



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 02:31 PM UTC

PDB ID : 7PI5 / pdb_00007pi5
EMDB ID : EMD-13430
Title : Unstacked stretched Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-19
Resolution : 2.78 Å (reported)
Based on initial model : 6KAC

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

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

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

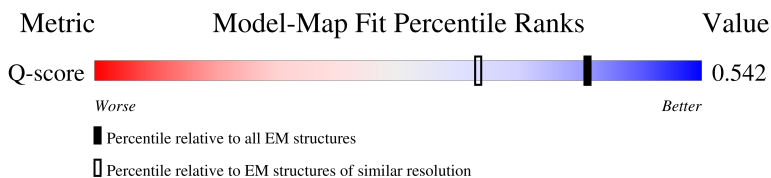
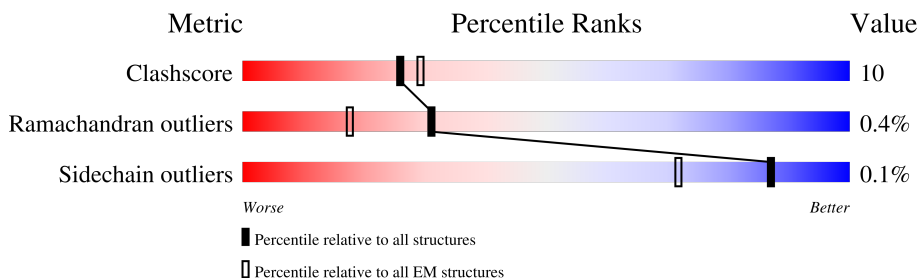
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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.



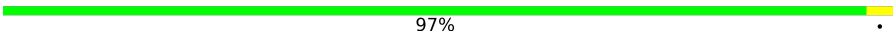
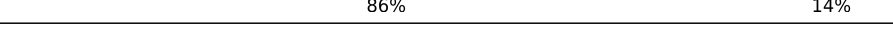
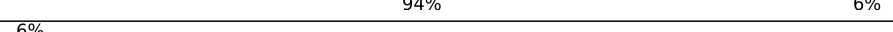
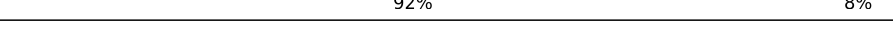
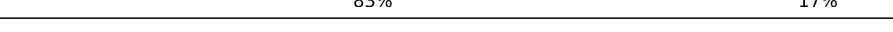
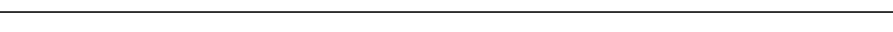
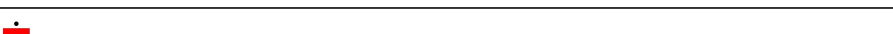
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	336	
1	a	336	
2	B	484	
2	b	484	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	V	32	 97%
3	v	32	 75% 25%
4	C	449	 75% 25%
4	c	449	 74% 26%
5	D	348	 78% 22%
5	d	348	 80% 20%
6	E	76	 84% 16%
6	e	76	 88% 12%
7	F	31	 84% 16%
7	f	31	 90% 10%
8	H	67	 82% 18%
8	h	67	 78% 22%
9	I	35	 6% 86% 14%
9	i	35	 94% 6%
10	J	36	 6% 92% 8%
10	j	36	 83% 17%
11	K	37	 73% 27%
11	k	37	 78% 22%
12	L	38	 87% 13%
12	l	38	 89% 11%
13	M	32	 88% 12%
13	m	32	 91% 9%
14	O	238	 5% 74% 25%
14	o	238	 74% 26%
15	P	187	 15% 81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	p	187	
16	T	30	
16	t	30	
17	W	44	
17	w	44	
18	X	30	
18	x	30	
19	Z	61	
19	z	61	
20	N	222	
20	n	222	
21	G	221	
21	g	221	
22	R	202	
22	r	202	
23	S	243	
23	s	243	
24	Y	222	
24	y	222	
25	U	27	
25	u	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	407	X	-	-	-
29	CLA	A	410	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	612	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	C	501	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	603	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	611	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	R	613	X	-	-	-
29	CLA	S	602	X	-	-	-
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	a	407	X	-	-	-
29	CLA	a	410	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	609	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	612	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-
29	CLA	c	501	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	503	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	506	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	511	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	c	513	X	-	-	-
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	612	X	-	-	-
29	CLA	g	613	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	n	612	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	603	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-
29	CLA	r	611	X	-	-	-
29	CLA	r	612	X	-	-	-
29	CLA	r	613	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	603	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	605	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	613	X	-	-	-
29	CLA	y	614	X	-	-	-
35	C7Z	B	620	X	-	-	-
35	C7Z	b	620	X	-	-	-
40	LMK	C	527	X	-	-	-
40	LMK	c	627	X	-	-	-
41	BCT	D	401	-	X	-	-
41	BCT	d	401	-	X	-	-
44	RRX	H	101	X	-	-	-
44	RRX	h	101	X	-	-	-
45	CHL	G	601	X	-	-	-
45	CHL	G	605	X	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CHL	y	607	X	-	-	-
45	CHL	y	609	X	-	-	-
46	LUT	S	620	X	-	-	-
46	LUT	s	620	X	-	-	-
47	XAT	G	622	X	-	-	-
47	XAT	N	622	X	-	-	-
47	XAT	R	621	X	-	-	-
47	XAT	Y	622	X	-	-	-
47	XAT	g	622	X	-	-	-
47	XAT	n	622	X	-	-	-
47	XAT	r	622	X	-	-	-
47	XAT	y	622	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 76287 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	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O		0	0
			297	207	43	47			
11	k	37	Total	C	N	O		0	0
			297	207	43	47			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O		0	0
			243	164	34	45			
13	m	32	Total	C	N	O		0	0
			243	164	34	45			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

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

- Molecule 15 is a protein called PsbP.

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

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

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

- Molecule 17 is a protein called PSII 6.1 kDa protein.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	65	MET	LEU	conflict	UNP A0A7S3QU88
W	96	TYR	PHE	conflict	UNP A0A7S3QU88
w	65	MET	LEU	conflict	UNP A0A7S3QU88

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
w	96	TYR	PHE	conflict	UNP A0A7S3QU88

- Molecule 18 is a protein called Hypothetical protein.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3
x	81	VAL	THR	conflict	UNP A0A7S3VKF3

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

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

- Molecule 20 is a protein called LHCII M3.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	56	ASP	GLU	conflict	UNP A0A7S3VRZ8
S	119	ILE	LEU	conflict	UNP A0A7S3VRZ8
S	209	LYS	GLN	conflict	UNP A0A7S3VRZ8
S	244	ILE	VAL	conflict	UNP A0A7S3VRZ8
S	245	ALA	GLY	conflict	UNP A0A7S3VRZ8
S	264	ILE	PHE	conflict	UNP A0A7S3VRZ8
S	268	LEU	ILE	conflict	UNP A0A7S3VRZ8
s	56	ASP	GLU	conflict	UNP A0A7S3VRZ8
s	119	ILE	LEU	conflict	UNP A0A7S3VRZ8
s	209	LYS	GLN	conflict	UNP A0A7S3VRZ8
s	244	ILE	VAL	conflict	UNP A0A7S3VRZ8
s	245	ALA	GLY	conflict	UNP A0A7S3VRZ8
s	264	ILE	PHE	conflict	UNP A0A7S3VRZ8
s	268	LEU	ILE	conflict	UNP A0A7S3VRZ8

- Molecule 24 is a protein called LHCII M1.

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

Continued on next page...

Continued from previous page...

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

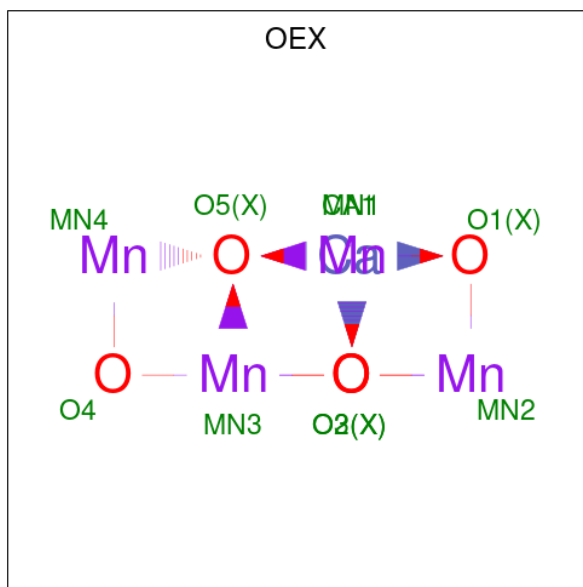
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	49	PHE	TYR	conflict	UNP A0A6S8N9J6
Y	52	SER	ALA	conflict	UNP A0A6S8N9J6
Y	73	THR	SER	conflict	UNP A0A6S8N9J6
Y	81	THR	ASN	conflict	UNP A0A6S8N9J6
Y	123	ILE	VAL	conflict	UNP A0A6S8N9J6
Y	220	LEU	PHE	conflict	UNP A0A6S8N9J6
Y	235	GLN	THR	conflict	UNP A0A6S8N9J6
Y	259	THR	SER	conflict	UNP A0A6S8N9J6
y	49	PHE	TYR	conflict	UNP A0A6S8N9J6
y	52	SER	ALA	conflict	UNP A0A6S8N9J6
y	73	THR	SER	conflict	UNP A0A6S8N9J6
y	81	THR	ASN	conflict	UNP A0A6S8N9J6
y	123	ILE	VAL	conflict	UNP A0A6S8N9J6
y	220	LEU	PHE	conflict	UNP A0A6S8N9J6
y	235	GLN	THR	conflict	UNP A0A6S8N9J6
y	259	THR	SER	conflict	UNP A0A6S8N9J6

- Molecule 25 is a protein called PsbU.

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

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

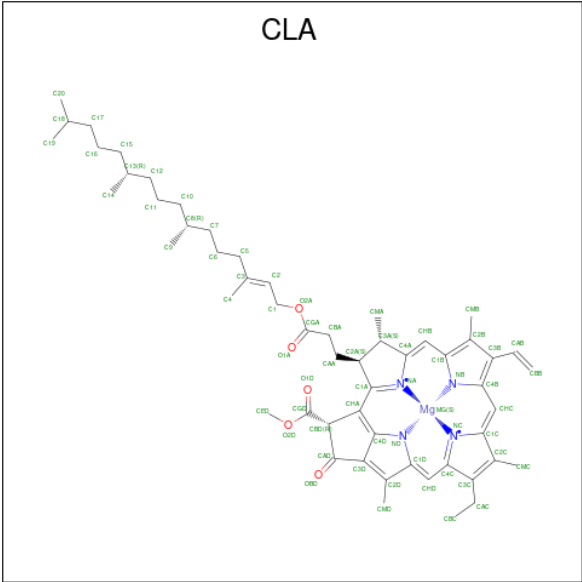
- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	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
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	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
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	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
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	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
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

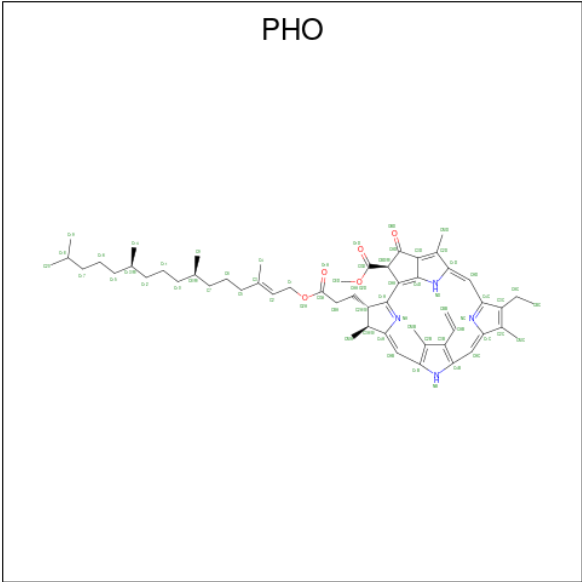
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 46	C 36	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

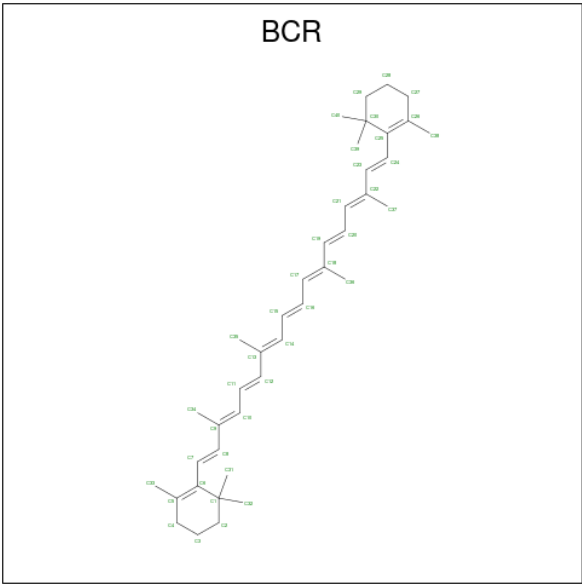
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



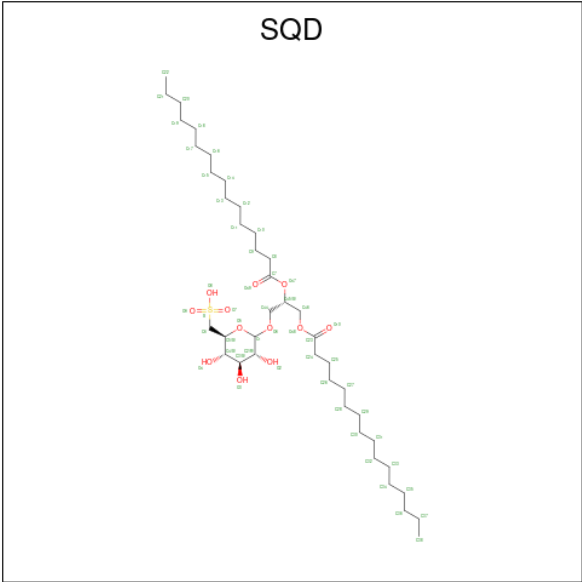
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



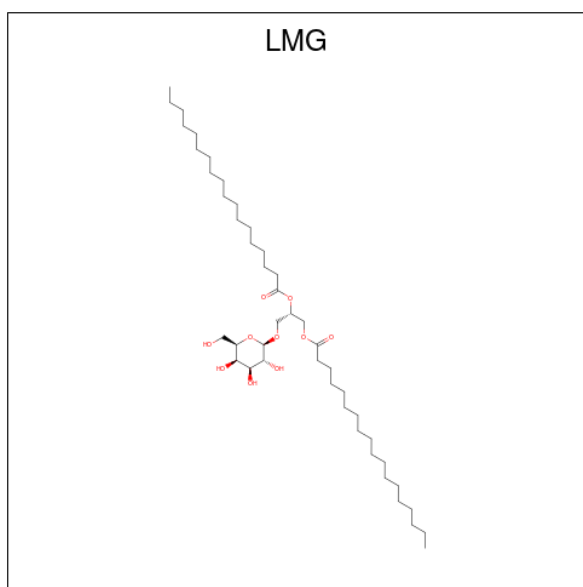
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C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

- Molecule 32 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
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			54	41	12	1	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	c	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

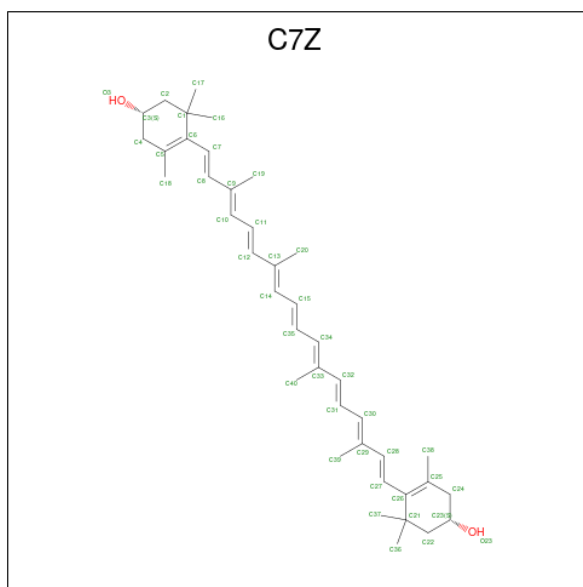


Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			44	34	10	
33	C	1	Total	C	O	0
			51	41	10	
33	D	1	Total	C	O	0
			46	36	10	
33	H	1	Total	C	O	0
			48	38	10	
33	J	1	Total	C	O	0
			45	35	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			44	34	10	
33	c	1	Total	C	O	0
			51	41	10	
33	d	1	Total	C	O	0
			46	36	10	
33	h	1	Total	C	O	0
			48	38	10	
33	j	1	Total	C	O	0
			45	35	10	

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

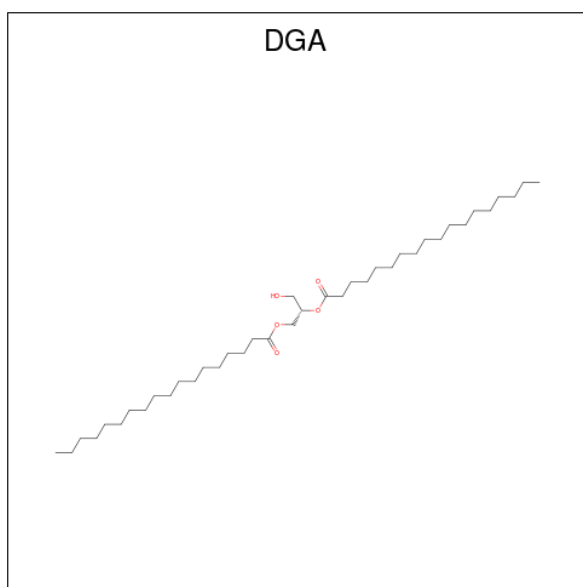
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Na	0
			1	1	
34	a	1	Total	Na	0
			1	1	

- Molecule 35 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



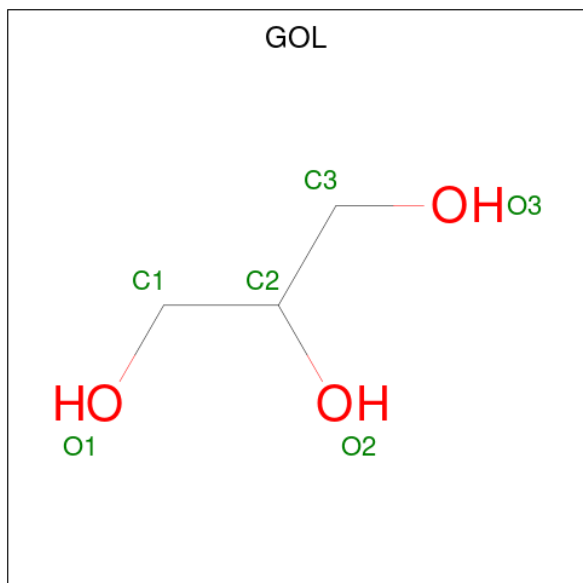
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			42	40	2	
35	b	1	Total	C	O	0
			42	40	2	

- Molecule 36 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



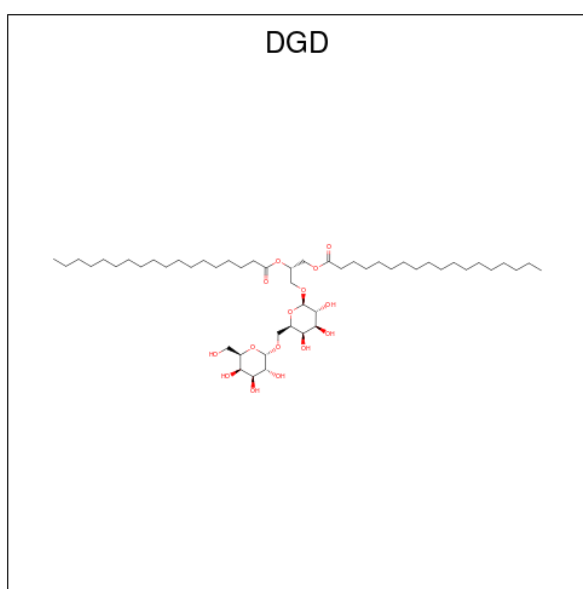
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			44	39	5	
36	C	1	Total	C	O	0
			44	39	5	
36	b	1	Total	C	O	0
			44	39	5	
36	c	1	Total	C	O	0
			44	39	5	

- Molecule 37 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			6	3	3	
37	b	1	Total	C	O	0
			6	3	3	
37	b	1	Total	C	O	0
			6	3	3	
37	y	1	Total	C	O	0
			6	3	3	

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



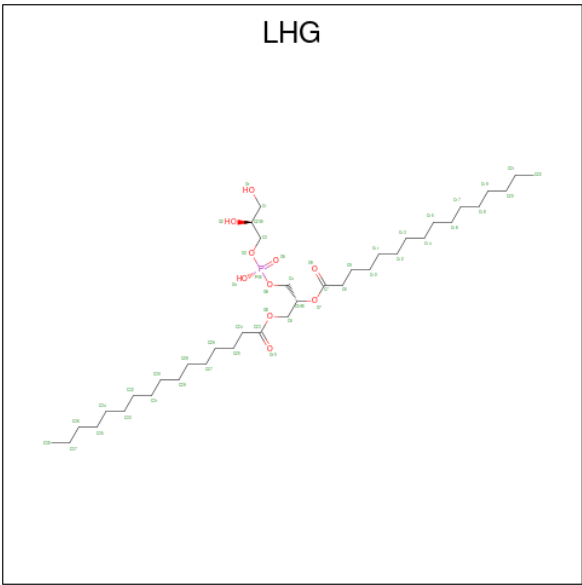
Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			62	47	15	
38	C	1	Total	C	O	0
			59	44	15	
38	C	1	Total	C	O	0
			66	51	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			59	44	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
38	c	1	Total	C	O	0
			66	51	15	

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



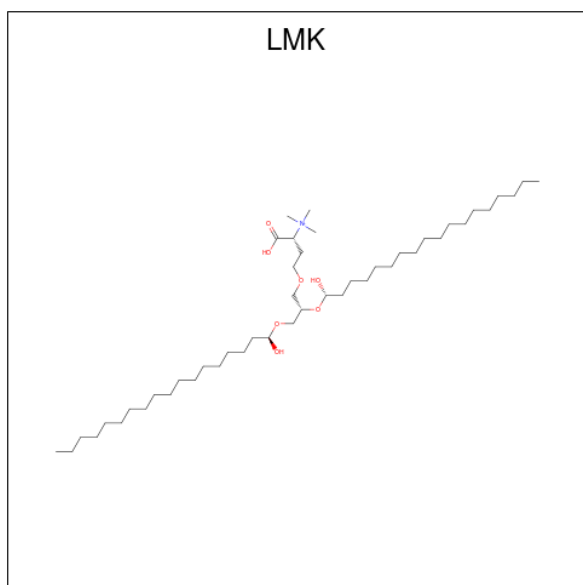
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	P	0
			47	36	10	1	
39	D	1	Total	C	O	P	0
			44	33	10	1	
39	D	1	Total	C	O	P	0
			49	38	10	1	
39	D	1	Total	C	O	P	0
			39	28	10	1	
39	L	1	Total	C	O	P	0
			49	38	10	1	
39	N	1	Total	C	O	P	0
			49	38	10	1	
39	G	1	Total	C	O	P	0
			49	38	10	1	
39	S	1	Total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

Continued on next page...

Continued from previous page...

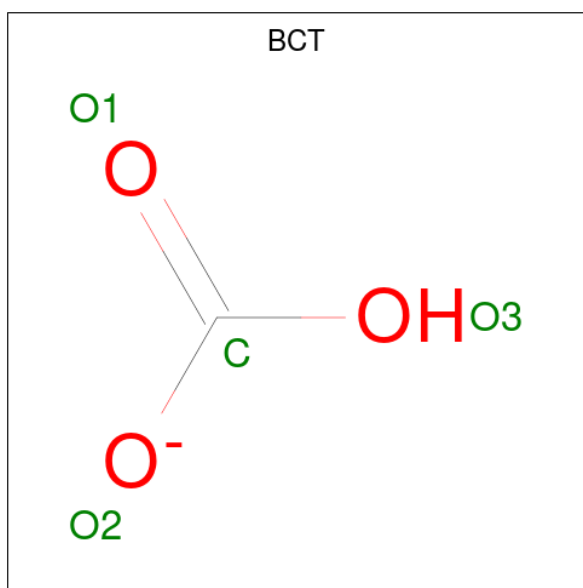
Mol	Chain	Residues	Atoms				AltConf
39	d	1	Total	C	O	P	0
			44	33	10	1	
39	d	1	Total	C	O	P	0
			49	38	10	1	
39	d	1	Total	C	O	P	0
			39	28	10	1	
39	l	1	Total	C	O	P	0
			49	38	10	1	
39	n	1	Total	C	O	P	0
			49	38	10	1	
39	g	1	Total	C	O	P	0
			49	38	10	1	
39	s	1	Total	C	O	P	0
			45	34	10	1	
39	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 40 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: C₄₆H₉₄NO₇).



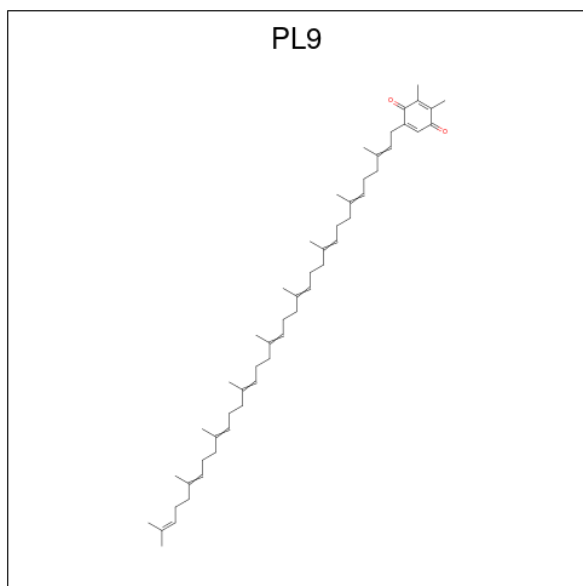
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			40	32	1	7	
40	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 41 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



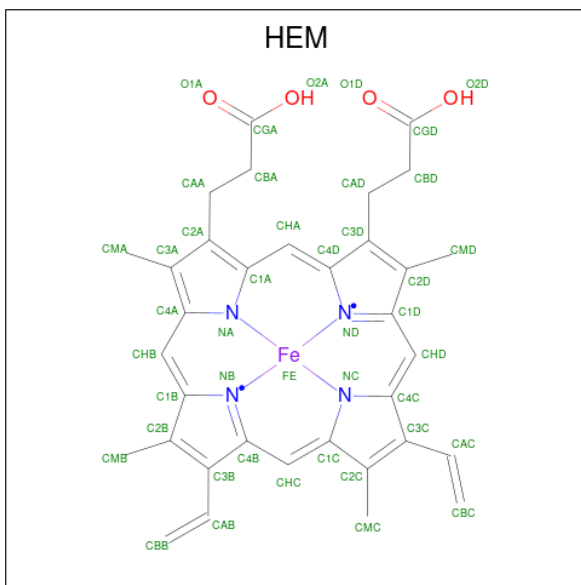
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			4	1	3	
41	d	1	Total	C	O	0
			4	1	3	

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



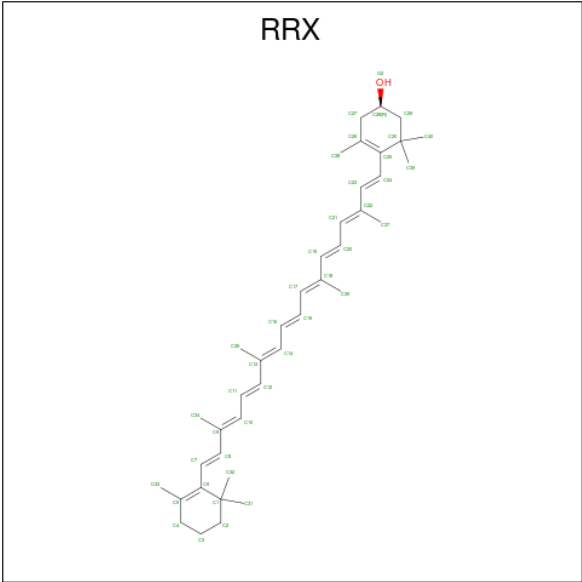
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			55	53	2	
42	d	1	Total	C	O	0
			55	53	2	

- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



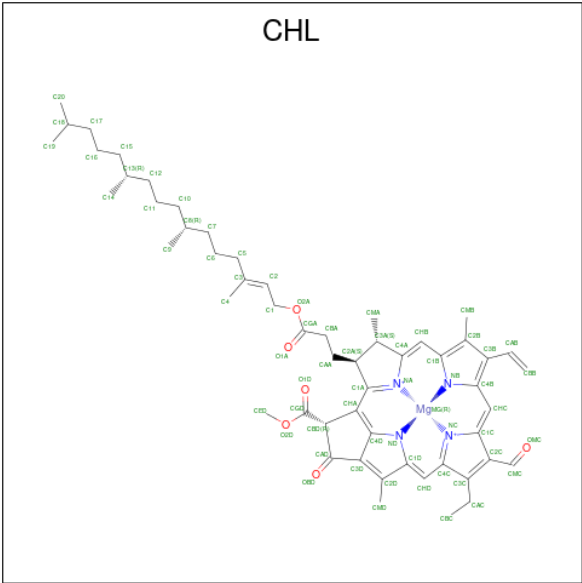
Mol	Chain	Residues	Atoms					AltConf
43	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
43	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 44 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



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

- Molecule 45 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
45	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
45	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
45	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
45	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
45	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

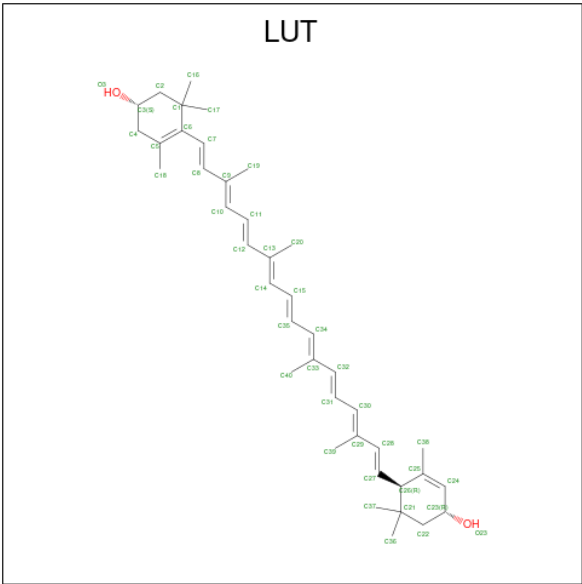
Mol	Chain	Residues	Atoms					AltConf
45	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
45	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	r	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
45	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
45	s	1	Total 44	C 35	Mg 1	N 4	O 4	0
45	s	1	Total 43	C 34	Mg 1	N 4	O 4	0
45	s	1	Total 61	C 50	Mg 1	N 4	O 6	0
45	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
45	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
45	y	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

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

- Molecule 46 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



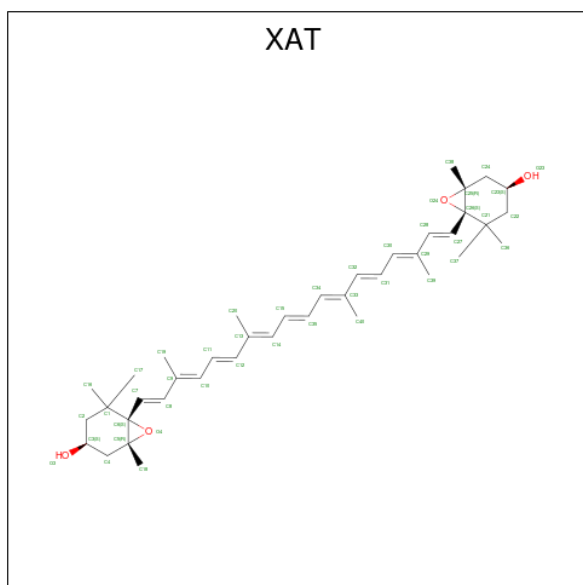
Mol	Chain	Residues	Atoms			AltConf
46	N	1	Total	C	O	0
			42	40	2	
46	N	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	R	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
46	n	1	Total	C	O	0
			42	40	2	
46	n	1	Total	C	O	0
			42	40	2	
46	g	1	Total	C	O	0
			42	40	2	
46	g	1	Total	C	O	0
			42	40	2	
46	r	1	Total	C	O	0
			42	40	2	
46	s	1	Total	C	O	0
			42	40	2	
46	s	1	Total	C	O	0
			42	40	2	
46	y	1	Total	C	O	0
			42	40	2	
46	y	1	Total	C	O	0
			42	40	2	

- Molecule 47 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).



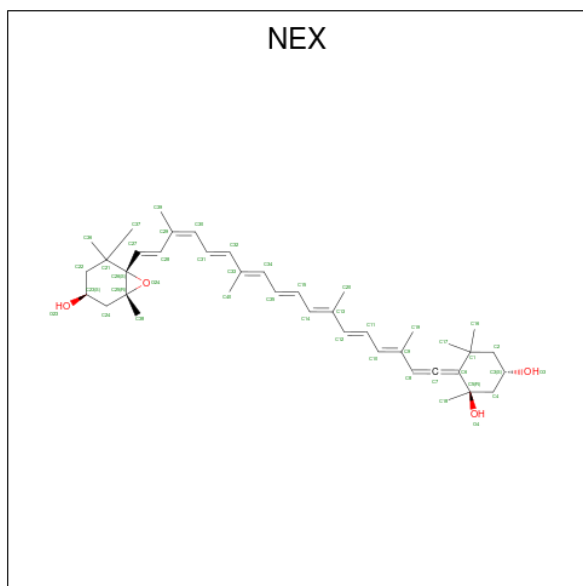
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			44	40	4	
47	G	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

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

- Molecule 48 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



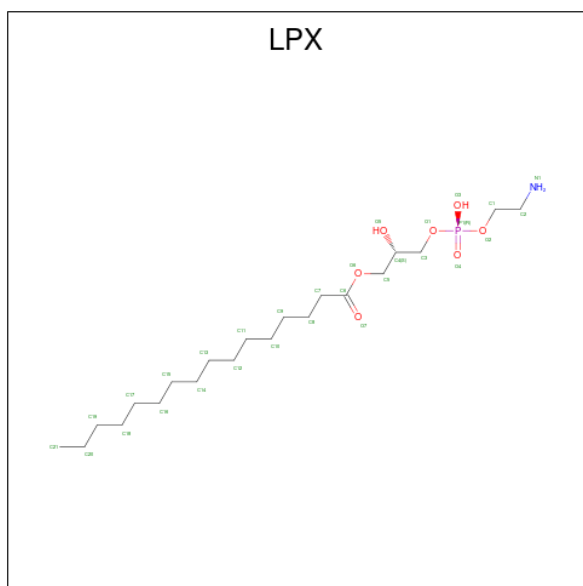
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			44	40	4	
48	S	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

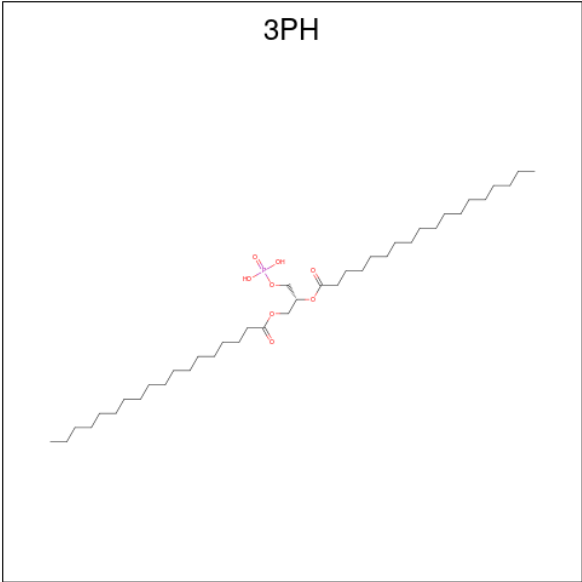
Mol	Chain	Residues	Atoms			AltConf
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			44	40	4	
48	s	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



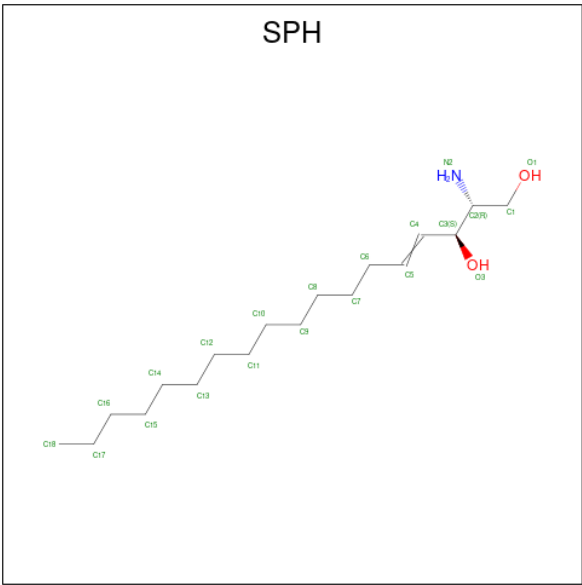
Mol	Chain	Residues	Atoms					AltConf
49	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
49	s	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 50 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
50	S	1	Total	C	O	P	0
			48	39	8	1	
50	i	1	Total	C	O	P	0
			48	39	8	1	
50	s	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 51 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



Mol	Chain	Residues	Atoms				AltConf
51	Y	1	Total	C	N	O	0
			21	18	1	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
51	y	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	43	Total	O	0
			43	43	
52	B	57	Total	O	0
			57	57	
52	C	55	Total	O	0
			55	55	
52	D	42	Total	O	0
			42	42	
52	E	7	Total	O	0
			7	7	
52	H	8	Total	O	0
			8	8	
52	I	4	Total	O	0
			4	4	
52	J	3	Total	O	0
			3	3	
52	K	2	Total	O	0
			2	2	
52	L	5	Total	O	0
			5	5	
52	M	4	Total	O	0
			4	4	
52	O	28	Total	O	0
			28	28	
52	P	10	Total	O	0
			10	10	
52	T	7	Total	O	0
			7	7	
52	W	5	Total	O	0
			5	5	
52	X	9	Total	O	0
			9	9	
52	Z	1	Total	O	0
			1	1	
52	N	5	Total	O	0
			5	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	G	4	Total 4	O 4	0
52	R	10	Total 10	O 10	0
52	S	8	Total 8	O 8	0
52	Y	14	Total 14	O 14	0
52	U	1	Total 1	O 1	0
52	a	59	Total 59	O 59	0
52	b	70	Total 70	O 70	0
52	v	3	Total 3	O 3	0
52	c	50	Total 50	O 50	0
52	d	41	Total 41	O 41	0
52	e	7	Total 7	O 7	0
52	f	1	Total 1	O 1	0
52	h	9	Total 9	O 9	0
52	i	3	Total 3	O 3	0
52	j	2	Total 2	O 2	0
52	k	1	Total 1	O 1	0
52	l	8	Total 8	O 8	0
52	m	4	Total 4	O 4	0
52	o	20	Total 20	O 20	0
52	p	15	Total 15	O 15	0
52	t	5	Total 5	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	w	3	Total 3	O 3	0
52	x	2	Total 2	O 2	0
52	n	13	Total 13	O 13	0
52	g	12	Total 12	O 12	0
52	r	15	Total 15	O 15	0
52	s	21	Total 21	O 21	0
52	y	22	Total 22	O 22	0

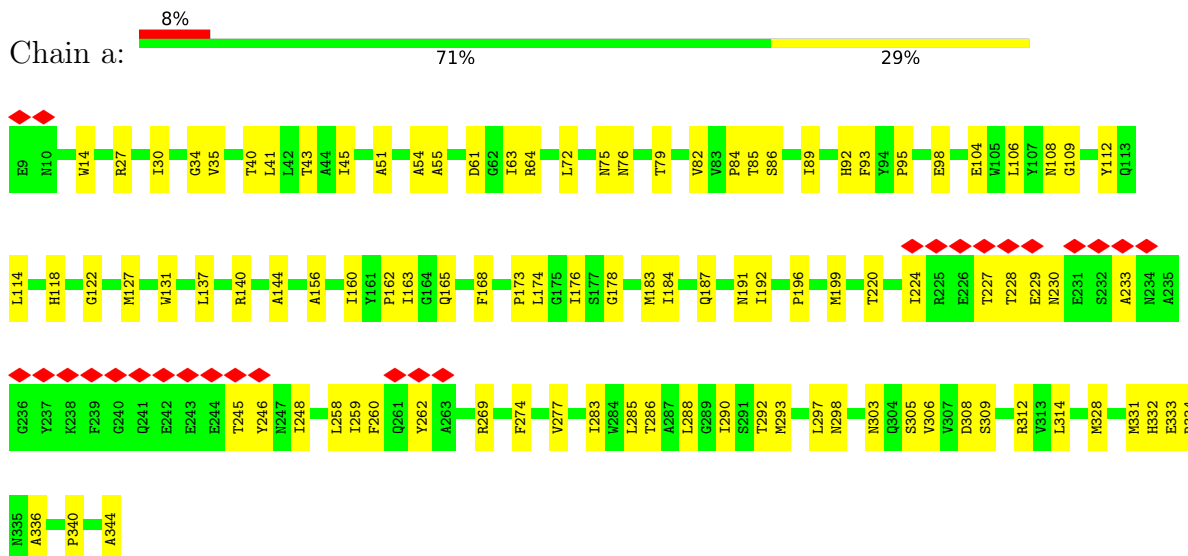
3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1

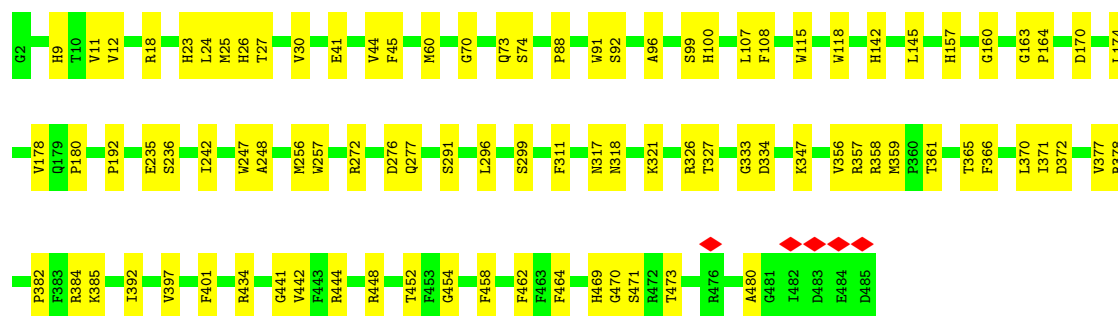


- Molecule 1: Photosystem II protein D1



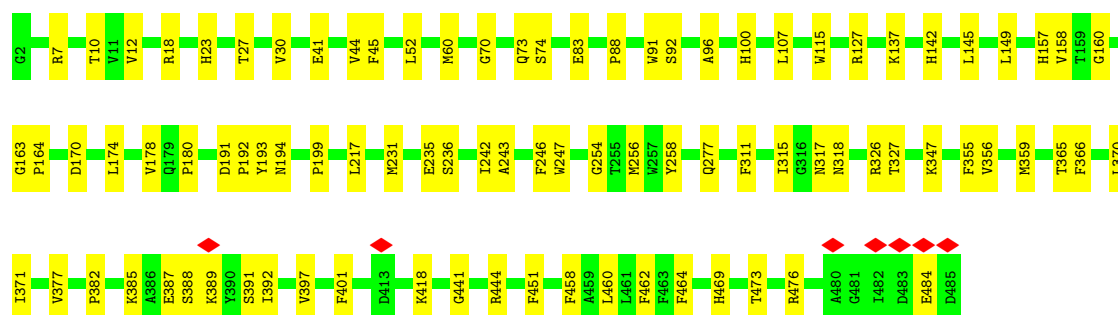
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  81% 19%

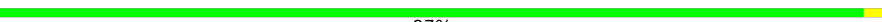


• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  81% 19%



• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  97%



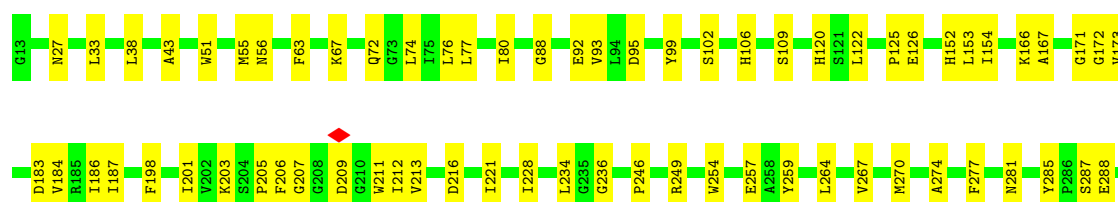
• Molecule 3: Photosystem II reaction center protein Ycf12

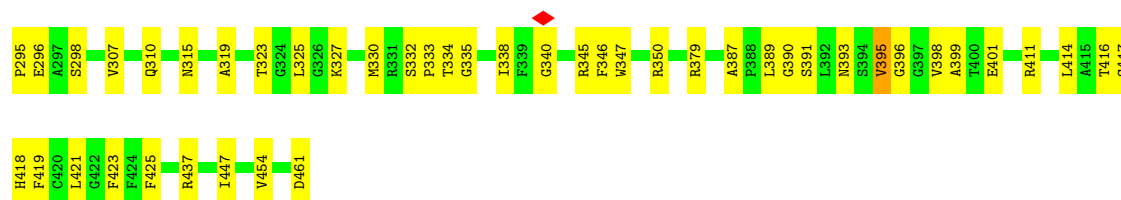
Chain v:  75% 25%



• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  75% 25%





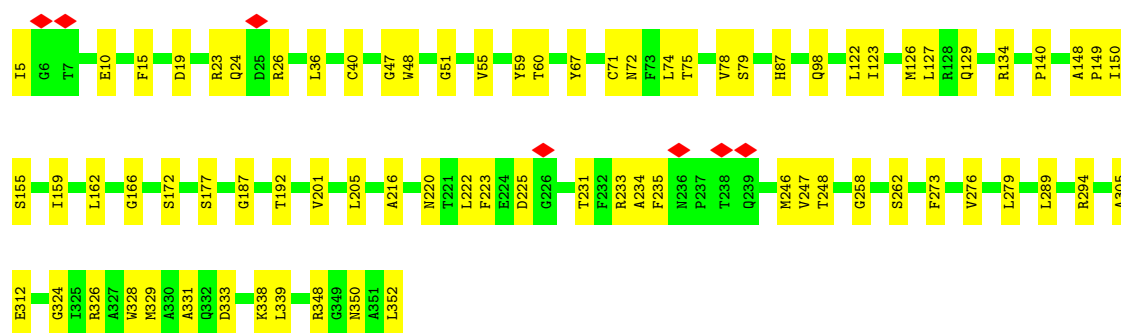
• Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 74% 26%



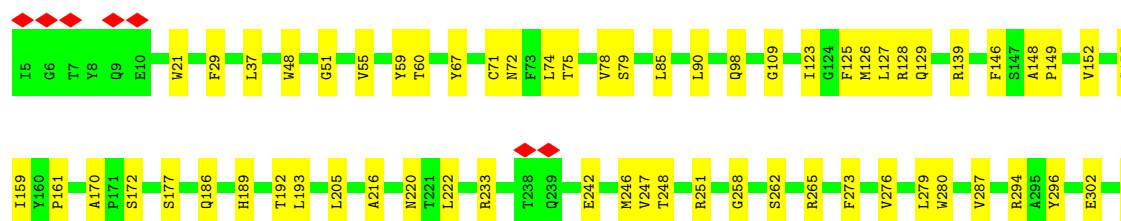
• Molecule 5: Photosystem II D2 protein

Chain D: 78% 22%



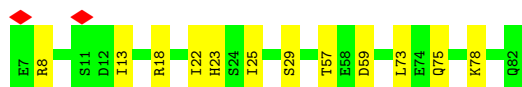
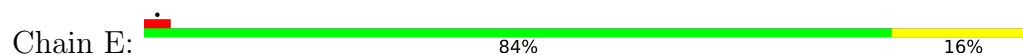
• Molecule 5: Photosystem II D2 protein

Chain d: 80% 20%

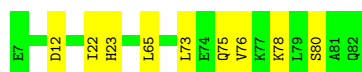
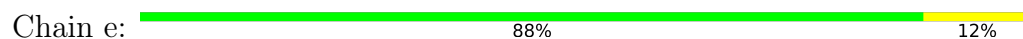




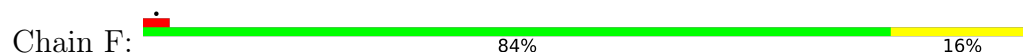
- Molecule 6: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit alpha



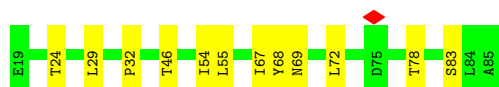
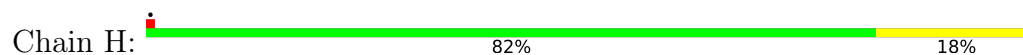
- Molecule 7: Cytochrome b559 subunit beta



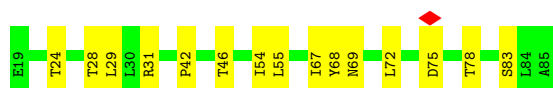
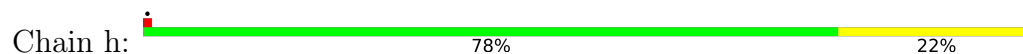
- Molecule 7: Cytochrome b559 subunit beta



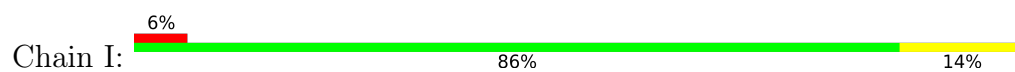
- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H



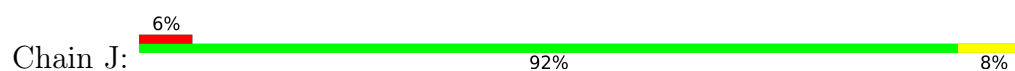
- Molecule 9: Photosystem II reaction center protein I



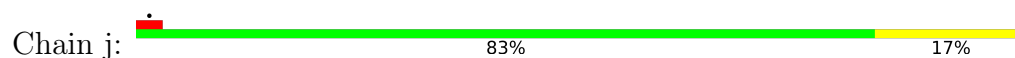
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



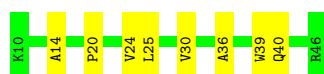
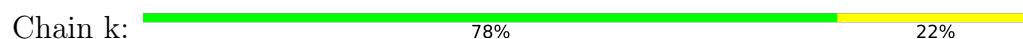
- Molecule 10: Photosystem II reaction center protein J



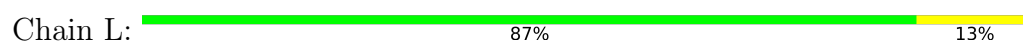
- Molecule 11: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein K

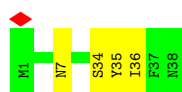


- Molecule 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L

Chain l:  89% 11%



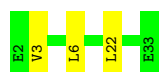
- Molecule 13: Photosystem II reaction center protein M

Chain M:  88% 12%



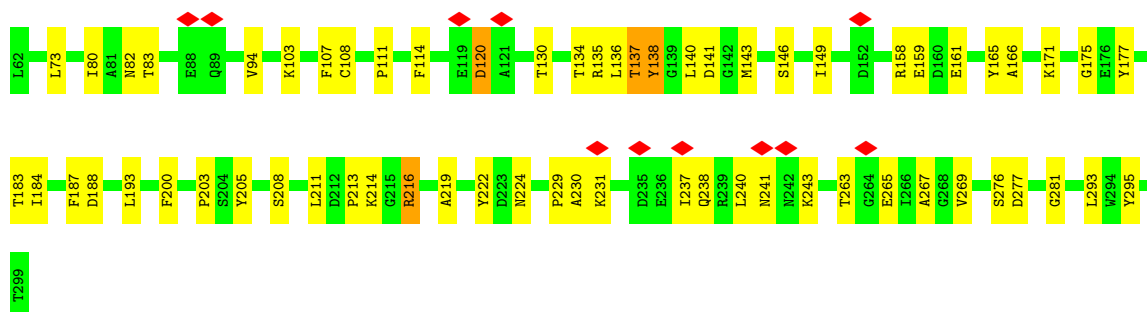
- Molecule 13: Photosystem II reaction center protein M

Chain m:  91% 9%



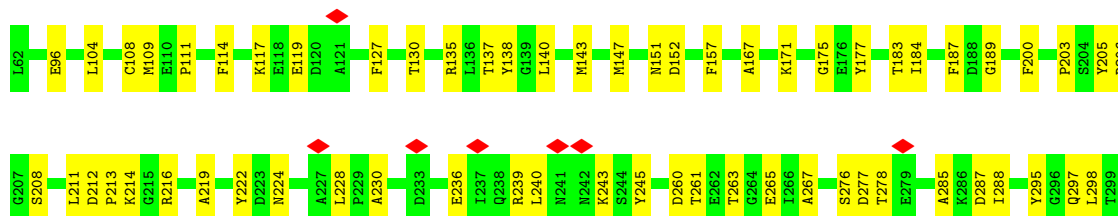
- Molecule 14: PsbO

Chain O:  5% 74% 25%



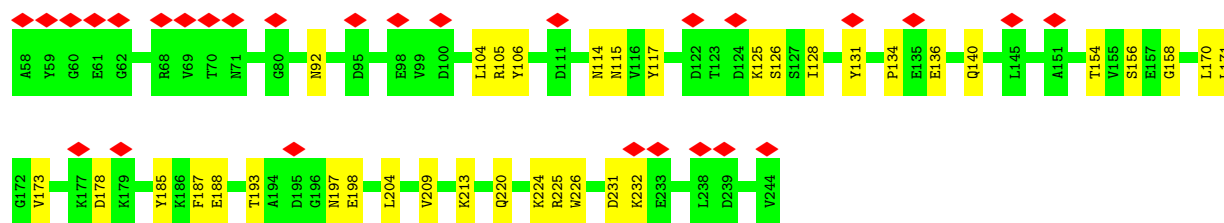
- Molecule 14: PsbO

Chain o:  74% 26%

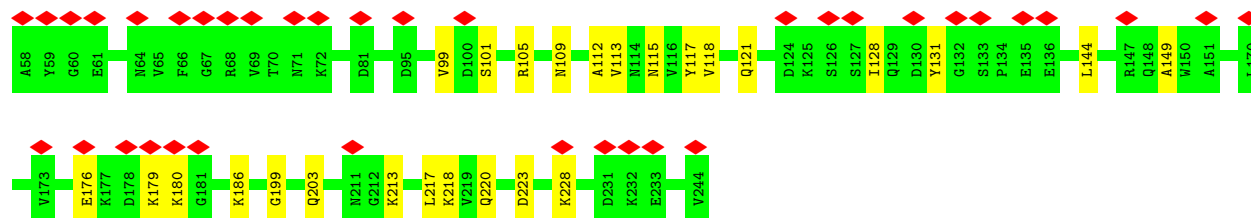
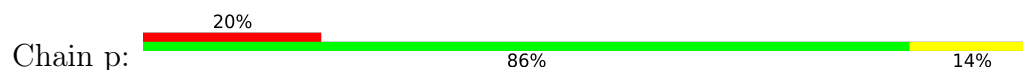


- Molecule 15: PsbP

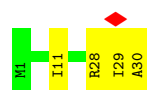
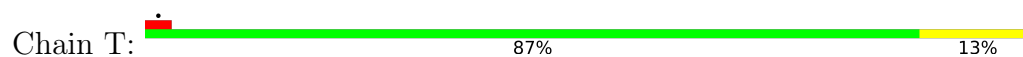
Chain P:  15% 81% 19%



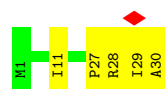
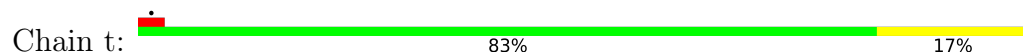
- Molecule 15: PsbP



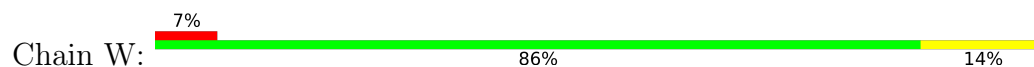
- Molecule 16: Photosystem II reaction center protein T



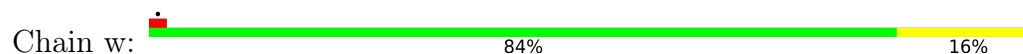
- Molecule 16: Photosystem II reaction center protein T



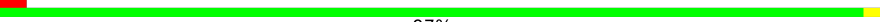
- Molecule 17: PSII 6.1 kDa protein

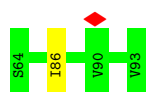


- Molecule 17: PSII 6.1 kDa protein



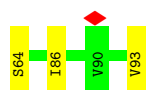
- Molecule 18: Hypothetical protein

Chain X:  97%



- Molecule 18: Hypothetical protein

Chain x:  90% 10%



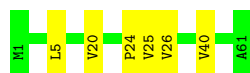
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  90% 10%



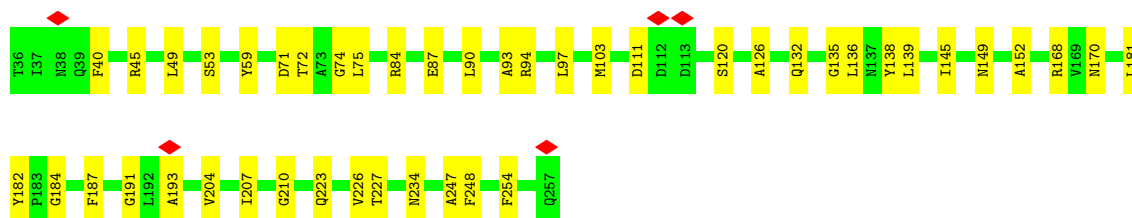
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  90% 10%



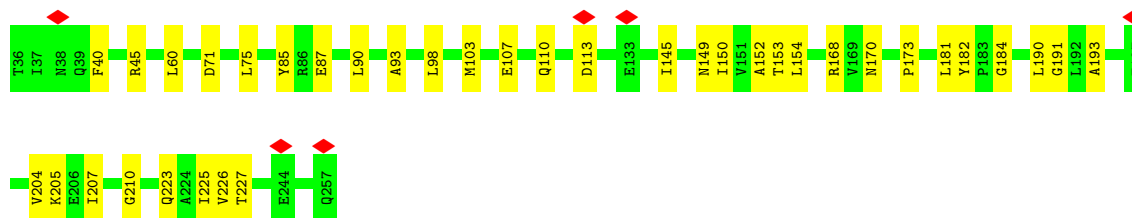
- Molecule 20: LHCII M3

Chain N:  80% 20%



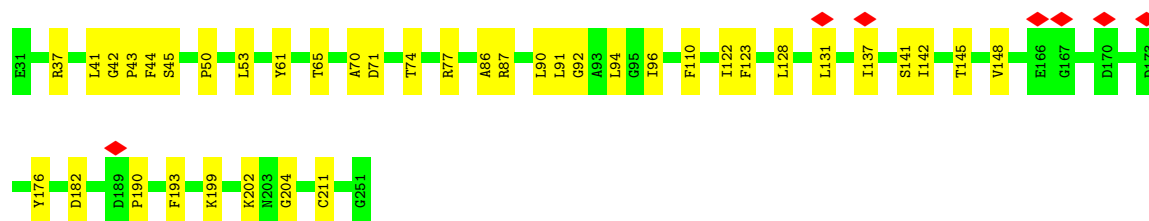
- Molecule 20: LHCII M3

Chain n:  83% 17%



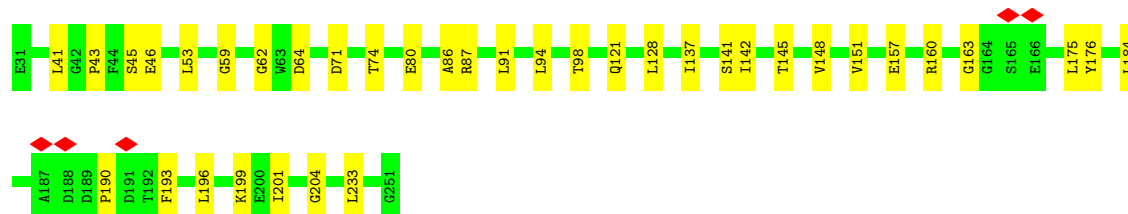
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G:  82% 18%



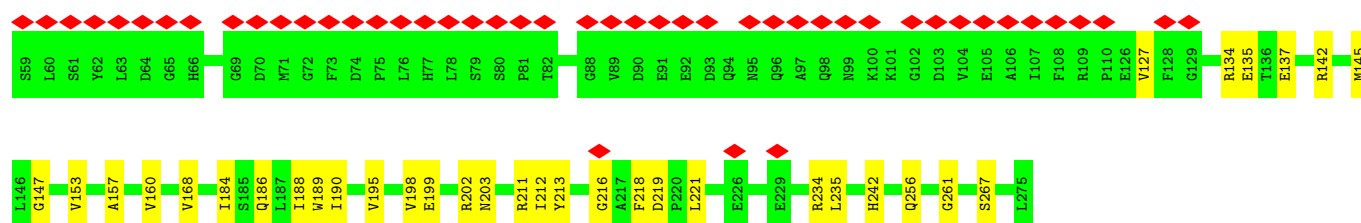
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain g:  83% 17%



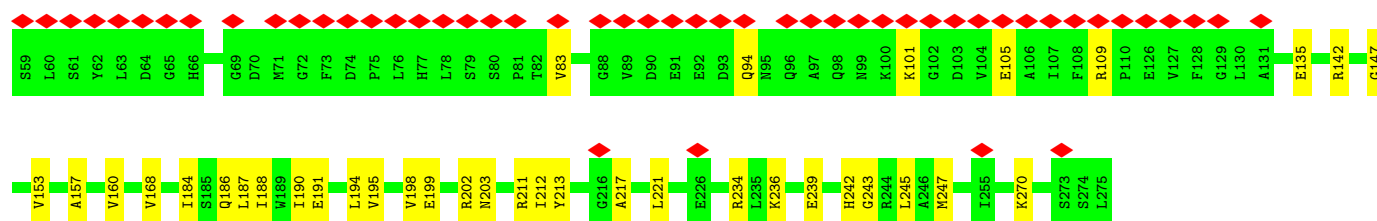
- Molecule 22: CP29

Chain R:  24% 83% 17%



- Molecule 22: CP29

Chain r:  26% 82% 18%



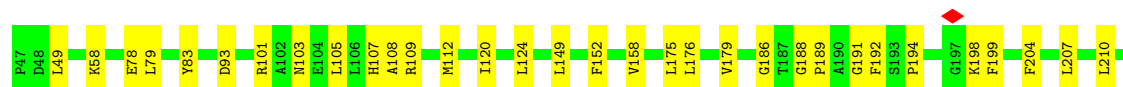
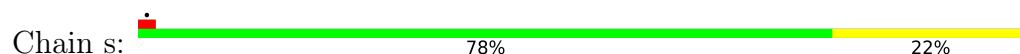
- Molecule 23: CP26

Chain S:  83% 17%

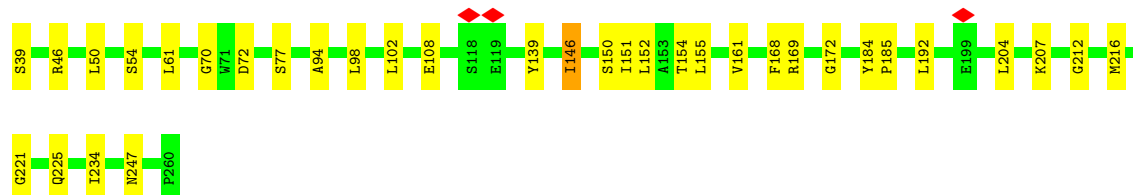
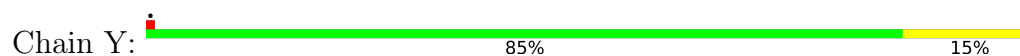




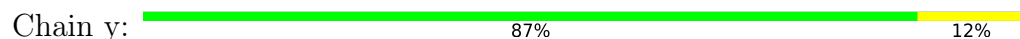
• Molecule 23: CP26



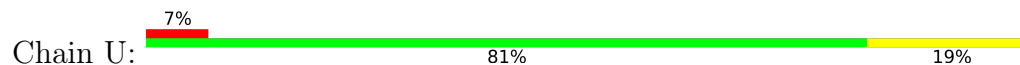
• Molecule 24: LHCII M1



• Molecule 24: LHCII M1



• Molecule 25: PsbU



• Molecule 25: PsbU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	40.024	Depositor
Minimum map value	-28.419	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.896, 0.896, 0.896	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.23	0/2723	0.50	1/3715 (0.0%)
1	a	0.24	0/2723	0.54	1/3715 (0.0%)
2	B	0.18	0/3912	0.41	1/5327 (0.0%)
2	b	0.19	0/3912	0.41	0/5327
3	V	0.15	0/228	0.40	0/311
3	v	0.16	0/228	0.46	0/311
4	C	0.20	0/3602	0.51	1/4913 (0.0%)
4	c	0.20	0/3602	0.52	0/4913
5	D	0.21	0/2860	0.48	2/3899 (0.1%)
5	d	0.19	0/2860	0.44	2/3899 (0.1%)
6	E	0.17	0/639	0.48	0/870
6	e	0.19	0/639	0.51	0/870
7	F	0.18	0/259	0.41	0/351
7	f	0.18	0/259	0.38	0/351
8	H	0.18	0/513	0.41	0/703
8	h	0.20	0/513	0.42	0/703
9	I	0.19	0/287	0.41	0/386
9	i	0.17	0/287	0.40	0/386
10	J	0.12	0/272	0.30	0/369
10	j	0.14	0/272	0.36	0/369
11	K	0.23	0/308	0.48	0/423
11	k	0.26	0/308	0.52	0/423
12	L	0.16	0/321	0.32	0/435
12	l	0.16	0/321	0.33	0/435
13	M	0.19	0/246	0.42	0/335
13	m	0.18	0/246	0.41	0/335
14	O	0.26	0/1855	0.55	2/2505 (0.1%)
14	o	0.20	0/1855	0.50	0/2505
15	P	0.20	0/1473	0.53	2/1988 (0.1%)
15	p	0.18	0/1473	0.51	0/1988
16	T	0.18	0/254	0.47	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.19	0/254	0.48	0/342
17	W	0.17	0/339	0.48	0/460
17	w	0.17	0/339	0.43	0/460
18	X	0.15	0/202	0.35	0/276
18	x	0.15	0/202	0.39	0/276
19	Z	0.16	0/469	0.39	0/641
19	z	0.15	0/469	0.37	0/641
20	N	0.17	0/1751	0.42	0/2386
20	n	0.16	0/1751	0.40	0/2386
21	G	0.18	0/1725	0.52	2/2348 (0.1%)
21	g	0.16	0/1725	0.40	0/2348
22	R	0.17	0/1561	0.43	0/2110
22	r	0.17	0/1561	0.43	0/2110
23	S	0.17	0/1895	0.42	0/2579
23	s	0.16	0/1902	0.38	0/2587
24	Y	0.21	0/1715	0.46	1/2338 (0.0%)
24	y	0.19	0/1715	0.43	0/2338
25	U	0.21	0/224	0.58	0/298
25	u	0.24	0/224	0.56	0/298
All	All	0.19	0/59273	0.46	15/80624 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	O	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	299	SER	N-CA-C	-6.96	105.98	114.75
5	D	59	TYR	CA-C-N	6.72	134.38	121.54
5	D	59	TYR	C-N-CA	6.72	134.38	121.54
5	d	59	TYR	CA-C-N	6.52	134.00	121.54
5	d	59	TYR	C-N-CA	6.52	134.00	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	O	136	LEU	Mainchain

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	2638	0	2541	81	0
1	a	2638	0	2541	83	0
2	B	3783	0	3663	74	0
2	b	3783	0	3663	77	0
3	V	227	0	261	1	0
3	v	227	0	261	7	0
4	C	3483	0	3376	90	0
4	c	3483	0	3376	88	0
5	D	2766	0	2655	63	0
5	d	2766	0	2654	61	0
6	E	621	0	605	10	0
6	e	621	0	605	8	0
7	F	252	0	265	4	0
7	f	252	0	265	3	0
8	H	503	0	532	13	0
8	h	503	0	532	15	0
9	I	279	0	288	5	0
9	i	279	0	288	2	0
10	J	266	0	286	2	0
10	j	266	0	286	5	0
11	K	297	0	312	8	0
11	k	297	0	312	8	0
12	L	313	0	325	5	0
12	l	313	0	325	4	0
13	M	243	0	264	3	0
13	m	243	0	264	2	0
14	O	1820	0	1776	48	0
14	o	1820	0	1776	45	0
15	P	1444	0	1403	26	0
15	p	1444	0	1403	21	0
16	T	247	0	260	4	0
16	t	247	0	260	5	0
17	W	332	0	323	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	w	332	0	323	5	0
18	X	201	0	224	1	0
18	x	201	0	224	3	0
19	Z	457	0	478	5	0
19	z	457	0	478	6	0
20	N	1703	0	1641	33	0
20	n	1703	0	1641	28	0
21	G	1680	0	1614	31	0
21	g	1680	0	1614	26	0
22	R	1533	0	1506	25	0
22	r	1533	0	1506	28	0
23	S	1849	0	1808	27	0
23	s	1856	0	1815	38	0
24	Y	1667	0	1624	29	0
24	y	1667	0	1624	23	0
25	U	224	0	226	5	0
25	u	224	0	226	12	0
26	A	10	0	0	0	0
26	a	10	0	0	1	0
27	A	1	0	0	0	0
27	a	1	0	0	0	0
28	A	2	0	0	0	0
28	a	2	0	0	0	0
29	A	239	0	240	18	0
29	B	1040	0	1149	68	0
29	C	845	0	932	60	0
29	D	130	0	144	10	0
29	G	446	0	428	15	0
29	N	468	0	467	17	0
29	R	501	0	455	18	0
29	S	625	0	586	19	0
29	Y	570	0	613	26	0
29	a	239	0	241	17	0
29	b	1040	0	1151	50	0
29	c	845	0	933	46	0
29	d	130	0	144	7	0
29	g	446	0	429	10	0
29	n	468	0	468	20	0
29	r	501	0	457	19	0
29	s	625	0	587	20	0
29	y	570	0	614	24	0
30	A	128	0	148	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	128	0	148	9	0
31	A	40	0	53	3	0
31	B	80	0	106	6	0
31	C	160	0	211	19	0
31	D	40	0	53	3	0
31	a	40	0	53	3	0
31	b	80	0	106	3	0
31	c	160	0	212	15	0
31	d	40	0	53	3	0
32	A	51	0	68	2	0
32	B	54	0	77	5	0
32	C	54	0	77	2	0
32	a	51	0	68	0	0
32	b	54	0	77	3	0
32	c	54	0	77	4	0
33	A	48	0	66	6	0
33	B	44	0	58	3	0
33	C	51	0	72	4	0
33	D	46	0	62	5	0
33	H	48	0	66	6	0
33	J	45	0	60	0	0
33	a	48	0	66	5	0
33	b	44	0	58	1	0
33	c	51	0	72	6	0
33	d	46	0	62	3	0
33	h	48	0	66	8	0
33	j	45	0	60	2	0
34	A	1	0	0	0	0
34	a	1	0	0	0	0
35	B	42	0	0	0	0
35	b	42	0	0	0	0
36	B	44	0	76	2	0
36	C	44	0	76	3	0
36	b	44	0	76	1	0
36	c	44	0	76	1	0
37	B	6	0	8	0	0
37	b	12	0	16	1	0
37	y	6	0	8	0	0
38	C	242	0	322	21	0
38	c	242	0	322	18	0
39	C	47	0	67	7	0
39	D	132	0	183	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G	49	0	74	4	0
39	L	49	0	74	6	0
39	N	49	0	74	2	0
39	S	45	0	63	8	0
39	Y	49	0	74	3	0
39	c	47	0	67	2	0
39	d	132	0	183	6	0
39	g	49	0	74	4	0
39	l	49	0	74	4	0
39	n	49	0	74	2	0
39	s	45	0	63	6	0
39	y	49	0	74	2	0
40	C	40	0	0	0	0
40	c	40	0	0	0	0
41	D	4	0	0	0	0
41	d	4	0	0	0	0
42	D	55	0	80	3	0
42	d	55	0	80	2	0
43	F	43	0	30	3	0
43	f	43	0	30	3	0
44	H	41	0	56	2	0
44	h	41	0	56	1	0
45	G	324	0	273	14	0
45	N	380	0	382	14	0
45	R	94	0	66	2	0
45	S	194	0	144	12	0
45	Y	310	0	306	15	0
45	g	324	0	272	15	0
45	n	380	0	382	18	0
45	r	94	0	66	3	0
45	s	194	0	144	8	0
45	y	310	0	306	13	0
46	G	84	0	110	6	0
46	N	84	0	110	12	0
46	R	42	0	55	4	0
46	S	84	0	110	12	0
46	Y	84	0	110	5	0
46	g	84	0	110	9	0
46	n	84	0	110	6	0
46	r	42	0	55	4	0
46	s	84	0	110	9	0
46	y	84	0	110	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	G	44	0	56	4	0
47	N	44	0	56	3	0
47	R	44	0	56	5	0
47	Y	44	0	56	1	0
47	g	44	0	56	2	0
47	n	44	0	56	3	0
47	r	44	0	56	5	0
47	y	44	0	56	2	0
48	G	44	0	54	0	0
48	N	44	0	54	2	0
48	R	44	0	54	2	0
48	S	44	0	54	2	0
48	Y	44	0	54	1	0
48	g	44	0	54	0	0
48	n	44	0	54	2	0
48	r	44	0	54	3	0
48	s	44	0	54	1	0
48	y	44	0	54	0	0
49	S	30	0	43	0	0
49	s	30	0	43	0	0
50	S	48	0	75	4	0
50	i	48	0	75	1	0
50	s	48	0	75	1	0
51	Y	21	0	37	2	0
51	y	21	0	37	3	0
52	A	43	0	0	5	0
52	B	57	0	0	3	0
52	C	55	0	0	4	0
52	D	42	0	0	4	0
52	E	7	0	0	0	0
52	G	4	0	0	0	0
52	H	8	0	0	0	0
52	I	4	0	0	0	0
52	J	3	0	0	0	0
52	K	2	0	0	0	0
52	L	5	0	0	0	0
52	M	4	0	0	0	0
52	N	5	0	0	0	0
52	O	28	0	0	2	0
52	P	10	0	0	1	0
52	R	10	0	0	0	0
52	S	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	T	7	0	0	0	0
52	U	1	0	0	0	0
52	W	5	0	0	0	0
52	X	9	0	0	0	0
52	Y	14	0	0	1	0
52	Z	1	0	0	0	0
52	a	59	0	0	2	0
52	b	70	0	0	4	0
52	c	50	0	0	4	0
52	d	41	0	0	11	0
52	e	7	0	0	0	0
52	f	1	0	0	0	0
52	g	12	0	0	1	0
52	h	9	0	0	0	0
52	i	3	0	0	0	0
52	j	2	0	0	0	0
52	k	1	0	0	0	0
52	l	8	0	0	0	0
52	m	4	0	0	0	0
52	n	13	0	0	1	0
52	o	20	0	0	0	0
52	p	15	0	0	4	0
52	r	15	0	0	1	0
52	s	21	0	0	1	0
52	t	5	0	0	0	0
52	v	3	0	0	1	0
52	w	3	0	0	0	0
52	x	2	0	0	0	0
52	y	22	0	0	3	0
All	All	76287	0	76145	1540	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 10.

The worst 5 of 1540 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:80:ILE:HD12	52:O:1027:HOH:O	1.42	1.20
15:p:109:ASN:ND2	52:p:1003:HOH:O	1.75	1.18
1:A:65:GLU:OE2	52:A:1026:HOH:O	1.63	1.16
14:O:80:ILE:CD1	52:O:1027:HOH:O	1.92	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:348:ARG:NH1	52:d:1031:HOH:O	1.74	1.13

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	335/336 (100%)	309 (92%)	26 (8%)	0	100	100
1	a	335/336 (100%)	310 (92%)	25 (8%)	0	100	100
2	B	482/484 (100%)	465 (96%)	16 (3%)	1 (0%)	43	70
2	b	482/484 (100%)	463 (96%)	18 (4%)	1 (0%)	43	70
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
4	C	447/449 (100%)	419 (94%)	25 (6%)	3 (1%)	18	44
4	c	447/449 (100%)	414 (93%)	29 (6%)	4 (1%)	14	37
5	D	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	36	63
5	d	346/348 (99%)	335 (97%)	10 (3%)	1 (0%)	36	63
6	E	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	9
13	m	30/32 (94%)	29 (97%)	0	1 (3%)	3	9
14	O	236/238 (99%)	208 (88%)	25 (11%)	3 (1%)	9	28
14	o	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	30	57
15	P	185/187 (99%)	169 (91%)	15 (8%)	1 (0%)	24	52
15	p	185/187 (99%)	172 (93%)	13 (7%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	8
16	t	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	8
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	52
20	n	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24	52
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	24	52
21	g	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	24	52
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100	100
22	r	198/202 (98%)	185 (93%)	13 (7%)	0	100	100
23	S	240/243 (99%)	220 (92%)	18 (8%)	2 (1%)	16	40
23	s	239/243 (98%)	221 (92%)	16 (7%)	2 (1%)	16	40
24	Y	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	52
24	y	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	52
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7351/7456 (99%)	6934 (94%)	387 (5%)	30 (0%)	31	57

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
15	P	126	SER
16	T	29	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	274 (99%)	2 (1%)	76	90
2	B	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	193 (99%)	2 (1%)	68	86
14	o	195/195 (100%)	194 (100%)	1 (0%)	81	92
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	158/158 (100%)	158 (100%)	0	100	100
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	189 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	y	167/167 (100%)	165 (99%)	2 (1%)	63	84
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5953/5952 (100%)	5946 (100%)	7 (0%)	87	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	332	HIS
14	o	119	GLU
24	y	149	GLN
24	y	76	LEU
1	a	92	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
20	n	132	GLN
24	y	138	ASN
20	n	234	ASN
22	r	98	GLN
25	u	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 343 ligands modelled in this entry, 8 are monoatomic - leaving 335 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$
36	DGA	c	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.53	3 (6%)
29	CLA	B	613	-	69,73,73	1.34	7 (10%)	82,113,113	1.84	16 (19%)
35	C7Z	b	620	-	43,43,43	5.50	26 (60%)	56,60,60	2.03	14 (25%)
45	CHL	n	608	-	44,58,74	1.47	7 (15%)	37,94,114	2.02	11 (29%)
29	CLA	N	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	19 (23%)
29	CLA	c	502	-	69,73,73	1.38	6 (8%)	82,113,113	1.99	16 (19%)
29	CLA	c	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	20 (24%)
29	CLA	R	603	-	64,68,73	1.42	7 (10%)	76,107,113	1.94	18 (23%)
29	CLA	S	602	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	20 (26%)
29	CLA	b	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	16 (19%)
39	LHG	s	624	-	44,44,48	0.42	0	47,50,54	1.12	3 (6%)
29	CLA	y	608	-	54,58,73	1.54	6 (11%)	64,95,113	2.08	20 (31%)
45	CHL	g	601	21	60,74,74	1.32	9 (15%)	58,114,114	1.72	11 (18%)
29	CLA	n	614	-	53,57,73	1.55	8 (15%)	61,93,113	2.19	21 (34%)
29	CLA	b	612	-	69,73,73	1.37	6 (8%)	82,113,113	1.90	16 (19%)
29	CLA	R	604	-	53,57,73	1.53	6 (11%)	61,93,113	2.20	19 (31%)
38	DGD	C	519	-	63,63,67	1.23	7 (11%)	77,77,81	1.07	4 (5%)
29	CLA	r	609	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	16 (21%)
29	CLA	S	603	-	69,73,73	1.38	8 (11%)	82,113,113	1.85	15 (18%)
29	CLA	S	613	-	59,63,73	1.46	6 (10%)	70,101,113	2.23	19 (27%)
29	CLA	B	605	-	69,73,73	1.38	7 (10%)	82,113,113	2.02	17 (20%)
29	CLA	A	405	-	69,73,73	1.35	7 (10%)	82,113,113	1.86	17 (20%)
29	CLA	s	610	-	69,73,73	1.37	8 (11%)	82,113,113	1.88	22 (26%)
45	CHL	g	607	-	44,58,74	1.39	7 (15%)	37,94,114	2.11	11 (29%)
29	CLA	s	604	-	59,63,73	1.46	6 (10%)	70,101,113	1.95	16 (22%)
29	CLA	b	608	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	y	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.84	21 (25%)
29	CLA	R	612	-	64,68,73	1.41	7 (10%)	76,107,113	1.98	17 (22%)
38	DGD	c	520	-	60,60,67	1.16	6 (10%)	74,74,81	0.99	2 (2%)
49	LPX	s	625	-	29,29,29	1.00	2 (6%)	31,33,33	0.99	1 (3%)
37	GOL	b	625	-	5,5,5	0.59	0	5,5,5	0.30	0
45	CHL	s	601	23	40,54,74	1.70	8 (20%)	34,90,114	2.17	11 (32%)
38	DGD	c	518	-	56,56,67	1.06	4 (7%)	70,70,81	1.06	3 (4%)
29	CLA	S	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.87	21 (25%)
45	CHL	R	606	-	38,52,74	1.76	9 (23%)	31,87,114	2.28	11 (35%)
45	CHL	Y	609	-	60,74,74	1.30	8 (13%)	58,114,114	1.68	12 (20%)
29	CLA	b	607	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	18 (21%)
29	CLA	n	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	22 (26%)
29	CLA	S	604	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	16 (22%)
29	CLA	S	605	-	54,58,73	1.55	8 (14%)	64,95,113	2.29	19 (29%)
29	CLA	y	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	16 (19%)
48	NEX	R	622	-	40,46,46	2.70	11 (27%)	50,70,70	1.67	11 (22%)
31	BCR	A	411	-	41,41,41	1.62	4 (9%)	56,56,56	4.38	13 (23%)
32	SQD	B	621	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
45	CHL	n	609	-	60,74,74	1.19	7 (11%)	58,114,114	1.79	13 (22%)
31	BCR	a	411	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	13 (23%)
29	CLA	c	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	20 (24%)
29	CLA	c	507	52	69,73,73	1.37	7 (10%)	82,113,113	1.88	19 (23%)
45	CHL	S	606	-	38,52,74	1.68	8 (21%)	31,87,114	2.16	10 (32%)
29	CLA	A	406	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	15 (18%)
46	LUT	Y	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.79	15 (29%)
29	CLA	a	407	-	53,57,73	1.54	6 (11%)	61,93,113	2.14	20 (32%)
43	HEM	F	101	6,7	50,50,50	1.51	6 (12%)	67,82,82	1.27	6 (8%)
29	CLA	y	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	19 (23%)
32	SQD	c	626	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
29	CLA	B	607	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	18 (21%)
48	NEX	S	622	-	40,46,46	2.66	11 (27%)	50,70,70	1.78	12 (24%)
29	CLA	R	608	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	19 (25%)
29	CLA	C	507	52	69,73,73	1.37	6 (8%)	82,113,113	1.87	19 (23%)
51	SPH	Y	625	-	19,20,20	0.64	0	18,21,21	1.11	1 (5%)
32	SQD	C	526	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	BCT	d	401	27	3,3,3	3.21	1 (33%)	2,3,3	2.76	2 (100%)
31	BCR	C	515	-	41,41,41	1.60	4 (9%)	56,56,56	4.38	12 (21%)
39	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
32	SQD	A	412	-	49,51,54	0.83	0	59,62,65	0.87	3 (5%)
45	CHL	s	607	-	37,51,74	1.61	8 (21%)	30,86,114	2.36	11 (36%)
50	3PH	S	626	-	47,47,47	0.87	4 (8%)	50,52,52	1.15	2 (4%)
29	CLA	N	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	18 (21%)
44	RRX	h	101	-	42,42,42	5.00	24 (57%)	56,58,58	2.06	18 (32%)
29	CLA	C	501	-	69,73,73	1.36	8 (11%)	82,113,113	1.98	20 (24%)
31	BCR	b	618	-	41,41,41	1.59	4 (9%)	56,56,56	4.47	13 (23%)
31	BCR	c	517	-	41,41,41	1.60	4 (9%)	56,56,56	4.27	17 (30%)
29	CLA	B	609	-	69,73,73	1.37	6 (8%)	82,113,113	1.98	18 (21%)
29	CLA	B	602	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	18 (21%)
29	CLA	n	613	-	69,73,73	1.36	8 (11%)	82,113,113	1.90	18 (21%)
46	LUT	G	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.89	11 (21%)
29	CLA	g	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
33	LMG	A	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.18	5 (8%)
45	CHL	S	607	-	37,51,74	1.54	8 (21%)	30,86,114	2.32	11 (36%)
46	LUT	G	621	-	42,43,43	2.47	1 (2%)	51,60,60	1.84	13 (25%)
29	CLA	D	403	-	69,73,73	1.37	7 (10%)	82,113,113	1.87	19 (23%)
39	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
46	LUT	g	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.84	12 (23%)
39	LHG	S	624	-	44,44,48	0.42	0	47,50,54	1.12	3 (6%)
29	CLA	Y	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	21 (25%)
46	LUT	S	621	-	42,43,43	2.40	1 (2%)	51,60,60	1.87	16 (31%)
29	CLA	N	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.15	18 (29%)
29	CLA	s	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	17 (20%)
37	GOL	B	627	-	5,5,5	0.59	0	5,5,5	0.24	0
29	CLA	b	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	18 (21%)
33	LMG	D	411	-	46,46,55	1.03	4 (8%)	54,54,63	1.13	2 (3%)
29	CLA	G	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.19	19 (31%)
45	CHL	g	606	-	44,58,74	1.38	7 (15%)	37,94,114	2.13	12 (32%)
47	XAT	G	622	-	41,47,47	0.69	1 (2%)	54,74,74	1.92	14 (25%)
29	CLA	B	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	16 (19%)
39	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.04	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	C	514	-	41,41,41	1.59	4 (9%)	56,56,56	4.59	11 (19%)
46	LUT	s	621	-	42,43,43	2.41	1 (2%)	51,60,60	1.87	14 (27%)
48	NEX	g	623	-	40,46,46	2.67	11 (27%)	50,70,70	1.77	11 (22%)
29	CLA	N	612	-	49,53,73	1.61	8 (16%)	58,89,113	2.07	13 (22%)
29	CLA	s	614	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	17 (24%)
45	CHL	S	608	-	55,69,74	1.38	8 (14%)	52,108,114	1.77	12 (23%)
30	PHO	a	409	-	58,69,69	2.16	10 (17%)	55,99,99	1.75	8 (14%)
40	LMK	C	527	-	39,39,53	1.54	3 (7%)	39,46,60	1.33	2 (5%)
29	CLA	B	617	-	69,73,73	1.35	7 (10%)	82,113,113	3.99	18 (21%)
29	CLA	b	604	-	69,73,73	1.38	7 (10%)	82,113,113	1.80	17 (20%)
32	SQD	a	412	-	49,51,54	0.80	0	59,62,65	0.84	2 (3%)
45	CHL	s	606	-	38,52,74	1.65	8 (21%)	31,87,114	2.17	10 (32%)
29	CLA	S	614	-	59,63,73	1.47	6 (10%)	70,101,113	1.99	15 (21%)
29	CLA	G	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.86	19 (23%)
45	CHL	N	608	-	44,58,74	1.44	7 (15%)	37,94,114	2.07	11 (29%)
29	CLA	G	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
46	LUT	Y	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.86	14 (27%)
31	BCR	B	619	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	19 (33%)
29	CLA	B	606	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	14 (17%)
45	CHL	G	608	-	38,52,74	1.66	8 (21%)	31,87,114	2.24	10 (32%)
29	CLA	R	602	-	64,68,73	1.41	7 (10%)	76,107,113	1.99	20 (26%)
33	LMG	d	411	-	46,46,55	1.03	4 (8%)	54,54,63	1.11	2 (3%)
29	CLA	B	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	17 (20%)
39	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
29	CLA	A	407	-	53,57,73	1.54	6 (11%)	61,93,113	2.16	20 (32%)
45	CHL	Y	601	24	60,74,74	1.32	8 (13%)	58,114,114	1.75	12 (20%)
29	CLA	c	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
48	NEX	s	623	-	40,46,46	2.72	12 (30%)	50,70,70	1.70	10 (20%)
39	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.05	3 (5%)
32	SQD	b	621	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
29	CLA	Y	608	-	54,58,73	1.54	8 (14%)	64,95,113	2.09	21 (32%)
38	DGD	C	518	-	56,56,67	1.07	4 (7%)	70,70,81	1.05	3 (4%)
29	CLA	c	509	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	16 (19%)
42	PL9	d	405	-	55,55,55	1.19	5 (9%)	68,69,69	1.45	11 (16%)
31	BCR	c	516	-	41,41,41	1.61	4 (9%)	56,56,56	4.48	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	g	603	-	69,73,73	1.35	8 (11%)	82,113,113	1.92	20 (24%)
29	CLA	d	402	-	69,73,73	1.35	7 (10%)	82,113,113	1.81	16 (19%)
46	LUT	N	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.79	15 (29%)
33	LMG	h	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.10	2 (3%)
29	CLA	C	509	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	17 (20%)
47	XAT	Y	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.72	16 (29%)
29	CLA	R	610	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	22 (28%)
26	OEX	a	401	4,52,1	0,15,15	-	-	-		
35	C7Z	B	620	-	43,43,43	5.51	26 (60%)	56,60,60	2.04	16 (28%)
30	PHO	A	408	-	58,69,69	2.15	10 (17%)	55,99,99	1.49	8 (14%)
48	NEX	Y	623	-	40,46,46	2.67	11 (27%)	50,70,70	1.79	10 (20%)
30	PHO	a	408	-	58,69,69	2.15	10 (17%)	55,99,99	1.55	7 (12%)
29	CLA	G	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.93	20 (24%)
45	CHL	N	607	-	60,74,74	1.15	7 (11%)	58,114,114	1.78	13 (22%)
29	CLA	g	612	-	47,51,73	1.64	7 (14%)	55,86,113	2.10	16 (29%)
33	LMG	j	101	-	45,45,55	0.99	3 (6%)	53,53,63	1.05	2 (3%)
29	CLA	B	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	17 (20%)
47	XAT	R	621	-	41,47,47	0.68	1 (2%)	54,74,74	2.20	19 (35%)
33	LMG	b	622	-	44,44,55	0.96	3 (6%)	52,52,63	1.07	3 (5%)
29	CLA	c	510	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	16 (19%)
29	CLA	B	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
29	CLA	r	611	-	50,54,73	1.59	8 (16%)	59,90,113	2.04	15 (25%)
45	CHL	R	607	-	44,58,74	1.60	8 (18%)	37,94,114	2.11	12 (32%)
46	LUT	y	621	-	42,43,43	2.45	1 (2%)	51,60,60	1.86	12 (23%)
31	BCR	C	517	-	41,41,41	1.60	4 (9%)	56,56,56	4.40	13 (23%)
51	SPH	y	625	-	19,20,20	0.66	0	18,21,21	1.11	1 (5%)
37	GOL	y	626	-	5,5,5	0.58	0	5,5,5	0.28	0
29	CLA	N	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	23 (28%)
29	CLA	b	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.90	18 (21%)
29	CLA	r	612	-	64,68,73	1.42	7 (10%)	76,107,113	1.93	21 (27%)
29	CLA	C	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	20 (24%)
39	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.93	2 (3%)
45	CHL	r	607	-	44,58,74	1.48	8 (18%)	37,94,114	2.20	12 (32%)
39	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.12	4 (7%)
45	CHL	g	609	-	60,74,74	1.40	9 (15%)	58,114,114	1.60	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	G	611	-	49,53,73	1.60	7 (14%)	58,89,113	2.10	17 (29%)
29	CLA	s	605	-	54,58,73	1.55	8 (14%)	64,95,113	2.26	19 (29%)
29	CLA	b	616	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	18 (21%)
29	CLA	a	410	-	64,68,73	1.40	7 (10%)	76,107,113	2.00	18 (23%)
29	CLA	B	611	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	18 (21%)
40	LMK	c	627	-	39,39,53	1.54	3 (7%)	39,46,60	1.37	2 (5%)
29	CLA	Y	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.91	21 (25%)
33	LMG	B	622	-	44,44,55	0.95	3 (6%)	52,52,63	1.07	3 (5%)
45	CHL	Y	606	-	60,74,74	1.37	9 (15%)	58,114,114	1.75	13 (22%)
29	CLA	y	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	19 (23%)
29	CLA	b	615	-	69,73,73	1.36	6 (8%)	82,113,113	2.02	18 (21%)
45	CHL	G	609	-	60,74,74	1.40	9 (15%)	58,114,114	1.61	11 (18%)
39	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.02	2 (4%)
48	NEX	r	623	-	40,46,46	2.67	11 (27%)	50,70,70	1.51	7 (14%)
29	CLA	c	511	-	69,73,73	1.36	6 (8%)	82,113,113	1.96	19 (23%)
39	LHG	D	408	-	43,43,48	0.42	0	46,49,54	1.15	3 (6%)
29	CLA	B	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	17 (20%)
45	CHL	n	601	-	60,74,74	1.33	8 (13%)	58,114,114	1.77	12 (20%)
47	XAT	g	622	-	41,47,47	0.71	1 (2%)	54,74,74	1.90	13 (24%)
29	CLA	Y	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	21 (25%)
29	CLA	r	613	-	50,54,73	1.58	6 (12%)	59,90,113	2.10	17 (28%)
29	CLA	g	611	-	49,53,73	1.60	6 (12%)	58,89,113	2.10	16 (27%)
29	CLA	S	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	16 (19%)
48	NEX	n	623	-	40,46,46	2.73	12 (30%)	50,70,70	1.69	10 (20%)
29	CLA	b	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
29	CLA	N	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	21 (25%)
29	CLA	Y	604	-	69,73,73	1.35	8 (11%)	82,113,113	1.83	18 (21%)
46	LUT	n	620	-	42,43,43	2.47	1 (2%)	51,60,60	1.73	17 (33%)
33	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.08	2 (3%)
29	CLA	s	602	-	64,68,73	1.39	7 (10%)	76,107,113	1.92	19 (25%)
29	CLA	Y	612	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	17 (20%)
29	CLA	n	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
29	CLA	n	604	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	21 (25%)
26	OEX	A	401	52,1	0,15,15	-	-	-	-	-
45	CHL	N	601	-	60,74,74	1.29	8 (13%)	58,114,114	1.80	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	y	605	24	40,54,74	1.67	7 (17%)	34,90,114	2.11	10 (29%)
45	CHL	y	606	-	60,74,74	1.34	8 (13%)	58,114,114	1.75	13 (22%)
29	CLA	B	608	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	16 (19%)
29	CLA	g	604	-	53,57,73	1.55	7 (13%)	61,93,113	2.16	18 (29%)
50	3PH	i	101	-	47,47,47	0.87	4 (8%)	50,52,52	1.16	2 (4%)
45	CHL	n	605	20	60,74,74	1.38	8 (13%)	58,114,114	1.69	11 (18%)
48	NEX	N	623	-	40,46,46	2.67	11 (27%)	50,70,70	1.74	11 (22%)
29	CLA	N	611	-	53,57,73	1.54	8 (15%)	61,93,113	2.14	18 (29%)
45	CHL	G	601	21	60,74,74	1.28	8 (13%)	58,114,114	1.72	11 (18%)
29	CLA	s	613	-	59,63,73	1.47	7 (11%)	70,101,113	2.21	17 (24%)
29	CLA	C	511	-	69,73,73	1.36	6 (8%)	82,113,113	1.99	21 (25%)
31	BCR	c	515	-	41,41,41	1.60	4 (9%)	56,56,56	4.39	14 (25%)
29	CLA	c	508	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	17 (20%)
29	CLA	b	609	-	69,73,73	1.36	6 (8%)	82,113,113	2.03	17 (20%)
45	CHL	N	605	20	60,74,74	1.33	8 (13%)	58,114,114	1.70	11 (18%)
29	CLA	G	604	-	53,57,73	1.55	6 (11%)	61,93,113	2.19	20 (32%)
39	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.08	2 (4%)
29	CLA	b	617	-	69,73,73	1.36	6 (8%)	82,113,113	3.97	16 (19%)
29	CLA	C	510	-	69,73,73	1.34	6 (8%)	82,113,113	1.96	18 (21%)
37	GOL	b	624	-	5,5,5	0.60	0	5,5,5	0.25	0
29	CLA	C	505	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	15 (18%)
29	CLA	R	613	-	50,54,73	1.59	6 (12%)	59,90,113	2.09	16 (27%)
39	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.05	2 (4%)
29	CLA	c	506	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	17 (20%)
36	DGA	B	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.51	3 (6%)
45	CHL	y	601	24	60,74,74	1.29	8 (13%)	58,114,114	1.79	12 (20%)
41	BCT	D	401	27	3,3,3	3.20	1 (33%)	2,3,3	2.73	2 (100%)
29	CLA	r	604	-	53,57,73	1.53	7 (13%)	61,93,113	2.16	19 (31%)
43	HEM	f	101	6,7	50,50,50	1.49	6 (12%)	67,82,82	1.30	7 (10%)
29	CLA	s	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	15 (18%)
29	CLA	b	606	-	69,73,73	1.34	7 (10%)	82,113,113	1.93	14 (17%)
45	CHL	y	607	-	60,74,74	1.17	7 (11%)	58,114,114	1.74	14 (24%)
36	DGA	C	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.53	3 (6%)
29	CLA	C	508	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	16 (19%)
29	CLA	c	504	-	69,73,73	1.34	6 (8%)	82,113,113	1.90	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	S	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.94	20 (26%)
46	LUT	y	620	-	42,43,43	2.42	1 (2%)	51,60,60	1.79	16 (31%)
29	CLA	a	406	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	17 (20%)
29	CLA	s	612	-	49,53,73	1.61	6 (12%)	58,89,113	2.05	17 (29%)
29	CLA	C	504	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
45	CHL	Y	605	24	40,54,74	1.72	8 (20%)	34,90,114	2.04	10 (29%)
46	LUT	n	621	-	42,43,43	2.42	1 (2%)	51,60,60	1.71	11 (21%)
29	CLA	r	608	-	64,68,73	1.42	6 (9%)	76,107,113	1.93	17 (22%)
29	CLA	s	609	-	64,68,73	1.41	7 (10%)	76,107,113	1.91	18 (23%)
29	CLA	A	410	-	64,68,73	1.40	8 (12%)	76,107,113	2.00	19 (25%)
46	LUT	r	620	-	42,43,43	2.45	1 (2%)	51,60,60	2.18	12 (23%)
31	BCR	b	619	-	41,41,41	1.61	4 (9%)	56,56,56	4.55	18 (32%)
29	CLA	Y	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.81	15 (18%)
29	CLA	b	605	-	69,73,73	1.38	7 (10%)	82,113,113	1.98	15 (18%)
29	CLA	S	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.04	14 (24%)
29	CLA	s	617	-	54,58,73	1.53	7 (12%)	64,95,113	2.12	20 (31%)
48	NEX	y	623	-	40,46,46	2.72	12 (30%)	50,70,70	1.66	11 (22%)
45	CHL	G	607	-	44,58,74	1.35	7 (15%)	37,94,114	2.13	10 (27%)
29	CLA	g	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	18 (21%)
45	CHL	s	608	-	55,69,74	1.39	8 (14%)	52,108,114	1.80	12 (23%)
29	CLA	n	611	-	53,57,73	1.54	8 (15%)	61,93,113	2.19	18 (29%)
29	CLA	C	506	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	17 (20%)
50	3PH	s	626	-	47,47,47	0.88	4 (8%)	50,52,52	1.17	2 (4%)
46	LUT	N	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.75	14 (27%)
29	CLA	D	402	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	16 (19%)
29	CLA	C	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.79	18 (21%)
29	CLA	Y	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
29	CLA	S	617	-	54,58,73	1.54	8 (14%)	64,95,113	2.12	19 (29%)
38	DGD	c	523	-	67,67,67	1.30	7 (10%)	81,81,81	0.99	2 (2%)
29	CLA	b	611	-	69,73,73	1.37	7 (10%)	82,113,113	1.87	20 (24%)
31	BCR	B	618	-	41,41,41	1.58	4 (9%)	56,56,56	4.46	14 (25%)
47	XAT	y	622	-	41,47,47	0.68	1 (2%)	54,74,74	3.75	17 (31%)
45	CHL	N	609	-	60,74,74	1.22	8 (13%)	58,114,114	1.66	11 (18%)
45	CHL	Y	607	-	60,74,74	1.14	7 (11%)	58,114,114	1.78	13 (22%)
47	XAT	n	622	-	41,47,47	0.69	1 (2%)	54,74,74	1.97	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	y	609	-	60,74,74	1.31	8 (13%)	58,114,114	1.66	12 (20%)
42	PL9	D	405	-	55,55,55	1.15	5 (9%)	68,69,69	1.46	11 (16%)
45	CHL	N	606	-	60,74,74	1.38	8 (13%)	58,114,114	1.76	13 (22%)
39	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.17	3 (7%)
38	DGD	C	523	-	67,67,67	1.30	7 (10%)	81,81,81	0.99	2 (2%)
45	CHL	G	606	-	44,58,74	1.69	9 (20%)	37,94,114	2.07	12 (32%)
45	CHL	n	606	-	60,74,74	1.46	8 (13%)	58,114,114	1.68	13 (22%)
36	DGA	b	623	-	43,43,43	1.15	2 (4%)	45,45,45	1.51	3 (6%)
45	CHL	S	601	23	40,54,74	1.66	8 (20%)	34,90,114	2.13	10 (29%)
39	LHG	d	408	-	43,43,48	0.42	0	46,49,54	1.16	3 (6%)
29	CLA	B	615	-	69,73,73	1.36	7 (10%)	82,113,113	2.02	18 (21%)
29	CLA	Y	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.83	21 (25%)
48	NEX	G	623	-	40,46,46	2.68	12 (30%)	50,70,70	1.77	12 (24%)
29	CLA	n	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.97	21 (25%)
39	LHG	l	101	-	48,48,48	0.41	0	51,54,54	0.94	2 (3%)
29	CLA	d	403	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	19 (23%)
39	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
29	CLA	R	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.93	17 (22%)
29	CLA	N	602	-	69,73,73	1.37	6 (8%)	82,113,113	1.88	18 (21%)
30	PHO	A	409	-	58,69,69	2.16	9 (15%)	55,99,99	1.64	7 (12%)
29	CLA	C	502	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	17 (20%)
45	CHL	g	608	-	38,52,74	1.62	8 (21%)	31,87,114	2.26	10 (32%)
29	CLA	G	612	-	47,51,73	1.64	7 (14%)	55,86,113	2.10	16 (29%)
29	CLA	y	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	21 (25%)
29	CLA	B	616	-	69,73,73	1.37	6 (8%)	82,113,113	1.87	19 (23%)
45	CHL	G	605	21	42,56,74	1.52	8 (19%)	36,92,114	2.11	11 (30%)
31	BCR	D	404	-	41,41,41	1.60	4 (9%)	56,56,56	4.18	17 (30%)
46	LUT	R	620	-	42,43,43	2.45	1 (2%)	51,60,60	2.10	11 (21%)
46	LUT	s	620	-	42,43,43	2.49	1 (2%)	51,60,60	1.97	15 (29%)
29	CLA	R	611	-	50,54,73	1.59	8 (16%)	59,90,113	2.03	16 (27%)
49	LPX	S	625	-	29,29,29	1.01	2 (6%)	31,33,33	0.99	1 (3%)
29	CLA	g	602	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	20 (24%)
33	LMG	J	101	-	45,45,55	1.00	3 (6%)	53,53,63	1.02	2 (3%)
33	LMG	c	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.12	4 (6%)
29	CLA	b	613	-	69,73,73	1.34	7 (10%)	82,113,113	1.85	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	r	602	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	20 (26%)
33	LMG	a	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.13	3 (5%)
39	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.12	3 (5%)
29	CLA	r	603	-	64,68,73	1.42	7 (10%)	76,107,113	1.93	18 (23%)
31	BCR	C	516	-	41,41,41	1.60	4 (9%)	56,56,56	4.53	15 (26%)
29	CLA	y	610	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	20 (24%)
33	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.10	4 (6%)
46	LUT	S	620	-	42,43,43	2.47	1 (2%)	51,60,60	1.99	13 (25%)
29	CLA	y	604	-	69,73,73	1.35	6 (8%)	82,113,113	1.83	18 (21%)
38	DGD	c	519	-	63,63,67	1.23	7 (11%)	77,77,81	1.04	3 (3%)
29	CLA	y	612	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	19 (23%)
31	BCR	d	404	-	41,41,41	1.60	4 (9%)	56,56,56	4.25	17 (30%)
47	XAT	N	622	-	41,47,47	0.68	1 (2%)	54,74,74	1.96	12 (22%)
29	CLA	n	612	-	49,53,73	1.60	6 (12%)	58,89,113	2.03	16 (27%)
45	CHL	n	607	-	60,74,74	1.13	7 (11%)	58,114,114	1.83	12 (20%)
38	DGD	C	520	-	60,60,67	1.17	6 (10%)	74,74,81	0.99	2 (2%)
46	LUT	g	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.88	12 (23%)
31	BCR	c	514	-	41,41,41	1.60	4 (9%)	56,56,56	4.54	14 (25%)
45	CHL	g	605	21	42,56,74	1.52	8 (19%)	36,92,114	2.10	11 (30%)
47	XAT	r	622	-	41,47,47	0.71	1 (2%)	54,74,74	2.17	20 (37%)
29	CLA	g	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.17	18 (29%)
29	CLA	C	503	-	69,73,73	1.36	6 (8%)	82,113,113	1.93	21 (25%)
44	RRX	H	101	-	42,42,42	5.00	24 (57%)	56,58,58	2.07	18 (32%)
29	CLA	c	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	19 (23%)
29	CLA	r	610	-	64,68,73	1.41	8 (12%)	76,107,113	2.03	22 (28%)
29	CLA	G	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	22 (26%)
29	CLA	a	405	-	69,73,73	1.36	7 (10%)	82,113,113	1.85	19 (23%)
29	CLA	c	505	-	69,73,73	1.36	6 (8%)	82,113,113	1.93	16 (19%)
45	CHL	r	606	-	38,52,74	1.73	9 (23%)	31,87,114	2.20	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGA	c	524	-	-	19/45/45/45	-
29	CLA	B	613	-	1/1/15/20	14/39/115/115	-
35	C7Z	b	620	-	1/1/12/26	9/29/67/67	0/2/2/2
45	CHL	n	608	-	3/3/16/26	4/20/118/137	-
29	CLA	N	610	-	1/1/15/20	8/39/115/115	-
29	CLA	c	502	-	1/1/15/20	16/39/115/115	-
29	CLA	c	503	-	1/1/15/20	20/39/115/115	-
29	CLA	R	603	-	1/1/14/20	14/33/109/115	-
29	CLA	S	602	-	1/1/14/20	12/33/109/115	-
29	CLA	b	610	-	1/1/15/20	14/39/115/115	-
39	LHG	s	624	-	-	28/49/49/53	-
29	CLA	y	608	-	1/1/12/20	8/21/97/115	-
45	CHL	g	601	21	4/4/20/26	9/39/137/137	-
29	CLA	n	614	-	1/1/11/20	7/20/96/115	-
29	CLA	b	612	-	1/1/15/20	14/39/115/115	-
29	CLA	R	604	-	1/1/11/20	13/20/96/115	-
38	DGD	C	519	-	-	18/51/91/95	0/2/2/2
29	CLA	r	609	-	1/1/14/20	18/33/109/115	-
29	CLA	S	603	-	1/1/15/20	15/39/115/115	-
29	CLA	S	613	-	1/1/13/20	12/27/103/115	-
29	CLA	B	605	-	1/1/15/20	18/39/115/115	-
29	CLA	A	405	-	1/1/15/20	16/39/115/115	-
29	CLA	s	610	-	1/1/15/20	20/39/115/115	-
45	CHL	g	607	-	3/3/16/26	2/20/118/137	-
29	CLA	s	604	-	1/1/13/20	12/27/103/115	-
29	CLA	b	608	-	1/1/15/20	23/39/115/115	-
29	CLA	y	602	-	1/1/15/20	19/39/115/115	-
29	CLA	R	612	-	1/1/14/20	15/33/109/115	-
38	DGD	c	520	-	-	12/48/88/95	0/2/2/2
49	LPX	s	625	-	-	9/31/31/31	-
37	GOL	b	625	-	-	1/4/4/4	-
45	CHL	s	601	23	3/3/16/26	6/15/113/137	-
38	DGD	c	518	-	-	10/44/84/95	0/2/2/2
29	CLA	S	610	-	1/1/15/20	11/39/115/115	-
45	CHL	R	606	-	3/3/15/26	2/13/111/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	Y	609	-	4/4/20/26	7/39/137/137	-
29	CLA	b	607	-	1/1/15/20	14/39/115/115	-
29	CLA	n	602	-	1/1/15/20	16/39/115/115	-
29	CLA	S	604	-	1/1/13/20	10/27/103/115	-
29	CLA	S	605	-	1/1/12/20	15/21/97/115	-
29	CLA	y	611	-	1/1/15/20	17/39/115/115	-
48	NEX	R	622	-	-	8/27/83/83	0/3/3/3
31	BCR	A	411	-	-	11/29/63/63	0/2/2/2
32	SQD	B	621	-	-	19/49/69/69	0/1/1/1
45	CHL	n	609	-	4/4/20/26	8/39/137/137	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
29	CLA	c	501	-	1/1/15/20	13/39/115/115	-
29	CLA	c	507	52	1/1/15/20	21/39/115/115	-
45	CHL	S	606	-	3/3/15/26	0/13/111/137	-
29	CLA	A	406	-	1/1/15/20	11/39/115/115	-
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	a	407	-	1/1/11/20	4/20/96/115	-
43	HEM	F	101	6,7	-	3/14/54/54	-
29	CLA	y	614	-	1/1/15/20	15/39/115/115	-
32	SQD	c	626	-	-	14/49/69/69	0/1/1/1
29	CLA	B	607	-	1/1/15/20	14/39/115/115	-
48	NEX	S	622	-	-	11/27/83/83	0/3/3/3
29	CLA	R	608	-	1/1/14/20	16/33/109/115	-
29	CLA	C	507	52	1/1/15/20	20/39/115/115	-
51	SPH	Y	625	-	-	10/21/21/21	-
32	SQD	C	526	-	-	18/49/69/69	0/1/1/1
31	BCR	C	515	-	-	11/29/63/63	0/2/2/2
39	LHG	D	409	-	-	29/53/53/53	-
32	SQD	A	412	-	-	12/46/66/69	0/1/1/1
45	CHL	s	607	-	4/4/15/26	3/12/110/137	-
50	3PH	S	626	-	-	19/49/49/49	-
29	CLA	N	613	-	1/1/15/20	19/39/115/115	-
44	RRX	h	101	-	1/1/11/25	10/29/65/65	0/2/2/2
29	CLA	C	501	-	1/1/15/20	19/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	b	618	-	-	11/29/63/63	0/2/2/2
31	BCR	c	517	-	-	8/29/63/63	0/2/2/2
29	CLA	B	609	-	1/1/15/20	14/39/115/115	-
29	CLA	B	602	-	1/1/15/20	19/39/115/115	-
29	CLA	n	613	-	1/1/15/20	14/39/115/115	-
46	LUT	G	620	-	-	6/29/67/67	0/2/2/2
29	CLA	g	613	-	1/1/15/20	21/39/115/115	-
33	LMG	A	413	-	-	14/43/63/70	0/1/1/1
45	CHL	S	607	-	4/4/15/26	3/12/110/137	-
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
29	CLA	D	403	-	1/1/15/20	14/39/115/115	-
39	LHG	g	624	-	-	27/53/53/53	-
46	LUT	g	620	-	-	3/29/67/67	0/2/2/2
39	LHG	S	624	-	-	26/49/49/53	-
29	CLA	Y	613	-	1/1/15/20	18/39/115/115	-
46	LUT	S	621	-	-	2/29/67/67	0/2/2/2
29	CLA	N	614	-	1/1/11/20	9/20/96/115	-
29	CLA	s	611	-	1/1/15/20	12/39/115/115	-
37	GOL	B	627	-	-	0/4/4/4	-
29	CLA	b	614	-	1/1/15/20	10/39/115/115	-
33	LMG	D	411	-	-	7/41/61/70	0/1/1/1
29	CLA	G	614	-	1/1/11/20	11/20/96/115	-
45	CHL	g	606	-	3/3/16/26	5/20/118/137	-
47	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	B	612	-	1/1/15/20	18/39/115/115	-
39	LHG	y	624	-	-	28/53/53/53	-
31	BCR	C	514	-	-	11/29/63/63	0/2/2/2
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
48	NEX	g	623	-	-	3/27/83/83	0/3/3/3
29	CLA	N	612	-	1/1/11/20	7/15/91/115	-
29	CLA	s	614	-	1/1/13/20	10/27/103/115	-
45	CHL	S	608	-	4/4/19/26	2/33/131/137	-
30	PHO	a	409	-	-	9/37/103/103	0/5/6/6
40	LMK	C	527	-	1/1/6/6	11/46/46/60	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	617	-	1/1/15/20	19/39/115/115	-
29	CLA	b	604	-	1/1/15/20	16/39/115/115	-
32	SQD	a	412	-	-	13/46/66/69	0/1/1/1
45	CHL	s	606	-	3/3/15/26	1/13/111/137	-
29	CLA	S	614	-	1/1/13/20	10/27/103/115	-
29	CLA	G	602	-	1/1/15/20	24/39/115/115	-
45	CHL	N	608	-	3/3/16/26	4/20/118/137	-
29	CLA	G	603	-	1/1/15/20	18/39/115/115	-
46	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
31	BCR	B	619	-	-	10/29/63/63	0/2/2/2
29	CLA	B	606	-	1/1/15/20	10/39/115/115	-
45	CHL	G	608	-	3/3/15/26	2/13/111/137	-
29	CLA	R	602	-	1/1/14/20	15/33/109/115	-
33	LMG	d	411	-	-	12/41/61/70	0/1/1/1
29	CLA	B	603	-	1/1/15/20	14/39/115/115	-
39	LHG	G	630	-	-	30/53/53/53	-
29	CLA	A	407	-	1/1/11/20	4/20/96/115	-
45	CHL	Y	601	24	4/4/20/26	6/39/137/137	-
29	CLA	c	513	-	1/1/15/20	19/39/115/115	-
48	NEX	s	623	-	-	13/27/83/83	0/3/3/3
39	LHG	Y	624	-	-	29/53/53/53	-
32	SQD	b	621	-	-	19/49/69/69	0/1/1/1
29	CLA	Y	608	-	1/1/12/20	6/21/97/115	-
38	DGD	C	518	-	-	9/44/84/95	0/2/2/2
29	CLA	c	509	-	1/1/15/20	10/39/115/115	-
42	PL9	d	405	-	-	11/53/73/73	0/1/1/1
31	BCR	c	516	-	-	14/29/63/63	0/2/2/2
29	CLA	g	603	-	1/1/15/20	21/39/115/115	-
29	CLA	d	402	-	1/1/15/20	10/39/115/115	-
46	LUT	N	620	-	-	2/29/67/67	0/2/2/2
33	LMG	h	102	-	-	13/43/63/70	0/1/1/1
29	CLA	C	509	-	1/1/15/20	9/39/115/115	-
47	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
29	CLA	R	610	-	1/1/14/20	10/33/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
30	PHO	A	408	-	-	6/37/103/103	0/5/6/6
48	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
29	CLA	G	610	-	1/1/15/20	13/39/115/115	-
45	CHL	N	607	-	4/4/20/26	6/39/137/137	-
29	CLA	g	612	-	1/1/10/20	6/13/89/115	-
33	LMG	j	101	-	-	12/40/60/70	0/1/1/1
29	CLA	B	610	-	1/1/15/20	14/39/115/115	-
47	XAT	R	621	-	1/1/12/26	11/31/93/93	0/4/4/4
33	LMG	b	622	-	-	11/39/59/70	0/1/1/1
29	CLA	c	510	-	1/1/15/20	10/39/115/115	-
29	CLA	B	614	-	1/1/15/20	11/39/115/115	-
29	CLA	r	611	-	1/1/11/20	7/17/93/115	-
45	CHL	R	607	-	3/3/16/26	3/20/118/137	-
46	LUT	y	621	-	-	2/29/67/67	0/2/2/2
31	BCR	C	517	-	-	8/29/63/63	0/2/2/2
51	SPH	y	625	-	-	11/21/21/21	-
37	GOL	y	626	-	-	1/4/4/4	-
29	CLA	N	603	-	1/1/15/20	15/39/115/115	-
29	CLA	b	602	-	1/1/15/20	19/39/115/115	-
29	CLA	r	612	-	1/1/14/20	14/33/109/115	-
29	CLA	C	513	-	1/1/15/20	19/39/115/115	-
39	LHG	L	101	-	-	30/53/53/53	-
45	CHL	r	607	-	3/3/16/26	5/20/118/137	-
39	LHG	n	624	-	-	26/53/53/53	-
45	CHL	g	609	-	4/4/20/26	2/39/137/137	-
29	CLA	G	611	-	1/1/11/20	6/15/91/115	-
29	CLA	s	605	-	1/1/12/20	10/21/97/115	-
29	CLA	b	616	-	1/1/15/20	10/39/115/115	-
29	CLA	a	410	-	1/1/14/20	8/33/109/115	-
29	CLA	B	611	-	1/1/15/20	9/39/115/115	-
40	LMK	c	627	-	1/1/6/6	10/46/46/60	-
29	CLA	Y	603	-	1/1/15/20	16/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B	622	-	-	11/39/59/70	0/1/1/1
45	CHL	Y	606	-	4/4/20/26	5/39/137/137	-
29	CLA	y	613	-	1/1/15/20	16/39/115/115	-
29	CLA	b	615	-	1/1/15/20	9/39/115/115	-
45	CHL	G	609	-	4/4/20/26	7/39/137/137	-
39	LHG	c	625	-	-	27/51/51/53	-
48	NEX	r	623	-	-	8/27/83/83	0/3/3/3
29	CLA	c	511	-	1/1/15/20	13/39/115/115	-
39	LHG	D	408	-	-	30/48/48/53	-
29	CLA	B	604	-	1/1/15/20	19/39/115/115	-
45	CHL	n	601	-	4/4/20/26	8/39/137/137	-
47	XAT	g	622	-	2/2/12/26	0/31/93/93	0/4/4/4
29	CLA	Y	610	-	1/1/15/20	21/39/115/115	-
29	CLA	r	613	-	1/1/11/20	10/17/93/115	-
29	CLA	g	611	-	1/1/11/20	6/15/91/115	-
29	CLA	S	611	-	1/1/15/20	11/39/115/115	-
48	NEX	n	623	-	-	2/27/83/83	0/3/3/3
29	CLA	b	603	-	1/1/15/20	16/39/115/115	-
29	CLA	N	604	-	1/1/15/20	19/39/115/115	-
29	CLA	Y	604	-	1/1/15/20	18/39/115/115	-
46	LUT	n	620	-	-	6/29/67/67	0/2/2/2
33	LMG	H	102	-	-	12/43/63/70	0/1/1/1
29	CLA	s	602	-	1/1/14/20	10/33/109/115	-
29	CLA	Y	612	-	1/1/15/20	12/39/115/115	-
29	CLA	n	610	-	1/1/15/20	12/39/115/115	-
29	CLA	n	604	-	1/1/15/20	18/39/115/115	-
45	CHL	y	605	24	3/3/16/26	3/15/113/137	-
45	CHL	N	601	-	4/4/20/26	4/39/137/137	-
45	CHL	y	606	-	4/4/20/26	6/39/137/137	-
29	CLA	B	608	-	1/1/15/20	23/39/115/115	-
29	CLA	g	604	-	1/1/11/20	12/20/96/115	-
50	3PH	i	101	-	-	20/49/49/49	-
45	CHL	n	605	20	4/4/20/26	10/39/137/137	-
48	NEX	N	623	-	-	2/27/83/83	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	611	-	1/1/11/20	12/20/96/115	-
45	CHL	G	601	21	4/4/20/26	5/39/137/137	-
29	CLA	s	613	-	1/1/13/20	12/27/103/115	-
29	CLA	C	511	-	1/1/15/20	14/39/115/115	-
31	BCR	c	515	-	-	11/29/63/63	0/2/2/2
29	CLA	c	508	-	1/1/15/20	9/39/115/115	-
29	CLA	b	609	-	1/1/15/20	15/39/115/115	-
45	CHL	N	605	20	4/4/20/26	11/39/137/137	-
29	CLA	G	604	-	1/1/11/20	10/20/96/115	-
39	LHG	D	410	-	-	26/43/43/53	-
29	CLA	b	617	-	1/1/15/20	17/39/115/115	-
29	CLA	C	510	-	1/1/15/20	15/39/115/115	-
37	GOL	b	624	-	-	0/4/4/4	-
29	CLA	C	505	-	1/1/15/20	13/39/115/115	-
29	CLA	R	613	-	1/1/11/20	10/17/93/115	-
39	LHG	C	525	-	-	28/51/51/53	-
29	CLA	c	506	-	1/1/15/20	22/39/115/115	-
36	DGA	B	625	-	-	24/45/45/45	-
45	CHL	y	601	24	4/4/20/26	4/39/137/137	-
29	CLA	r	604	-	1/1/11/20	13/20/96/115	-
43	HEM	f	101	6,7	-	3/14/54/54	-
29	CLA	s	603	-	1/1/15/20	14/39/115/115	-
29	CLA	b	606	-	1/1/15/20	10/39/115/115	-
45	CHL	y	607	-	4/4/20/26	7/39/137/137	-
36	DGA	C	524	-	-	18/45/45/45	-
29	CLA	C	508	-	1/1/15/20	10/39/115/115	-
29	CLA	c	504	-	1/1/15/20	15/39/115/115	-
29	CLA	S	609	-	1/1/14/20	10/33/109/115	-
46	LUT	y	620	-	-	1/29/67/67	0/2/2/2
29	CLA	a	406	-	1/1/15/20	11/39/115/115	-
29	CLA	s	612	-	1/1/11/20	8/15/91/115	-
29	CLA	C	504	-	1/1/15/20	14/39/115/115	-
45	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
46	LUT	n	621	-	-	4/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	r	608	-	1/1/14/20	13/33/109/115	-
29	CLA	s	609	-	1/1/14/20	15/33/109/115	-
29	CLA	A	410	-	1/1/14/20	12/33/109/115	-
46	LUT	r	620	-	-	9/29/67/67	0/2/2/2
31	BCR	b	619	-	-	8/29/63/63	0/2/2/2
29	CLA	Y	611	-	1/1/15/20	17/39/115/115	-
29	CLA	b	605	-	1/1/15/20	20/39/115/115	-
29	CLA	S	612	-	1/1/11/20	6/15/91/115	-
29	CLA	s	617	-	1/1/12/20	9/21/97/115	-
48	NEX	y	623	-	-	3/27/83/83	0/3/3/3
45	CHL	G	607	-	3/3/16/26	3/20/118/137	-
29	CLA	g	610	-	1/1/15/20	11/39/115/115	-
45	CHL	s	608	-	4/4/19/26	2/33/131/137	-
29	CLA	n	611	-	1/1/11/20	12/20/96/115	-
29	CLA	C	506	-	1/1/15/20	22/39/115/115	-
50	3PH	s	626	-	-	27/49/49/49	-
46	LUT	N	621	-	-	2/29/67/67	0/2/2/2
29	CLA	D	402	-	1/1/15/20	12/39/115/115	-
29	CLA	C	512	-	1/1/15/20	13/39/115/115	-
29	CLA	Y	614	-	1/1/15/20	14/39/115/115	-
29	CLA	S	617	-	1/1/12/20	10/21/97/115	-
38	DGD	c	523	-	-	18/55/95/95	0/2/2/2
29	CLA	b	611	-	1/1/15/20	11/39/115/115	-
31	BCR	B	618	-	-	12/29/63/63	0/2/2/2
47	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
45	CHL	N	609	-	4/4/20/26	8/39/137/137	-
45	CHL	Y	607	-	4/4/20/26	4/39/137/137	-
47	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
45	CHL	y	609	-	4/4/20/26	6/39/137/137	-
42	PL9	D	405	-	-	13/53/73/73	0/1/1/1
45	CHL	N	606	-	4/4/20/26	5/39/137/137	-
39	LHG	d	410	-	-	32/43/43/53	-
38	DGD	C	523	-	-	16/55/95/95	0/2/2/2
45	CHL	G	606	-	4/4/16/26	3/20/118/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	n	606	-	4/4/20/26	5/39/137/137	-
36	DGA	b	623	-	-	26/45/45/45	-
45	CHL	S	601	23	3/3/16/26	2/15/113/137	-
39	LHG	d	408	-	-	27/48/48/53	-
29	CLA	B	615	-	1/1/15/20	8/39/115/115	-
29	CLA	Y	602	-	1/1/15/20	18/39/115/115	-
48	NEX	G	623	-	-	3/27/83/83	0/3/3/3
29	CLA	n	603	-	1/1/15/20	20/39/115/115	-
39	LHG	l	101	-	-	29/53/53/53	-
29	CLA	d	403	-	1/1/15/20	15/39/115/115	-
39	LHG	d	409	-	-	28/53/53/53	-
29	CLA	R	609	-	1/1/14/20	15/33/109/115	-
29	CLA	N	602	-	1/1/15/20	18/39/115/115	-
30	PHO	A	409	-	-	10/37/103/103	0/5/6/6
29	CLA	C	502	-	1/1/15/20	12/39/115/115	-
45	CHL	g	608	-	3/3/15/26	3/13/111/137	-
29	CLA	G	612	-	1/1/10/20	6/13/89/115	-
29	CLA	y	603	-	1/1/15/20	13/39/115/115	-
29	CLA	B	616	-	1/1/15/20	11/39/115/115	-
45	CHL	G	605	21	3/3/16/26	3/18/116/137	-
31	BCR	D	404	-	-	11/29/63/63	0/2/2/2
46	LUT	R	620	-	-	8/29/67/67	0/2/2/2
46	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
29	CLA	R	611	-	1/1/11/20	7/17/93/115	-
49	LPX	S	625	-	-	9/31/31/31	-
29	CLA	g	602	-	1/1/15/20	21/39/115/115	-
33	LMG	J	101	-	-	12/40/60/70	0/1/1/1
33	LMG	c	521	-	-	18/46/66/70	0/1/1/1
29	CLA	b	613	-	1/1/15/20	16/39/115/115	-
29	CLA	r	602	-	1/1/14/20	11/33/109/115	-
33	LMG	a	413	-	-	14/43/63/70	0/1/1/1
39	LHG	N	624	-	-	29/53/53/53	-
29	CLA	r	603	-	1/1/14/20	17/33/109/115	-
31	BCR	C	516	-	-	15/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	610	-	1/1/15/20	22/39/115/115	-
46	LUT	S	620	-	1/1/12/27	4/29/67/67	0/2/2/2
33	LMG	C	521	-	-	19/46/66/70	0/1/1/1
29	CLA	y	604	-	1/1/15/20	17/39/115/115	-
38	DGD	c	519	-	-	21/51/91/95	0/2/2/2
29	CLA	y	612	-	1/1/15/20	13/39/115/115	-
31	BCR	d	404	-	-	12/29/63/63	0/2/2/2
47	XAT	N	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	n	612	-	1/1/11/20	8/15/91/115	-
45	CHL	n	607	-	4/4/20/26	10/39/137/137	-
38	DGD	C	520	-	-	12/48/88/95	0/2/2/2
46	LUT	g	621	-	-	2/29/67/67	0/2/2/2
31	BCR	c	514	-	-	11/29/63/63	0/2/2/2
45	CHL	g	605	21	3/3/16/26	2/18/116/137	-
47	XAT	r	622	-	1/1/12/26	11/31/93/93	0/4/4/4
29	CLA	g	614	-	1/1/11/20	11/20/96/115	-
29	CLA	C	503	-	1/1/15/20	19/39/115/115	-
44	RRX	H	101	-	1/1/11/25	9/29/65/65	0/2/2/2
29	CLA	c	512	-	1/1/15/20	17/39/115/115	-
29	CLA	r	610	-	1/1/14/20	11/33/109/115	-
29	CLA	G	613	-	1/1/15/20	20/39/115/115	-
29	CLA	a	405	-	1/1/15/20	15/39/115/115	-
29	CLA	c	505	-	1/1/15/20	16/39/115/115	-
45	CHL	r	606	-	3/3/15/26	0/13/111/137	-

