



wwPDB EM Validation Summary Report i

Feb 23, 2023 – 02:45 pm GMT

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 i 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](#) ①) were used in the production of this report:

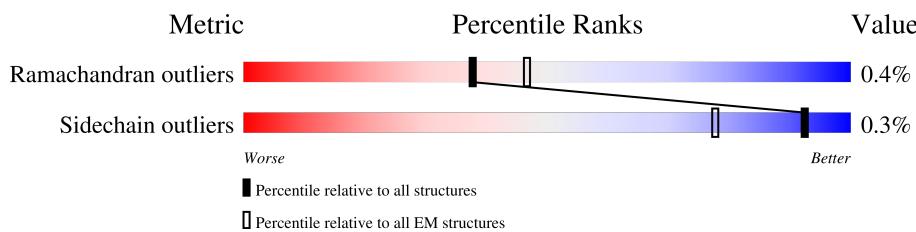
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance

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

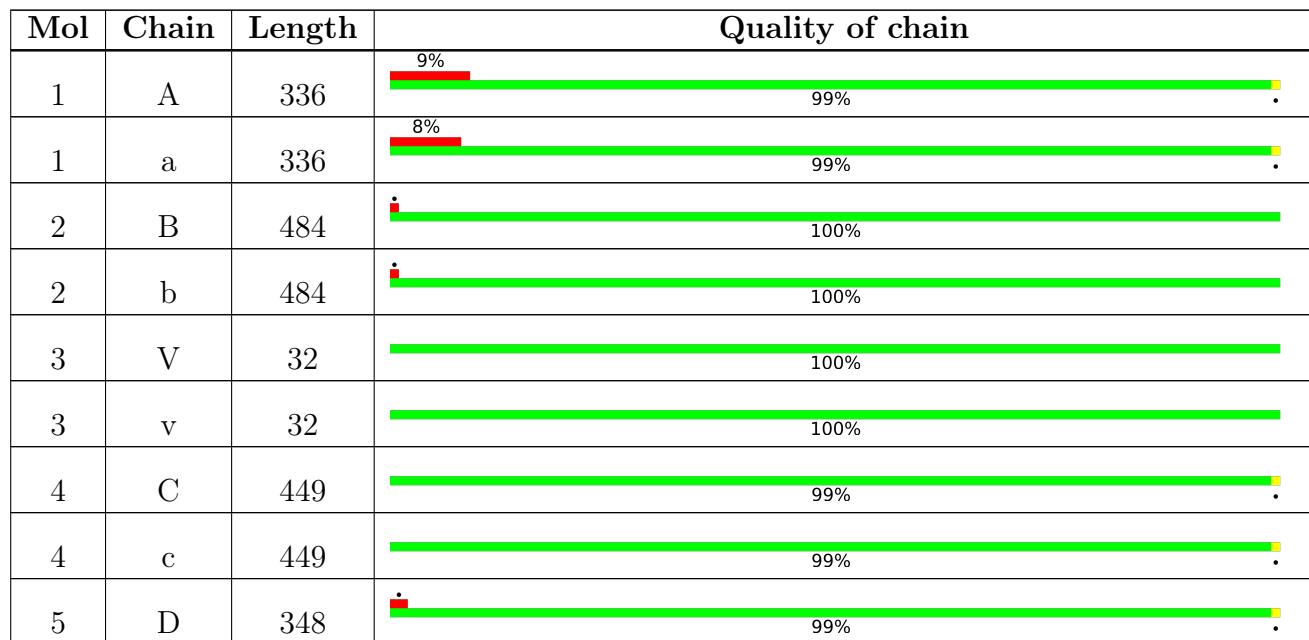
The reported resolution of this entry is 2.78 Å.

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.



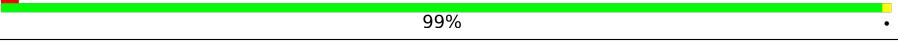
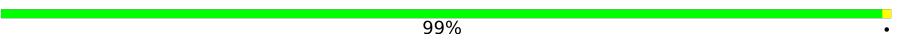
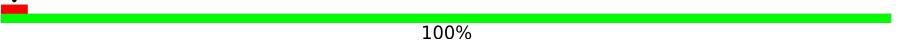
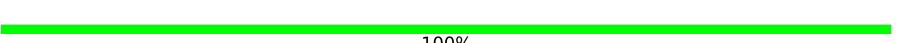
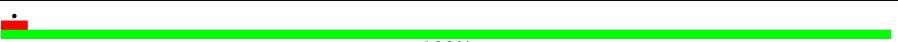
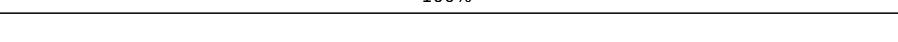
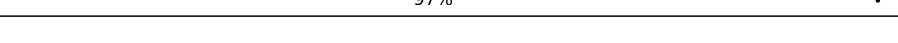
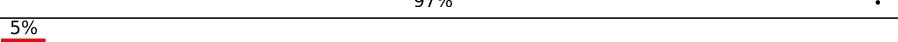
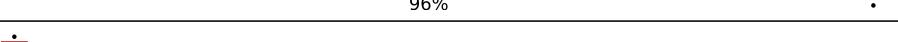
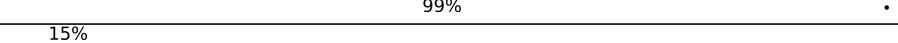
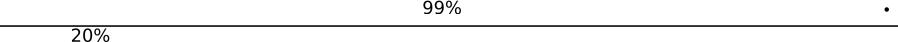
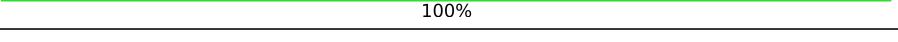
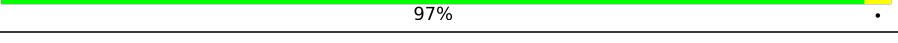
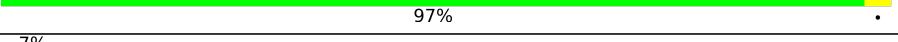
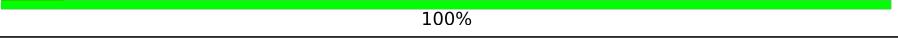
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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.



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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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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 [\(i\)](#)

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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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			

Mol	Chain	Residues	Atoms					AltConf	Trace
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	S	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total	C	N	O	S	0	0

- 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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

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

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 457 312 68 76 1	0	0
19	z	61	Total C N O S 457 312 68 76 1	0	0

- Molecule 20 is a protein called LHCII M3.

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

- 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 1680 1085 271 321 3	0	0
21	g	221	Total C N O S 1680 1085 271 321 3	0	0

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:

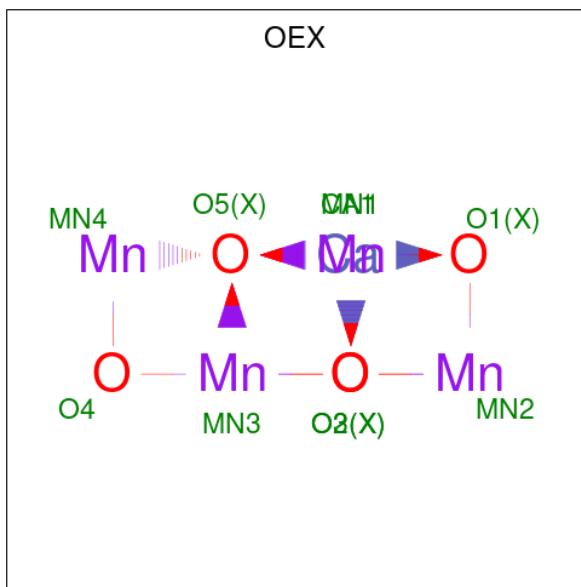
Chain	Residue	Modelled	Actual	Comment	Reference
Y	49	PHE	TYR	conflict	UNP A0A6S8N9J6
Y	52	SER	ALA	conflict	UNP A0A6S8N9J6
Y	73	THR	SER	conflict	UNP A0A6S8N9J6
Y	81	THR	ASN	conflict	UNP A0A6S8N9J6
Y	123	ILE	VAL	conflict	UNP A0A6S8N9J6
Y	220	LEU	PHE	conflict	UNP A0A6S8N9J6
Y	235	GLN	THR	conflict	UNP A0A6S8N9J6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

Mol	Chain	Residues	Atoms					AltConf	Trace
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: CaMn₄O₅).



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

Mol	Chain	Residues	Atoms				AltConf
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			

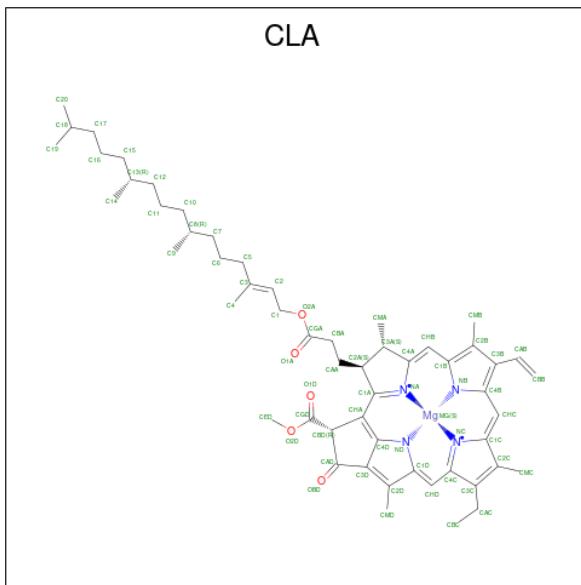
Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	Fe			0
			1	1			

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

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

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

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



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

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Mol	Chain	Residues	Atoms					AltConf
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0

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

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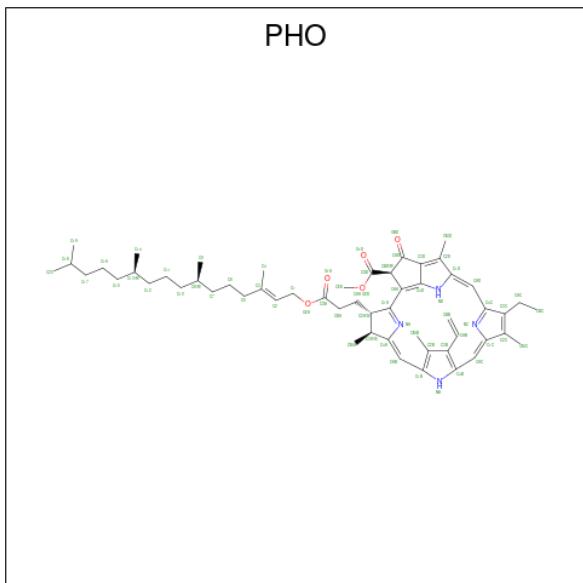
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0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

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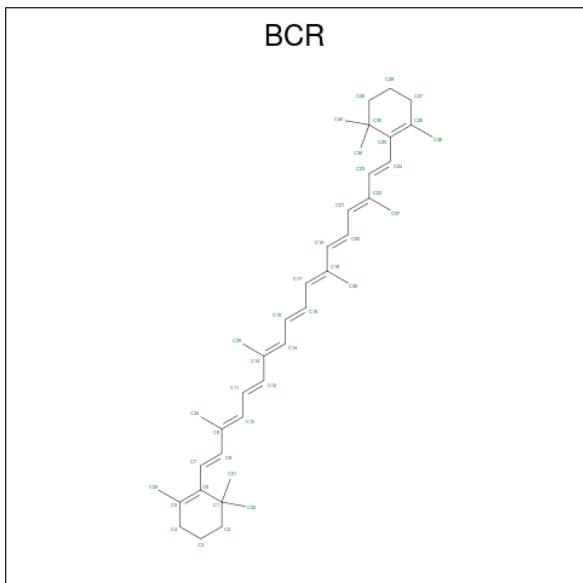
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0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

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



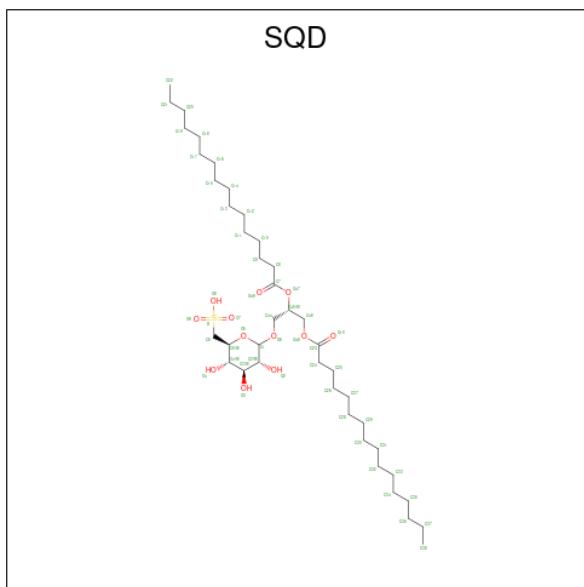
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total 64	C 55	N 4	O 5	0
30	A	1	Total 64	C 55	N 4	O 5	0
30	a	1	Total 64	C 55	N 4	O 5	0
30	a	1	Total 64	C 55	N 4	O 5	0

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



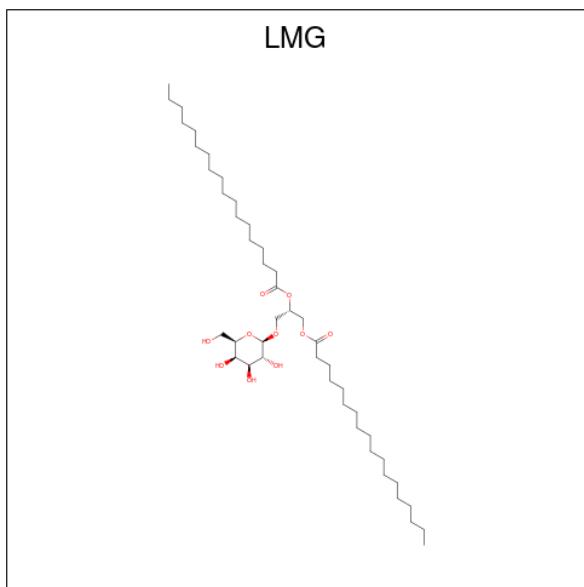
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C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

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (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).

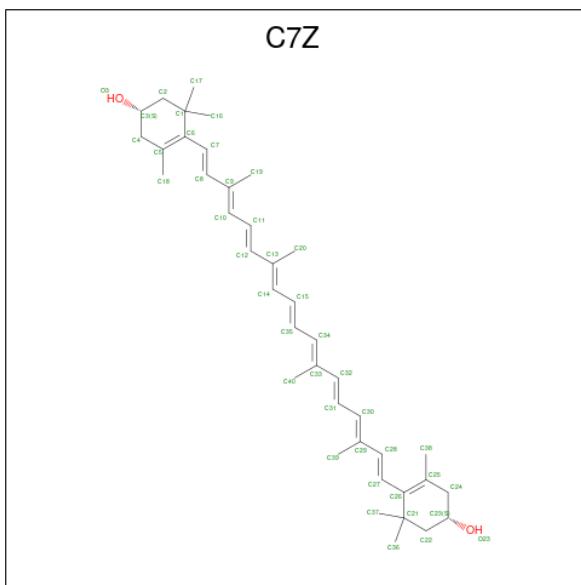


Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			44	34	10	
33	C	1	Total	C	O	0
			51	41	10	
33	D	1	Total	C	O	0
			46	36	10	
33	H	1	Total	C	O	0
			48	38	10	
33	J	1	Total	C	O	0
			45	35	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			44	34	10	
33	c	1	Total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

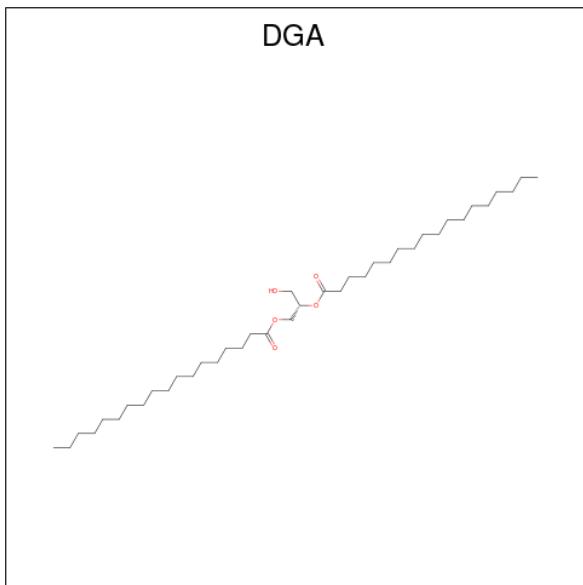
Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total Na		0
34	a	1	Total Na		0

- 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: C₄₀H₅₆O₂).



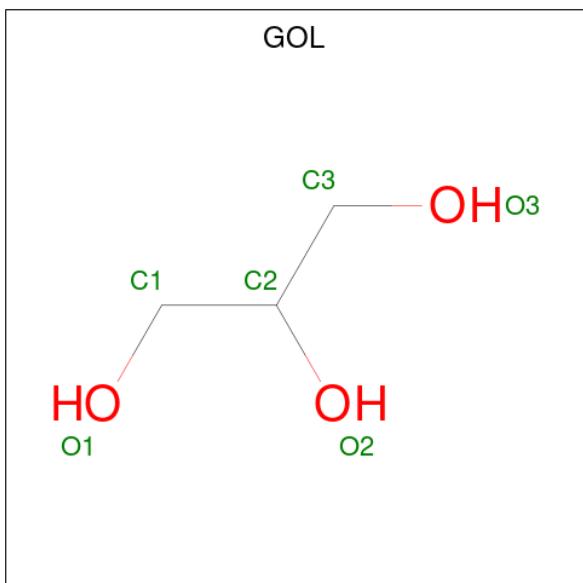
Mol	Chain	Residues	Atoms		AltConf
35	B	1	Total C O		0
35	b	1	Total C O		0

- Molecule 36 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



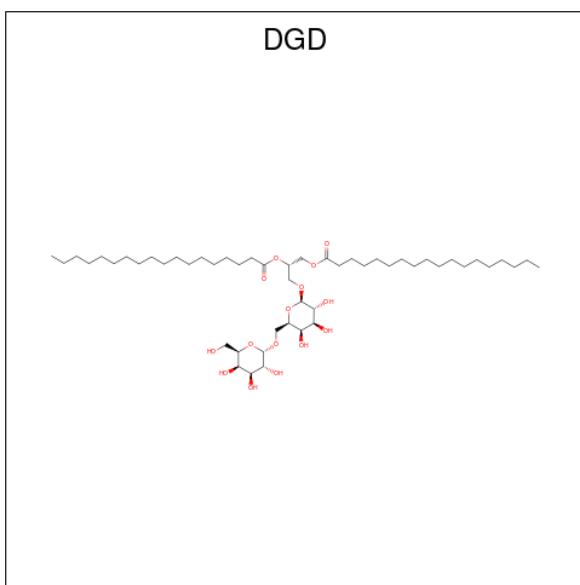
Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total C O 44 39 5	0
36	C	1	Total C O 44 39 5	0
36	b	1	Total C O 44 39 5	0
36	c	1	Total C O 44 39 5	0

- Molecule 37 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



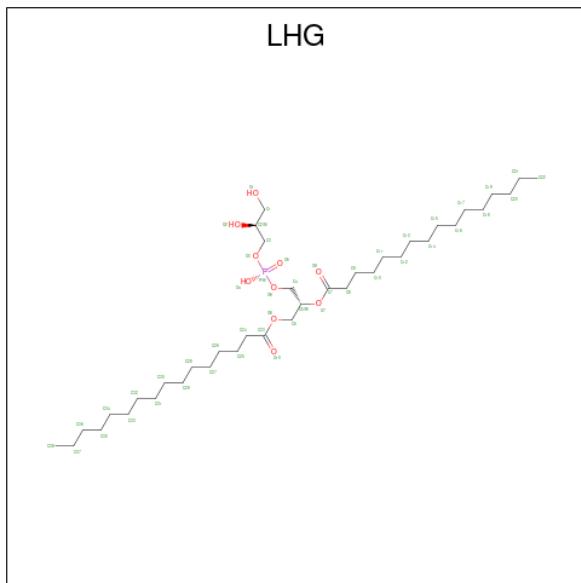
Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			62	47	15	
38	C	1	Total	C	O	0
			59	44	15	
38	C	1	Total	C	O	0
			66	51	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			59	44	15	

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

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



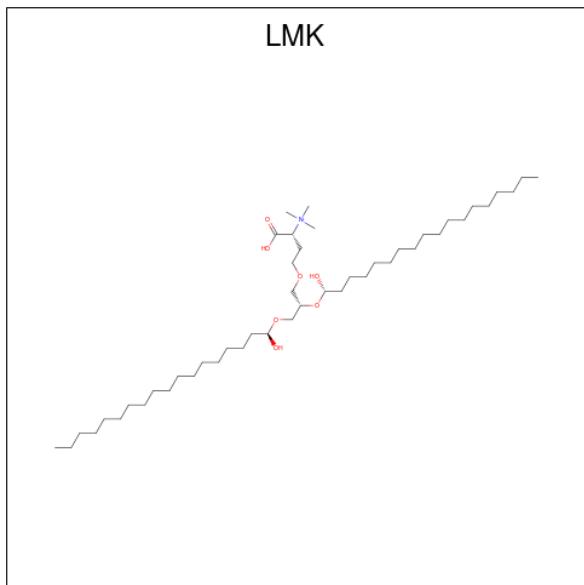
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	P	0
			47	36	10	1	
39	D	1	Total	C	O	P	0
			44	33	10	1	
39	D	1	Total	C	O	P	0
			49	38	10	1	
39	D	1	Total	C	O	P	0
			39	28	10	1	
39	L	1	Total	C	O	P	0
			49	38	10	1	
39	N	1	Total	C	O	P	0
			49	38	10	1	
39	G	1	Total	C	O	P	0
			49	38	10	1	
39	S	1	Total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

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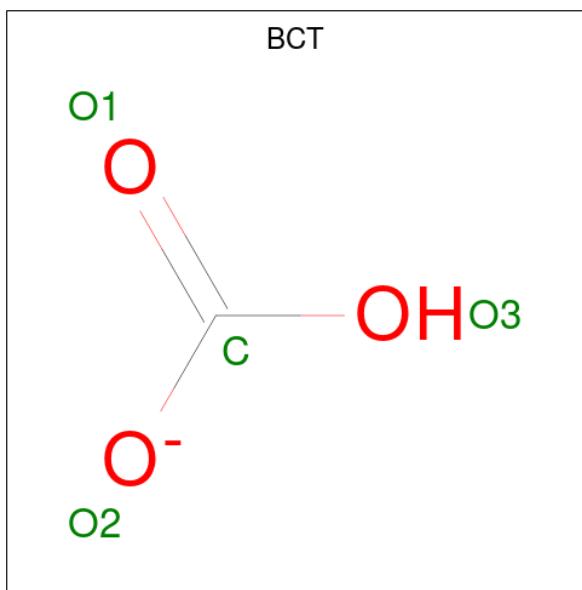
Mol	Chain	Residues	Atoms				AltConf
39	d	1	Total	C	O	P	0
			44	33	10	1	
39	d	1	Total	C	O	P	0
			49	38	10	1	
39	d	1	Total	C	O	P	0
			39	28	10	1	
39	l	1	Total	C	O	P	0
			49	38	10	1	
39	n	1	Total	C	O	P	0
			49	38	10	1	
39	g	1	Total	C	O	P	0
			49	38	10	1	
39	s	1	Total	C	O	P	0
			45	34	10	1	
39	y	1	Total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

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



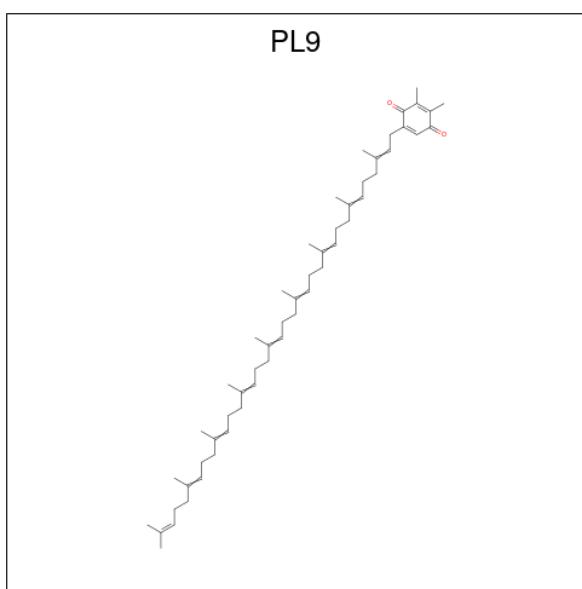
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			40	32	1	7	
40	c	1	Total	C	N	O	0
			40	32	1	7	

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



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

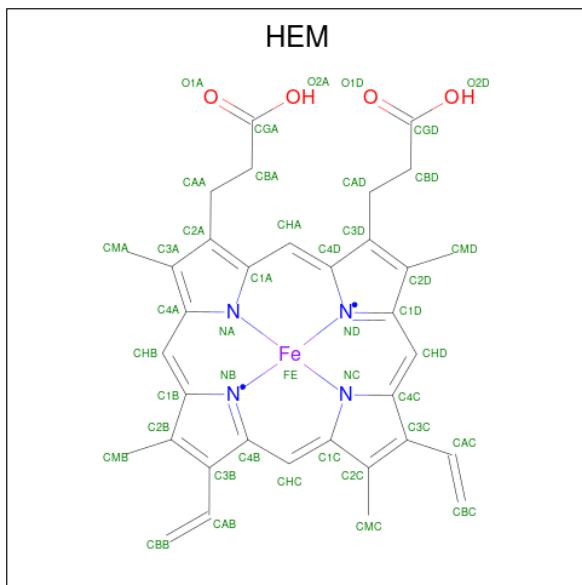
- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

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

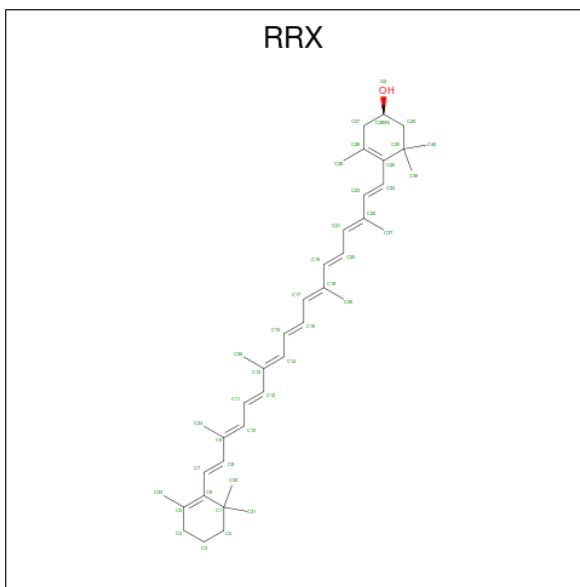
- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

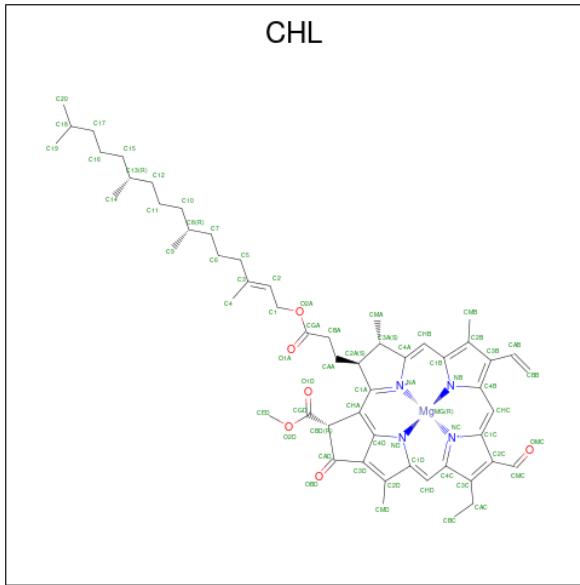
Mol	Chain	Residues	Atoms					AltConf
43	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



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

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



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

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

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

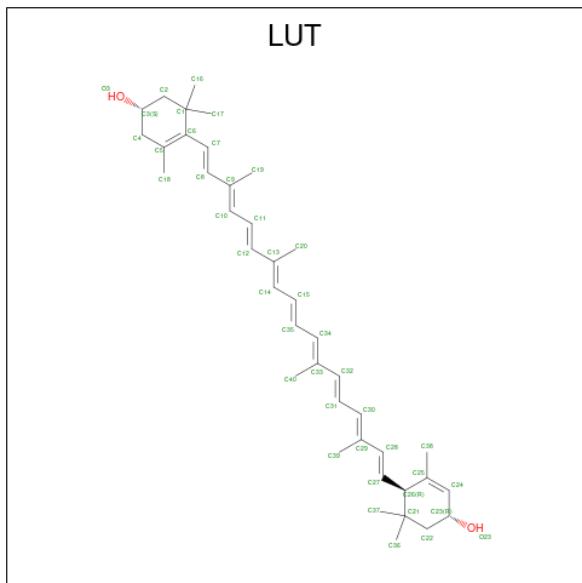
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Mol	Chain	Residues	Atoms					AltConf
45	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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

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



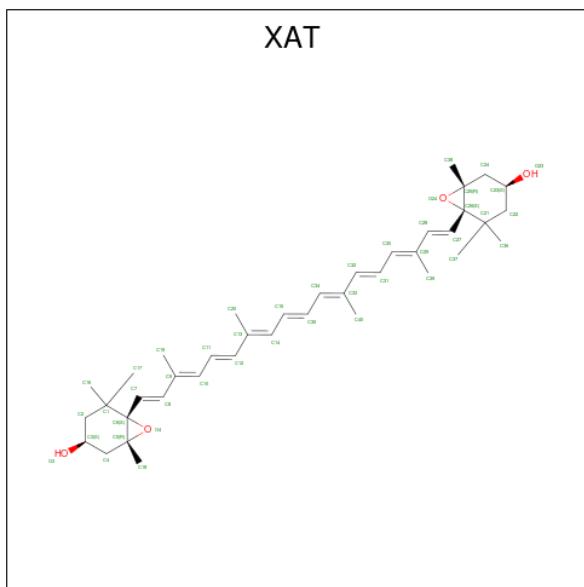
Mol	Chain	Residues	Atoms			AltConf
46	N	1	Total	C	O	0
			42	40	2	
46	N	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	R	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0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

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

- 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).



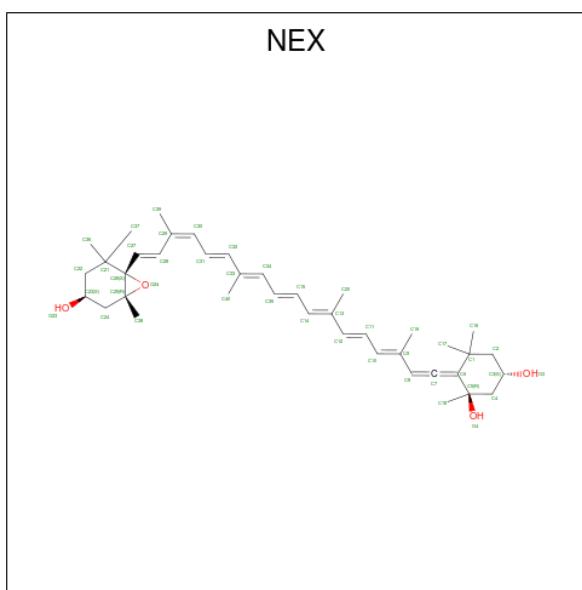
Mol	Chain	Residues	Atoms	AltConf
47	N	1	Total C O 44 40 4	0
47	G	1	Total C O 44 40 4	0

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

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



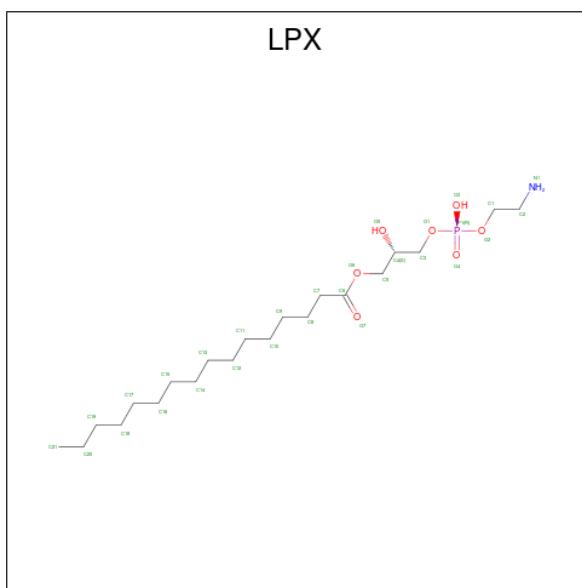
Mol	Chain	Residues	Atoms	AltConf
48	N	1	Total C O 44 40 4	0
48	G	1	Total C O 44 40 4	0
48	R	1	Total C O 44 40 4	0
48	S	1	Total C O 44 40 4	0

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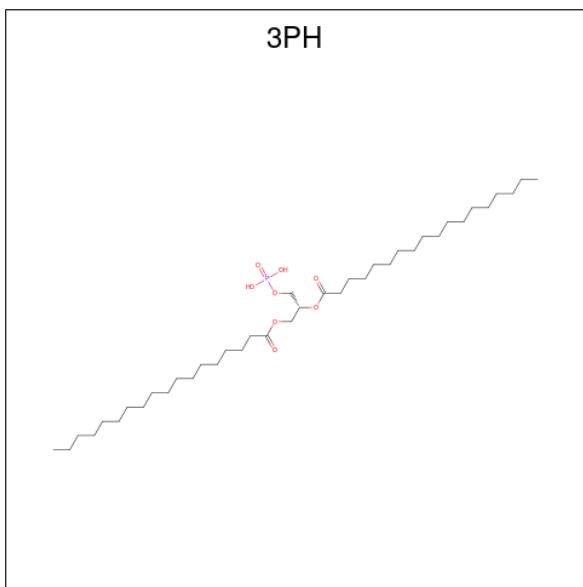
Mol	Chain	Residues	Atoms	AltConf
48	Y	1	Total C O 44 40 4	0
48	n	1	Total C O 44 40 4	0
48	g	1	Total C O 44 40 4	0
48	r	1	Total C O 44 40 4	0
48	s	1	Total C O 44 40 4	0
48	y	1	Total C O 44 40 4	0

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



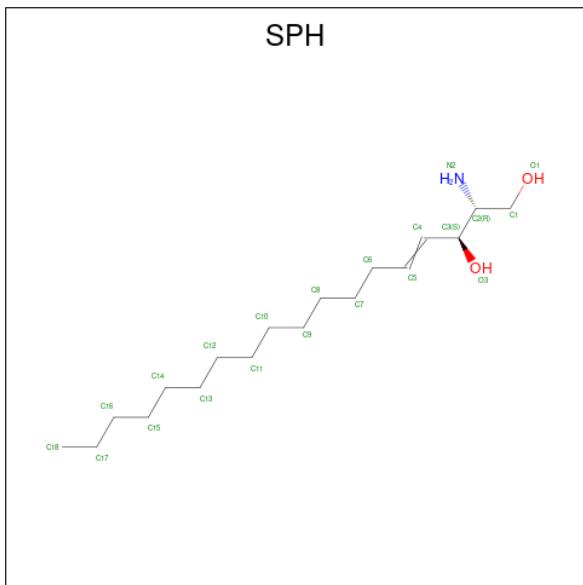
Mol	Chain	Residues	Atoms	AltConf
49	S	1	Total C N O P 30 21 1 7 1	0
49	s	1	Total C N O P 30 21 1 7 1	0

- 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
			48	39	8	1
50	i	1	Total	C	O	P
			48	39	8	1
50	s	1	Total	C	O	P
			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
			21	18	1	2

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

- Molecule 52 is water.

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

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

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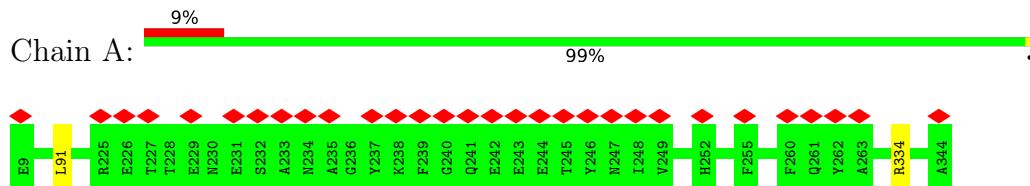
Continued from previous page...

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

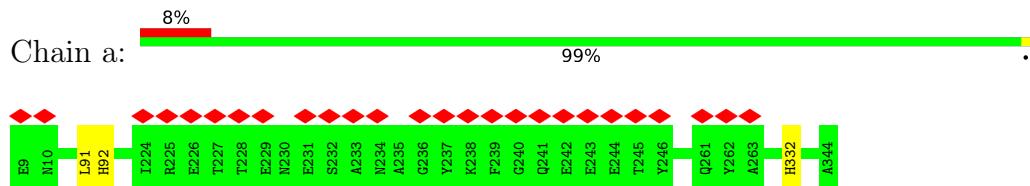
3 Residue-property plots [\(i\)](#)

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.

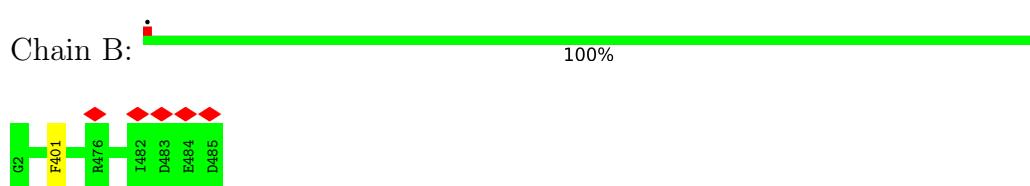
- Molecule 1: Photosystem II protein D1



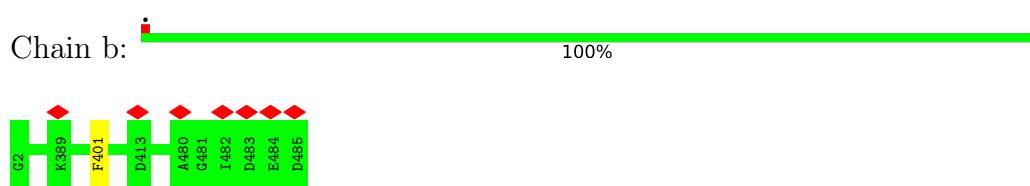
- Molecule 1: Photosystem II protein D1



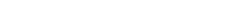
- Molecule 2: Photosystem II CP47 reaction center protein



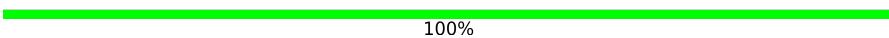
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

- There are no outlier residues recorded for this chain.

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  99%

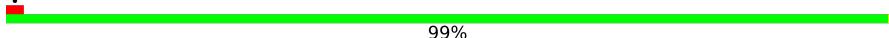


- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  99%



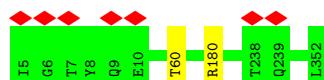
- Molecule 5: Photosystem II D2 protein

Chain D:  99%



- Molecule 5: Photosystem II D2 protein

Chain d:  99%

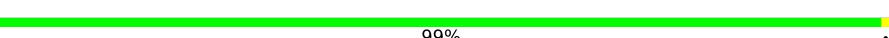


- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  99%



- Molecule 7: Cytochrome b559 subunit beta



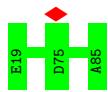
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein I



There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

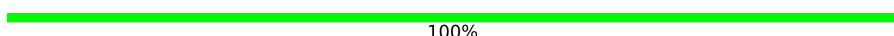
There are no outlier residues recorded for this chain.

- 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%

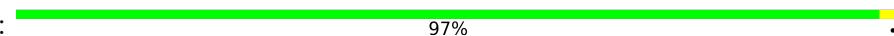
There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain l:  100%



- Molecule 13: Photosystem II reaction center protein M

Chain M:  97%

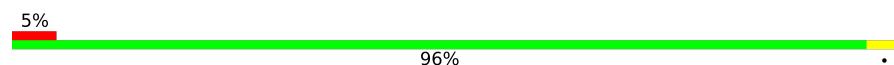


- Molecule 13: Photosystem II reaction center protein M

Chain m:  97%



- Molecule 14: PsbO

Chain O:  96%
5%



- Molecule 14: PsbO

Chain o: 99%



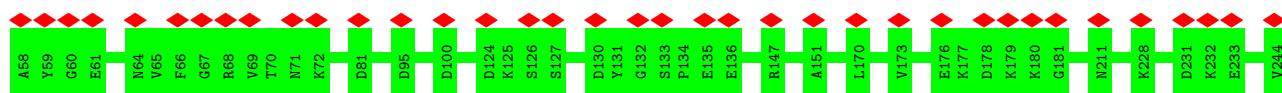
- Molecule 15: PsbP

Chain P: 15% 99%



- Molecule 15: PsbP

Chain p: 20% 100%



- Molecule 16: Photosystem II reaction center protein T

Chain T: 97%



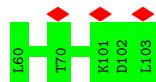
- Molecule 16: Photosystem II reaction center protein T

Chain t: 97%



- Molecule 17: PSII 6.1 kDa protein

Chain W: 7% 100%

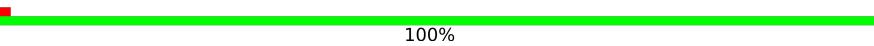


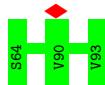
- Molecule 17: PSII 6.1 kDa protein

Chain w:  100%



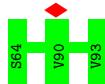
- Molecule 18: Hypothetical protein

Chain X:  100%

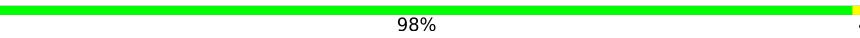


- Molecule 18: Hypothetical protein

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%

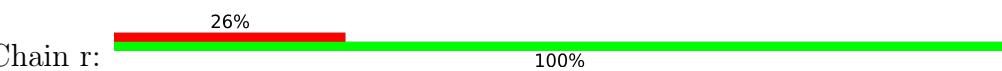


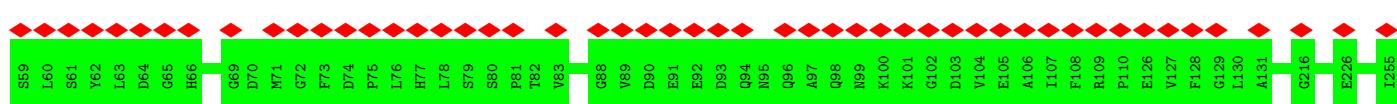
- Molecule 22: CP29

Chain R:  24%



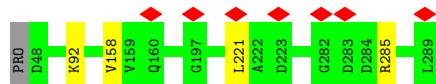
- Molecule 22: CP29

Chain r:  26%



- Molecule 23: CP26

Chain S:  98%



- Molecule 23: CP26

Chain s:  99%



- Molecule 24: LHCII M1

Chain Y:  99%



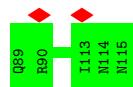
- Molecule 24: LHCII M1

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 (i)

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 i

5.1 Standard geometry i

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

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 [\(i\)](#)

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 [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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
31	BCR	c	516	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	15 (26%)
29	CLA	y	608	-	50,58,73	1.55	8 (16%)	58,95,113	2.22	18 (31%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
36	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)
29	CLA	y	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	21 (27%)
39	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
29	CLA	r	611	-	46,54,73	1.61	10 (21%)	53,90,113	2.12	14 (26%)
29	CLA	n	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	20 (26%)
29	CLA	b	609	-	65,73,73	1.34	7 (10%)	76,113,113	2.14	17 (22%)
29	CLA	g	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.20	13 (25%)
29	CLA	Y	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	19 (25%)
29	CLA	a	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.01	19 (25%)
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%)
29	CLA	g	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
30	PHO	a	409	-	51,69,69	0.98	3 (5%)	47,99,99	1.24	5 (10%)
33	LMG	h	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.09	2 (3%)
32	SQD	B	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
31	BCR	c	517	-	41,41,41	1.81	4 (9%)	56,56,56	4.10	19 (33%)
29	CLA	R	612	-	60,68,73	1.42	8 (13%)	70,107,113	2.07	16 (22%)
29	CLA	y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.97	17 (22%)
45	CHL	G	601	21	66,74,74	0.81	3 (4%)	73,114,114	1.24	11 (15%)
46	LUT	G	621	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	13 (25%)
29	CLA	b	610	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	15 (19%)
41	BCT	D	401	27	2,3,3	1.27	0	2,3,3	2.64	2 (100%)
29	CLA	R	611	-	46,54,73	1.62	10 (21%)	53,90,113	2.10	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	y	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.02	19 (25%)
29	CLA	G	613	-	65,73,73	1.35	9 (13%)	76,113,113	2.02	18 (23%)
31	BCR	D	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.04	17 (30%)
41	BCT	d	401	27	2,3,3	1.26	0	2,3,3	2.67	2 (100%)
39	LHG	l	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
29	CLA	R	603	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	18 (25%)
50	3PH	i	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
29	CLA	G	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.19	15 (28%)
45	CHL	y	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.22	10 (13%)
46	LUT	y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.03	12 (23%)
29	CLA	c	503	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	18 (23%)
51	SPH	y	625	-	19,20,20	0.64	0	18,21,21	1.10	1 (5%)
45	CHL	Y	605	24	46,54,74	1.01	3 (6%)	49,90,114	1.41	10 (20%)
30	PHO	A	409	-	51,69,69	1.00	3 (5%)	47,99,99	1.20	3 (6%)
29	CLA	y	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	19 (25%)
29	CLA	C	507	52	65,73,73	1.37	7 (10%)	76,113,113	1.96	18 (23%)
29	CLA	S	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.96	19 (25%)
29	CLA	c	505	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	15 (19%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	13 (23%)
39	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
45	CHL	r	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.36	9 (19%)
39	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.00	2 (4%)
29	CLA	G	602	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	18 (23%)
29	CLA	Y	613	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	20 (26%)
38	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.05	3 (4%)
29	CLA	g	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
29	CLA	C	504	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
29	CLA	Y	603	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	19 (25%)
29	CLA	r	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.02	14 (20%)
29	CLA	G	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.18	12 (24%)
29	CLA	s	604	-	55,63,73	1.48	7 (12%)	64,101,113	2.07	14 (21%)
48	NEX	r	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.54	9 (18%)
45	CHL	s	601	23	46,54,74	1.03	4 (8%)	49,90,114	1.37	9 (18%)
40	LMK	C	527	-	38,39,53	1.48	2 (5%)	41,46,60	1.30	2 (4%)
44	RRX	h	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.03	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	Y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.21	9 (12%)
29	CLA	N	612	-	45,53,73	1.63	9 (20%)	52,89,113	2.14	11 (21%)
30	PHO	A	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.15	4 (8%)
29	CLA	C	512	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	17 (22%)
33	LMG	A	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.17	4 (7%)
45	CHL	s	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.24	9 (13%)
46	LUT	s	620	-	42,43,43	2.41	1 (2%)	51,60,60	2.12	16 (31%)
46	LUT	n	621	-	42,43,43	2.33	1 (2%)	51,60,60	1.85	11 (21%)
43	HEM	F	101	6,7	41,50,50	1.55	3 (7%)	45,82,82	1.51	6 (13%)
26	OEX	a	401	52,1,4	0,15,15	-	-	-	-	-
42	PL9	D	405	-	55,55,55	1.17	5 (9%)	68,69,69	1.50	13 (19%)
29	CLA	B	609	-	65,73,73	1.34	8 (12%)	76,113,113	2.10	17 (22%)
29	CLA	B	614	-	65,73,73	1.32	6 (9%)	76,113,113	2.01	18 (23%)
29	CLA	n	613	-	65,73,73	1.36	10 (15%)	76,113,113	2.01	16 (21%)
29	CLA	g	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.19	13 (26%)
29	CLA	C	505	-	65,73,73	1.36	9 (13%)	76,113,113	2.03	16 (21%)
45	CHL	n	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.21	8 (10%)
29	CLA	s	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.40	18 (31%)
39	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.03	2 (4%)
29	CLA	c	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	18 (23%)
47	XAT	R	621	-	39,47,47	0.69	1 (2%)	54,74,74	2.22	17 (31%)
47	XAT	n	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	a	406	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	17 (22%)
45	CHL	G	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.19	10 (13%)
29	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	21 (27%)
29	CLA	b	607	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	19 (25%)
45	CHL	s	606	-	44,52,74	1.01	3 (6%)	46,87,114	1.43	10 (21%)
29	CLA	G	610	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	18 (23%)
29	CLA	b	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.97	16 (21%)
32	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.89	2 (3%)
29	CLA	s	612	-	45,53,73	1.61	8 (17%)	52,89,113	2.16	15 (28%)
46	LUT	S	621	-	42,43,43	2.31	1 (2%)	51,60,60	1.97	15 (29%)
37	GOL	y	626	-	5,5,5	0.57	0	5,5,5	0.25	0
29	CLA	S	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.03	17 (24%)
33	LMG	c	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	c	504	-	65,73,73	1.32	7 (10%)	76,113,113	2.05	19 (25%)
29	CLA	c	510	-	65,73,73	1.33	8 (12%)	76,113,113	2.03	16 (21%)
45	CHL	g	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.23	10 (13%)
29	CLA	c	511	-	65,73,73	1.34	7 (10%)	76,113,113	2.08	20 (26%)
29	CLA	Y	604	-	65,73,73	1.35	9 (13%)	76,113,113	1.93	18 (23%)
29	CLA	s	614	-	55,63,73	1.46	7 (12%)	64,101,113	2.17	15 (23%)
45	CHL	S	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.40	9 (19%)
45	CHL	N	608	-	50,58,74	0.89	2 (4%)	52,94,114	1.41	11 (21%)
31	BCR	C	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.43	12 (21%)
29	CLA	C	513	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	19 (25%)
45	CHL	S	608	-	61,69,74	0.87	3 (4%)	67,108,114	1.26	10 (14%)
46	LUT	Y	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.95	14 (27%)
32	SQD	A	412	-	50,51,54	0.84	0	59,62,65	0.94	3 (5%)
45	CHL	N	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.25	11 (15%)
29	CLA	b	614	-	65,73,73	1.33	6 (9%)	76,113,113	2.00	18 (23%)
45	CHL	n	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.28	10 (13%)
33	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.07	2 (3%)
29	CLA	Y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
48	NEX	G	623	-	38,46,46	3.31	10 (26%)	50,70,70	1.77	11 (22%)
45	CHL	N	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.27	10 (13%)
29	CLA	c	512	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	19 (25%)
39	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
29	CLA	g	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	18 (23%)
29	CLA	N	614	-	49,57,73	1.55	8 (16%)	55,93,113	2.26	16 (29%)
29	CLA	G	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	19 (25%)
31	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.36	18 (32%)
39	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
29	CLA	N	604	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	20 (26%)
29	CLA	y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
29	CLA	S	614	-	55,63,73	1.47	8 (14%)	64,101,113	2.12	15 (23%)
31	BCR	B	618	-	41,41,41	1.81	4 (9%)	56,56,56	4.29	15 (26%)
47	XAT	r	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.18	19 (35%)
31	BCR	C	515	-	41,41,41	1.84	4 (9%)	56,56,56	4.22	13 (23%)
47	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.70	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.10	1 (5%)
46	LUT	N	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.92	13 (25%)
29	CLA	n	602	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	22 (28%)
45	CHL	R	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.33	8 (17%)
48	NEX	Y	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.80	11 (22%)
29	CLA	R	604	-	49,57,73	1.52	8 (16%)	55,93,113	2.33	18 (32%)
48	NEX	g	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.81	13 (26%)
29	CLA	b	605	-	65,73,73	1.38	8 (12%)	76,113,113	2.08	16 (21%)
36	DGA	b	623	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)
29	CLA	A	407	-	49,57,73	1.56	7 (14%)	55,93,113	2.25	16 (29%)
29	CLA	B	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	15 (19%)
29	CLA	S	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	15 (19%)
36	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
26	OEX	A	401	52,1	0,15,15	-	-	-	-	-
29	CLA	a	407	-	49,57,73	1.56	8 (16%)	55,93,113	2.24	18 (32%)
49	LPX	s	625	-	29,29,29	0.98	2 (6%)	31,33,33	0.98	1 (3%)
29	CLA	N	611	-	49,57,73	1.57	10 (20%)	55,93,113	2.22	15 (27%)
29	CLA	b	604	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	18 (23%)
46	LUT	R	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.16	14 (27%)
45	CHL	g	607	-	50,58,74	0.88	2 (4%)	52,94,114	1.41	10 (19%)
29	CLA	d	402	-	65,73,73	1.35	8 (12%)	76,113,113	1.90	14 (18%)
29	CLA	b	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
38	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.04	3 (4%)
29	CLA	C	506	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	19 (25%)
29	CLA	s	603	-	65,73,73	1.38	10 (15%)	76,113,113	1.89	14 (18%)
29	CLA	N	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	20 (26%)
29	CLA	B	617	-	65,73,73	1.34	8 (12%)	76,113,113	4.31	17 (22%)
29	CLA	C	508	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	16 (21%)
29	CLA	c	506	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	19 (25%)
29	CLA	r	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.28	17 (30%)
33	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	3 (5%)
29	CLA	n	610	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	17 (22%)
29	CLA	C	503	-	65,73,73	1.36	9 (13%)	76,113,113	2.02	19 (25%)
29	CLA	A	406	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	16 (21%)
39	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.07	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CHL	r	607	-	50,58,74	0.94	3 (6%)	52,94,114	1.37	9 (17%)
45	CHL	n	608	-	50,58,74	0.90	2 (4%)	52,94,114	1.41	11 (21%)
50	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
29	CLA	b	617	-	65,73,73	1.35	7 (10%)	76,113,113	4.30	17 (22%)
29	CLA	B	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	14 (18%)
29	CLA	B	615	-	65,73,73	1.34	8 (12%)	76,113,113	2.17	20 (26%)
39	LHG	d	410	-	38,38,48	0.41	0	41,44,54	1.15	3 (7%)
32	SQD	c	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	s	610	-	65,73,73	1.37	9 (13%)	76,113,113	1.97	19 (25%)
29	CLA	R	609	-	60,68,73	1.42	7 (11%)	70,107,113	2.02	15 (21%)
47	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
47	XAT	N	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.96	13 (24%)
29	CLA	S	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.14	12 (23%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.12	3 (5%)
33	LMG	b	622	-	44,44,55	0.85	3 (6%)	52,52,63	1.07	3 (5%)
45	CHL	Y	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.16	9 (12%)
45	CHL	N	605	20	66,74,74	0.83	3 (4%)	73,114,114	1.20	10 (13%)
46	LUT	r	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.20	15 (29%)
48	NEX	n	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	12 (24%)
29	CLA	g	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.27	17 (30%)
33	LMG	j	101	-	45,45,55	0.89	3 (6%)	53,53,63	1.04	2 (3%)
45	CHL	R	607	-	50,58,74	0.96	3 (6%)	52,94,114	1.38	8 (15%)
46	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.94	15 (29%)
45	CHL	y	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.20	8 (10%)
29	CLA	b	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.16	19 (25%)
37	GOL	b	625	-	5,5,5	0.58	0	5,5,5	0.28	0
29	CLA	B	605	-	65,73,73	1.39	8 (12%)	76,113,113	2.10	15 (19%)
48	NEX	R	622	-	38,46,46	3.42	10 (26%)	50,70,70	1.69	11 (22%)
29	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
46	LUT	g	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.95	11 (21%)
39	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.03	3 (5%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.11	17 (30%)
45	CHL	g	605	21	48,56,74	0.95	3 (6%)	51,92,114	1.41	10 (19%)
29	CLA	C	510	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	16 (21%)
29	CLA	B	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	NEX	y	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	13 (26%)
29	CLA	Y	614	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	17 (22%)
45	CHL	G	605	21	48,56,74	0.96	2 (4%)	51,92,114	1.38	10 (19%)
29	CLA	s	611	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
42	PL9	d	405	-	55,55,55	1.21	4 (7%)	68,69,69	1.49	12 (17%)
39	LHG	S	624	-	44,44,48	0.41	0	47,50,54	1.10	3 (6%)
29	CLA	r	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	15 (21%)
29	CLA	C	502	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	16 (21%)
29	CLA	B	613	-	65,73,73	1.32	7 (10%)	76,113,113	1.95	16 (21%)
29	CLA	b	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	18 (23%)
29	CLA	c	502	-	65,73,73	1.36	7 (10%)	76,113,113	2.13	16 (21%)
45	CHL	N	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.17	9 (12%)
29	CLA	s	613	-	55,63,73	1.49	8 (14%)	64,101,113	2.32	16 (25%)
29	CLA	G	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.30	17 (30%)
29	CLA	c	508	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	18 (23%)
29	CLA	N	613	-	65,73,73	1.37	10 (15%)	76,113,113	1.99	16 (21%)
37	GOL	b	624	-	5,5,5	0.59	0	5,5,5	0.22	0
35	C7Z	B	620	-	43,43,43	5.41	26 (60%)	58,60,60	2.04	19 (32%)
44	RRX	H	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.04	18 (31%)
35	C7Z	b	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.05	17 (29%)
39	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
45	CHL	G	607	-	50,58,74	0.87	2 (4%)	52,94,114	1.42	11 (21%)
46	LUT	G	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.96	12 (23%)
29	CLA	a	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.11	17 (24%)
29	CLA	b	613	-	65,73,73	1.32	8 (12%)	76,113,113	1.96	17 (22%)
30	PHO	a	408	-	51,69,69	1.00	4 (7%)	47,99,99	1.15	6 (12%)
46	LUT	S	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.09	12 (23%)
29	CLA	B	602	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	17 (22%)
31	BCR	C	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	16 (28%)
31	BCR	b	619	-	41,41,41	1.83	4 (9%)	56,56,56	4.38	17 (30%)
43	HEM	f	101	6,7	41,50,50	1.54	4 (9%)	45,82,82	1.55	7 (15%)
45	CHL	n	606	-	66,74,74	0.89	4 (6%)	73,114,114	1.17	9 (12%)
29	CLA	s	602	-	60,68,73	1.38	8 (13%)	70,107,113	2.05	17 (24%)
47	XAT	g	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.88	15 (27%)
47	XAT	y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.73	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	18 (23%)
45	CHL	N	601	-	66,74,74	0.82	3 (4%)	73,114,114	1.17	8 (10%)
45	CHL	y	605	24	46,54,74	1.00	2 (4%)	49,90,114	1.38	8 (16%)
48	NEX	S	622	-	38,46,46	3.28	9 (23%)	50,70,70	1.80	12 (24%)
29	CLA	b	608	-	65,73,73	1.34	6 (9%)	76,113,113	2.05	17 (22%)
29	CLA	S	603	-	65,73,73	1.39	10 (15%)	76,113,113	1.91	14 (18%)
29	CLA	n	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.11	14 (26%)
31	BCR	c	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	13 (23%)
46	LUT	n	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.82	14 (27%)
29	CLA	s	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	16 (22%)
31	BCR	b	618	-	41,41,41	1.82	4 (9%)	56,56,56	4.30	15 (26%)
29	CLA	B	610	-	65,73,73	1.34	8 (12%)	76,113,113	1.99	16 (21%)
29	CLA	r	613	-	46,54,73	1.60	9 (19%)	53,90,113	2.19	15 (28%)
45	CHL	n	605	20	66,74,74	0.84	3 (4%)	73,114,114	1.18	10 (13%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	14 (25%)
29	CLA	B	604	-	65,73,73	1.36	9 (13%)	76,113,113	1.92	17 (22%)
29	CLA	S	604	-	55,63,73	1.45	7 (12%)	64,101,113	2.18	17 (26%)
39	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.11	2 (3%)
31	BCR	A	411	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	15 (26%)
38	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.98	2 (2%)
45	CHL	g	608	-	44,52,74	0.99	3 (6%)	46,87,114	1.42	9 (19%)
29	CLA	b	612	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
33	LMG	J	101	-	45,45,55	0.90	3 (6%)	53,53,63	1.00	2 (3%)
29	CLA	b	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	14 (18%)
29	CLA	d	403	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	16 (21%)
38	DGD	C	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
29	CLA	r	603	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	17 (24%)
37	GOL	B	627	-	5,5,5	0.58	0	5,5,5	0.21	0
29	CLA	R	613	-	46,54,73	1.61	8 (17%)	53,90,113	2.18	14 (26%)
45	CHL	g	606	-	50,58,74	0.89	2 (4%)	52,94,114	1.39	9 (17%)
29	CLA	b	602	-	65,73,73	1.37	9 (13%)	76,113,113	1.98	17 (22%)
29	CLA	y	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	16 (21%)
29	CLA	S	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.04	17 (24%)
29	CLA	C	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.11	19 (25%)
29	CLA	r	612	-	60,68,73	1.43	9 (15%)	70,107,113	2.03	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	LUT	s	621	-	42,43,43	2.32	1 (2%)	51,60,60	1.99	14 (27%)
29	CLA	B	608	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	16 (21%)
29	CLA	B	616	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	15 (19%)
45	CHL	y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.22	10 (13%)
45	CHL	y	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.23	12 (16%)
39	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
29	CLA	R	610	-	60,68,73	1.42	9 (15%)	70,107,113	2.07	20 (28%)
33	LMG	B	622	-	44,44,55	0.85	2 (4%)	52,52,63	1.06	3 (5%)
29	CLA	g	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
38	DGD	c	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
49	LPX	S	625	-	29,29,29	0.99	2 (6%)	31,33,33	0.98	1 (3%)
46	LUT	Y	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
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	1.06	6 (10%)	74,74,81	0.98	2 (2%)
29	CLA	C	501	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	18 (23%)
29	CLA	Y	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	13 (17%)
45	CHL	Y	609	-	66,74,74	0.81	3 (4%)	73,114,114	1.23	12 (16%)
29	CLA	g	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
29	CLA	r	610	-	60,68,73	1.40	10 (16%)	70,107,113	2.15	20 (28%)
29	CLA	R	602	-	60,68,73	1.42	9 (15%)	70,107,113	2.10	18 (25%)
38	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.03	3 (3%)
39	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.02	3 (5%)
39	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
29	CLA	y	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
45	CHL	n	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.33	13 (17%)
50	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
45	CHL	G	608	-	44,52,74	1.00	3 (6%)	46,87,114	1.41	9 (19%)
29	CLA	N	610	-	65,73,73	1.36	8 (12%)	76,113,113	2.01	18 (23%)
36	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
29	CLA	A	410	-	60,68,73	1.41	9 (15%)	70,107,113	2.10	16 (22%)
45	CHL	Y	601	24	66,74,74	0.80	2 (3%)	73,114,114	1.20	9 (12%)
29	CLA	y	604	-	65,73,73	1.34	6 (9%)	76,113,113	1.95	18 (23%)
29	CLA	n	611	-	49,57,73	1.56	9 (18%)	55,93,113	2.27	15 (27%)
29	CLA	R	608	-	60,68,73	1.43	9 (15%)	70,107,113	2.01	16 (22%)
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
46	LUT	N	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.92	13 (25%)
45	CHL	s	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.44	7 (15%)
29	CLA	n	614	-	49,57,73	1.55	10 (20%)	55,93,113	2.30	18 (32%)
48	NEX	s	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.72	11 (22%)
29	CLA	S	613	-	55,63,73	1.48	8 (14%)	64,101,113	2.33	16 (25%)
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%)
29	CLA	Y	608	-	50,58,73	1.55	8 (16%)	58,95,113	2.22	19 (32%)
29	CLA	s	617	-	50,58,73	1.53	9 (18%)	58,95,113	2.27	19 (32%)
45	CHL	S	601	23	46,54,74	1.02	4 (8%)	49,90,114	1.35	9 (18%)
29	CLA	n	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	19 (25%)
29	CLA	A	405	-	65,73,73	1.32	6 (9%)	76,113,113	2.03	18 (23%)
39	LHG	s	624	-	44,44,48	0.42	0	47,50,54	1.11	3 (6%)
29	CLA	C	509	-	65,73,73	1.33	6 (9%)	76,113,113	2.04	19 (25%)
46	LUT	g	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	12 (23%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	14 (25%)
39	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
33	LMG	D	411	-	46,46,55	0.92	4 (8%)	54,54,63	1.11	2 (3%)
40	LMK	c	627	-	38,39,53	1.48	2 (5%)	41,46,60	1.33	2 (4%)
29	CLA	c	509	-	65,73,73	1.32	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	B	612	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
29	CLA	G	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.28	16 (29%)
29	CLA	c	513	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
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%)
33	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	2 (3%)
48	NEX	N	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.76	14 (28%)
29	CLA	D	402	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	15 (19%)
45	CHL	S	607	-	43,51,74	1.01	3 (6%)	45,86,114	1.45	8 (17%)

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
31	BCR	c	516	-	-	13/29/63/63	0/2/2/2
29	CLA	y	608	-	1/1/12/20	8/19/97/115	-
32	SQD	a	412	-	-	13/46/66/69	0/1/1/1
36	DGA	B	625	-	-	24/45/45/45	-
29	CLA	y	602	-	1/1/15/20	15/37/115/115	-
39	LHG	D	409	-	-	30/53/53/53	-
29	CLA	r	611	-	1/1/11/20	5/15/93/115	-
29	CLA	n	604	-	1/1/15/20	16/37/115/115	-
29	CLA	b	609	-	1/1/15/20	15/37/115/115	-
29	CLA	g	611	-	1/1/11/20	4/13/91/115	-
29	CLA	Y	602	-	1/1/15/20	15/37/115/115	-
29	CLA	a	405	-	1/1/15/20	14/37/115/115	-
29	CLA	S	617	-	1/1/12/20	10/19/97/115	-
29	CLA	D	403	-	1/1/15/20	12/37/115/115	-
29	CLA	g	614	-	1/1/11/20	9/18/96/115	-
30	PHO	a	409	-	-	9/37/103/103	0/5/6/6
33	LMG	h	102	-	-	14/43/63/70	0/1/1/1
32	SQD	B	621	-	-	19/49/69/69	0/1/1/1
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	R	612	-	1/1/14/20	13/31/109/115	-
29	CLA	y	610	-	1/1/15/20	24/37/115/115	-
45	CHL	G	601	21	4/4/20/26	8/39/137/137	-
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
29	CLA	b	610	-	1/1/15/20	15/37/115/115	-
29	CLA	R	611	-	1/1/11/20	5/15/93/115	-
29	CLA	y	603	-	1/1/15/20	13/37/115/115	-
29	CLA	G	613	-	1/1/15/20	20/37/115/115	-
31	BCR	D	404	-	-	11/29/63/63	0/2/2/2
39	LHG	l	101	-	-	29/53/53/53	-
29	CLA	R	603	-	1/1/14/20	16/31/109/115	-
50	3PH	i	101	-	-	20/49/49/49	-
29	CLA	G	611	-	1/1/11/20	5/13/91/115	-
45	CHL	y	606	-	4/4/20/26	8/39/137/137	-
46	LUT	y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	c	503	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SPH	y	625	-	-	11/21/21/21	-
45	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
30	PHO	A	409	-	-	10/37/103/103	0/5/6/6
29	CLA	y	613	-	1/1/15/20	19/37/115/115	-
29	CLA	C	507	52	1/1/15/20	17/37/115/115	-
29	CLA	S	610	-	1/1/15/20	11/37/115/115	-
29	CLA	c	505	-	1/1/15/20	15/37/115/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
39	LHG	d	408	-	-	29/48/48/53	-
45	CHL	r	606	-	3/3/15/26	1/13/111/137	-
39	LHG	c	625	-	-	27/51/51/53	-
29	CLA	G	602	-	1/1/15/20	21/37/115/115	-
29	CLA	Y	613	-	1/1/15/20	21/37/115/115	-
38	DGD	c	518	-	-	11/44/84/95	0/2/2/2
29	CLA	g	613	-	1/1/15/20	21/37/115/115	-
29	CLA	C	504	-	1/1/15/20	14/37/115/115	-
29	CLA	Y	603	-	1/1/15/20	15/37/115/115	-
29	CLA	r	609	-	1/1/14/20	18/31/109/115	-
29	CLA	G	612	-	1/1/10/20	4/11/89/115	-
29	CLA	s	604	-	1/1/13/20	12/25/103/115	-
48	NEX	r	623	-	-	7/27/83/83	0/3/3/3
45	CHL	s	601	23	3/3/16/26	7/15/113/137	-
40	LMK	C	527	-	1/1/6/6	10/46/46/60	-
44	RRX	h	101	-	1/1/11/25	10/29/65/65	0/2/2/2
45	CHL	Y	607	-	4/4/20/26	4/39/137/137	-
29	CLA	N	612	-	1/1/11/20	5/13/91/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	C	512	-	1/1/15/20	17/37/115/115	-
33	LMG	A	413	-	-	14/43/63/70	0/1/1/1
45	CHL	s	608	-	4/4/19/26	1/33/131/137	-
46	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
46	LUT	n	621	-	-	4/29/67/67	0/2/2/2
43	HEM	F	101	6,7	-	2/12/54/54	-
42	PL9	D	405	-	-	12/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	609	-	1/1/15/20	14/37/115/115	-
29	CLA	B	614	-	1/1/15/20	12/37/115/115	-
29	CLA	n	613	-	1/1/15/20	14/37/115/115	-
29	CLA	g	612	-	1/1/10/20	4/11/89/115	-
29	CLA	C	505	-	1/1/15/20	12/37/115/115	-
45	CHL	n	601	-	4/4/20/26	10/39/137/137	-
29	CLA	s	605	-	1/1/12/20	8/19/97/115	-
39	LHG	C	525	-	-	28/51/51/53	-
29	CLA	c	501	-	1/1/15/20	11/37/115/115	-
47	XAT	R	621	-	1/1/12/26	11/31/93/93	0/4/4/4
47	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	a	406	-	1/1/15/20	13/37/115/115	-
45	CHL	G	609	-	4/4/20/26	9/39/137/137	-
29	CLA	N	603	-	1/1/15/20	14/37/115/115	-
29	CLA	b	607	-	1/1/15/20	14/37/115/115	-
45	CHL	s	606	-	3/3/15/26	1/13/111/137	-
29	CLA	G	610	-	1/1/15/20	13/37/115/115	-
29	CLA	b	616	-	1/1/15/20	10/37/115/115	-
32	SQD	C	526	-	-	19/49/69/69	0/1/1/1
29	CLA	s	612	-	1/1/11/20	6/13/91/115	-
46	LUT	S	621	-	-	4/29/67/67	0/2/2/2
37	GOL	y	626	-	-	0/4/4/4	-
29	CLA	S	602	-	1/1/14/20	12/31/109/115	-
33	LMG	c	521	-	-	18/46/66/70	0/1/1/1
32	SQD	b	621	-	-	19/49/69/69	0/1/1/1
29	CLA	c	504	-	1/1/15/20	17/37/115/115	-
29	CLA	c	510	-	1/1/15/20	12/37/115/115	-
45	CHL	g	609	-	4/4/20/26	6/39/137/137	-
29	CLA	c	511	-	1/1/15/20	13/37/115/115	-
29	CLA	Y	604	-	1/1/15/20	18/37/115/115	-
29	CLA	s	614	-	1/1/13/20	8/25/103/115	-
45	CHL	S	606	-	3/3/15/26	0/13/111/137	-
45	CHL	N	608	-	3/3/16/26	3/20/118/137	-
31	BCR	C	514	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	513	-	1/1/15/20	19/37/115/115	-
45	CHL	S	608	-	4/4/19/26	2/33/131/137	-
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
32	SQD	A	412	-	-	12/46/66/69	0/1/1/1
45	CHL	N	609	-	4/4/20/26	7/39/137/137	-
29	CLA	b	614	-	1/1/15/20	10/37/115/115	-
45	CHL	n	607	-	4/4/20/26	10/39/137/137	-
33	LMG	H	102	-	-	12/43/63/70	0/1/1/1
29	CLA	Y	610	-	1/1/15/20	22/37/115/115	-
48	NEX	G	623	-	-	3/27/83/83	0/3/3/3
45	CHL	N	607	-	4/4/20/26	7/39/137/137	-
29	CLA	c	512	-	1/1/15/20	19/37/115/115	-
39	LHG	L	101	-	-	30/53/53/53	-
29	CLA	g	603	-	1/1/15/20	17/37/115/115	-
29	CLA	N	614	-	1/1/11/20	7/18/96/115	-
29	CLA	G	603	-	1/1/15/20	18/37/115/115	-
31	BCR	B	619	-	-	11/29/63/63	0/2/2/2
39	LHG	g	624	-	-	28/53/53/53	-
29	CLA	N	604	-	1/1/15/20	19/37/115/115	-
29	CLA	y	612	-	1/1/15/20	11/37/115/115	-
29	CLA	S	614	-	1/1/13/20	8/25/103/115	-
47	XAT	r	622	-	1/1/12/26	11/31/93/93	0/4/4/4
31	BCR	B	618	-	-	13/29/63/63	0/2/2/2
31	BCR	C	515	-	-	11/29/63/63	0/2/2/2
47	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
51	SPH	Y	625	-	-	10/21/21/21	-
46	LUT	N	620	-	-	3/29/67/67	0/2/2/2
29	CLA	n	602	-	1/1/15/20	16/37/115/115	-
45	CHL	R	606	-	3/3/15/26	4/13/111/137	-
48	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
29	CLA	R	604	-	1/1/11/20	12/18/96/115	-
48	NEX	g	623	-	-	3/27/83/83	0/3/3/3
29	CLA	b	605	-	1/1/15/20	20/37/115/115	-
36	DGA	b	623	-	-	26/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	407	-	1/1/11/20	4/18/96/115	-
29	CLA	B	611	-	1/1/15/20	9/37/115/115	-
29	CLA	S	611	-	1/1/15/20	12/37/115/115	-
36	DGA	c	524	-	-	19/45/45/45	-
29	CLA	a	407	-	1/1/11/20	4/18/96/115	-
49	LPX	s	625	-	-	10/31/31/31	-
29	CLA	N	611	-	1/1/11/20	10/18/96/115	-
29	CLA	b	604	-	1/1/15/20	14/37/115/115	-
46	LUT	R	620	-	-	8/29/67/67	0/2/2/2
45	CHL	g	607	-	3/3/16/26	3/20/118/137	-
29	CLA	d	402	-	1/1/15/20	13/37/115/115	-
29	CLA	b	611	-	1/1/15/20	9/37/115/115	-
38	DGD	C	518	-	-	8/44/84/95	0/2/2/2
29	CLA	C	506	-	1/1/15/20	21/37/115/115	-
29	CLA	s	603	-	1/1/15/20	15/37/115/115	-
29	CLA	N	602	-	1/1/15/20	17/37/115/115	-
29	CLA	B	617	-	1/1/15/20	17/37/115/115	-
29	CLA	C	508	-	1/1/15/20	12/37/115/115	-
29	CLA	c	506	-	1/1/15/20	22/37/115/115	-
29	CLA	r	604	-	1/1/11/20	12/18/96/115	-
33	LMG	C	521	-	-	18/46/66/70	0/1/1/1
29	CLA	n	610	-	1/1/15/20	12/37/115/115	-
29	CLA	C	503	-	1/1/15/20	19/37/115/115	-
29	CLA	A	406	-	1/1/15/20	13/37/115/115	-
39	LHG	D	410	-	-	26/43/43/53	-
45	CHL	r	607	-	3/3/16/26	8/20/118/137	-
45	CHL	n	608	-	3/3/16/26	3/20/118/137	-
50	3PH	s	626	-	-	27/49/49/49	-
29	CLA	b	617	-	1/1/15/20	16/37/115/115	-
29	CLA	B	606	-	1/1/15/20	12/37/115/115	-
29	CLA	B	615	-	1/1/15/20	8/37/115/115	-
39	LHG	d	410	-	-	33/43/43/53	-
32	SQD	c	626	-	-	16/49/69/69	0/1/1/1
29	CLA	s	610	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	R	609	-	1/1/14/20	15/31/109/115	-
47	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
47	XAT	N	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	S	612	-	1/1/11/20	5/13/91/115	-
33	LMG	a	413	-	-	13/43/63/70	0/1/1/1
33	LMG	b	622	-	-	11/39/59/70	0/1/1/1
45	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
45	CHL	N	605	20	4/4/20/26	10/39/137/137	-
46	LUT	r	620	-	-	9/29/67/67	0/2/2/2
48	NEX	n	623	-	-	2/27/83/83	0/3/3/3
29	CLA	g	604	-	1/1/11/20	12/18/96/115	-
33	LMG	j	101	-	-	12/40/60/70	0/1/1/1
45	CHL	R	607	-	3/3/16/26	5/20/118/137	-
46	LUT	y	620	-	-	4/29/67/67	0/2/2/2
45	CHL	y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	b	615	-	1/1/15/20	12/37/115/115	-
37	GOL	b	625	-	-	1/4/4/4	-
29	CLA	B	605	-	1/1/15/20	18/37/115/115	-
48	NEX	R	622	-	-	8/27/83/83	0/3/3/3
29	CLA	Y	612	-	1/1/15/20	10/37/115/115	-
46	LUT	g	620	-	-	3/29/67/67	0/2/2/2
39	LHG	Y	624	-	-	31/53/53/53	-
31	BCR	d	404	-	-	12/29/63/63	0/2/2/2
45	CHL	g	605	21	3/3/16/26	4/18/116/137	-
29	CLA	C	510	-	1/1/15/20	14/37/115/115	-
29	CLA	B	603	-	1/1/15/20	16/37/115/115	-
48	NEX	y	623	-	-	3/27/83/83	0/3/3/3
29	CLA	Y	614	-	1/1/15/20	13/37/115/115	-
45	CHL	G	605	21	3/3/16/26	1/18/116/137	-
29	CLA	s	611	-	1/1/15/20	11/37/115/115	-
42	PL9	d	405	-	-	10/53/73/73	0/1/1/1
39	LHG	S	624	-	-	28/49/49/53	-
29	CLA	r	608	-	1/1/14/20	13/31/109/115	-
29	CLA	C	502	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	613	-	1/1/15/20	15/37/115/115	-
29	CLA	b	603	-	1/1/15/20	16/37/115/115	-
29	CLA	c	502	-	1/1/15/20	20/37/115/115	-
45	CHL	N	606	-	4/4/20/26	4/39/137/137	-
29	CLA	s	613	-	1/1/13/20	10/25/103/115	-
29	CLA	G	604	-	1/1/11/20	8/18/96/115	-
29	CLA	c	508	-	1/1/15/20	12/37/115/115	-
29	CLA	N	613	-	1/1/15/20	19/37/115/115	-
37	GOL	b	624	-	-	0/4/4/4	-
35	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
44	RRX	H	101	-	1/1/11/25	9/29/65/65	0/2/2/2
35	C7Z	b	620	-	1/1/12/26	9/29/67/67	0/2/2/2
39	LHG	n	624	-	-	27/53/53/53	-
45	CHL	G	607	-	3/3/16/26	3/20/118/137	-
46	LUT	G	620	-	-	6/29/67/67	0/2/2/2
29	CLA	a	410	-	1/1/14/20	9/31/109/115	-
29	CLA	b	613	-	1/1/15/20	17/37/115/115	-
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
46	LUT	S	620	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CLA	B	602	-	1/1/15/20	21/37/115/115	-
31	BCR	C	516	-	-	15/29/63/63	0/2/2/2
31	BCR	b	619	-	-	8/29/63/63	0/2/2/2
43	HEM	f	101	6,7	-	2/12/54/54	-
45	CHL	n	606	-	4/4/20/26	5/39/137/137	-
29	CLA	s	602	-	1/1/14/20	10/31/109/115	-
47	XAT	g	622	-	2/2/12/26	0/31/93/93	0/4/4/4
47	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	B	607	-	1/1/15/20	12/37/115/115	-
45	CHL	N	601	-	4/4/20/26	5/39/137/137	-
45	CHL	y	605	24	3/3/16/26	3/15/113/137	-
48	NEX	S	622	-	-	11/27/83/83	0/3/3/3
29	CLA	b	608	-	1/1/15/20	25/37/115/115	-
29	CLA	S	603	-	1/1/15/20	15/37/115/115	-
29	CLA	n	612	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	c	515	-	-	11/29/63/63	0/2/2/2
46	LUT	n	620	-	-	6/29/67/67	0/2/2/2
29	CLA	s	609	-	1/1/14/20	14/31/109/115	-
31	BCR	b	618	-	-	13/29/63/63	0/2/2/2
29	CLA	B	610	-	1/1/15/20	15/37/115/115	-
29	CLA	r	613	-	1/1/11/20	9/15/93/115	-
45	CHL	n	605	20	4/4/20/26	8/39/137/137	-
31	BCR	C	517	-	-	8/29/63/63	0/2/2/2
29	CLA	B	604	-	1/1/15/20	17/37/115/115	-
29	CLA	S	604	-	1/1/13/20	9/25/103/115	-
39	LHG	N	624	-	-	30/53/53/53	-
31	BCR	A	411	-	-	11/29/63/63	0/2/2/2
38	DGD	C	520	-	-	12/48/88/95	0/2/2/2
45	CHL	g	608	-	3/3/15/26	1/13/111/137	-
29	CLA	b	612	-	1/1/15/20	19/37/115/115	-
33	LMG	J	101	-	-	12/40/60/70	0/1/1/1
29	CLA	b	606	-	1/1/15/20	12/37/115/115	-
29	CLA	d	403	-	1/1/15/20	13/37/115/115	-
38	DGD	C	523	-	-	17/55/95/95	0/2/2/2
29	CLA	r	603	-	1/1/14/20	17/31/109/115	-
37	GOL	B	627	-	-	0/4/4/4	-
29	CLA	R	613	-	1/1/11/20	8/15/93/115	-
45	CHL	g	606	-	3/3/16/26	5/20/118/137	-
29	CLA	b	602	-	1/1/15/20	21/37/115/115	-
29	CLA	y	614	-	1/1/15/20	15/37/115/115	-
29	CLA	S	609	-	1/1/14/20	8/31/109/115	-
29	CLA	C	511	-	1/1/15/20	15/37/115/115	-
29	CLA	r	612	-	1/1/14/20	12/31/109/115	-
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
29	CLA	B	608	-	1/1/15/20	25/37/115/115	-
29	CLA	B	616	-	1/1/15/20	10/37/115/115	-
45	CHL	y	607	-	4/4/20/26	5/39/137/137	-
45	CHL	y	609	-	4/4/20/26	7/39/137/137	-
39	LHG	G	630	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	R	610	-	1/1/14/20	10/31/109/115	-
33	LMG	B	622	-	-	11/39/59/70	0/1/1/1
29	CLA	g	610	-	1/1/15/20	11/37/115/115	-
38	DGD	c	523	-	-	18/55/95/95	0/2/2/2
49	LPX	S	625	-	-	10/31/31/31	-
46	LUT	Y	620	-	-	4/29/67/67	0/2/2/2
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	C	501	-	1/1/15/20	18/37/115/115	-
29	CLA	Y	611	-	1/1/15/20	17/37/115/115	-
45	CHL	Y	609	-	4/4/20/26	7/39/137/137	-
29	CLA	g	602	-	1/1/15/20	18/37/115/115	-
29	CLA	r	610	-	1/1/14/20	11/31/109/115	-
29	CLA	R	602	-	1/1/14/20	13/31/109/115	-
38	DGD	c	519	-	-	21/51/91/95	0/2/2/2
39	LHG	y	624	-	-	30/53/53/53	-
39	LHG	D	408	-	-	30/48/48/53	-
29	CLA	y	611	-	1/1/15/20	15/37/115/115	-
45	CHL	n	609	-	4/4/20/26	7/39/137/137	-
50	3PH	S	626	-	-	19/49/49/49	-
45	CHL	G	608	-	3/3/15/26	0/13/111/137	-
29	CLA	N	610	-	1/1/15/20	8/37/115/115	-
36	DGA	C	524	-	-	18/45/45/45	-
29	CLA	A	410	-	1/1/14/20	10/31/109/115	-
45	CHL	Y	601	24	4/4/20/26	8/39/137/137	-
29	CLA	y	604	-	1/1/15/20	20/37/115/115	-
29	CLA	n	611	-	1/1/11/20	10/18/96/115	-
29	CLA	R	608	-	1/1/14/20	16/31/109/115	-
45	CHL	G	606	-	4/4/16/26	5/20/118/137	-
46	LUT	N	621	-	-	2/29/67/67	0/2/2/2
45	CHL	s	607	-	4/4/15/26	1/12/110/137	-
29	CLA	n	614	-	1/1/11/20	5/18/96/115	-
48	NEX	s	623	-	-	13/27/83/83	0/3/3/3
29	CLA	S	613	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
29	CLA	Y	608	-	1/1/12/20	6/19/97/115	-
29	CLA	s	617	-	1/1/12/20	9/19/97/115	-
45	CHL	S	601	23	3/3/16/26	3/15/113/137	-
29	CLA	n	603	-	1/1/15/20	22/37/115/115	-
29	CLA	A	405	-	1/1/15/20	16/37/115/115	-
39	LHG	s	624	-	-	31/49/49/53	-
29	CLA	C	509	-	1/1/15/20	10/37/115/115	-
46	LUT	g	621	-	-	2/29/67/67	0/2/2/2
31	BCR	c	514	-	-	12/29/63/63	0/2/2/2
39	LHG	d	409	-	-	29/53/53/53	-
33	LMG	D	411	-	-	8/41/61/70	0/1/1/1
40	LMK	c	627	-	1/1/6/6	9/46/46/60	-
29	CLA	c	509	-	1/1/15/20	11/37/115/115	-
29	CLA	B	612	-	1/1/15/20	21/37/115/115	-
29	CLA	G	614	-	1/1/11/20	10/18/96/115	-
29	CLA	c	513	-	1/1/15/20	18/37/115/115	-
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	-
33	LMG	d	411	-	-	12/41/61/70	0/1/1/1
48	NEX	N	623	-	-	2/27/83/83	0/3/3/3
29	CLA	D	402	-	1/1/15/20	11/37/115/115	-
45	CHL	S	607	-	4/4/15/26	1/12/110/137	-

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

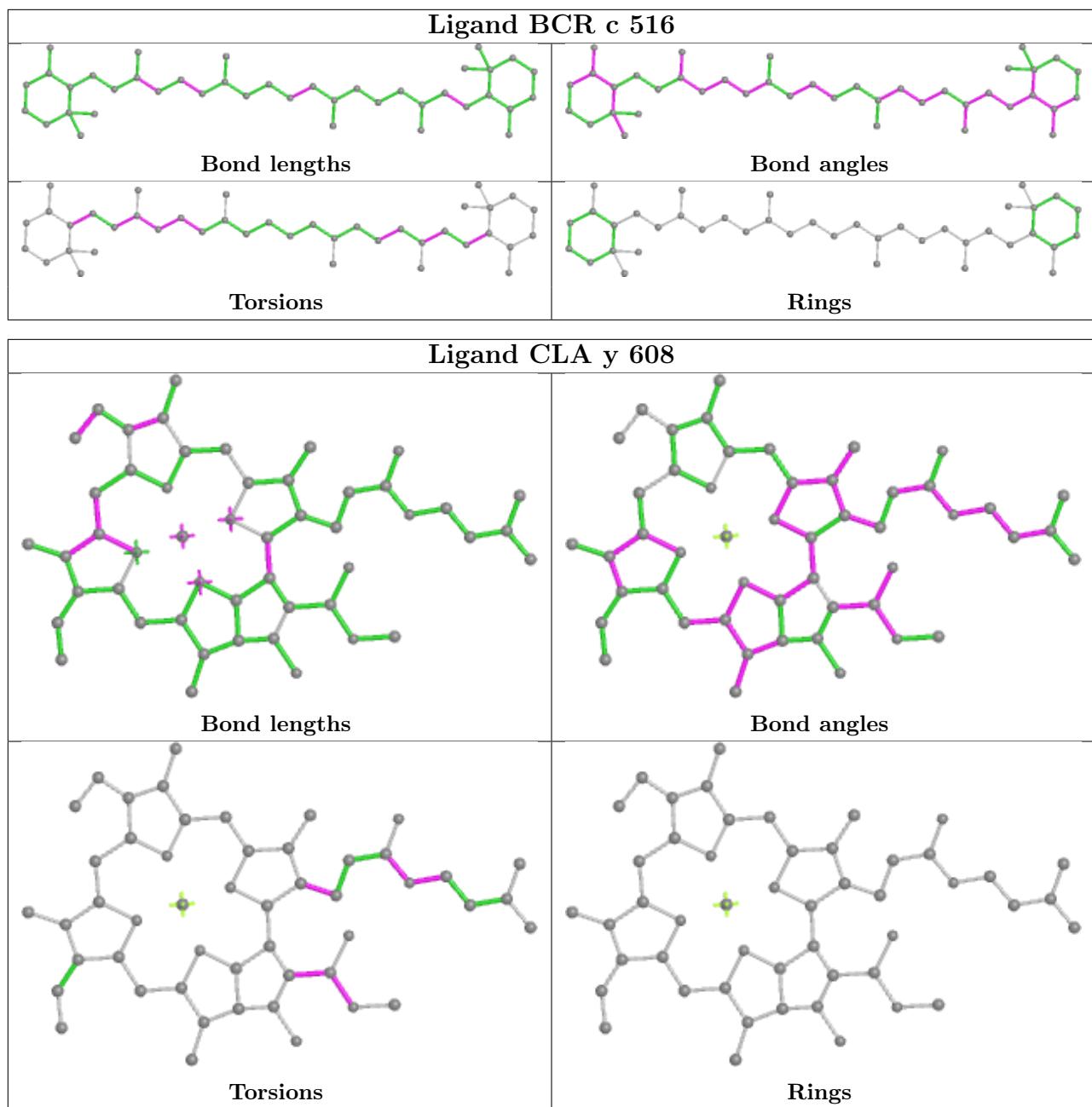
5 of 3918 torsion outliers are listed below:

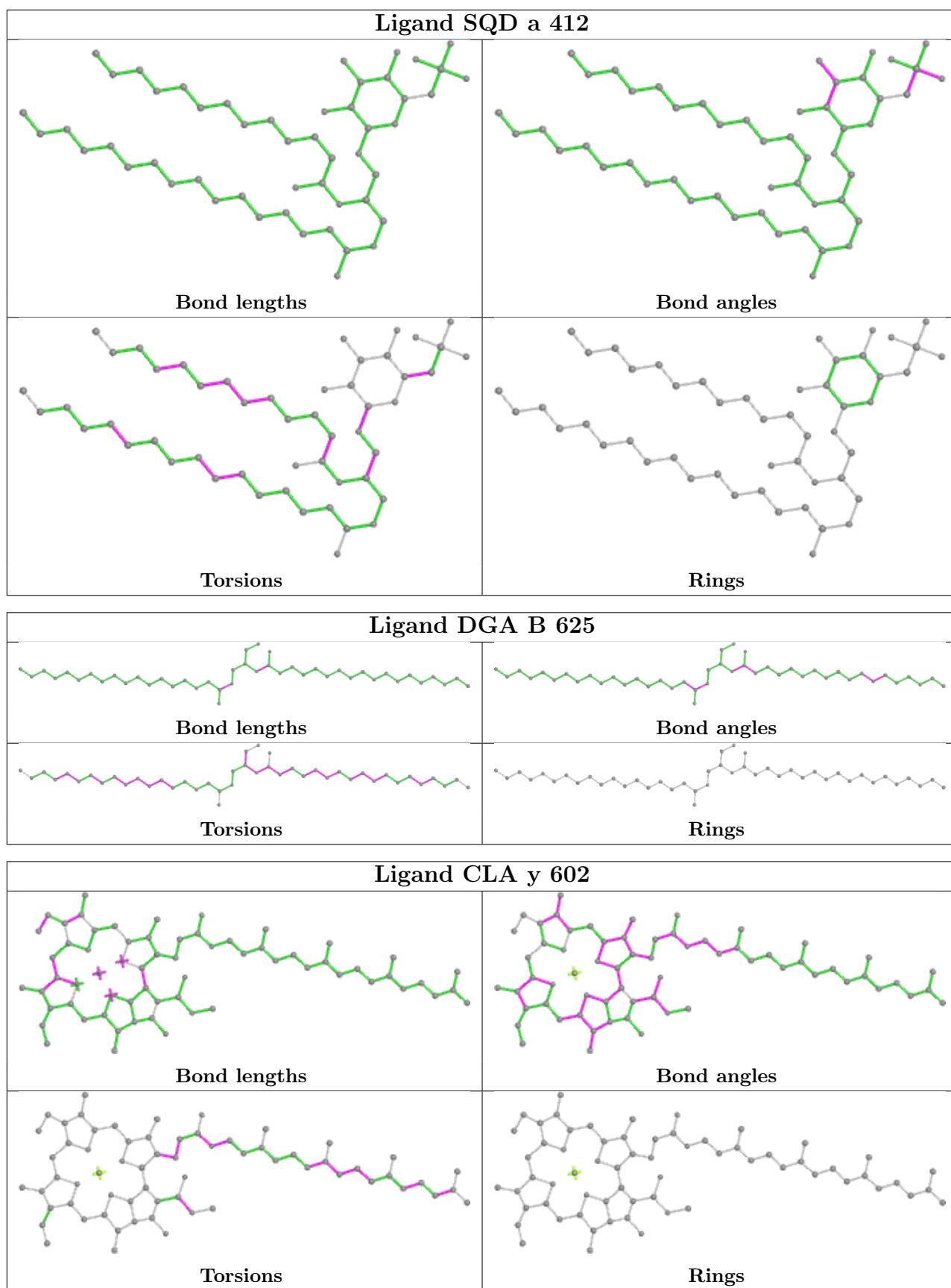
Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D

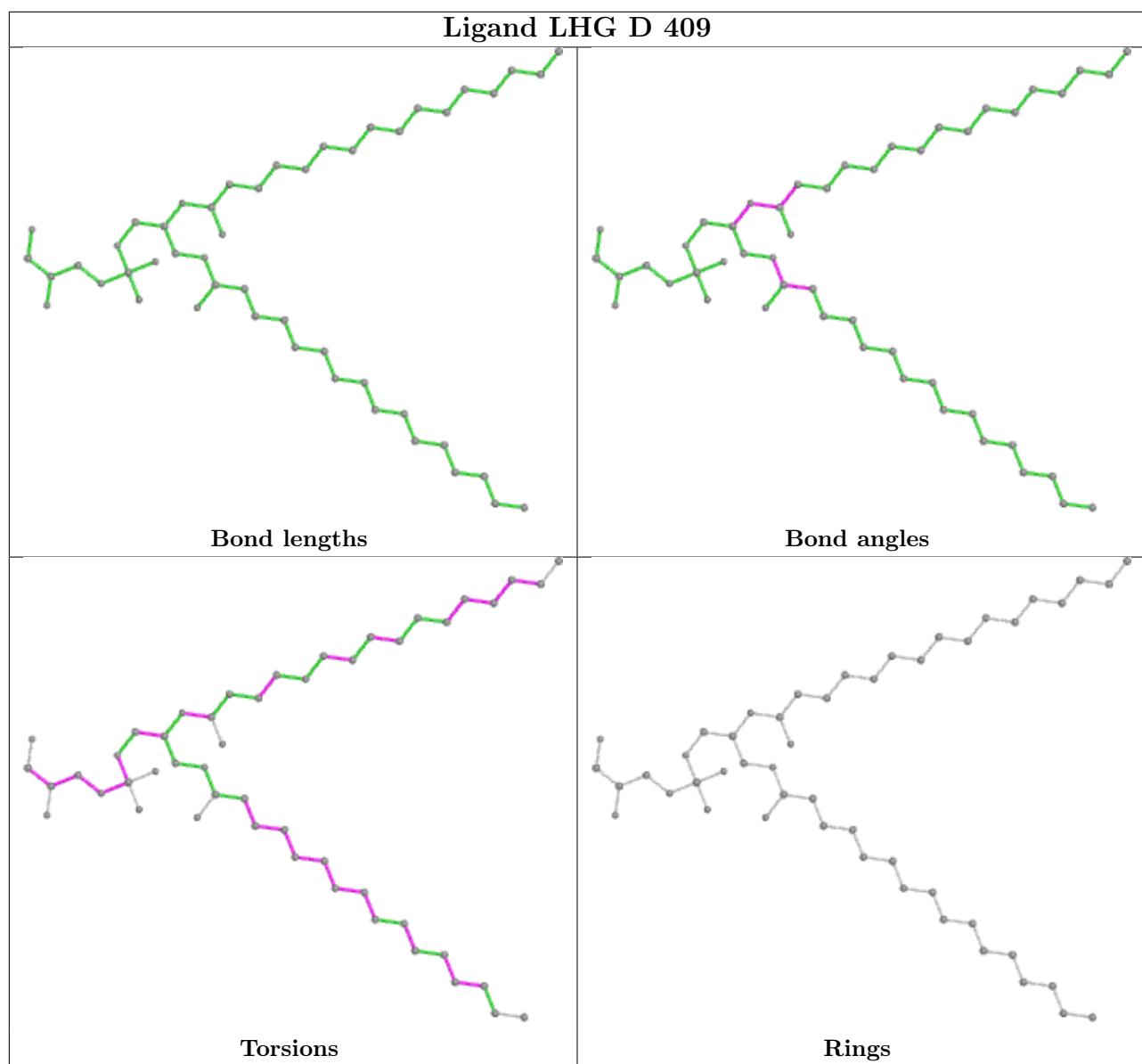
There are no ring outliers.

