



wwPDB EM Validation Summary Report ⓘ

Aug 10, 2022 – 03:30 pm BST

PDB ID : 7PI5
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:

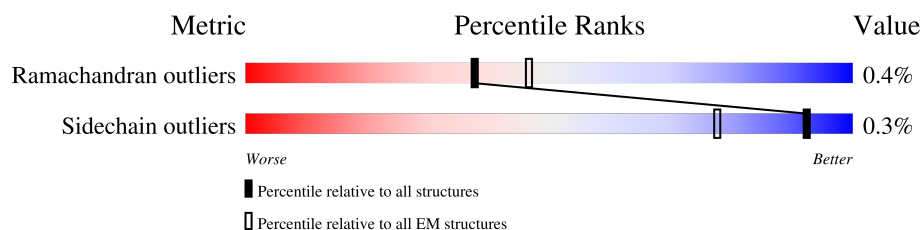
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

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.



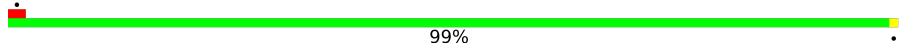
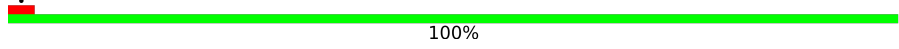
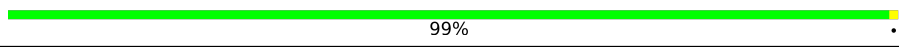
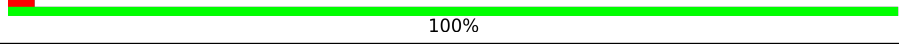
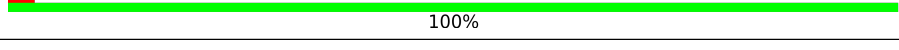
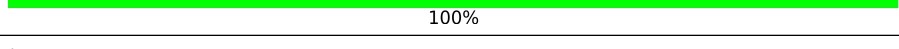
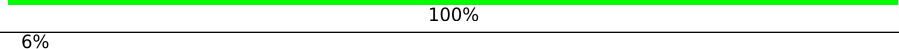
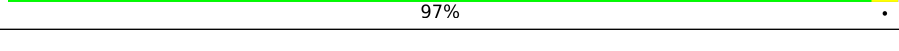
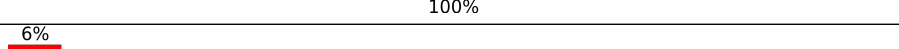
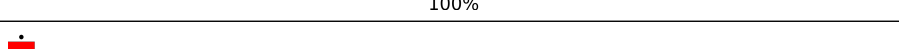
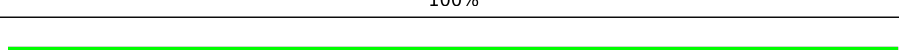
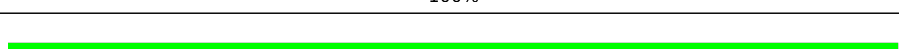
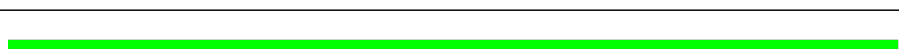
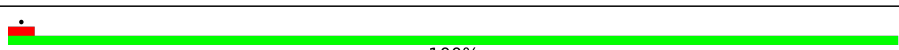
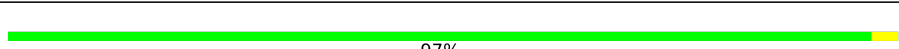

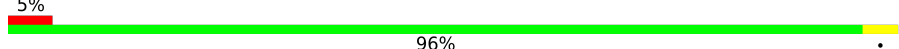
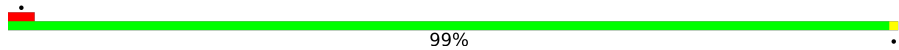
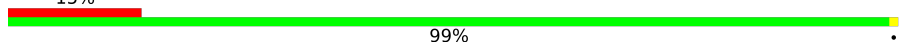
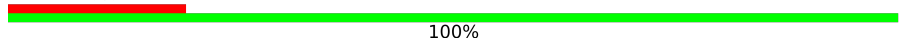
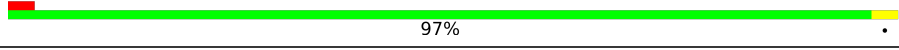
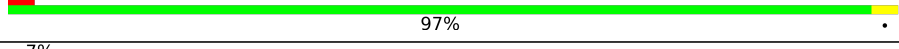
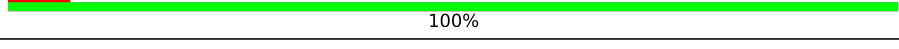
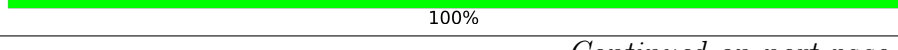

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>9%</div> <div>99%</div> <div>.</div> </div>
1	a	336	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
2	B	484	<div> <div>100%</div> </div>
2	b	484	<div> <div>100%</div> </div>
3	V	32	<div> <div>100%</div> </div>
3	v	32	<div> <div>100%</div> </div>
4	C	449	<div> <div>99%</div> <div>.</div> </div>
4	c	449	<div> <div>99%</div> <div>.</div> </div>
5	D	348	<div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	d	348	 99%
6	E	76	 100%
6	e	76	 99%
7	F	31	 100%
7	f	31	 100%
8	H	67	 100%
8	h	67	 100%
9	I	35	 97%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 100%
12	l	38	 100%
13	M	32	 97%
13	m	32	 97%
14	O	238	 96%
14	o	238	 99%
15	P	187	 99%
15	p	187	 100%
16	T	30	 97%
16	t	30	 97%
17	W	44	 100%
17	w	44	 100%

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Mol	Chain	Length	Quality of chain
18	X	30	 100%
18	x	30	 100%
19	Z	61	 98%
19	z	61	 100%
20	N	222	 99%
20	n	222	 100%
21	G	221	 99%
21	g	221	 100%
22	R	202	 24% 100%
22	r	202	 26% 100%
23	S	243	 98%
23	s	243	 99%
24	Y	222	 99%
24	y	222	 99%
25	U	27	 7% 100%
25	u	27	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	R	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
44	RRX	H	101	X	-	-	-
44	RRX	h	101	X	-	-	-
45	CHL	G	601	X	-	-	-
45	CHL	G	605	X	-	-	-
45	CHL	G	606	X	-	-	-
45	CHL	G	607	X	-	-	-
45	CHL	G	608	X	-	-	-
45	CHL	G	609	X	-	-	-
45	CHL	N	601	X	-	-	-
45	CHL	N	605	X	-	-	-
45	CHL	N	606	X	-	-	-
45	CHL	N	607	X	-	-	-
45	CHL	N	608	X	-	-	-
45	CHL	N	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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		

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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

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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		

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

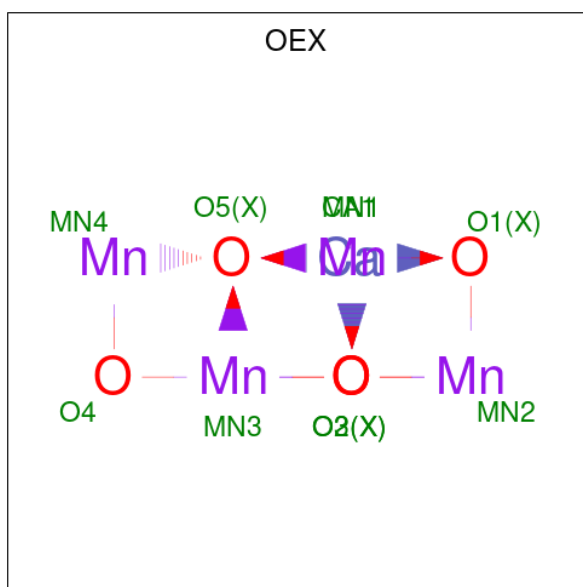
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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	

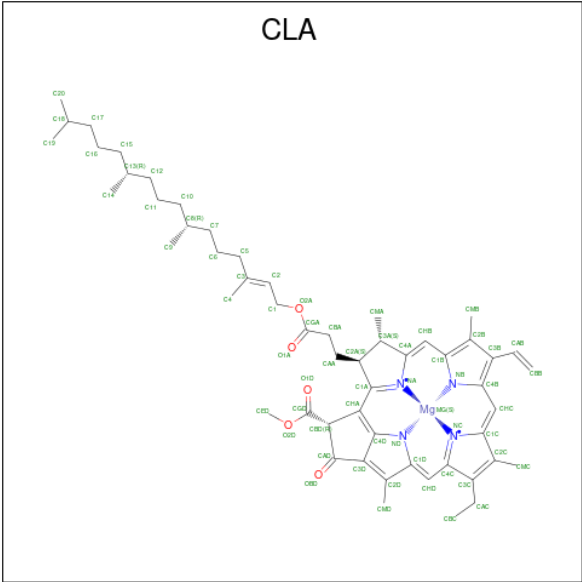
- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	G	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	R	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	R	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	R	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	R	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	R	1	Total 501	C 411	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total	C	Mg	N	O	0
			501	411	9	36	45	
29	R	1	Total	C	Mg	N	O	0
			501	411	9	36	45	
29	R	1	Total	C	Mg	N	O	0
			501	411	9	36	45	
29	R	1	Total	C	Mg	N	O	0
			501	411	9	36	45	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	S	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	Y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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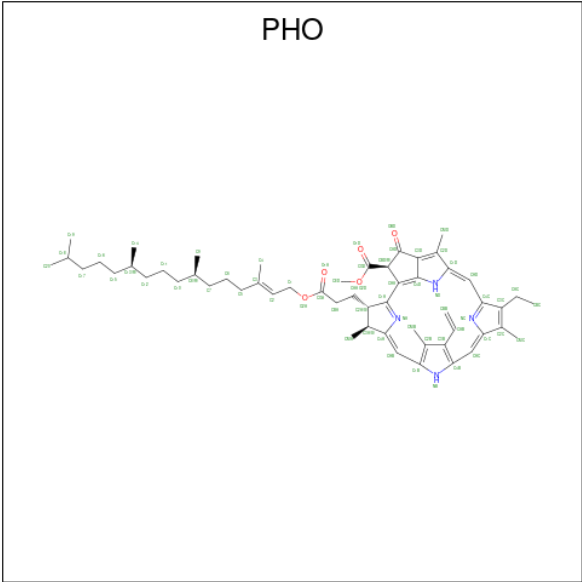
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	g	1	Total 446	C 368	Mg 8	N 32	O 38	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0
29	r	1	Total 501	C 411	Mg 9	N 36	O 45	0

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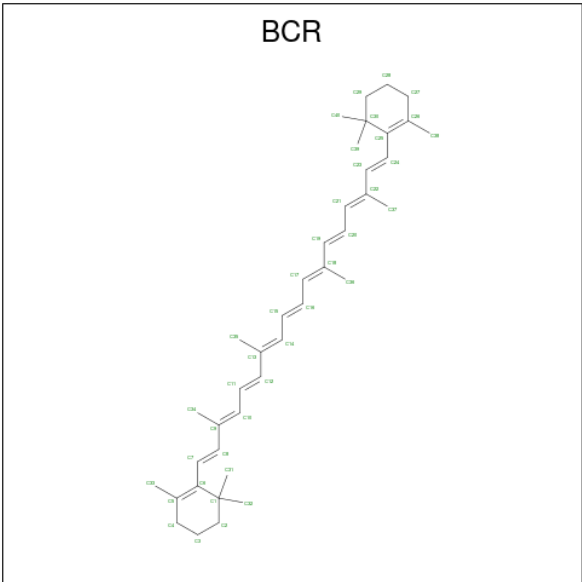
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C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

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



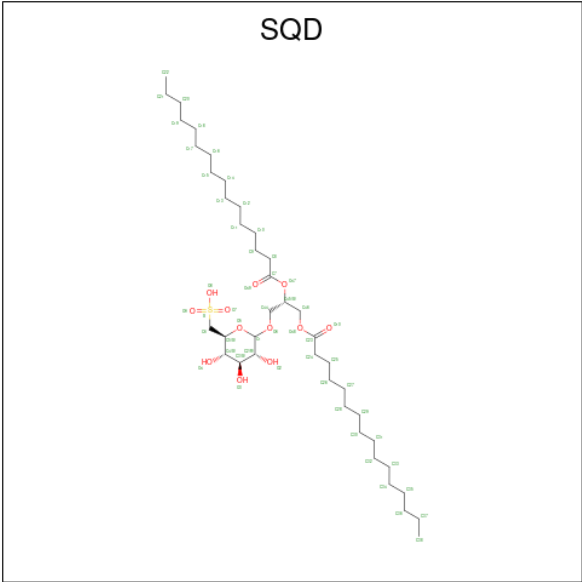
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



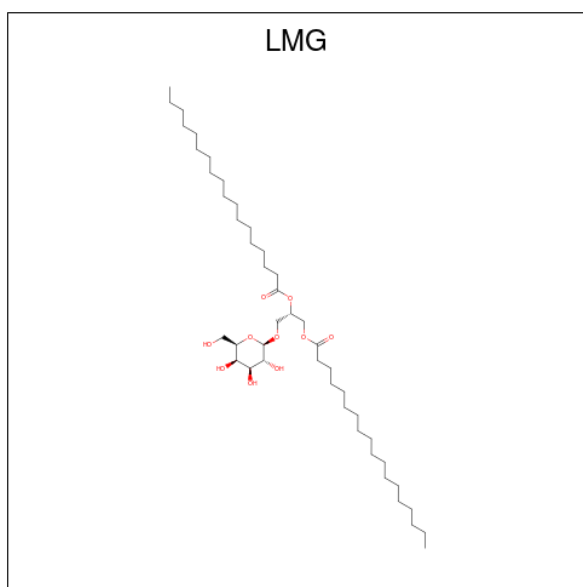
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 80 80	0
31	B	1	Total C 80 80	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 80 80	0
31	b	1	Total C 80 80	0
31	c	1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

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: 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 (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).

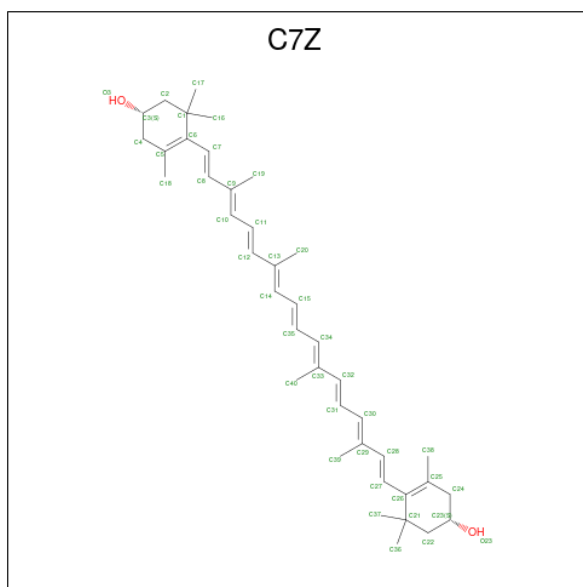


Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			44	34	10	
33	C	1	Total	C	O	0
			51	41	10	
33	D	1	Total	C	O	0
			46	36	10	
33	H	1	Total	C	O	0
			48	38	10	
33	J	1	Total	C	O	0
			45	35	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			44	34	10	
33	c	1	Total	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 (three-letter code: NA) (formula: Na).

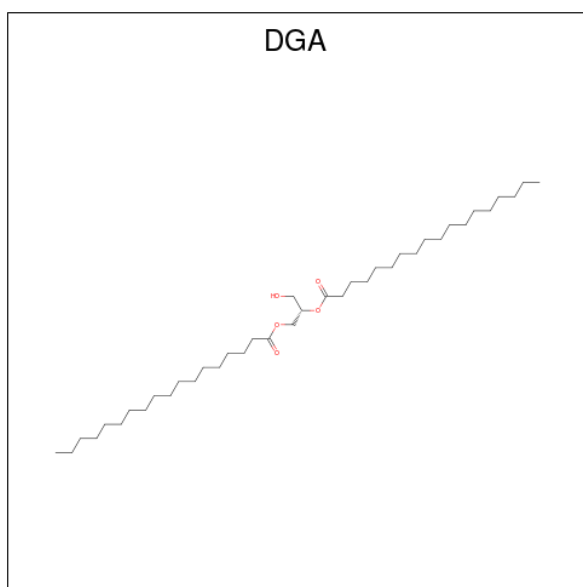
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Na	0
			1	1	
34	a	1	Total	Na	0
			1	1	

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



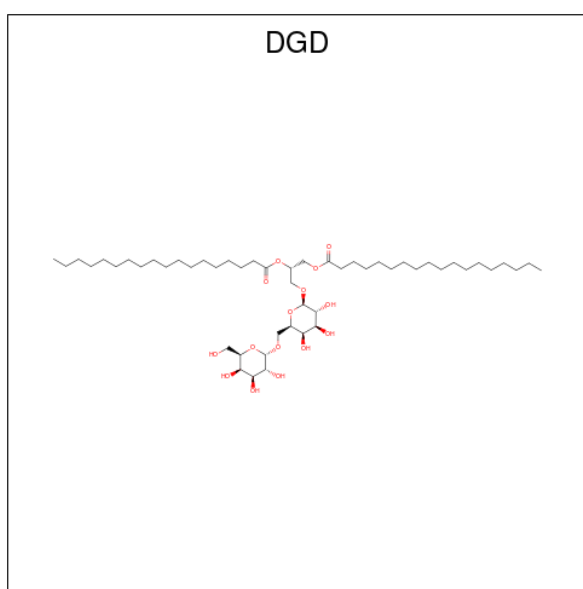
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			44	39	5	
36	C	1	Total	C	O	0
			44	39	5	
36	b	1	Total	C	O	0
			44	39	5	
36	c	1	Total	C	O	0
			44	39	5	

- Molecule 37 is GLYCEROL (three-letter code: 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
			12	6	6	
37	b	1	Total	C	O	0
			12	6	6	
37	y	1	Total	C	O	0
			6	3	3	

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



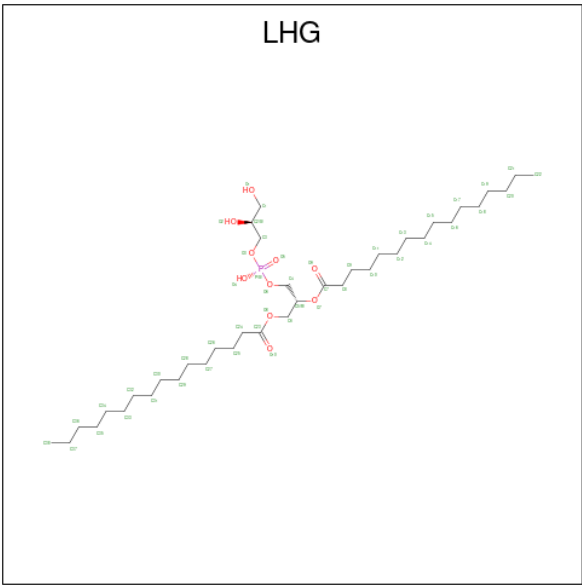
Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			242	182	60	
38	C	1	Total	C	O	0
			242	182	60	
38	C	1	Total	C	O	0
			242	182	60	
38	C	1	Total	C	O	0
			242	182	60	
38	c	1	Total	C	O	0
			242	182	60	
38	c	1	Total	C	O	0
			242	182	60	
38	c	1	Total	C	O	0
			242	182	60	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	c	1	242	182	60	0

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



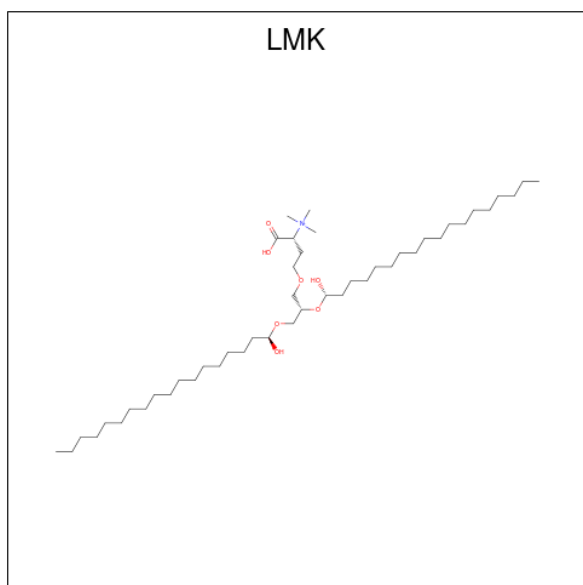
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
39	C	1	47	36	10	1	0
39	D	1	132	99	30	3	0
39	D	1	132	99	30	3	0
39	D	1	132	99	30	3	0
39	L	1	49	38	10	1	0
39	N	1	49	38	10	1	0
39	G	1	49	38	10	1	0
39	S	1	45	34	10	1	0
39	Y	1	49	38	10	1	0
39	c	1	47	36	10	1	0

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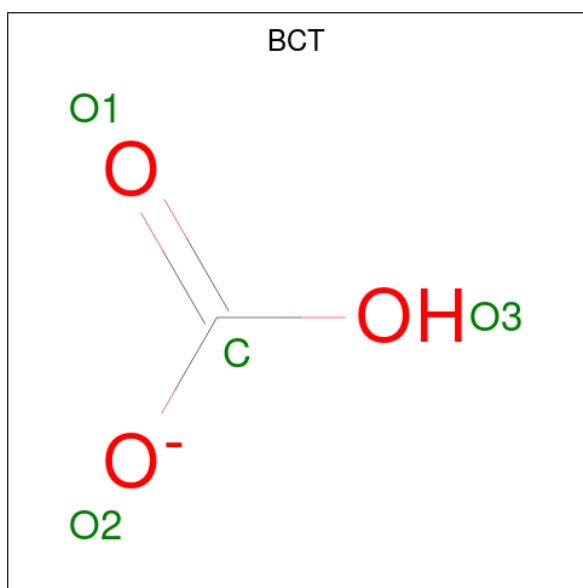
Mol	Chain	Residues	Atoms				AltConf
39	d	1	Total	C	O	P	0
			132	99	30	3	
39	d	1	Total	C	O	P	0
			132	99	30	3	
39	d	1	Total	C	O	P	0
			132	99	30	3	
39	l	1	Total	C	O	P	0
			49	38	10	1	
39	n	1	Total	C	O	P	0
			49	38	10	1	
39	g	1	Total	C	O	P	0
			49	38	10	1	
39	s	1	Total	C	O	P	0
			45	34	10	1	
39	y	1	Total	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-oxidan-1-yl]octadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula: C₄₆H₉₄NO₇).



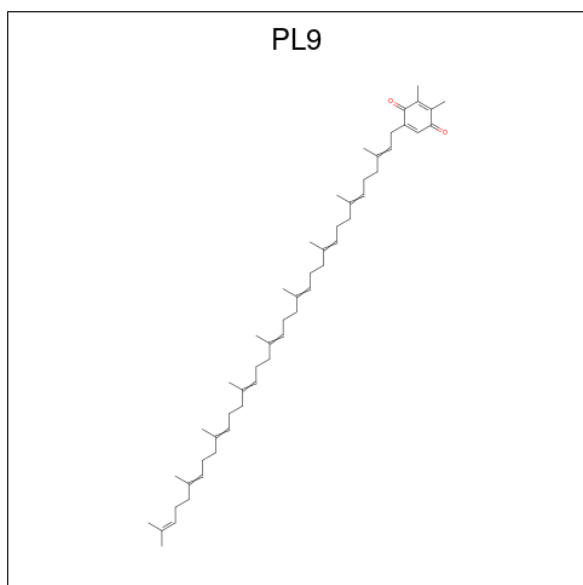
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			40	32	1	7	
40	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 41 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



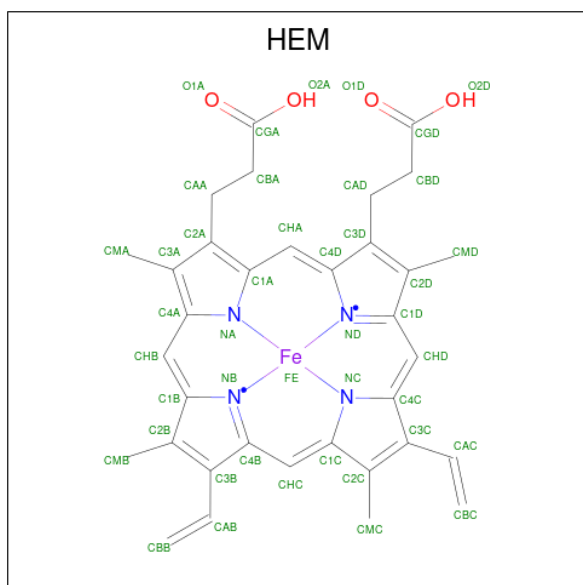
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			4	1	3	
41	d	1	Total	C	O	0
			4	1	3	

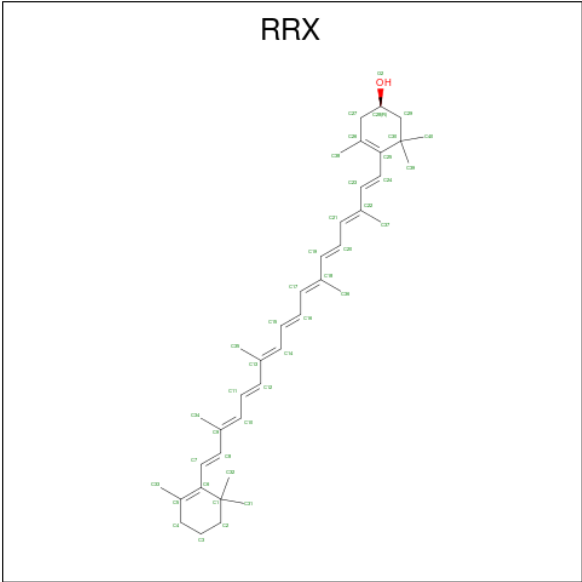
- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

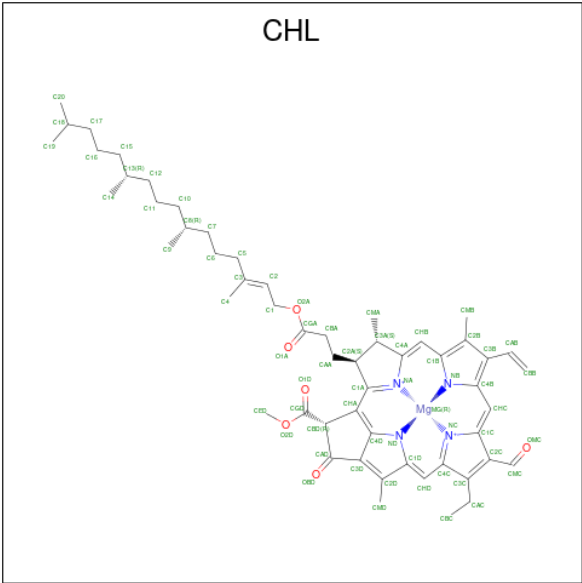
- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





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

- Molecule 45 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
45	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
45	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
45	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0

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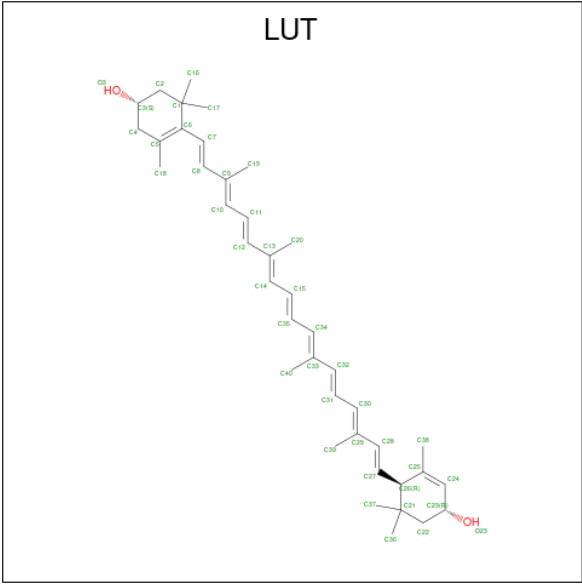
Mol	Chain	Residues	Atoms					AltConf
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
45	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
45	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
45	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
45	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
45	y	1	Total 310	C 255	Mg 5	N 20	O 30	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
45	y	1	310	255	5	20	30	0
45	y	1	310	255	5	20	30	0

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



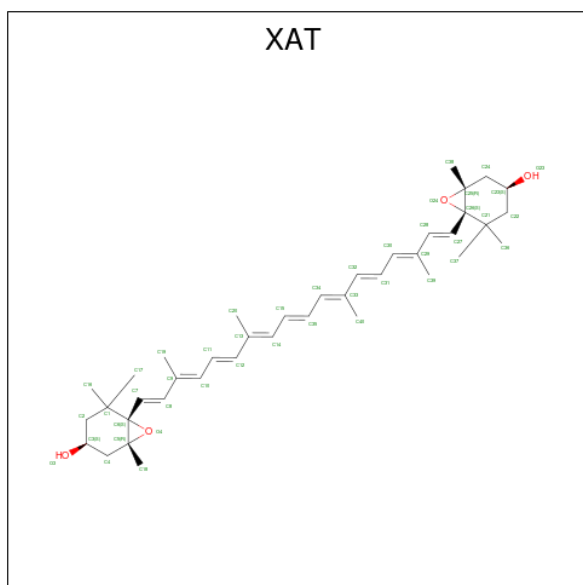
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	N	1	84	80	4	0
46	N	1	84	80	4	0
46	G	1	84	80	4	0
46	G	1	84	80	4	0
46	R	1	42	40	2	0
46	S	1	84	80	4	0
46	S	1	84	80	4	0
46	Y	1	84	80	4	0
46	Y	1	84	80	4	0

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

- 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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



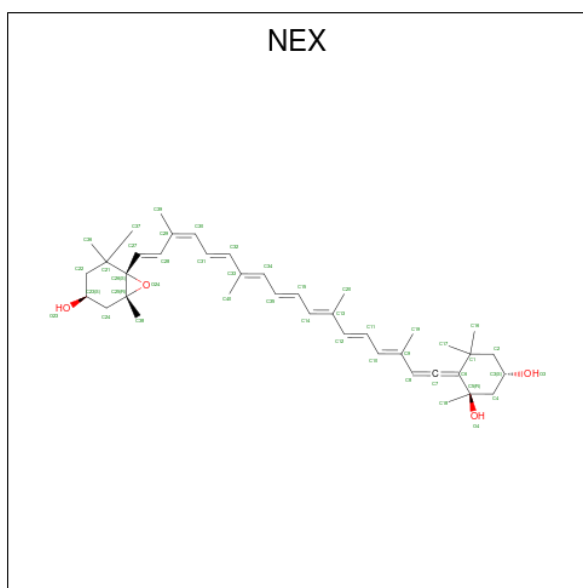
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			44	40	4	
47	G	1	Total	C	O	0
			44	40	4	

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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 (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



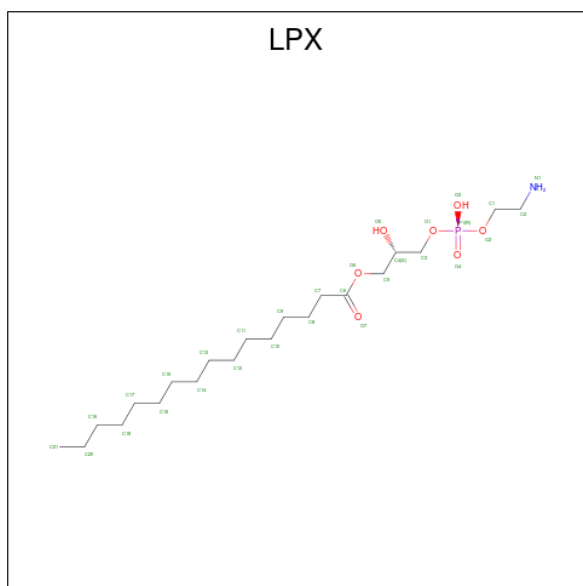
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			44	40	4	
48	S	1	Total	C	O	0
			44	40	4	

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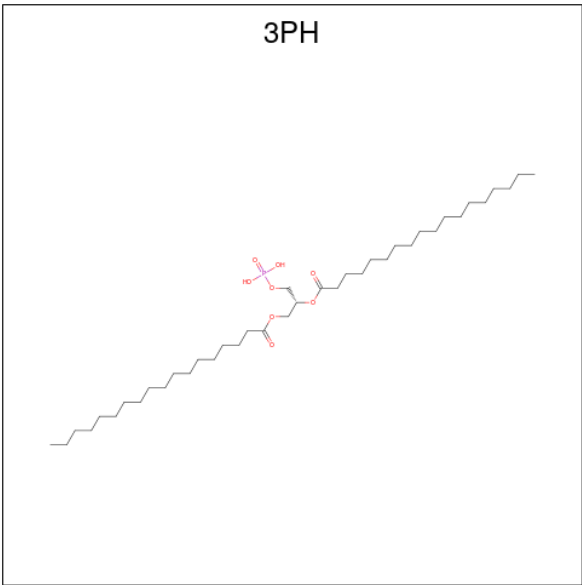
Mol	Chain	Residues	Atoms			AltConf
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			44	40	4	
48	s	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

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



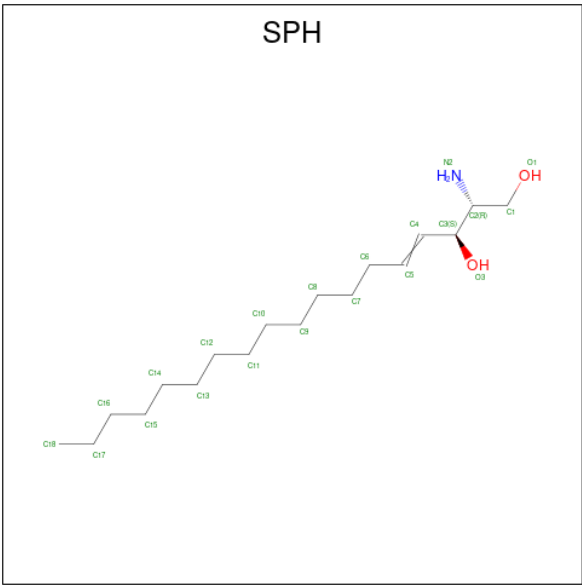
Mol	Chain	Residues	Atoms					AltConf
49	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
49	s	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 50 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 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 (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



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

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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	

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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

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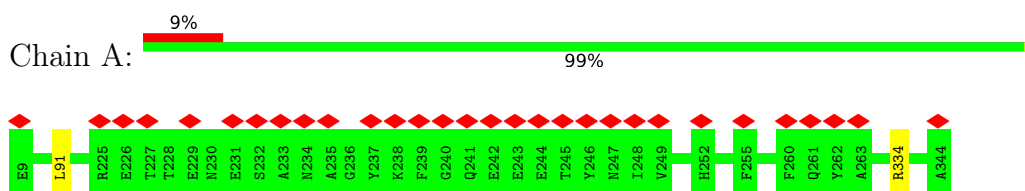
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Mol	Chain	Residues	Atoms		AltConf
52	w	3	Total 3	O 3	0
52	x	2	Total 2	O 2	0
52	n	13	Total 13	O 13	0
52	g	12	Total 12	O 12	0
52	r	15	Total 15	O 15	0
52	s	21	Total 21	O 21	0
52	y	22	Total 22	O 22	0

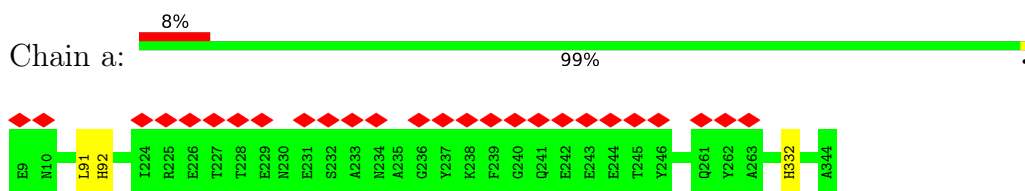
3 Residue-property plots [i](#)

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

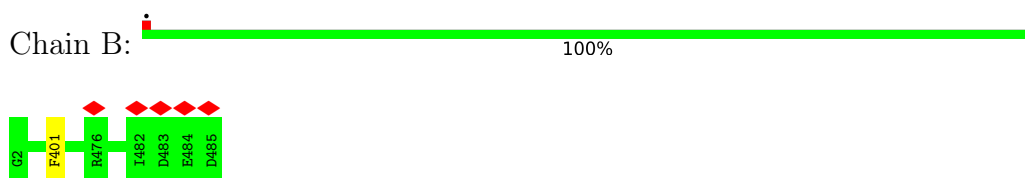
- Molecule 1: Photosystem II protein D1



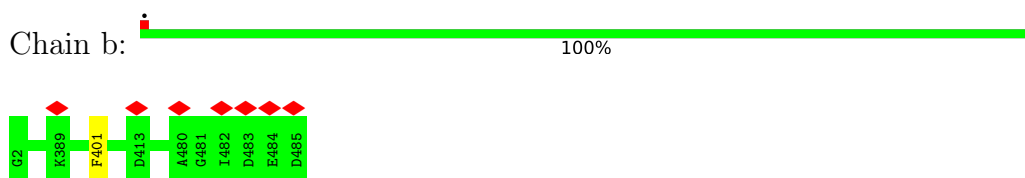
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II reaction center protein Ycf12



There are no outlier residues recorded for this chain.

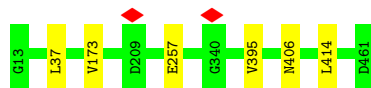
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  99%



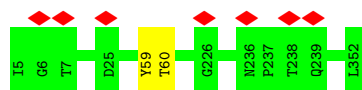
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  99%



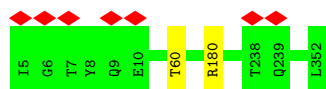
- Molecule 5: Photosystem II D2 protein

Chain D:  99%



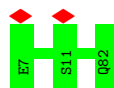
- Molecule 5: Photosystem II D2 protein

Chain d:  99%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  99%



- Molecule 7: Cytochrome b559 subunit beta

Chain F:  100%



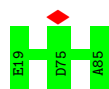
- Molecule 7: Cytochrome b559 subunit beta

Chain f:  100%



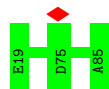
- Molecule 8: Photosystem II reaction center protein H

Chain H:  100%



- Molecule 8: Photosystem II reaction center protein H

Chain h:  100%



- Molecule 9: Photosystem II reaction center protein I

Chain I:  6% 97%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein J

Chain J:  6% 100%



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain l:  100%



- Molecule 13: Photosystem II reaction center protein M

Chain M:  97%



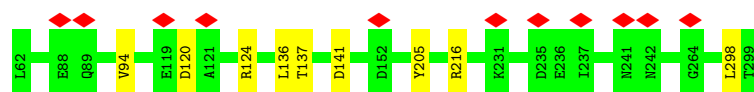
- Molecule 13: Photosystem II reaction center protein M

Chain m:  97%



- Molecule 14: PsbO

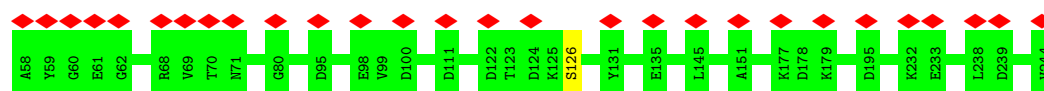
Chain O:  5% 96%



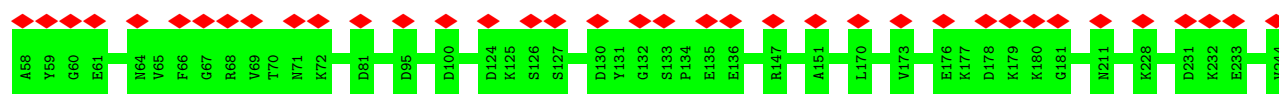
- Molecule 14: PsbO



- Molecule 15: PsbP



- Molecule 15: PsbP



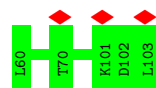
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T

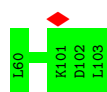


- Molecule 17: PSII 6.1 kDa protein



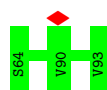
- Molecule 17: PSII 6.1 kDa protein

Chain w:  100%



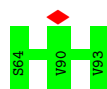
- Molecule 18: Hypothetical protein

Chain X:  100%



- Molecule 18: Hypothetical protein

Chain x:  100%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  98%



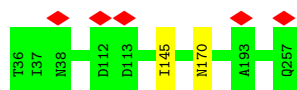
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: LHCII M3

Chain N:  99%



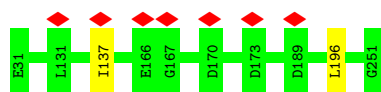
- Molecule 20: LHCII M3

Chain n:  100%



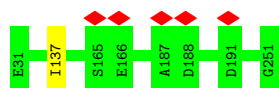
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G:  99%



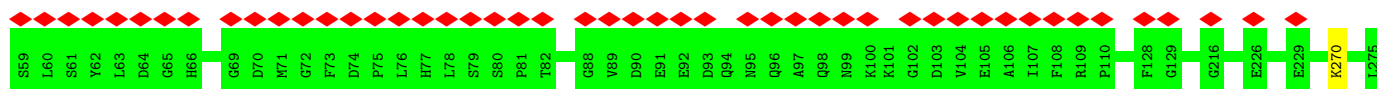
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain g:  100%



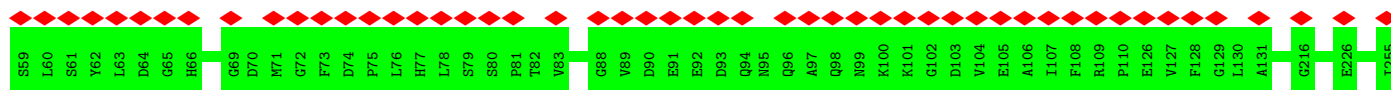
- Molecule 22: CP29

Chain R:  24%  100%



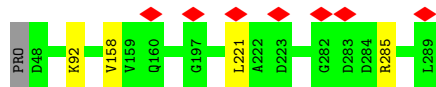
- Molecule 22: CP29

Chain r:  26%  100%



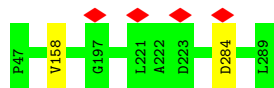
- Molecule 23: CP26

Chain S:  98%



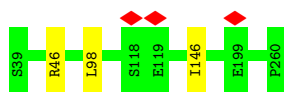
- Molecule 23: CP26

Chain s:  99%



- Molecule 24: LHCII M1

Chain Y:  99%



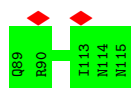
- Molecule 24: LHCII M1

Chain y:  99%



- Molecule 25: PsbU

Chain U:  7%  100%



- Molecule 25: PsbU

Chain u:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 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 (\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 (\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: OEX, HEM, LMG, 3PH, SPH, PHO, C7Z, CHL, RRX, BCT, XAT, PL9, LUT, CLA, LPX, DGA, NEX, LHG, DGD, NA, BCR, LMK, CL, SQD, FE2, GOL

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	0.29	0/2723	0.55	1/3715 (0.0%)
1	a	0.32	0/2723	0.57	1/3715 (0.0%)
2	B	0.30	0/3912	0.52	0/5327
2	b	0.30	0/3912	0.52	0/5327
3	V	0.25	0/228	0.57	0/311
3	v	0.24	0/228	0.61	0/311
4	C	0.29	0/3602	0.56	2/4913 (0.0%)
4	c	0.30	0/3602	0.58	1/4913 (0.0%)
5	D	0.30	0/2860	0.54	1/3899 (0.0%)
5	d	0.30	0/2860	0.53	0/3899
6	E	0.27	0/639	0.54	0/870
6	e	0.27	0/639	0.61	1/870 (0.1%)
7	F	0.27	0/259	0.54	0/351
7	f	0.26	0/259	0.49	0/351
8	H	0.27	0/513	0.53	0/703
8	h	0.29	0/513	0.52	0/703
9	I	0.30	0/287	0.50	0/386
9	i	0.29	0/287	0.51	0/386
10	J	0.25	0/272	0.46	0/369
10	j	0.25	0/272	0.55	0/369
11	K	0.32	0/308	0.52	0/423
11	k	0.34	0/308	0.58	0/423
12	L	0.27	0/321	0.45	0/435
12	l	0.27	0/321	0.47	0/435
13	M	0.26	0/246	0.48	0/335
13	m	0.25	0/246	0.46	0/335
14	O	0.31	0/1855	0.63	2/2505 (0.1%)
14	o	0.29	0/1855	0.59	1/2505 (0.0%)
15	P	0.28	0/1473	0.59	0/1988
15	p	0.27	0/1473	0.55	0/1988
16	T	0.29	0/254	0.50	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.29	0/254	0.51	0/342
17	W	0.25	0/339	0.51	0/460
17	w	0.27	0/339	0.51	0/460
18	X	0.25	0/202	0.39	0/276
18	x	0.25	0/202	0.41	0/276
19	Z	0.27	0/469	0.44	0/641
19	z	0.26	0/469	0.47	0/641
20	N	0.27	0/1751	0.53	0/2386
20	n	0.27	0/1751	0.51	0/2386
21	G	0.28	0/1725	0.57	1/2348 (0.0%)
21	g	0.27	0/1725	0.50	0/2348
22	R	0.28	0/1561	0.56	0/2110
22	r	0.27	0/1561	0.56	0/2110
23	S	0.27	0/1895	0.52	1/2579 (0.0%)
23	s	0.27	0/1902	0.49	0/2587
24	Y	0.28	0/1715	0.57	1/2338 (0.0%)
24	y	0.28	0/1715	0.53	0/2338
25	U	0.29	0/224	0.70	0/298
25	u	0.35	0/224	0.67	0/298
All	All	0.29	0/59273	0.54	13/80624 (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 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	98	LEU	CA-CB-CG	8.32	134.44	115.30
21	G	196	LEU	CA-CB-CG	7.56	132.68	115.30
6	e	79	LEU	CA-CB-CG	7.15	131.74	115.30
4	C	37	LEU	CA-CB-CG	5.88	128.84	115.30
14	O	298	LEU	CA-CB-CG	5.84	128.74	115.30

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 [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	47	76
2	b	482/484 (100%)	463 (96%)	18 (4%)	1 (0%)	47	76
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%)	22	50
4	c	447/449 (100%)	414 (93%)	29 (6%)	4 (1%)	17	44
5	D	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	41	70
5	d	346/348 (99%)	335 (97%)	10 (3%)	1 (0%)	41	70
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	34/36 (94%)	34 (100%)	0	0	100	100
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%)	4	11
13	m	30/32 (94%)	29 (97%)	0	1 (3%)	4	11
14	O	236/238 (99%)	208 (88%)	25 (11%)	3 (1%)	12	33
14	o	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	34	64
15	P	185/187 (99%)	169 (91%)	15 (8%)	1 (0%)	29	58
15	p	185/187 (99%)	172 (93%)	13 (7%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	3	10
16	t	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	3	10
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%)	29	58
20	n	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	58
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	29	58
21	g	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	29	58
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%)	19	47
23	s	239/243 (98%)	221 (92%)	16 (7%)	2 (1%)	19	47
24	Y	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	58
24	y	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	29	58
25	U	25/27 (93%)	25 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
All	All	7351/7456 (99%)	6934 (94%)	387 (5%)	30 (0%)	38	64

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%)	275 (100%)	1 (0%)	91	96
1	a	276/275 (100%)	274 (99%)	2 (1%)	84	94
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%)	349 (100%)	1 (0%)	92	97
4	c	350/350 (100%)	349 (100%)	1 (0%)	92	97
5	D	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	278 (100%)	1 (0%)	91	96
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	30 (97%)	1 (3%)	39	70
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%)	192 (98%)	3 (2%)	65	87
14	o	195/195 (100%)	194 (100%)	1 (0%)	88	95
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%)	49 (98%)	1 (2%)	55	82
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	170 (99%)	1 (1%)	86	95
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%)	157 (99%)	1 (1%)	86	95
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	188 (100%)	1 (0%)	88	95
23	s	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	167/167 (100%)	166 (99%)	1 (1%)	86	95
24	y	167/167 (100%)	165 (99%)	2 (1%)	71	90
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%)	5935 (100%)	18 (0%)	92	97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	d	180	ARG
24	y	149	GLN
24	y	76	LEU
22	R	270	LYS
4	c	406	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
20	n	170	ASN
15	p	109	ASN
1	a	181	ASN
8	h	69	ASN
1	a	92	HIS

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 monosaccharides 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$
40	LMK	C	527	-	38,39,53	1.48	2 (5%)	41,46,60	1.30	2 (4%)
33	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	3 (5%)
48	NEX	G	623	-	38,46,46	3.31	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	N	612	-	45,53,73	1.63	9 (20%)	52,89,113	2.14	11 (21%)
29	CLA	y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.97	17 (22%)
39	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.03	2 (4%)
29	CLA	y	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	16 (21%)
29	CLA	c	504	-	65,73,73	1.32	7 (10%)	76,113,113	2.05	19 (25%)
29	CLA	n	614	-	49,57,73	1.55	10 (20%)	55,93,113	2.30	18 (32%)
37	GOL	B	627	-	5,5,5	0.58	0	5,5,5	0.21	0
39	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
48	NEX	r	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.54	9 (18%)
45	CHL	y	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.20	8 (10%)
29	CLA	G	613	-	65,73,73	1.35	9 (13%)	76,113,113	2.02	18 (23%)
31	BCR	C	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	16 (28%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	13 (23%)
45	CHL	N	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.25	11 (15%)
51	SPH	y	625	-	19,20,20	0.64	0	18,21,21	1.10	1 (5%)
45	CHL	s	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.44	7 (15%)
39	LHG	S	624	-	44,44,48	0.41	0	47,50,54	1.10	3 (6%)
46	LUT	s	621	-	42,43,43	2.32	1 (2%)	51,60,60	1.99	14 (27%)
46	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.94	15 (29%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
29	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	21 (27%)
45	CHL	y	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.22	10 (13%)
49	LPX	S	625	-	29,29,29	0.99	2 (6%)	31,33,33	0.98	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	D	402	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	15 (19%)
45	CHL	G	605	21	48,56,74	0.96	2 (4%)	51,92,114	1.38	10 (19%)
45	CHL	n	608	-	50,58,74	0.90	2 (4%)	52,94,114	1.41	11 (21%)
30	PHO	A	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.15	4 (8%)
29	CLA	r	613	-	46,54,73	1.60	9 (19%)	53,90,113	2.19	15 (28%)
29	CLA	Y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
29	CLA	a	406	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	17 (22%)
29	CLA	R	610	-	60,68,73	1.42	9 (15%)	70,107,113	2.07	20 (28%)
29	CLA	r	610	-	60,68,73	1.40	10 (16%)	70,107,113	2.15	20 (28%)
36	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)
33	LMG	B	622	-	44,44,55	0.85	2 (4%)	52,52,63	1.06	3 (5%)
45	CHL	y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.22	10 (13%)
41	BCT	D	401	27	2,3,3	1.27	0	2,3,3	2.64	2 (100%)
29	CLA	s	603	-	65,73,73	1.38	10 (15%)	76,113,113	1.89	14 (18%)
29	CLA	R	609	-	60,68,73	1.42	7 (11%)	70,107,113	2.02	15 (21%)
29	CLA	r	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.02	14 (20%)
29	CLA	Y	604	-	65,73,73	1.35	9 (13%)	76,113,113	1.93	18 (23%)
29	CLA	C	506	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	19 (25%)
29	CLA	s	611	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
47	XAT	n	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	R	603	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	18 (25%)
39	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
33	LMG	b	622	-	44,44,55	0.85	3 (6%)	52,52,63	1.07	3 (5%)
38	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.03	3 (3%)
37	GOL	y	626	-	5,5,5	0.57	0	5,5,5	0.25	0
47	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
35	C7Z	B	620	-	43,43,43	5.41	26 (60%)	58,60,60	2.04	19 (32%)
45	CHL	g	601	21	66,74,74	0.82	3 (4%)	73,114,114	1.24	10 (13%)
29	CLA	S	605	-	50,58,73	1.58	9 (18%)	58,95,113	2.44	18 (31%)
45	CHL	Y	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.16	9 (12%)
29	CLA	C	507	52	65,73,73	1.37	7 (10%)	76,113,113	1.96	18 (23%)
31	BCR	C	515	-	41,41,41	1.84	4 (9%)	56,56,56	4.22	13 (23%)
38	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.05	3 (4%)
46	LUT	g	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.95	11 (21%)
36	DGA	b	623	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PHO	a	408	-	51,69,69	1.00	4 (7%)	47,99,99	1.15	6 (12%)
29	CLA	y	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
29	CLA	B	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	18 (23%)
29	CLA	C	510	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	16 (21%)
45	CHL	Y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.21	9 (12%)
29	CLA	S	603	-	65,73,73	1.39	10 (15%)	76,113,113	1.91	14 (18%)
39	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.03	3 (5%)
45	CHL	N	601	-	66,74,74	0.82	3 (4%)	73,114,114	1.17	8 (10%)
29	CLA	n	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.11	14 (26%)
29	CLA	G	602	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	18 (23%)
29	CLA	c	510	-	65,73,73	1.33	8 (12%)	76,113,113	2.03	16 (21%)
29	CLA	Y	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	13 (17%)
46	LUT	n	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.82	14 (27%)
29	CLA	B	609	-	65,73,73	1.34	8 (12%)	76,113,113	2.10	17 (22%)
29	CLA	Y	614	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	17 (22%)
29	CLA	G	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.18	12 (24%)
45	CHL	g	607	-	50,58,74	0.88	2 (4%)	52,94,114	1.41	10 (19%)
29	CLA	s	617	-	50,58,73	1.53	9 (18%)	58,95,113	2.27	19 (32%)
29	CLA	c	508	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	18 (23%)
43	HEM	F	101	7,6	41,50,50	1.55	3 (7%)	45,82,82	1.51	6 (13%)
29	CLA	B	608	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	16 (21%)
29	CLA	c	507	52	65,73,73	1.37	9 (13%)	76,113,113	1.97	19 (25%)
29	CLA	r	602	-	60,68,73	1.41	9 (15%)	70,107,113	2.03	17 (24%)
44	RRX	H	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.04	18 (31%)
29	CLA	c	509	-	65,73,73	1.32	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	C	508	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	16 (21%)
33	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	2 (3%)
45	CHL	g	608	-	44,52,74	0.99	3 (6%)	46,87,114	1.42	9 (19%)
36	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
47	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.70	16 (29%)
48	NEX	n	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	12 (24%)
38	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.04	3 (4%)
29	CLA	b	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	14 (18%)
37	GOL	b	625	-	5,5,5	0.58	0	5,5,5	0.28	0
42	PL9	d	405	-	55,55,55	1.21	4 (7%)	68,69,69	1.49	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	J	101	-	45,45,55	0.90	3 (6%)	53,53,63	1.00	2 (3%)
45	CHL	N	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.27	10 (13%)
46	LUT	N	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.92	13 (25%)
46	LUT	N	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.92	13 (25%)
29	CLA	s	614	-	55,63,73	1.46	7 (12%)	64,101,113	2.17	15 (23%)
45	CHL	g	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.23	10 (13%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	14 (25%)
29	CLA	n	611	-	49,57,73	1.56	9 (18%)	55,93,113	2.27	15 (27%)
32	SQD	c	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
32	SQD	A	412	-	50,51,54	0.84	0	59,62,65	0.94	3 (5%)
49	LPX	s	625	-	29,29,29	0.98	2 (6%)	31,33,33	0.98	1 (3%)
29	CLA	g	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.20	13 (25%)
29	CLA	g	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.27	17 (30%)
45	CHL	N	605	20	66,74,74	0.83	3 (4%)	73,114,114	1.20	10 (13%)
45	CHL	S	601	23	46,54,74	1.02	4 (8%)	49,90,114	1.35	9 (18%)
29	CLA	S	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.14	12 (23%)
29	CLA	s	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	16 (22%)
39	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
29	CLA	R	604	-	49,57,73	1.52	8 (16%)	55,93,113	2.33	18 (32%)
29	CLA	s	610	-	65,73,73	1.37	9 (13%)	76,113,113	1.97	19 (25%)
29	CLA	c	502	-	65,73,73	1.36	7 (10%)	76,113,113	2.13	16 (21%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.12	3 (5%)
29	CLA	G	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.30	17 (30%)
39	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.02	3 (5%)
46	LUT	R	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.16	14 (27%)
31	BCR	B	618	-	41,41,41	1.81	4 (9%)	56,56,56	4.29	15 (26%)
26	OEX	a	401	4,52,1	0,15,15	-	-	-	-	-
29	CLA	N	611	-	49,57,73	1.57	10 (20%)	55,93,113	2.22	15 (27%)
29	CLA	G	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	19 (25%)
29	CLA	c	506	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	19 (25%)
46	LUT	g	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	12 (23%)
29	CLA	b	604	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	18 (23%)
48	NEX	y	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	13 (26%)
29	CLA	b	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.16	19 (25%)
45	CHL	G	606	-	50,58,74	0.99	4 (8%)	52,94,114	1.38	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	N	608	-	50,58,74	0.89	2 (4%)	52,94,114	1.41	11 (21%)
29	CLA	s	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.40	18 (31%)
29	CLA	S	617	-	50,58,73	1.55	9 (18%)	58,95,113	2.25	16 (27%)
29	CLA	D	403	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	16 (21%)
45	CHL	G	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.19	10 (13%)
33	LMG	A	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.17	4 (7%)
29	CLA	B	615	-	65,73,73	1.34	8 (12%)	76,113,113	2.17	20 (26%)
45	CHL	R	607	-	50,58,74	0.96	3 (6%)	52,94,114	1.38	8 (15%)
45	CHL	r	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.36	9 (19%)
45	CHL	S	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.40	9 (19%)
29	CLA	y	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	19 (25%)
45	CHL	s	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.24	9 (13%)
29	CLA	B	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	14 (18%)
37	GOL	b	624	-	5,5,5	0.59	0	5,5,5	0.22	0
39	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
29	CLA	G	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.28	16 (29%)
45	CHL	N	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.17	9 (12%)
31	BCR	c	516	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	15 (26%)
47	XAT	R	621	-	39,47,47	0.69	1 (2%)	54,74,74	2.22	17 (31%)
29	CLA	n	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	20 (26%)
50	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
29	CLA	c	503	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	18 (23%)
29	CLA	C	505	-	65,73,73	1.36	9 (13%)	76,113,113	2.03	16 (21%)
29	CLA	r	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.28	17 (30%)
29	CLA	b	614	-	65,73,73	1.33	6 (9%)	76,113,113	2.00	18 (23%)
38	DGD	C	519	-	63,63,67	1.12	6 (9%)	77,77,81	1.06	4 (5%)
38	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.98	2 (2%)
29	CLA	g	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
41	BCT	d	401	27	2,3,3	1.26	0	2,3,3	2.67	2 (100%)
48	NEX	Y	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.80	11 (22%)
29	CLA	g	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
29	CLA	n	602	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	22 (28%)
33	LMG	c	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.10	3 (5%)
29	CLA	C	504	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
48	NEX	g	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.81	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	LUT	s	620	-	42,43,43	2.41	1 (2%)	51,60,60	2.12	16 (31%)
29	CLA	B	614	-	65,73,73	1.32	6 (9%)	76,113,113	2.01	18 (23%)
29	CLA	N	604	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	20 (26%)
33	LMG	h	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.09	2 (3%)
38	DGD	c	520	-	60,60,67	1.06	6 (10%)	74,74,81	0.98	2 (2%)
32	SQD	B	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	S	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.96	19 (25%)
45	CHL	s	606	-	44,52,74	1.01	3 (6%)	46,87,114	1.43	10 (21%)
31	BCR	C	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.43	12 (21%)
47	XAT	g	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.88	15 (27%)
36	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
45	CHL	S	608	-	61,69,74	0.87	3 (4%)	67,108,114	1.26	10 (14%)
29	CLA	Y	613	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	20 (26%)
29	CLA	S	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.04	17 (24%)
29	CLA	n	613	-	65,73,73	1.36	10 (15%)	76,113,113	2.01	16 (21%)
47	XAT	r	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.18	19 (35%)
31	BCR	b	619	-	41,41,41	1.83	4 (9%)	56,56,56	4.38	17 (30%)
48	NEX	s	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.72	11 (22%)
33	LMG	D	411	-	46,46,55	0.92	4 (8%)	54,54,63	1.11	2 (3%)
31	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.36	18 (32%)
45	CHL	S	607	-	43,51,74	1.01	3 (6%)	45,86,114	1.45	8 (17%)
45	CHL	n	605	20	66,74,74	0.84	3 (4%)	73,114,114	1.18	10 (13%)
32	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.89	2 (3%)
47	XAT	N	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.96	13 (24%)
29	CLA	S	614	-	55,63,73	1.47	8 (14%)	64,101,113	2.12	15 (23%)
30	PHO	A	409	-	51,69,69	1.00	3 (5%)	47,99,99	1.20	3 (6%)
38	DGD	c	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
39	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.00	2 (4%)
29	CLA	r	603	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	17 (24%)
45	CHL	G	601	21	66,74,74	0.81	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	c	512	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	19 (25%)
29	CLA	b	608	-	65,73,73	1.34	6 (9%)	76,113,113	2.05	17 (22%)
29	CLA	B	610	-	65,73,73	1.34	8 (12%)	76,113,113	1.99	16 (21%)
39	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.11	2 (3%)
29	CLA	n	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	N	614	-	49,57,73	1.55	8 (16%)	55,93,113	2.26	16 (29%)
46	LUT	G	621	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	13 (25%)
29	CLA	g	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.19	13 (26%)
48	NEX	S	622	-	38,46,46	3.28	9 (23%)	50,70,70	1.80	12 (24%)
29	CLA	C	512	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	17 (22%)
45	CHL	Y	609	-	66,74,74	0.81	3 (4%)	73,114,114	1.23	12 (16%)
29	CLA	b	613	-	65,73,73	1.32	8 (12%)	76,113,113	1.96	17 (22%)
29	CLA	C	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.11	19 (25%)
29	CLA	b	612	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
39	LHG	s	624	-	44,44,48	0.42	0	47,50,54	1.11	3 (6%)
29	CLA	S	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	15 (19%)
29	CLA	B	612	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
29	CLA	c	511	-	65,73,73	1.34	7 (10%)	76,113,113	2.08	20 (26%)
45	CHL	G	607	-	50,58,74	0.87	2 (4%)	52,94,114	1.42	11 (21%)
39	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
29	CLA	G	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.19	15 (28%)
29	CLA	N	613	-	65,73,73	1.37	10 (15%)	76,113,113	1.99	16 (21%)
29	CLA	N	610	-	65,73,73	1.36	8 (12%)	76,113,113	2.01	18 (23%)
50	3PH	i	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
29	CLA	b	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
29	CLA	c	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	18 (23%)
29	CLA	y	604	-	65,73,73	1.34	6 (9%)	76,113,113	1.95	18 (23%)
29	CLA	a	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.01	19 (25%)
29	CLA	r	612	-	60,68,73	1.43	9 (15%)	70,107,113	2.03	17 (24%)
29	CLA	Y	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	19 (25%)
39	LHG	l	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
29	CLA	C	502	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	16 (21%)
29	CLA	B	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	15 (19%)
29	CLA	s	613	-	55,63,73	1.49	8 (14%)	64,101,113	2.32	16 (25%)
29	CLA	A	406	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	16 (21%)
29	CLA	a	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.11	17 (24%)
29	CLA	C	513	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	19 (25%)
35	C7Z	b	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.05	17 (29%)
29	CLA	C	503	-	65,73,73	1.36	9 (13%)	76,113,113	2.02	19 (25%)
29	CLA	a	407	-	49,57,73	1.56	8 (16%)	55,93,113	2.24	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	R	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.33	8 (17%)
45	CHL	y	605	24	46,54,74	1.00	2 (4%)	49,90,114	1.38	8 (16%)
29	CLA	R	613	-	46,54,73	1.61	8 (17%)	53,90,113	2.18	14 (26%)
29	CLA	S	604	-	55,63,73	1.45	7 (12%)	64,101,113	2.18	17 (26%)
29	CLA	c	513	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
29	CLA	y	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	21 (27%)
29	CLA	R	608	-	60,68,73	1.43	9 (15%)	70,107,113	2.01	16 (22%)
46	LUT	n	621	-	42,43,43	2.33	1 (2%)	51,60,60	1.85	11 (21%)
29	CLA	d	402	-	65,73,73	1.35	8 (12%)	76,113,113	1.90	14 (18%)
33	LMG	j	101	-	45,45,55	0.89	3 (6%)	53,53,63	1.04	2 (3%)
29	CLA	C	501	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	18 (23%)
29	CLA	S	613	-	55,63,73	1.48	8 (14%)	64,101,113	2.33	16 (25%)
29	CLA	y	608	-	50,58,73	1.55	8 (16%)	58,95,113	2.22	18 (31%)
45	CHL	n	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.33	13 (17%)
29	CLA	B	605	-	65,73,73	1.39	8 (12%)	76,113,113	2.10	15 (19%)
46	LUT	G	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.96	12 (23%)
45	CHL	Y	605	24	46,54,74	1.01	3 (6%)	49,90,114	1.41	10 (20%)
29	CLA	R	602	-	60,68,73	1.42	9 (15%)	70,107,113	2.10	18 (25%)
48	NEX	R	622	-	38,46,46	3.42	10 (26%)	50,70,70	1.69	11 (22%)
29	CLA	s	604	-	55,63,73	1.48	7 (12%)	64,101,113	2.07	14 (21%)
46	LUT	S	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.09	12 (23%)
45	CHL	G	608	-	44,52,74	1.00	3 (6%)	46,87,114	1.41	9 (19%)
29	CLA	Y	603	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	19 (25%)
31	BCR	b	618	-	41,41,41	1.82	4 (9%)	56,56,56	4.30	15 (26%)
32	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
45	CHL	g	606	-	50,58,74	0.89	2 (4%)	52,94,114	1.39	9 (17%)
45	CHL	n	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.21	8 (10%)
29	CLA	g	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
29	CLA	A	410	-	60,68,73	1.41	9 (15%)	70,107,113	2.10	16 (22%)
46	LUT	Y	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
39	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
46	LUT	r	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.20	15 (29%)
29	CLA	b	607	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	19 (25%)
29	CLA	A	407	-	49,57,73	1.56	7 (14%)	55,93,113	2.25	16 (29%)
29	CLA	n	610	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.07	2 (4%)
39	LHG	d	410	-	38,38,48	0.41	0	41,44,54	1.15	3 (7%)
29	CLA	Y	608	-	50,58,73	1.55	8 (16%)	58,95,113	2.22	19 (32%)
29	CLA	b	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.97	16 (21%)
29	CLA	B	602	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	17 (22%)
46	LUT	y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.03	12 (23%)
29	CLA	C	509	-	65,73,73	1.33	6 (9%)	76,113,113	2.04	19 (25%)
45	CHL	g	605	21	48,56,74	0.95	3 (6%)	51,92,114	1.41	10 (19%)
29	CLA	y	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.02	19 (25%)
29	CLA	c	505	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	15 (19%)
45	CHL	r	607	-	50,58,74	0.94	3 (6%)	52,94,114	1.37	9 (17%)
45	CHL	n	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.28	10 (13%)
29	CLA	b	602	-	65,73,73	1.37	9 (13%)	76,113,113	1.98	17 (22%)
29	CLA	A	405	-	65,73,73	1.32	6 (9%)	76,113,113	2.03	18 (23%)
30	PHO	a	409	-	51,69,69	0.98	3 (5%)	47,99,99	1.24	5 (10%)
45	CHL	y	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.23	12 (16%)
29	CLA	g	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	18 (23%)
29	CLA	y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
31	BCR	A	411	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	15 (26%)
29	CLA	S	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.03	17 (24%)
26	OEX	A	401	52,1	0,15,15	-	-	-	-	-
39	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
43	HEM	f	101	7,6	41,50,50	1.54	4 (9%)	45,82,82	1.55	7 (15%)
46	LUT	Y	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.95	14 (27%)
29	CLA	G	610	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	18 (23%)
48	NEX	N	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.76	14 (28%)
44	RRX	h	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.03	19 (33%)
31	BCR	D	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.04	17 (30%)
29	CLA	N	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	20 (26%)
29	CLA	b	610	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	15 (19%)
45	CHL	Y	601	24	66,74,74	0.80	2 (3%)	73,114,114	1.20	9 (12%)
31	BCR	c	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	13 (23%)
29	CLA	R	612	-	60,68,73	1.42	8 (13%)	70,107,113	2.07	16 (22%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	14 (25%)
29	CLA	r	611	-	46,54,73	1.61	10 (21%)	53,90,113	2.12	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LMK	c	627	-	38,39,53	1.48	2 (5%)	41,46,60	1.33	2 (4%)
51	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.10	1 (5%)
29	CLA	B	613	-	65,73,73	1.32	7 (10%)	76,113,113	1.95	16 (21%)
29	CLA	b	609	-	65,73,73	1.34	7 (10%)	76,113,113	2.14	17 (22%)
39	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
45	CHL	n	606	-	66,74,74	0.89	4 (6%)	73,114,114	1.17	9 (12%)
29	CLA	d	403	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	16 (21%)
29	CLA	r	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	15 (21%)
29	CLA	b	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	18 (23%)
29	CLA	s	602	-	60,68,73	1.38	8 (13%)	70,107,113	2.05	17 (24%)
47	XAT	y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.73	19 (35%)
50	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
33	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.07	2 (3%)
46	LUT	S	621	-	42,43,43	2.31	1 (2%)	51,60,60	1.97	15 (29%)
29	CLA	b	605	-	65,73,73	1.38	8 (12%)	76,113,113	2.08	16 (21%)
29	CLA	B	604	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	17 (22%)
29	CLA	b	617	-	65,73,73	1.35	7 (10%)	76,113,113	4.30	17 (22%)
29	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
45	CHL	s	601	23	46,54,74	1.03	4 (8%)	49,90,114	1.37	9 (18%)
29	CLA	B	617	-	65,73,73	1.34	8 (12%)	76,113,113	4.31	17 (22%)
29	CLA	s	612	-	45,53,73	1.61	8 (17%)	52,89,113	2.16	15 (28%)
38	DGD	C	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
29	CLA	B	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	18 (23%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.11	17 (30%)
29	CLA	B	616	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	15 (19%)
29	CLA	R	611	-	46,54,73	1.62	10 (21%)	53,90,113	2.10	14 (26%)
31	BCR	c	517	-	41,41,41	1.81	4 (9%)	56,56,56	4.10	19 (33%)
29	CLA	g	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
42	PL9	D	405	-	55,55,55	1.17	5 (9%)	68,69,69	1.50	13 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LMK	C	527	-	1/1/6/6	10/46/46/60	-
33	LMG	C	521	-	-	18/46/66/70	0/1/1/1
48	NEX	G	623	-	-	3/27/83/83	0/3/3/3
29	CLA	N	612	-	1/1/11/20	5/13/91/115	-
29	CLA	y	610	-	1/1/15/20	24/37/115/115	-
39	LHG	C	525	-	-	28/51/51/53	-
29	CLA	y	614	-	1/1/15/20	15/37/115/115	-
29	CLA	c	504	-	1/1/15/20	17/37/115/115	-
29	CLA	n	614	-	1/1/11/20	5/18/96/115	-
37	GOL	B	627	-	-	0/4/4/4	-
39	LHG	D	409	-	-	30/53/53/53	-
48	NEX	r	623	-	-	7/27/83/83	0/3/3/3
45	CHL	y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	G	613	-	1/1/15/20	20/37/115/115	-
45	CHL	N	609	-	4/4/20/26	7/39/137/137	-
31	BCR	C	516	-	-	15/29/63/63	0/2/2/2
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
51	SPH	y	625	-	-	11/21/21/21	-
45	CHL	s	607	-	4/4/15/26	1/12/110/137	-
39	LHG	S	624	-	-	28/49/49/53	-
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
46	LUT	y	620	-	-	4/29/67/67	0/2/2/2
32	SQD	a	412	-	-	13/46/66/69	0/1/1/1
29	CLA	N	603	-	1/1/15/20	14/37/115/115	-
45	CHL	y	606	-	4/4/20/26	8/39/137/137	-
49	LPX	S	625	-	-	10/31/31/31	-
29	CLA	D	402	-	1/1/15/20	11/37/115/115	-
45	CHL	G	605	21	3/3/16/26	1/18/116/137	-
45	CHL	n	608	-	3/3/16/26	3/20/118/137	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	r	613	-	1/1/11/20	9/15/93/115	-
29	CLA	Y	610	-	1/1/15/20	22/37/115/115	-
29	CLA	a	406	-	1/1/15/20	13/37/115/115	-
29	CLA	R	610	-	1/1/14/20	10/31/109/115	-
29	CLA	r	610	-	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGA	B	625	-	-	24/45/45/45	-
33	LMG	B	622	-	-	11/39/59/70	0/1/1/1
45	CHL	y	607	-	4/4/20/26	5/39/137/137	-
29	CLA	s	603	-	1/1/15/20	15/37/115/115	-
29	CLA	R	609	-	1/1/14/20	15/31/109/115	-
29	CLA	r	609	-	1/1/14/20	18/31/109/115	-
29	CLA	Y	604	-	1/1/15/20	18/37/115/115	-
29	CLA	C	506	-	1/1/15/20	21/37/115/115	-
29	CLA	s	611	-	1/1/15/20	11/37/115/115	-
47	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	R	603	-	1/1/14/20	16/31/109/115	-
39	LHG	L	101	-	-	30/53/53/53	-
33	LMG	b	622	-	-	11/39/59/70	0/1/1/1
38	DGD	c	519	-	-	21/51/91/95	0/2/2/2
37	GOL	y	626	-	-	0/4/4/4	-
47	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
35	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
45	CHL	g	601	21	4/4/20/26	12/39/137/137	-
29	CLA	S	605	-	1/1/12/20	12/19/97/115	-
45	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
29	CLA	C	507	52	1/1/15/20	17/37/115/115	-
31	BCR	C	515	-	-	11/29/63/63	0/2/2/2
38	DGD	c	518	-	-	11/44/84/95	0/2/2/2
46	LUT	g	620	-	-	3/29/67/67	0/2/2/2
36	DGA	b	623	-	-	26/45/45/45	-
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
29	CLA	y	611	-	1/1/15/20	15/37/115/115	-
29	CLA	B	607	-	1/1/15/20	12/37/115/115	-
29	CLA	C	510	-	1/1/15/20	14/37/115/115	-
45	CHL	Y	607	-	4/4/20/26	4/39/137/137	-
29	CLA	S	603	-	1/1/15/20	15/37/115/115	-
39	LHG	Y	624	-	-	31/53/53/53	-
45	CHL	N	601	-	4/4/20/26	5/39/137/137	-
29	CLA	n	612	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	602	-	1/1/15/20	21/37/115/115	-
29	CLA	c	510	-	1/1/15/20	12/37/115/115	-
29	CLA	Y	611	-	1/1/15/20	17/37/115/115	-
46	LUT	n	620	-	-	6/29/67/67	0/2/2/2
29	CLA	B	609	-	1/1/15/20	14/37/115/115	-
29	CLA	Y	614	-	1/1/15/20	13/37/115/115	-
29	CLA	G	612	-	1/1/10/20	4/11/89/115	-
45	CHL	g	607	-	3/3/16/26	3/20/118/137	-
29	CLA	s	617	-	1/1/12/20	9/19/97/115	-
29	CLA	c	508	-	1/1/15/20	12/37/115/115	-
43	HEM	F	101	7,6	-	2/12/54/54	-
29	CLA	B	608	-	1/1/15/20	25/37/115/115	-
29	CLA	c	507	52	1/1/15/20	19/37/115/115	-
29	CLA	r	602	-	1/1/14/20	9/31/109/115	-
44	RRX	H	101	-	1/1/11/25	9/29/65/65	0/2/2/2
29	CLA	c	509	-	1/1/15/20	11/37/115/115	-
29	CLA	C	508	-	1/1/15/20	12/37/115/115	-
33	LMG	d	411	-	-	12/41/61/70	0/1/1/1
45	CHL	g	608	-	3/3/15/26	1/13/111/137	-
36	DGA	c	524	-	-	19/45/45/45	-
47	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
48	NEX	n	623	-	-	2/27/83/83	0/3/3/3
38	DGD	C	518	-	-	8/44/84/95	0/2/2/2
29	CLA	b	606	-	1/1/15/20	12/37/115/115	-
37	GOL	b	625	-	-	1/4/4/4	-
42	PL9	d	405	-	-	10/53/73/73	0/1/1/1
33	LMG	J	101	-	-	12/40/60/70	0/1/1/1
45	CHL	N	607	-	4/4/20/26	7/39/137/137	-
46	LUT	N	620	-	-	3/29/67/67	0/2/2/2
46	LUT	N	621	-	-	2/29/67/67	0/2/2/2
29	CLA	s	614	-	1/1/13/20	8/25/103/115	-
45	CHL	g	609	-	4/4/20/26	6/39/137/137	-
31	BCR	C	517	-	-	8/29/63/63	0/2/2/2
29	CLA	n	611	-	1/1/11/20	10/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	c	626	-	-	16/49/69/69	0/1/1/1
32	SQD	A	412	-	-	12/46/66/69	0/1/1/1
49	LPX	s	625	-	-	10/31/31/31	-
29	CLA	g	611	-	1/1/11/20	4/13/91/115	-
29	CLA	g	604	-	1/1/11/20	12/18/96/115	-
45	CHL	N	605	20	4/4/20/26	10/39/137/137	-
45	CHL	S	601	23	3/3/16/26	3/15/113/137	-
29	CLA	S	612	-	1/1/11/20	5/13/91/115	-
29	CLA	s	609	-	1/1/14/20	14/31/109/115	-
39	LHG	G	630	-	-	31/53/53/53	-
29	CLA	R	604	-	1/1/11/20	12/18/96/115	-
29	CLA	s	610	-	1/1/15/20	20/37/115/115	-
29	CLA	c	502	-	1/1/15/20	20/37/115/115	-
33	LMG	a	413	-	-	13/43/63/70	0/1/1/1
29	CLA	G	604	-	1/1/11/20	8/18/96/115	-
39	LHG	y	624	-	-	30/53/53/53	-
46	LUT	R	620	-	-	8/29/67/67	0/2/2/2
31	BCR	B	618	-	-	13/29/63/63	0/2/2/2
29	CLA	N	611	-	1/1/11/20	10/18/96/115	-
29	CLA	G	603	-	1/1/15/20	18/37/115/115	-
29	CLA	c	506	-	1/1/15/20	22/37/115/115	-
46	LUT	g	621	-	-	2/29/67/67	0/2/2/2
29	CLA	b	604	-	1/1/15/20	14/37/115/115	-
48	NEX	y	623	-	-	3/27/83/83	0/3/3/3
29	CLA	b	615	-	1/1/15/20	12/37/115/115	-
45	CHL	G	606	-	4/4/16/26	5/20/118/137	-
45	CHL	N	608	-	3/3/16/26	3/20/118/137	-
29	CLA	s	605	-	1/1/12/20	8/19/97/115	-
29	CLA	S	617	-	1/1/12/20	10/19/97/115	-
29	CLA	D	403	-	1/1/15/20	12/37/115/115	-
45	CHL	G	609	-	4/4/20/26	9/39/137/137	-
33	LMG	A	413	-	-	14/43/63/70	0/1/1/1
29	CLA	B	615	-	1/1/15/20	8/37/115/115	-
45	CHL	R	607	-	3/3/16/26	5/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	r	606	-	3/3/15/26	1/13/111/137	-
45	CHL	S	606	-	3/3/15/26	0/13/111/137	-
29	CLA	y	613	-	1/1/15/20	19/37/115/115	-
45	CHL	s	608	-	4/4/19/26	1/33/131/137	-
29	CLA	B	606	-	1/1/15/20	12/37/115/115	-
37	GOL	b	624	-	-	0/4/4/4	-
39	LHG	g	624	-	-	28/53/53/53	-
29	CLA	G	614	-	1/1/11/20	10/18/96/115	-
45	CHL	N	606	-	4/4/20/26	4/39/137/137	-
31	BCR	c	516	-	-	13/29/63/63	0/2/2/2
47	XAT	R	621	-	1/1/12/26	11/31/93/93	0/4/4/4
29	CLA	n	604	-	1/1/15/20	16/37/115/115	-
50	3PH	S	626	-	-	19/49/49/49	-
29	CLA	c	503	-	1/1/15/20	20/37/115/115	-
29	CLA	C	505	-	1/1/15/20	12/37/115/115	-
29	CLA	r	604	-	1/1/11/20	12/18/96/115	-
29	CLA	b	614	-	1/1/15/20	10/37/115/115	-
38	DGD	C	519	-	-	19/51/91/95	0/2/2/2
38	DGD	C	520	-	-	12/48/88/95	0/2/2/2
29	CLA	g	614	-	1/1/11/20	9/18/96/115	-
48	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
29	CLA	g	613	-	1/1/15/20	21/37/115/115	-
29	CLA	n	602	-	1/1/15/20	16/37/115/115	-
33	LMG	c	521	-	-	18/46/66/70	0/1/1/1
29	CLA	C	504	-	1/1/15/20	14/37/115/115	-
48	NEX	g	623	-	-	3/27/83/83	0/3/3/3
46	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
29	CLA	B	614	-	1/1/15/20	12/37/115/115	-
29	CLA	N	604	-	1/1/15/20	19/37/115/115	-
33	LMG	h	102	-	-	14/43/63/70	0/1/1/1
38	DGD	c	520	-	-	12/48/88/95	0/2/2/2
32	SQD	B	621	-	-	19/49/69/69	0/1/1/1
29	CLA	S	610	-	1/1/15/20	11/37/115/115	-
45	CHL	s	606	-	3/3/15/26	1/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	514	-	-	11/29/63/63	0/2/2/2
47	XAT	g	622	-	2/2/12/26	0/31/93/93	0/4/4/4
36	DGA	C	524	-	-	18/45/45/45	-
45	CHL	S	608	-	4/4/19/26	2/33/131/137	-
29	CLA	Y	613	-	1/1/15/20	21/37/115/115	-
29	CLA	S	609	-	1/1/14/20	8/31/109/115	-
29	CLA	n	613	-	1/1/15/20	14/37/115/115	-
47	XAT	r	622	-	1/1/12/26	11/31/93/93	0/4/4/4
31	BCR	b	619	-	-	8/29/63/63	0/2/2/2
48	NEX	s	623	-	-	13/27/83/83	0/3/3/3
33	LMG	D	411	-	-	8/41/61/70	0/1/1/1
31	BCR	B	619	-	-	11/29/63/63	0/2/2/2
45	CHL	S	607	-	4/4/15/26	1/12/110/137	-
45	CHL	n	605	20	4/4/20/26	8/39/137/137	-
32	SQD	C	526	-	-	19/49/69/69	0/1/1/1
47	XAT	N	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	S	614	-	1/1/13/20	8/25/103/115	-
30	PHO	A	409	-	-	10/37/103/103	0/5/6/6
38	DGD	c	523	-	-	18/55/95/95	0/2/2/2
39	LHG	c	625	-	-	27/51/51/53	-
29	CLA	r	603	-	1/1/14/20	17/31/109/115	-
45	CHL	G	601	21	4/4/20/26	8/39/137/137	-
29	CLA	c	512	-	1/1/15/20	19/37/115/115	-
29	CLA	b	608	-	1/1/15/20	25/37/115/115	-
29	CLA	B	610	-	1/1/15/20	15/37/115/115	-
39	LHG	N	624	-	-	30/53/53/53	-
29	CLA	n	603	-	1/1/15/20	22/37/115/115	-
29	CLA	N	614	-	1/1/11/20	7/18/96/115	-
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
29	CLA	g	612	-	1/1/10/20	4/11/89/115	-
48	NEX	S	622	-	-	11/27/83/83	0/3/3/3
29	CLA	C	512	-	1/1/15/20	17/37/115/115	-
45	CHL	Y	609	-	4/4/20/26	7/39/137/137	-
29	CLA	b	613	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	511	-	1/1/15/20	15/37/115/115	-
29	CLA	b	612	-	1/1/15/20	19/37/115/115	-
39	LHG	s	624	-	-	31/49/49/53	-
29	CLA	S	611	-	1/1/15/20	12/37/115/115	-
29	CLA	B	612	-	1/1/15/20	21/37/115/115	-
29	CLA	c	511	-	1/1/15/20	13/37/115/115	-
45	CHL	G	607	-	3/3/16/26	3/20/118/137	-
39	LHG	D	408	-	-	30/48/48/53	-
29	CLA	G	611	-	1/1/11/20	5/13/91/115	-
29	CLA	N	613	-	1/1/15/20	19/37/115/115	-
29	CLA	N	610	-	1/1/15/20	8/37/115/115	-
50	3PH	i	101	-	-	20/49/49/49	-
29	CLA	b	611	-	1/1/15/20	9/37/115/115	-
29	CLA	c	501	-	1/1/15/20	11/37/115/115	-
29	CLA	y	604	-	1/1/15/20	20/37/115/115	-
29	CLA	a	405	-	1/1/15/20	14/37/115/115	-
29	CLA	r	612	-	1/1/14/20	12/31/109/115	-
29	CLA	Y	602	-	1/1/15/20	15/37/115/115	-
39	LHG	l	101	-	-	29/53/53/53	-
29	CLA	C	502	-	1/1/15/20	14/37/115/115	-
29	CLA	B	611	-	1/1/15/20	9/37/115/115	-
29	CLA	s	613	-	1/1/13/20	10/25/103/115	-
29	CLA	A	406	-	1/1/15/20	13/37/115/115	-
29	CLA	a	410	-	1/1/14/20	9/31/109/115	-
29	CLA	C	513	-	1/1/15/20	19/37/115/115	-
35	C7Z	b	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	C	503	-	1/1/15/20	19/37/115/115	-
29	CLA	a	407	-	1/1/11/20	4/18/96/115	-
45	CHL	R	606	-	3/3/15/26	4/13/111/137	-
45	CHL	y	605	24	3/3/16/26	3/15/113/137	-
29	CLA	R	613	-	1/1/11/20	8/15/93/115	-
29	CLA	S	604	-	1/1/13/20	9/25/103/115	-
29	CLA	c	513	-	1/1/15/20	18/37/115/115	-
29	CLA	y	602	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	R	608	-	1/1/14/20	16/31/109/115	-
46	LUT	n	621	-	-	4/29/67/67	0/2/2/2
29	CLA	d	402	-	1/1/15/20	13/37/115/115	-
33	LMG	j	101	-	-	12/40/60/70	0/1/1/1
29	CLA	C	501	-	1/1/15/20	18/37/115/115	-
29	CLA	S	613	-	1/1/13/20	10/25/103/115	-
29	CLA	y	608	-	1/1/12/20	8/19/97/115	-
45	CHL	n	609	-	4/4/20/26	7/39/137/137	-
29	CLA	B	605	-	1/1/15/20	18/37/115/115	-
46	LUT	G	620	-	-	6/29/67/67	0/2/2/2
45	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
29	CLA	R	602	-	1/1/14/20	13/31/109/115	-
48	NEX	R	622	-	-	8/27/83/83	0/3/3/3
29	CLA	s	604	-	1/1/13/20	12/25/103/115	-
46	LUT	S	620	-	1/1/12/27	4/29/67/67	0/2/2/2
45	CHL	G	608	-	3/3/15/26	0/13/111/137	-
29	CLA	Y	603	-	1/1/15/20	15/37/115/115	-
31	BCR	b	618	-	-	13/29/63/63	0/2/2/2
32	SQD	b	621	-	-	19/49/69/69	0/1/1/1
45	CHL	g	606	-	3/3/16/26	5/20/118/137	-
45	CHL	n	601	-	4/4/20/26	10/39/137/137	-
29	CLA	g	602	-	1/1/15/20	18/37/115/115	-
29	CLA	A	410	-	1/1/14/20	10/31/109/115	-
46	LUT	Y	620	-	-	4/29/67/67	0/2/2/2
39	LHG	d	408	-	-	29/48/48/53	-
46	LUT	r	620	-	-	9/29/67/67	0/2/2/2
29	CLA	b	607	-	1/1/15/20	14/37/115/115	-
29	CLA	A	407	-	1/1/11/20	4/18/96/115	-
29	CLA	n	610	-	1/1/15/20	12/37/115/115	-
39	LHG	D	410	-	-	26/43/43/53	-
39	LHG	d	410	-	-	33/43/43/53	-
29	CLA	Y	608	-	1/1/12/20	6/19/97/115	-
29	CLA	b	616	-	1/1/15/20	10/37/115/115	-
29	CLA	B	602	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	LUT	y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	C	509	-	1/1/15/20	10/37/115/115	-
45	CHL	g	605	21	3/3/16/26	4/18/116/137	-
29	CLA	y	603	-	1/1/15/20	13/37/115/115	-
29	CLA	c	505	-	1/1/15/20	15/37/115/115	-
45	CHL	r	607	-	3/3/16/26	8/20/118/137	-
45	CHL	n	607	-	4/4/20/26	10/39/137/137	-
29	CLA	b	602	-	1/1/15/20	21/37/115/115	-
29	CLA	A	405	-	1/1/15/20	16/37/115/115	-
30	PHO	a	409	-	-	9/37/103/103	0/5/6/6
45	CHL	y	609	-	4/4/20/26	7/39/137/137	-
29	CLA	g	603	-	1/1/15/20	17/37/115/115	-
29	CLA	y	612	-	1/1/15/20	11/37/115/115	-
31	BCR	A	411	-	-	11/29/63/63	0/2/2/2
29	CLA	S	602	-	1/1/14/20	12/31/109/115	-
39	LHG	d	409	-	-	29/53/53/53	-
43	HEM	f	101	7,6	-	2/12/54/54	-
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	G	610	-	1/1/15/20	13/37/115/115	-
48	NEX	N	623	-	-	2/27/83/83	0/3/3/3
44	RRX	h	101	-	1/1/11/25	10/29/65/65	0/2/2/2
31	BCR	D	404	-	-	11/29/63/63	0/2/2/2
29	CLA	N	602	-	1/1/15/20	17/37/115/115	-
29	CLA	b	610	-	1/1/15/20	15/37/115/115	-
45	CHL	Y	601	24	4/4/20/26	8/39/137/137	-
31	BCR	c	515	-	-	11/29/63/63	0/2/2/2
29	CLA	R	612	-	1/1/14/20	13/31/109/115	-
31	BCR	c	514	-	-	12/29/63/63	0/2/2/2
29	CLA	r	611	-	1/1/11/20	5/15/93/115	-
40	LMK	c	627	-	1/1/6/6	9/46/46/60	-
51	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	B	613	-	1/1/15/20	15/37/115/115	-
29	CLA	b	609	-	1/1/15/20	15/37/115/115	-
39	LHG	n	624	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	n	606	-	4/4/20/26	5/39/137/137	-
29	CLA	d	403	-	1/1/15/20	13/37/115/115	-
29	CLA	r	608	-	1/1/14/20	13/31/109/115	-
29	CLA	b	603	-	1/1/15/20	16/37/115/115	-
29	CLA	s	602	-	1/1/14/20	10/31/109/115	-
47	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
50	3PH	s	626	-	-	27/49/49/49	-
33	LMG	H	102	-	-	12/43/63/70	0/1/1/1
46	LUT	S	621	-	-	4/29/67/67	0/2/2/2
29	CLA	b	605	-	1/1/15/20	20/37/115/115	-
29	CLA	B	604	-	1/1/15/20	17/37/115/115	-
29	CLA	b	617	-	1/1/15/20	16/37/115/115	-
29	CLA	Y	612	-	1/1/15/20	10/37/115/115	-
45	CHL	s	601	23	3/3/16/26	7/15/113/137	-
29	CLA	B	617	-	1/1/15/20	17/37/115/115	-
29	CLA	s	612	-	1/1/11/20	6/13/91/115	-
38	DGD	C	523	-	-	17/55/95/95	0/2/2/2
29	CLA	B	603	-	1/1/15/20	16/37/115/115	-
31	BCR	d	404	-	-	12/29/63/63	0/2/2/2
29	CLA	B	616	-	1/1/15/20	10/37/115/115	-
29	CLA	R	611	-	1/1/11/20	5/15/93/115	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	g	610	-	1/1/15/20	11/37/115/115	-
42	PL9	D	405	-	-	12/53/73/73	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	620	C7Z	C25-C26	16.16	1.62	1.34
35	b	620	C7Z	C25-C26	16.13	1.62	1.34
44	h	101	RRX	C26-C25	15.49	1.61	1.34
44	H	101	RRX	C26-C25	15.48	1.61	1.34
35	b	620	C7Z	C5-C6	15.32	1.61	1.34

The worst 5 of 4140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	617	CLA	C4-C3-C5	-22.25	77.84	115.27
29	b	617	CLA	C4-C3-C5	-22.23	77.87	115.27
29	b	617	CLA	C5-C3-C2	18.79	159.15	121.12
29	B	617	CLA	C5-C3-C2	18.73	159.01	121.12
31	C	517	BCR	C10-C11-C12	17.71	178.49	123.22

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

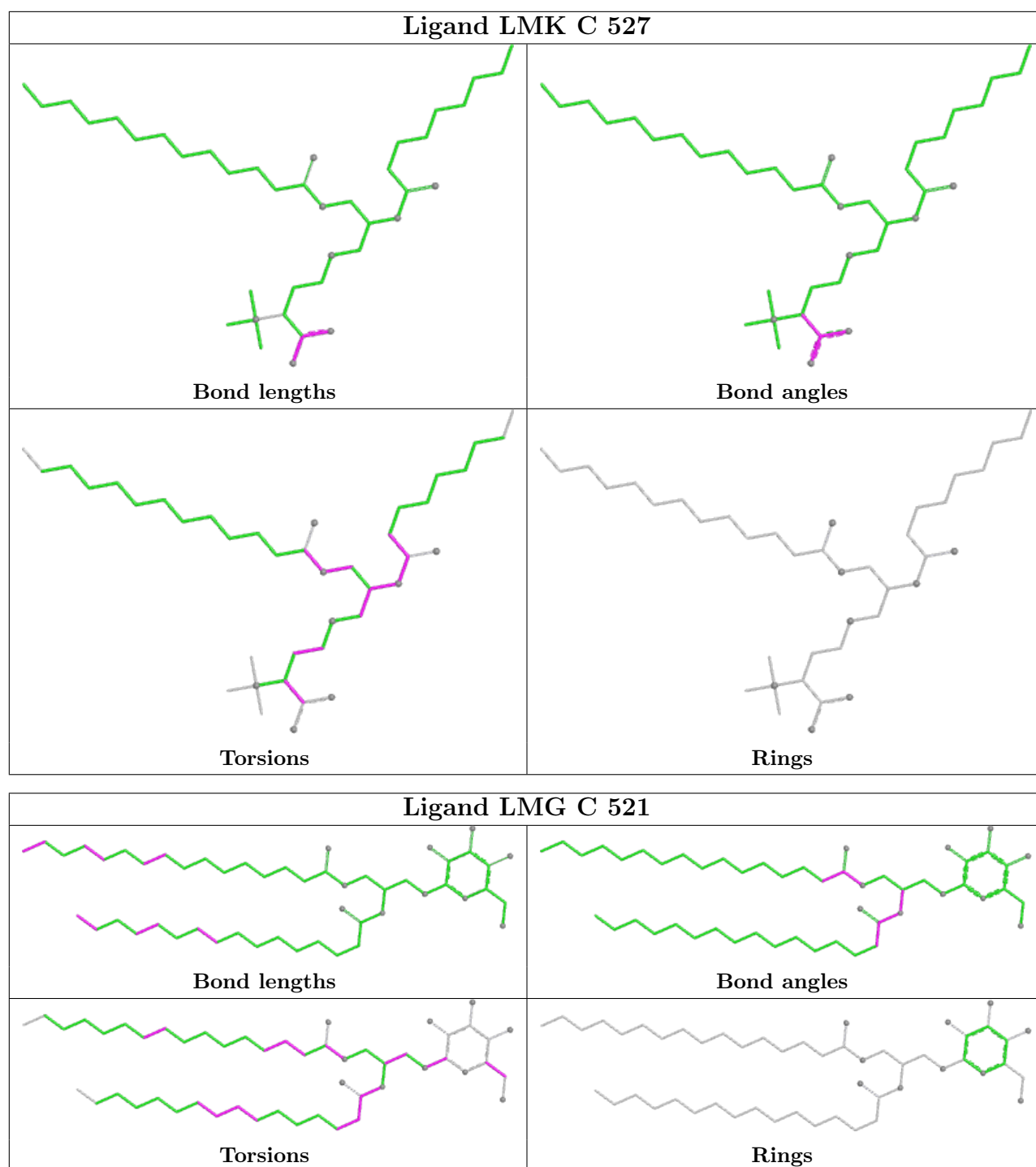
5 of 3918 torsion outliers are listed below:

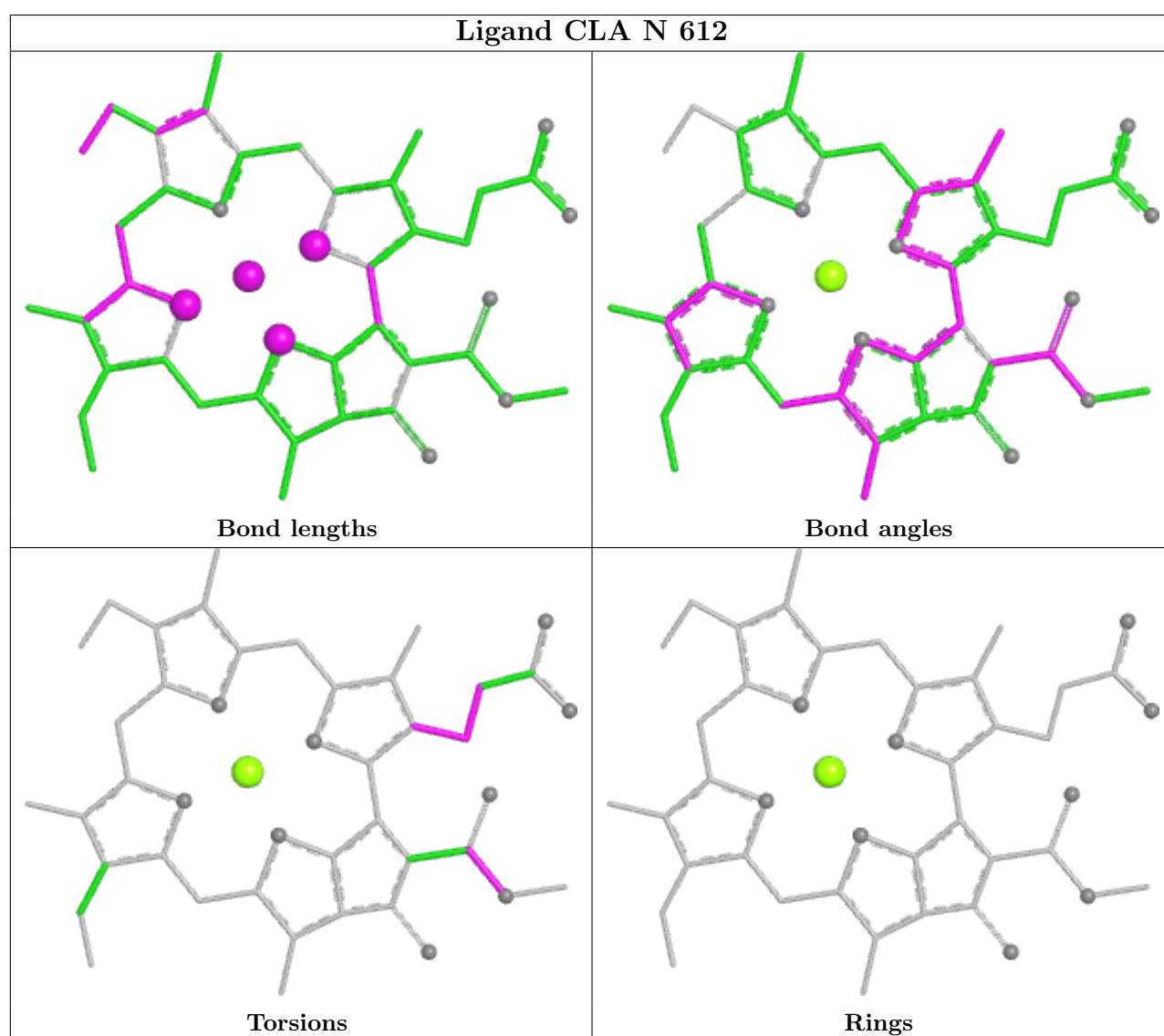
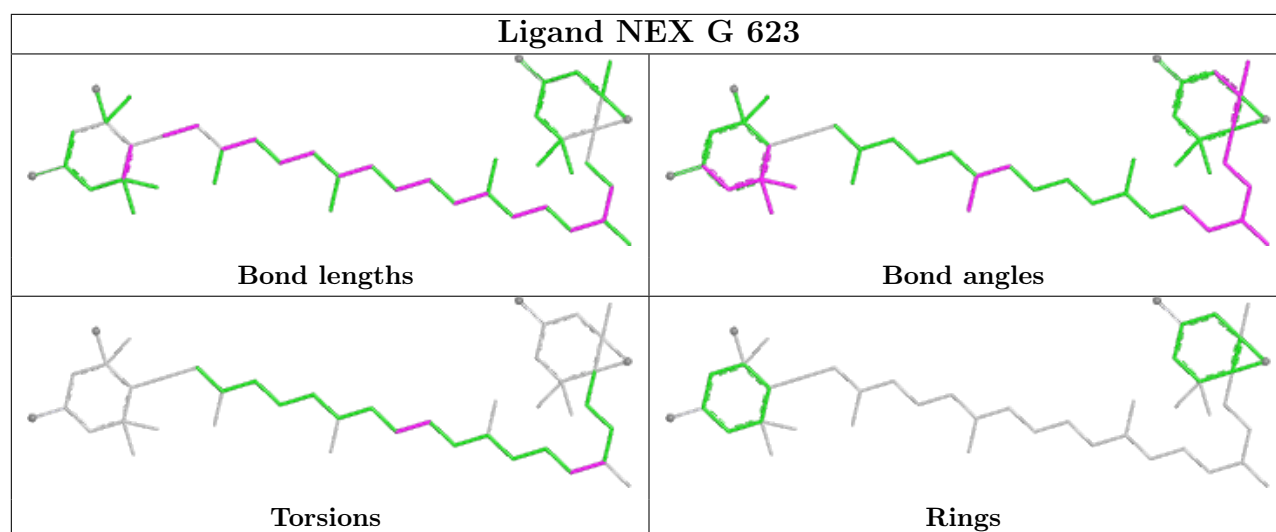
Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D

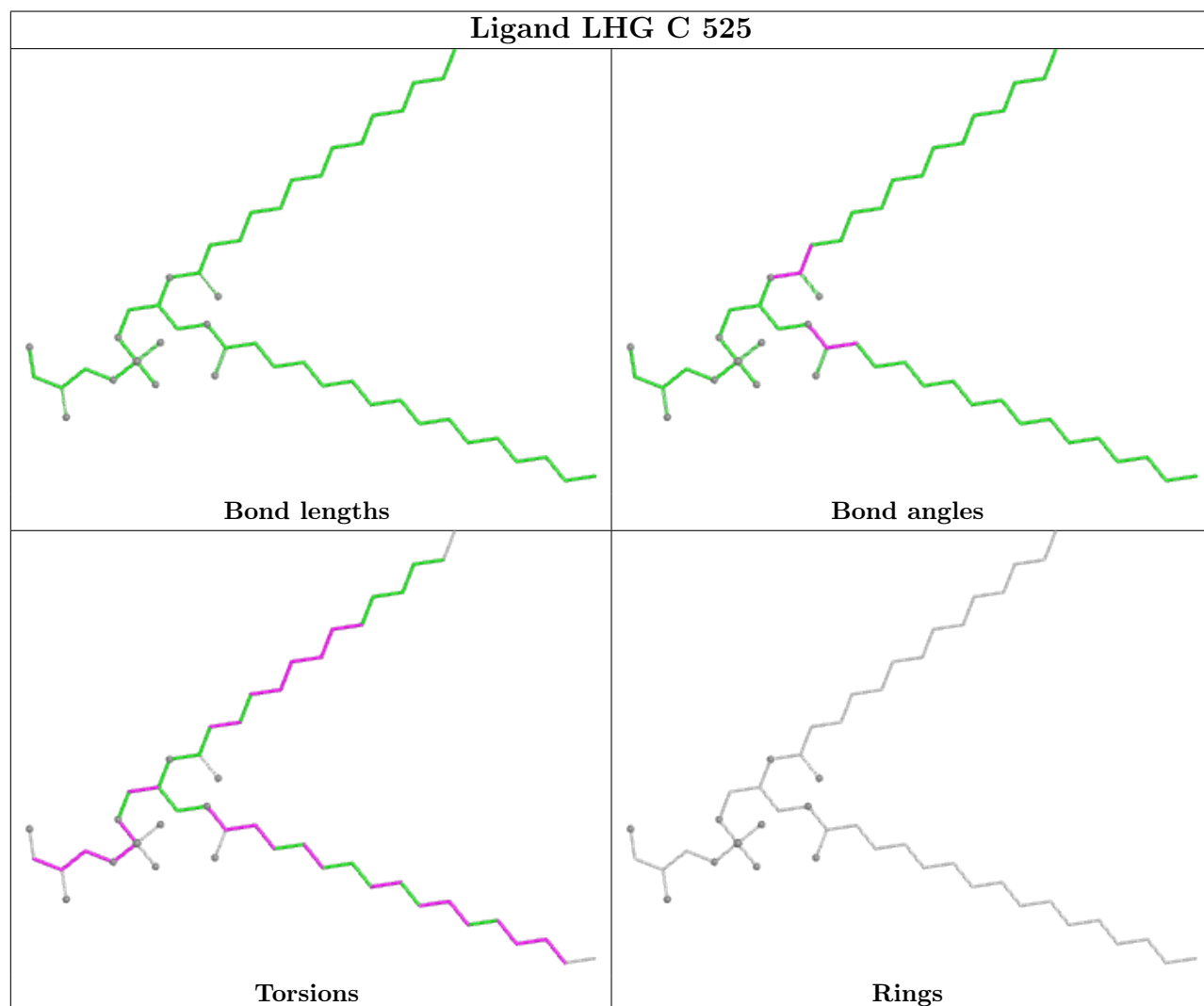
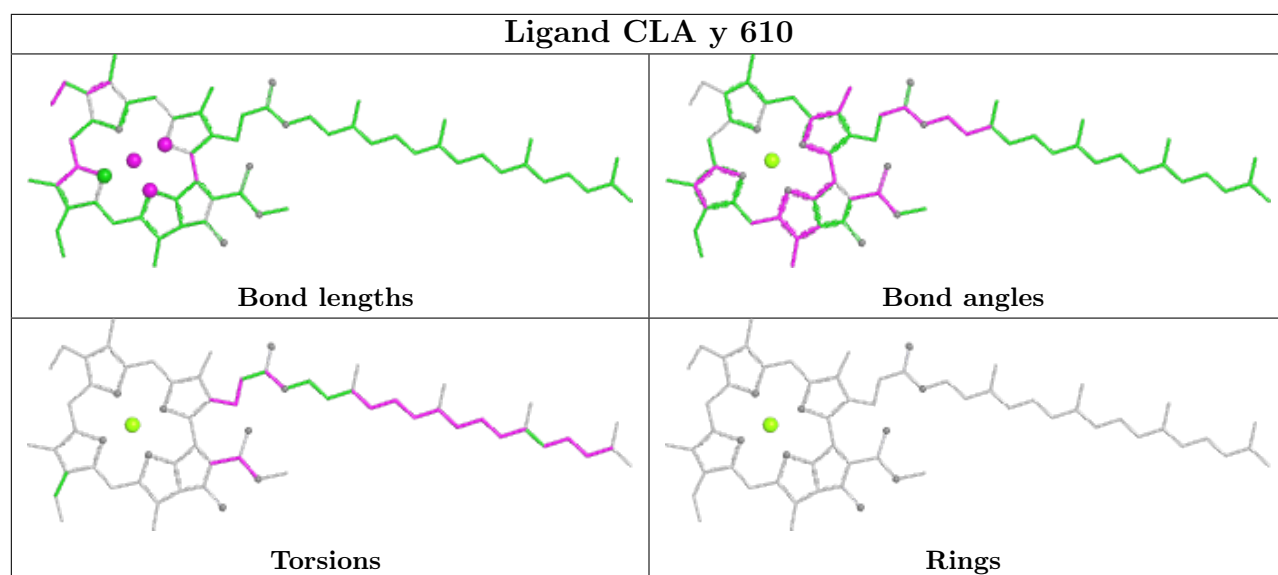
There are no ring outliers.