The worst 5 of 1954 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	620	C7Z	C25-C26	16.66	1.62	1.34
35	b	620	C7Z	C25-C26	16.62	1.62	1.34
44	h	101	RRX	C26-C25	15.97	1.61	1.34
44	H	101	RRX	C26-C25	15.95	1.61	1.34
35	b	620	C7Z	C5-C6	15.78	1.61	1.34

The worst 5 of 4413 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	617	CLA	C4-C3-C5	-21.54	77.84	115.23
29	b	617	CLA	C4-C3-C5	-21.52	77.87	115.23
31	C	517	BCR	C10-C11-C12	19.08	178.49	123.20
31	c	516	BCR	C10-C11-C12	19.08	178.47	123.20
31	C	516	BCR	C10-C11-C12	18.91	177.99	123.20

5 of 343 chirality outliers are listed below:

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

5 of 3913 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	B	602	CLA	CBD-CGD-O2D-CED
29	B	603	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

301 monomers are involved in 799 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	524	DGA	1	0
29	B	613	CLA	5	0
45	n	608	CHL	1	0
29	N	610	CLA	6	0
29	c	502	CLA	5	0
29	c	503	CLA	2	0
29	R	603	CLA	1	0
29	S	602	CLA	4	0
29	b	610	CLA	4	0
39	s	624	LHG	6	0
29	y	608	CLA	1	0
45	g	601	CHL	5	0
29	b	612	CLA	5	0
29	R	604	CLA	1	0
38	C	519	DGD	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	r	609	CLA	3	0
29	S	603	CLA	3	0
29	S	613	CLA	3	0
29	B	605	CLA	5	0
29	A	405	CLA	7	0
29	s	610	CLA	3	0
45	g	607	CHL	1	0
29	s	604	CLA	2	0
29	b	608	CLA	2	0
29	y	602	CLA	2	0
29	R	612	CLA	2	0
38	c	520	DGD	4	0
37	b	625	GOL	1	0
45	s	601	CHL	2	0
38	c	518	DGD	5	0
29	S	610	CLA	4	0
45	R	606	CHL	1	0
45	Y	609	CHL	7	0
29	b	607	CLA	4	0
29	n	602	CLA	3	0
29	S	604	CLA	1	0
29	y	611	CLA	2	0
48	R	622	NEX	2	0
31	A	411	BCR	3	0
32	B	621	SQD	5	0
45	n	609	CHL	4	0
31	a	411	BCR	3	0
29	c	501	CLA	3	0
29	c	507	CLA	2	0
45	S	606	CHL	4	0
29	A	406	CLA	5	0
46	Y	621	LUT	3	0
29	a	407	CLA	1	0
43	F	101	HEM	3	0
29	y	614	CLA	5	0
32	c	626	SQD	4	0
29	B	607	CLA	9	0
48	S	622	NEX	2	0
29	R	608	CLA	3	0
29	C	507	CLA	6	0
51	Y	625	SPH	2	0
32	C	526	SQD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	515	BCR	4	0
39	D	409	LHG	3	0
32	A	412	SQD	2	0
45	s	607	CHL	2	0
50	S	626	3PH	4	0
44	h	101	RRX	1	0
29	C	501	CLA	7	0
31	b	618	BCR	2	0
31	c	517	BCR	3	0
29	B	609	CLA	6	0
29	B	602	CLA	3	0
29	n	613	CLA	4	0
46	G	620	LUT	3	0
29	g	613	CLA	2	0
33	A	413	LMG	6	0
45	S	607	CHL	3	0
46	G	621	LUT	3	0
29	D	403	CLA	3	0
39	g	624	LHG	4	0
46	g	620	LUT	4	0
39	S	624	LHG	8	0
29	Y	613	CLA	4	0
46	S	621	LUT	7	0
29	N	614	CLA	1	0
29	s	611	CLA	3	0
29	b	614	CLA	2	0
33	D	411	LMG	5	0
29	G	614	CLA	1	0
45	g	606	CHL	2	0
47	G	622	XAT	4	0
29	B	612	CLA	7	0
39	y	624	LHG	2	0
31	C	514	BCR	6	0
46	s	621	LUT	6	0
29	N	612	CLA	1	0
29	s	614	CLA	2	0
45	S	608	CHL	4	0
30	a	409	PHO	4	0
29	B	617	CLA	7	0
29	b	604	CLA	2	0
45	s	606	CHL	2	0
29	S	614	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	G	602	CLA	4	0
45	N	608	CHL	2	0
29	G	603	CLA	2	0
46	Y	620	LUT	2	0
31	B	619	BCR	3	0
29	B	606	CLA	6	0
45	G	608	CHL	1	0
29	R	602	CLA	3	0
33	d	411	LMG	3	0
29	B	603	CLA	2	0
39	G	630	LHG	4	0
29	A	407	CLA	1	0
45	Y	601	CHL	1	0
29	c	513	CLA	7	0
48	s	623	NEX	1	0
39	Y	624	LHG	3	0
32	b	621	SQD	3	0
29	Y	608	CLA	3	0
38	C	518	DGD	5	0
29	c	509	CLA	2	0
42	d	405	PL9	2	0
31	c	516	BCR	4	0
29	g	603	CLA	1	0
29	d	402	CLA	4	0
46	N	620	LUT	6	0
33	h	102	LMG	8	0
29	C	509	CLA	4	0
47	Y	622	XAT	1	0
29	R	610	CLA	4	0
26	a	401	OEX	1	0
30	A	408	PHO	6	0
48	Y	623	NEX	1	0
30	a	408	PHO	5	0
29	G	610	CLA	3	0
45	N	607	CHL	3	0
33	j	101	LMG	2	0
29	B	610	CLA	3	0
47	R	621	XAT	5	0
33	b	622	LMG	1	0
29	c	510	CLA	5	0
29	B	614	CLA	3	0
45	R	607	CHL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	y	621	LUT	2	0
31	C	517	BCR	5	0
51	y	625	SPH	3	0
29	N	603	CLA	3	0
29	b	602	CLA	1	0
29	r	612	CLA	2	0
29	C	513	CLA	10	0
39	L	101	LHG	6	0
45	r	607	CHL	1	0
39	n	624	LHG	2	0
45	g	609	CHL	3	0
29	b	616	CLA	7	0
29	a	410	CLA	4	0
29	B	611	CLA	3	0
29	Y	603	CLA	2	0
33	B	622	LMG	3	0
45	Y	606	CHL	2	0
29	y	613	CLA	5	0
29	b	615	CLA	1	0
45	G	609	CHL	3	0
39	c	625	LHG	2	0
48	r	623	NEX	3	0
29	c	511	CLA	6	0
39	D	408	LHG	3	0
29	B	604	CLA	3	0
45	n	601	CHL	3	0
47	g	622	XAT	2	0
29	Y	610	CLA	2	0
29	r	613	CLA	1	0
29	S	611	CLA	2	0
48	n	623	NEX	2	0
29	b	603	CLA	1	0
29	N	604	CLA	1	0
29	Y	604	CLA	2	0
46	n	620	LUT	3	0
33	H	102	LMG	6	0
29	s	602	CLA	3	0
29	Y	612	CLA	3	0
29	n	610	CLA	4	0
29	n	604	CLA	1	0
45	N	601	CHL	2	0
45	y	605	CHL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	y	606	CHL	3	0
29	B	608	CLA	6	0
50	i	101	3PH	1	0
45	n	605	CHL	4	0
48	N	623	NEX	2	0
45	G	601	CHL	5	0
29	s	613	CLA	3	0
29	C	511	CLA	7	0
31	c	515	BCR	2	0
29	c	508	CLA	2	0
29	b	609	CLA	7	0
45	N	605	CHL	2	0
29	G	604	CLA	3	0
39	D	410	LHG	1	0
29	b	617	CLA	5	0
29	C	510	CLA	5	0
29	C	505	CLA	5	0
39	C	525	LHG	7	0
29	c	506	CLA	4	0
36	B	625	DGA	2	0
45	y	601	CHL	4	0
29	r	604	CLA	1	0
43	f	101	HEM	3	0
29	s	603	CLA	3	0
29	b	606	CLA	4	0
45	y	607	CHL	4	0
36	C	524	DGA	3	0
29	C	508	CLA	4	0
29	c	504	CLA	3	0
29	S	609	CLA	1	0
29	a	406	CLA	6	0
29	C	504	CLA	3	0
45	Y	605	CHL	2	0
46	n	621	LUT	3	0
29	r	608	CLA	4	0
29	s	609	CLA	2	0
29	A	410	CLA	6	0
46	r	620	LUT	4	0
31	b	619	BCR	1	0
29	Y	611	CLA	4	0
29	b	605	CLA	5	0
29	S	612	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	s	617	CLA	1	0
29	g	610	CLA	2	0
45	s	608	CHL	3	0
29	C	506	CLA	3	0
50	s	626	3PH	1	0
46	N	621	LUT	6	0
29	D	402	CLA	7	0
29	C	512	CLA	3	0
29	Y	614	CLA	3	0
38	c	523	DGD	4	0
29	b	611	CLA	5	0
31	B	618	BCR	3	0
47	y	622	XAT	2	0
45	N	609	CHL	2	0
45	Y	607	CHL	7	0
47	n	622	XAT	3	0
45	y	609	CHL	2	0
42	D	405	PL9	3	0
45	N	606	CHL	4	0
39	d	410	LHG	2	0
38	C	523	DGD	5	0
45	G	606	CHL	2	0
45	n	606	CHL	2	0
36	b	623	DGA	1	0
45	S	601	CHL	2	0
39	d	408	LHG	3	0
29	B	615	CLA	4	0
29	Y	602	CLA	5	0
29	n	603	CLA	7	0
39	l	101	LHG	4	0
29	d	403	CLA	3	0
39	d	409	LHG	1	0
29	R	609	CLA	4	0
29	N	602	CLA	6	0
30	A	409	PHO	5	0
29	C	502	CLA	4	0
45	g	608	CHL	3	0
29	G	612	CLA	1	0
29	y	603	CLA	5	0
29	B	616	CLA	5	0
45	G	605	CHL	3	0
31	D	404	BCR	3	0

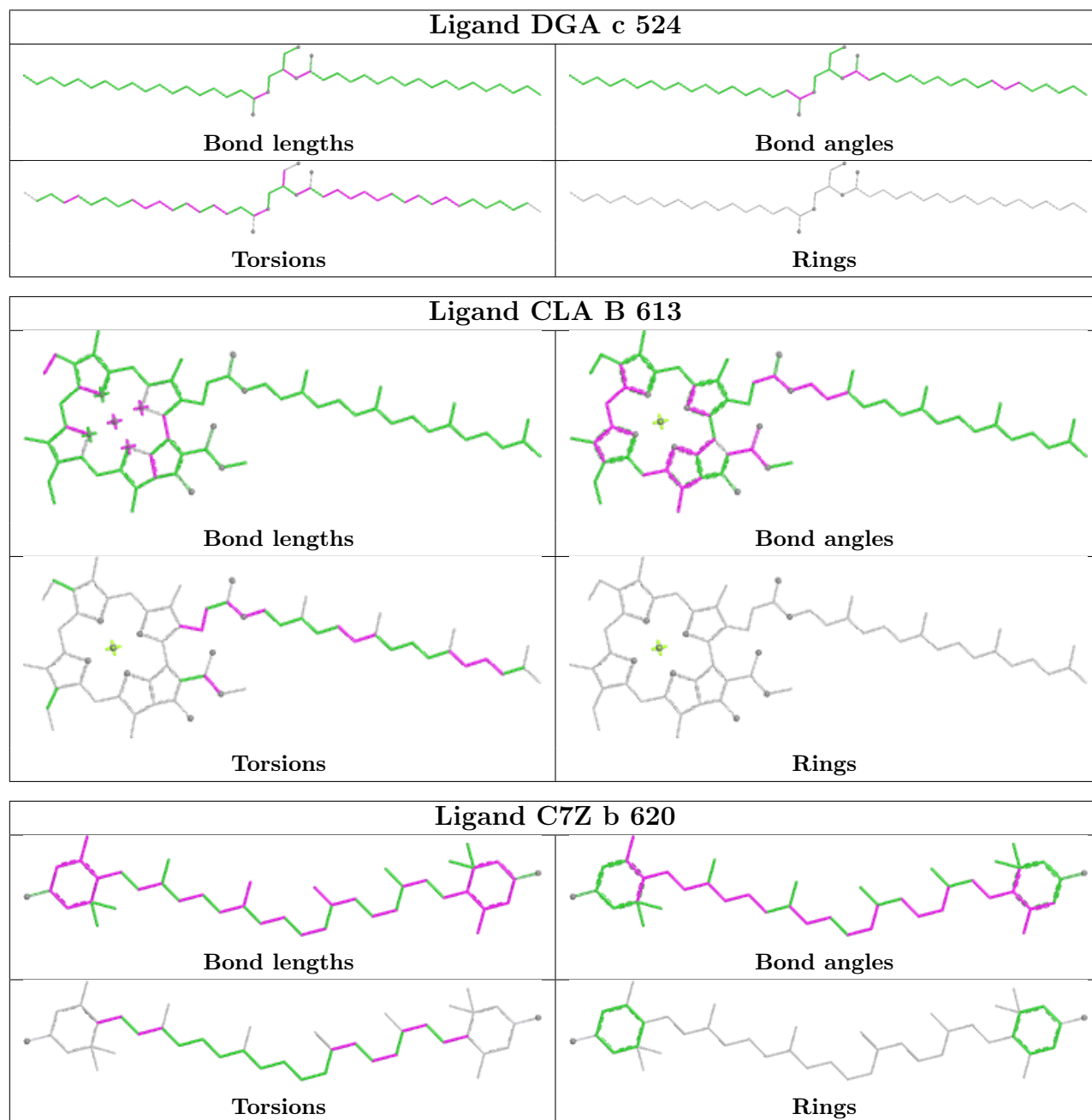
Continued on next page...

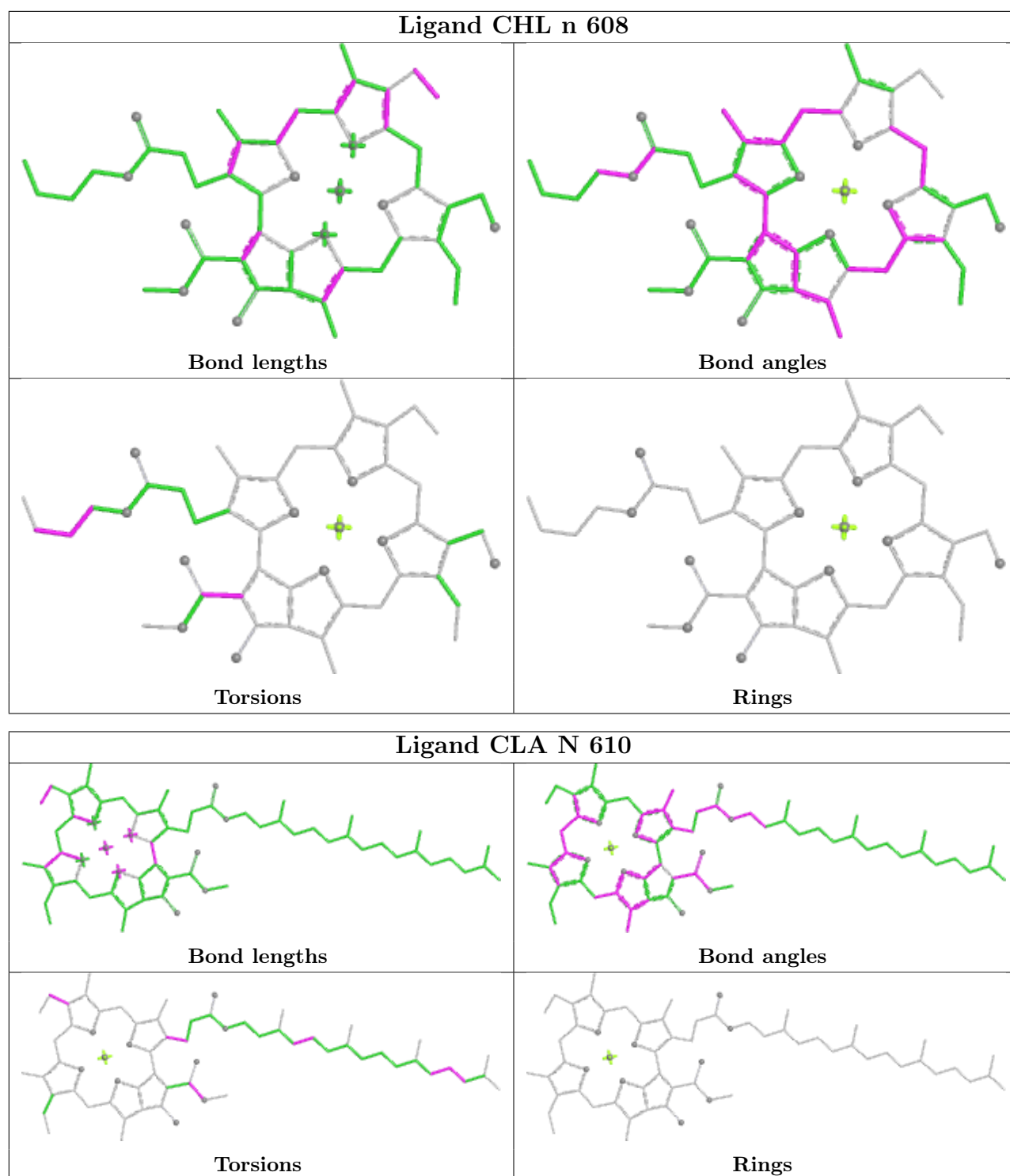
Continued from previous page...

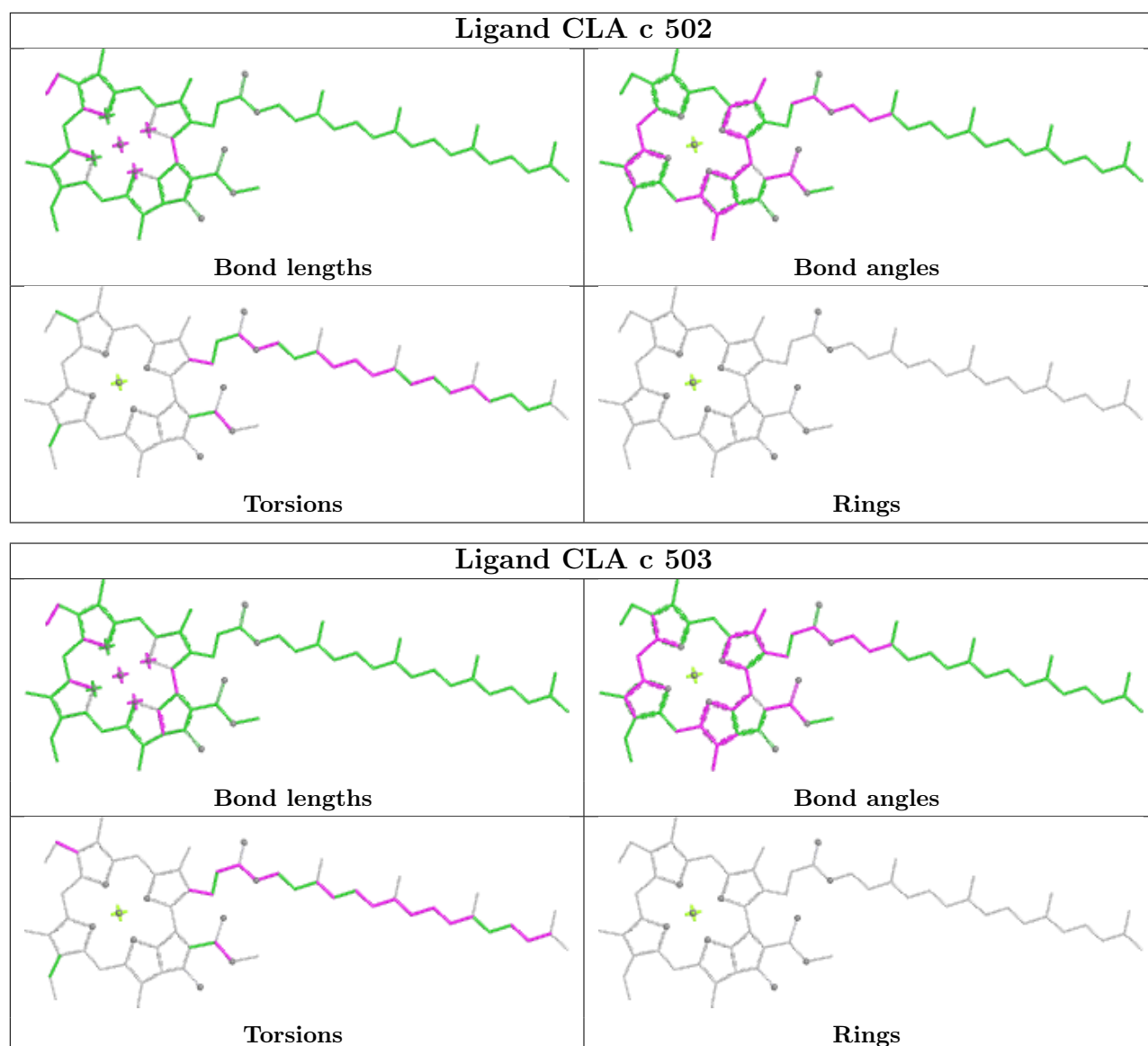
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	R	620	LUT	4	0
46	s	620	LUT	3	0
29	g	602	CLA	4	0
33	c	521	LMG	6	0
29	b	613	CLA	2	0
29	r	602	CLA	2	0
33	a	413	LMG	5	0
39	N	624	LHG	2	0
29	r	603	CLA	1	0
31	C	516	BCR	4	0
29	y	610	CLA	1	0
33	C	521	LMG	4	0
46	S	620	LUT	5	0
29	y	604	CLA	3	0
38	c	519	DGD	5	0
29	y	612	CLA	3	0
31	d	404	BCR	3	0
47	N	622	XAT	3	0
29	n	612	CLA	2	0
45	n	607	CHL	5	0
38	C	520	DGD	5	0
46	g	621	LUT	5	0
31	c	514	BCR	6	0
45	g	605	CHL	3	0
47	r	622	XAT	5	0
29	g	614	CLA	1	0
29	C	503	CLA	4	0
44	H	101	RRX	2	0
29	c	512	CLA	2	0
29	r	610	CLA	5	0
29	G	613	CLA	1	0
29	a	405	CLA	7	0
29	c	505	CLA	4	0
45	r	606	CHL	2	0

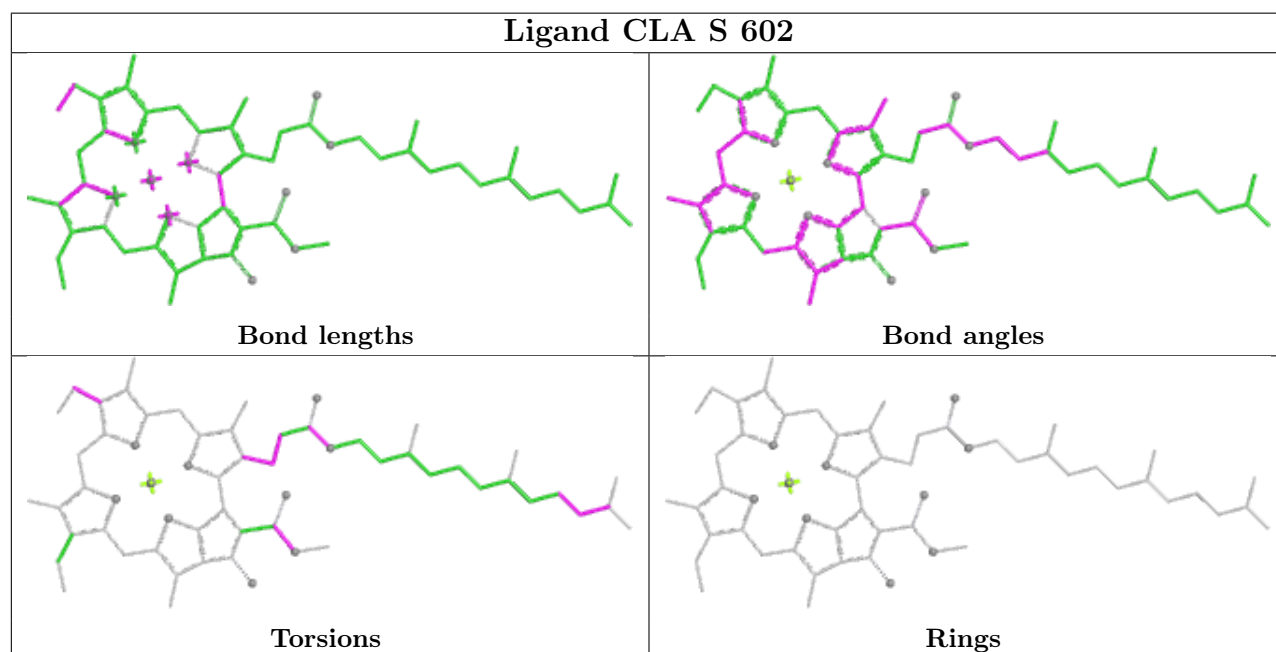
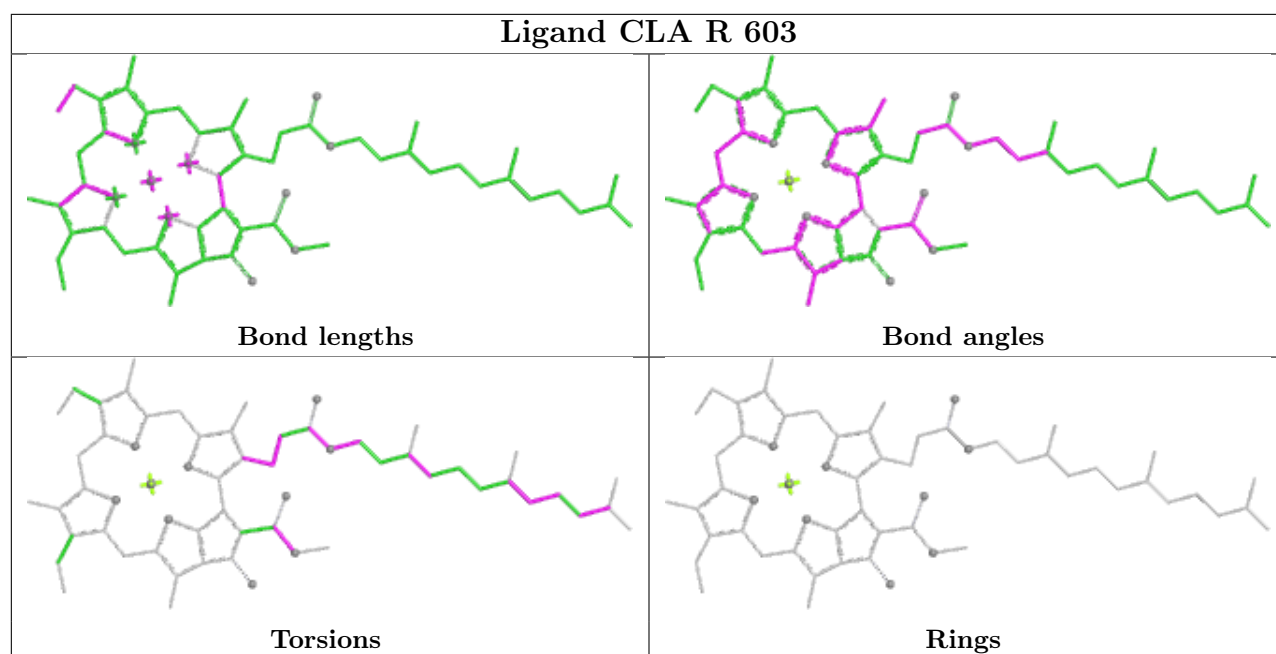
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

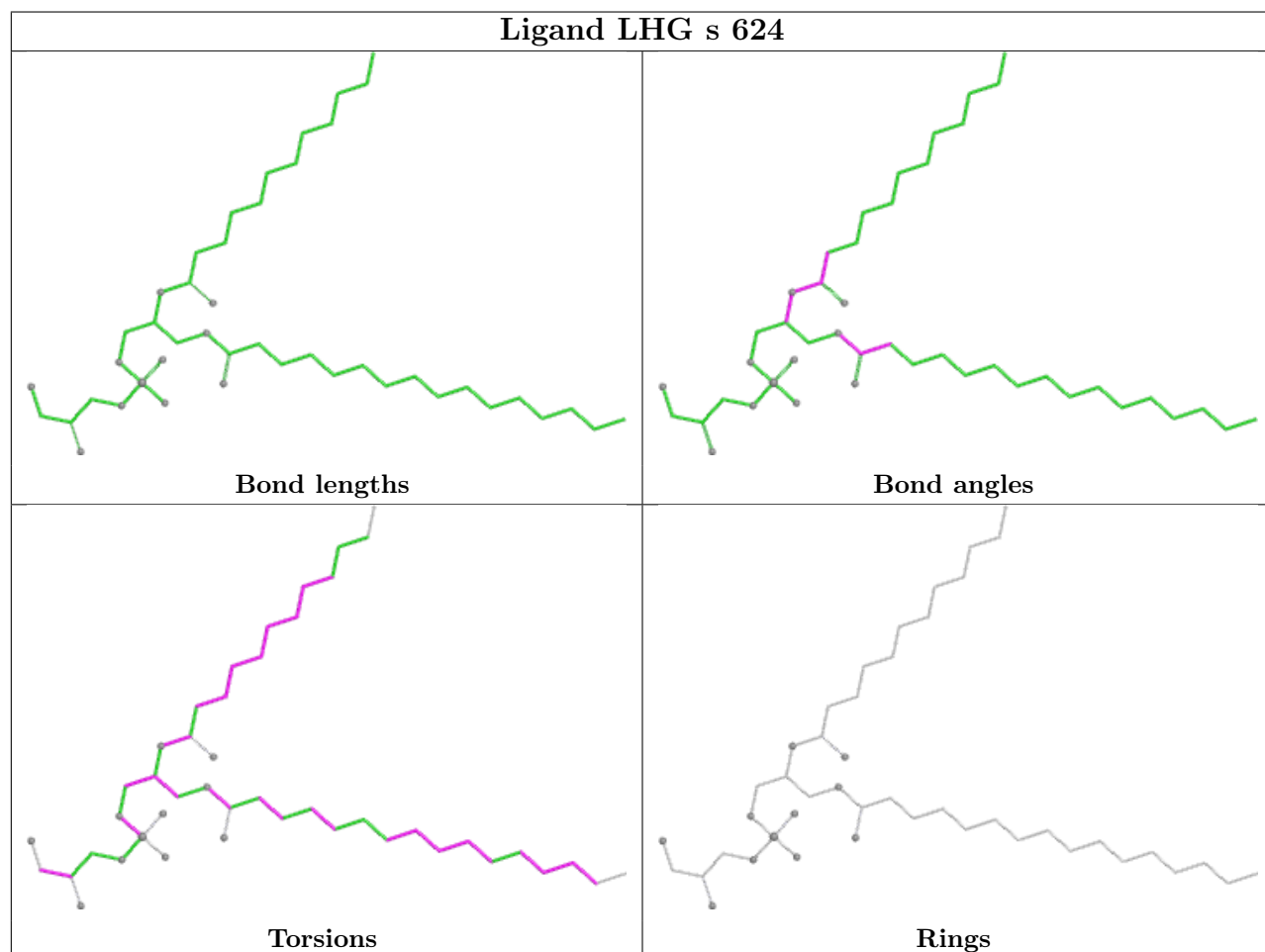
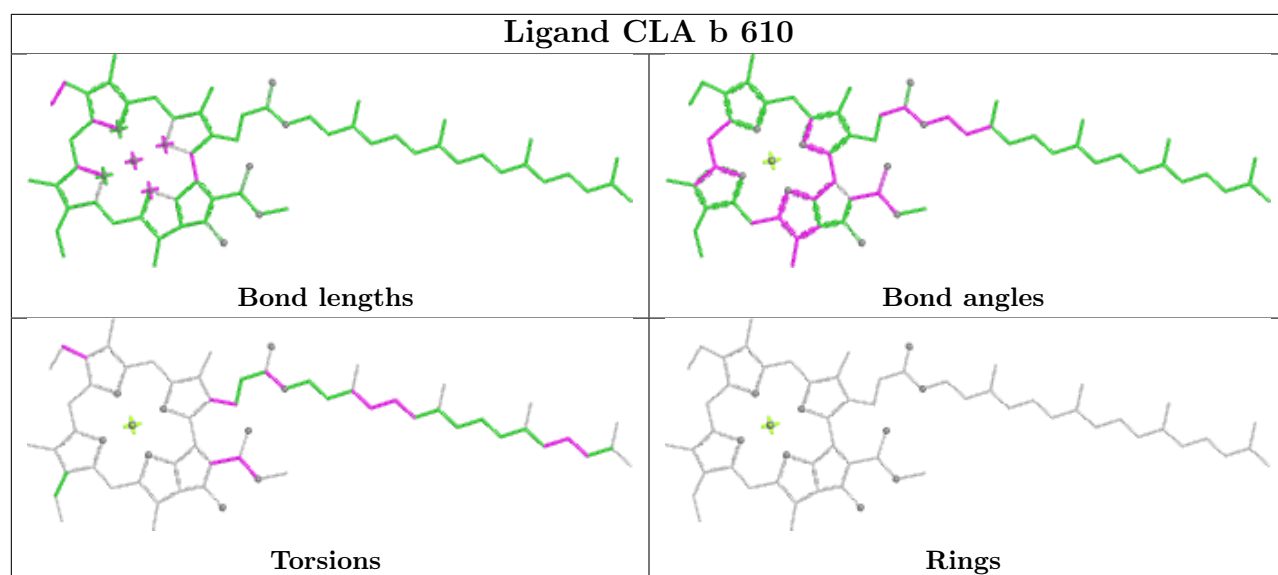
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



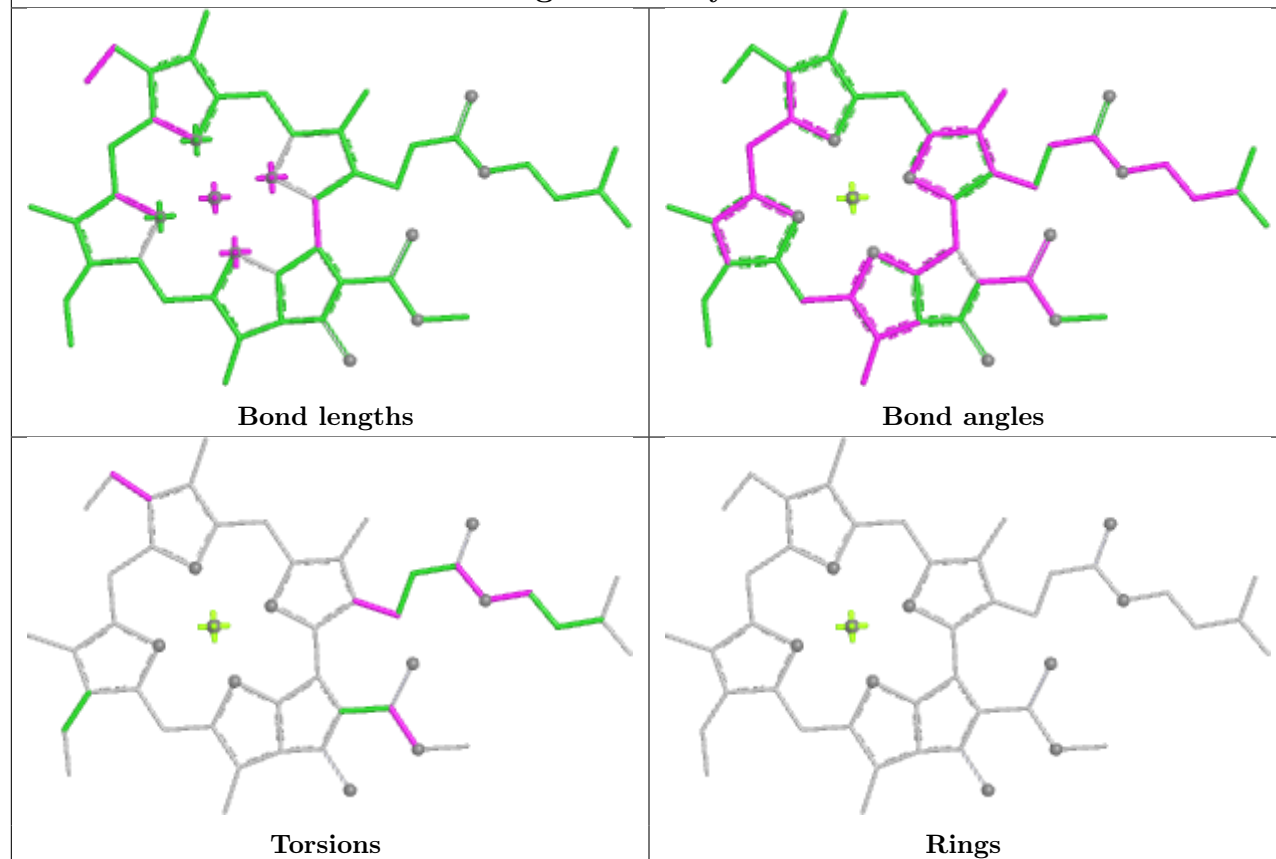




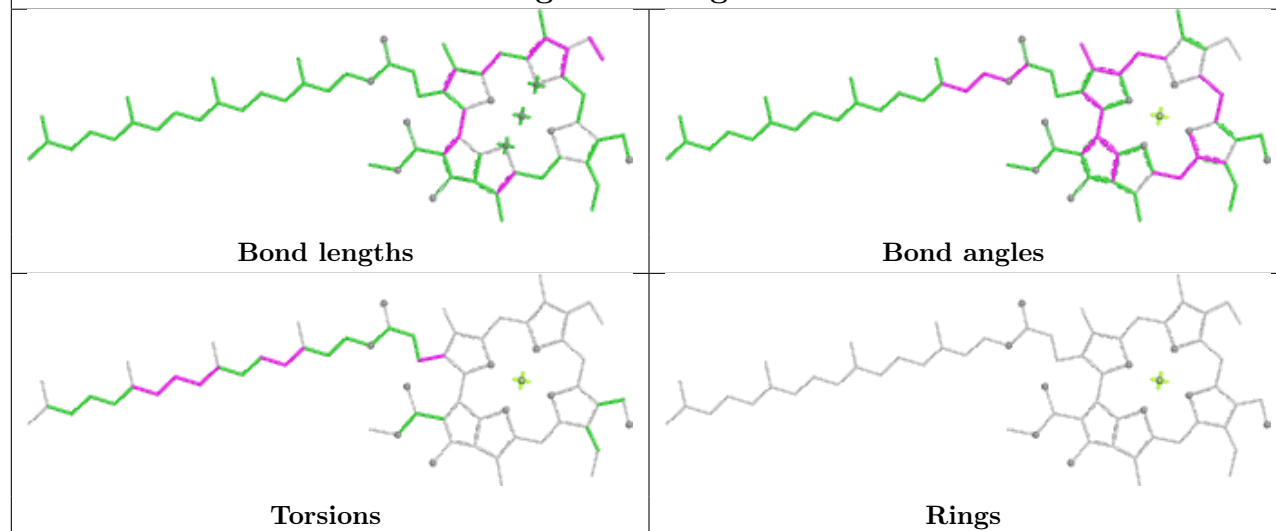




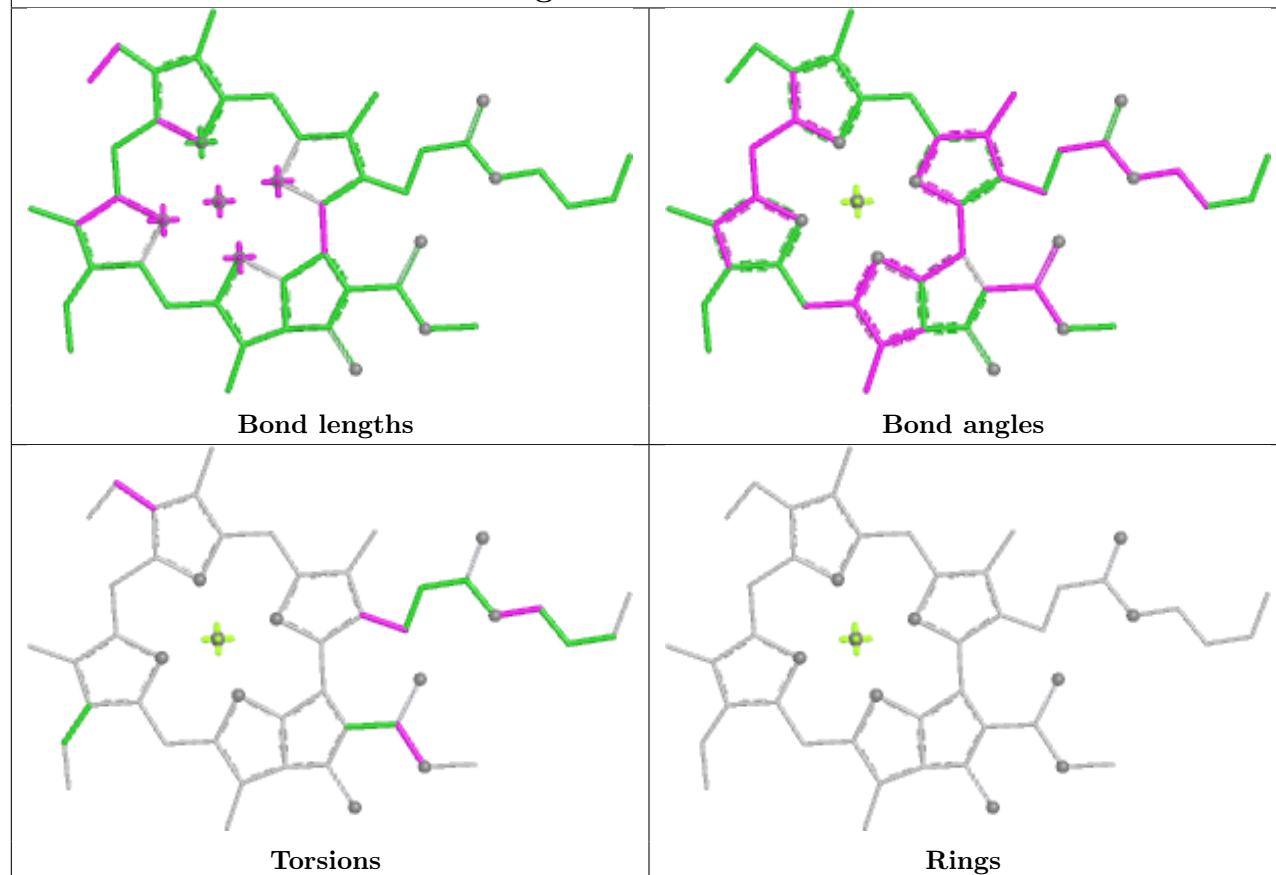
Ligand CLA y 608



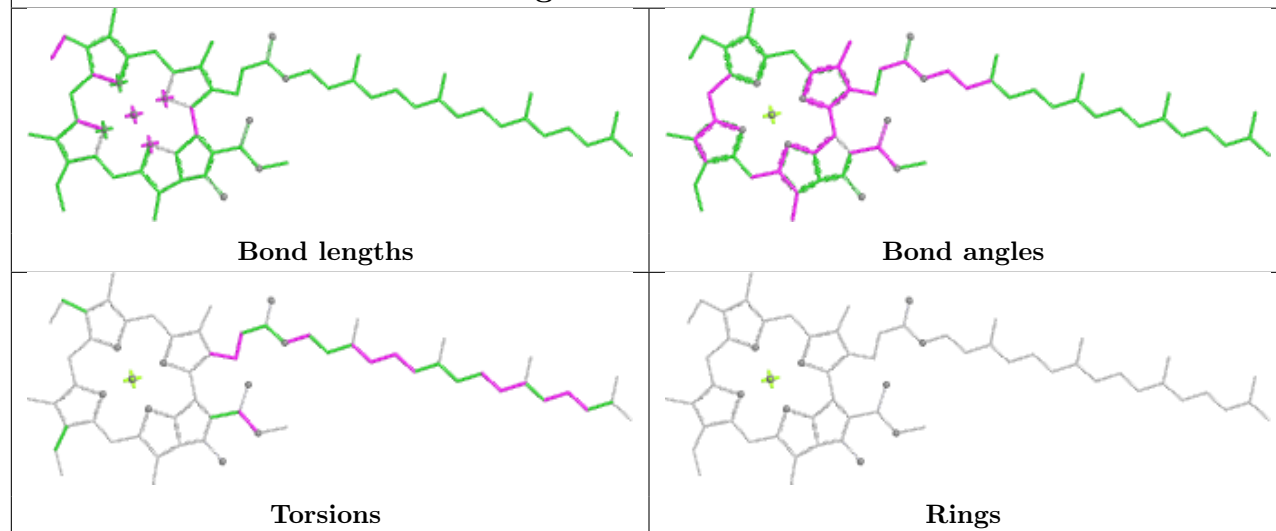
Ligand CHL g 601



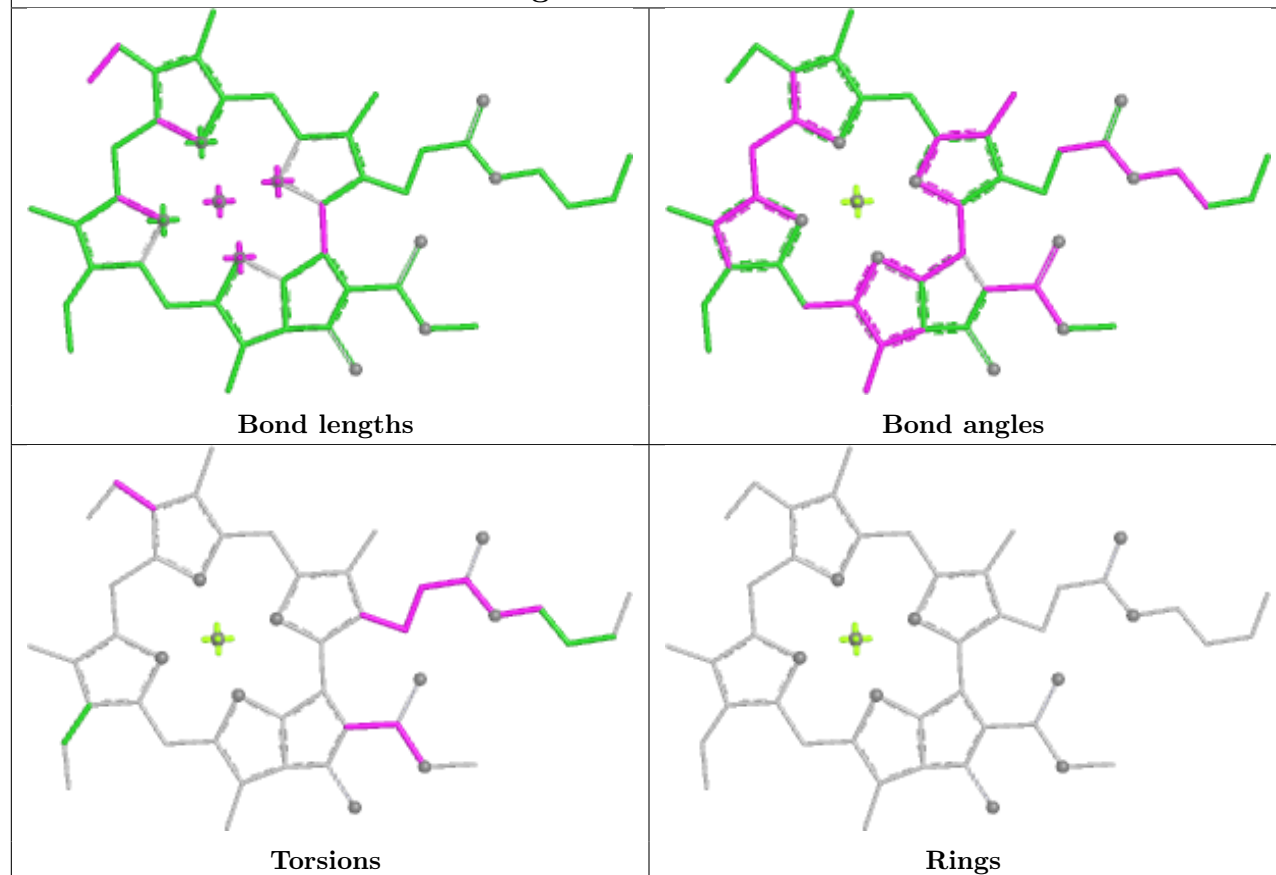
Ligand CLA n 614



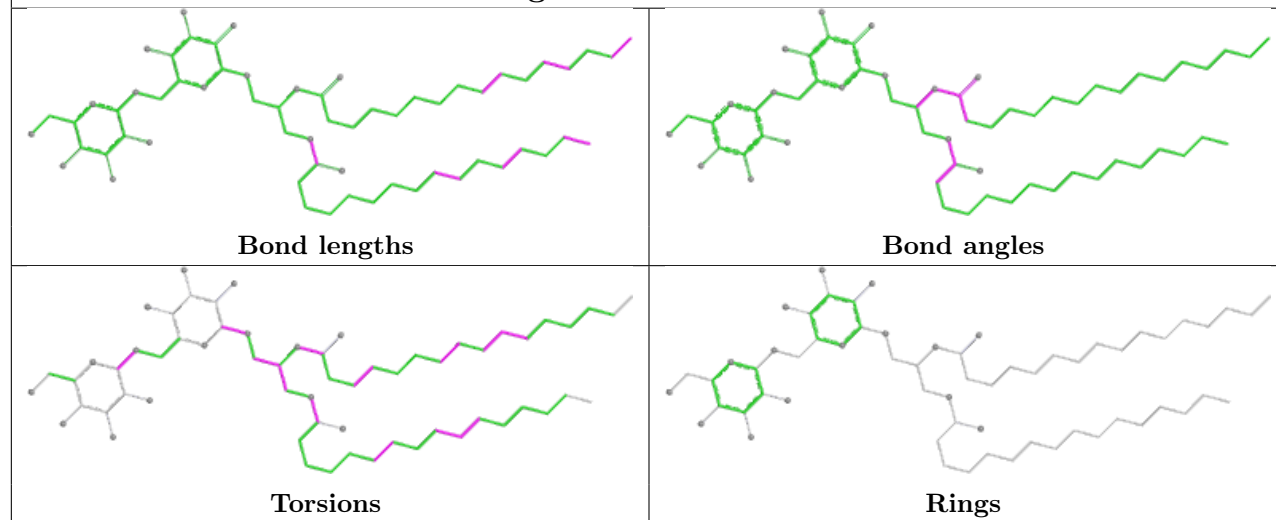
Ligand CLA b 612

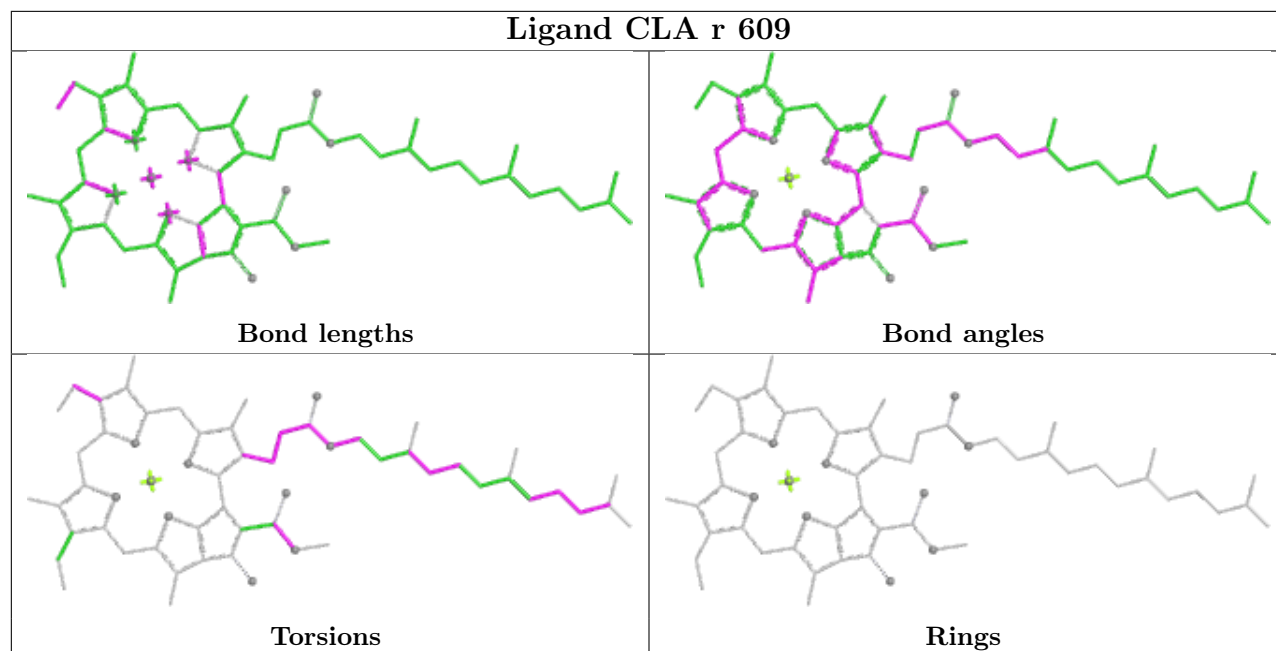
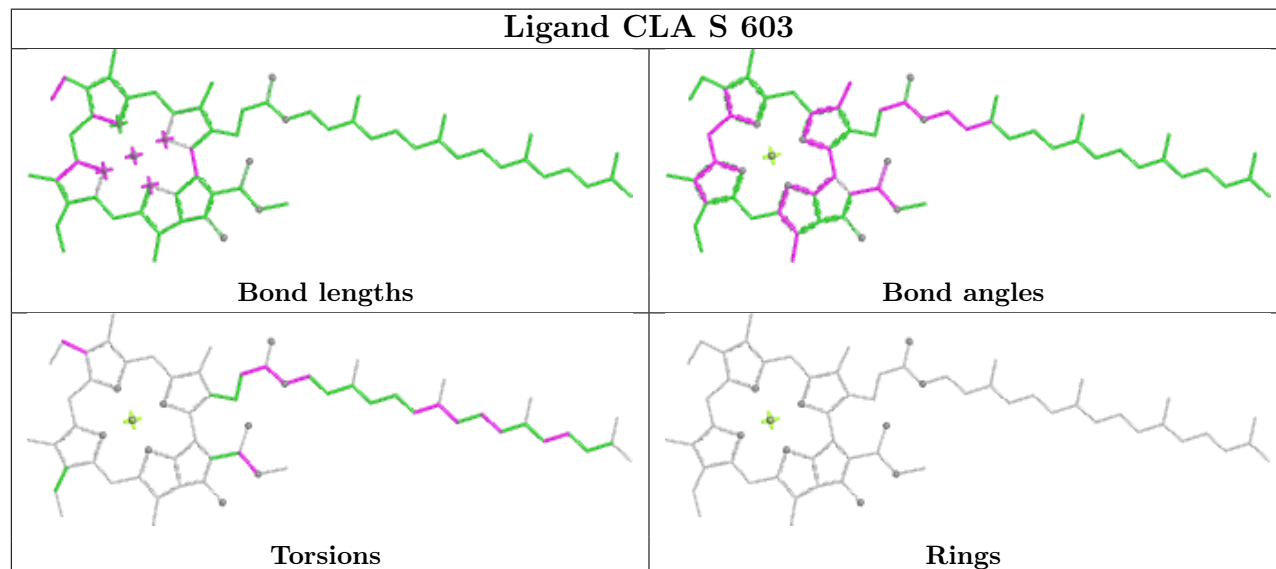


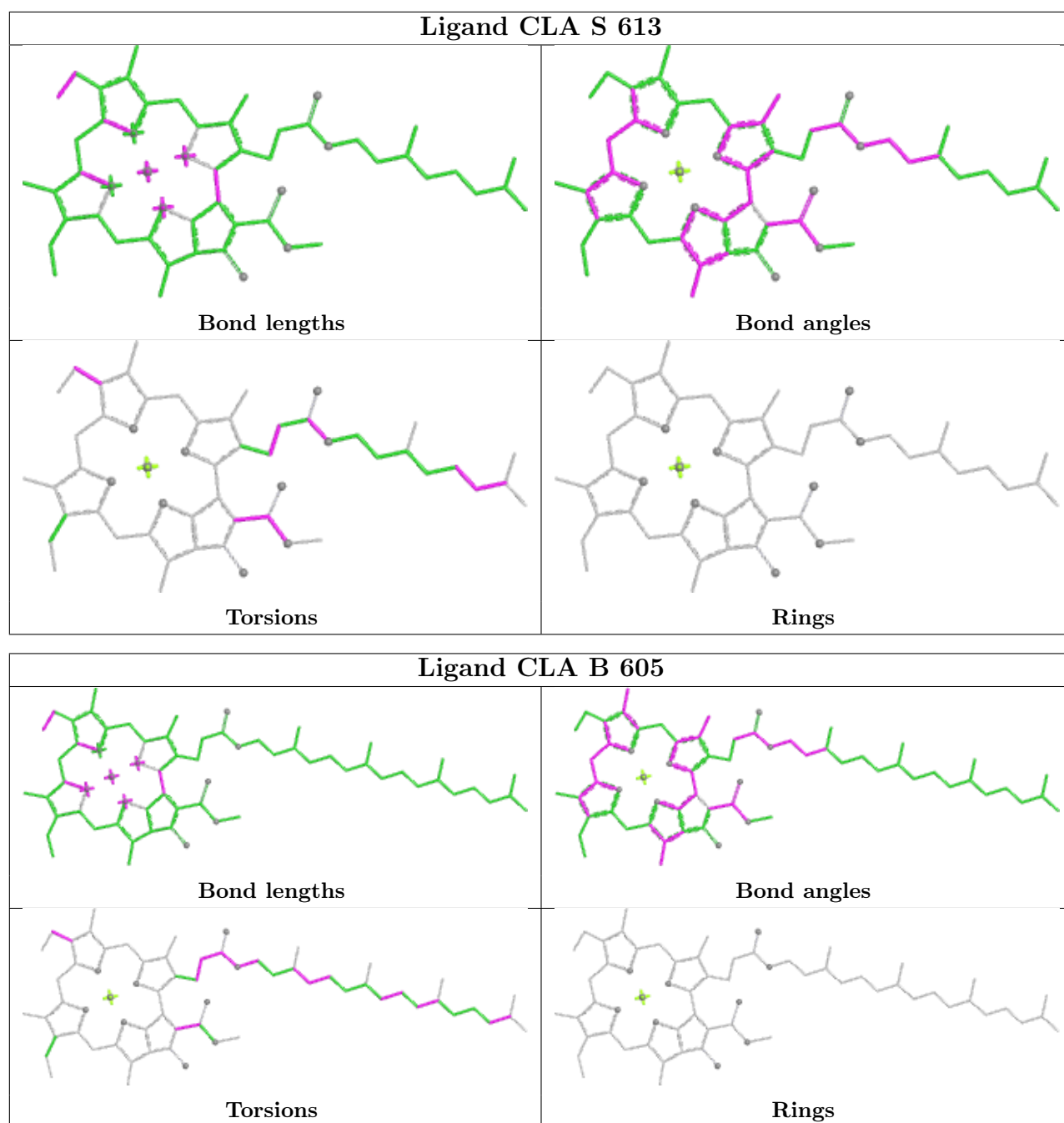
Ligand CLA R 604

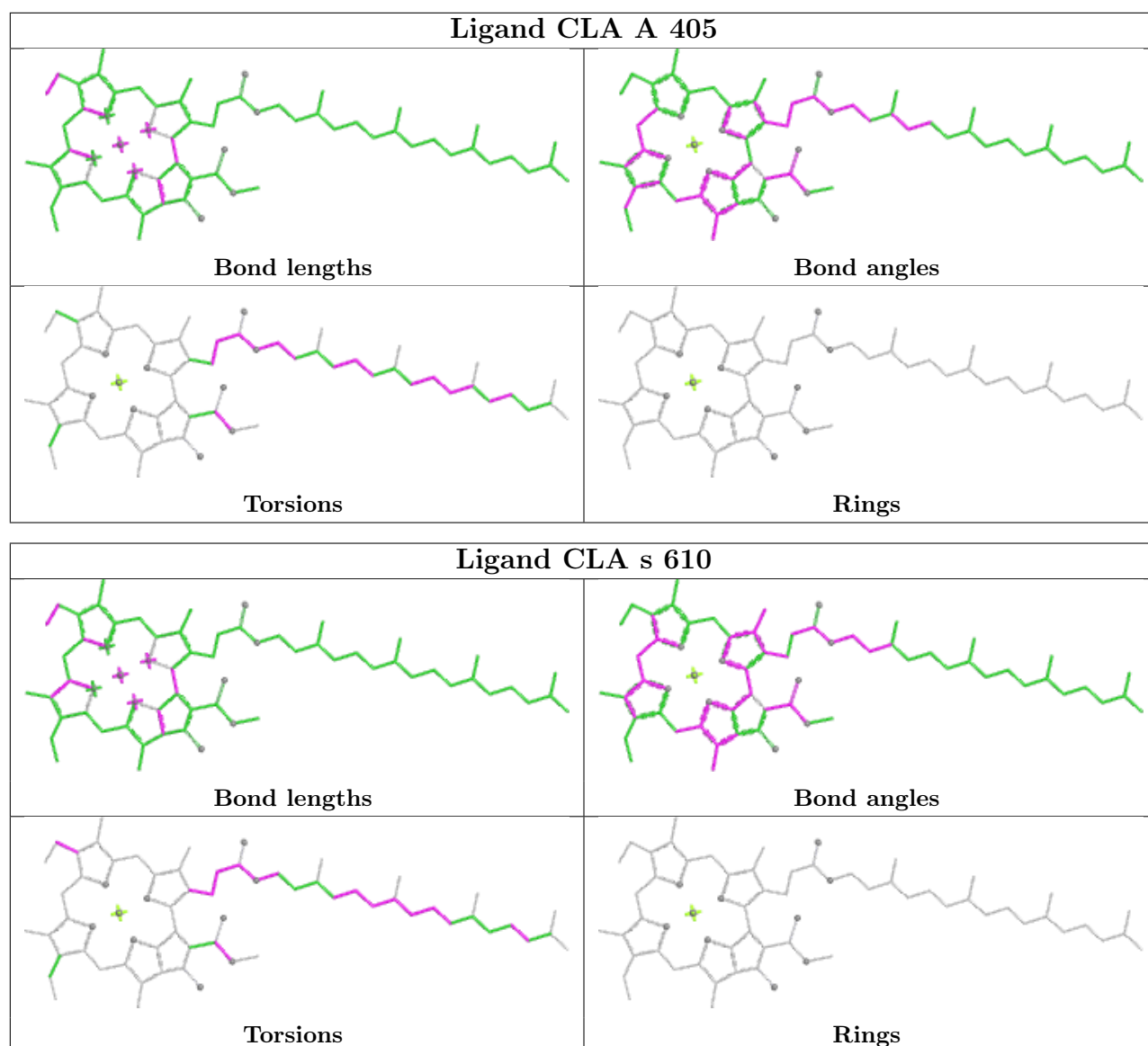


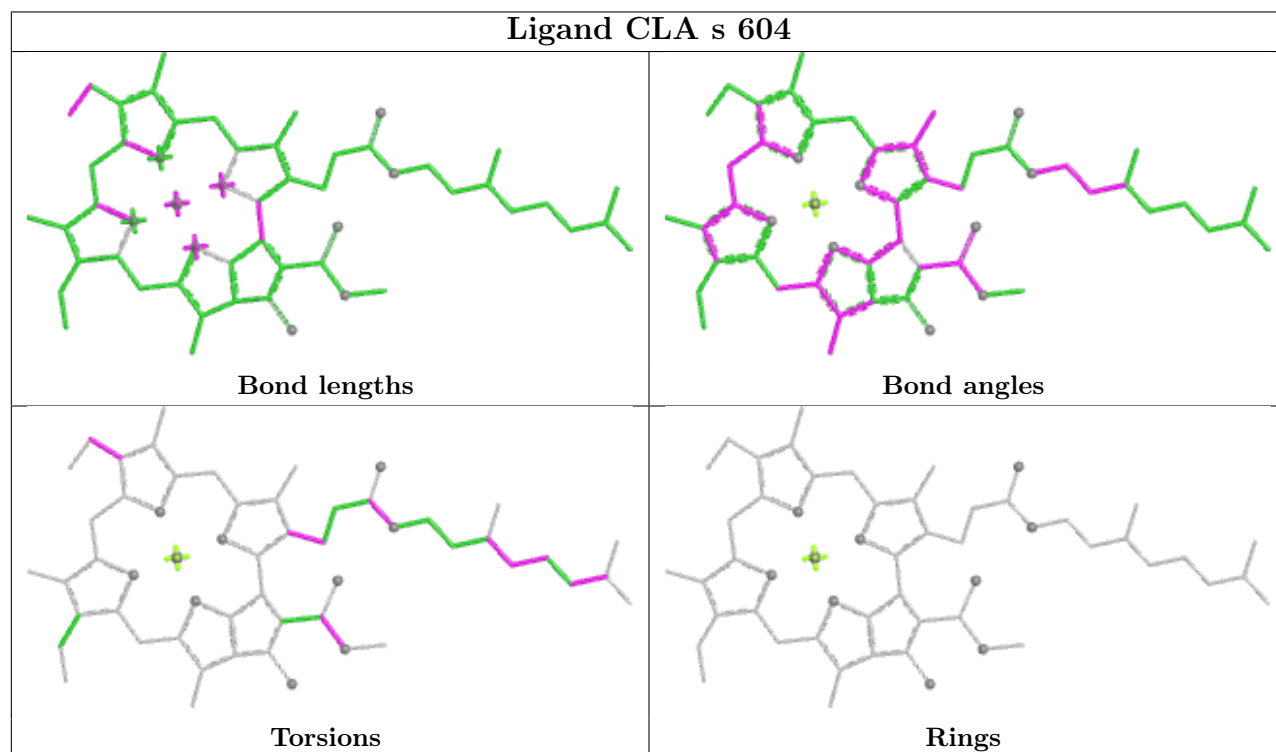
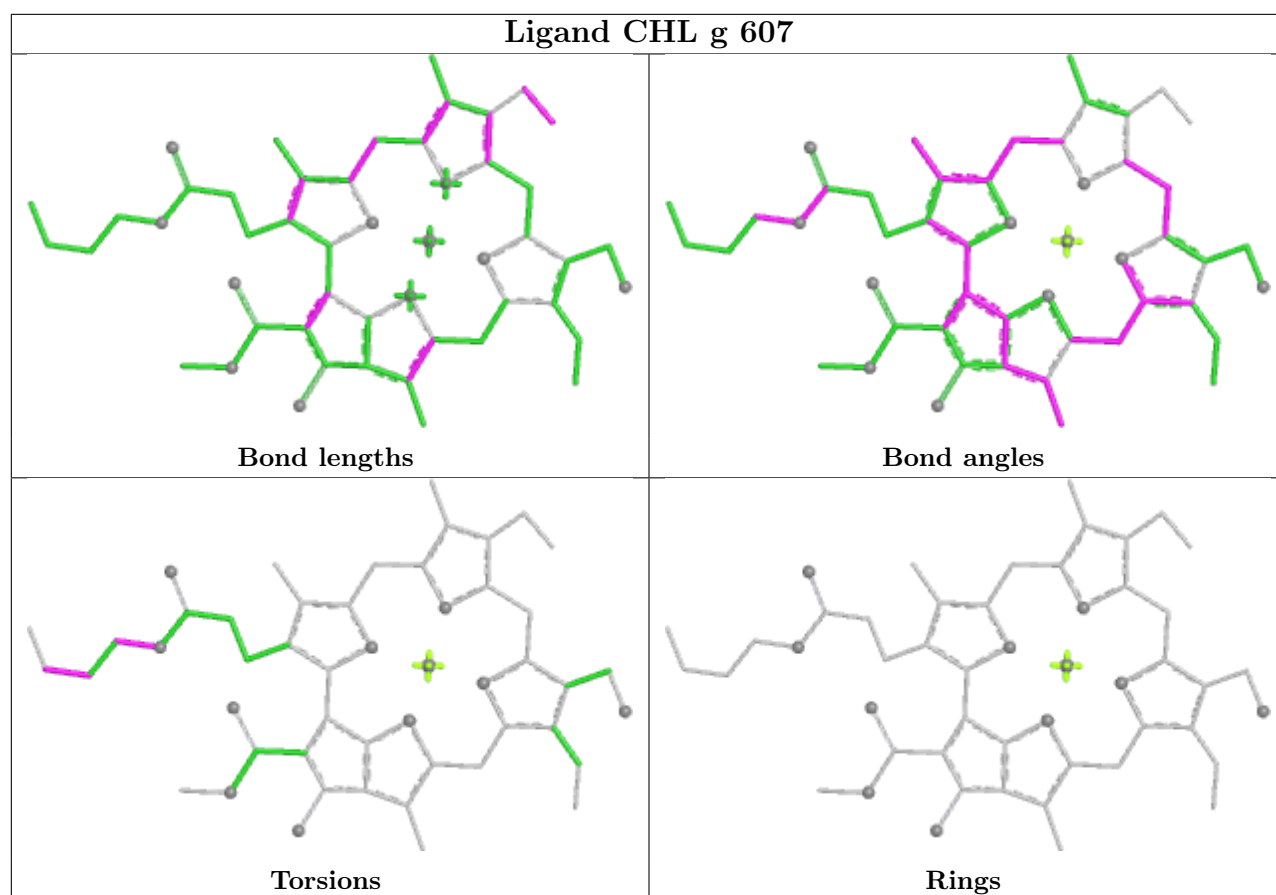
Ligand DGD C 519

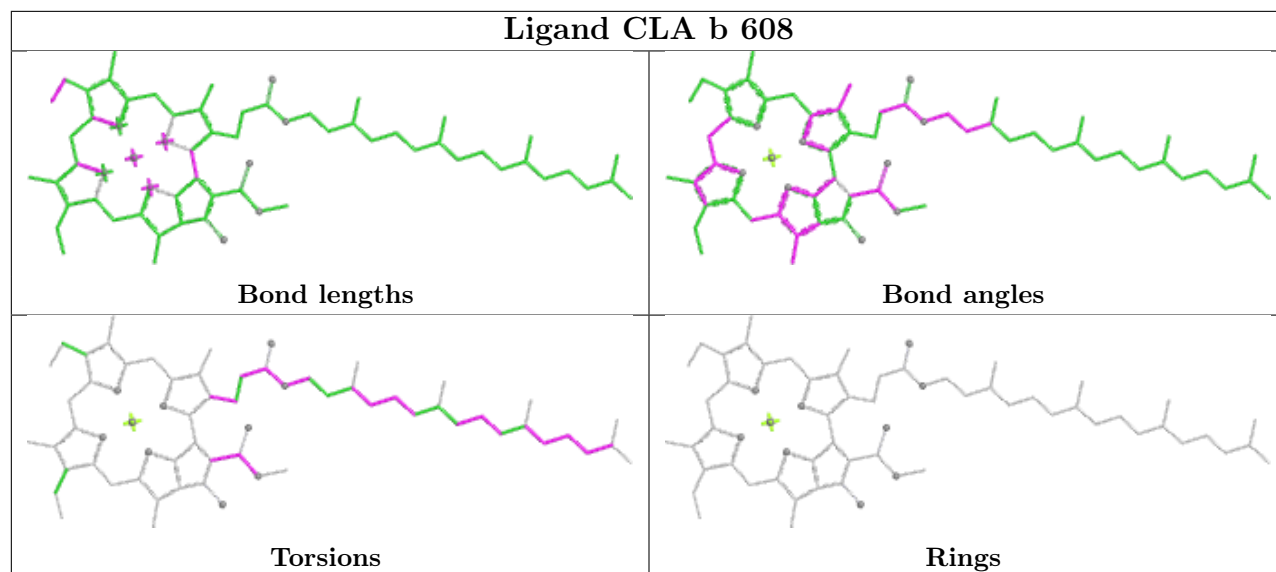
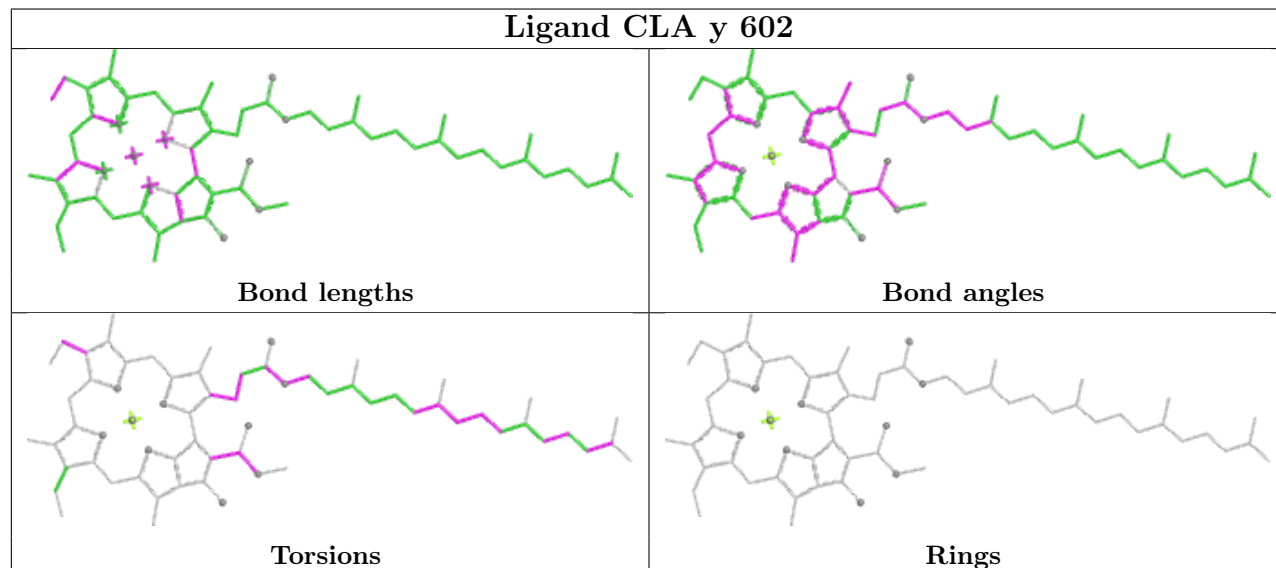


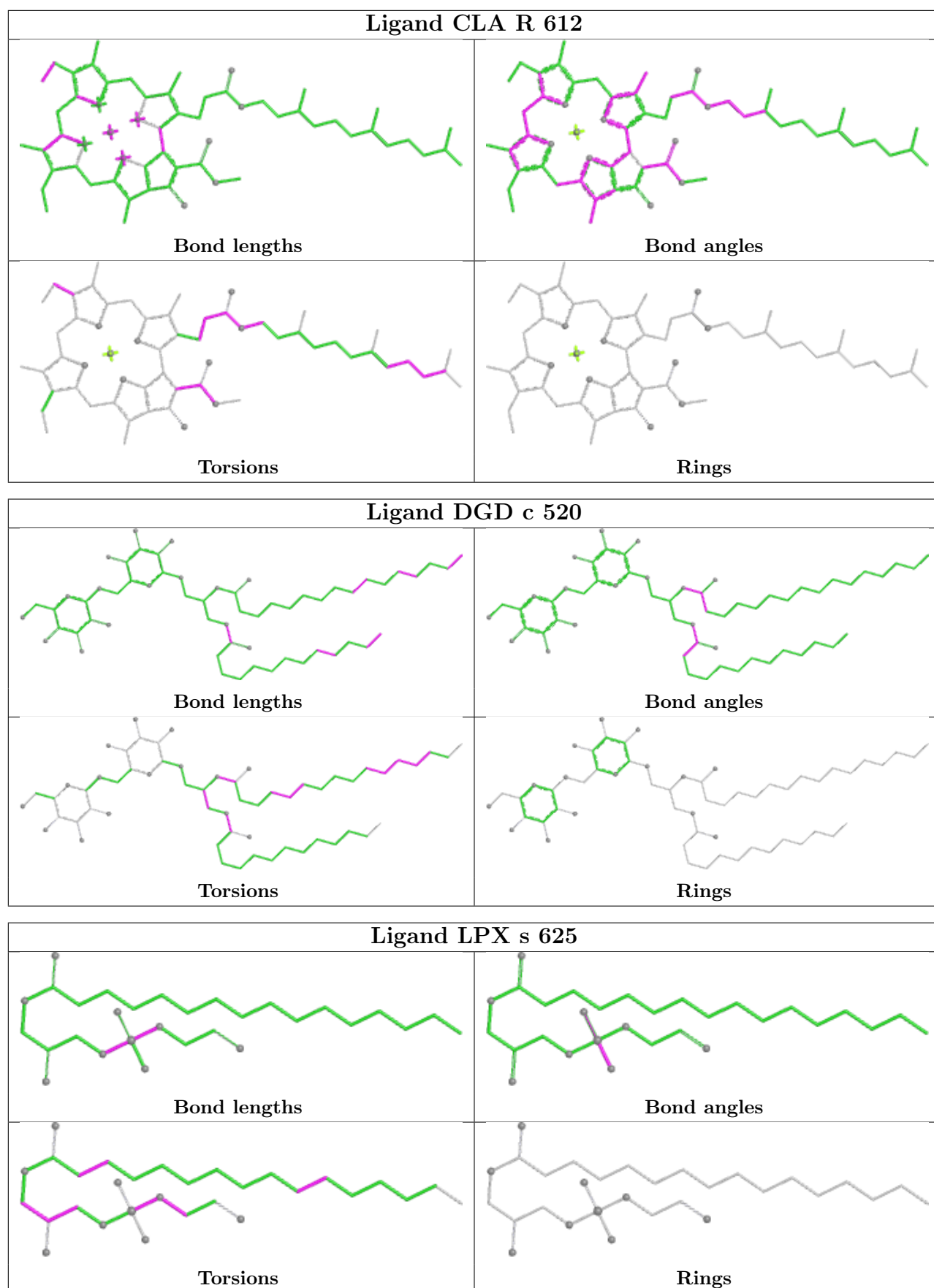
Ligand CLA r 609**Ligand CLA S 603**



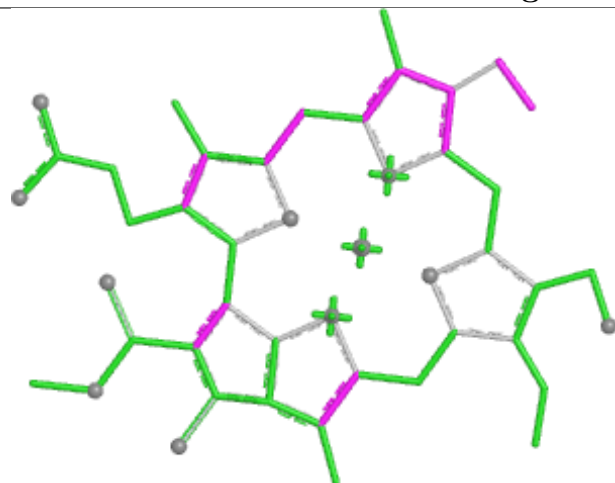




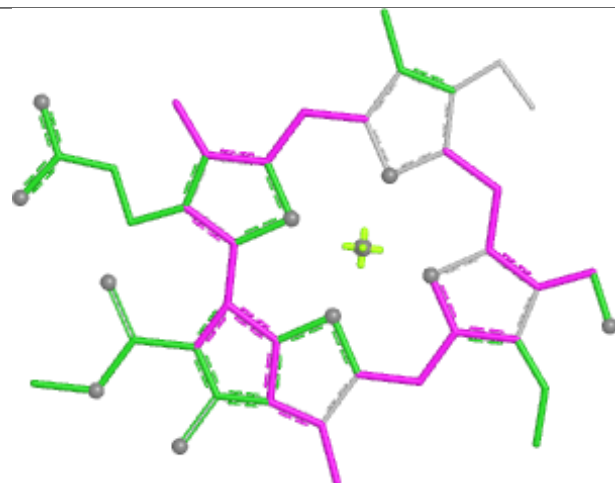
Ligand CLA b 608**Ligand CLA y 602**



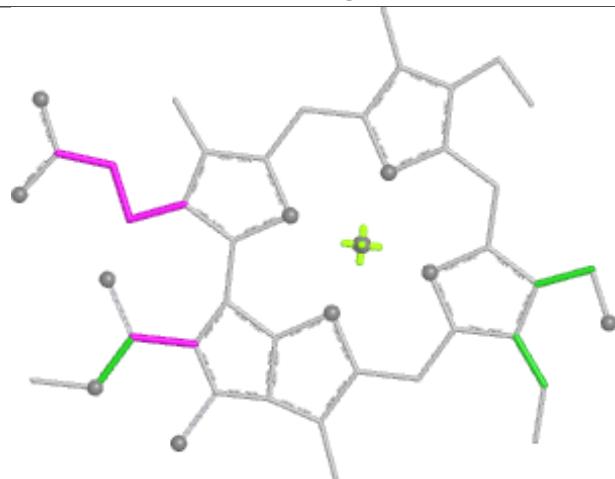
Ligand CHL s 601



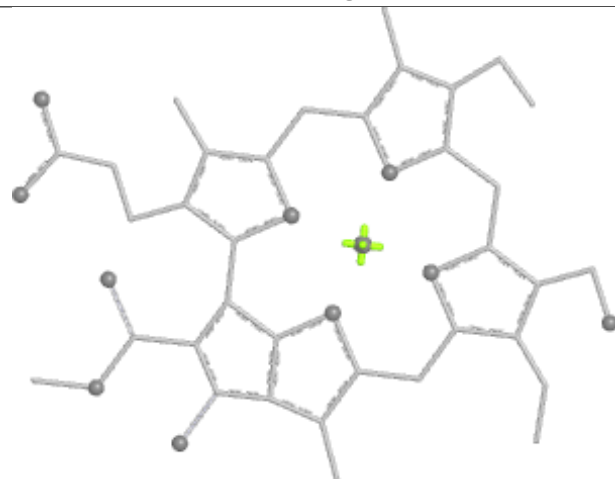
Bond lengths



Bond angles

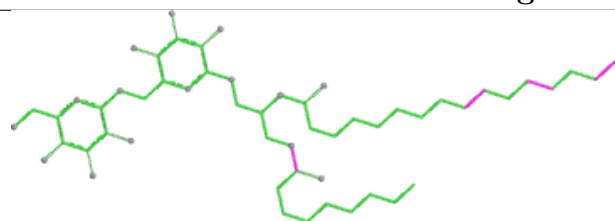


Torsions

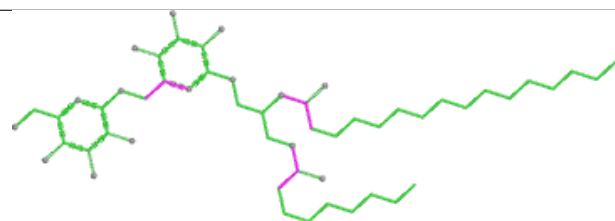


Rings

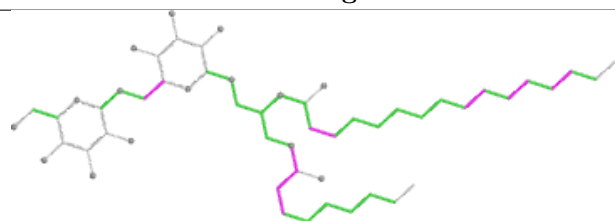
Ligand DGD c 518



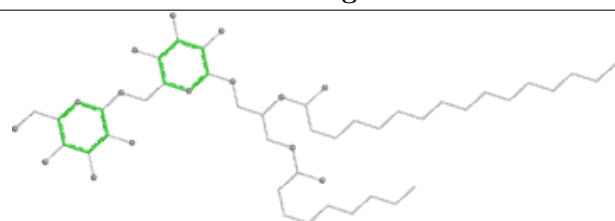
Bond lengths



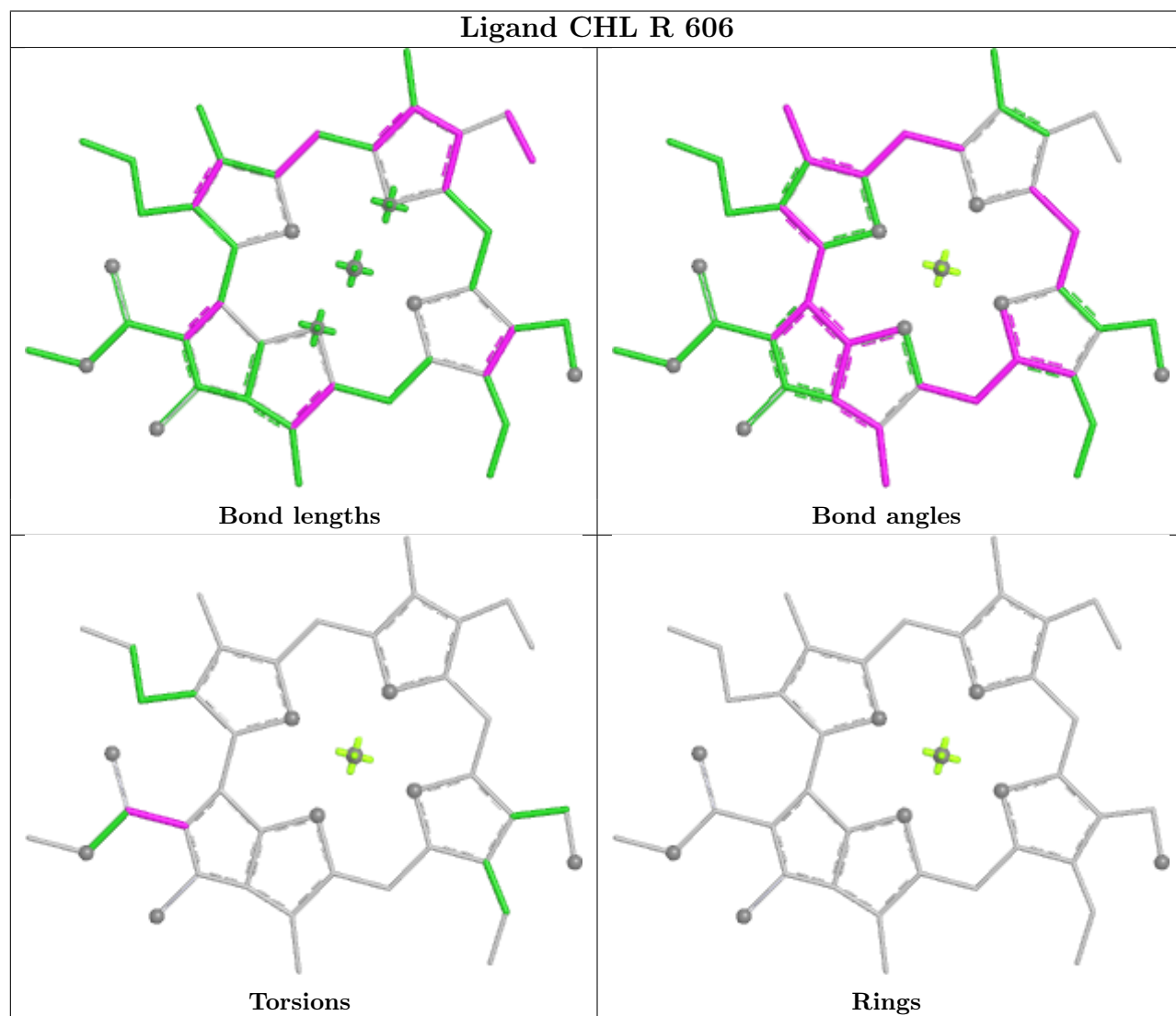
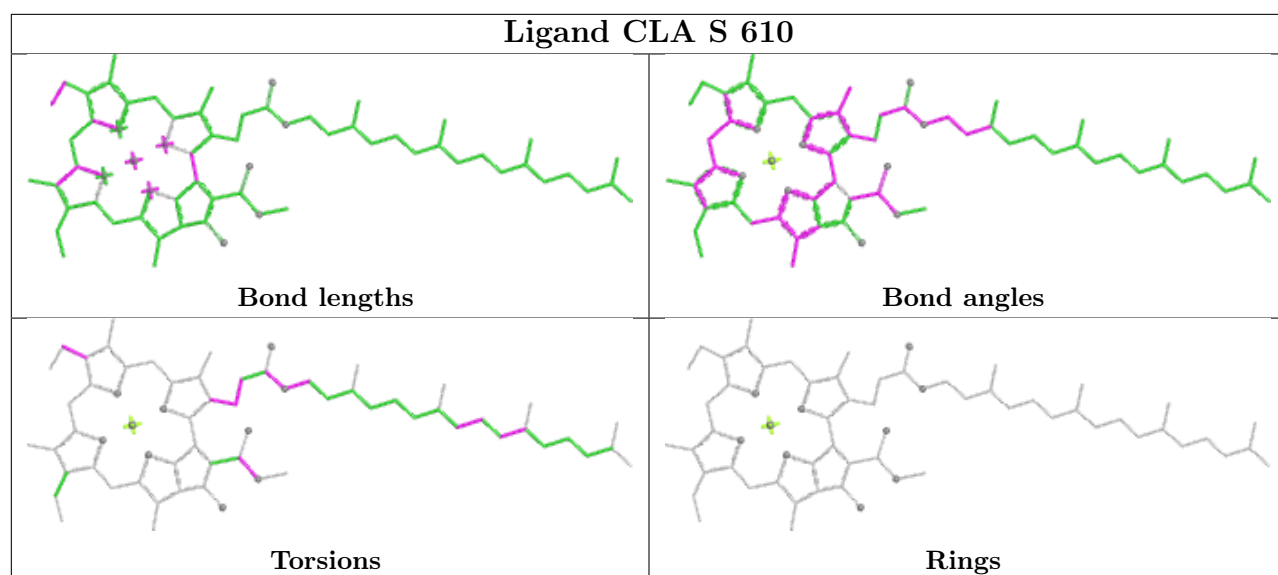
Bond angles