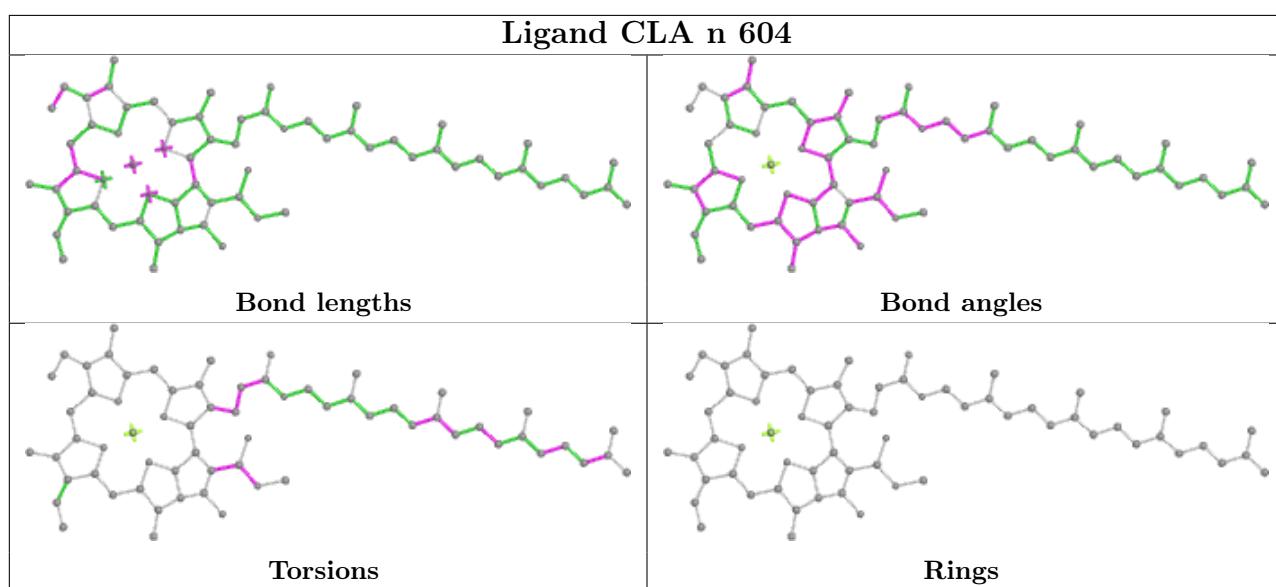
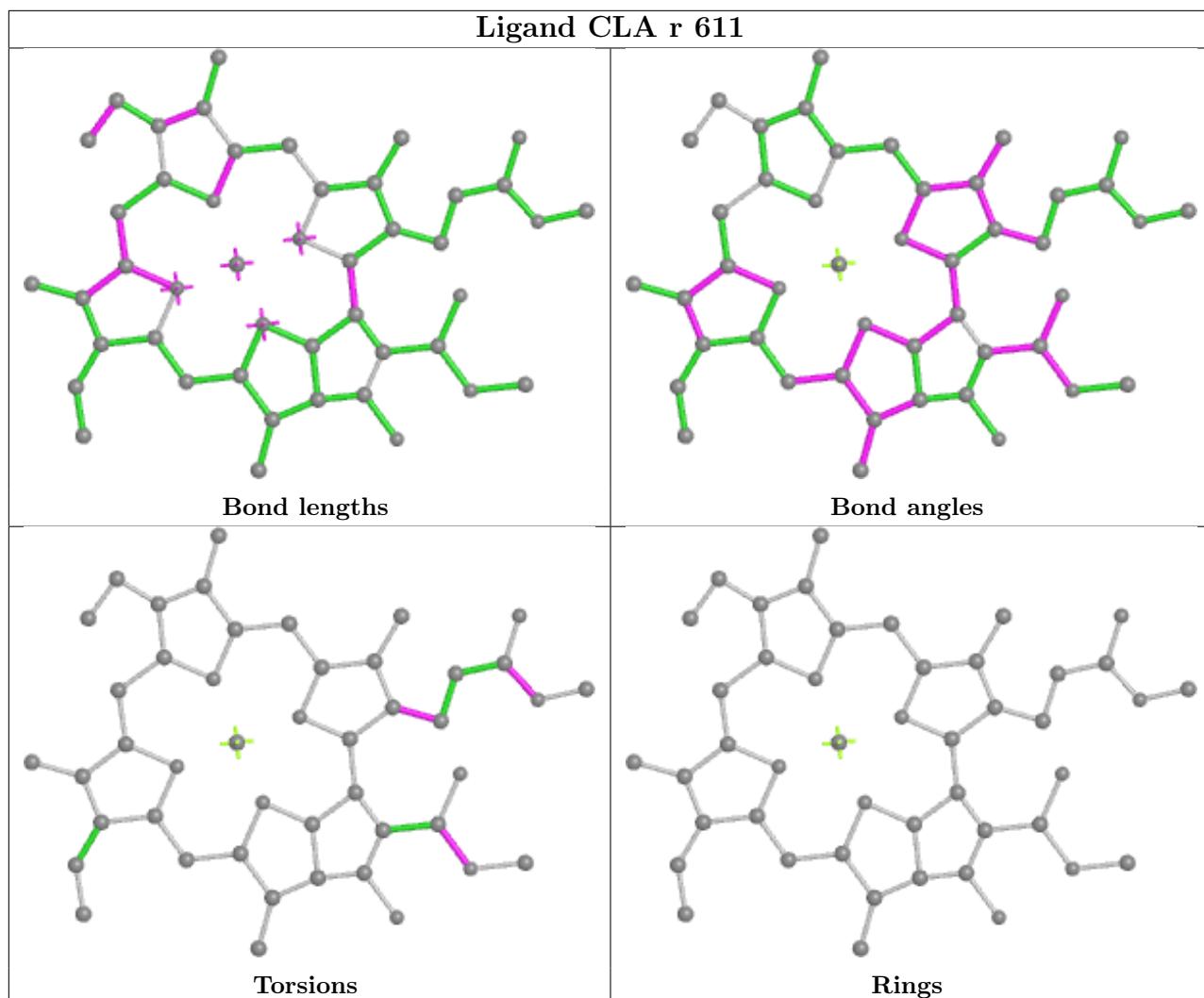
No monomer is involved in short contacts.

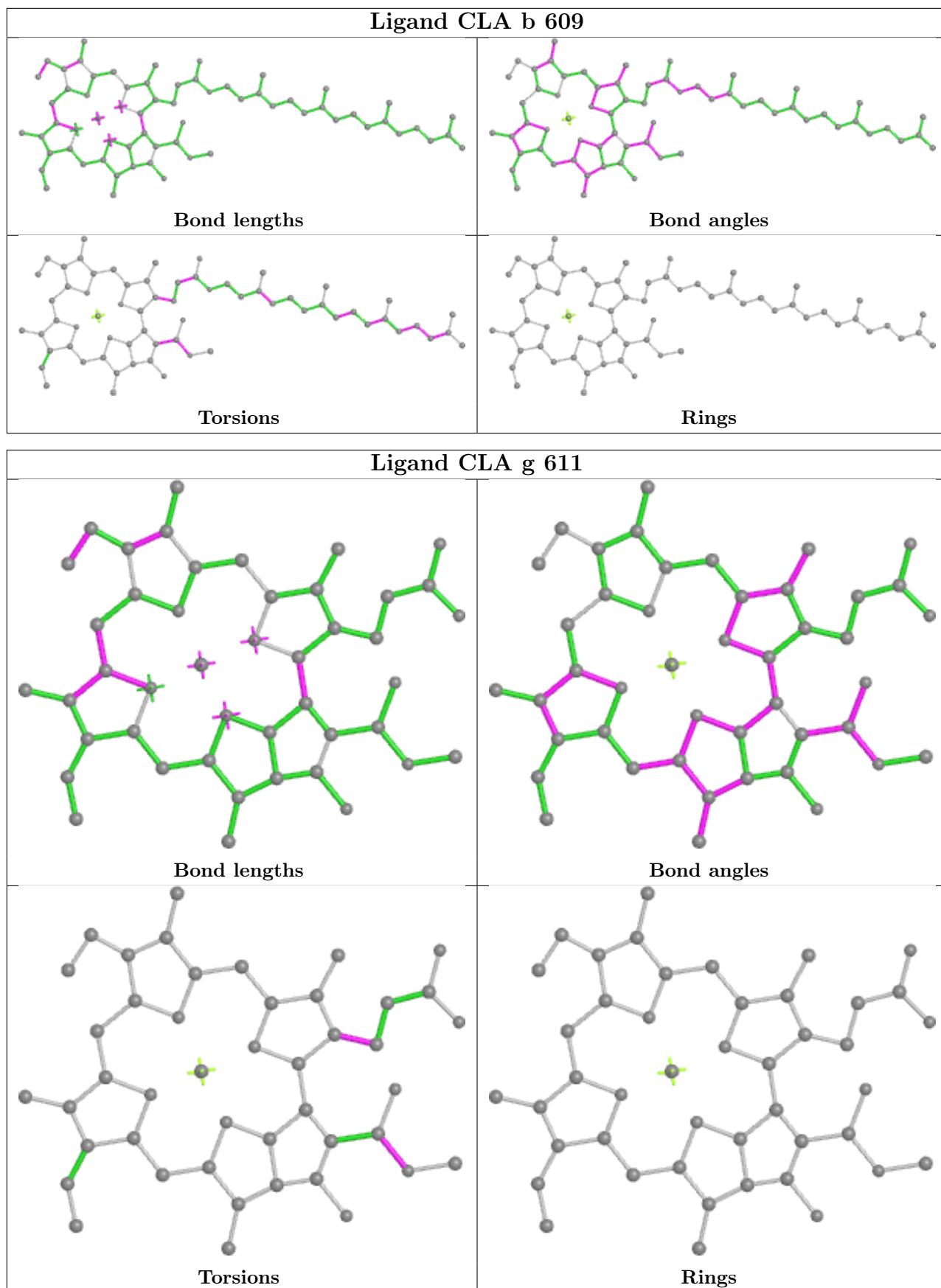
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

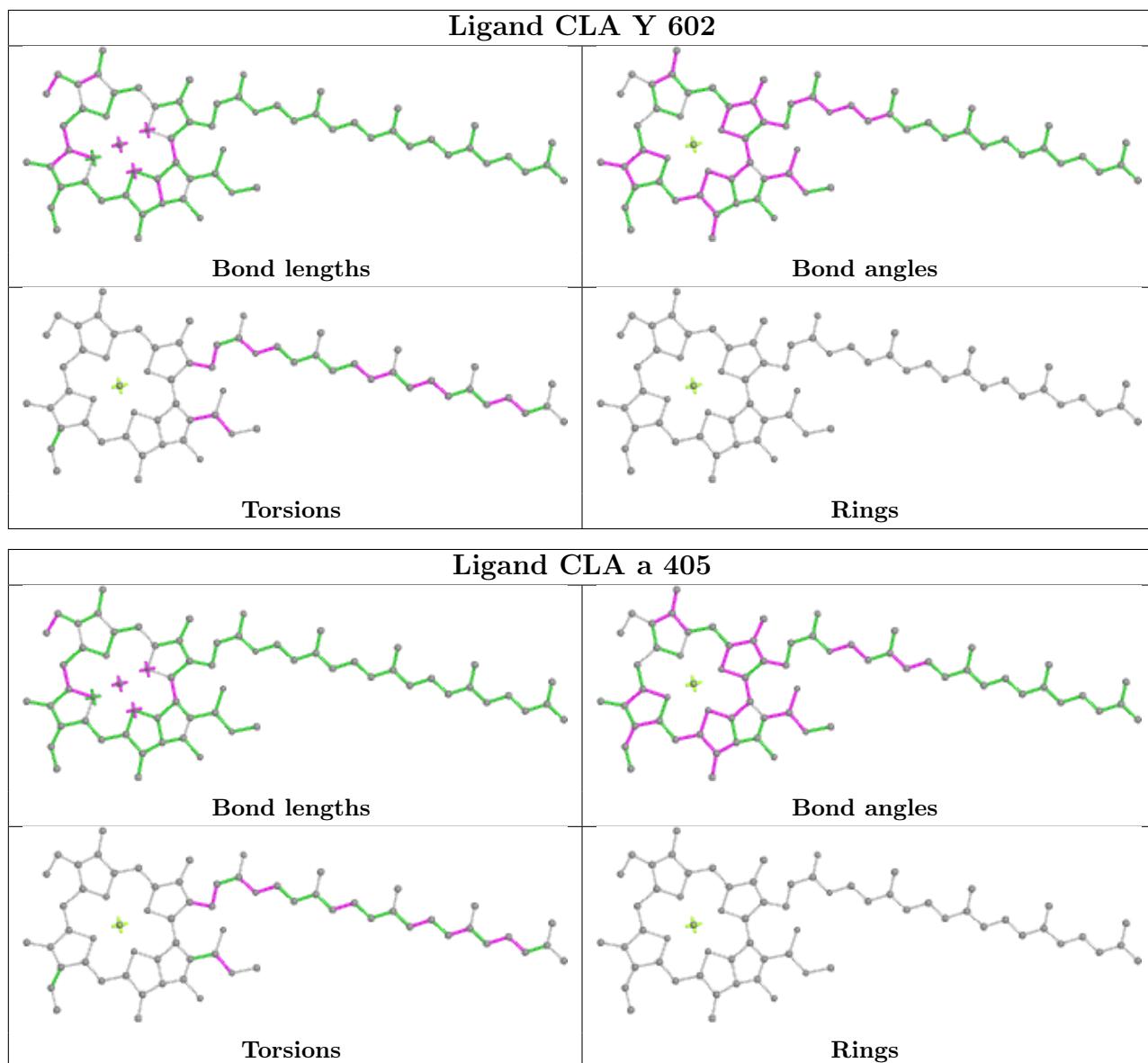


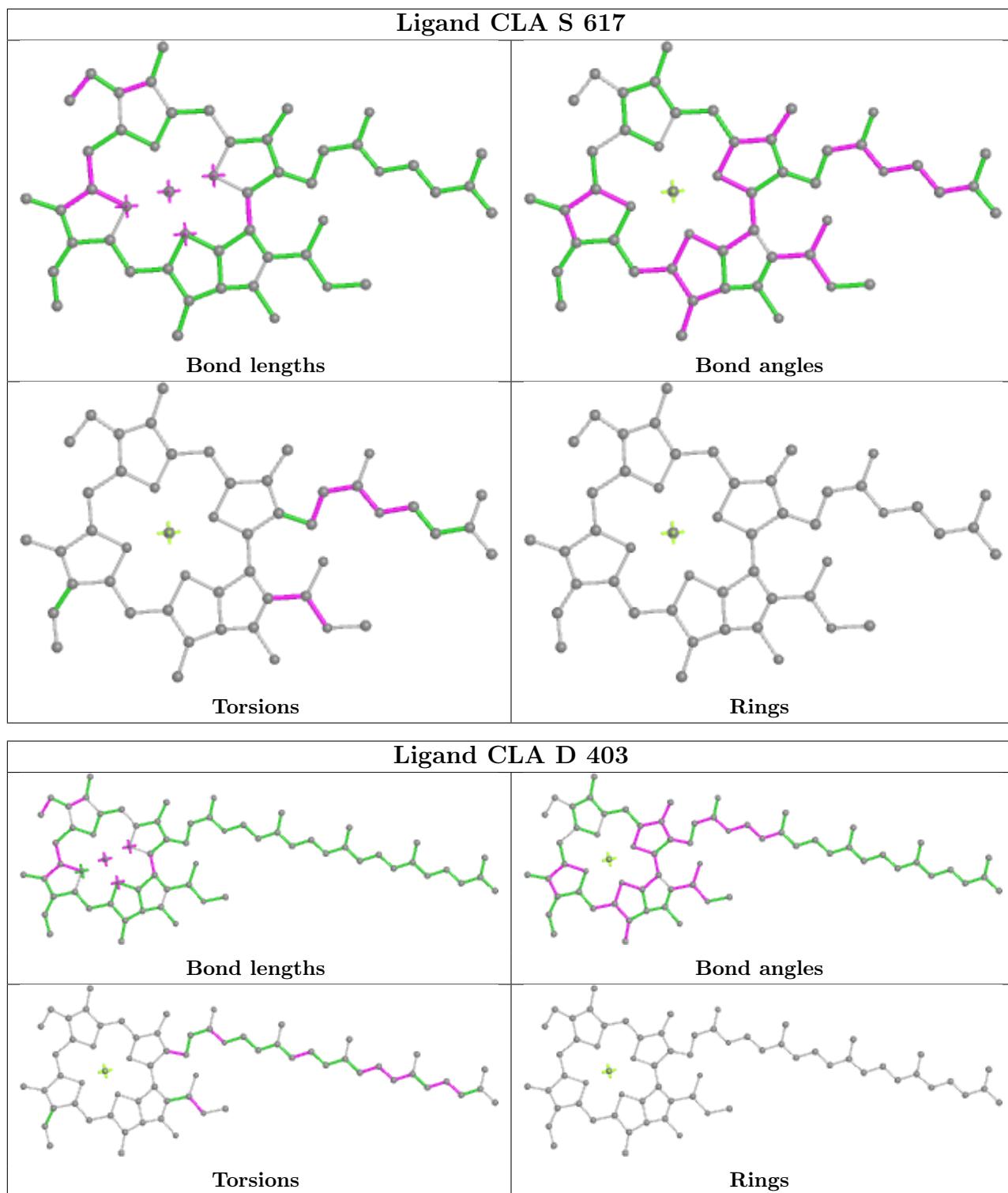


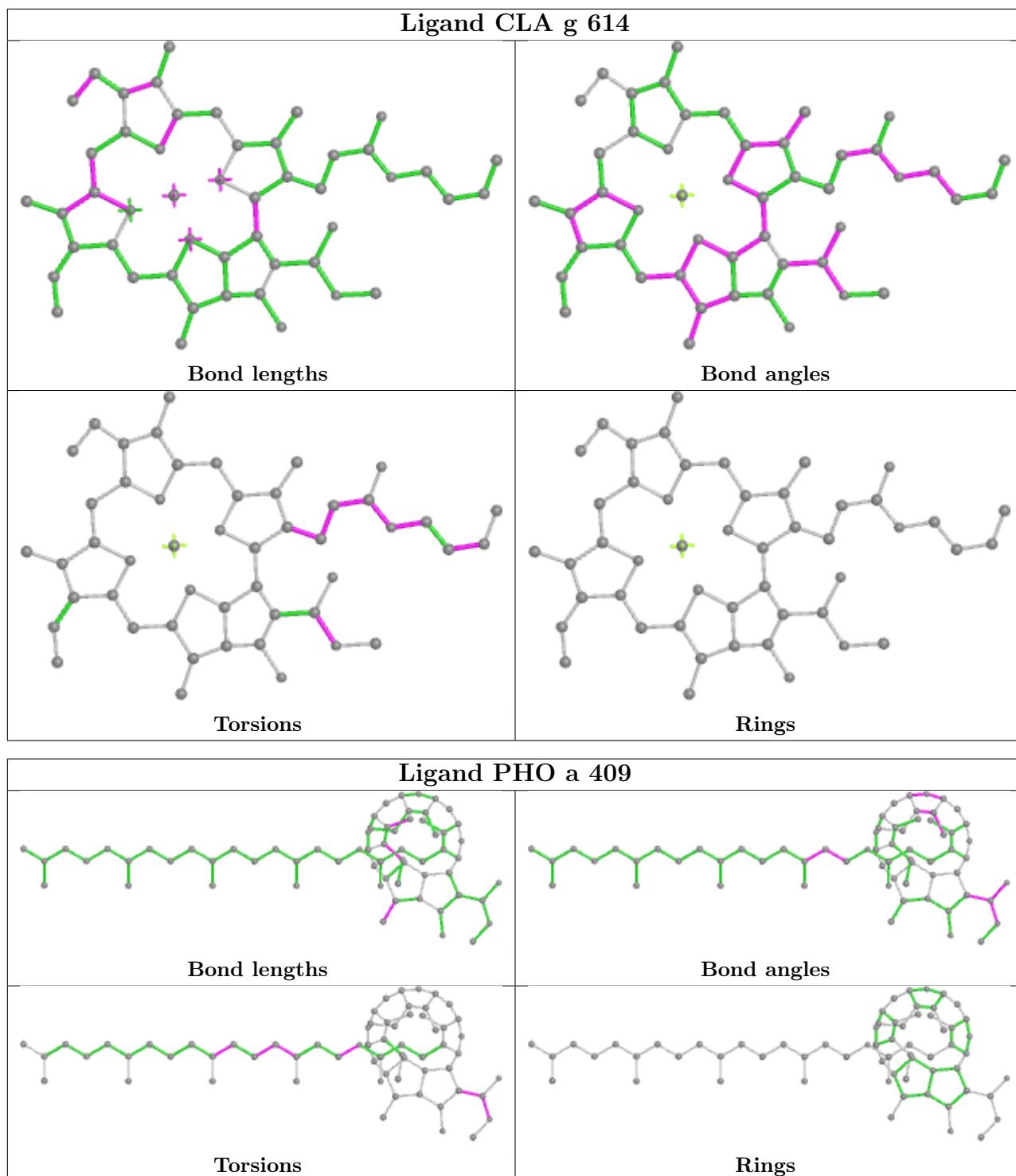


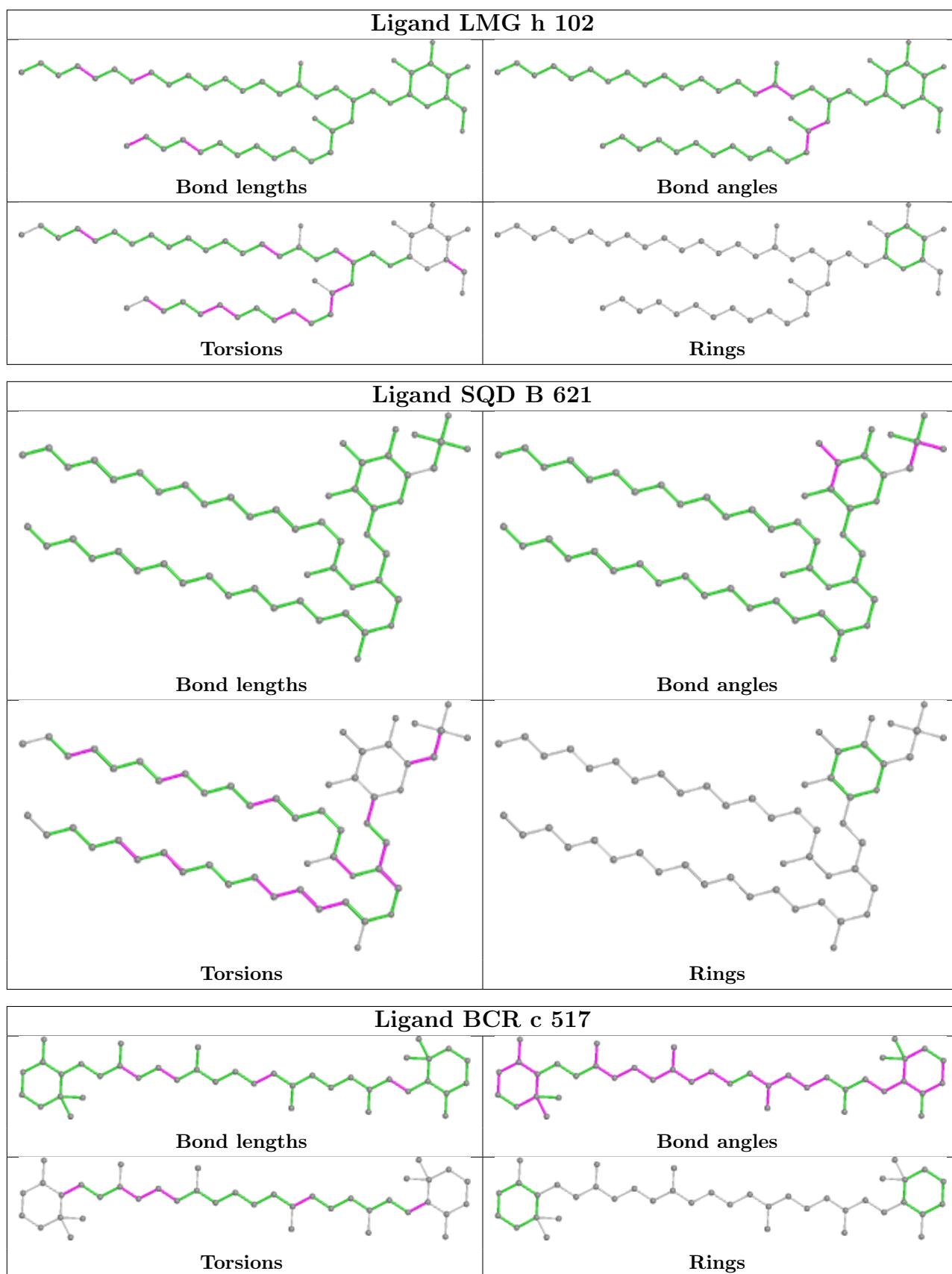


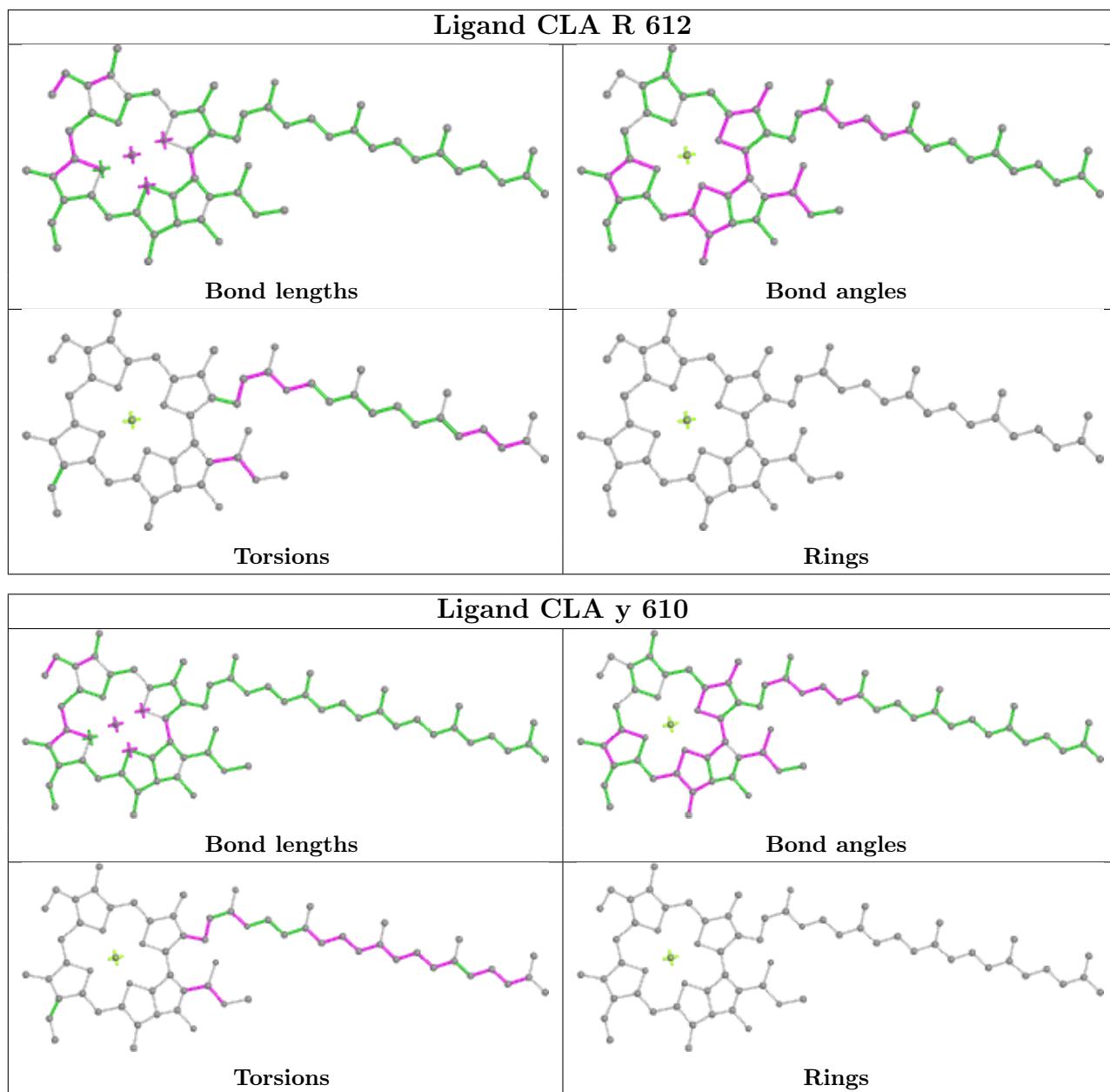


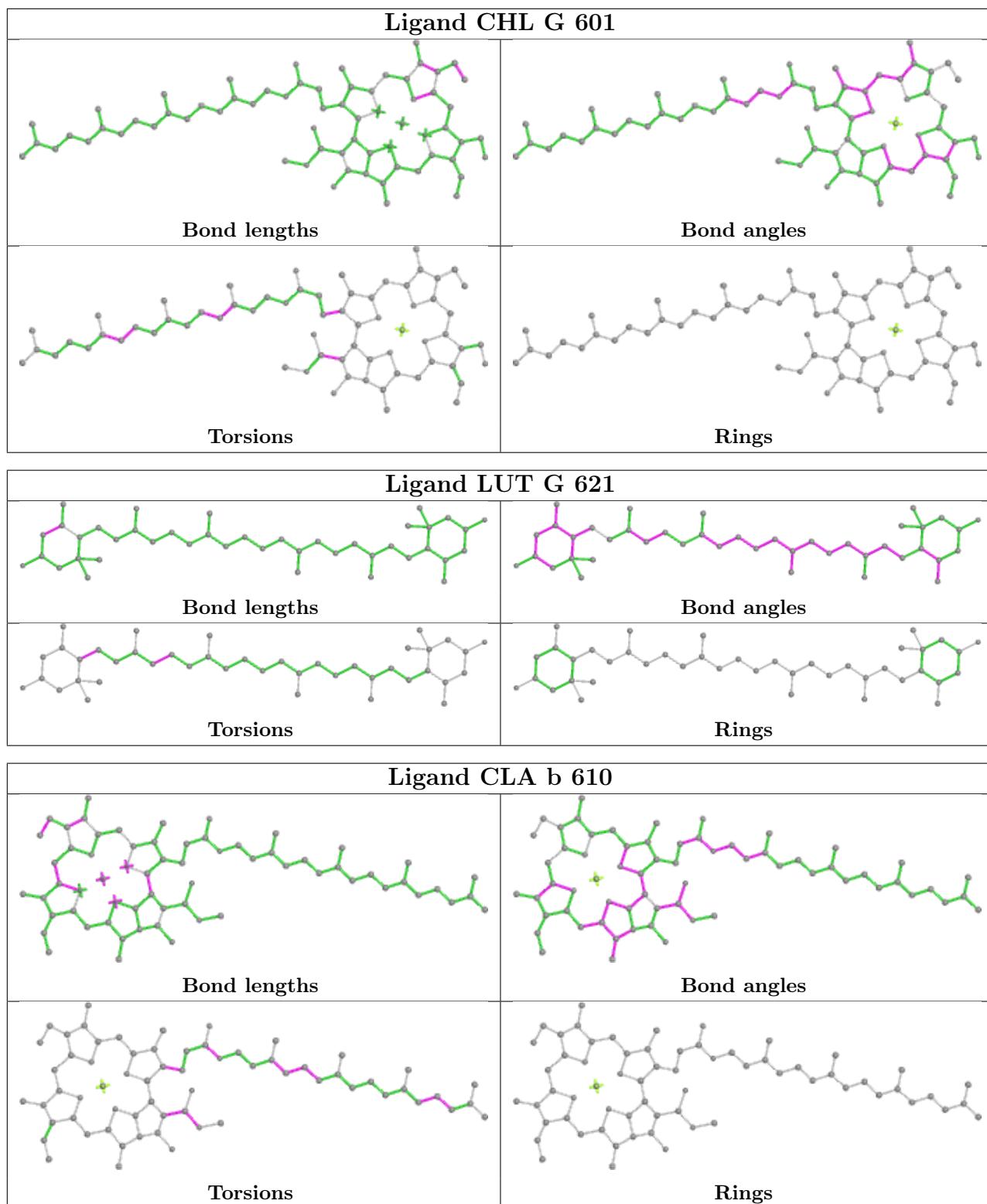


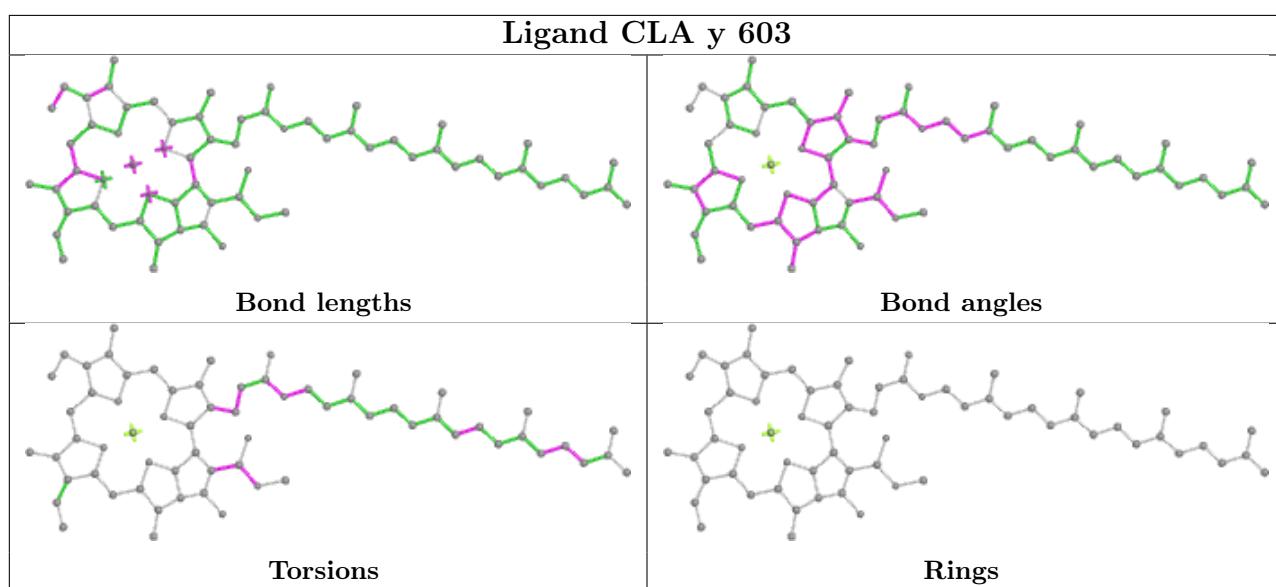
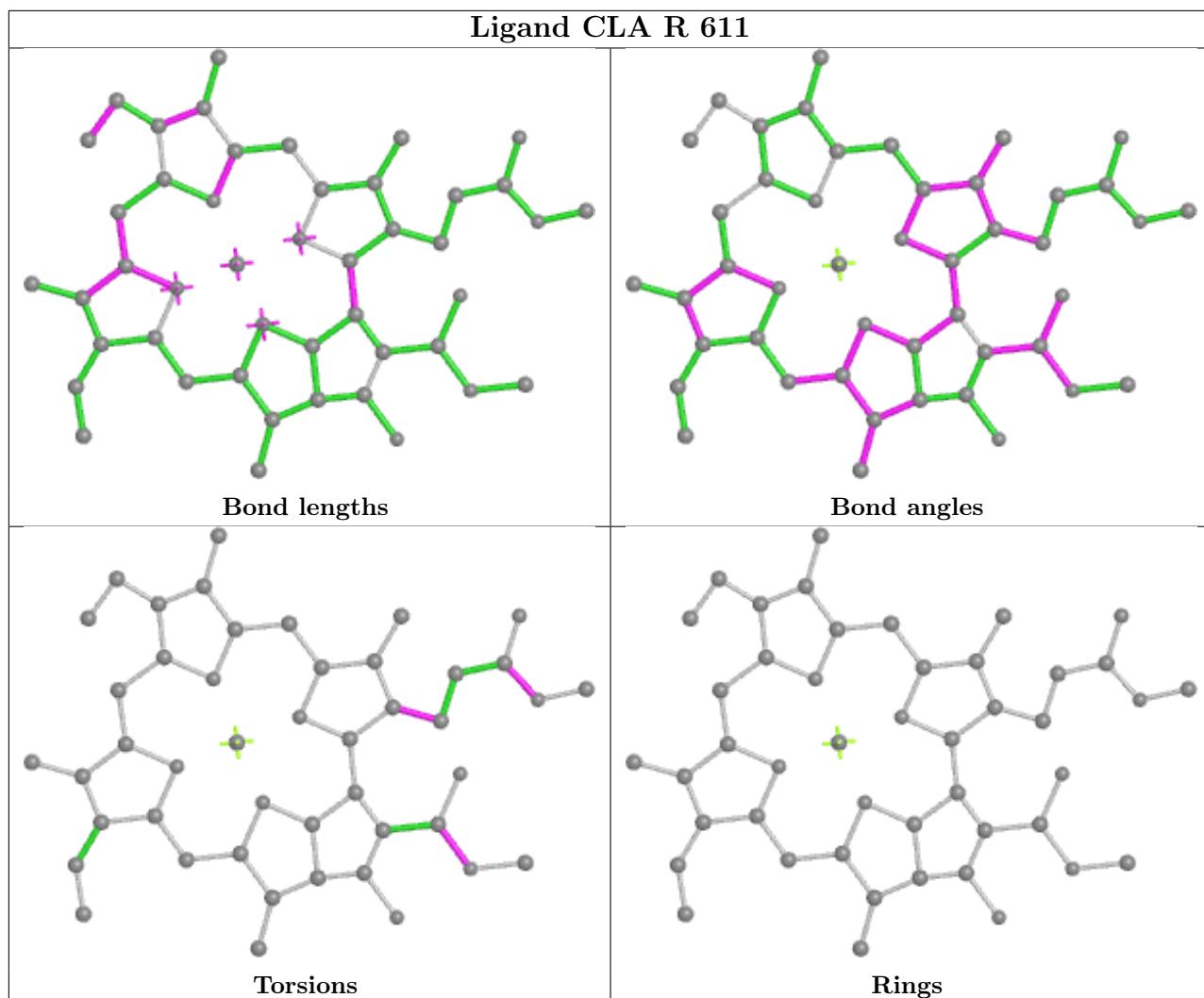


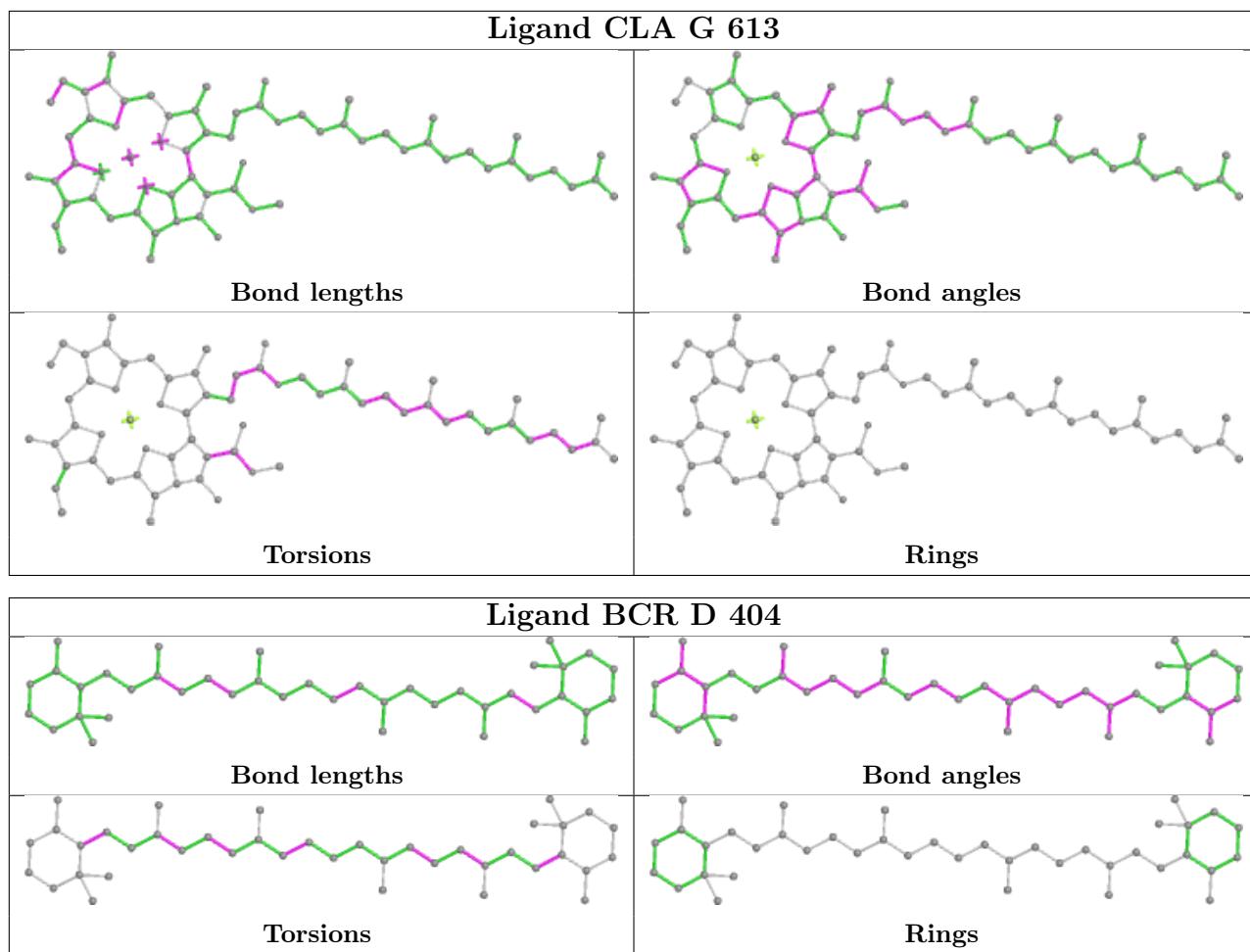


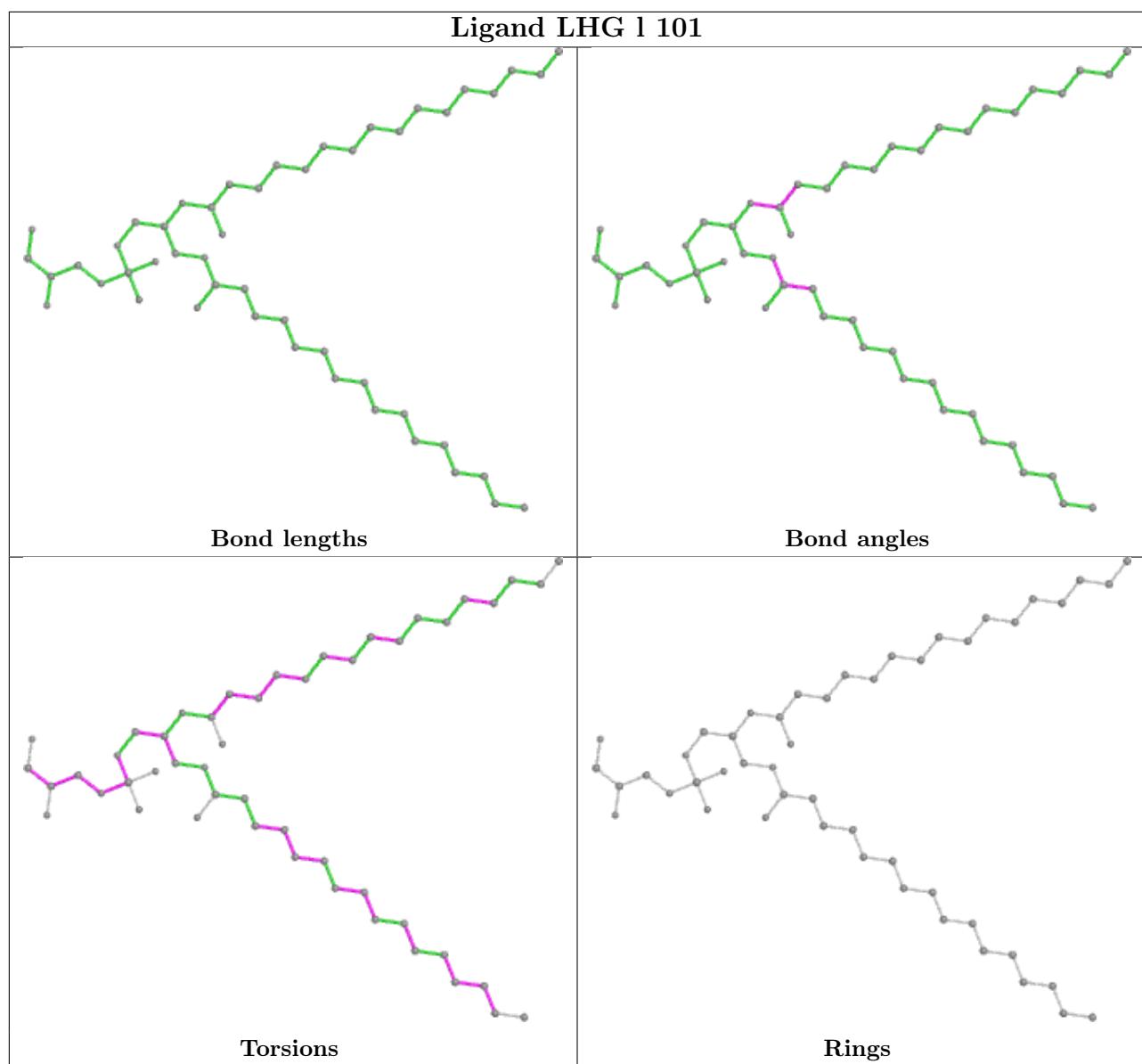


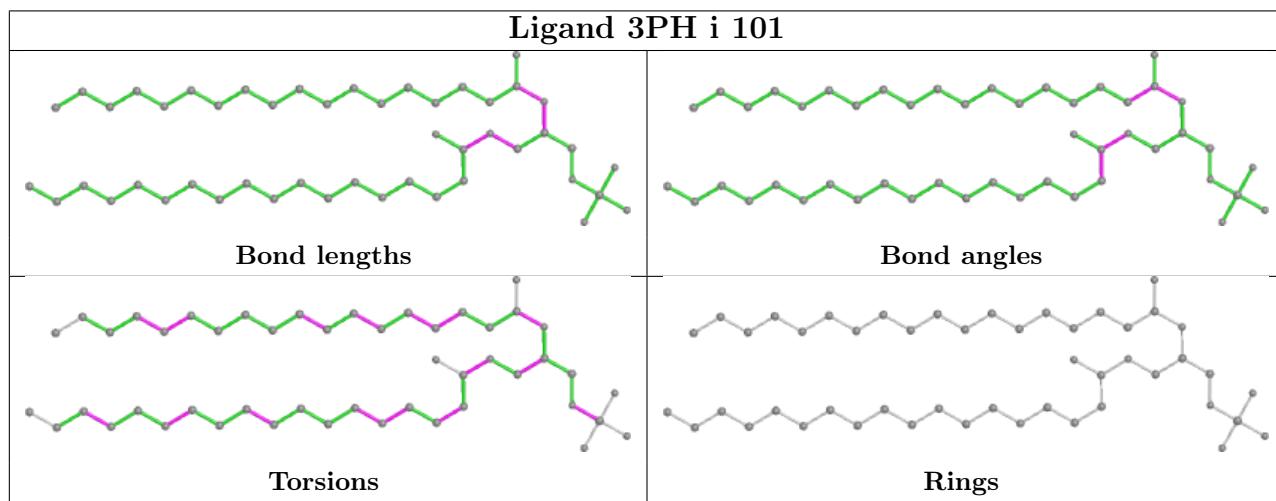
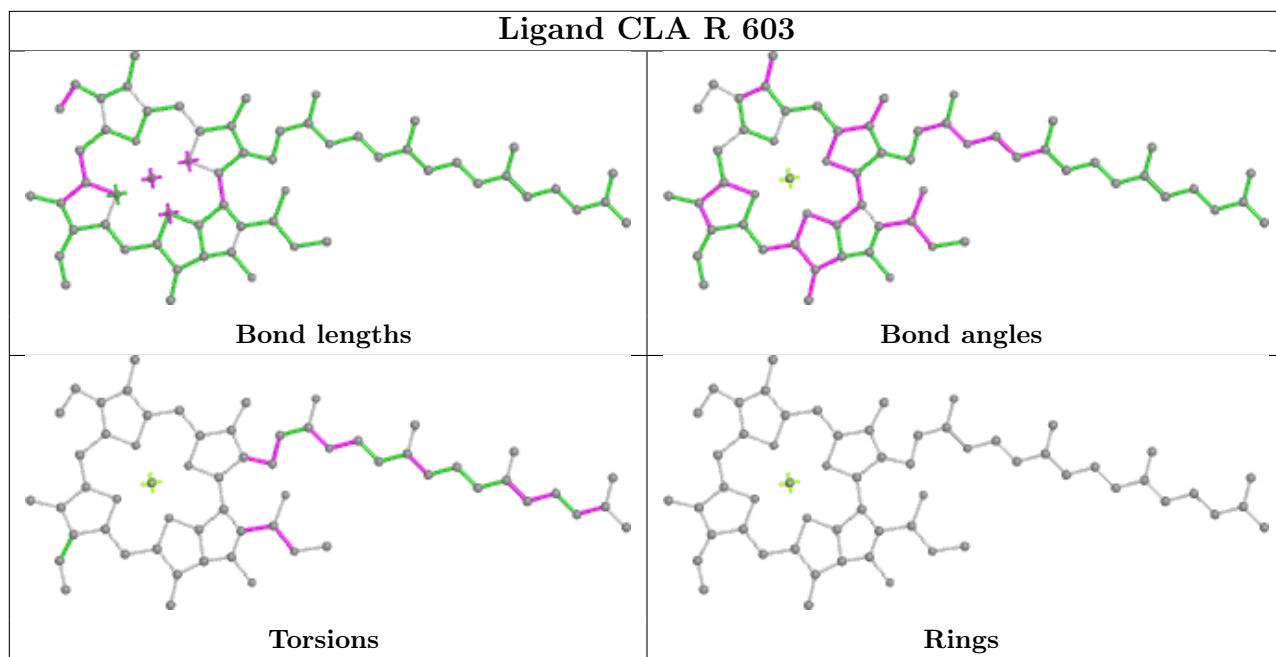


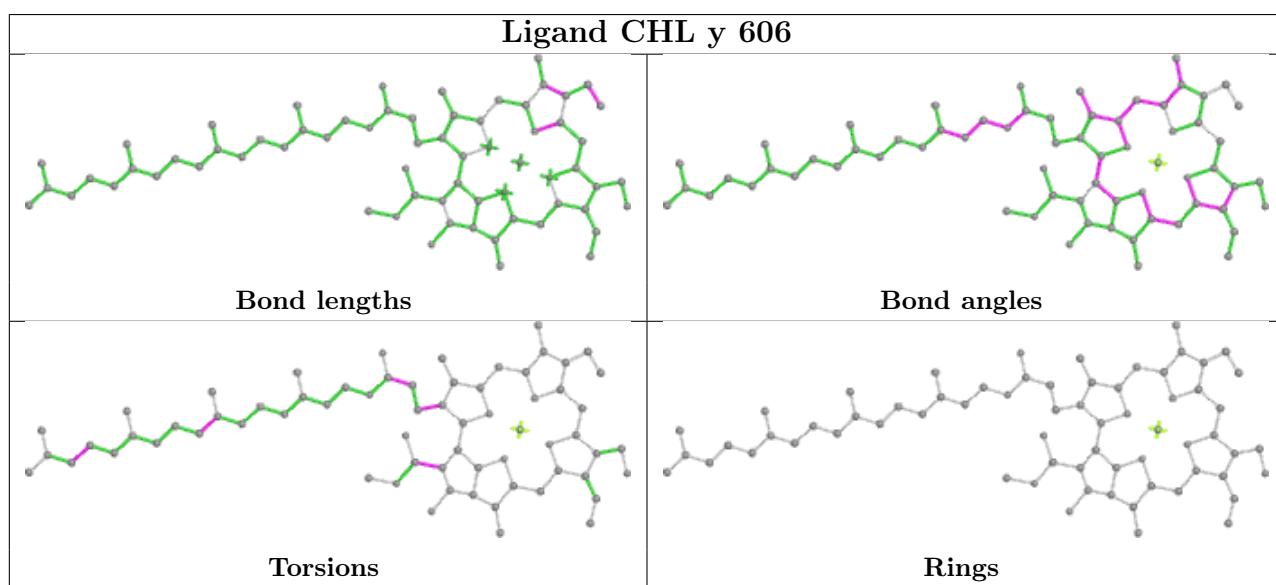
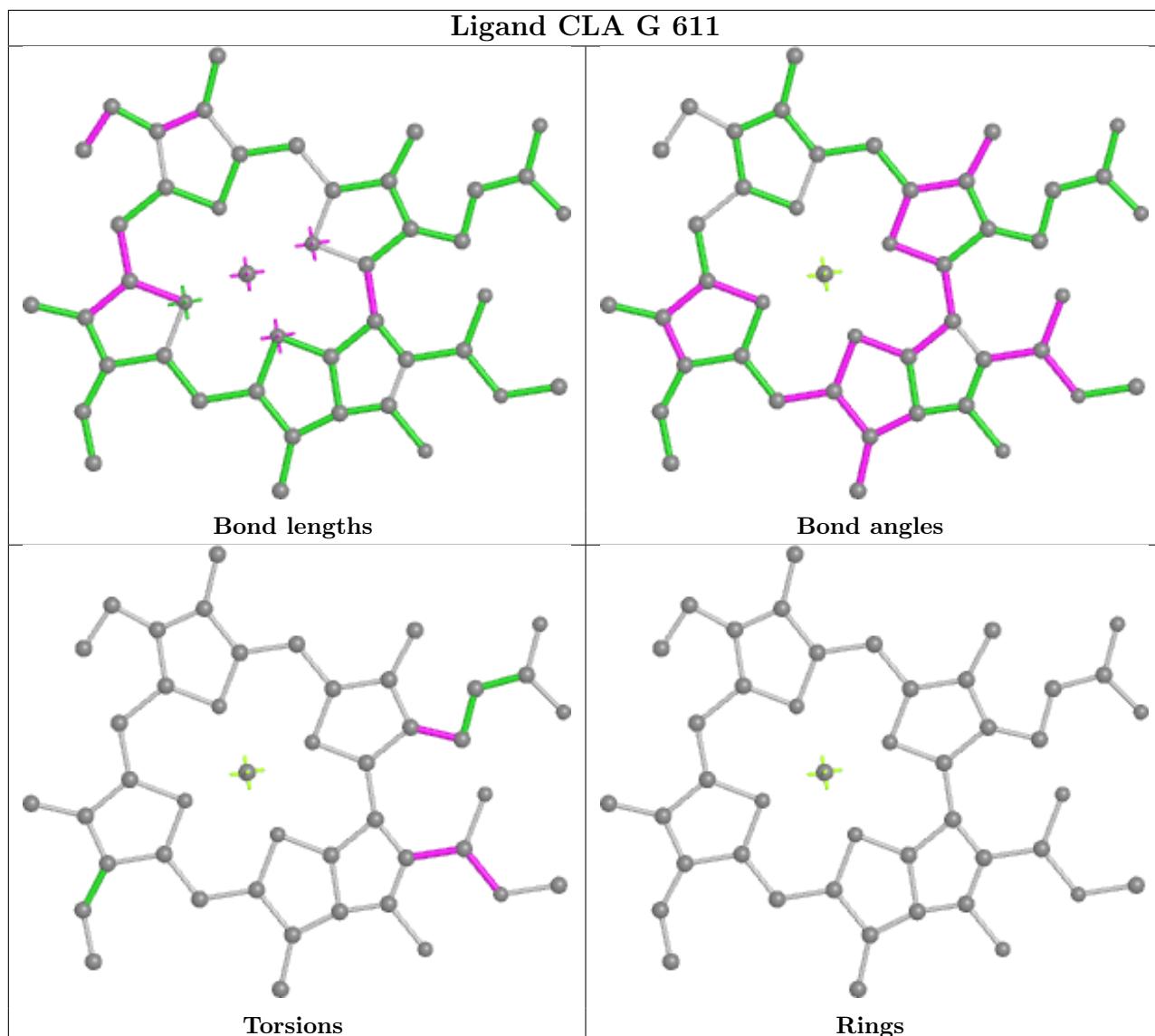


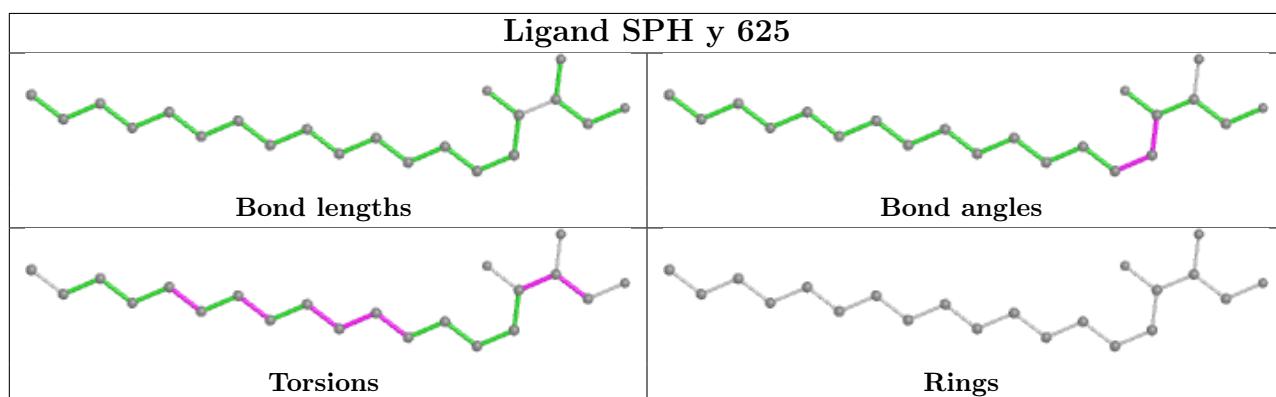
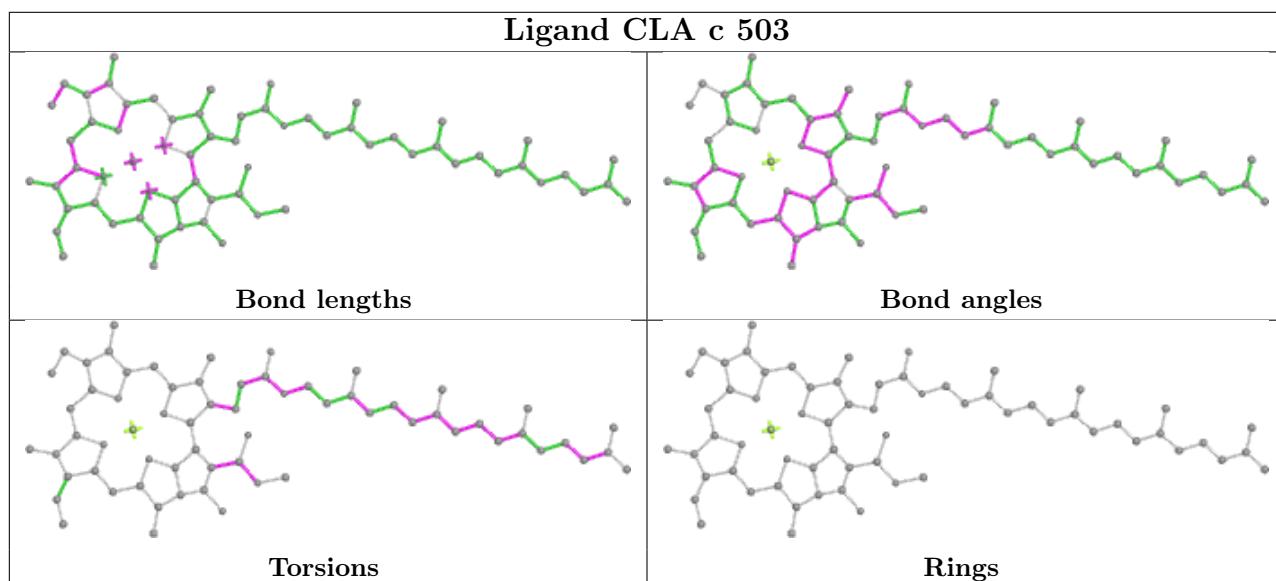
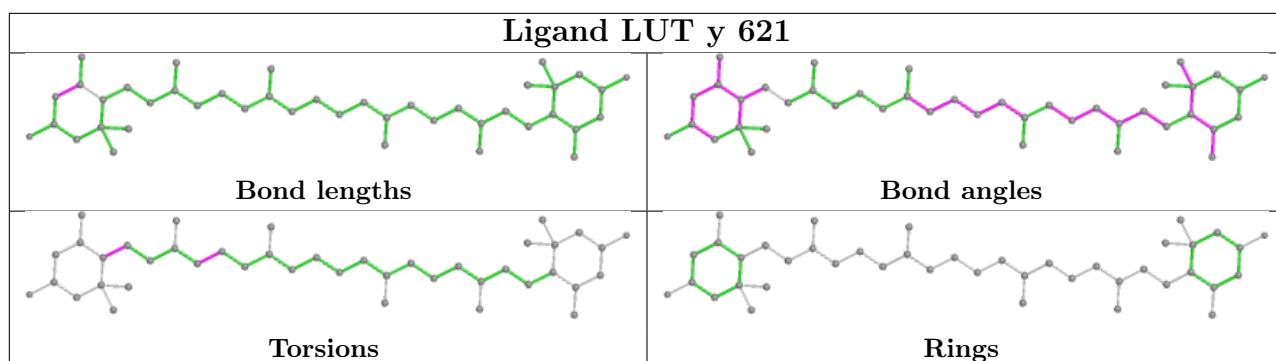


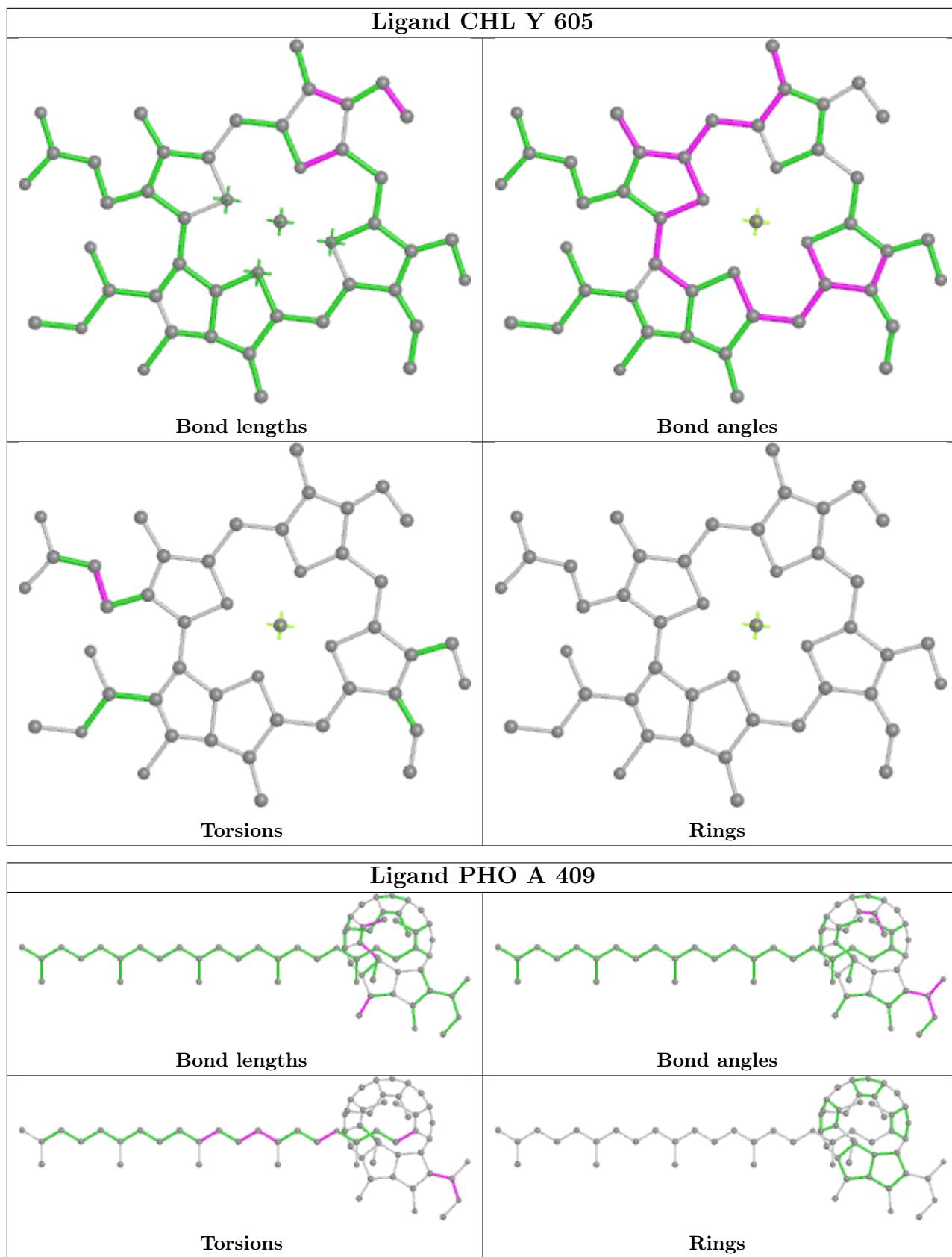


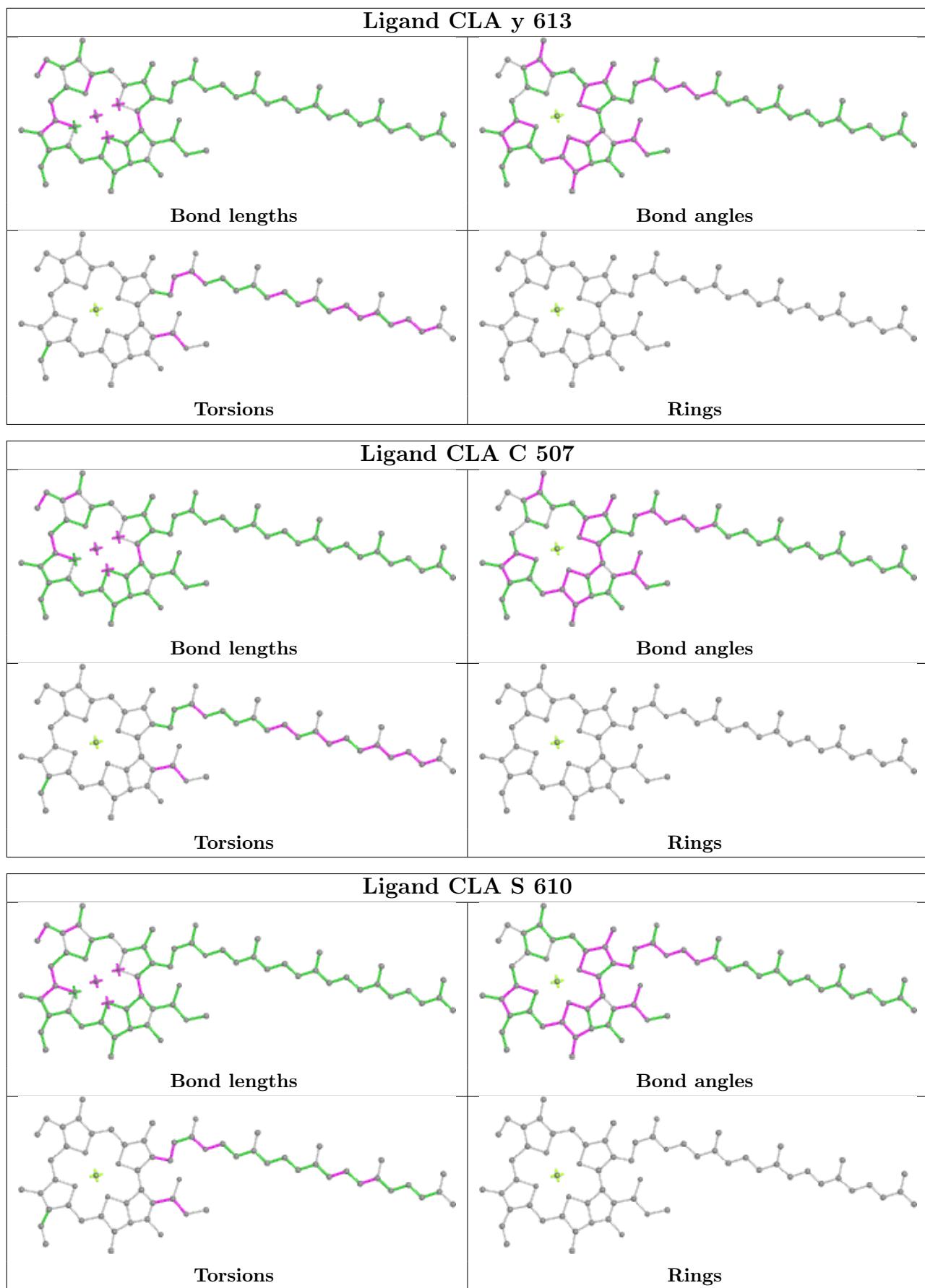


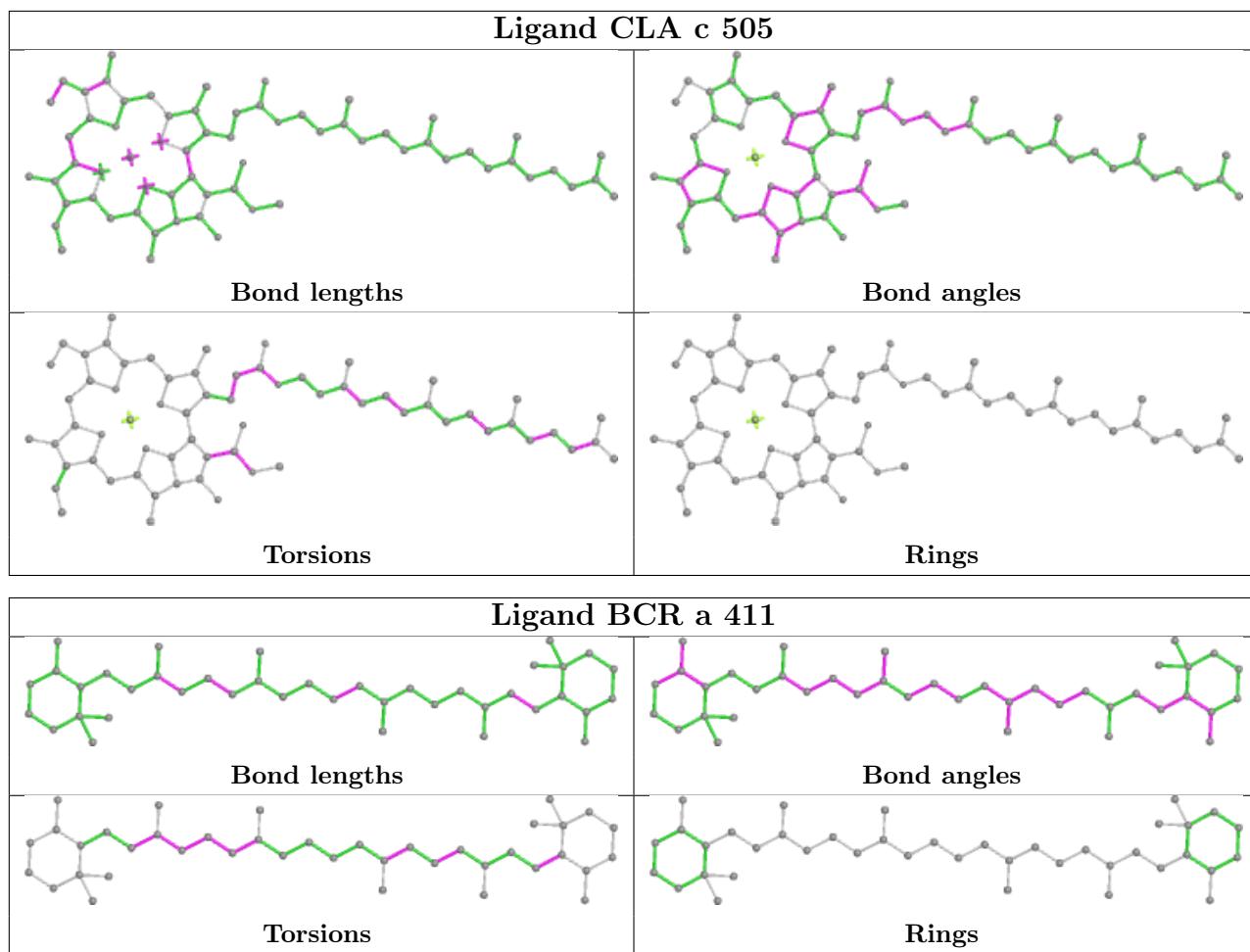


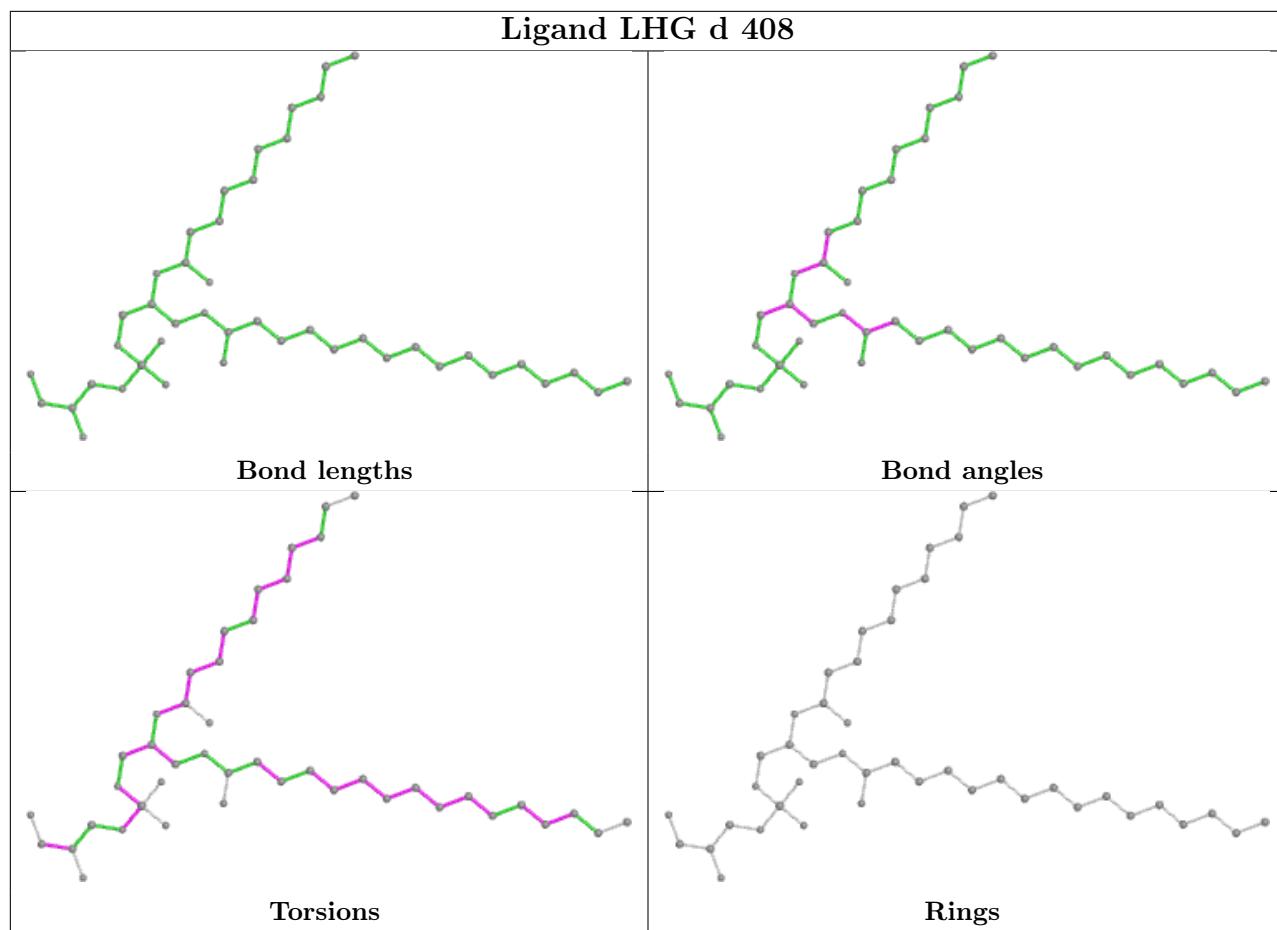


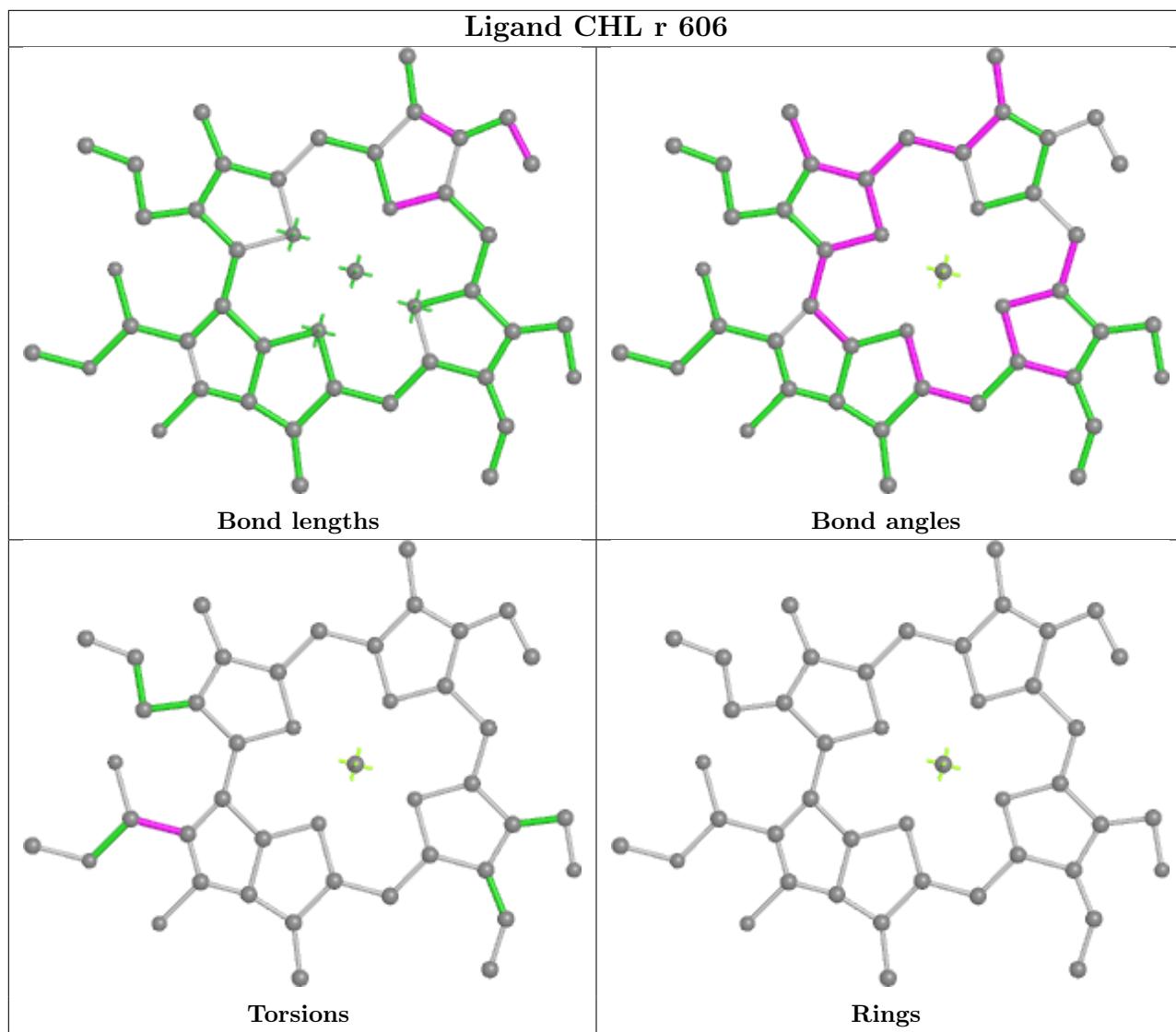


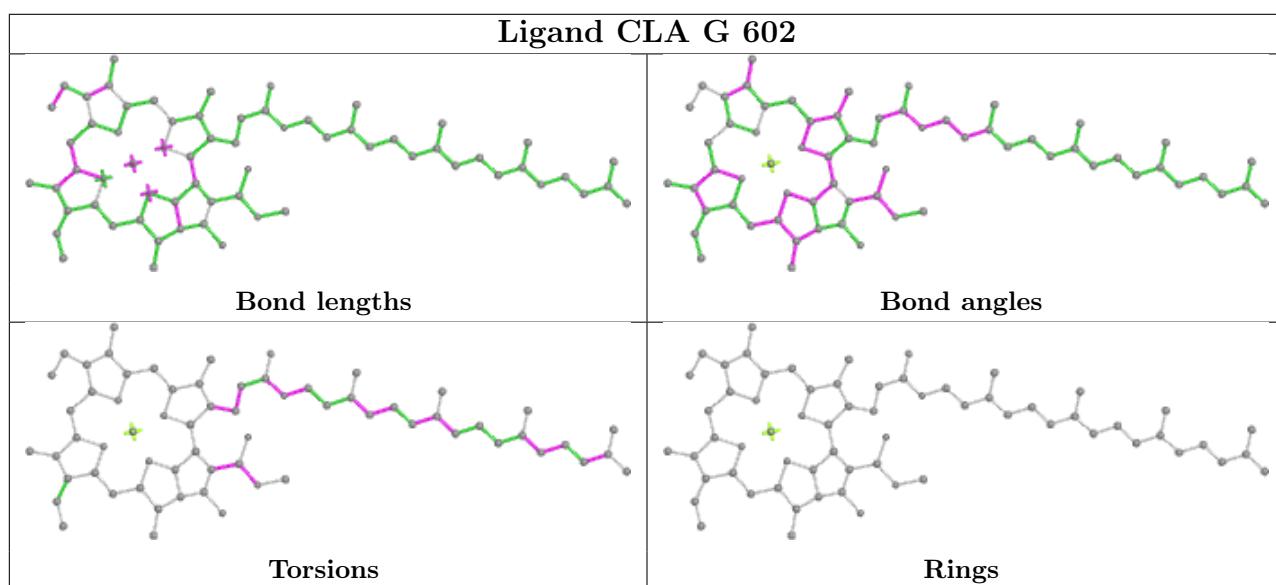
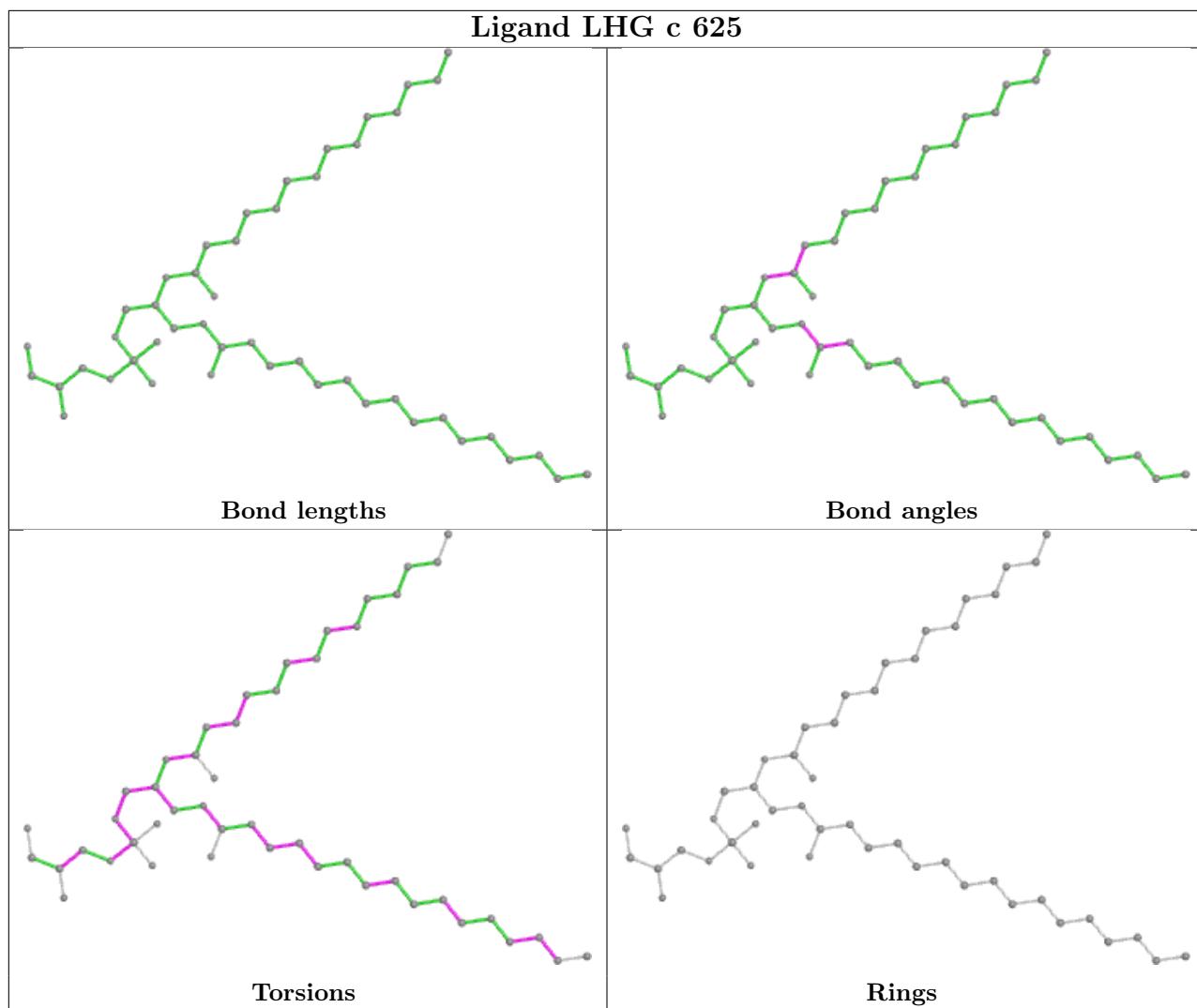


