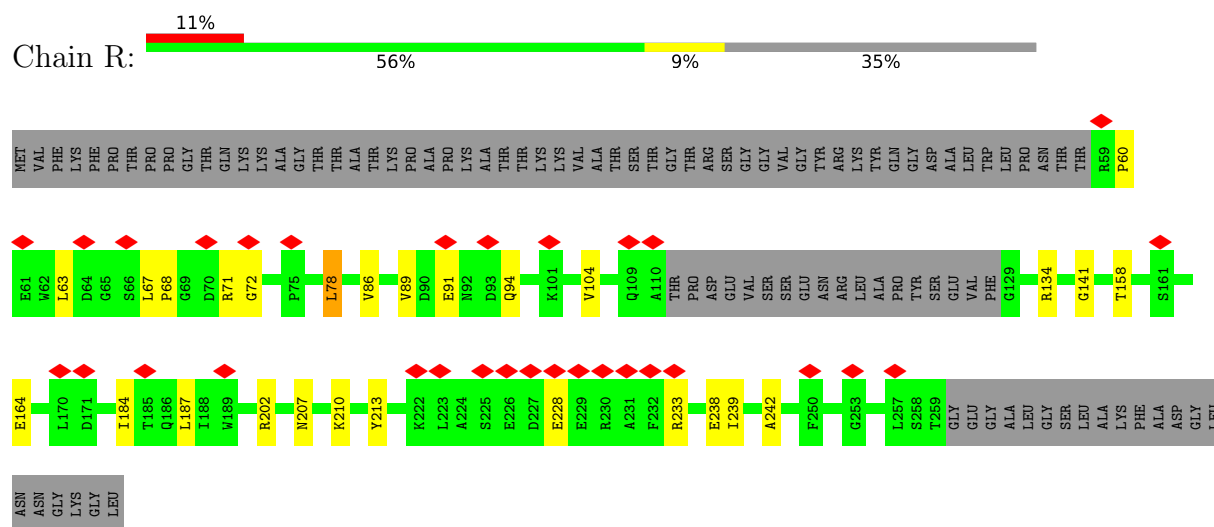
Chain Z: 



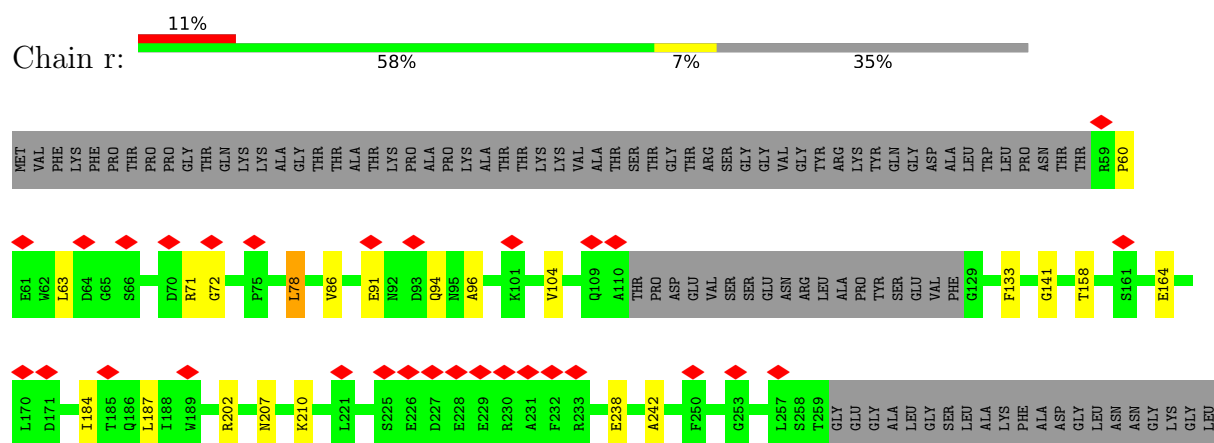
- Molecule 20: Photosystem II reaction center protein Z

Chain z: 

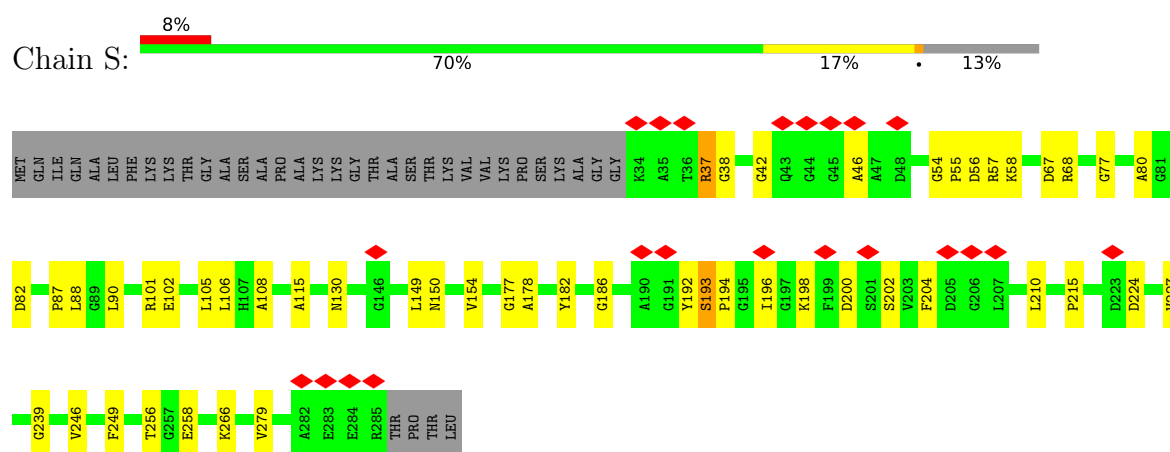
- Molecule 23: Chlorophyll a-b binding protein CP29



- Molecule 23: Chlorophyll a-b binding protein CP29



- Molecule 24: Chlorophyll a-b binding protein, chloroplastic



- Molecule 24: Chlorophyll a-b binding protein, chloroplastic



MET ALA HIS SER THR CYS SER SER GLY LYS ALA ALA VAL VAL VAL SER ARG ALA LYS THR THR ALA ARG PRO VAL ARG ARG MET SER VAL VAL VAL ALA SER SER ALA ALA PRO GLN GLY ASN ALA SER ARG ARG GLU LEU LEU GLY SER SER SER ALA VAL ALA ALA TRP VAL ALA SER LEU LEU LEU SER SER ARG ARG PRO

ALA HIS ALA ILE PHE GLY PHE ALA ASP ASP THR ALA VAL LEU PHE SER ASP THR HIS THR ALA ALA GLU SER PHE THR VAL ARG ARG MET SER LYS LYS VAL VAL ALA SER SER ALA ALA PRO GLN GLY ASN ALA SER ARG ARG GLU LEU LEU GLY SER SER SER ALA VAL ALA ALA TRP VAL ALA SER LEU LEU LEU SER SER ARG ARG PRO LYS VAL SER

GLY LYS PRO SER PHE GLY ASN THR TYR SER SER ALA ALA ASN ALA LEU LEU PHE SER ASP THR HIS THR PHE ASN SER PHE GLY THR ALA ALA THR ALA PRO ASP ILE LYS LYS LYS ARG LEU LEU GLU ARG GLN LYS GLU LEU ASP ASP ALA THR LEU LEU LEU THR ARG ASN ARG

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 1: 48% 92% 8%

G111 A118 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135

- Molecule 27: 10 kDa photosystem II polypeptide PsbR (potential)

Chain 0: 52% 100%

G111 A118 A119 G120 A121 A122 A123 A124 A125 A126 A127 A128 A129 A130 A131 A132 A133 A134 A135

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 4: 60% 92% 8%

A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A78 A79 A80 A83 A86 A87 A88

- Molecule 28: Unidentified Stromal Protein (USP)

Chain 3: 64% 100%

A64 A65 A66 A67 A68 A69 A70 A71 A72 A73 A74 A75 A76 A77 A80 A81 A82 A83 A86 A87 A88

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	258242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	399.36, 399.36, 399.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.46	0/2718	0.64	0/3706
1	a	0.46	0/2718	0.63	0/3706
2	B	0.37	0/3964	0.54	0/5397
2	b	0.37	0/3964	0.54	0/5397
3	V	0.26	0/224	0.56	0/307
3	v	0.26	0/224	0.57	0/307
4	C	0.42	0/3619	0.56	0/4931
4	c	0.42	0/3619	0.56	0/4931
5	D	0.44	0/2866	0.63	0/3909
5	d	0.43	0/2866	0.65	2/3909 (0.1%)
6	E	0.30	0/637	0.57	0/869
6	e	0.30	0/637	0.56	0/869
7	F	0.29	0/258	0.55	0/349
7	f	0.29	0/258	0.55	0/349
8	H	0.29	0/530	0.54	0/725
8	h	0.29	0/530	0.54	0/725
9	I	0.40	0/291	0.53	0/394
9	i	0.40	0/291	0.53	0/394
10	J	0.24	0/268	0.51	0/366
10	j	0.24	0/268	0.51	0/366
11	K	0.41	0/309	0.87	2/425 (0.5%)
11	k	0.41	0/309	0.87	2/425 (0.5%)
12	L	0.34	0/298	0.54	0/405
12	l	0.35	0/298	0.54	0/405
13	M	0.35	0/234	0.57	0/321
13	m	0.35	0/234	0.57	0/321
14	O	0.31	0/1839	0.59	2/2482 (0.1%)
14	o	0.31	0/1839	0.58	2/2482 (0.1%)
15	P	0.25	0/1473	0.48	0/1987
15	p	0.25	0/1473	0.48	0/1987
16	Q	0.23	0/1204	0.47	0/1616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	q	0.23	0/1204	0.47	0/1616
17	T	0.31	0/254	0.52	0/343
17	t	0.31	0/254	0.52	0/343
18	W	0.32	0/445	0.53	0/603
18	w	0.32	0/445	0.53	0/603
19	X	0.21	0/244	0.51	0/330
19	x	0.21	0/244	0.49	0/330
20	Z	0.24	0/469	0.54	0/644
20	z	0.24	0/469	0.51	0/644
21	N	0.28	0/1720	0.52	0/2341
21	n	0.28	0/1720	0.52	0/2341
22	G	0.24	0/1717	0.53	1/2337 (0.0%)
22	g	0.24	0/1717	0.51	0/2337
23	R	0.26	0/1429	0.54	0/1934
23	r	0.25	0/1429	0.53	0/1934
24	S	0.32	0/1968	0.57	0/2679
24	s	0.32	0/1968	0.58	0/2679
25	Y	0.33	0/1746	0.52	0/2375
25	y	0.33	0/1746	0.52	0/2375
26	U	0.28	0/184	0.73	0/246
26	u	0.29	0/184	0.73	0/246
27	0	0.11	0/120	0.31	0/164
27	1	0.11	0/120	0.30	0/164
28	3	0.26	0/174	0.78	0/237
28	4	0.25	0/174	0.69	0/237
All	All	0.35	0/62404	0.56	11/84844 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	27	VAL	CA-C-N	6.55	124.37	120.24
11	K	27	VAL	C-N-CA	6.55	124.37	120.24
11	k	27	VAL	CA-C-N	6.53	124.35	120.24
11	k	27	VAL	C-N-CA	6.53	124.35	120.24
14	o	214	TYR	CA-C-N	5.96	135.43	124.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2533	61	0
1	a	2636	0	2533	63	0
2	B	3836	0	3709	64	0
2	b	3836	0	3709	67	0
3	V	224	0	256	2	0
3	v	224	0	256	4	0
4	C	3498	0	3372	67	0
4	c	3498	0	3372	66	0
5	D	2771	0	2655	51	0
5	d	2771	0	2655	47	0
6	E	619	0	605	9	0
6	e	619	0	605	7	0
7	F	251	0	263	6	0
7	f	251	0	263	6	0
8	H	519	0	549	8	0
8	h	519	0	549	8	0
9	I	283	0	293	2	0
9	i	283	0	293	2	0
10	J	262	0	276	5	0
10	j	262	0	276	5	0
11	K	297	0	308	1	0
11	k	297	0	308	1	0
12	L	290	0	298	3	0
12	l	290	0	298	4	0
13	M	230	0	252	2	0
13	m	230	0	252	3	0
14	O	1808	0	1813	31	0
14	o	1808	0	1813	29	0
15	P	1444	0	1414	22	0
15	p	1444	0	1414	23	0
16	Q	1192	0	1216	16	0
16	q	1192	0	1216	13	0
17	T	247	0	260	4	0
17	t	247	0	260	5	0
18	W	434	0	411	7	0
18	w	434	0	411	6	0
19	X	242	0	266	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	x	242	0	266	3	0
20	Z	458	0	490	6	0
20	z	458	0	490	8	0
21	N	1672	0	1611	39	0
21	n	1672	0	1611	38	0
22	G	1667	0	1606	32	0
22	g	1667	0	1606	32	0
23	R	1400	0	1376	20	0
23	r	1400	0	1376	17	0
24	S	1914	0	1857	45	0
24	s	1914	0	1857	49	0
25	Y	1693	0	1629	26	0
25	y	1693	0	1629	28	0
26	U	184	0	190	2	0
26	u	184	0	190	2	0
27	0	121	0	116	0	0
27	1	121	0	116	1	0
28	3	169	0	148	0	0
28	4	169	0	148	2	0
29	A	10	0	0	1	0
29	a	10	0	0	1	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	A	2	0	0	0	0
31	a	2	0	0	0	0
32	A	239	0	242	6	0
32	B	1040	0	1152	44	0
32	C	845	0	936	28	0
32	D	130	0	144	6	0
32	G	446	0	432	10	0
32	N	468	0	471	11	0
32	R	244	0	199	8	0
32	S	471	0	363	6	0
32	Y	509	0	552	18	0
32	a	239	0	242	6	0
32	b	1040	0	1152	40	0
32	c	845	0	936	26	0
32	d	130	0	144	6	0
32	g	446	0	432	12	0
32	n	468	0	471	12	0
32	r	244	0	199	7	0
32	s	471	0	363	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	y	509	0	552	20	0
33	A	128	0	148	6	0
33	a	128	0	148	4	0
34	A	40	0	56	2	0
34	B	120	0	168	12	0
34	C	160	0	224	12	0
34	D	40	0	56	5	0
34	H	40	0	56	3	0
34	a	40	0	56	3	0
34	b	120	0	168	12	0
34	c	160	0	224	14	0
34	d	40	0	56	3	0
34	h	40	0	56	2	0
35	A	51	0	69	2	0
35	B	54	0	78	3	0
35	a	51	0	69	1	0
35	b	54	0	78	2	0
36	A	48	0	66	8	0
36	B	51	0	72	2	0
36	C	51	0	72	0	0
36	D	46	0	62	3	0
36	H	48	0	66	1	0
36	a	48	0	66	8	0
36	b	51	0	72	2	0
36	c	51	0	72	0	0
36	d	46	0	62	3	0
36	h	48	0	66	1	0
37	C	308	0	418	14	0
37	c	308	0	418	16	0
38	C	47	0	67	4	0
38	D	132	0	183	11	0
38	G	49	0	74	4	0
38	L	49	0	74	3	0
38	N	49	0	74	3	0
38	S	45	0	63	5	0
38	Y	49	0	74	3	0
38	c	47	0	67	4	0
38	d	132	0	183	11	0
38	g	49	0	74	5	0
38	l	49	0	74	4	0
38	n	49	0	74	4	0
38	s	45	0	63	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	y	49	0	74	3	0
39	D	4	0	0	0	0
39	d	4	0	0	0	0
40	D	55	0	80	3	0
40	d	55	0	80	4	0
41	F	43	0	30	0	0
41	f	43	0	30	0	0
42	Y	35	0	46	2	0
42	Z	70	0	92	1	0
42	y	35	0	46	1	0
42	z	70	0	92	2	0
43	G	324	0	278	14	0
43	N	360	0	348	18	0
43	R	140	0	99	3	0
43	S	182	0	125	4	0
43	Y	360	0	348	12	0
43	g	324	0	278	15	0
43	n	360	0	348	19	0
43	r	140	0	99	2	0
43	s	182	0	125	4	0
43	y	360	0	348	13	0
44	G	84	0	112	7	0
44	N	84	0	112	7	0
44	S	84	0	112	5	0
44	Y	84	0	112	7	0
44	g	84	0	112	7	0
44	n	84	0	112	6	0
44	s	84	0	112	6	0
44	y	84	0	112	6	0
45	G	44	0	56	4	0
45	N	44	0	56	4	0
45	R	44	0	56	3	0
45	Y	44	0	56	5	0
45	g	44	0	56	5	0
45	n	44	0	56	7	0
45	r	44	0	56	2	0
45	y	44	0	56	5	0
46	G	44	0	56	1	0
46	N	44	0	56	2	0
46	R	44	0	56	3	0
46	S	44	0	56	3	0
46	Y	44	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	g	44	0	56	1	0
46	n	44	0	56	2	0
46	r	44	0	56	3	0
46	s	44	0	56	1	0
46	y	44	0	56	2	0
47	A	40	0	0	0	0
47	B	57	0	0	6	0
47	C	28	0	0	2	0
47	D	28	0	0	1	0
47	E	6	0	0	0	0
47	F	3	0	0	0	0
47	G	6	0	0	0	0
47	H	7	0	0	0	0
47	I	5	0	0	0	0
47	J	1	0	0	0	0
47	L	1	0	0	0	0
47	M	3	0	0	0	0
47	N	3	0	0	0	0
47	O	43	0	0	7	0
47	P	23	0	0	2	0
47	Q	20	0	0	3	0
47	T	3	0	0	0	0
47	V	6	0	0	0	0
47	W	3	0	0	0	0
47	X	1	0	0	1	0
47	Y	8	0	0	0	0
47	Z	3	0	0	0	0
47	a	40	0	0	0	0
47	b	57	0	0	6	0
47	c	28	0	0	4	0
47	d	28	0	0	2	0
47	e	6	0	0	0	0
47	f	3	0	0	0	0
47	g	6	0	0	0	0
47	h	7	0	0	0	0
47	i	5	0	0	0	0
47	j	1	0	0	0	0
47	l	1	0	0	0	0
47	m	2	0	0	1	0
47	n	3	0	0	0	0
47	o	43	0	0	6	0
47	p	23	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	q	20	0	0	0	0
47	t	3	0	0	0	0
47	v	6	0	0	0	0
47	w	3	0	0	0	0
47	x	1	0	0	1	0
47	y	8	0	0	0	0
47	z	3	0	0	0	0
All	All	77947	0	77762	1245	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 8.

The worst 5 of 1245 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)
14:O:254:VAL:HG11	47:O:1039:HOH:O	1.24	1.38
14:o:254:VAL:HG11	47:o:1039:HOH:O	1.36	1.25
14:O:254:VAL:CG1	47:O:1039:HOH:O	1.74	1.12
16:Q:56:ASP:HB2	47:Q:1001:HOH:O	1.51	1.10
14:o:254:VAL:CG1	47:o:1039:HOH:O	1.94	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
1	a	334/352 (95%)	326 (98%)	8 (2%)	0	100	100
2	B	488/508 (96%)	477 (98%)	11 (2%)	0	100	100
2	b	488/508 (96%)	478 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
3	v	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
4	C	447/461 (97%)	421 (94%)	25 (6%)	1 (0%)	43	68
4	c	447/461 (97%)	422 (94%)	24 (5%)	1 (0%)	43	68
5	D	346/352 (98%)	334 (96%)	12 (4%)	0	100	100
5	d	346/352 (98%)	332 (96%)	14 (4%)	0	100	100
6	E	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
6	e	74/82 (90%)	68 (92%)	6 (8%)	0	100	100
7	F	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
7	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
8	H	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
8	h	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
9	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
9	i	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
10	J	34/42 (81%)	34 (100%)	0	0	100	100
10	j	34/42 (81%)	34 (100%)	0	0	100	100
11	K	35/46 (76%)	35 (100%)	0	0	100	100
11	k	35/46 (76%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
12	l	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
13	M	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
13	m	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
14	O	238/291 (82%)	224 (94%)	14 (6%)	0	100	100
14	o	238/291 (82%)	221 (93%)	17 (7%)	0	100	100
15	P	186/245 (76%)	180 (97%)	6 (3%)	0	100	100
15	p	186/245 (76%)	179 (96%)	7 (4%)	0	100	100
16	Q	146/199 (73%)	139 (95%)	7 (5%)	0	100	100
16	q	146/199 (73%)	138 (94%)	8 (6%)	0	100	100
17	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
17	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
18	W	54/115 (47%)	50 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	w	54/115 (47%)	50 (93%)	4 (7%)	0	100	100
19	X	33/101 (33%)	31 (94%)	2 (6%)	0	100	100
19	x	33/101 (33%)	32 (97%)	1 (3%)	0	100	100
20	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
21	N	217/257 (84%)	202 (93%)	15 (7%)	0	100	100
21	n	217/257 (84%)	201 (93%)	16 (7%)	0	100	100
22	G	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
22	g	217/249 (87%)	198 (91%)	19 (9%)	0	100	100
23	R	179/280 (64%)	169 (94%)	10 (6%)	0	100	100
23	r	179/280 (64%)	167 (93%)	12 (7%)	0	100	100
24	S	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	54
24	s	250/289 (86%)	235 (94%)	14 (6%)	1 (0%)	30	54
25	Y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
25	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
26	U	22/178 (12%)	19 (86%)	3 (14%)	0	100	100
26	u	22/178 (12%)	19 (86%)	3 (14%)	0	100	100
27	0	23/25 (92%)	23 (100%)	0	0	100	100
27	1	23/25 (92%)	23 (100%)	0	0	100	100
28	3	23/25 (92%)	17 (74%)	6 (26%)	0	100	100
28	4	23/25 (92%)	18 (78%)	5 (22%)	0	100	100
All	All	7742/9440 (82%)	7357 (95%)	381 (5%)	4 (0%)	49	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	211	TRP
4	c	211	TRP
24	S	193	SER
24	s	193	SER

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	274/289 (95%)	271 (99%)	3 (1%)	65	85
1	a	274/289 (95%)	271 (99%)	3 (1%)	65	85
2	B	392/407 (96%)	389 (99%)	3 (1%)	73	88
2	b	392/407 (96%)	389 (99%)	3 (1%)	73	88
3	V	26/27 (96%)	26 (100%)	0	100	100
3	v	26/27 (96%)	26 (100%)	0	100	100
4	C	352/362 (97%)	349 (99%)	3 (1%)	70	87
4	c	352/362 (97%)	349 (99%)	3 (1%)	70	87
5	D	278/281 (99%)	277 (100%)	1 (0%)	84	93
5	d	278/281 (99%)	277 (100%)	1 (0%)	84	93
6	E	67/71 (94%)	66 (98%)	1 (2%)	57	81
6	e	67/71 (94%)	66 (98%)	1 (2%)	57	81
7	F	25/37 (68%)	25 (100%)	0	100	100
7	f	25/37 (68%)	25 (100%)	0	100	100
8	H	58/75 (77%)	58 (100%)	0	100	100
8	h	58/75 (77%)	58 (100%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	100	100
9	i	32/34 (94%)	32 (100%)	0	100	100
10	J	27/32 (84%)	27 (100%)	0	100	100
10	j	27/32 (84%)	27 (100%)	0	100	100
11	K	31/38 (82%)	31 (100%)	0	100	100
11	k	31/38 (82%)	31 (100%)	0	100	100
12	L	33/35 (94%)	32 (97%)	1 (3%)	36	66
12	l	33/35 (94%)	32 (97%)	1 (3%)	36	66
13	M	26/30 (87%)	26 (100%)	0	100	100
13	m	26/30 (87%)	26 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	195/222 (88%)	192 (98%)	3 (2%)	57	81
14	o	195/222 (88%)	193 (99%)	2 (1%)	68	86
15	P	150/185 (81%)	149 (99%)	1 (1%)	76	90
15	p	150/185 (81%)	149 (99%)	1 (1%)	76	90
16	Q	126/157 (80%)	126 (100%)	0	100	100
16	q	126/157 (80%)	126 (100%)	0	100	100
17	T	27/28 (96%)	27 (100%)	0	100	100
17	t	27/28 (96%)	27 (100%)	0	100	100
18	W	44/87 (51%)	44 (100%)	0	100	100
18	w	44/87 (51%)	44 (100%)	0	100	100
19	X	25/67 (37%)	25 (100%)	0	100	100
19	x	25/67 (37%)	25 (100%)	0	100	100
20	Z	51/52 (98%)	51 (100%)	0	100	100
20	z	51/52 (98%)	51 (100%)	0	100	100
21	N	169/194 (87%)	169 (100%)	0	100	100
21	n	169/194 (87%)	169 (100%)	0	100	100
22	G	164/187 (88%)	164 (100%)	0	100	100
22	g	164/187 (88%)	163 (99%)	1 (1%)	78	91
23	R	144/218 (66%)	142 (99%)	2 (1%)	59	82
23	r	144/218 (66%)	142 (99%)	2 (1%)	59	82
24	S	190/217 (88%)	188 (99%)	2 (1%)	65	85
24	s	190/217 (88%)	188 (99%)	2 (1%)	65	85
25	Y	170/196 (87%)	170 (100%)	0	100	100
25	y	170/196 (87%)	170 (100%)	0	100	100
26	U	21/141 (15%)	21 (100%)	0	100	100
26	u	21/141 (15%)	21 (100%)	0	100	100
28	3	8/8 (100%)	8 (100%)	0	100	100
28	4	8/8 (100%)	8 (100%)	0	100	100
All	All	6210/7354 (84%)	6170 (99%)	40 (1%)	76	91

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	c	389	LEU
22	g	41	LEU
5	d	180	ARG
14	o	106	VAL
23	r	91	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	337	HIS
4	c	320	GLN
22	g	214	GLN
2	b	194	ASN
4	c	143	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 318 ligands modelled in this entry, 6 are monoatomic - leaving 312 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
32	CLA	C	507	47	69,73,73	1.13	9 (13%)	82,113,113	1.40	10 (12%)
32	CLA	Y	613	25	69,73,73	1.13	8 (11%)	82,113,113	1.27	7 (8%)
32	CLA	S	610	24	53,57,73	1.33	7 (13%)	61,93,113	1.21	7 (11%)
43	CHL	r	606	-	38,52,74	4.04	18 (47%)	31,87,114	3.08	16 (51%)
32	CLA	B	606	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
45	XAT	n	1622	-	41,47,47	0.93	2 (4%)	54,74,74	2.58	23 (42%)
32	CLA	y	603	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	8 (9%)
38	LHG	n	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
43	CHL	s	606	-	38,52,74	4.08	18 (47%)	31,87,114	2.93	13 (41%)
32	CLA	D	403	-	69,73,73	1.12	6 (8%)	82,113,113	1.23	7 (8%)
43	CHL	S	608	-	43,57,74	3.99	19 (44%)	37,93,114	2.76	12 (32%)
32	CLA	s	603	-	46,50,73	1.38	7 (15%)	53,85,113	1.40	7 (13%)
32	CLA	c	509	-	69,73,73	1.16	9 (13%)	82,113,113	1.39	10 (12%)
32	CLA	a	407	47	53,57,73	1.25	7 (13%)	61,93,113	1.44	6 (9%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.97	2 (2%)
44	LUT	N	1620	-	42,43,43	0.71	1 (2%)	51,60,60	1.67	14 (27%)
38	LHG	L	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.17	4 (7%)
32	CLA	B	607	-	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
32	CLA	b	607	-	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
32	CLA	c	508	-	69,73,73	1.11	6 (8%)	82,113,113	1.38	8 (9%)
46	NEX	g	1623	-	40,46,46	1.01	3 (7%)	50,70,70	2.23	16 (32%)
32	CLA	S	612	24	49,53,73	1.34	8 (16%)	58,89,113	1.38	7 (12%)
32	CLA	b	603	-	69,73,73	1.13	9 (13%)	82,113,113	1.17	8 (9%)
32	CLA	S	613	24	53,57,73	1.33	8 (15%)	61,93,113	1.29	5 (8%)
32	CLA	G	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	8 (9%)
36	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
32	CLA	N	602	21	69,73,73	1.15	7 (10%)	82,113,113	1.15	7 (8%)
32	CLA	s	614	-	52,56,73	1.29	7 (13%)	61,92,113	1.22	5 (8%)
43	CHL	n	607	-	60,74,74	3.20	20 (33%)	58,114,114	2.26	15 (25%)
32	CLA	S	602	24	53,57,73	1.27	8 (15%)	61,93,113	1.28	7 (11%)
46	NEX	R	625	-	40,46,46	0.99	3 (7%)	50,70,70	2.34	16 (32%)
43	CHL	y	608	-	44,58,74	3.85	19 (43%)	37,94,114	2.89	14 (37%)
41	HEM	f	101	7,6	50,50,50	1.38	7 (14%)	67,82,82	1.10	3 (4%)
32	CLA	S	614	-	52,56,73	1.29	7 (13%)	61,92,113	1.21	5 (8%)
32	CLA	B	617	-	69,73,73	1.13	7 (10%)	82,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	y	613	25	69,73,73	1.13	8 (11%)	82,113,113	1.27	7 (8%)
32	CLA	r	602	23	64,68,73	1.20	7 (10%)	76,107,113	1.20	6 (7%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	5 (7%)
32	CLA	G	611	38	49,53,73	1.34	6 (12%)	58,89,113	1.43	6 (10%)
38	LHG	s	2630	32	44,44,48	0.95	2 (4%)	47,50,54	1.01	2 (4%)
32	CLA	b	613	-	69,73,73	1.16	12 (17%)	82,113,113	1.48	9 (10%)
32	CLA	y	612	25	69,73,73	1.14	7 (10%)	82,113,113	1.19	5 (6%)
43	CHL	y	601	25	60,74,74	3.02	20 (33%)	58,114,114	2.78	17 (29%)
35	SQD	b	621	-	52,54,54	1.11	3 (5%)	62,65,65	1.00	2 (3%)
32	CLA	R	609	23	49,53,73	1.37	5 (10%)	58,89,113	1.37	8 (13%)
43	CHL	R	608	-	40,54,74	4.10	19 (47%)	34,90,114	2.62	11 (32%)
38	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.17	4 (7%)
32	CLA	b	606	-	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
32	CLA	S	605	24	54,58,73	1.27	7 (12%)	64,95,113	1.32	7 (10%)
46	NEX	n	1623	-	40,46,46	1.00	3 (7%)	50,70,70	2.19	15 (30%)
32	CLA	y	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.22	7 (8%)
32	CLA	N	613	21	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
45	XAT	G	1622	-	41,47,47	0.89	2 (4%)	54,74,74	2.76	22 (40%)
43	CHL	N	608	-	44,58,74	3.78	19 (43%)	37,94,114	2.91	12 (32%)
38	LHG	D	410	-	38,38,48	1.00	2 (5%)	41,44,54	1.01	2 (4%)
32	CLA	C	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	9 (10%)
43	CHL	g	605	22	42,56,74	4.21	20 (47%)	36,92,114	2.49	12 (33%)
32	CLA	G	614	-	53,57,73	1.30	6 (11%)	61,93,113	1.20	5 (8%)
32	CLA	Y	604	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	7 (8%)
43	CHL	Y	609	25	60,74,74	3.17	19 (31%)	58,114,114	2.53	15 (25%)
32	CLA	s	610	24	53,57,73	1.33	7 (13%)	61,93,113	1.22	8 (13%)
32	CLA	B	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	9 (10%)
32	CLA	g	604	-	53,57,73	1.32	8 (15%)	61,93,113	1.32	6 (9%)
32	CLA	y	611	38	69,73,73	1.14	9 (13%)	82,113,113	1.26	8 (9%)
32	CLA	r	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.29	6 (9%)
38	LHG	d	408	-	43,43,48	0.96	2 (4%)	46,49,54	1.04	2 (4%)
32	CLA	B	613	-	69,73,73	1.16	12 (17%)	82,113,113	1.48	9 (10%)
38	LHG	G	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
36	LMG	b	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
42	LMU	z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.15	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	G	605	22	42,56,74	4.20	20 (47%)	36,92,114	2.49	12 (33%)
38	LHG	D	408	-	43,43,48	0.96	2 (4%)	46,49,54	1.03	2 (4%)
32	CLA	A	410	-	64,68,73	1.16	8 (12%)	76,107,113	1.34	10 (13%)
34	BCR	B	619	-	41,41,41	0.70	0	56,56,56	1.95	13 (23%)
46	NEX	s	1623	-	40,46,46	1.12	4 (10%)	50,70,70	2.28	16 (32%)
43	CHL	y	607	-	60,74,74	3.15	19 (31%)	58,114,114	2.51	18 (31%)
34	BCR	B	620	-	41,41,41	0.70	0	56,56,56	1.76	13 (23%)
32	CLA	s	613	24	53,57,73	1.33	8 (15%)	61,93,113	1.30	5 (8%)
32	CLA	R	610	23	45,49,73	1.40	7 (15%)	54,84,113	1.24	4 (7%)
34	BCR	a	411	-	41,41,41	0.70	0	56,56,56	1.72	14 (25%)
44	LUT	G	1621	-	42,43,43	0.76	0	51,60,60	1.67	12 (23%)
32	CLA	d	402	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
32	CLA	B	609	-	69,73,73	1.11	9 (13%)	82,113,113	1.27	5 (6%)
32	CLA	C	502	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	3 (3%)
32	CLA	b	602	47	69,73,73	1.14	7 (10%)	82,113,113	1.28	6 (7%)
41	HEM	F	101	7,6	50,50,50	1.37	7 (14%)	67,82,82	1.10	3 (4%)
43	CHL	y	606	-	60,74,74	3.11	20 (33%)	58,114,114	2.40	15 (25%)
46	NEX	Y	1623	-	40,46,46	1.01	3 (7%)	50,70,70	2.34	17 (34%)
32	CLA	n	602	21	69,73,73	1.15	7 (10%)	82,113,113	1.15	7 (8%)
38	LHG	d	410	-	38,38,48	1.01	2 (5%)	41,44,54	1.01	2 (4%)
37	DGD	C	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	5 (7%)
33	PHO	a	409	-	58,69,69	2.05	10 (17%)	55,99,99	1.74	9 (16%)
45	XAT	g	1622	-	41,47,47	0.89	2 (4%)	54,74,74	2.75	23 (42%)
36	LMG	D	411	-	46,46,55	0.95	2 (4%)	54,54,63	1.16	4 (7%)
32	CLA	G	613	22	69,73,73	1.16	7 (10%)	82,113,113	1.38	4 (4%)
43	CHL	N	606	-	40,54,74	3.98	19 (47%)	34,90,114	3.12	14 (41%)
43	CHL	N	607	-	60,74,74	3.19	20 (33%)	58,114,114	2.26	15 (25%)
32	CLA	N	603	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
45	XAT	y	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.28	24 (44%)
34	BCR	C	516	-	41,41,41	0.77	1 (2%)	56,56,56	1.90	15 (26%)
32	CLA	c	511	4	69,73,73	1.13	8 (11%)	82,113,113	1.32	8 (9%)
34	BCR	b	618	-	41,41,41	0.68	0	56,56,56	1.86	17 (30%)
36	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	4 (6%)
43	CHL	Y	601	25	60,74,74	3.02	20 (33%)	58,114,114	2.78	17 (29%)
32	CLA	r	603	-	53,57,73	1.33	9 (16%)	61,93,113	1.40	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	Y	606	-	60,74,74	3.11	20 (33%)	58,114,114	2.40	15 (25%)
46	NEX	r	625	-	40,46,46	1.10	4 (10%)	50,70,70	2.35	17 (34%)
32	CLA	N	614	-	53,57,73	1.31	6 (11%)	61,93,113	1.25	5 (8%)
34	BCR	c	517	-	41,41,41	0.66	0	56,56,56	1.96	16 (28%)
43	CHL	n	601	21	60,74,74	3.26	19 (31%)	58,114,114	2.36	14 (24%)
42	LMU	Y	2632	-	36,36,36	1.13	2 (5%)	47,47,47	1.13	5 (10%)
44	LUT	Y	1620	-	42,43,43	0.77	0	51,60,60	2.05	17 (33%)
32	CLA	y	602	25	69,73,73	1.16	9 (13%)	82,113,113	1.20	9 (10%)
42	LMU	Z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.22	5 (10%)
38	LHG	d	409	-	48,48,48	0.89	3 (6%)	51,54,54	0.99	4 (7%)
42	LMU	Z	2635	-	36,36,36	1.21	2 (5%)	47,47,47	1.14	4 (8%)
32	CLA	b	609	-	69,73,73	1.11	9 (13%)	82,113,113	1.28	5 (6%)
32	CLA	c	513	-	69,73,73	1.11	8 (11%)	82,113,113	1.26	8 (9%)
32	CLA	N	611	38	53,57,73	1.30	7 (13%)	61,93,113	1.27	5 (8%)
32	CLA	A	406	47	69,73,73	1.14	9 (13%)	82,113,113	1.34	8 (9%)
34	BCR	b	620	-	41,41,41	0.71	0	56,56,56	1.75	13 (23%)
35	SQD	A	412	-	49,51,54	1.13	3 (6%)	59,62,65	3.32	10 (16%)
32	CLA	C	503	-	69,73,73	1.18	9 (13%)	82,113,113	1.26	11 (13%)
43	CHL	Y	608	-	44,58,74	3.84	19 (43%)	37,94,114	2.90	14 (37%)
32	CLA	C	511	4	69,73,73	1.13	8 (11%)	82,113,113	1.32	8 (9%)
44	LUT	y	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.80	11 (21%)
36	LMG	H	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.08	3 (5%)
32	CLA	c	505	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	9 (10%)
43	CHL	g	609	22	60,74,74	3.24	19 (31%)	58,114,114	2.50	16 (27%)
43	CHL	g	608	-	38,52,74	4.11	18 (47%)	31,87,114	2.95	14 (45%)
34	BCR	D	404	-	41,41,41	0.70	0	56,56,56	1.94	20 (35%)
34	BCR	b	619	-	41,41,41	0.69	0	56,56,56	1.96	13 (23%)
32	CLA	B	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.27	8 (9%)
44	LUT	g	1620	-	42,43,43	0.68	0	51,60,60	1.77	13 (25%)
32	CLA	B	615	-	69,73,73	1.14	8 (11%)	82,113,113	1.19	6 (7%)
32	CLA	Y	602	25	69,73,73	1.16	9 (13%)	82,113,113	1.20	8 (9%)
43	CHL	Y	607	-	60,74,74	3.15	19 (31%)	58,114,114	2.51	18 (31%)
35	SQD	a	412	-	49,51,54	1.13	3 (6%)	59,62,65	3.32	10 (16%)
32	CLA	c	501	-	69,73,73	1.15	8 (11%)	82,113,113	1.18	8 (9%)
43	CHL	y	605	25	40,54,74	4.09	19 (47%)	34,90,114	2.70	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	S	604	-	53,57,73	1.30	8 (15%)	61,93,113	1.33	6 (9%)
32	CLA	b	608	47	69,73,73	1.14	8 (11%)	82,113,113	1.23	7 (8%)
32	CLA	g	602	22	69,73,73	1.14	8 (11%)	82,113,113	1.14	6 (7%)
32	CLA	s	605	24	54,58,73	1.27	7 (12%)	64,95,113	1.32	7 (10%)
46	NEX	S	1623	-	40,46,46	1.07	3 (7%)	50,70,70	2.26	16 (32%)
32	CLA	c	507	47	69,73,73	1.13	8 (11%)	82,113,113	1.40	10 (12%)
32	CLA	C	513	-	69,73,73	1.11	8 (11%)	82,113,113	1.27	8 (9%)
32	CLA	G	604	-	53,57,73	1.33	8 (15%)	61,93,113	1.32	6 (9%)
43	CHL	G	609	22	60,74,74	3.24	19 (31%)	58,114,114	2.49	15 (25%)
32	CLA	C	508	-	69,73,73	1.11	6 (8%)	82,113,113	1.37	8 (9%)
32	CLA	B	603	-	69,73,73	1.13	9 (13%)	82,113,113	1.16	8 (9%)
32	CLA	D	402	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
32	CLA	b	611	47	69,73,73	1.15	8 (11%)	82,113,113	1.43	8 (9%)
44	LUT	S	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.83	18 (35%)
46	NEX	G	1623	-	40,46,46	1.12	4 (10%)	50,70,70	2.26	15 (30%)
32	CLA	S	611	38	53,57,73	1.27	8 (15%)	61,93,113	1.31	7 (11%)
32	CLA	n	604	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	7 (8%)
36	LMG	a	413	-	48,48,55	0.97	2 (4%)	56,56,63	1.07	4 (7%)
32	CLA	g	611	38	49,53,73	1.34	6 (12%)	58,89,113	1.42	6 (10%)
34	BCR	C	514	-	41,41,41	0.76	0	56,56,56	1.71	10 (17%)
32	CLA	S	609	24	45,49,73	1.42	6 (13%)	54,84,113	1.30	5 (9%)
32	CLA	n	613	21	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
32	CLA	N	612	21	49,53,73	1.37	7 (14%)	58,89,113	1.33	7 (12%)
44	LUT	n	1620	-	42,43,43	0.71	1 (2%)	51,60,60	1.67	14 (27%)
32	CLA	c	506	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	8 (9%)
40	PL9	D	405	-	55,55,55	1.96	14 (25%)	68,69,69	1.40	12 (17%)
34	BCR	d	404	-	41,41,41	0.69	0	56,56,56	1.94	20 (35%)
32	CLA	B	602	47	69,73,73	1.14	7 (10%)	82,113,113	1.27	6 (7%)
29	OEX	A	401	1,4	0,15,15	-	-	-	-	-
32	CLA	R	602	23	64,68,73	1.20	7 (10%)	76,107,113	1.20	6 (7%)
32	CLA	d	403	-	69,73,73	1.13	7 (10%)	82,113,113	1.22	7 (8%)
32	CLA	C	504	47	69,73,73	1.14	8 (11%)	82,113,113	1.24	5 (6%)
32	CLA	g	610	22	69,73,73	1.12	5 (7%)	82,113,113	1.18	5 (6%)
43	CHL	S	606	-	38,52,74	4.09	18 (47%)	31,87,114	2.93	13 (41%)
32	CLA	n	614	-	53,57,73	1.32	7 (13%)	61,93,113	1.26	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	h	101	-	41,41,41	0.65	0	56,56,56	2.02	13 (23%)
36	LMG	A	413	-	48,48,55	0.96	2 (4%)	56,56,63	1.08	4 (7%)
32	CLA	B	612	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
46	NEX	N	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.22	15 (30%)
43	CHL	R	606	-	38,52,74	4.04	18 (47%)	31,87,114	3.08	16 (51%)
37	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	6 (7%)
32	CLA	n	611	38	53,57,73	1.30	7 (13%)	61,93,113	1.28	5 (8%)
32	CLA	G	610	22	69,73,73	1.12	6 (8%)	82,113,113	1.19	5 (6%)
32	CLA	b	605	-	69,73,73	1.19	9 (13%)	82,113,113	1.36	8 (9%)
32	CLA	c	503	-	69,73,73	1.19	9 (13%)	82,113,113	1.25	11 (13%)
43	CHL	s	601	24	40,54,74	4.05	19 (47%)	34,90,114	2.96	14 (41%)
44	LUT	y	1620	-	42,43,43	0.77	0	51,60,60	2.05	16 (31%)
38	LHG	D	409	-	48,48,48	0.89	3 (6%)	51,54,54	0.99	3 (5%)
33	PHO	A	409	-	58,69,69	2.06	10 (17%)	55,99,99	1.75	9 (16%)
43	CHL	y	609	25	60,74,74	3.18	19 (31%)	58,114,114	2.53	15 (25%)
43	CHL	S	601	24	40,54,74	4.04	19 (47%)	34,90,114	2.97	15 (44%)
43	CHL	n	605	21	60,74,74	3.21	19 (31%)	58,114,114	2.54	17 (29%)
38	LHG	S	2630	32	44,44,48	0.95	2 (4%)	47,50,54	1.01	2 (4%)
32	CLA	y	610	25	69,73,73	1.11	8 (11%)	82,113,113	1.12	7 (8%)
32	CLA	b	604	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	9 (10%)
37	DGD	C	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	6 (7%)
44	LUT	S	1621	-	42,43,43	0.72	0	51,60,60	1.88	15 (29%)
32	CLA	b	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.29	8 (9%)
39	BCT	D	401	30	3,3,3	1.15	0	2,3,3	4.22	2 (100%)
43	CHL	G	601	22	60,74,74	3.14	19 (31%)	58,114,114	2.53	17 (29%)
43	CHL	g	601	22	60,74,74	3.14	19 (31%)	58,114,114	2.46	19 (32%)
38	LHG	c	2630	-	46,46,48	0.92	2 (4%)	49,52,54	1.04	4 (8%)
32	CLA	b	615	-	69,73,73	1.14	8 (11%)	82,113,113	1.18	6 (7%)
43	CHL	Y	605	25	40,54,74	4.09	19 (47%)	34,90,114	2.70	14 (41%)
43	CHL	s	607	-	37,51,74	4.21	17 (45%)	30,86,114	3.15	12 (40%)
43	CHL	n	606	-	40,54,74	3.97	19 (47%)	34,90,114	3.12	14 (41%)
44	LUT	G	1620	-	42,43,43	0.68	0	51,60,60	1.77	14 (27%)
33	PHO	a	408	-	58,69,69	2.03	10 (17%)	55,99,99	1.61	11 (20%)
34	BCR	c	515	-	41,41,41	0.79	1 (2%)	56,56,56	2.01	20 (35%)
32	CLA	G	612	22	47,51,73	1.38	7 (14%)	55,86,113	1.41	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	s	611	38	53,57,73	1.26	8 (15%)	61,93,113	1.30	7 (11%)
36	LMG	h	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.11	3 (5%)
32	CLA	Y	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	8 (9%)
43	CHL	g	606	-	44,58,74	3.82	19 (43%)	37,94,114	2.94	14 (37%)
32	CLA	a	405	-	69,73,73	1.22	9 (13%)	82,113,113	1.39	10 (12%)
43	CHL	g	607	-	44,58,74	3.87	19 (43%)	37,94,114	2.78	18 (48%)
34	BCR	c	514	-	41,41,41	0.76	0	56,56,56	1.71	10 (17%)
32	CLA	y	614	-	58,62,73	1.24	8 (13%)	68,99,113	1.23	6 (8%)
43	CHL	G	608	-	38,52,74	4.11	18 (47%)	31,87,114	2.94	13 (41%)
32	CLA	g	613	22	69,73,73	1.16	8 (11%)	82,113,113	1.38	3 (3%)
43	CHL	N	609	21	60,74,74	3.14	19 (31%)	58,114,114	2.28	12 (20%)
32	CLA	R	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.29	5 (8%)
38	LHG	C	2630	-	46,46,48	0.92	2 (4%)	49,52,54	1.05	4 (8%)
36	LMG	B	622	-	51,51,55	0.90	2 (3%)	59,59,63	1.11	4 (6%)
38	LHG	N	2630	32	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
40	PL9	d	405	-	55,55,55	1.97	13 (23%)	68,69,69	1.40	12 (17%)
32	CLA	R	603	-	53,57,73	1.32	9 (16%)	61,93,113	1.40	8 (13%)
34	BCR	c	516	-	41,41,41	0.77	1 (2%)	56,56,56	1.91	16 (28%)
43	CHL	S	607	-	37,51,74	4.21	17 (45%)	30,86,114	3.15	12 (40%)
34	BCR	A	411	-	41,41,41	0.71	0	56,56,56	1.72	14 (25%)
45	XAT	r	624	-	41,47,47	0.87	2 (4%)	54,74,74	2.59	20 (37%)
38	LHG	y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.21	6 (11%)
32	CLA	r	609	23	49,53,73	1.37	6 (12%)	58,89,113	1.38	8 (13%)
32	CLA	g	614	-	53,57,73	1.30	6 (11%)	61,93,113	1.21	5 (8%)
32	CLA	G	602	22	69,73,73	1.14	8 (11%)	82,113,113	1.15	7 (8%)
34	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	2.01	20 (35%)
44	LUT	n	1621	-	42,43,43	0.74	0	51,60,60	1.65	9 (17%)
43	CHL	G	607	-	44,58,74	3.86	19 (43%)	37,94,114	2.79	18 (48%)
32	CLA	s	609	24	45,49,73	1.41	6 (13%)	54,84,113	1.30	5 (9%)
34	BCR	B	618	-	41,41,41	0.68	0	56,56,56	1.87	17 (30%)
37	DGD	C	524	-	67,67,67	0.83	2 (2%)	81,81,81	1.00	4 (4%)
29	OEX	a	401	1,4	0,15,15	-	-	-	-	-
44	LUT	s	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.83	17 (33%)
44	LUT	N	1621	-	42,43,43	0.74	0	51,60,60	1.65	9 (17%)
34	BCR	C	517	-	41,41,41	0.66	0	56,56,56	1.96	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	d	411	-	46,46,55	0.96	2 (4%)	54,54,63	1.16	4 (7%)
32	CLA	a	410	-	64,68,73	1.15	8 (12%)	76,107,113	1.33	10 (13%)
32	CLA	C	501	-	69,73,73	1.16	7 (10%)	82,113,113	1.16	8 (9%)
32	CLA	N	610	21	69,73,73	1.12	7 (10%)	82,113,113	1.17	7 (8%)
32	CLA	B	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
32	CLA	S	603	-	46,50,73	1.38	7 (15%)	53,85,113	1.41	7 (13%)
44	LUT	g	1621	-	42,43,43	0.76	0	51,60,60	1.67	12 (23%)
43	CHL	R	607	-	44,58,74	3.98	19 (43%)	37,94,114	2.66	14 (37%)
43	CHL	N	605	21	60,74,74	3.21	19 (31%)	58,114,114	2.54	17 (29%)
44	LUT	s	1621	-	42,43,43	0.72	0	51,60,60	1.88	15 (29%)
32	CLA	N	604	-	69,73,73	1.16	8 (11%)	82,113,113	1.17	7 (8%)
32	CLA	s	602	24	53,57,73	1.27	8 (15%)	61,93,113	1.29	7 (11%)
32	CLA	Y	610	25	69,73,73	1.11	7 (10%)	82,113,113	1.12	7 (8%)
43	CHL	n	608	-	44,58,74	3.78	19 (43%)	37,94,114	2.93	12 (32%)
46	NEX	y	1623	-	40,46,46	0.96	3 (7%)	50,70,70	2.33	17 (34%)
33	PHO	A	408	-	58,69,69	2.02	10 (17%)	55,99,99	1.61	10 (18%)
32	CLA	Y	611	38	69,73,73	1.13	8 (11%)	82,113,113	1.27	7 (8%)
32	CLA	b	614	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
32	CLA	r	610	23	45,49,73	1.39	7 (15%)	54,84,113	1.25	5 (9%)
43	CHL	N	601	21	60,74,74	3.27	19 (31%)	58,114,114	2.36	15 (25%)
32	CLA	n	612	21	49,53,73	1.37	7 (14%)	58,89,113	1.33	7 (12%)
32	CLA	b	617	-	69,73,73	1.14	7 (10%)	82,113,113	1.27	8 (9%)
32	CLA	c	504	47	69,73,73	1.14	8 (11%)	82,113,113	1.24	5 (6%)
32	CLA	B	608	47	69,73,73	1.14	8 (11%)	82,113,113	1.22	7 (8%)
32	CLA	C	509	-	69,73,73	1.16	10 (14%)	82,113,113	1.40	10 (12%)
32	CLA	c	512	-	69,73,73	1.13	7 (10%)	82,113,113	1.33	8 (9%)
37	DGD	C	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.98	2 (2%)
43	CHL	n	609	21	60,74,74	3.14	19 (31%)	58,114,114	2.27	12 (20%)
38	LHG	g	2630	32	48,48,48	0.93	2 (4%)	51,54,54	0.97	3 (5%)
32	CLA	b	610	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	8 (9%)
32	CLA	Y	614	-	58,62,73	1.24	8 (13%)	68,99,113	1.23	6 (8%)
32	CLA	b	612	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
32	CLA	B	610	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	8 (9%)
32	CLA	c	510	-	69,73,73	1.15	6 (8%)	82,113,113	1.34	6 (7%)
32	CLA	g	612	22	47,51,73	1.38	7 (14%)	55,86,113	1.41	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	CHL	s	608	-	43,57,74	3.99	19 (44%)	37,93,114	2.75	12 (32%)
45	XAT	N	1622	-	41,47,47	0.92	2 (4%)	54,74,74	2.57	23 (42%)
32	CLA	s	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.33	6 (9%)
32	CLA	C	510	-	69,73,73	1.15	7 (10%)	82,113,113	1.33	6 (7%)
32	CLA	C	506	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	8 (9%)
42	LMU	y	2632	-	36,36,36	1.14	2 (5%)	47,47,47	1.13	5 (10%)
32	CLA	a	406	47	69,73,73	1.14	9 (13%)	82,113,113	1.34	8 (9%)
32	CLA	s	612	24	49,53,73	1.34	8 (16%)	58,89,113	1.38	7 (12%)
35	SQD	B	621	-	52,54,54	1.11	3 (5%)	62,65,65	1.01	2 (3%)
32	CLA	c	502	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	4 (4%)
38	LHG	Y	2630	32	48,48,48	0.91	2 (4%)	51,54,54	1.21	5 (9%)
32	CLA	n	610	21	69,73,73	1.12	7 (10%)	82,113,113	1.16	7 (8%)
32	CLA	C	512	-	69,73,73	1.13	8 (11%)	82,113,113	1.32	9 (10%)
37	DGD	c	524	-	67,67,67	0.83	2 (2%)	81,81,81	1.00	4 (4%)
43	CHL	G	606	-	44,58,74	3.82	19 (43%)	37,94,114	2.94	14 (37%)
43	CHL	r	608	-	40,54,74	4.11	20 (50%)	34,90,114	2.60	12 (35%)
32	CLA	B	611	47	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
42	LMU	z	2634	-	36,36,36	1.20	2 (5%)	47,47,47	1.22	5 (10%)
32	CLA	g	603	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	9 (10%)
45	XAT	Y	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.27	24 (44%)
32	CLA	Y	612	25	69,73,73	1.15	8 (11%)	82,113,113	1.19	5 (6%)
37	DGD	C	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
34	BCR	H	101	-	41,41,41	0.65	0	56,56,56	2.02	13 (23%)
32	CLA	n	603	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
44	LUT	Y	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.80	11 (21%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	0.91	3 (3%)
39	BCT	d	401	30	3,3,3	1.15	0	2,3,3	4.22	2 (100%)
45	XAT	R	624	-	41,47,47	0.87	2 (4%)	54,74,74	2.58	20 (37%)
32	CLA	A	407	47	53,57,73	1.25	7 (13%)	61,93,113	1.45	6 (9%)
32	CLA	B	605	-	69,73,73	1.19	9 (13%)	82,113,113	1.36	10 (12%)
32	CLA	A	405	-	69,73,73	1.21	9 (13%)	82,113,113	1.37	9 (10%)
43	CHL	r	607	-	44,58,74	3.98	19 (43%)	37,94,114	2.66	14 (37%)

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
32	CLA	C	507	47	1/1/15/20	10/39/115/115	-
32	CLA	Y	613	25	-	7/39/115/115	-
32	CLA	S	610	24	1/1/11/20	6/20/96/115	-
43	CHL	r	606	-	3/3/15/26	7/13/111/137	-
32	CLA	B	606	-	1/1/15/20	10/39/115/115	-
45	XAT	n	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	y	603	-	1/1/15/20	15/39/115/115	-
43	CHL	s	606	-	3/3/15/26	5/13/111/137	-
38	LHG	n	2630	32	-	11/53/53/53	-
32	CLA	D	403	-	-	14/39/115/115	-
43	CHL	S	608	-	3/3/16/26	8/19/117/137	-
32	CLA	s	603	-	1/1/10/20	6/12/88/115	-
32	CLA	c	509	-	1/1/15/20	7/39/115/115	-
32	CLA	a	407	47	1/1/11/20	1/20/96/115	-
37	DGD	c	520	-	-	14/48/88/95	0/2/2/2
44	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
38	LHG	L	101	-	-	19/53/53/53	-
32	CLA	B	607	-	1/1/15/20	10/39/115/115	-
32	CLA	b	607	-	1/1/15/20	10/39/115/115	-
32	CLA	c	508	-	1/1/15/20	13/39/115/115	-
46	NEX	g	1623	-	-	3/27/83/83	0/3/3/3
32	CLA	S	612	24	1/1/11/20	6/15/91/115	-
32	CLA	b	603	-	1/1/15/20	15/39/115/115	-
32	CLA	S	613	24	-	10/20/96/115	-
32	CLA	G	603	-	1/1/15/20	15/39/115/115	-
36	LMG	C	521	-	-	5/46/66/70	0/1/1/1
32	CLA	N	602	21	1/1/15/20	12/39/115/115	-
32	CLA	s	614	-	1/1/11/20	5/19/95/115	-
43	CHL	n	607	-	3/3/20/26	21/39/137/137	-
32	CLA	S	602	24	1/1/11/20	8/20/96/115	-
46	NEX	R	625	-	-	5/27/83/83	0/3/3/3
43	CHL	y	608	-	3/3/16/26	4/20/118/137	-
41	HEM	f	101	7,6	-	2/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	S	614	-	1/1/11/20	5/19/95/115	-
32	CLA	B	617	-	1/1/15/20	16/39/115/115	-
32	CLA	y	613	25	-	7/39/115/115	-
32	CLA	r	602	23	1/1/14/20	7/33/109/115	-
37	DGD	c	518	-	-	11/44/84/95	0/2/2/2
32	CLA	G	611	38	1/1/11/20	4/15/91/115	-
38	LHG	s	2630	32	-	6/49/49/53	-
32	CLA	b	613	-	1/1/15/20	7/39/115/115	-
32	CLA	y	612	25	1/1/15/20	18/39/115/115	-
43	CHL	y	601	25	3/3/20/26	20/39/137/137	-
35	SQD	b	621	-	-	15/49/69/69	0/1/1/1
32	CLA	R	609	23	1/1/11/20	7/15/91/115	-
43	CHL	R	608	-	3/3/16/26	5/15/113/137	-
38	LHG	l	101	-	-	19/53/53/53	-
32	CLA	b	606	-	1/1/15/20	10/39/115/115	-
32	CLA	S	605	24	1/1/12/20	6/21/97/115	-
46	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
32	CLA	y	604	-	1/1/15/20	14/39/115/115	-
32	CLA	N	613	21	-	14/39/115/115	-
45	XAT	G	1622	-	-	1/31/93/93	0/4/4/4
43	CHL	N	608	-	3/3/16/26	6/20/118/137	-
38	LHG	D	410	-	-	13/43/43/53	-
32	CLA	C	505	-	-	13/39/115/115	-
43	CHL	g	605	22	3/3/16/26	4/18/116/137	-
32	CLA	G	614	-	1/1/11/20	12/20/96/115	-
32	CLA	Y	604	-	1/1/15/20	14/39/115/115	-
43	CHL	Y	609	25	3/3/20/26	19/39/137/137	-
32	CLA	s	610	24	1/1/11/20	6/20/96/115	-
32	CLA	B	604	-	-	14/39/115/115	-
32	CLA	g	604	-	1/1/11/20	8/20/96/115	-
32	CLA	y	611	38	1/1/15/20	13/39/115/115	-
32	CLA	r	604	-	1/1/11/20	11/20/96/115	-
38	LHG	d	408	-	-	18/48/48/53	-
32	CLA	B	613	-	1/1/15/20	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	G	2630	32	-	17/53/53/53	-
36	LMG	b	622	-	-	3/46/66/70	0/1/1/1
42	LMU	z	2635	-	-	10/21/61/61	0/2/2/2
43	CHL	G	605	22	3/3/16/26	4/18/116/137	-
38	LHG	D	408	-	-	18/48/48/53	-
32	CLA	A	410	-	-	4/33/109/115	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
46	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
43	CHL	y	607	-	3/3/20/26	22/39/137/137	-
34	BCR	B	620	-	-	3/29/63/63	0/2/2/2
32	CLA	s	613	24	-	10/20/96/115	-
32	CLA	R	610	23	1/1/10/20	4/10/86/115	-
34	BCR	a	411	-	-	3/29/63/63	0/2/2/2
44	LUT	G	1621	-	-	5/29/67/67	0/2/2/2
32	CLA	d	402	-	1/1/15/20	9/39/115/115	-
32	CLA	B	609	-	1/1/15/20	14/39/115/115	-
32	CLA	C	502	-	-	6/39/115/115	-
32	CLA	b	602	47	1/1/15/20	15/39/115/115	-
41	HEM	F	101	7,6	-	2/14/54/54	-
43	CHL	y	606	-	3/3/20/26	15/39/137/137	-
46	NEX	Y	1623	-	-	8/27/83/83	0/3/3/3
32	CLA	n	602	21	1/1/15/20	12/39/115/115	-
38	LHG	d	410	-	-	12/43/43/53	-
37	DGD	C	518	-	-	12/44/84/95	0/2/2/2
33	PHO	a	409	-	-	4/37/103/103	0/5/6/6
45	XAT	g	1622	-	-	1/31/93/93	0/4/4/4
36	LMG	D	411	-	-	10/41/61/70	0/1/1/1
32	CLA	G	613	22	-	15/39/115/115	-
43	CHL	N	606	-	3/3/16/26	7/15/113/137	-
43	CHL	N	607	-	3/3/20/26	21/39/137/137	-
32	CLA	N	603	-	1/1/15/20	18/39/115/115	-
45	XAT	y	1622	-	-	4/31/93/93	0/4/4/4
34	BCR	C	516	-	-	8/29/63/63	0/2/2/2
32	CLA	c	511	4	-	9/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	b	618	-	-	2/29/63/63	0/2/2/2
36	LMG	c	521	-	-	5/46/66/70	0/1/1/1
43	CHL	Y	601	25	3/3/20/26	20/39/137/137	-
32	CLA	r	603	-	1/1/11/20	14/20/96/115	-
43	CHL	Y	606	-	3/3/20/26	16/39/137/137	-
46	NEX	r	625	-	-	5/27/83/83	0/3/3/3
32	CLA	N	614	-	1/1/11/20	8/20/96/115	-
34	BCR	c	517	-	-	1/29/63/63	0/2/2/2
43	CHL	n	601	21	3/3/20/26	14/39/137/137	-
42	LMU	Y	2632	-	-	9/21/61/61	0/2/2/2
44	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	y	602	25	1/1/15/20	11/39/115/115	-
42	LMU	Z	2634	-	-	8/21/61/61	0/2/2/2
38	LHG	d	409	-	-	18/53/53/53	-
42	LMU	Z	2635	-	-	10/21/61/61	0/2/2/2
32	CLA	b	609	-	1/1/15/20	14/39/115/115	-
32	CLA	c	513	-	1/1/15/20	16/39/115/115	-
32	CLA	N	611	38	1/1/11/20	11/20/96/115	-
32	CLA	A	406	47	-	5/39/115/115	-
34	BCR	b	620	-	-	3/29/63/63	0/2/2/2
35	SQD	A	412	-	-	15/46/66/69	0/1/1/1
32	CLA	C	503	-	1/1/15/20	10/39/115/115	-
43	CHL	Y	608	-	3/3/16/26	4/20/118/137	-
32	CLA	C	511	4	-	10/39/115/115	-
44	LUT	y	1621	-	-	5/29/67/67	0/2/2/2
36	LMG	H	102	-	-	14/43/63/70	0/1/1/1
32	CLA	c	505	-	-	13/39/115/115	-
43	CHL	g	609	22	3/3/20/26	21/39/137/137	-
43	CHL	g	608	-	3/3/15/26	7/13/111/137	-
34	BCR	D	404	-	-	2/29/63/63	0/2/2/2
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
32	CLA	B	616	-	1/1/15/20	11/39/115/115	-
44	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	B	615	-	1/1/15/20	18/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Y	602	25	1/1/15/20	11/39/115/115	-
43	CHL	Y	607	-	3/3/20/26	22/39/137/137	-
35	SQD	a	412	-	-	15/46/66/69	0/1/1/1
32	CLA	c	501	-	1/1/15/20	17/39/115/115	-
43	CHL	y	605	25	3/3/16/26	10/15/113/137	-
32	CLA	S	604	-	1/1/11/20	6/20/96/115	-
32	CLA	b	608	47	1/1/15/20	11/39/115/115	-
32	CLA	g	602	22	1/1/15/20	17/39/115/115	-
32	CLA	s	605	24	1/1/12/20	6/21/97/115	-
46	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
32	CLA	c	507	47	1/1/15/20	10/39/115/115	-
32	CLA	C	513	-	1/1/15/20	16/39/115/115	-
32	CLA	G	604	-	1/1/11/20	8/20/96/115	-
43	CHL	G	609	22	3/3/20/26	21/39/137/137	-
32	CLA	C	508	-	1/1/15/20	13/39/115/115	-
32	CLA	B	603	-	1/1/15/20	13/39/115/115	-
32	CLA	D	402	-	1/1/15/20	9/39/115/115	-
32	CLA	b	611	47	1/1/15/20	9/39/115/115	-
44	LUT	S	1620	-	-	3/29/67/67	0/2/2/2
46	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
32	CLA	S	611	38	1/1/11/20	7/20/96/115	-
32	CLA	n	604	-	1/1/15/20	10/39/115/115	-
36	LMG	a	413	-	-	15/43/63/70	0/1/1/1
32	CLA	g	611	38	1/1/11/20	4/15/91/115	-
34	BCR	C	514	-	-	2/29/63/63	0/2/2/2
32	CLA	S	609	24	1/1/10/20	4/10/86/115	-
32	CLA	n	613	21	-	14/39/115/115	-
32	CLA	N	612	21	1/1/11/20	6/15/91/115	-
44	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
32	CLA	c	506	-	-	4/39/115/115	-
40	PL9	D	405	-	-	14/53/73/73	0/1/1/1
34	BCR	d	404	-	-	2/29/63/63	0/2/2/2
32	CLA	B	602	47	1/1/15/20	15/39/115/115	-
32	CLA	R	602	23	1/1/14/20	7/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	g	610	22	1/1/15/20	12/39/115/115	-
32	CLA	d	403	-	-	14/39/115/115	-
32	CLA	C	504	47	1/1/15/20	13/39/115/115	-
43	CHL	S	606	-	3/3/15/26	5/13/111/137	-
32	CLA	n	614	-	1/1/11/20	8/20/96/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
36	LMG	A	413	-	-	16/43/63/70	0/1/1/1
32	CLA	B	612	-	1/1/15/20	11/39/115/115	-
46	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
43	CHL	R	606	-	3/3/15/26	7/13/111/137	-
37	DGD	c	519	-	-	11/51/91/95	0/2/2/2
32	CLA	n	611	38	1/1/11/20	11/20/96/115	-
32	CLA	G	610	22	1/1/15/20	12/39/115/115	-
32	CLA	b	605	-	1/1/15/20	11/39/115/115	-
32	CLA	c	503	-	1/1/15/20	10/39/115/115	-
43	CHL	s	601	24	3/3/16/26	7/15/113/137	-
44	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
38	LHG	D	409	-	-	18/53/53/53	-
33	PHO	A	409	-	-	2/37/103/103	0/5/6/6
43	CHL	y	609	25	3/3/20/26	19/39/137/137	-
43	CHL	S	601	24	3/3/16/26	7/15/113/137	-
43	CHL	n	605	21	3/3/20/26	20/39/137/137	-
38	LHG	S	2630	32	-	8/49/49/53	-
32	CLA	y	610	25	1/1/15/20	7/39/115/115	-
32	CLA	b	604	-	-	14/39/115/115	-
37	DGD	C	519	-	-	11/51/91/95	0/2/2/2
44	LUT	S	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	b	616	-	1/1/15/20	11/39/115/115	-
43	CHL	G	601	22	3/3/20/26	12/39/137/137	-
43	CHL	g	601	22	3/3/20/26	12/39/137/137	-
38	LHG	c	2630	-	-	15/51/51/53	-
32	CLA	b	615	-	1/1/15/20	18/39/115/115	-
43	CHL	Y	605	25	3/3/16/26	10/15/113/137	-
43	CHL	s	607	-	3/3/15/26	3/12/110/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CHL	n	606	-	3/3/16/26	7/15/113/137	-
44	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
33	PHO	a	408	-	-	11/37/103/103	0/5/6/6
34	BCR	c	515	-	-	7/29/63/63	0/2/2/2
32	CLA	G	612	22	1/1/10/20	6/13/89/115	-
32	CLA	s	611	38	1/1/11/20	7/20/96/115	-
36	LMG	h	102	-	-	15/43/63/70	0/1/1/1
32	CLA	Y	603	-	1/1/15/20	15/39/115/115	-
43	CHL	g	606	-	3/3/16/26	8/20/118/137	-
32	CLA	a	405	-	1/1/15/20	15/39/115/115	-
43	CHL	g	607	-	3/3/16/26	7/20/118/137	-
34	BCR	c	514	-	-	2/29/63/63	0/2/2/2
32	CLA	y	614	-	1/1/12/20	7/26/102/115	-
43	CHL	G	608	-	3/3/15/26	7/13/111/137	-
32	CLA	g	613	22	-	15/39/115/115	-
43	CHL	N	609	21	3/3/20/26	21/39/137/137	-
32	CLA	R	604	-	1/1/11/20	11/20/96/115	-
38	LHG	C	2630	-	-	15/51/51/53	-
36	LMG	B	622	-	-	3/46/66/70	0/1/1/1
38	LHG	N	2630	32	-	11/53/53/53	-
40	PL9	d	405	-	-	14/53/73/73	0/1/1/1
32	CLA	R	603	-	1/1/11/20	14/20/96/115	-
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
43	CHL	S	607	-	3/3/15/26	3/12/110/137	-
34	BCR	A	411	-	-	3/29/63/63	0/2/2/2
45	XAT	r	624	-	-	1/31/93/93	0/4/4/4
38	LHG	y	2630	32	-	17/53/53/53	-
32	CLA	r	609	23	1/1/11/20	7/15/91/115	-
32	CLA	g	614	-	1/1/11/20	12/20/96/115	-
32	CLA	G	602	22	1/1/15/20	17/39/115/115	-
34	BCR	C	515	-	-	7/29/63/63	0/2/2/2
44	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
43	CHL	G	607	-	3/3/16/26	7/20/118/137	-
32	CLA	s	609	24	1/1/10/20	4/10/86/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	B	618	-	-	2/29/63/63	0/2/2/2
37	DGD	C	524	-	-	10/55/95/95	0/2/2/2
44	LUT	s	1620	-	-	3/29/67/67	0/2/2/2
44	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
34	BCR	C	517	-	-	1/29/63/63	0/2/2/2
36	LMG	d	411	-	-	10/41/61/70	0/1/1/1
32	CLA	a	410	-	-	4/33/109/115	-
32	CLA	C	501	-	1/1/15/20	17/39/115/115	-
32	CLA	N	610	21	1/1/15/20	3/39/115/115	-
32	CLA	B	614	-	1/1/15/20	10/39/115/115	-
32	CLA	S	603	-	1/1/10/20	6/12/88/115	-
44	LUT	g	1621	-	-	4/29/67/67	0/2/2/2
43	CHL	R	607	-	3/3/16/26	7/20/118/137	-
43	CHL	N	605	21	3/3/20/26	20/39/137/137	-
44	LUT	s	1621	-	-	3/29/67/67	0/2/2/2
32	CLA	N	604	-	1/1/15/20	10/39/115/115	-
32	CLA	s	602	24	1/1/11/20	8/20/96/115	-
32	CLA	Y	610	25	1/1/15/20	7/39/115/115	-
43	CHL	n	608	-	3/3/16/26	6/20/118/137	-
46	NEX	y	1623	-	-	9/27/83/83	0/3/3/3
33	PHO	A	408	-	-	13/37/103/103	0/5/6/6
32	CLA	Y	611	38	1/1/15/20	13/39/115/115	-
32	CLA	b	614	-	1/1/15/20	10/39/115/115	-
32	CLA	r	610	23	1/1/10/20	4/10/86/115	-
43	CHL	N	601	21	3/3/20/26	14/39/137/137	-
32	CLA	n	612	21	1/1/11/20	6/15/91/115	-
32	CLA	b	617	-	1/1/15/20	16/39/115/115	-
32	CLA	c	504	47	1/1/15/20	13/39/115/115	-
32	CLA	B	608	47	1/1/15/20	11/39/115/115	-
32	CLA	C	509	-	1/1/15/20	7/39/115/115	-
32	CLA	c	512	-	1/1/15/20	14/39/115/115	-
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
43	CHL	n	609	21	3/3/20/26	21/39/137/137	-
38	LHG	g	2630	32	-	17/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	610	-	-	13/39/115/115	-
32	CLA	Y	614	-	1/1/12/20	7/26/102/115	-
32	CLA	b	612	-	1/1/15/20	11/39/115/115	-
32	CLA	c	510	-	1/1/15/20	13/39/115/115	-
32	CLA	B	610	-	-	13/39/115/115	-
32	CLA	g	612	22	1/1/10/20	6/13/89/115	-
43	CHL	s	608	-	3/3/16/26	8/19/117/137	-
45	XAT	N	1622	-	-	1/31/93/93	0/4/4/4
32	CLA	s	604	-	1/1/11/20	6/20/96/115	-
32	CLA	C	510	-	1/1/15/20	14/39/115/115	-
32	CLA	C	506	-	-	4/39/115/115	-
42	LMU	y	2632	-	-	9/21/61/61	0/2/2/2
32	CLA	a	406	47	-	7/39/115/115	-
32	CLA	s	612	24	1/1/11/20	6/15/91/115	-
35	SQD	B	621	-	-	17/49/69/69	0/1/1/1
32	CLA	c	502	-	-	6/39/115/115	-
38	LHG	Y	2630	32	-	17/53/53/53	-
32	CLA	n	610	21	1/1/15/20	3/39/115/115	-
32	CLA	C	512	-	1/1/15/20	14/39/115/115	-
37	DGD	c	524	-	-	10/55/95/95	0/2/2/2
43	CHL	G	606	-	3/3/16/26	8/20/118/137	-
43	CHL	r	608	-	3/3/16/26	5/15/113/137	-
32	CLA	B	611	47	1/1/15/20	9/39/115/115	-
42	LMU	z	2634	-	-	8/21/61/61	0/2/2/2
32	CLA	g	603	-	1/1/15/20	15/39/115/115	-
45	XAT	Y	1622	-	-	4/31/93/93	0/4/4/4
32	CLA	Y	612	25	1/1/15/20	18/39/115/115	-
37	DGD	C	523	-	-	15/55/95/95	0/2/2/2
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
32	CLA	n	603	-	1/1/15/20	18/39/115/115	-
44	LUT	Y	1621	-	-	5/29/67/67	0/2/2/2
37	DGD	c	523	-	-	15/55/95/95	0/2/2/2
45	XAT	R	624	-	-	1/31/93/93	0/4/4/4
32	CLA	A	407	47	1/1/11/20	1/20/96/115	-
32	CLA	B	605	-	1/1/15/20	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	A	405	-	1/1/15/20	15/39/115/115	-
43	CHL	r	607	-	3/3/16/26	7/20/118/137	-

The worst 5 of 2334 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	g	605	CHL	C2C-C3C	11.03	1.47	1.36
43	G	605	CHL	C2C-C3C	10.95	1.47	1.36
43	G	605	CHL	C1D-C2D	10.51	1.51	1.39
43	s	608	CHL	C2C-C3C	10.48	1.46	1.36
43	S	608	CHL	C2C-C3C	10.43	1.46	1.36

The worst 5 of 2866 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	y	1622	XAT	C37-C21-C36	-17.36	82.16	107.37
45	Y	1622	XAT	C37-C21-C36	-17.35	82.17	107.37
35	A	412	SQD	O9-S-C6	-16.02	82.84	106.76
35	a	412	SQD	O9-S-C6	-15.94	82.95	106.76
45	y	1622	XAT	C37-C21-C22	-14.83	82.91	108.97

5 of 272 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	407	CLA	ND
32	B	602	CLA	ND
32	B	603	CLA	ND
32	B	605	CLA	ND

5 of 2925 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	B	604	CLA	C4-C3-C5-C6
32	B	605	CLA	C1A-C2A-CAA-CBA
32	B	605	CLA	CAD-CBD-CGD-O1D
32	B	605	CLA	CAD-CBD-CGD-O2D
32	B	610	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

257 monomers are involved in 577 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	507	CLA	2	0
32	Y	613	CLA	3	0
43	r	606	CHL	1	0
32	B	606	CLA	4	0
45	n	1622	XAT	7	0
32	y	603	CLA	3	0
38	n	2630	LHG	4	0
43	s	606	CHL	2	0
43	S	608	CHL	2	0
32	s	603	CLA	1	0
37	c	520	DGD	4	0
44	N	1620	LUT	4	0
38	L	101	LHG	3	0
32	B	607	CLA	2	0
32	b	607	CLA	1	0
32	c	508	CLA	4	0
46	g	1623	NEX	1	0
32	b	603	CLA	2	0
32	G	603	CLA	3	0
32	N	602	CLA	3	0
32	s	614	CLA	1	0
43	n	607	CHL	5	0
46	R	625	NEX	3	0
32	S	614	CLA	1	0
32	B	617	CLA	2	0
32	y	613	CLA	4	0
32	r	602	CLA	4	0
37	c	518	DGD	2	0
38	s	2630	LHG	3	0
32	b	613	CLA	6	0
32	y	612	CLA	3	0
43	y	601	CHL	2	0
35	b	621	SQD	2	0
32	R	609	CLA	1	0
43	R	608	CHL	1	0
38	l	101	LHG	4	0
32	b	606	CLA	4	0
46	n	1623	NEX	2	0
32	y	604	CLA	3	0
32	N	613	CLA	1	0
45	G	1622	XAT	4	0
38	D	410	LHG	3	0
32	C	505	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	Y	604	CLA	3	0
43	Y	609	CHL	5	0
32	B	604	CLA	5	0
32	g	604	CLA	2	0
32	y	611	CLA	4	0
32	r	604	CLA	1	0
38	d	408	LHG	5	0
32	B	613	CLA	7	0
38	G	2630	LHG	4	0
36	b	622	LMG	2	0
42	z	2635	LMU	2	0
38	D	408	LHG	4	0
32	A	410	CLA	2	0
34	B	619	BCR	4	0
46	s	1623	NEX	1	0
43	y	607	CHL	2	0
34	B	620	BCR	2	0
32	R	610	CLA	2	0
34	a	411	BCR	3	0
44	G	1621	LUT	4	0
32	d	402	CLA	6	0
32	B	609	CLA	2	0
32	b	602	CLA	1	0
43	y	606	CHL	3	0
46	Y	1623	NEX	2	0
32	n	602	CLA	3	0
38	d	410	LHG	2	0
37	C	518	DGD	2	0
33	a	409	PHO	2	0
45	g	1622	XAT	5	0
36	D	411	LMG	3	0
43	N	606	CHL	2	0
43	N	607	CHL	5	0
32	N	603	CLA	3	0
45	y	1622	XAT	5	0
34	C	516	BCR	4	0
32	c	511	CLA	3	0
34	b	618	BCR	6	0
43	Y	601	CHL	2	0
43	Y	606	CHL	3	0
46	r	625	NEX	3	0
34	c	517	BCR	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	n	601	CHL	6	0
42	Y	2632	LMU	2	0
44	Y	1620	LUT	3	0
32	y	602	CLA	2	0
38	d	409	LHG	4	0
42	Z	2635	LMU	1	0
32	b	609	CLA	2	0
32	c	513	CLA	4	0
32	A	406	CLA	3	0
34	b	620	BCR	3	0
35	A	412	SQD	2	0
32	C	503	CLA	3	0
32	C	511	CLA	4	0
44	y	1621	LUT	4	0
36	H	102	LMG	1	0
32	c	505	CLA	3	0
43	g	609	CHL	5	0
43	g	608	CHL	1	0
34	D	404	BCR	5	0
34	b	619	BCR	3	0
32	B	616	CLA	2	0
44	g	1620	LUT	4	0
32	B	615	CLA	3	0
32	Y	602	CLA	2	0
43	Y	607	CHL	2	0
35	a	412	SQD	1	0
32	c	501	CLA	1	0
43	y	605	CHL	1	0
32	S	604	CLA	1	0
32	b	608	CLA	3	0
32	g	602	CLA	6	0
46	S	1623	NEX	3	0
32	c	507	CLA	2	0
32	C	513	CLA	5	0
32	G	604	CLA	2	0
43	G	609	CHL	4	0
32	C	508	CLA	4	0
32	B	603	CLA	3	0
32	D	402	CLA	6	0
32	b	611	CLA	1	0
46	G	1623	NEX	1	0
32	S	611	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	n	604	CLA	4	0
36	a	413	LMG	8	0
34	C	514	BCR	2	0
32	S	609	CLA	1	0
32	n	613	CLA	1	0
44	n	1620	LUT	3	0
32	c	506	CLA	2	0
40	D	405	PL9	3	0
34	d	404	BCR	3	0
32	B	602	CLA	1	0
29	A	401	OEX	1	0
32	R	602	CLA	4	0
32	C	504	CLA	3	0
32	g	610	CLA	2	0
43	S	606	CHL	2	0
34	h	101	BCR	2	0
36	A	413	LMG	8	0
32	B	612	CLA	3	0
46	N	1623	NEX	2	0
43	R	606	CHL	1	0
37	c	519	DGD	6	0
32	G	610	CLA	2	0
32	b	605	CLA	5	0
32	c	503	CLA	4	0
44	y	1620	LUT	2	0
38	D	409	LHG	4	0
33	A	409	PHO	2	0
43	y	609	CHL	6	0
43	n	605	CHL	2	0
38	S	2630	LHG	5	0
32	y	610	CLA	1	0
32	b	604	CLA	3	0
37	C	519	DGD	4	0
44	S	1621	LUT	5	0
32	b	616	CLA	1	0
43	G	601	CHL	6	0
43	g	601	CHL	6	0
38	c	2630	LHG	4	0
32	b	615	CLA	3	0
43	Y	605	CHL	1	0
43	n	606	CHL	2	0
44	G	1620	LUT	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	408	PHO	2	0
34	c	515	BCR	3	0
32	s	611	CLA	1	0
36	h	102	LMG	1	0
32	Y	603	CLA	2	0
32	a	405	CLA	1	0
43	g	607	CHL	3	0
34	c	514	BCR	3	0
32	y	614	CLA	3	0
43	G	608	CHL	1	0
43	N	609	CHL	5	0
32	R	604	CLA	1	0
38	C	2630	LHG	4	0
36	B	622	LMG	2	0
38	N	2630	LHG	3	0
40	d	405	PL9	4	0
34	c	516	BCR	4	0
34	A	411	BCR	2	0
45	r	624	XAT	2	0
38	y	2630	LHG	3	0
32	r	609	CLA	1	0
32	G	602	CLA	4	0
34	C	515	BCR	2	0
44	n	1621	LUT	3	0
43	G	607	CHL	3	0
32	s	609	CLA	1	0
34	B	618	BCR	6	0
37	C	524	DGD	2	0
29	a	401	OEX	1	0
44	s	1620	LUT	1	0
44	N	1621	LUT	3	0
34	C	517	BCR	4	0
36	d	411	LMG	3	0
32	a	410	CLA	3	0
32	C	501	CLA	1	0
32	N	610	CLA	1	0
32	B	614	CLA	4	0
32	S	603	CLA	1	0
44	g	1621	LUT	3	0
43	R	607	CHL	2	0
43	N	605	CHL	2	0
44	s	1621	LUT	5	0

Continued on next page...

Continued from previous page...

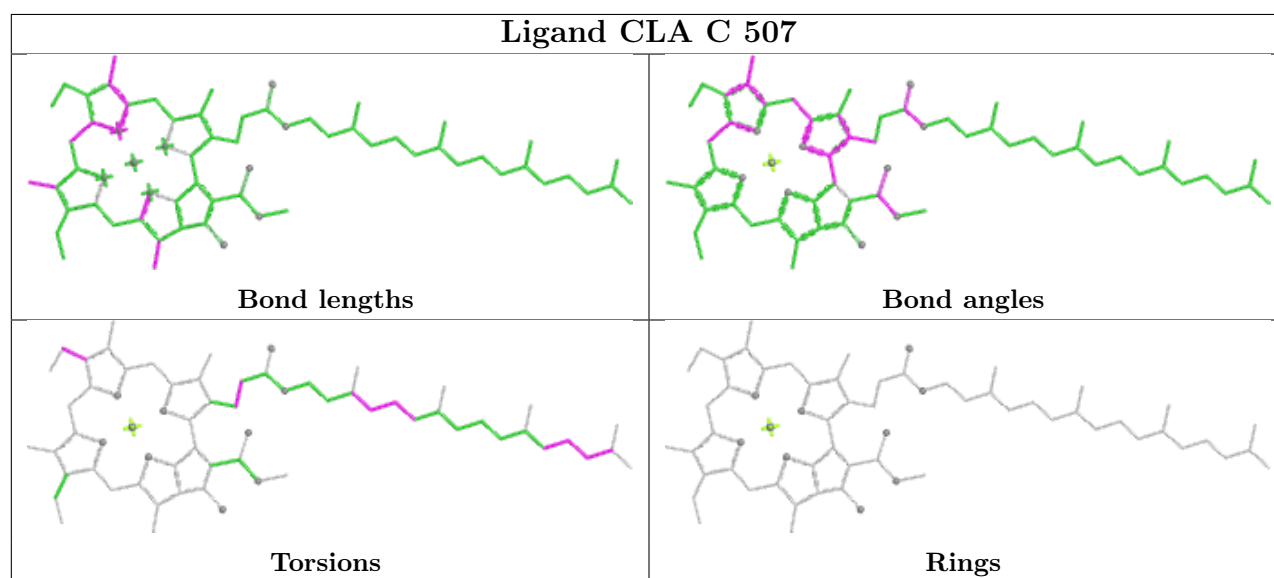
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	N	604	CLA	3	0
32	Y	610	CLA	1	0
46	y	1623	NEX	2	0
33	A	408	PHO	4	0
32	Y	611	CLA	4	0
32	b	614	CLA	5	0
32	r	610	CLA	1	0
43	N	601	CHL	5	0
32	b	617	CLA	1	0
32	c	504	CLA	3	0
32	B	608	CLA	3	0
32	c	512	CLA	1	0
37	C	520	DGD	5	0
43	n	609	CHL	6	0
38	g	2630	LHG	5	0
32	b	610	CLA	4	0
32	Y	614	CLA	3	0
32	b	612	CLA	4	0
32	B	610	CLA	4	0
32	c	510	CLA	2	0
43	s	608	CHL	2	0
45	N	1622	XAT	4	0
32	s	604	CLA	1	0
32	C	510	CLA	3	0
32	C	506	CLA	1	0
42	y	2632	LMU	1	0
32	a	406	CLA	2	0
35	B	621	SQD	3	0
38	Y	2630	LHG	3	0
32	n	610	CLA	1	0
32	C	512	CLA	1	0
37	c	524	DGD	2	0
32	B	611	CLA	1	0
42	z	2634	LMU	1	0
32	g	603	CLA	3	0
45	Y	1622	XAT	5	0
32	Y	612	CLA	3	0
37	C	523	DGD	3	0
34	H	101	BCR	3	0
32	n	603	CLA	3	0
44	Y	1621	LUT	4	0
37	c	523	DGD	4	0

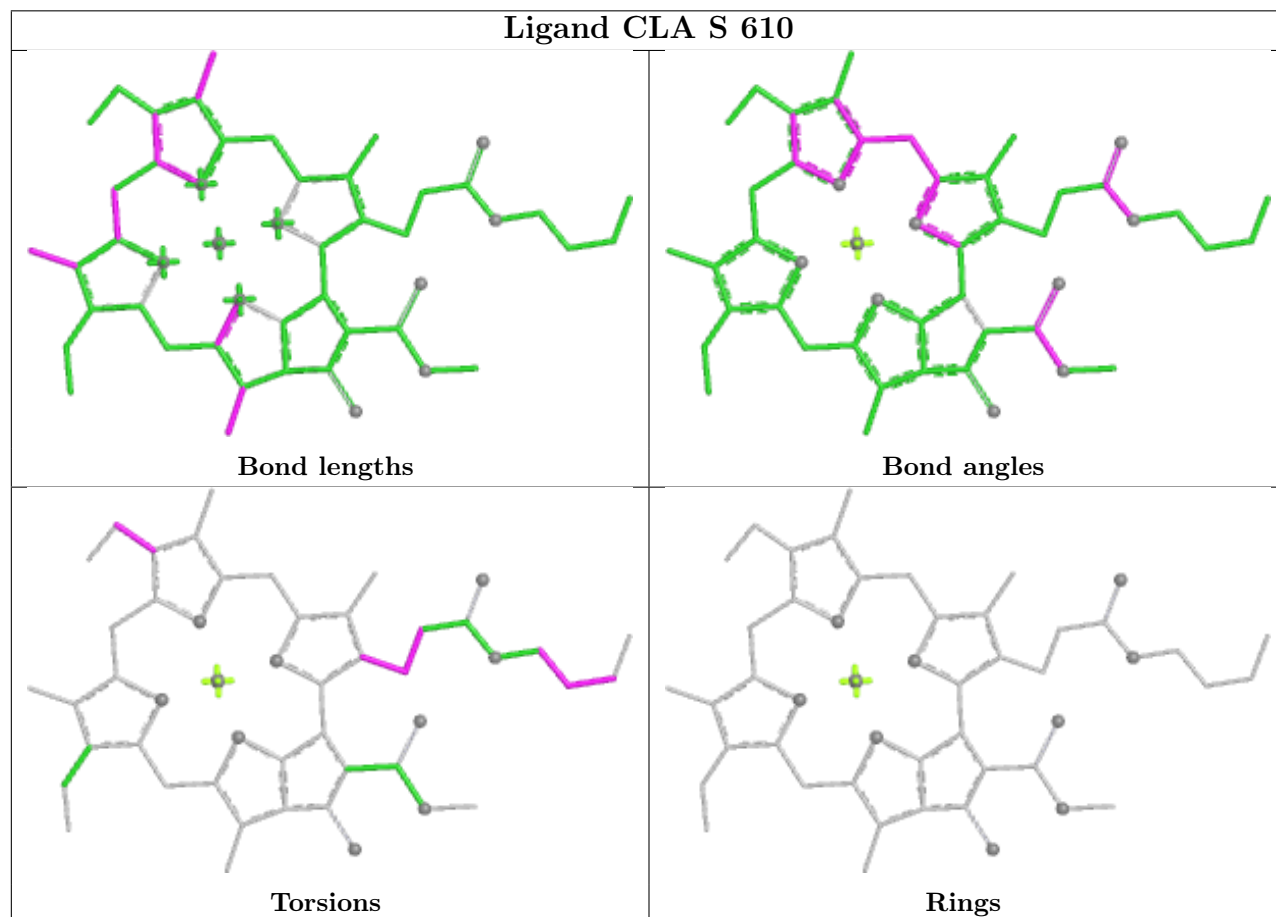
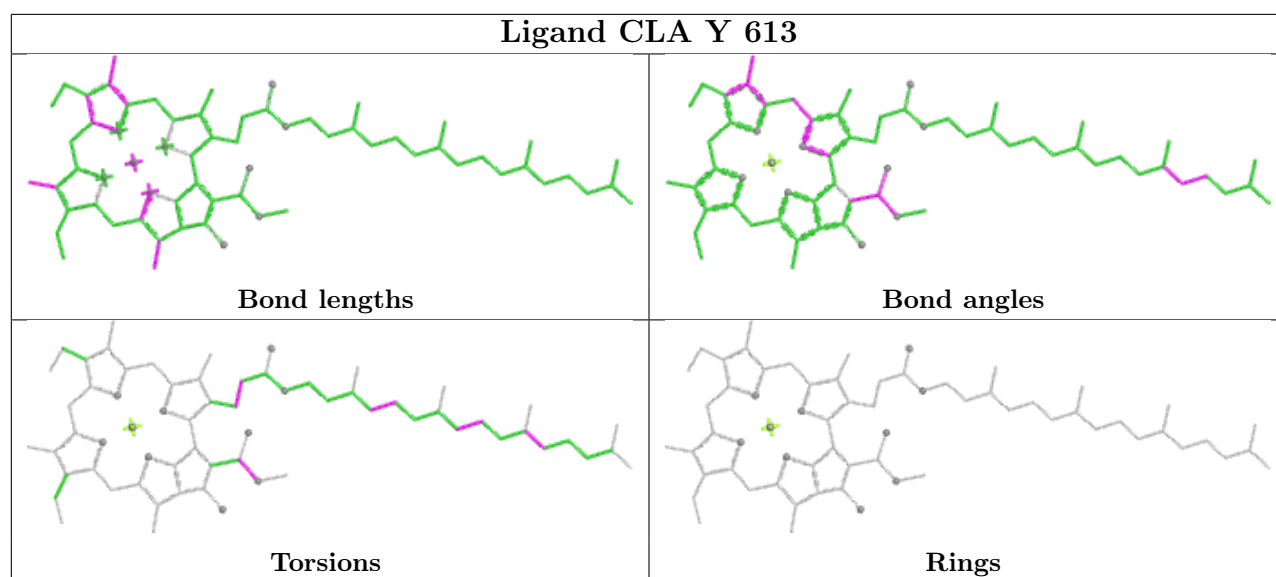
Continued on next page...

Continued from previous page...

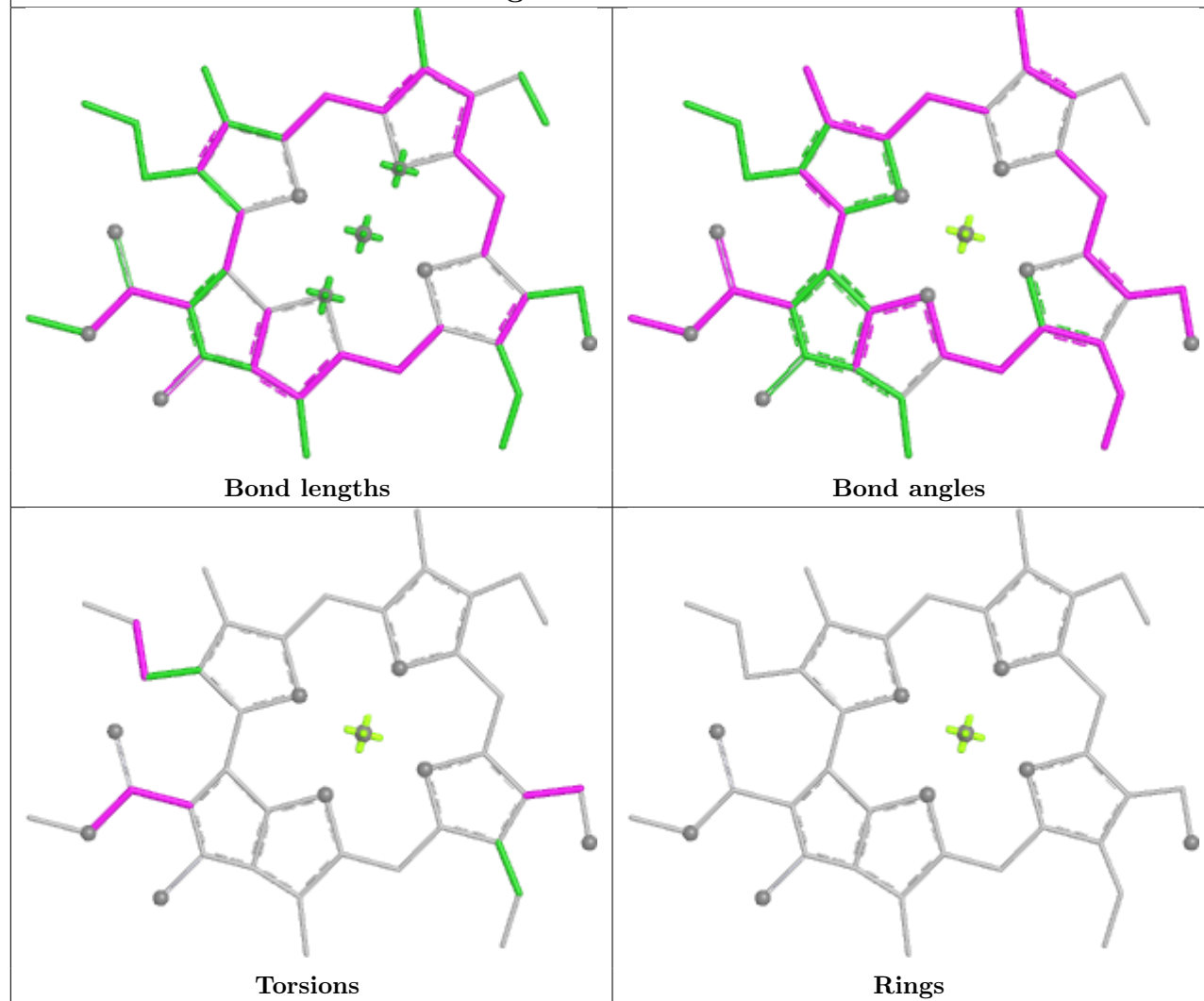
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	R	624	XAT	3	0
32	B	605	CLA	4	0
32	A	405	CLA	1	0
43	r	607	CHL	2	0

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.