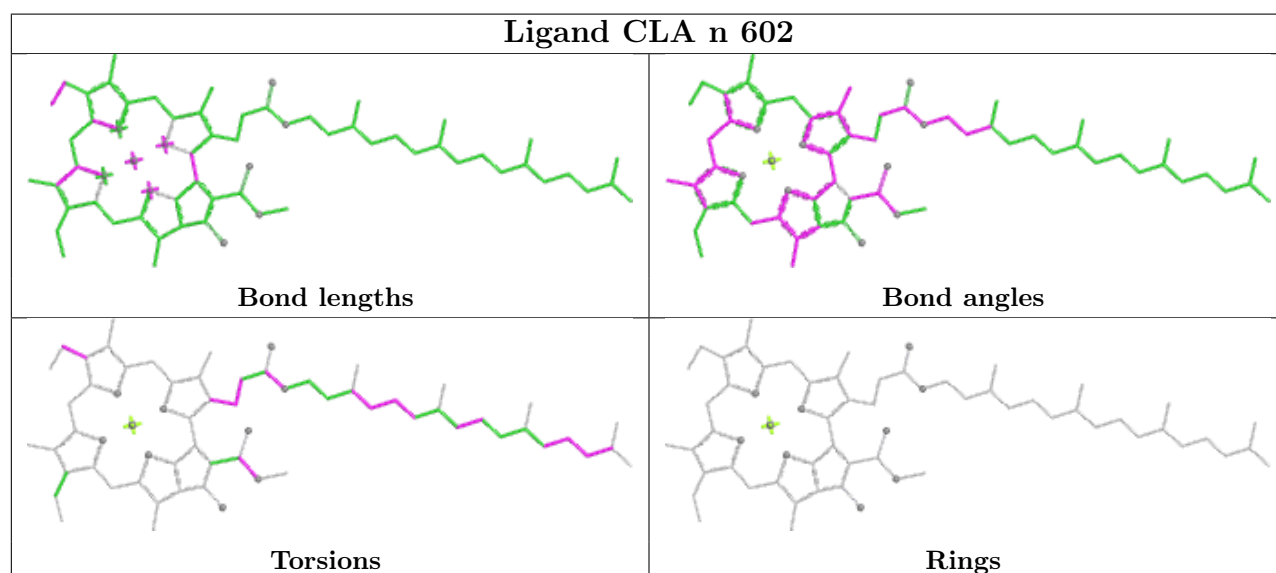
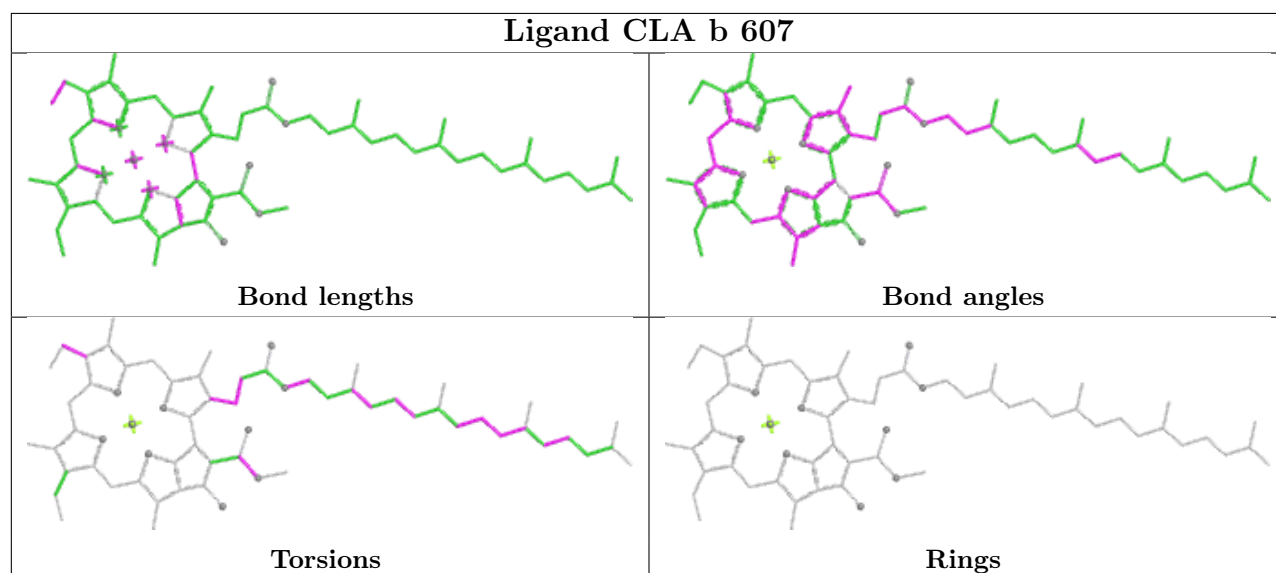
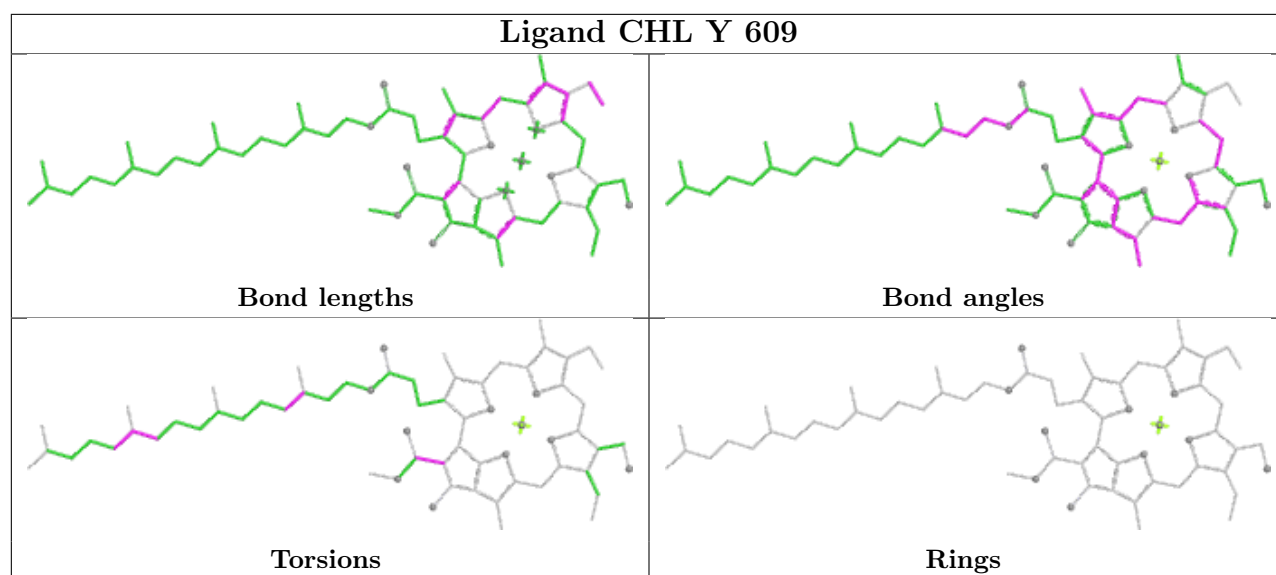


Torsions

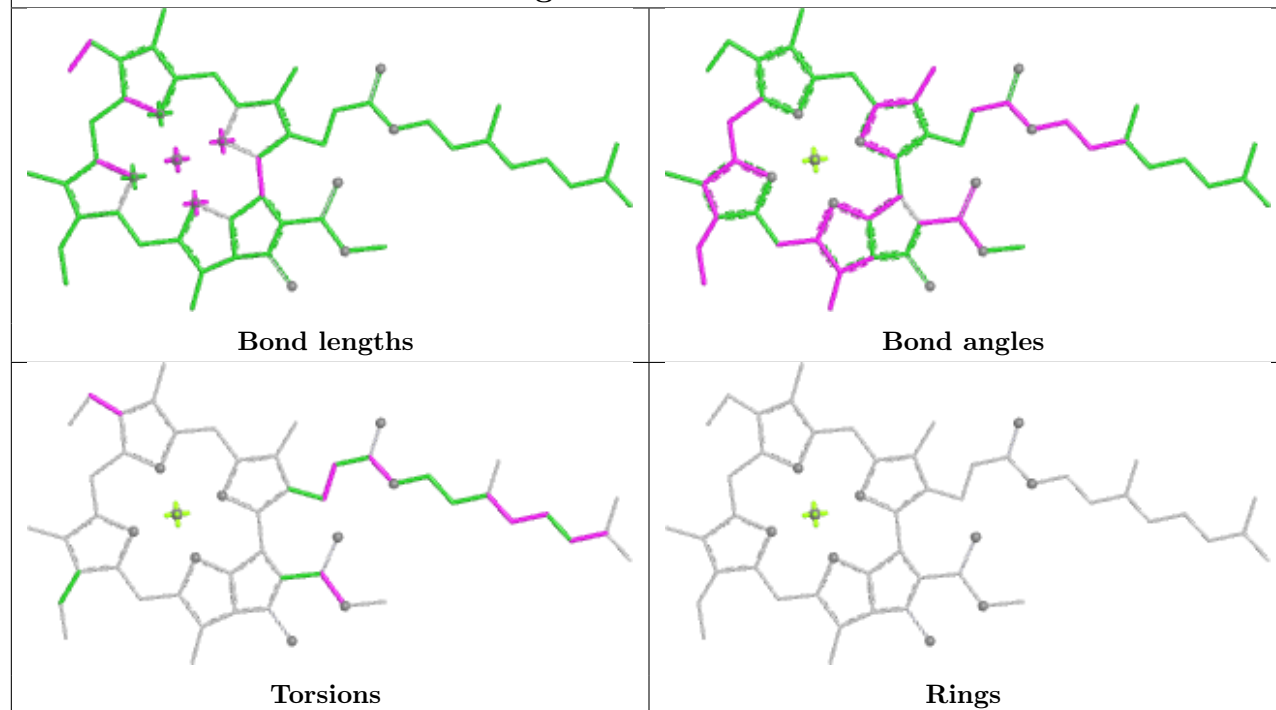


Rings

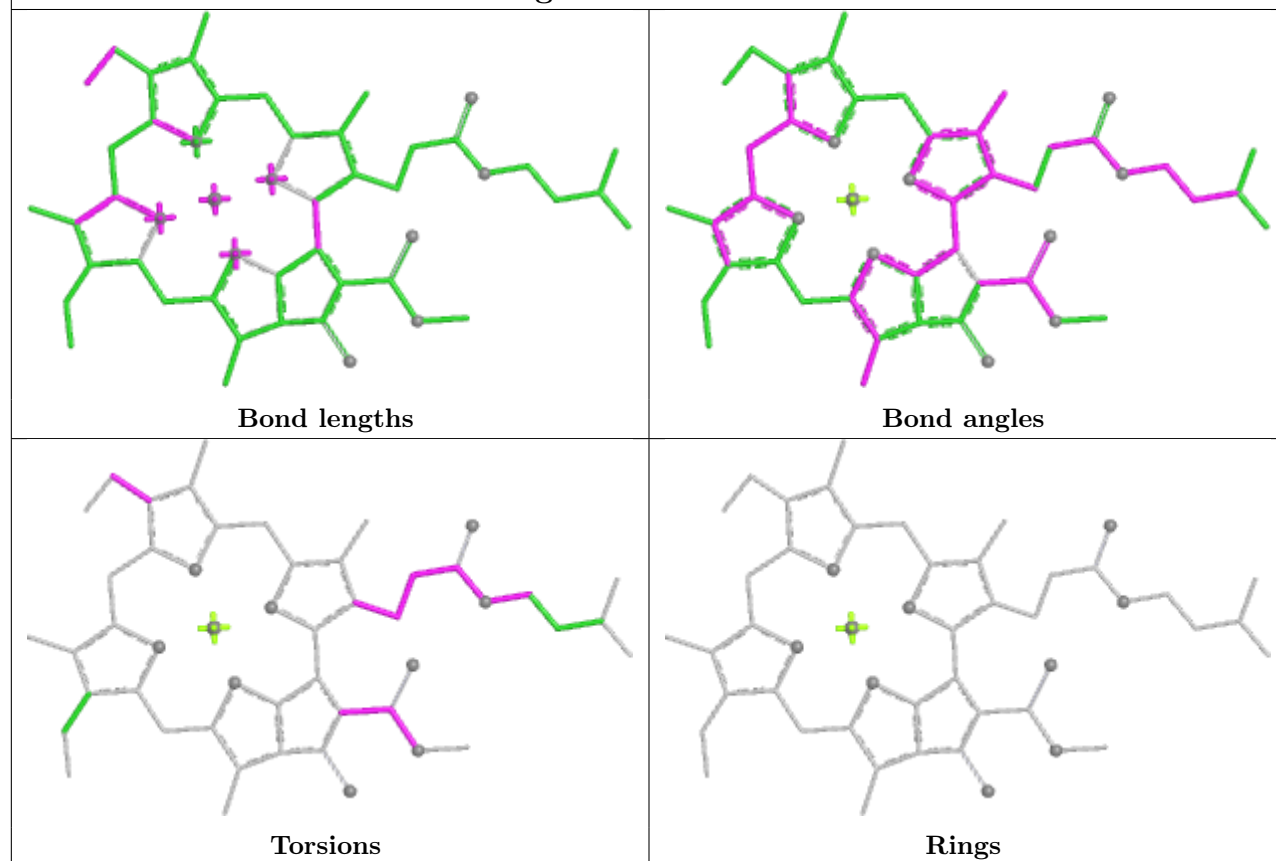


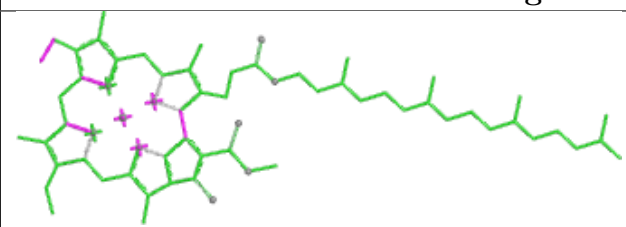
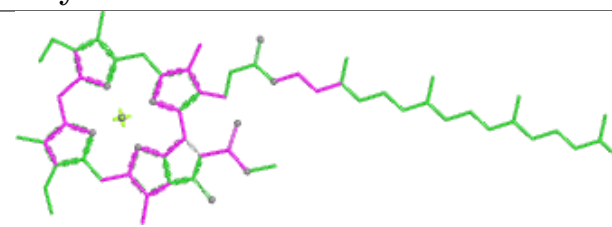
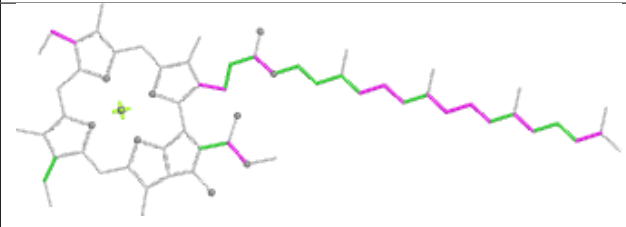
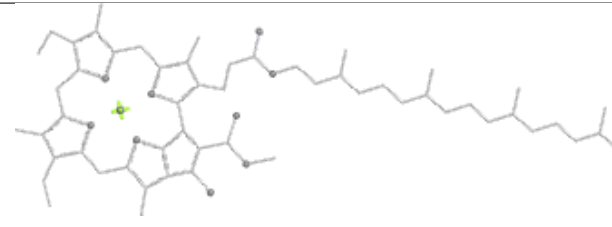


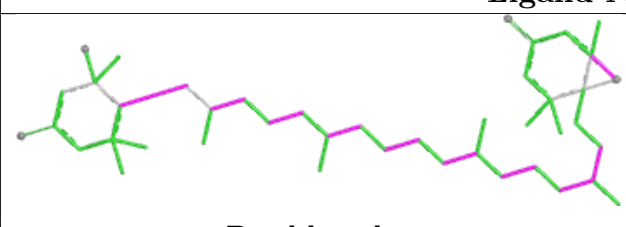
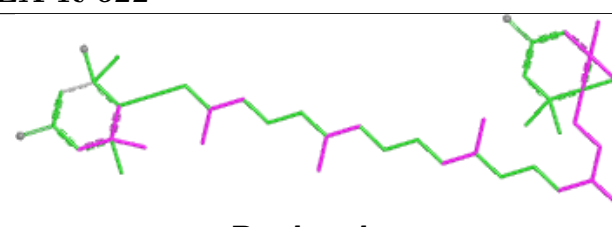
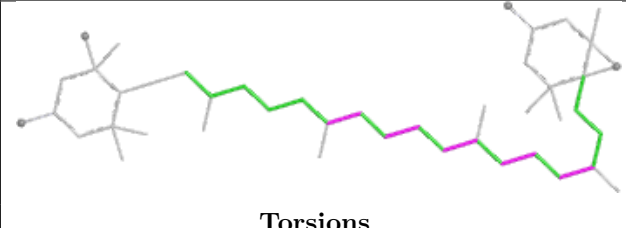
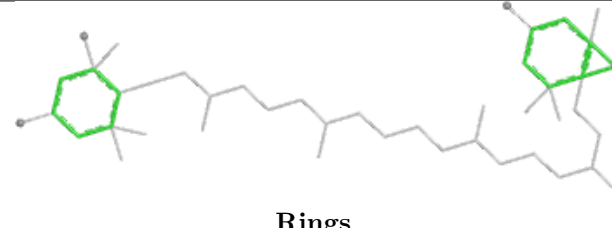
Ligand CLA S 604

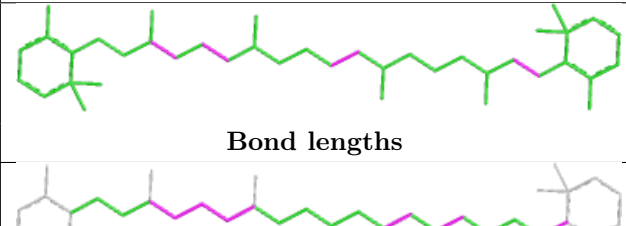
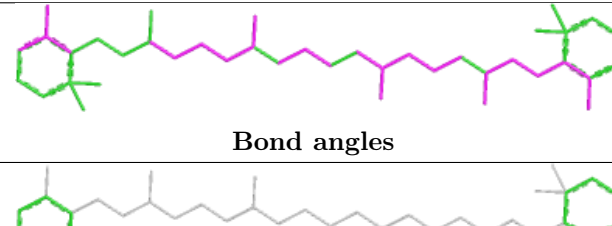


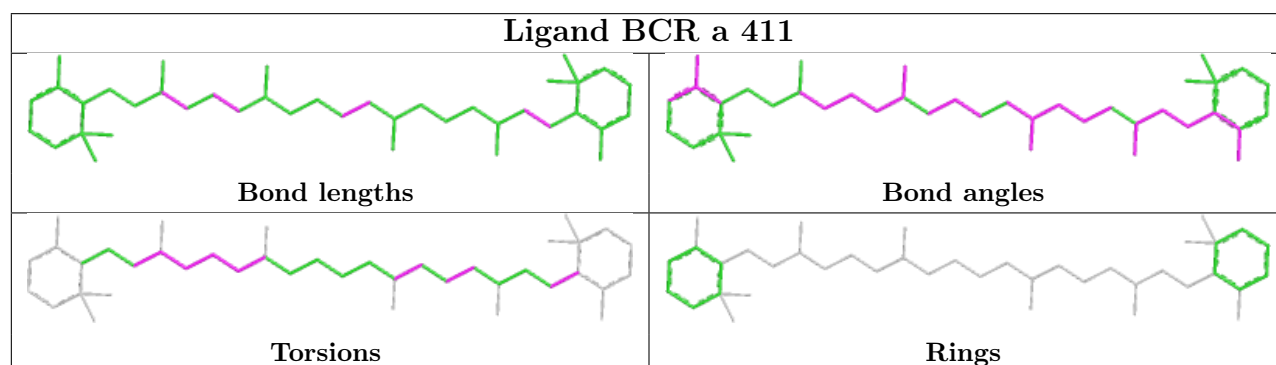
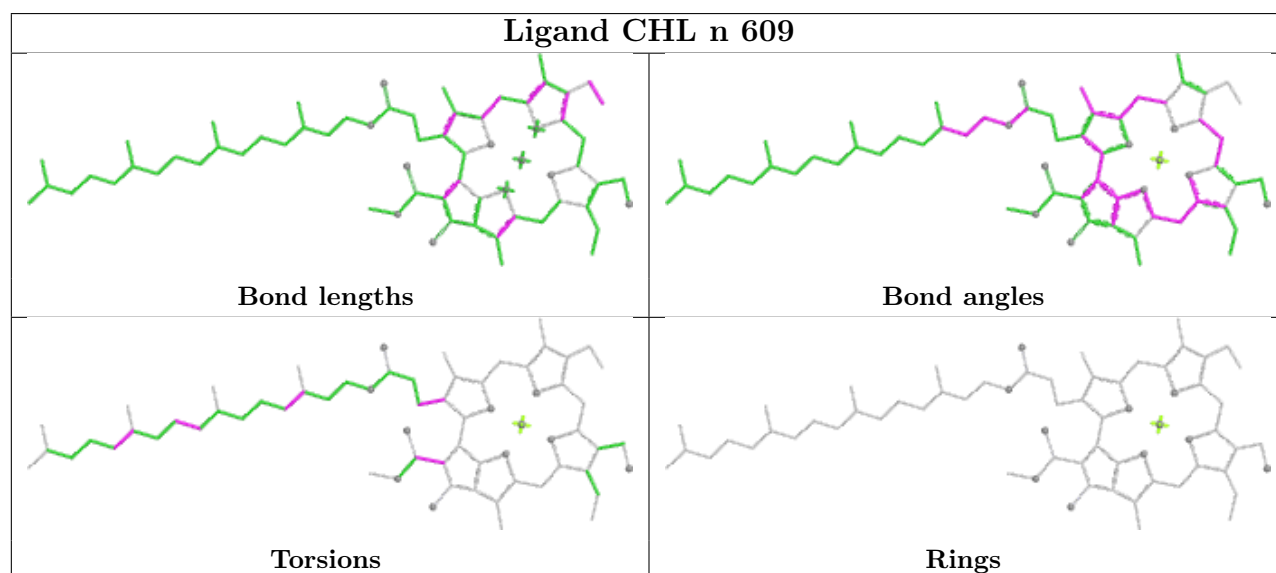
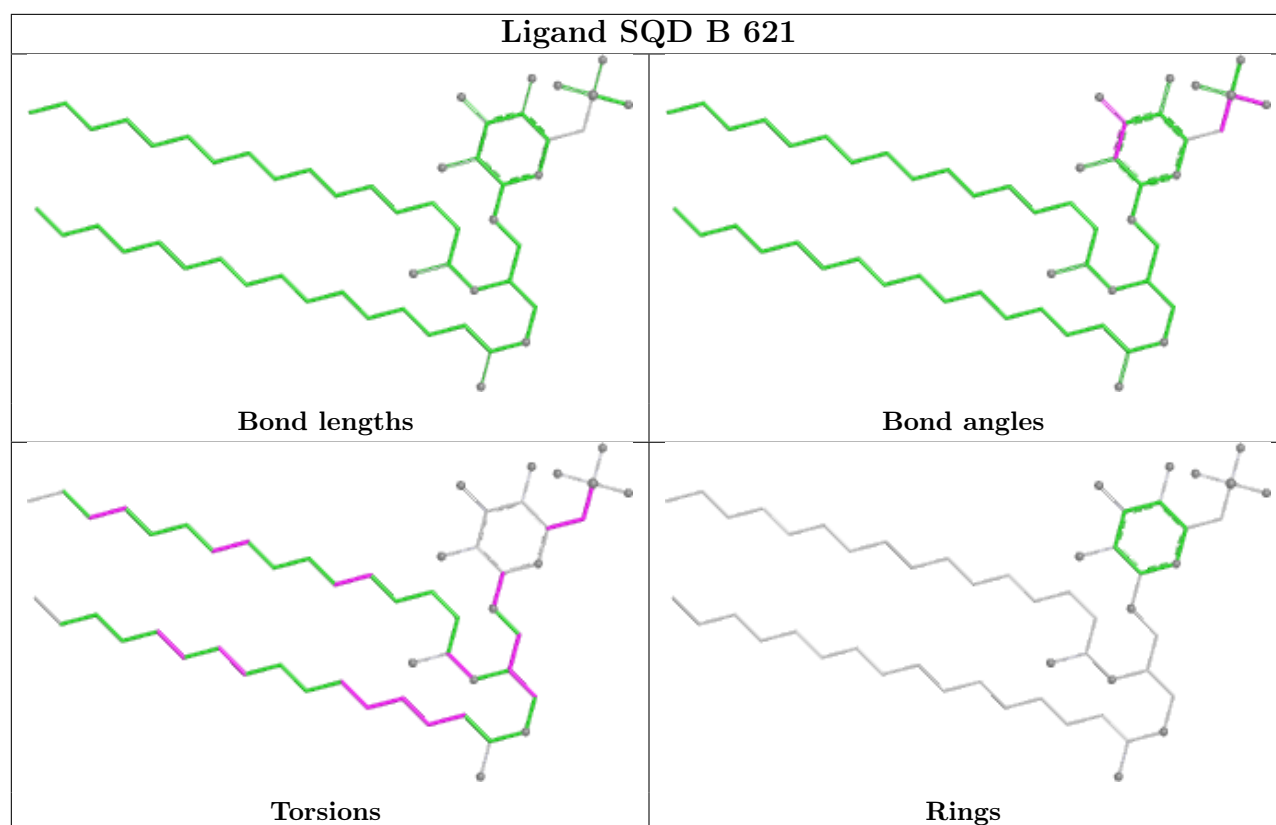
Ligand CLA S 605

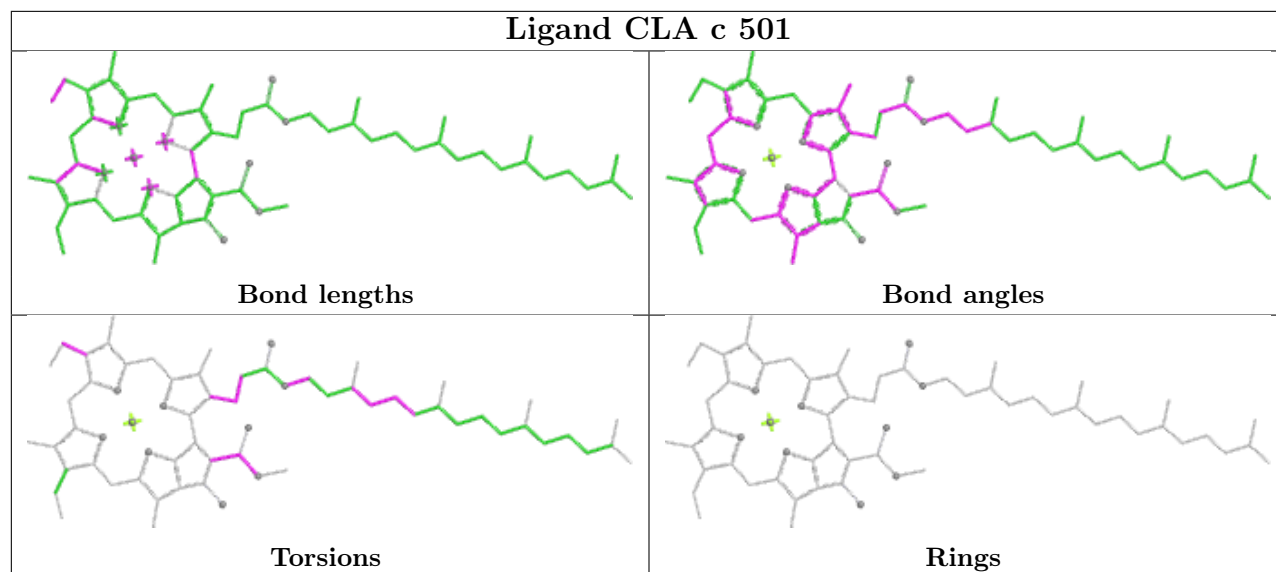
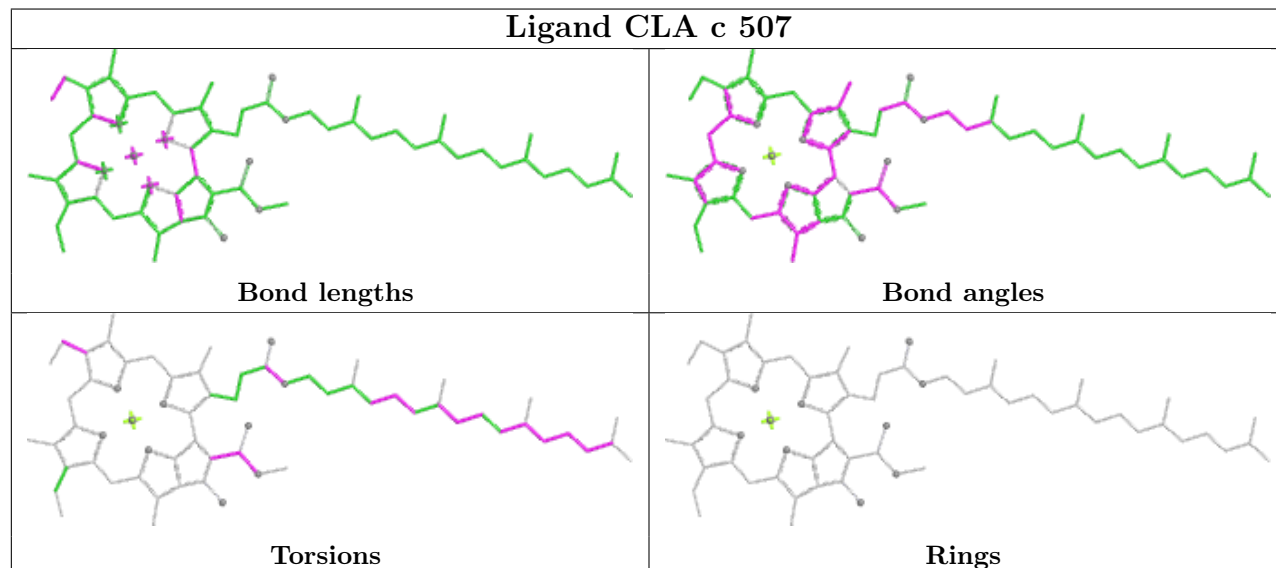


Ligand CLA y 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

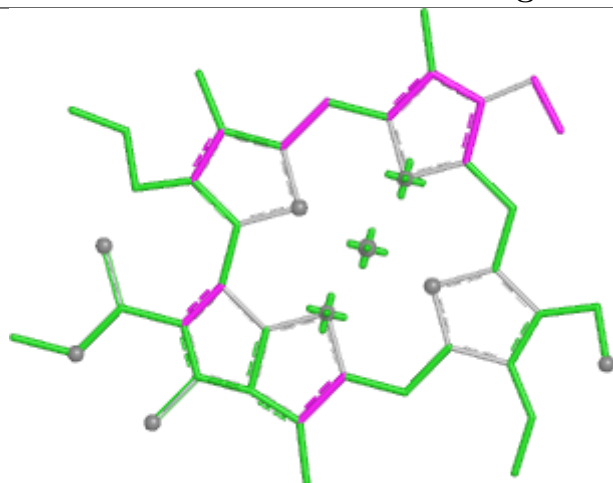
Ligand NEX R 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

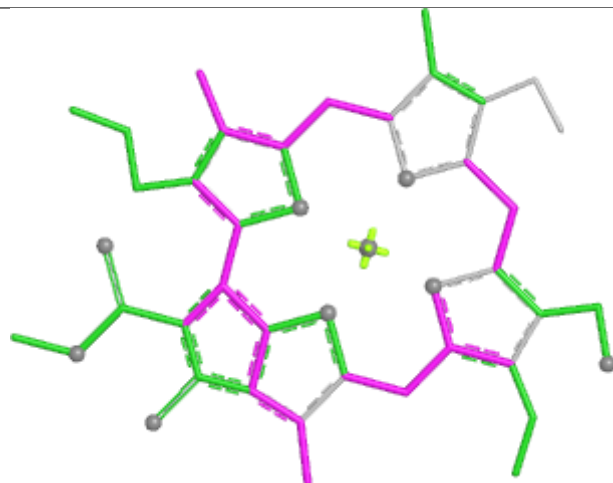


Ligand CLA c 501**Ligand CLA c 507**

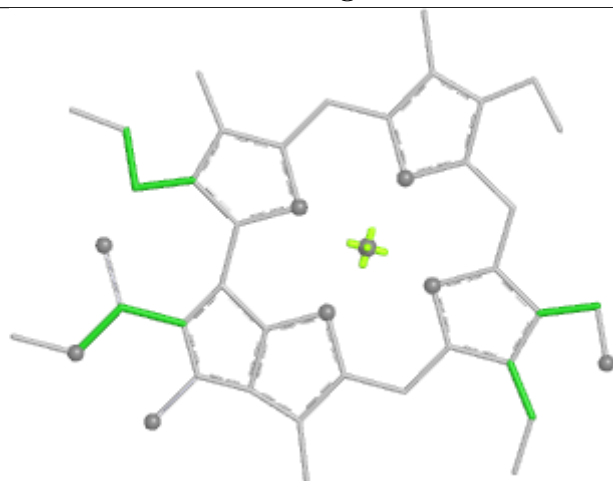
Ligand CHL S 606



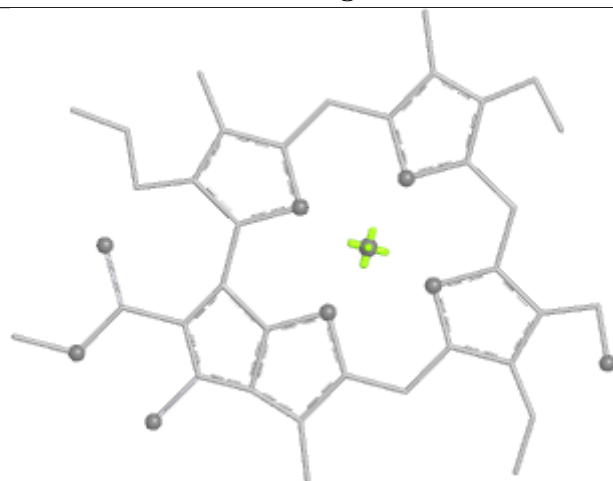
Bond lengths



Bond angles

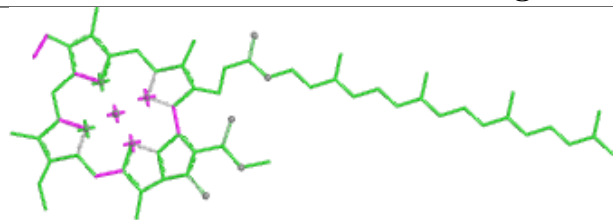


Torsions

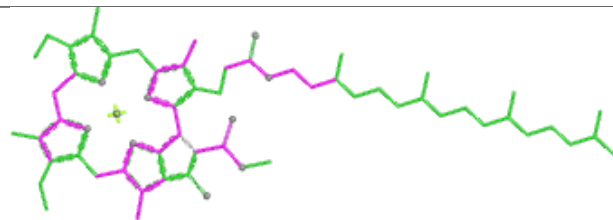


Rings

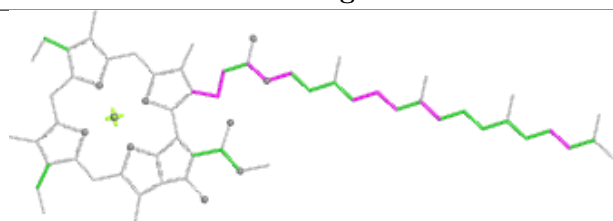
Ligand CLA A 406



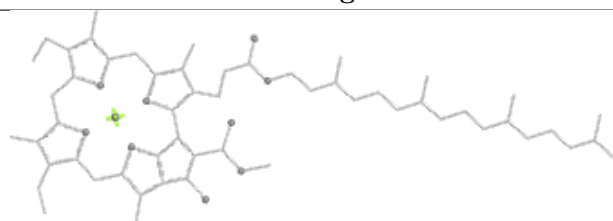
Bond lengths



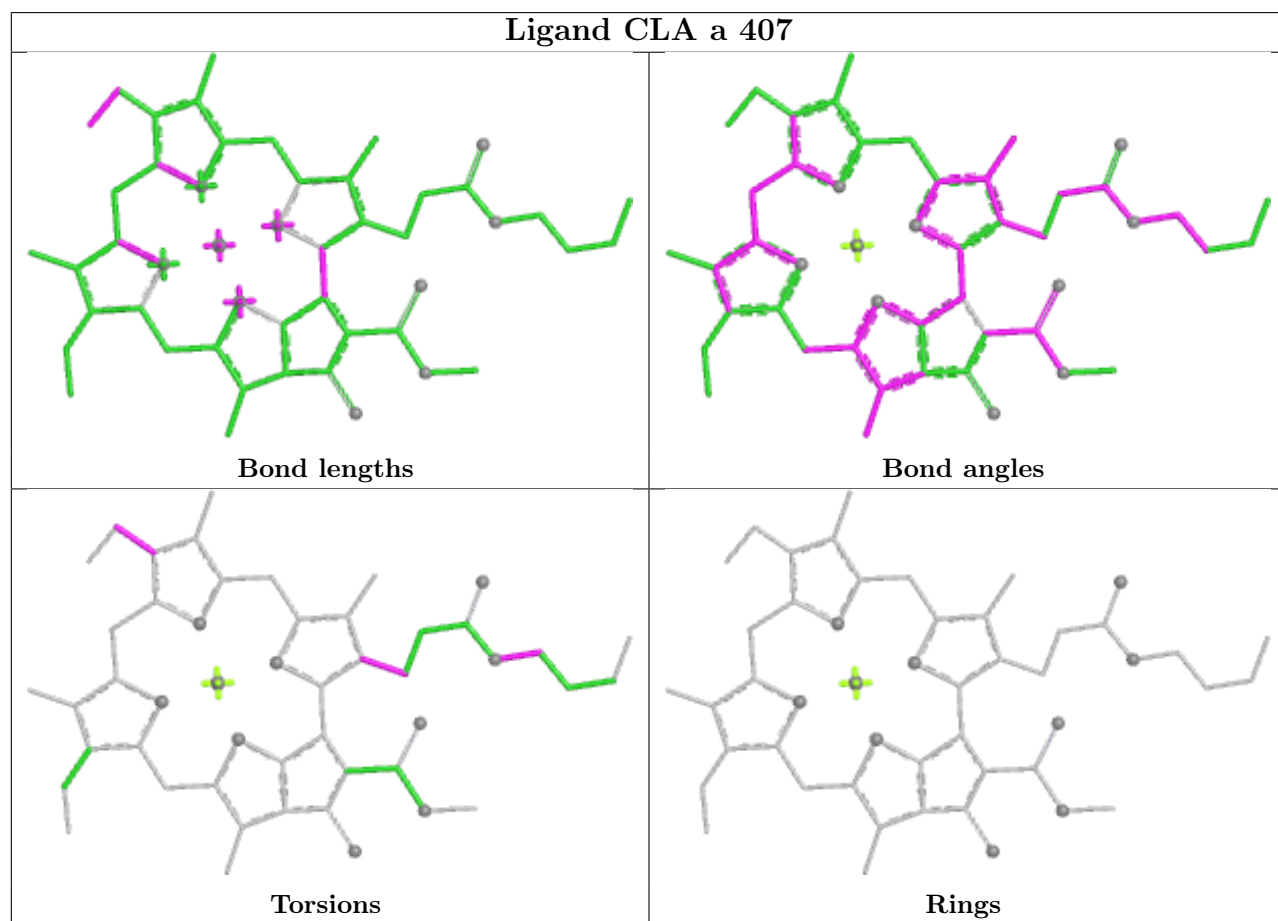
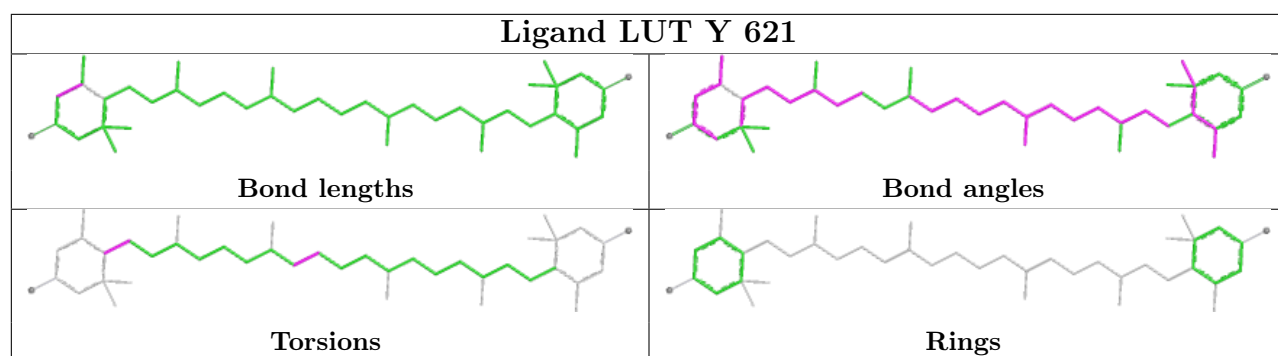
Bond angles

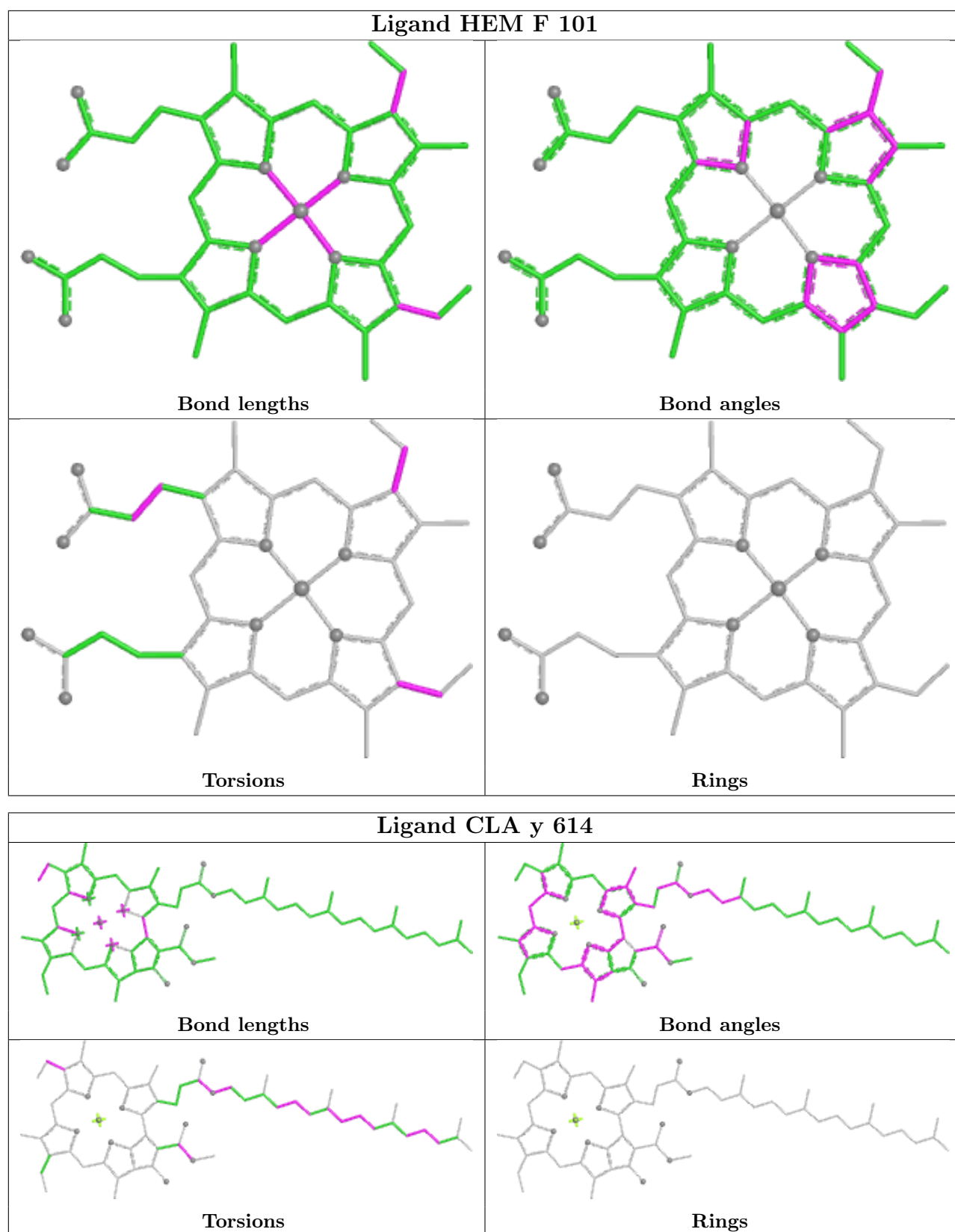


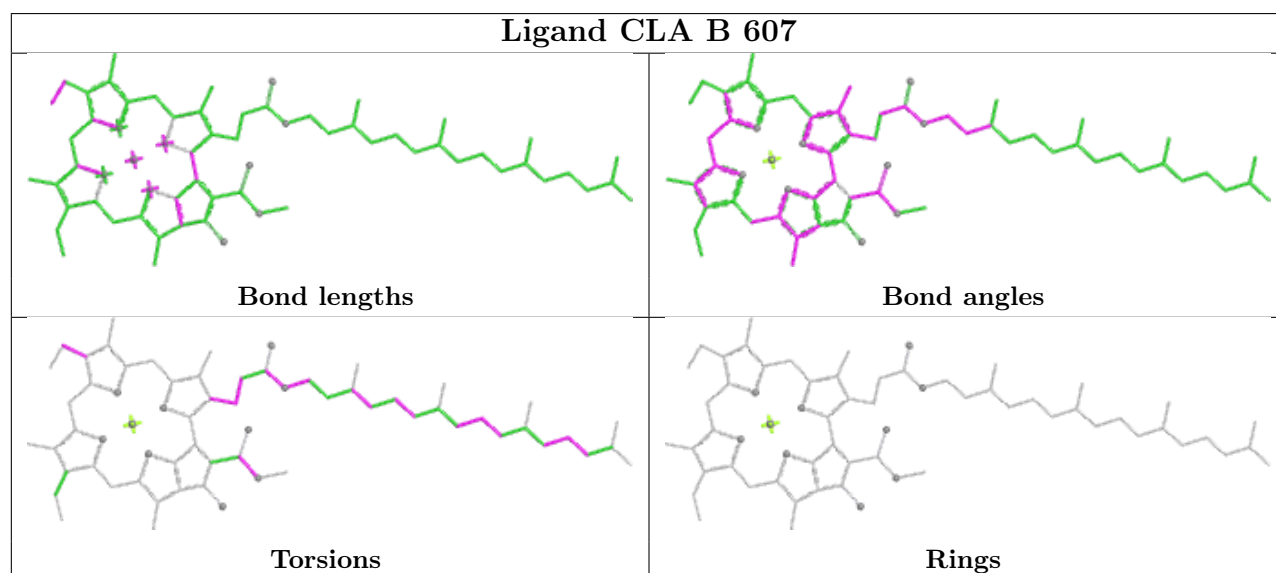
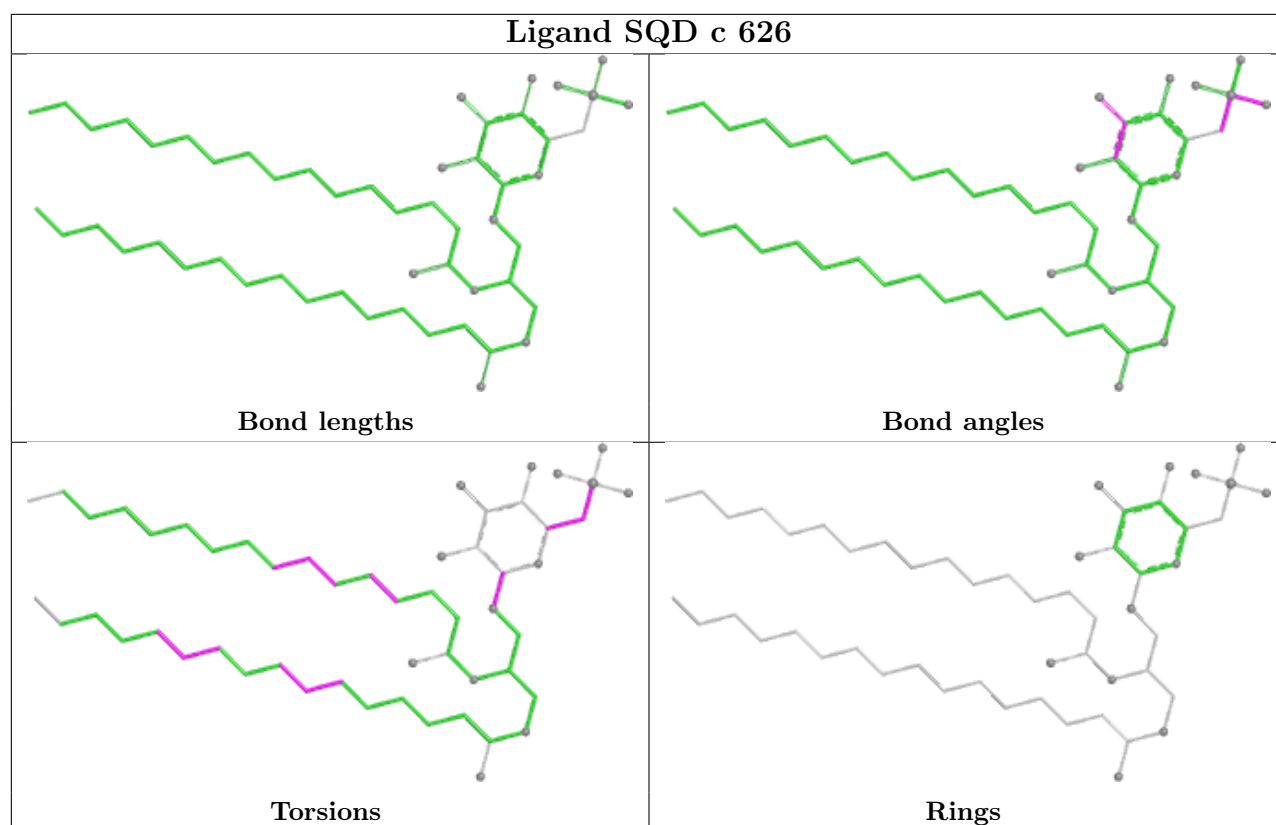
Torsions

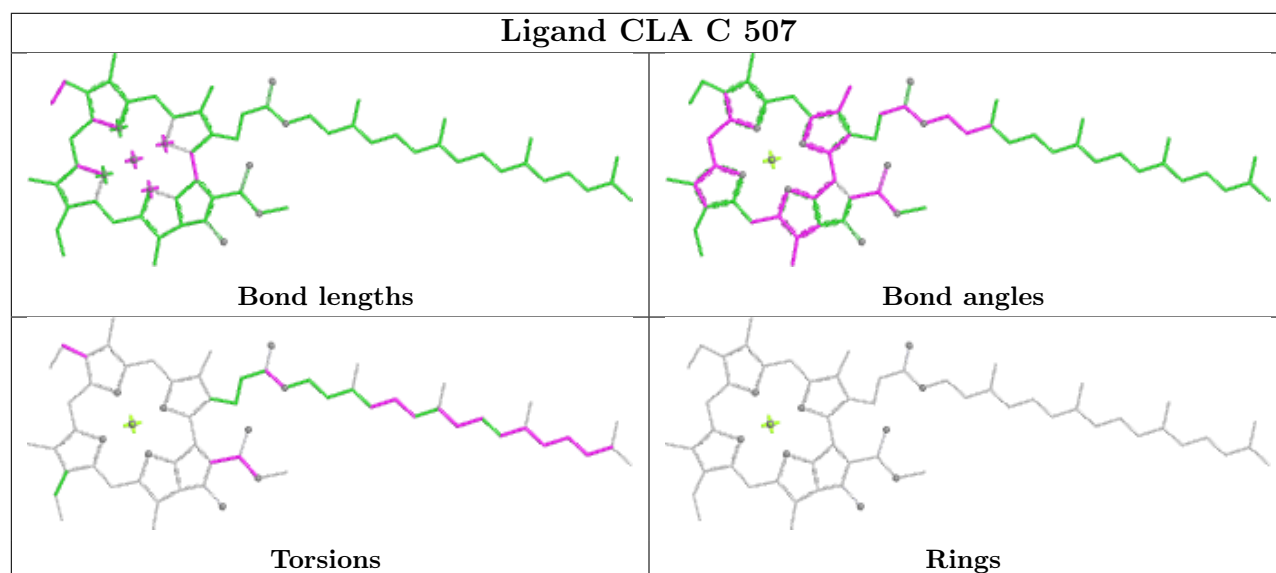
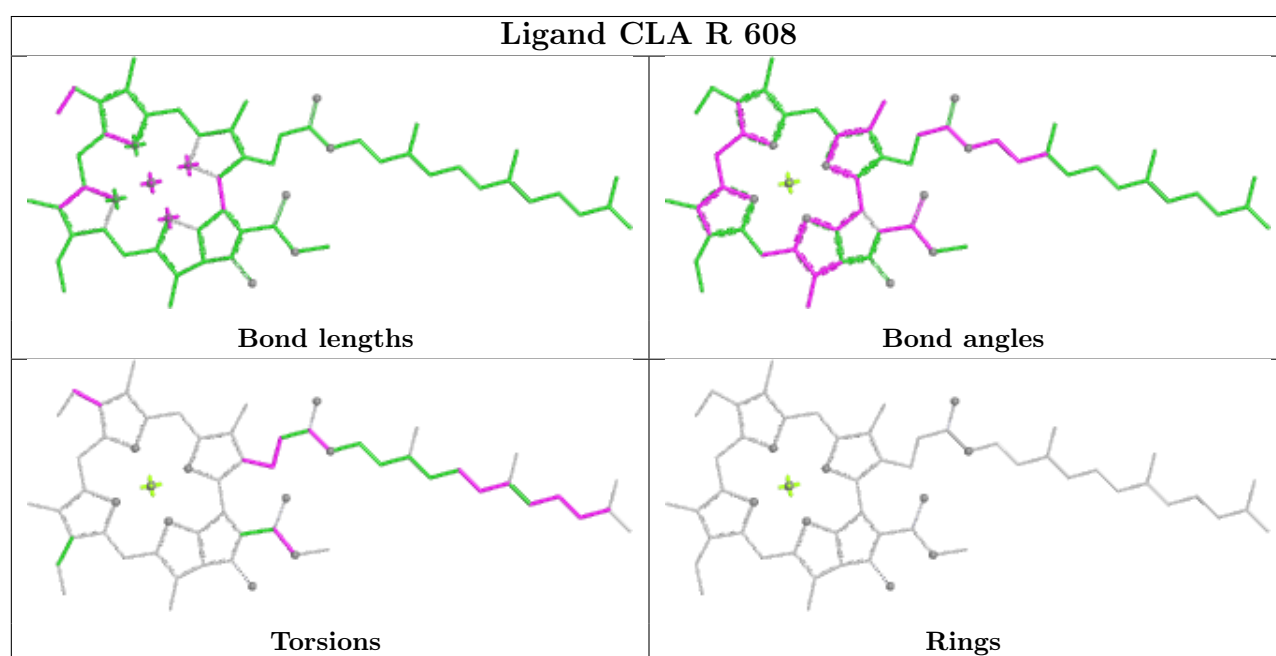
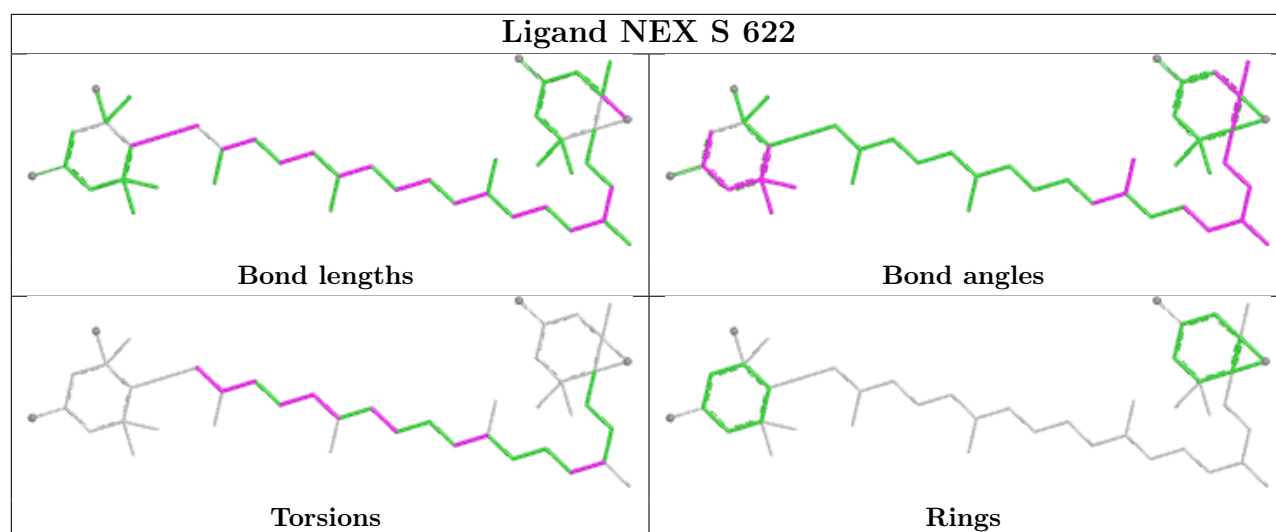


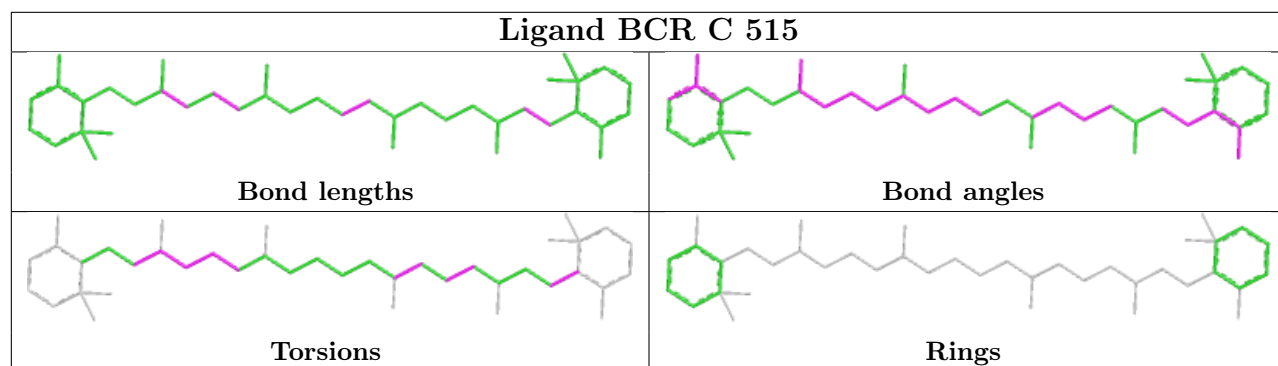
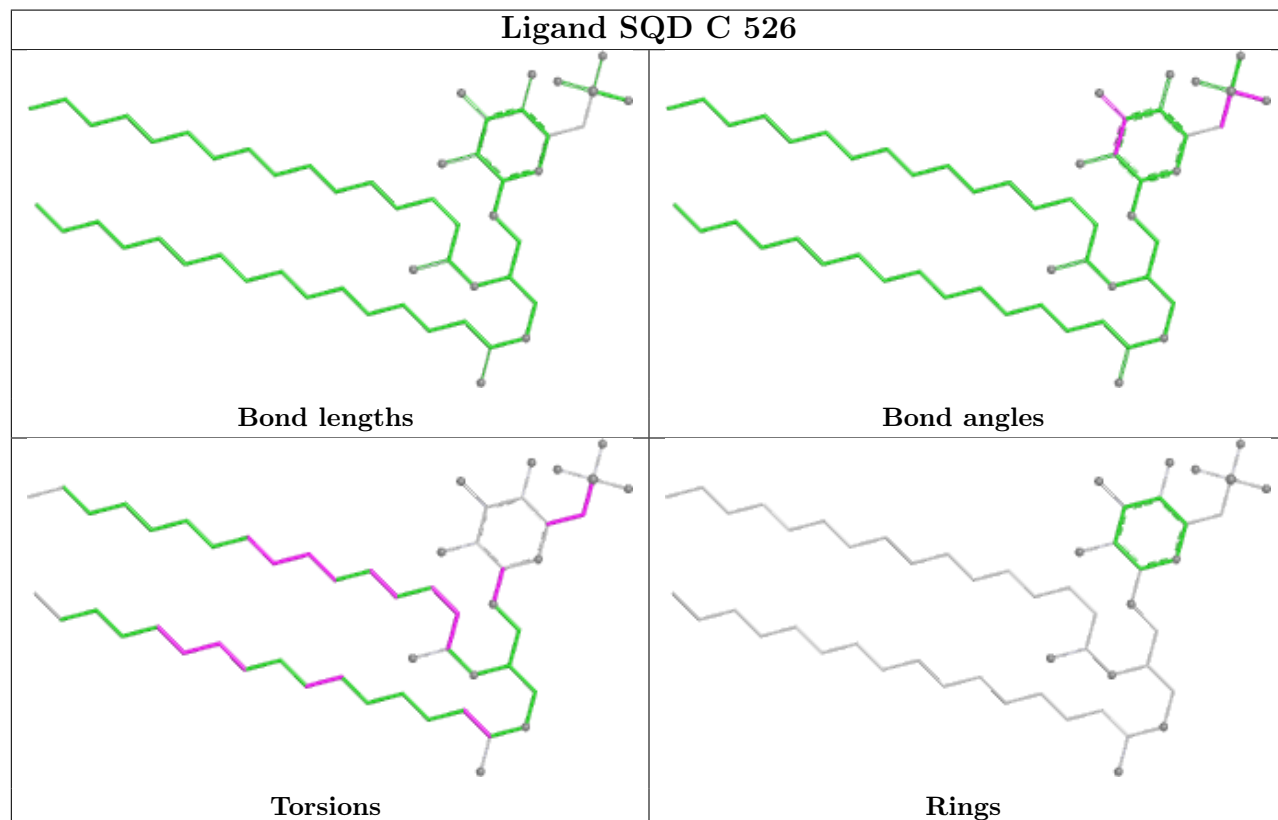
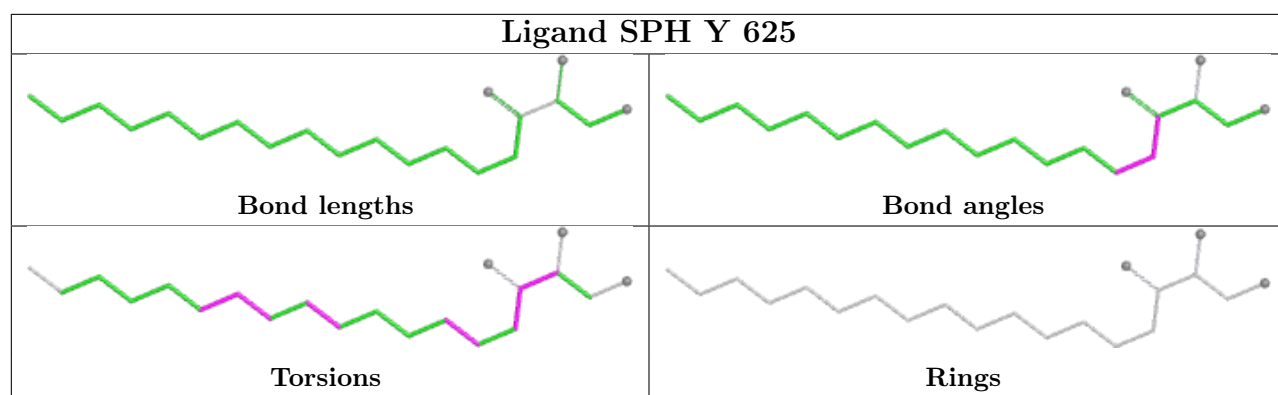
Rings

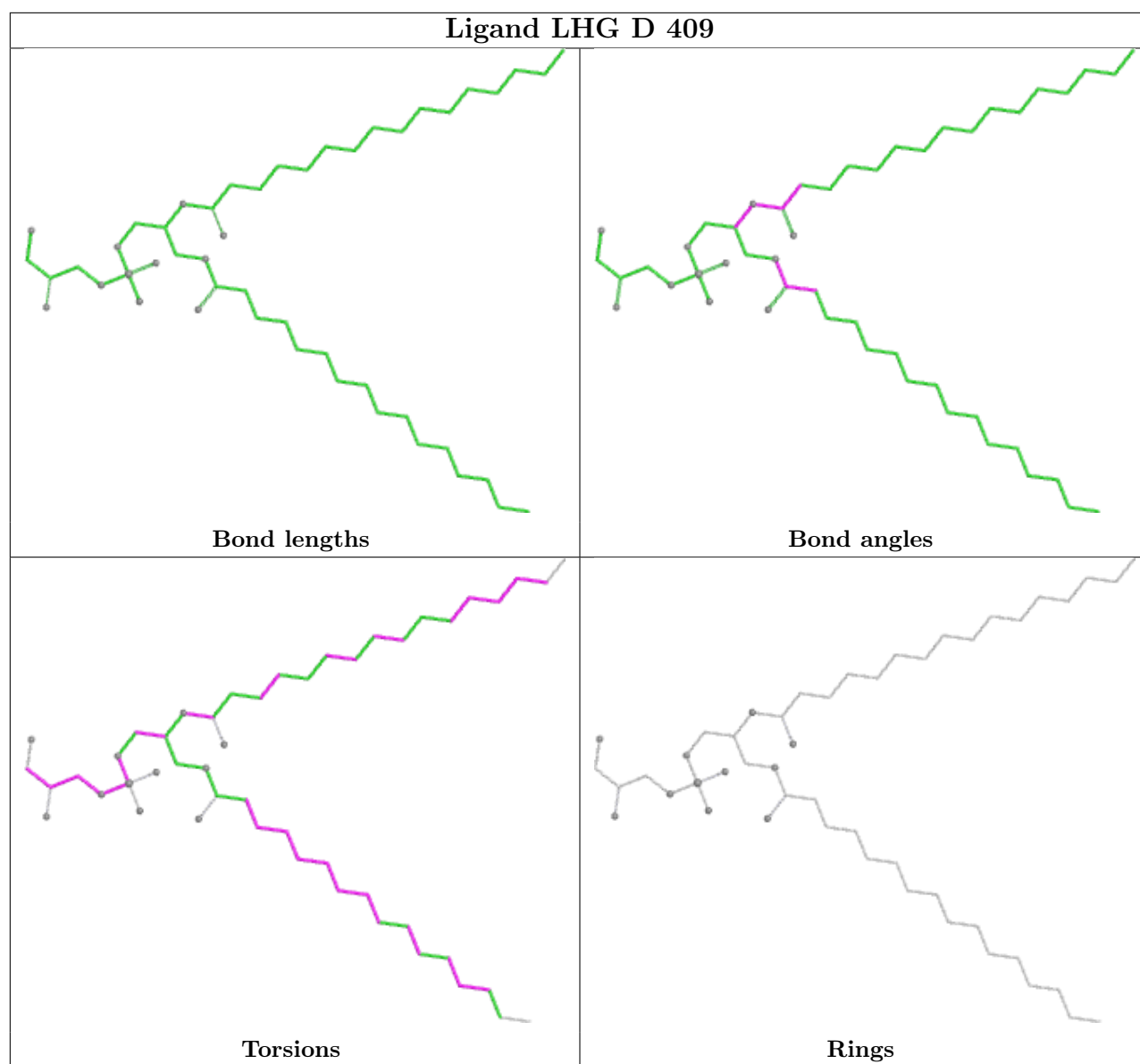


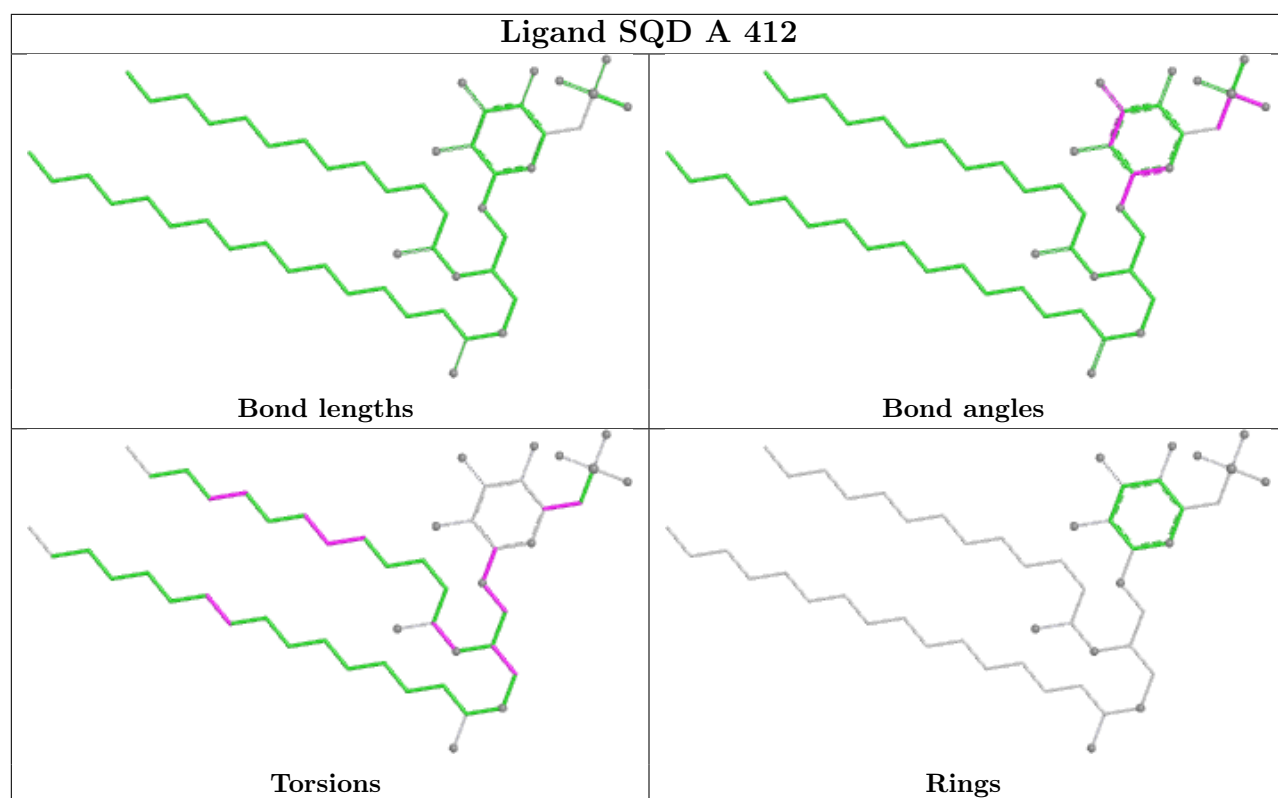


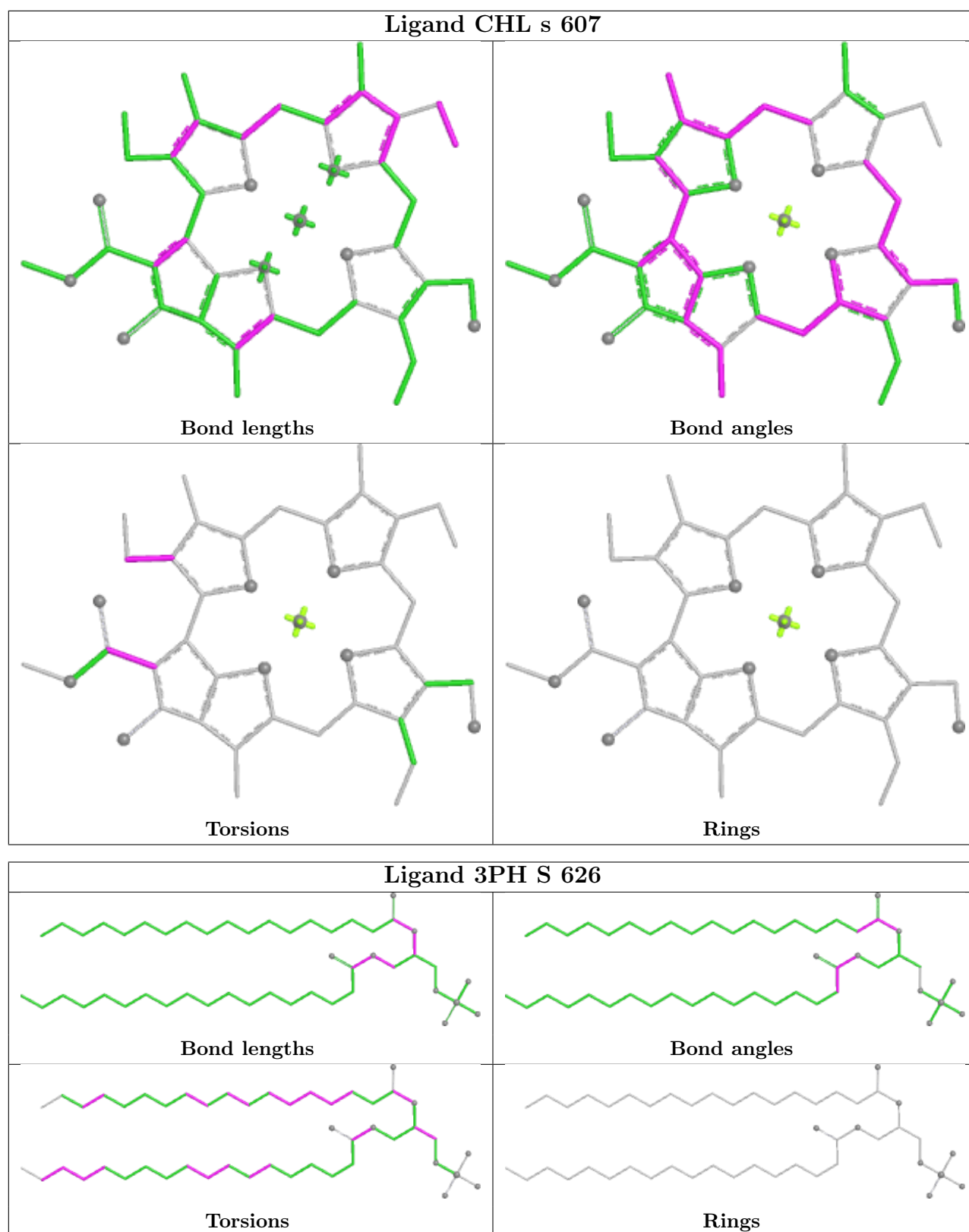


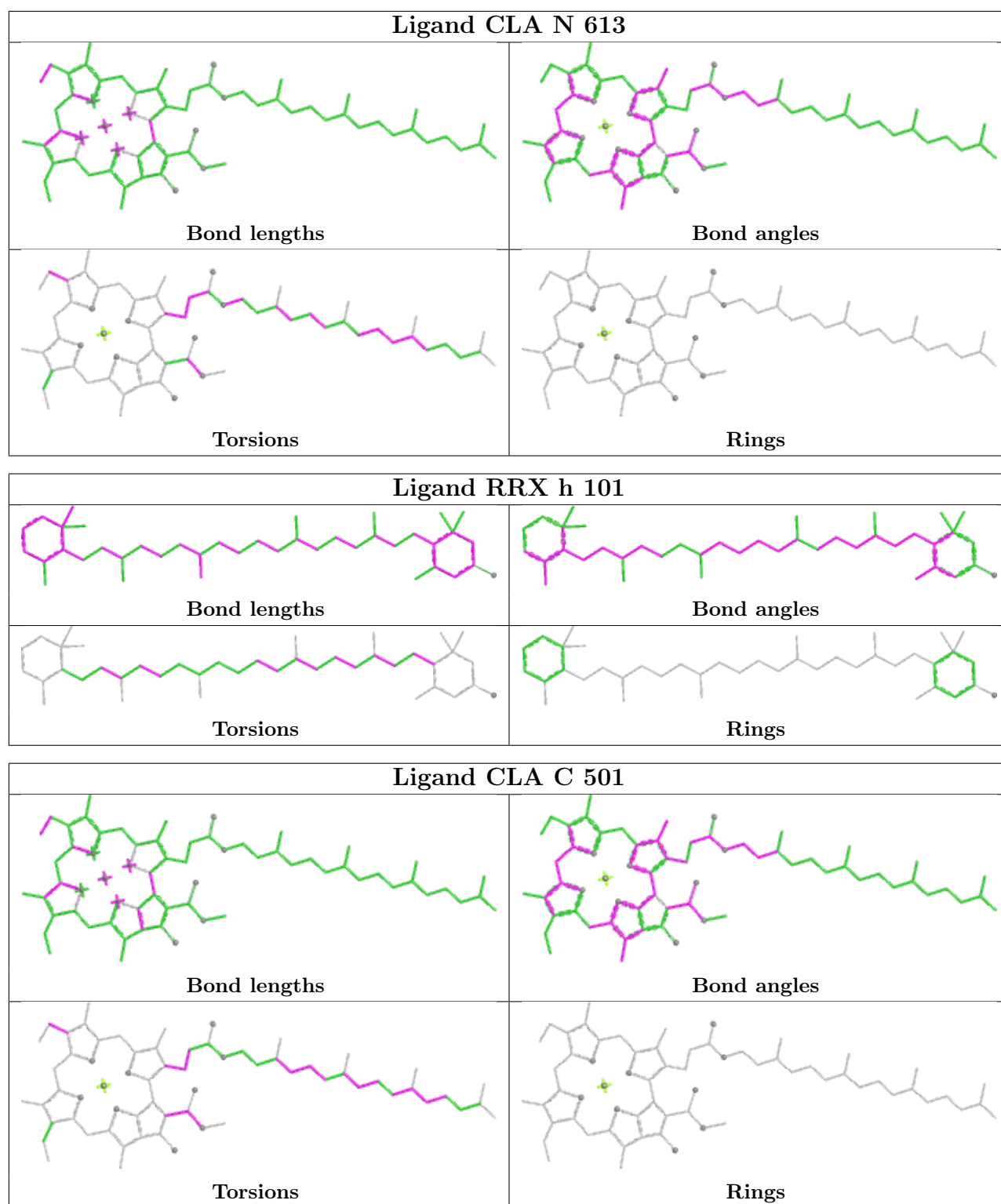


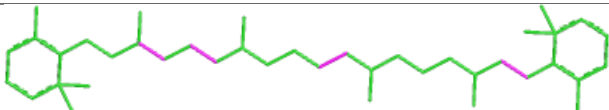
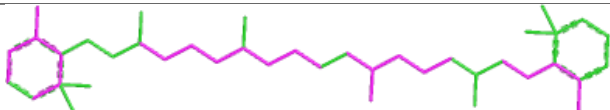
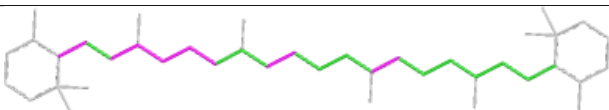
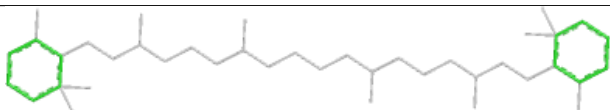


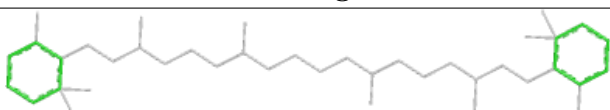


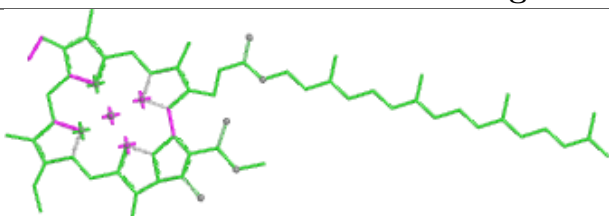
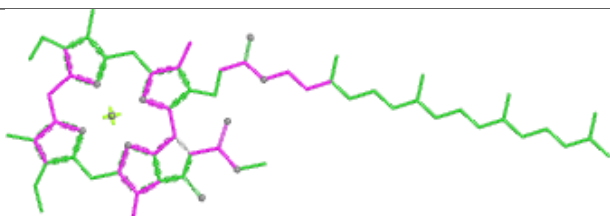
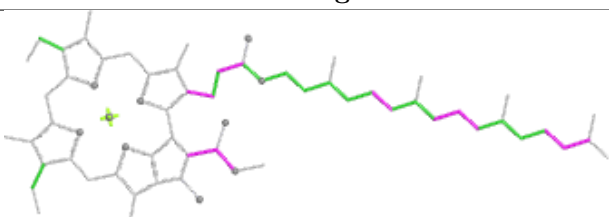
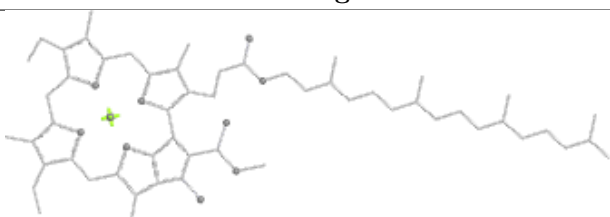


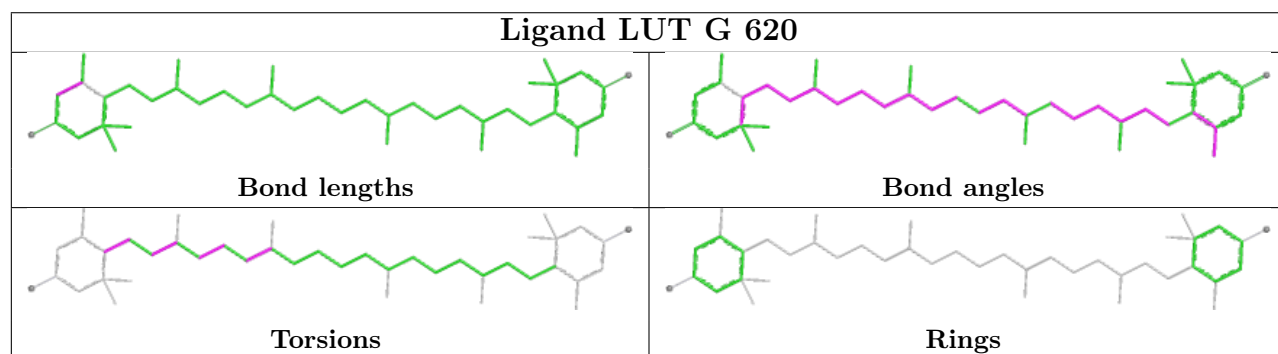
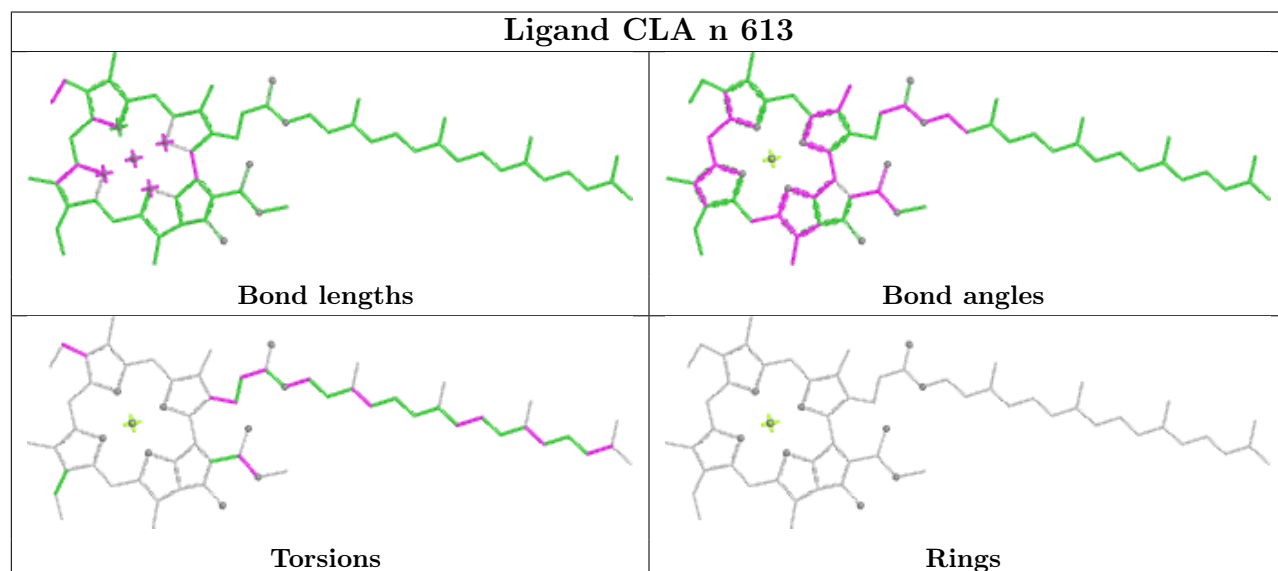
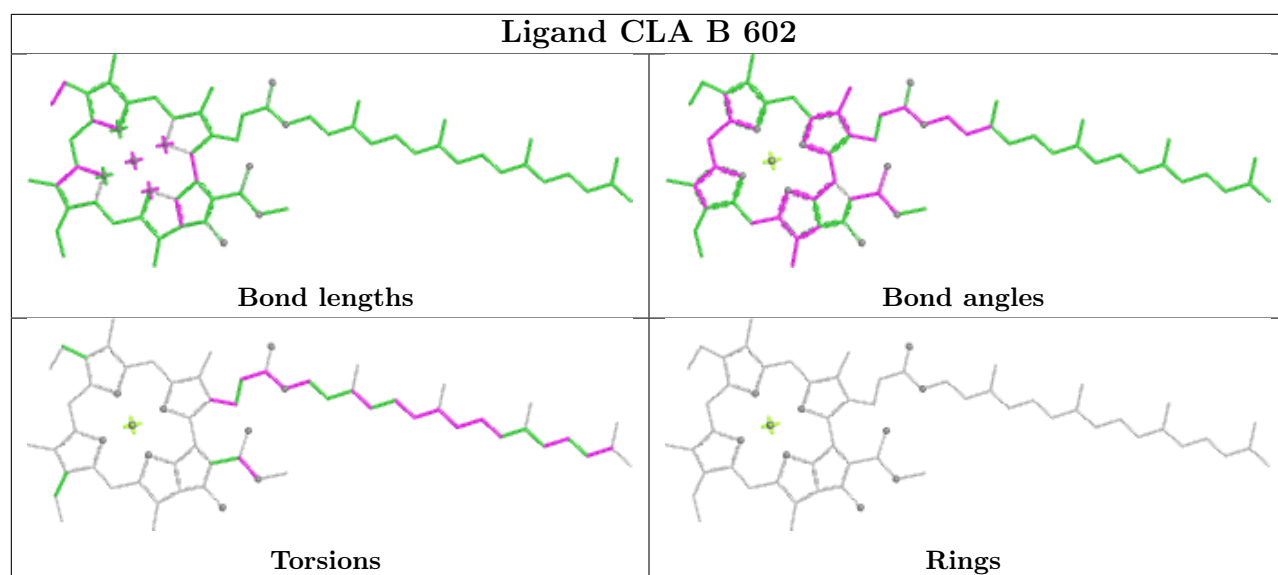


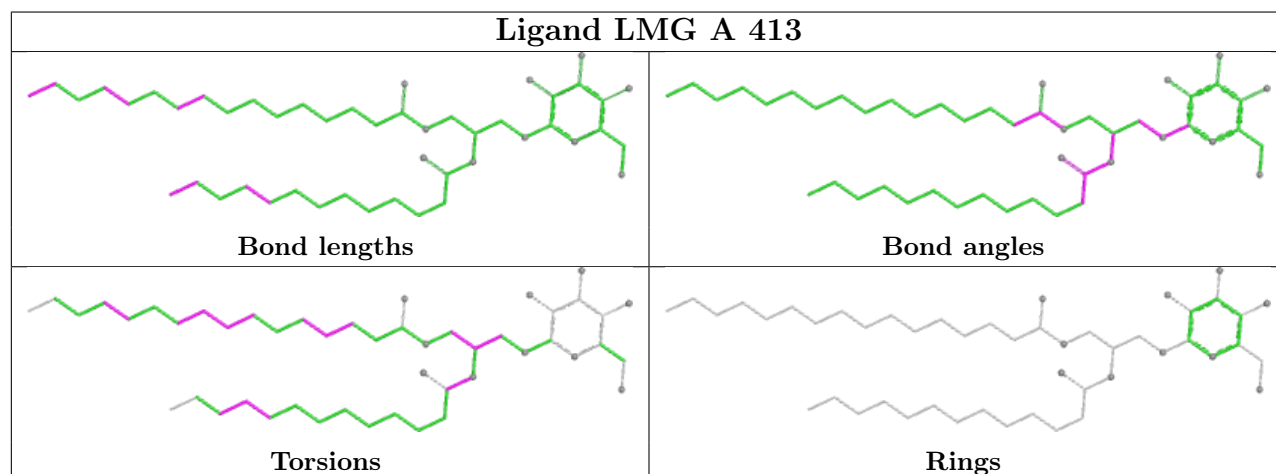
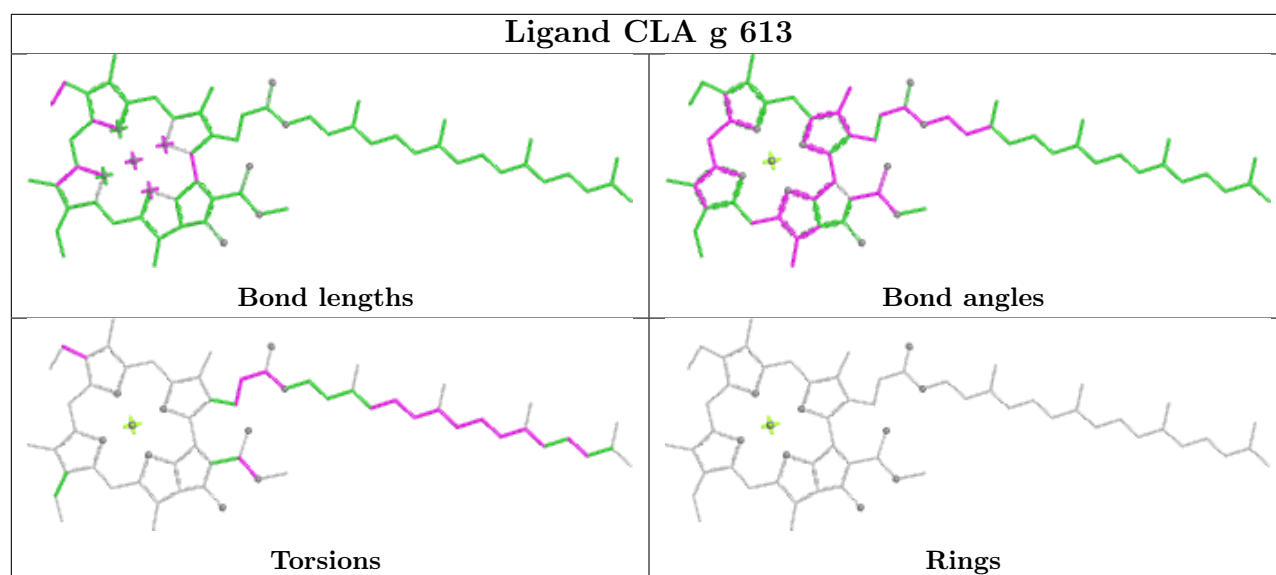


Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

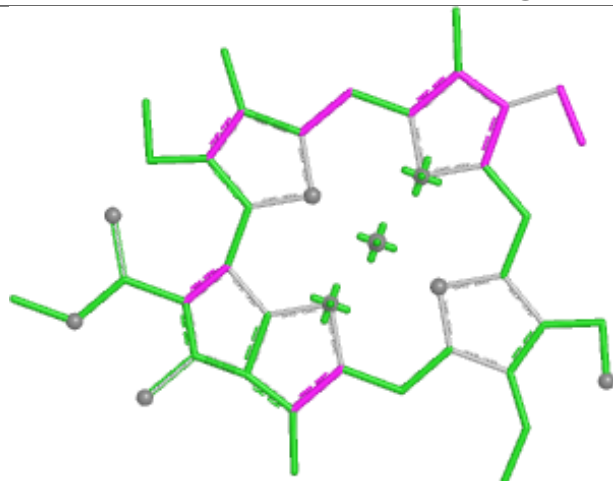
Ligand BCR c 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

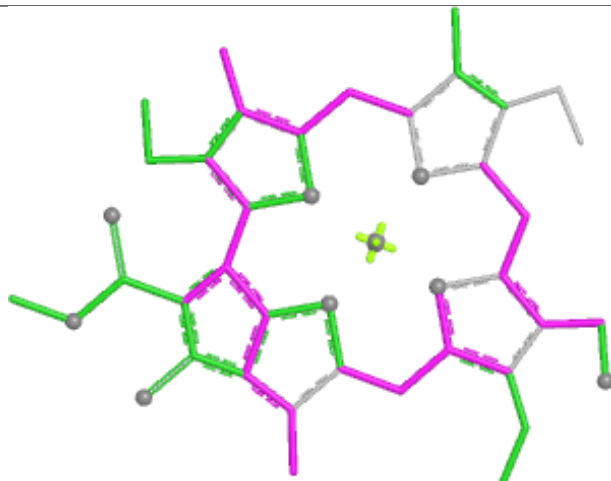




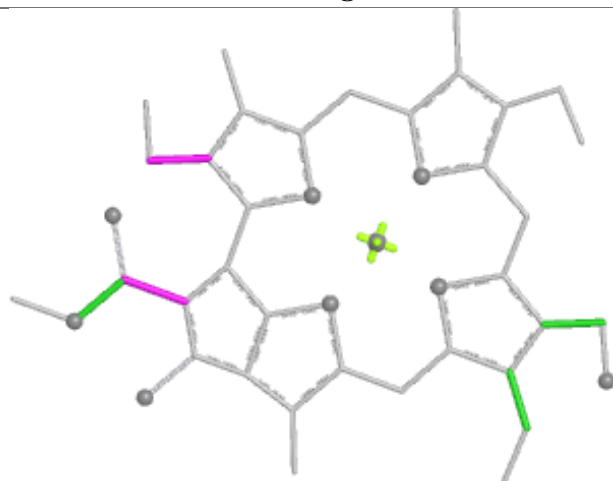
Ligand CHL S 607



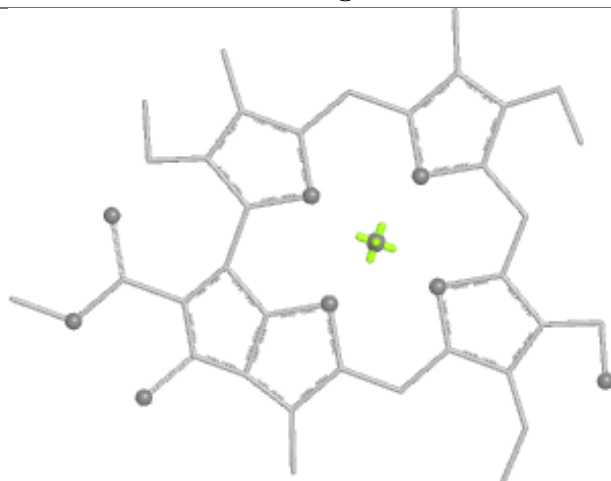
Bond lengths



Bond angles

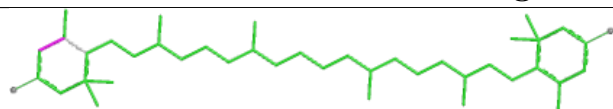


Torsions

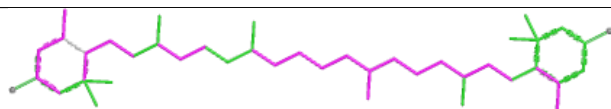


Rings

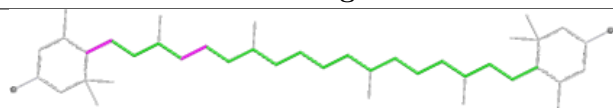
Ligand LUT G 621



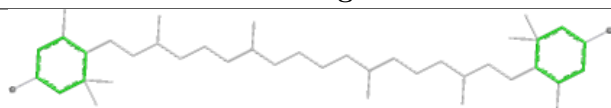
Bond lengths



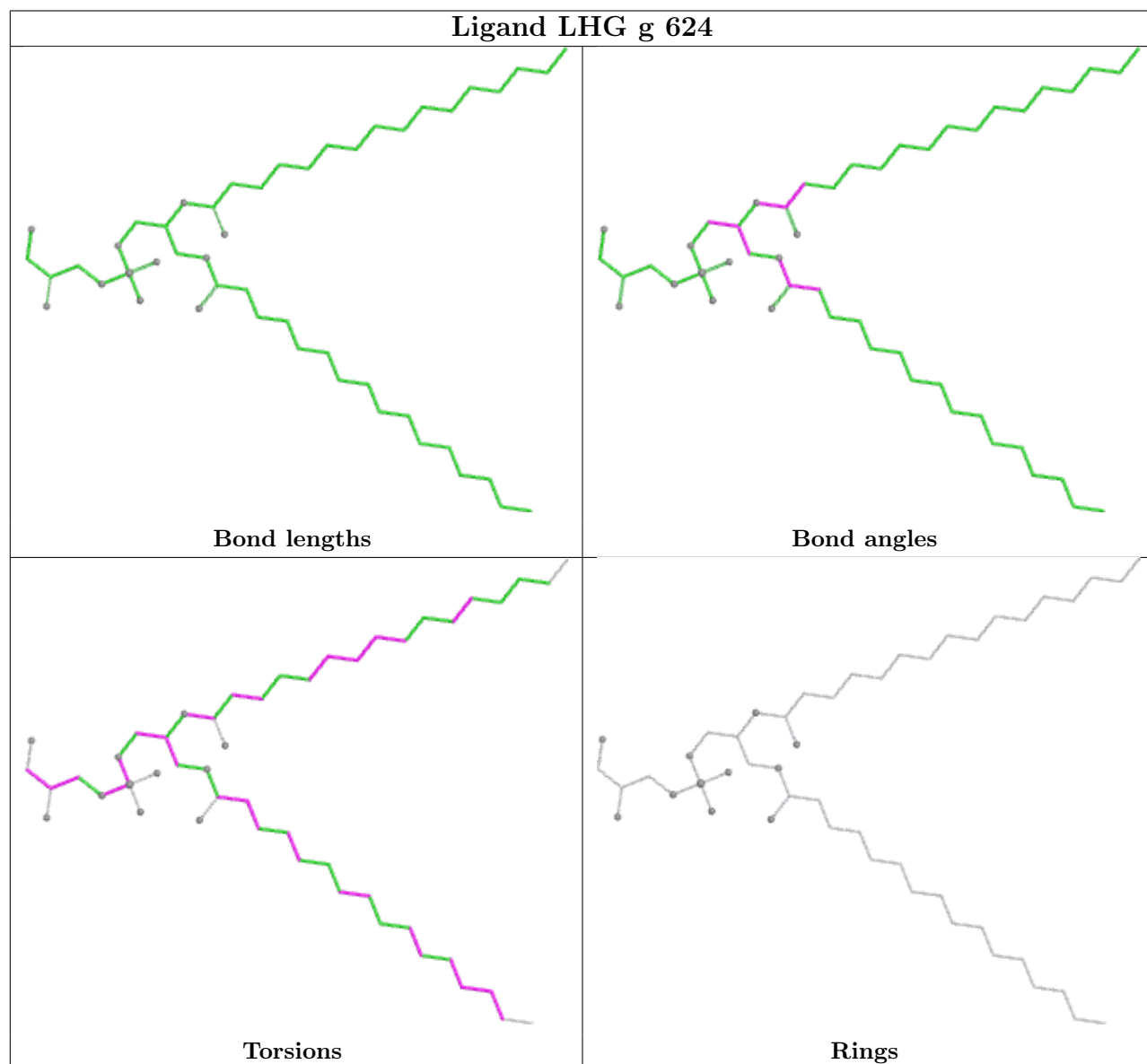
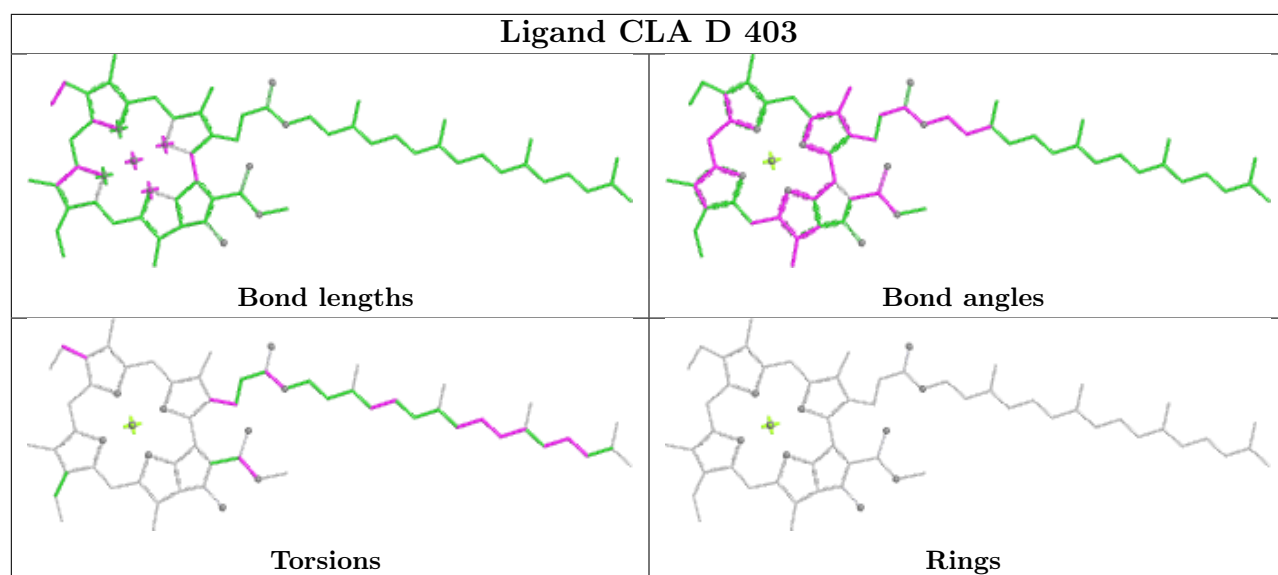
Bond angles

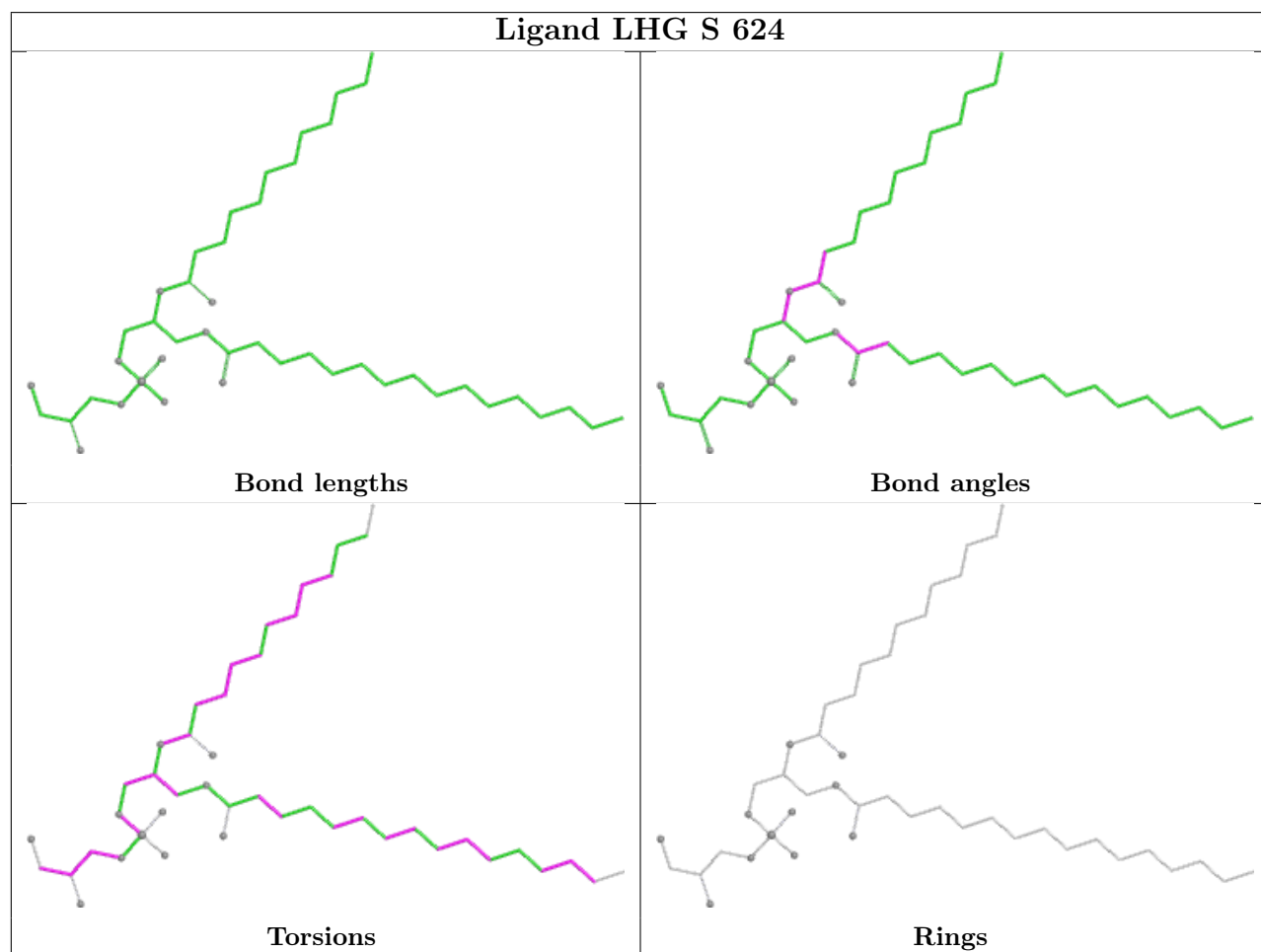
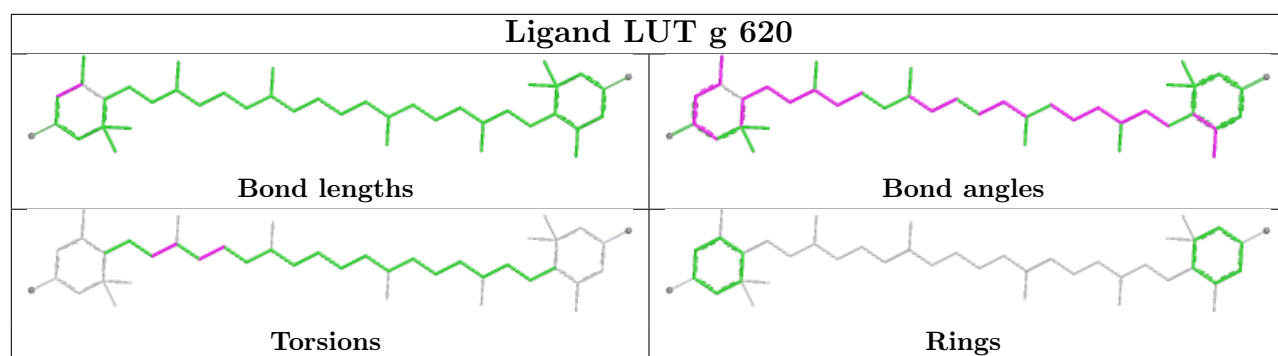