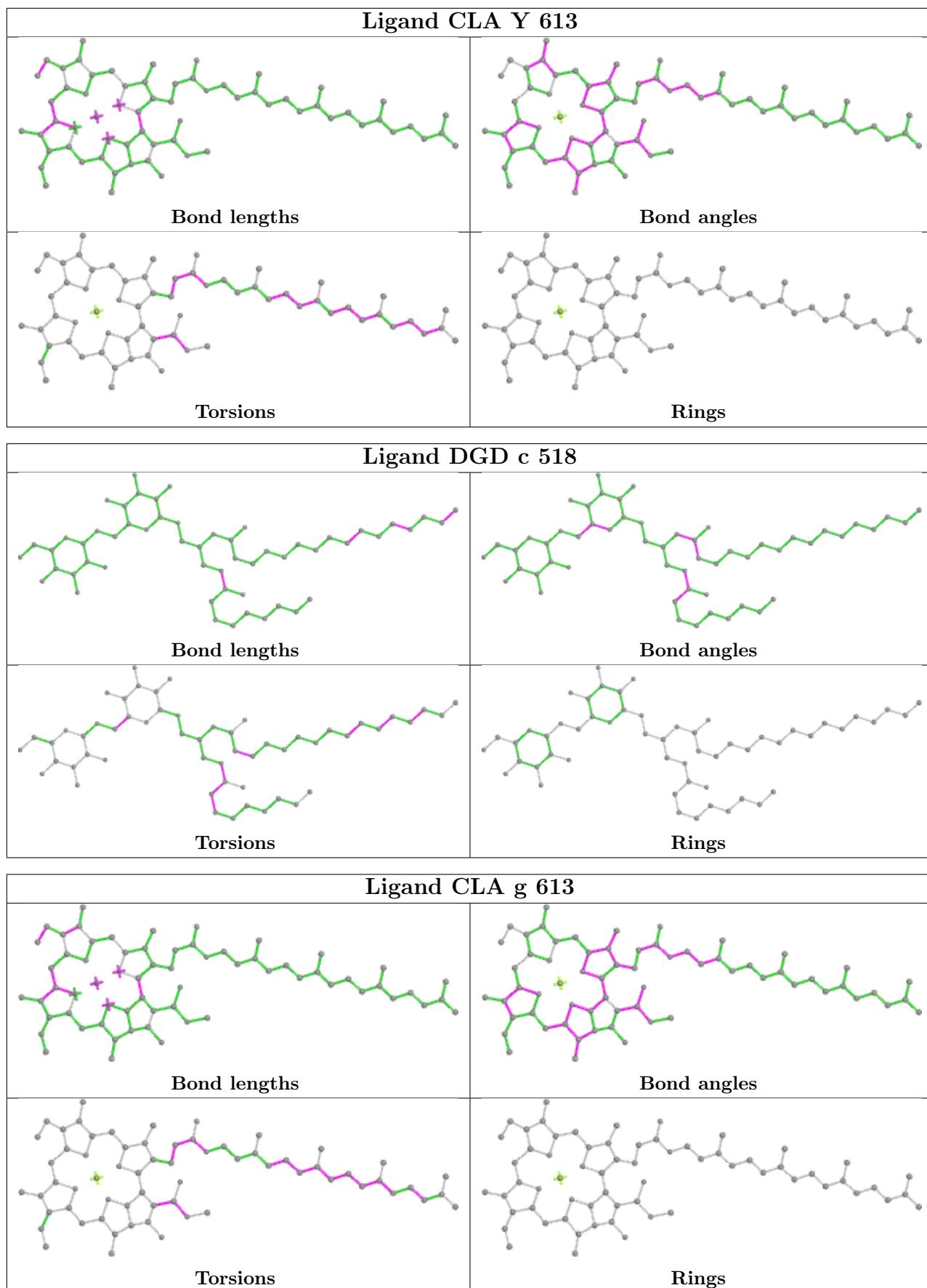


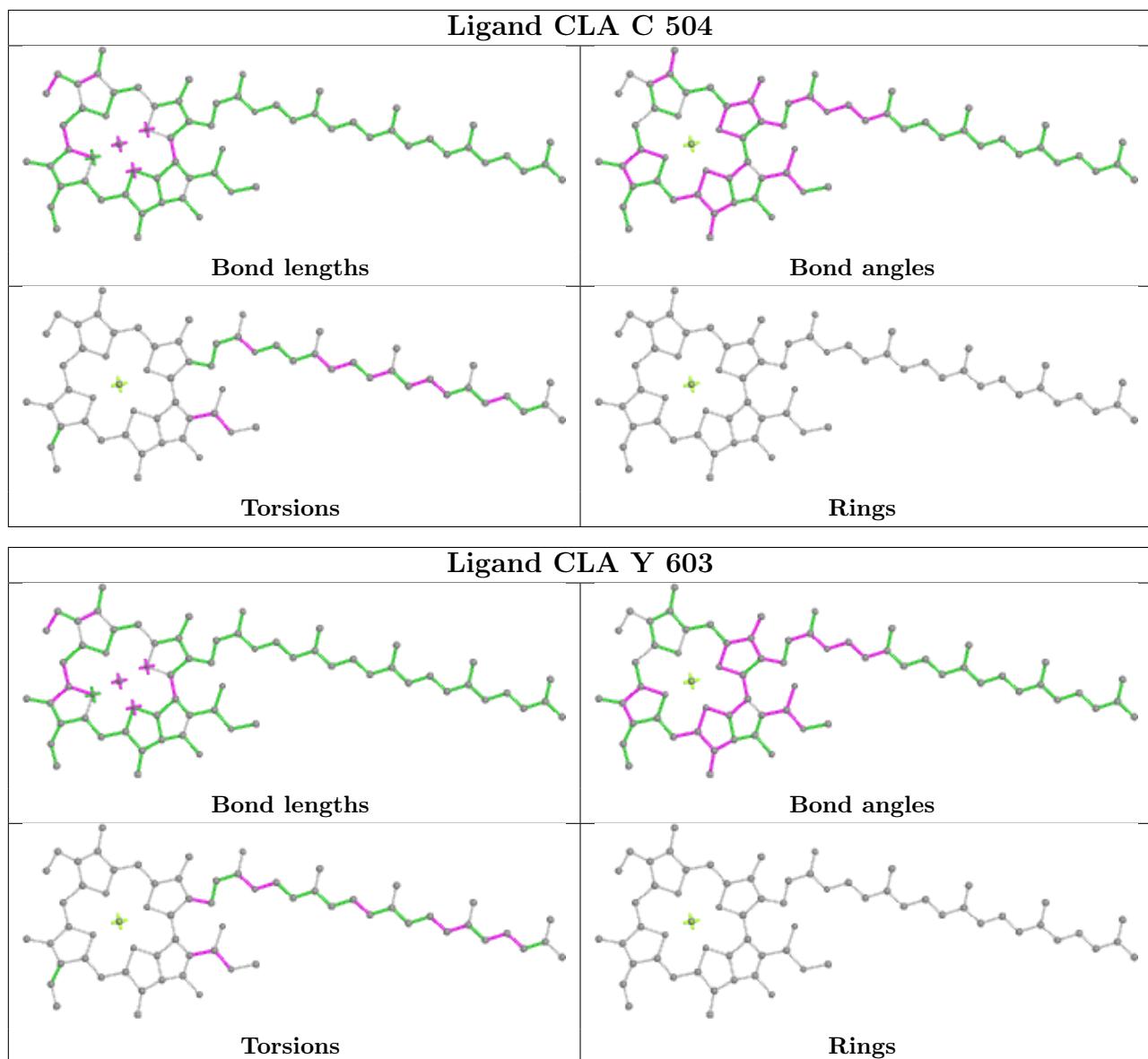


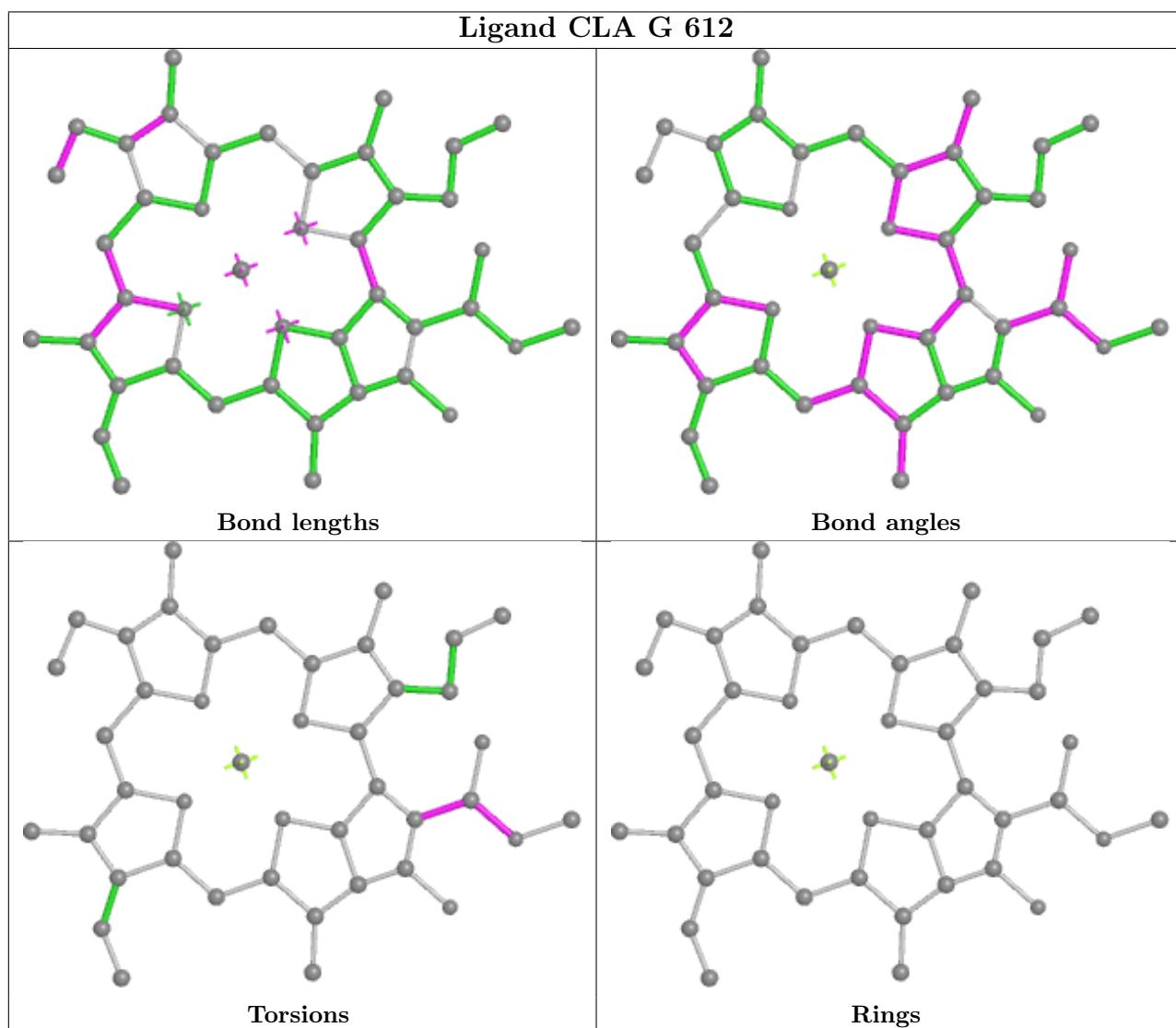
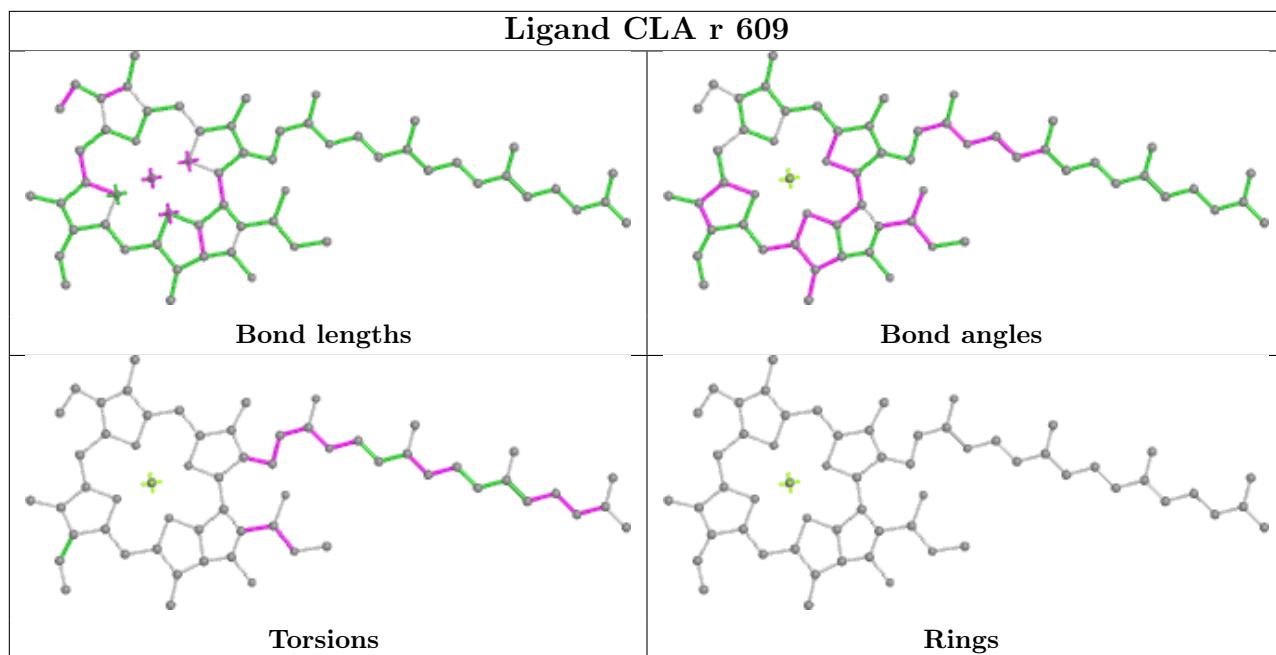


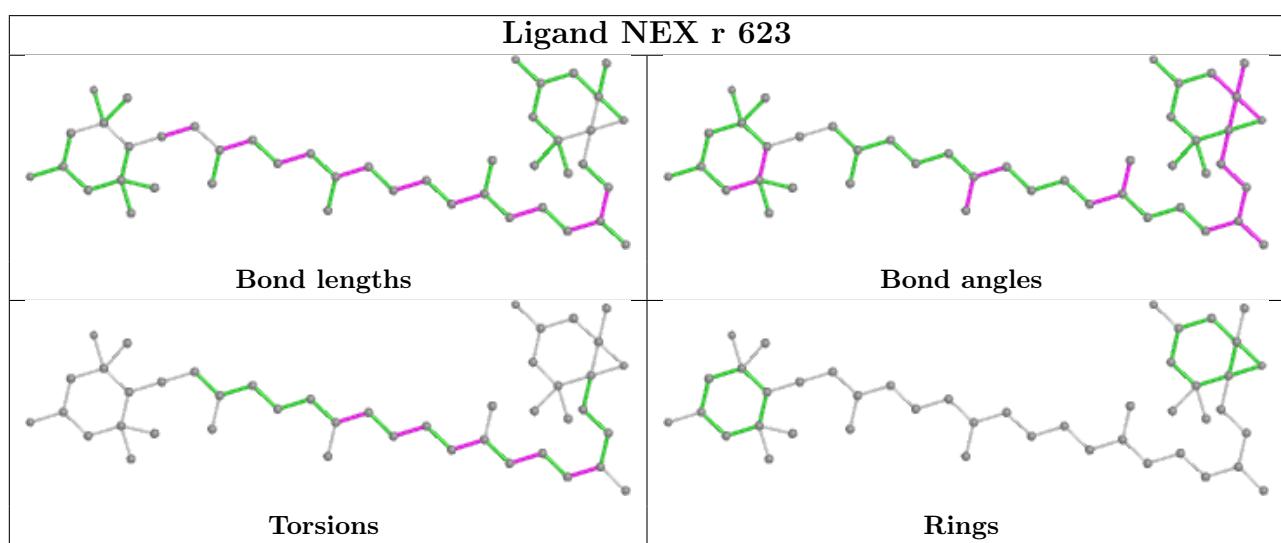
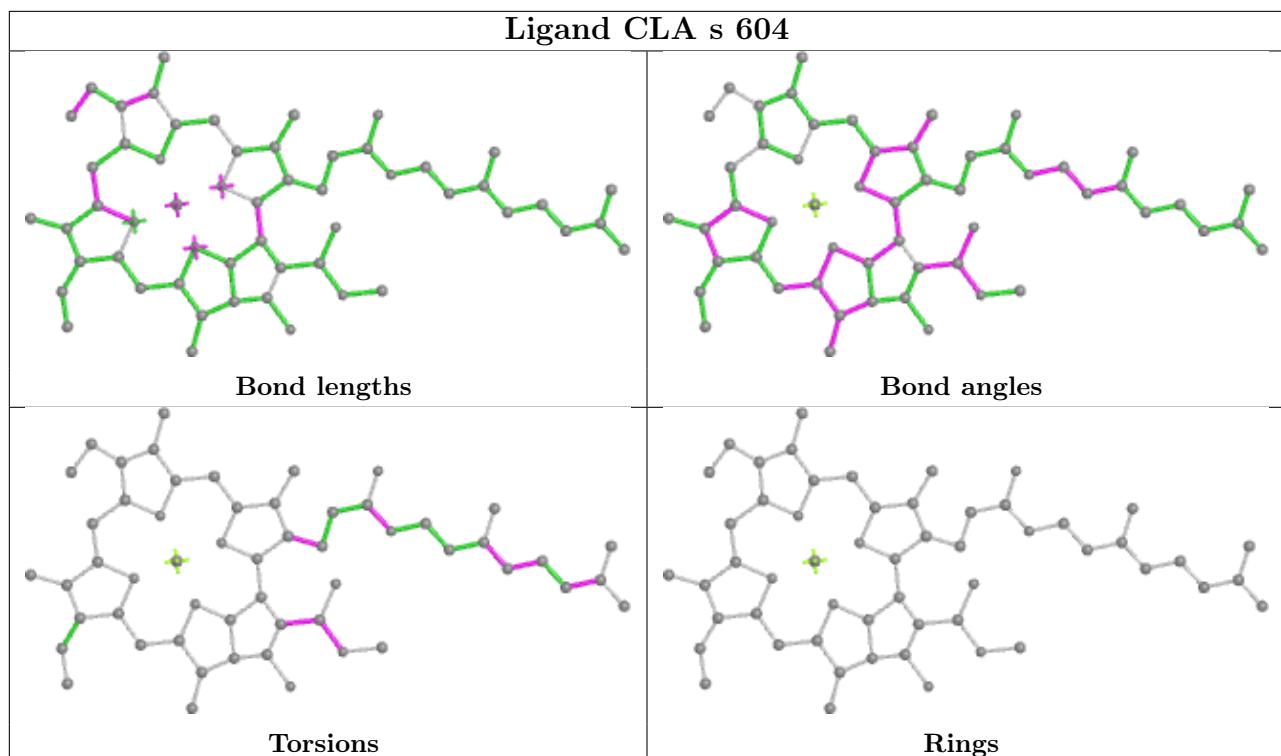


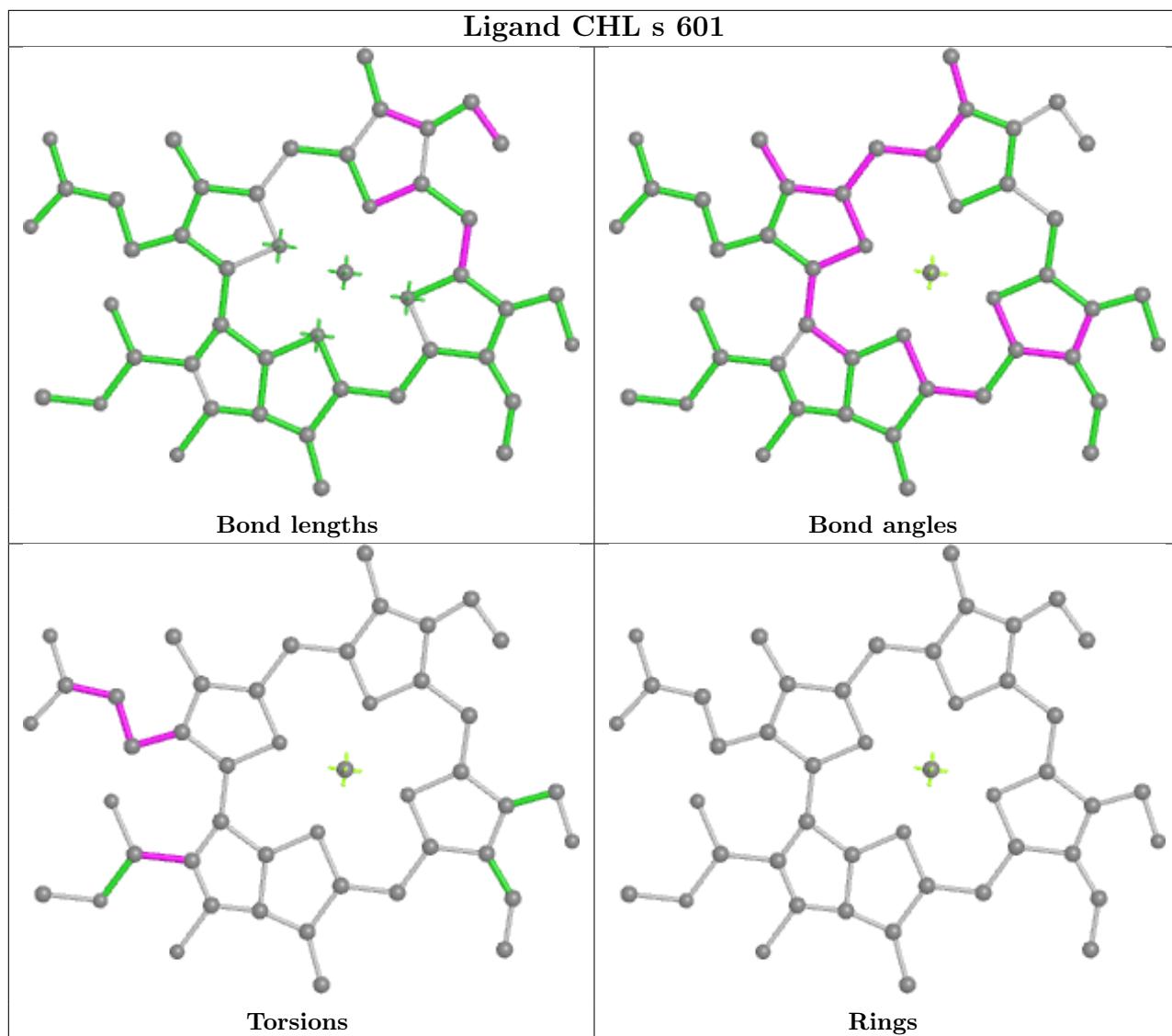


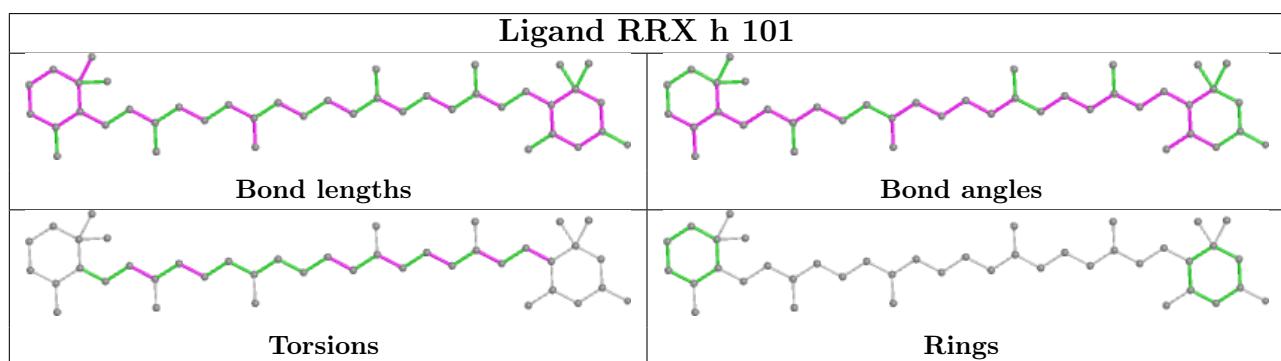
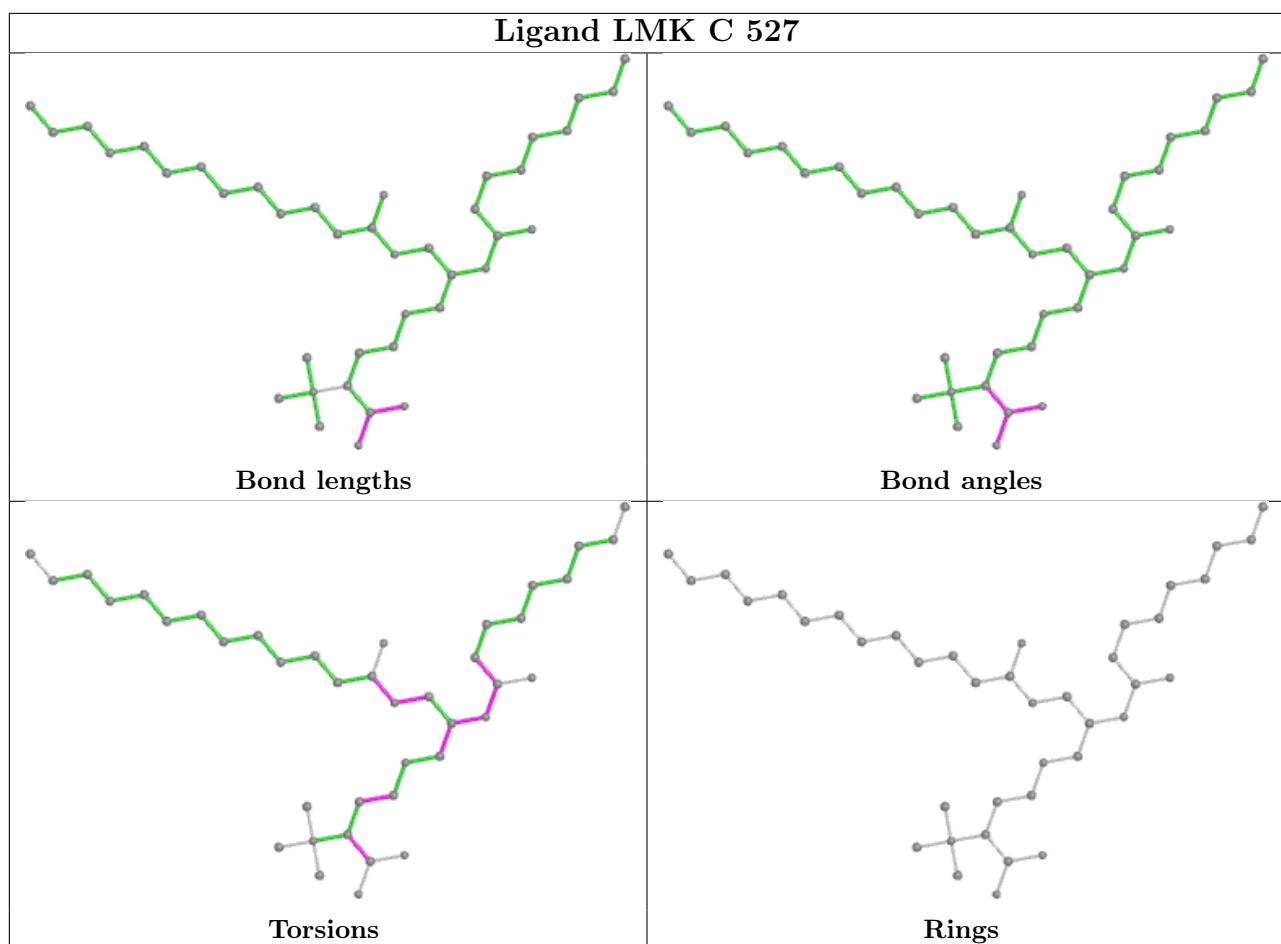


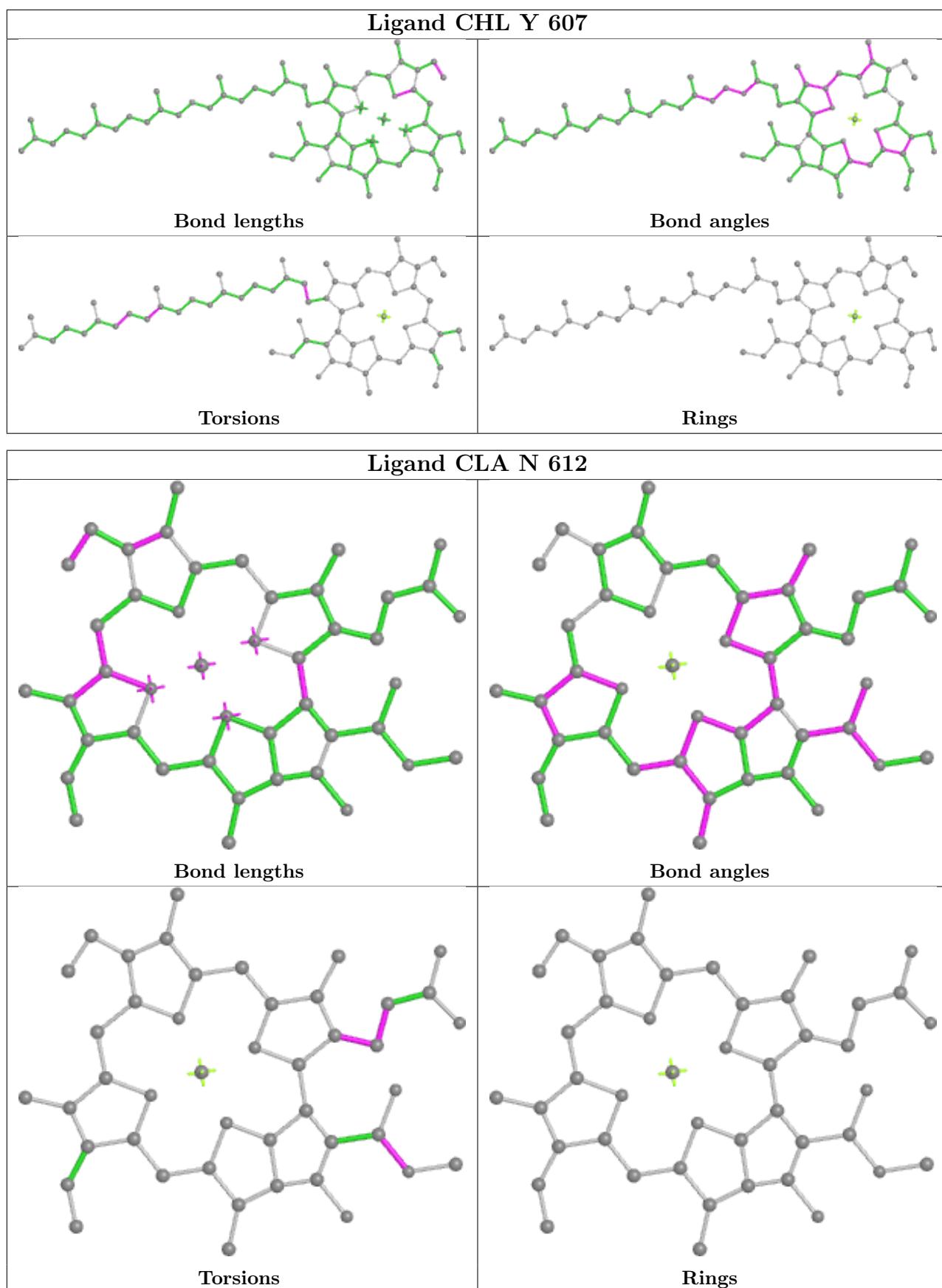


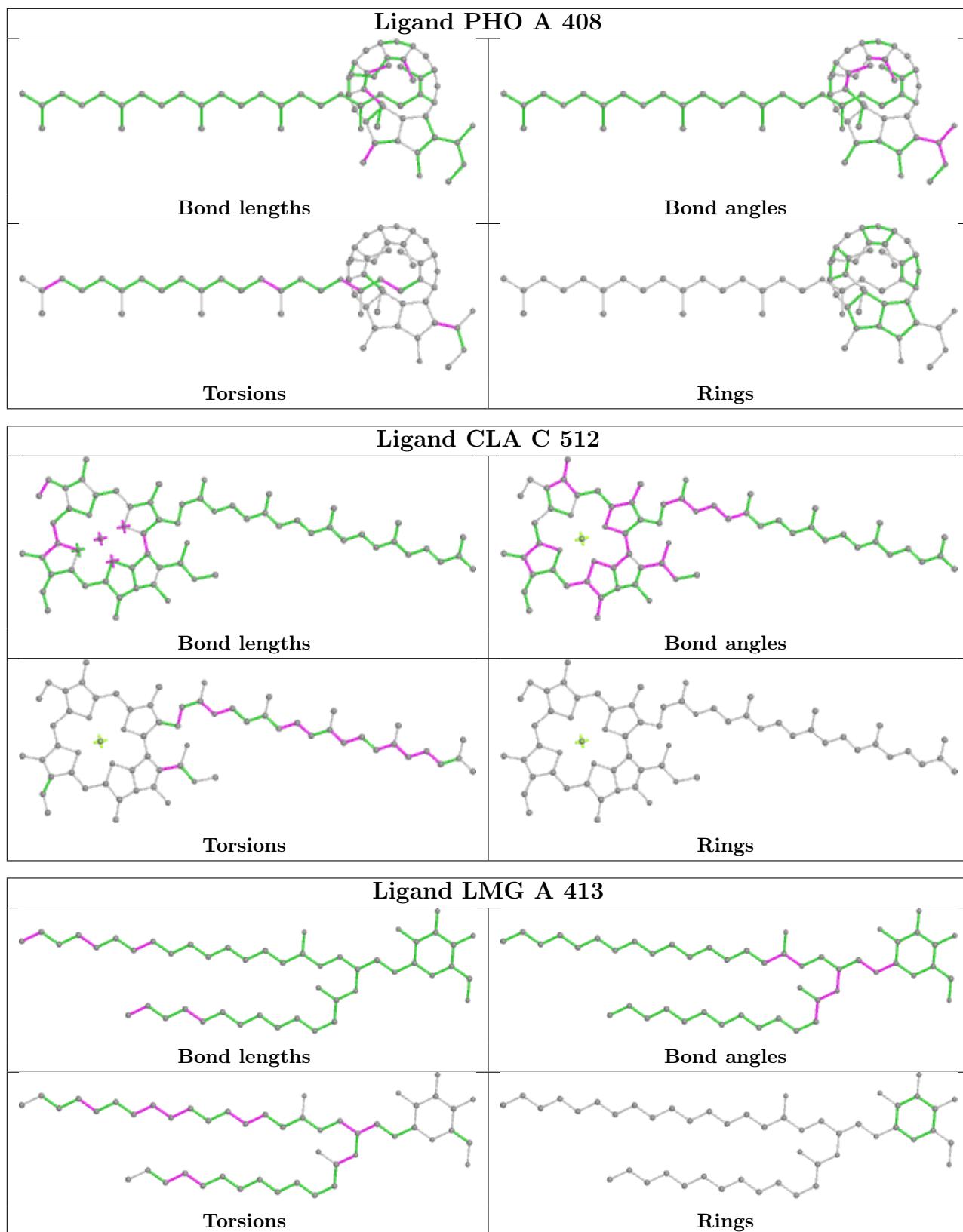


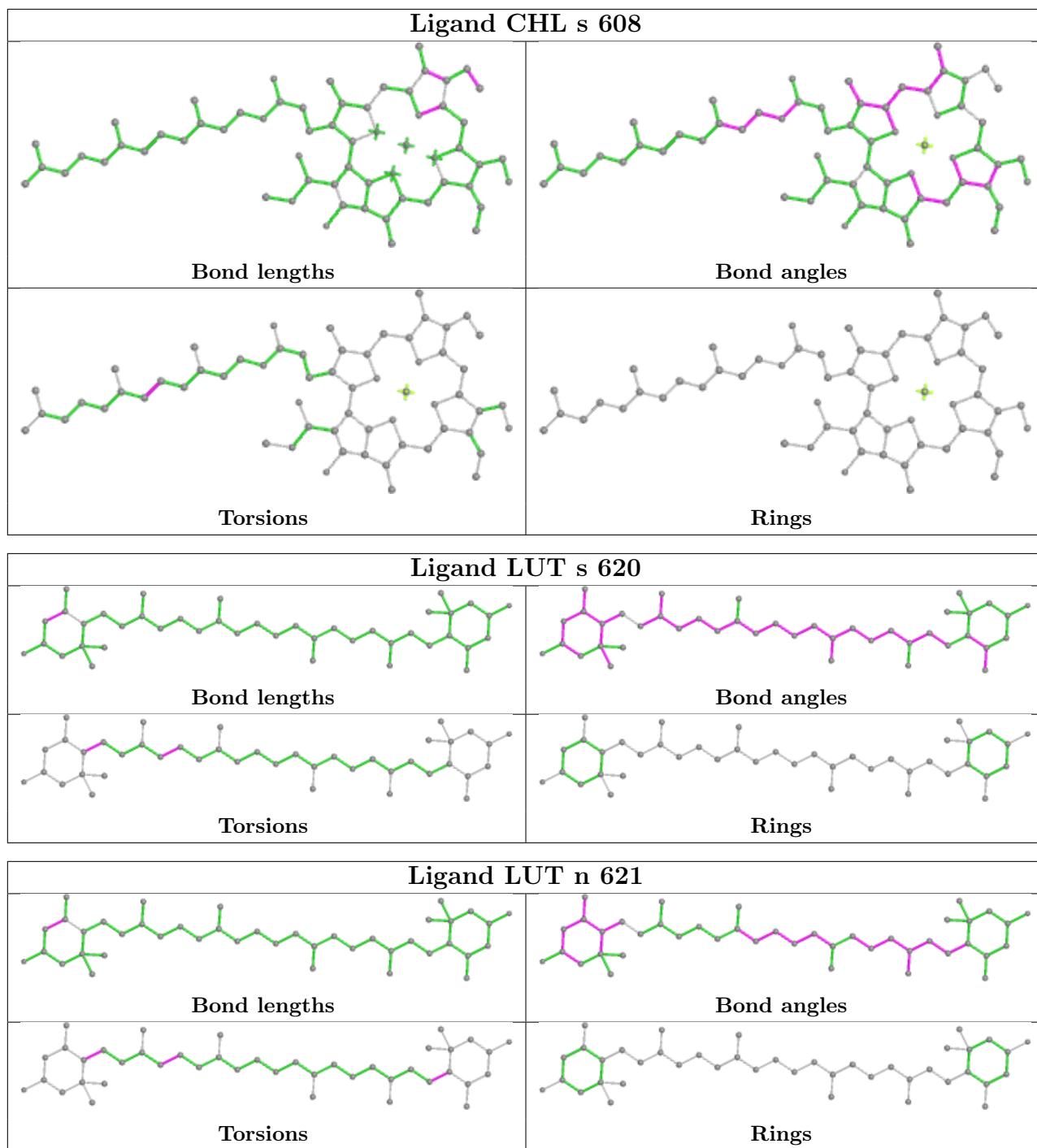


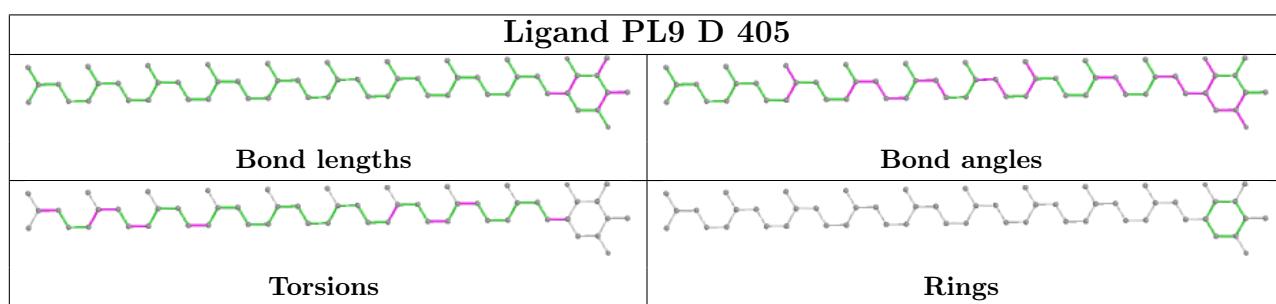
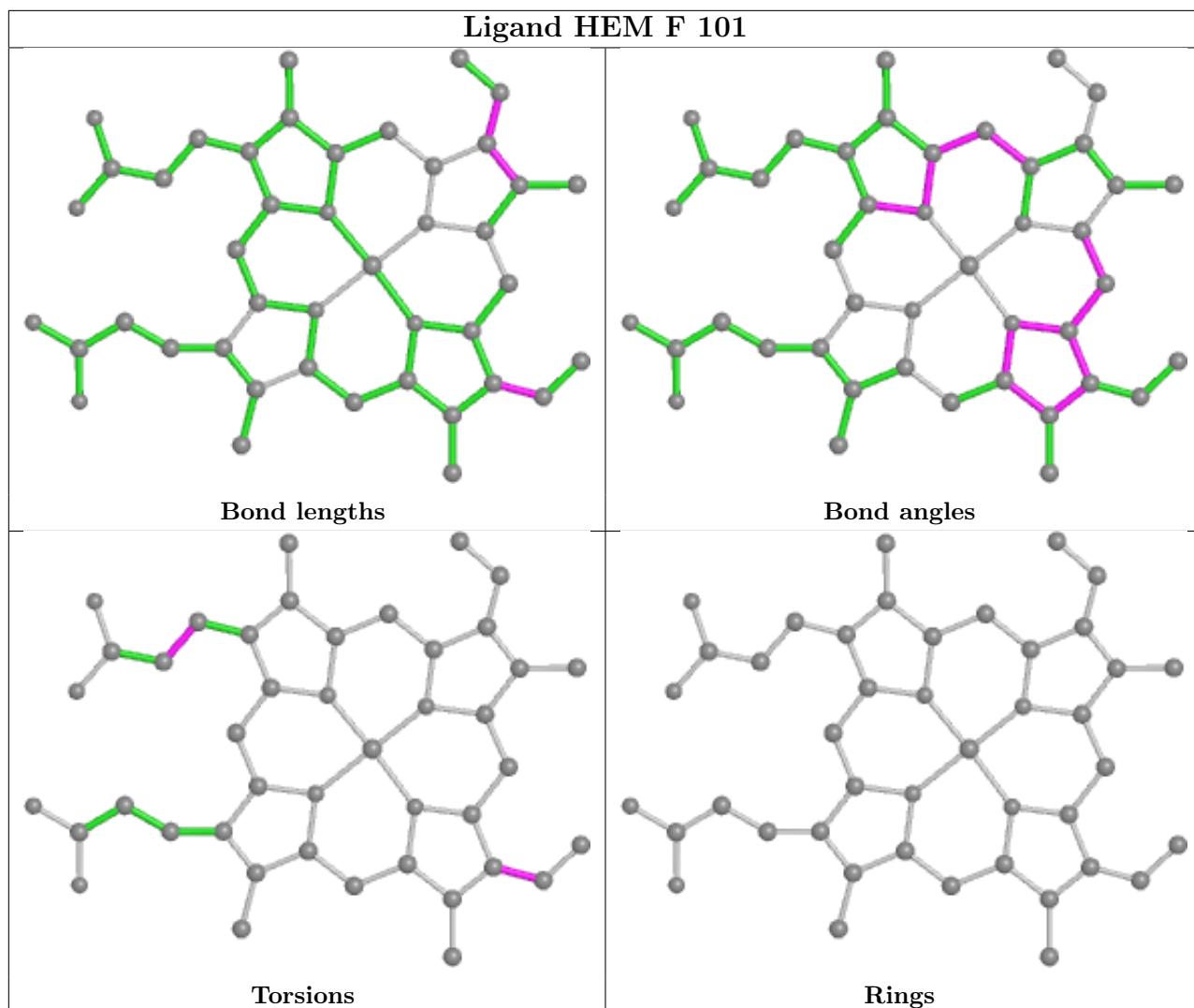


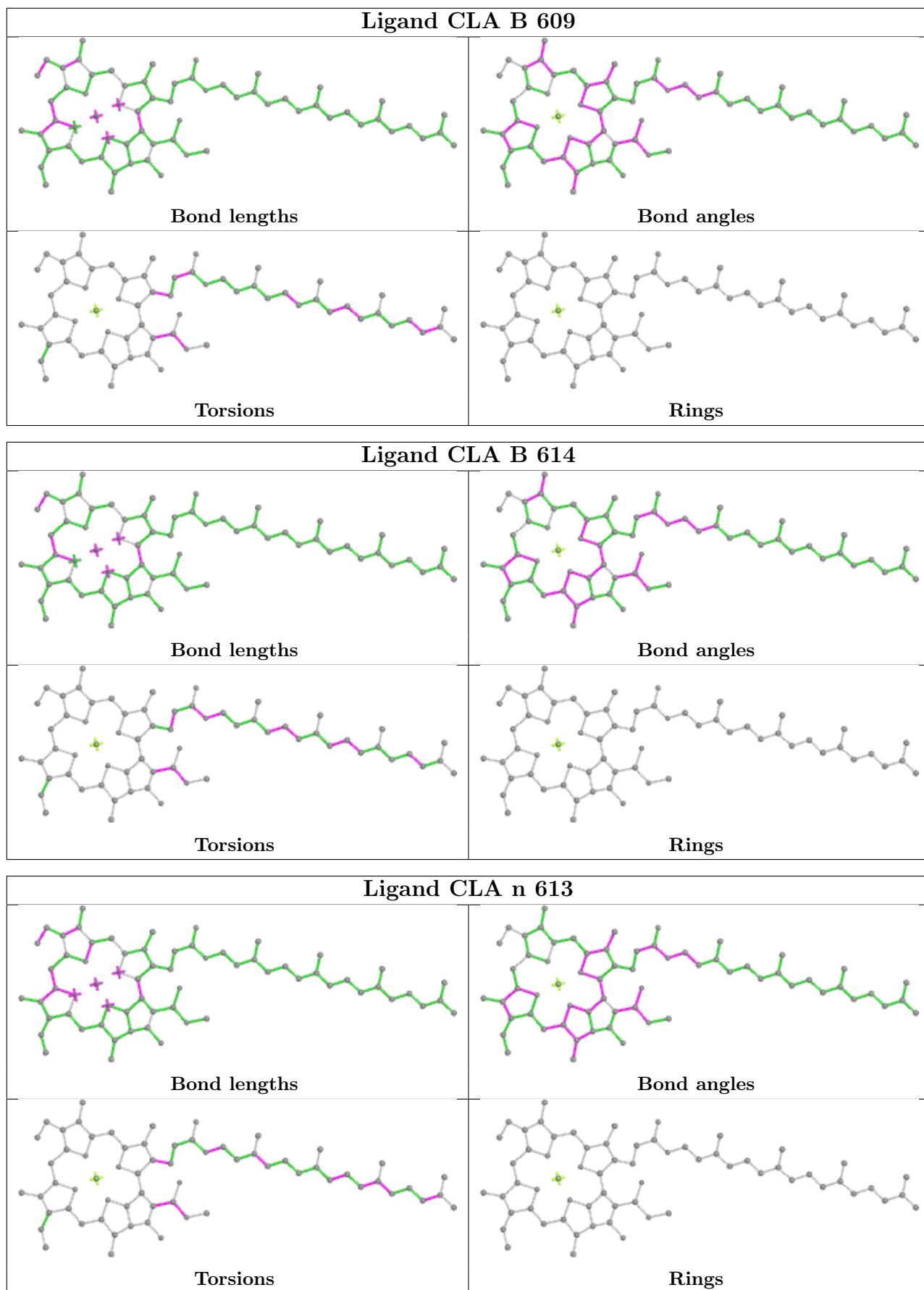


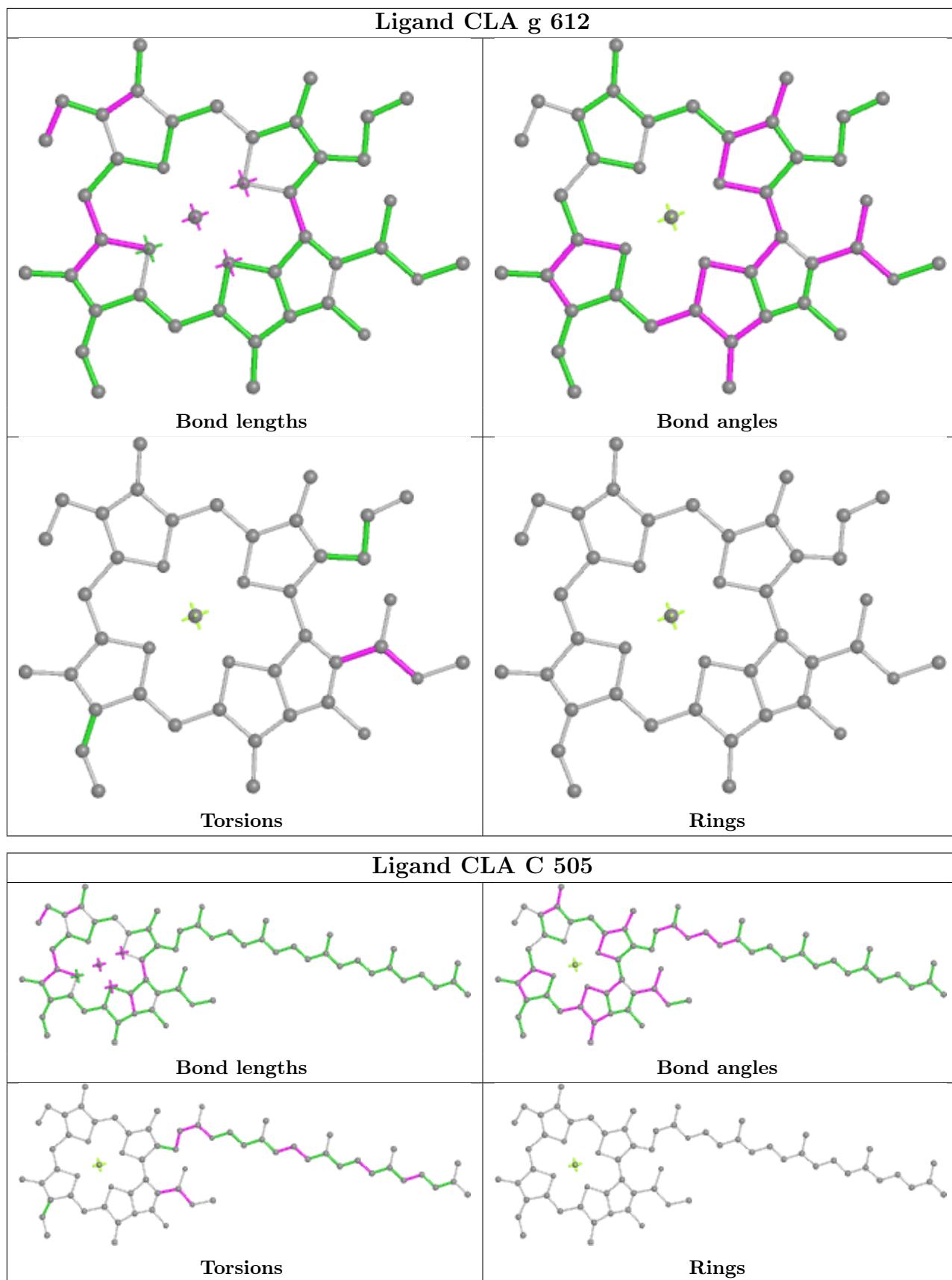


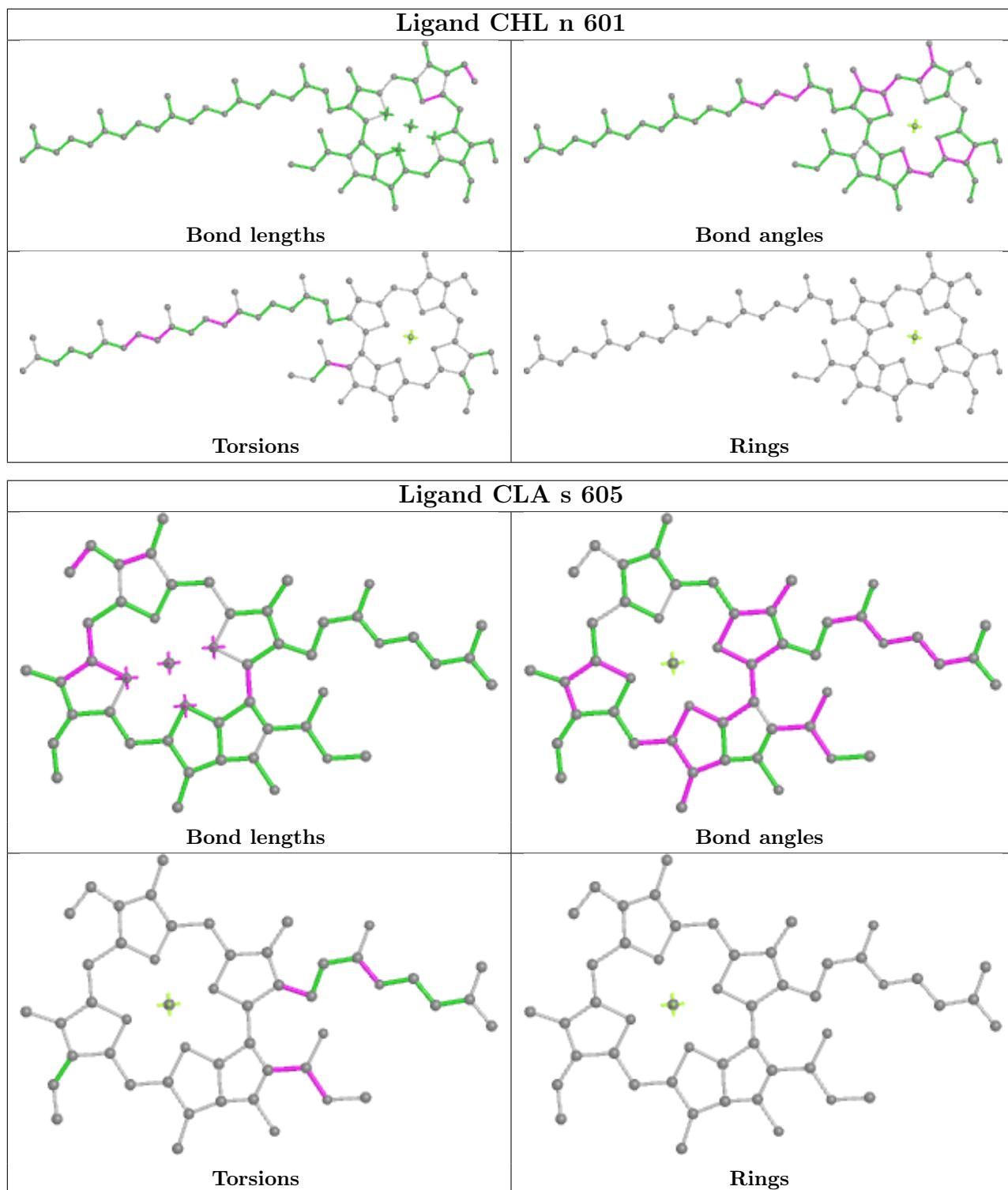


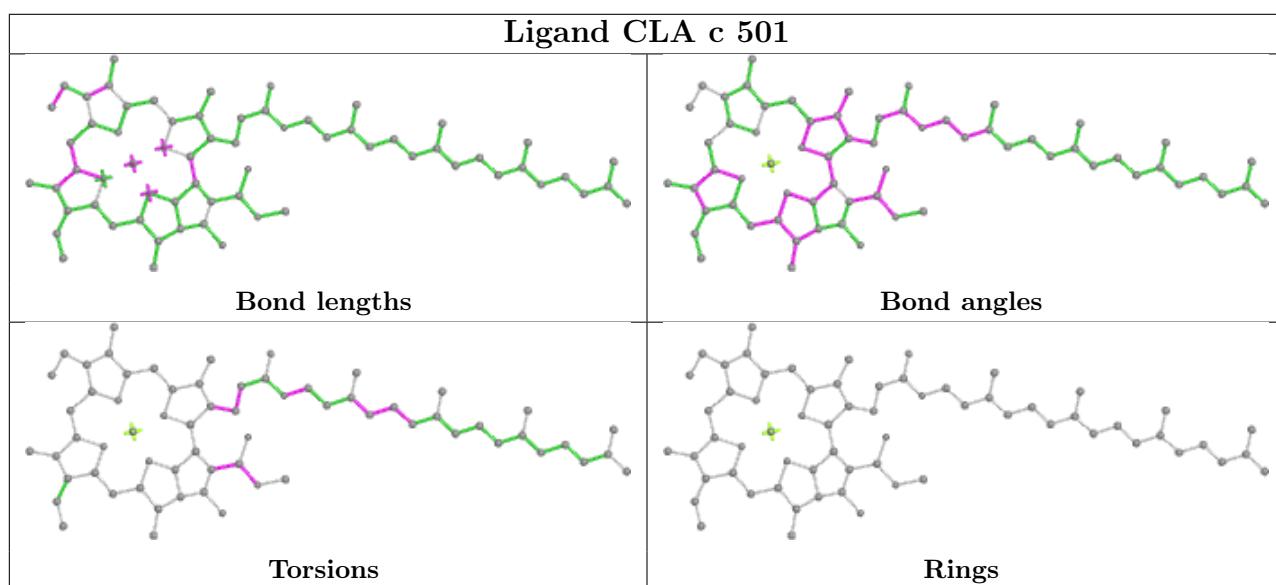
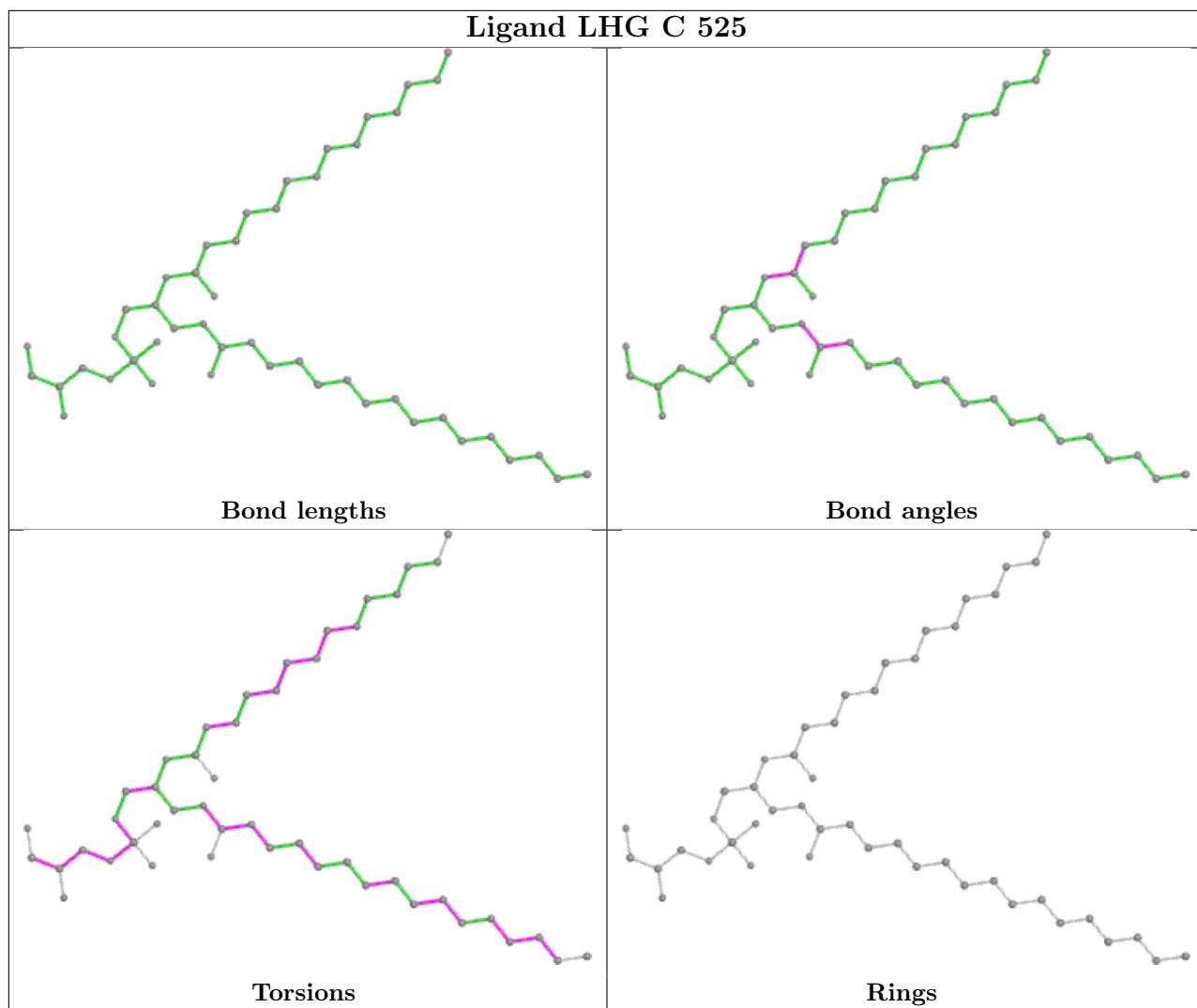


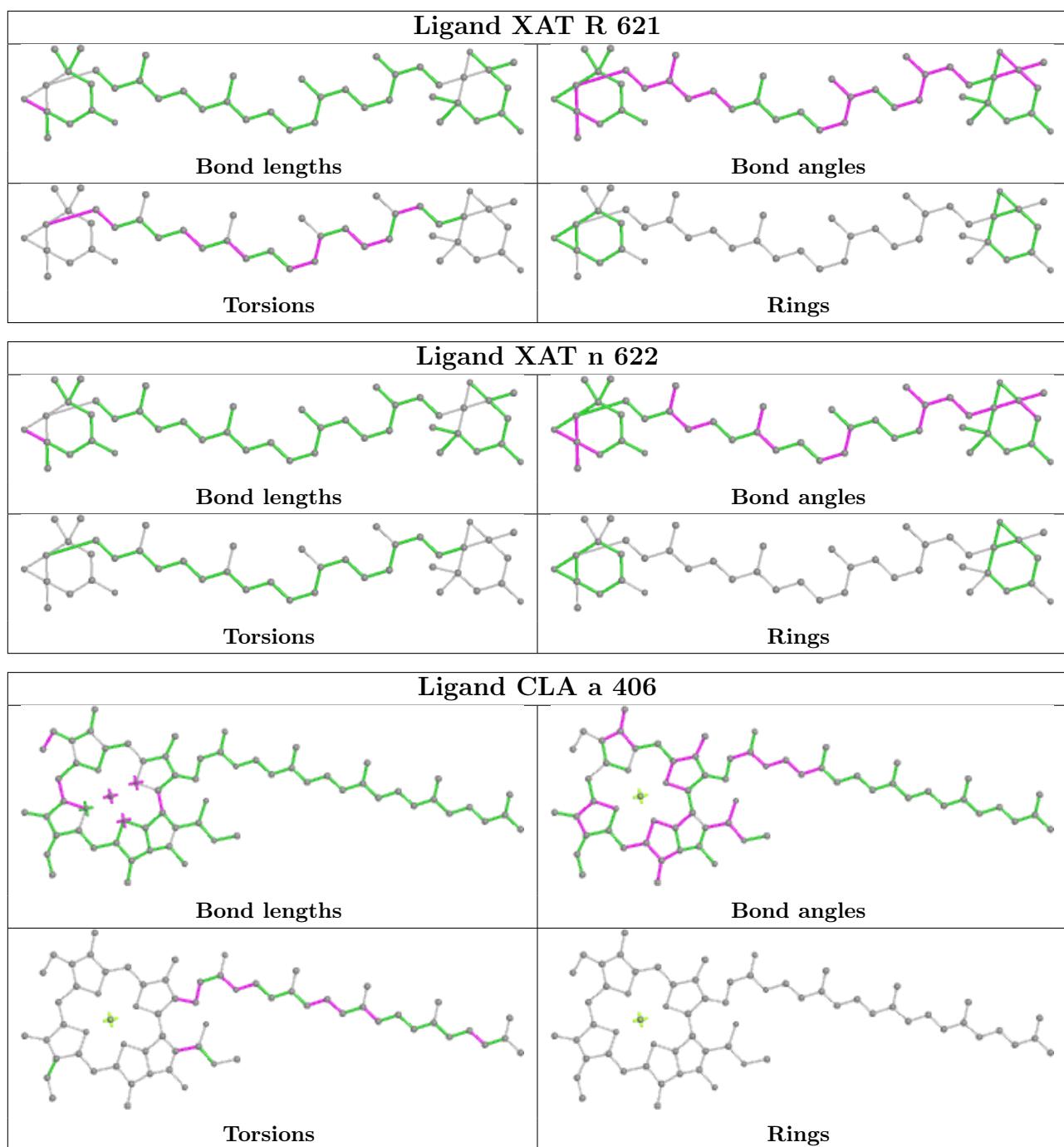


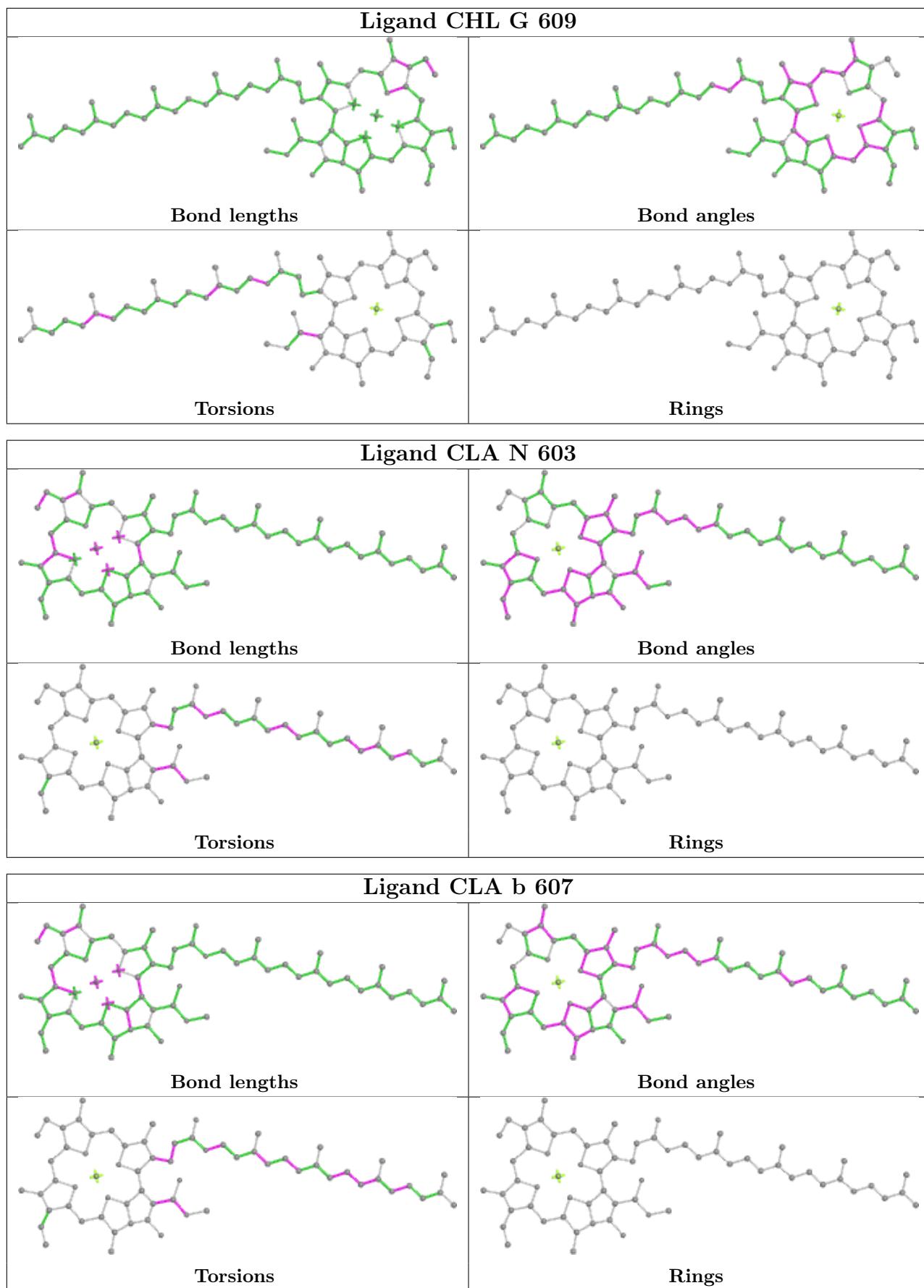


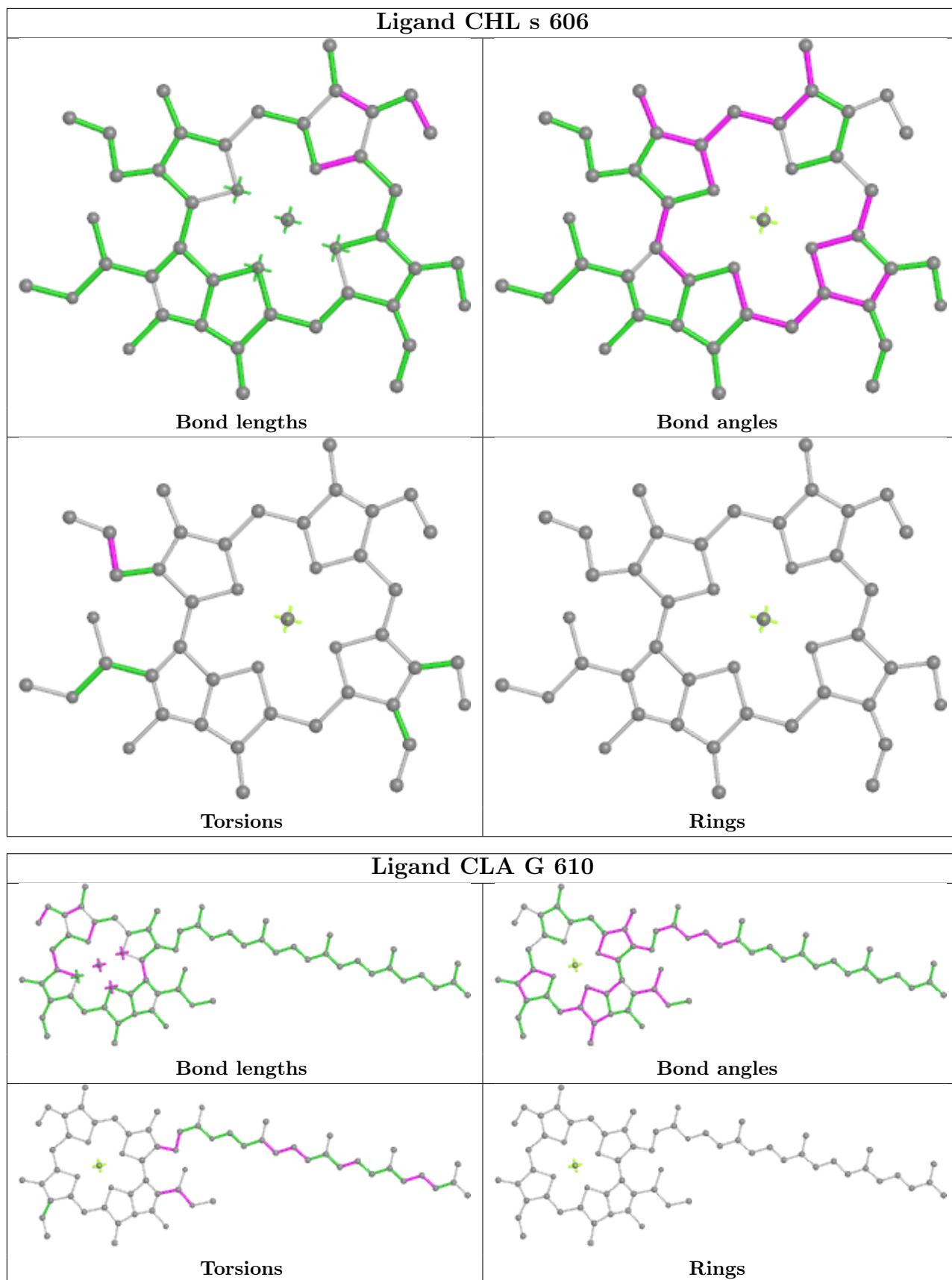


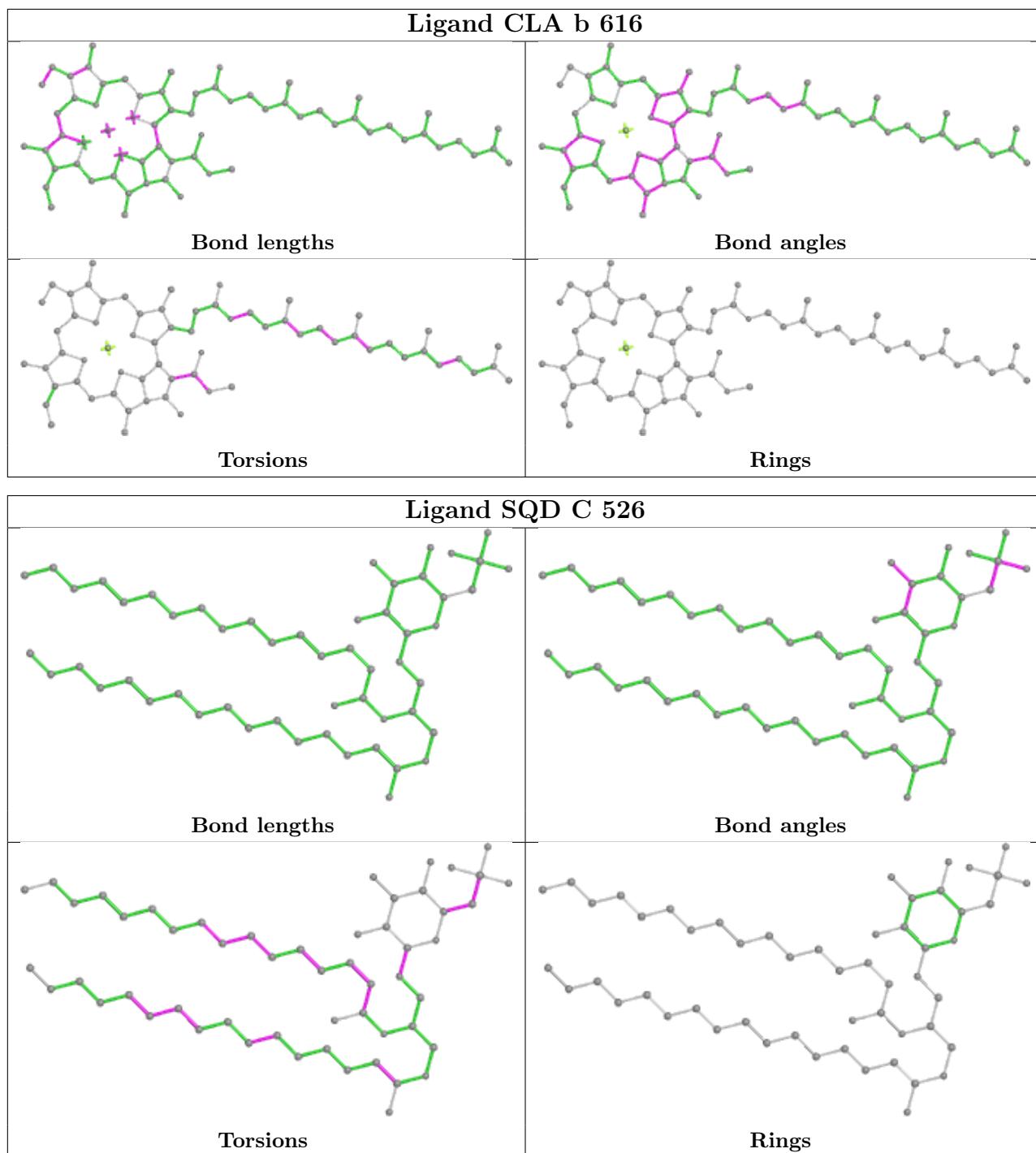


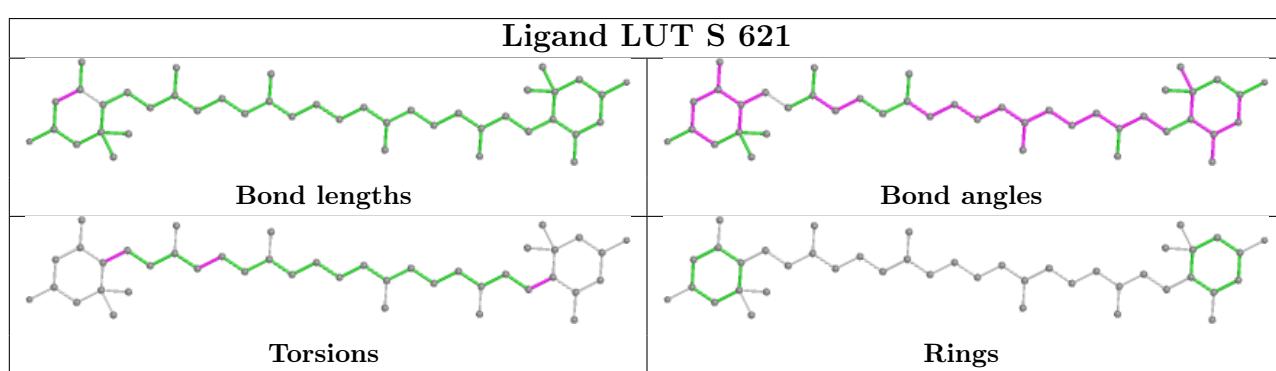
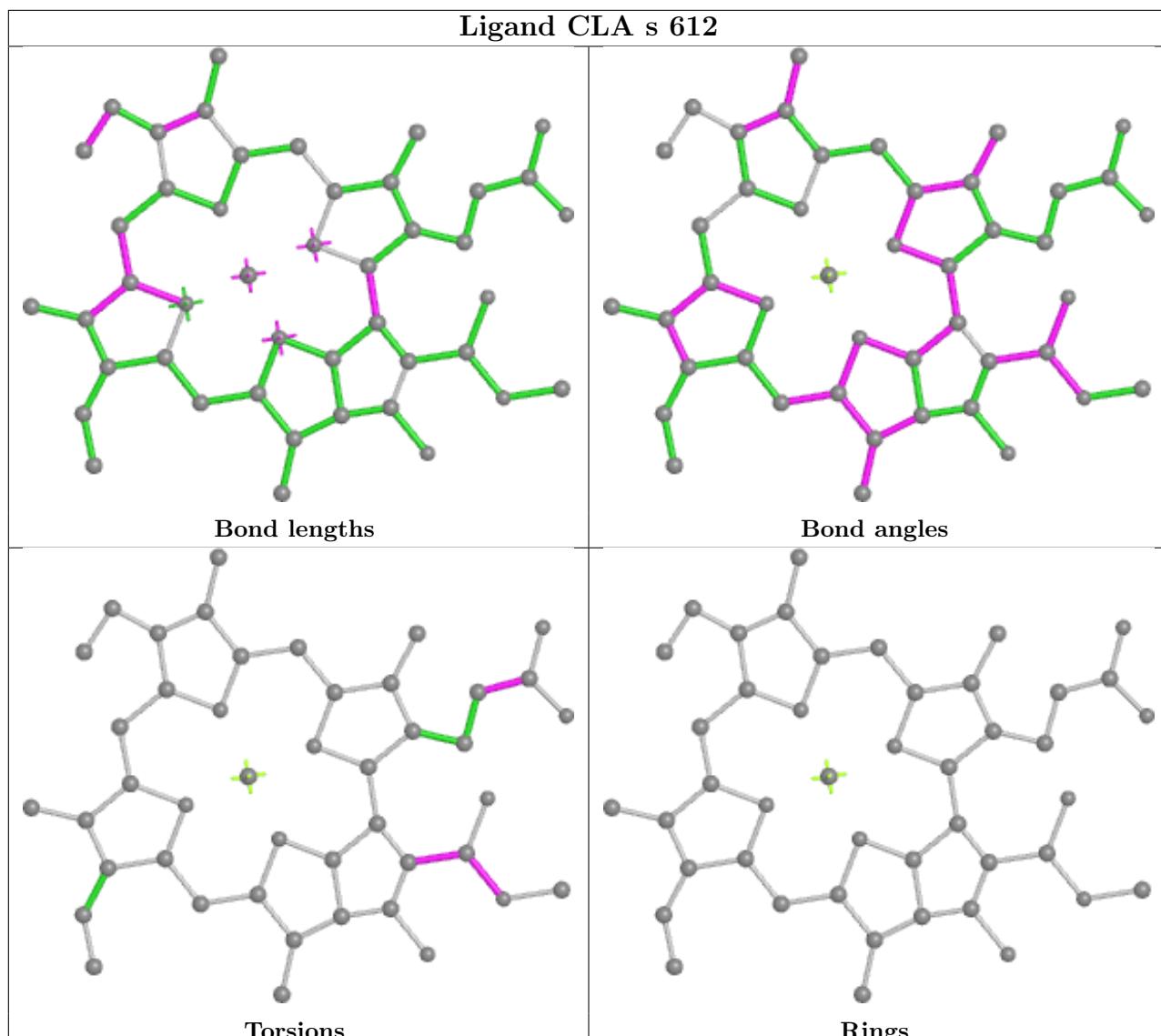


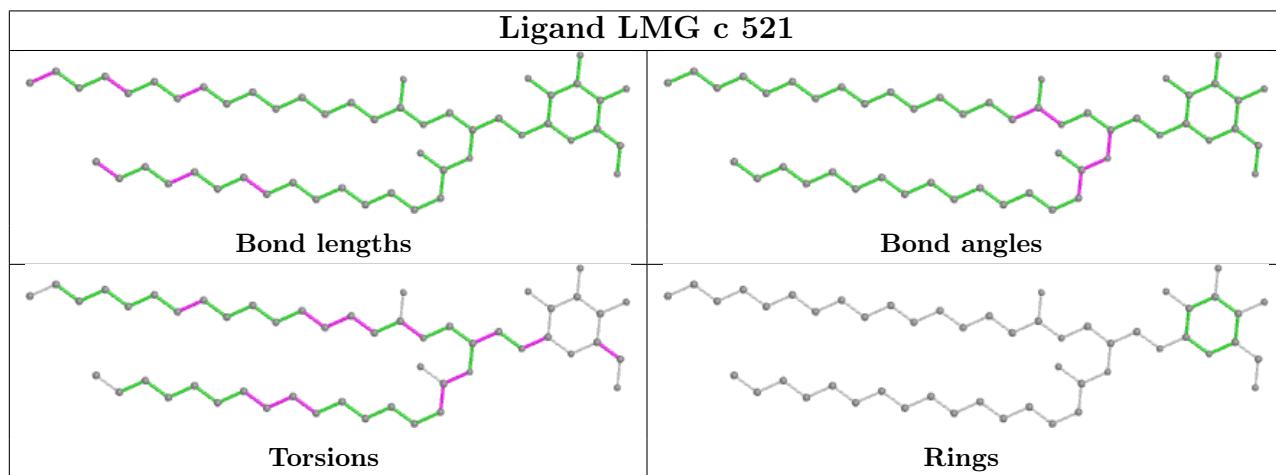
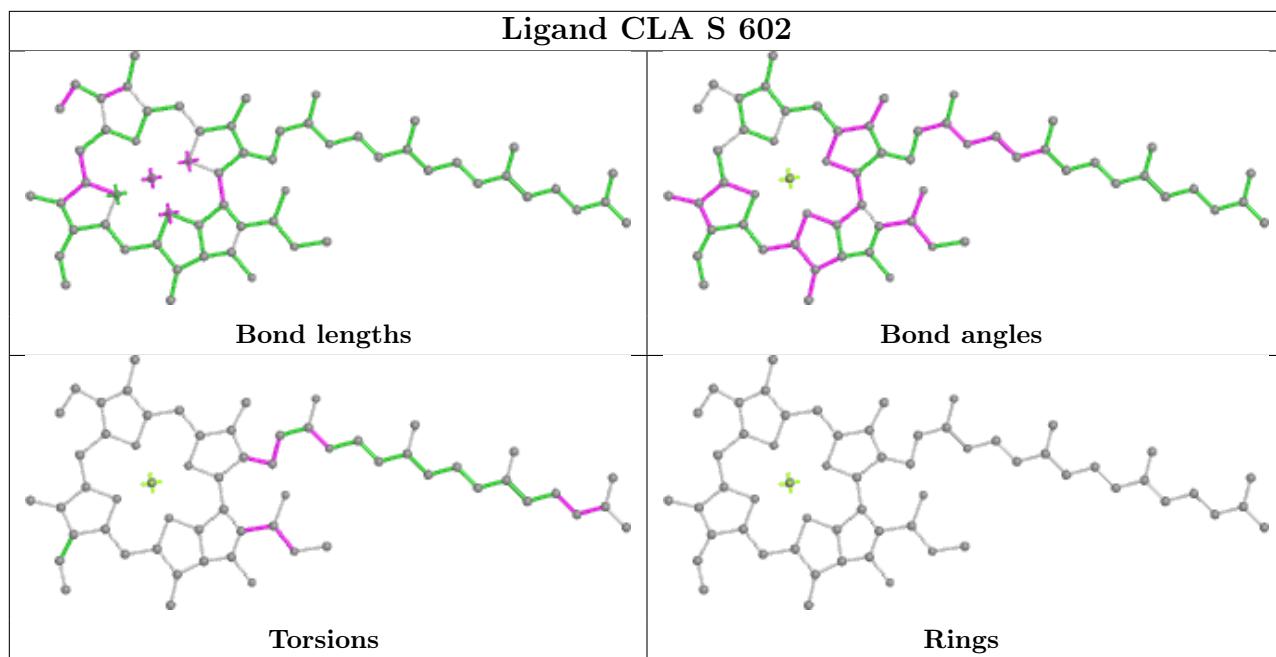