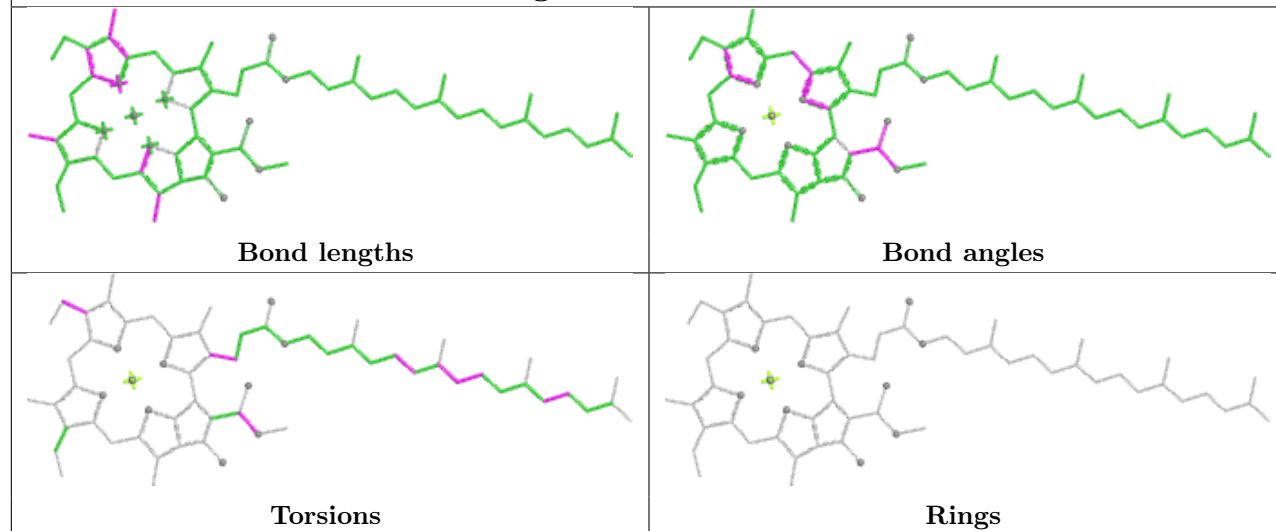


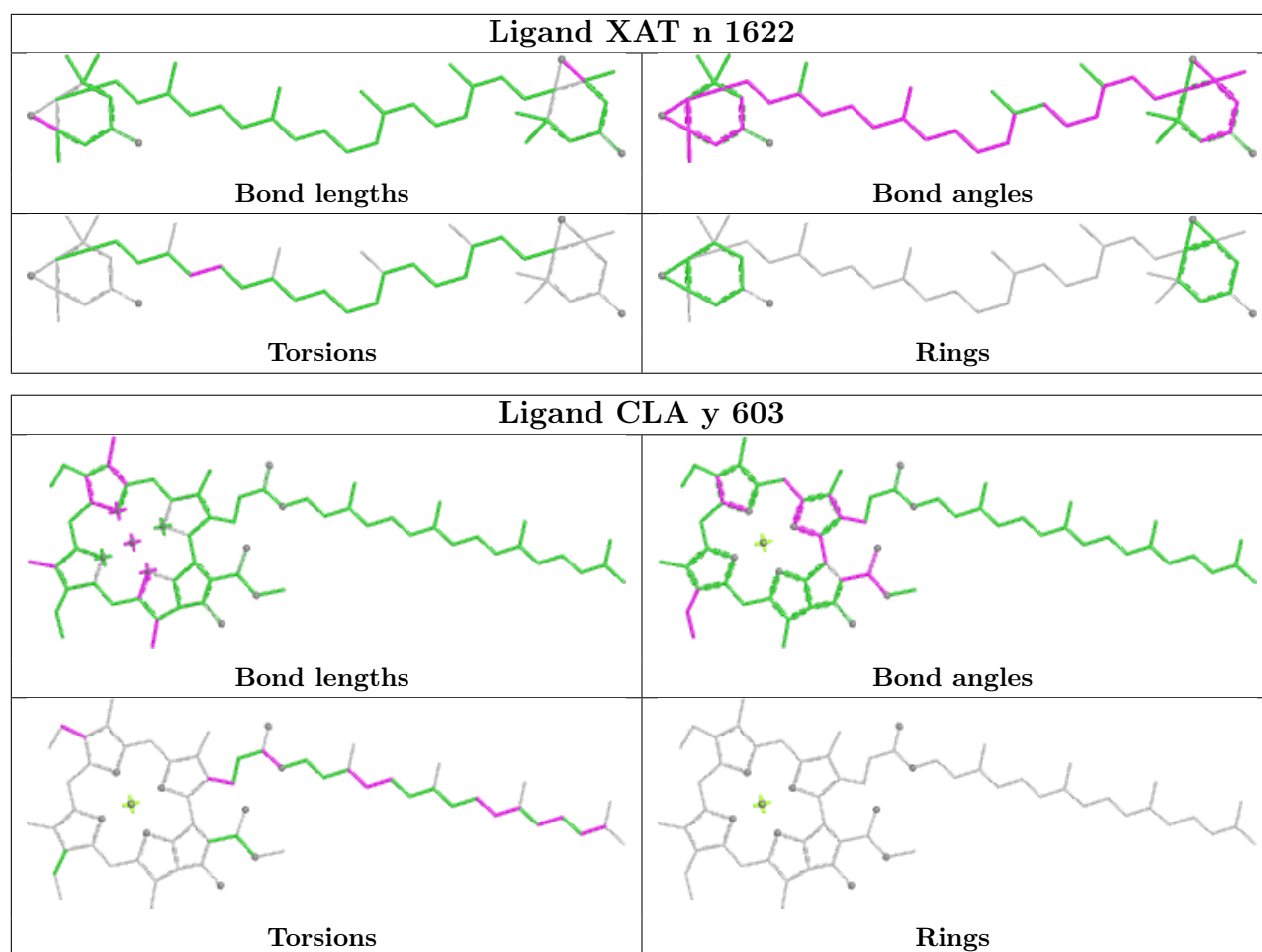


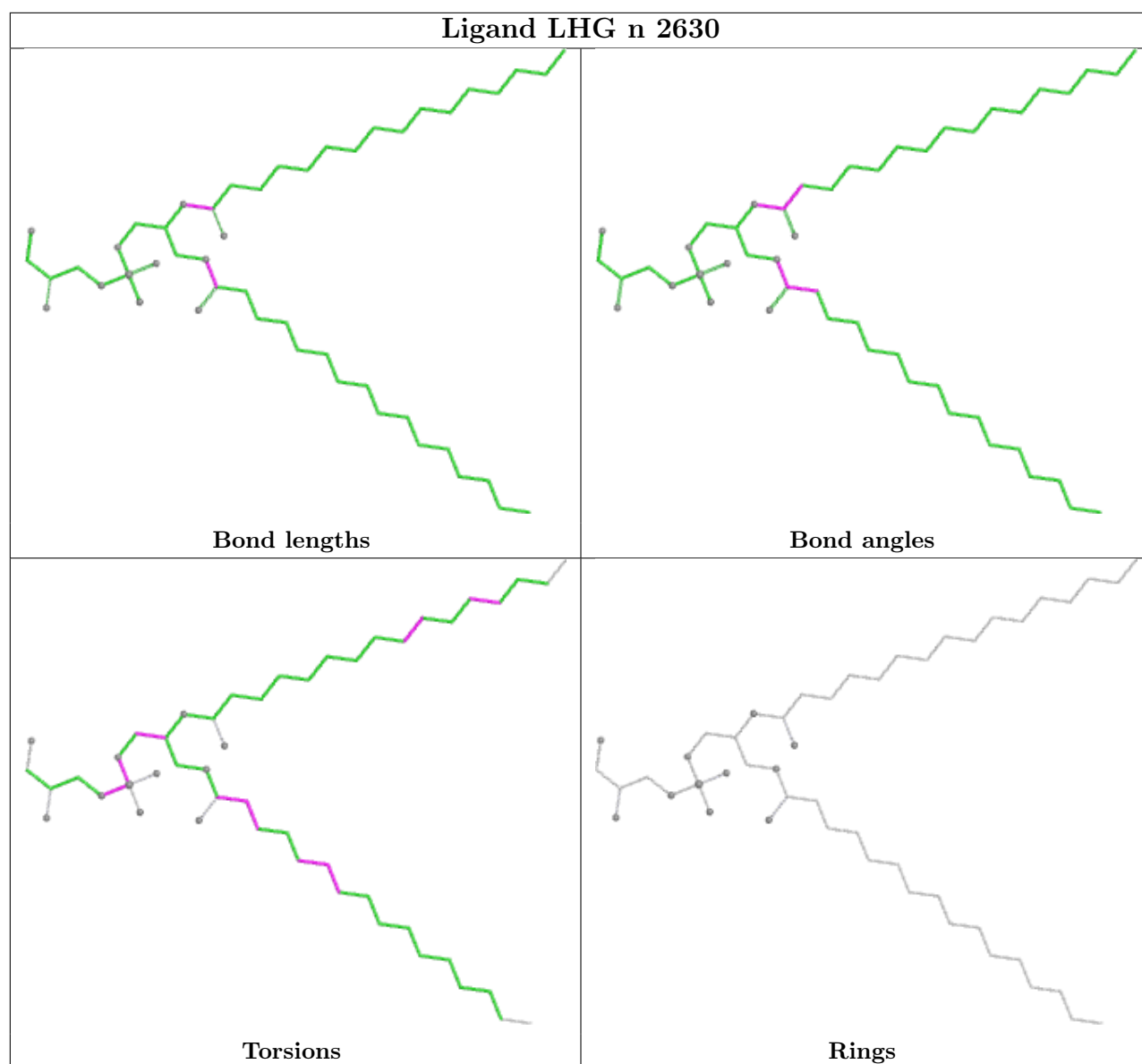
Ligand CHL r 606



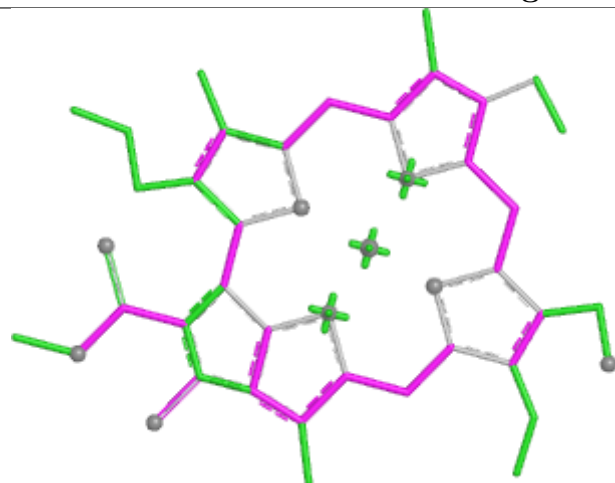
Ligand CLA B 606



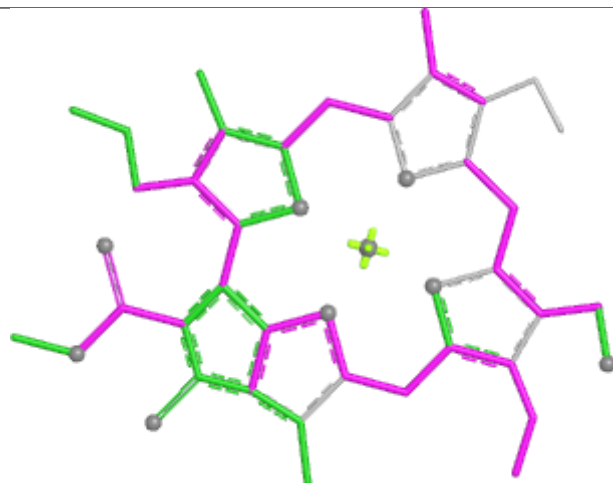




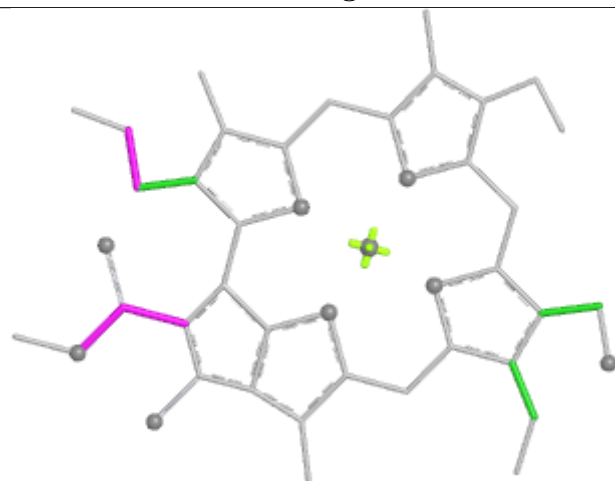
Ligand CHL s 606



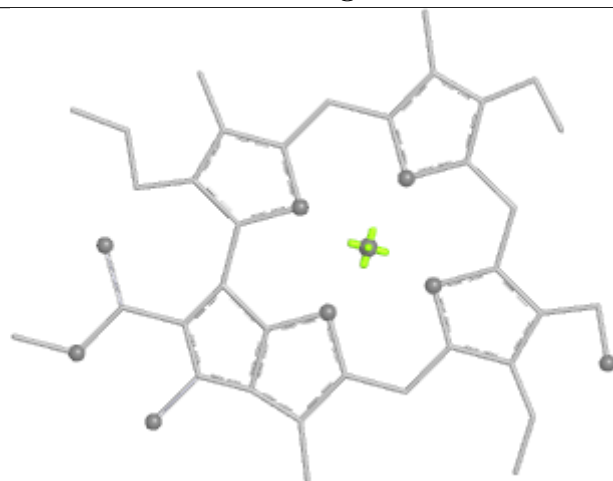
Bond lengths



Bond angles

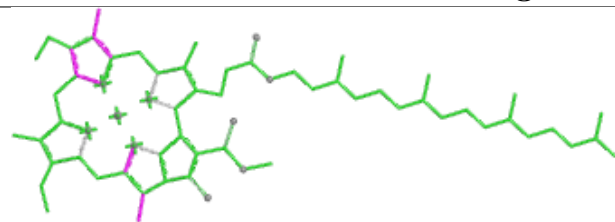


Torsions

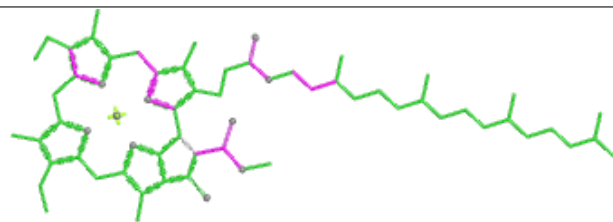


Rings

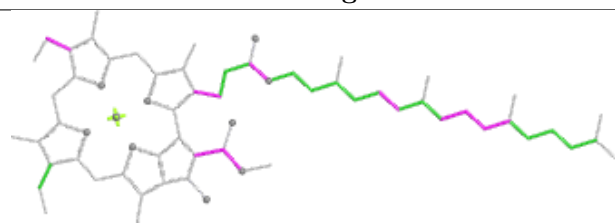
Ligand CLA D 403



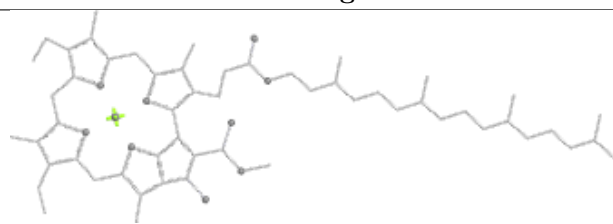
Bond lengths



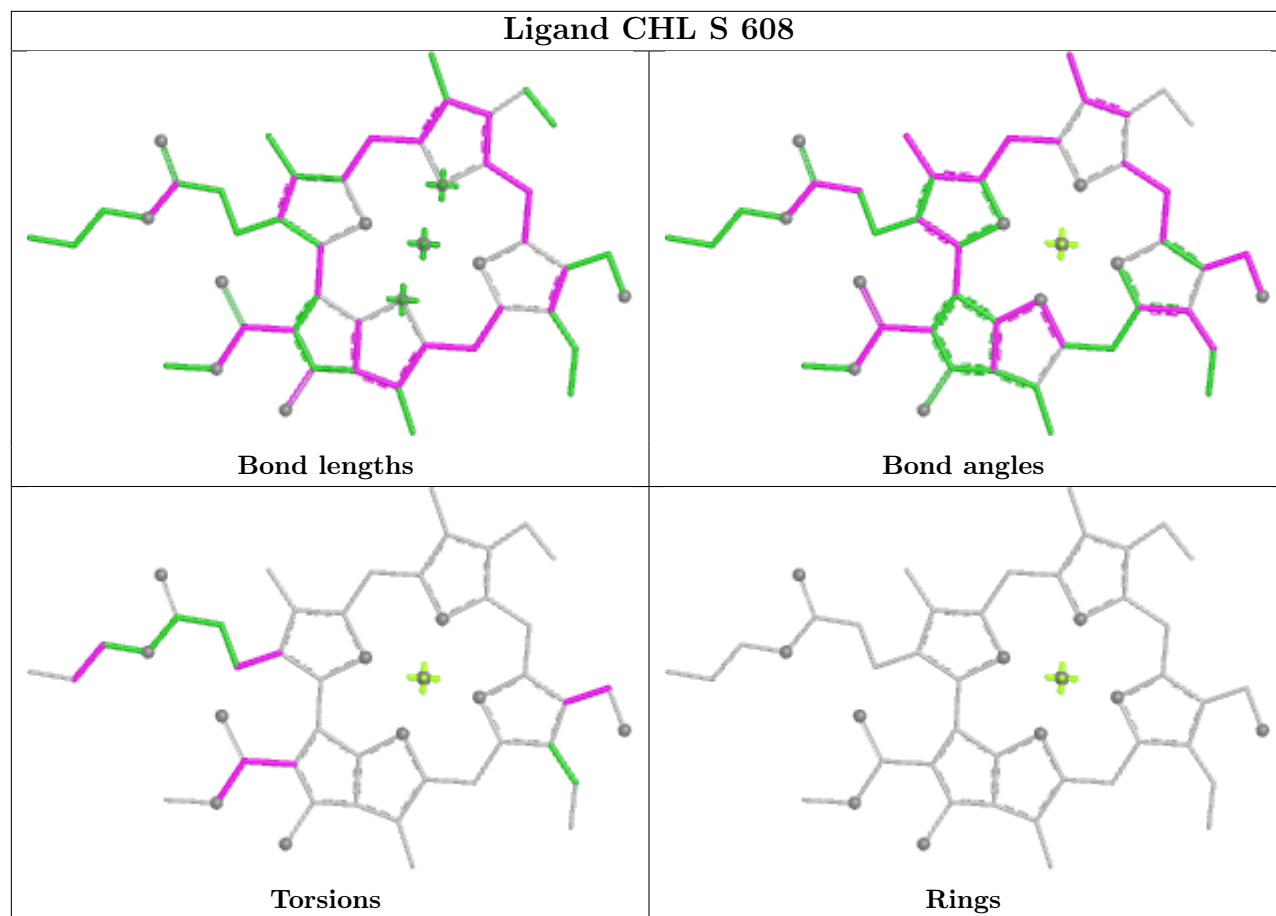
Bond angles



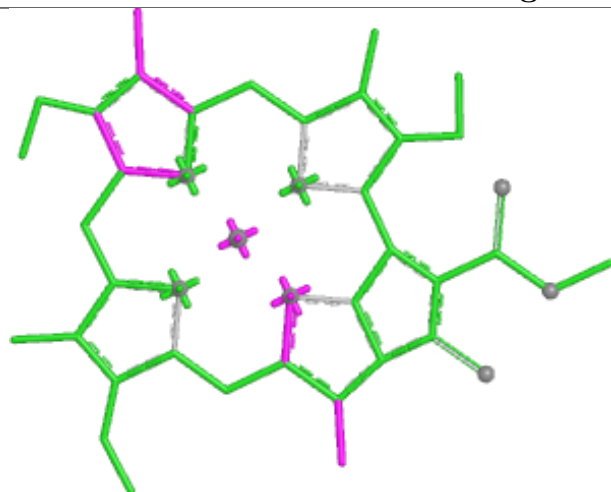
Torsions



Rings



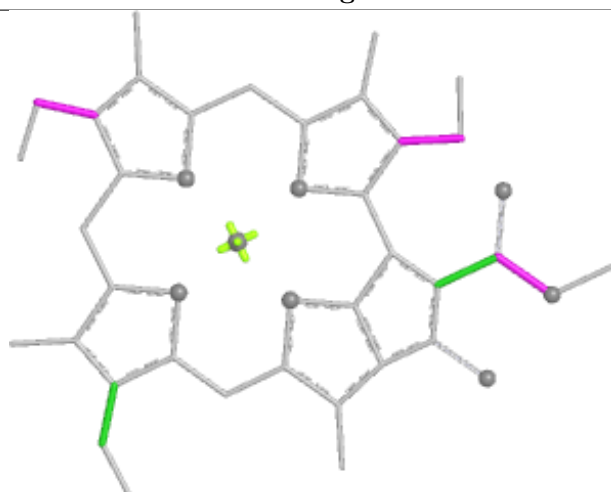
Ligand CLA s 603



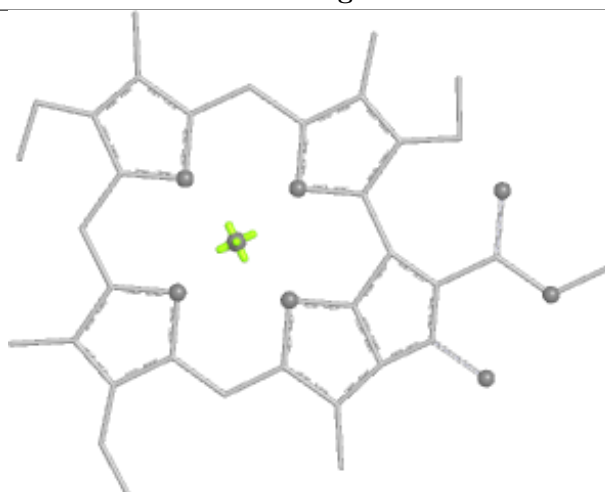
Bond lengths



Bond angles

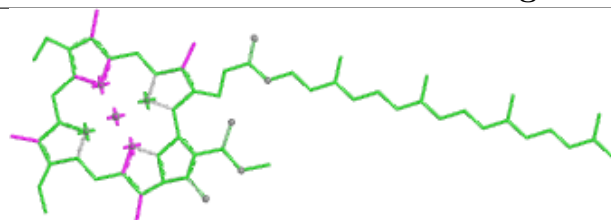


Torsions

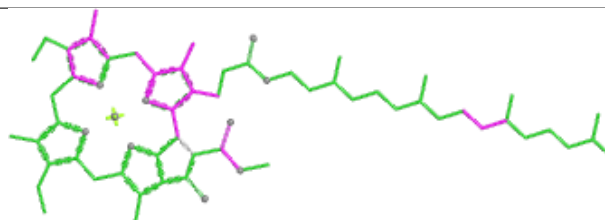


Rings

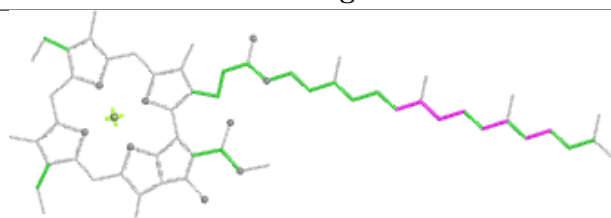
Ligand CLA c 509



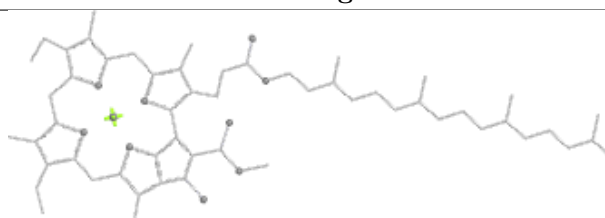
Bond lengths



Bond angles

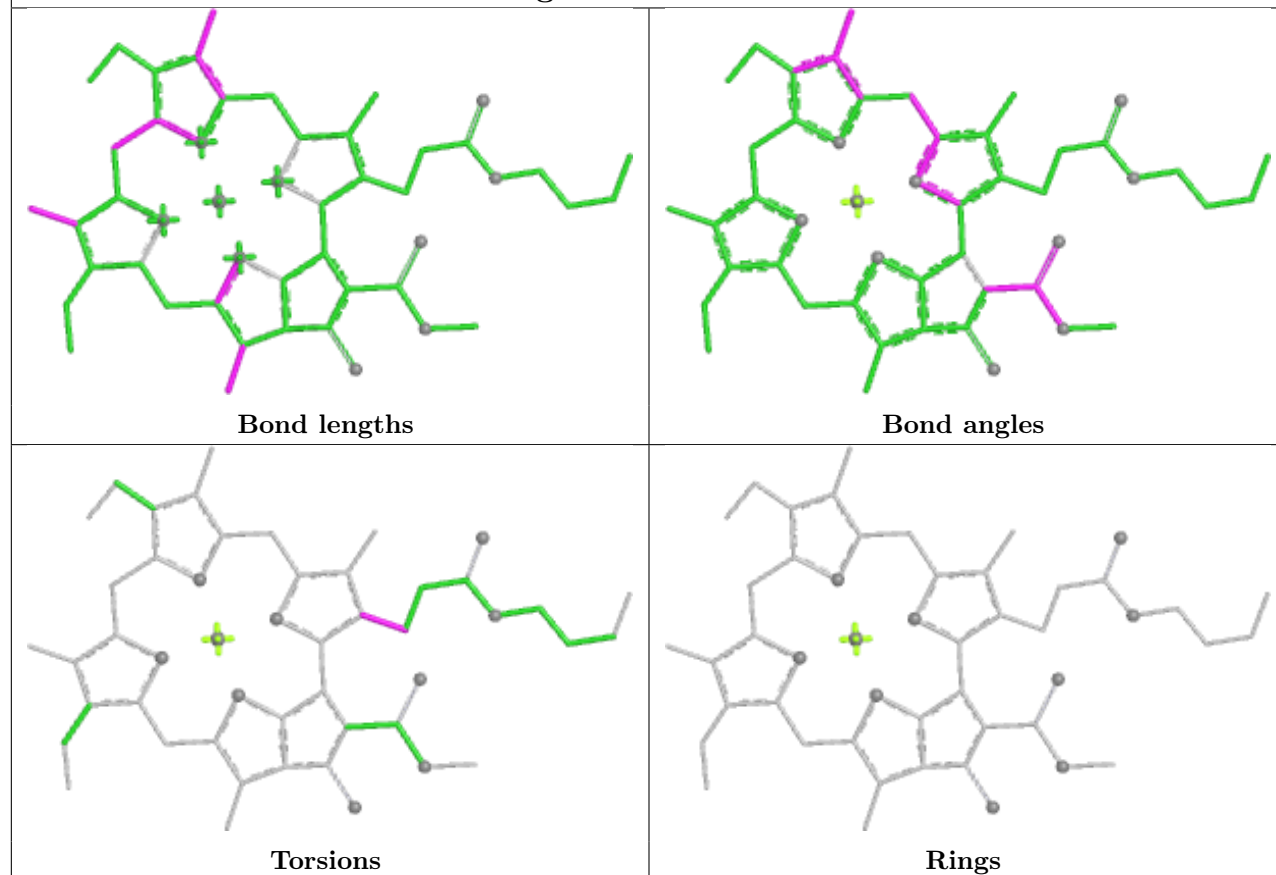


Torsions

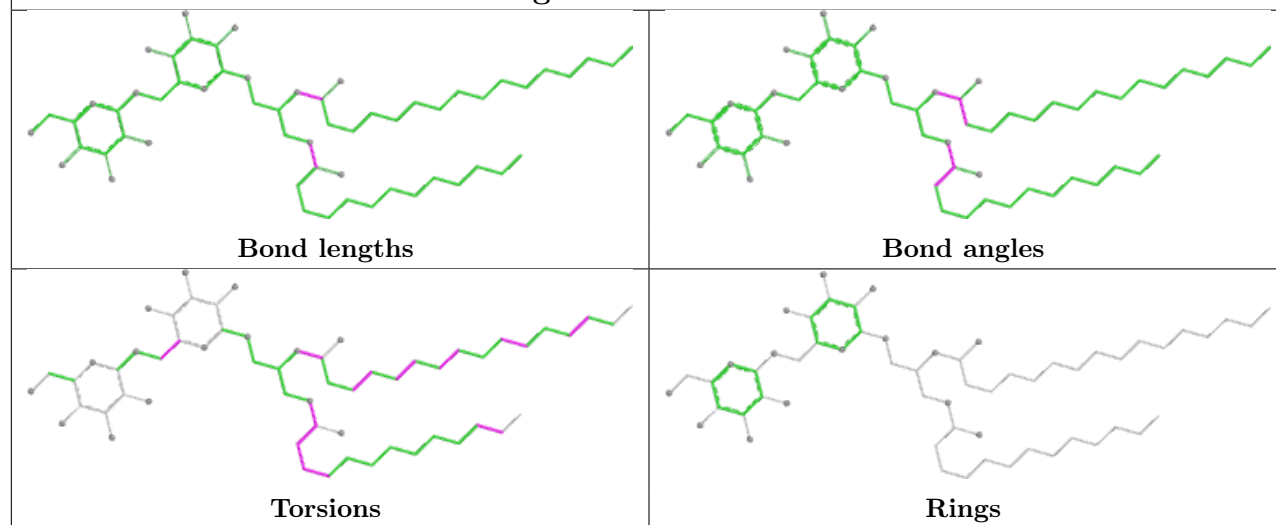


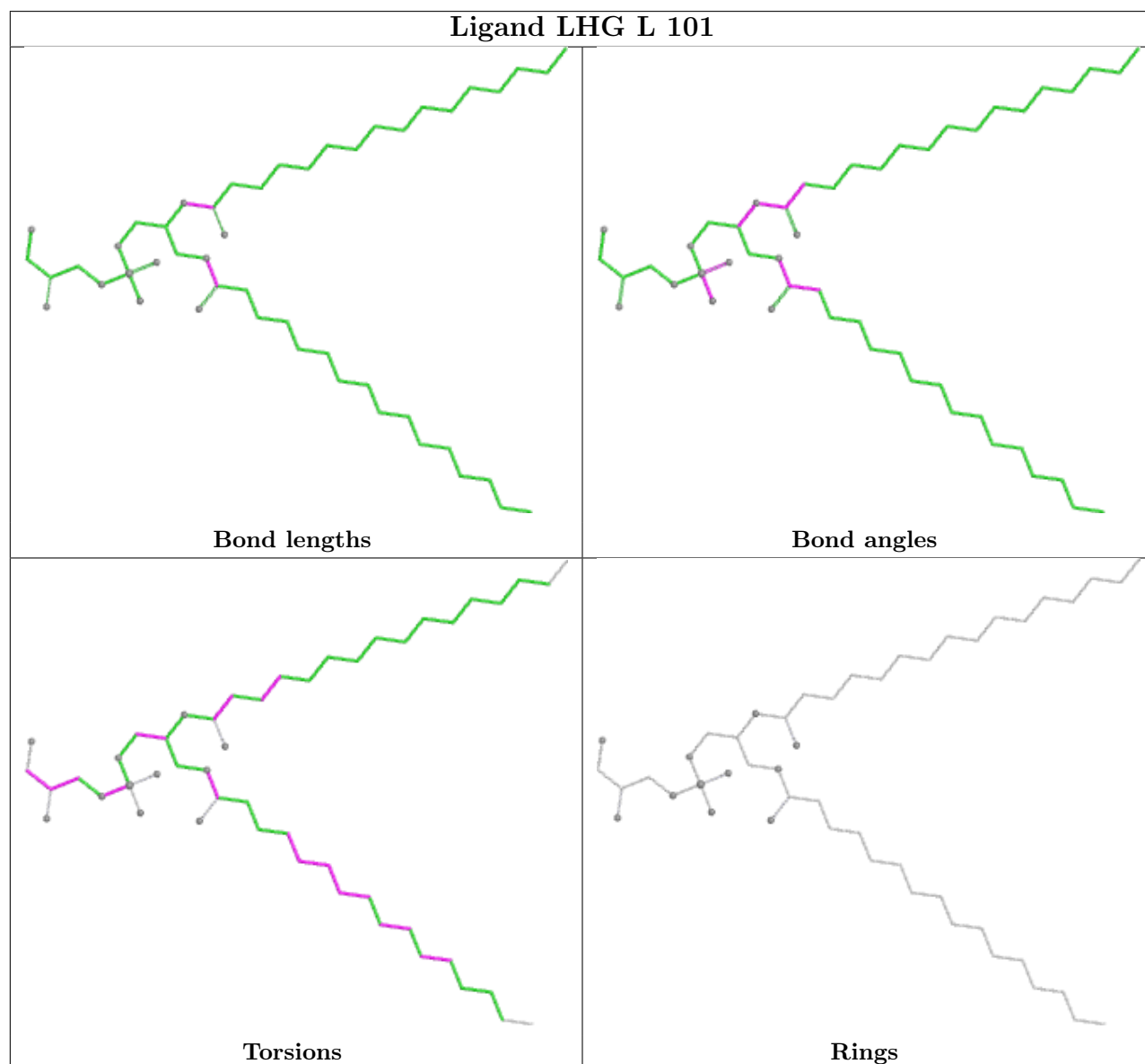
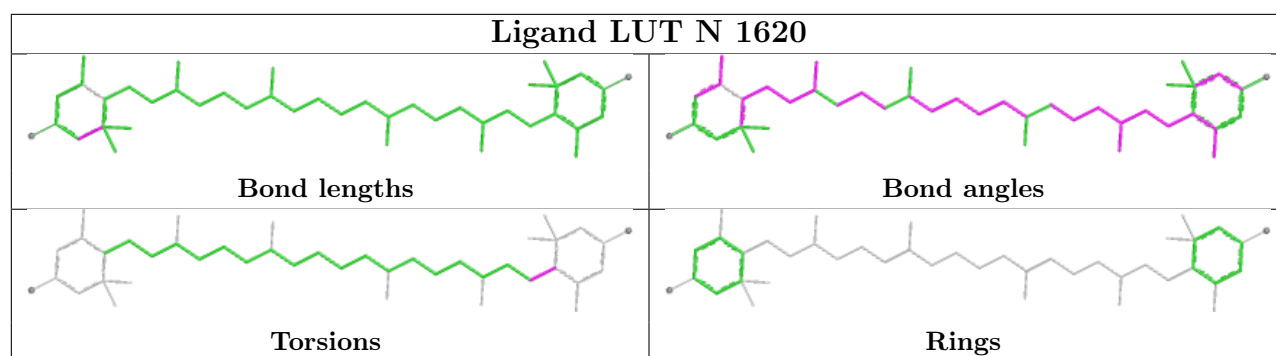
Rings

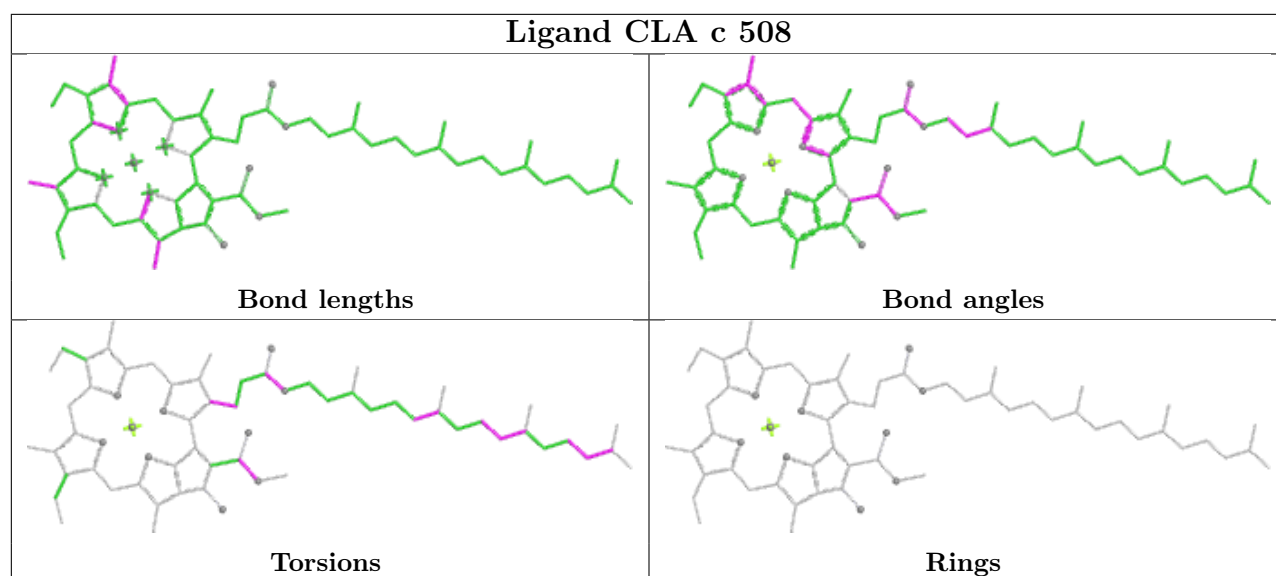
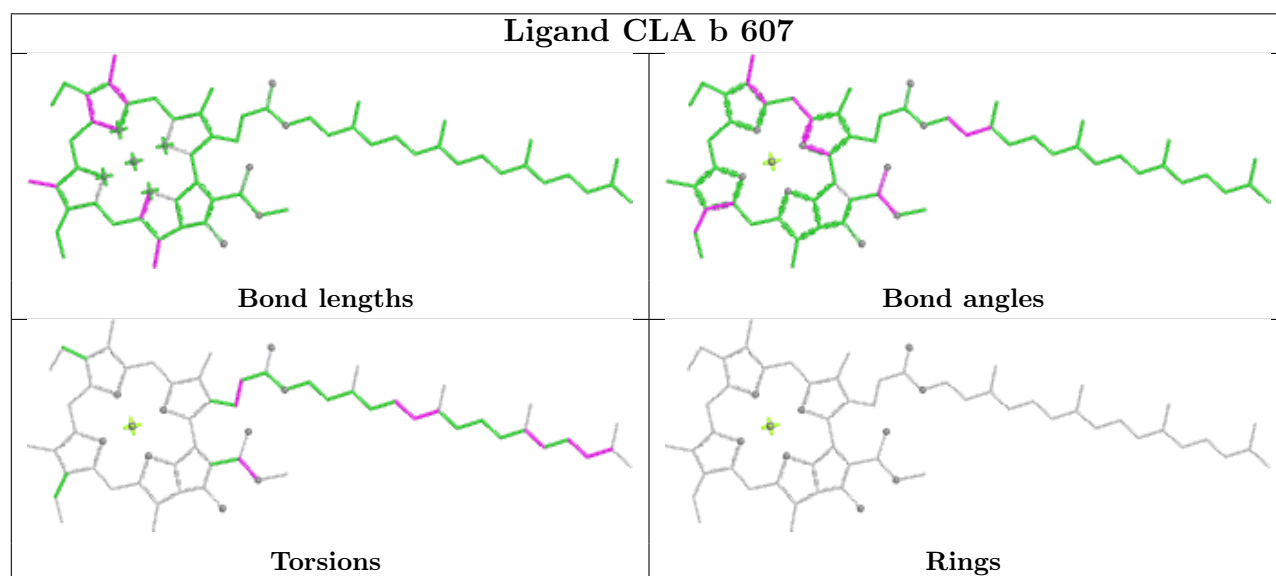
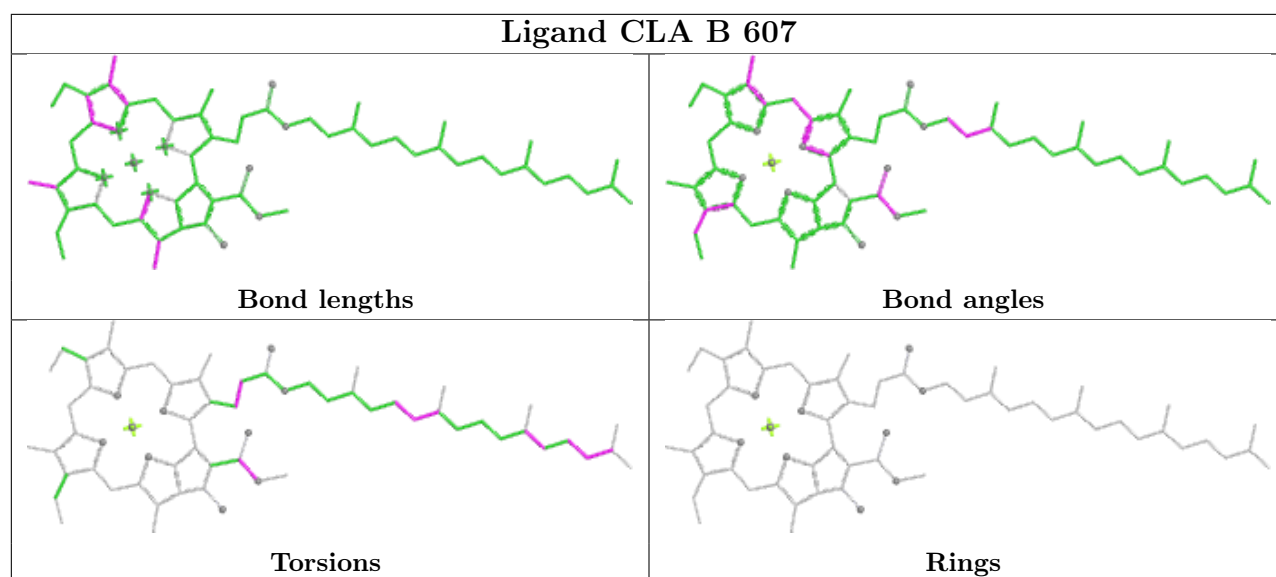
Ligand CLA a 407

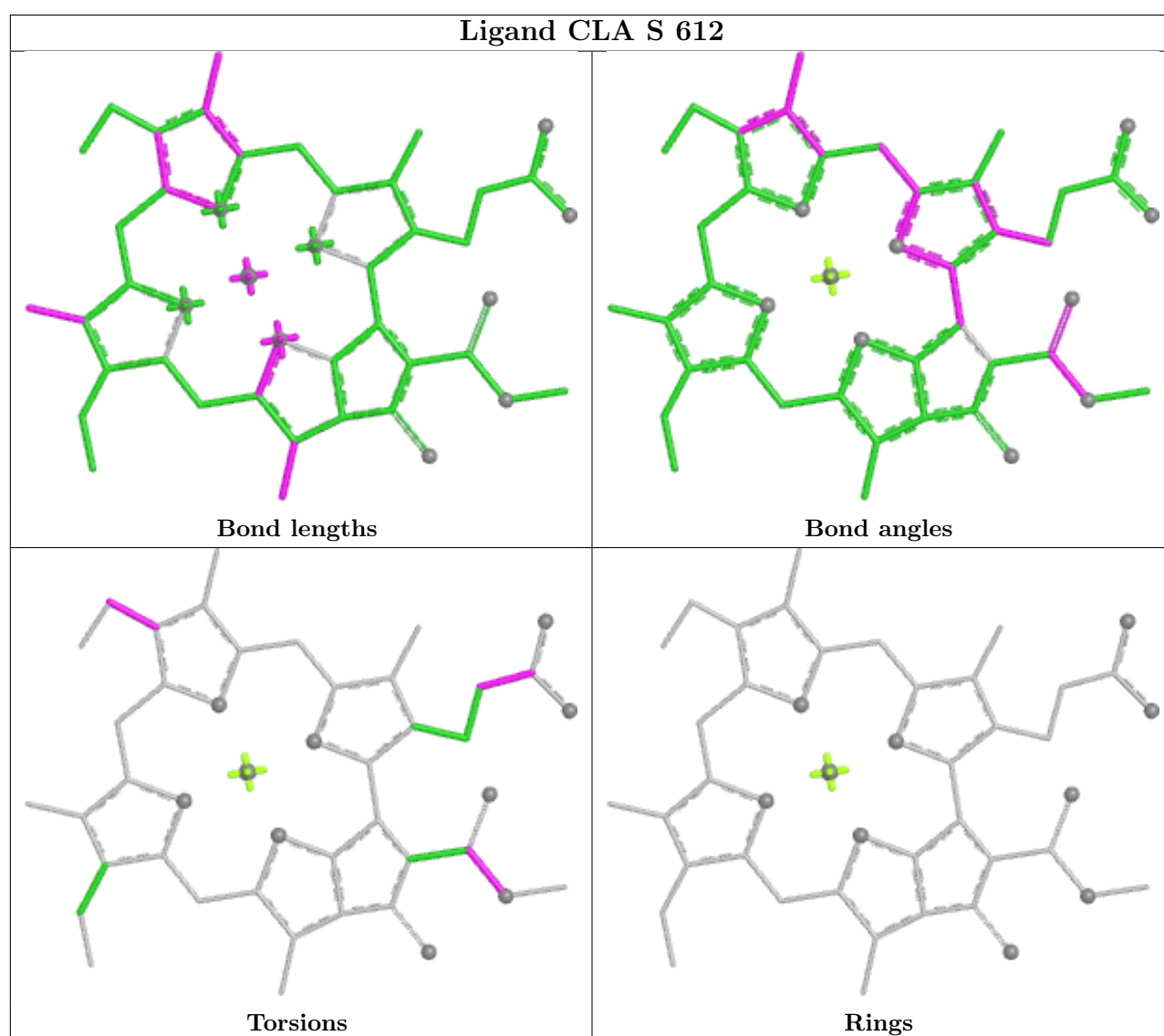
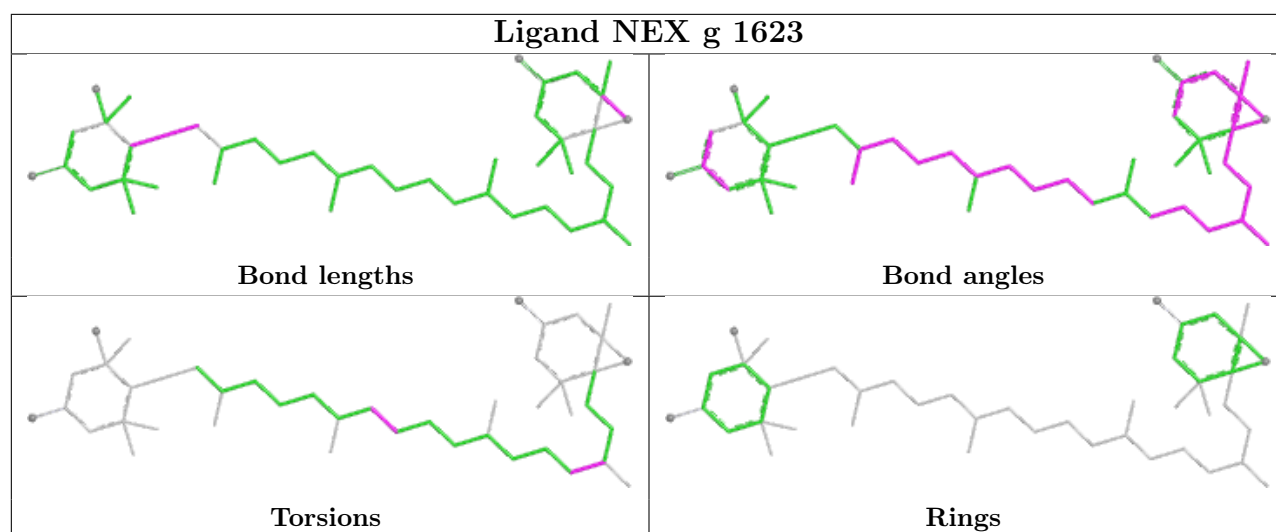


Ligand DGD c 520

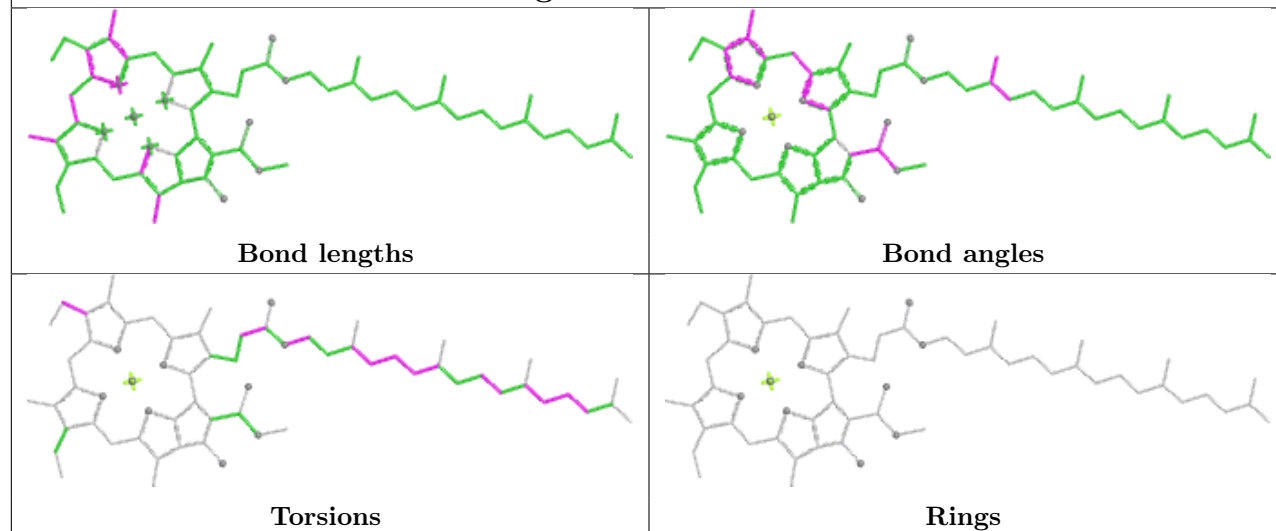




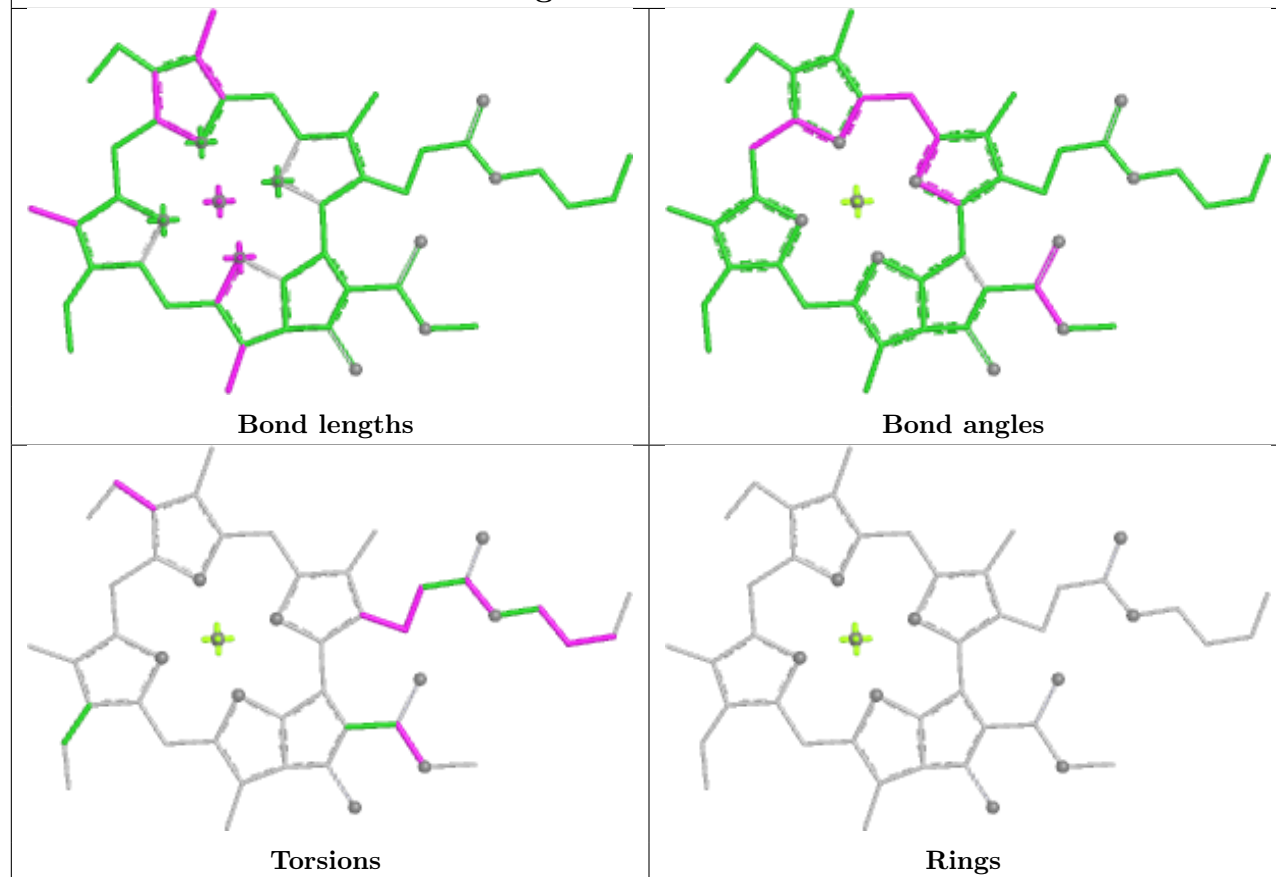


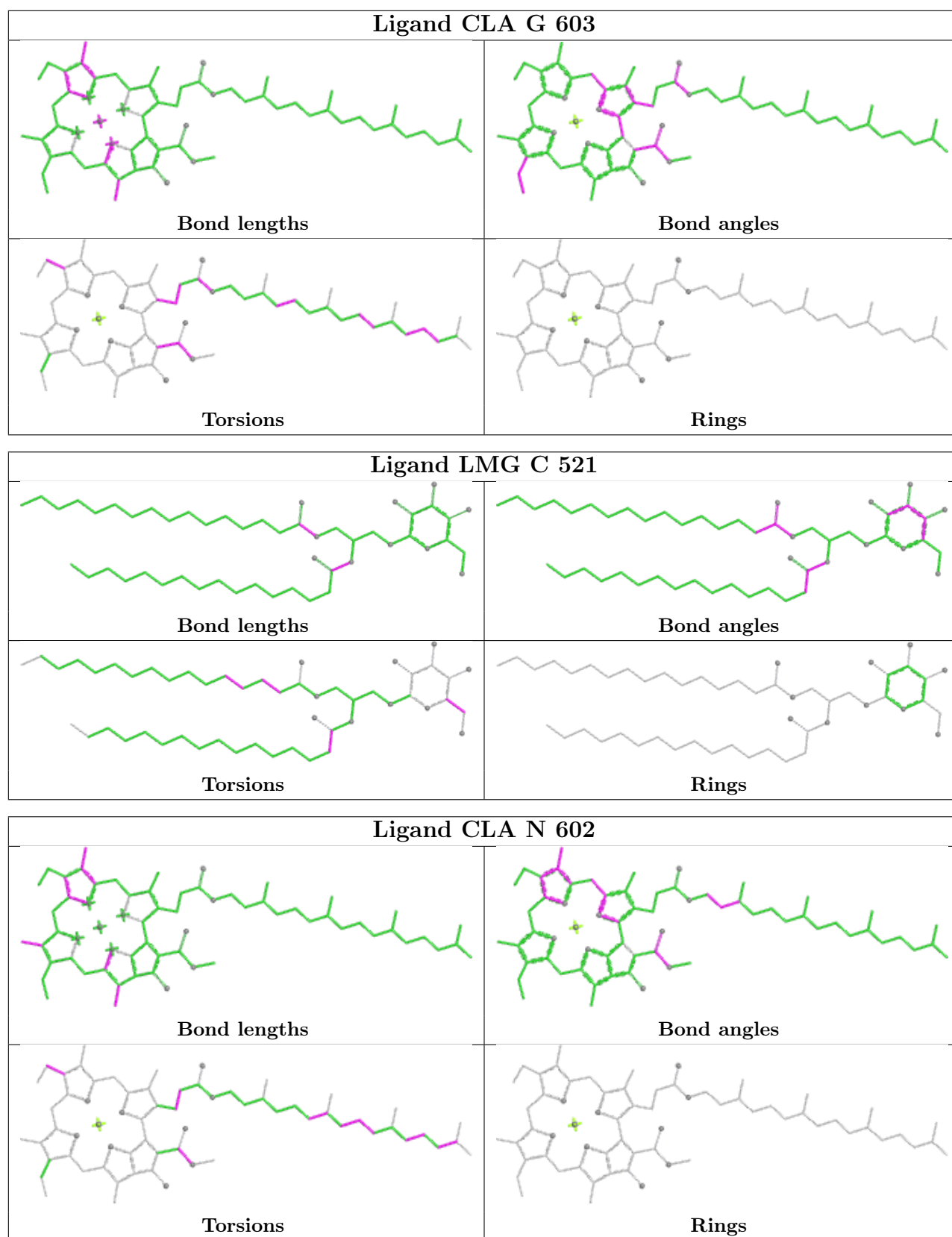


Ligand CLA b 603

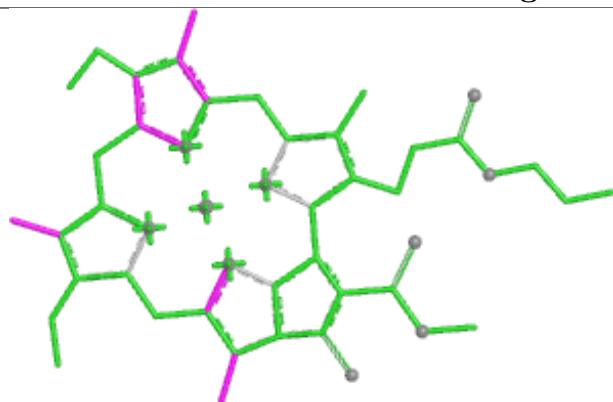


Ligand CLA S 613

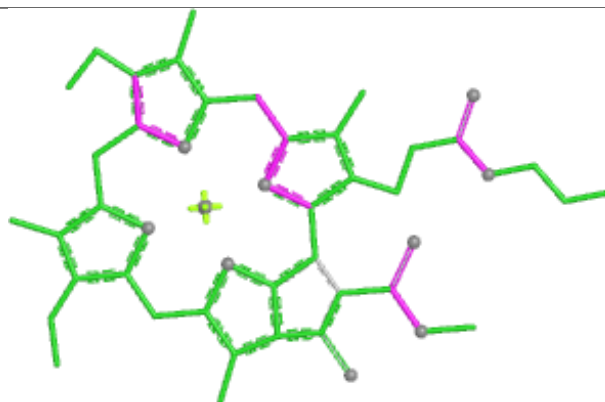




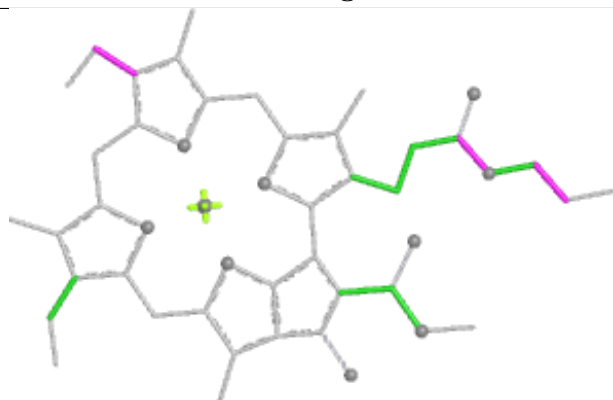
Ligand CLA s 614



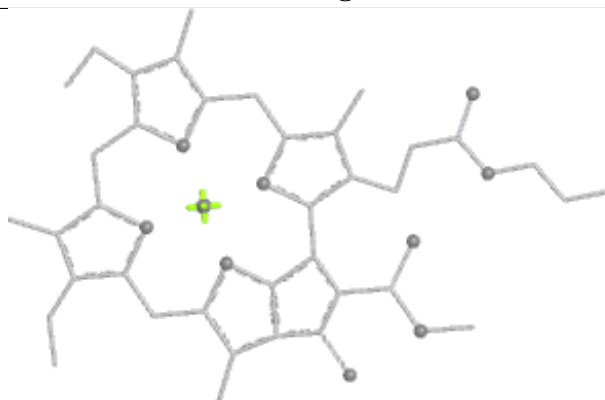
Bond lengths



Bond angles

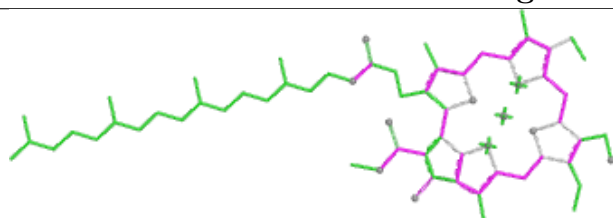


Torsions

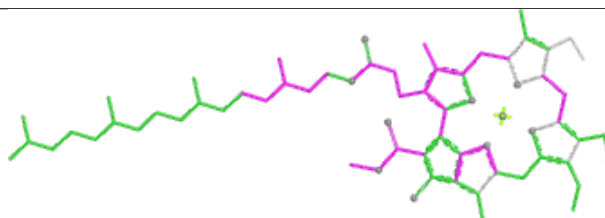


Rings

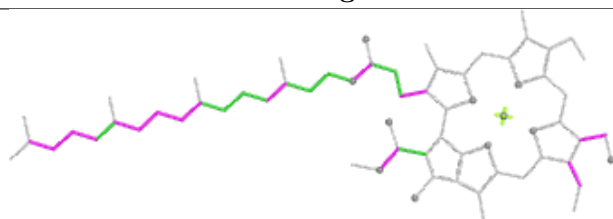
Ligand CHL n 607



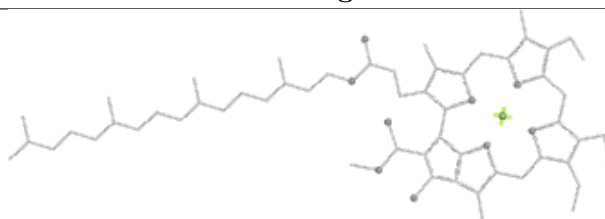
Bond lengths



Bond angles

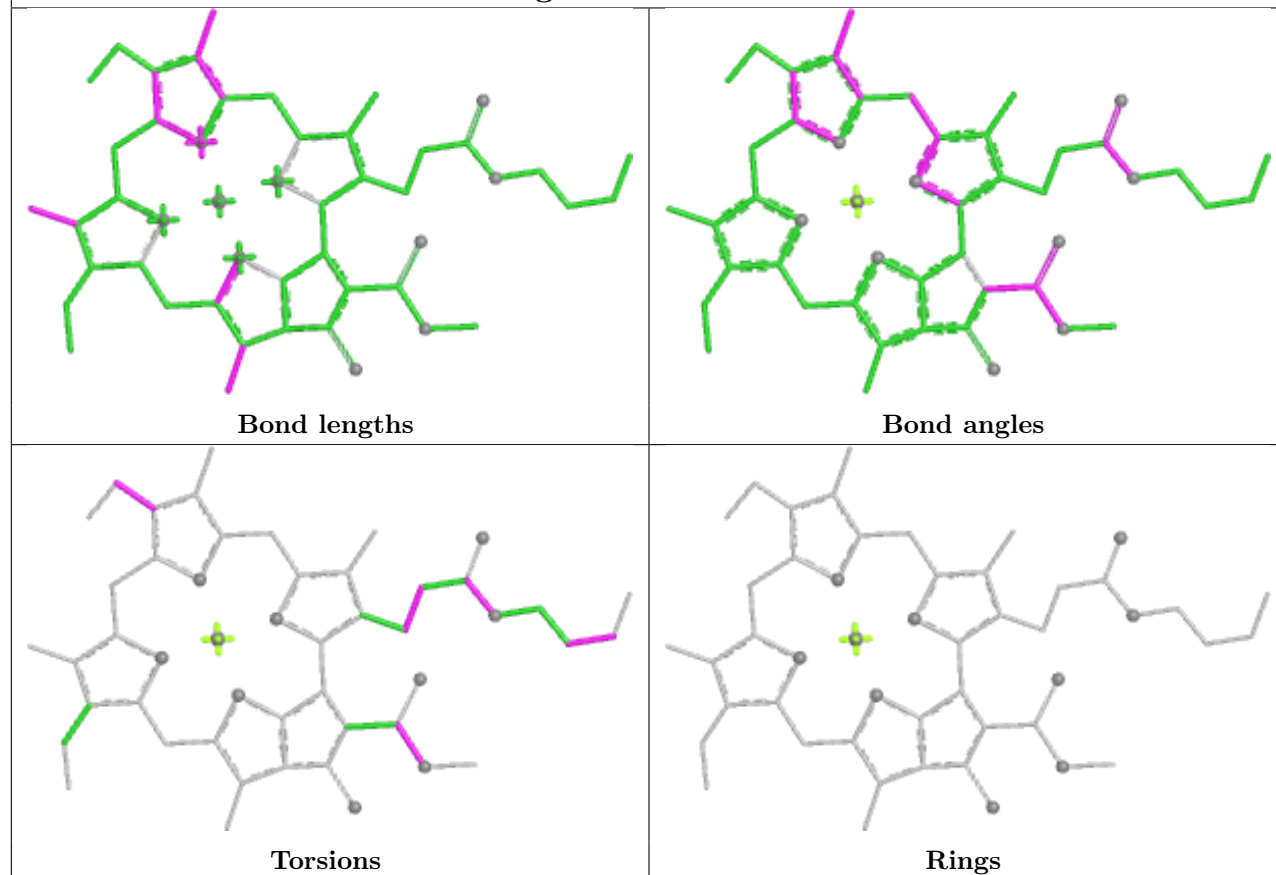


Torsions

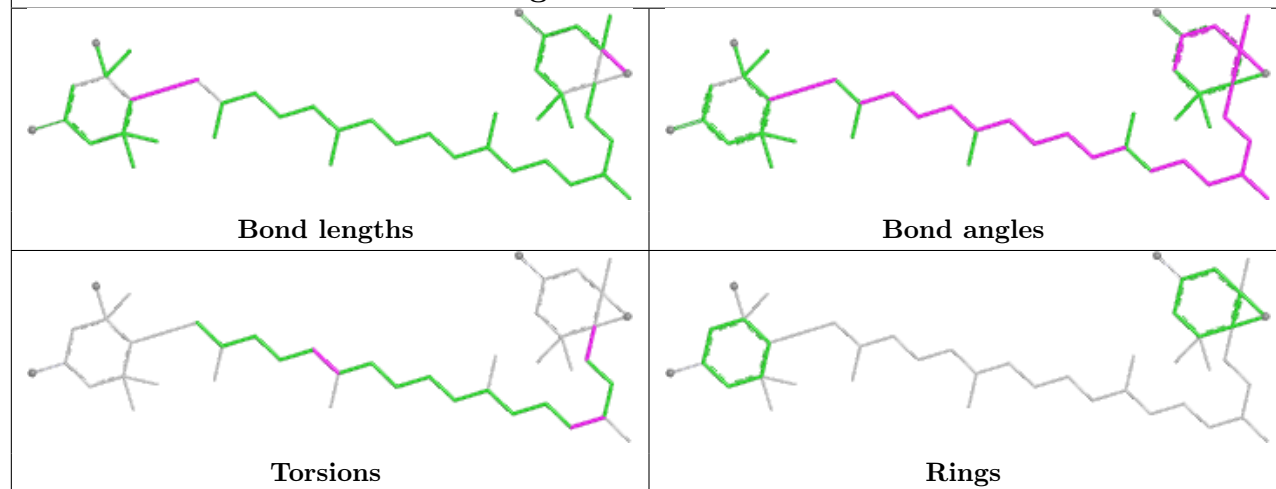


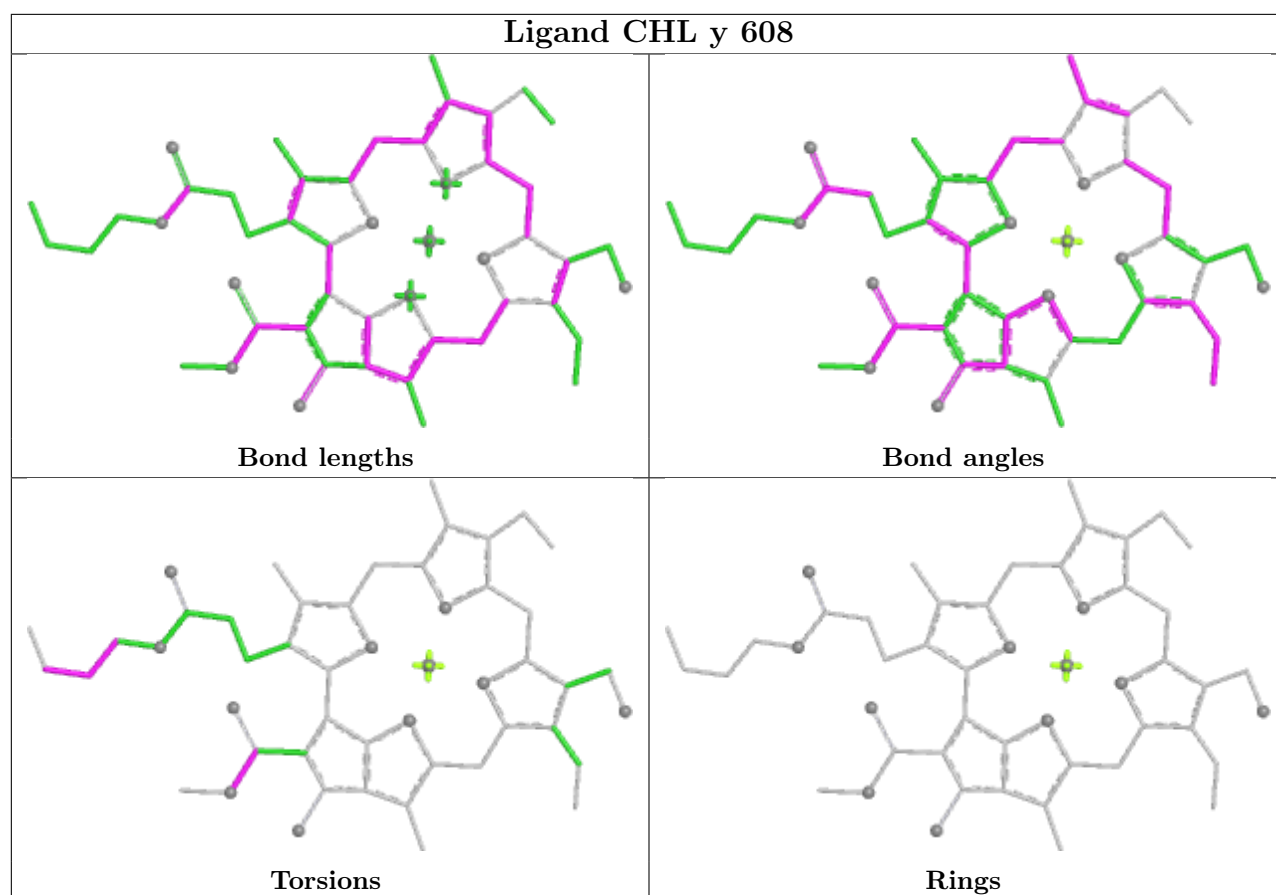
Rings

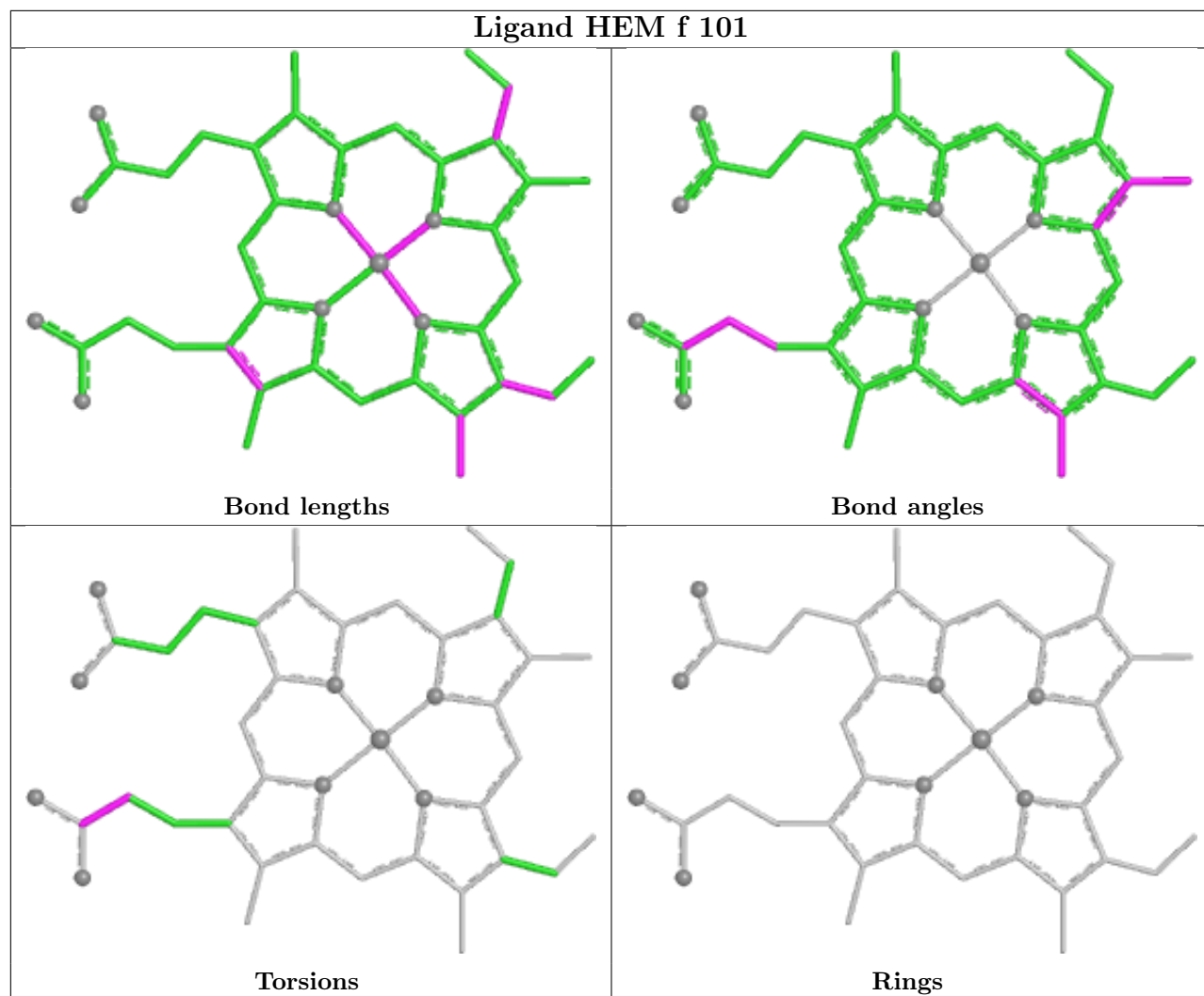
Ligand CLA S 602



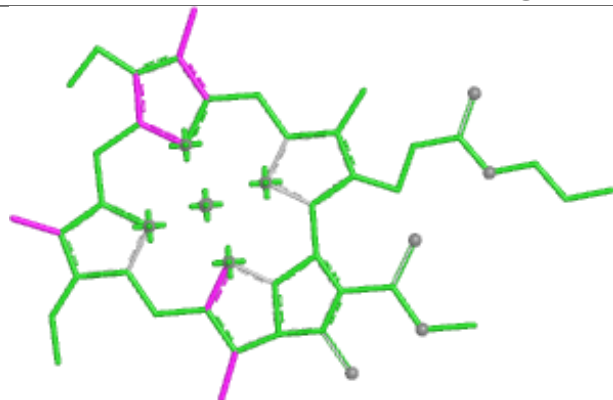
Ligand NEX R 625



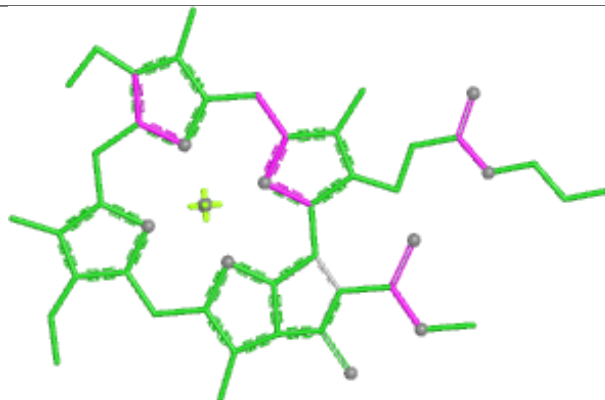




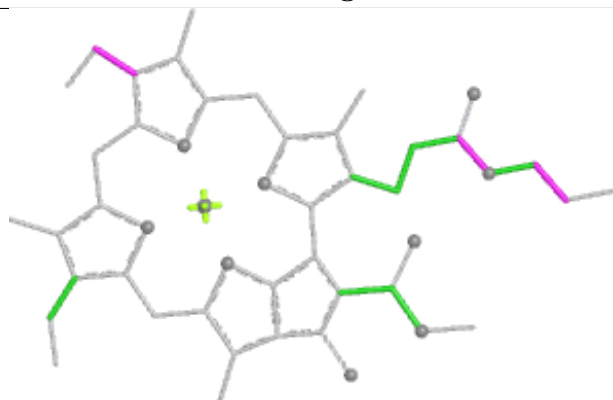
Ligand CLA S 614



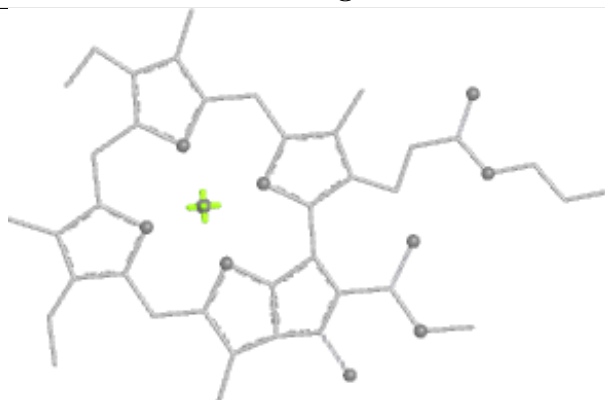
Bond lengths



Bond angles

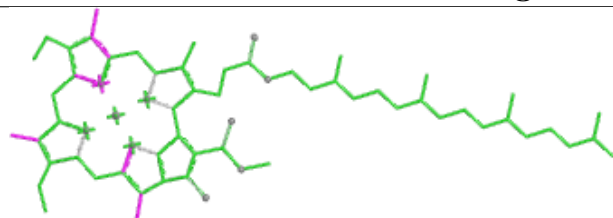


Torsions

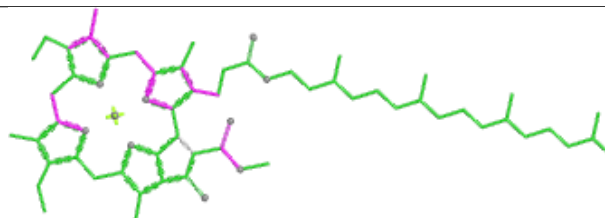


Rings

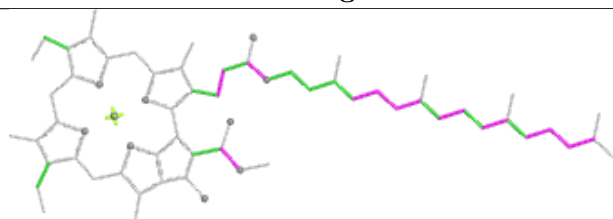
Ligand CLA B 617



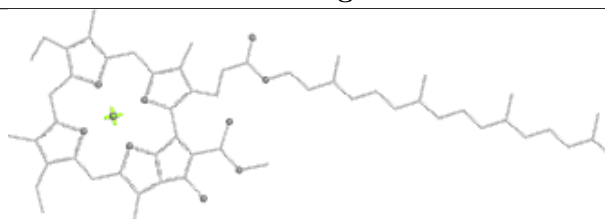
Bond lengths



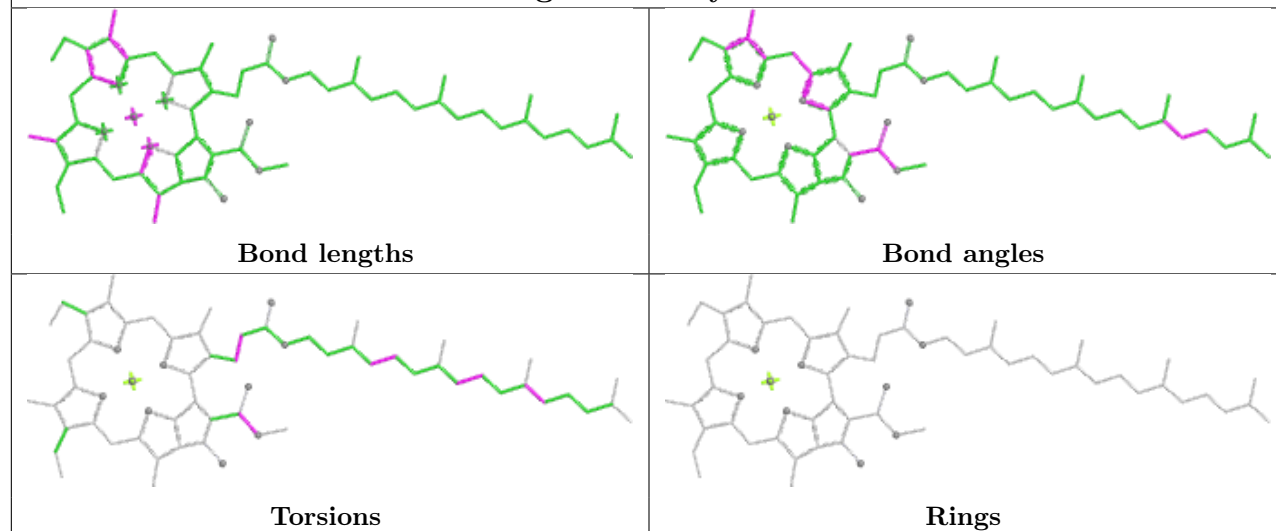
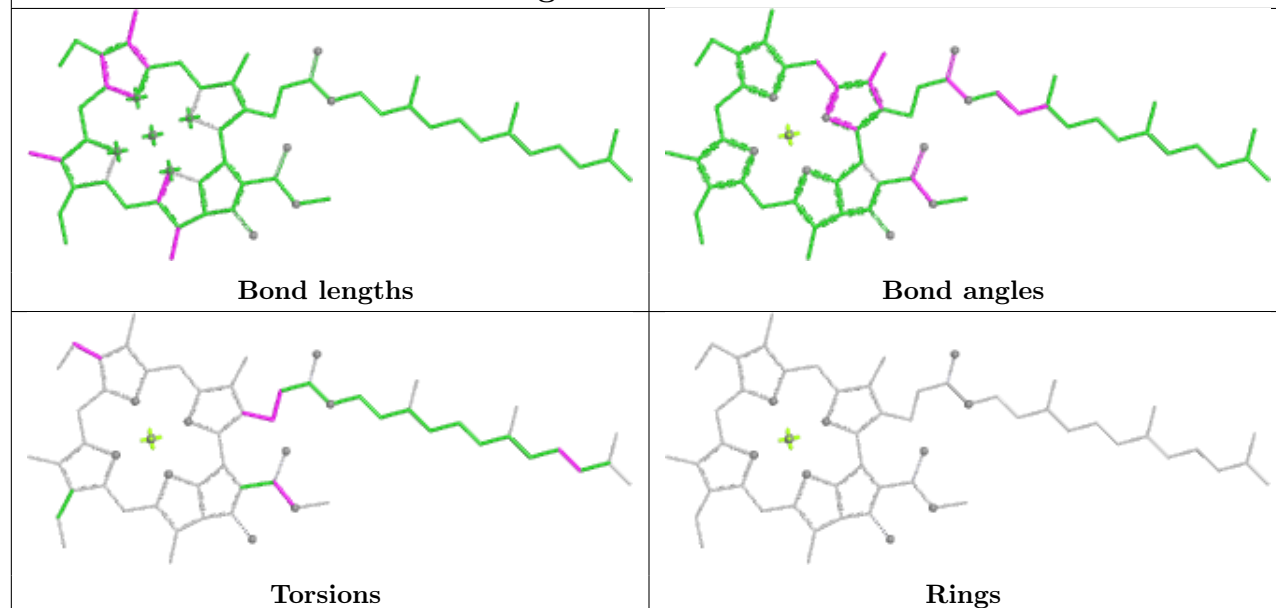
Bond angles

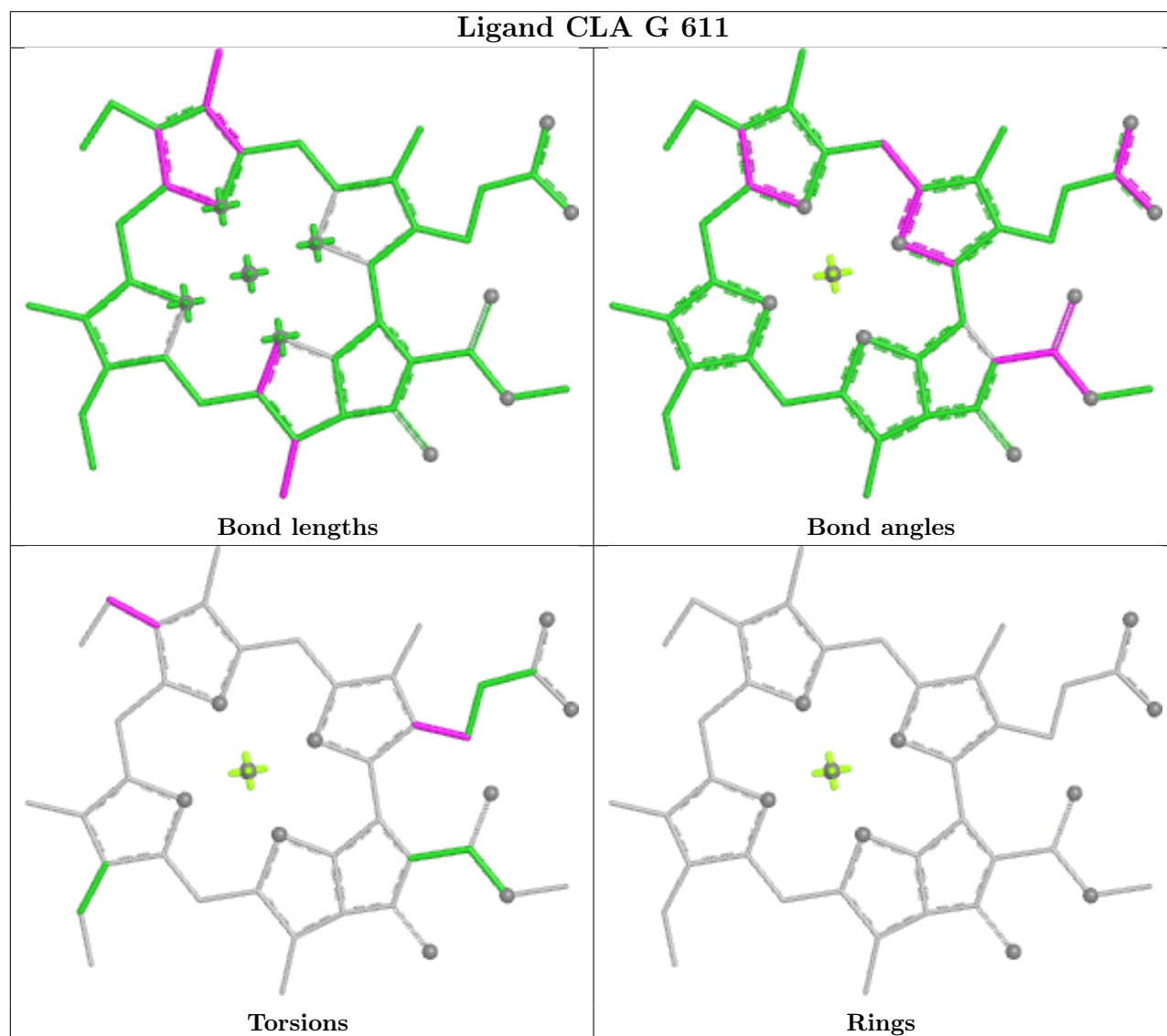
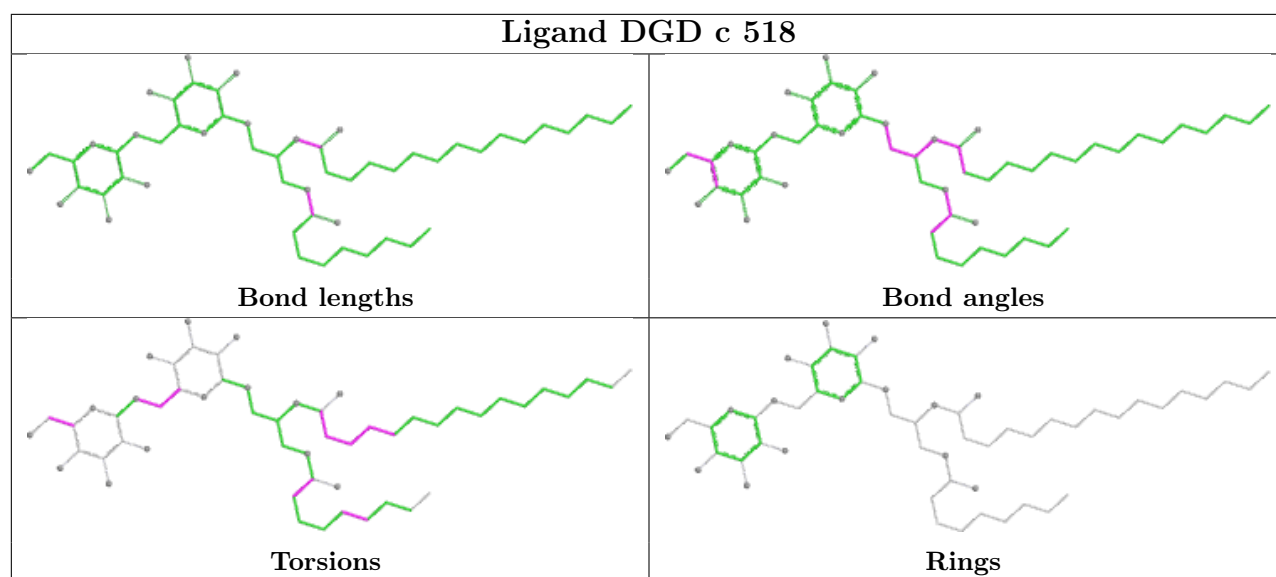


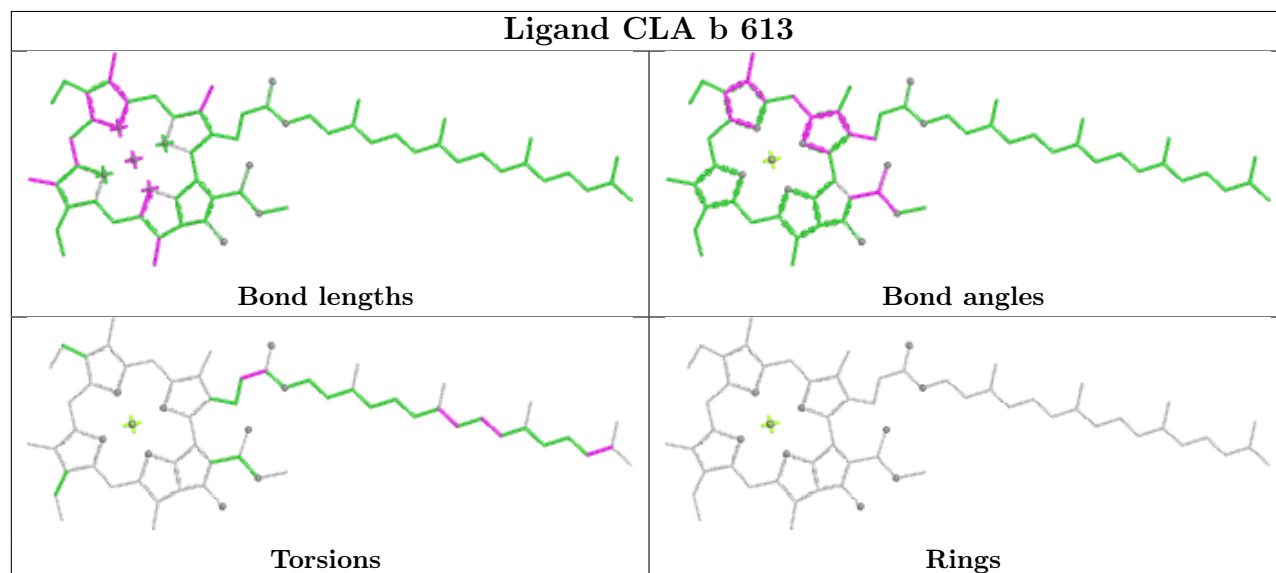
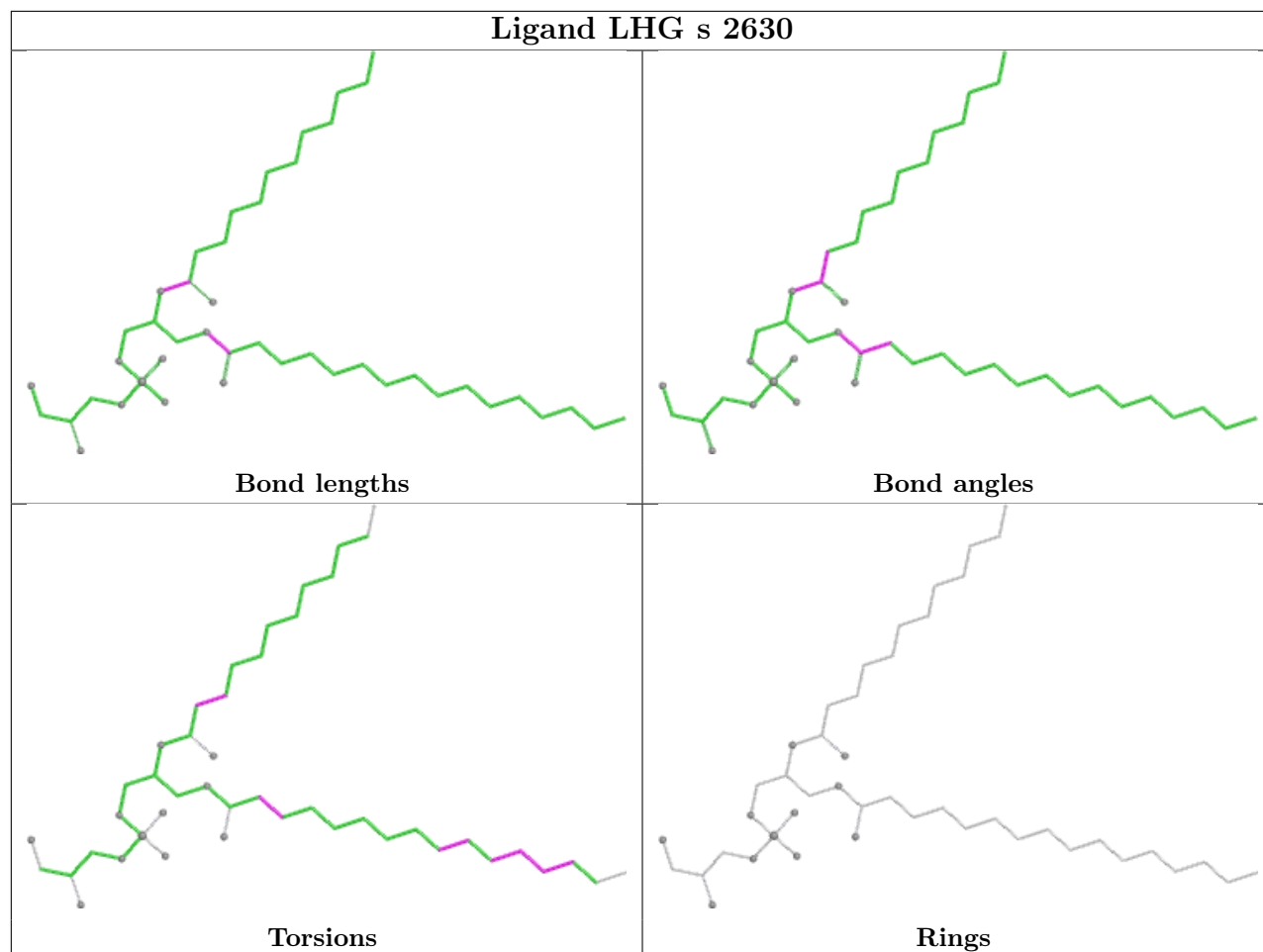
Torsions

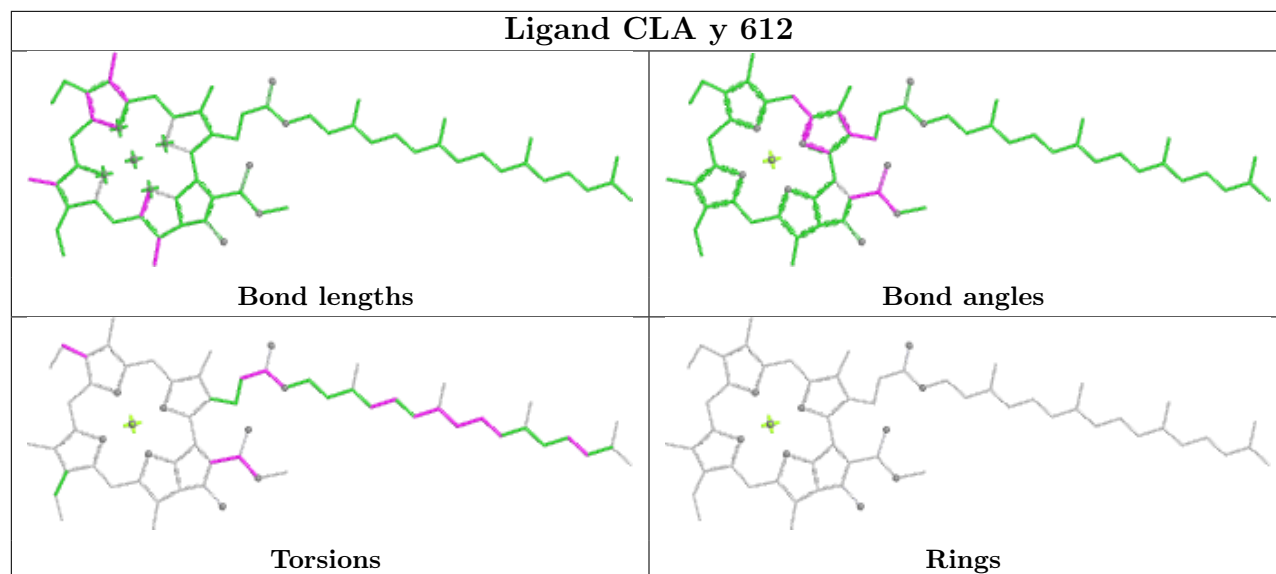
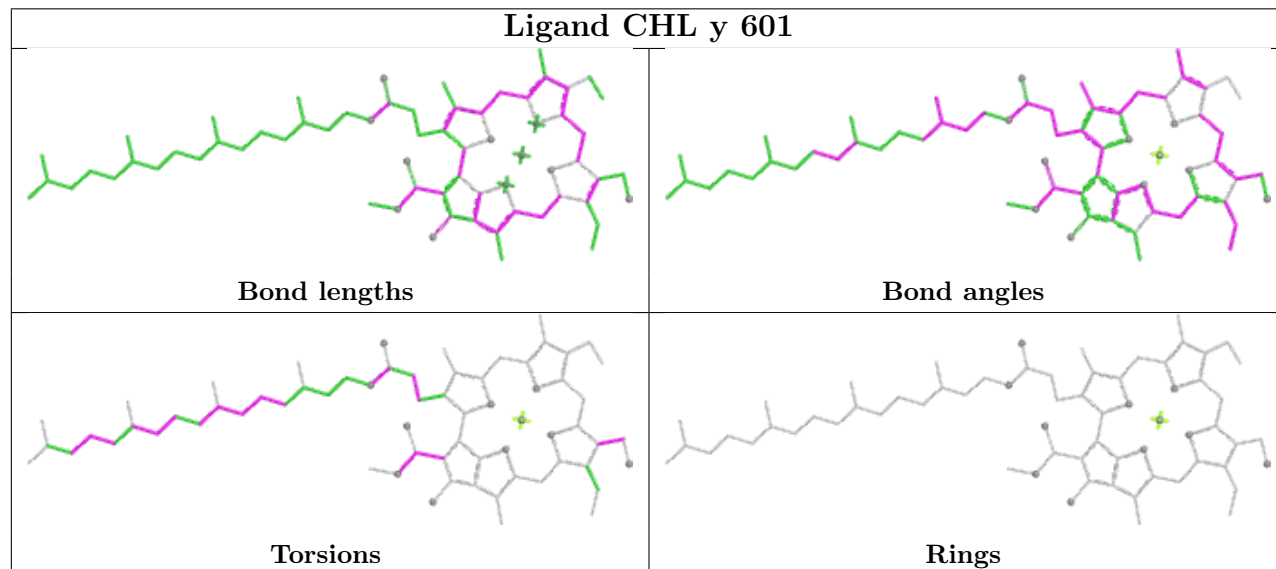


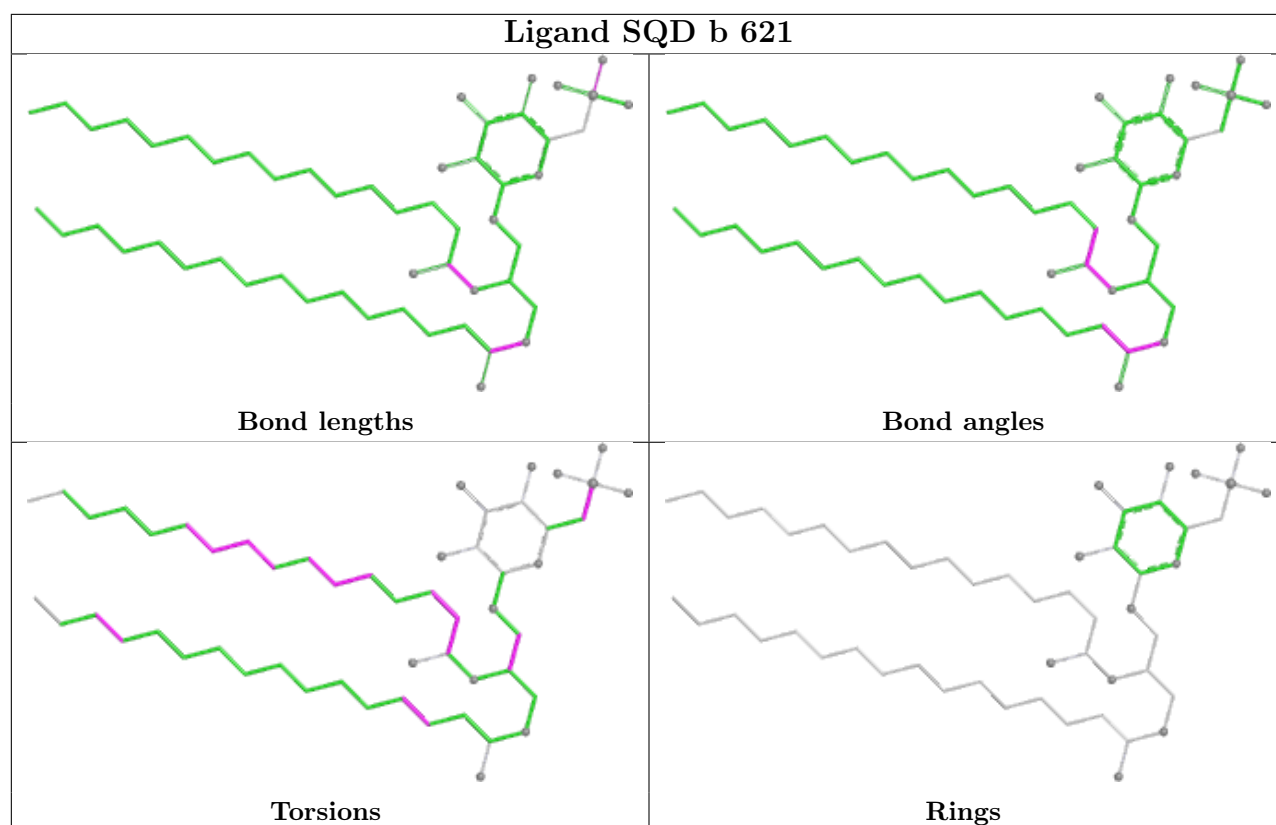
Rings

Ligand CLA y 613**Ligand CLA r 602**

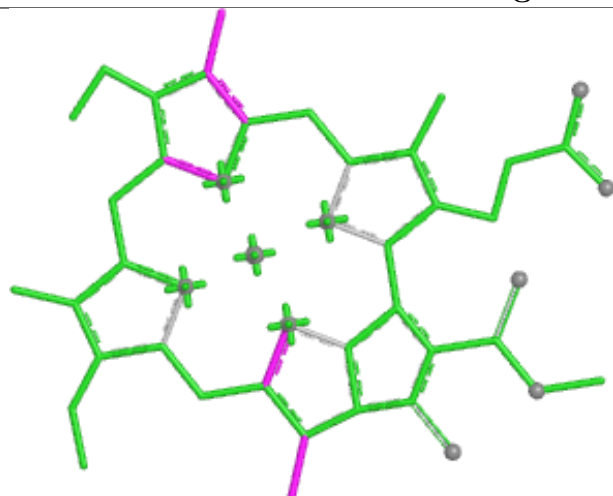




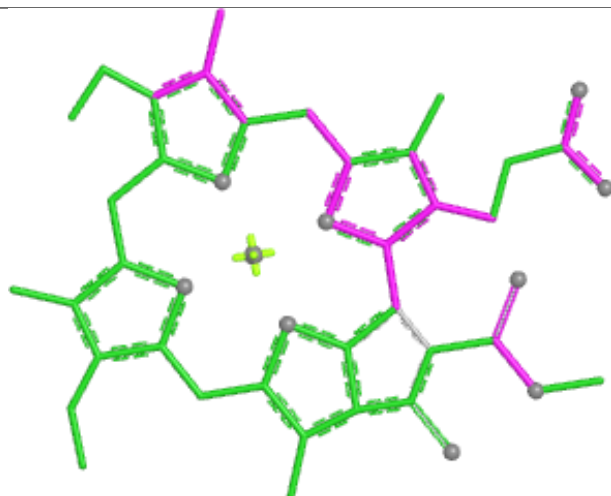
Ligand CLA y 612**Ligand CHL y 601**



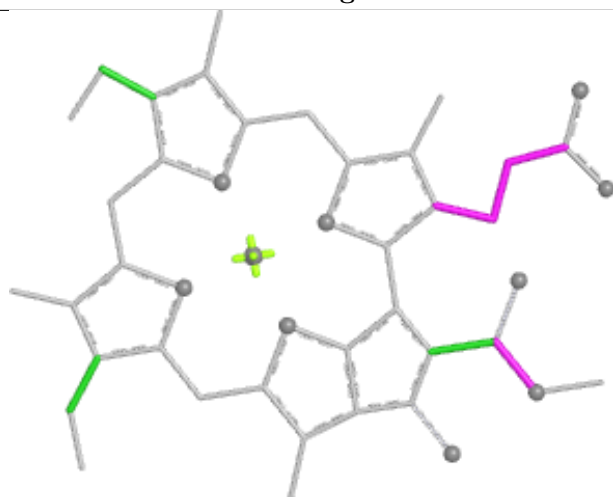
Ligand CLA R 609



Bond lengths



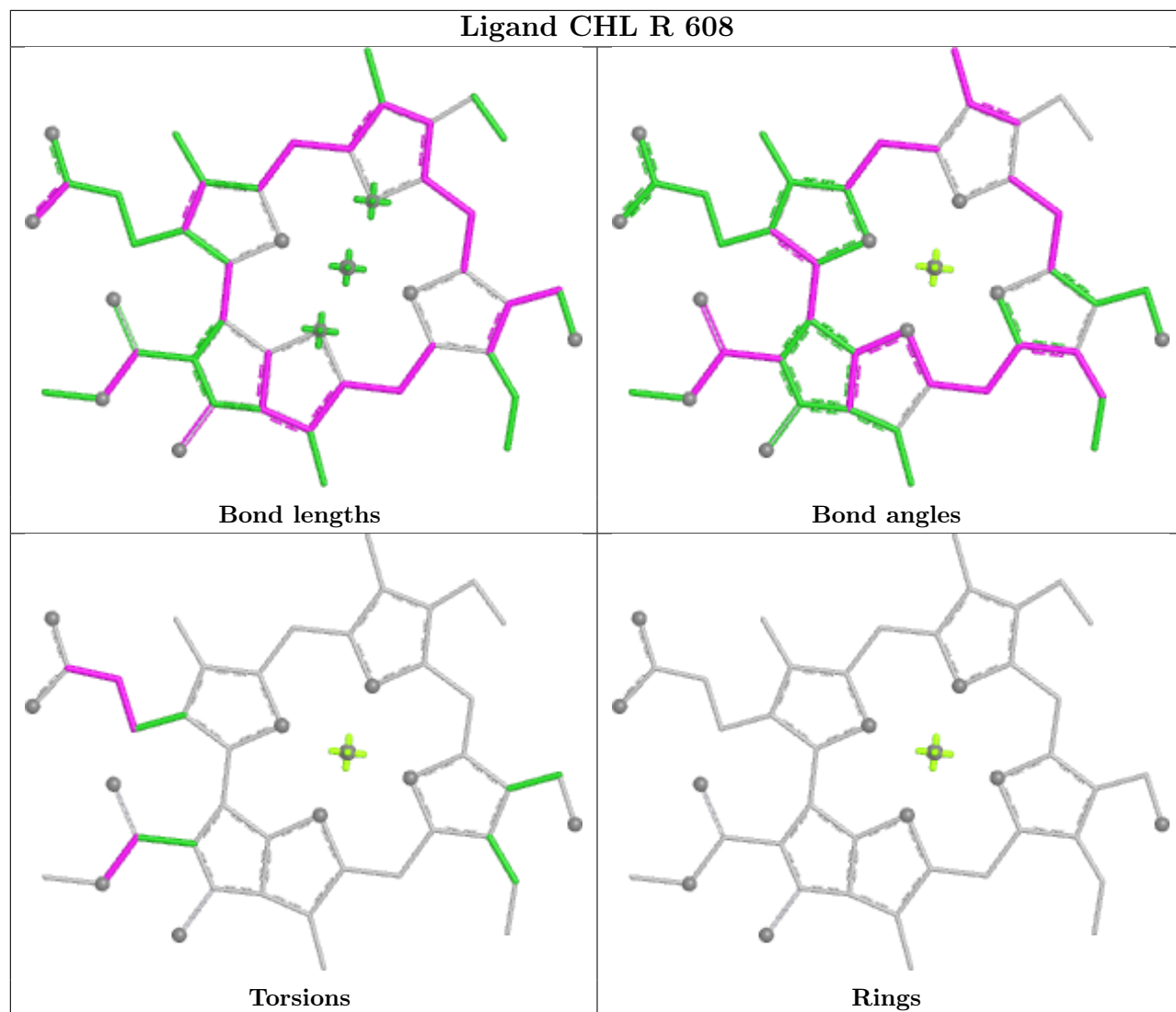
Bond angles

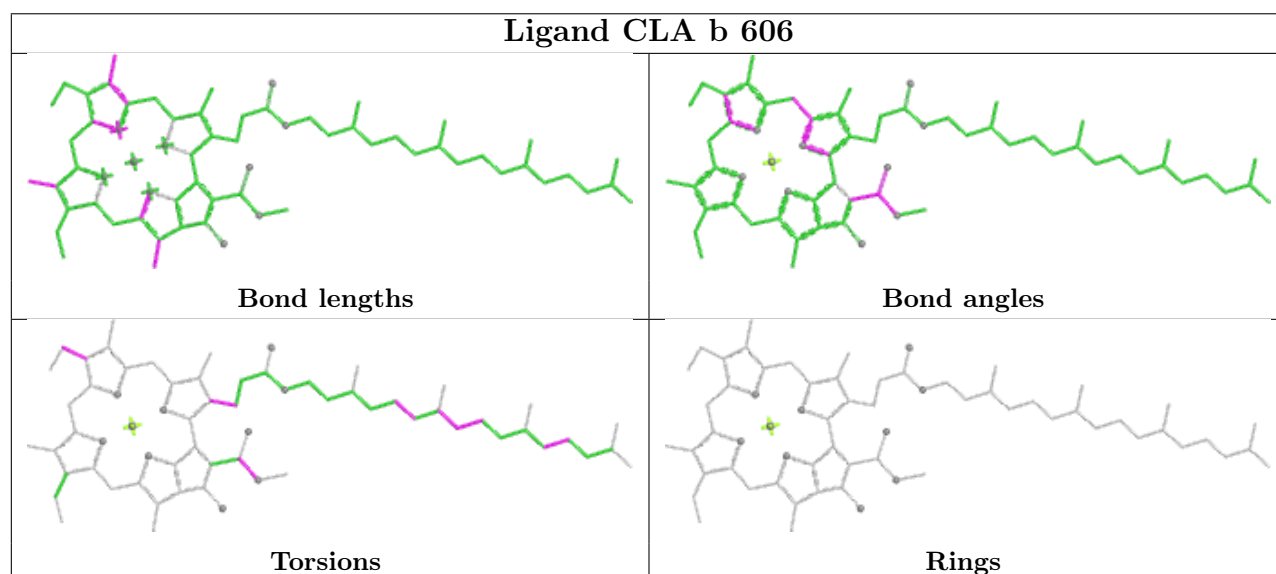
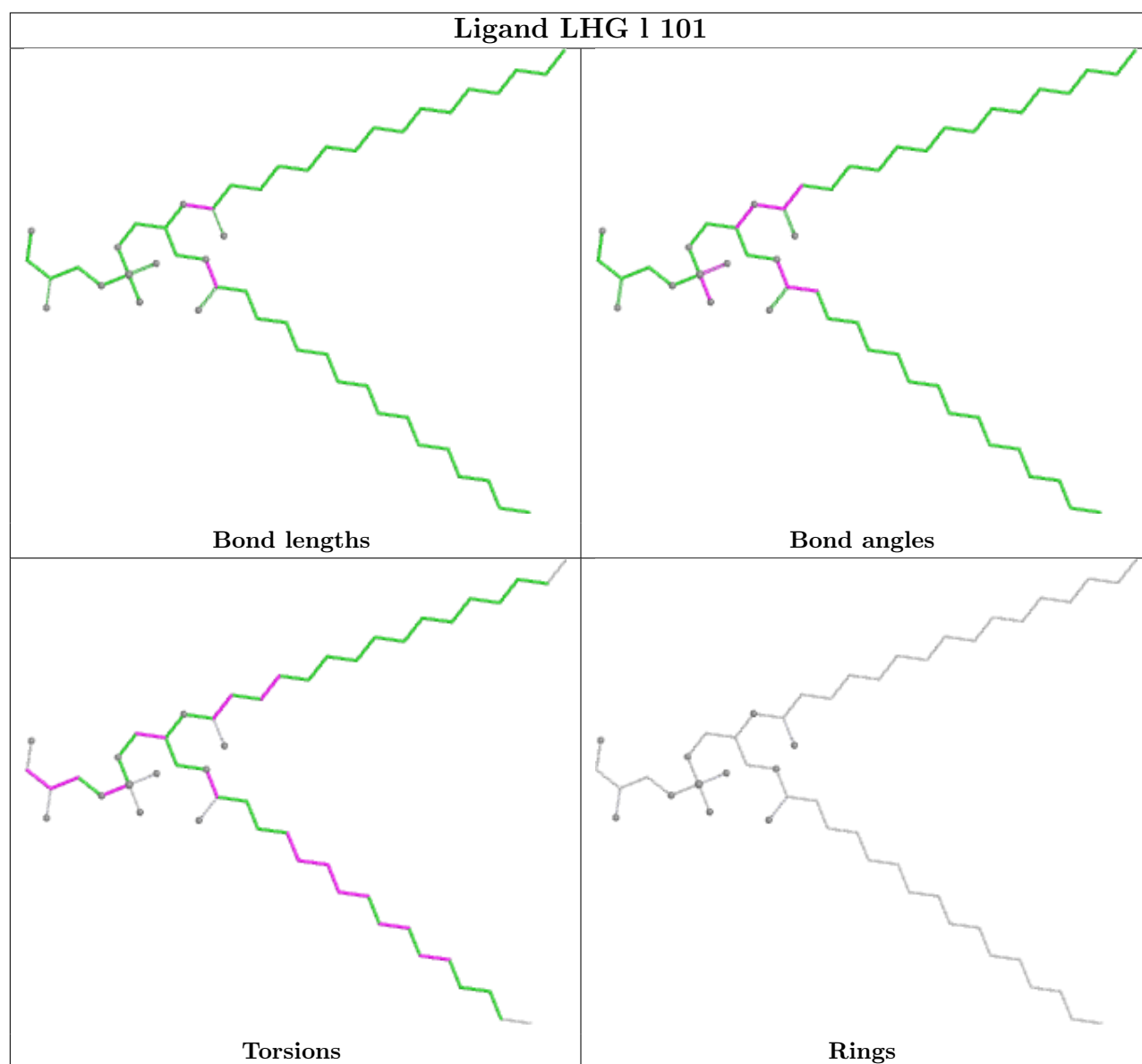