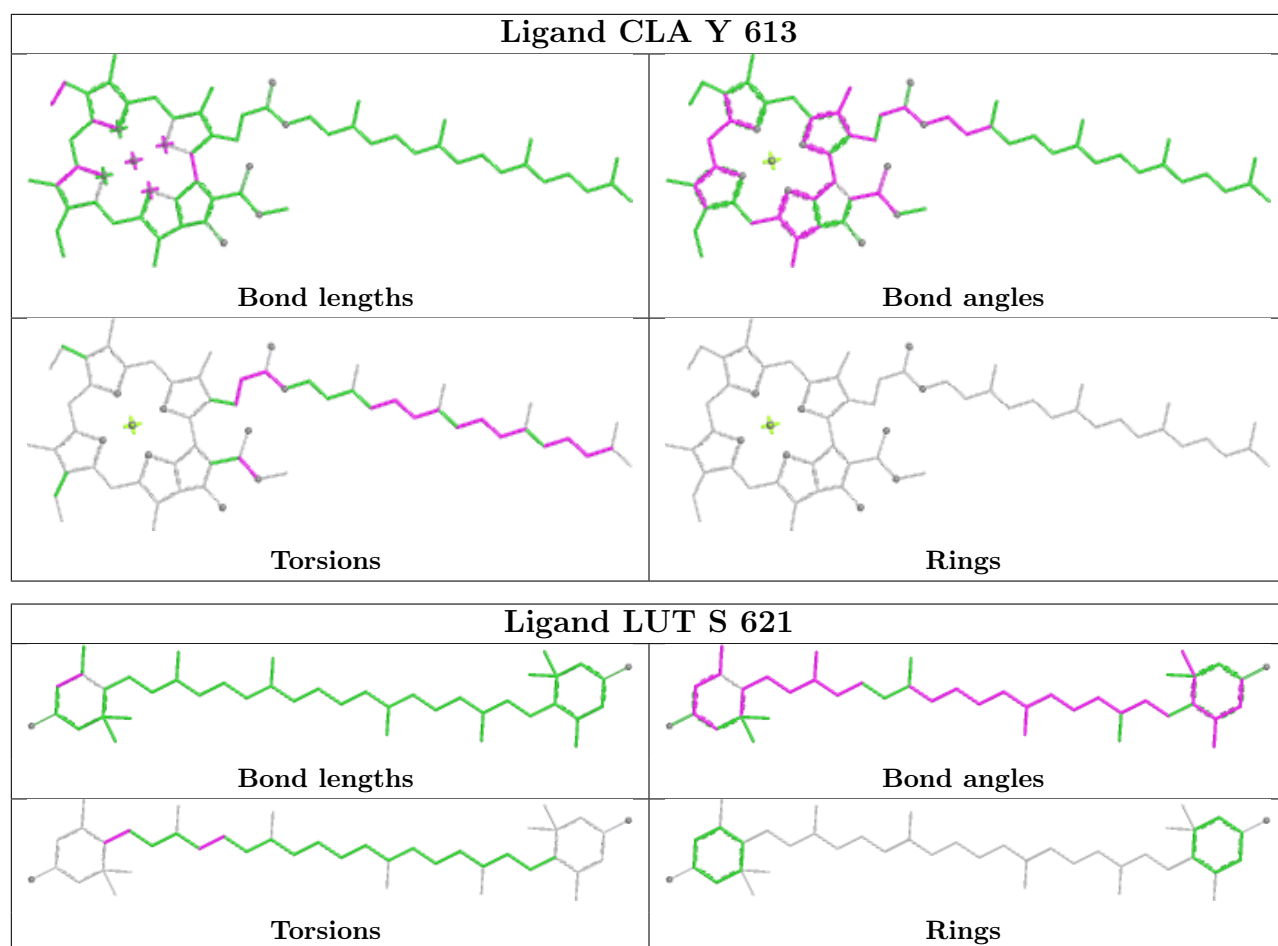
Torsions



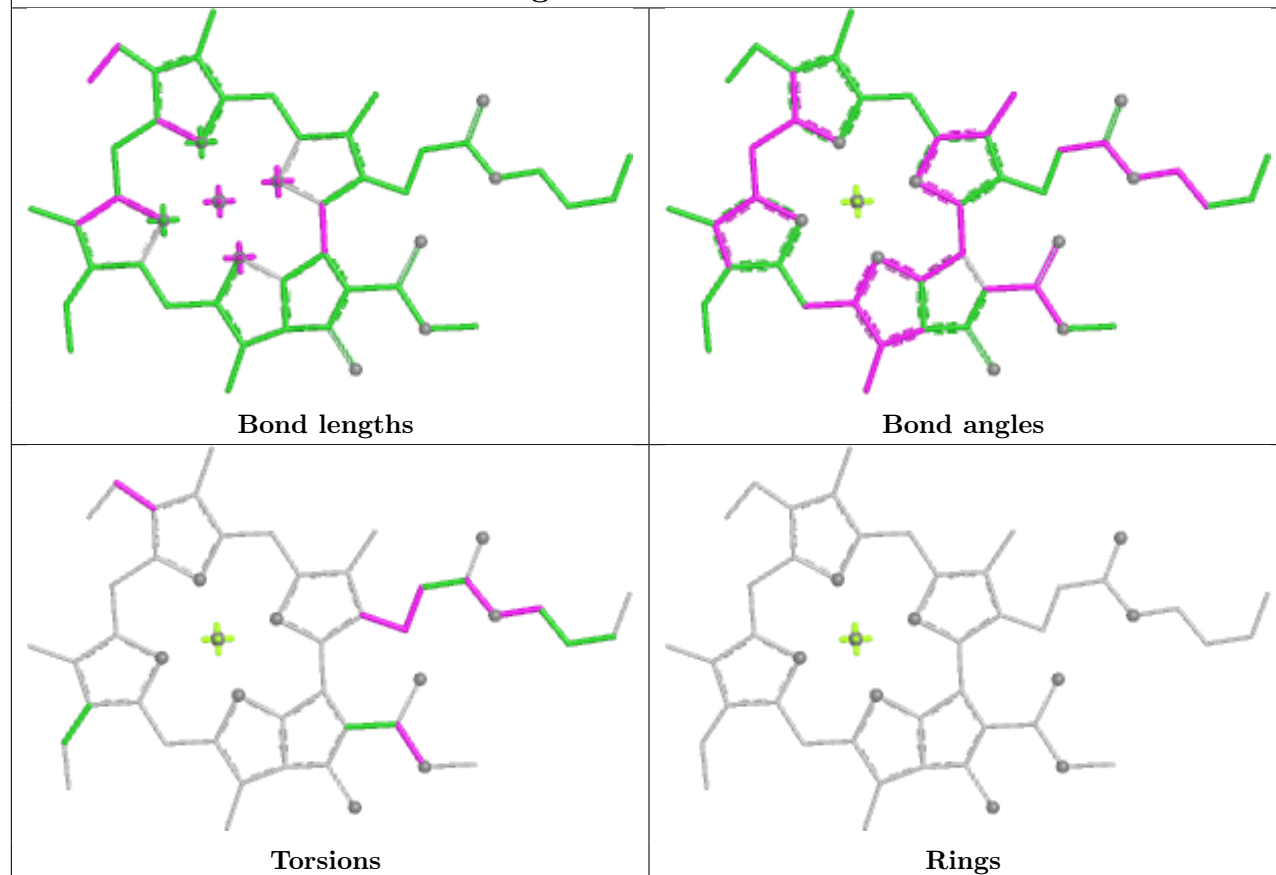
Rings



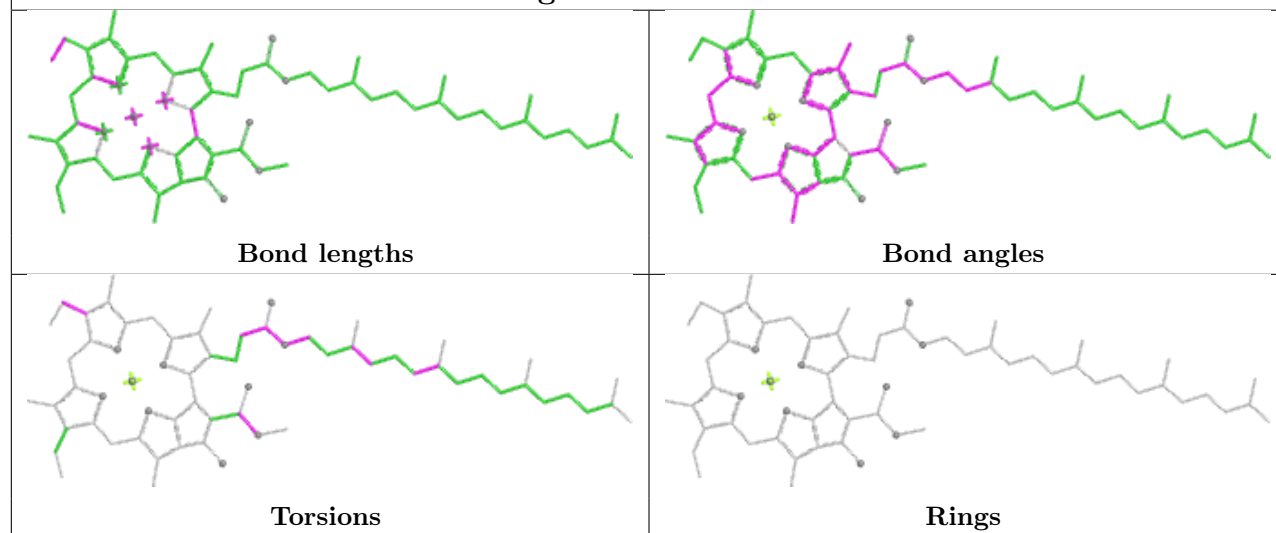


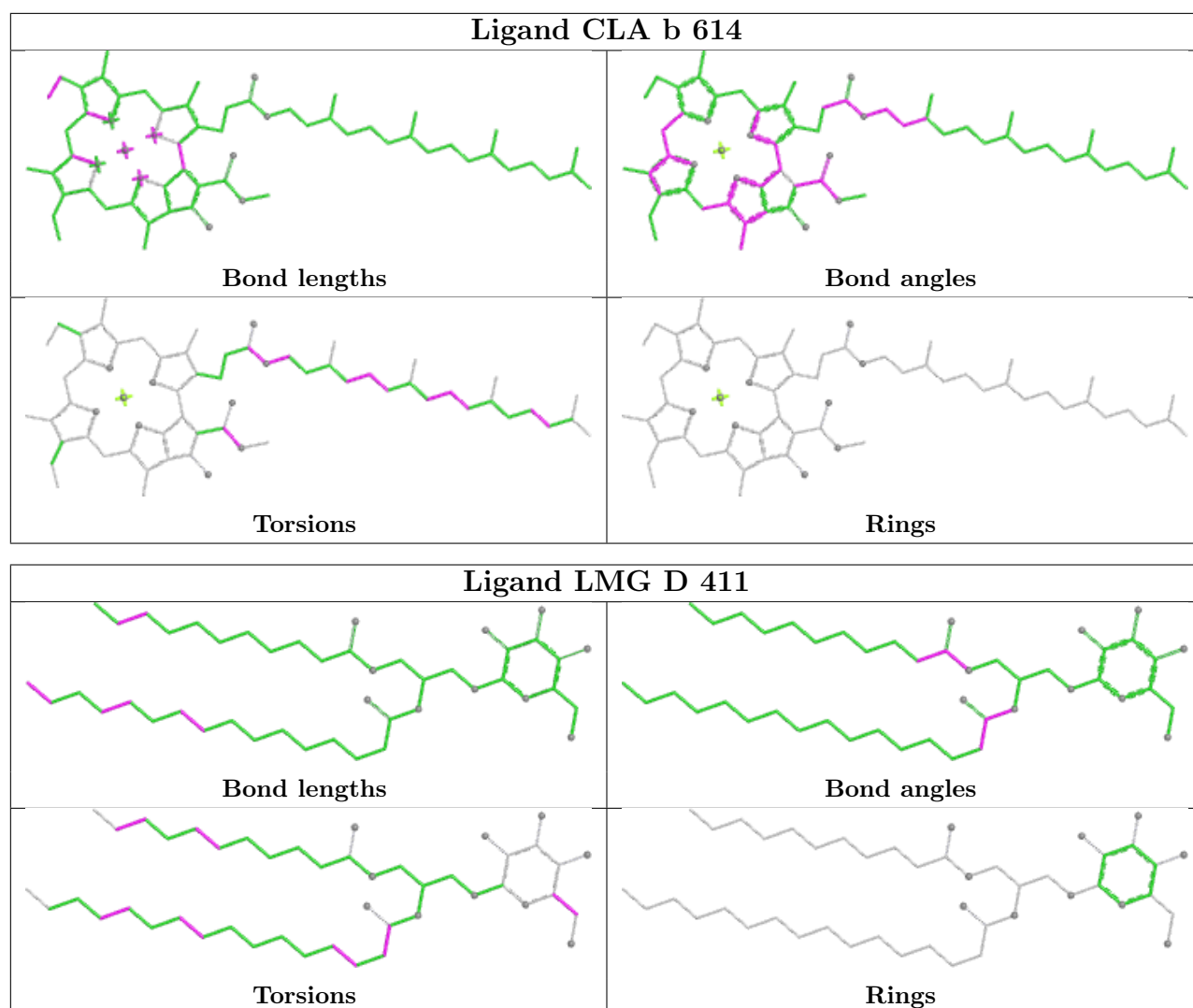


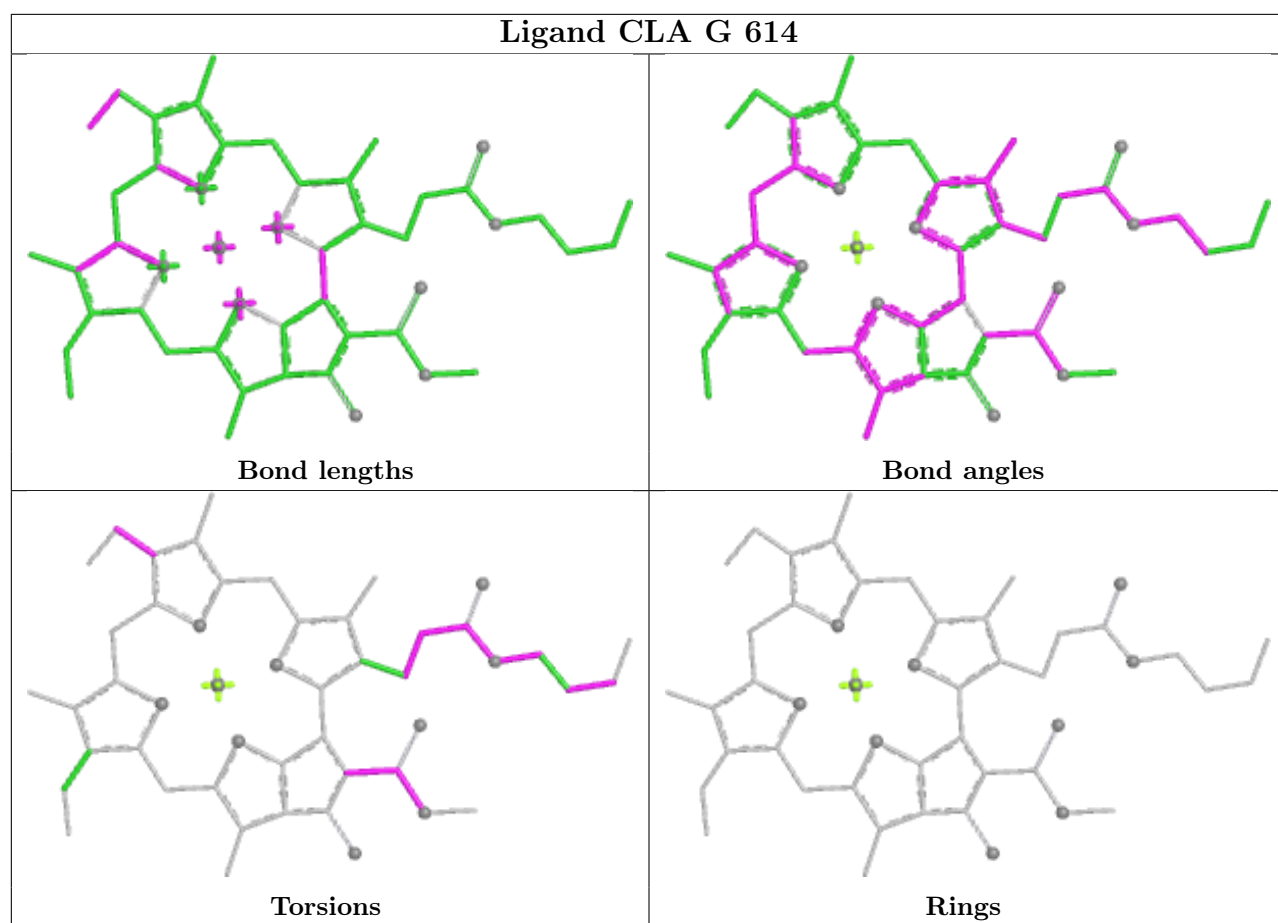
Ligand CLA N 614

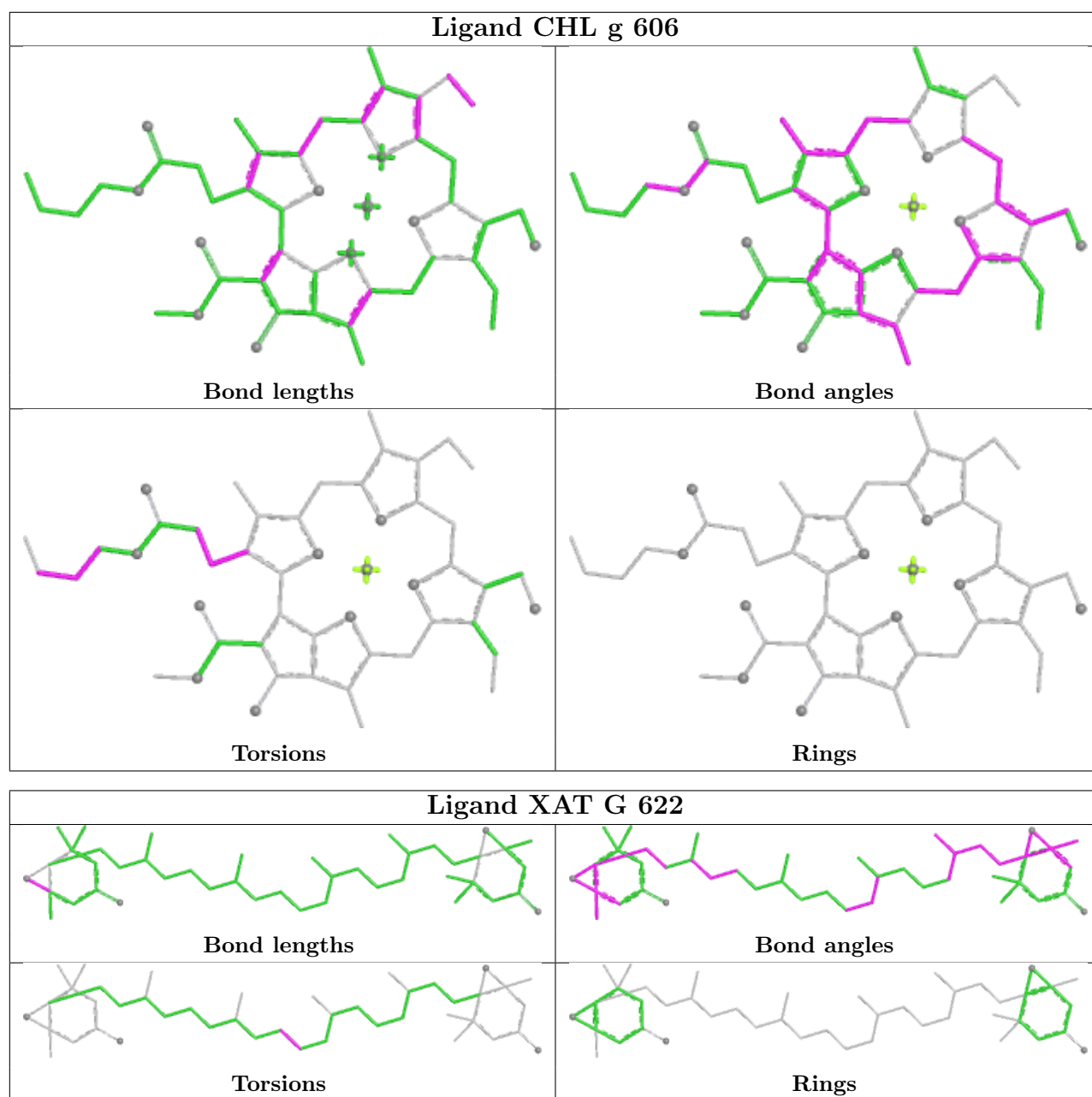


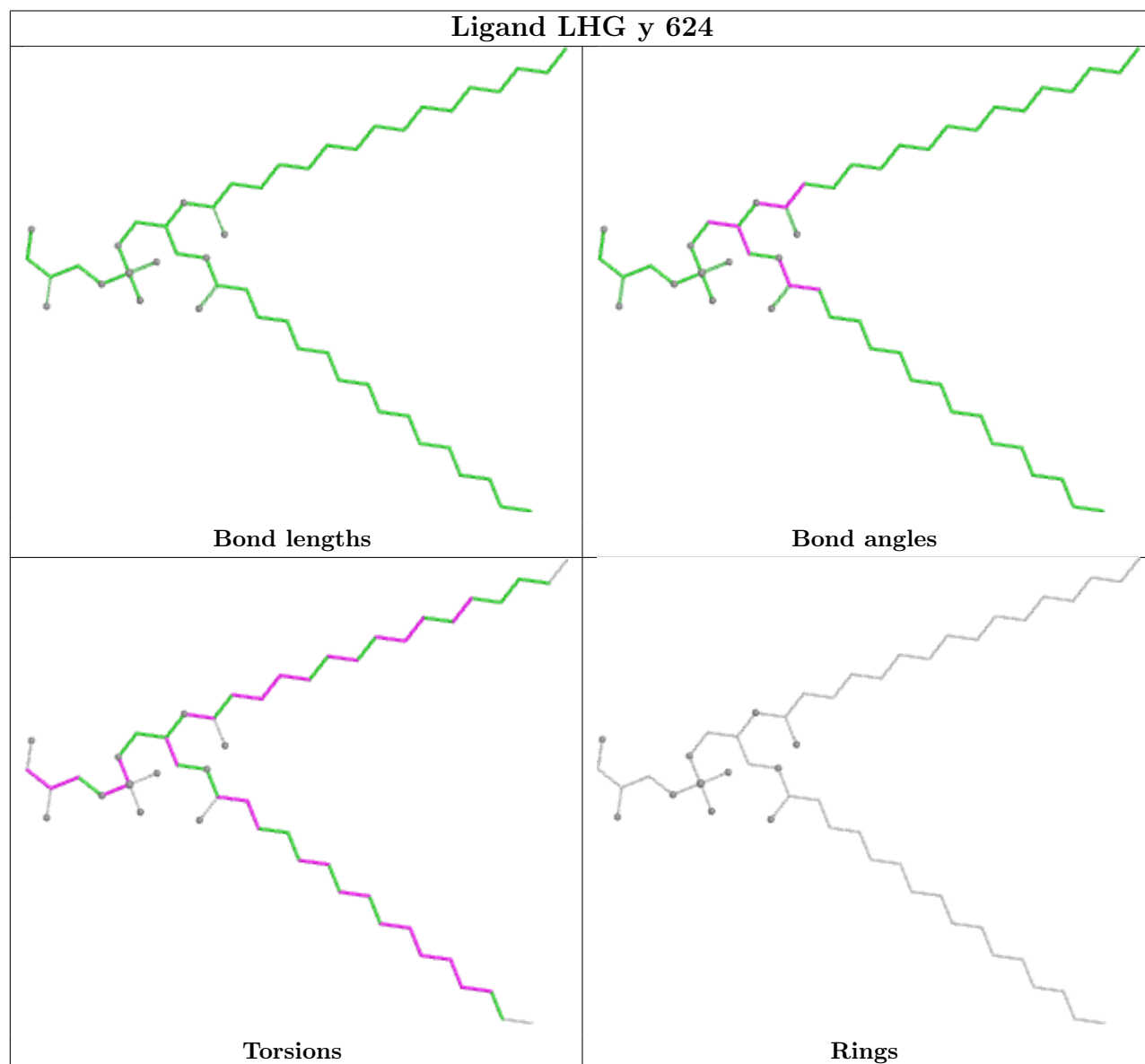
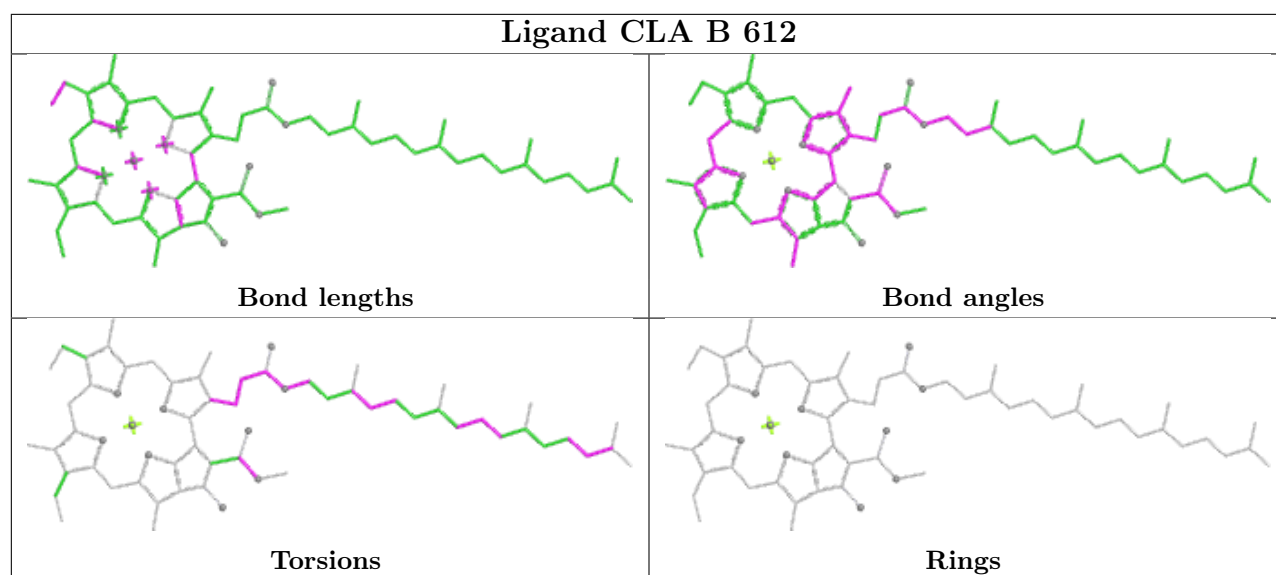
Ligand CLA s 611

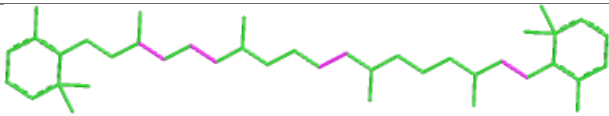
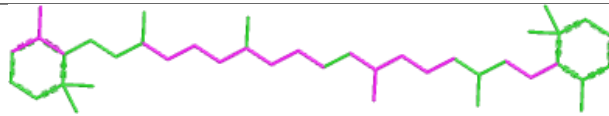
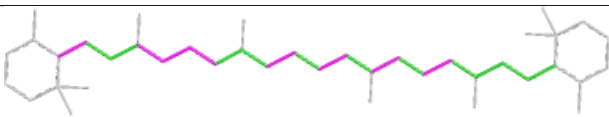
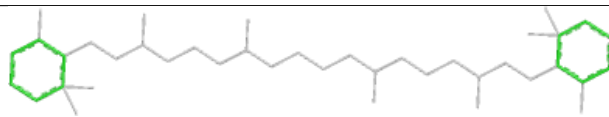


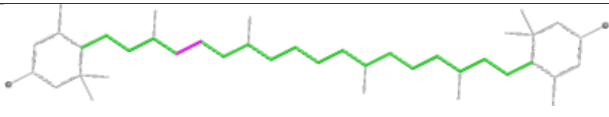
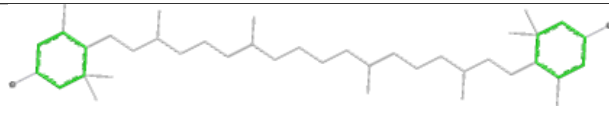


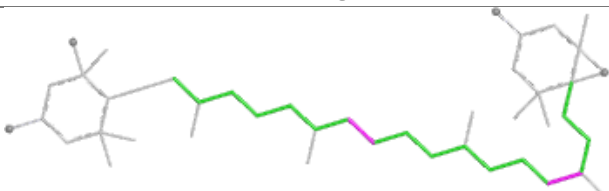
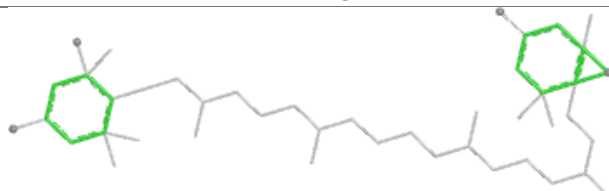


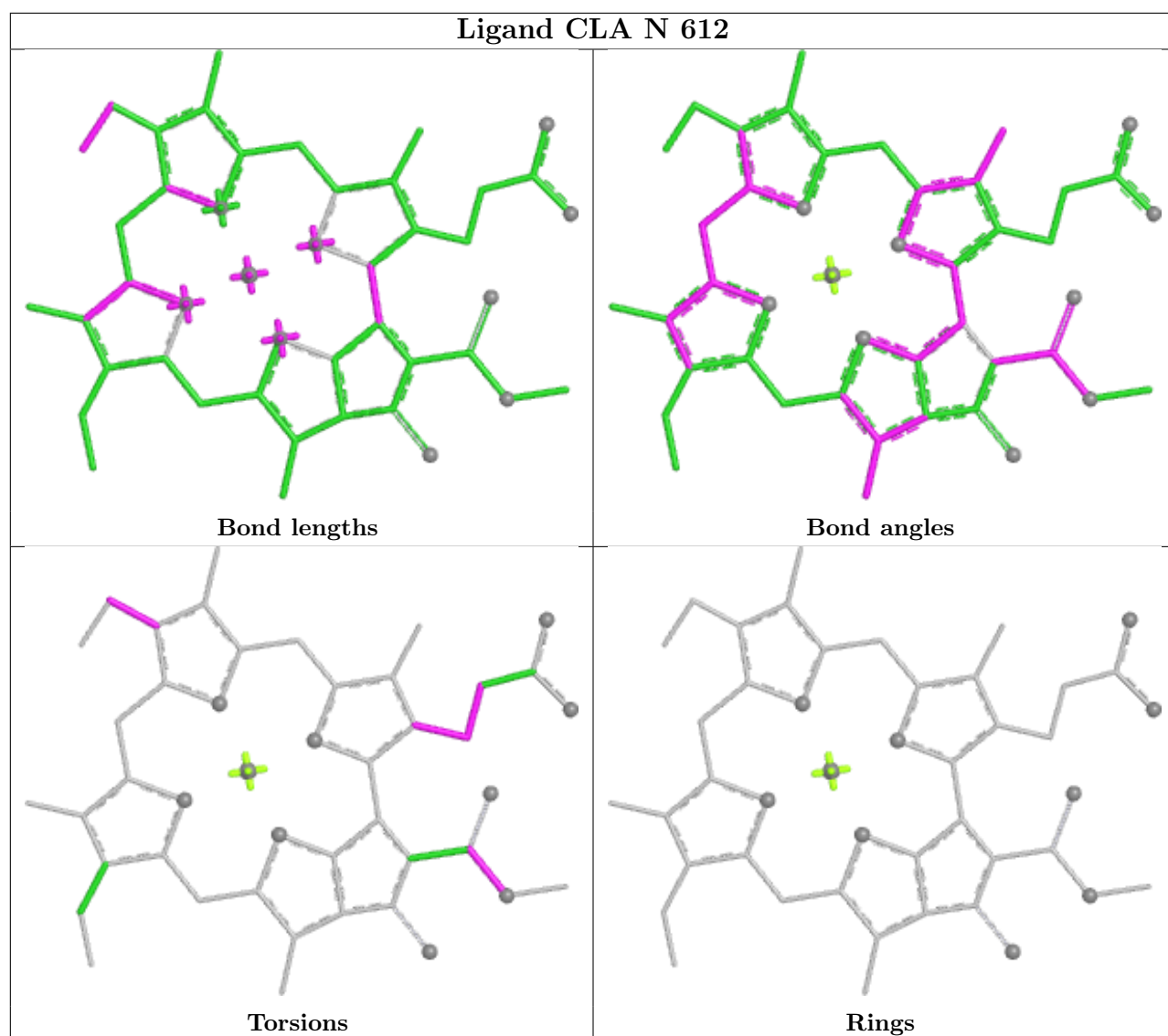


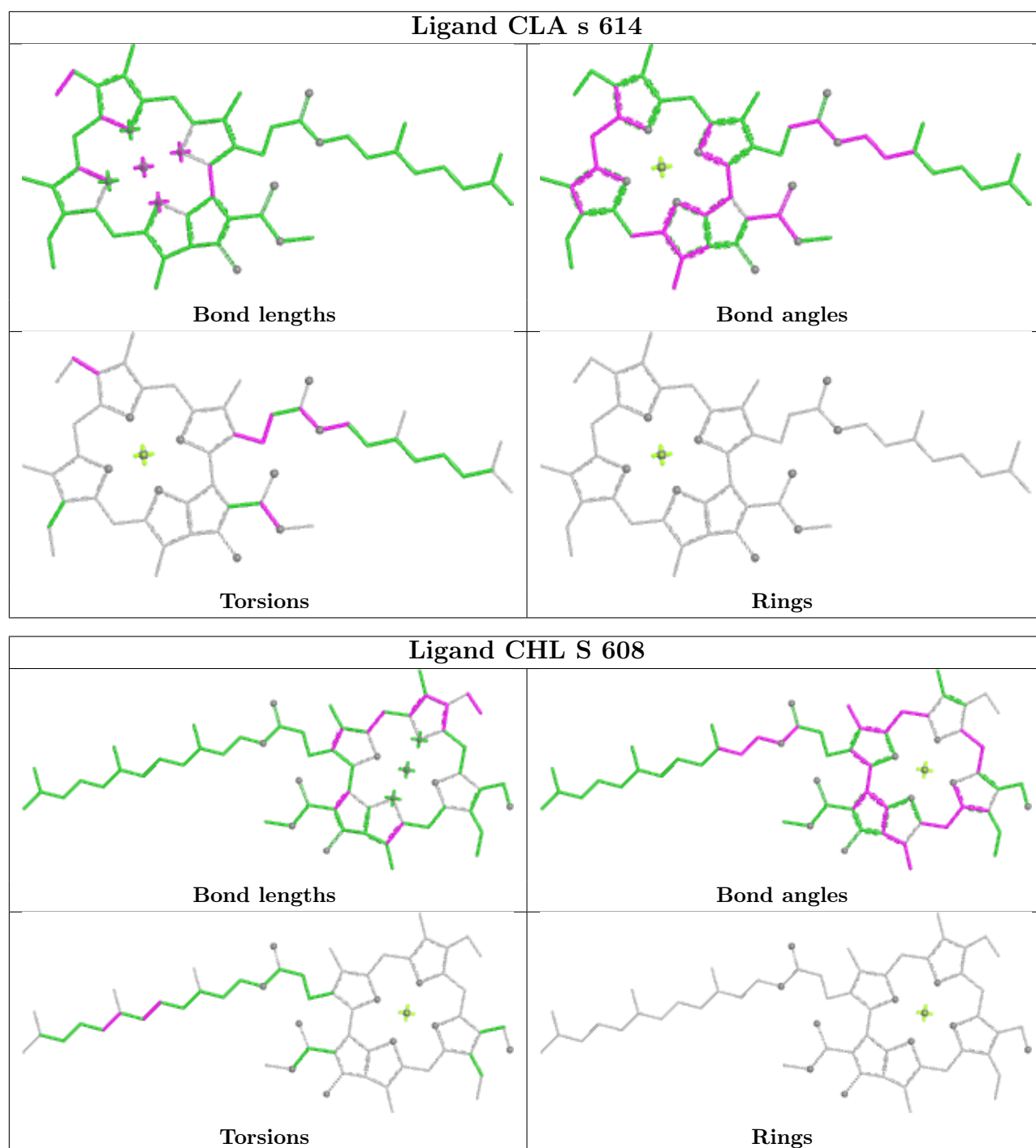


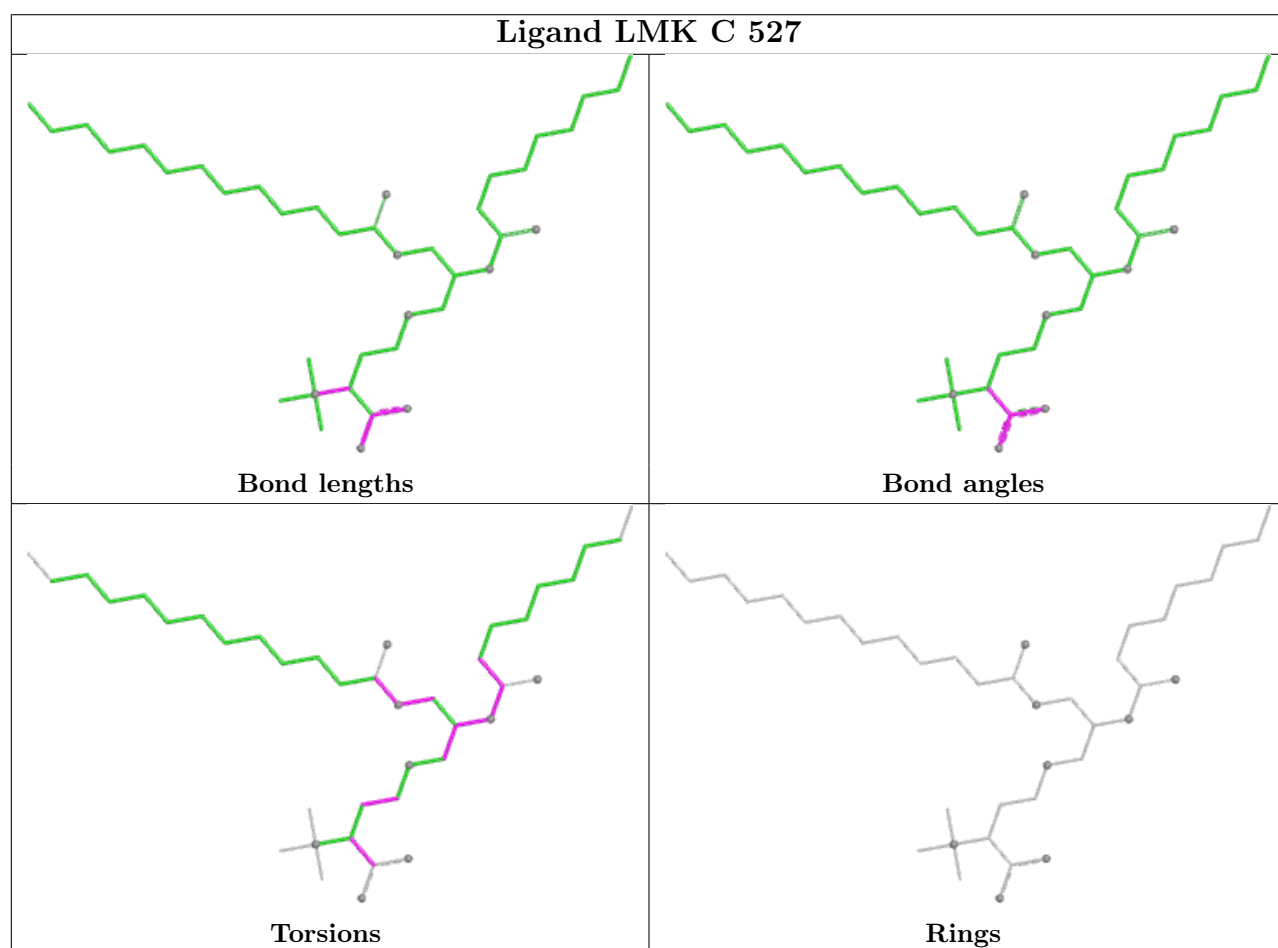
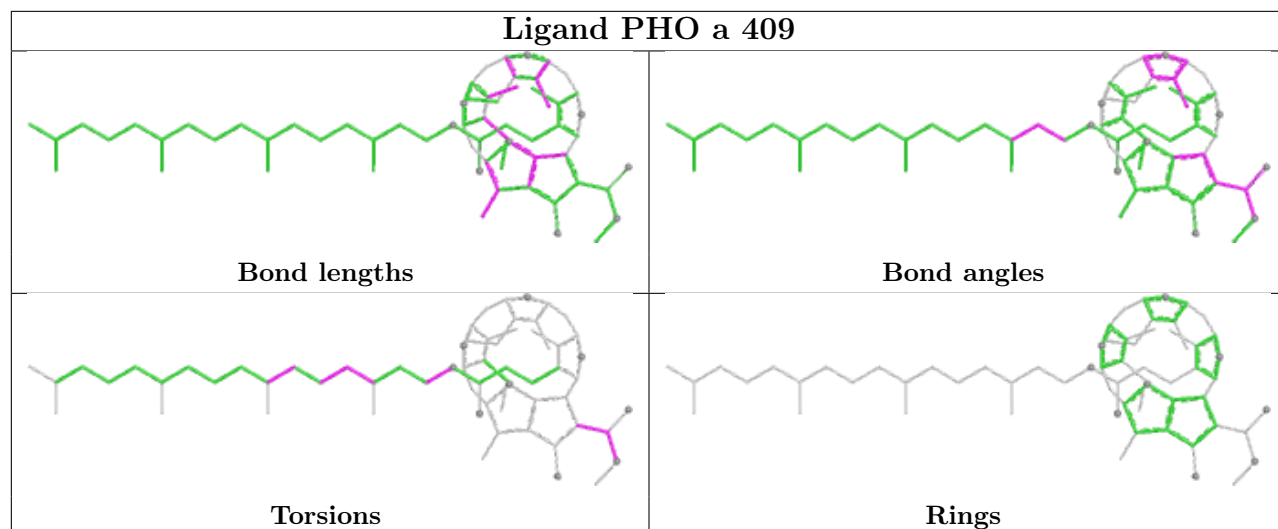
Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

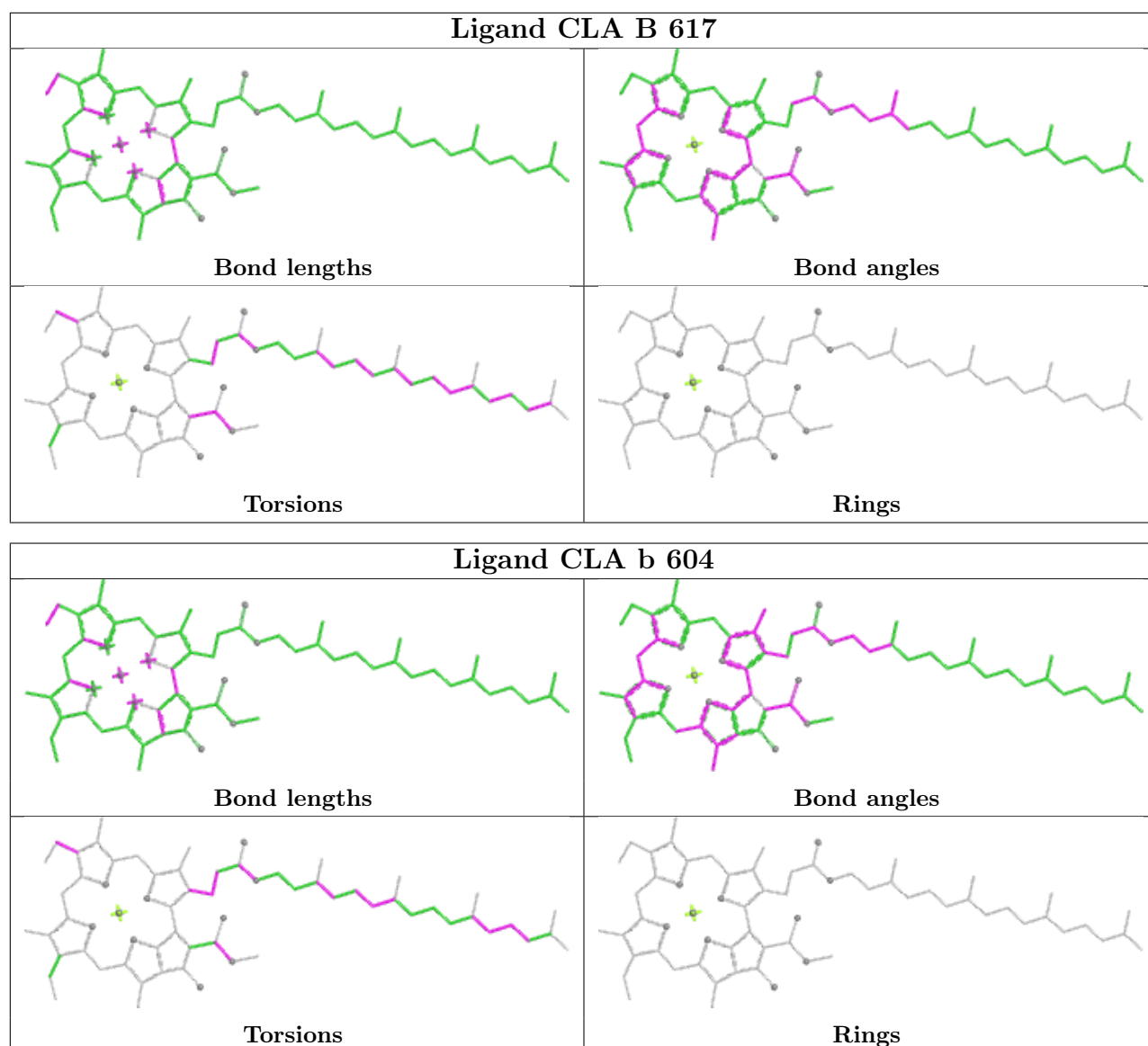
Ligand LUT s 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

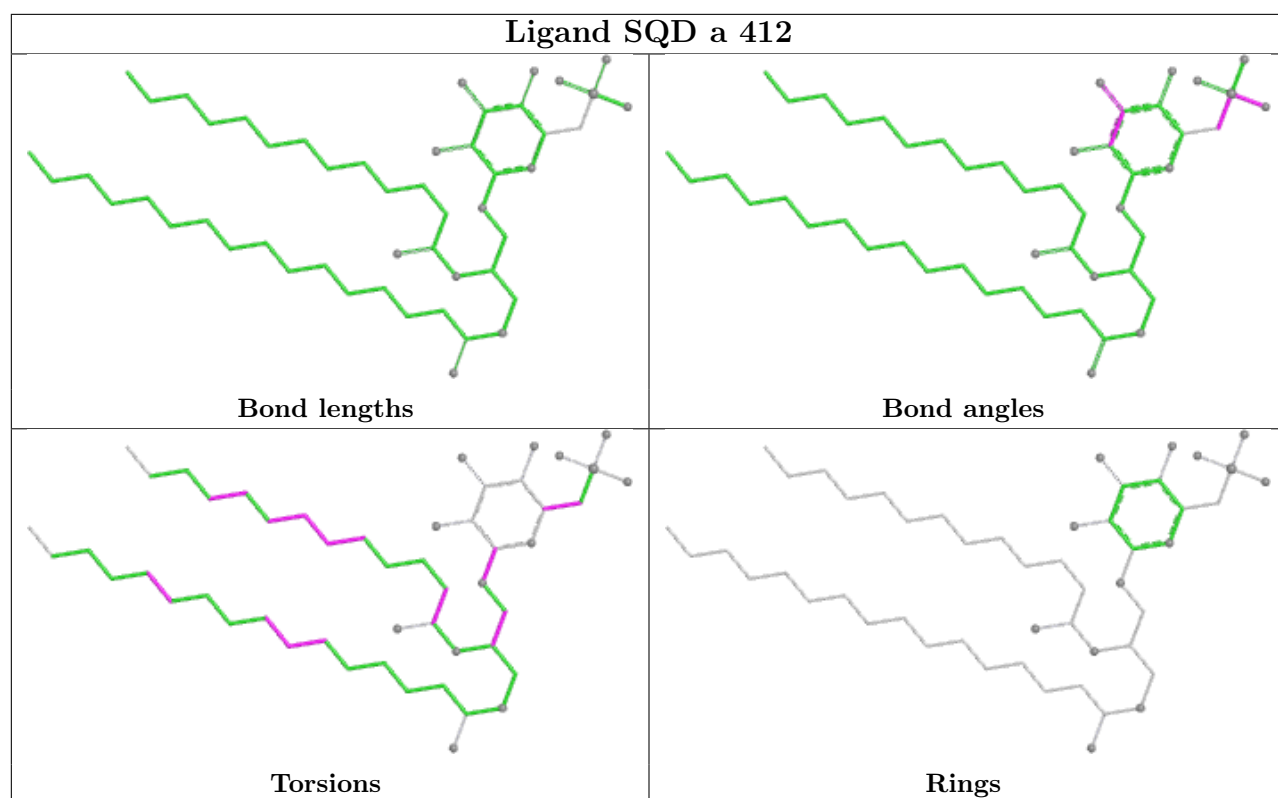
Ligand NEX g 623	
	
Bond lengths	Bond angles
	
Torsions	Rings



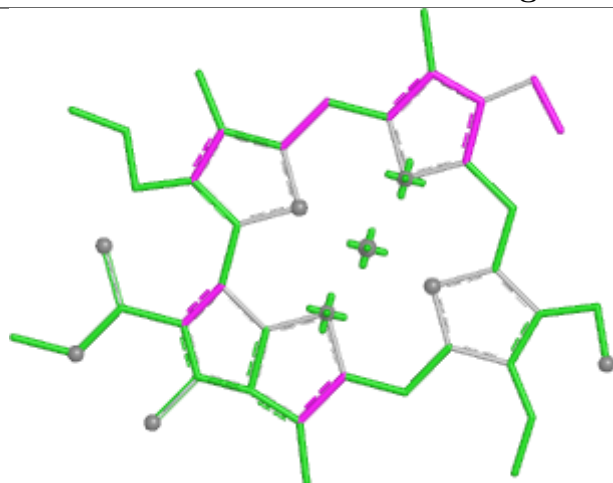




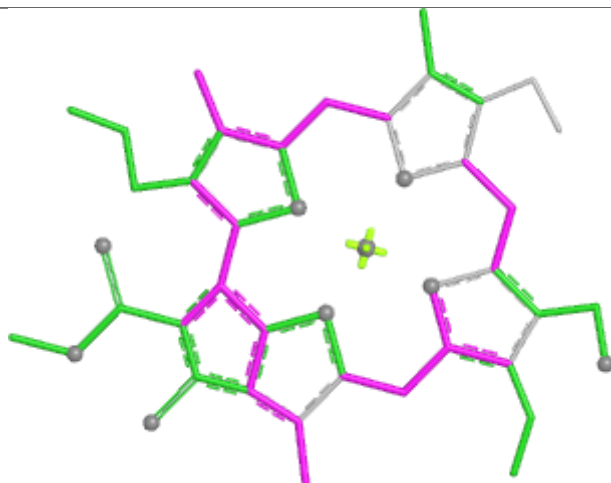




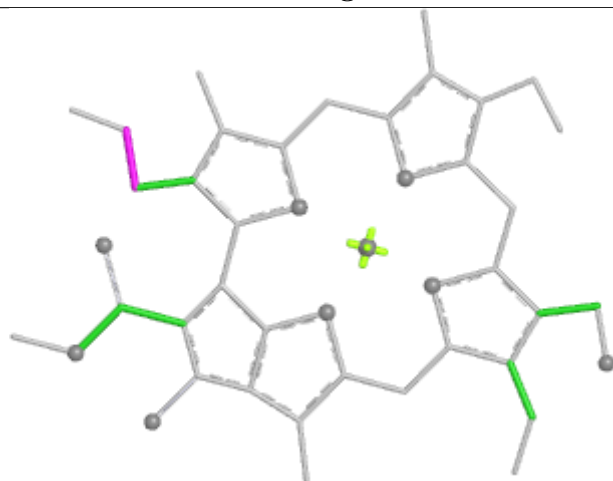
Ligand CHL s 606



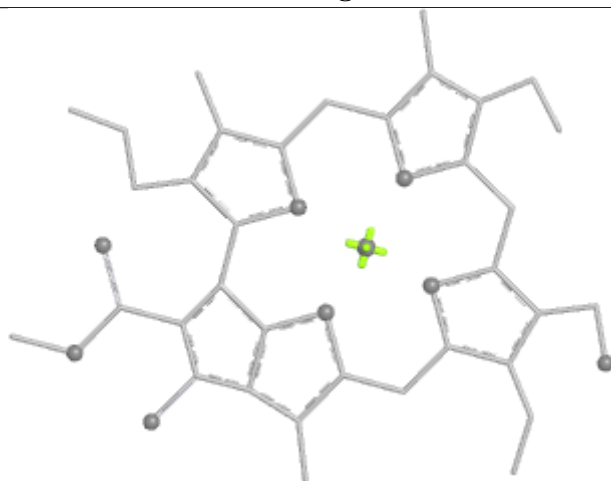
Bond lengths



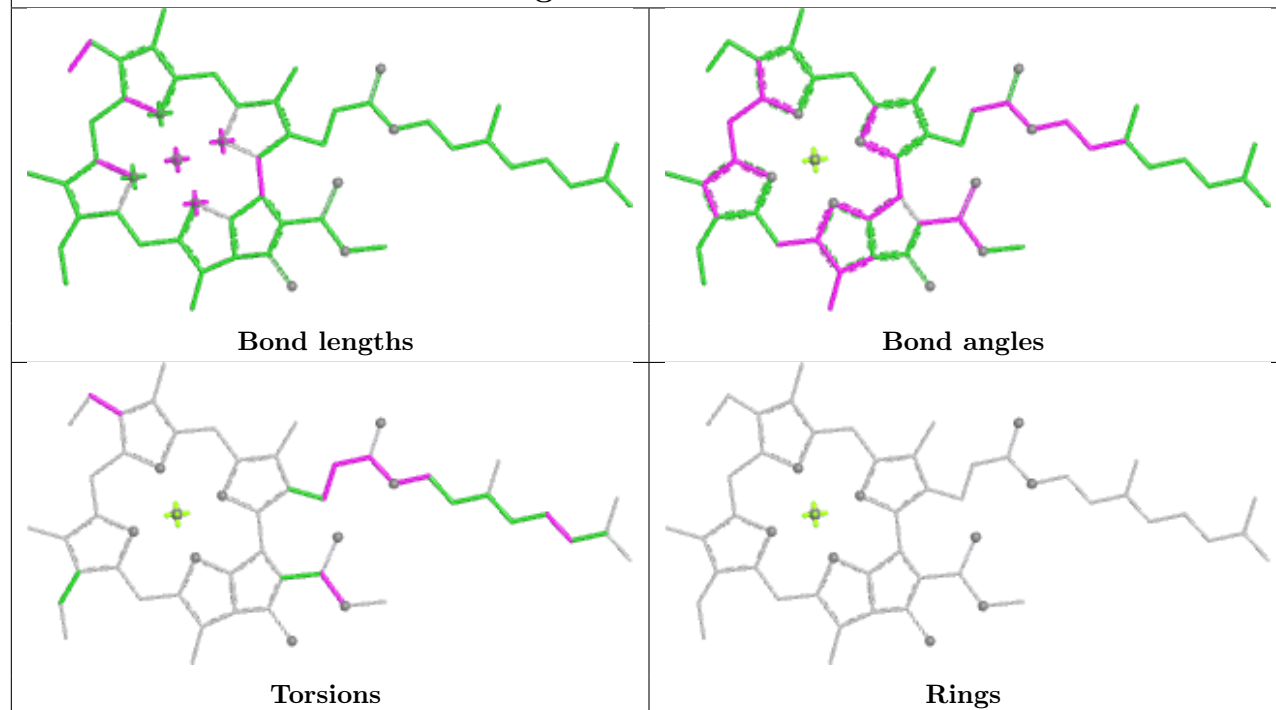
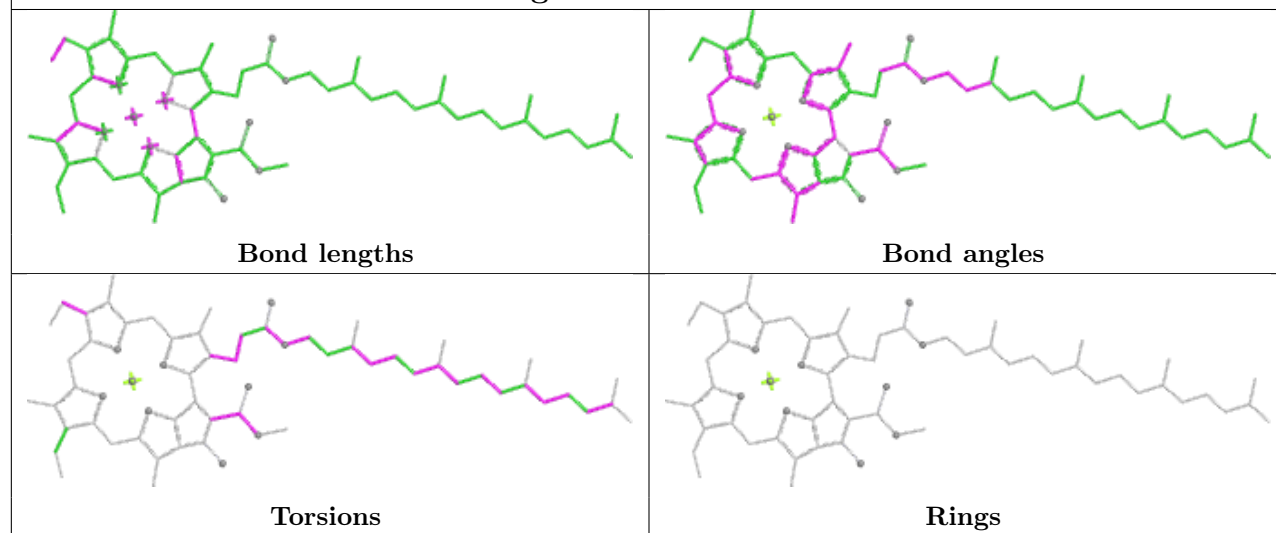
Bond angles

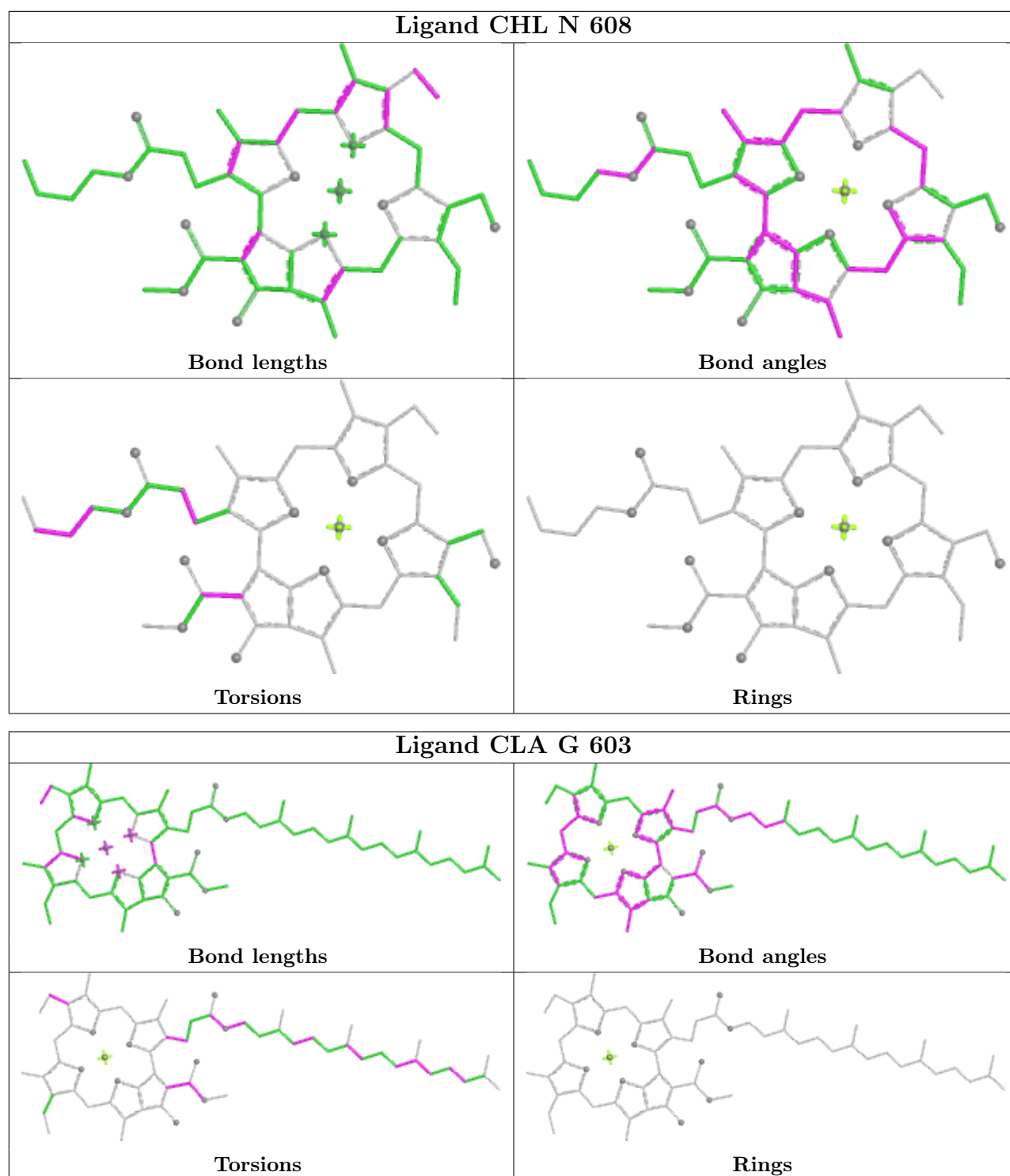


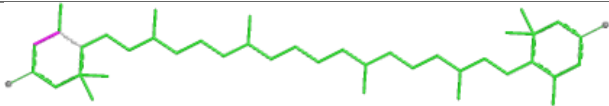
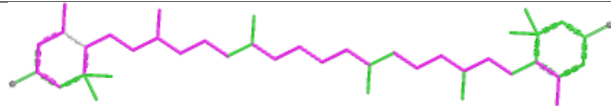
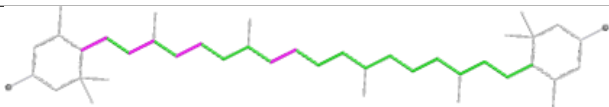
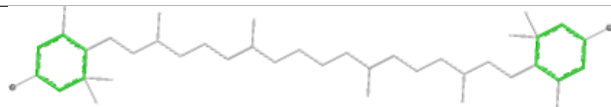
Torsions

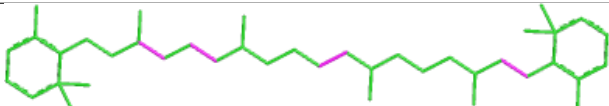
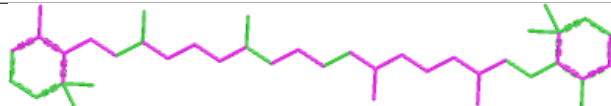
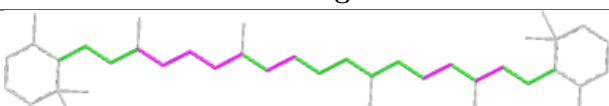
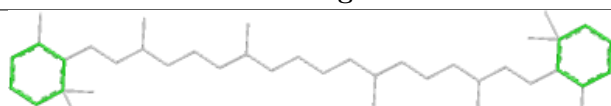


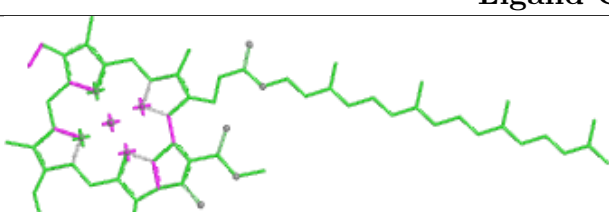
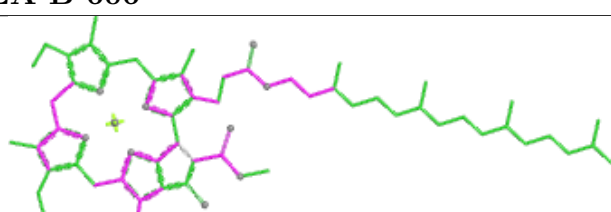
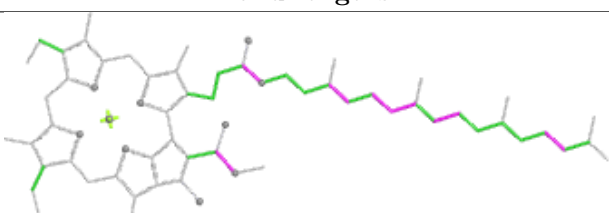
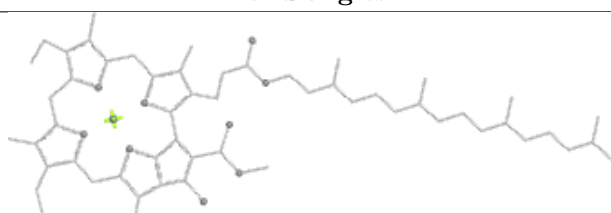
Rings

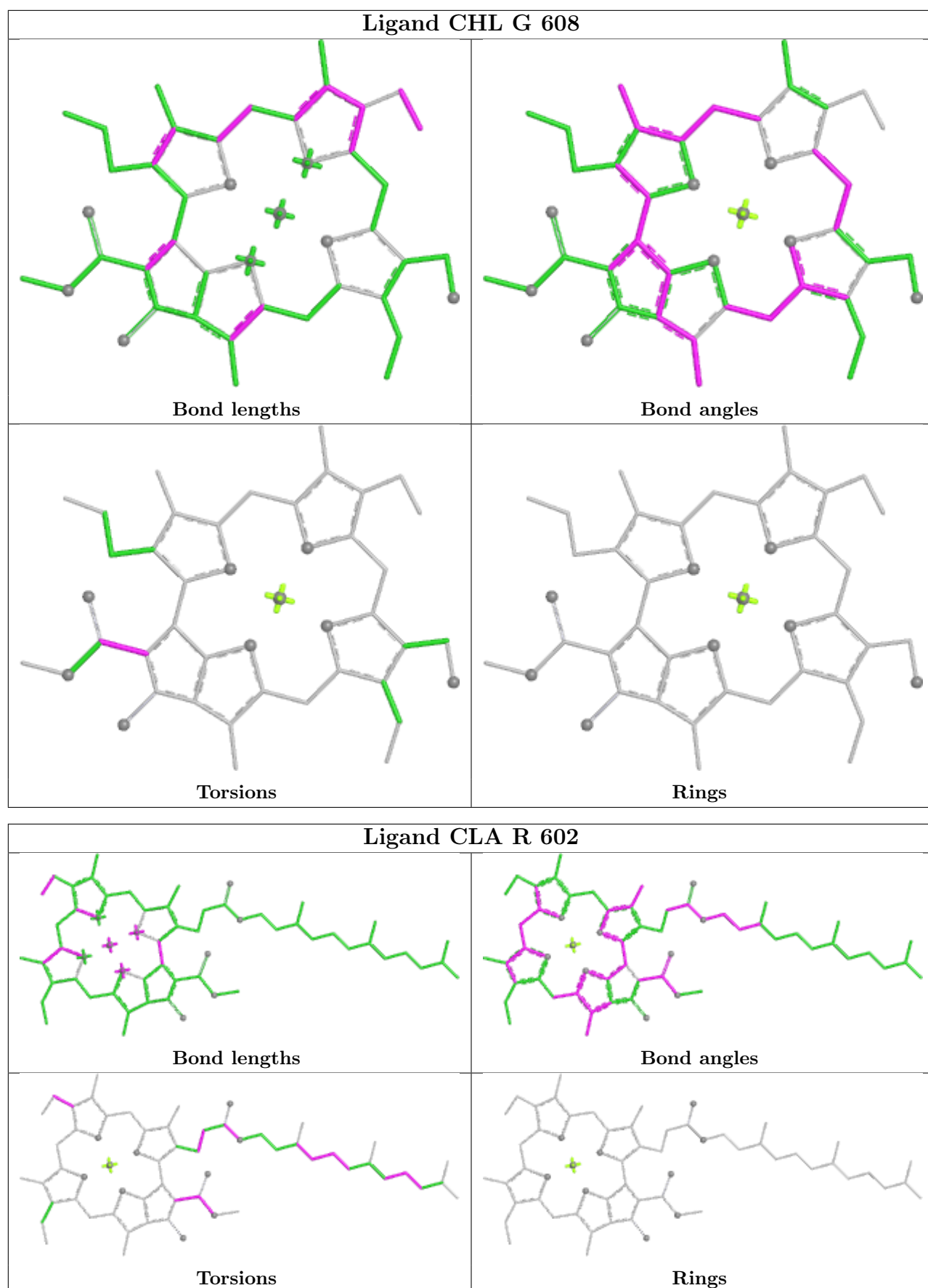
Ligand CLA S 614**Ligand CLA G 602**

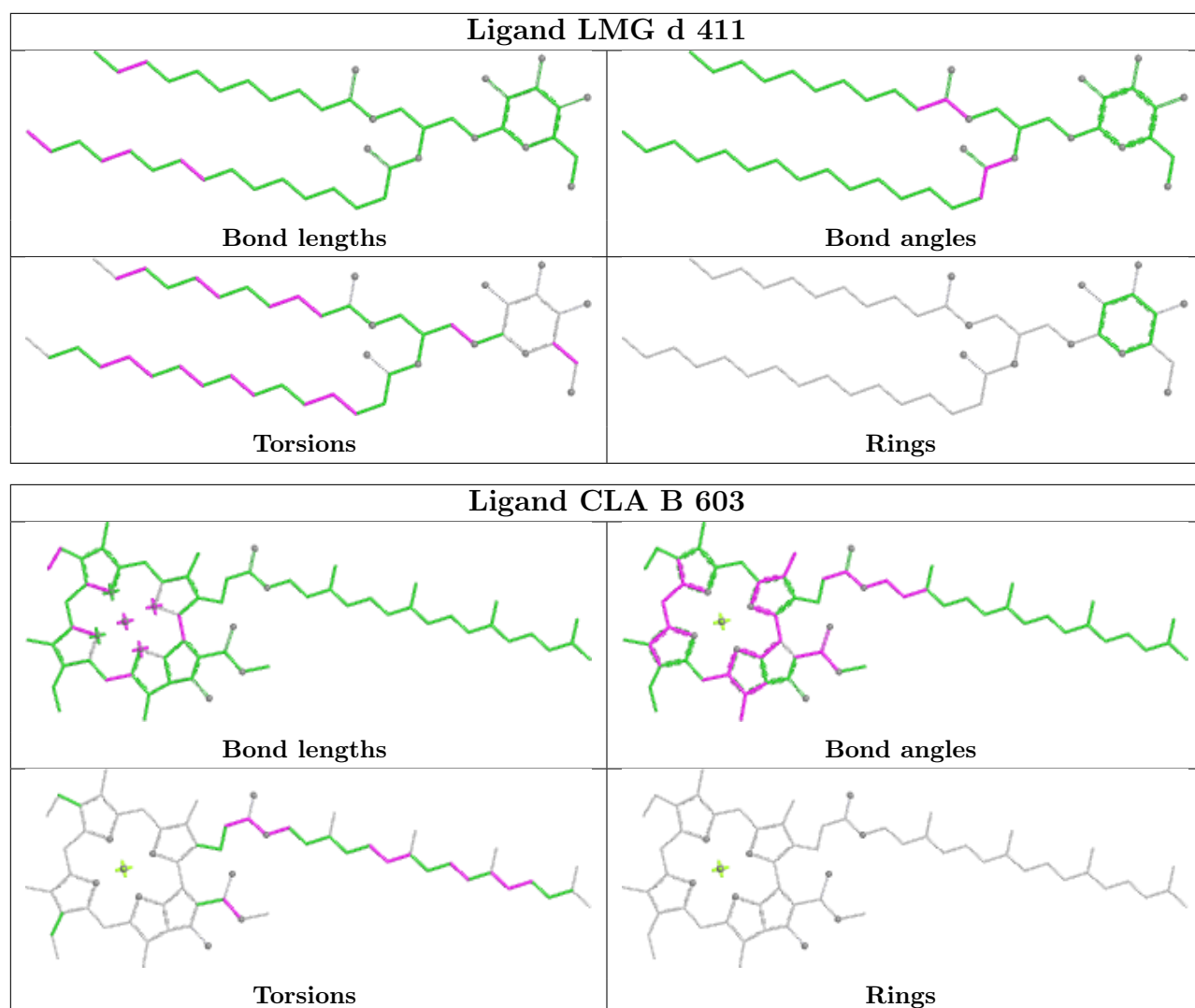


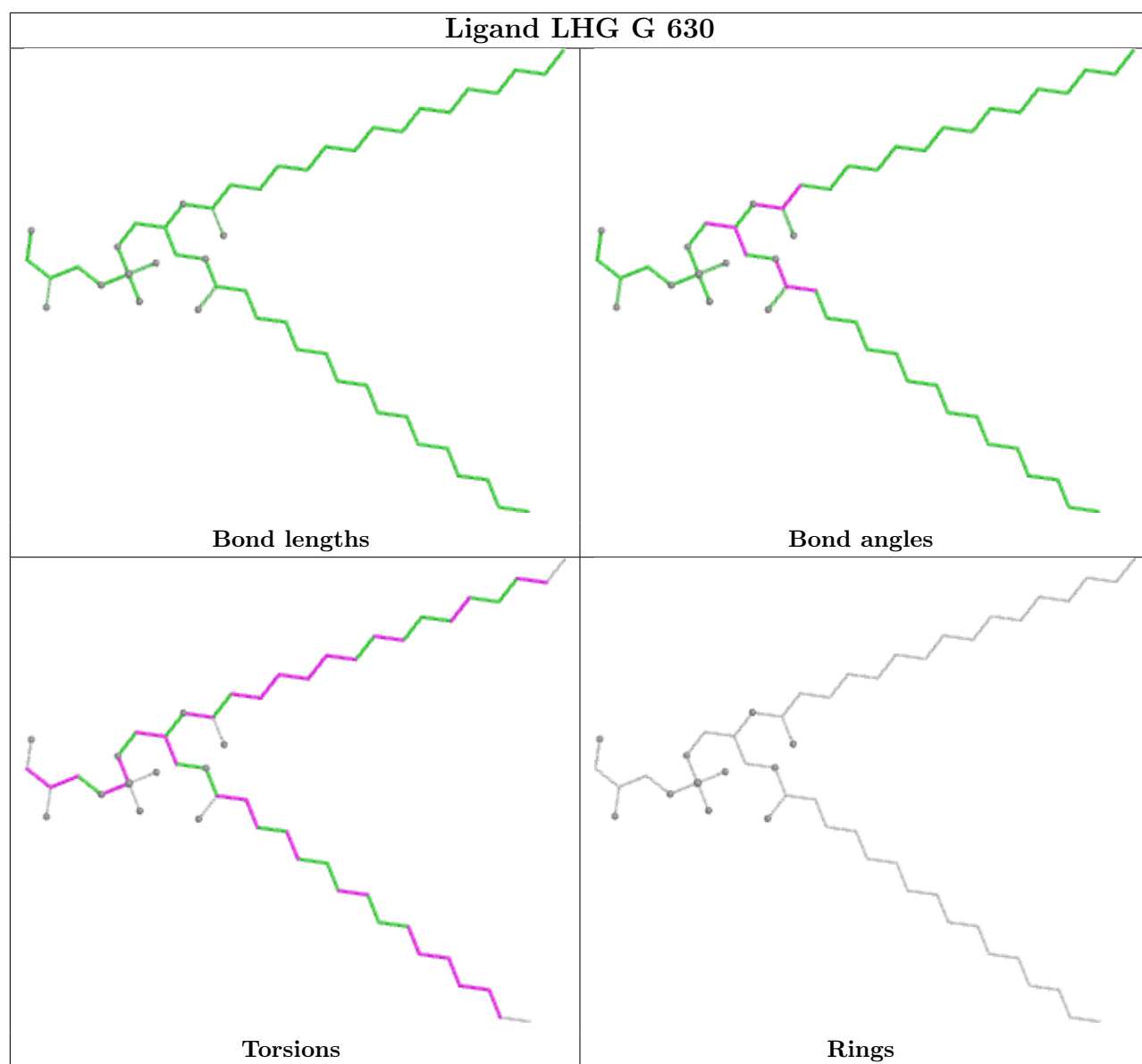
Ligand LUT Y 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

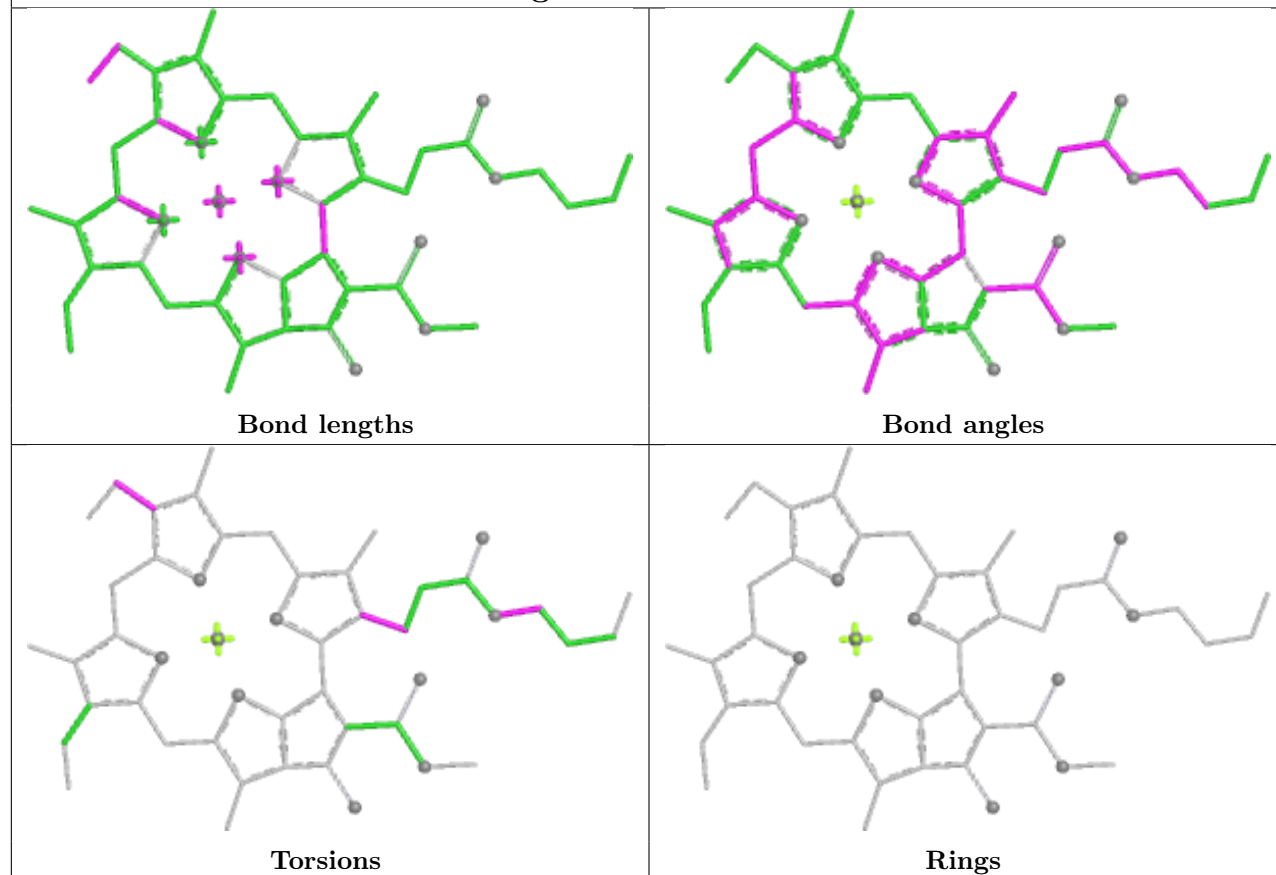
Ligand CLA B 606	
	
Bond lengths	Bond angles
	
Torsions	Rings



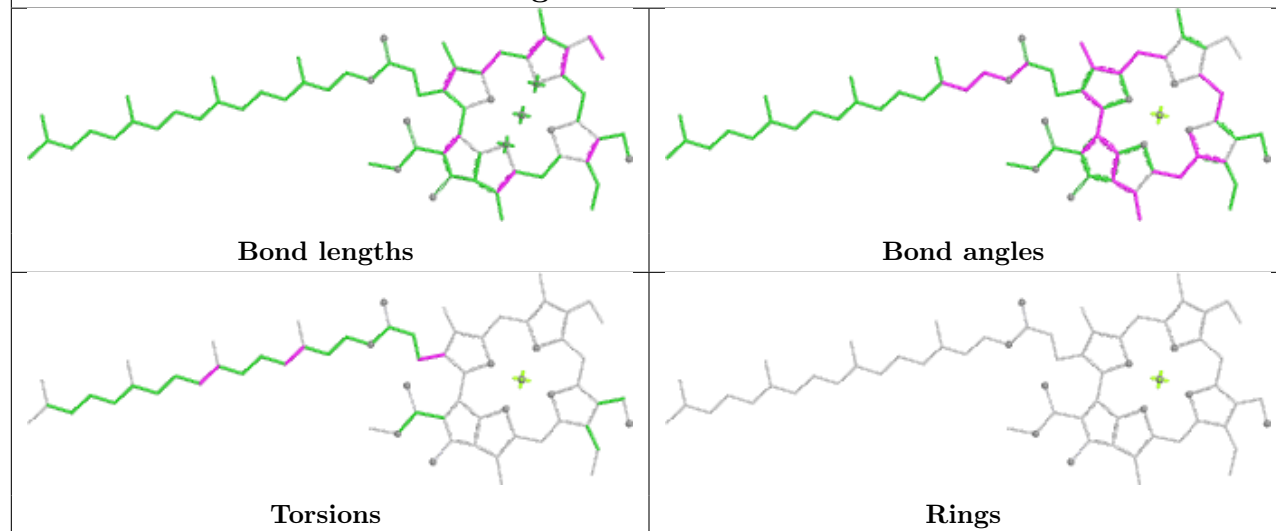


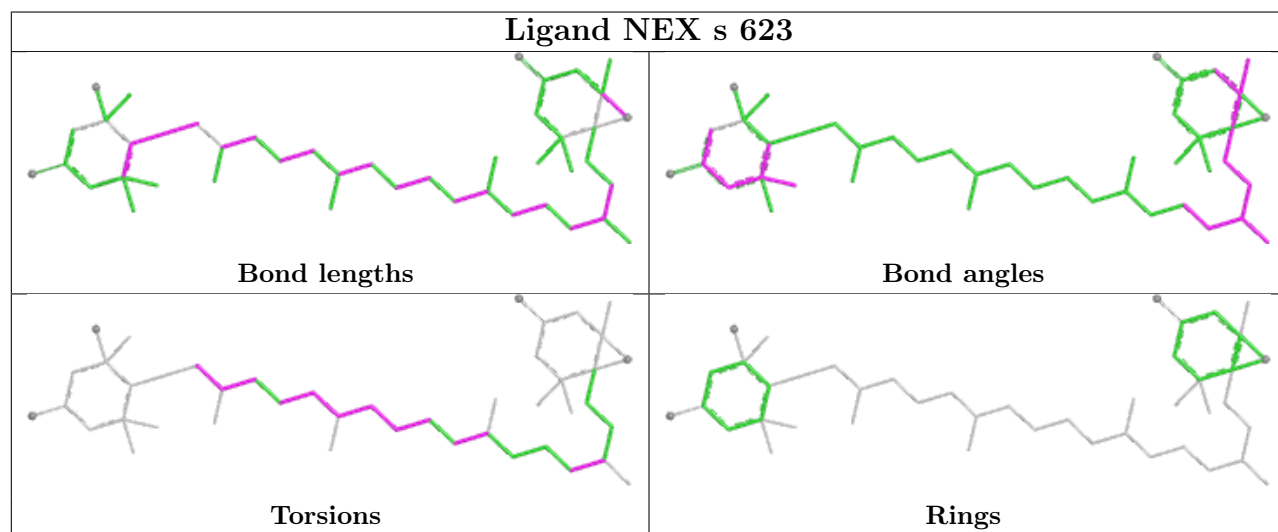
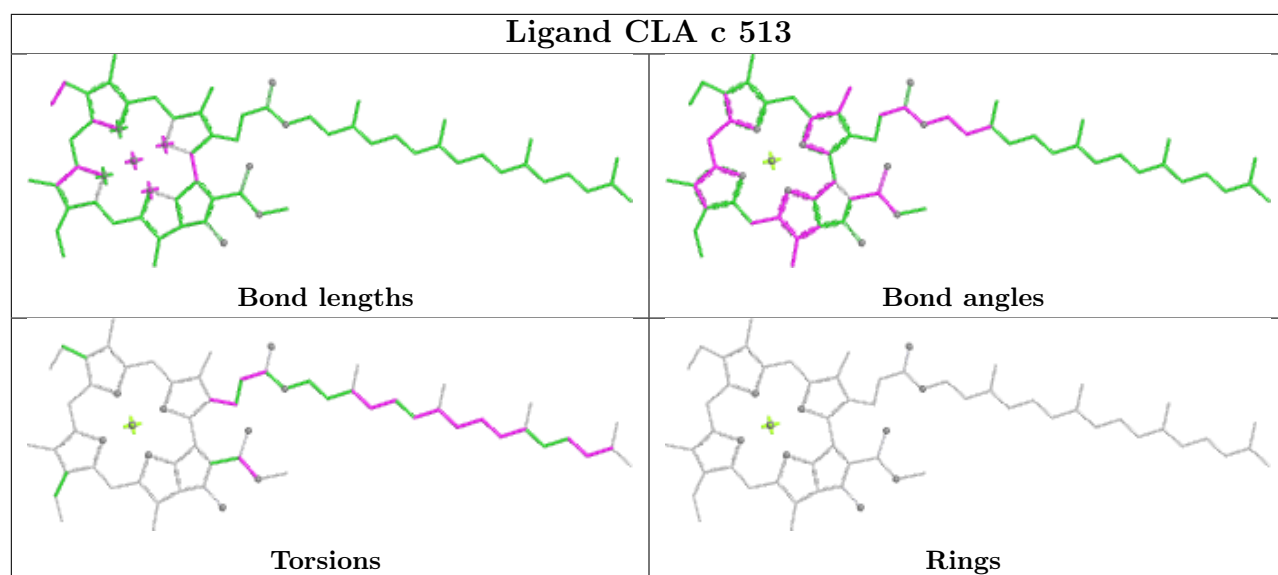


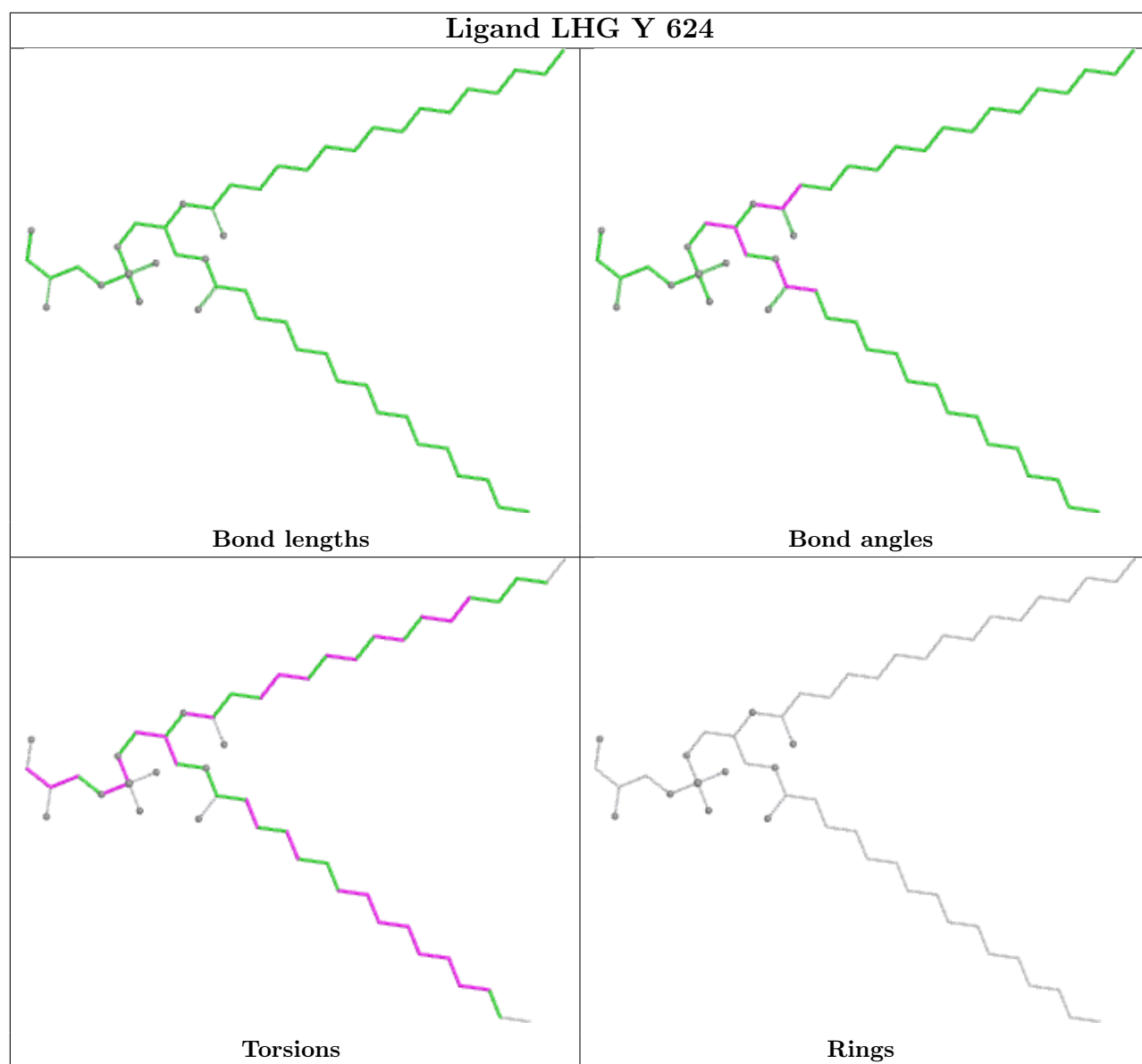
Ligand CLA A 407

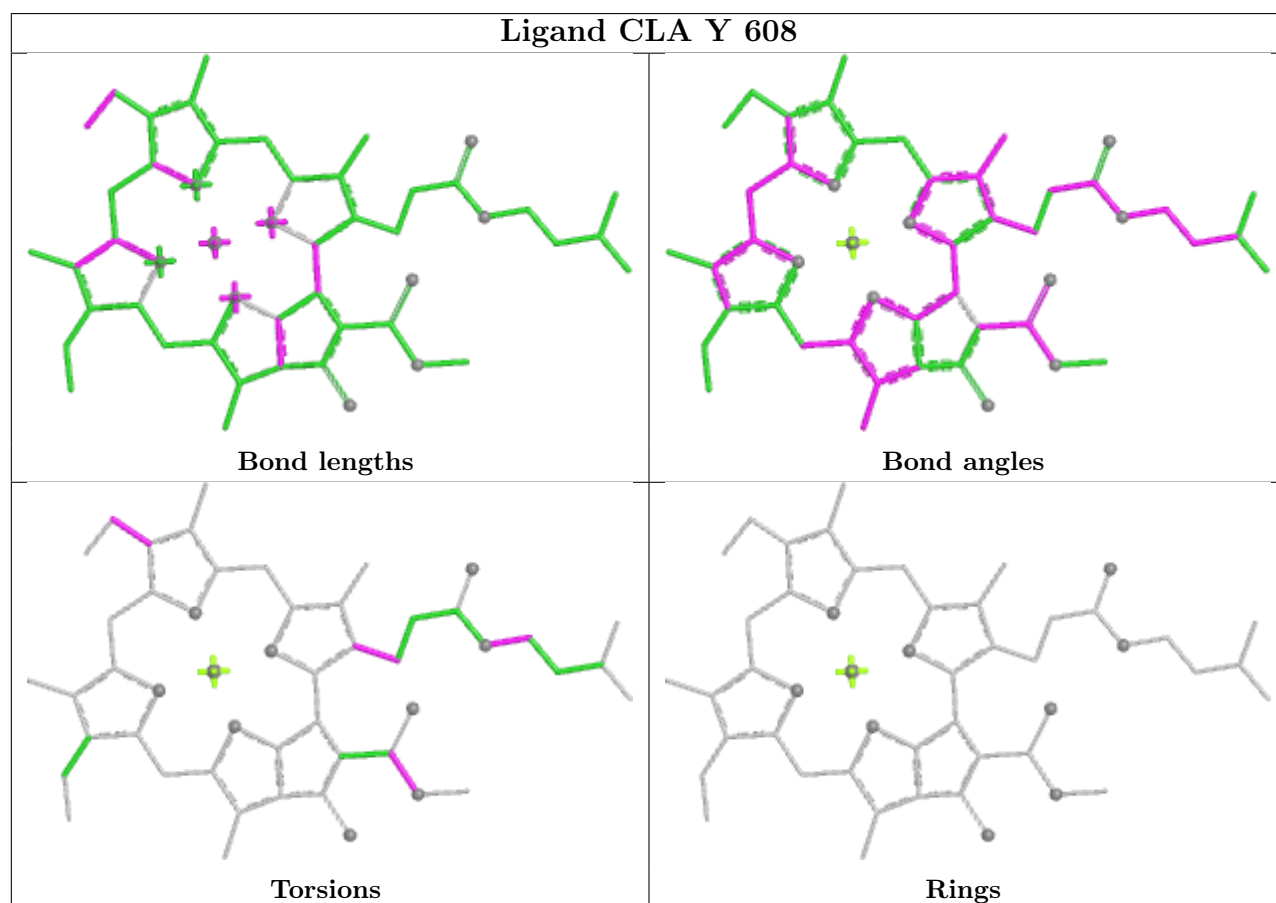
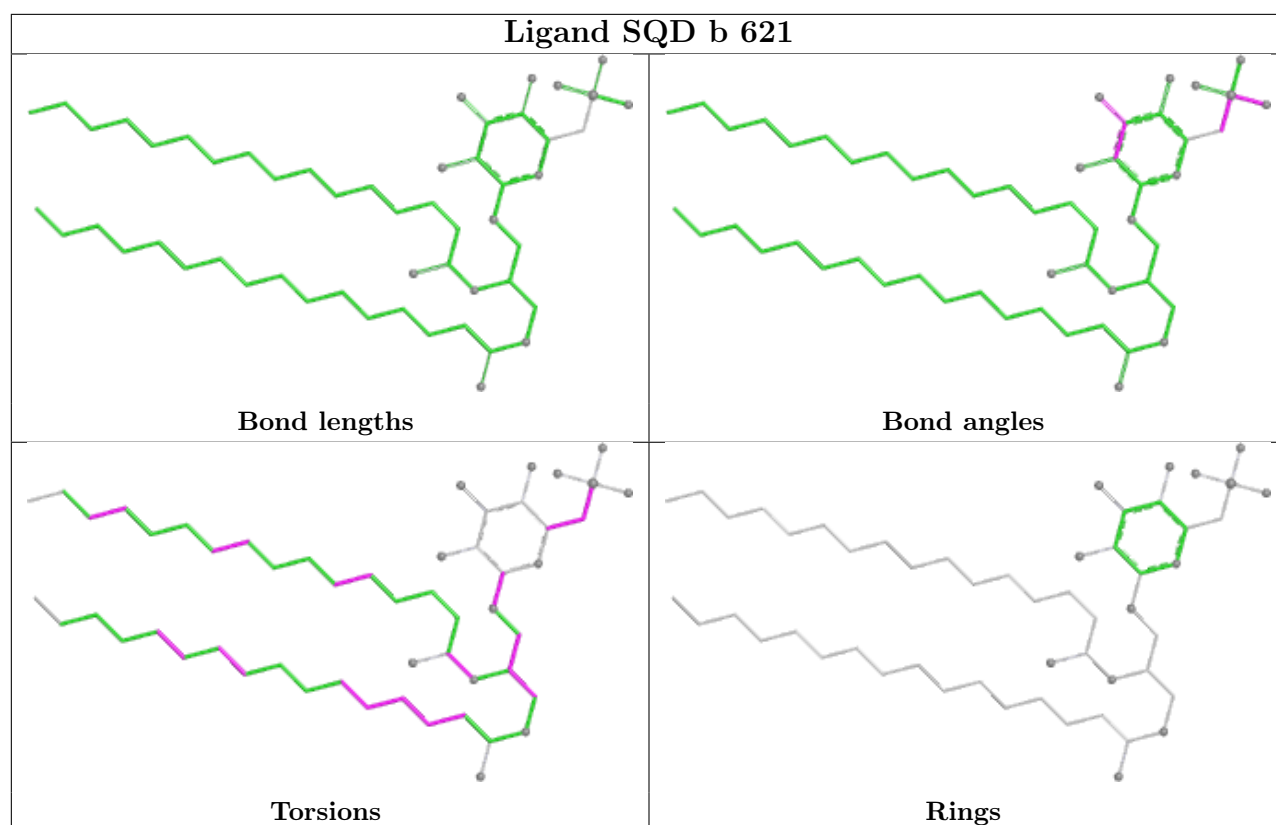


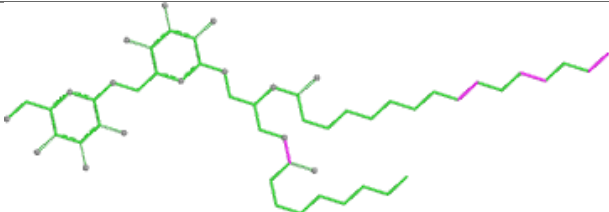
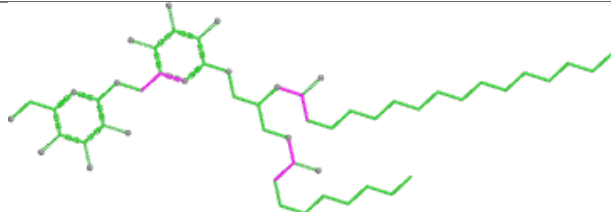
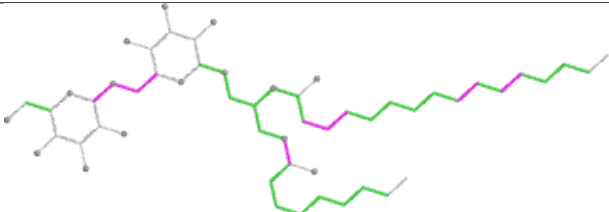
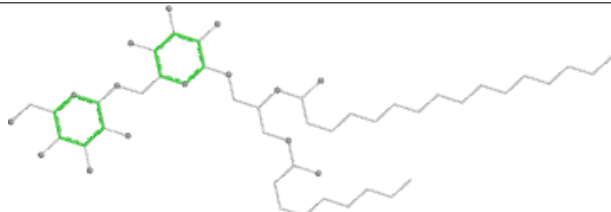
Ligand CHL Y 601

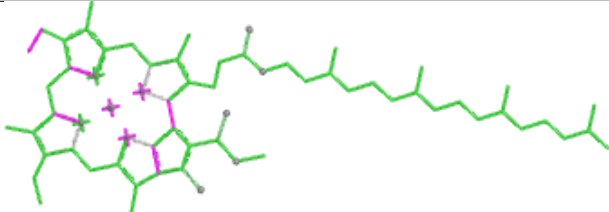
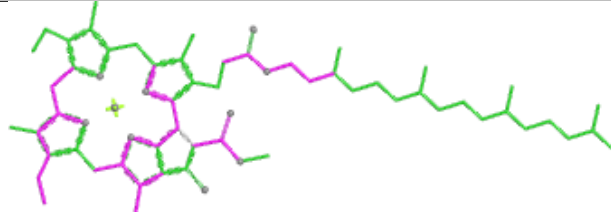
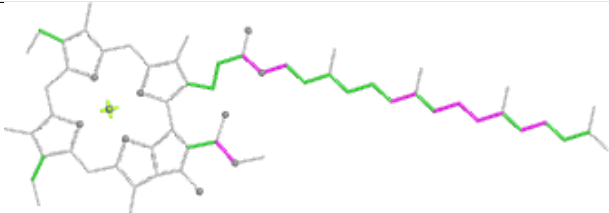
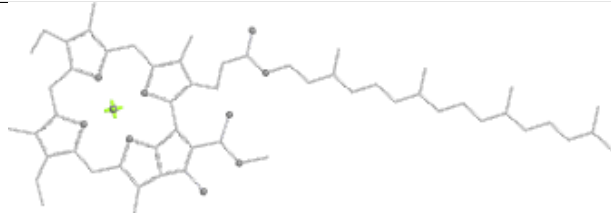


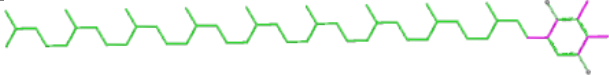
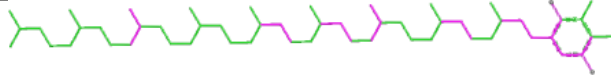
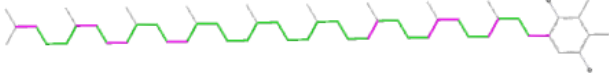
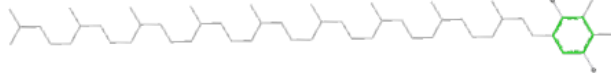


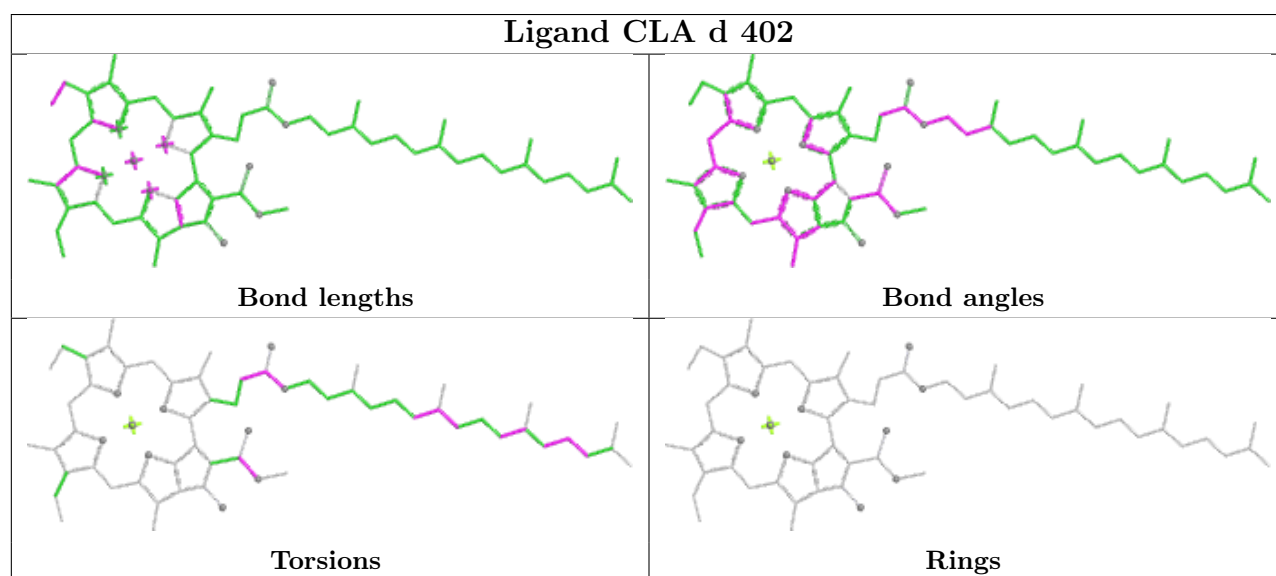
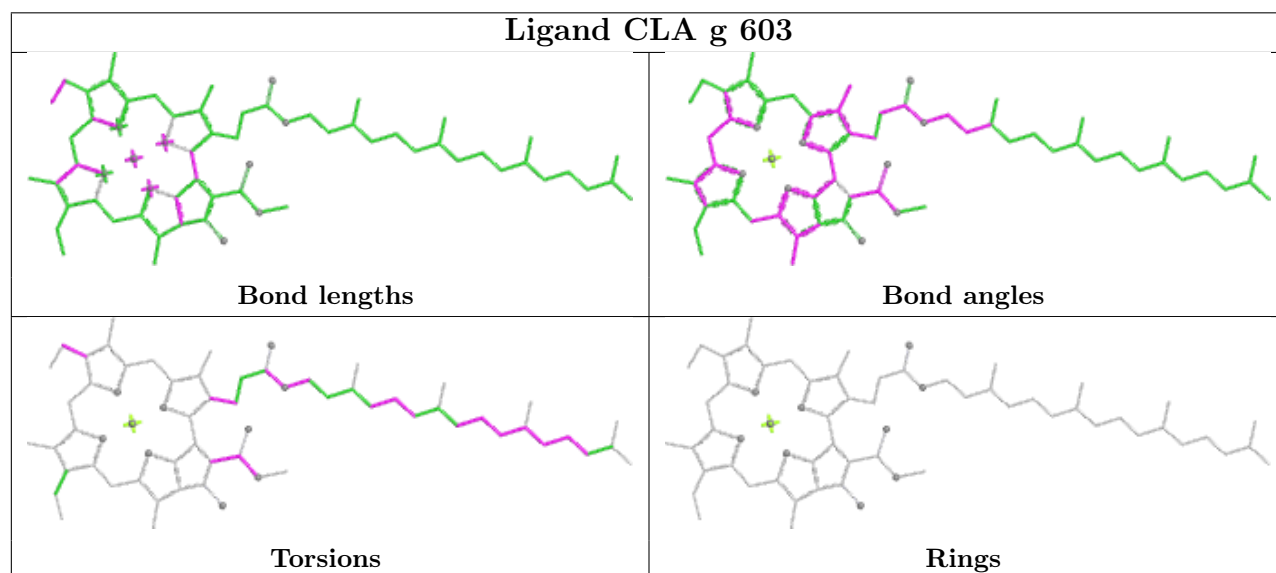
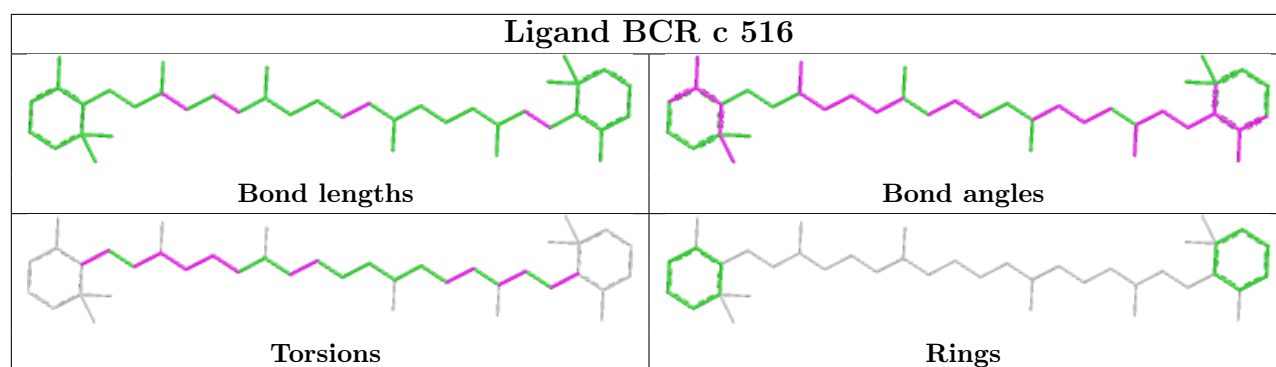


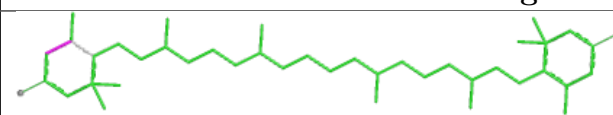
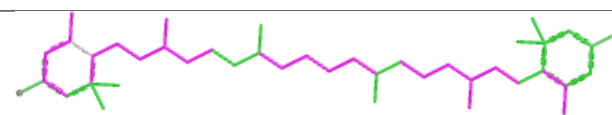
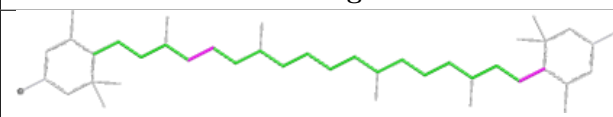
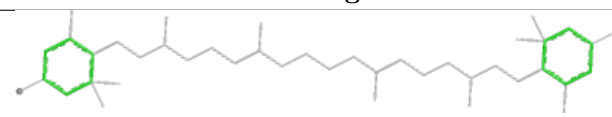


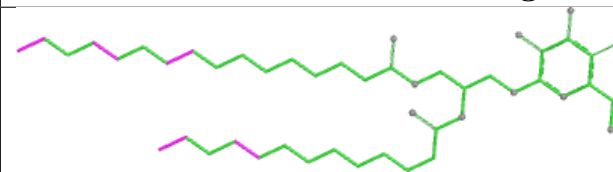
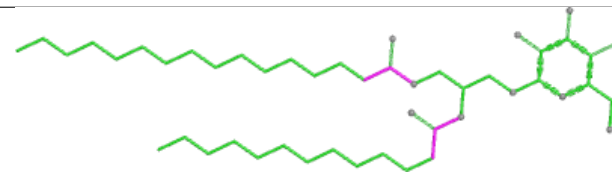
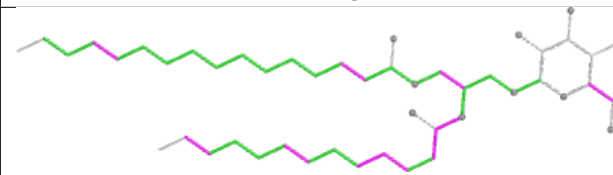
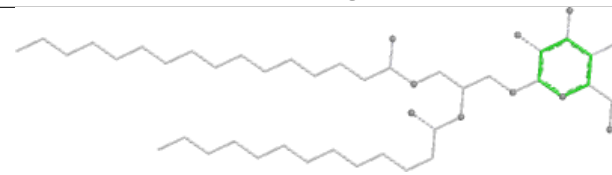
Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

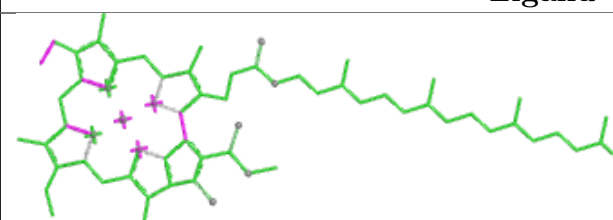
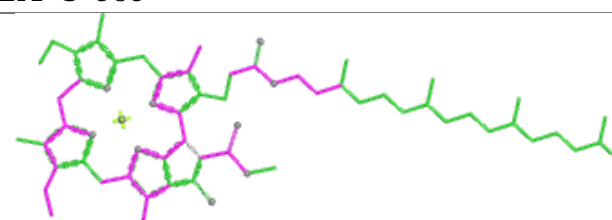
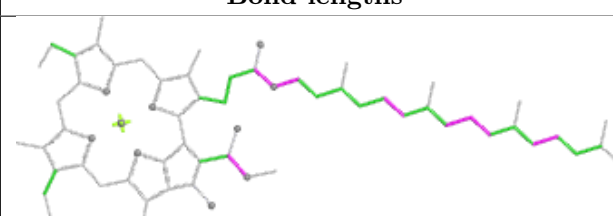
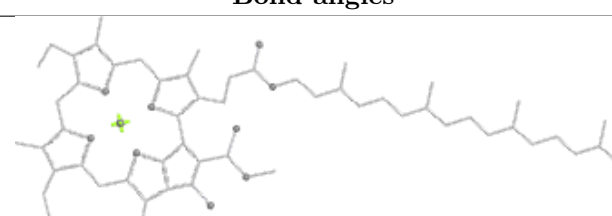
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

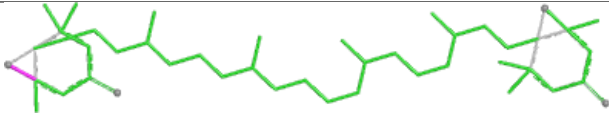
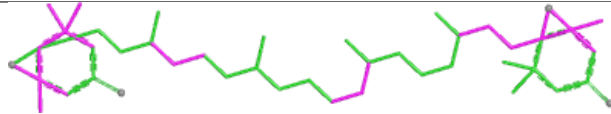
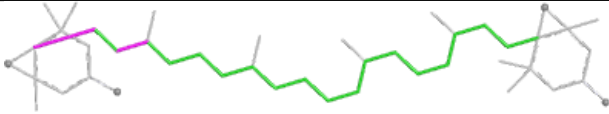
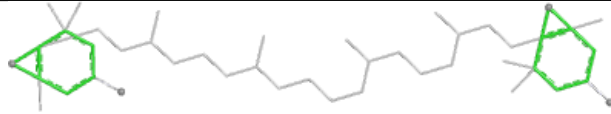
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