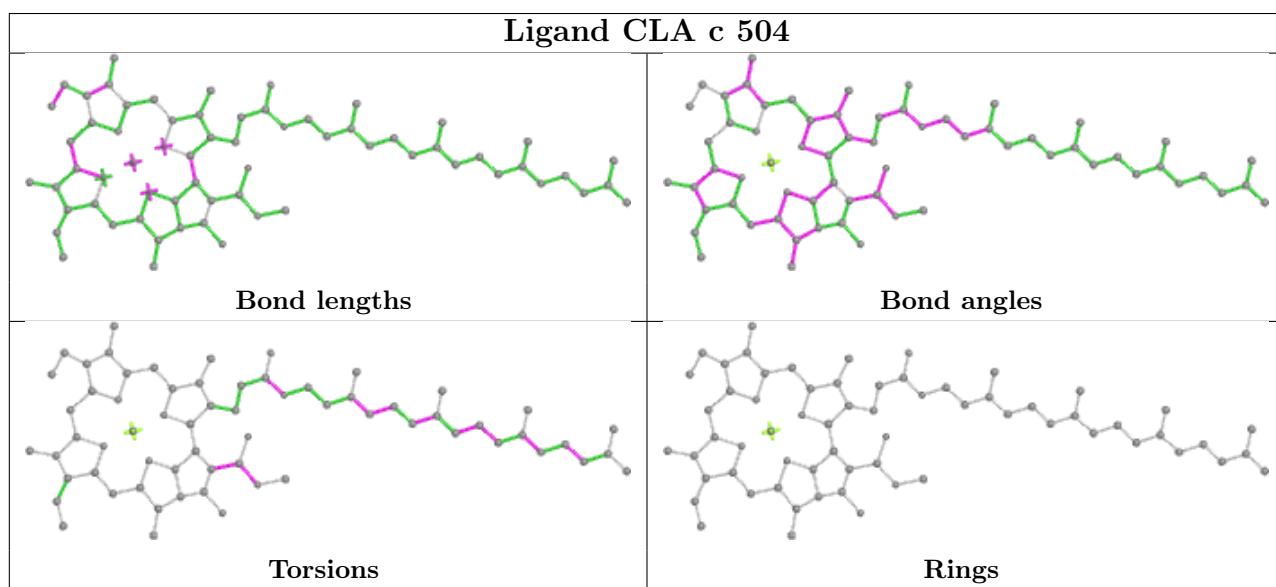
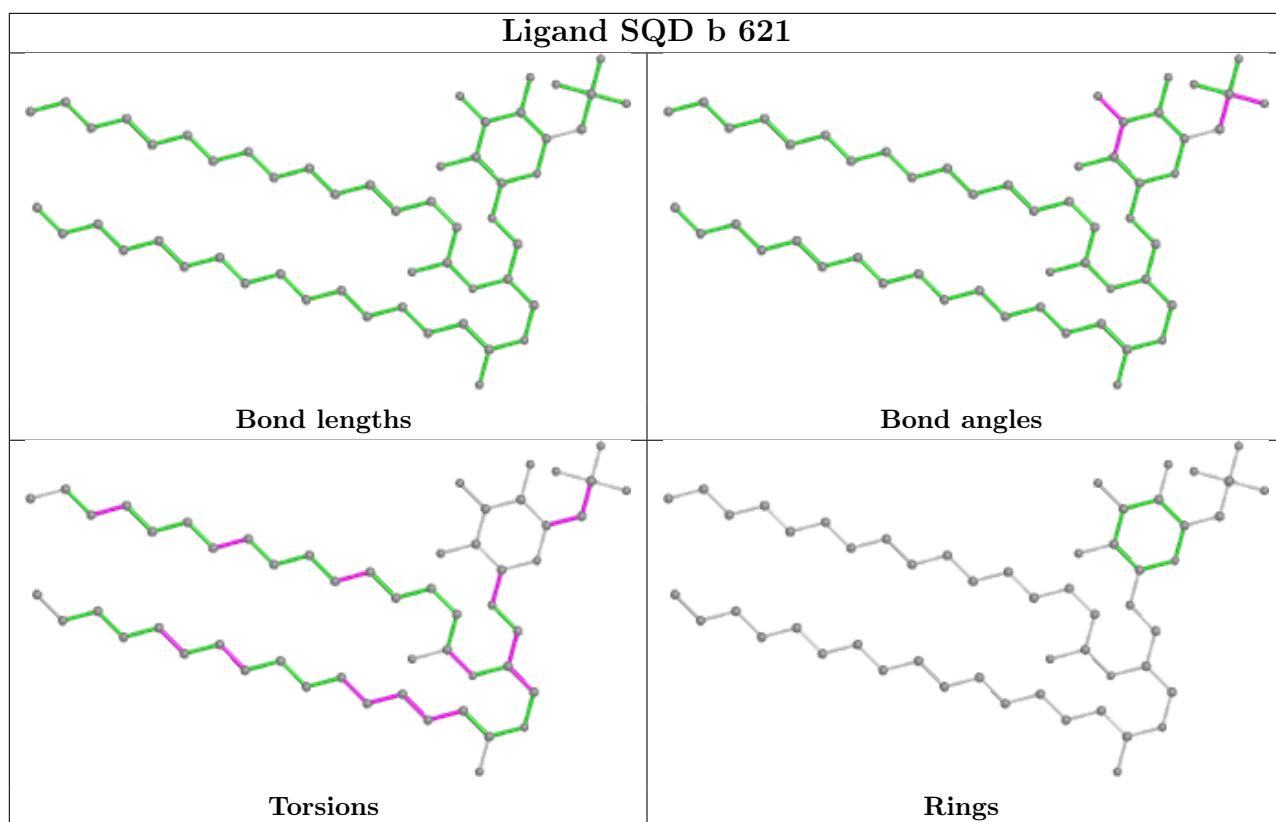


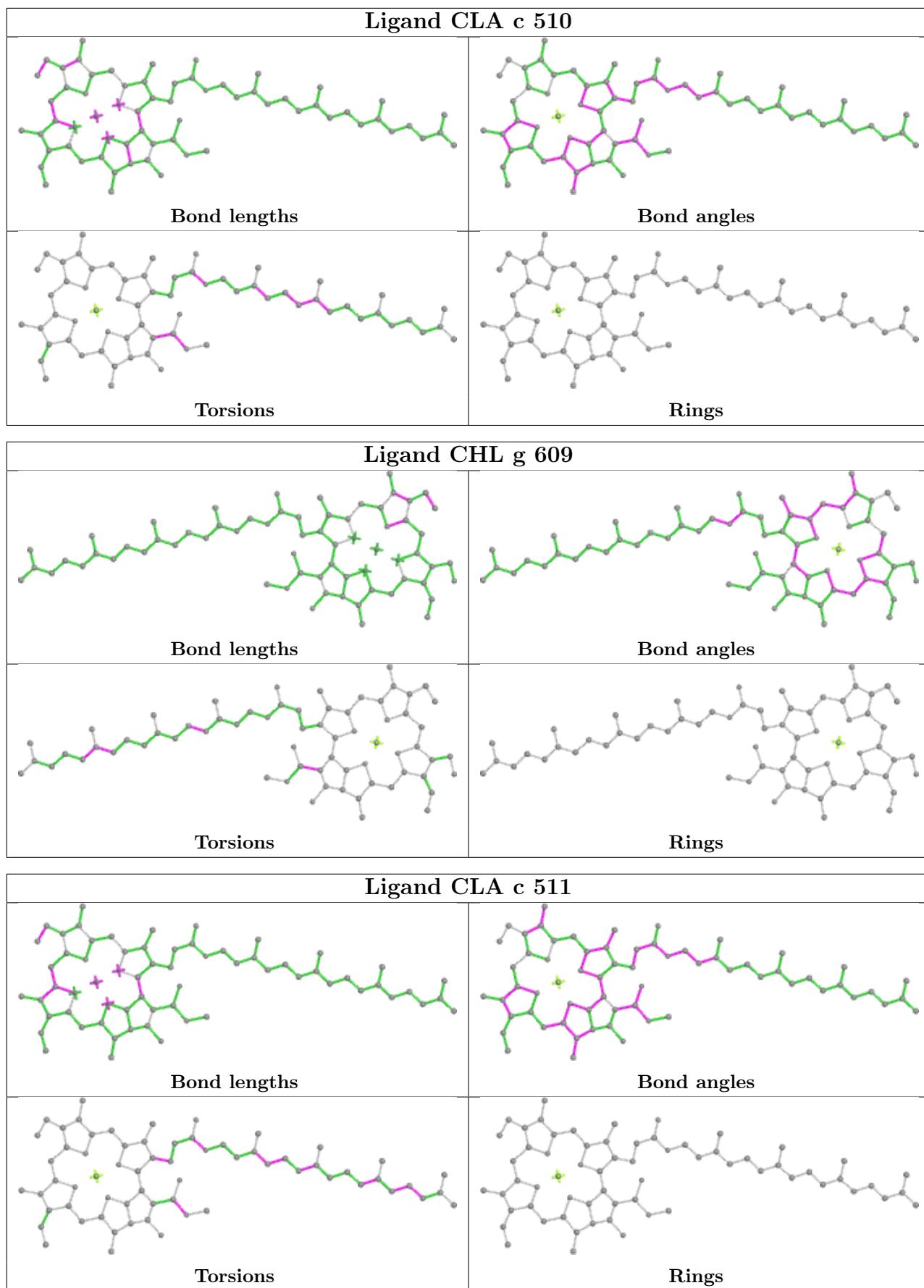


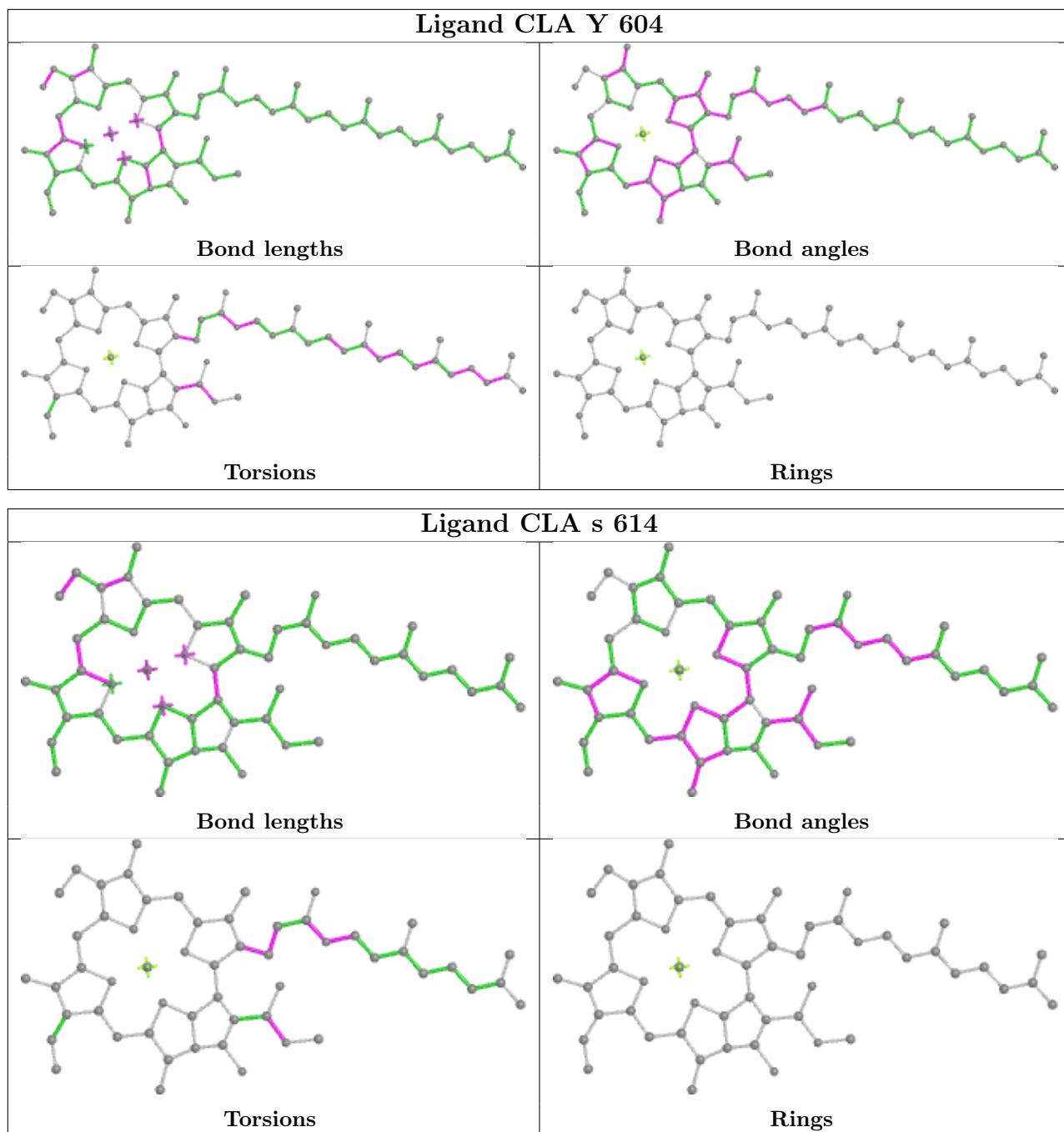


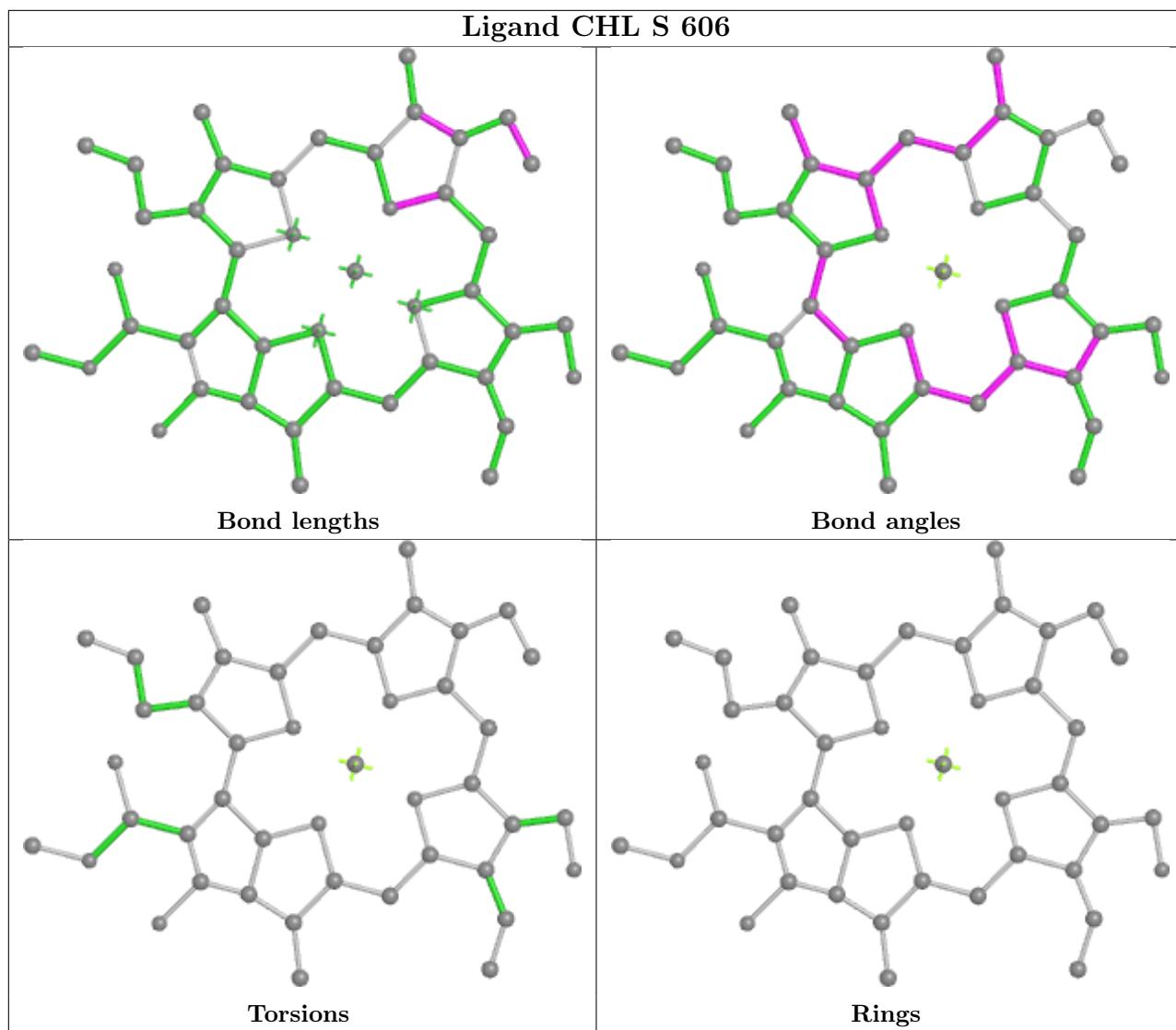


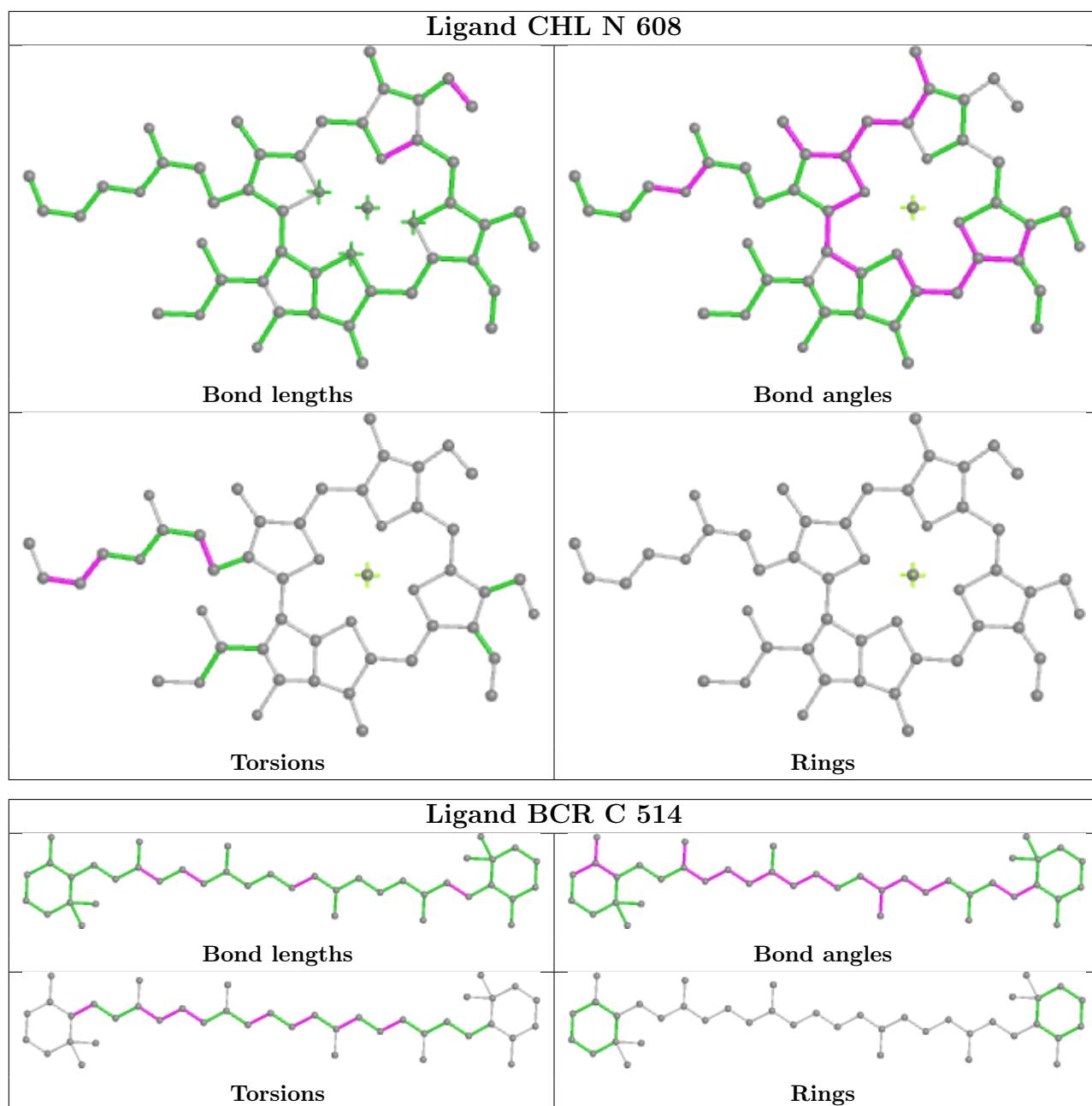


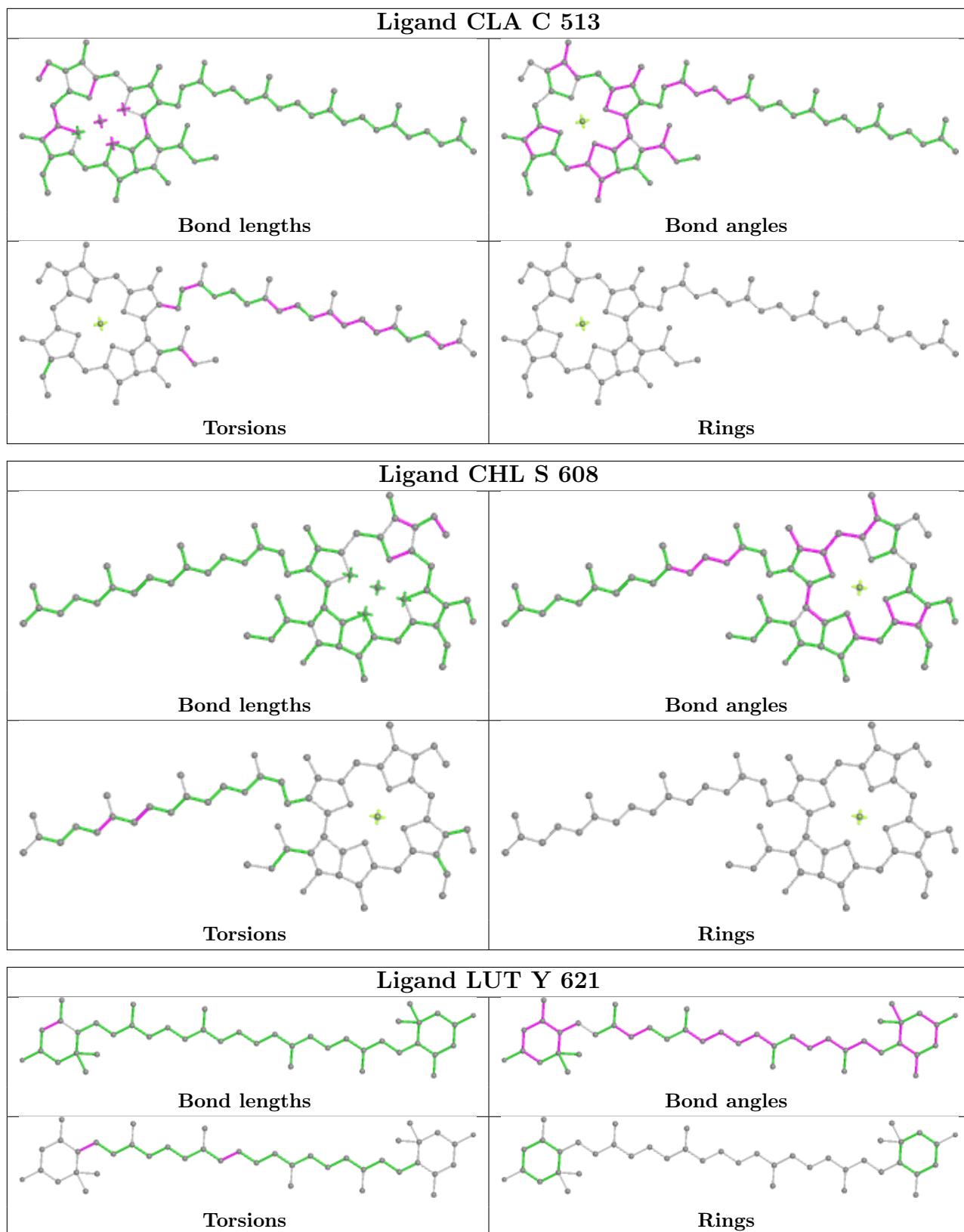


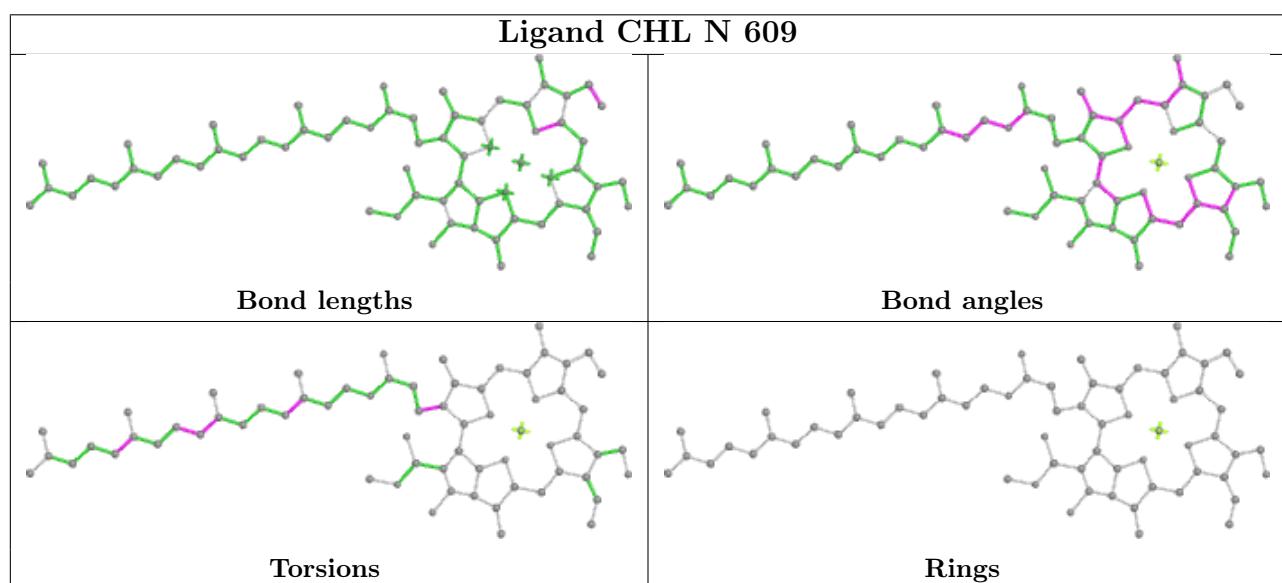
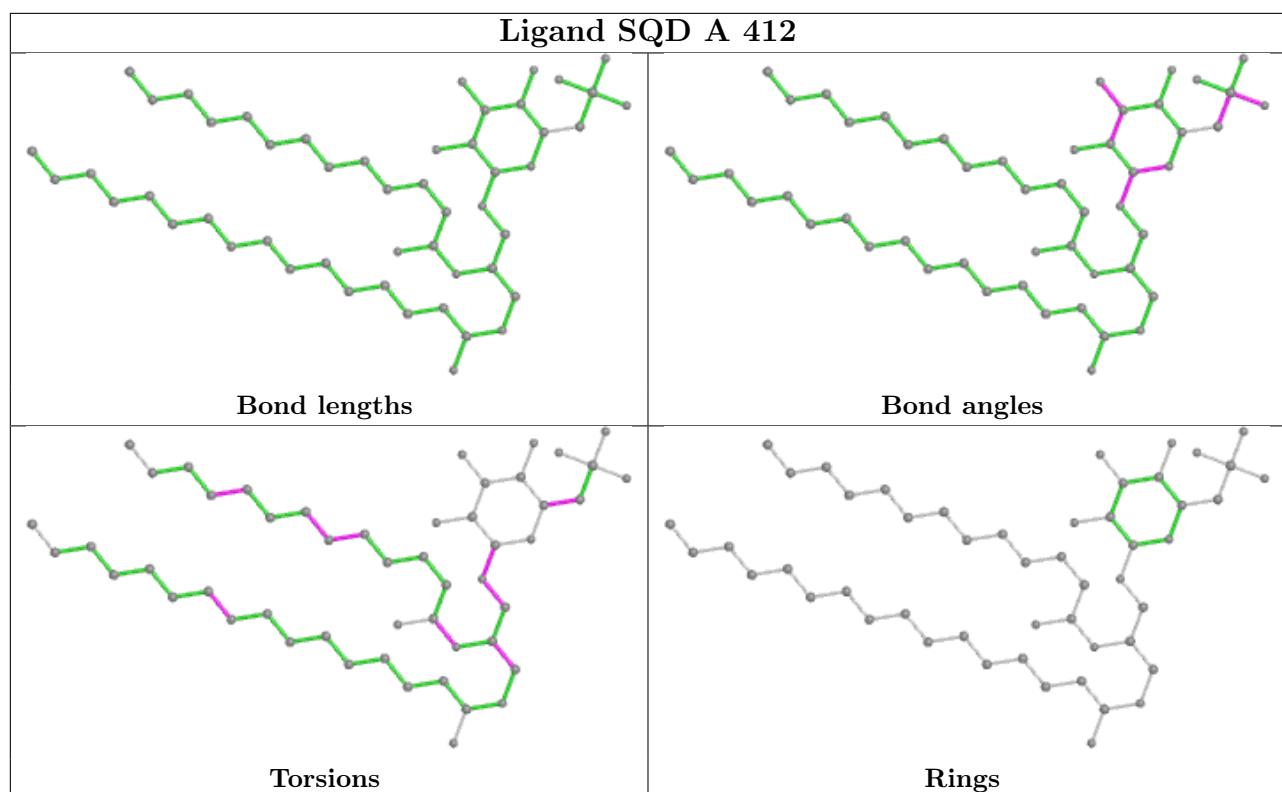


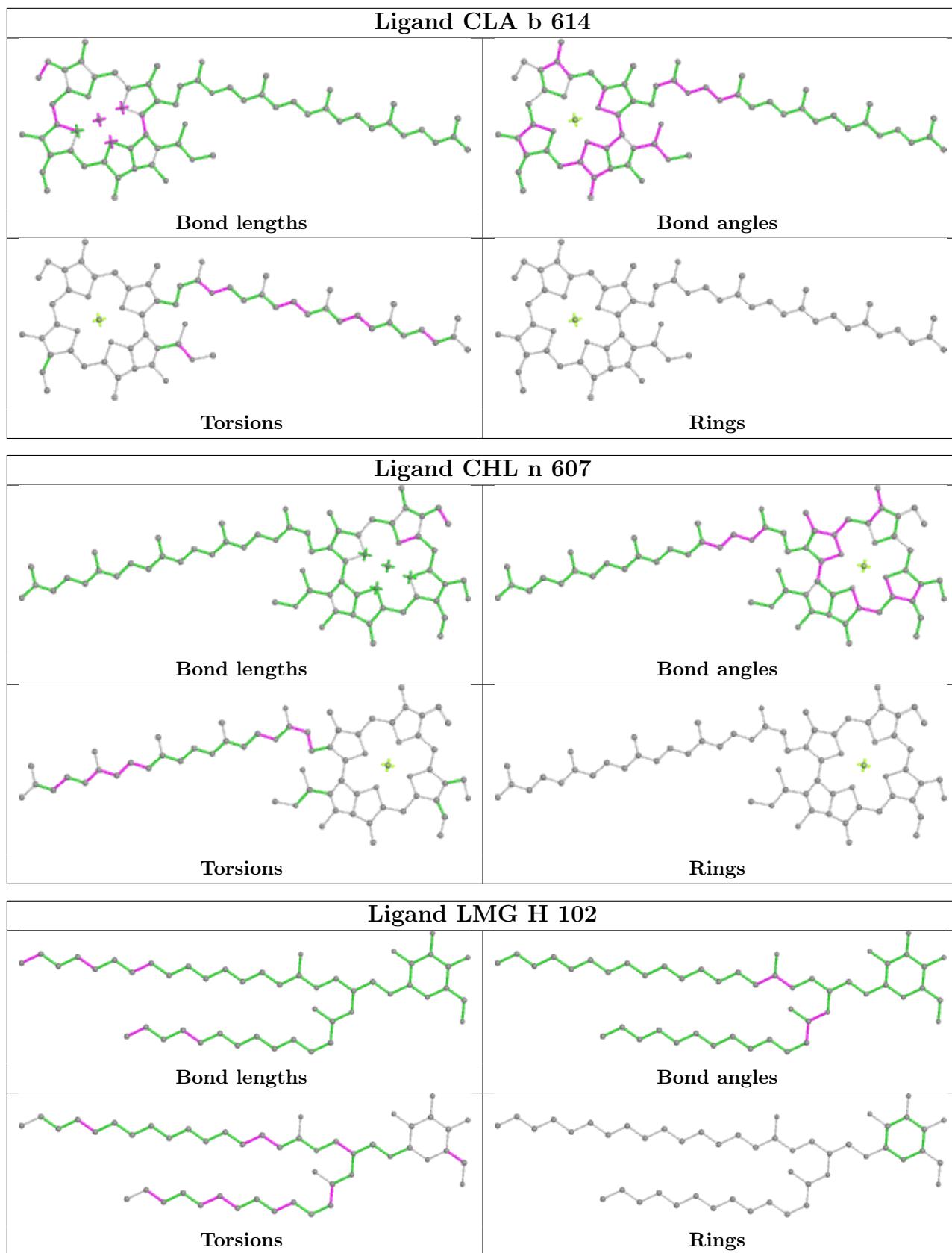


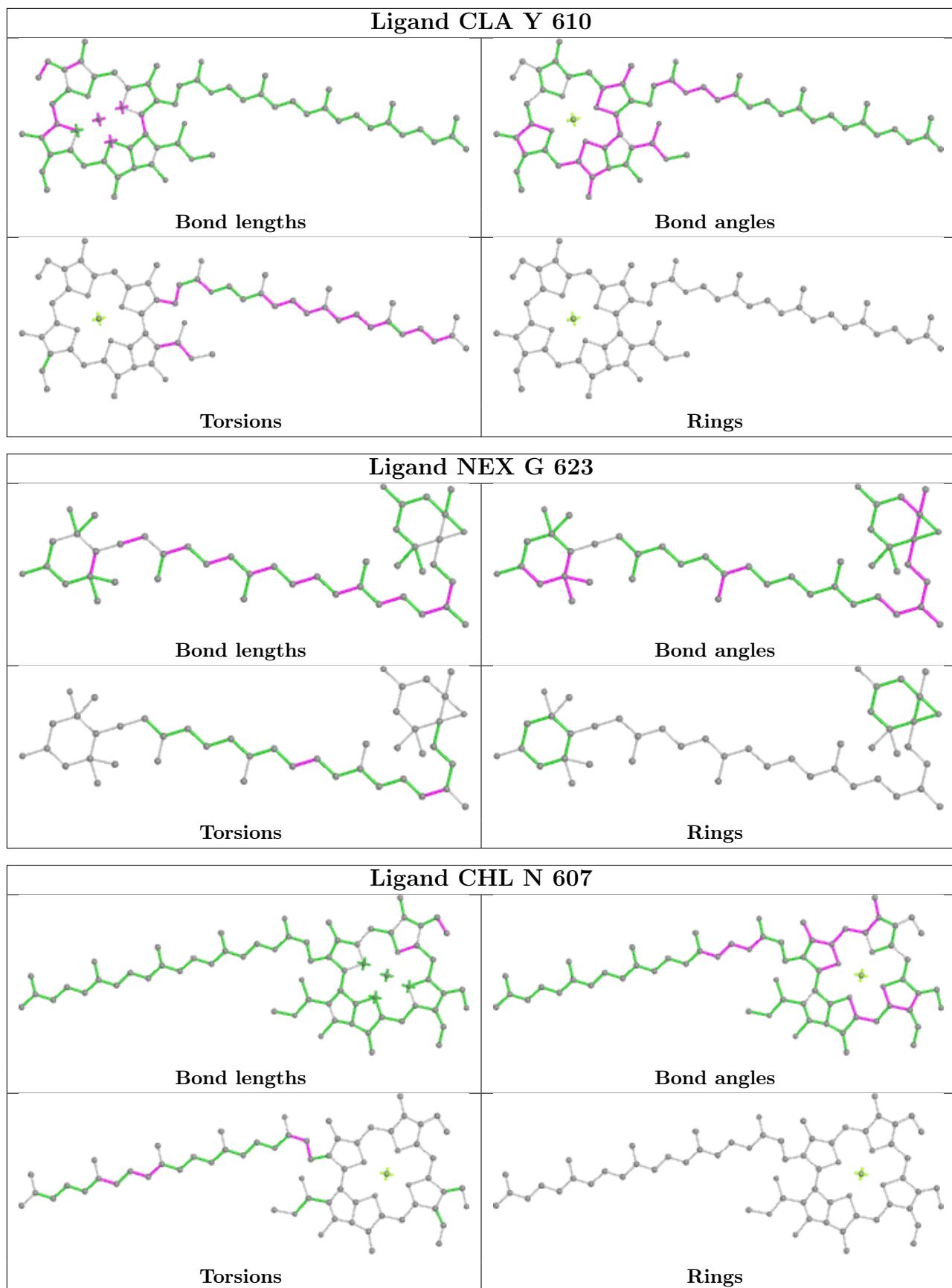


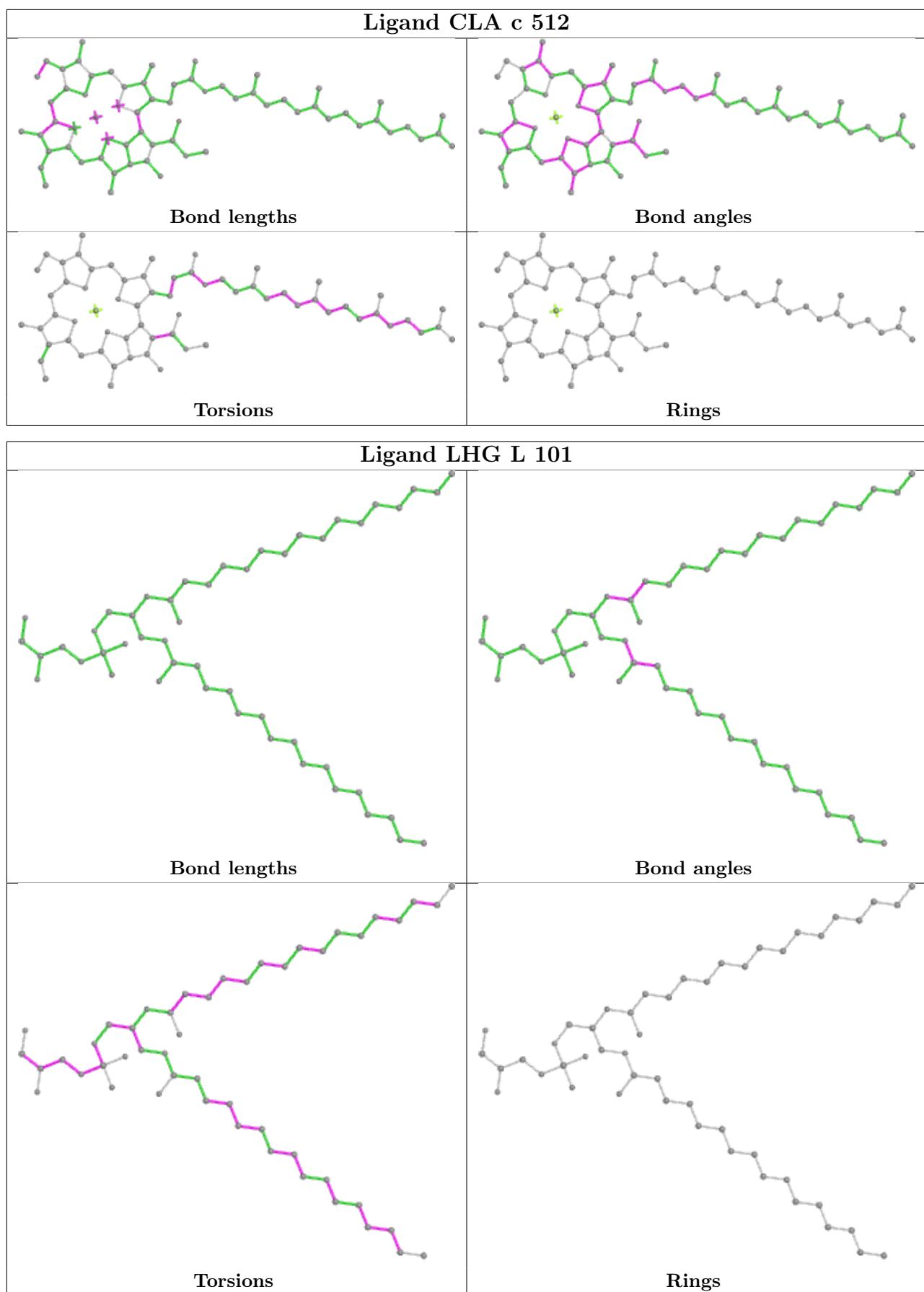


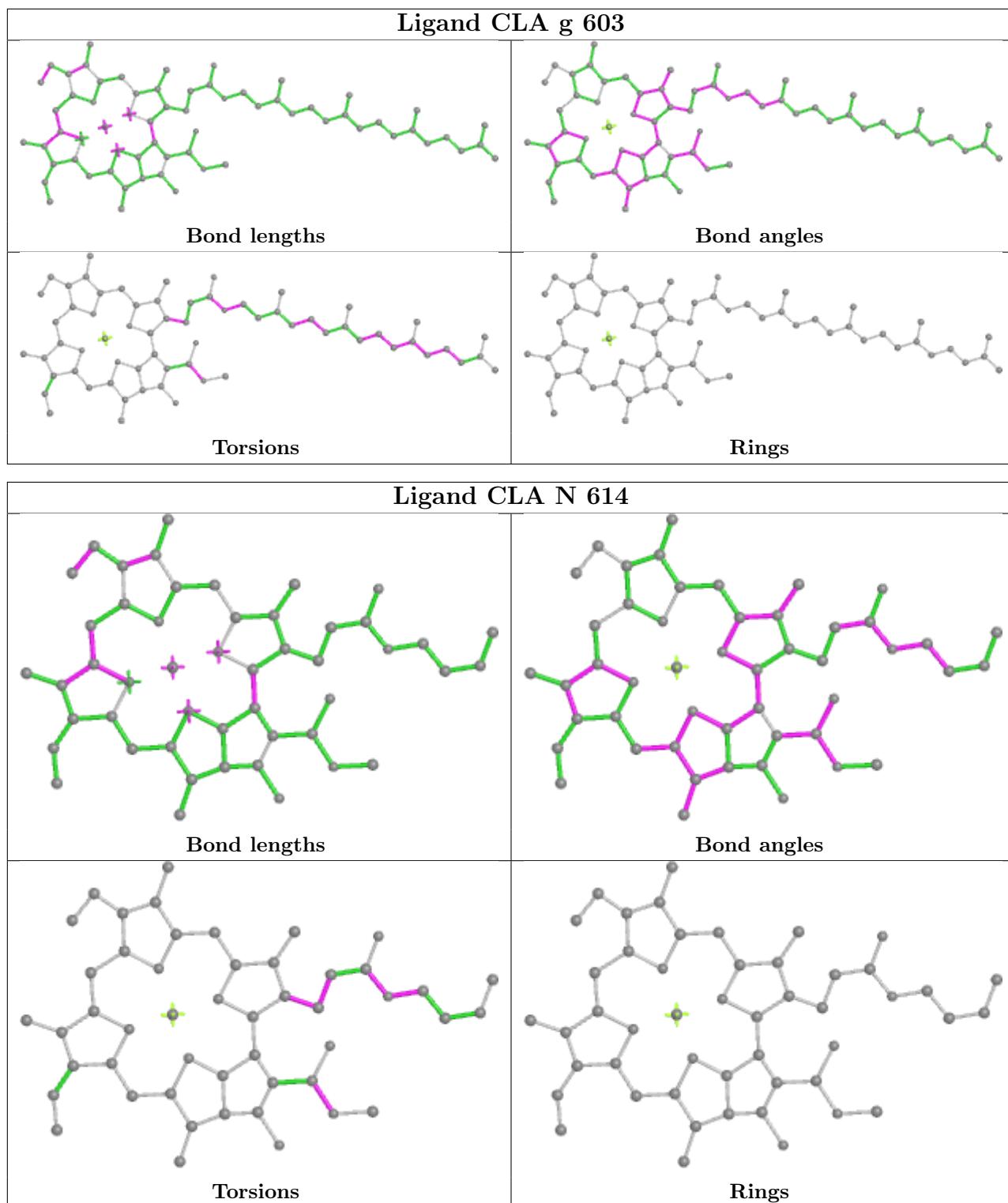


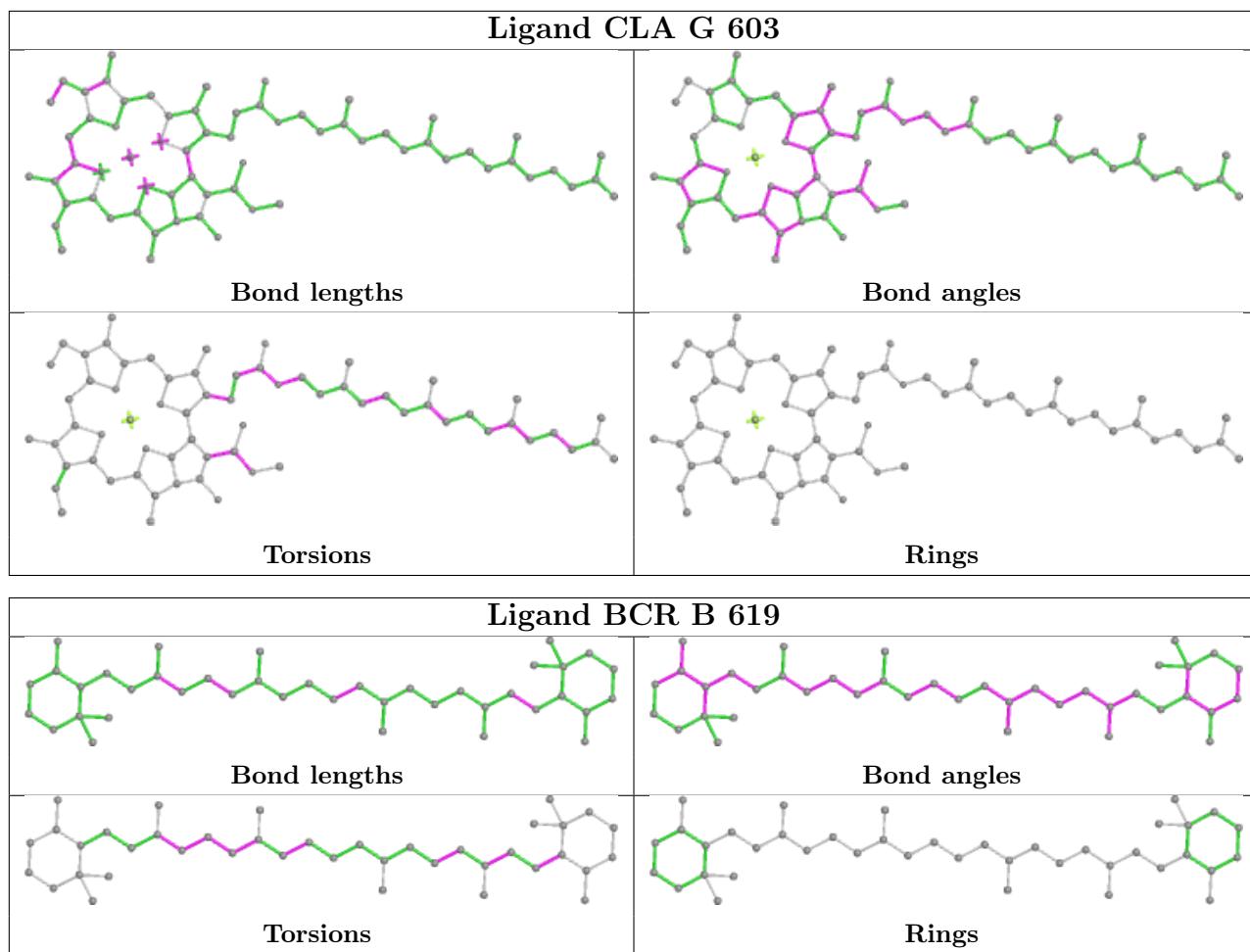


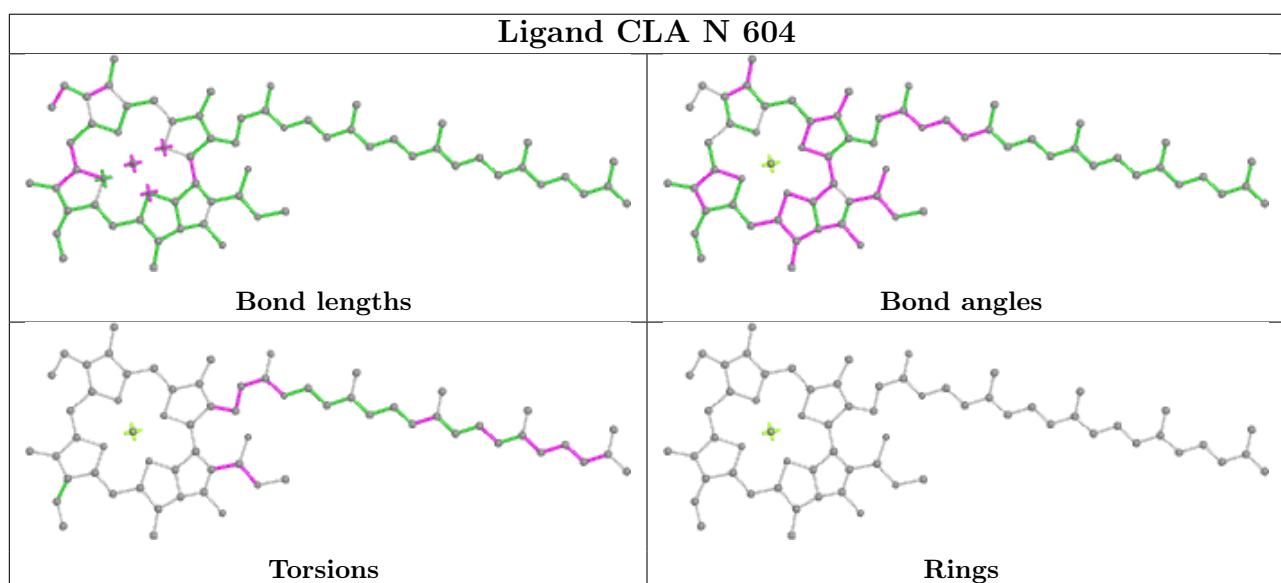
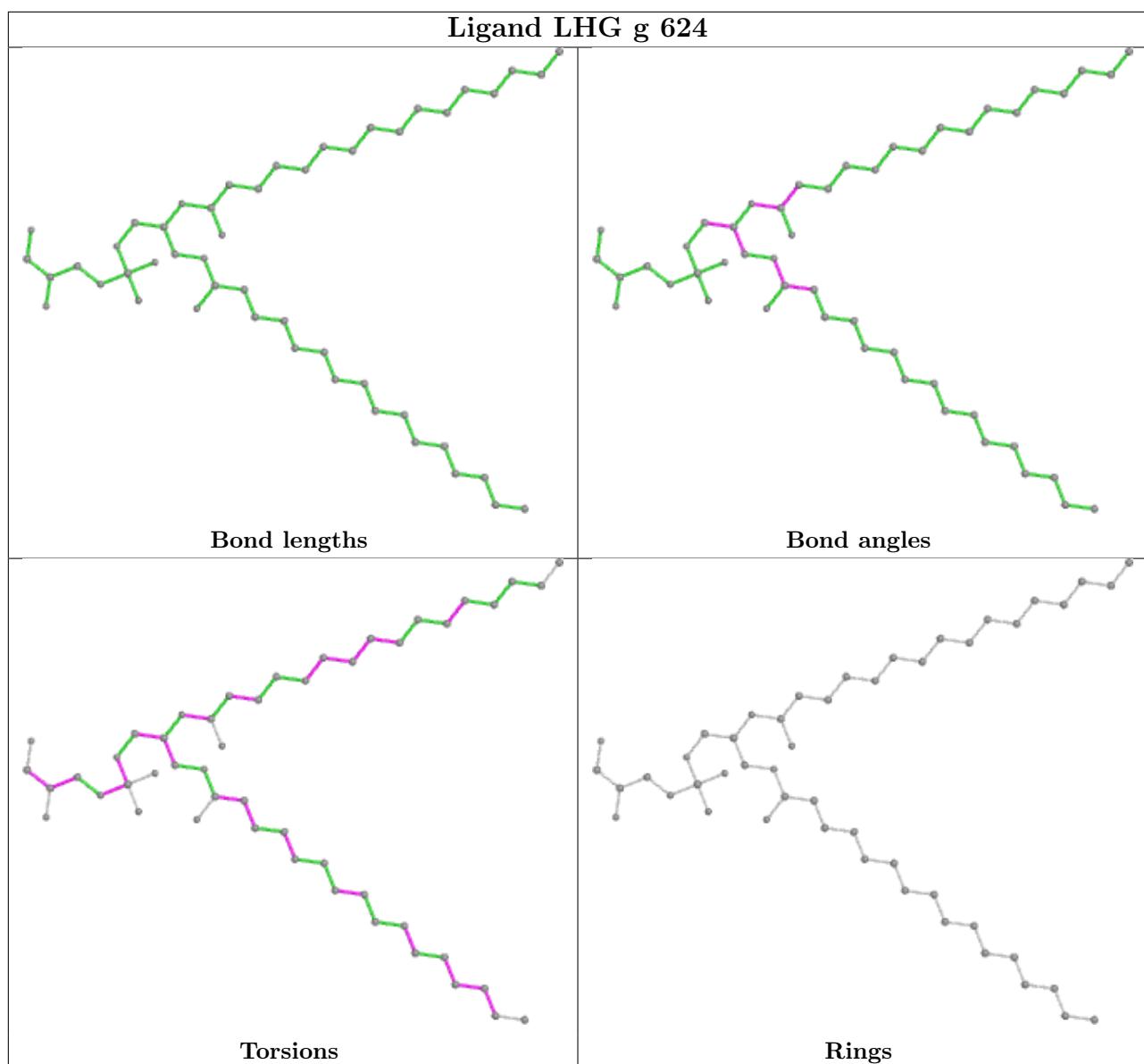


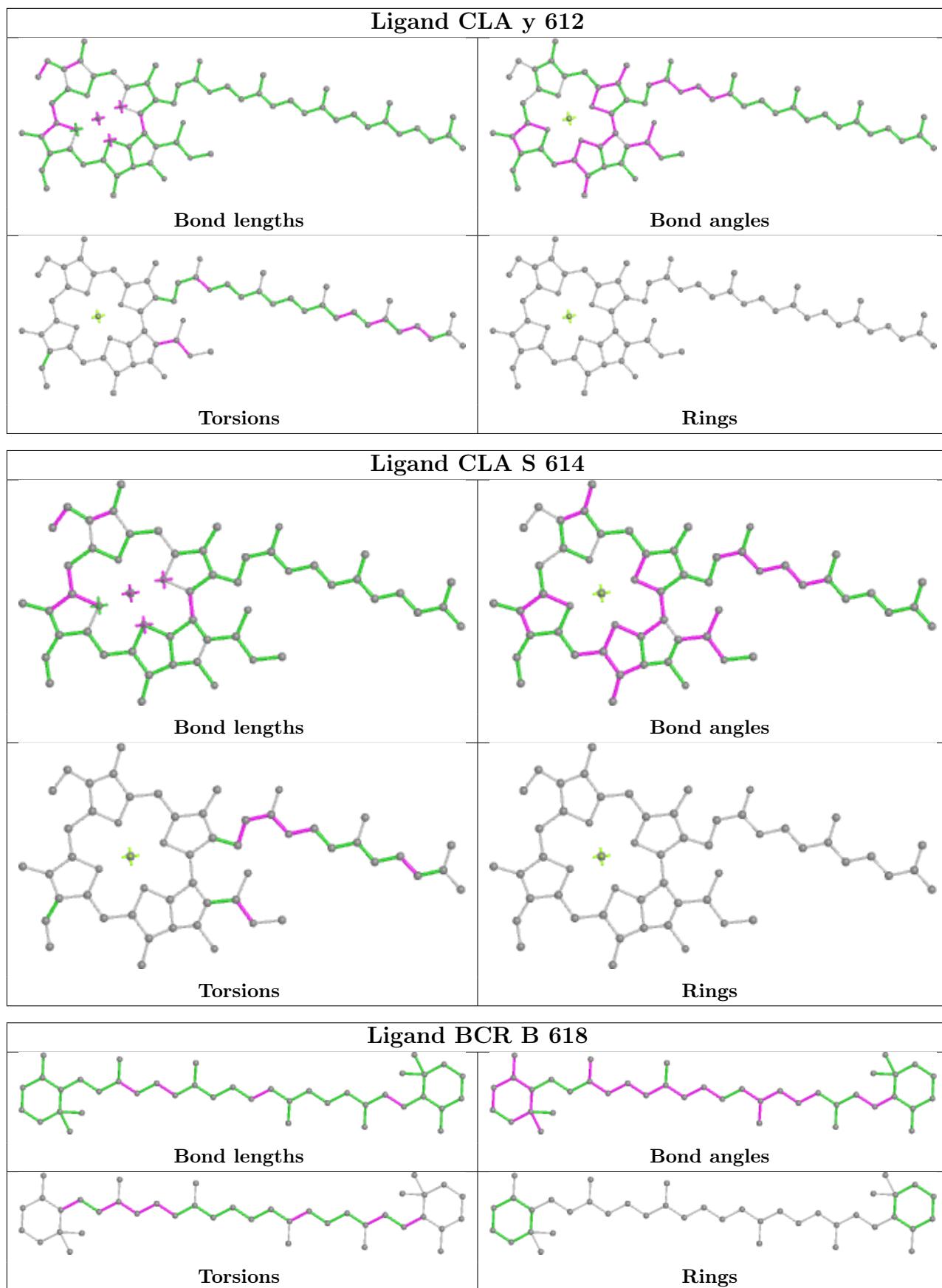


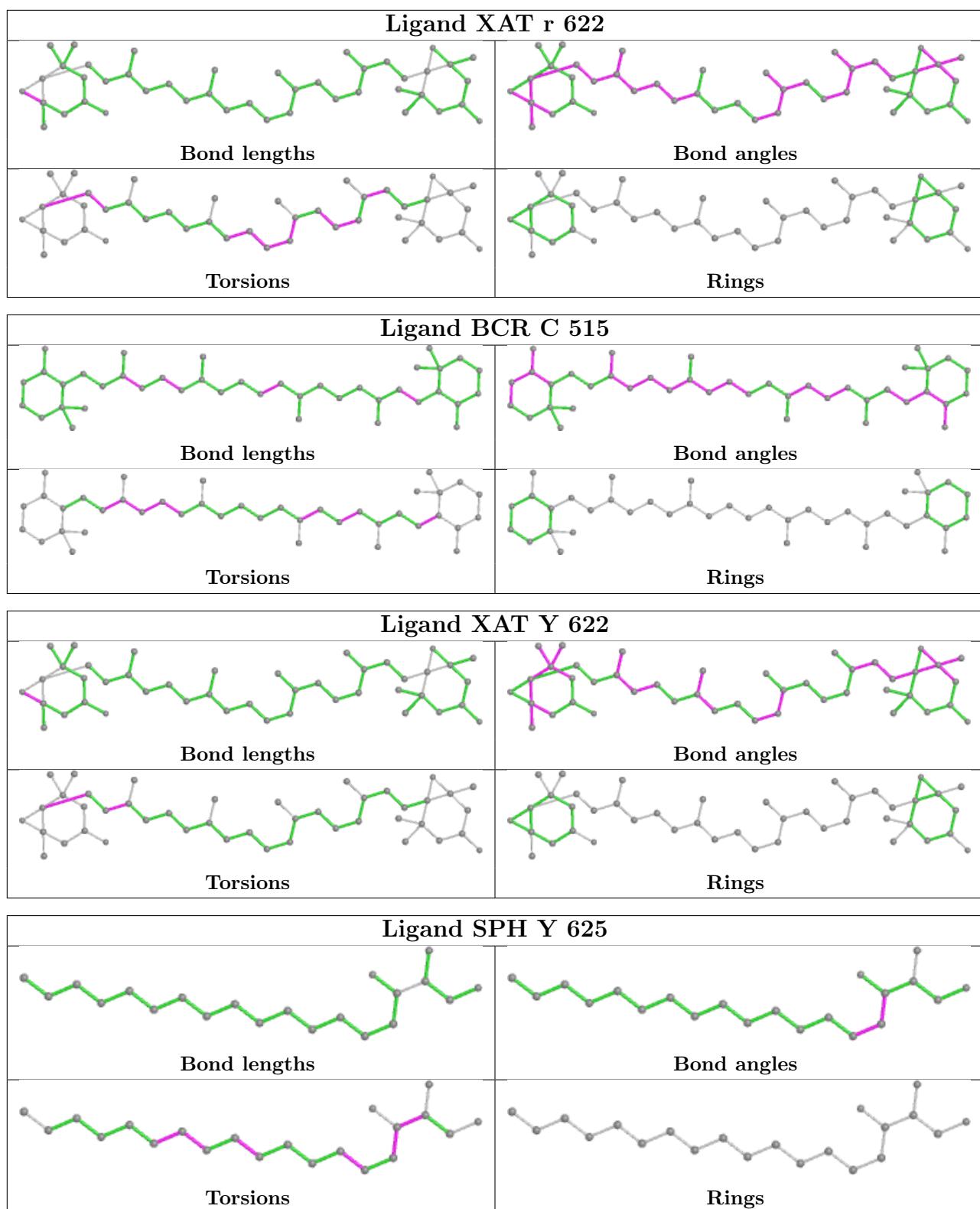


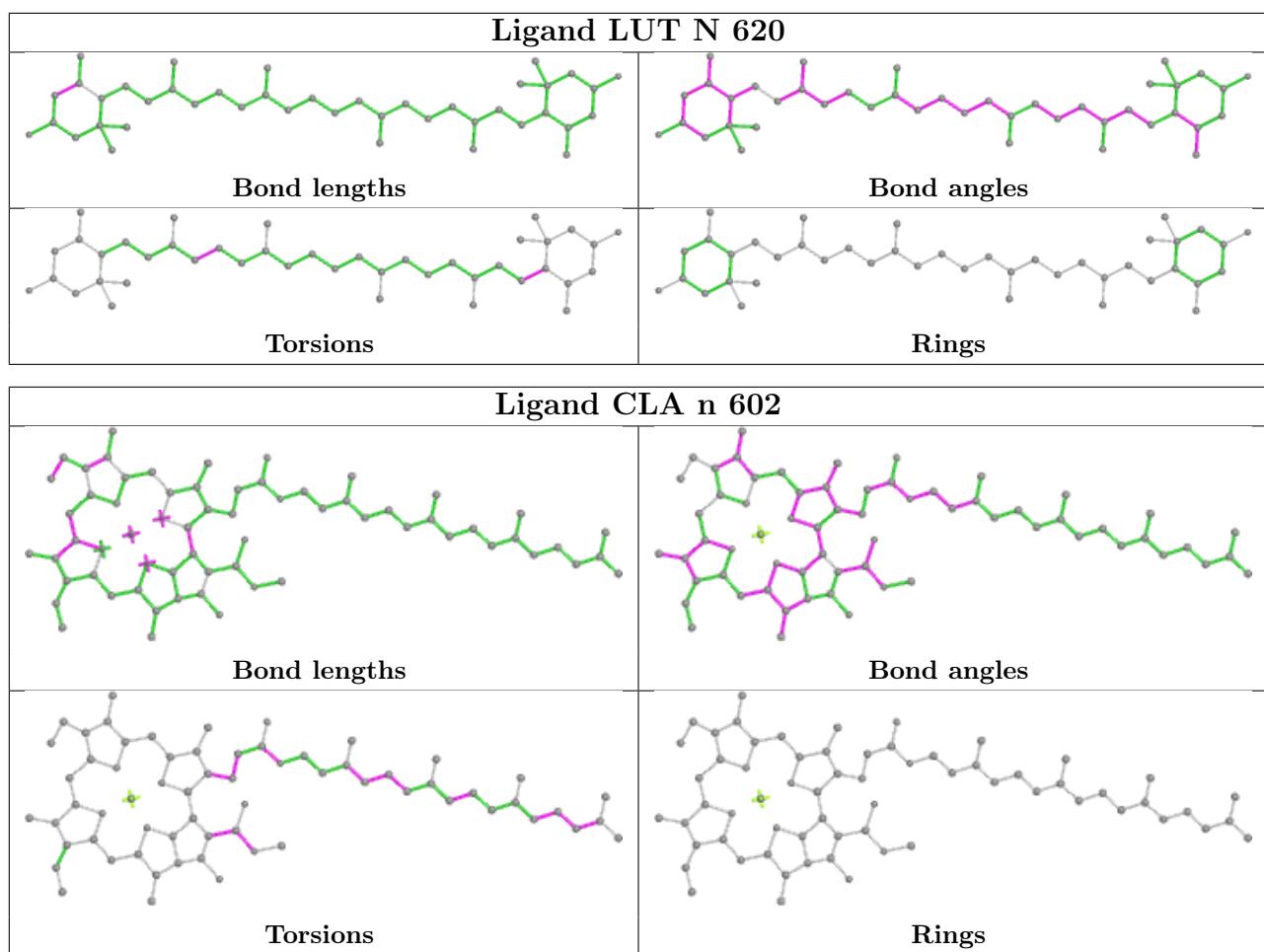


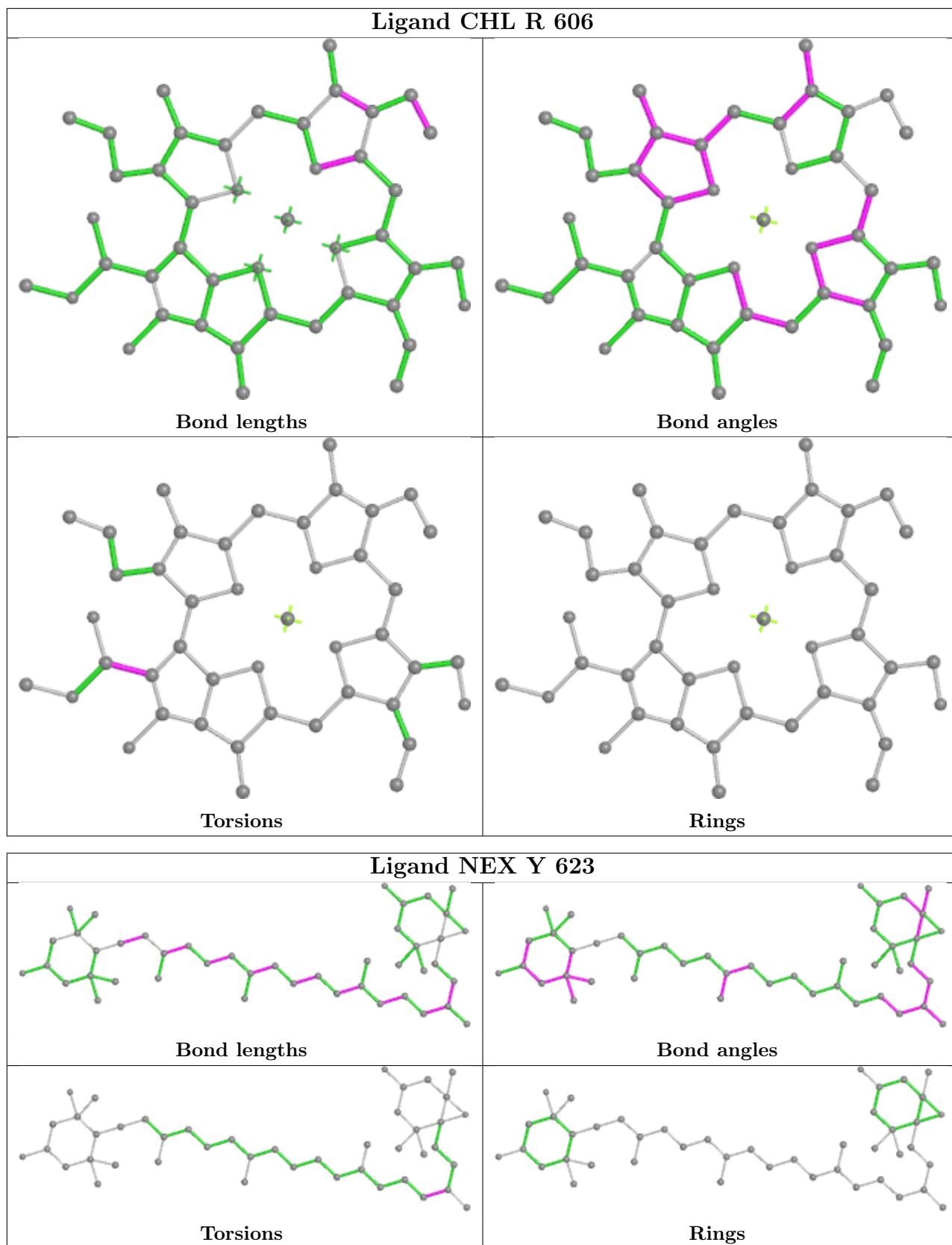


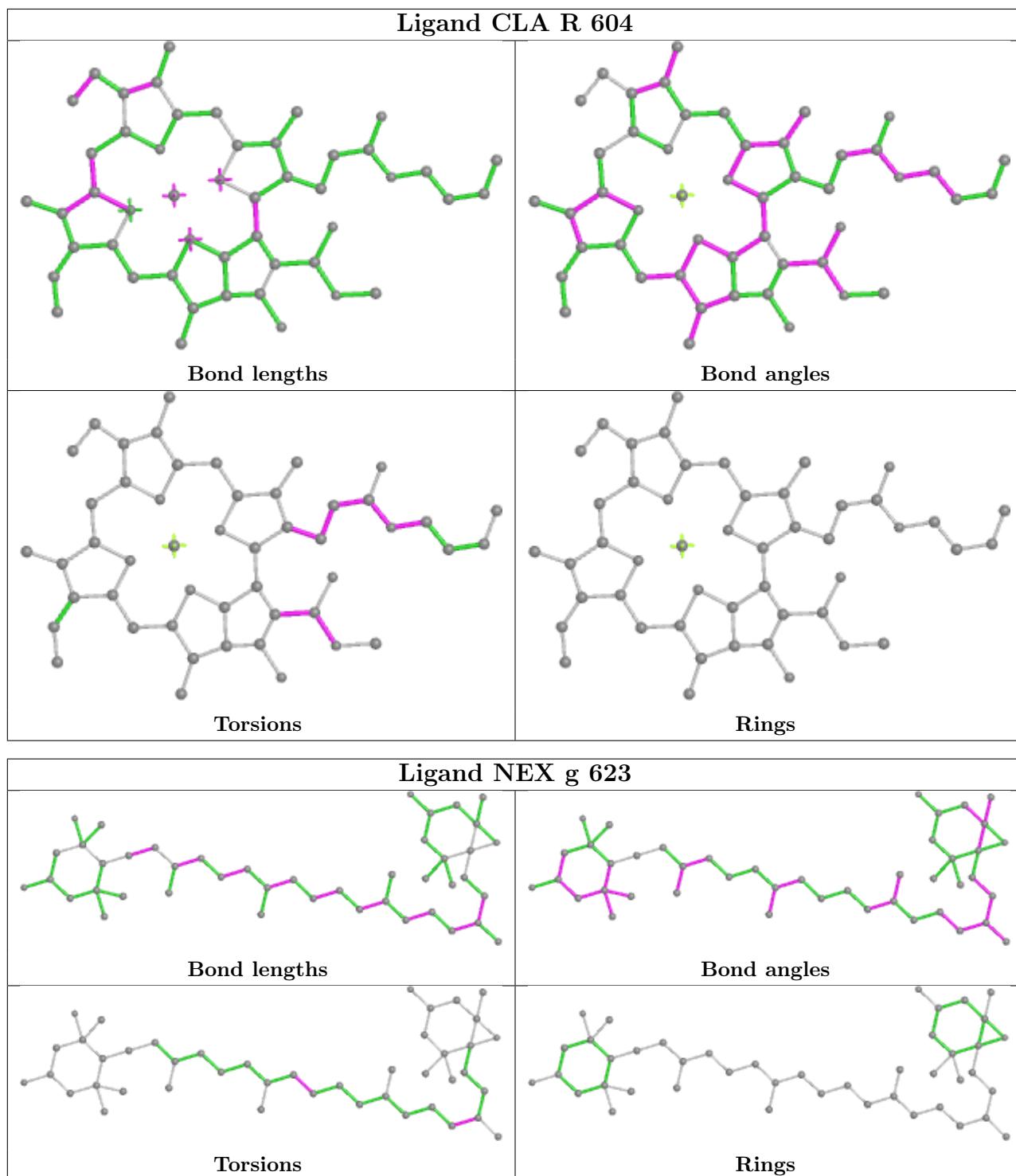


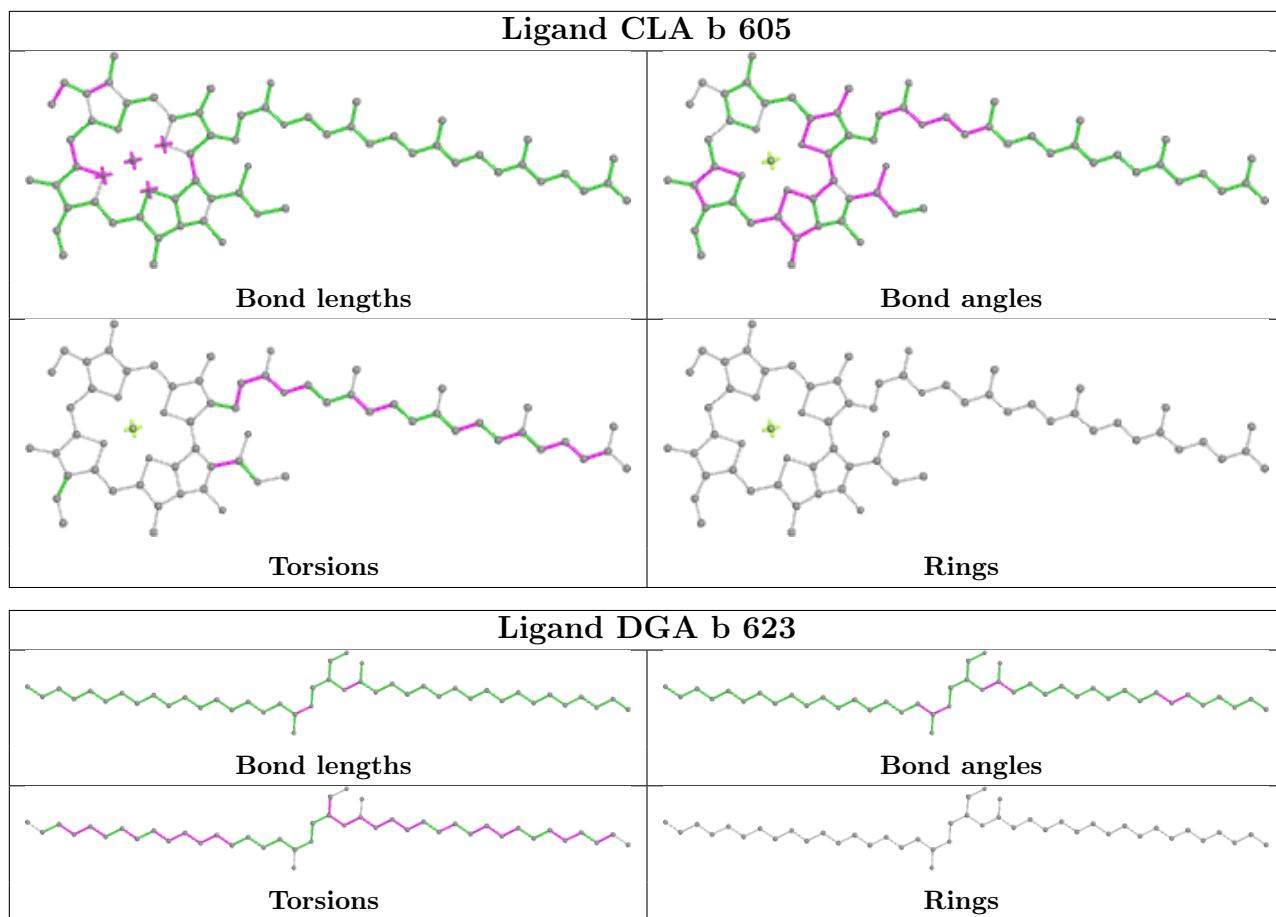


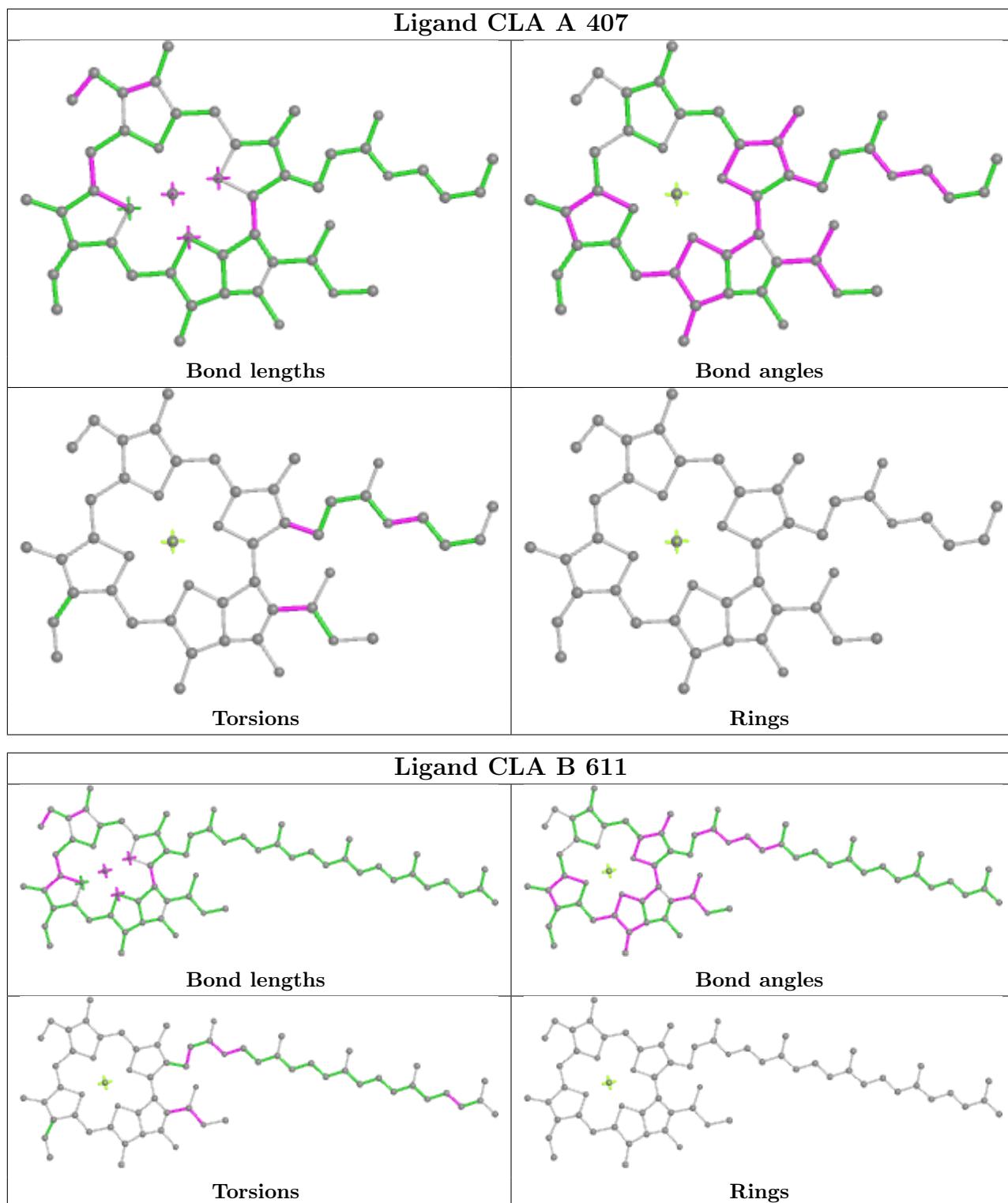


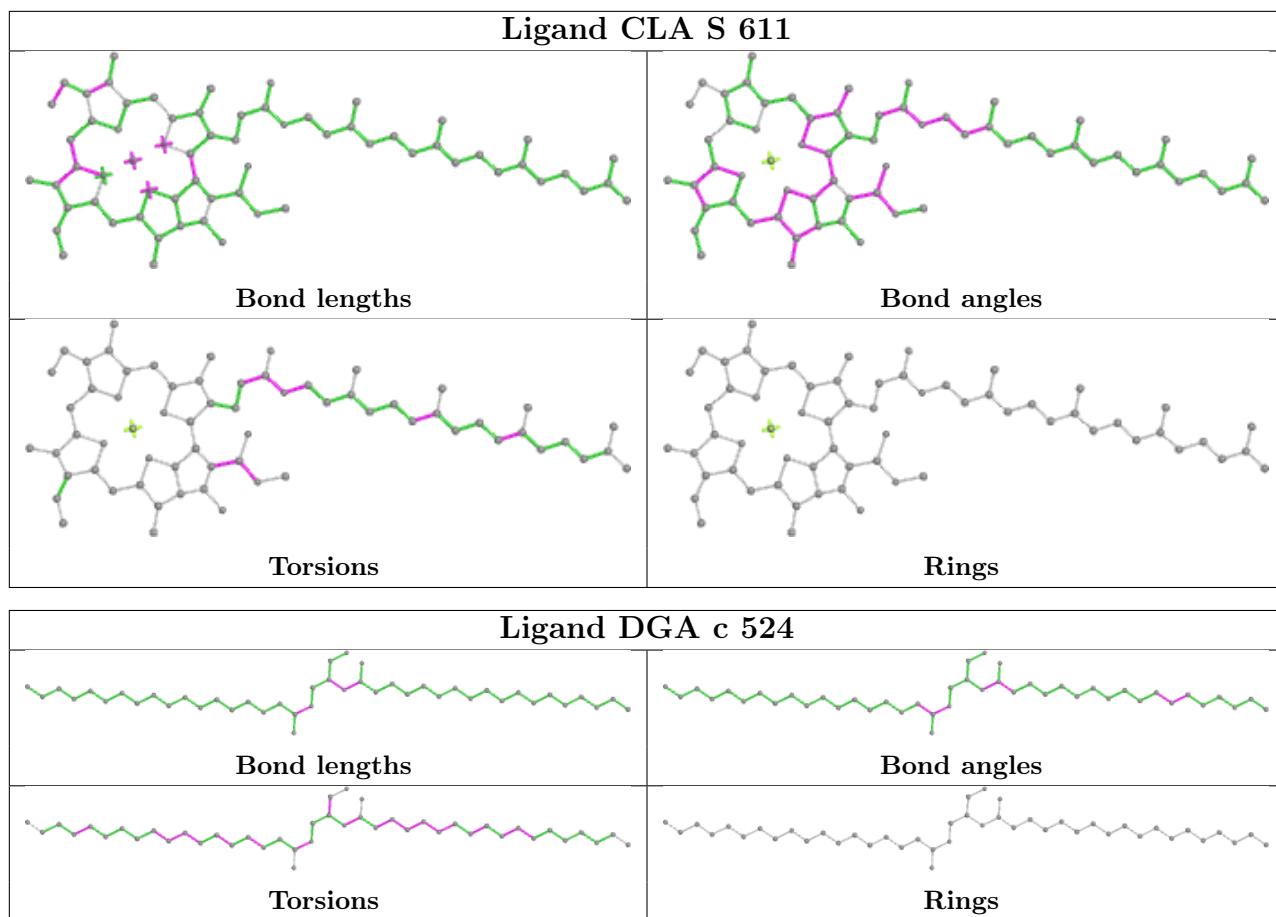


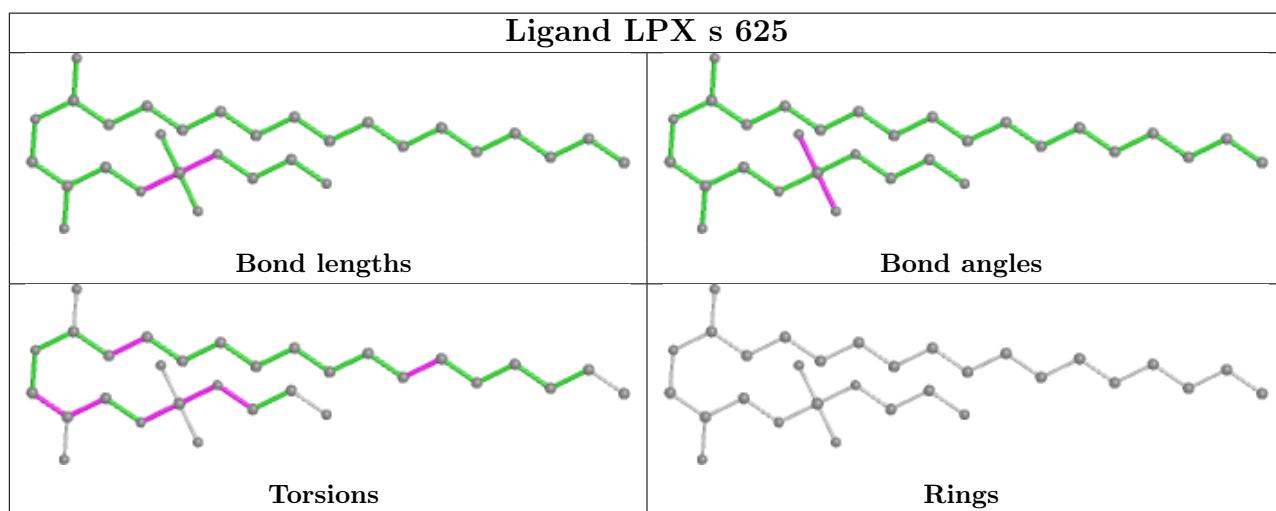
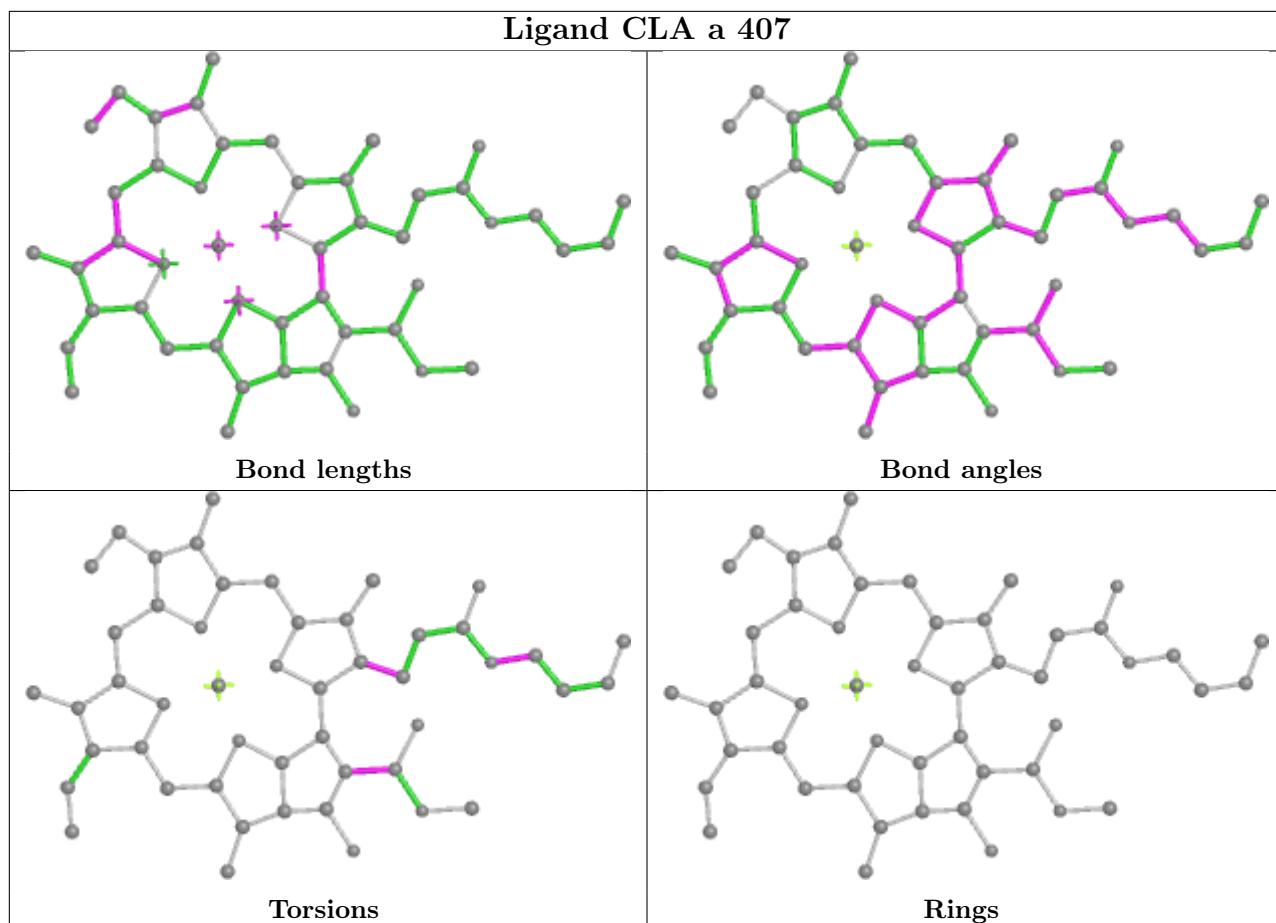