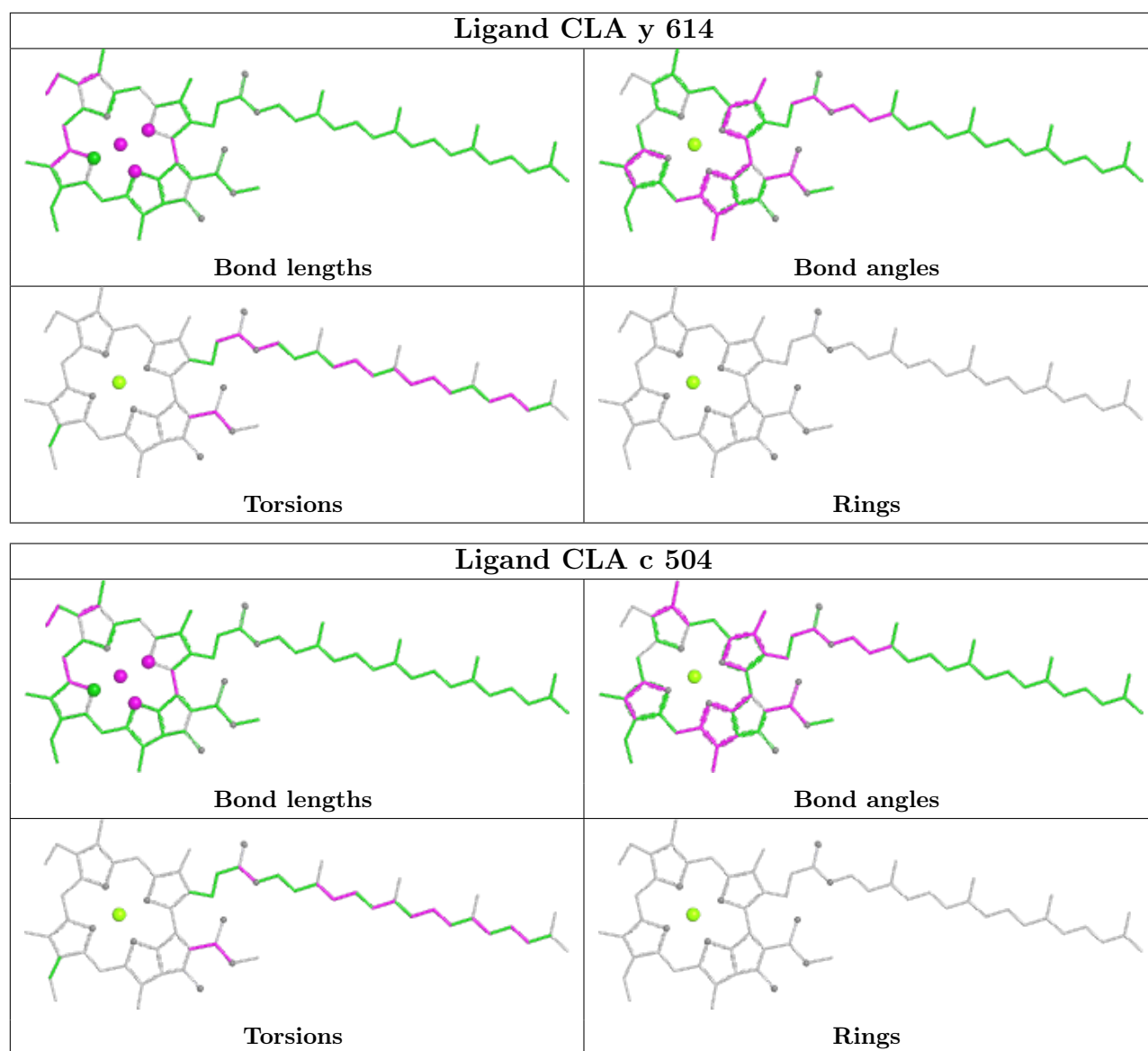
No monomer is involved in short contacts.

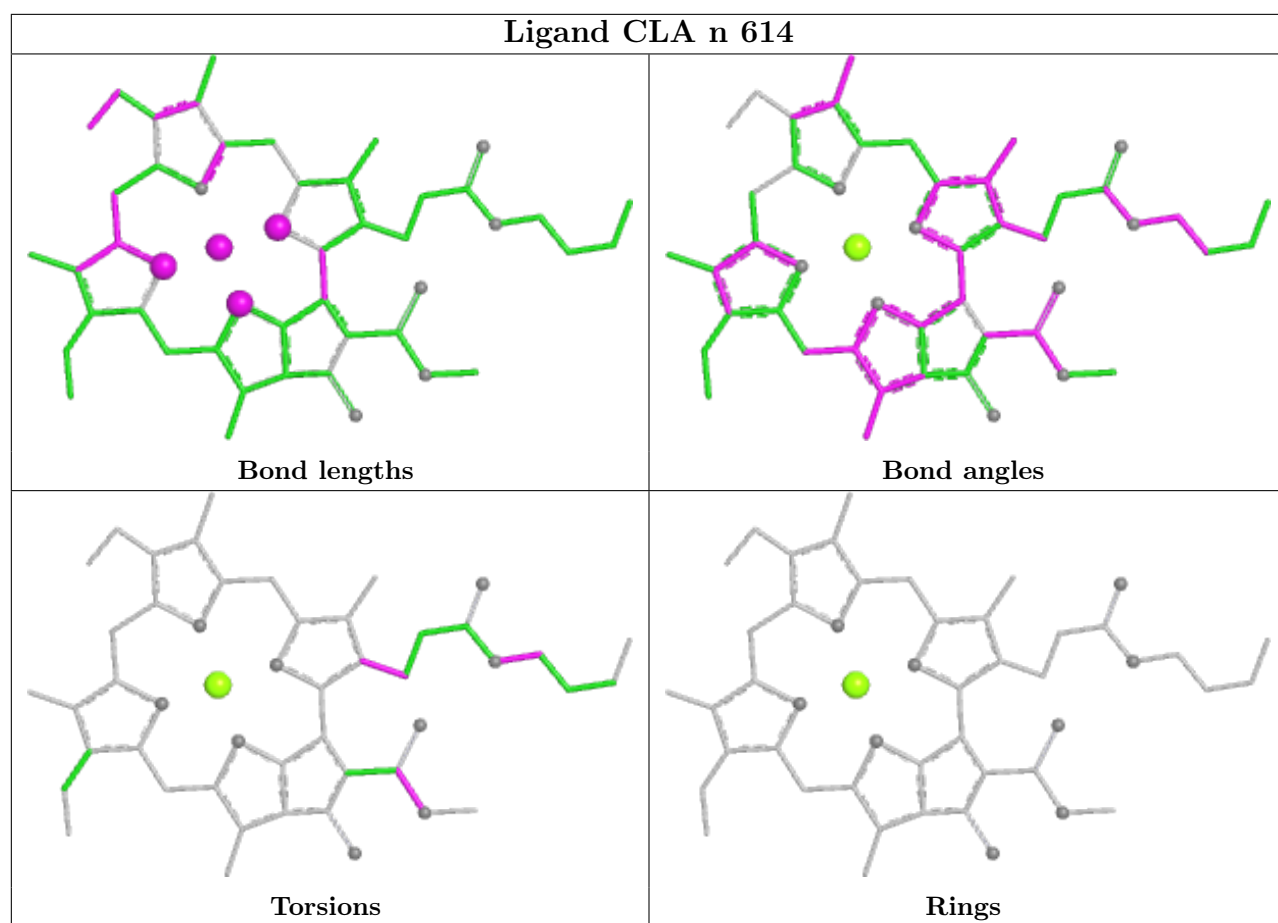
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

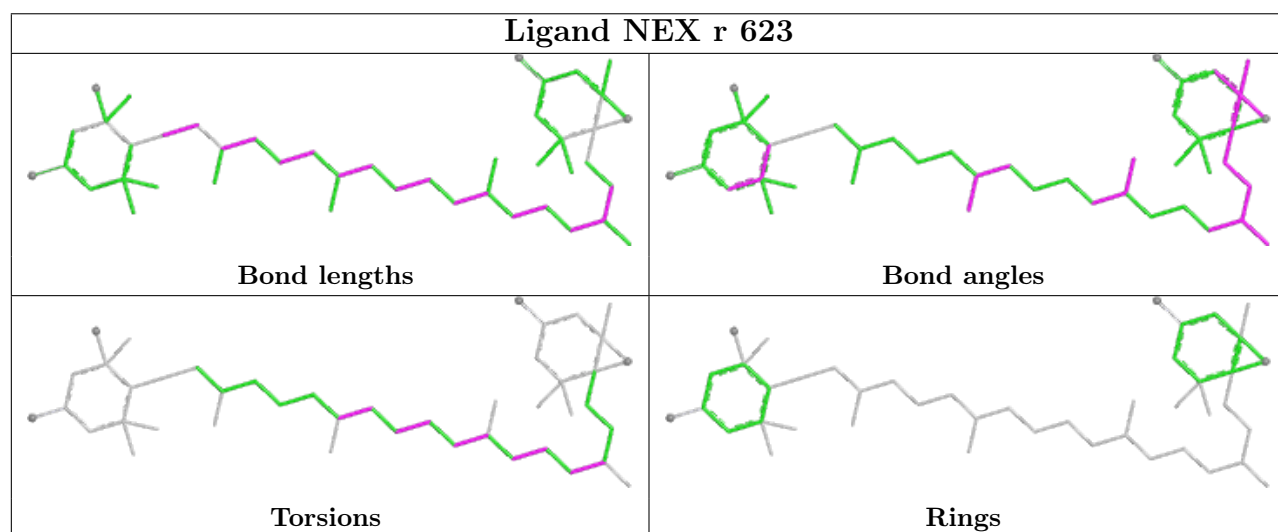
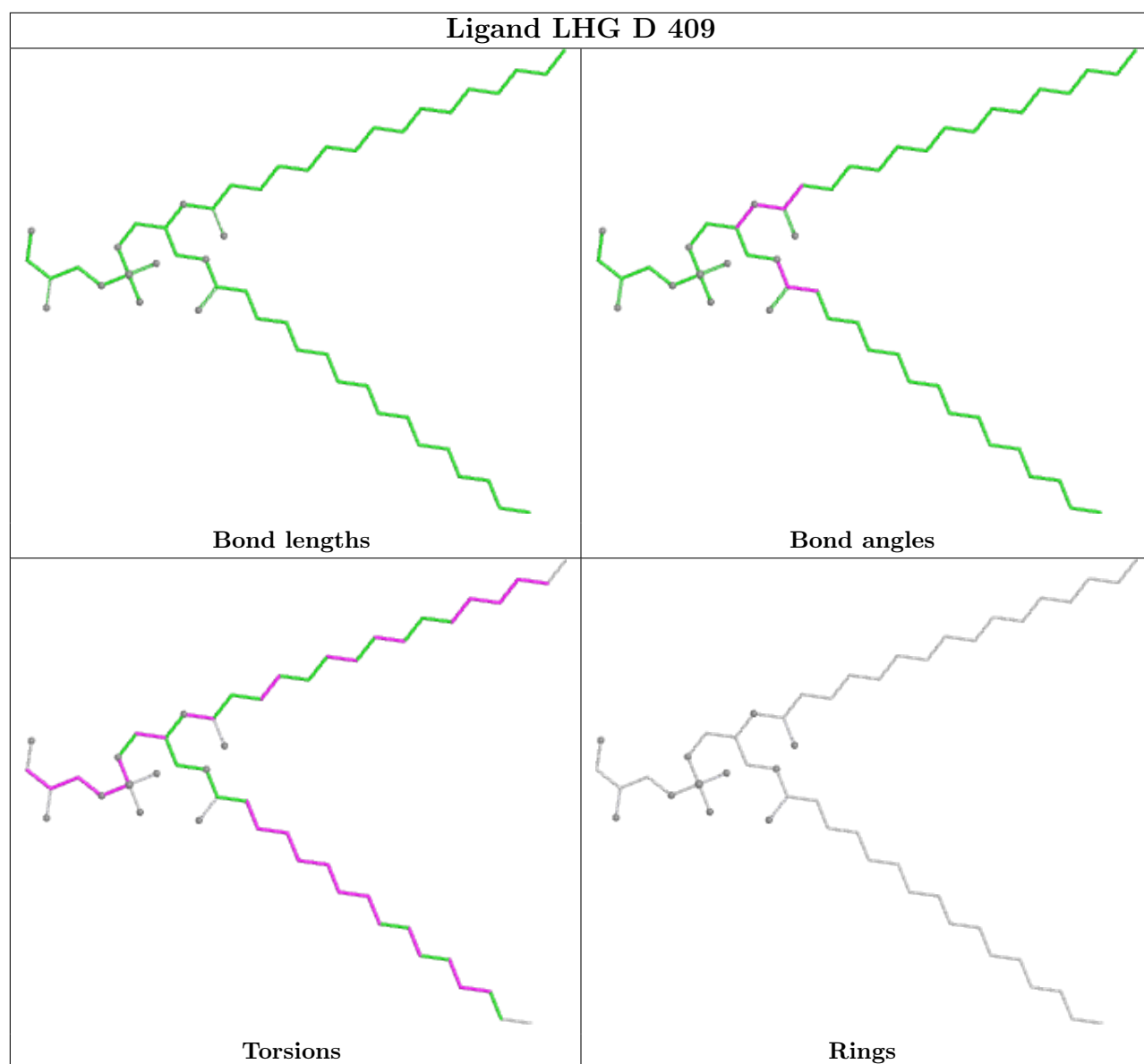


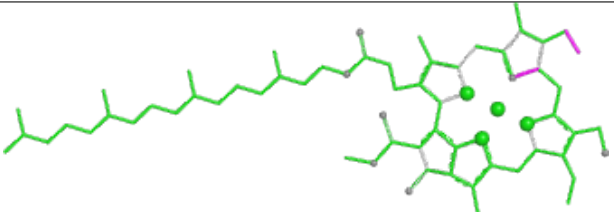
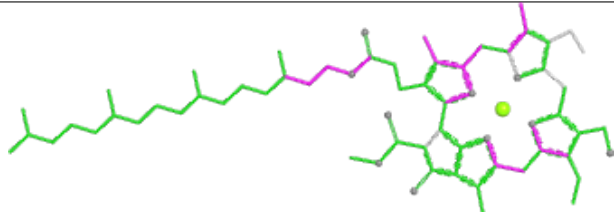
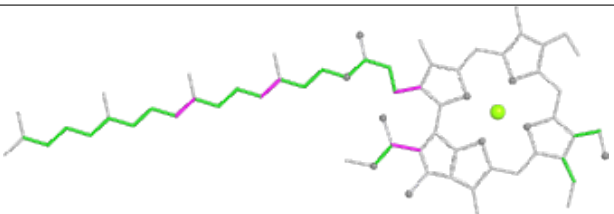
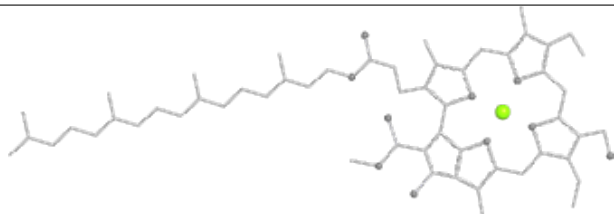


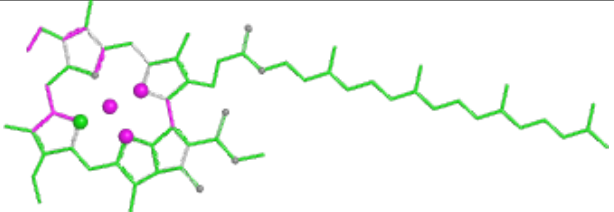
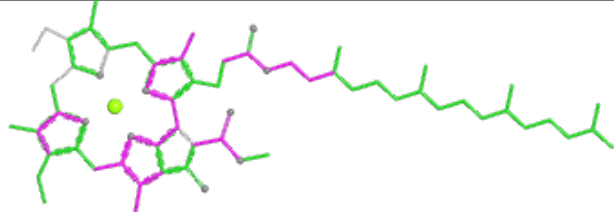
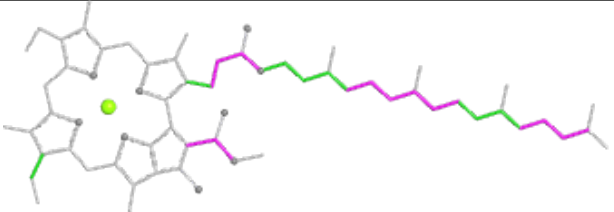
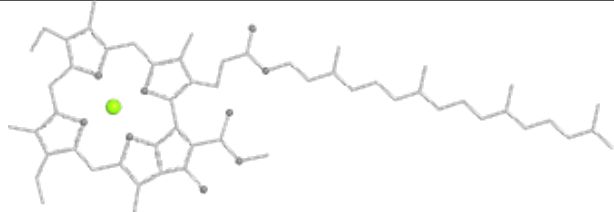


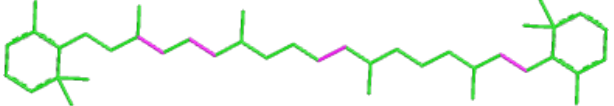
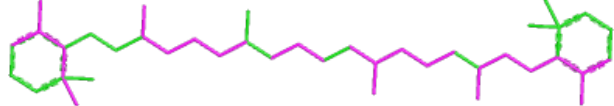
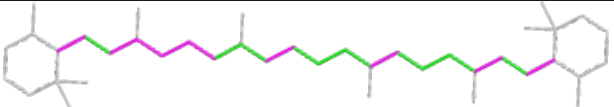
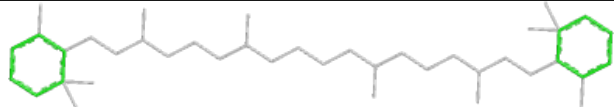


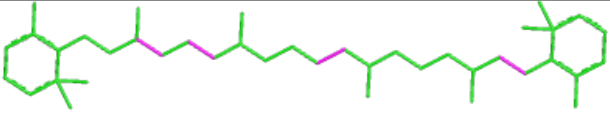
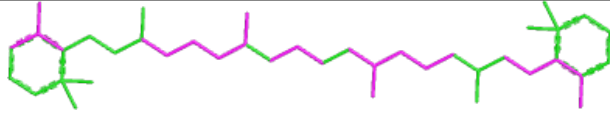
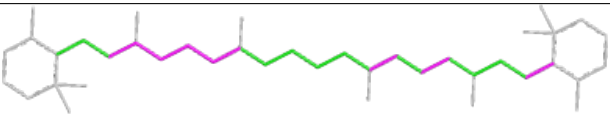
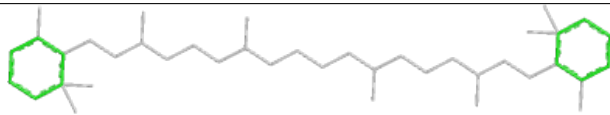
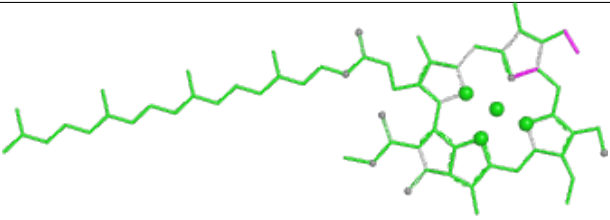
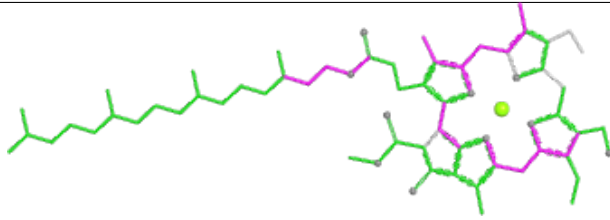
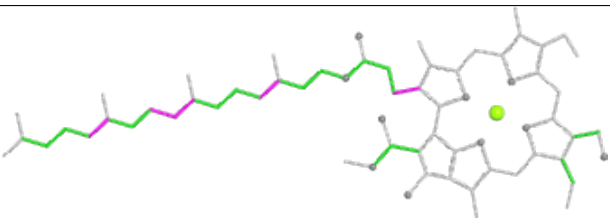
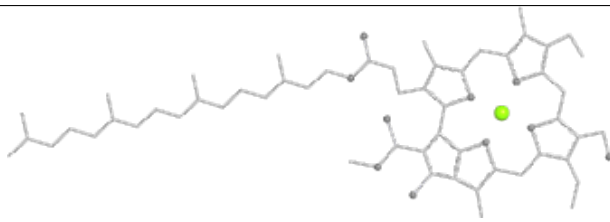
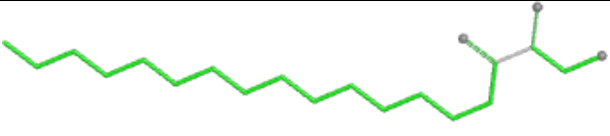
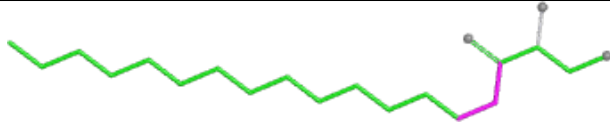
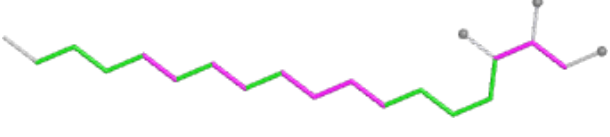
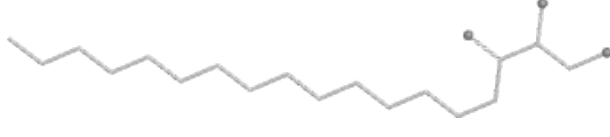




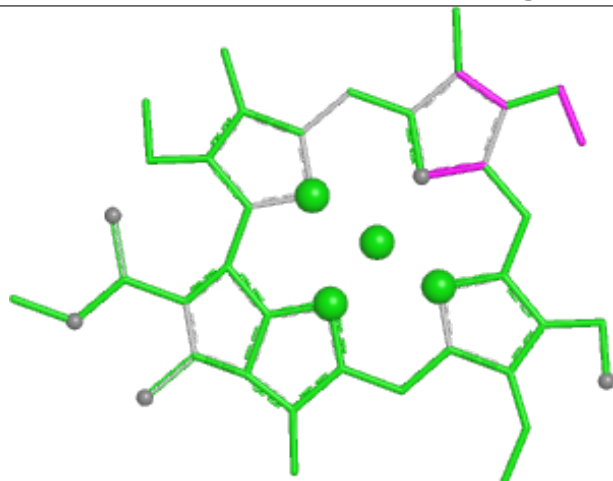
Ligand CHL y 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

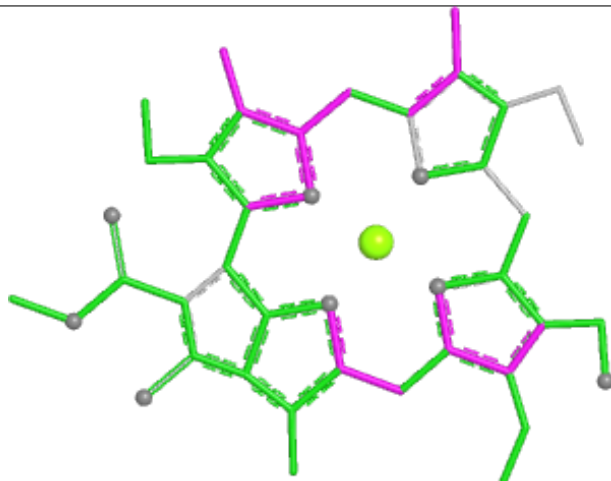
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL N 609	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand SPH y 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

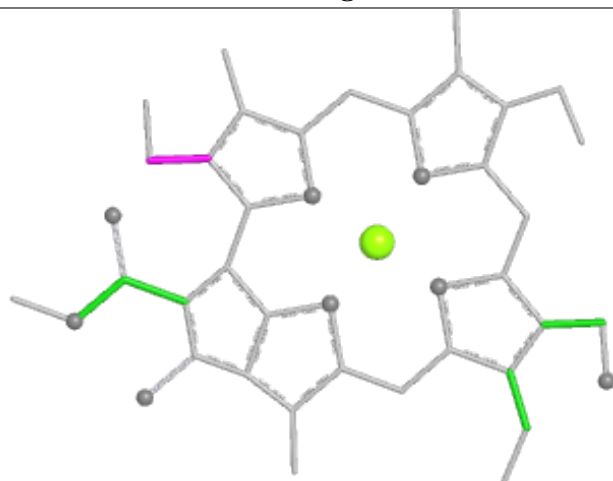
Ligand CHL s 607



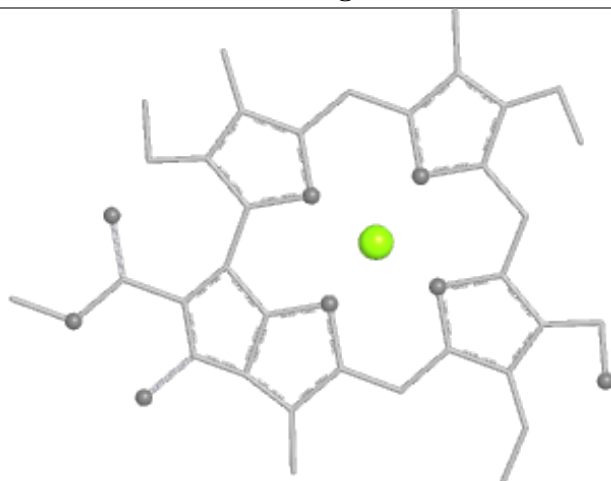
Bond lengths



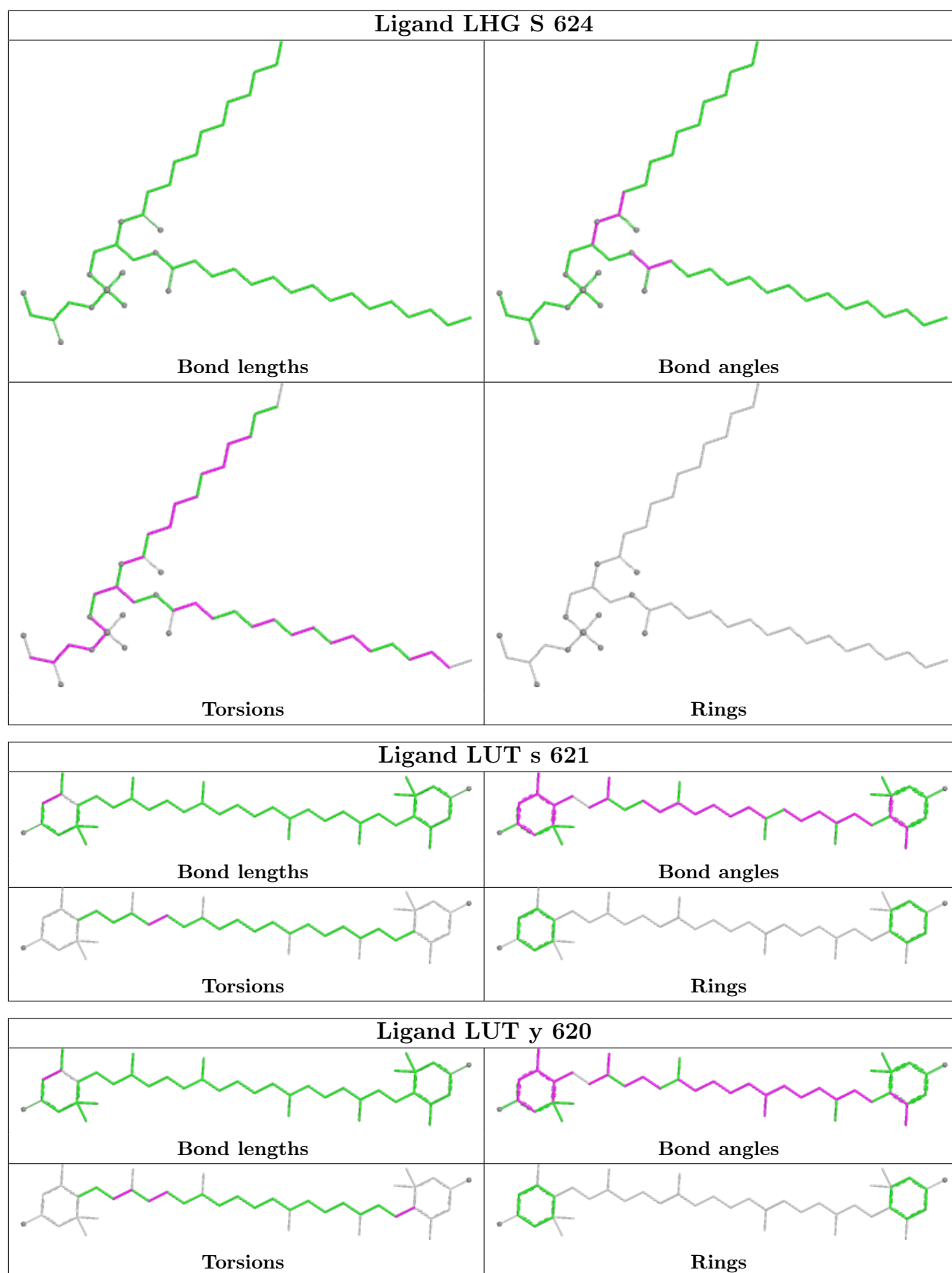
Bond angles

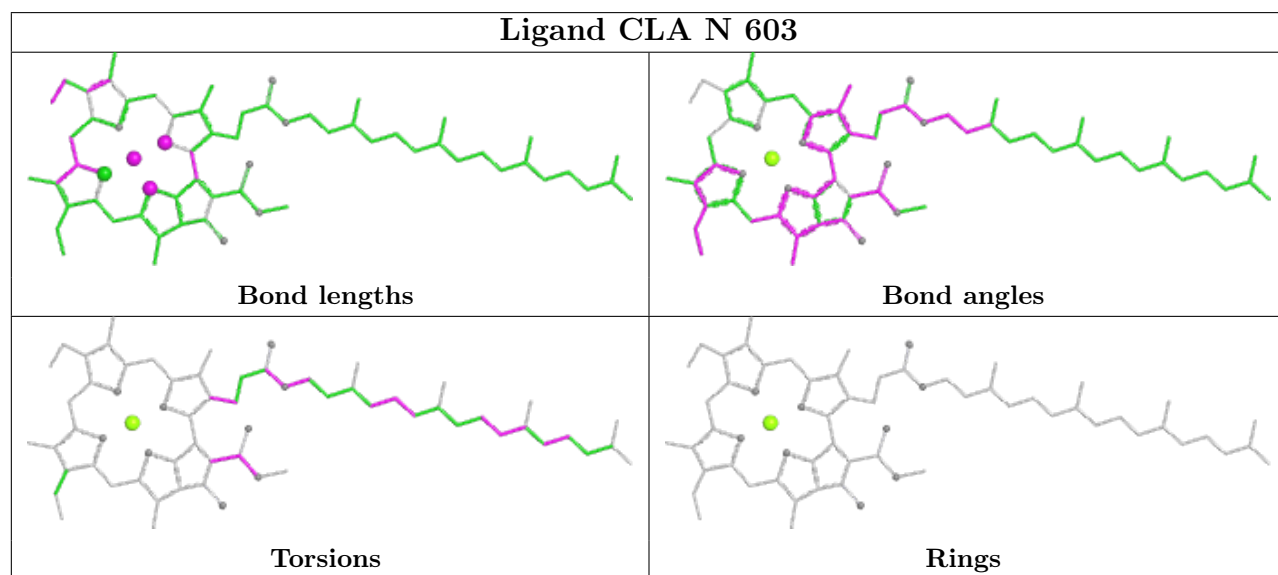
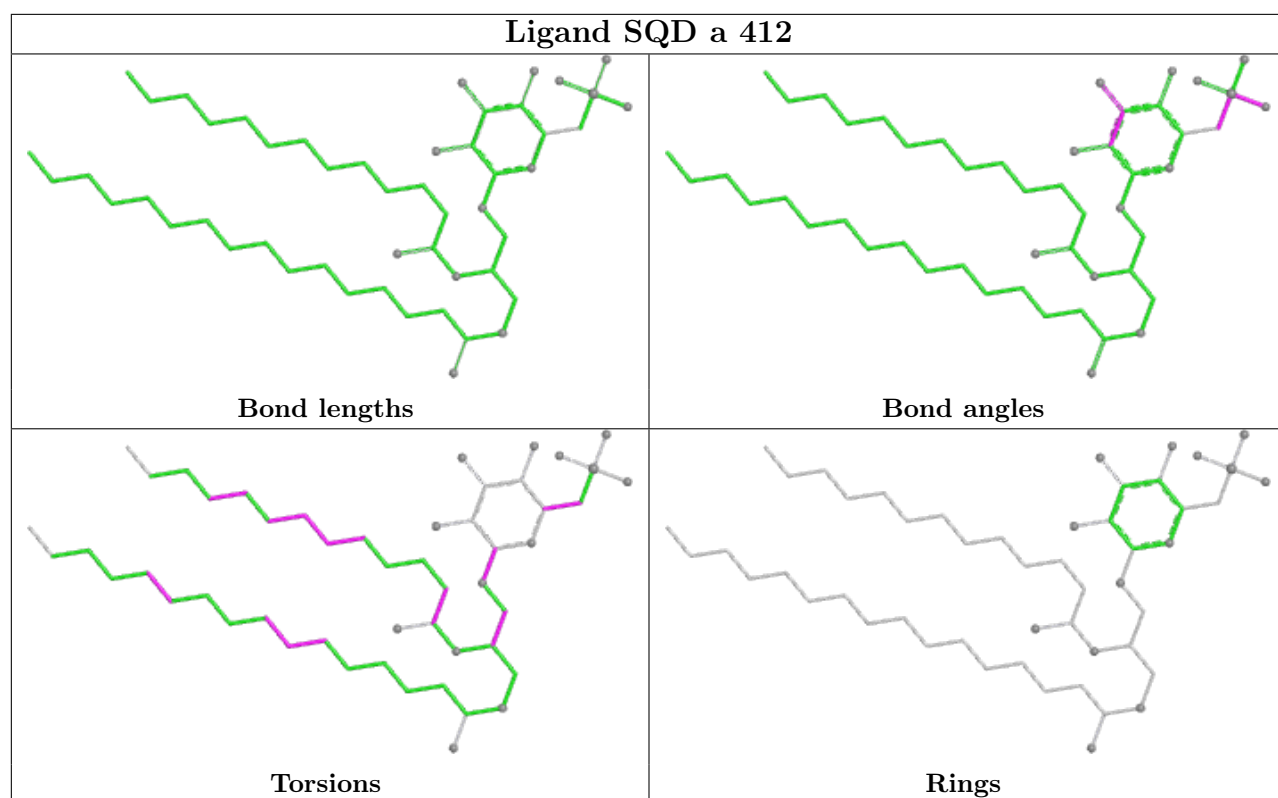


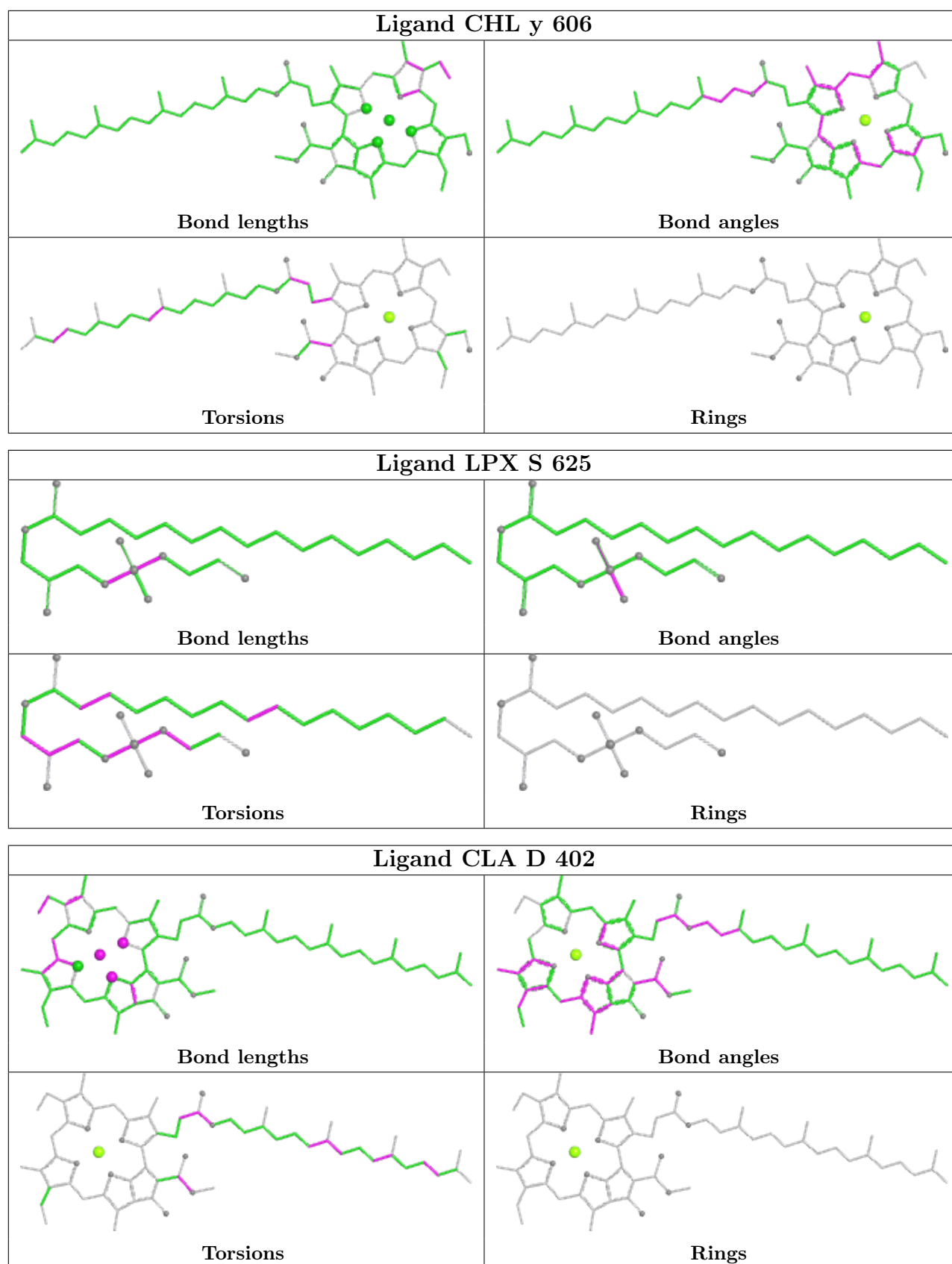
Torsions

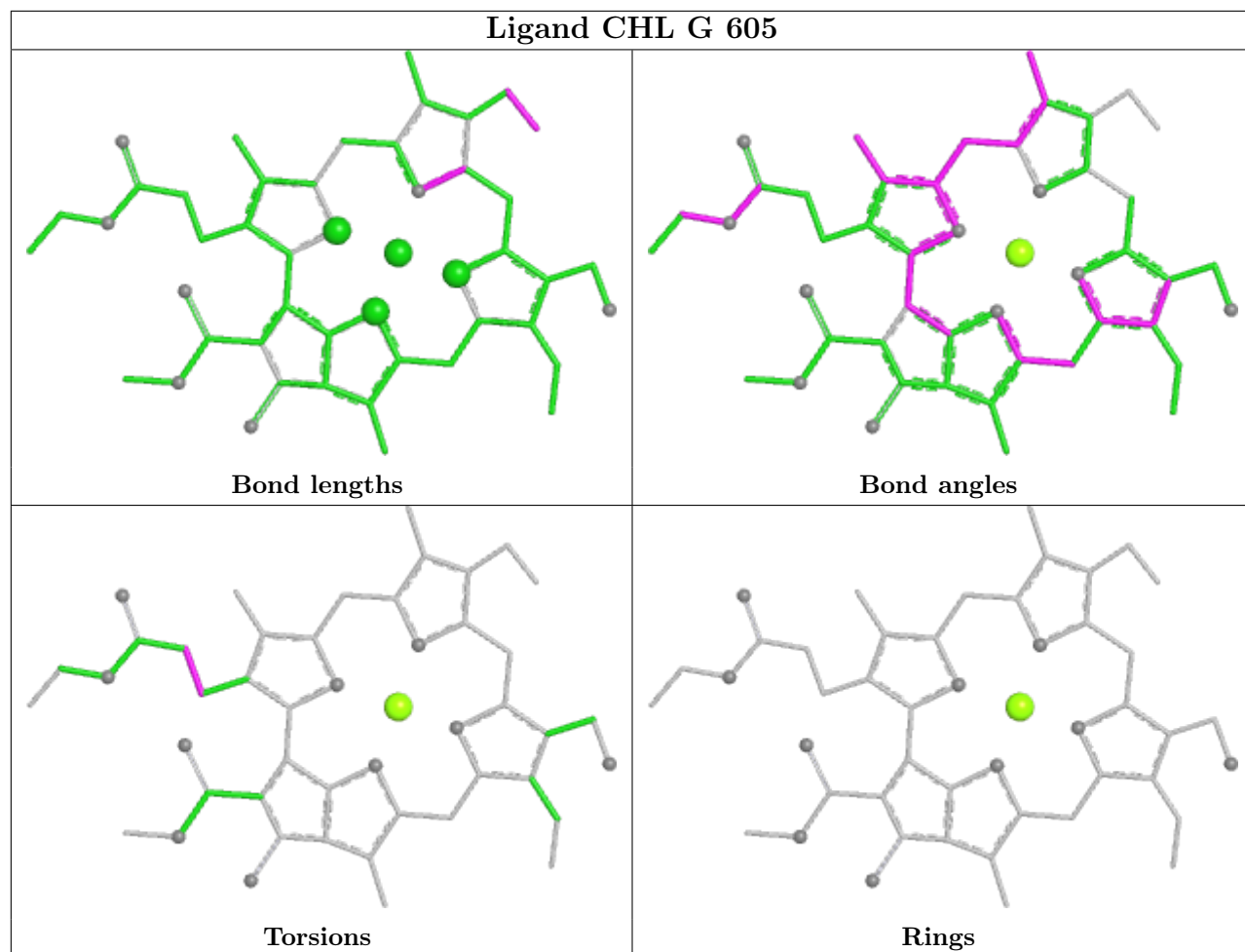


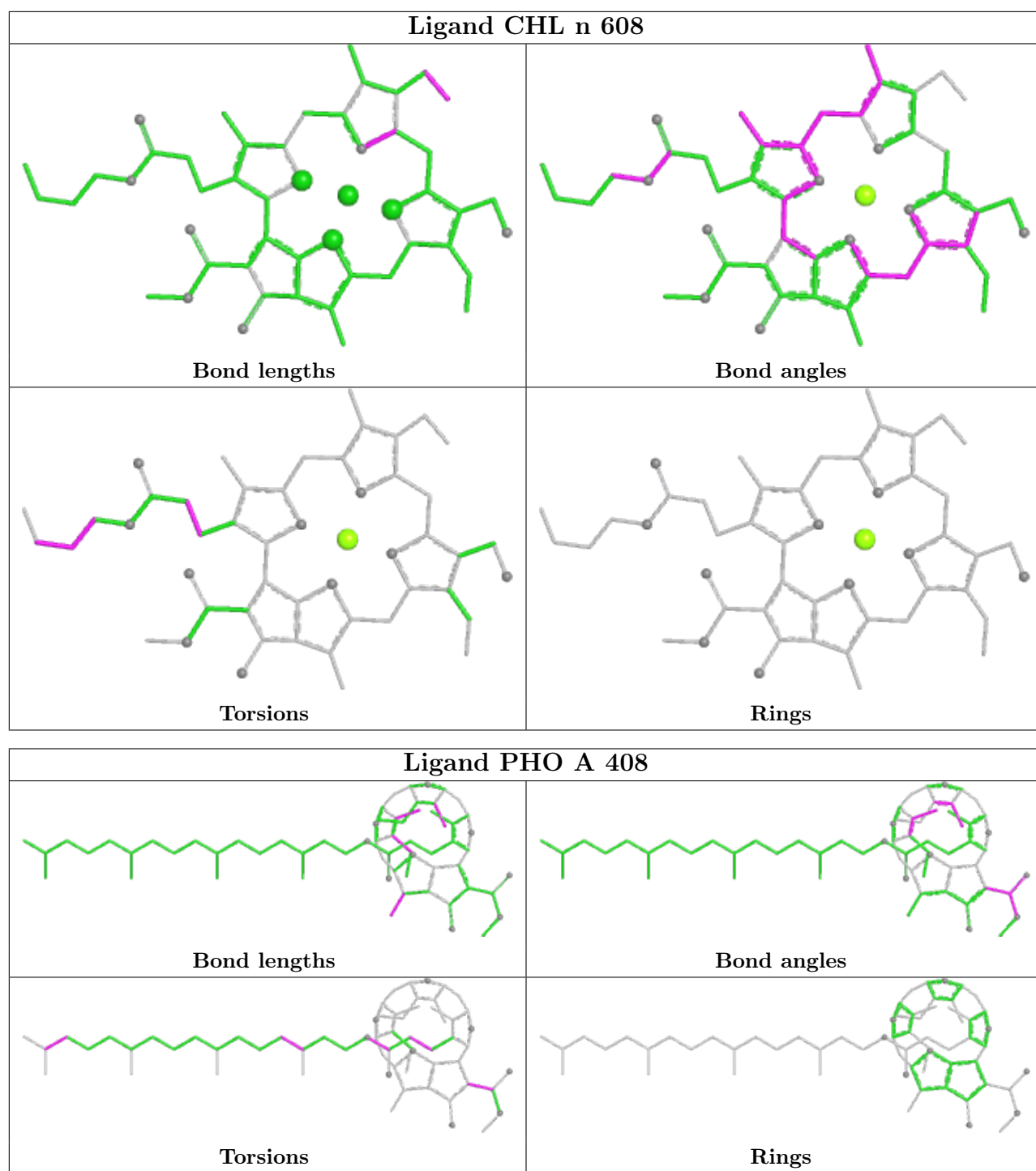
Rings



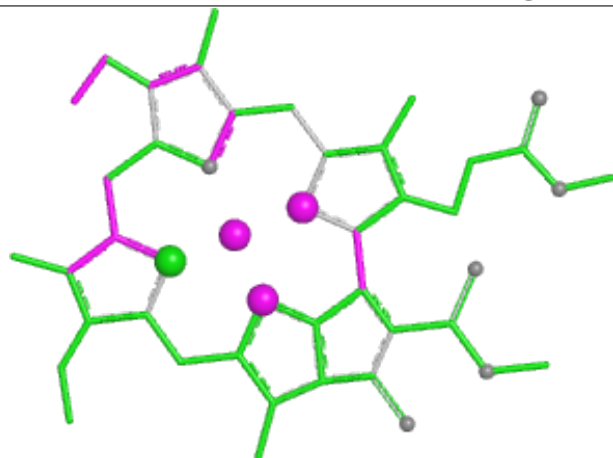




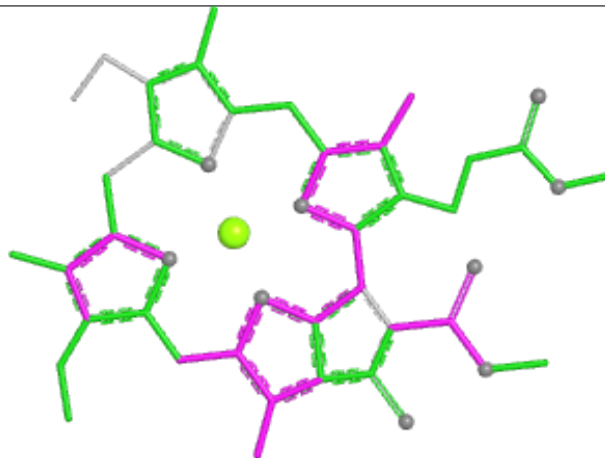




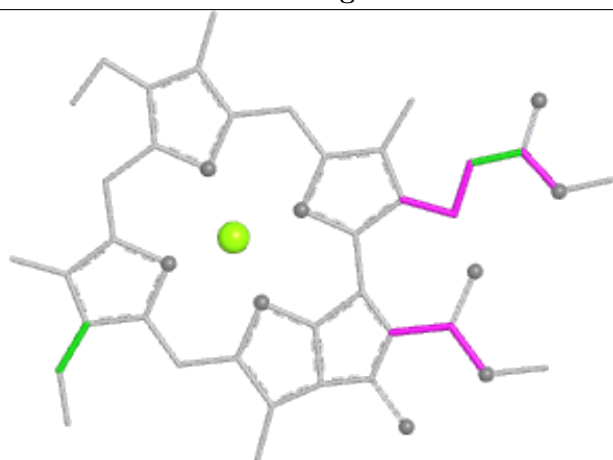
Ligand CLA r 613



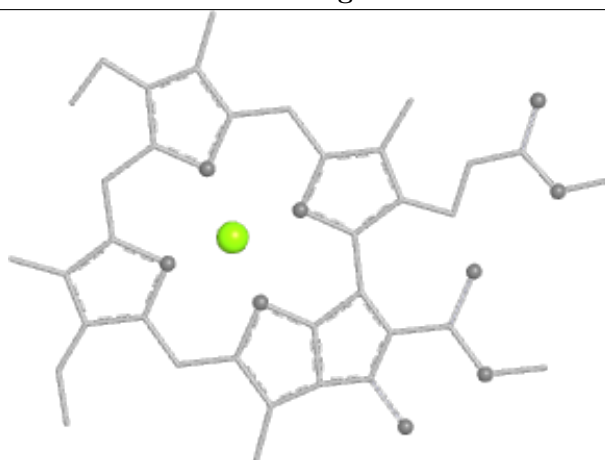
Bond lengths



Bond angles

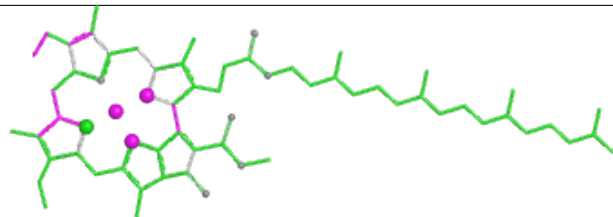


Torsions

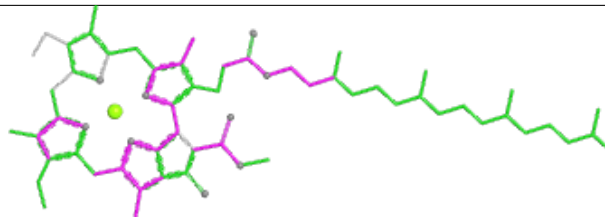


Rings

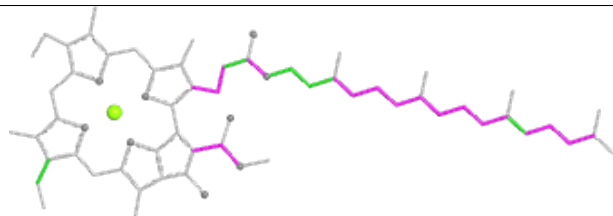
Ligand CLA Y 610



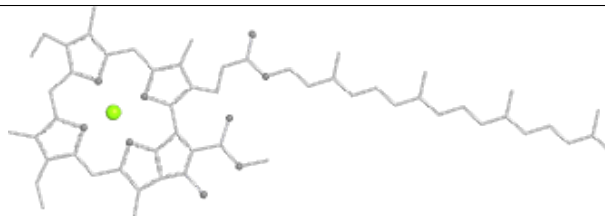
Bond lengths



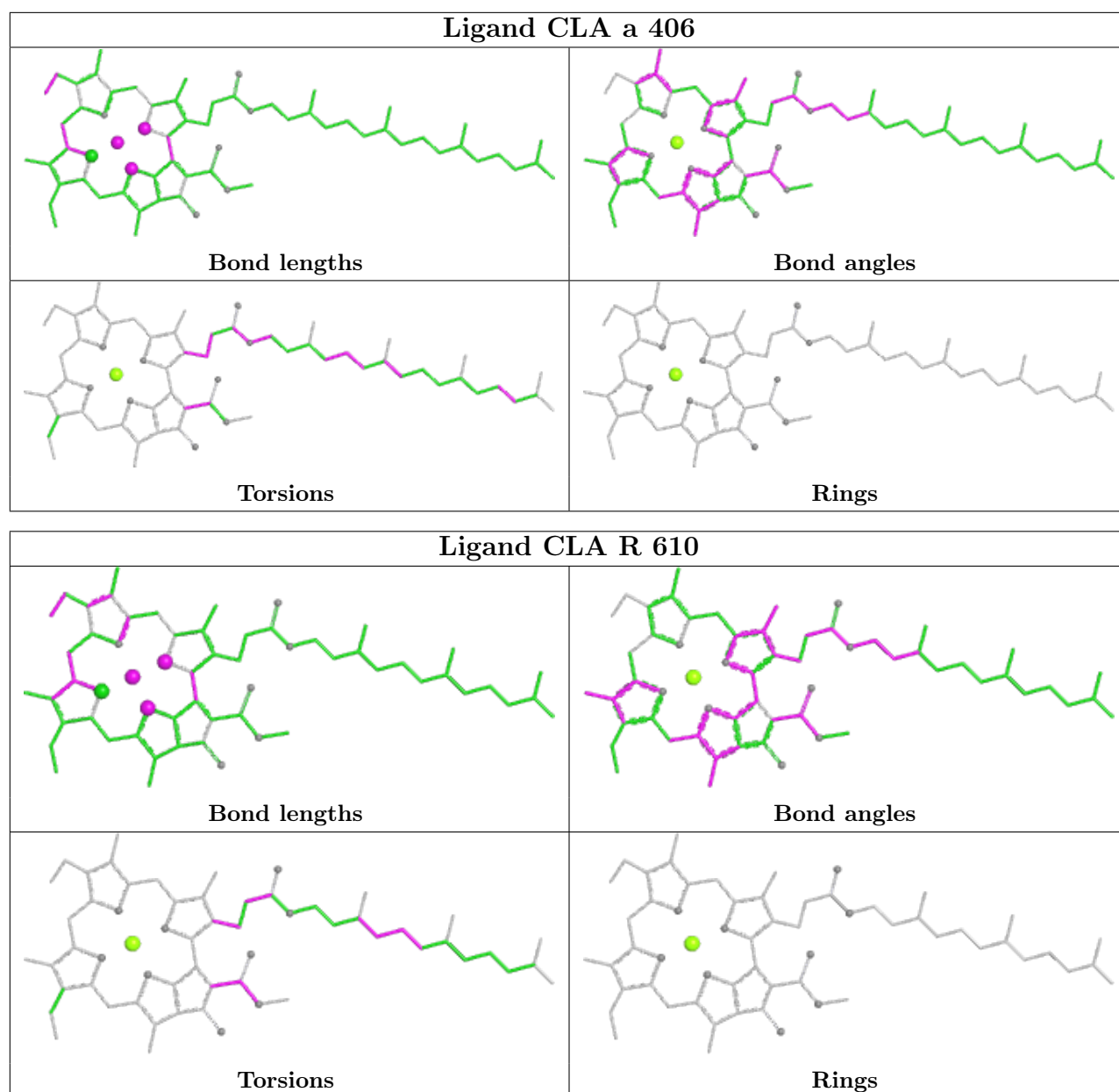
Bond angles

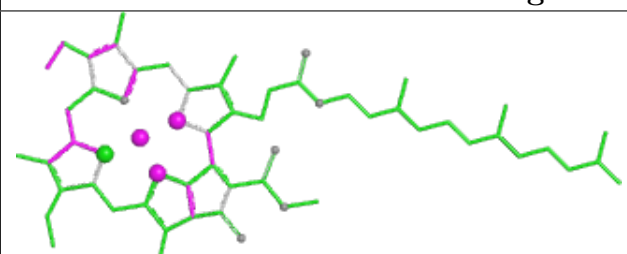
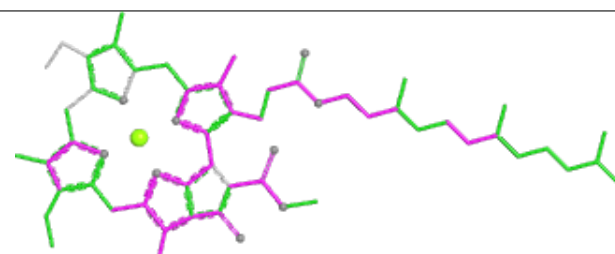
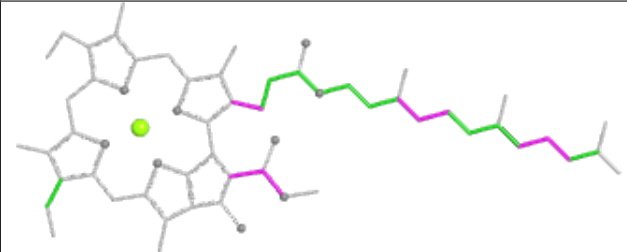
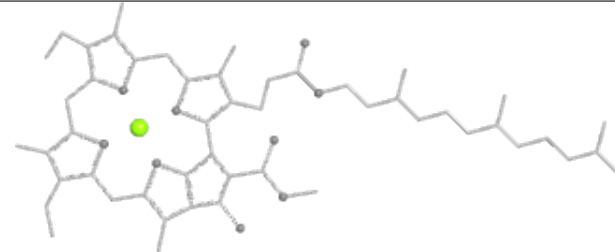


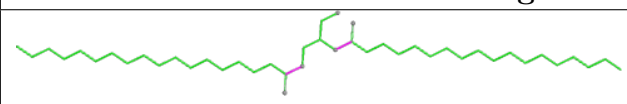
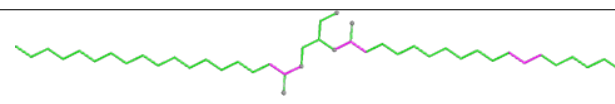
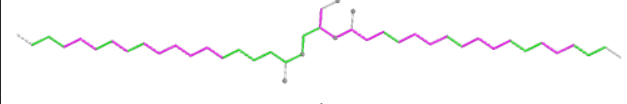
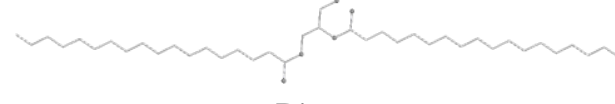
Torsions

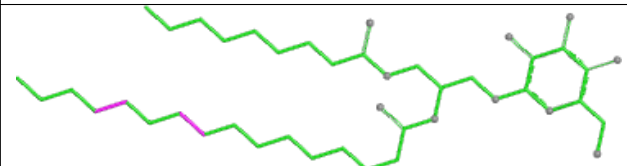
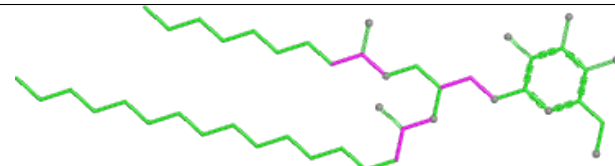
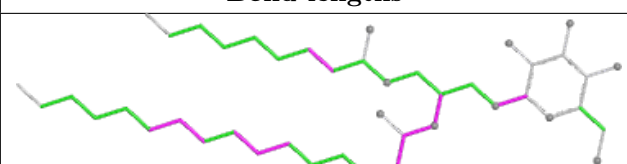
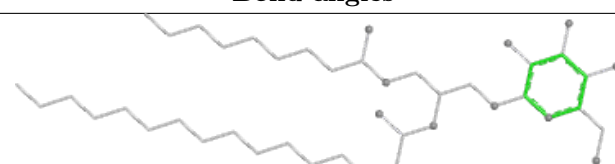


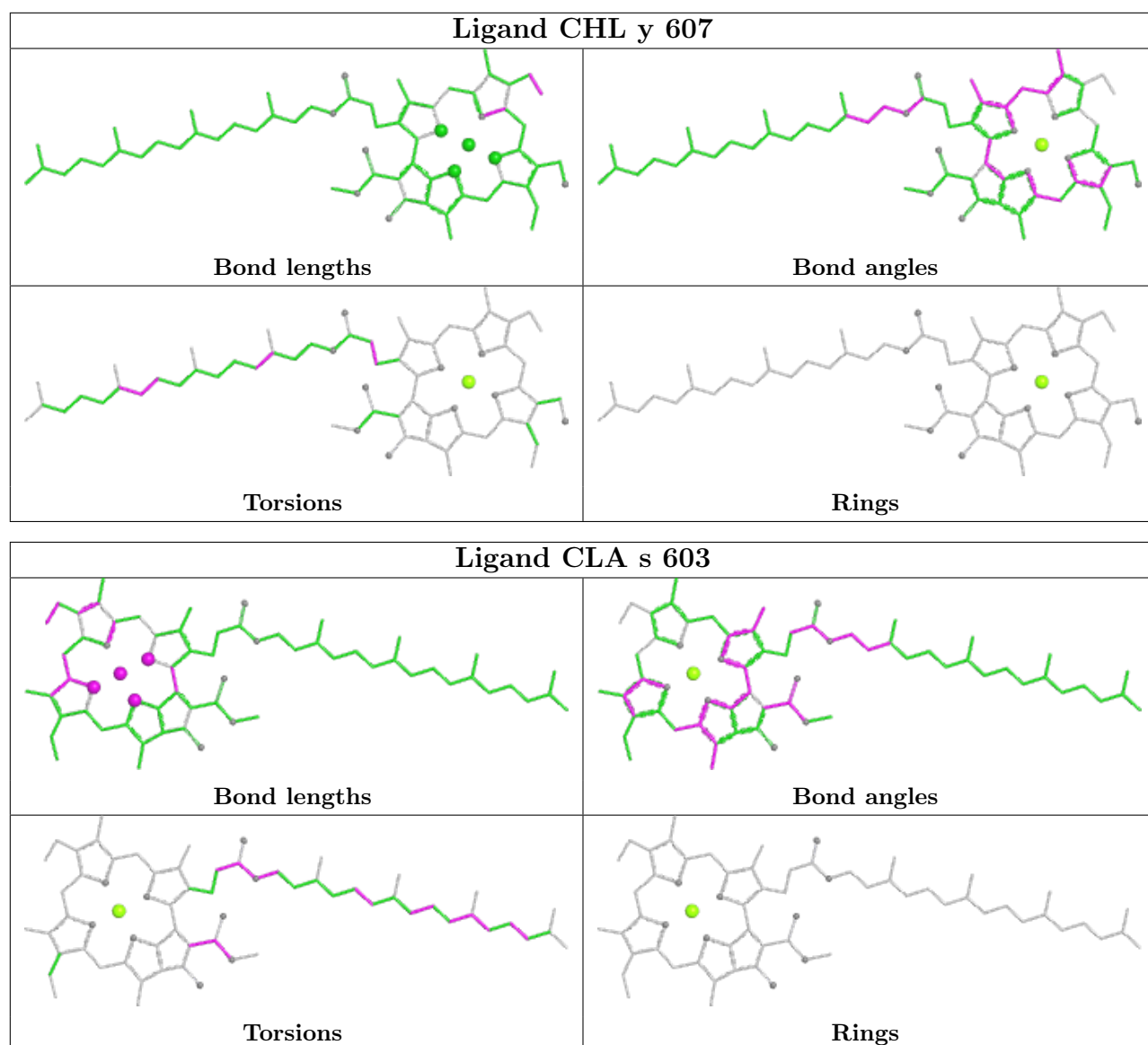
Rings

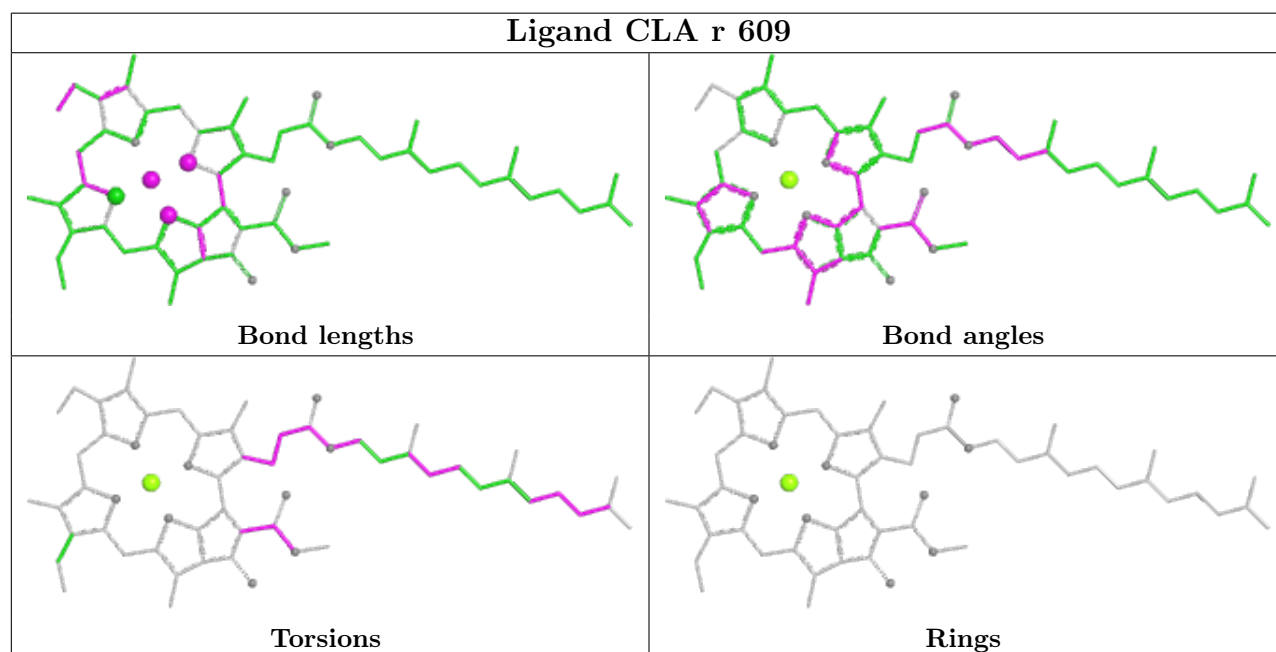
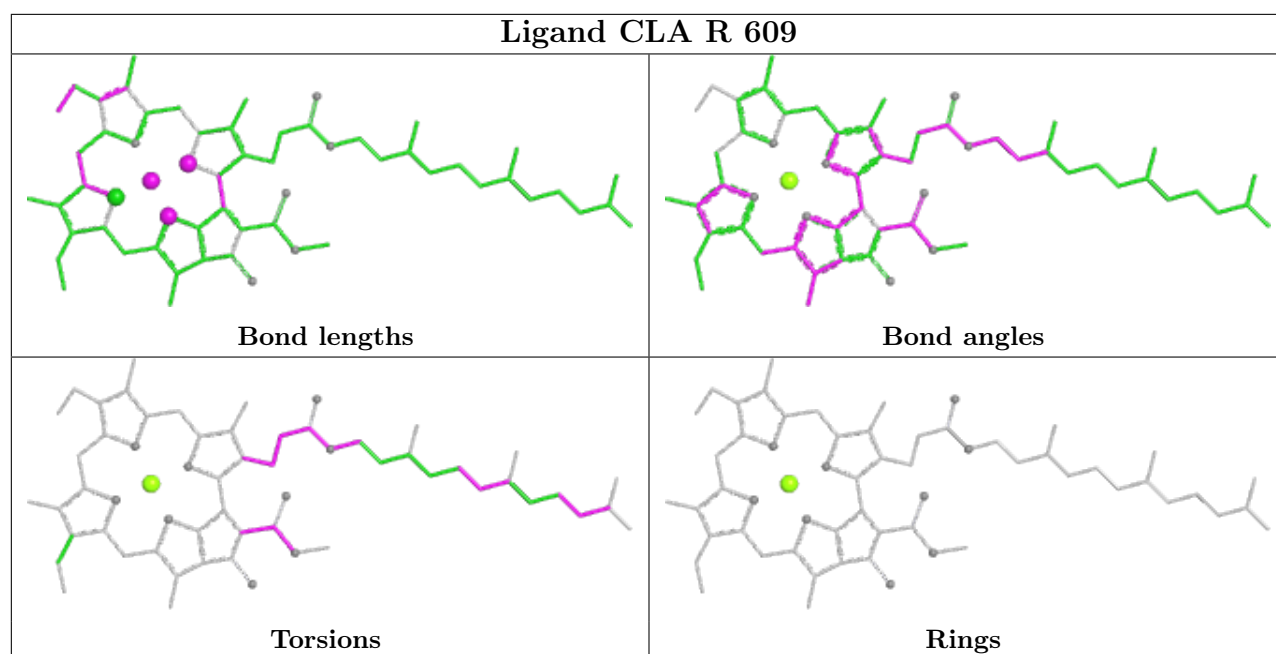


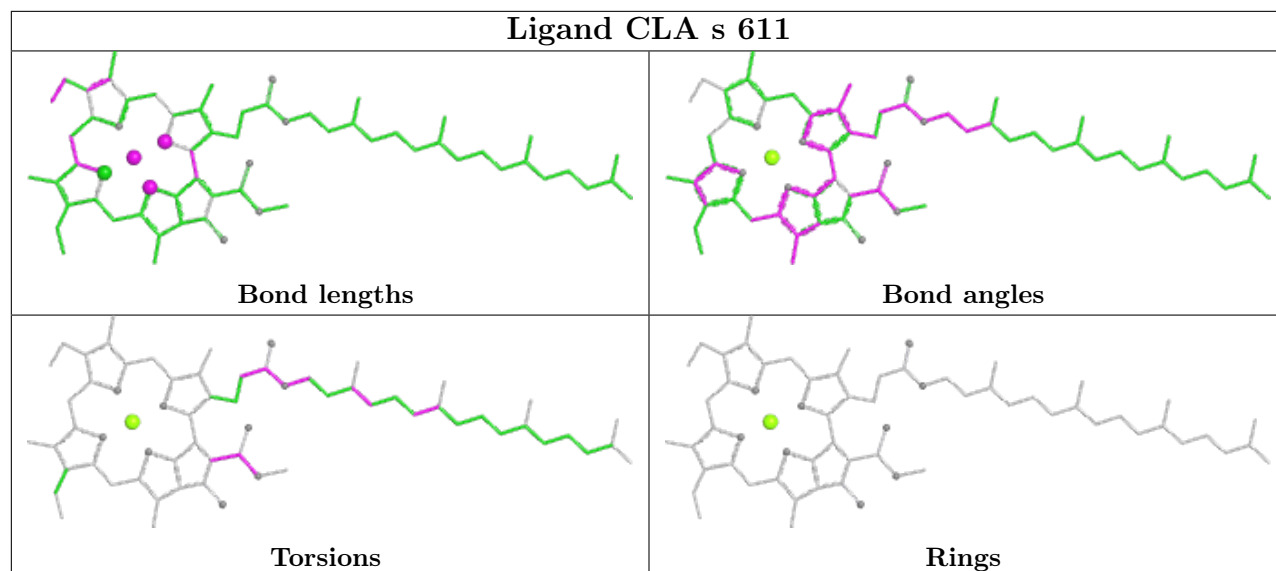
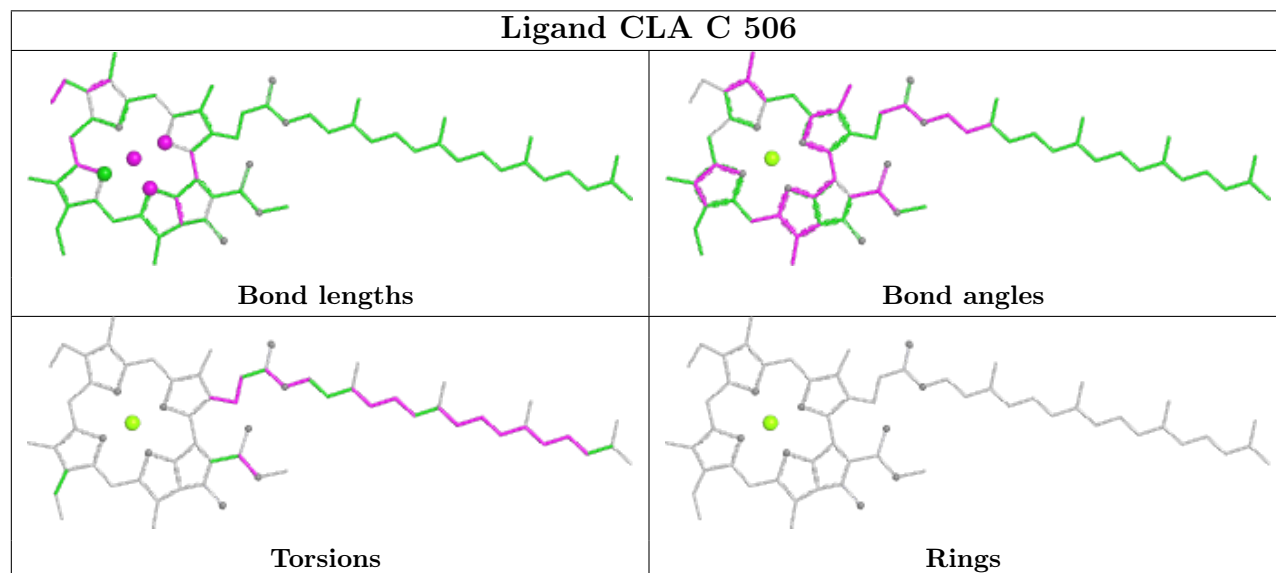
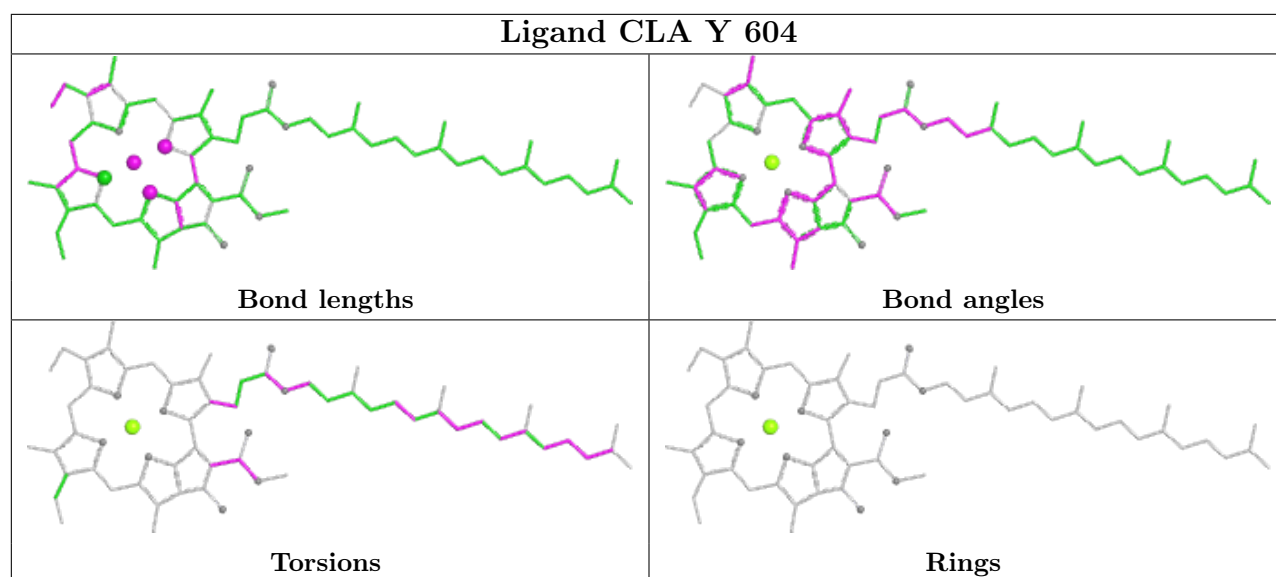
Ligand CLA r 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

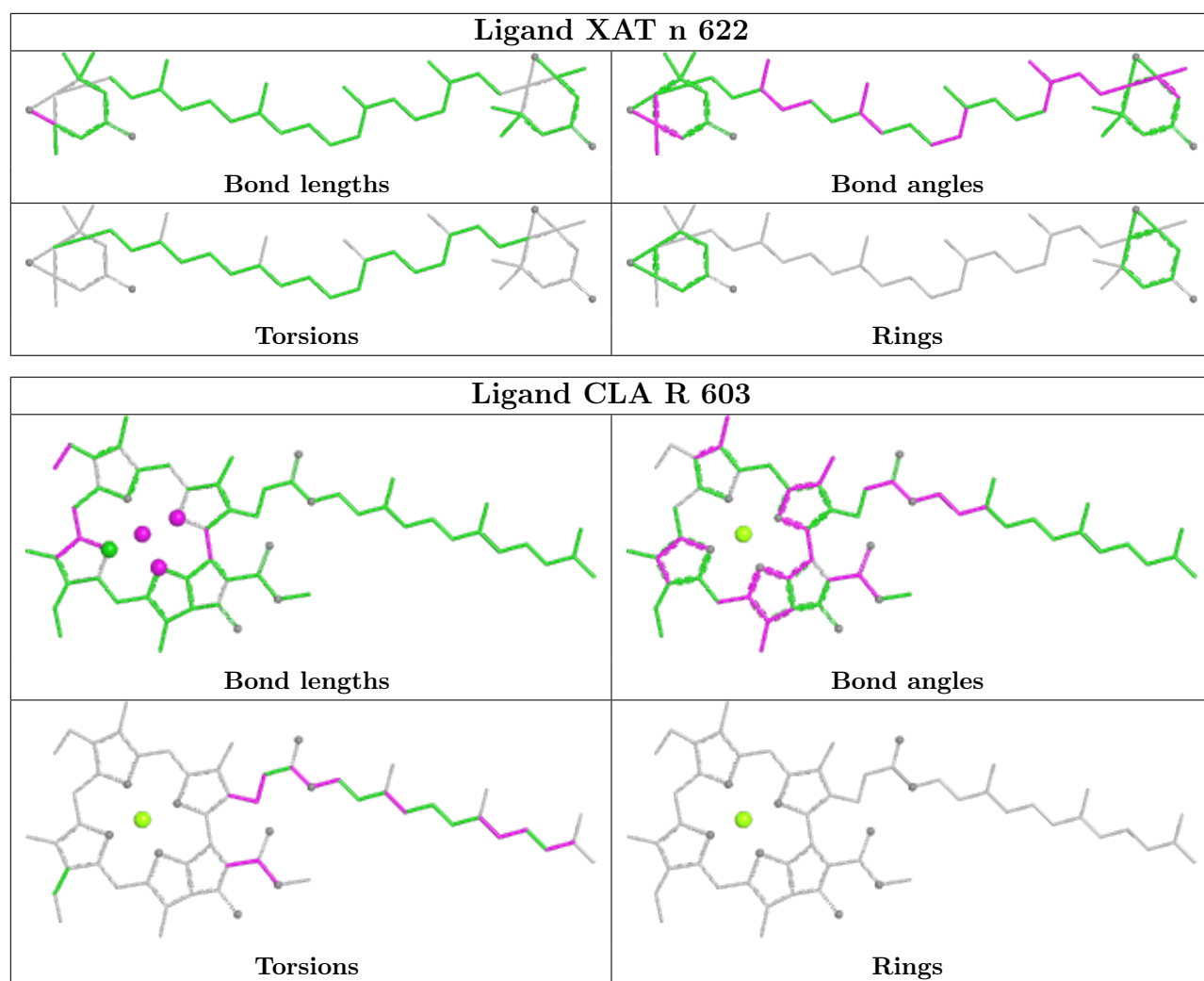
Ligand DGA B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

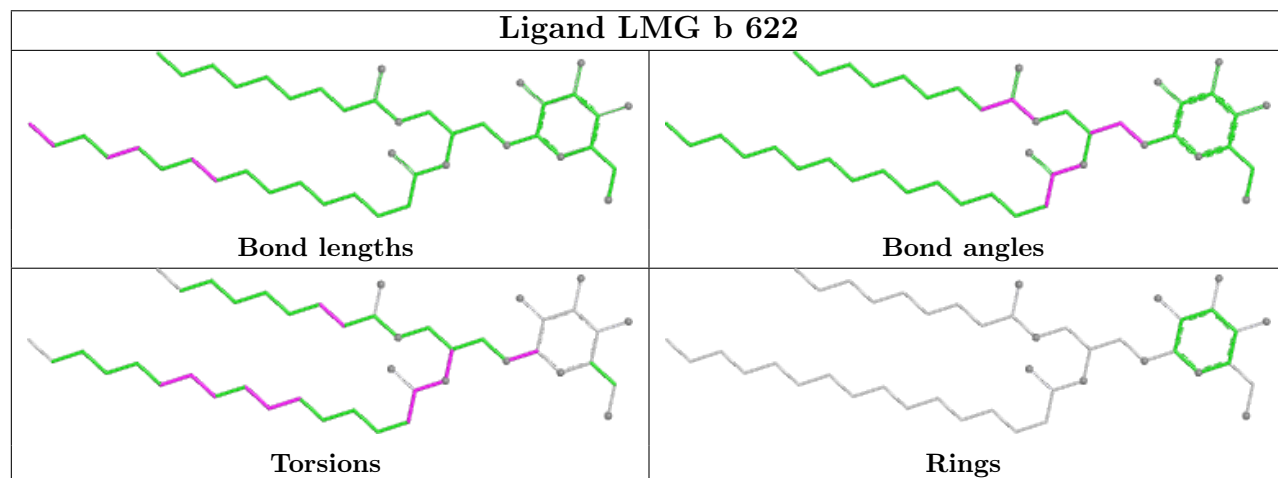
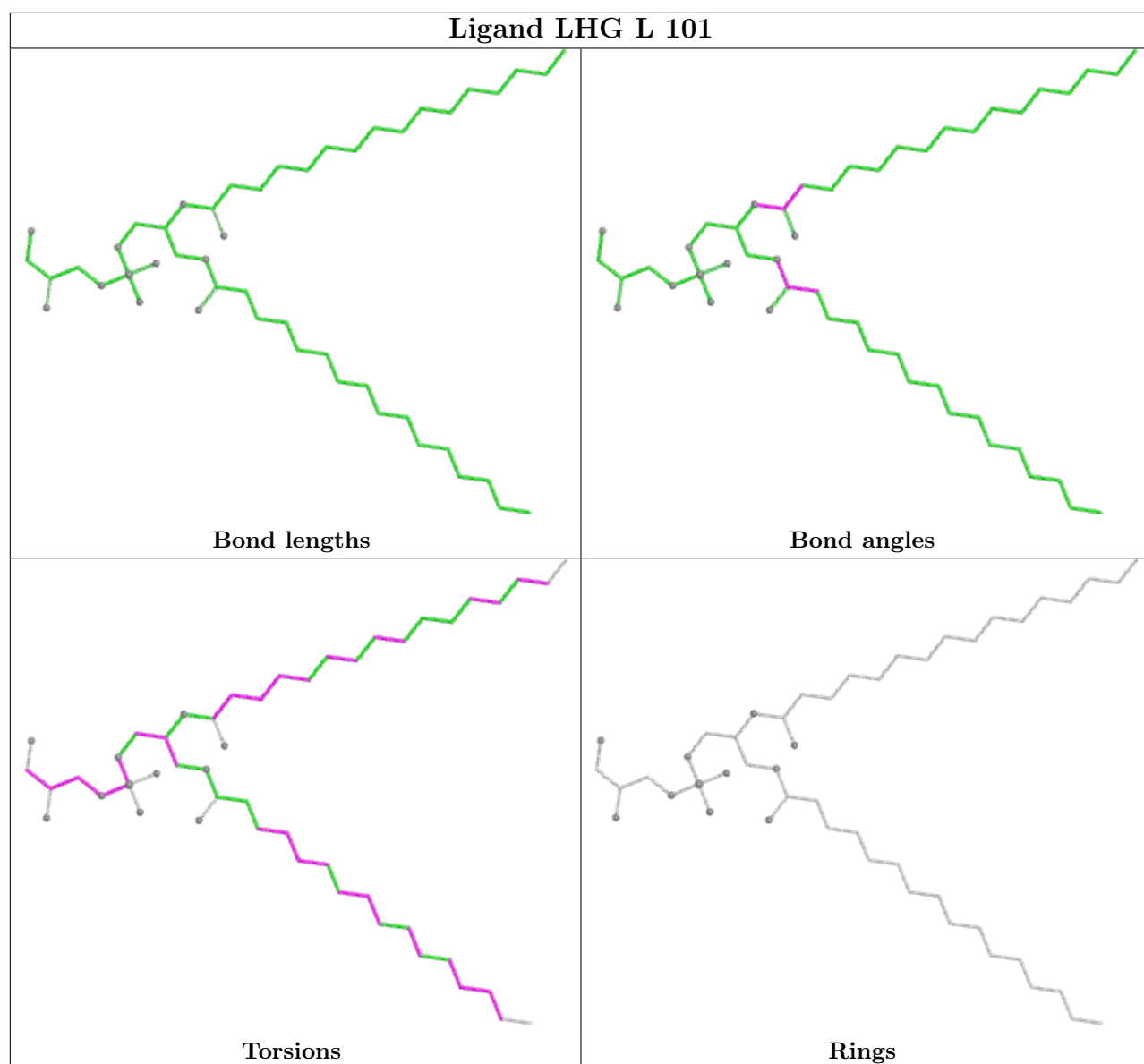
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

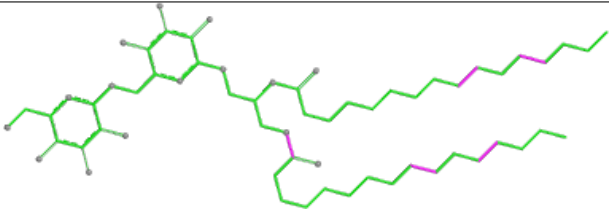
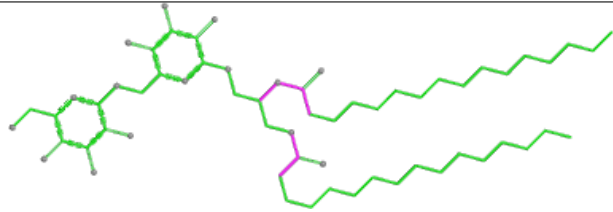
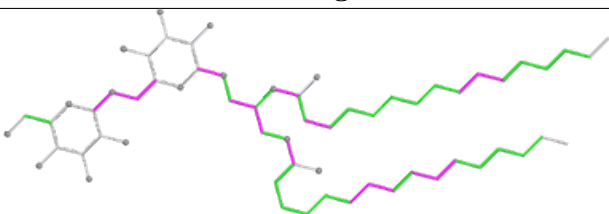
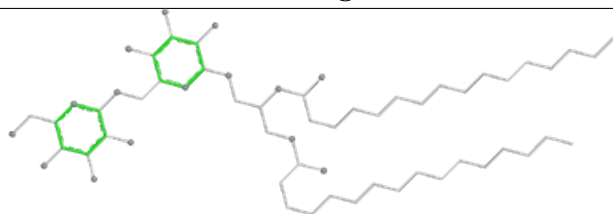


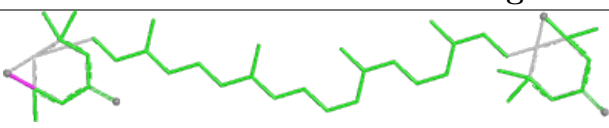
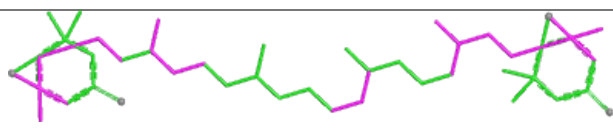
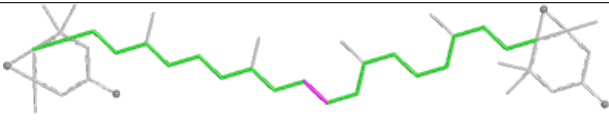
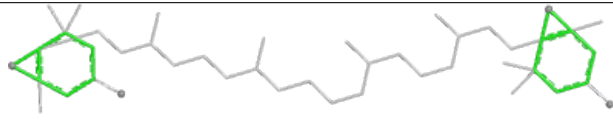


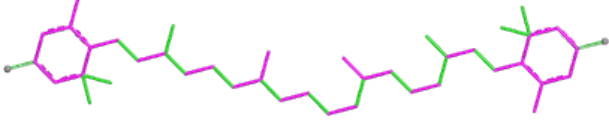
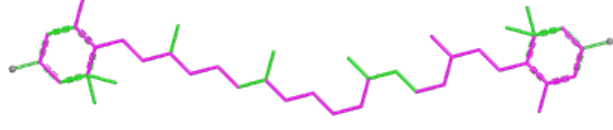
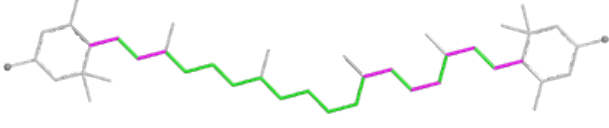
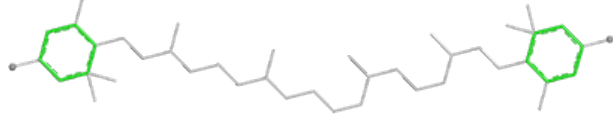


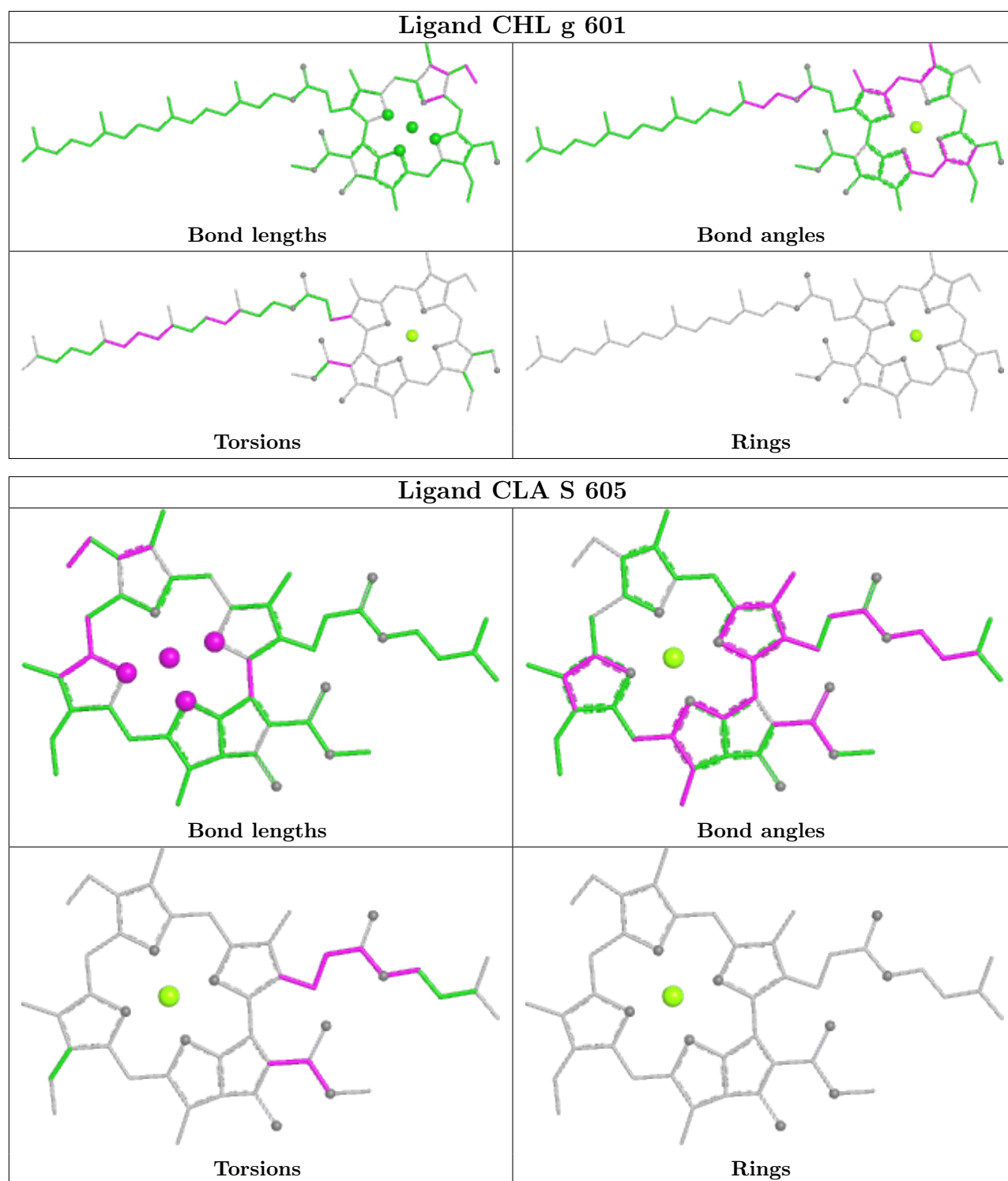


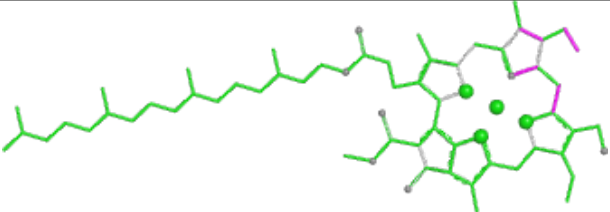
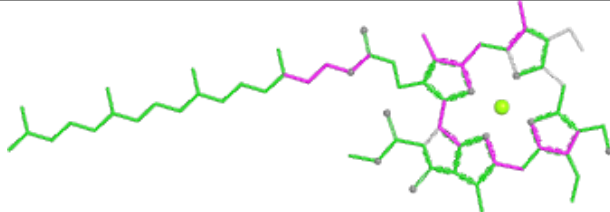
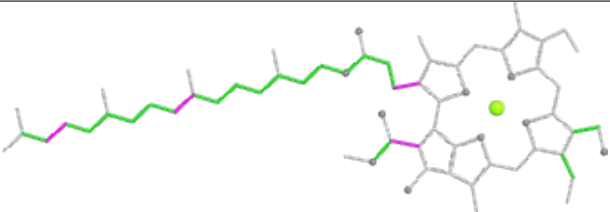
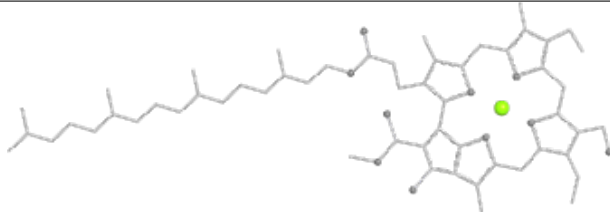
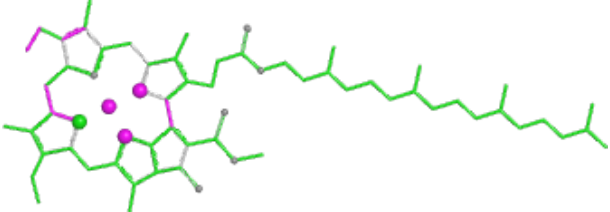
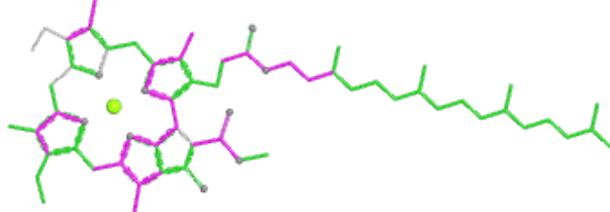
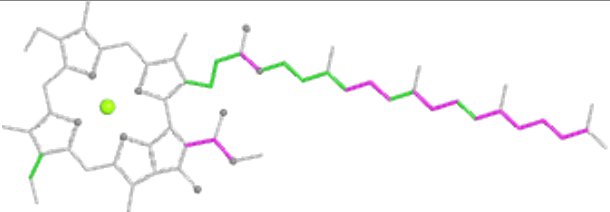
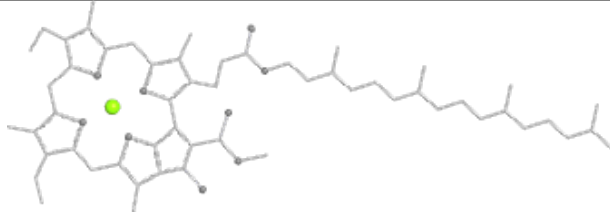
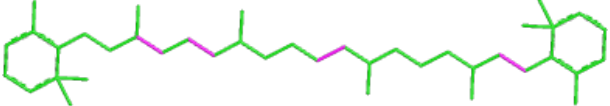
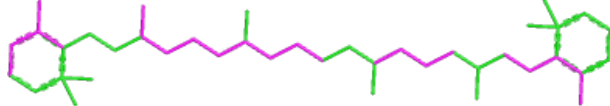
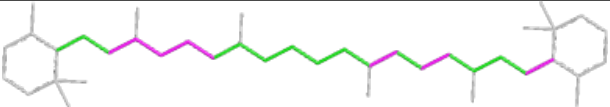
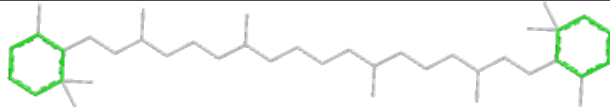


