



wwPDB EM Validation Summary Report i

Dec 18, 2022 – 09:42 pm GMT

PDB ID : 7OUI
EMDB ID : EMD-13078
Title : Structure of C2S2M2-type Photosystem supercomplex from *Arabidopsis thaliana* (digitonin-extracted)
Authors : Graca, A.T.; Hall, M.; Persson, K.; Schroder, W.P.
Deposited on : 2021-06-11
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the 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:

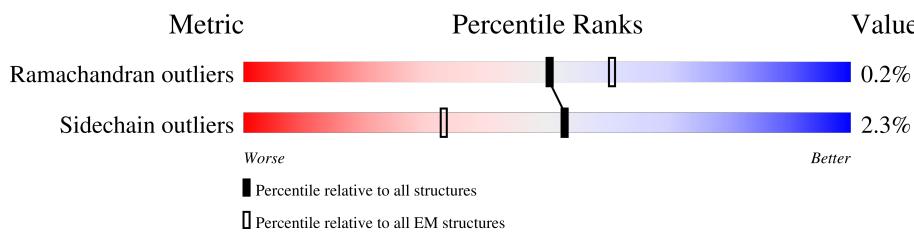
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

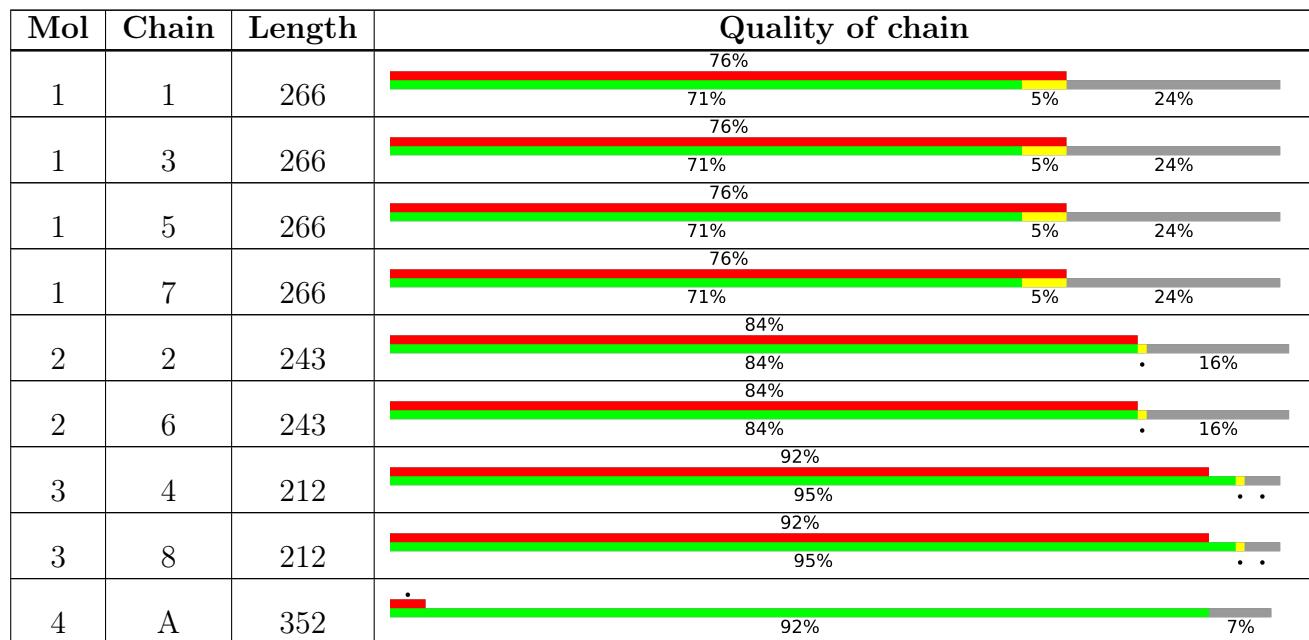
The reported resolution of this entry is 2.79 Å.

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.



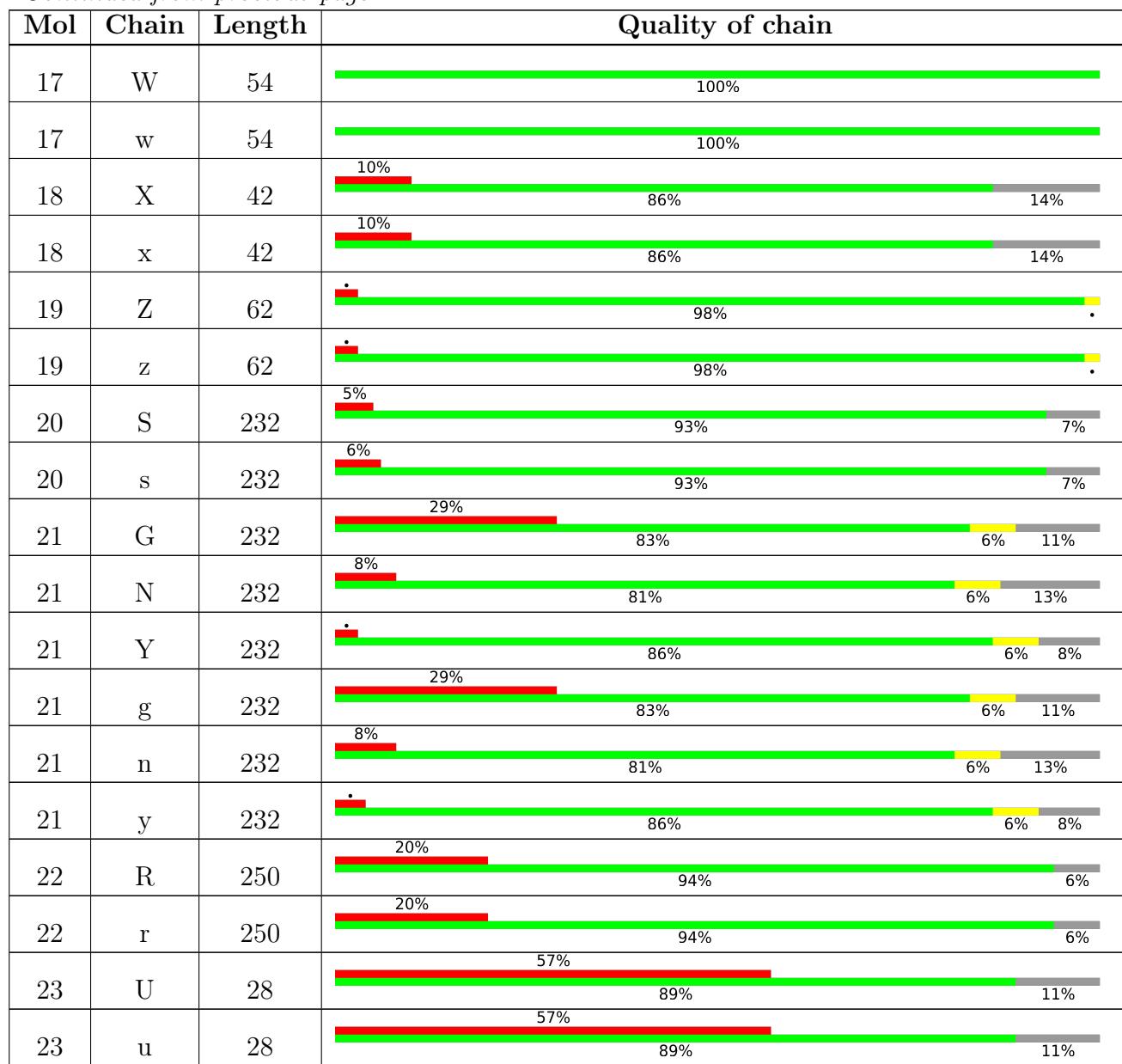
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Mol	Chain	Length	Quality of chain	
4	a	352	92%	7%
5	B	508	95%	.
5	b	508	95%	.
6	C	459	94%	6%
6	c	459	94%	6%
7	D	352	97%	.
7	d	352	97%	.
8	E	83	80%	20%
8	e	83	80%	20%
9	F	39	74%	26%
9	f	39	74%	26%
10	H	72	83%	17%
10	h	72	83%	17%
11	I	36	97%	.
11	i	36	97%	.
12	K	37	100%	
12	k	37	100%	
13	L	38	95%	5%
13	l	38	95%	5%
14	M	34	91%	6%
14	m	34	91%	6%
15	O	247	79%	20%
15	o	247	79%	20%
16	T	33	88%	12%
16	t	33	88%	12%

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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
24	CHL	1	301	X	-	-	-
24	CHL	1	302	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	603	X	-	-	-
24	CHL	5	301	X	-	-	-
24	CHL	5	302	X	-	-	-
24	CHL	6	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	6	603	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	605	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	613	X	-	-	-
24	CHL	S	302	X	-	-	-
24	CHL	S	306	X	-	-	-
24	CHL	S	307	X	-	-	-
24	CHL	S	308	X	-	-	-
24	CHL	Y	302	X	-	-	-
24	CHL	Y	306	X	-	-	-
24	CHL	Y	307	X	-	-	-
24	CHL	Y	308	X	-	-	-
24	CHL	Y	309	X	-	-	-
24	CHL	Y	310	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	605	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	r	613	X	-	-	-
24	CHL	s	302	X	-	-	-
24	CHL	s	306	X	-	-	-
24	CHL	s	307	X	-	-	-
24	CHL	s	308	X	-	-	-
24	CHL	y	302	X	-	-	-
24	CHL	y	306	X	-	-	-
24	CHL	y	307	X	-	-	-
24	CHL	y	308	X	-	-	-
24	CHL	y	309	X	-	-	-
24	CHL	y	310	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	605	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	A	401	X	-	-	-
25	CLA	A	402	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	608	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	614	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	304	X	-	-	-
25	CLA	S	305	X	-	-	-
25	CLA	S	309	X	-	-	-
25	CLA	S	310	X	-	-	-
25	CLA	S	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	S	314	X	-	-	-
25	CLA	Y	303	X	-	-	-
25	CLA	Y	304	X	-	-	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	311	X	-	-	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-
25	CLA	a	403	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	608	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	614	X	-	-	-
25	CLA	s	303	X	-	-	-
25	CLA	s	304	X	-	-	-
25	CLA	s	305	X	-	-	-
25	CLA	s	309	X	-	-	-
25	CLA	s	310	X	-	-	-
25	CLA	s	311	X	-	-	-
25	CLA	s	312	X	-	-	-
25	CLA	s	313	X	-	-	-
25	CLA	s	314	X	-	-	-
25	CLA	y	303	X	-	-	-
25	CLA	y	304	X	-	-	-
25	CLA	y	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	y	311	X	-	-	-
25	CLA	y	312	X	-	-	-
25	CLA	y	313	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-

2 Entry composition [\(i\)](#)

There are 42 unique types of molecules in this entry. The entry contains 85897 atoms, of which 1470 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 Lhcb1.4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	3	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	5	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		
1	7	202	Total	C	N	O	S	0	0
			1537	996	250	286	5		

- Molecule 2 is a protein called Lhcb3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		
2	6	205	Total	C	N	O	S	0	0
			1593	1040	258	290	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
3	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		
4	a	326	Total	C	N	O	S	0	0
			2548	1664	419	452	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	487	3810	2495	644	659	12	0	0
5	b	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	433	3373	2221	563	578	11	0	0
6	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	342	2722	1800	445	465	12	0	0
7	d	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
8	E	66	543	357	88	98		0	0
8	e	66	Total	C	N	O		0	0
			543	357	88	98			

- Molecule 9 is a protein called Cytochrome b559 subunit beta (PsbF).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	29	224	147	40	36	1	0	0
9	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	60	Total	C	N	O	S	
			446	293	70	81	2	0

Mol	Chain	Residues	Atoms				AltConf	Trace
10	h	60	Total	C	N	O	S	
			446	293	70	81	2	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	I	35	Total	C	N	O	S	
			286	195	44	46	1	0

Mol	Chain	Residues	Atoms				AltConf	Trace
11	i	35	Total	C	N	O	S	
			286	195	44	46	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	K	37	Total	C	N	O	S	
			301	211	44	45	1	0

Mol	Chain	Residues	Atoms				AltConf	Trace
12	k	37	Total	C	N	O	S	
			301	211	44	45	1	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	36	Total	C	N	O		
			302	200	47	55	0	0

Mol	Chain	Residues	Atoms				AltConf	Trace
13	l	36	Total	C	N	O		
			302	200	47	55	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	32	Total	C	N	O	S	
			250	173	35	41	1	0

Mol	Chain	Residues	Atoms				AltConf	Trace
14	m	32	Total	C	N	O	S	
			250	173	35	41	1	0

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	197	Total	C	N	O	S	
			1516	969	241	302	4	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	197	1516	969	241	302	4	0	0

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

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

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

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

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
18	X	36	248	162	39	47		0	0
18	x	36	248	162	39	47		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	62	464	313	69	81	1	0	0
19	z	62	464	313	69	81	1	0	0

- Molecule 20 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	216	1670	1091	272	303	4	0	0
20	s	216	1670	1091	272	303	4	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	206	Total	C	N	O	S		
			1562	1010	255	292	5	0	0
21	N	202	Total	C	N	O	S		
			1536	994	251	286	5	0	0
21	Y	213	Total	C	N	O	S		
			1621	1048	266	302	5	0	0
21	g	206	Total	C	N	O	S		
			1562	1010	255	292	5	0	0
21	n	202	Total	C	N	O	S		
			1536	994	251	286	5	0	0
21	y	213	Total	C	N	O	S		
			1621	1048	266	302	5	0	0

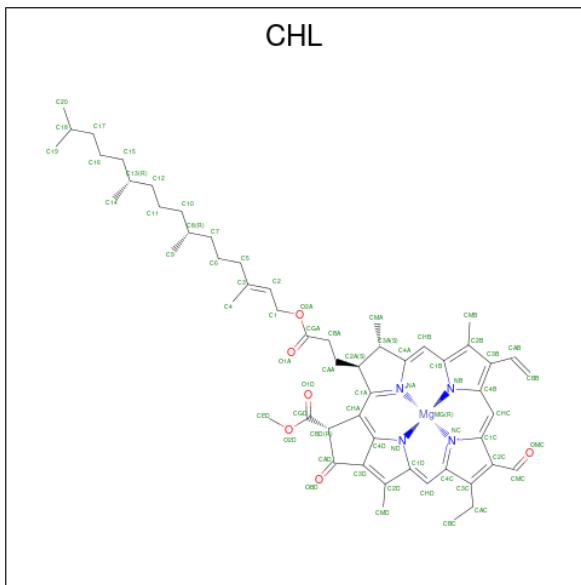
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	235	Total	C	N	O	S		
			1827	1183	298	343	3	0	0
22	r	235	Total	C	N	O	S		
			1827	1183	298	343	3	0	0

- Molecule 23 is a protein called PsbTn.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	25	Total	C	N	O	S		
			194	122	36	33	3	0	0
23	u	25	Total	C	N	O	S		
			194	122	36	33	3	0	0

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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Mol	Chain	Residues	Atoms						AltConf
24	N	1	Total	C	Mg	N	O		0
			348	282	6	24	36		
24	N	1	Total	C	Mg	N	O		0
			348	282	6	24	36		
24	N	1	Total	C	Mg	N	O		0
			348	282	6	24	36		
24	N	1	Total	C	Mg	N	O		0
			348	282	6	24	36		
24	N	1	Total	C	Mg	N	O		0
			348	282	6	24	36		
24	Y	1	Total	C	Mg	N	O		0
			344	278	6	24	36		
24	Y	1	Total	C	Mg	N	O		0
			344	278	6	24	36		
24	Y	1	Total	C	Mg	N	O		0
			344	278	6	24	36		
24	Y	1	Total	C	Mg	N	O		0
			344	278	6	24	36		
24	Y	1	Total	C	Mg	N	O		0
			344	278	6	24	36		
24	R	1	Total	C	Mg	N	O		0
			195	153	4	16	22		
24	R	1	Total	C	Mg	N	O		0
			195	153	4	16	22		
24	R	1	Total	C	Mg	N	O		0
			195	153	4	16	22		
24	R	1	Total	C	Mg	N	O		0
			195	153	4	16	22		
24	5	1	Total	C	Mg	N	O		0
			92	70	2	8	12		
24	5	1	Total	C	Mg	N	O		0
			92	70	2	8	12		
24	6	1	Total	C	Mg	N	O		0
			110	88	2	8	12		
24	6	1	Total	C	Mg	N	O		0
			110	88	2	8	12		
24	s	1	Total	C	Mg	N	O		0
			184	140	4	16	24		

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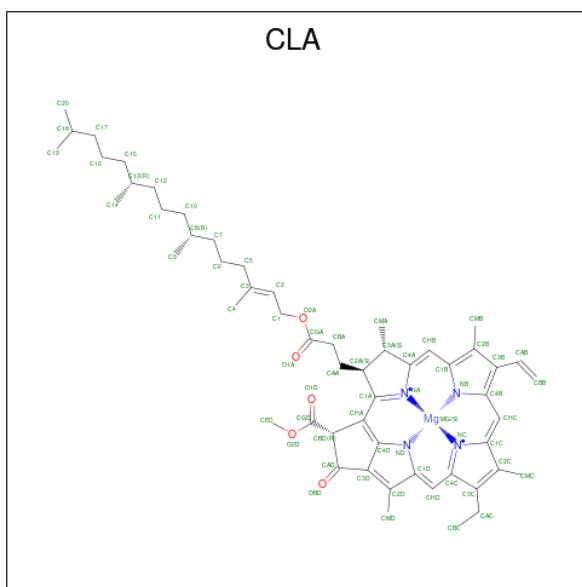
Mol	Chain	Residues	Atoms					AltConf
24	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
24	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
24	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			335	269	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			348	282	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			348	282	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			348	282	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			348	282	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			348	282	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			344	278	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total 195	C 153	Mg 4	N 16	O 22	0
24	r	1	Total 195	C 153	Mg 4	N 16	O 22	0
24	r	1	Total 195	C 153	Mg 4	N 16	O 22	0
24	r	1	Total 195	C 153	Mg 4	N 16	O 22	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 163	C 133	Mg 3	N 12	O 15	0
25	2	1	Total 163	C 133	Mg 3	N 12	O 15	0
25	2	1	Total 163	C 133	Mg 3	N 12	O 15	0
25	A	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	A	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	A	1	Total 190	C 160	Mg 3	N 12	O 15	0
25	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			840	710	13	52	65	

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Mol	Chain	Residues	Atoms						AltConf
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	C	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	D	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	D	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	D	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	S	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	G	1	Total	C	Mg	N	O		0
			472	392	8	32	40		
25	G	1	Total	C	Mg	N	O		0
			472	392	8	32	40		

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Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	a	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
25	a	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
25	a	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			840	710	13	52	65	

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Mol	Chain	Residues	Atoms						AltConf
25	c	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	c	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	c	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	c	1	Total	C	Mg	N	O		0
			840	710	13	52	65		
25	d	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	d	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	d	1	Total	C	Mg	N	O		0
			180	150	3	12	15		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	s	1	Total	C	Mg	N	O		0
			465	375	9	36	45		
25	g	1	Total	C	Mg	N	O		0
			472	392	8	32	40		
25	g	1	Total	C	Mg	N	O		0
			472	392	8	32	40		
25	g	1	Total	C	Mg	N	O		0
			472	392	8	32	40		
25	g	1	Total	C	Mg	N	O		0
			472	392	8	32	40		
25	g	1	Total	C	Mg	N	O		0
			472	392	8	32	40		

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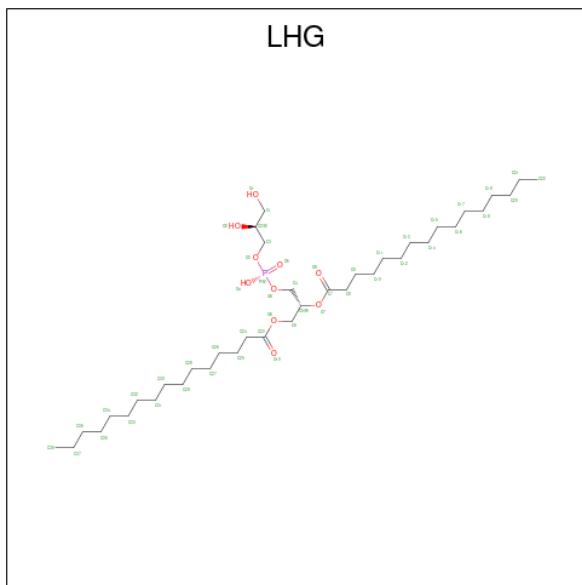
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			470	390	8	32	40	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total 47				0
26	B	1	Total 142				0
26	B	1	Total 142				0

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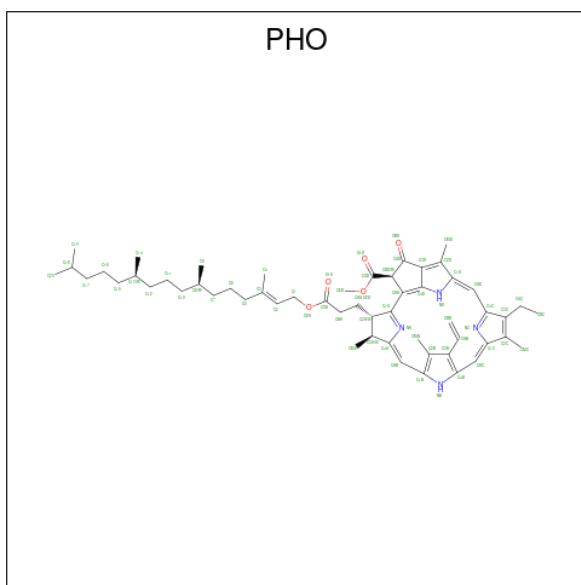
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C O P 142 109 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	C	1	Total C H O P 221 114 74 30 3	0
26	D	1	Total C O P 49 38 10 1	0
26	L	1	Total C O P 49 38 10 1	0
26	S	1	Total C O P 98 76 20 2	0
26	S	1	Total C O P 98 76 20 2	0
26	N	1	Total C O P 49 38 10 1	0
26	Y	1	Total C O P 98 76 20 2	0
26	Y	1	Total C O P 98 76 20 2	0
26	R	1	Total C O P 42 31 10 1	0
26	6	1	Total C O P 47 36 10 1	0
26	b	1	Total C O P 142 109 30 3	0
26	b	1	Total C O P 142 109 30 3	0
26	b	1	Total C O P 142 109 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	c	1	Total C H O P 221 114 74 30 3	0
26	d	1	Total C O P 49 38 10 1	0
26	l	1	Total C O P 49 38 10 1	0

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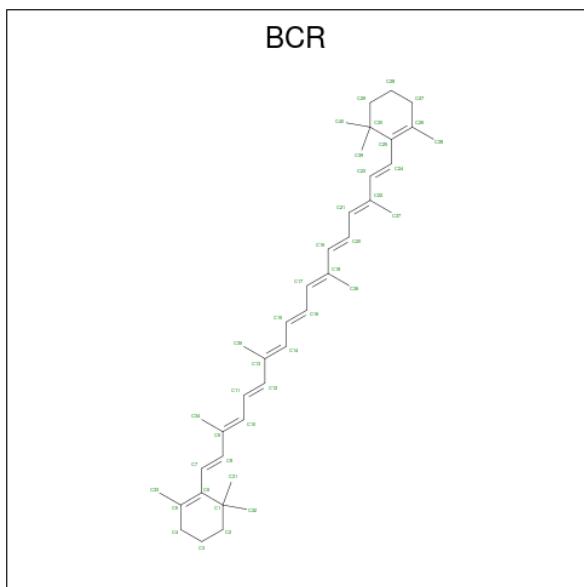
Mol	Chain	Residues	Atoms				AltConf
26	s	1	Total	C	O	P	0
			98	76	20	2	
26	s	1	Total	C	O	P	0
			98	76	20	2	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			98	76	20	2	
26	y	1	Total	C	O	P	0
			98	76	20	2	
26	r	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 27 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



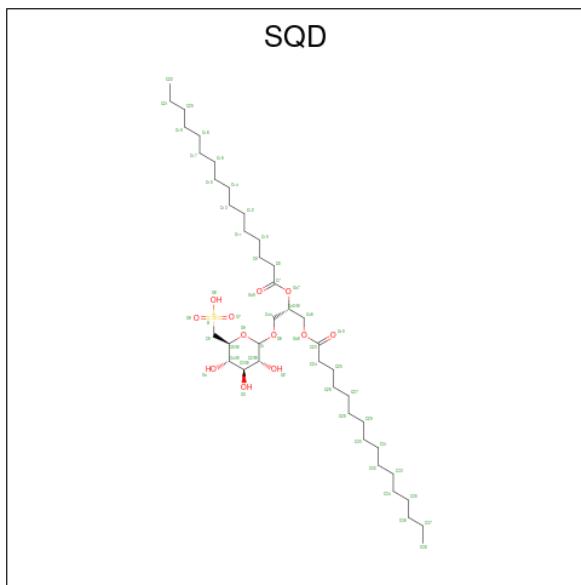
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 120 120	0
28	B	1	Total C 120 120	0
28	B	1	Total C 120 120	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	H	1	Total C 40 40	0
28	I	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	T	1	Total C 40 40	0
28	Z	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 120 120	0
28	b	1	Total C 120 120	0

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Mol	Chain	Residues	Atoms	AltConf
28	b	1	Total C 120 120	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	i	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0
28	z	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