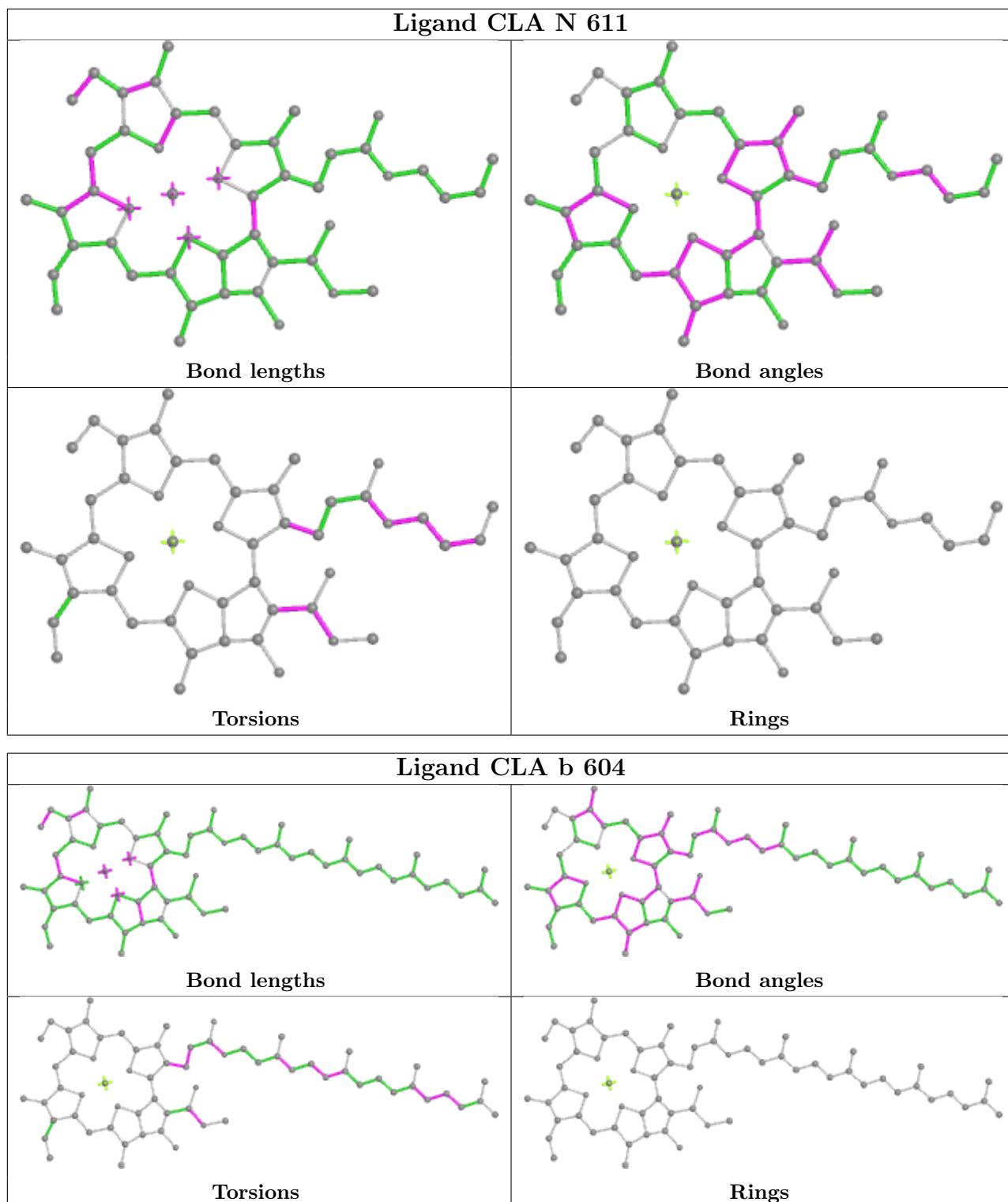


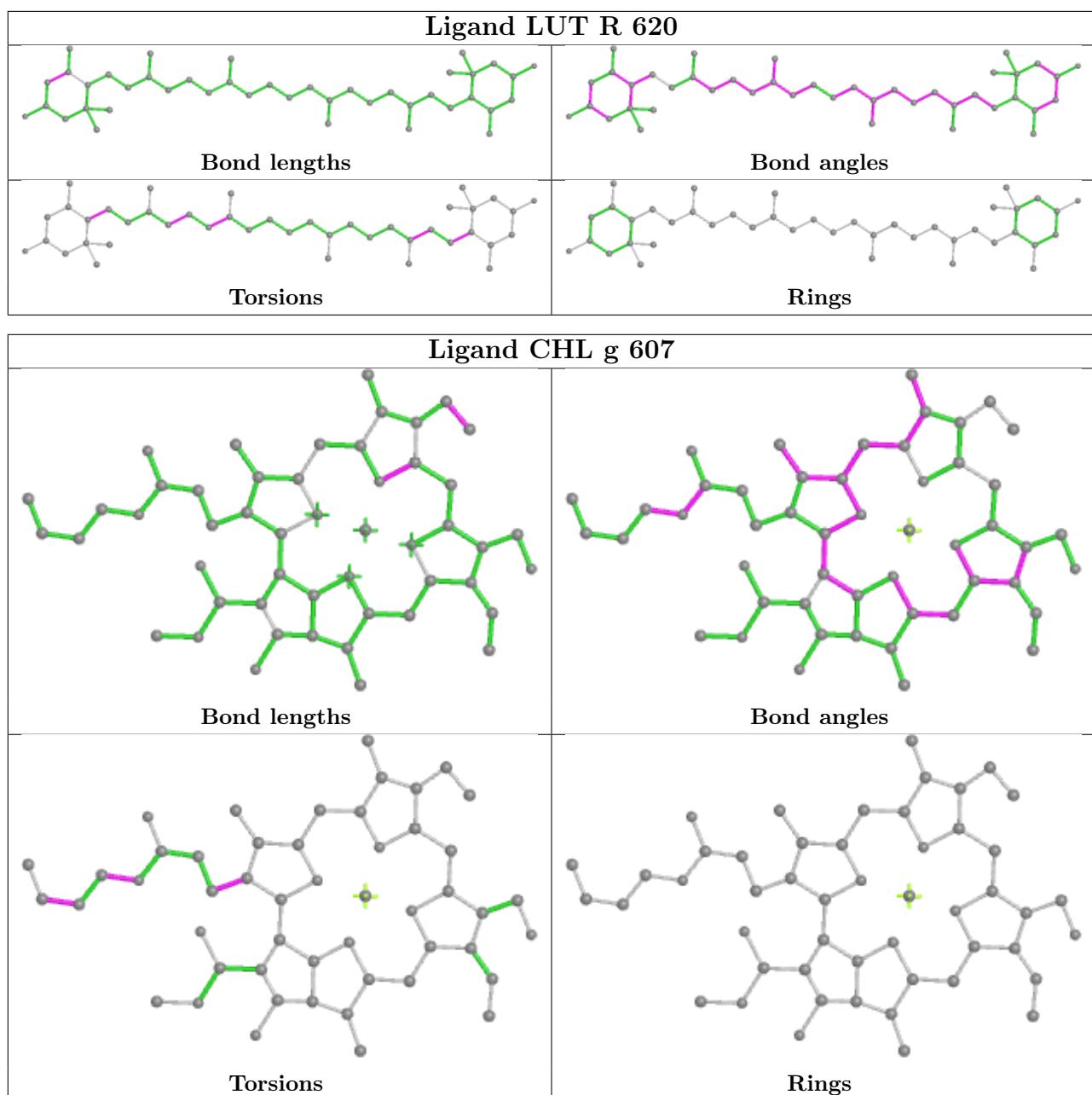


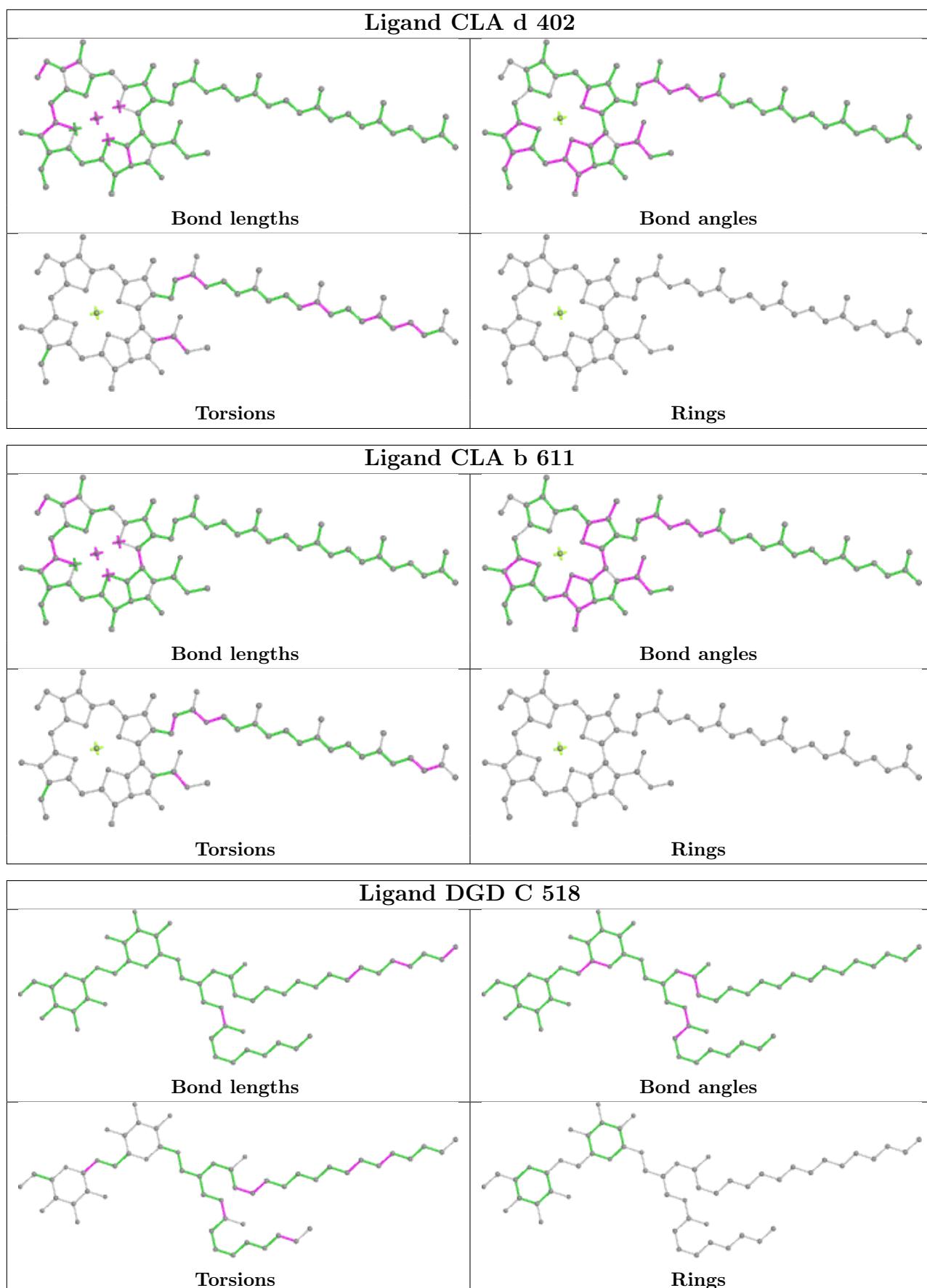


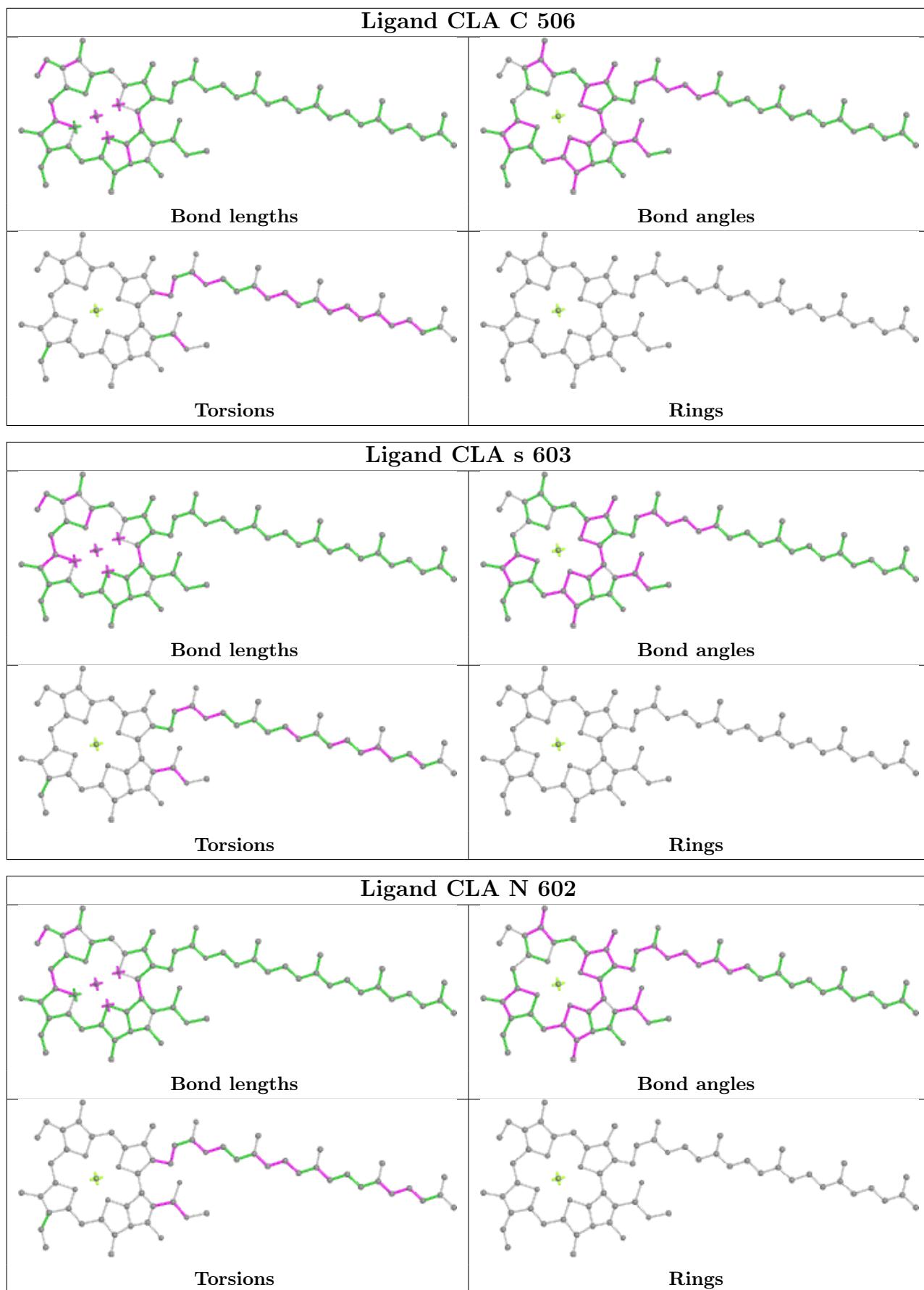


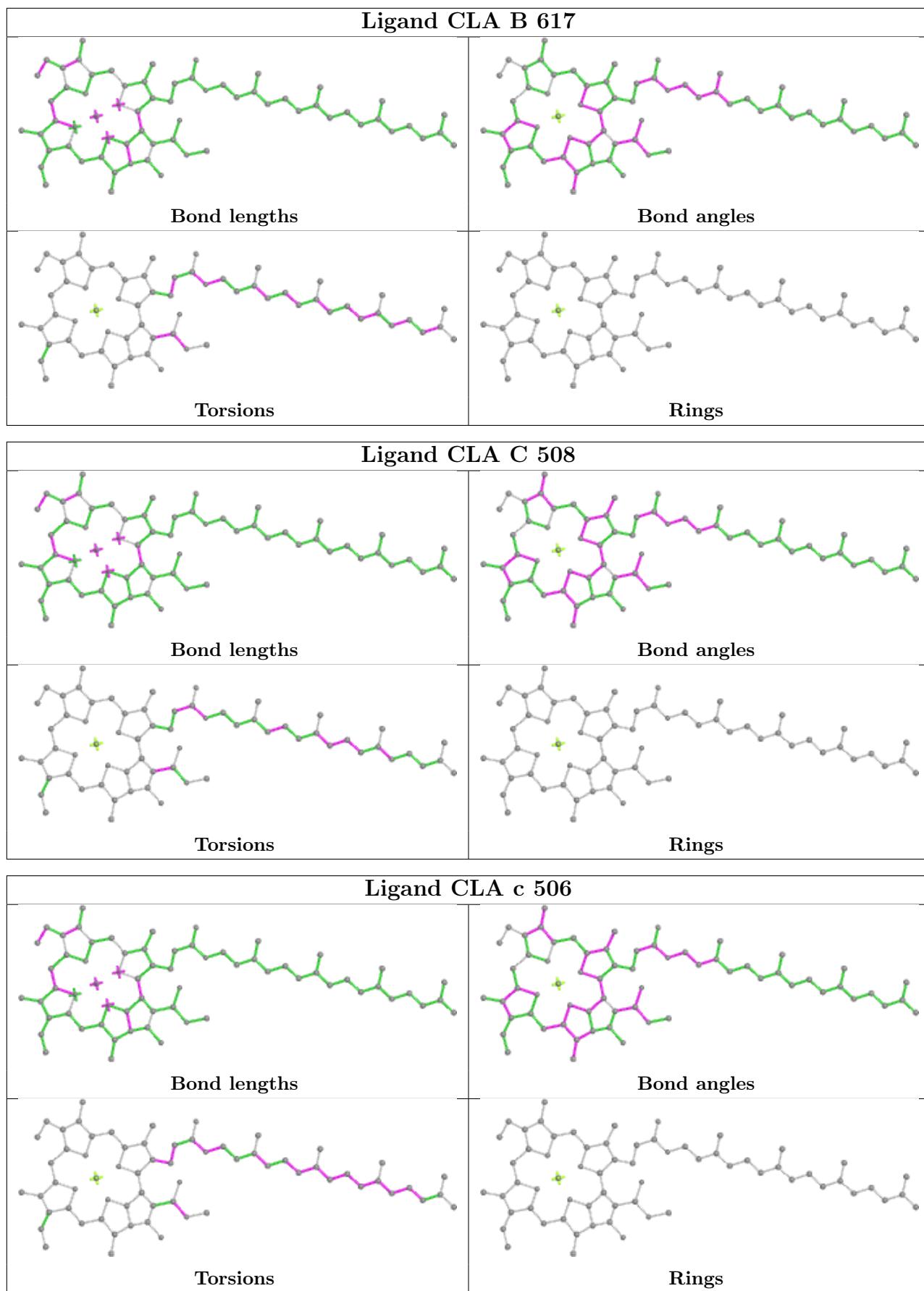


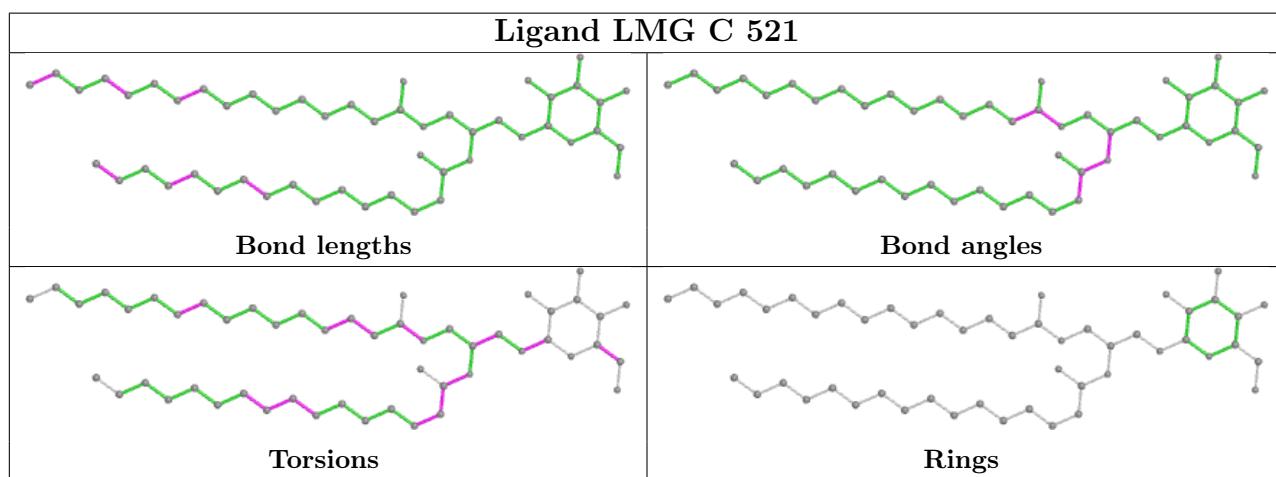
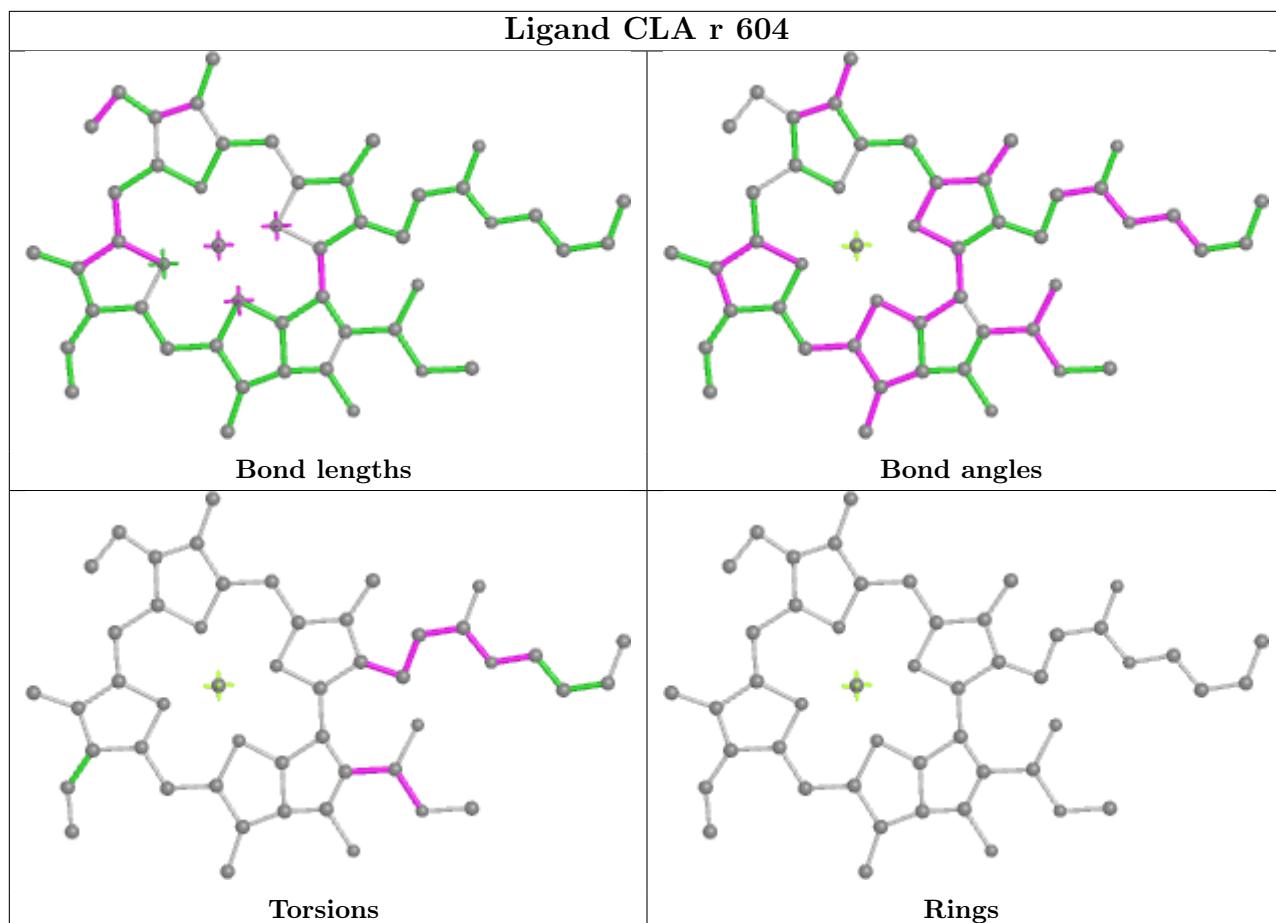


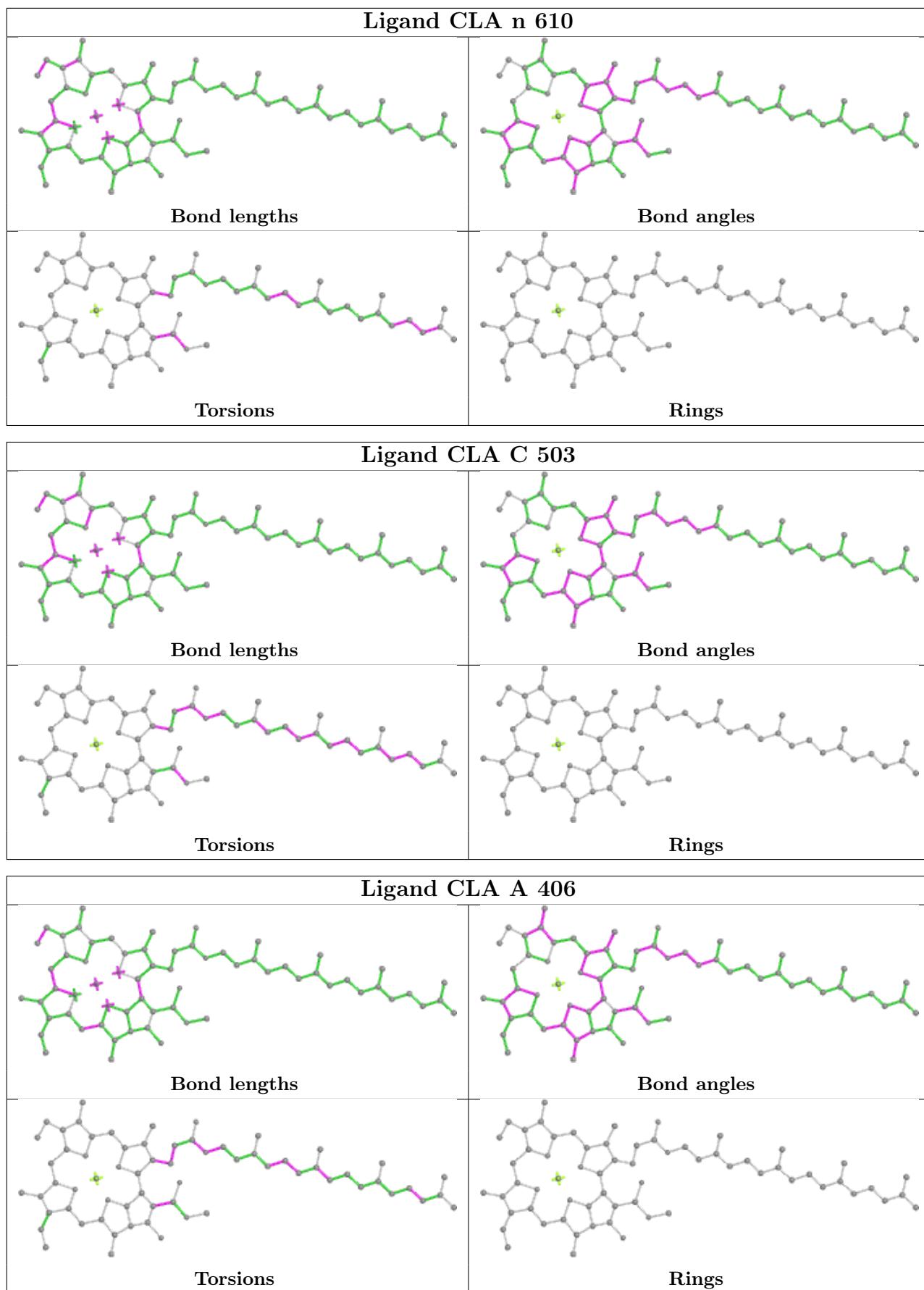


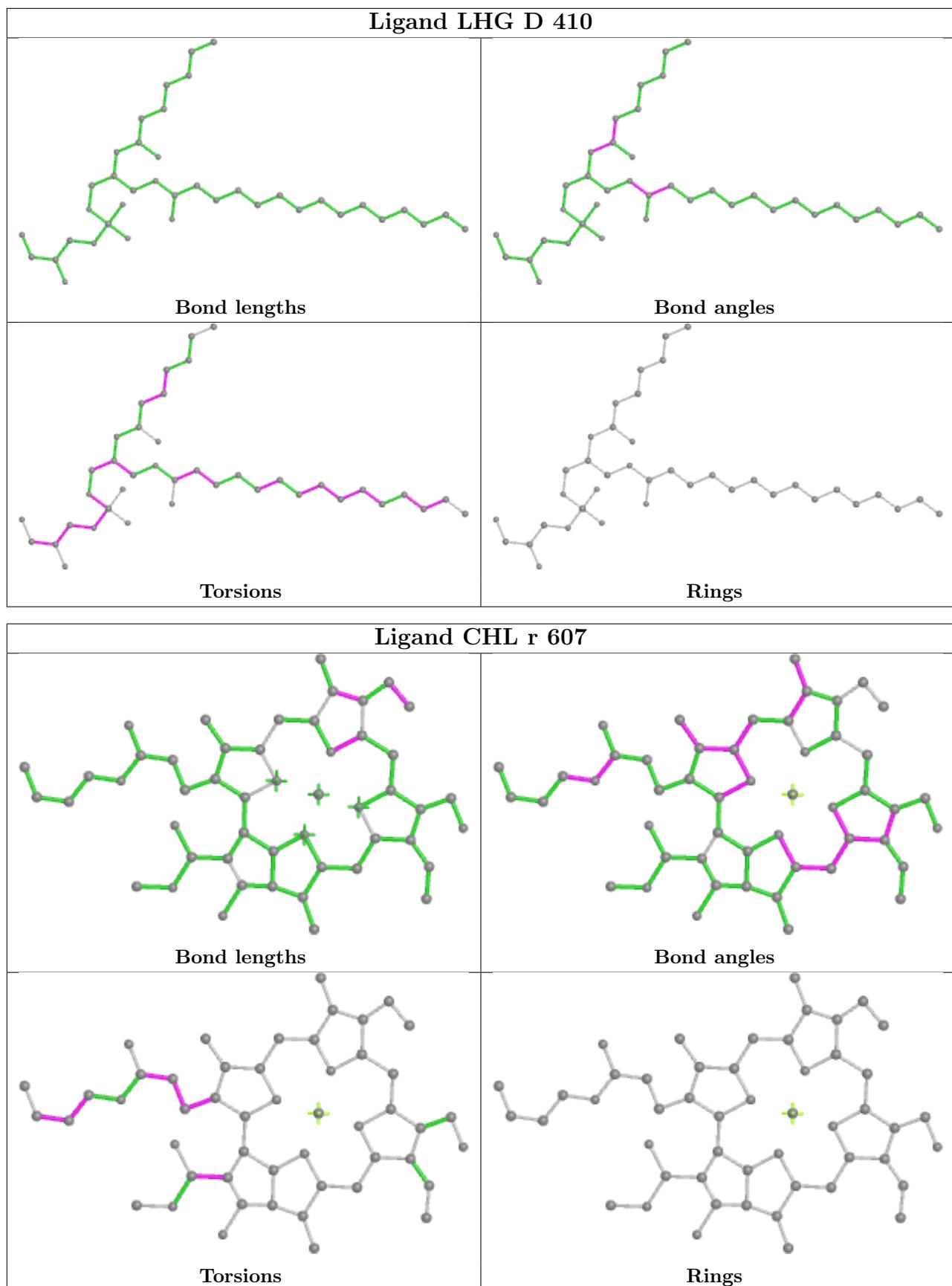


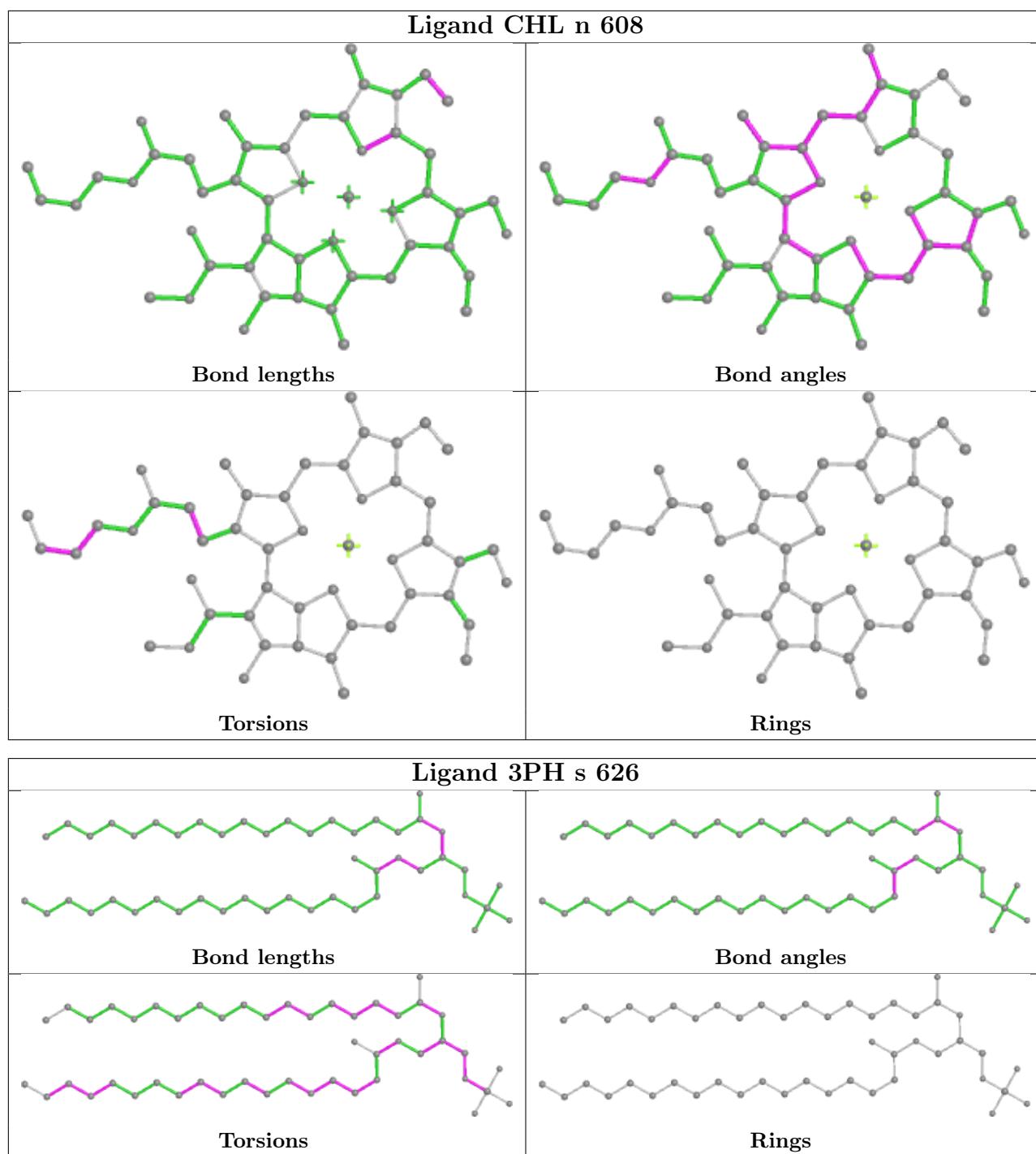


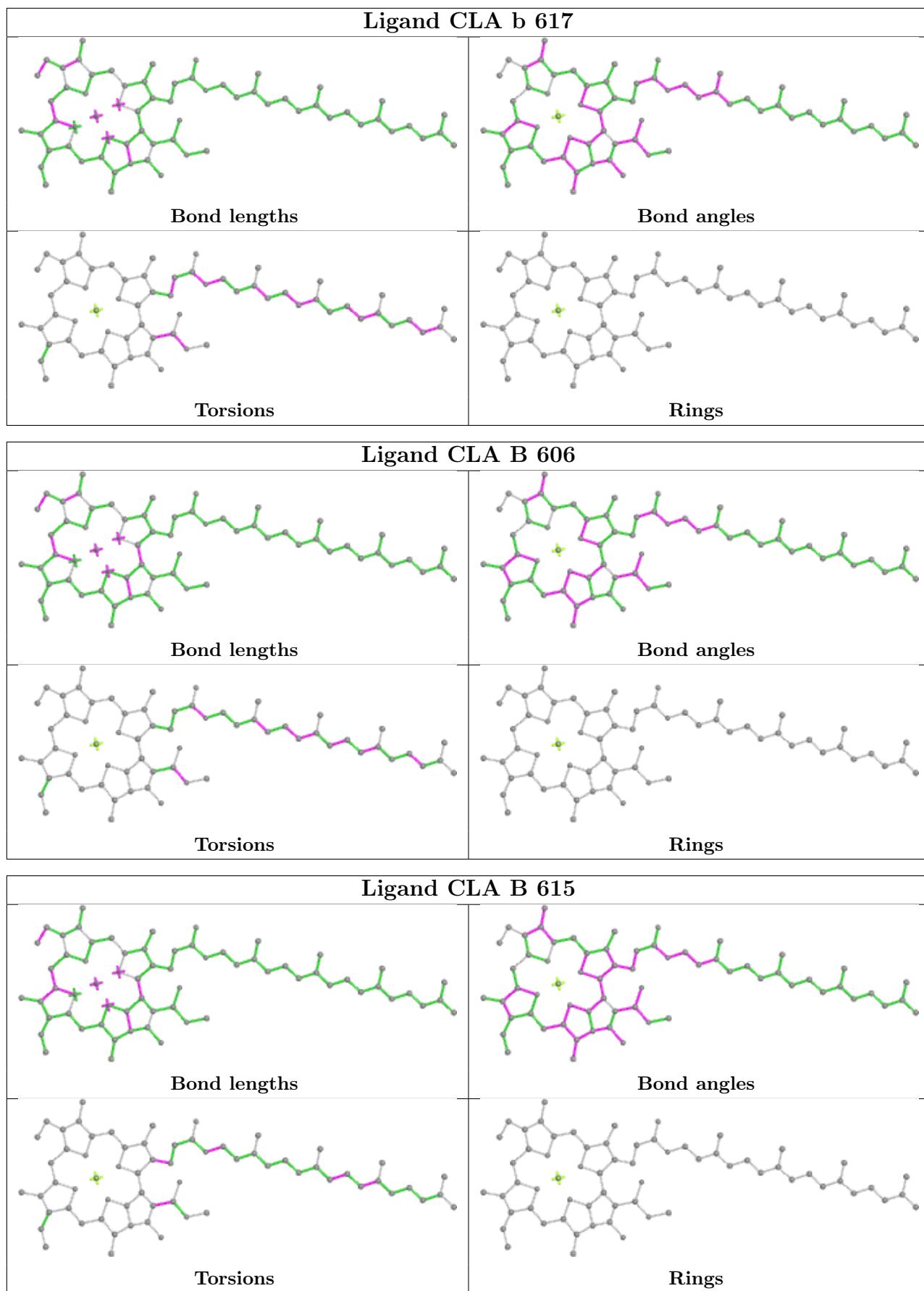


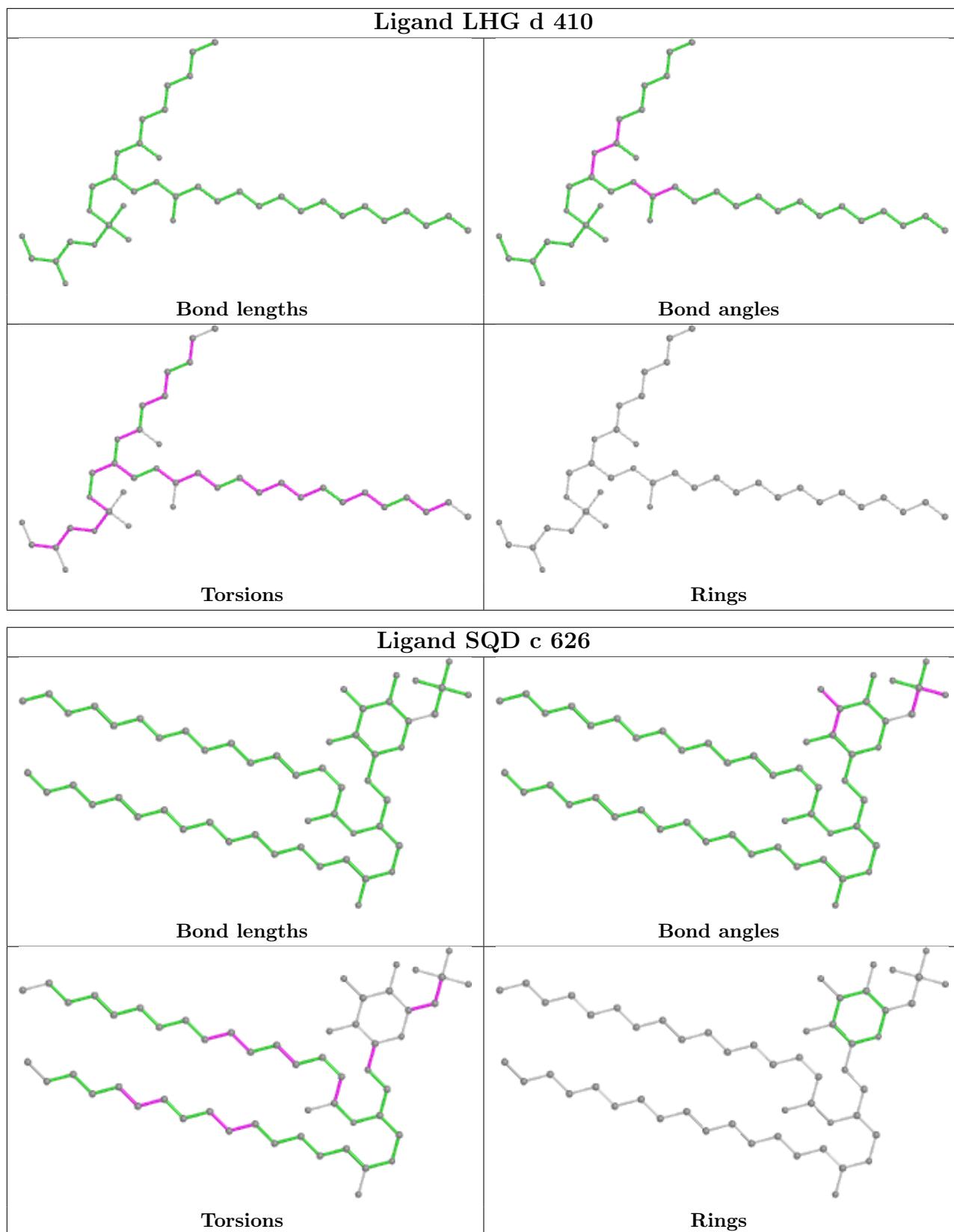


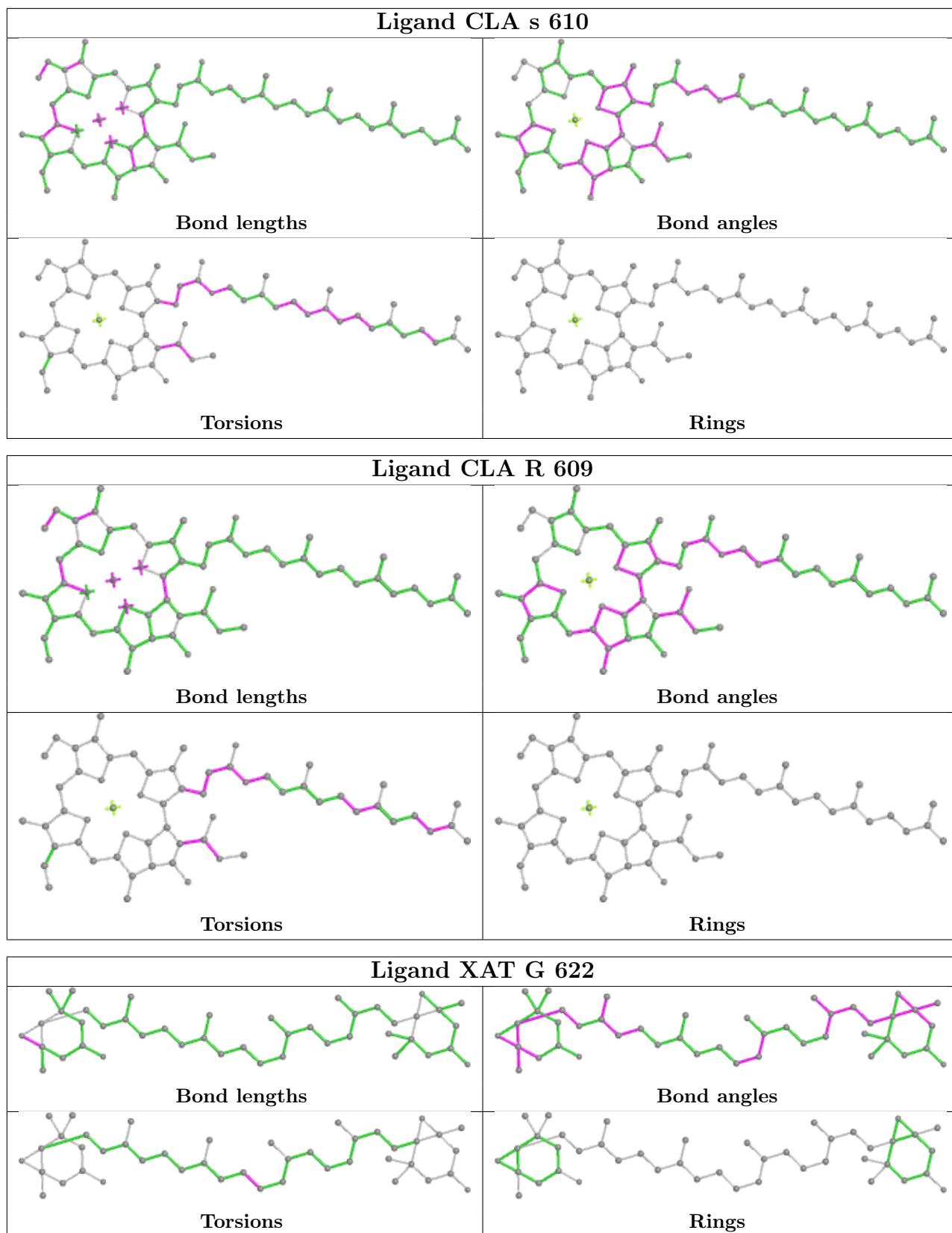


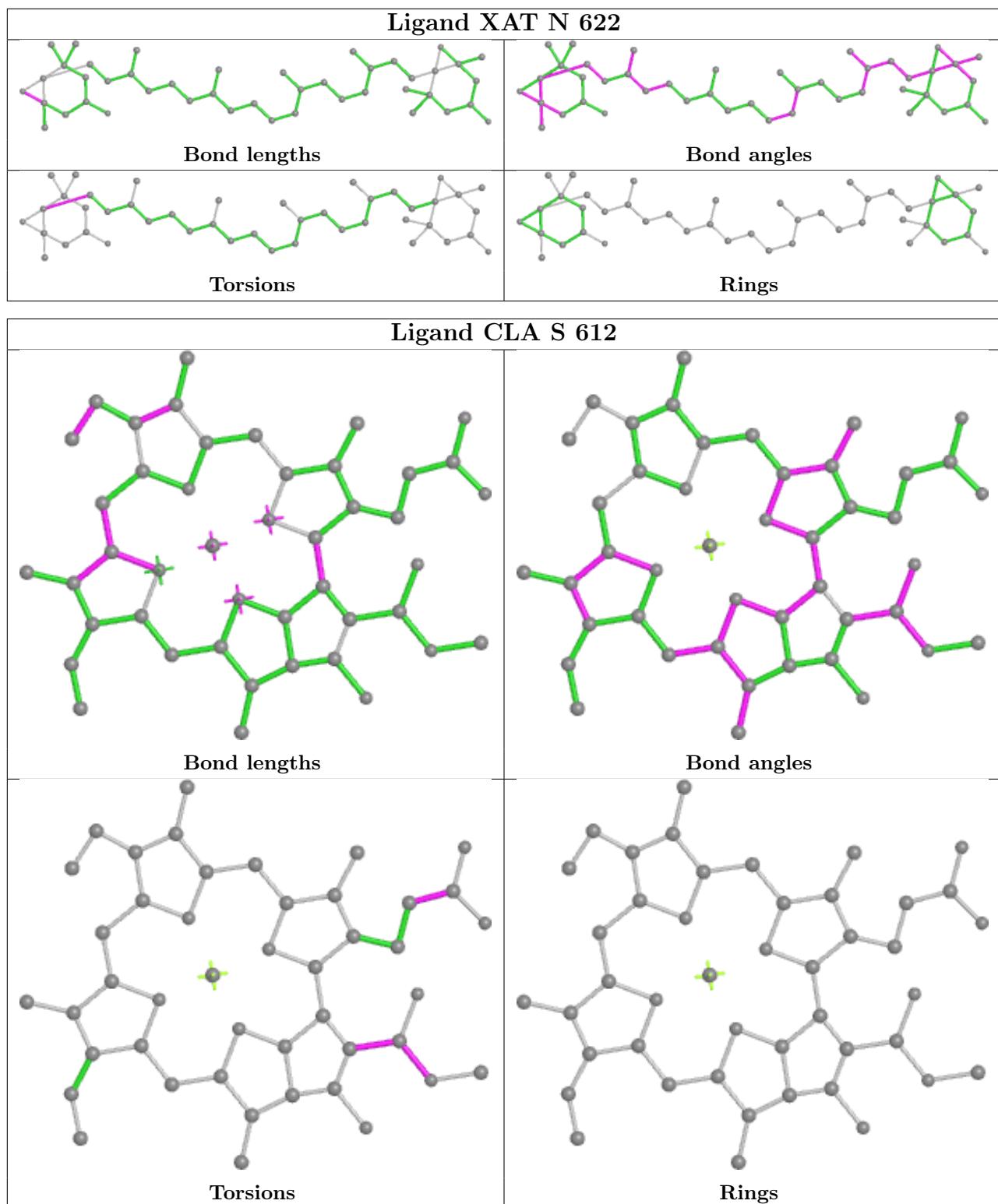


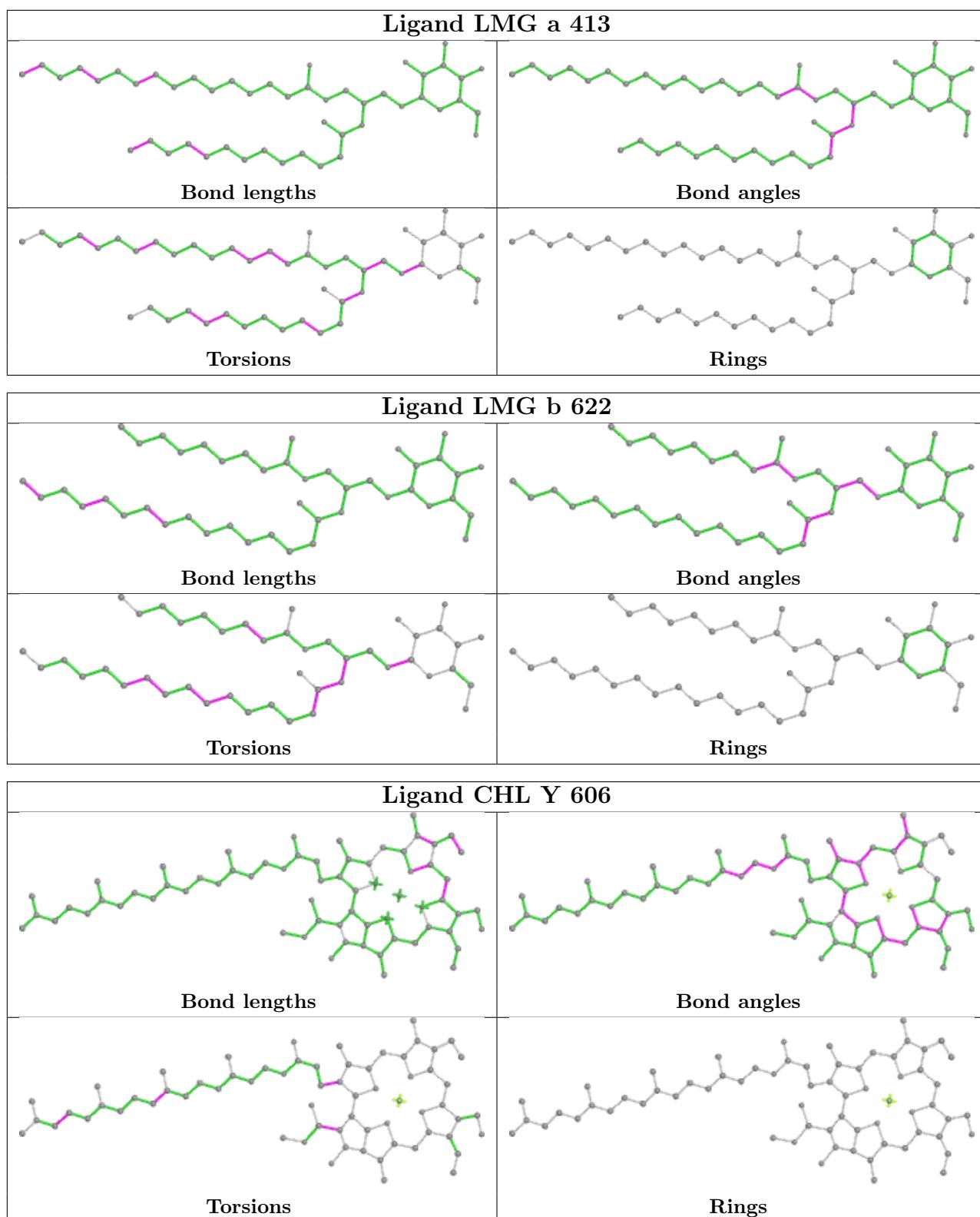


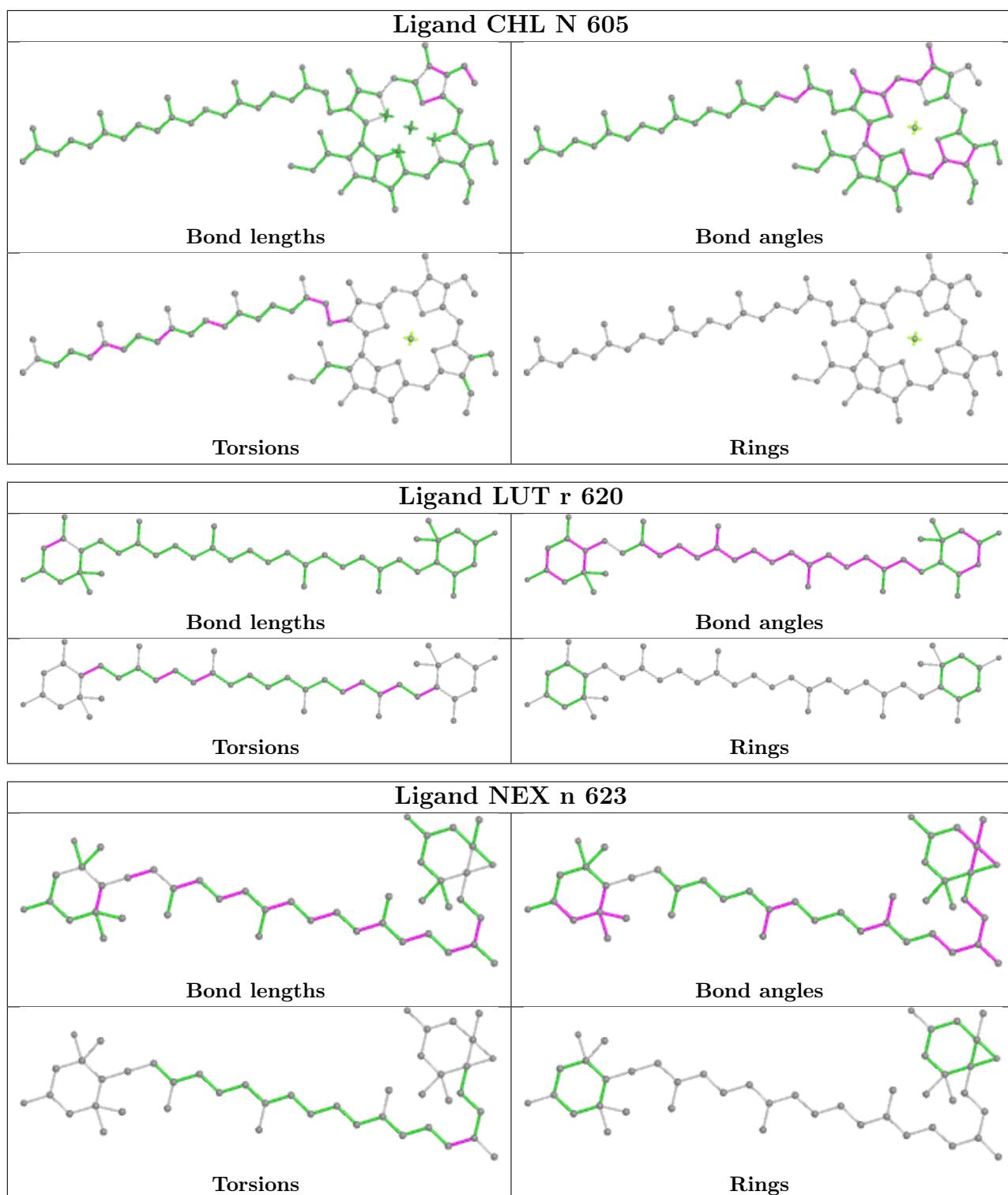


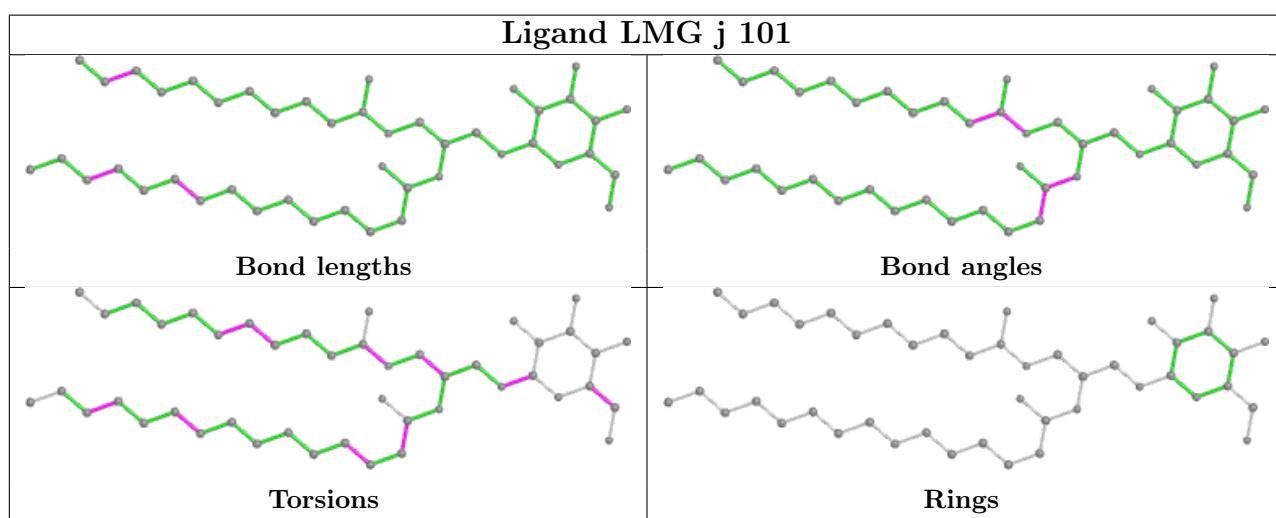
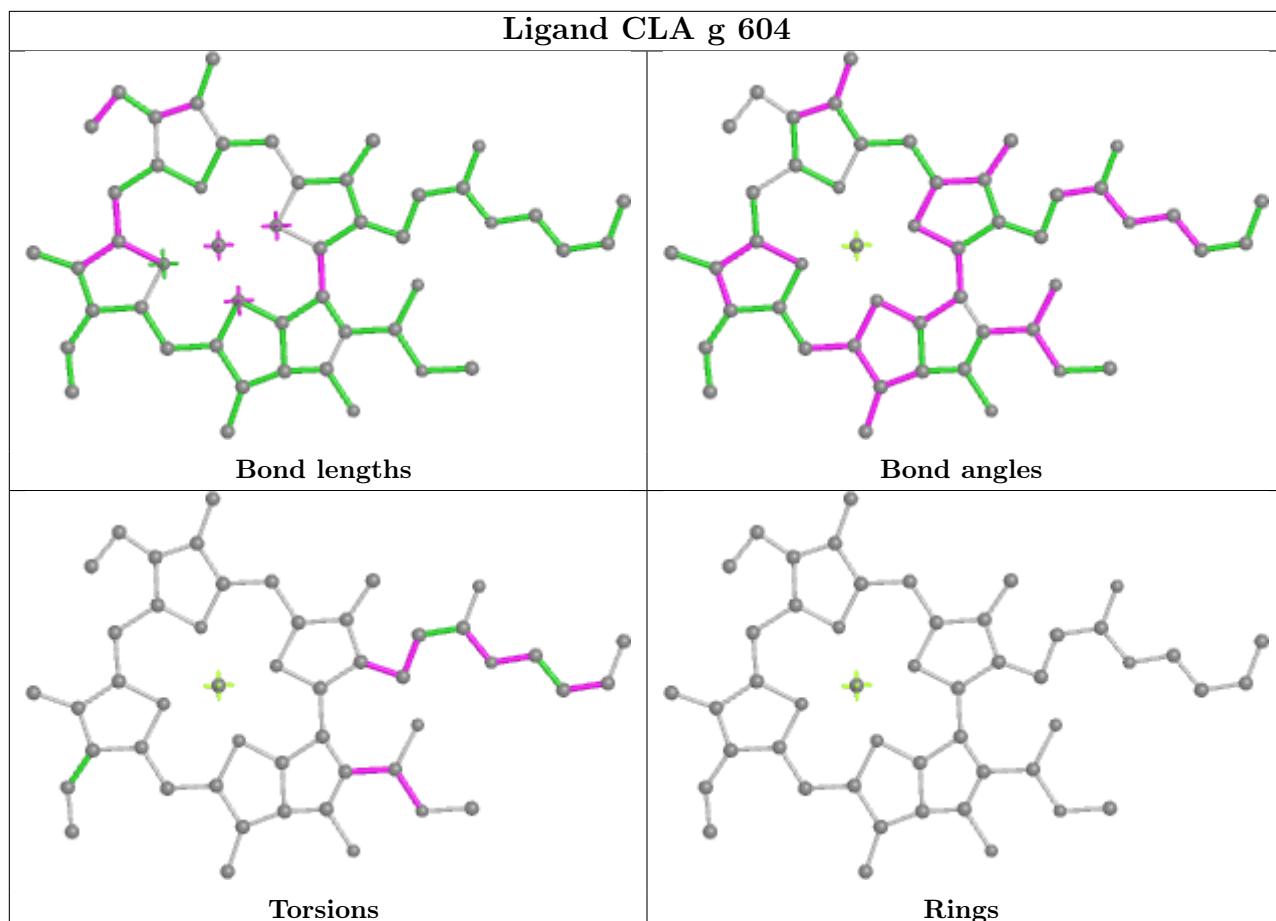