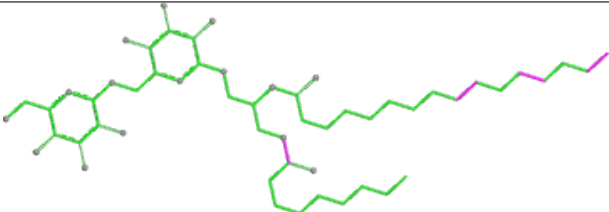
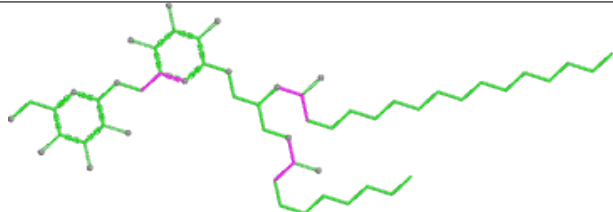
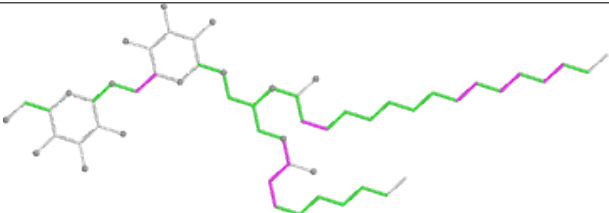
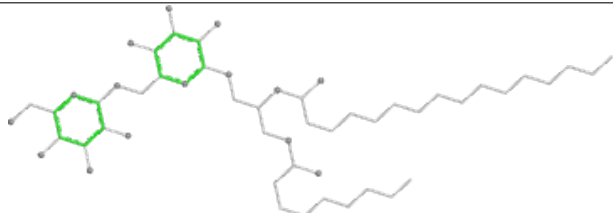
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

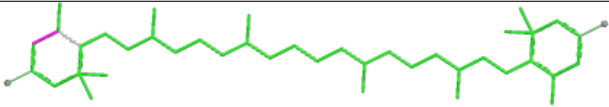
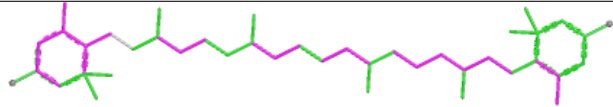
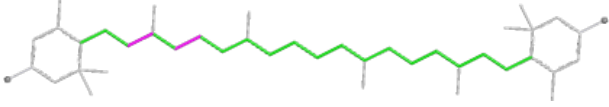
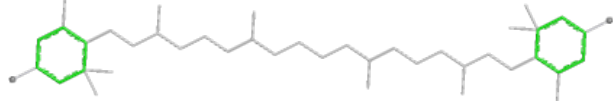
Ligand XAT G 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

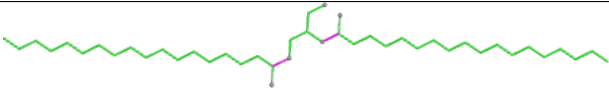
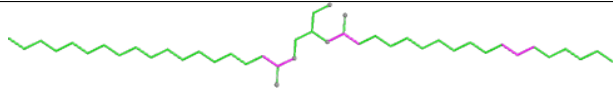
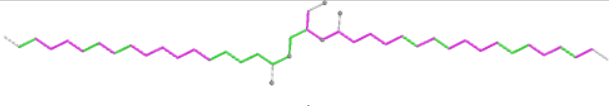
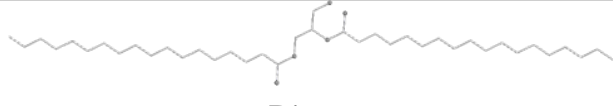
Ligand C7Z B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

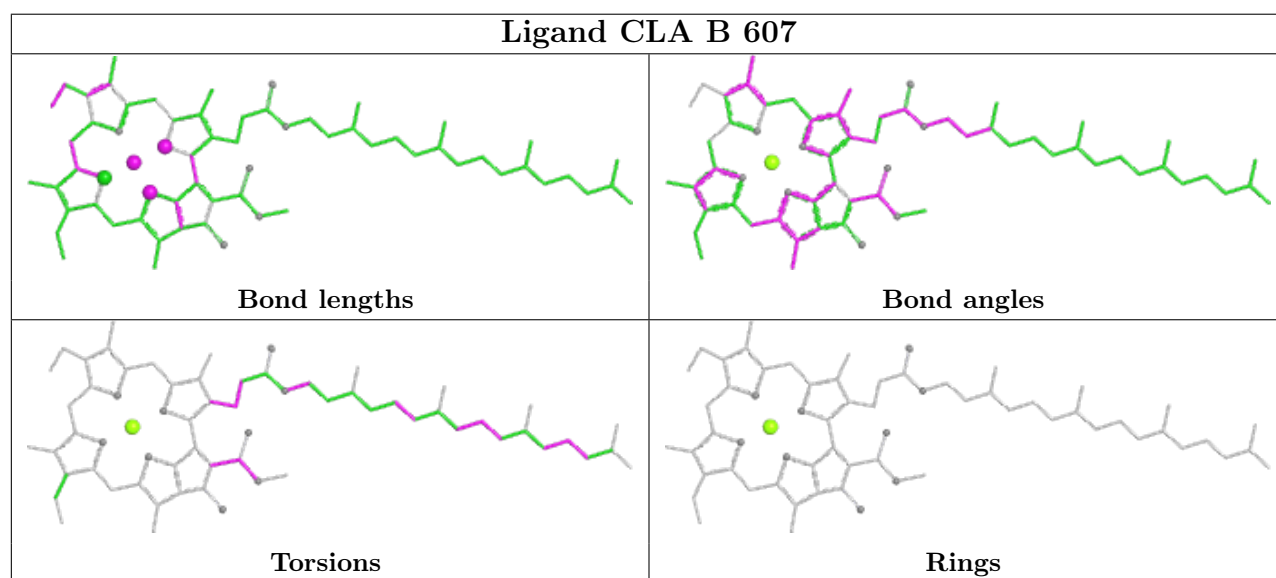
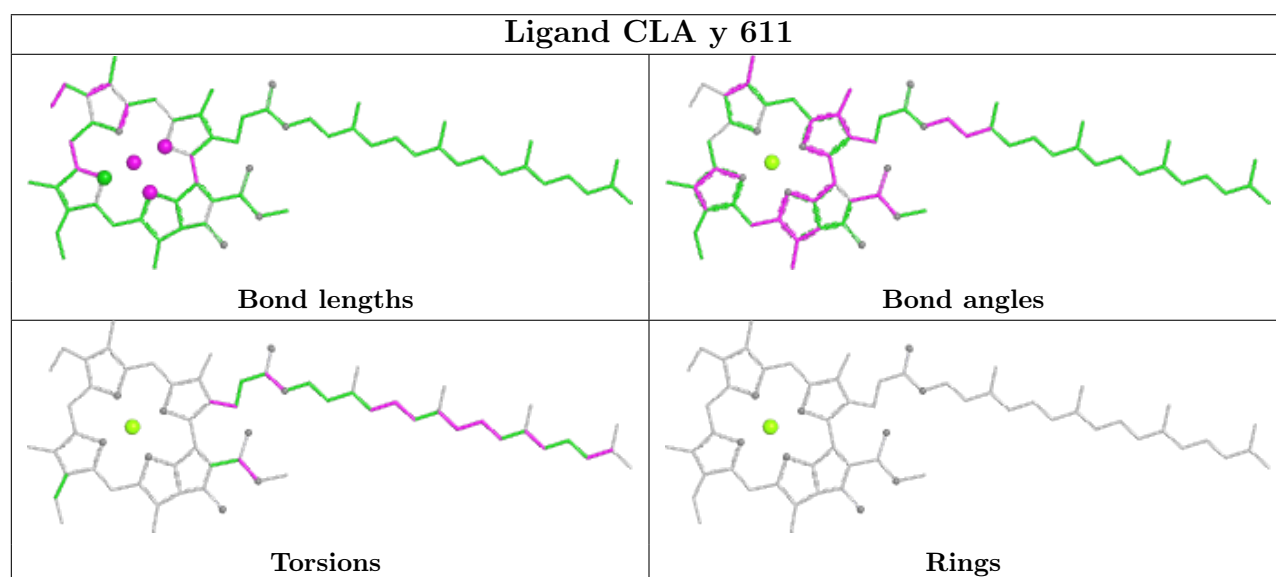
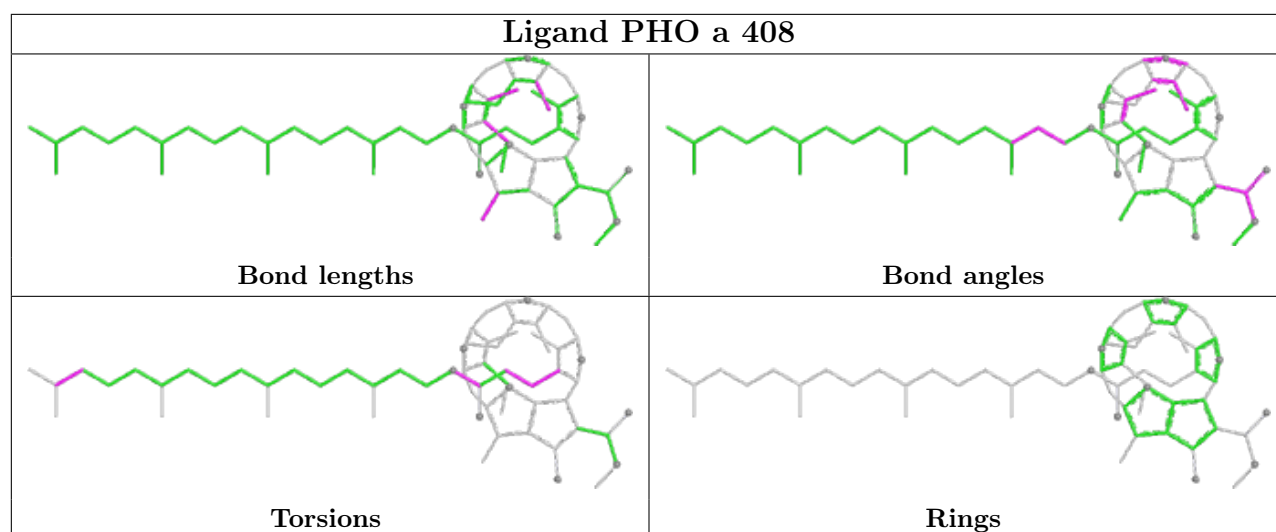


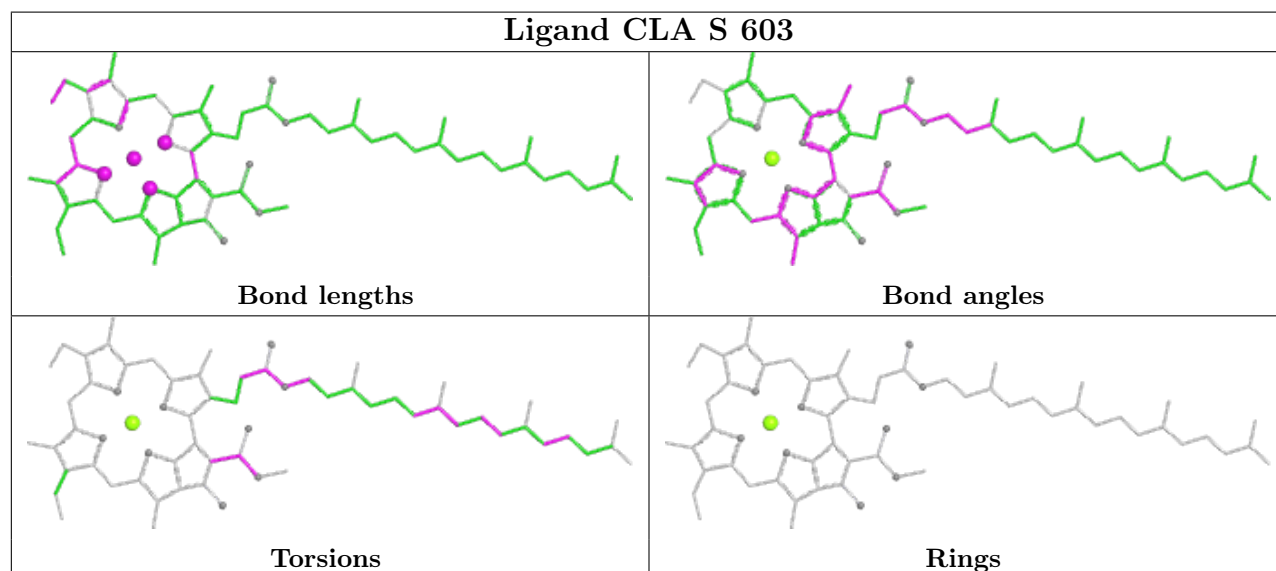
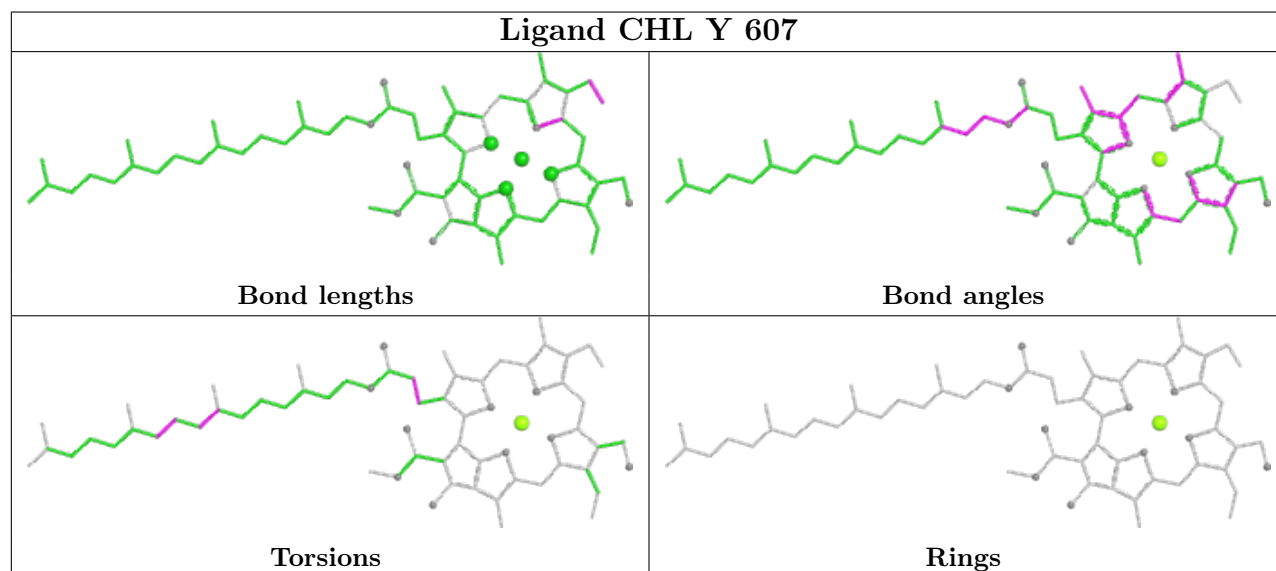
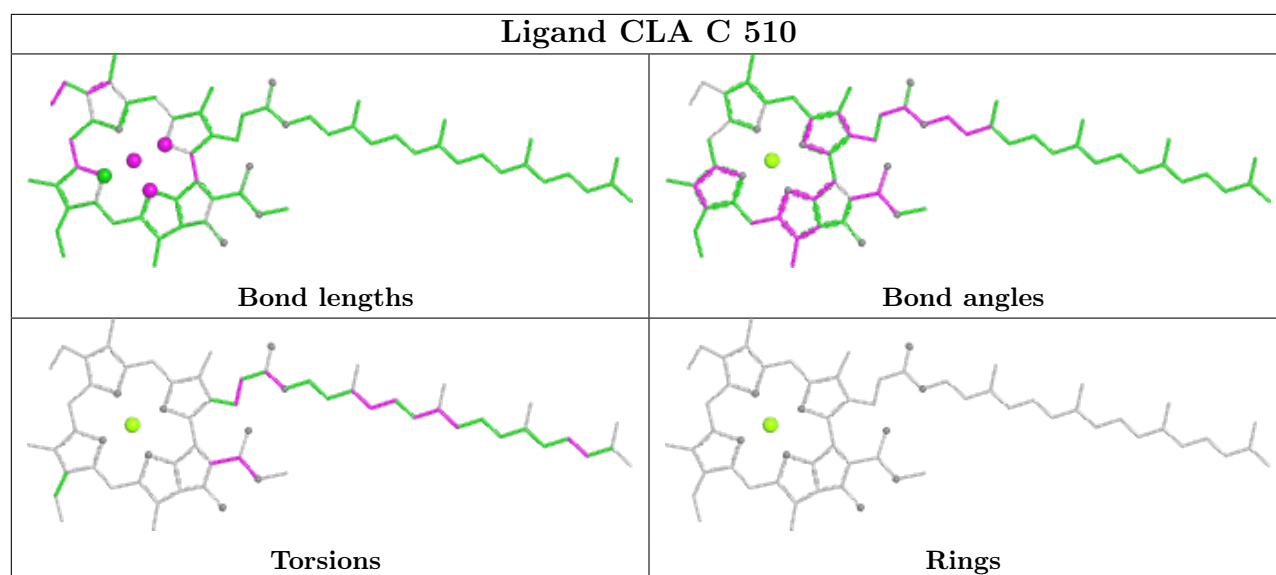
Ligand CHL Y 606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA C 507	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

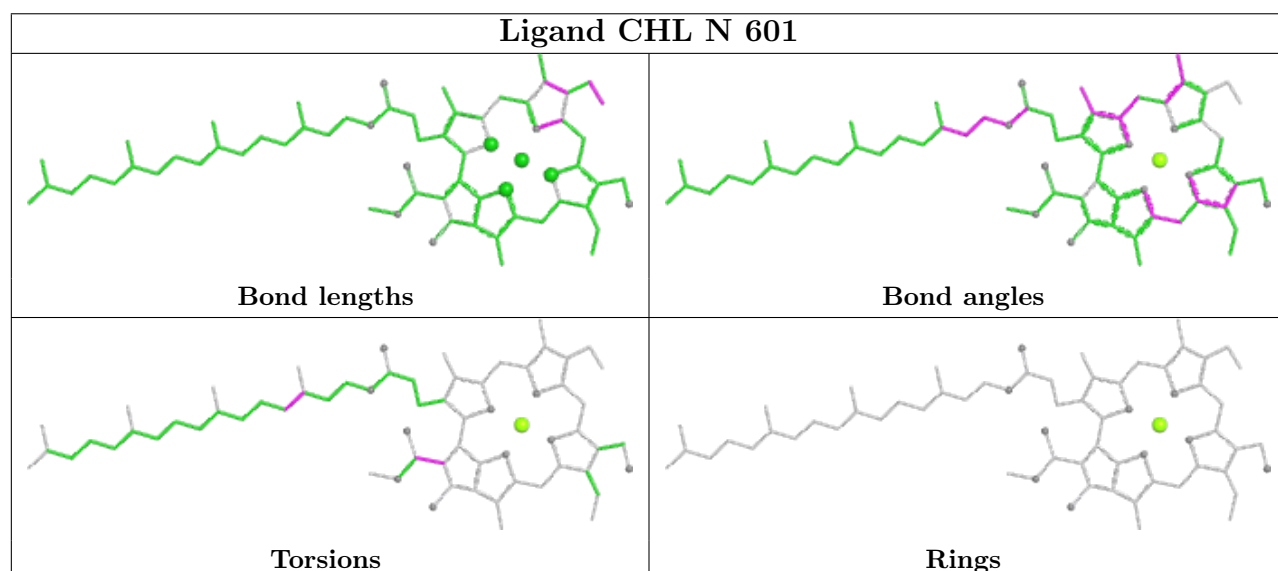
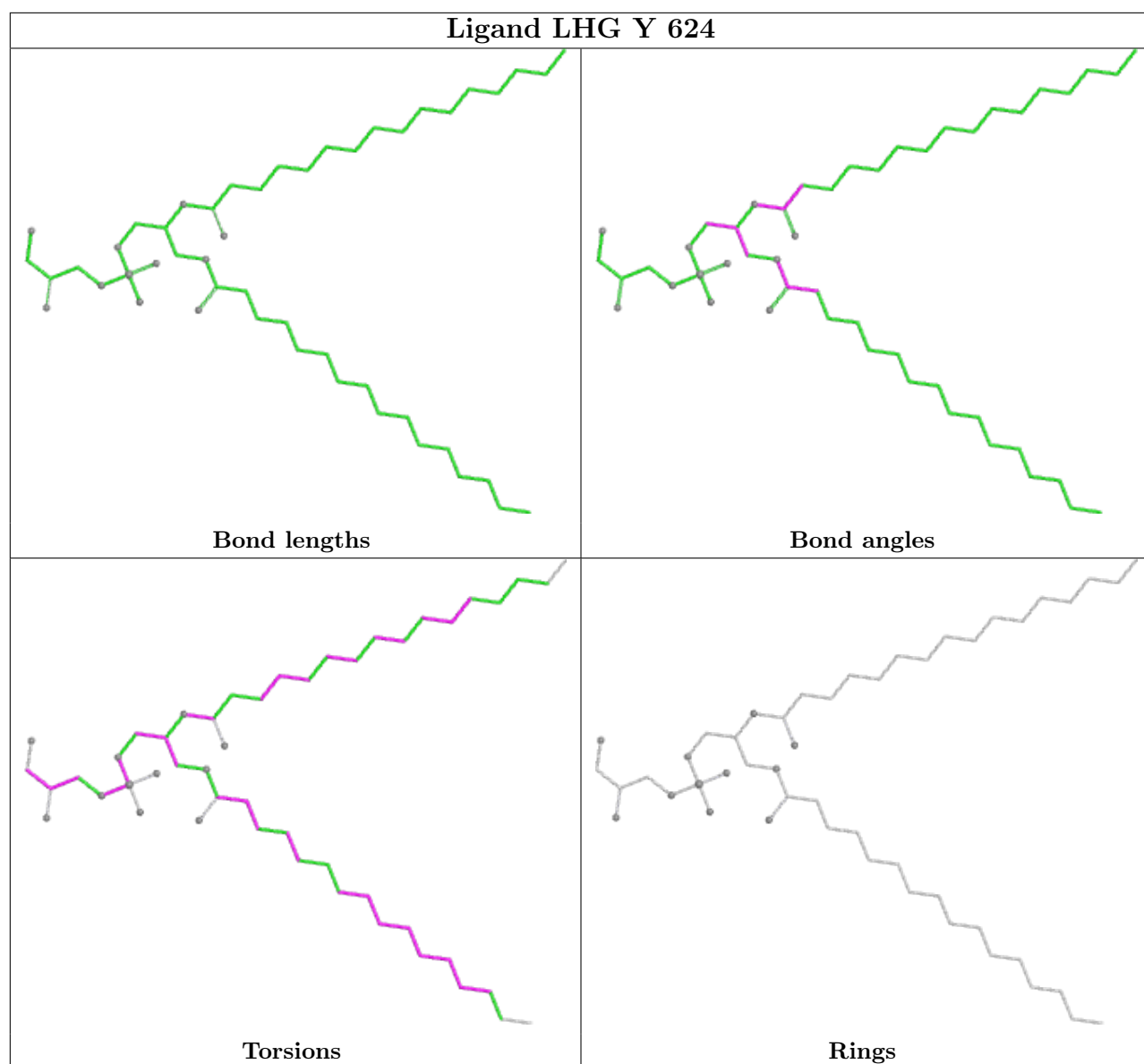
Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT g 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

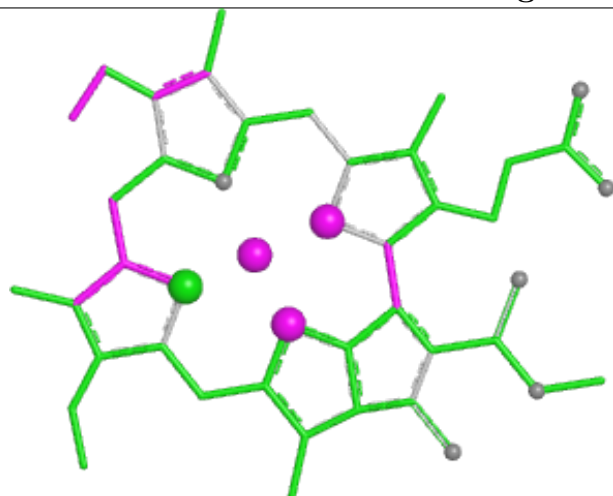
Ligand DGA b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings



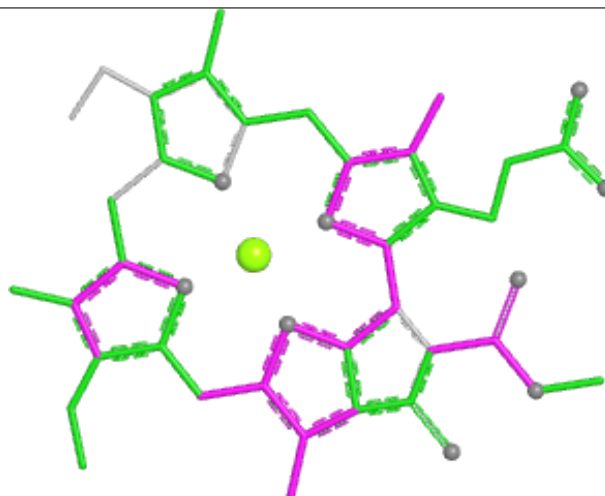




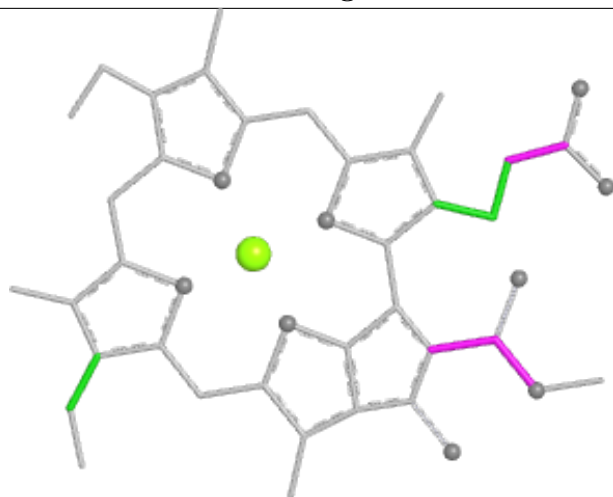
Ligand CLA n 612



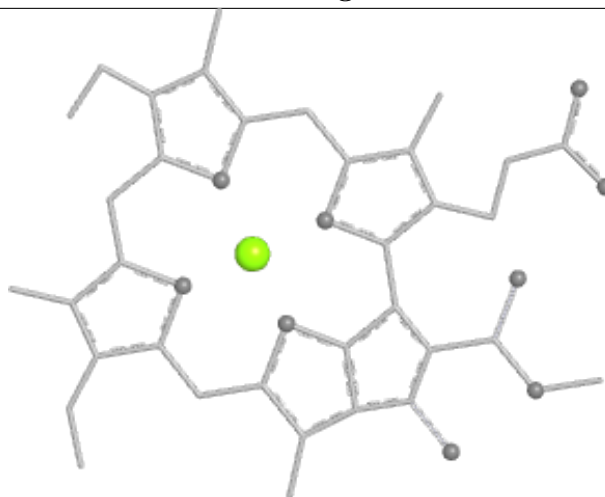
Bond lengths



Bond angles

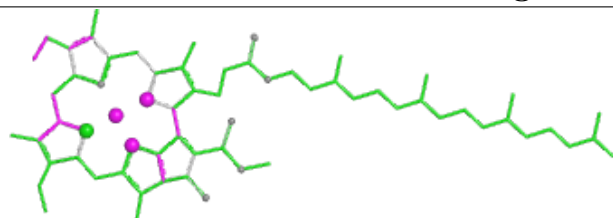


Torsions

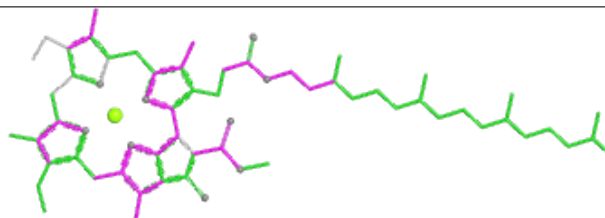


Rings

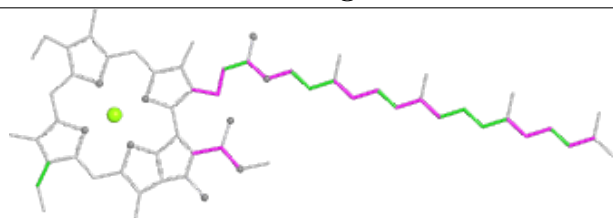
Ligand CLA G 602



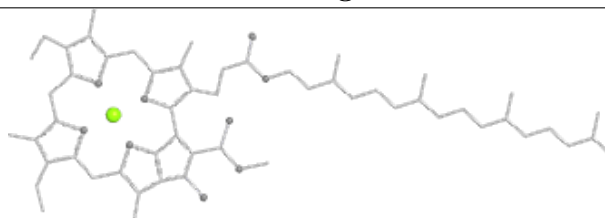
Bond lengths



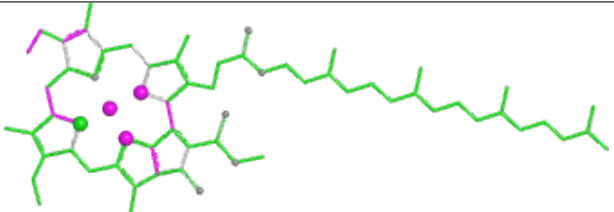
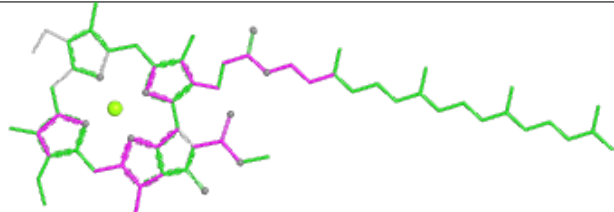
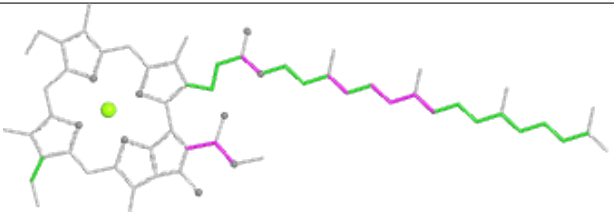
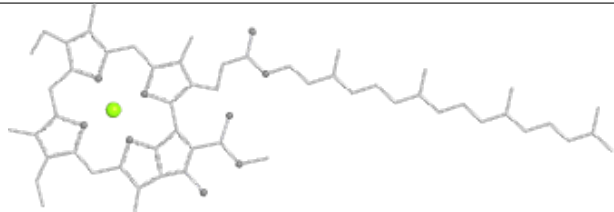
Bond angles

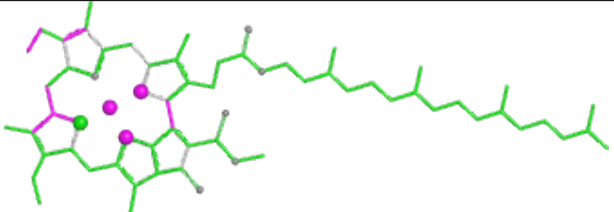
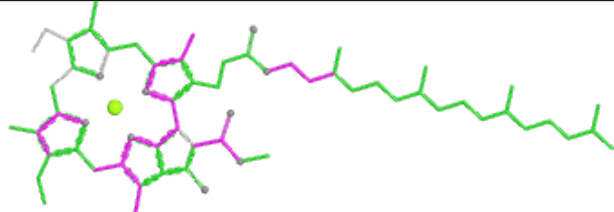
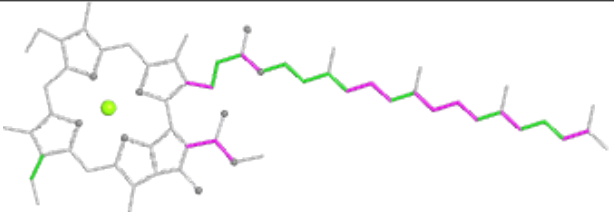
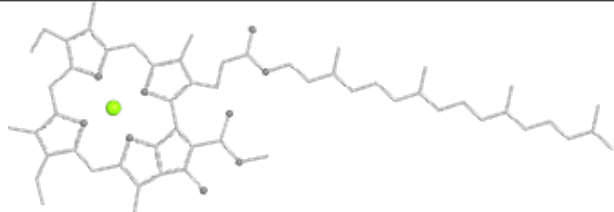


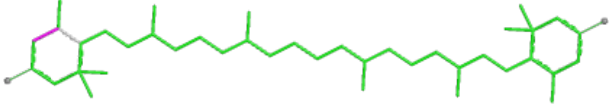
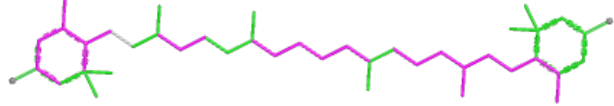
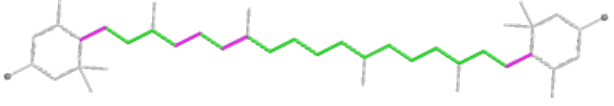
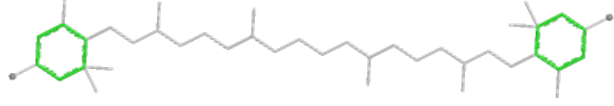
Torsions

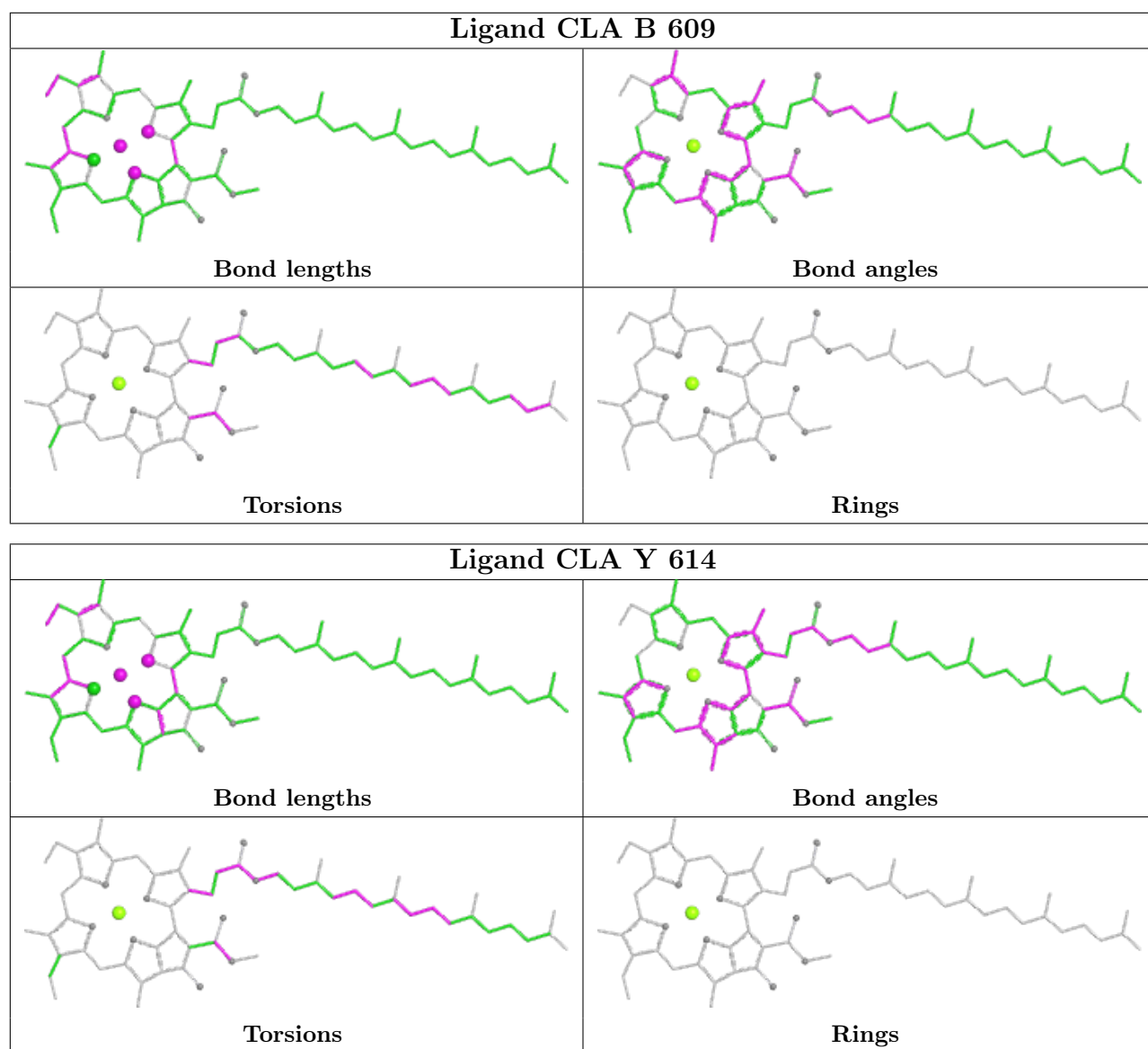


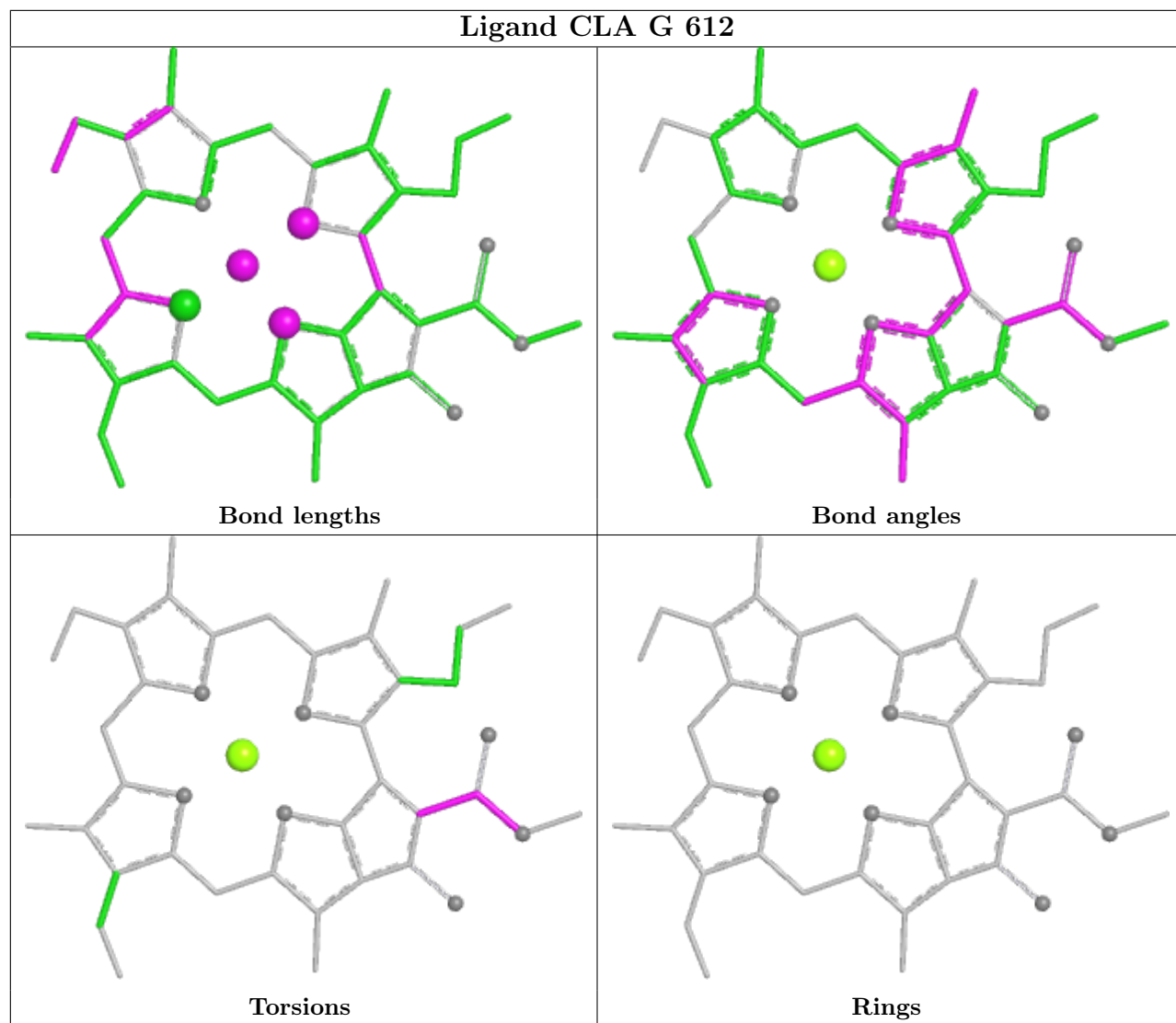
Rings

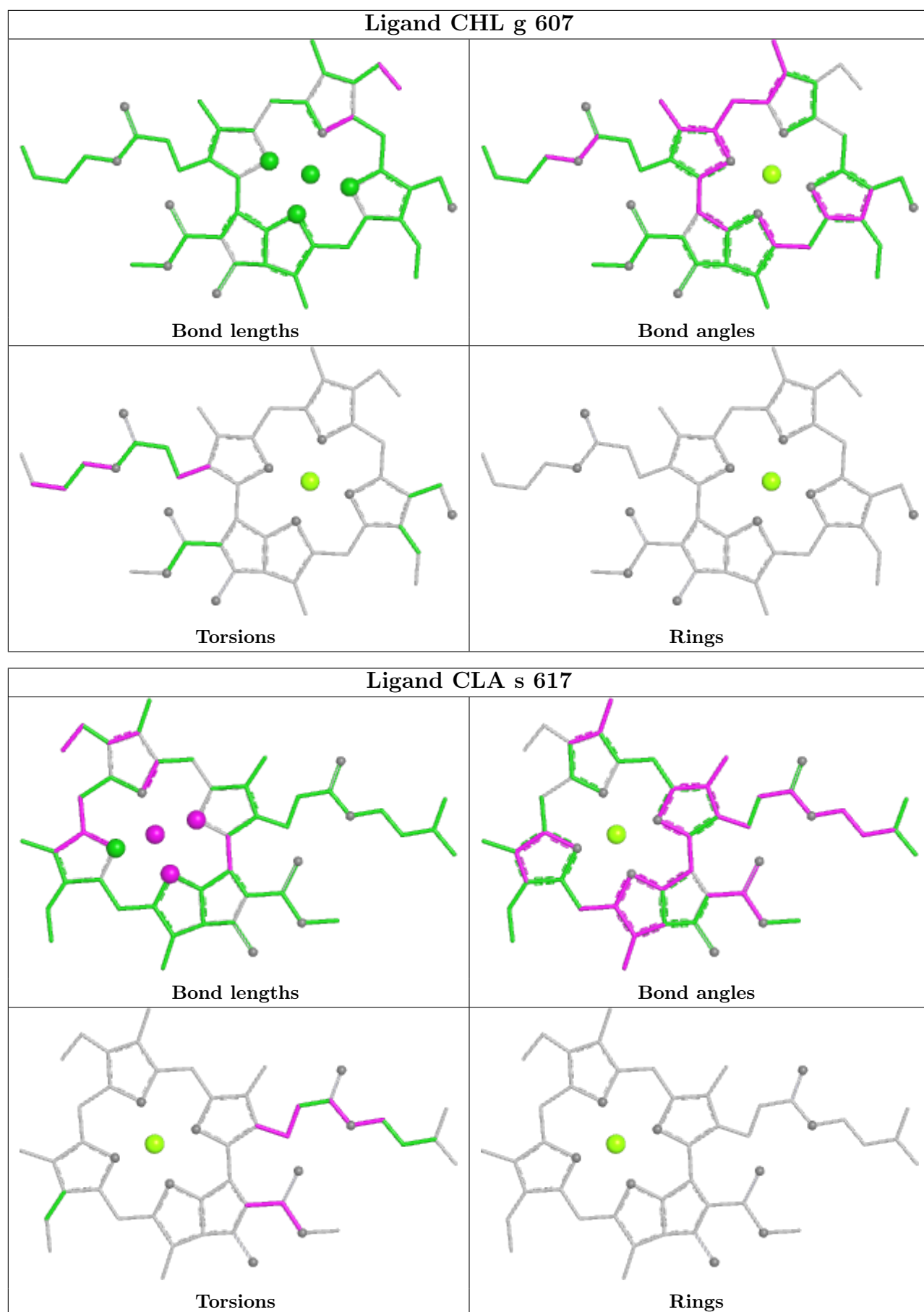
Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

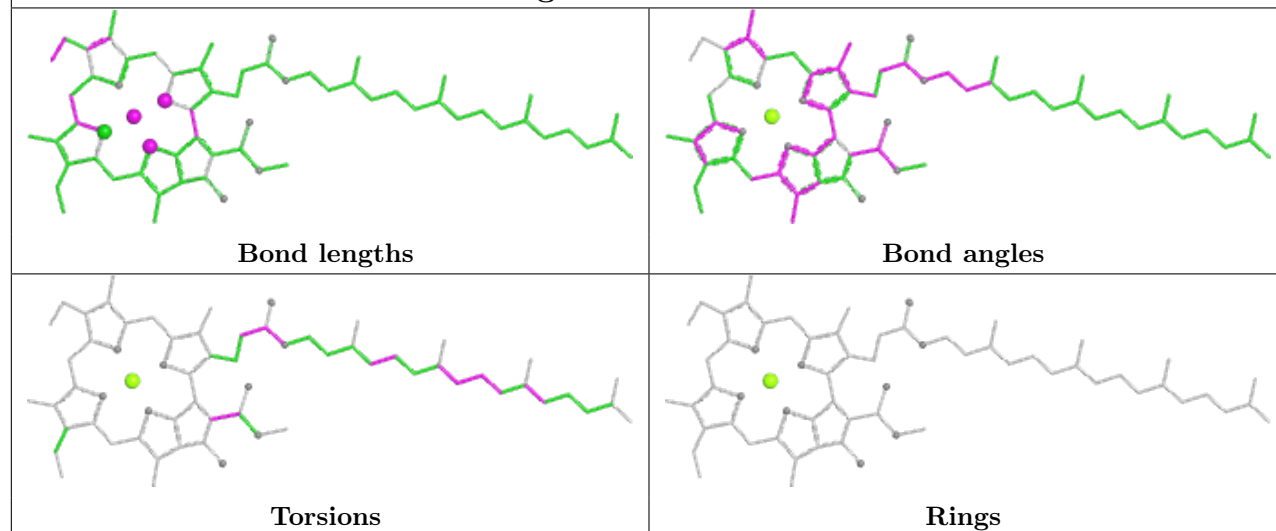
Ligand LUT n 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



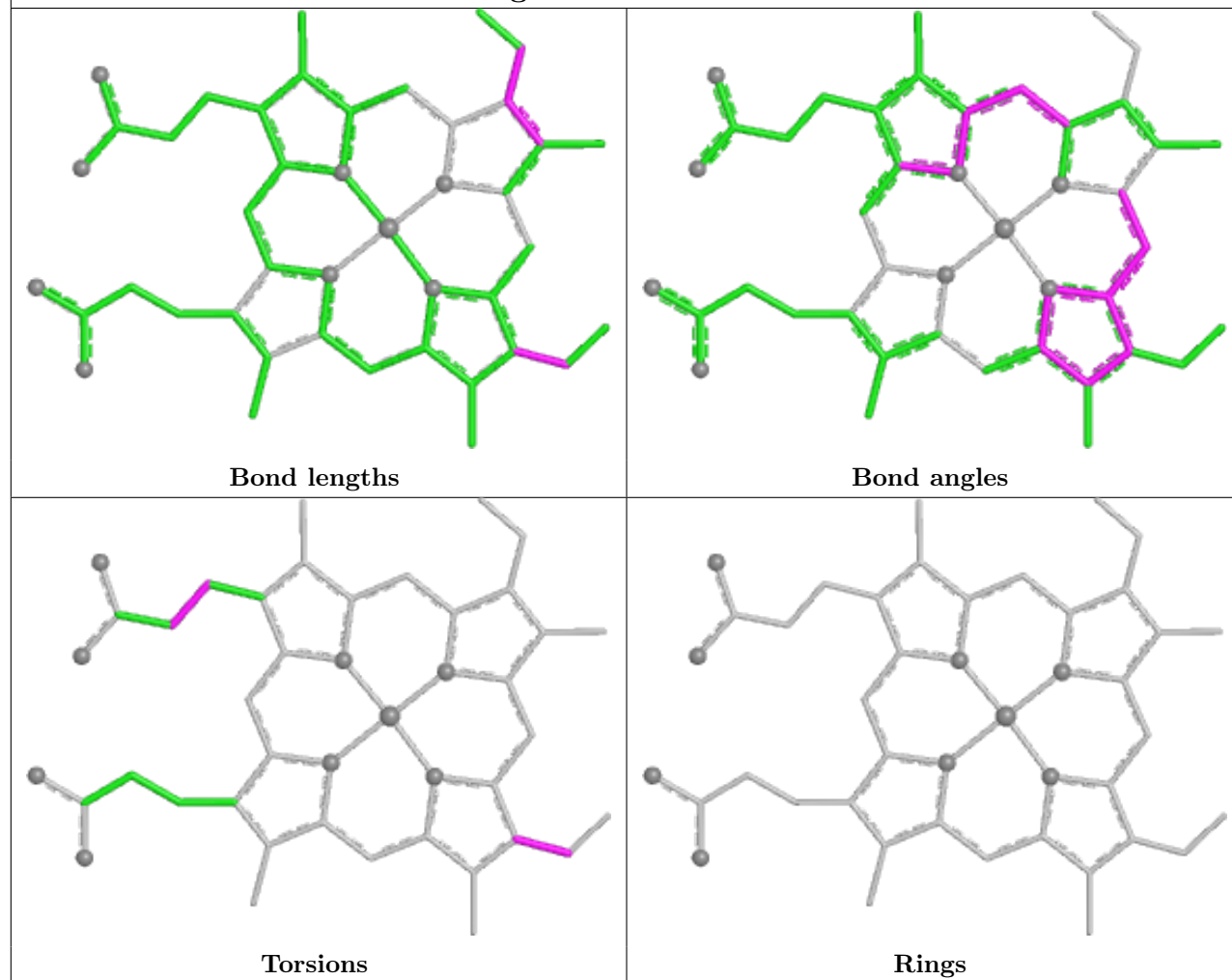


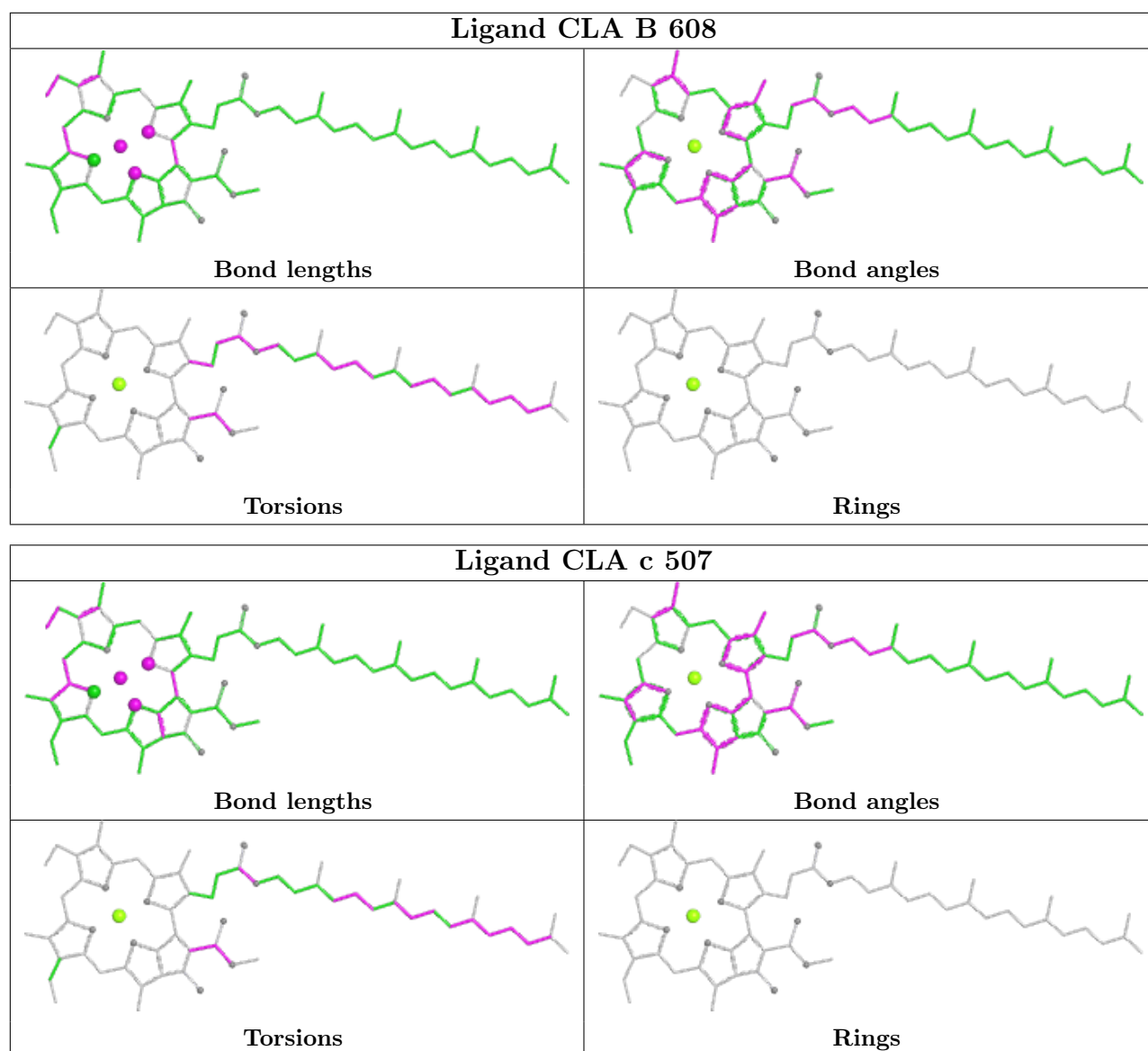


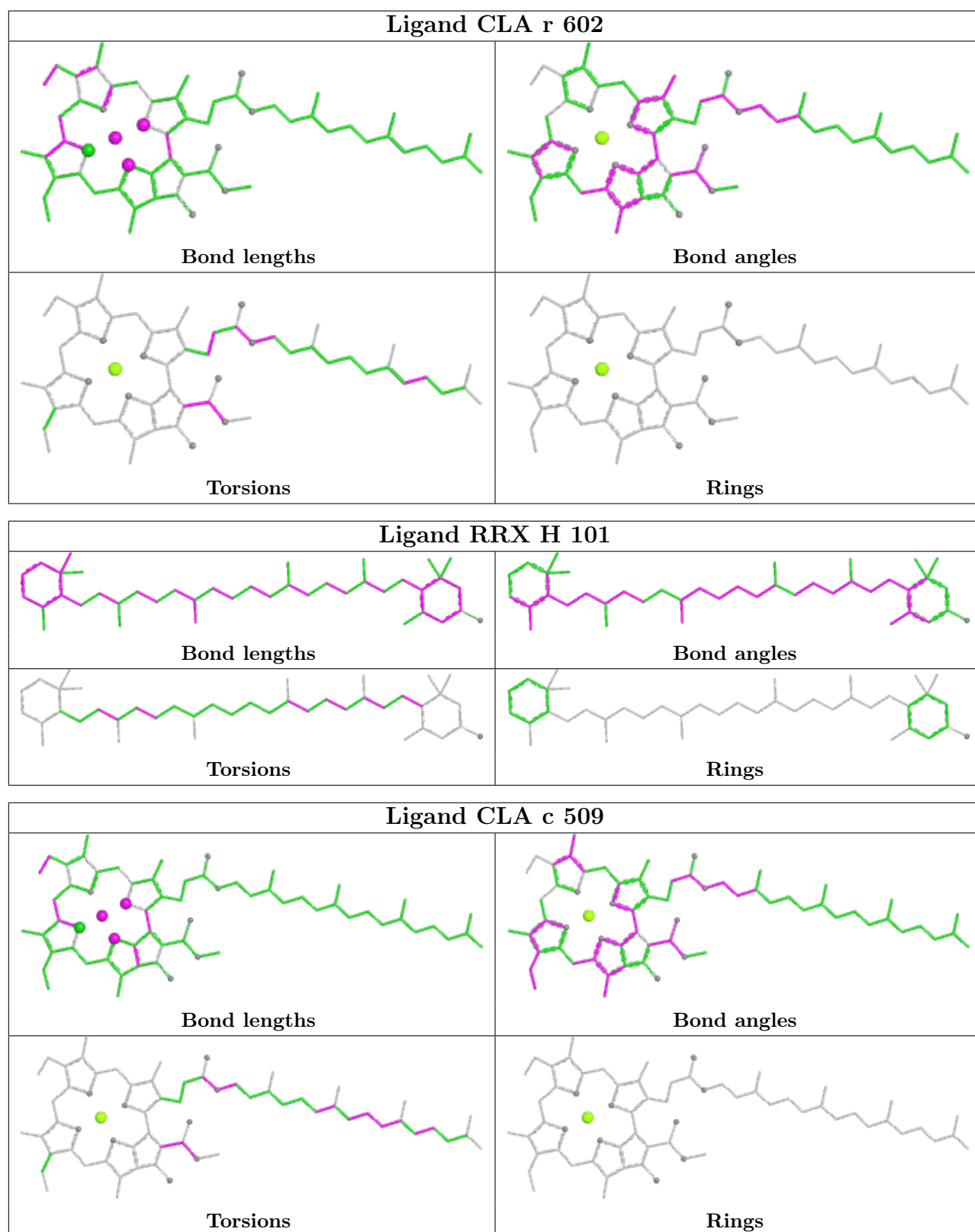
Ligand CLA c 508

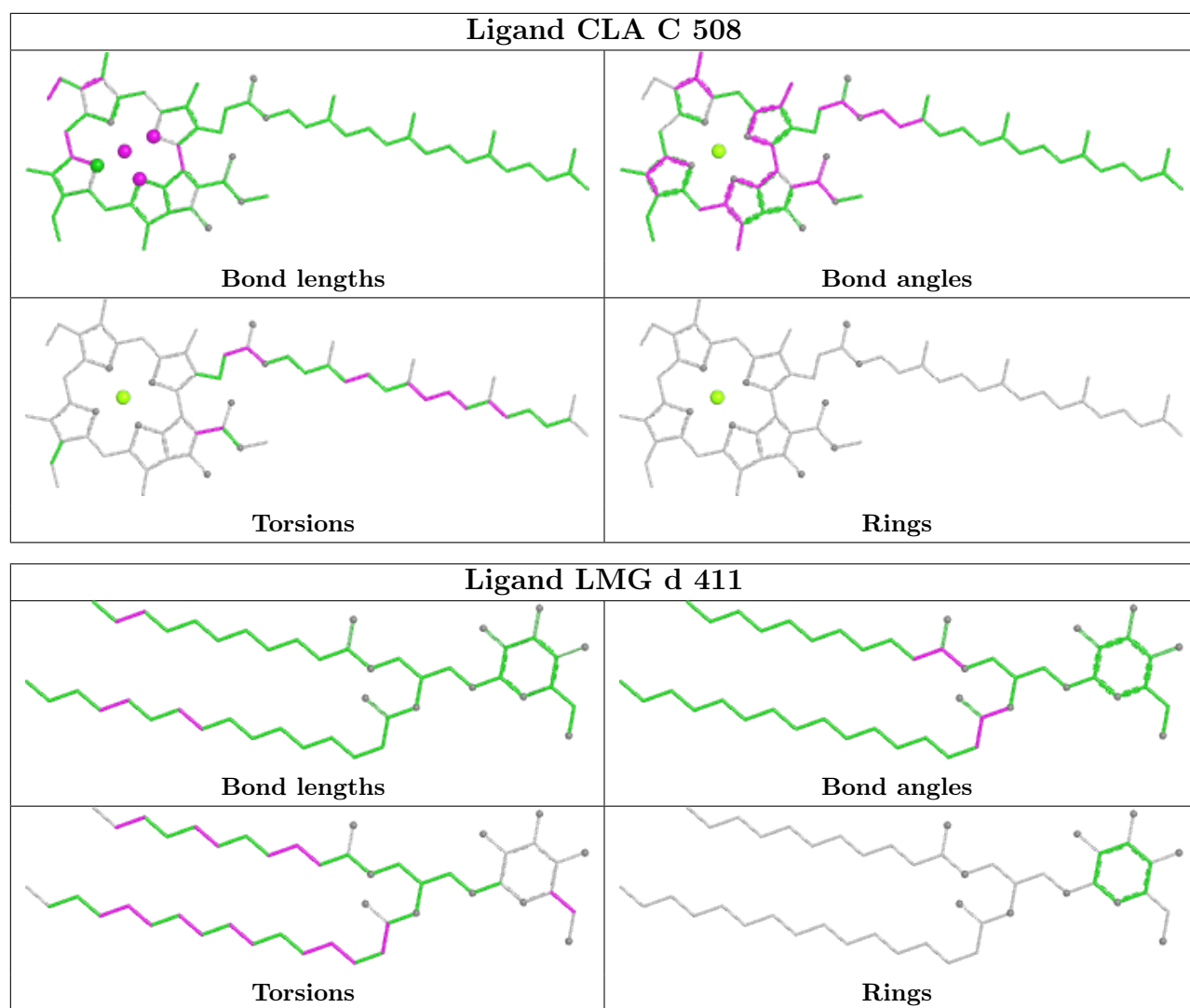


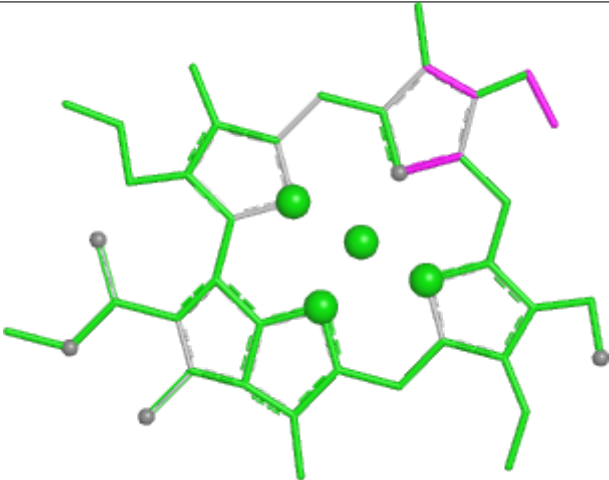
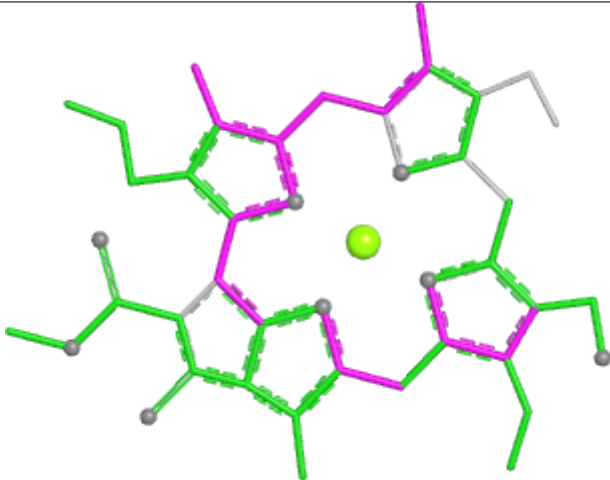
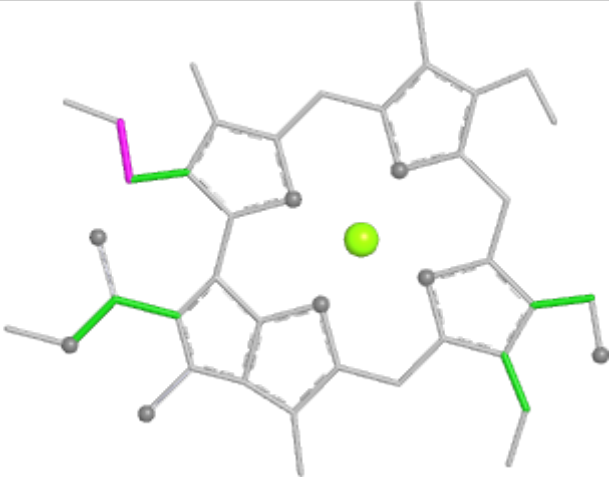
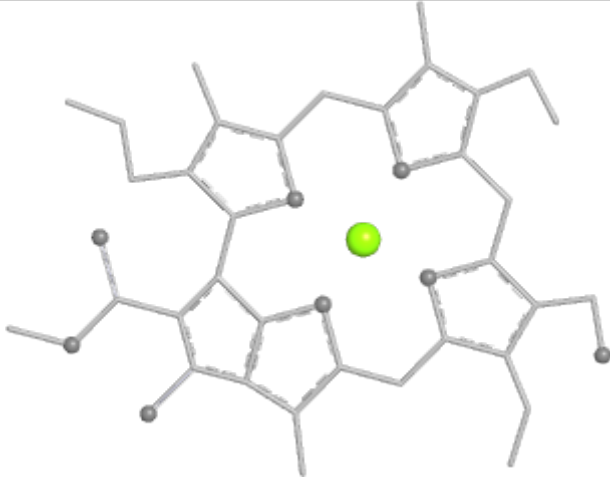
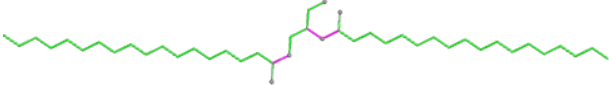
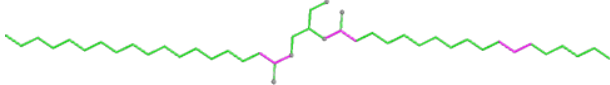
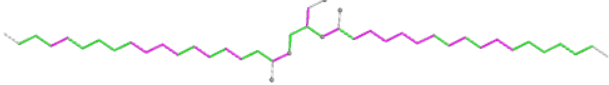
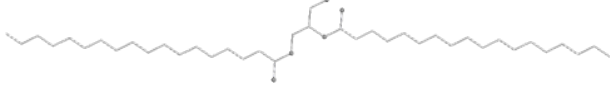
Ligand HEM F 101

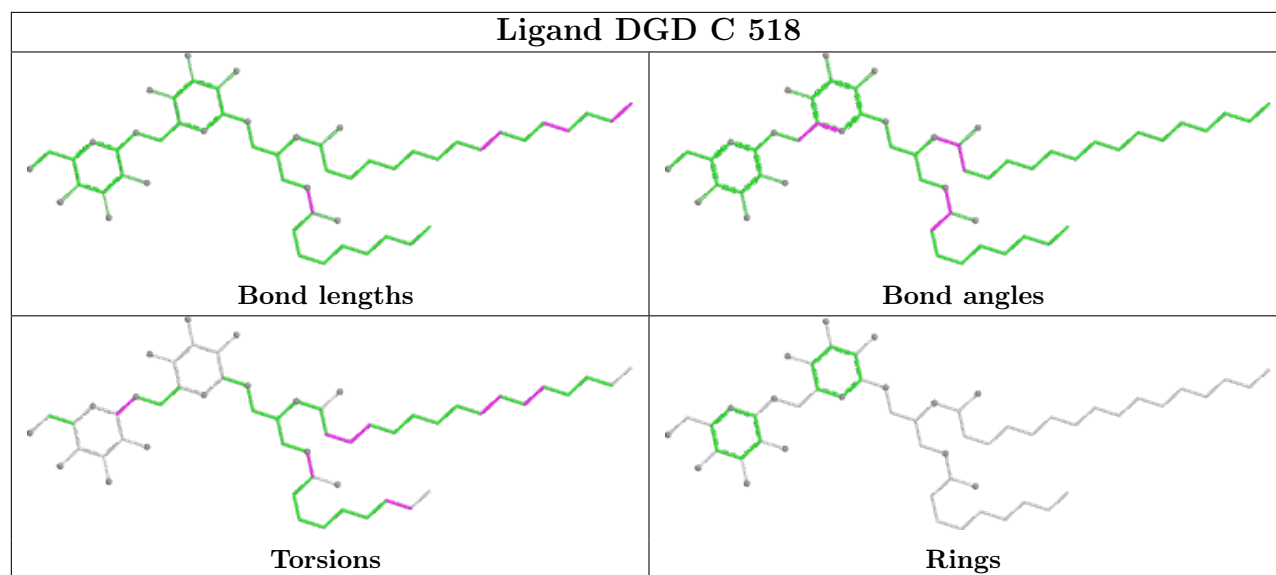
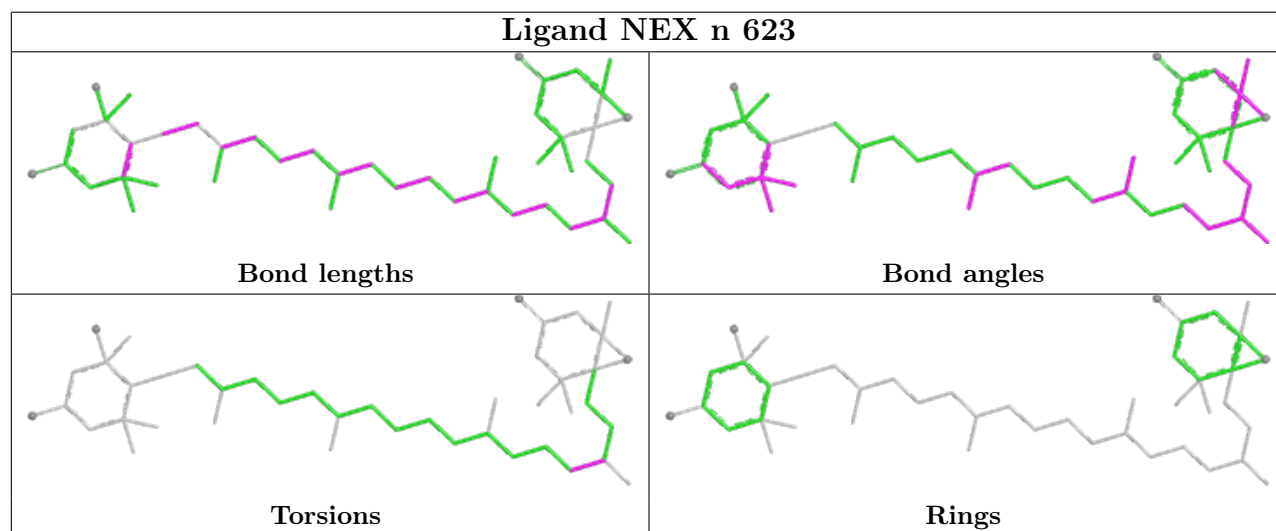
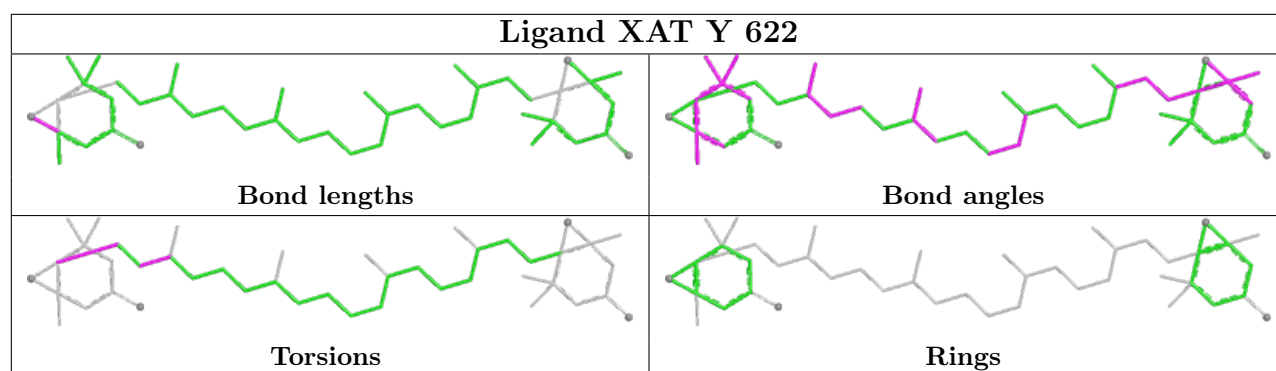


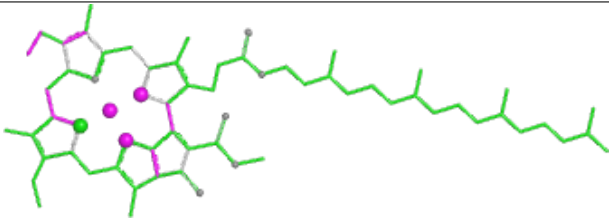
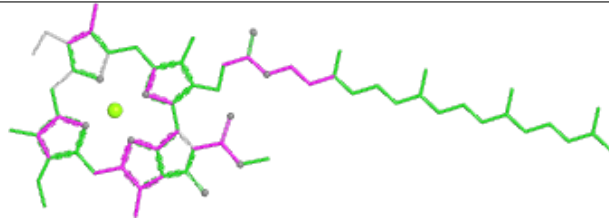
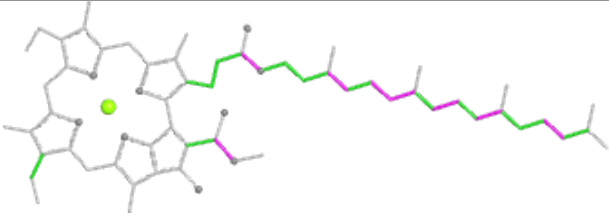
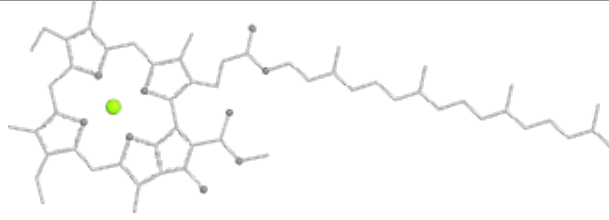


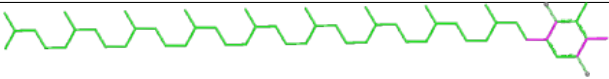
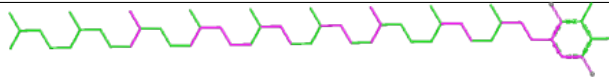
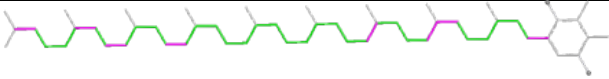
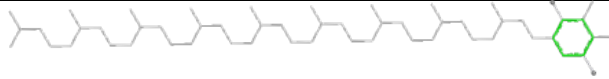


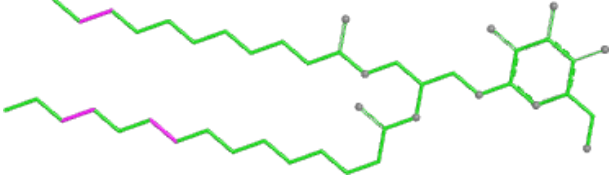
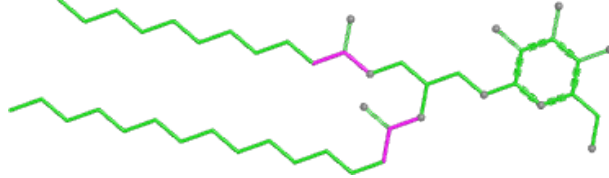
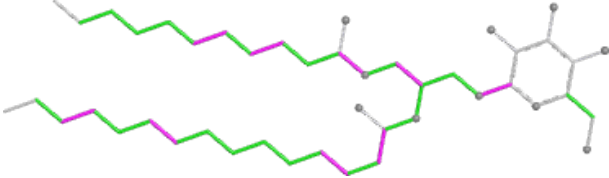
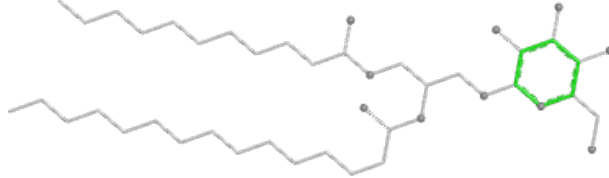


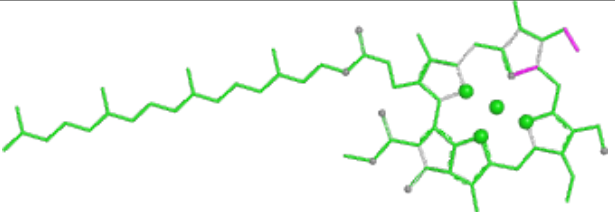
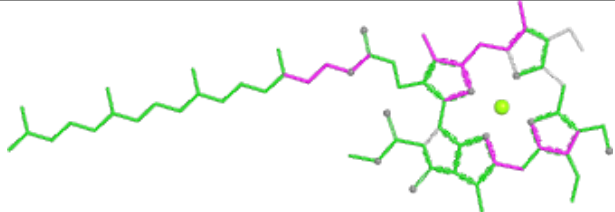
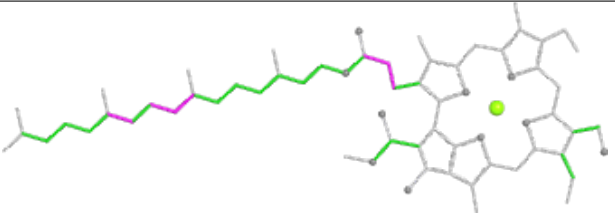
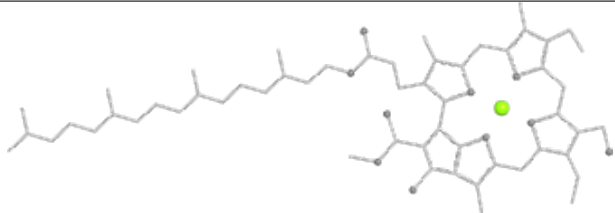
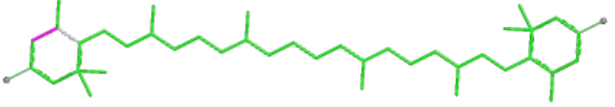
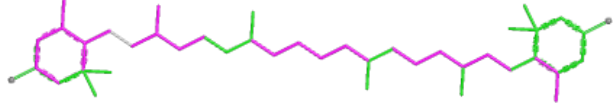
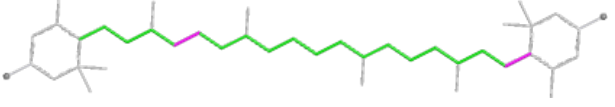
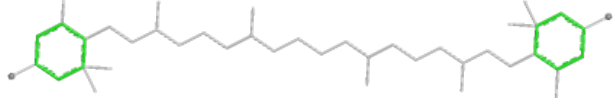
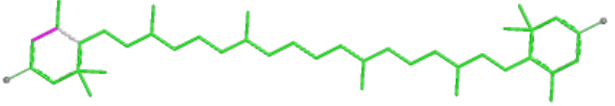
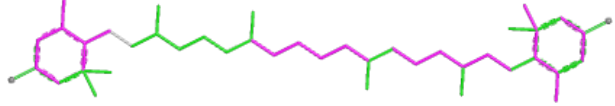
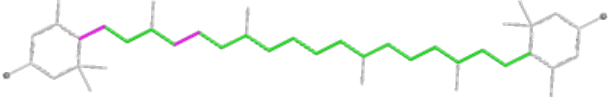
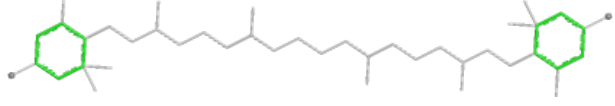
Ligand CHL g 608	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand DGA c 524	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings

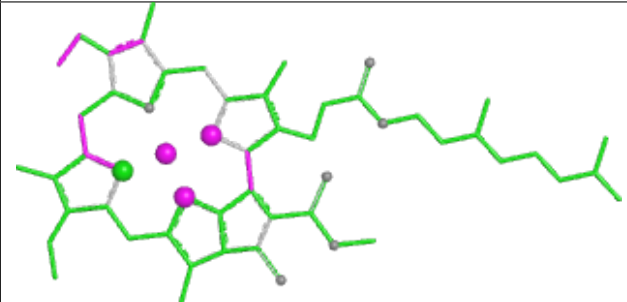
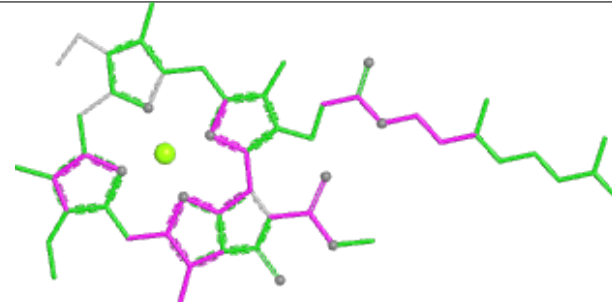
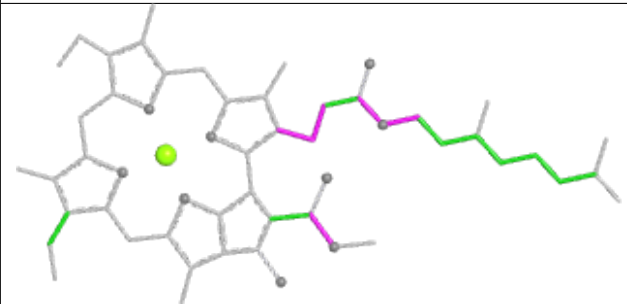
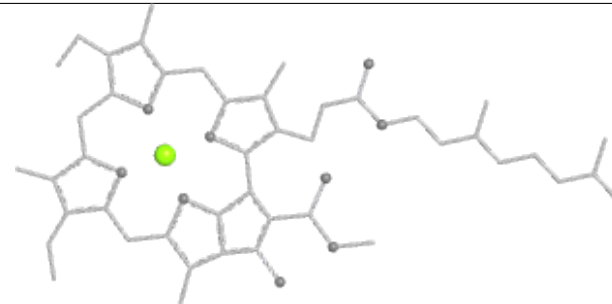


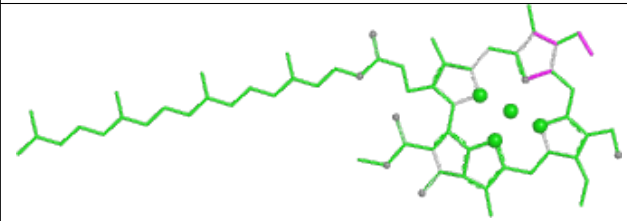
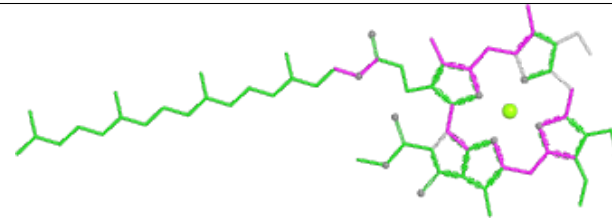
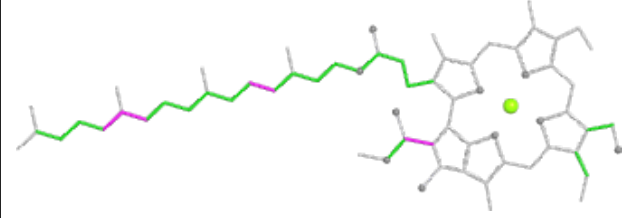
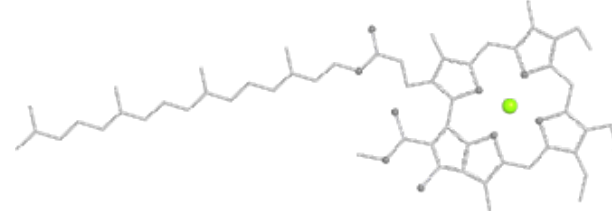
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

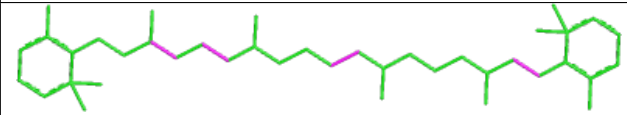
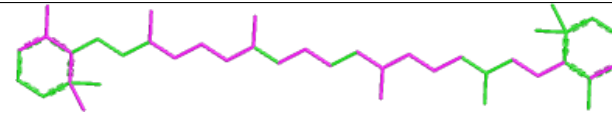
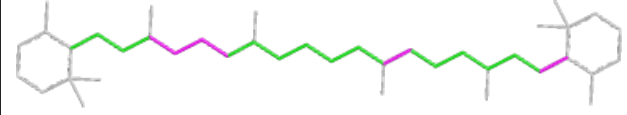
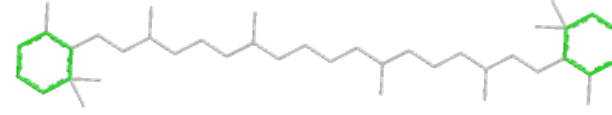
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

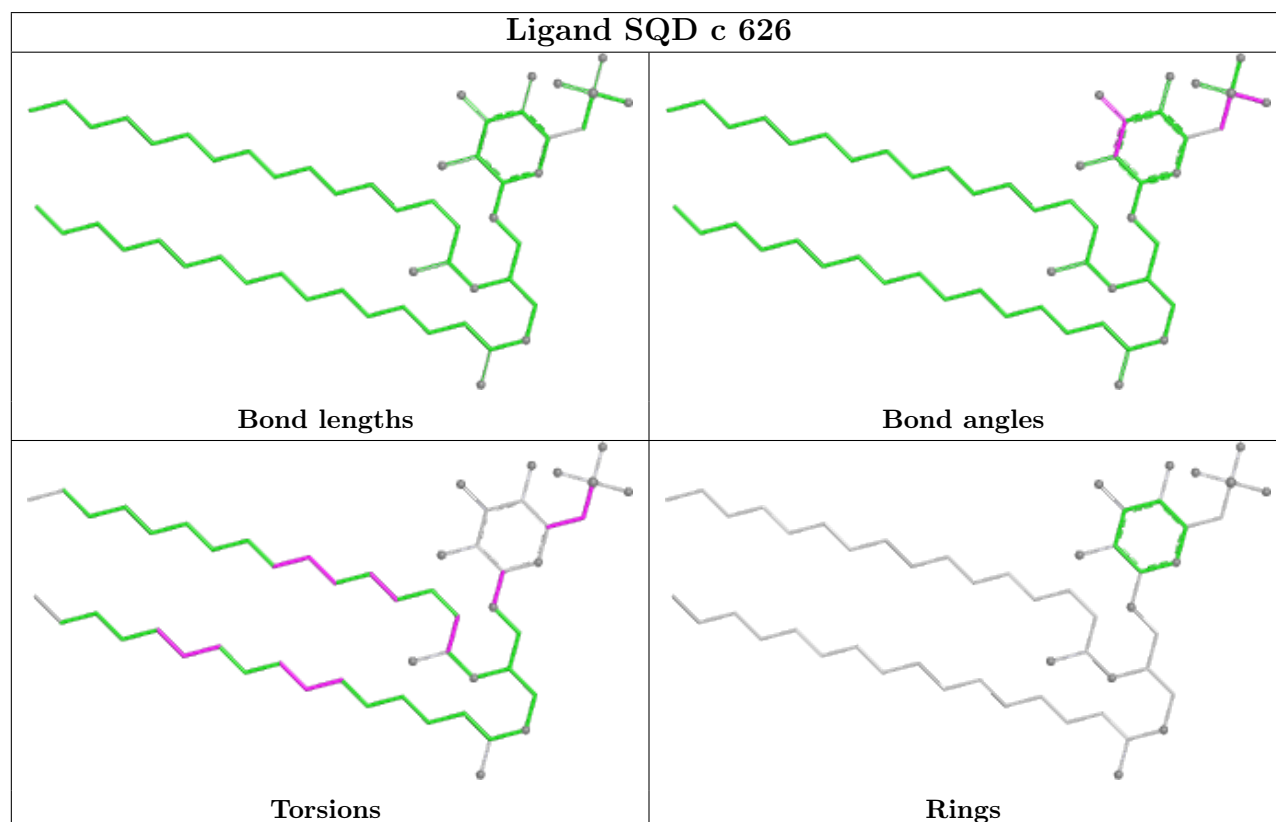
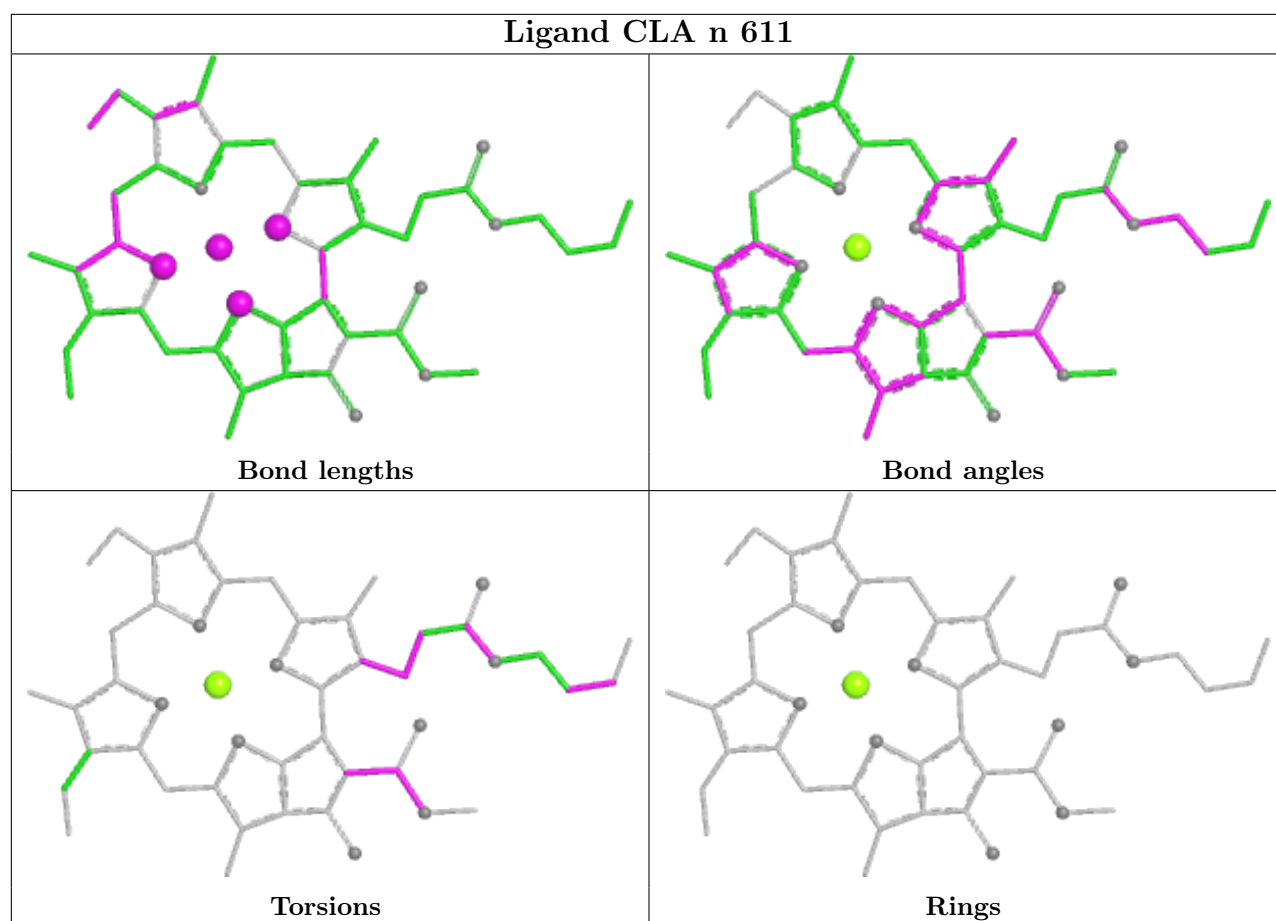
Ligand LMG J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

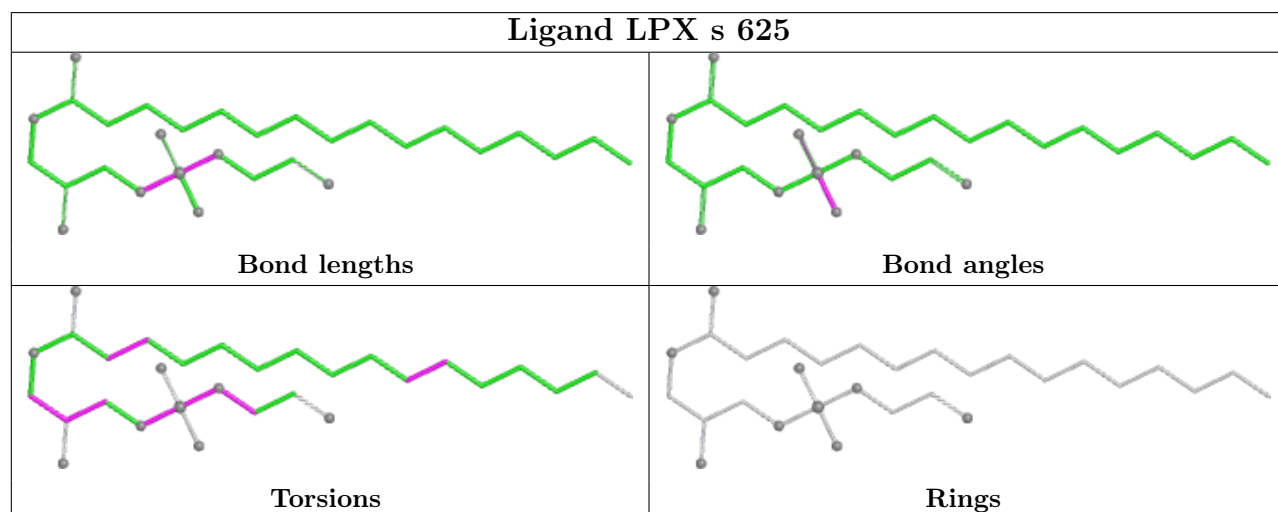
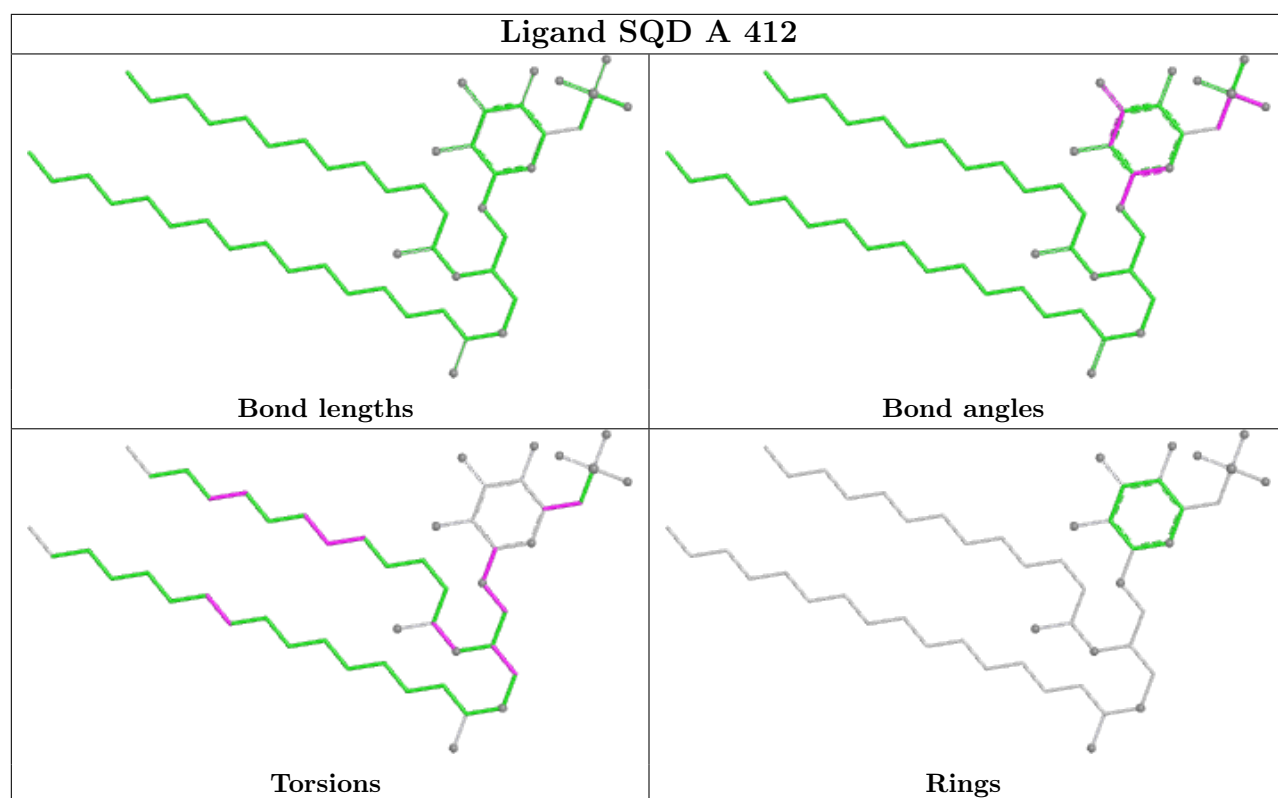
Ligand CHL N 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT N 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT N 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA s 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

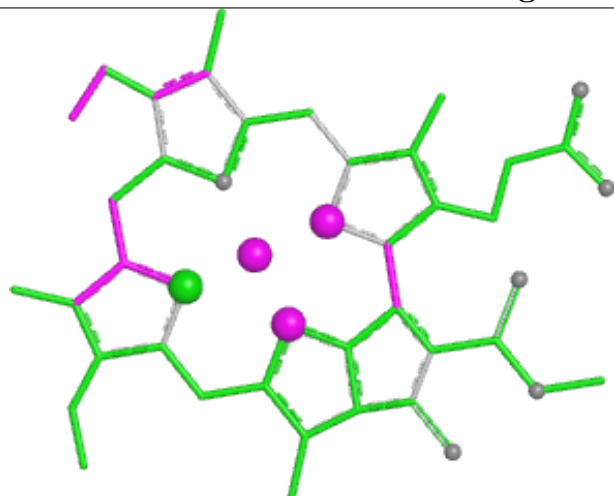
Ligand CHL g 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