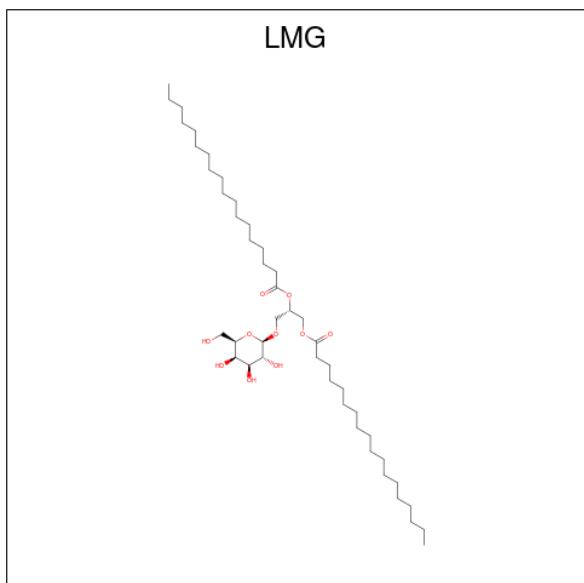
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O S 104 78 24 2	0
29	A	1	Total C O S 104 78 24 2	0
29	L	1	Total C O S 96 70 24 2	0

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Mol	Chain	Residues	Atoms				AltConf
29	L	1	Total	C	O	S	0
			96	70	24	2	
29	a	1	Total	C	O	S	0
			104	78	24	2	
29	a	1	Total	C	O	S	0
			104	78	24	2	
29	l	1	Total	C	O	S	0
			96	70	24	2	
29	l	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



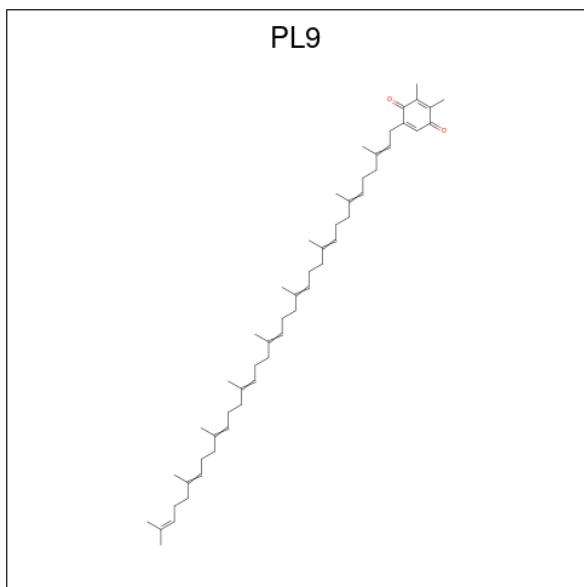
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O		0
			88	68	20		
30	A	1	Total	C	O		0
			88	68	20		
30	B	1	Total	C	O		0
			106	86	20		
30	B	1	Total	C	O		0
			106	86	20		
30	C	1	Total	C	O		0
			51	41	10		
30	D	1	Total	C	O		0
			46	36	10		

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Mol	Chain	Residues	Atoms	AltConf
30	a	1	Total C O 88 68 20	0
30	a	1	Total C O 88 68 20	0
30	b	1	Total C O 106 86 20	0
30	b	1	Total C O 106 86 20	0
30	c	1	Total C O 51 41 10	0
30	d	1	Total C O 46 36 10	0

- Molecule 31 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: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 13 11 2	0
31	D	1	Total C O 55 53 2	0
31	a	1	Total C O 13 11 2	0
31	d	1	Total C O 55 53 2	0

- Molecule 32 is a ligand with the chemical component id AJP but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for AJP. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

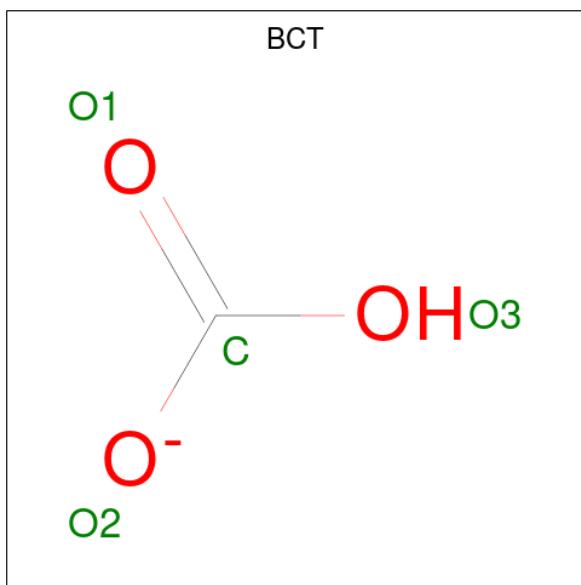
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total 177	C 56	H 92	O 29	0
32	B	1	Total 177	C 56	H 92	O 29	0
32	S	1	Total 95	C 33	H 53	O 9	0
32	G	1	Total 95	C 33	H 53	O 9	0
32	N	1	Total 190	C 66	H 106	O 18	0
32	N	1	Total 190	C 66	H 106	O 18	0
32	Y	1	Total 475	C 165	H 265	O 45	0
32	Y	1	Total 475	C 165	H 265	O 45	0
32	Y	1	Total 475	C 165	H 265	O 45	0
32	Y	1	Total 475	C 165	H 265	O 45	0
32	a	1	Total 177	C 56	H 92	O 29	0
32	b	1	Total 177	C 56	H 92	O 29	0
32	s	1	Total 95	C 33	H 53	O 9	0
32	g	1	Total 95	C 33	H 53	O 9	0
32	n	1	Total 190	C 66	H 106	O 18	0
32	n	1	Total 190	C 66	H 106	O 18	0
32	y	1	Total 475	C 165	H 265	O 45	0
32	y	1	Total 475	C 165	H 265	O 45	0
32	y	1	Total 475	C 165	H 265	O 45	0

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Mol	Chain	Residues	Atoms	AltConf
32	y	1	Total C H O 475 165 265 45	0
32	y	1	Total C H O 475 165 265 45	0

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

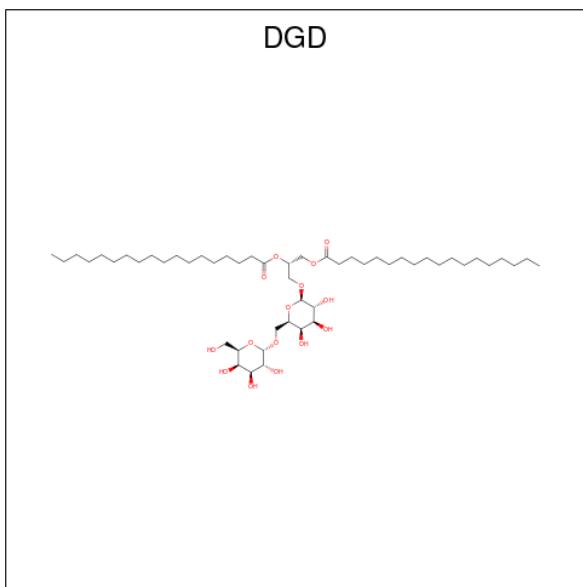


Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 4 1 3	0
33	a	1	Total C O 4 1 3	0

- Molecule 34 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			59	44	15	
35	B	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			117	87	30	
35	C	1	Total	C	O	0
			117	87	30	
35	a	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			117	87	30	
35	c	1	Total	C	O	0
			117	87	30	

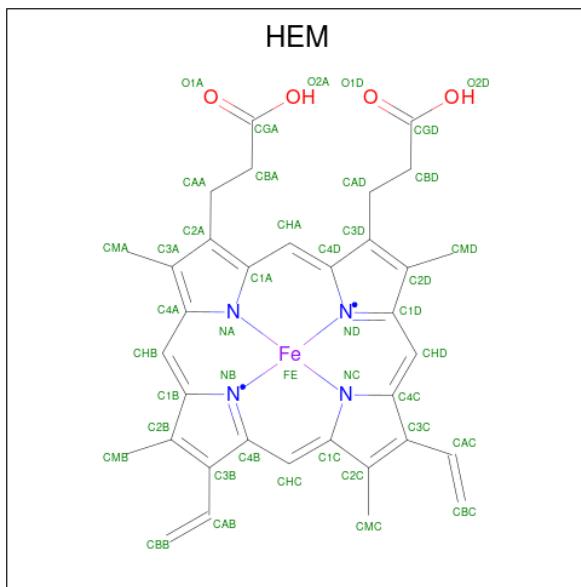
- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	Ca		0
			1	1		
36	B	1	Total	Ca		0
			1	1		
36	a	1	Total	Ca		0
			1	1		
36	b	1	Total	Ca		0
			1	1		

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total 1	Cl 1	0
37	d	1	Total 1	Cl 1	0

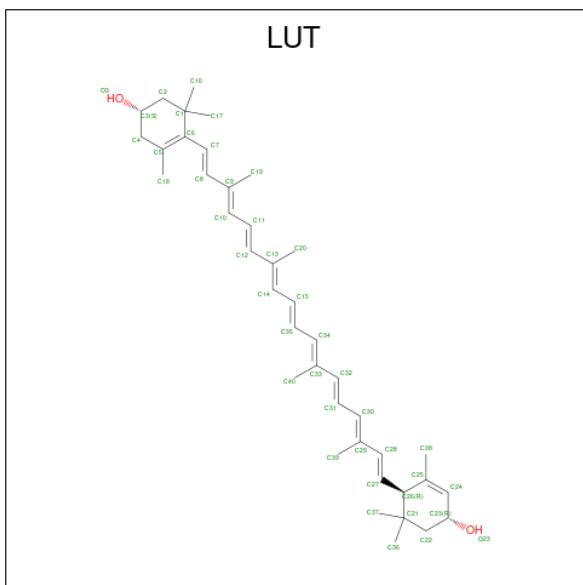
- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



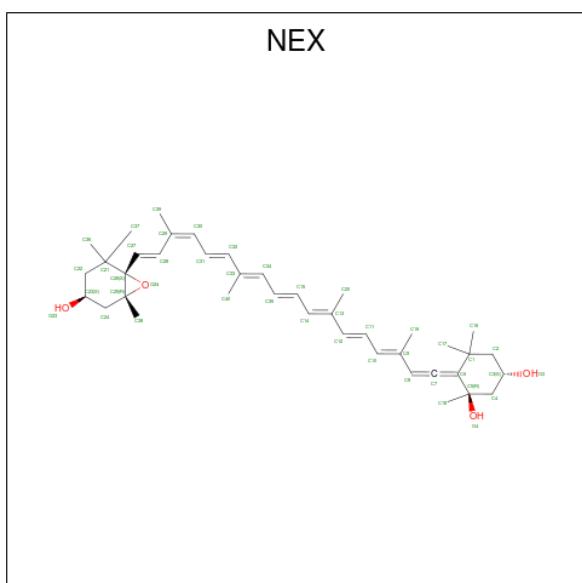
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total 84	C 80	O 4	0
39	S	1	Total 84	C 80	O 4	0
39	G	1	Total 84	C 80	O 4	0
39	G	1	Total 84	C 80	O 4	0
39	N	1	Total 84	C 80	O 4	0
39	N	1	Total 84	C 80	O 4	0
39	Y	1	Total 84	C 80	O 4	0
39	Y	1	Total 84	C 80	O 4	0
39	R	1	Total 42	C 40	O 2	0
39	s	1	Total 84	C 80	O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

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

- Molecule 40 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



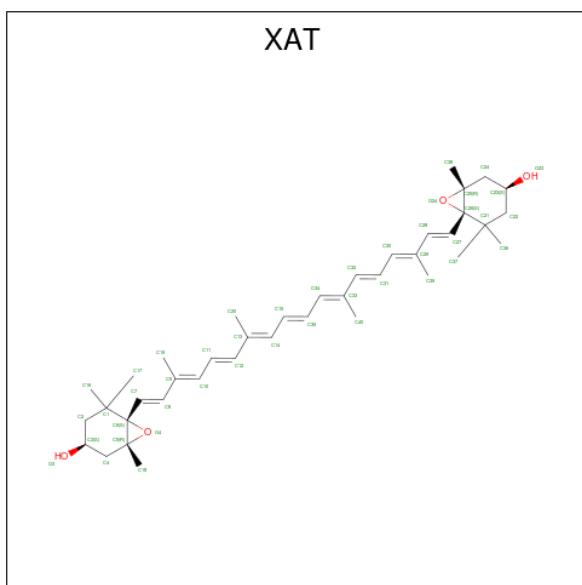
Mol	Chain	Residues	Atoms	AltConf
40	S	1	Total C O 44 40 4	0
40	G	1	Total C O 44 40 4	0
40	N	1	Total C O 44 40 4	0
40	Y	1	Total C O 44 40 4	0
40	R	1	Total C O 44 40 4	0
40	s	1	Total C O 44 40 4	0

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

- Molecule 41 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
41	R	1	Total C O 44 40 4	0
41	r	1	Total C O 44 40 4	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	AltConf
42	A	23	Total O 23 23	0
42	B	10	Total O 10 10	0
42	C	14	Total O 14 14	0

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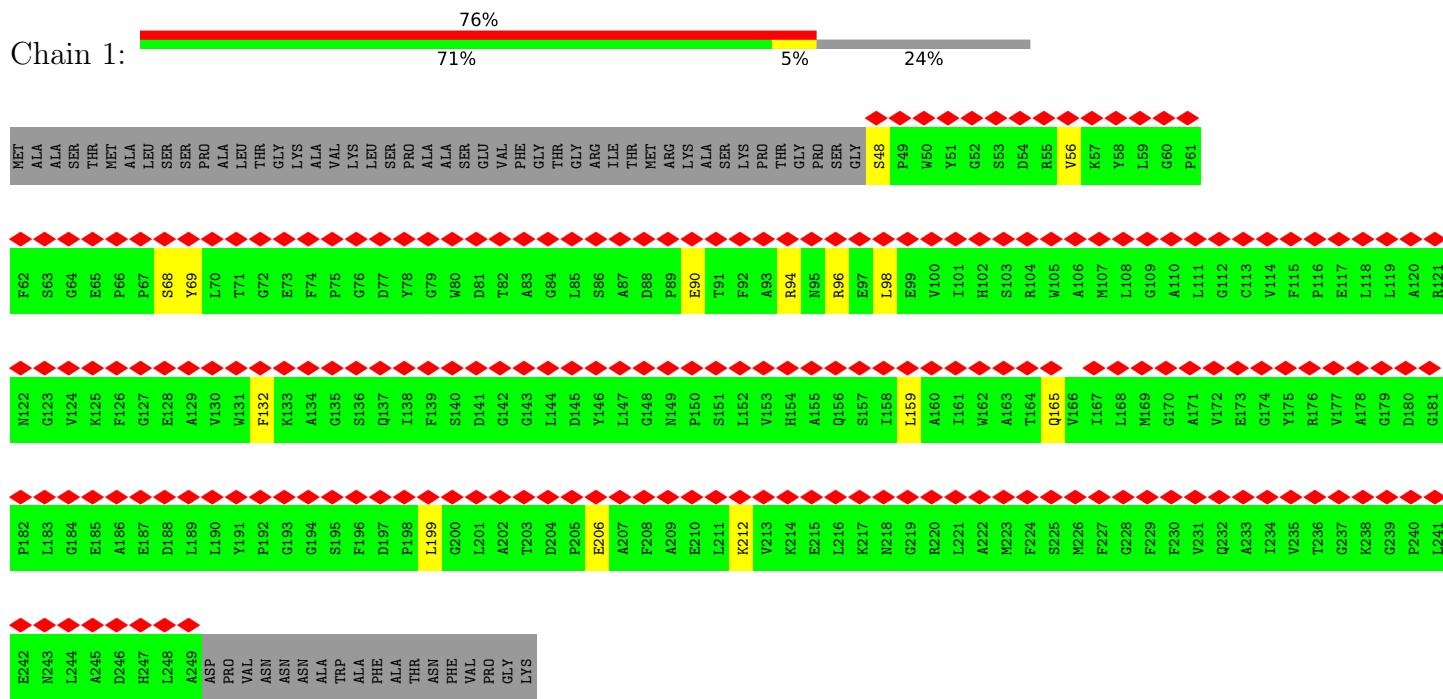
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Mol	Chain	Residues	Atoms	AltConf
42	D	14	Total O 14 14	0
42	H	1	Total O 1 1	0
42	I	1	Total O 1 1	0
42	L	3	Total O 3 3	0
42	M	1	Total O 1 1	0
42	T	1	Total O 1 1	0
42	W	1	Total O 1 1	0
42	a	23	Total O 23 23	0
42	b	10	Total O 10 10	0
42	c	14	Total O 14 14	0
42	d	14	Total O 14 14	0
42	h	1	Total O 1 1	0
42	i	1	Total O 1 1	0
42	l	3	Total O 3 3	0
42	m	2	Total O 2 2	0
42	t	1	Total O 1 1	0
42	w	1	Total O 1 1	0

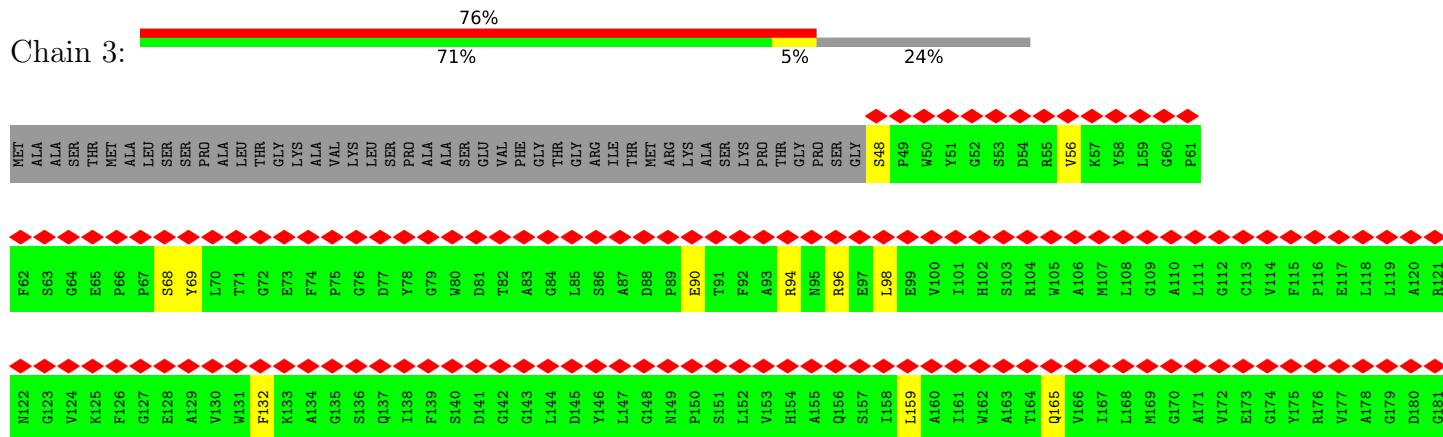
3 Residue-property plots

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

- Molecule 1: Lhcb1.4



- Molecule 1: Lhcb1.4



- Molecule 1: LhcB1.4



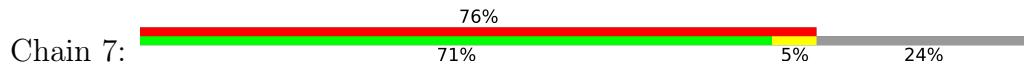
MET	ALA	ALA	ALA	SER	THR	MET	ALA	LEU	SER	SER	PRO	ALA	LEU	THR	GLY	LYS	ALA	VAL	LYS	LEU	SER	PRO	ALA	ALA	SER	GLU	VAL	PHE	GLY	GLY	THR	GLY	ARG	ILE	THR	MET	ARG	LYS	ALA	SER	LYS	PRO	THR	GLY	PRO	SER	GLY	S48	P49	W50	Y51	G52	S53	D54	R55	V56	K57	L59	Y58	D61
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F62	S63	G64	E65	P66	P67	S68	Y69	L70	T71	G72	E73	F74	P75	G76	D77	Y78	G79	R80	D81	T82	A83	G84	L85	S86	A87	D88	P89	E90	T91	F92	A93	R94	N95	R96	E97	L98	E99	V100	I101	H102	S103	R104	W105	A106	M107	L108	G109	C110	L111	G112	C113	V114	F115	P116	E117	L118	C119	A120	R121
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G123
V124
K125
F126
G127
E128
A129
V130
W131
F132

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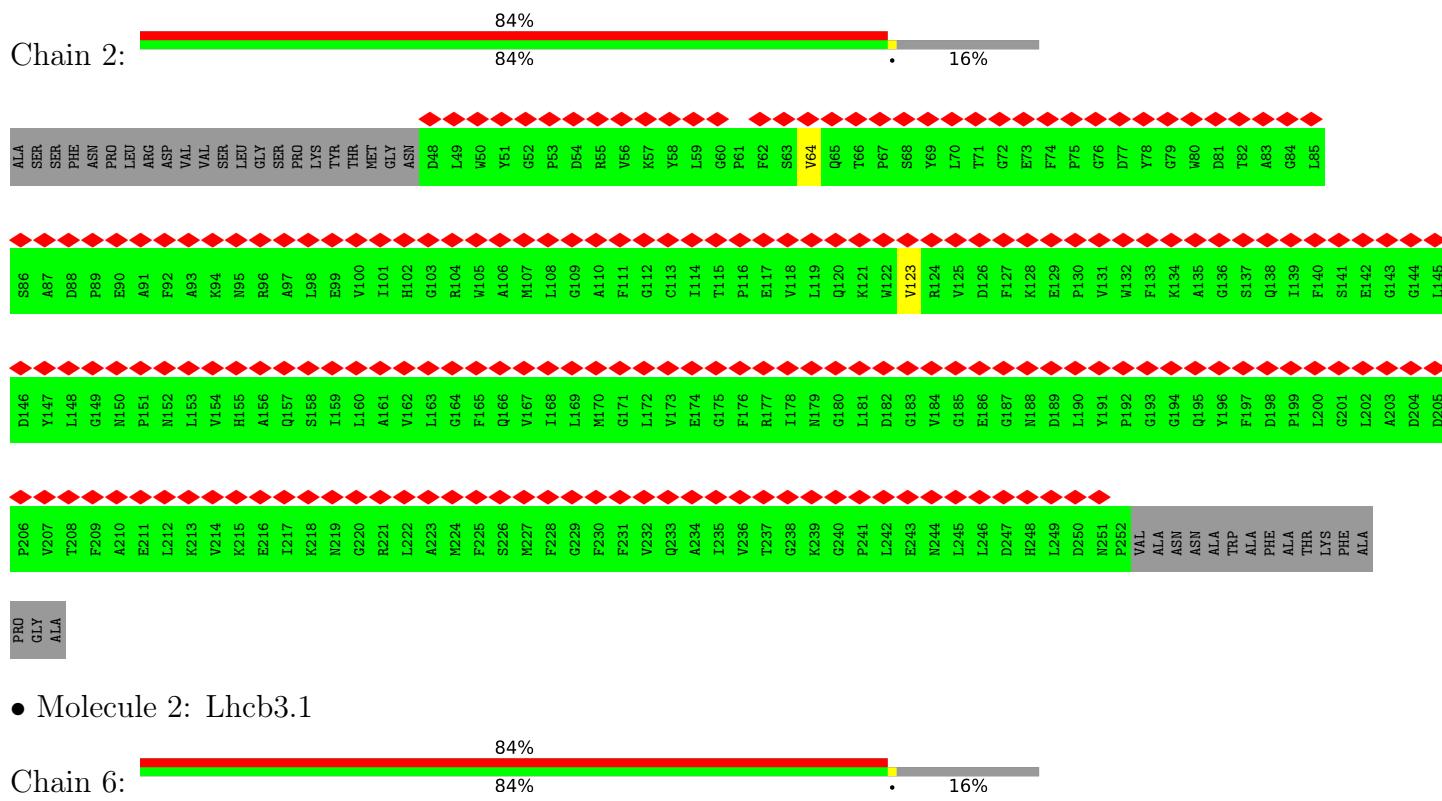
- Molecule 1: Lhcb1.4



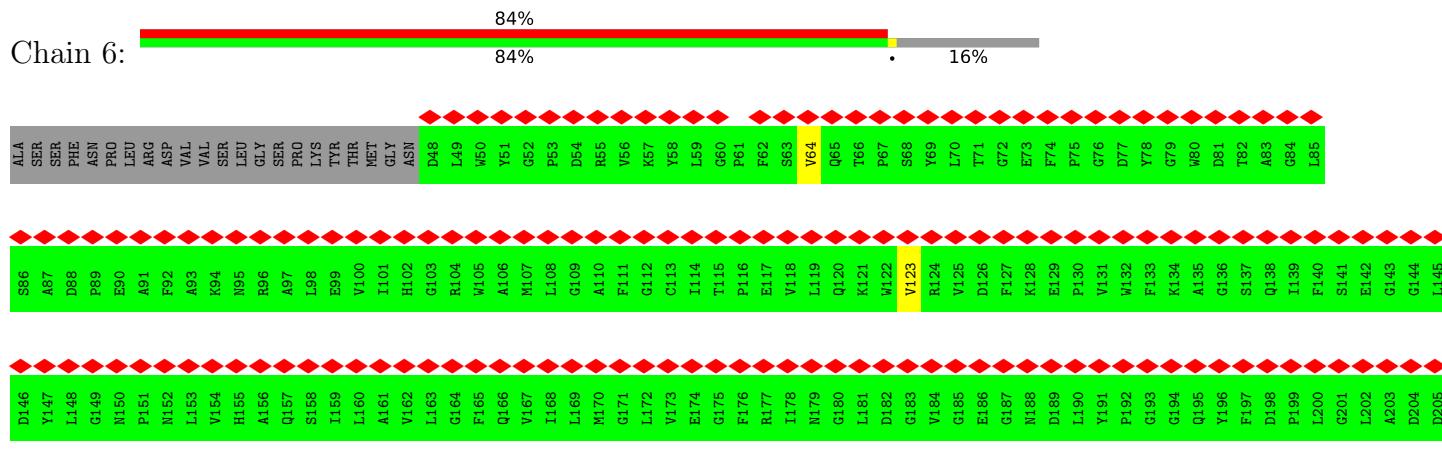
F62	S63	G64	E65	P66	P67	S68	L70	T71	G72	E73	F74	P75	G76	D77	Y78	G79	W80	D81	T82	A83	G84	L85	S86	A87	D88	P89	E90	T91	F92	A93	R94	N95	R96	E97	E98	E99	V100	I101	H102	S103	R104	W105	A106	M107	L108	G109	A110	L111	G112	C113	V114	F115	P116	E117	L118	J119	A120	R121
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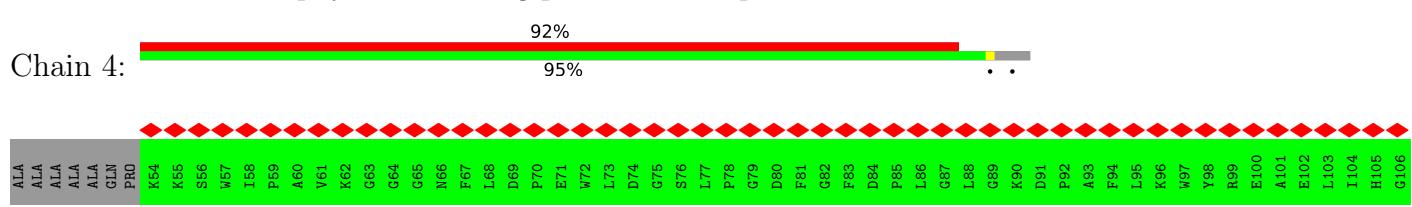
- Molecule 2: LhcB3.1