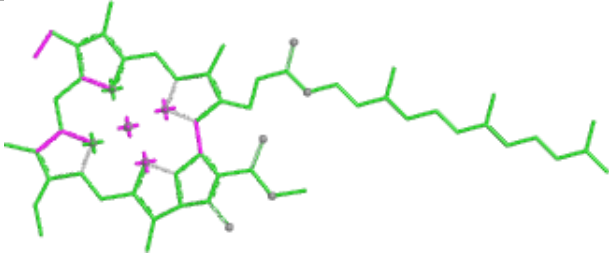
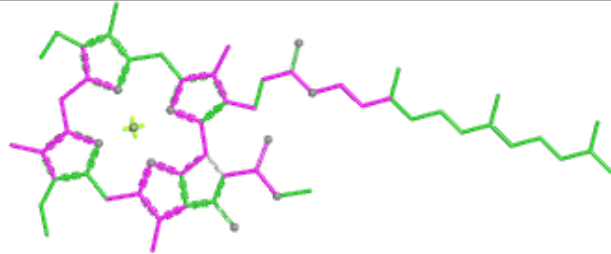
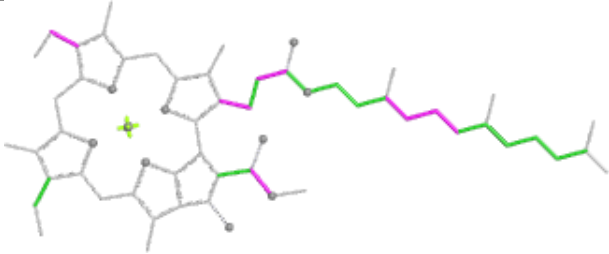
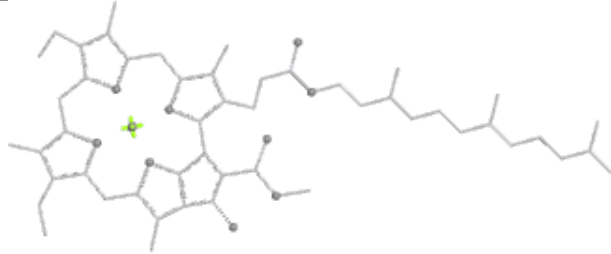


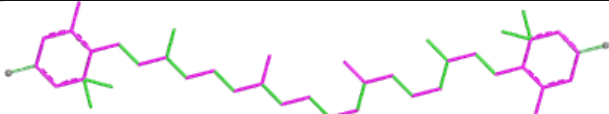
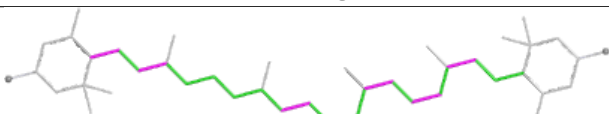
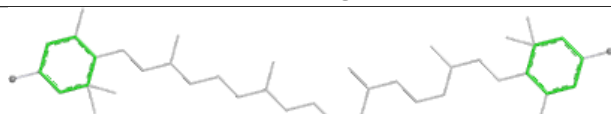
Ligand LUT N 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

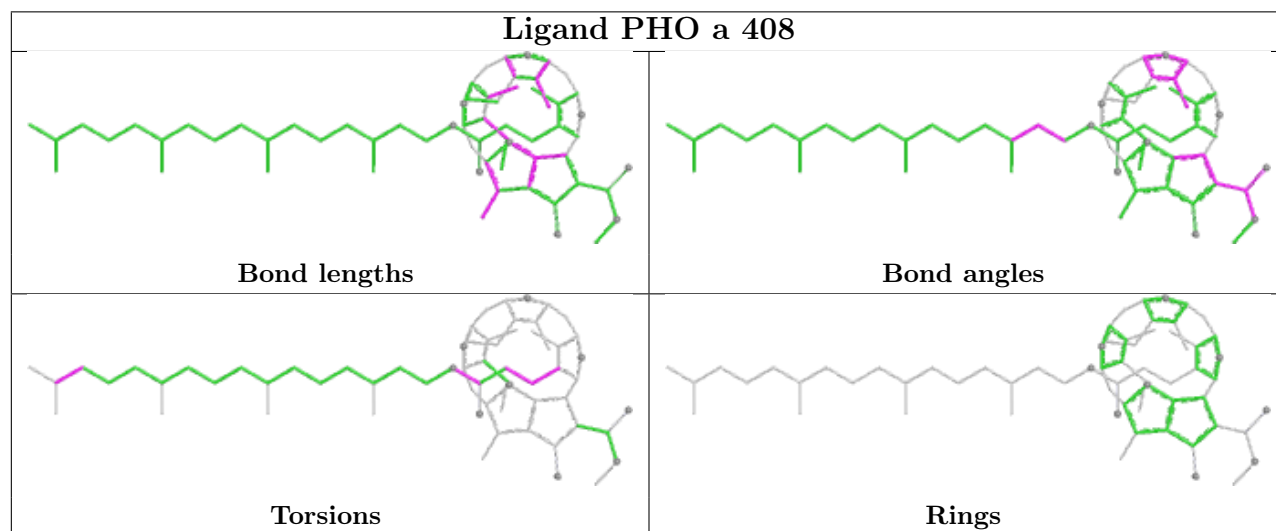
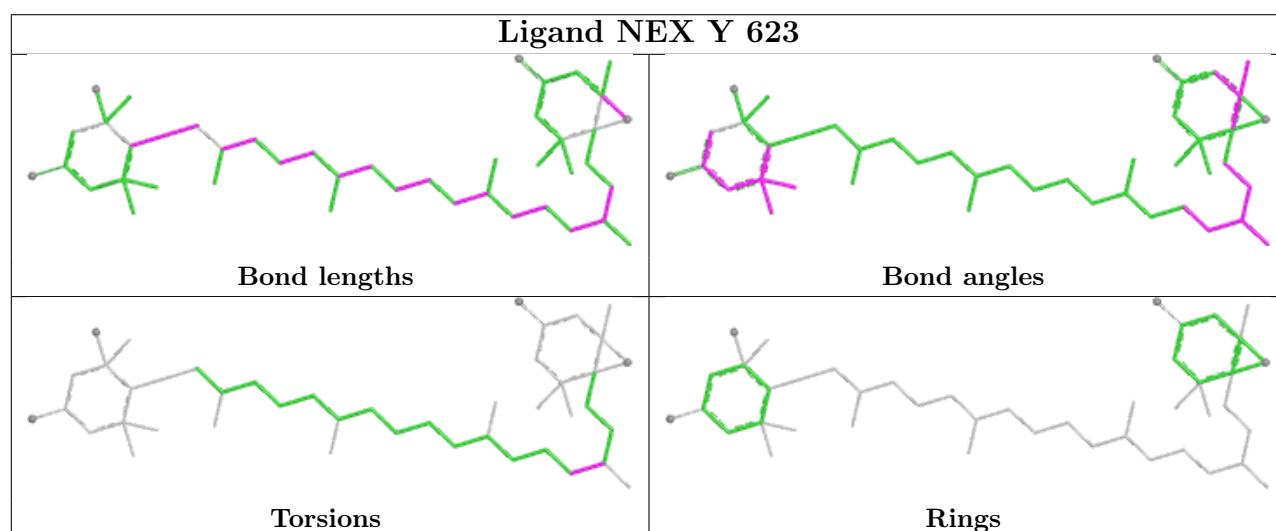
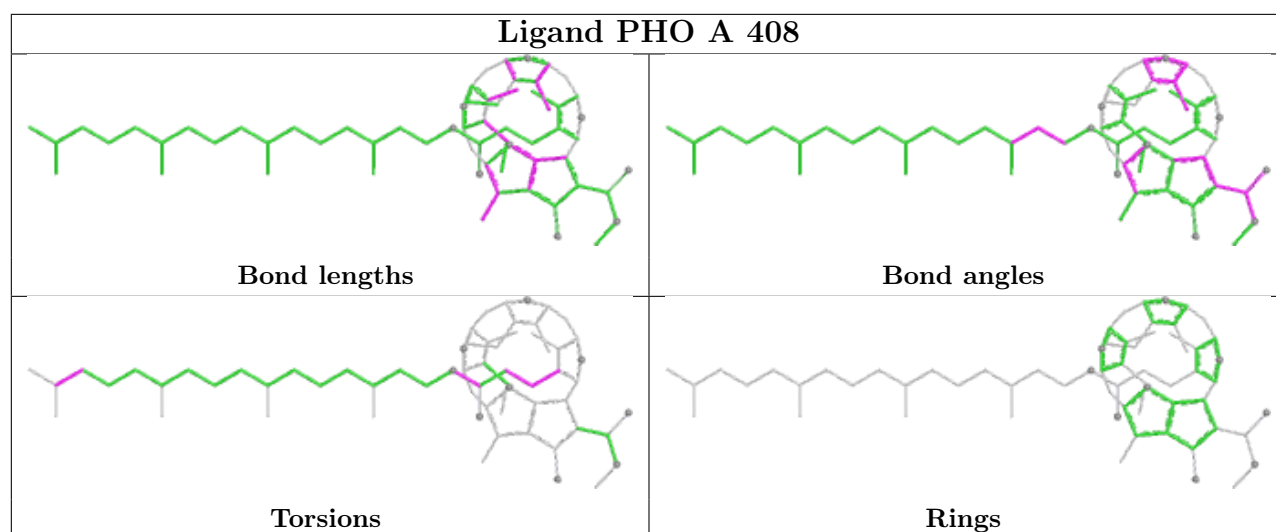
Ligand LMG h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

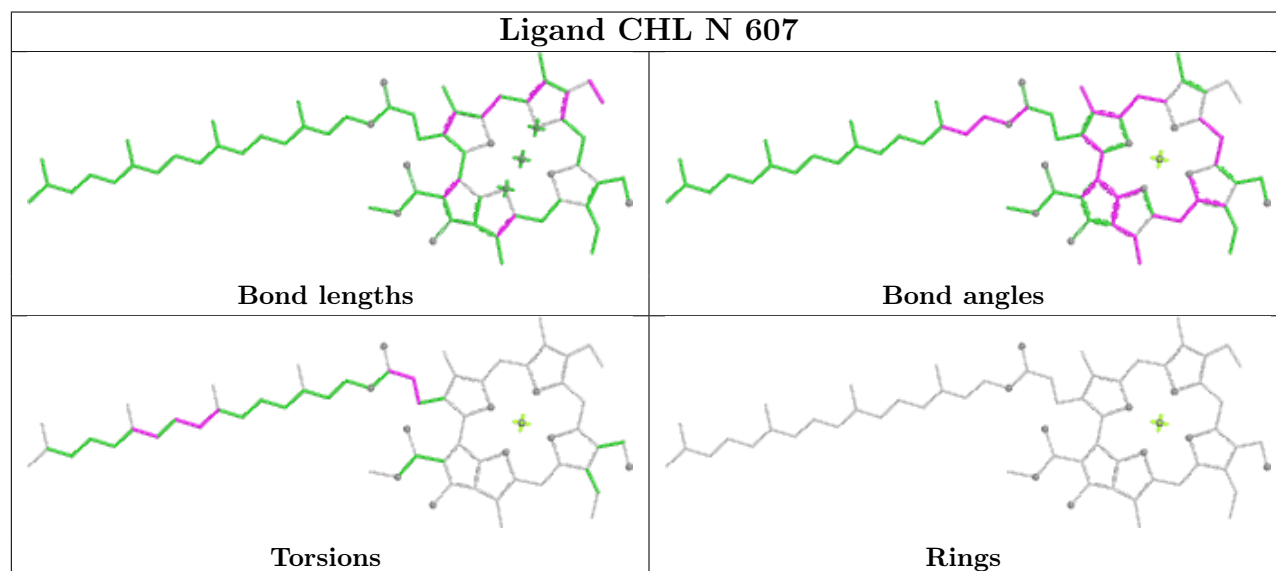
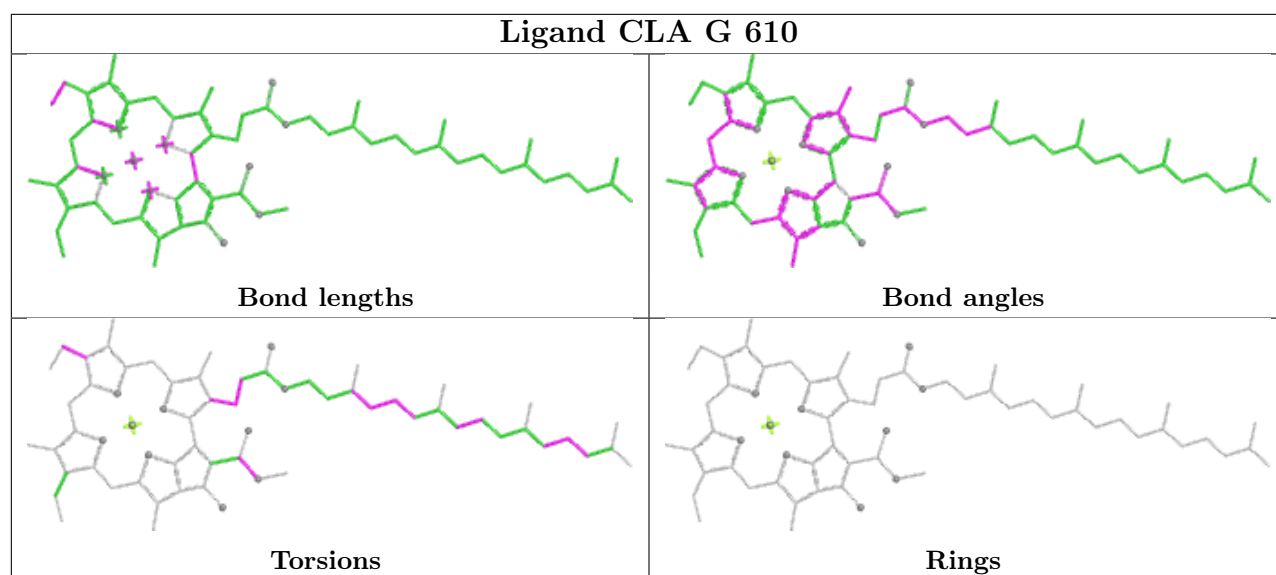
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT Y 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

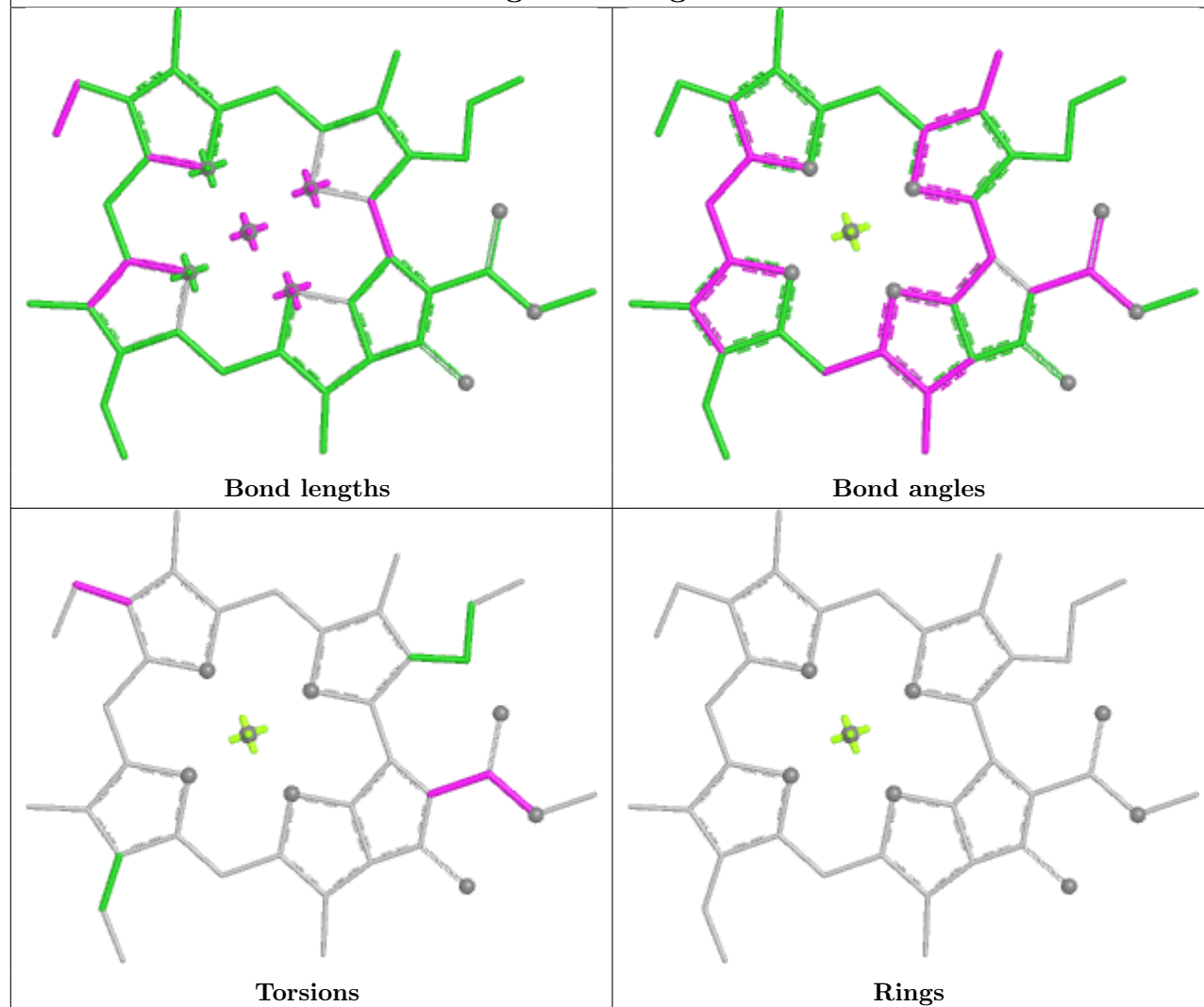
Ligand CLA R 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C7Z B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

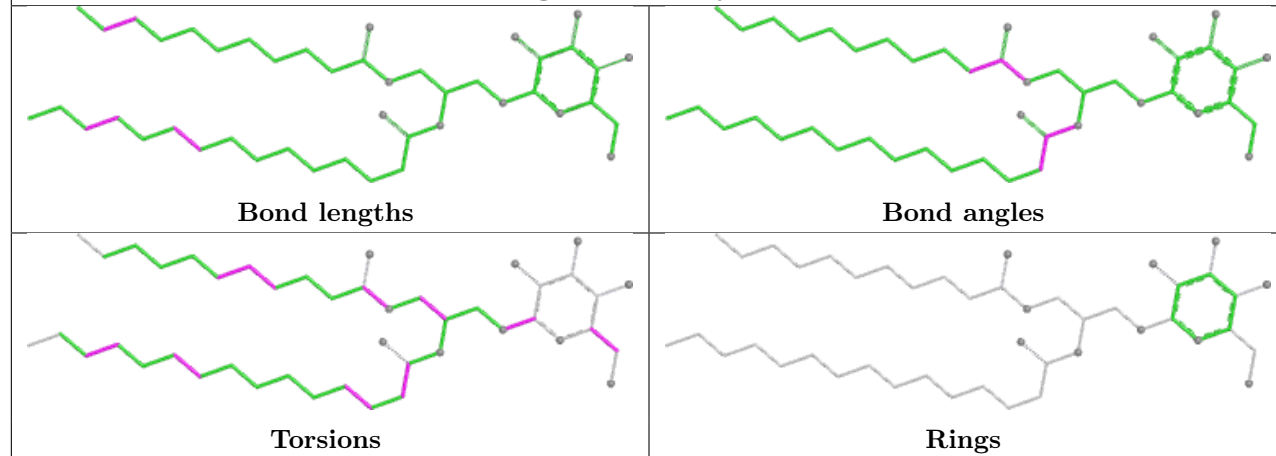


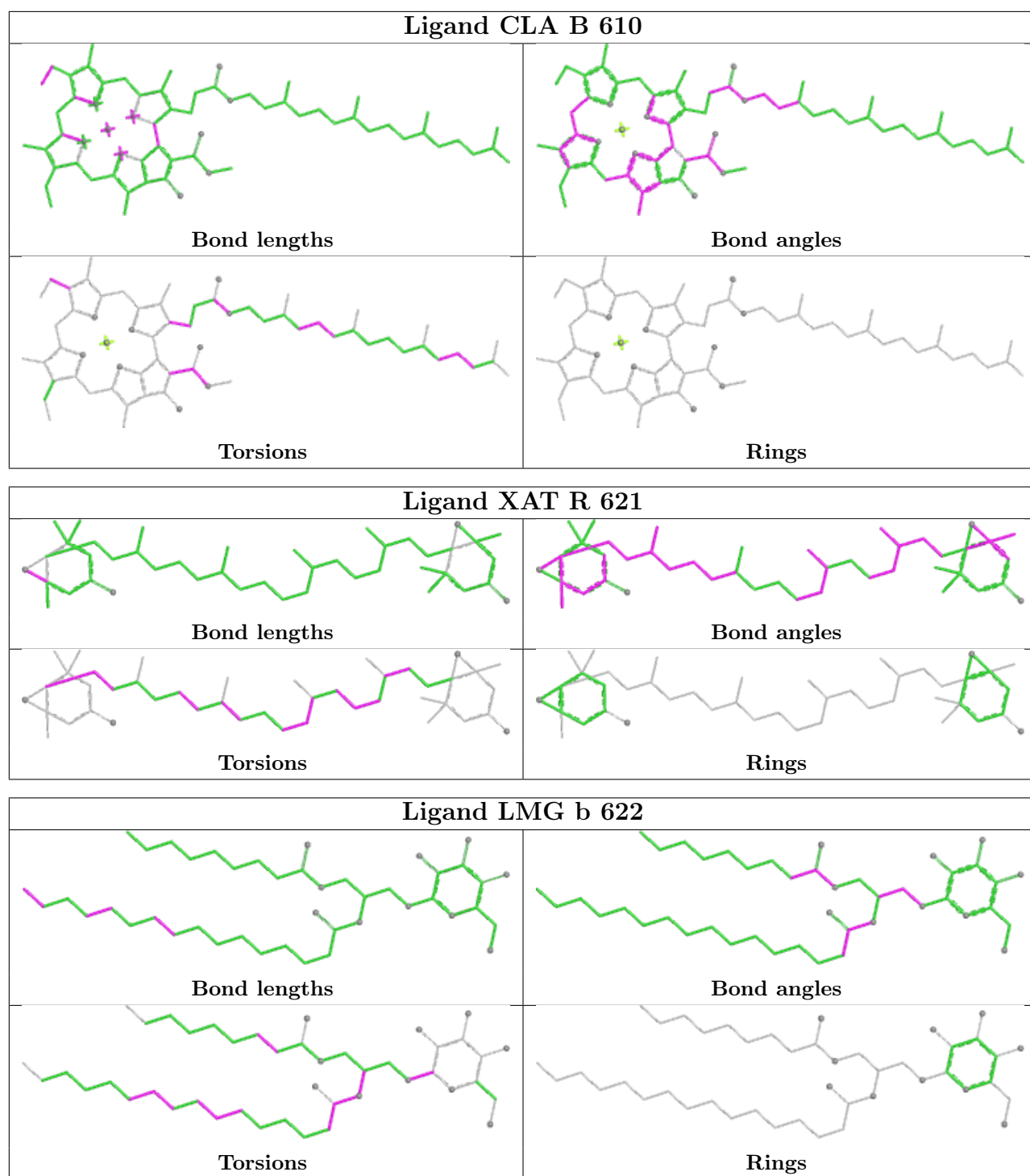


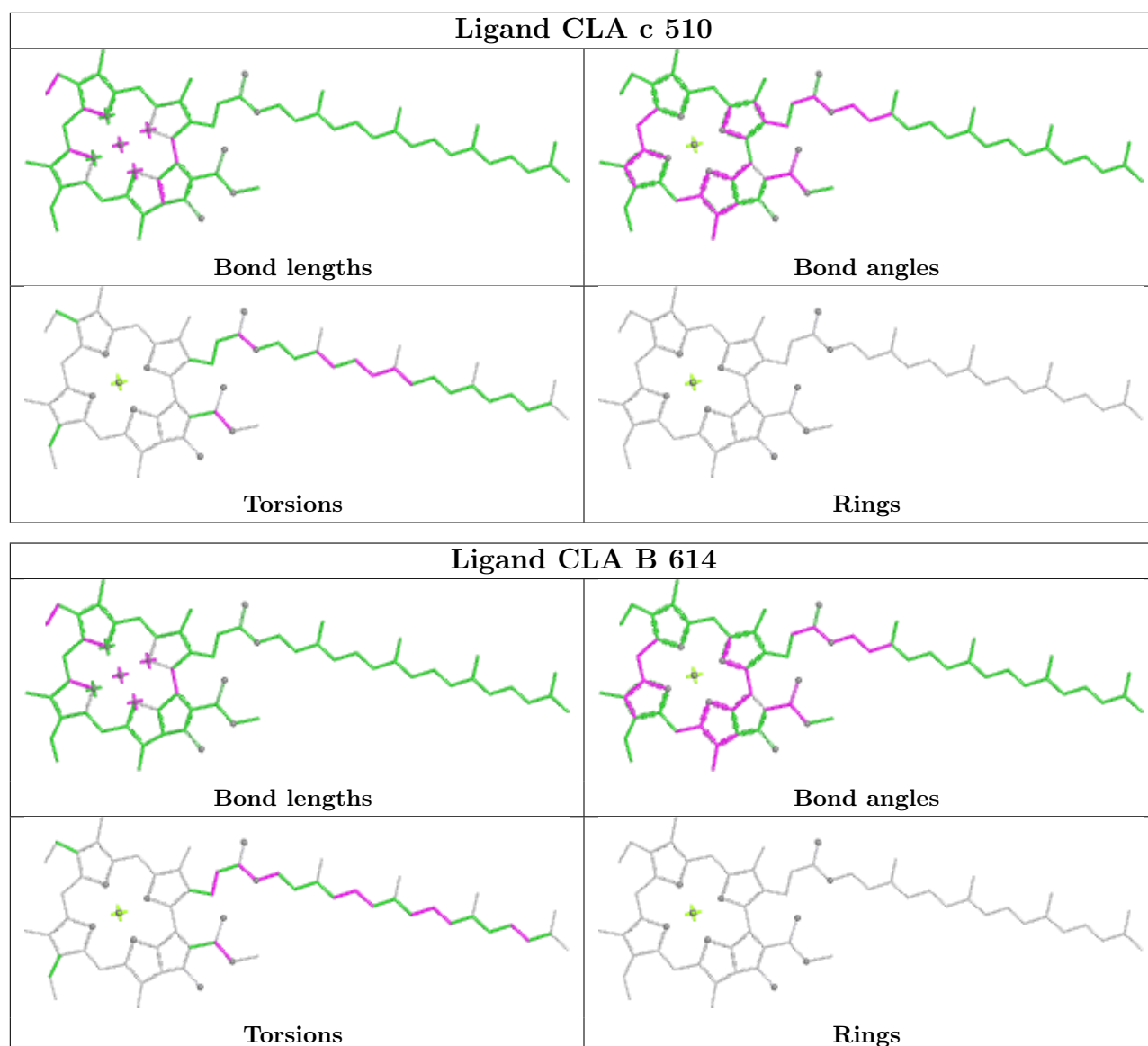
Ligand CLA g 612



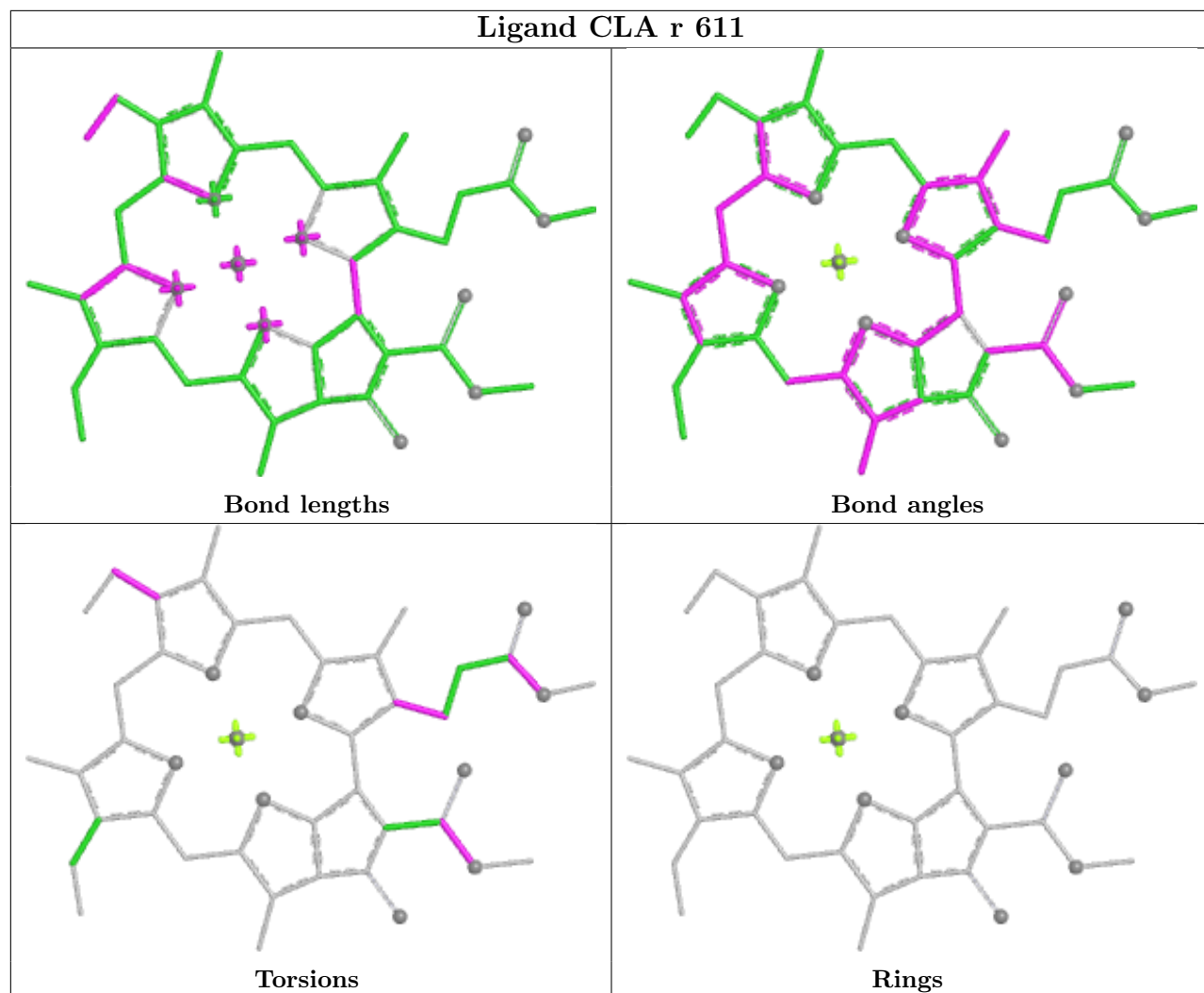
Ligand LMG j 101

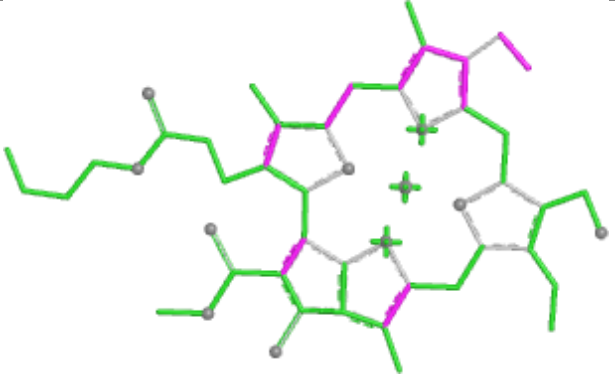
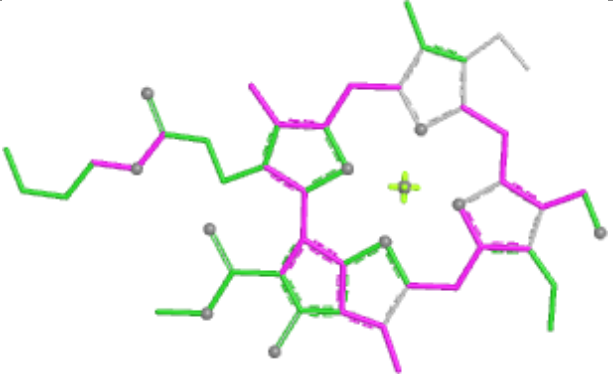
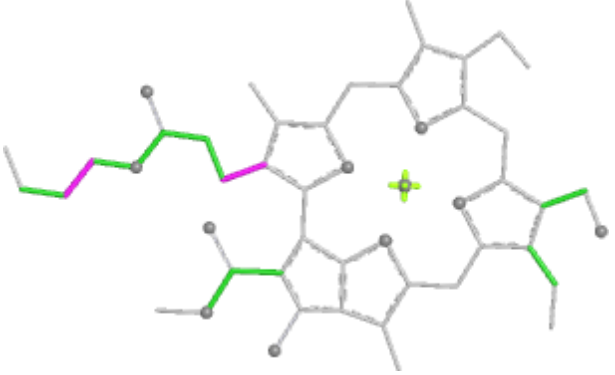
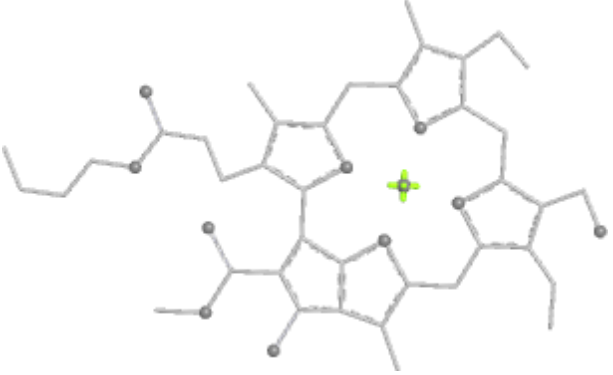
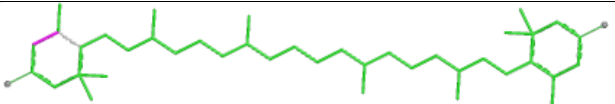
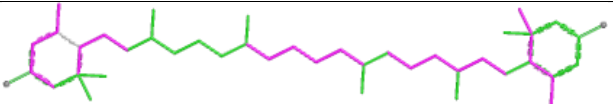
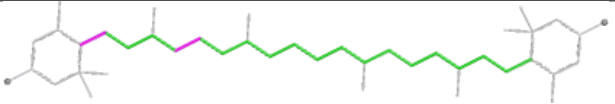
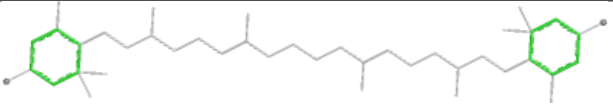
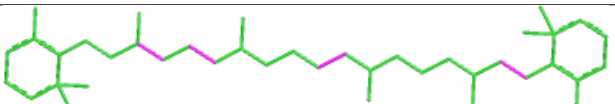
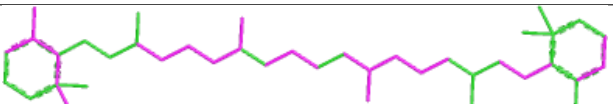
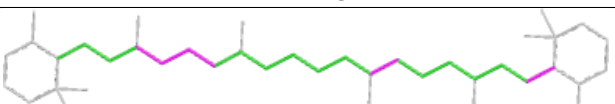
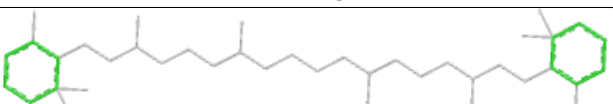


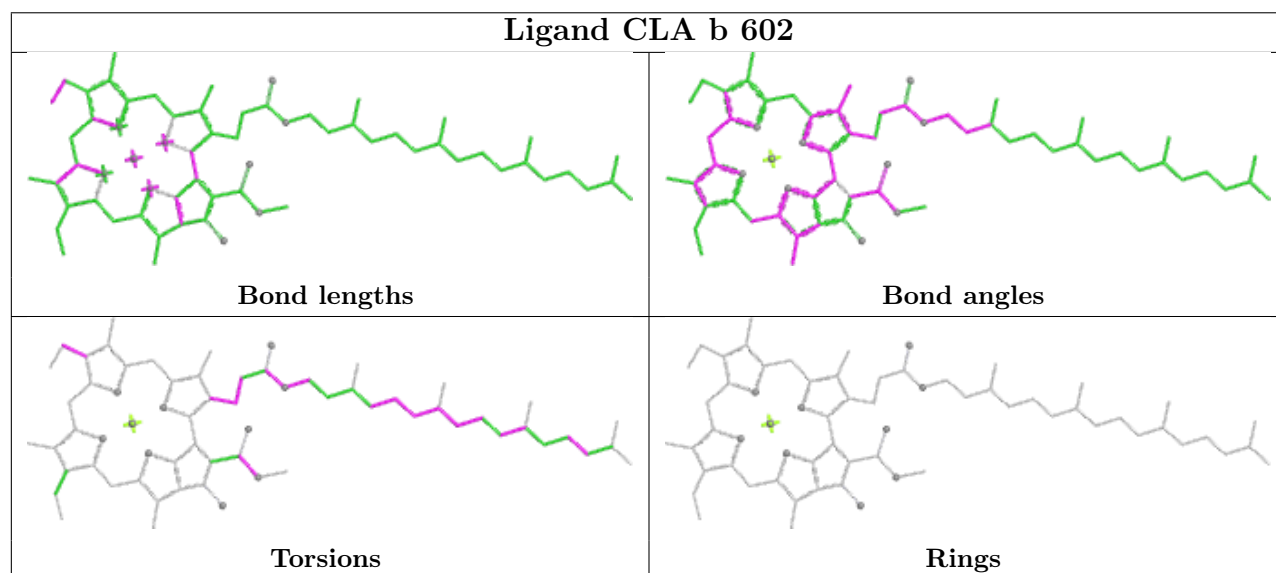
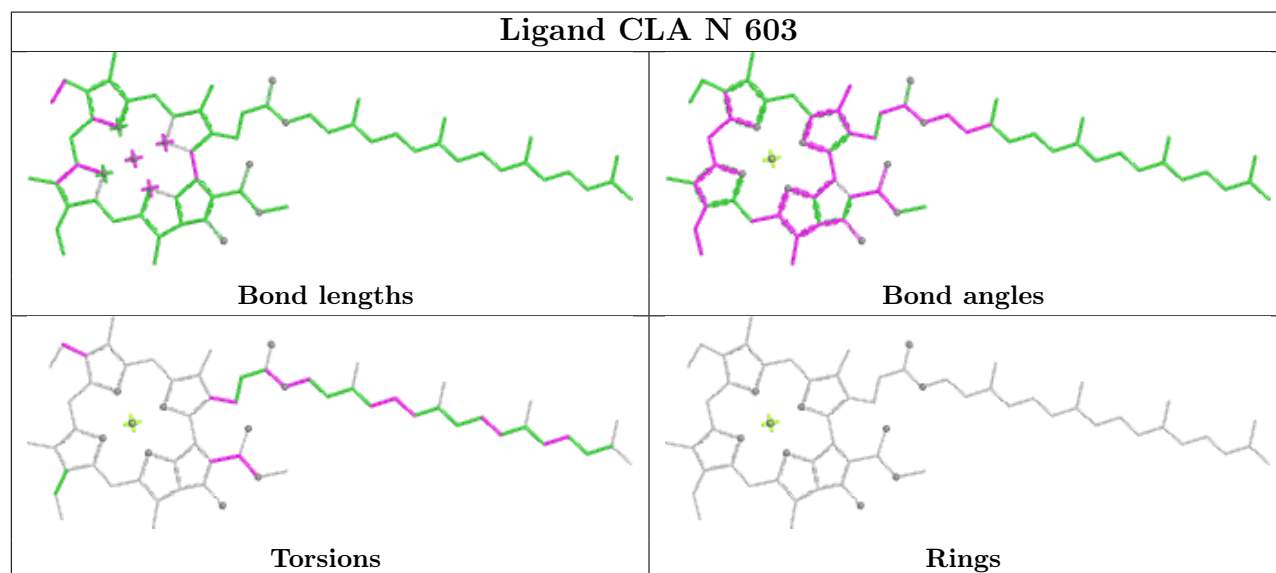
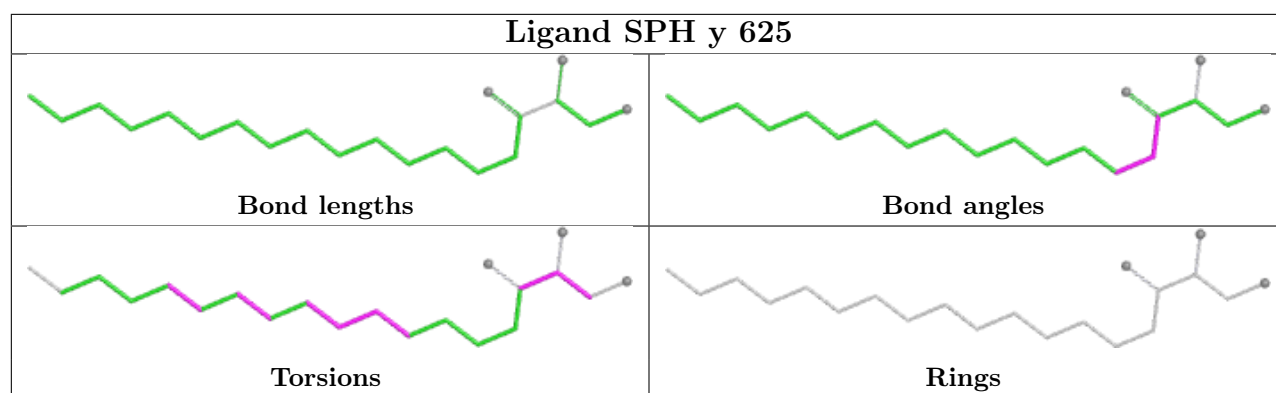


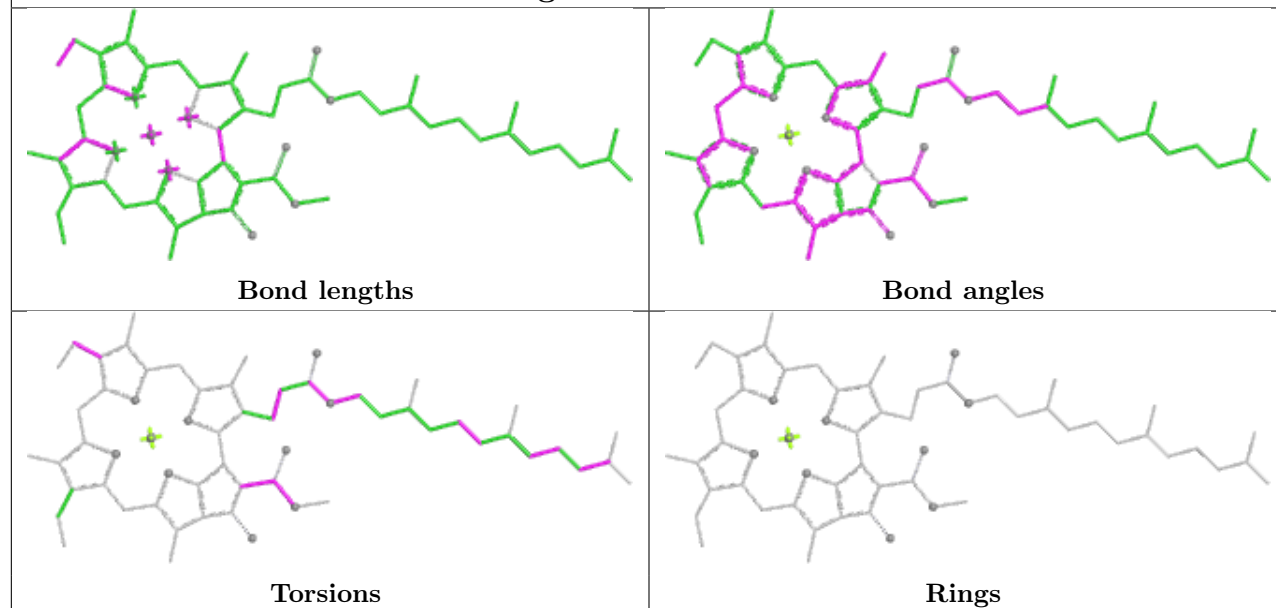
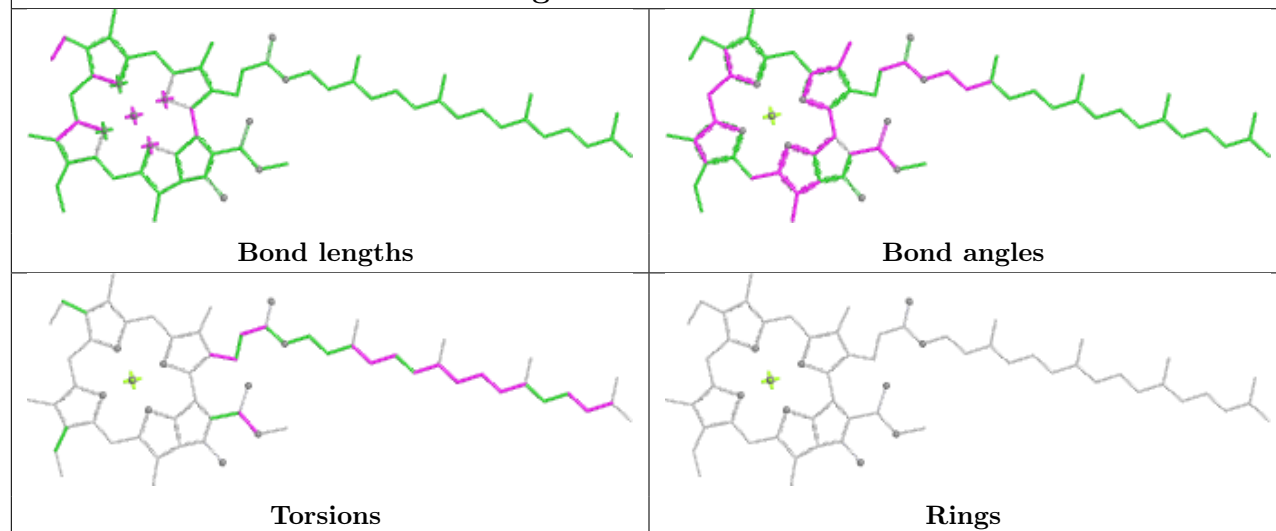


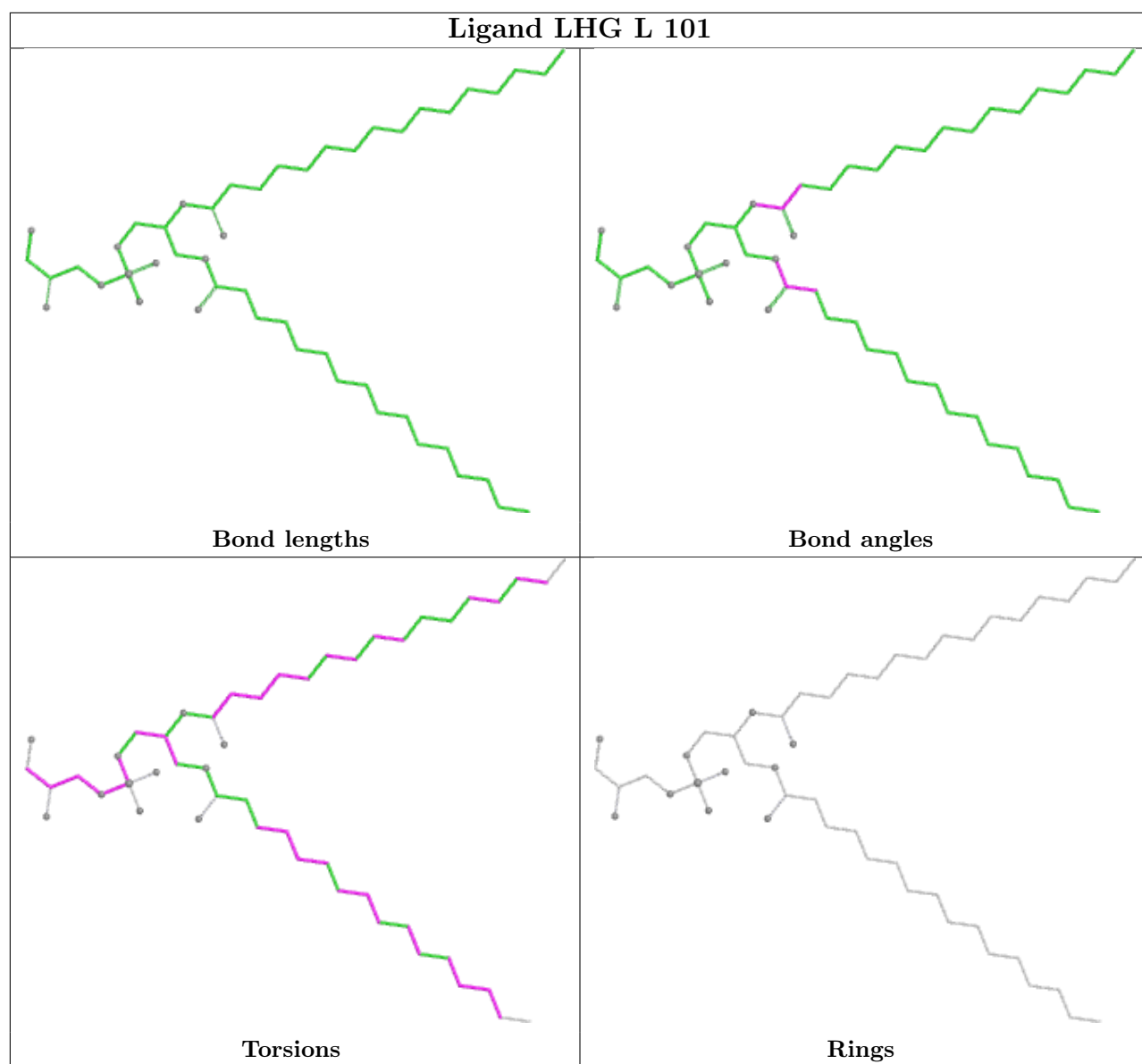
Ligand CLA r 611

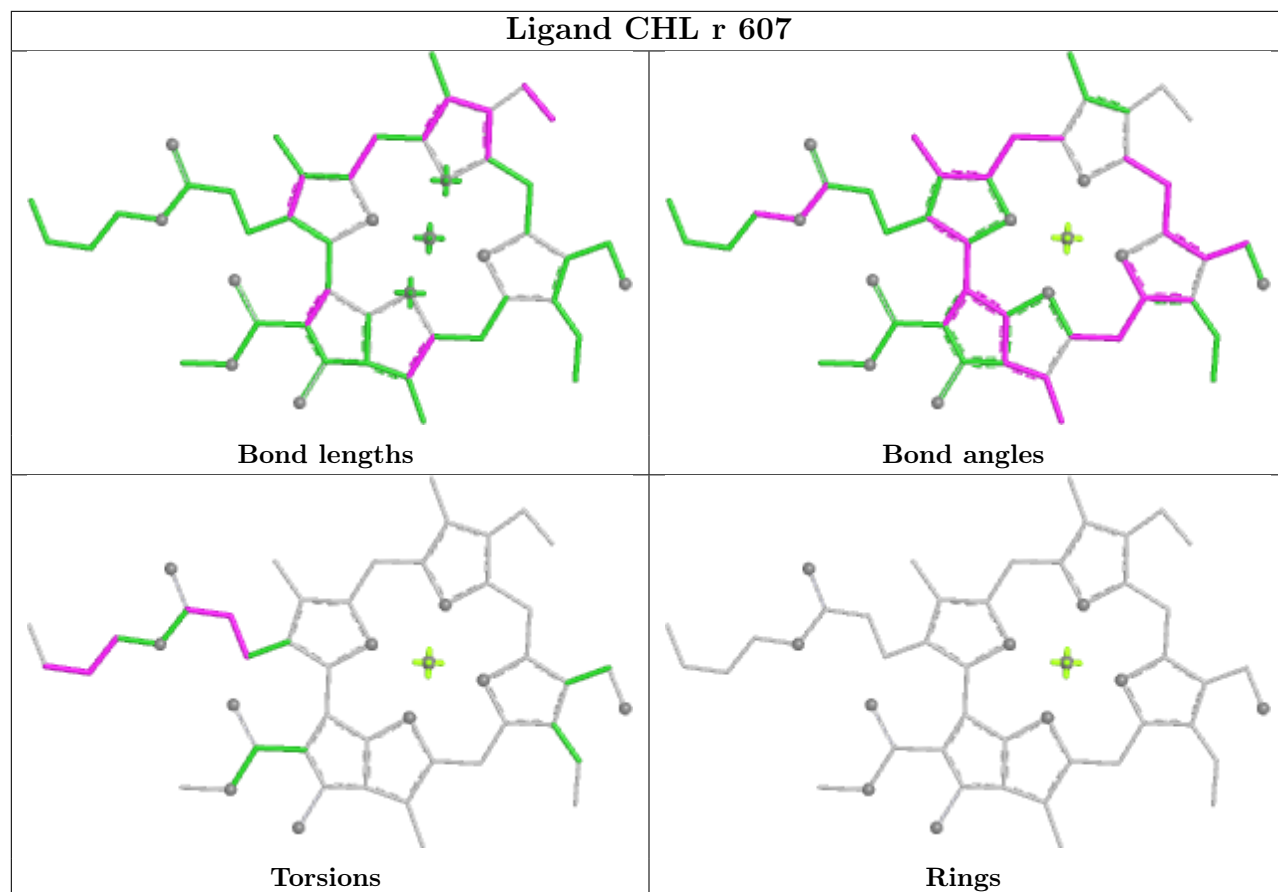


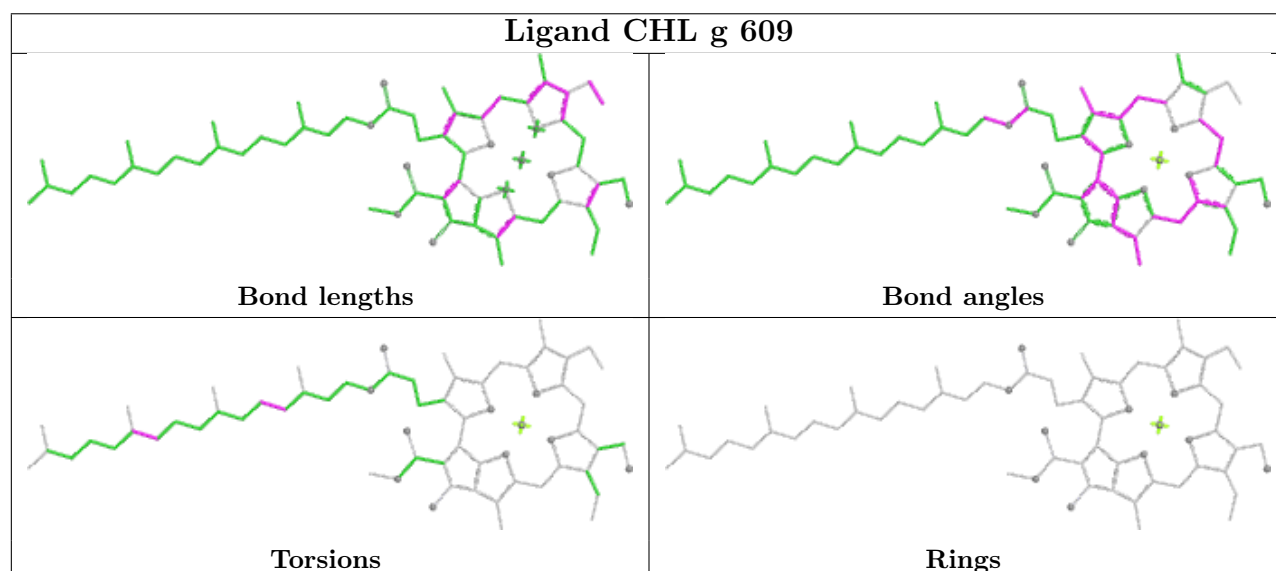
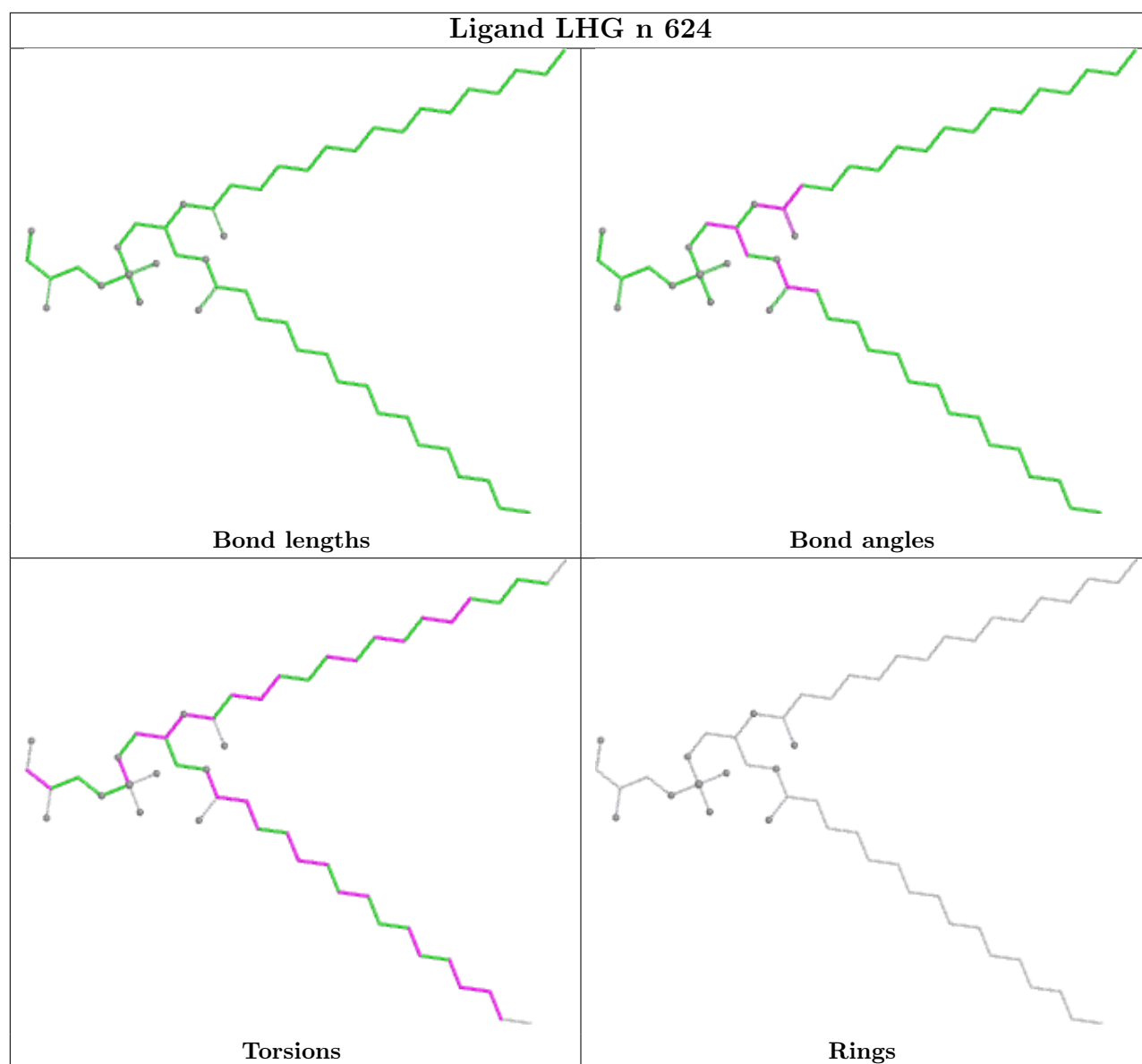
Ligand CHL R 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT y 621	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings



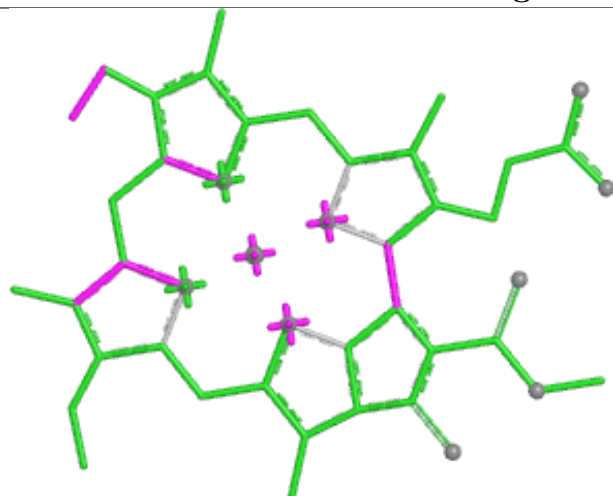
Ligand CLA r 612**Ligand CLA C 513**



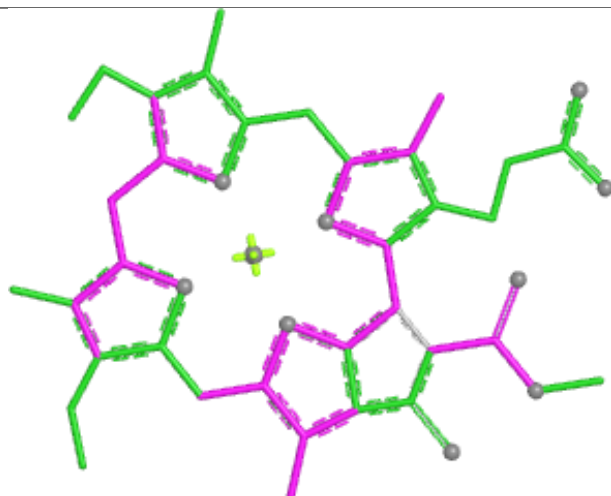




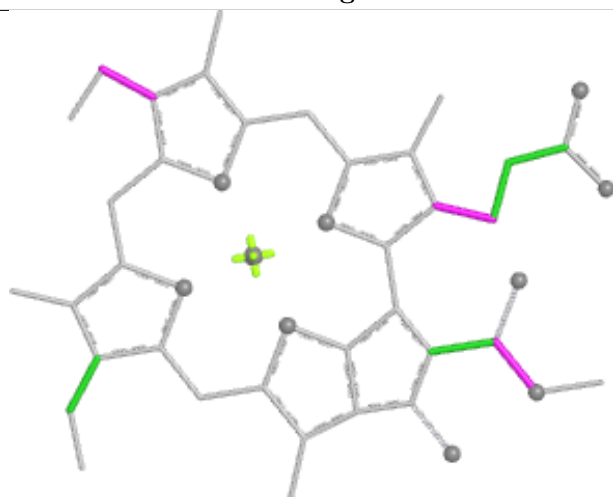
Ligand CLA G 611



Bond lengths



Bond angles

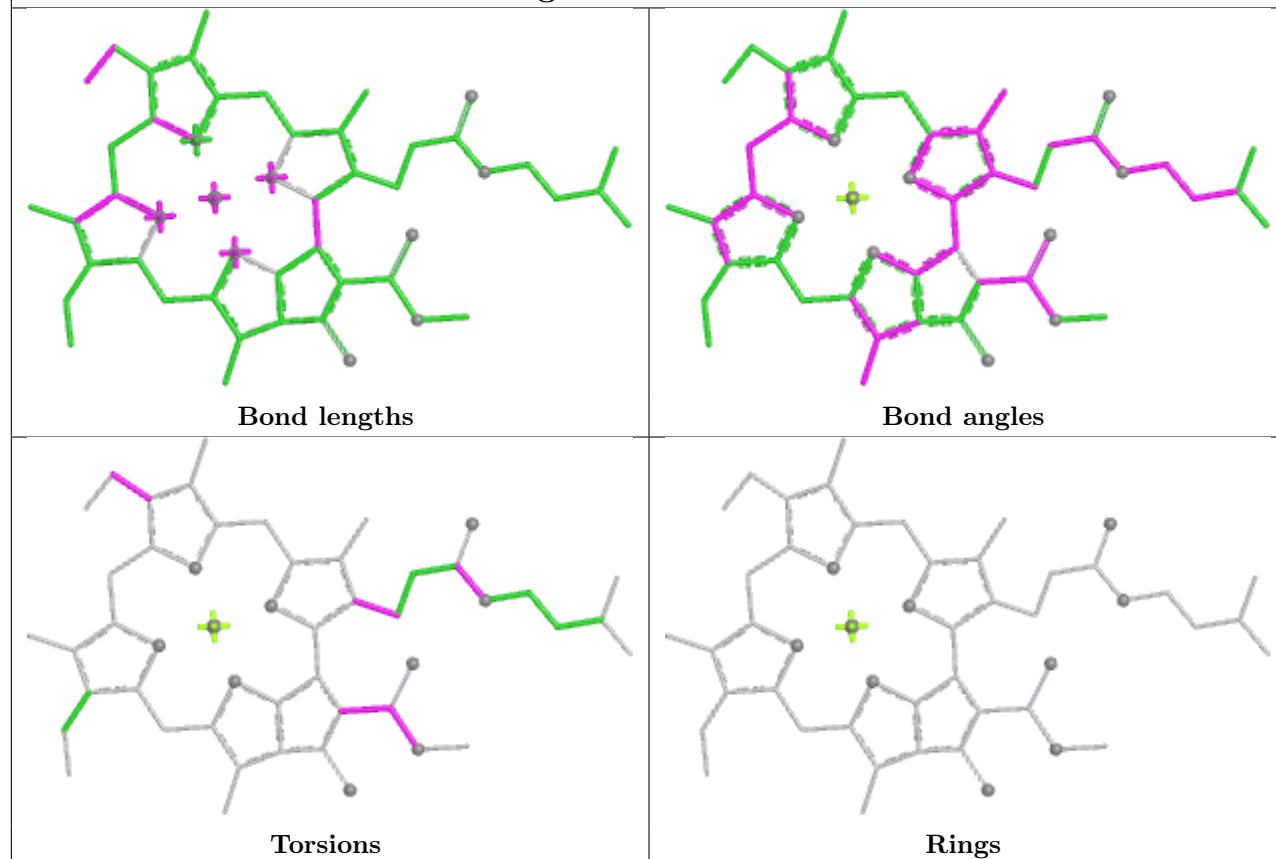


Torsions

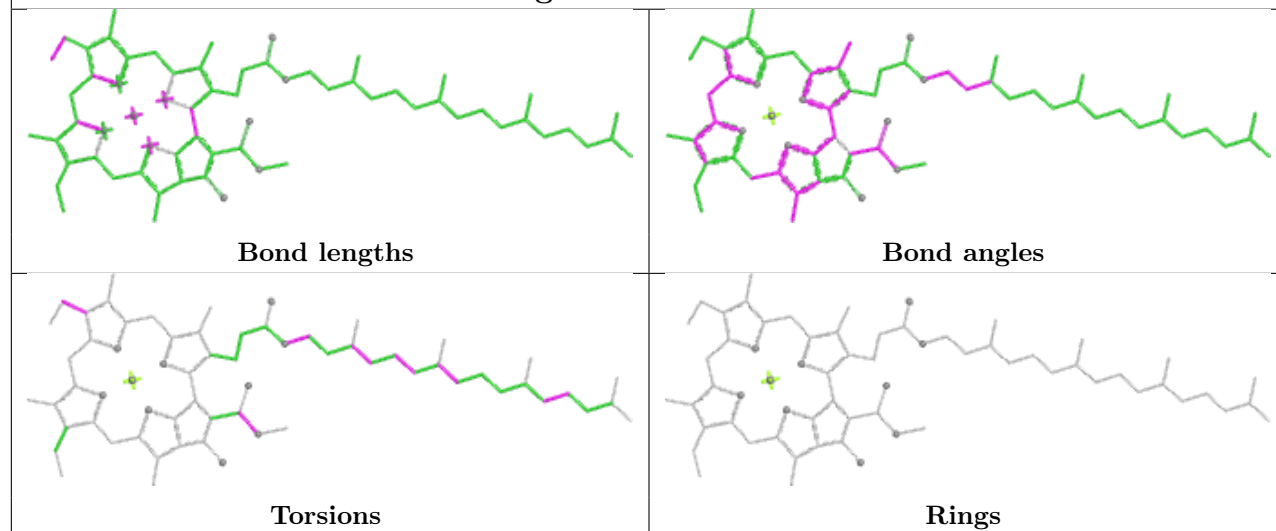


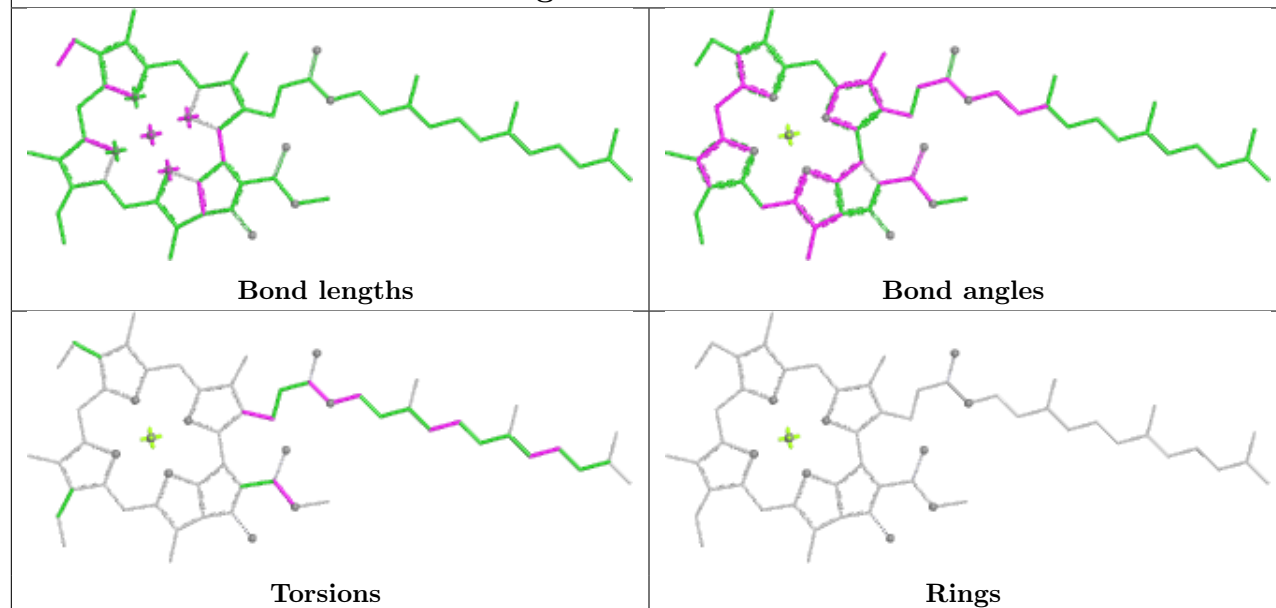
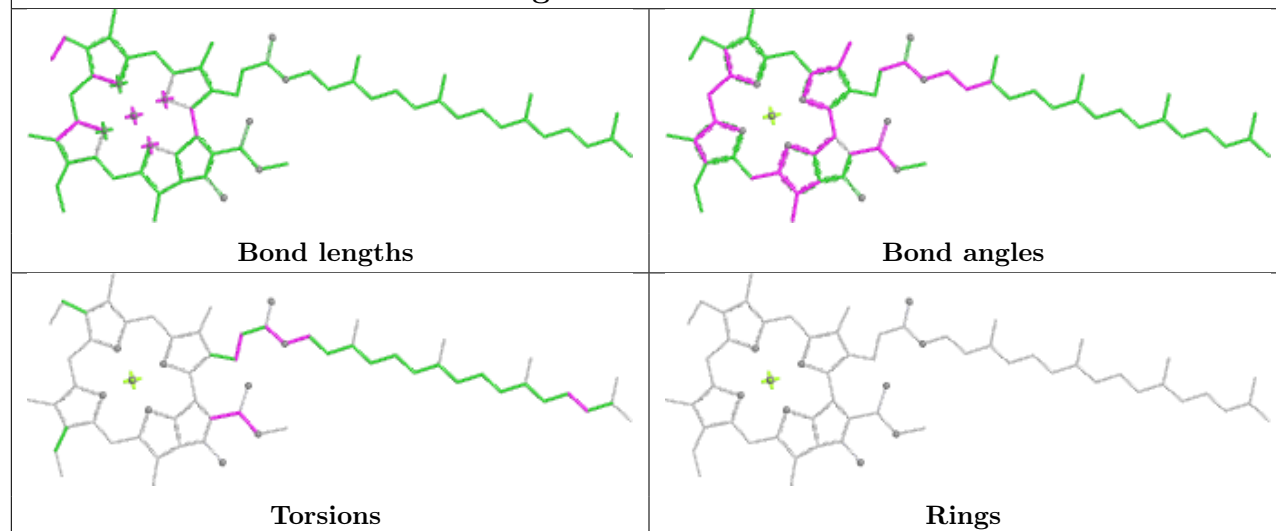
Rings

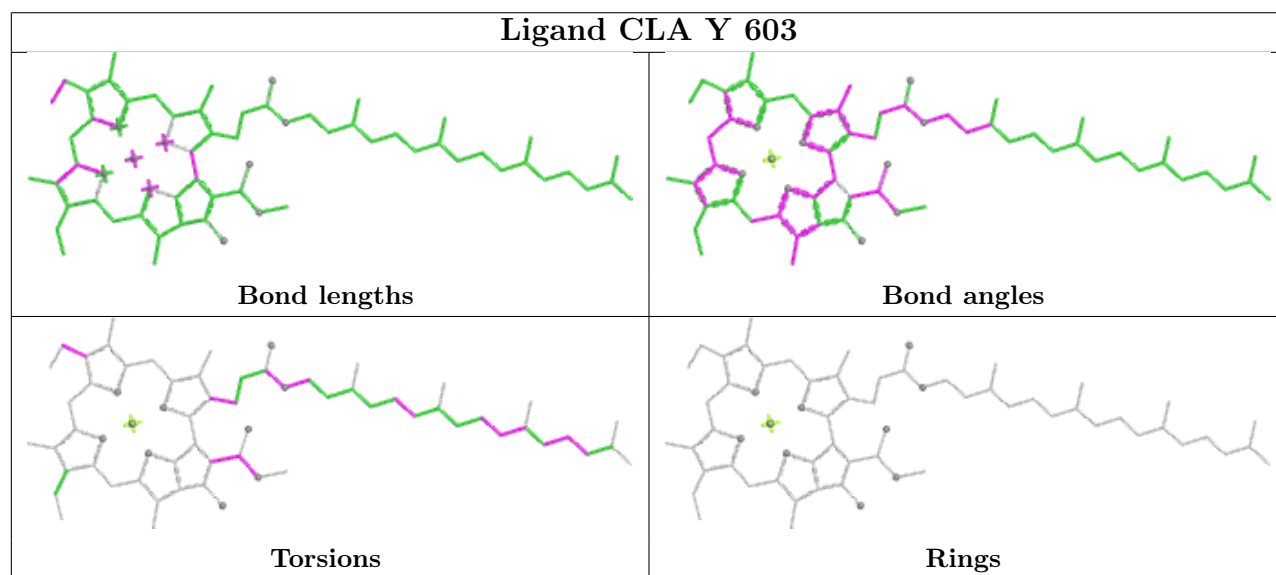
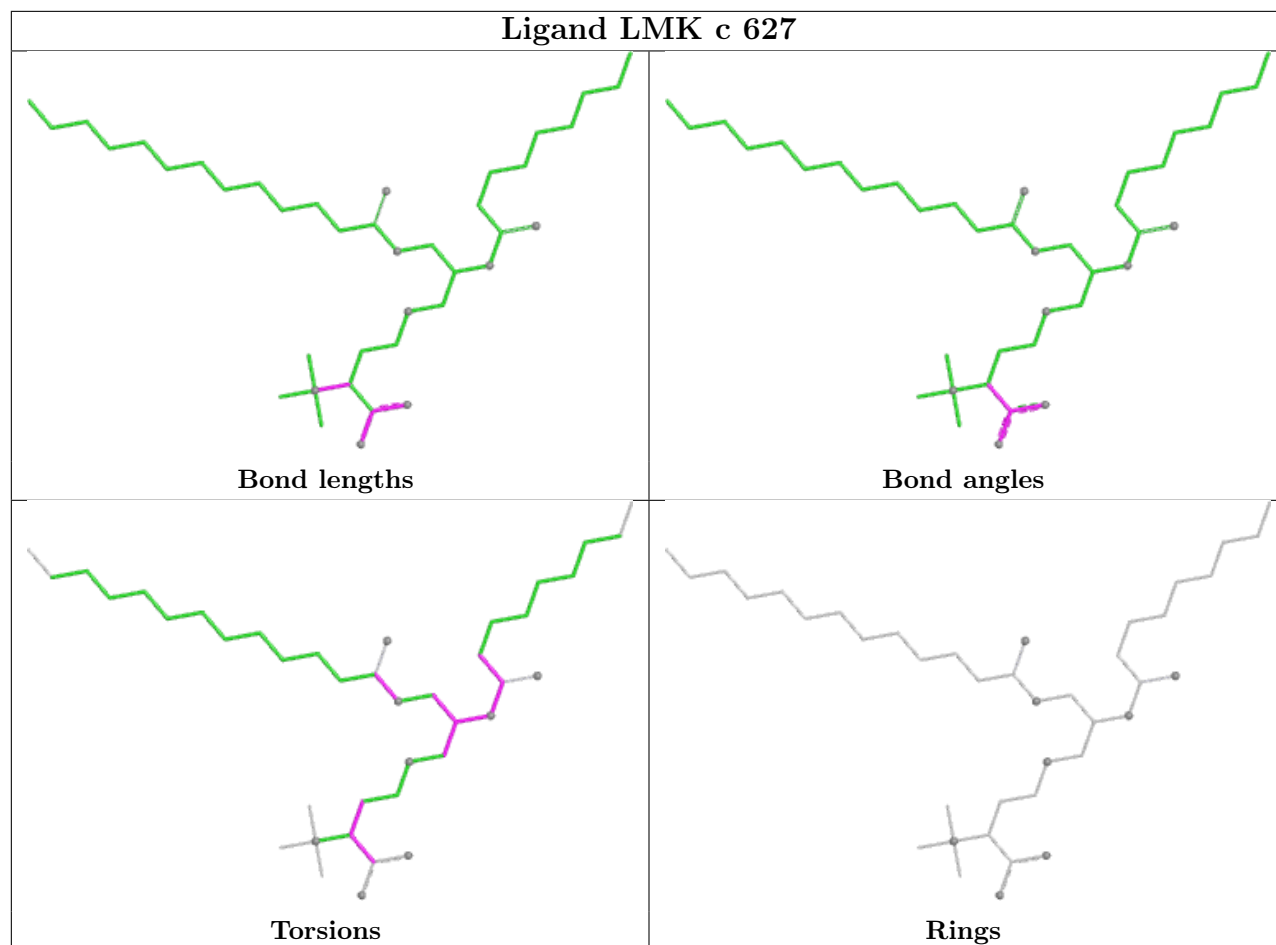
Ligand CLA s 605

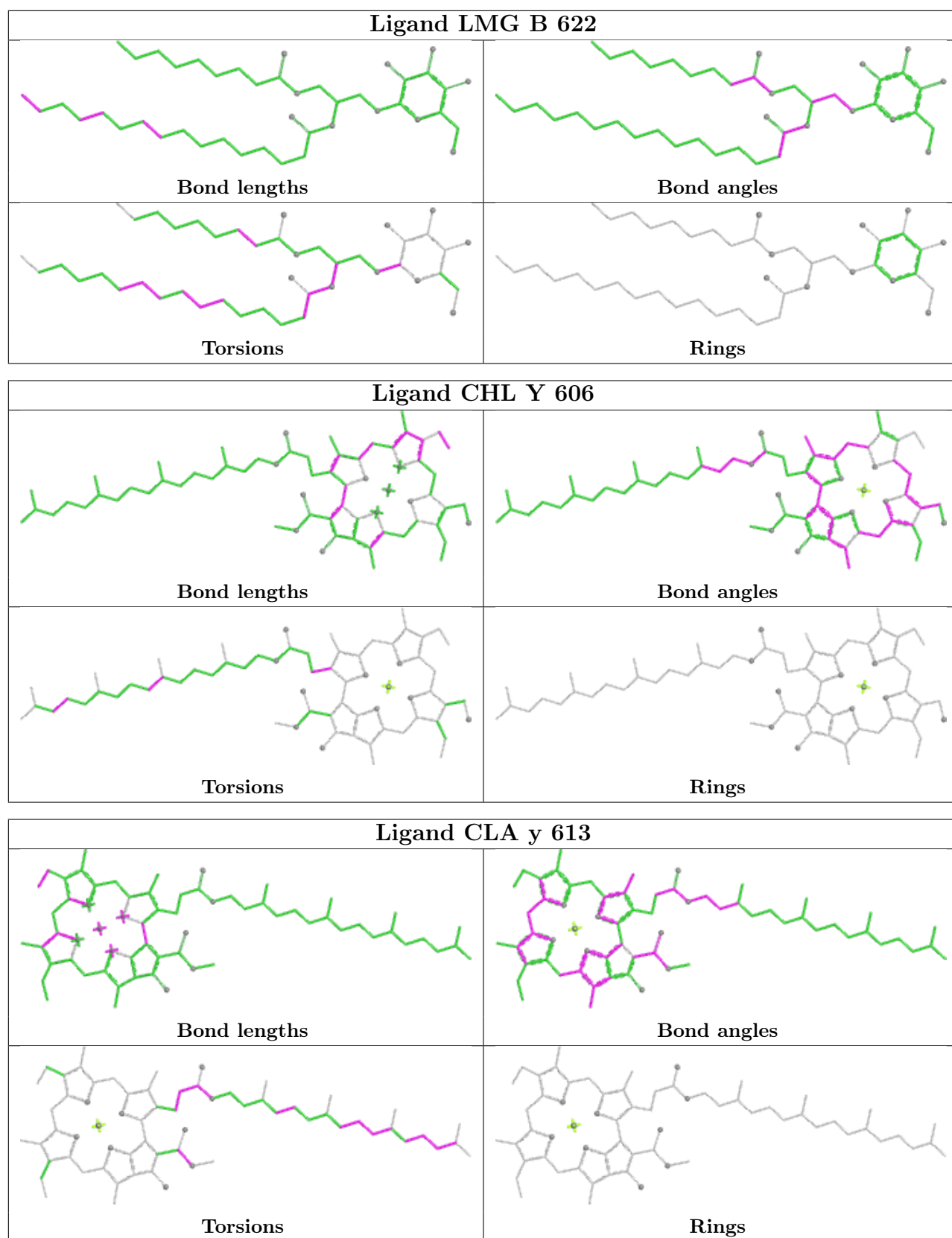


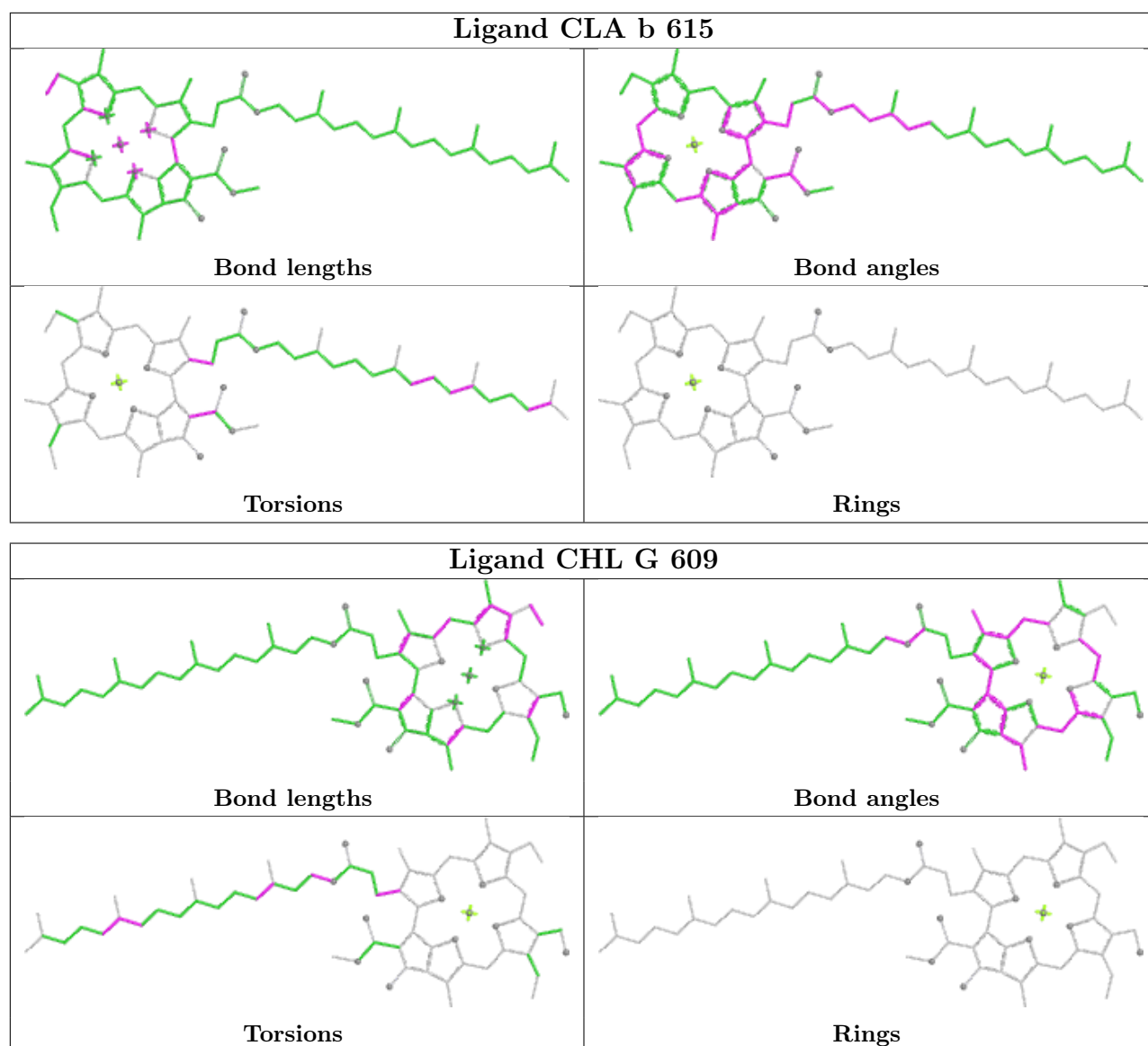
Ligand CLA b 616

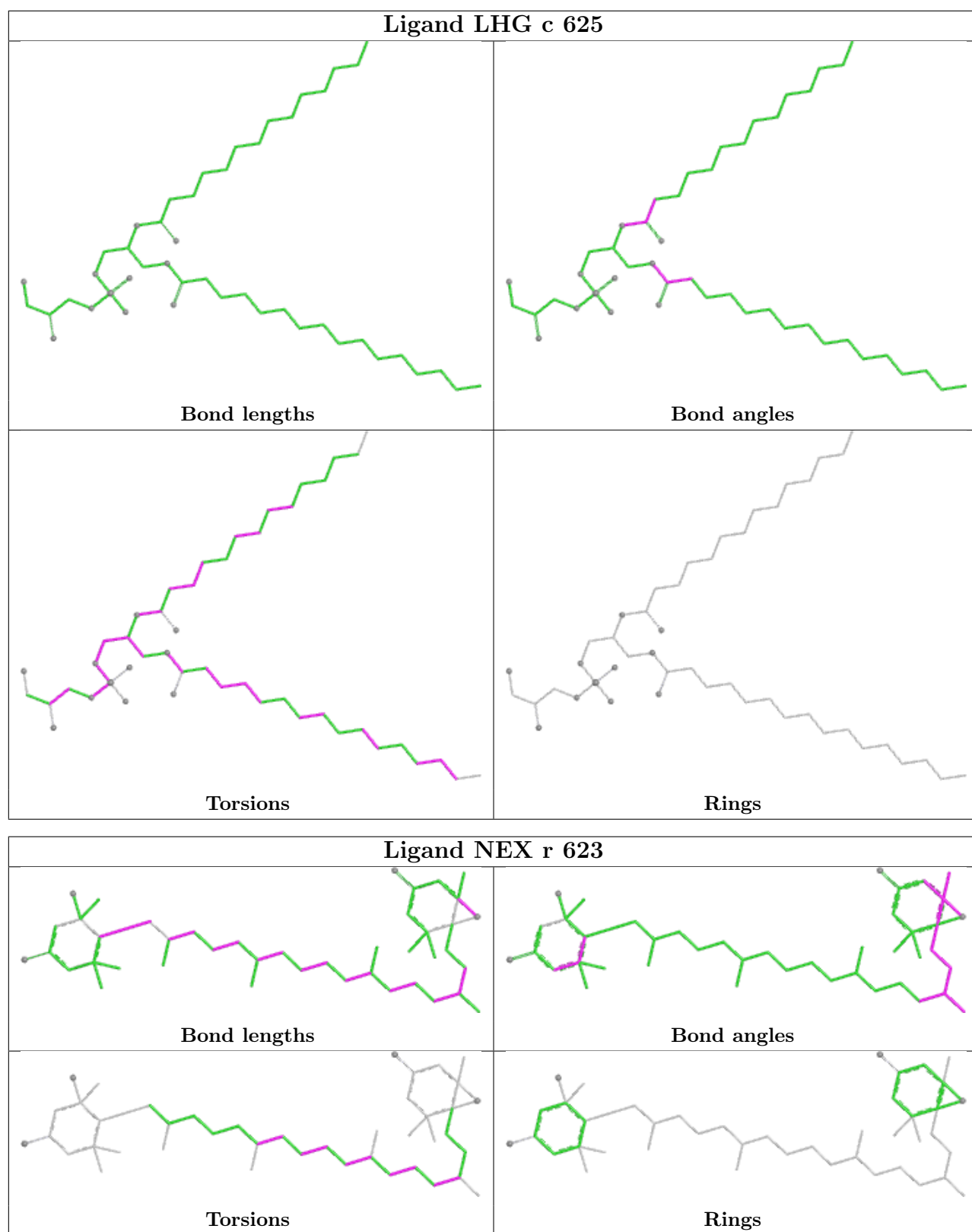


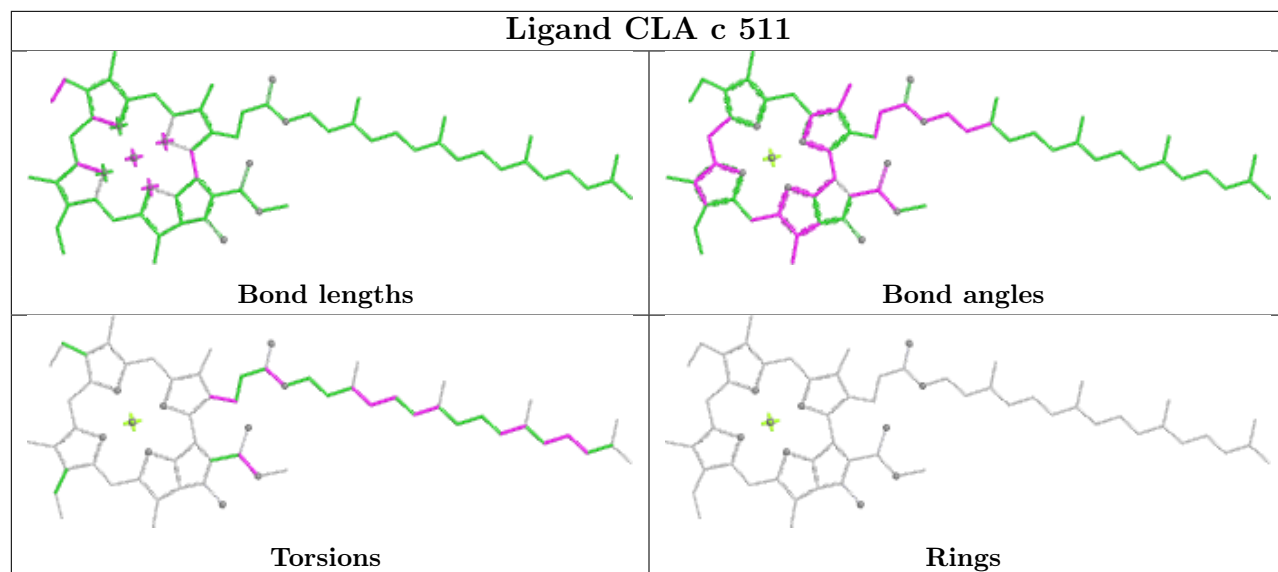
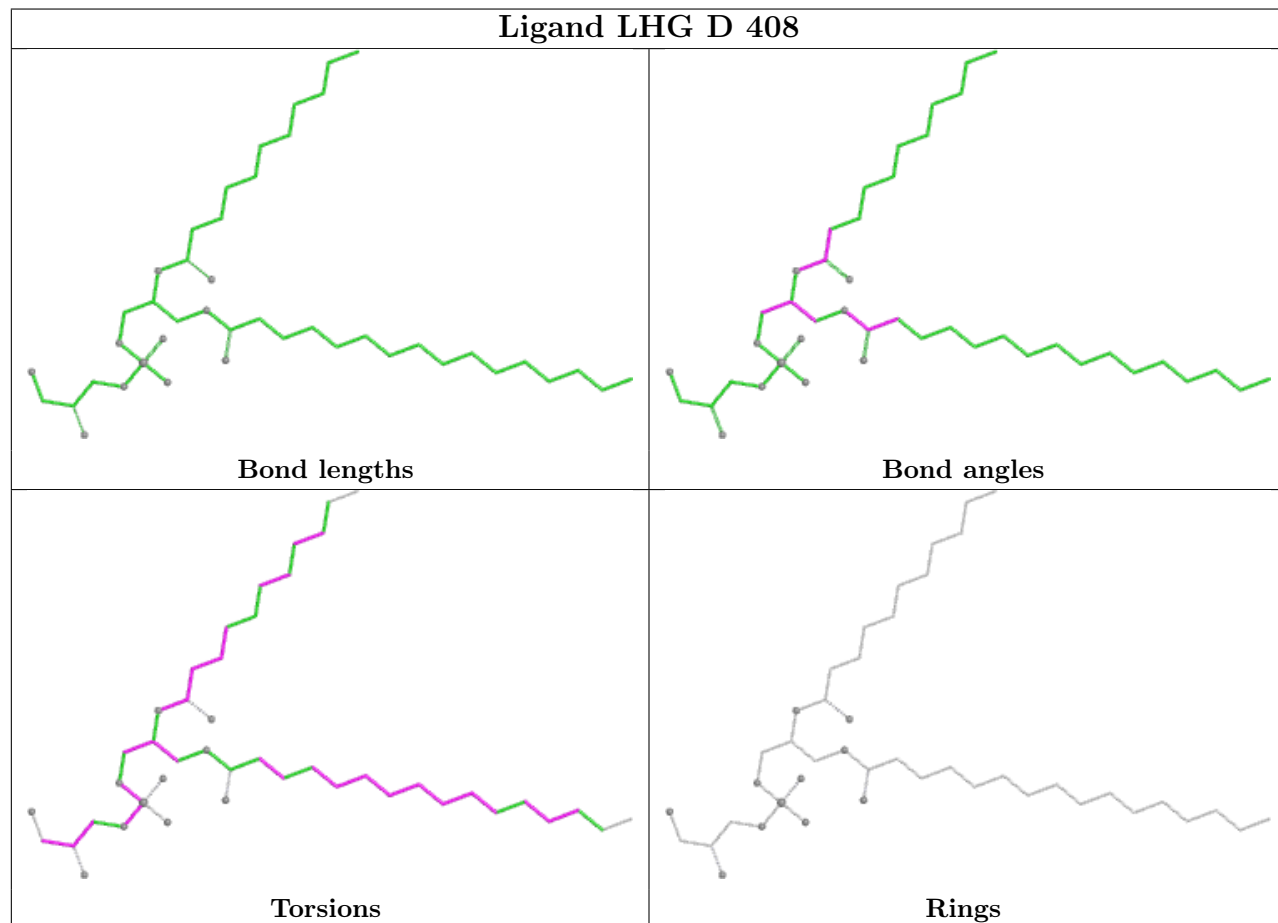
Ligand CLA a 410**Ligand CLA B 611**

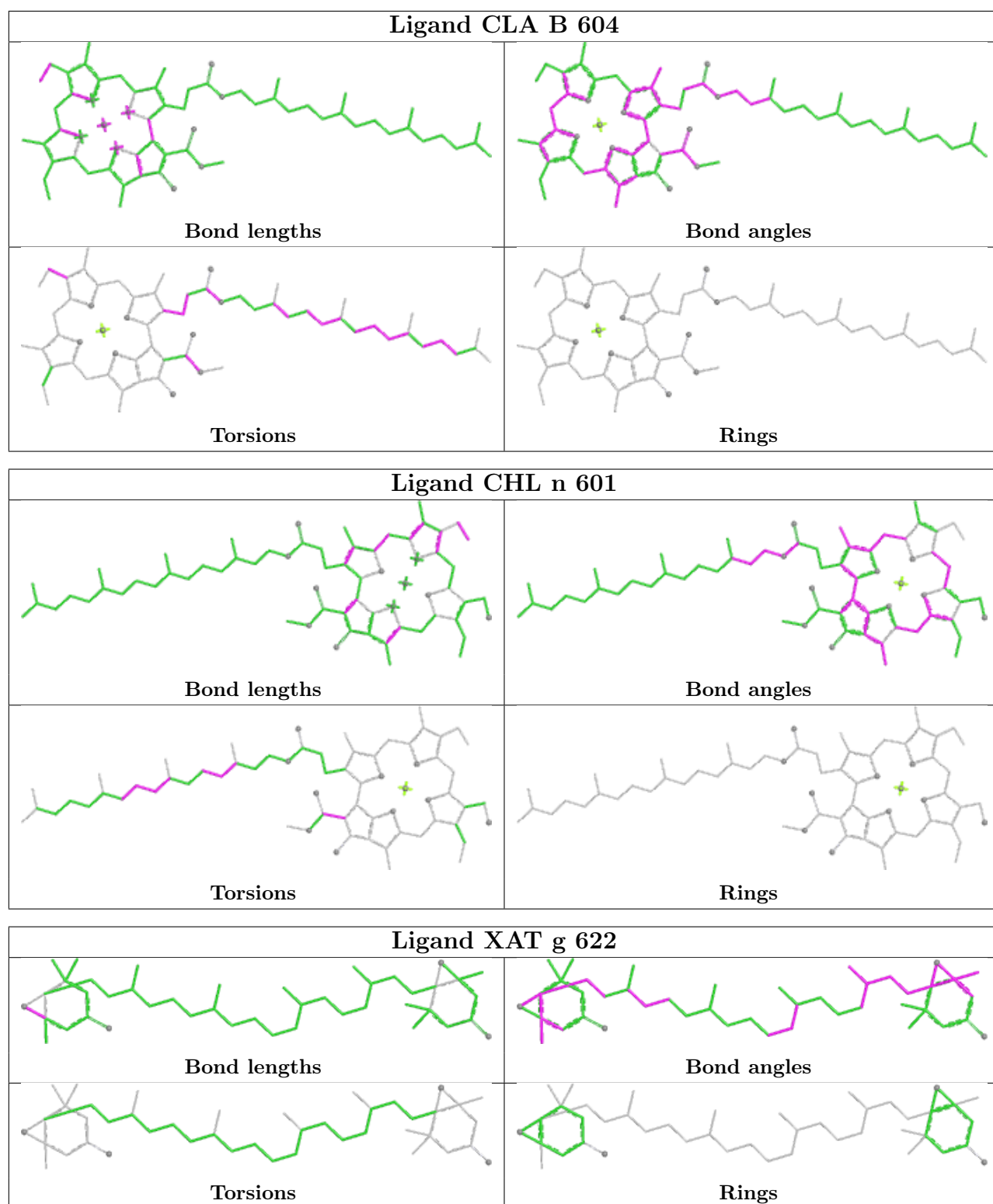


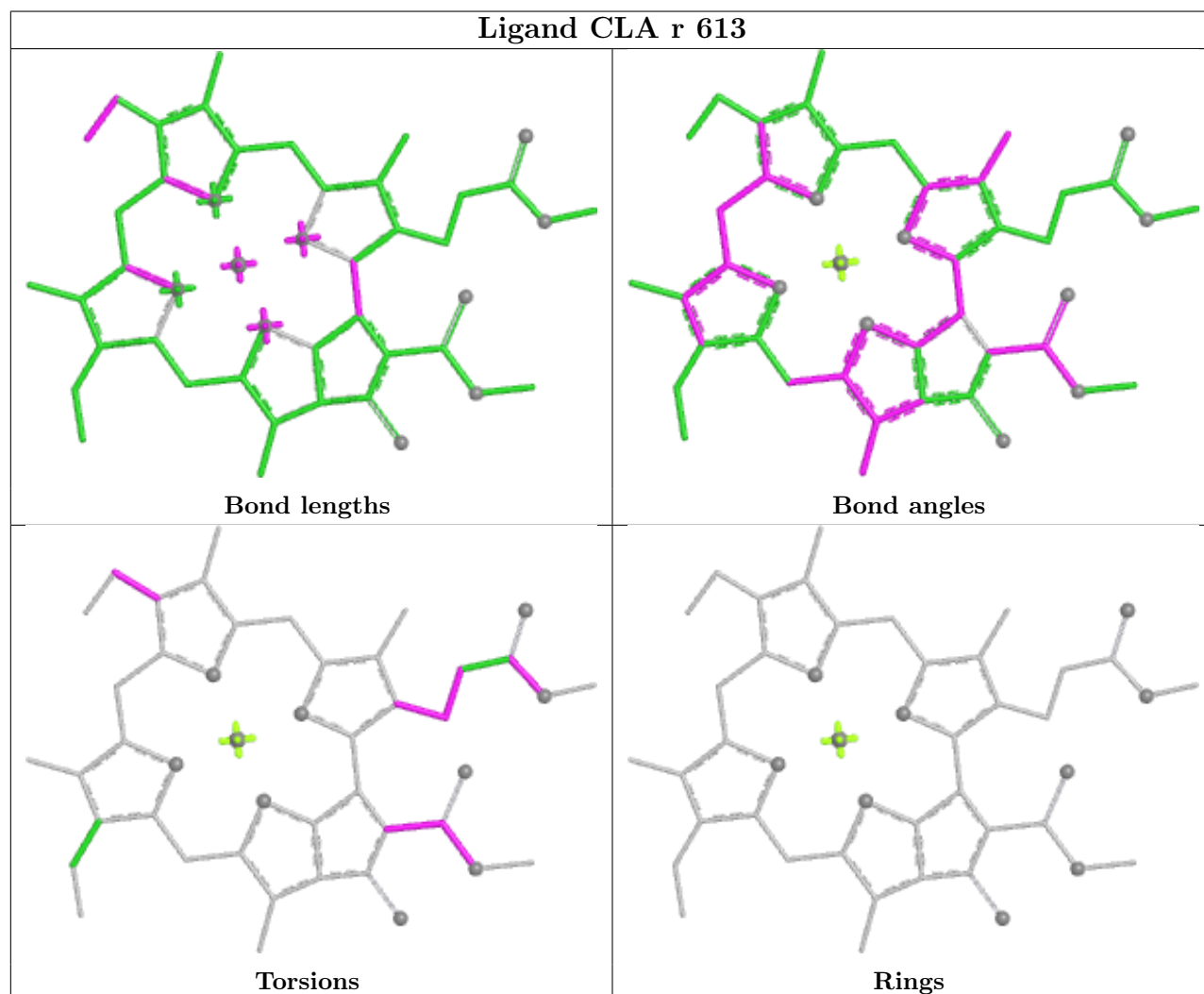
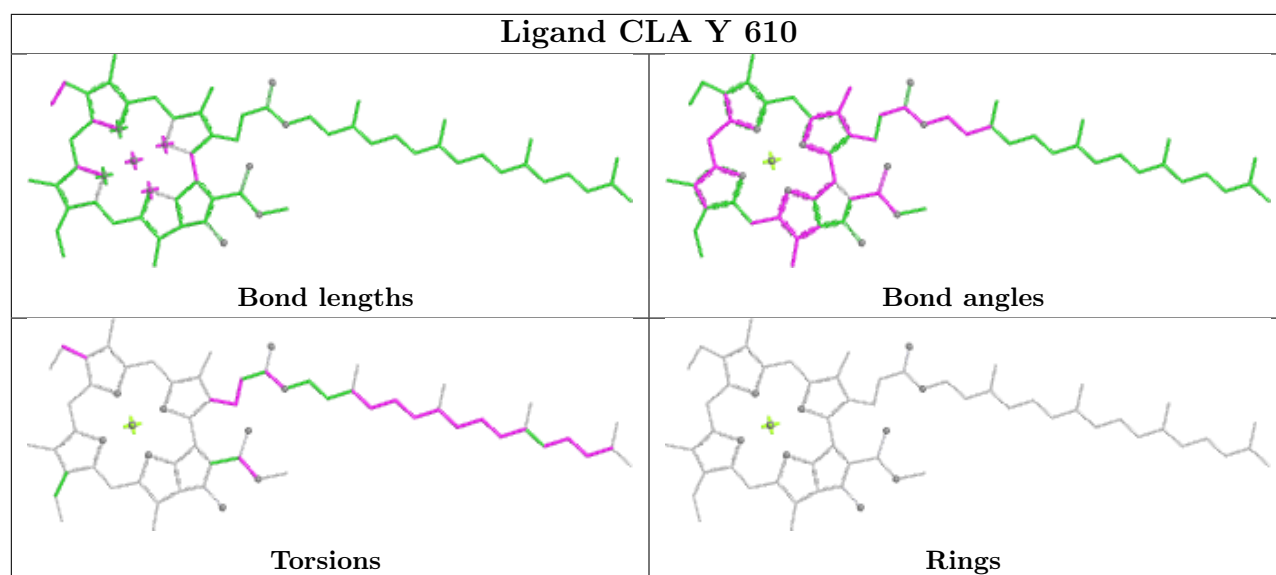