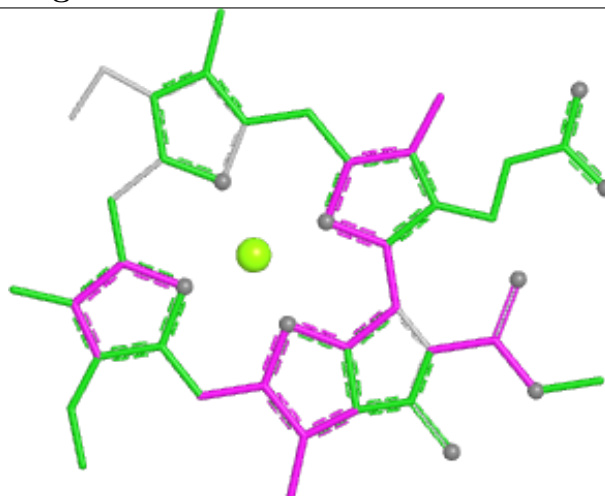




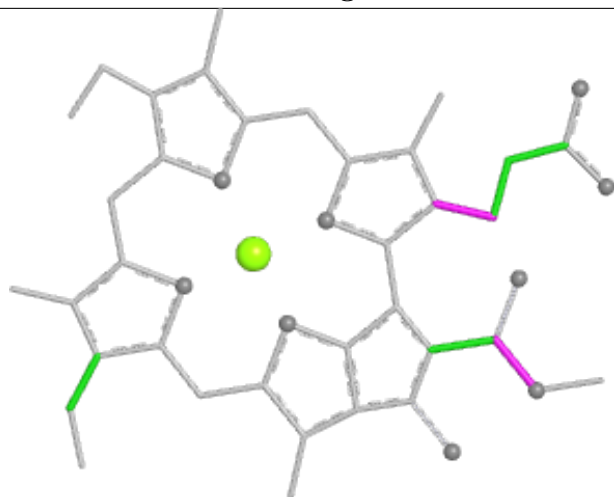
Ligand CLA g 611



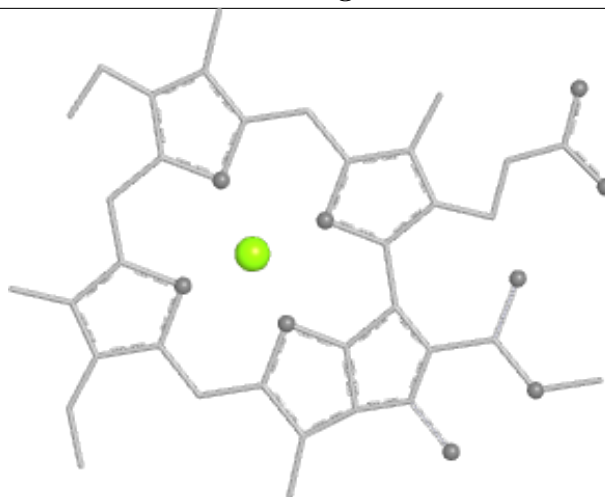
Bond lengths



Bond angles

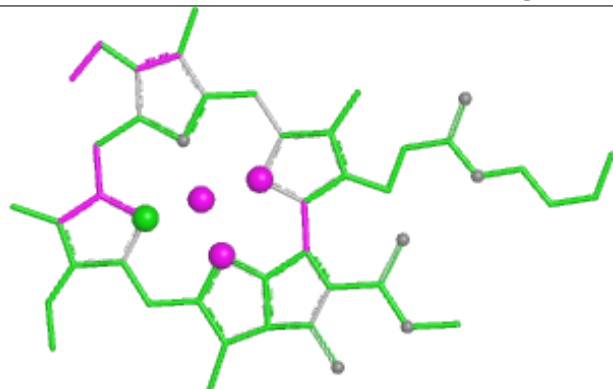


Torsions

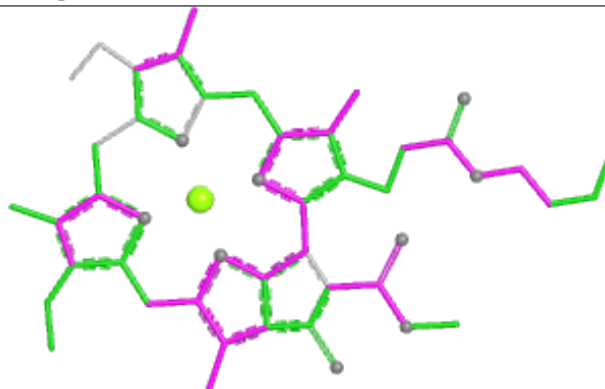


Rings

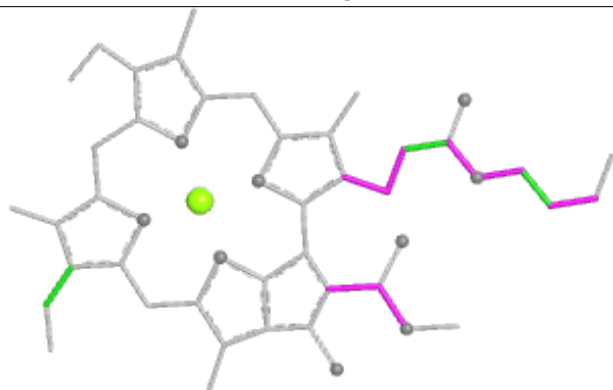
Ligand CLA g 604



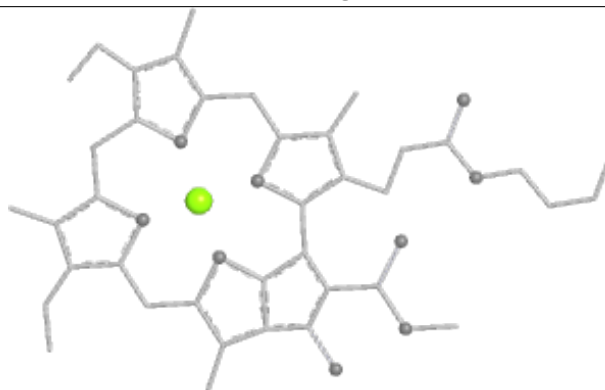
Bond lengths



Bond angles

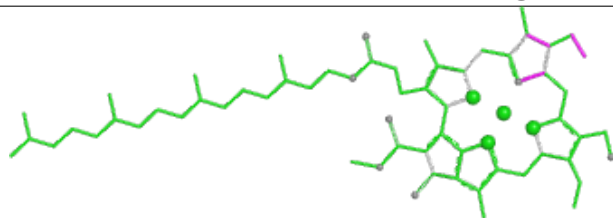


Torsions

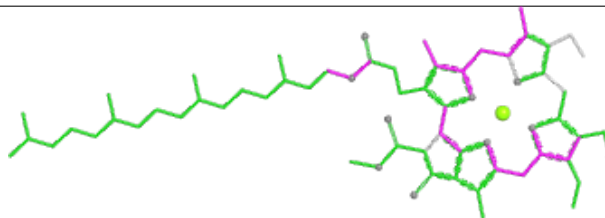


Rings

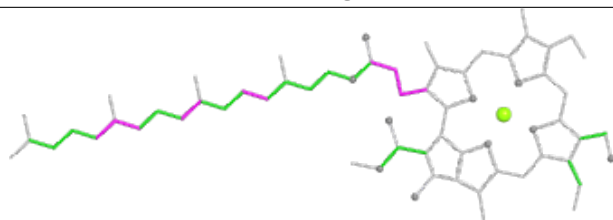
Ligand CHL N 605



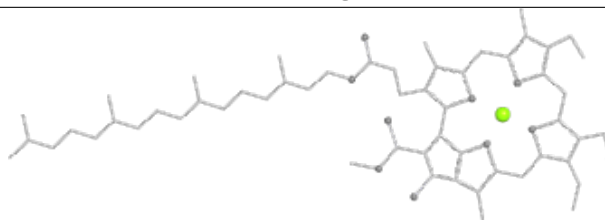
Bond lengths



Bond angles

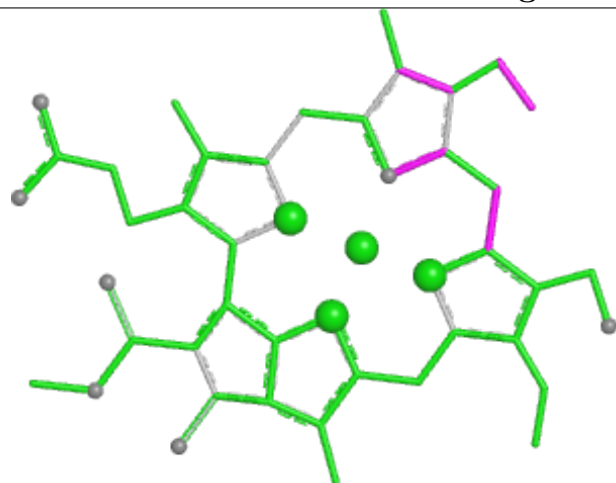


Torsions

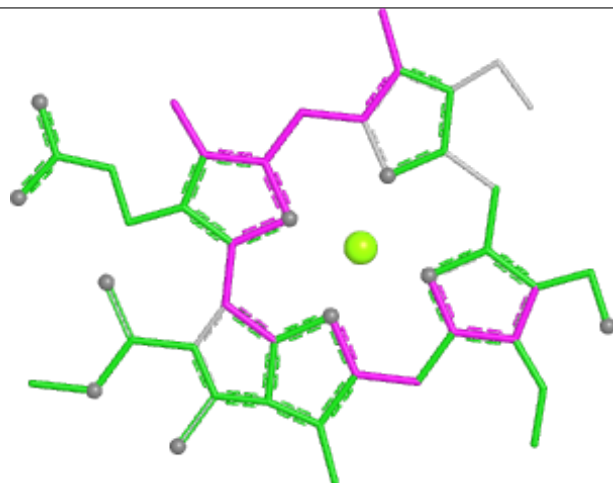


Rings

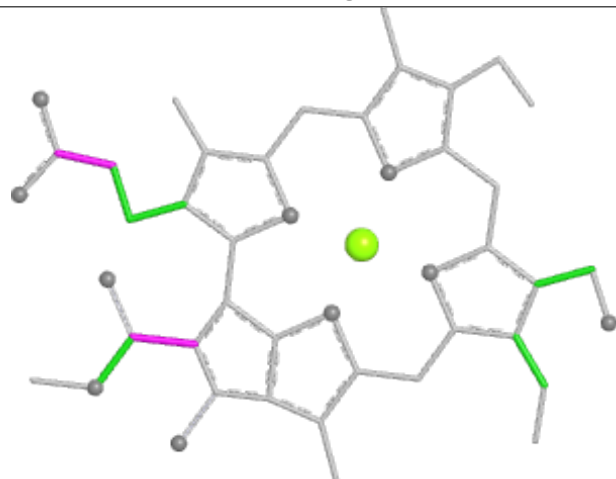
Ligand CHL S 601



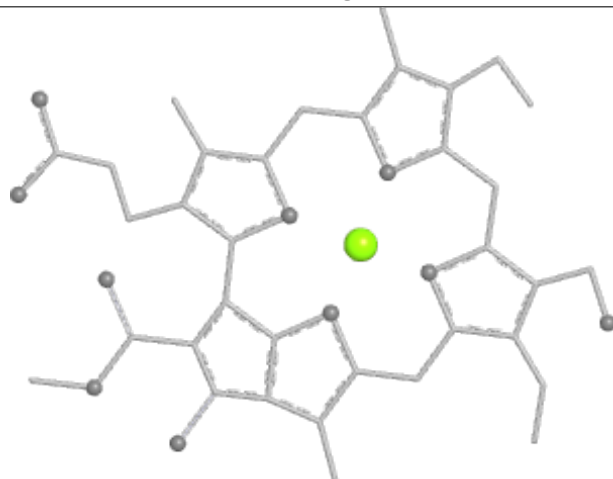
Bond lengths



Bond angles

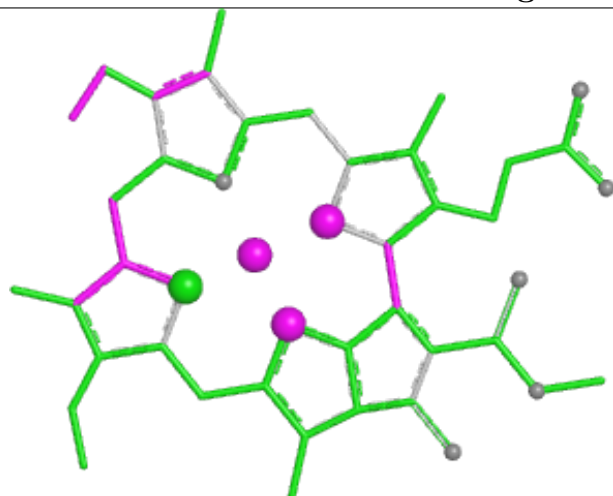


Torsions

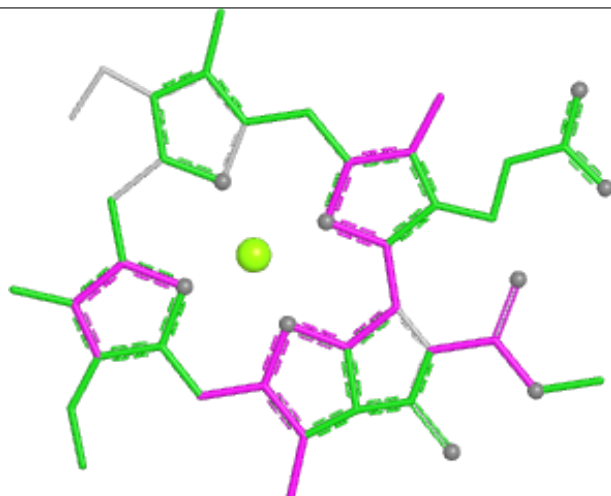


Rings

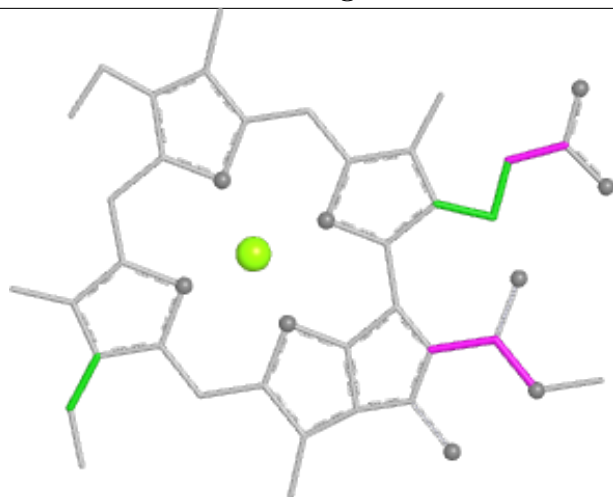
Ligand CLA S 612



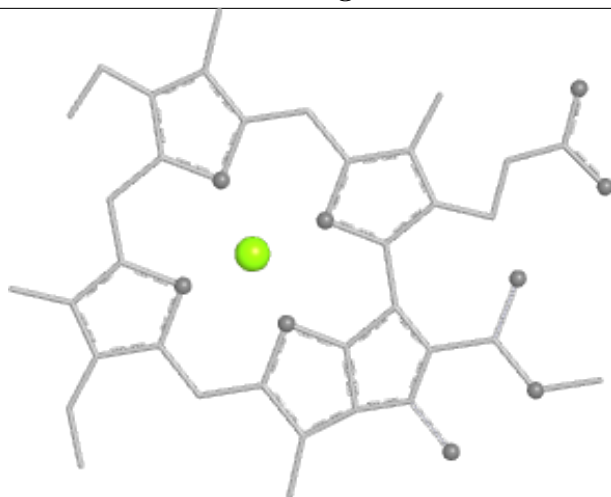
Bond lengths



Bond angles

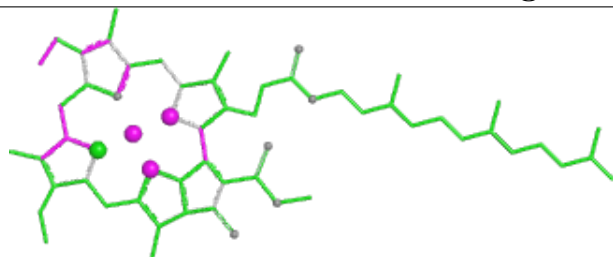


Torsions

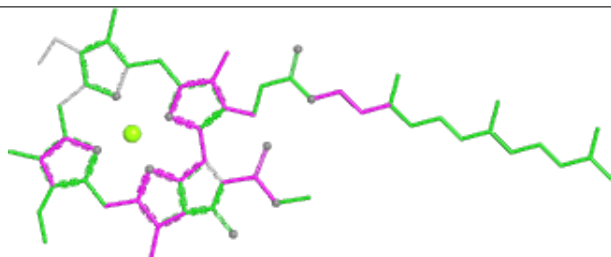


Rings

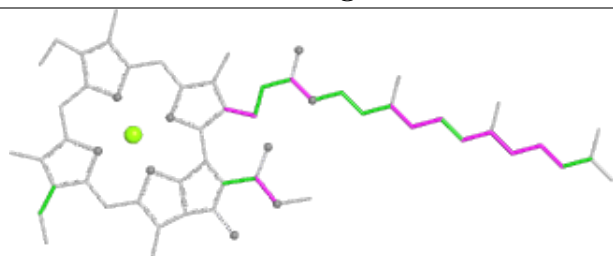
Ligand CLA s 609



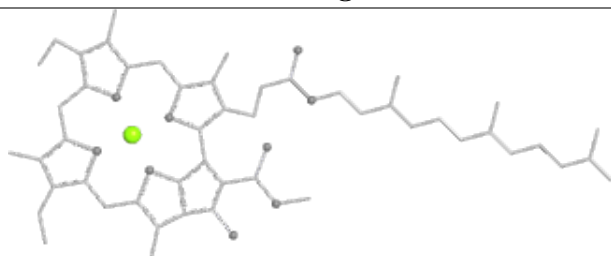
Bond lengths



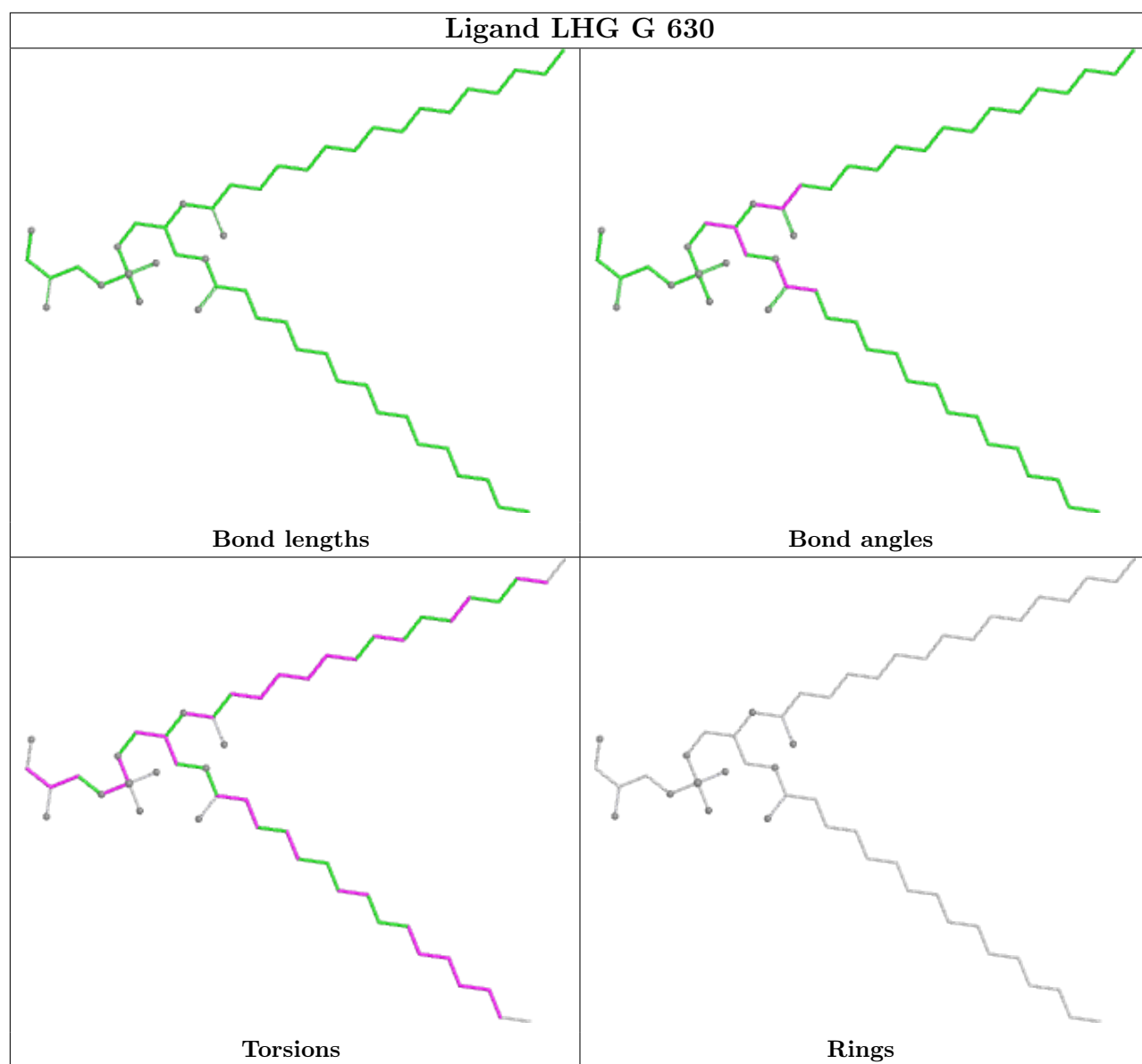
Bond angles



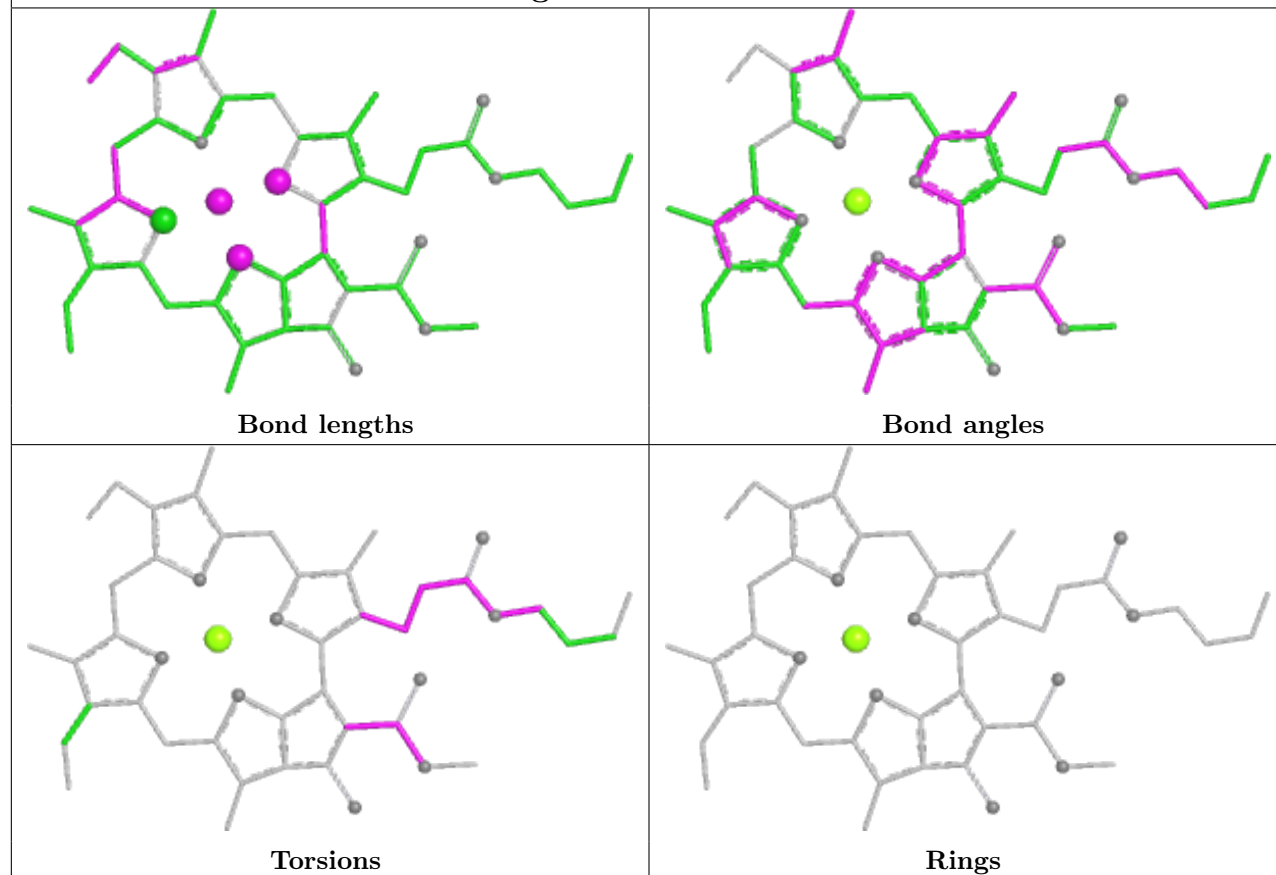
Torsions



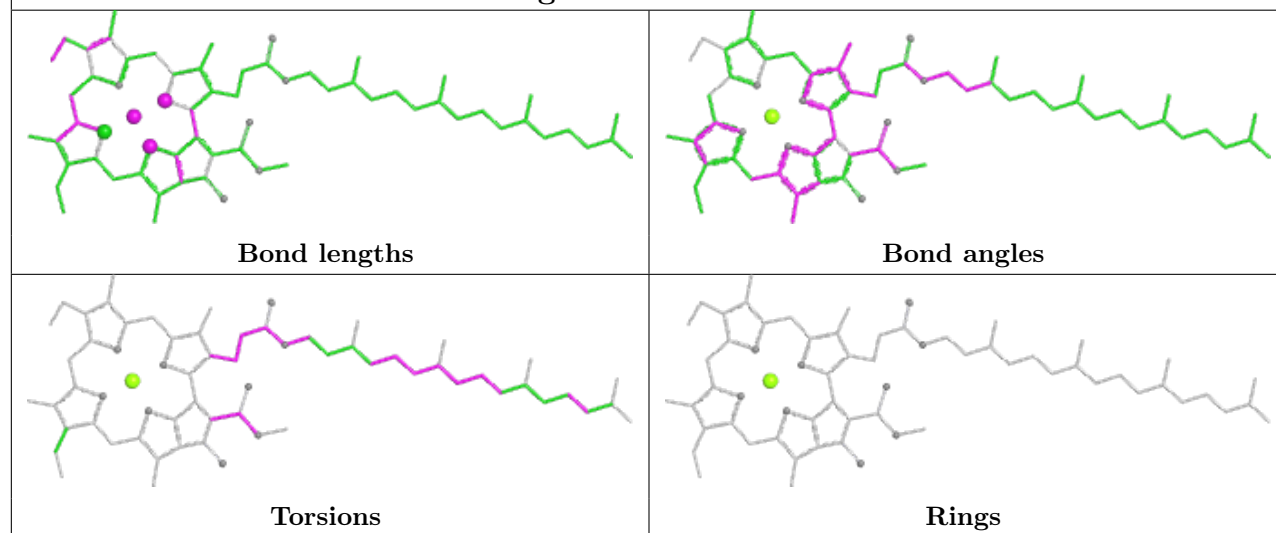
Rings

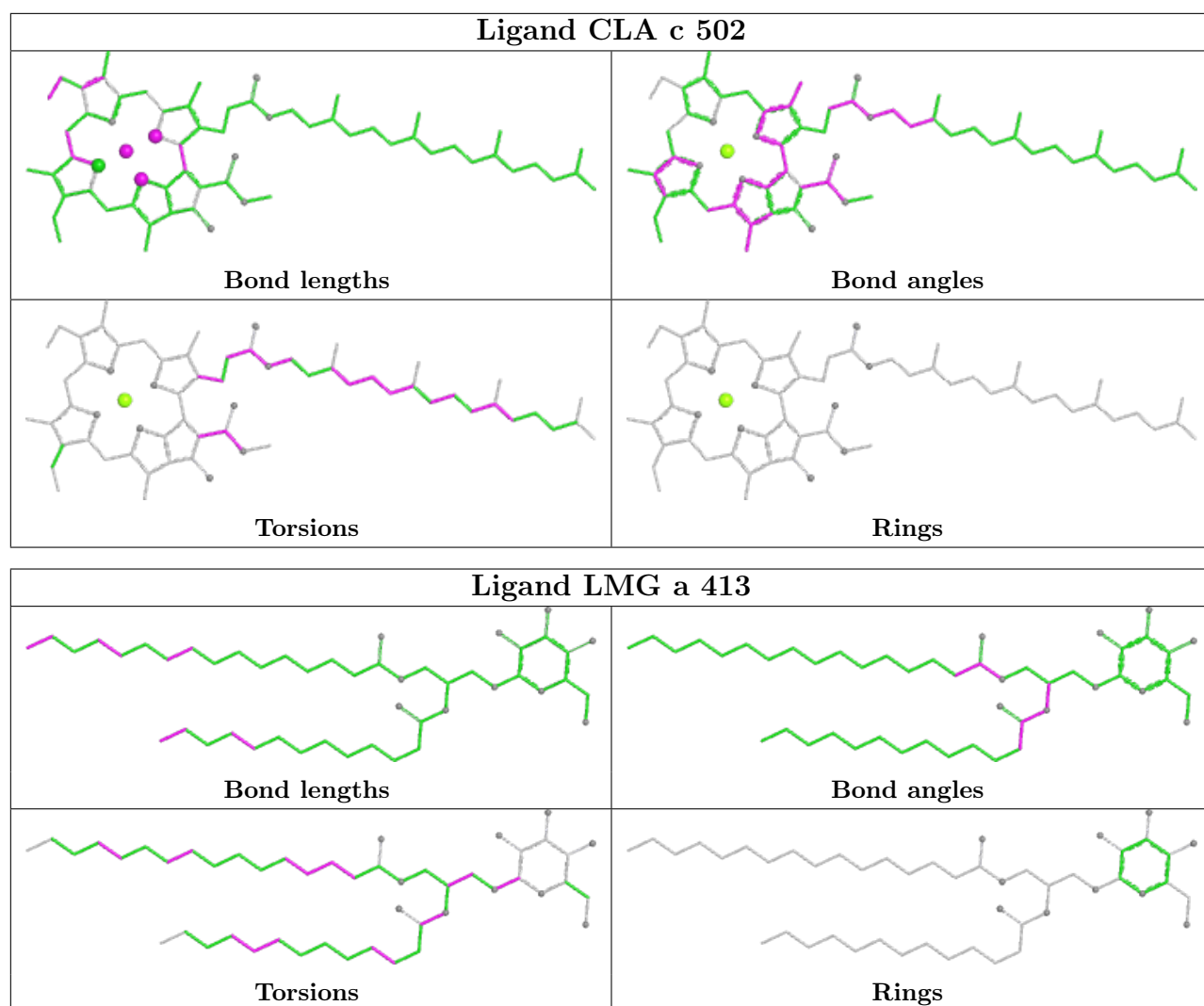


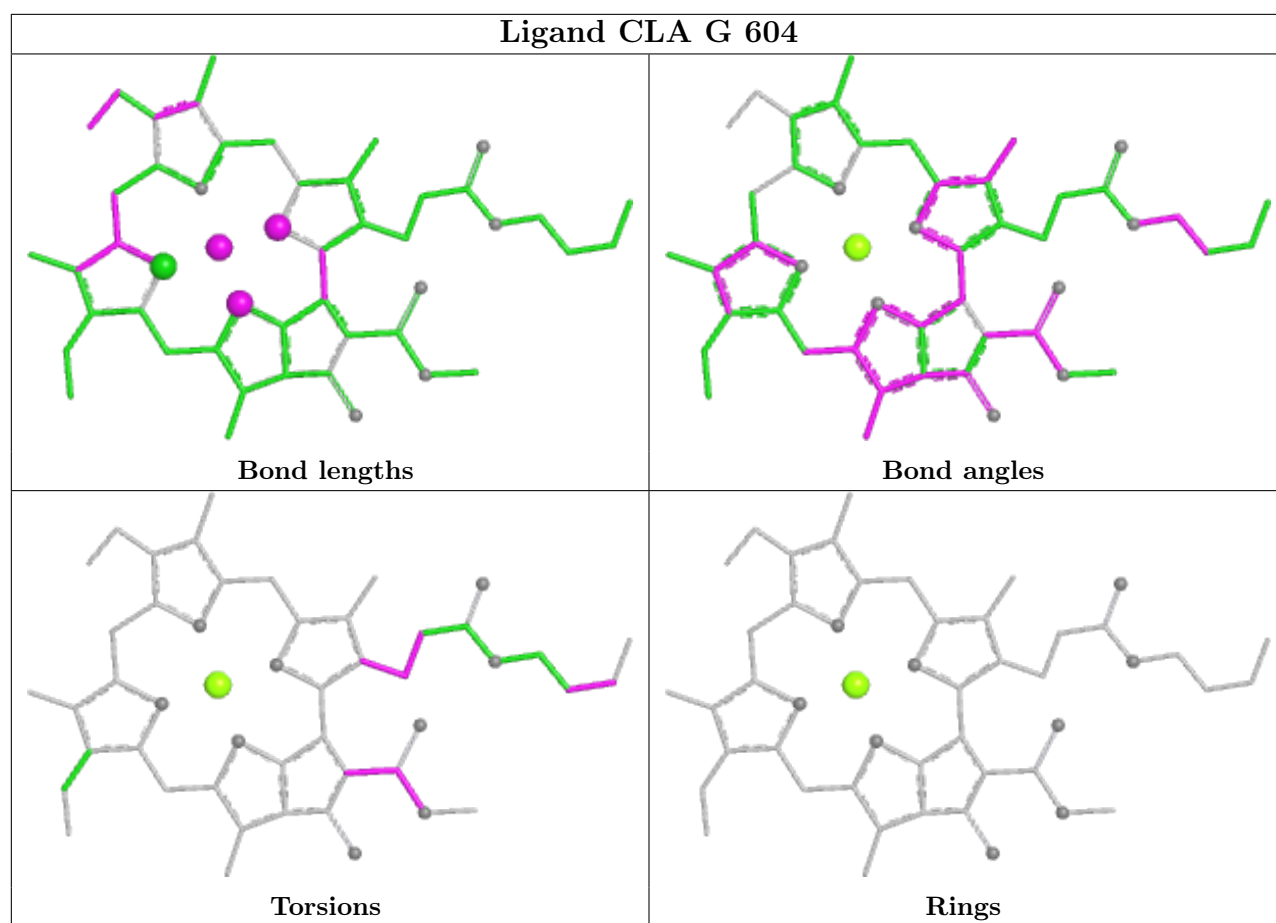
Ligand CLA R 604

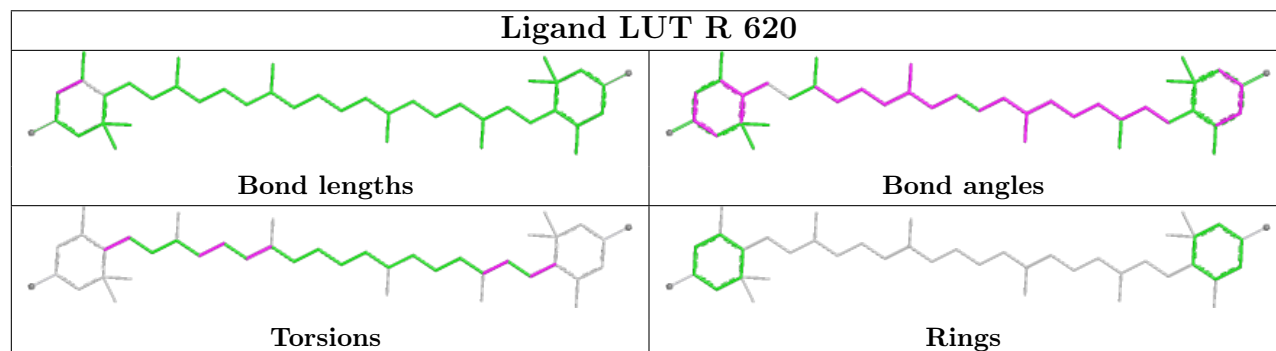
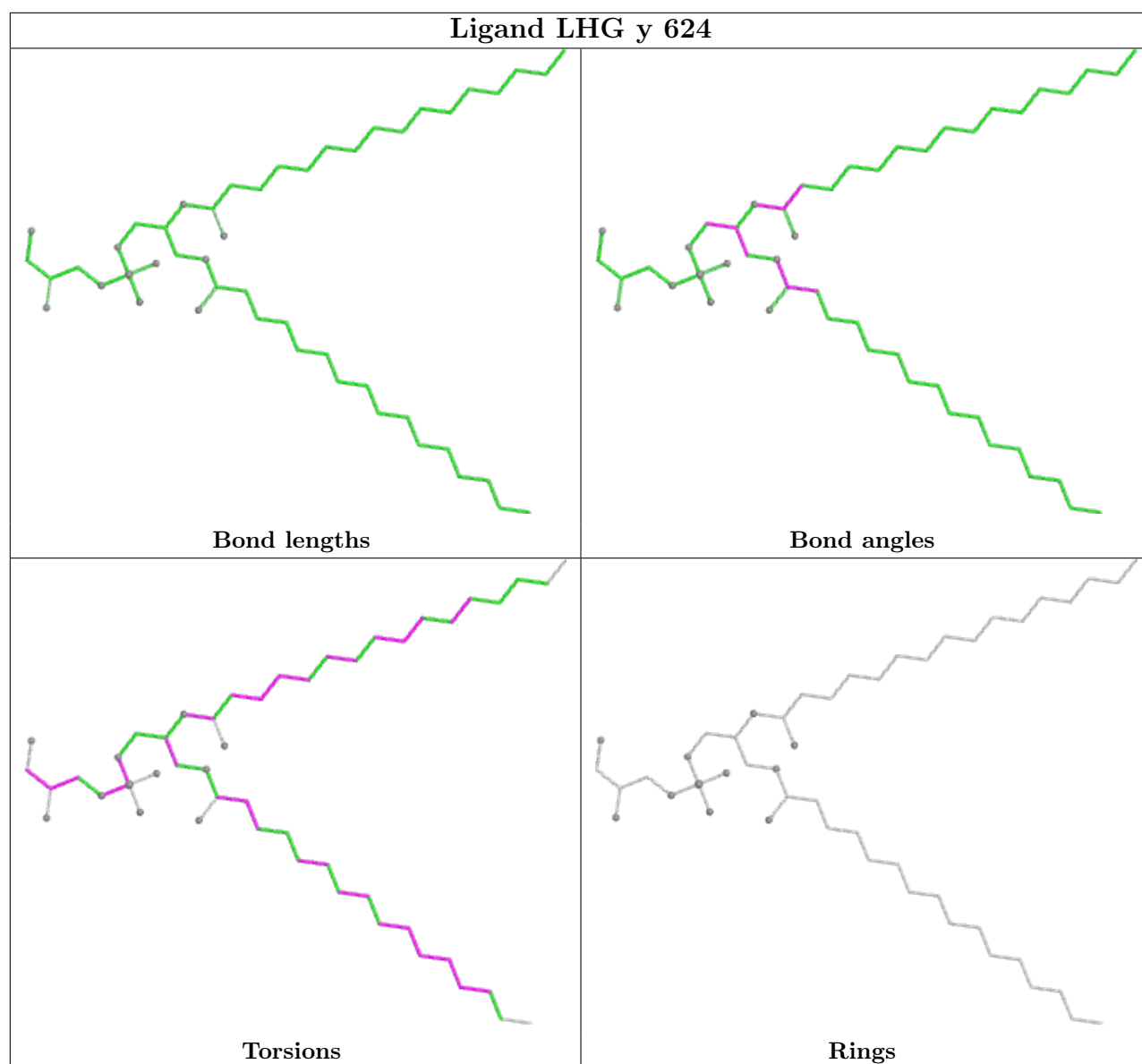


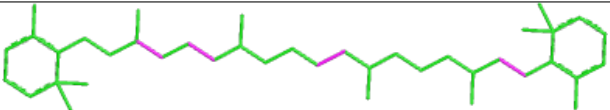
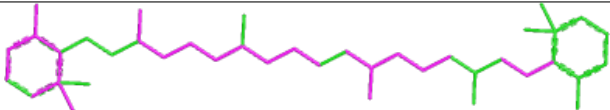
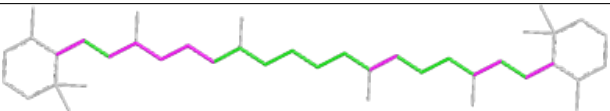
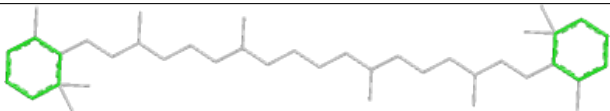
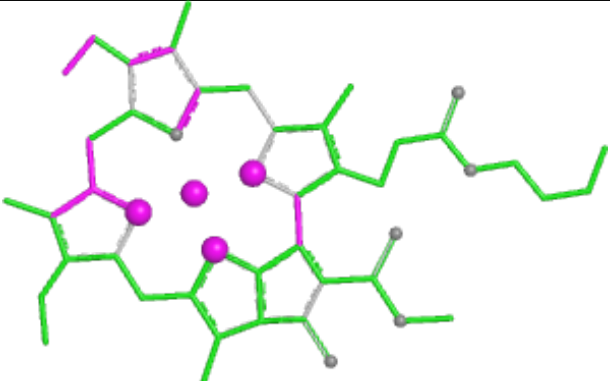
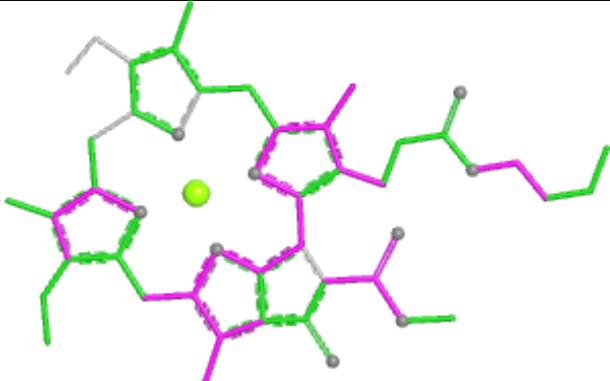
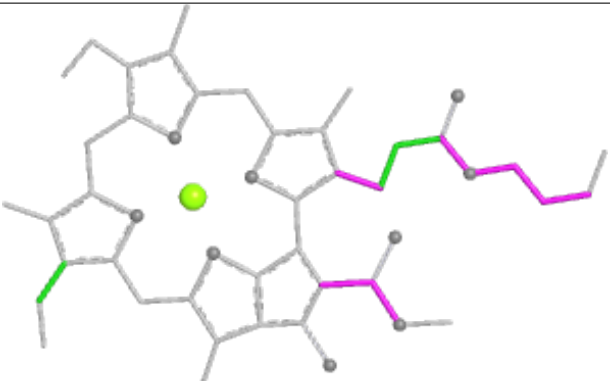
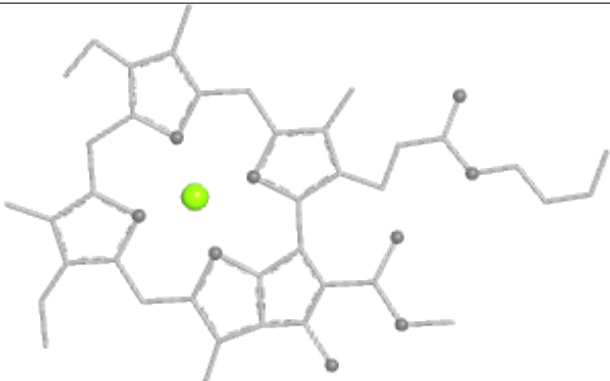
Ligand CLA s 610

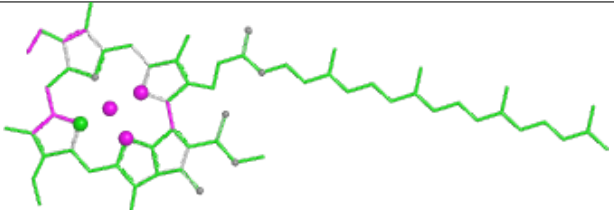
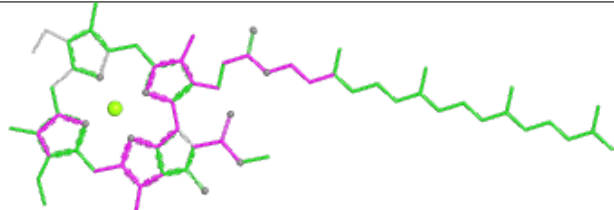
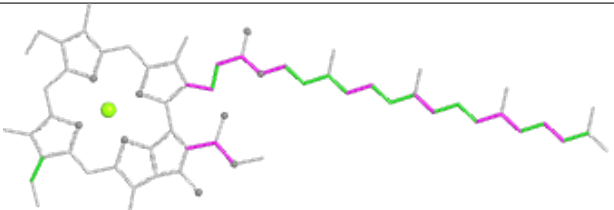
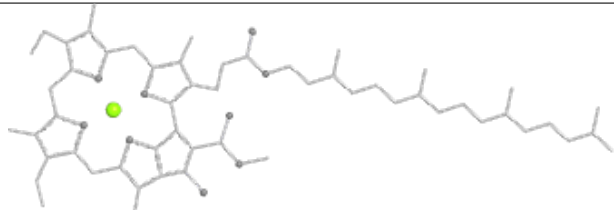


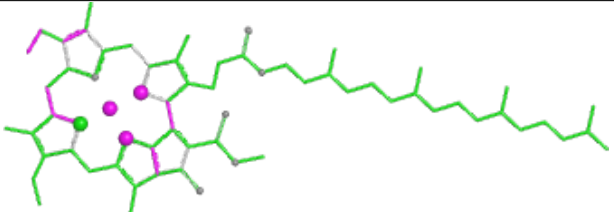
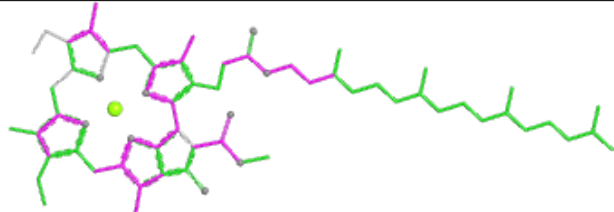
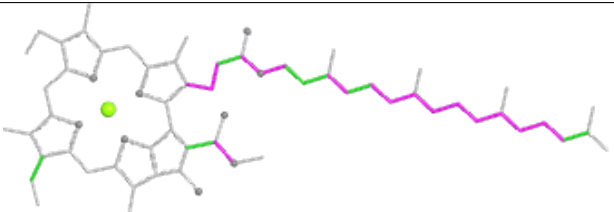
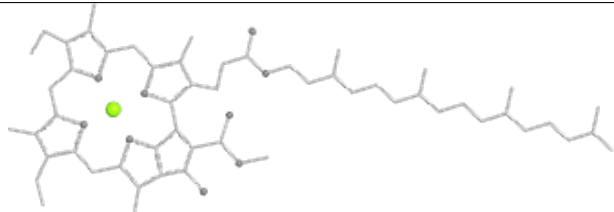


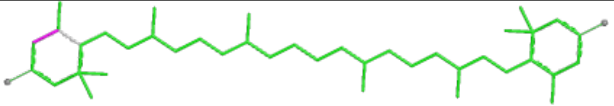
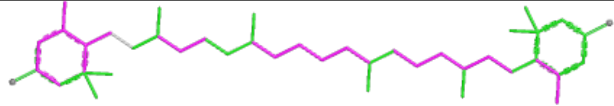
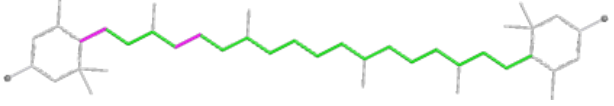
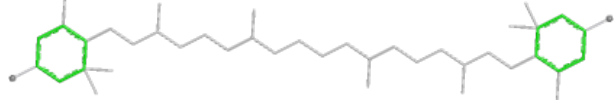


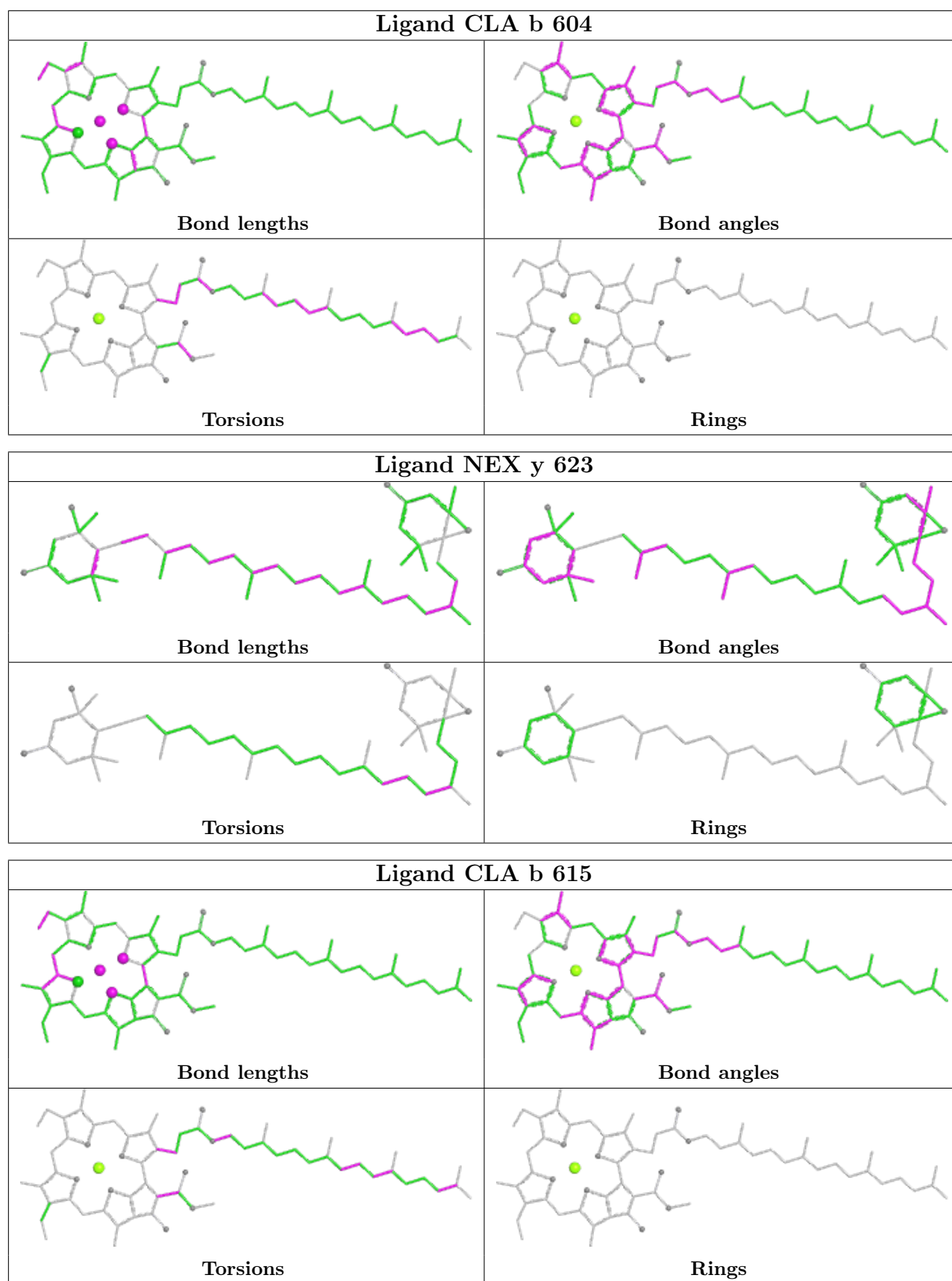


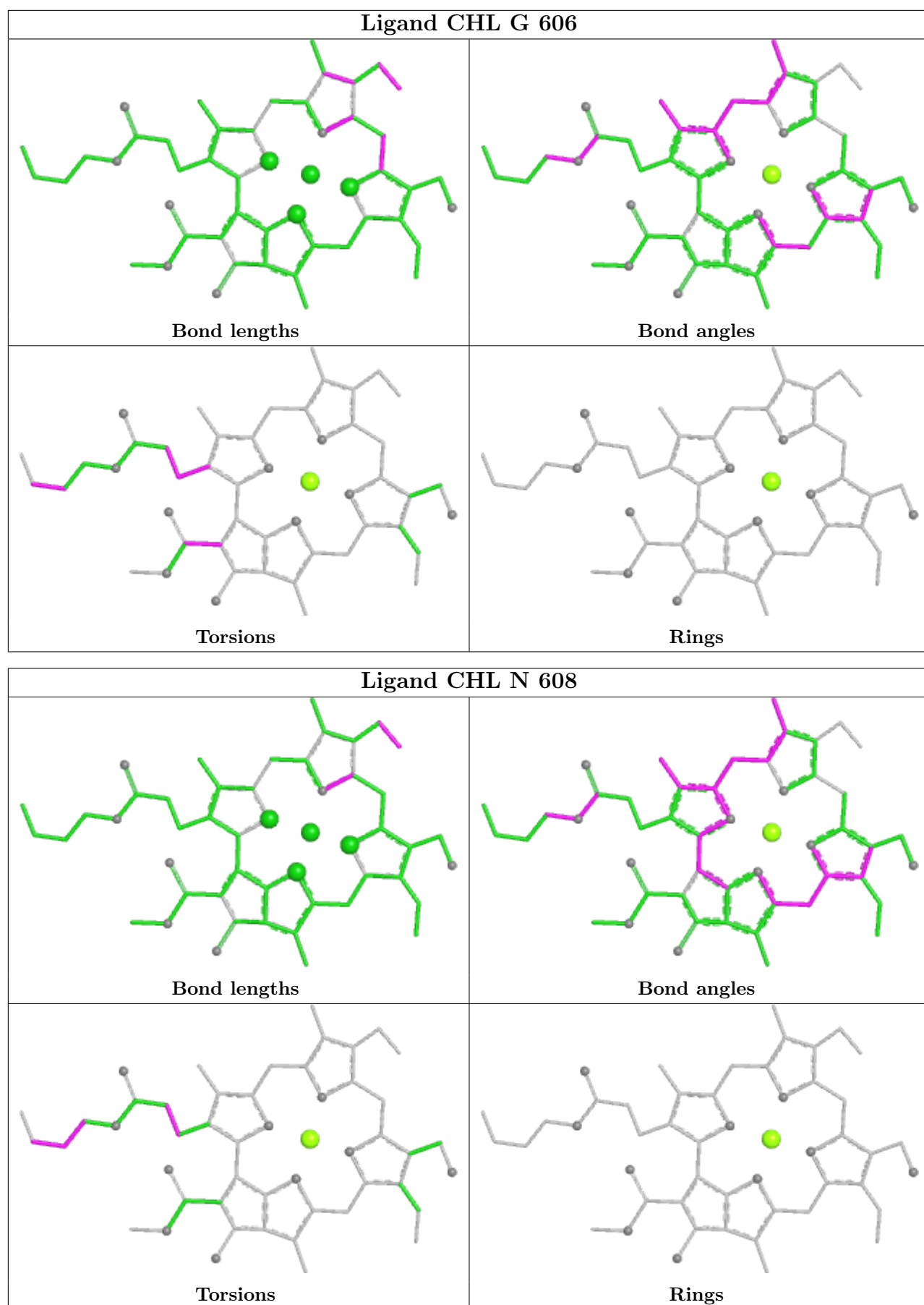
Ligand BCR B 618	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA N 611	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

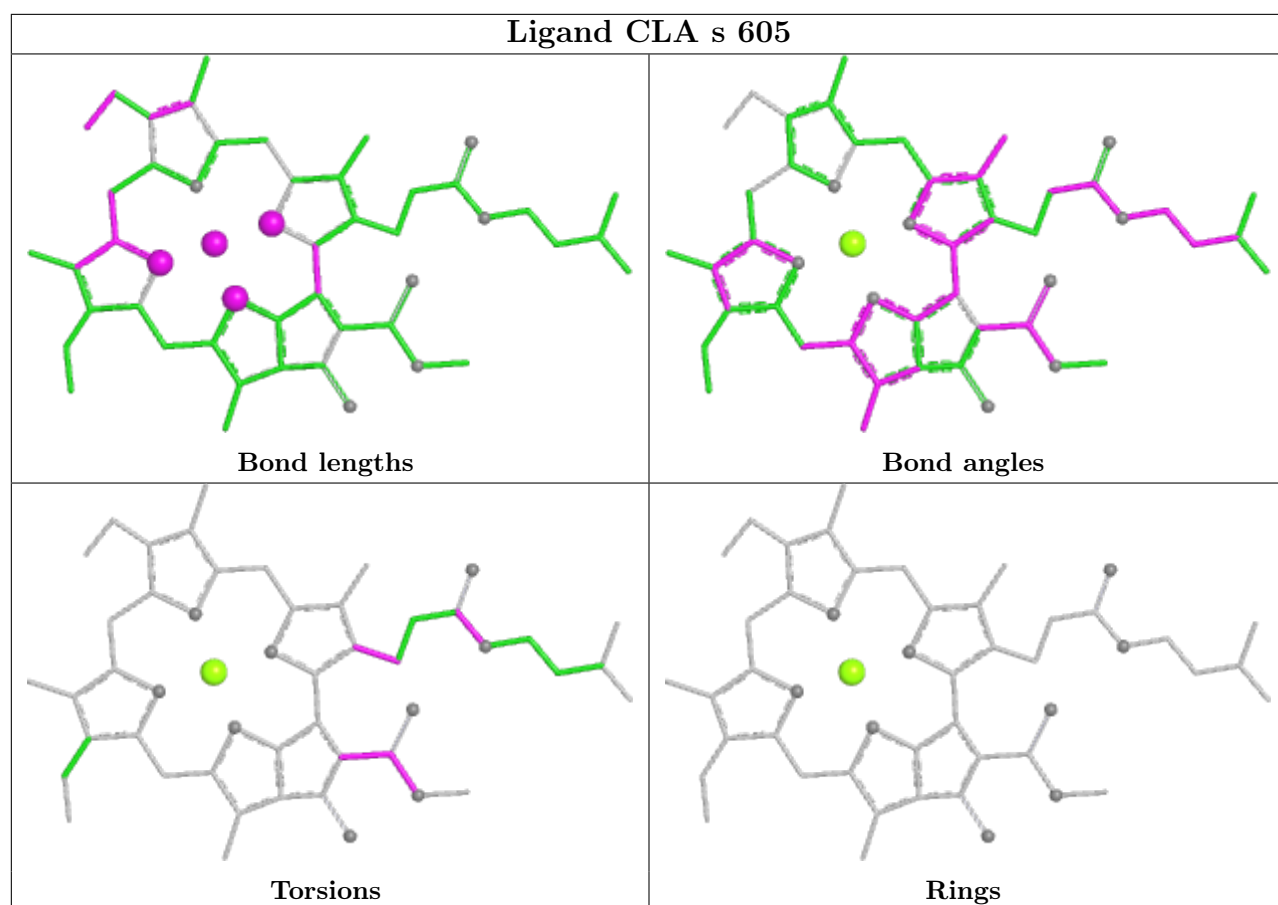
Ligand CLA G 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

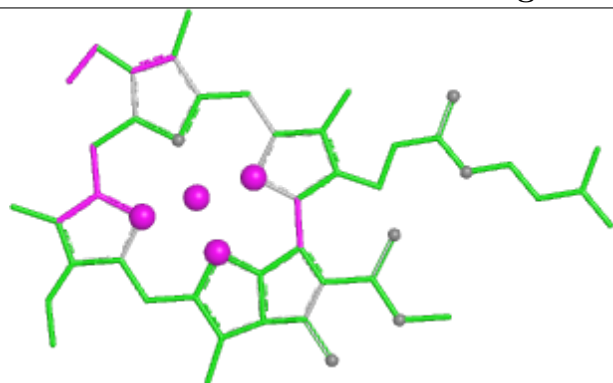
Ligand LUT g 621	
	
Bond lengths	Bond angles
	
Torsions	Rings



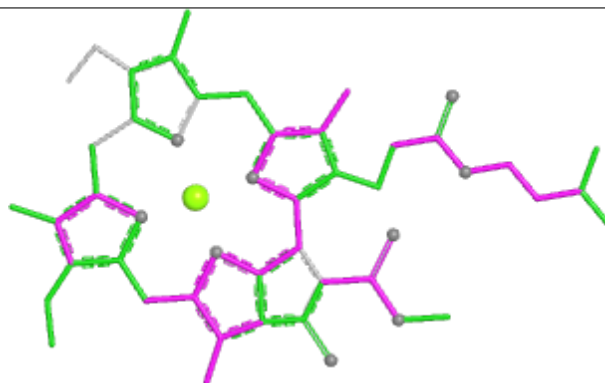




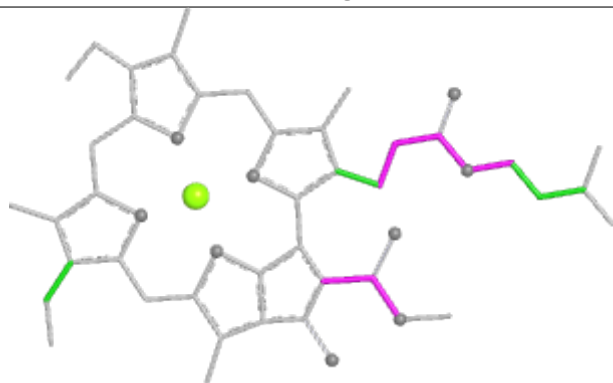
Ligand CLA S 617



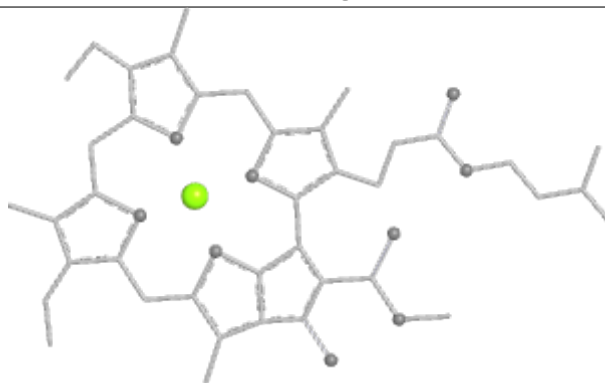
Bond lengths



Bond angles

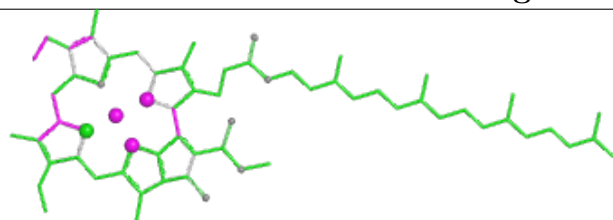


Torsions

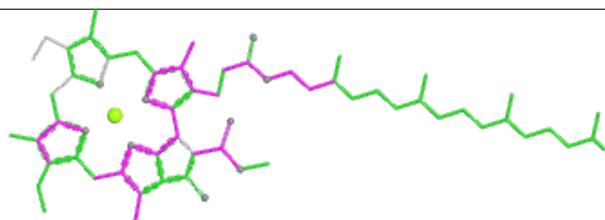


Rings

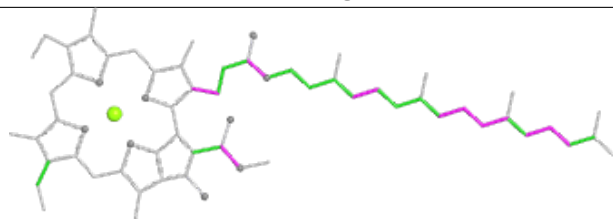
Ligand CLA D 403



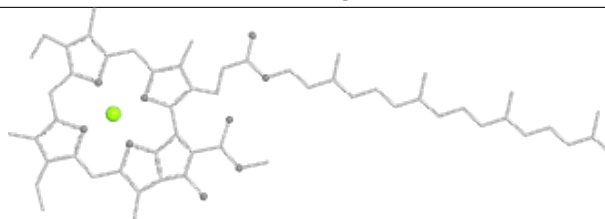
Bond lengths



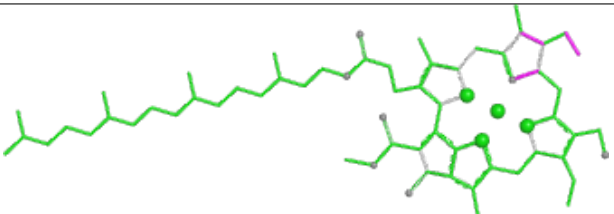
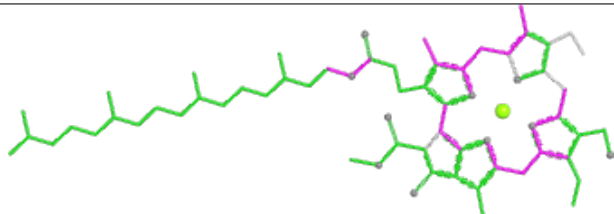
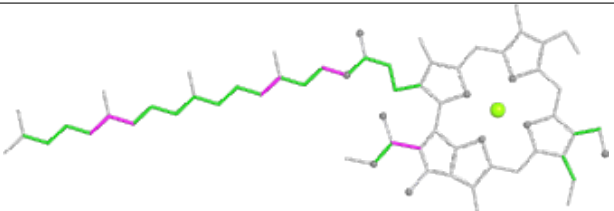
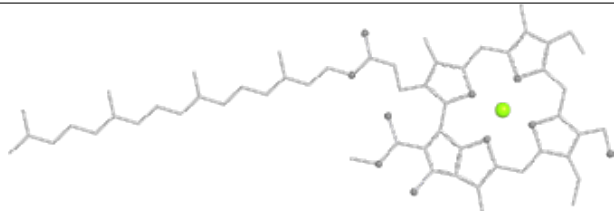
Bond angles

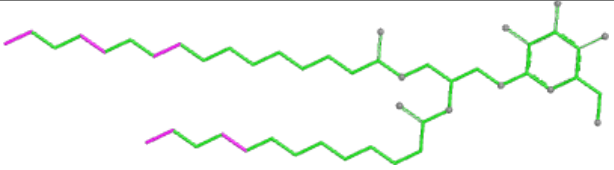
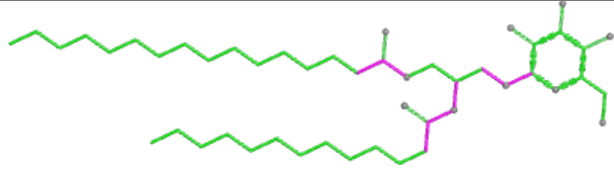
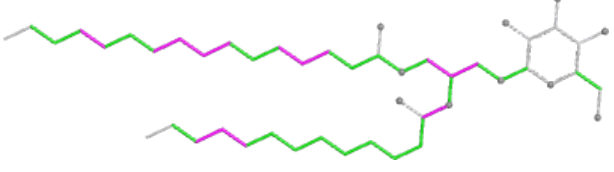
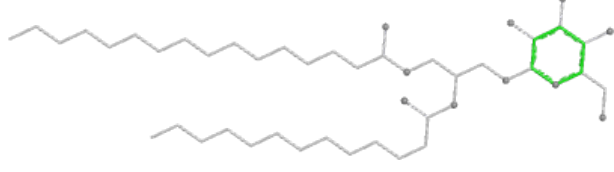


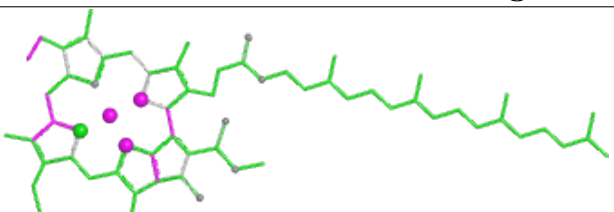
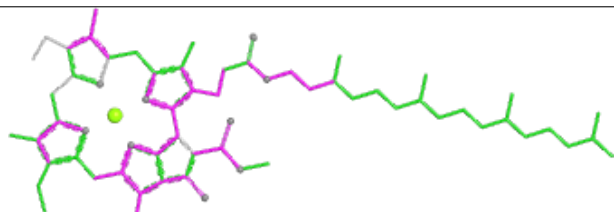
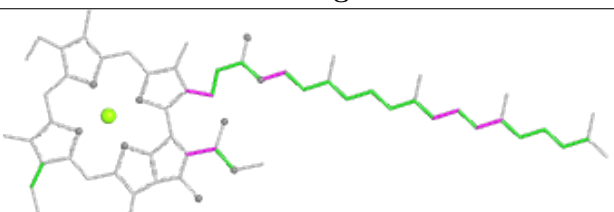
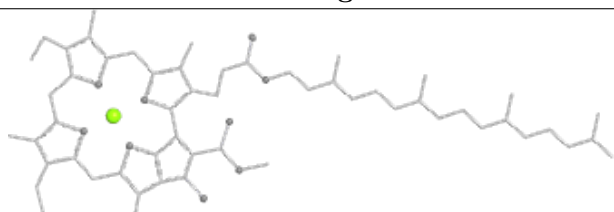
Torsions

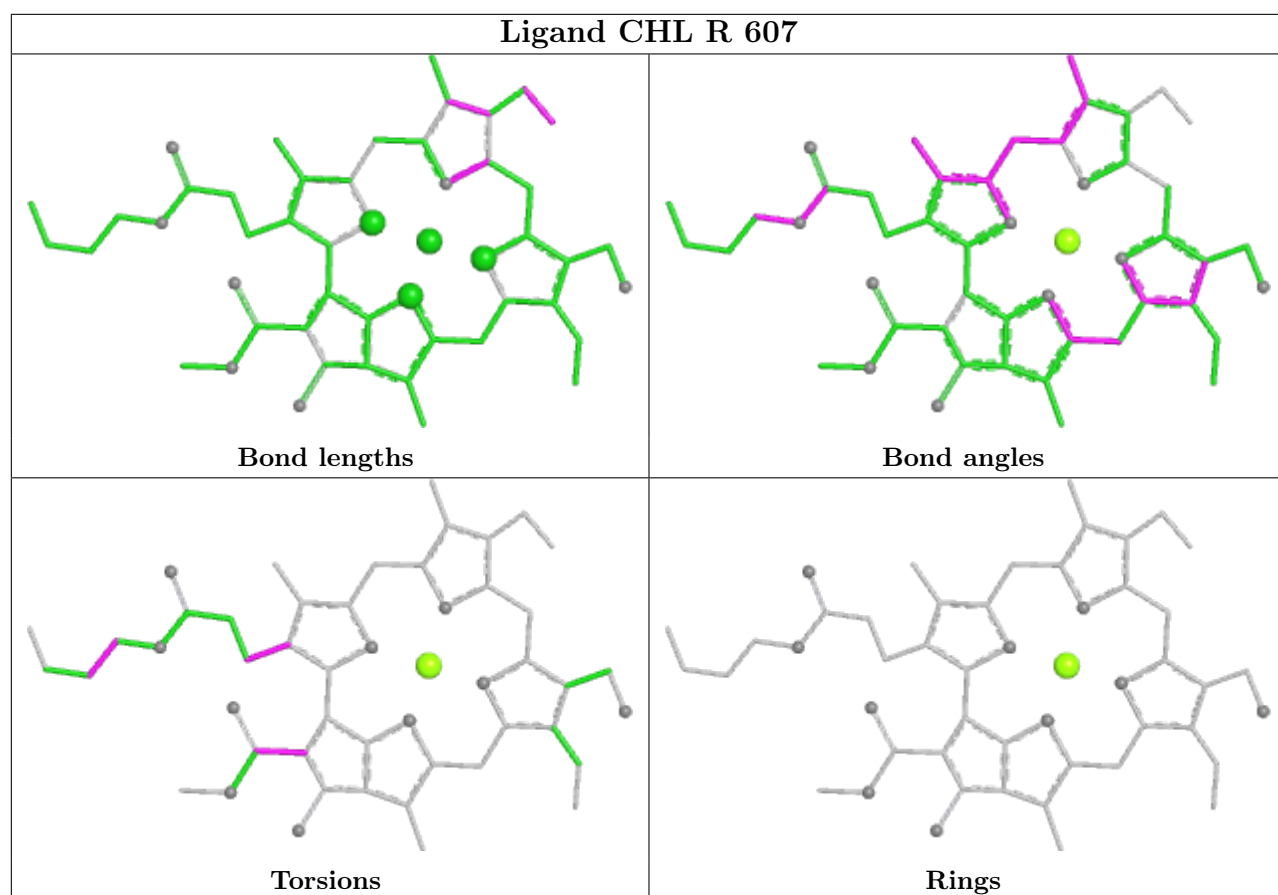


Rings

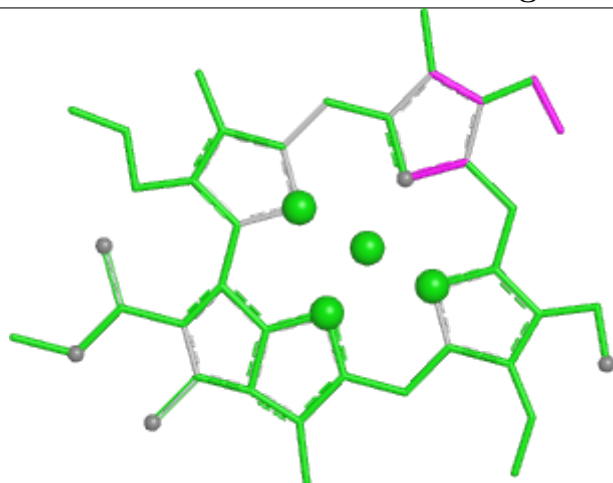
Ligand CHL G 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

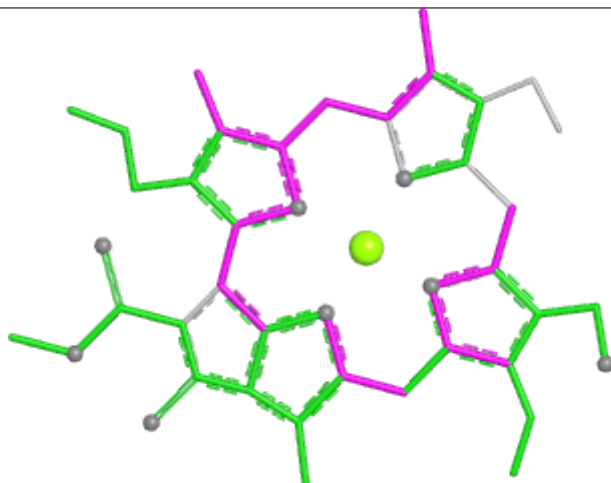
Ligand CLA B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings



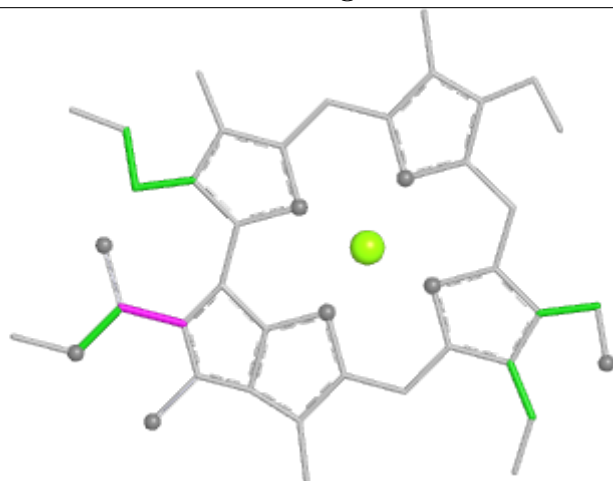
Ligand CHL r 606



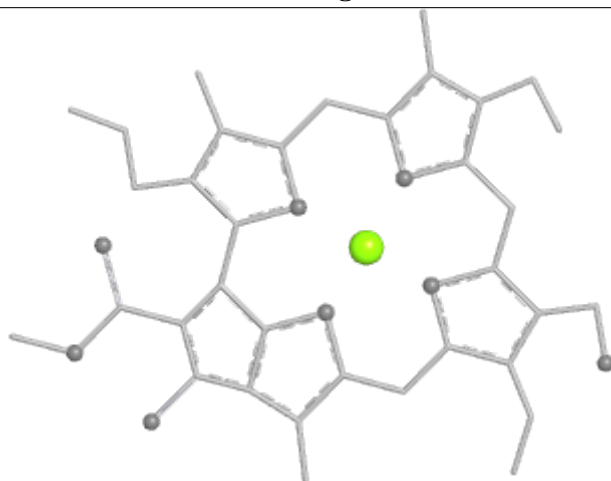
Bond lengths



Bond angles

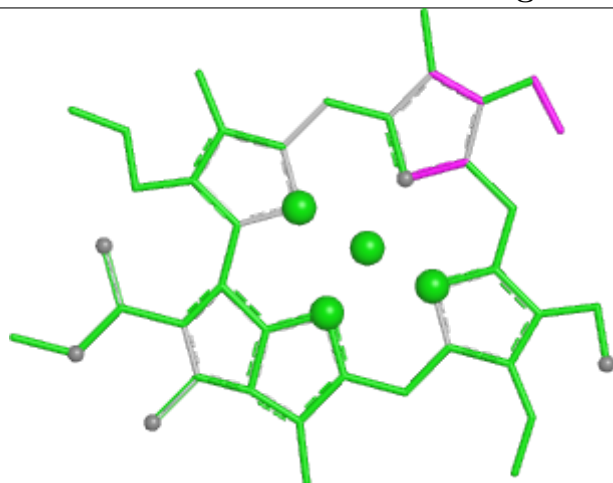


Torsions

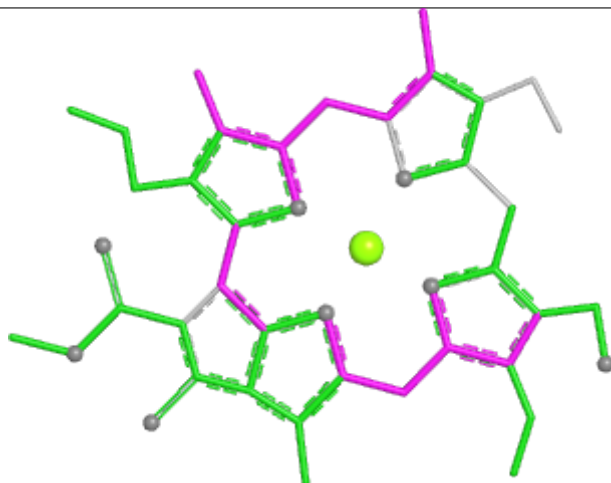


Rings

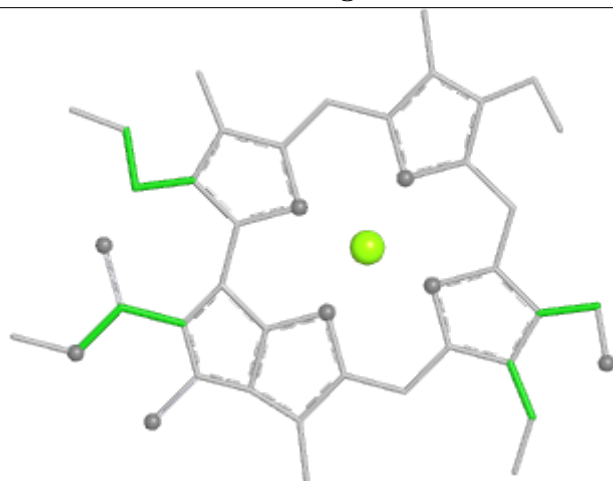
Ligand CHL S 606



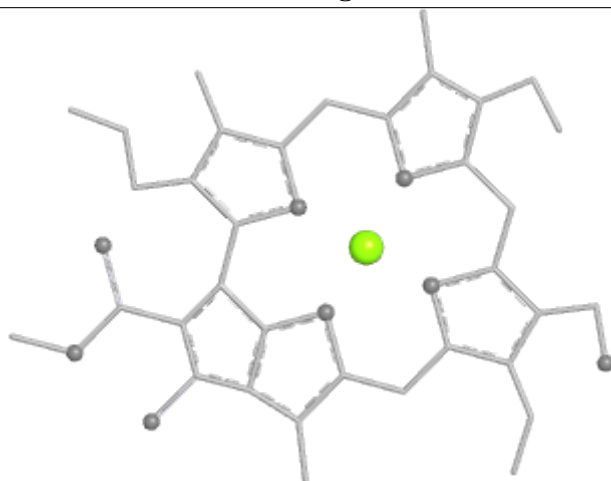
Bond lengths



Bond angles

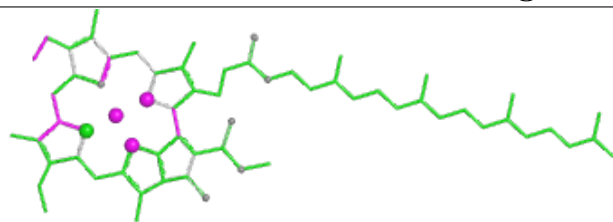


Torsions

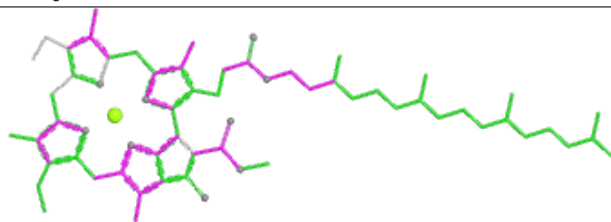


Rings

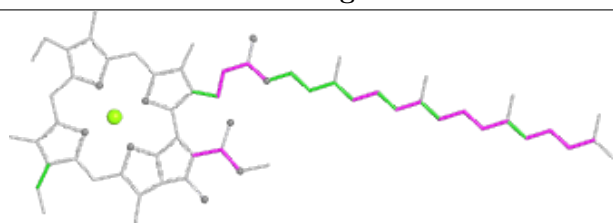
Ligand CLA y 613



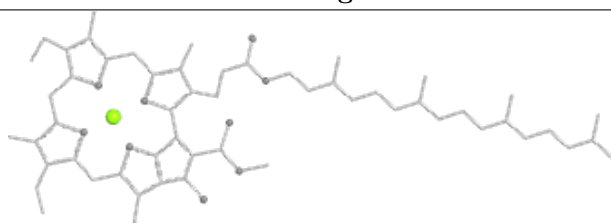
Bond lengths



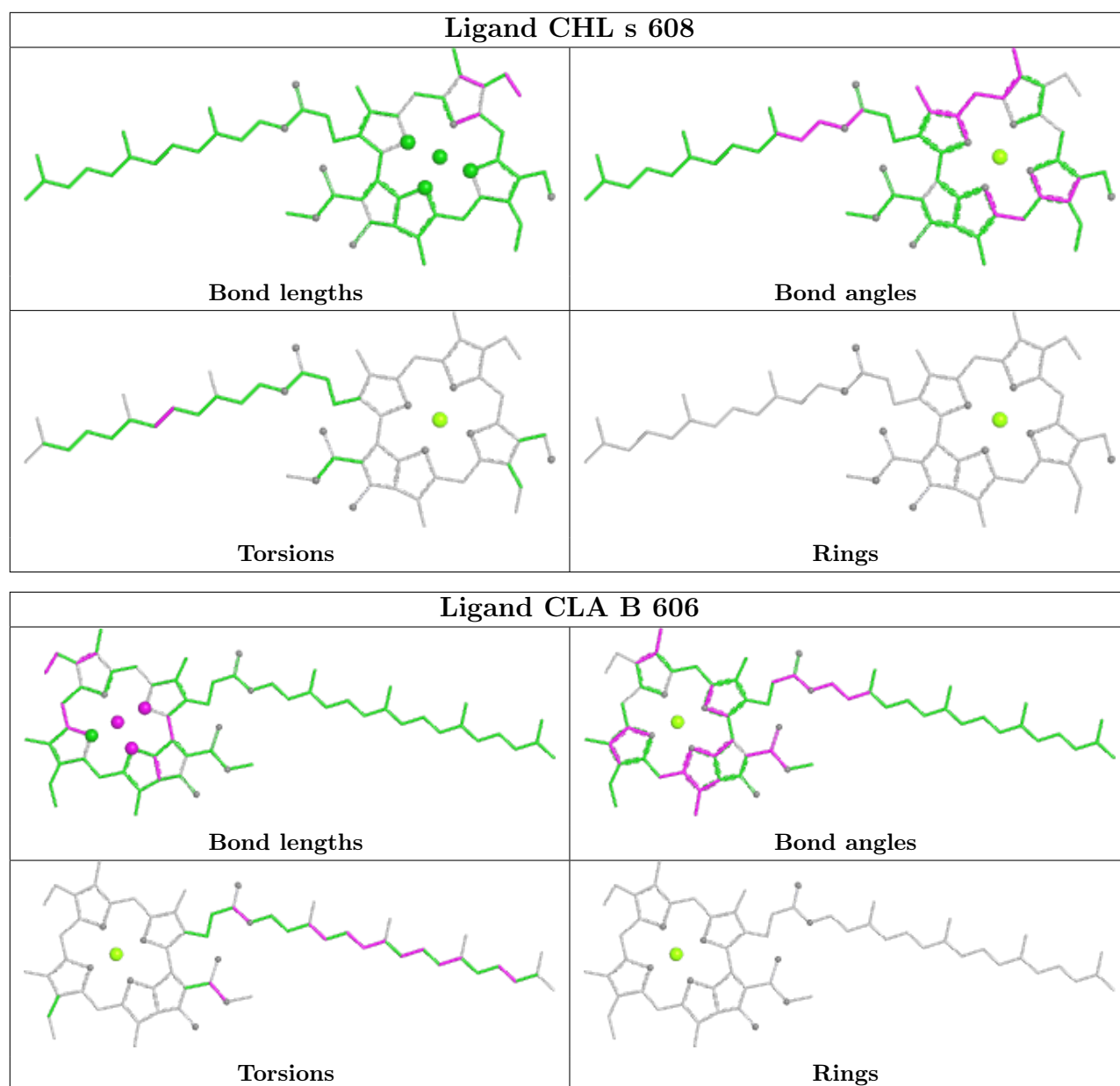
Bond angles

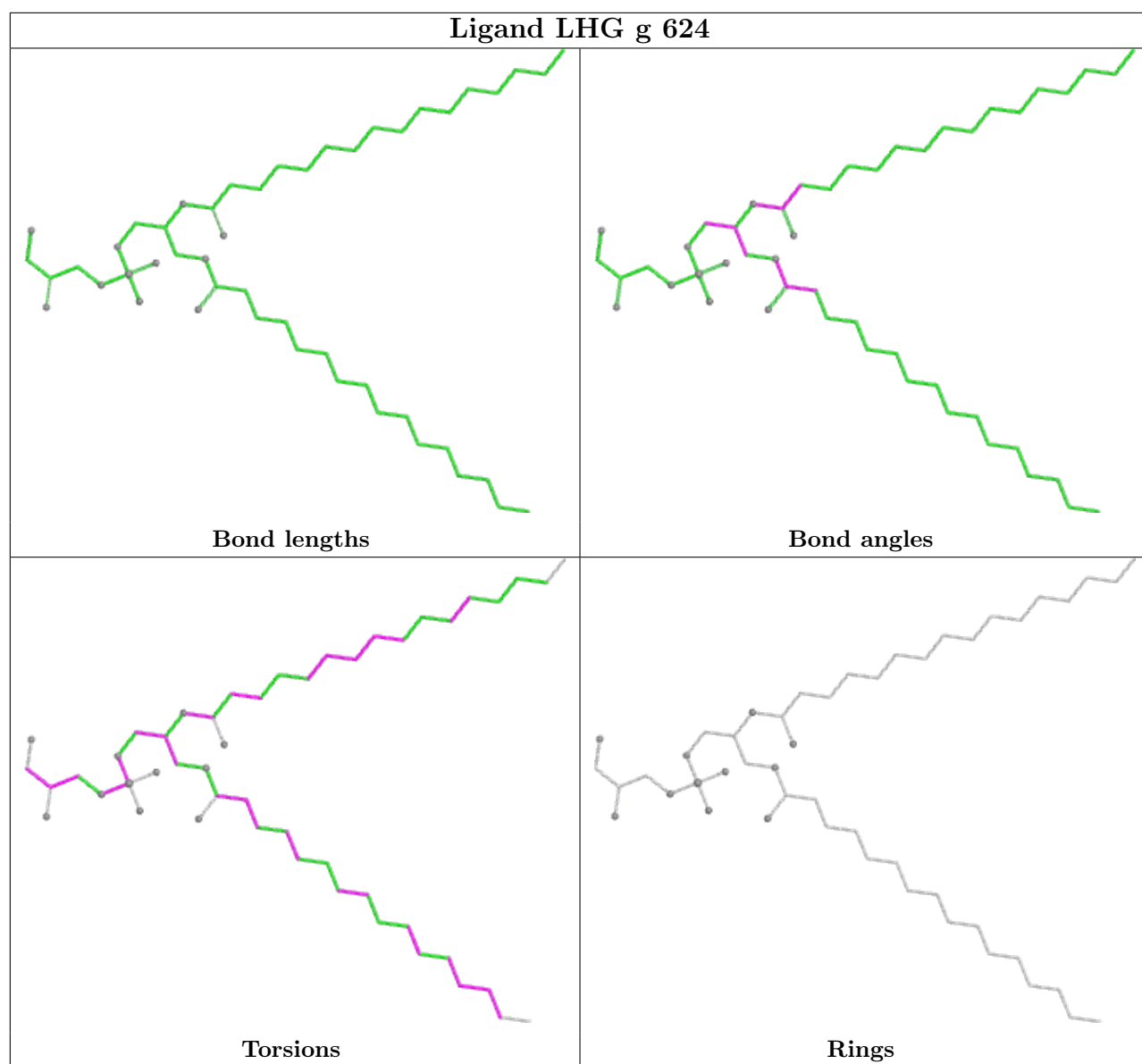


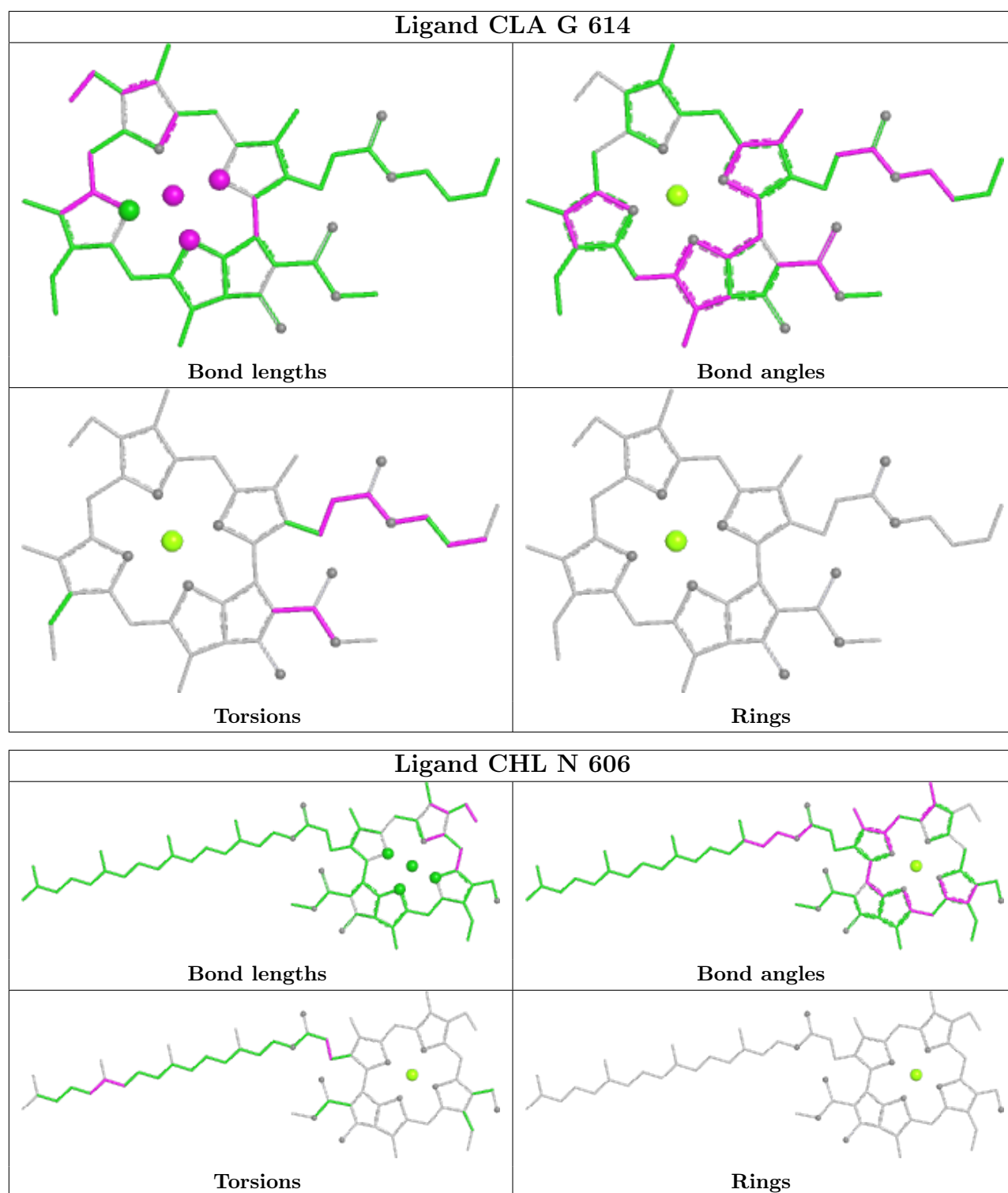
Torsions

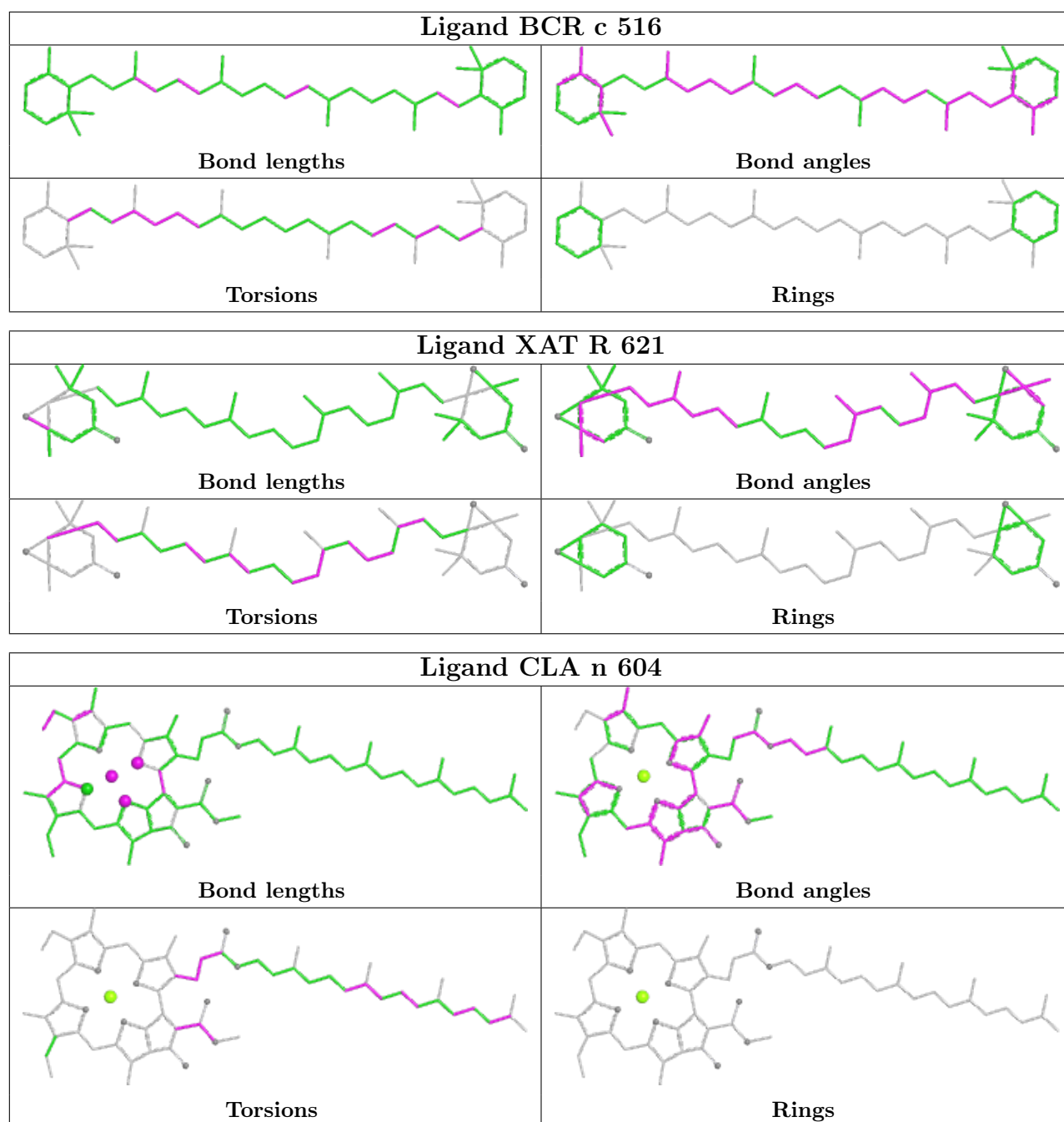


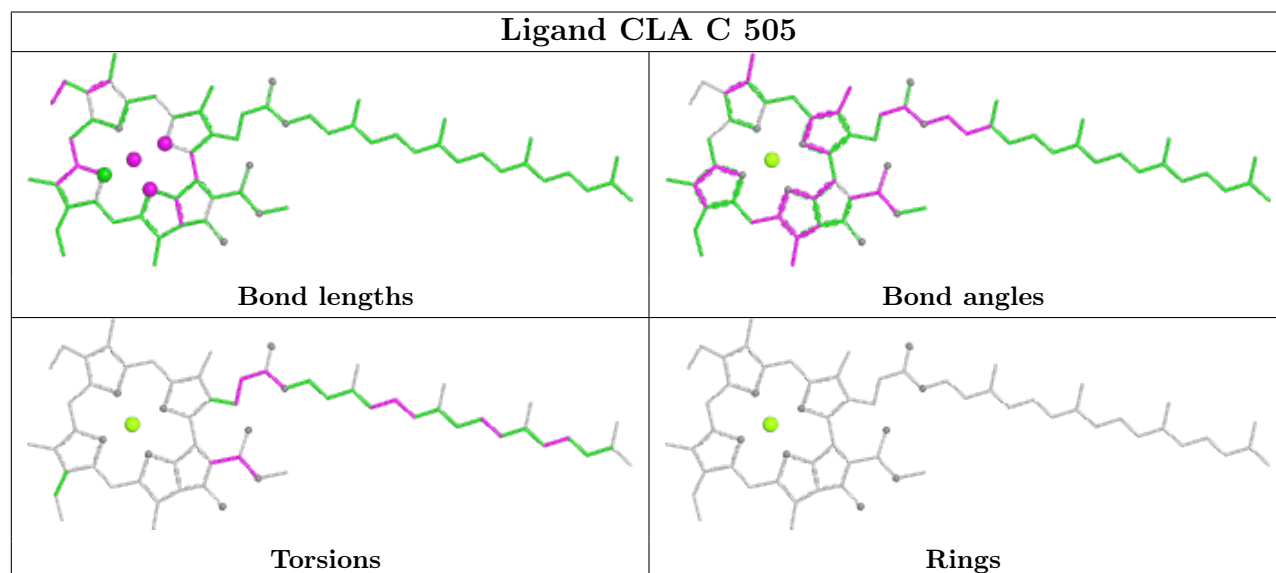
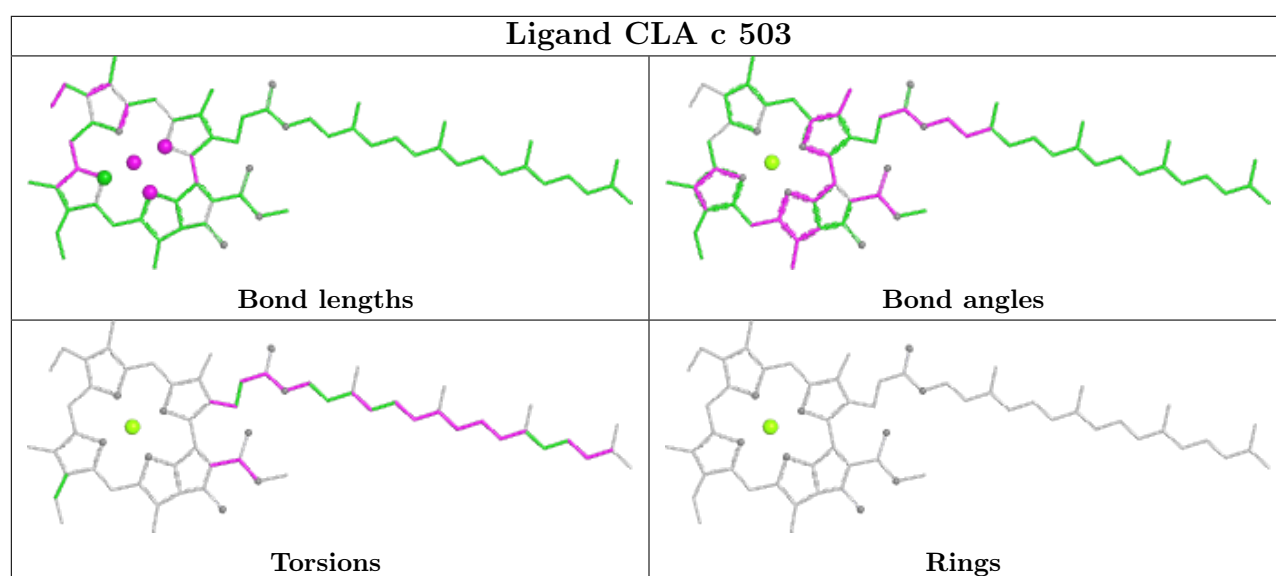
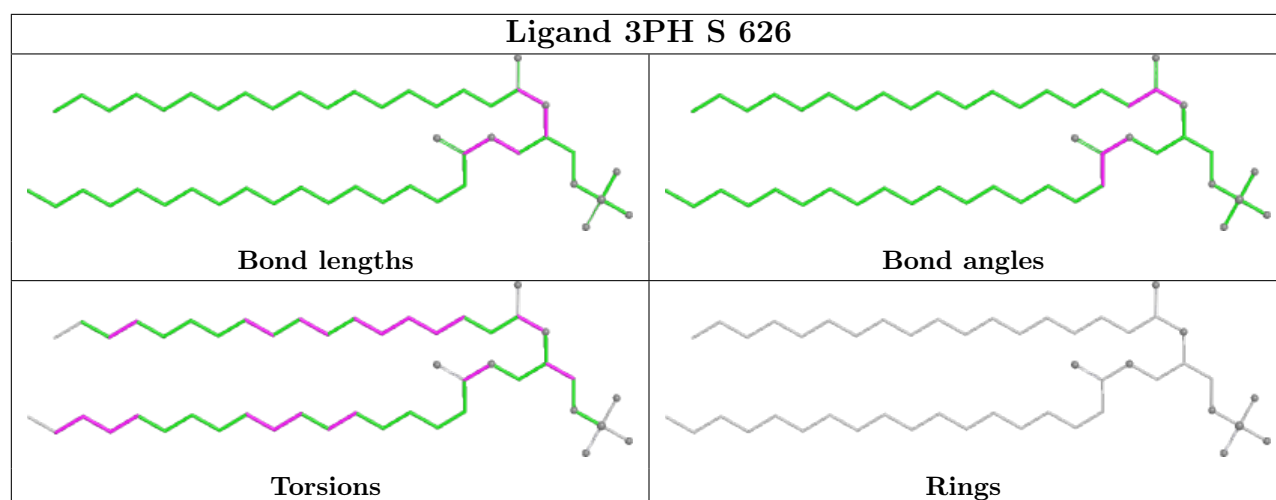
Rings