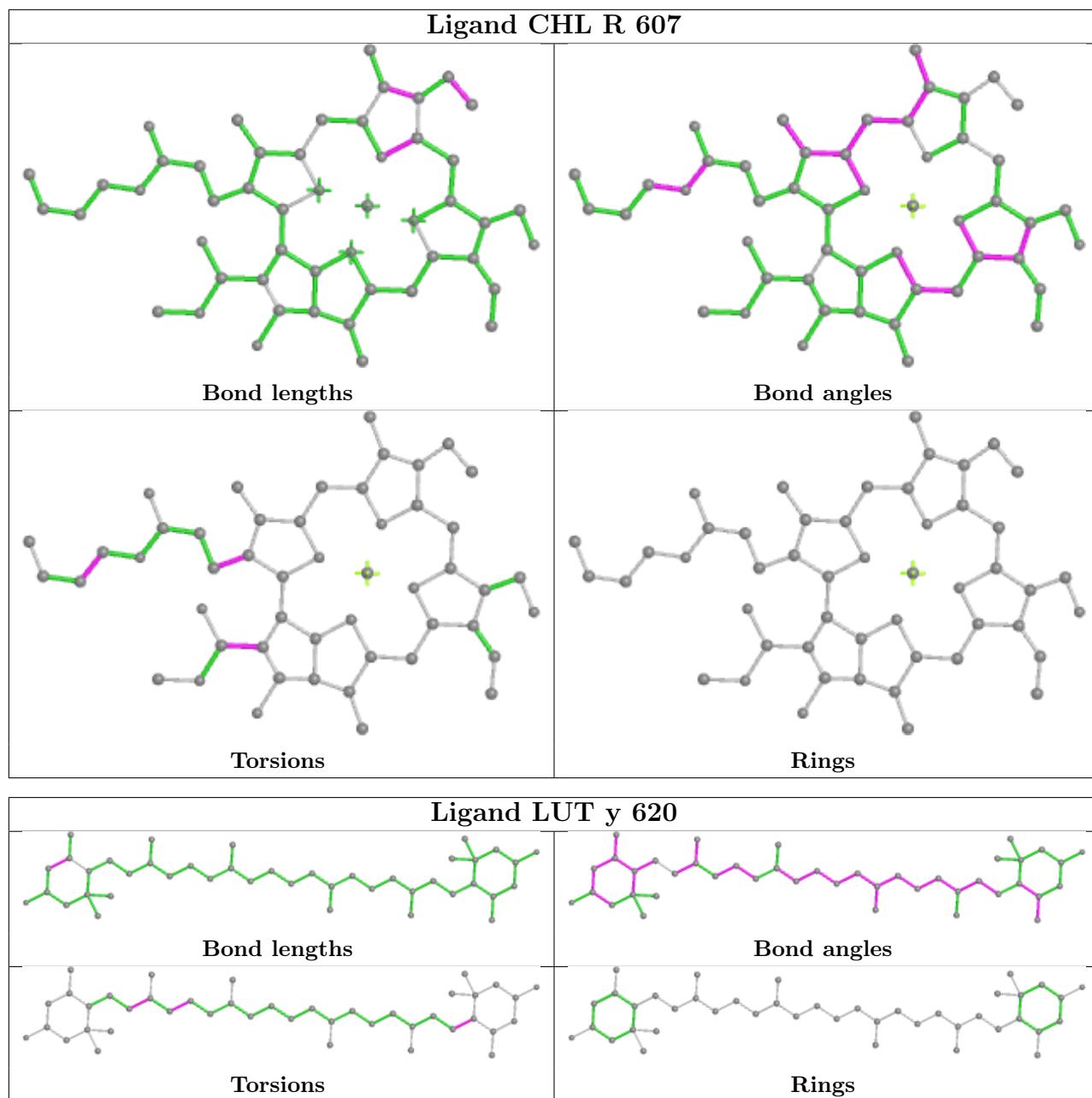


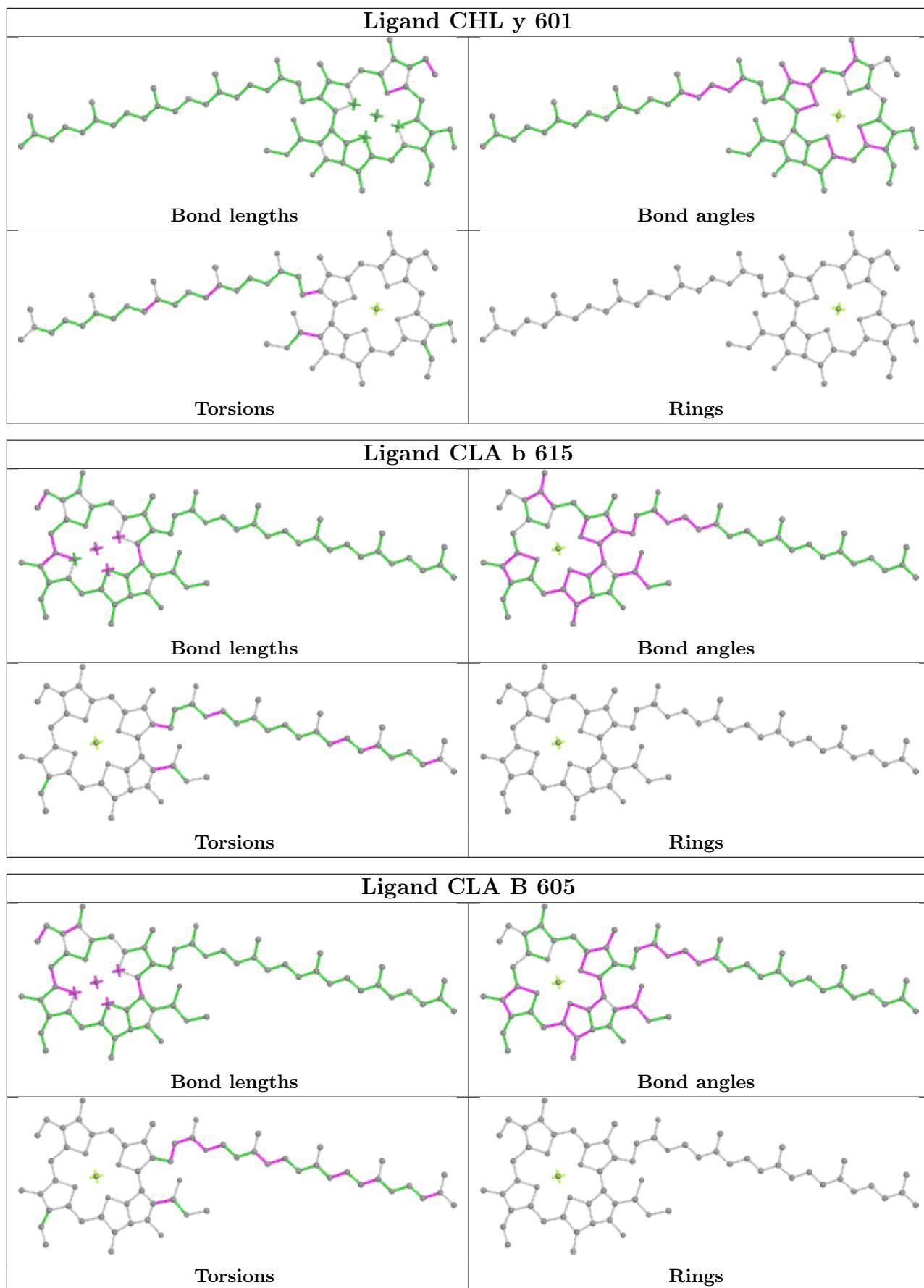


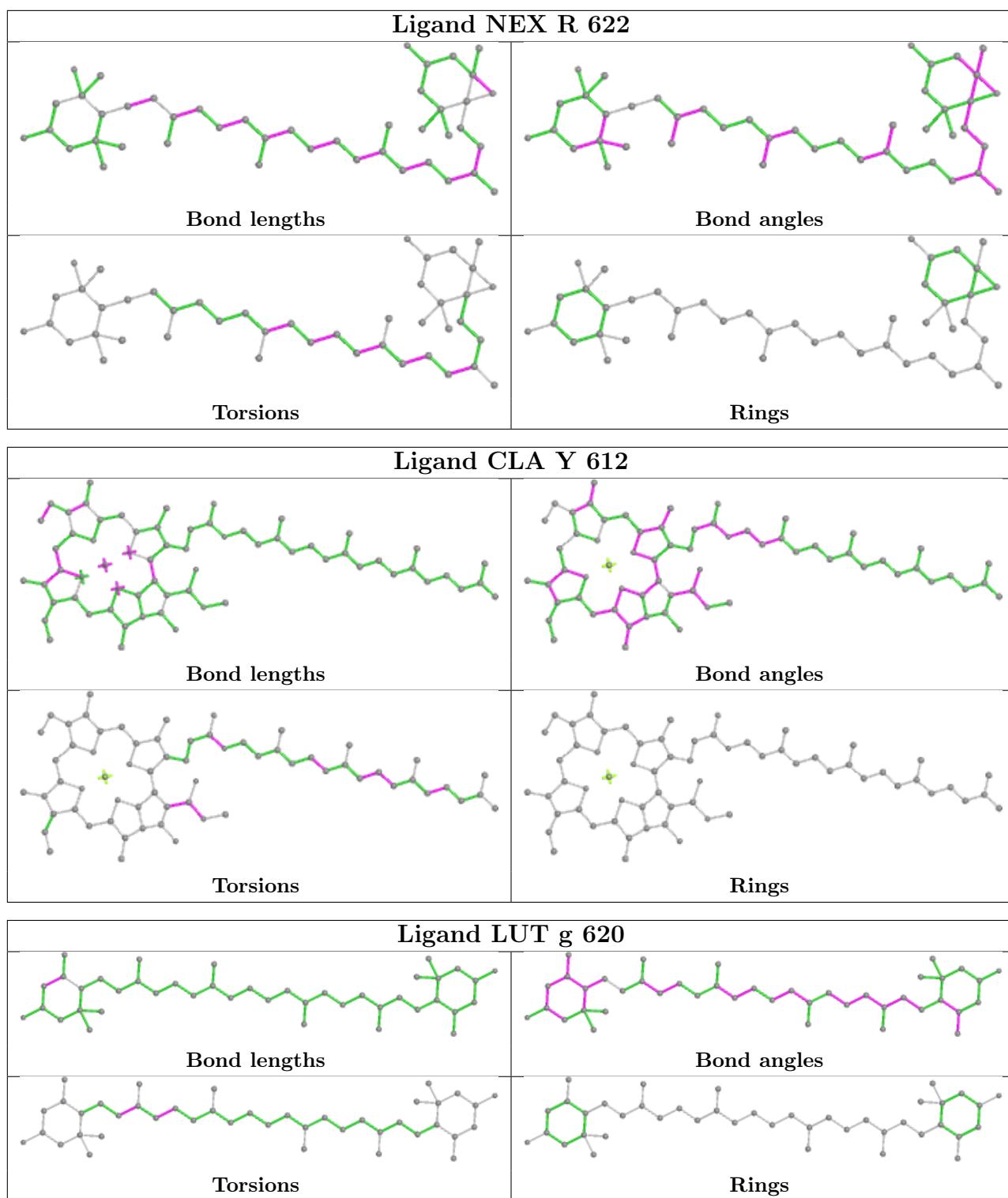


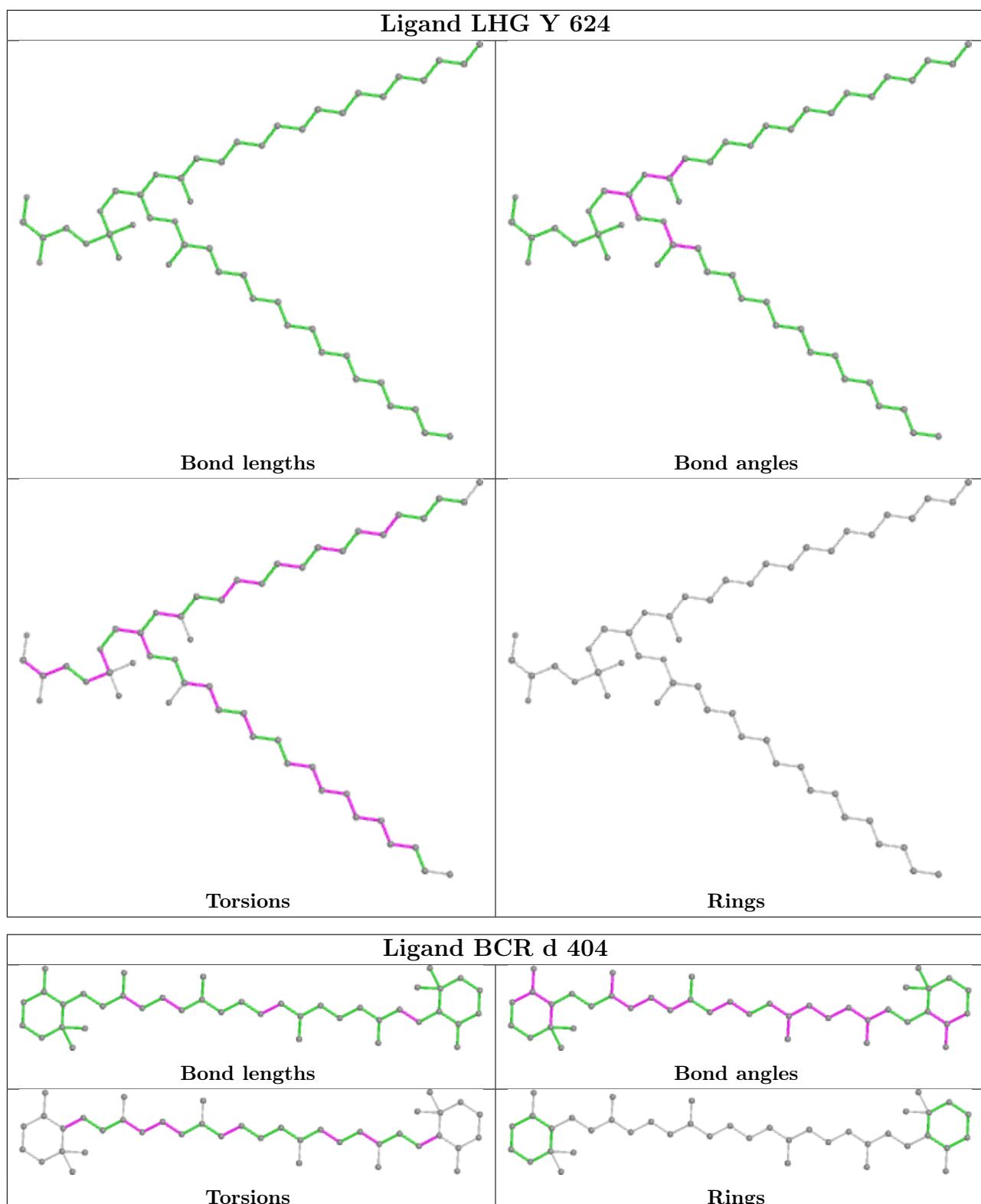


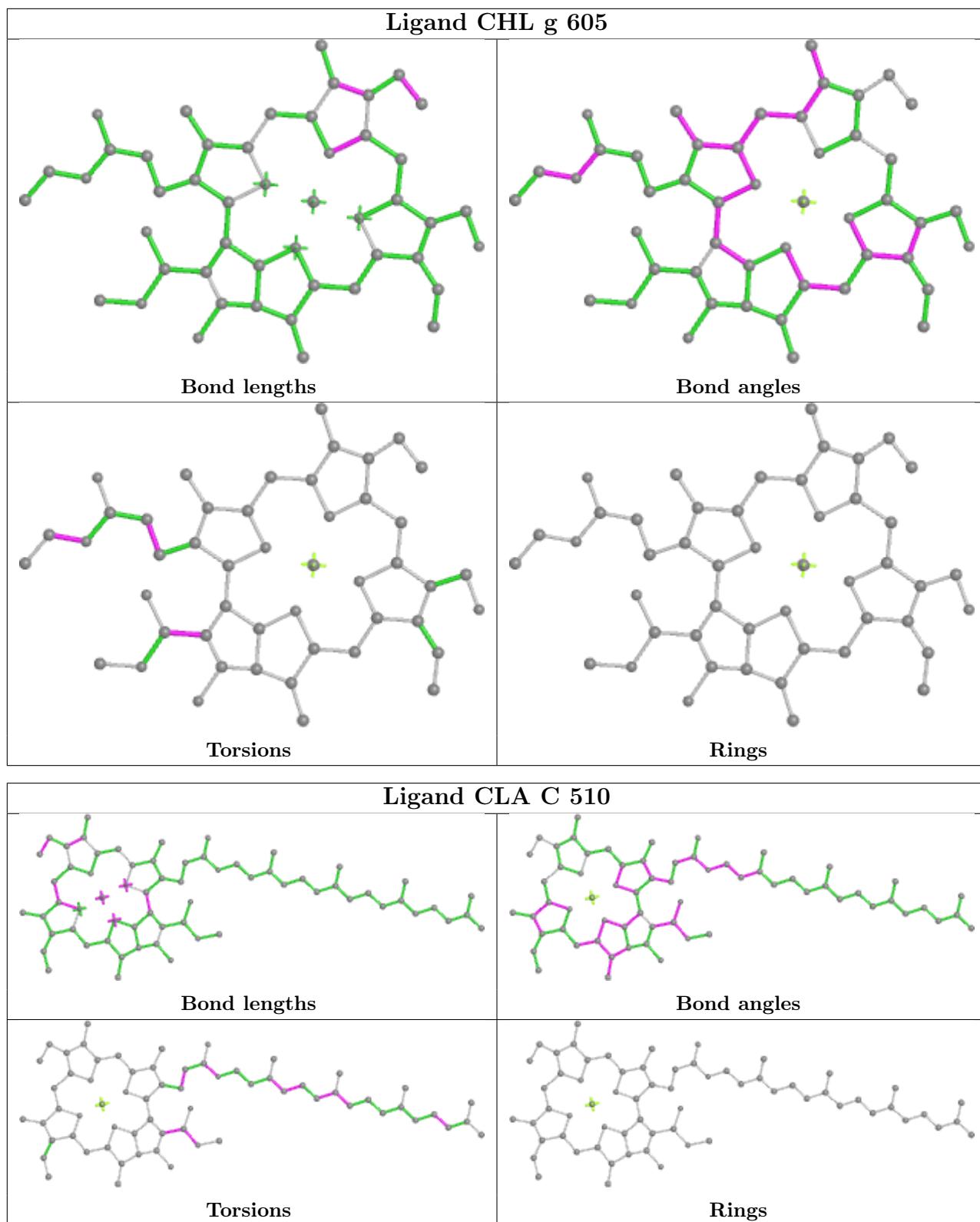


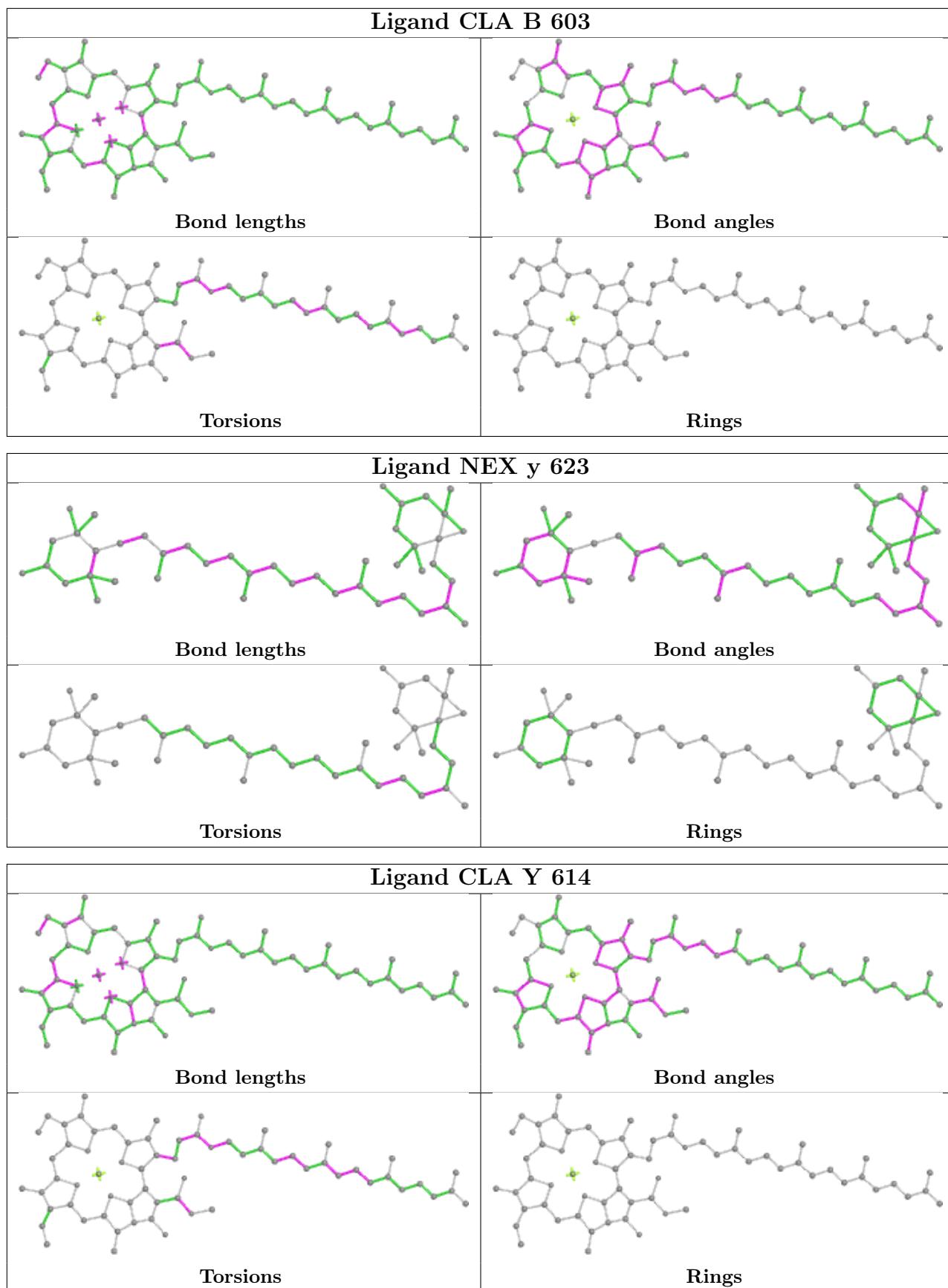


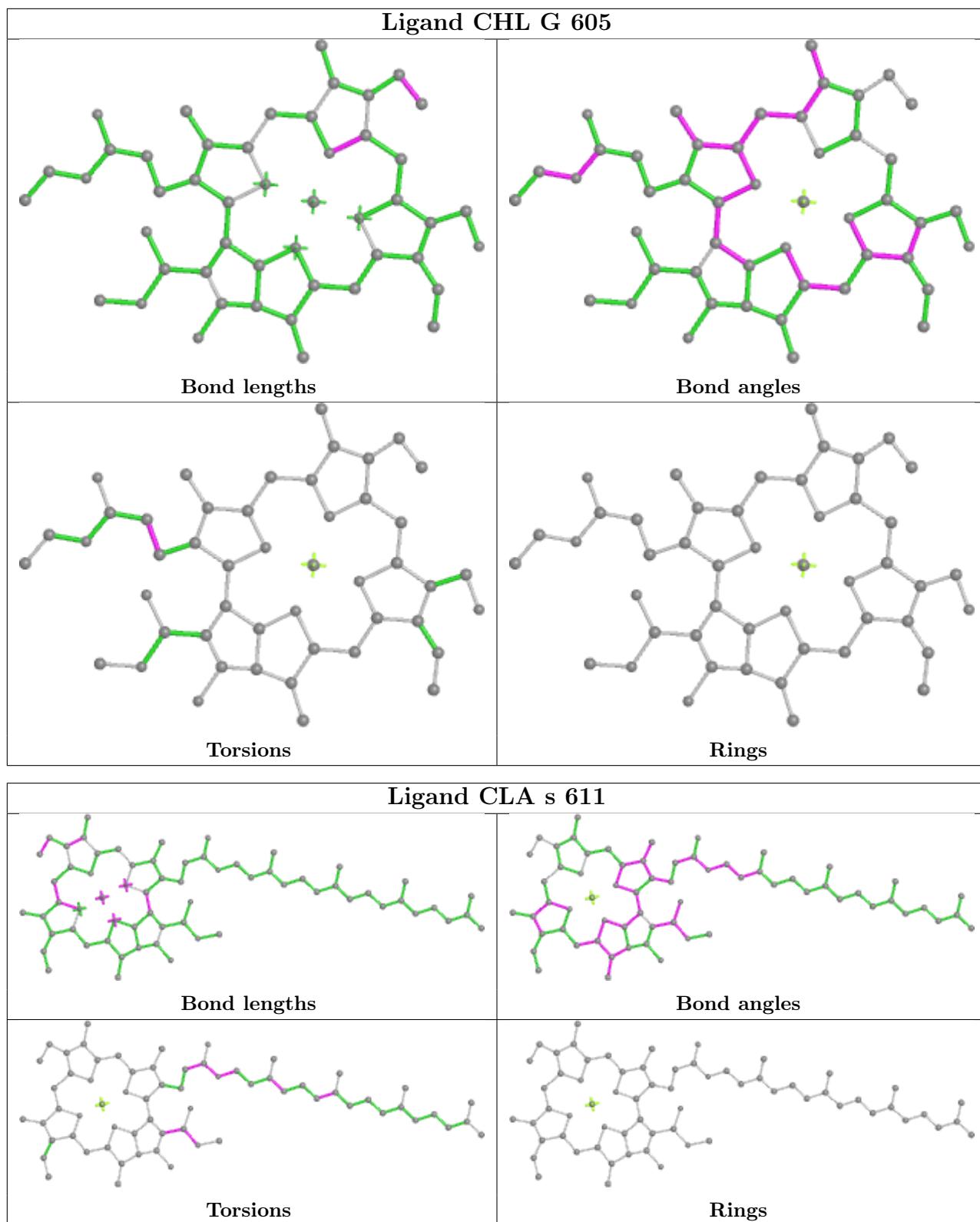


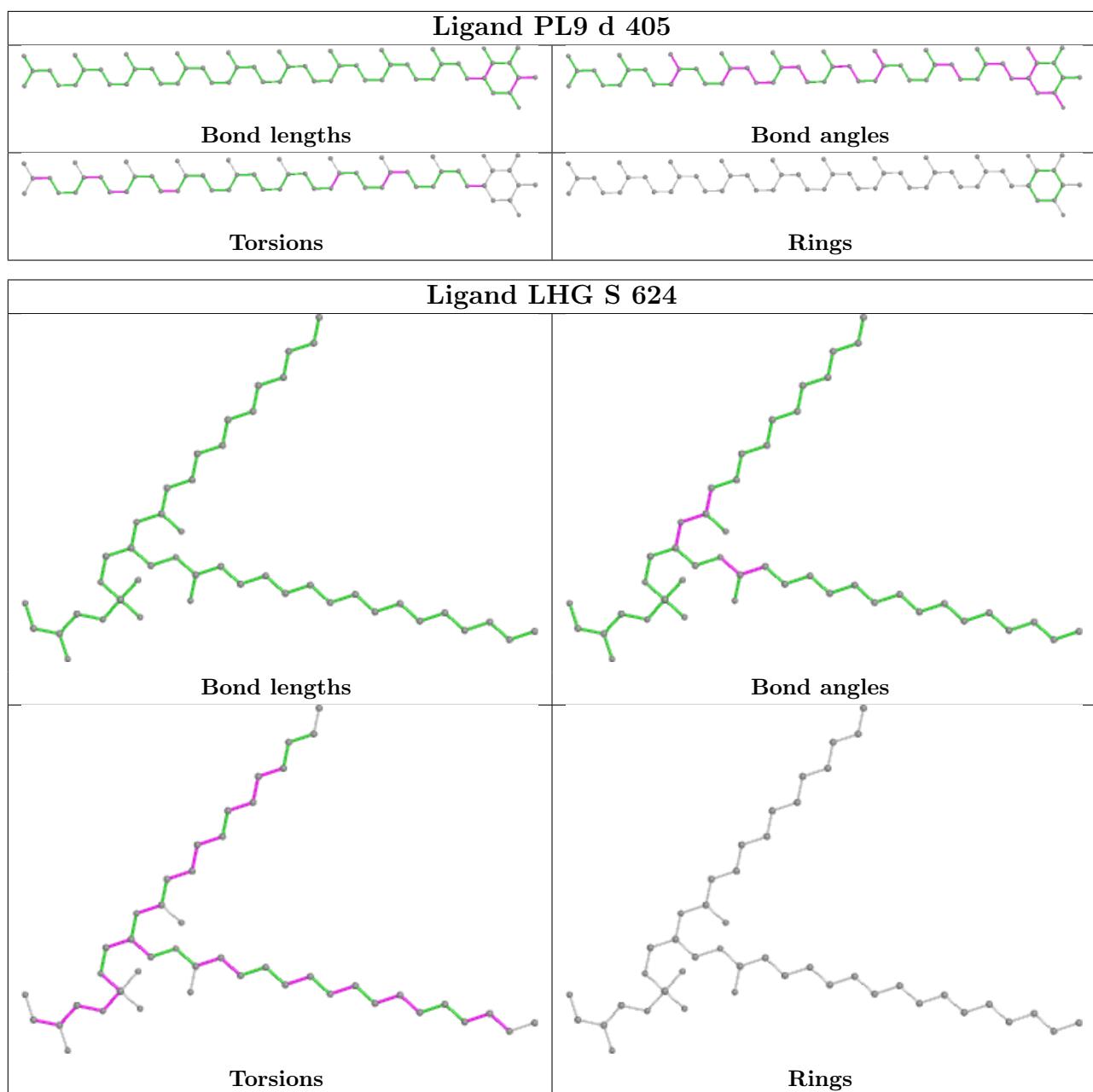


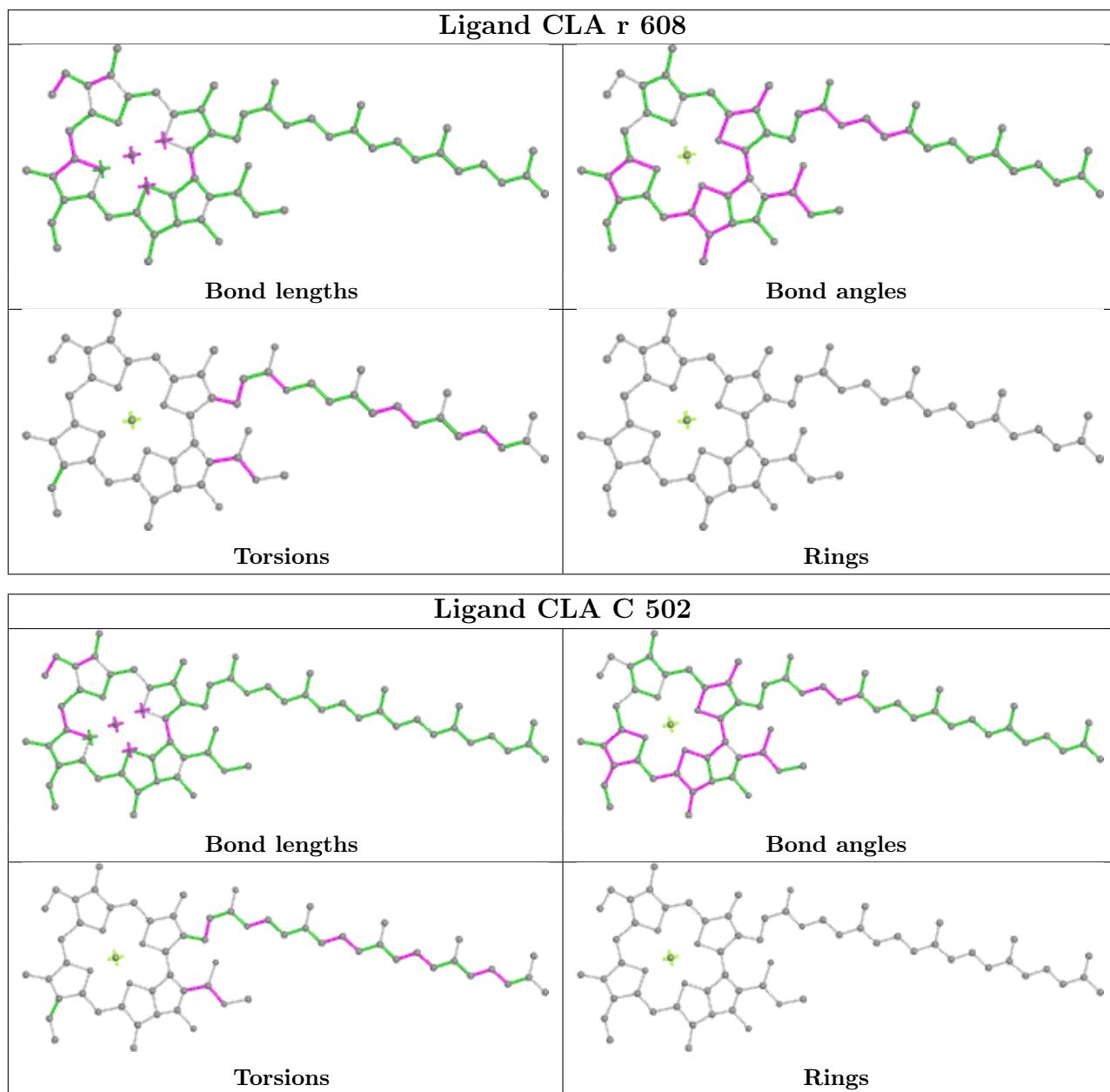


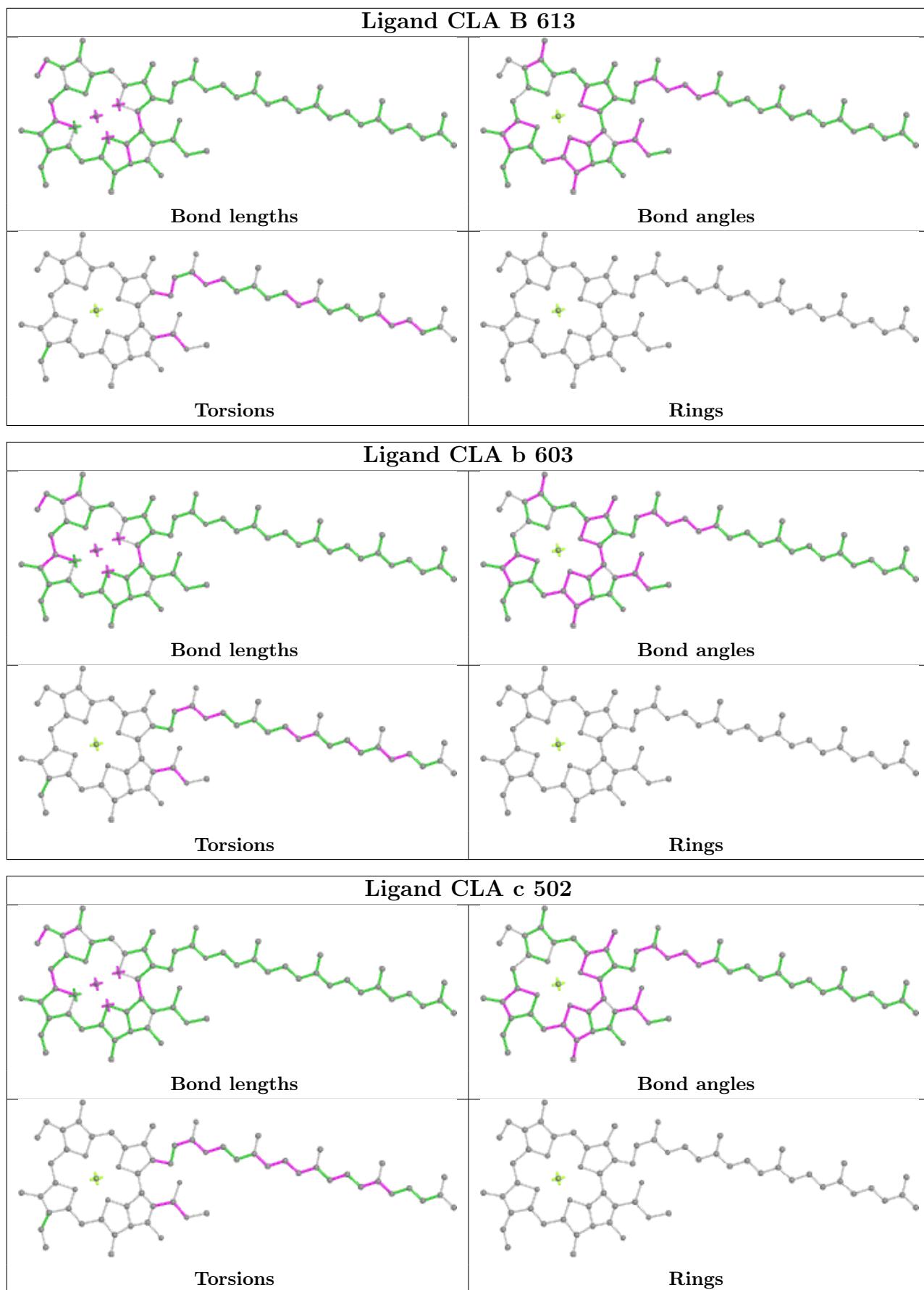


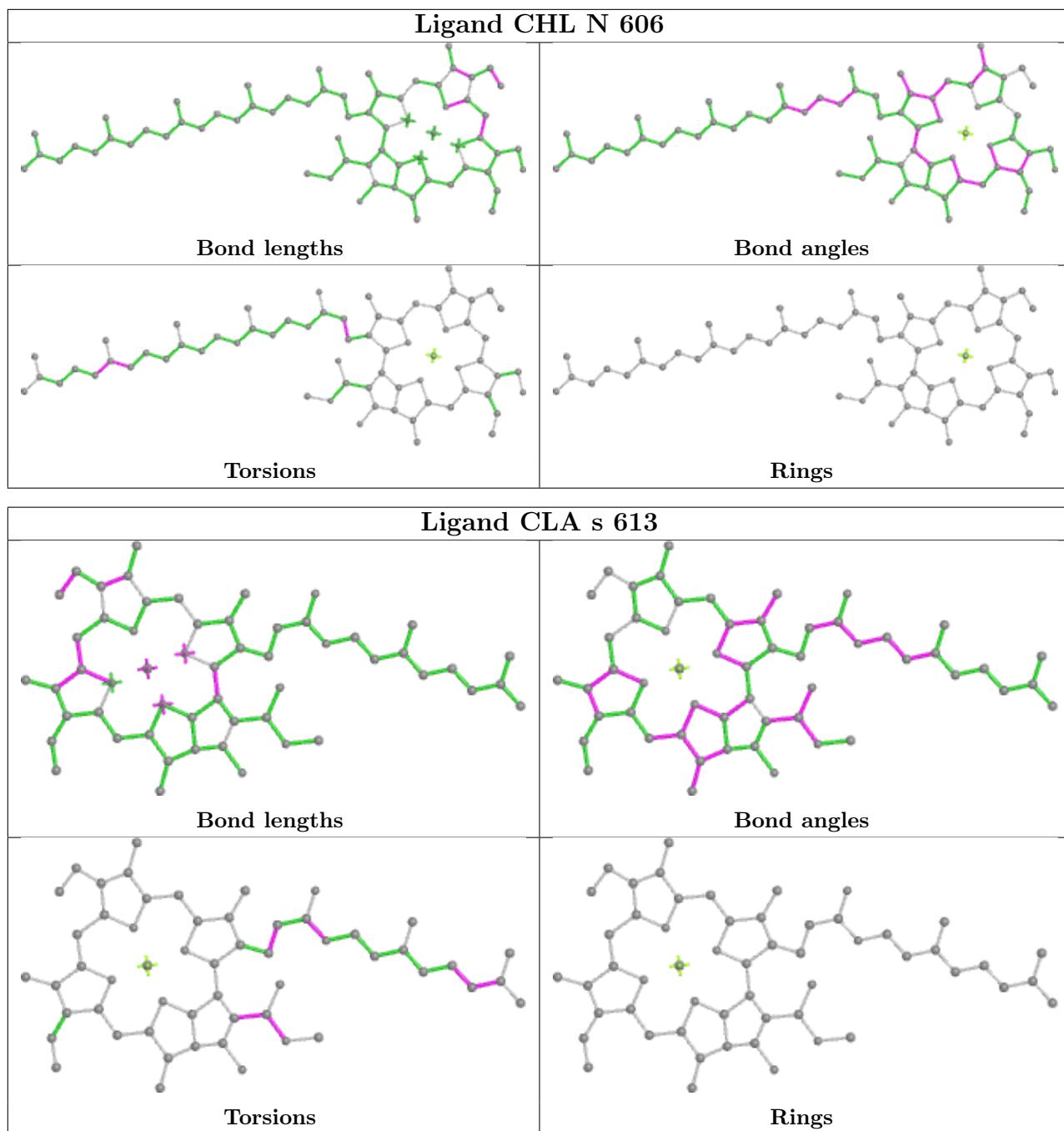


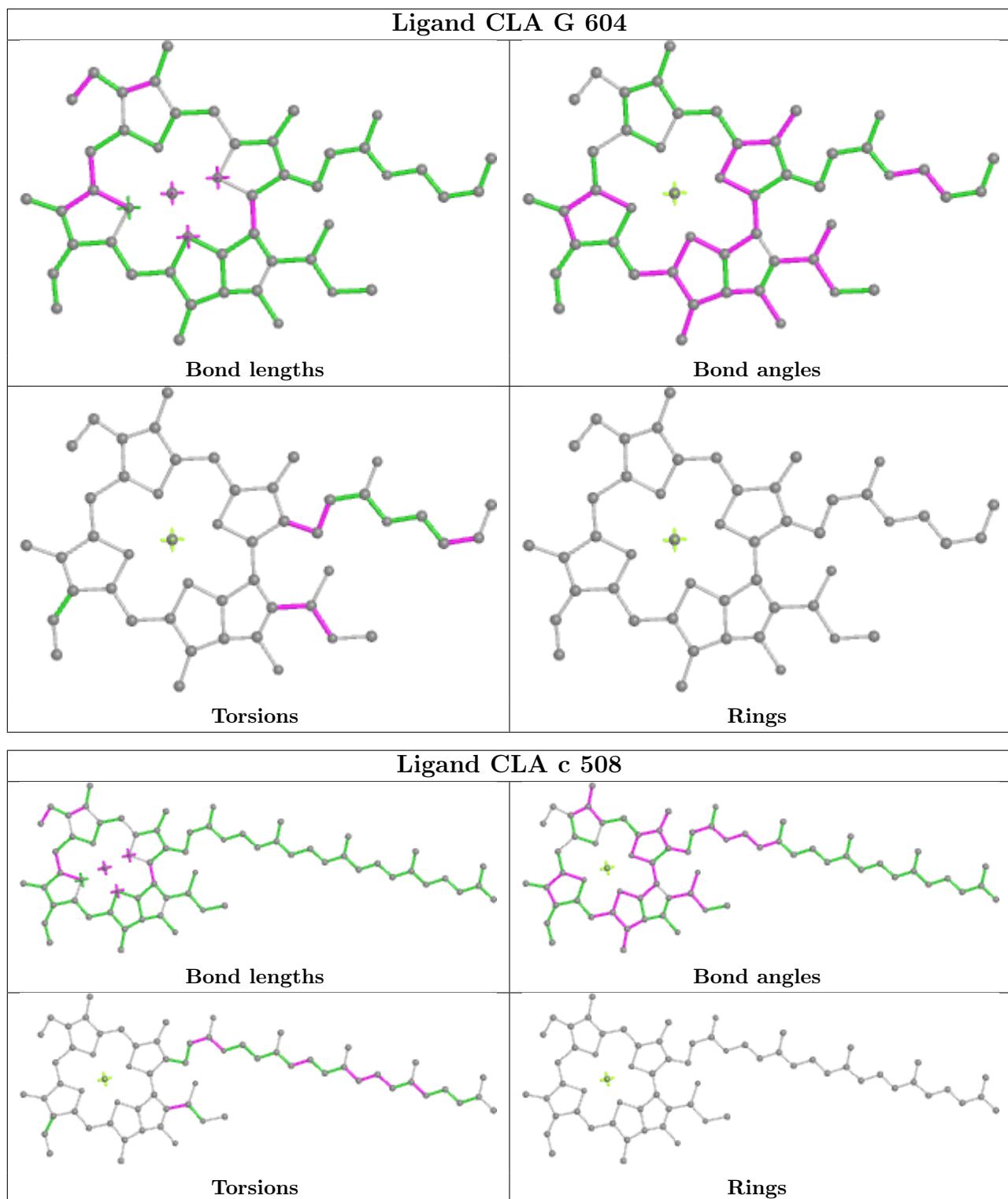


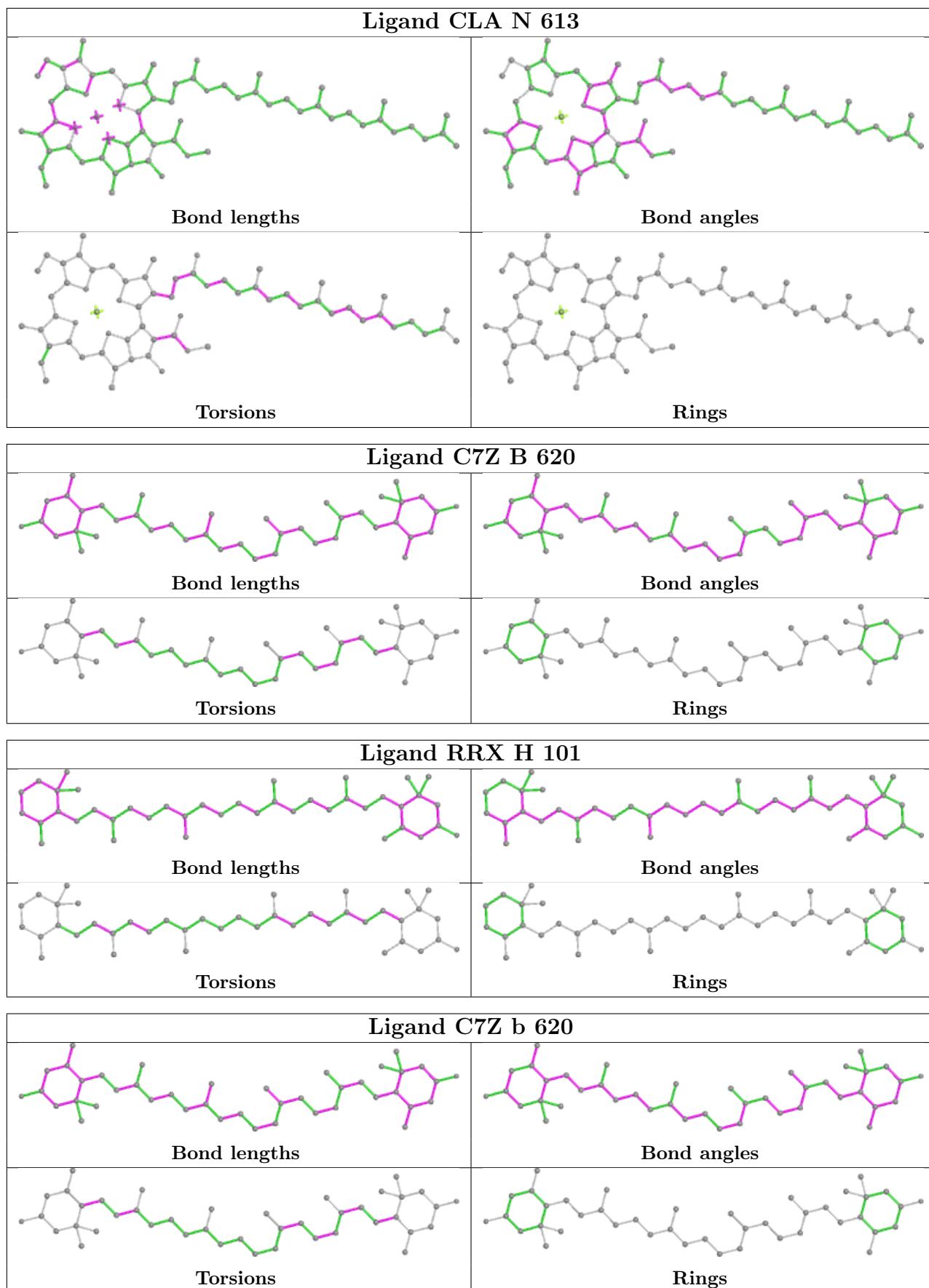


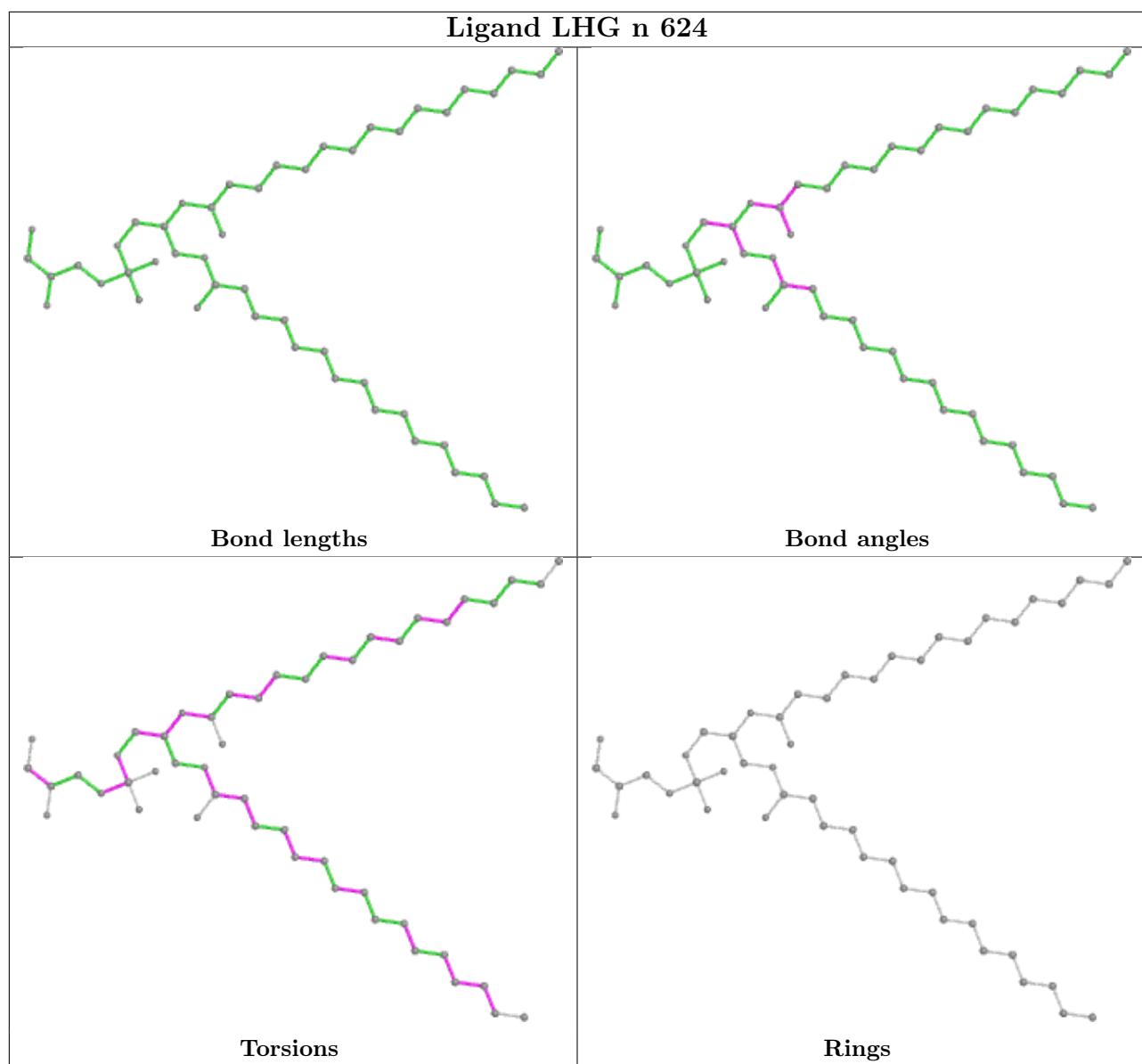


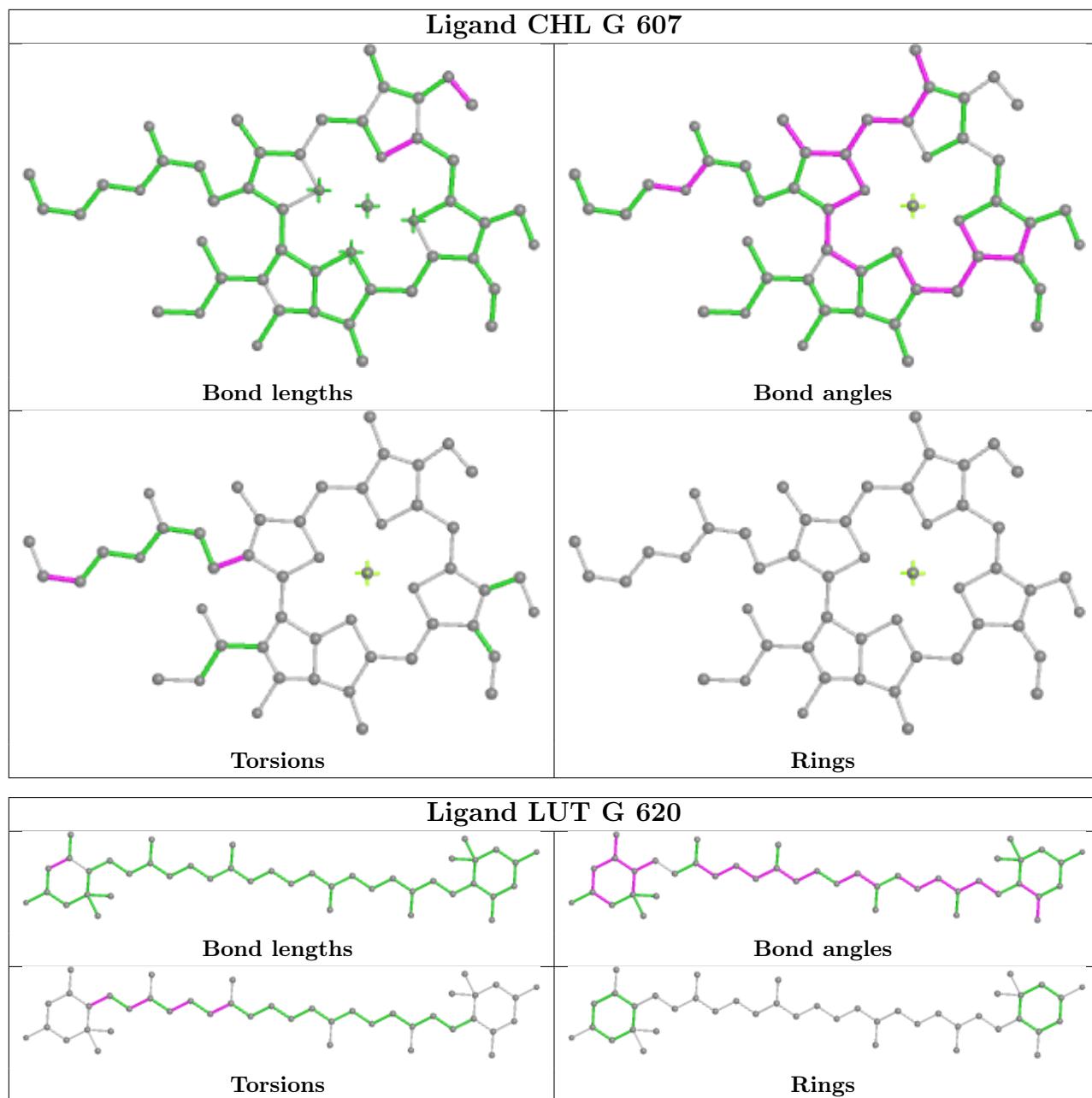


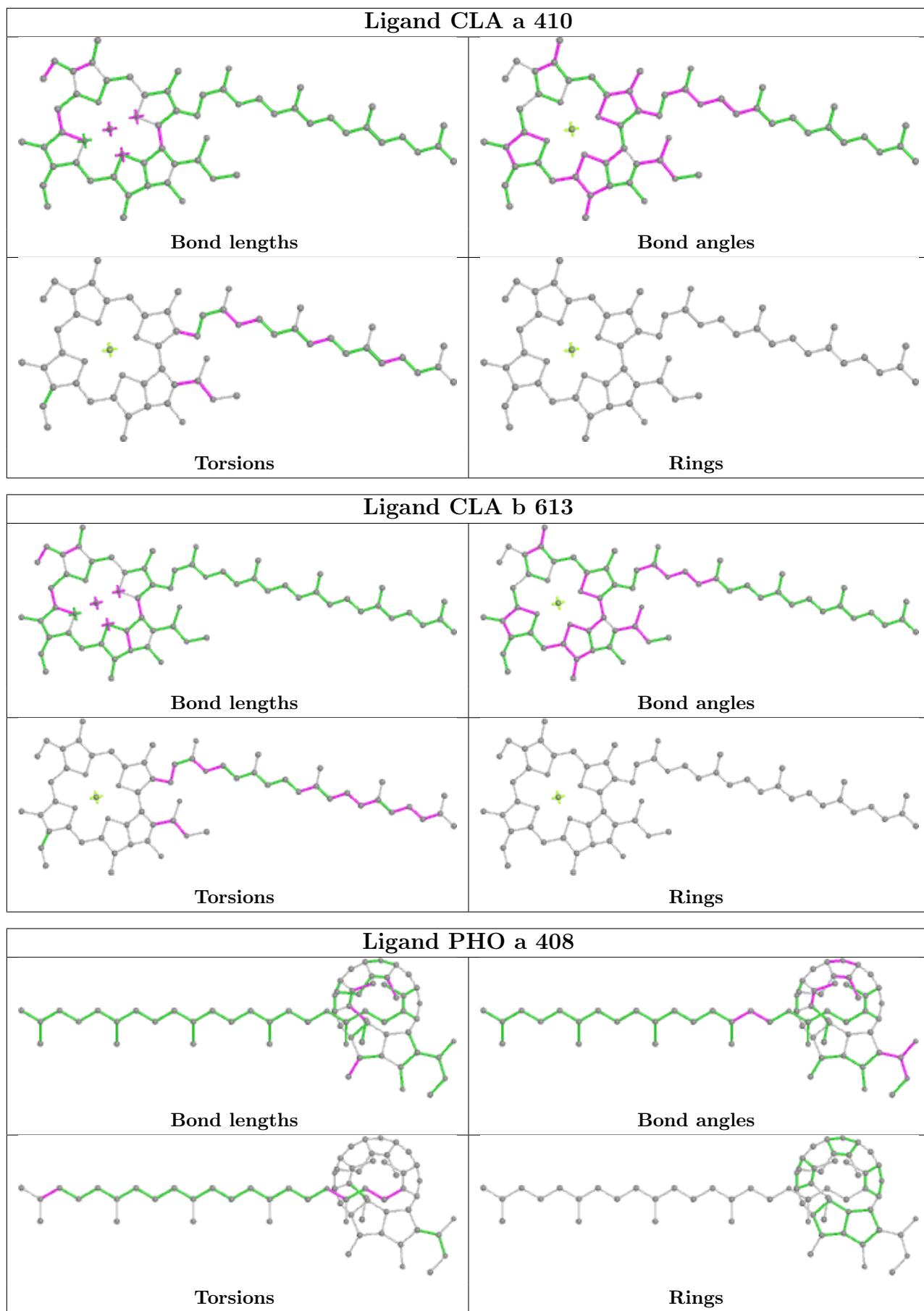


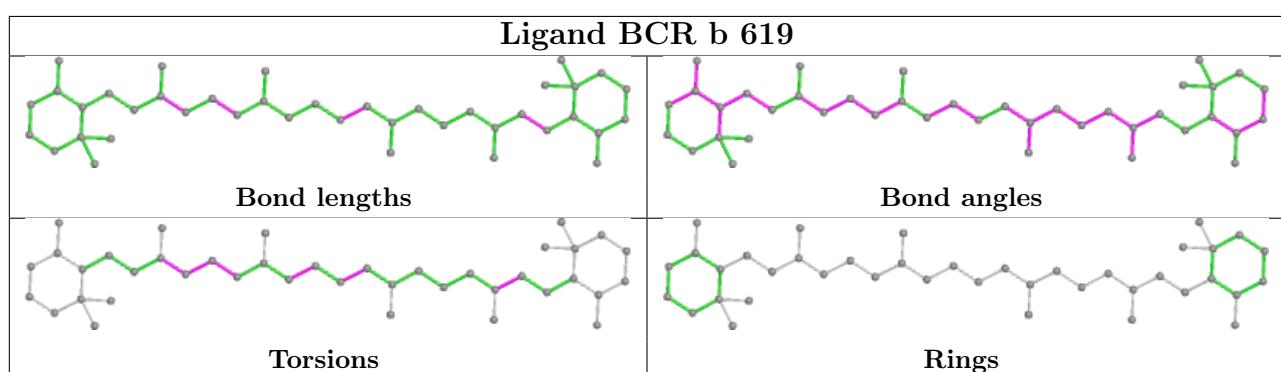
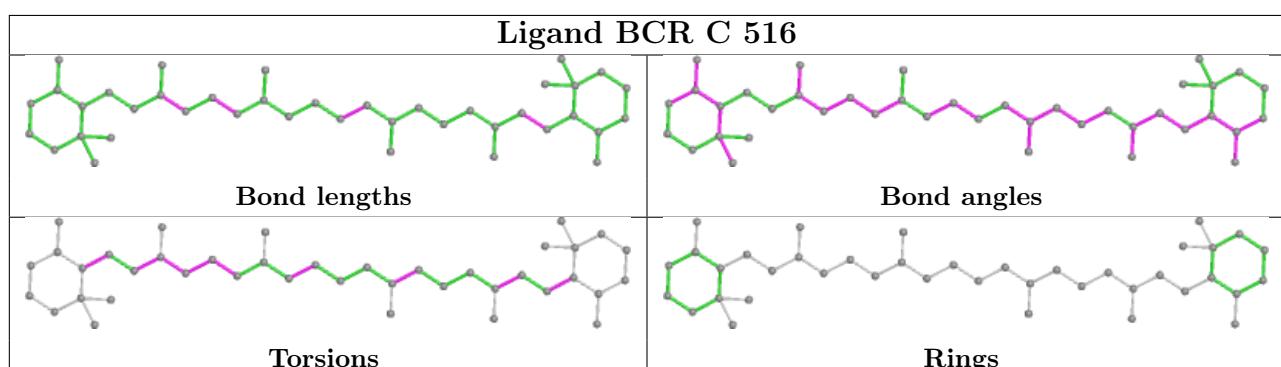
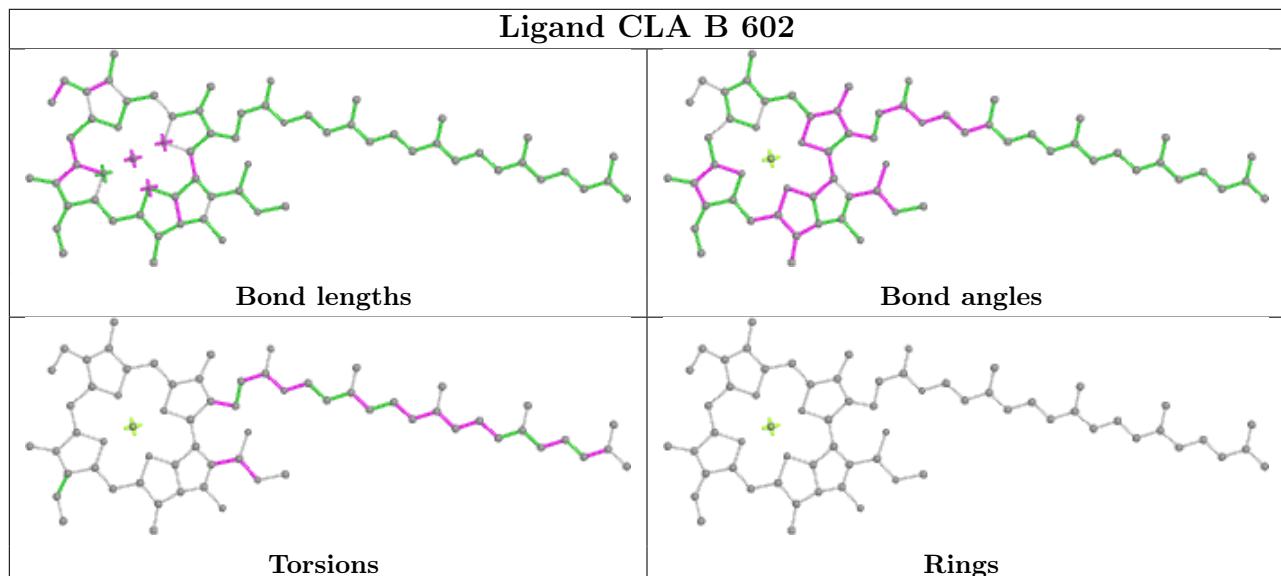
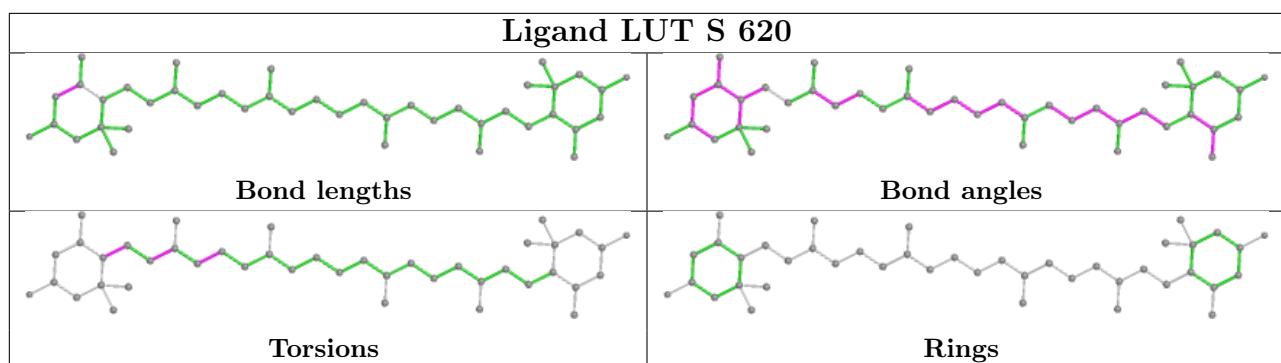


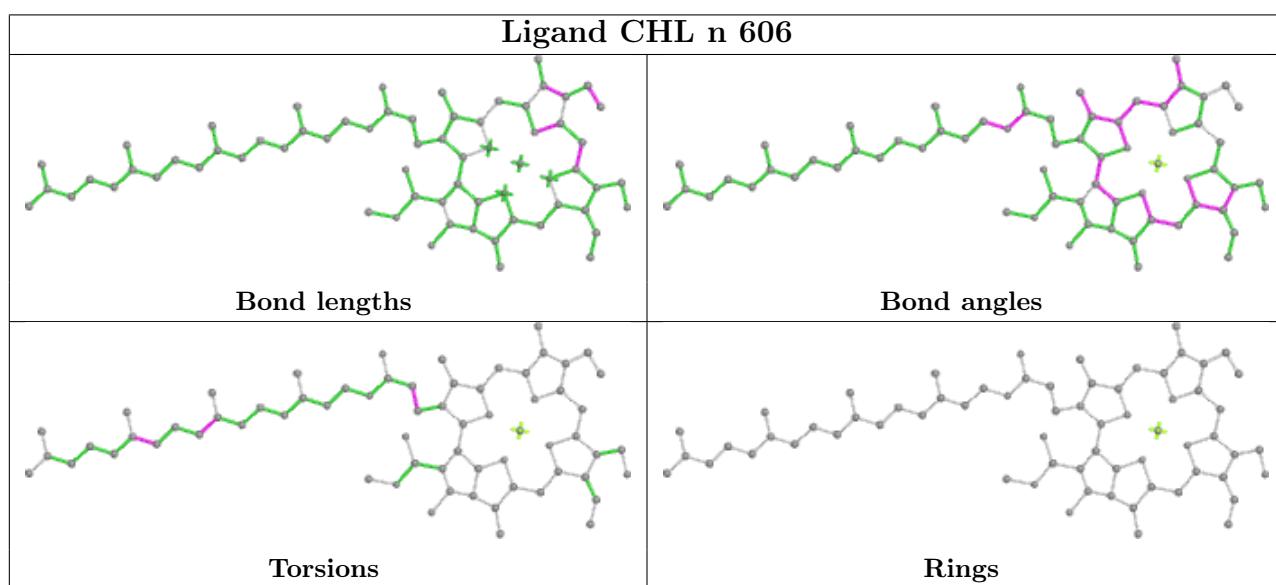
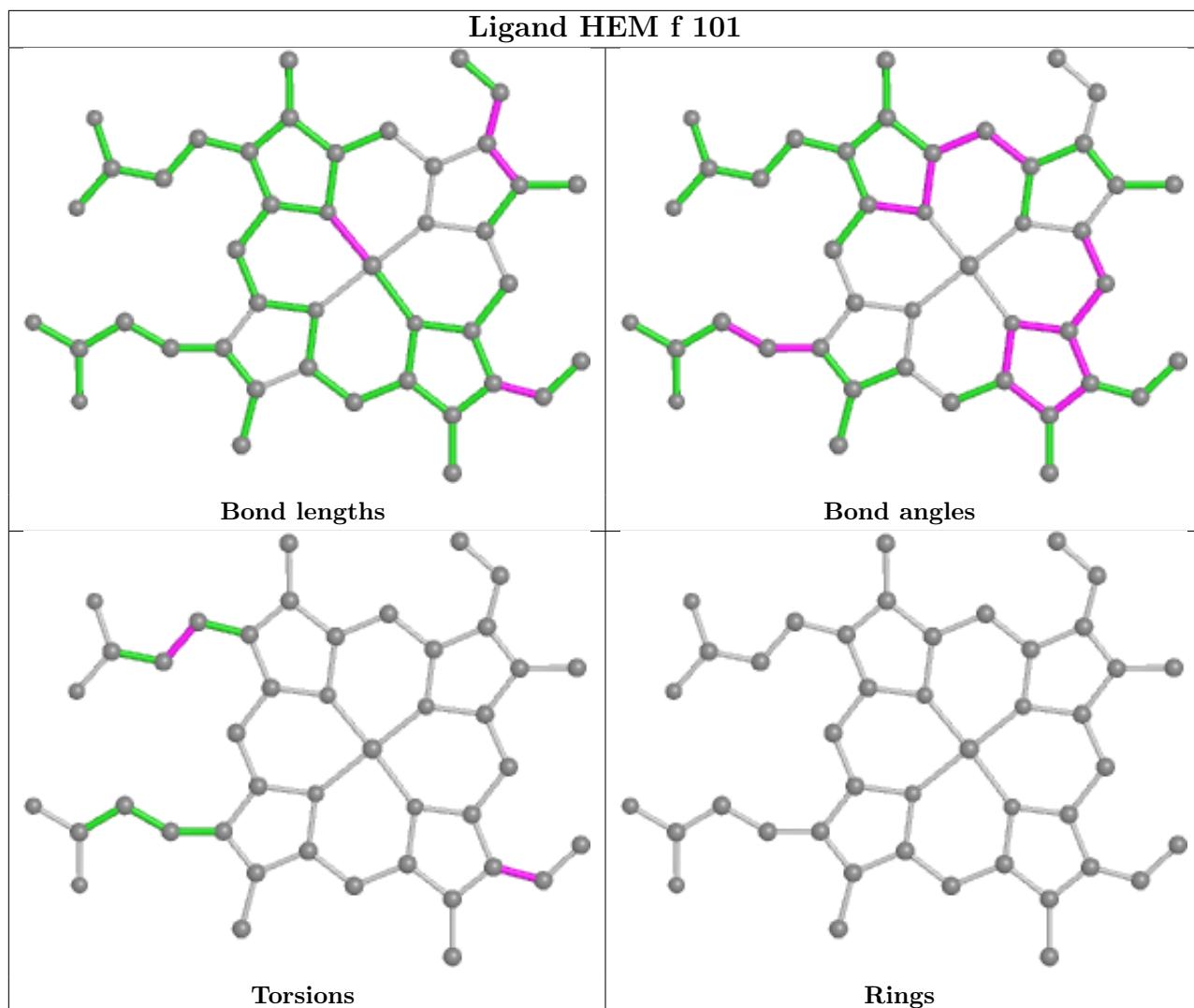


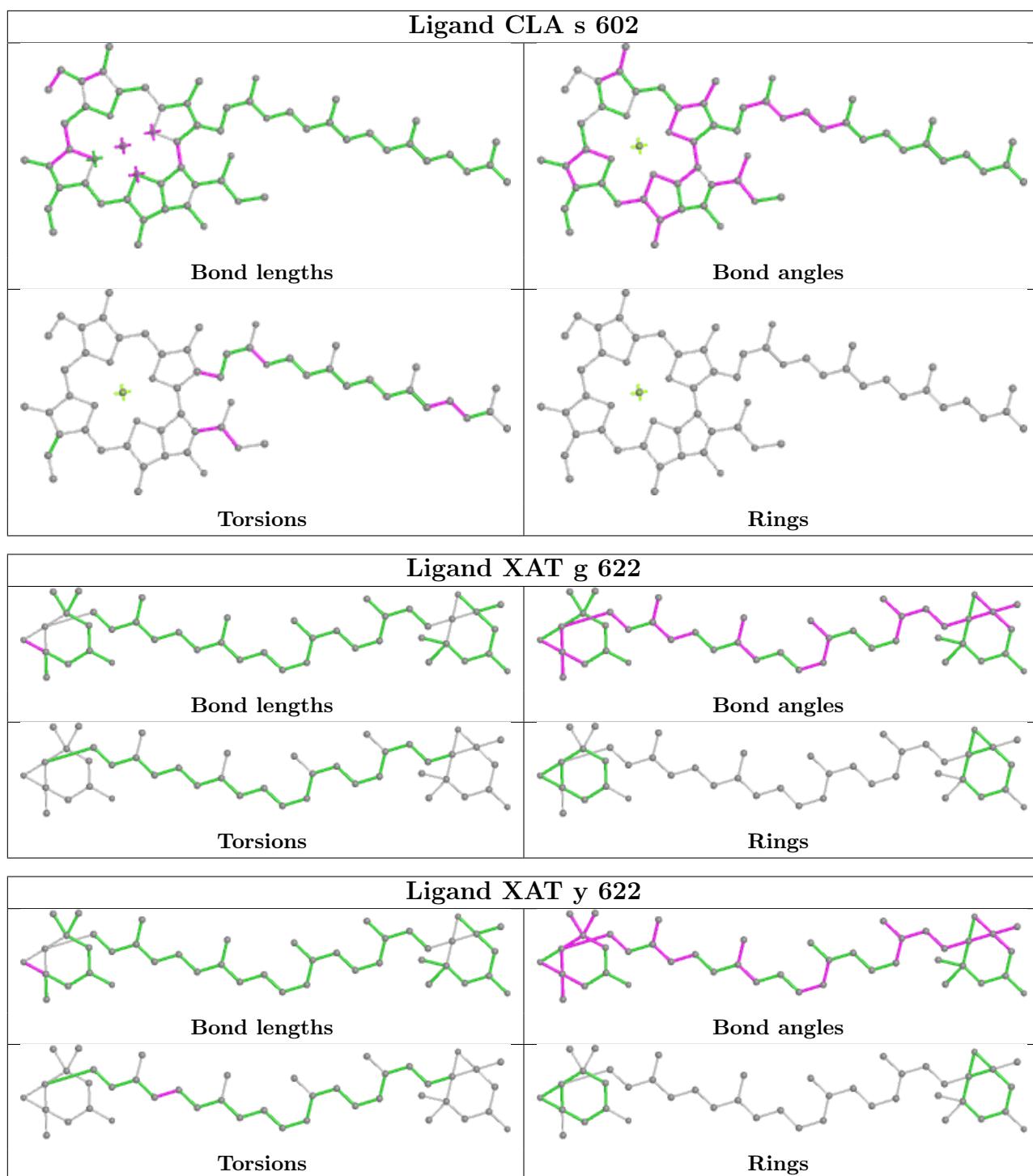


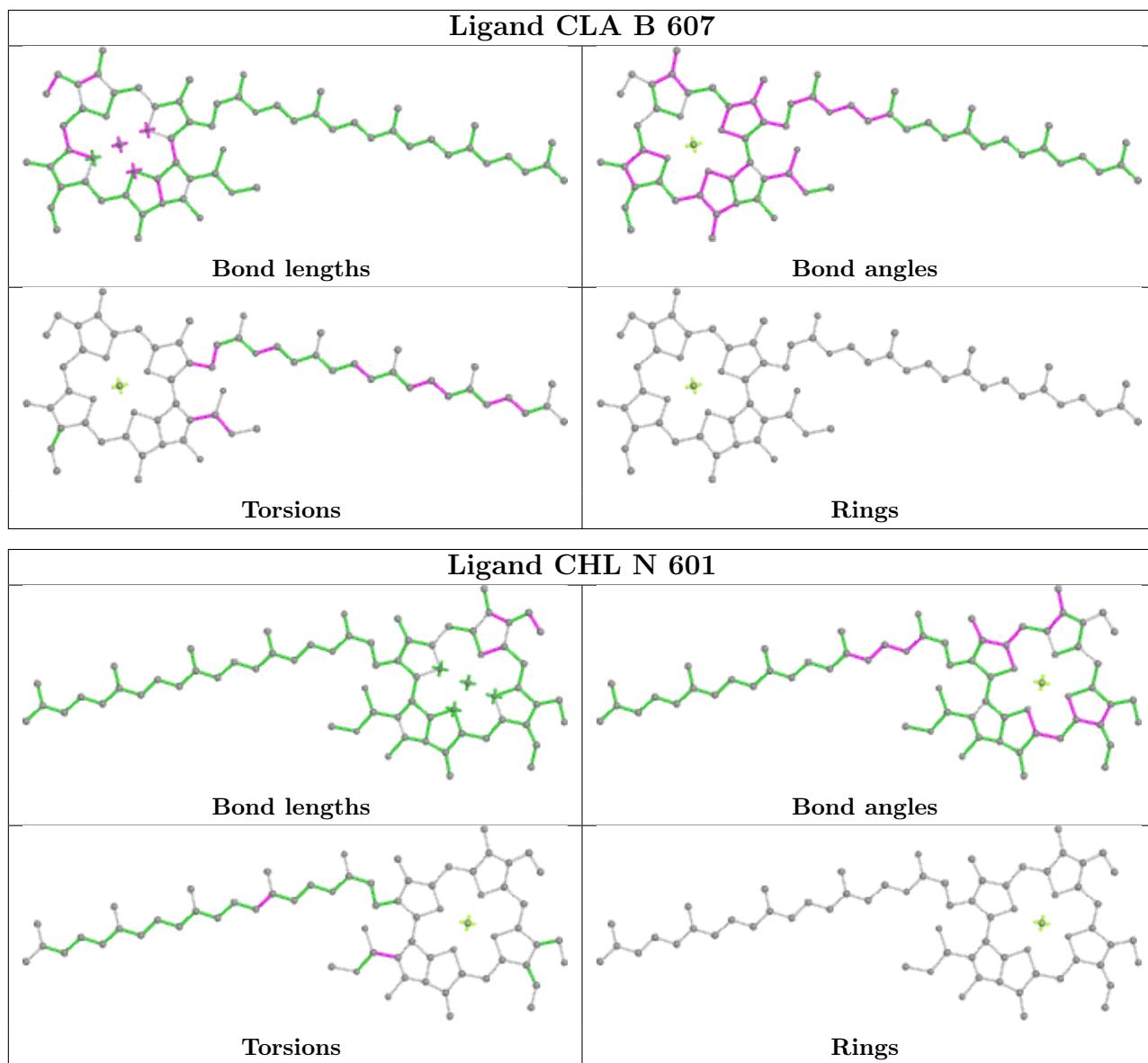


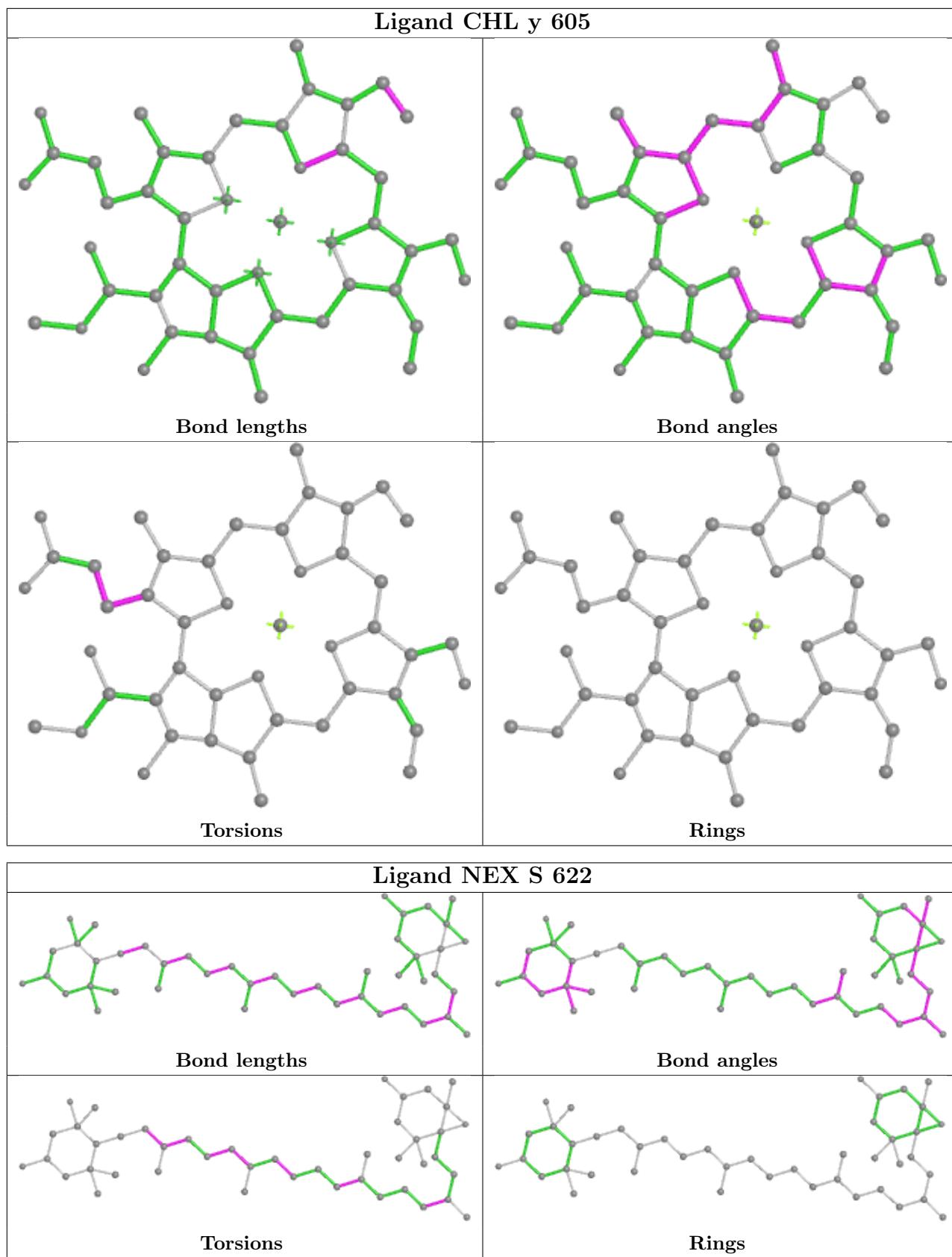


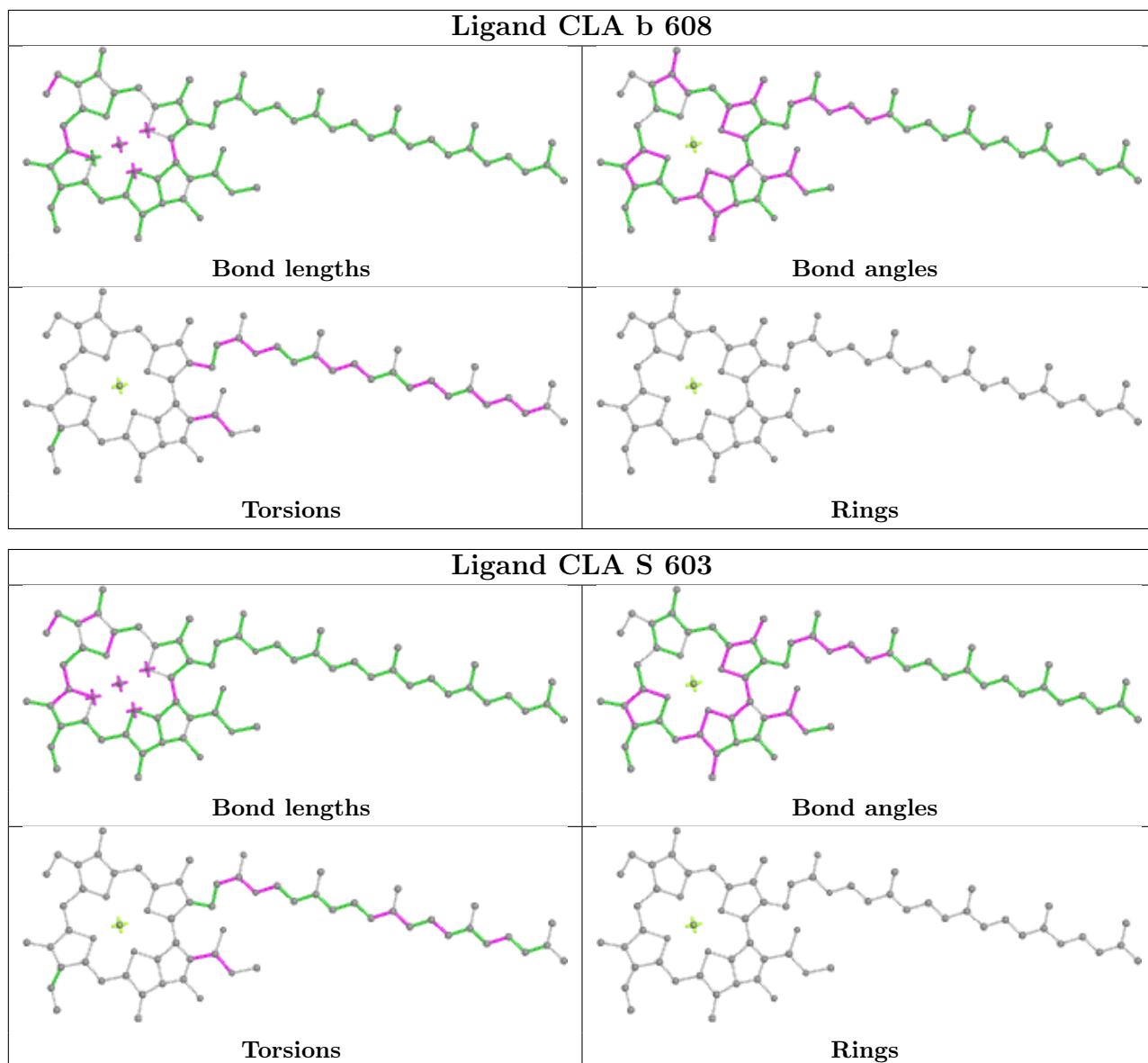


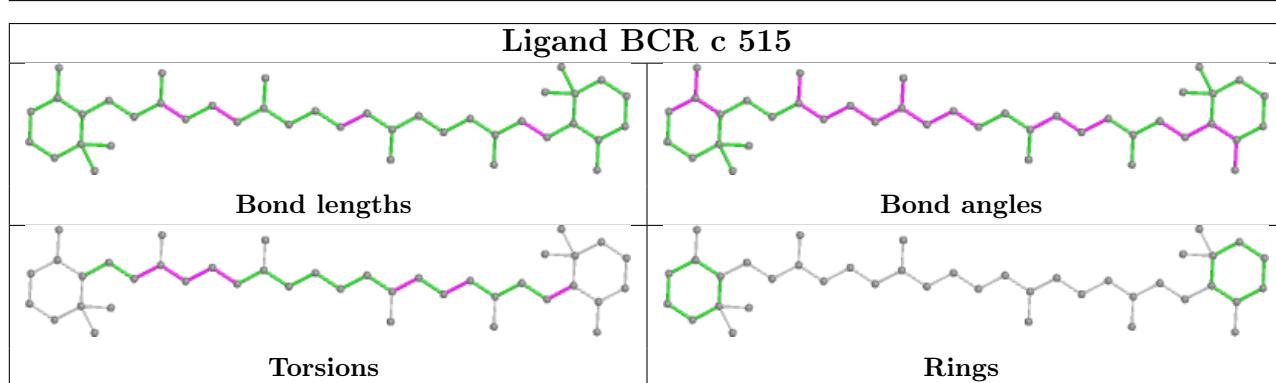
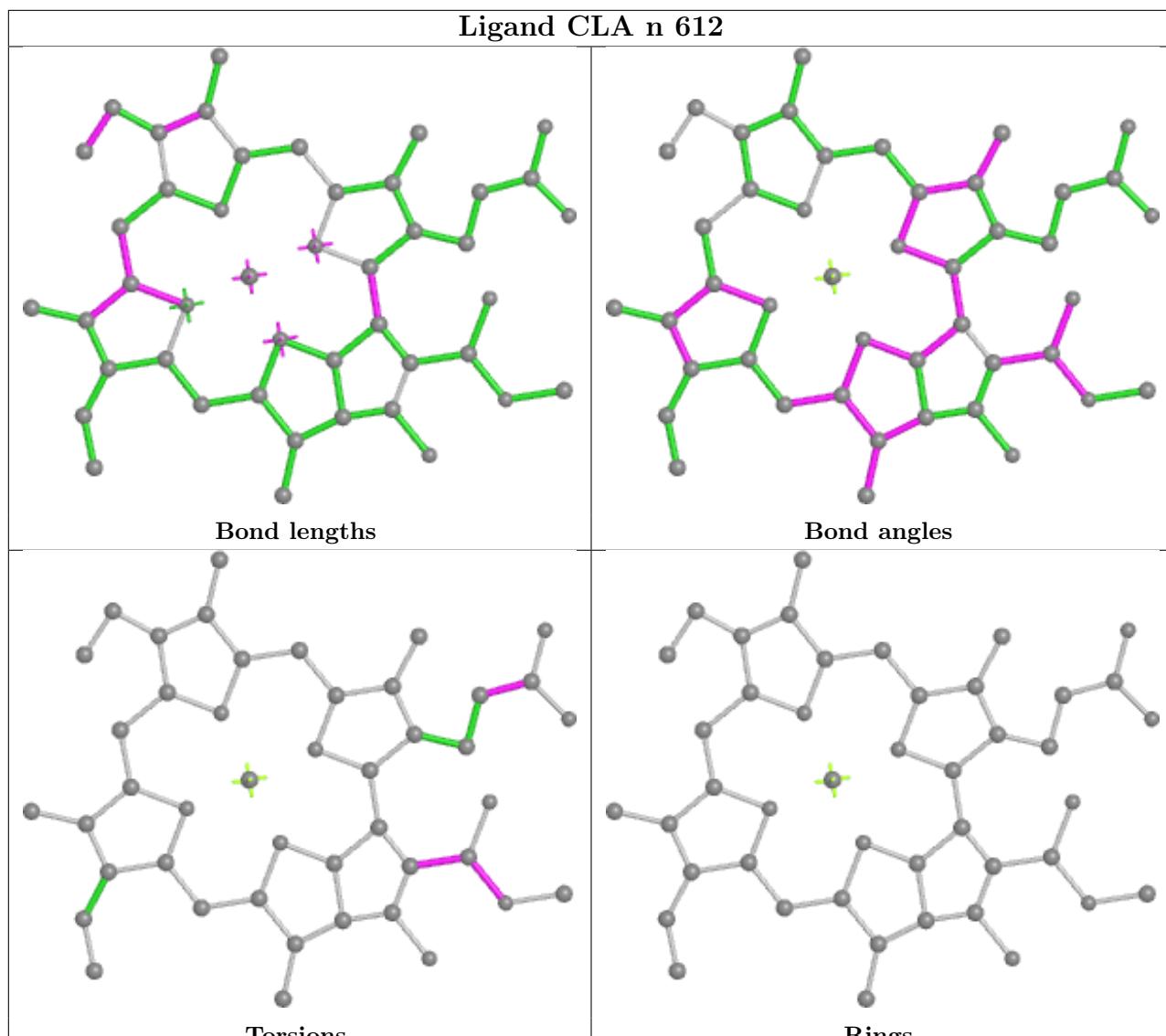


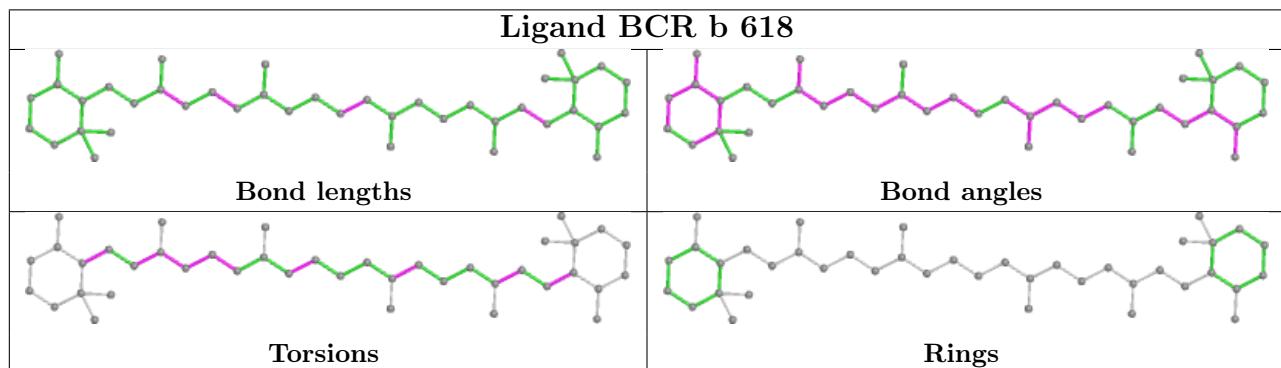
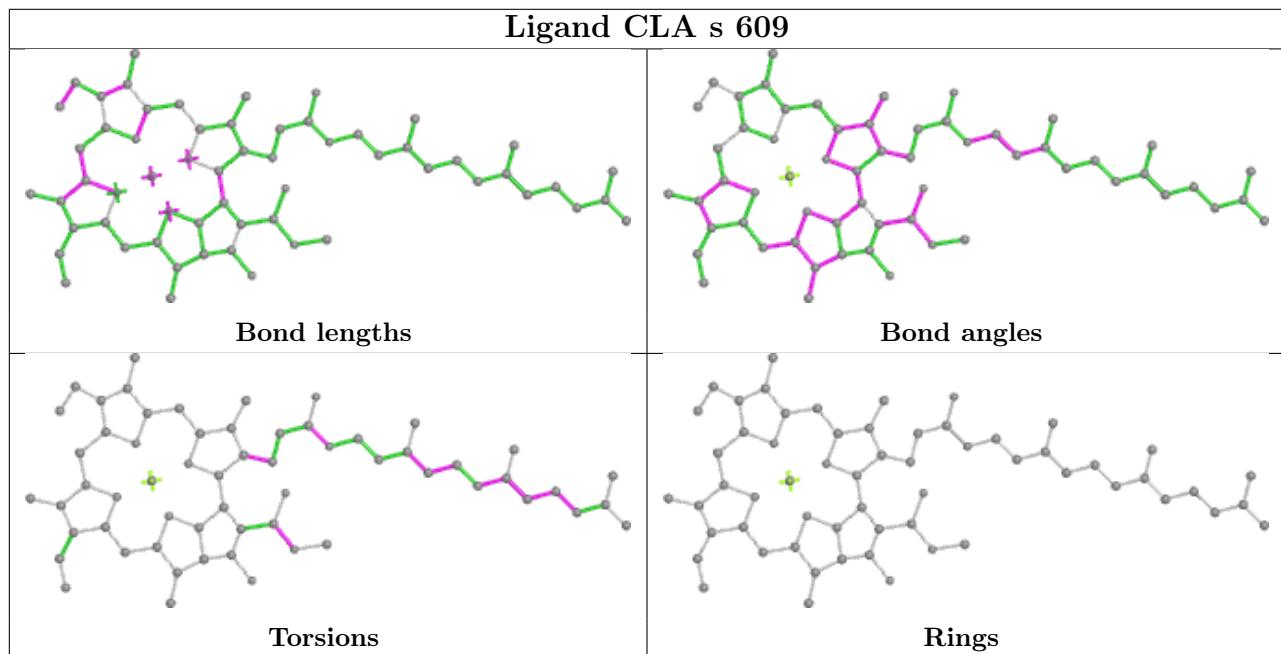
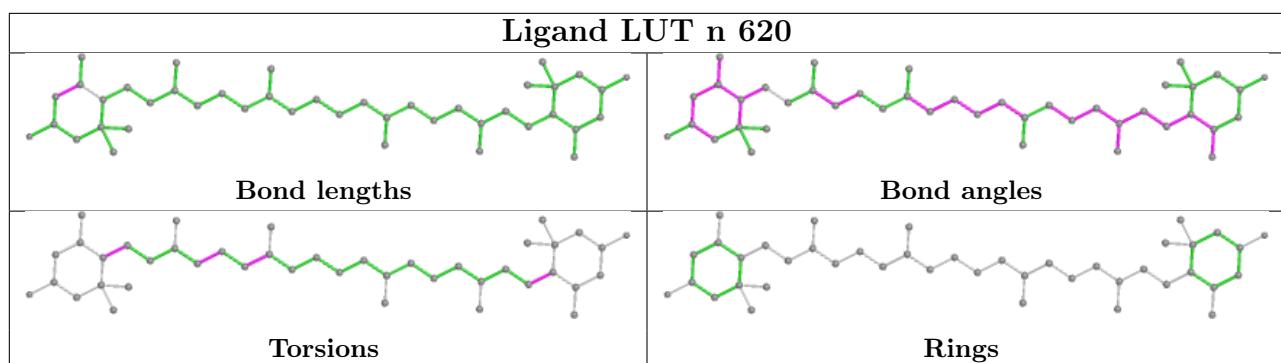


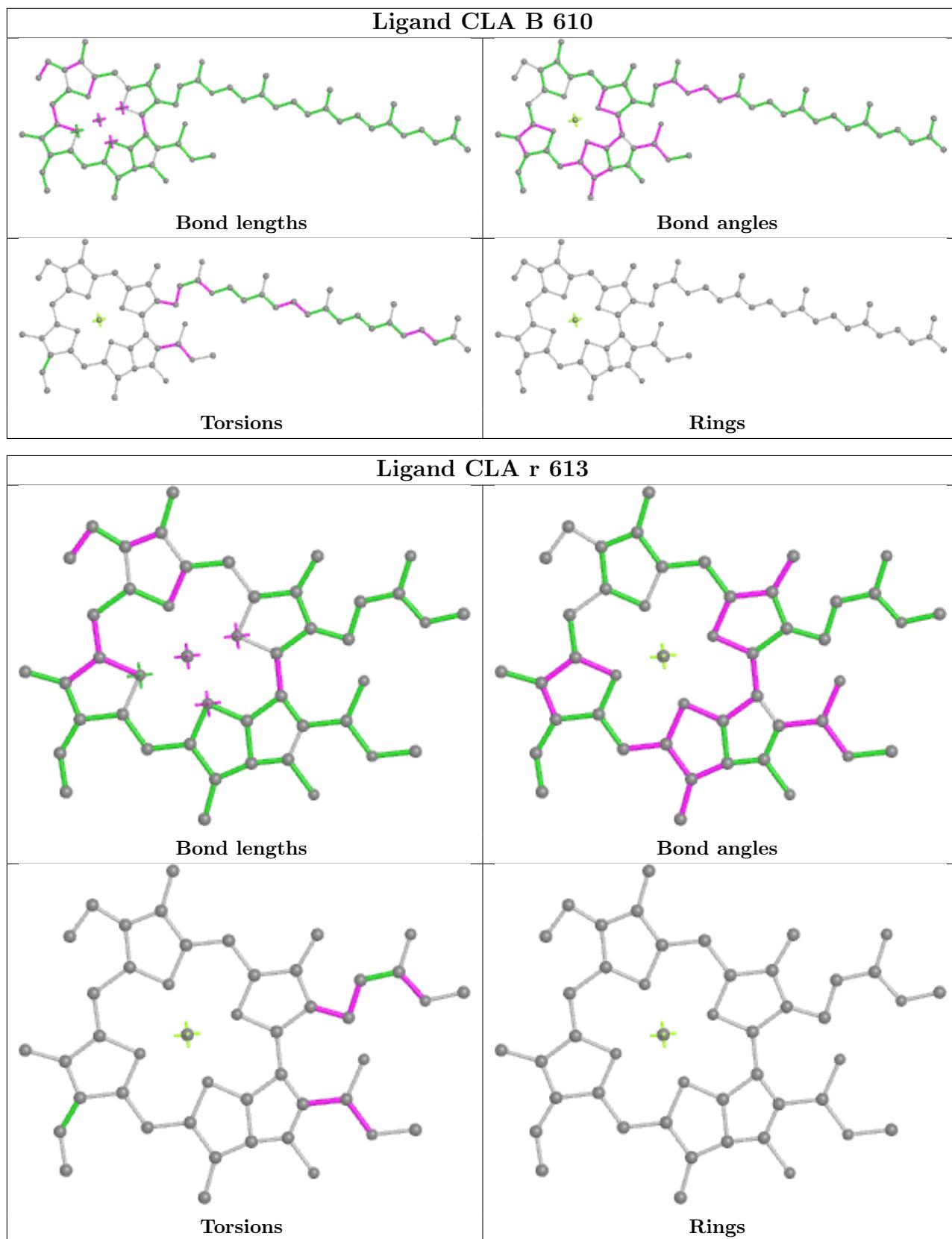


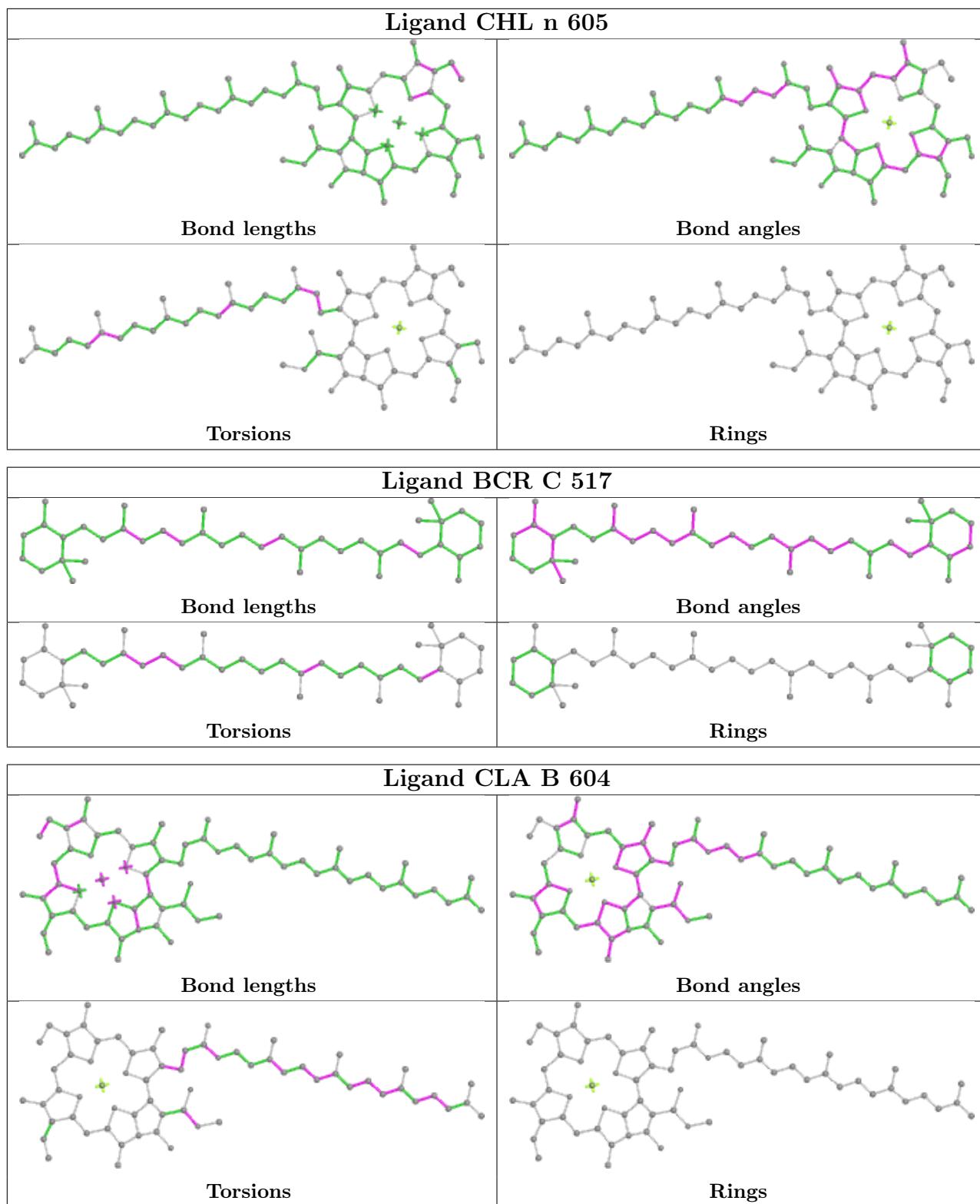


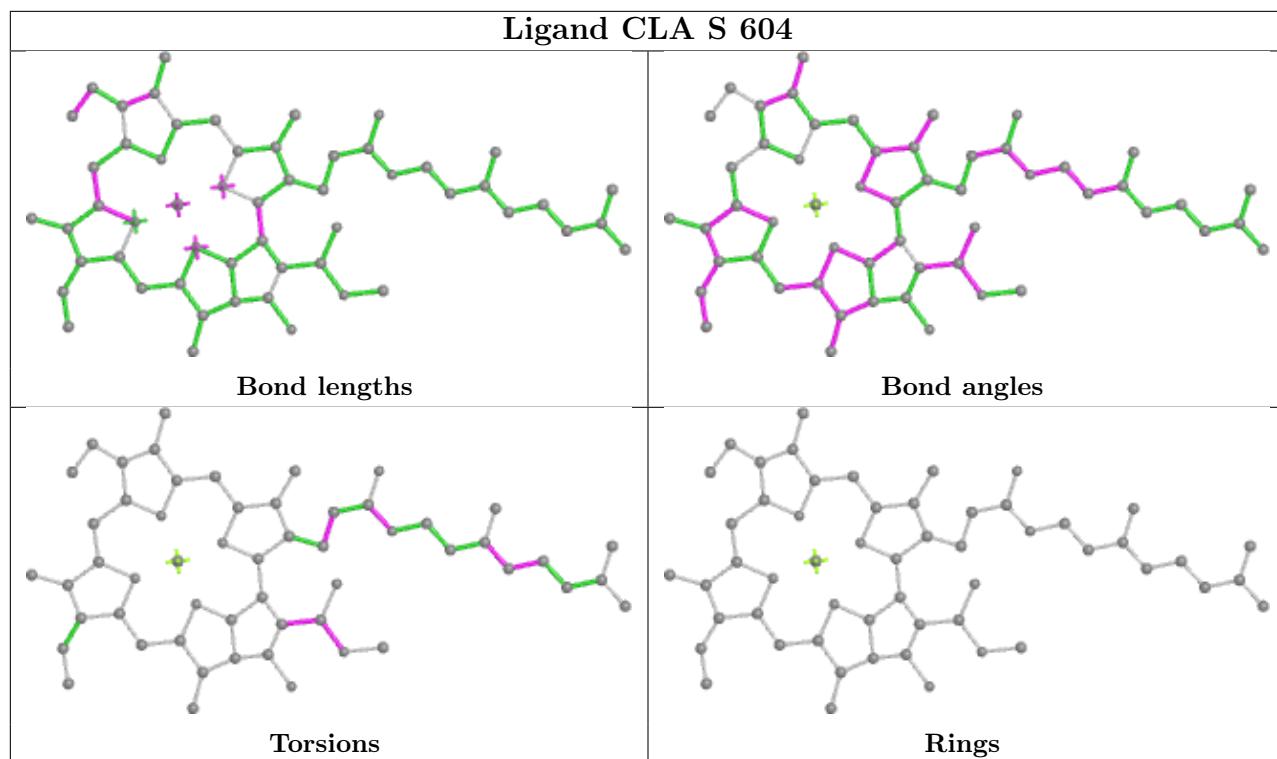


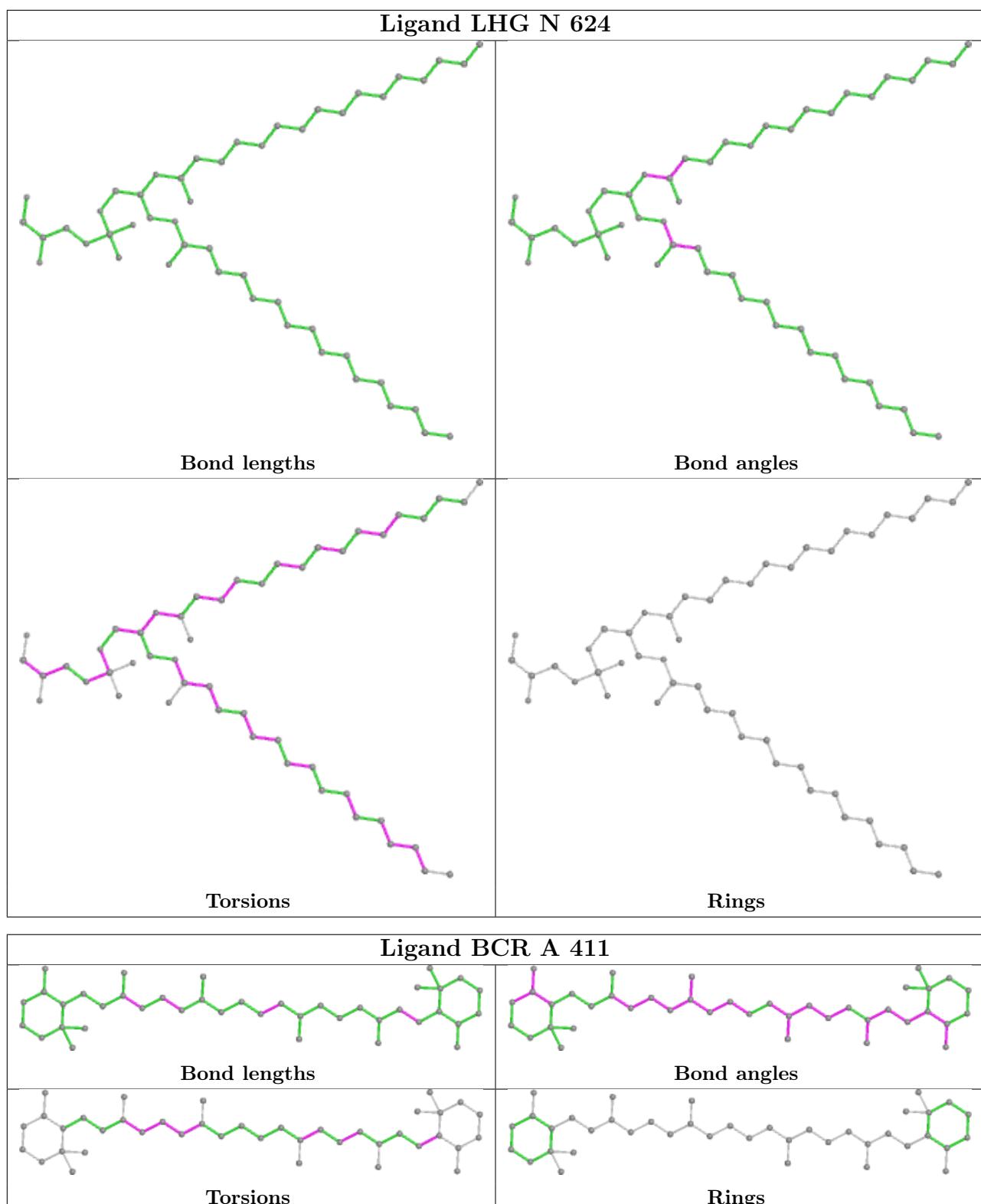


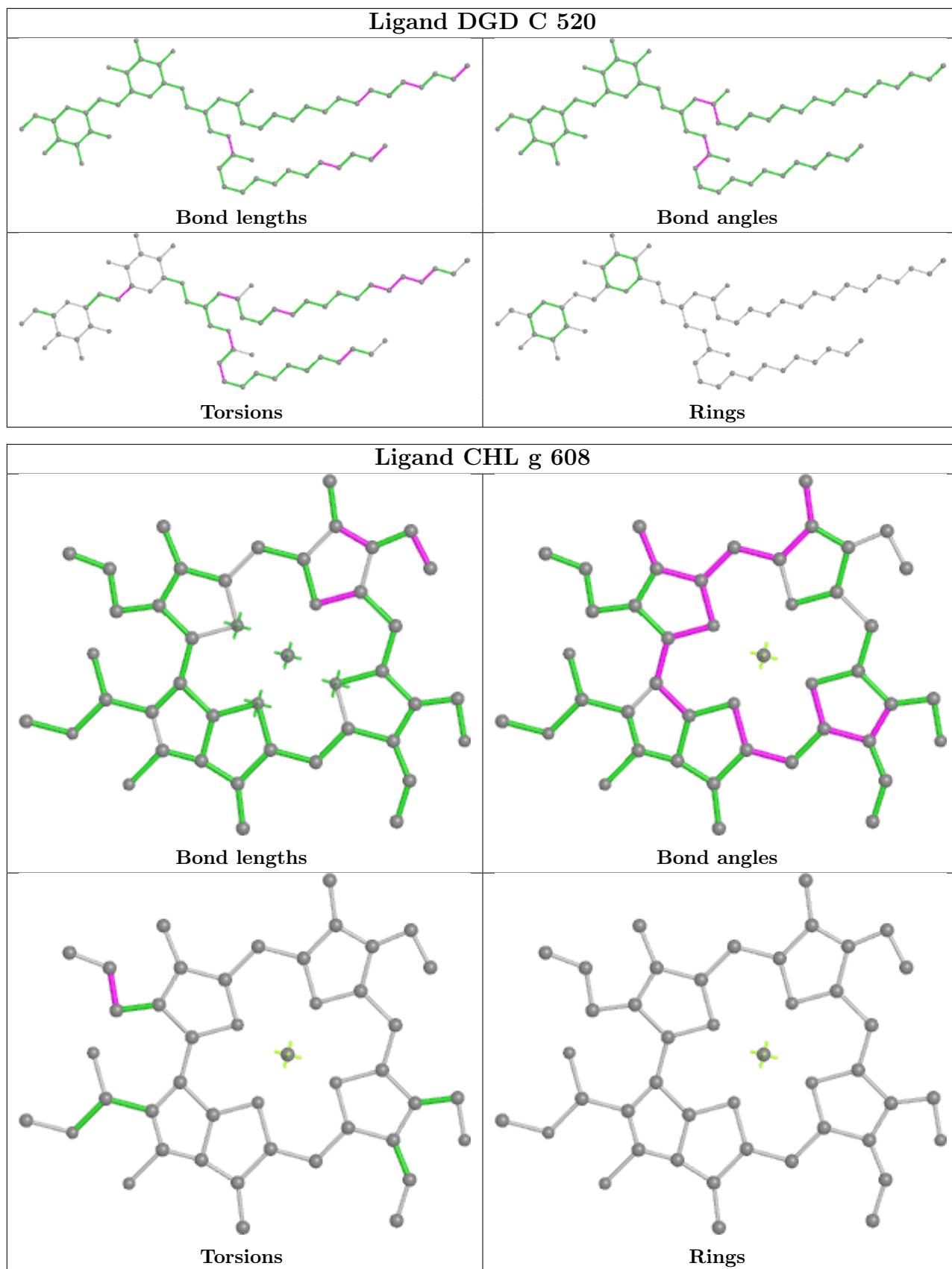


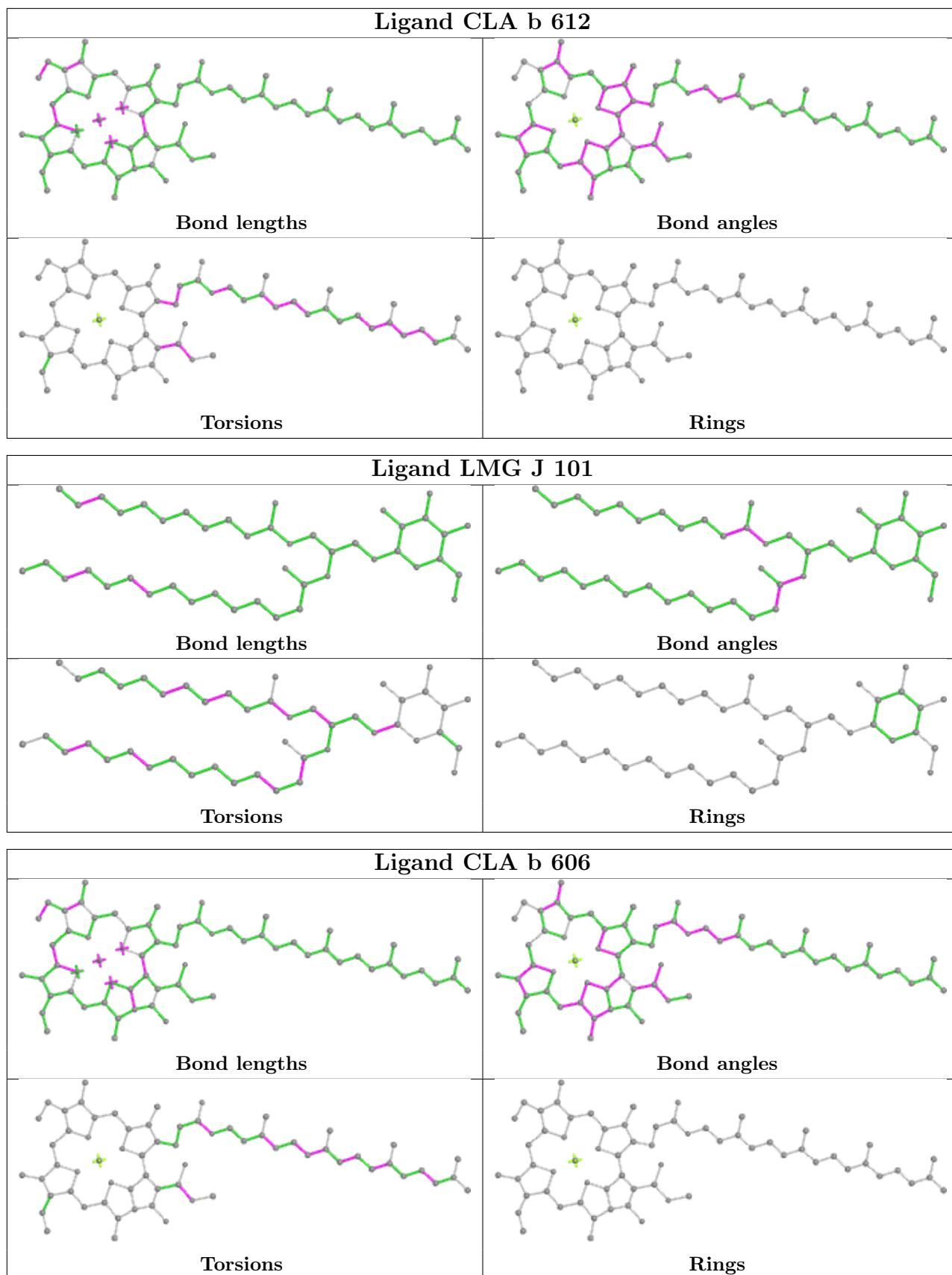


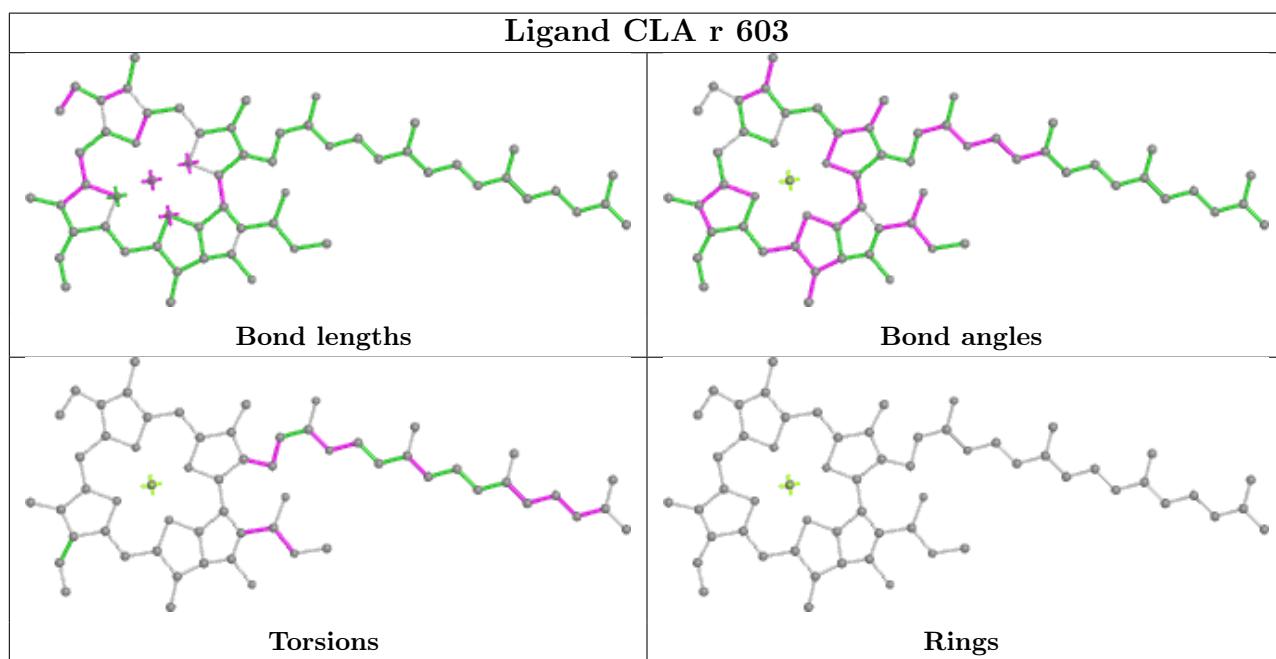
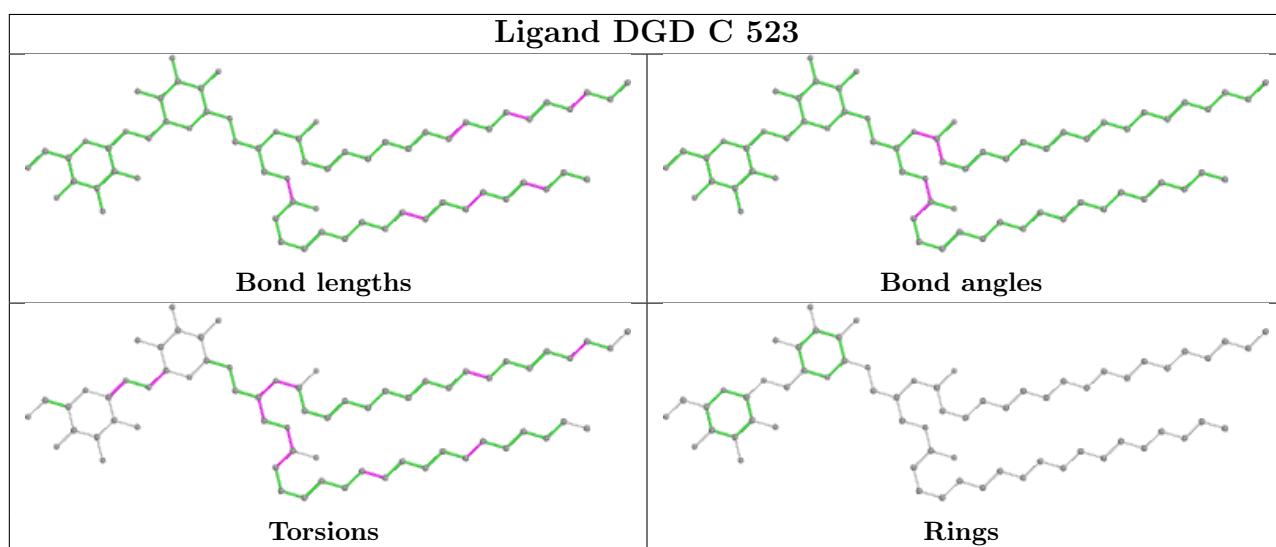
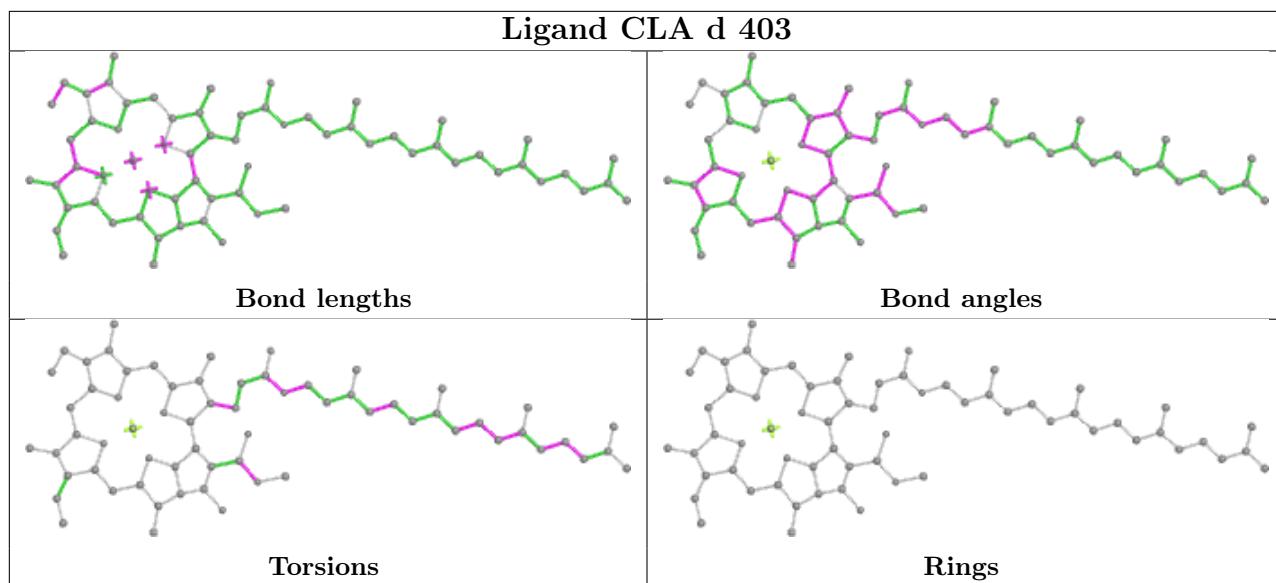