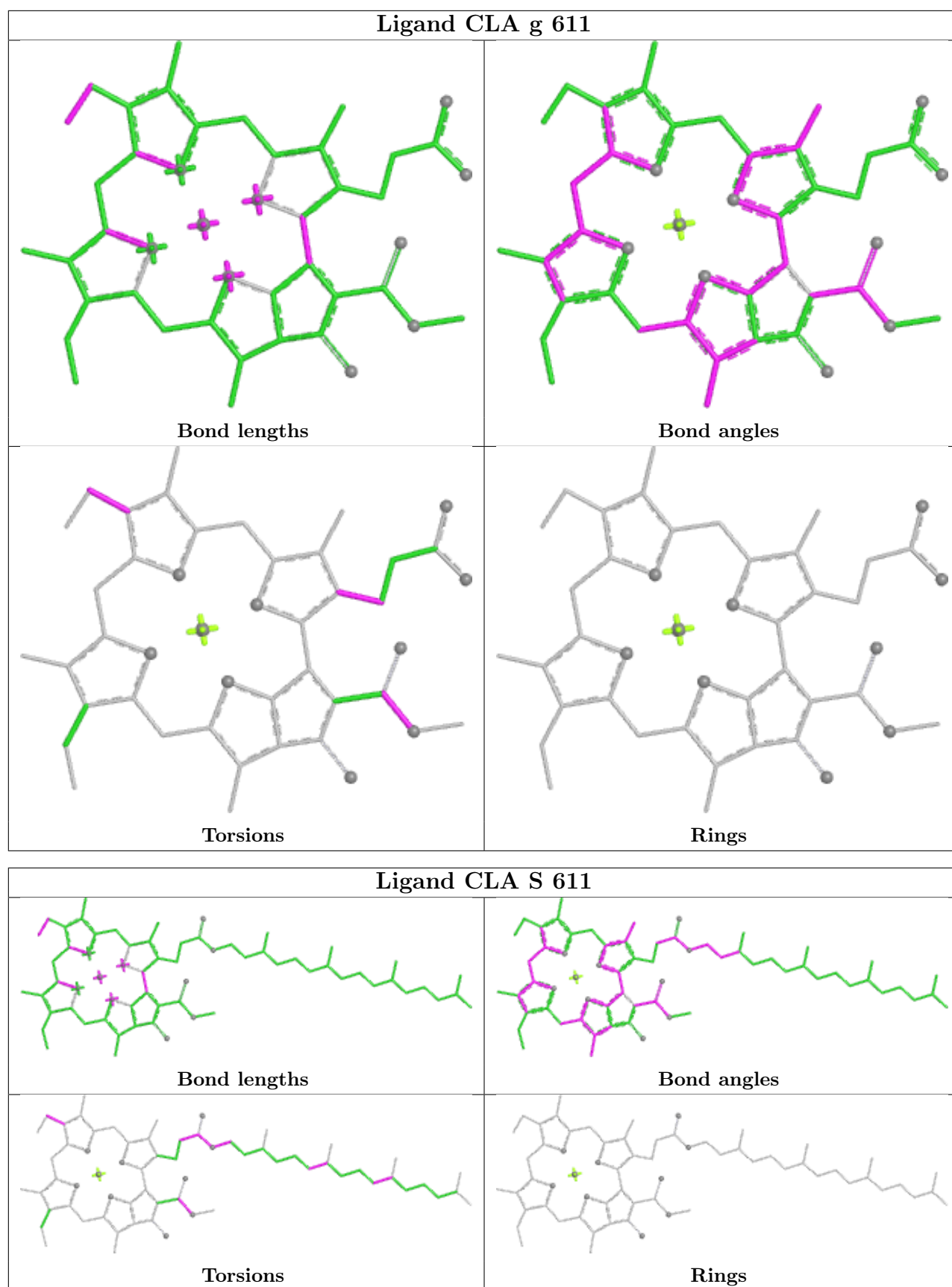


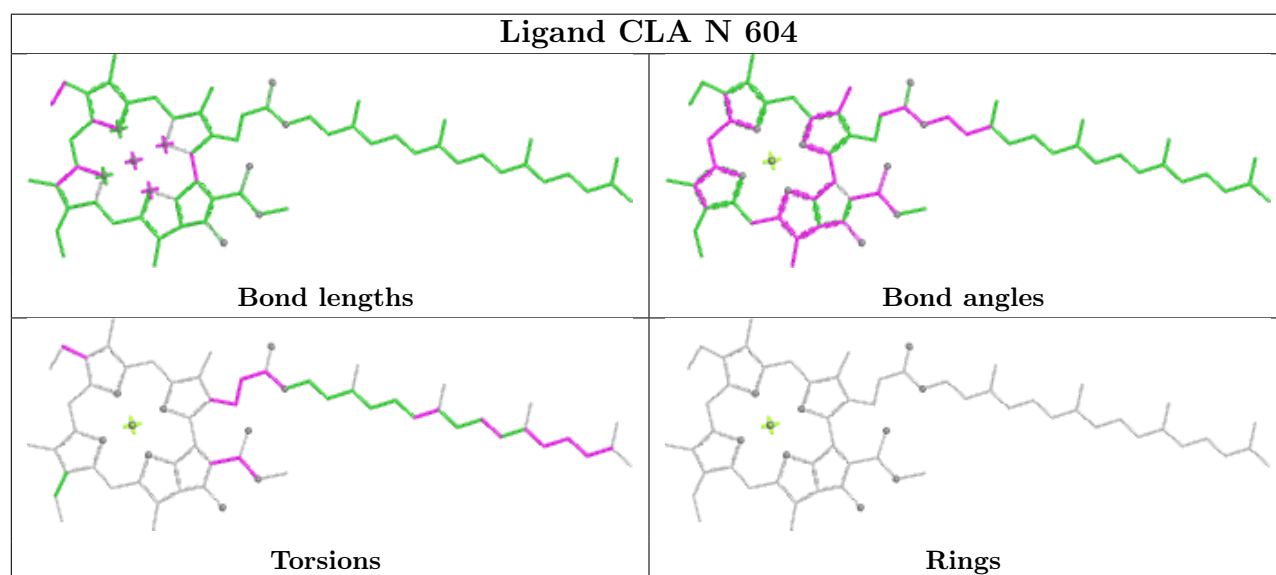
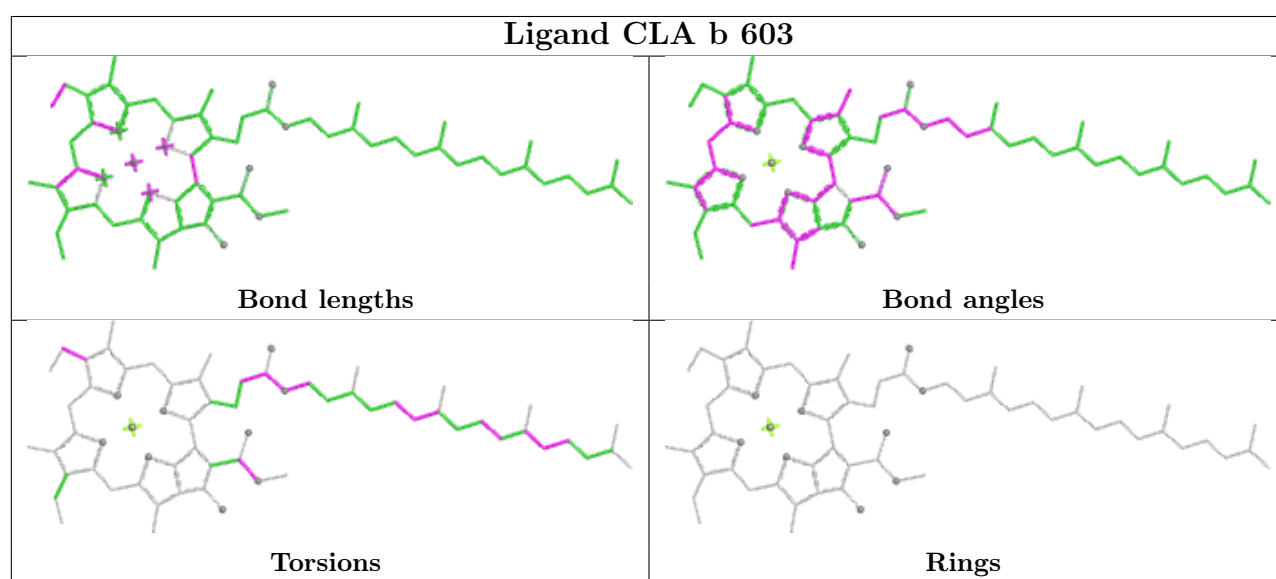
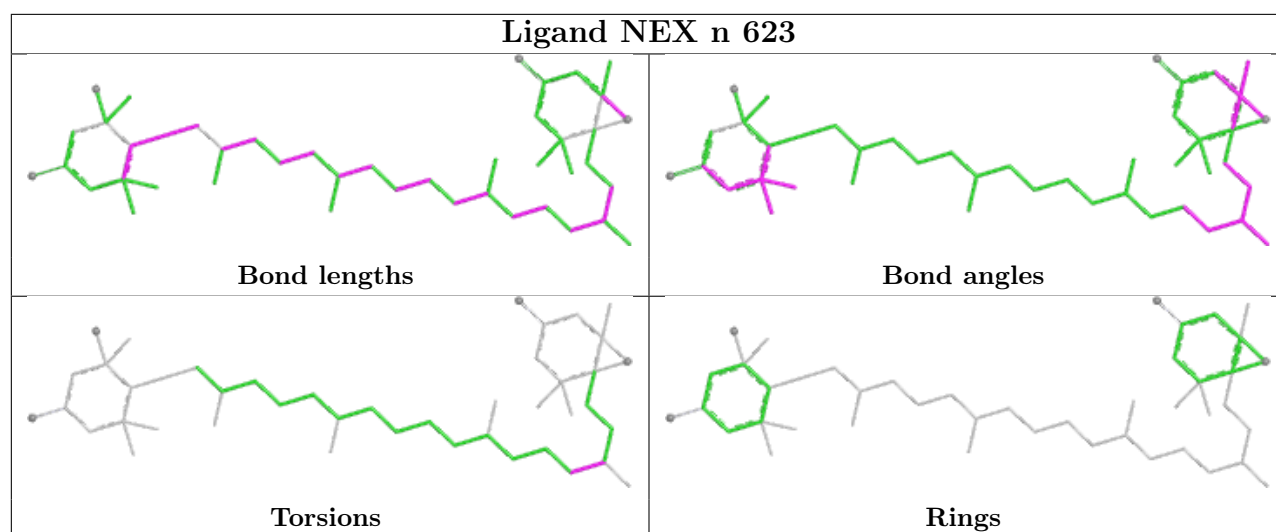


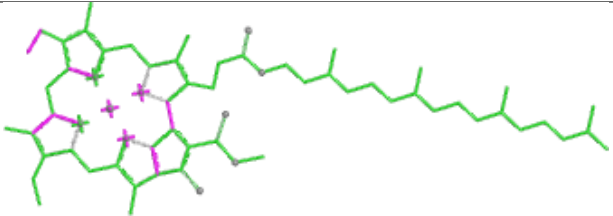
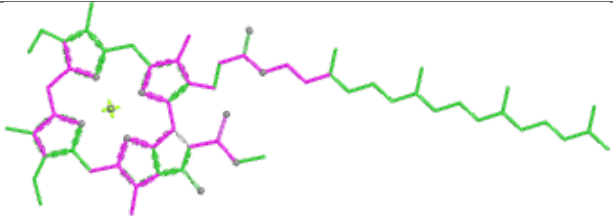
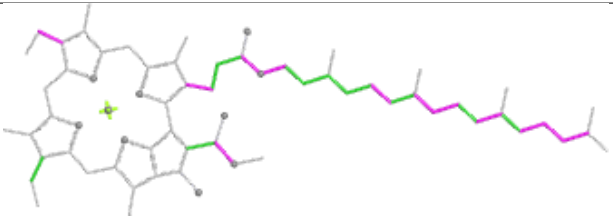
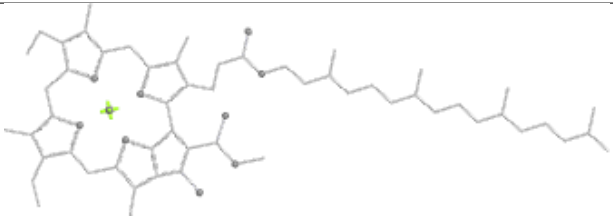
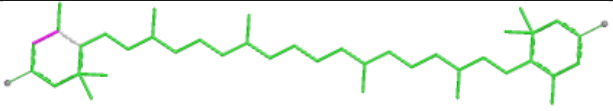
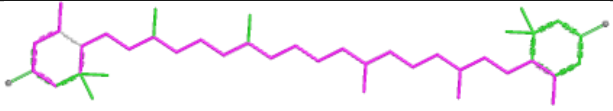
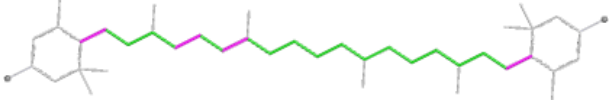
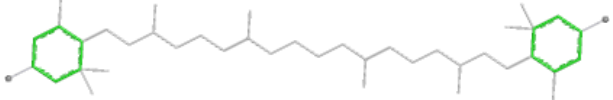
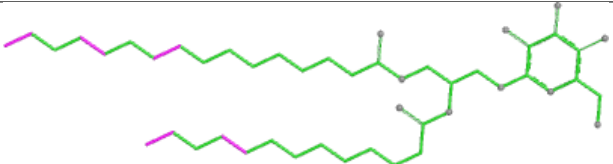
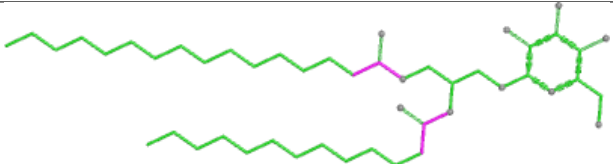
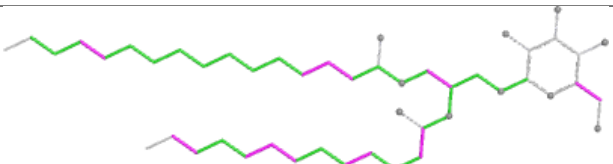
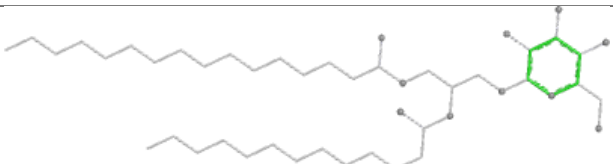
Ligand CLA c 511**Ligand LHG D 408**

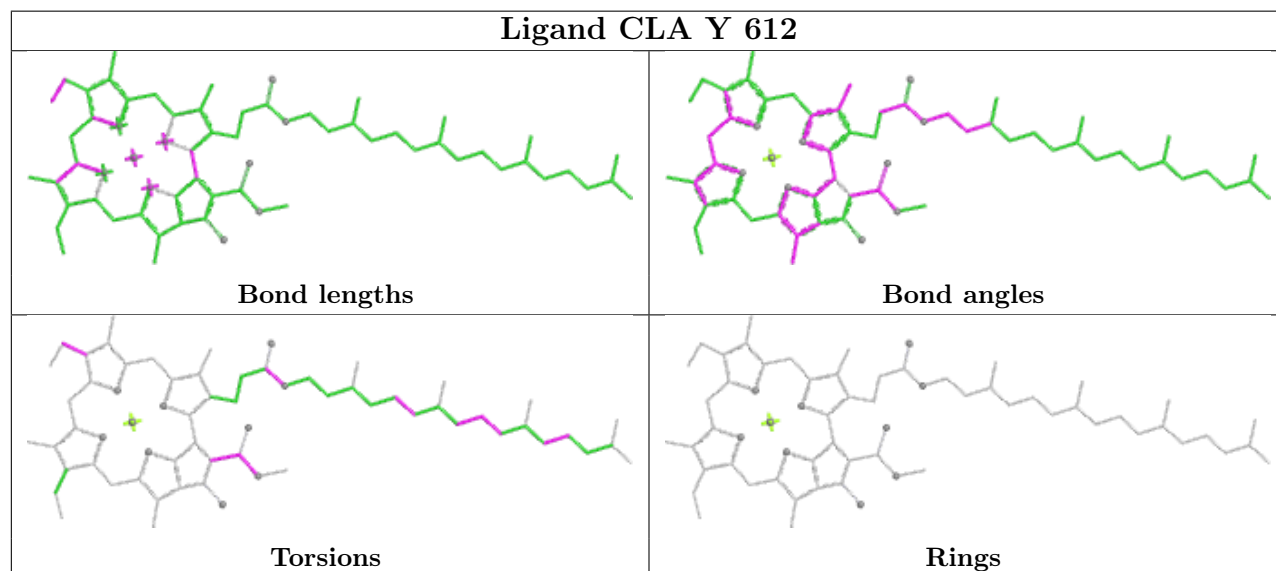
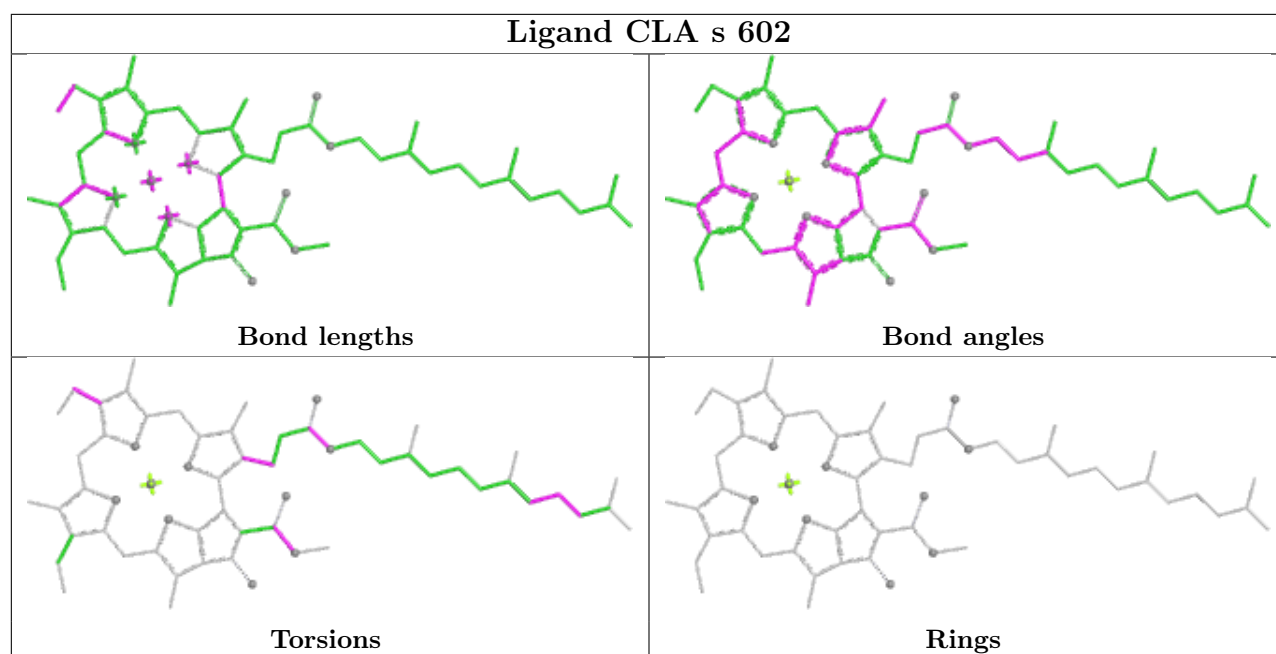


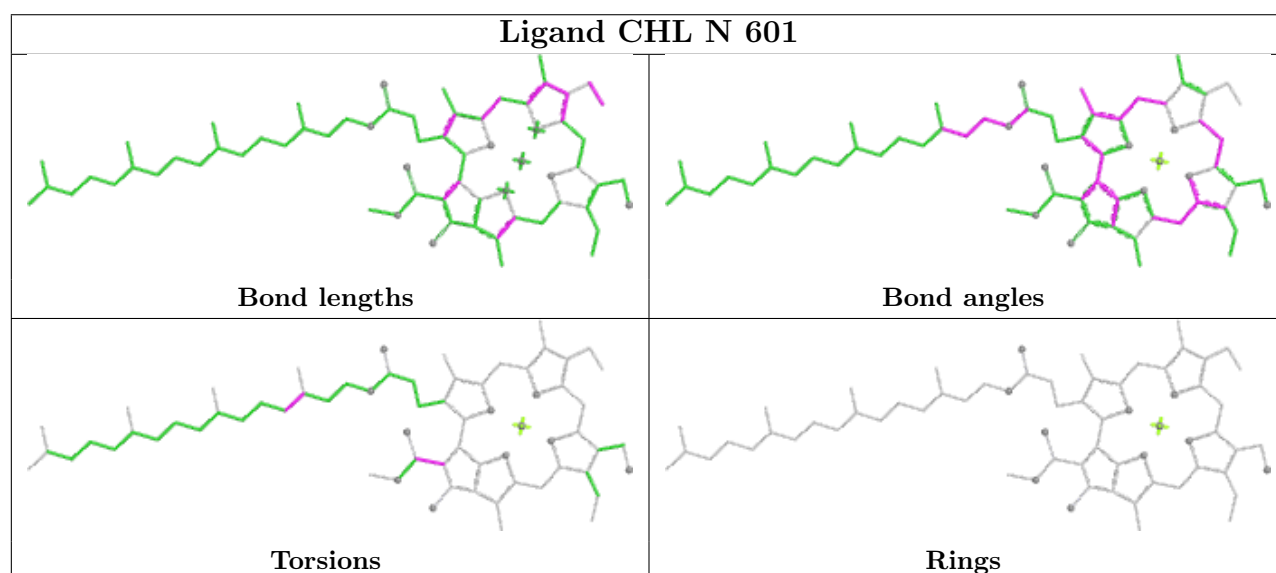
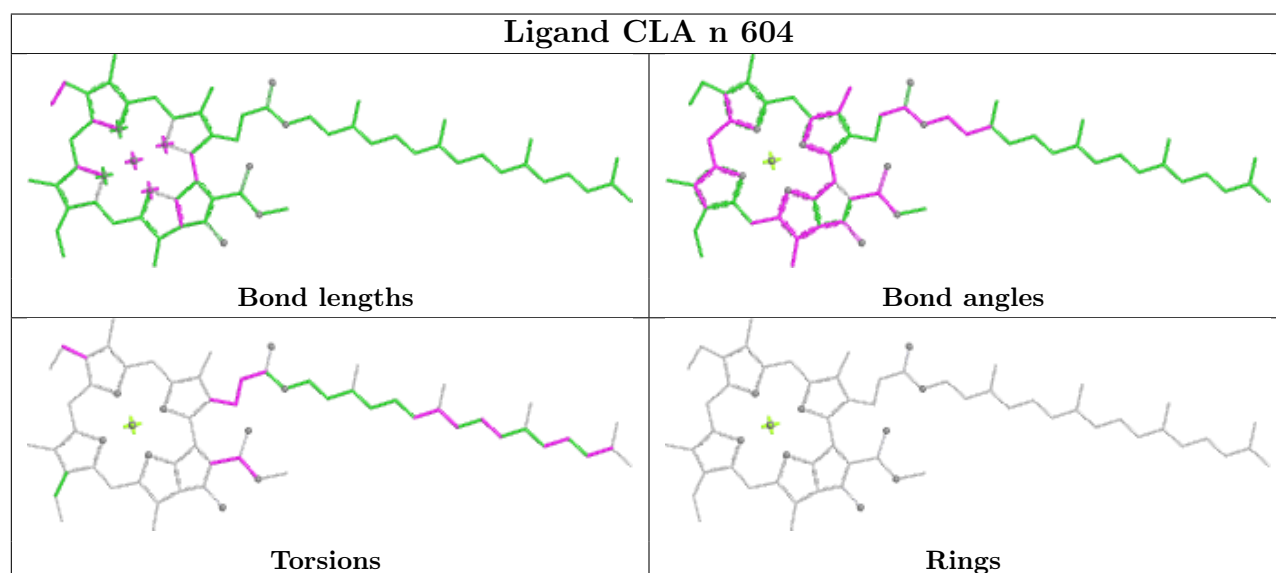
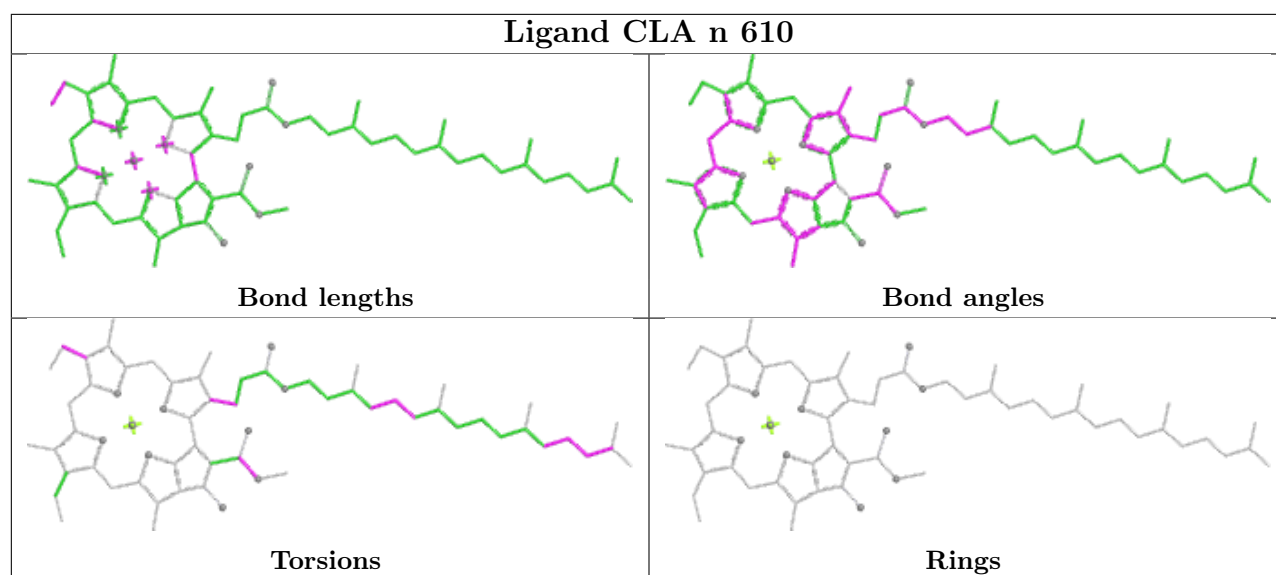


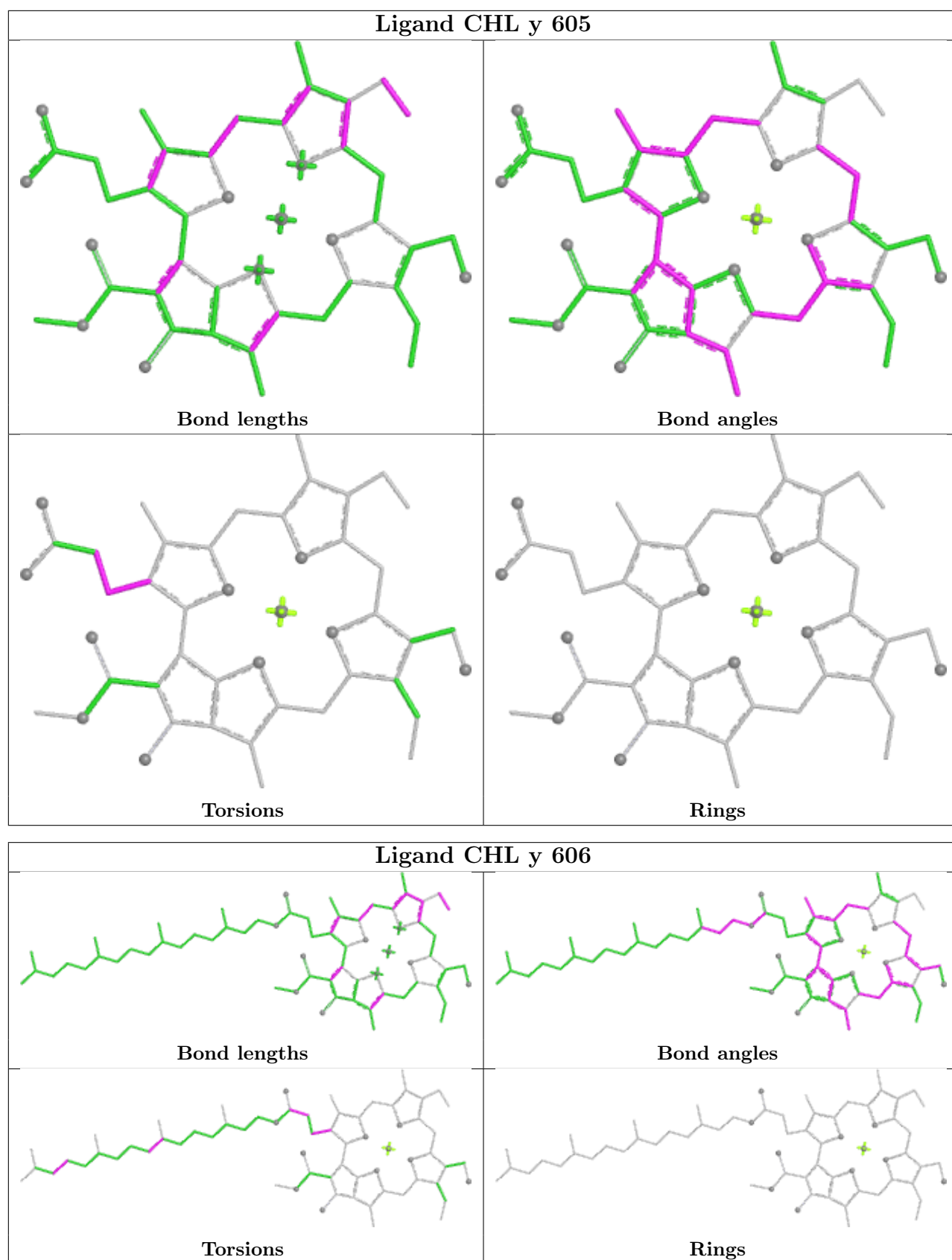




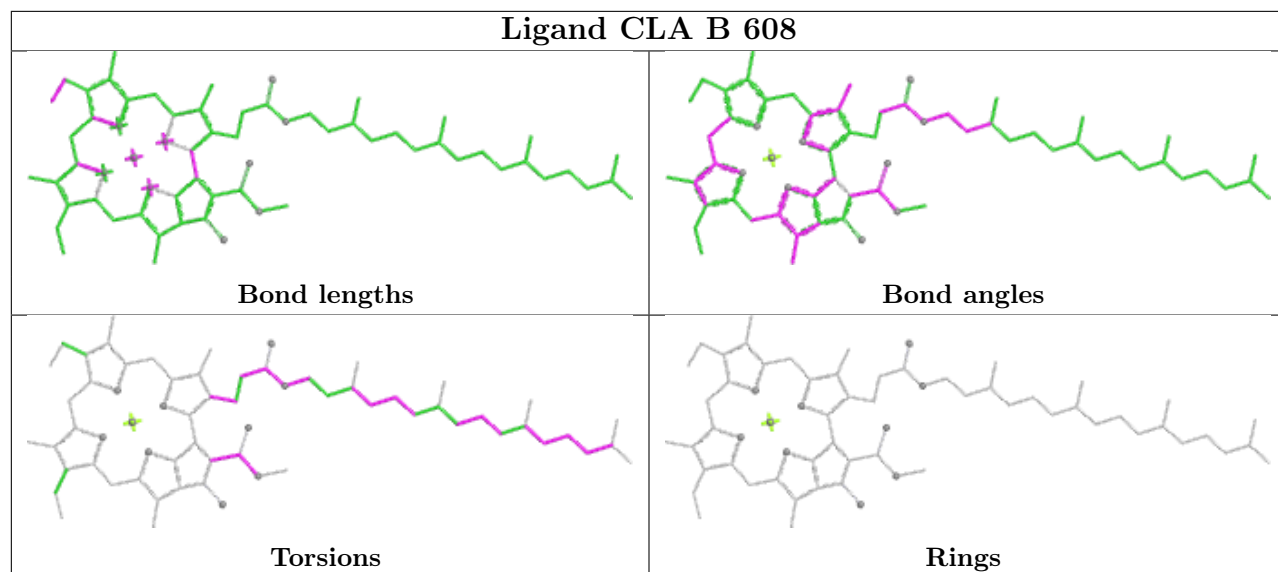
Ligand CLA Y 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT n 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



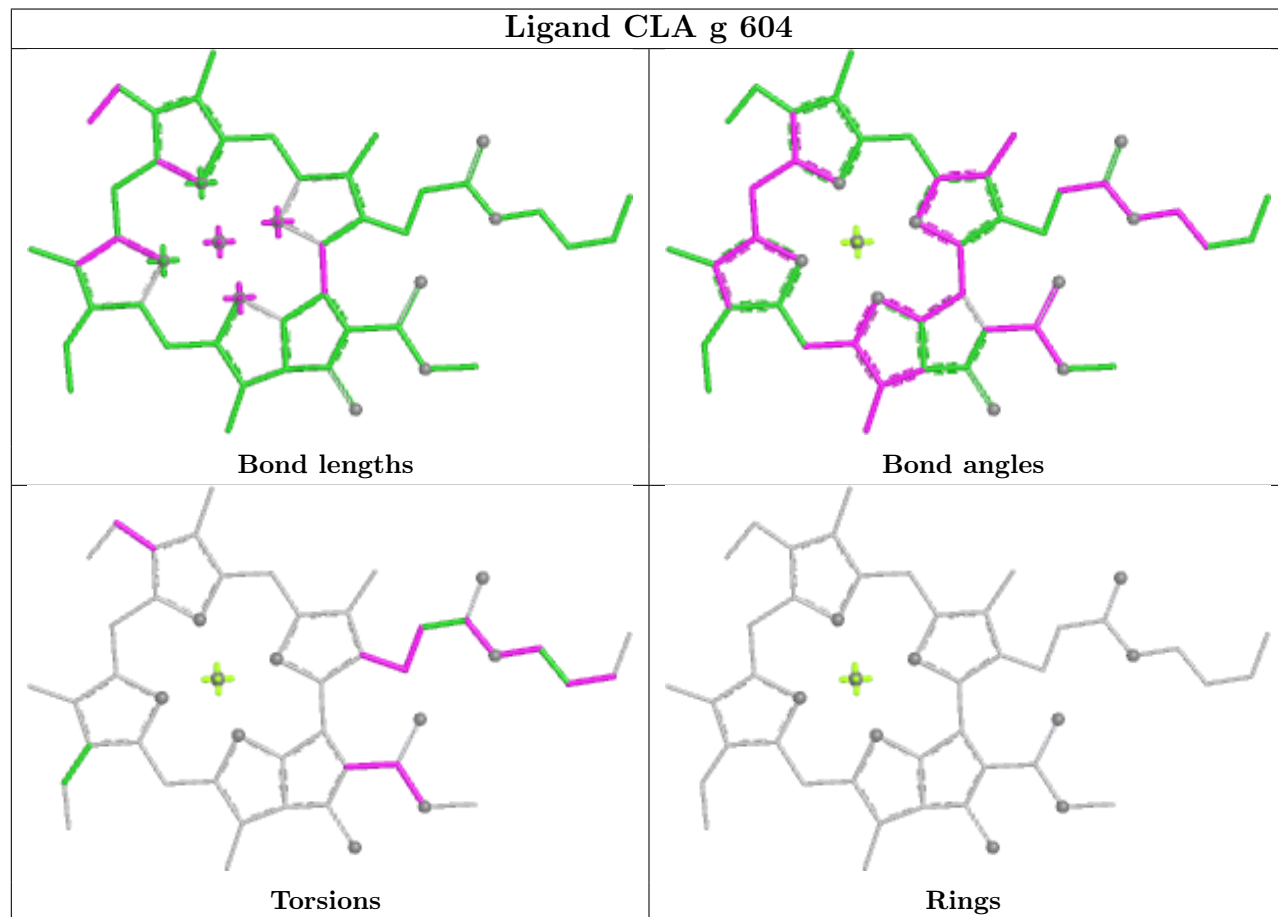


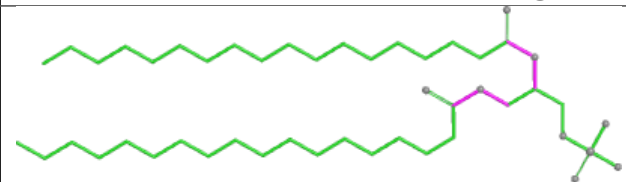
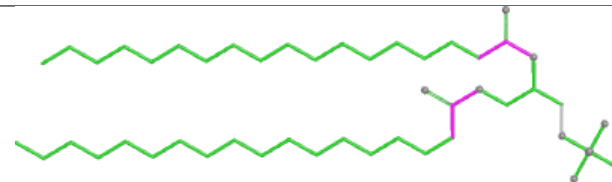
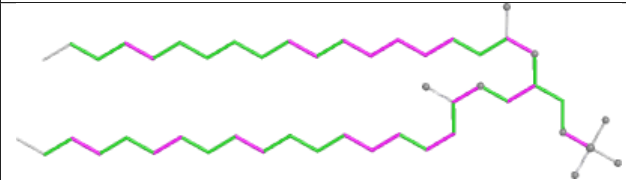
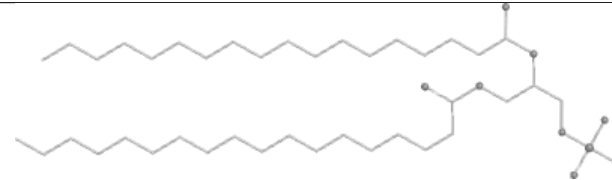


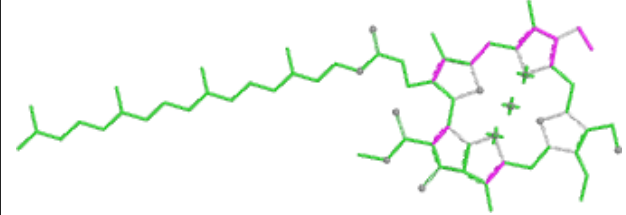
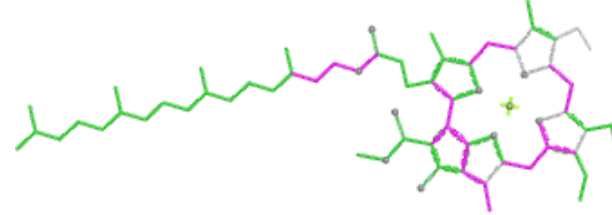
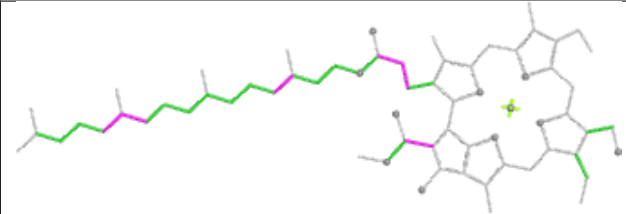
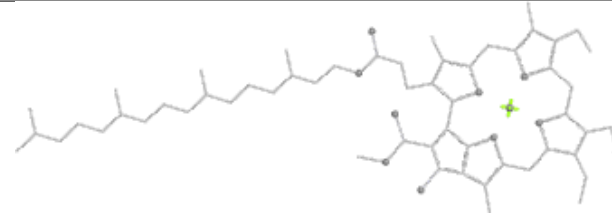
Ligand CLA B 608

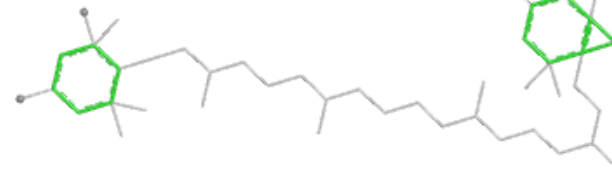


Ligand CLA g 604

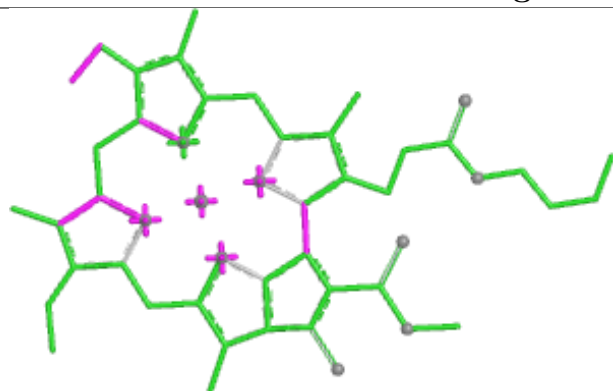


Ligand 3PH i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

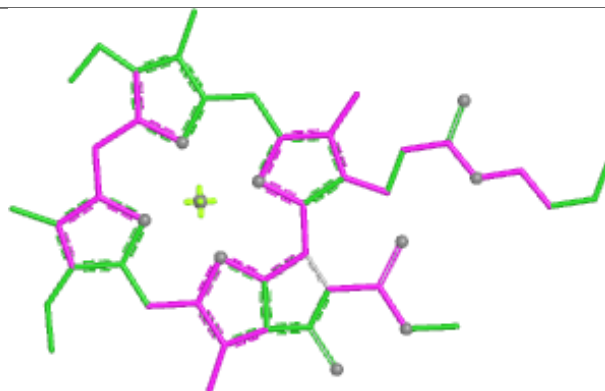
Ligand CHL n 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX N 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

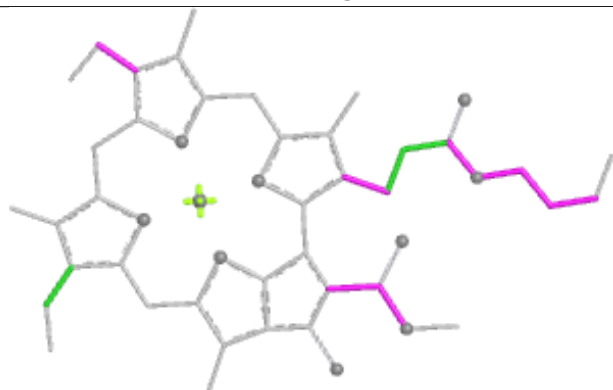
Ligand CLA N 611



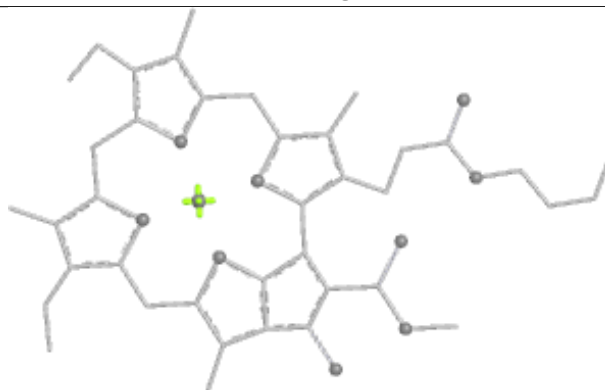
Bond lengths



Bond angles

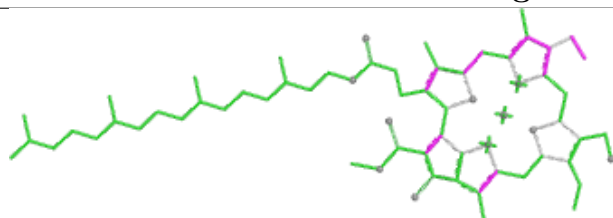


Torsions

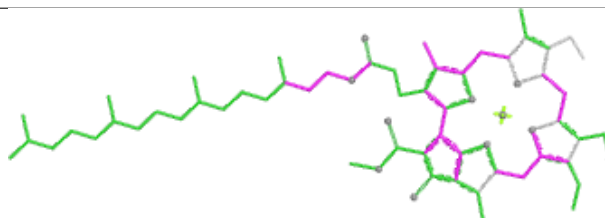


Rings

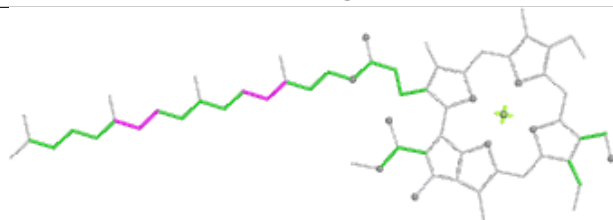
Ligand CHL G 601



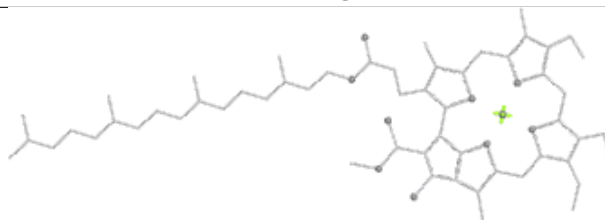
Bond lengths



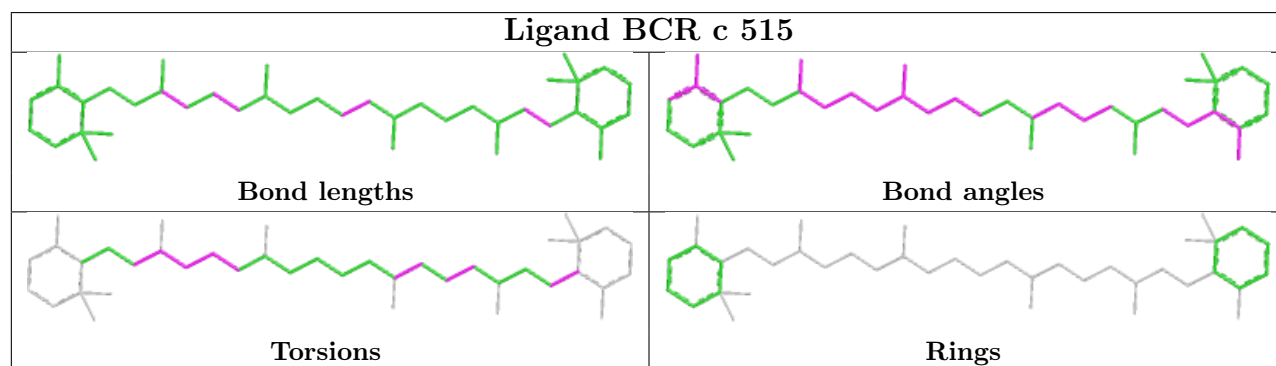
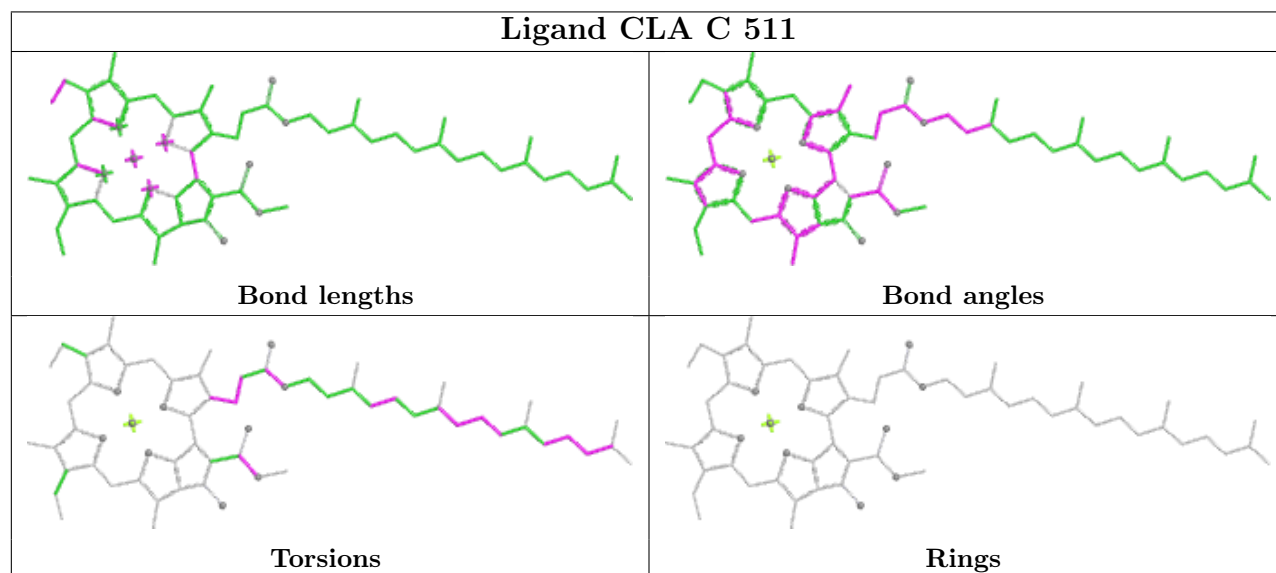
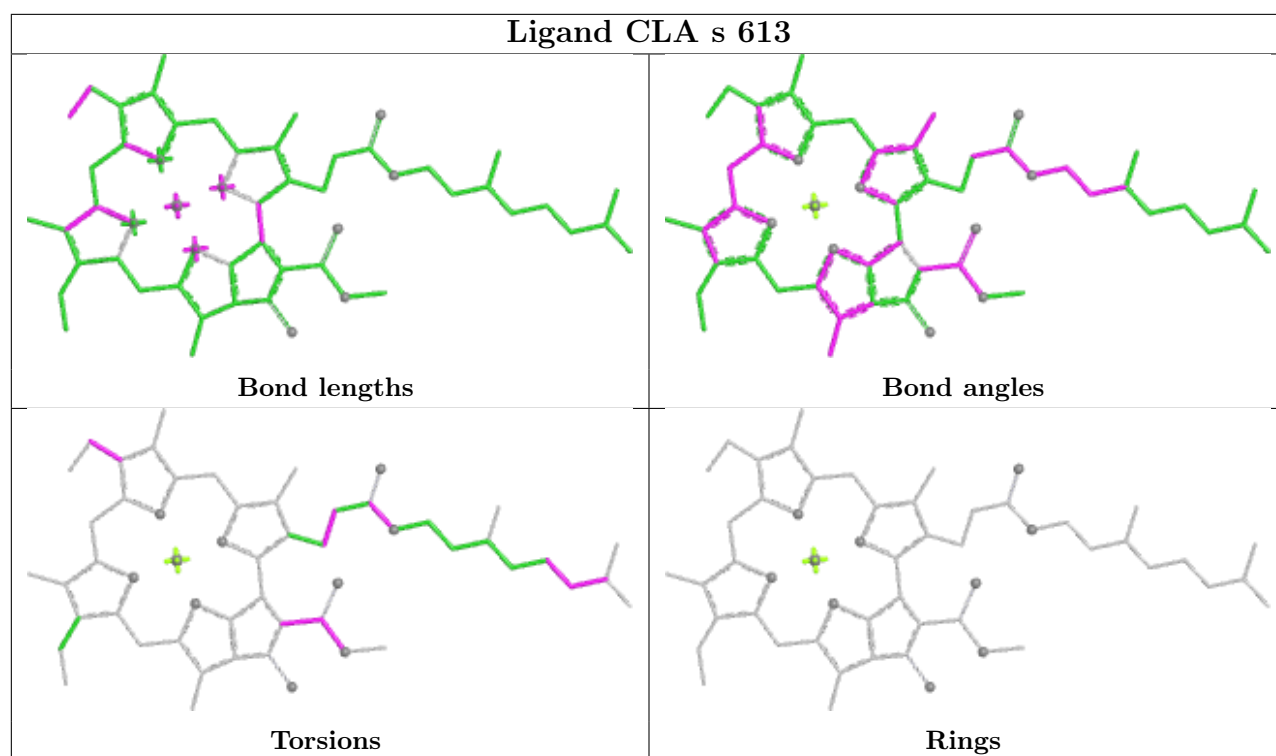
Bond angles

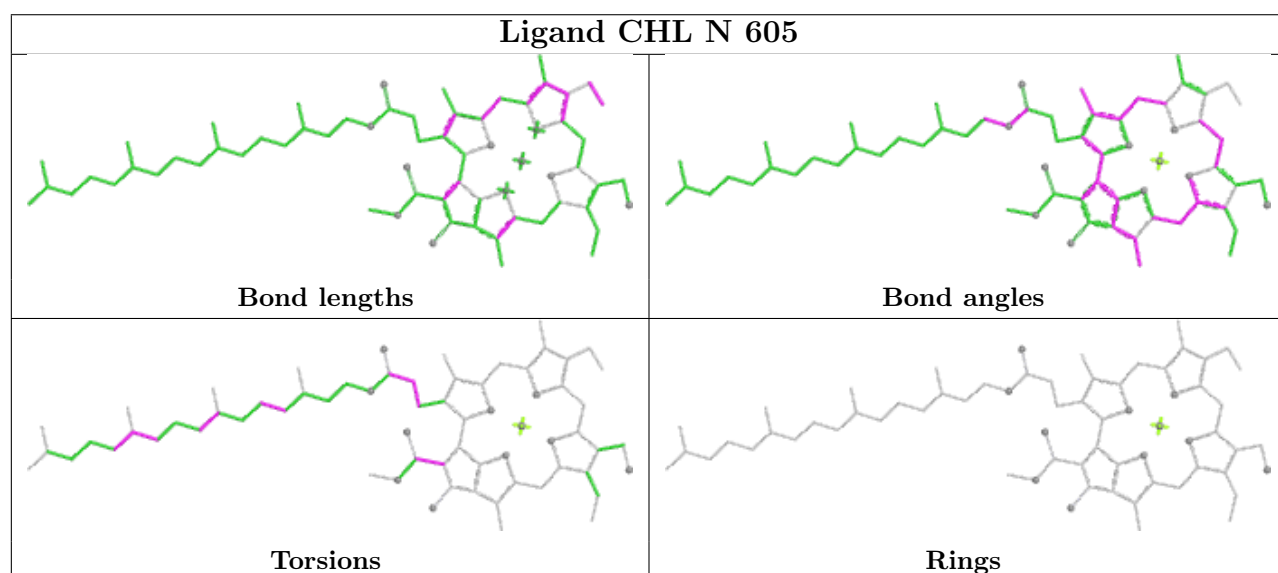
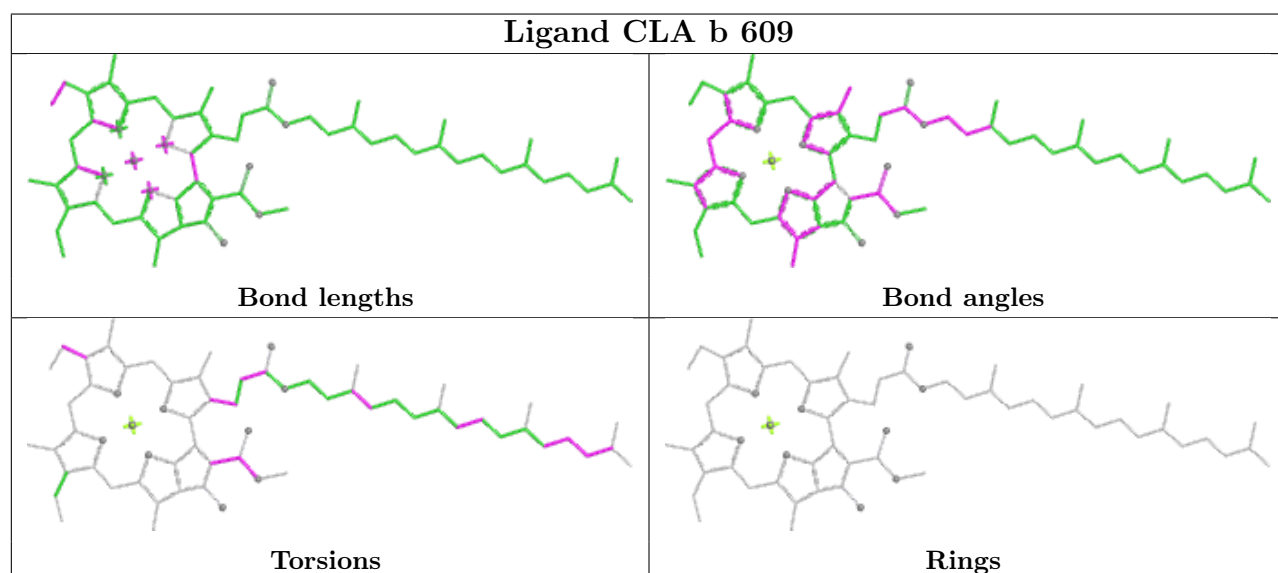
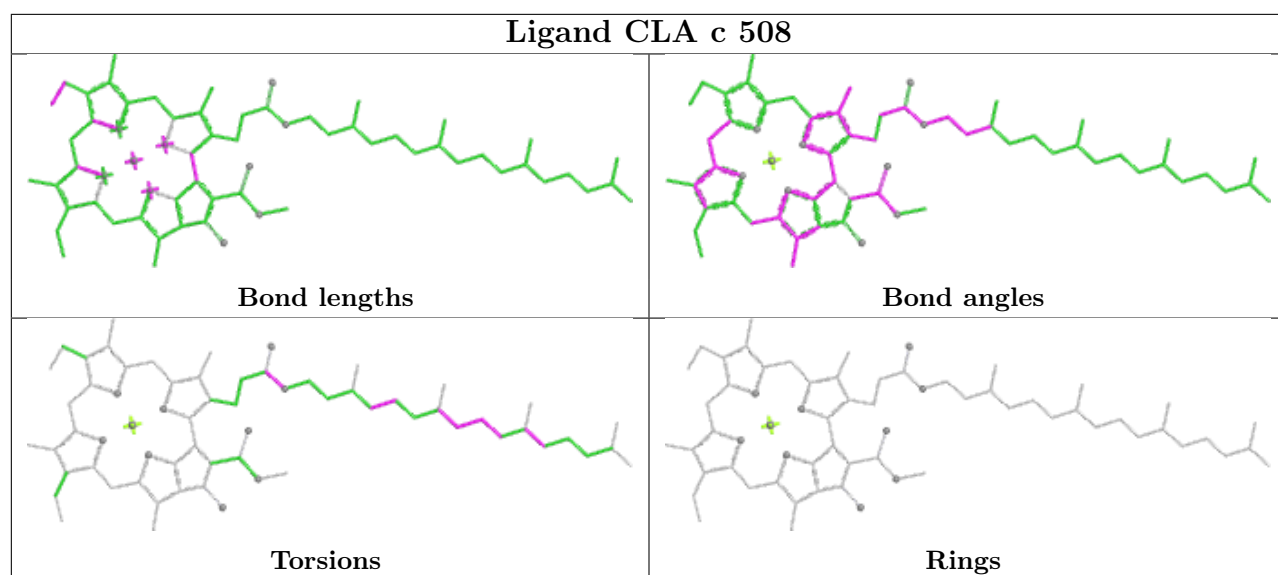


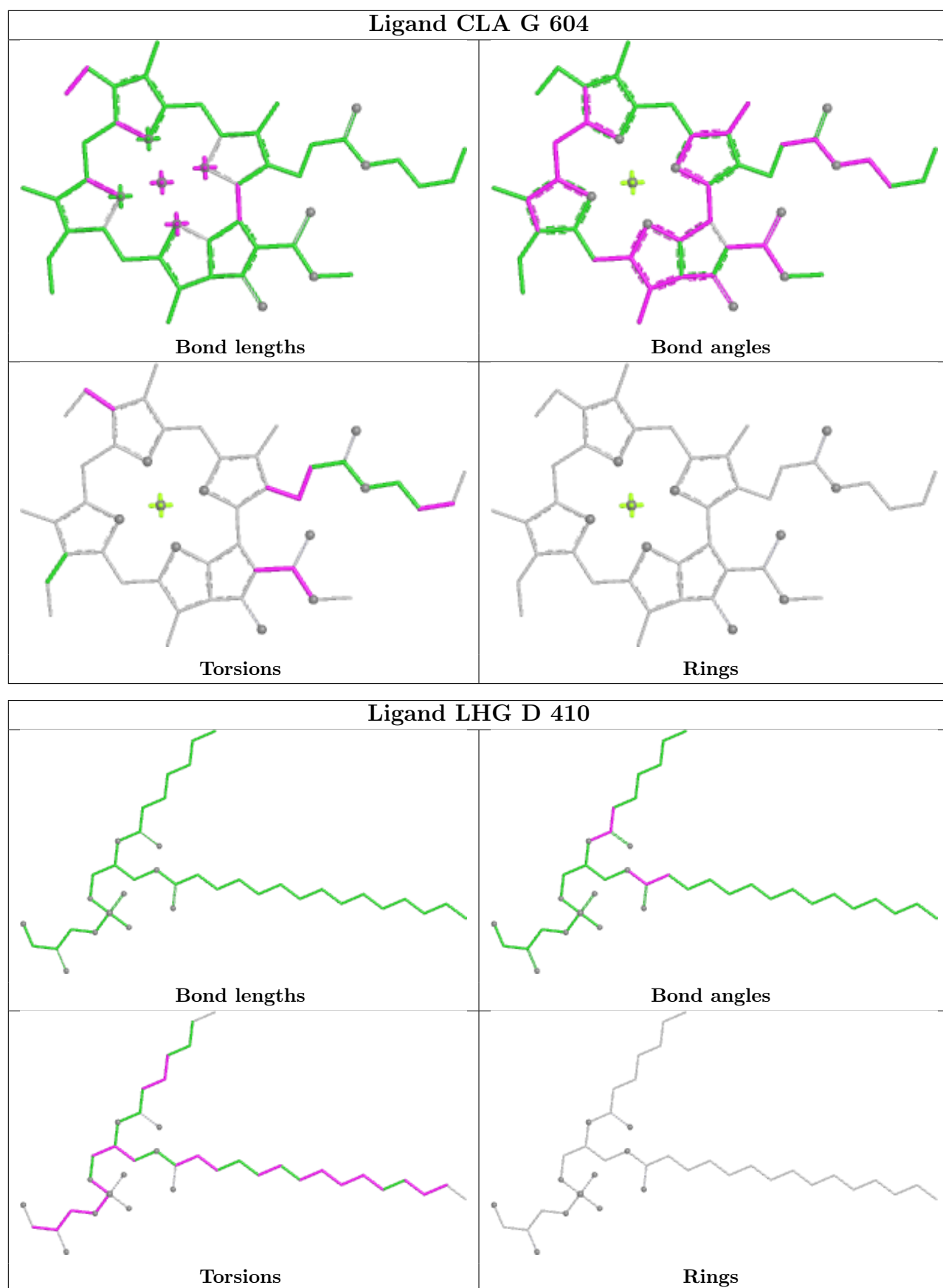
Torsions

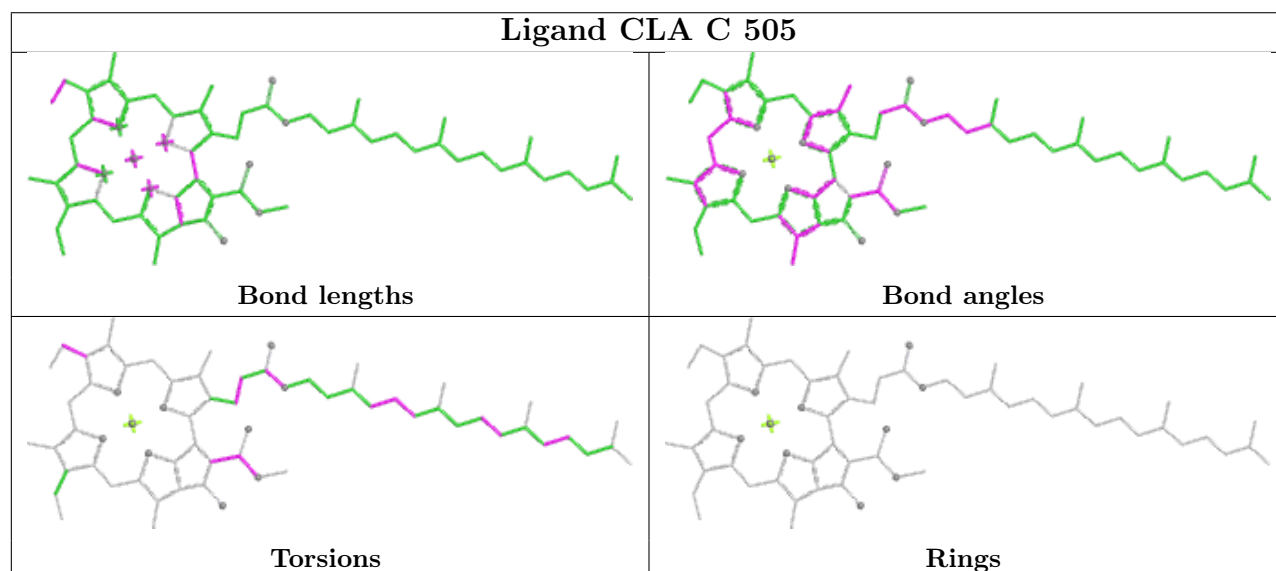
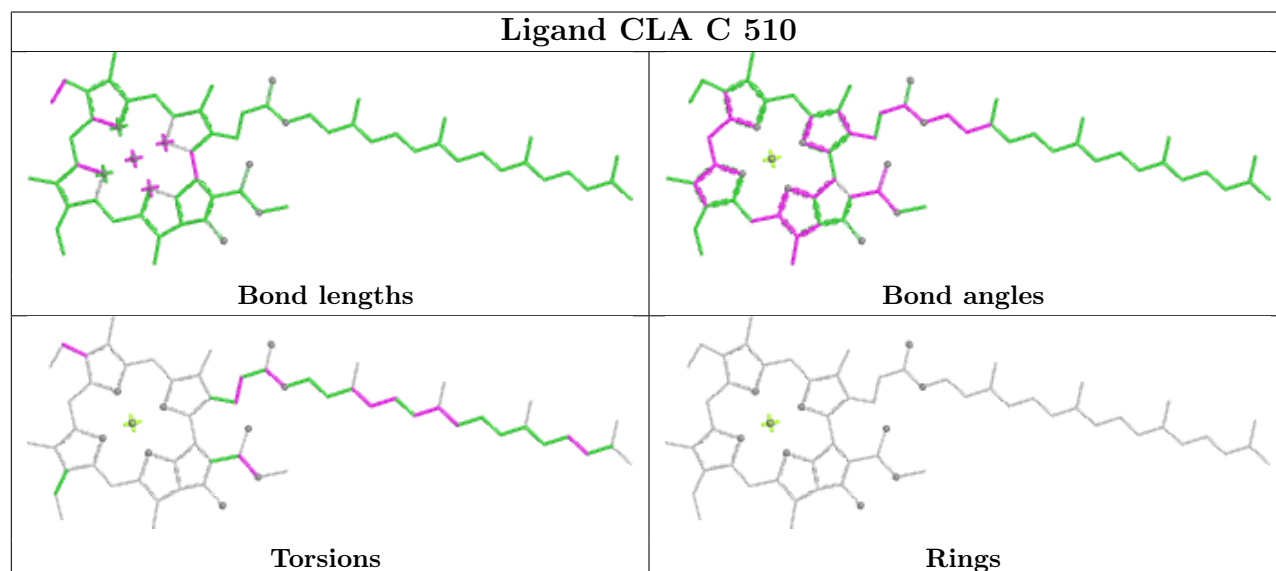
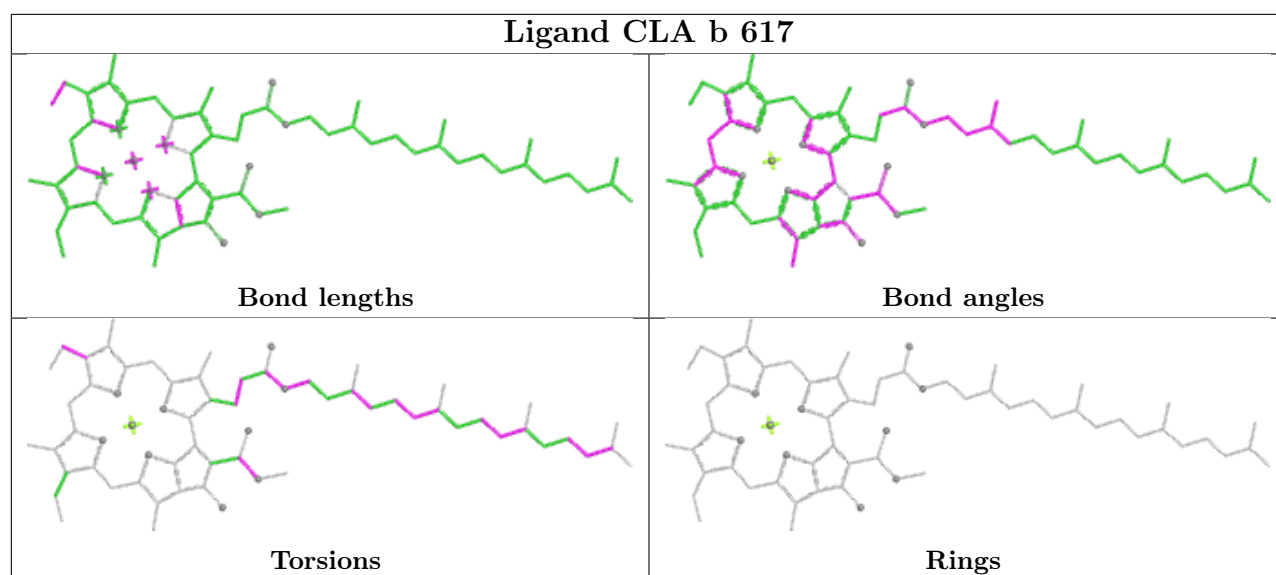


Rings

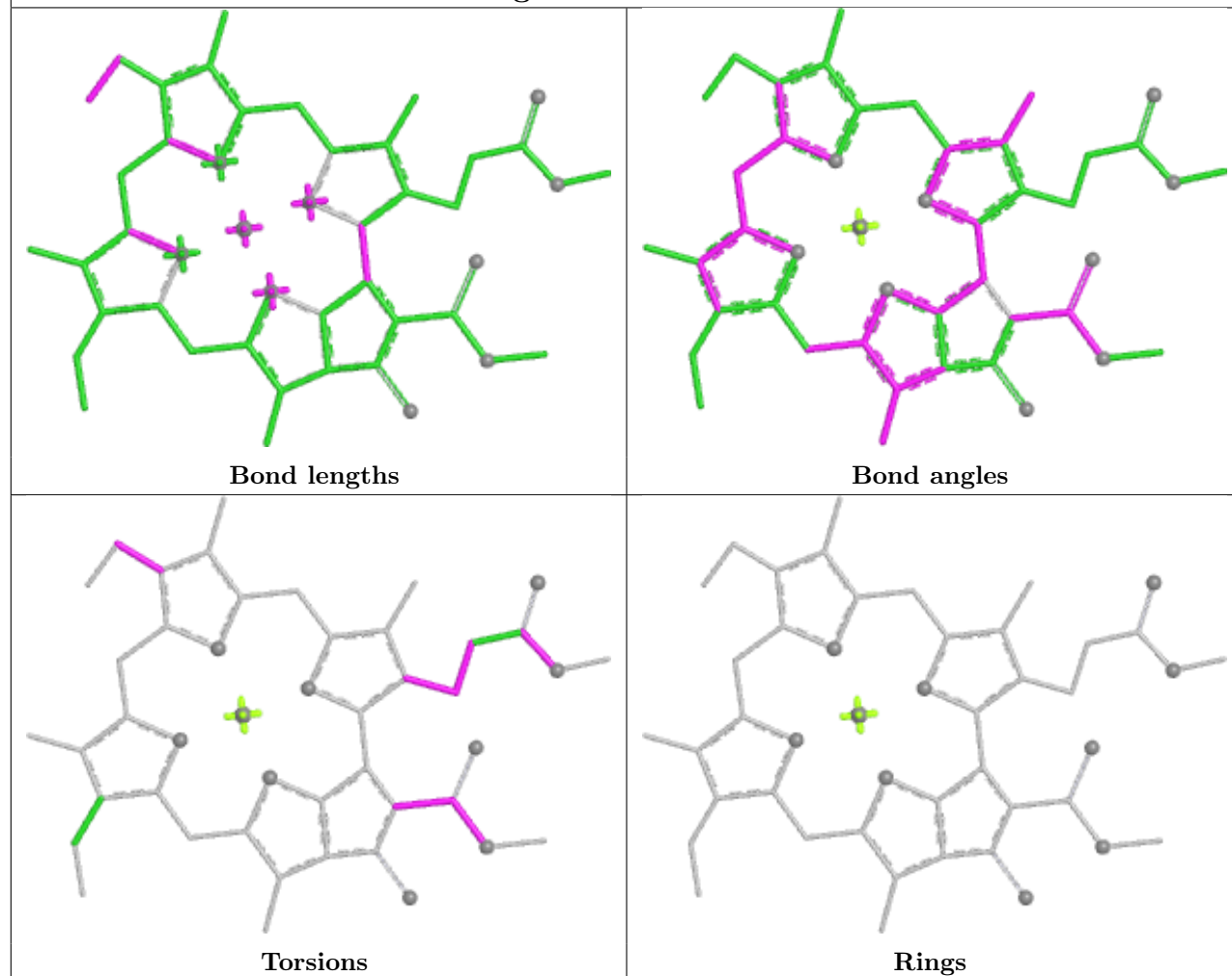


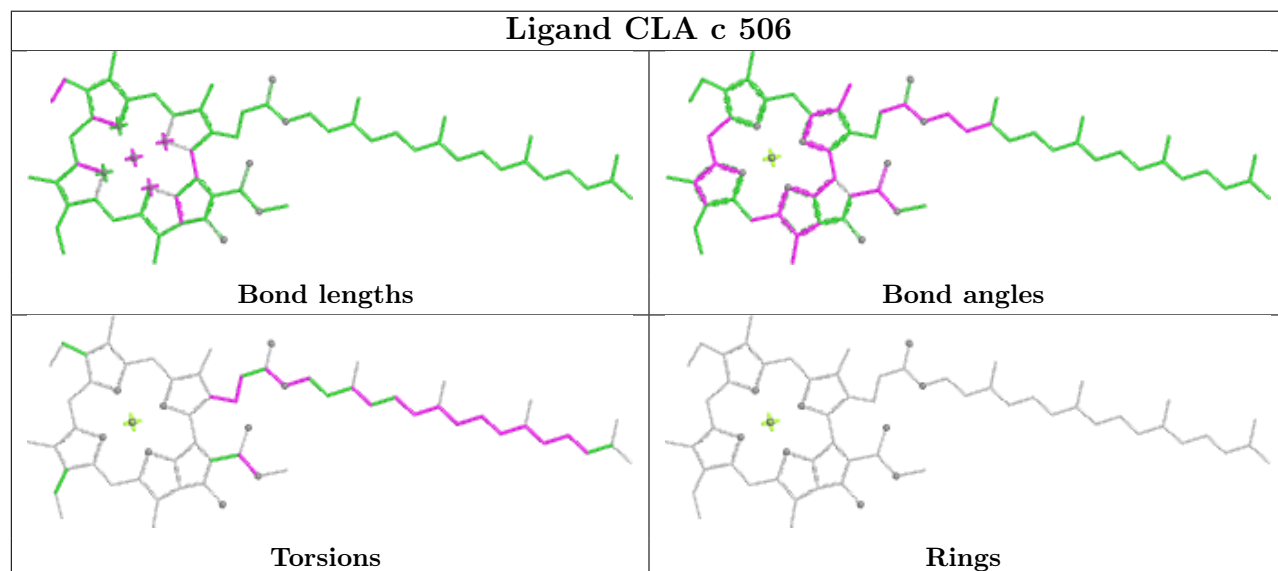
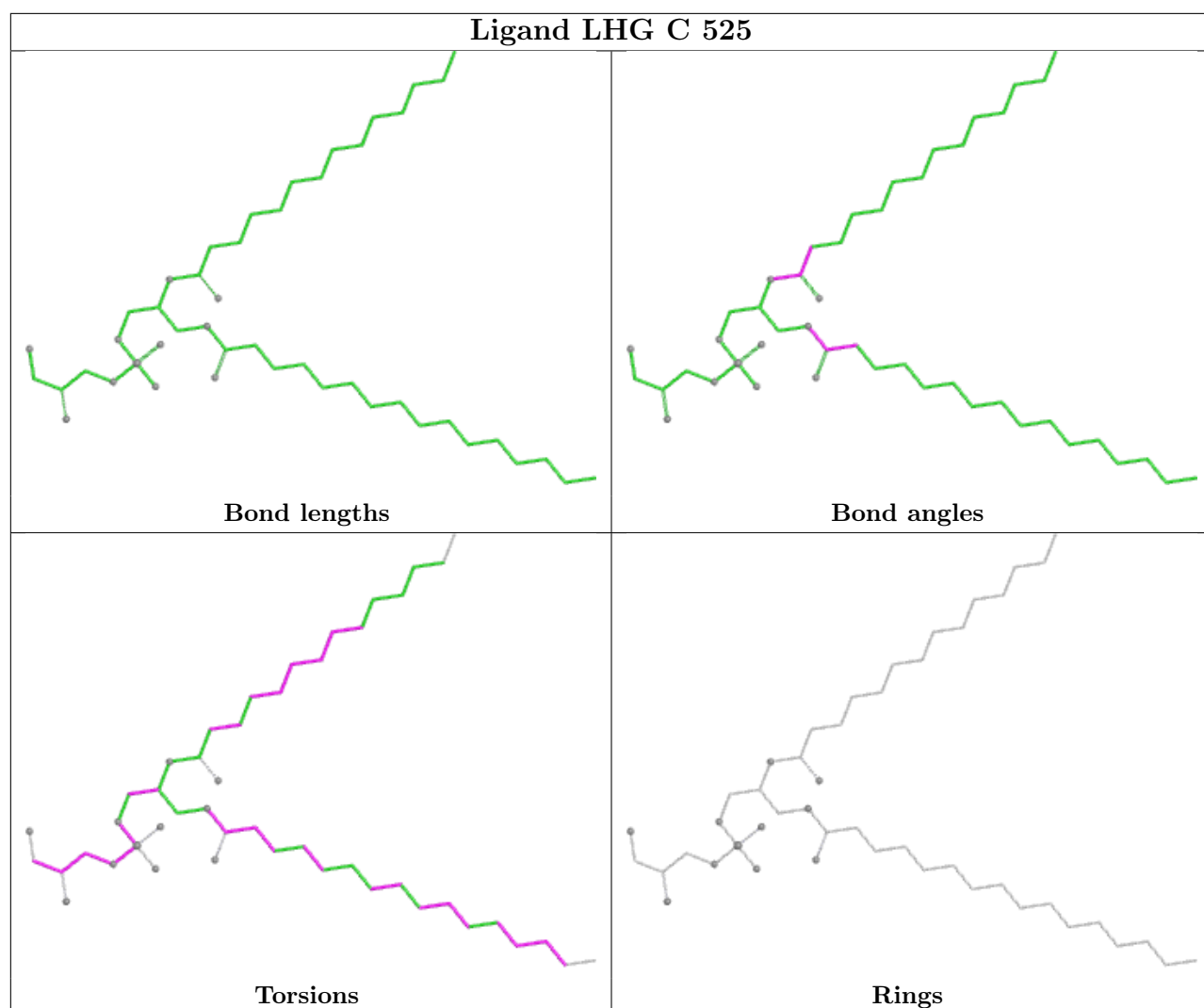


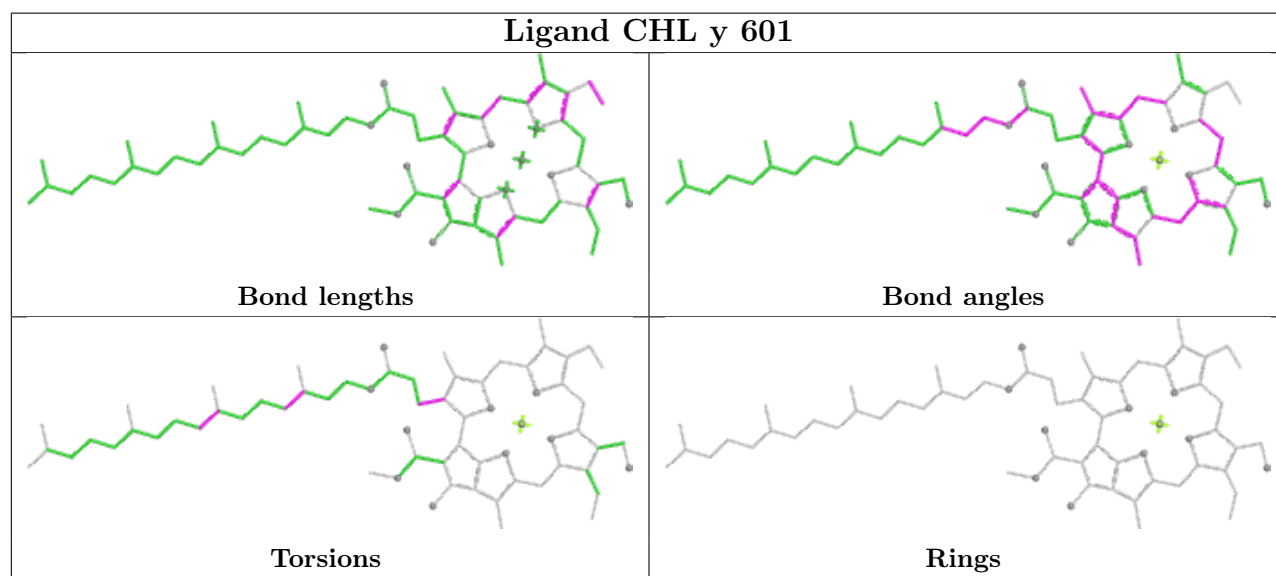
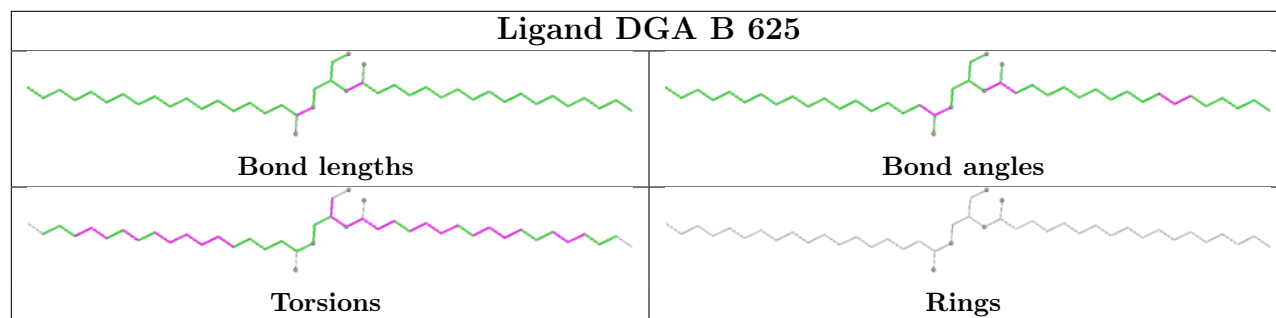


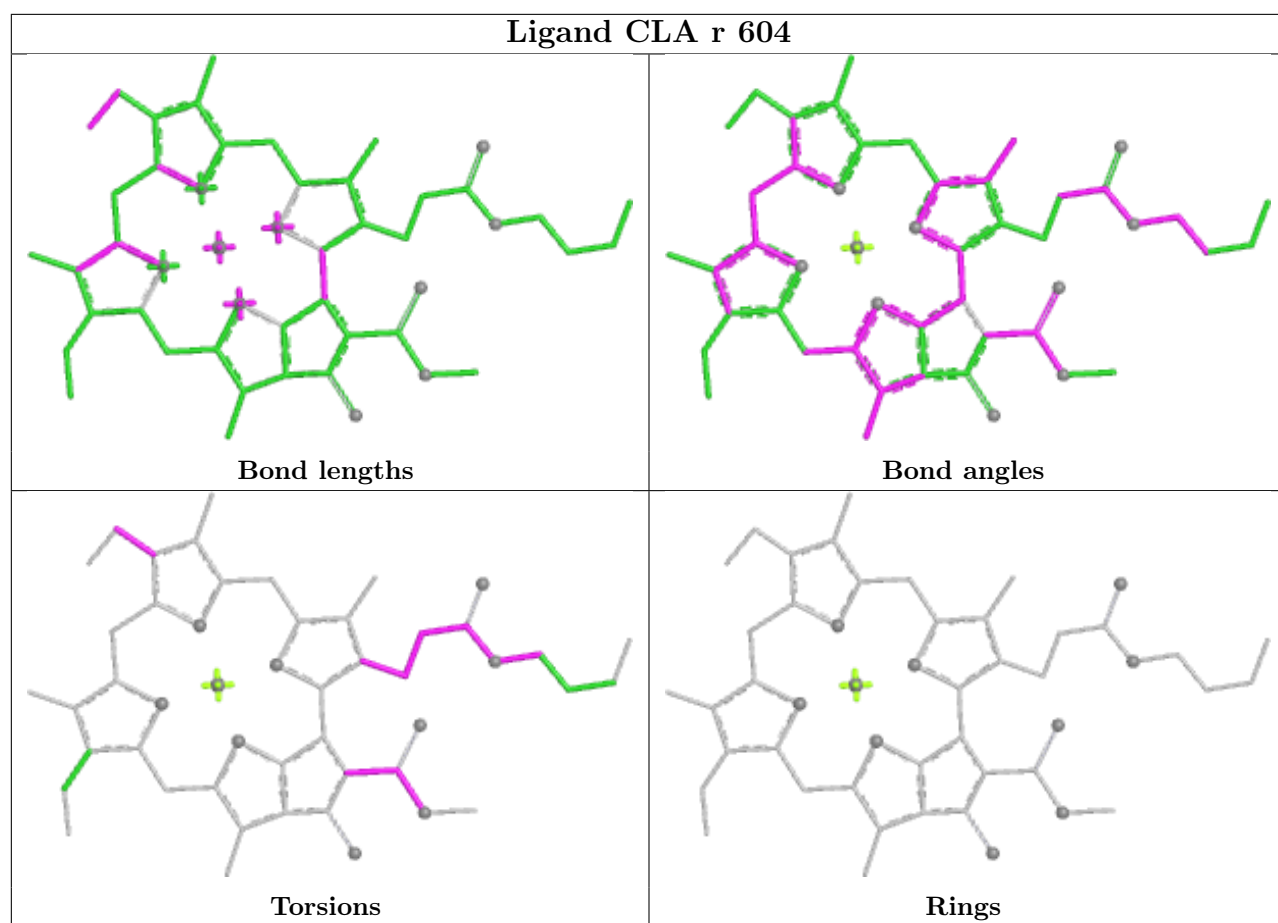


Ligand CLA R 613

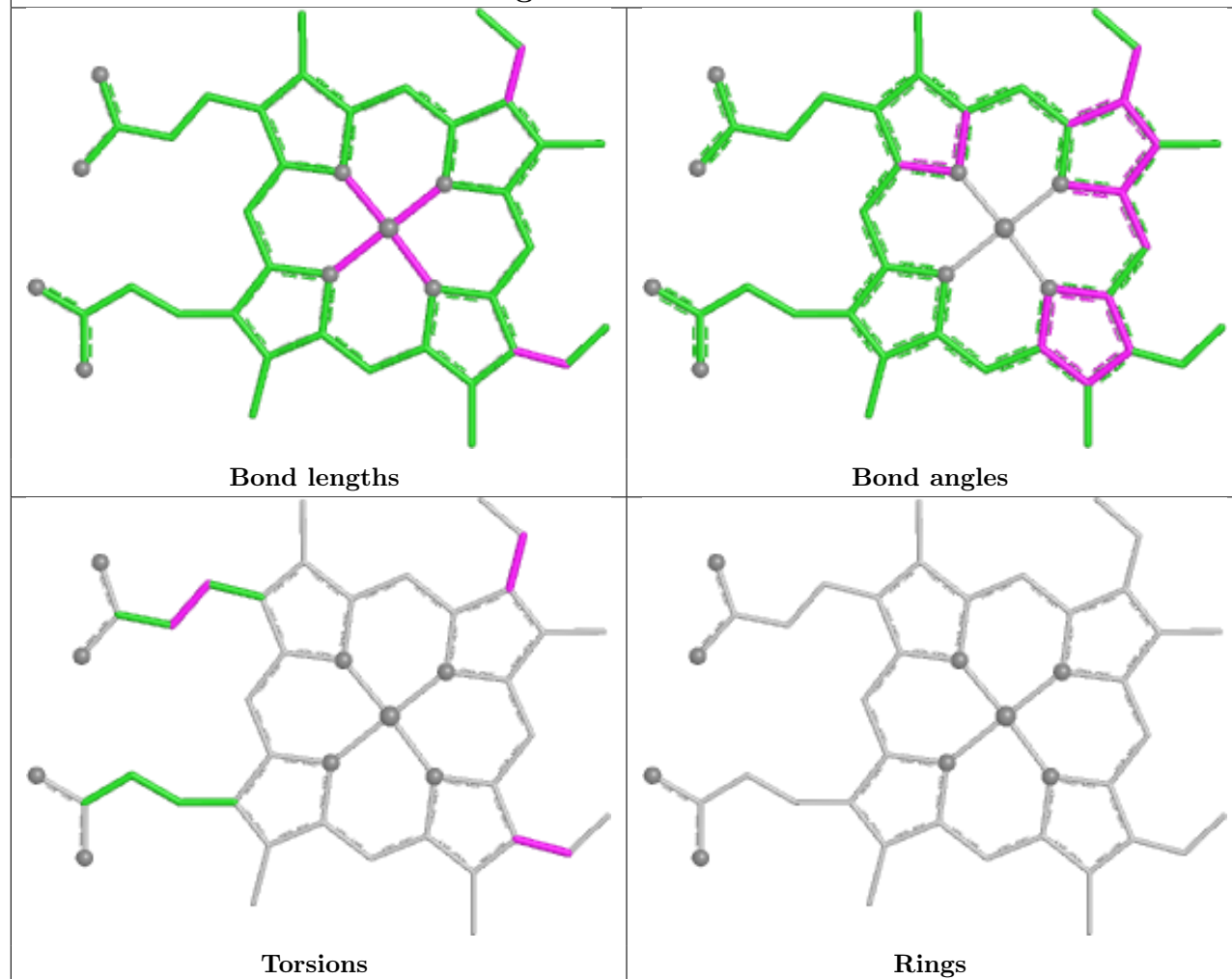




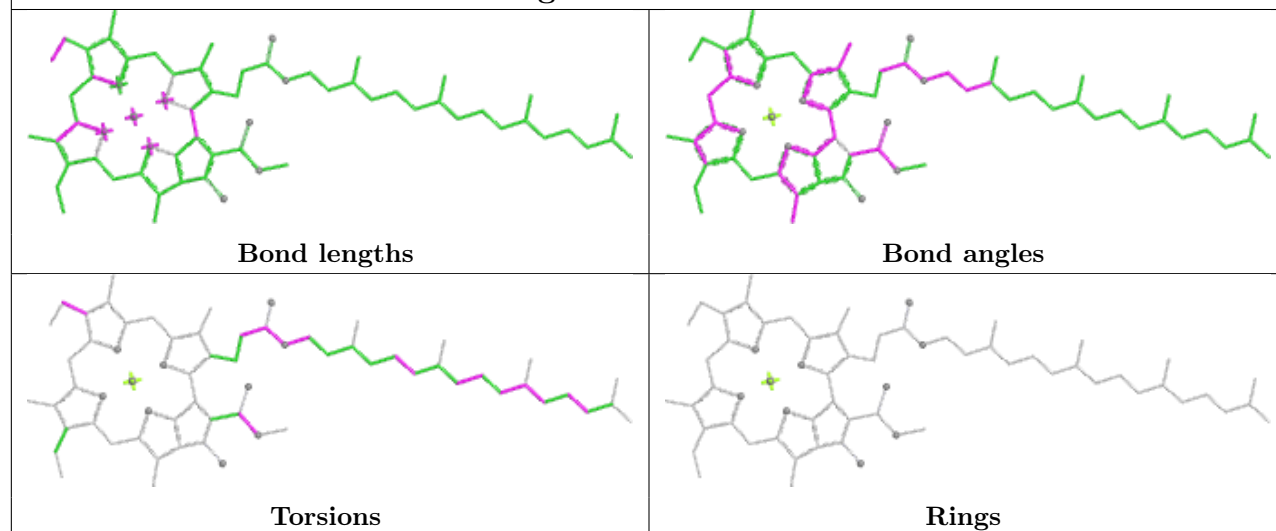


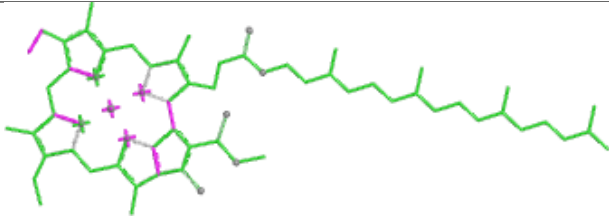
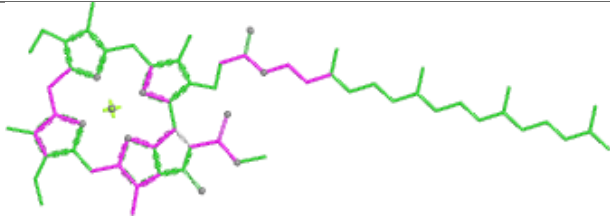
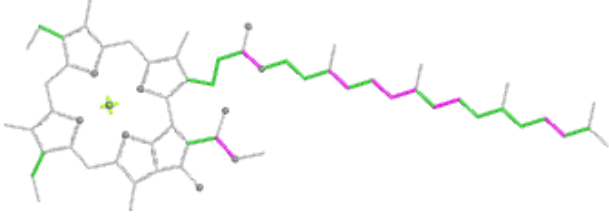
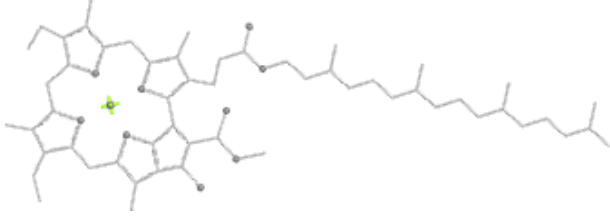
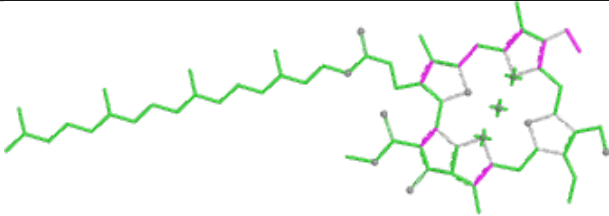
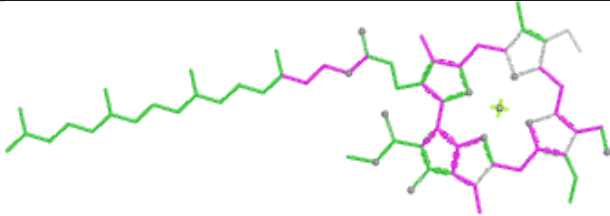
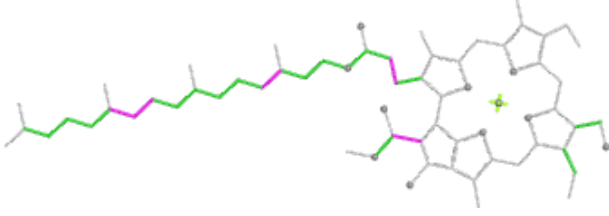
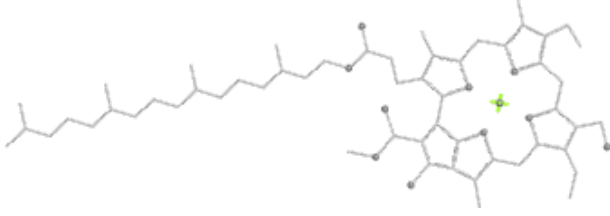
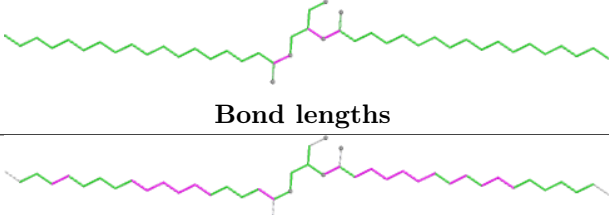
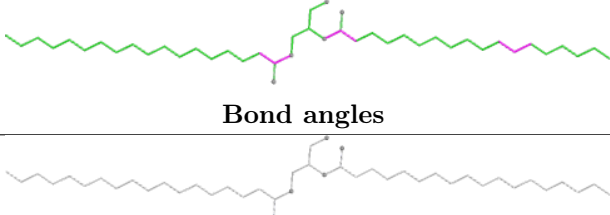


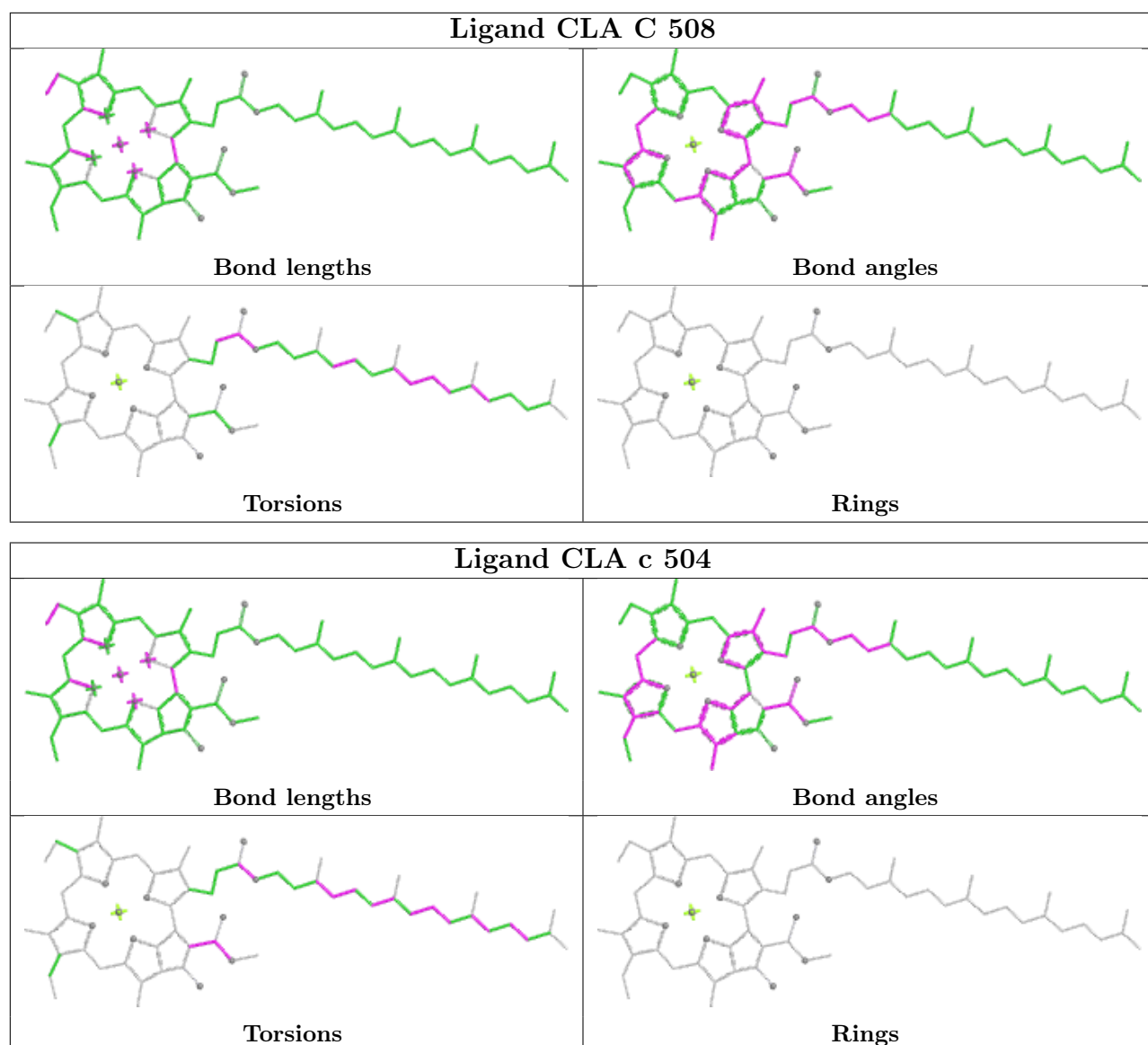
Ligand HEM f 101

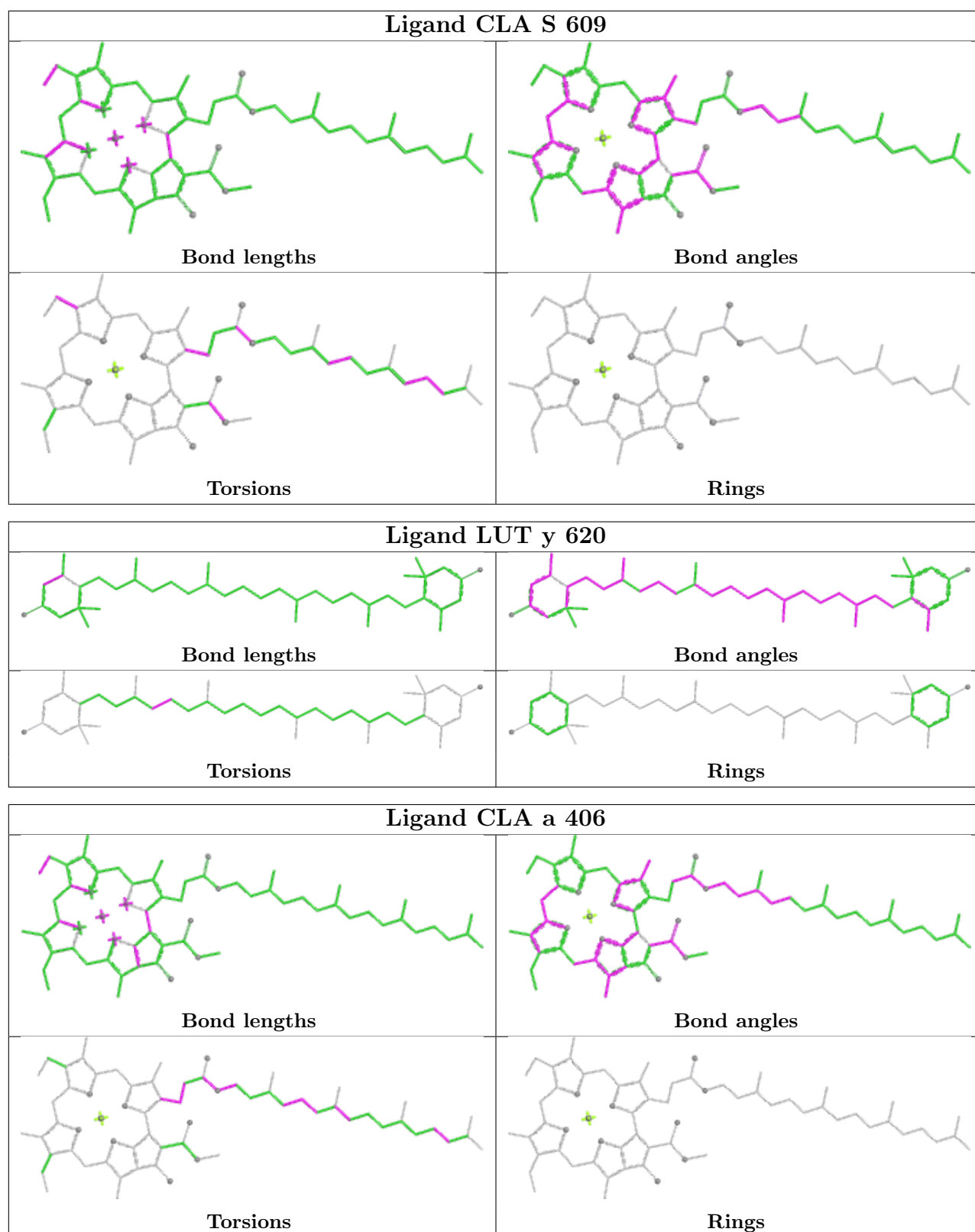


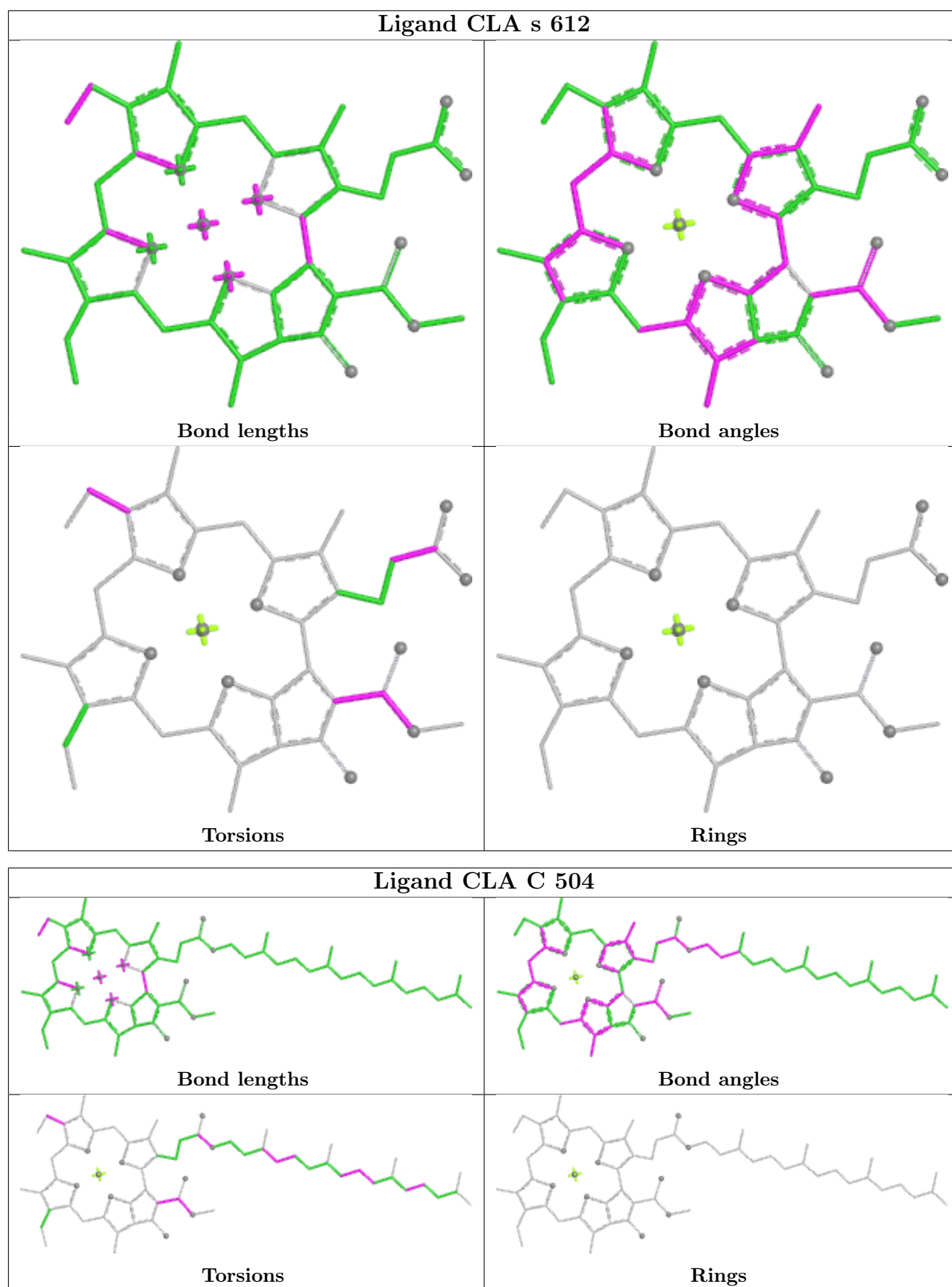
Ligand CLA s 603

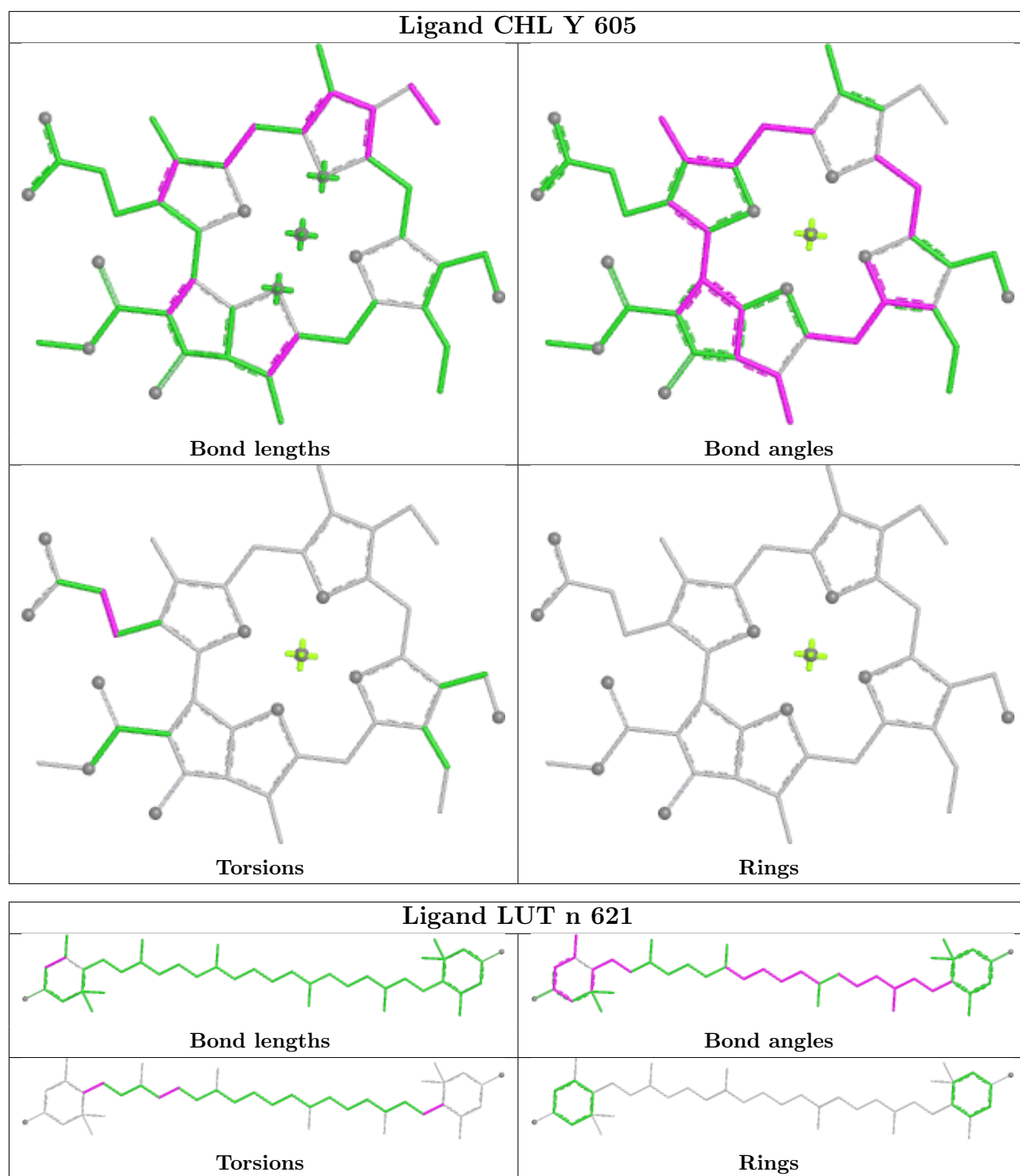


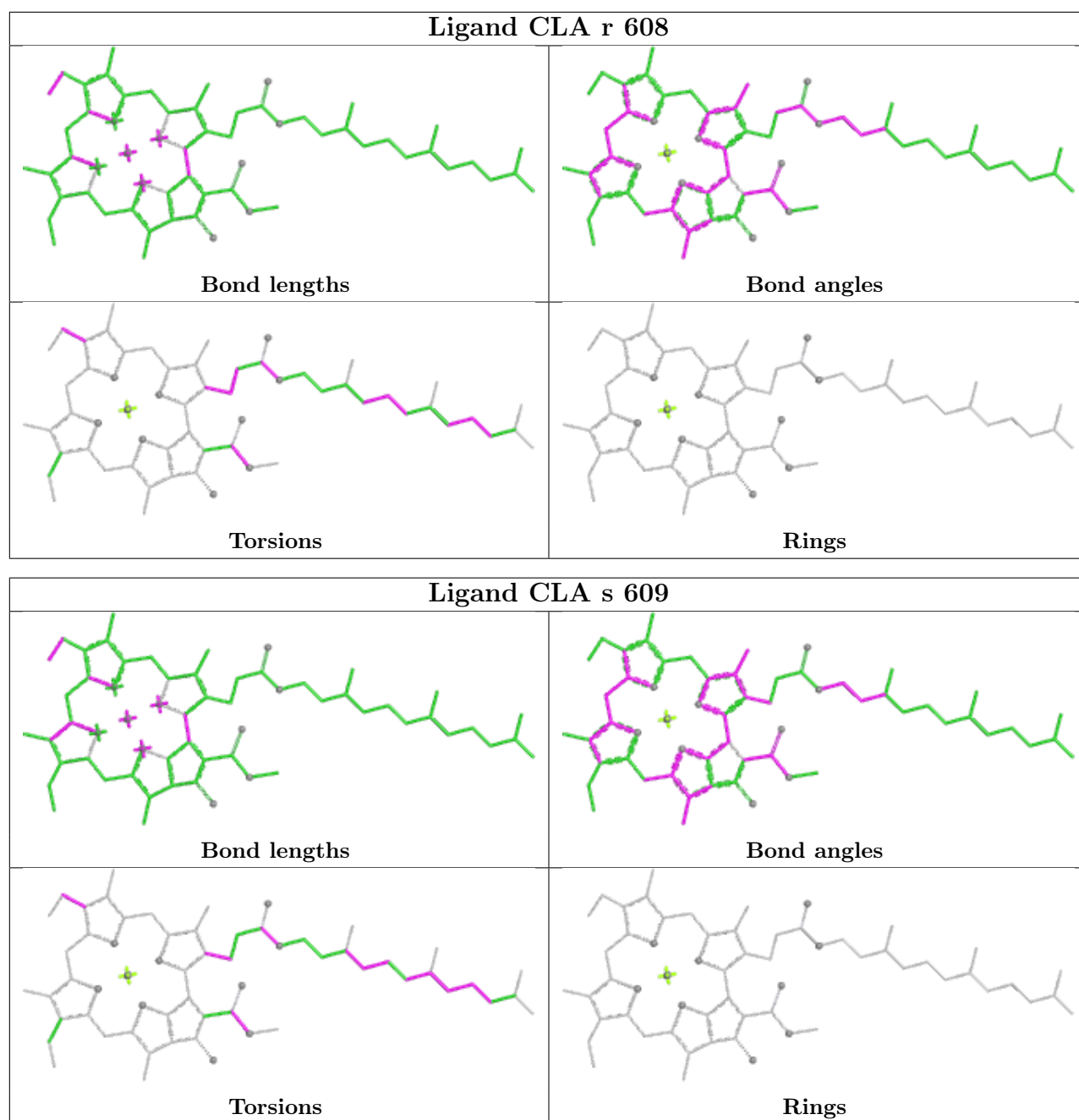
Ligand CLA b 606	
	
Bond lengths	
Bond angles	
Torsions	
Rings	
Ligand CHL y 607	
	
Bond lengths	
Bond angles	
Torsions	
Rings	
Ligand DGA C 524	
	
Bond lengths	
Bond angles	
Torsions	
Rings	

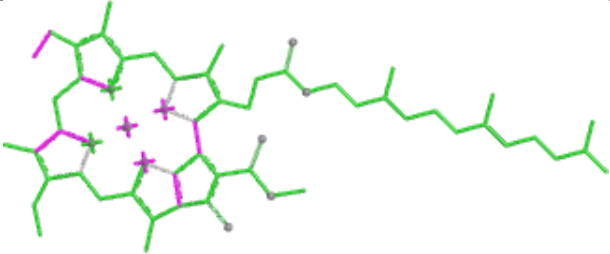
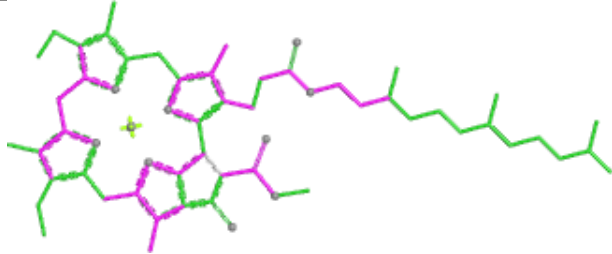
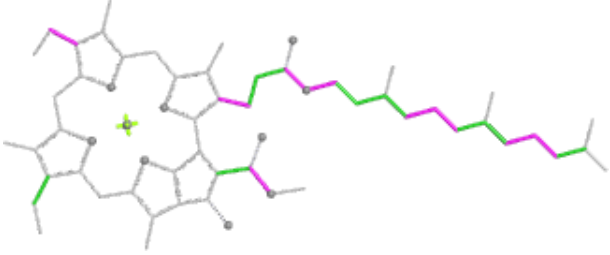
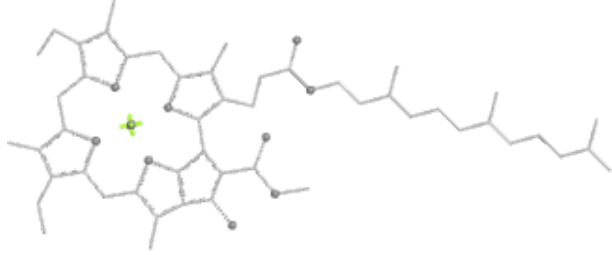
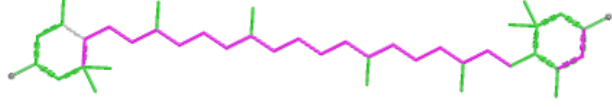
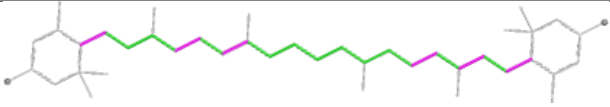
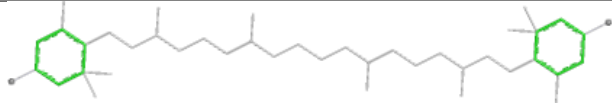
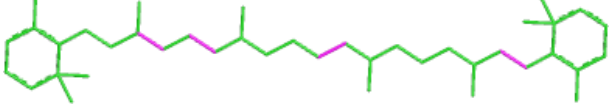
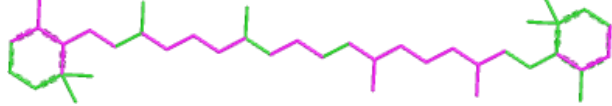
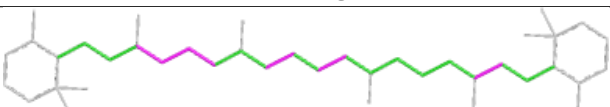
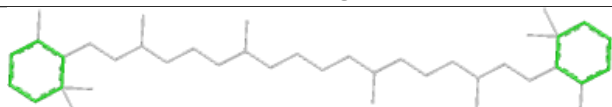