- Molecule 2: LhcB3.1

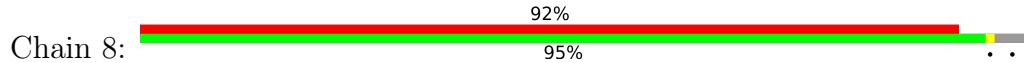


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



R107	P167	D168	S169	K230	H231	S232	R233	E234	K54	E173	V113	V114
ALA	ALA	ALA	ALA	ALA	ALA	GLN	PRO	ALA	ALA	ALA	ALA	ALA
ALA	V108	A109	A110	M110	M110	A111	A111	A112	A112	E173	V113	V114
ILE	I229	I230	H231	S232	V172	E173	V173	E174	V174	V174	V174	V174
LEU	S168	S169	Q170	A171	V172	E173	V173	E174	V174	V174	V174	V174
GLU	I229	K230	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S171	S171	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S232	S232	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
GLU	M233	M233	V172	V172	V172	E173	V173	E174	V174	V174	V174	V174
SER	L234	L234	E173	V173	V173	E174	V174	E174	V174	V174	V174	V174
SER	A235	A235	V174	V174	V174	E174	V174	E174	V174	V174	V174	V174
E11	M236											

- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



R107	P167	D168	S169	K230	H231	S232	R233	E234	K54	E173	V113	V114
ALA	ALA	ALA	ALA	ALA	ALA	GLN	PRO	ALA	ALA	ALA	ALA	ALA
ALA	V108	A109	A110	M110	M110	A111	A111	A112	A112	E173	V113	V114
ILE	I229	I230	H231	S232	V172	E173	V173	E174	V174	V174	V174	V174
LEU	S168	S169	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
GLU	I229	K230	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S171	S171	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S232	S232	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
GLU	M233	M233	V172	V172	V172	E173	V173	E174	V174	V174	V174	V174
SER	L234	L234	E173	V173	V173	E174	V174	E174	V174	V174	V174	V174
SER	A235	A235	V174	V174	V174	E174	V174	E174	V174	V174	V174	V174
E11	M236											

P167	P177	D178	S179	K230	H231	S232	R233	E234	K54	E173	V113	V114
ALA	ALA	ALA	ALA	ALA	ALA	GLN	PRO	ALA	ALA	ALA	ALA	ALA
ALA	V108	A109	A110	M110	M110	A111	A111	A112	A112	E173	V113	V114
ILE	I229	I230	H231	S232	V172	E173	V173	E174	V174	V174	V174	V174
LEU	S168	S169	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
GLU	I229	K230	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S171	S171	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S232	S232	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
GLU	M233	M233	V172	V172	V172	E173	V173	E174	V174	V174	V174	V174
SER	L234	L234	E173	V173	V173	E174	V174	E174	V174	V174	V174	V174
SER	A235	A235	V174	V174	V174	E174	V174	E174	V174	V174	V174	V174
E11	M236											

P167	P177	D178	S179	K230	H231	S232	R233	E234	K54	E173	V113	V114
ALA	ALA	ALA	ALA	ALA	ALA	GLN	PRO	ALA	ALA	ALA	ALA	ALA
ALA	V108	A109	A110	M110	M110	A111	A111	A112	A112	E173	V113	V114
ILE	I229	I230	H231	S232	V172	E173	V173	E174	V174	V174	V174	V174
LEU	S168	S169	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
GLU	I229	K230	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S171	S171	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
ARG	S232	S232	A171	A172	A172	E173	V173	E174	V174	V174	V174	V174
GLU	M233	M233	V172	V172	V172	E173	V173	E174	V174	V174	V174	V174
SER	L234	L234	E173	V173	V173	E174	V174	E174	V174	V174	V174	V174
SER	A235	A235	V174	V174	V174	E174	V174	E174	V174	V174	V174	V174
E11	M236											

- Molecule 4: Photosystem II protein D1



C18	C18	E226	E226	E226	R238	R238	H282	H282	Y282	Y282	A283	A283
THR	ALA											
ALA	V108	A109	A110	M110	M110	A111	A111	A112	A112	E173	V113	V114
ILE	I229	I230	H231	S232	V172	E173	V173	E174	V174	V174	V174	V174
LEU	S168	S169	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
GLU	I229	K230	Q170	A171	A172	E173	V173	E174	V174	V174	V174	V174
ASP	E226											
PRO	F285											
PHE	M286											
PRO	G287											
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
ASP	A336											
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ALA	V113	A114	A115	M115	M115	A116	A116	A117	A117	E173	V113	V114
ILE	I114	I115	E173	I114	I115							
GLU	I114	I115	E173	I114	I115							
ASP	P164	E173	P164	P164								
PRO	R164	E173	R164	R164								
SER	E164	E173	E164	E164								
THR	K164	E173	K164	K164								
VAL	K220	E173	K220	K220								
GLU	M166	E173	M166	M166								
ALA	V162	E173	V162	V162								
ALA	R223	E173	R223	R223								

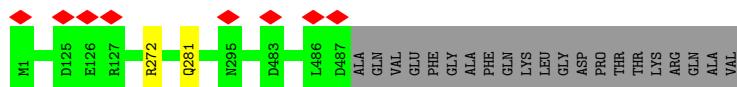
- Molecule 5: Photosystem II CP47 reaction center protein





- Molecule 5: Photosystem II CP47 reaction center protein

Chain b:



- Molecule 6: Photosystem II CP43 reaction center protein

Chain C:



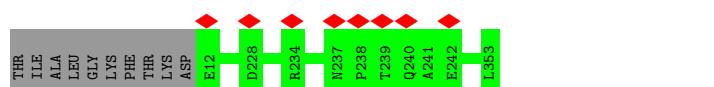
- Molecule 6: Photosystem II CP43 reaction center protein

Chain c:



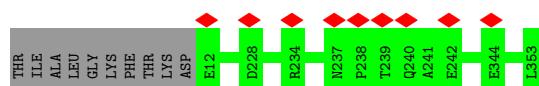
- Molecule 7: Photosystem II D2 protein

Chain D:



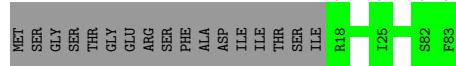
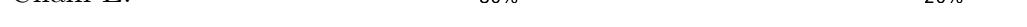
- Molecule 7: Photosystem II D2 protein

Chain d:

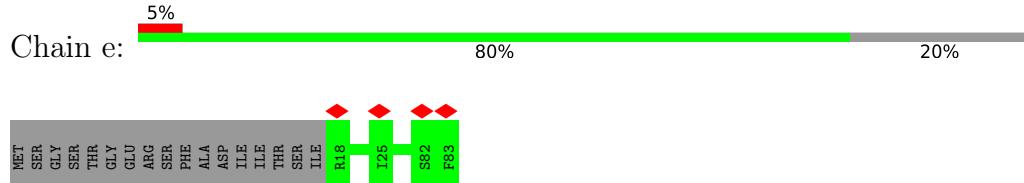


- Molecule 8: Cytochrome b559 subunit alpha

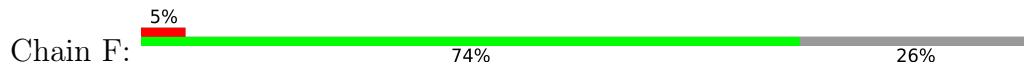
卷之三



- Molecule 8: Cytochrome b559 subunit alpha



- Molecule 9: Cytochrome b559 subunit beta (PsbF)



MET-THR-ILE-ASP-ARG-THR-PRO-ILE-PHE-T11

Q38 R39

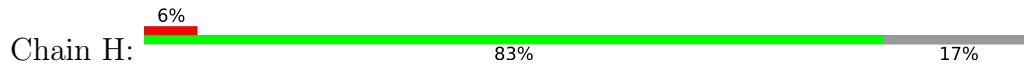
- Molecule 9: Cytochrome b559 subunit beta (PsbF)



MET THR ILE ASP ARG THR TYR PRO ILE PHE T11

R39

- Molecule 10: Photosystem II reaction center protein H



P14

ALA THR GLN THR VAL GLU ASP SER SER ARG SER GLY

- Molecule 10: Photosystem II reaction center protein H

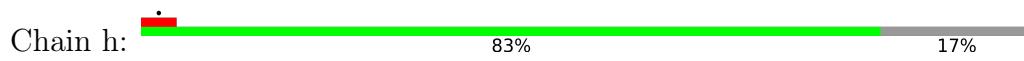
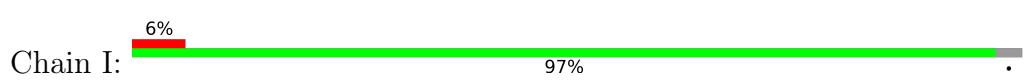


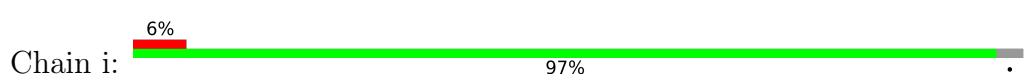
Diagram illustrating the P14 loop sequence: GLY-P14-SER-VAL-GLU-ASP-SER-ARG-SER-GLY. Red diamonds above the loop indicate mutations at positions 14, 15, 16, and 17.

- Molecule 11: Photosystem II reaction center protein L



FM1
R34
E35
GLU

- Molecule 11: Photosystem II reaction center protein L



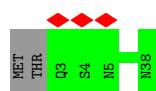
- Molecule 12: Photosystem II reaction center protein K



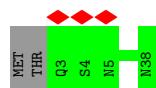
- Molecule 12: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein L



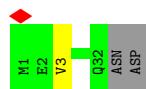
- Molecule 13: Photosystem II reaction center protein L



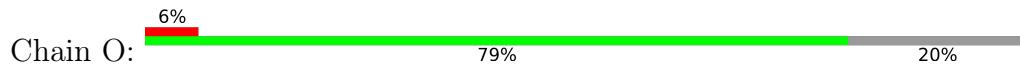
- Molecule 14: Photosystem II reaction center protein M



- Molecule 14: Photosystem II reaction center protein M



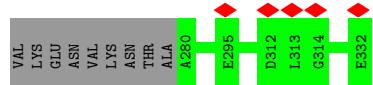
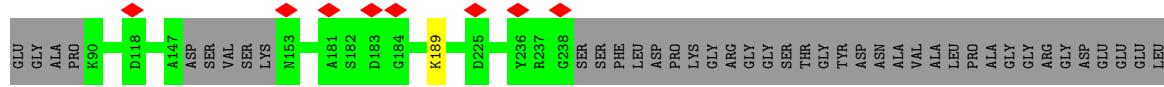
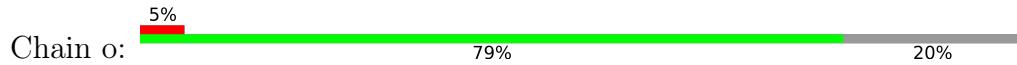
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



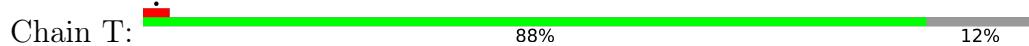


-

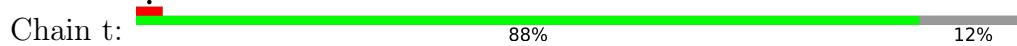
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T



- Molecule 17: Photosystem II reaction center W protein, chloroplastic

Chain W: 100%

- There are no outlier residues recorded for this chain.

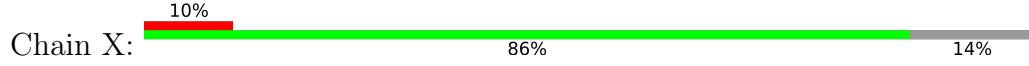
• Molecule 17: Photosystem II reaction center

- Chain w:



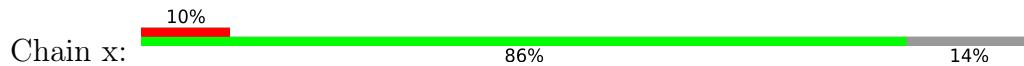
There are no outlier residues recorded for this chain.

- Molecule 18: PsbX

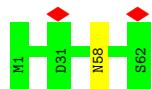




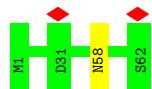
- Molecule 18: PsbX



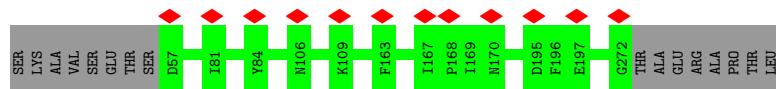
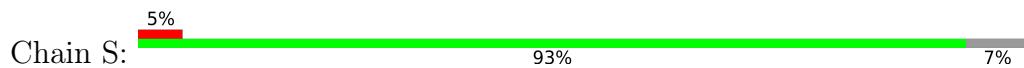
- Molecule 19: Photosystem II reaction center protein Z



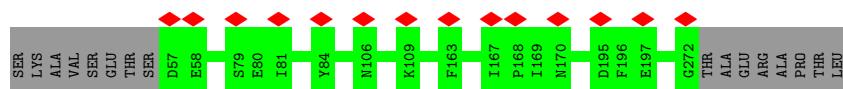
- Molecule 19: Photosystem II reaction center protein Z



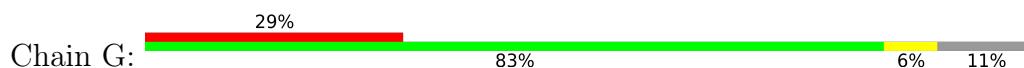
- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

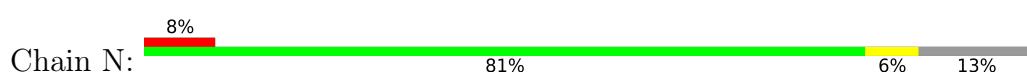


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

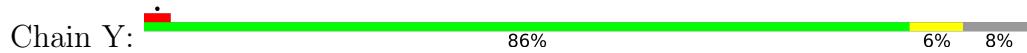




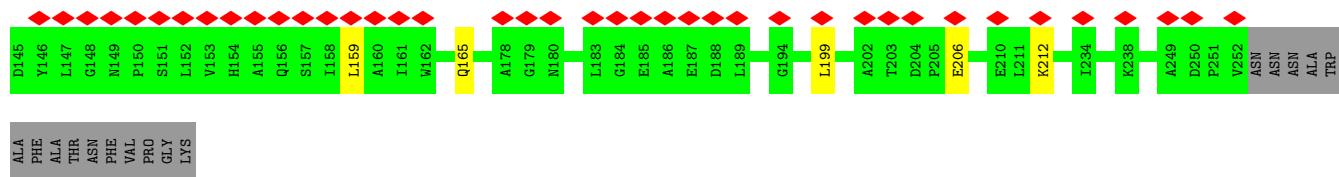
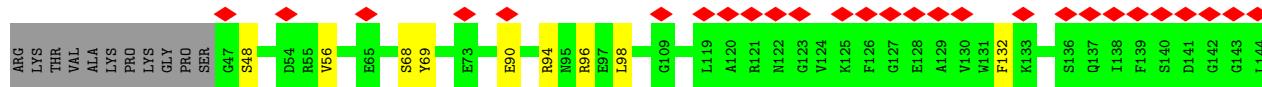
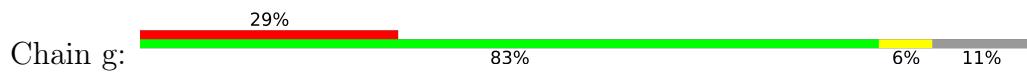
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



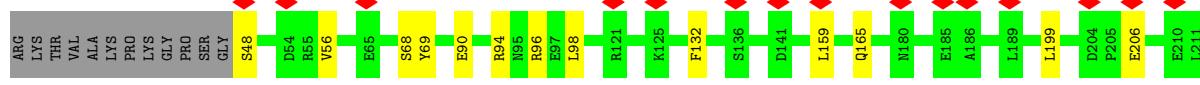
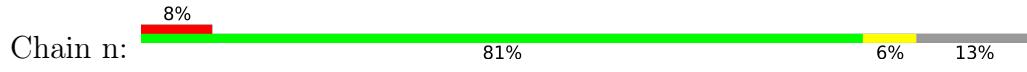
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

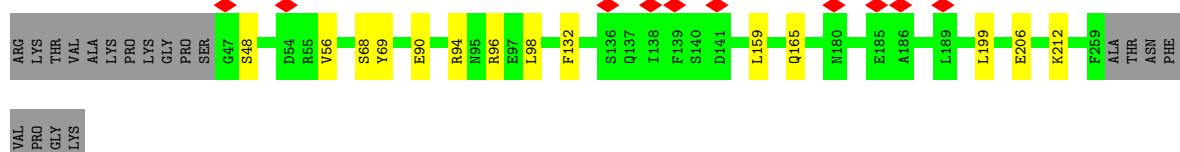
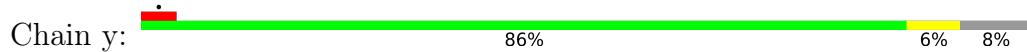


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

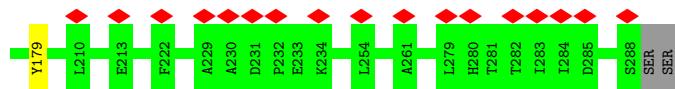
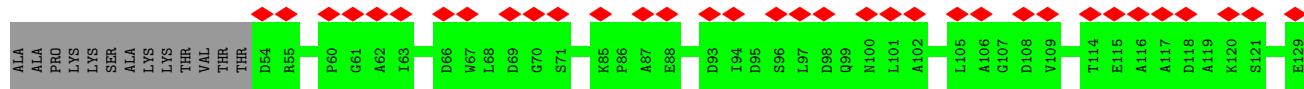




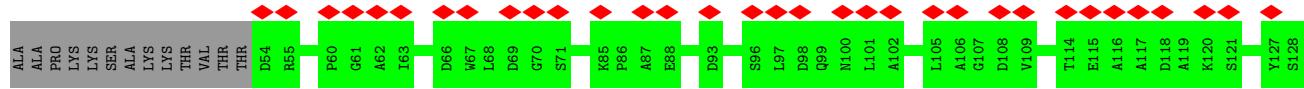
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



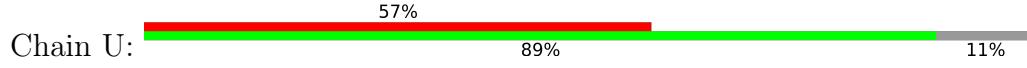
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



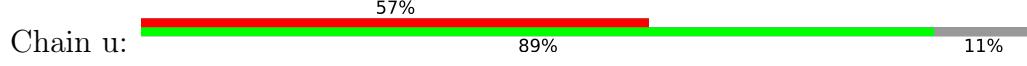
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



- Molecule 23: PsbTn



- Molecule 23: PsbTn



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100712	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 ($e^-/\text{\AA}^2$)	1.49	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	33.682	Depositor
Minimum map value	-19.496	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.976	Depositor
Recommended contour level	4.0	Depositor
Map size (\AA)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	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: BCR, PL9, AJP, CA, SQD, LHG, CHL, LUT, CLA, BCT, PHO, CL, DGD, LMG, FE2, XAT, NEX, HEM

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	1	0.31	0/1582	0.51	0/2150
1	3	0.31	0/1582	0.51	0/2150
1	5	0.31	0/1582	0.52	0/2150
1	7	0.31	0/1582	0.51	0/2150
2	2	0.27	0/1640	0.47	0/2229
2	6	0.27	0/1640	0.47	0/2229
3	4	0.28	0/1652	0.48	0/2242
3	8	0.28	0/1652	0.49	0/2242
4	A	0.25	0/2626	0.45	0/3580
4	a	0.26	0/2626	0.45	0/3580
5	B	0.25	0/3940	0.46	0/5368
5	b	0.25	0/3940	0.46	0/5368
6	C	0.25	0/3487	0.44	0/4750
6	c	0.25	0/3487	0.44	0/4750
7	D	0.26	0/2815	0.45	0/3837
7	d	0.26	0/2815	0.45	0/3837
8	E	0.25	0/561	0.47	0/763
8	e	0.25	0/561	0.47	0/763
9	F	0.24	0/229	0.45	0/311
9	f	0.24	0/229	0.45	0/311
10	H	0.24	0/455	0.45	0/619
10	h	0.24	0/455	0.45	0/619
11	I	0.26	0/294	0.48	0/397
11	i	0.26	0/294	0.49	0/397
12	K	0.26	0/312	0.39	0/428
12	k	0.26	0/312	0.39	0/428
13	L	0.24	0/310	0.37	0/421
13	l	0.24	0/310	0.37	0/421
14	M	0.25	0/254	0.38	0/347
14	m	0.25	0/254	0.38	0/347
15	O	0.26	0/1548	0.48	0/2091

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.26	0/1548	0.48	0/2091
16	T	0.27	0/246	0.39	0/333
16	t	0.27	0/246	0.39	0/333
17	W	0.25	0/438	0.41	0/594
17	w	0.25	0/438	0.41	0/594
18	X	0.25	0/250	0.43	0/339
18	x	0.25	0/250	0.43	0/339
19	Z	0.25	0/474	0.36	0/649
19	z	0.25	0/474	0.36	0/649
20	S	0.26	0/1715	0.43	0/2328
20	s	0.26	0/1715	0.43	0/2328
21	G	0.30	0/1607	0.51	0/2184
21	N	0.30	0/1580	0.52	0/2146
21	Y	0.30	0/1669	0.51	0/2270
21	g	0.30	0/1607	0.51	0/2184
21	n	0.30	0/1580	0.51	0/2146
21	y	0.30	0/1669	0.51	0/2270
22	R	0.27	0/1878	0.46	0/2561
22	r	0.27	0/1878	0.46	0/2561
23	U	0.23	0/196	0.49	0/261
23	u	0.23	0/196	0.49	0/261
All	All	0.27	0/66680	0.47	0/90696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	200/266 (75%)	188 (94%)	12 (6%)	0	100 100
1	3	200/266 (75%)	188 (94%)	12 (6%)	0	100 100
1	5	200/266 (75%)	188 (94%)	12 (6%)	0	100 100
1	7	200/266 (75%)	188 (94%)	12 (6%)	0	100 100
2	2	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	15 44
2	6	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	15 44
3	4	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	29 61
3	8	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	29 61
4	A	324/352 (92%)	309 (95%)	14 (4%)	1 (0%)	41 72
4	a	324/352 (92%)	308 (95%)	15 (5%)	1 (0%)	41 72
5	B	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	47 78
5	b	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	47 78
6	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	47 78
6	c	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	47 78
7	D	340/352 (97%)	330 (97%)	10 (3%)	0	100 100
7	d	340/352 (97%)	330 (97%)	10 (3%)	0	100 100
8	E	64/83 (77%)	61 (95%)	3 (5%)	0	100 100
8	e	64/83 (77%)	61 (95%)	3 (5%)	0	100 100
9	F	27/39 (69%)	27 (100%)	0	0	100 100
9	f	27/39 (69%)	27 (100%)	0	0	100 100
10	H	58/72 (81%)	52 (90%)	6 (10%)	0	100 100
10	h	58/72 (81%)	52 (90%)	6 (10%)	0	100 100
11	I	33/36 (92%)	28 (85%)	5 (15%)	0	100 100
11	i	33/36 (92%)	28 (85%)	5 (15%)	0	100 100
12	K	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
12	k	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
13	L	34/38 (90%)	32 (94%)	2 (6%)	0	100 100
13	l	34/38 (90%)	32 (94%)	2 (6%)	0	100 100
14	M	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	4 13
14	m	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	4 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	O	191/247 (77%)	183 (96%)	8 (4%)	0	100 100
15	o	191/247 (77%)	183 (96%)	8 (4%)	0	100 100
16	T	27/33 (82%)	25 (93%)	2 (7%)	0	100 100
16	t	27/33 (82%)	25 (93%)	2 (7%)	0	100 100
17	W	52/54 (96%)	50 (96%)	2 (4%)	0	100 100
17	w	52/54 (96%)	50 (96%)	2 (4%)	0	100 100
18	X	34/42 (81%)	33 (97%)	1 (3%)	0	100 100
18	x	34/42 (81%)	33 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	54 (90%)	6 (10%)	0	100 100
19	z	60/62 (97%)	54 (90%)	6 (10%)	0	100 100
20	S	214/232 (92%)	204 (95%)	10 (5%)	0	100 100
20	s	214/232 (92%)	203 (95%)	11 (5%)	0	100 100
21	G	204/232 (88%)	192 (94%)	12 (6%)	0	100 100
21	N	200/232 (86%)	189 (94%)	11 (6%)	0	100 100
21	Y	211/232 (91%)	200 (95%)	11 (5%)	0	100 100
21	g	204/232 (88%)	192 (94%)	12 (6%)	0	100 100
21	n	200/232 (86%)	189 (94%)	11 (6%)	0	100 100
21	y	211/232 (91%)	200 (95%)	11 (5%)	0	100 100
22	R	233/250 (93%)	223 (96%)	10 (4%)	0	100 100
22	r	233/250 (93%)	223 (96%)	10 (4%)	0	100 100
23	U	23/28 (82%)	19 (83%)	4 (17%)	0	100 100
23	u	23/28 (82%)	19 (83%)	4 (17%)	0	100 100
All	All	8226/9282 (89%)	7790 (95%)	422 (5%)	14 (0%)	50 78