Torsions

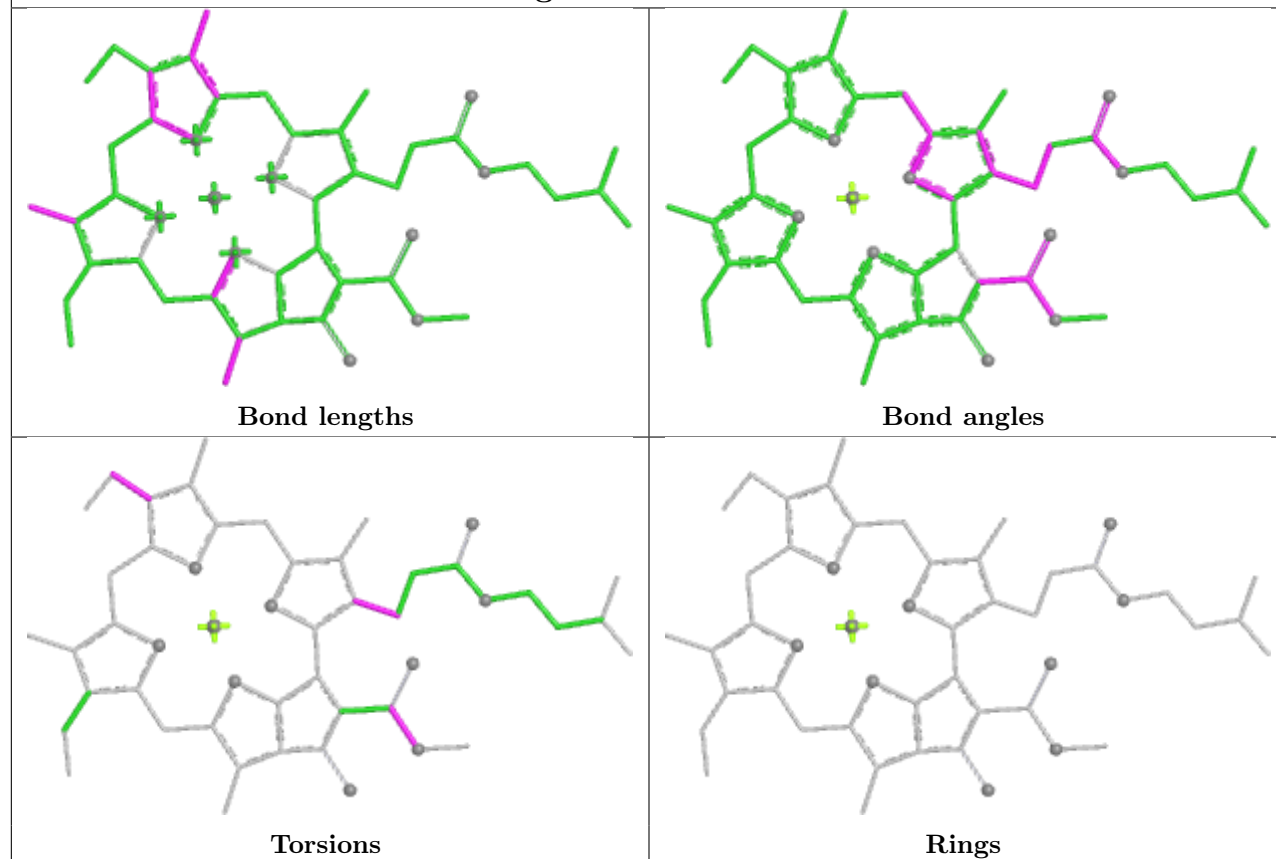


Rings

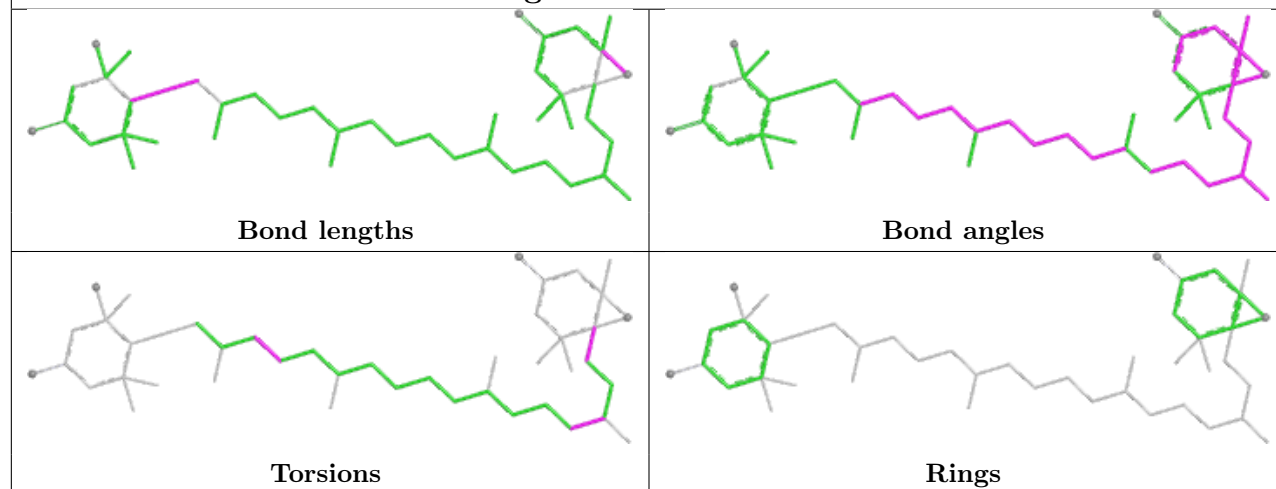


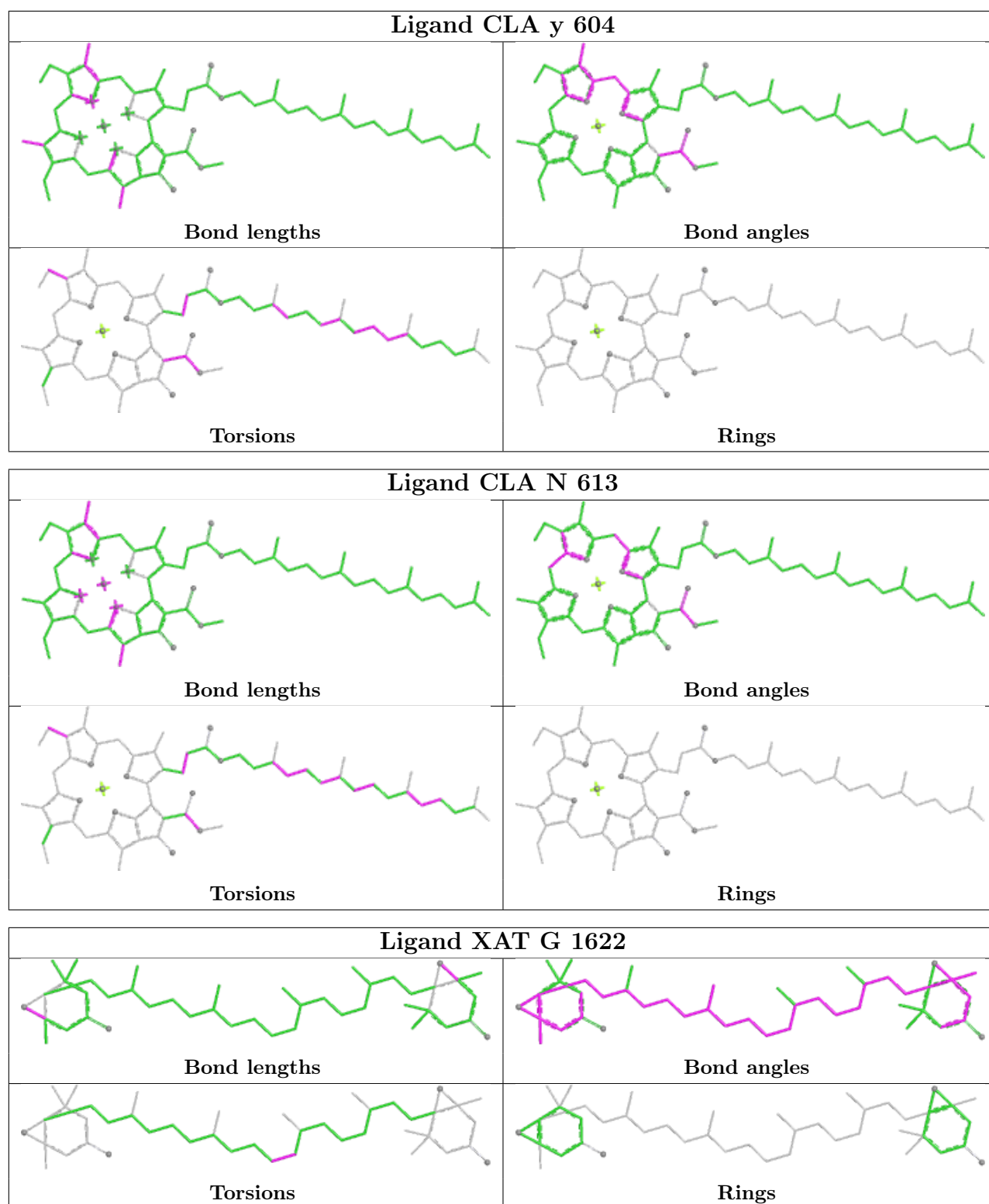


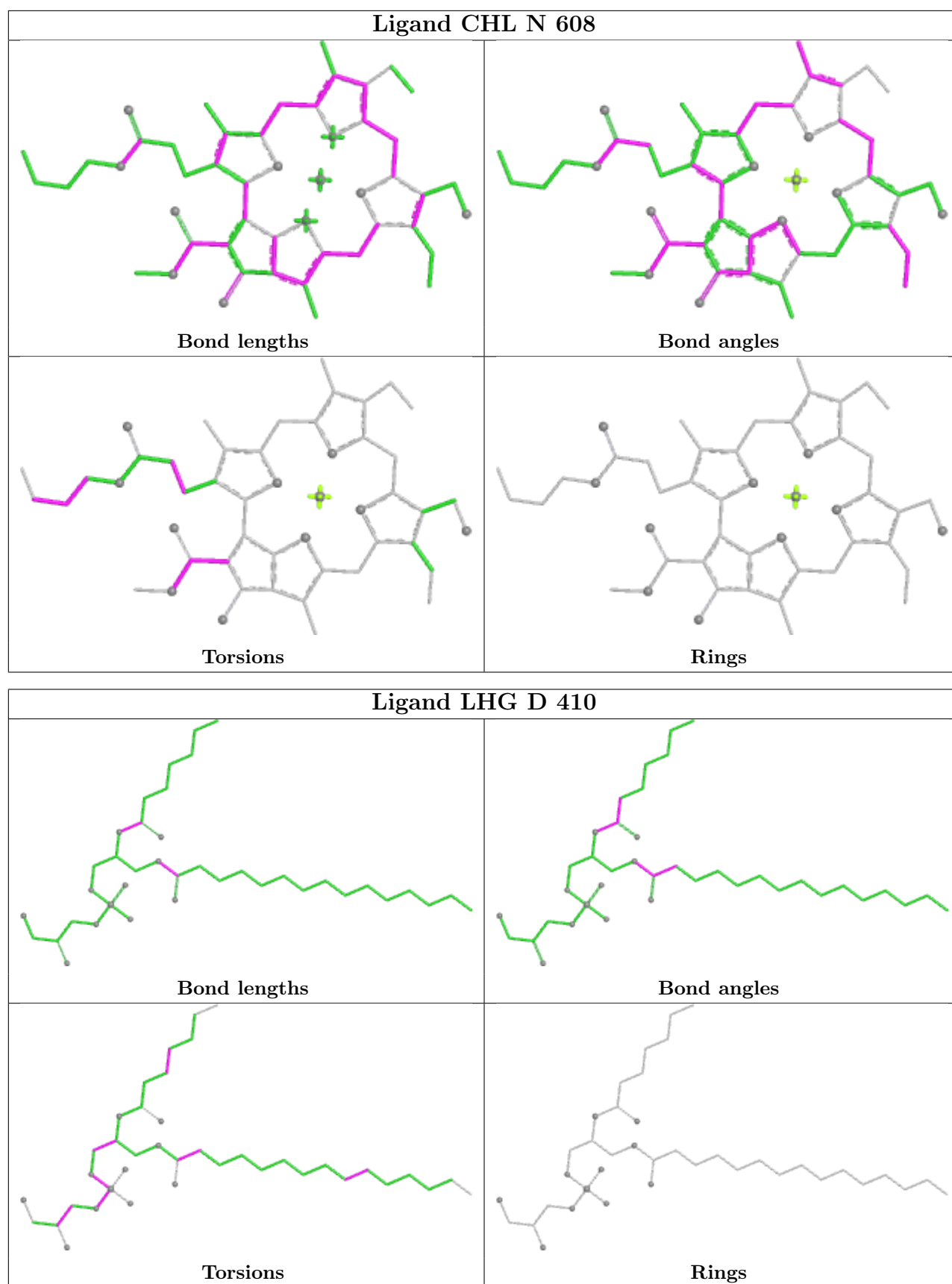
Ligand CLA S 605

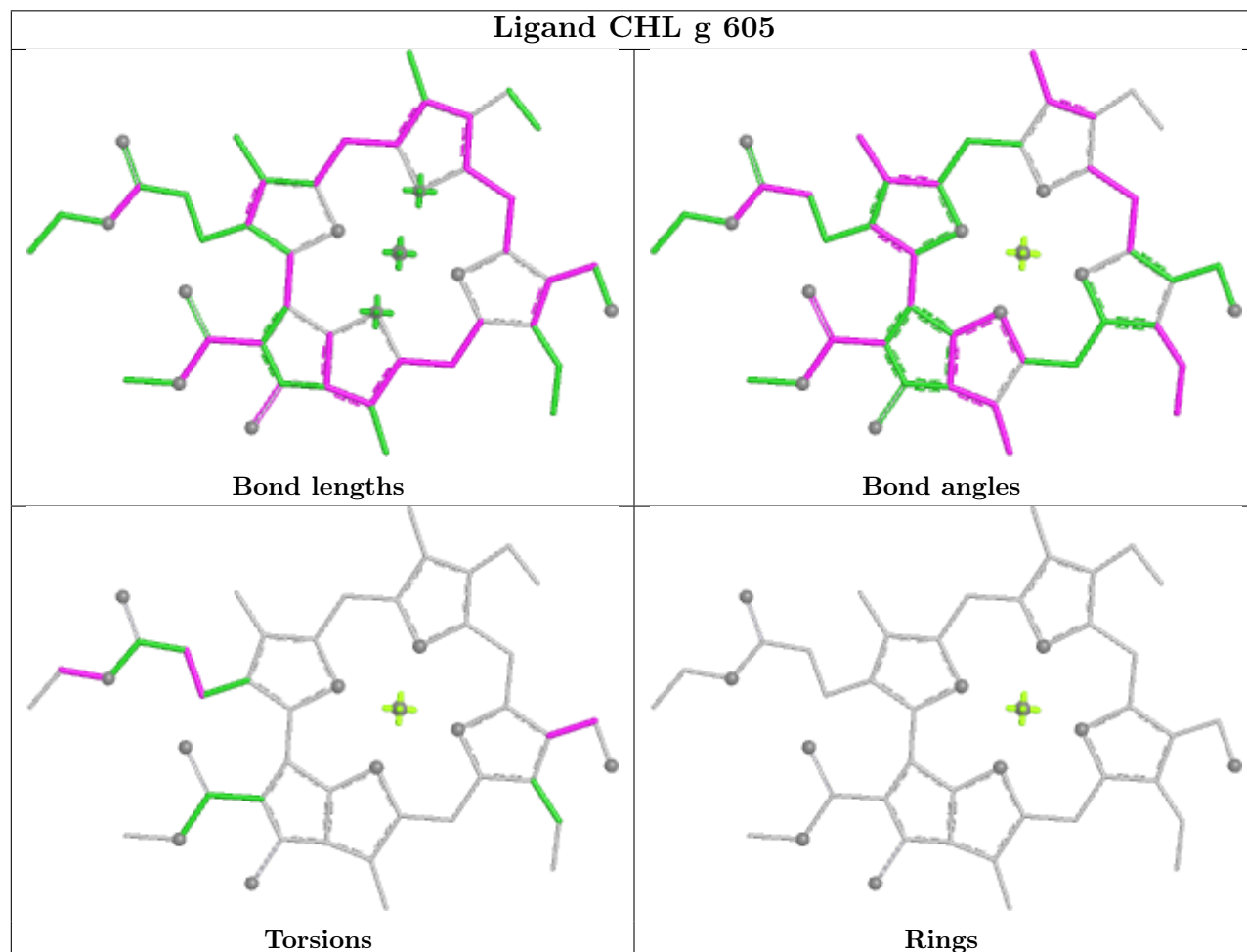
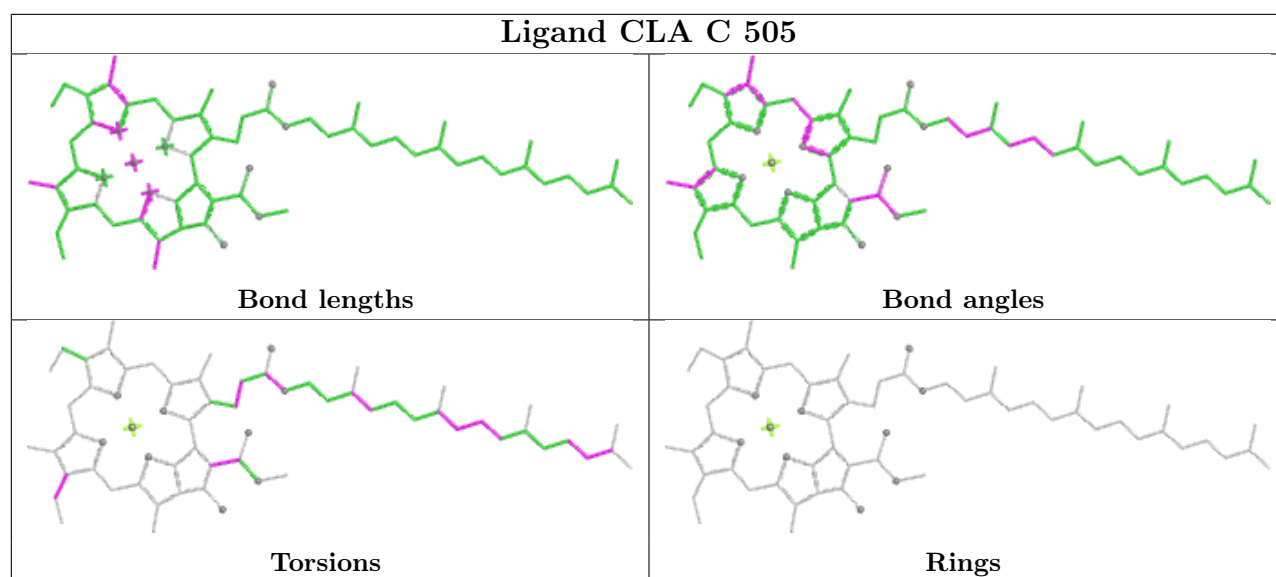


Ligand NEX n 1623

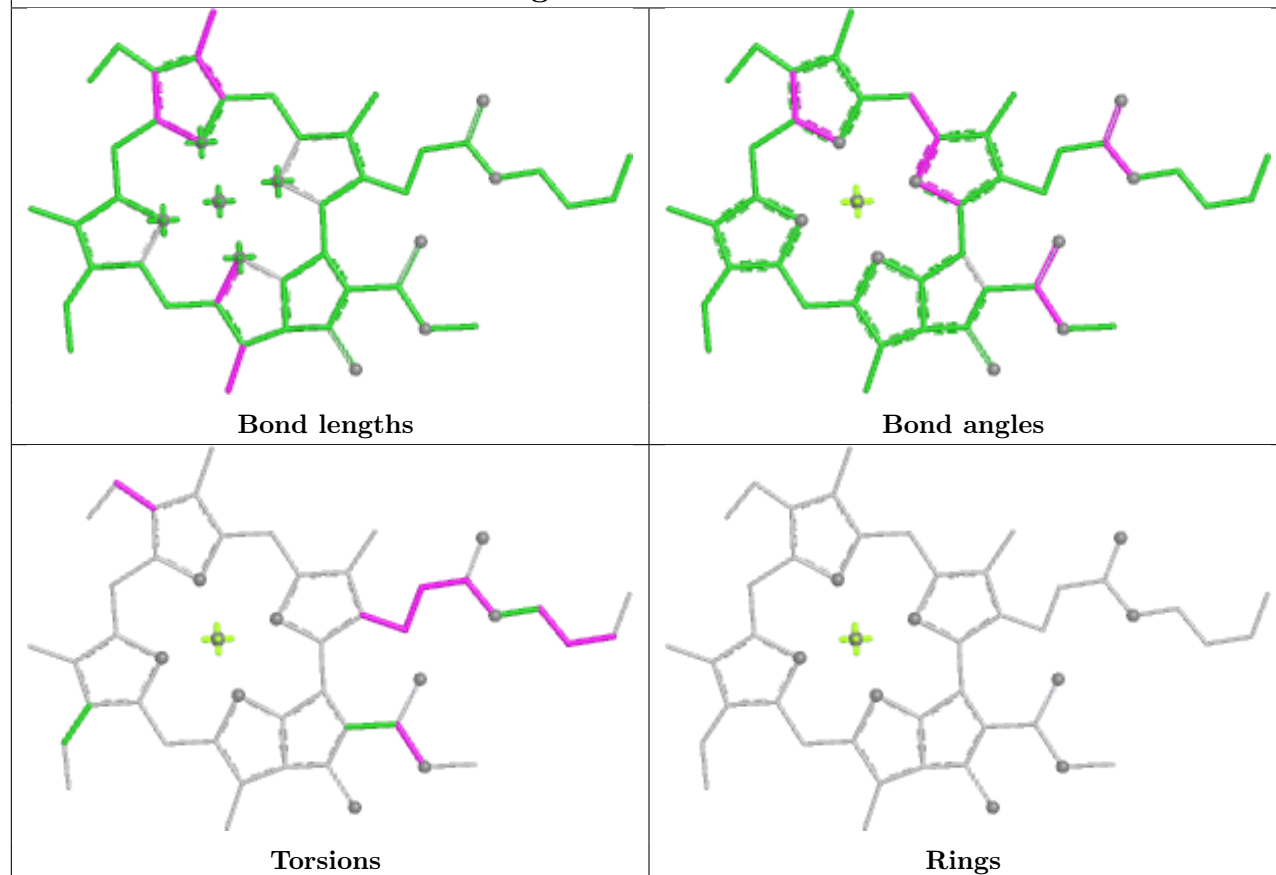




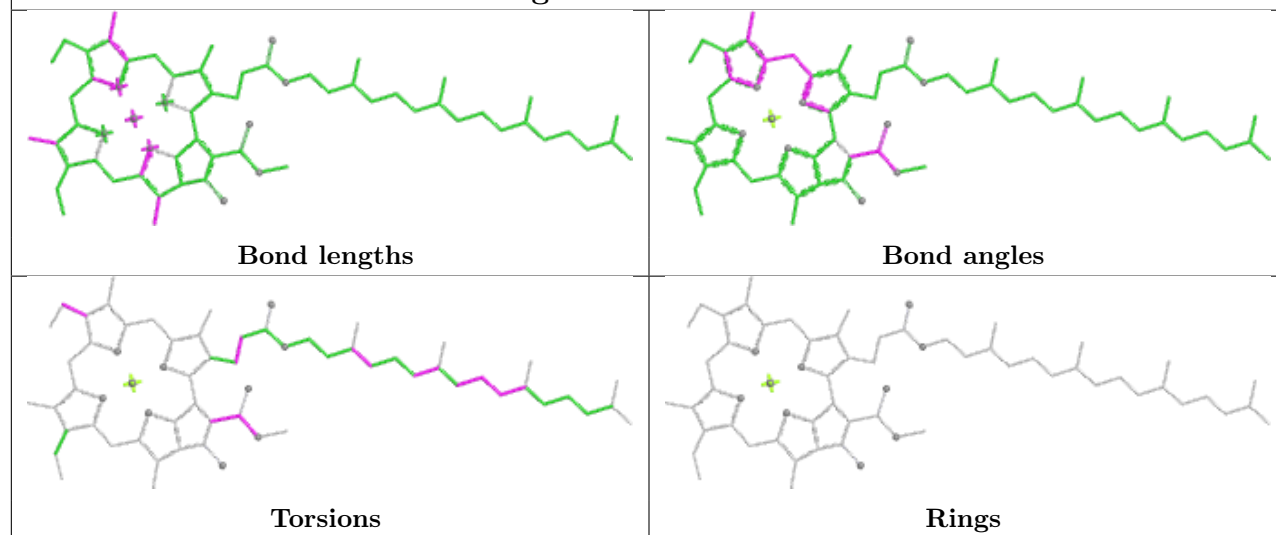


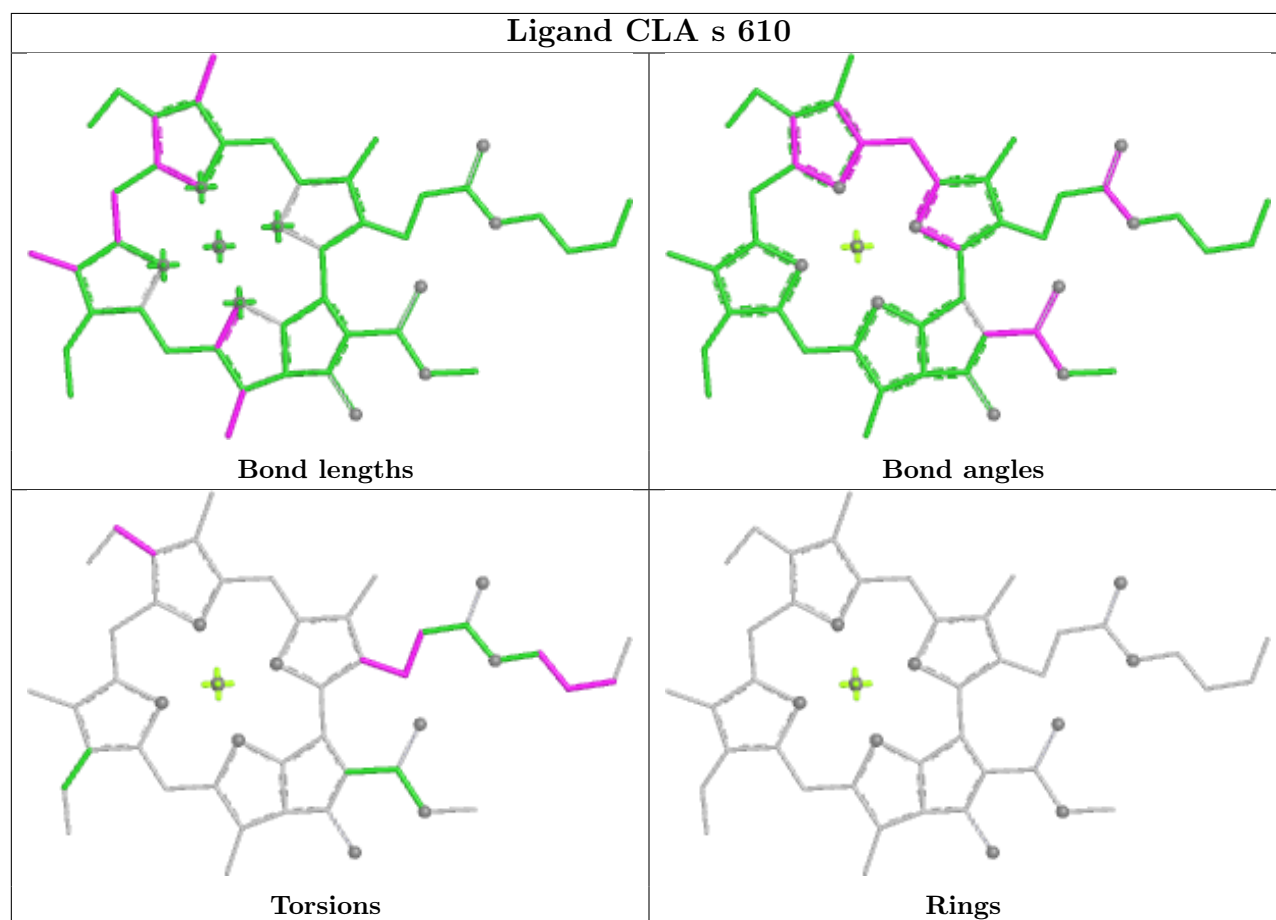
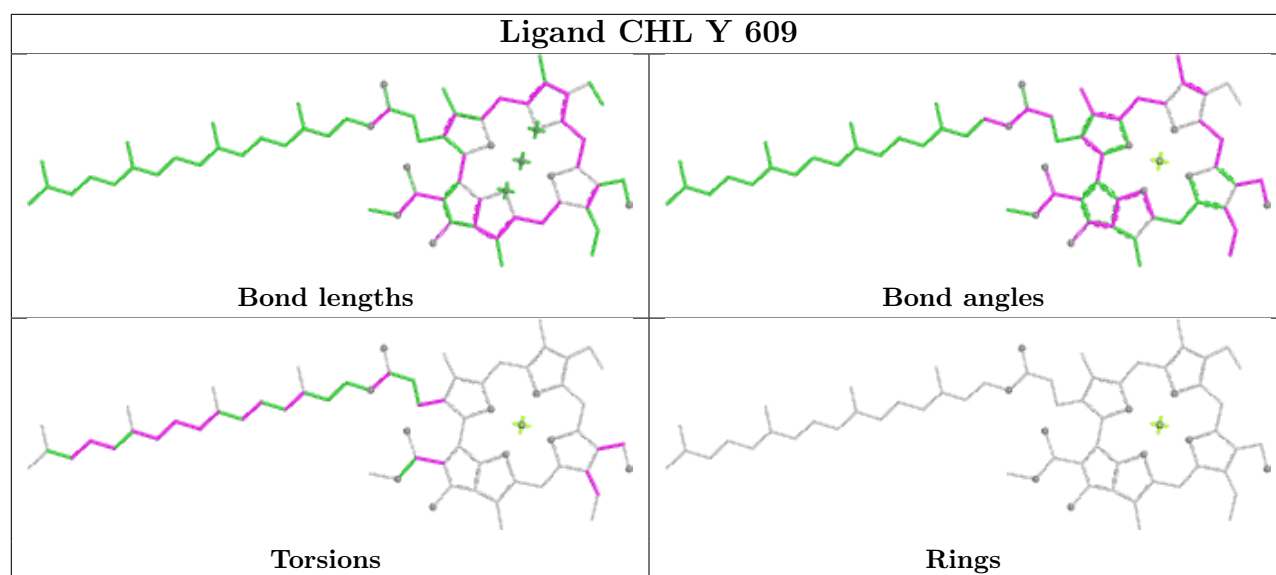


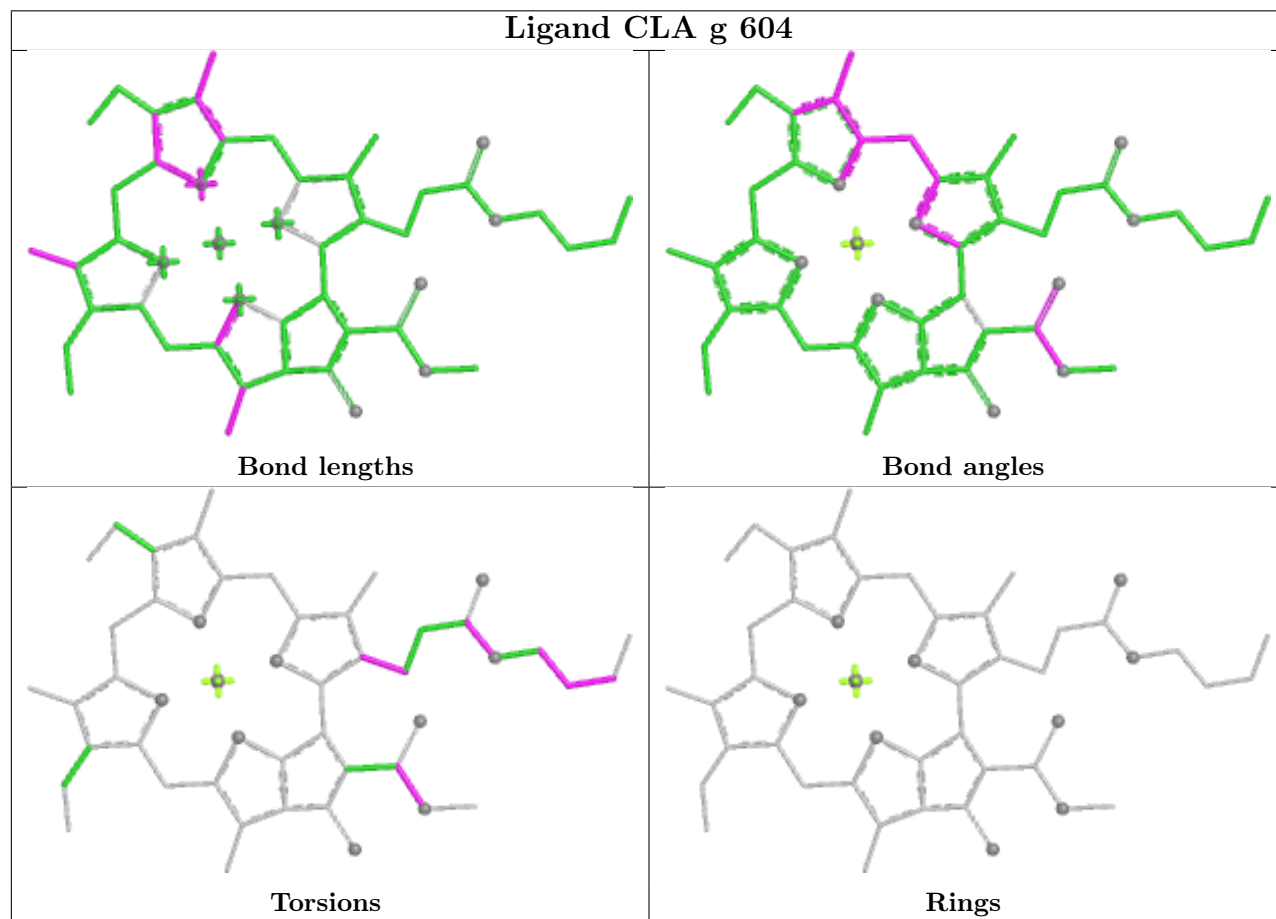
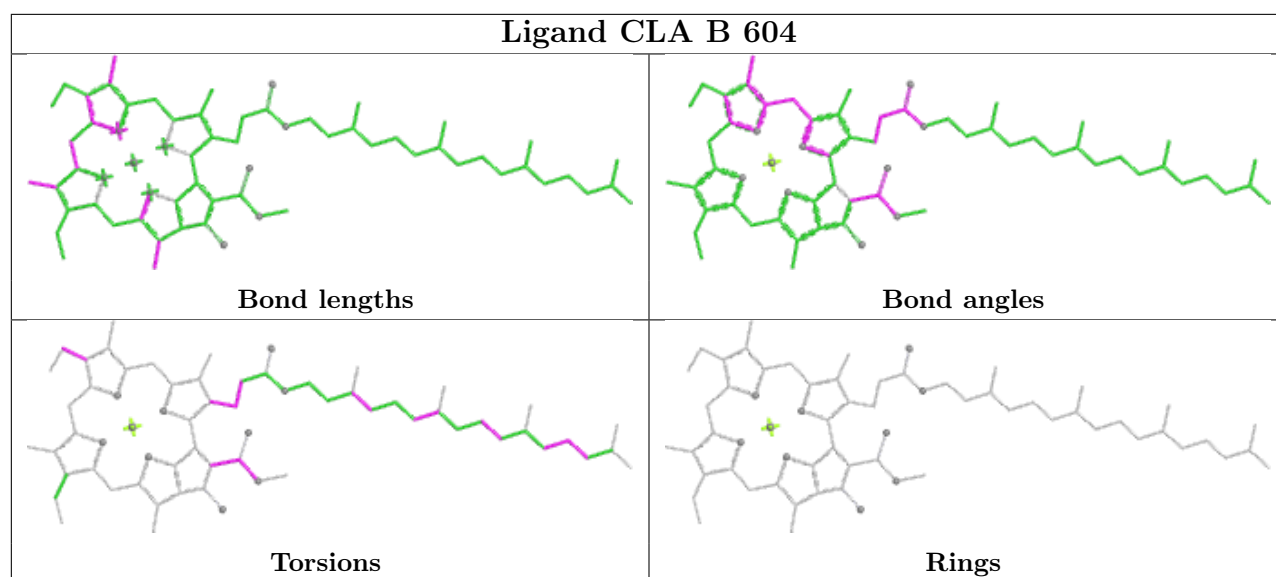
Ligand CLA G 614

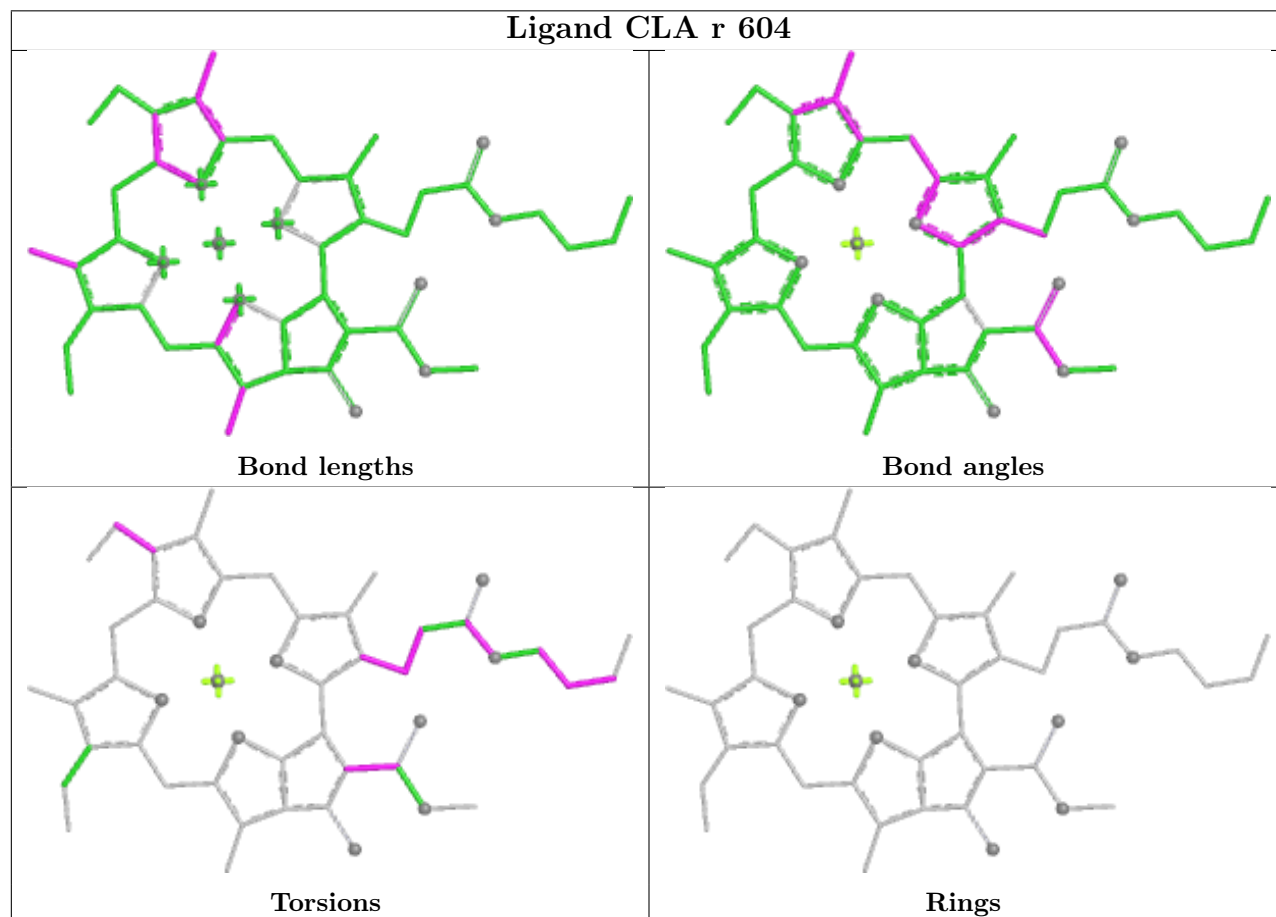
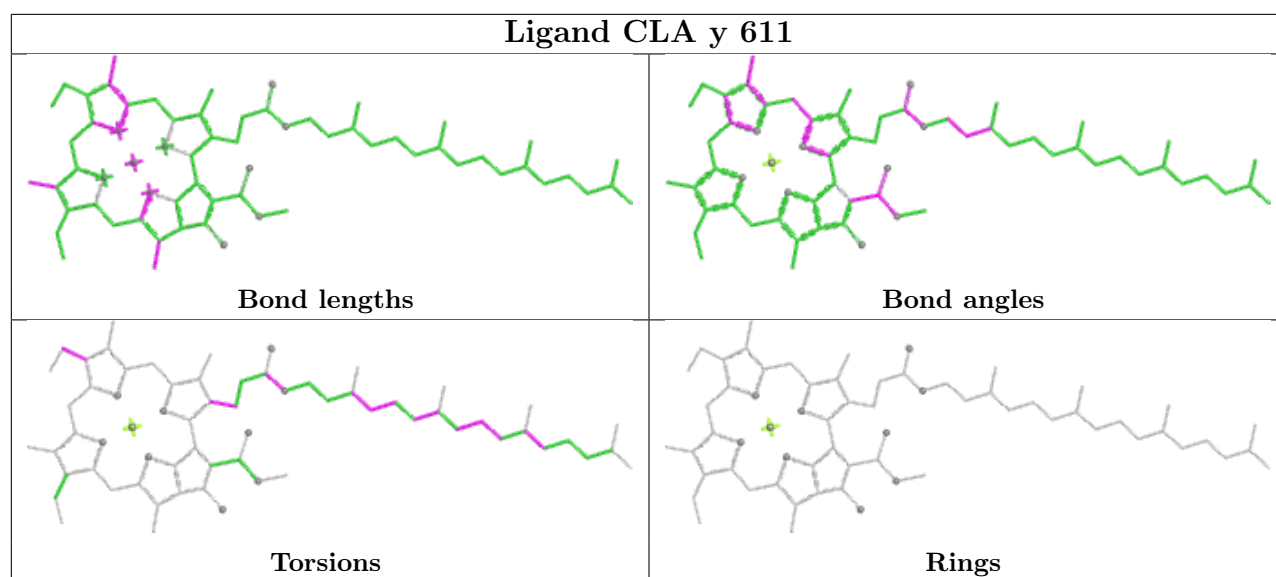


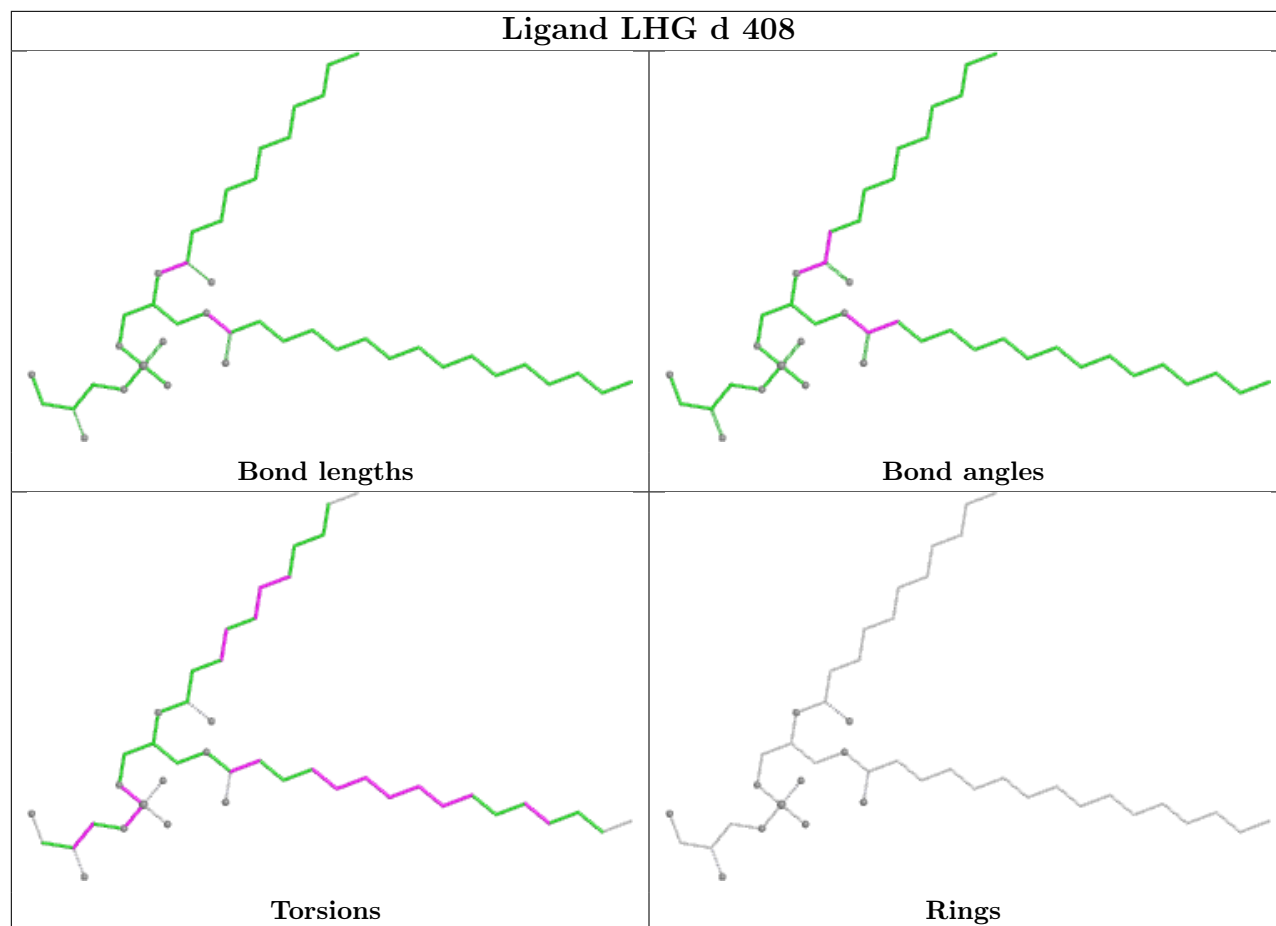
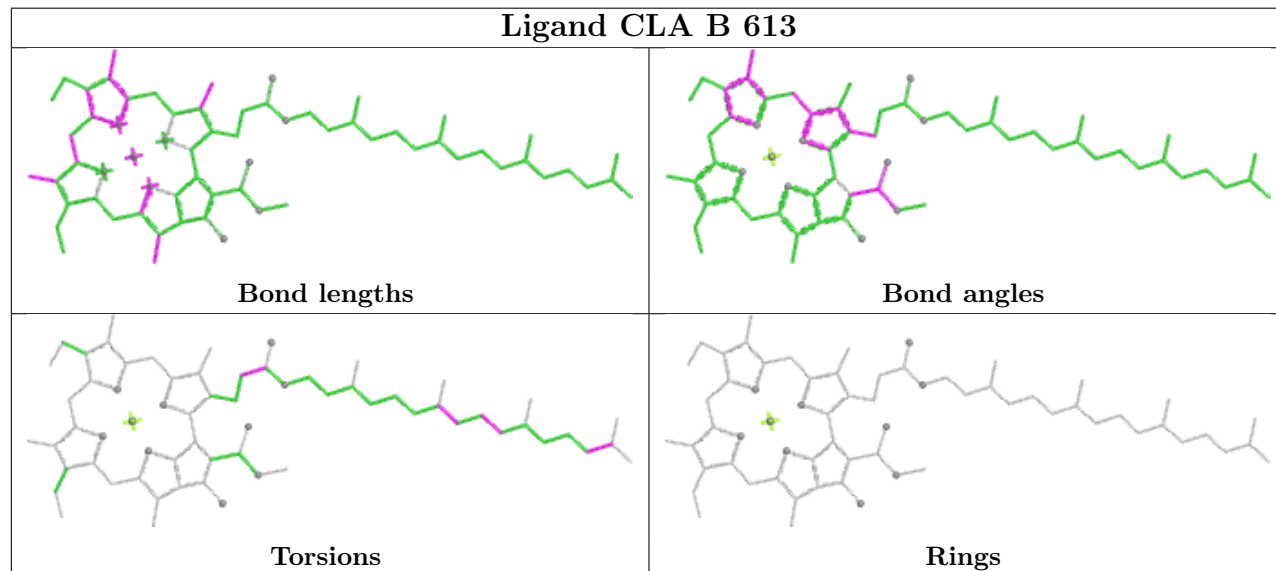
Ligand CLA Y 604

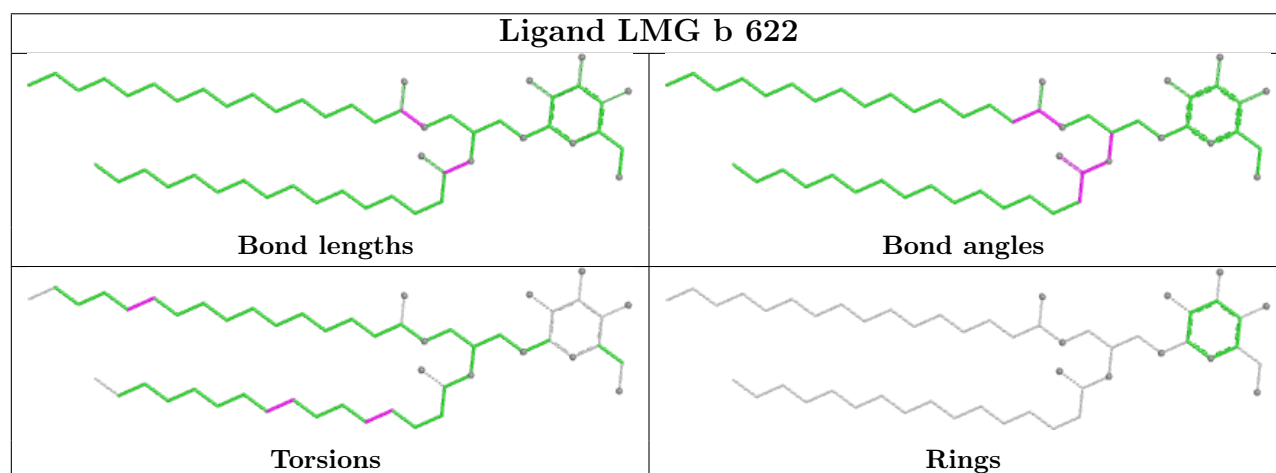
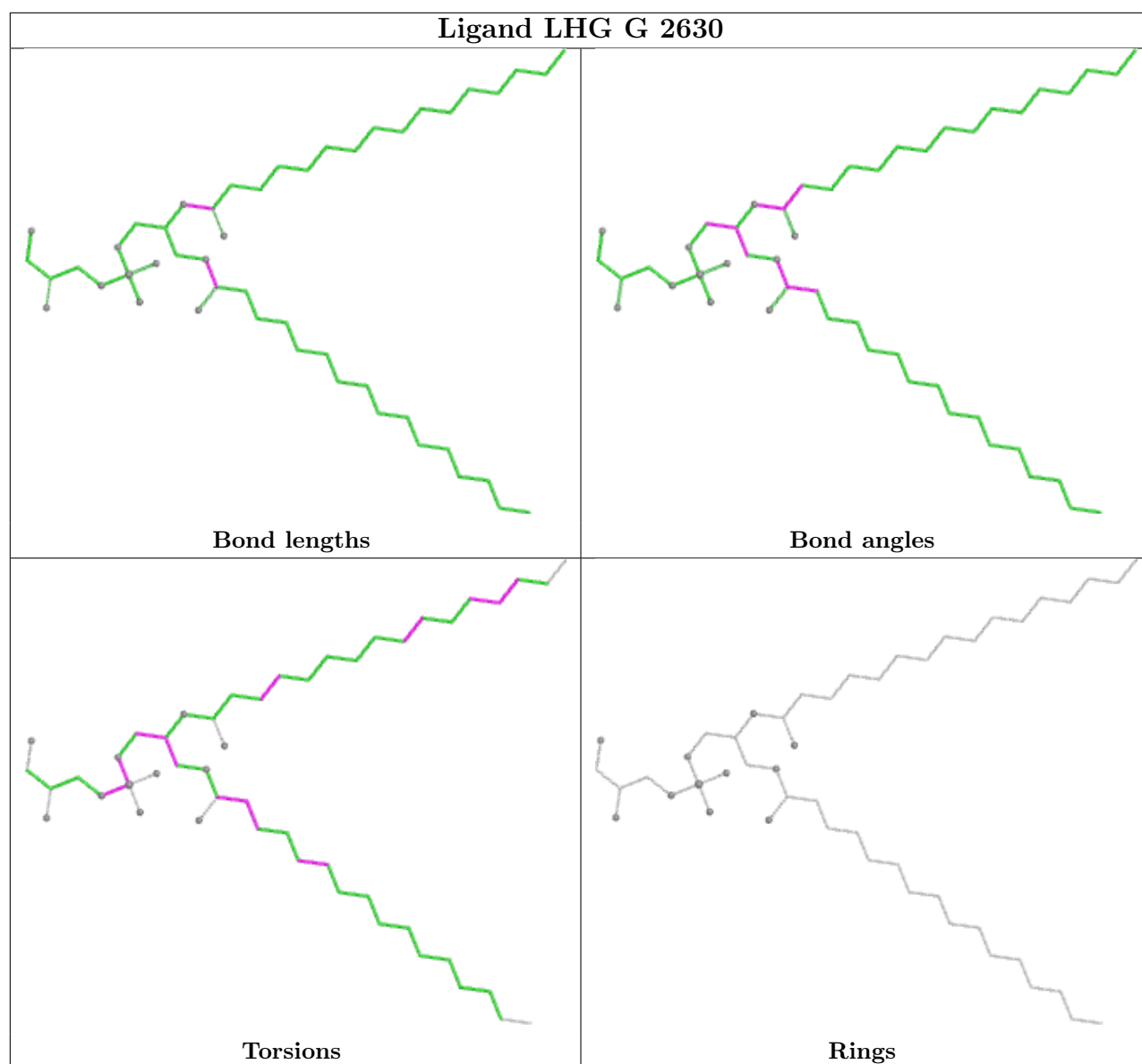


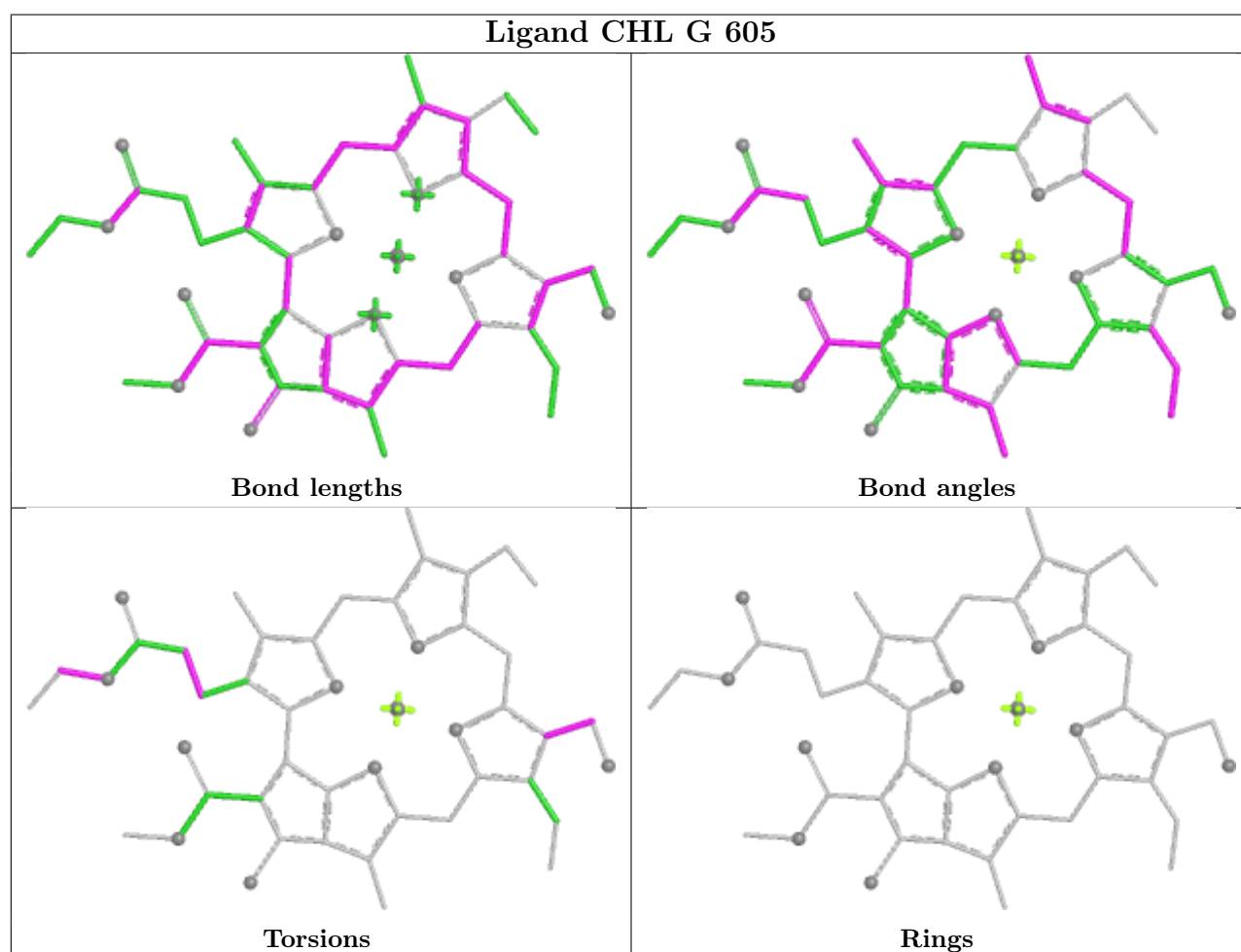
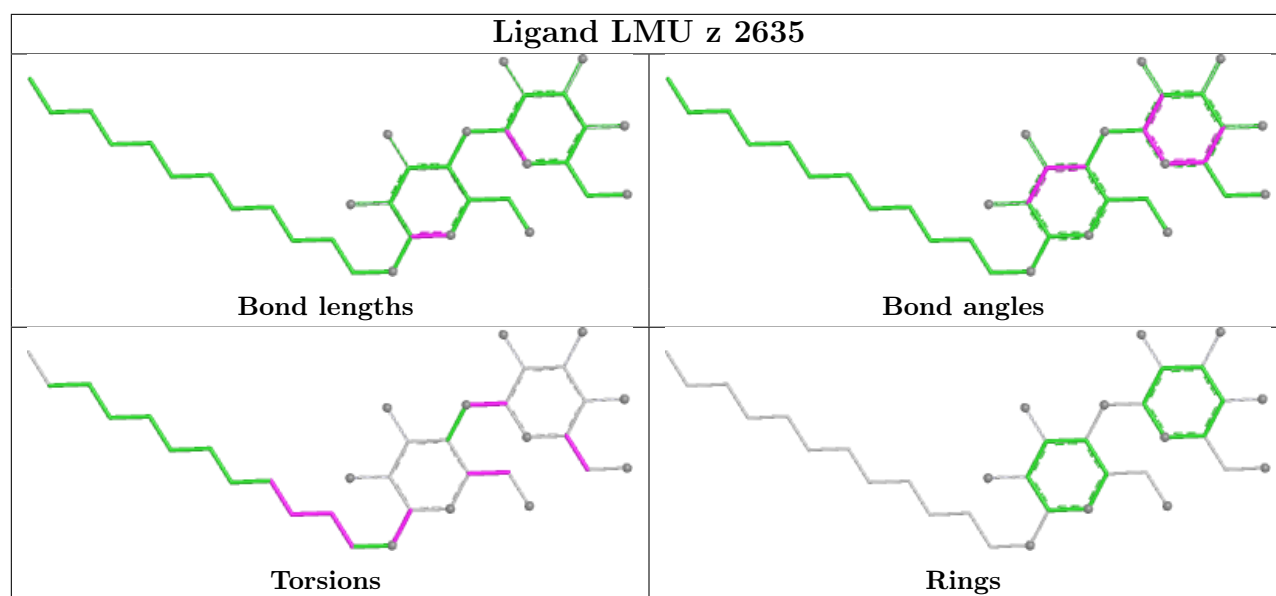


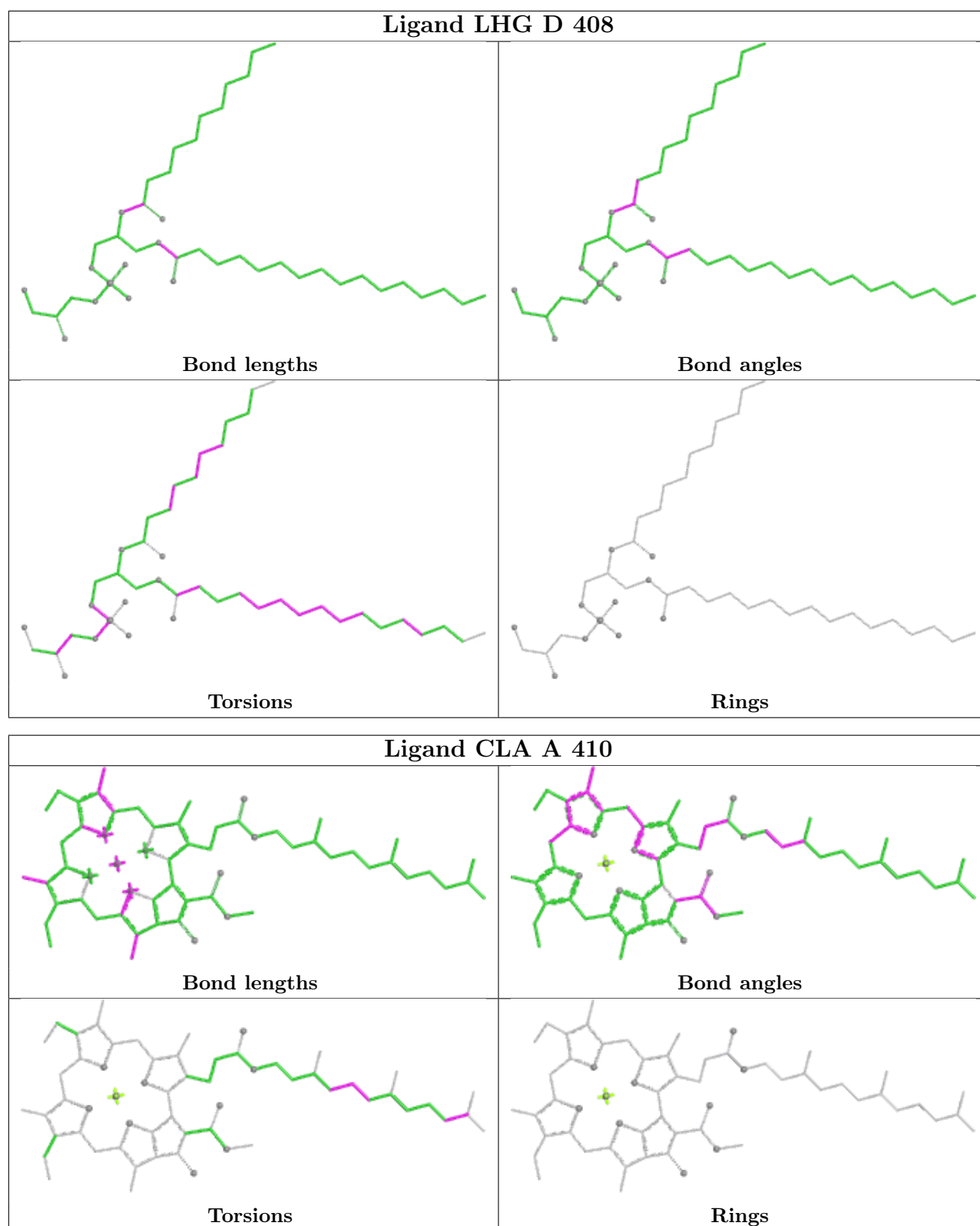


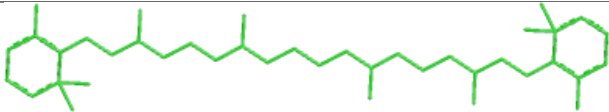
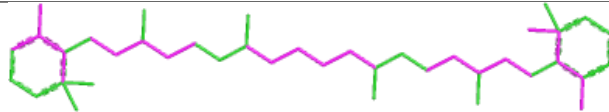
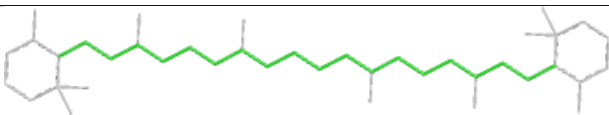
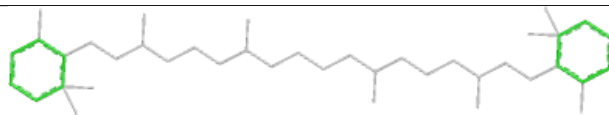


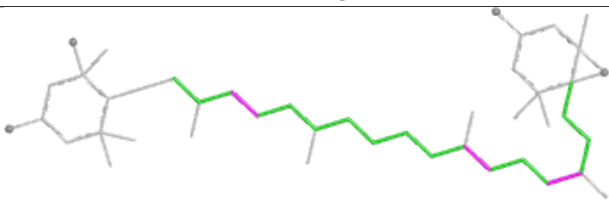
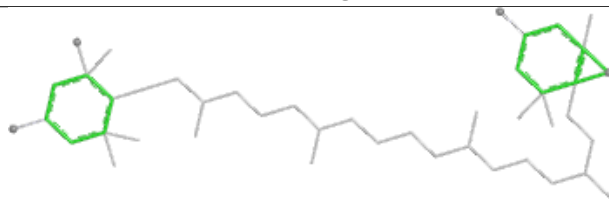
Ligand LHG d 408**Ligand CLA B 613**

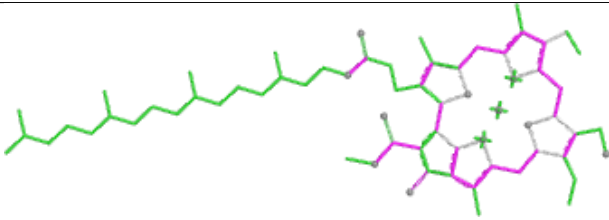
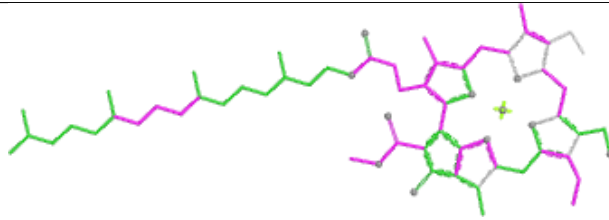
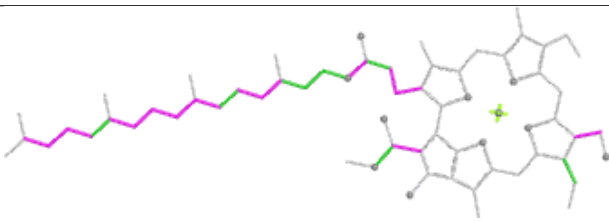
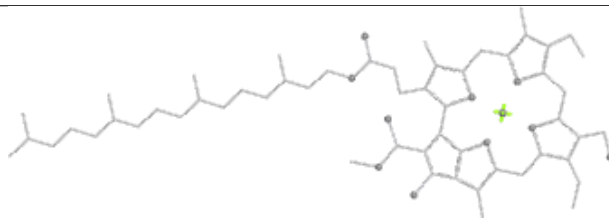


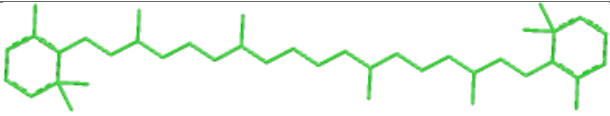
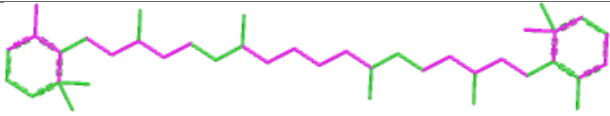
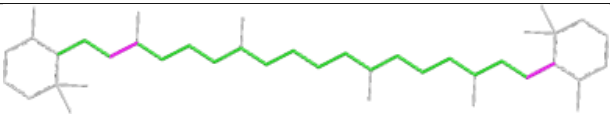
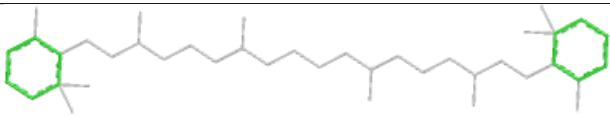
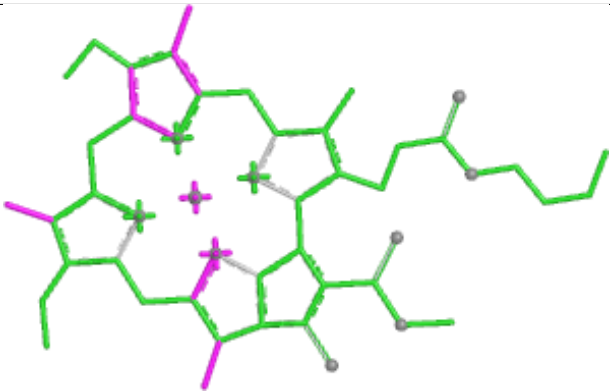
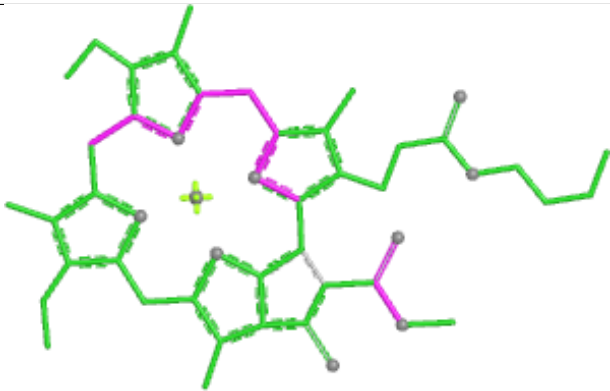
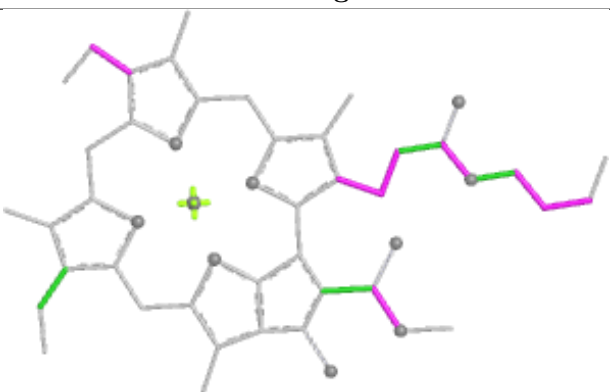
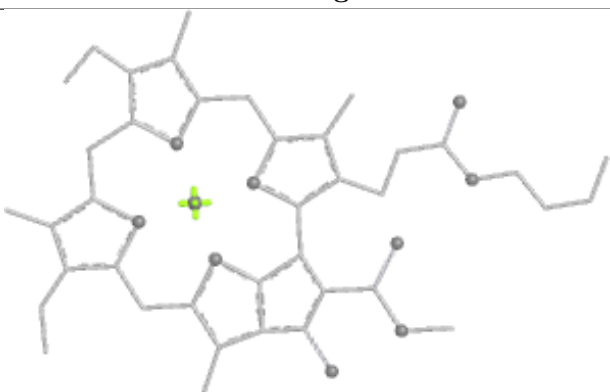




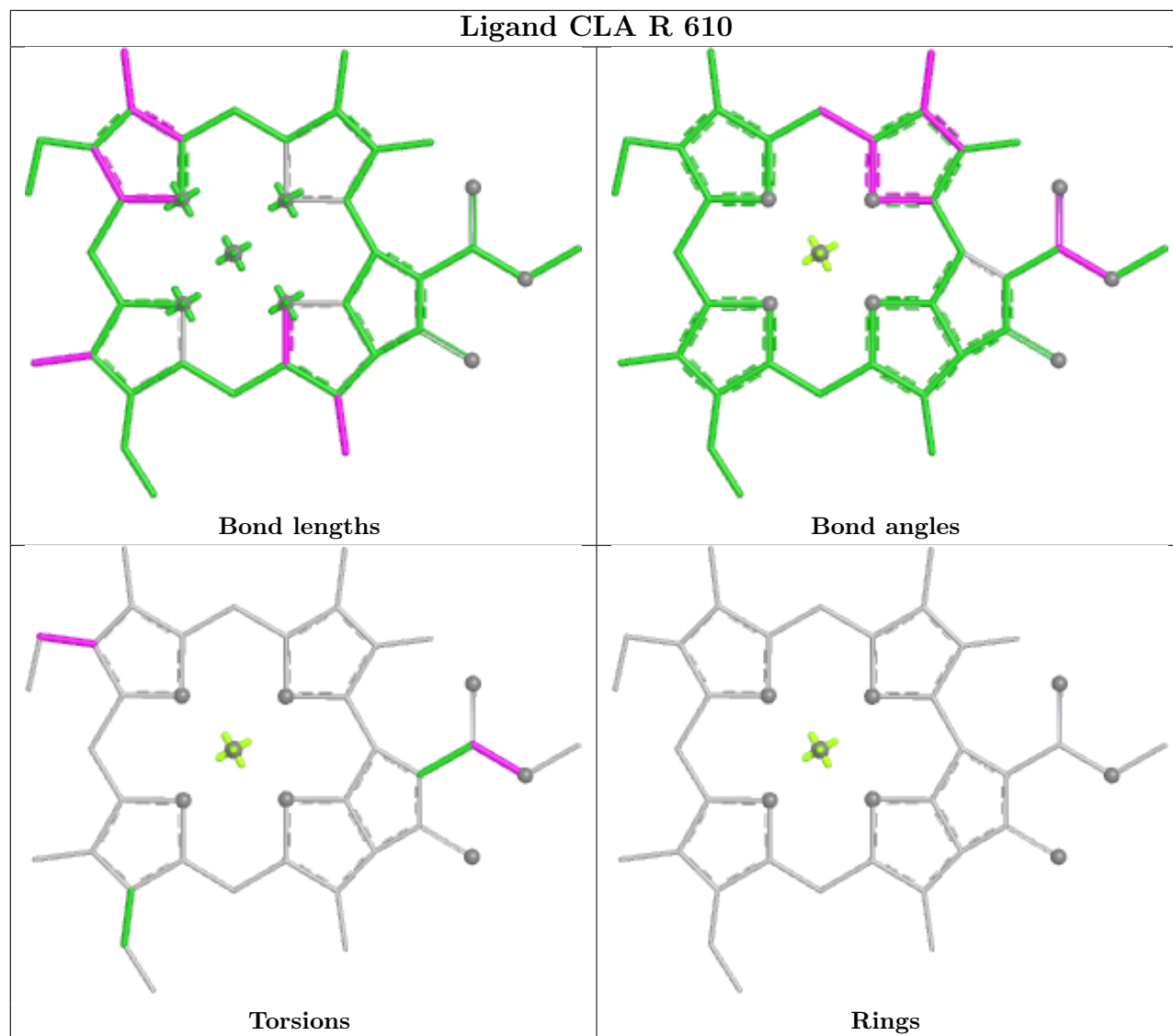
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX s 1623	
	
Bond lengths	Bond angles
	
Torsions	Rings

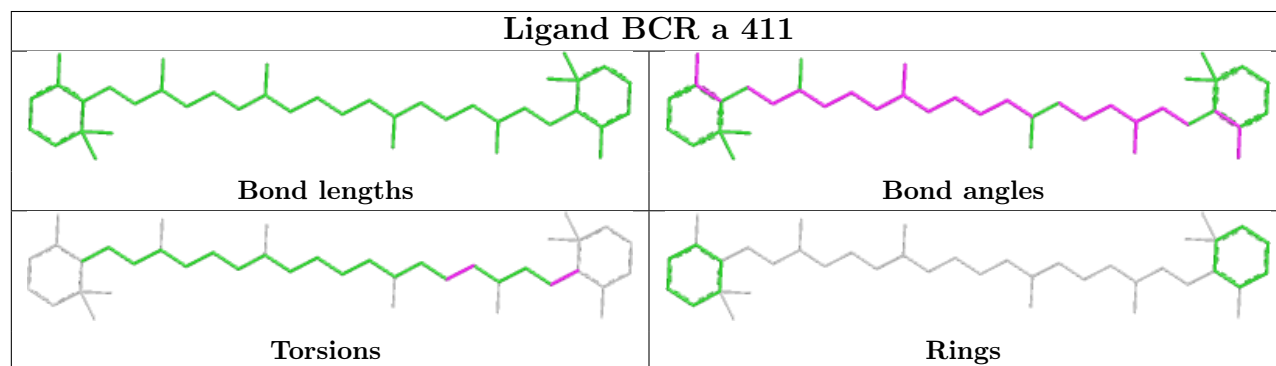
Ligand CHL y 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

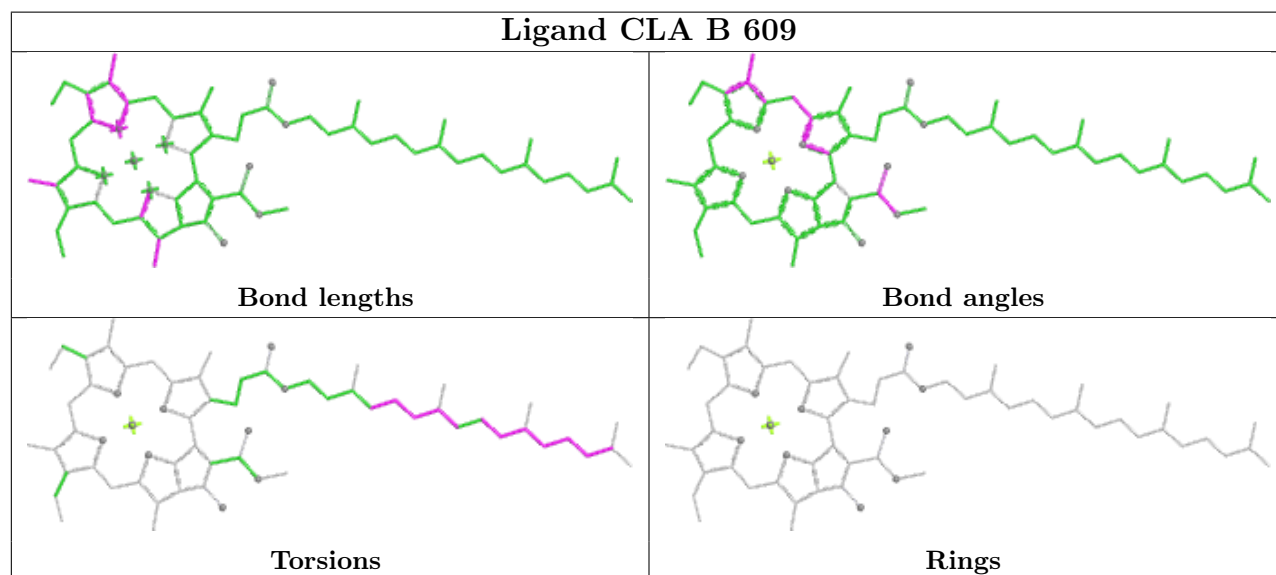
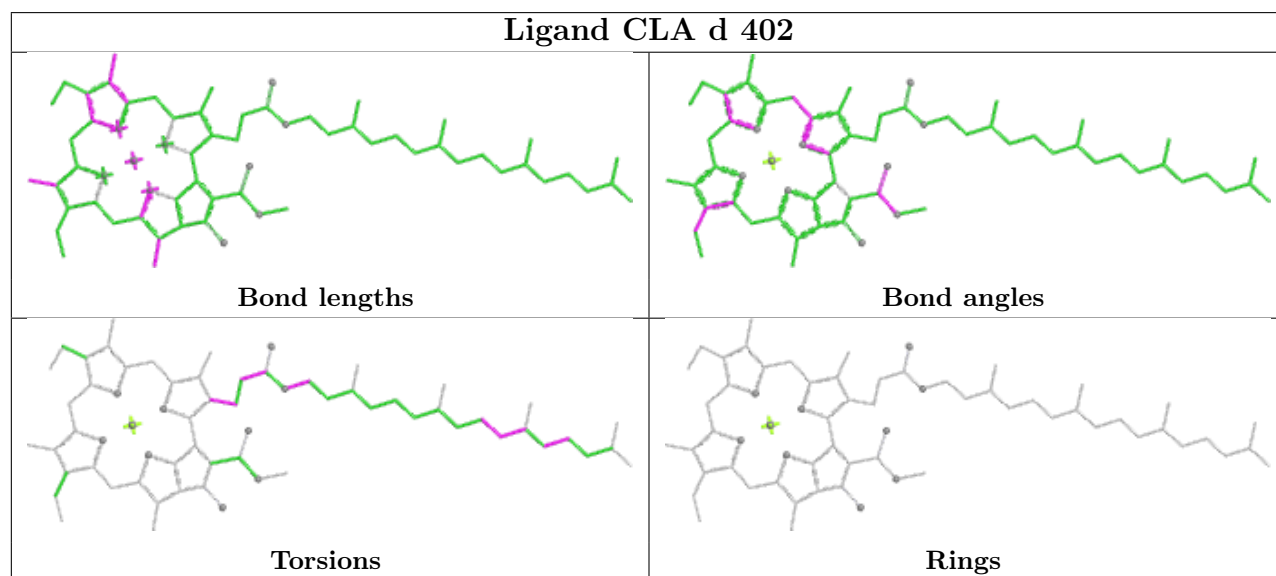
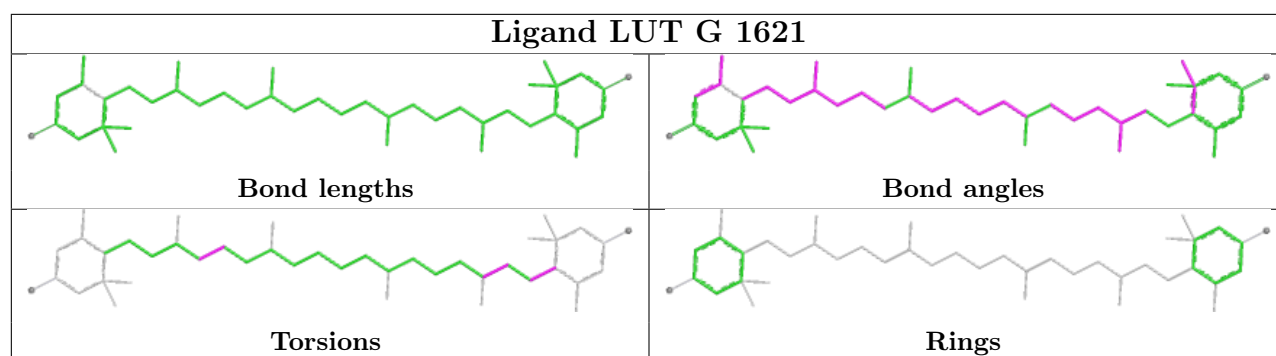
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA s 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

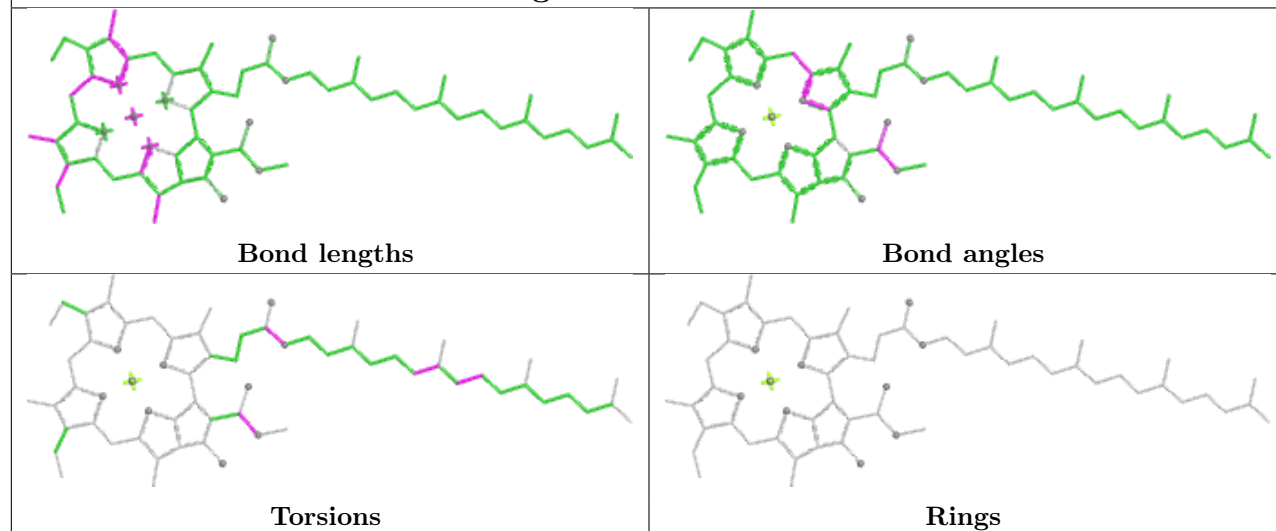
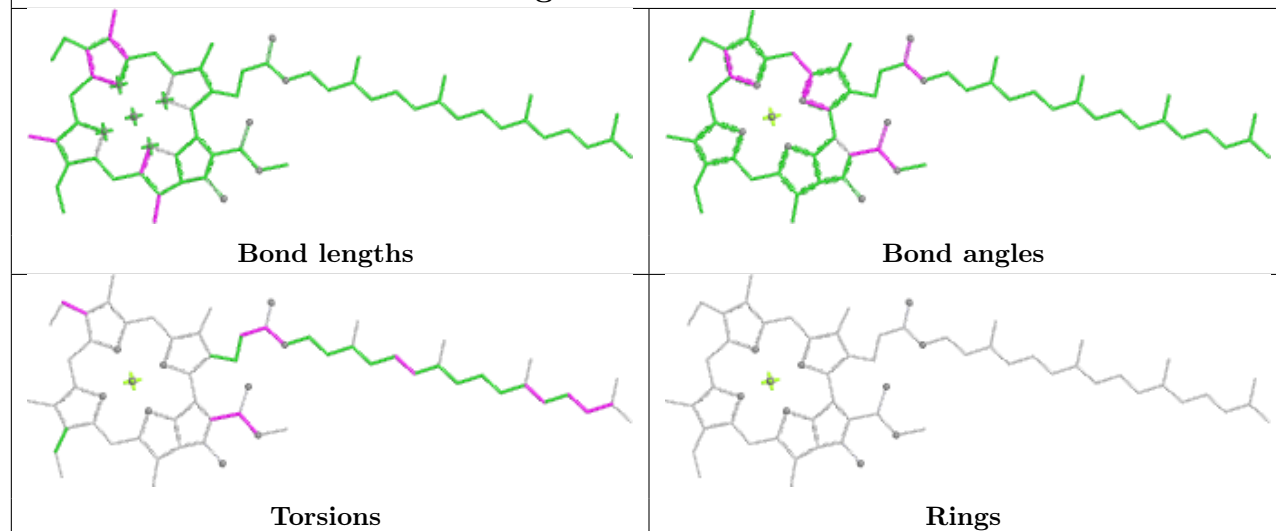
Ligand CLA R 610

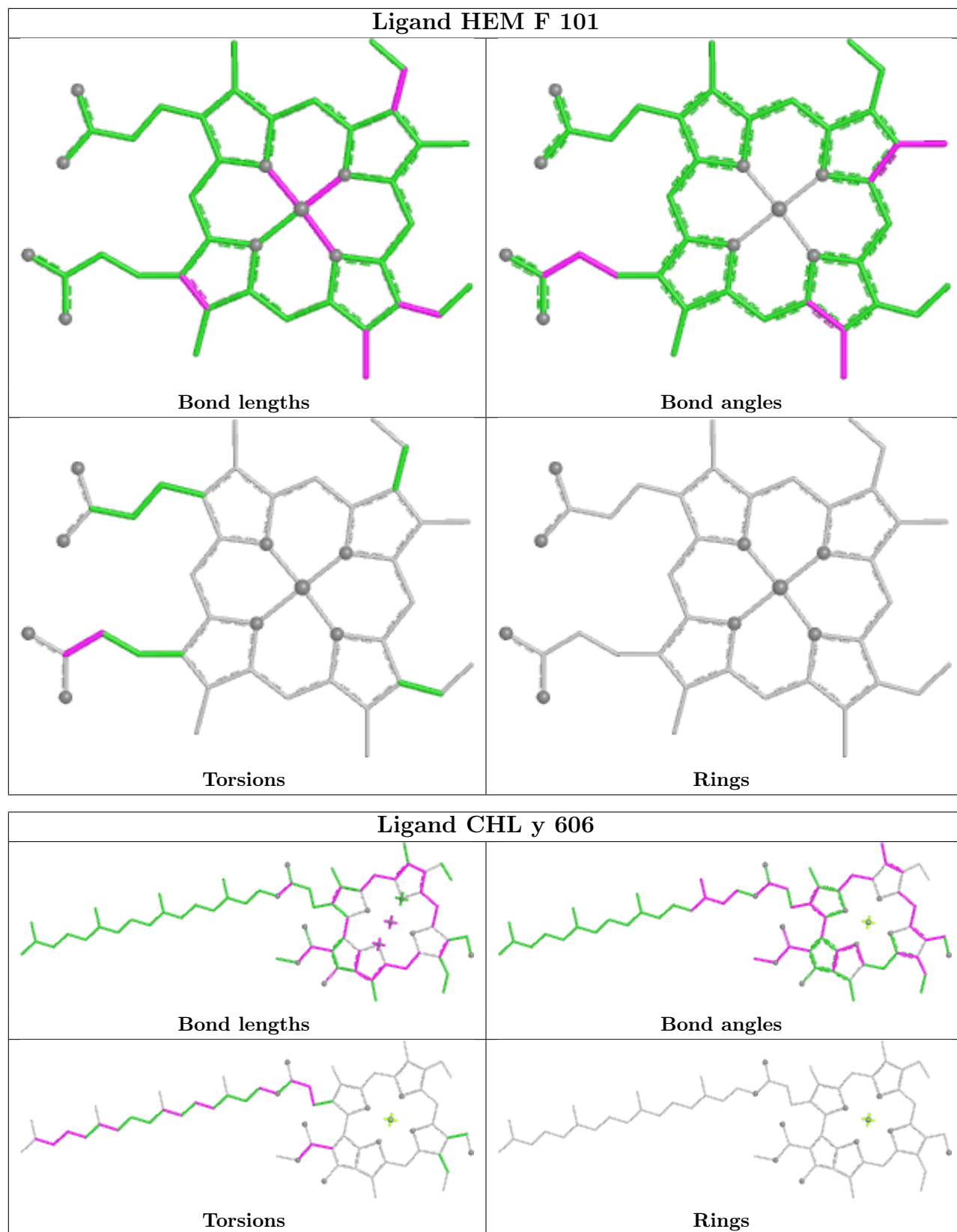


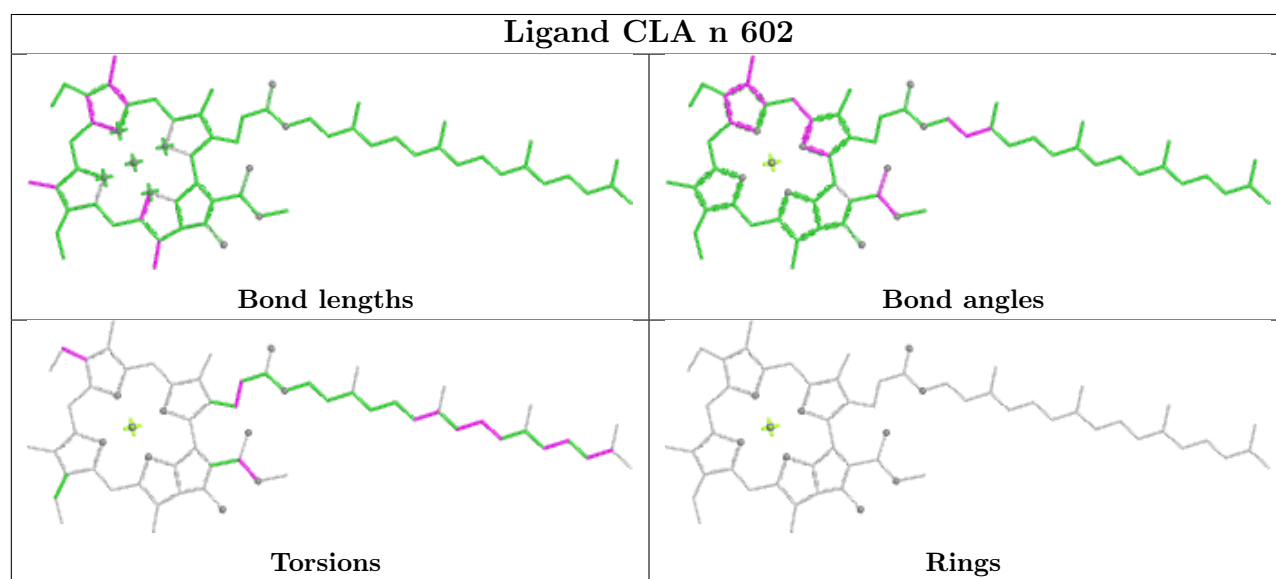
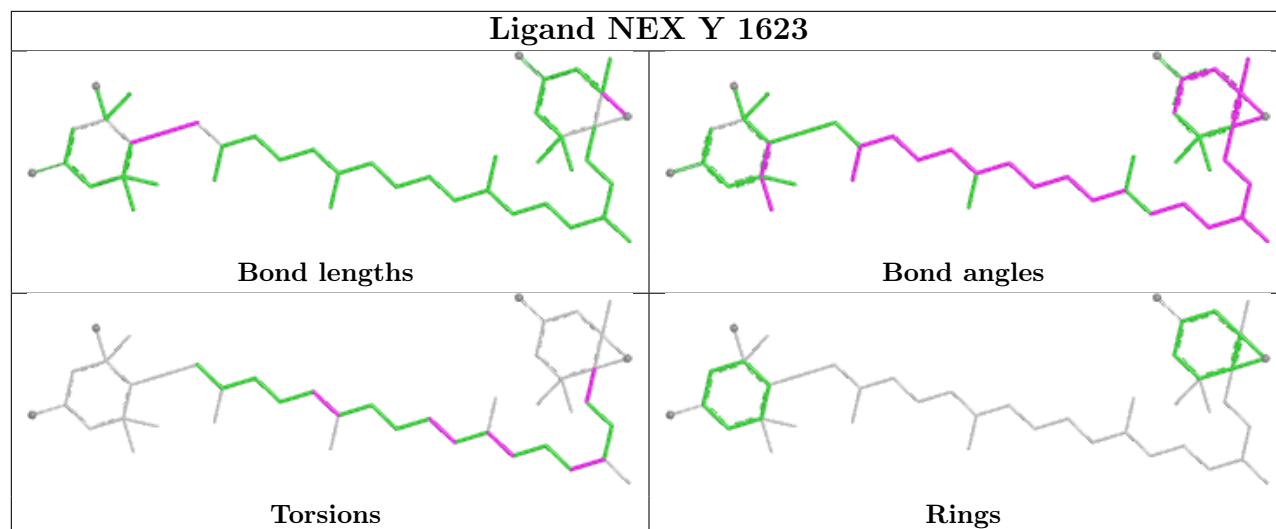
Ligand BCR a 411

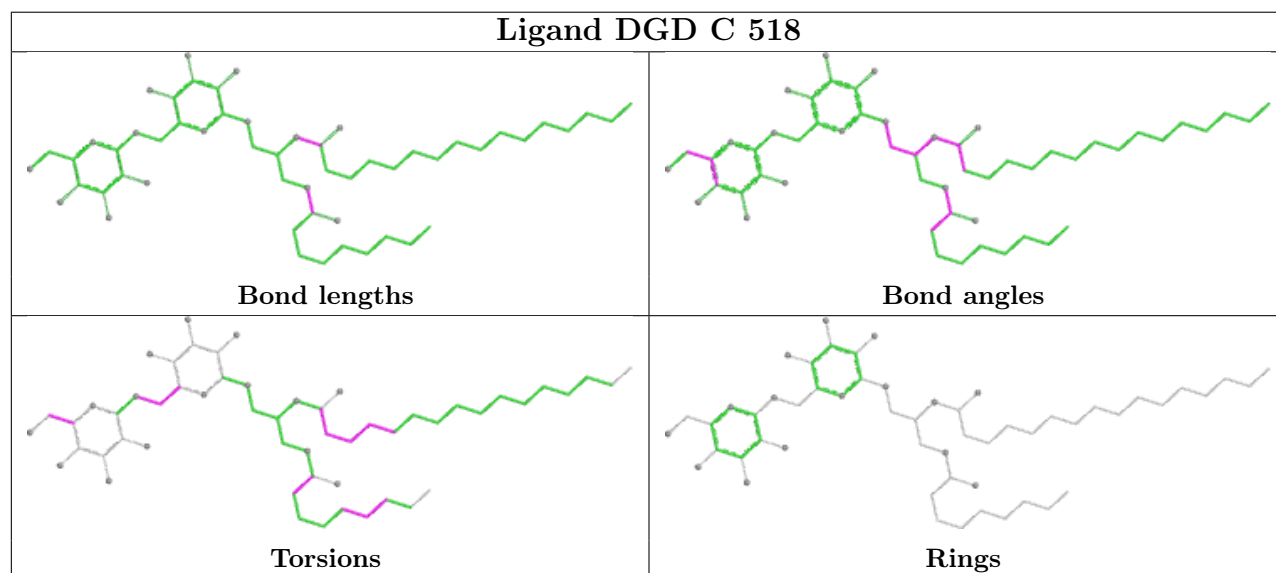
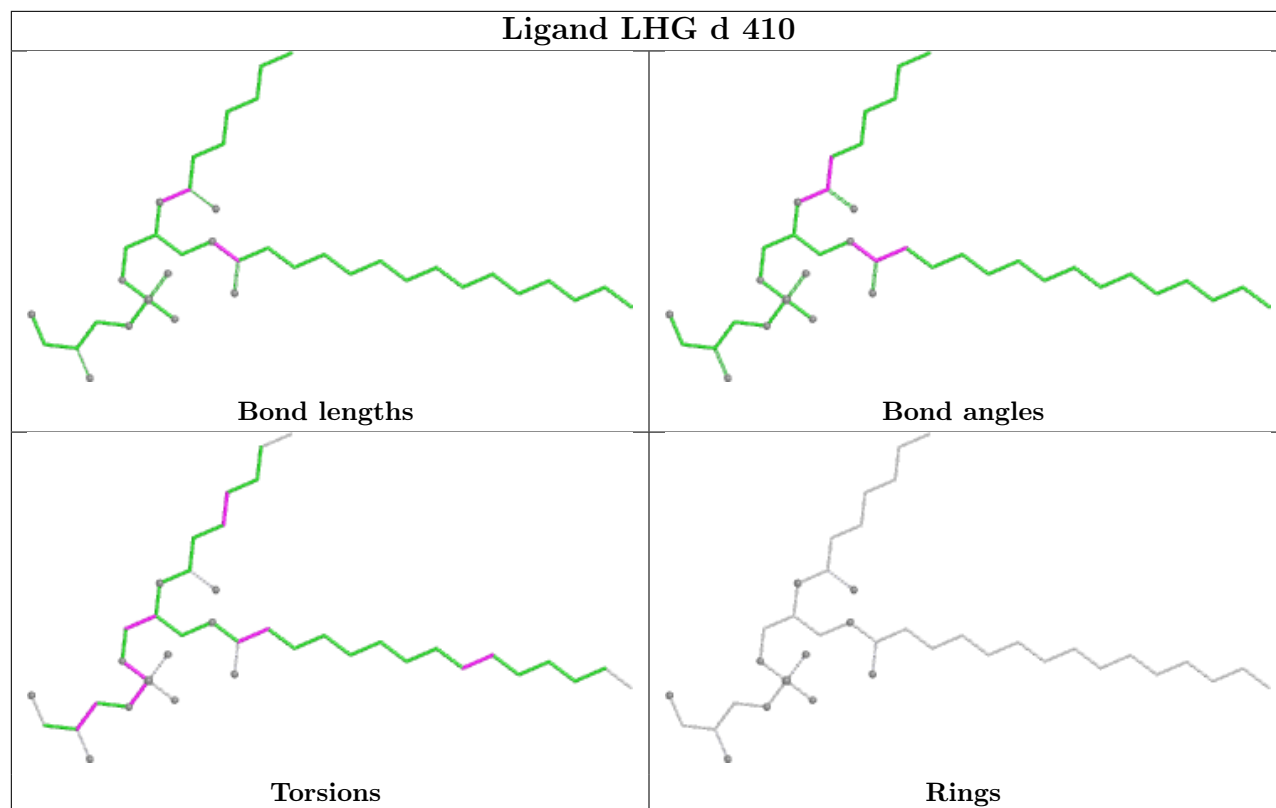