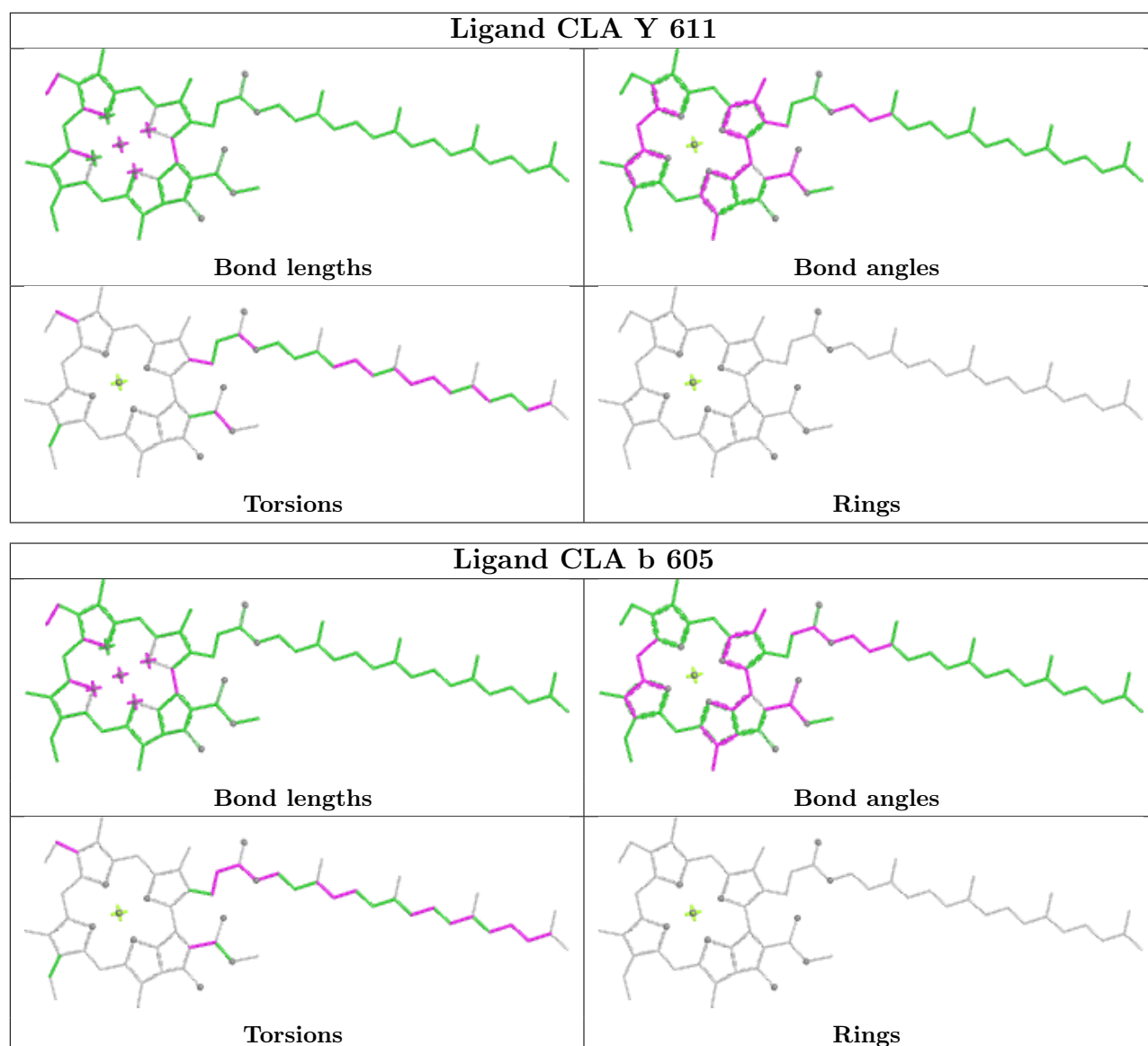




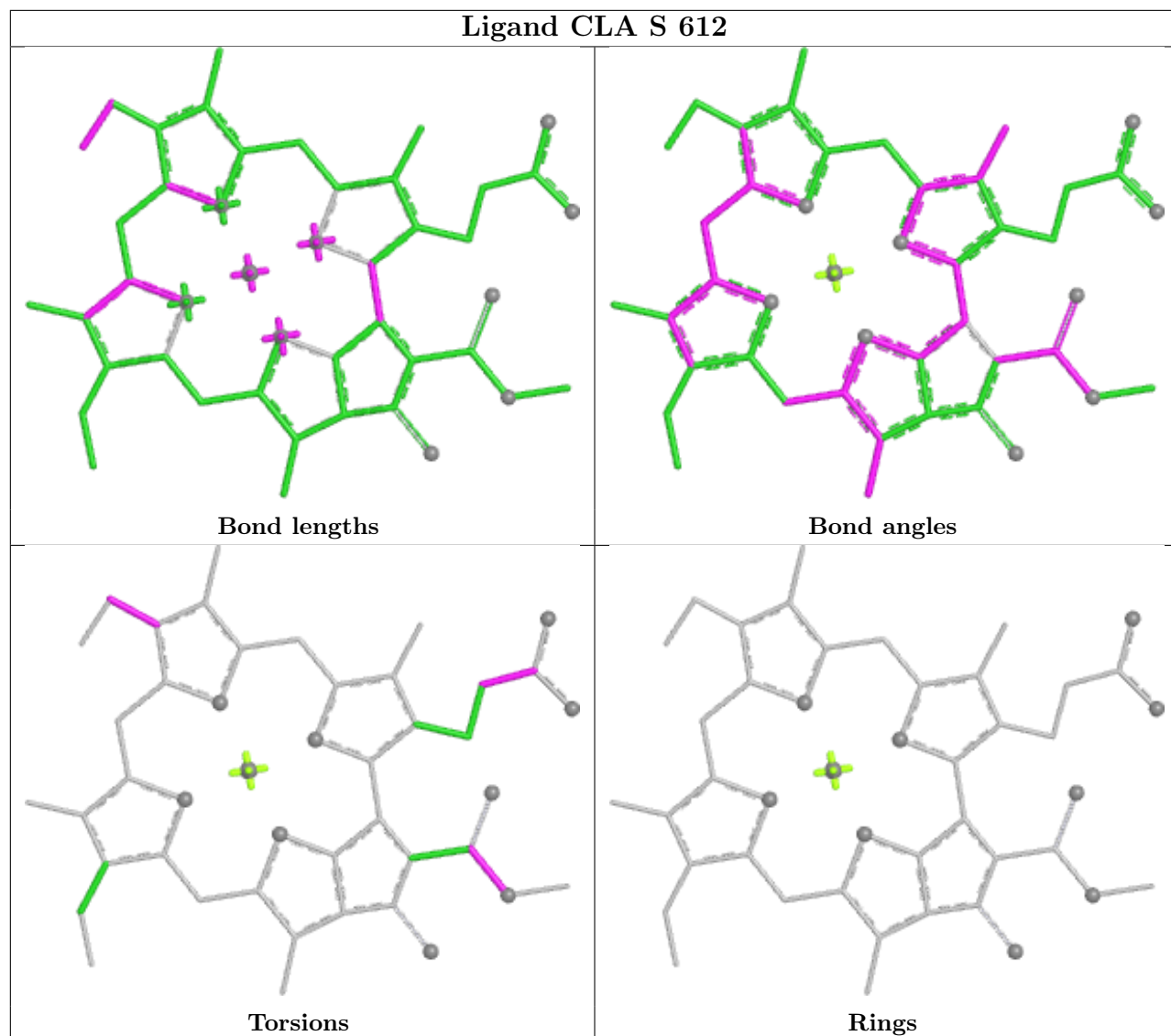


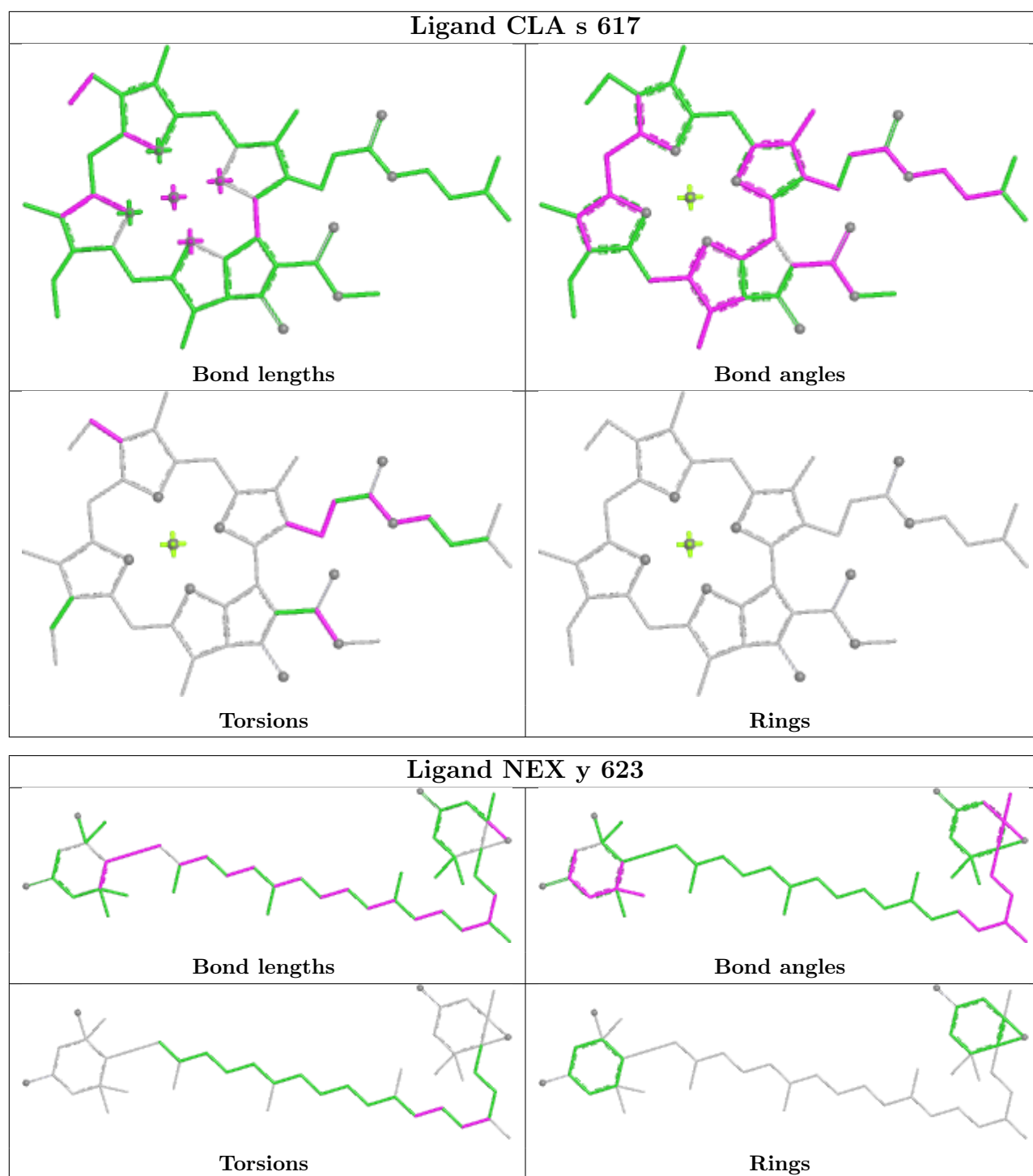


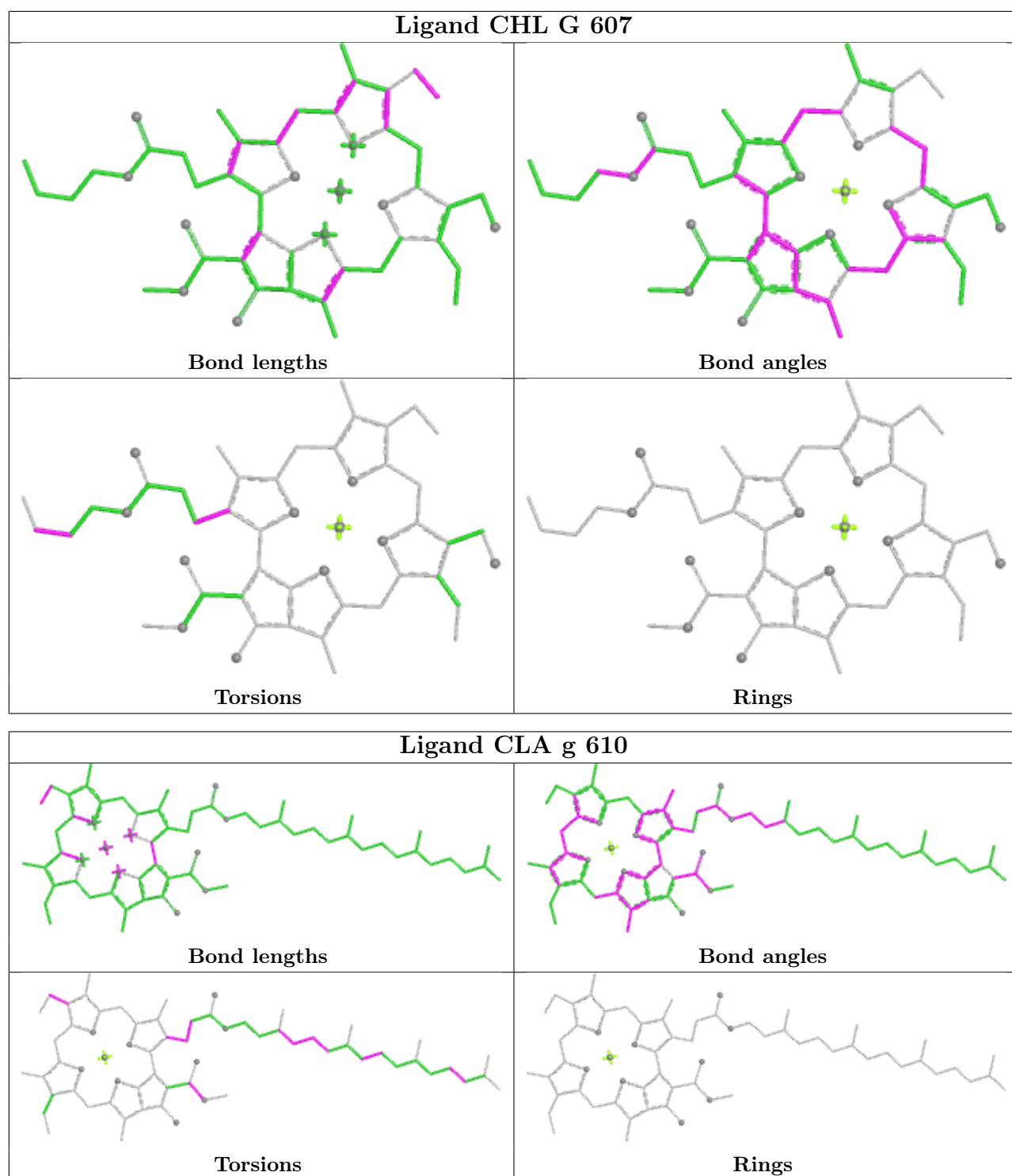
Ligand CLA A 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT r 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

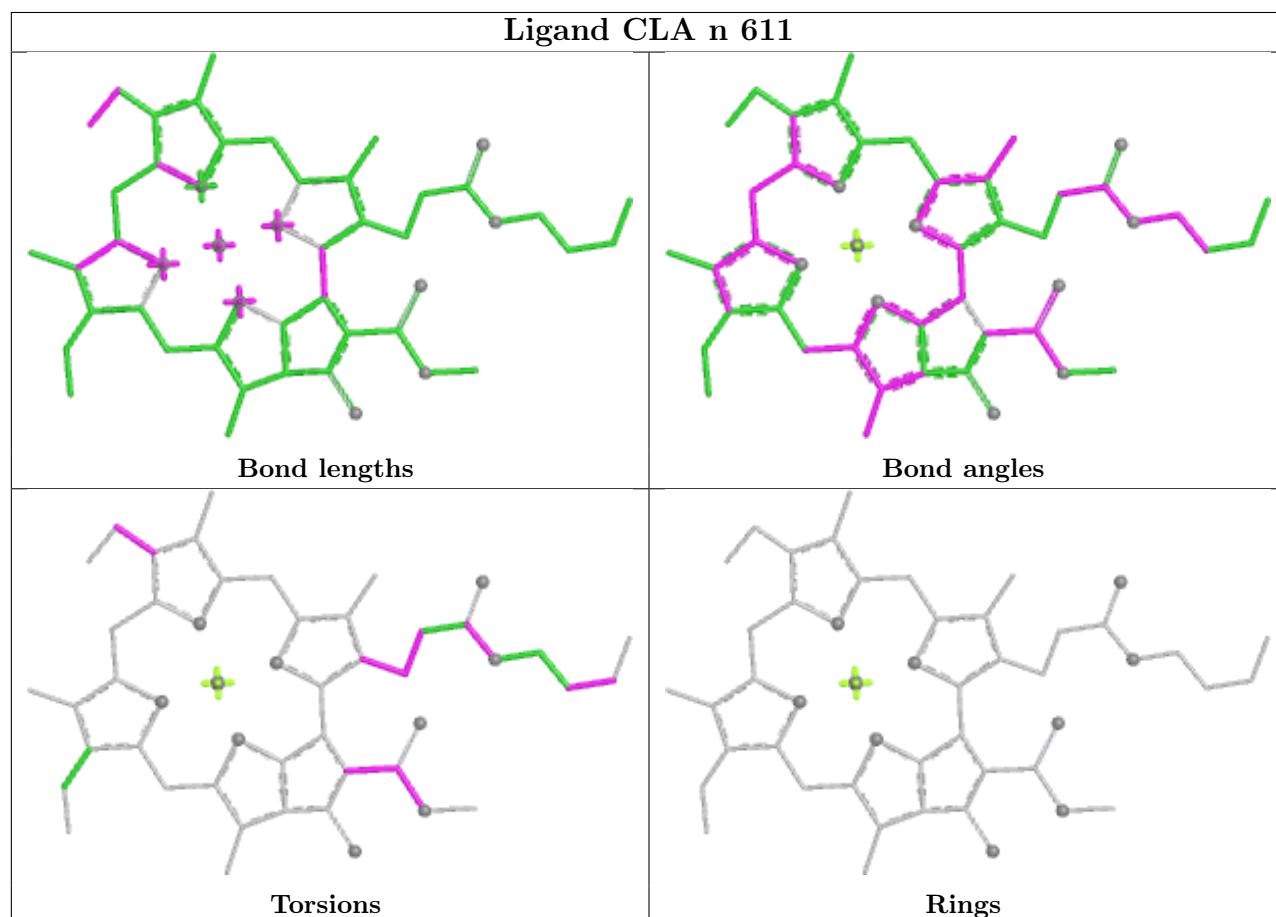
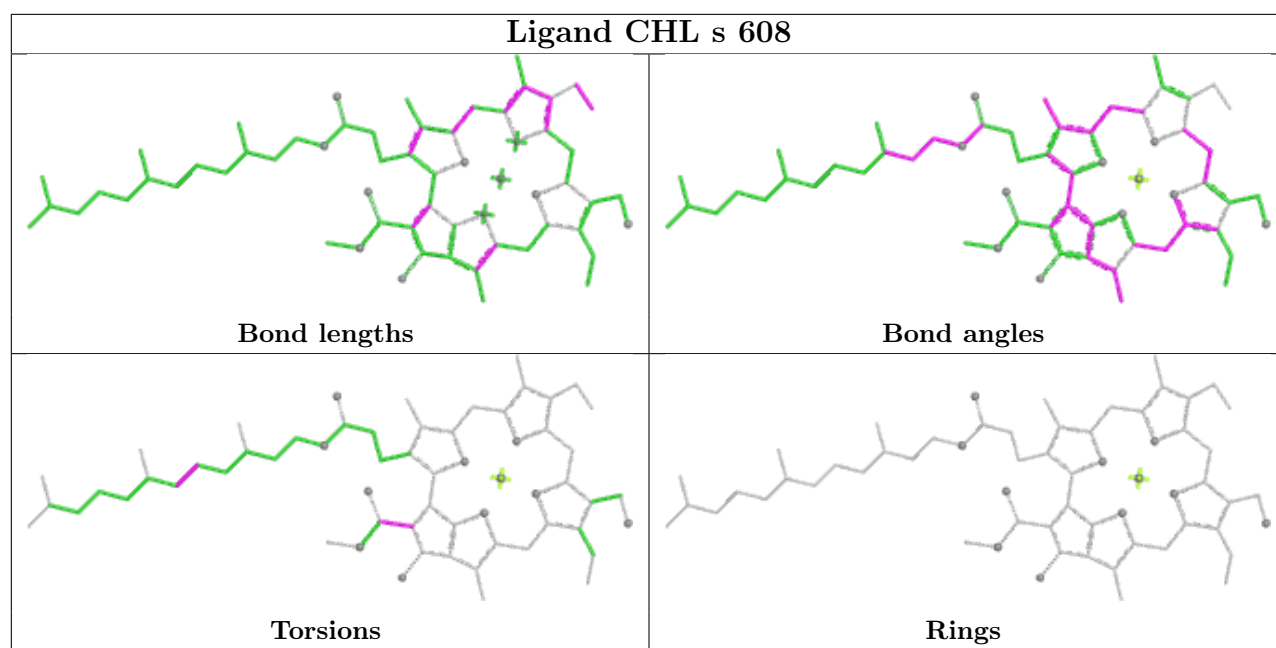


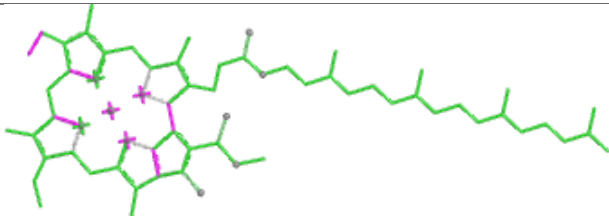
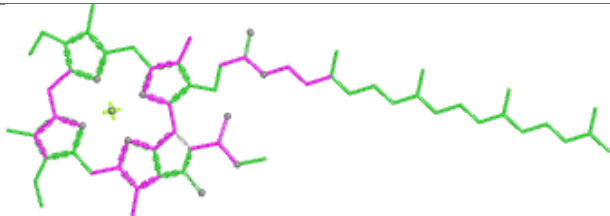
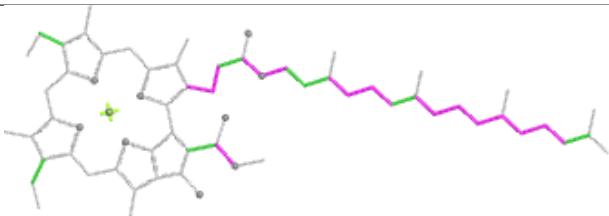
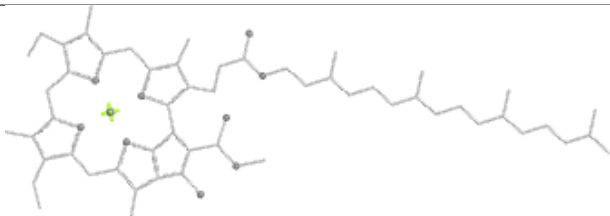
Ligand CLA S 612

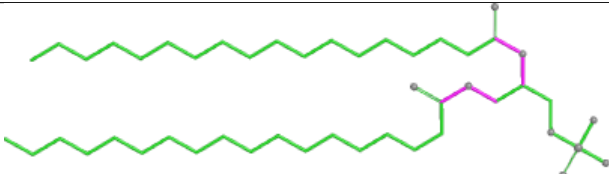
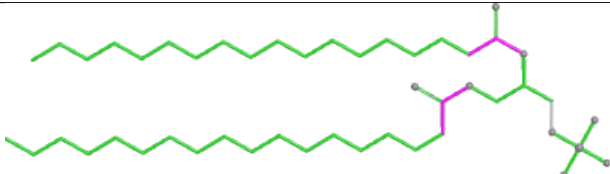
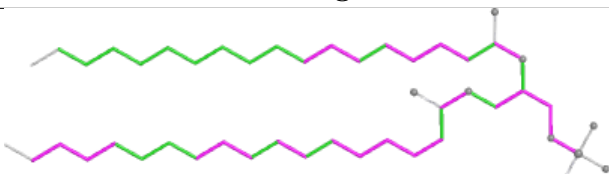
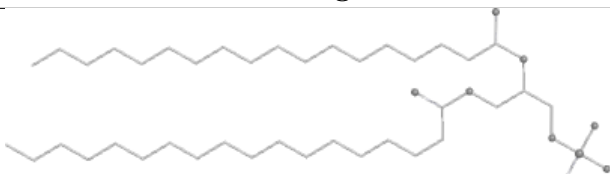


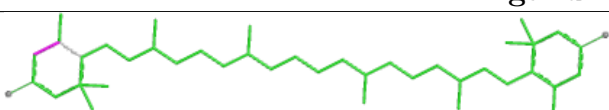
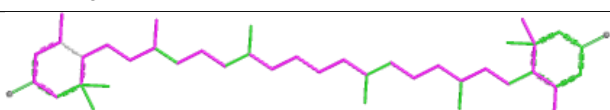
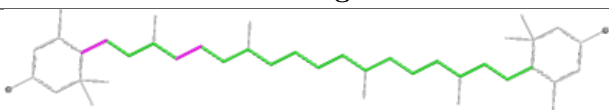
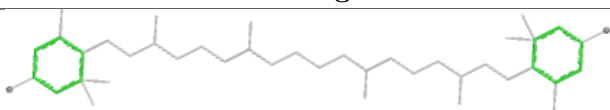


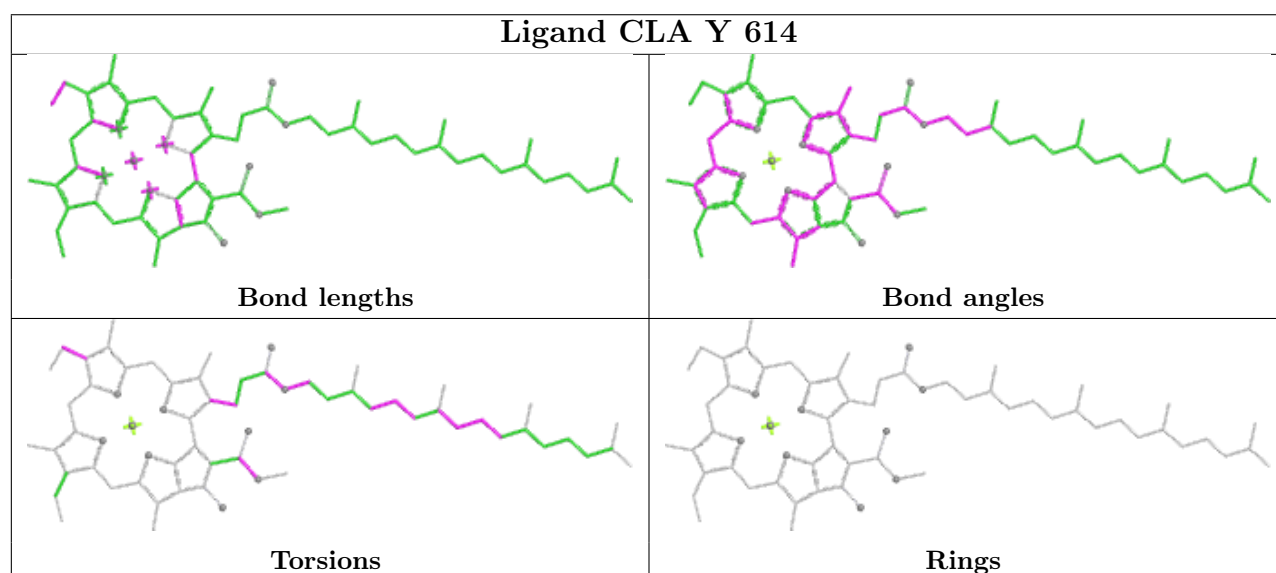
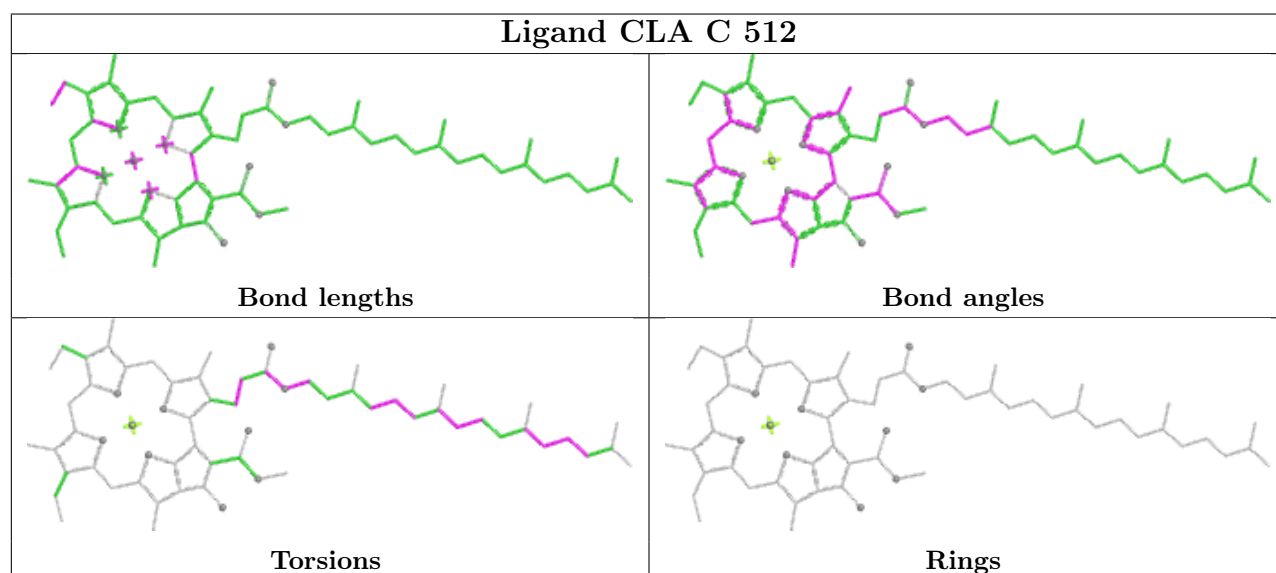
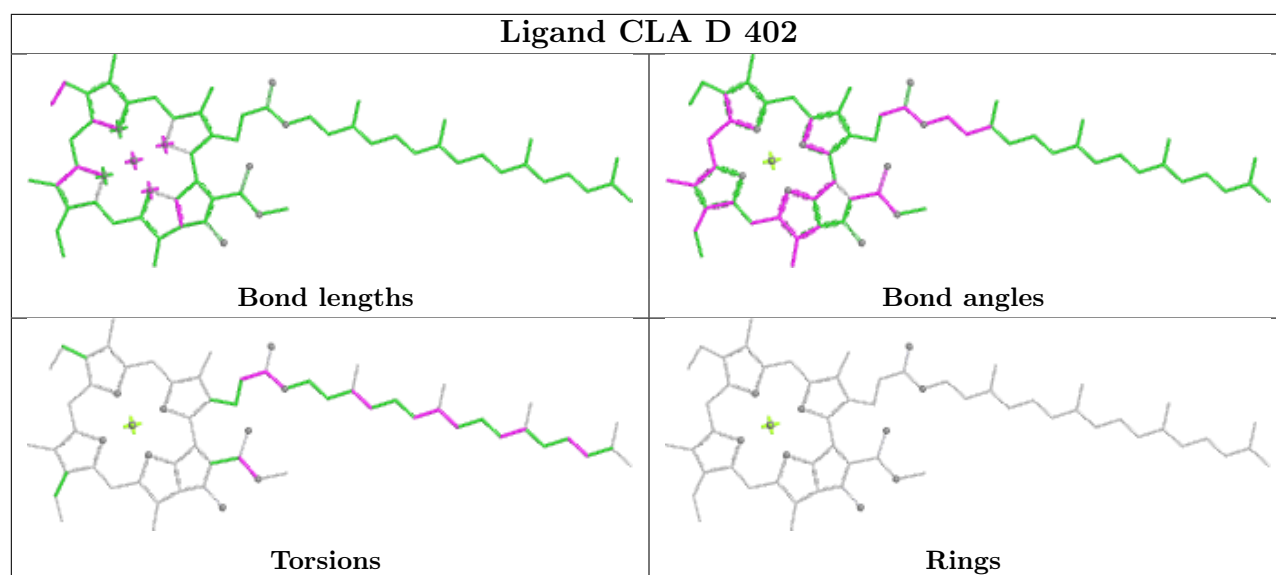




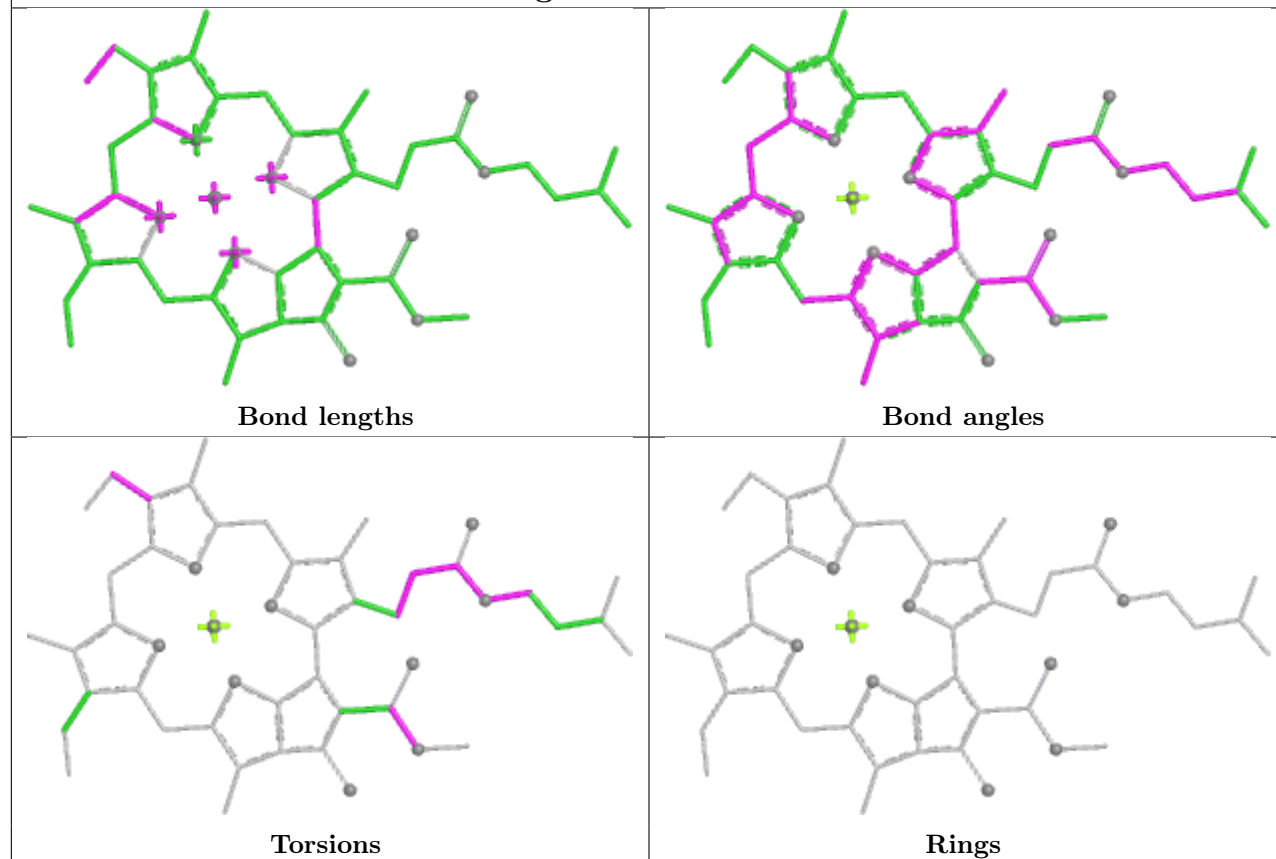
Ligand CLA C 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PH s 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

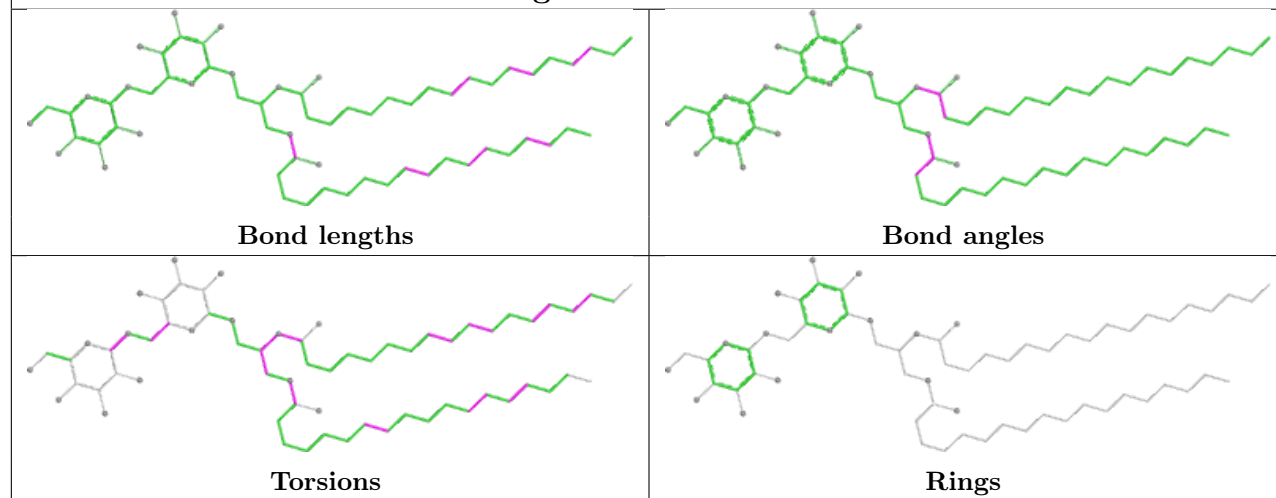
Ligand LUT N 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

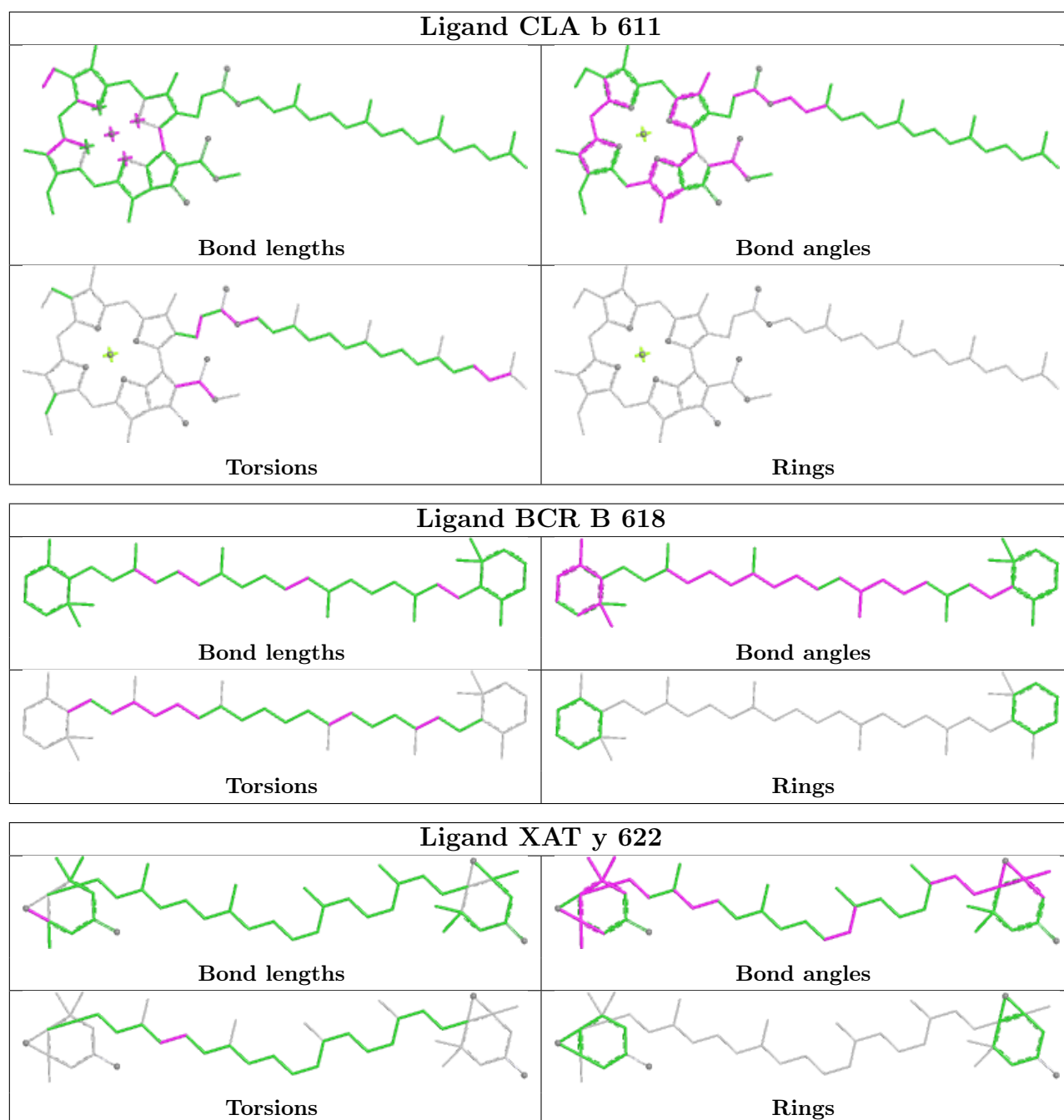


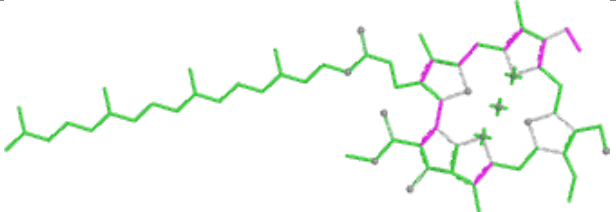
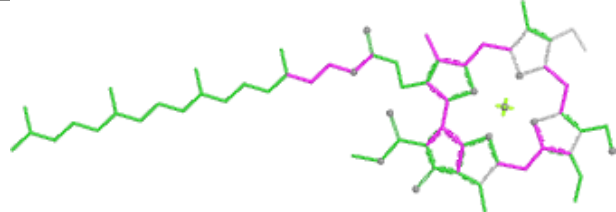
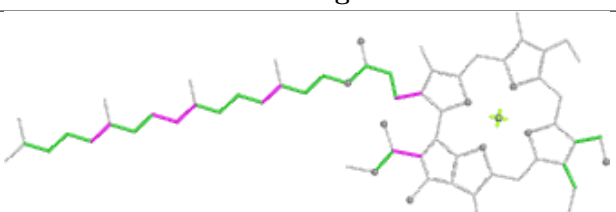
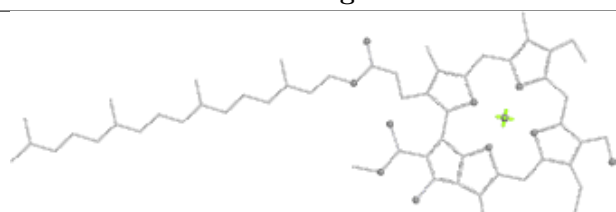
Ligand CLA S 617

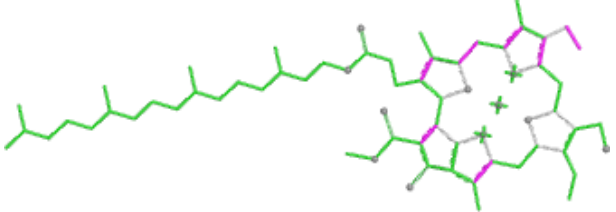
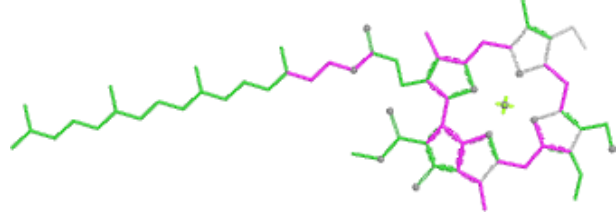
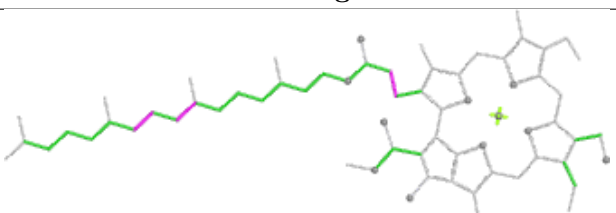
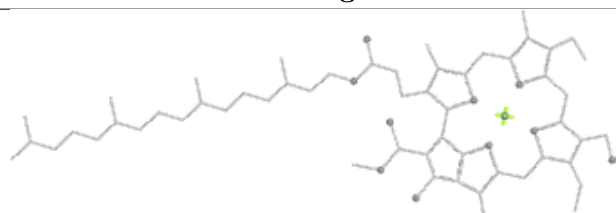


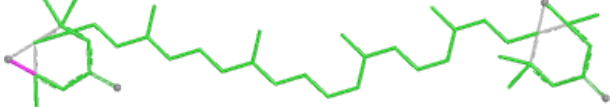
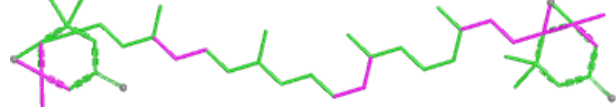
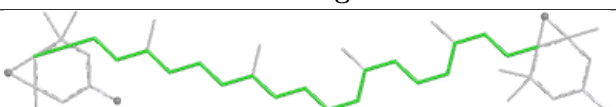
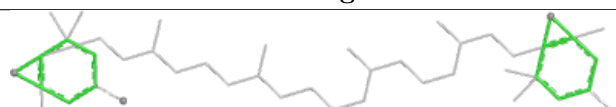
Ligand DGD c 523

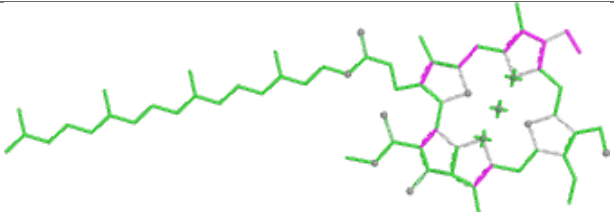
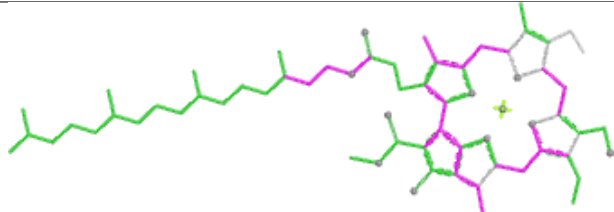
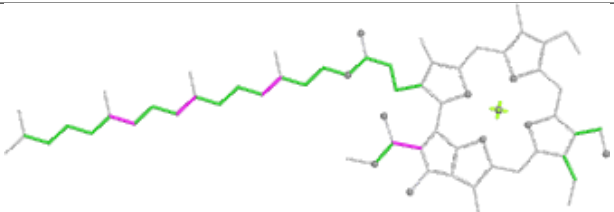
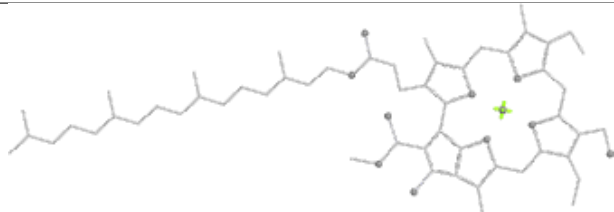


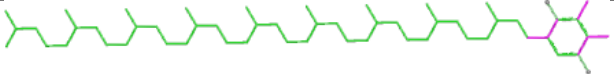
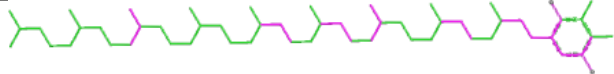
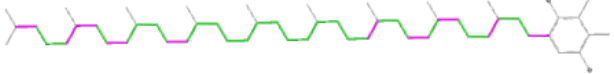
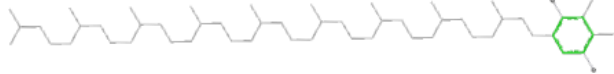


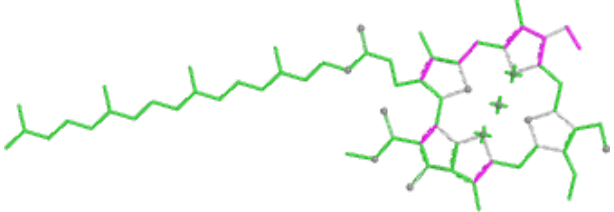
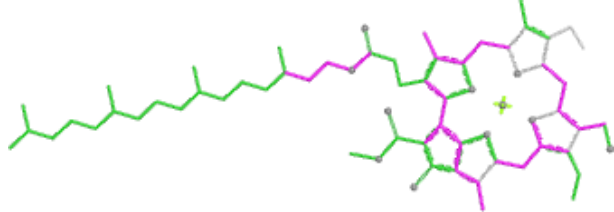
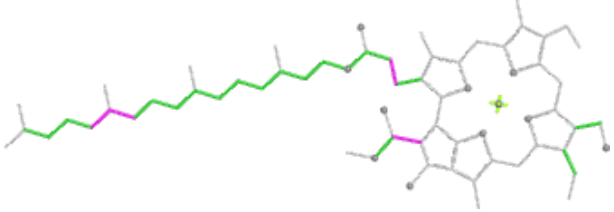
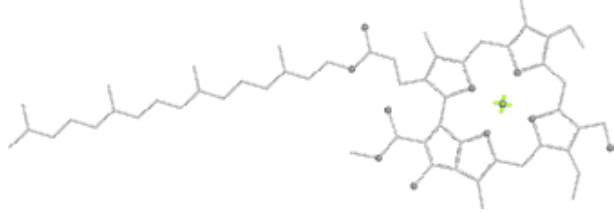
Ligand CHL N 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

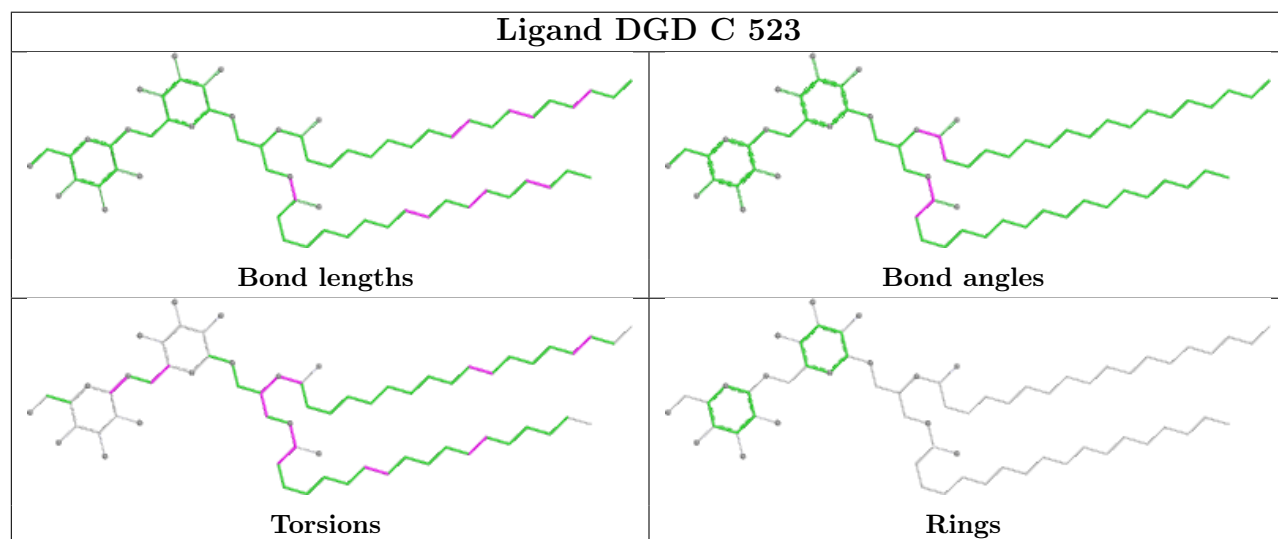
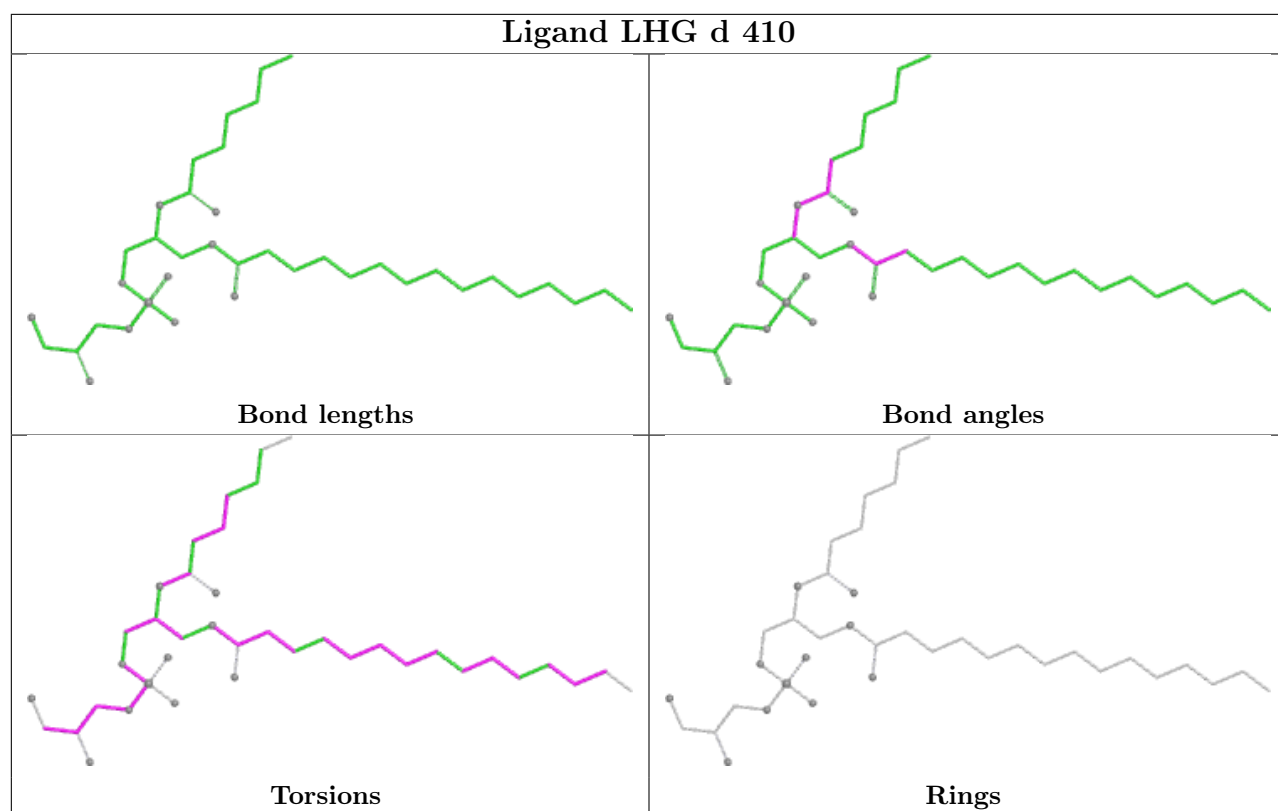
Ligand CHL Y 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

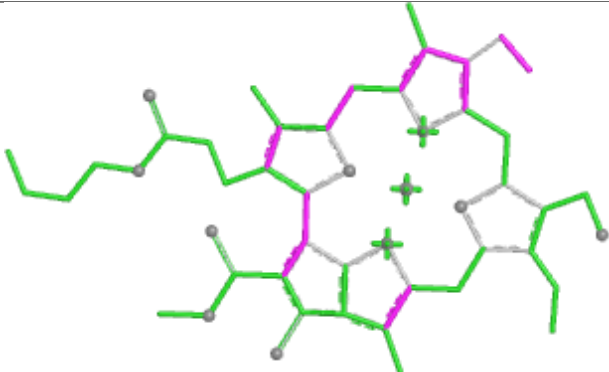
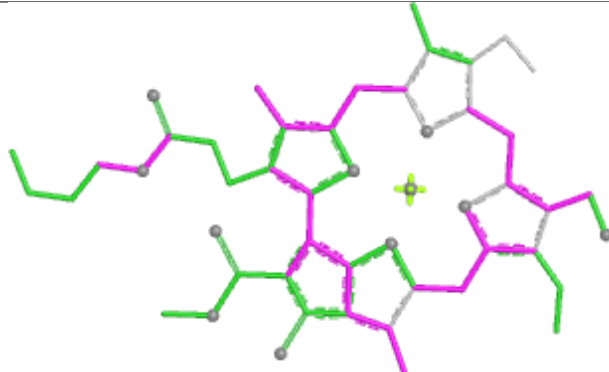
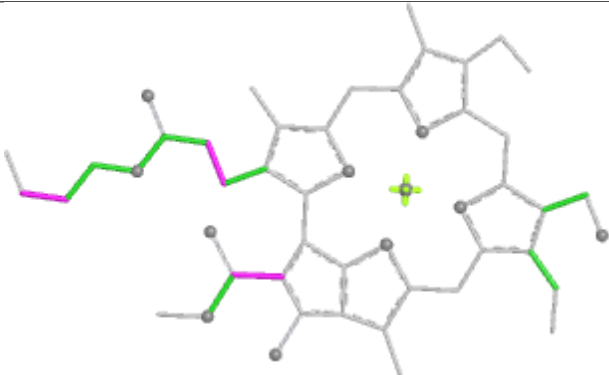
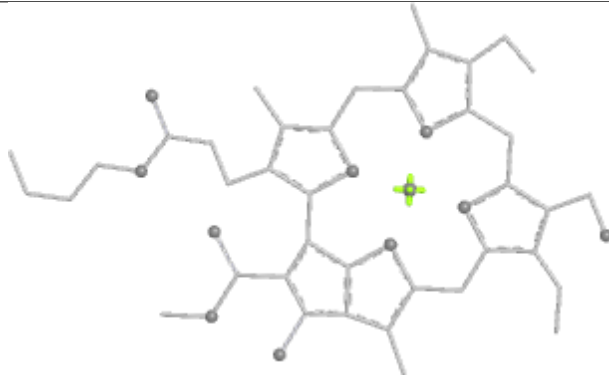
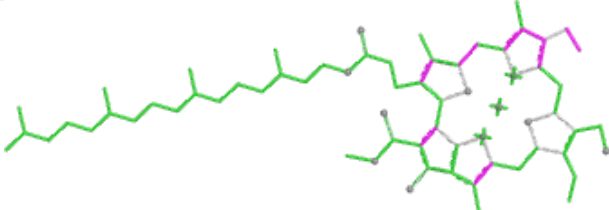
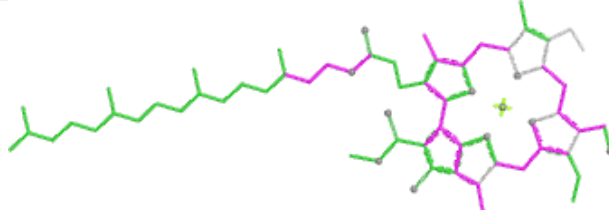
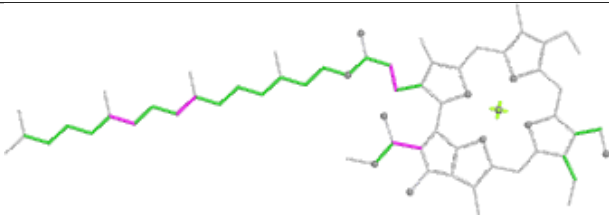
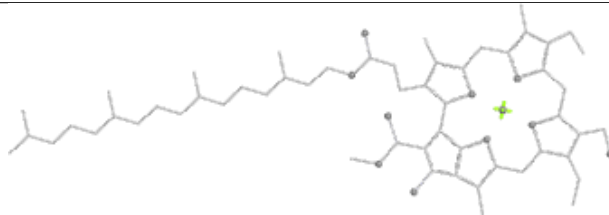
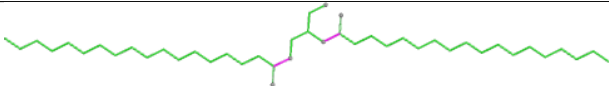
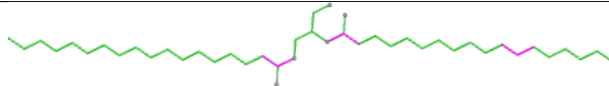
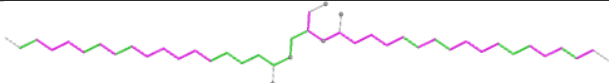
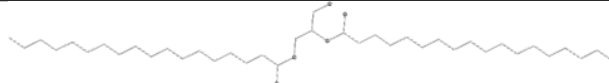
Ligand XAT n 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL y 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

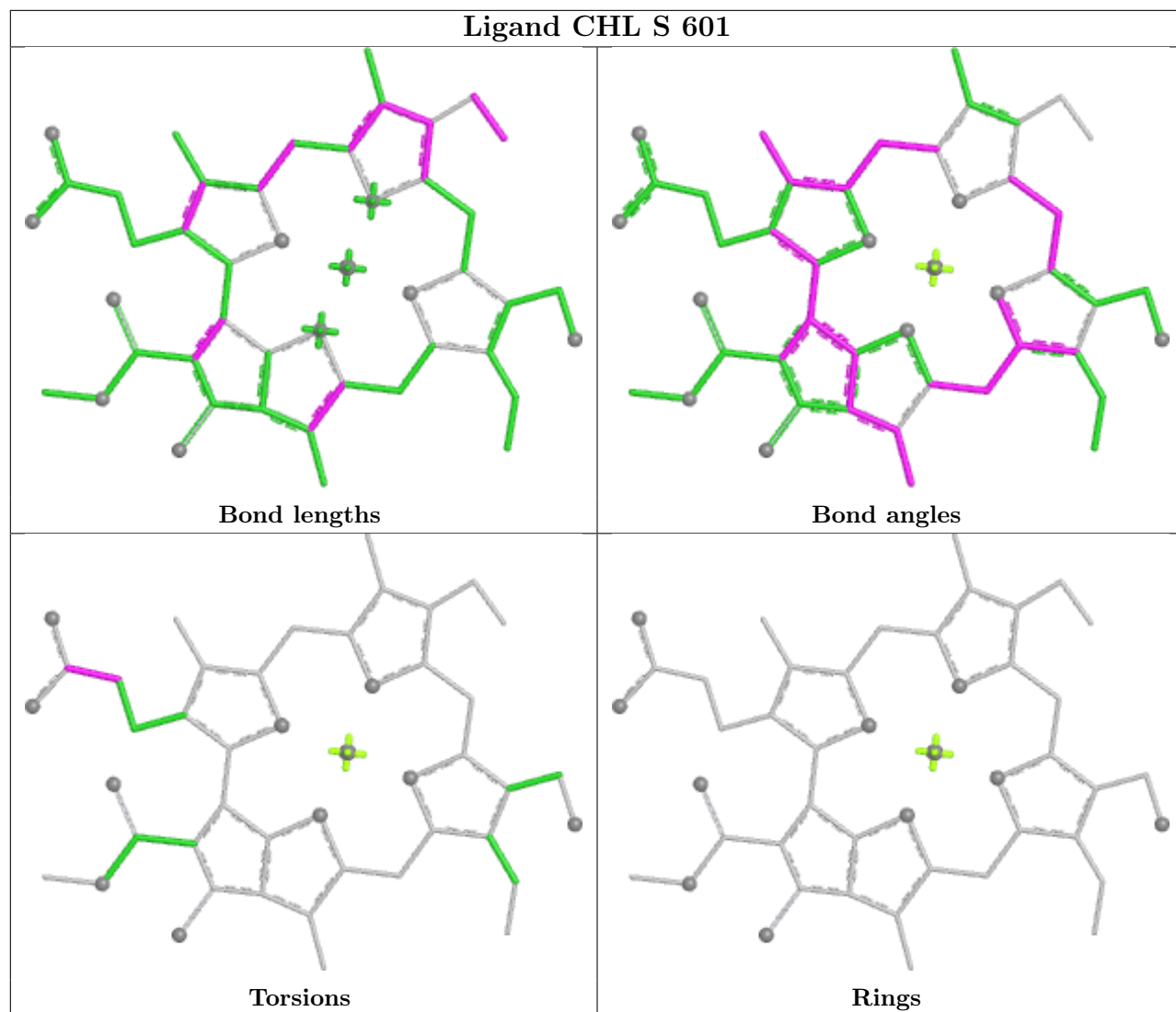
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

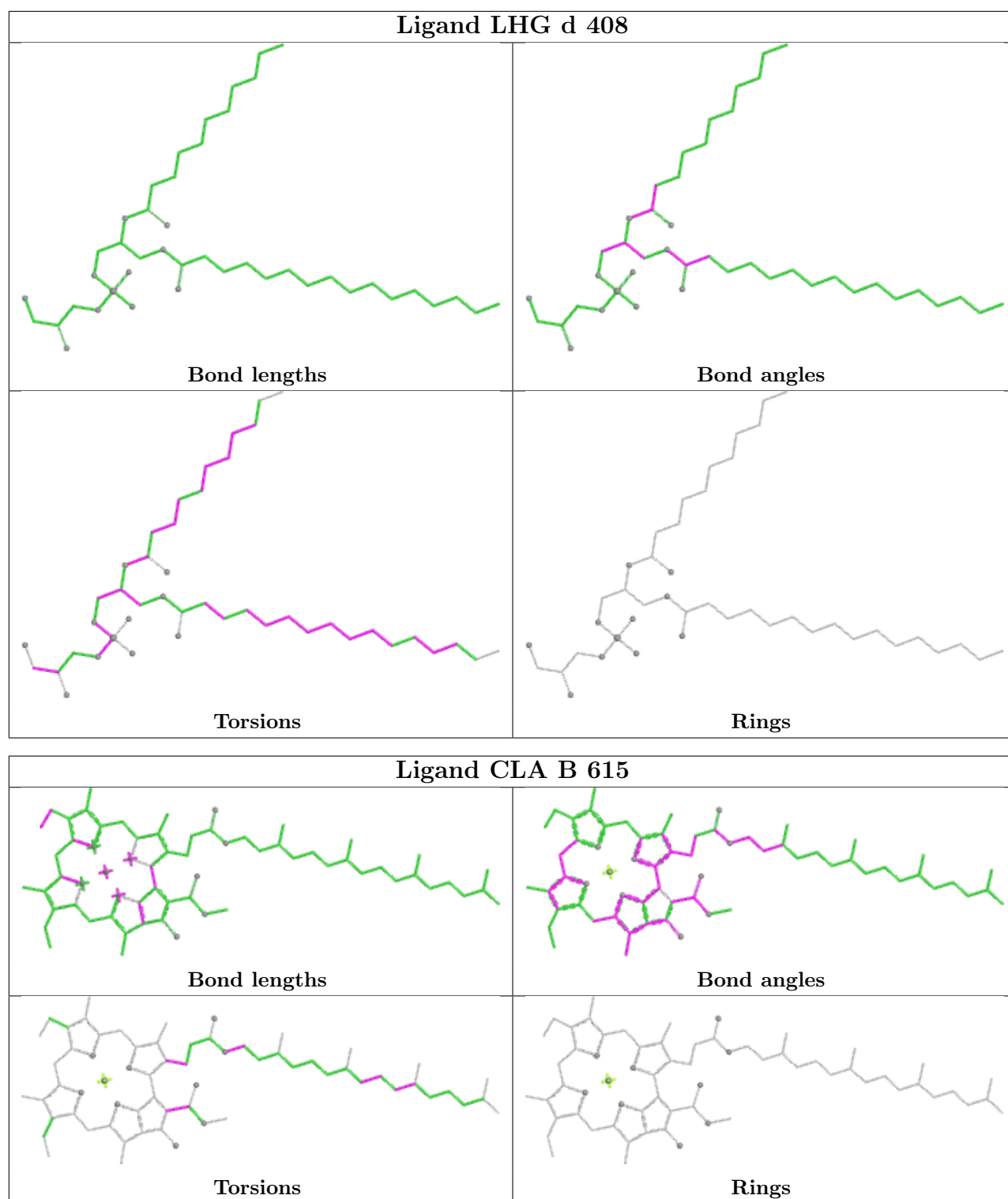
Ligand CHL N 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

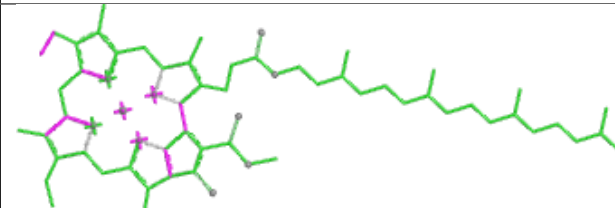
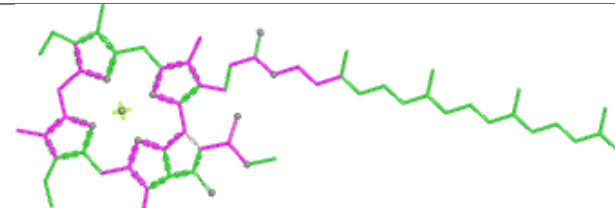
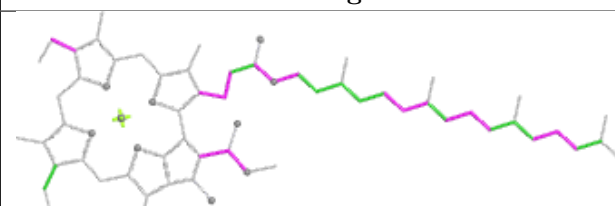
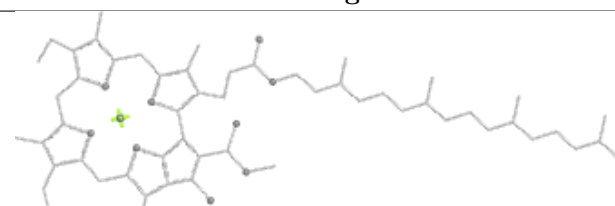


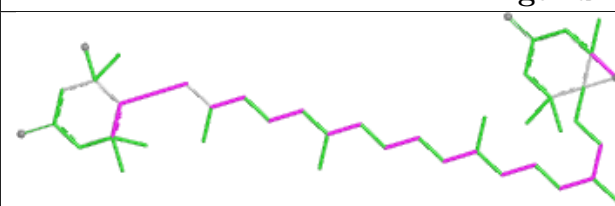
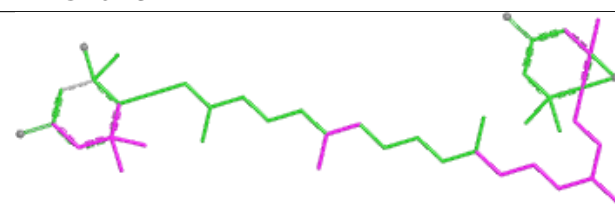
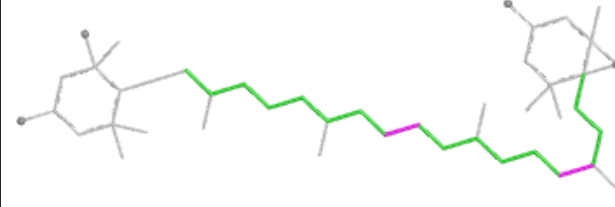
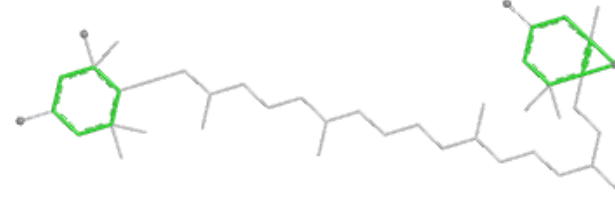
Ligand CHL G 606	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL n 606	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand DGA b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

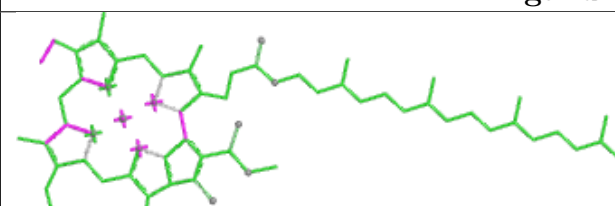
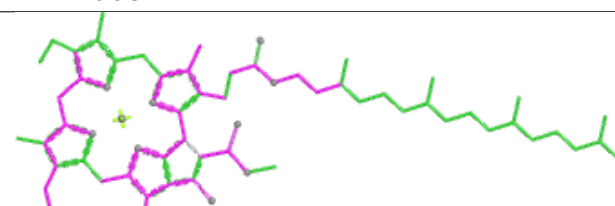
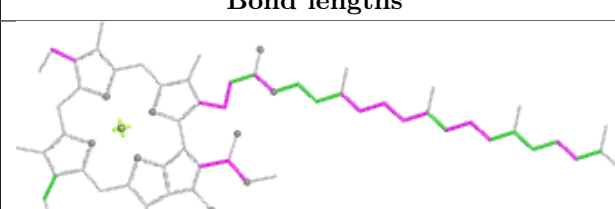
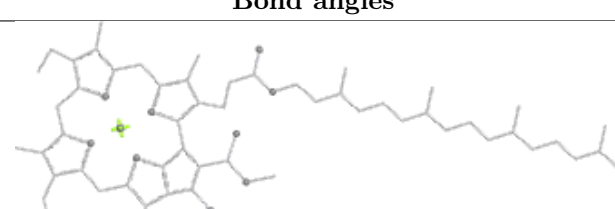
Ligand CHL S 601

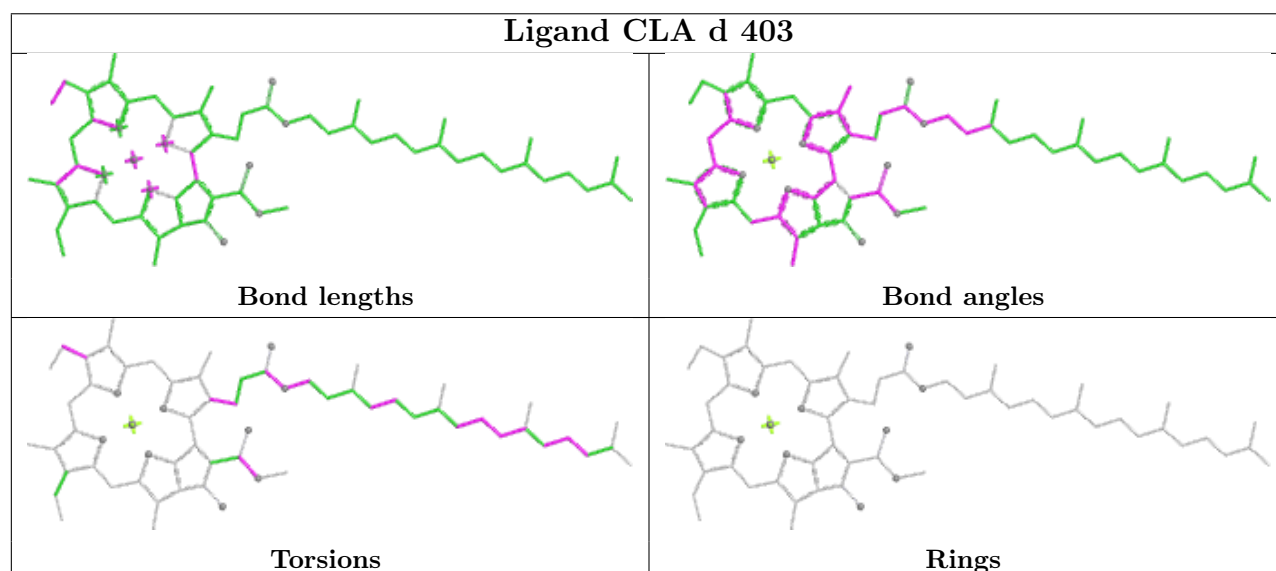
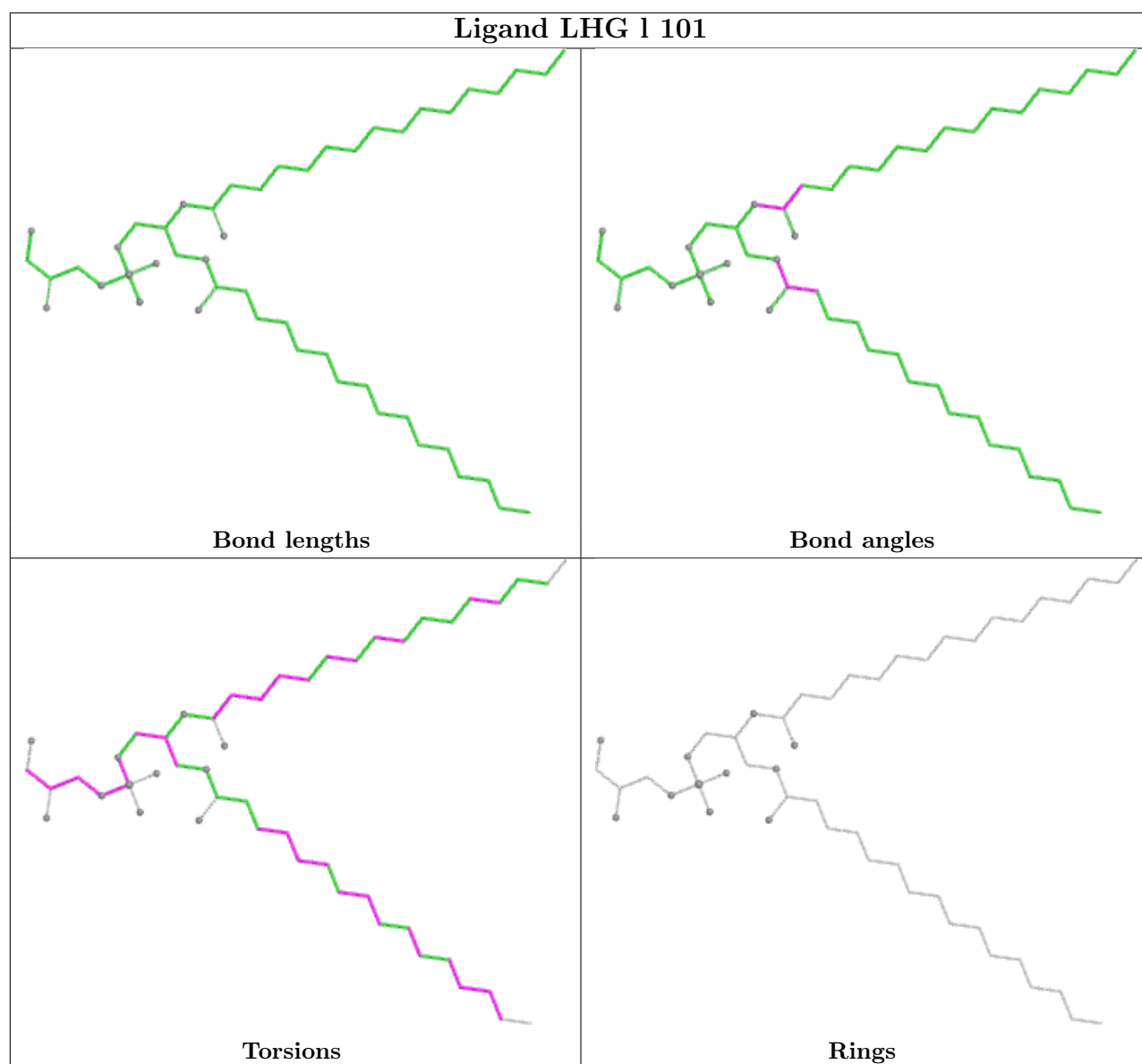


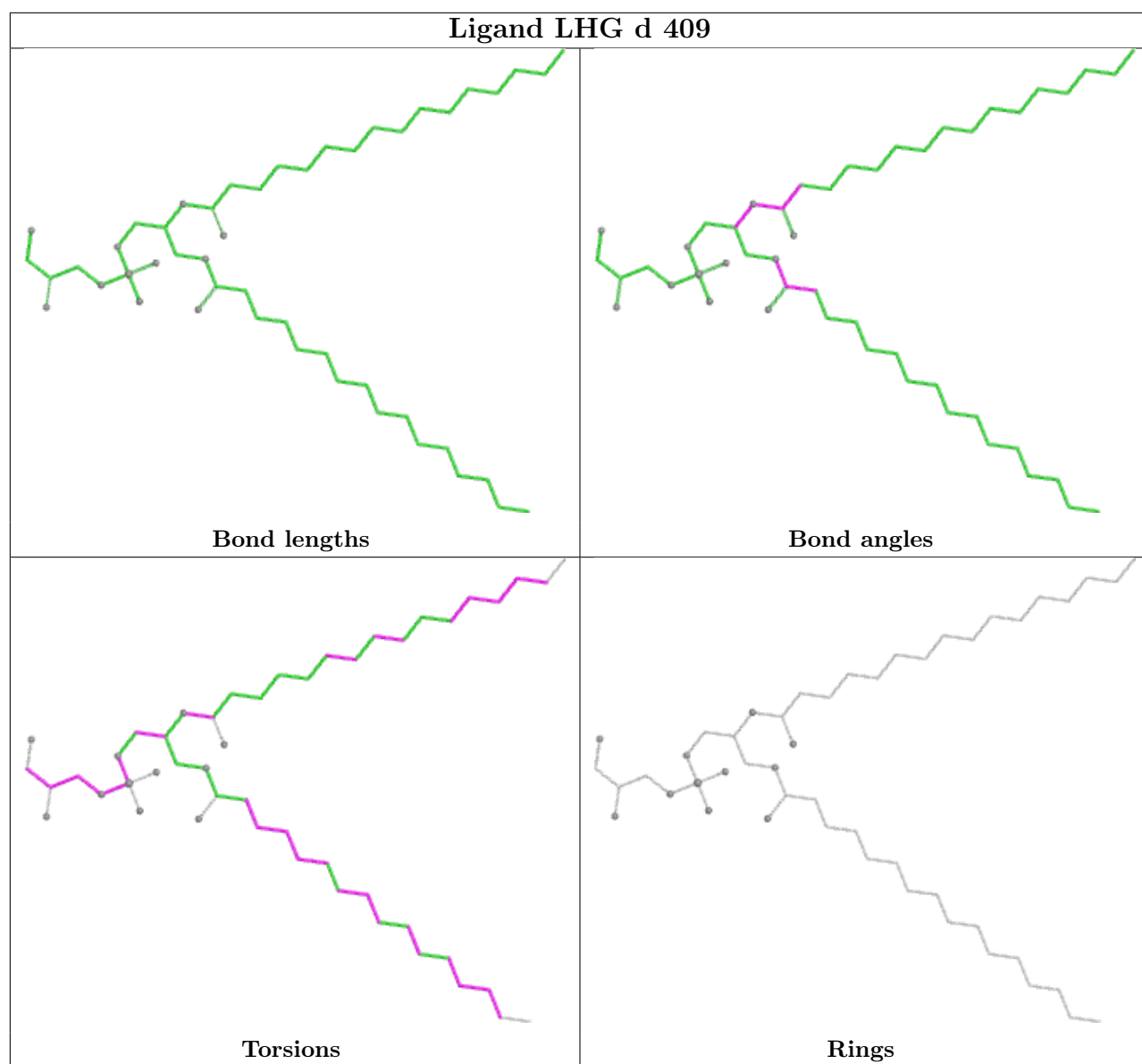


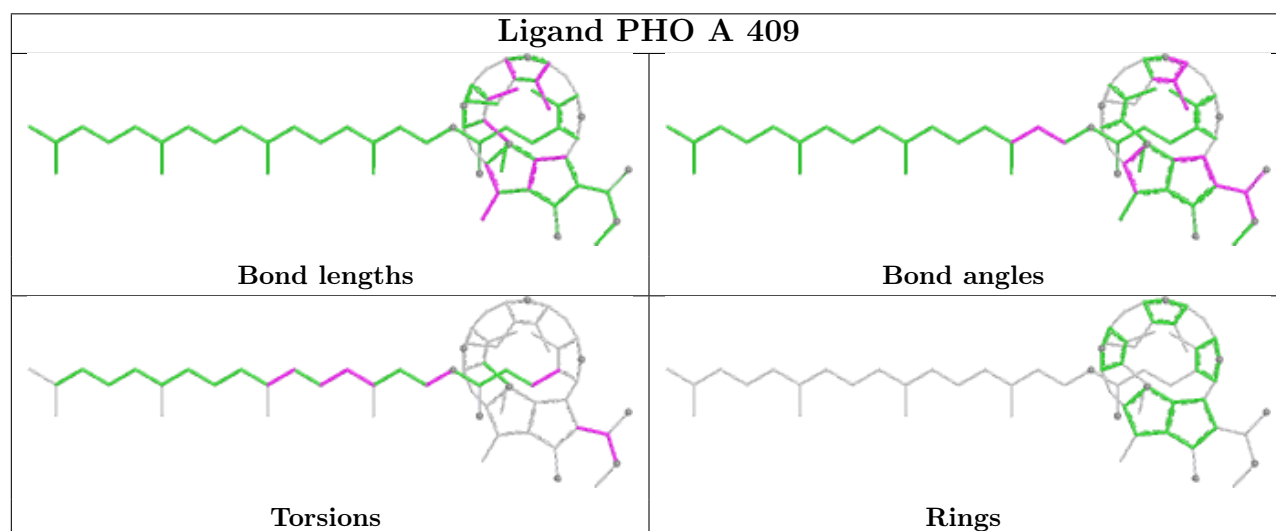
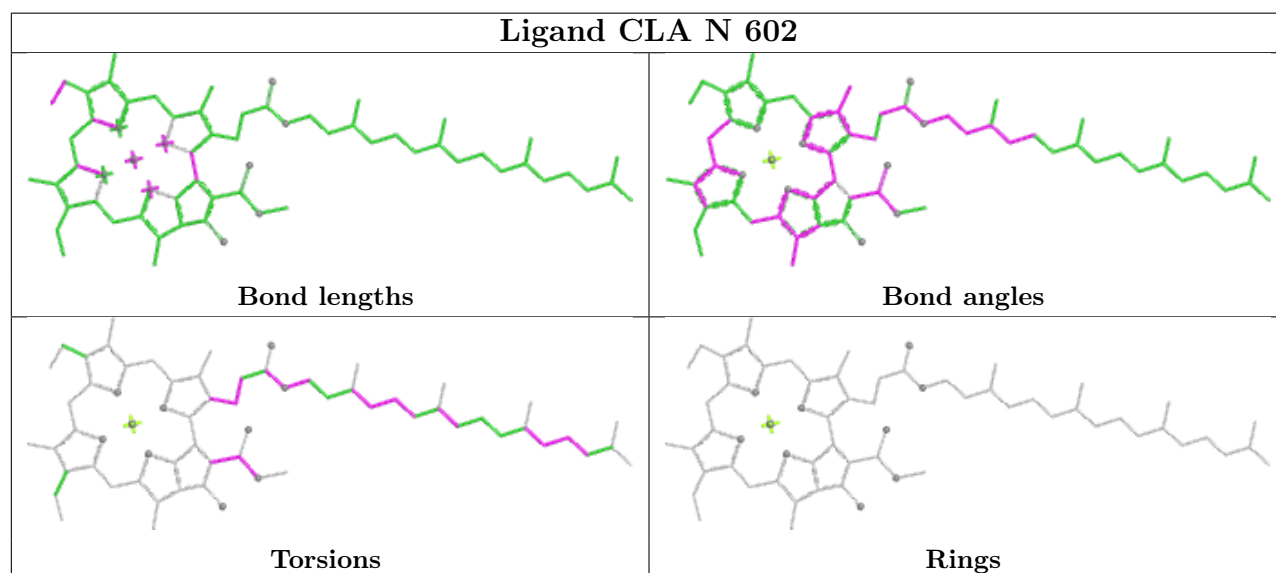
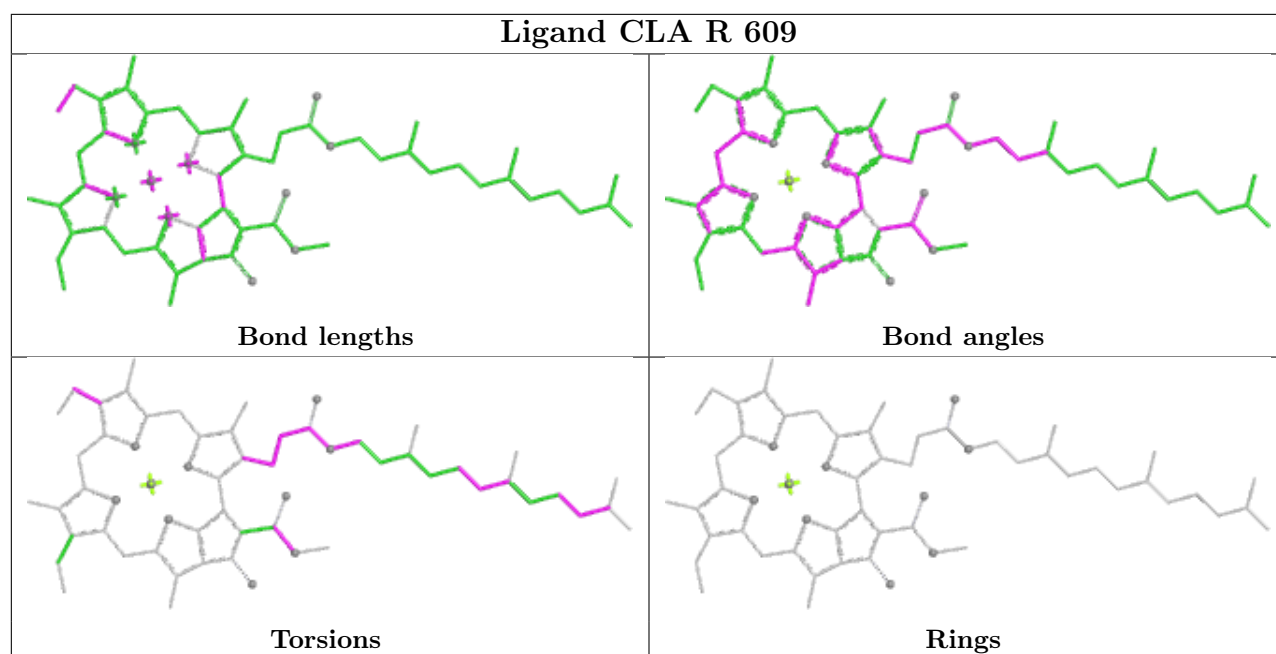
Ligand CLA Y 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

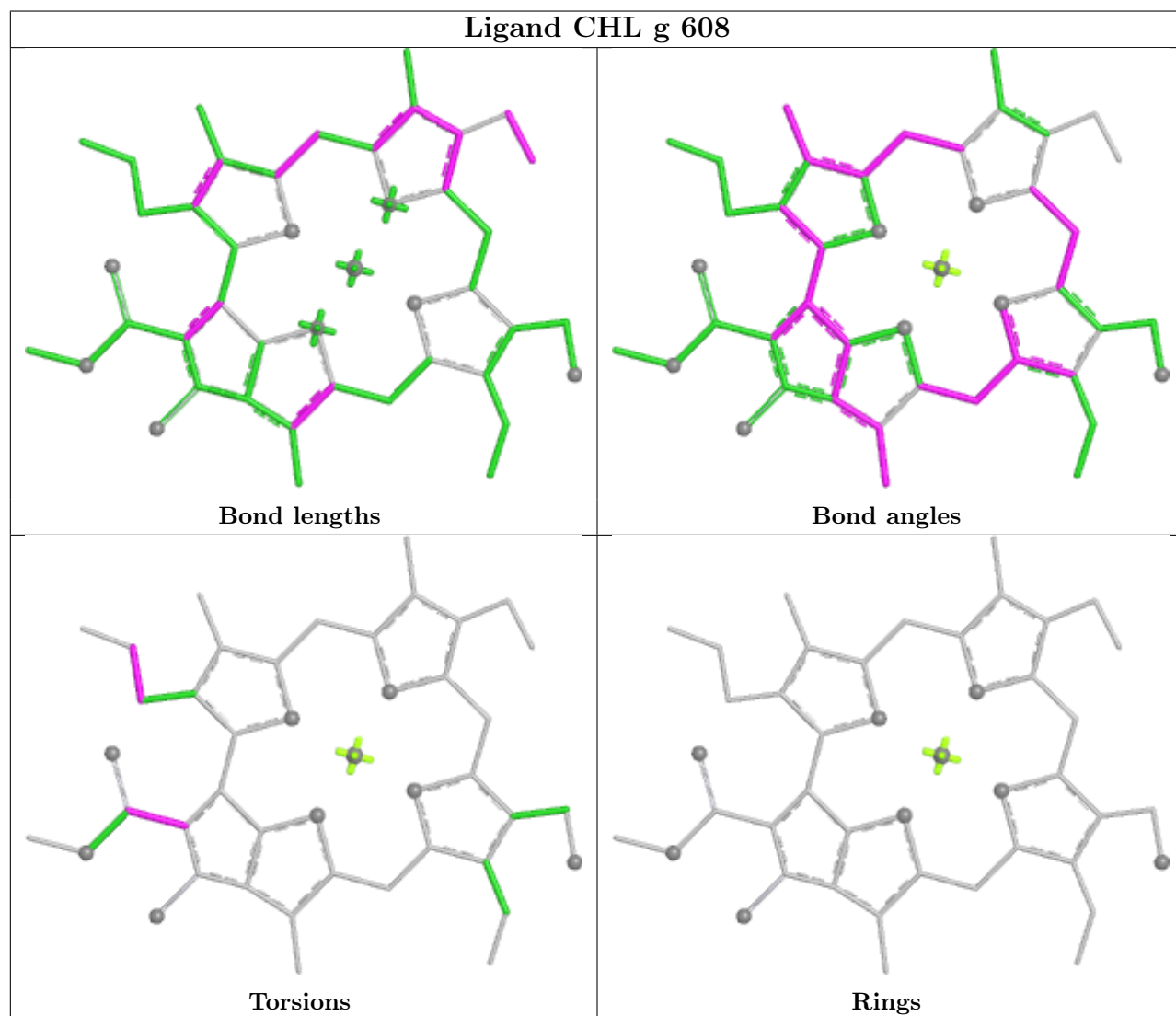
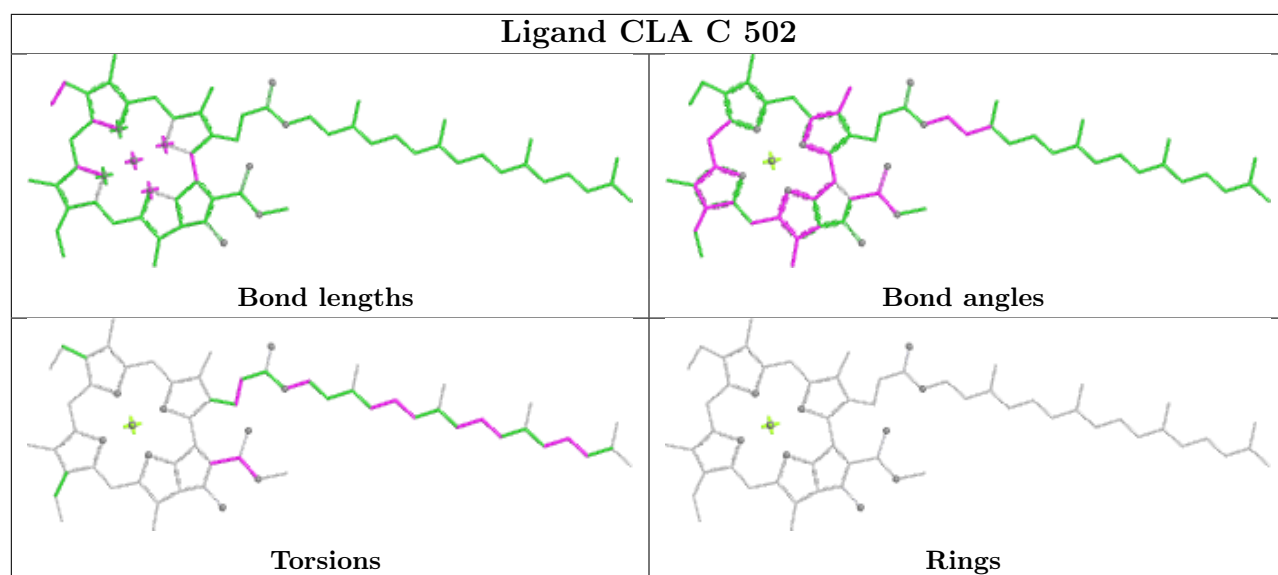
Ligand NEX G 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

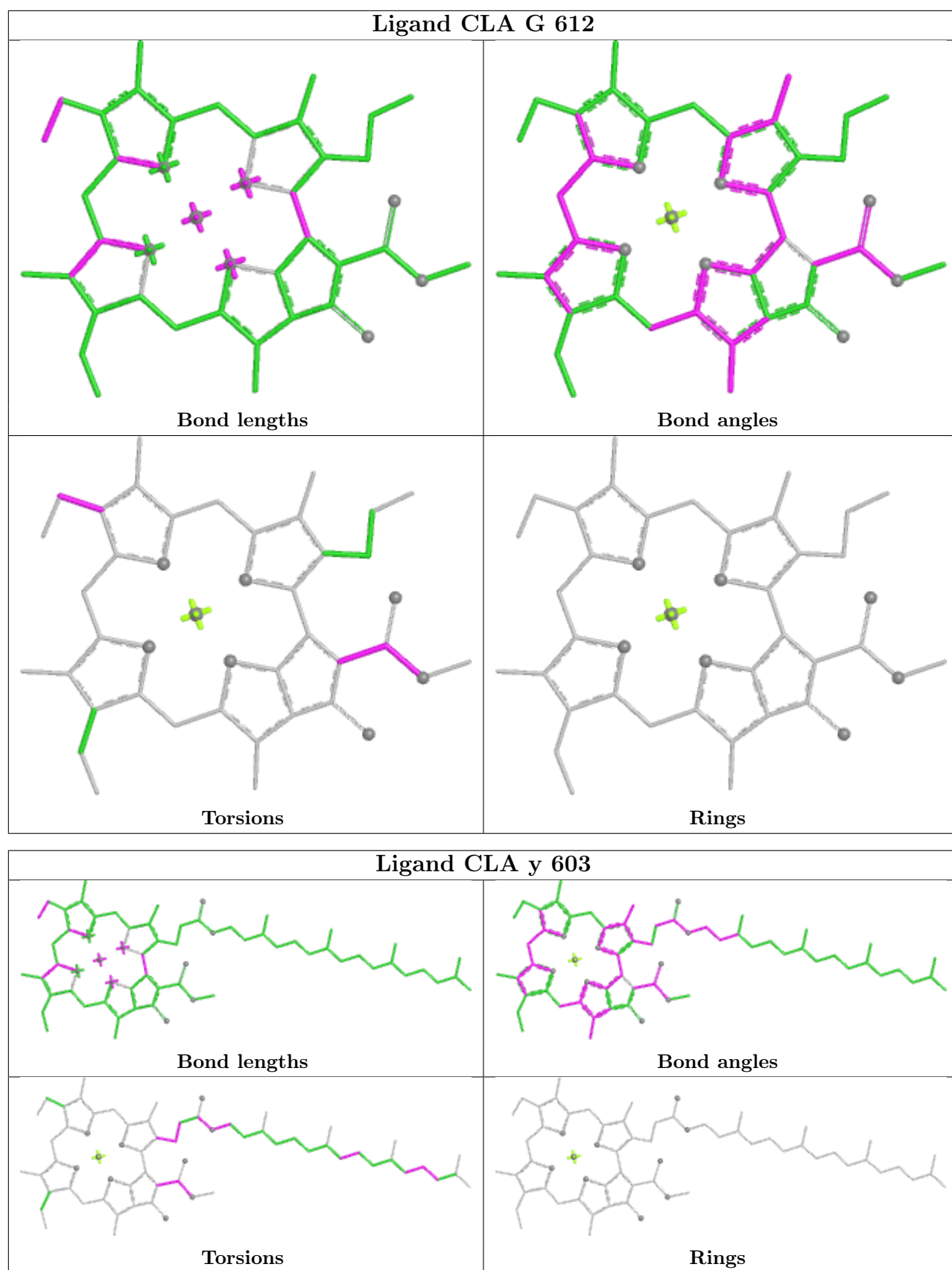
Ligand CLA n 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

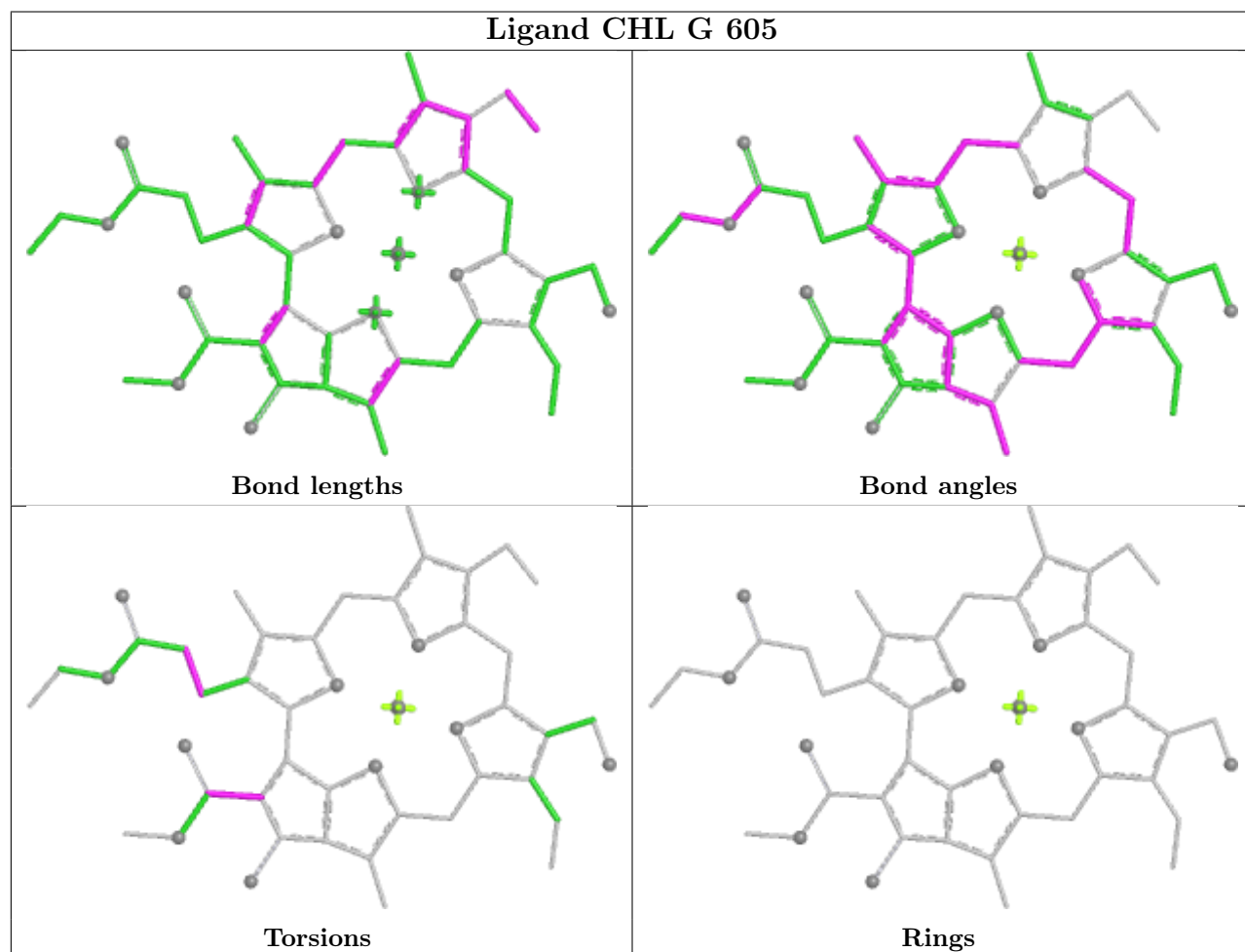
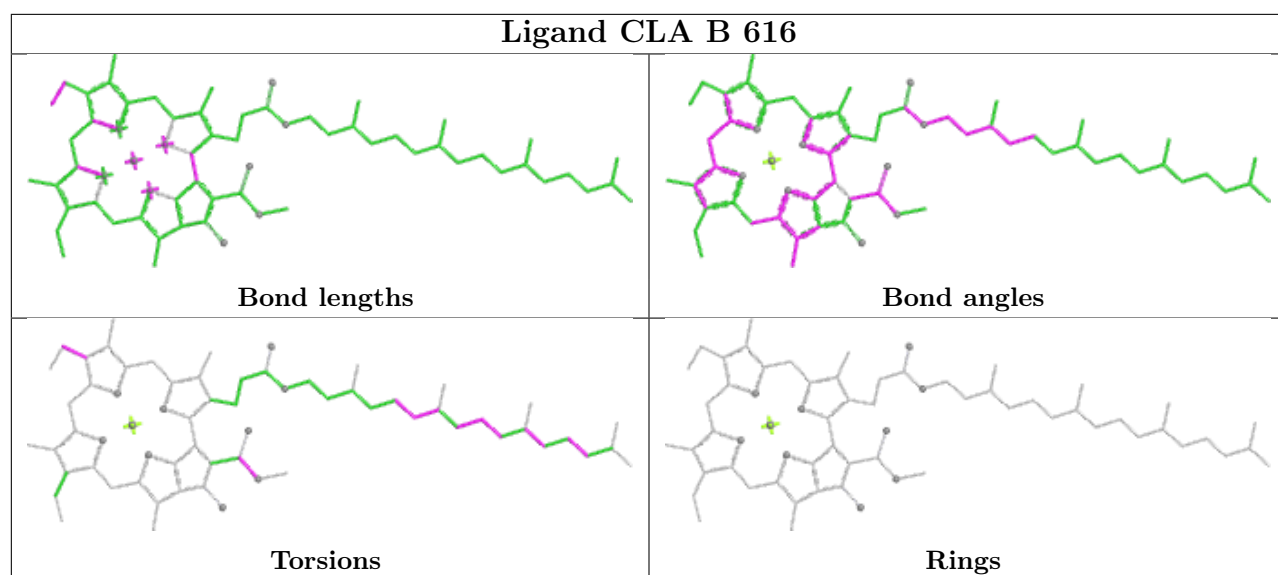