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	123	VAL
3	4	182	ALA
4	A	18	CYS
14	M	3	VAL
2	6	123	VAL

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	1	154/201 (77%)	140 (91%)	14 (9%)	9 27
1	3	154/201 (77%)	140 (91%)	14 (9%)	9 27
1	5	154/201 (77%)	140 (91%)	14 (9%)	9 27
1	7	154/201 (77%)	140 (91%)	14 (9%)	9 27
2	2	164/192 (85%)	164 (100%)	0	100 100
2	6	164/192 (85%)	164 (100%)	0	100 100
3	4	156/159 (98%)	155 (99%)	1 (1%)	86 96
3	8	156/159 (98%)	155 (99%)	1 (1%)	86 96
4	A	263/284 (93%)	263 (100%)	0	100 100
4	a	263/284 (93%)	263 (100%)	0	100 100
5	B	384/402 (96%)	383 (100%)	1 (0%)	92 98
5	b	384/402 (96%)	383 (100%)	1 (0%)	92 98
6	C	340/359 (95%)	340 (100%)	0	100 100
6	c	340/359 (95%)	340 (100%)	0	100 100
7	D	274/282 (97%)	274 (100%)	0	100 100
7	d	274/282 (97%)	274 (100%)	0	100 100
8	E	59/73 (81%)	59 (100%)	0	100 100
8	e	59/73 (81%)	59 (100%)	0	100 100
9	F	24/34 (71%)	24 (100%)	0	100 100
9	f	24/34 (71%)	24 (100%)	0	100 100
10	H	50/60 (83%)	50 (100%)	0	100 100
10	h	50/60 (83%)	50 (100%)	0	100 100
11	I	32/33 (97%)	32 (100%)	0	100 100
11	i	32/33 (97%)	32 (100%)	0	100 100
12	K	32/32 (100%)	32 (100%)	0	100 100
12	k	32/32 (100%)	32 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	L	34/36 (94%)	34 (100%)	0	100	100
13	l	34/36 (94%)	34 (100%)	0	100	100
14	M	28/30 (93%)	28 (100%)	0	100	100
14	m	28/30 (93%)	28 (100%)	0	100	100
15	O	167/204 (82%)	166 (99%)	1 (1%)	86	96
15	o	167/204 (82%)	166 (99%)	1 (1%)	86	96
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	W	47/47 (100%)	47 (100%)	0	100	100
17	w	47/47 (100%)	47 (100%)	0	100	100
18	X	29/34 (85%)	29 (100%)	0	100	100
18	x	29/34 (85%)	29 (100%)	0	100	100
19	Z	54/54 (100%)	53 (98%)	1 (2%)	57	85
19	z	54/54 (100%)	53 (98%)	1 (2%)	57	85
20	S	167/180 (93%)	167 (100%)	0	100	100
20	s	167/180 (93%)	167 (100%)	0	100	100
21	G	157/177 (89%)	143 (91%)	14 (9%)	9	28
21	N	154/177 (87%)	140 (91%)	14 (9%)	9	27
21	Y	162/177 (92%)	148 (91%)	14 (9%)	10	30
21	g	157/177 (89%)	143 (91%)	14 (9%)	9	28
21	n	154/177 (87%)	140 (91%)	14 (9%)	9	27
21	y	162/177 (92%)	148 (91%)	14 (9%)	10	30
22	R	189/201 (94%)	188 (100%)	1 (0%)	88	96
22	r	189/201 (94%)	188 (100%)	1 (0%)	88	96
23	U	20/23 (87%)	20 (100%)	0	100	100
23	u	20/23 (87%)	20 (100%)	0	100	100
All	All	6640/7364 (90%)	6490 (98%)	150 (2%)	53	82