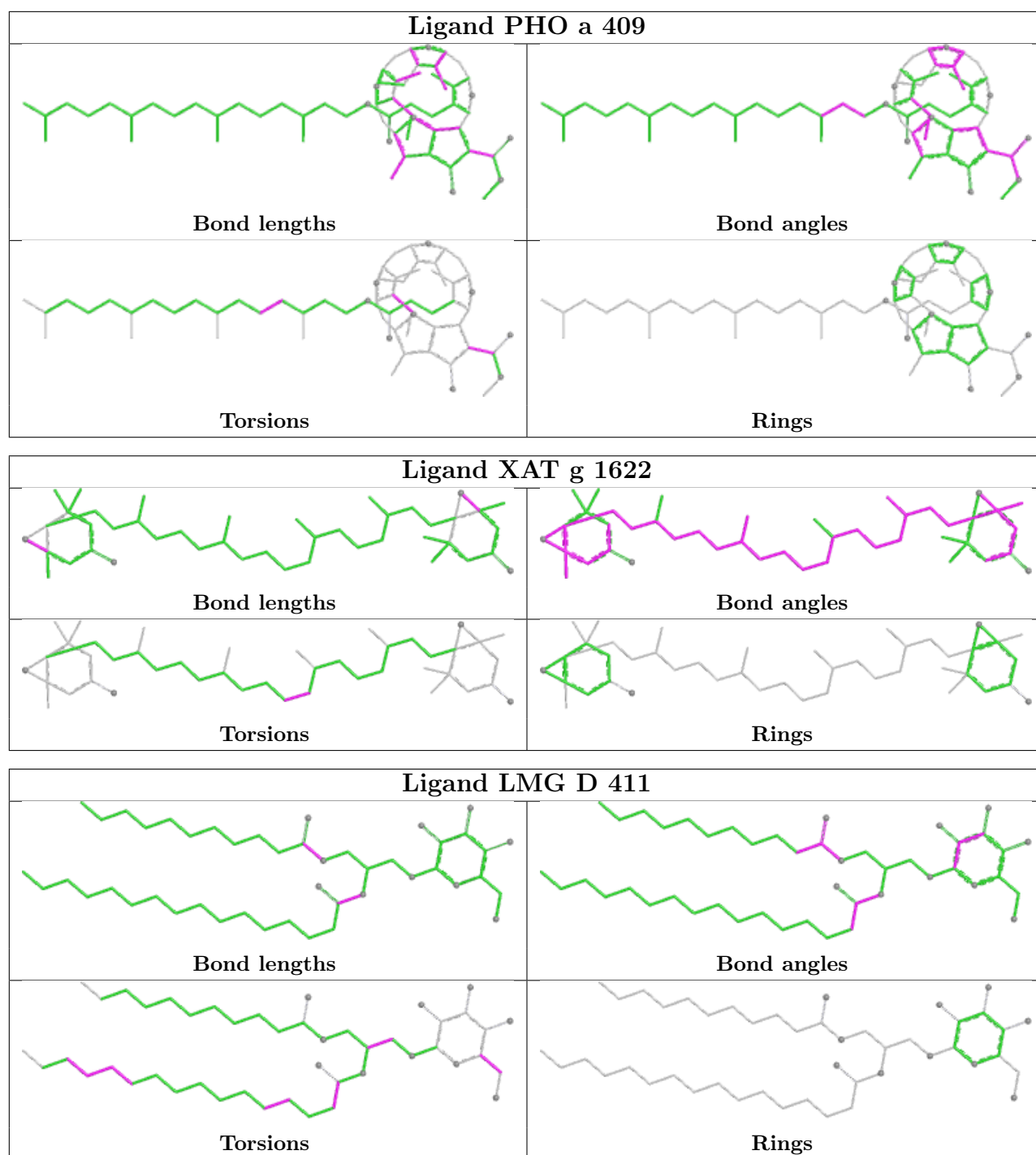


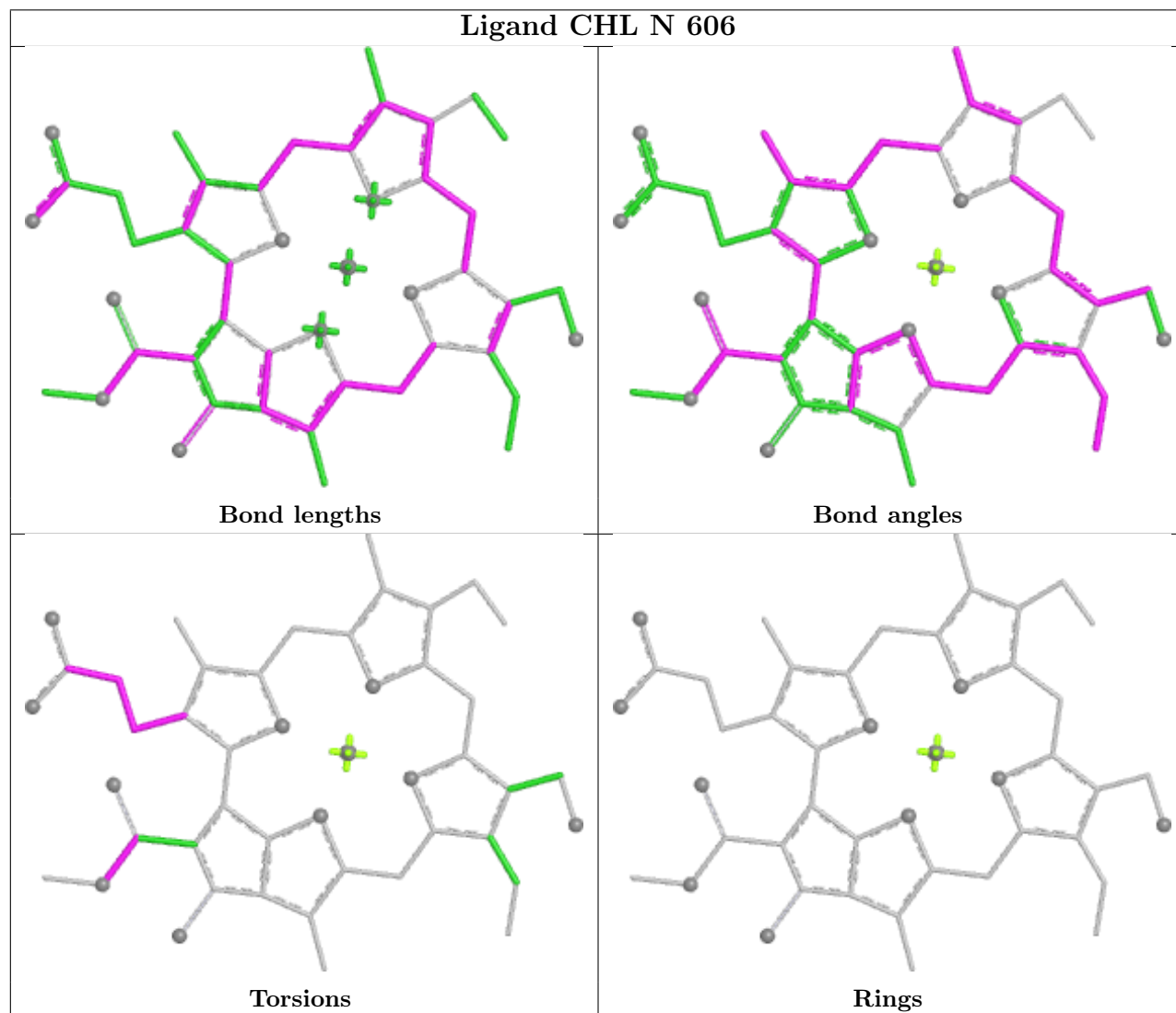
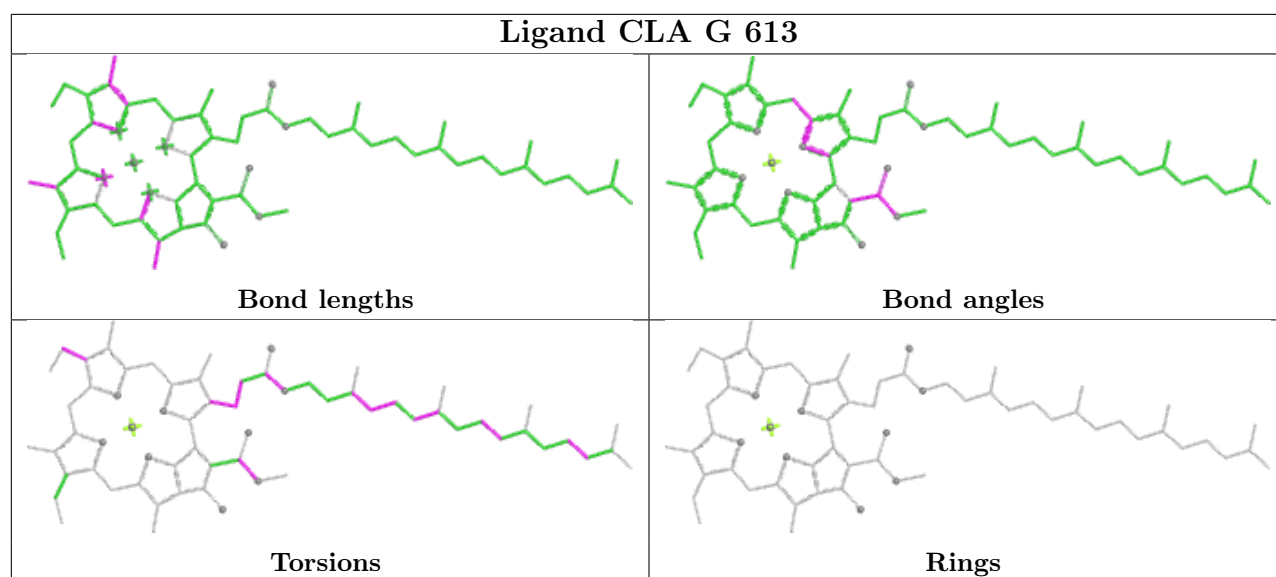
Ligand CLA C 502**Ligand CLA b 602**

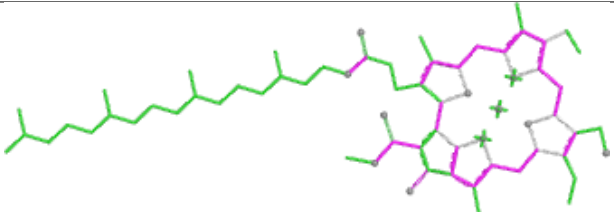
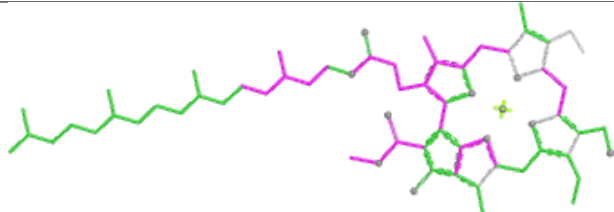
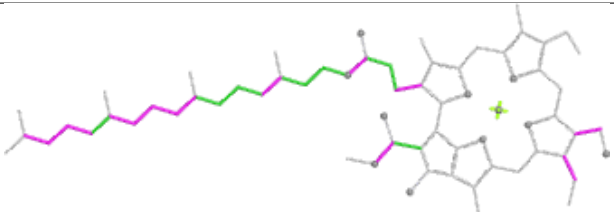
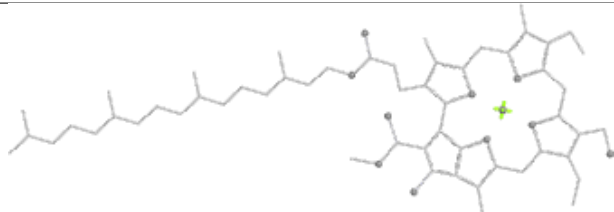


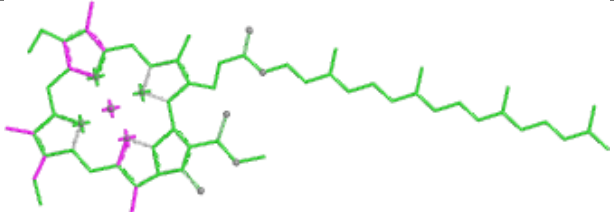
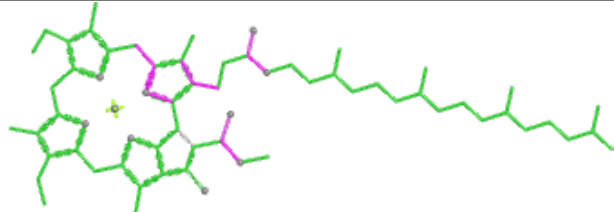
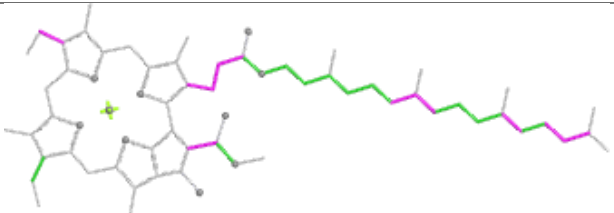
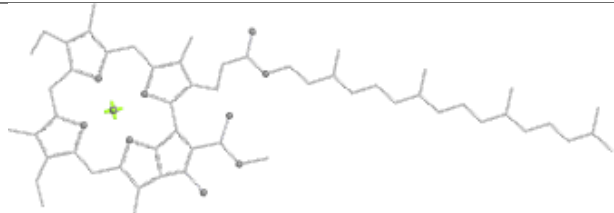


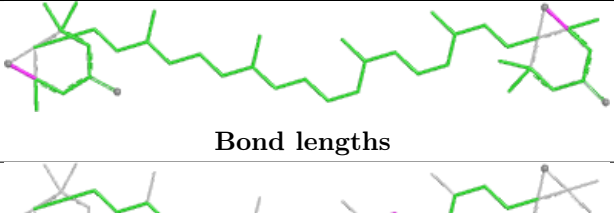
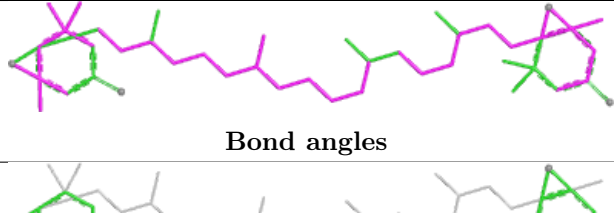
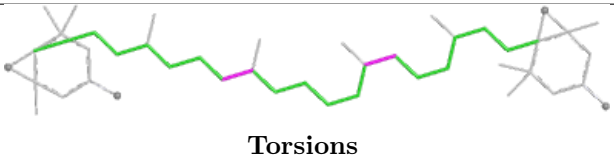
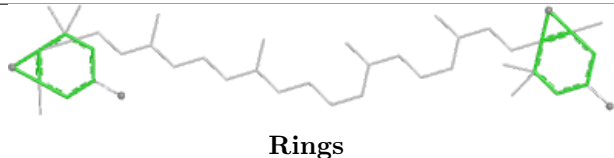


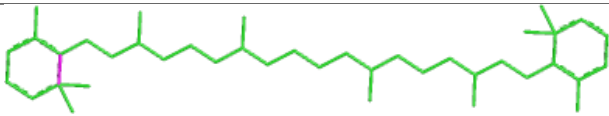
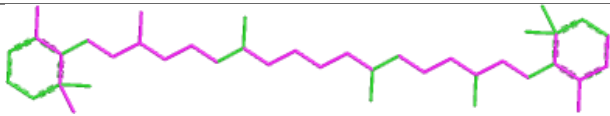
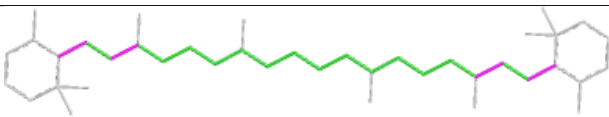
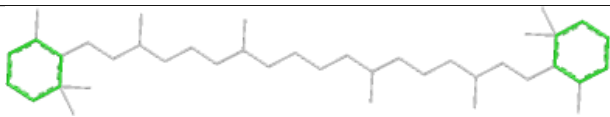


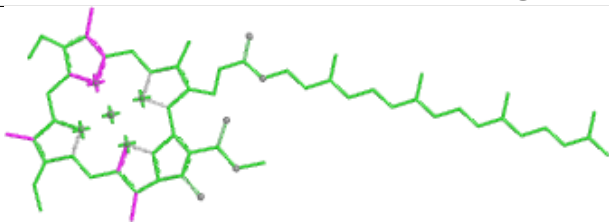
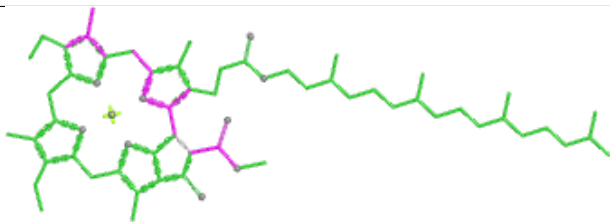
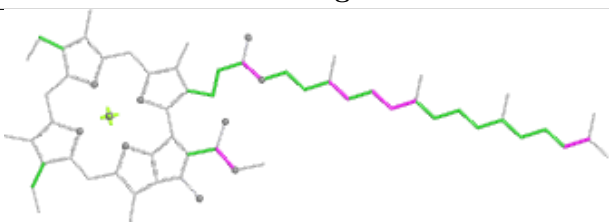
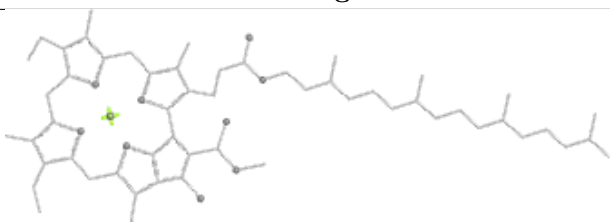


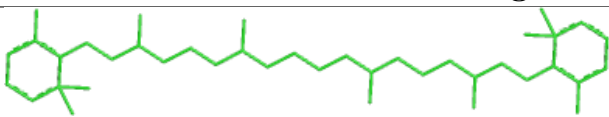
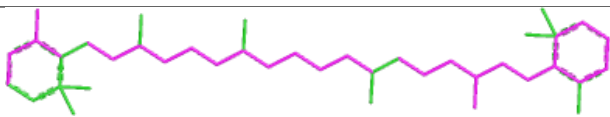
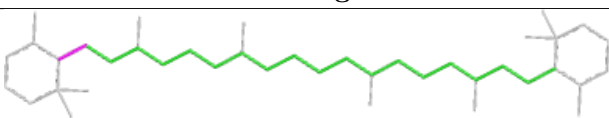
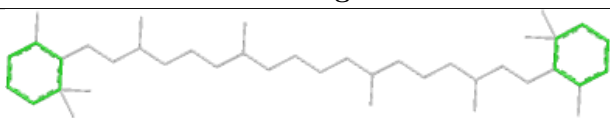
Ligand CHL N 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

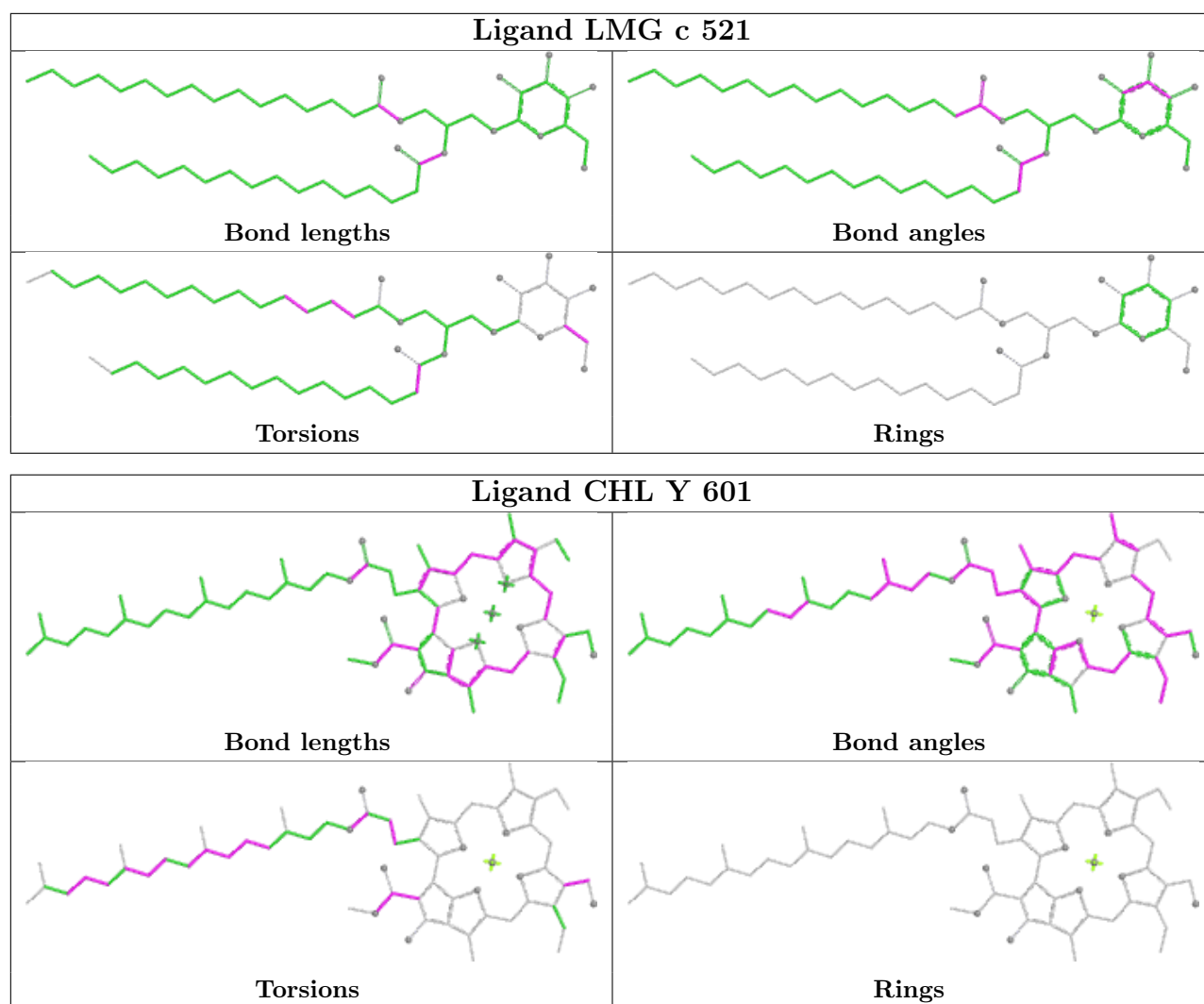
Ligand CLA N 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT y 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

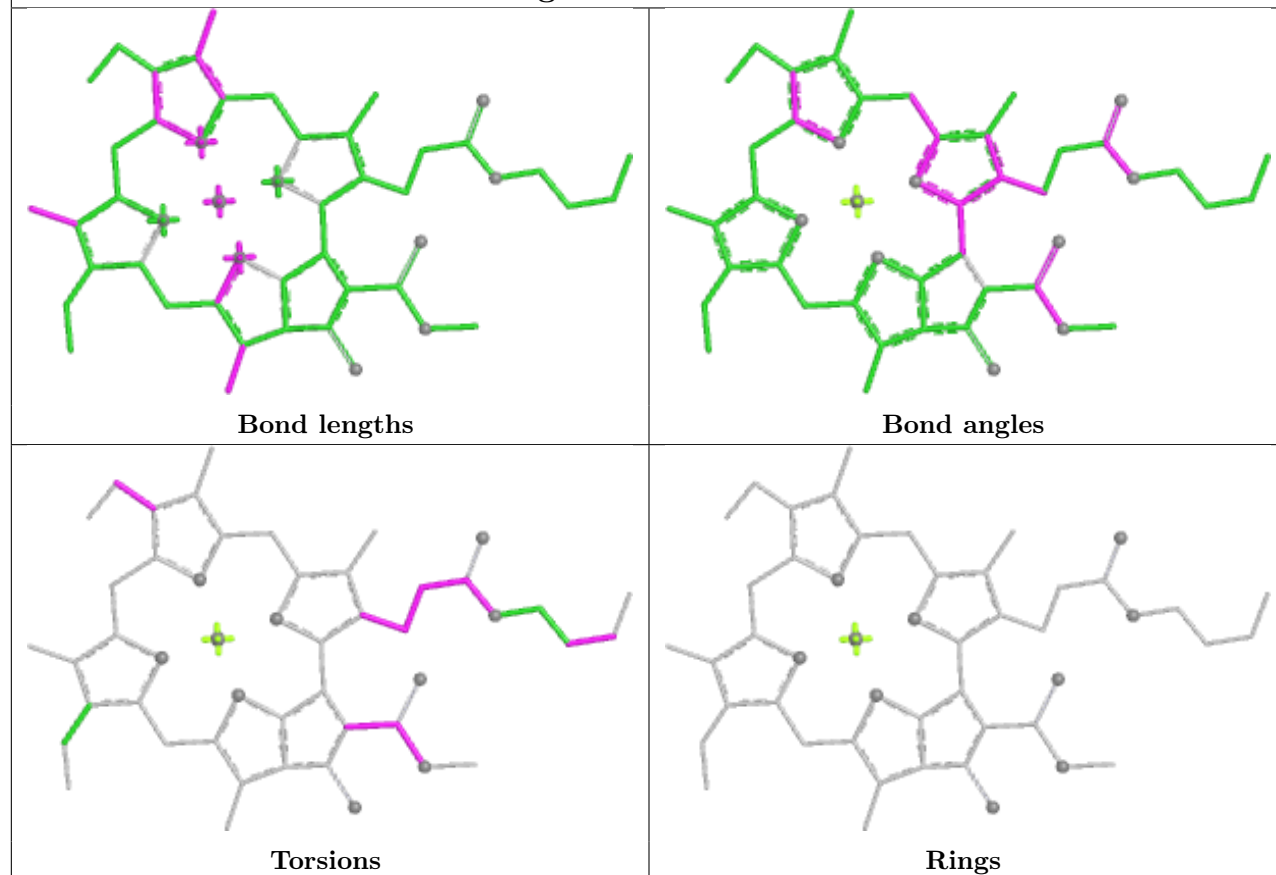
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

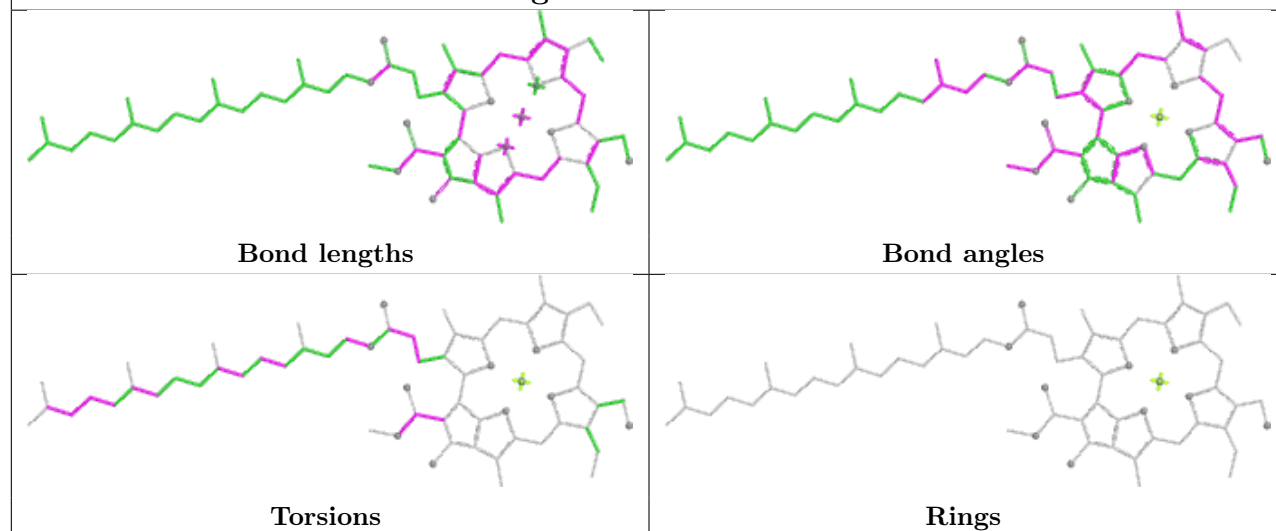
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

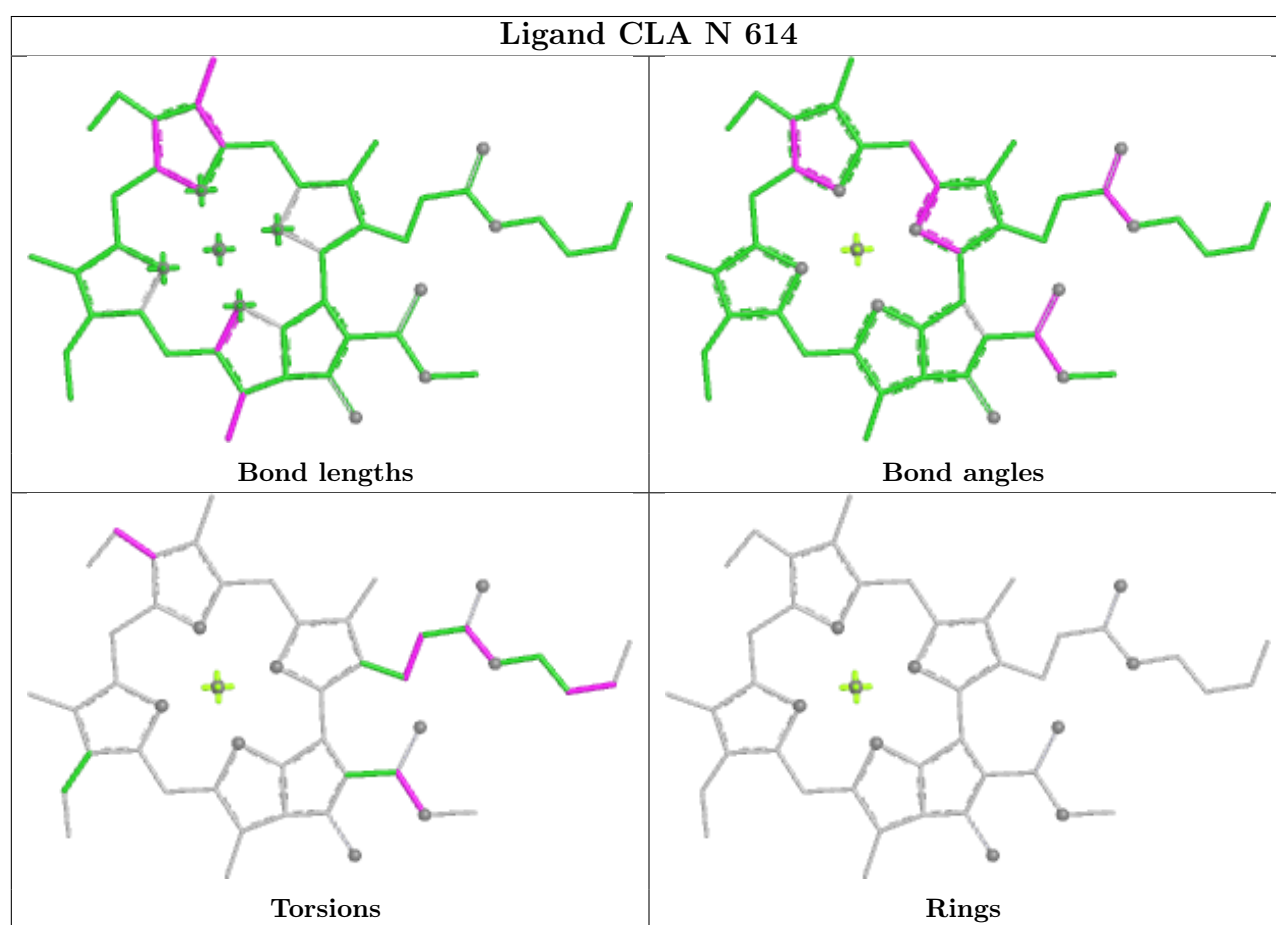
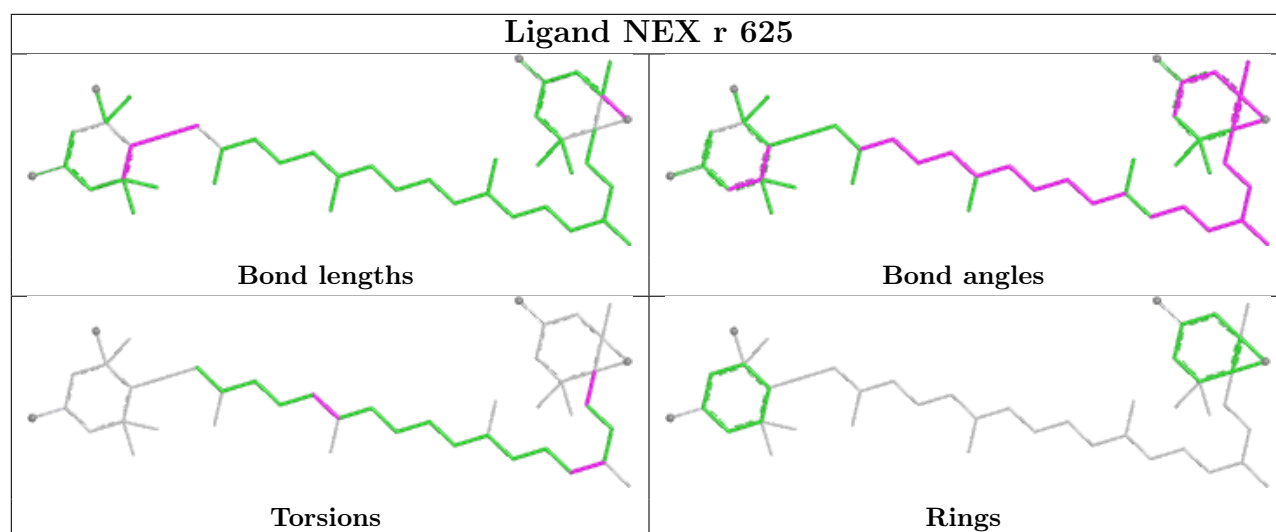


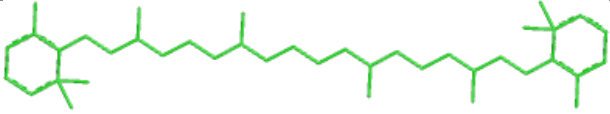
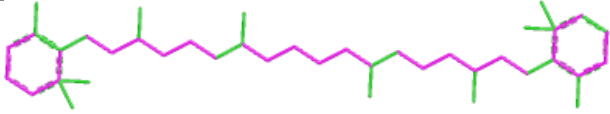
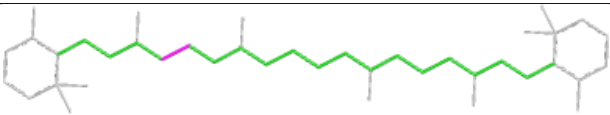
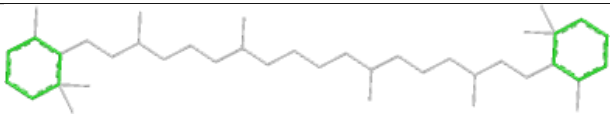
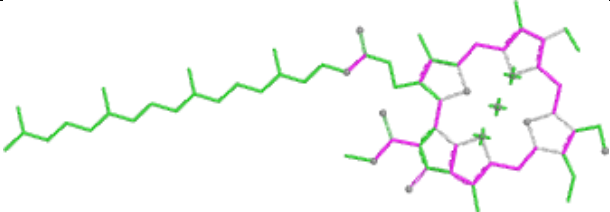
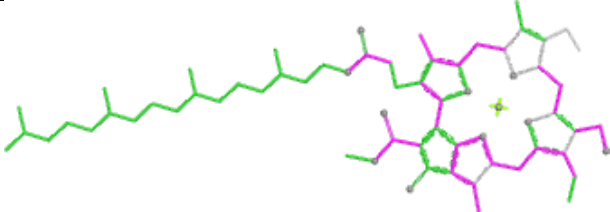
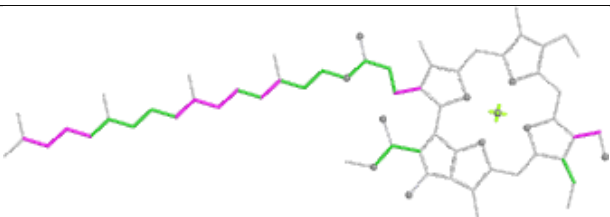
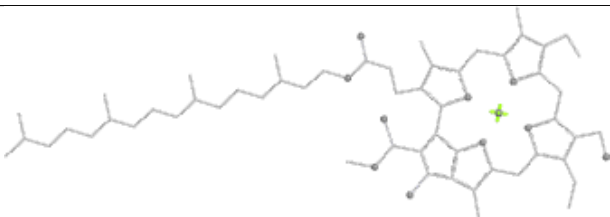
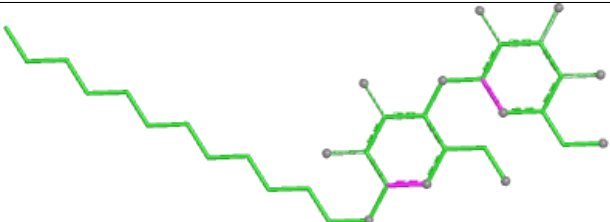
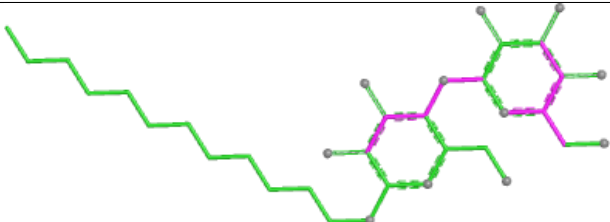
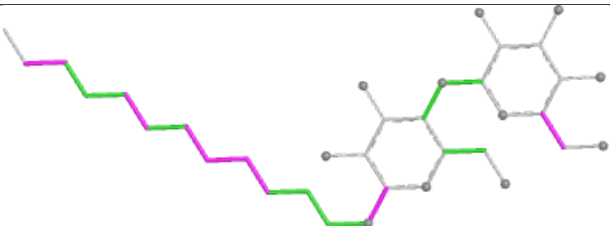
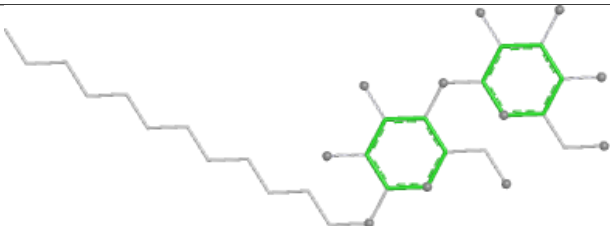
Ligand CLA r 603

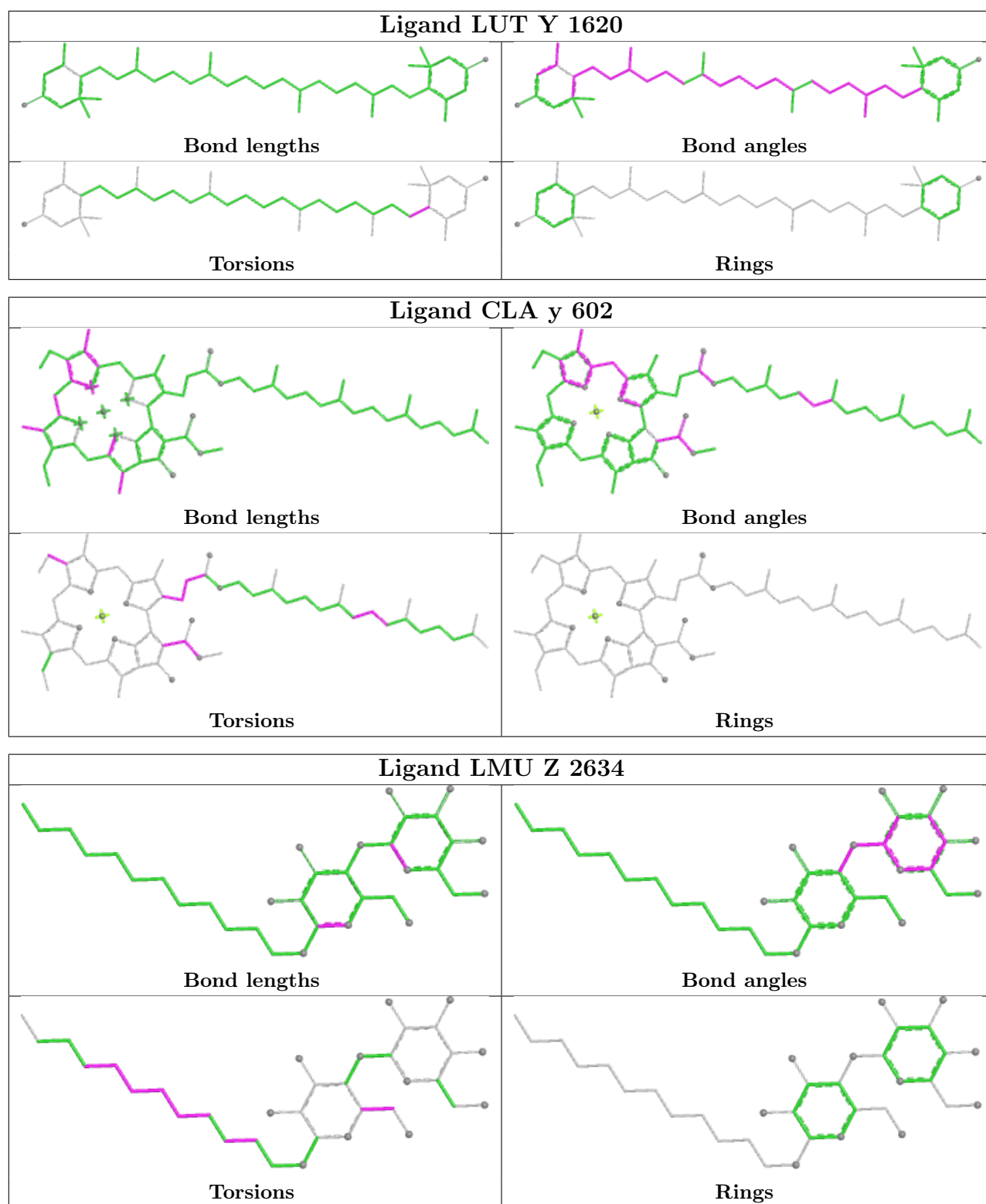


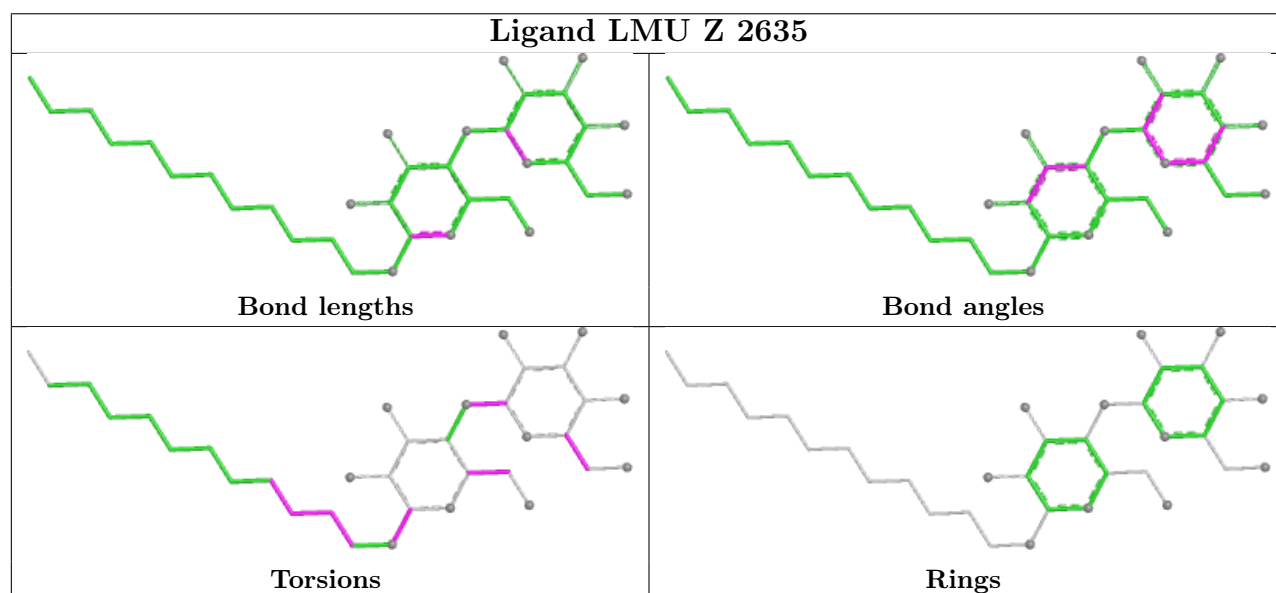
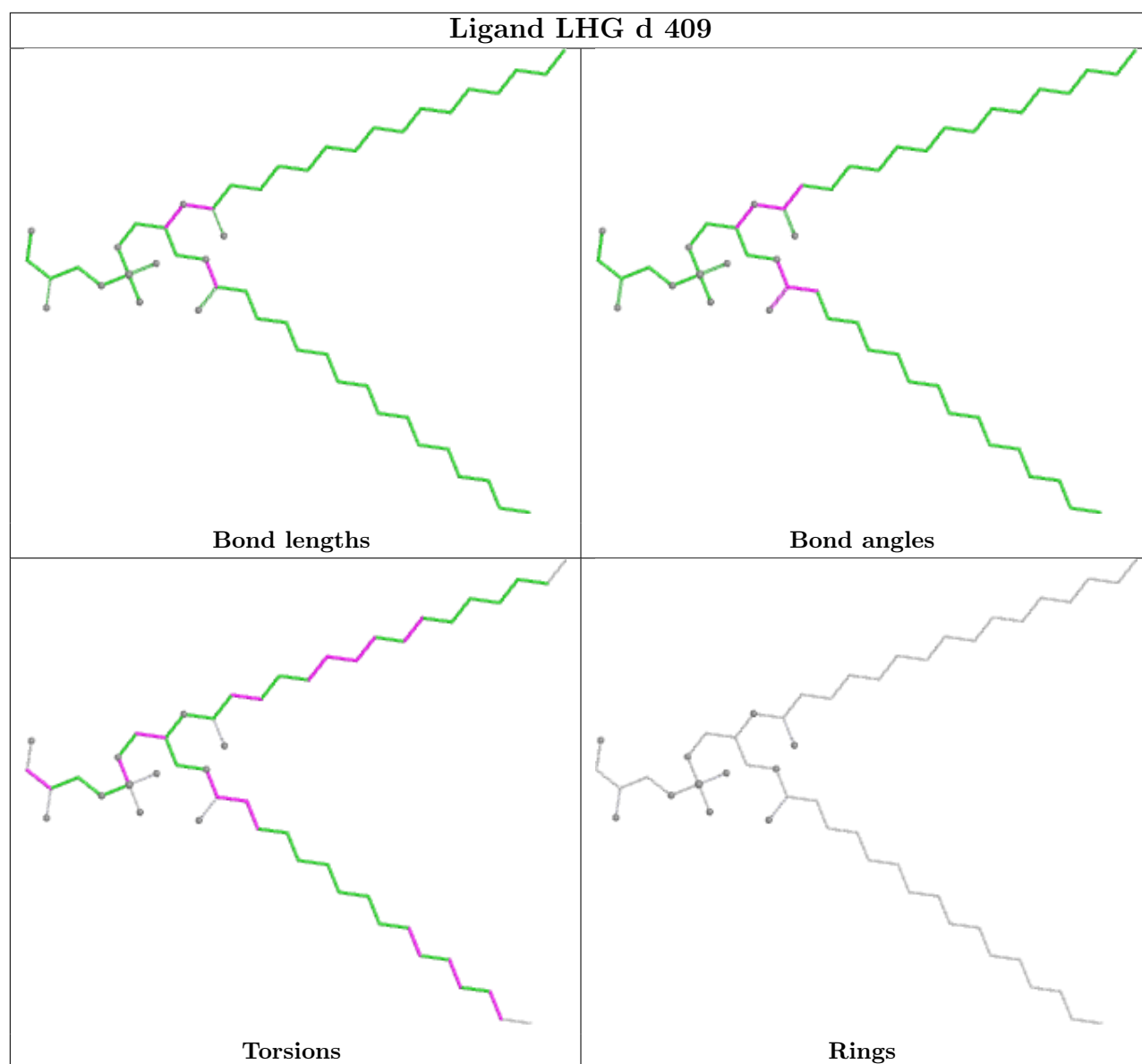
Ligand CHL Y 606

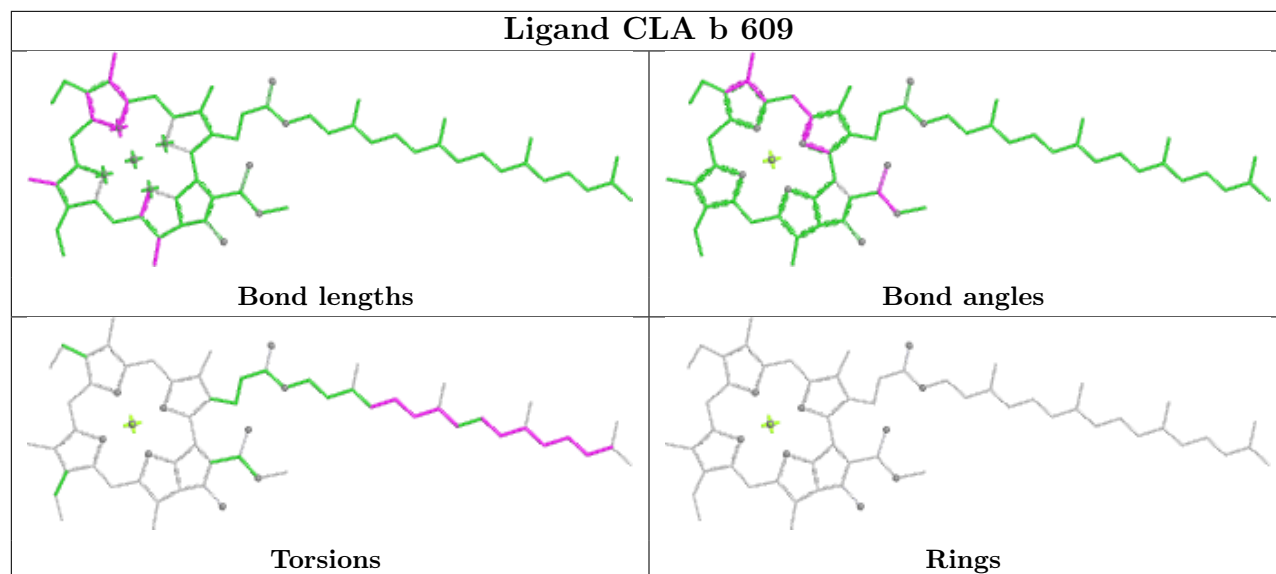
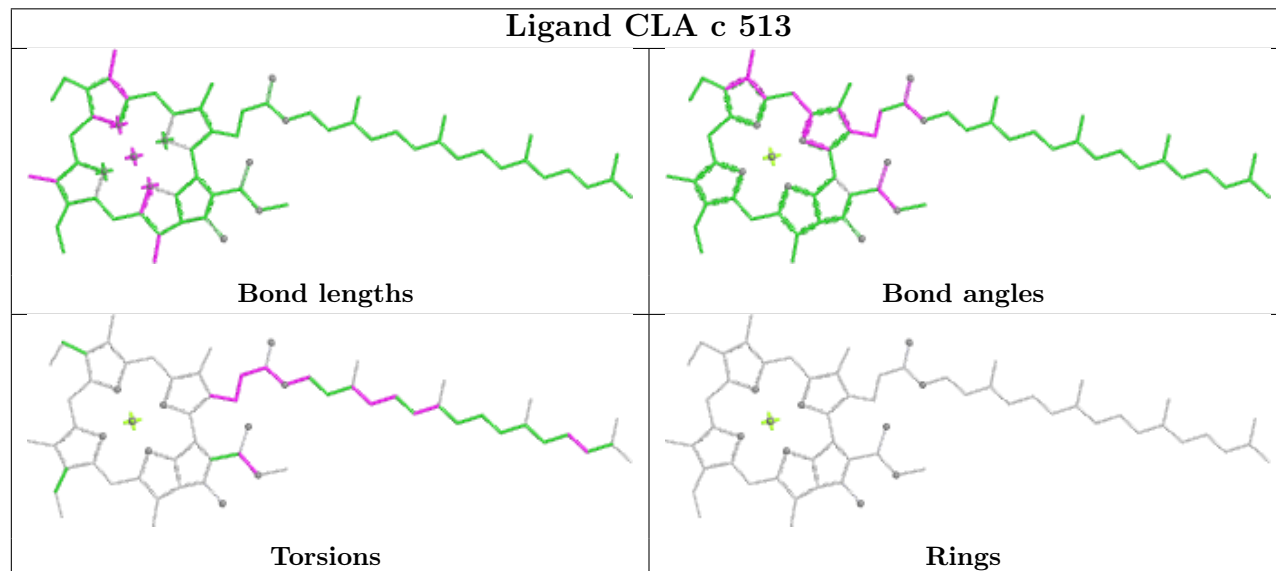




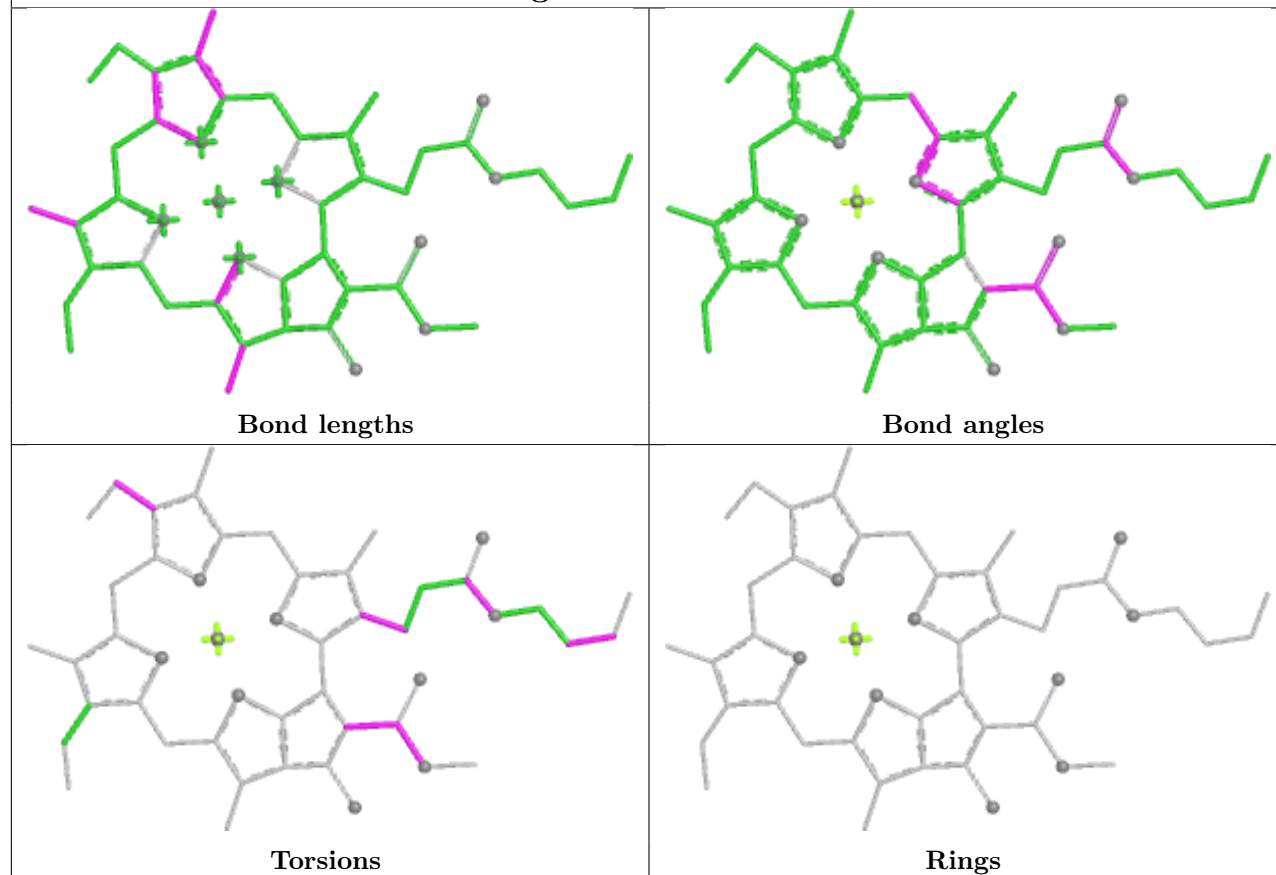
Ligand BCR c 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL n 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMU Y 2632	
 Bond lengths	 Bond angles
 Torsions	 Rings



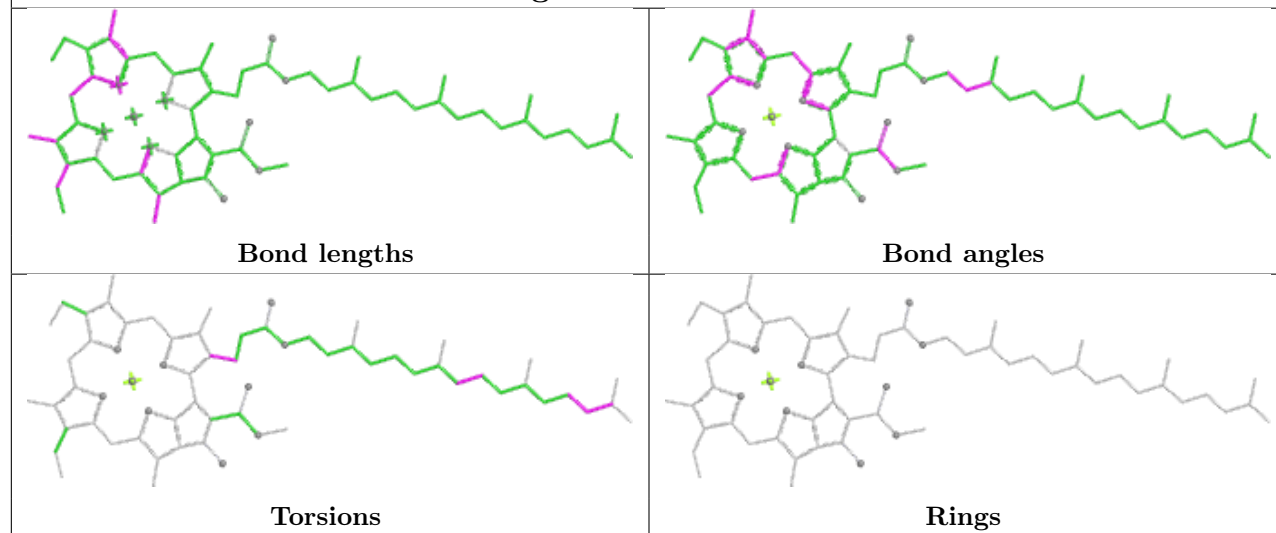


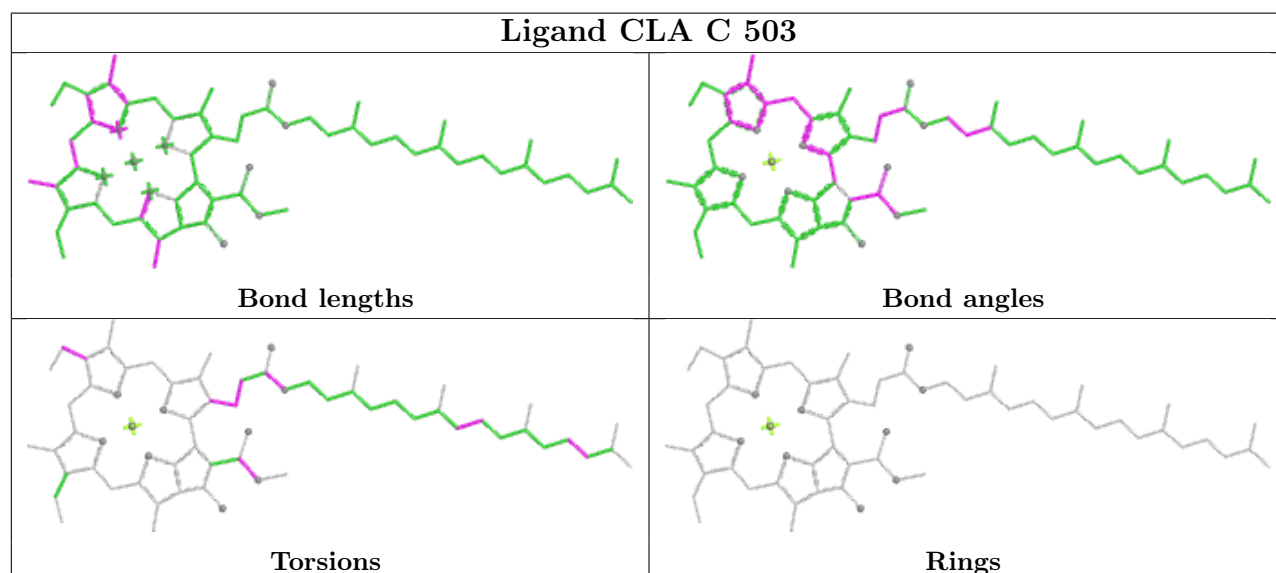
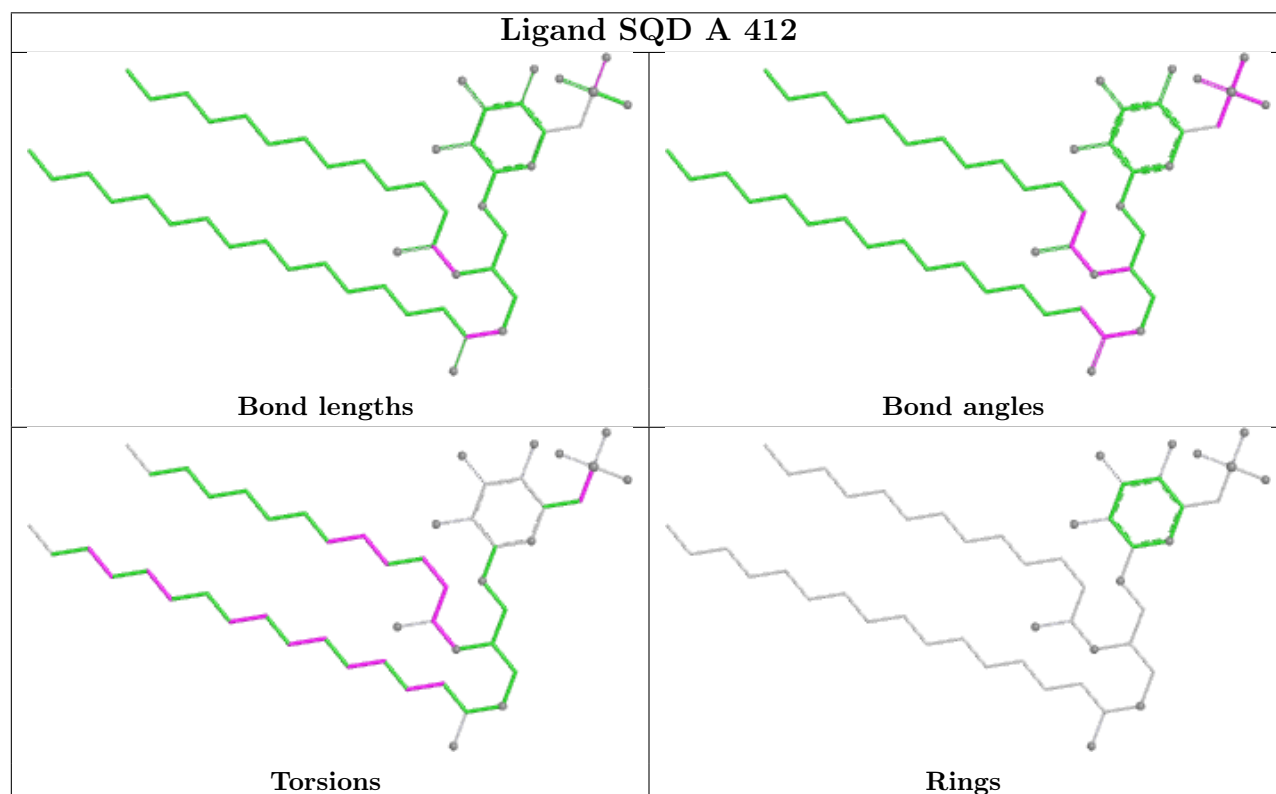
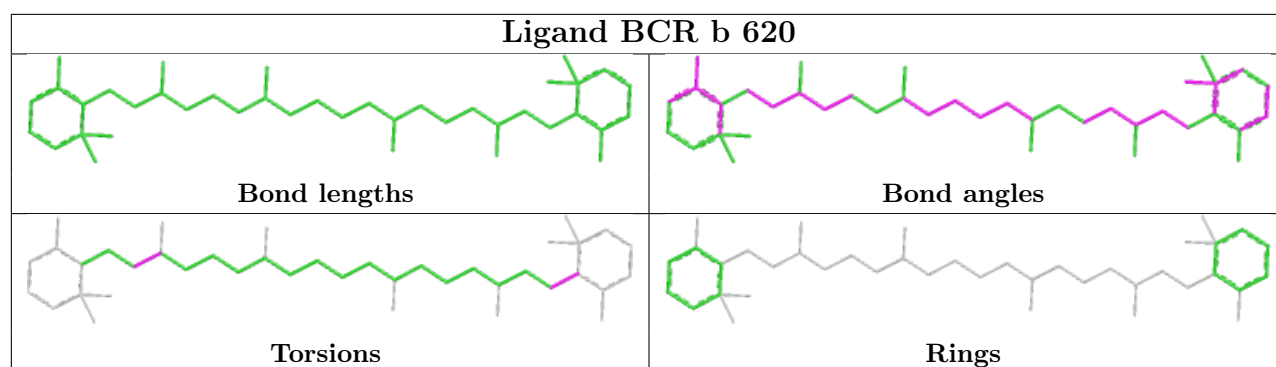
Ligand CLA b 609**Ligand CLA c 513**

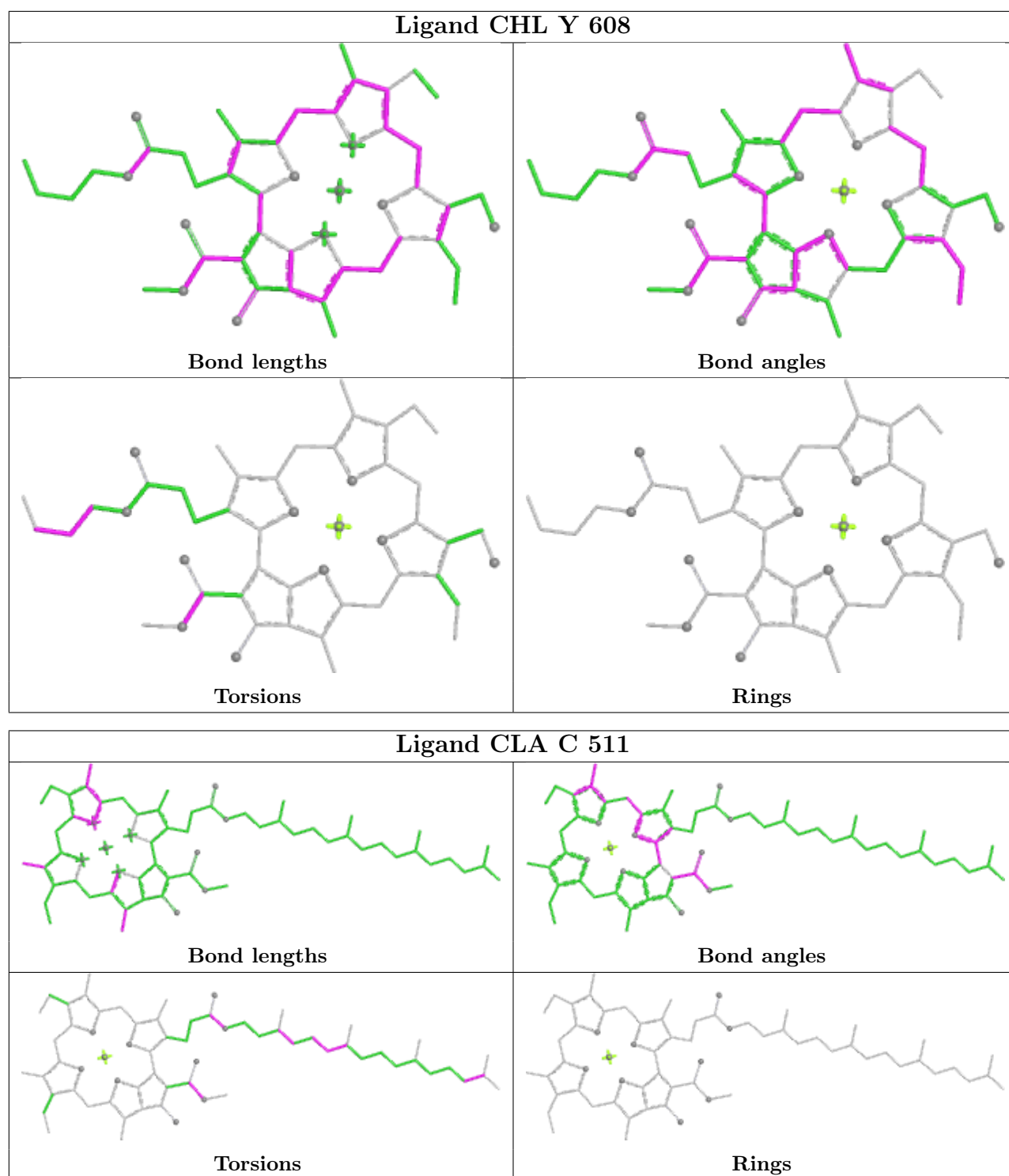
Ligand CLA N 611

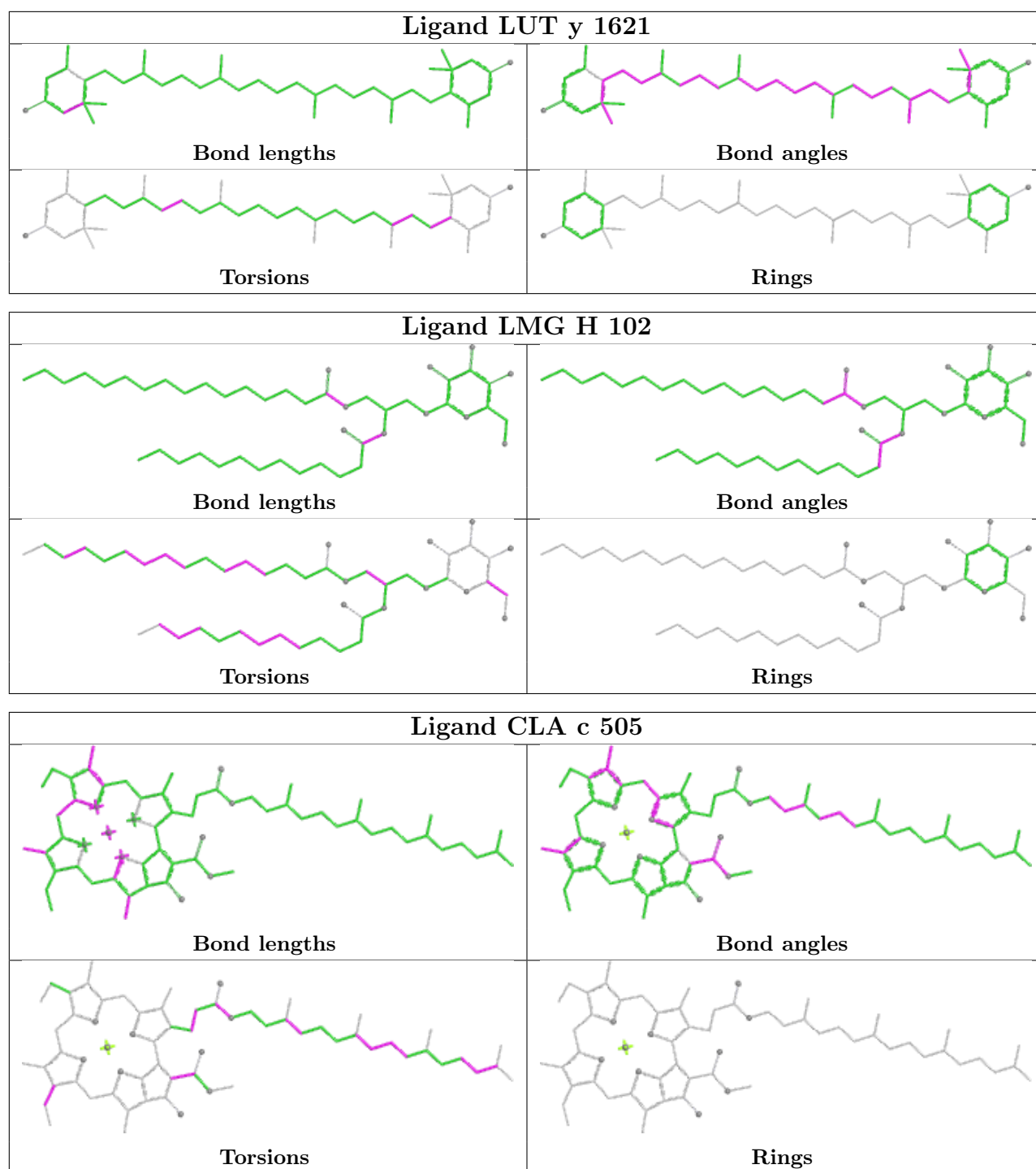


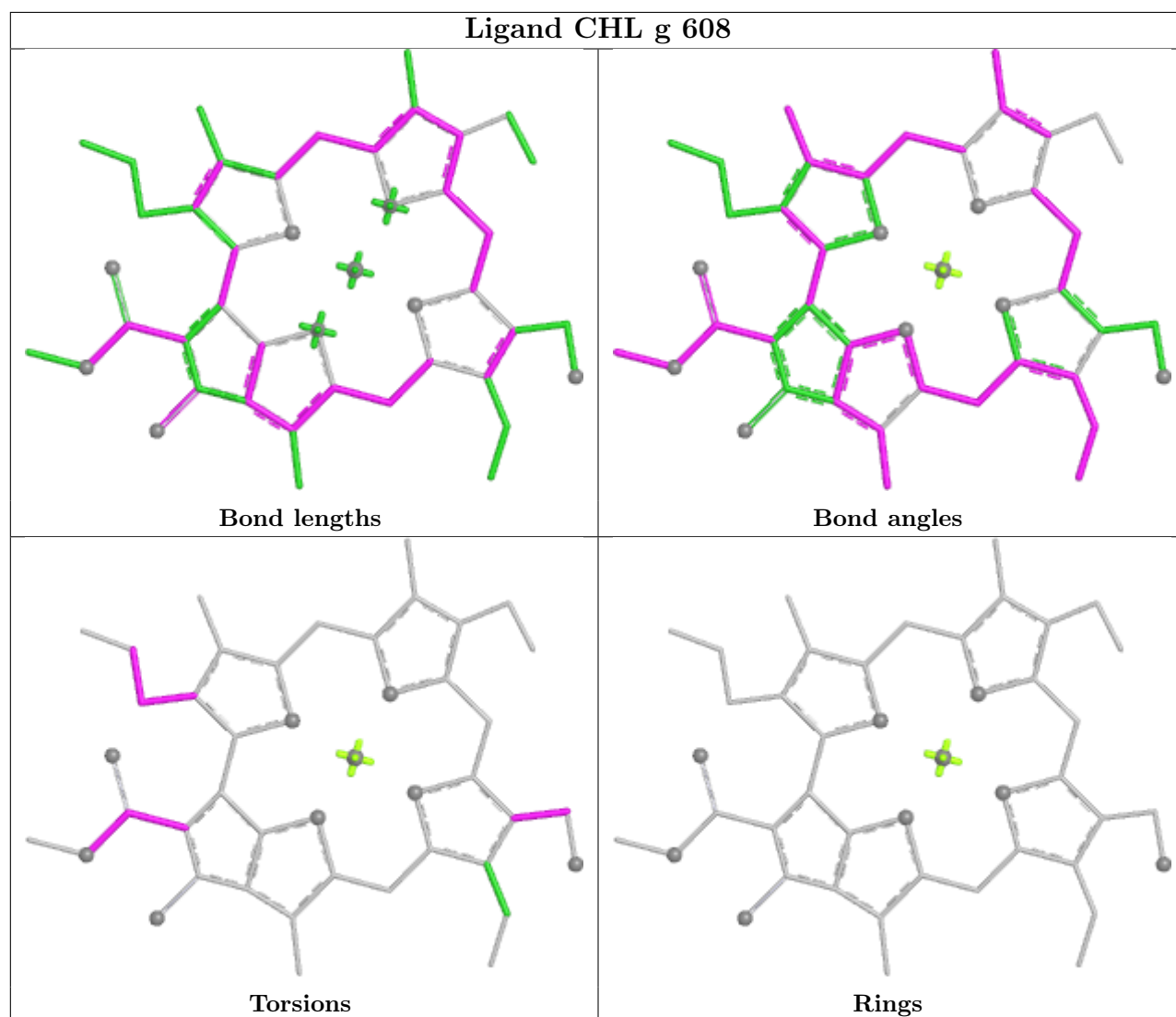
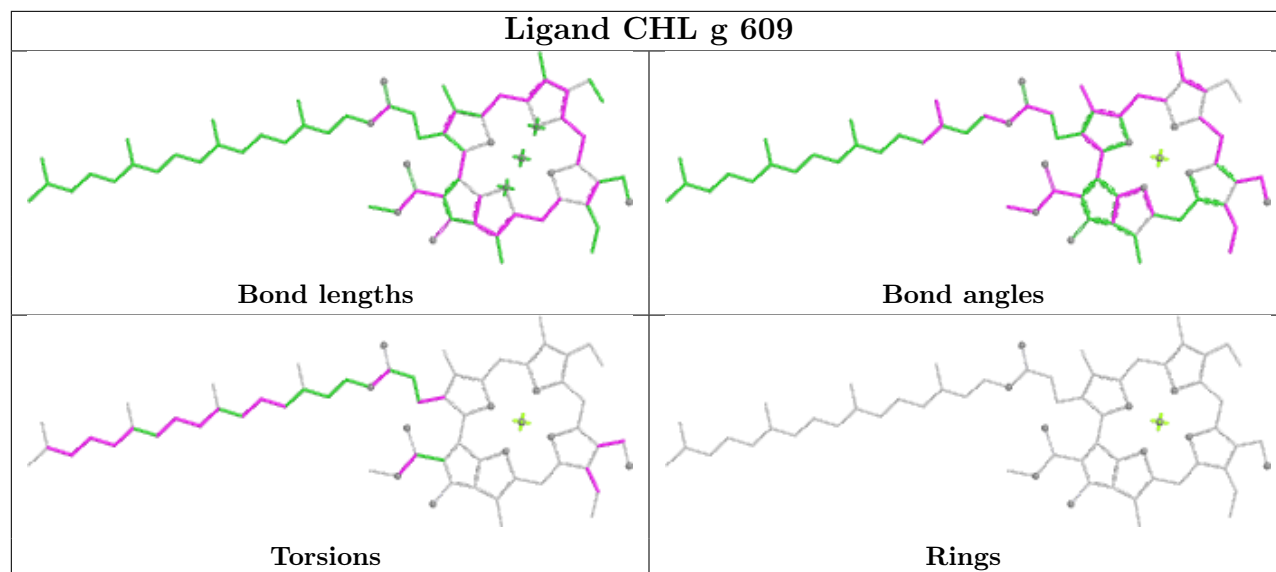
Ligand CLA A 406

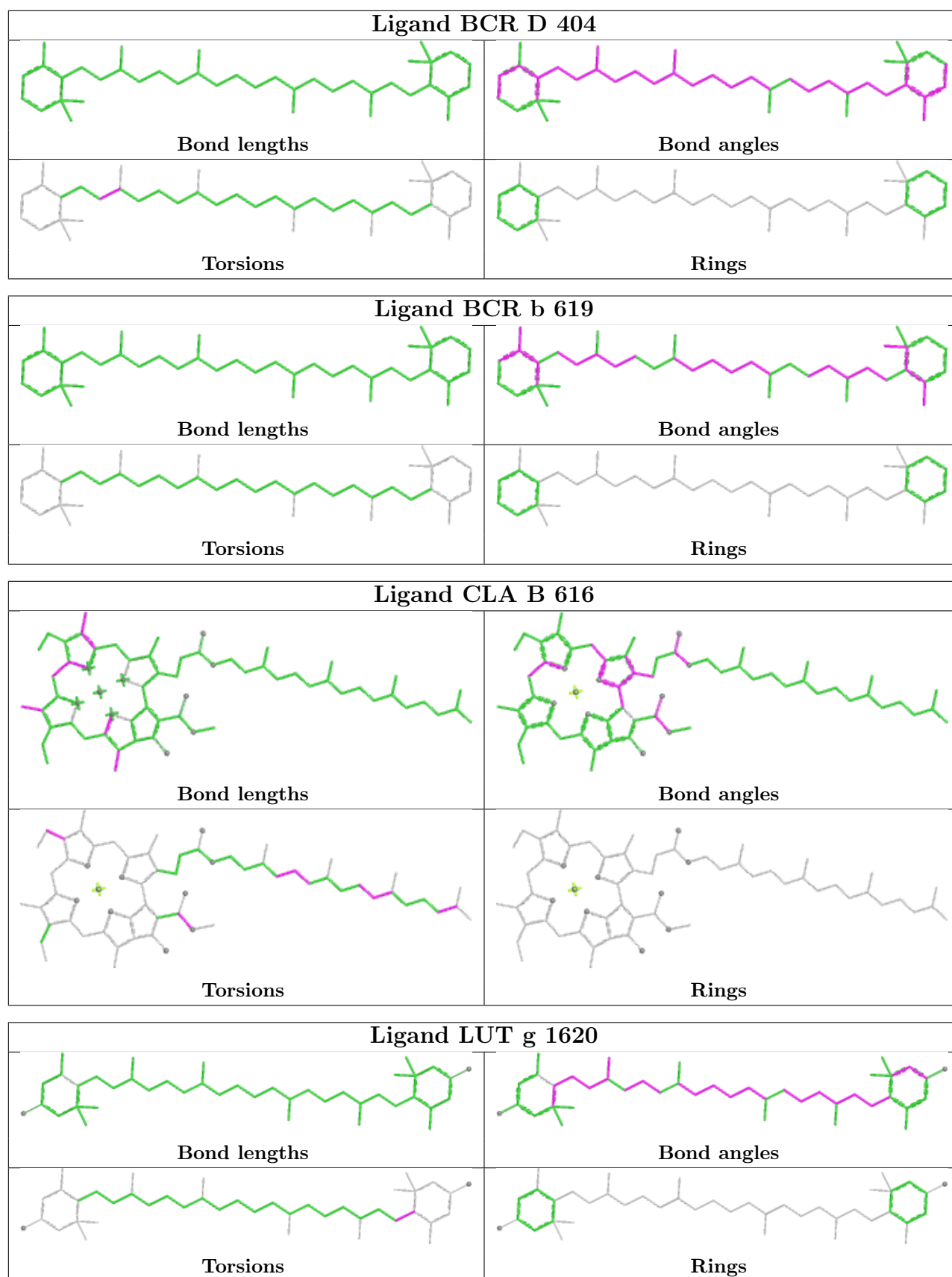


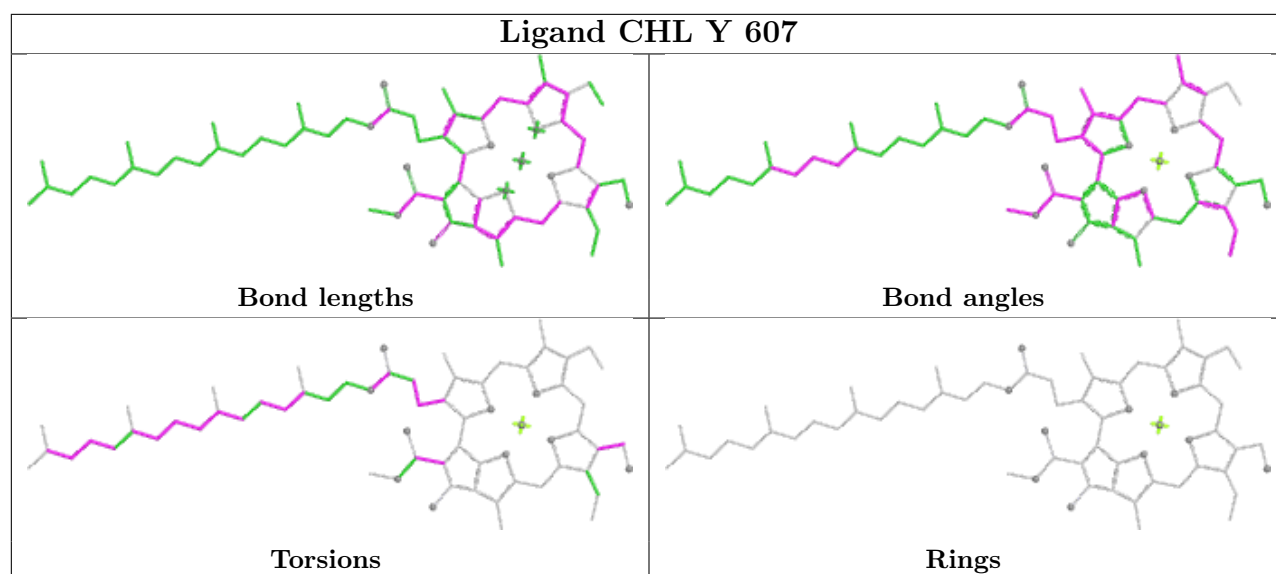
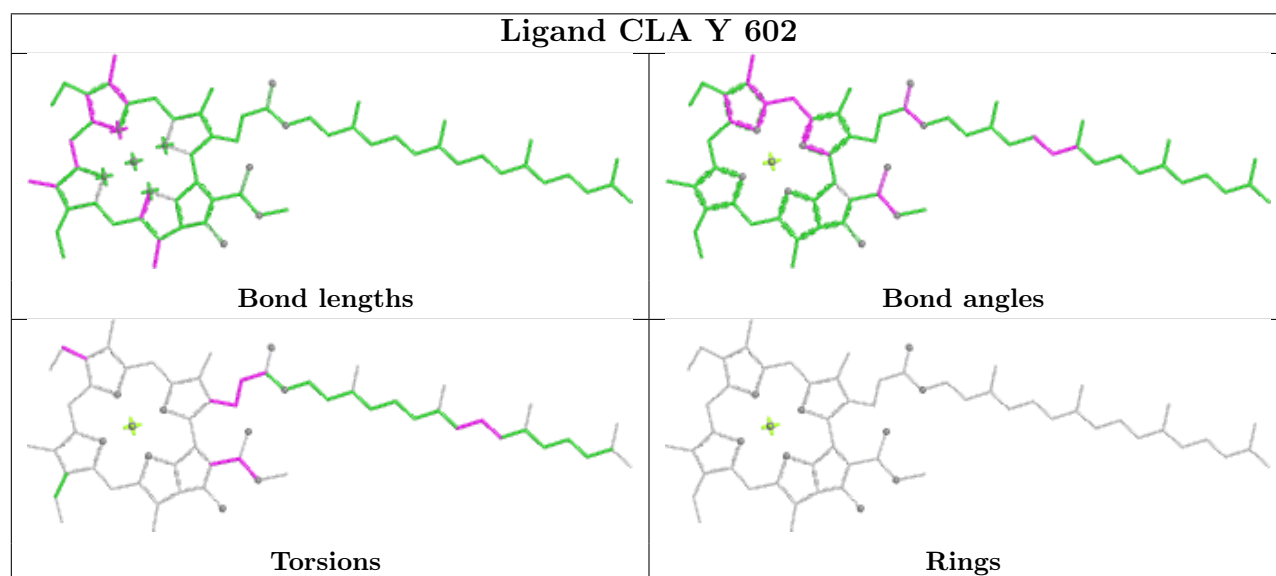
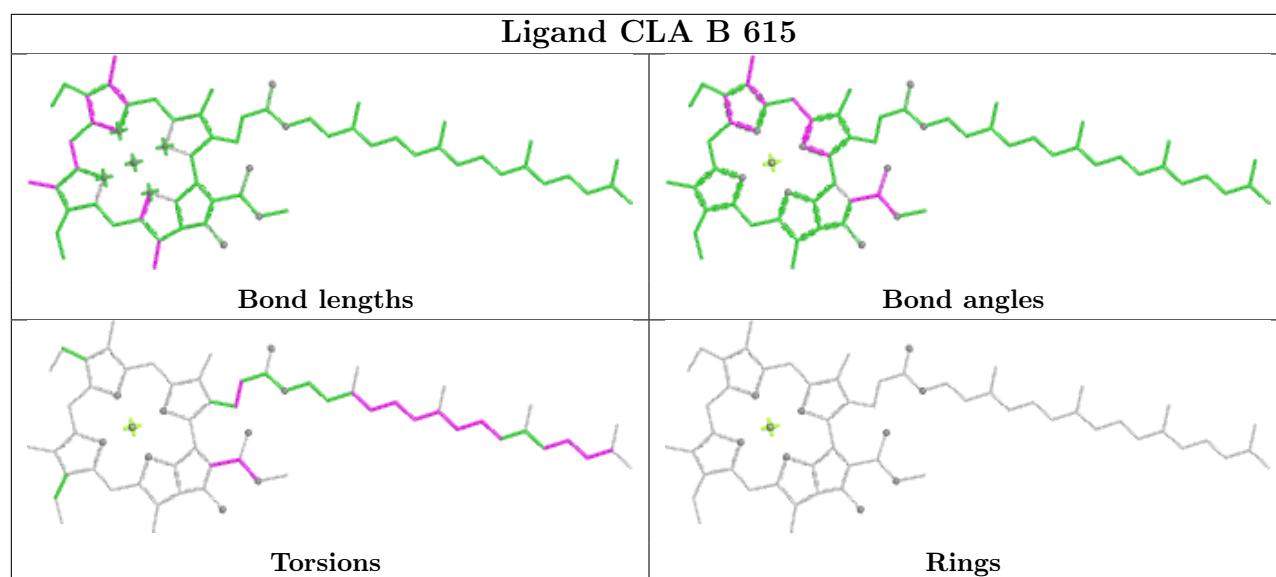


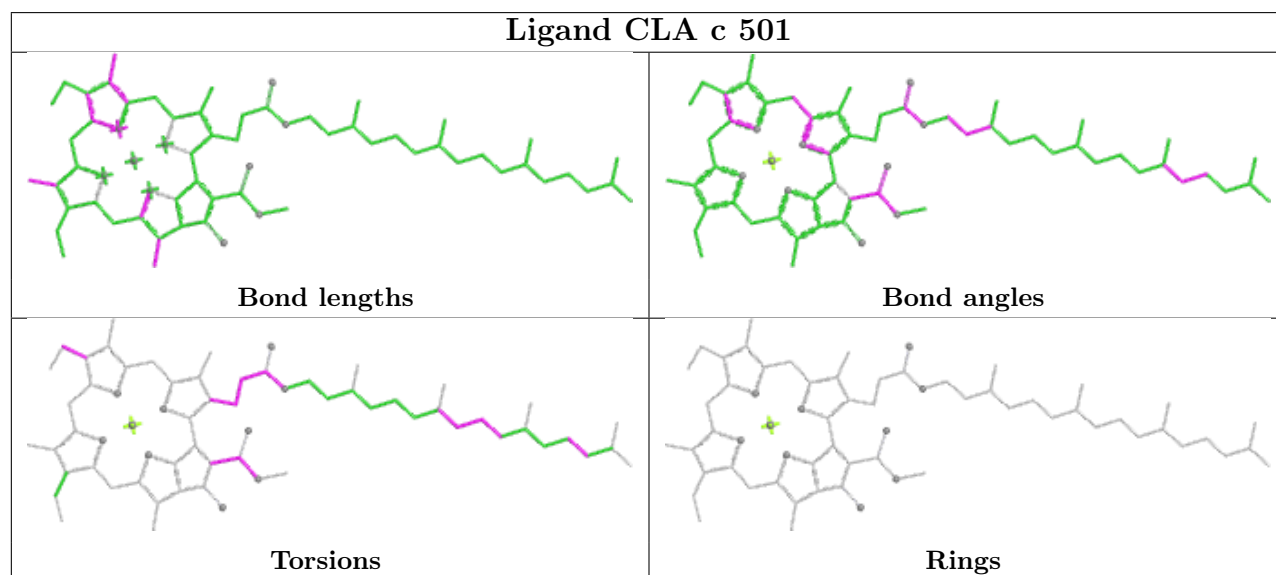
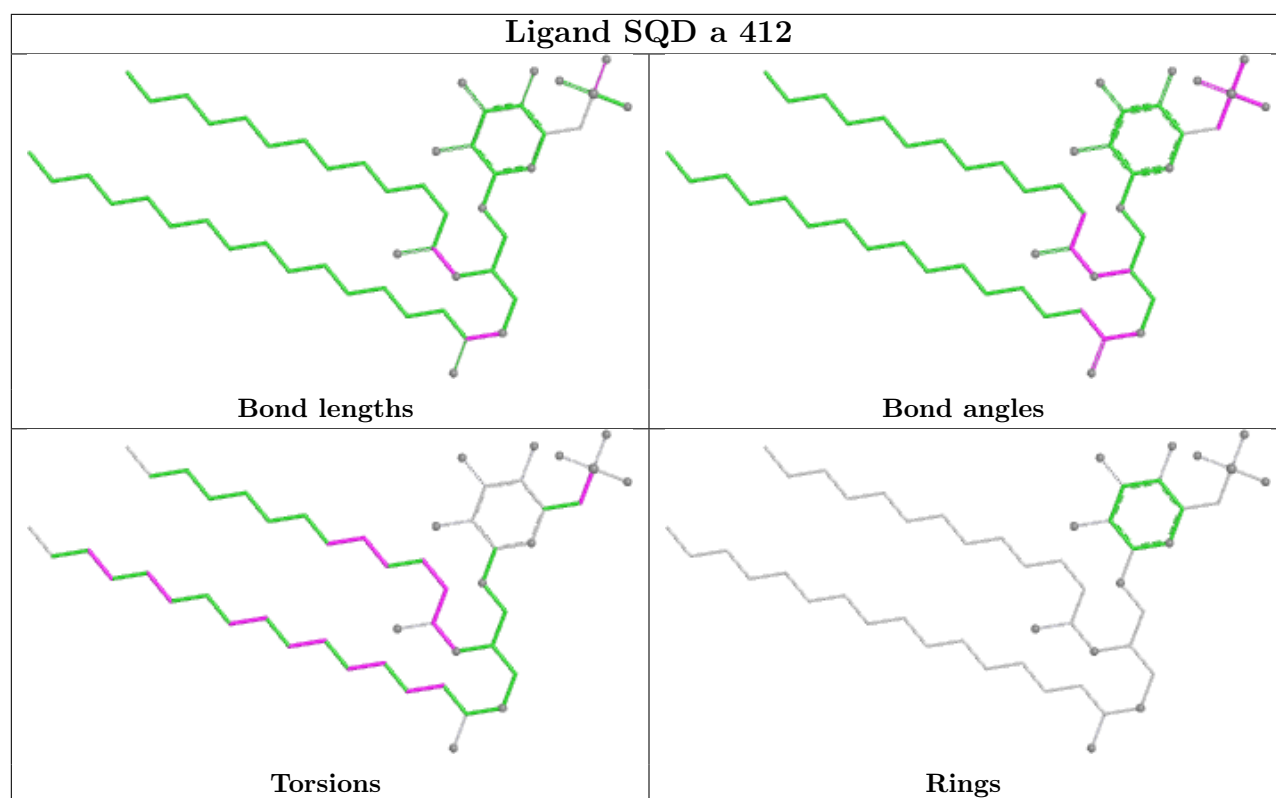