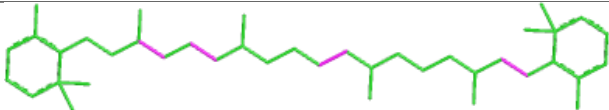
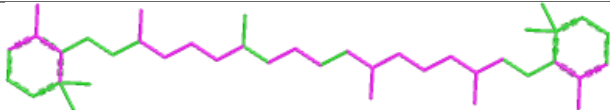
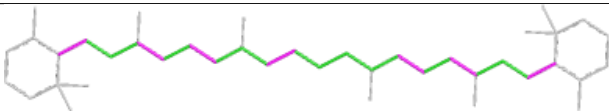
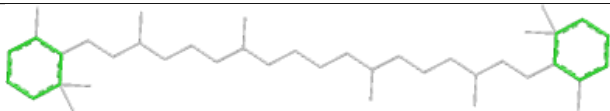


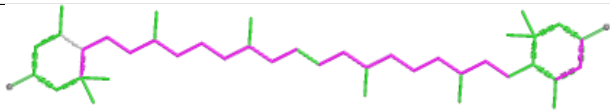
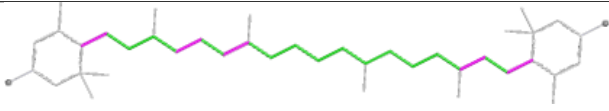
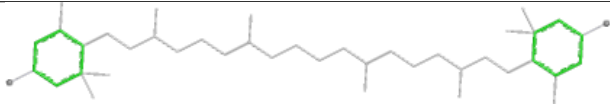


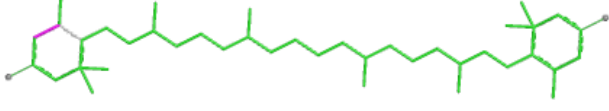
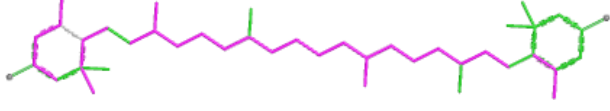
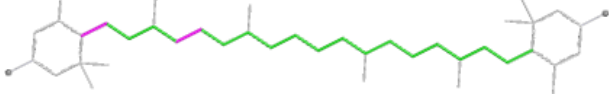
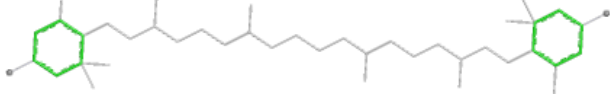




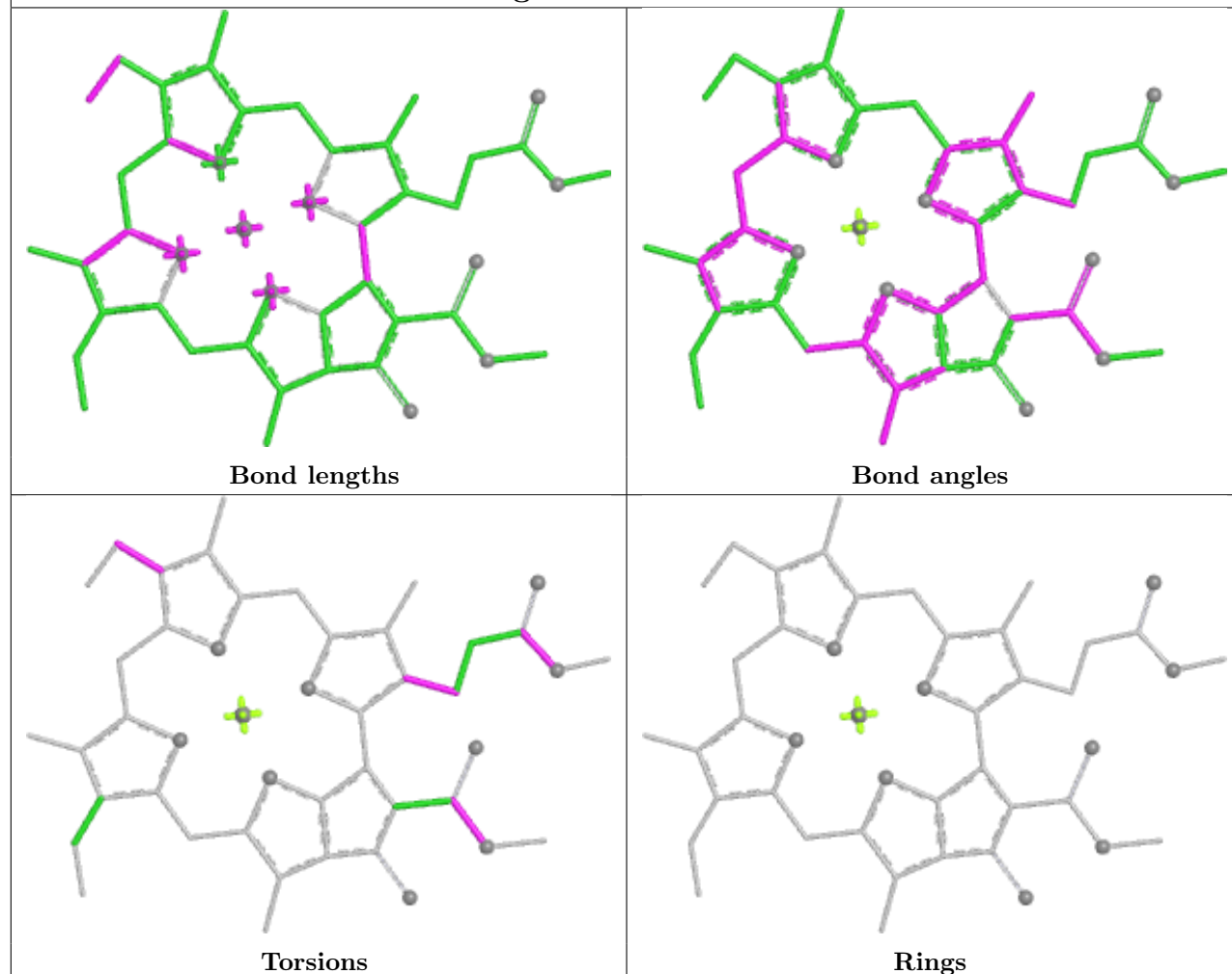


Ligand BCR D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

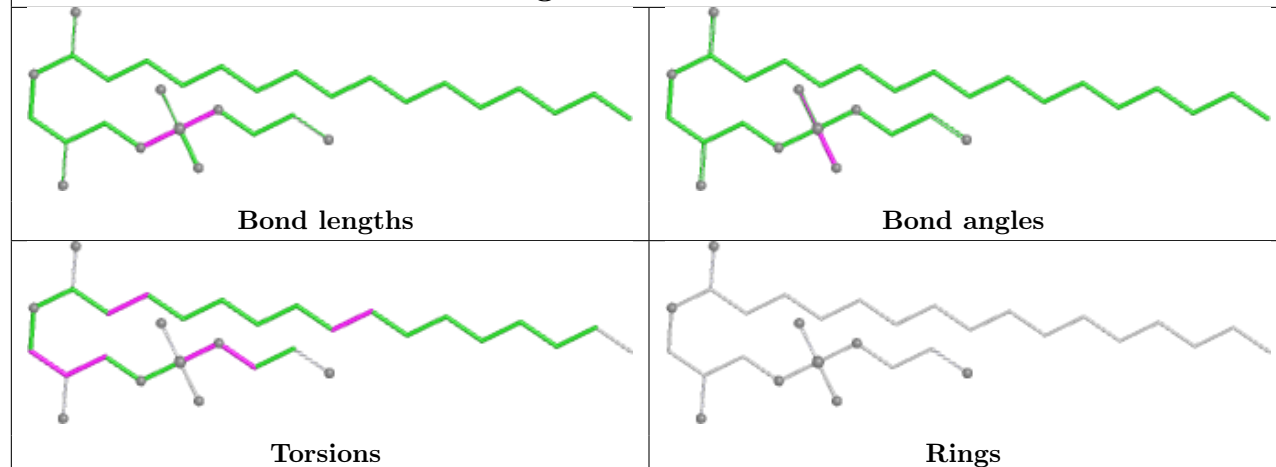
Ligand LUT R 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

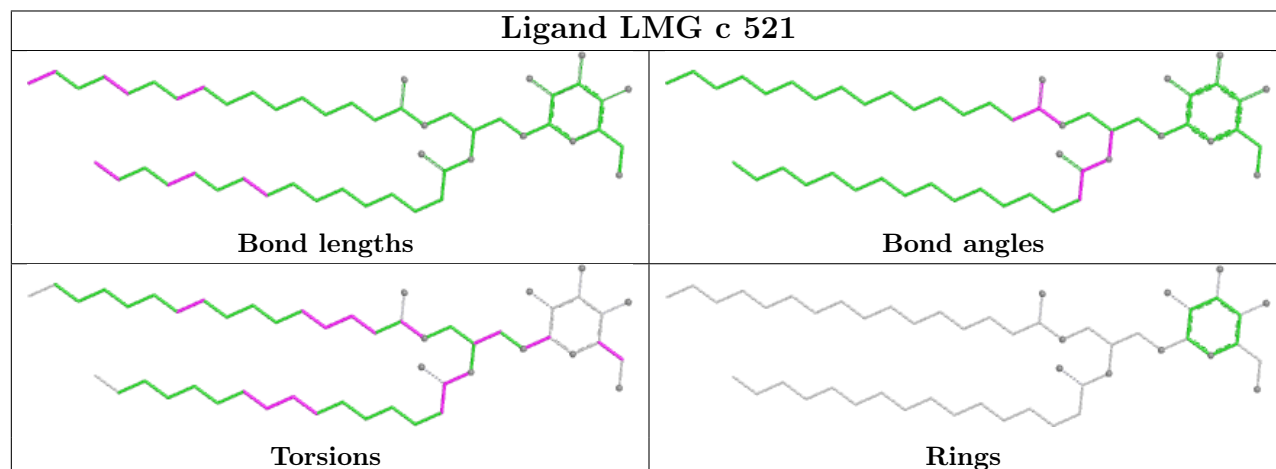
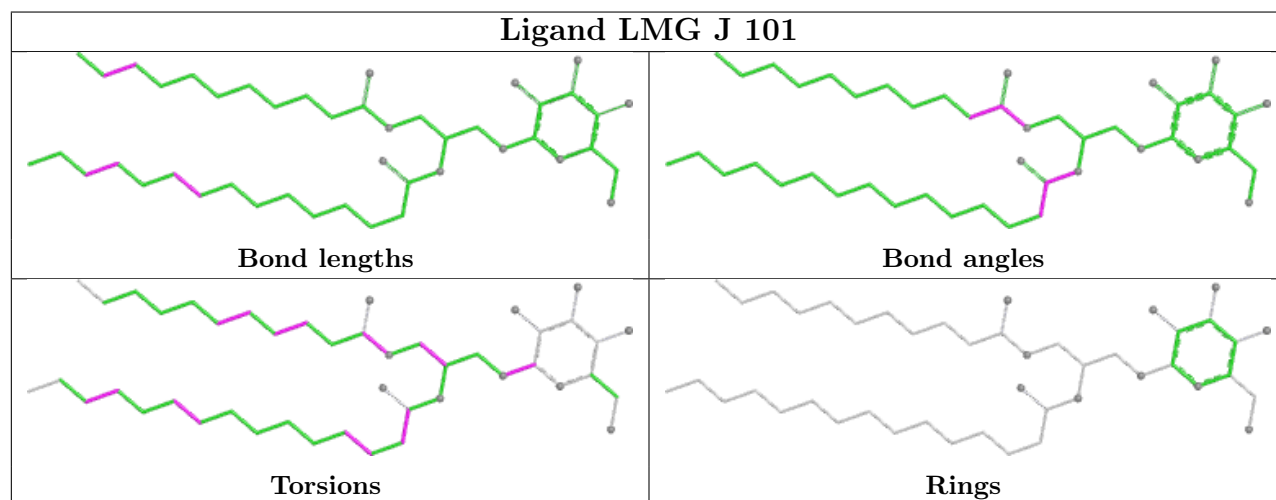
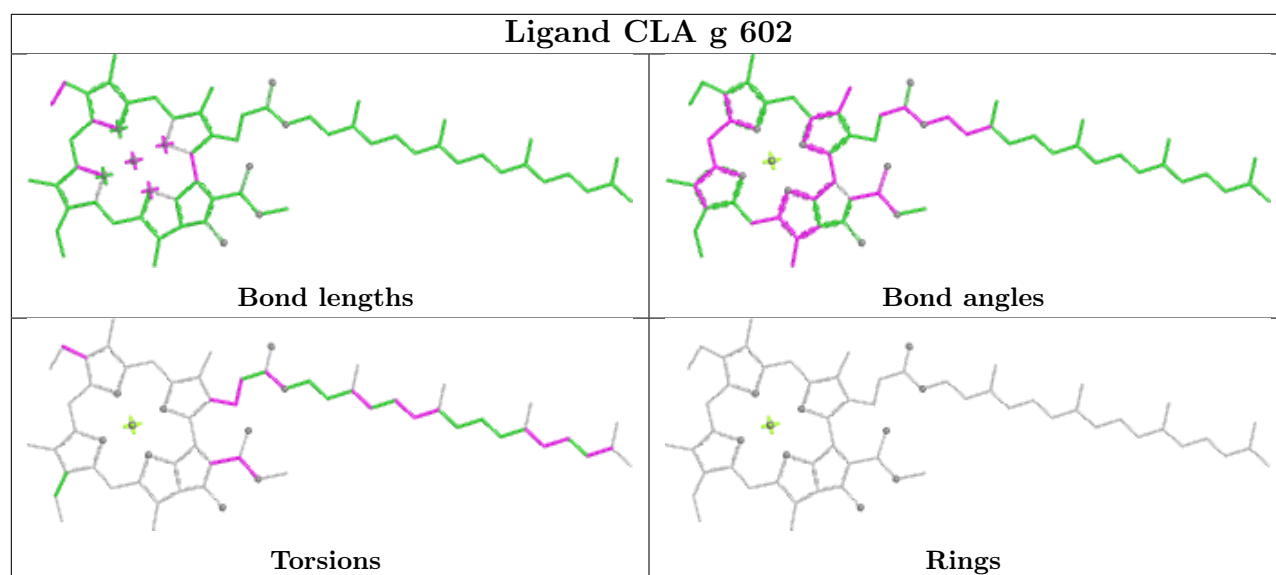
Ligand LUT s 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

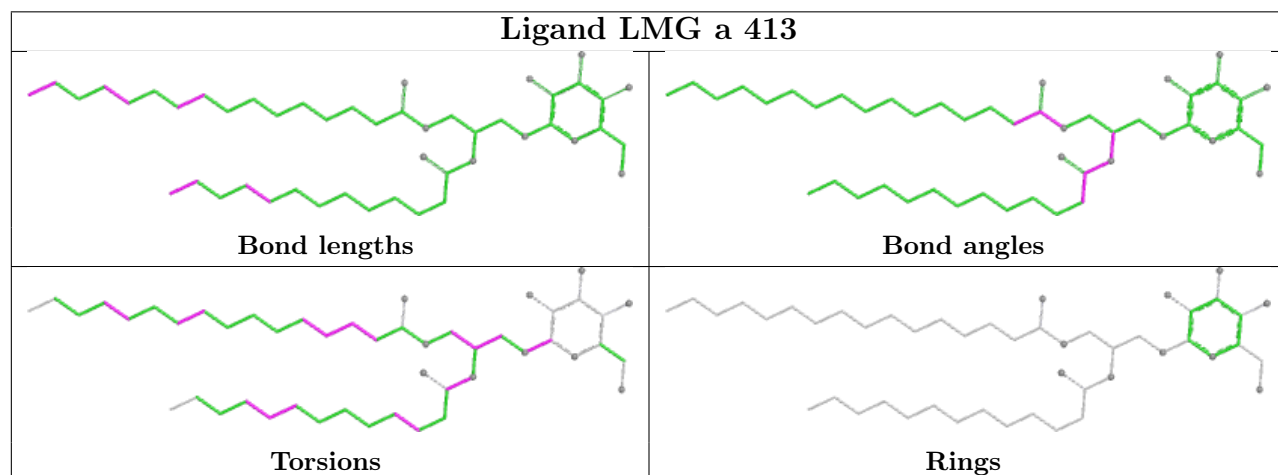
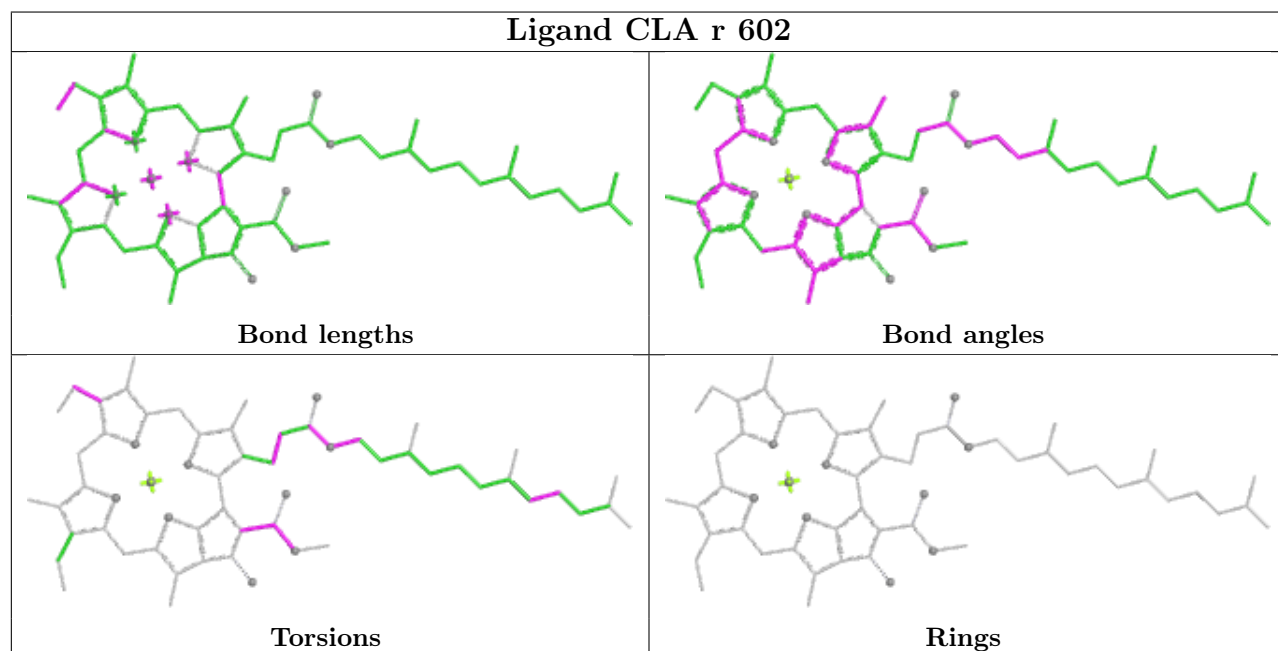
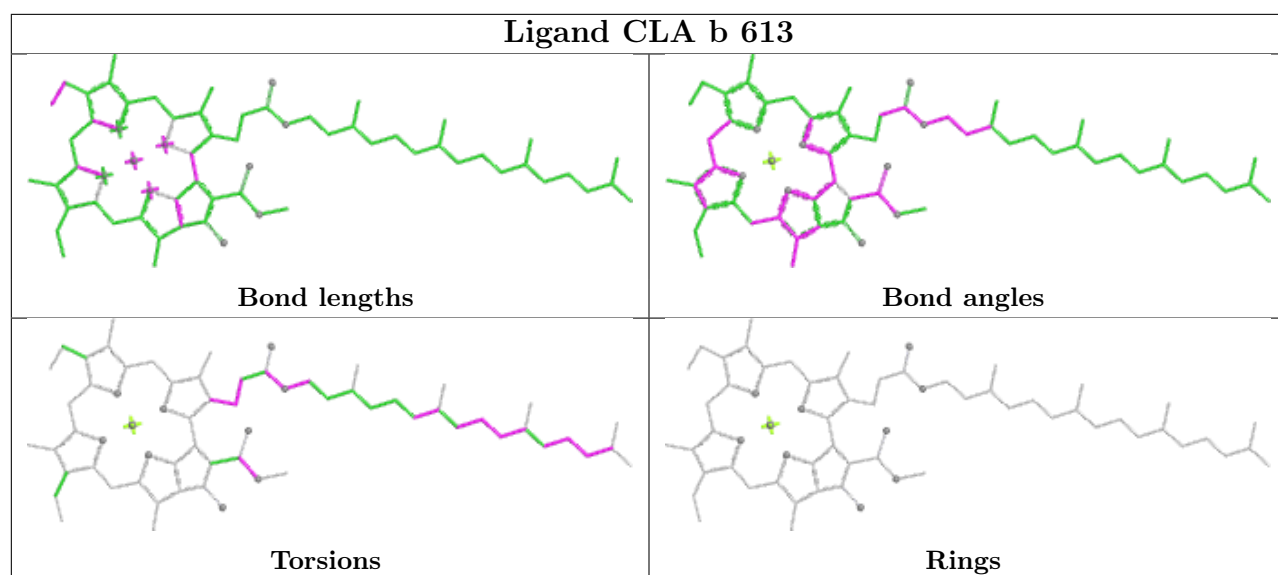
Ligand CLA R 611

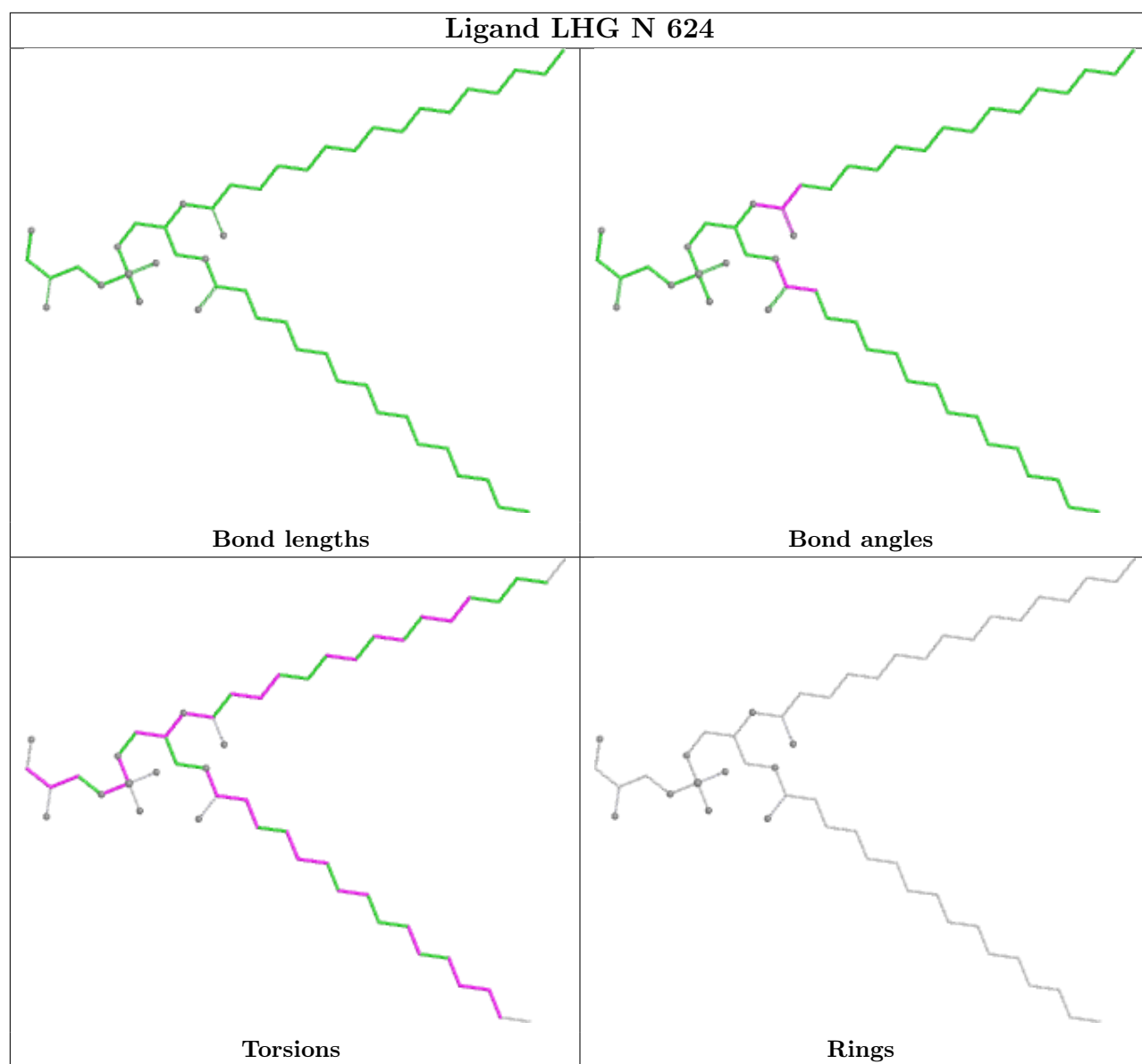


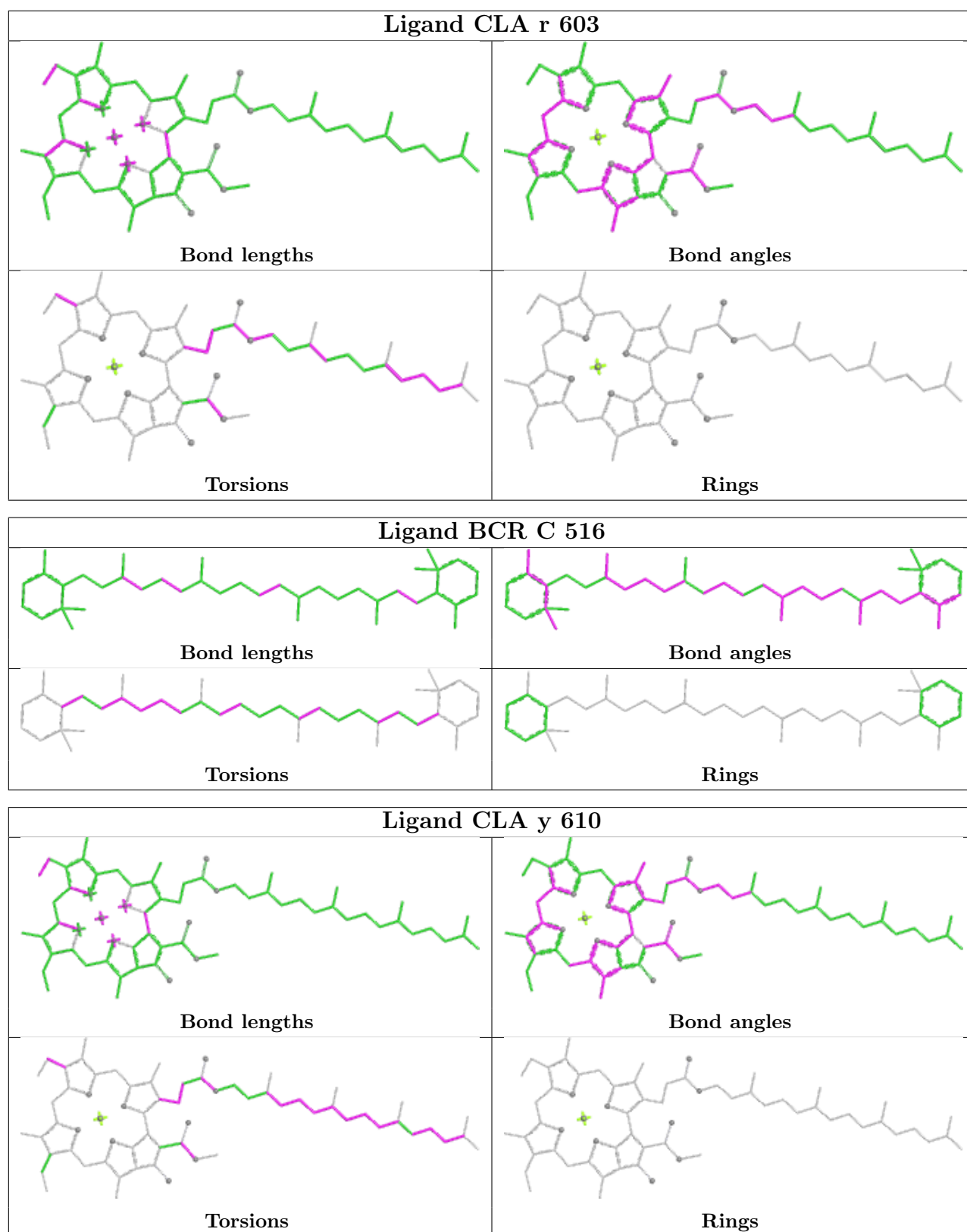
Ligand LPX S 625

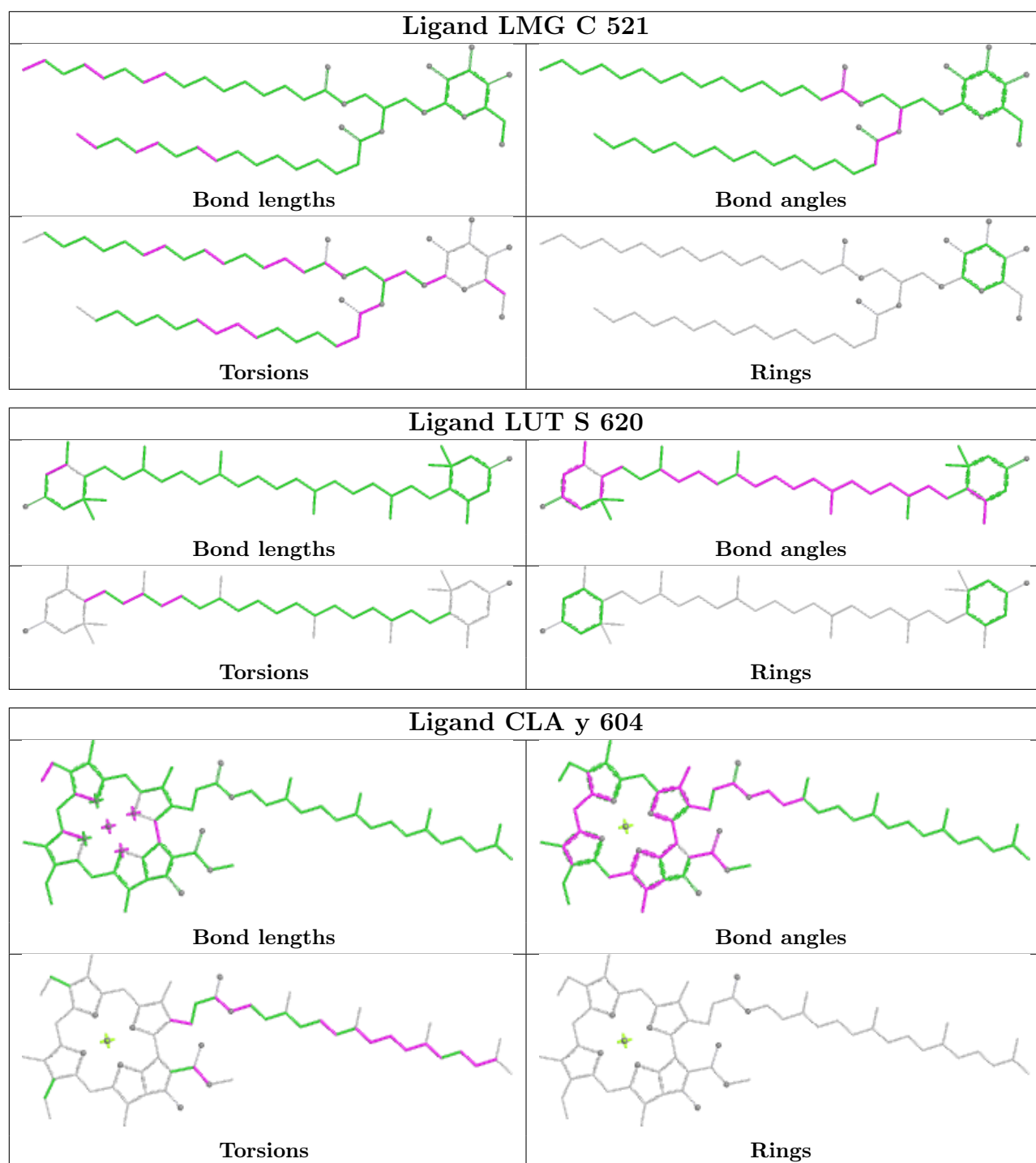


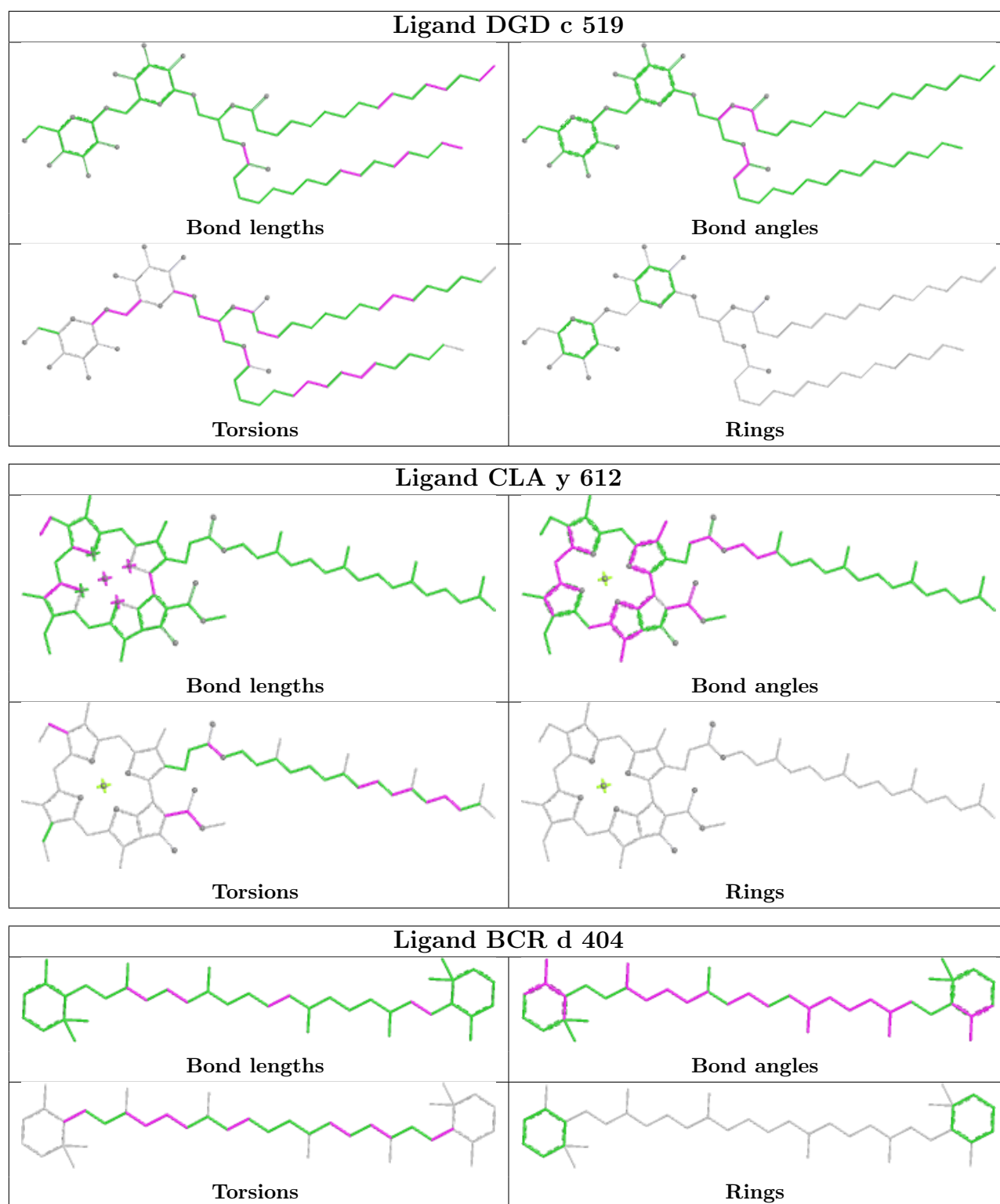


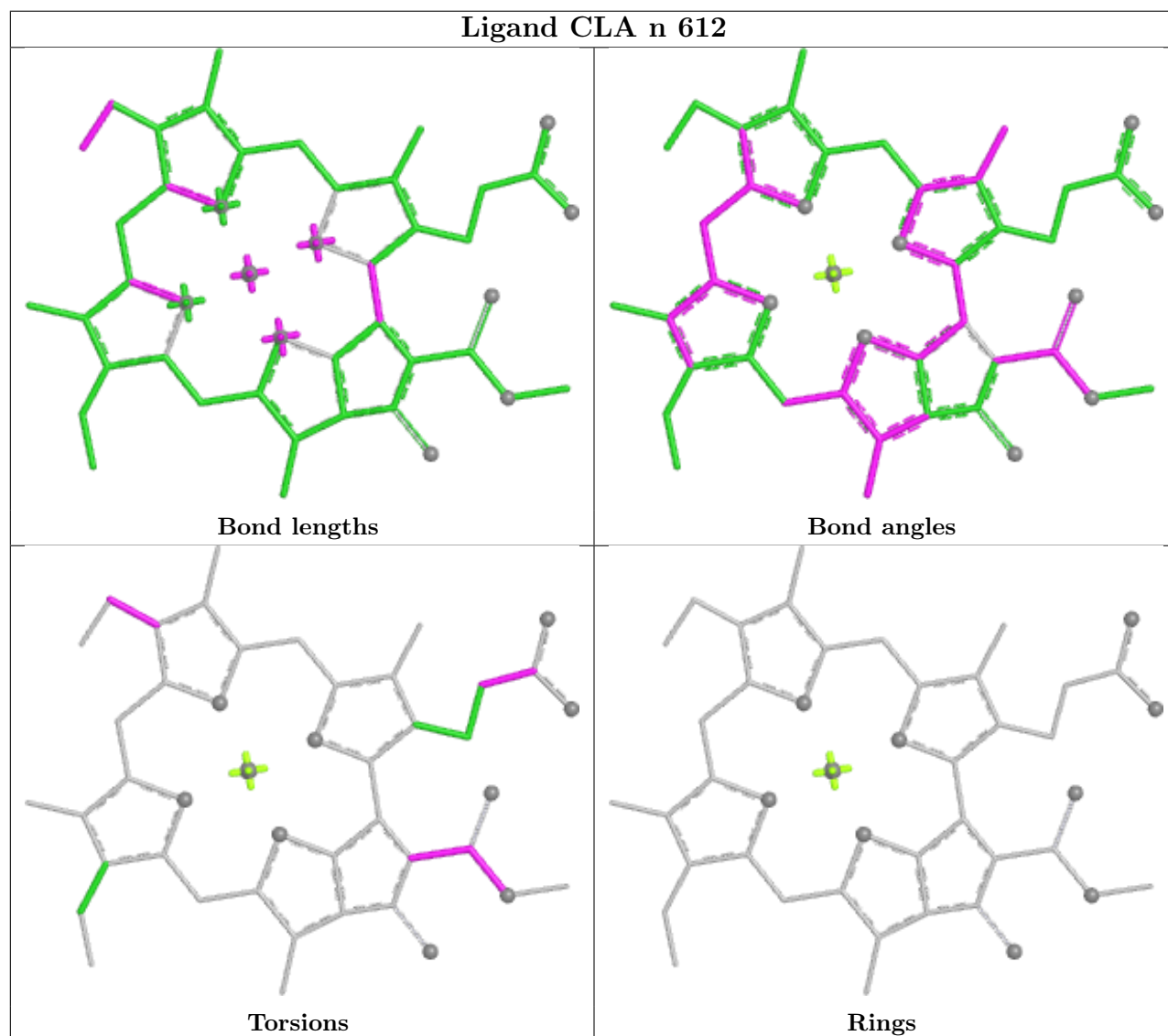
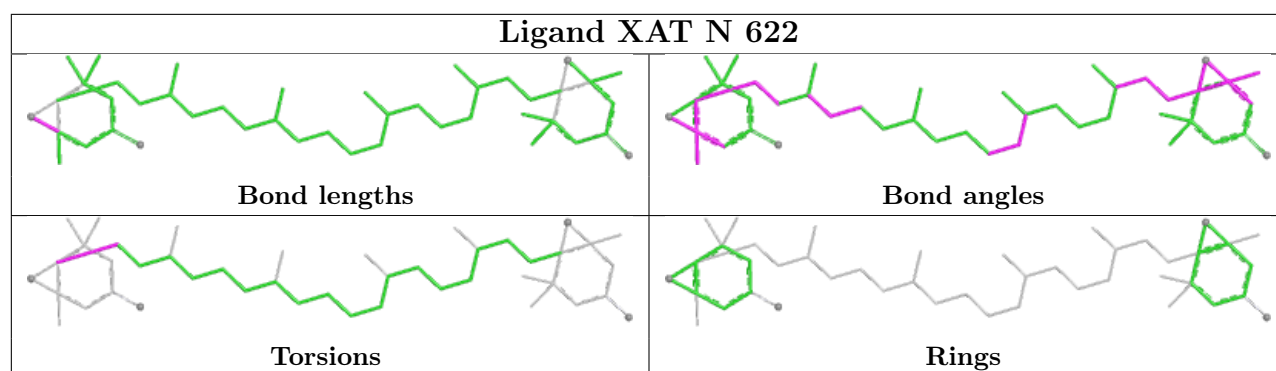


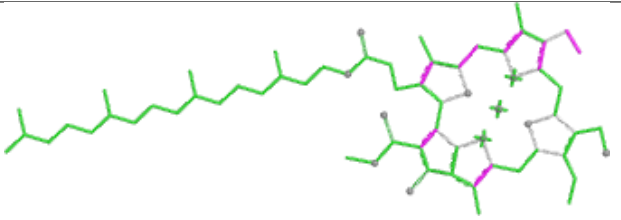
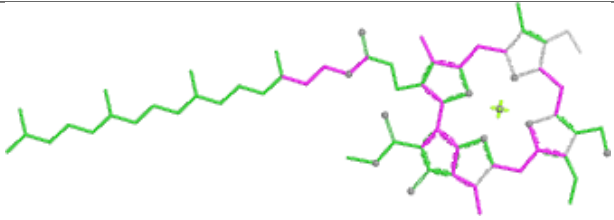
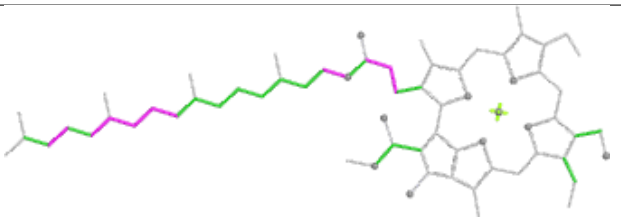
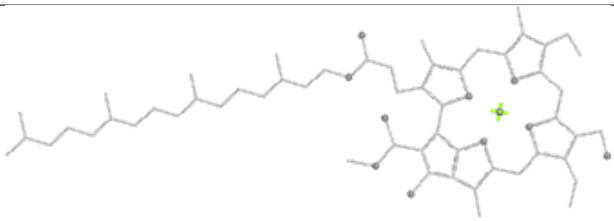


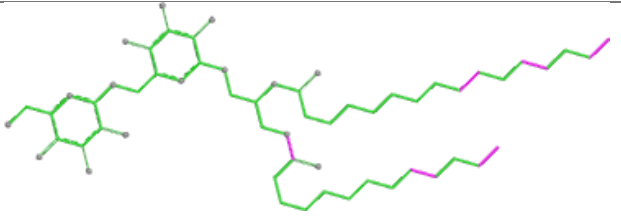
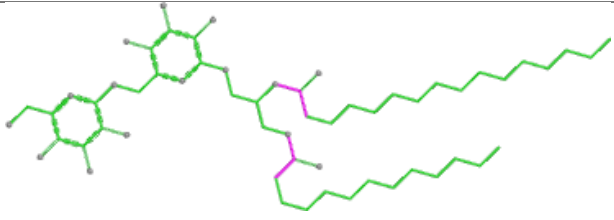
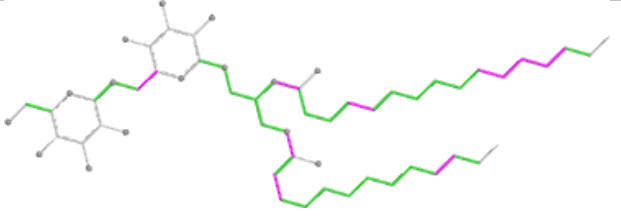
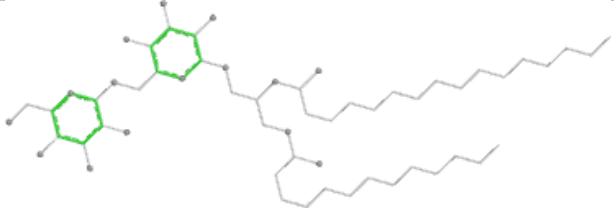


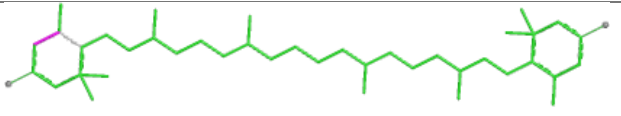
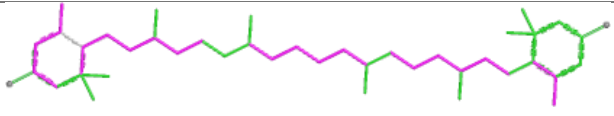
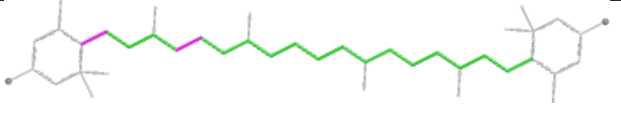
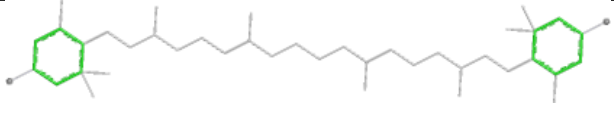


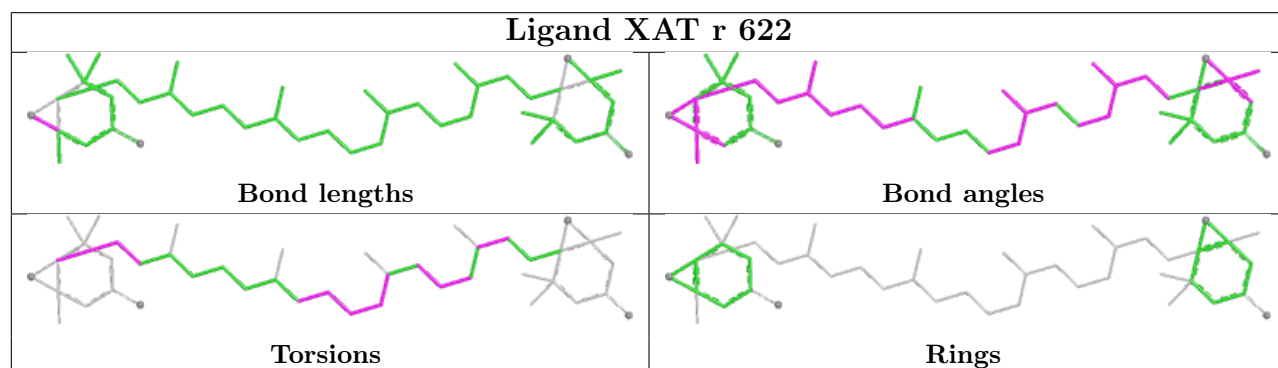
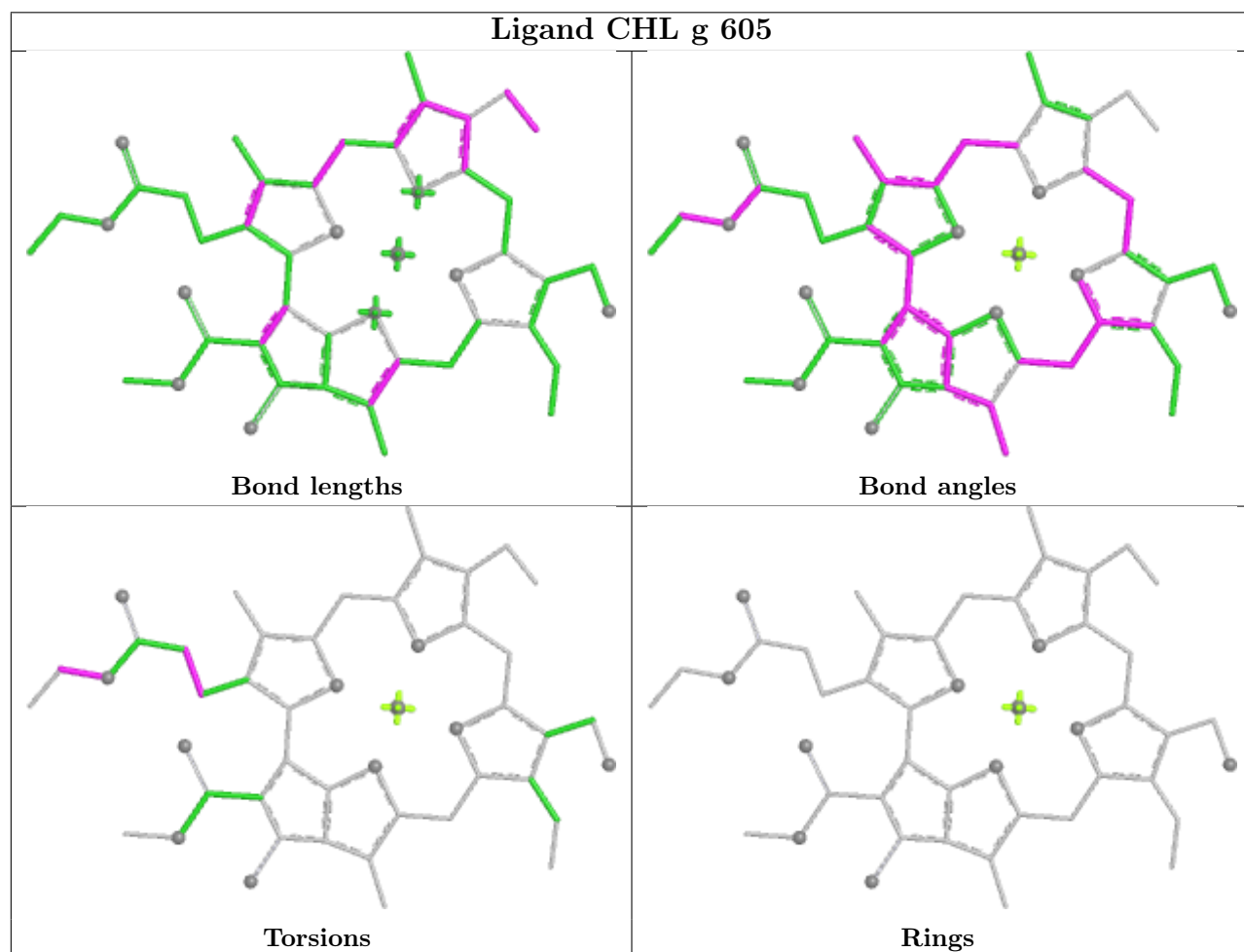
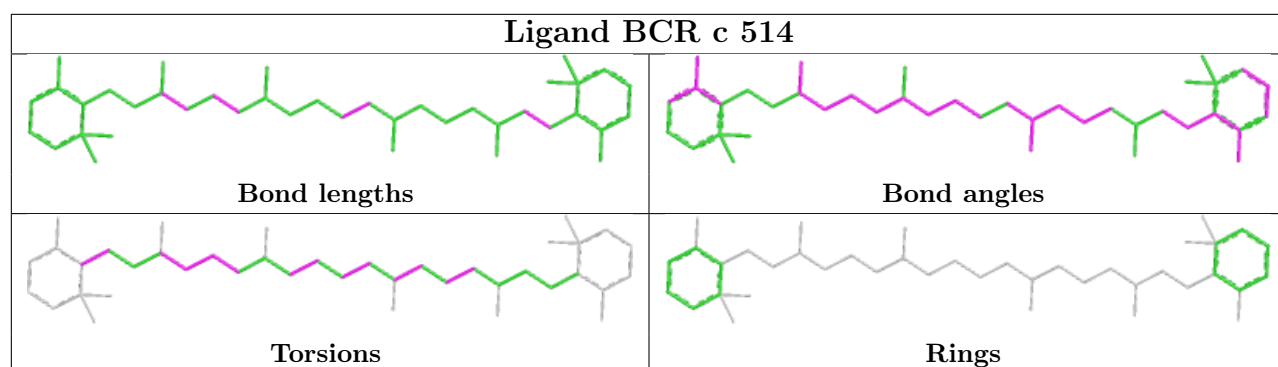




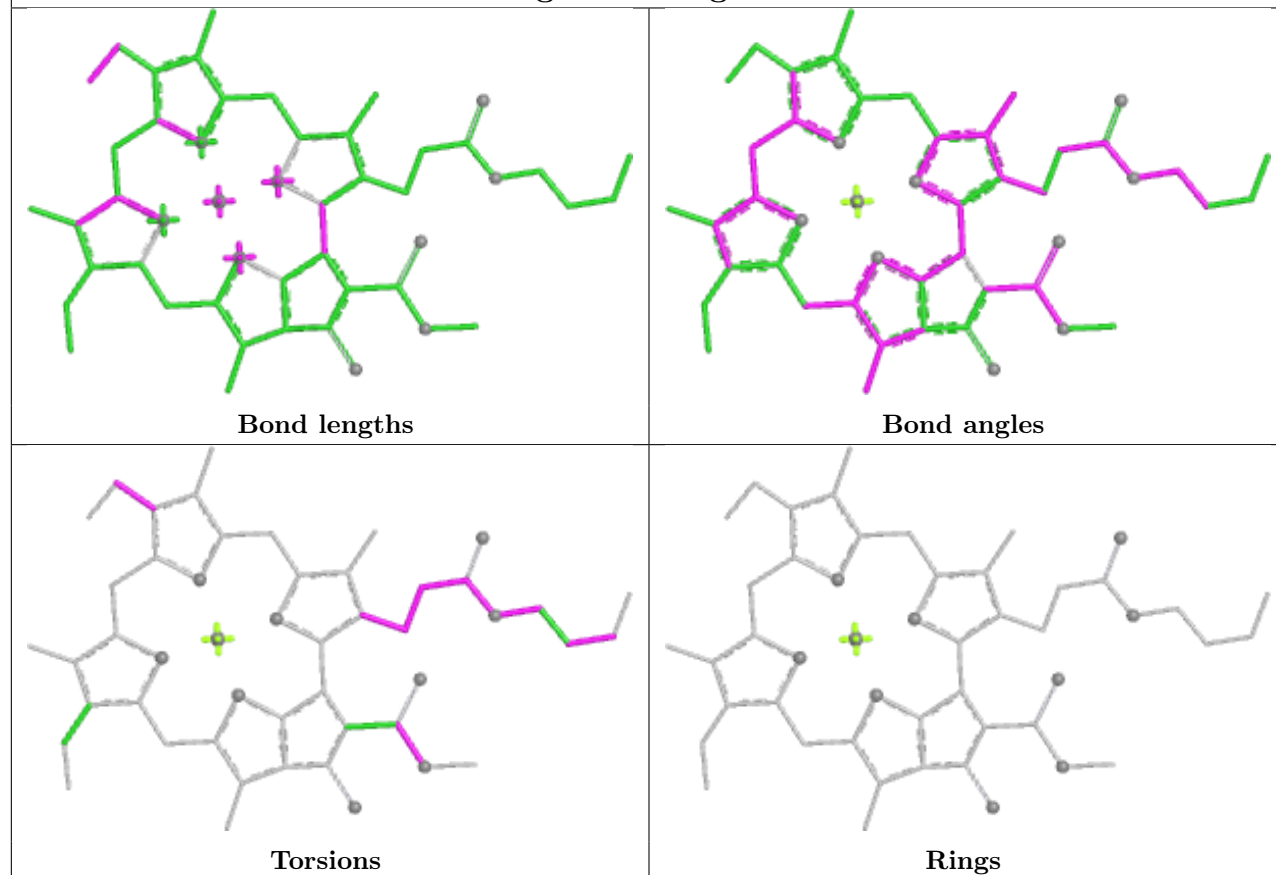
Ligand CHL n 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

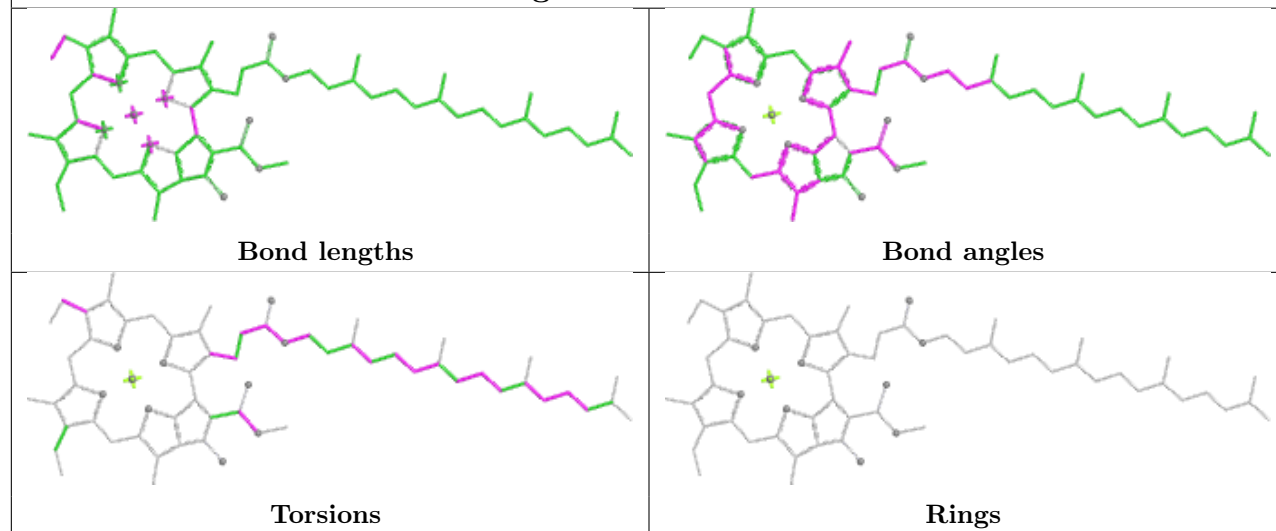
Ligand LUT g 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

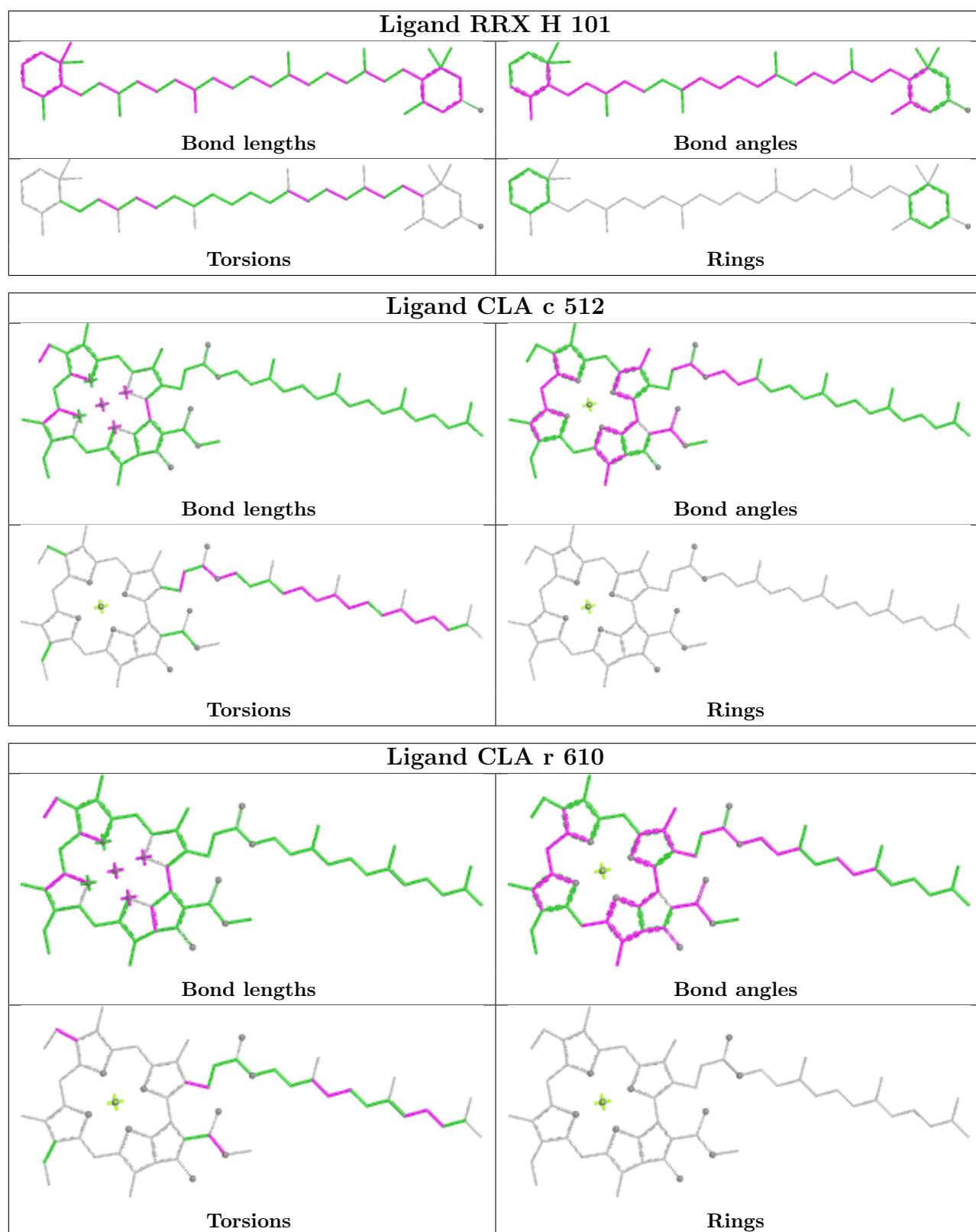


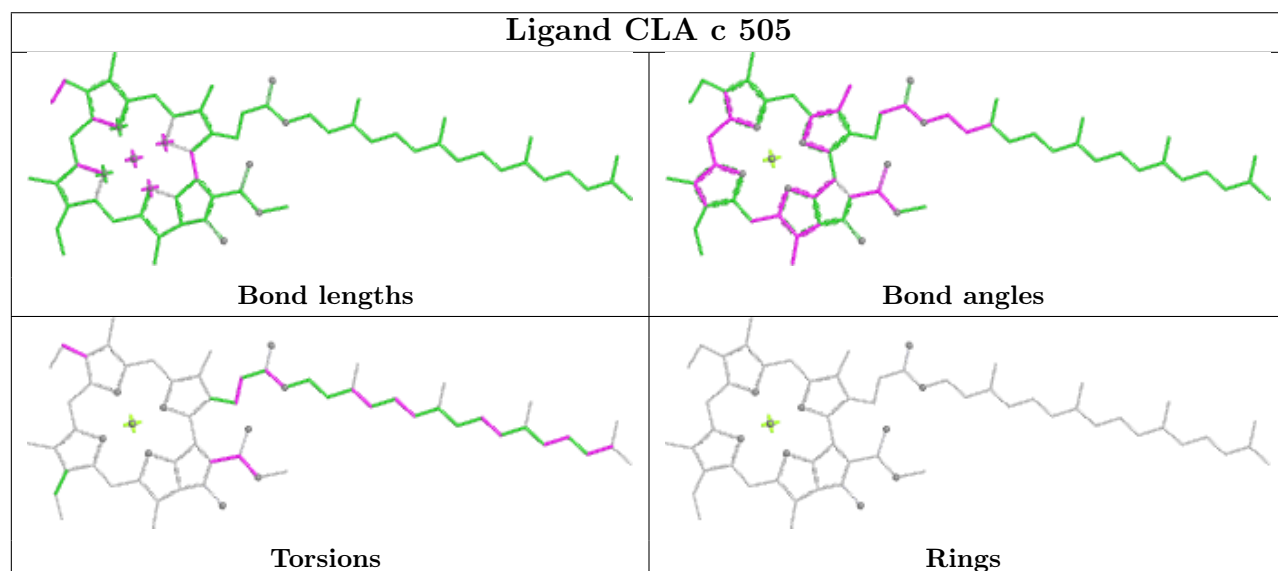
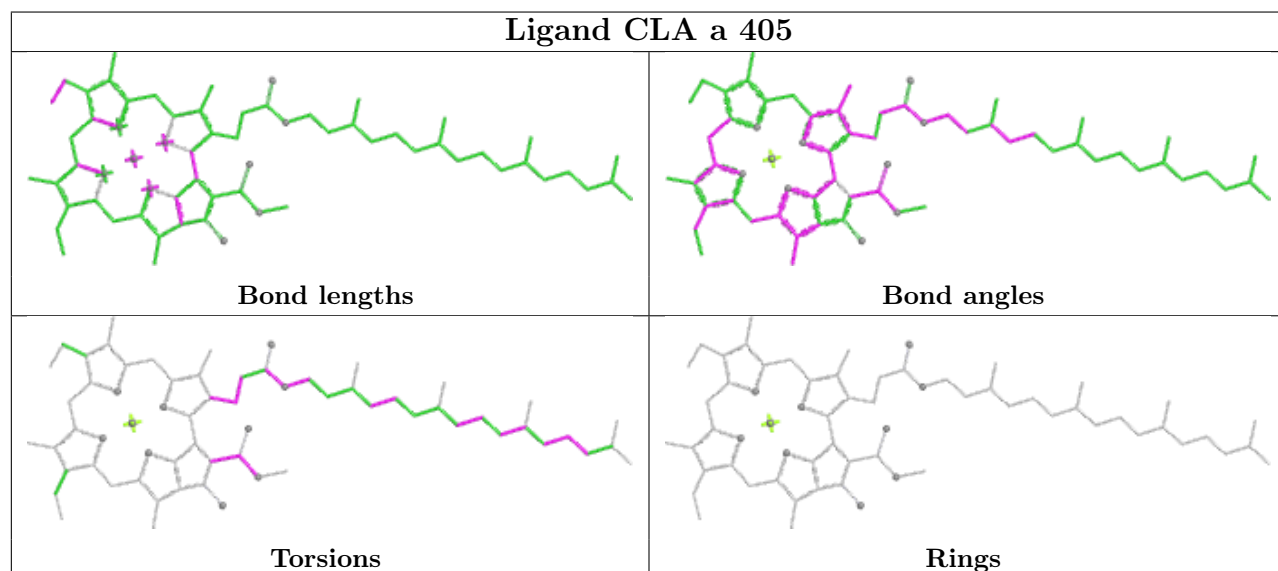
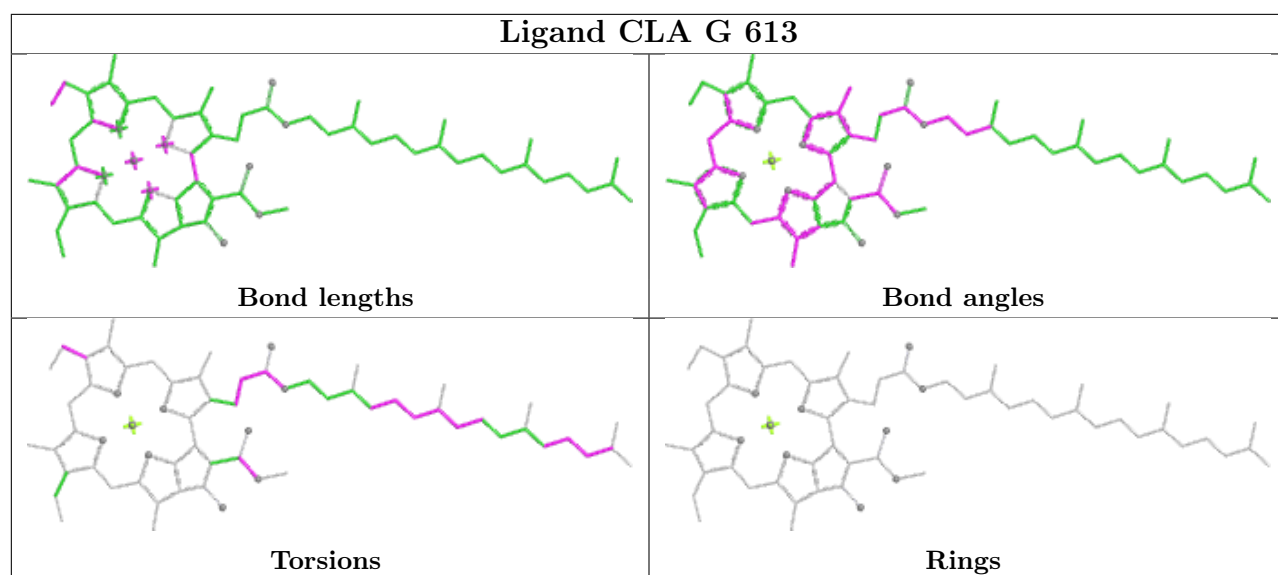
Ligand CLA g 614

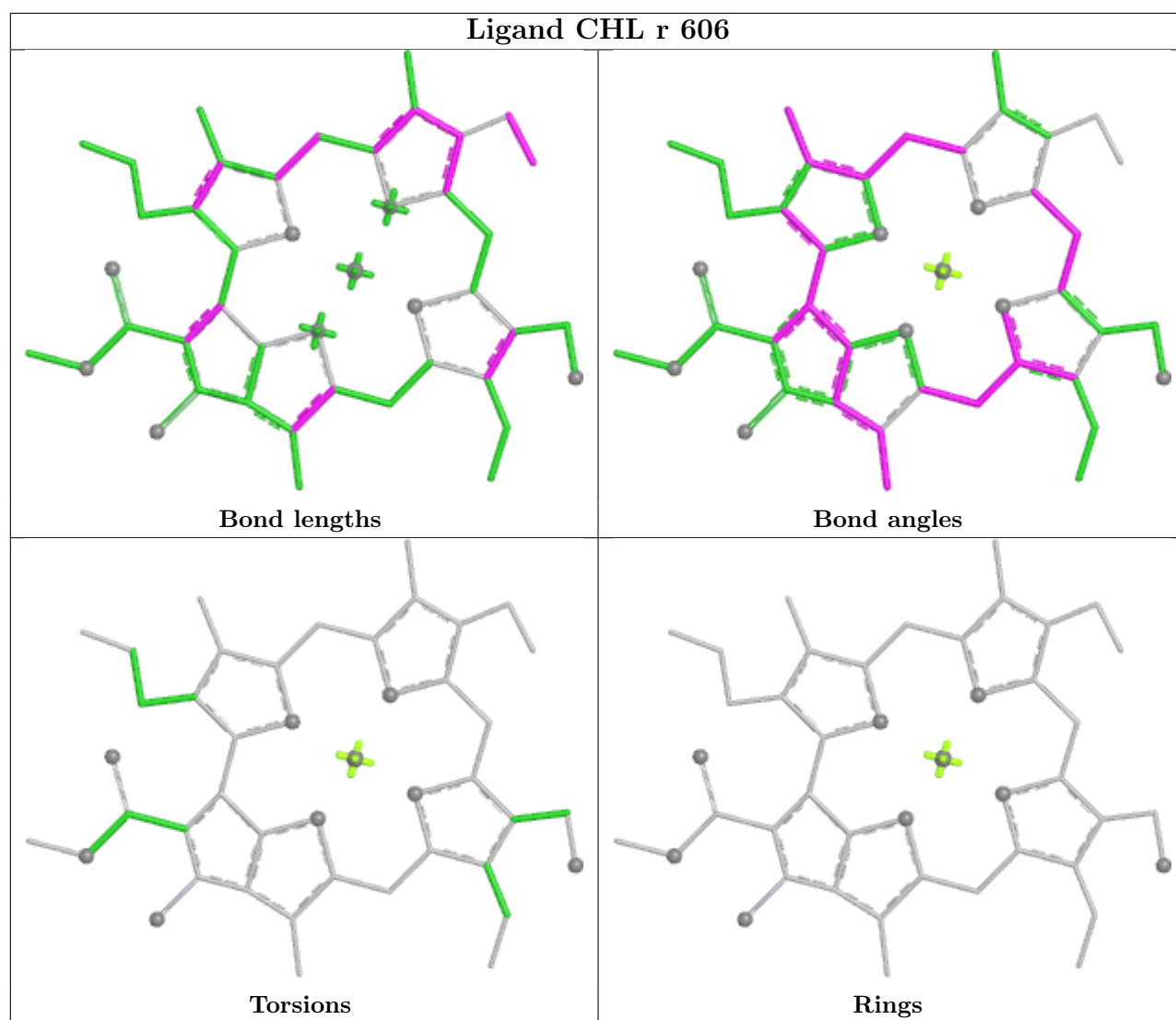


Ligand CLA C 503









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	R	1
22	r	1
23	s	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	110:PRO	C	126:GLU	N	17.87
1	r	110:PRO	C	126:GLU	N	17.80
1	s	285:ARG	C	286:VAL	N	3.20

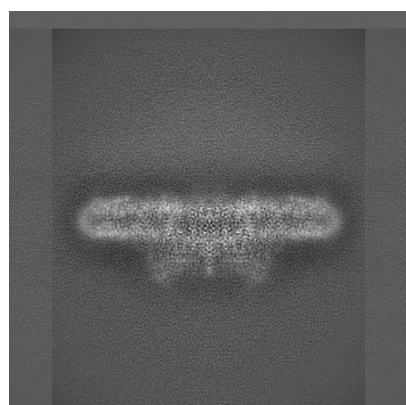
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13430. These allow visual inspection of the internal detail of the map and identification of artifacts.

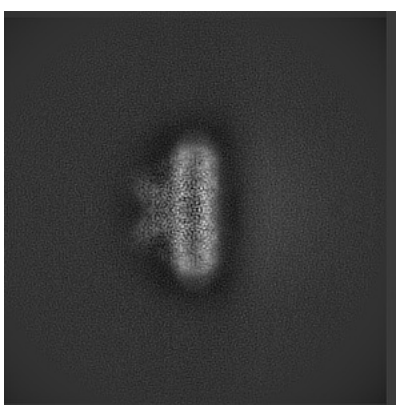
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

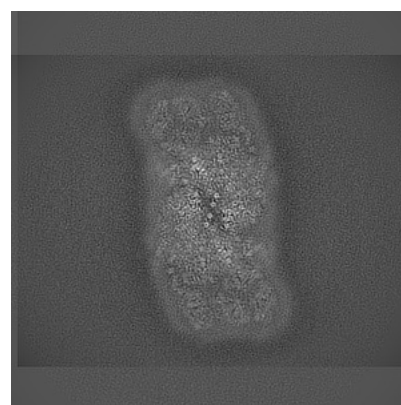
6.1.1 Primary map



X



Y

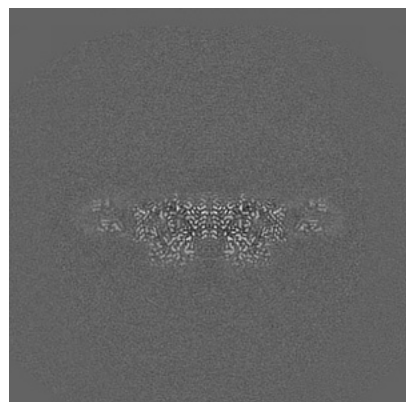


Z

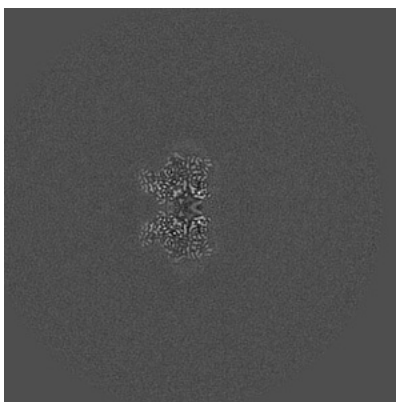
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

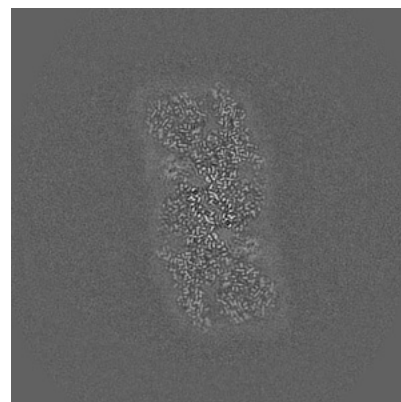
6.2.1 Primary map



X Index: 250



Y Index: 250

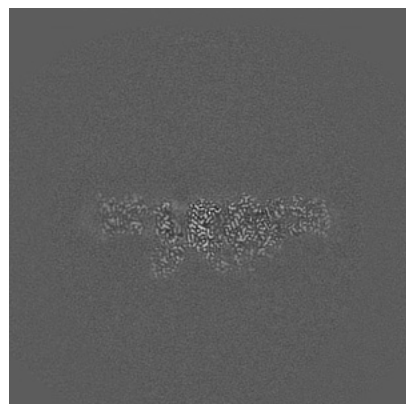


Z Index: 250

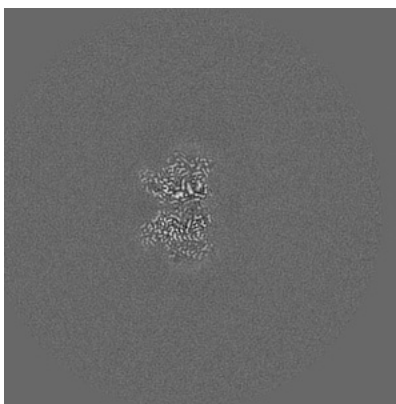
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

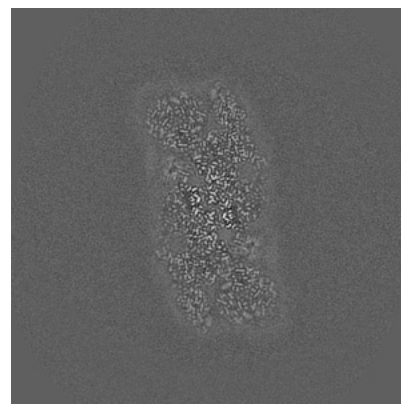
6.3.1 Primary map



X Index: 268



Y Index: 248

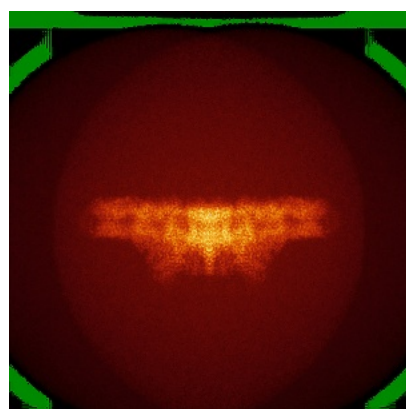


Z Index: 249

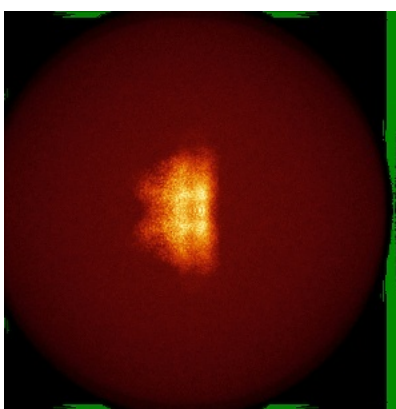
The images above show the largest variance slices of the map in three orthogonal directions.

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

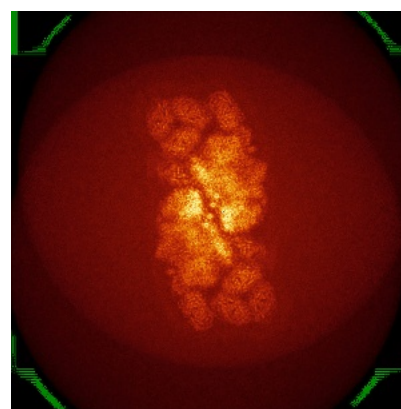
6.4.1 Primary map



X



Y

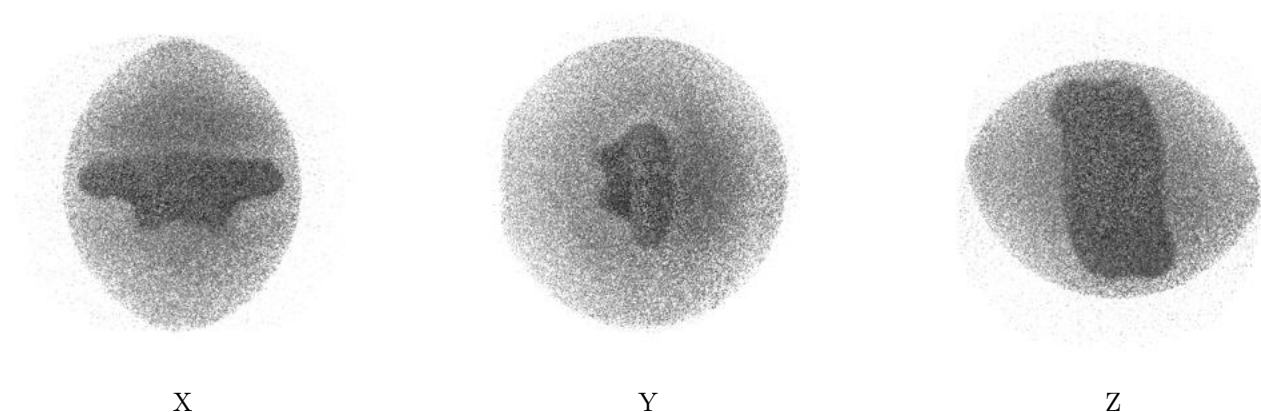


Z

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

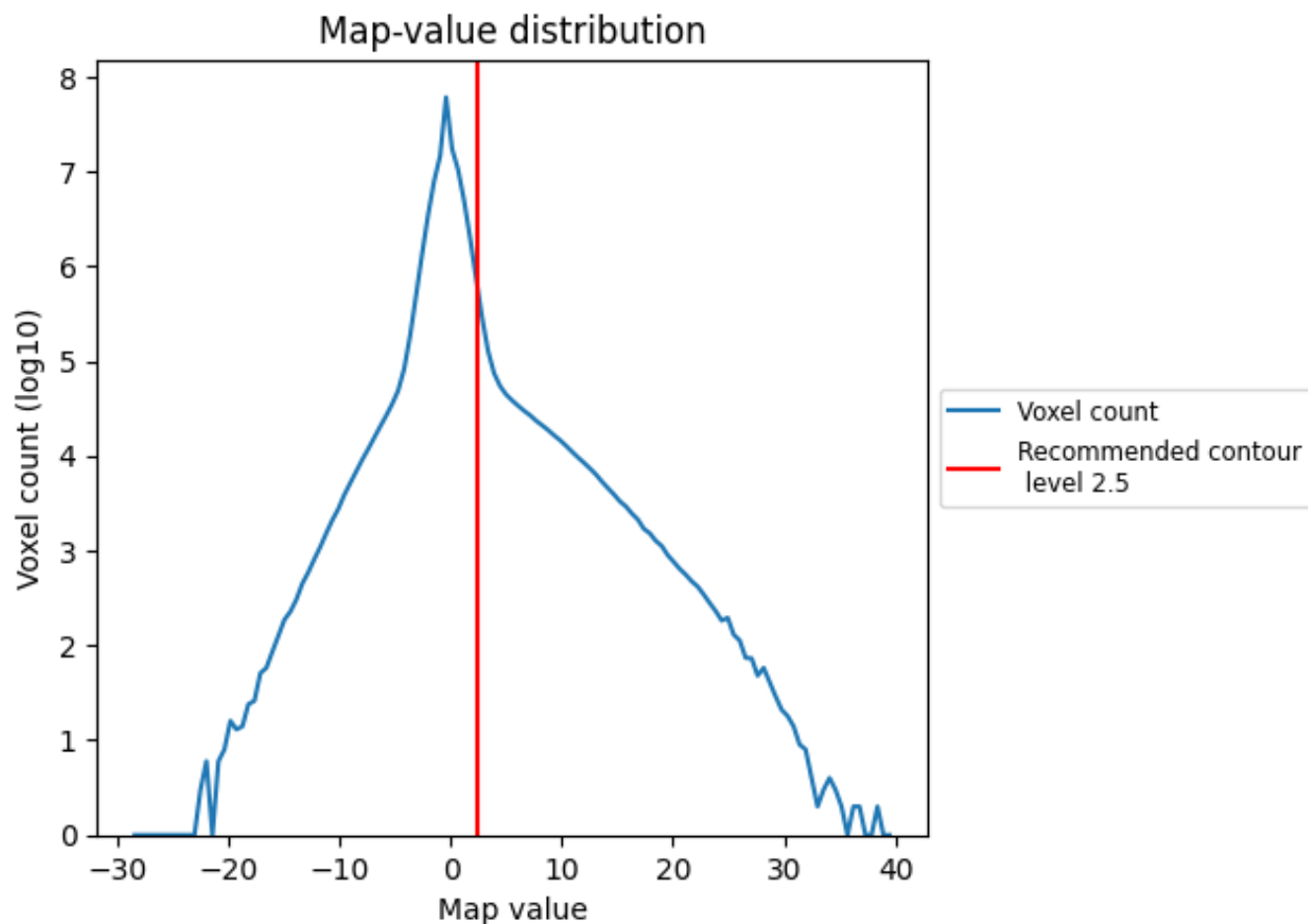
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

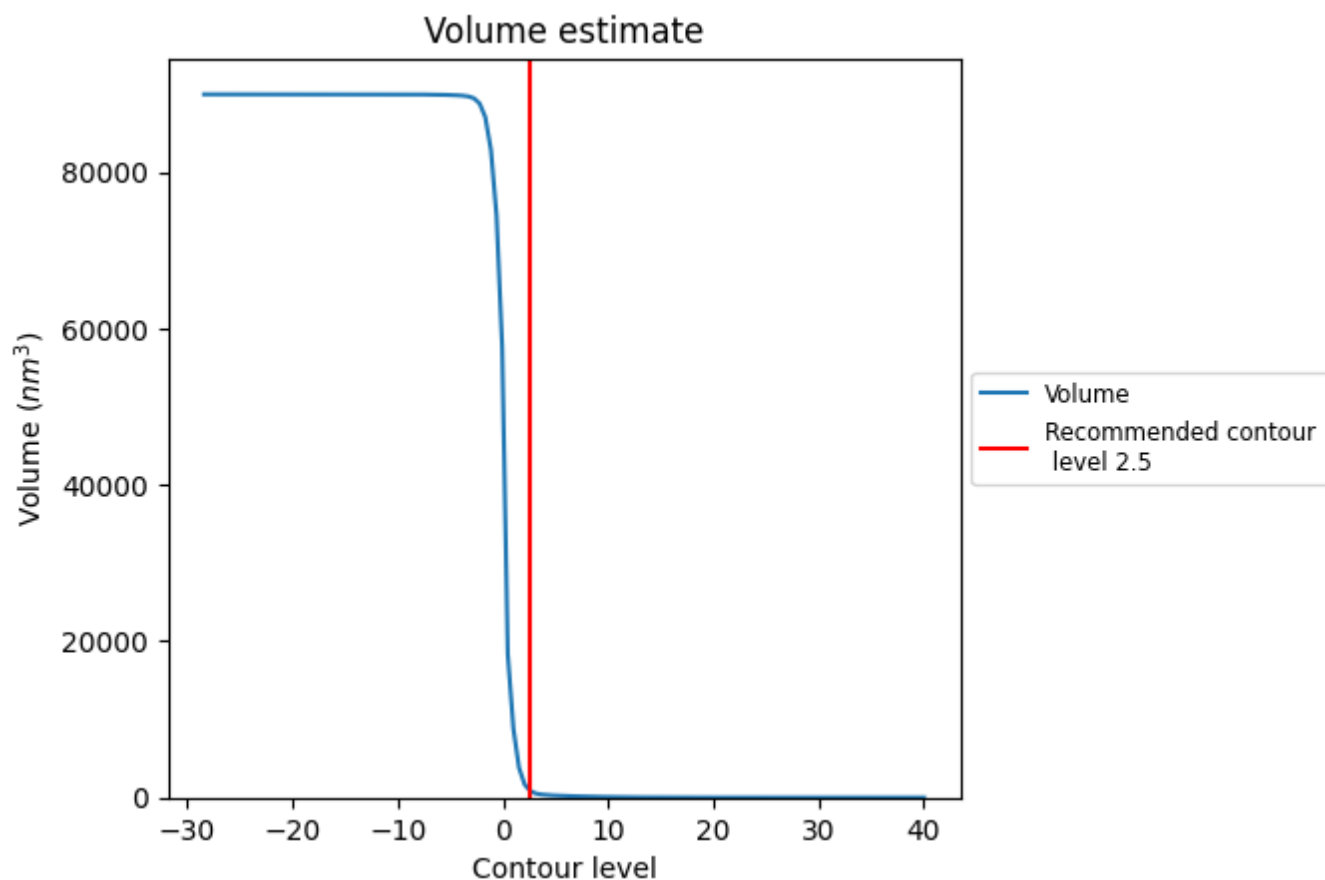
This section contains the results of statistical analysis of the map.

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.

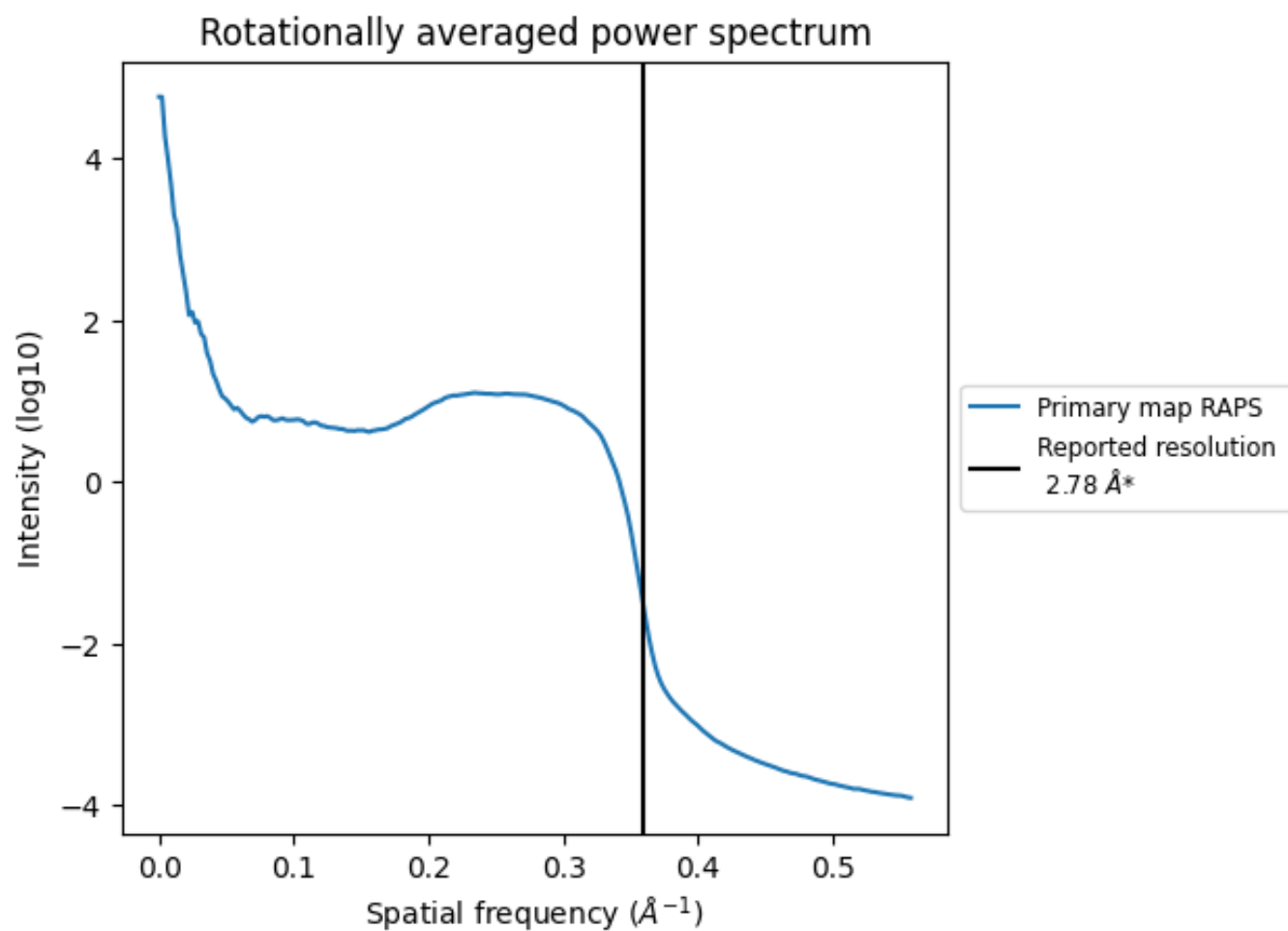
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 980 nm^3 ; this corresponds to an approximate mass of 885 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 ⓘ

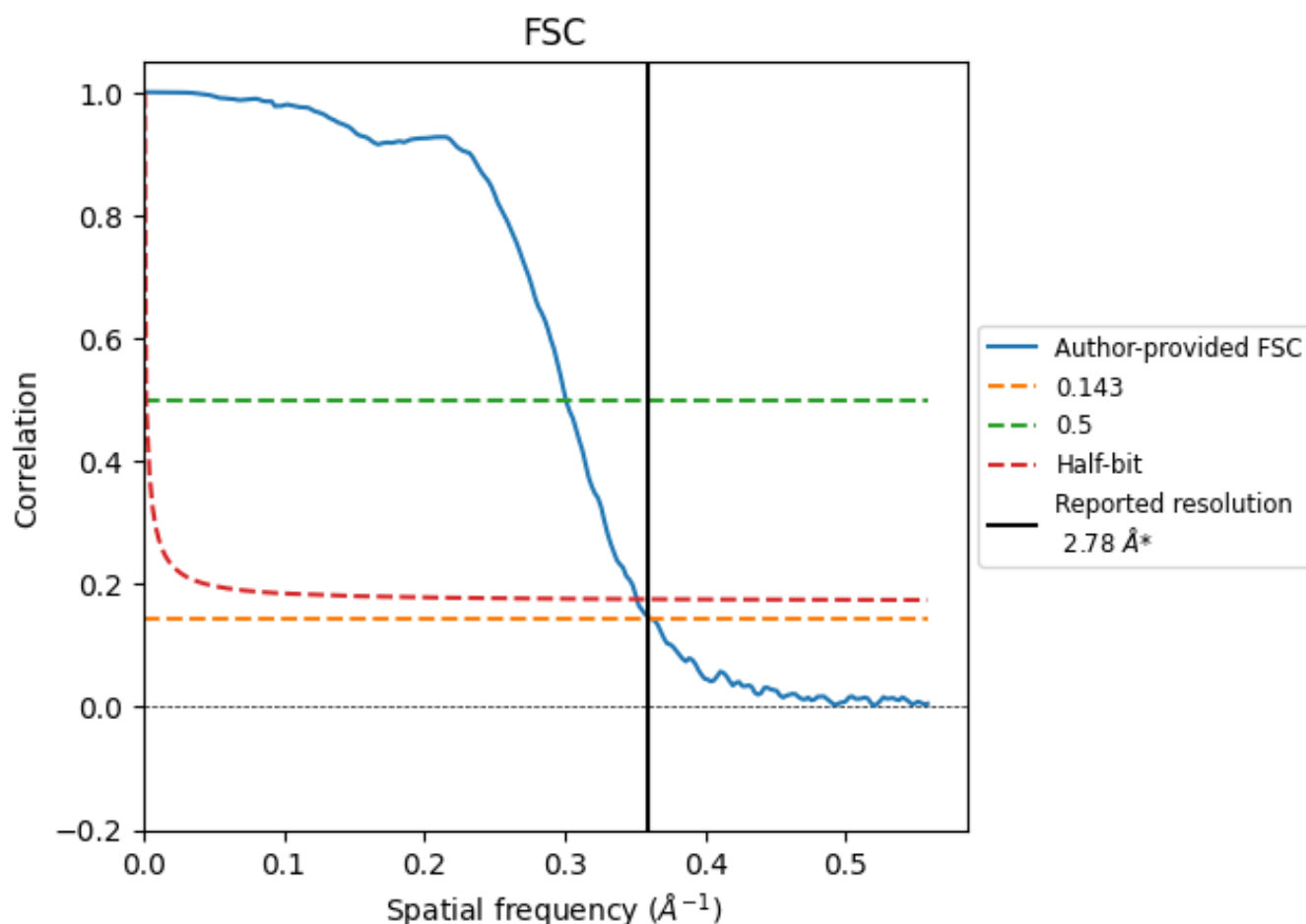


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

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 0.360 Å⁻¹

8.2 Resolution estimates [i](#)

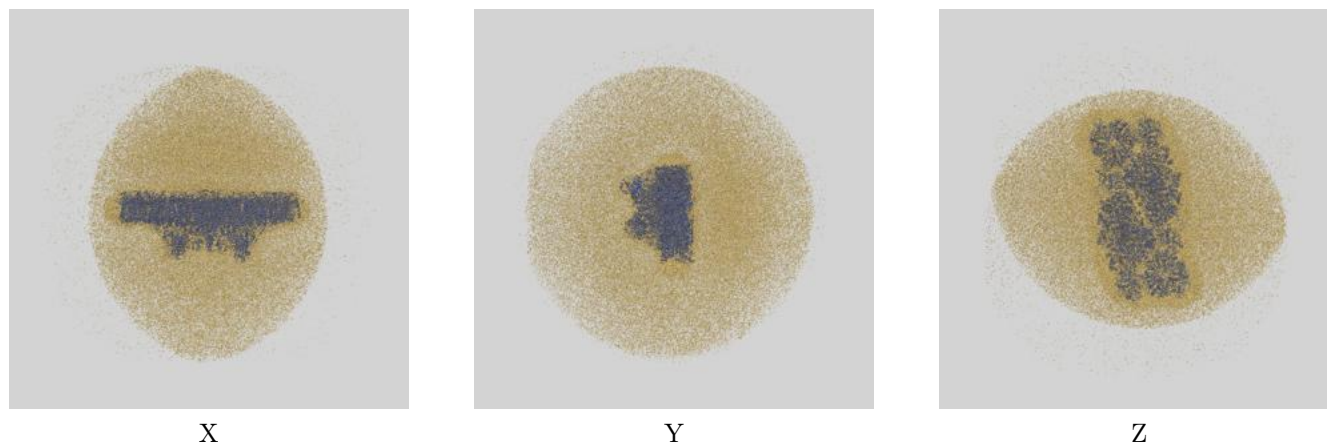
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.77	3.32	2.85
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

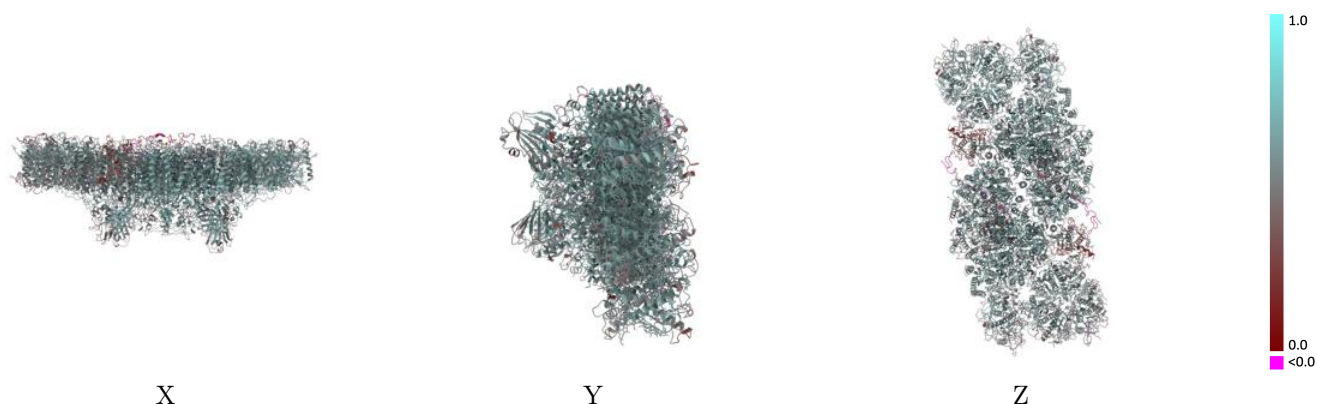
This section contains information regarding the fit between EMDB map EMD-13430 and PDB model 7PI5. Per-residue inclusion information can be found in section [3](#) on page [49](#).

9.1 Map-model overlay [i](#)



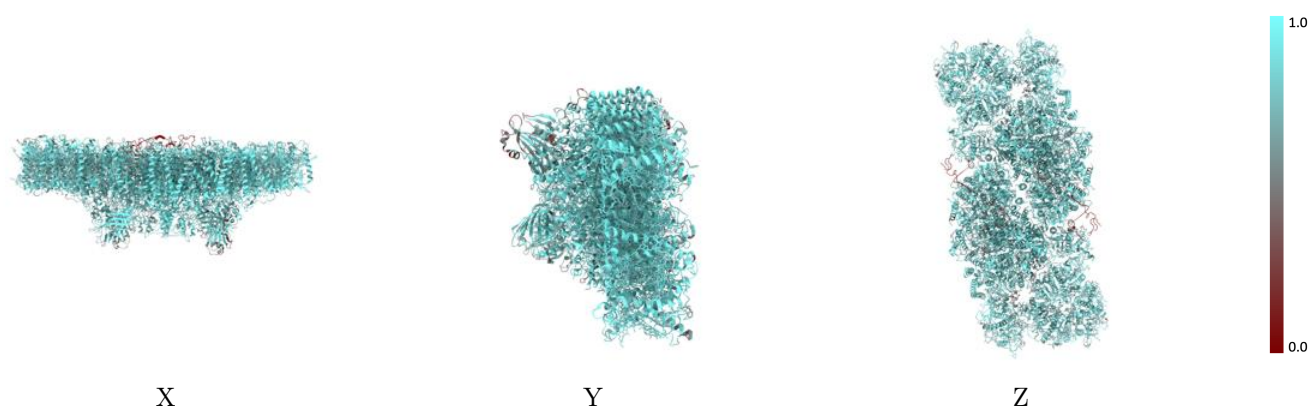
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



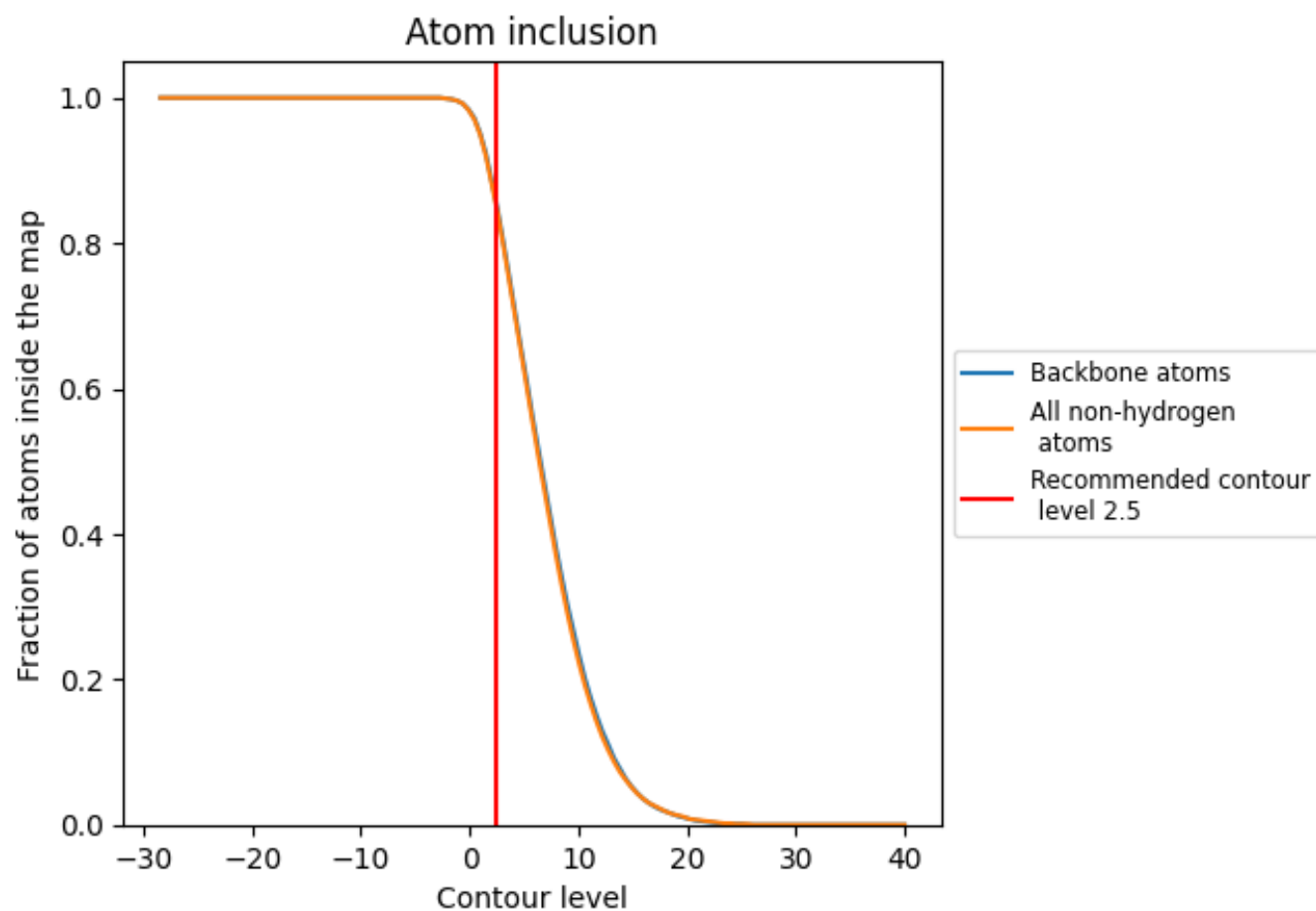
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.5420
A	 0.8520	 0.5510
B	 0.9210	 0.5880
C	 0.8770	 0.5650
D	 0.8960	 0.5800
E	 0.8730	 0.5320
F	 0.8500	 0.5380
G	 0.7990	 0.4950
H	 0.8770	 0.5610
I	 0.8800	 0.5740
J	 0.8170	 0.5330
K	 0.8700	 0.5590
L	 0.9350	 0.5800
M	 0.9130	 0.5710
N	 0.8080	 0.5170
O	 0.8090	 0.4940
P	 0.6310	 0.4770
R	 0.6810	 0.3480
S	 0.8070	 0.5130
T	 0.9300	 0.5740
U	 0.6610	 0.4280
V	 0.8400	 0.5450
W	 0.8200	 0.5230
X	 0.7860	 0.5080
Y	 0.8590	 0.5380
Z	 0.8700	 0.5380
a	 0.8720	 0.5630
b	 0.9230	 0.5900
c	 0.8990	 0.5810
d	 0.9150	 0.5920
e	 0.8760	 0.5540
f	 0.8990	 0.5730
g	 0.8360	 0.5390
h	 0.8910	 0.5730
i	 0.9470	 0.5810



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.8460	 0.5670
k	 0.8770	 0.5850
l	 0.9320	 0.5910
m	 0.9050	 0.5660
n	 0.8520	 0.5550
o	 0.8460	 0.5340
p	 0.6150	 0.4980
r	 0.6650	 0.3580
s	 0.8420	 0.5460
t	 0.9170	 0.5760
u	 0.7480	 0.4740
v	 0.8760	 0.5630
w	 0.8590	 0.5380
x	 0.8260	 0.5260
y	 0.8810	 0.5690
z	 0.9010	 0.5730