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	g	132	PHE
21	y	132	PHE

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Mol	Chain	Res	Type
21	g	206	GLU
21	n	159	LEU
21	N	68	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
7	d	264	ASN
20	s	135	ASN
7	d	351	ASN
15	o	113	GLN
22	r	245	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 374 ligands modelled in this entry, 22 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 8 are monoatomic - leaving 344 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
25	CLA	y	305	-	50,58,73	1.89	9 (18%)	58,95,113	1.85	14 (24%)
26	LHG	C	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
25	CLA	B	614	30	65,73,73	1.62	9 (13%)	76,113,113	1.82	13 (17%)
25	CLA	y	315	-	45,53,73	2.01	10 (22%)	52,89,113	1.82	13 (25%)
24	CHL	G	607	-	46,54,74	1.71	10 (21%)	49,90,114	2.02	12 (24%)
28	BCR	T	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.28	8 (14%)
25	CLA	y	313	-	60,68,73	1.79	10 (16%)	70,107,113	1.75	15 (21%)
25	CLA	c	505	-	65,73,73	1.64	9 (13%)	76,113,113	1.77	15 (19%)
28	BCR	b	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
24	CHL	S	307	-	46,54,74	1.74	10 (21%)	49,90,114	2.14	10 (20%)
24	CHL	n	605	21	48,56,74	1.66	9 (18%)	51,92,114	2.06	12 (23%)
40	NEX	s	317	-	38,46,46	1.62	8 (21%)	50,70,70	2.23	11 (22%)
25	CLA	6	605	2	48,56,73	1.87	9 (18%)	55,92,113	1.94	11 (20%)
25	CLA	c	507	-	65,73,73	1.65	9 (13%)	76,113,113	1.66	14 (18%)
25	CLA	B	601	-	65,73,73	1.58	9 (13%)	76,113,113	1.92	15 (19%)
25	CLA	b	609	-	65,73,73	1.62	9 (13%)	76,113,113	1.81	17 (22%)
28	BCR	b	617	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	6 (10%)
26	LHG	2	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	n	611	26	60,68,73	1.72	10 (16%)	70,107,113	1.69	16 (22%)
25	CLA	c	511	6	65,73,73	1.59	9 (13%)	76,113,113	2.20	16 (21%)
25	CLA	S	309	20	45,53,73	2.05	9 (20%)	52,89,113	2.10	13 (25%)
25	CLA	b	602	-	65,73,73	1.67	9 (13%)	76,113,113	1.75	16 (21%)
35	DGD	B	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)
39	LUT	s	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
25	CLA	r	610	26	49,57,73	1.85	8 (16%)	55,93,113	3.07	16 (29%)
24	CHL	y	302	21	66,74,74	1.47	11 (16%)	73,114,114	1.79	15 (20%)
27	PHO	A	403	-	51,69,69	0.52	0	47,99,99	1.72	5 (10%)
25	CLA	Y	315	-	45,53,73	2.00	10 (22%)	52,89,113	1.83	13 (25%)
25	CLA	6	604	2,26	55,63,73	1.75	8 (14%)	64,101,113	2.08	19 (29%)
25	CLA	s	313	-	55,63,73	1.72	10 (18%)	64,101,113	2.40	15 (23%)
26	LHG	D	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
30	LMG	A	408	-	48,48,55	0.44	0	56,56,63	1.20	5 (8%)
25	CLA	G	613	-	65,73,73	1.58	10 (15%)	76,113,113	1.92	15 (19%)
24	CHL	N	608	-	66,74,74	1.48	10 (15%)	73,114,114	1.77	9 (12%)
25	CLA	c	506	-	65,73,73	1.69	9 (13%)	76,113,113	1.70	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	Y	305	-	50,58,73	1.89	9 (18%)	58,95,113	1.85	14 (24%)
25	CLA	Y	312	26	60,68,73	1.73	10 (16%)	70,107,113	1.71	16 (22%)
33	BCT	A	413	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
24	CHL	g	609	21	61,69,74	1.55	10 (16%)	67,108,114	1.94	12 (17%)
28	BCR	H	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	S	310	20	55,63,73	1.81	9 (16%)	64,101,113	1.76	12 (18%)
25	CLA	N	604	-	50,58,73	1.81	10 (20%)	58,95,113	2.12	15 (25%)
25	CLA	B	607	-	65,73,73	1.61	9 (13%)	76,113,113	1.77	15 (19%)
25	CLA	C	509	-	65,73,73	1.62	10 (15%)	76,113,113	1.79	13 (17%)
30	LMG	b	620	25	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
25	CLA	c	509	-	65,73,73	1.63	10 (15%)	76,113,113	1.79	12 (15%)
25	CLA	B	613	-	65,73,73	1.64	9 (13%)	76,113,113	1.63	14 (18%)
25	CLA	R	612	-	60,68,73	1.64	10 (16%)	70,107,113	2.06	16 (22%)
25	CLA	b	613	-	65,73,73	1.63	9 (13%)	76,113,113	1.63	14 (18%)
24	CHL	y	310	21	56,64,74	1.62	11 (19%)	61,102,114	1.85	11 (18%)
26	LHG	R	618	25	41,41,48	0.45	0	44,47,54	1.23	4 (9%)
25	CLA	B	616	-	65,73,73	1.64	9 (13%)	76,113,113	1.69	13 (17%)
25	CLA	Y	303	21	65,73,73	1.69	10 (15%)	76,113,113	1.75	15 (19%)
25	CLA	6	602	2	60,68,73	1.71	9 (15%)	70,107,113	2.47	26 (37%)
25	CLA	c	503	-	65,73,73	1.61	9 (13%)	76,113,113	1.85	16 (21%)
26	LHG	Y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
28	BCR	c	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	7 (12%)
40	NEX	R	617	-	38,46,46	1.68	7 (18%)	50,70,70	3.06	17 (34%)
25	CLA	Y	304	-	65,73,73	1.63	10 (15%)	76,113,113	1.76	15 (19%)
24	CHL	N	609	21	66,74,74	1.48	9 (13%)	73,114,114	1.69	13 (17%)
26	LHG	B	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	d	402	-	65,73,73	1.69	10 (15%)	76,113,113	1.82	17 (22%)
28	BCR	A	406	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	10 (17%)
25	CLA	r	603	-	60,68,73	1.65	8 (13%)	70,107,113	2.75	19 (27%)
25	CLA	s	304	-	45,53,73	1.92	9 (20%)	52,89,113	2.10	10 (19%)
26	LHG	b	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
24	CHL	S	308	-	46,54,74	1.75	12 (26%)	49,90,114	2.18	12 (24%)
39	LUT	Y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.73	9 (17%)
25	CLA	b	601	-	65,73,73	1.57	9 (13%)	76,113,113	1.92	15 (19%)
25	CLA	C	513	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	g	601	21	66,74,74	1.46	10 (15%)	73,114,114	1.74	13 (17%)
25	CLA	b	610	-	65,73,73	1.69	9 (13%)	76,113,113	1.64	13 (17%)
25	CLA	S	314	-	49,57,73	1.92	10 (20%)	55,93,113	1.82	13 (23%)
24	CHL	y	306	21	48,56,74	1.67	10 (20%)	51,92,114	2.05	11 (21%)
25	CLA	b	604	-	65,73,73	1.63	9 (13%)	76,113,113	1.79	16 (21%)
24	CHL	Y	308	-	58,66,74	1.60	10 (17%)	63,104,114	1.92	13 (20%)
24	CHL	N	601	21	56,64,74	1.60	11 (19%)	61,102,114	1.83	12 (19%)
25	CLA	Y	314	21	65,73,73	1.57	9 (13%)	76,113,113	1.89	14 (18%)
26	LHG	c	517	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
28	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	10 (17%)
25	CLA	s	305	-	50,58,73	1.83	8 (16%)	58,95,113	3.36	19 (32%)
24	CHL	n	607	-	66,74,74	1.50	11 (16%)	73,114,114	1.75	12 (16%)
25	CLA	A	405	-	60,68,73	1.68	10 (16%)	70,107,113	1.83	15 (21%)
24	CHL	y	307	21	50,58,74	1.70	10 (20%)	52,94,114	1.89	14 (26%)
39	LUT	N	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.73	9 (17%)
29	SQD	A	407	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
26	LHG	c	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
30	LMG	a	409	-	48,48,55	0.44	0	56,56,63	1.19	5 (8%)
35	DGD	C	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
25	CLA	n	613	-	60,68,73	1.63	10 (16%)	70,107,113	1.91	18 (25%)
26	LHG	S	318	25	48,48,48	0.42	0	51,54,54	1.19	4 (7%)
26	LHG	d	406	-	48,48,48	0.43	0	51,54,54	1.18	4 (7%)
25	CLA	N	603	-	65,73,73	1.61	10 (15%)	76,113,113	1.73	16 (21%)
24	CHL	1	302	-	46,54,74	1.74	11 (23%)	49,90,114	2.12	10 (20%)
25	CLA	c	502	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	15 (19%)
25	CLA	R	608	22	58,66,73	1.77	9 (15%)	67,104,113	1.86	16 (23%)
25	CLA	2	605	2	48,56,73	1.87	9 (18%)	55,92,113	1.94	12 (21%)
25	CLA	D	401	42	50,58,73	1.81	10 (20%)	58,95,113	2.07	14 (24%)
30	LMG	B	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
25	CLA	C	507	-	65,73,73	1.65	9 (13%)	76,113,113	1.66	14 (18%)
31	PL9	D	405	-	55,55,55	0.50	0	68,69,69	0.79	0
25	CLA	b	612	-	65,73,73	1.62	10 (15%)	76,113,113	1.78	15 (19%)
25	CLA	s	303	20	61,69,73	1.71	9 (14%)	71,108,113	1.74	15 (21%)
24	CHL	n	608	-	66,74,74	1.48	10 (15%)	73,114,114	1.77	9 (12%)
26	LHG	Y	301	21	48,48,48	0.44	0	51,54,54	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	G	608	-	66,74,74	1.50	12 (18%)	73,114,114	1.77	12 (16%)
25	CLA	d	401	42	50,58,73	1.81	10 (20%)	58,95,113	2.07	14 (24%)
25	CLA	b	615	-	65,73,73	1.70	8 (12%)	76,113,113	1.70	16 (21%)
39	LUT	g	615	-	42,43,43	0.86	2 (4%)	51,60,60	1.65	8 (15%)
25	CLA	C	510	-	65,73,73	1.58	10 (15%)	76,113,113	1.75	15 (19%)
26	LHG	b	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
29	SQD	L	101	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	y	311	21	60,68,73	1.77	9 (15%)	70,107,113	1.80	16 (22%)
25	CLA	b	605	-	65,73,73	1.59	9 (13%)	76,113,113	1.90	14 (18%)
25	CLA	C	512	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	19 (25%)
25	CLA	n	604	-	50,58,73	1.81	10 (20%)	58,95,113	2.12	15 (25%)
25	CLA	C	511	6	65,73,73	1.60	9 (13%)	76,113,113	2.21	17 (22%)
25	CLA	G	604	40	50,58,73	1.87	9 (18%)	58,95,113	1.98	14 (24%)
40	NEX	G	617	25	38,46,46	1.52	8 (21%)	50,70,70	2.76	14 (28%)
28	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	R	603	-	60,68,73	1.66	8 (13%)	70,107,113	2.74	19 (27%)
40	NEX	S	317	-	38,46,46	1.61	8 (21%)	50,70,70	2.23	11 (22%)
25	CLA	B	610	-	65,73,73	1.70	9 (13%)	76,113,113	1.64	13 (17%)
25	CLA	B	604	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)
25	CLA	R	604	-	48,56,73	1.80	10 (20%)	55,92,113	1.95	16 (29%)
39	LUT	y	316	-	42,43,43	0.83	2 (4%)	51,60,60	1.74	8 (15%)
25	CLA	r	608	22	58,66,73	1.78	9 (15%)	67,104,113	1.86	16 (23%)
25	CLA	c	510	-	65,73,73	1.58	10 (15%)	76,113,113	1.75	15 (19%)
24	CHL	Y	309	-	66,74,74	1.49	11 (16%)	73,114,114	1.71	13 (17%)
25	CLA	s	309	20	45,53,73	2.05	9 (20%)	52,89,113	2.09	13 (25%)
25	CLA	b	614	30	65,73,73	1.62	9 (13%)	76,113,113	1.82	13 (17%)
29	SQD	a	408	-	49,50,54	0.82	1 (2%)	58,61,65	0.95	3 (5%)
28	BCR	C	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
41	XAT	r	616	-	39,47,47	1.16	6 (15%)	54,74,74	2.42	16 (29%)
25	CLA	B	602	-	65,73,73	1.67	9 (13%)	76,113,113	1.75	17 (22%)
31	PL9	d	405	-	55,55,55	0.50	0	68,69,69	0.78	0
28	BCR	z	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	B	615	-	65,73,73	1.70	8 (12%)	76,113,113	1.71	16 (21%)
35	DGD	A	415	-	60,60,67	0.49	0	74,74,81	1.22	5 (6%)
25	CLA	r	602	22	60,68,73	1.72	9 (15%)	70,107,113	1.88	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LUT	Y	317	-	42,43,43	0.92	4 (9%)	51,60,60	1.50	6 (11%)
24	CHL	g	608	-	66,74,74	1.50	12 (18%)	73,114,114	1.76	12 (16%)
25	CLA	B	608	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)
24	CHL	r	613	-	42,50,74	1.71	9 (21%)	44,85,114	2.27	10 (22%)
25	CLA	n	612	-	60,68,73	1.77	9 (15%)	70,107,113	1.88	15 (21%)
25	CLA	g	604	40	50,58,73	1.88	9 (18%)	58,95,113	1.97	14 (24%)
25	CLA	a	406	-	60,68,73	1.68	10 (16%)	70,107,113	1.83	15 (21%)
25	CLA	R	602	22	60,68,73	1.72	9 (15%)	70,107,113	1.89	18 (25%)
28	BCR	b	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
24	CHL	R	613	-	42,50,74	1.72	8 (19%)	44,85,114	2.28	10 (22%)
25	CLA	b	608	-	65,73,73	1.62	10 (15%)	76,113,113	1.78	15 (19%)
24	CHL	Y	302	21	66,74,74	1.46	11 (16%)	73,114,114	1.79	15 (20%)
25	CLA	r	609	22	65,73,73	1.69	9 (13%)	76,113,113	1.73	17 (22%)
30	LMG	c	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
25	CLA	R	614	22	45,53,73	2.06	8 (17%)	52,89,113	1.75	14 (26%)
30	LMG	B	620	25	51,51,55	0.44	0	59,59,63	1.21	4 (6%)
24	CHL	s	302	20	46,54,74	1.72	11 (23%)	49,90,114	2.08	11 (22%)
25	CLA	r	614	22	45,53,73	2.06	8 (17%)	52,89,113	1.75	14 (26%)
25	CLA	N	610	21	65,73,73	1.71	9 (13%)	76,113,113	1.74	16 (21%)
24	CHL	n	601	21	56,64,74	1.60	11 (19%)	61,102,114	1.82	12 (19%)
24	CHL	G	605	21	46,54,74	1.73	10 (21%)	49,90,114	2.03	9 (18%)
29	SQD	a	412	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
33	BCT	a	414	34	2,3,3	1.20	0	2,3,3	4.33	2 (100%)
24	CHL	s	306	-	46,54,74	1.74	12 (26%)	49,90,114	2.13	13 (26%)
25	CLA	G	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.77	16 (21%)
25	CLA	N	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.71	17 (22%)
25	CLA	N	614	-	48,56,73	1.81	9 (18%)	55,92,113	2.03	12 (21%)
24	CHL	6	601	2	64,72,74	1.51	11 (17%)	70,111,114	2.05	14 (20%)
25	CLA	g	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.77	16 (21%)
26	LHG	C	518	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
28	BCR	B	617	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	6 (10%)
26	LHG	6	606	25	46,46,48	0.44	0	49,52,54	1.19	4 (8%)
25	CLA	B	603	-	65,73,73	1.62	9 (13%)	76,113,113	1.70	15 (19%)
25	CLA	c	504	-	60,68,73	1.65	8 (13%)	70,107,113	2.68	21 (30%)
35	DGD	C	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LUT	S	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
39	LUT	s	316	-	42,43,43	0.89	4 (9%)	51,60,60	1.65	8 (15%)
25	CLA	r	601	-	49,57,73	1.84	9 (18%)	55,93,113	3.32	18 (32%)
25	CLA	S	313	-	55,63,73	1.72	10 (18%)	64,101,113	2.39	15 (23%)
31	PL9	A	409	-	13,13,55	0.96	0	17,17,69	0.72	0
38	HEM	F	101	9	41,50,50	1.91	8 (19%)	45,82,82	1.71	6 (13%)
25	CLA	C	505	-	65,73,73	1.64	9 (13%)	76,113,113	1.76	15 (19%)
26	LHG	y	319	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	R	610	26	49,57,73	1.85	8 (16%)	55,93,113	3.07	16 (29%)
25	CLA	g	603	-	60,68,73	1.67	9 (15%)	70,107,113	1.81	14 (20%)
24	CHL	Y	310	21	56,64,74	1.62	10 (17%)	61,102,114	1.84	11 (18%)
30	LMG	b	623	-	55,55,55	0.43	0	63,63,63	1.23	4 (6%)
25	CLA	Y	313	-	60,68,73	1.79	10 (16%)	70,107,113	1.75	15 (21%)
25	CLA	b	603	-	65,73,73	1.62	9 (13%)	76,113,113	1.71	15 (19%)
40	NEX	N	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
25	CLA	B	611	-	65,73,73	1.60	9 (13%)	76,113,113	1.80	16 (21%)
25	CLA	R	611	-	49,57,73	1.96	10 (20%)	55,93,113	3.54	22 (40%)
24	CHL	r	605	-	46,54,74	1.74	10 (21%)	49,90,114	2.19	13 (26%)
35	DGD	a	401	-	60,60,67	0.48	0	74,74,81	1.22	5 (6%)
40	NEX	y	318	-	38,46,46	1.73	9 (23%)	50,70,70	2.21	18 (36%)
25	CLA	s	314	-	49,57,73	1.93	10 (20%)	55,93,113	1.82	13 (23%)
24	CHL	r	606	-	46,54,74	1.73	9 (19%)	49,90,114	2.00	9 (18%)
25	CLA	r	612	-	60,68,73	1.64	10 (16%)	70,107,113	2.06	16 (22%)
26	LHG	b	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
26	LHG	r	618	25	41,41,48	0.46	0	44,47,54	1.22	4 (9%)
25	CLA	g	614	-	48,56,73	1.89	9 (18%)	55,92,113	1.80	13 (23%)
29	SQD	l	101	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)
24	CHL	R	605	-	46,54,74	1.74	11 (23%)	49,90,114	2.19	13 (26%)
38	HEM	f	101	9	41,50,50	1.91	9 (21%)	45,82,82	1.71	6 (13%)
24	CHL	y	308	-	58,66,74	1.60	11 (18%)	63,104,114	1.92	13 (20%)
29	SQD	A	411	-	53,54,54	0.80	1 (1%)	62,65,65	0.97	2 (3%)
24	CHL	2	601	2	64,72,74	1.50	10 (15%)	70,111,114	2.05	14 (20%)
25	CLA	g	611	-	60,68,73	1.67	10 (16%)	70,107,113	1.79	20 (28%)
25	CLA	n	603	-	65,73,73	1.61	10 (15%)	76,113,113	1.73	16 (21%)
25	CLA	S	304	-	45,53,73	1.92	10 (22%)	52,89,113	2.09	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	l	103	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
24	CHL	s	307	-	46,54,74	1.74	11 (23%)	49,90,114	2.13	11 (22%)
26	LHG	n	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
24	CHL	1	301	1	46,54,74	1.74	11 (23%)	49,90,114	2.02	11 (22%)
35	DGD	c	515	-	56,56,67	0.48	0	70,70,81	1.23	6 (8%)
24	CHL	5	302	-	46,54,74	1.74	11 (23%)	49,90,114	2.11	9 (18%)
25	CLA	y	314	21	65,73,73	1.58	9 (13%)	76,113,113	1.90	14 (18%)
24	CHL	Y	307	21	50,58,74	1.70	10 (20%)	52,94,114	1.88	14 (26%)
26	LHG	N	618	25	48,48,48	0.43	0	51,54,54	1.15	4 (7%)
28	BCR	h	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	n	610	21	65,73,73	1.71	9 (13%)	76,113,113	1.75	16 (21%)
25	CLA	y	312	26	60,68,73	1.73	10 (16%)	70,107,113	1.71	16 (22%)
27	PHO	A	404	-	51,69,69	0.52	0	47,99,99	1.71	7 (14%)
25	CLA	C	501	-	65,73,73	1.58	8 (12%)	76,113,113	2.48	20 (26%)
25	CLA	C	503	-	65,73,73	1.60	9 (13%)	76,113,113	1.85	16 (21%)
24	CHL	G	609	21	61,69,74	1.55	11 (18%)	67,108,114	1.92	13 (19%)
25	CLA	N	611	26	60,68,73	1.72	10 (16%)	70,107,113	1.69	16 (22%)
25	CLA	Y	311	21	60,68,73	1.77	9 (15%)	70,107,113	1.80	16 (22%)
25	CLA	G	610	-	64,72,73	1.60	8 (12%)	74,111,113	2.00	17 (22%)
25	CLA	B	612	-	65,73,73	1.63	10 (15%)	76,113,113	1.78	15 (19%)
25	CLA	B	609	-	65,73,73	1.62	9 (13%)	76,113,113	1.81	17 (22%)
25	CLA	G	611	-	60,68,73	1.66	8 (13%)	70,107,113	1.78	20 (28%)
28	BCR	D	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	g	613	-	65,73,73	1.59	10 (15%)	76,113,113	1.92	14 (18%)
24	CHL	Y	306	21	48,56,74	1.67	10 (20%)	51,92,114	2.05	11 (21%)
26	LHG	y	301	21	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
31	PL9	a	410	-	13,13,55	0.96	0	17,17,69	0.72	0
28	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.28	9 (16%)
40	NEX	r	617	-	38,46,46	1.68	8 (21%)	50,70,70	3.05	17 (34%)
24	CHL	S	302	20	46,54,74	1.72	10 (21%)	49,90,114	2.08	11 (22%)
25	CLA	2	604	2,26	55,63,73	1.75	8 (14%)	64,101,113	2.08	19 (29%)
40	NEX	n	617	-	38,46,46	1.67	7 (18%)	50,70,70	2.43	18 (36%)
28	BCR	i	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.27	9 (16%)
28	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	9 (16%)
30	LMG	a	411	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	r	611	-	49,57,73	1.95	10 (20%)	55,93,113	3.54	22 (40%)
25	CLA	S	312	-	49,57,73	1.98	9 (18%)	55,93,113	1.89	14 (25%)
26	LHG	c	519	6	48,48,48	0.45	0	51,54,54	1.18	4 (7%)
24	CHL	n	606	-	46,54,74	1.73	12 (26%)	49,90,114	2.13	14 (28%)
25	CLA	R	609	22	65,73,73	1.68	9 (13%)	76,113,113	1.72	17 (22%)
24	CHL	R	607	-	61,69,74	1.55	11 (18%)	67,108,114	1.91	13 (19%)
25	CLA	g	610	-	64,72,73	1.61	8 (12%)	74,111,113	2.00	16 (21%)
24	CHL	G	601	21	66,74,74	1.46	11 (16%)	73,114,114	1.75	14 (19%)
24	CHL	N	605	21	48,56,74	1.67	10 (20%)	51,92,114	2.07	12 (23%)
24	CHL	N	606	-	46,54,74	1.73	12 (26%)	49,90,114	2.11	13 (26%)
39	LUT	R	615	-	42,43,43	0.96	3 (7%)	51,60,60	1.67	9 (17%)
39	LUT	n	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
25	CLA	c	512	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	18 (23%)
26	LHG	S	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	G	612	21	60,68,73	1.77	9 (15%)	70,107,113	1.71	12 (17%)
25	CLA	S	303	20	61,69,73	1.71	10 (16%)	71,108,113	1.74	14 (19%)
26	LHG	L	102	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
28	BCR	B	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	8 (14%)
41	XAT	R	616	-	39,47,47	1.17	6 (15%)	54,74,74	2.41	16 (29%)
25	CLA	N	612	-	60,68,73	1.76	9 (15%)	70,107,113	1.87	15 (21%)
25	CLA	C	508	-	65,73,73	1.58	9 (13%)	76,113,113	1.88	17 (22%)
39	LUT	n	615	-	42,43,43	0.88	2 (4%)	51,60,60	1.72	9 (17%)
25	CLA	a	403	-	65,73,73	1.59	10 (15%)	76,113,113	1.80	16 (21%)
24	CHL	r	607	-	61,69,74	1.55	11 (18%)	67,108,114	1.90	13 (19%)
26	LHG	s	318	25	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	D	402	-	65,73,73	1.69	10 (15%)	76,113,113	1.82	17 (22%)
39	LUT	N	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.53	6 (11%)
25	CLA	c	501	-	65,73,73	1.58	8 (12%)	76,113,113	2.48	20 (26%)
24	CHL	2	603	2	46,54,74	1.86	13 (28%)	49,90,114	2.53	17 (34%)
25	CLA	S	305	-	50,58,73	1.83	8 (16%)	58,95,113	3.36	19 (32%)
26	LHG	B	622	-	48,48,48	0.45	0	51,54,54	1.15	4 (7%)
24	CHL	g	606	-	50,58,74	1.65	9 (18%)	52,94,114	2.14	11 (21%)
26	LHG	C	517	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	R	601	-	49,57,73	1.84	9 (18%)	55,93,113	3.30	18 (32%)
25	CLA	G	614	-	48,56,73	1.89	9 (18%)	55,92,113	1.80	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	616	-	65,73,73	1.64	9 (13%)	76,113,113	1.69	13 (17%)
25	CLA	D	403	-	65,73,73	1.60	8 (12%)	76,113,113	2.73	21 (27%)
25	CLA	c	508	-	65,73,73	1.58	9 (13%)	76,113,113	1.88	16 (21%)
25	CLA	g	612	21	60,68,73	1.77	8 (13%)	70,107,113	1.71	12 (17%)
39	LUT	G	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
35	DGD	b	626	-	63,63,67	0.49	0	77,77,81	1.29	6 (7%)
39	LUT	g	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.44	4 (7%)
27	PHO	a	405	-	51,69,69	0.52	0	47,99,99	1.71	7 (14%)
29	SQD	l	102	-	41,42,54	0.88	1 (2%)	50,53,65	1.11	3 (6%)
25	CLA	2	602	2	60,68,73	1.71	9 (15%)	70,107,113	2.47	26 (37%)
25	CLA	n	602	21	65,73,73	1.70	10 (15%)	76,113,113	1.72	17 (22%)
25	CLA	n	614	-	48,56,73	1.81	9 (18%)	55,92,113	2.02	12 (21%)
40	NEX	g	617	25	38,46,46	1.61	8 (21%)	50,70,70	2.77	15 (30%)
39	LUT	G	615	-	42,43,43	0.87	3 (7%)	51,60,60	1.65	8 (15%)
25	CLA	c	513	-	65,73,73	1.63	10 (15%)	76,113,113	1.81	17 (22%)
29	SQD	L	103	-	53,54,54	0.80	1 (1%)	62,65,65	1.01	3 (4%)
25	CLA	s	310	20	55,63,73	1.80	9 (16%)	64,101,113	1.76	11 (17%)
30	LMG	A	410	-	40,40,55	0.48	0	48,48,63	1.28	4 (8%)
24	CHL	N	607	-	66,74,74	1.50	11 (16%)	73,114,114	1.75	12 (16%)
24	CHL	g	607	-	46,54,74	1.71	9 (19%)	49,90,114	2.02	12 (24%)
25	CLA	A	402	-	65,73,73	1.59	10 (15%)	76,113,113	1.80	16 (21%)
24	CHL	G	606	-	50,58,74	1.65	9 (18%)	52,94,114	2.13	12 (23%)
25	CLA	s	311	26	56,64,73	1.71	9 (16%)	65,102,113	2.18	13 (20%)
24	CHL	S	306	-	46,54,74	1.75	12 (26%)	49,90,114	2.13	13 (26%)
24	CHL	R	606	-	46,54,74	1.74	10 (21%)	49,90,114	2.01	9 (18%)
24	CHL	y	309	-	66,74,74	1.49	11 (16%)	73,114,114	1.70	13 (17%)
25	CLA	a	402	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	16 (21%)
24	CHL	6	603	2	46,54,74	1.86	13 (28%)	49,90,114	2.53	17 (34%)
25	CLA	C	504	-	60,68,73	1.66	8 (13%)	70,107,113	2.67	21 (30%)
24	CHL	s	308	-	46,54,74	1.75	12 (26%)	49,90,114	2.18	12 (24%)
30	LMG	C	520	-	51,51,55	0.45	0	59,59,63	1.23	4 (6%)
26	LHG	B	621	-	46,46,48	0.45	0	49,52,54	1.18	4 (8%)
39	LUT	r	615	-	42,43,43	0.95	3 (7%)	51,60,60	1.68	9 (17%)
25	CLA	C	502	-	65,73,73	1.63	9 (13%)	76,113,113	1.81	15 (19%)
25	CLA	N	613	-	60,68,73	1.63	10 (16%)	70,107,113	1.91	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	Z	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
40	NEX	Y	318	-	38,46,46	1.73	8 (21%)	50,70,70	2.21	18 (36%)
25	CLA	s	312	-	49,57,73	1.98	9 (18%)	55,93,113	1.89	14 (25%)
39	LUT	S	315	-	42,43,43	0.92	3 (7%)	51,60,60	1.57	8 (15%)
25	CLA	A	401	-	65,73,73	1.60	10 (15%)	76,113,113	1.74	16 (21%)
28	BCR	k	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.30	9 (16%)
25	CLA	y	304	-	65,73,73	1.63	10 (15%)	76,113,113	1.76	15 (19%)
25	CLA	B	606	-	65,73,73	1.57	9 (13%)	76,113,113	1.81	14 (18%)
25	CLA	r	604	-	48,56,73	1.79	9 (18%)	55,92,113	1.95	16 (29%)
30	LMG	D	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
27	PHO	a	404	-	51,69,69	0.52	0	47,99,99	1.72	5 (10%)
25	CLA	S	311	26	56,64,73	1.72	9 (16%)	65,102,113	2.18	13 (20%)
25	CLA	b	611	-	65,73,73	1.60	9 (13%)	76,113,113	1.80	16 (21%)
24	CHL	n	609	21	66,74,74	1.48	10 (15%)	73,114,114	1.69	13 (17%)
26	LHG	s	301	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	b	607	-	65,73,73	1.62	9 (13%)	76,113,113	1.77	15 (19%)
25	CLA	d	403	-	65,73,73	1.60	8 (12%)	76,113,113	2.73	21 (27%)
25	CLA	y	303	21	65,73,73	1.69	10 (15%)	76,113,113	1.75	15 (19%)
24	CHL	g	605	21	46,54,74	1.72	11 (23%)	49,90,114	2.04	9 (18%)
25	CLA	B	605	-	65,73,73	1.60	9 (13%)	76,113,113	1.90	14 (18%)
30	LMG	d	407	-	46,46,55	0.44	0	54,54,63	1.21	4 (7%)
25	CLA	C	506	-	65,73,73	1.69	9 (13%)	76,113,113	1.70	16 (21%)
25	CLA	G	603	-	60,68,73	1.67	9 (15%)	70,107,113	1.81	14 (20%)
35	DGD	c	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
25	CLA	b	606	-	65,73,73	1.57	9 (13%)	76,113,113	1.81	14 (18%)
24	CHL	5	301	1	46,54,74	1.74	10 (21%)	49,90,114	2.02	11 (22%)
39	LUT	y	317	-	42,43,43	0.92	3 (7%)	51,60,60	1.50	6 (11%)
28	BCR	t	101	16	41,41,41	1.15	3 (7%)	56,56,56	1.27	8 (14%)
28	BCR	a	407	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	10 (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
25	CLA	y	305	-	1/1/12/20	7/19/97/115	-
26	LHG	C	519	6	-	21/53/53/53	-
25	CLA	B	614	30	1/1/15/20	13/37/115/115	-
25	CLA	y	315	-	1/1/11/20	8/13/91/115	-
24	CHL	G	607	-	2/2/16/26	6/15/113/137	-
28	BCR	T	101	16	-	17/29/63/63	0/2/2/2
25	CLA	y	313	-	1/1/14/20	11/31/109/115	-
25	CLA	c	505	-	1/1/15/20	12/37/115/115	-
28	BCR	b	618	-	-	3/29/63/63	0/2/2/2
24	CHL	S	307	-	3/3/16/26	7/15/113/137	-
24	CHL	n	605	21	3/3/16/26	7/18/116/137	-
40	NEX	s	317	-	-	6/27/83/83	0/3/3/3
25	CLA	6	605	2	1/1/11/20	10/17/95/115	-
25	CLA	c	507	-	1/1/15/20	15/37/115/115	-
25	CLA	B	601	-	1/1/15/20	16/37/115/115	-
25	CLA	b	609	-	1/1/15/20	11/37/115/115	-
28	BCR	b	617	-	-	3/29/63/63	0/2/2/2
26	LHG	2	606	25	-	25/51/51/53	-
25	CLA	n	611	26	1/1/14/20	12/31/109/115	-
25	CLA	c	511	6	1/1/15/20	7/37/115/115	-
25	CLA	S	309	20	1/1/11/20	5/13/91/115	-
25	CLA	b	602	-	1/1/15/20	14/37/115/115	-
35	DGD	B	626	-	-	23/51/91/95	0/2/2/2
39	LUT	s	315	-	-	4/29/67/67	0/2/2/2
25	CLA	r	610	26	1/1/11/20	9/18/96/115	-
24	CHL	y	302	21	2/2/20/26	23/39/137/137	-
27	PHO	A	403	-	-	12/37/103/103	0/5/6/6
25	CLA	Y	315	-	1/1/11/20	8/13/91/115	-
25	CLA	6	604	2,26	1/1/13/20	9/25/103/115	-
25	CLA	s	313	-	1/1/13/20	10/25/103/115	-
26	LHG	D	406	-	-	18/53/53/53	-
30	LMG	A	408	-	-	18/43/63/70	0/1/1/1
25	CLA	G	613	-	1/1/15/20	16/37/115/115	-
24	CHL	N	608	-	3/3/20/26	15/39/137/137	-
25	CLA	c	506	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Y	305	-	1/1/12/20	7/19/97/115	-
25	CLA	Y	312	26	1/1/14/20	11/31/109/115	-
24	CHL	g	609	21	3/3/19/26	10/33/131/137	-
28	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	CLA	S	310	20	1/1/13/20	9/25/103/115	-
25	CLA	N	604	-	1/1/12/20	6/19/97/115	-
25	CLA	B	607	-	1/1/15/20	16/37/115/115	-
25	CLA	C	509	-	1/1/15/20	7/37/115/115	-
30	LMG	b	620	25	-	15/46/66/70	0/1/1/1
25	CLA	c	509	-	1/1/15/20	7/37/115/115	-
25	CLA	B	613	-	1/1/15/20	15/37/115/115	-
25	CLA	R	612	-	1/1/14/20	11/31/109/115	-
25	CLA	b	613	-	1/1/15/20	15/37/115/115	-
24	CHL	y	310	21	3/3/18/26	11/27/125/137	-
26	LHG	R	618	25	-	12/46/46/53	-
25	CLA	B	616	-	1/1/15/20	17/37/115/115	-
25	CLA	Y	303	21	1/1/15/20	12/37/115/115	-
25	CLA	6	602	2	1/1/14/20	13/31/109/115	-
25	CLA	c	503	-	1/1/15/20	9/37/115/115	-
26	LHG	Y	319	25	-	23/53/53/53	-
28	BCR	c	514	-	-	2/29/63/63	0/2/2/2
40	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	Y	304	-	1/1/15/20	22/37/115/115	-
24	CHL	N	609	21	2/2/20/26	15/39/137/137	-
26	LHG	B	625	-	-	14/50/50/53	-
25	CLA	d	402	-	1/1/15/20	10/37/115/115	-
28	BCR	A	406	-	-	5/29/63/63	0/2/2/2
25	CLA	r	603	-	1/1/14/20	13/31/109/115	-
25	CLA	s	304	-	1/1/11/20	2/13/91/115	-
26	LHG	b	622	-	-	18/53/53/53	-
24	CHL	S	308	-	3/3/16/26	2/15/113/137	-
39	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
25	CLA	b	601	-	1/1/15/20	16/37/115/115	-
25	CLA	C	513	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	601	21	2/2/20/26	24/39/137/137	-
25	CLA	b	610	-	1/1/15/20	9/37/115/115	-
25	CLA	S	314	-	1/1/11/20	3/18/96/115	-
24	CHL	y	306	21	3/3/16/26	9/18/116/137	-
25	CLA	b	604	-	1/1/15/20	15/37/115/115	-
24	CHL	Y	308	-	2/2/18/26	8/30/128/137	-
24	CHL	N	601	21	2/2/18/26	13/27/125/137	-
25	CLA	Y	314	21	1/1/15/20	16/37/115/115	-
26	LHG	c	517	-	-	17/53/53/53	-
28	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	s	305	-	1/1/12/20	9/19/97/115	-
24	CHL	n	607	-	2/2/20/26	18/39/137/137	-
25	CLA	A	405	-	1/1/14/20	9/31/109/115	-
24	CHL	y	307	21	3/3/16/26	3/20/118/137	-
39	LUT	N	615	-	-	8/29/67/67	0/2/2/2
29	SQD	A	407	-	-	21/45/65/69	0/1/1/1
26	LHG	c	518	-	-	12/53/53/53	-
30	LMG	a	409	-	-	18/43/63/70	0/1/1/1
35	DGD	C	516	-	-	28/51/91/95	0/2/2/2
25	CLA	n	613	-	1/1/14/20	21/31/109/115	-
26	LHG	S	318	25	-	20/53/53/53	-
26	LHG	d	406	-	-	18/53/53/53	-
25	CLA	N	603	-	1/1/15/20	17/37/115/115	-
24	CHL	1	302	-	3/3/16/26	5/15/113/137	-
25	CLA	c	502	-	1/1/15/20	6/37/115/115	-
25	CLA	R	608	22	1/1/13/20	15/29/107/115	-
25	CLA	2	605	2	1/1/11/20	10/17/95/115	-
25	CLA	D	401	42	1/1/12/20	2/19/97/115	-
30	LMG	B	623	-	-	28/50/70/70	0/1/1/1
25	CLA	C	507	-	1/1/15/20	15/37/115/115	-
31	PL9	D	405	-	-	5/53/73/73	0/1/1/1
25	CLA	b	612	-	1/1/15/20	8/37/115/115	-
25	CLA	s	303	20	1/1/14/20	16/33/111/115	-
24	CHL	n	608	-	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	Y	301	21	-	16/53/53/53	-
24	CHL	G	608	-	3/3/20/26	22/39/137/137	-
25	CLA	d	401	42	1/1/12/20	2/19/97/115	-
25	CLA	b	615	-	1/1/15/20	10/37/115/115	-
39	LUT	g	615	-	-	5/29/67/67	0/2/2/2
25	CLA	C	510	-	1/1/15/20	14/37/115/115	-
26	LHG	b	621	-	-	19/51/51/53	-
29	SQD	L	101	-	-	13/37/57/69	0/1/1/1
25	CLA	y	311	21	1/1/14/20	10/31/109/115	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-
25	CLA	C	512	-	1/1/15/20	12/37/115/115	-
25	CLA	n	604	-	1/1/12/20	6/19/97/115	-
25	CLA	C	511	6	1/1/15/20	7/37/115/115	-
25	CLA	G	604	40	1/1/12/20	11/19/97/115	-
40	NEX	G	617	25	-	11/27/83/83	0/3/3/3
28	BCR	d	404	-	-	5/29/63/63	0/2/2/2
25	CLA	R	603	-	1/1/14/20	13/31/109/115	-
40	NEX	S	317	-	-	6/27/83/83	0/3/3/3
25	CLA	B	610	-	1/1/15/20	9/37/115/115	-
25	CLA	B	604	-	1/1/15/20	15/37/115/115	-
25	CLA	R	604	-	1/1/11/20	4/17/95/115	-
39	LUT	y	316	-	-	3/29/67/67	0/2/2/2
25	CLA	r	608	22	1/1/13/20	15/29/107/115	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
24	CHL	Y	309	-	3/3/20/26	20/39/137/137	-
25	CLA	s	309	20	1/1/11/20	5/13/91/115	-
25	CLA	b	614	30	1/1/15/20	13/37/115/115	-
29	SQD	a	408	-	-	21/45/65/69	0/1/1/1
28	BCR	C	514	-	-	2/29/63/63	0/2/2/2
41	XAT	r	616	-	-	2/31/93/93	0/4/4/4
25	CLA	B	602	-	1/1/15/20	14/37/115/115	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
28	BCR	z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	A	415	-	-	27/48/88/95	0/2/2/2
25	CLA	r	602	22	1/1/14/20	10/31/109/115	-
39	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
24	CHL	g	608	-	3/3/20/26	22/39/137/137	-
25	CLA	B	608	-	1/1/15/20	12/37/115/115	-
24	CHL	r	613	-	3/3/15/26	6/10/108/137	-
25	CLA	n	612	-	1/1/14/20	18/31/109/115	-
25	CLA	g	604	40	1/1/12/20	11/19/97/115	-
25	CLA	a	406	-	1/1/14/20	9/31/109/115	-
25	CLA	R	602	22	1/1/14/20	10/31/109/115	-
28	BCR	b	619	-	-	3/29/63/63	0/2/2/2
24	CHL	R	613	-	3/3/15/26	6/10/108/137	-
25	CLA	b	608	-	1/1/15/20	12/37/115/115	-
24	CHL	Y	302	21	2/2/20/26	23/39/137/137	-
25	CLA	r	609	22	1/1/15/20	14/37/115/115	-
30	LMG	c	520	-	-	18/46/66/70	0/1/1/1
25	CLA	R	614	22	1/1/11/20	8/13/91/115	-
30	LMG	B	620	25	-	15/46/66/70	0/1/1/1
24	CHL	s	302	20	2/2/16/26	4/15/113/137	-
25	CLA	r	614	22	1/1/11/20	8/13/91/115	-
25	CLA	N	610	21	1/1/15/20	15/37/115/115	-
24	CHL	n	601	21	2/2/18/26	13/27/125/137	-
24	CHL	G	605	21	3/3/16/26	9/15/113/137	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
24	CHL	s	306	-	3/3/16/26	7/15/113/137	-
25	CLA	G	602	21	1/1/15/20	15/37/115/115	-
25	CLA	N	602	21	1/1/15/20	13/37/115/115	-
25	CLA	N	614	-	1/1/11/20	4/17/95/115	-
24	CHL	6	601	2	3/3/19/26	16/37/135/137	-
25	CLA	g	602	21	1/1/15/20	15/37/115/115	-
26	LHG	C	518	-	-	12/53/53/53	-
28	BCR	B	617	-	-	3/29/63/63	0/2/2/2
26	LHG	6	606	25	-	25/51/51/53	-
25	CLA	B	603	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	504	-	1/1/14/20	14/31/109/115	-
35	DGD	C	515	-	-	17/44/84/95	0/2/2/2
39	LUT	S	316	-	-	4/29/67/67	0/2/2/2
39	LUT	s	316	-	-	4/29/67/67	0/2/2/2
25	CLA	r	601	-	1/1/11/20	11/18/96/115	-
25	CLA	S	313	-	1/1/13/20	10/25/103/115	-
31	PL9	A	409	-	-	2/5/18/73	0/1/1/1
38	HEM	F	101	9	-	1/12/54/54	-
25	CLA	C	505	-	1/1/15/20	12/37/115/115	-
26	LHG	y	319	25	-	23/53/53/53	-
25	CLA	R	610	26	1/1/11/20	9/18/96/115	-
25	CLA	g	603	-	1/1/14/20	11/31/109/115	-
24	CHL	Y	310	21	3/3/18/26	11/27/125/137	-
30	LMG	b	623	-	-	28/50/70/70	0/1/1/1
25	CLA	Y	313	-	1/1/14/20	11/31/109/115	-
25	CLA	b	603	-	1/1/15/20	11/37/115/115	-
40	NEX	N	617	-	-	10/27/83/83	0/3/3/3
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
25	CLA	R	611	-	1/1/11/20	11/18/96/115	-
24	CHL	r	605	-	3/3/16/26	3/15/113/137	-
35	DGD	a	401	-	-	27/48/88/95	0/2/2/2
40	NEX	y	318	-	-	7/27/83/83	1/3/3/3
25	CLA	s	314	-	1/1/11/20	3/18/96/115	-
24	CHL	r	606	-	3/3/16/26	11/15/113/137	-
25	CLA	r	612	-	1/1/14/20	11/31/109/115	-
26	LHG	b	625	-	-	14/50/50/53	-
26	LHG	r	618	25	-	12/46/46/53	-
25	CLA	g	614	-	1/1/11/20	9/17/95/115	-
29	SQD	l	101	-	-	27/49/69/69	0/1/1/1
24	CHL	R	605	-	3/3/16/26	3/15/113/137	-
38	HEM	f	101	9	-	1/12/54/54	-
24	CHL	y	308	-	2/2/18/26	8/30/128/137	-
29	SQD	A	411	-	-	22/49/69/69	0/1/1/1
24	CHL	2	601	2	3/3/19/26	16/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	g	611	-	1/1/14/20	16/31/109/115	-
25	CLA	n	603	-	1/1/15/20	17/37/115/115	-
25	CLA	S	304	-	1/1/11/20	2/13/91/115	-
26	LHG	l	103	-	-	29/53/53/53	-
24	CHL	s	307	-	3/3/16/26	7/15/113/137	-
26	LHG	n	618	25	-	29/53/53/53	-
24	CHL	1	301	1	3/3/16/26	4/15/113/137	-
35	DGD	c	515	-	-	17/44/84/95	0/2/2/2
24	CHL	5	302	-	3/3/16/26	5/15/113/137	-
25	CLA	y	314	21	1/1/15/20	16/37/115/115	-
24	CHL	Y	307	21	3/3/16/26	3/20/118/137	-
26	LHG	N	618	25	-	29/53/53/53	-
28	BCR	h	101	-	-	6/29/63/63	0/2/2/2
25	CLA	n	610	21	1/1/15/20	15/37/115/115	-
25	CLA	y	312	26	1/1/14/20	11/31/109/115	-
27	PHO	A	404	-	-	1/37/103/103	0/5/6/6
25	CLA	C	501	-	1/1/15/20	7/37/115/115	-
25	CLA	C	503	-	1/1/15/20	9/37/115/115	-
24	CHL	G	609	21	3/3/19/26	10/33/131/137	-
25	CLA	N	611	26	1/1/14/20	12/31/109/115	-
25	CLA	Y	311	21	1/1/14/20	9/31/109/115	-
25	CLA	G	610	-	1/1/14/20	14/36/114/115	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
25	CLA	B	609	-	1/1/15/20	11/37/115/115	-
25	CLA	G	611	-	1/1/14/20	16/31/109/115	-
28	BCR	D	404	-	-	5/29/63/63	0/2/2/2
25	CLA	g	613	-	1/1/15/20	16/37/115/115	-
24	CHL	Y	306	21	3/3/16/26	9/18/116/137	-
26	LHG	y	301	21	-	16/53/53/53	-
31	PL9	a	410	-	-	2/5/18/73	0/1/1/1
28	BCR	I	101	-	-	5/29/63/63	0/2/2/2
40	NEX	r	617	-	-	6/27/83/83	0/3/3/3
24	CHL	S	302	20	2/2/16/26	4/15/113/137	-
25	CLA	2	604	2,26	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	NEX	n	617	-	-	10/27/83/83	0/3/3/3
28	BCR	i	101	-	-	4/29/63/63	0/2/2/2
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LMG	a	411	-	-	13/35/55/70	0/1/1/1
25	CLA	r	611	-	1/1/11/20	11/18/96/115	-
25	CLA	S	312	-	1/1/11/20	7/18/96/115	-
26	LHG	c	519	6	-	21/53/53/53	-
24	CHL	n	606	-	2/2/16/26	4/15/113/137	-
25	CLA	R	609	22	1/1/15/20	14/37/115/115	-
24	CHL	R	607	-	3/3/19/26	13/33/131/137	-
25	CLA	g	610	-	1/1/14/20	14/36/114/115	-
24	CHL	G	601	21	2/2/20/26	24/39/137/137	-
24	CHL	N	605	21	3/3/16/26	7/18/116/137	-
24	CHL	N	606	-	2/2/16/26	4/15/113/137	-
39	LUT	R	615	-	-	4/29/67/67	0/2/2/2
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
25	CLA	c	512	-	1/1/15/20	12/37/115/115	-
26	LHG	S	301	-	-	21/53/53/53	-
25	CLA	G	612	21	1/1/14/20	11/31/109/115	-
25	CLA	S	303	20	1/1/14/20	16/33/111/115	-
26	LHG	L	102	-	-	29/53/53/53	-
28	BCR	B	619	-	-	3/29/63/63	0/2/2/2
41	XAT	R	616	-	-	2/31/93/93	0/4/4/4
25	CLA	N	612	-	1/1/14/20	18/31/109/115	-
25	CLA	C	508	-	1/1/15/20	12/37/115/115	-
39	LUT	n	615	-	-	8/29/67/67	0/2/2/2
25	CLA	a	403	-	1/1/15/20	7/37/115/115	-
24	CHL	r	607	-	3/3/19/26	13/33/131/137	-
26	LHG	s	318	25	-	21/53/53/53	-
25	CLA	D	402	-	1/1/15/20	10/37/115/115	-
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
25	CLA	c	501	-	1/1/15/20	7/37/115/115	-
24	CHL	2	603	2	3/3/16/26	10/15/113/137	-
25	CLA	S	305	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	B	622	-	-	18/53/53/53	-
24	CHL	g	606	-	3/3/16/26	3/20/118/137	-
26	LHG	C	517	-	-	16/53/53/53	-
25	CLA	R	601	-	1/1/11/20	11/18/96/115	-
25	CLA	G	614	-	1/1/11/20	9/17/95/115	-
25	CLA	b	616	-	1/1/15/20	17/37/115/115	-
25	CLA	D	403	-	1/1/15/20	12/37/115/115	-
25	CLA	c	508	-	1/1/15/20	12/37/115/115	-
25	CLA	g	612	21	1/1/14/20	11/31/109/115	-
39	LUT	G	616	-	-	0/29/67/67	0/2/2/2
35	DGD	b	626	-	-	23/51/91/95	0/2/2/2
39	LUT	g	616	-	-	0/29/67/67	0/2/2/2
27	PHO	a	405	-	-	1/37/103/103	0/5/6/6
29	SQD	l	102	-	-	13/37/57/69	0/1/1/1
25	CLA	2	602	2	1/1/14/20	13/31/109/115	-
25	CLA	n	602	21	1/1/15/20	13/37/115/115	-
25	CLA	n	614	-	1/1/11/20	4/17/95/115	-
40	NEX	g	617	25	-	11/27/83/83	0/3/3/3
39	LUT	G	615	-	-	5/29/67/67	0/2/2/2
25	CLA	c	513	-	1/1/15/20	13/37/115/115	-
29	SQD	L	103	-	-	27/49/69/69	0/1/1/1
25	CLA	s	310	20	1/1/13/20	9/25/103/115	-
30	LMG	A	410	-	-	13/35/55/70	0/1/1/1
24	CHL	N	607	-	2/2/20/26	18/39/137/137	-
24	CHL	g	607	-	2/2/16/26	6/15/113/137	-
25	CLA	A	402	-	1/1/15/20	7/37/115/115	-
24	CHL	G	606	-	3/3/16/26	3/20/118/137	-
25	CLA	s	311	26	1/1/13/20	12/27/105/115	-
24	CHL	S	306	-	3/3/16/26	7/15/113/137	-
24	CHL	R	606	-	3/3/16/26	11/15/113/137	-
24	CHL	y	309	-	3/3/20/26	20/39/137/137	-
25	CLA	a	402	-	1/1/15/20	7/37/115/115	-
24	CHL	6	603	2	3/3/16/26	10/15/113/137	-
25	CLA	C	504	-	1/1/14/20	14/31/109/115	-
24	CHL	s	308	-	3/3/16/26	2/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	C	520	-	-	18/46/66/70	0/1/1/1
26	LHG	B	621	-	-	19/51/51/53	-
39	LUT	r	615	-	-	4/29/67/67	0/2/2/2
25	CLA	C	502	-	1/1/15/20	6/37/115/115	-
25	CLA	N	613	-	1/1/14/20	21/31/109/115	-
28	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
40	NEX	Y	318	-	-	7/27/83/83	1/3/3/3
25	CLA	s	312	-	1/1/11/20	7/18/96/115	-
39	LUT	S	315	-	-	4/29/67/67	0/2/2/2
25	CLA	A	401	-	1/1/15/20	7/37/115/115	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
25	CLA	y	304	-	1/1/15/20	22/37/115/115	-
25	CLA	B	606	-	1/1/15/20	11/37/115/115	-
25	CLA	r	604	-	1/1/11/20	4/17/95/115	-
30	LMG	D	407	-	-	16/41/61/70	0/1/1/1
27	PHO	a	404	-	-	12/37/103/103	0/5/6/6
25	CLA	S	311	26	1/1/13/20	12/27/105/115	-
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
24	CHL	n	609	21	2/2/20/26	15/39/137/137	-
26	LHG	s	301	-	-	21/53/53/53	-
25	CLA	b	607	-	1/1/15/20	16/37/115/115	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
25	CLA	y	303	21	1/1/15/20	12/37/115/115	-
24	CHL	g	605	21	3/3/16/26	9/15/113/137	-
25	CLA	B	605	-	1/1/15/20	7/37/115/115	-
30	LMG	d	407	-	-	16/41/61/70	0/1/1/1
25	CLA	C	506	-	1/1/15/20	11/37/115/115	-
25	CLA	G	603	-	1/1/14/20	12/31/109/115	-
35	DGD	c	516	-	-	28/51/91/95	0/2/2/2
25	CLA	b	606	-	1/1/15/20	11/37/115/115	-
24	CHL	5	301	1	3/3/16/26	4/15/113/137	-
39	LUT	y	317	-	-	3/29/67/67	0/2/2/2
28	BCR	t	101	16	-	17/29/63/63	0/2/2/2
28	BCR	a	407	-	-	5/29/63/63	0/2/2/2