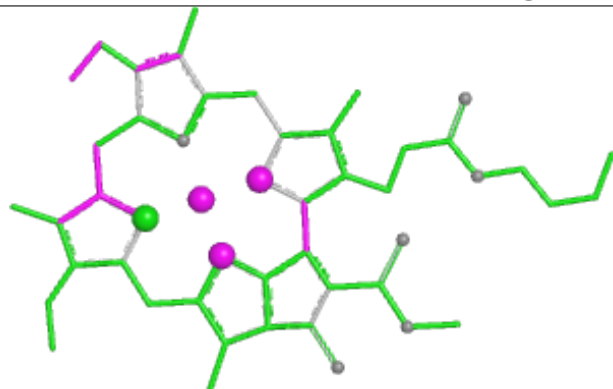




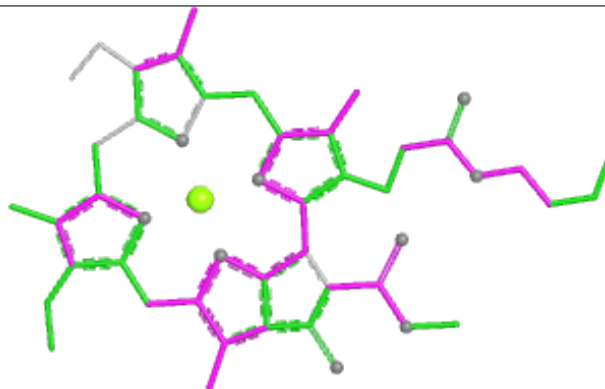




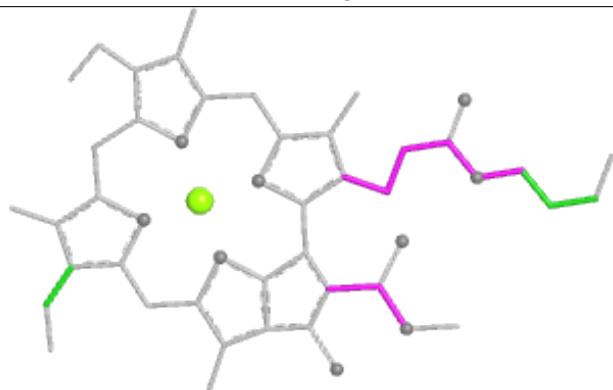
Ligand CLA r 604



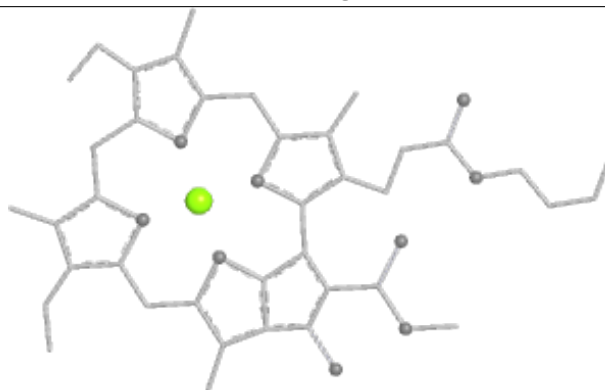
Bond lengths



Bond angles

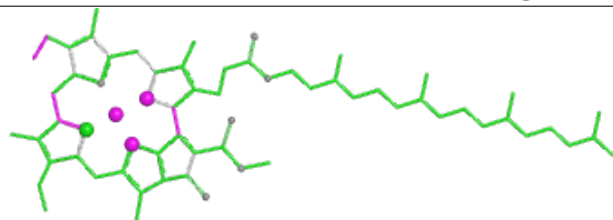


Torsions

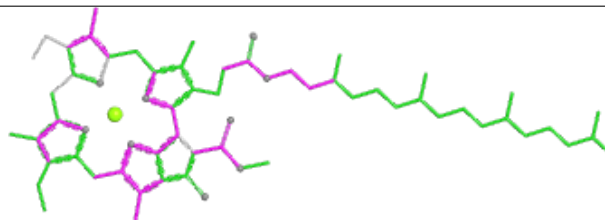


Rings

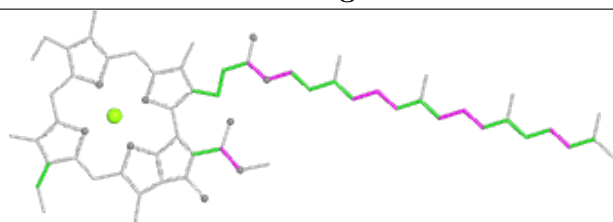
Ligand CLA b 614



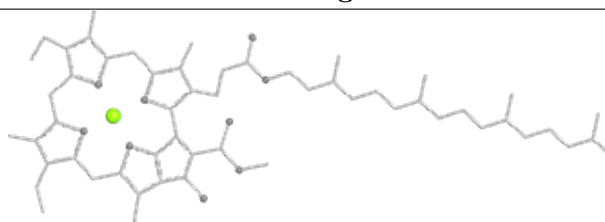
Bond lengths



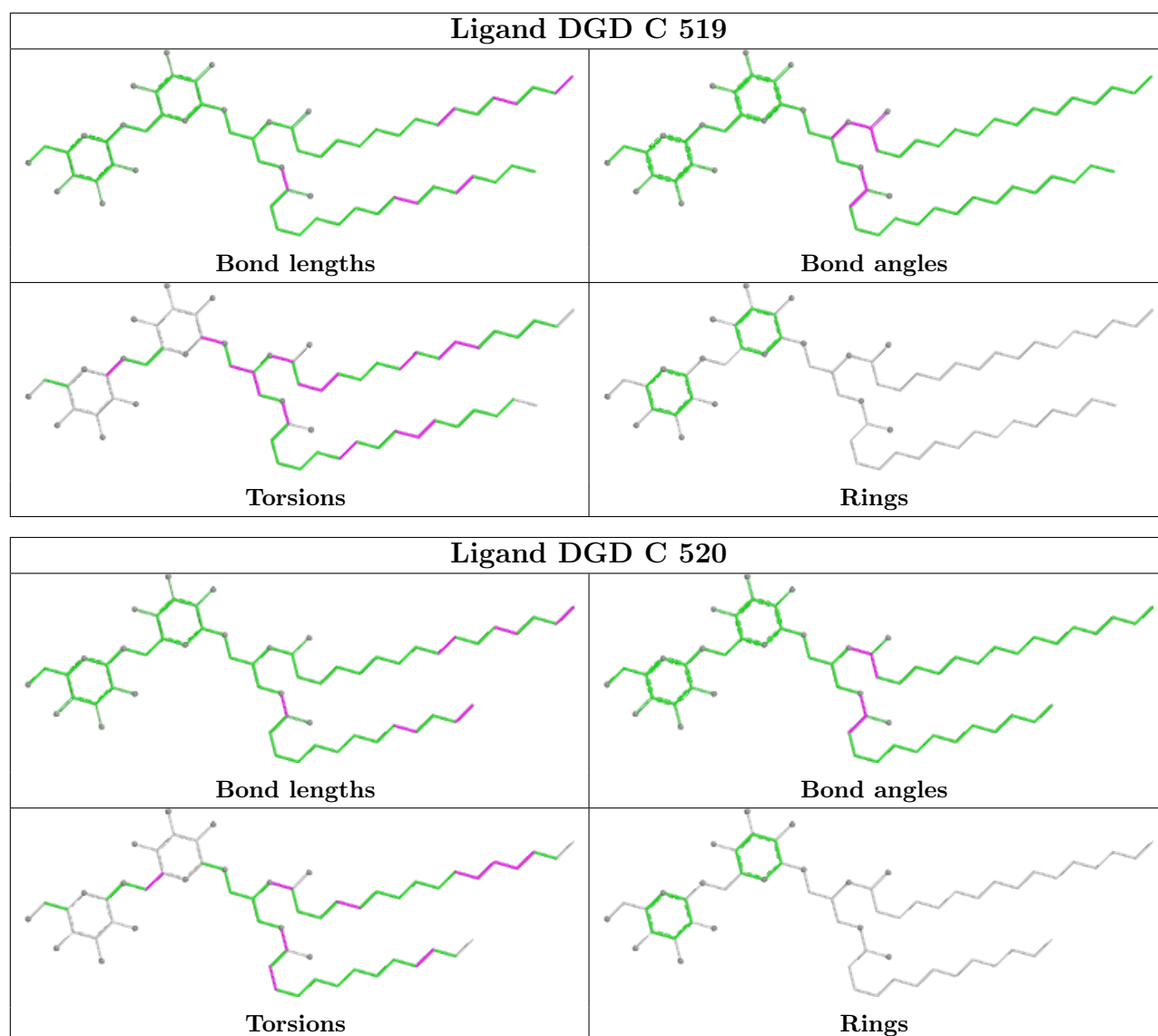
Bond angles

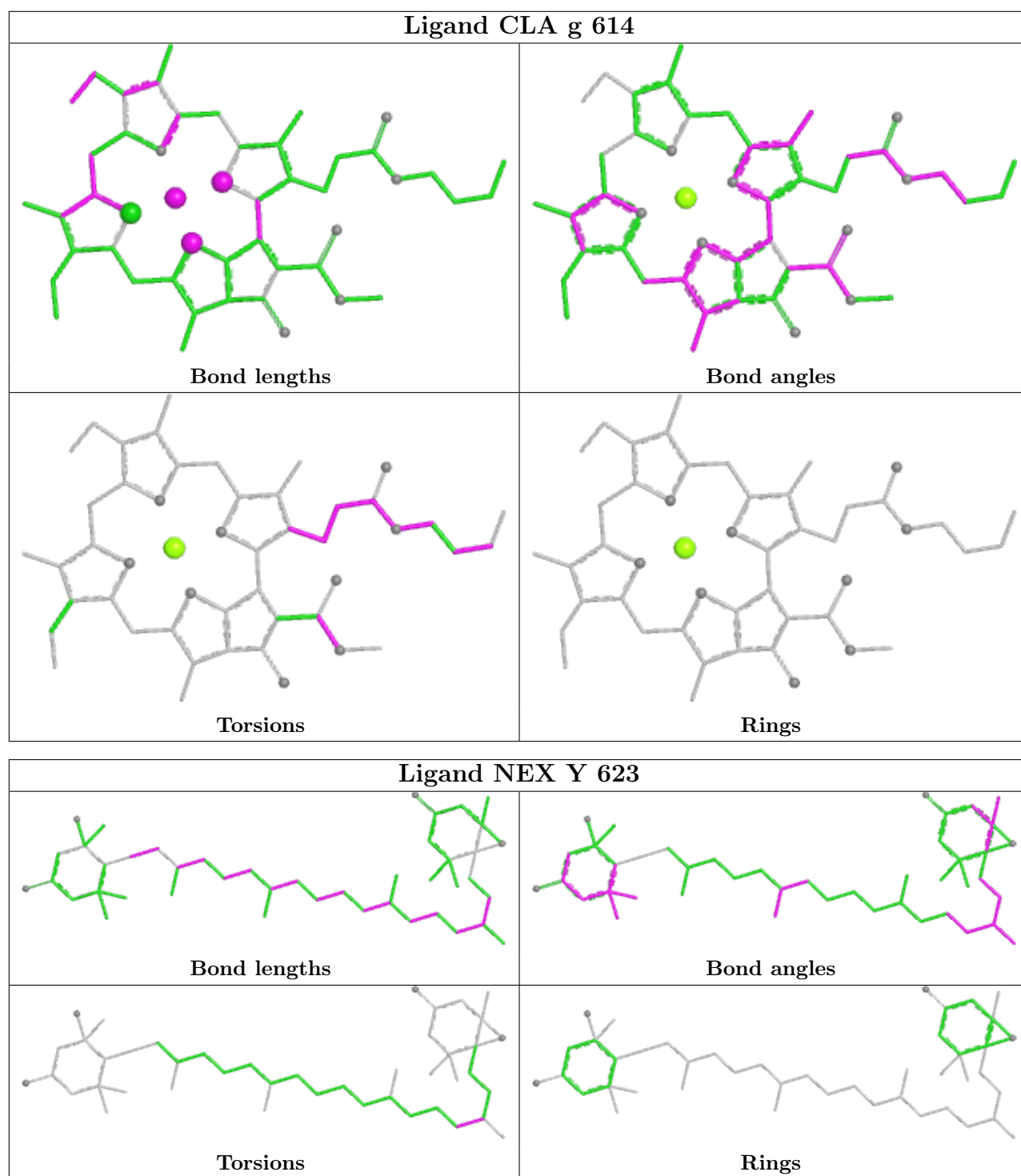


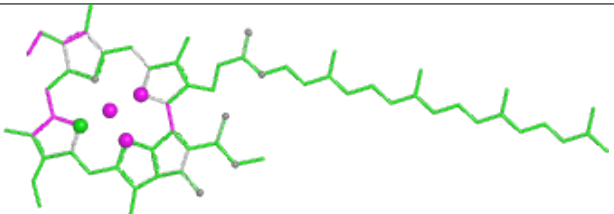
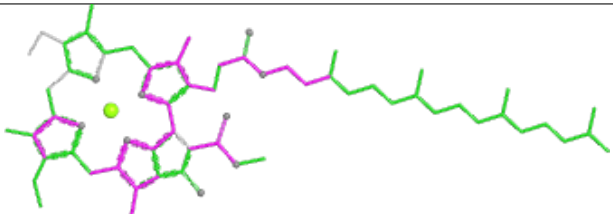
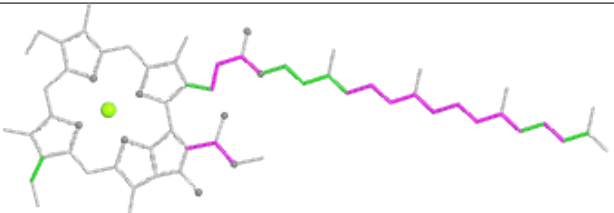
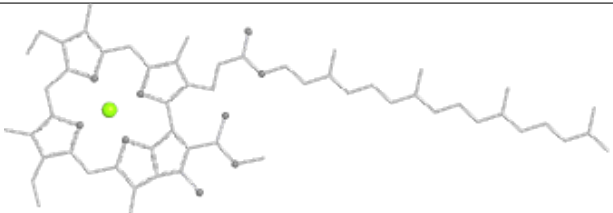
Torsions

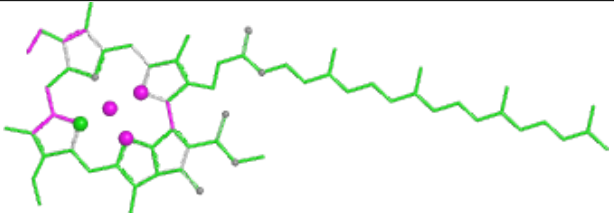
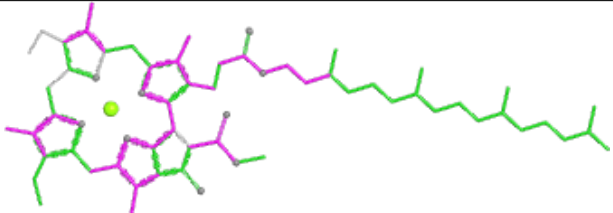
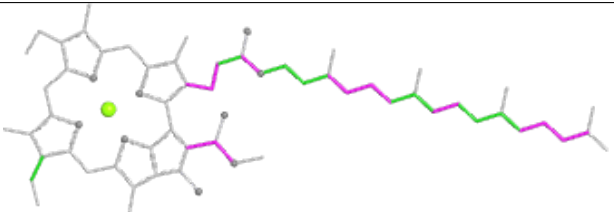
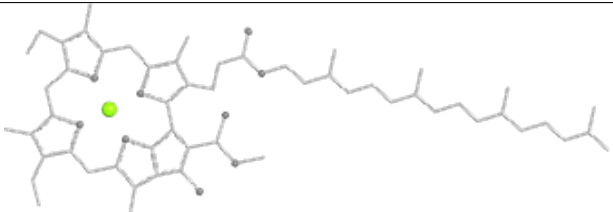


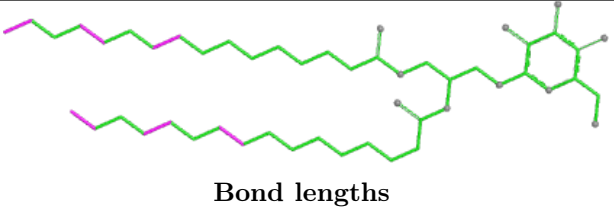
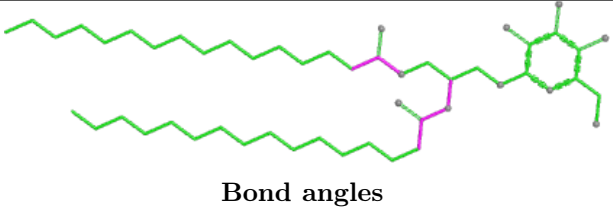
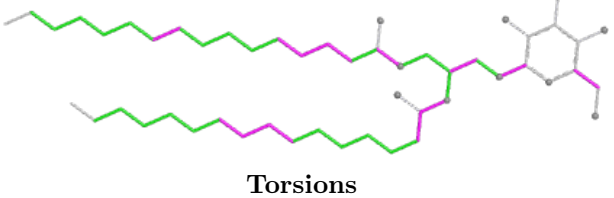
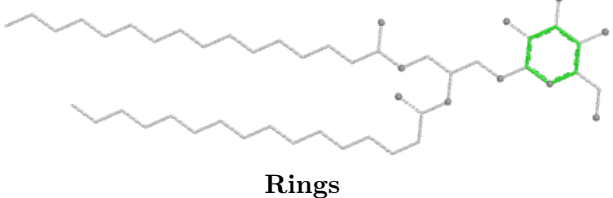
Rings

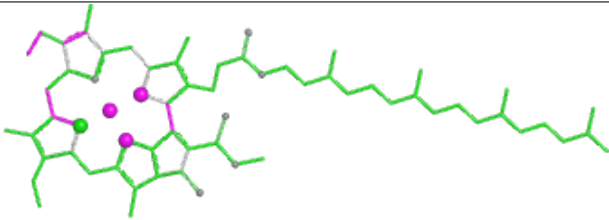
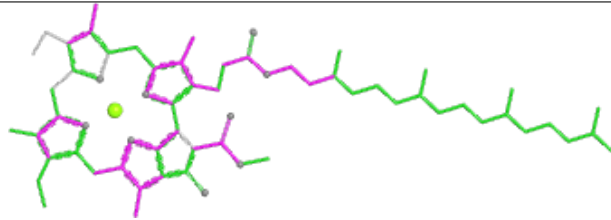
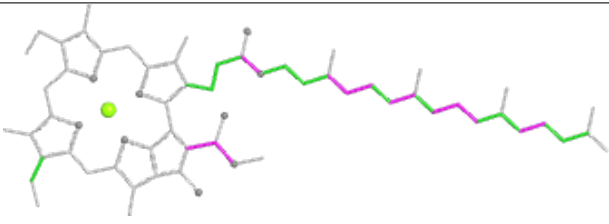
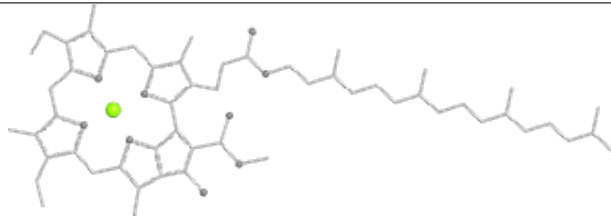


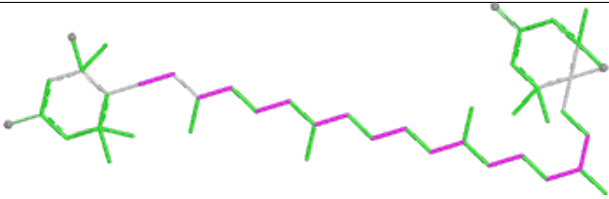
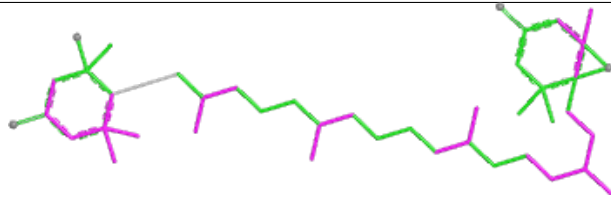
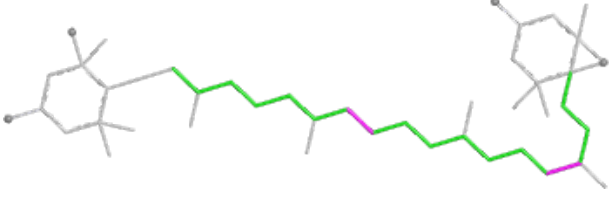
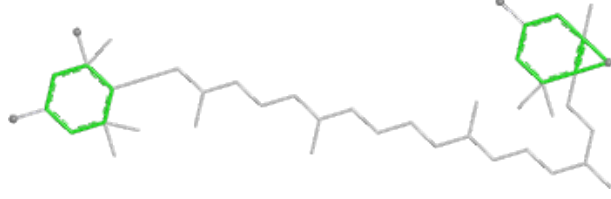


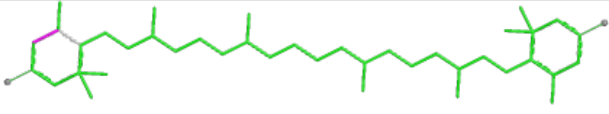
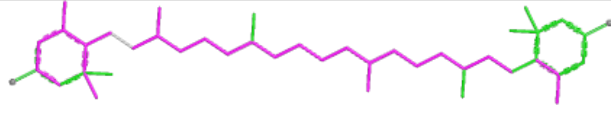
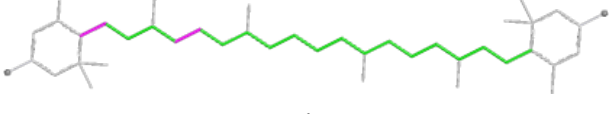
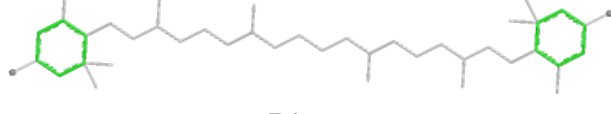
Ligand CLA g 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

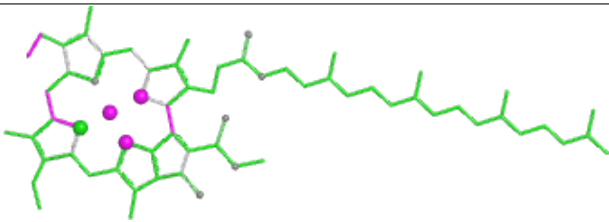
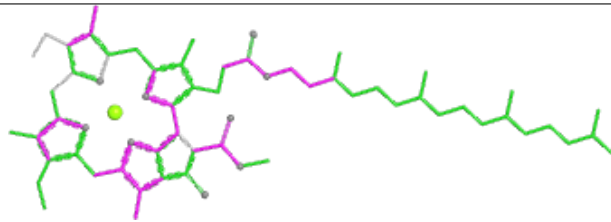
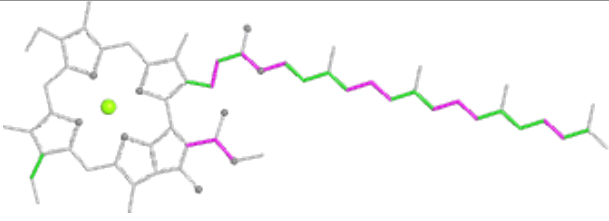
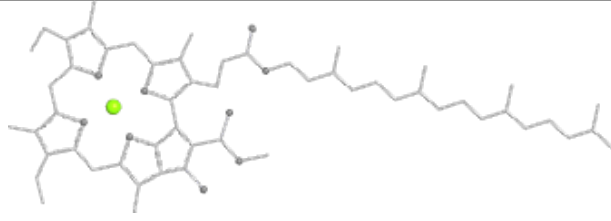
Ligand CLA n 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

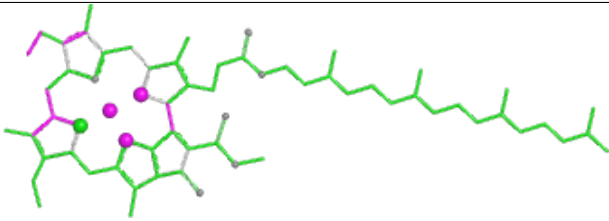
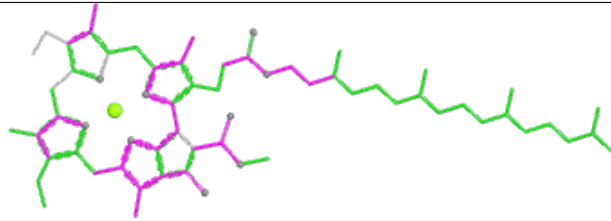
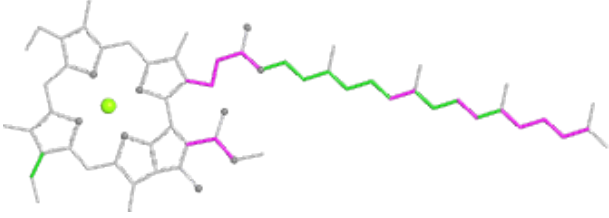
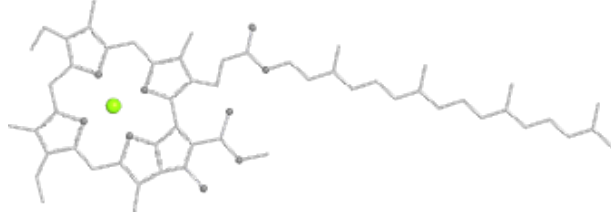
Ligand LMG c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

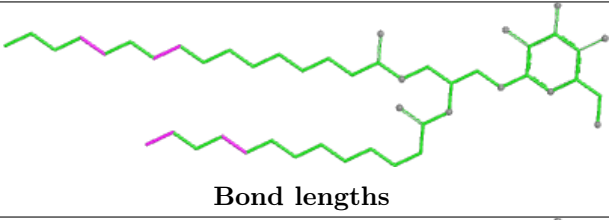
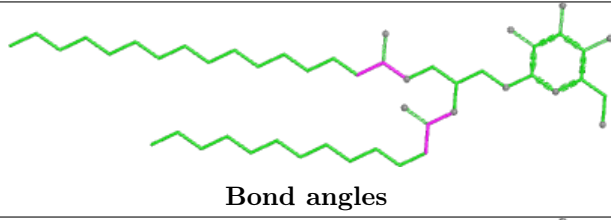
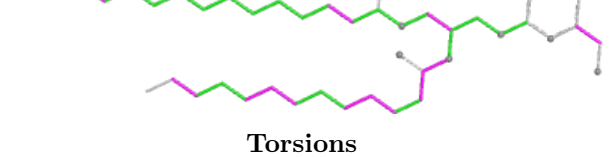

Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

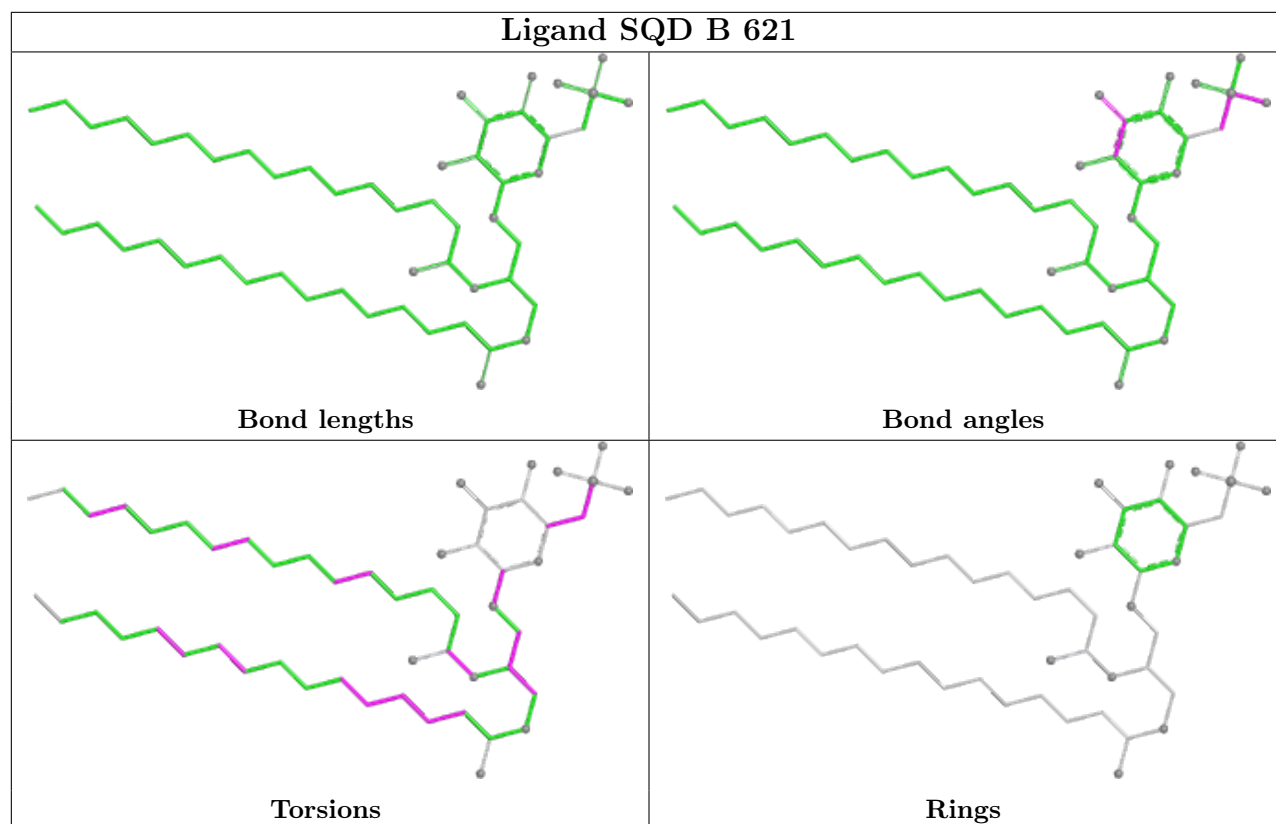
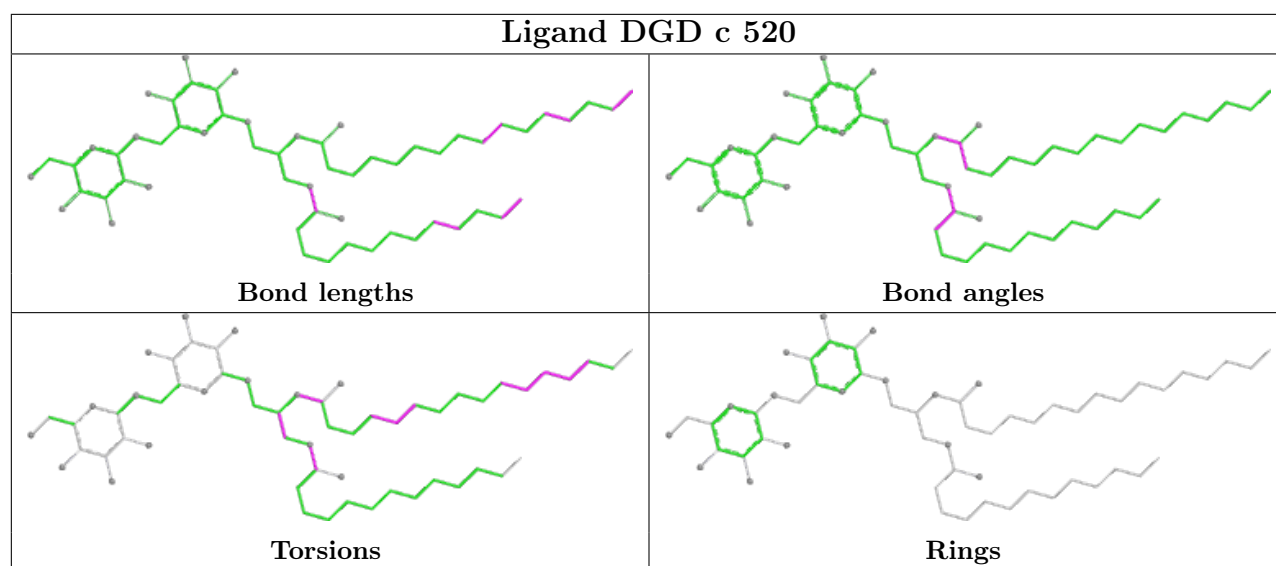
Ligand NEX g 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

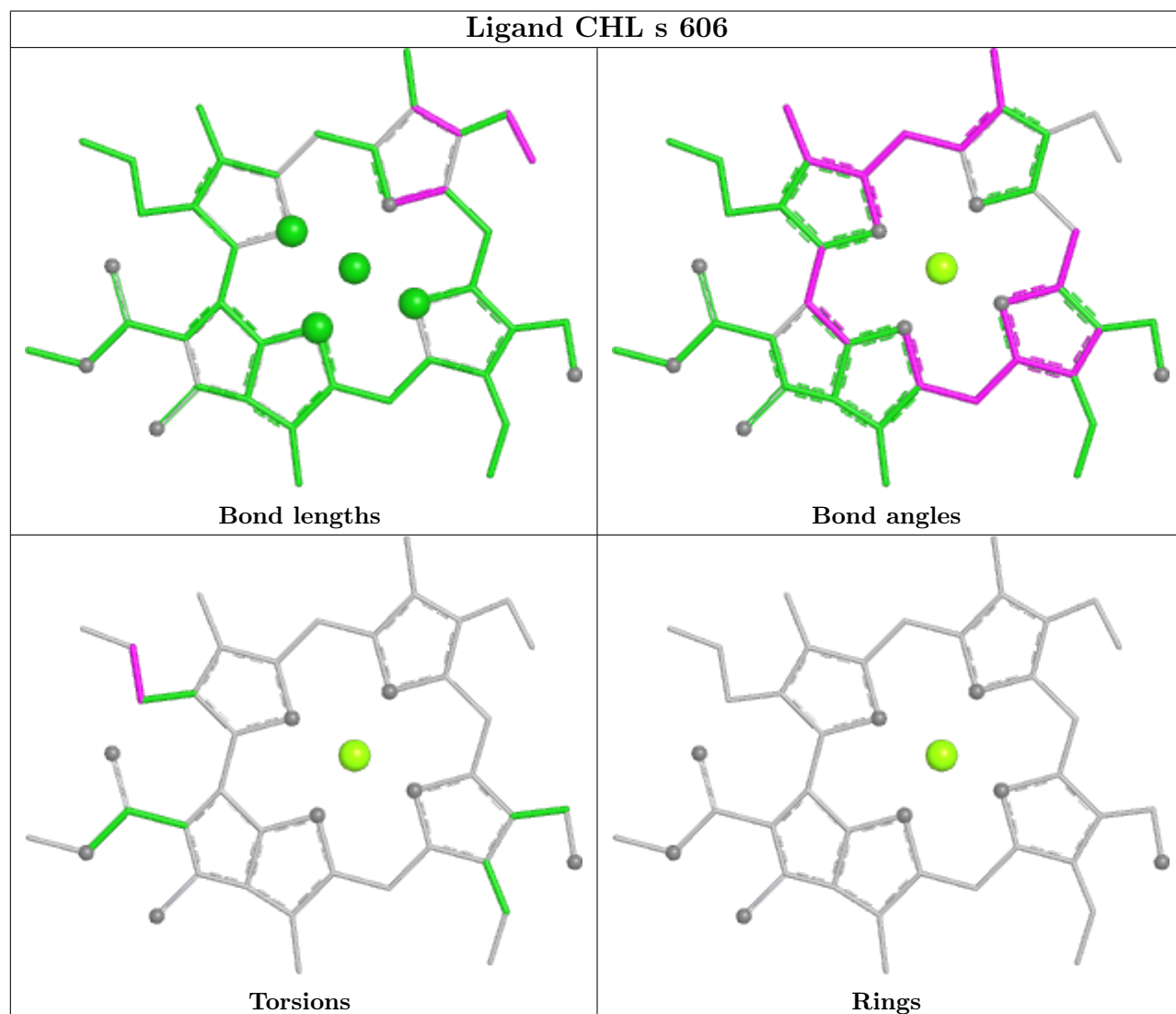
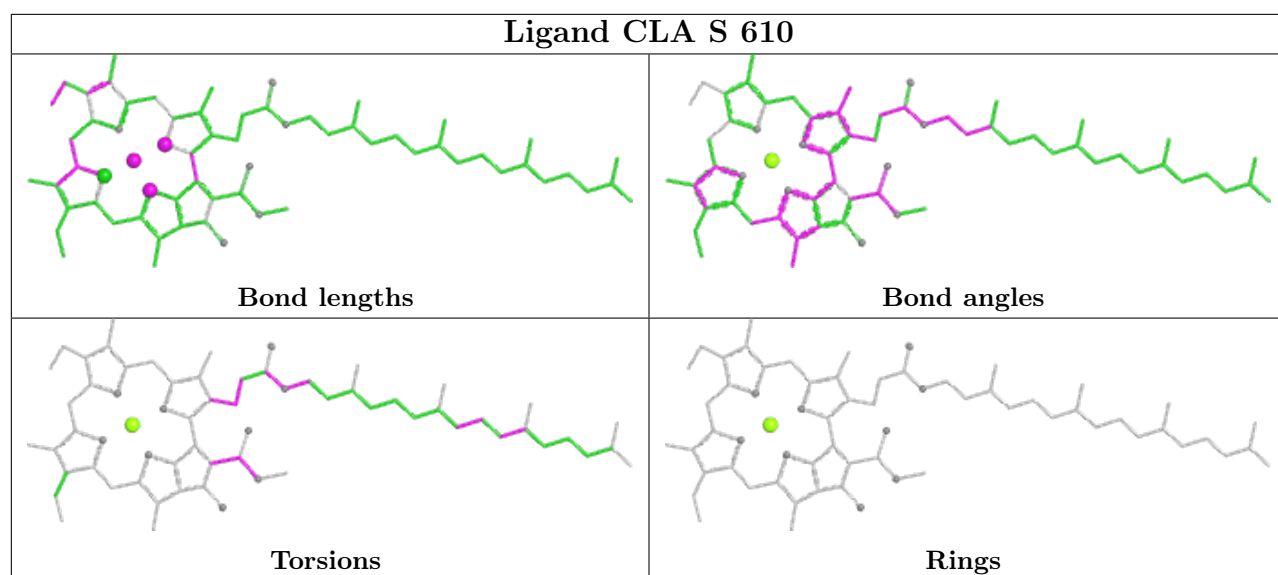
Ligand LUT s 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

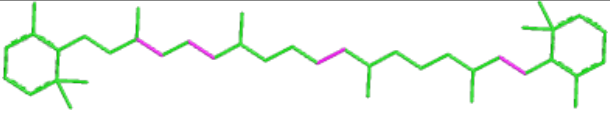
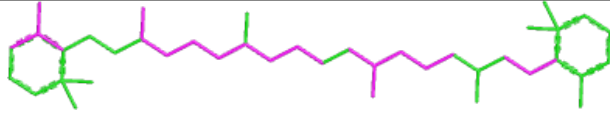
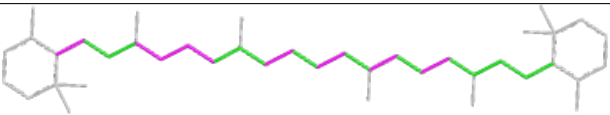
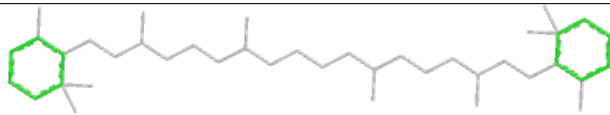
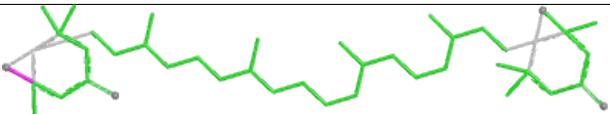
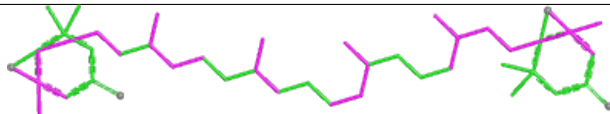
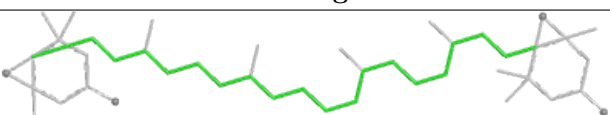
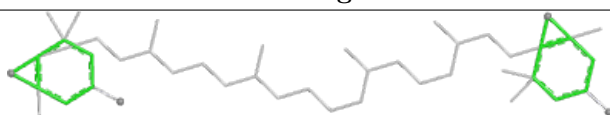
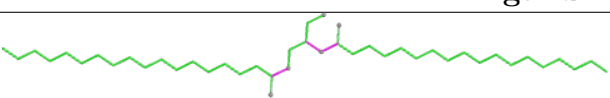
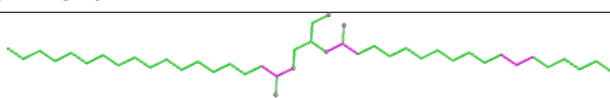
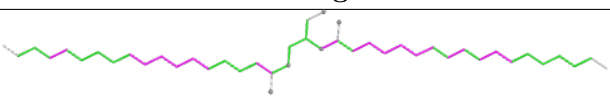
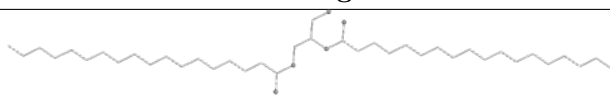
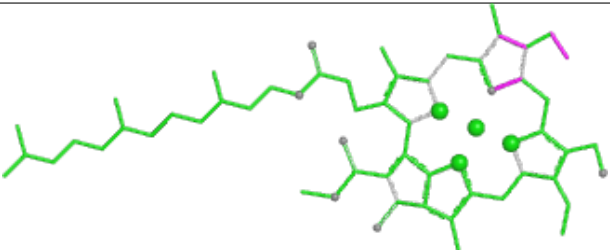
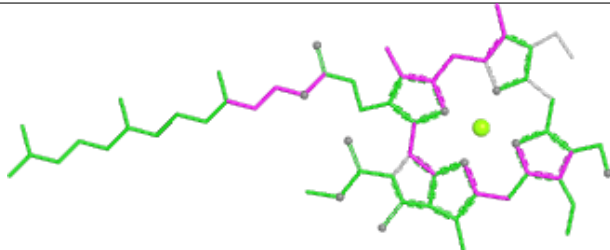
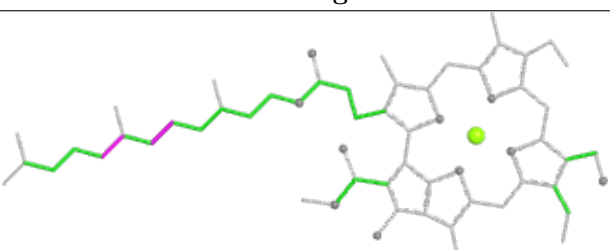
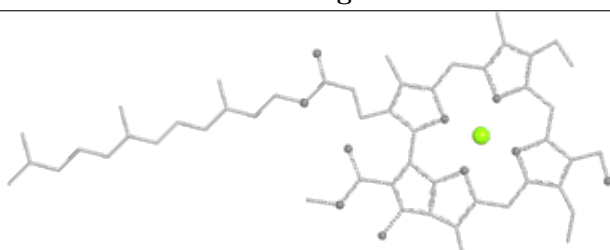
Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

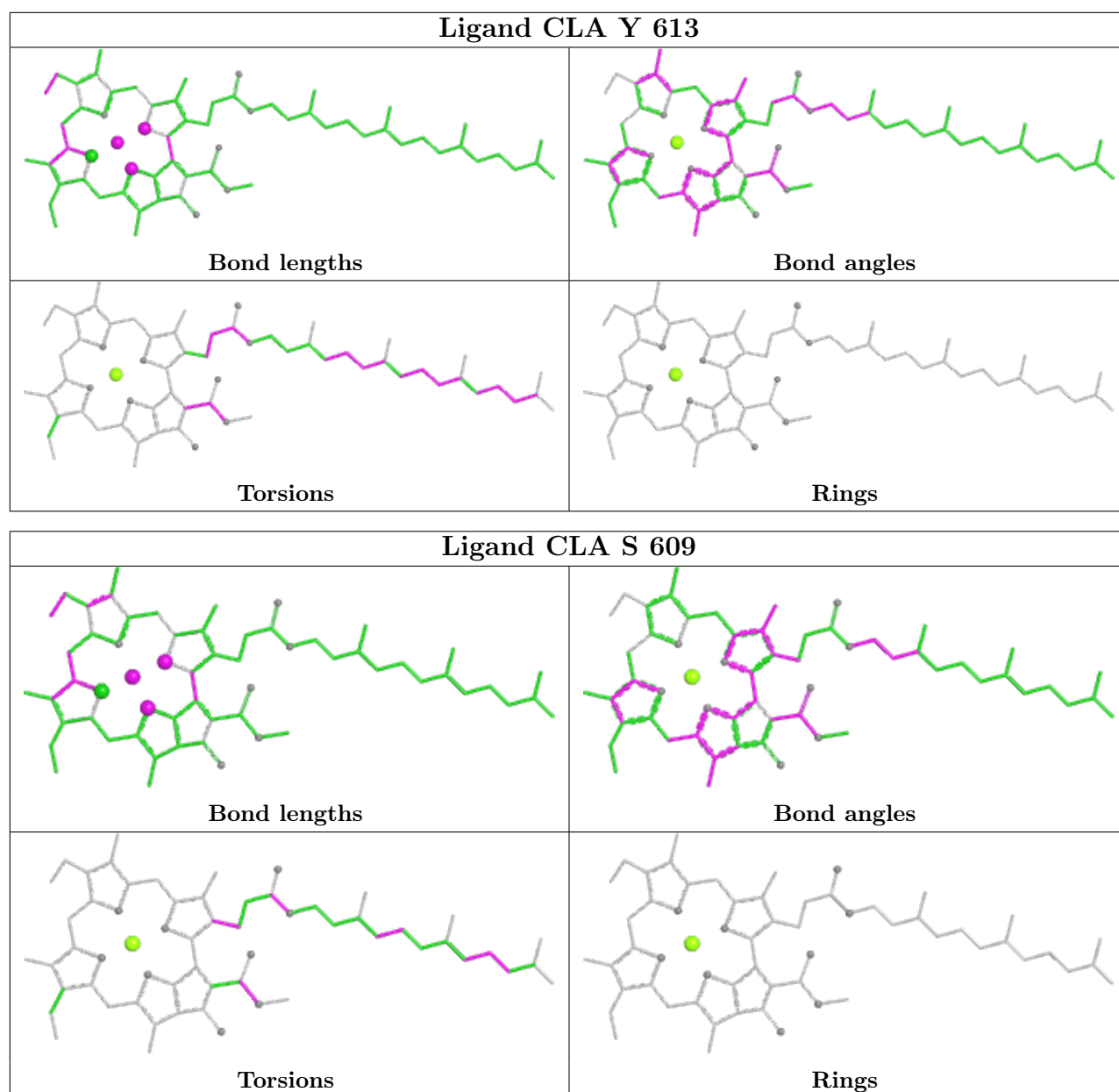
Ligand CLA N 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

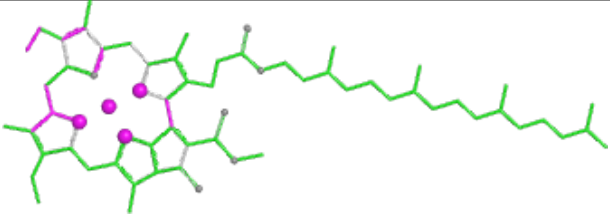
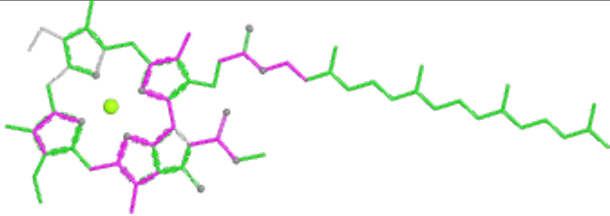
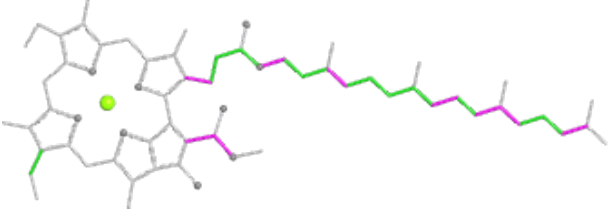
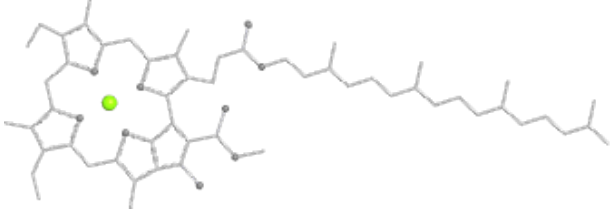
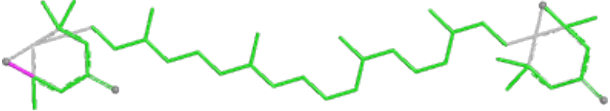
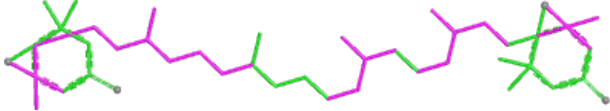
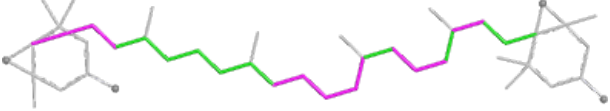
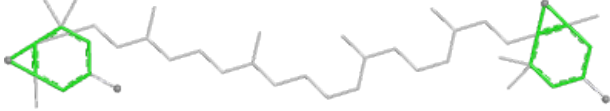
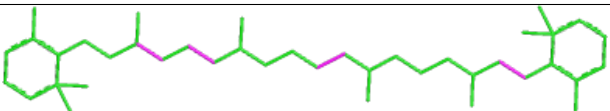
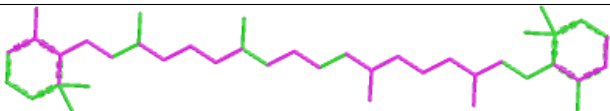
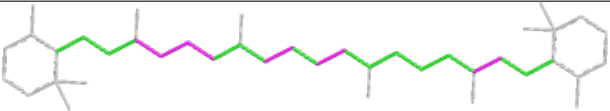
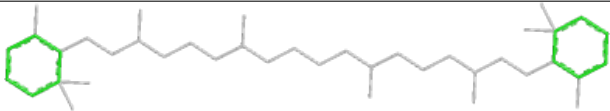
Ligand LMG h 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

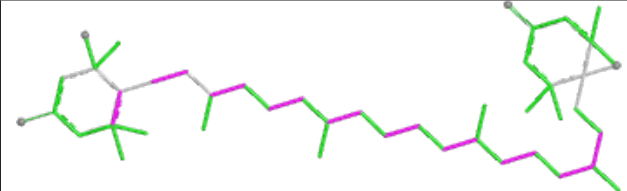

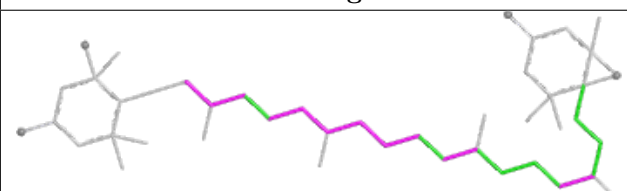
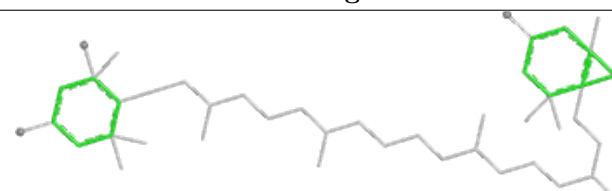


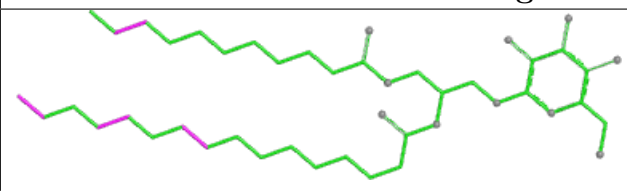
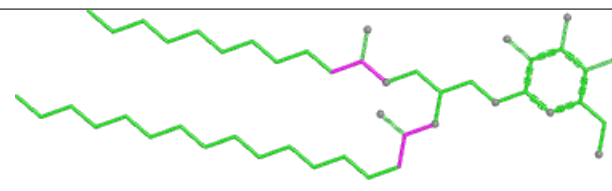
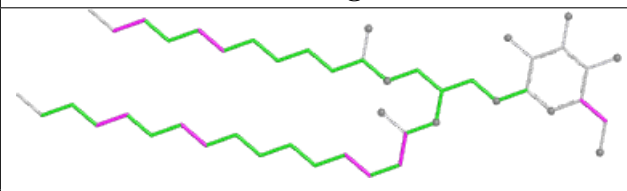
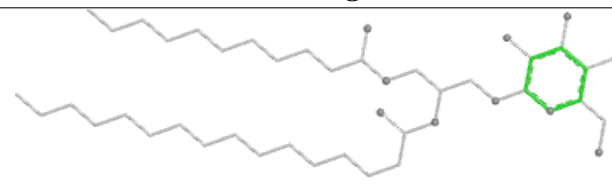


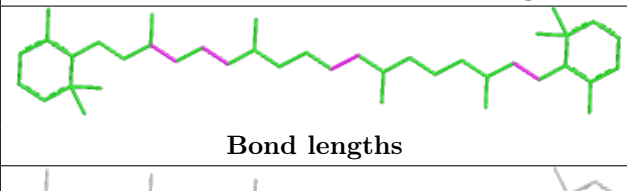
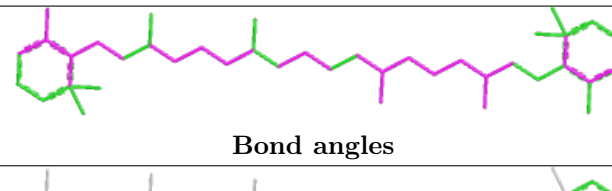
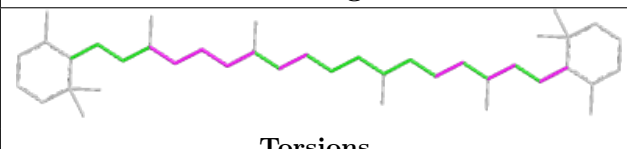
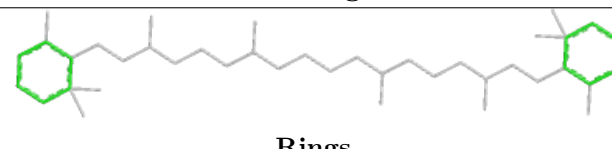
Ligand BCR C 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand XAT g 622	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGA C 524	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL S 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

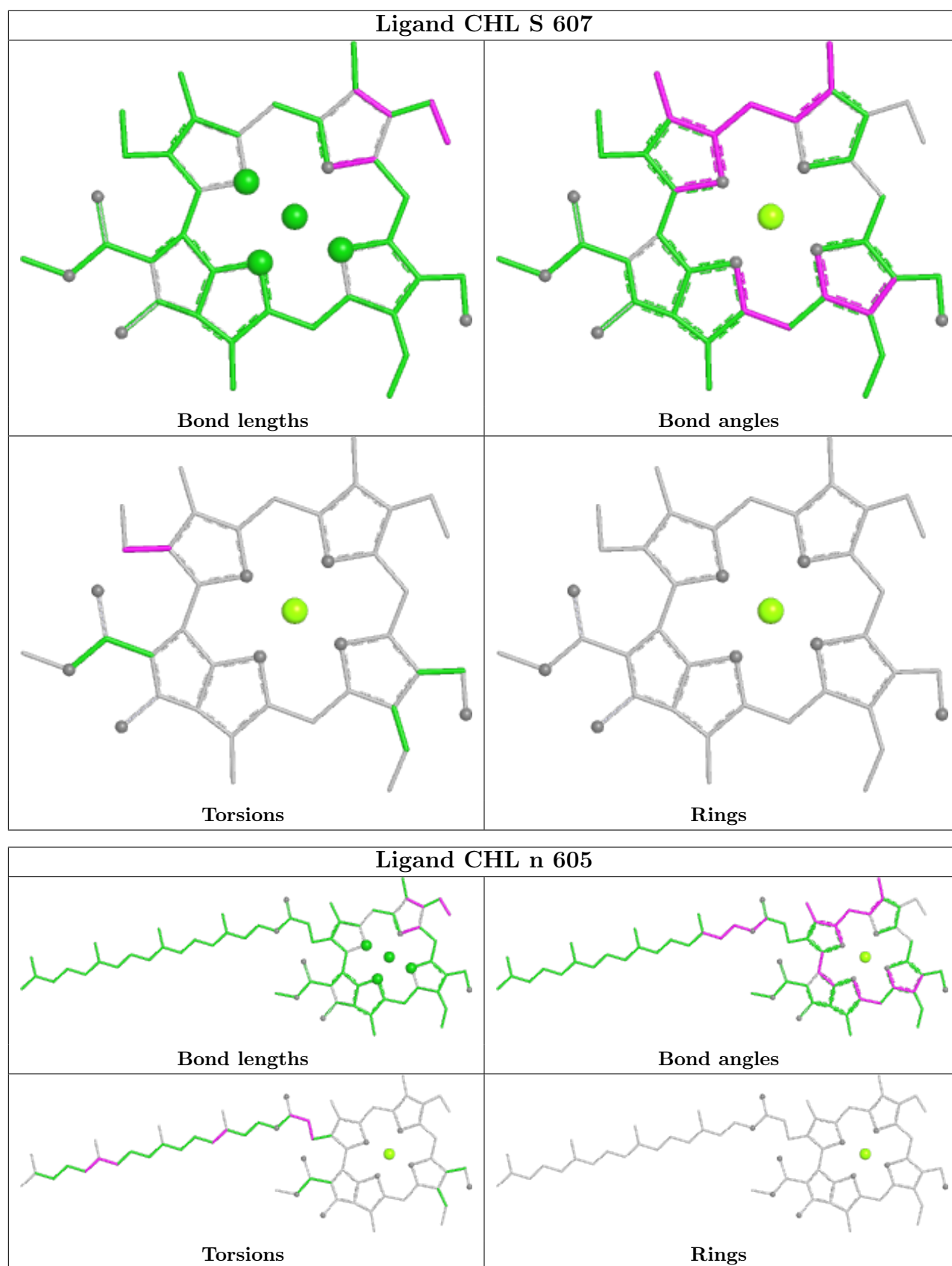


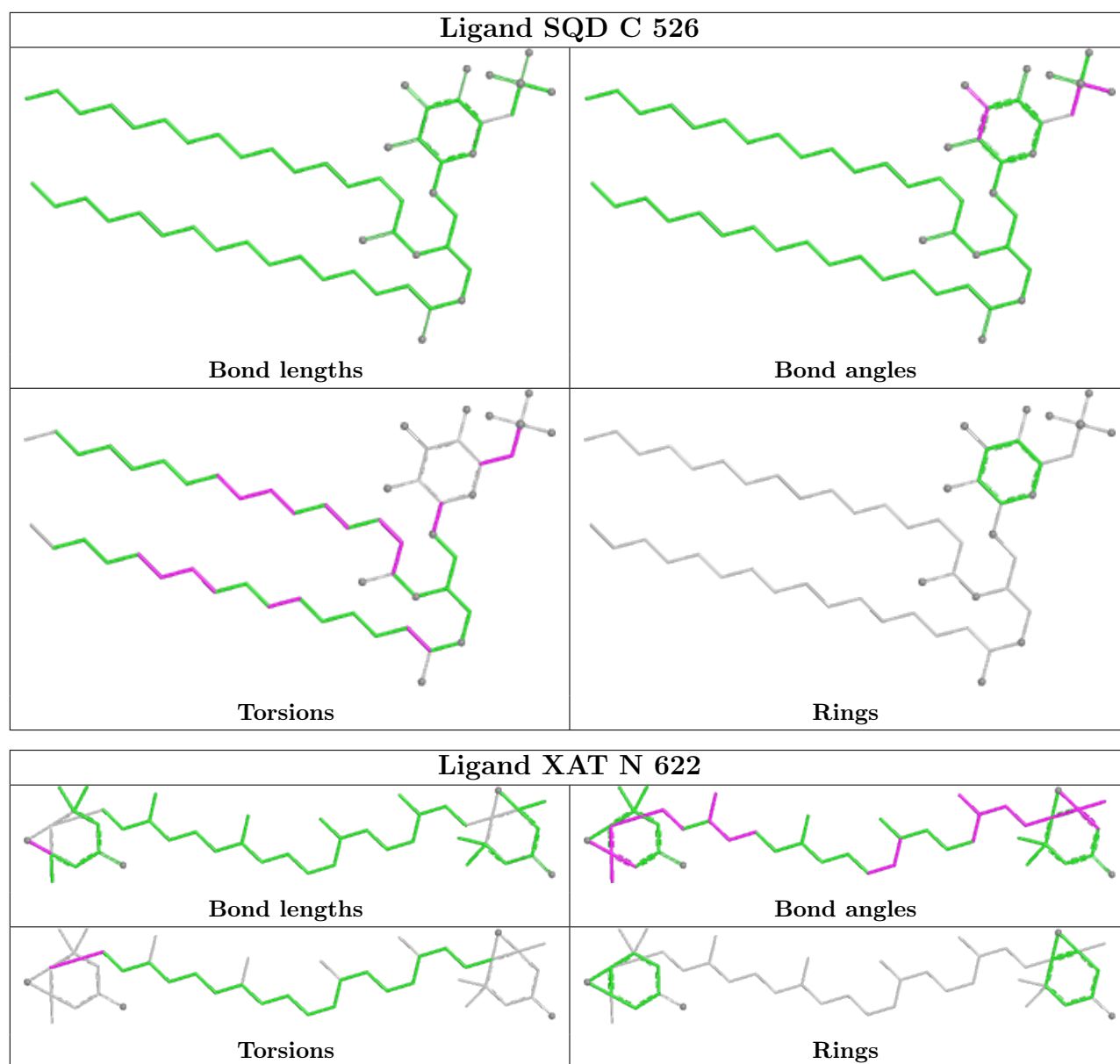
Ligand CLA n 613	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand XAT r 622	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

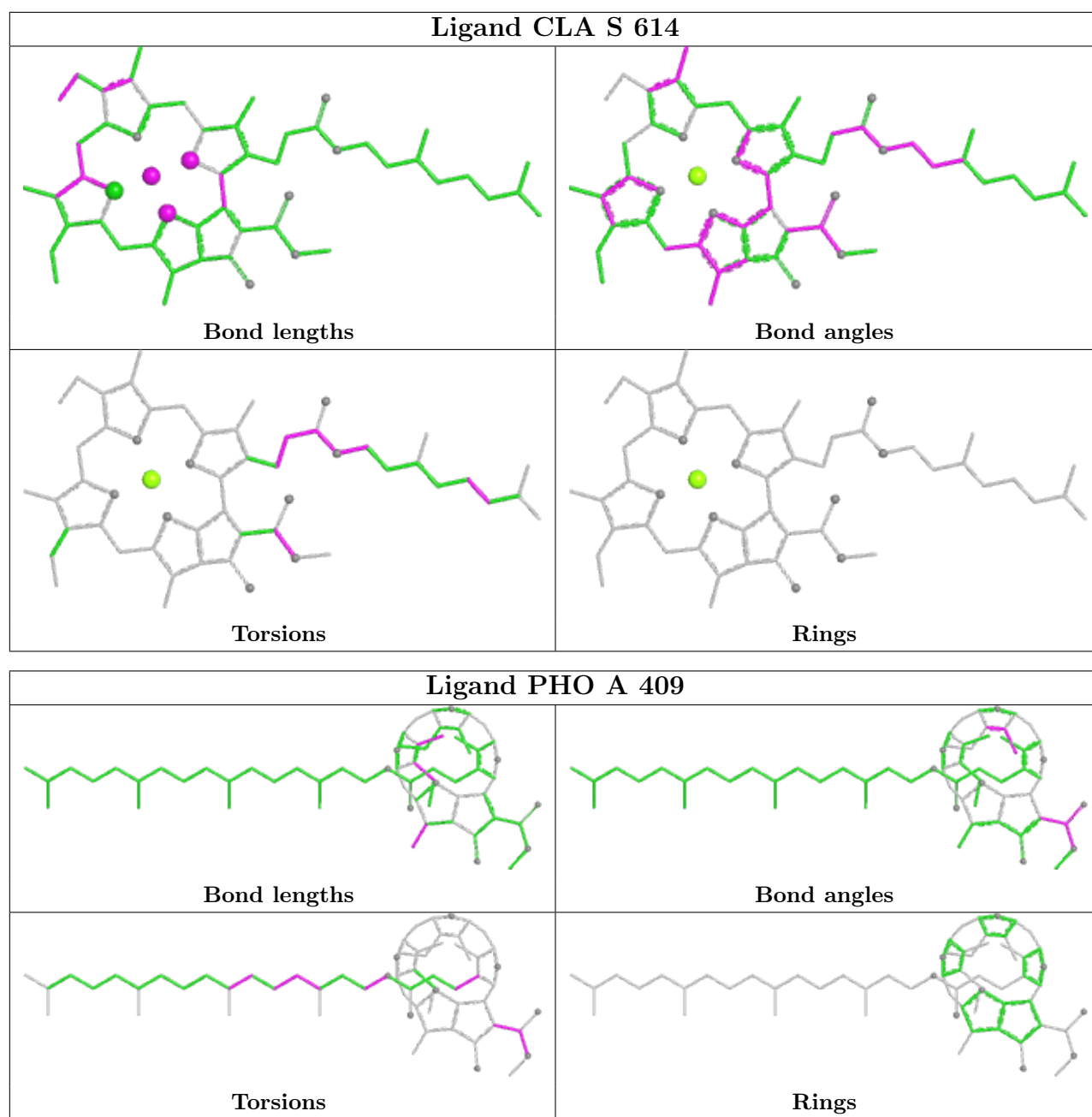
Ligand NEX s 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

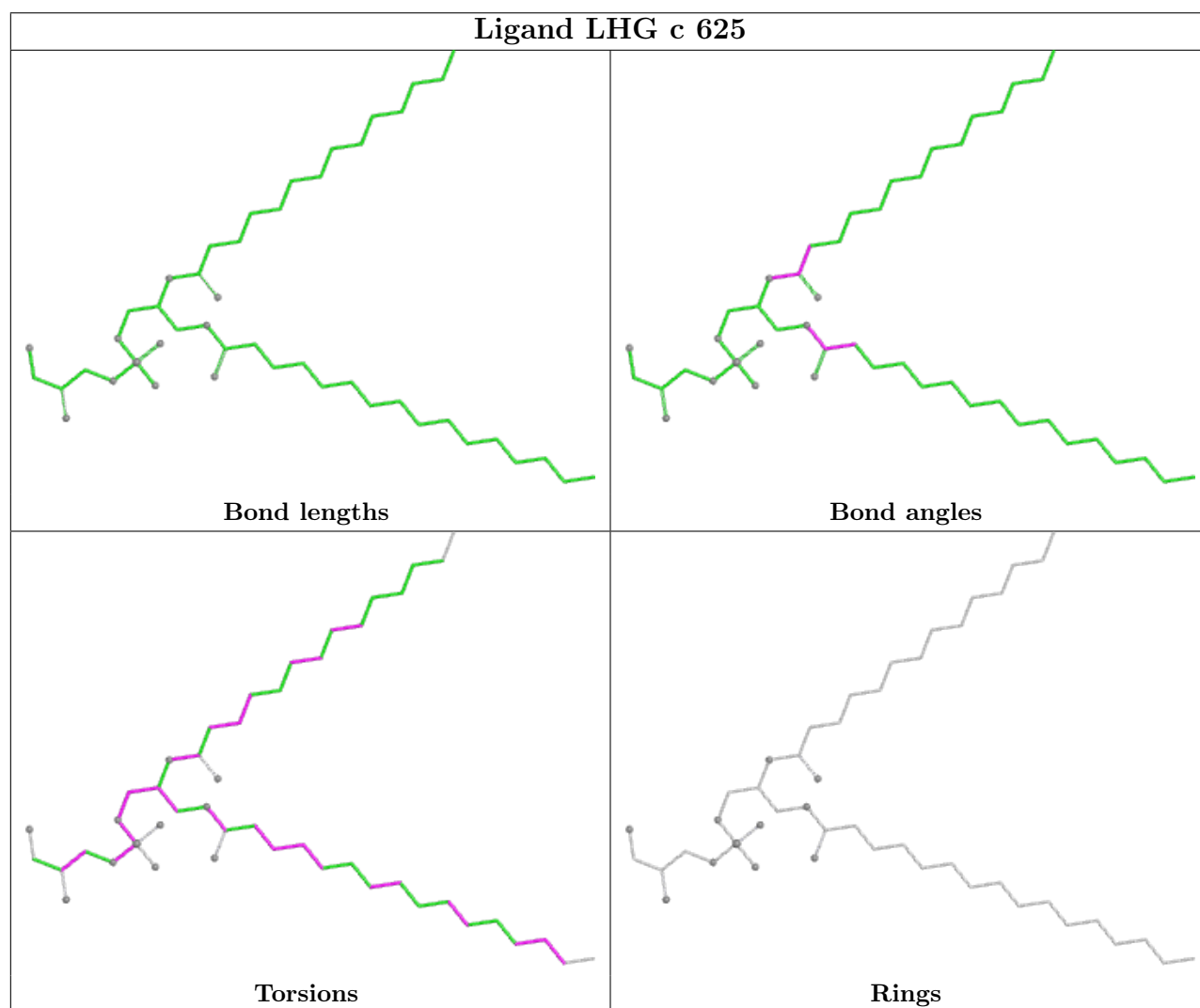
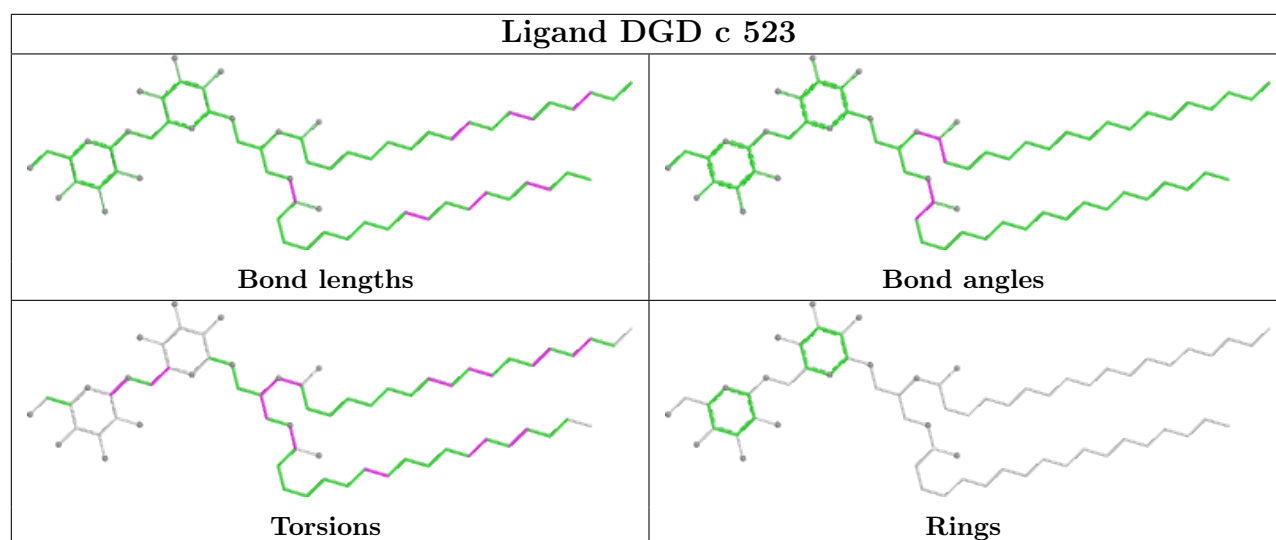
Ligand LMG D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

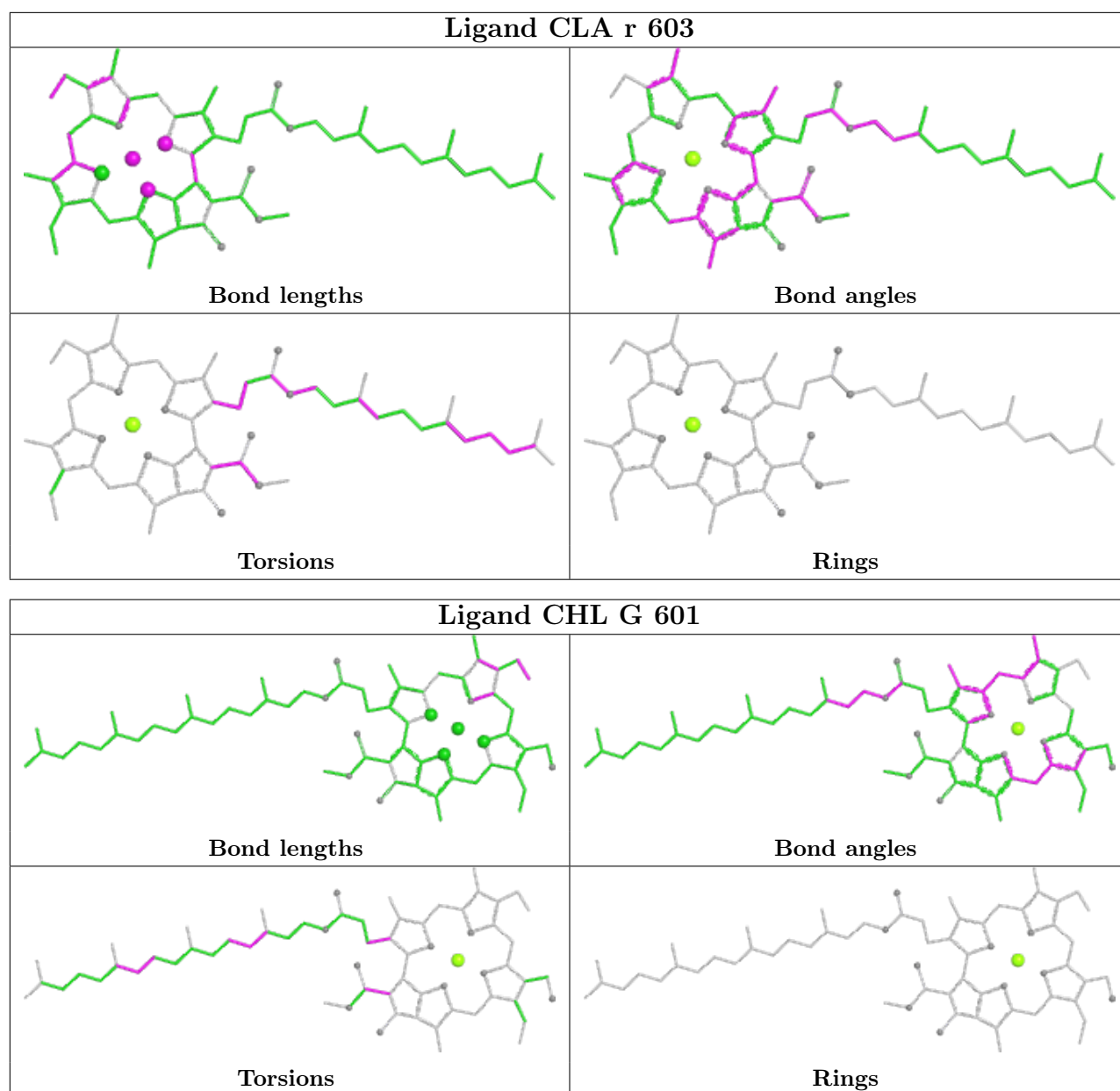
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

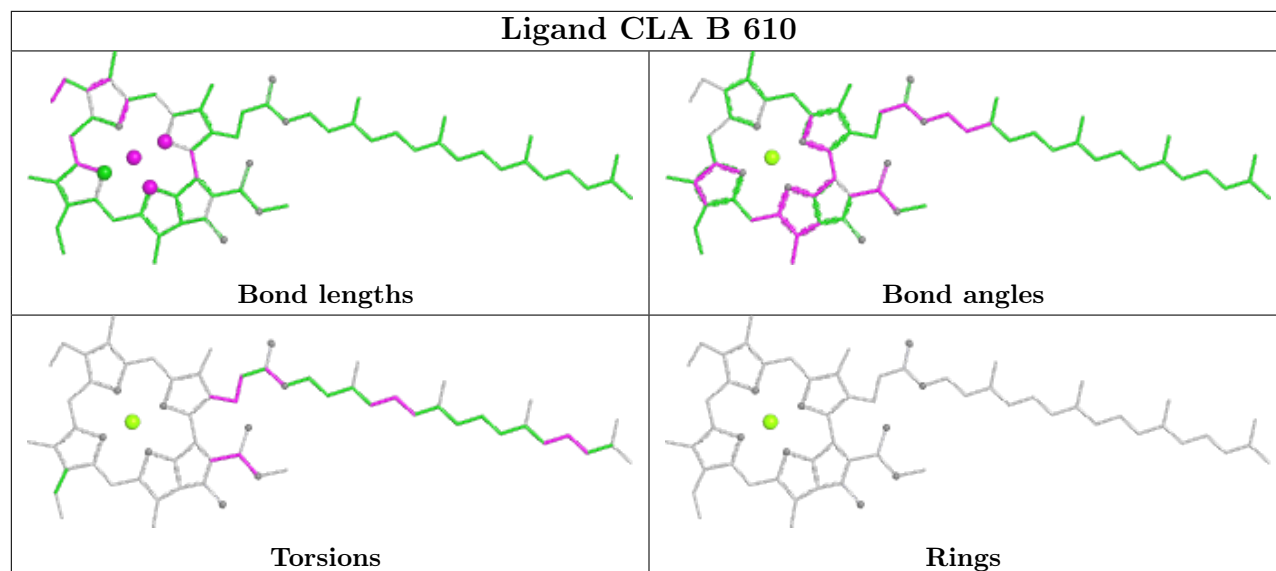
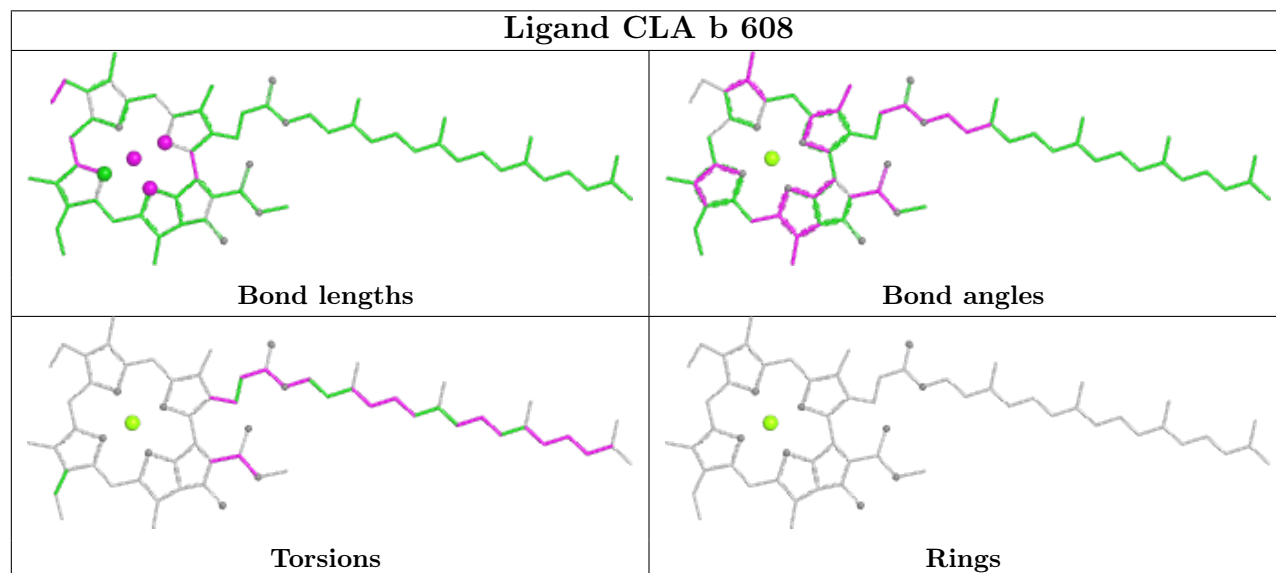
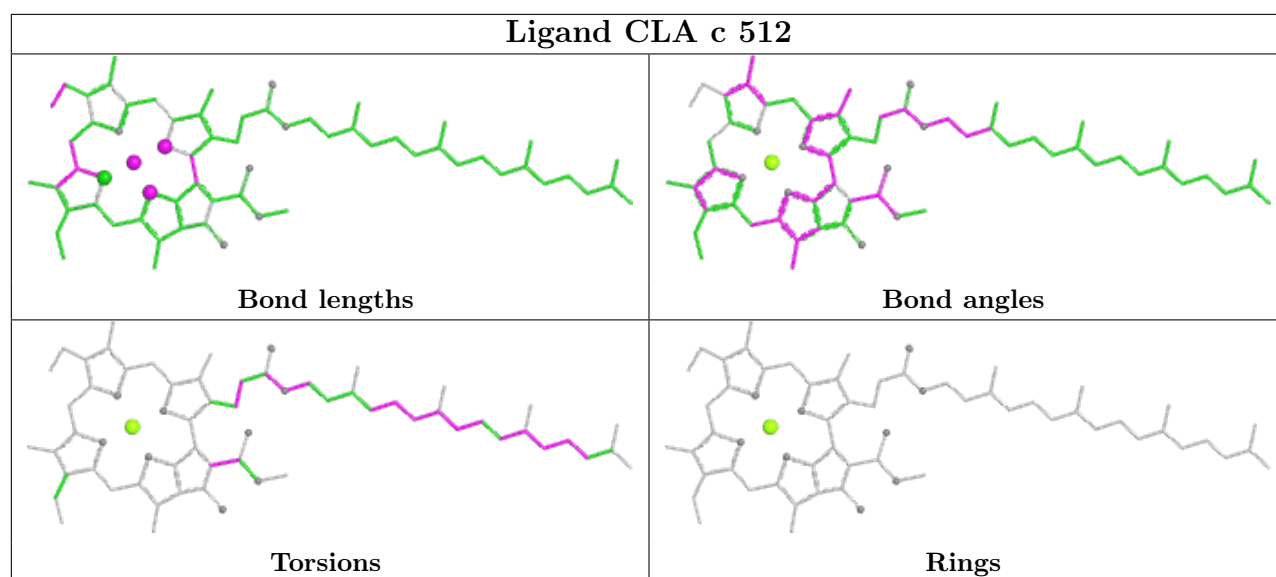


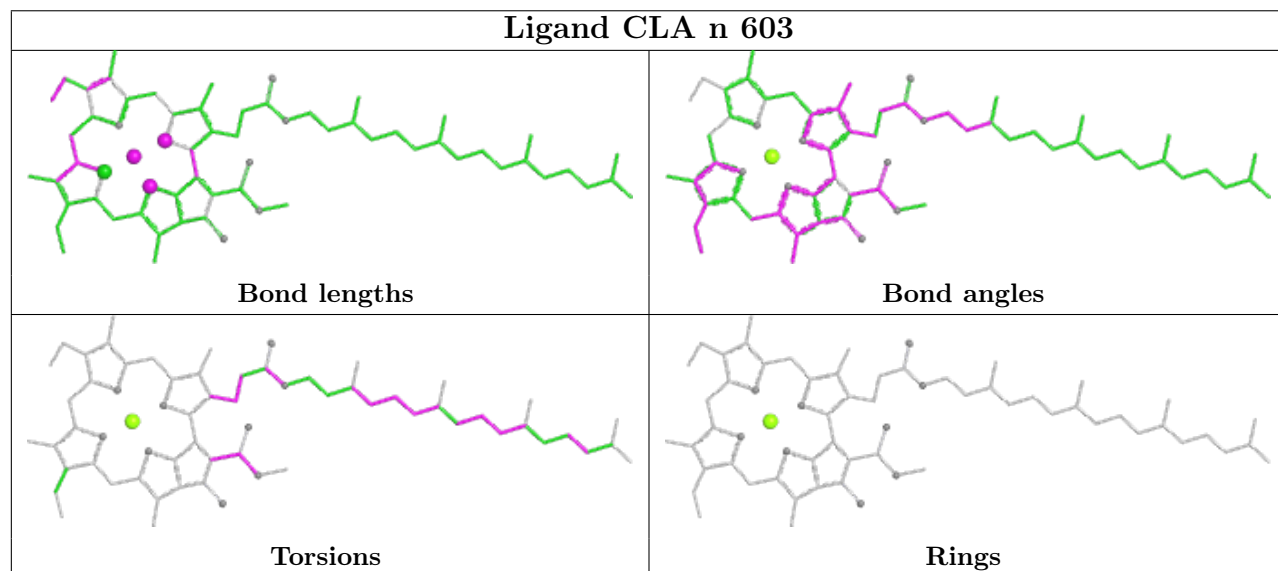
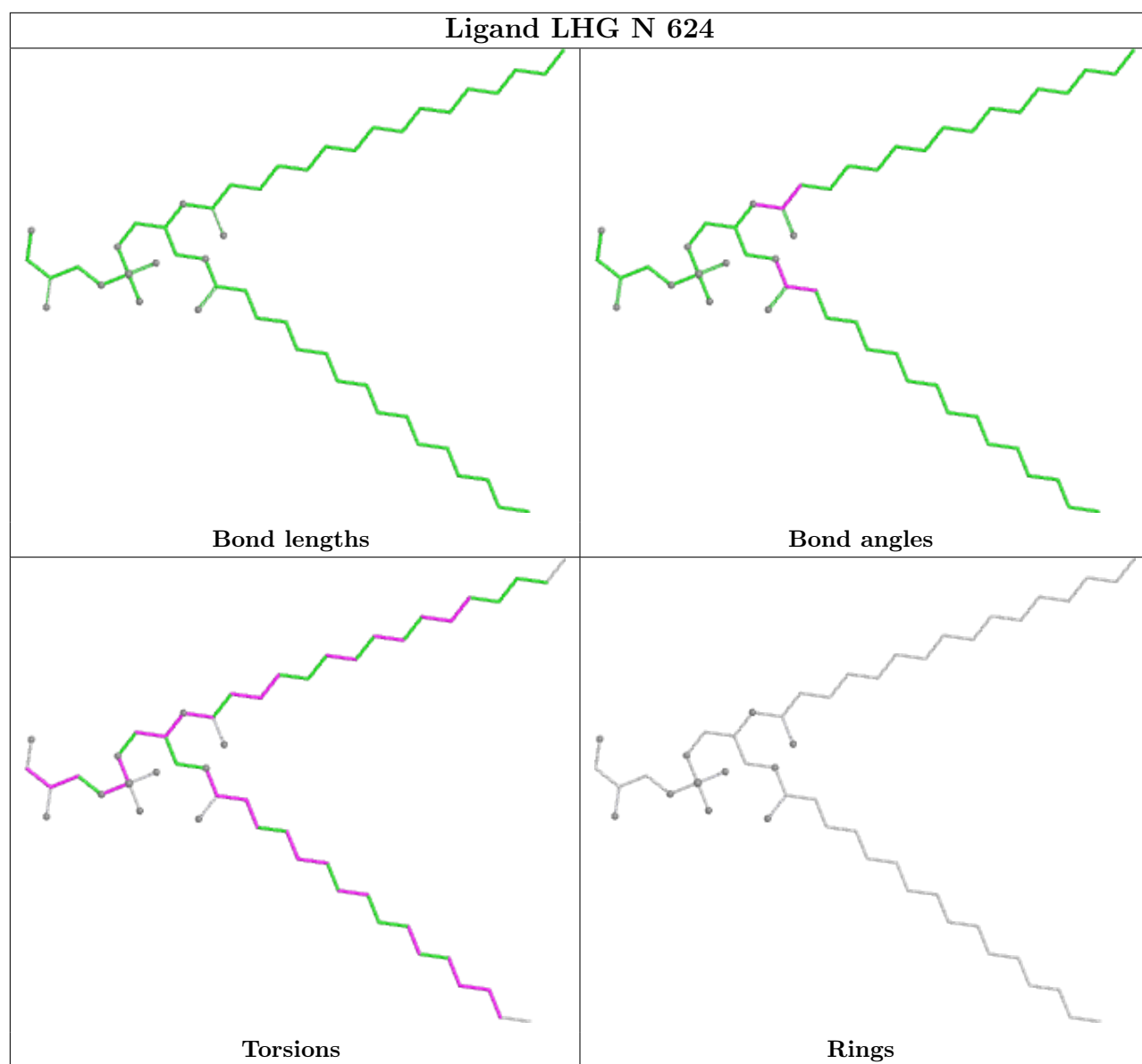


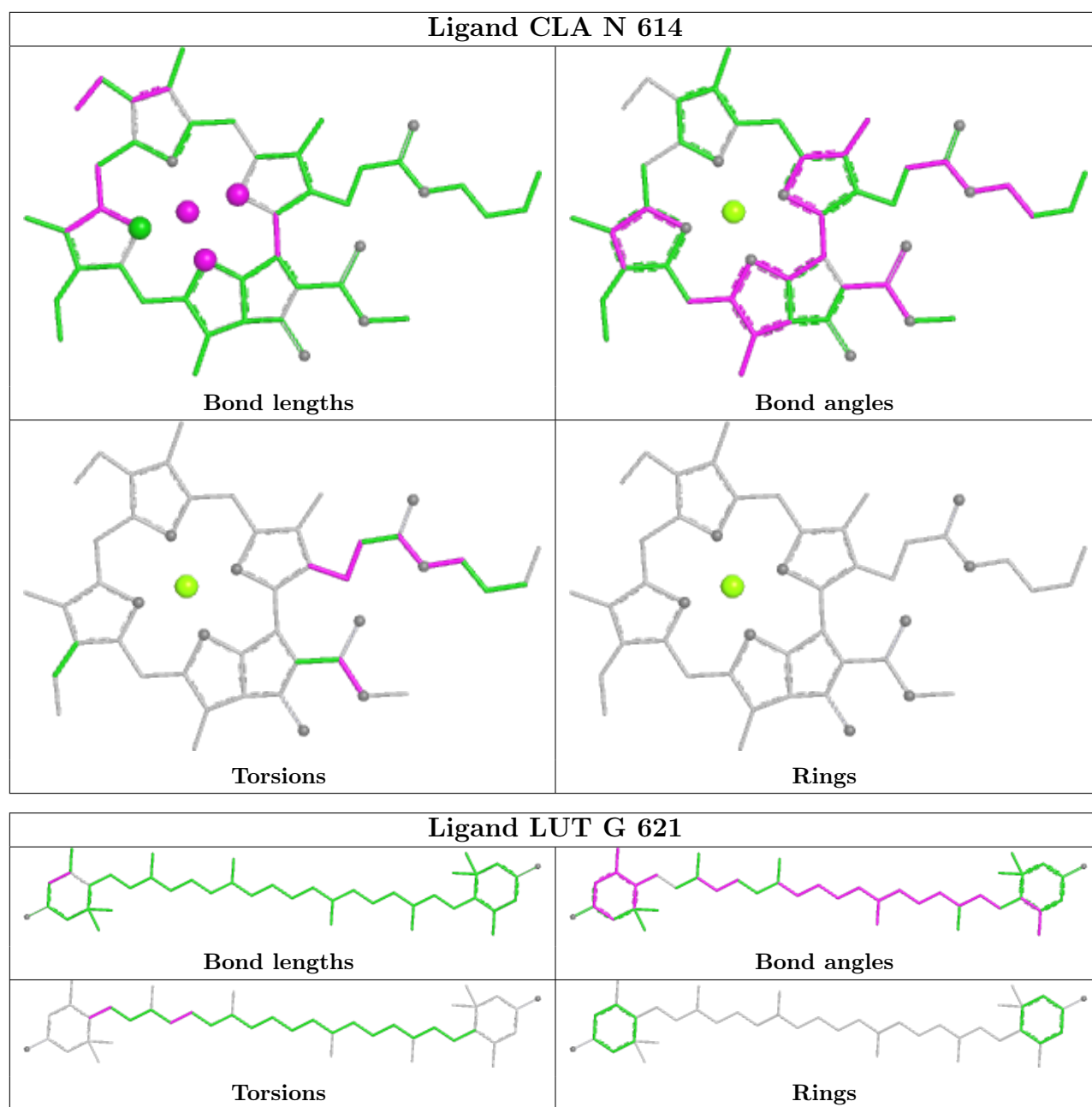




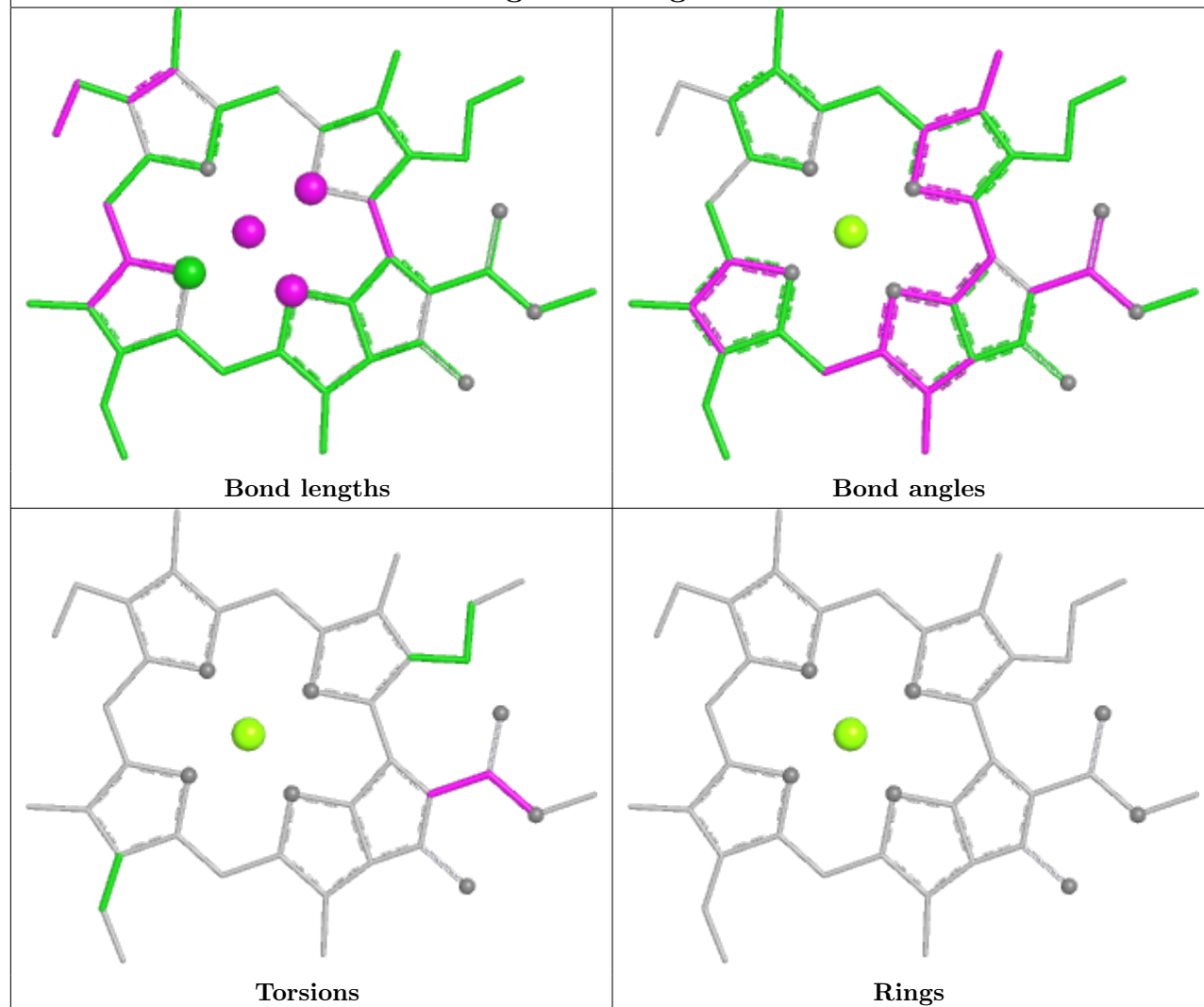




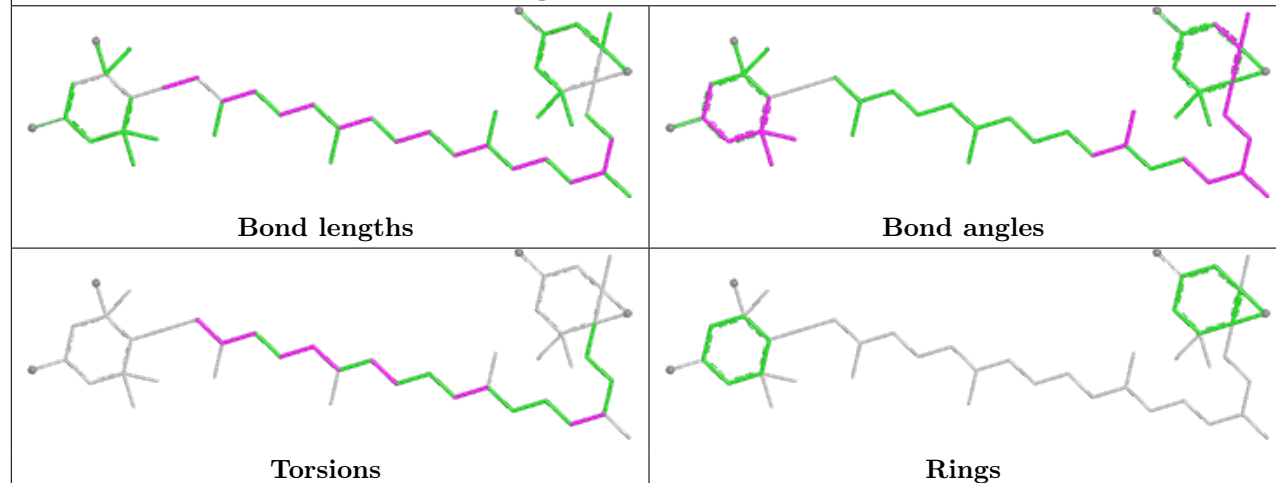


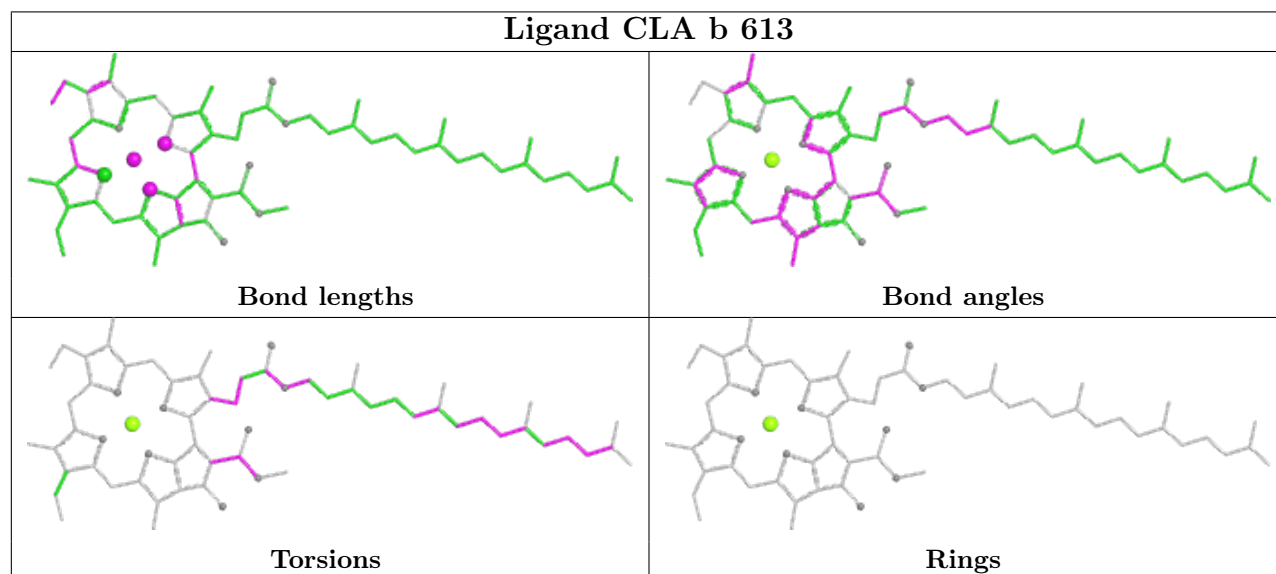
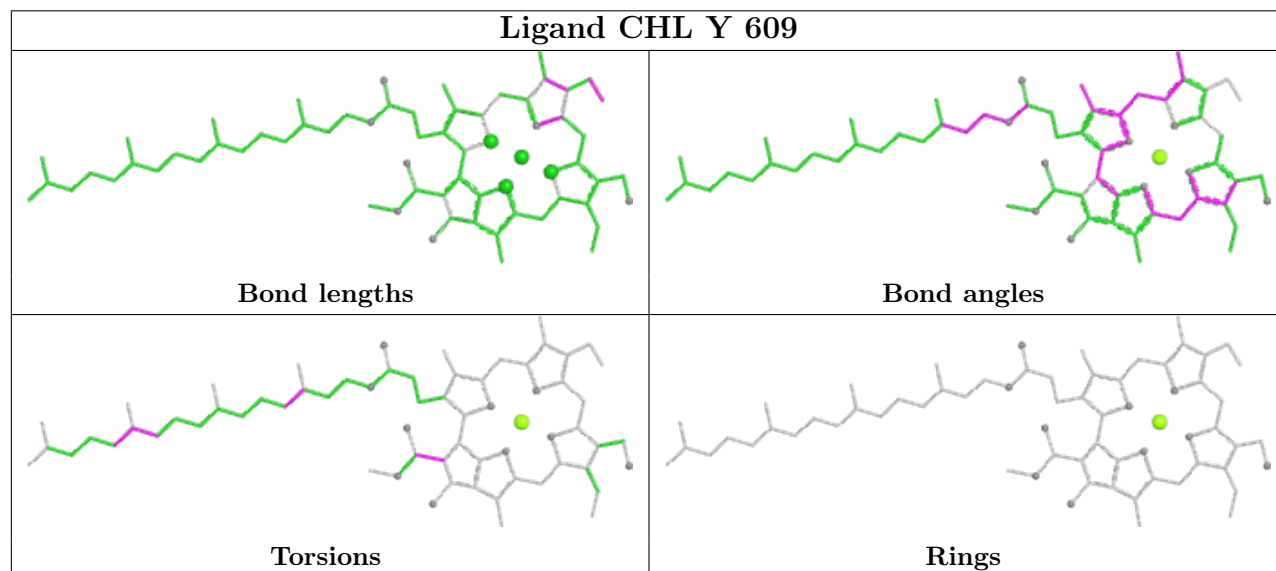
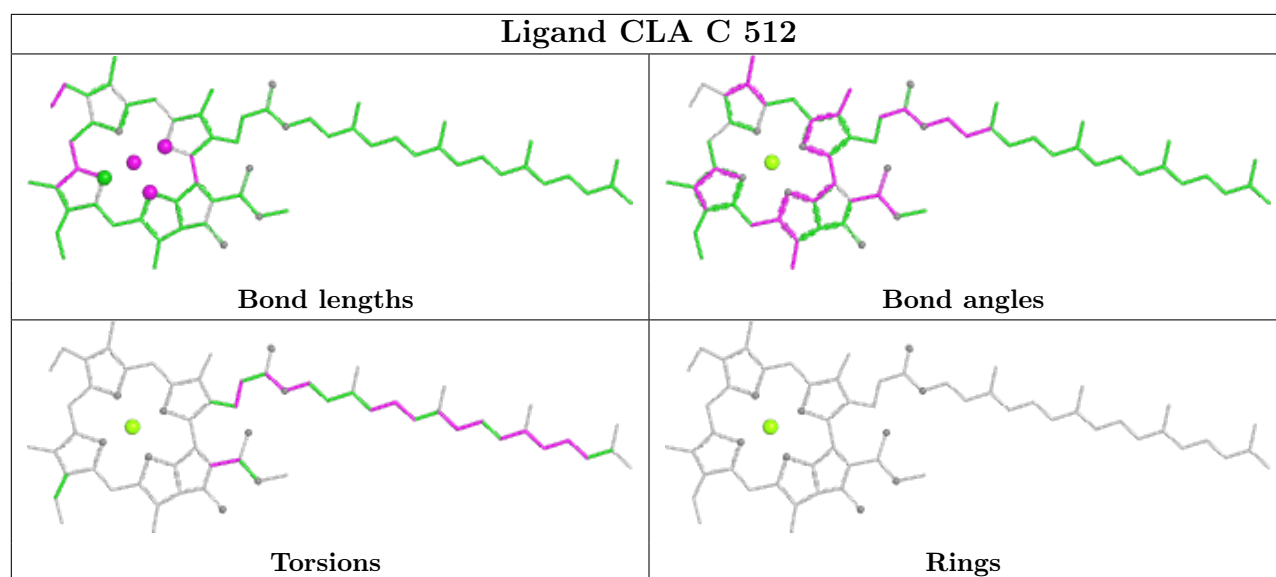