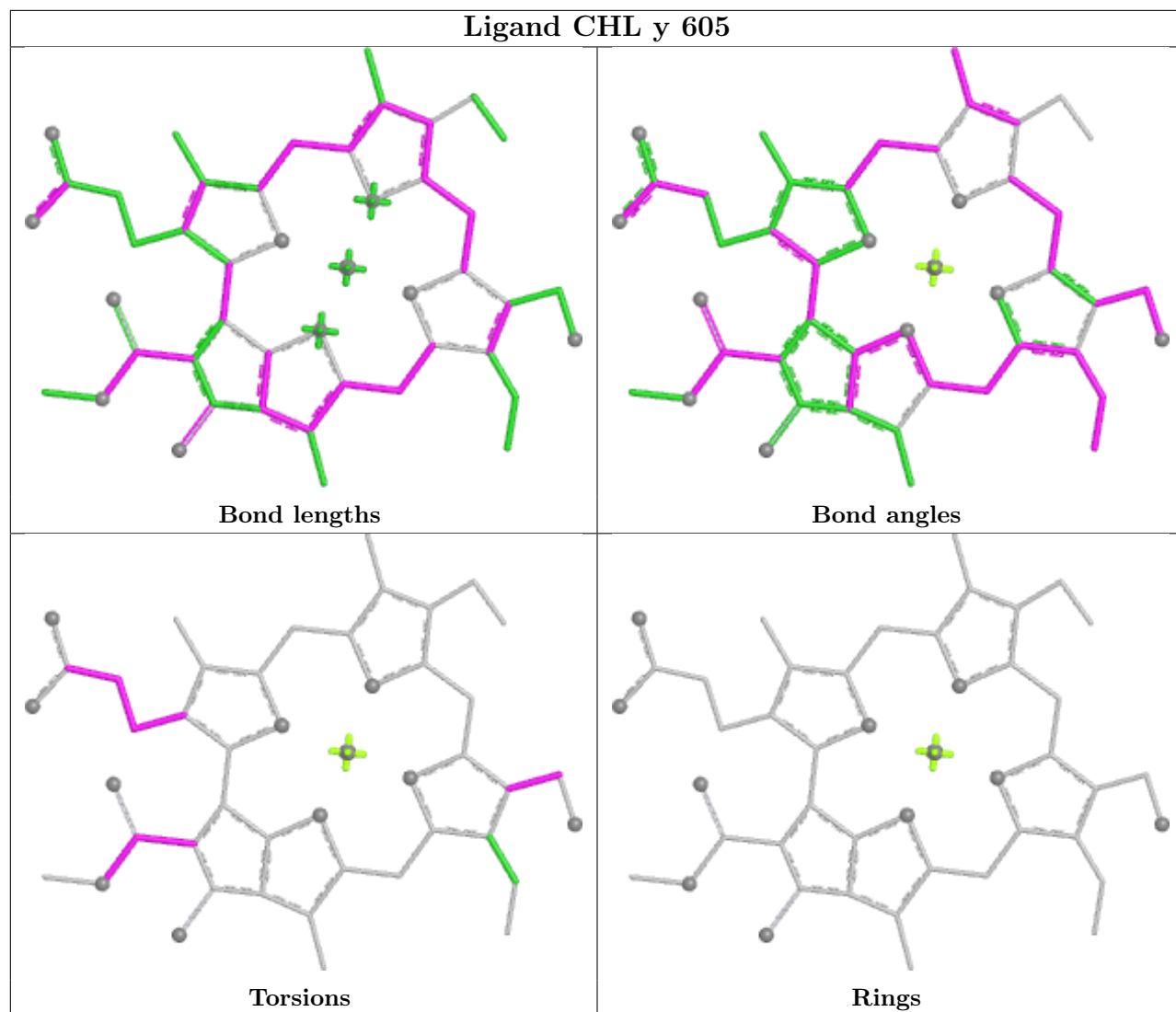




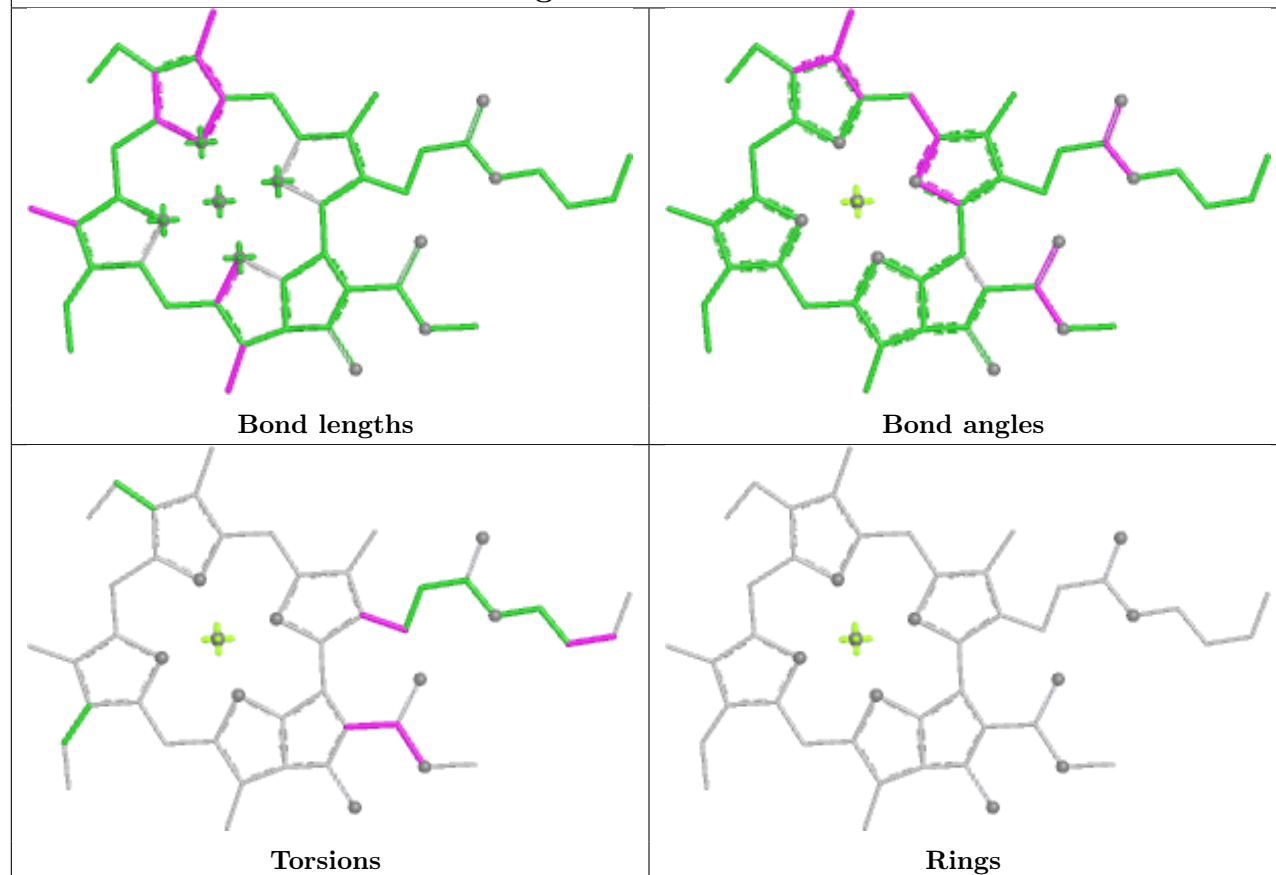




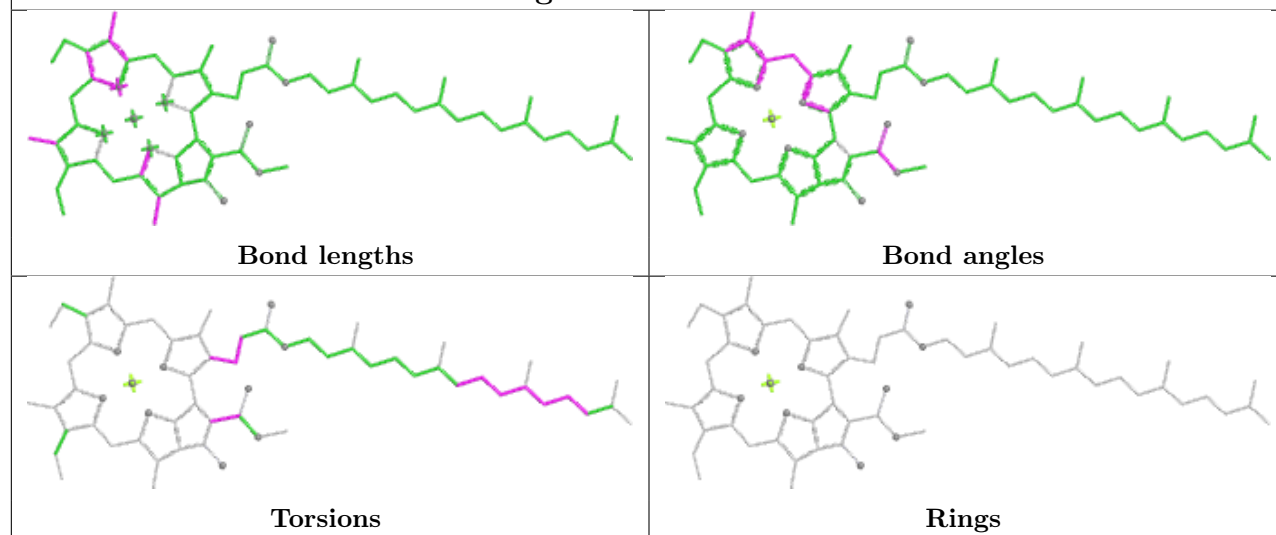
Ligand CHL y 605



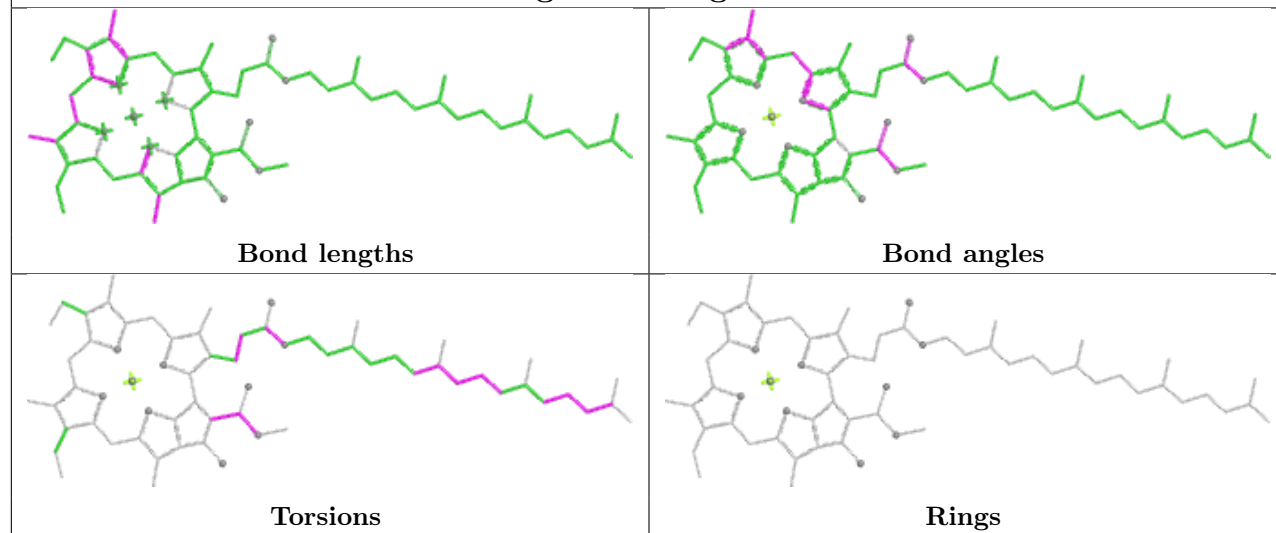
Ligand CLA S 604



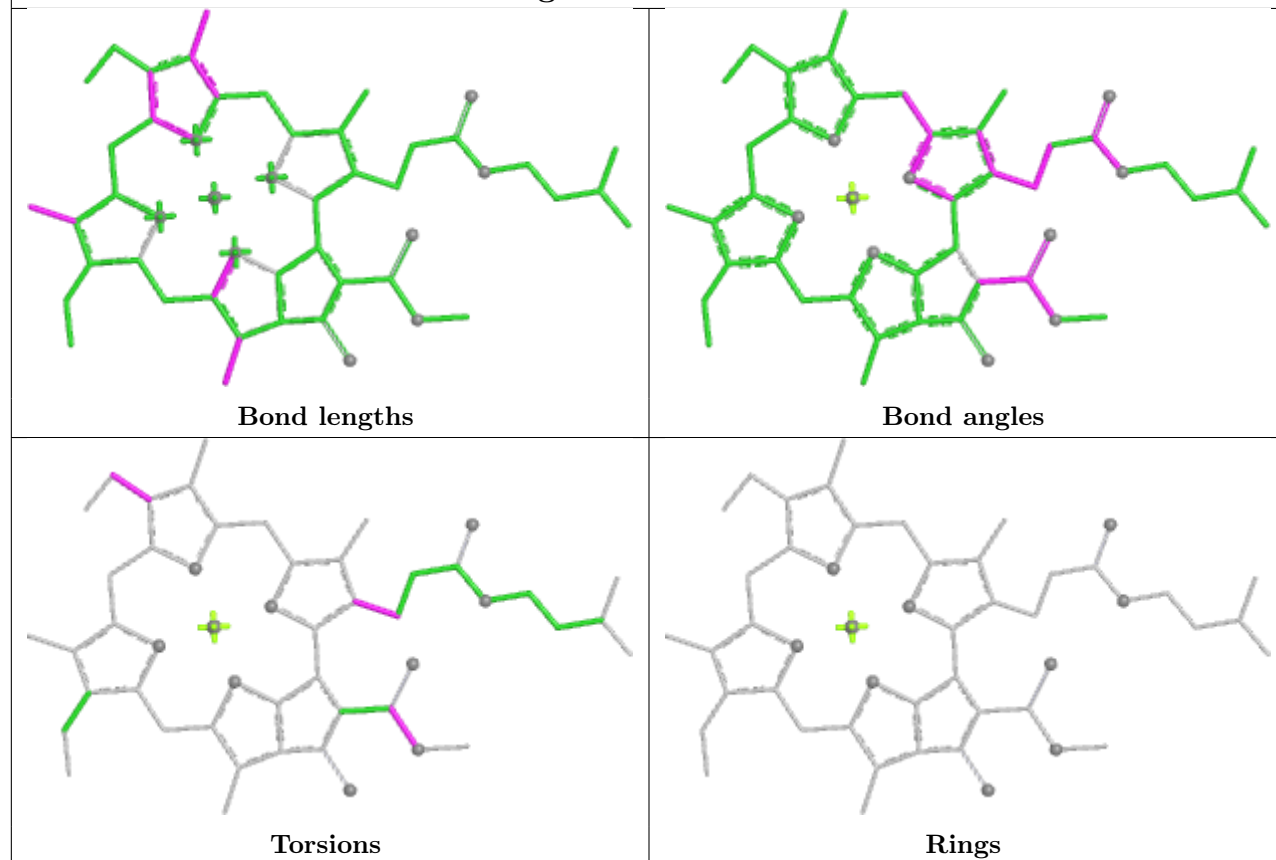
Ligand CLA b 608

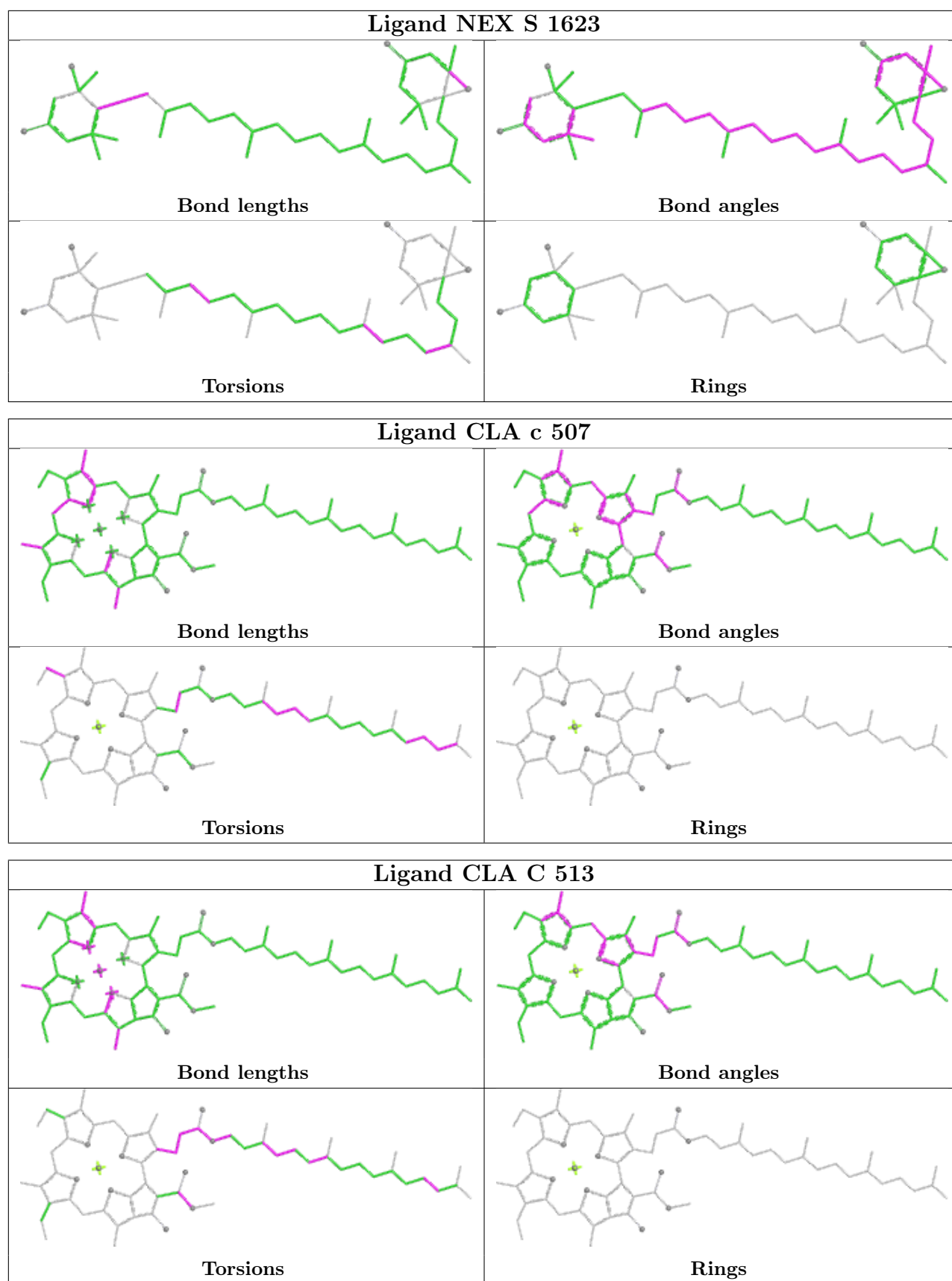


Ligand CLA g 602

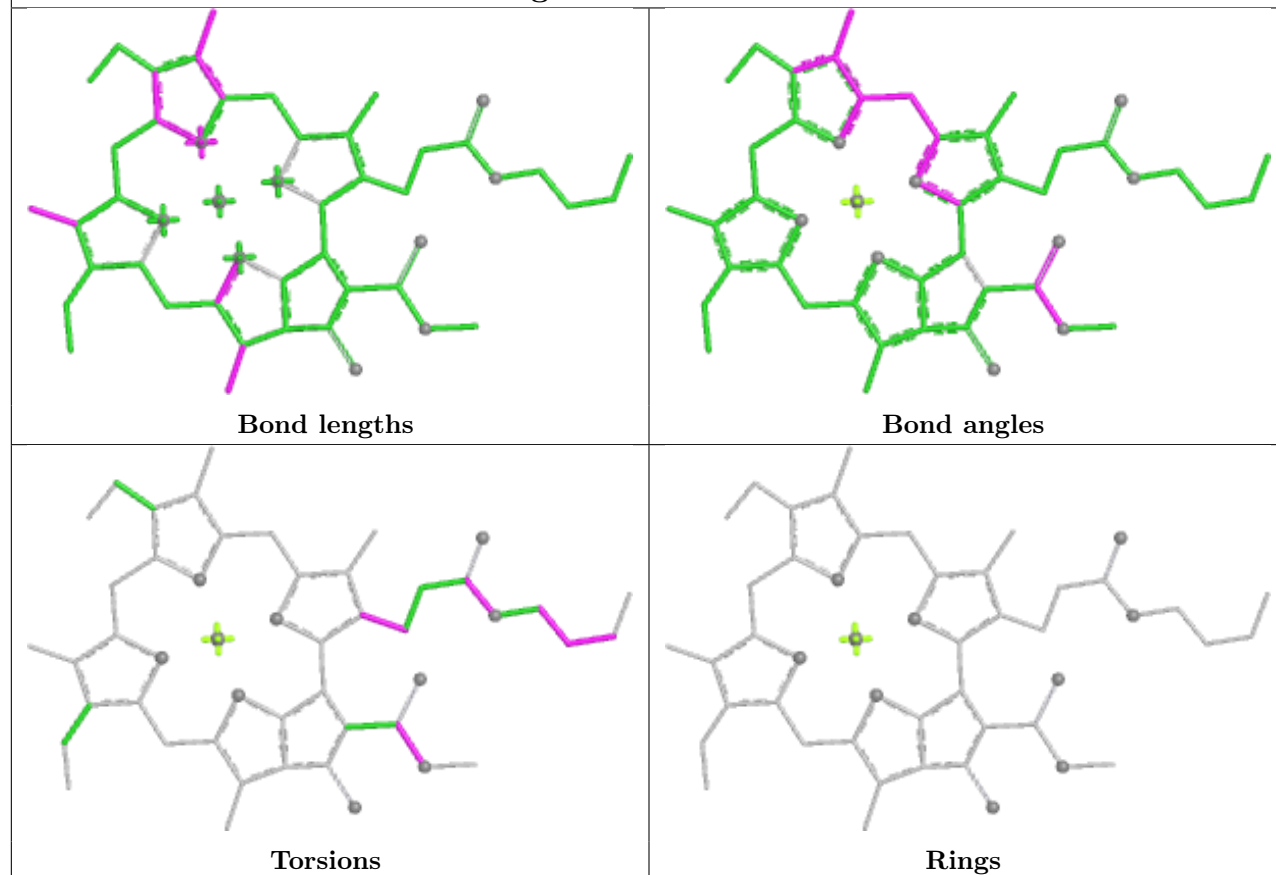


Ligand CLA s 605

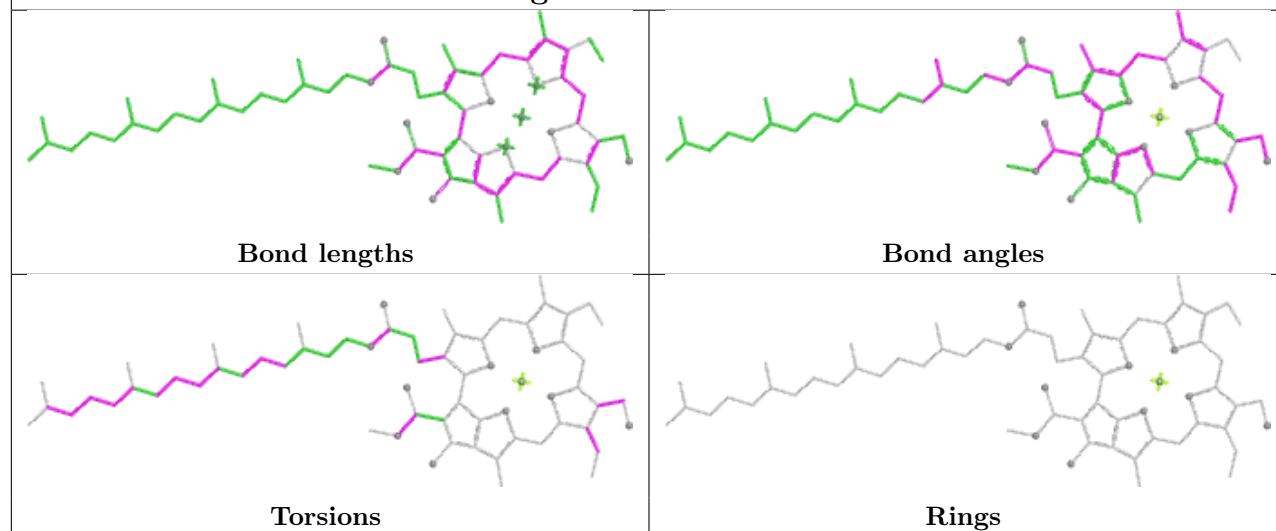


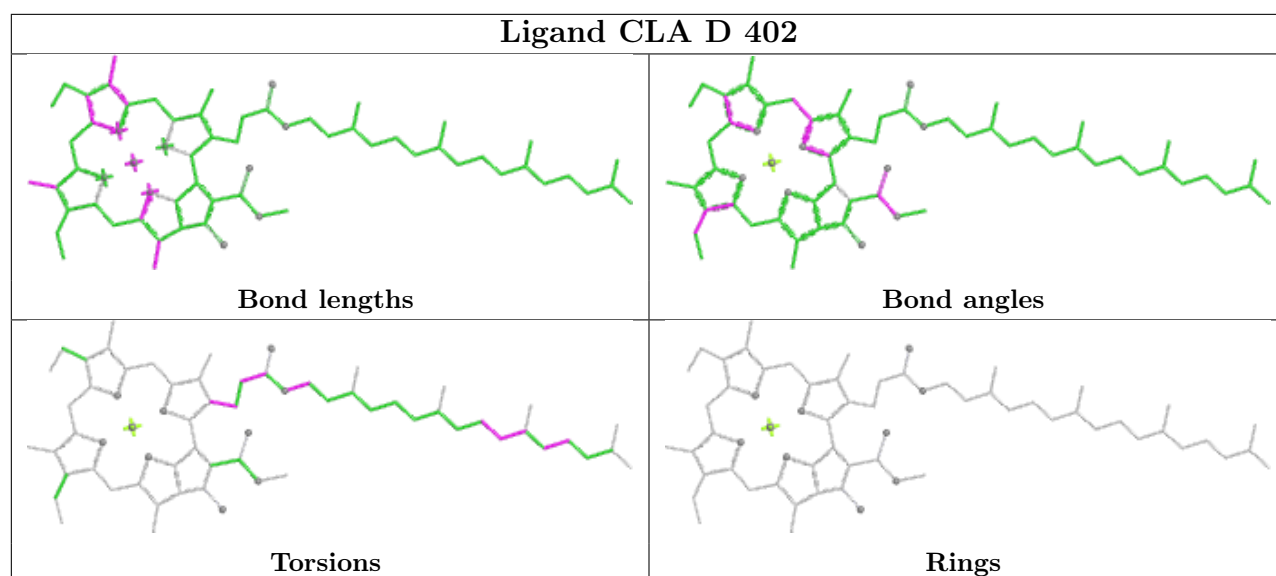
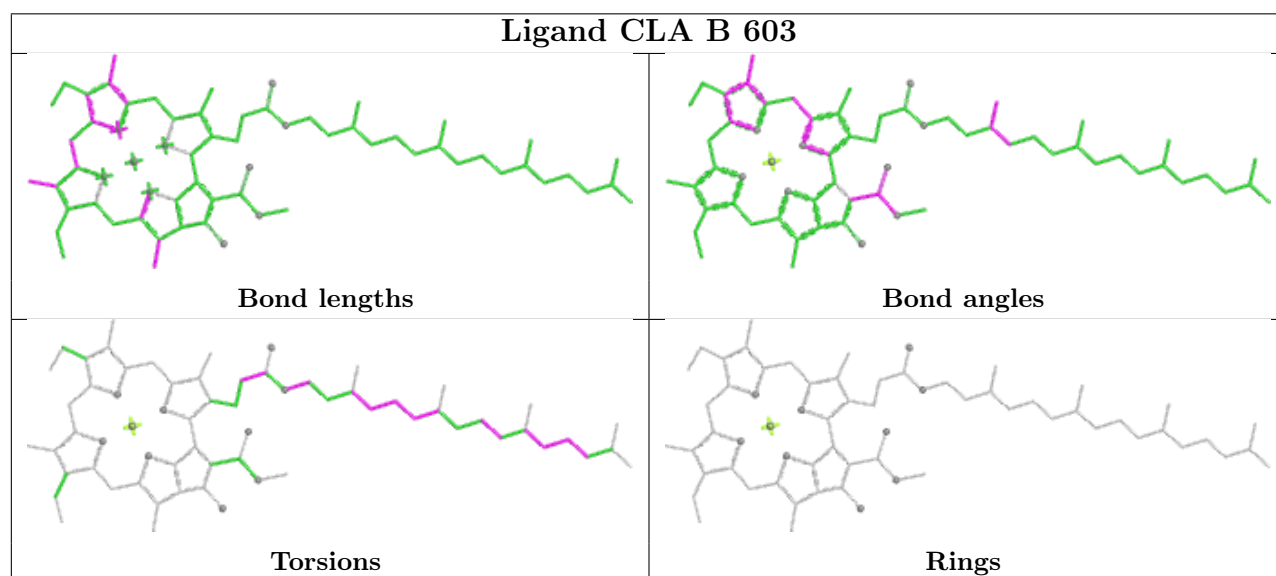
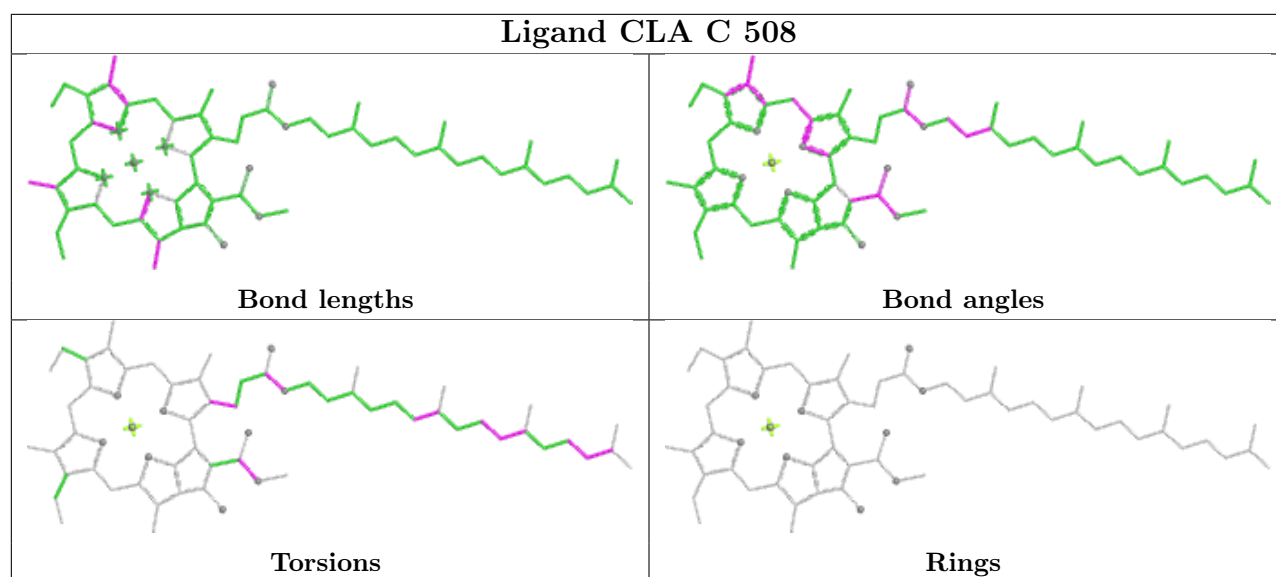


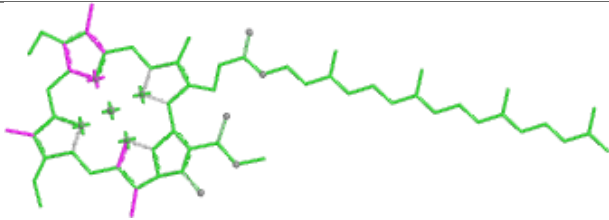
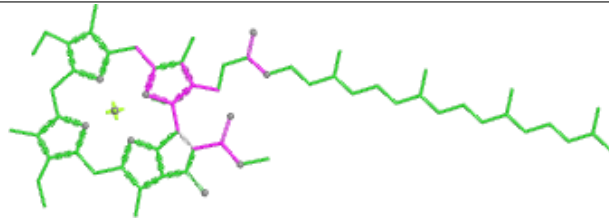
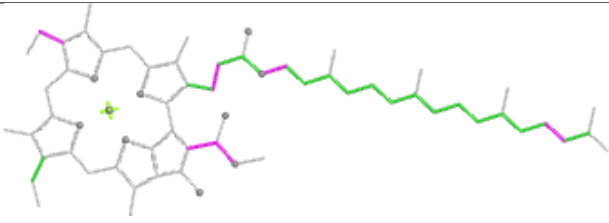
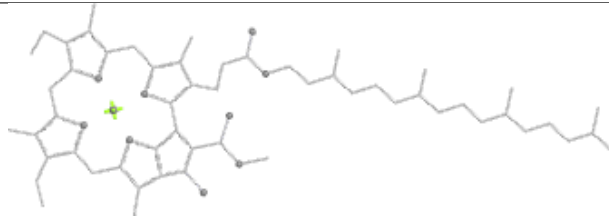
Ligand CLA G 604

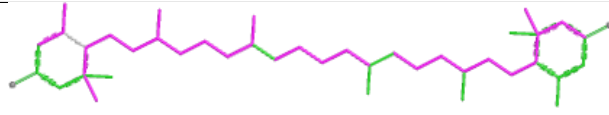
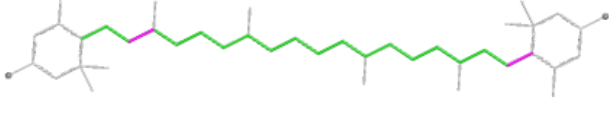
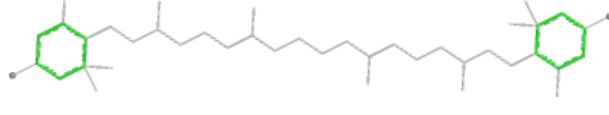


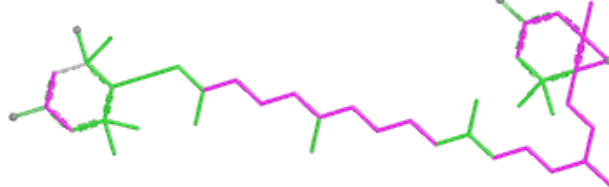
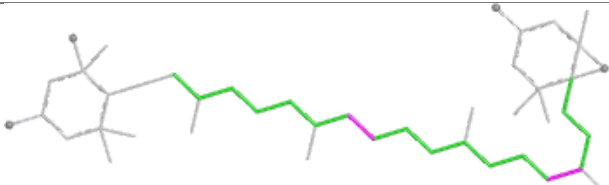
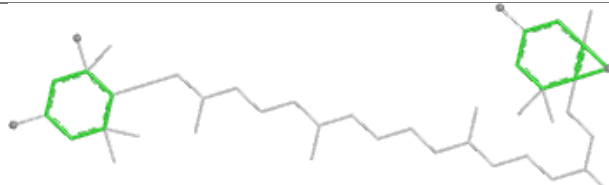
Ligand CHL G 609



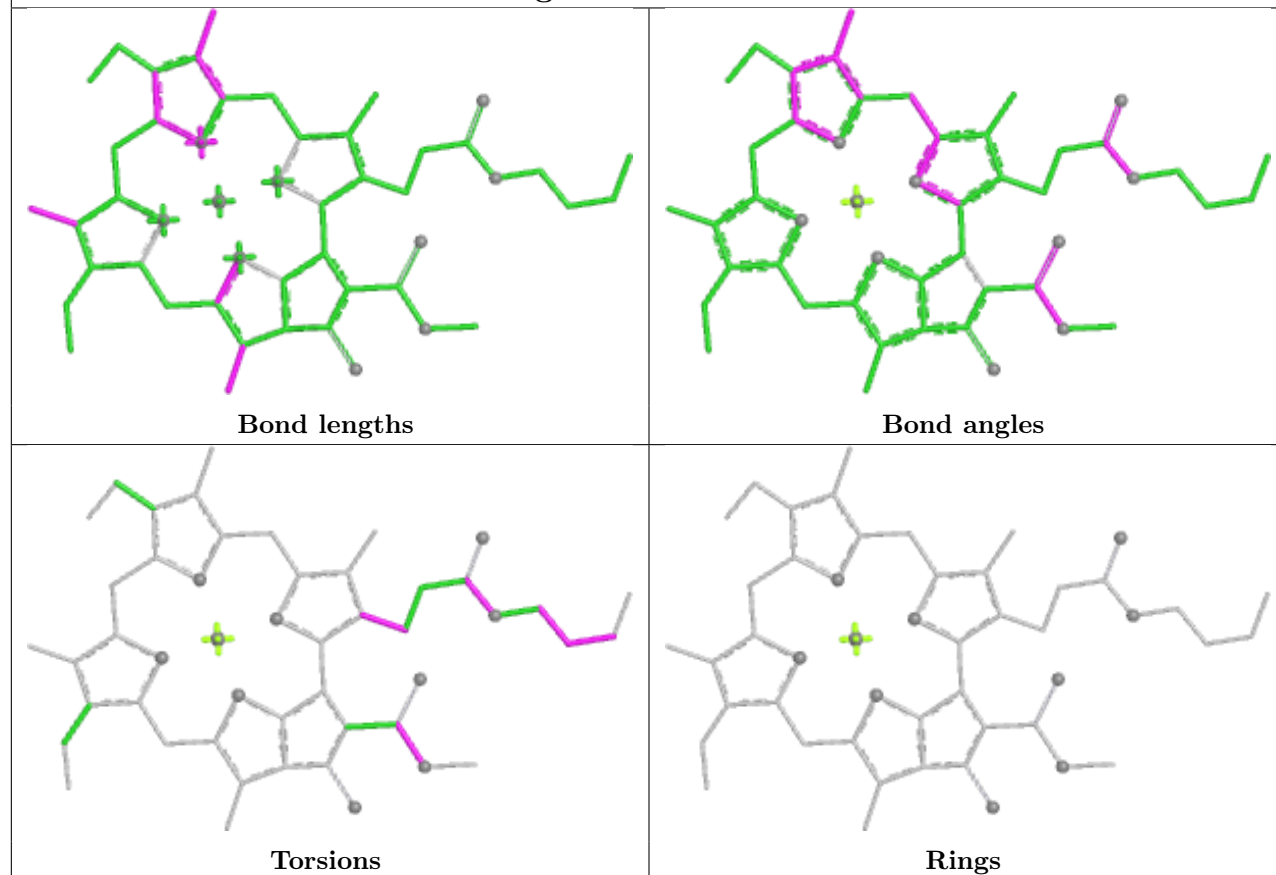


Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

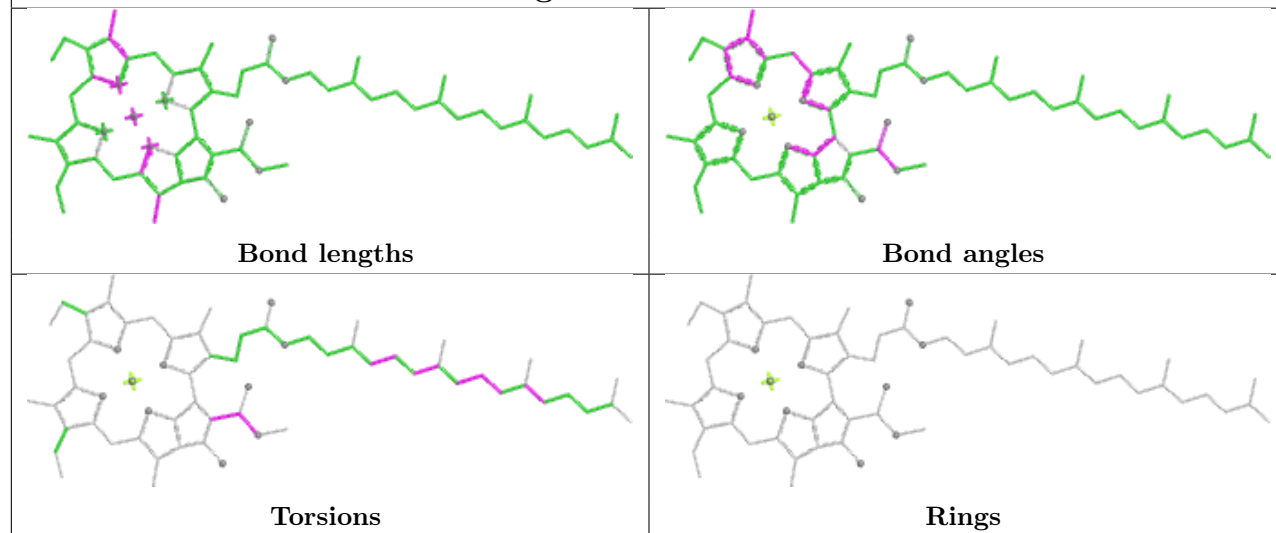
Ligand LUT S 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

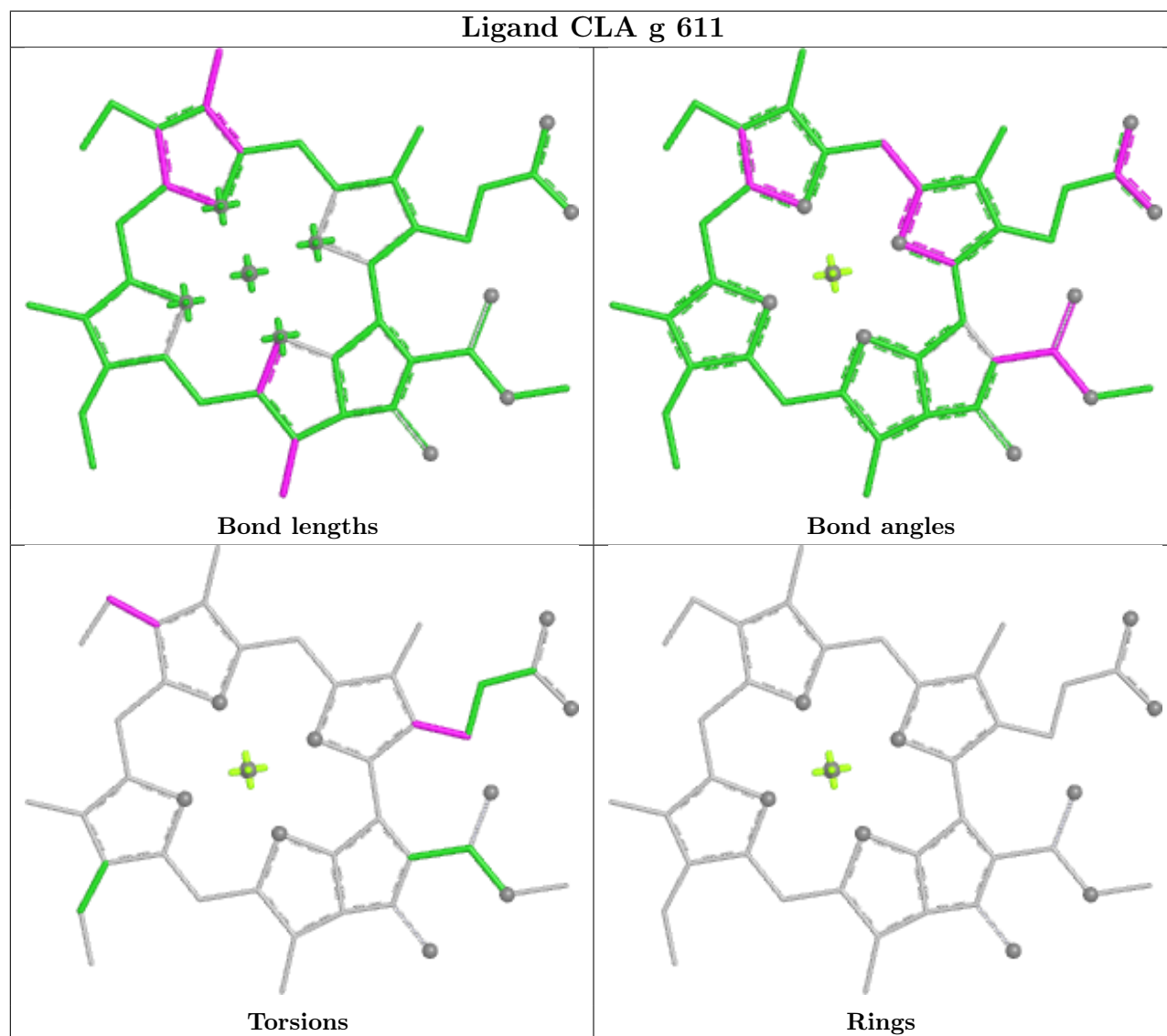
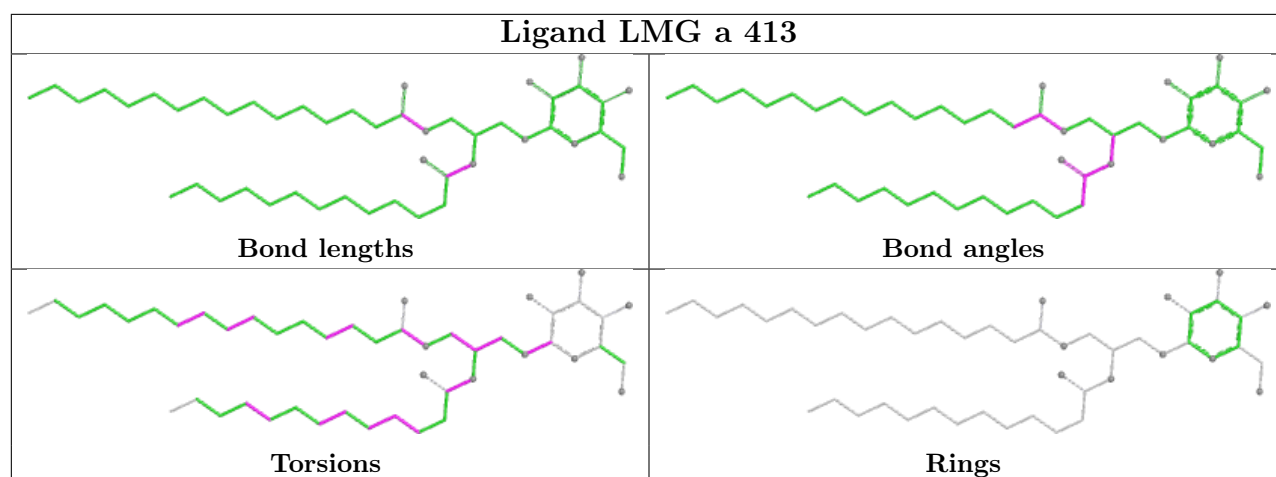
Ligand NEX G 1623	
	
Bond lengths	Bond angles
	
Torsions	Rings

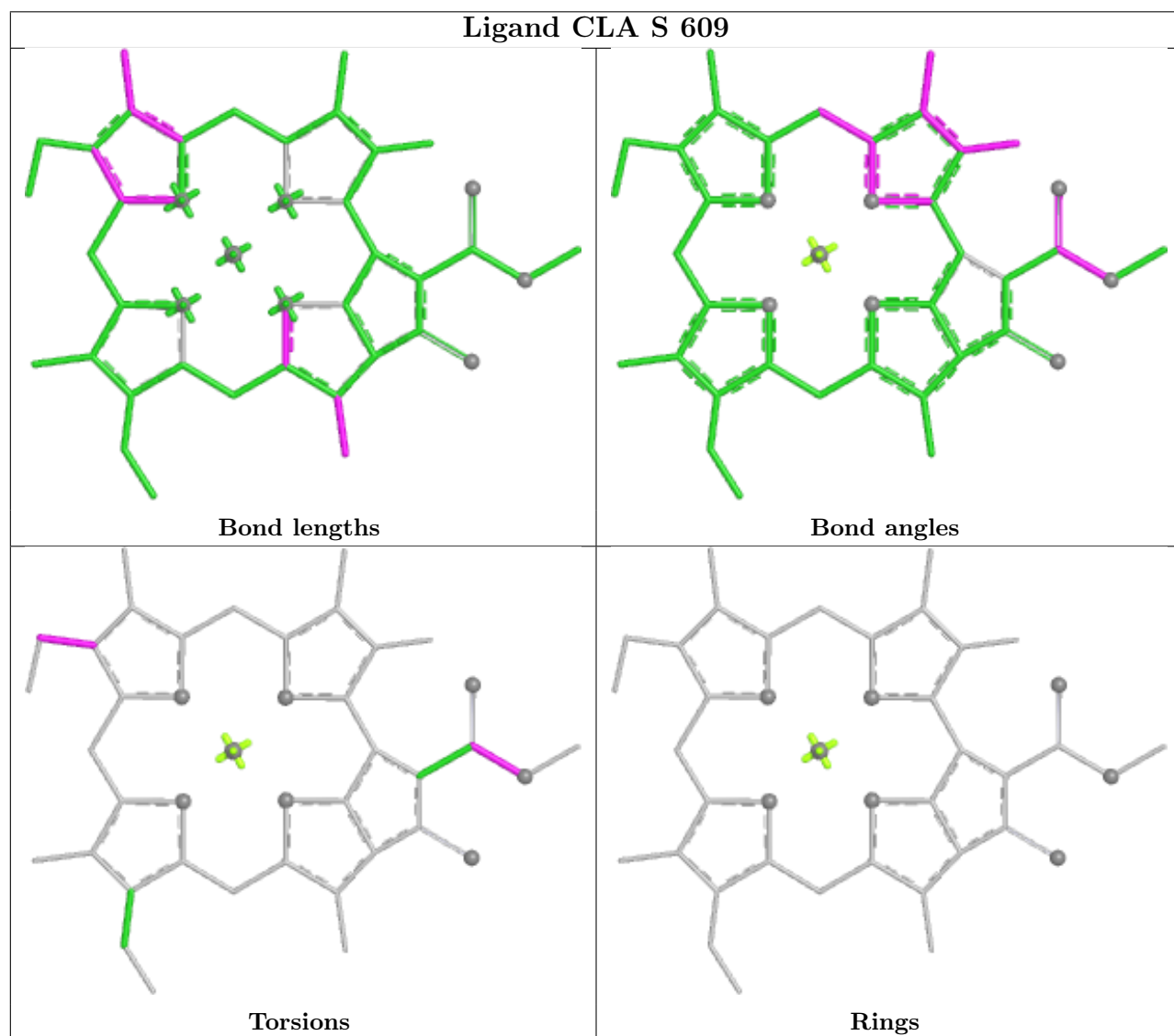
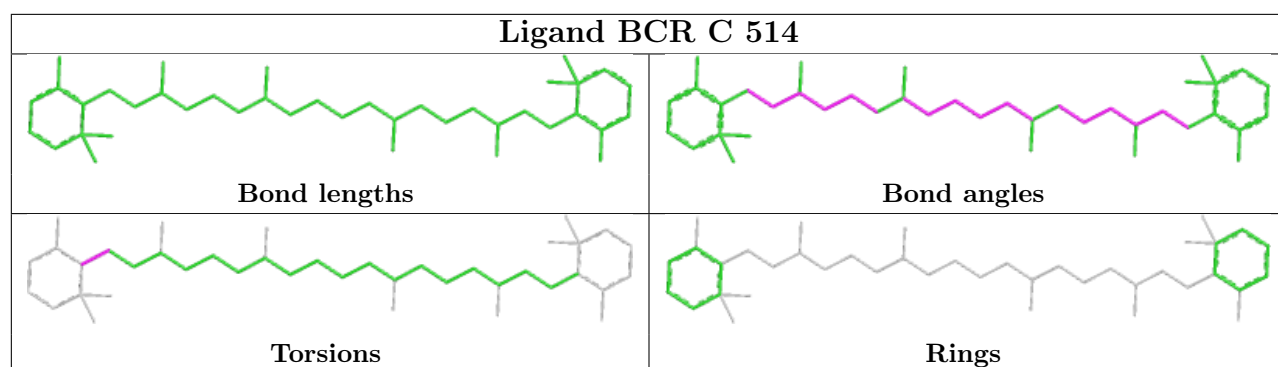
Ligand CLA S 611



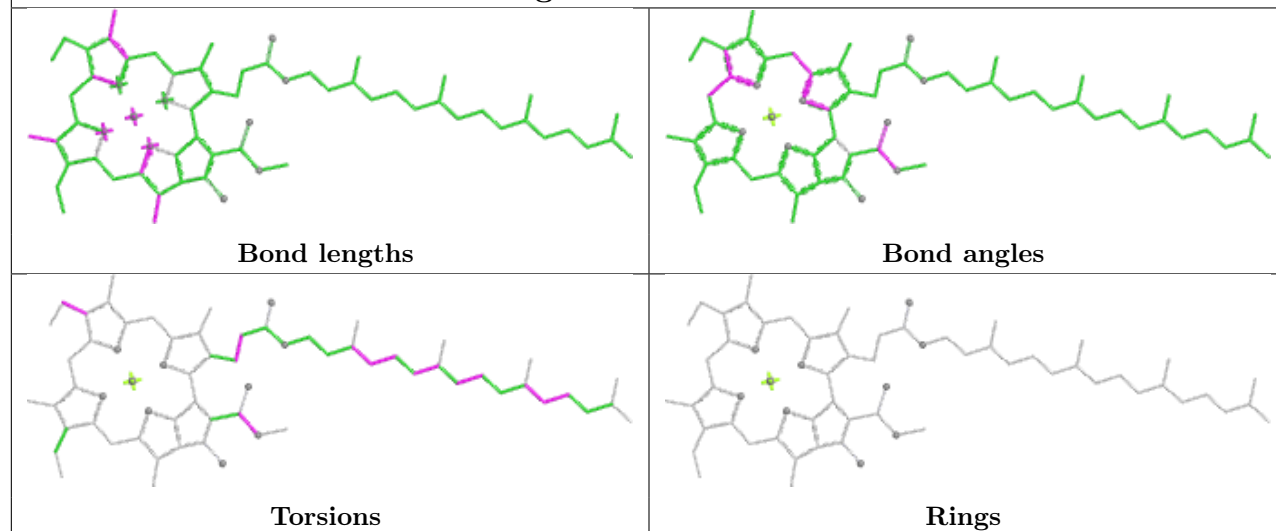
Ligand CLA n 604



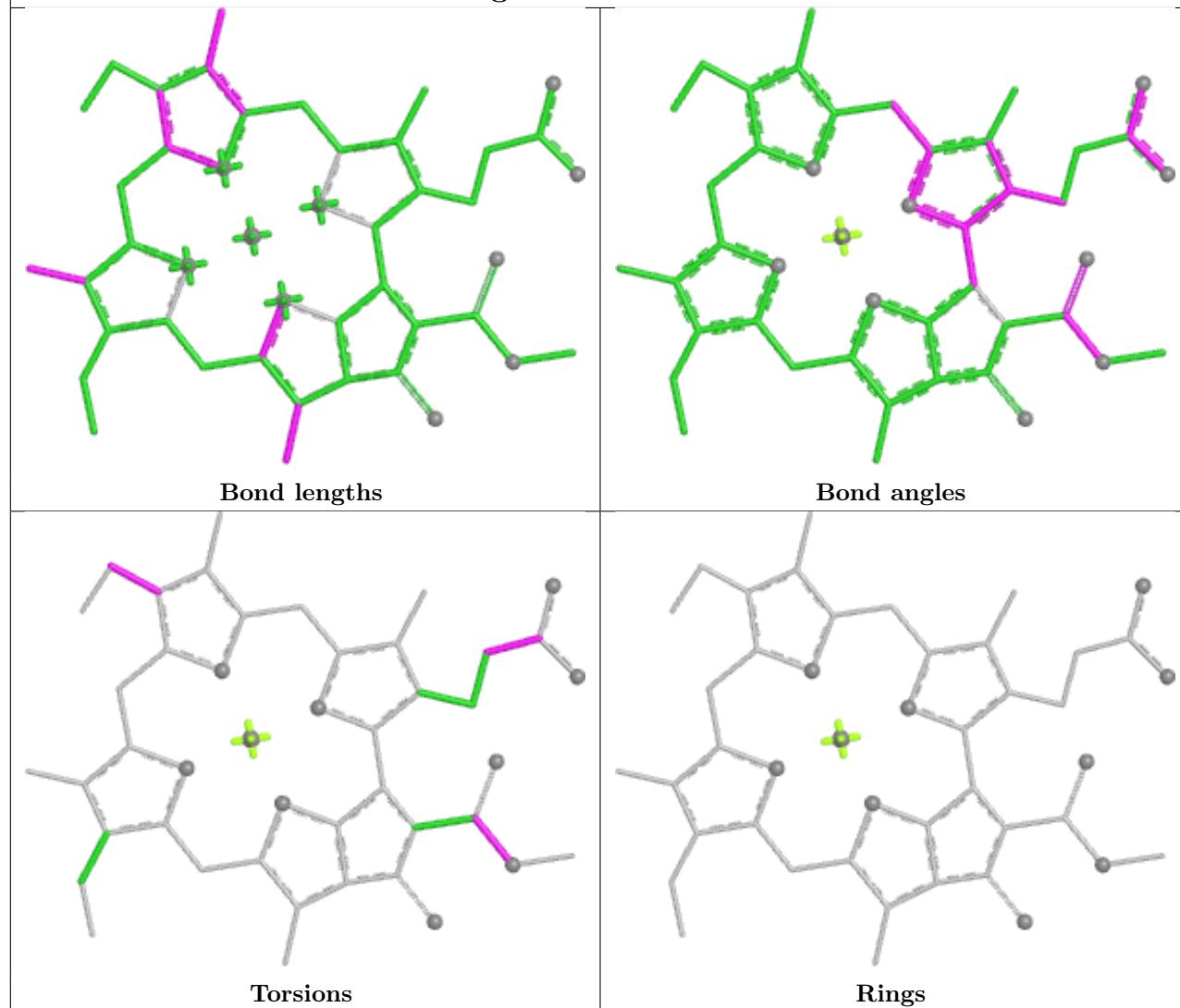


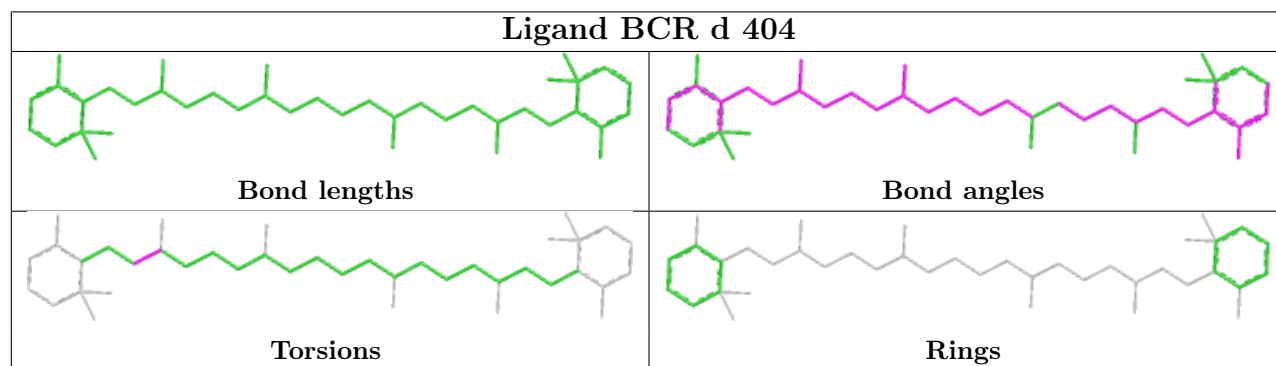
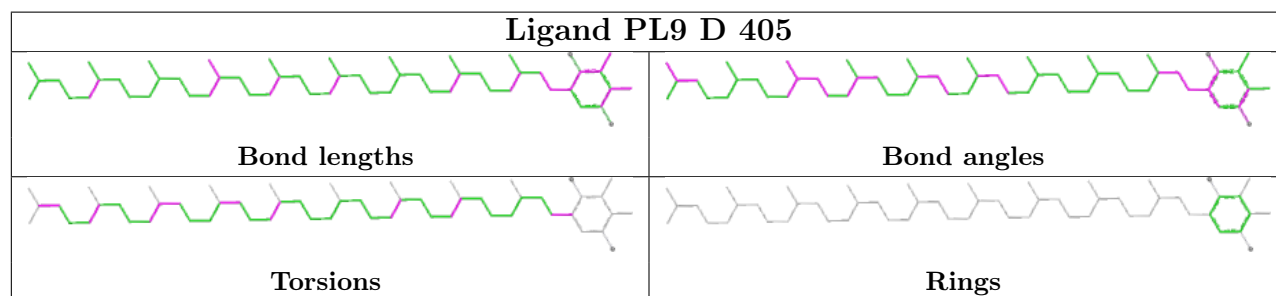
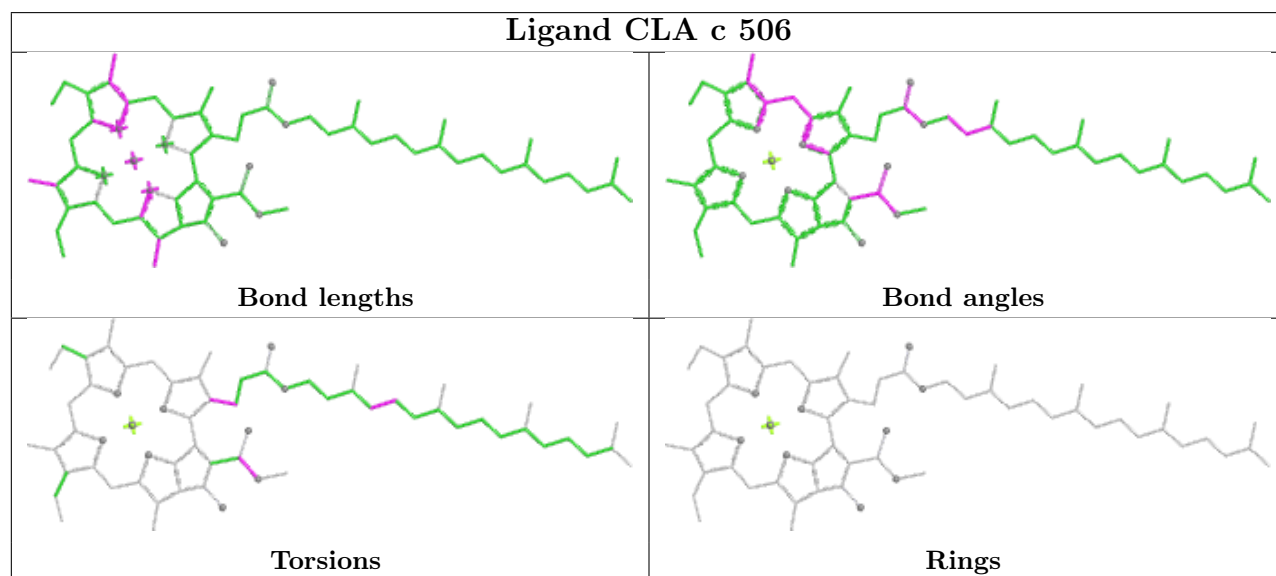
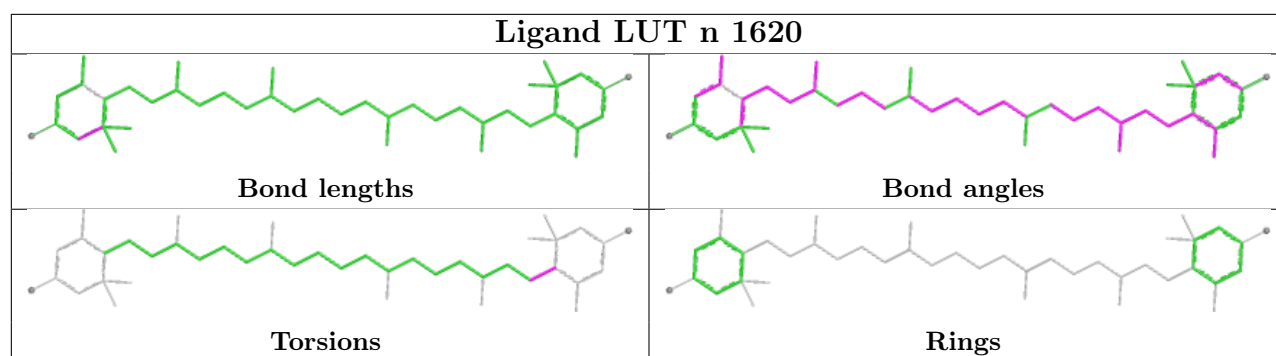


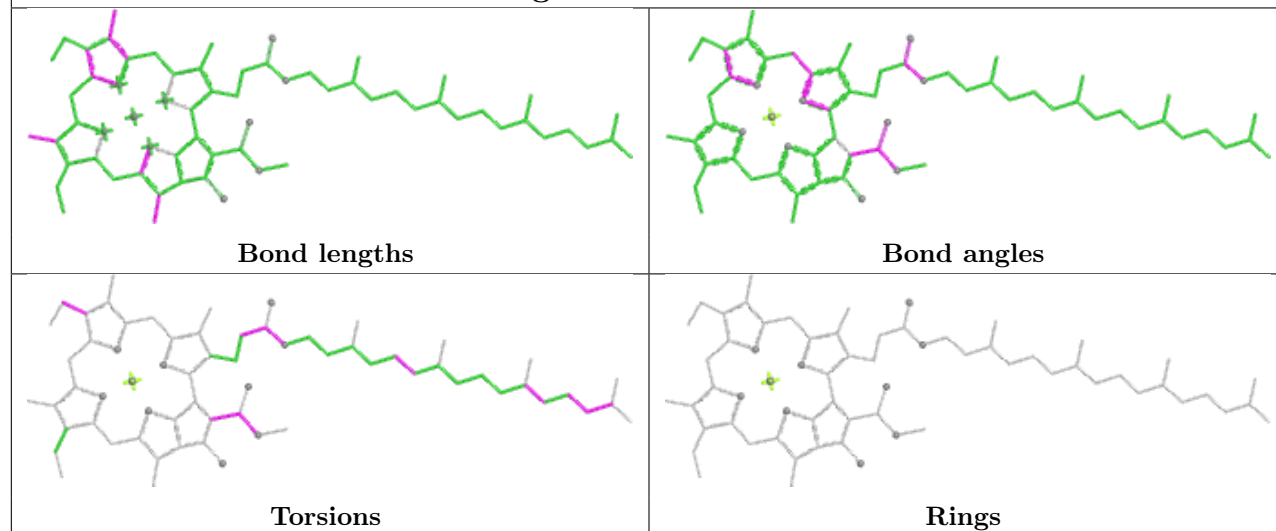
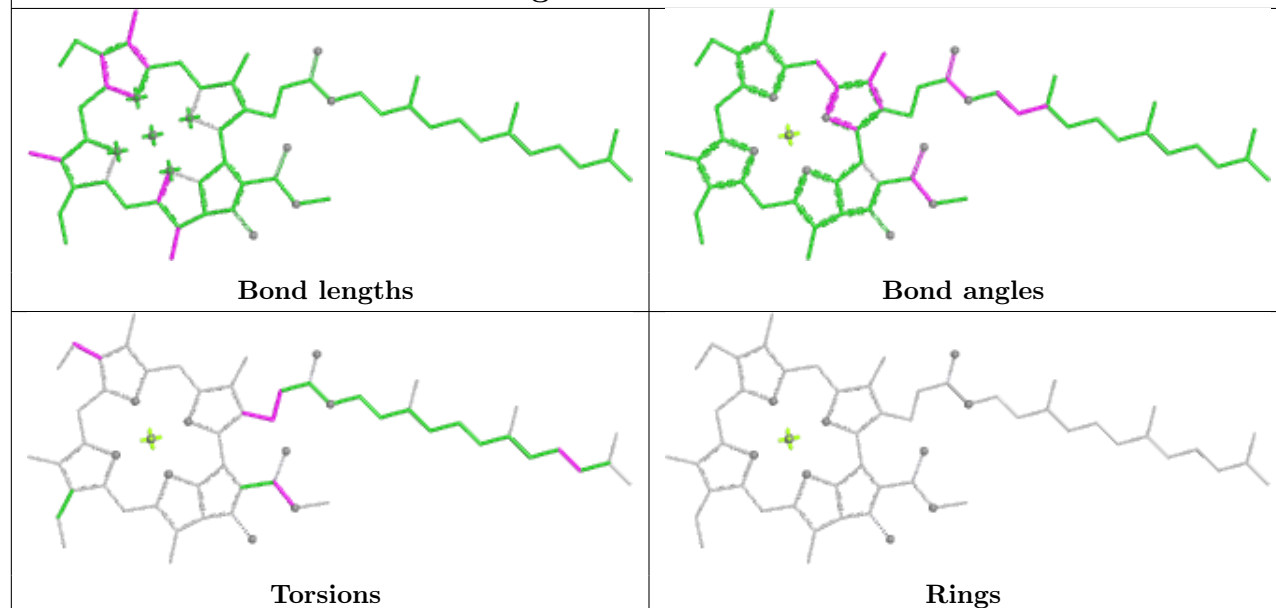
Ligand CLA n 613



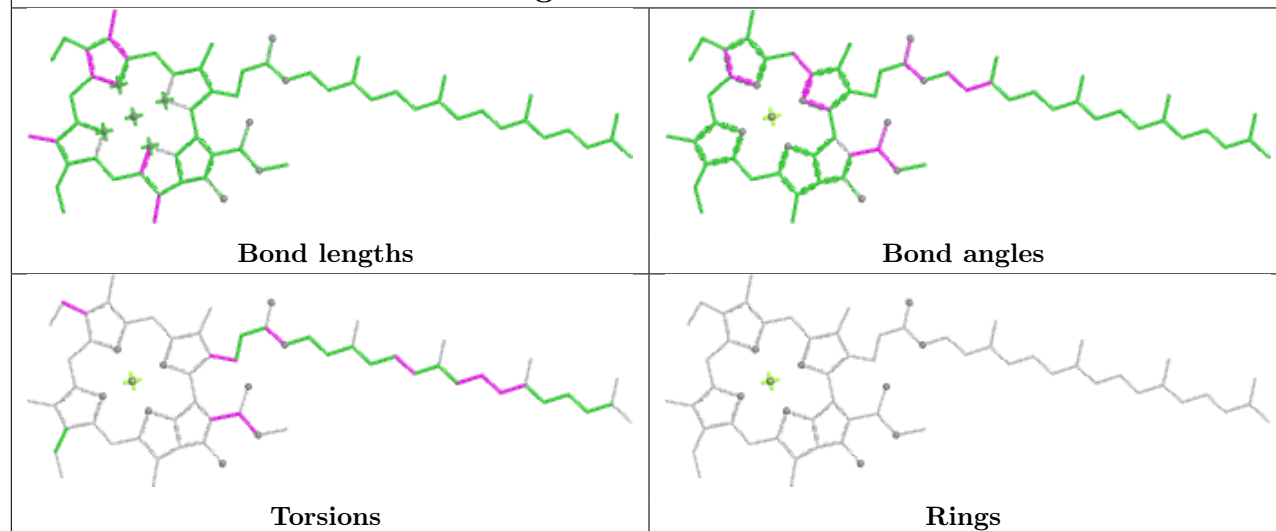
Ligand CLA N 612



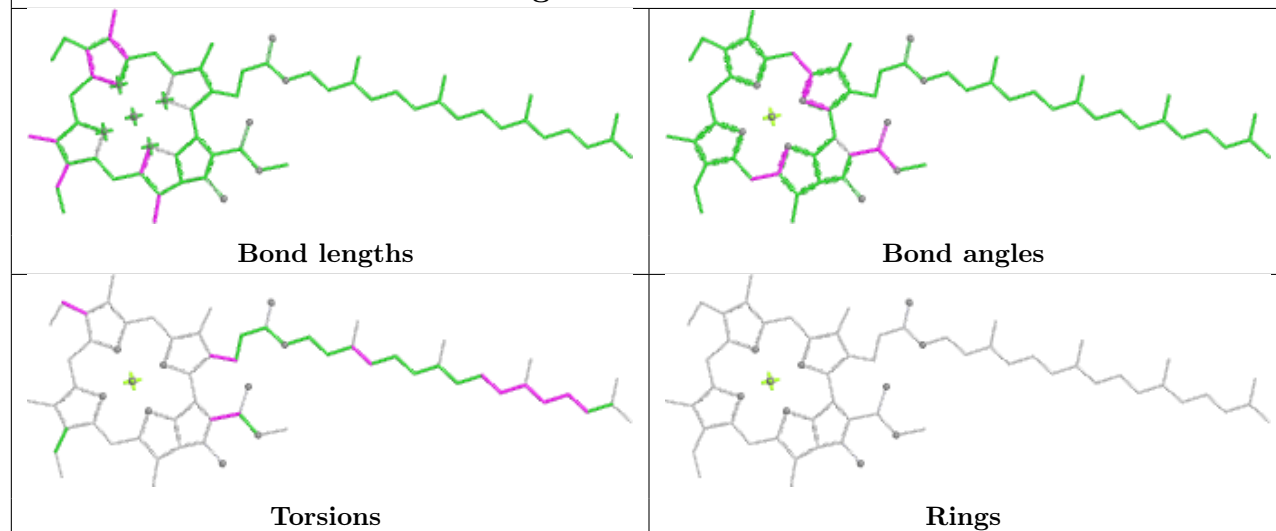


Ligand CLA B 602**Ligand CLA R 602**

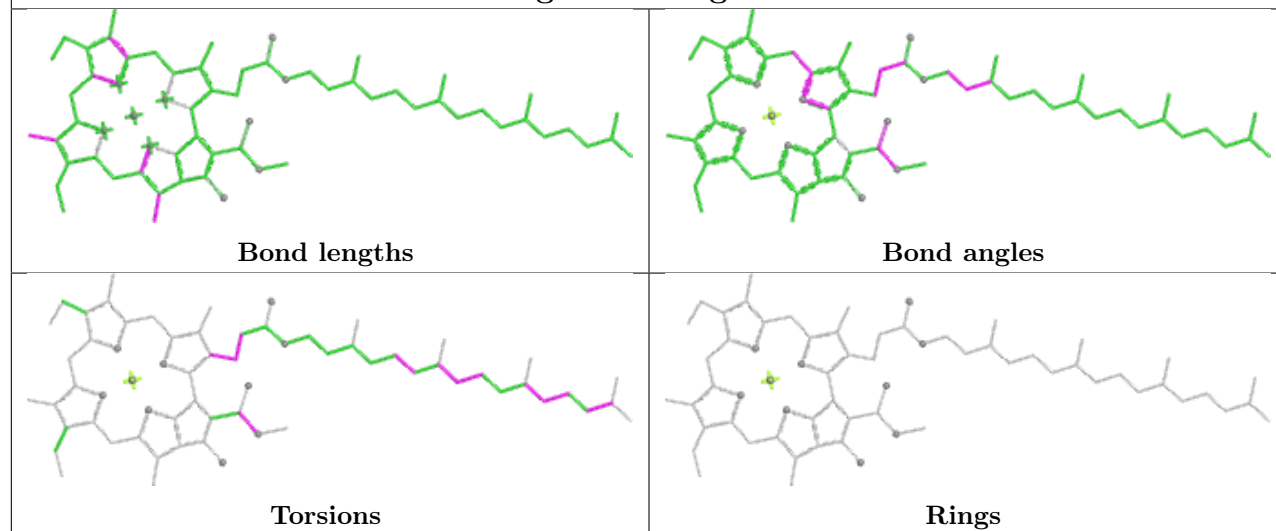
Ligand CLA d 403



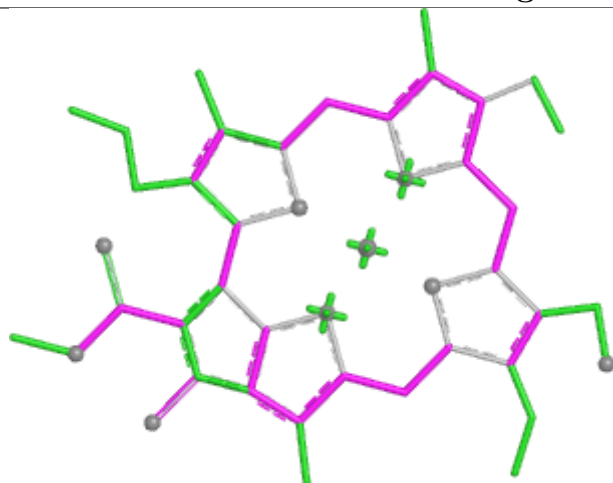
Ligand CLA C 504



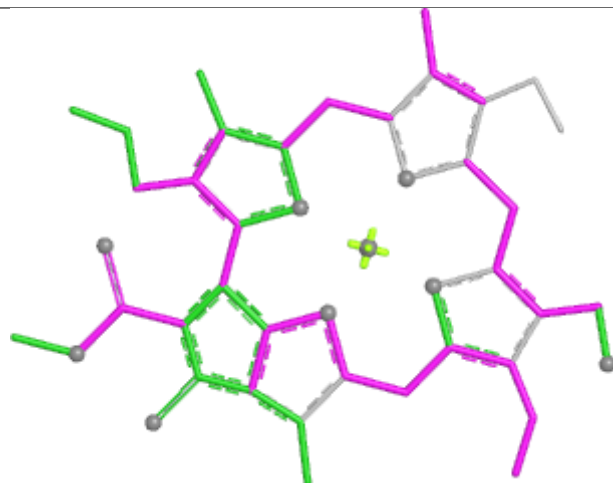
Ligand CLA g 610



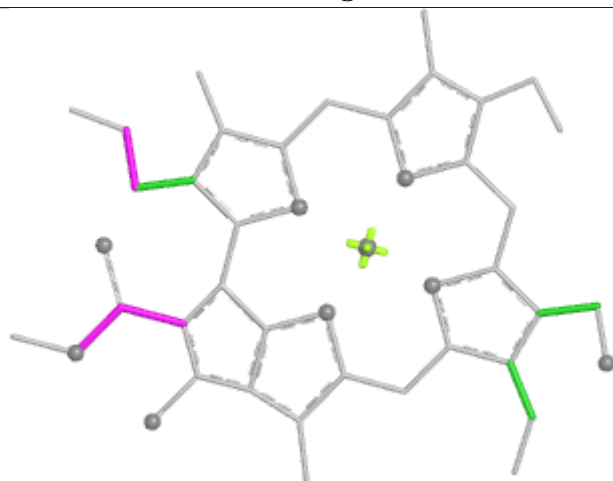
Ligand CHL S 606



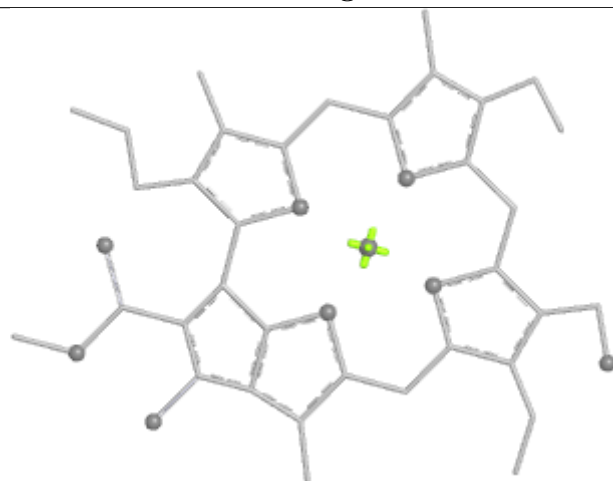
Bond lengths



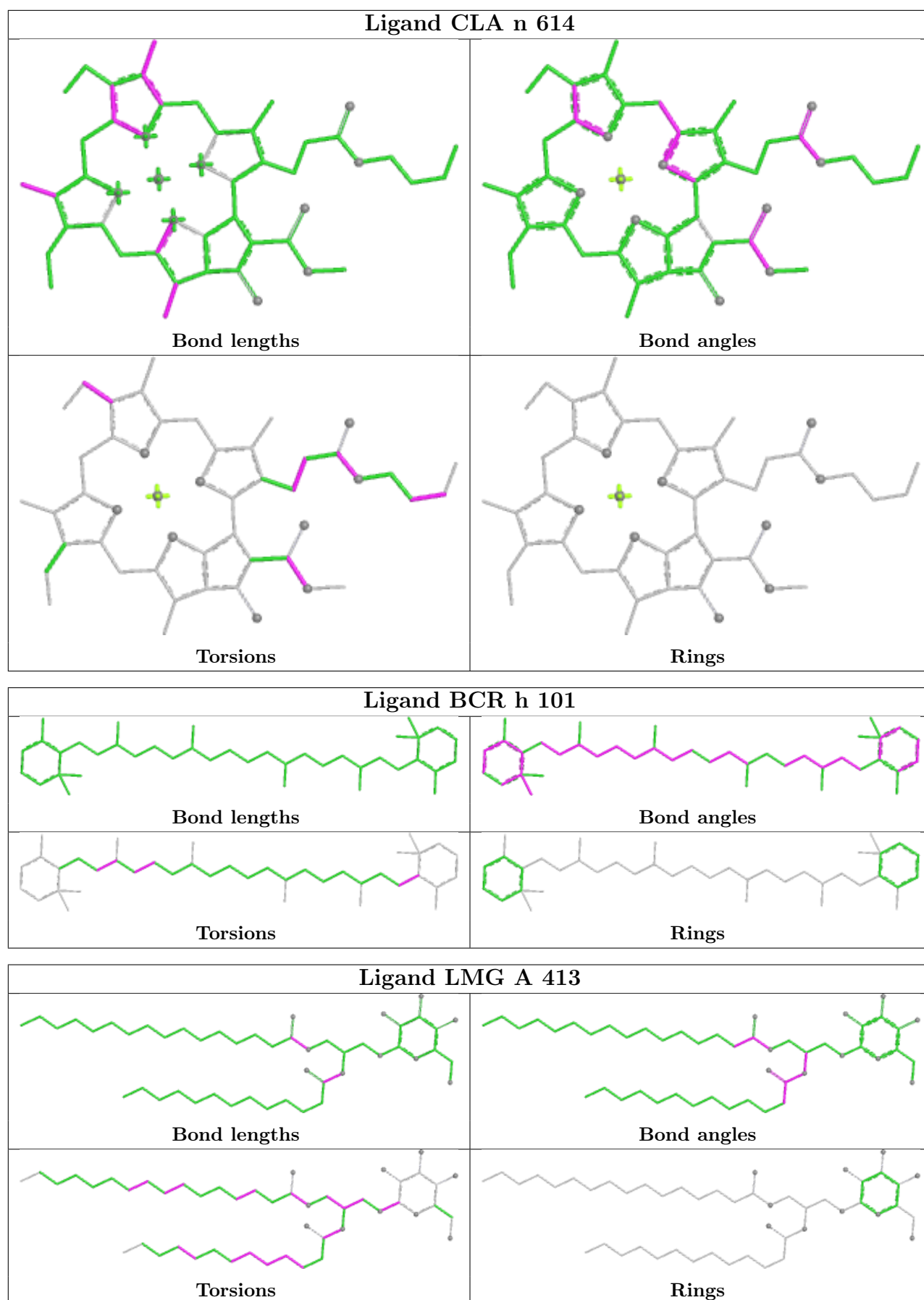
Bond angles

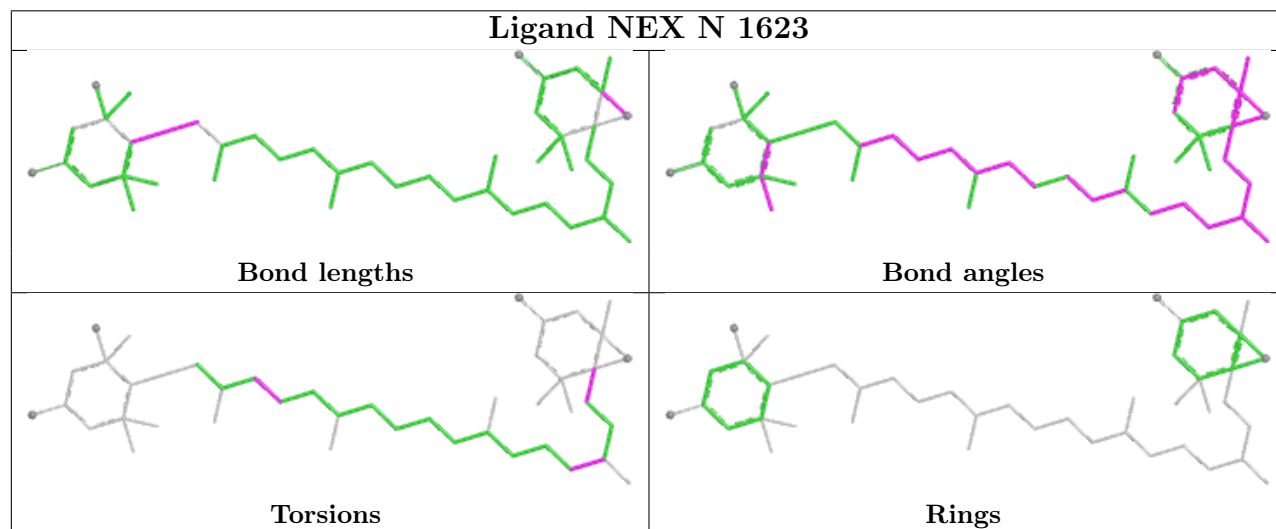
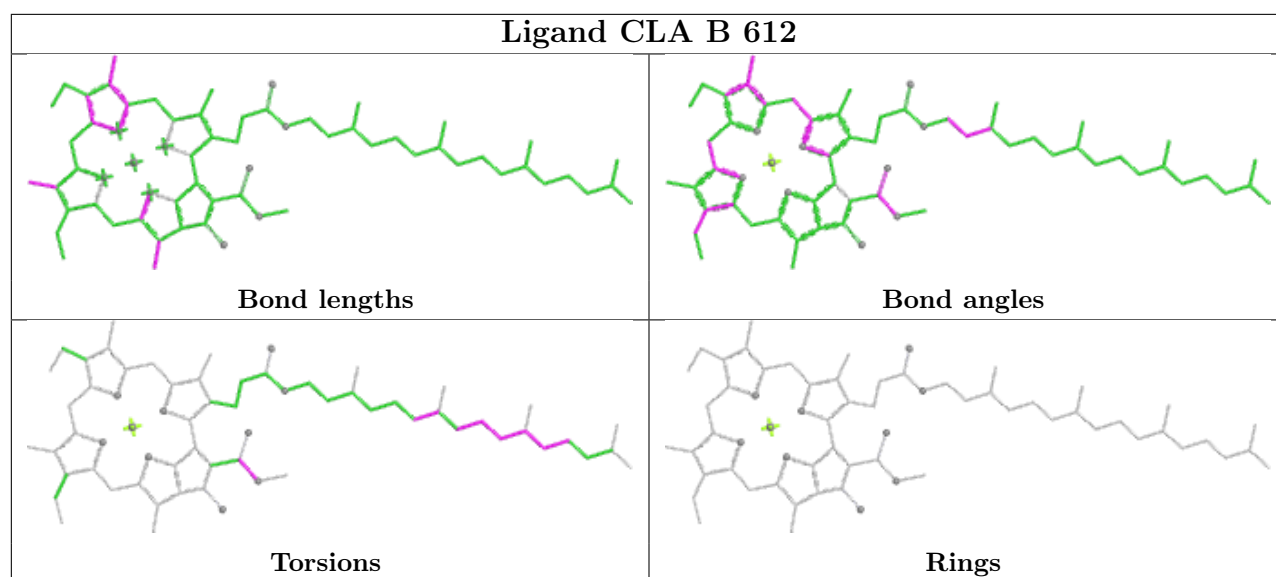


Torsions

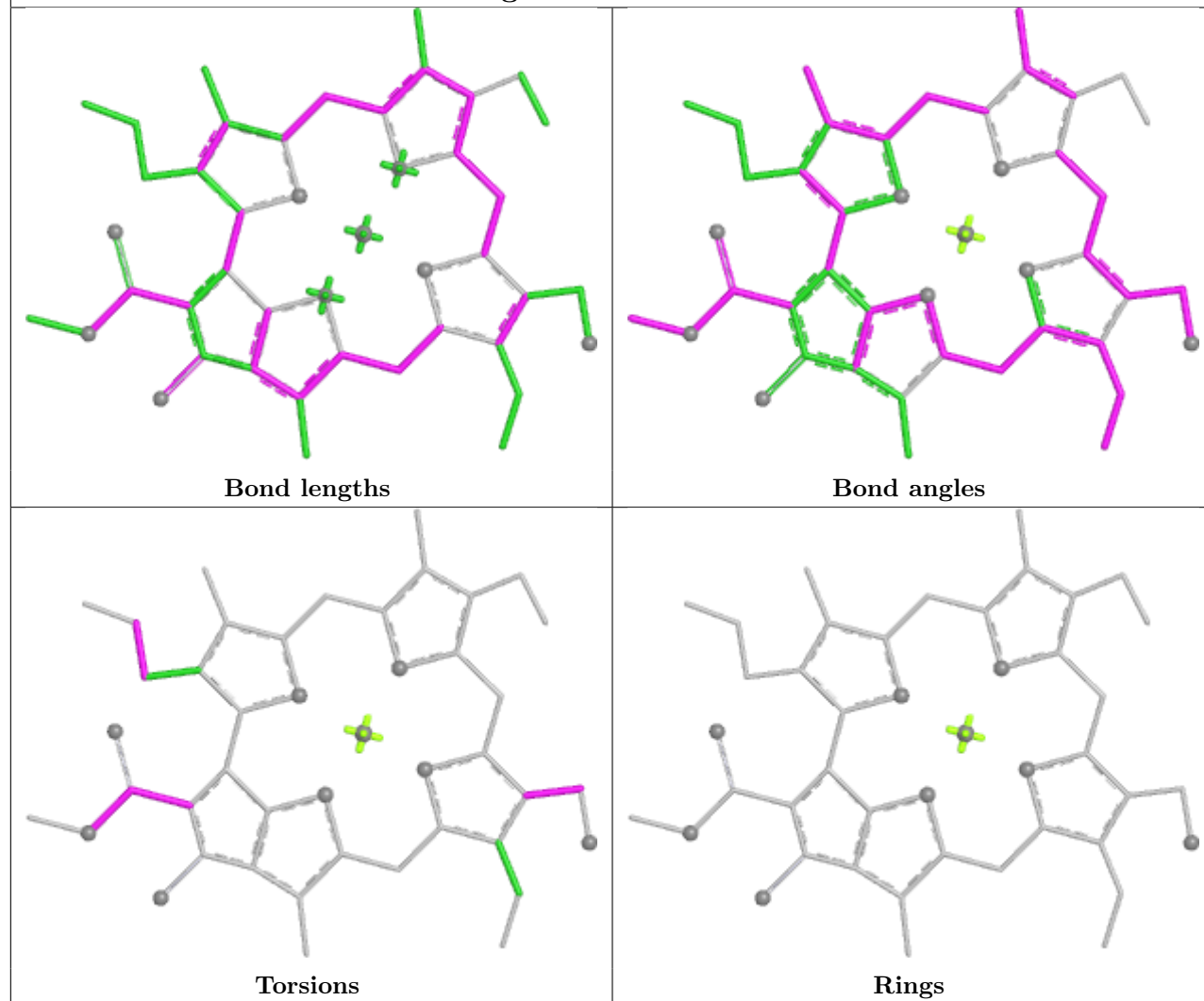


Rings

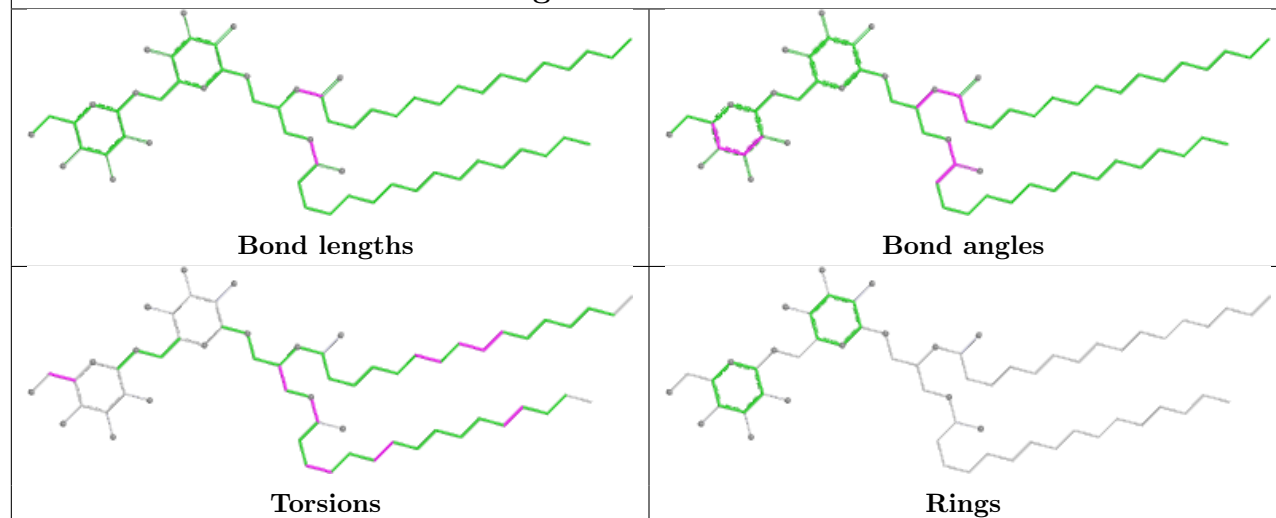




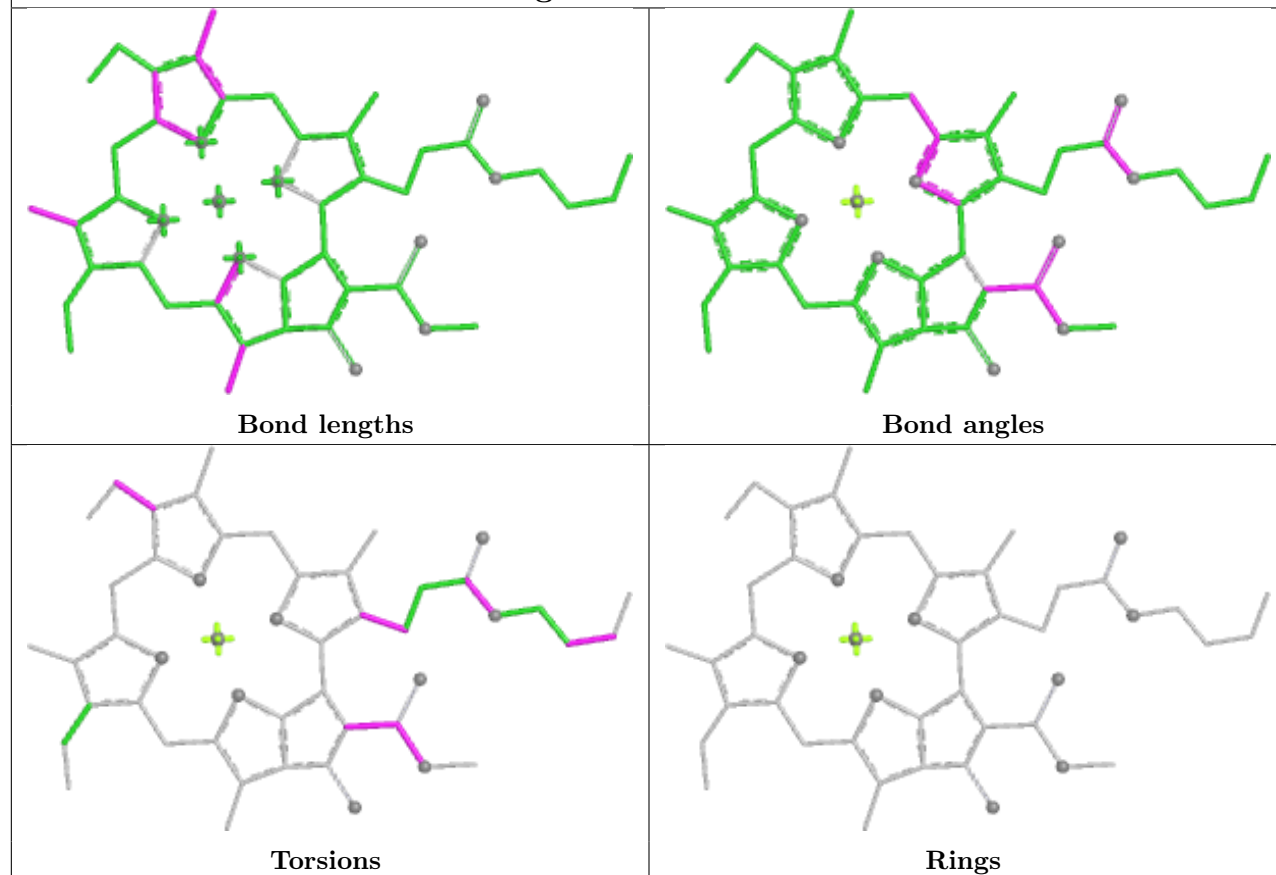
Ligand CHL R 606



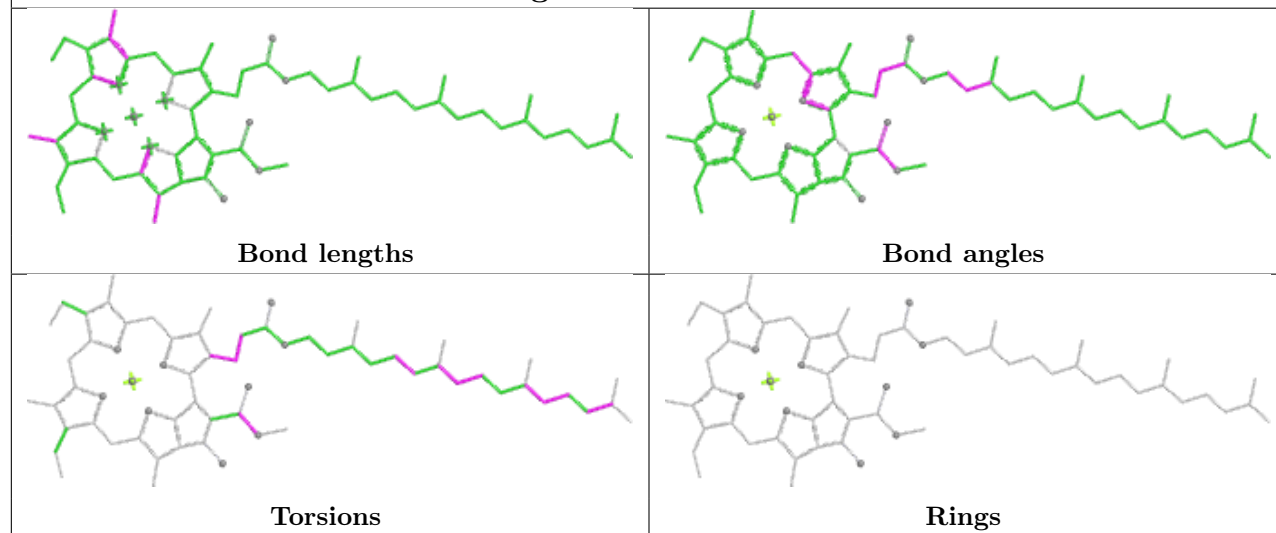
Ligand DGD c 519

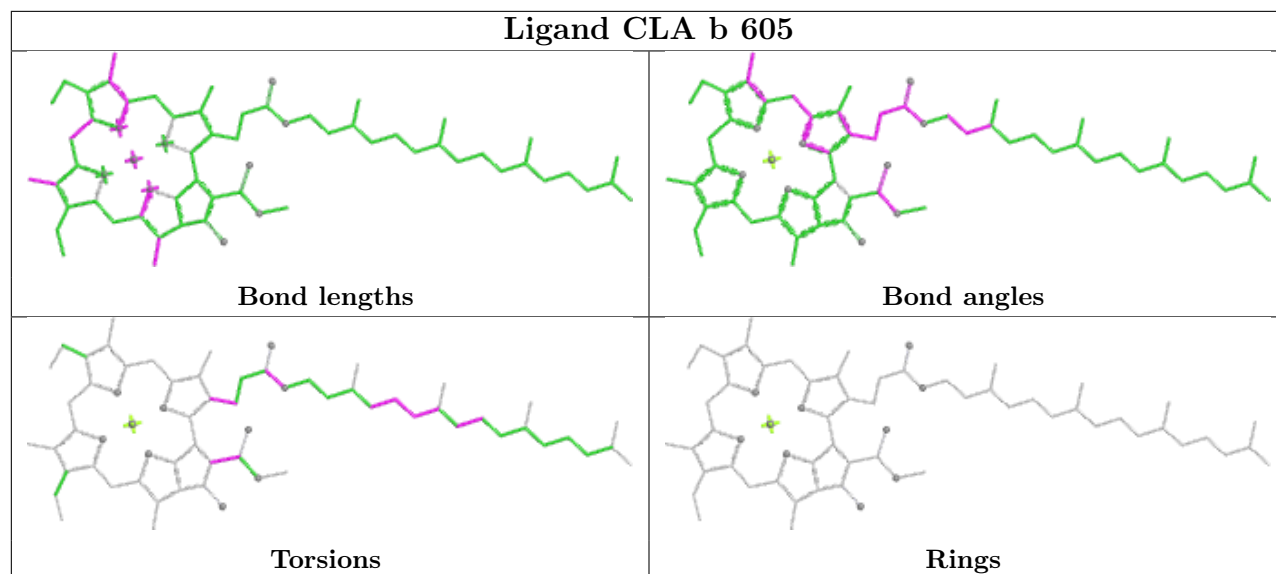
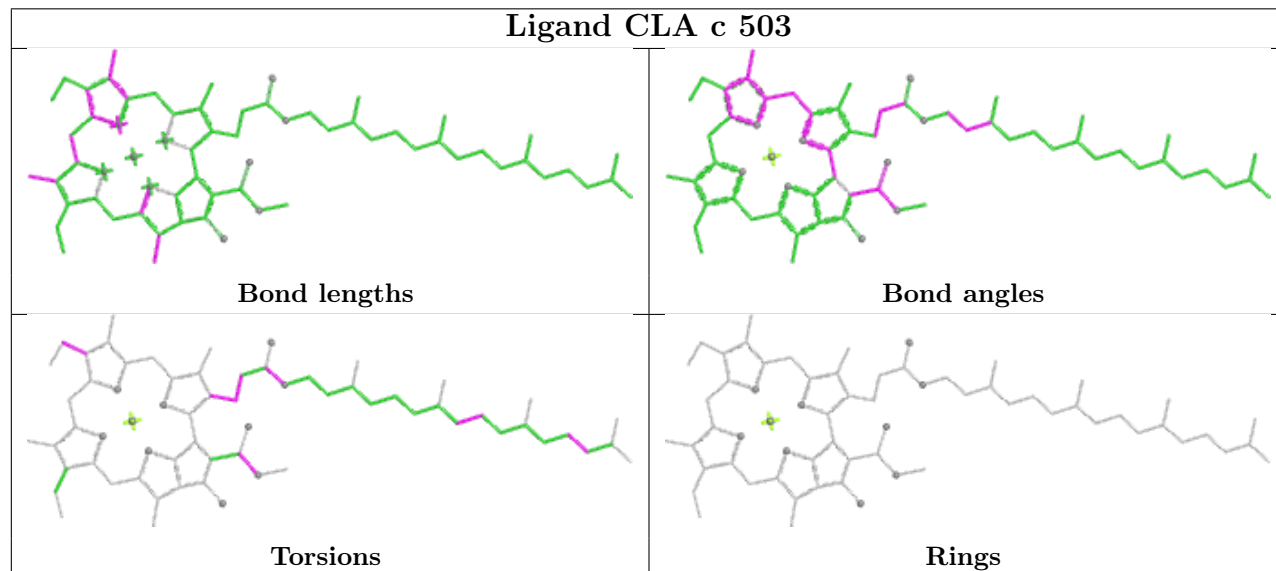


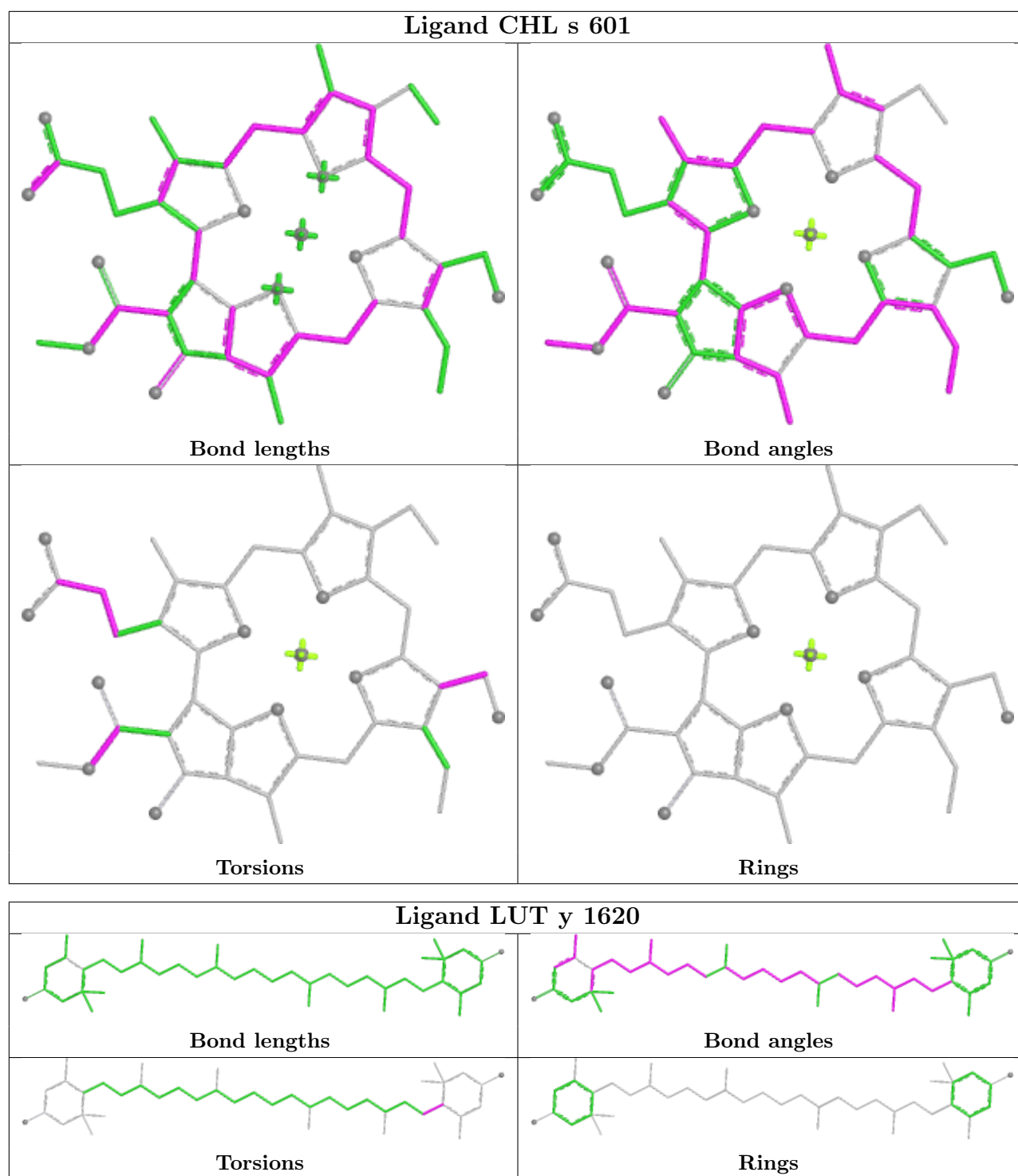
Ligand CLA n 611

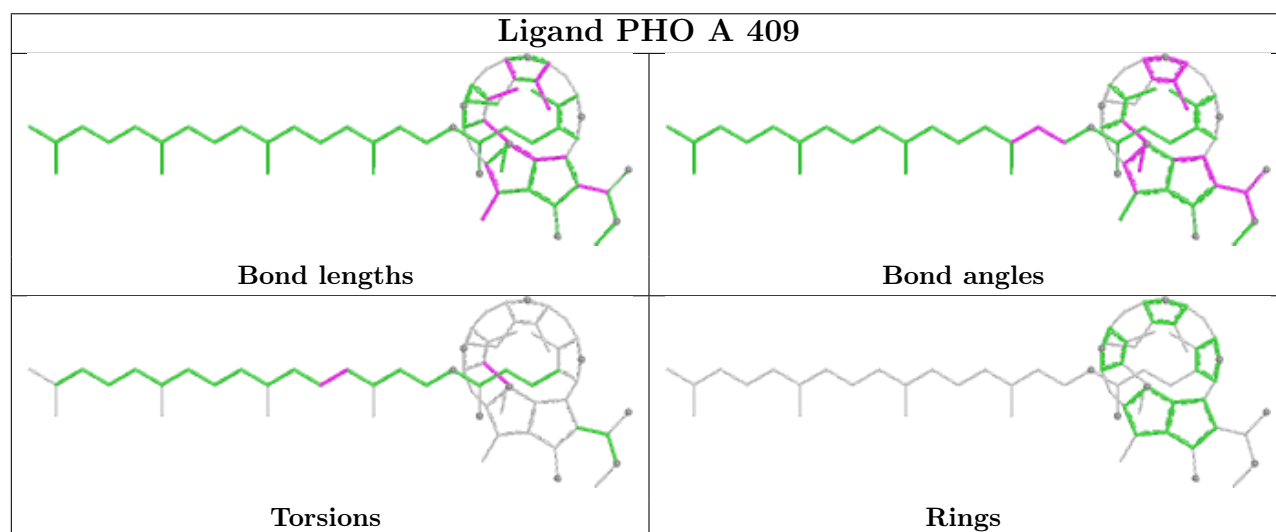
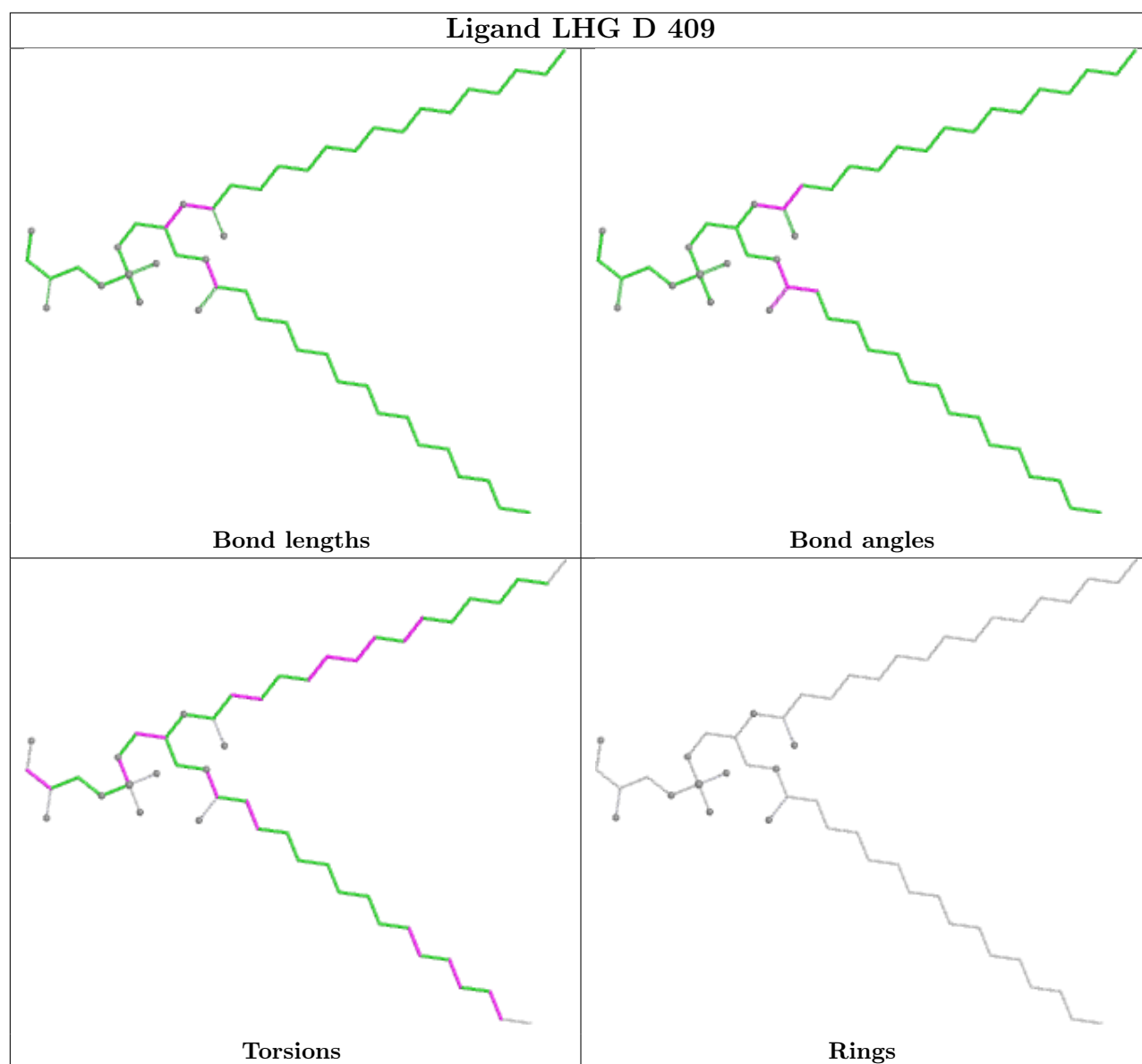