The worst 5 of 2344 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	101	HEM	FE-NB	8.66	2.39	1.96
38	f	101	HEM	FE-NB	8.66	2.39	1.96
25	N	610	CLA	C1B-NB	7.29	1.41	1.35
25	n	610	CLA	C1B-NB	7.26	1.41	1.35
25	y	311	CLA	C1B-NB	7.19	1.41	1.35

The worst 5 of 4029 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	305	CLA	C4A-NA-C1A	-18.81	98.25	106.71
25	S	305	CLA	C4A-NA-C1A	-18.75	98.28	106.71
25	r	601	CLA	C4A-NA-C1A	-17.30	98.93	106.71
25	R	601	CLA	C4A-NA-C1A	-17.14	99.00	106.71
25	R	610	CLA	C4A-NA-C1A	-16.34	99.36	106.71

5 of 324 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	301	CHL	ND
24	1	301	CHL	NA
24	1	301	CHL	NC
24	1	302	CHL	ND
24	1	302	CHL	NA

5 of 3889 torsion outliers are listed below:

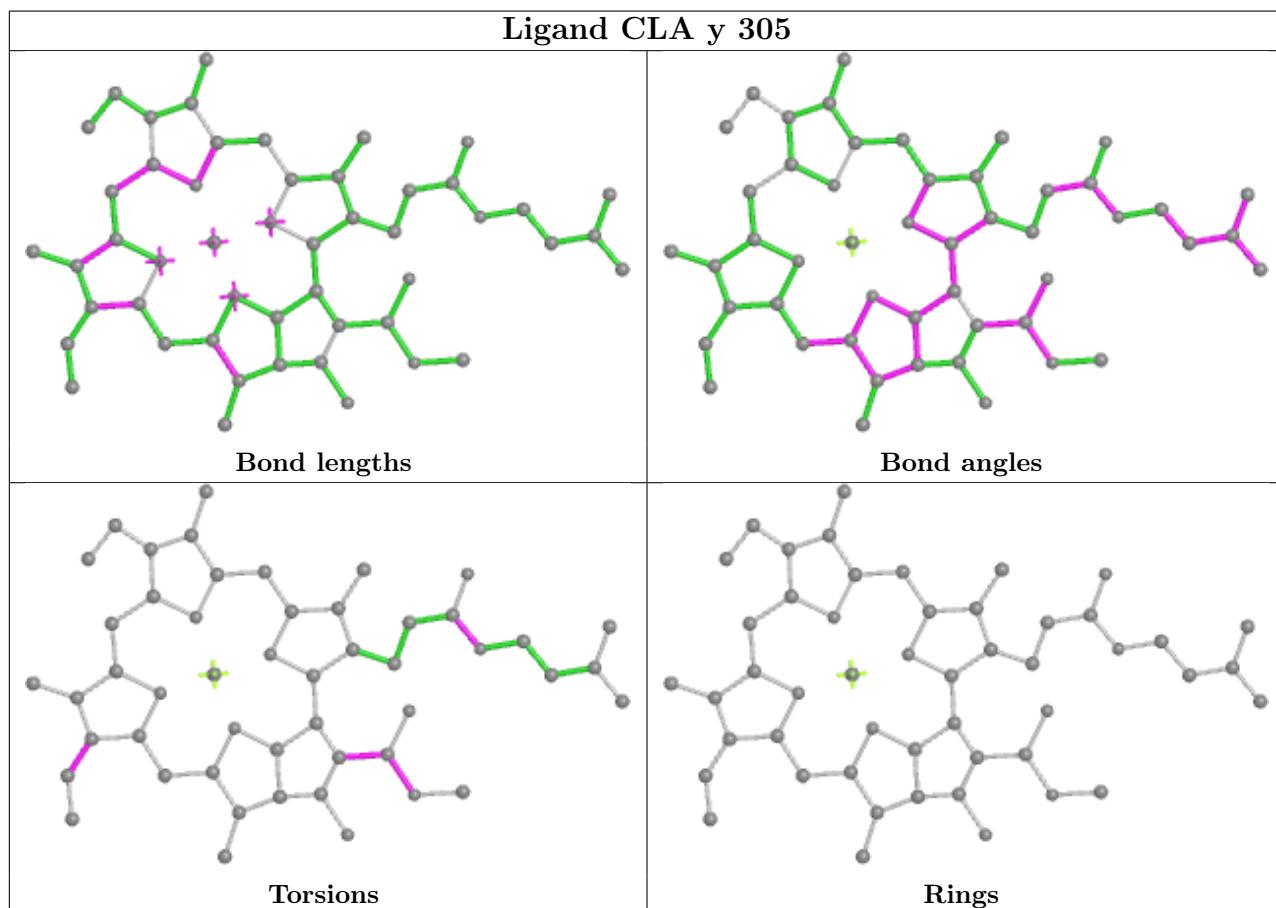
Mol	Chain	Res	Type	Atoms
24	1	302	CHL	C1A-C2A-CAA-CBA
24	1	302	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	CHA-CBD-CGD-O2D

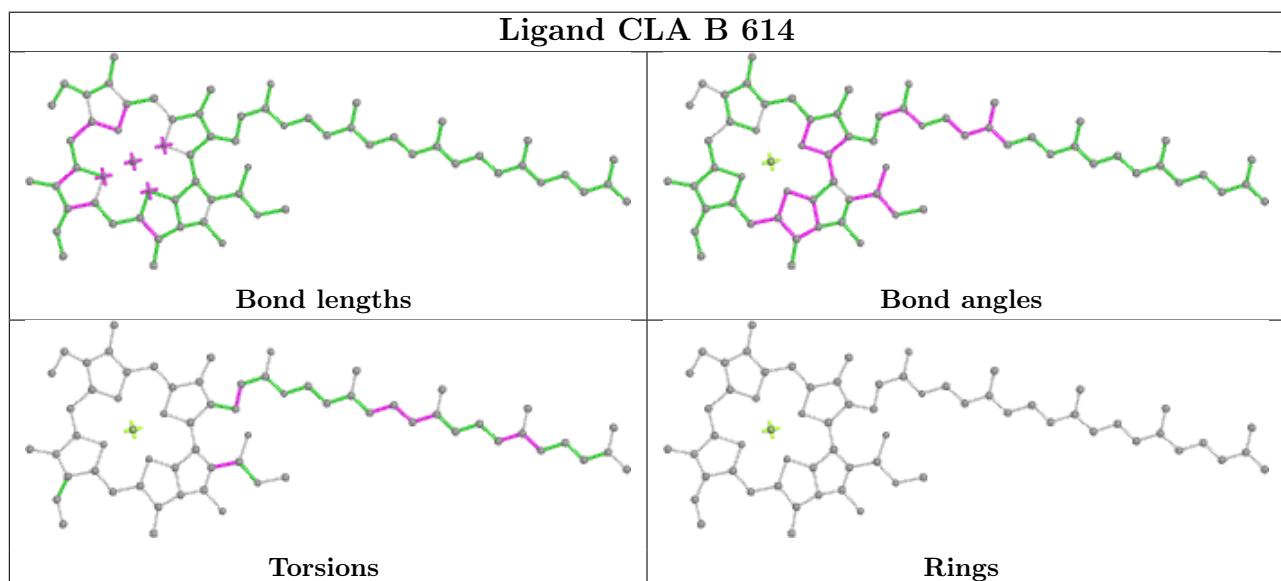
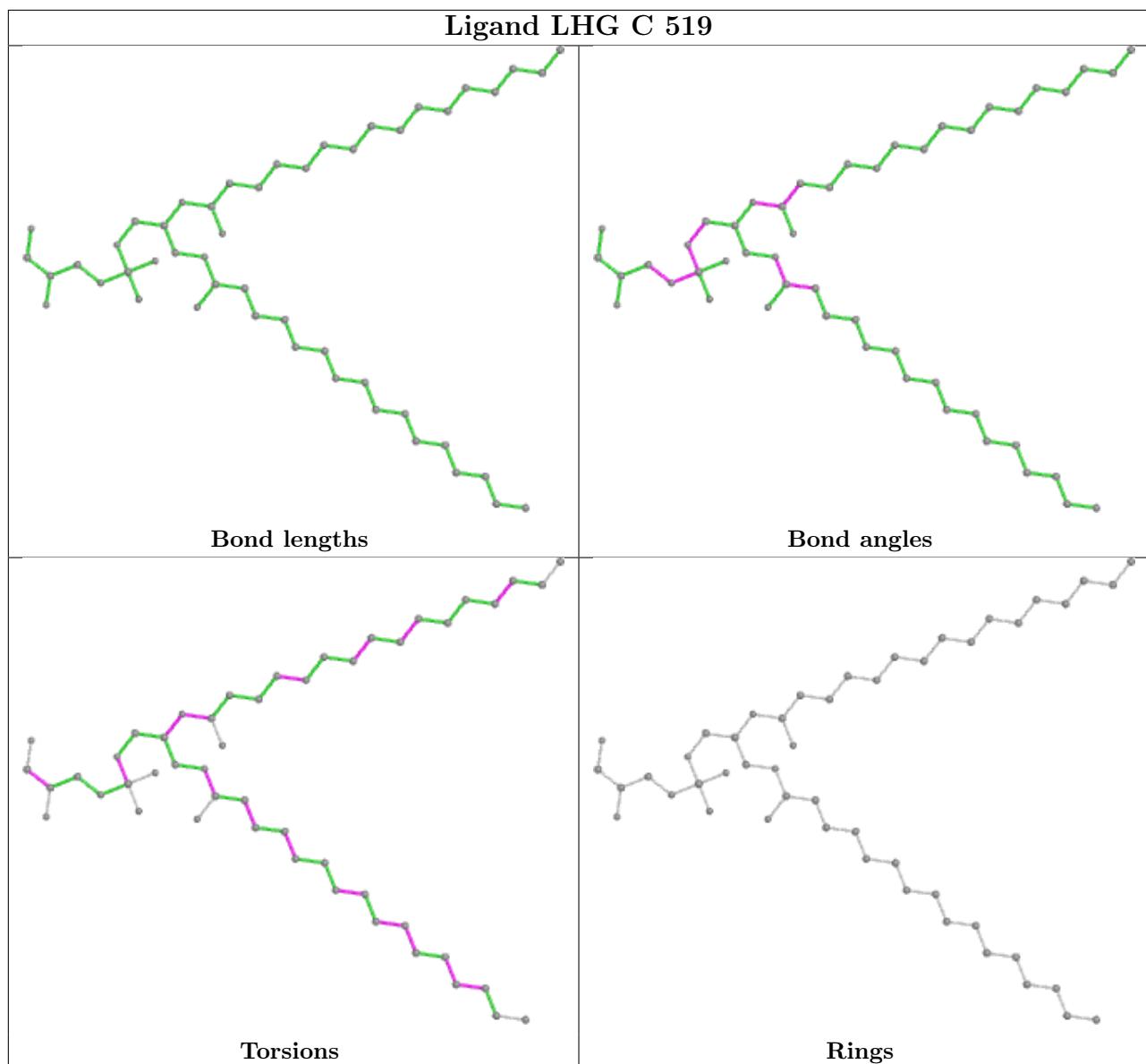
All (2) ring outliers are listed below:

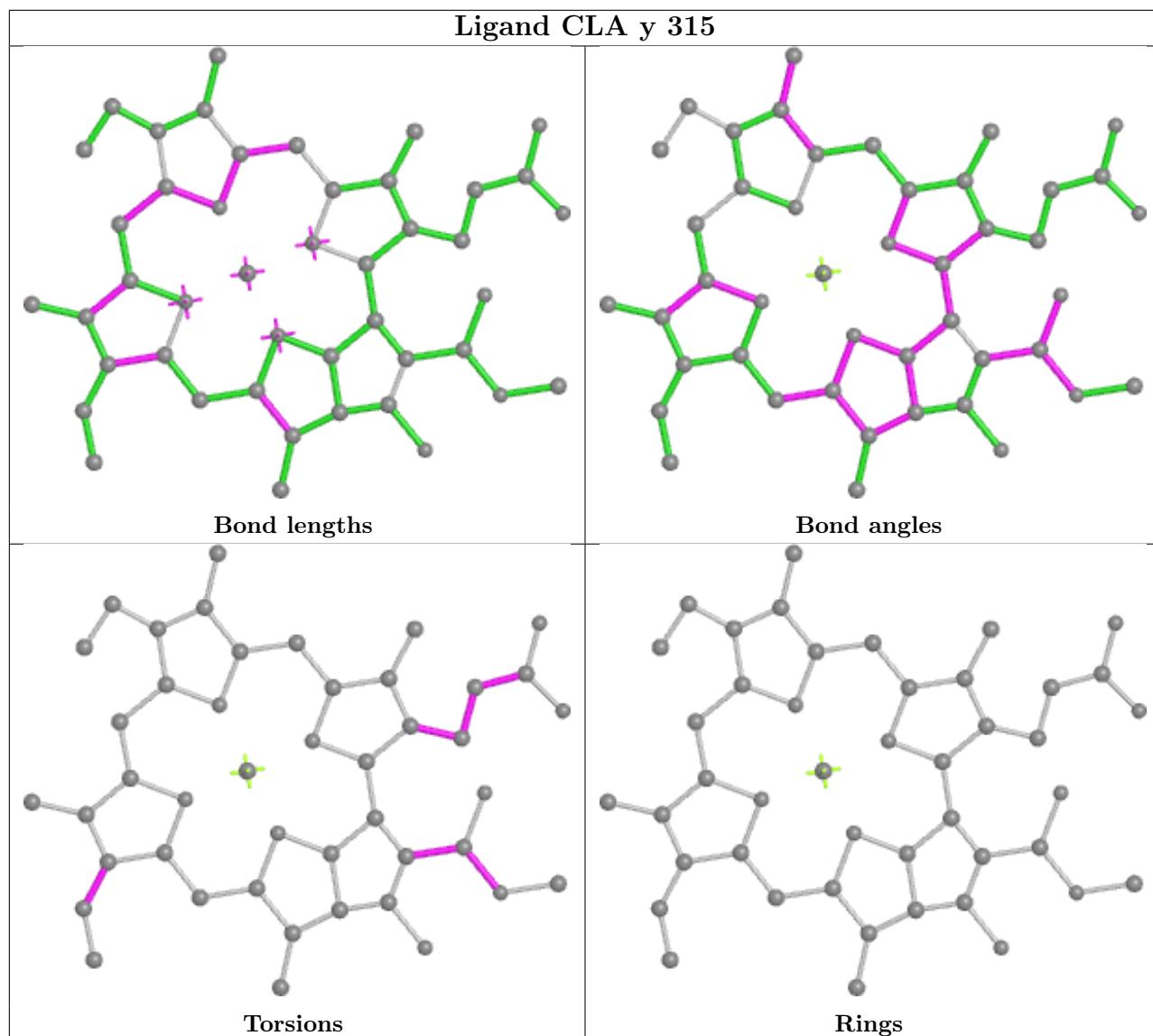
Mol	Chain	Res	Type	Atoms
40	Y	318	NEX	C1-C2-C3-C4-C5-C6
40	y	318	NEX	C1-C2-C3-C4-C5-C6

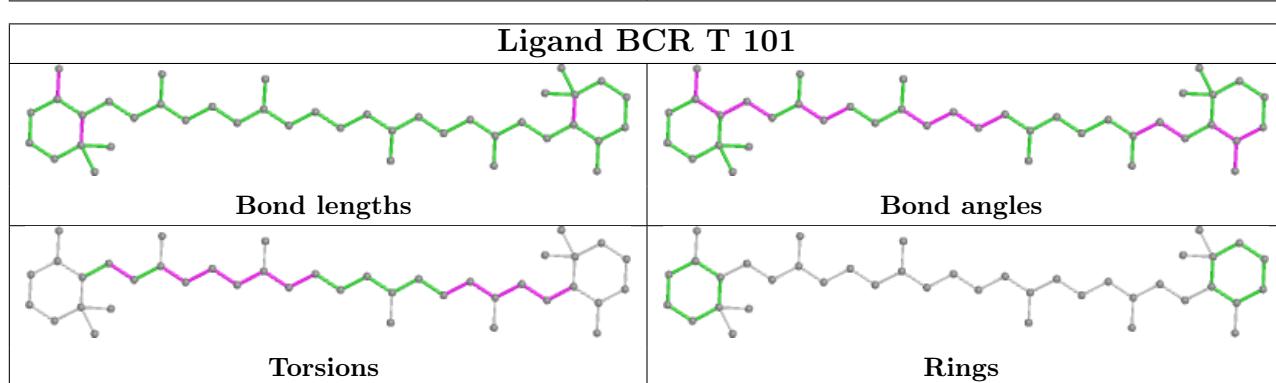
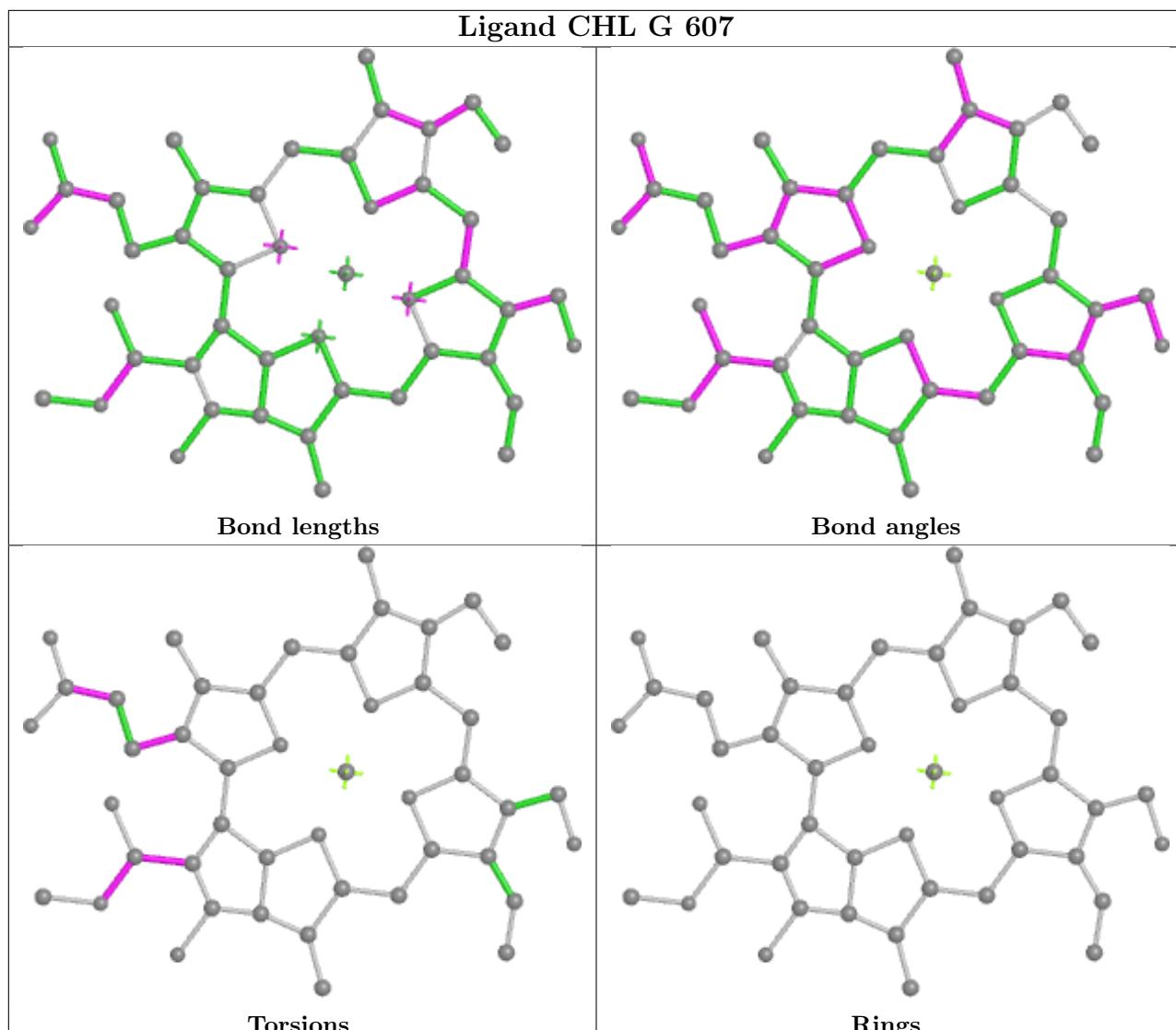
No monomer is involved in short contacts.