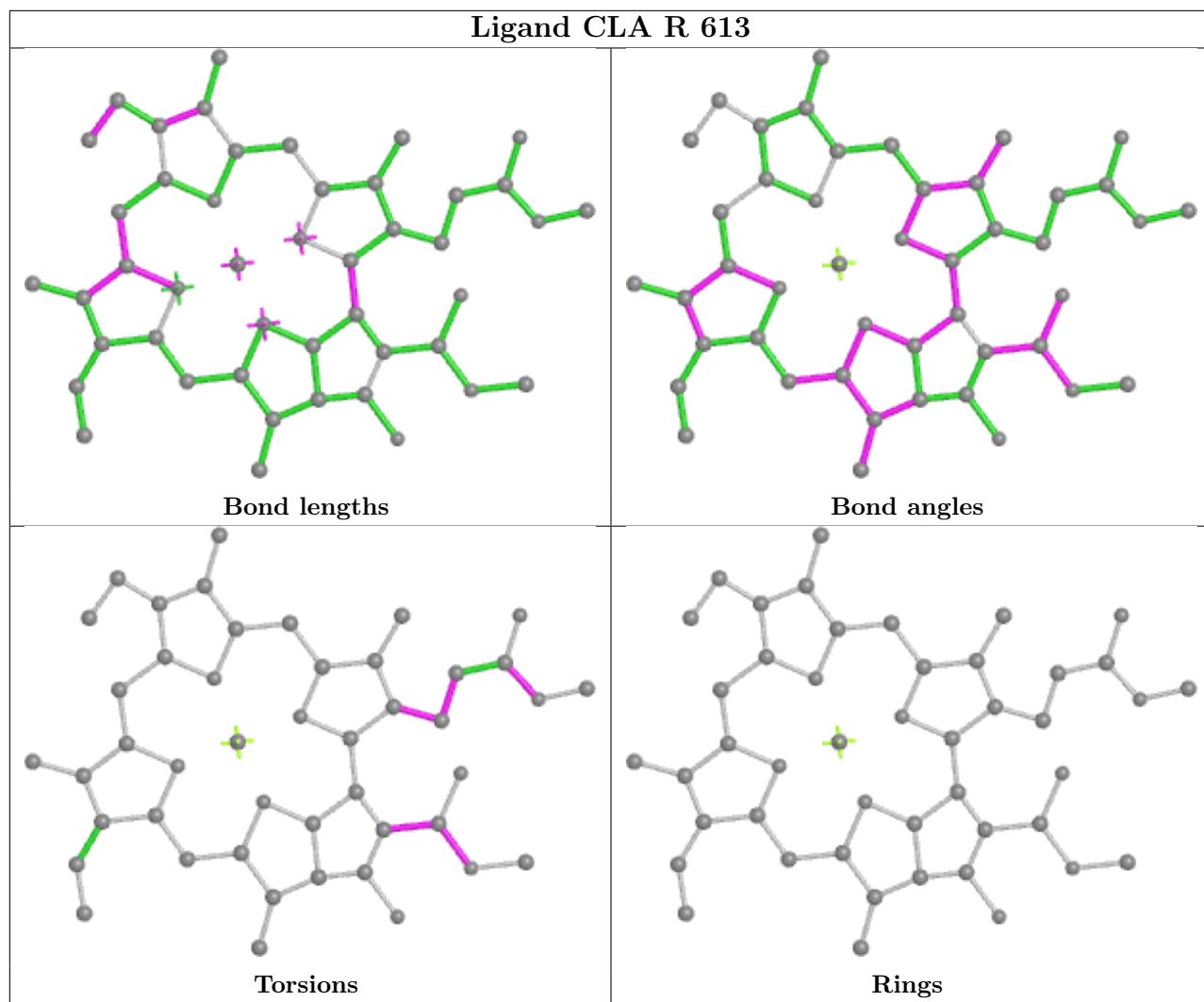


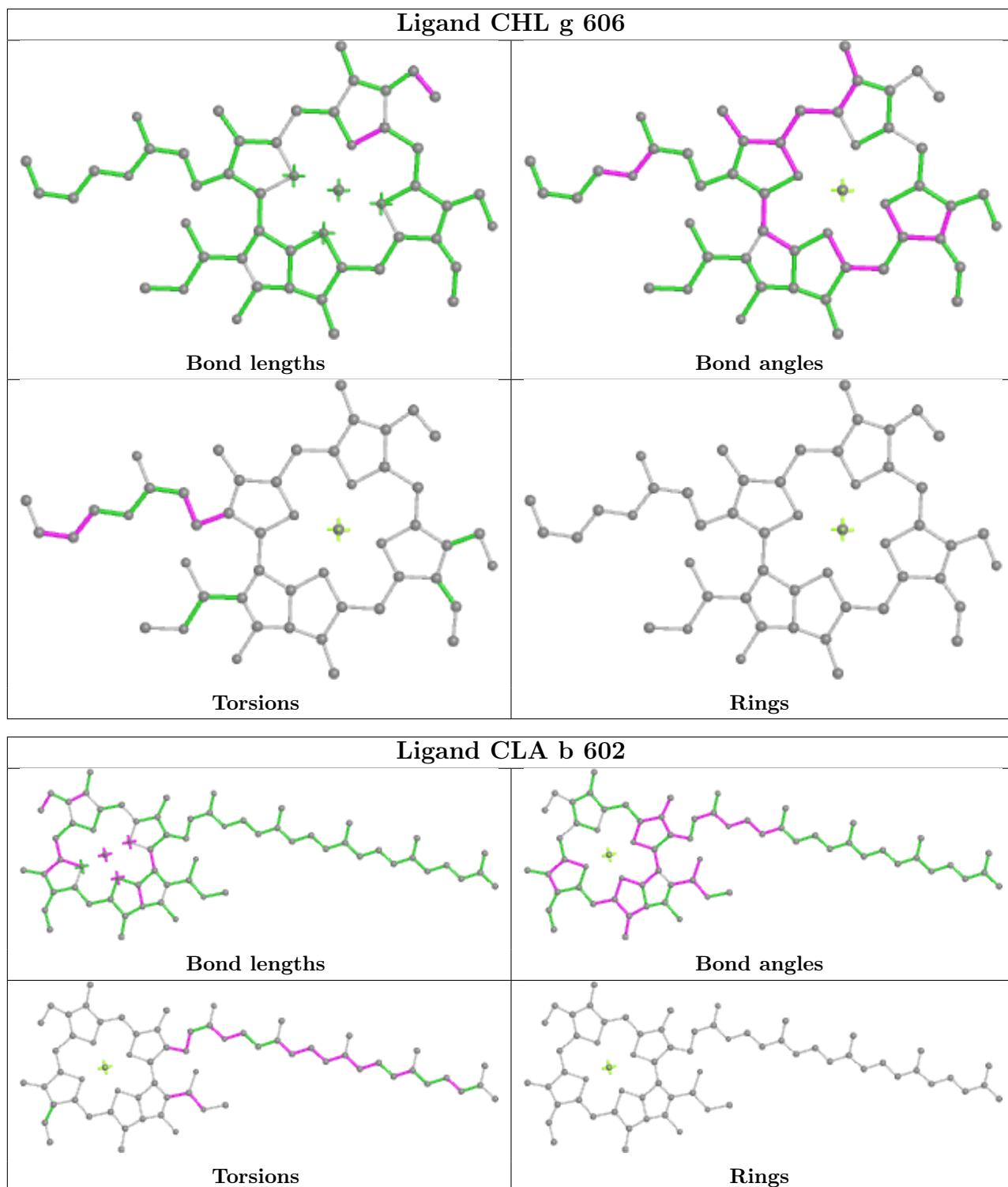


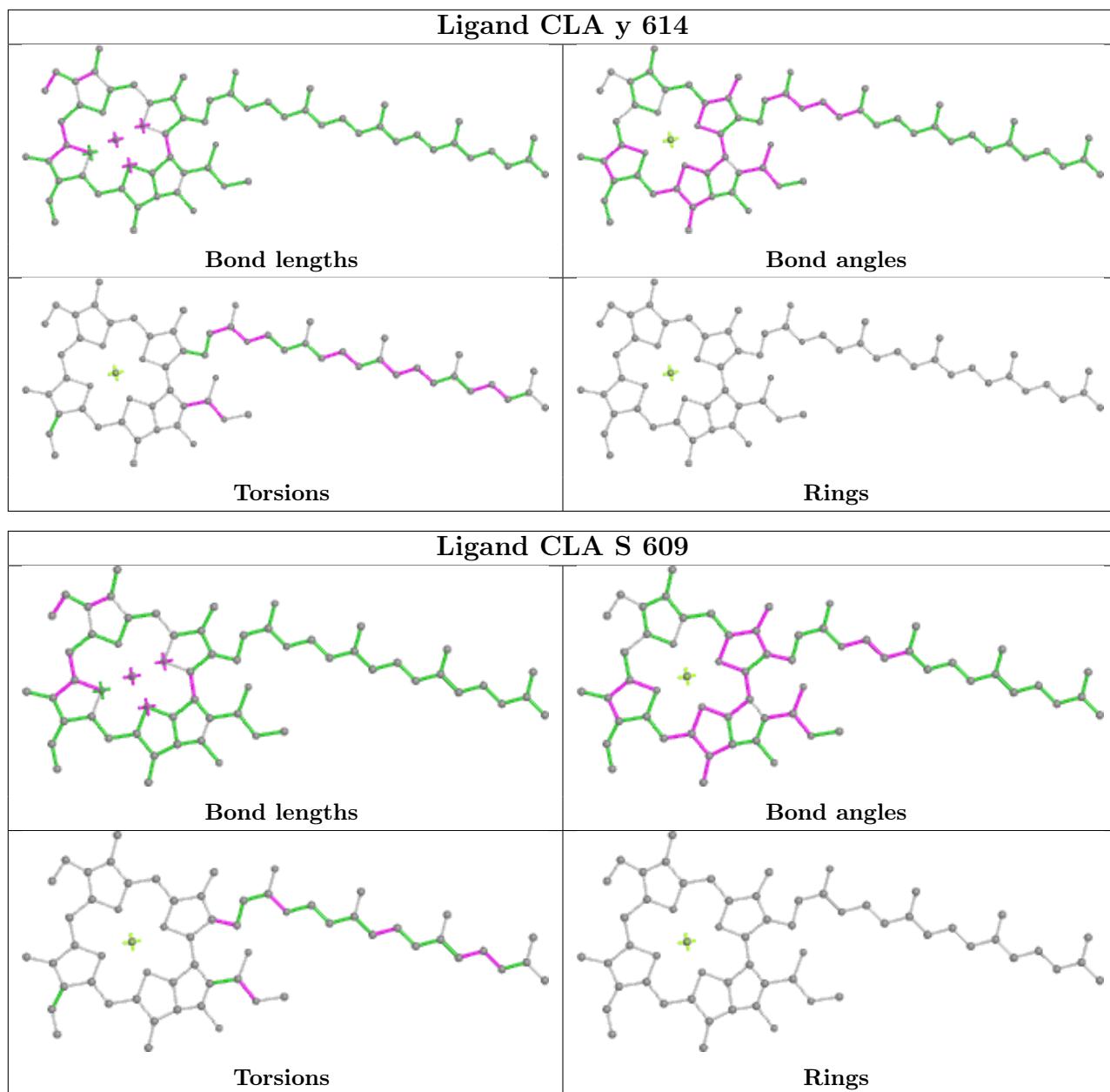


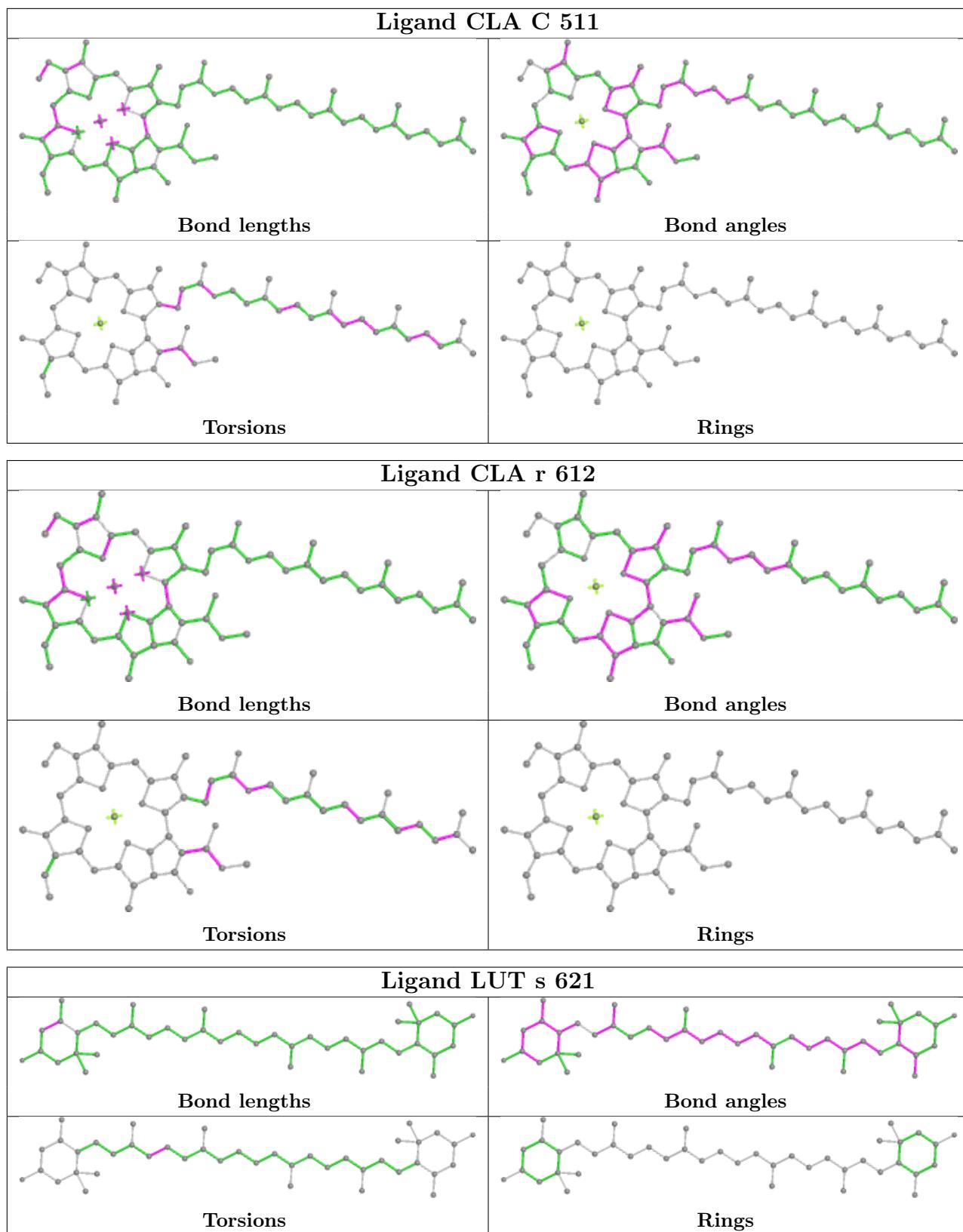


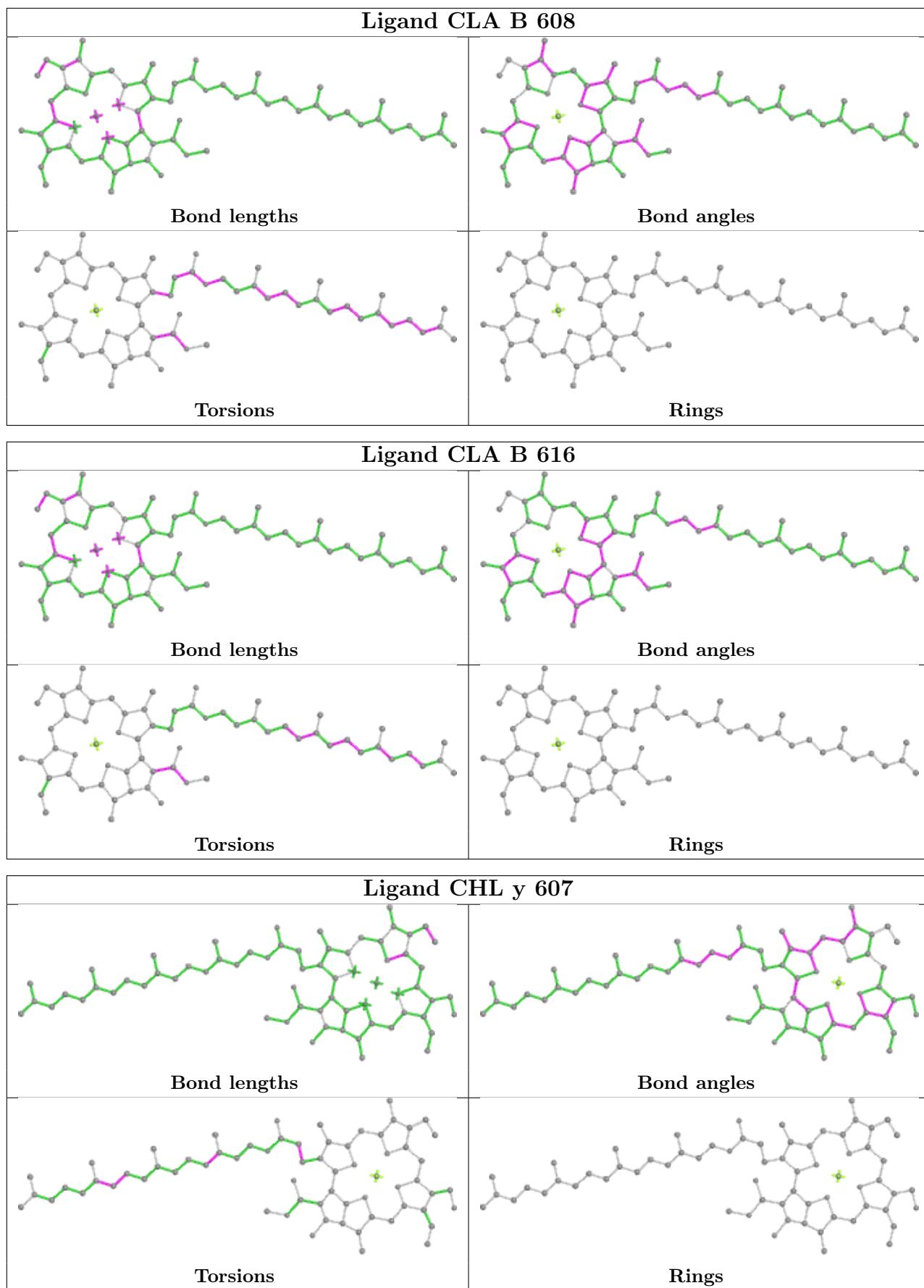


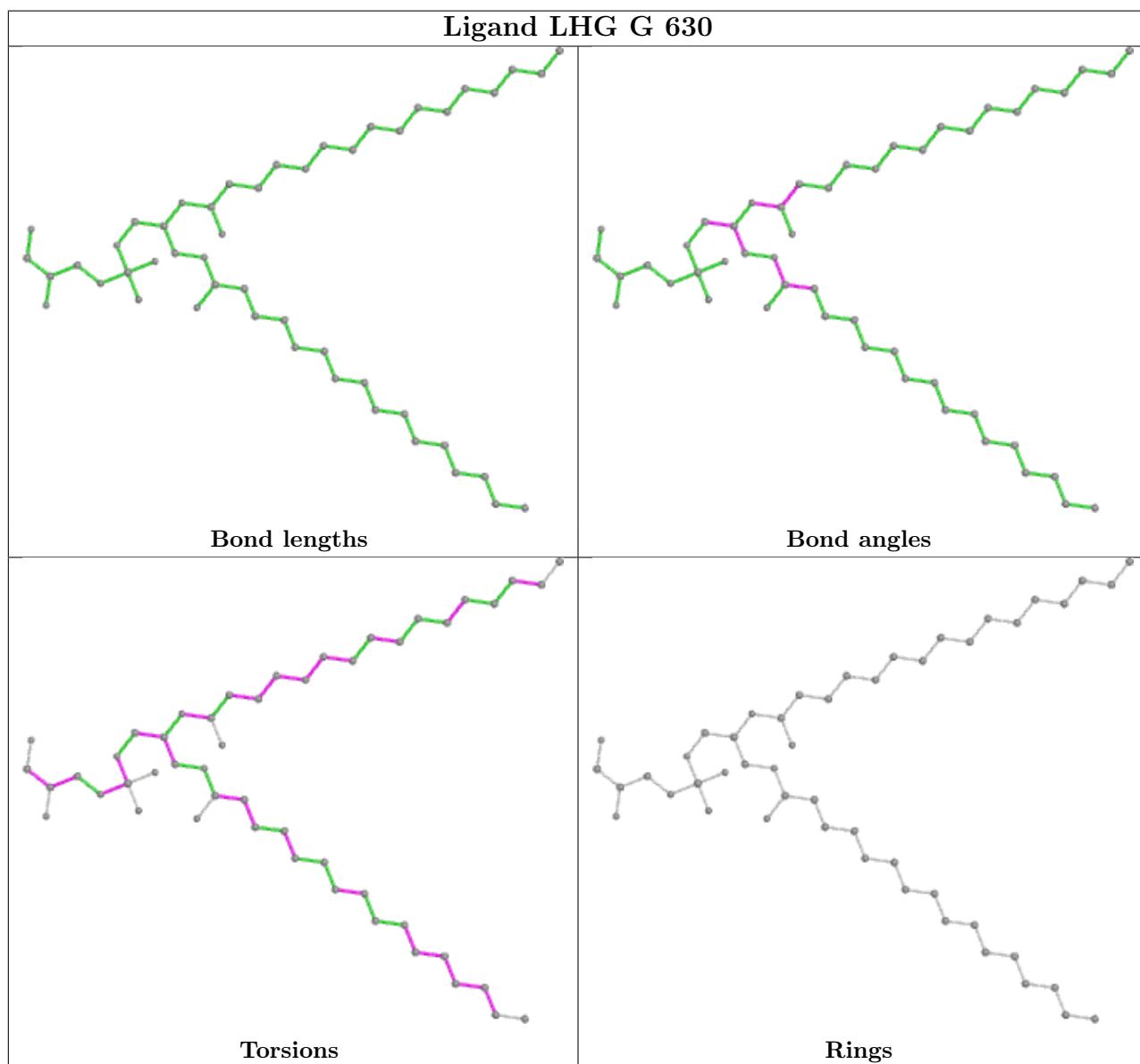
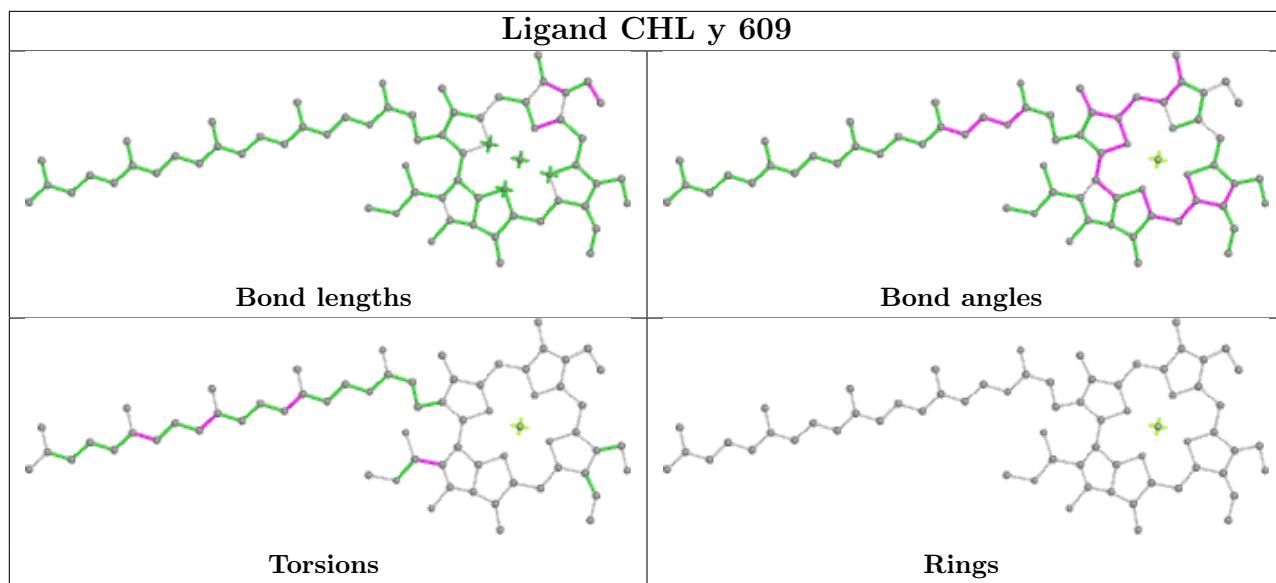


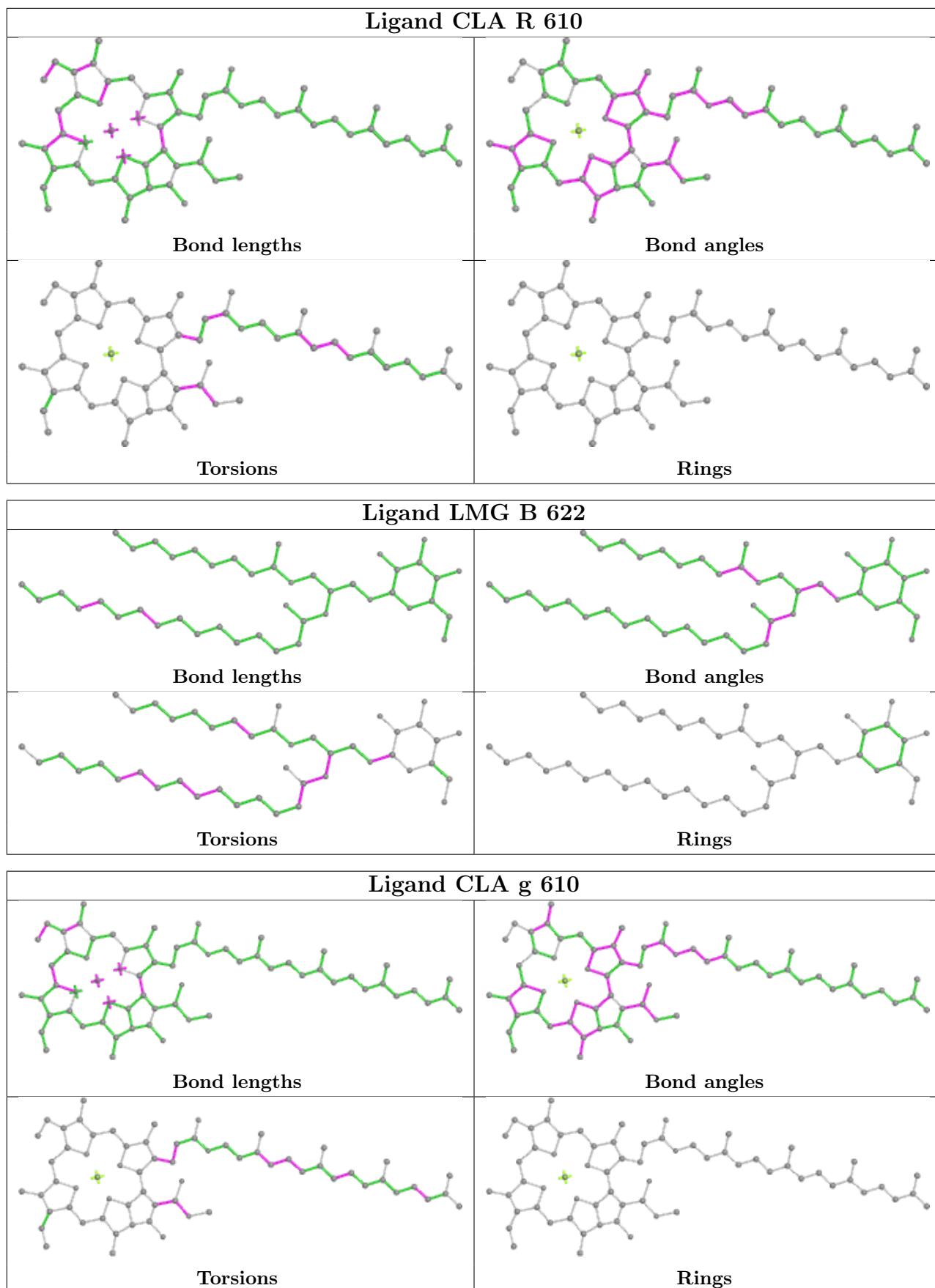


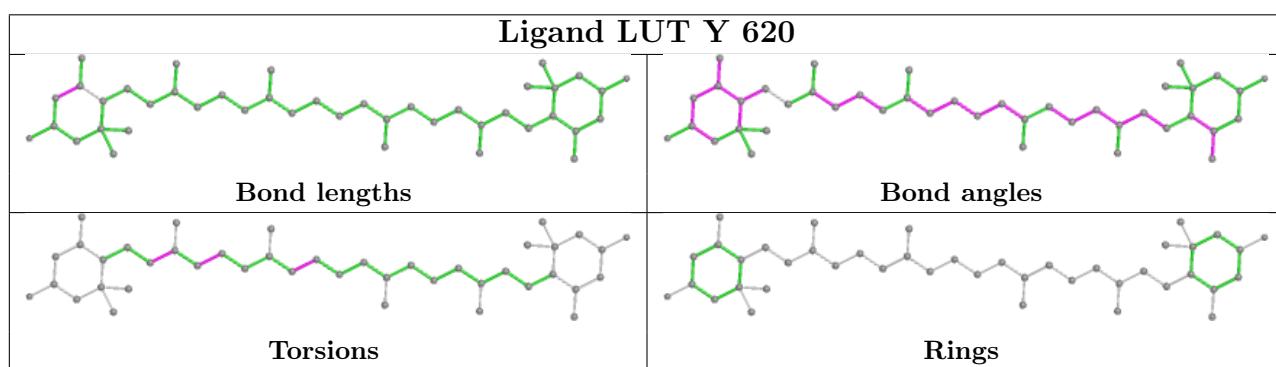
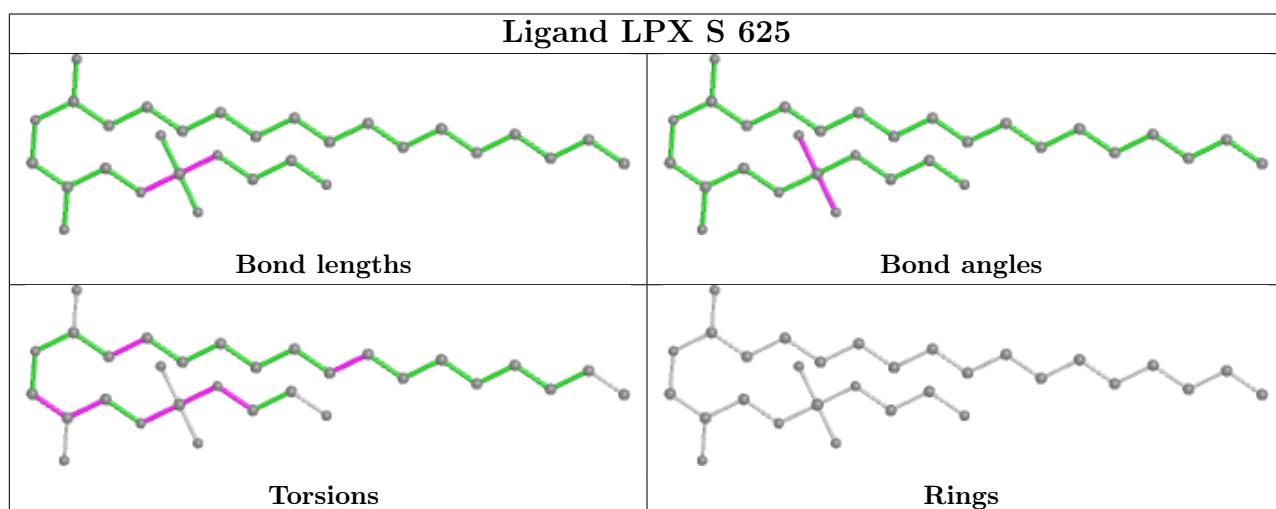
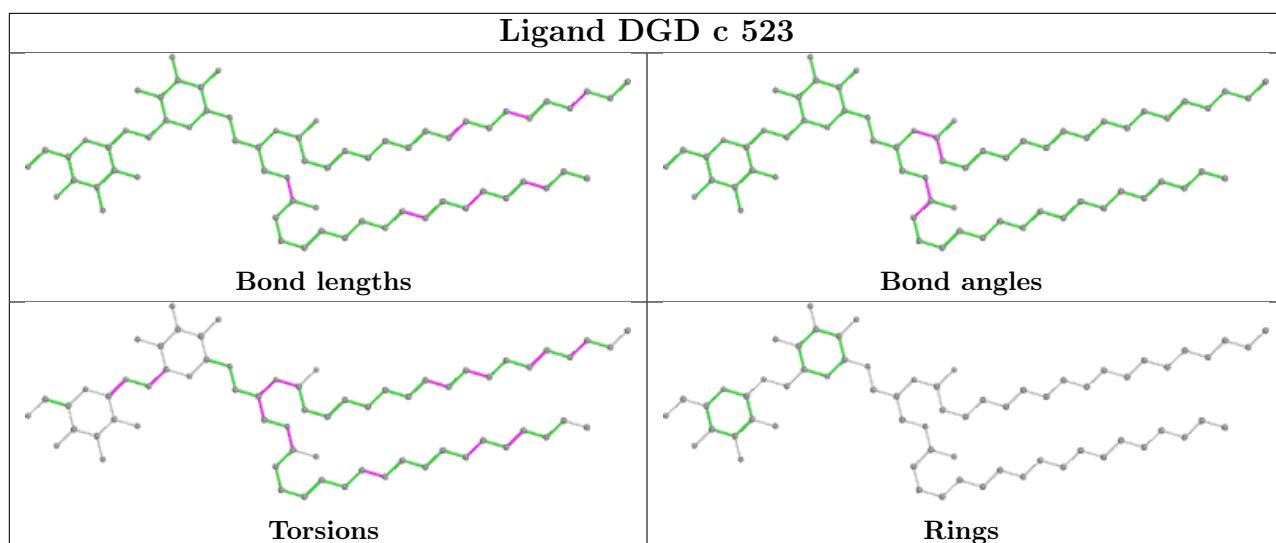


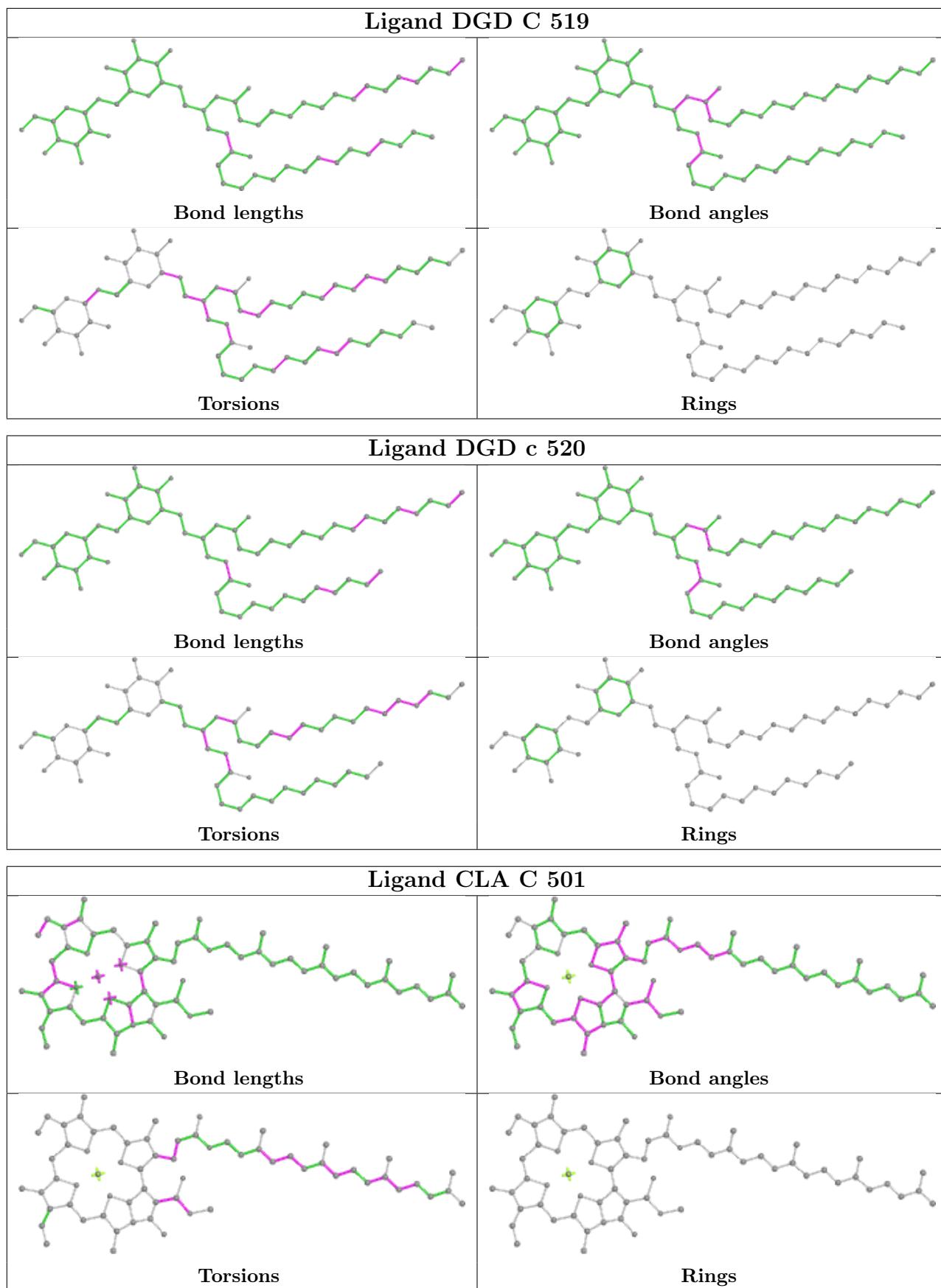


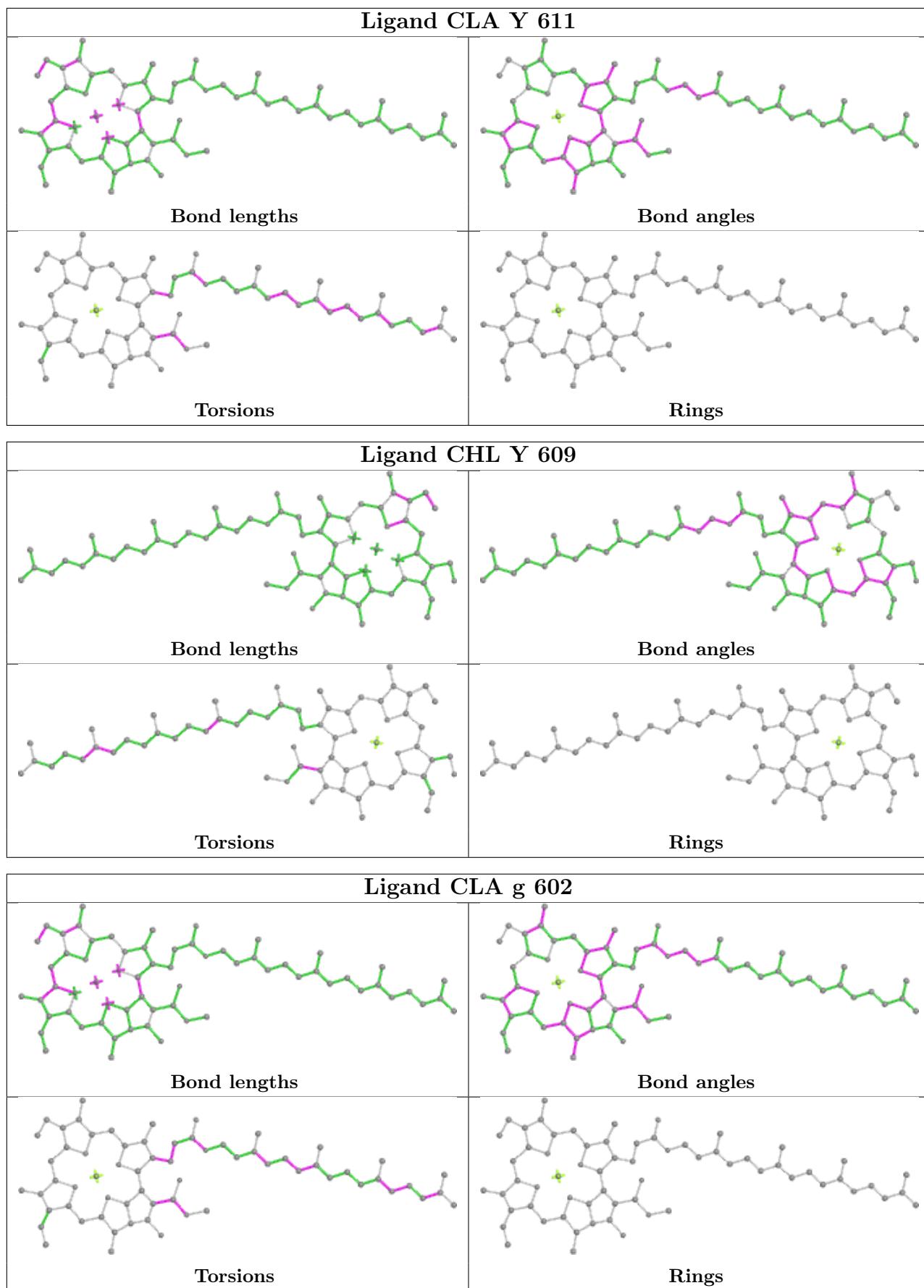


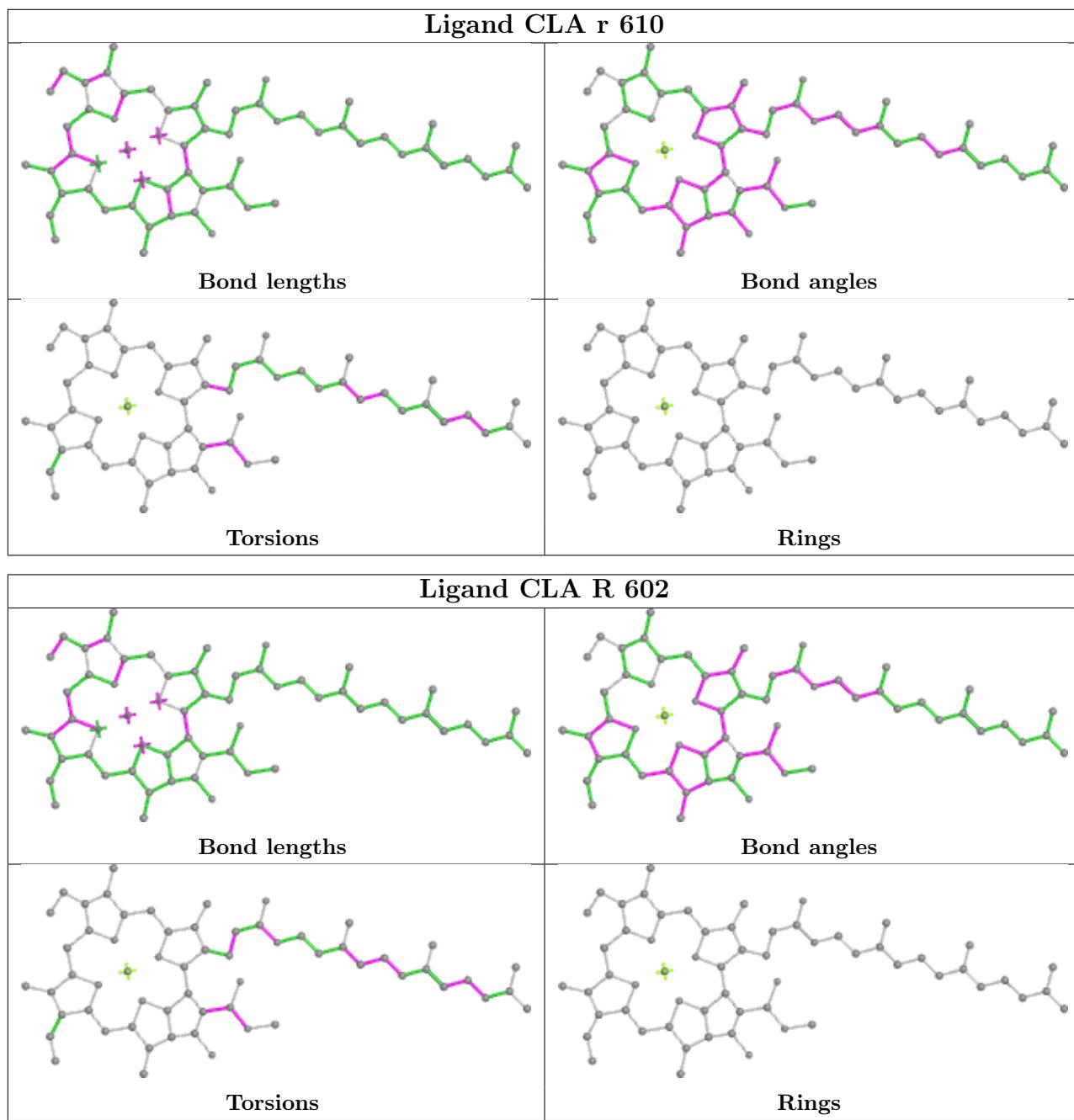


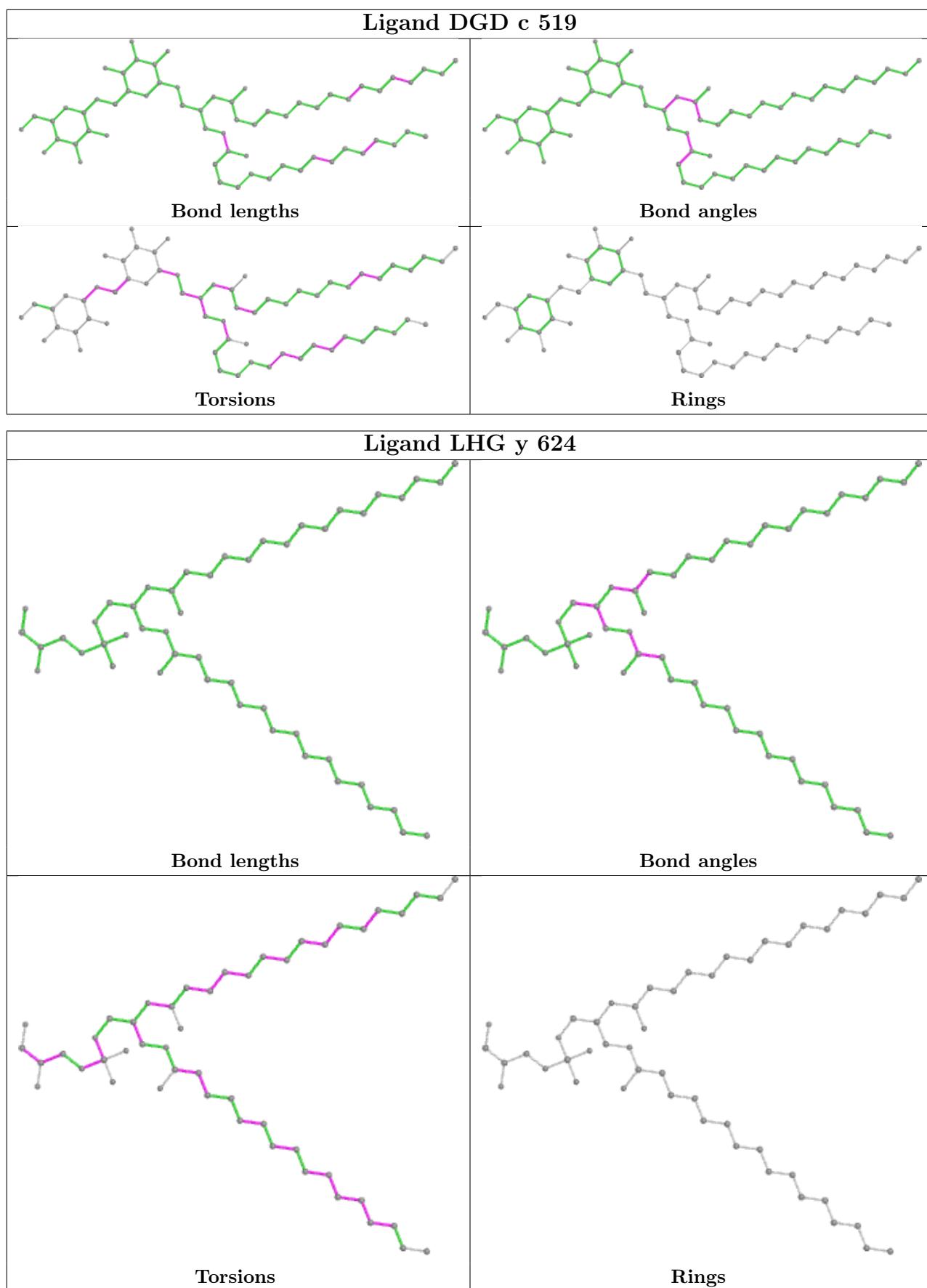


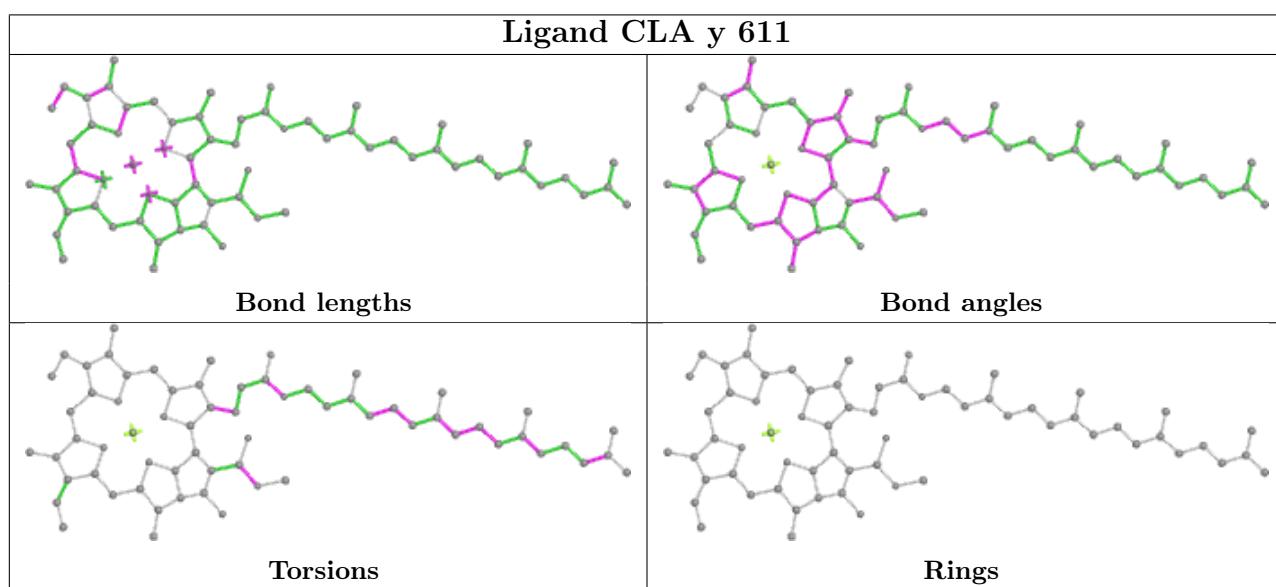
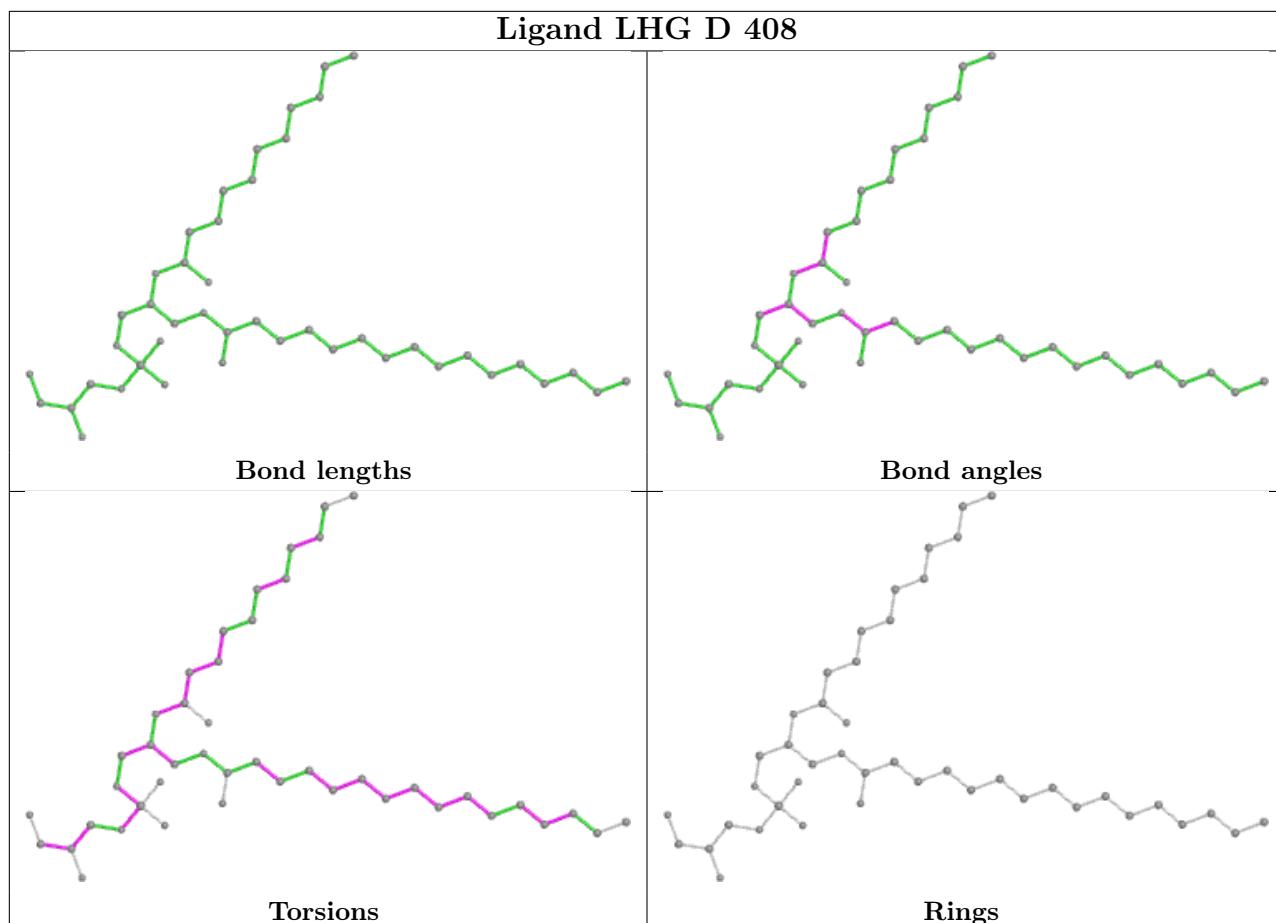


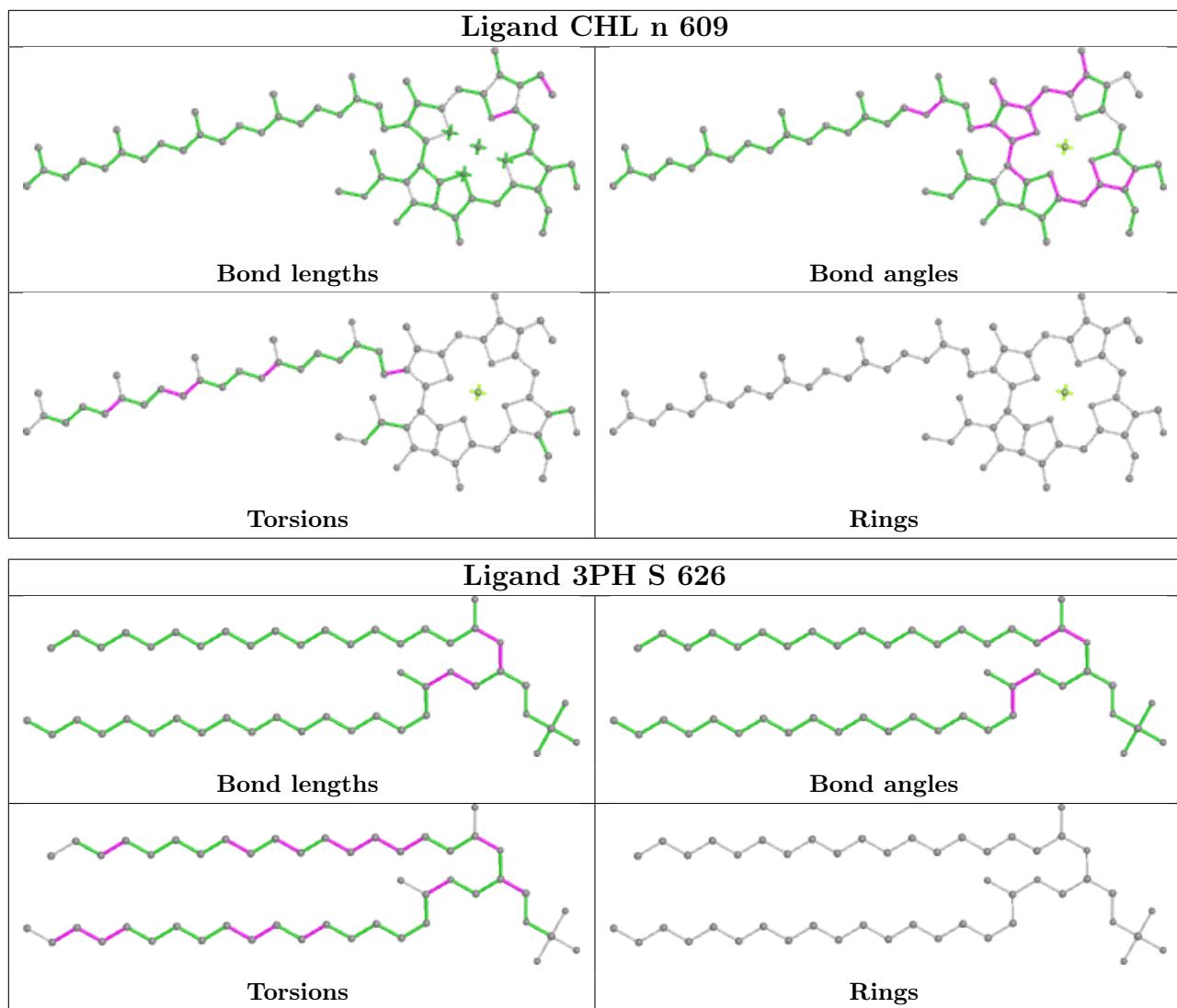


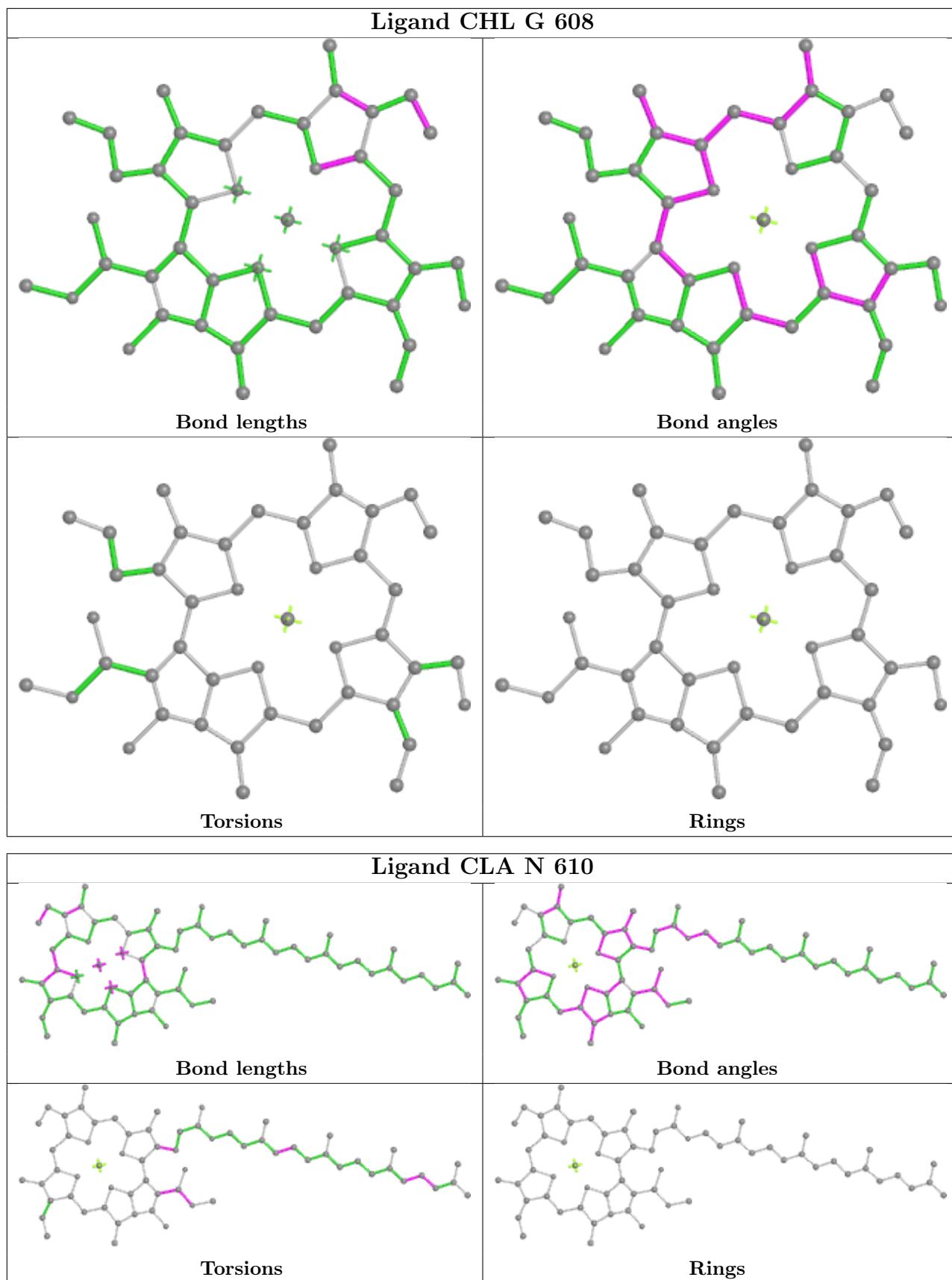


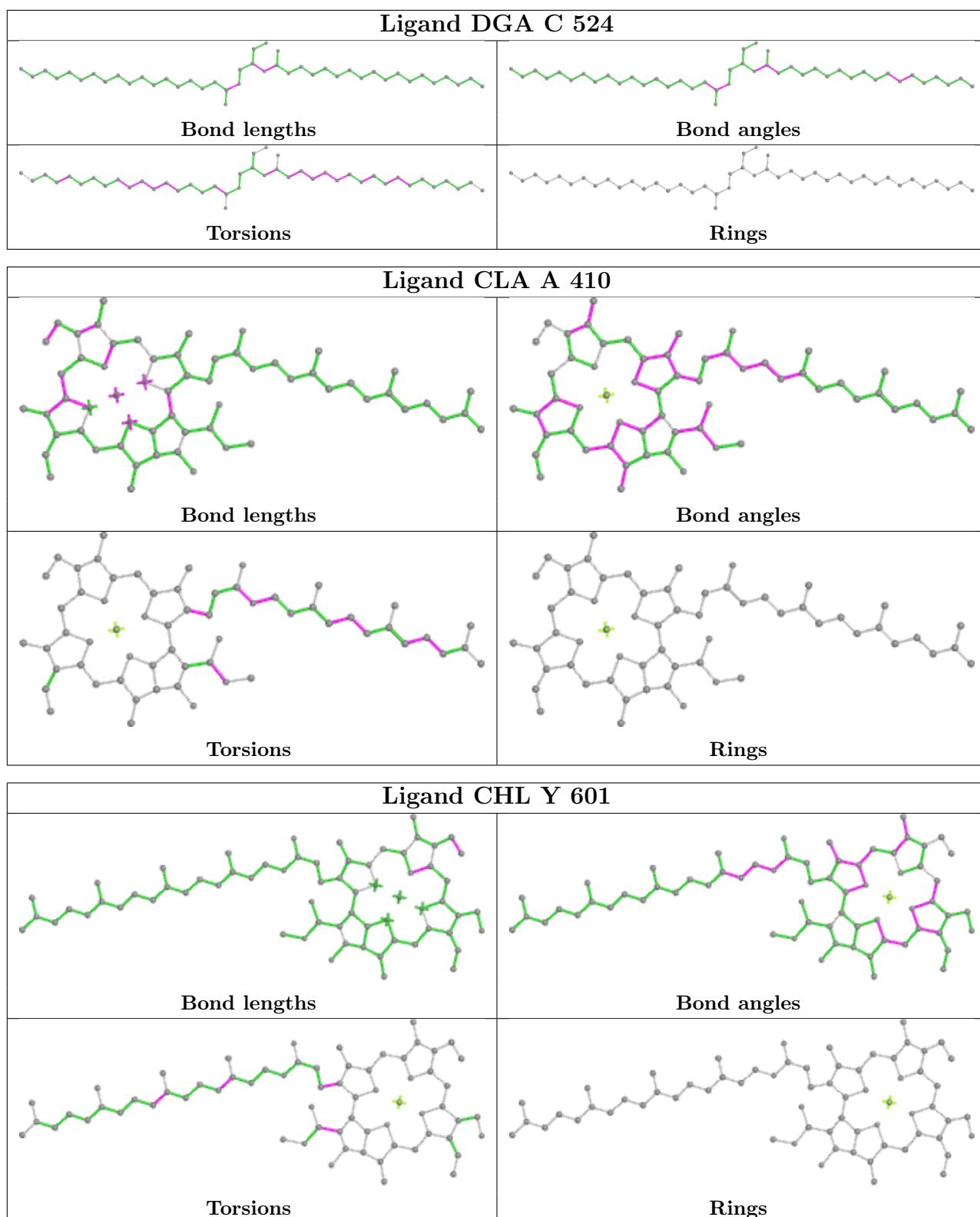


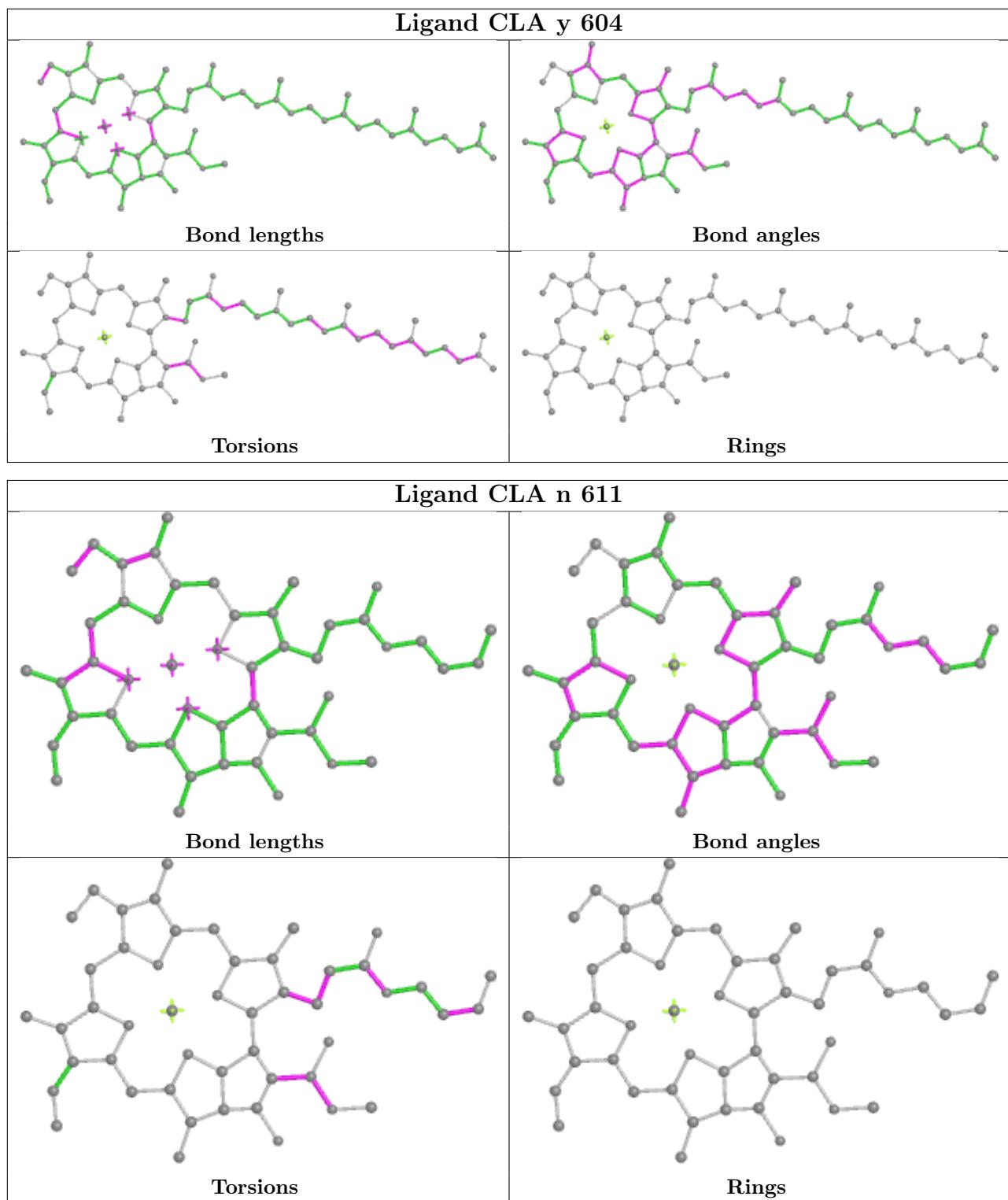


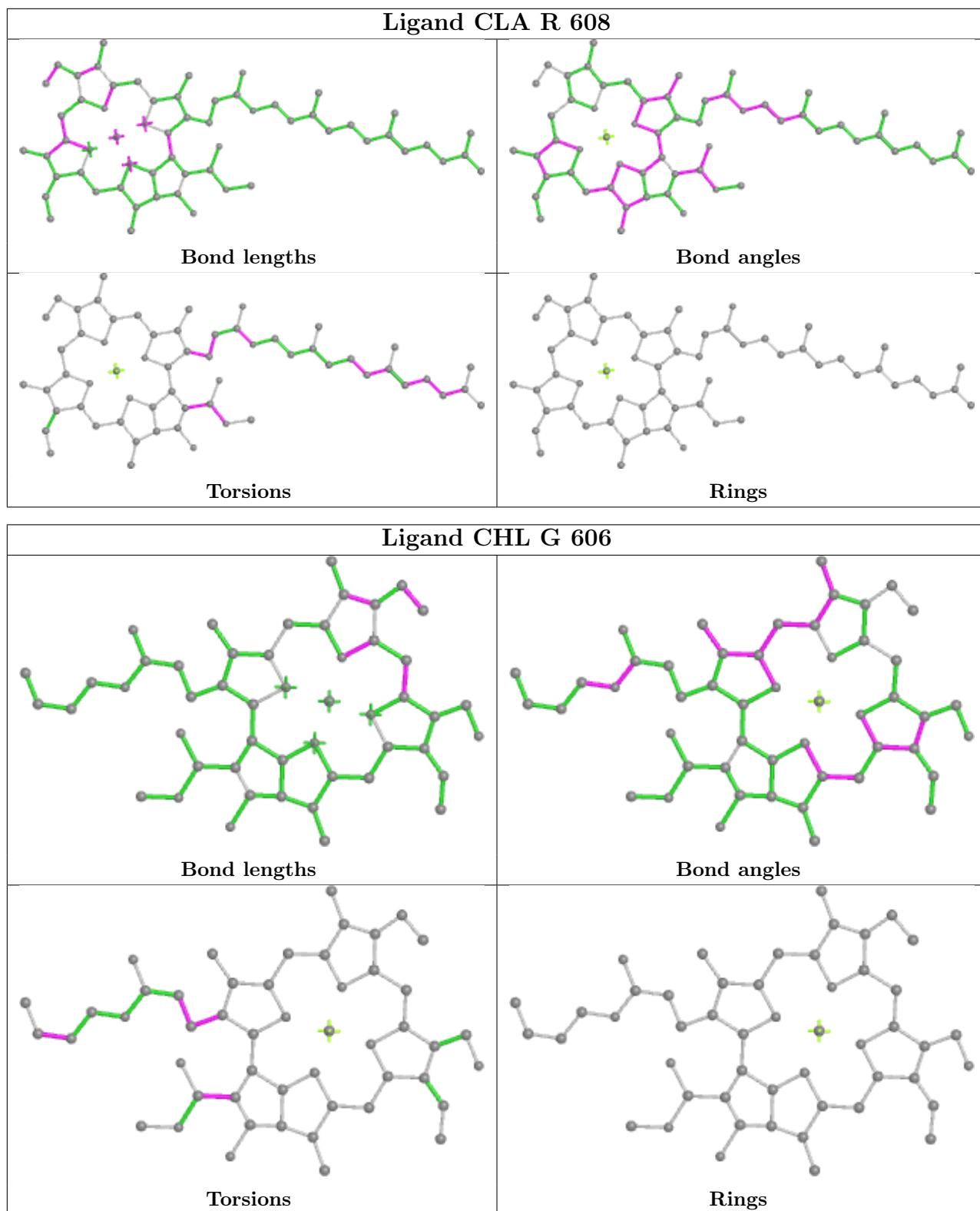


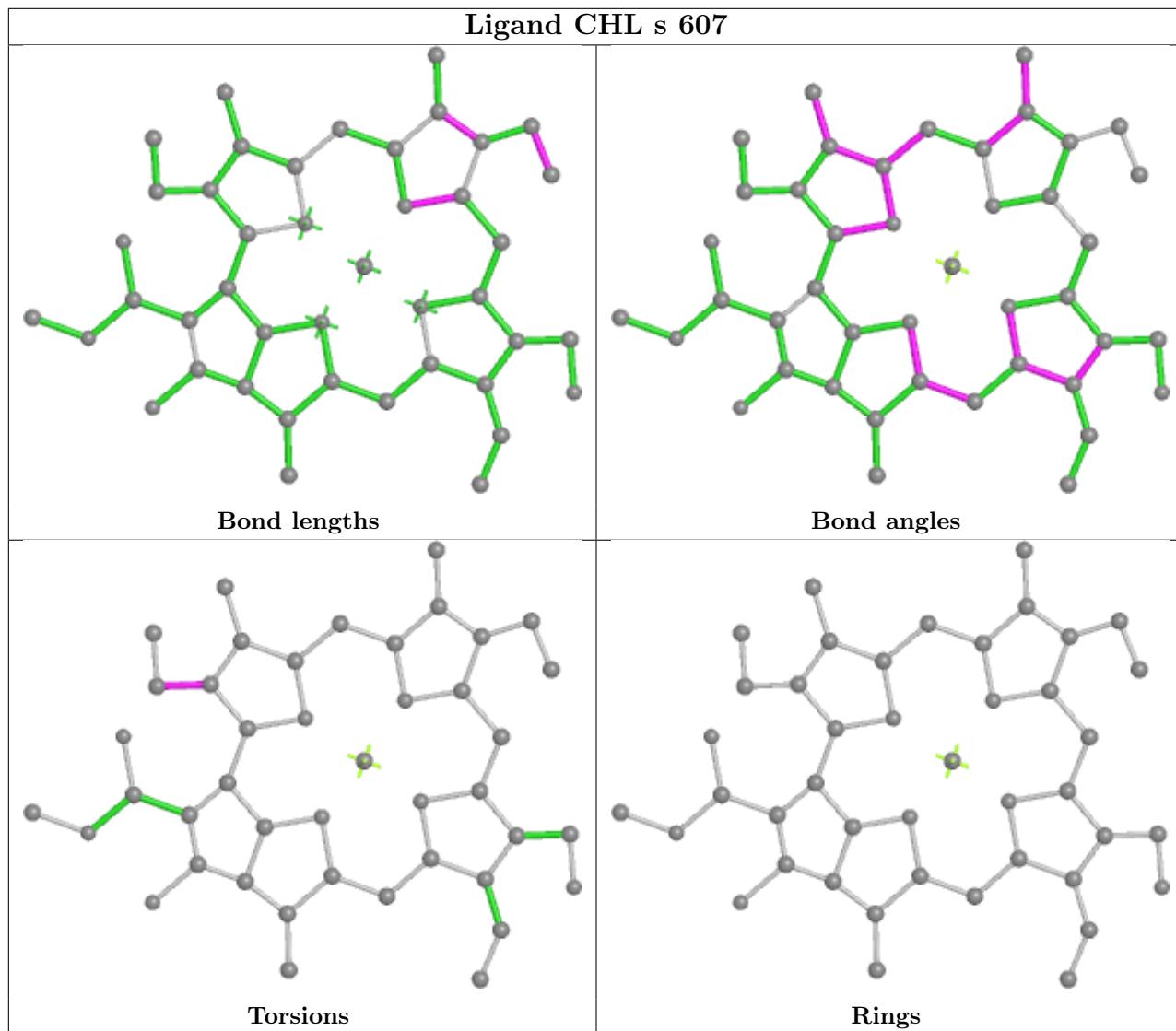
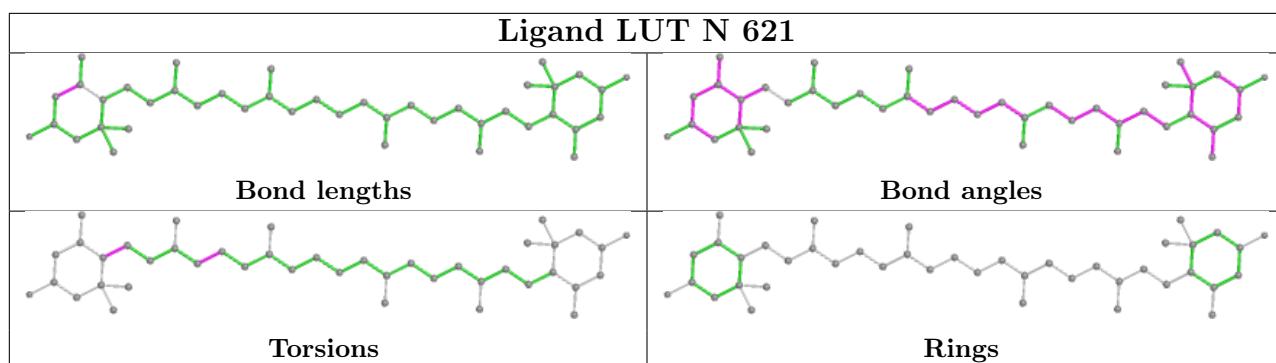