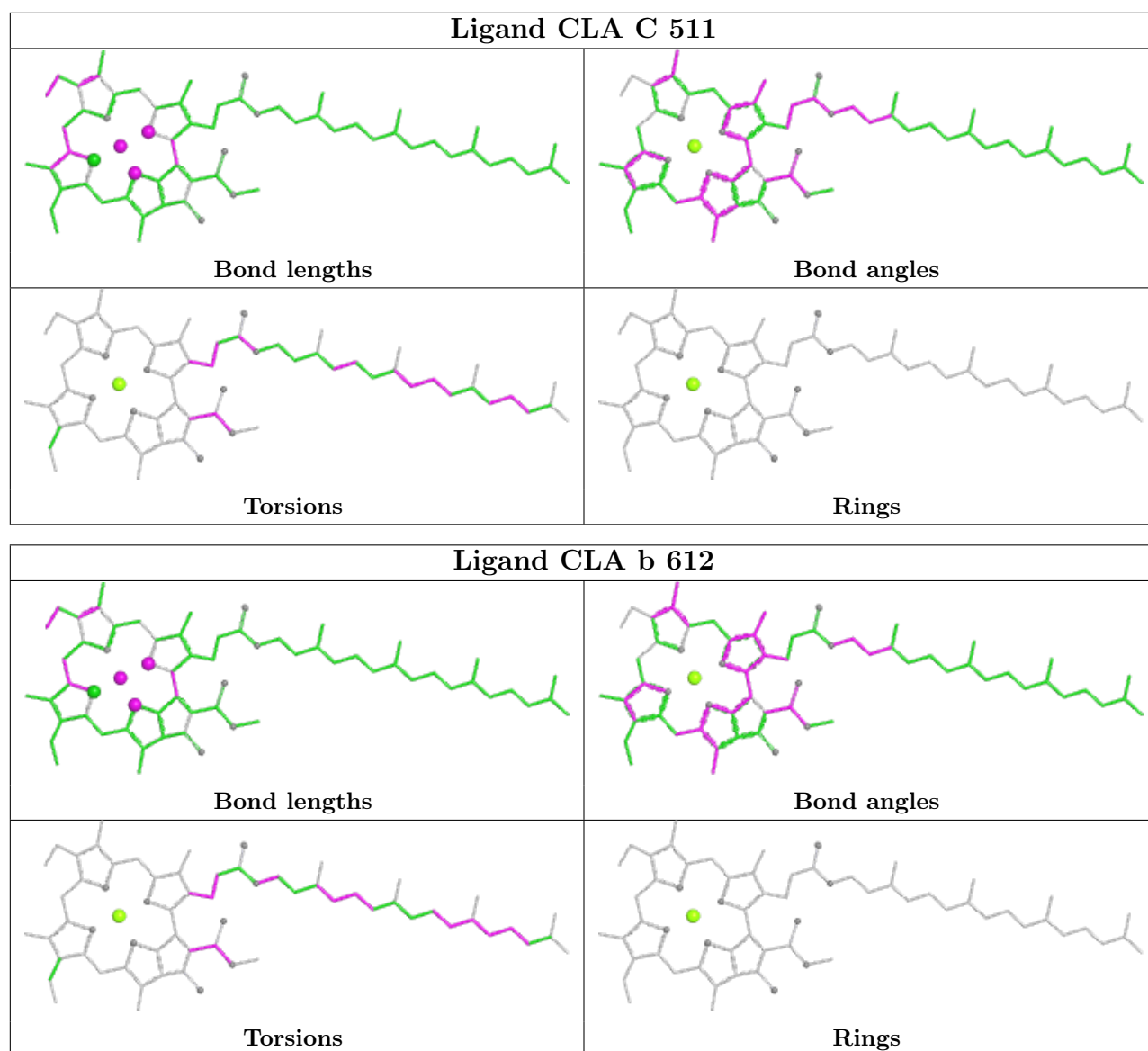
Ligand CLA g 612

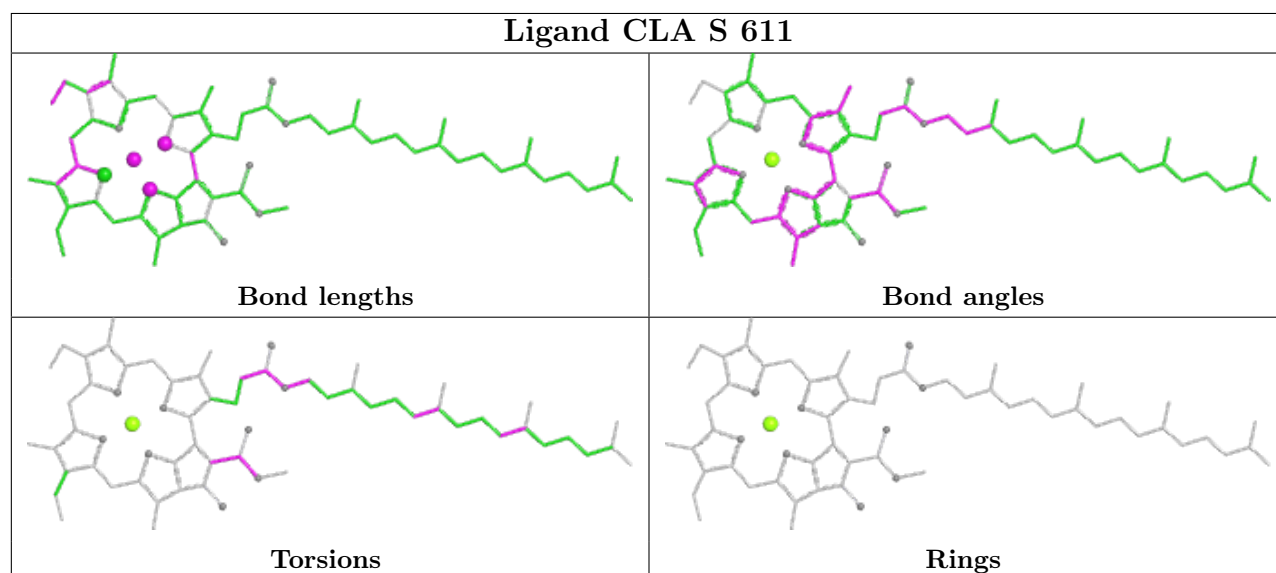
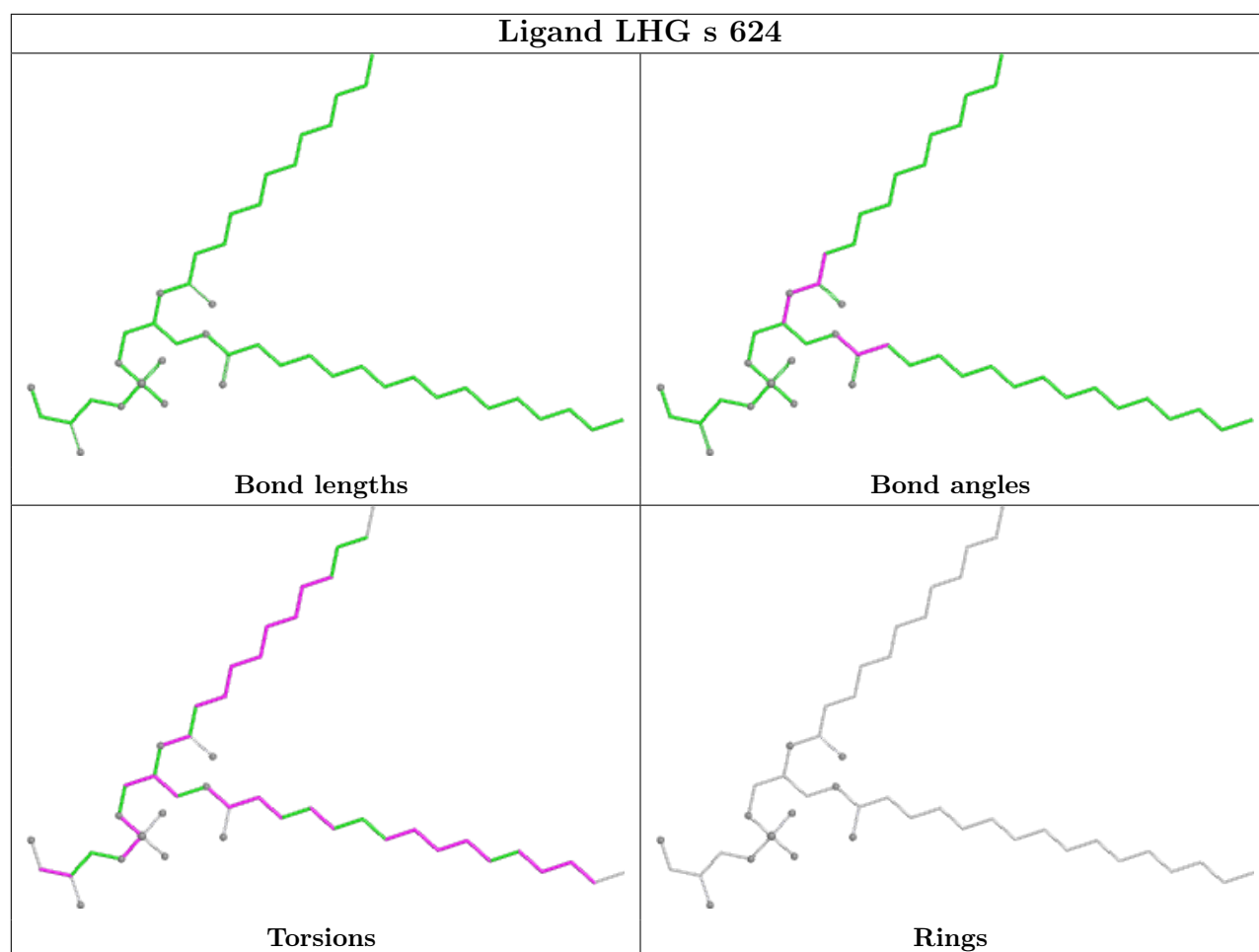


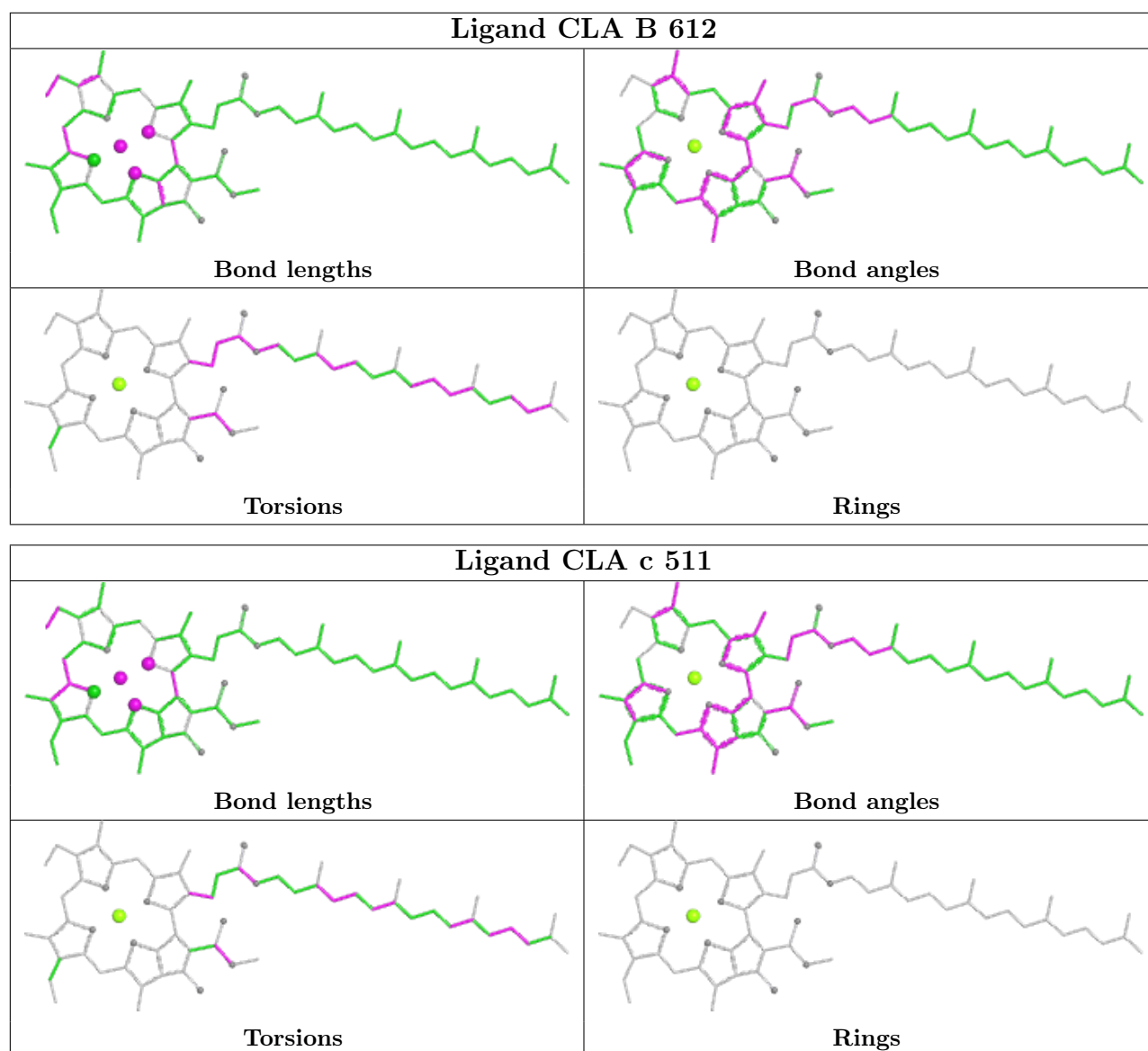
Ligand NEX S 622

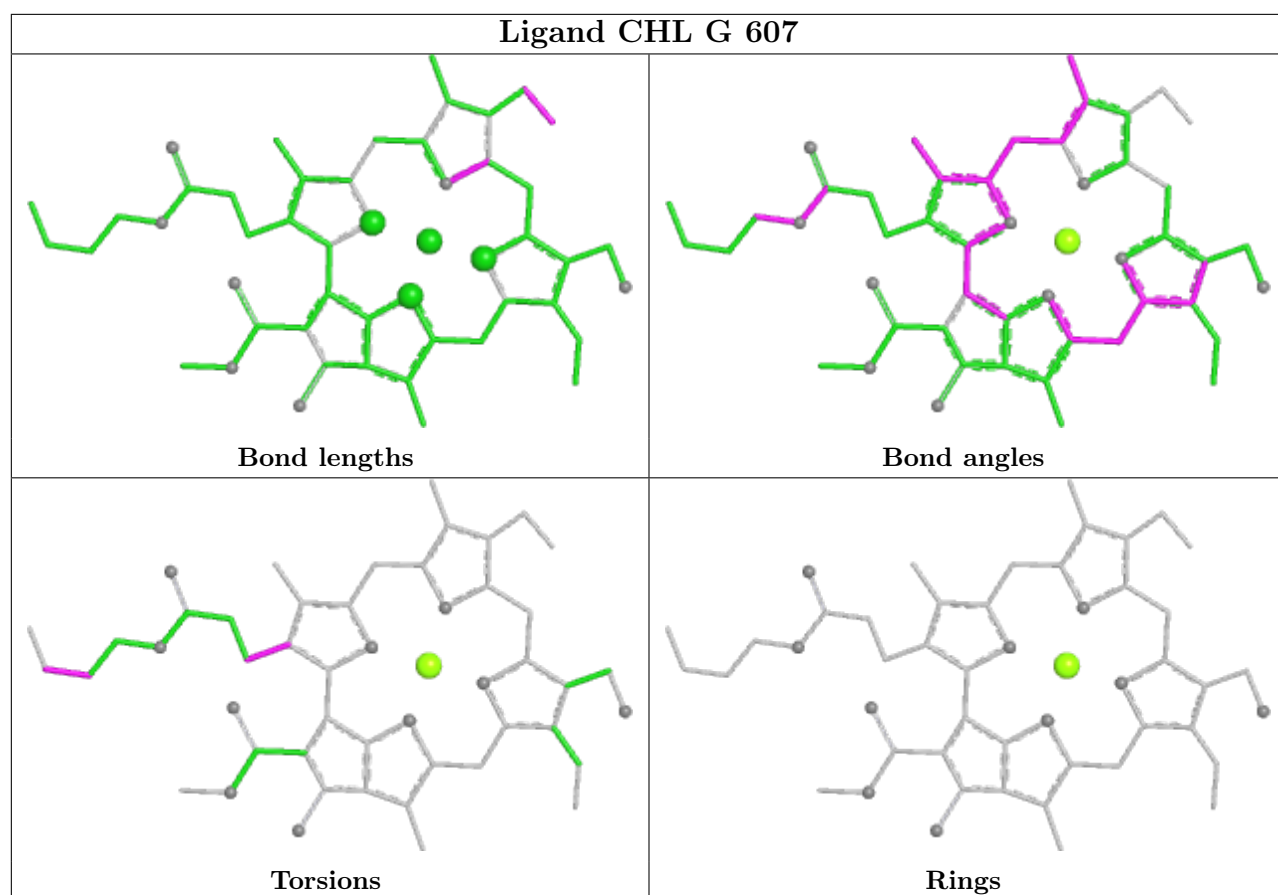


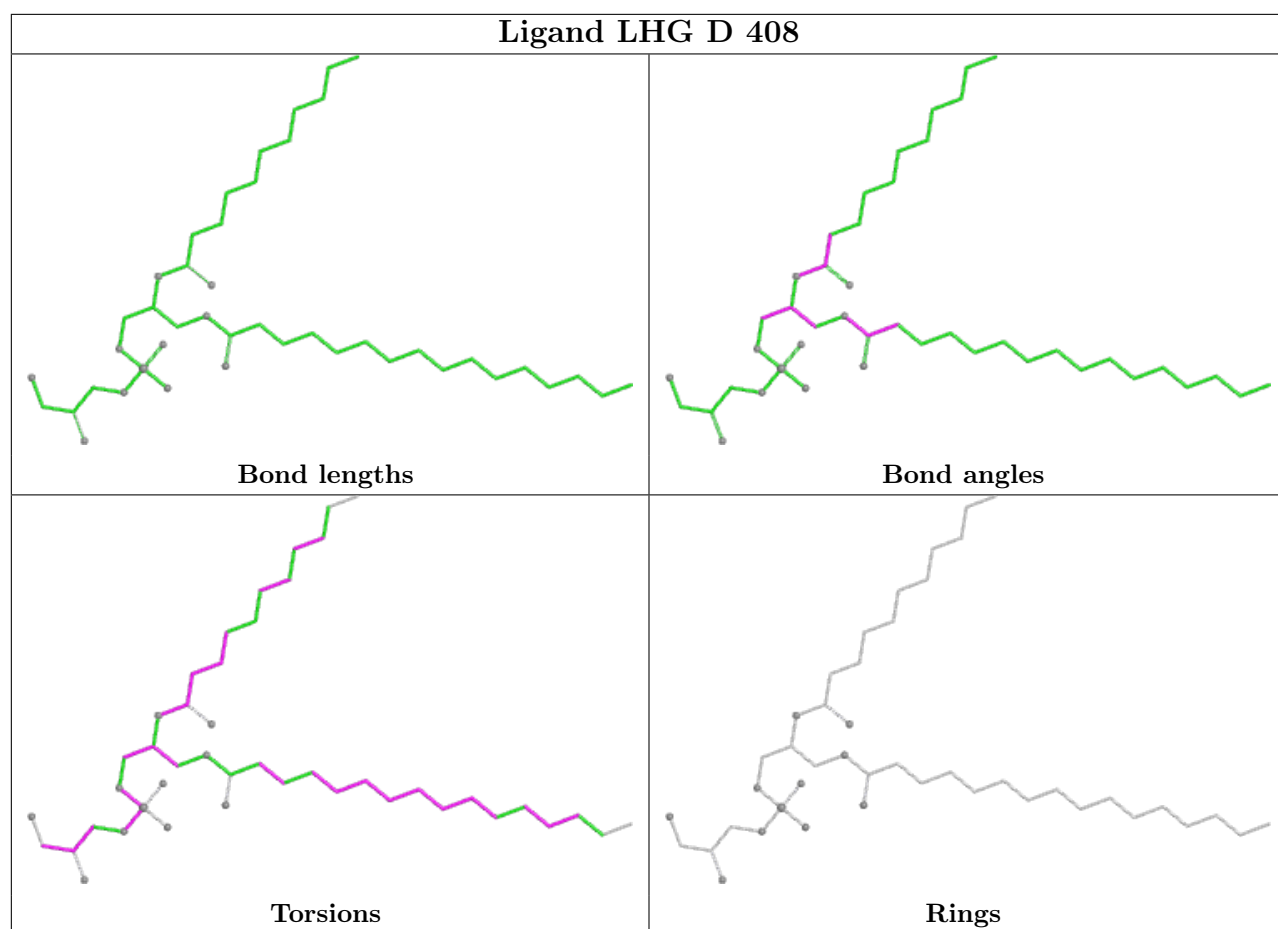


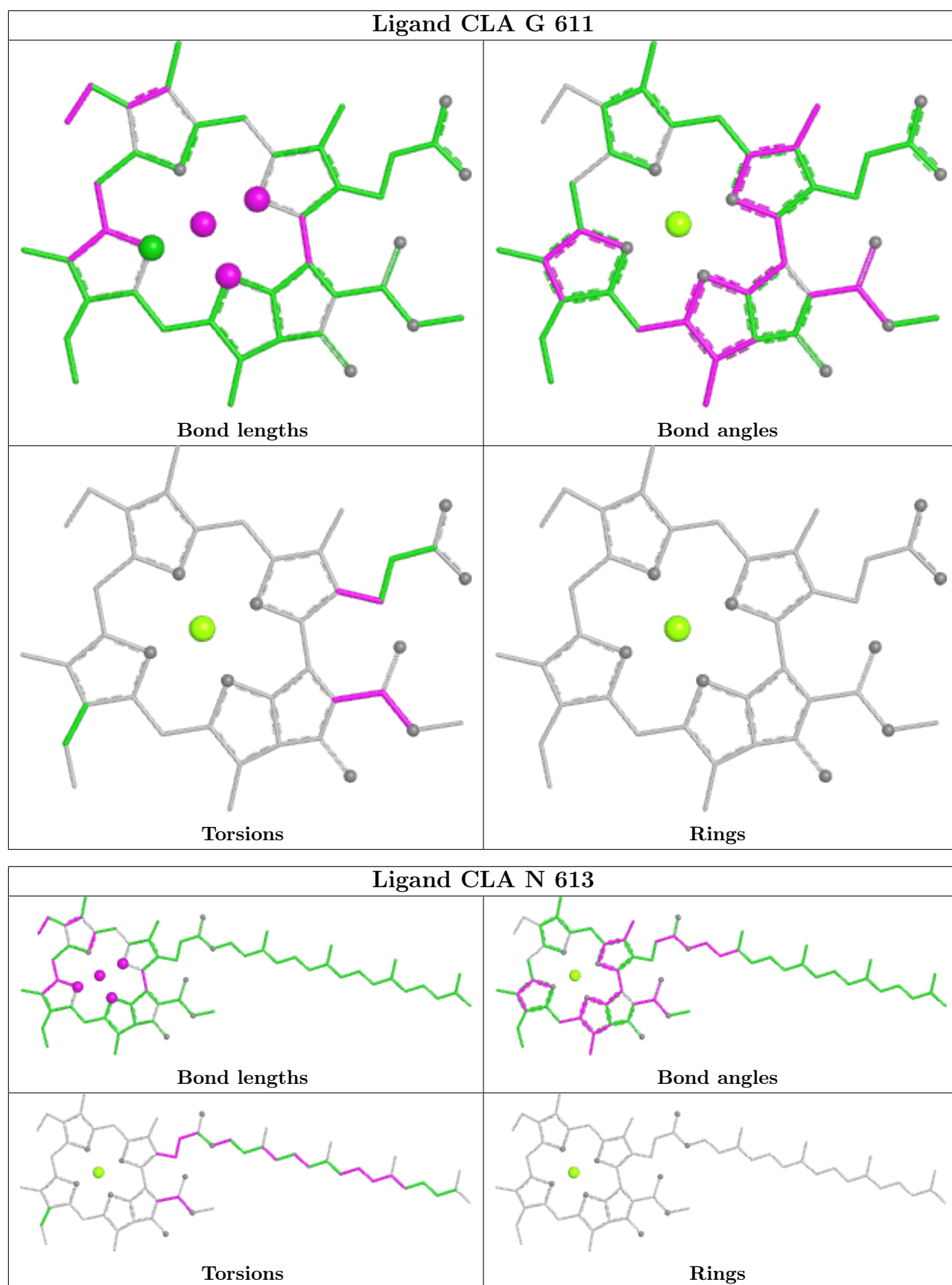


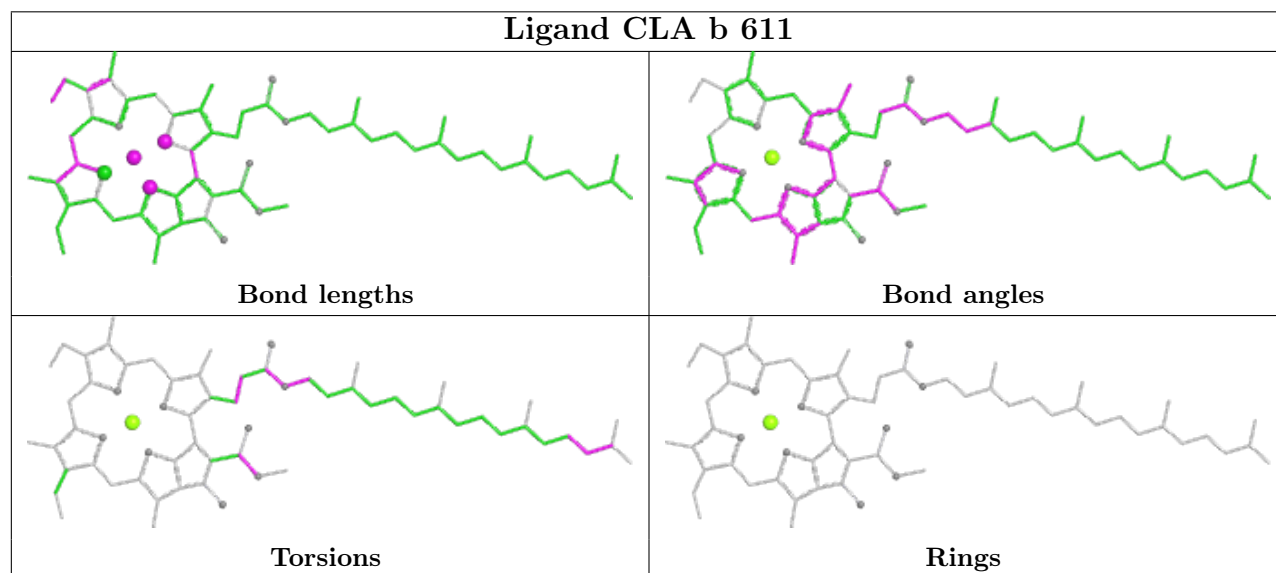
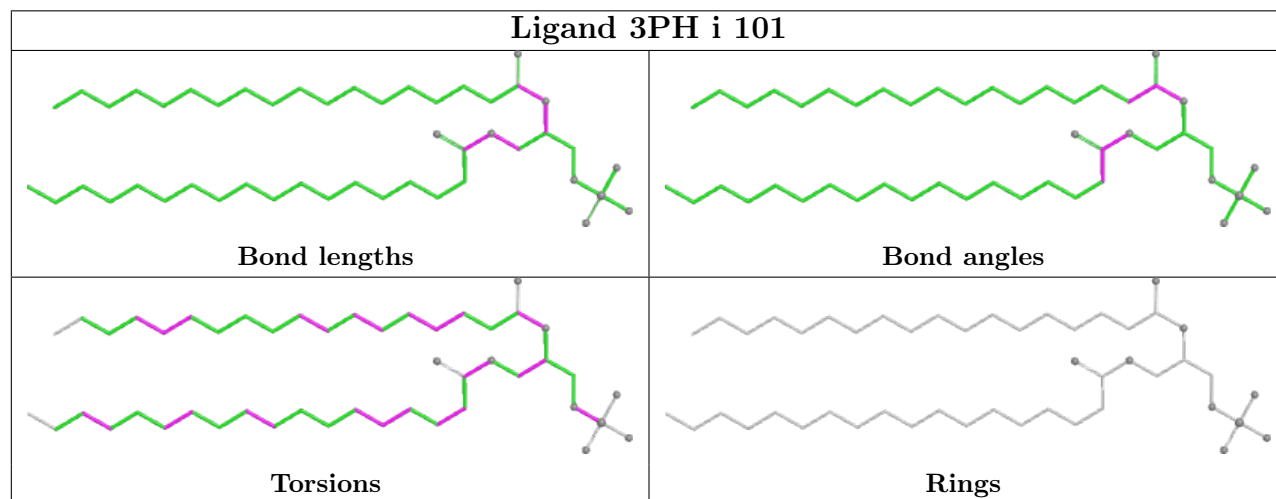
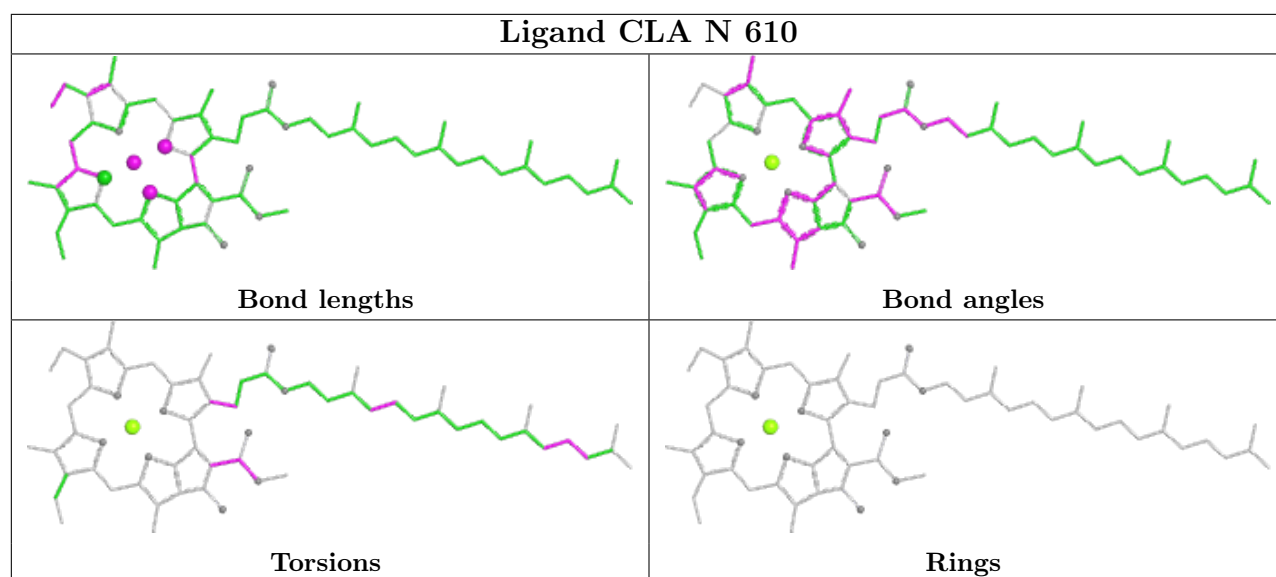


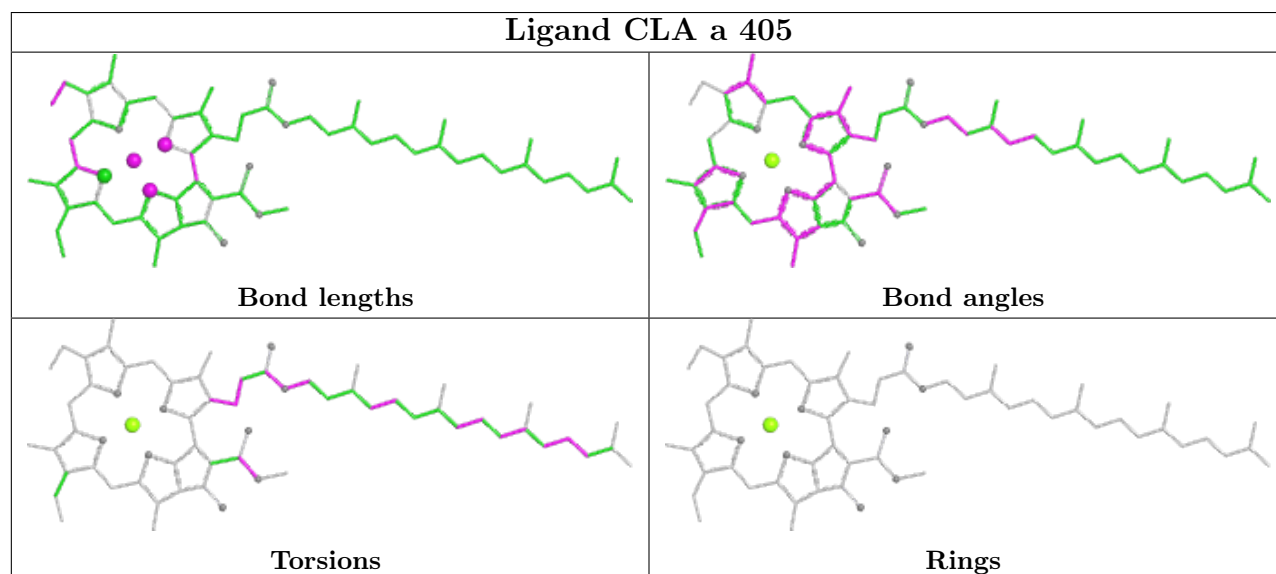
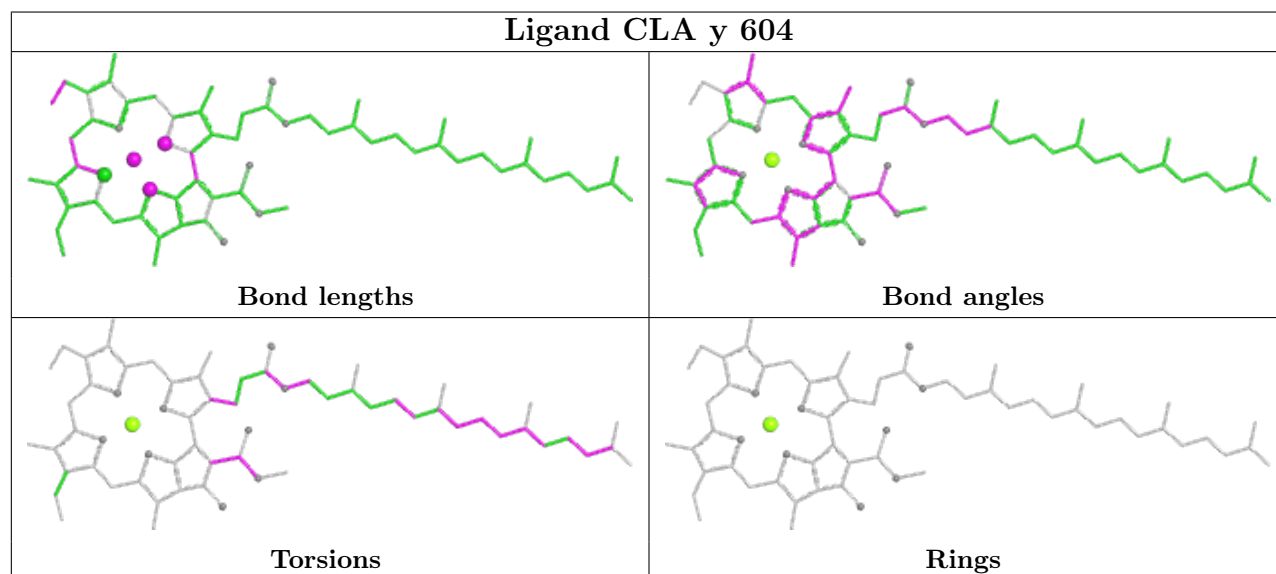
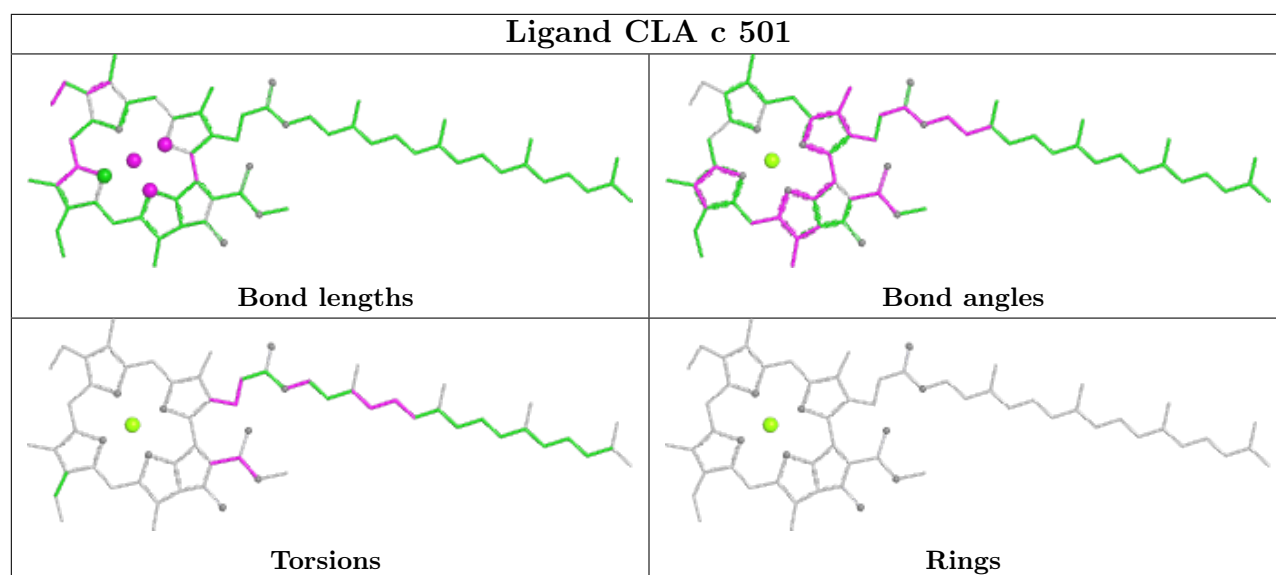


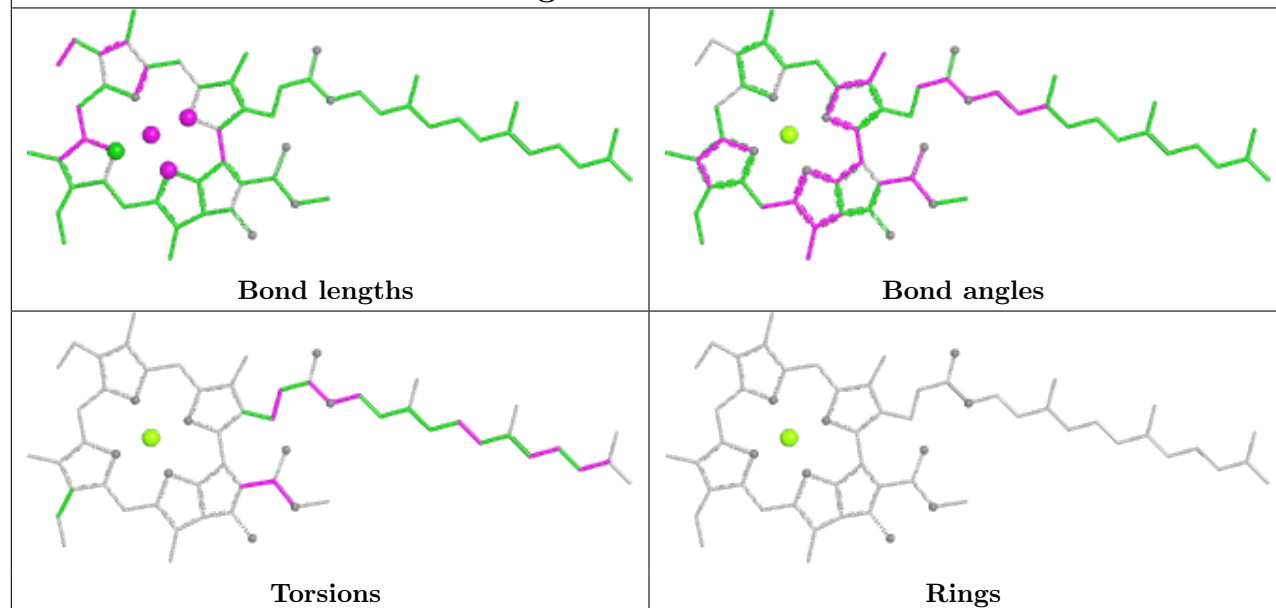
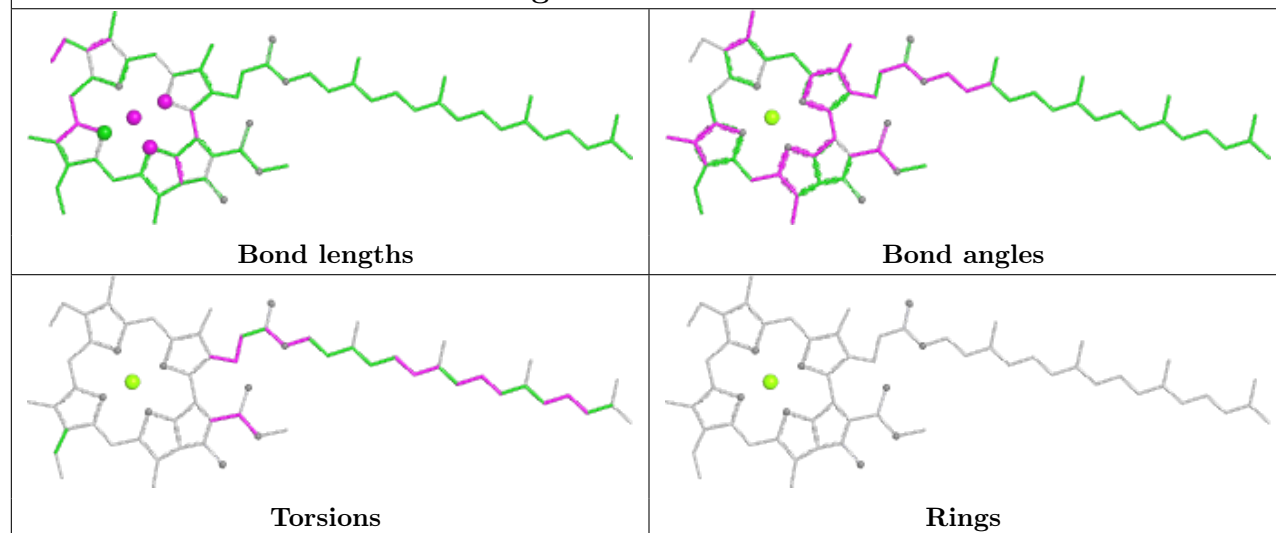


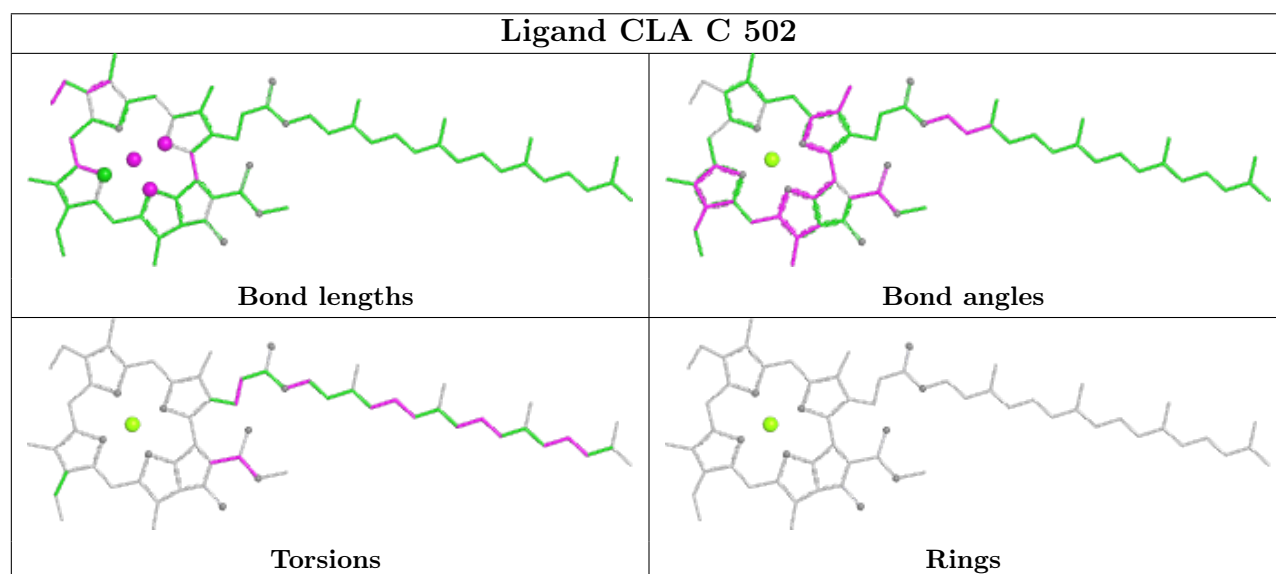
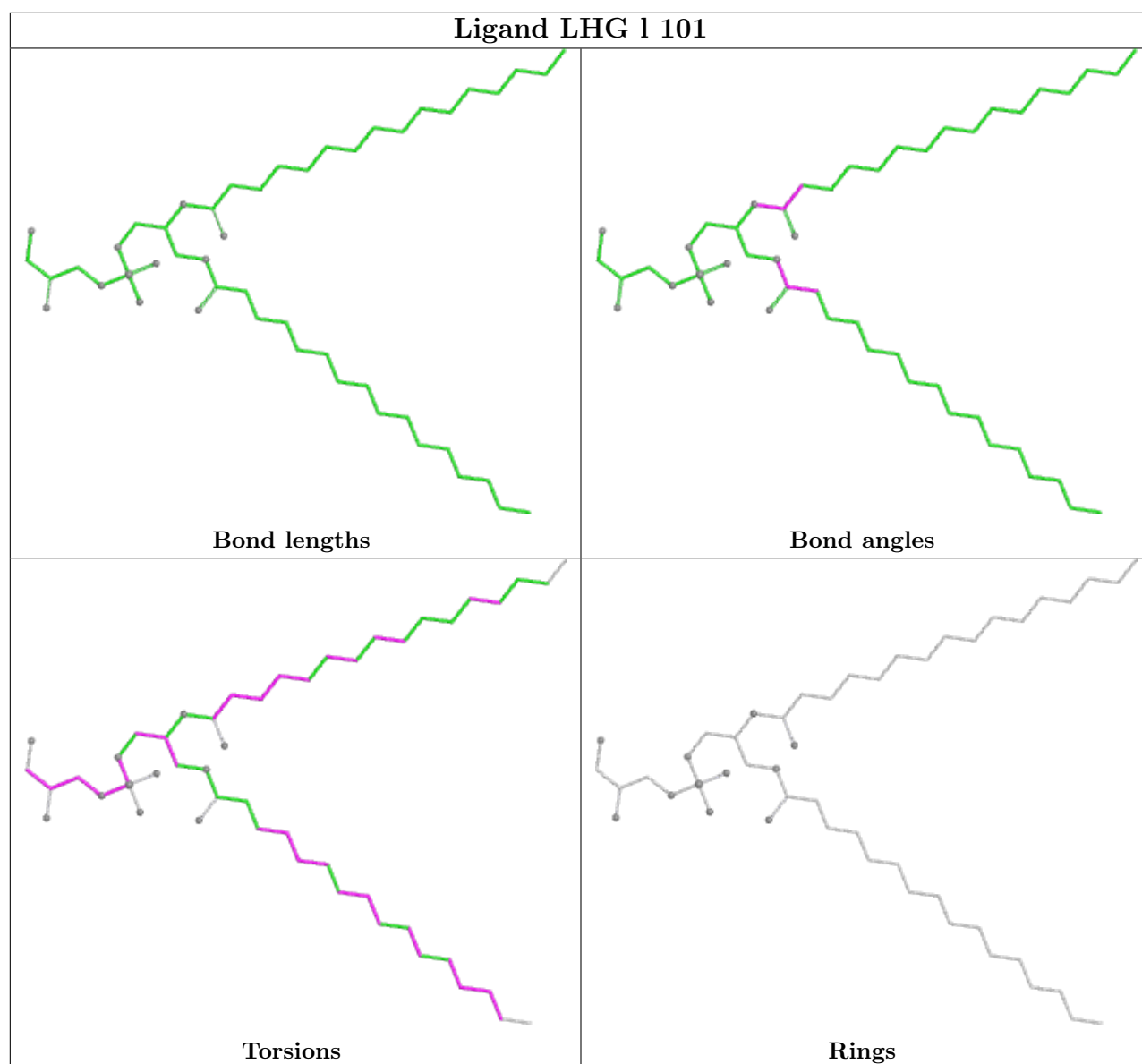


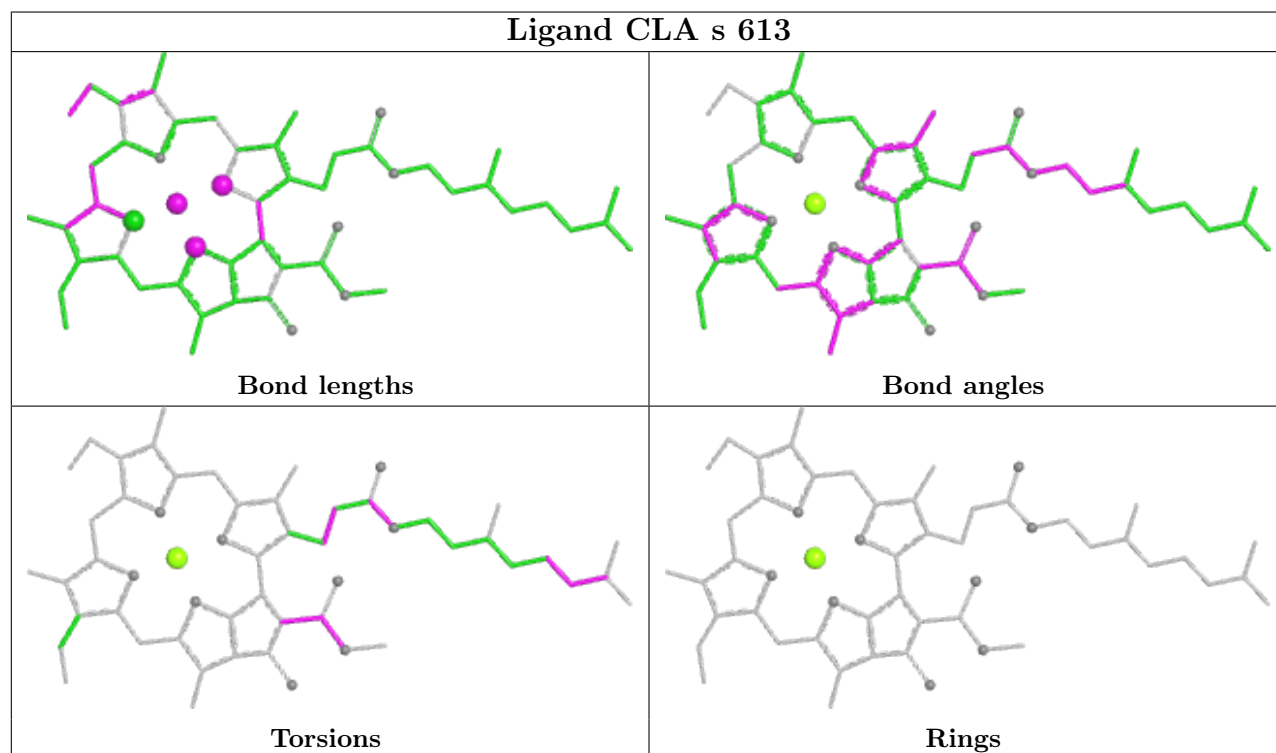
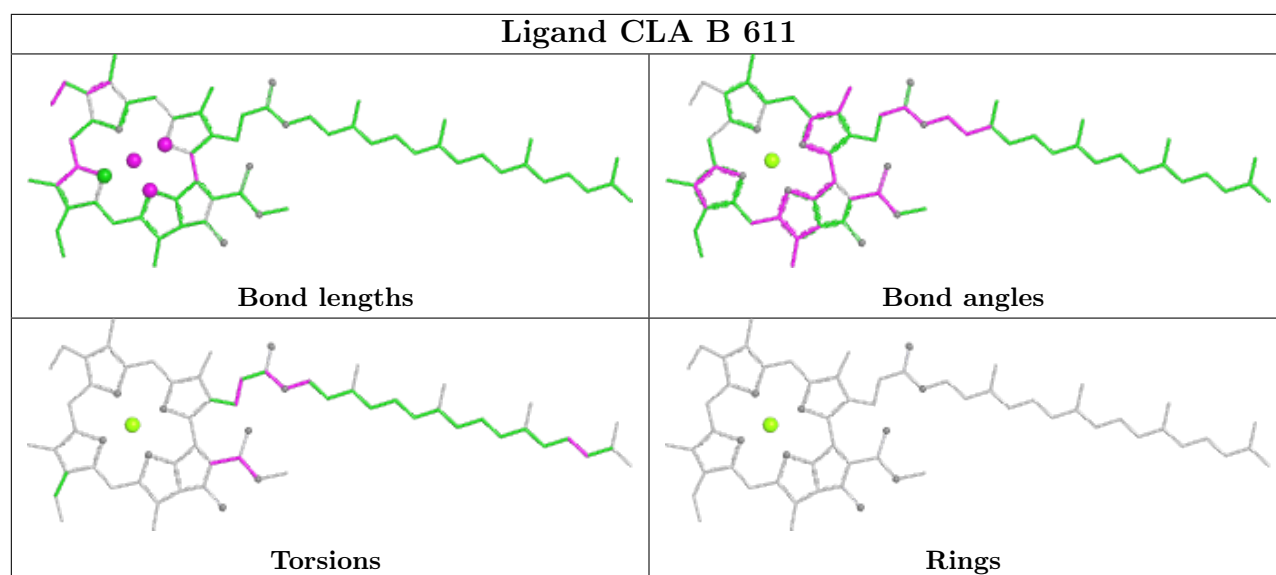


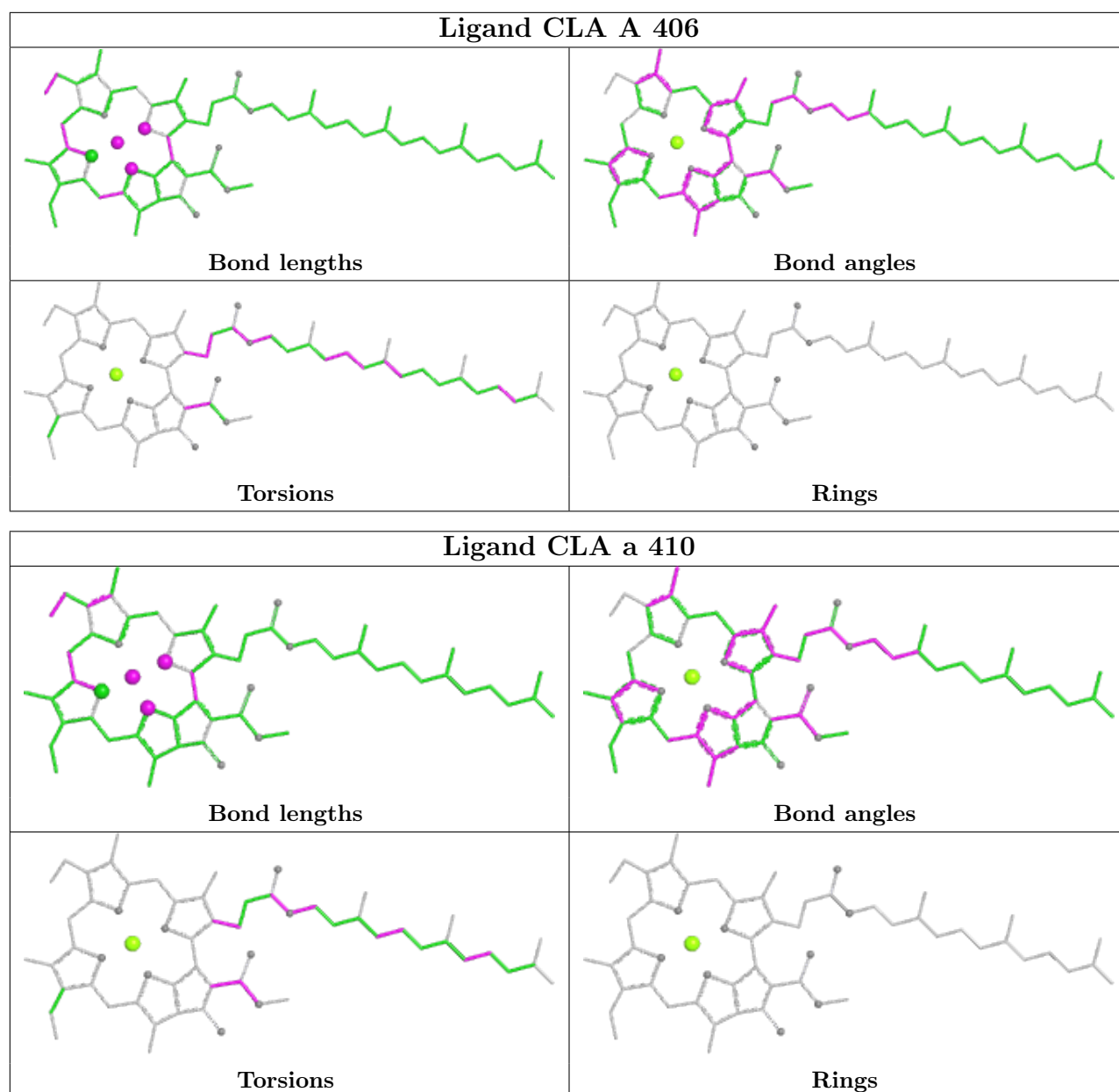


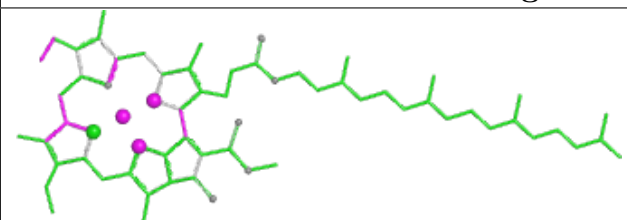
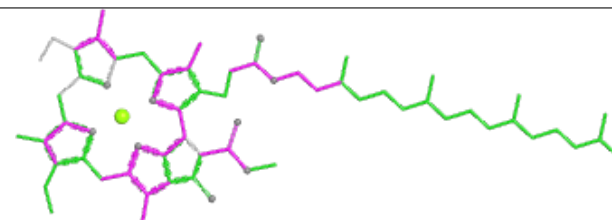
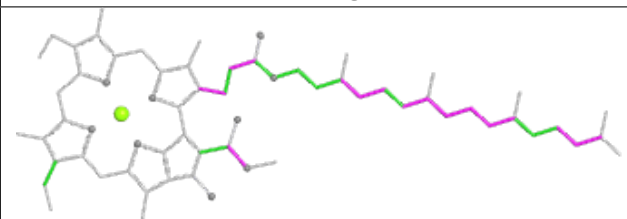
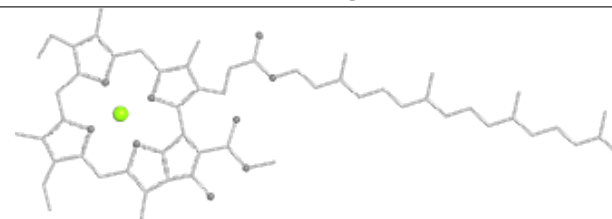


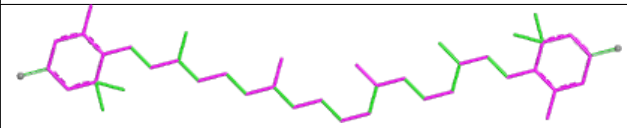
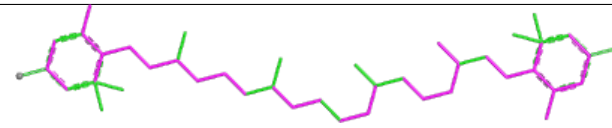
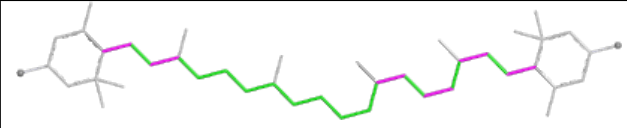
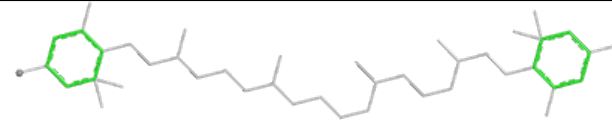
Ligand CLA r 612**Ligand CLA Y 602**

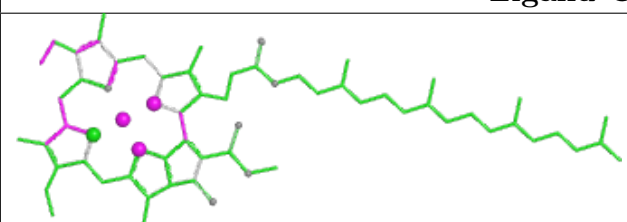
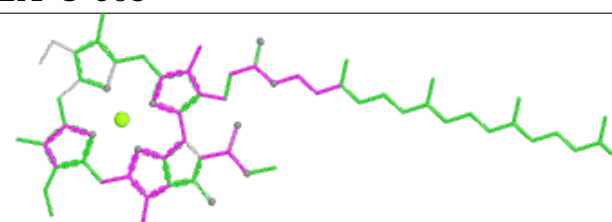
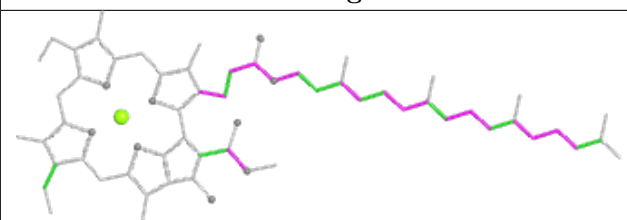
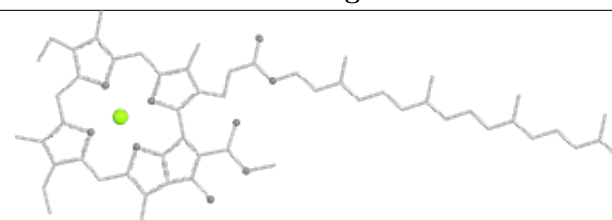


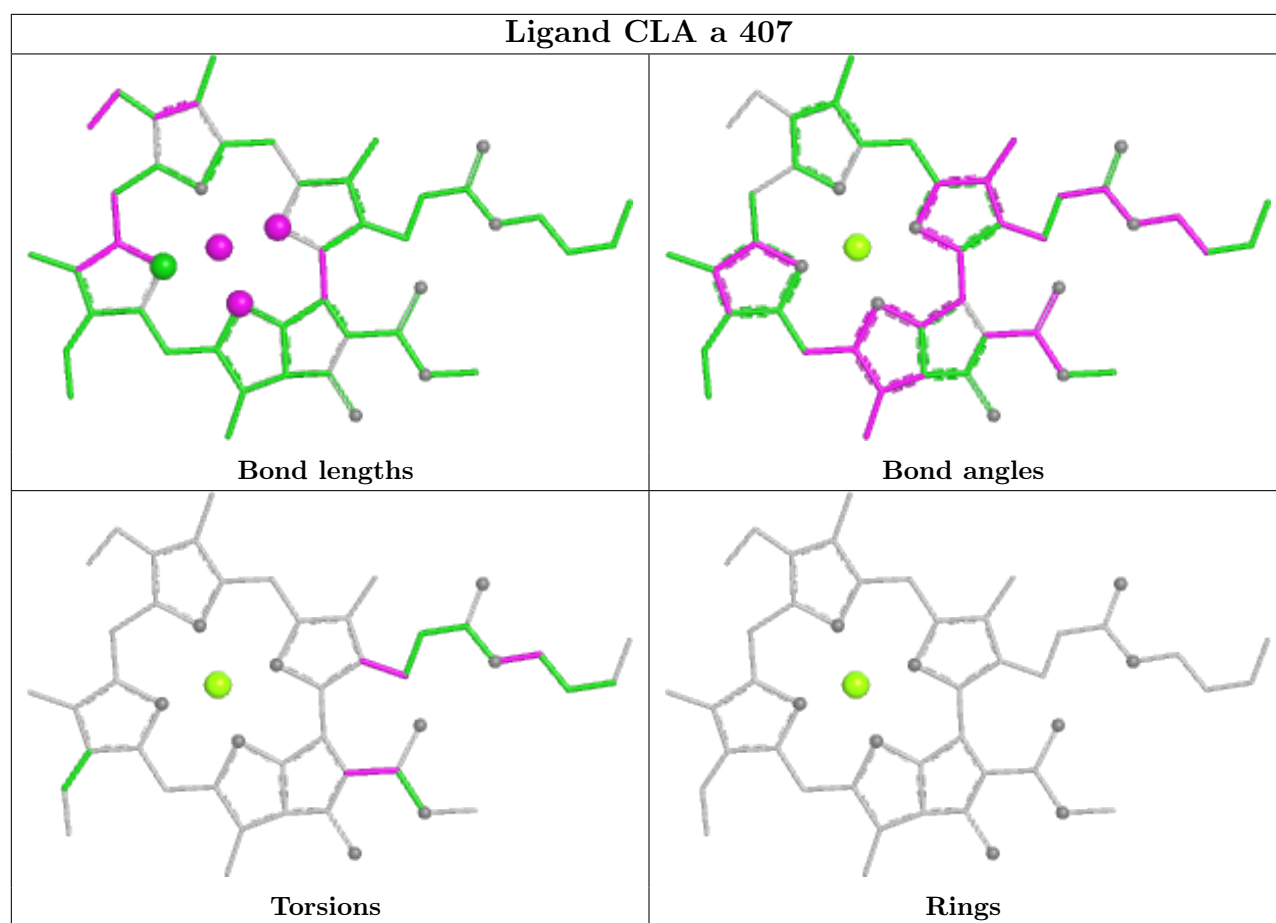




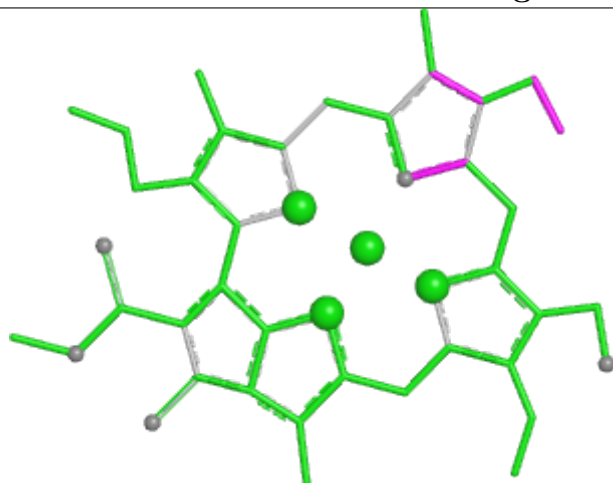
Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C7Z b 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

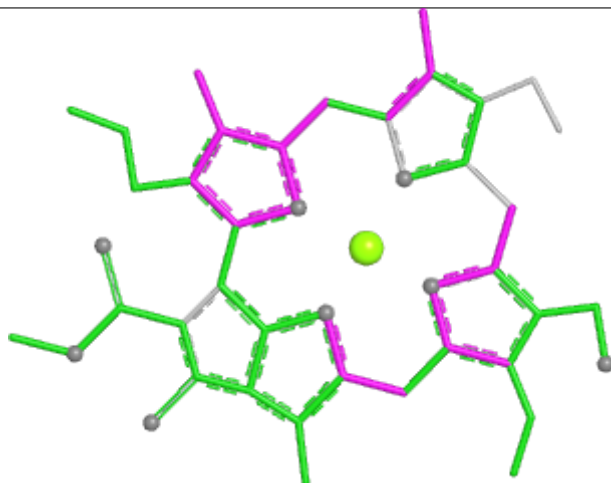
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings



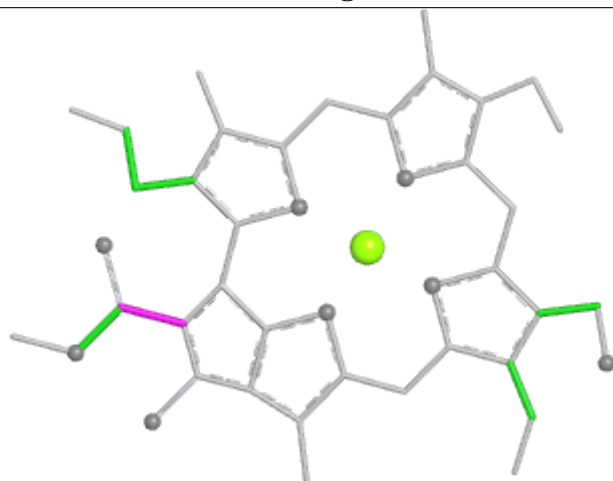
Ligand CHL R 606



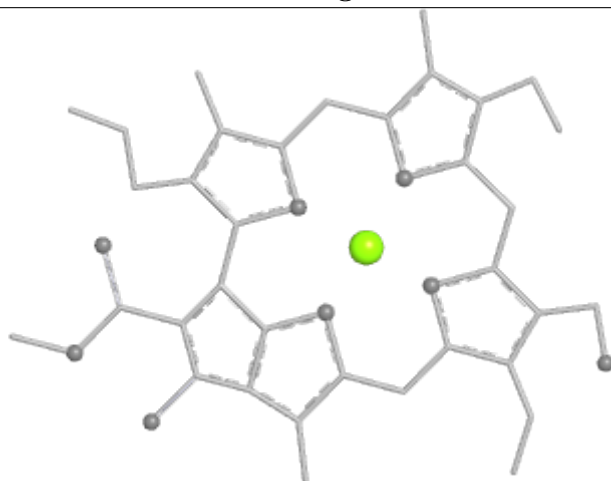
Bond lengths



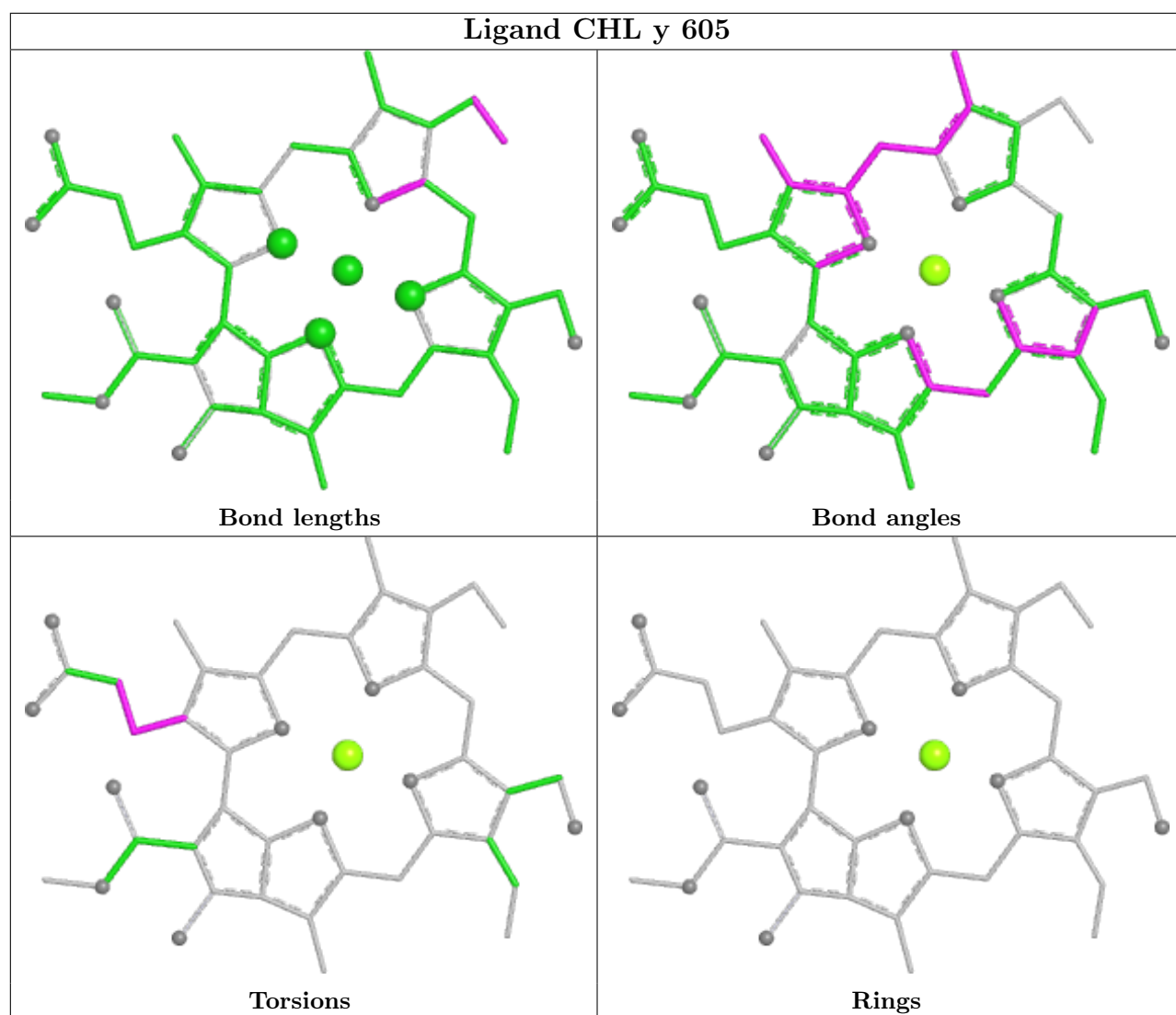
Bond angles



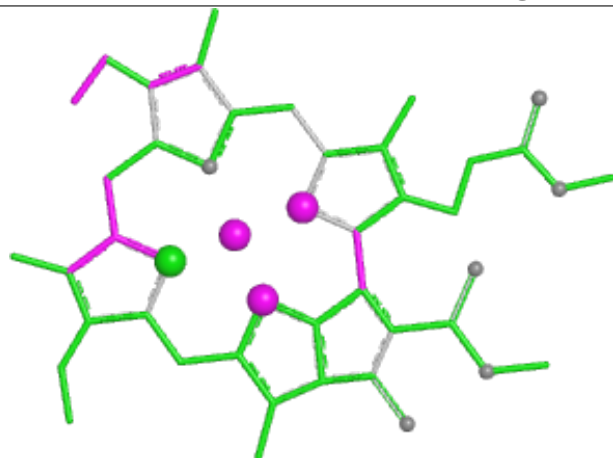
Torsions



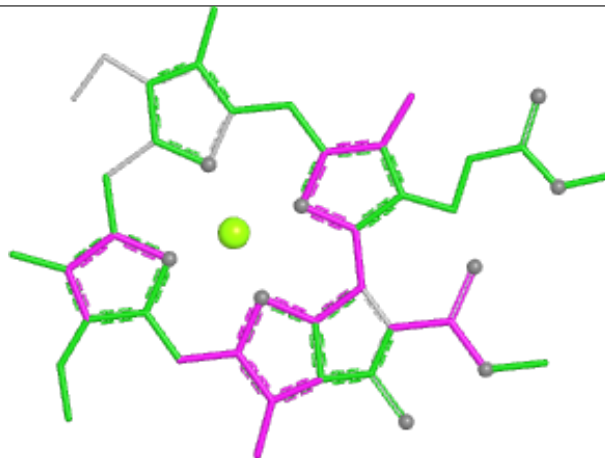
Rings



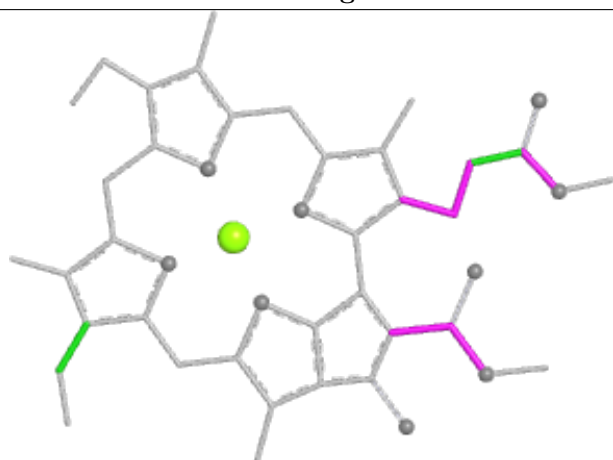
Ligand CLA R 613



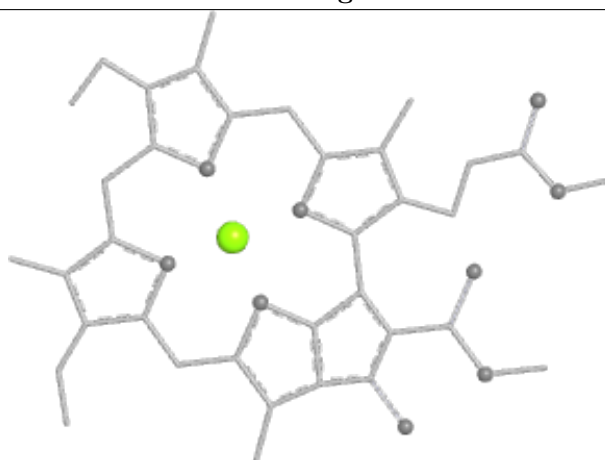
Bond lengths



Bond angles

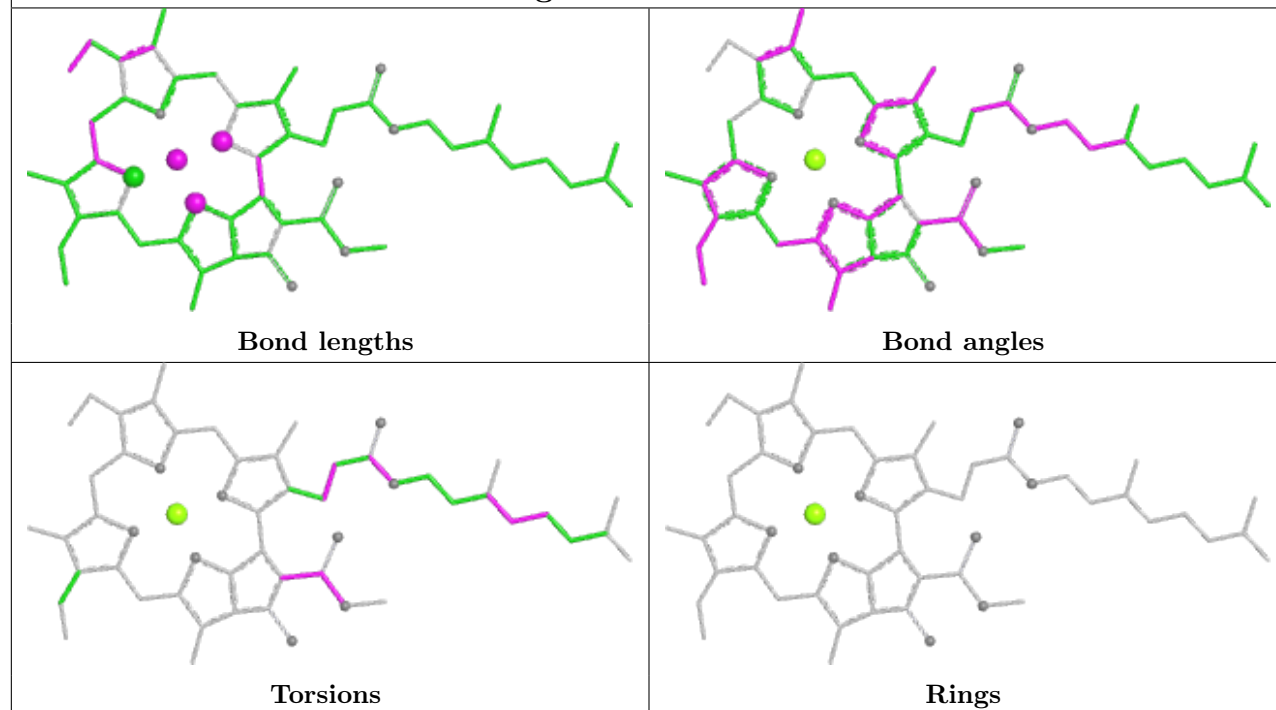


Torsions

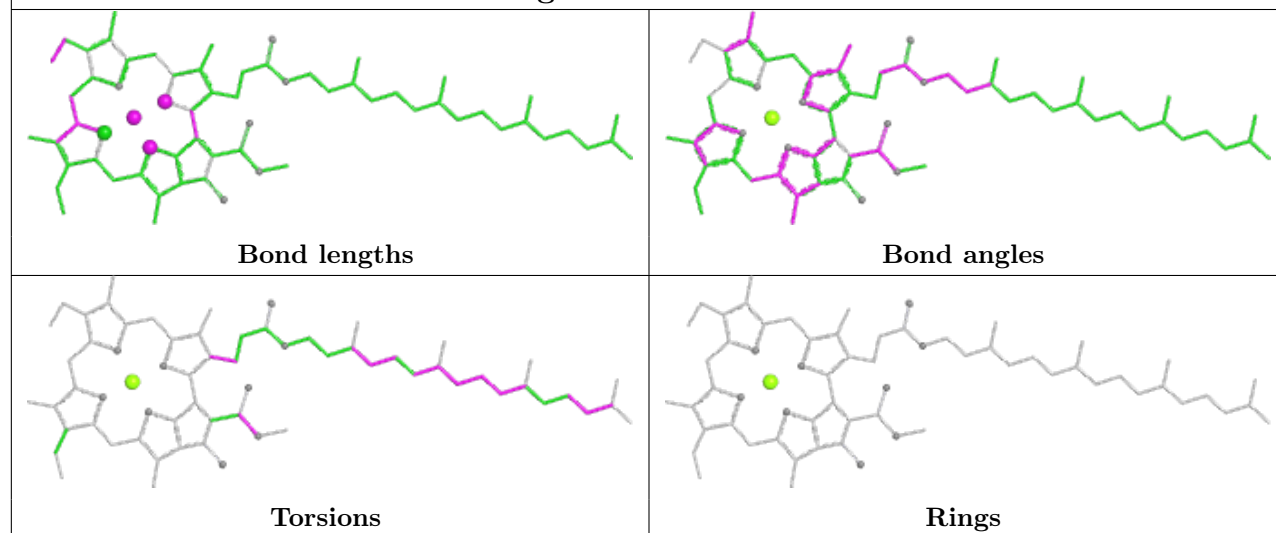


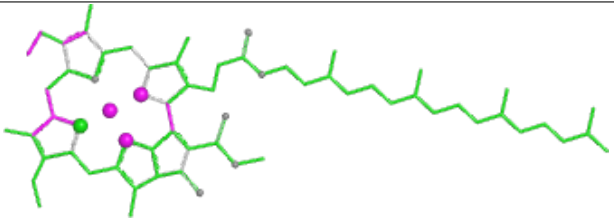
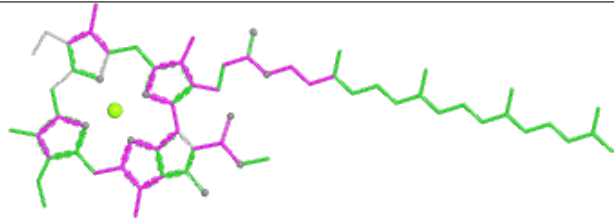
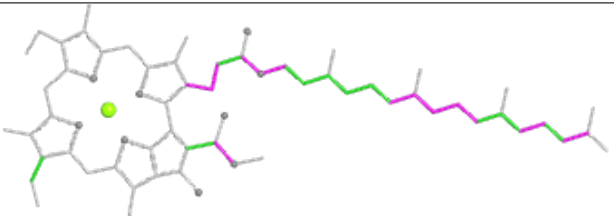
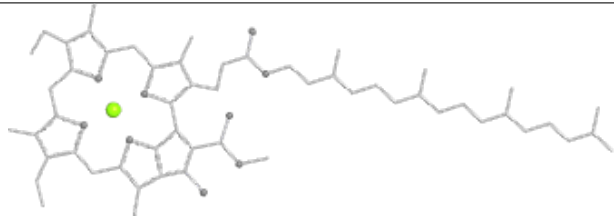
Rings

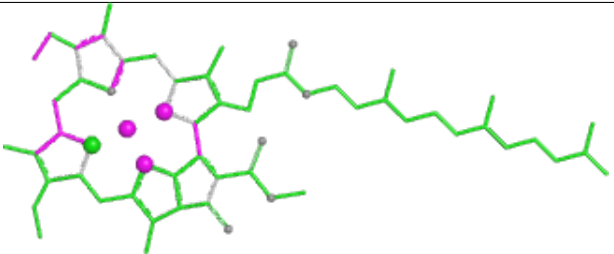
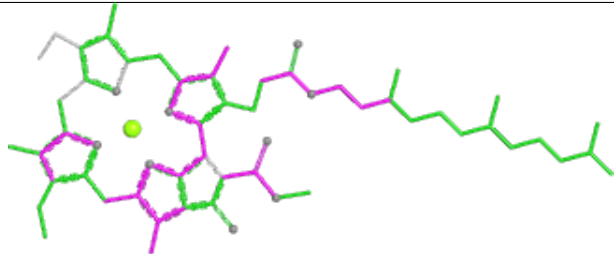
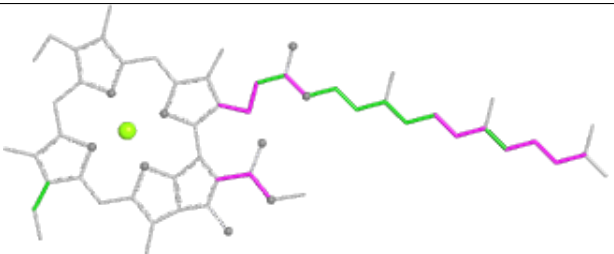
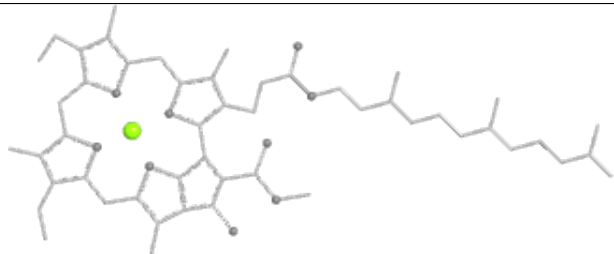
Ligand CLA S 604

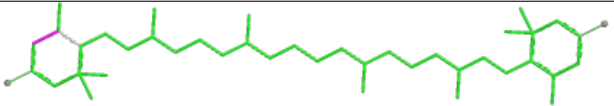
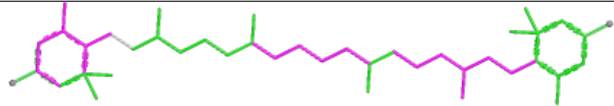
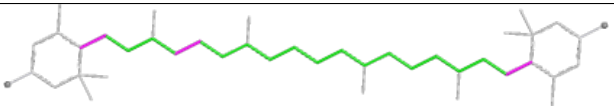
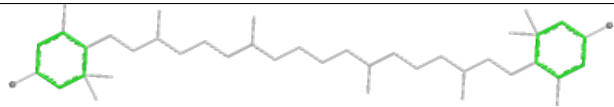


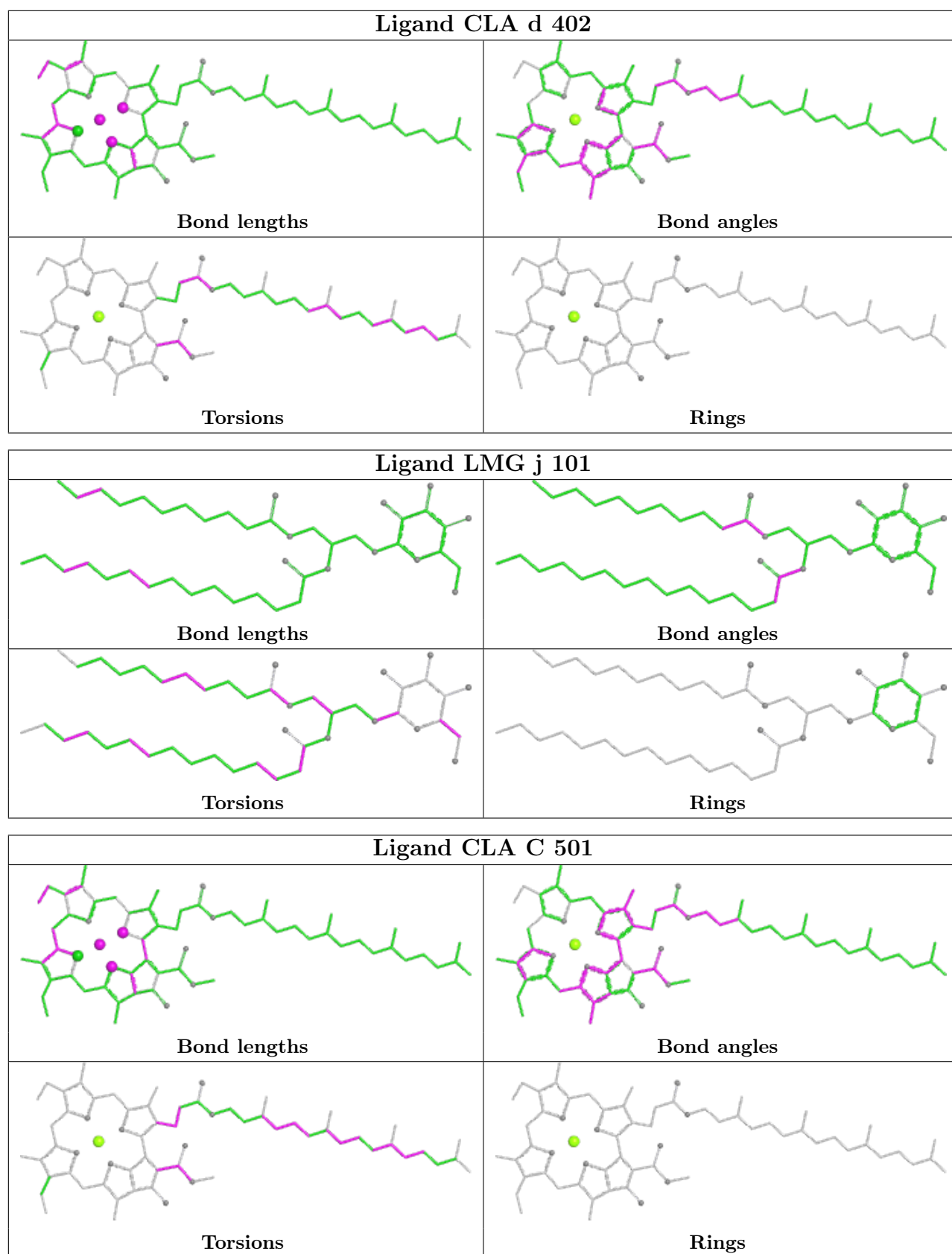
Ligand CLA c 513



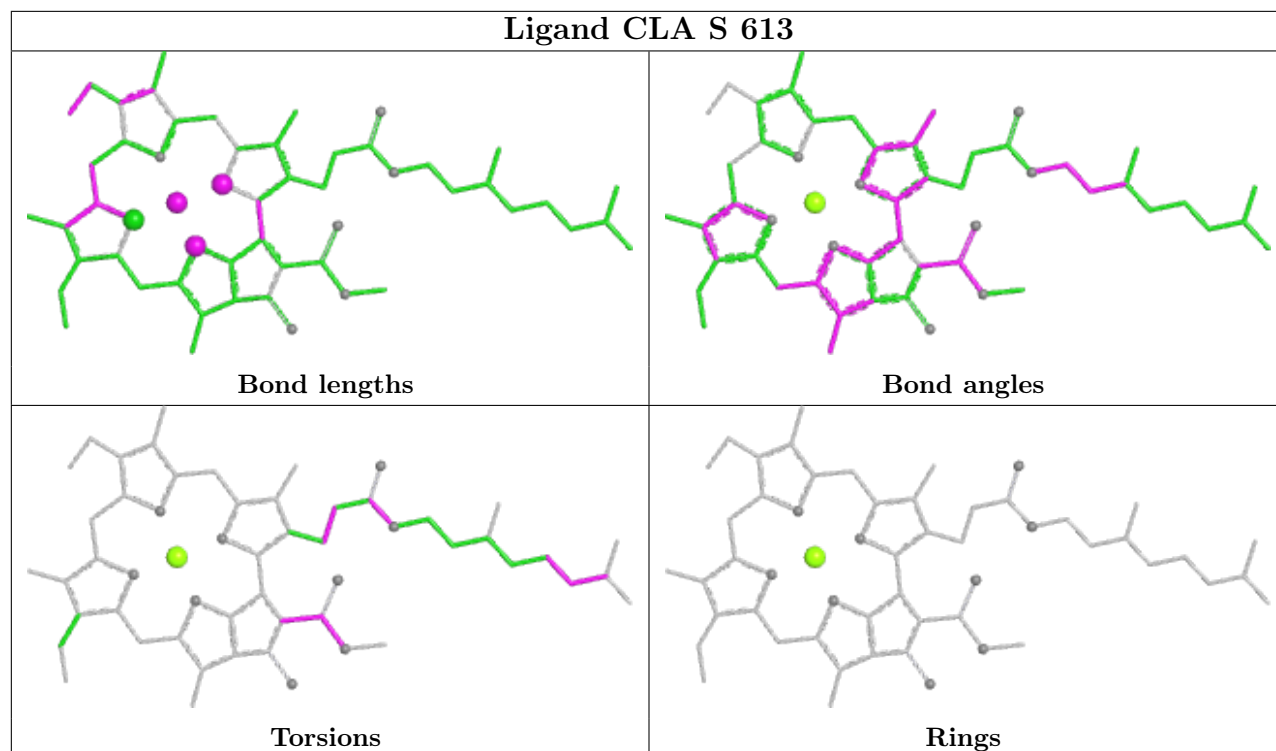
Ligand CLA y 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