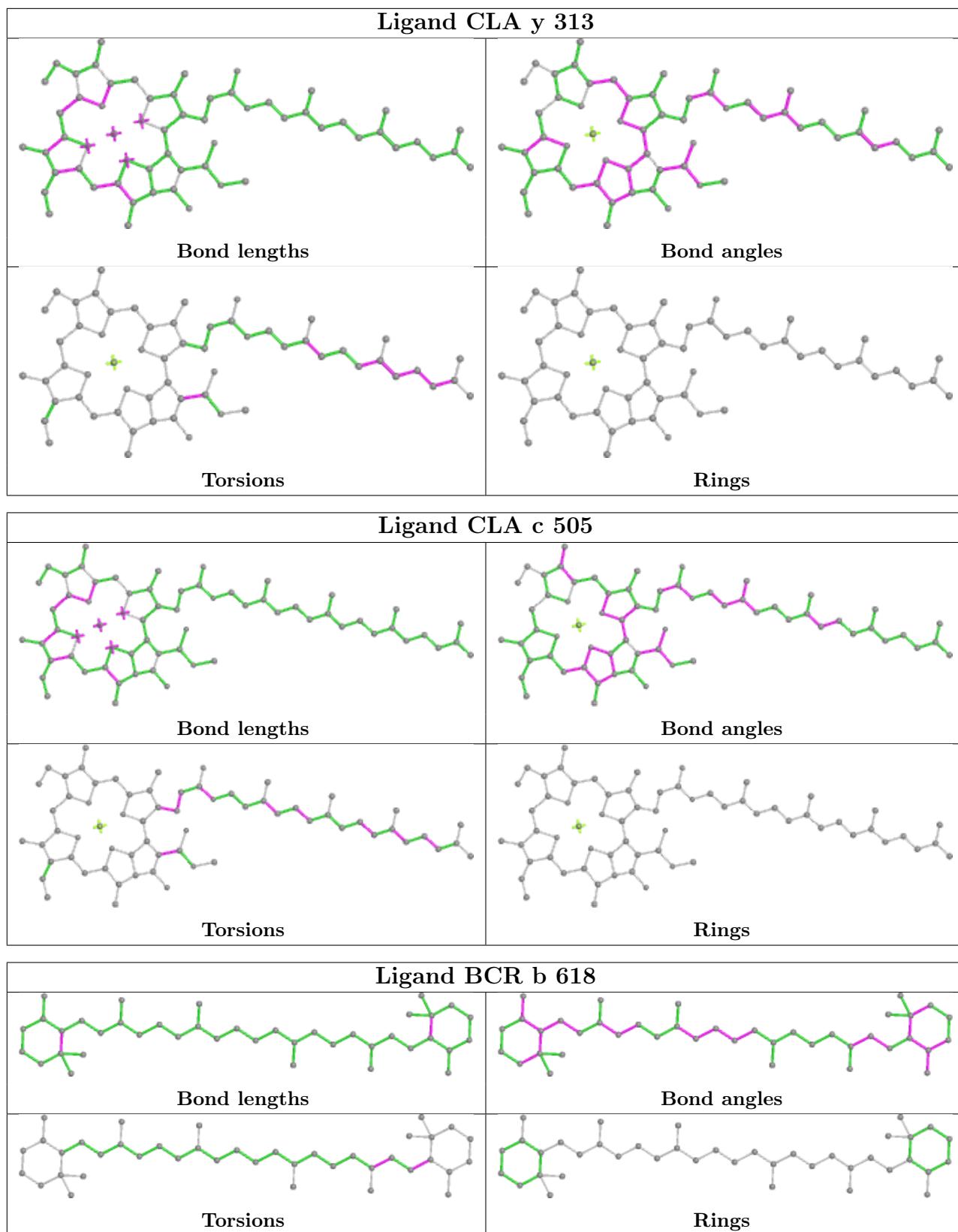
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

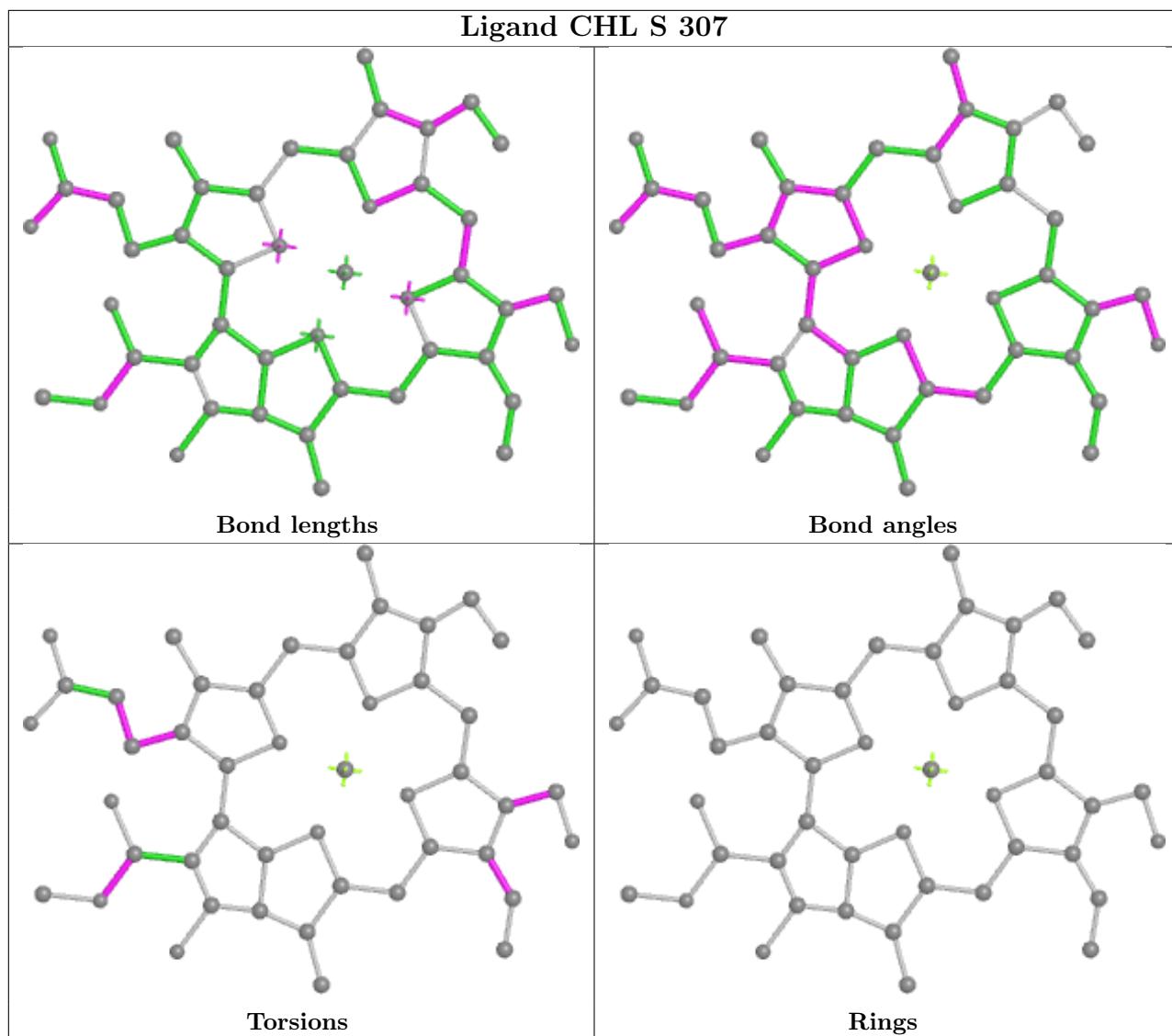


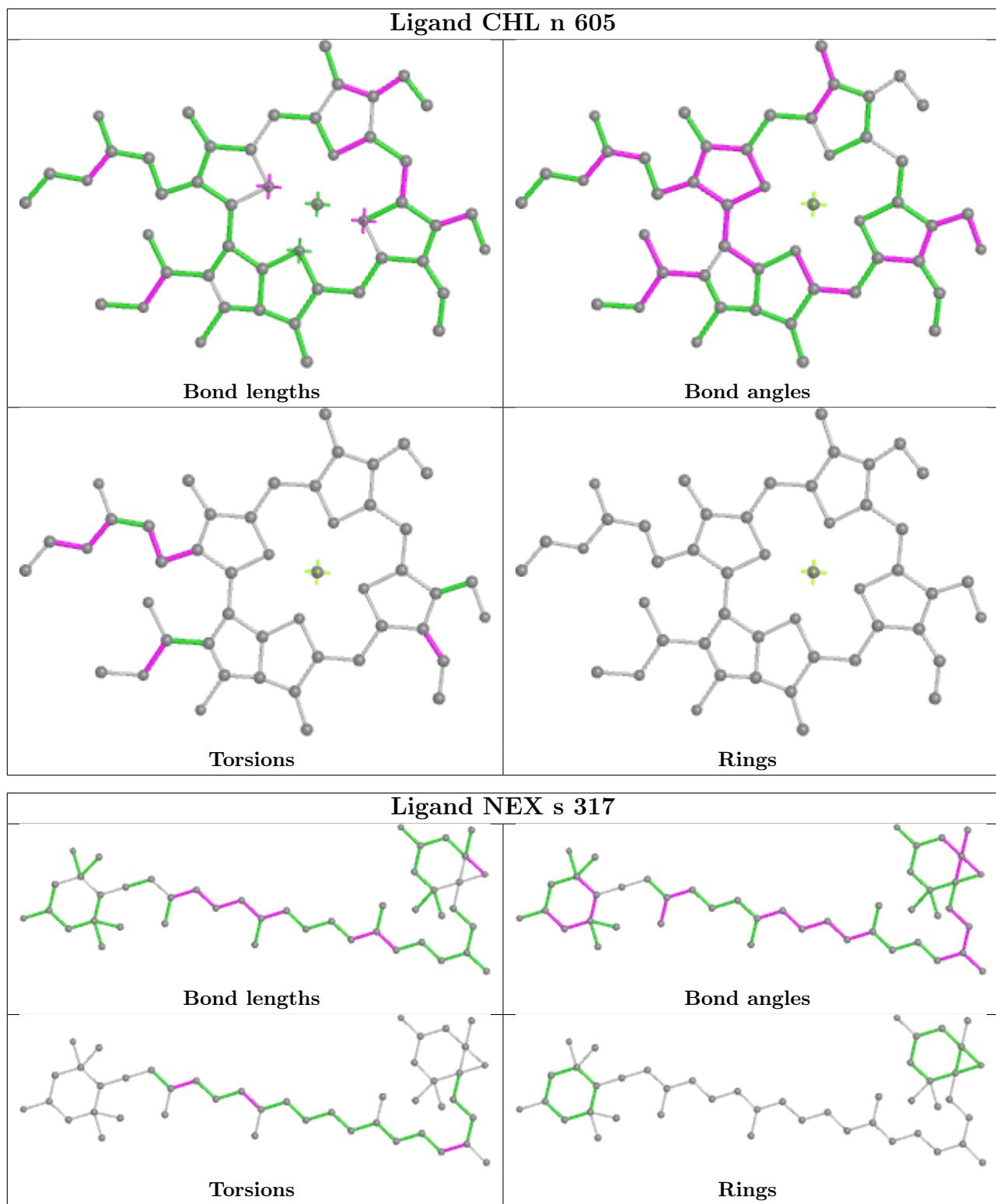


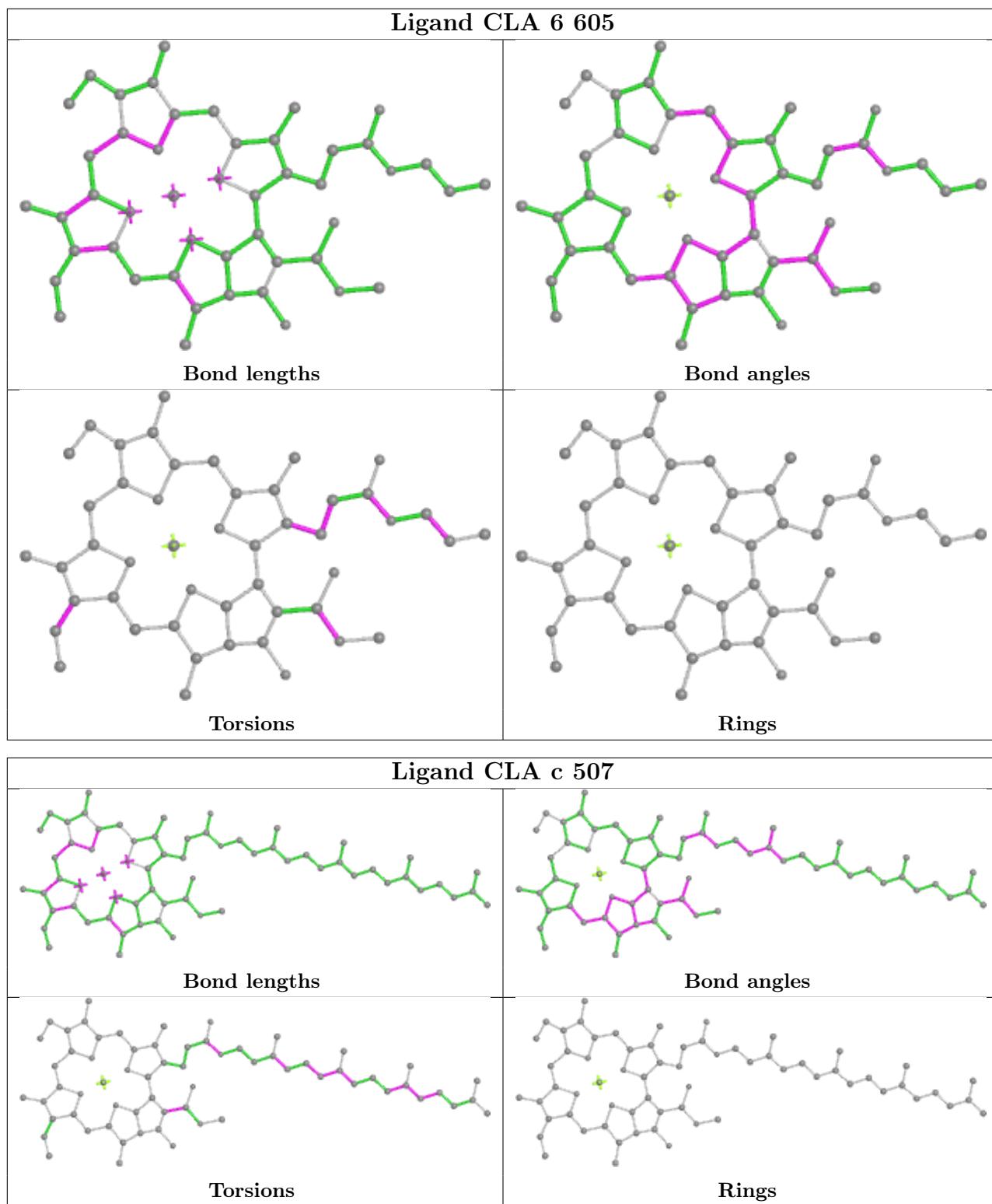


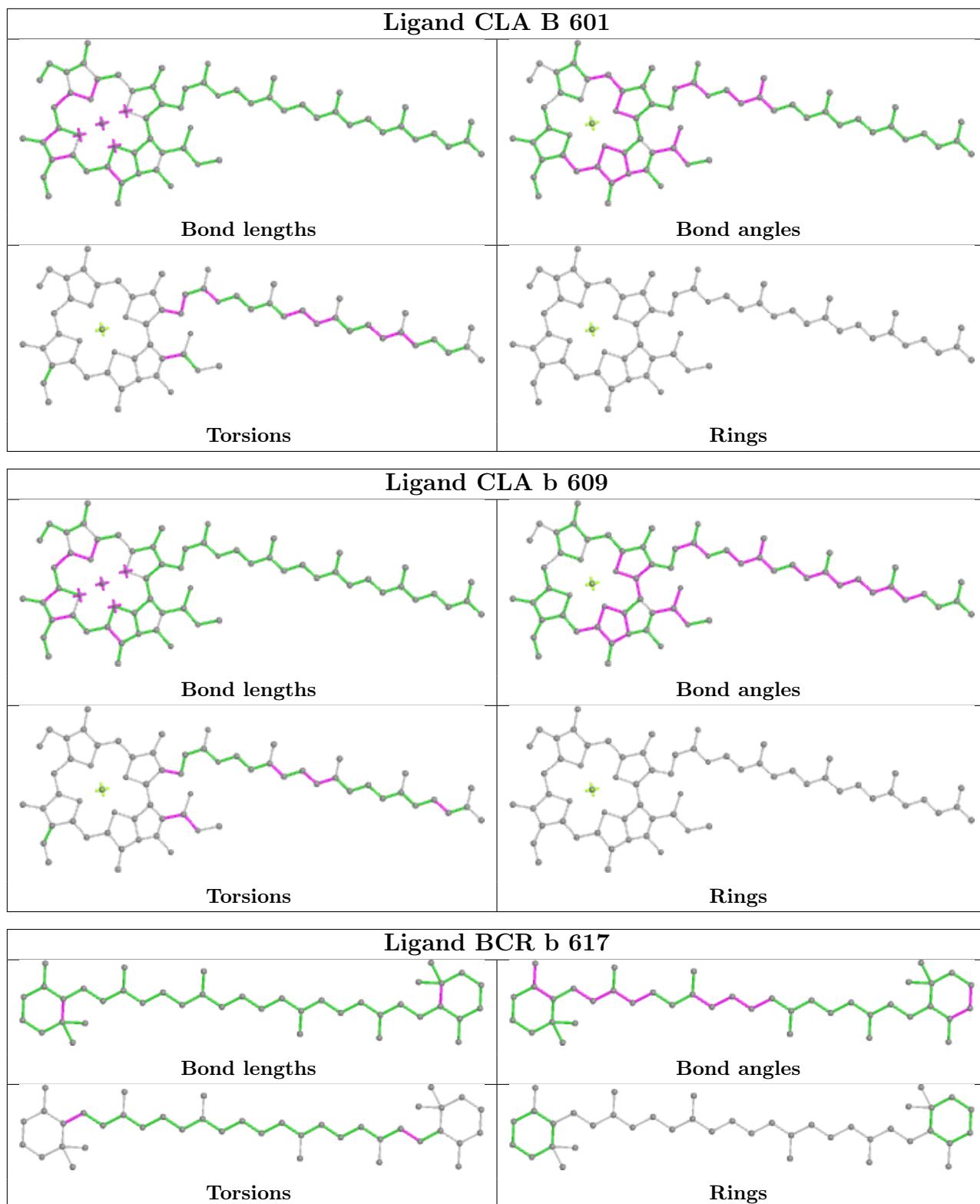


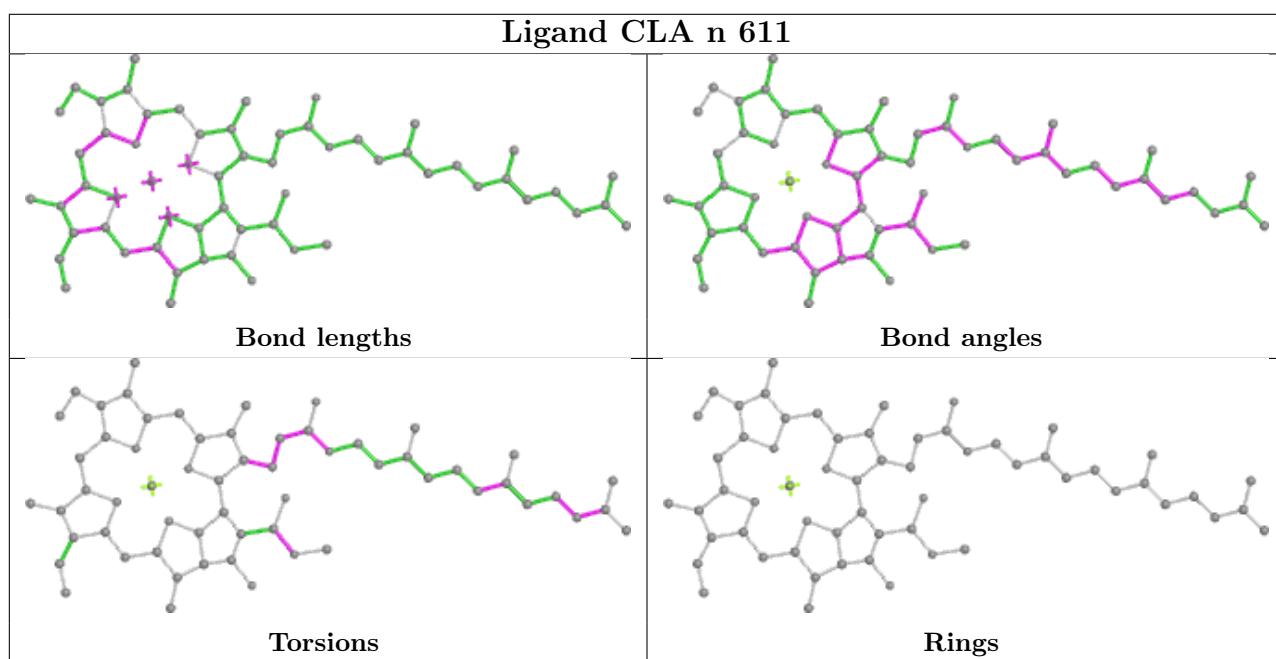
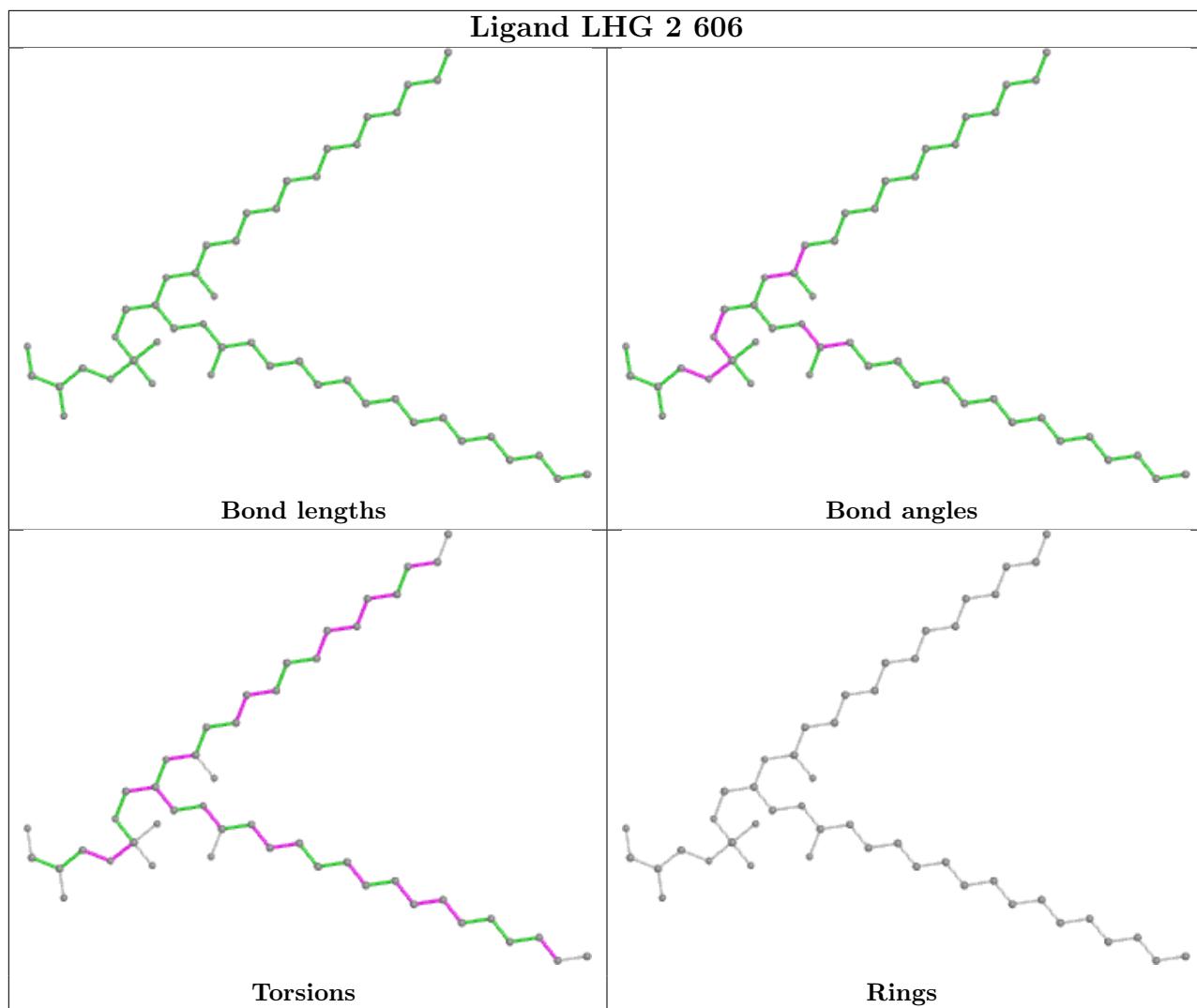