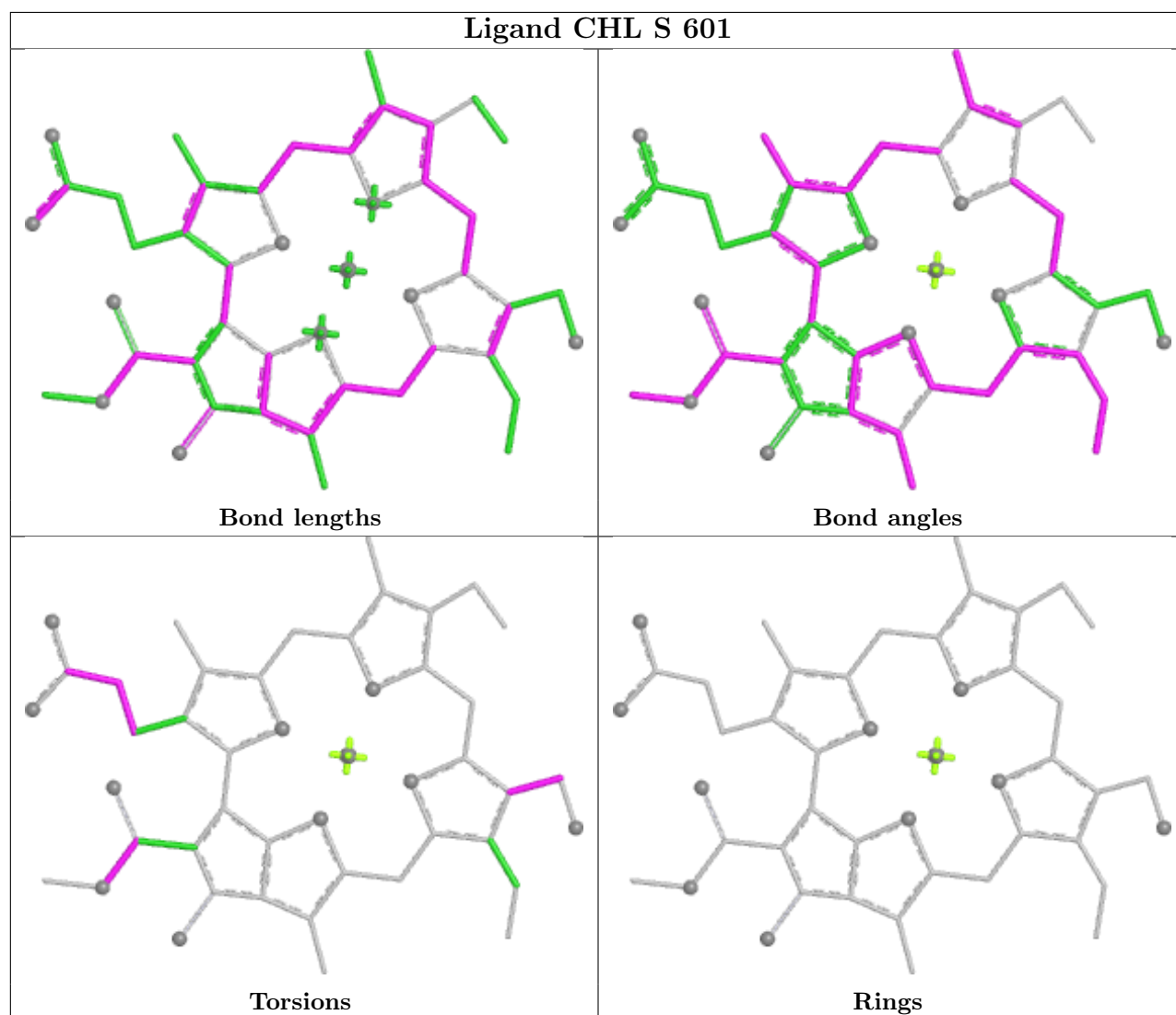
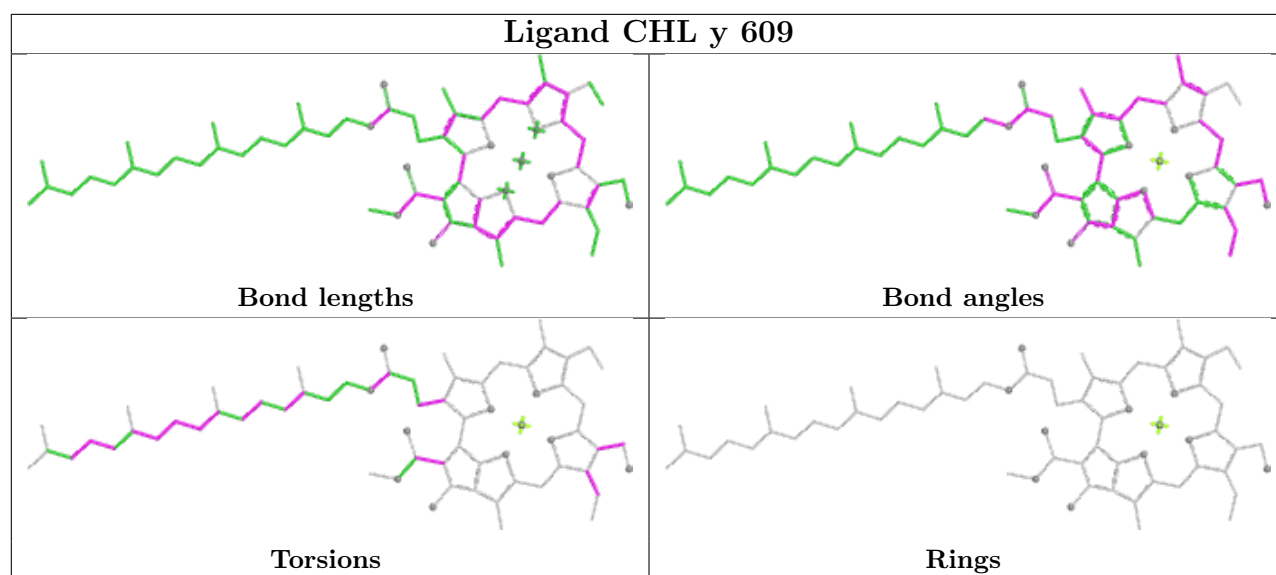
Ligand CLA G 610

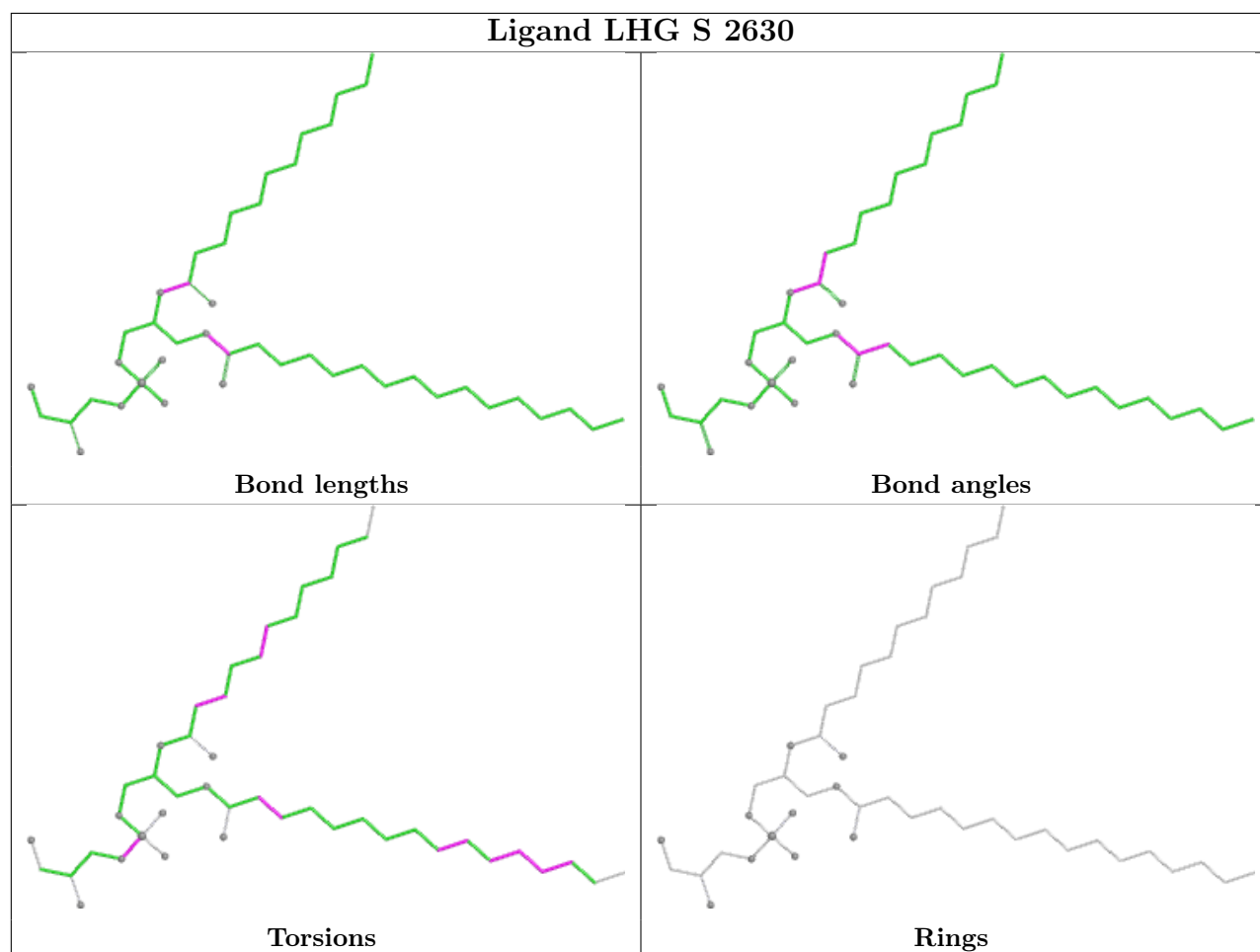
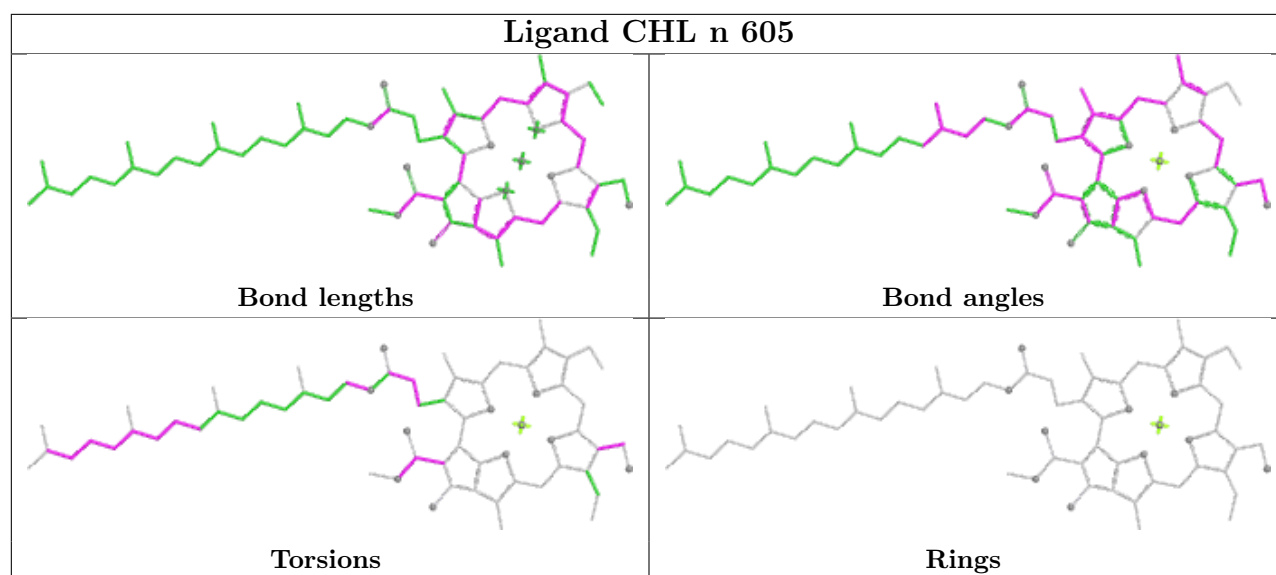


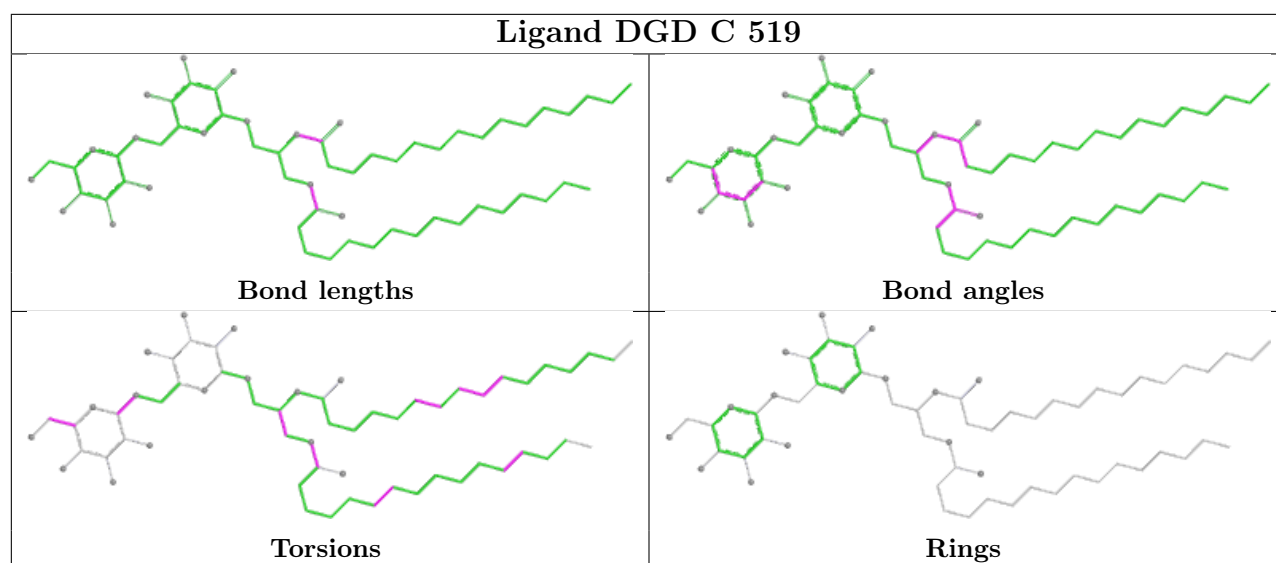
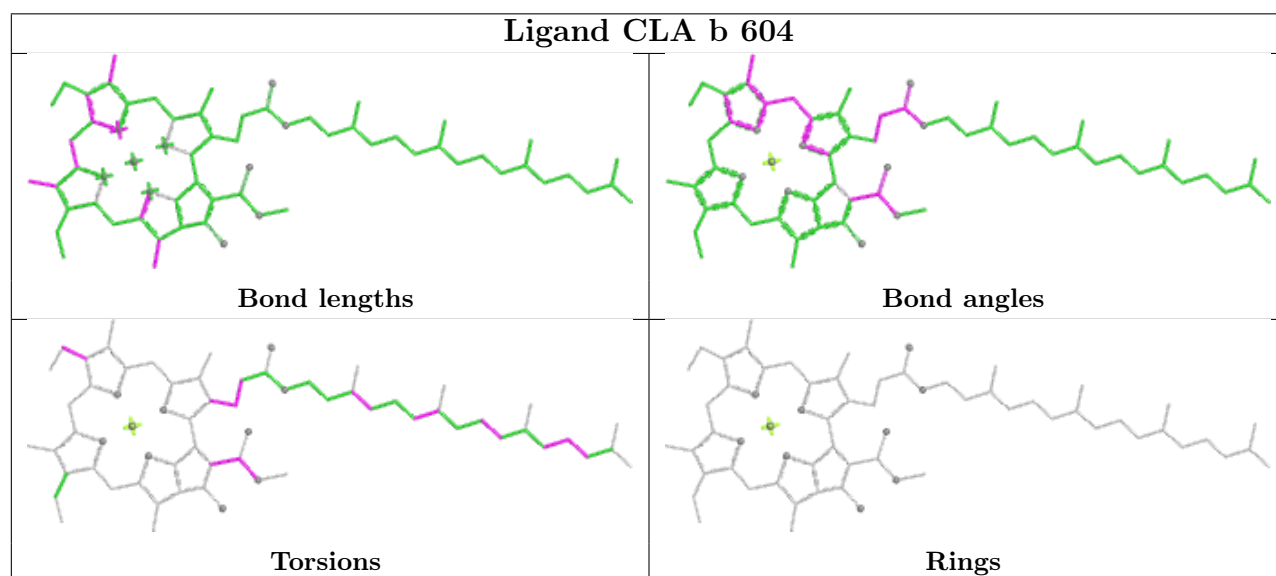
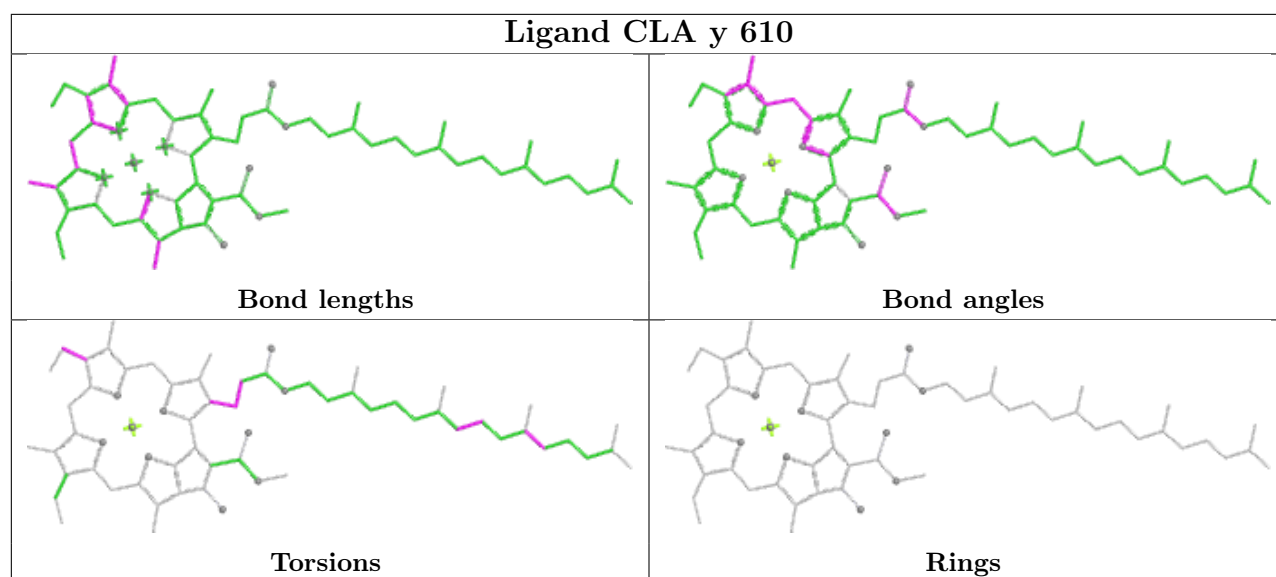
Ligand CLA b 605**Ligand CLA c 503**

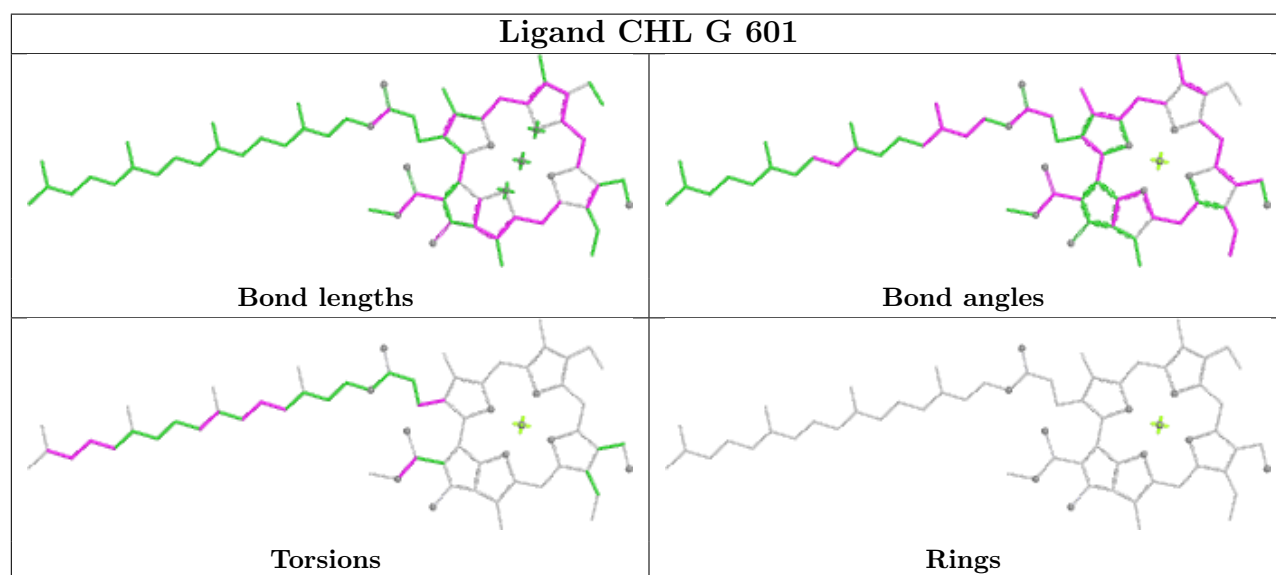
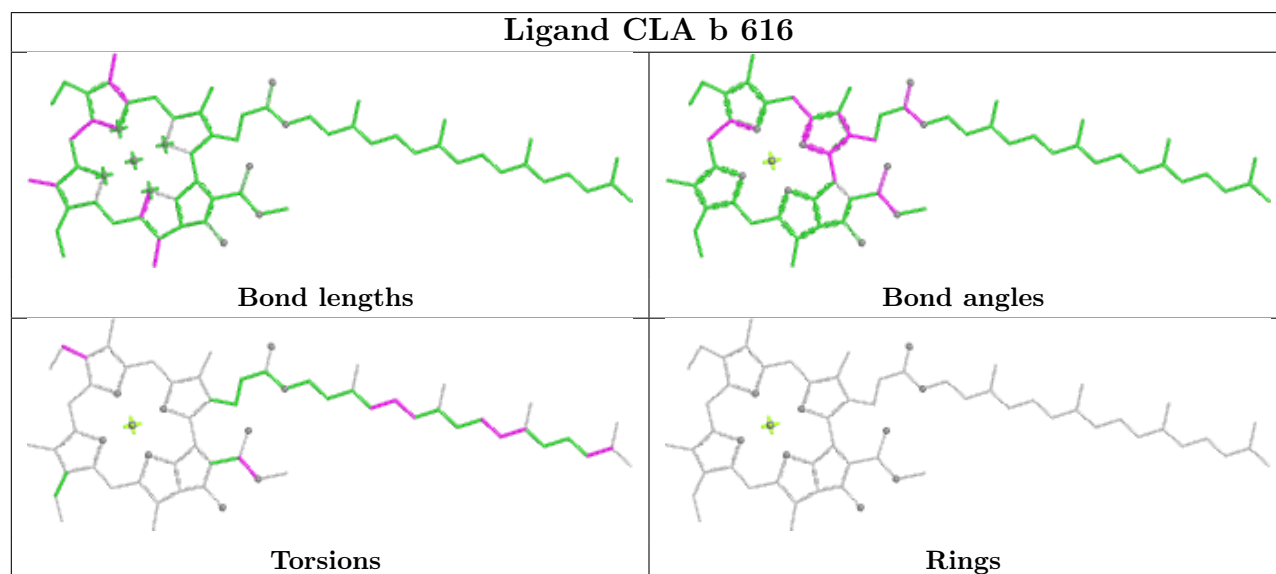
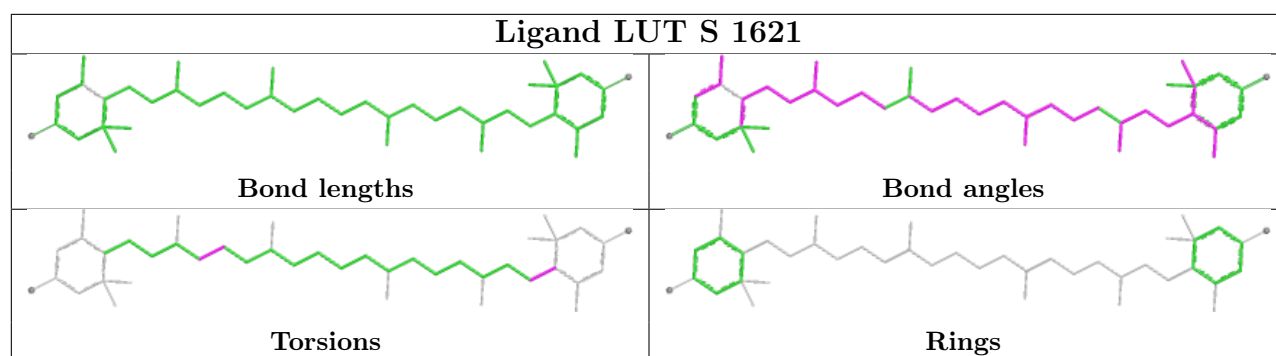


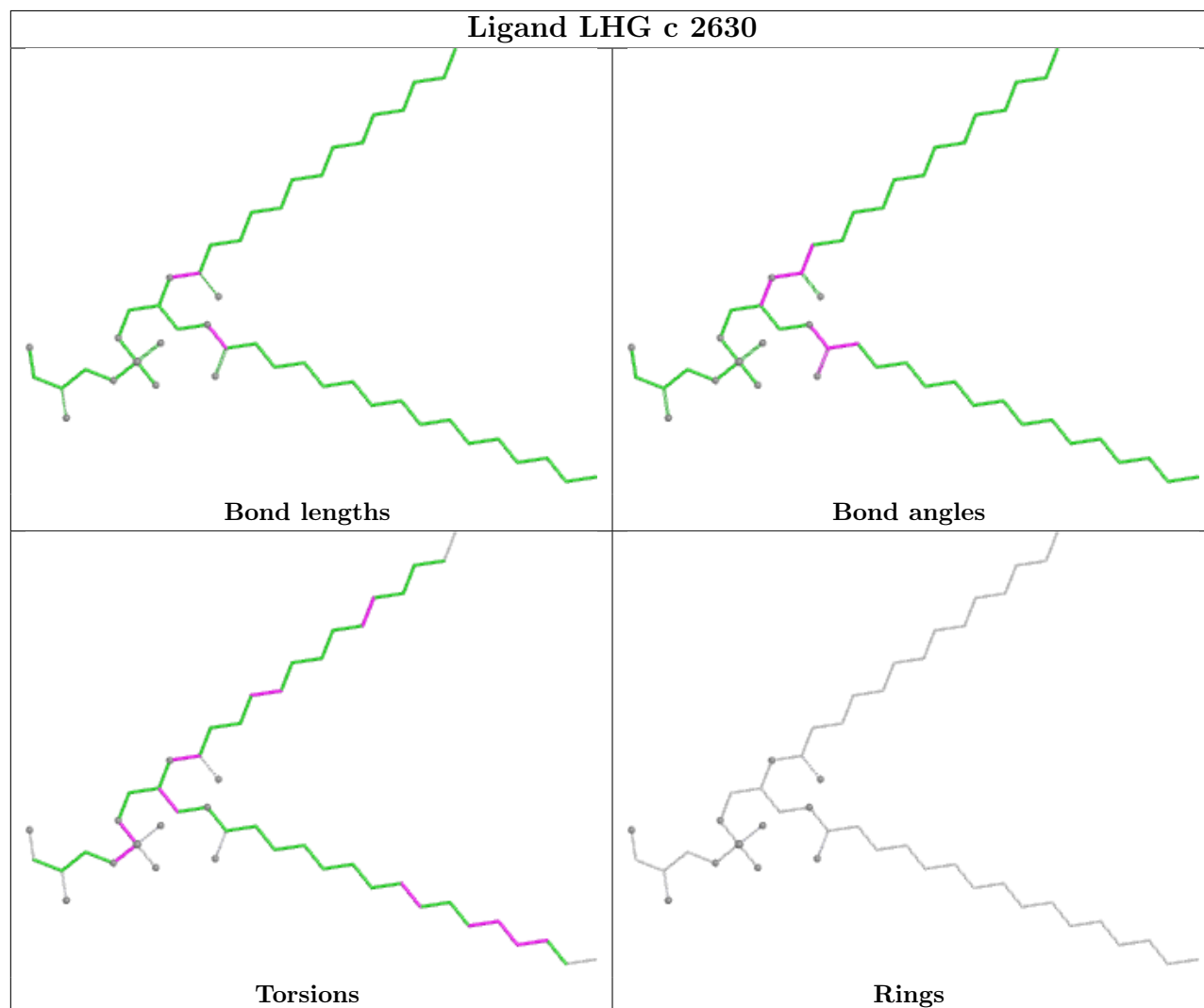
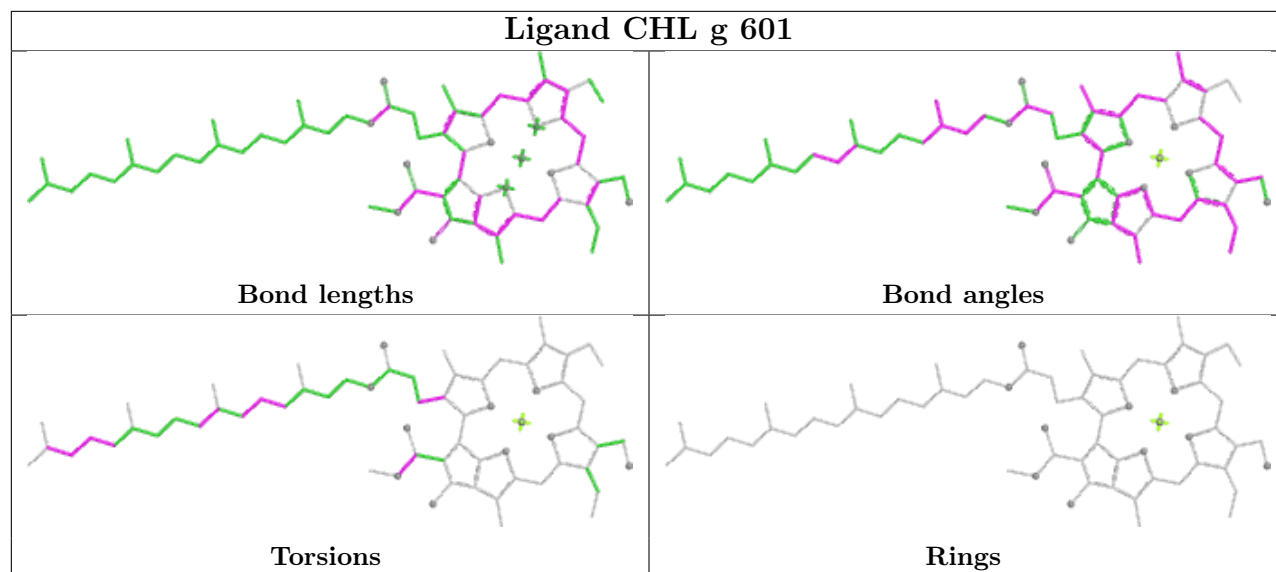




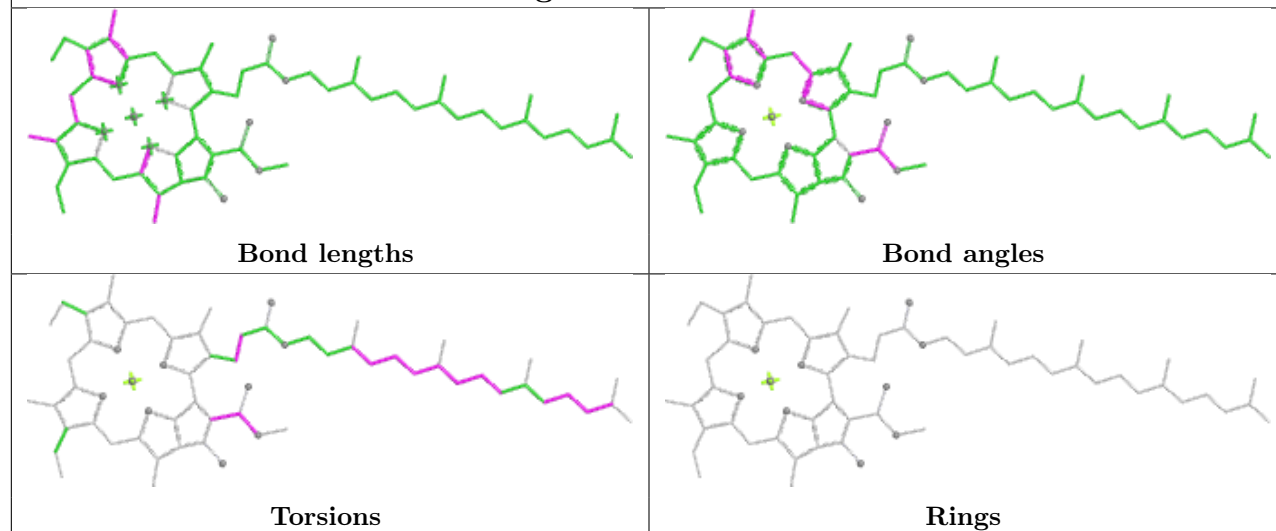




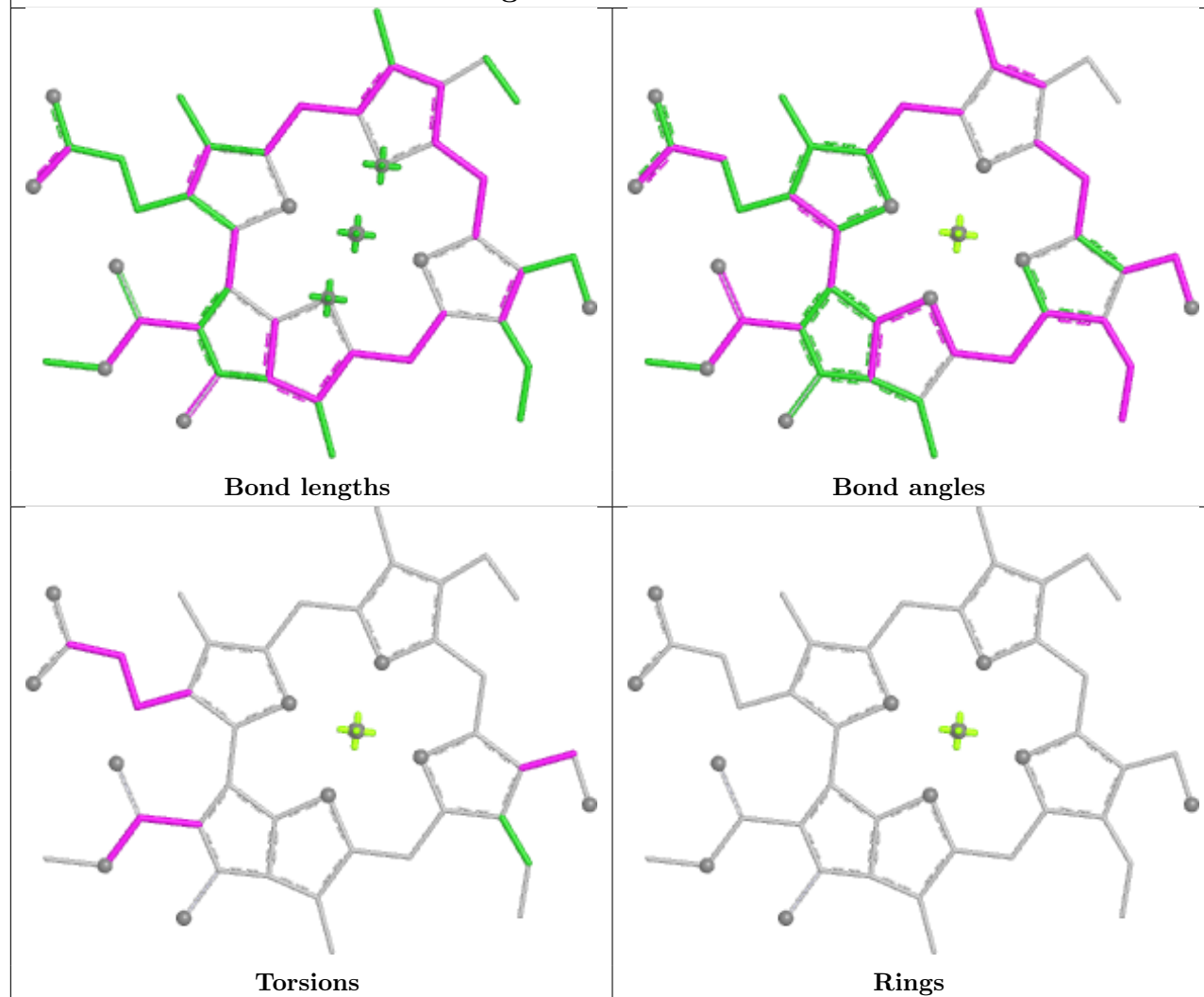




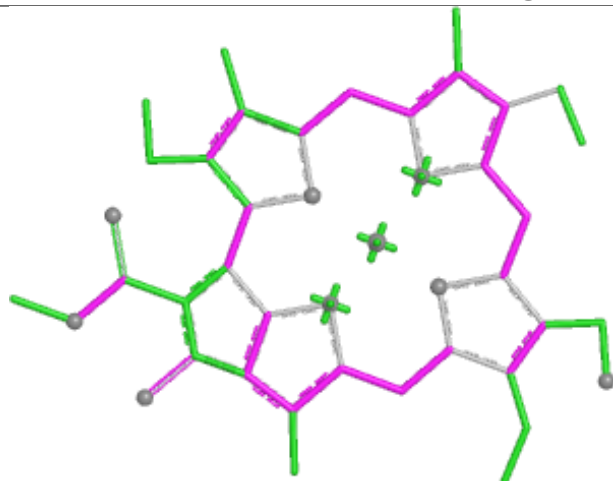
Ligand CLA b 615



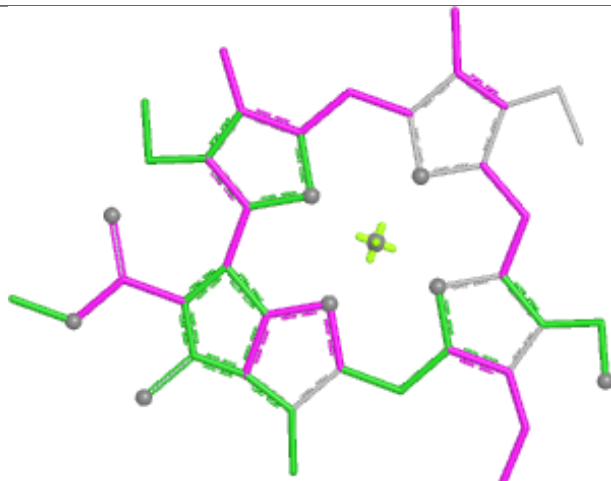
Ligand CHL Y 605



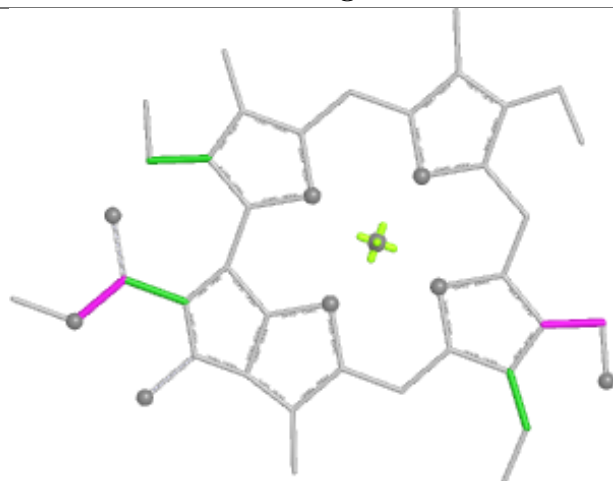
Ligand CHL s 607



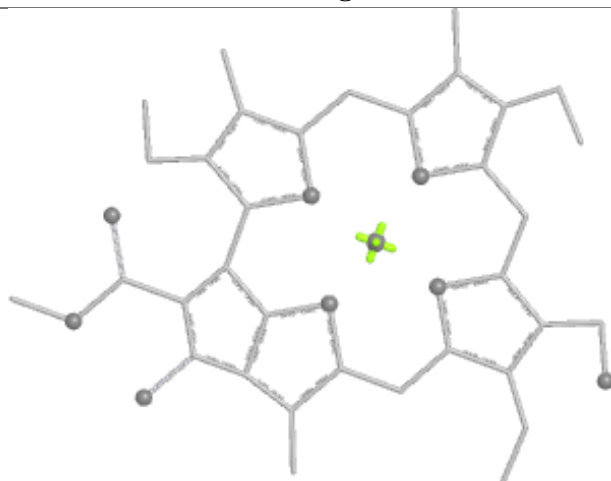
Bond lengths



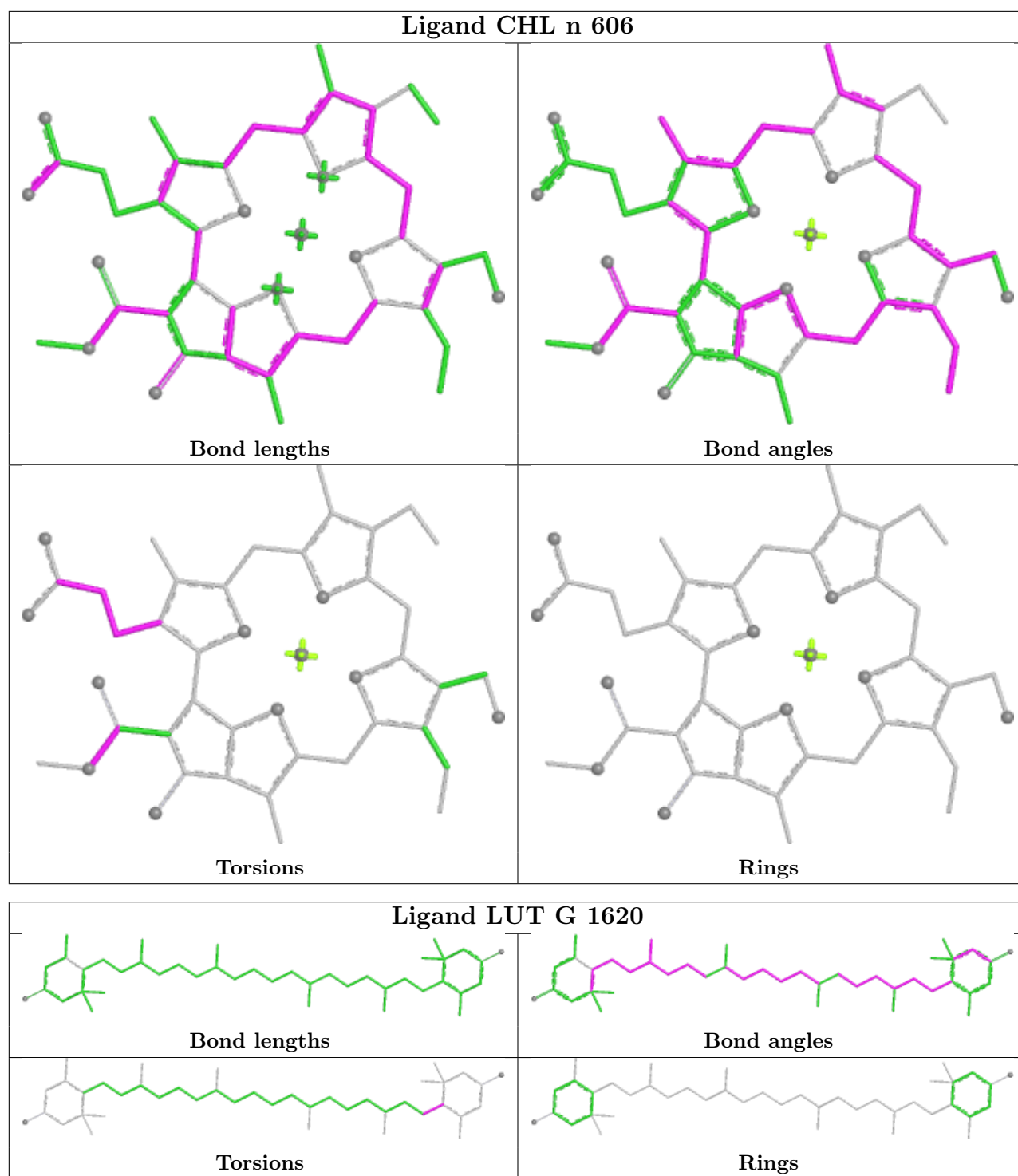
Bond angles

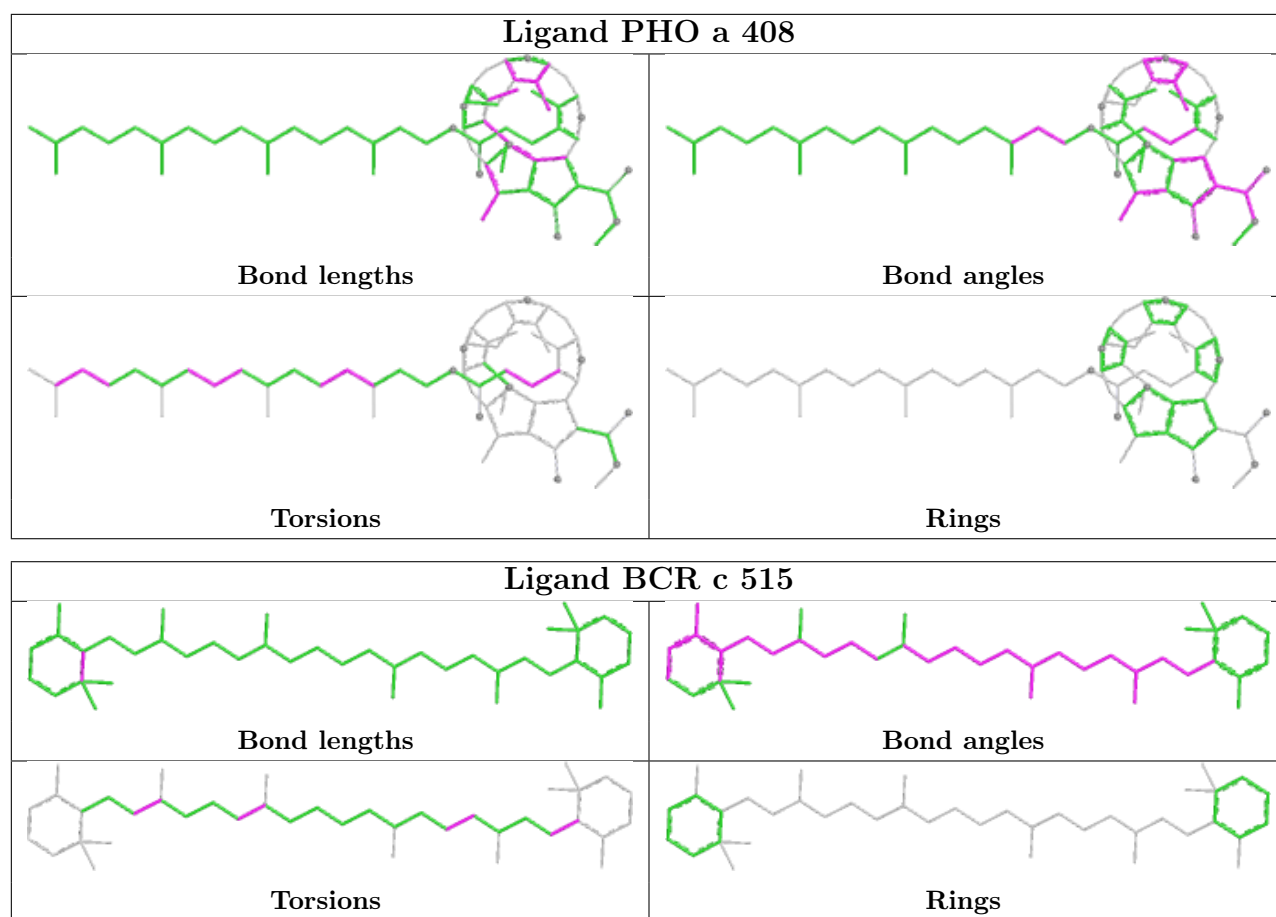


Torsions

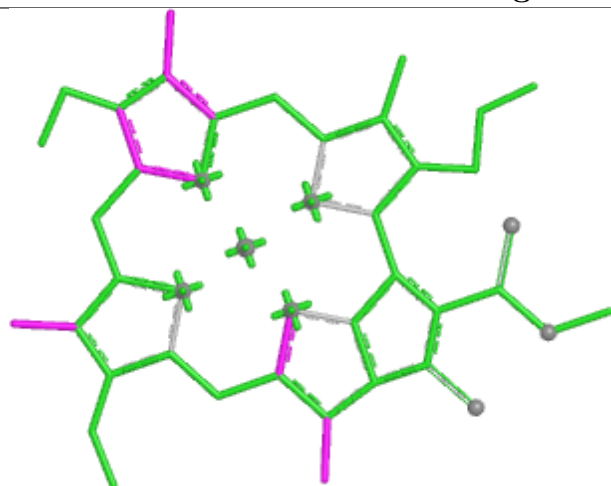


Rings

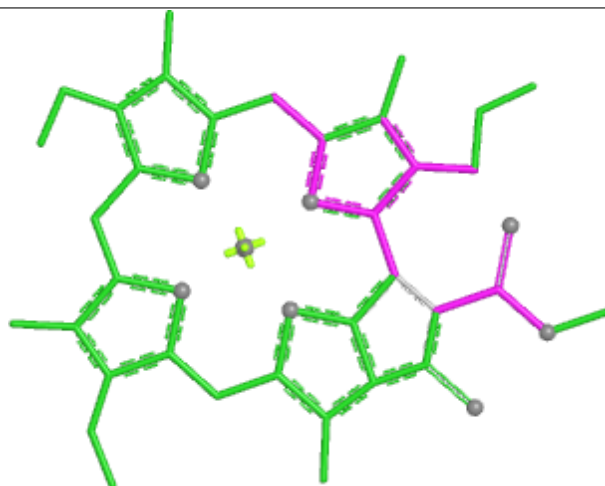




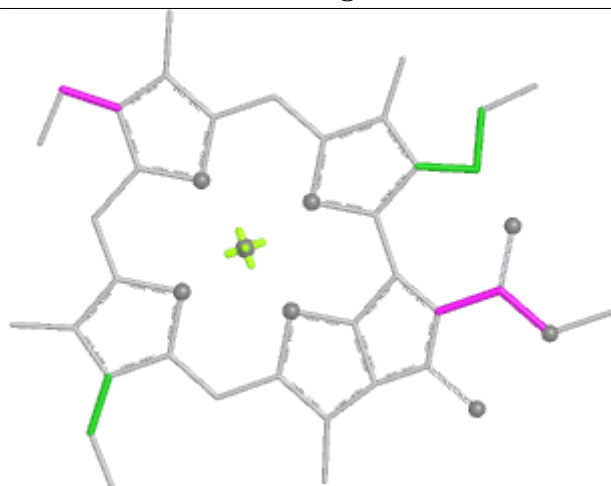
Ligand CLA G 612



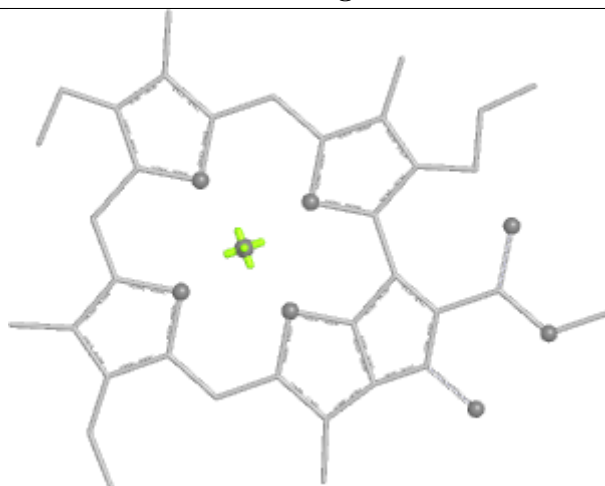
Bond lengths



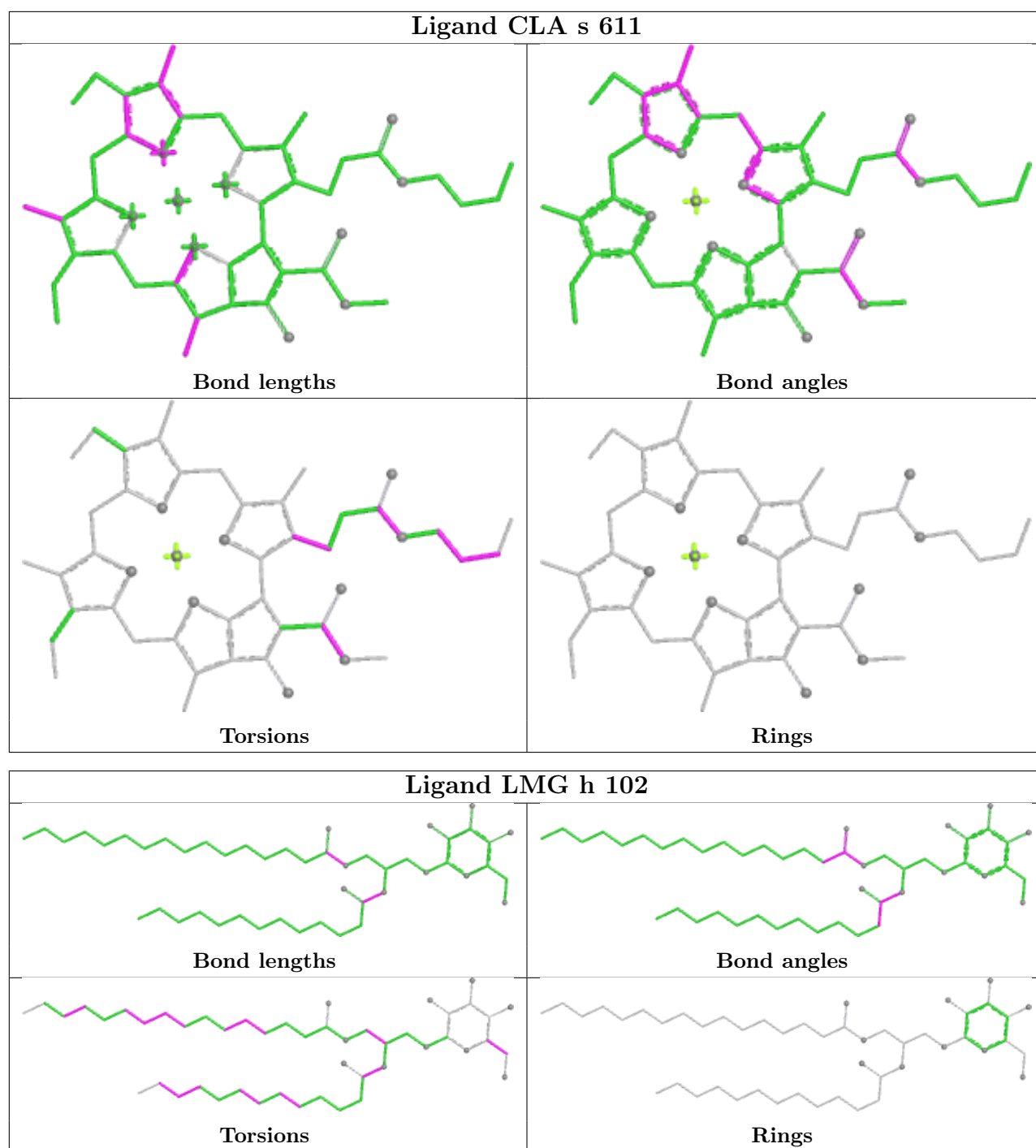
Bond angles

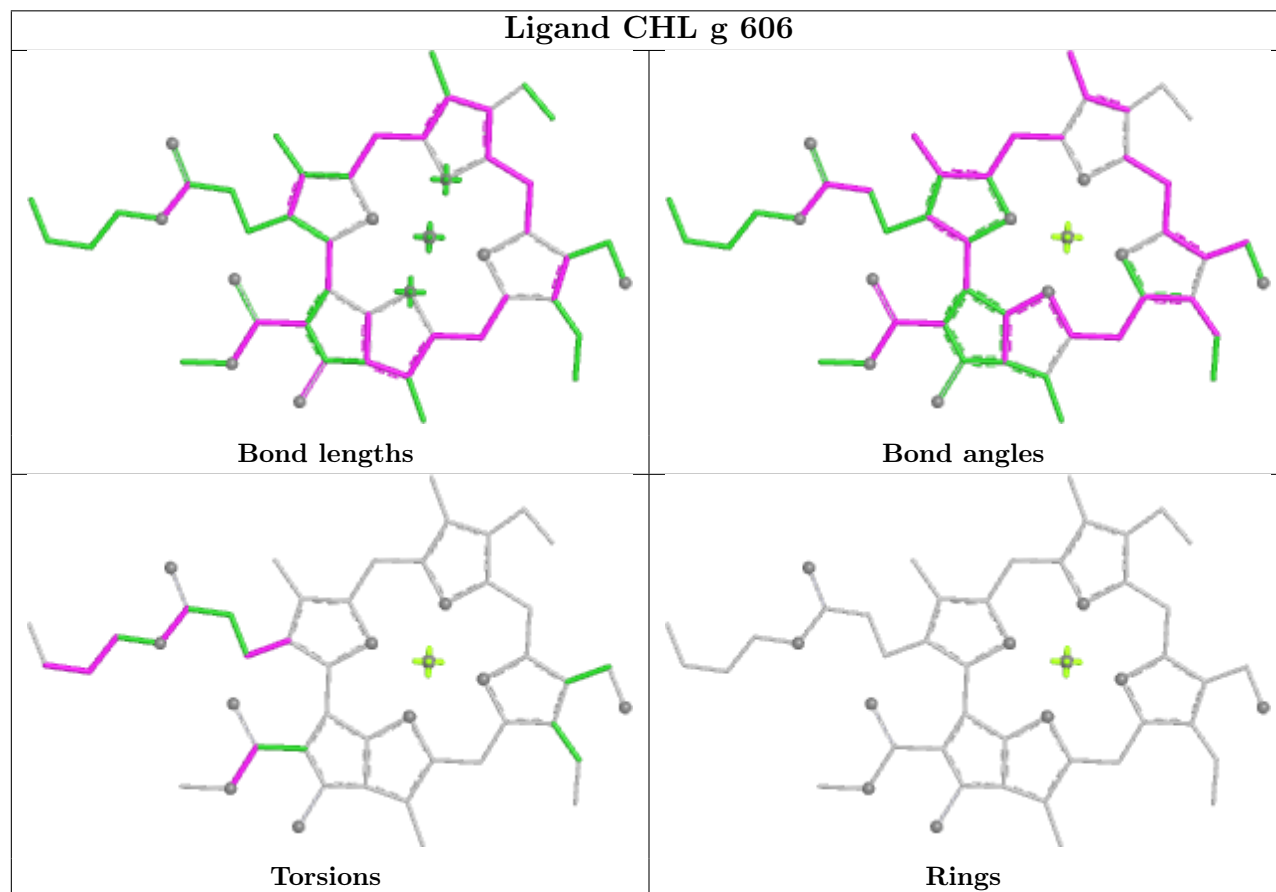
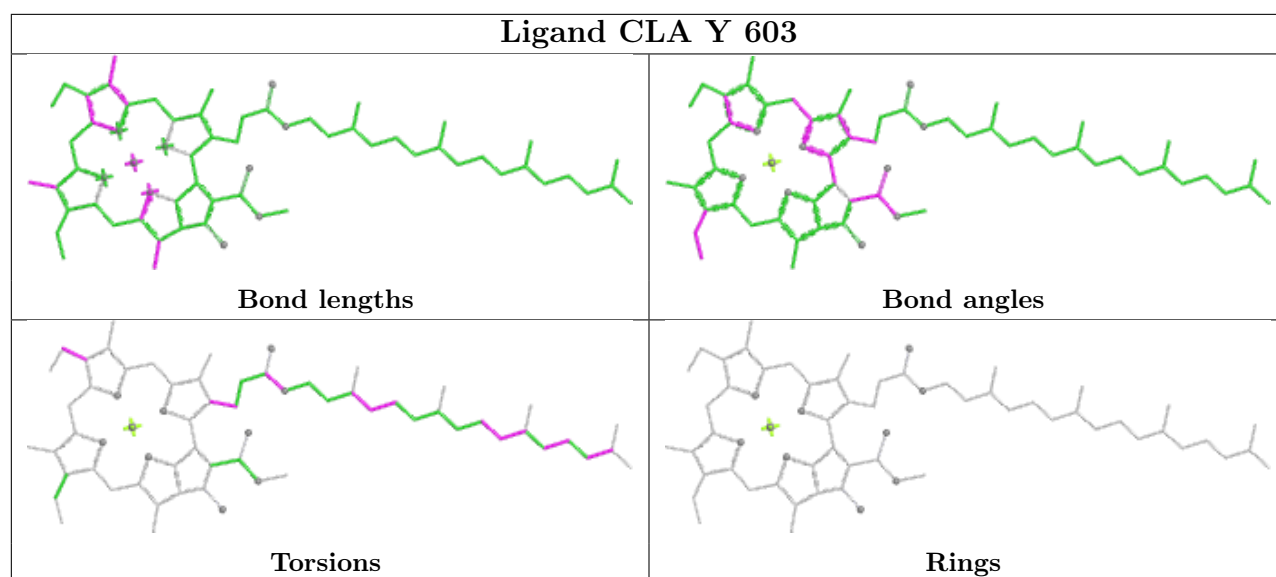


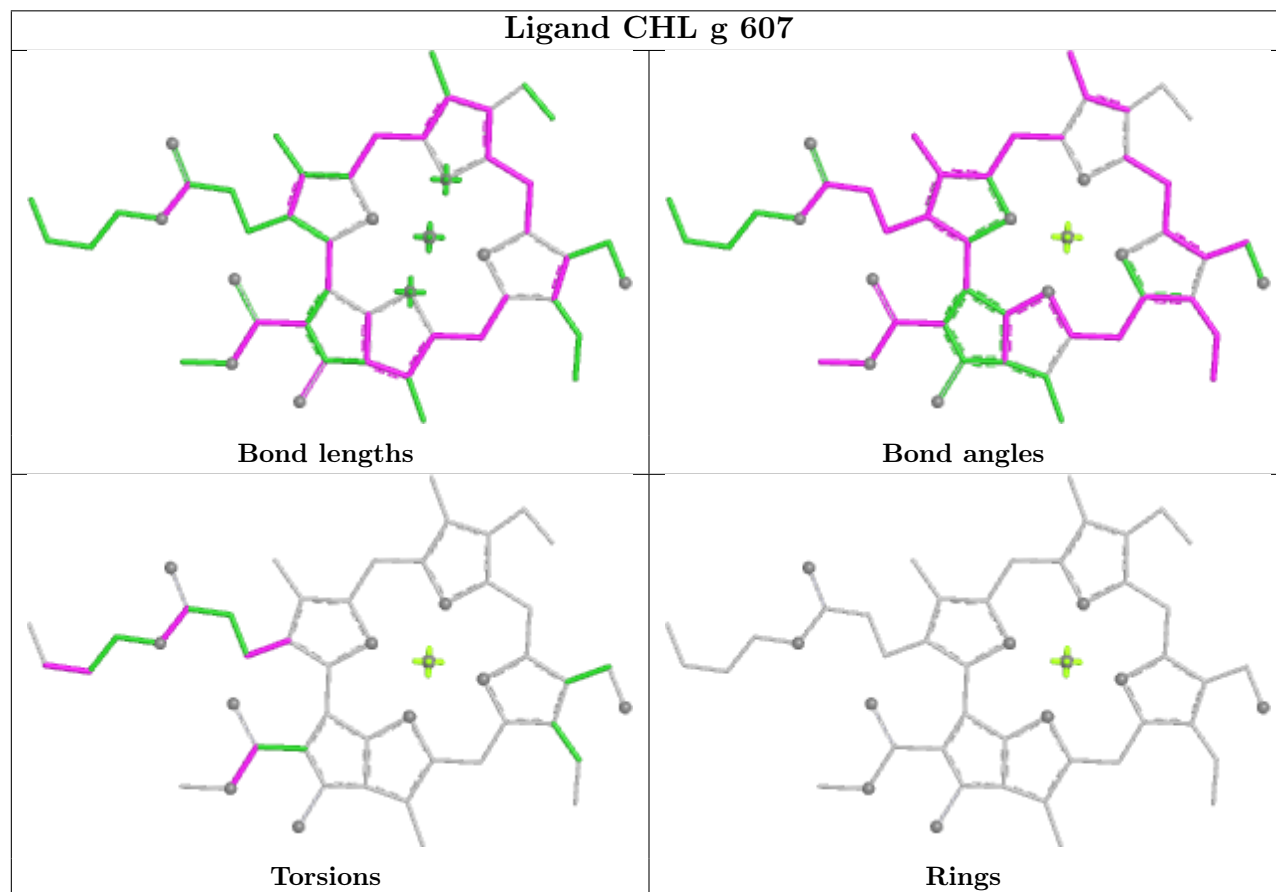
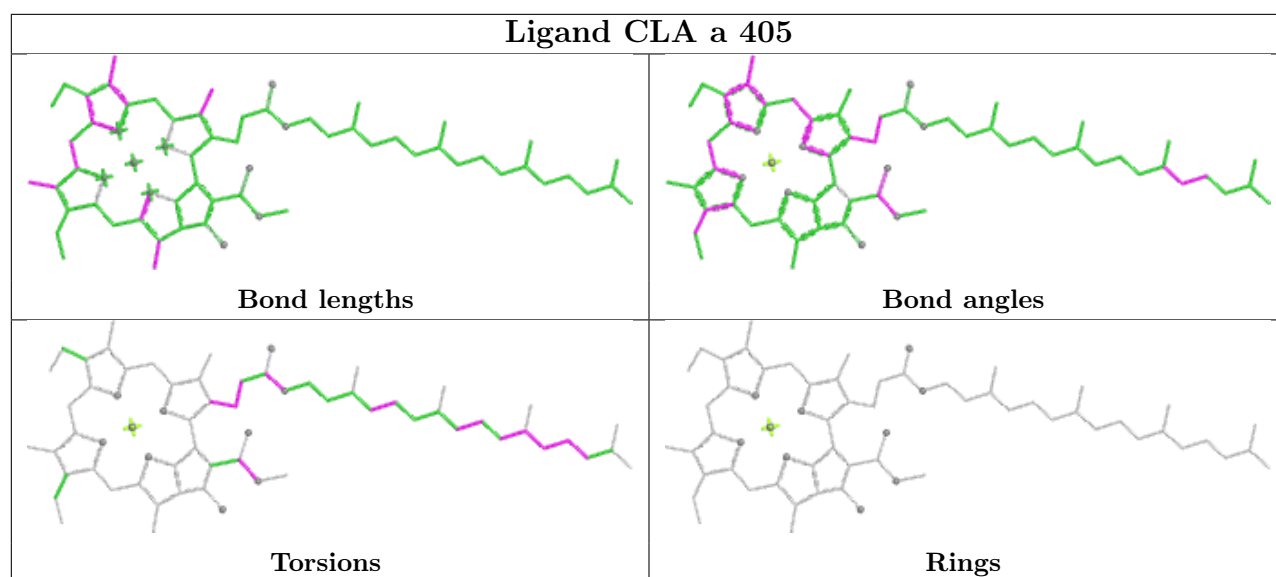
Torsions

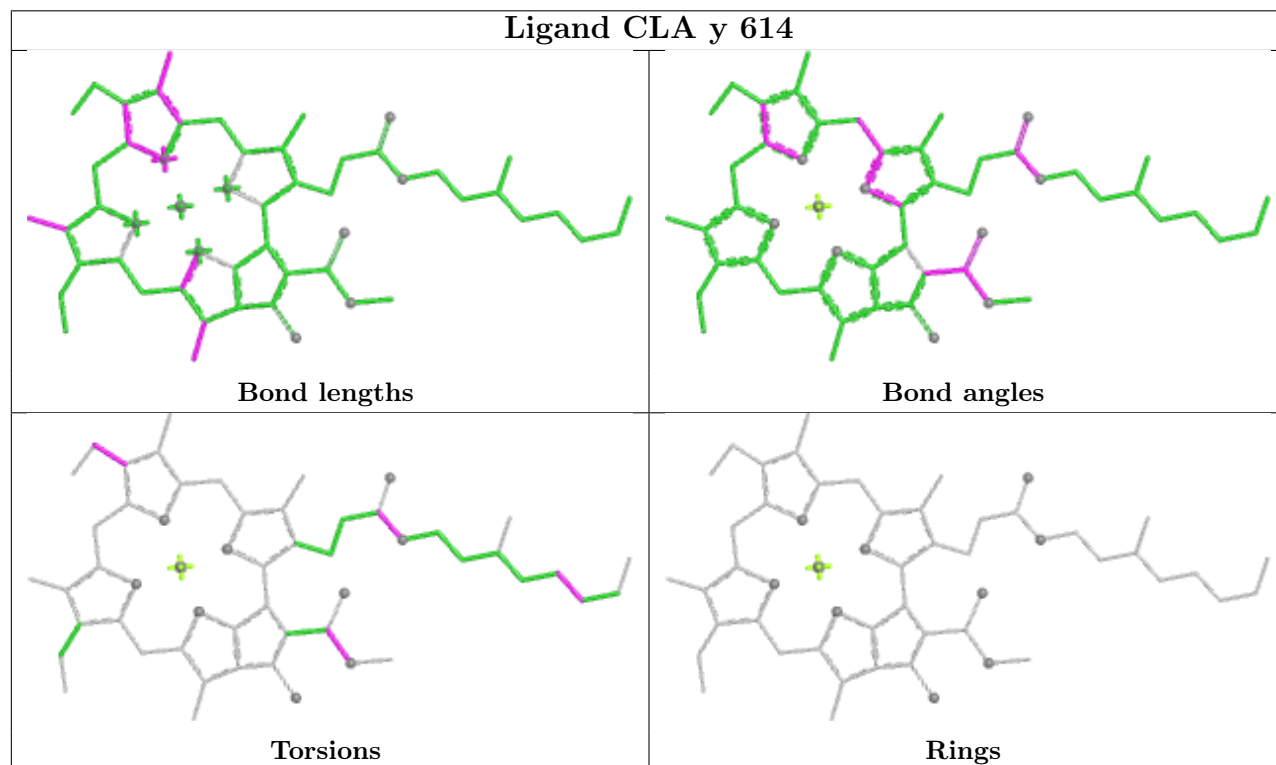
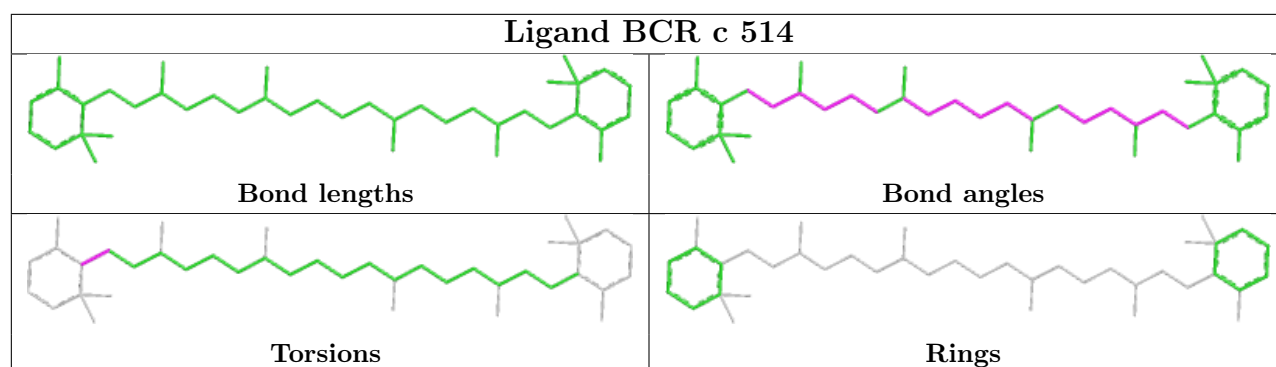


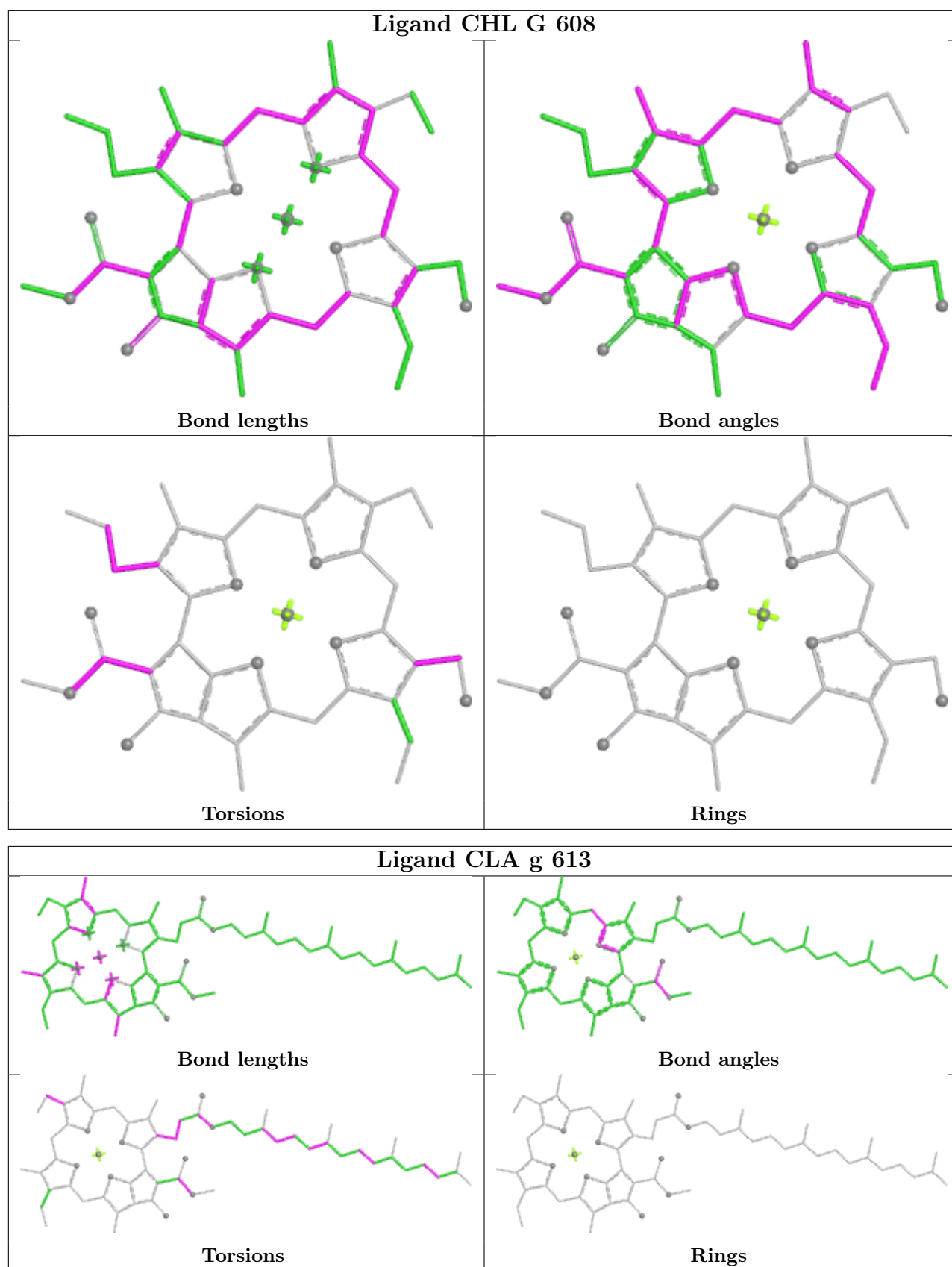
Rings

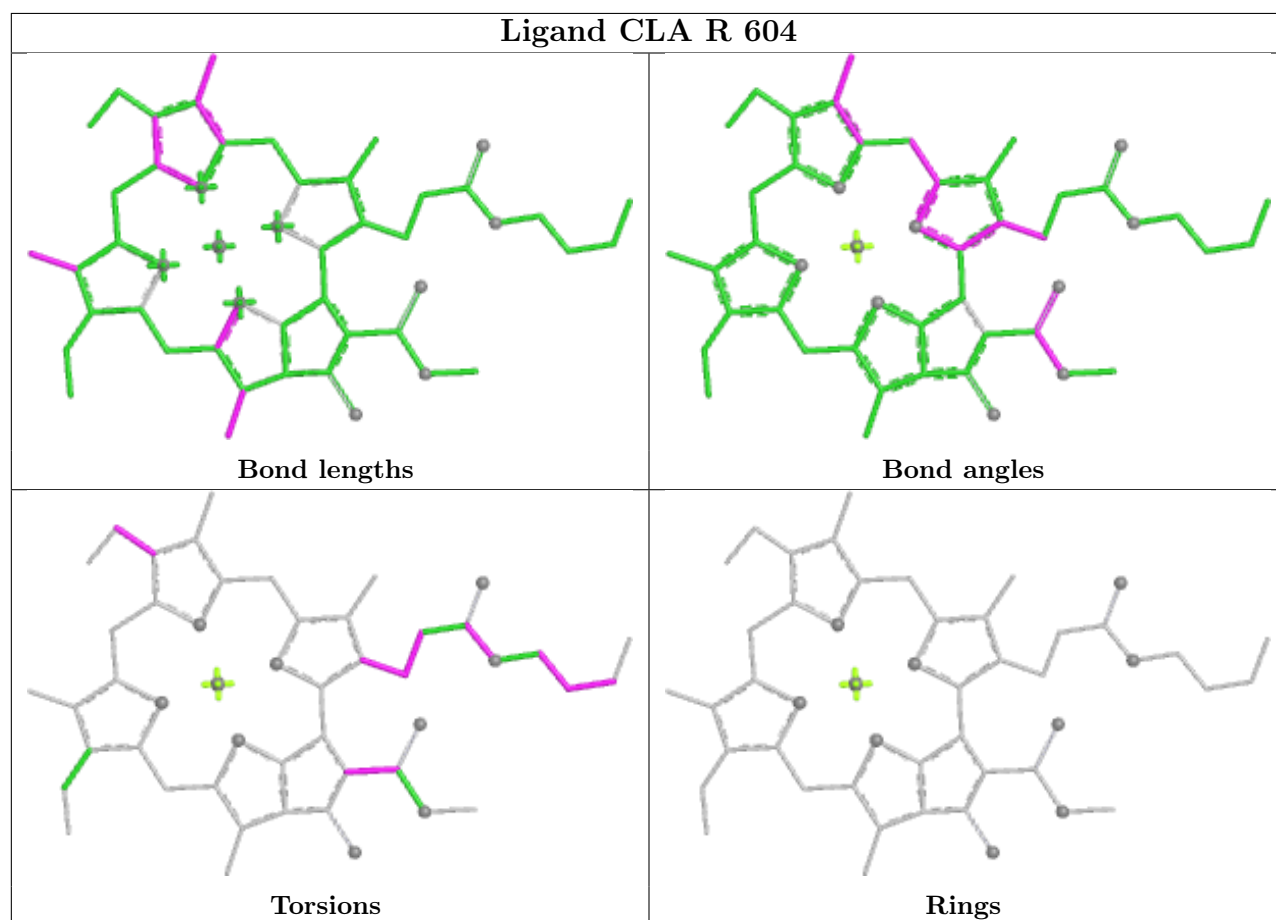
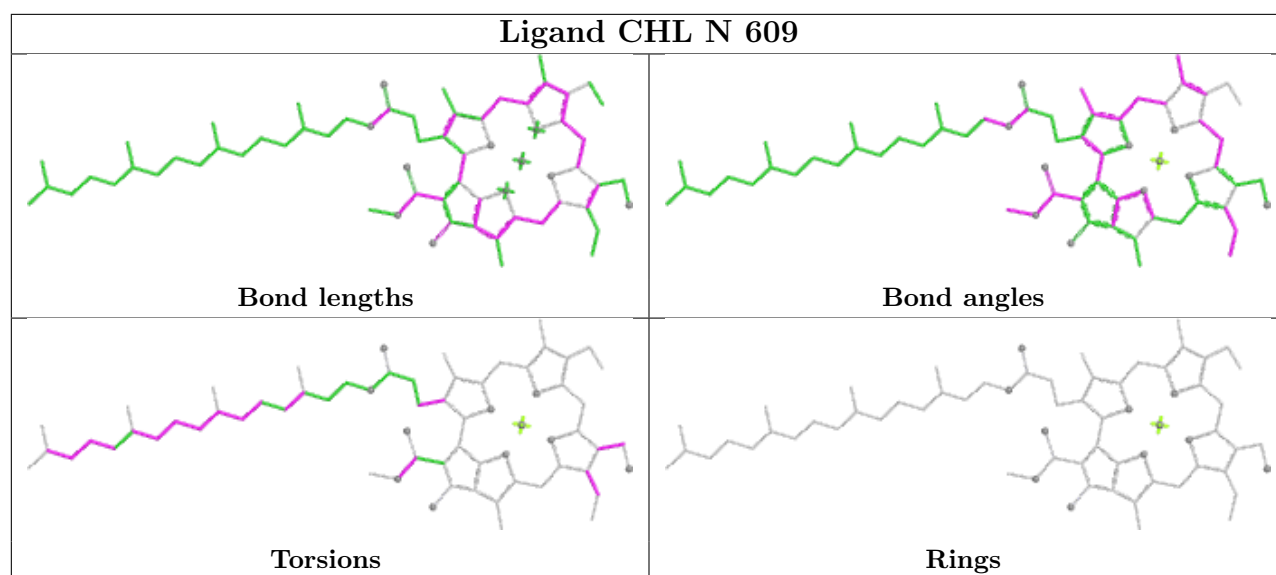


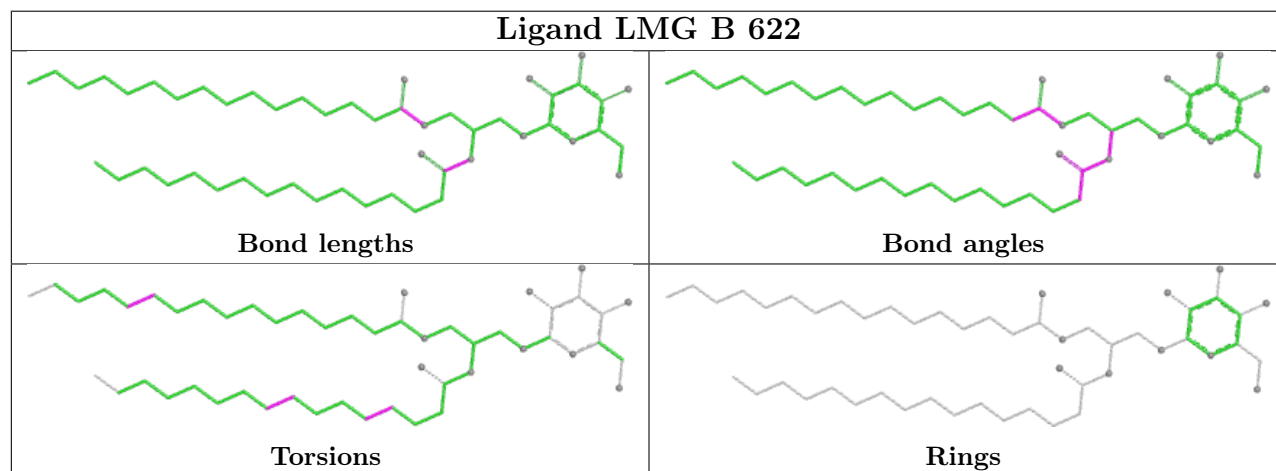
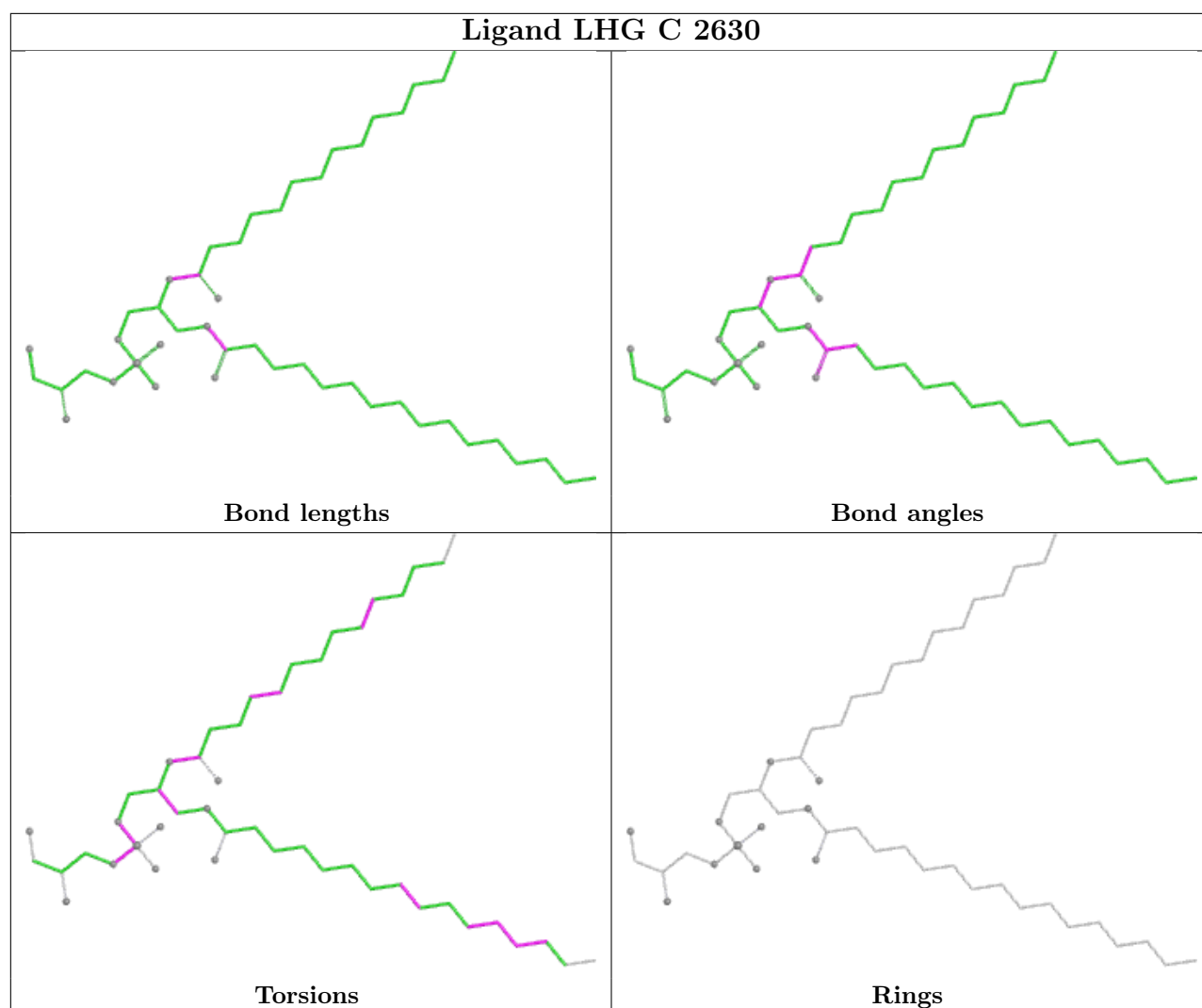


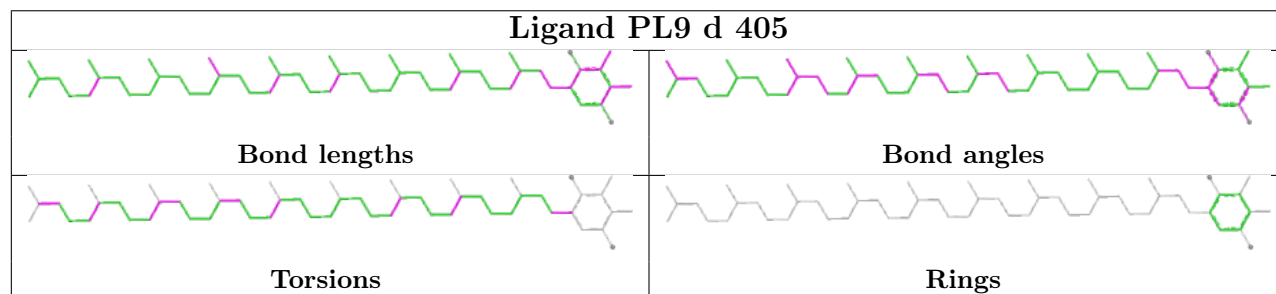
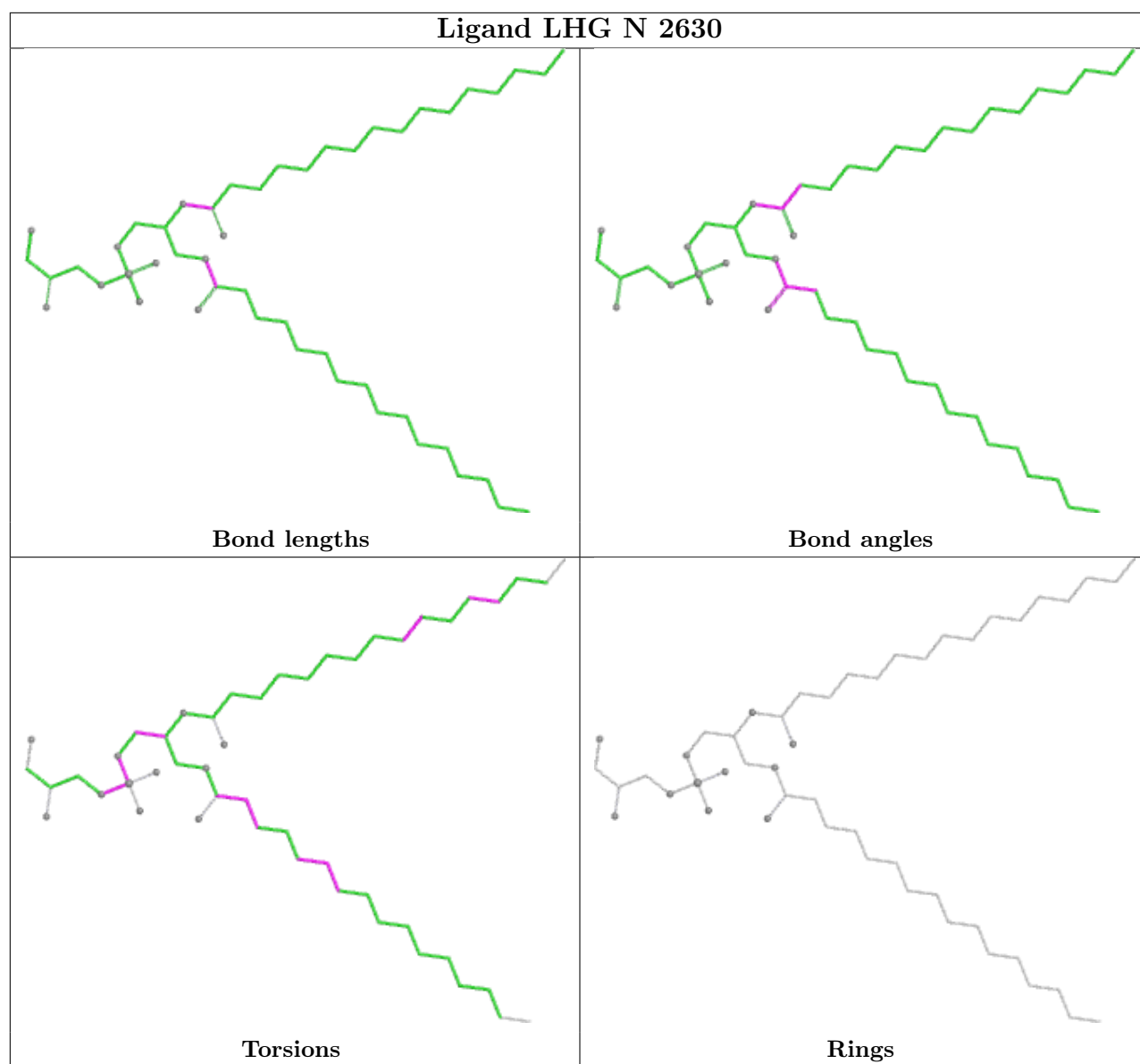




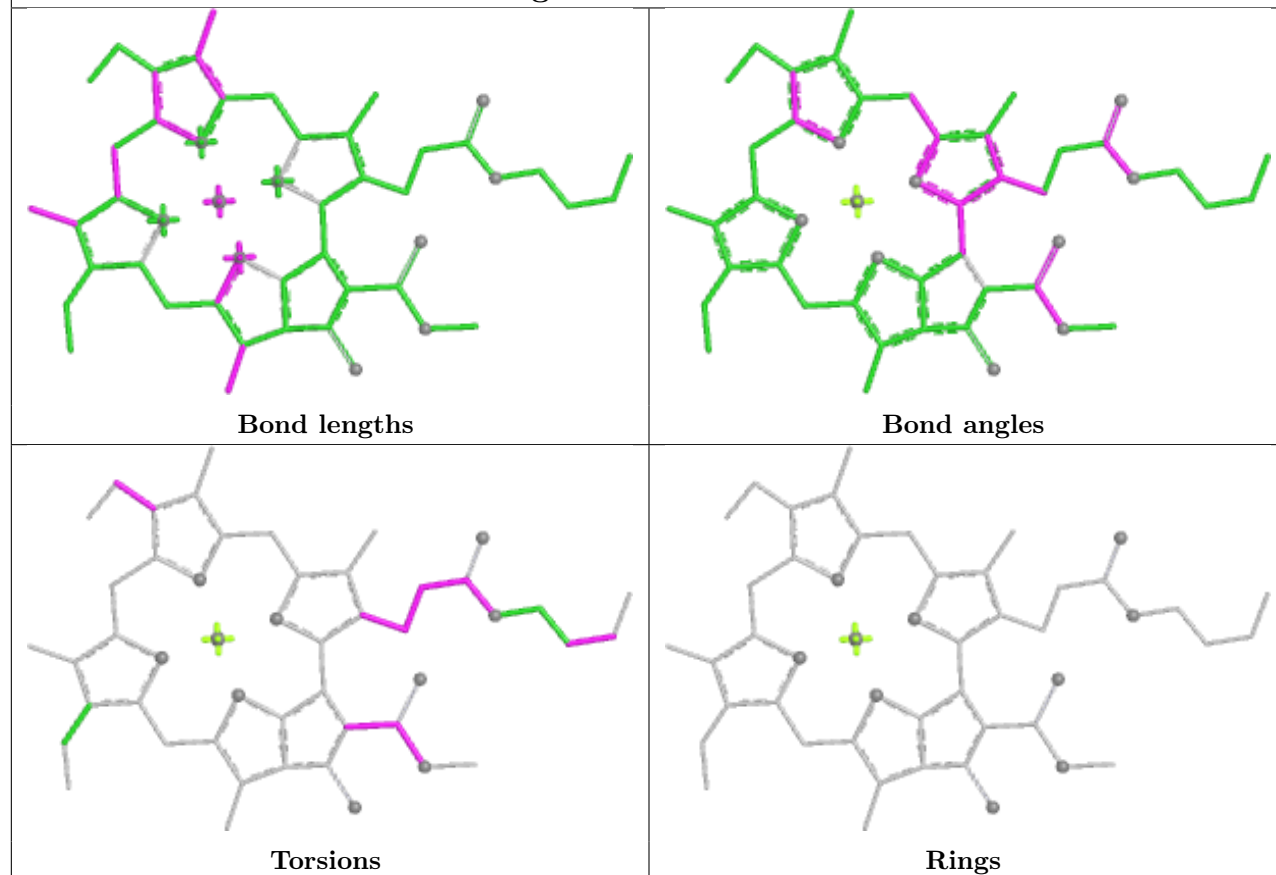




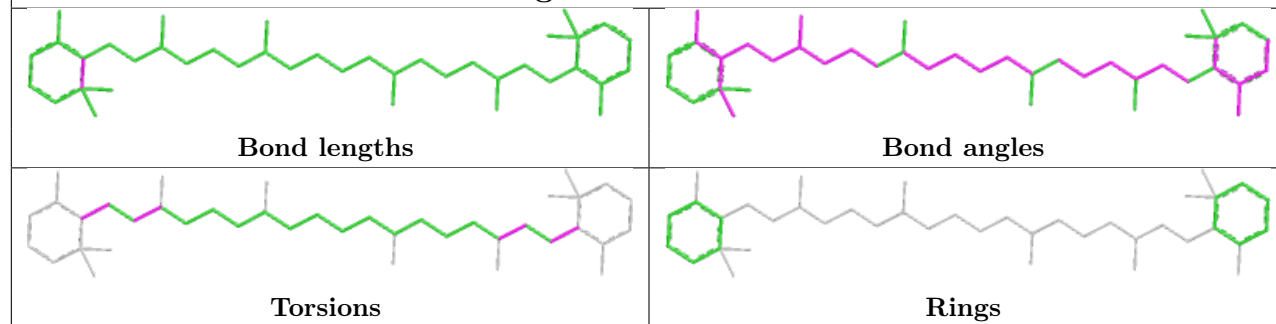




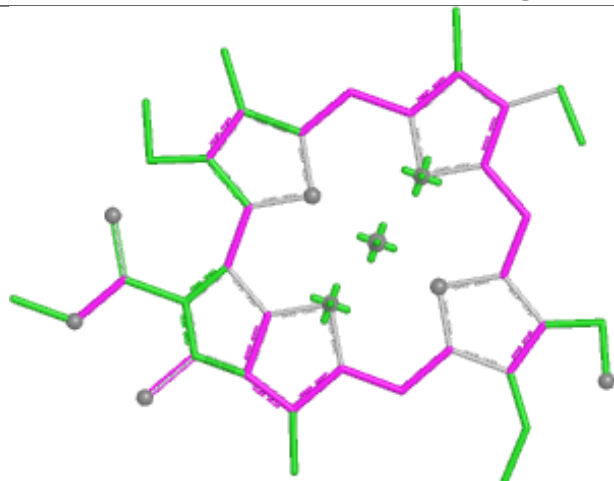
Ligand CLA R 603



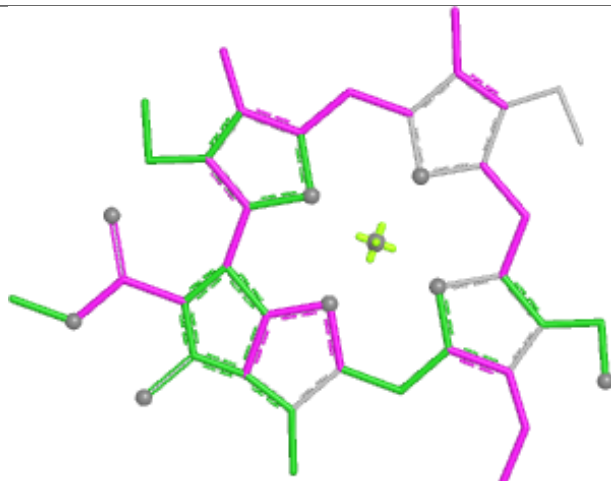
Ligand BCR c 516



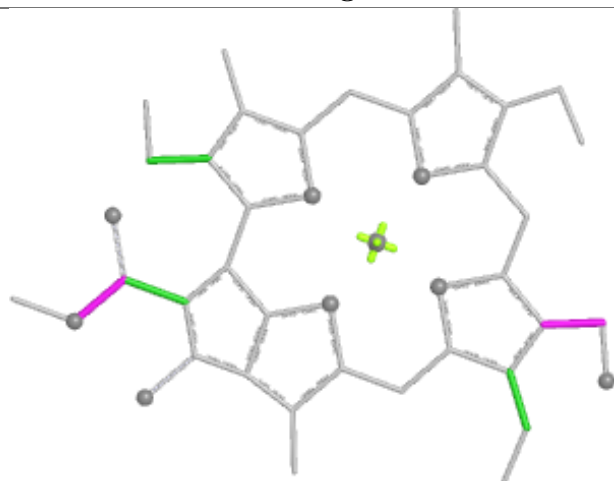
Ligand CHL S 607



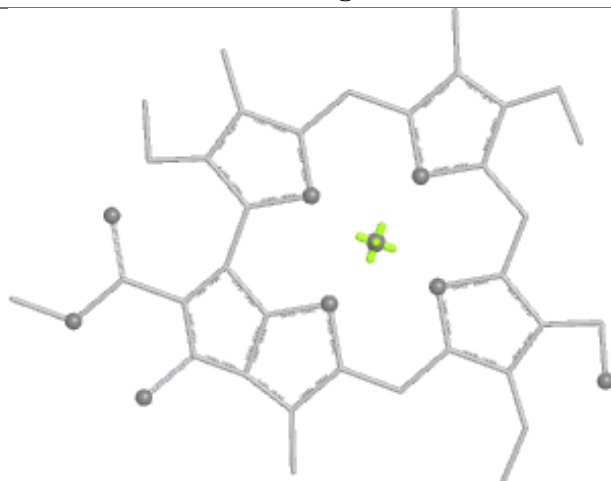
Bond lengths



Bond angles

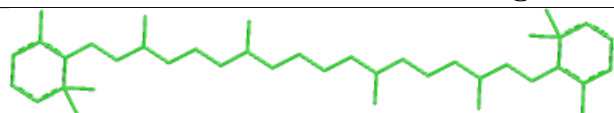


Torsions

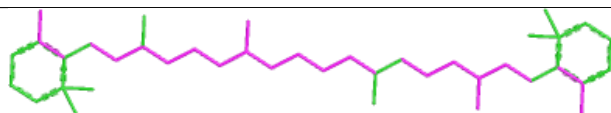


Rings

Ligand BCR A 411



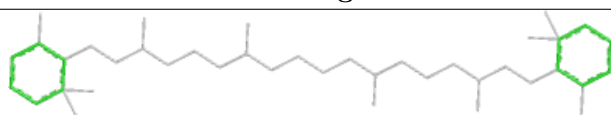
Bond lengths



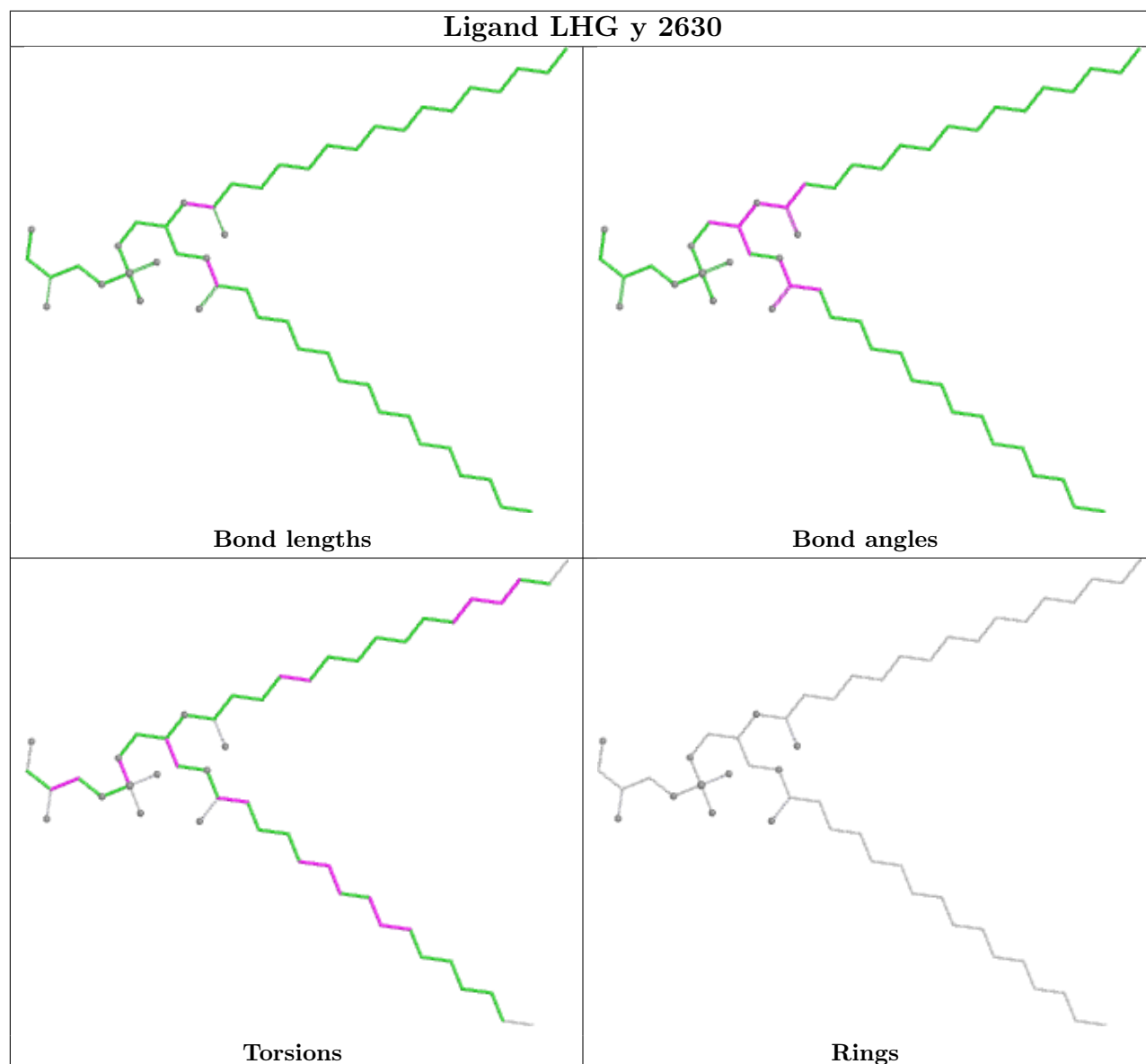
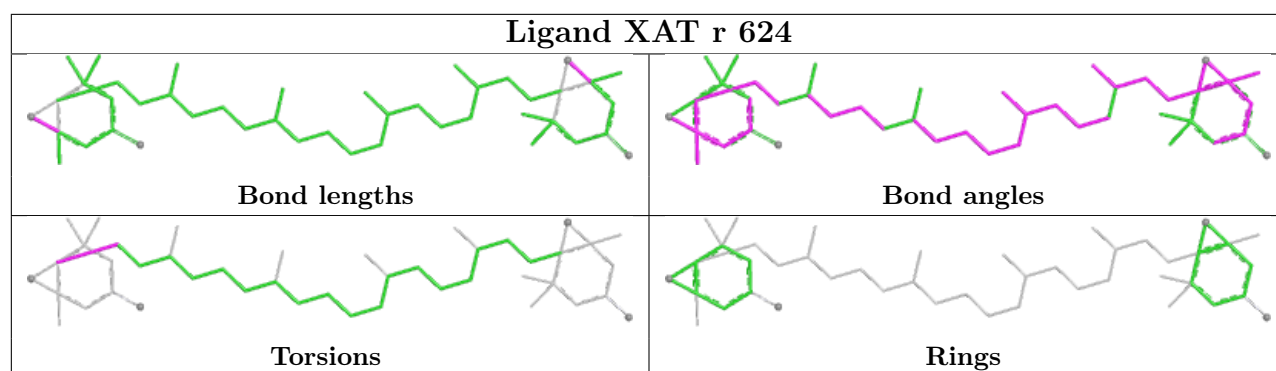
Bond angles