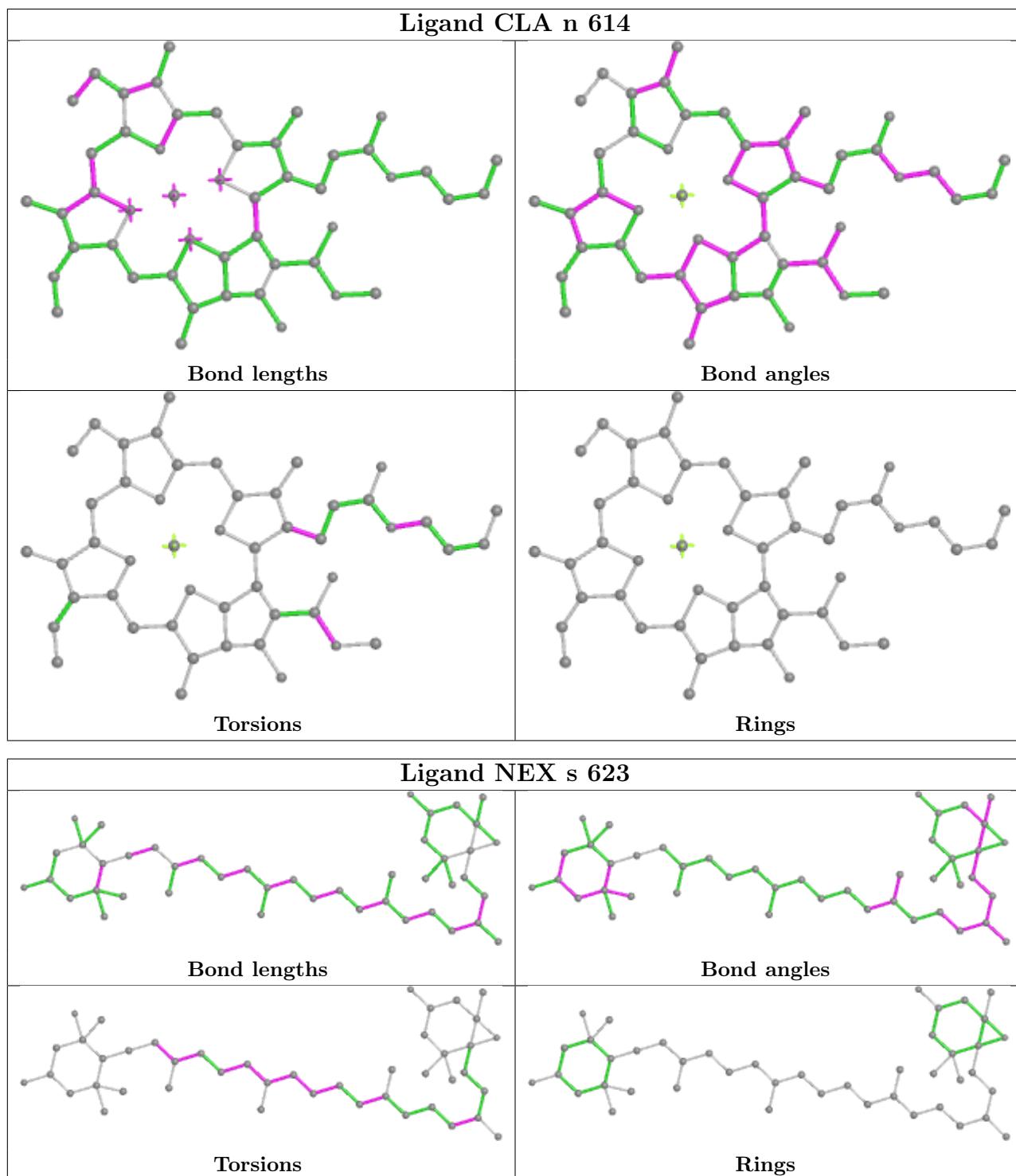


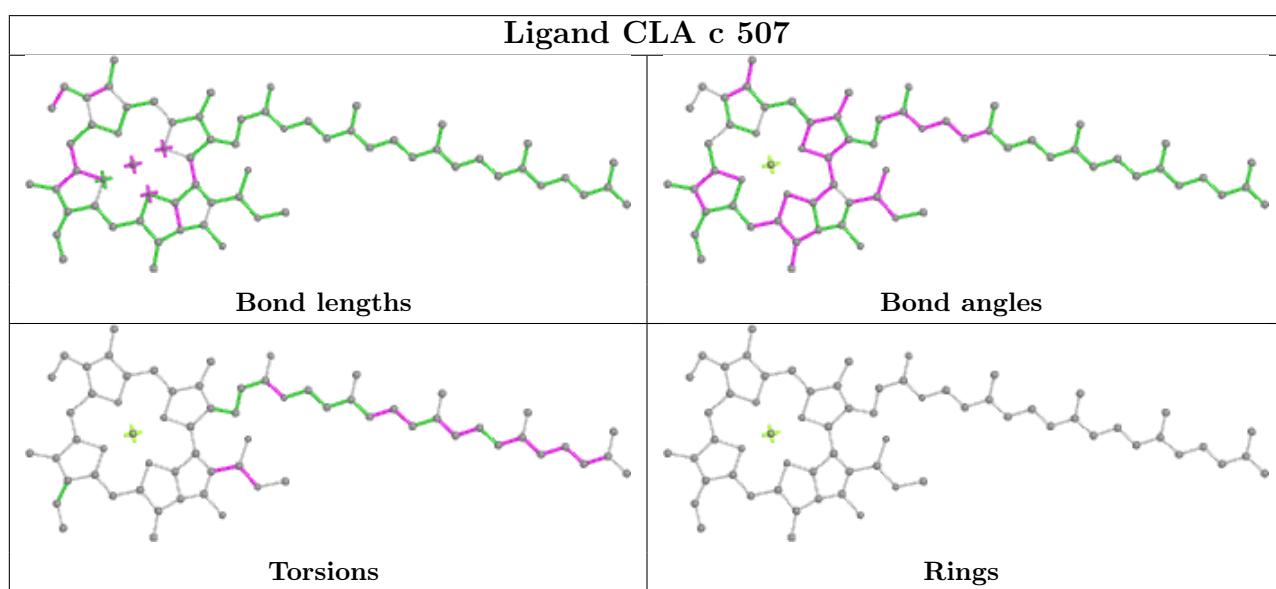
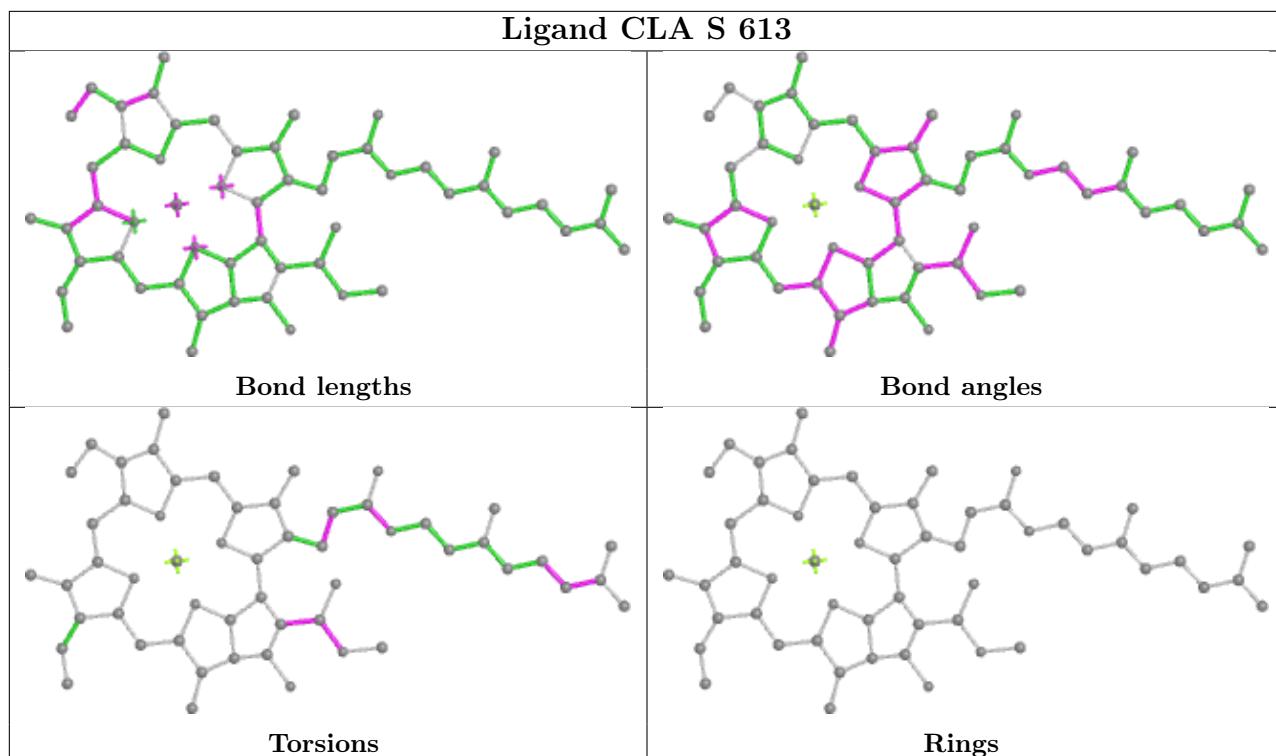


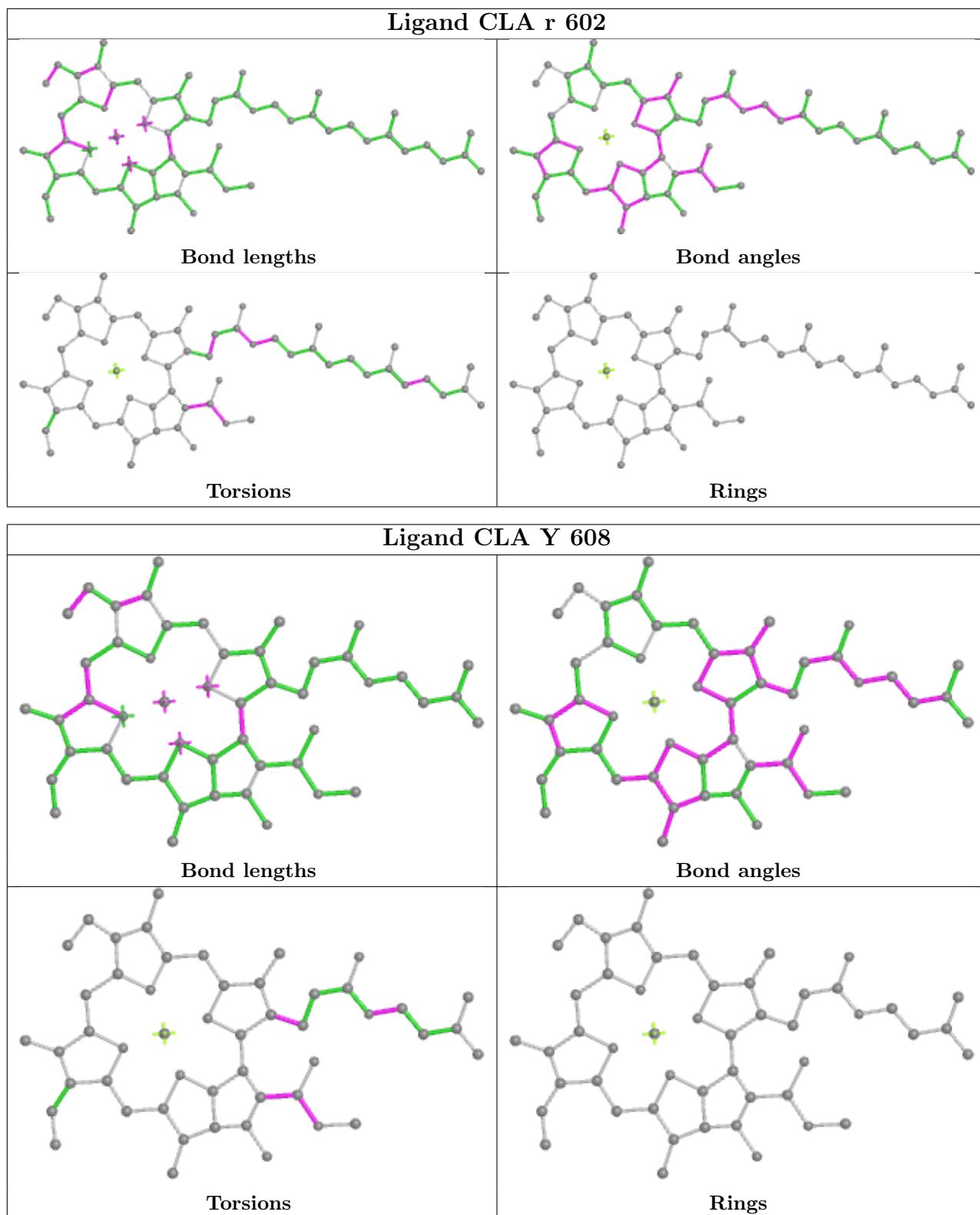


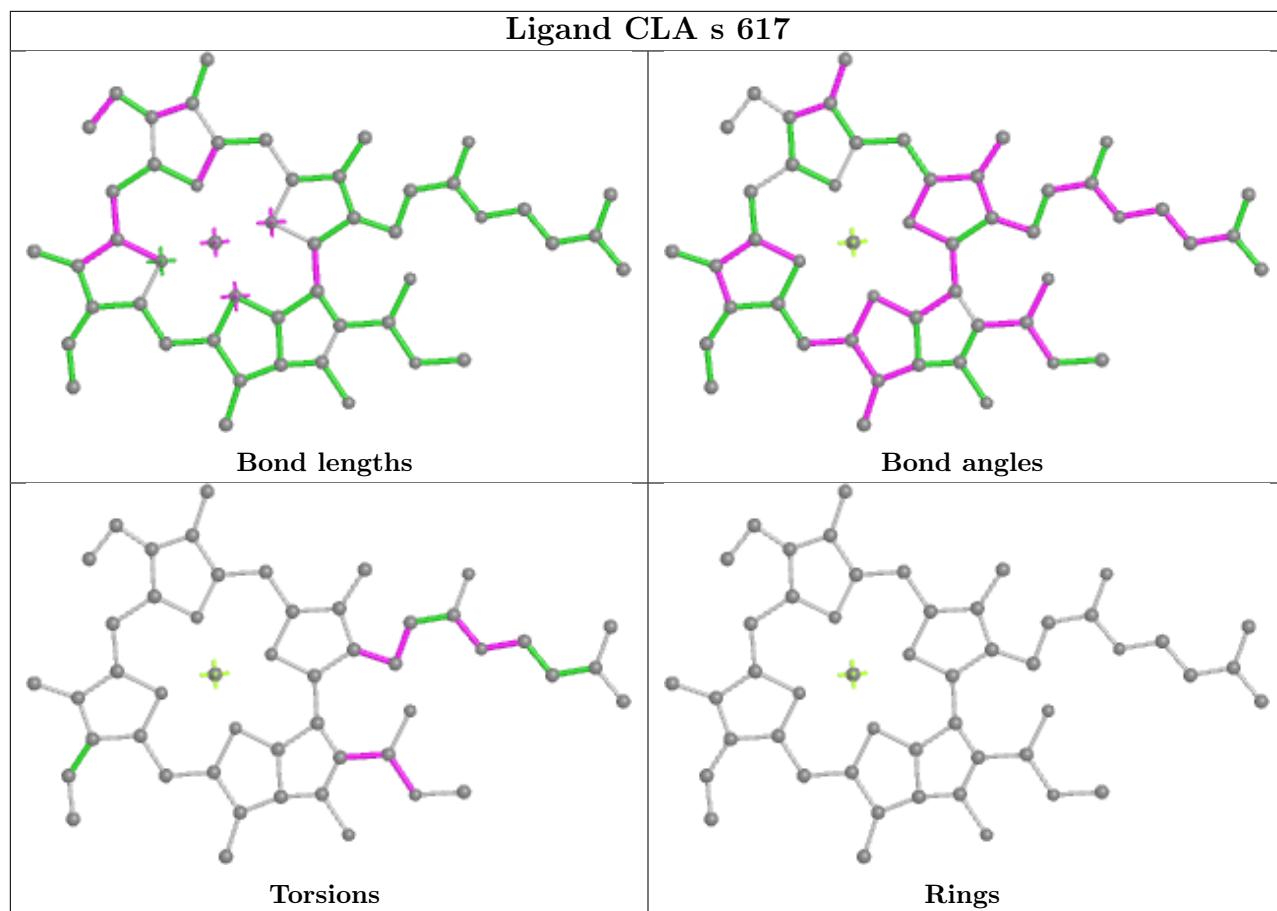


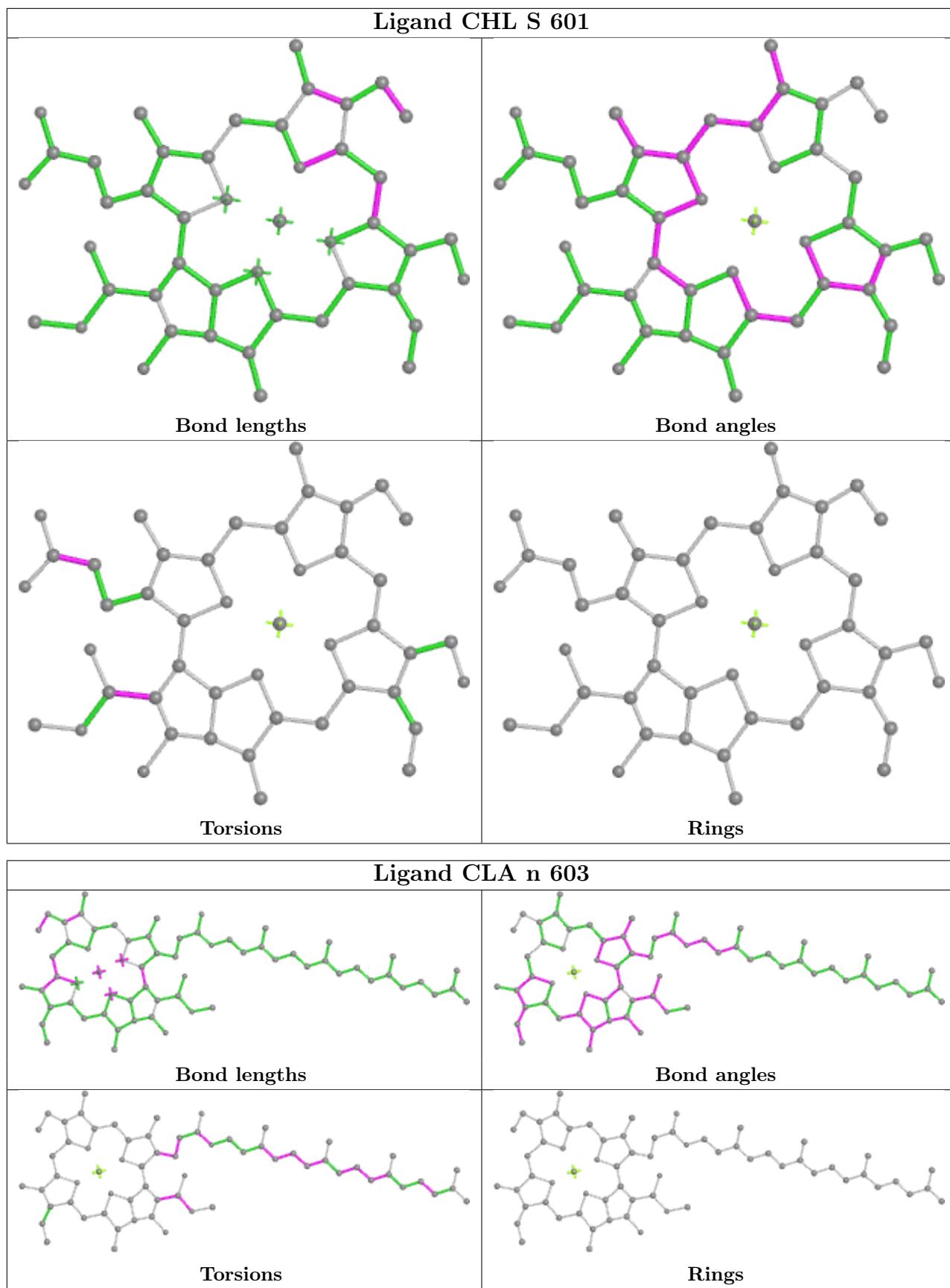


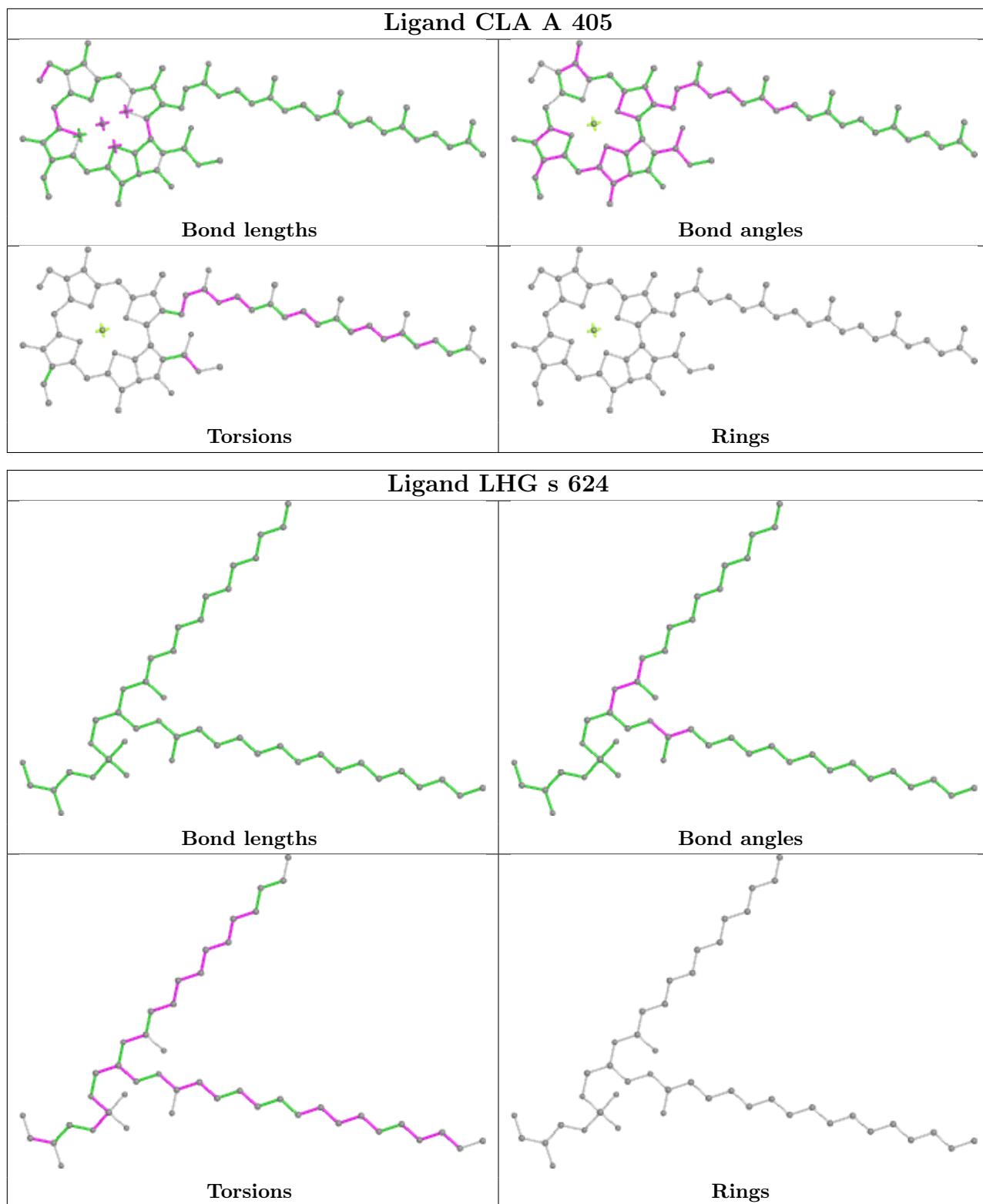


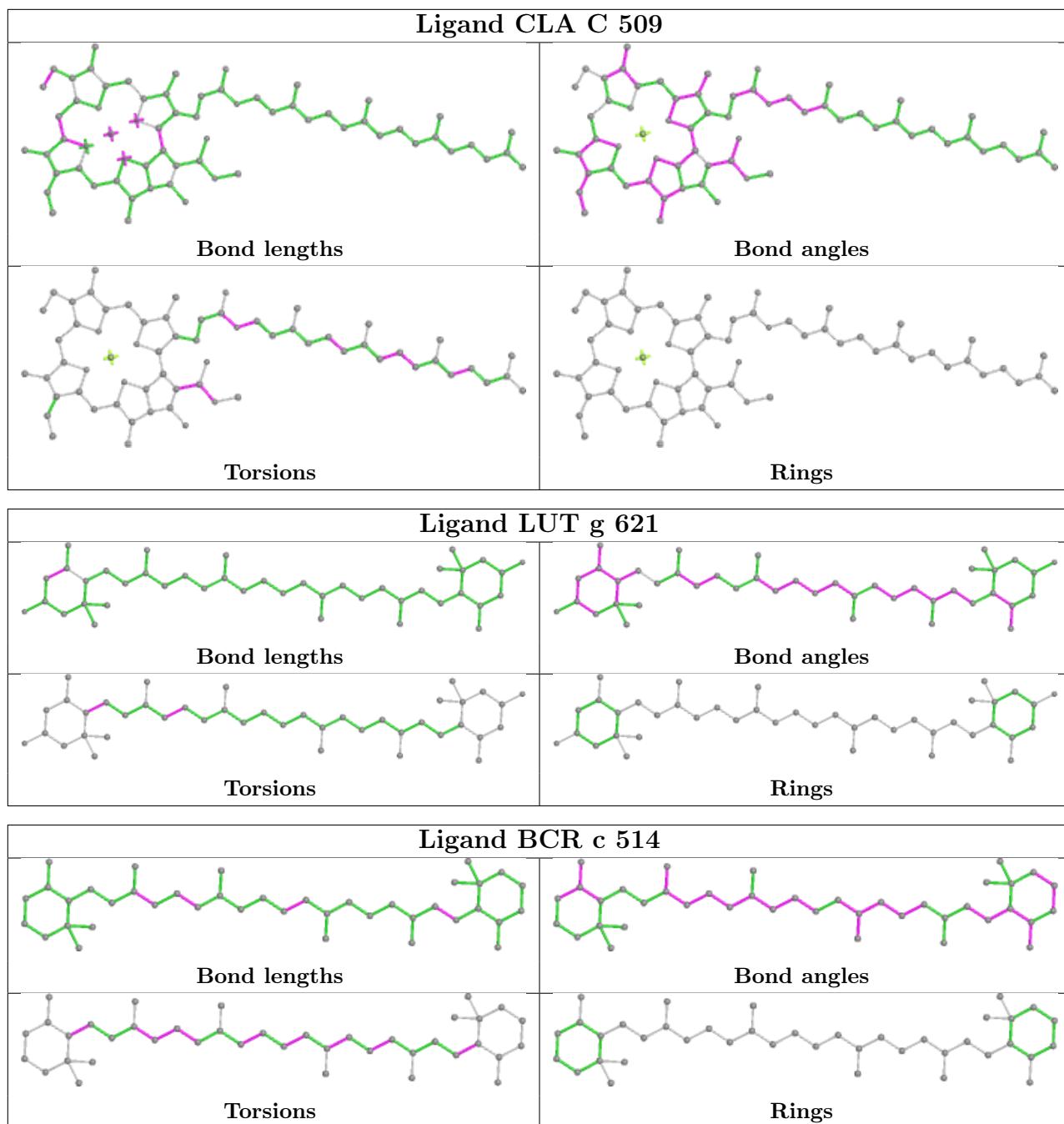


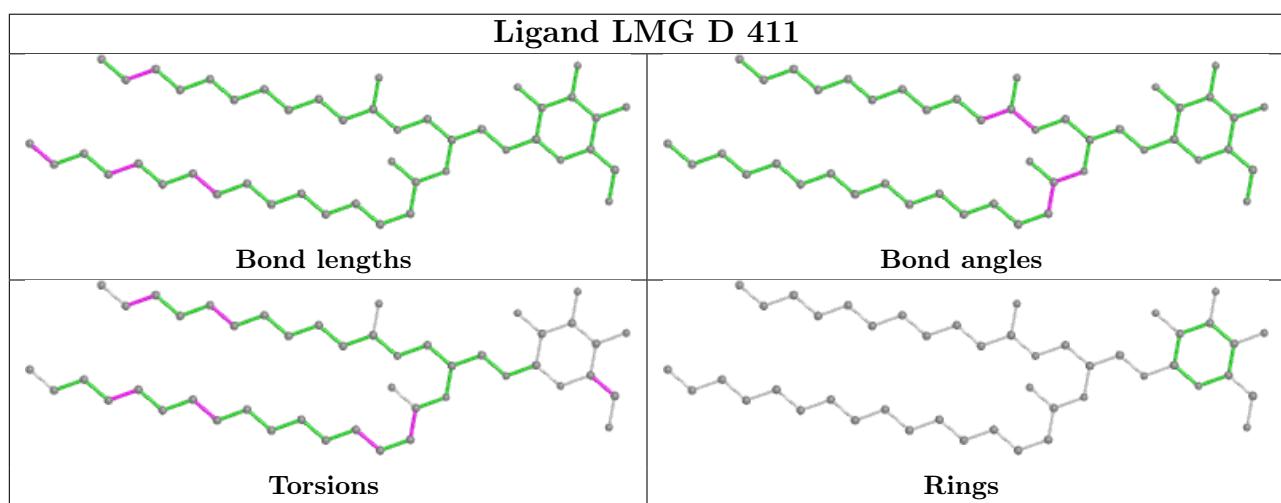
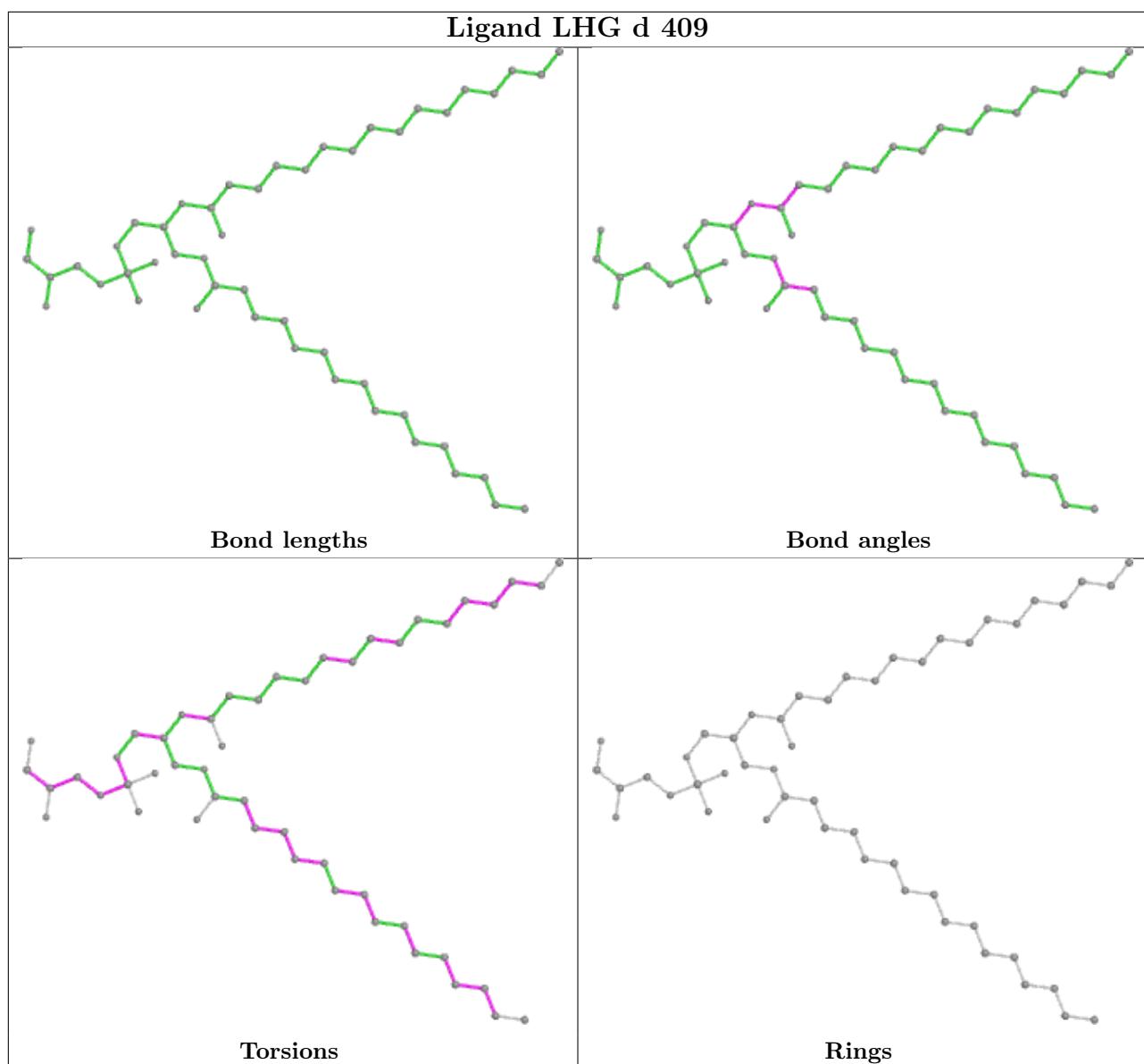


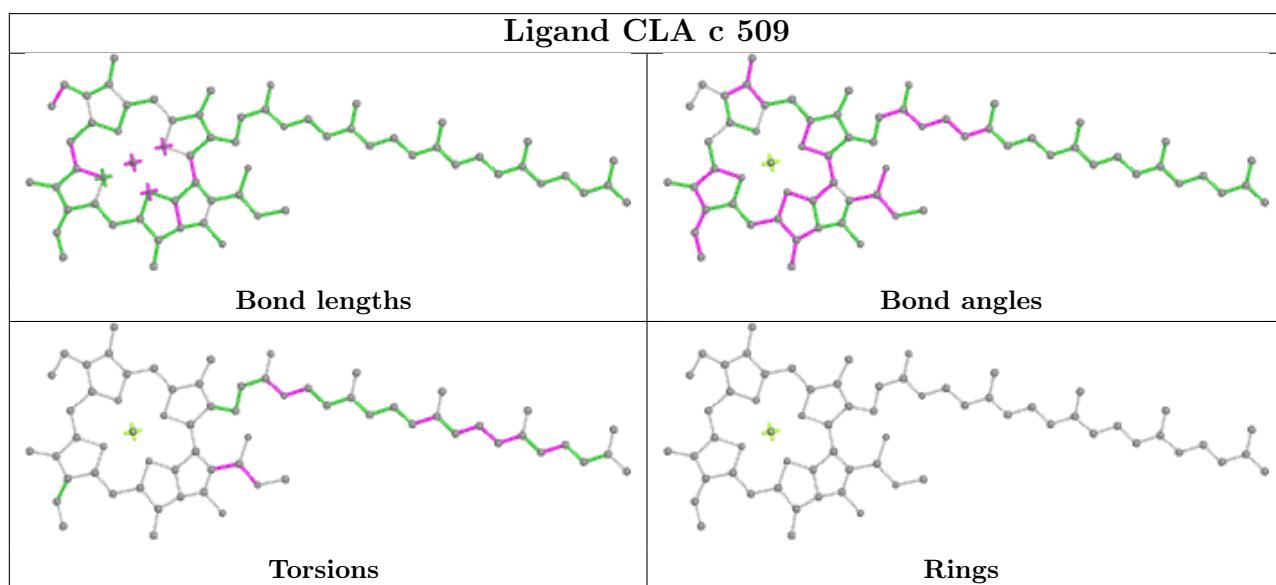
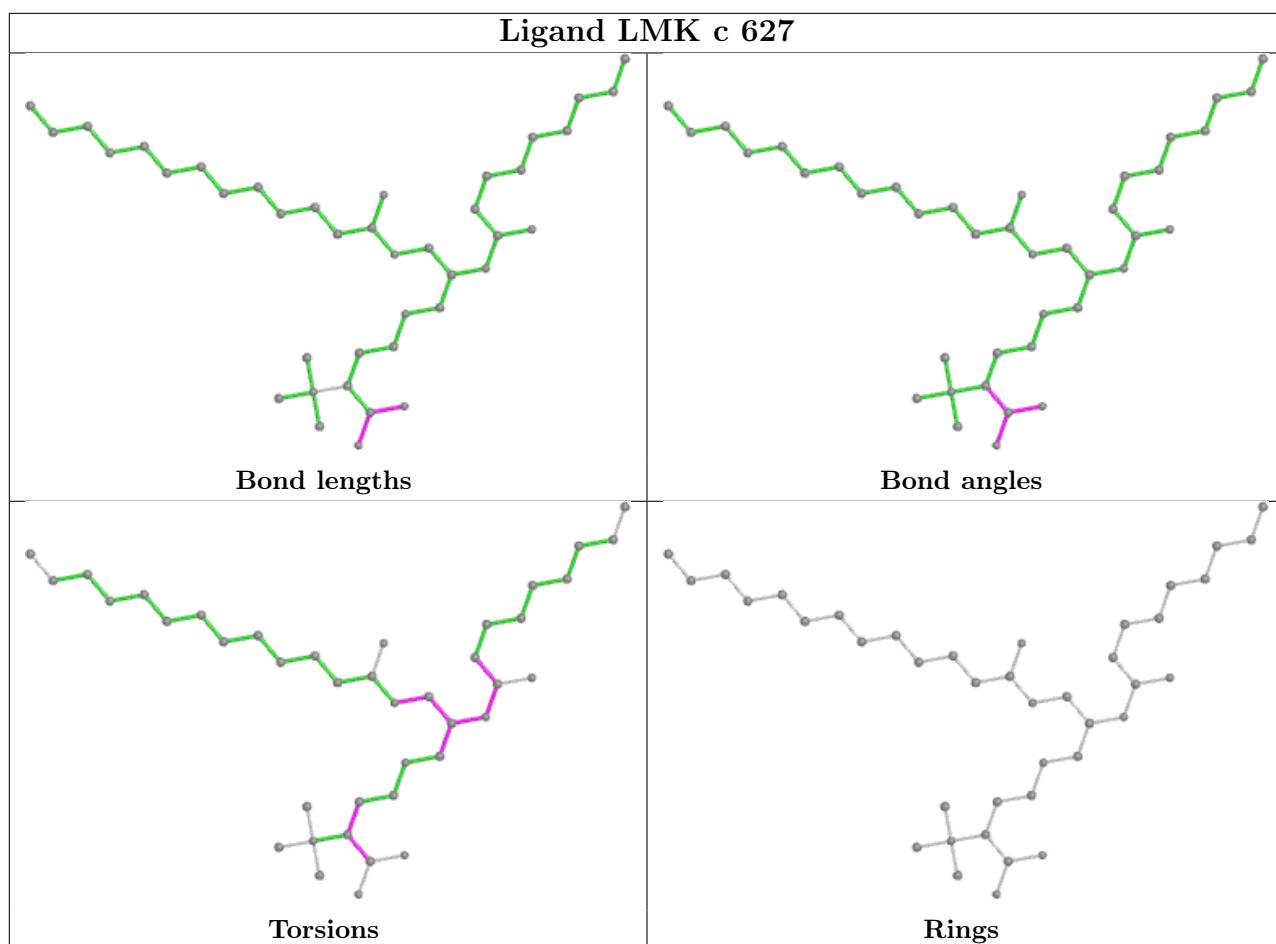


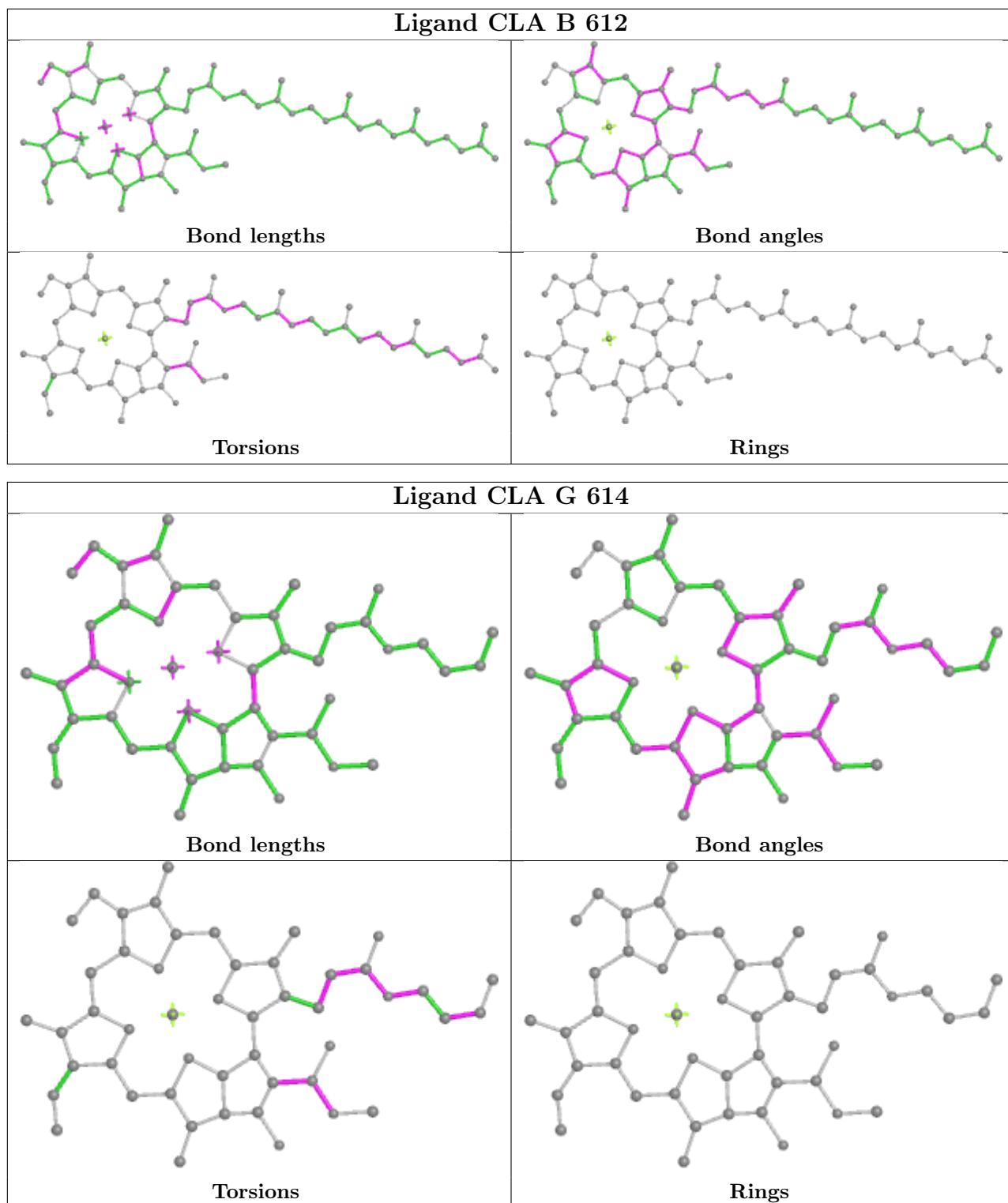


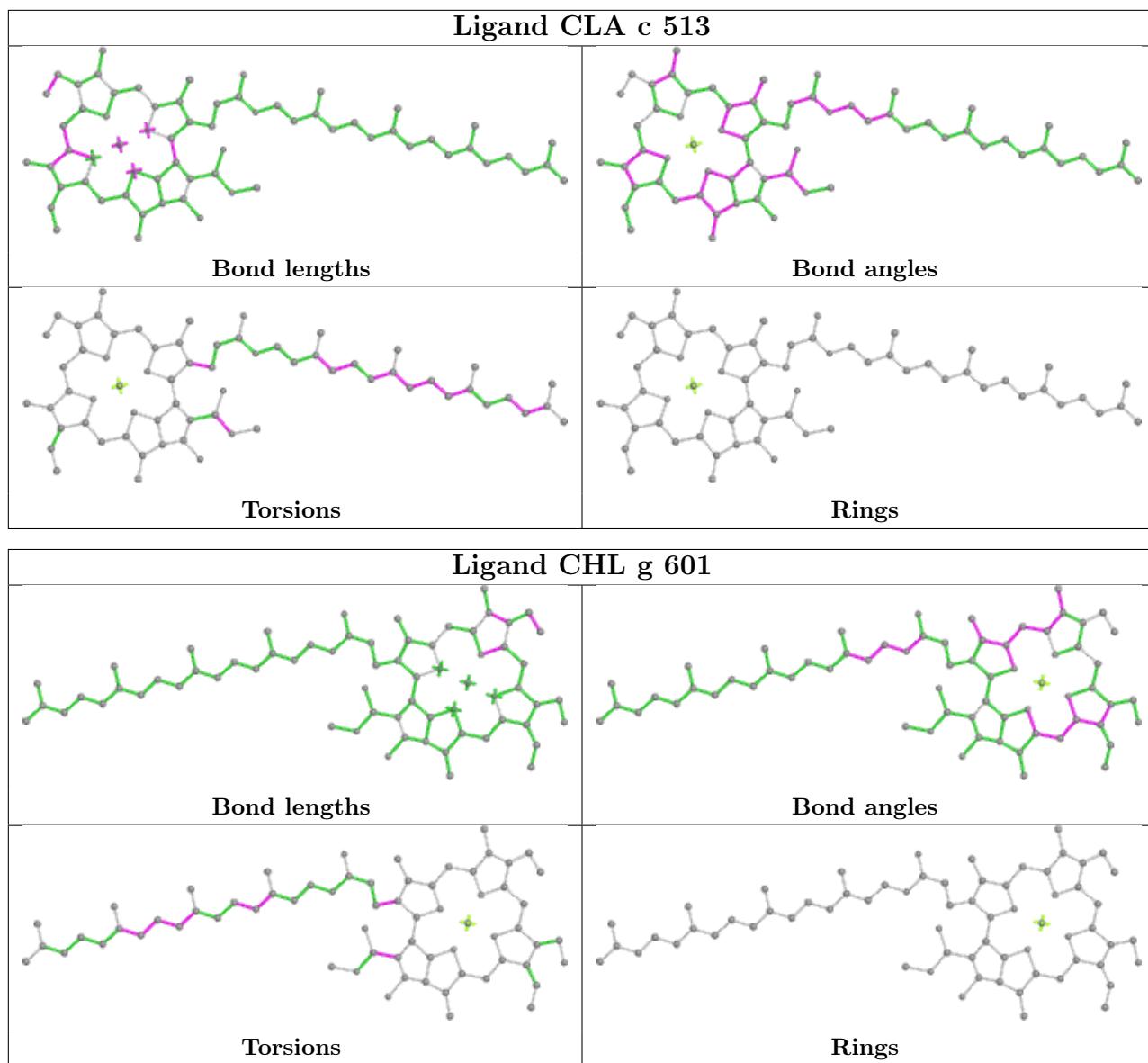


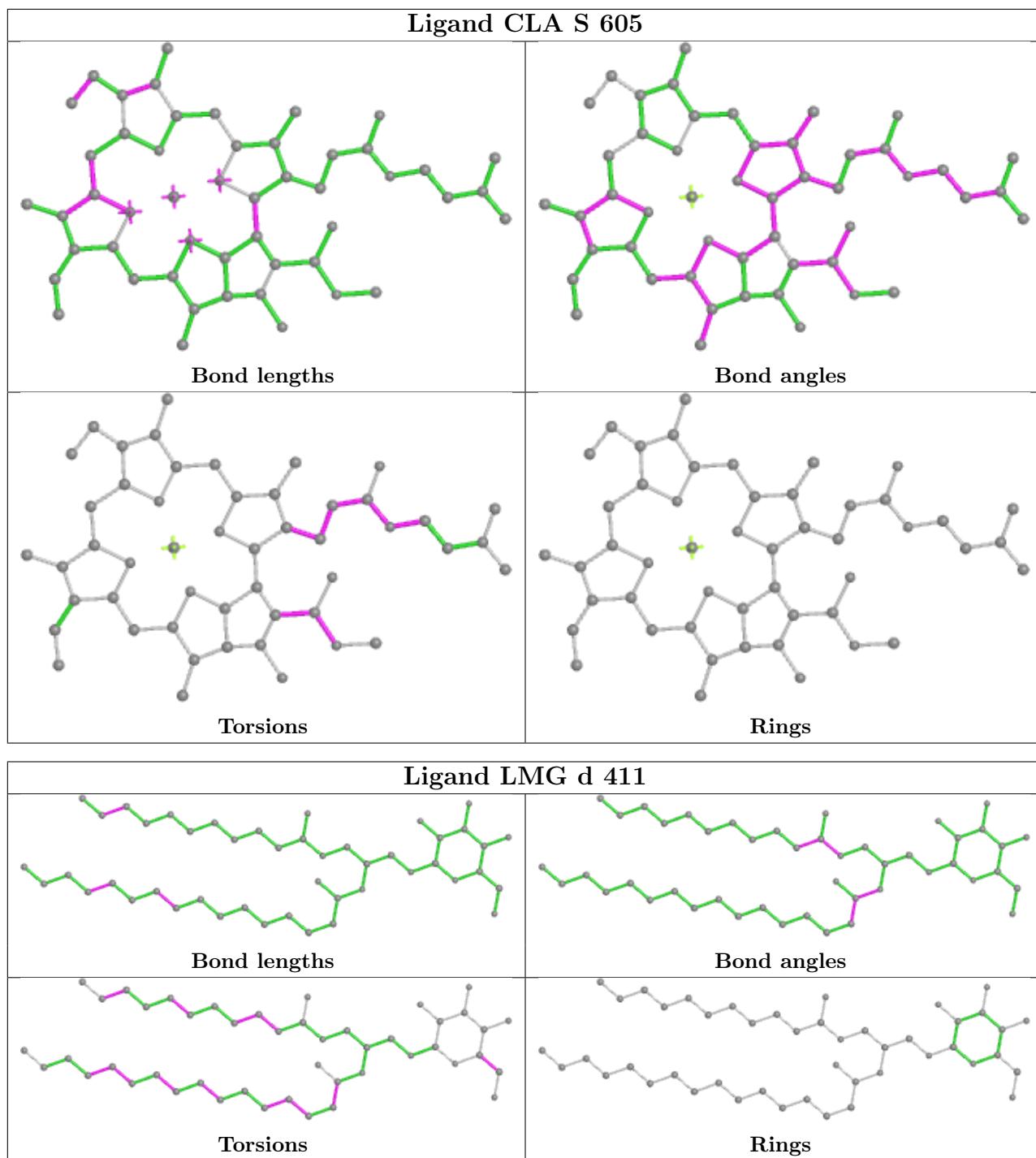


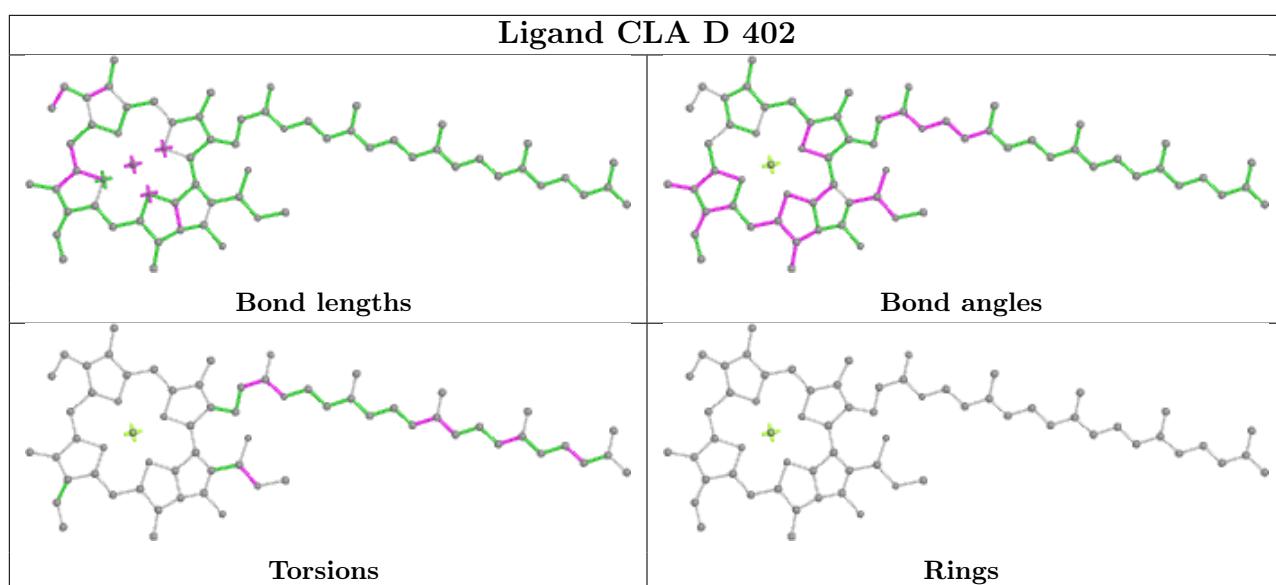
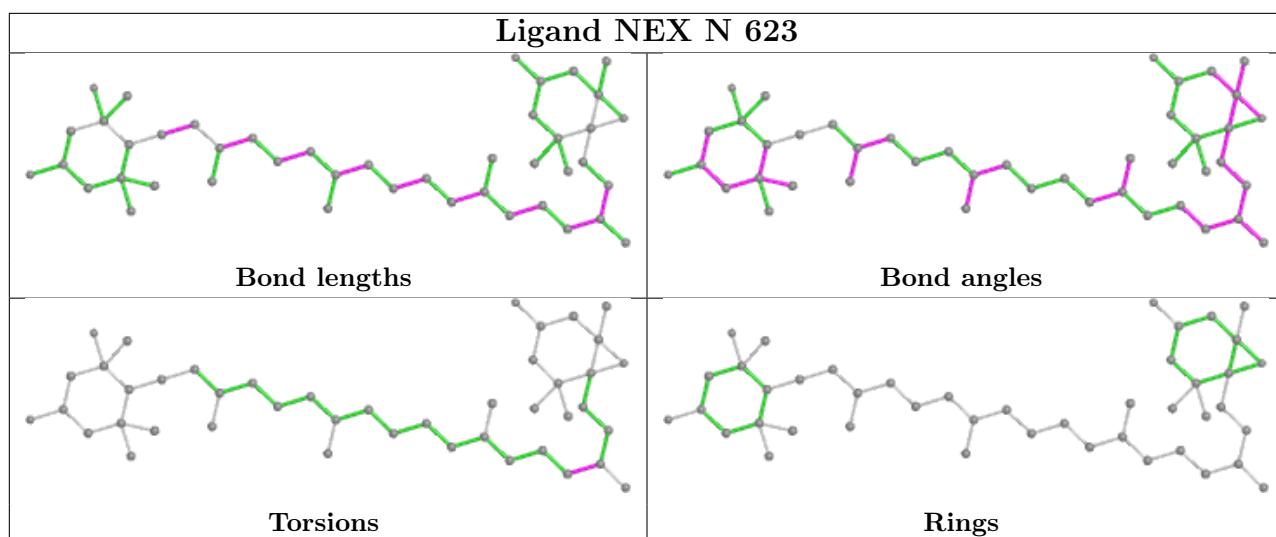


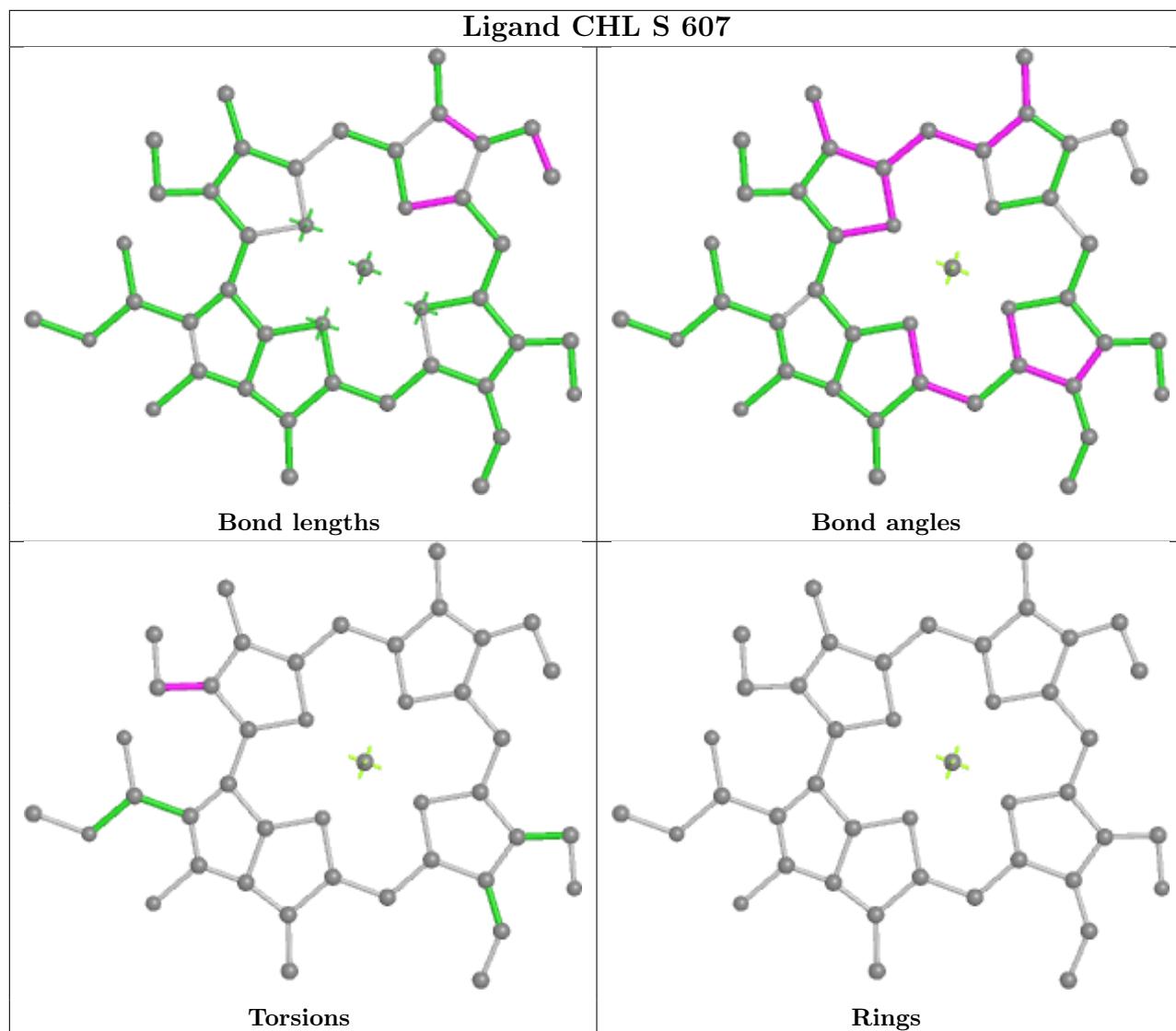












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

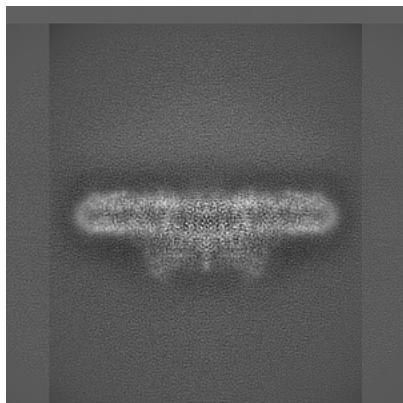
6 Map visualisation (i)

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

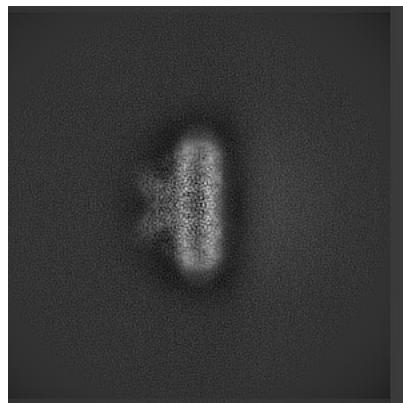
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

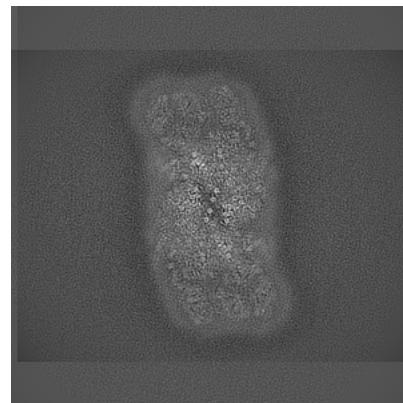
6.1.1 Primary map



X



Y

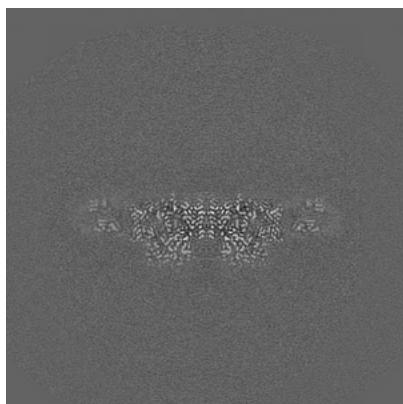


Z

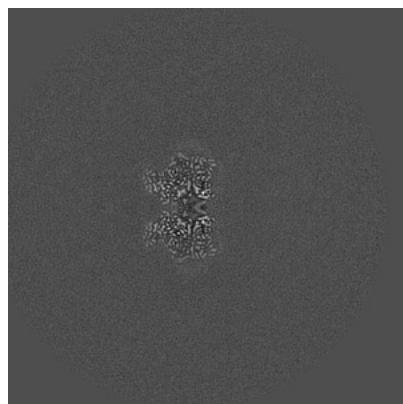
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

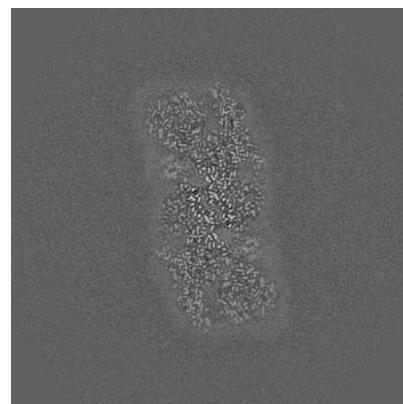
6.2.1 Primary map



X Index: 250



Y Index: 250

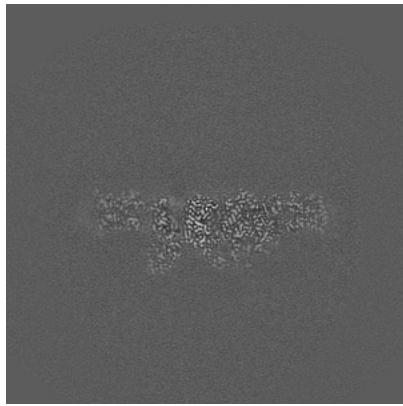


Z Index: 250

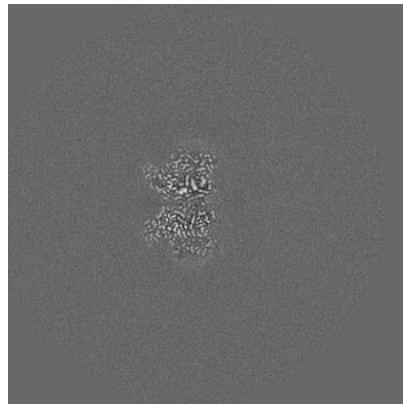
The images above show central slices of the map in three orthogonal directions.

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

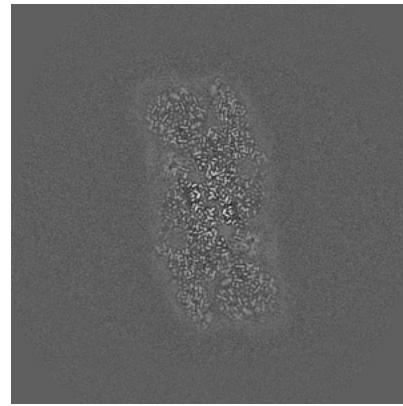
6.3.1 Primary map



X Index: 268



Y Index: 248

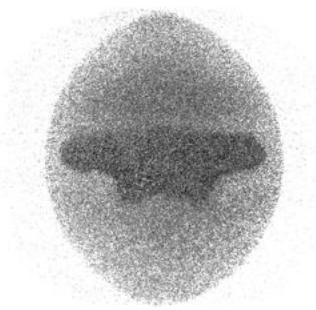


Z Index: 249

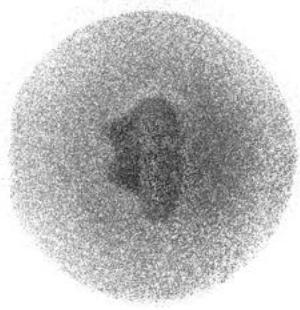
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [\(i\)](#)

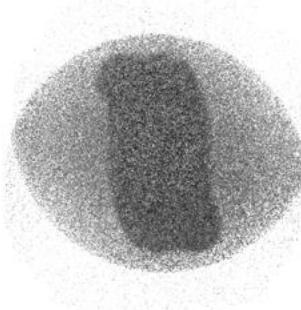
6.4.1 Primary map



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.

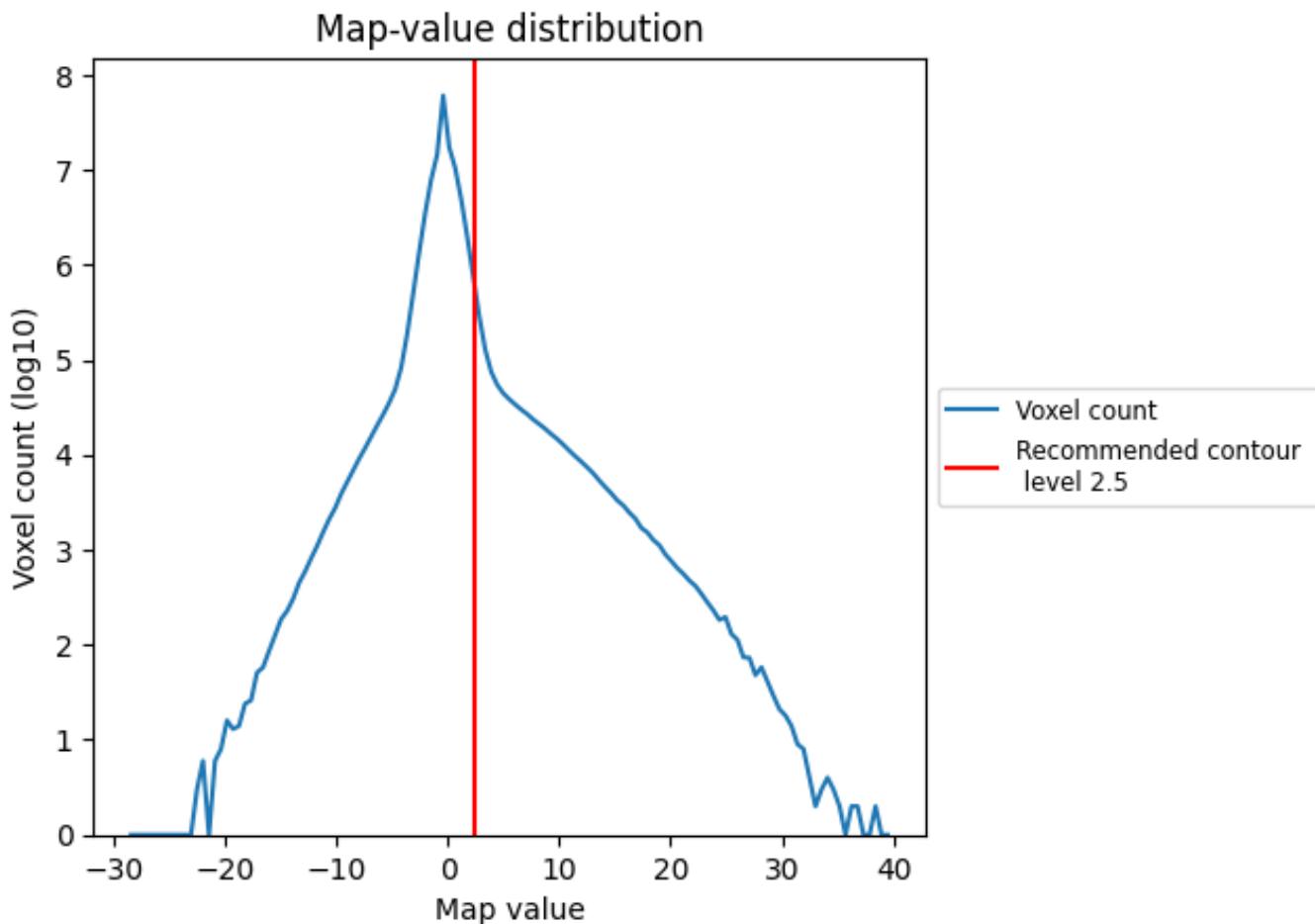
6.5 Mask visualisation

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

7 Map analysis (i)

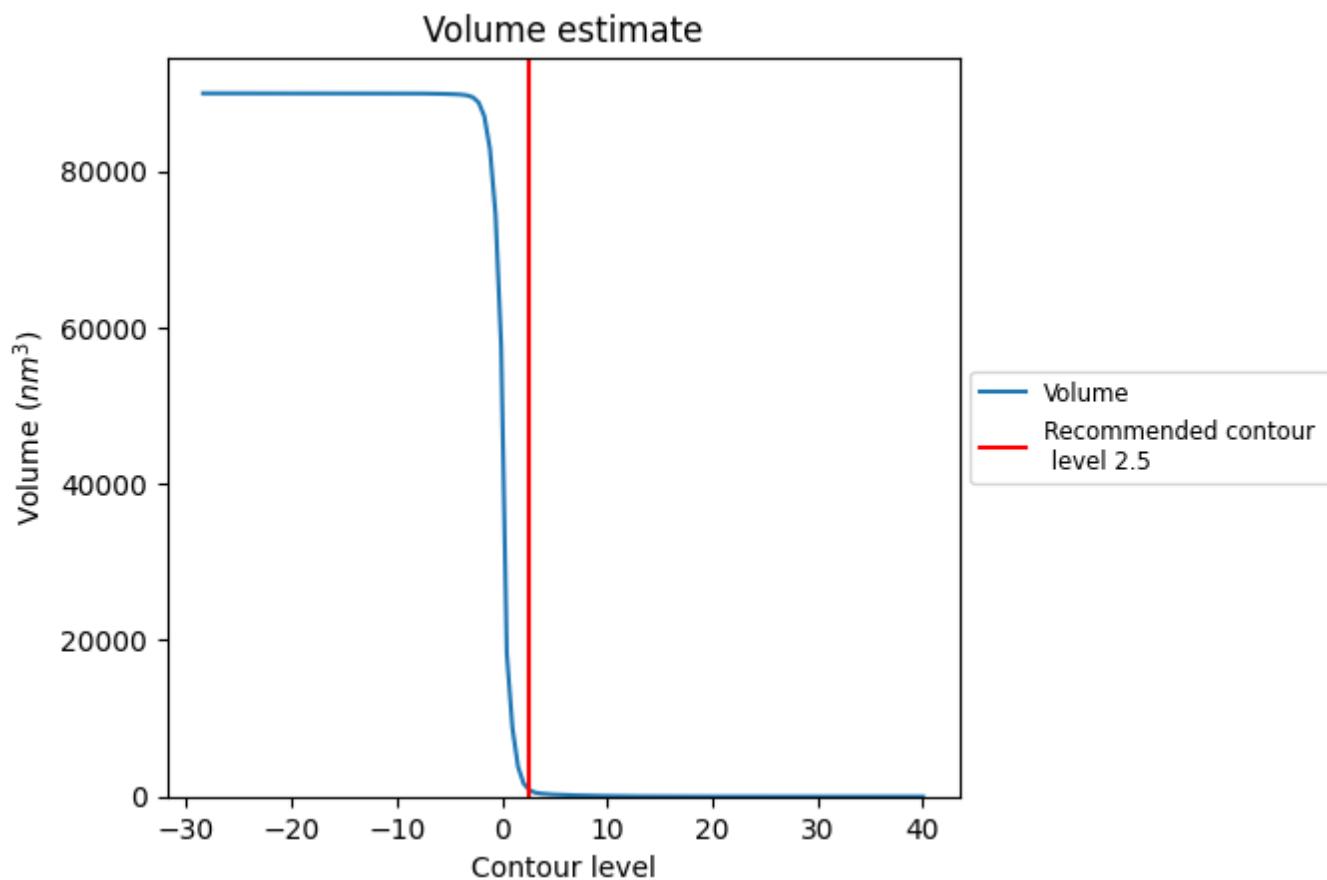
This section contains the results of statistical analysis of the map.

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.

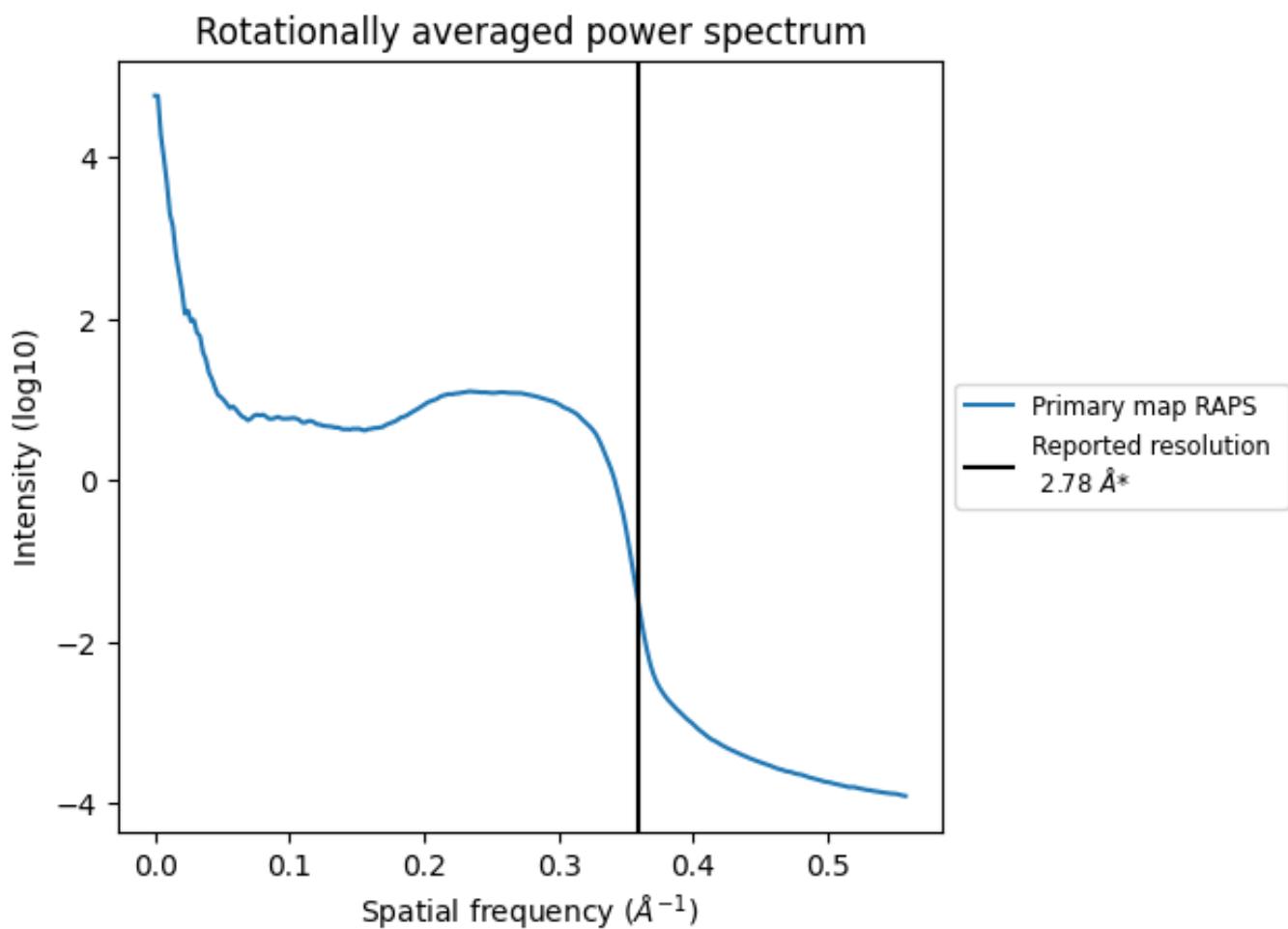
7.2 Volume estimate (i)



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

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

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

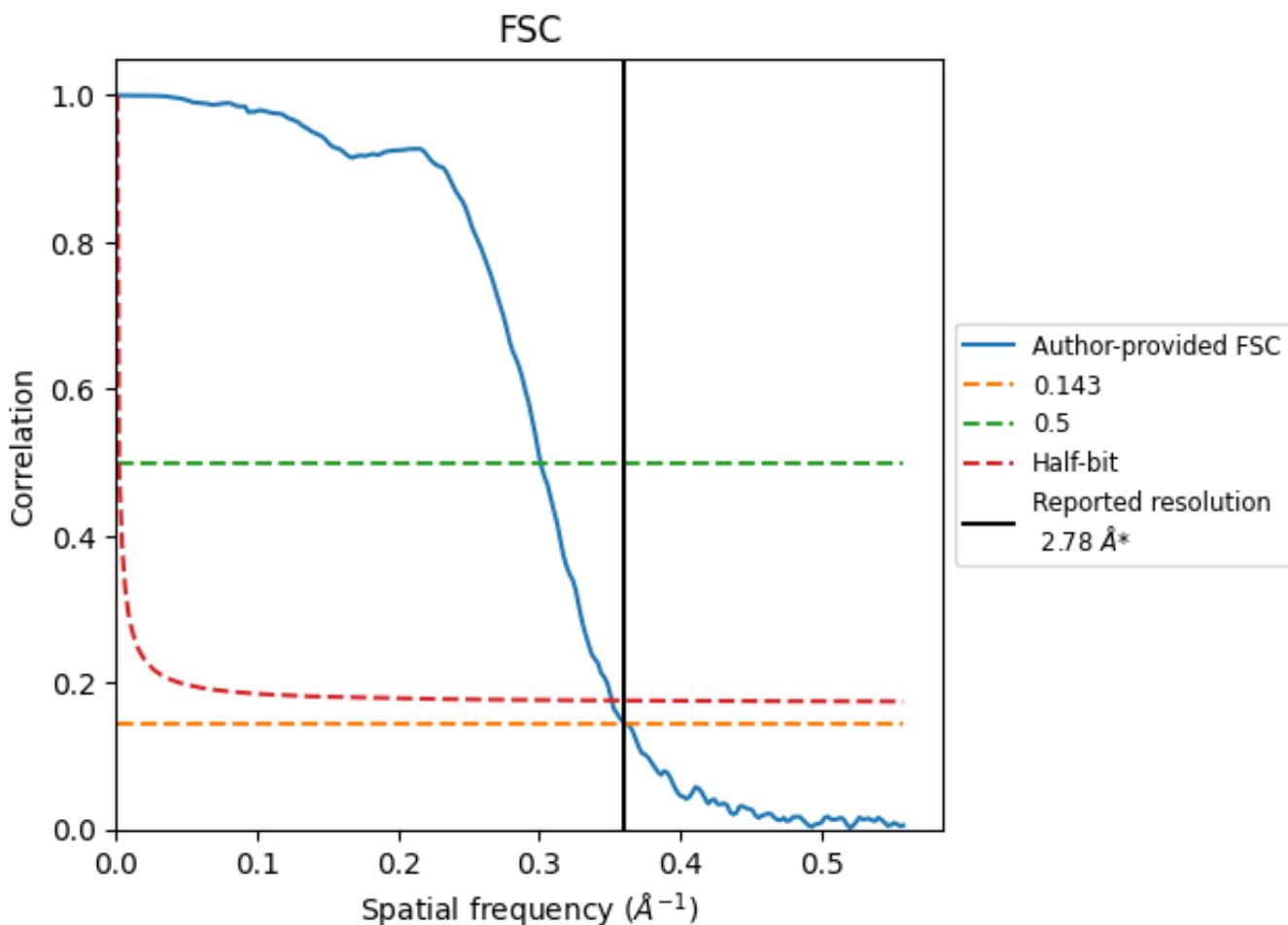


*Reported resolution corresponds to spatial frequency of 0.360 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

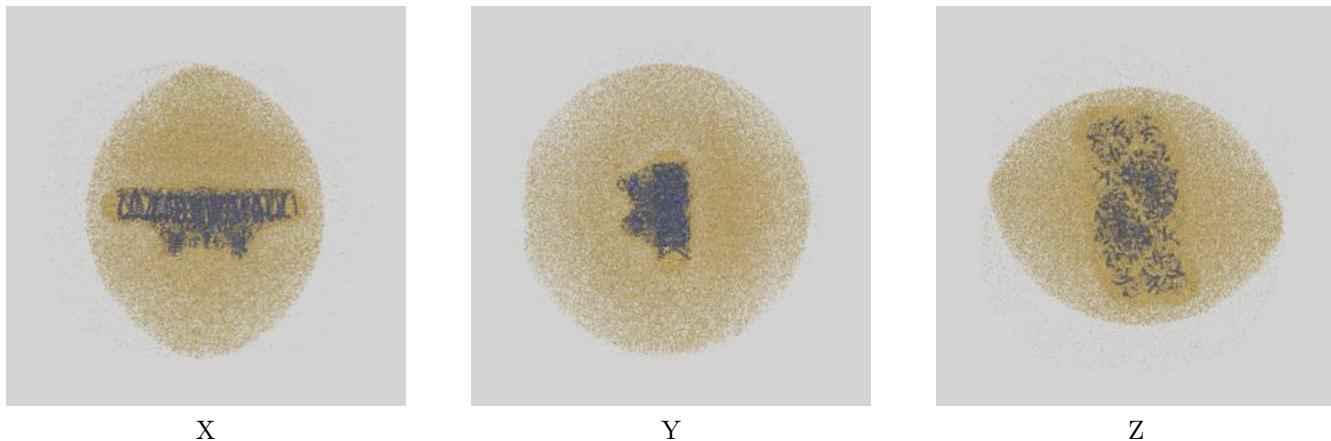
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.77	3.32	2.85
Unmasked-calculated*	-	-	-

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

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

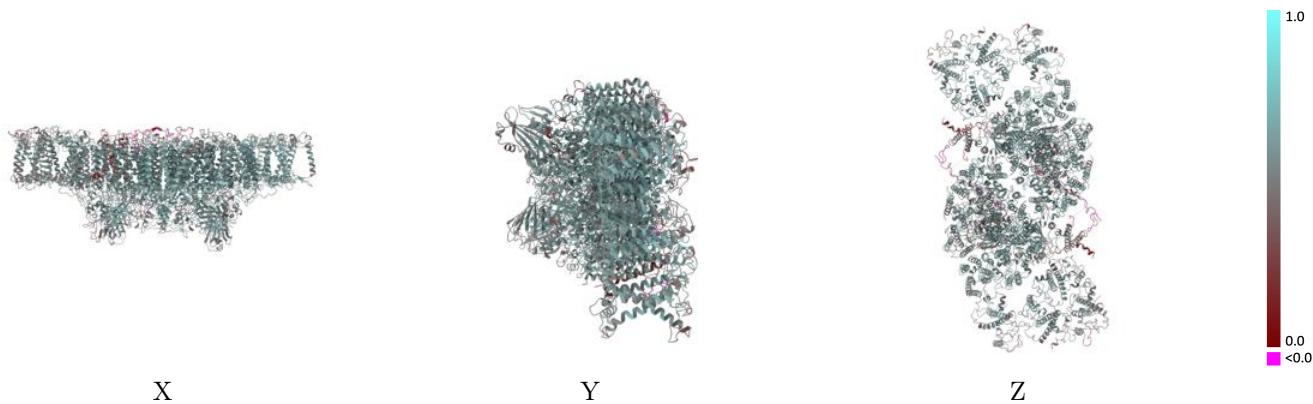
This section contains information regarding the fit between EMDB map EMD-13430 and PDB model 7PI5. Per-residue inclusion information can be found in section [3](#) on page [49](#).

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



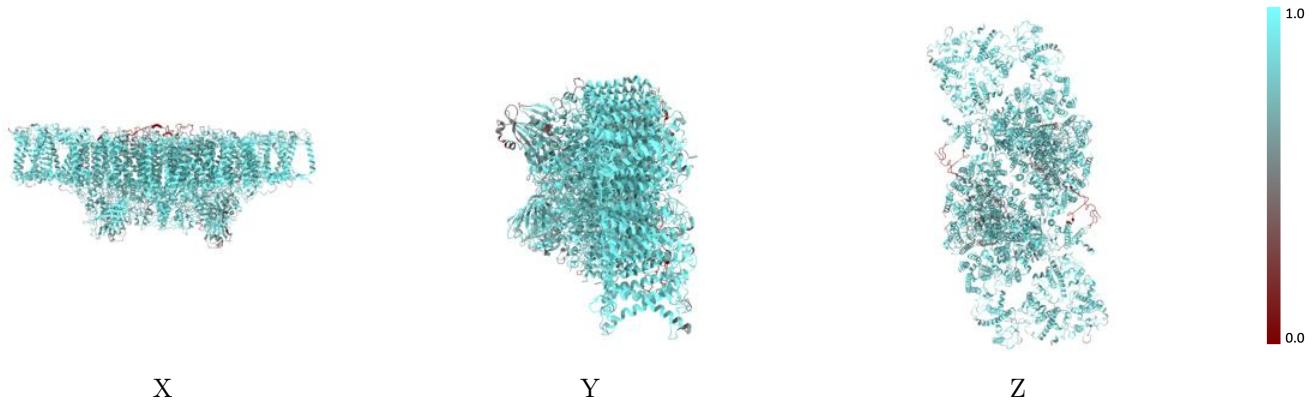
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



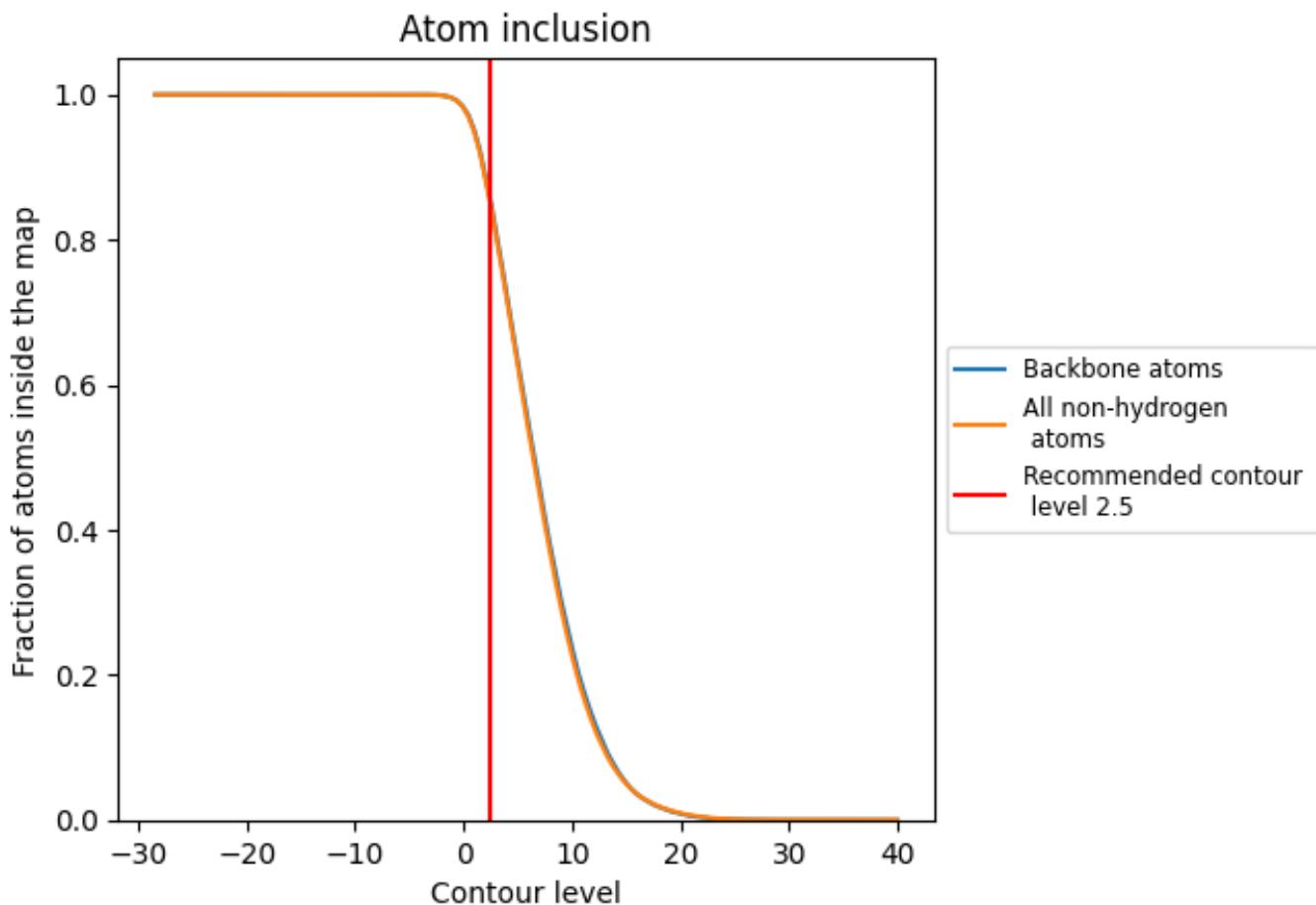
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion [\(i\)](#)



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

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.8488	0.5420
A	0.8524	0.5510
B	0.9214	0.5880
C	0.8768	0.5650
D	0.8959	0.5800
E	0.8729	0.5320
F	0.8497	0.5380
G	0.7994	0.4950
H	0.8773	0.5610
I	0.8804	0.5740
J	0.8170	0.5330
K	0.8703	0.5590
L	0.9352	0.5800
M	0.9132	0.5710
N	0.8079	0.5170
O	0.8095	0.4940
P	0.6310	0.4770
R	0.6807	0.3480
S	0.8071	0.5130
T	0.9298	0.5740
U	0.6606	0.4280
V	0.8400	0.5450
W	0.8196	0.5230
X	0.7861	0.5080
Y	0.8587	0.5380
Z	0.8703	0.5380
a	0.8719	0.5630
b	0.9228	0.5900
c	0.8992	0.5810
d	0.9148	0.5920
e	0.8762	0.5540
f	0.8986	0.5730
g	0.8356	0.5390
h	0.8910	0.5730
i	0.9472	0.5810



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Chain	Atom inclusion	Q-score
j	0.8464	0.5670
k	0.8771	0.5850
l	0.9324	0.5910
m	0.9050	0.5660
n	0.8517	0.5550
o	0.8457	0.5340
p	0.6148	0.4980
r	0.6647	0.3580
s	0.8424	0.5460
t	0.9174	0.5760
u	0.7477	0.4740
v	0.8756	0.5630
w	0.8593	0.5380
x	0.8259	0.5260
y	0.8811	0.5690
z	0.9011	0.5730