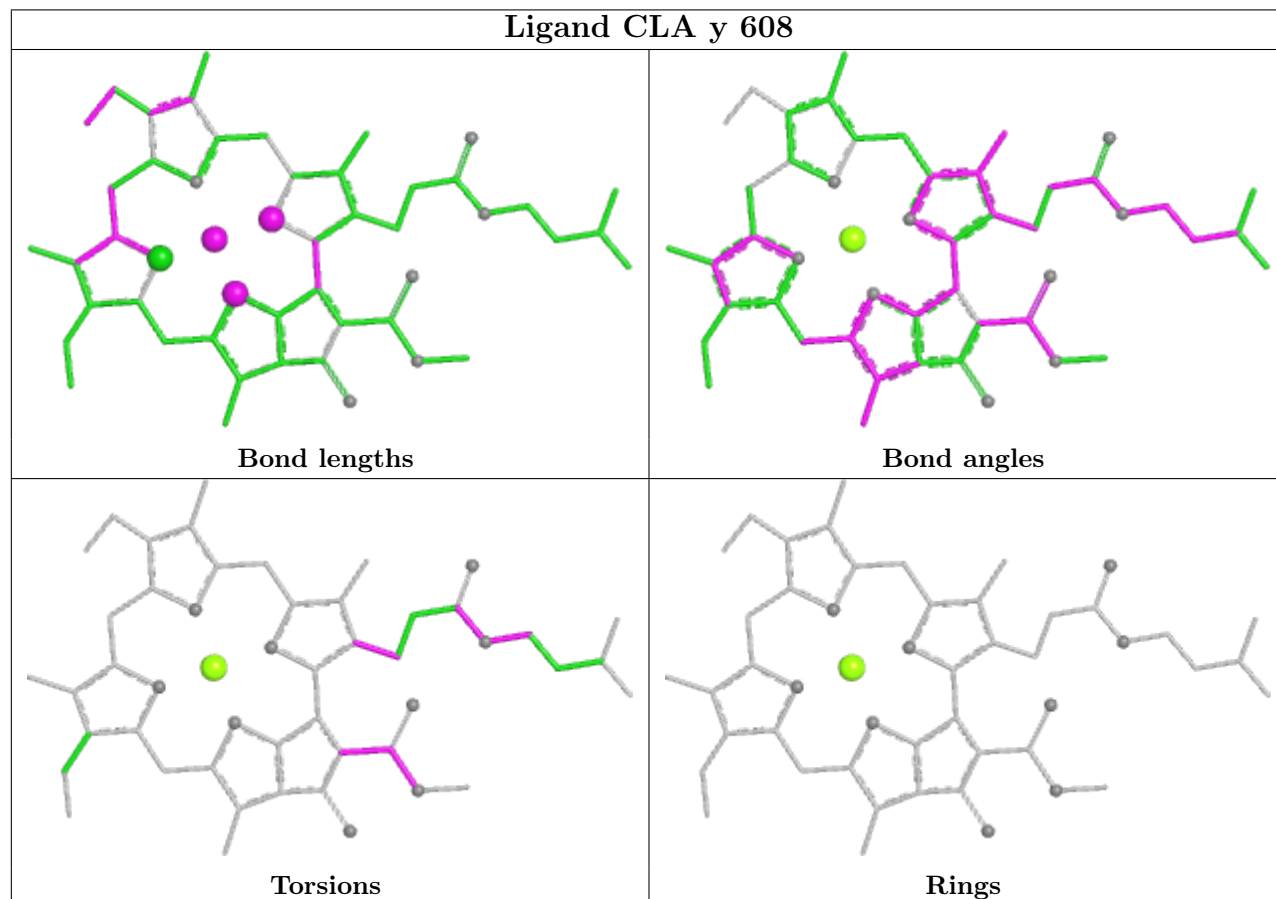
Ligand LUT n 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

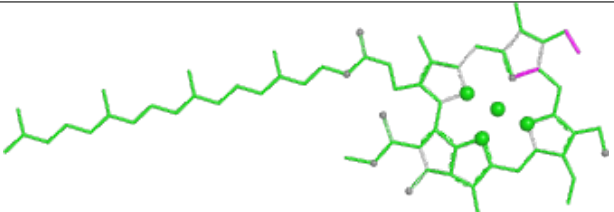
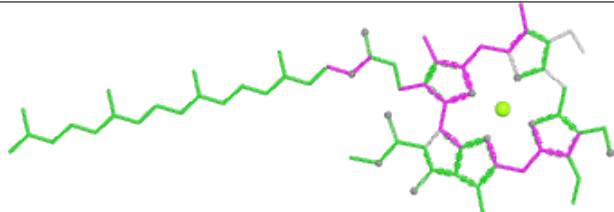
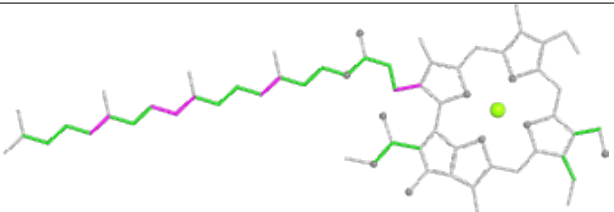
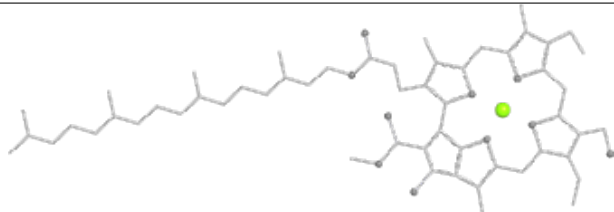


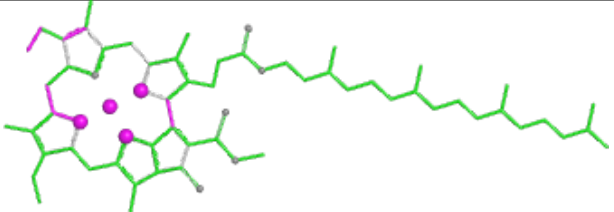
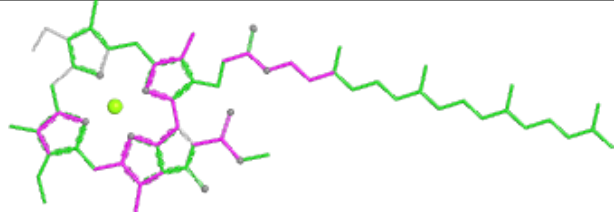
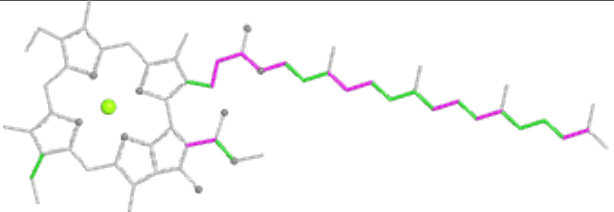
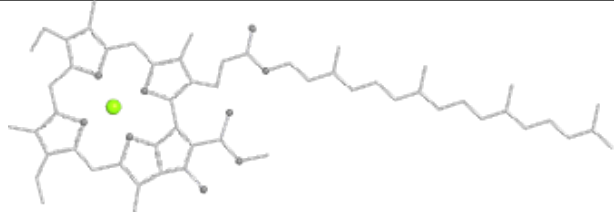
Ligand CLA S 613

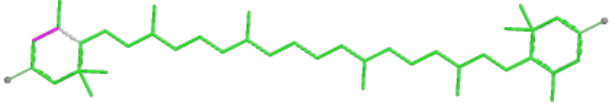
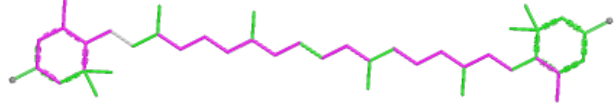
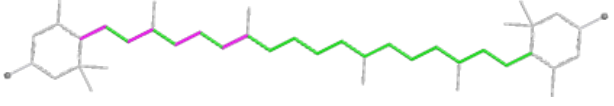
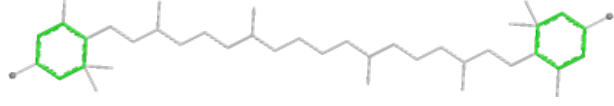


Ligand CLA y 608

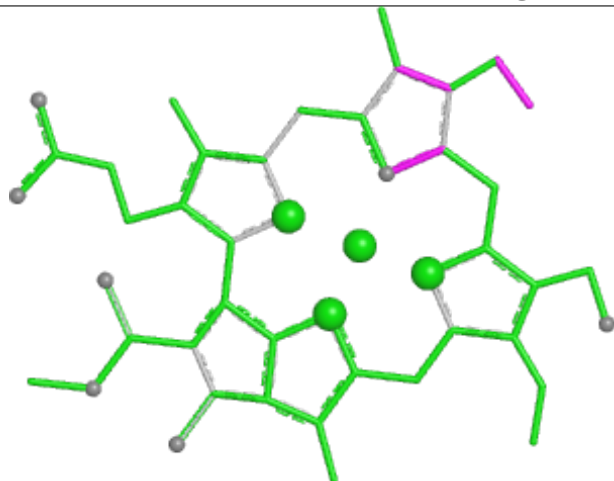


Ligand CHL n 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

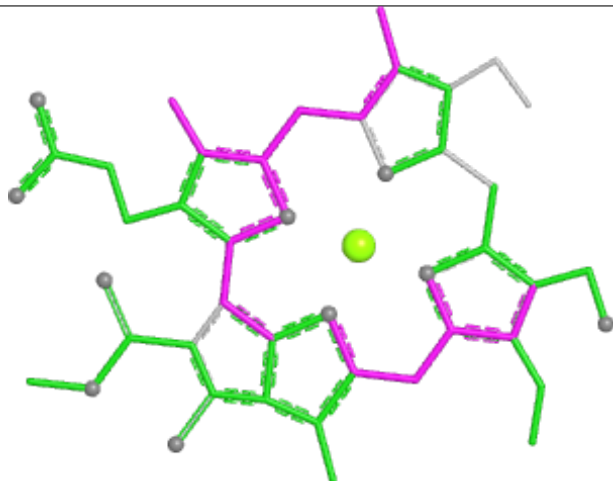
Ligand CLA B 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT G 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

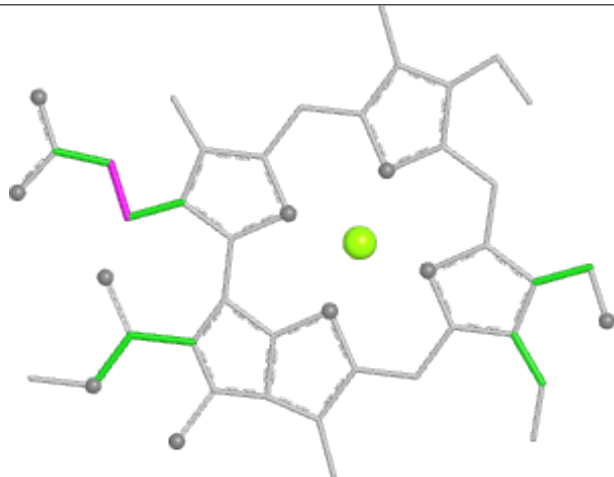
Ligand CHL Y 605



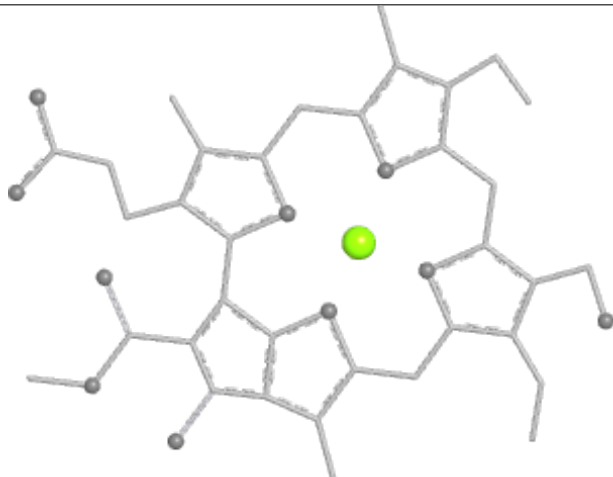
Bond lengths



Bond angles

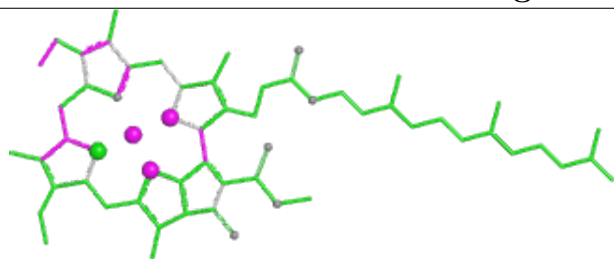


Torsions

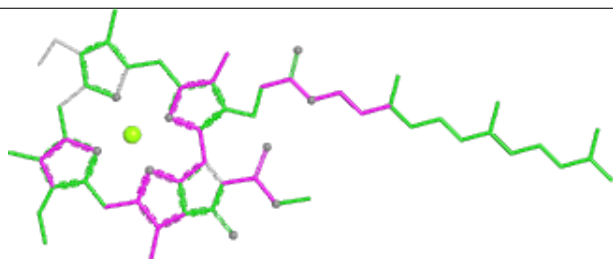


Rings

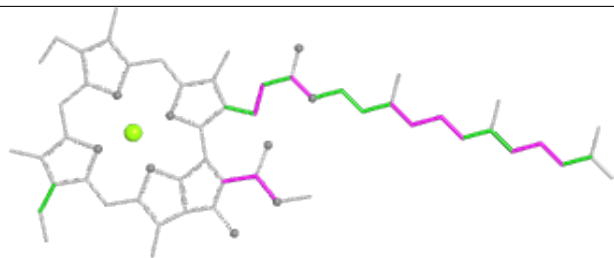
Ligand CLA R 602



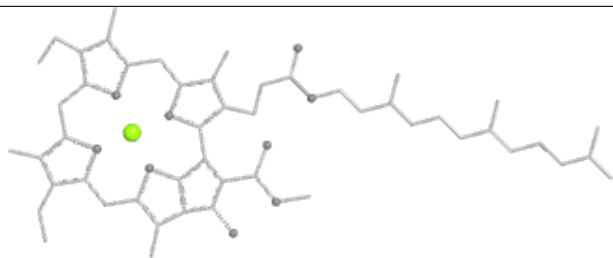
Bond lengths



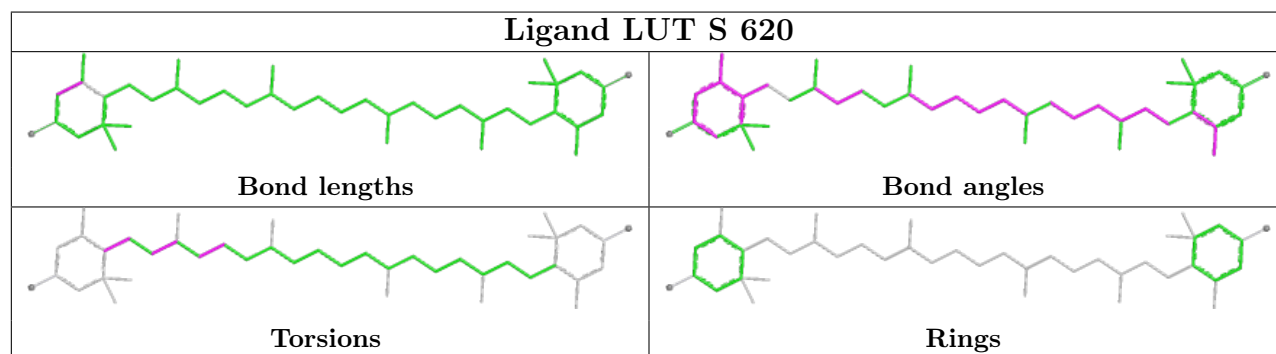
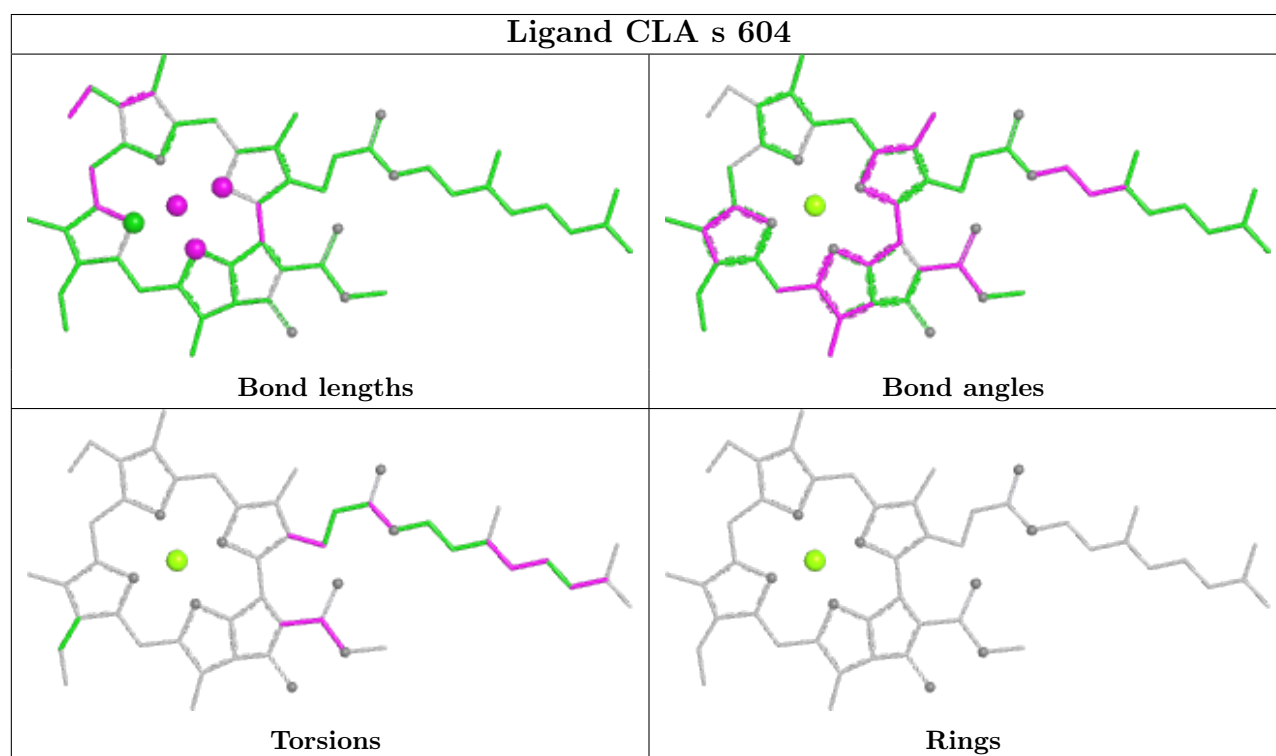
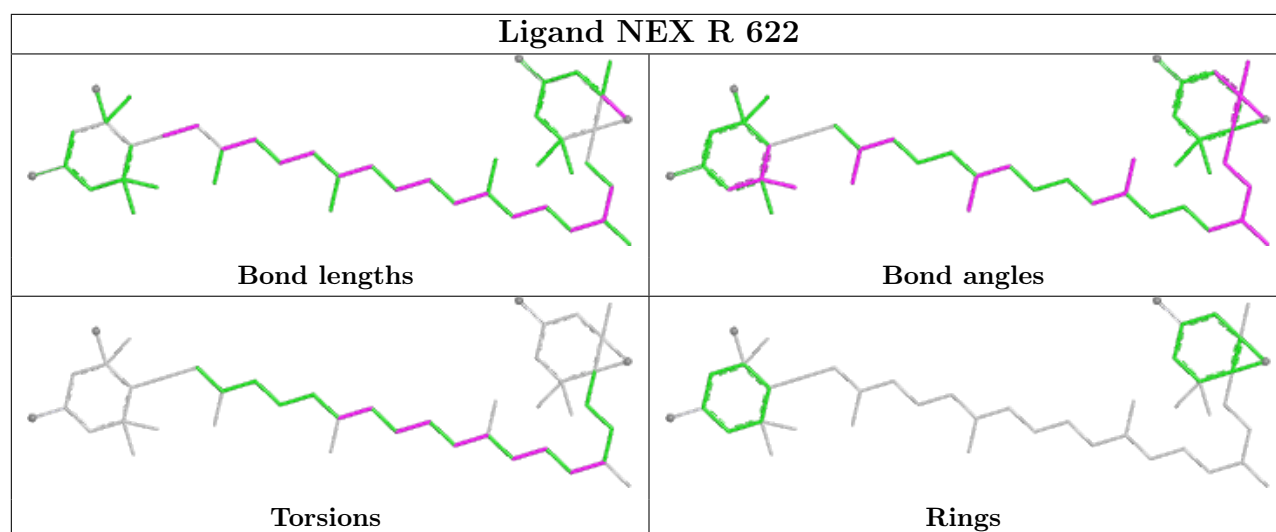
Bond angles

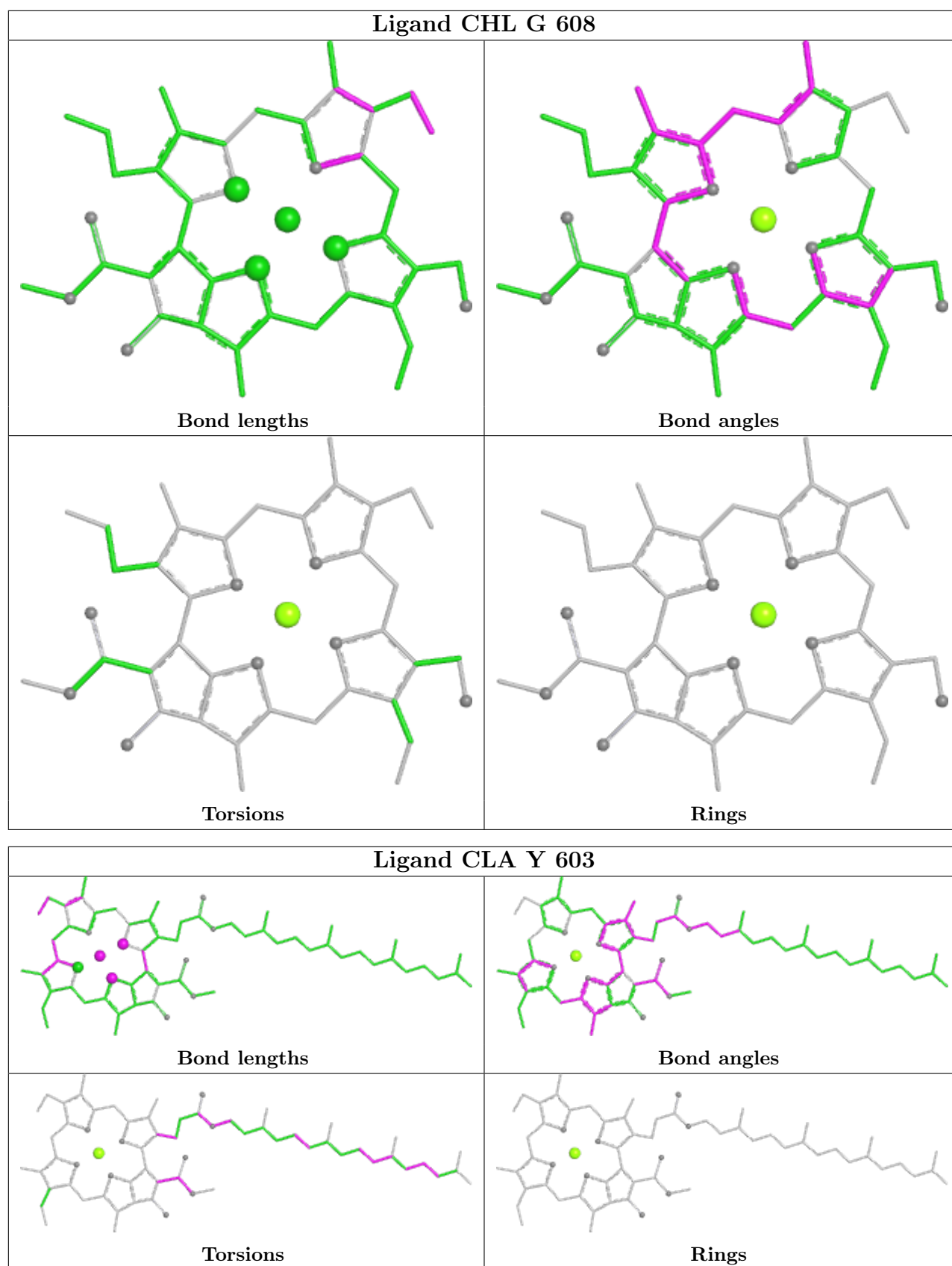


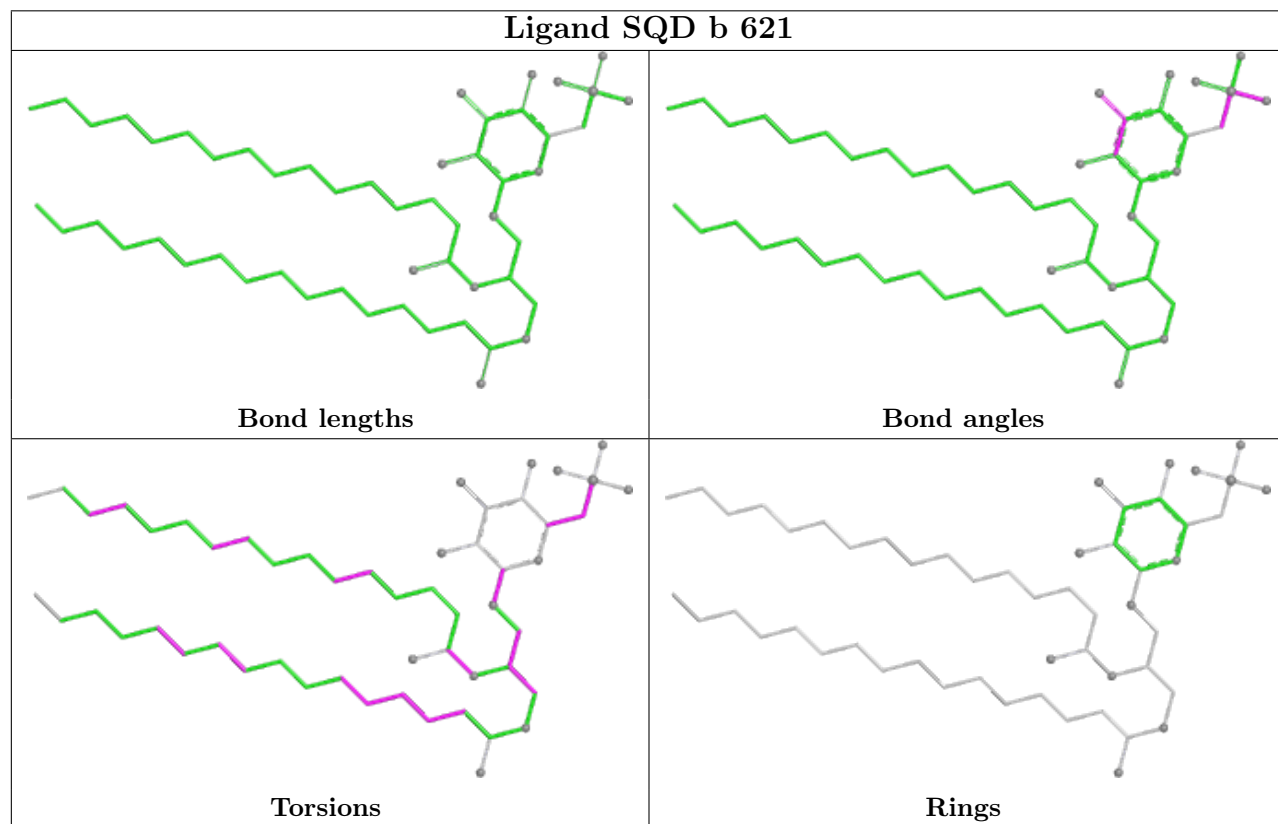
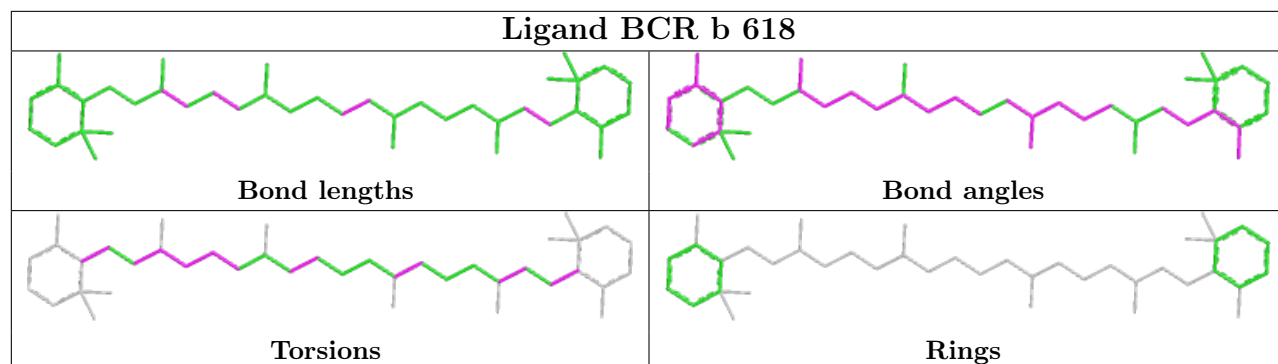
Torsions

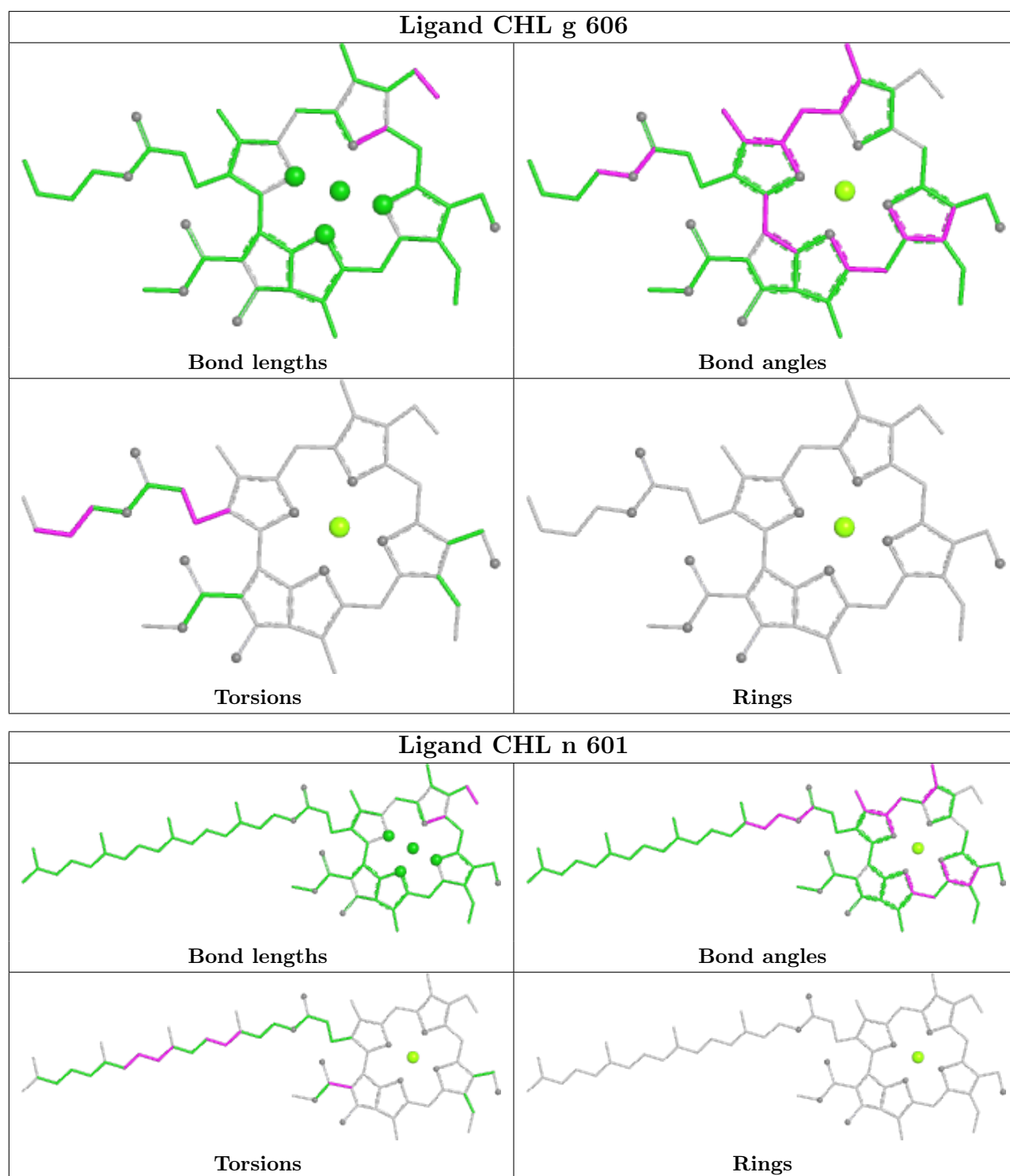


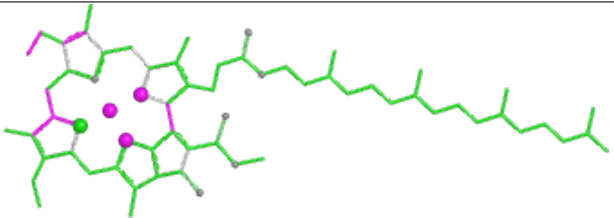
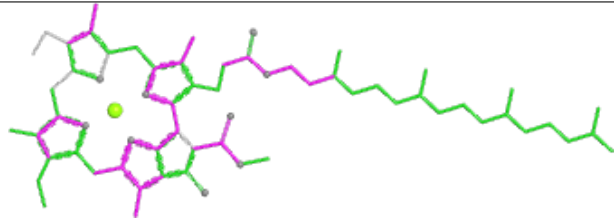
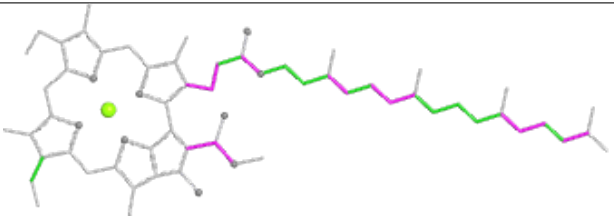
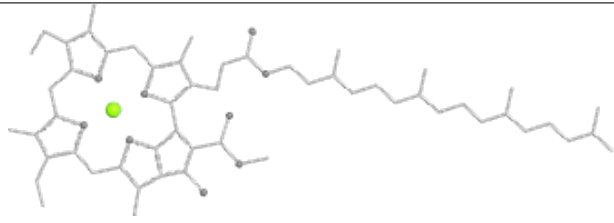
Rings

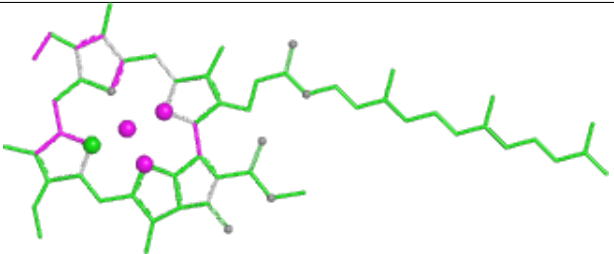
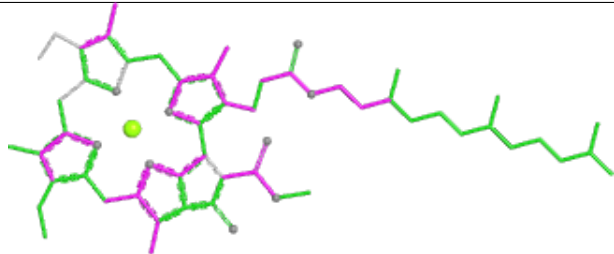
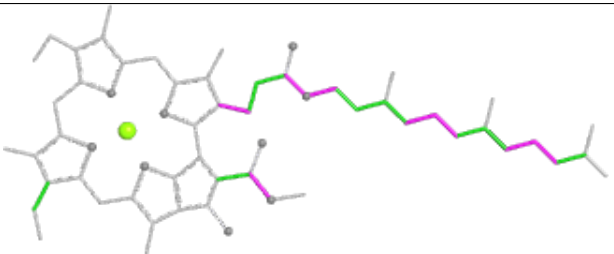
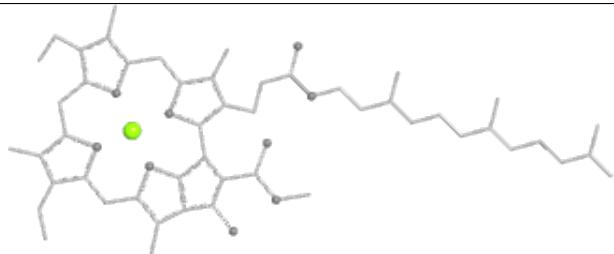


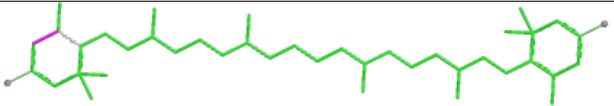
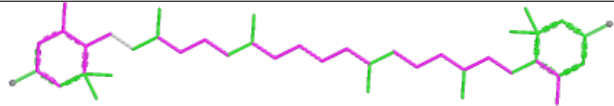
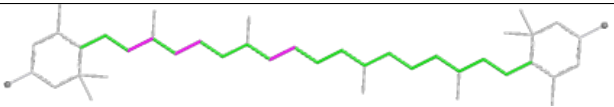
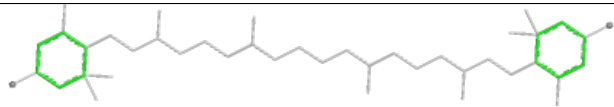


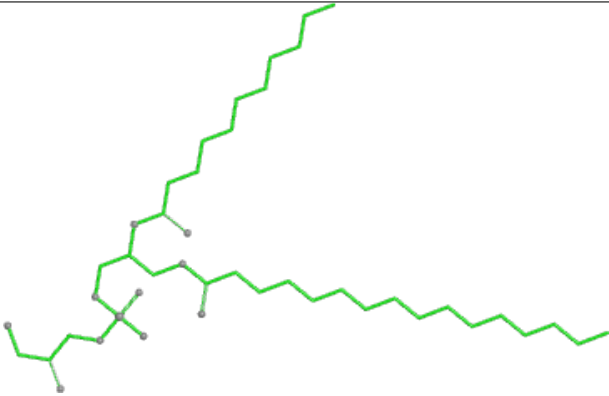
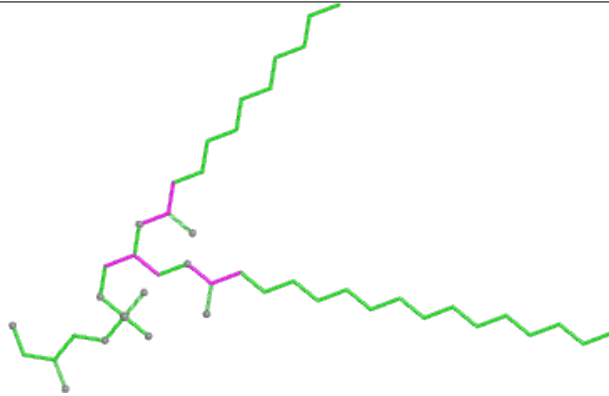
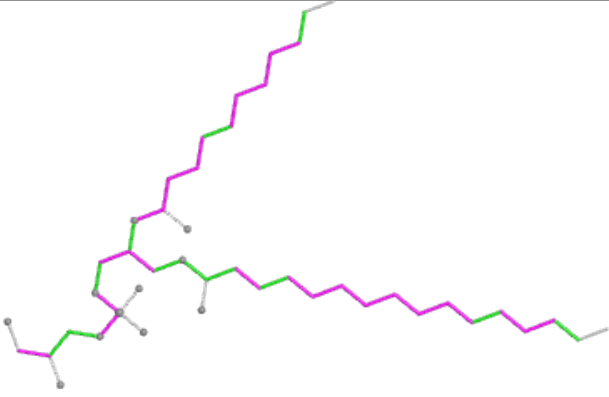
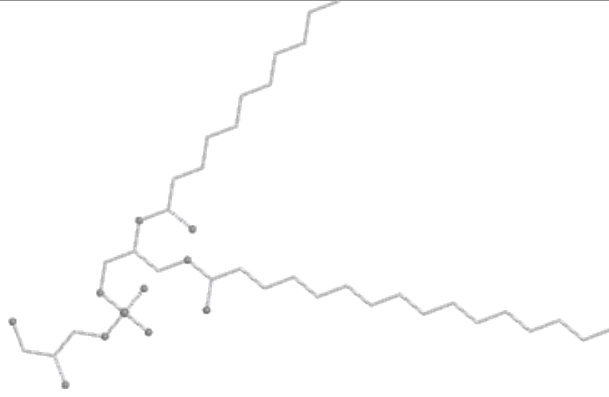


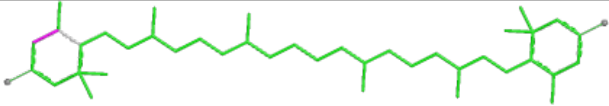
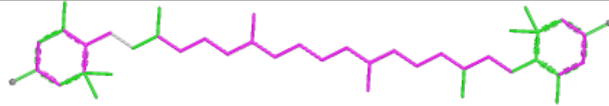
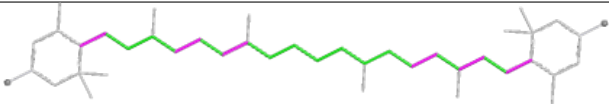
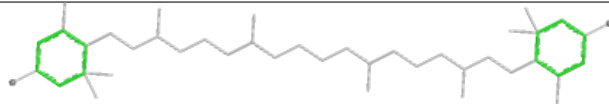


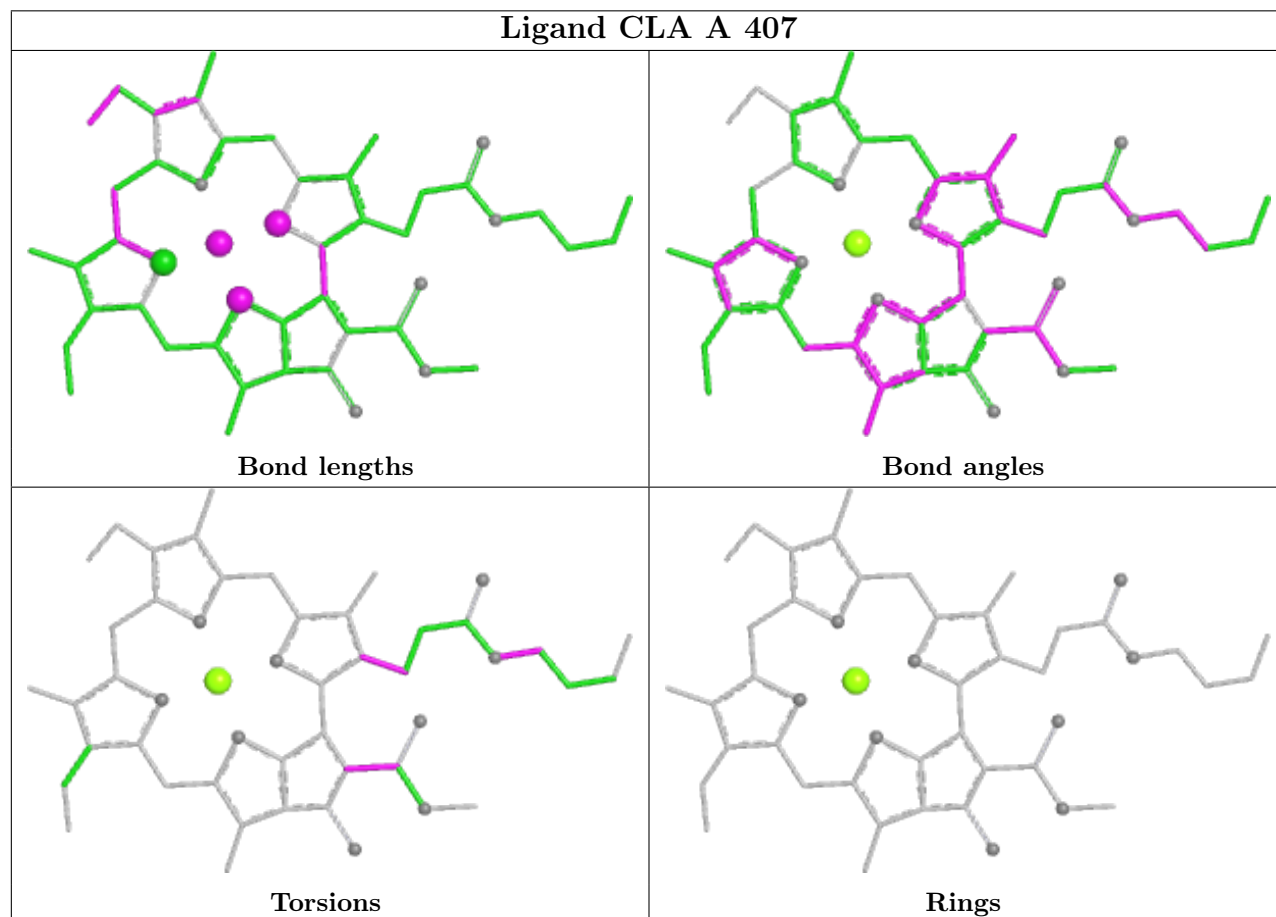
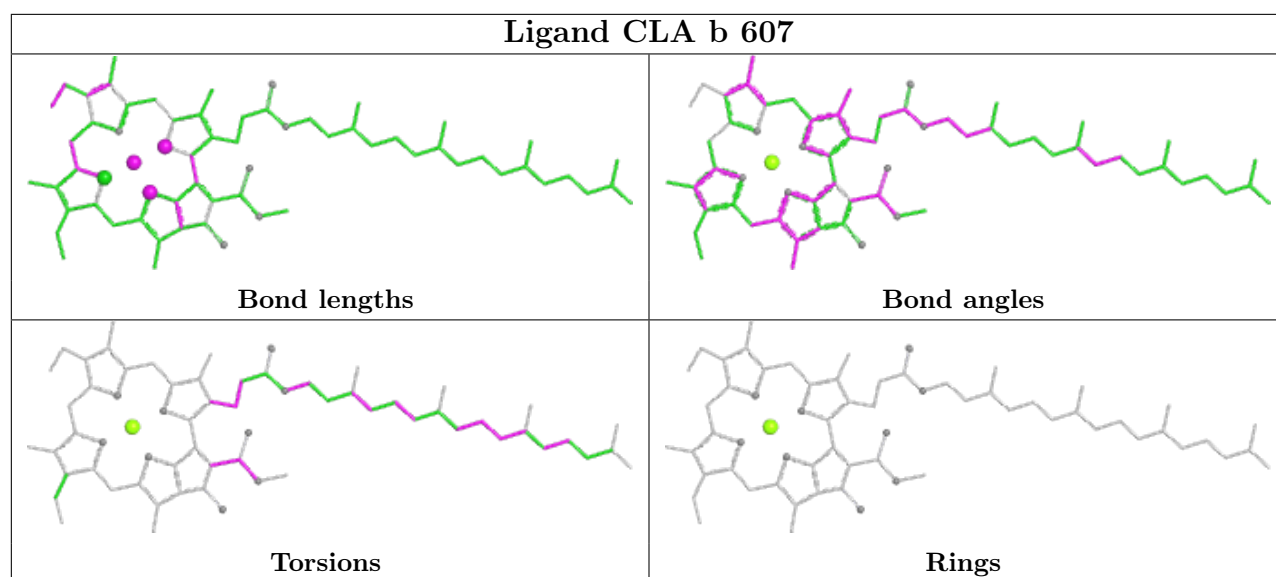
Ligand CLA g 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

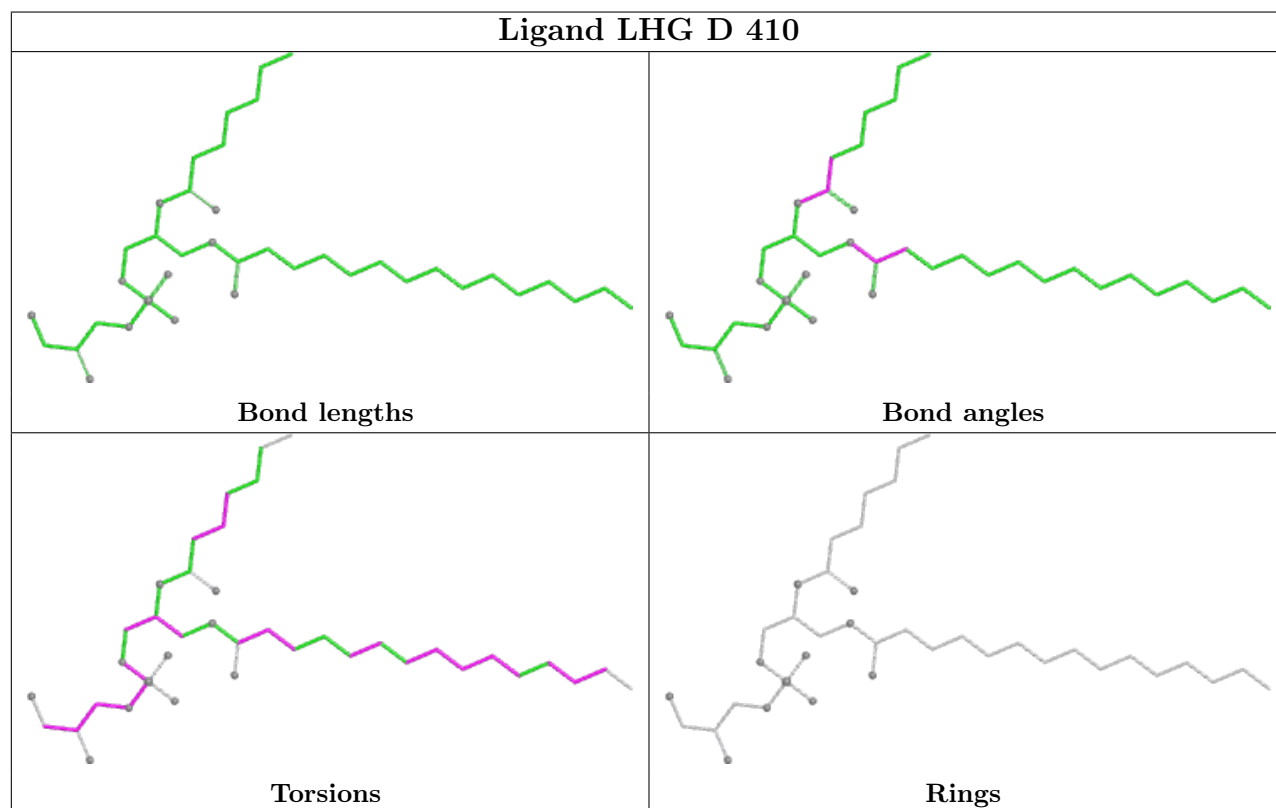
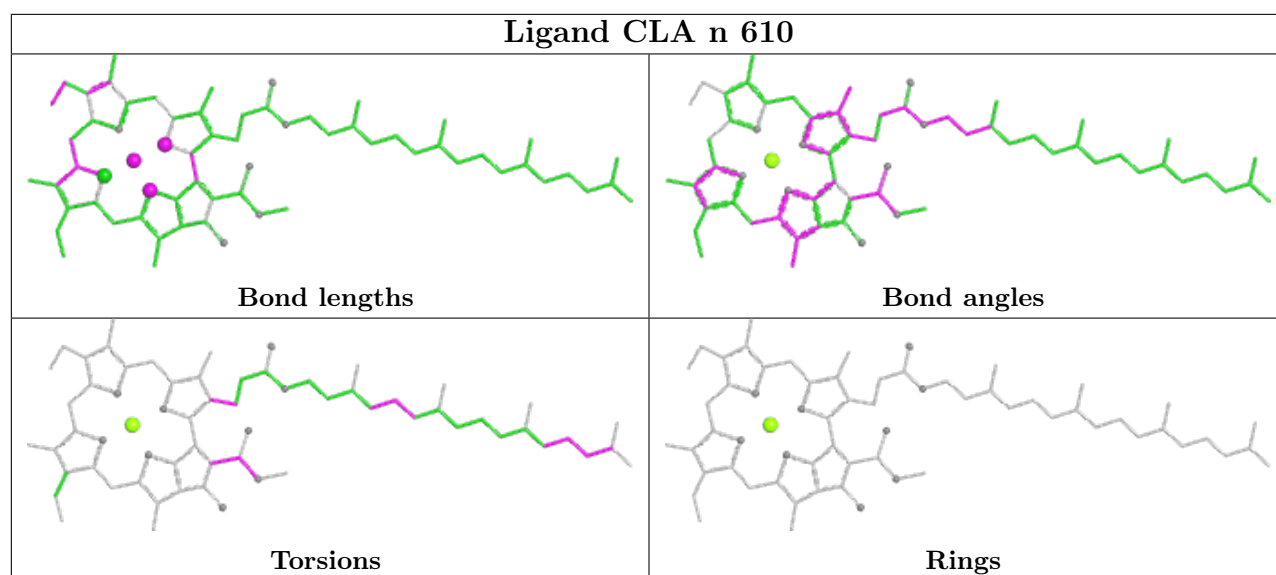
Ligand CLA A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

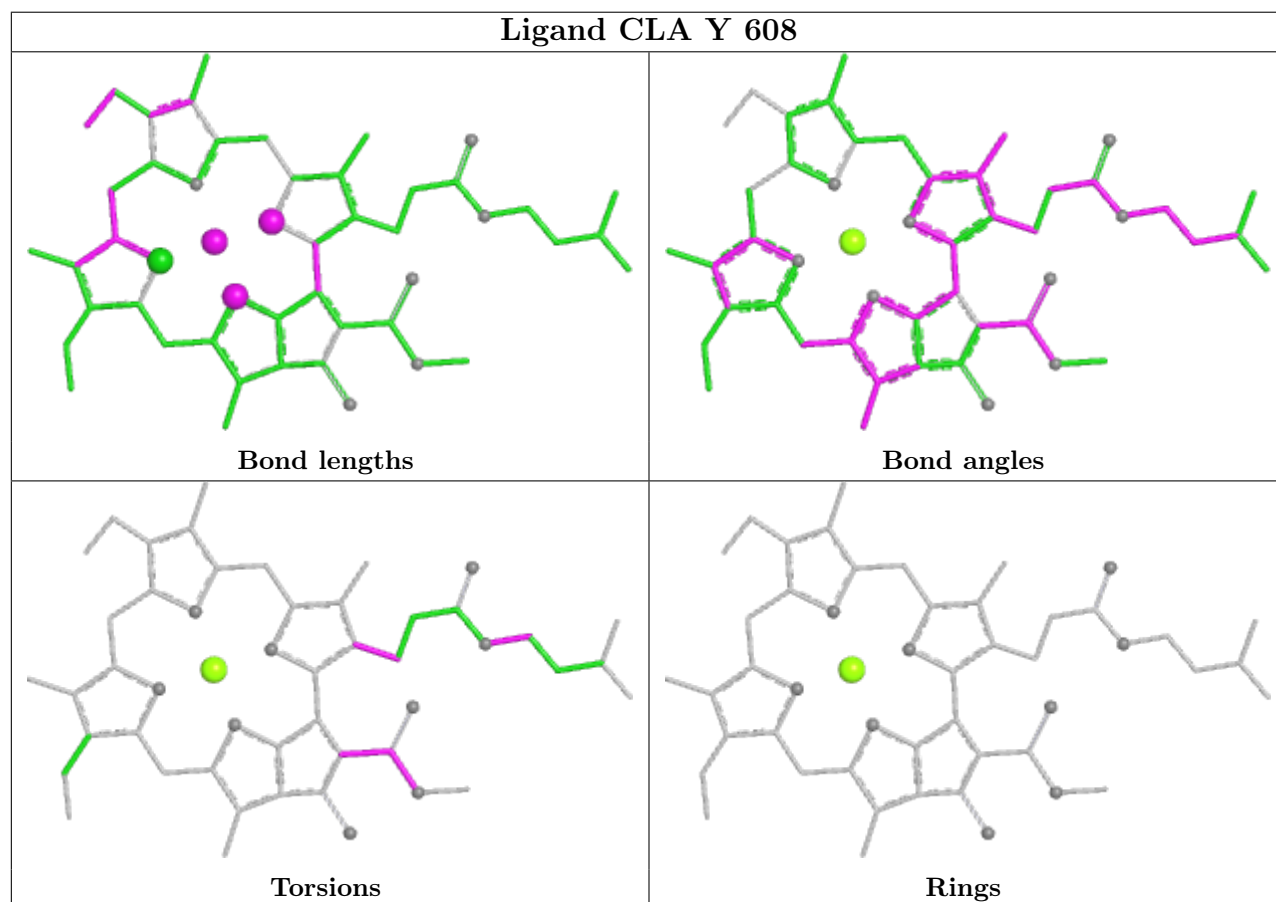
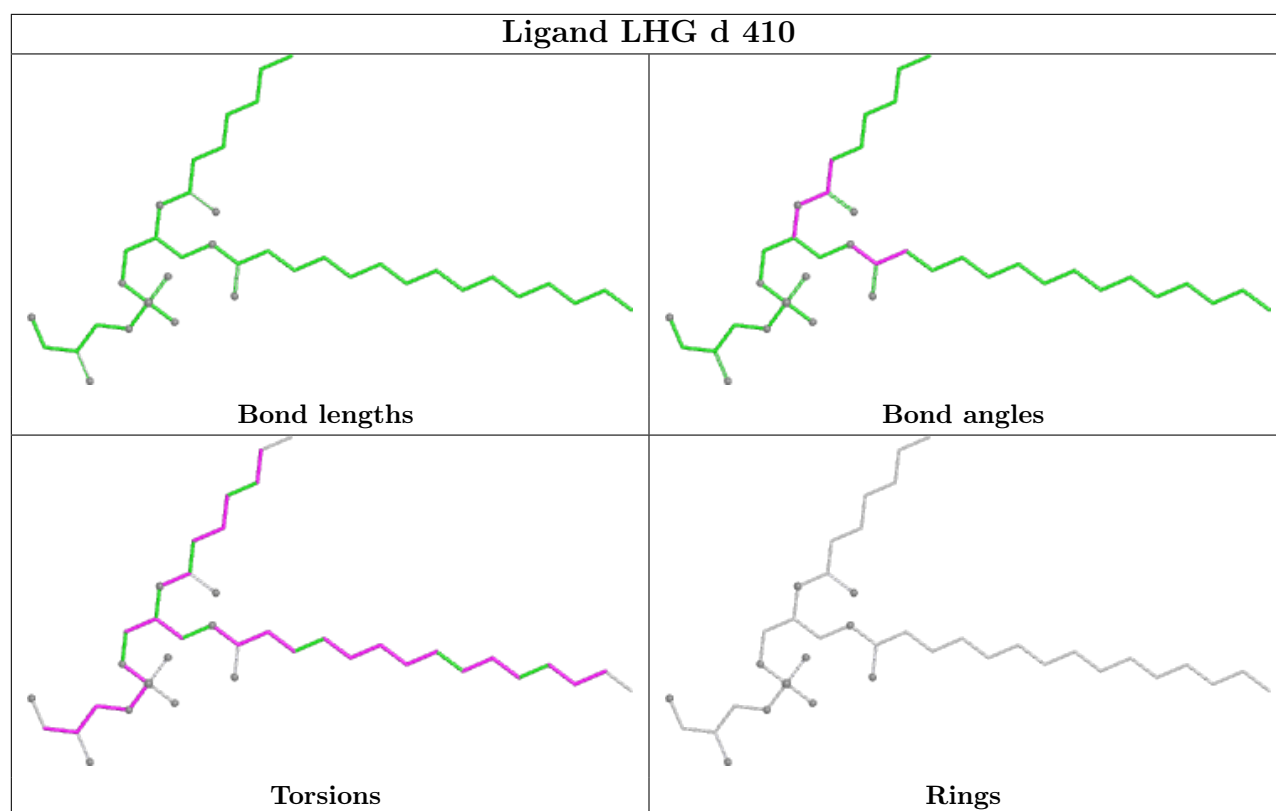
Ligand LUT Y 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

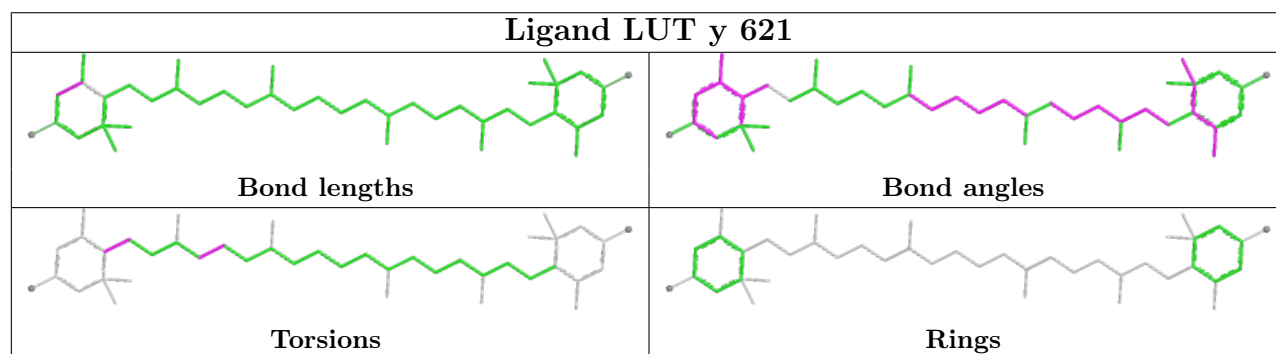
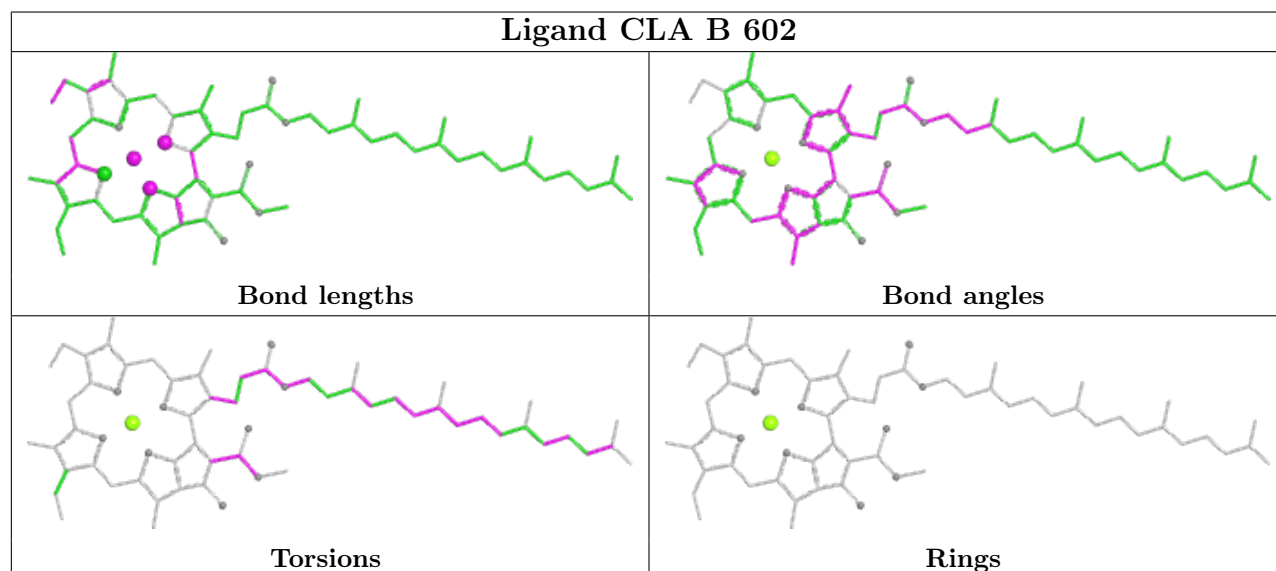
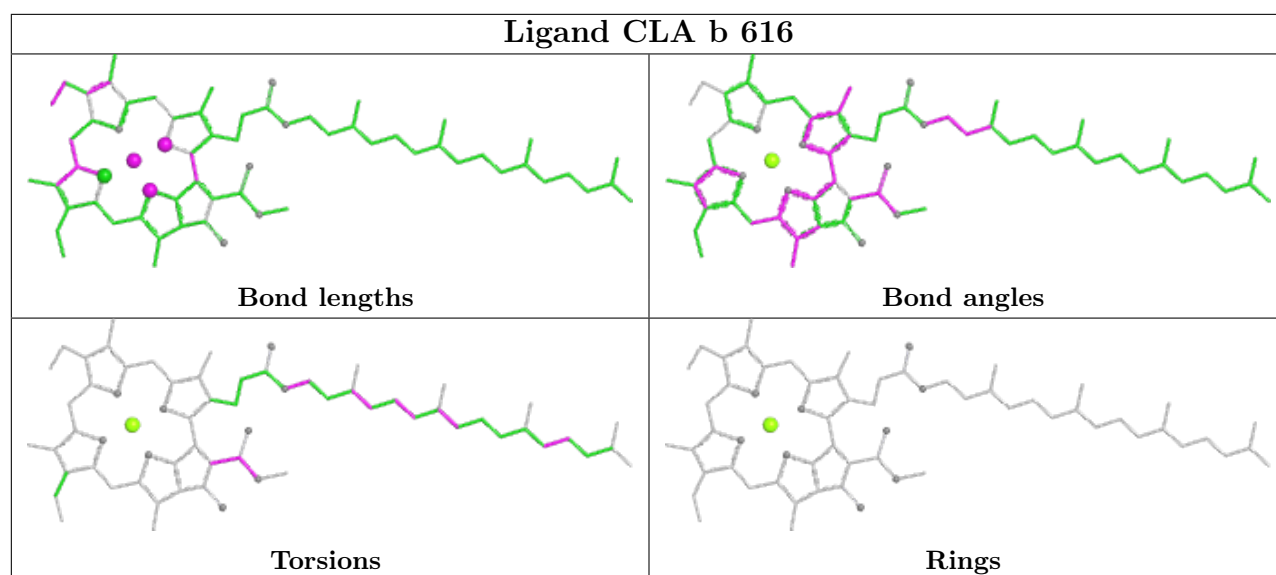
Ligand LHG d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

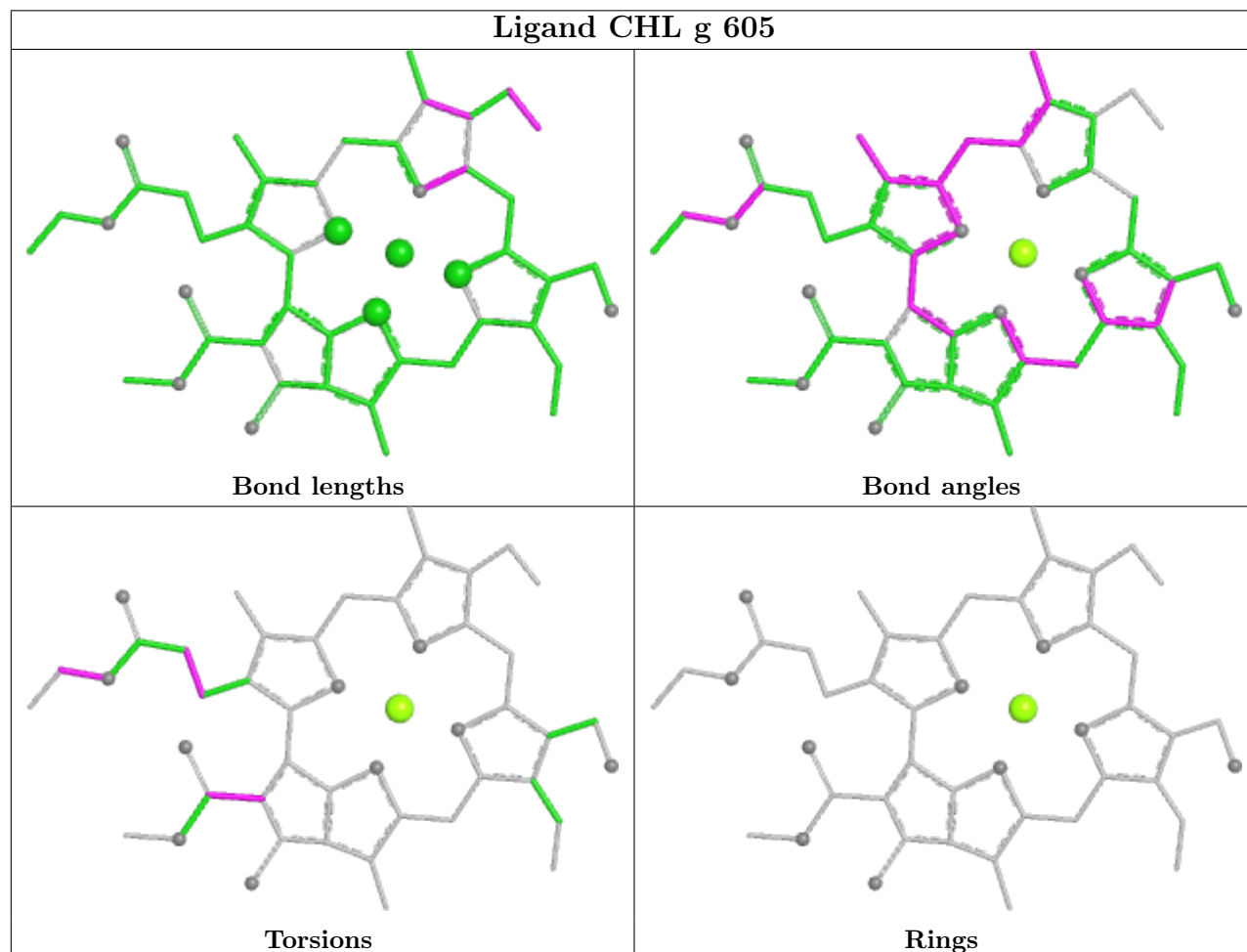
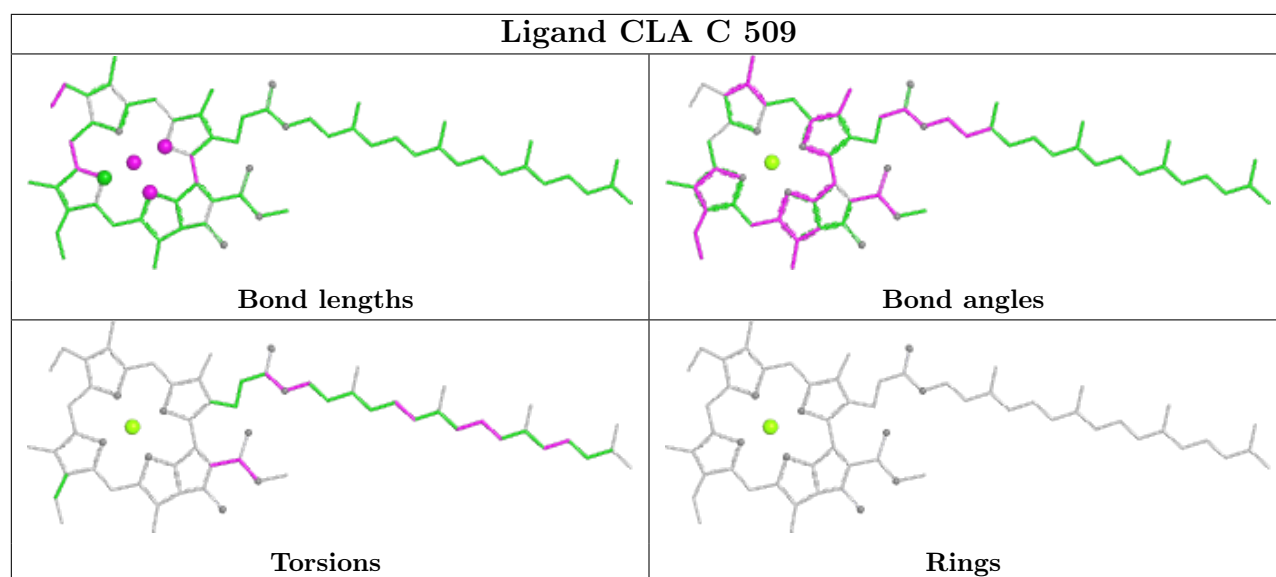
Ligand LUT r 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

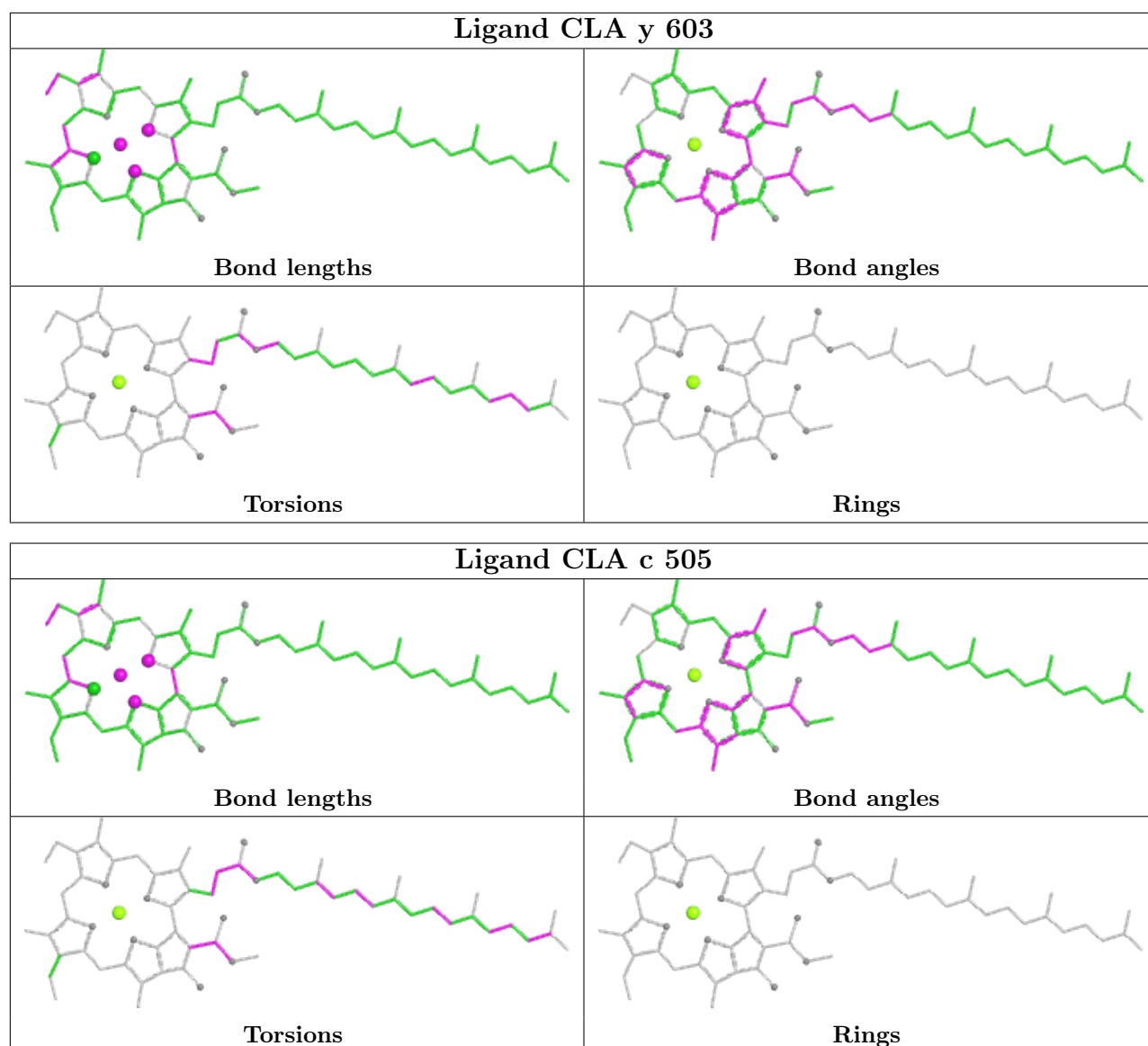


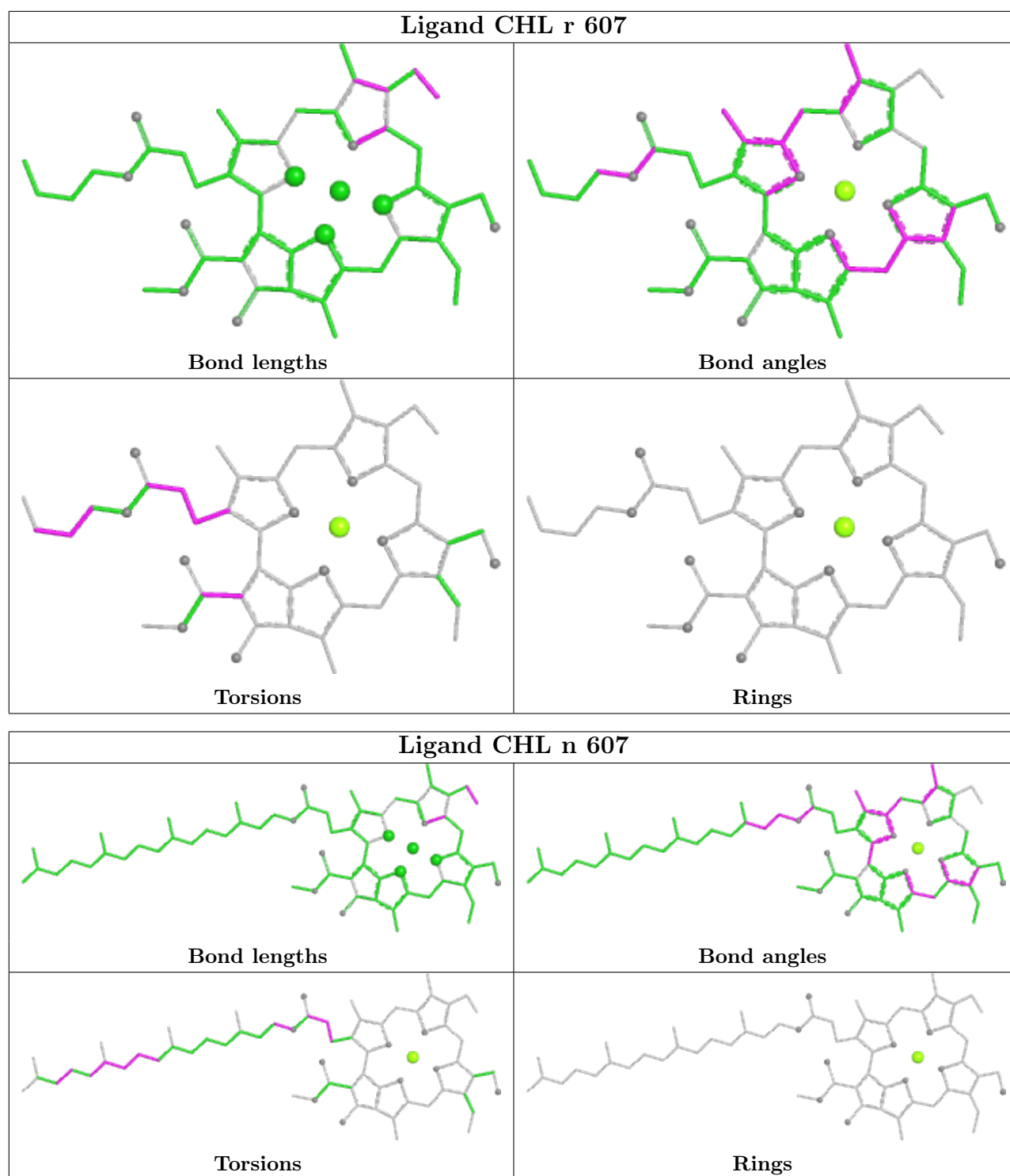


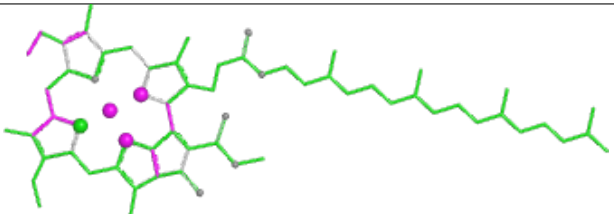
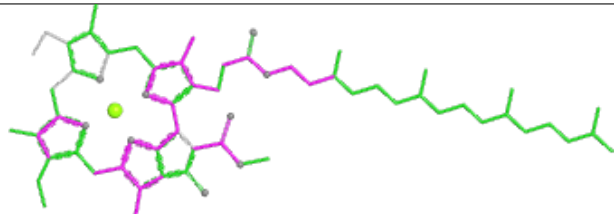
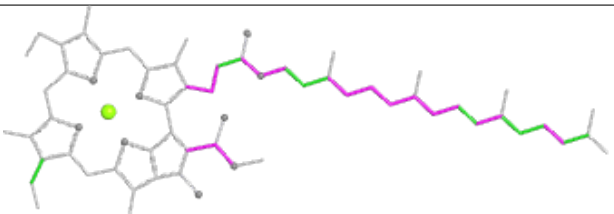
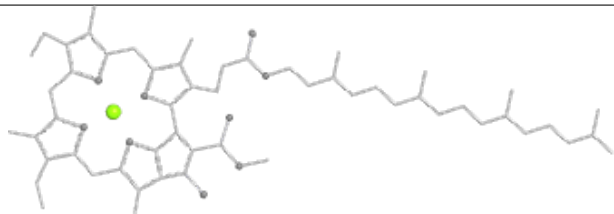


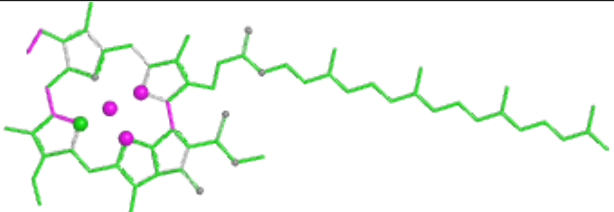
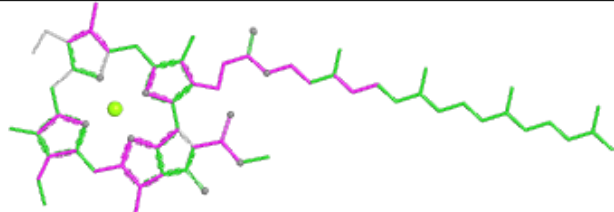
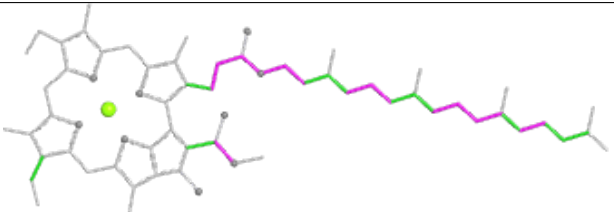
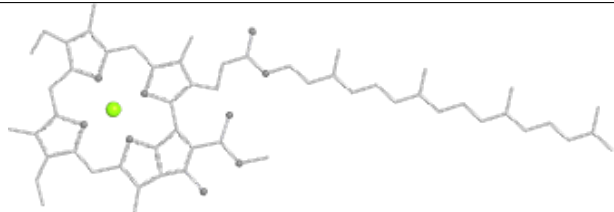


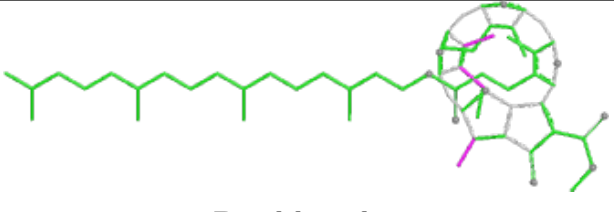
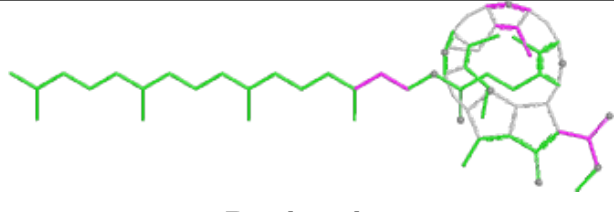
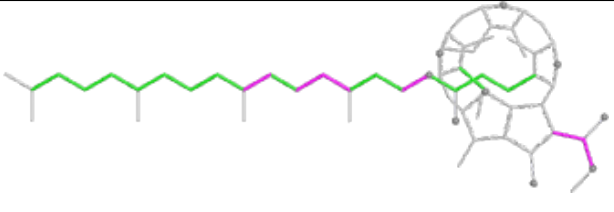
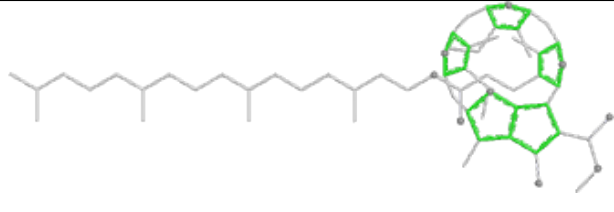


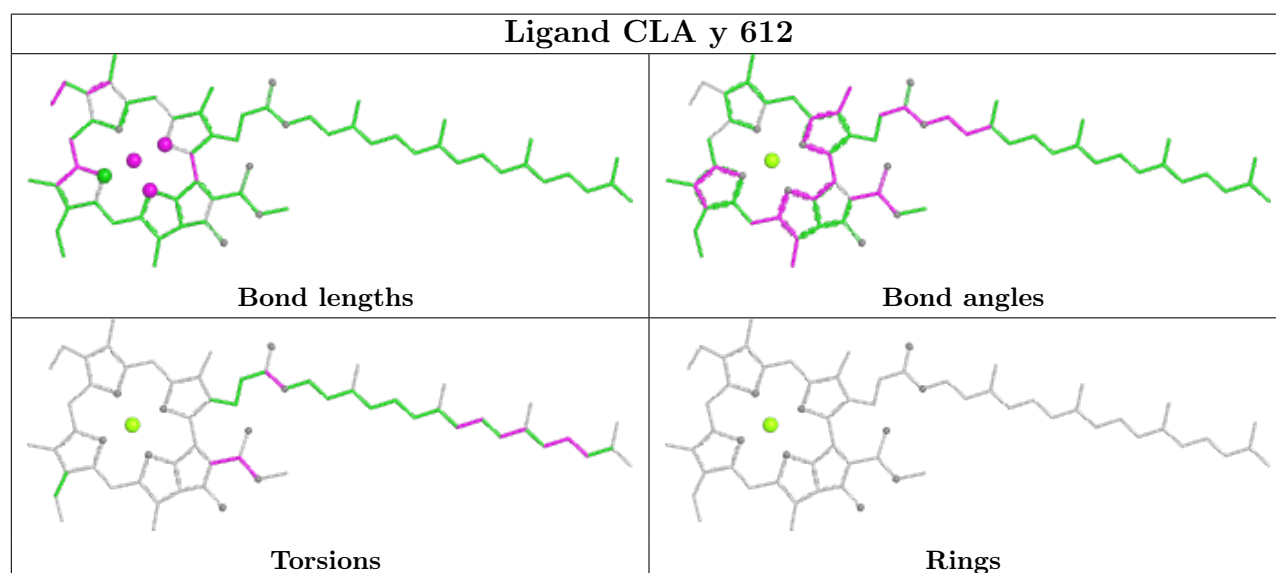
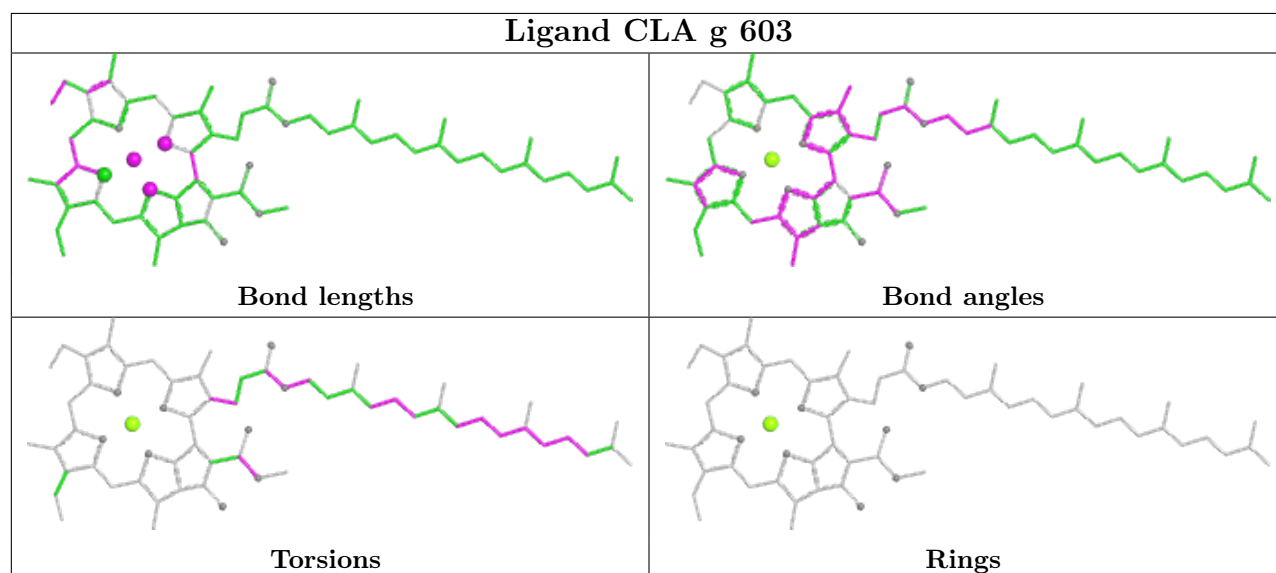
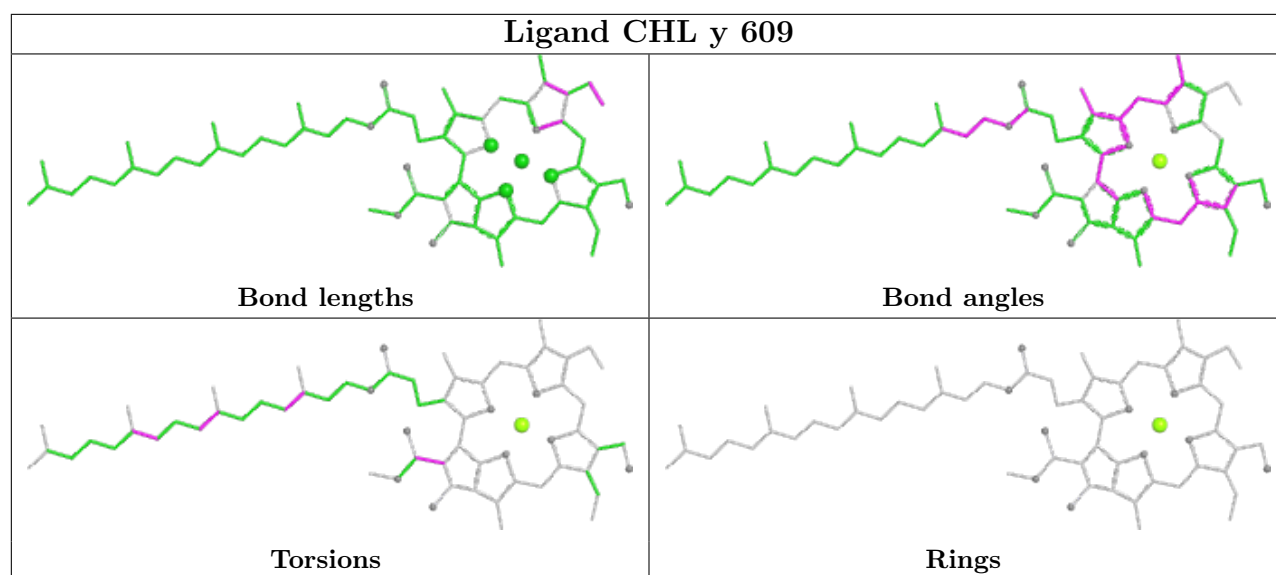


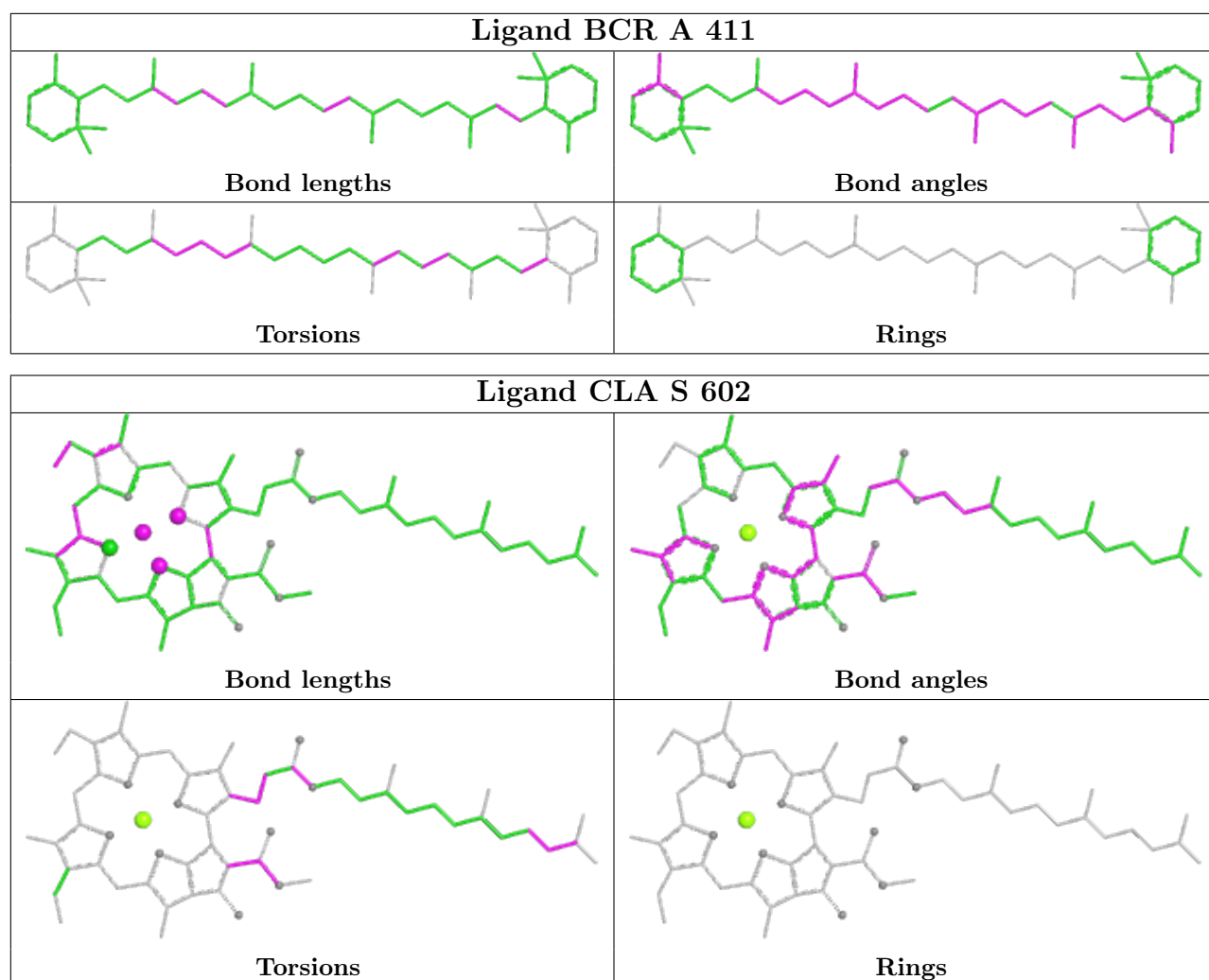


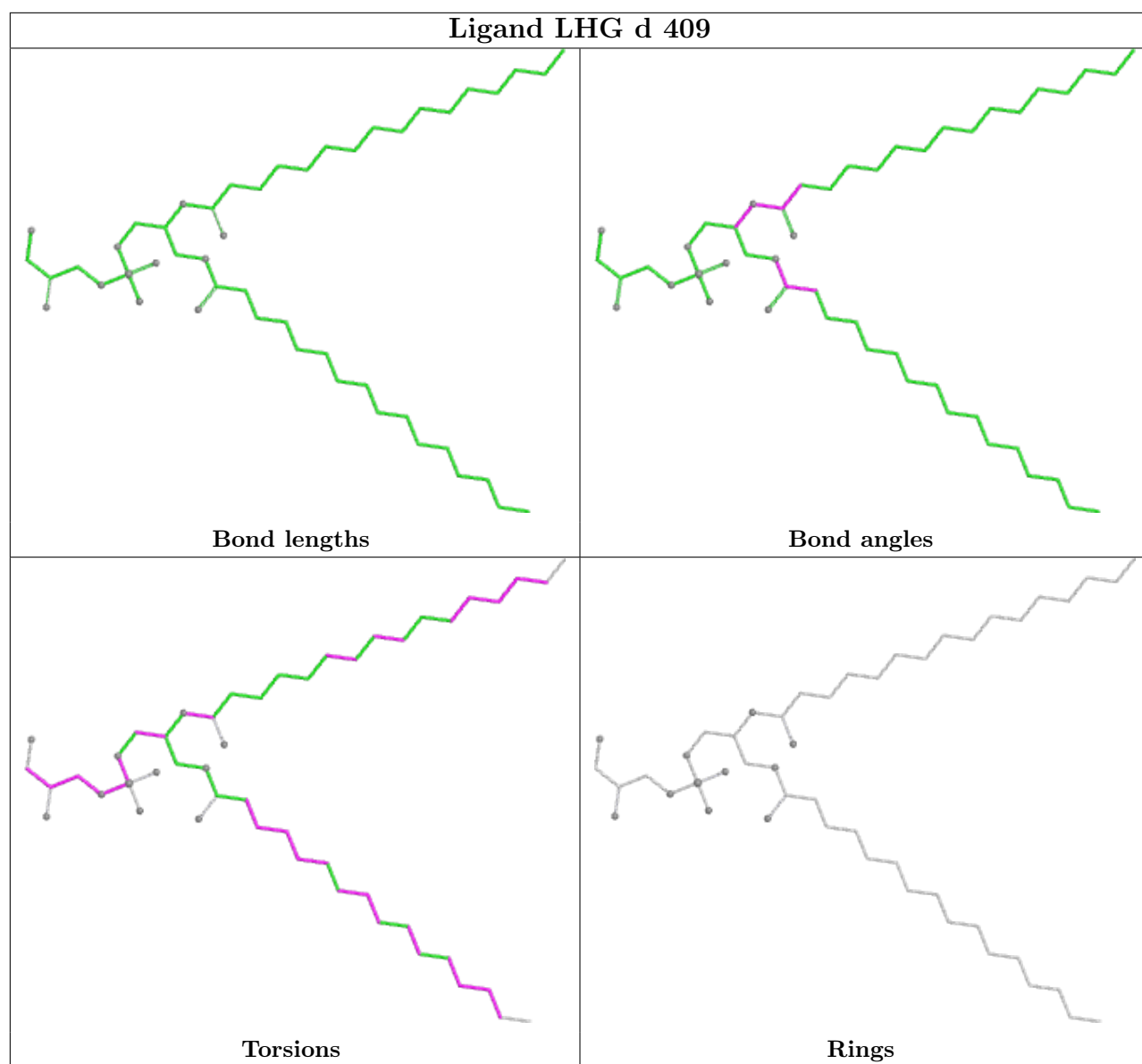
Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

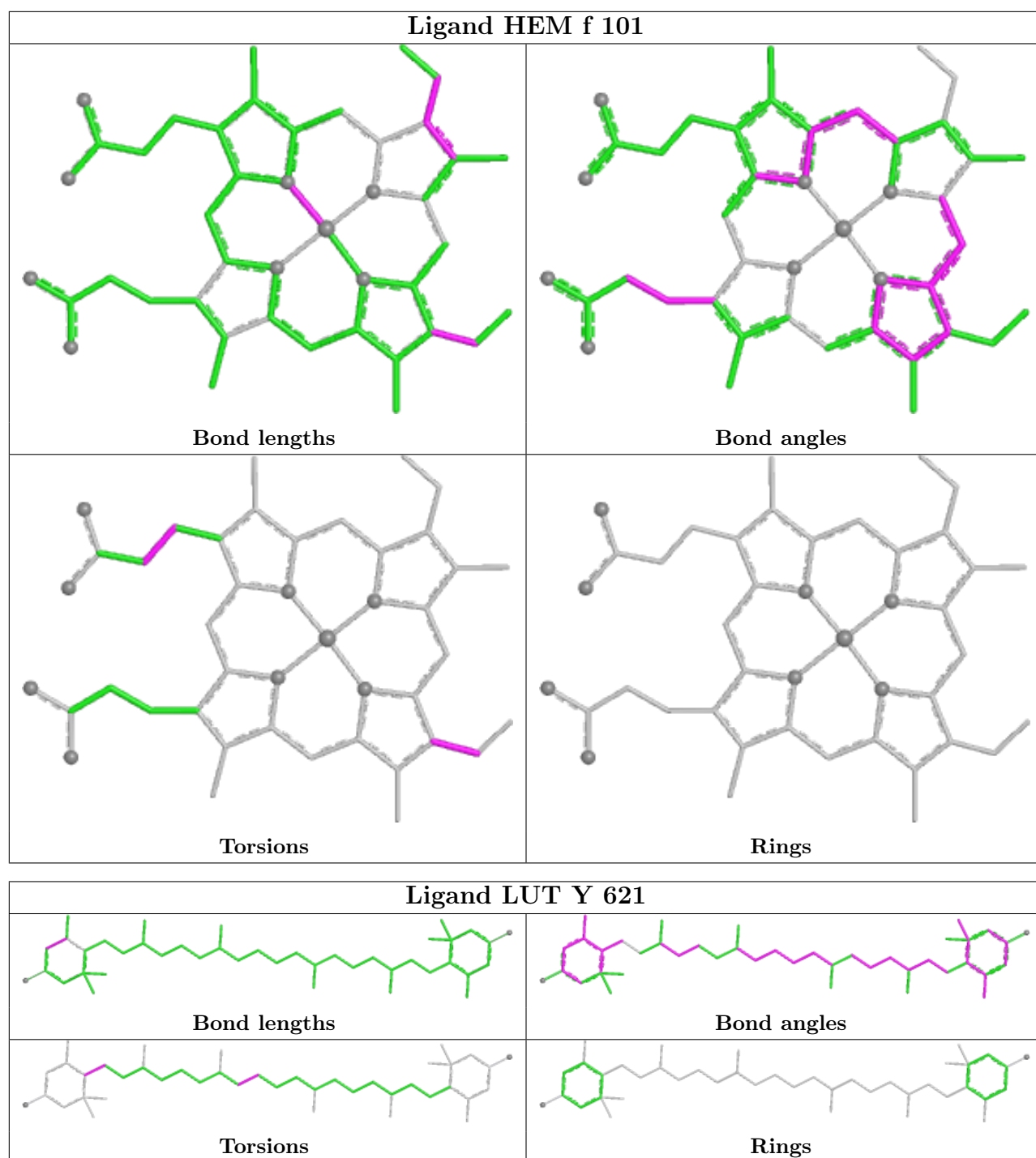
Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