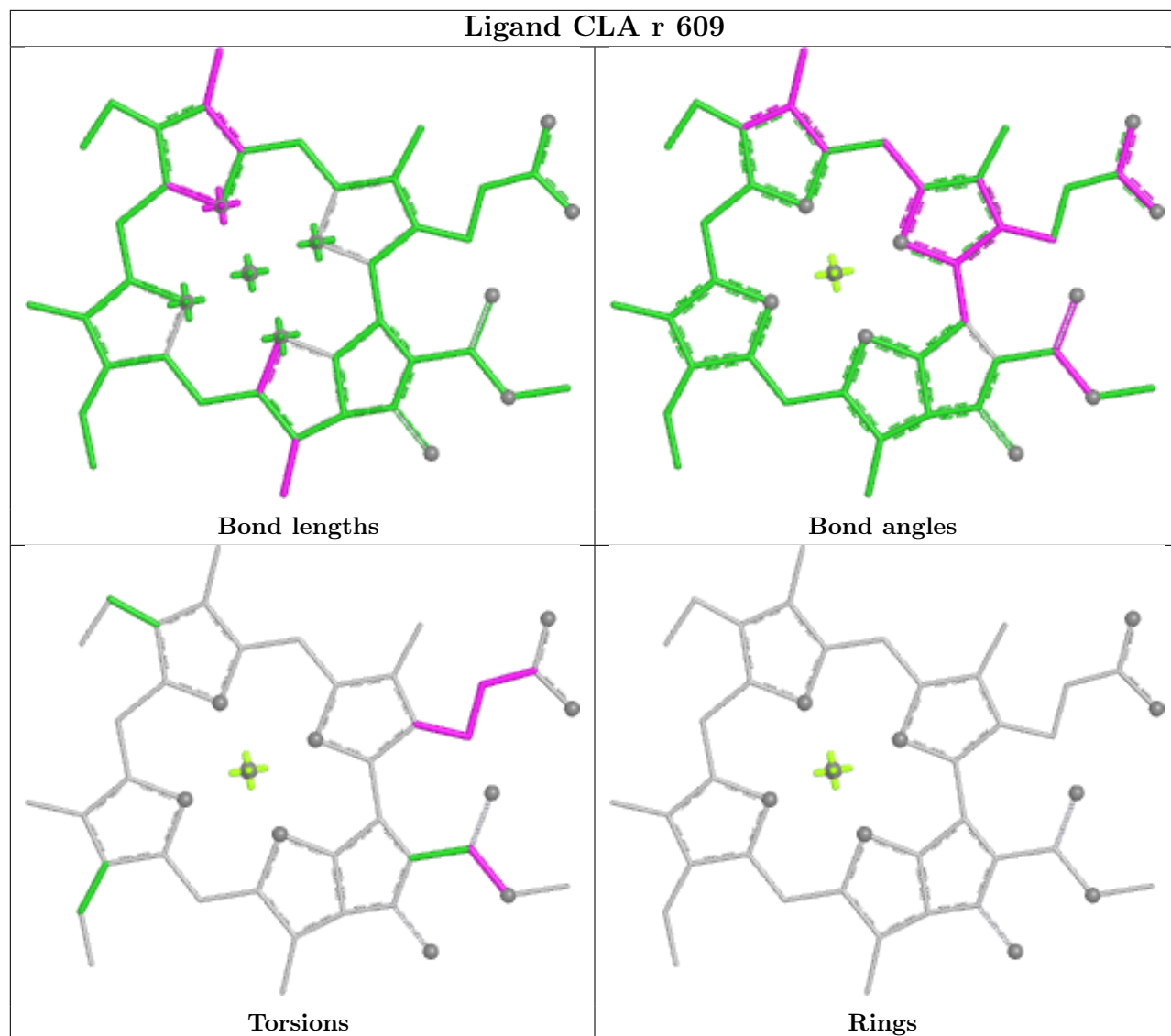
Torsions



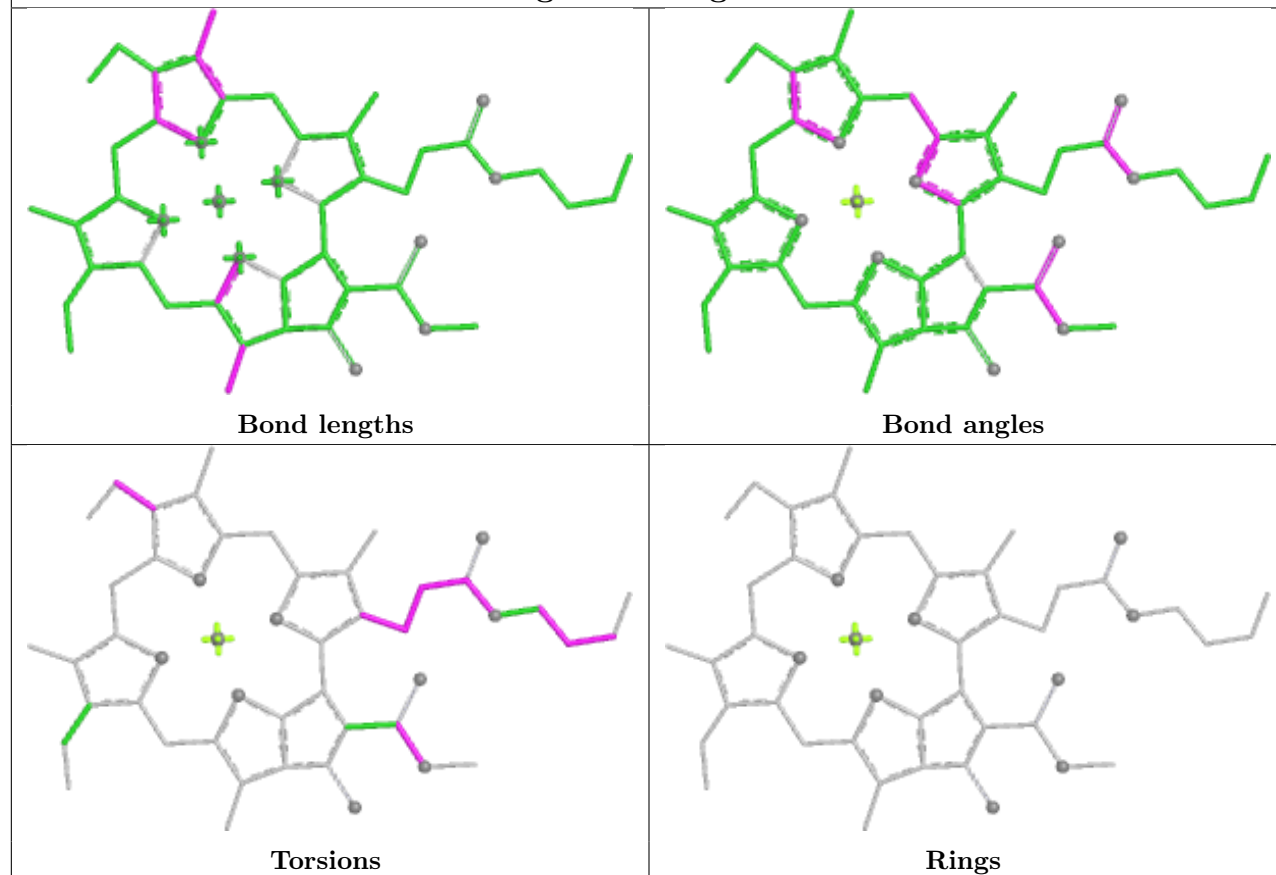
Rings



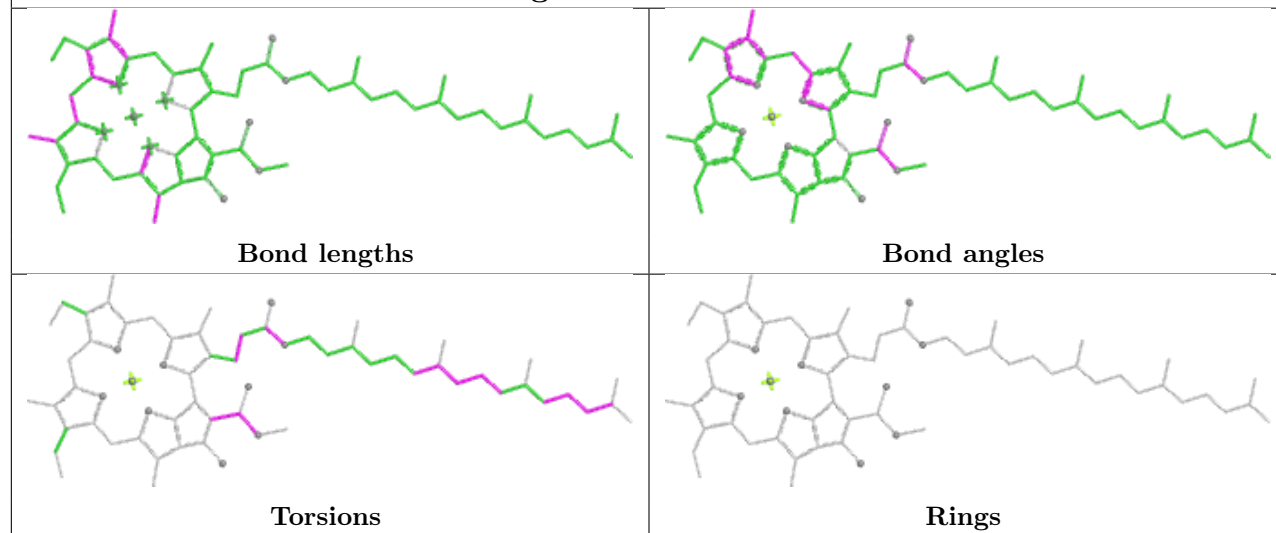
Ligand CLA r 609

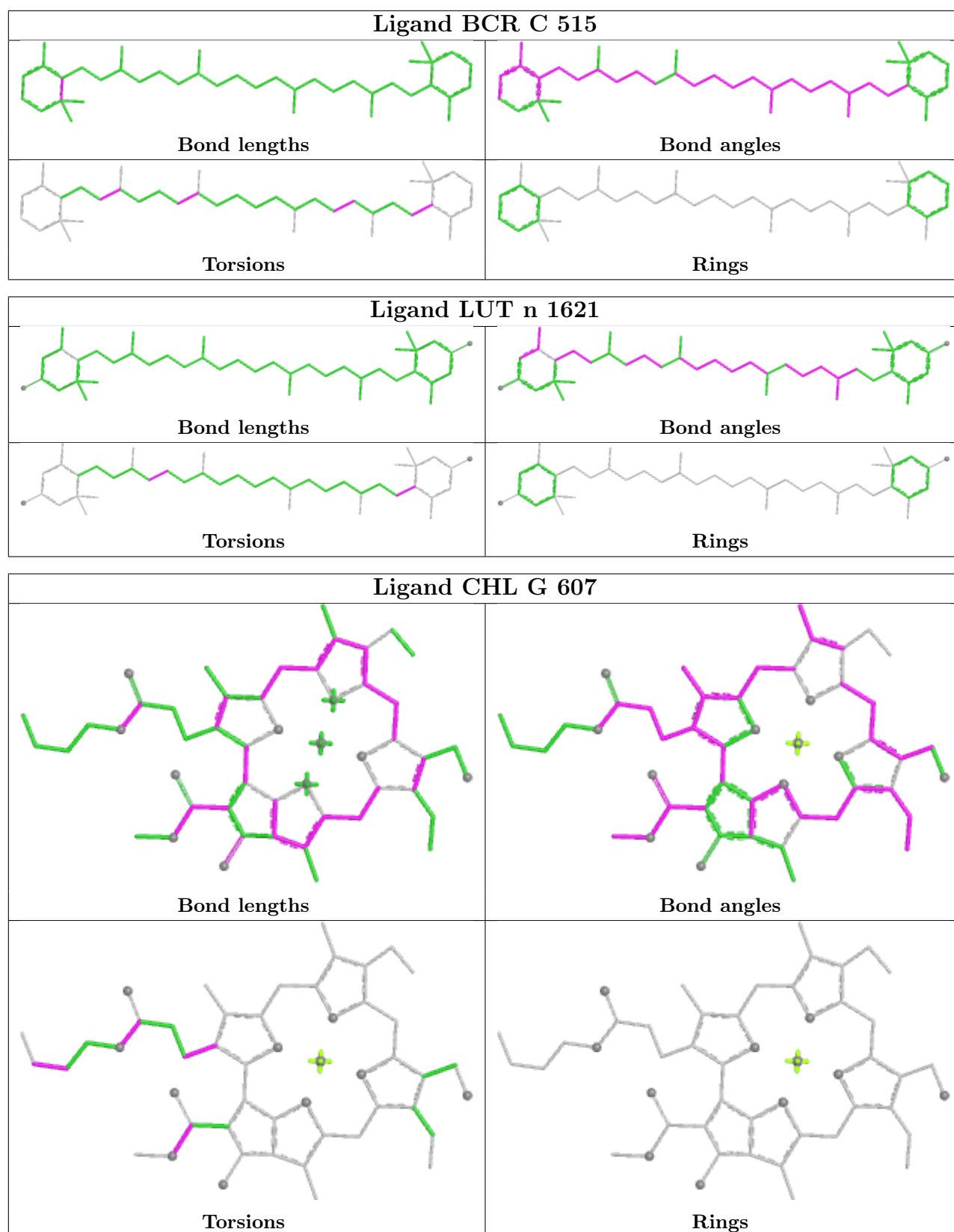


Ligand CLA g 614

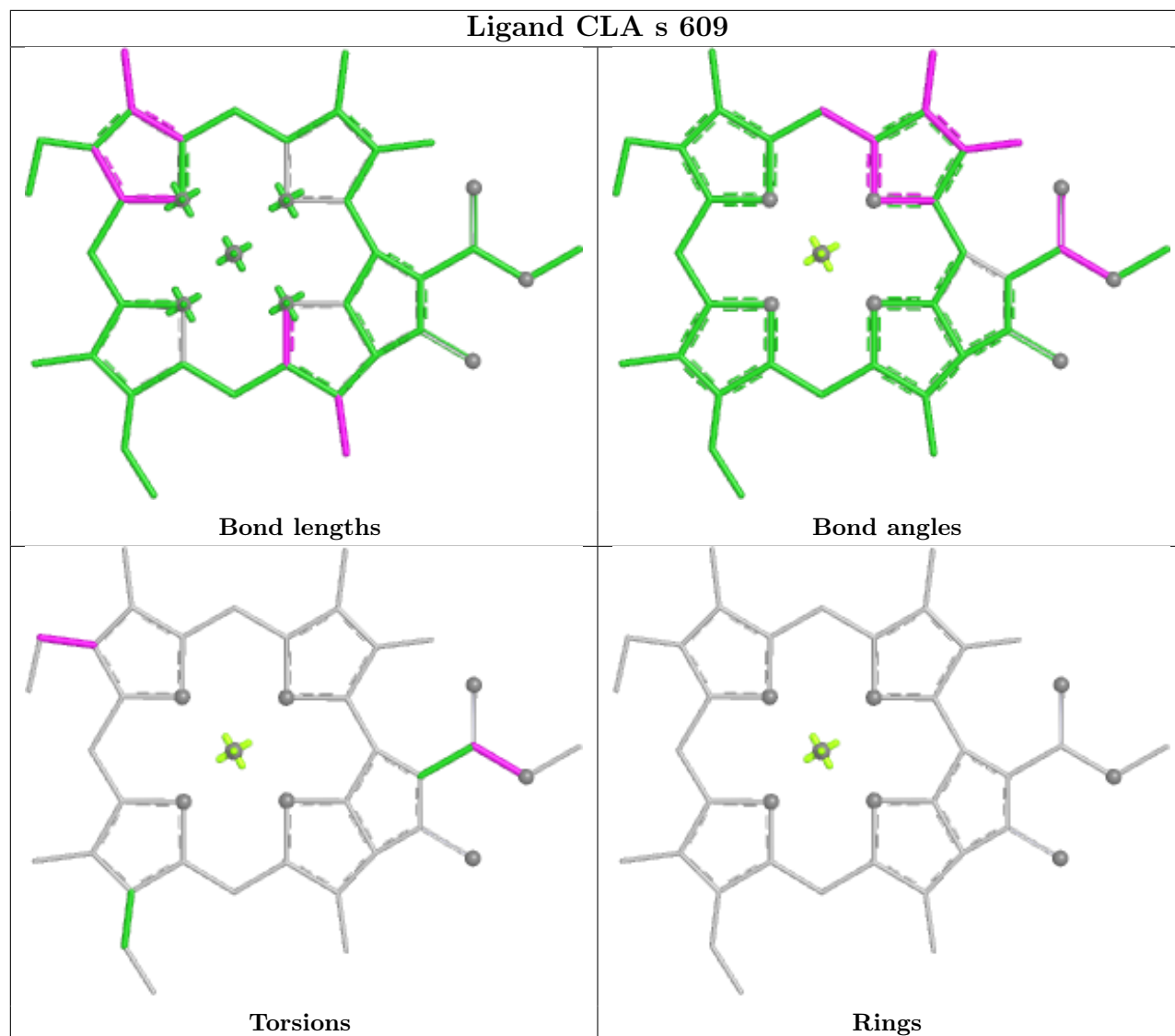


Ligand CLA G 602

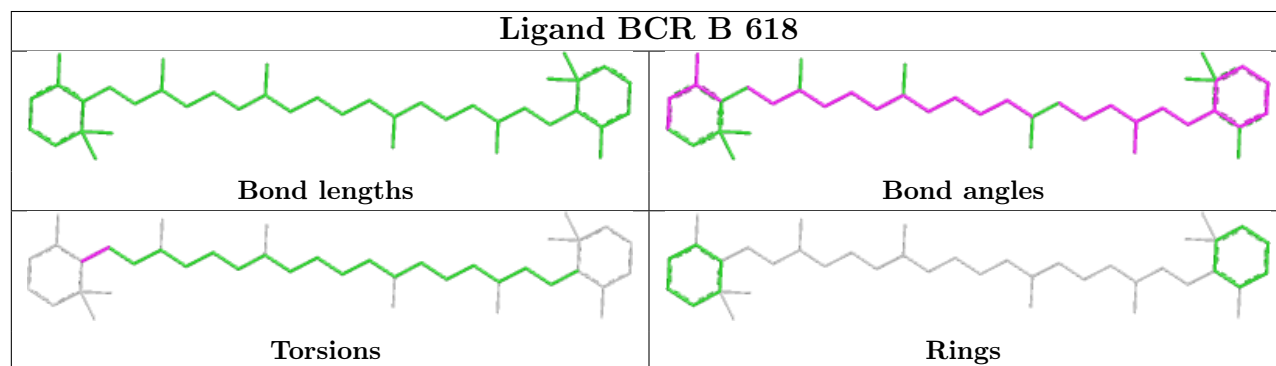


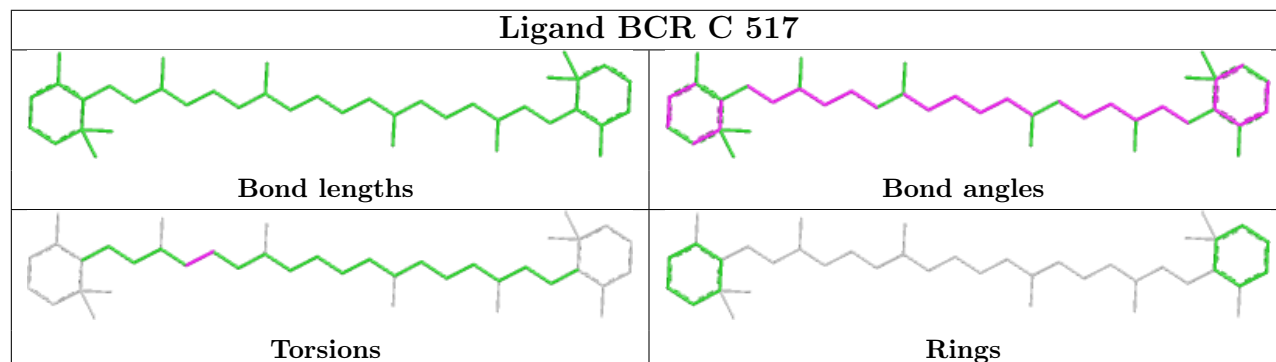
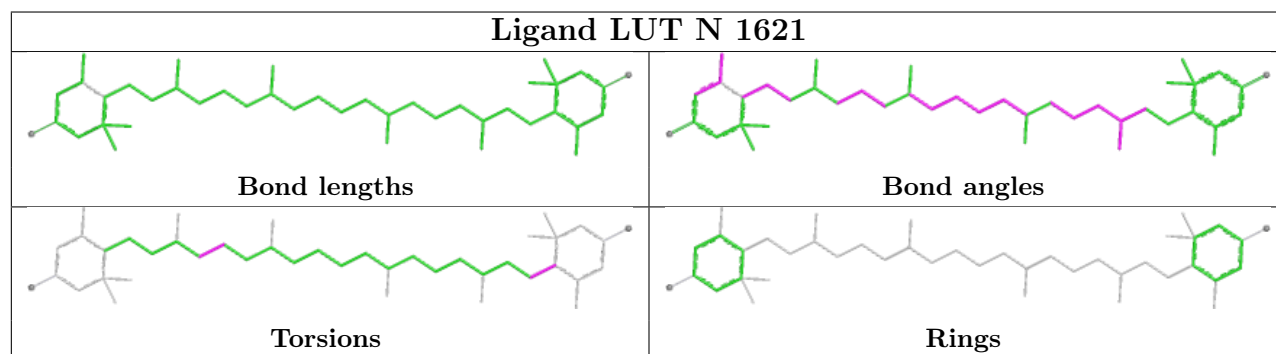
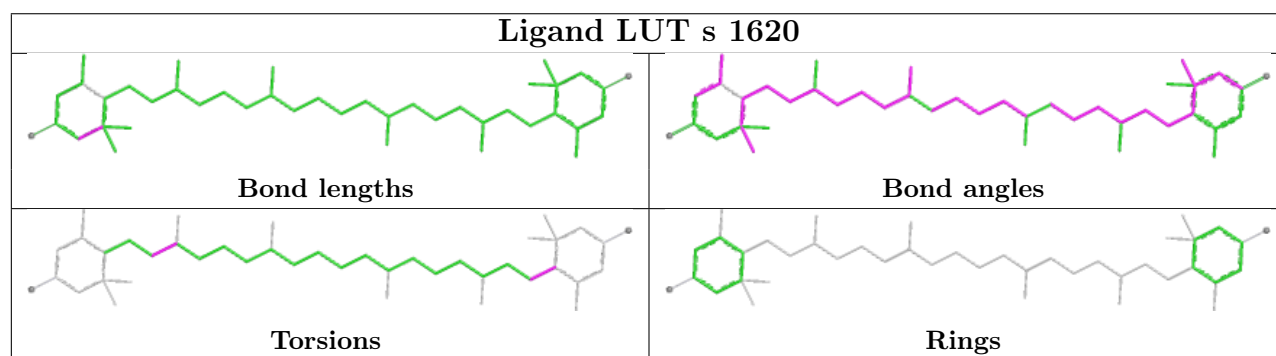
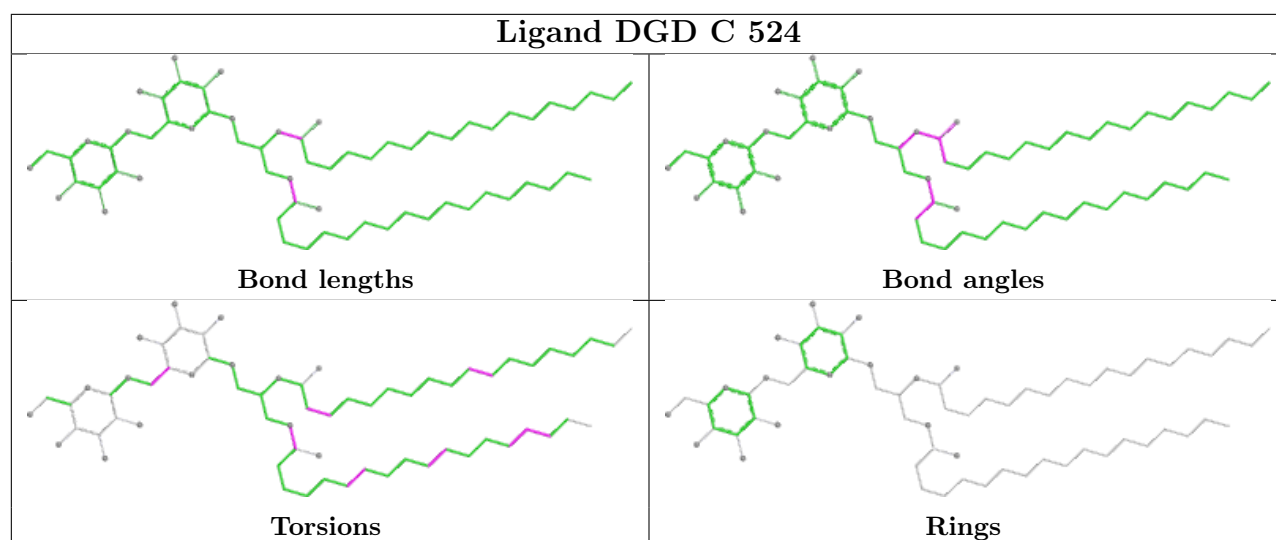


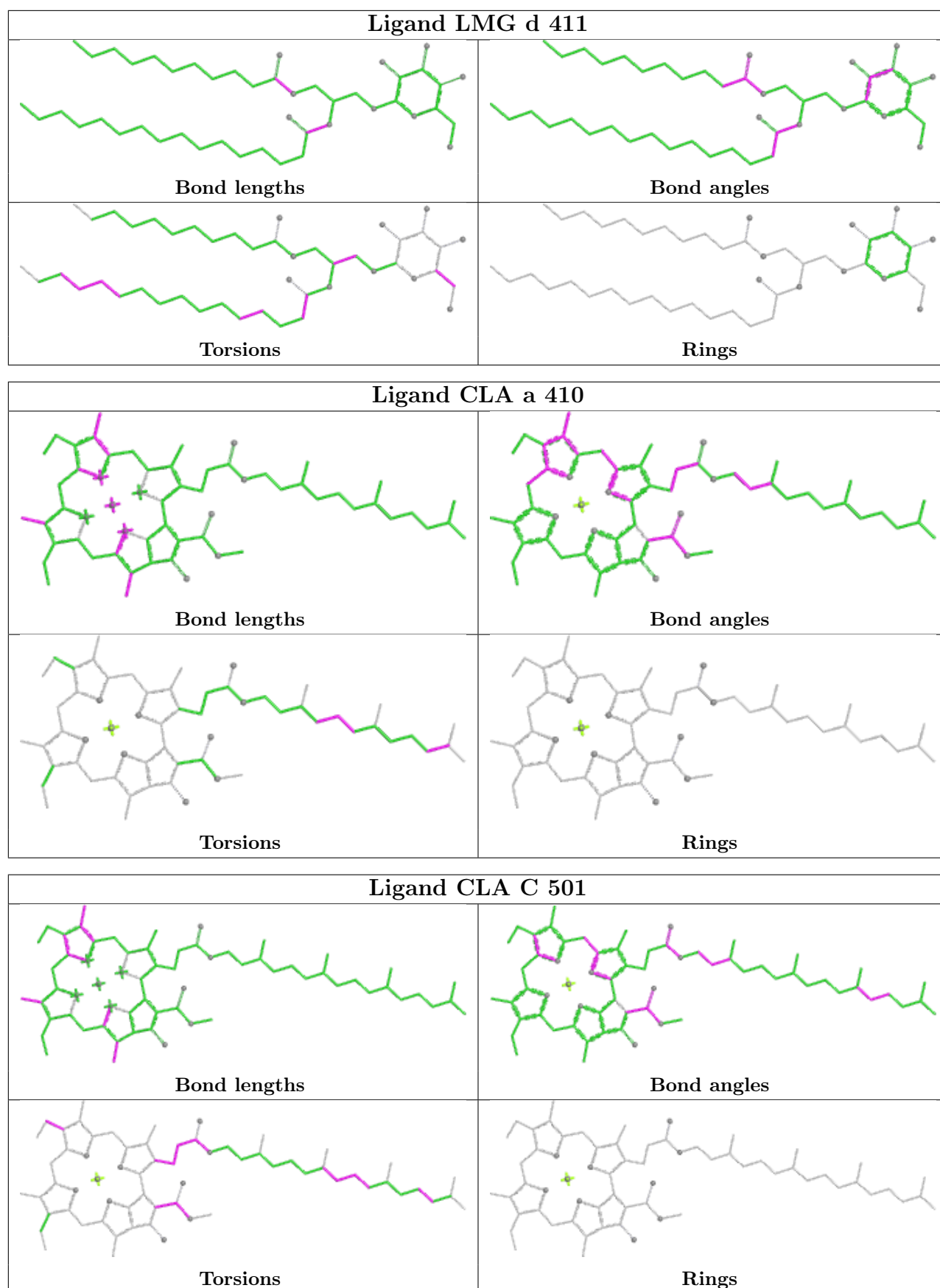
Ligand CLA s 609

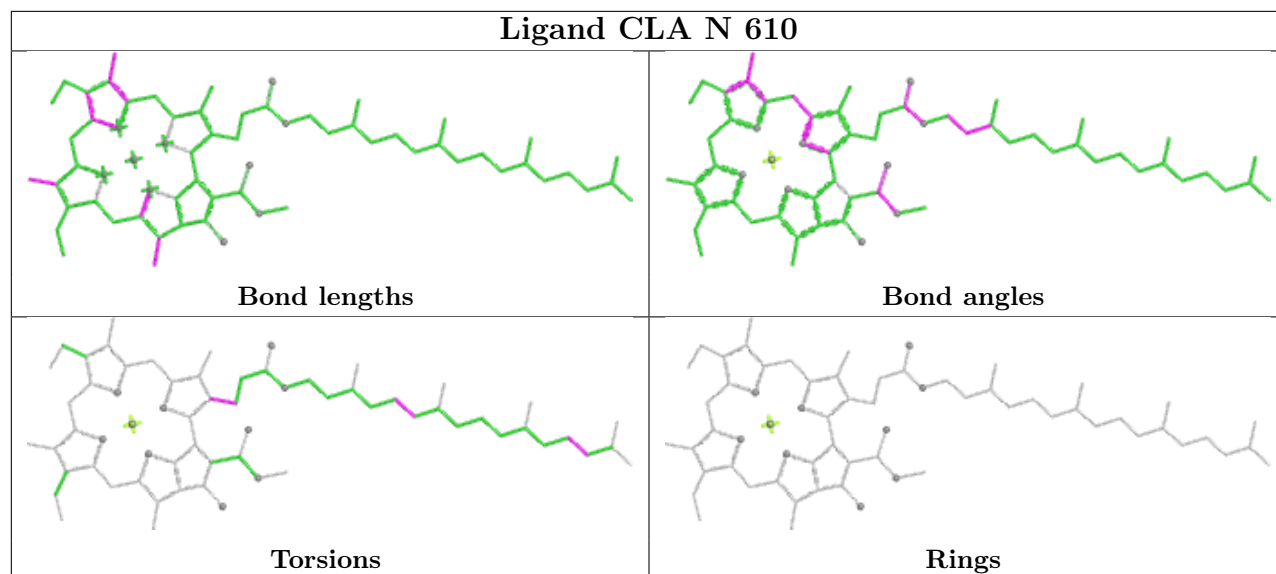
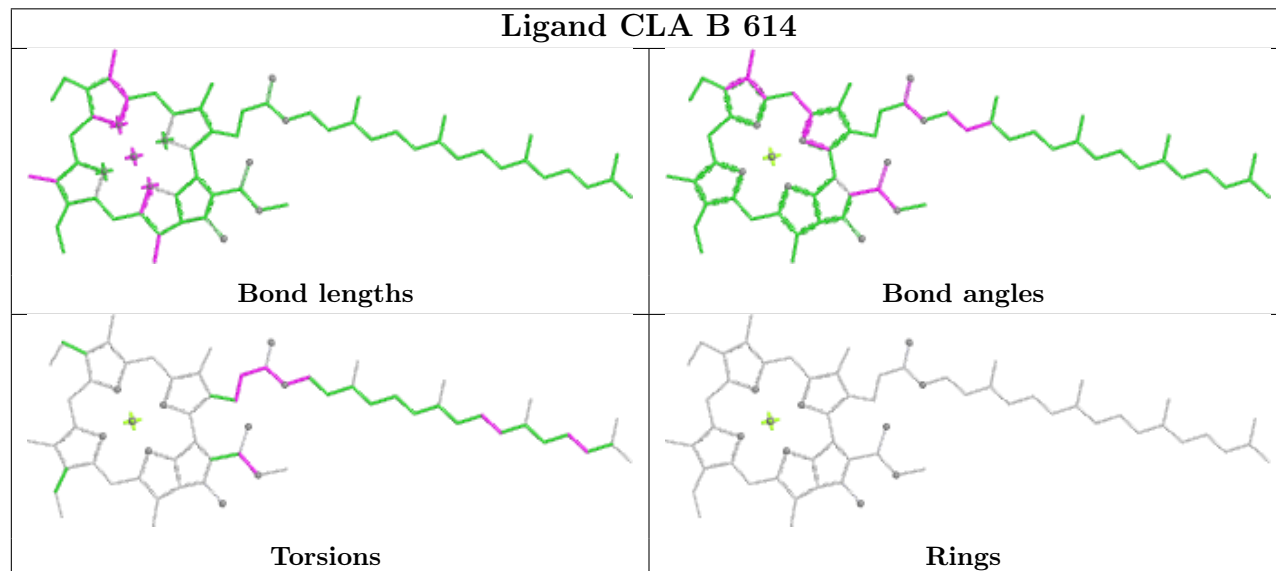


Ligand BCR B 618

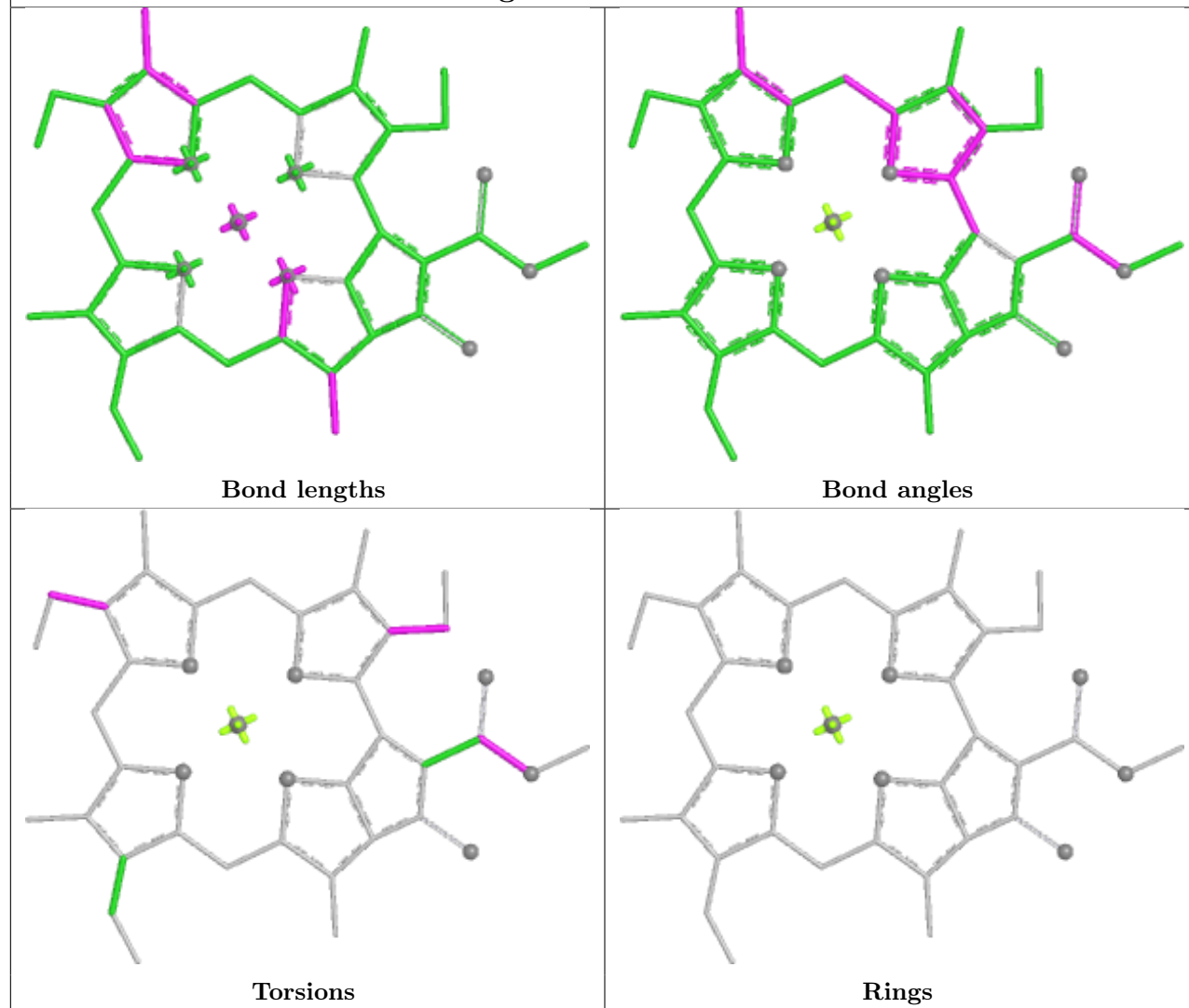




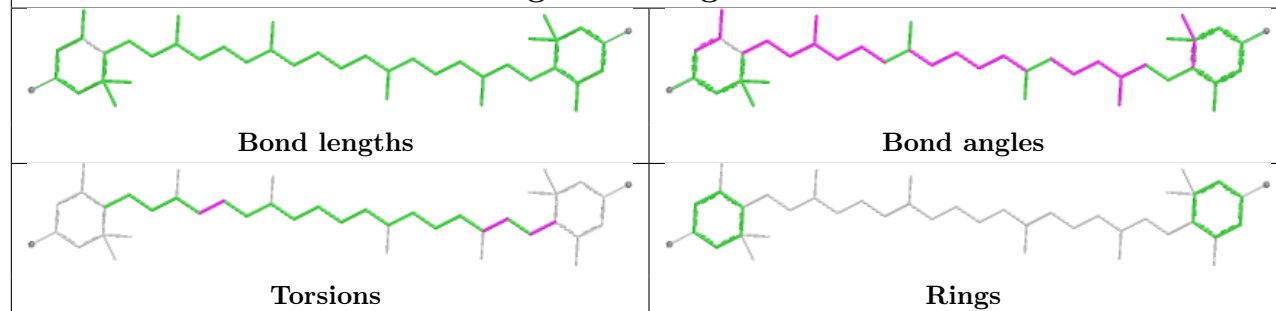


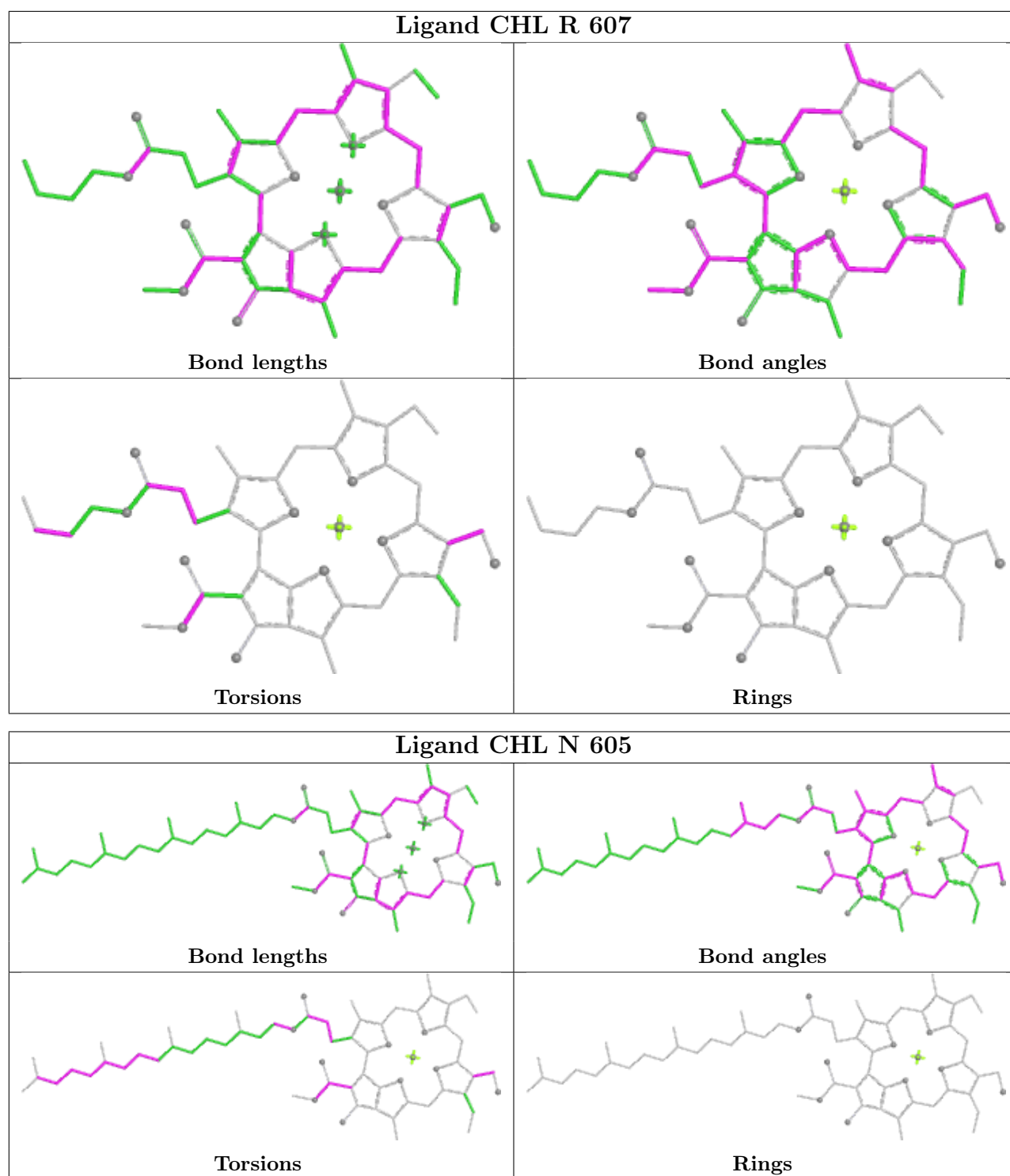
Ligand CLA N 610**Ligand CLA B 614**

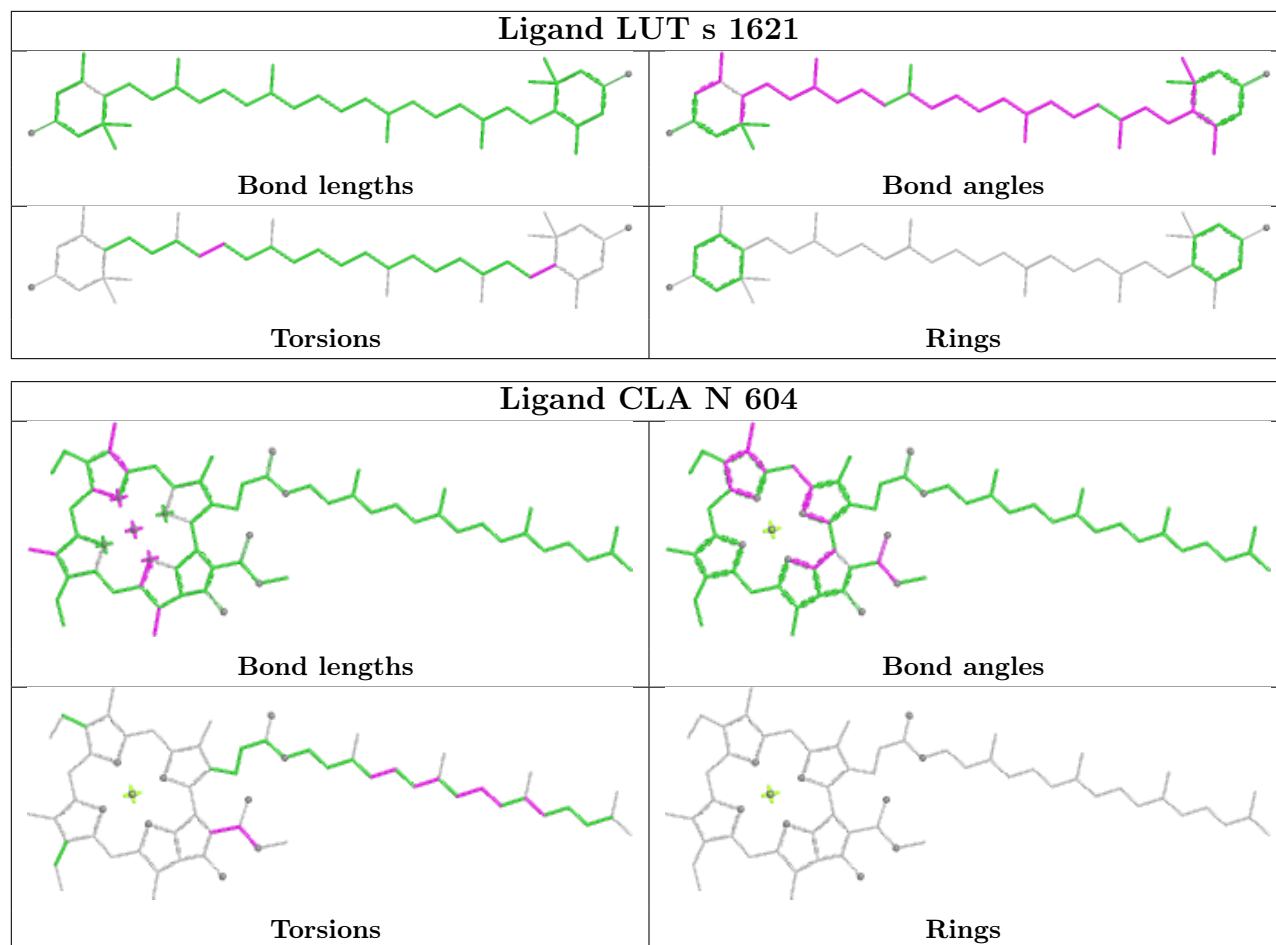
Ligand CLA S 603



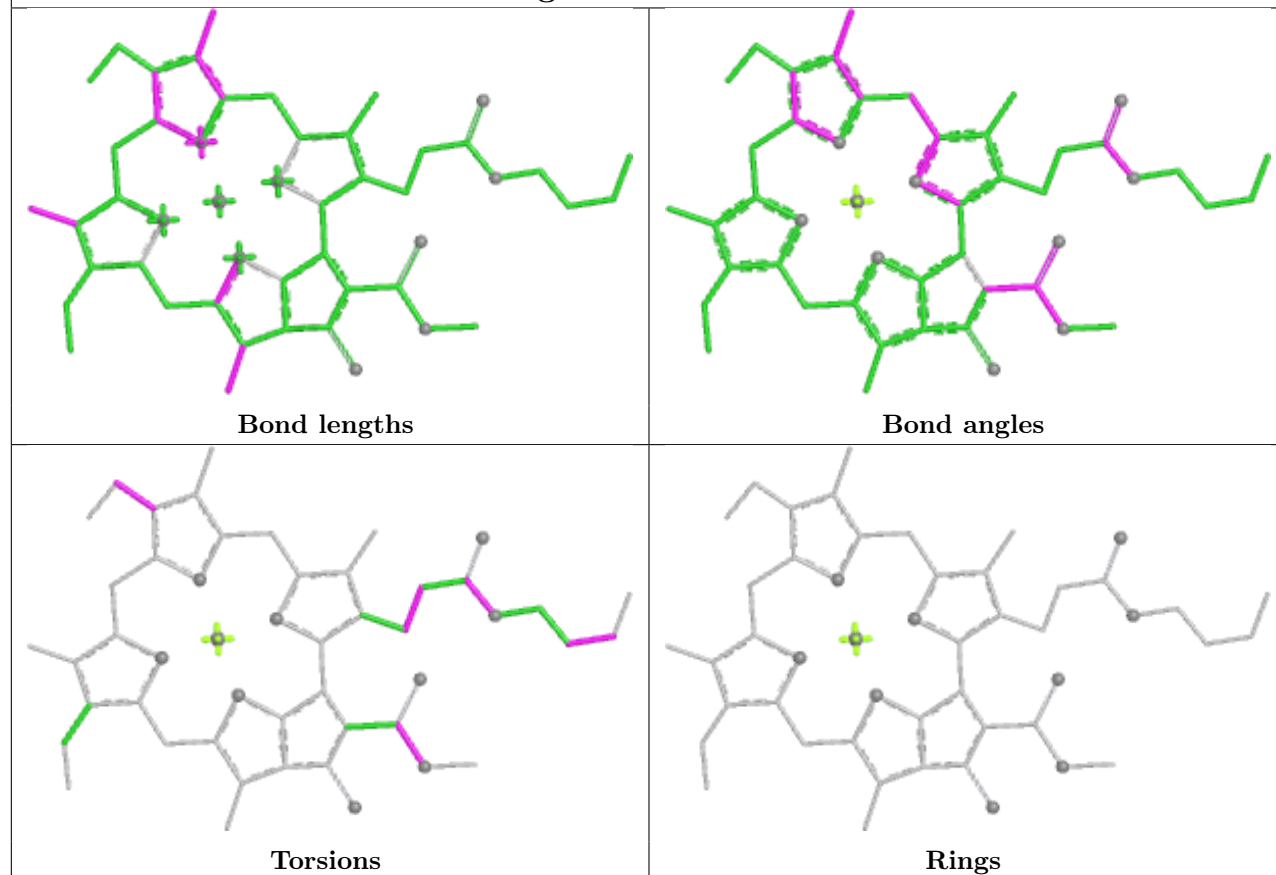
Ligand LUT g 1621



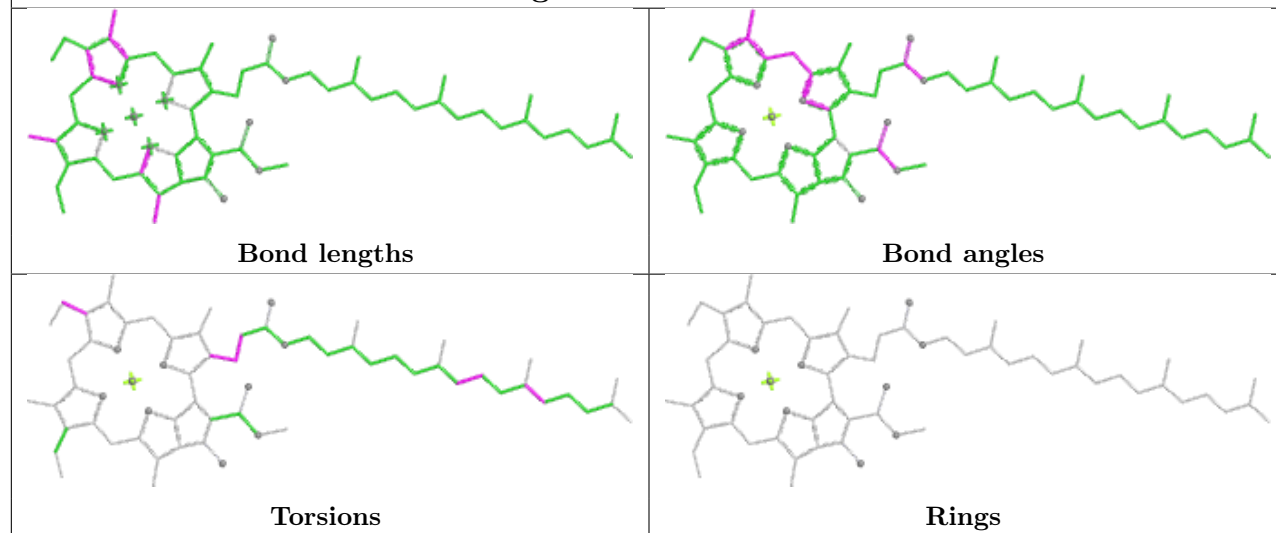


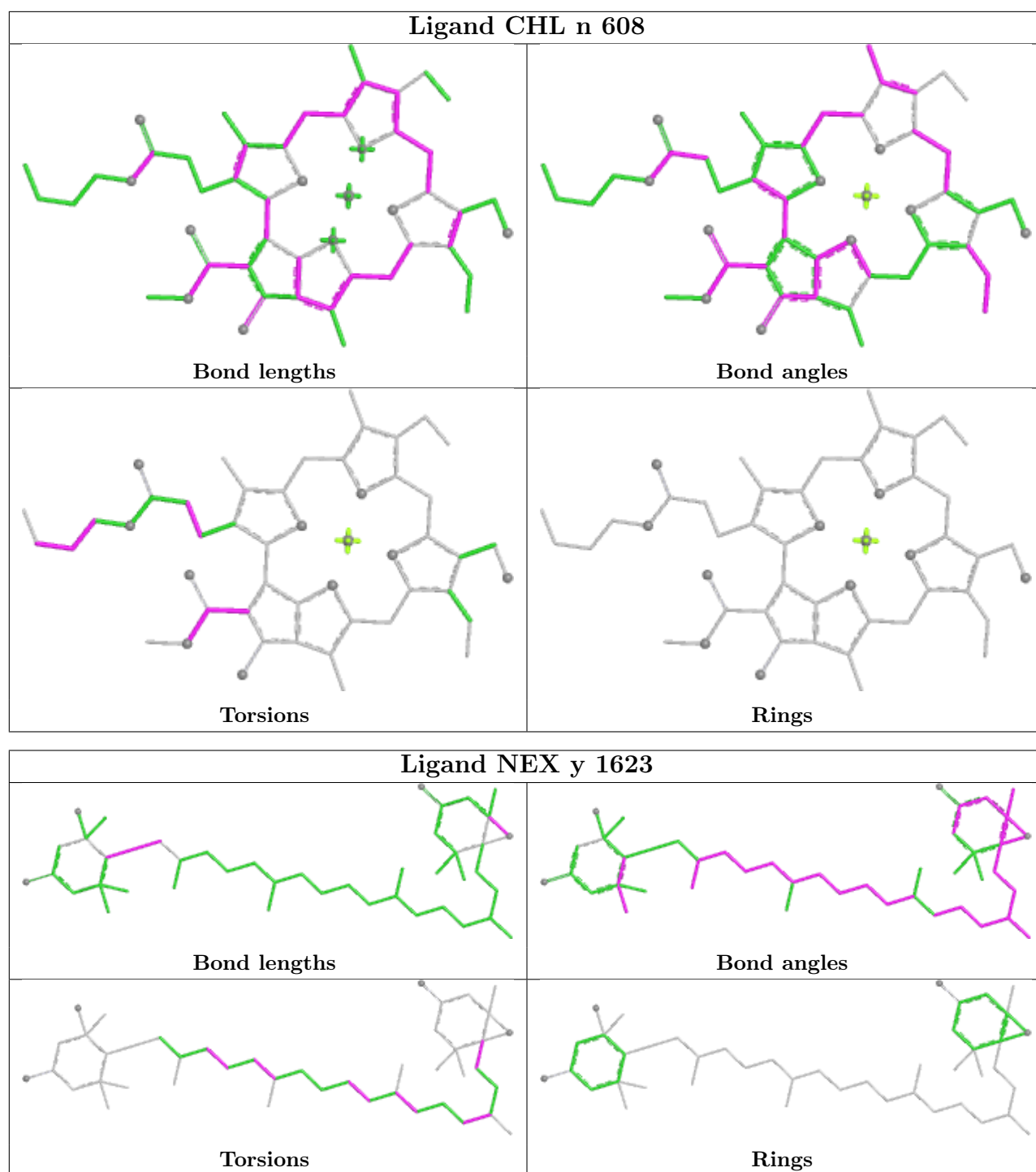


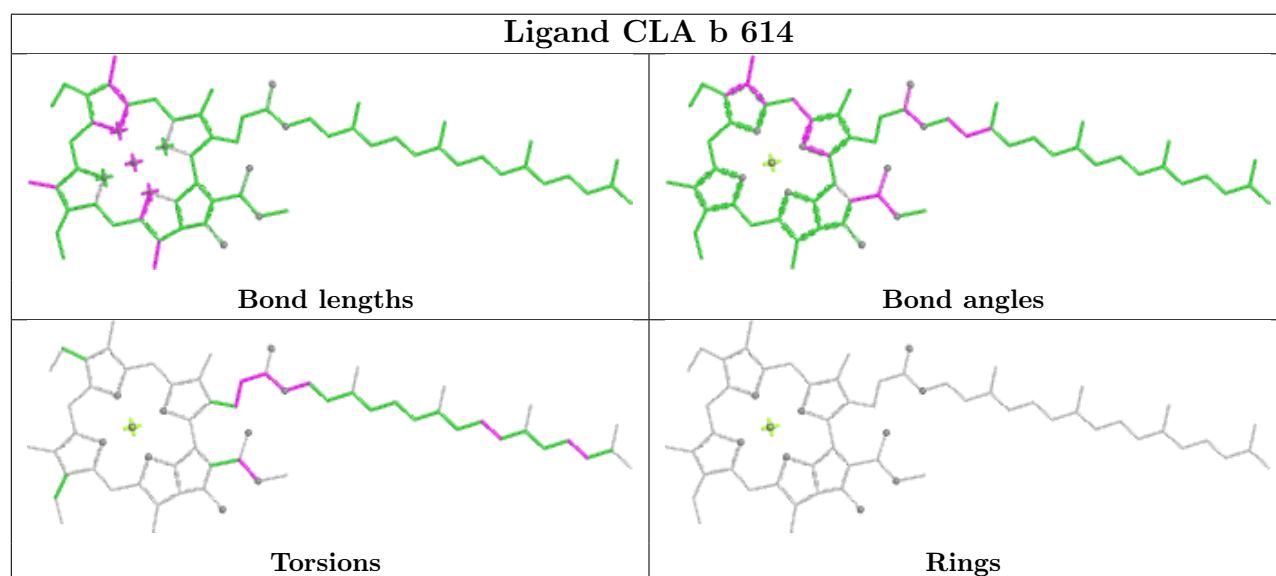
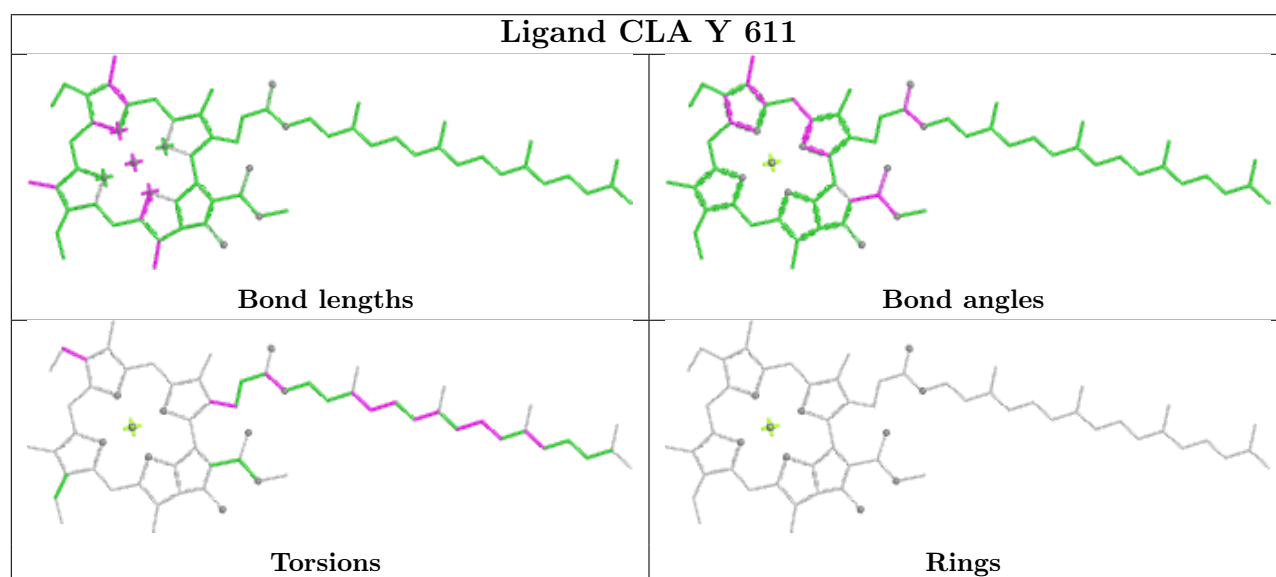
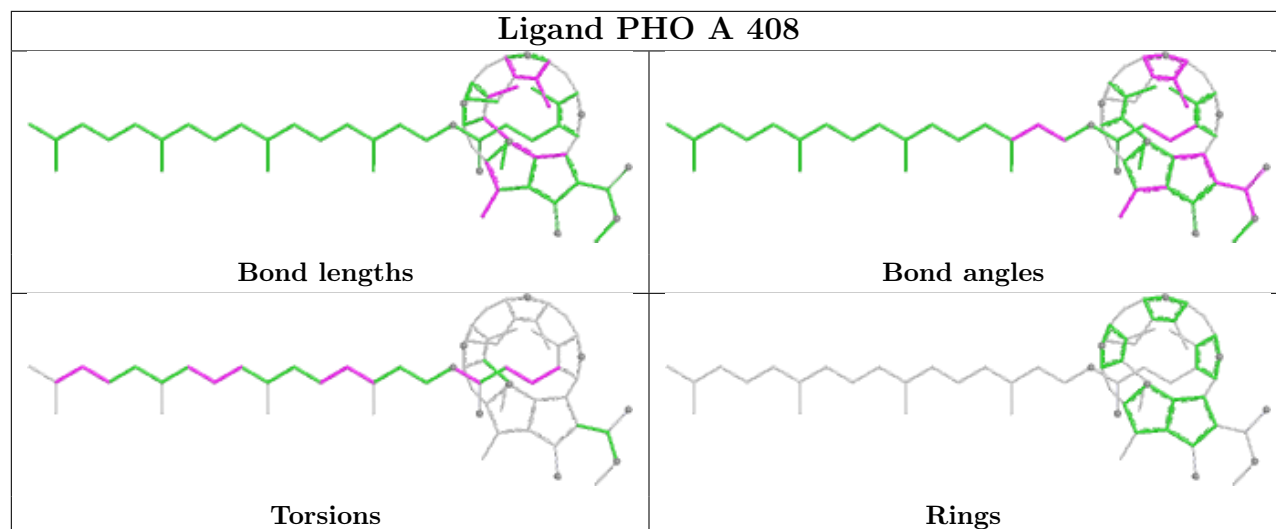
Ligand CLA s 602



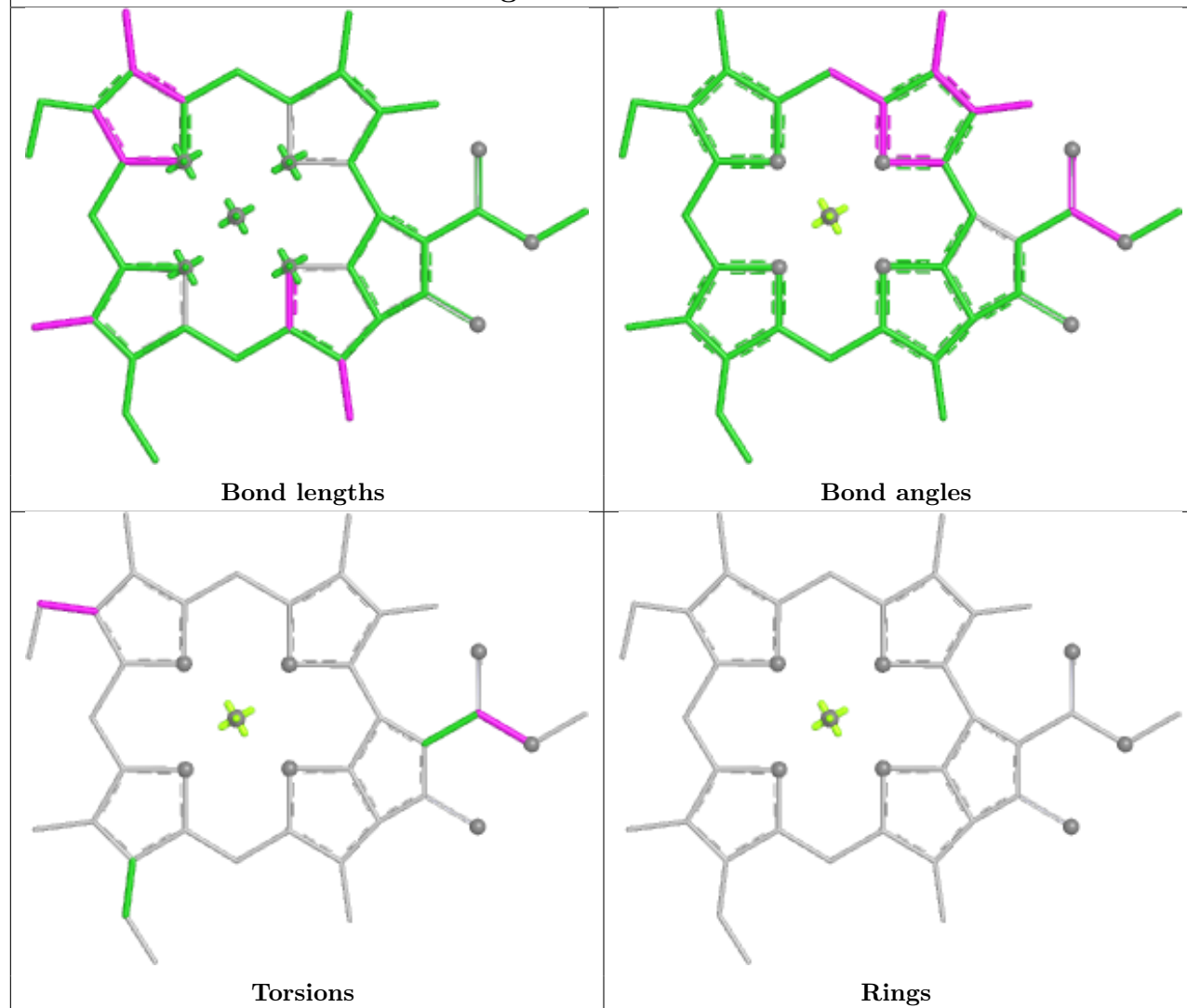
Ligand CLA Y 610



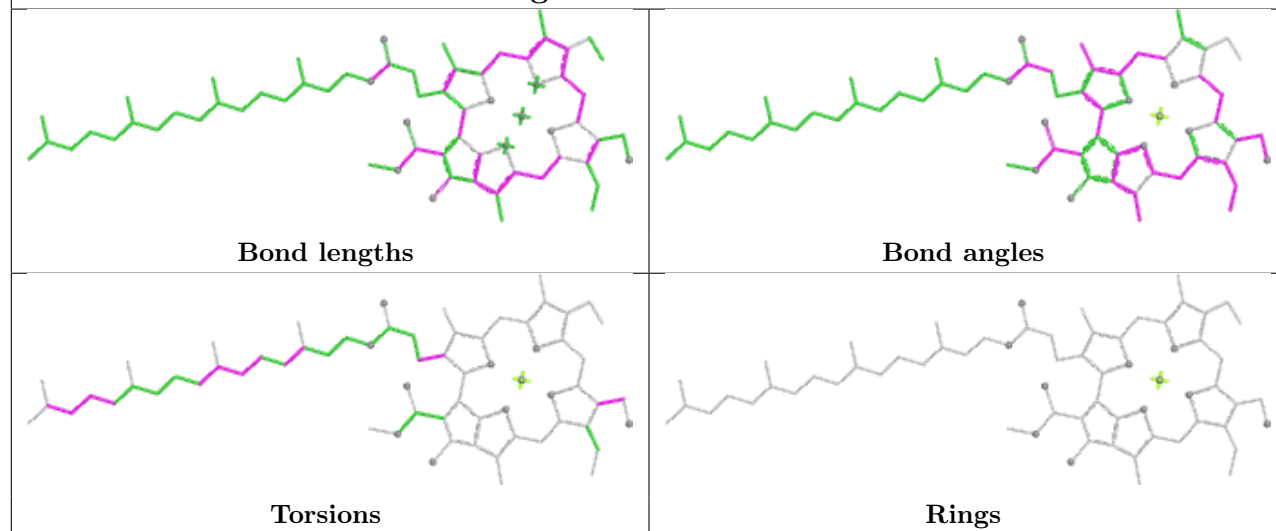




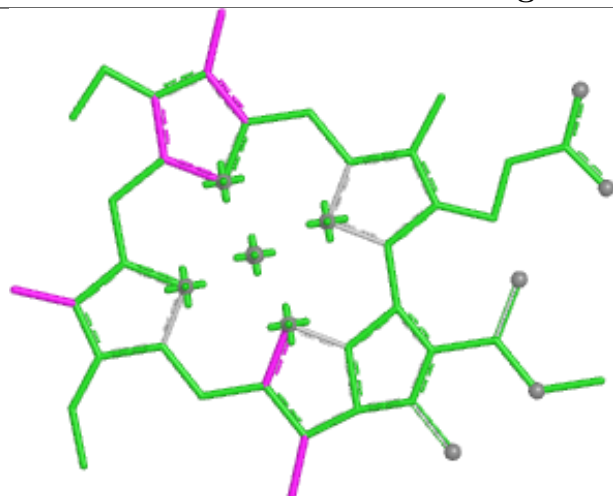
Ligand CLA r 610



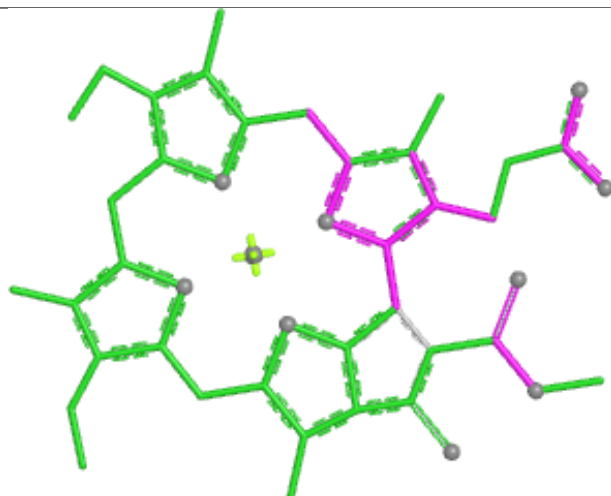
Ligand CHL N 601



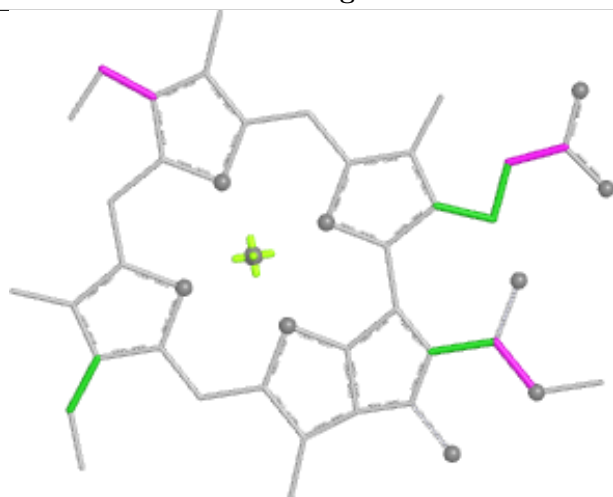
Ligand CLA n 612



Bond lengths



Bond angles

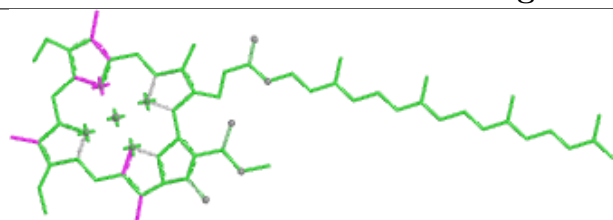


Torsions

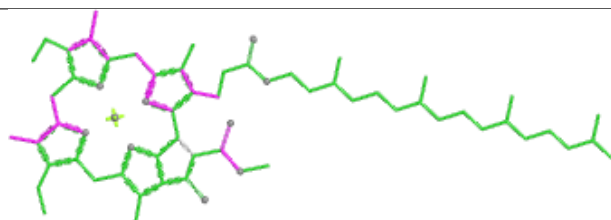


Rings

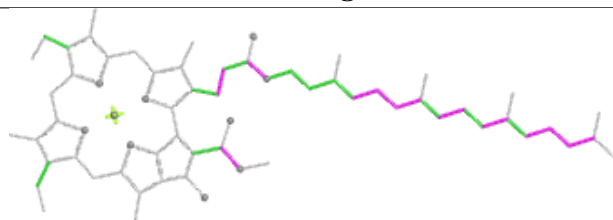
Ligand CLA b 617



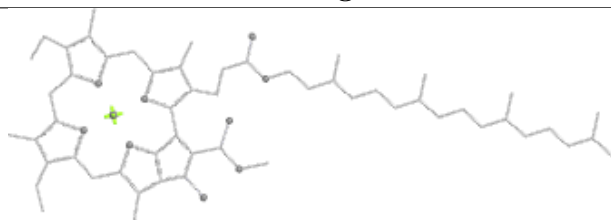
Bond lengths



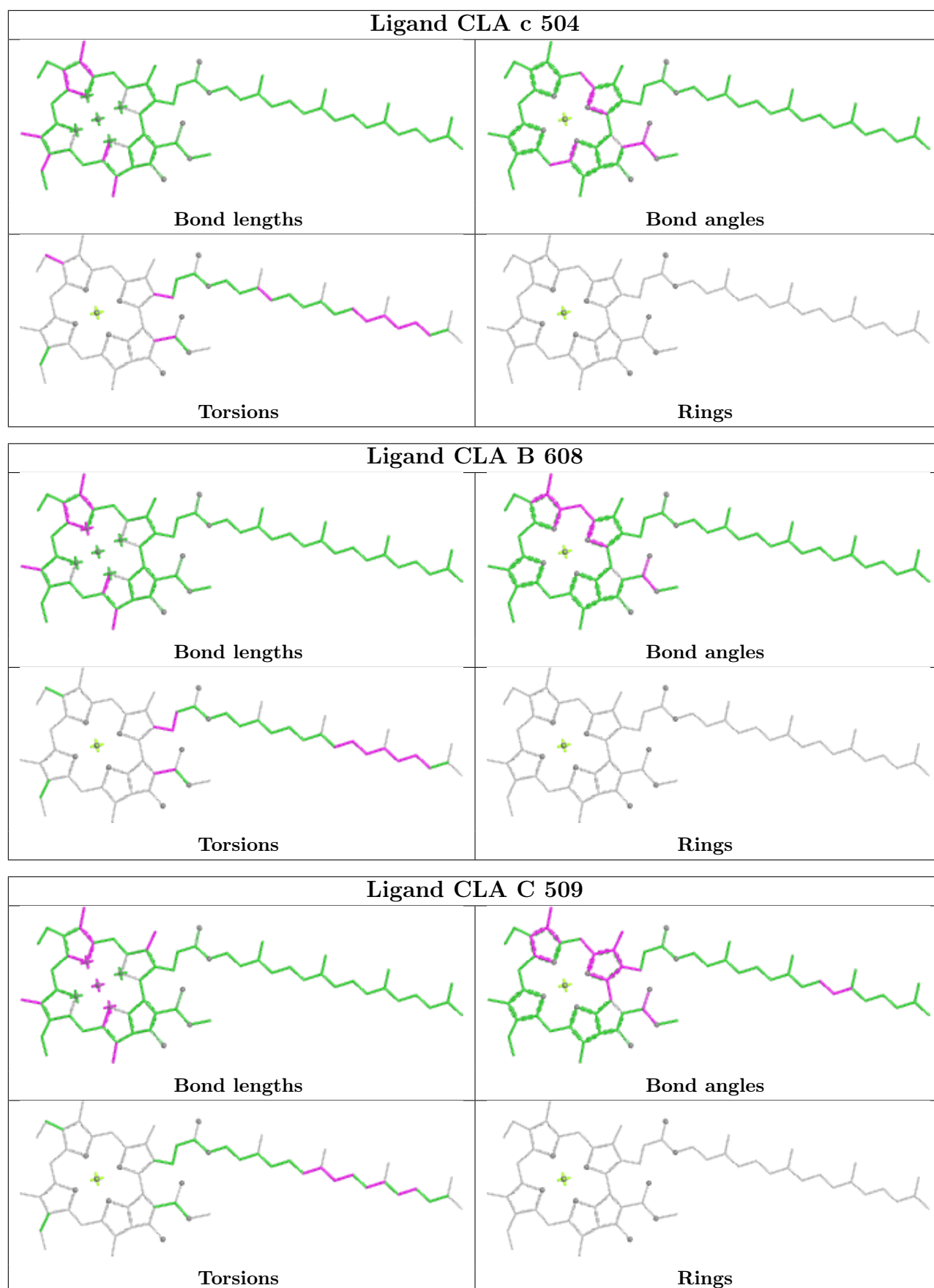
Bond angles

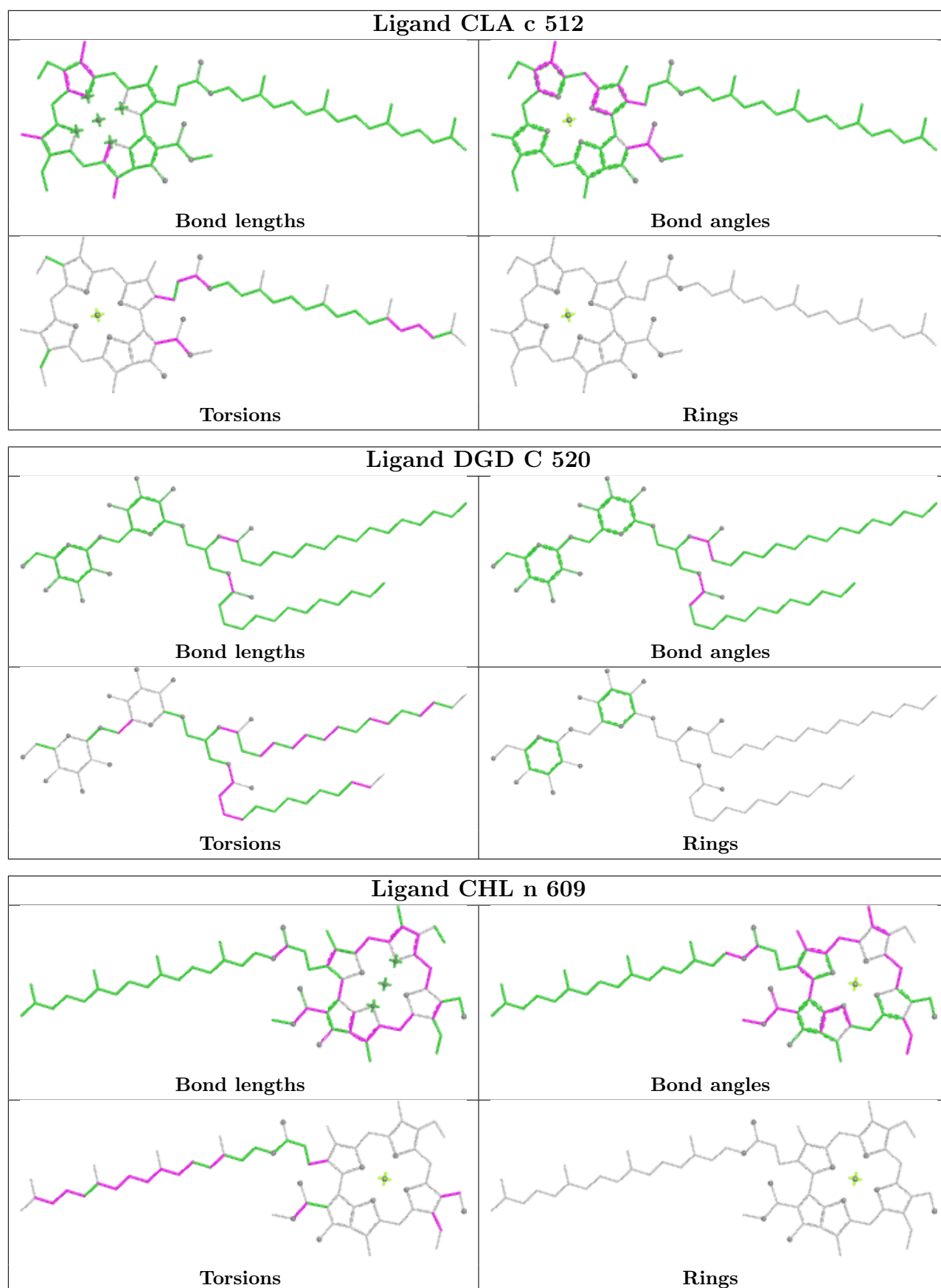


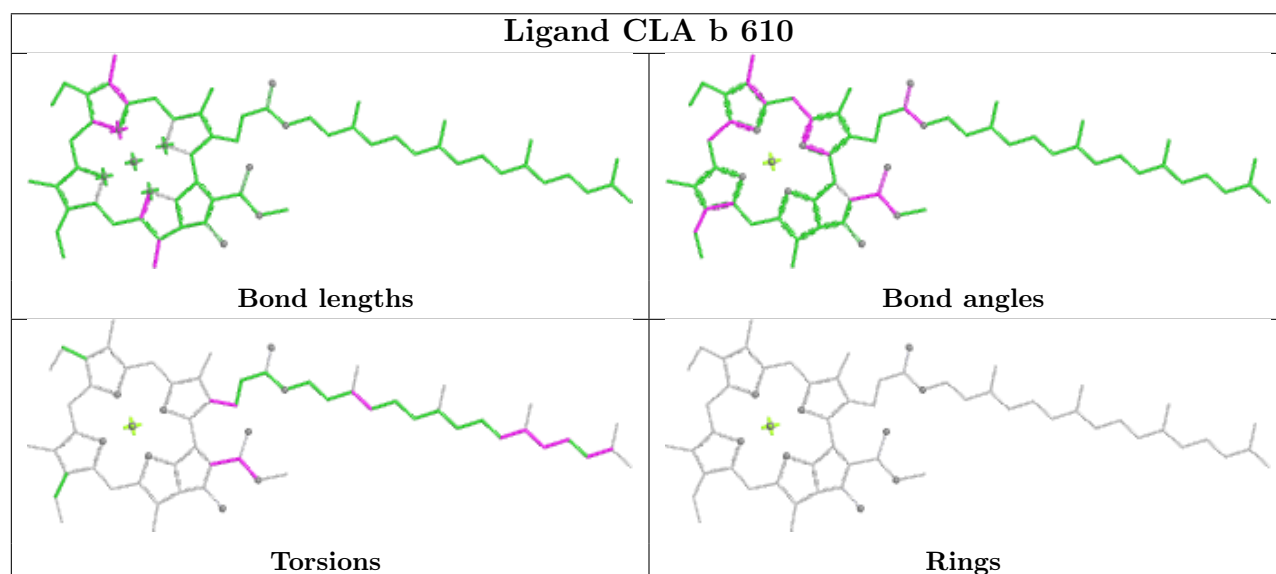
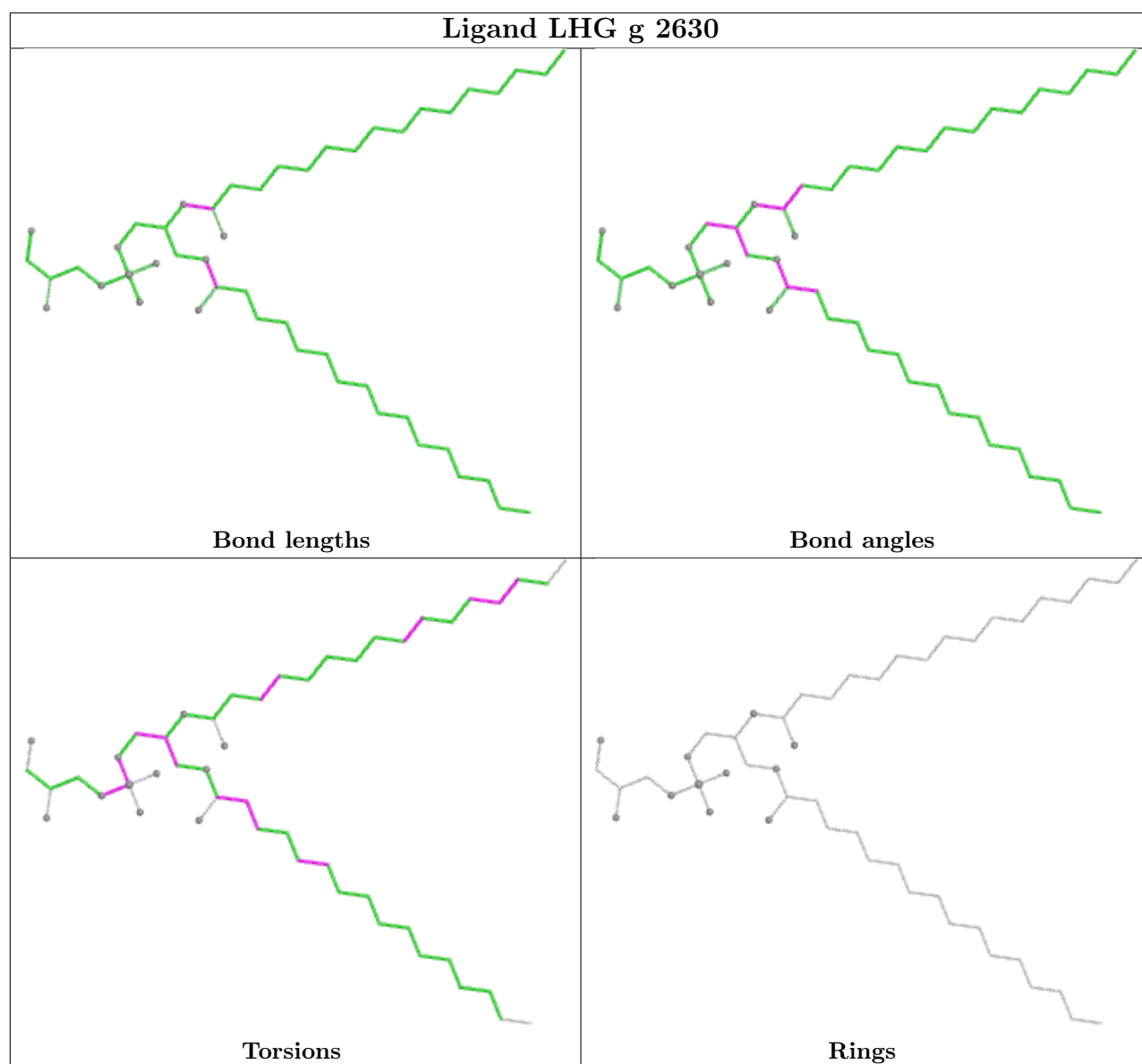
Torsions

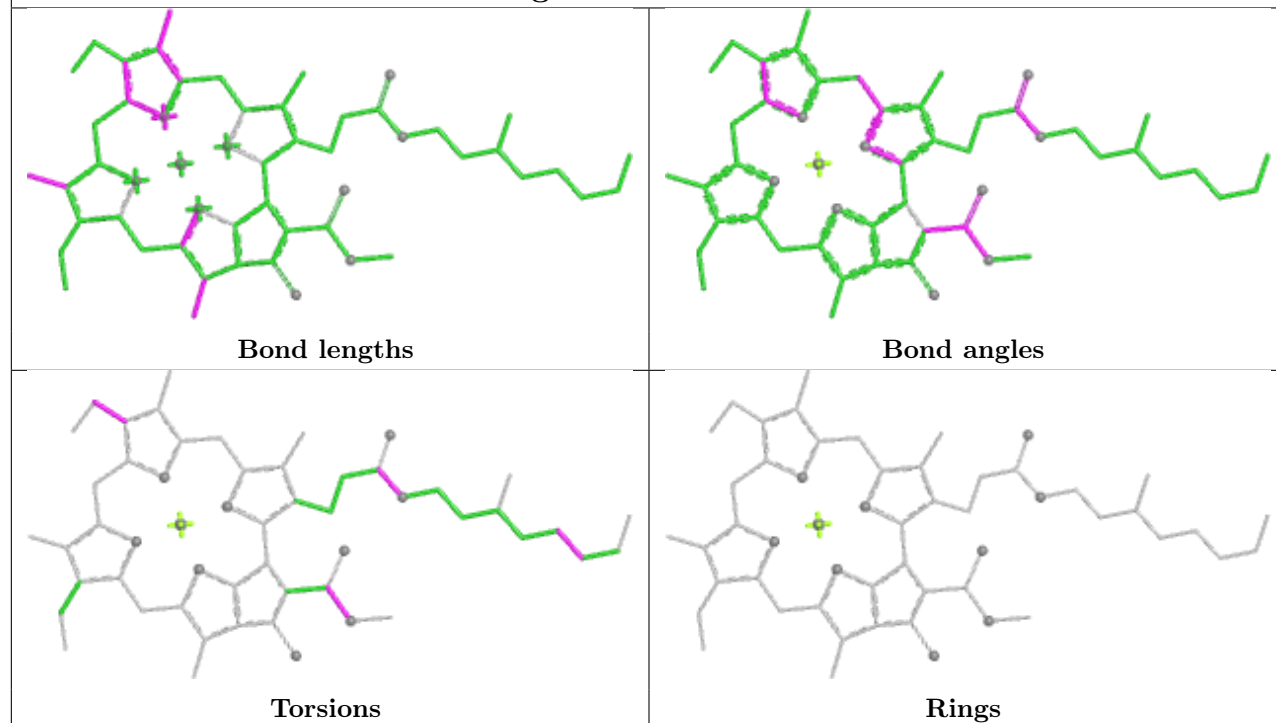
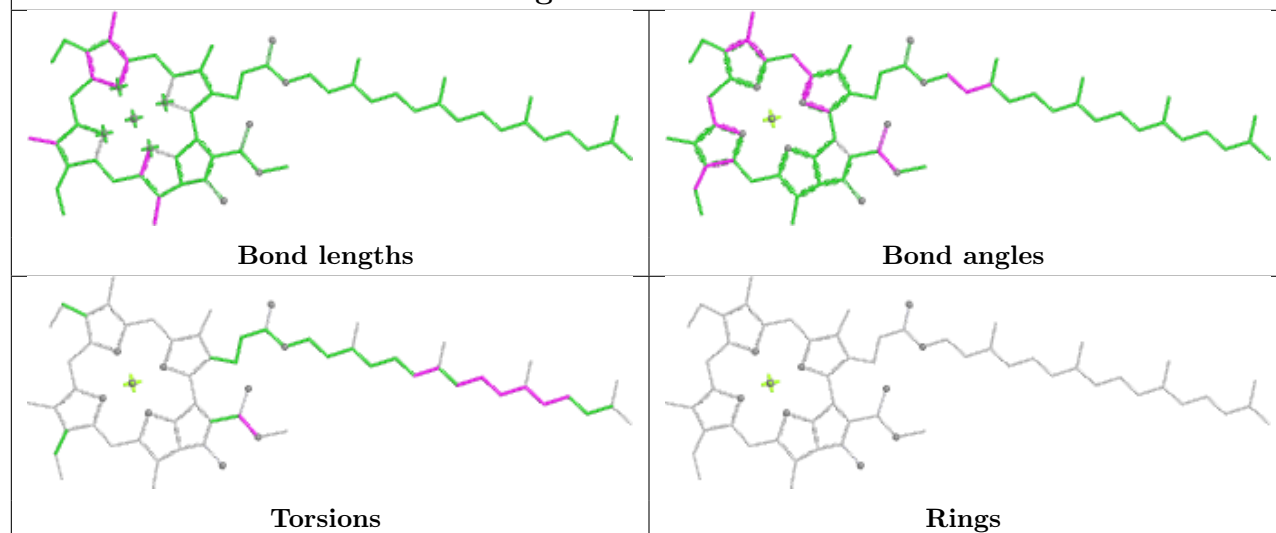


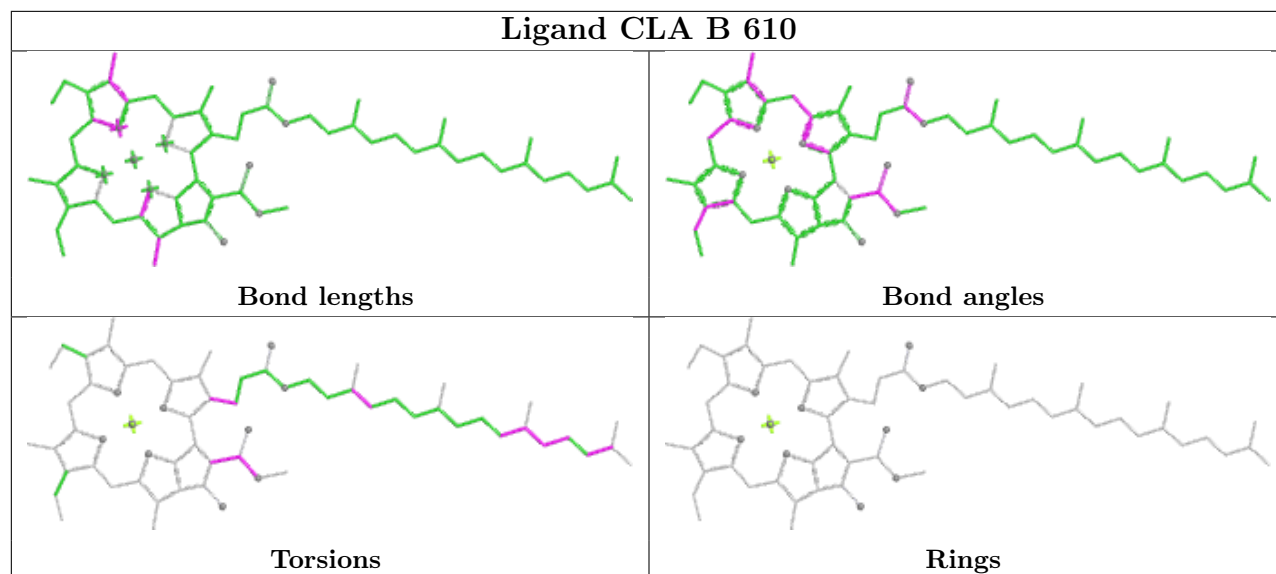
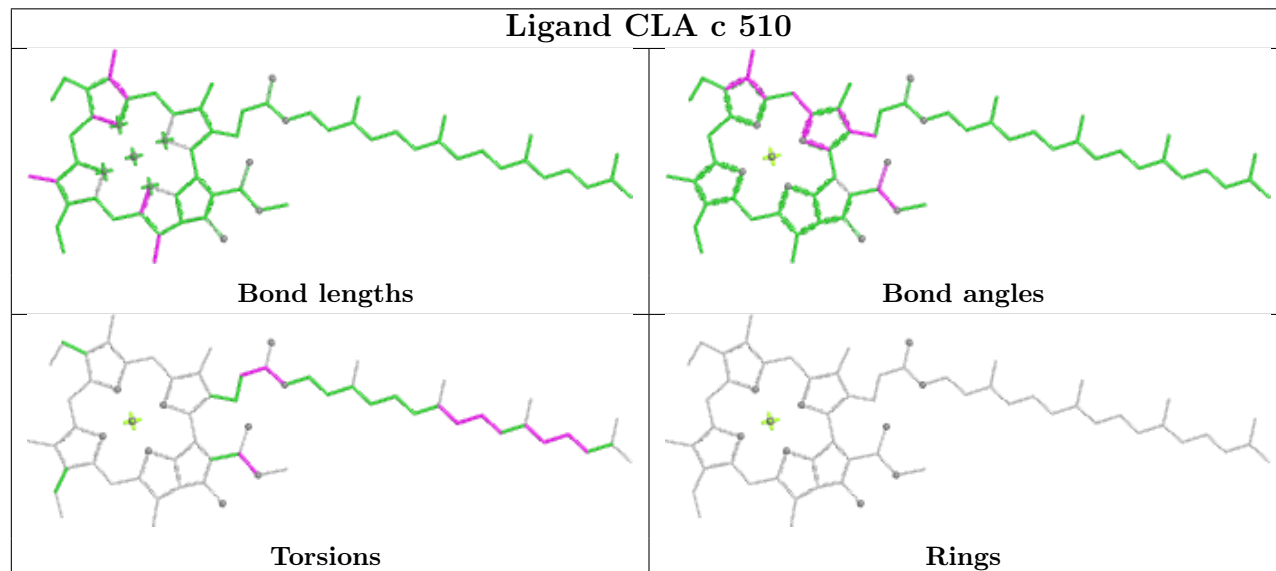
Rings