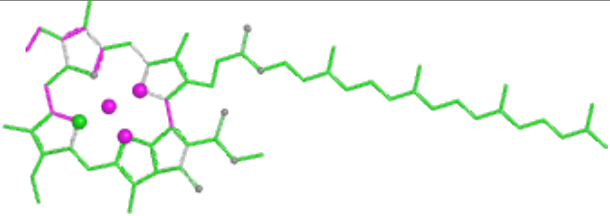
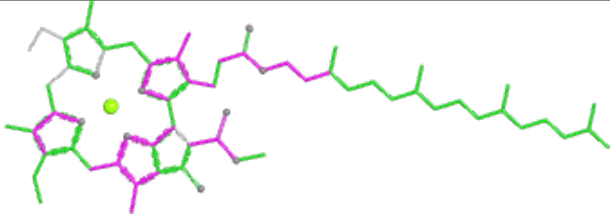
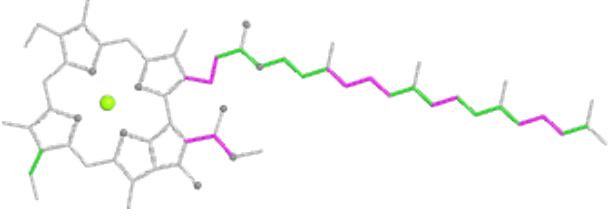
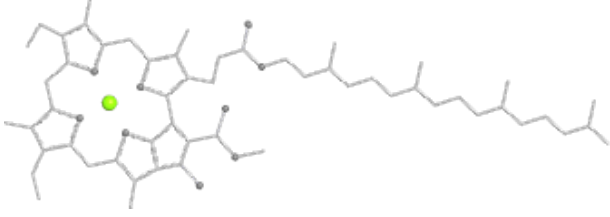
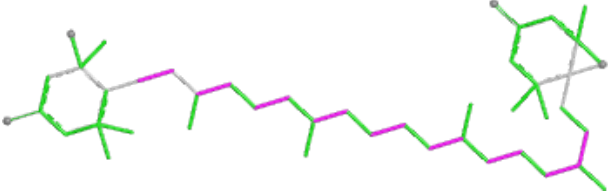


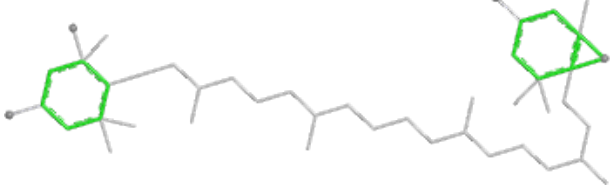
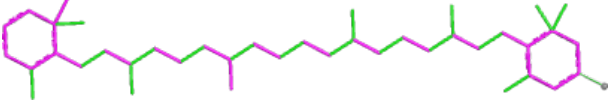
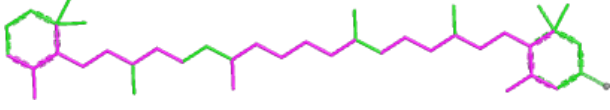
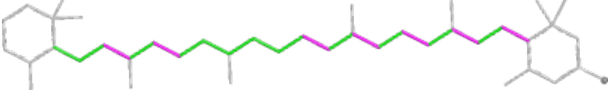
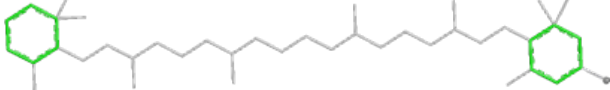
Ligand PHO a 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

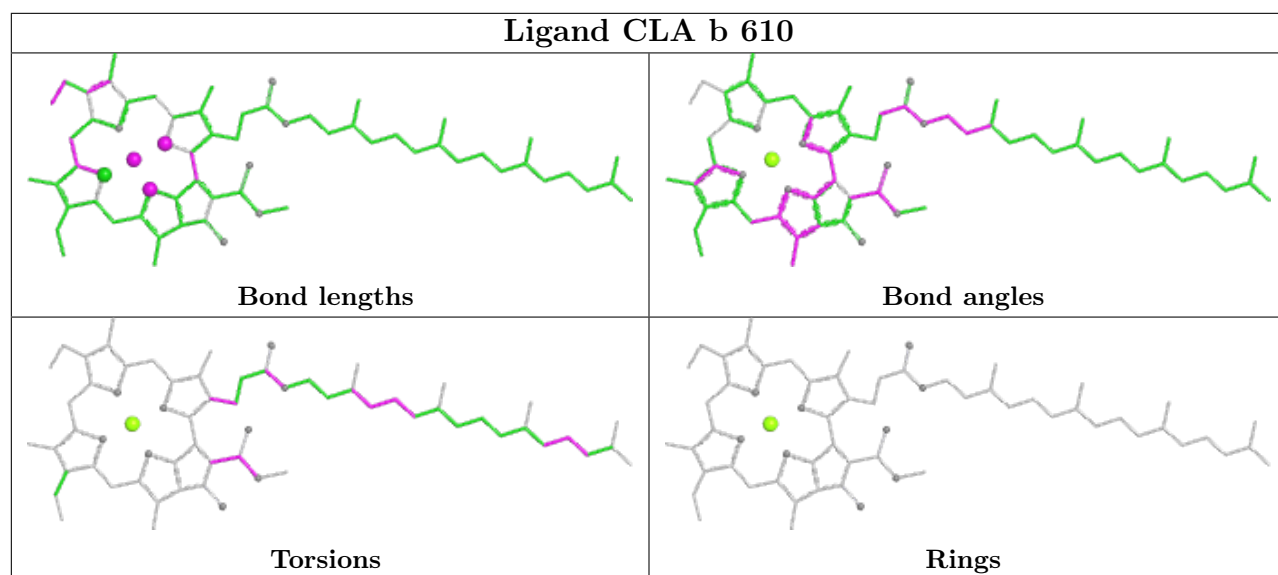
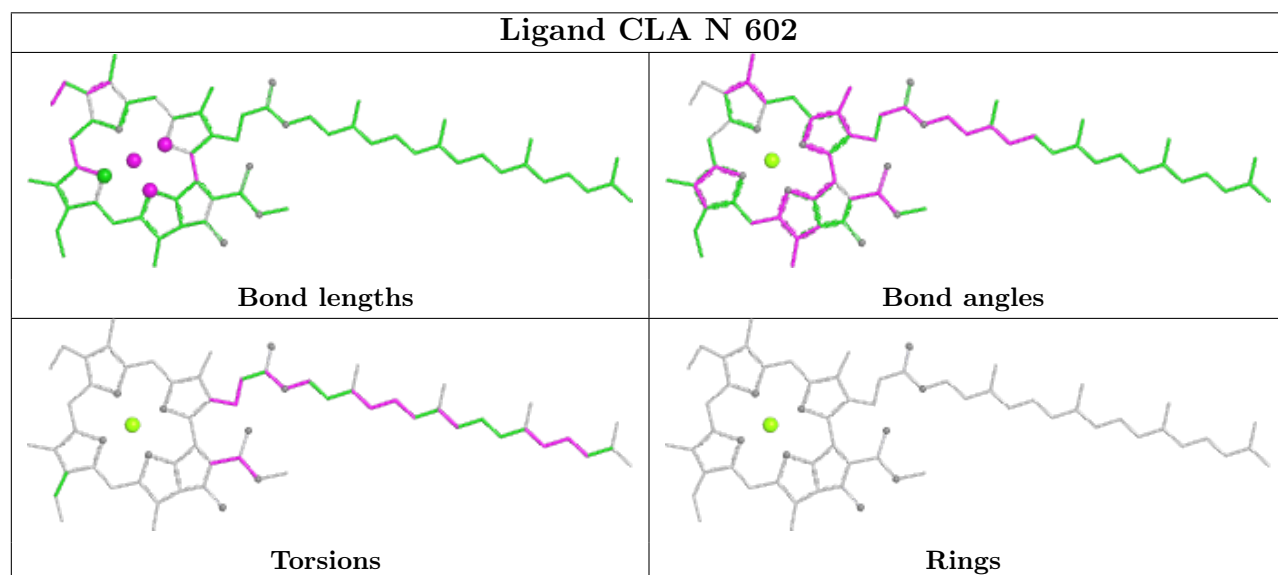
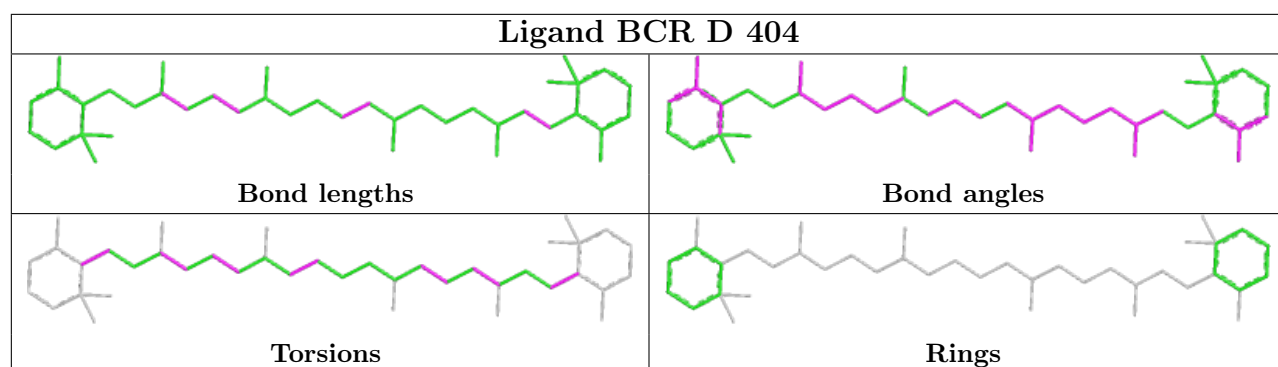


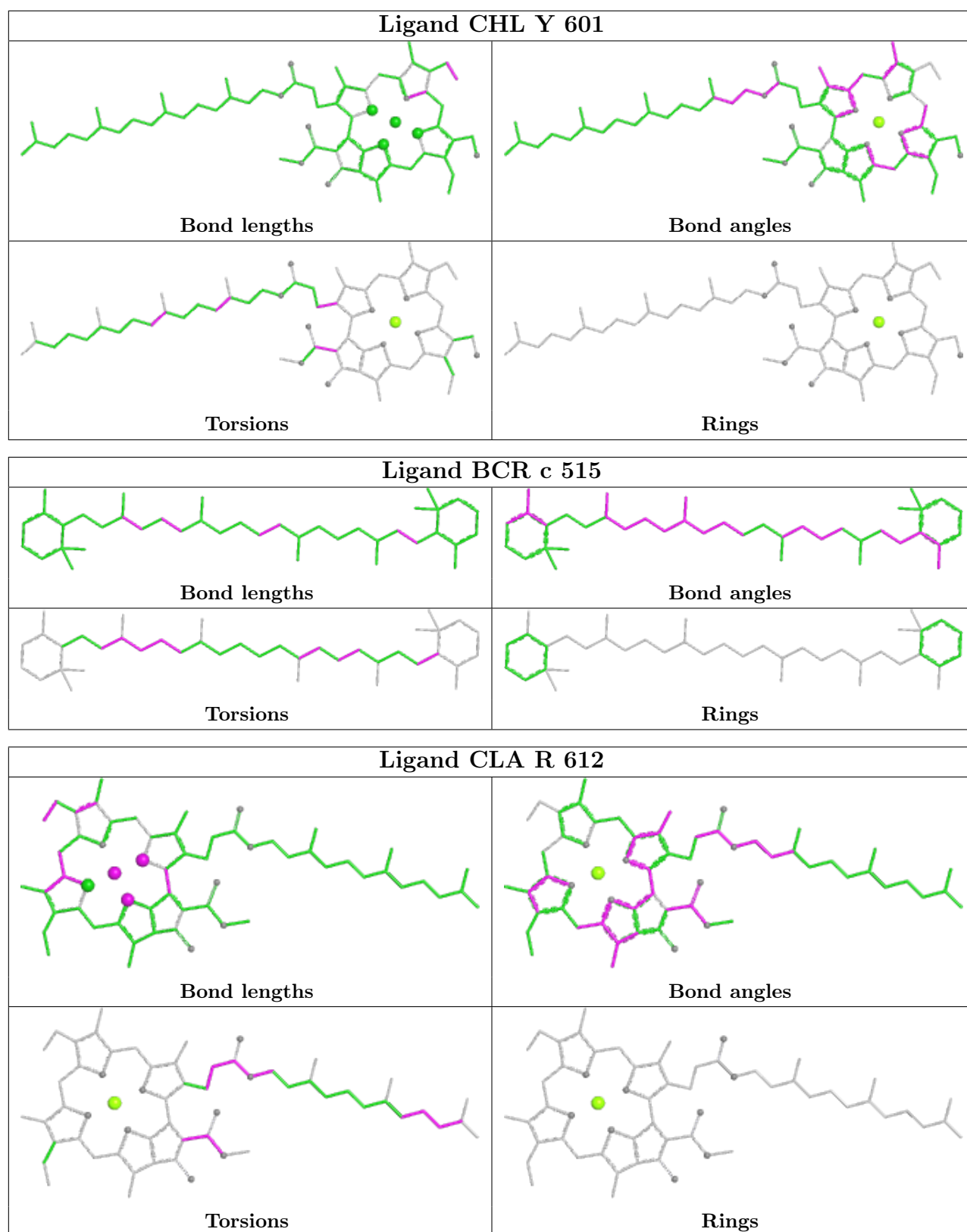


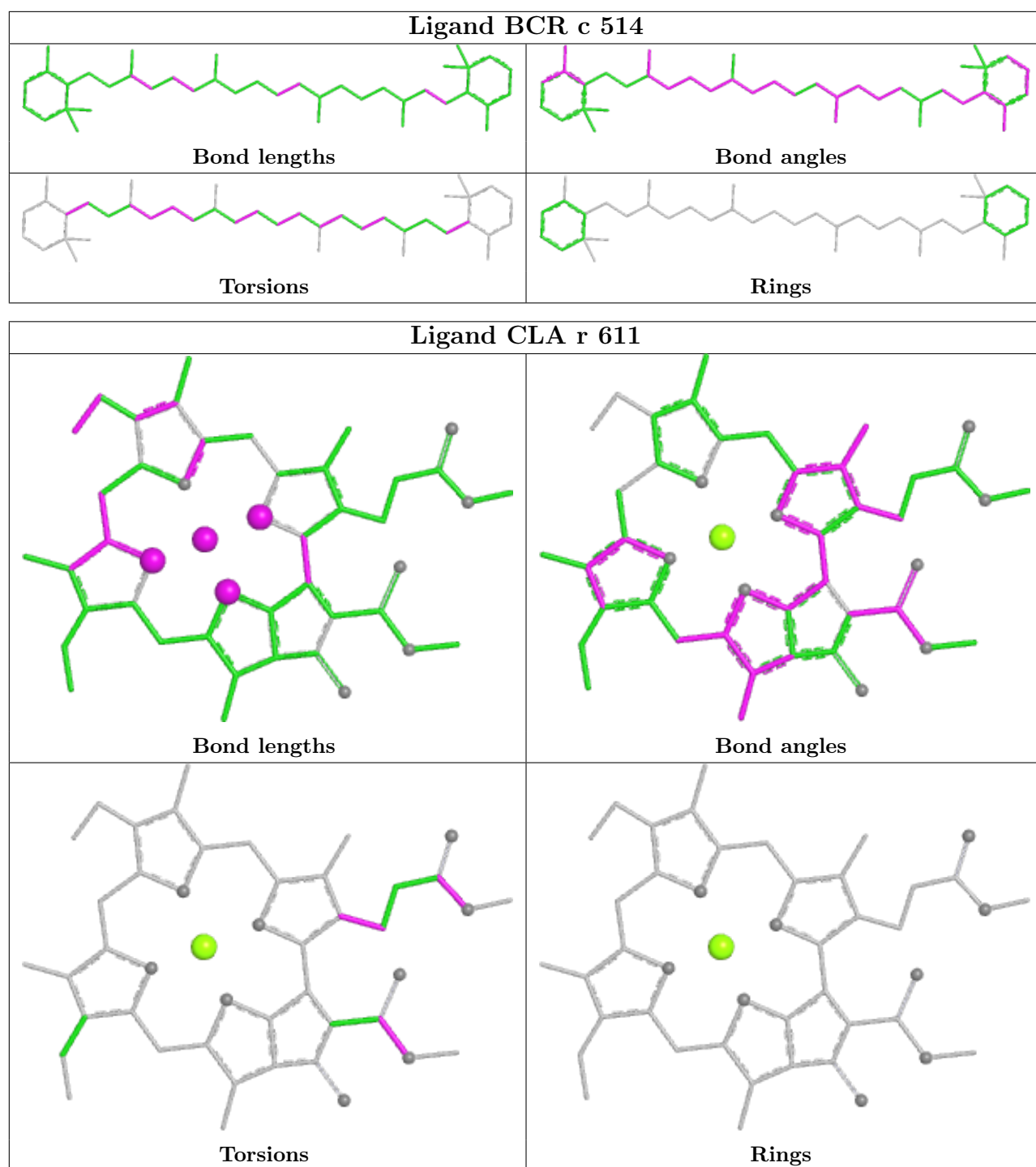


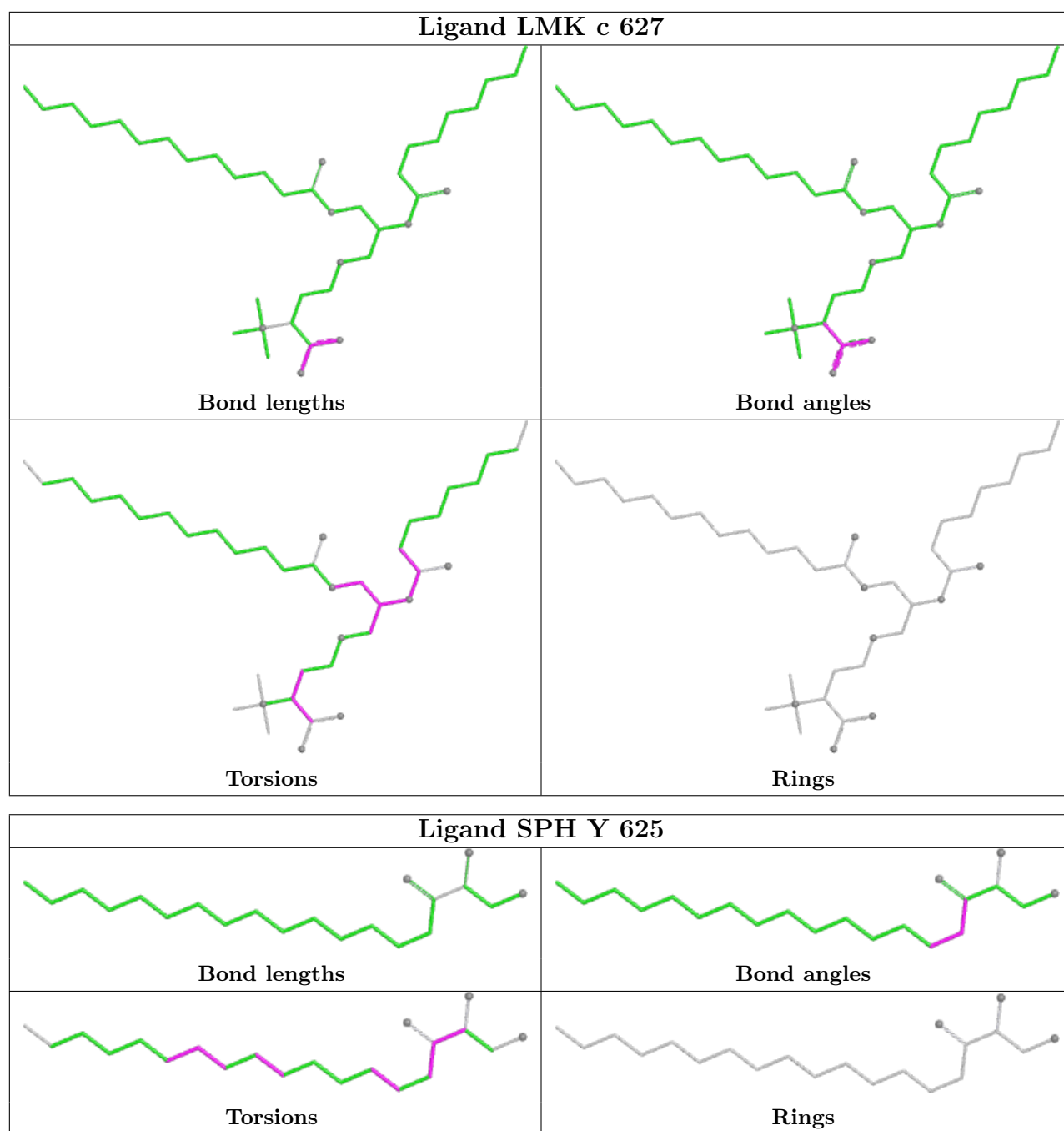


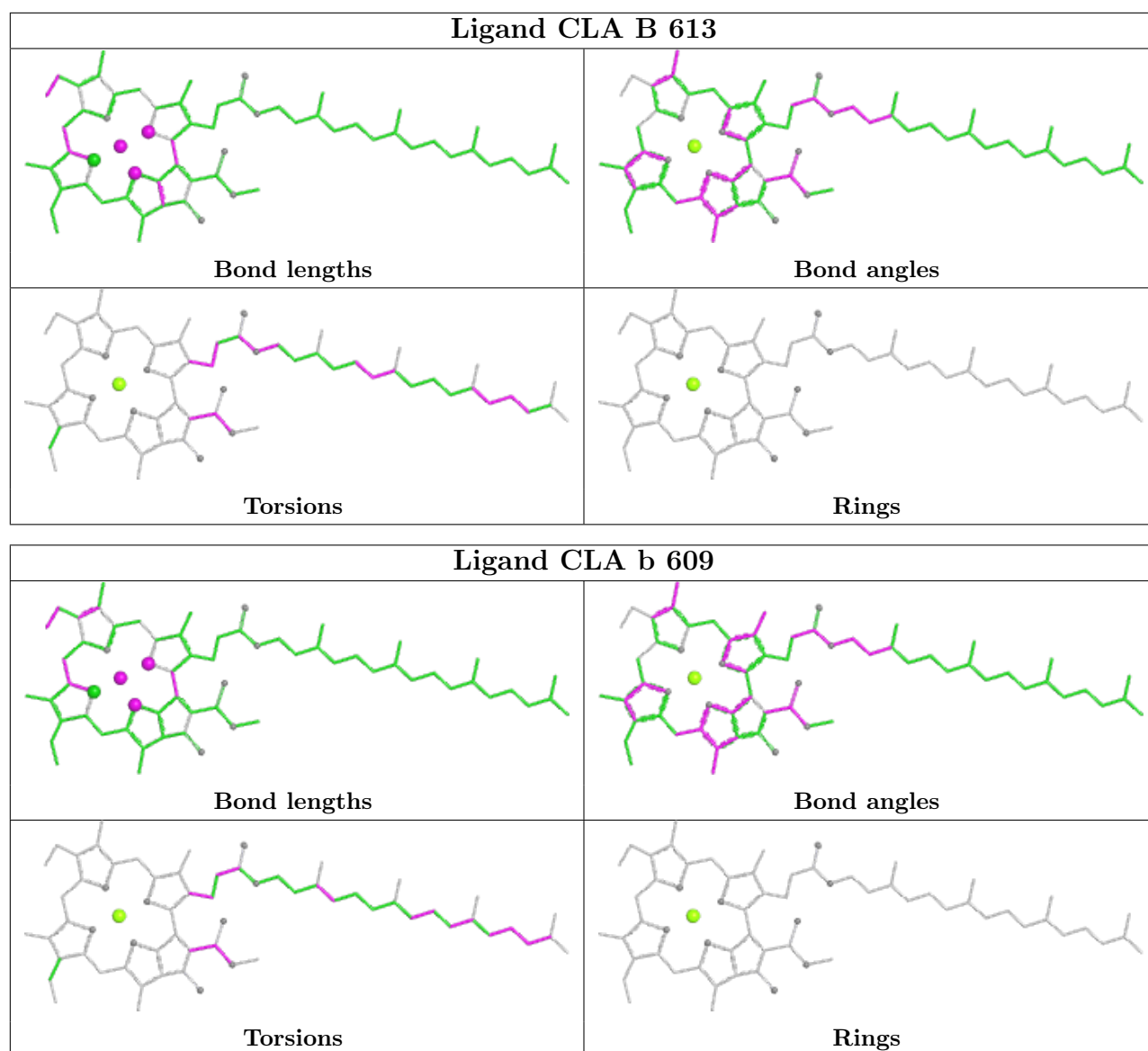
Ligand CLA G 610	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand NEX N 623	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand RRX h 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

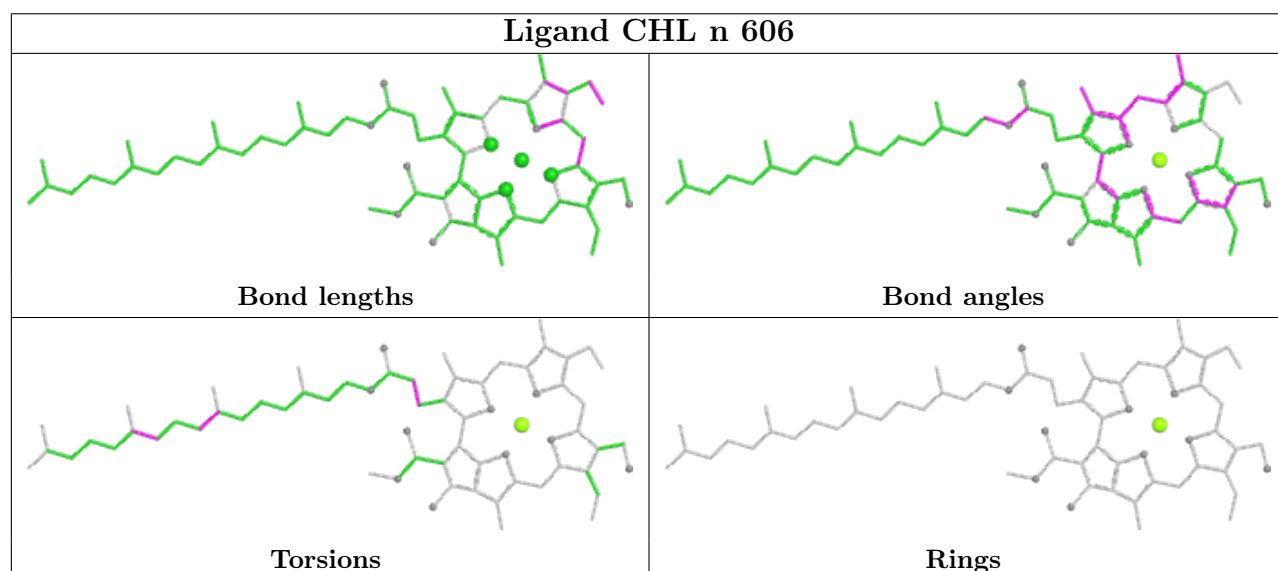
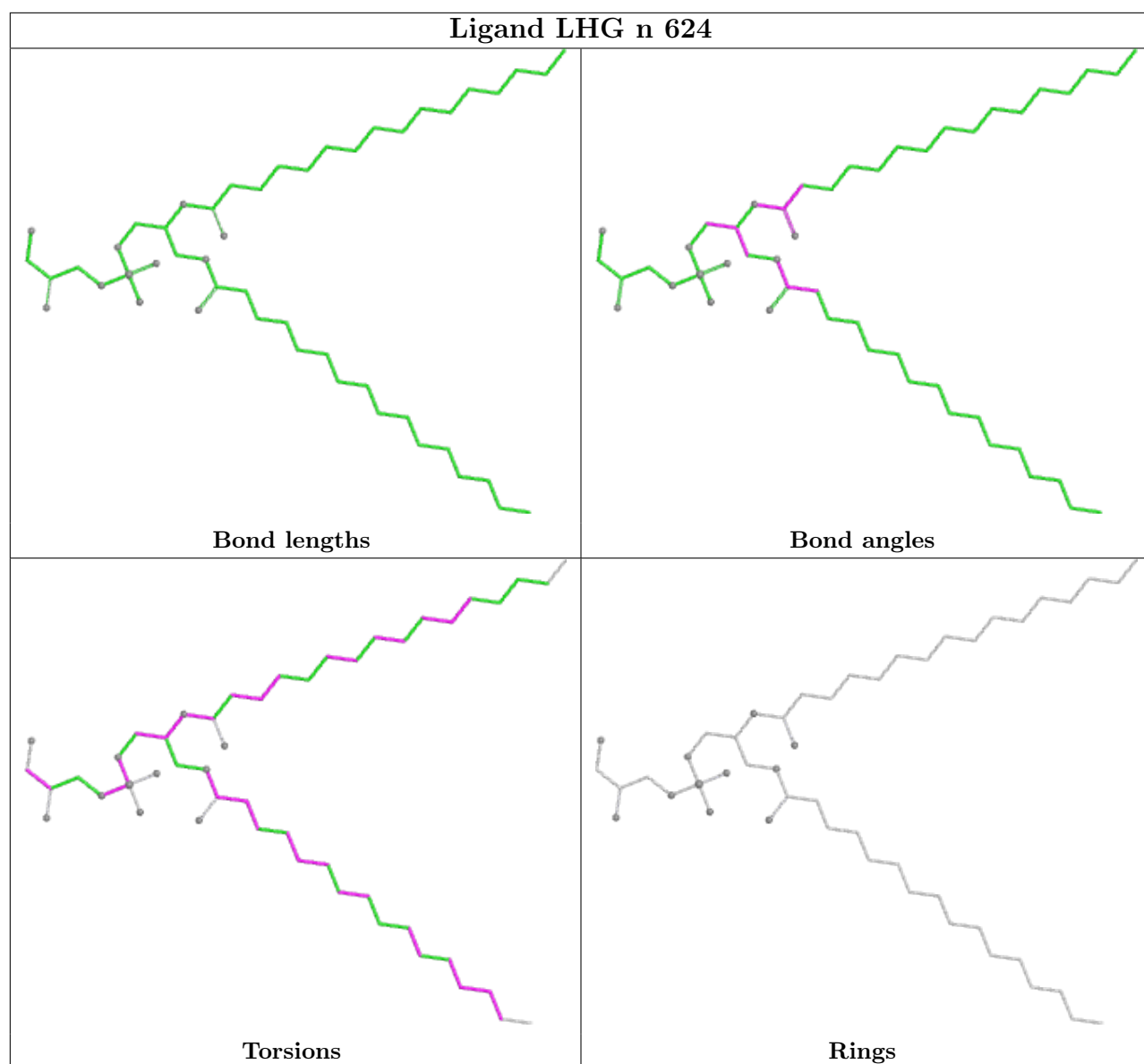


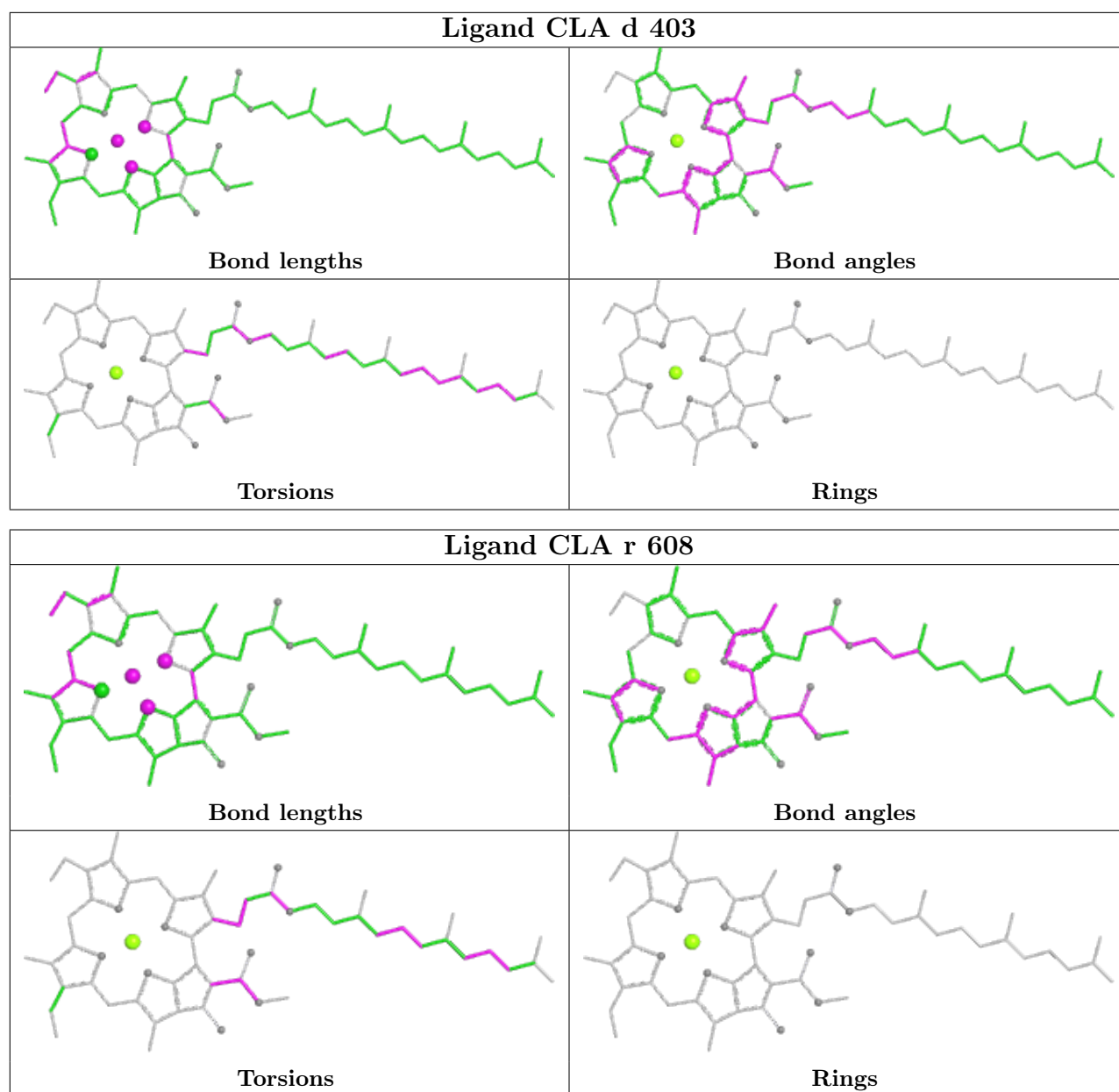


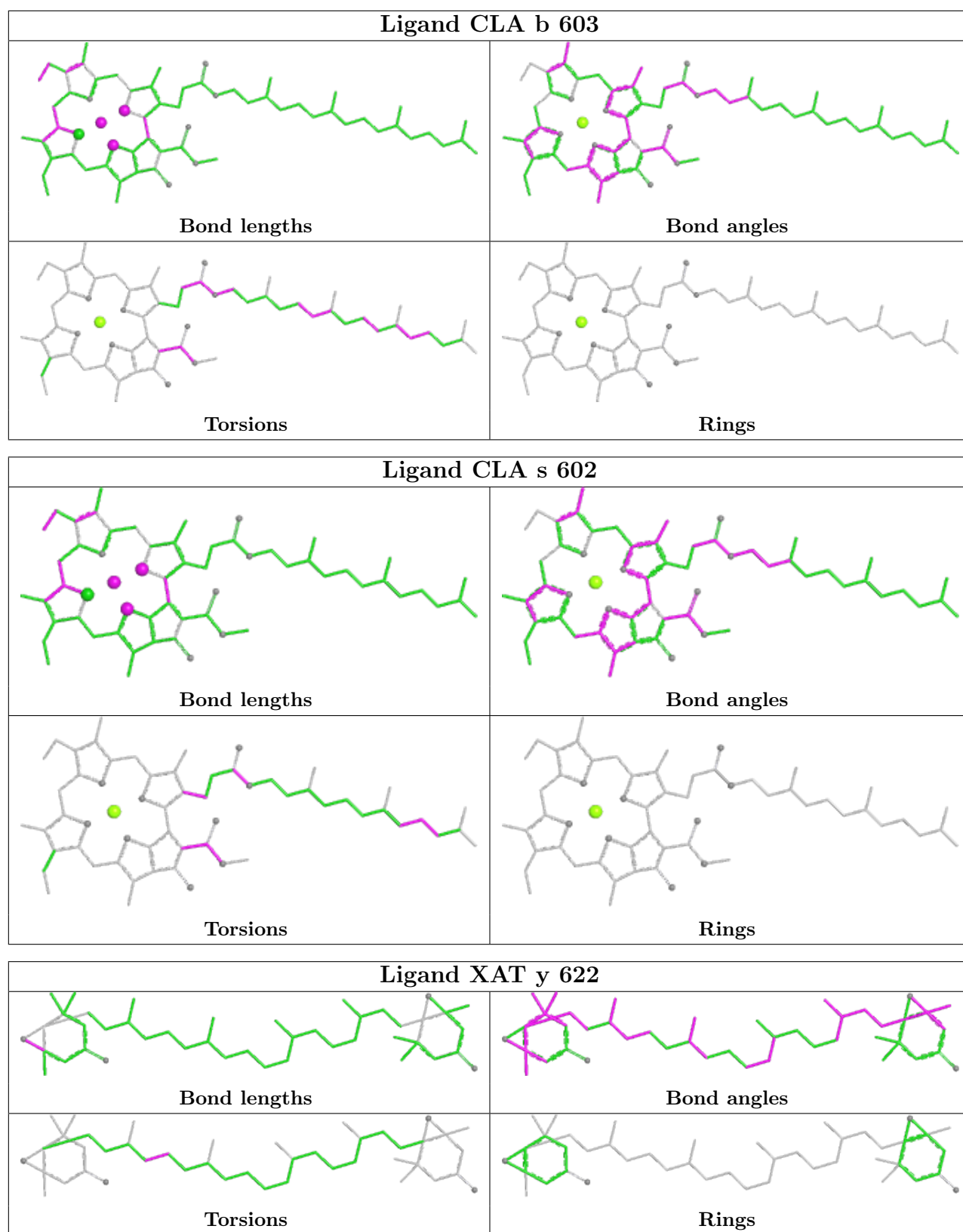


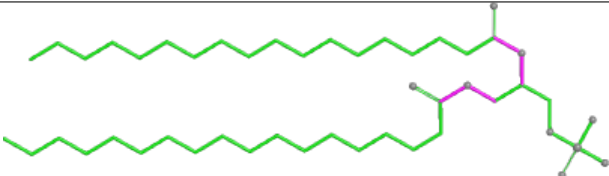

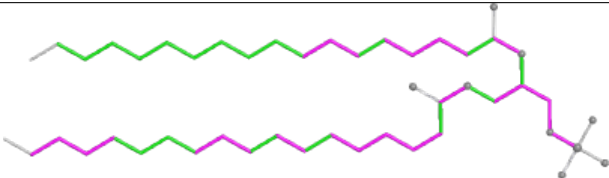
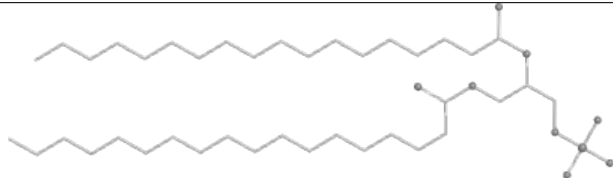
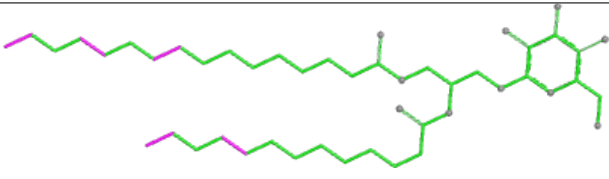
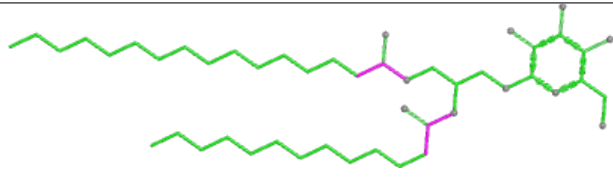
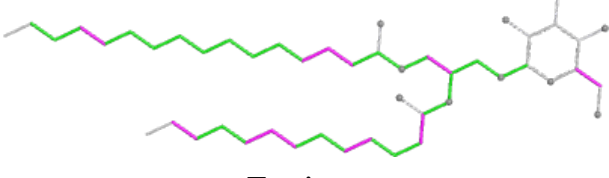
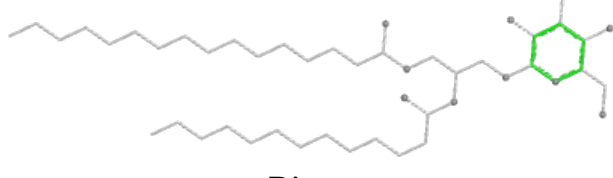
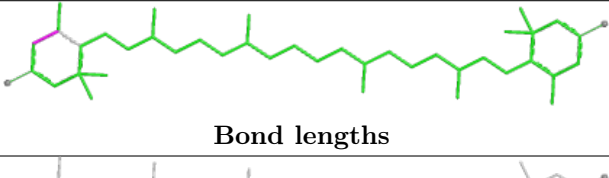
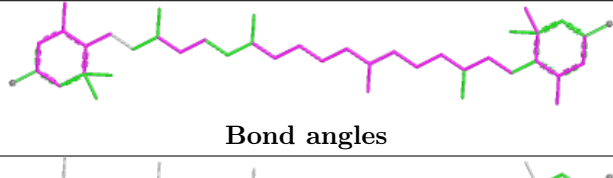




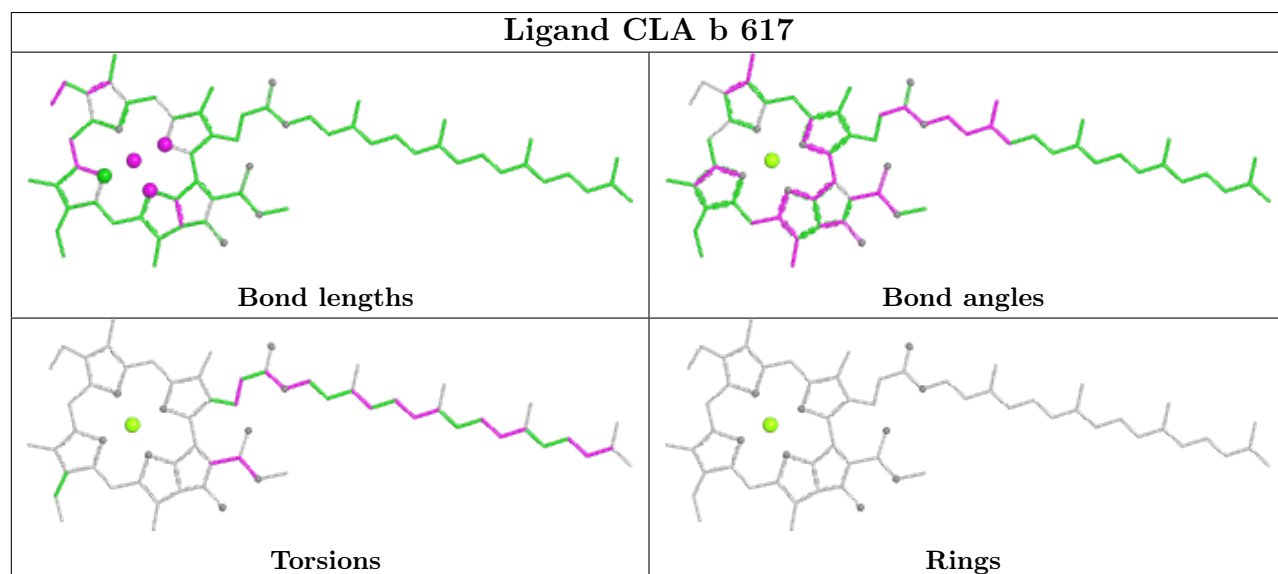
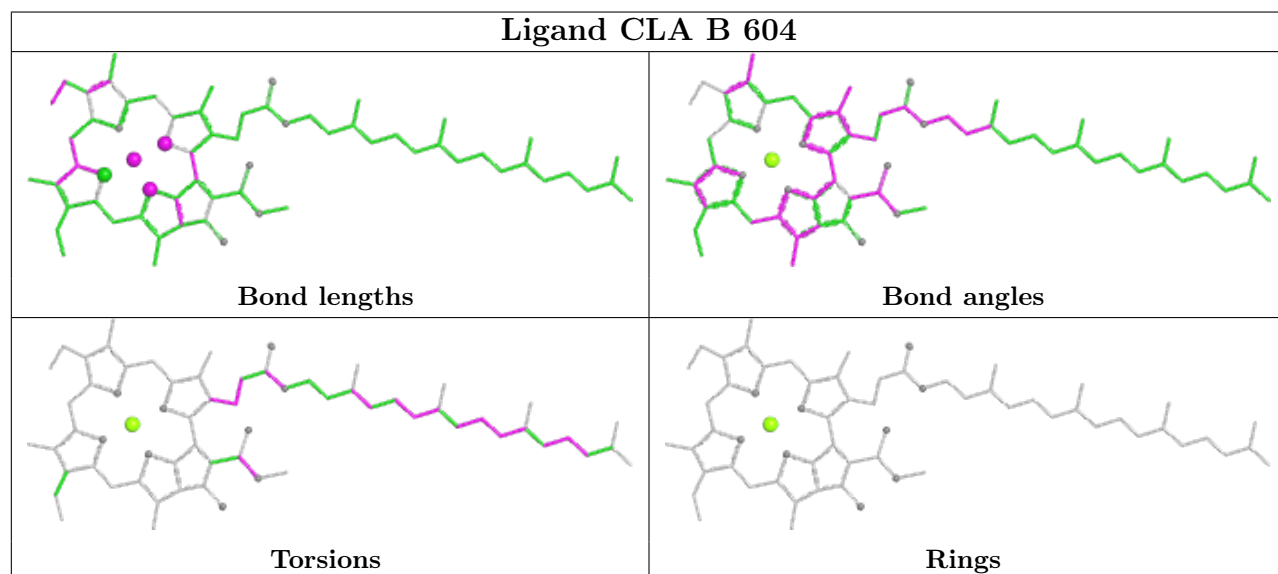
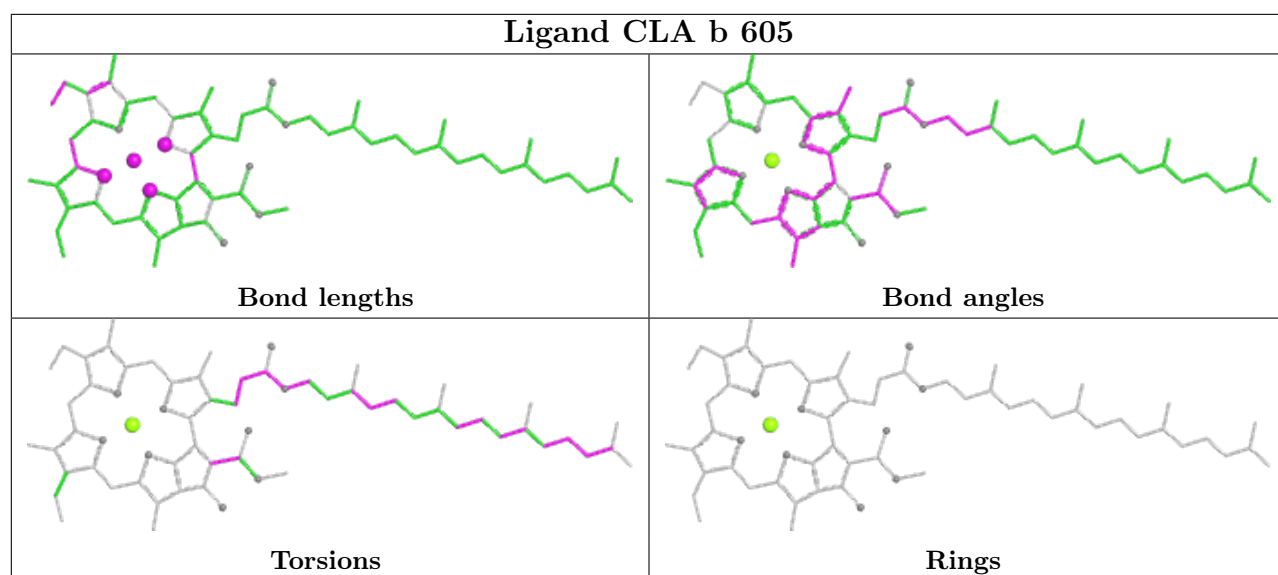


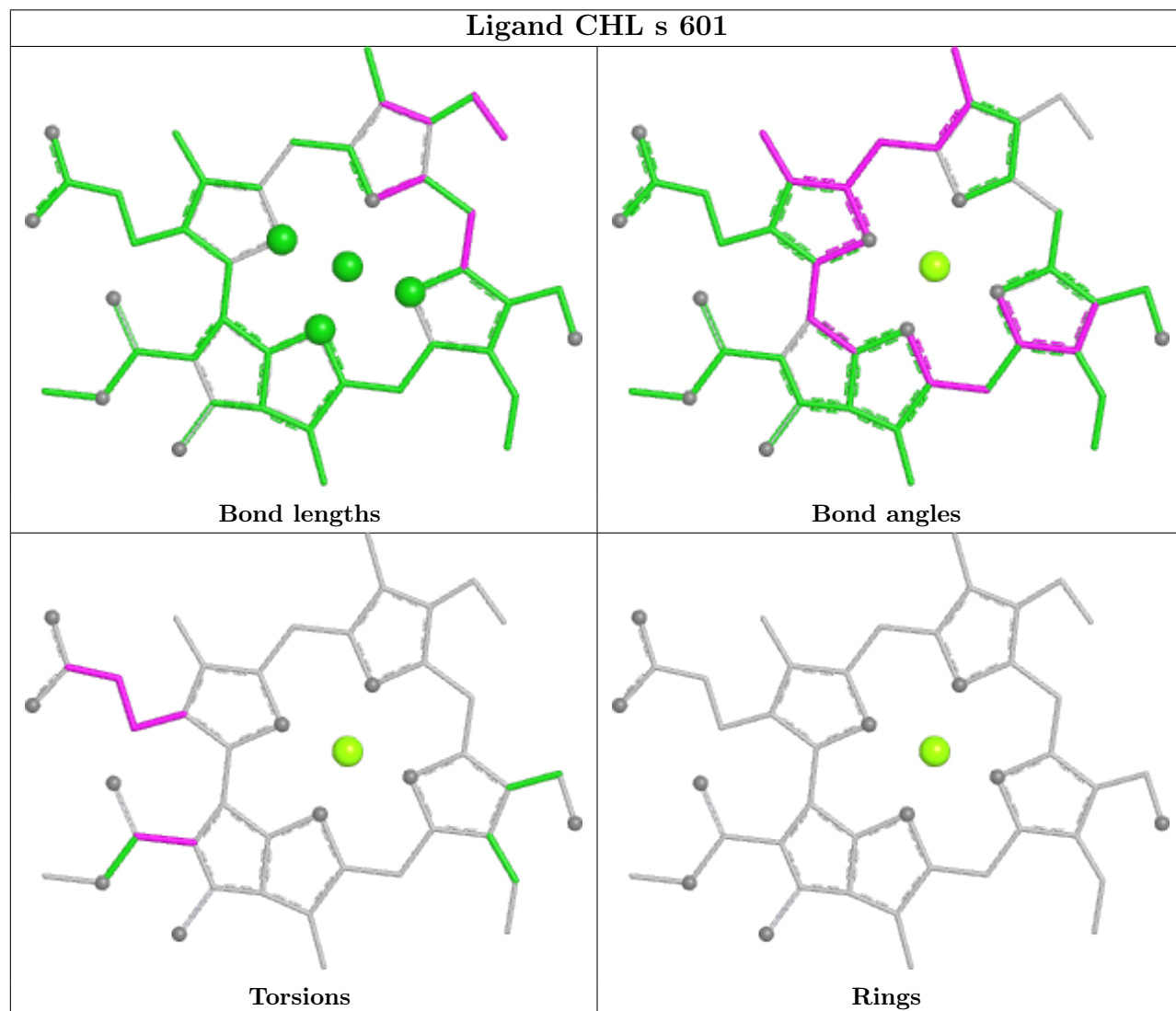
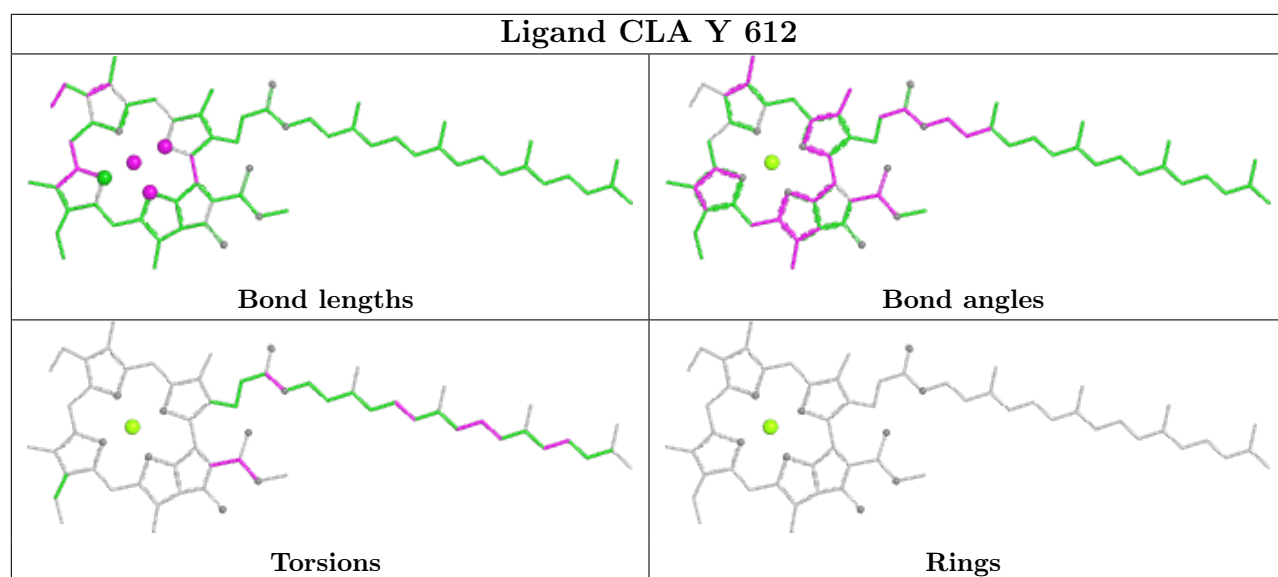


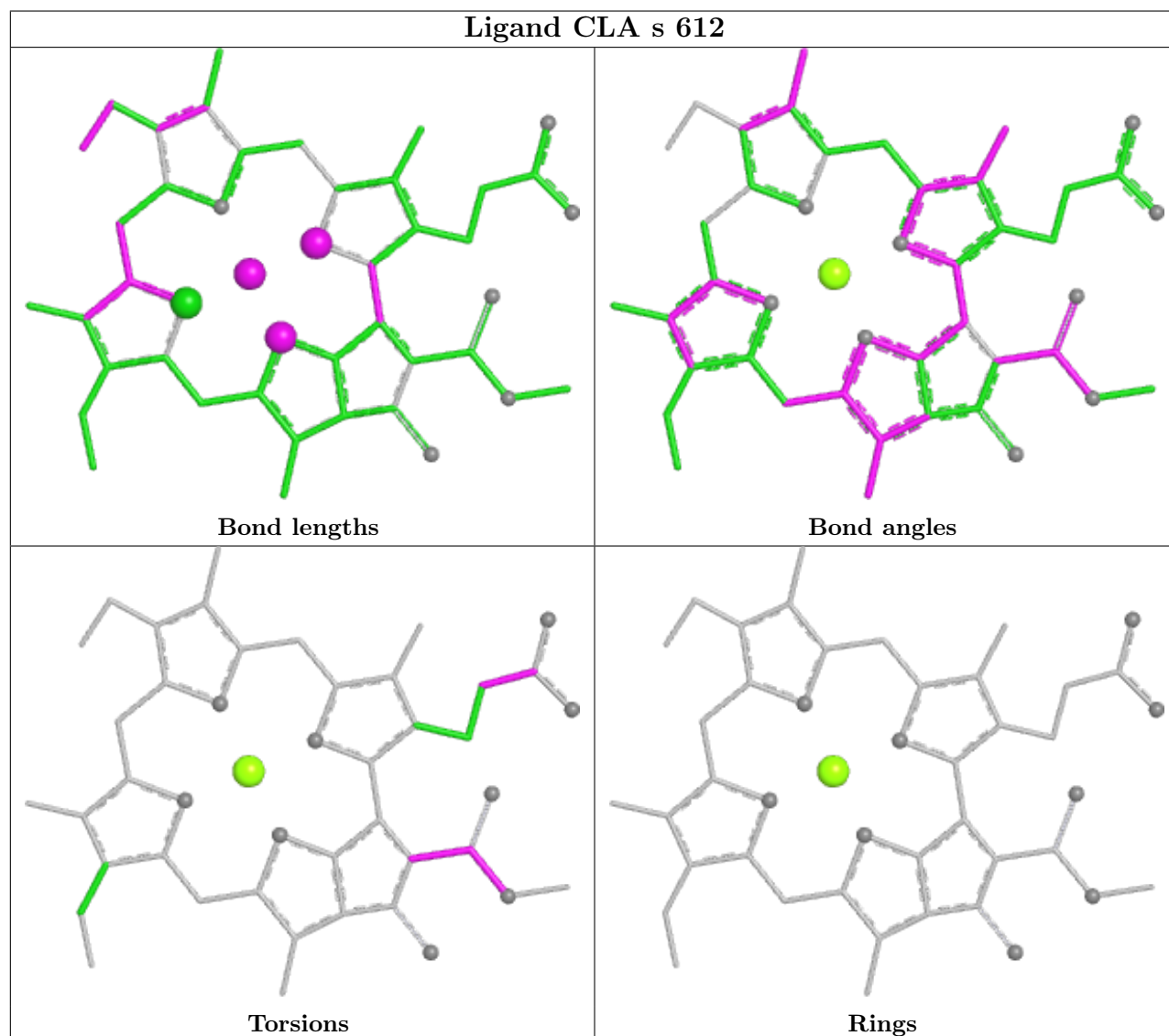
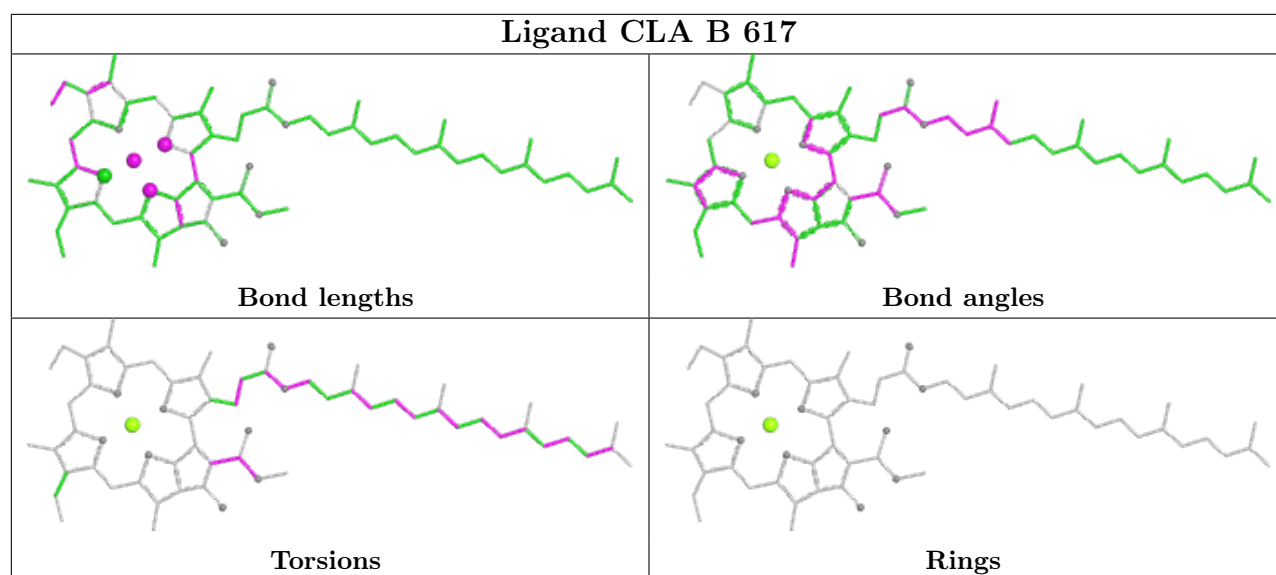


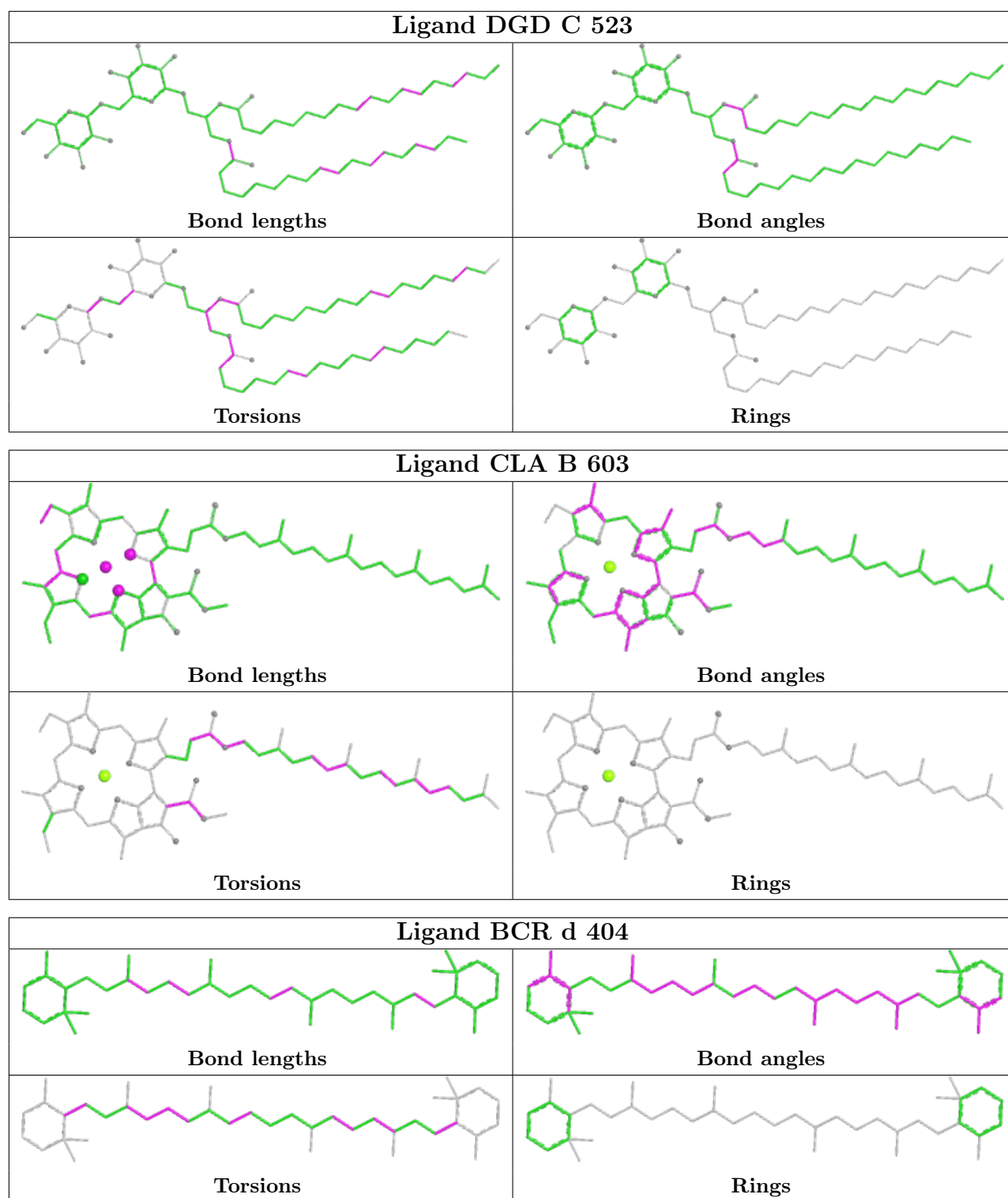


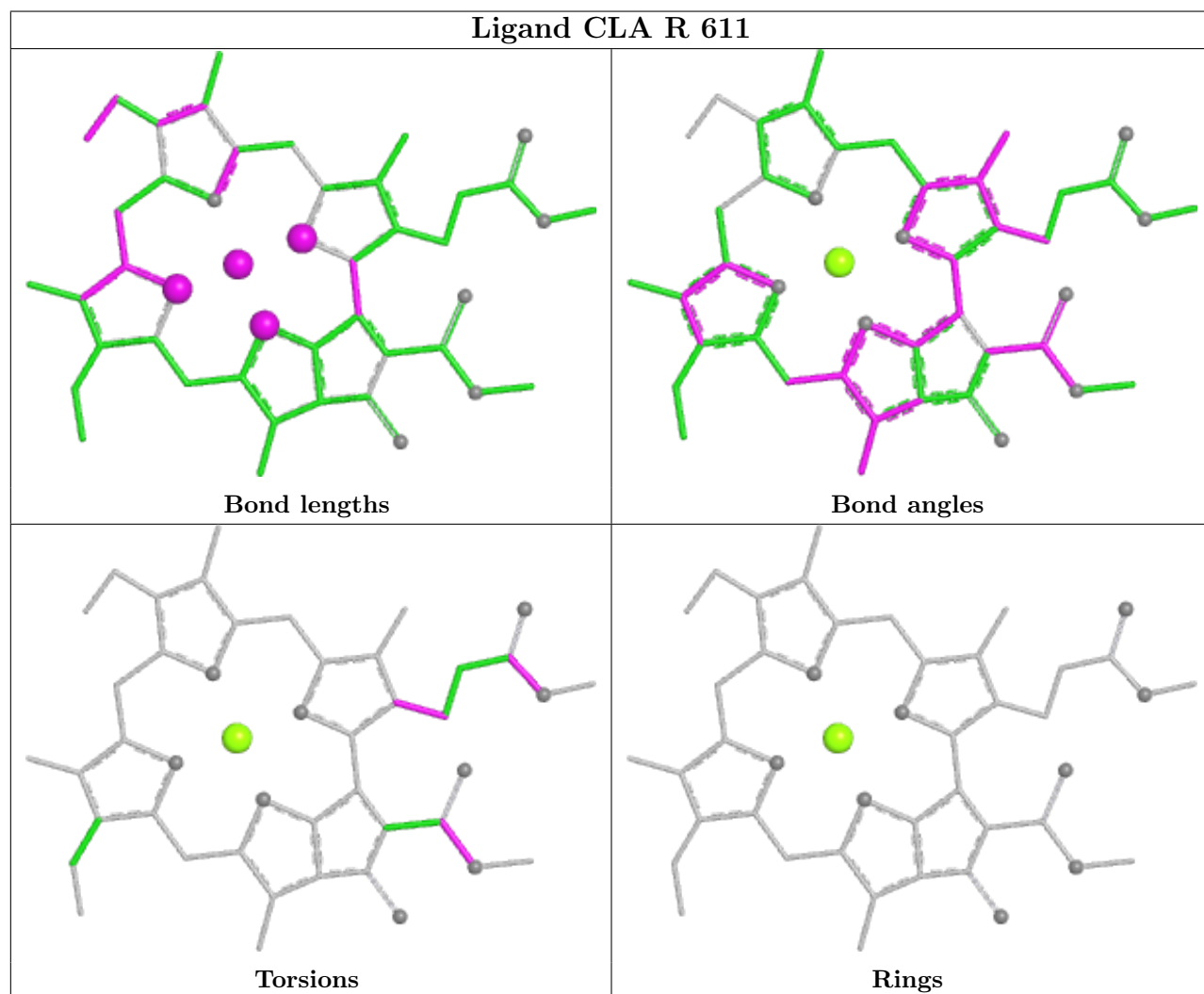
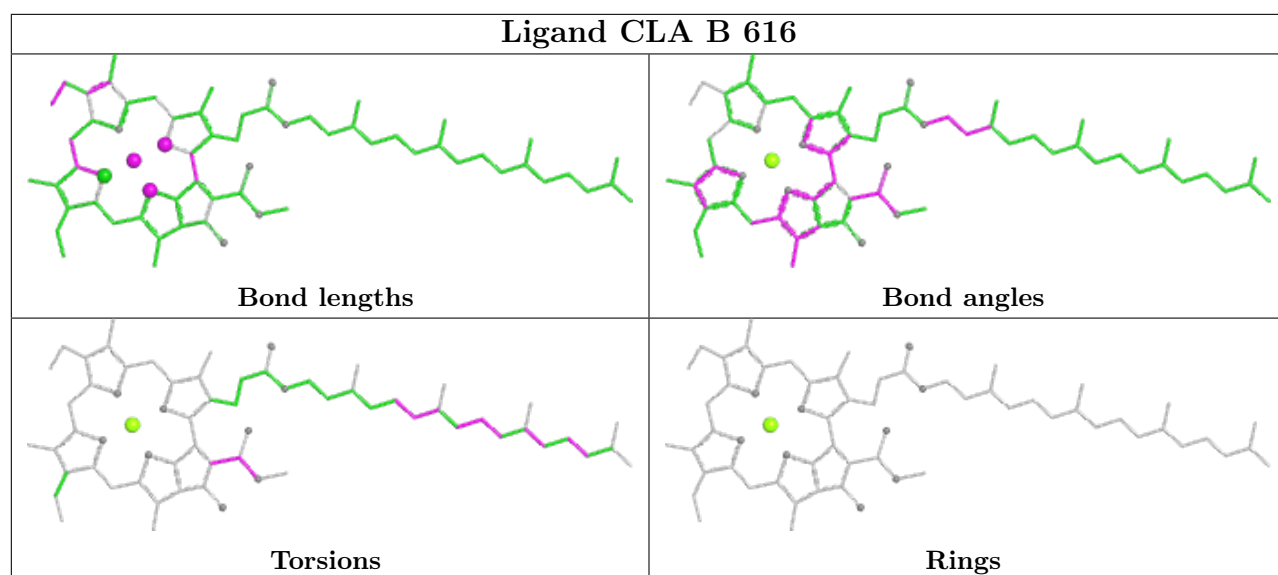
Ligand 3PH s 626	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG H 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

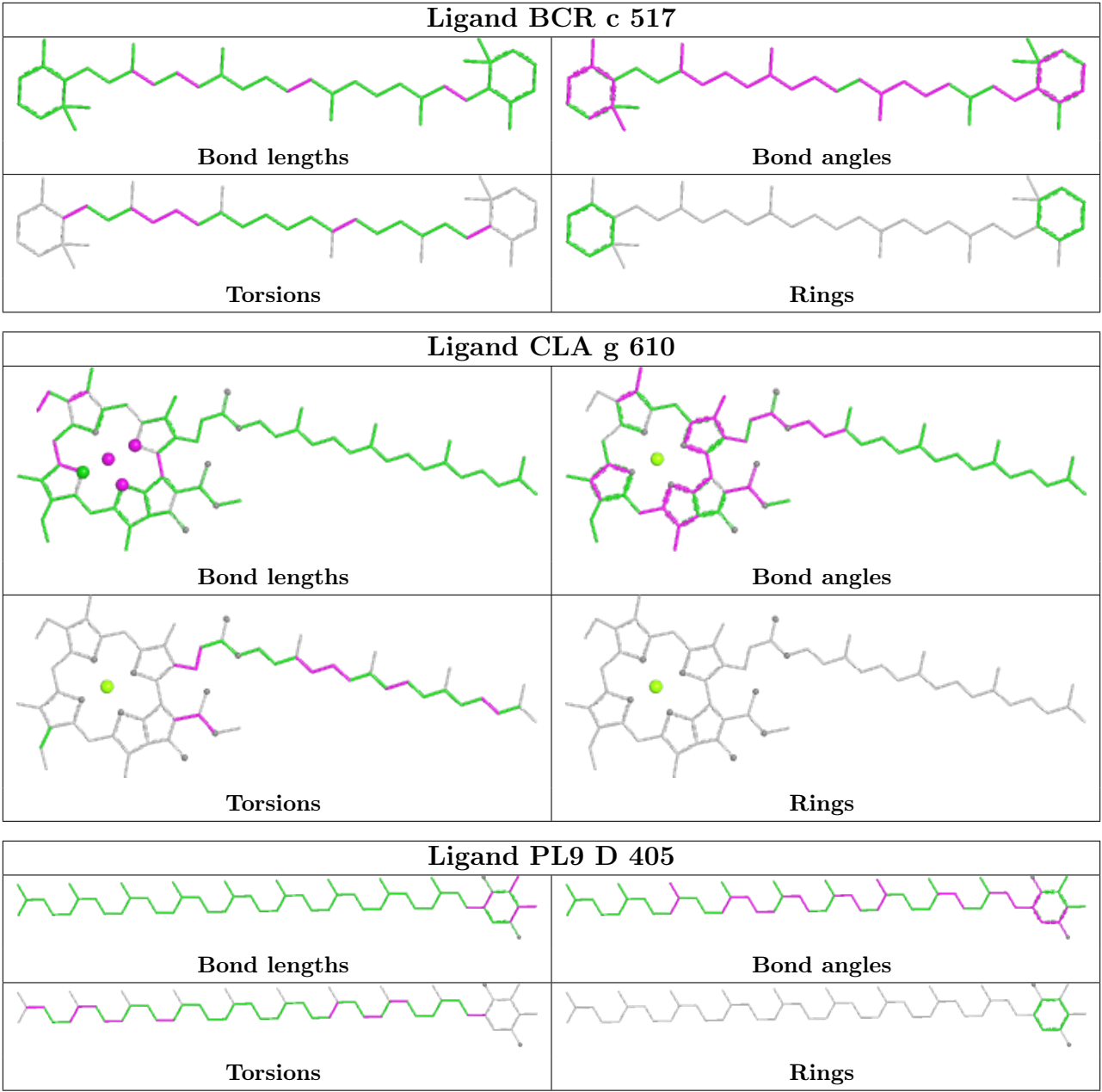












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	R	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
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

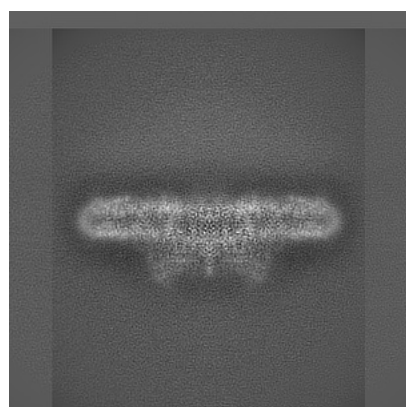
6 Map visualisation [i](#)

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.

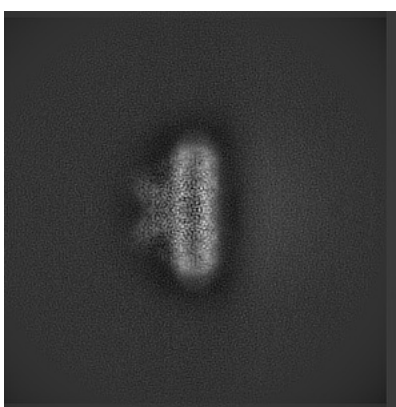
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

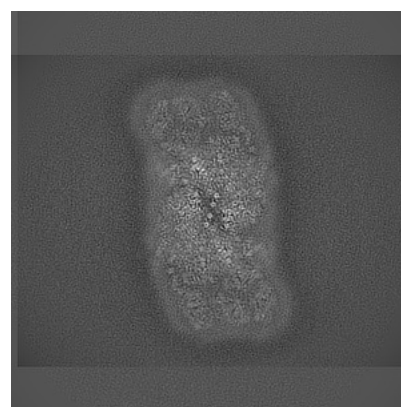
6.1.1 Primary map



X



Y

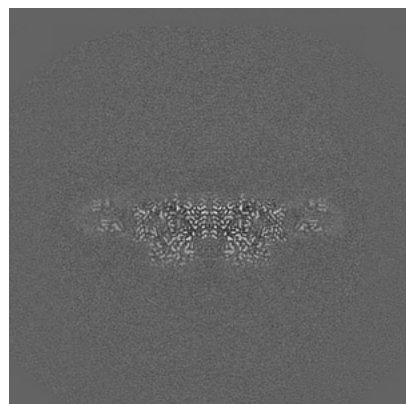


Z

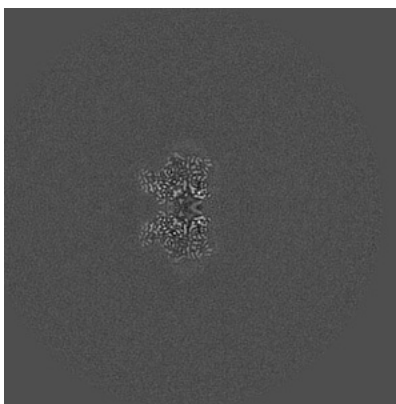
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

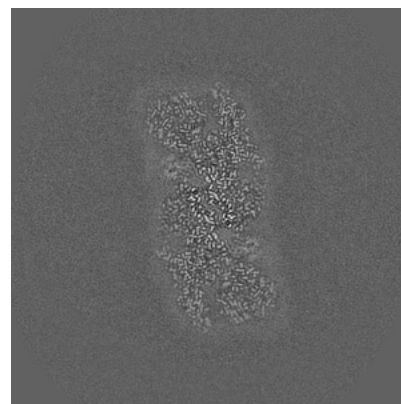
6.2.1 Primary map



X Index: 250



Y Index: 250

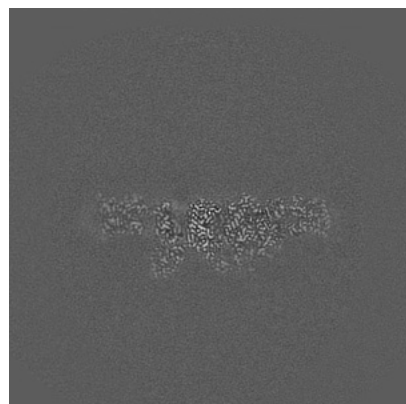


Z Index: 250

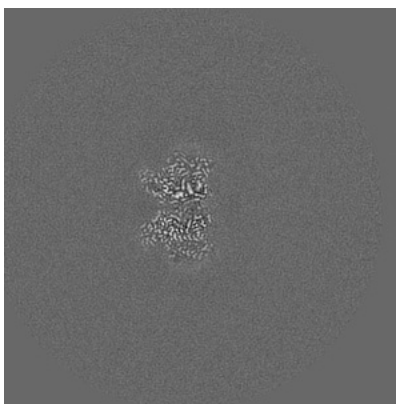
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

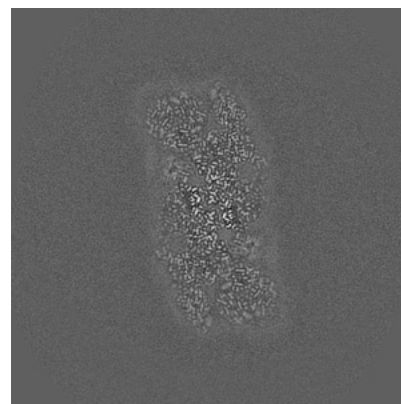
6.3.1 Primary map



X Index: 268



Y Index: 248

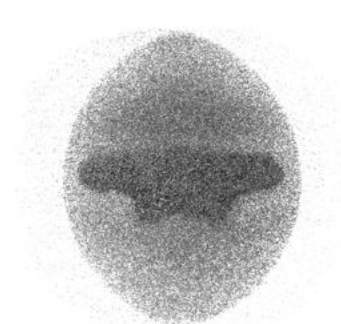


Z Index: 249

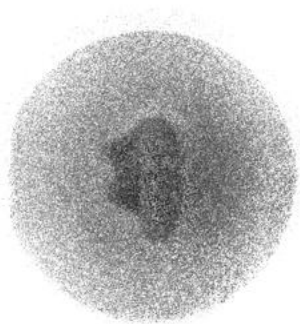
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

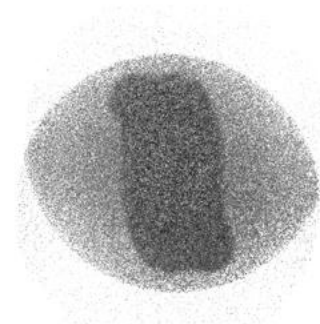
6.4.1 Primary map



X



Y



Z

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

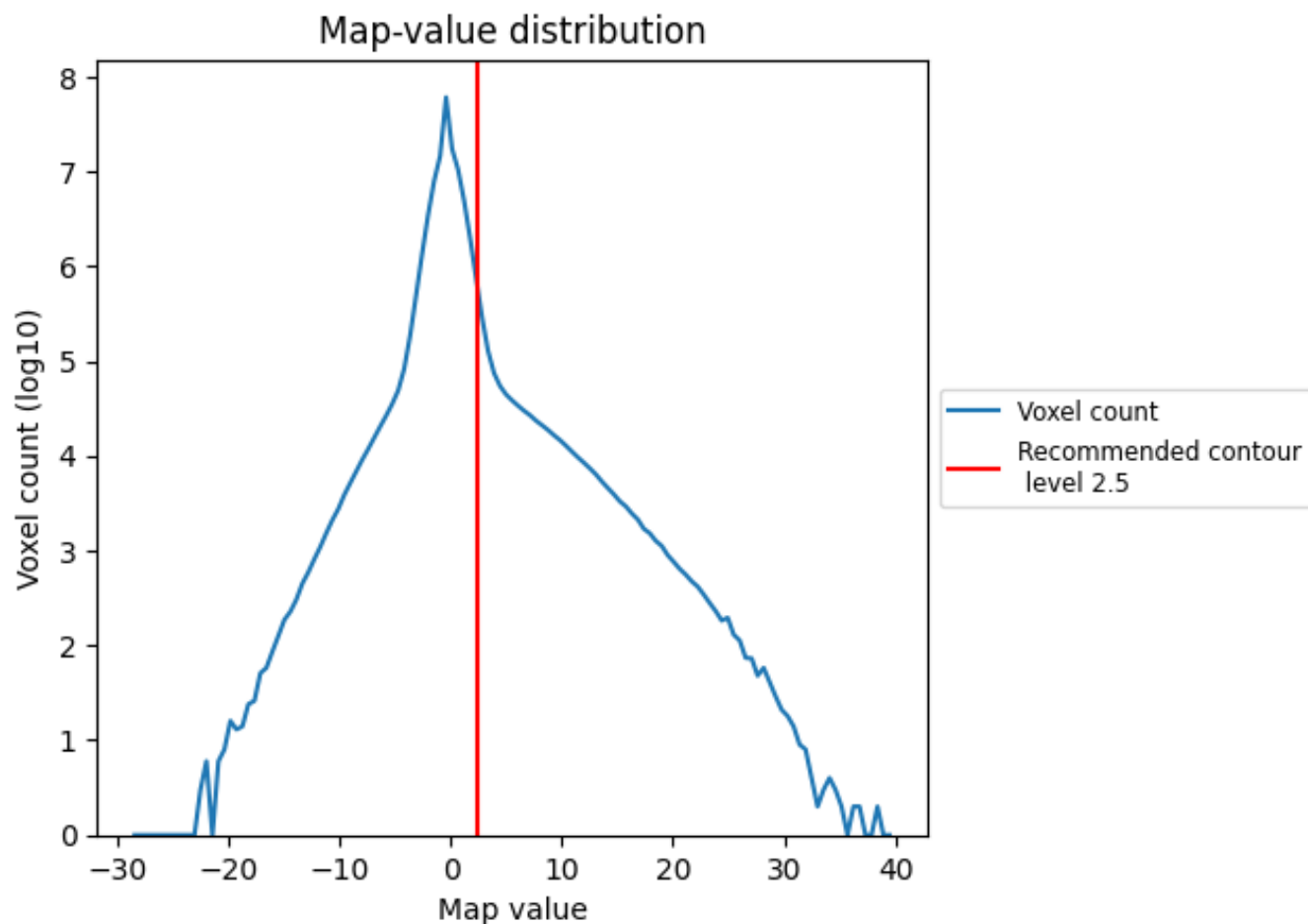
6.5 Mask visualisation

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

7 Map analysis [i](#)

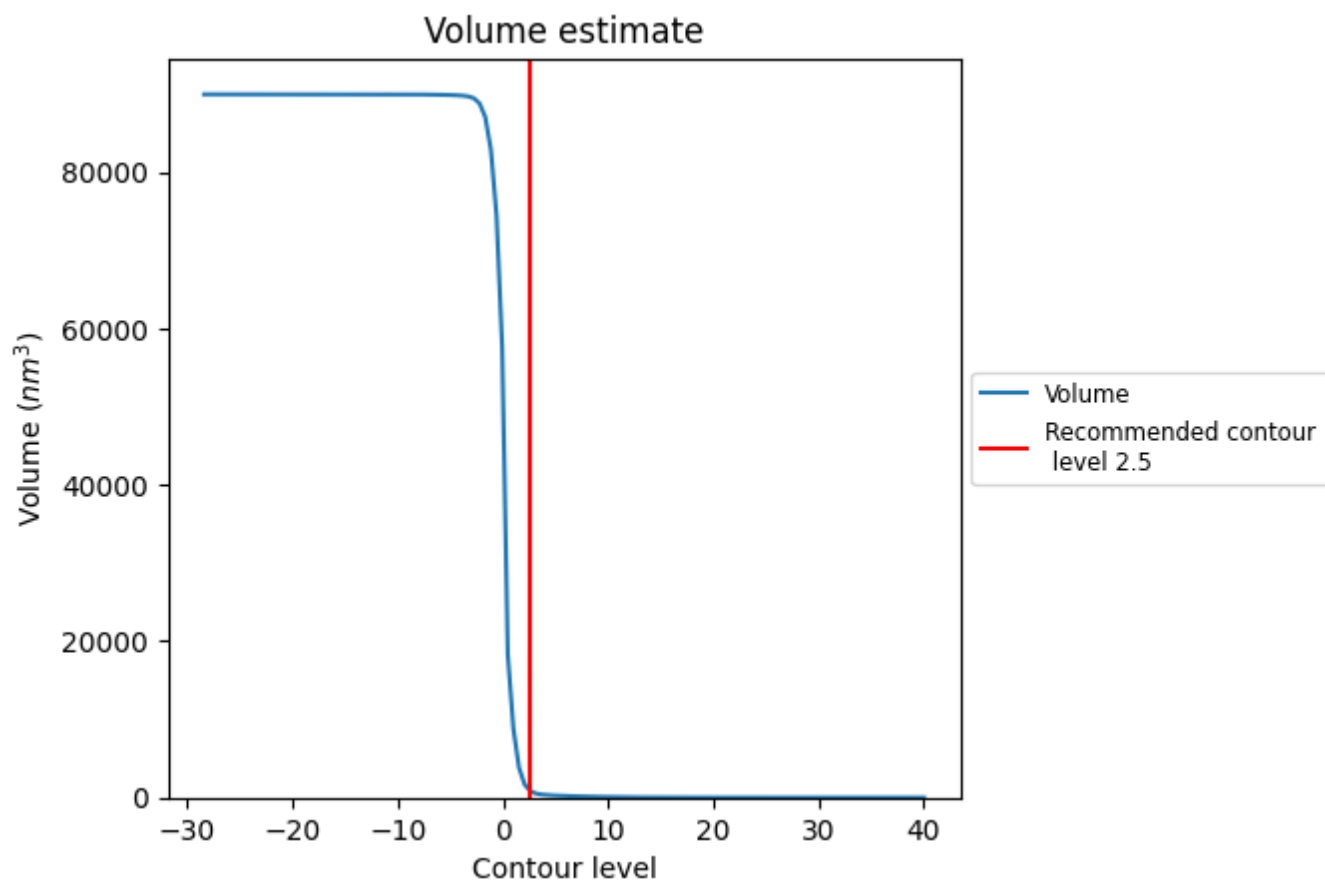
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

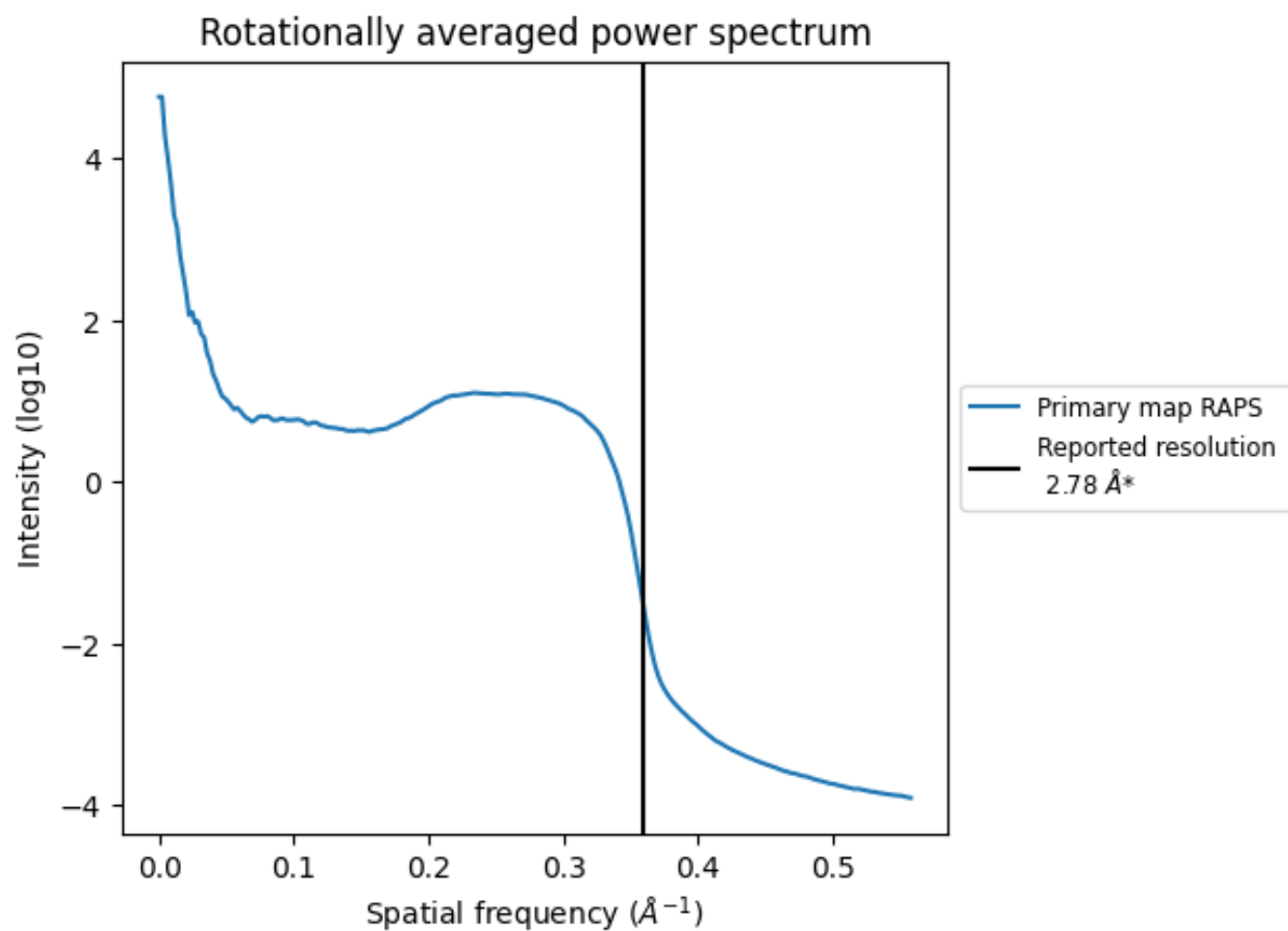
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 980 nm³; 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 ⓘ

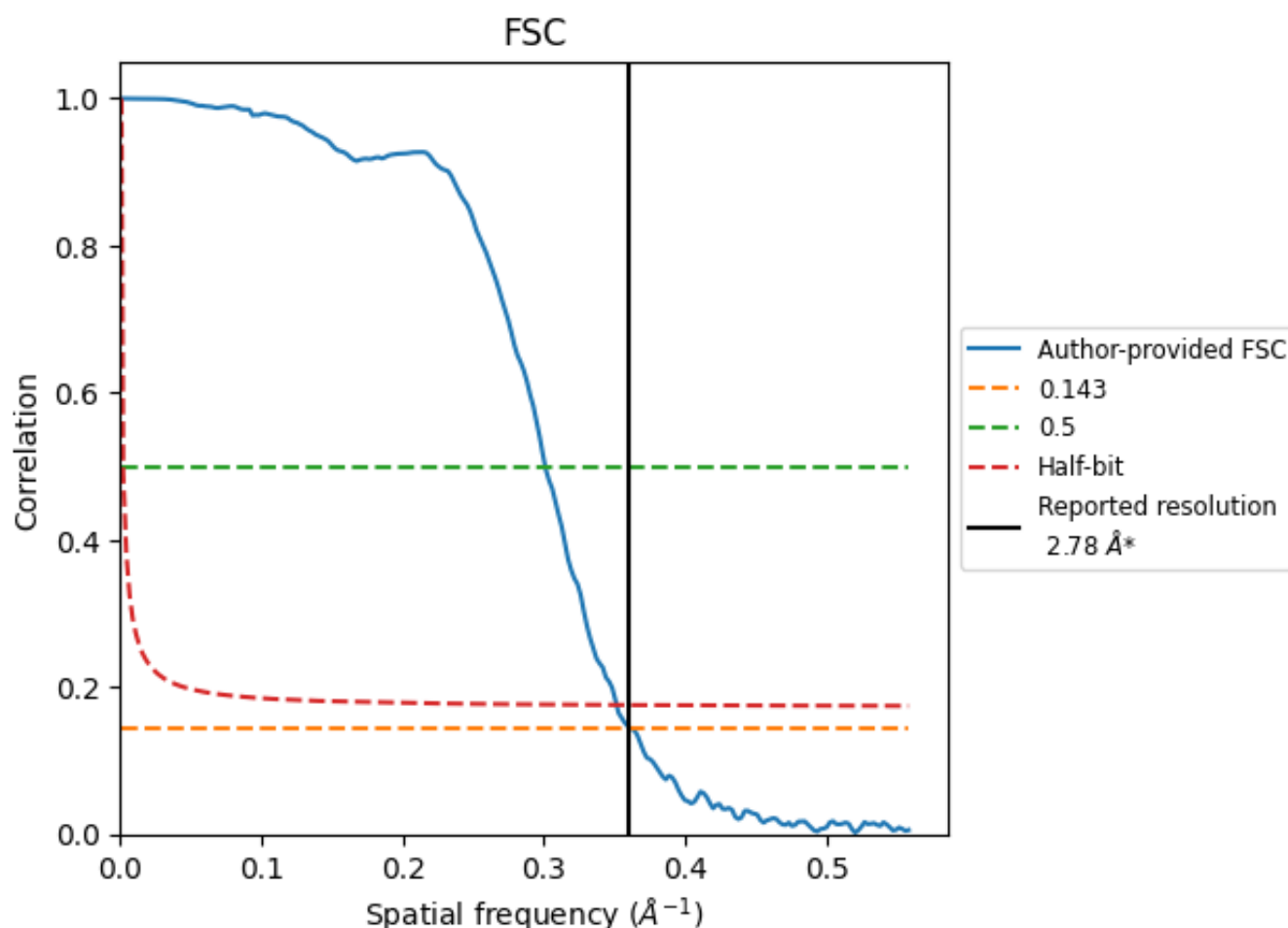


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

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](#)

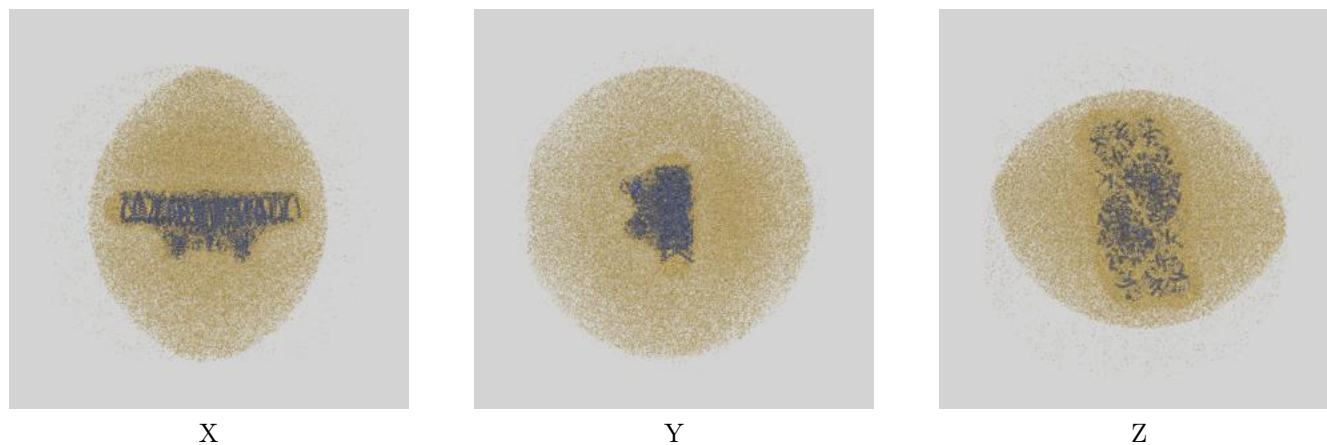
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.77	3.32	2.85
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

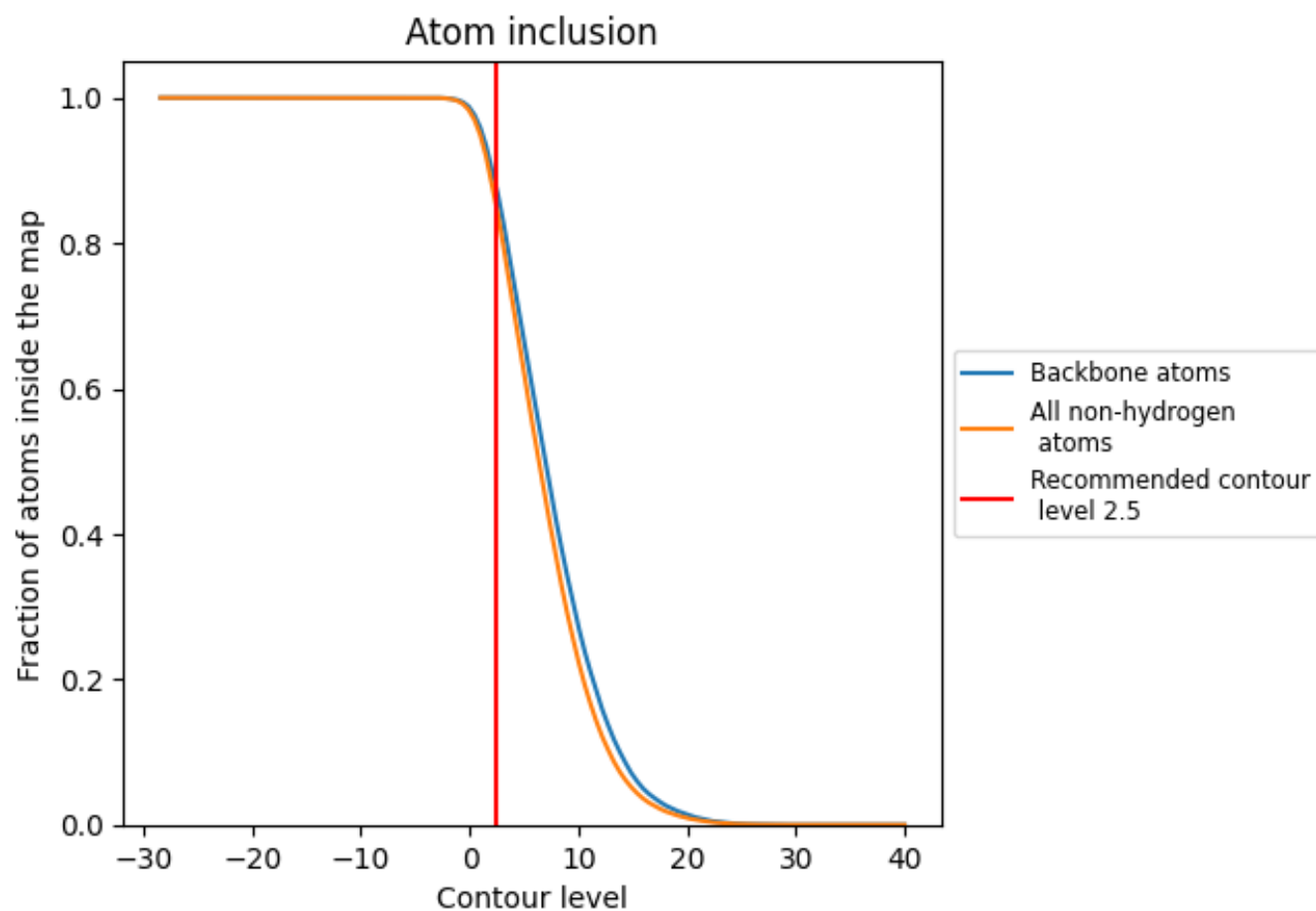
This section contains information regarding the fit between EMDB map EMD-13430 and PDB model 7PI5. Per-residue inclusion information can be found in section [3](#) on page [49](#).

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 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.