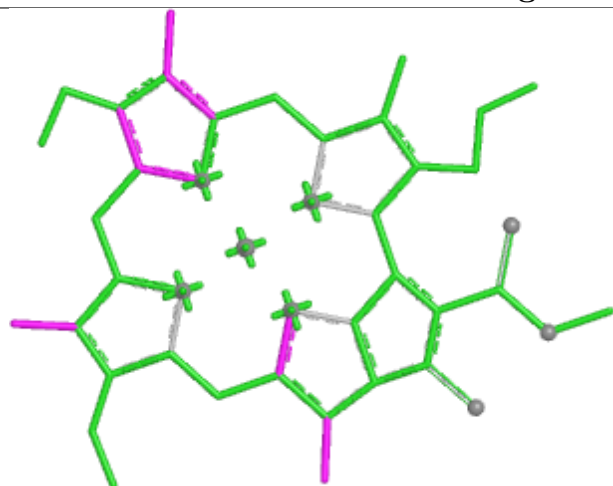




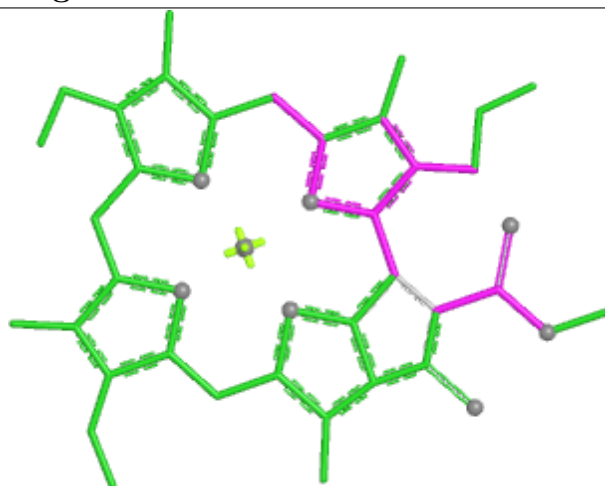
Ligand CLA Y 614**Ligand CLA b 612**

Ligand CLA B 610**Ligand CLA c 510**

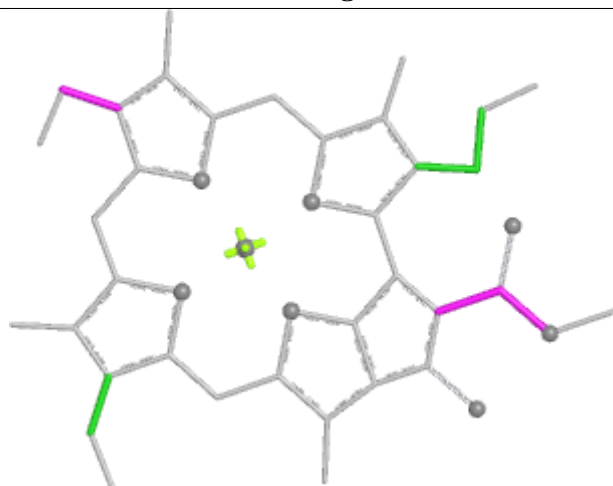
Ligand CLA g 612



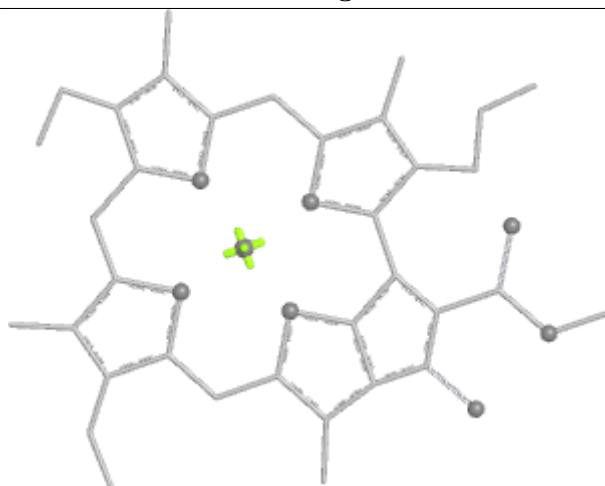
Bond lengths



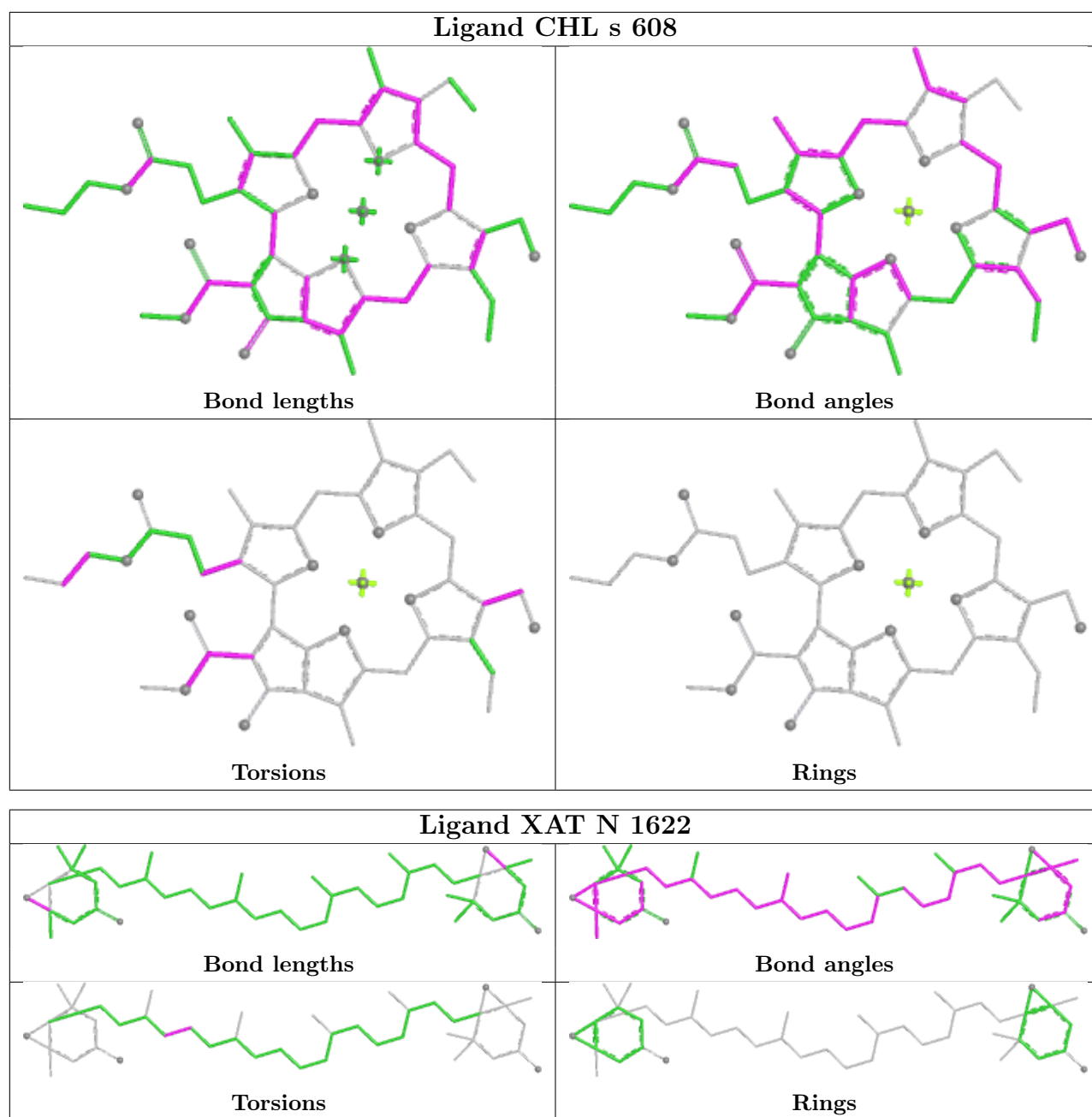
Bond angles



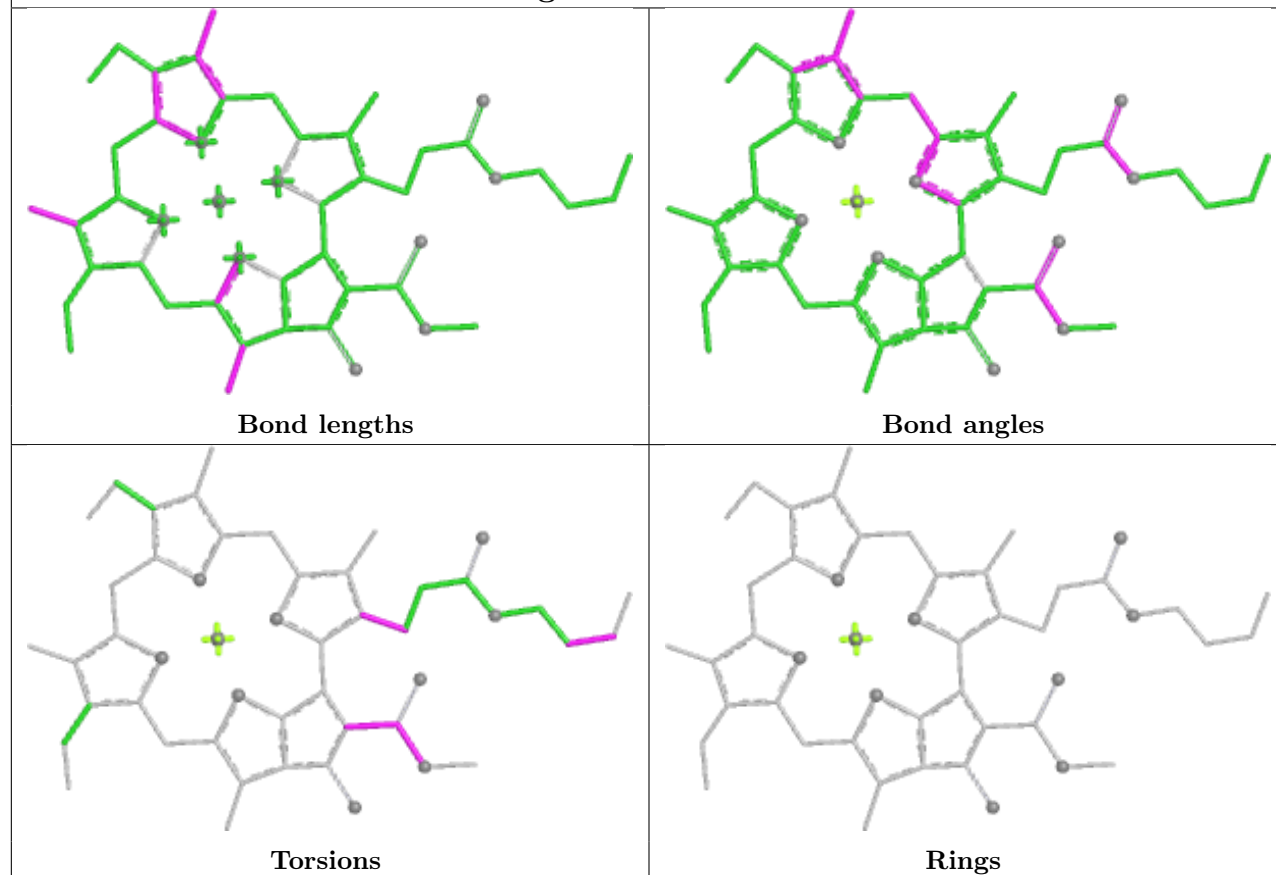
Torsions



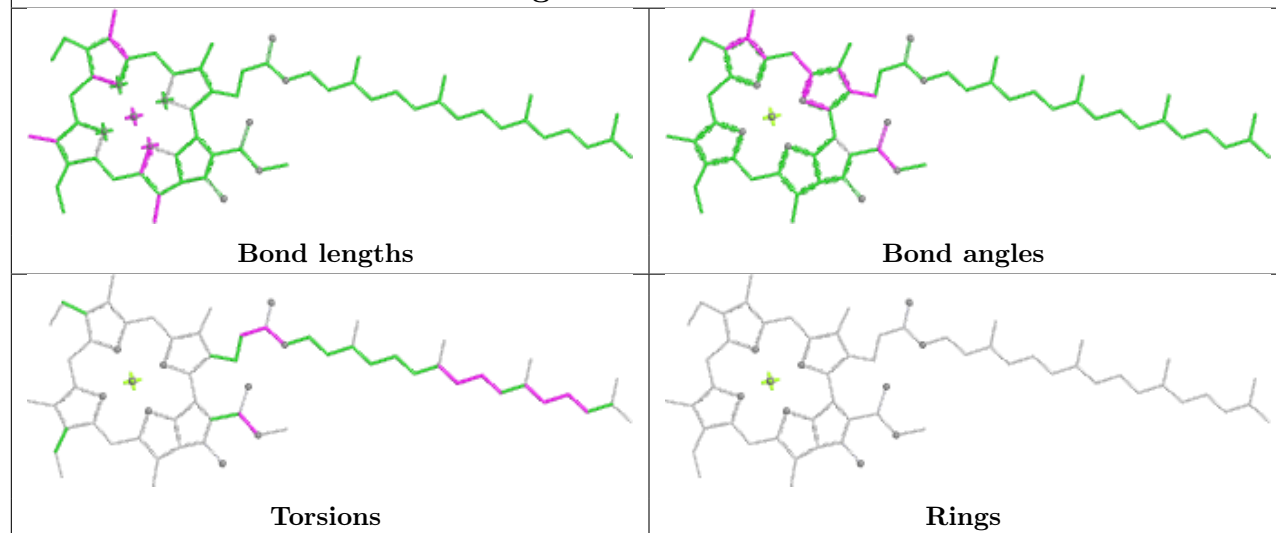
Rings

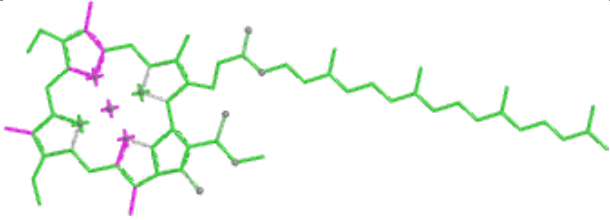
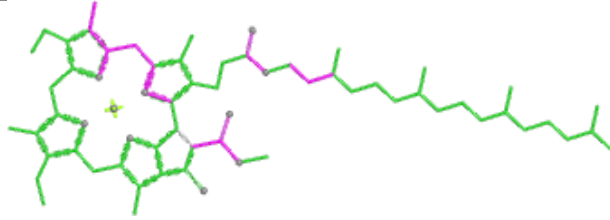
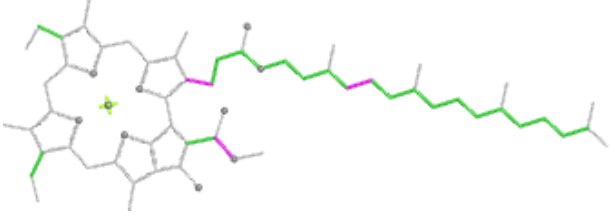
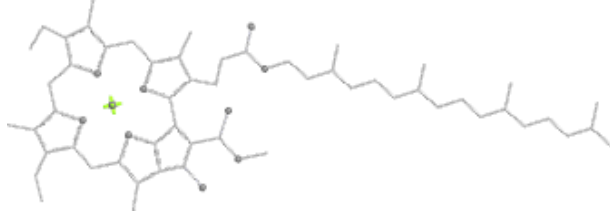
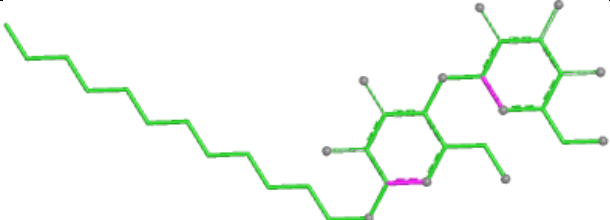
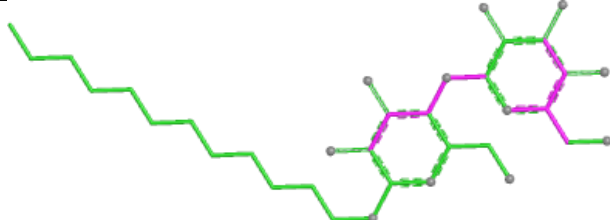
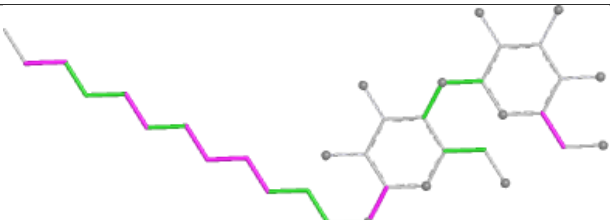
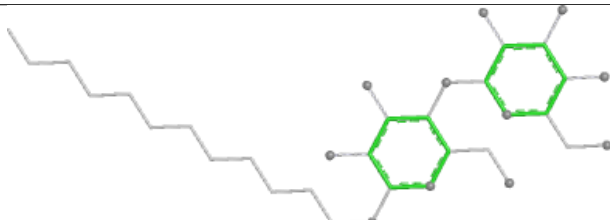
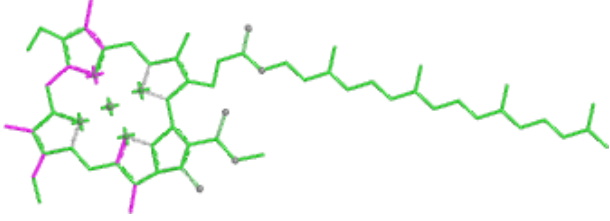
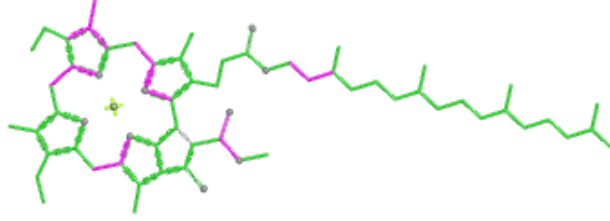
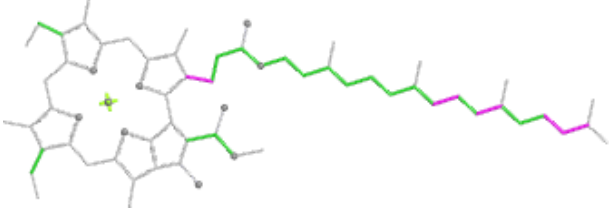
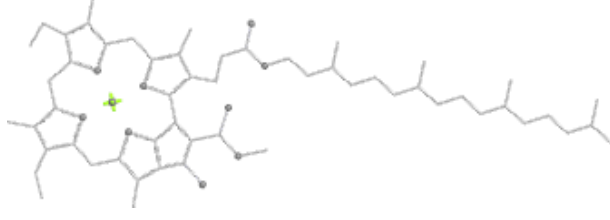


Ligand CLA s 604

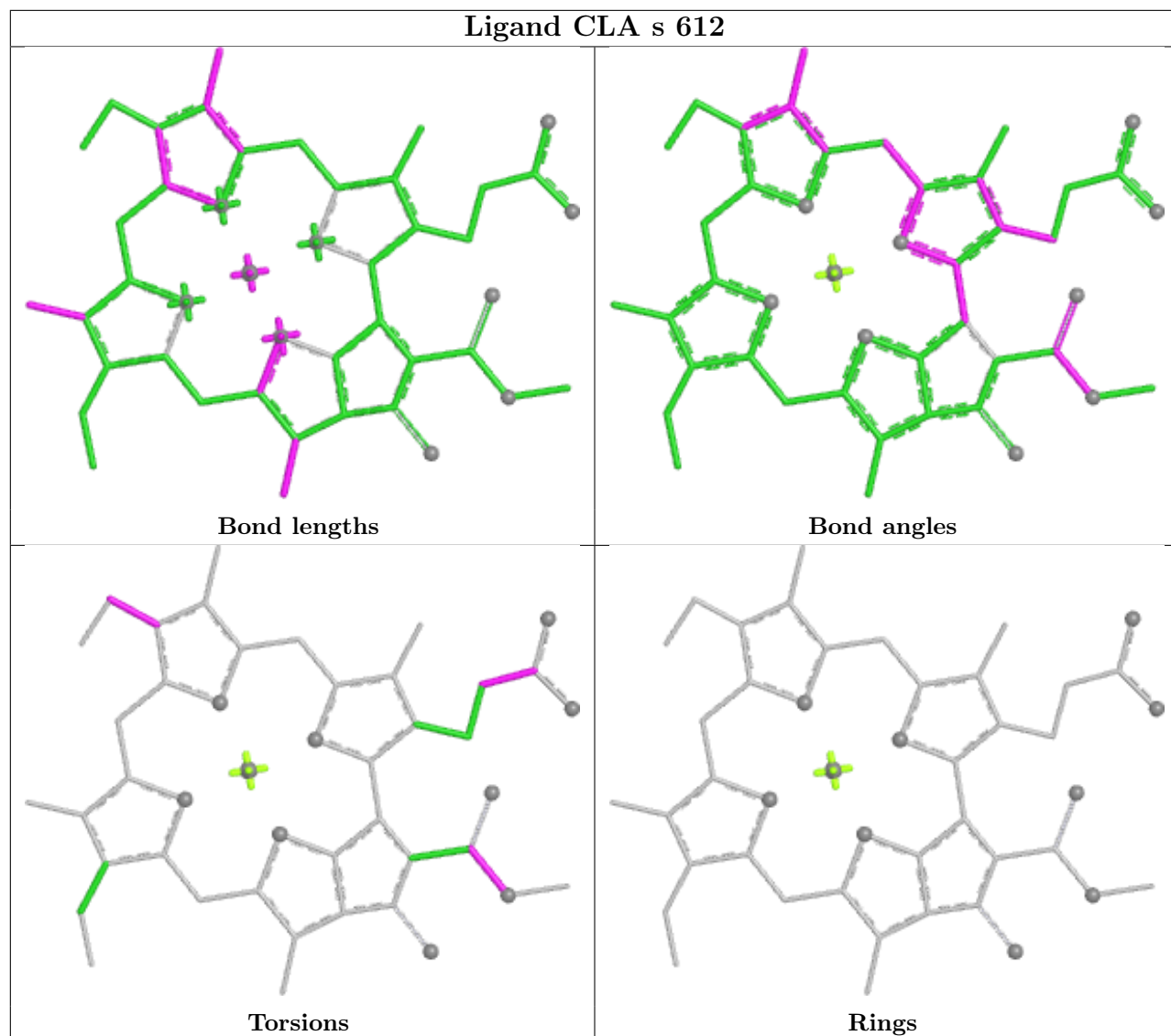


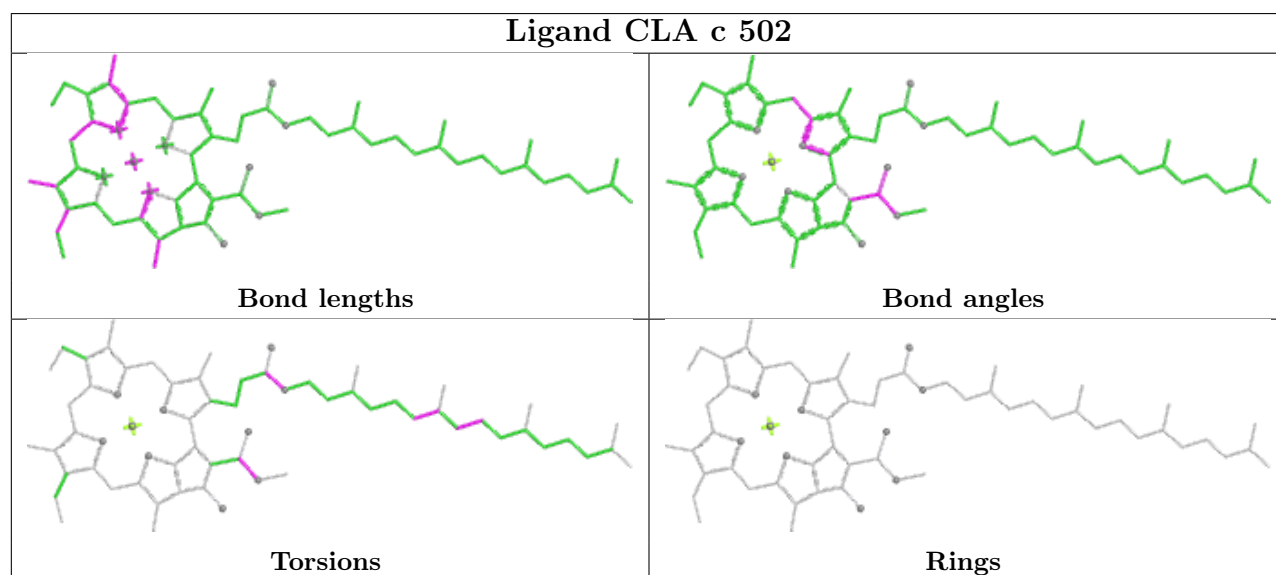
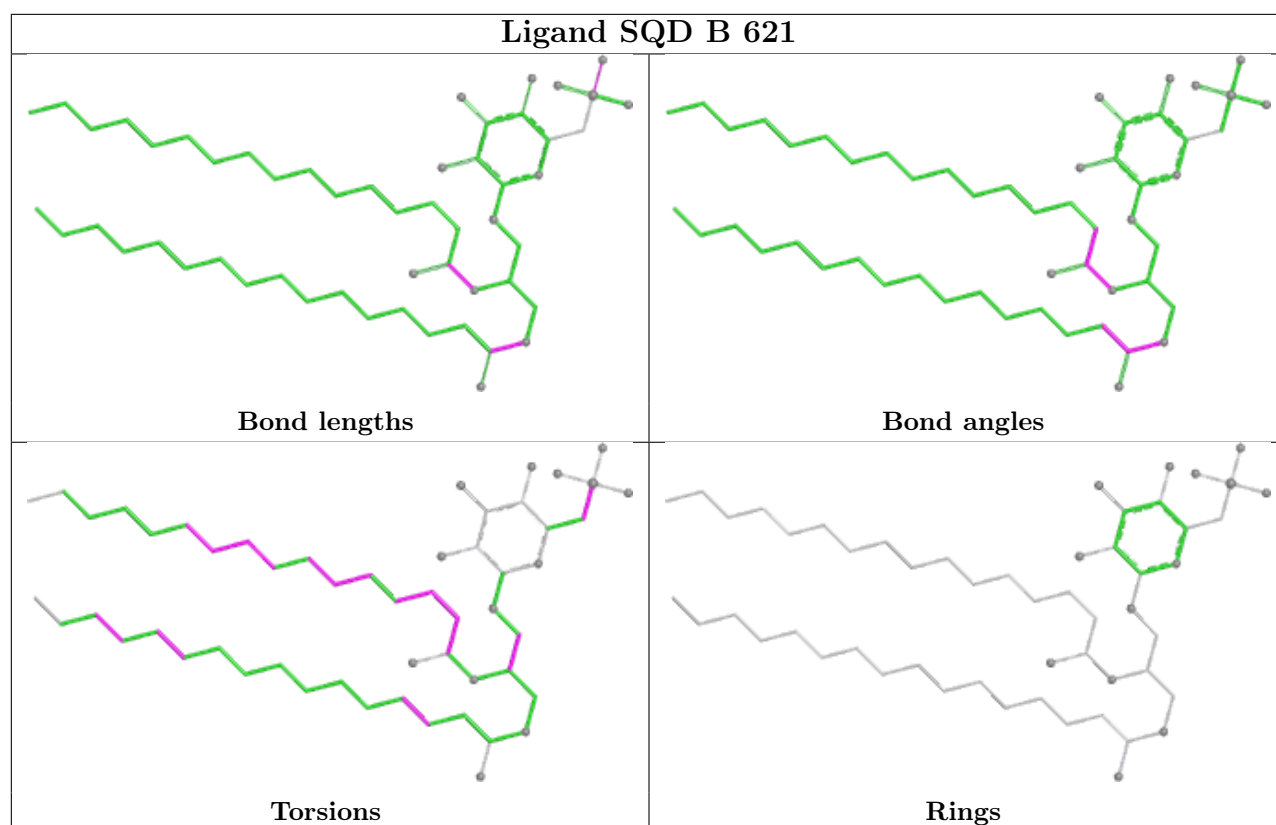
Ligand CLA C 510

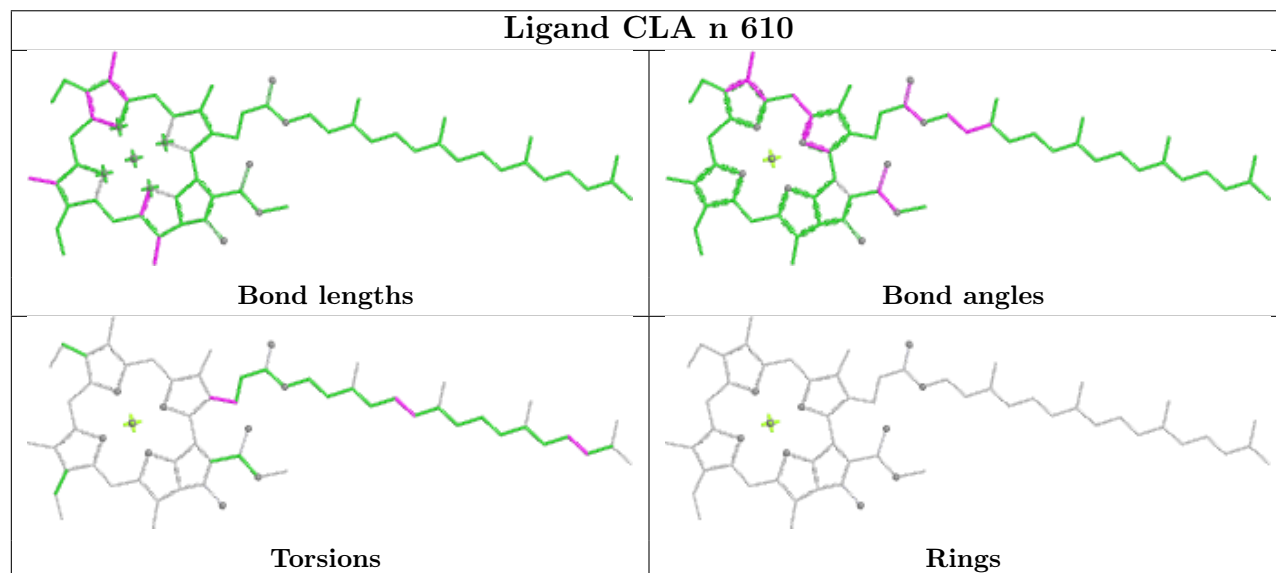
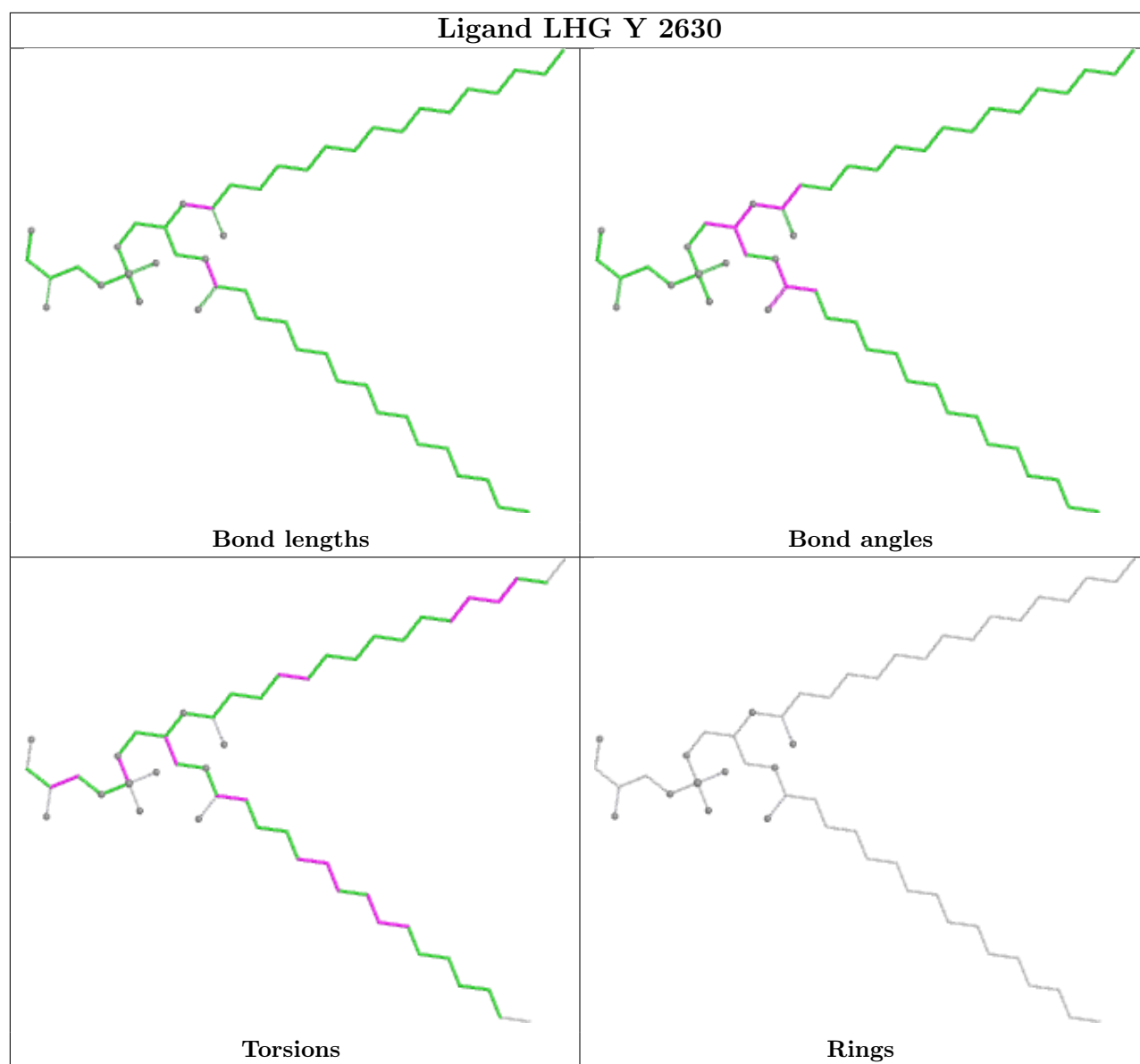


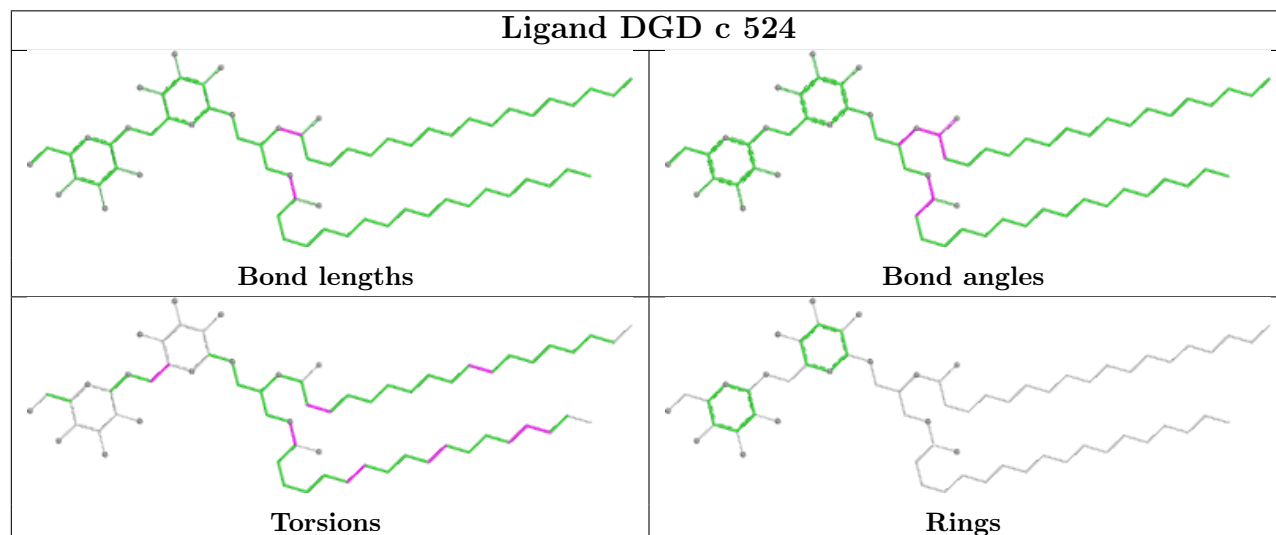
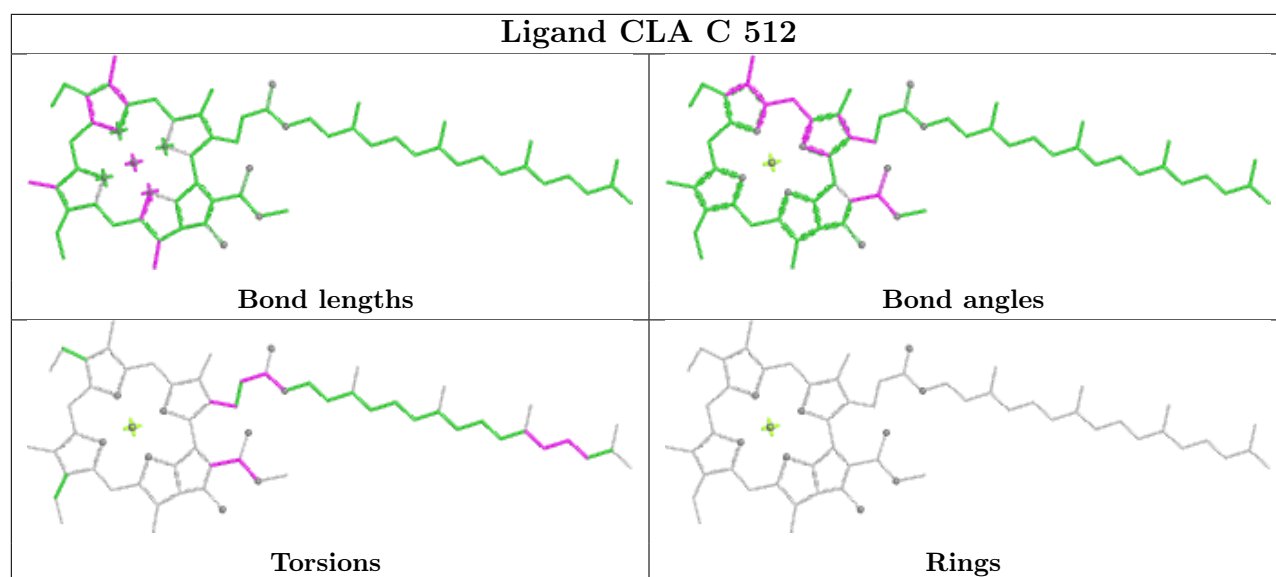
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMU y 2632	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

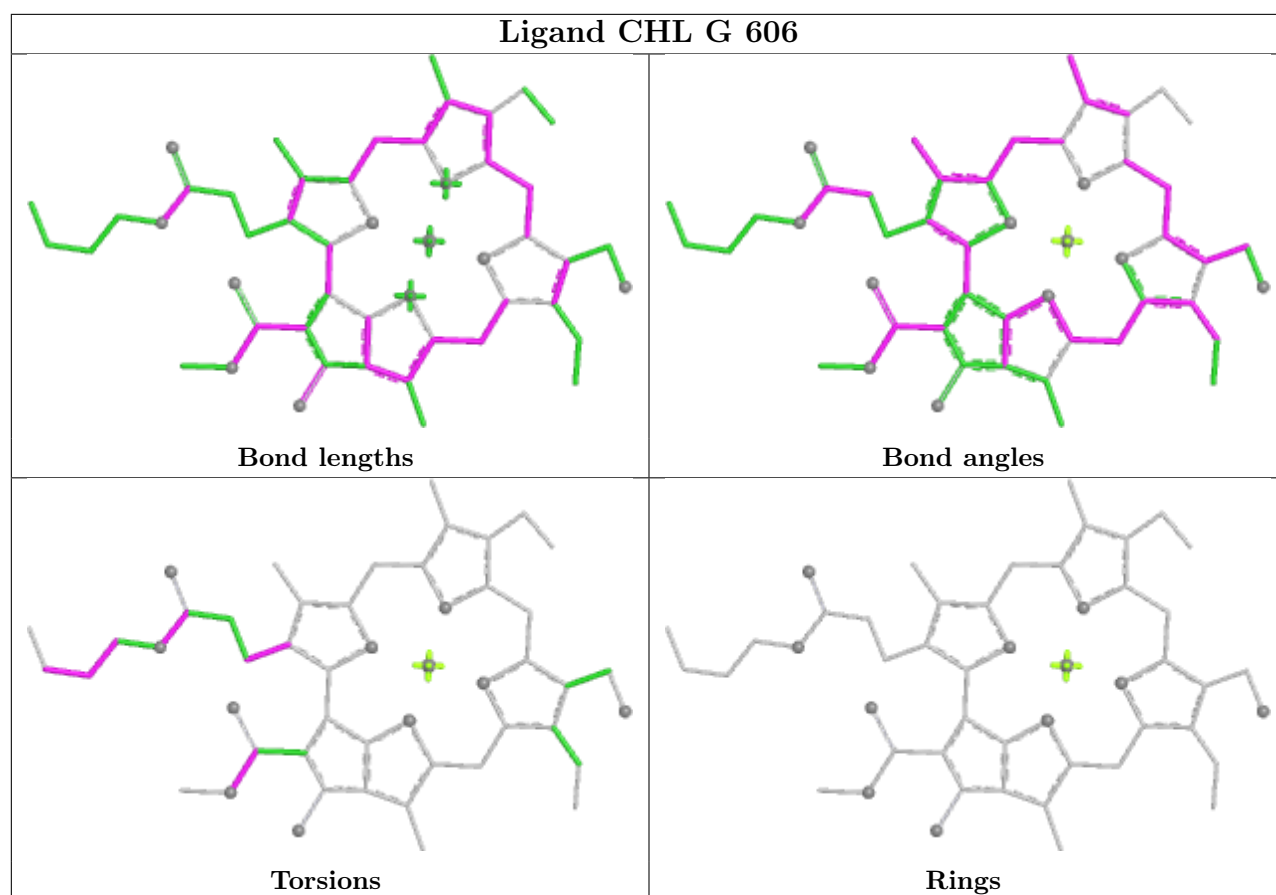
Ligand CLA s 612



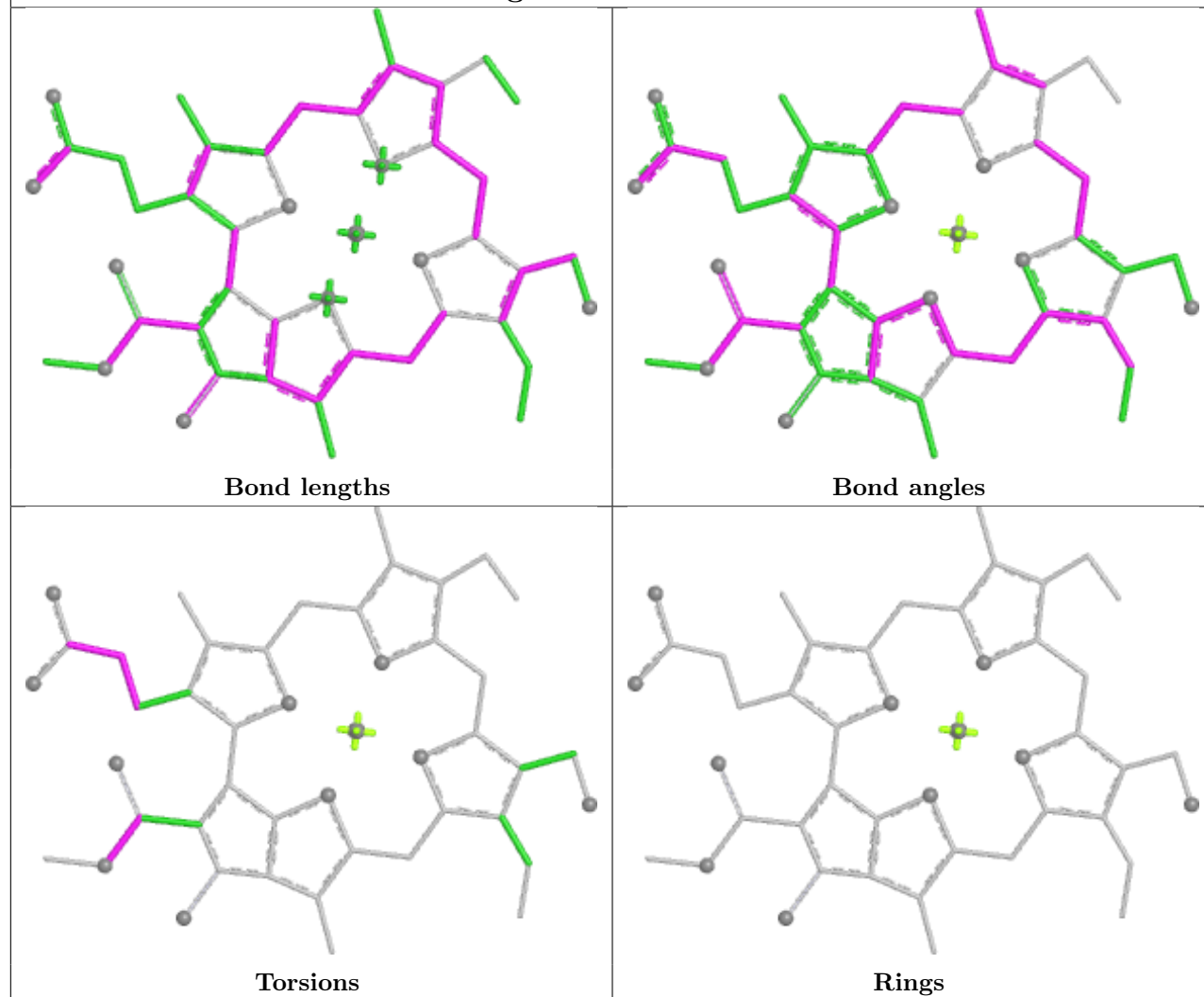




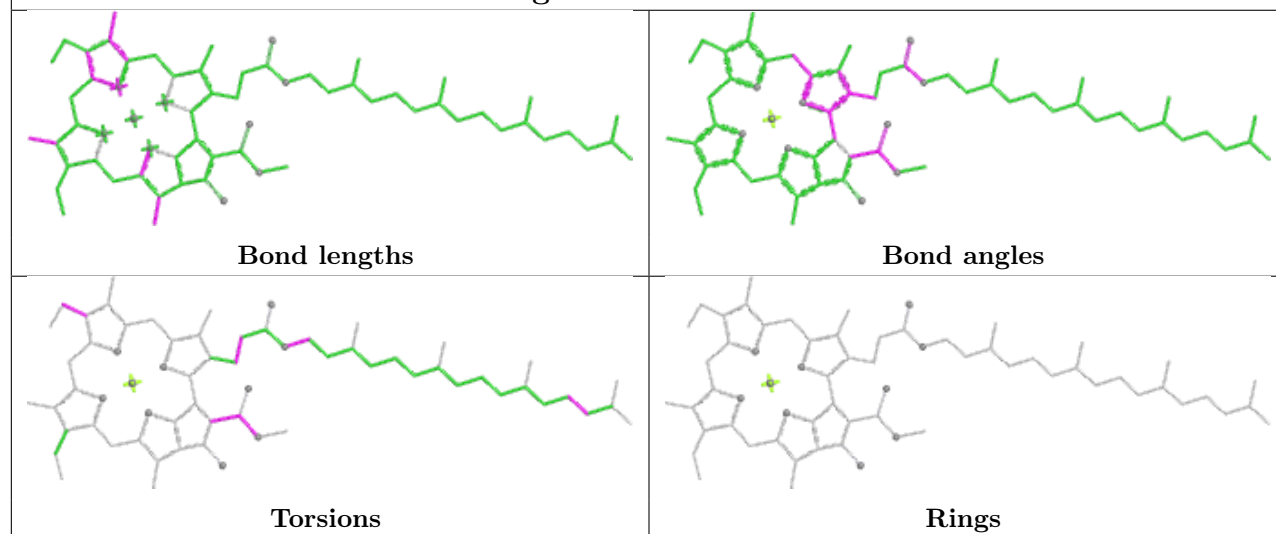


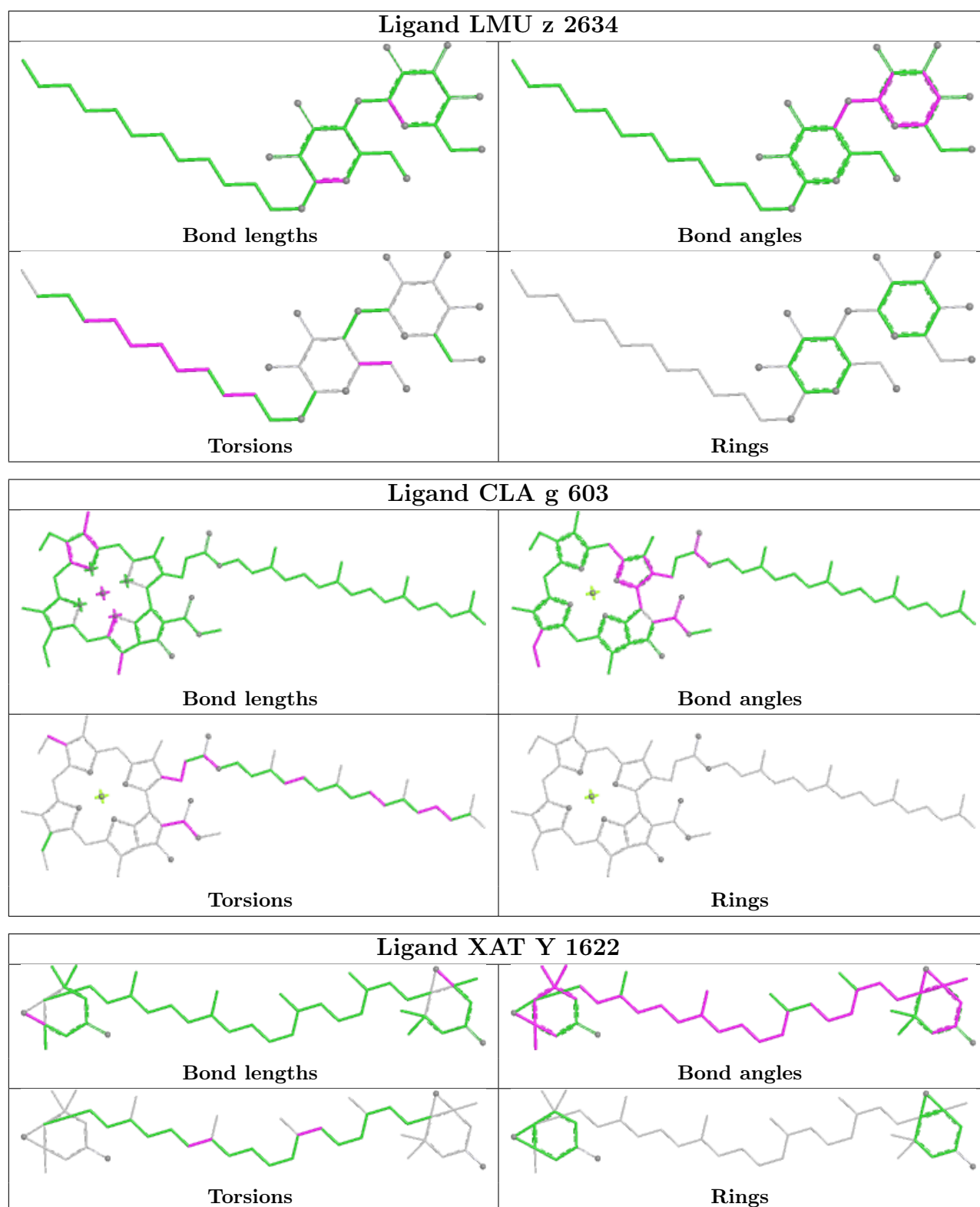


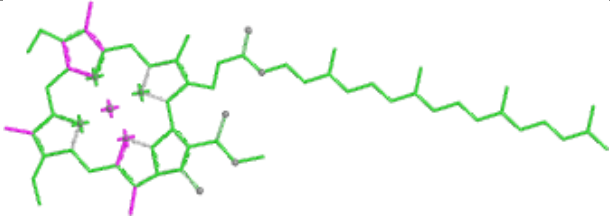
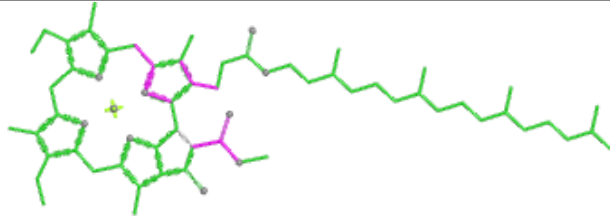
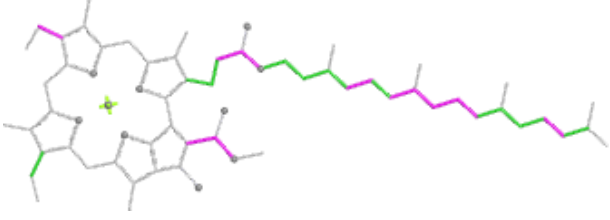
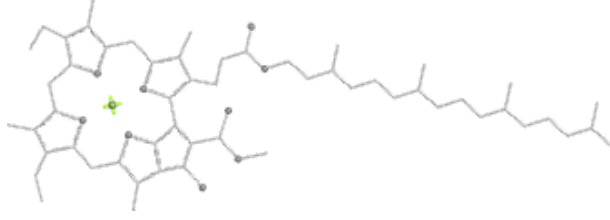
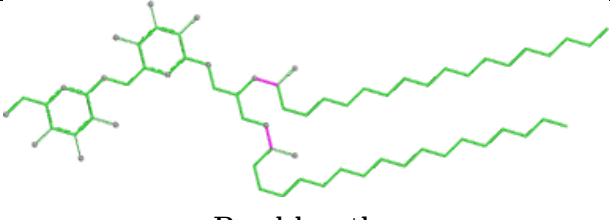
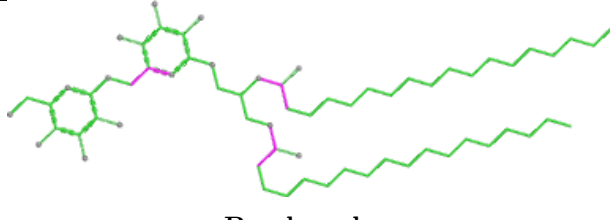
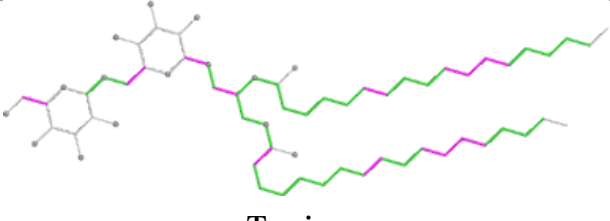
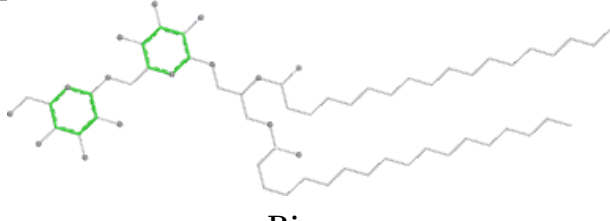
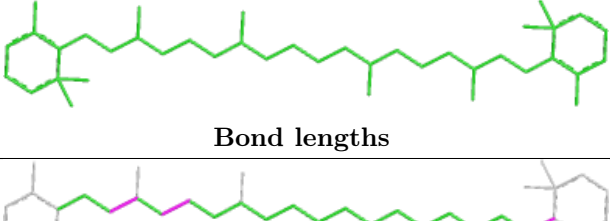
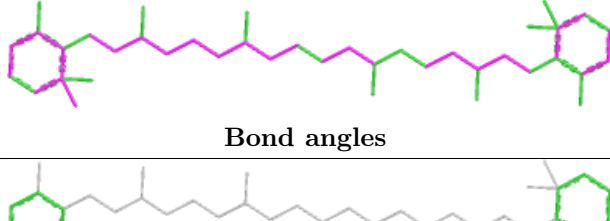
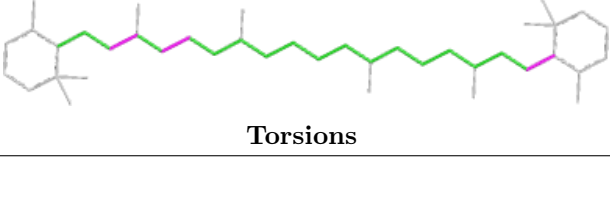
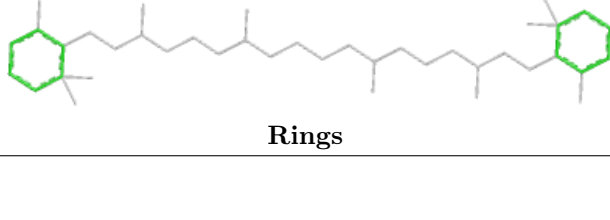
Ligand CHL r 608

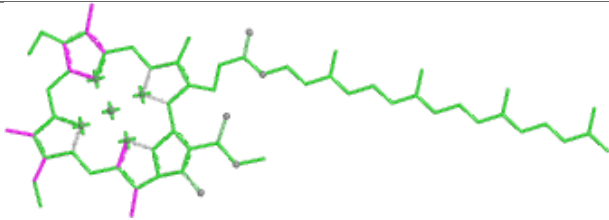
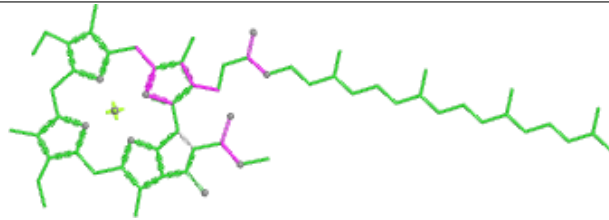
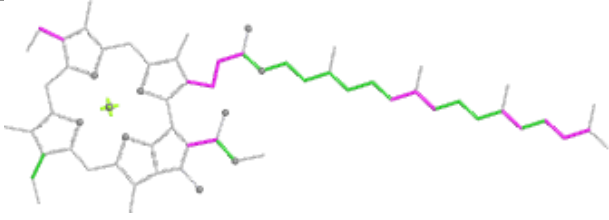
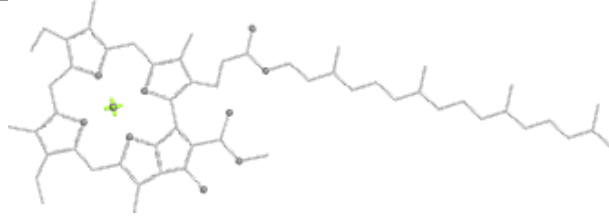


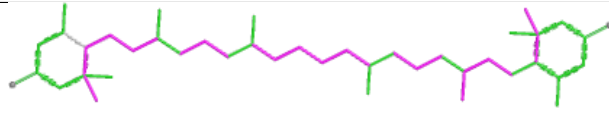
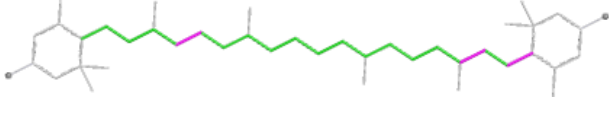
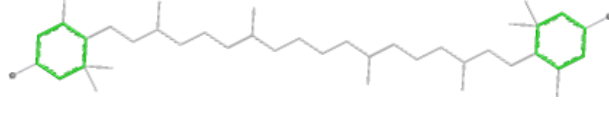
Ligand CLA B 611

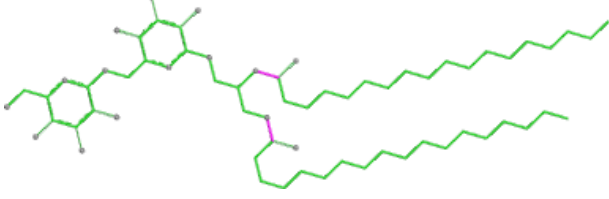
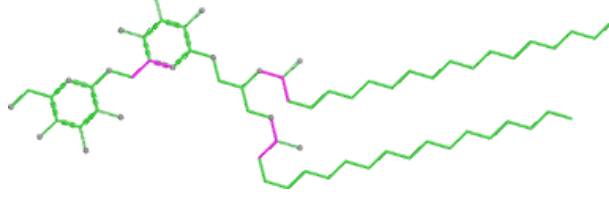
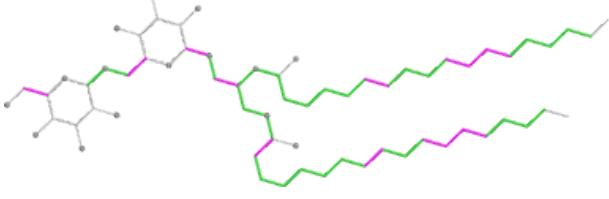
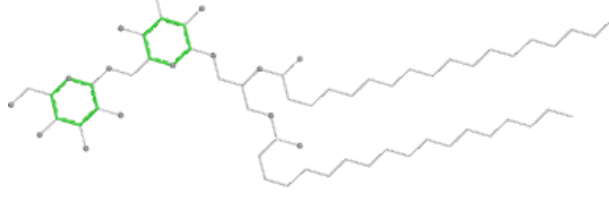


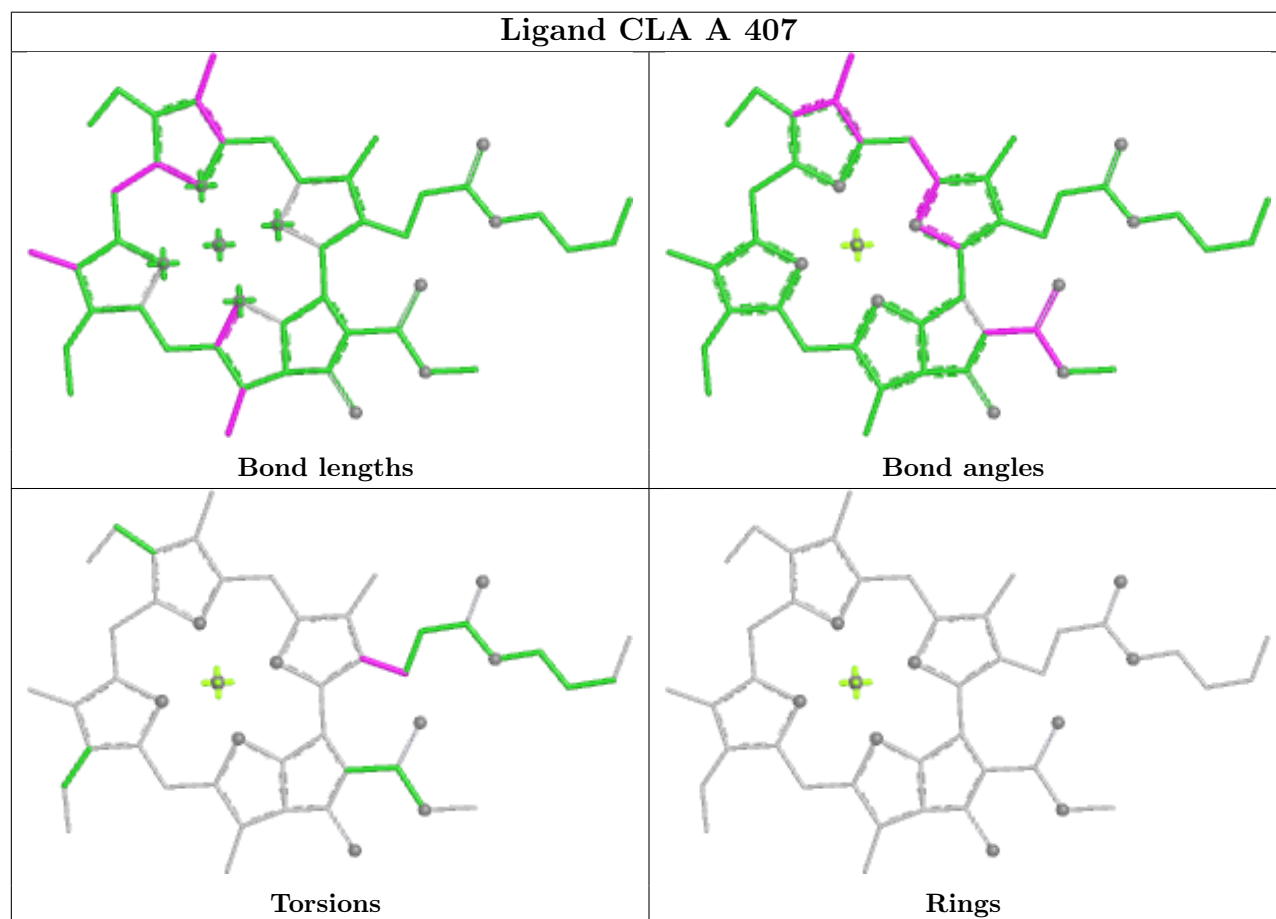
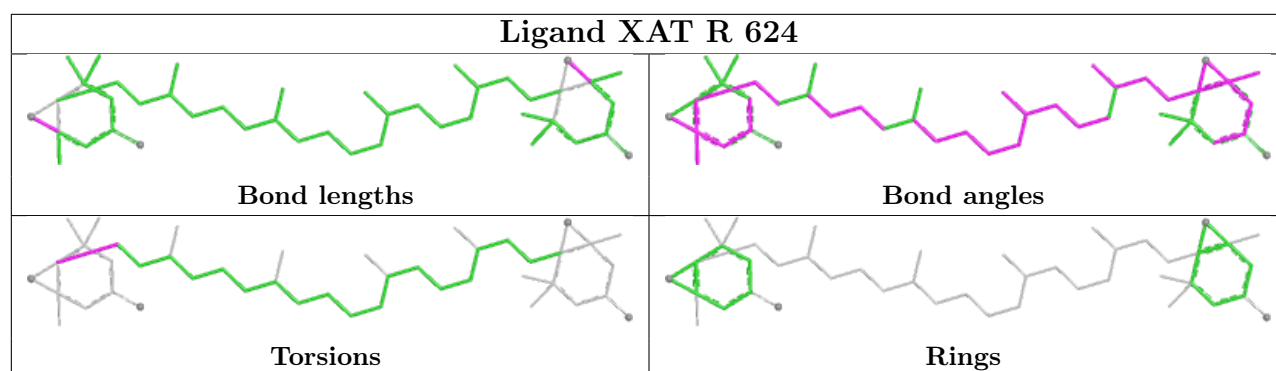


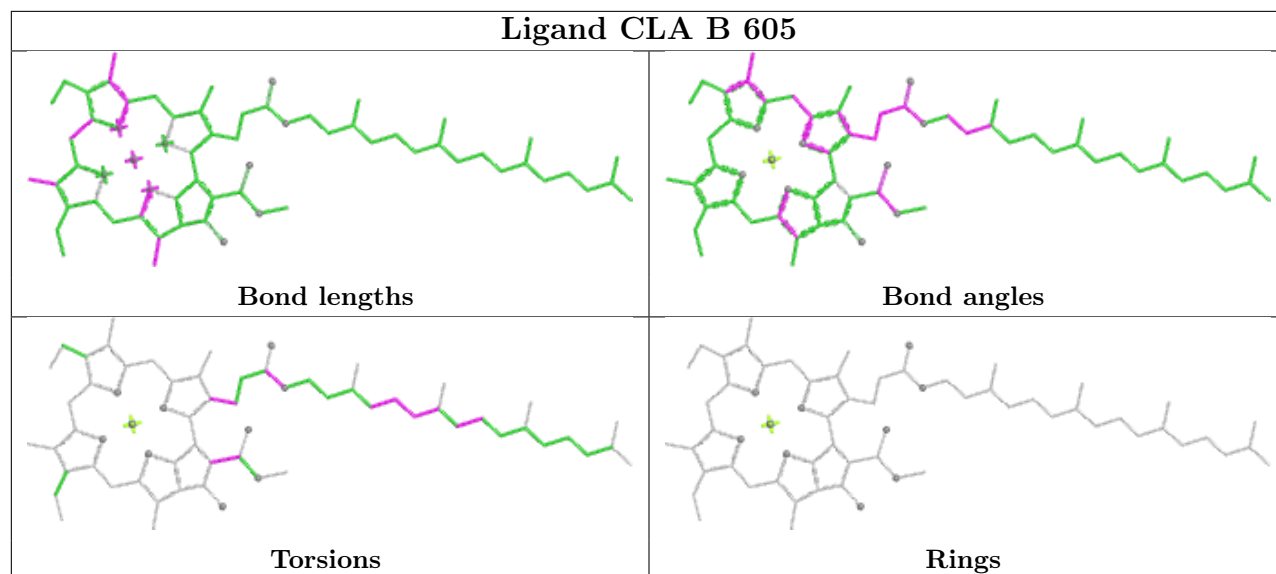
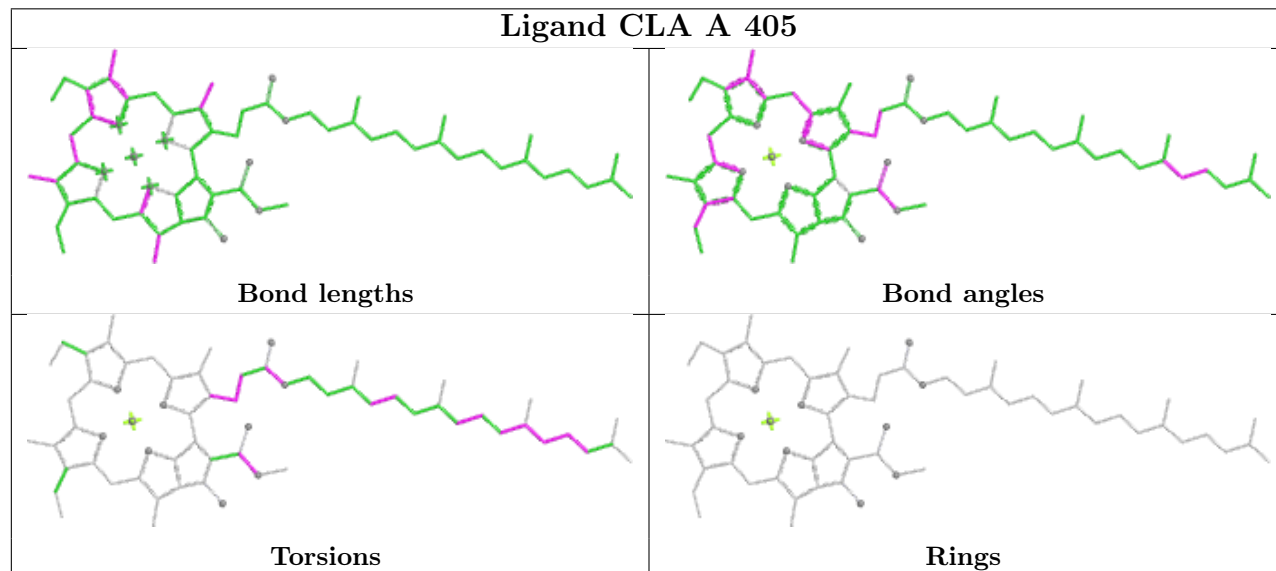
Ligand CLA Y 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD C 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

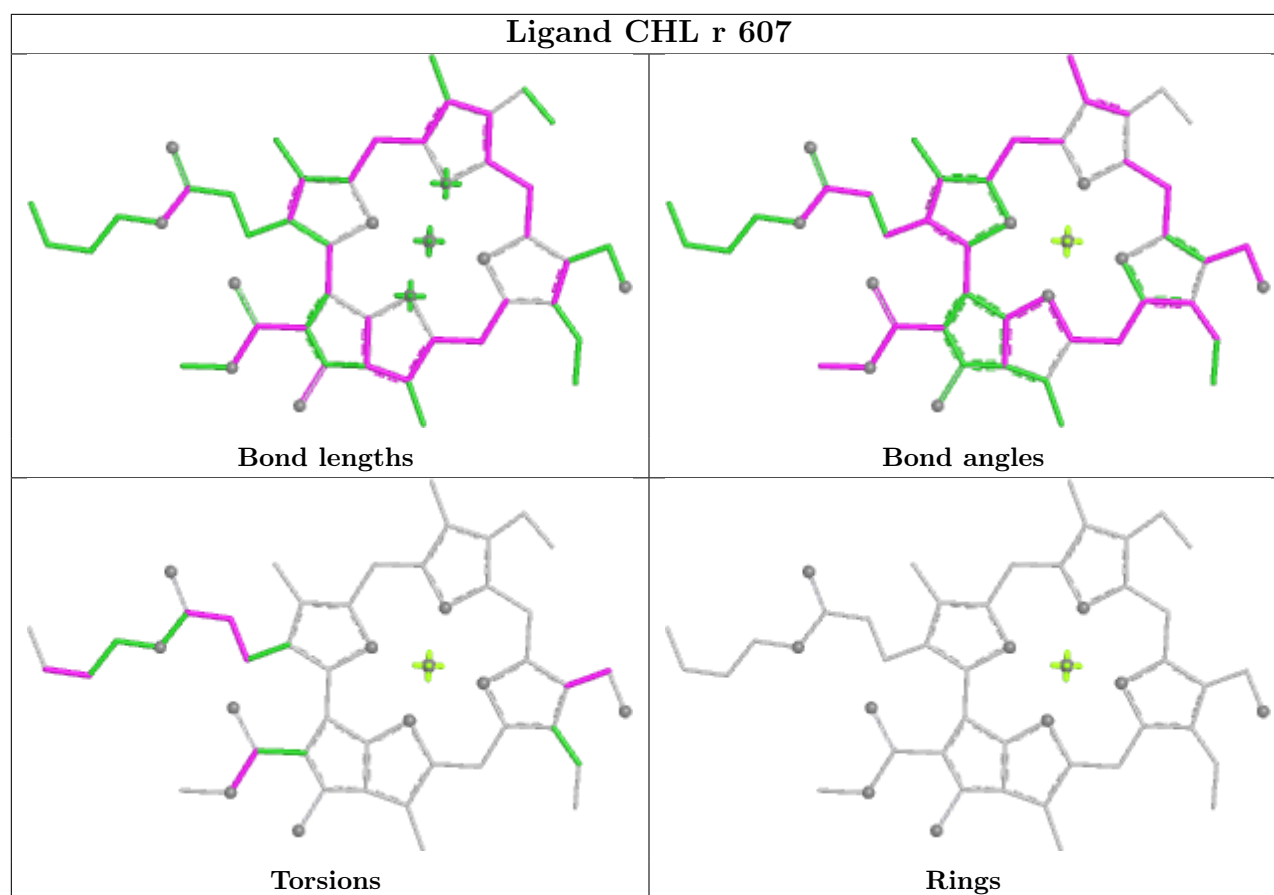
Ligand CLA n 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT Y 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings



Ligand CLA B 605**Ligand CLA A 405**



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.

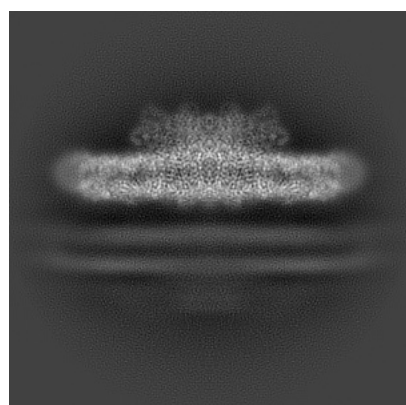
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9955. These allow visual inspection of the internal detail of the map and identification of artifacts.

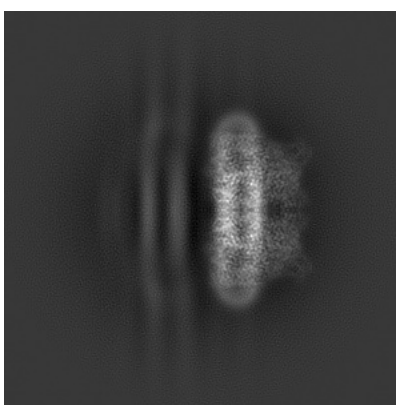
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

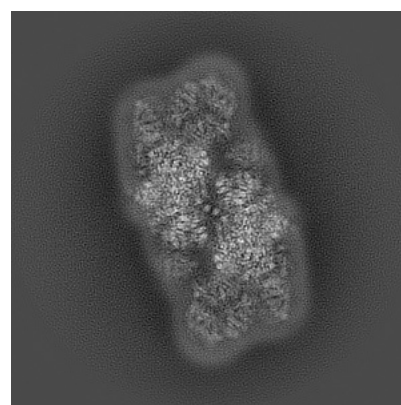
6.1.1 Primary map



X



Y

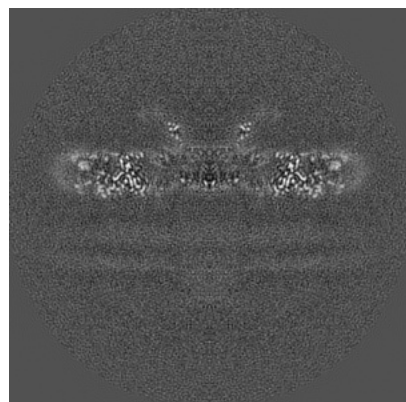


Z

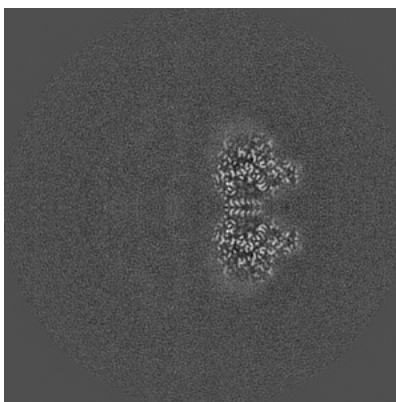
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

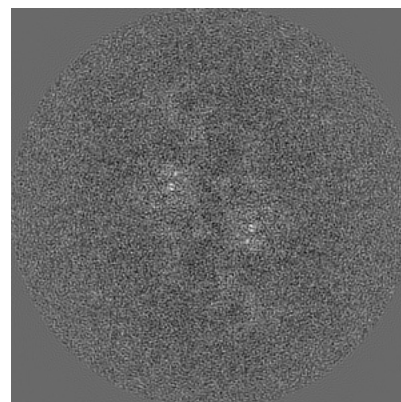
6.2.1 Primary map



X Index: 192



Y Index: 192

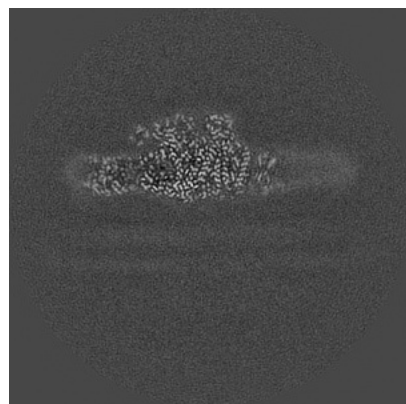


Z Index: 192

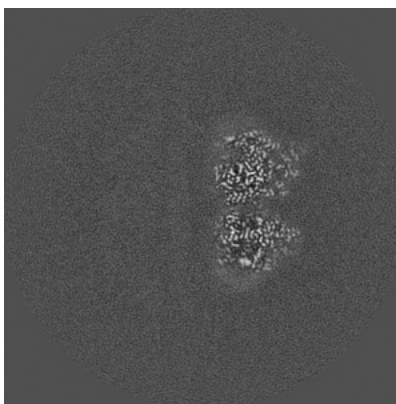
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

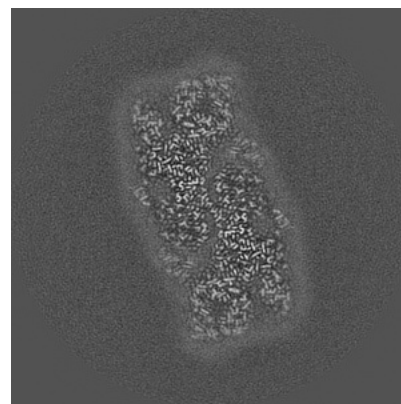
6.3.1 Primary map



X Index: 220



Y Index: 183

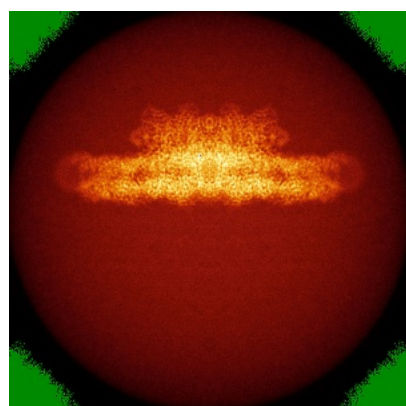


Z Index: 215

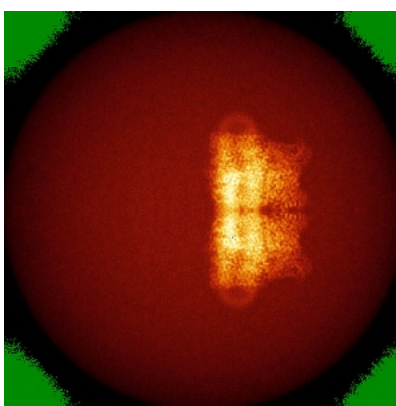
The images above show the largest variance slices of the map in three orthogonal directions.

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

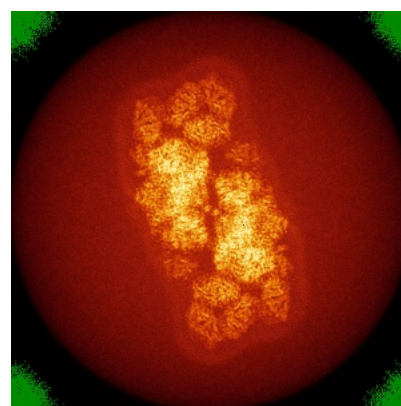
6.4.1 Primary map



X



Y

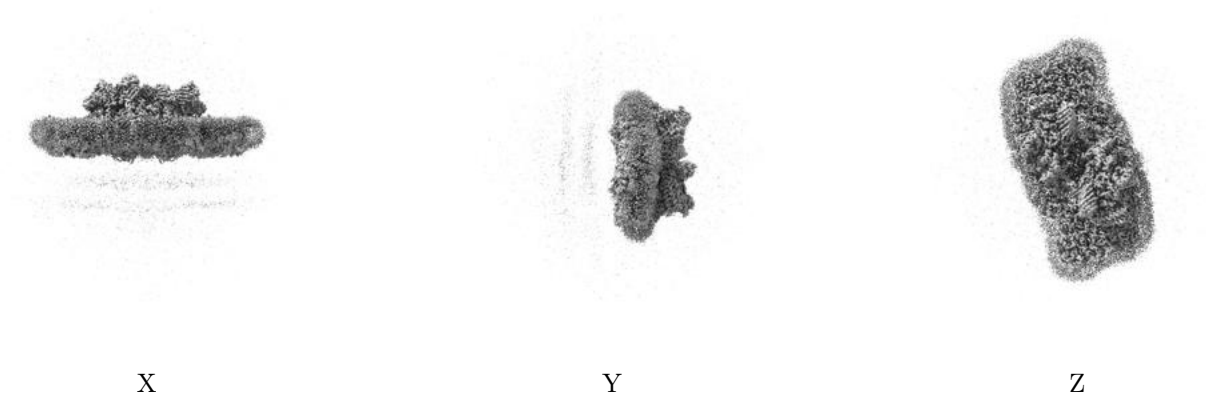


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

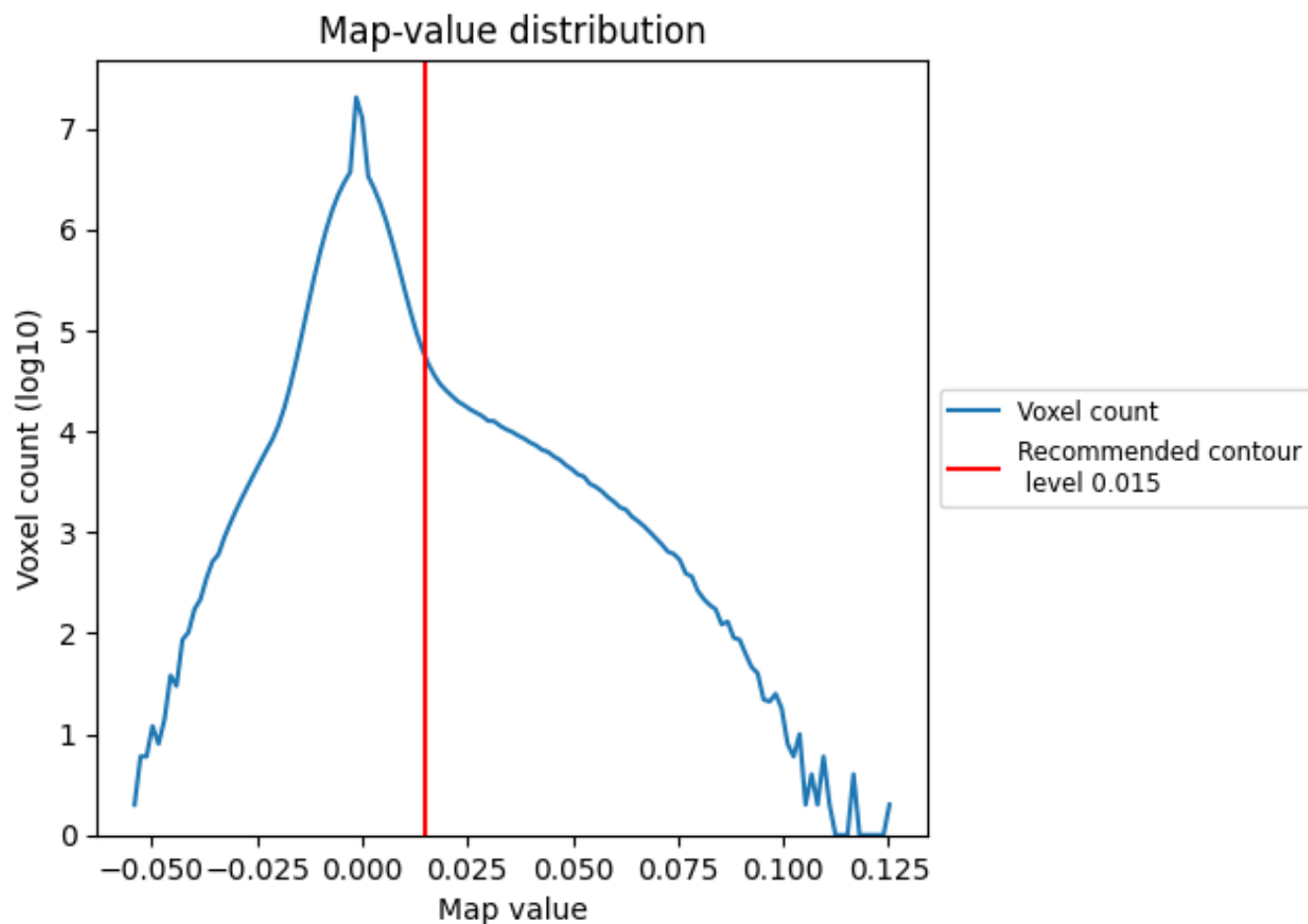
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

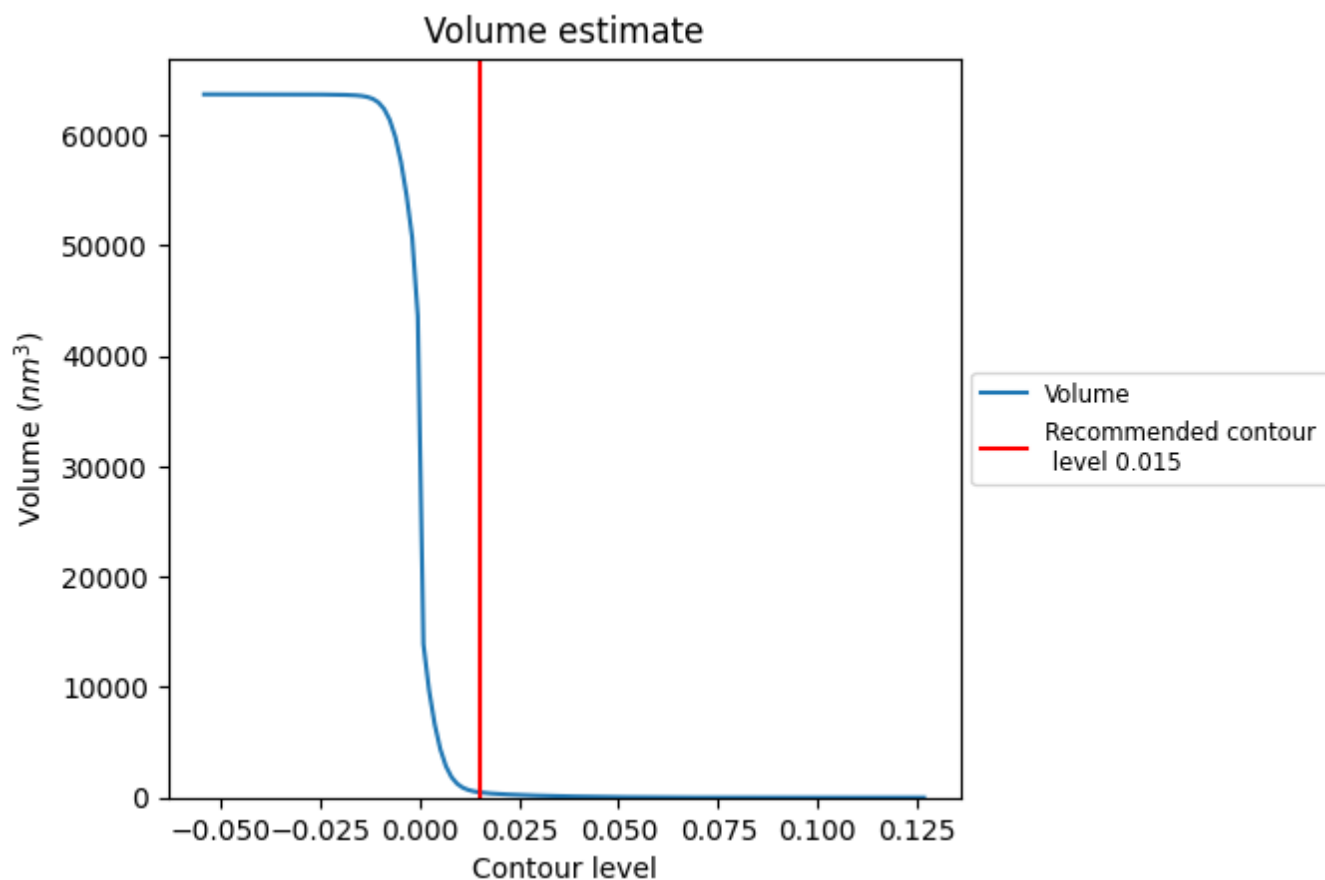
This section contains the results of statistical analysis of the map.

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.

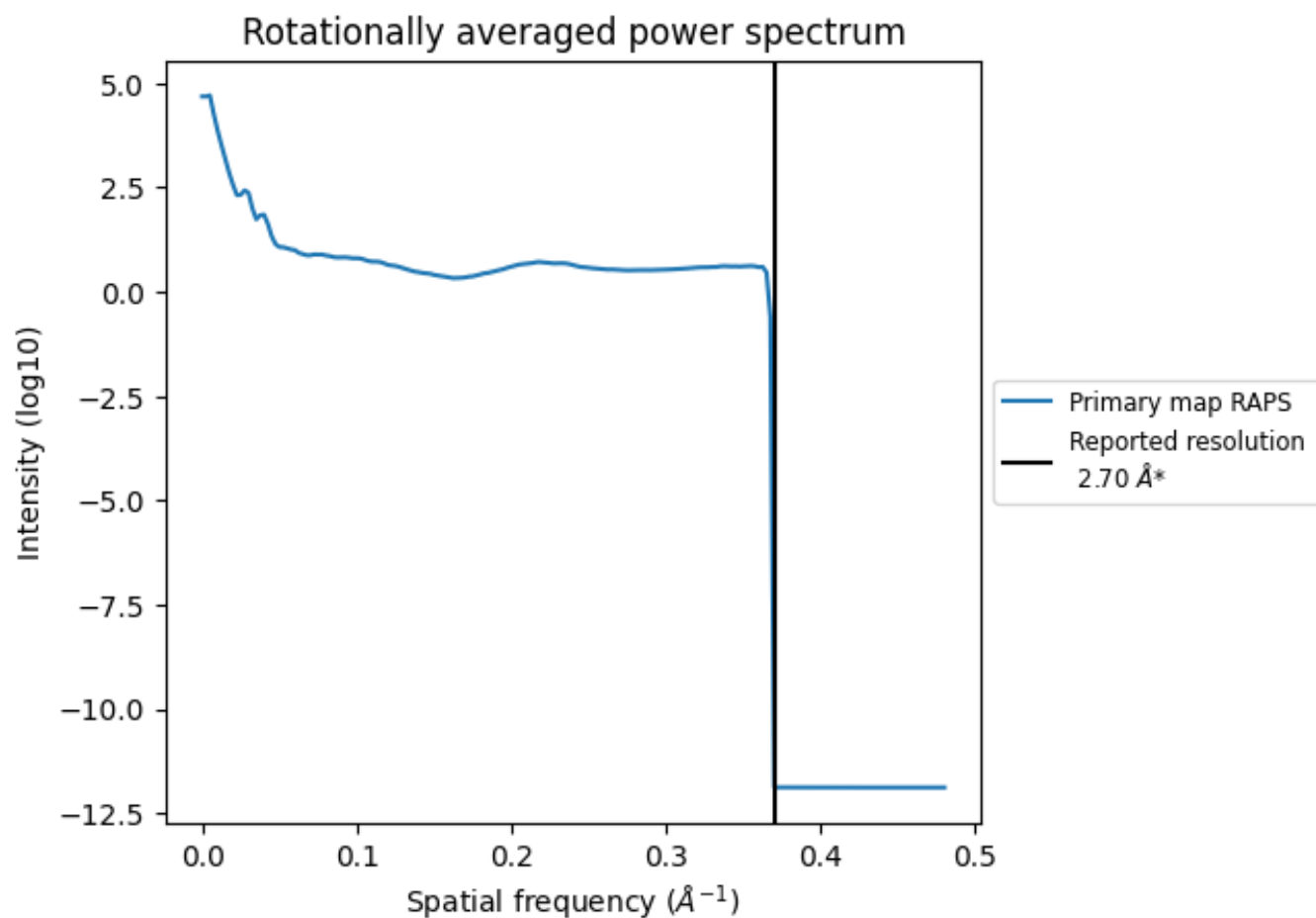
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 436 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 ⓘ

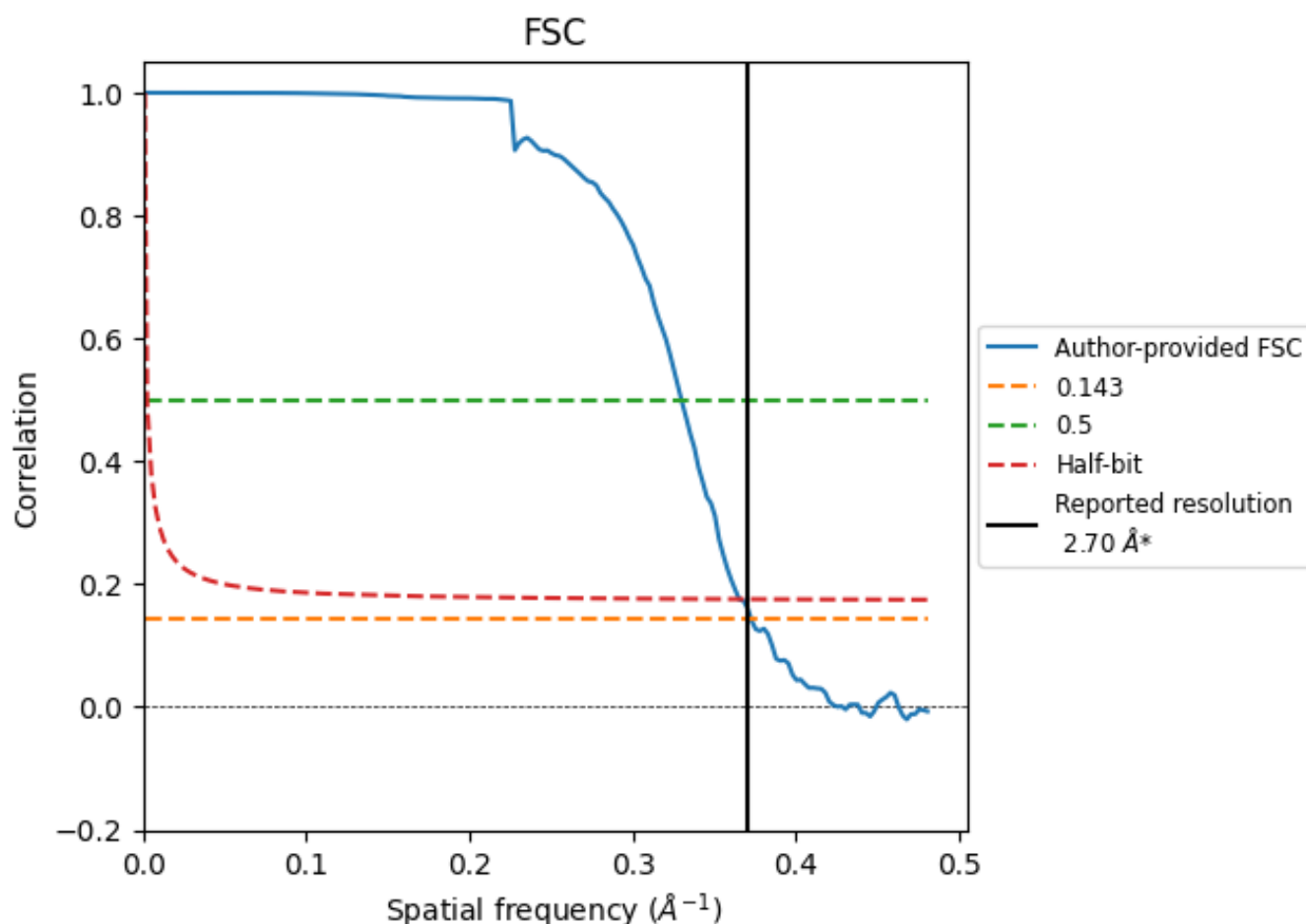


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

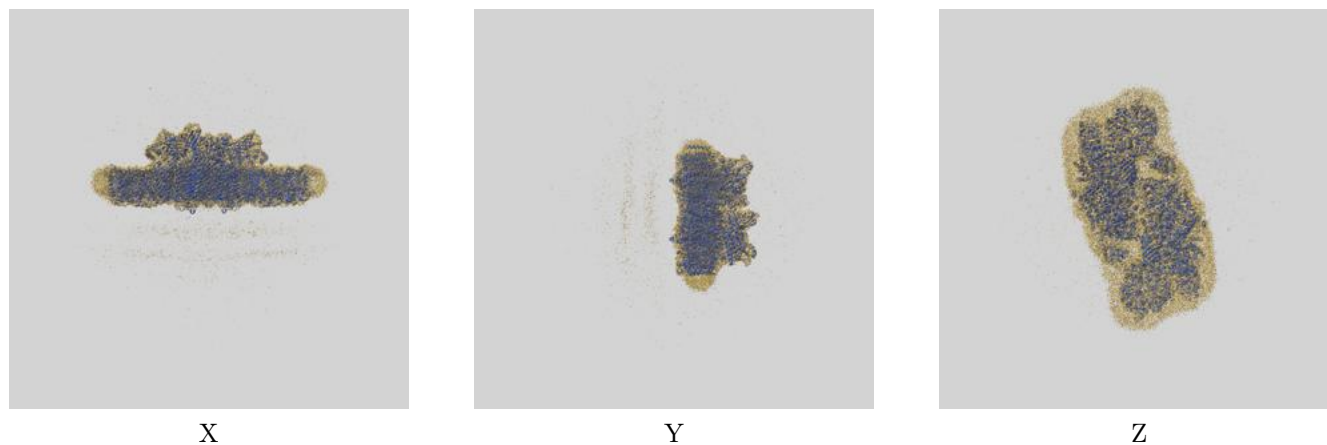
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.03	2.74
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

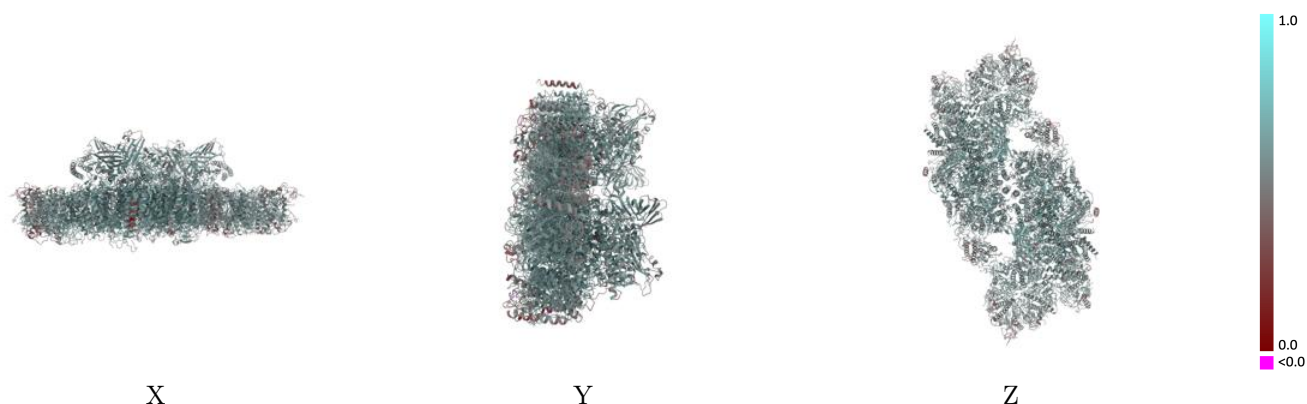
This section contains information regarding the fit between EMDB map EMD-9955 and PDB model 6KAC. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

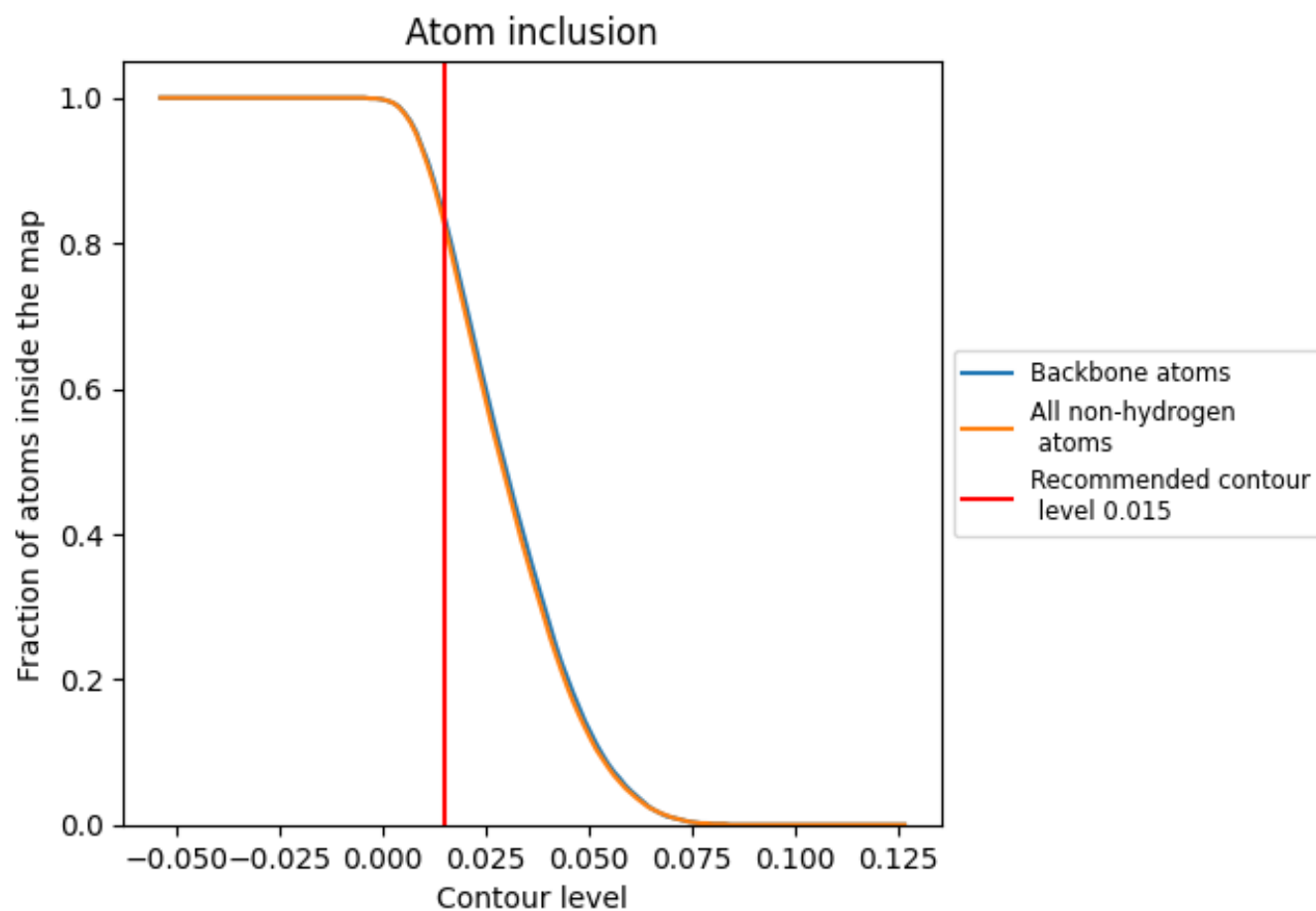


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5690
0	 0.4210	 0.3430
1	 0.4380	 0.3500
3	 0.4380	 0.4680
4	 0.4200	 0.4720
A	 0.9180	 0.6230
B	 0.8710	 0.5950
C	 0.8960	 0.6150
D	 0.9050	 0.6150
E	 0.8210	 0.5420
F	 0.8390	 0.5680
G	 0.7530	 0.5100
H	 0.8060	 0.5620
I	 0.9320	 0.6130
J	 0.8050	 0.5710
K	 0.8870	 0.5810
L	 0.8680	 0.5980
M	 0.8290	 0.5800
N	 0.7990	 0.5510
O	 0.8170	 0.5610
P	 0.7760	 0.5490
Q	 0.6930	 0.5330
R	 0.6500	 0.4630
S	 0.7750	 0.5110
T	 0.8060	 0.5920
U	 0.4560	 0.4770
V	 0.7210	 0.5200
W	 0.8170	 0.5660
X	 0.6490	 0.4910
Y	 0.8410	 0.5930
Z	 0.8000	 0.5640
a	 0.9170	 0.6220
b	 0.8710	 0.5950
c	 0.8960	 0.6140
d	 0.9020	 0.6140



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.8210	 0.5450
f	 0.8420	 0.5600
g	 0.7510	 0.5110
h	 0.8060	 0.5590
i	 0.9320	 0.6190
j	 0.8050	 0.5700
k	 0.8870	 0.5790
l	 0.8680	 0.6000
m	 0.8290	 0.5830
n	 0.7990	 0.5490
o	 0.8150	 0.5610
p	 0.7760	 0.5500
q	 0.6920	 0.5340
r	 0.6500	 0.4670
s	 0.7760	 0.5100
t	 0.8060	 0.5940
u	 0.4510	 0.4770
v	 0.7160	 0.5210
w	 0.8170	 0.5690
x	 0.6450	 0.4970
y	 0.8410	 0.5920
z	 0.8000	 0.5620