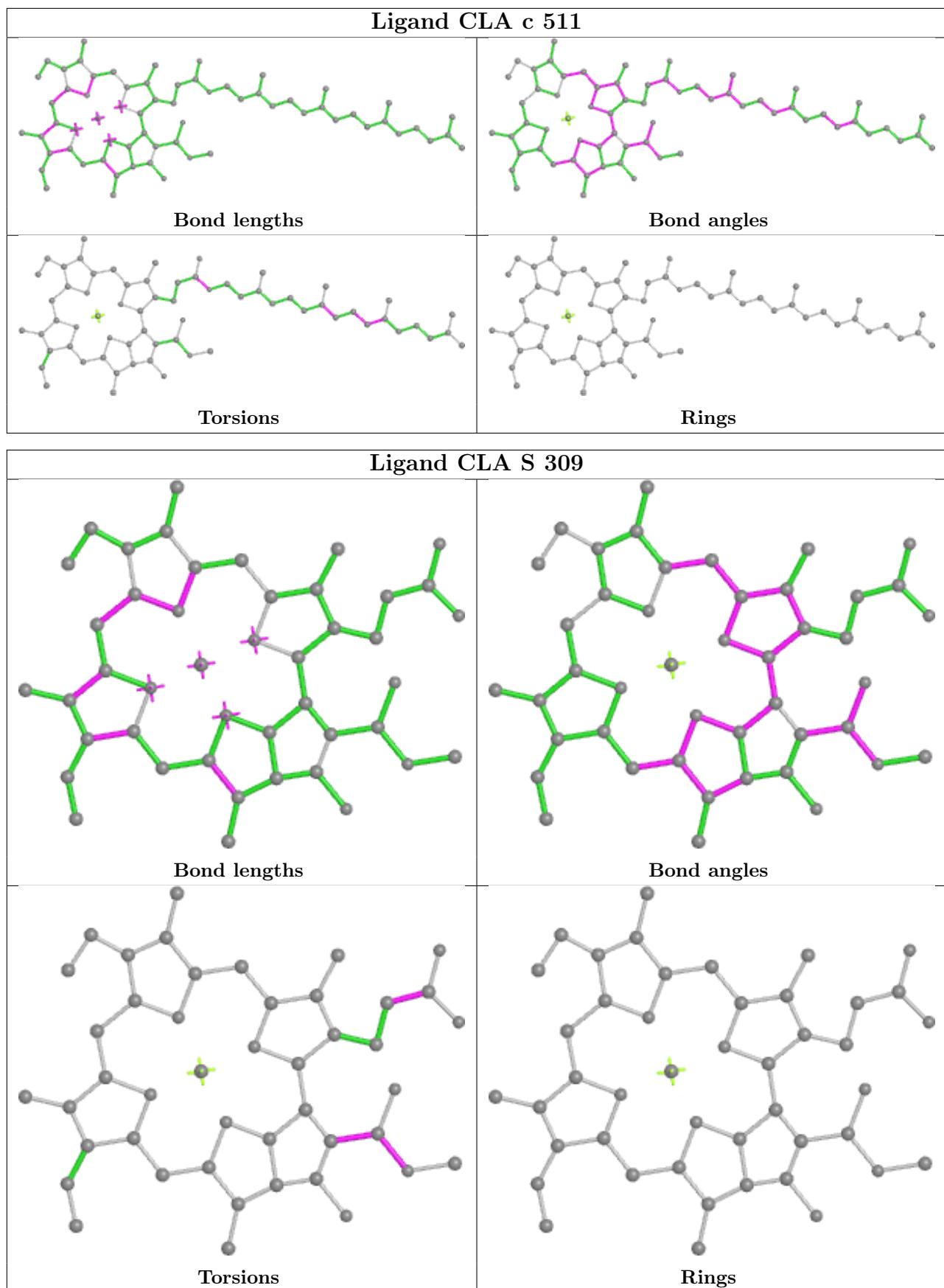


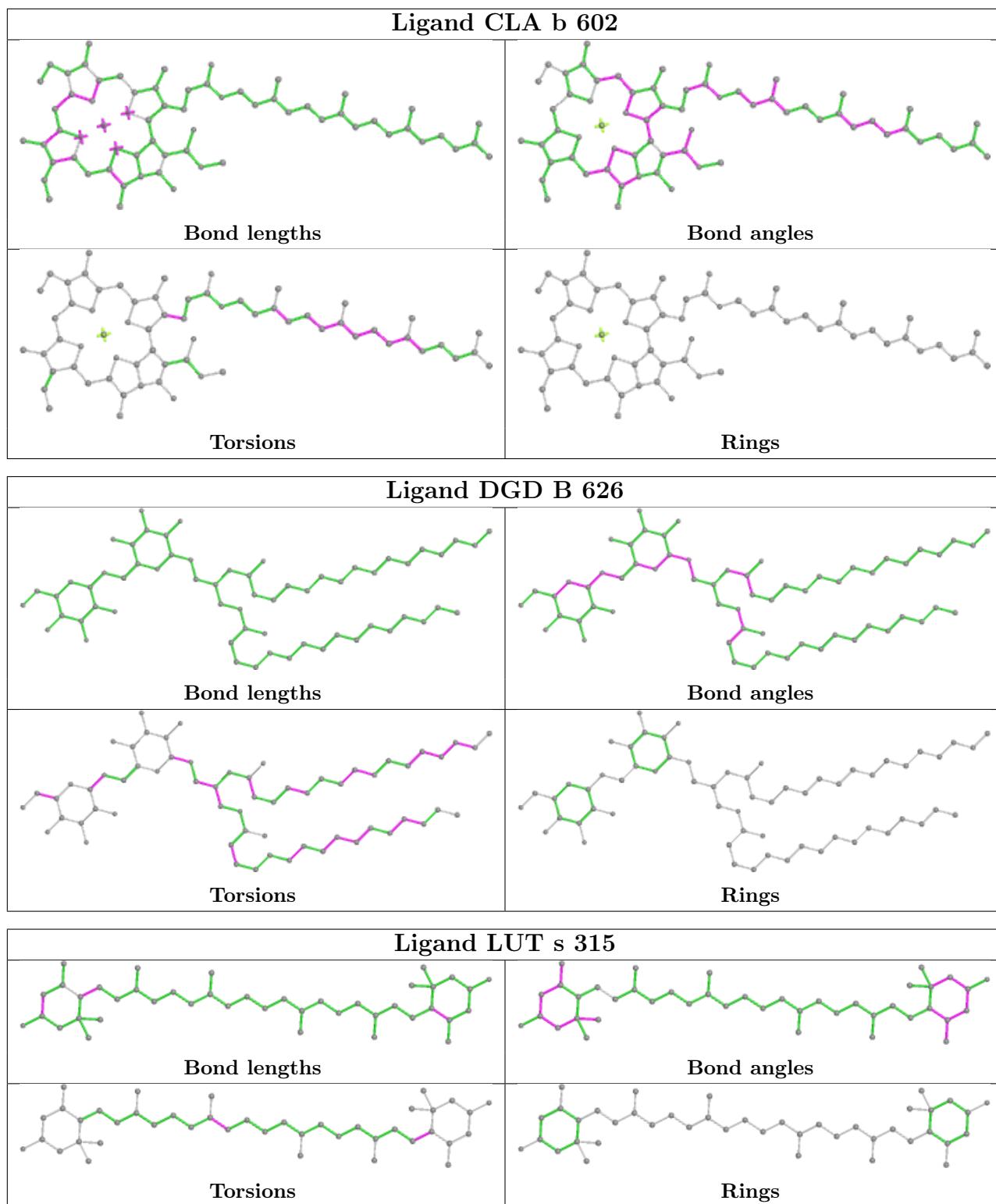


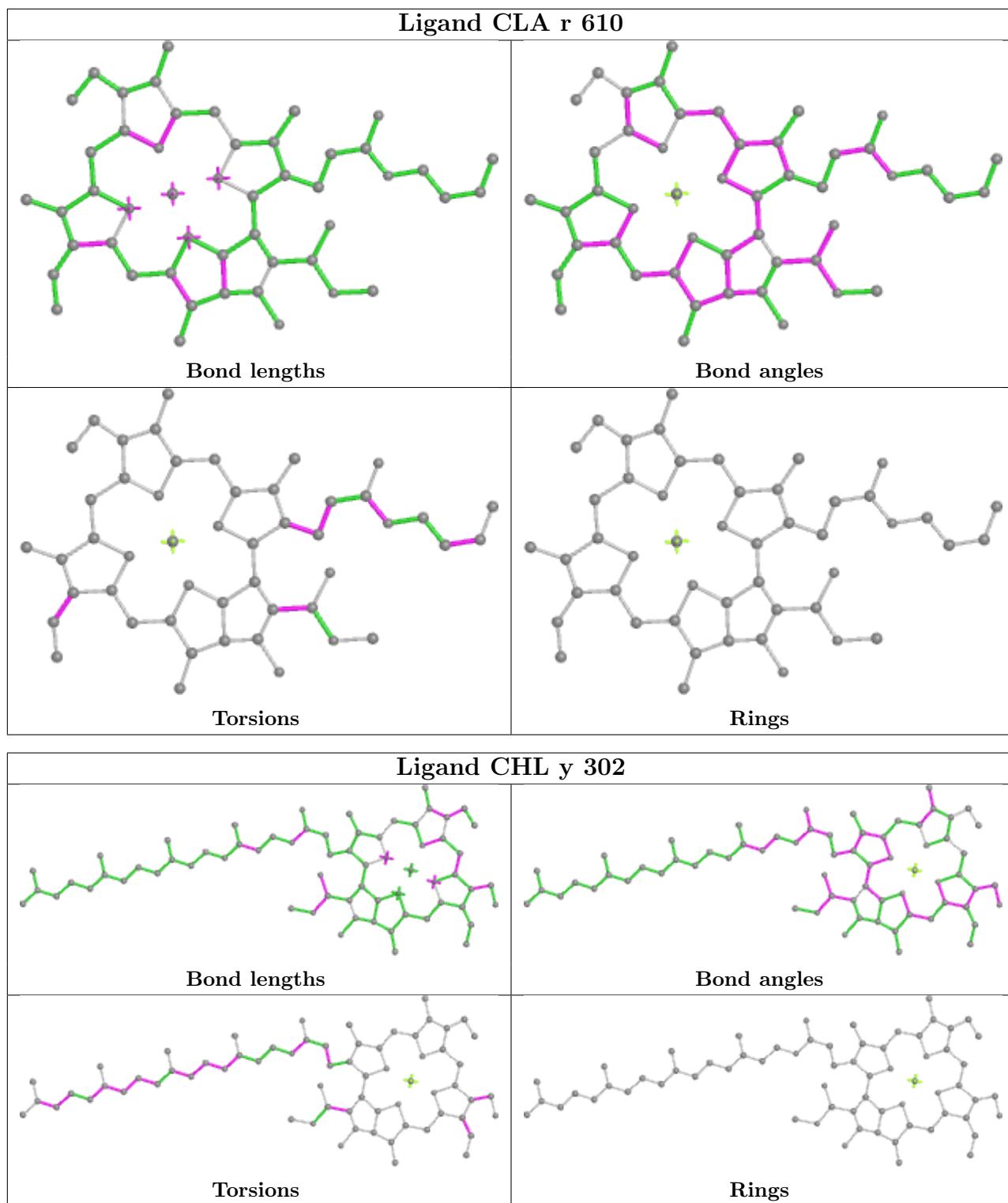


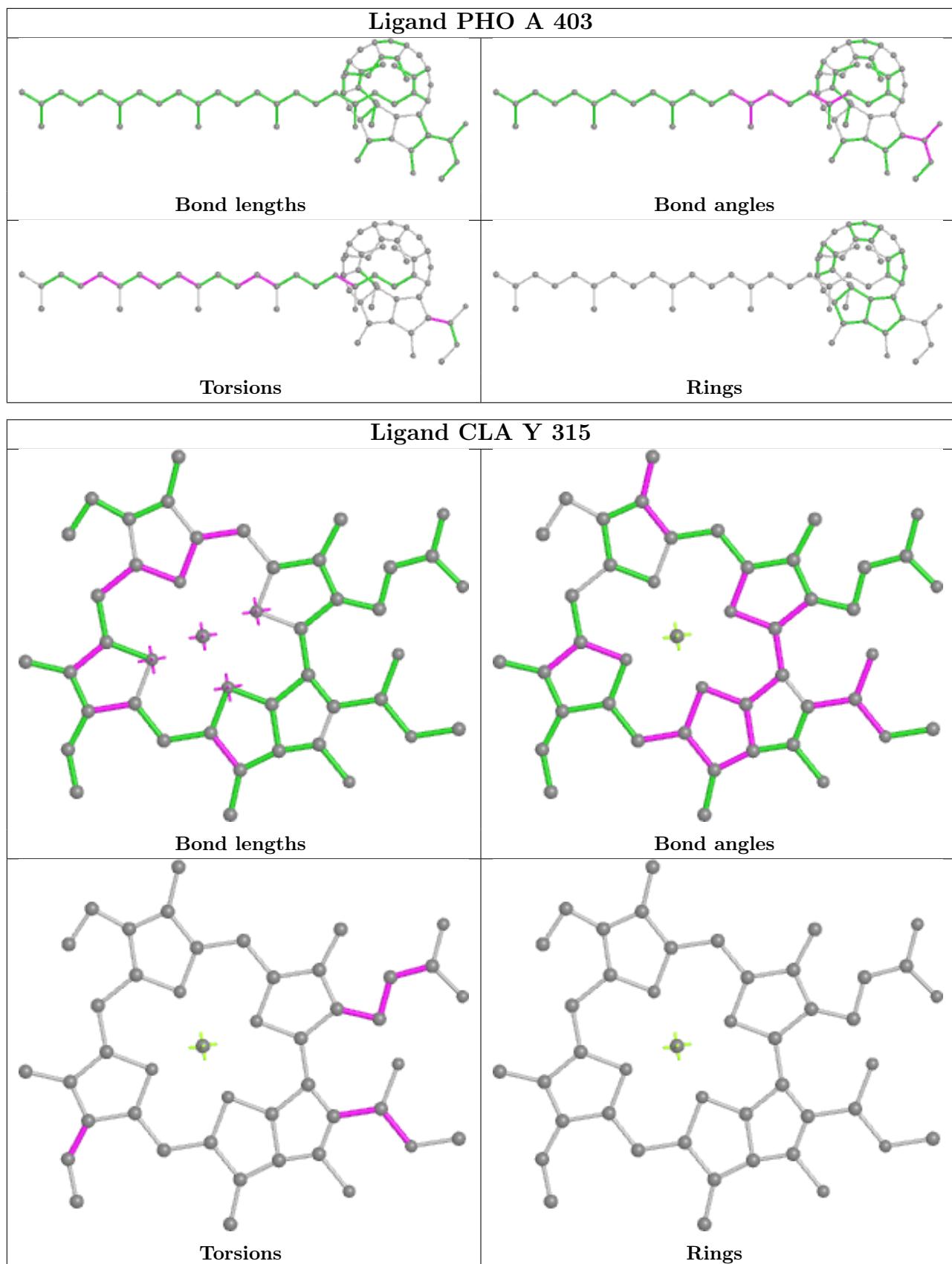


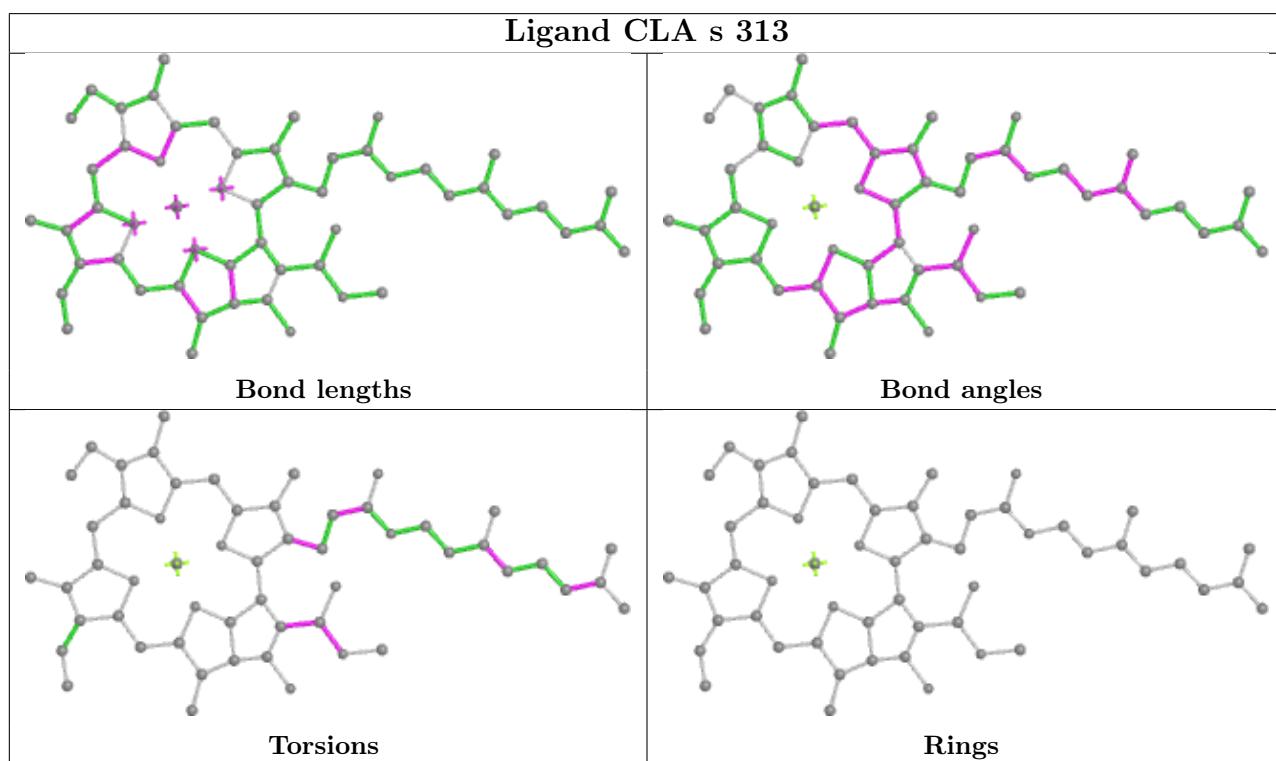
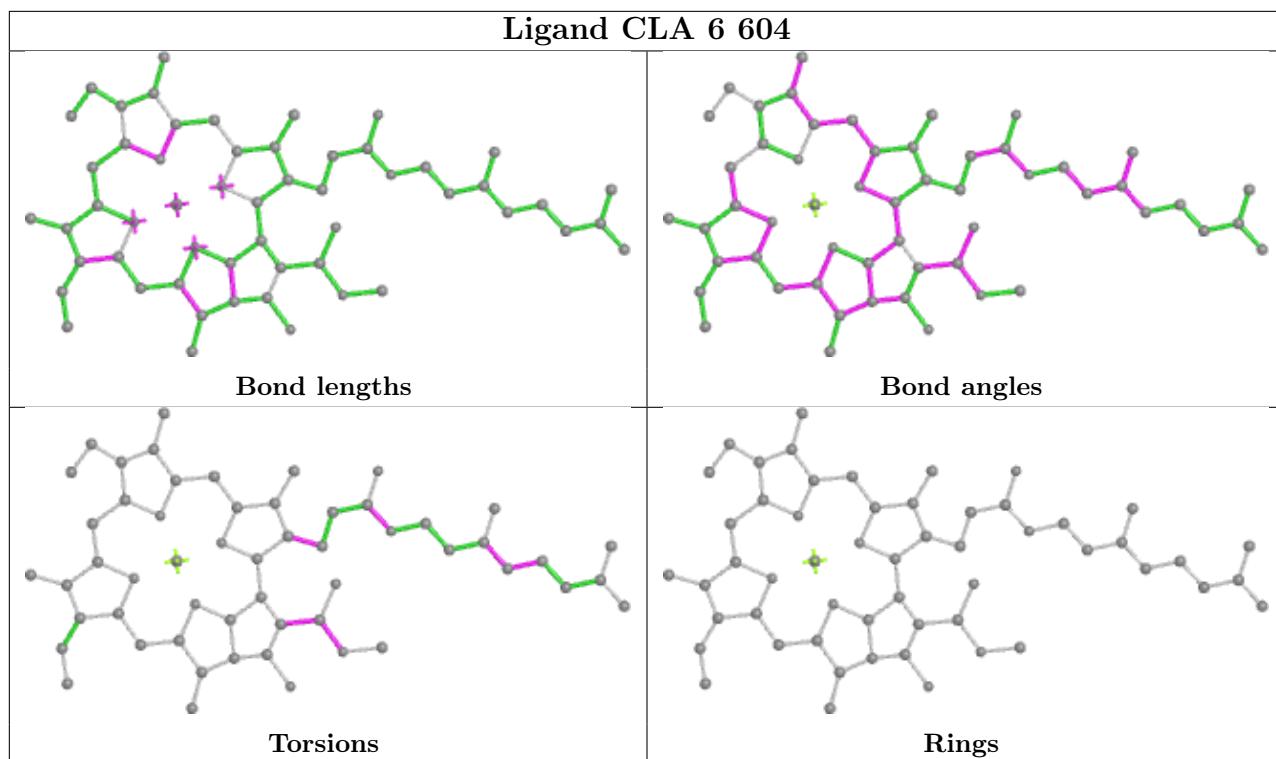


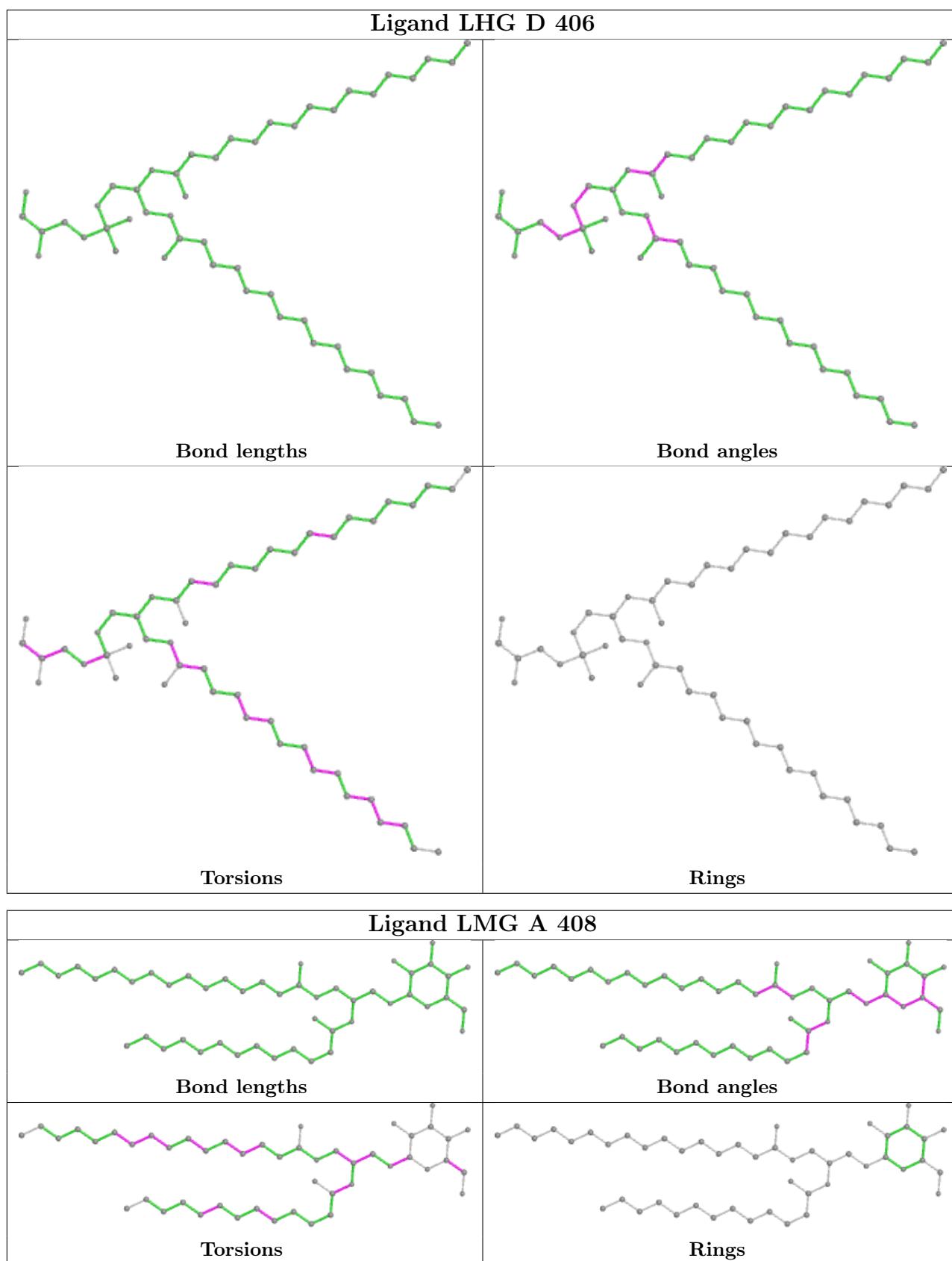


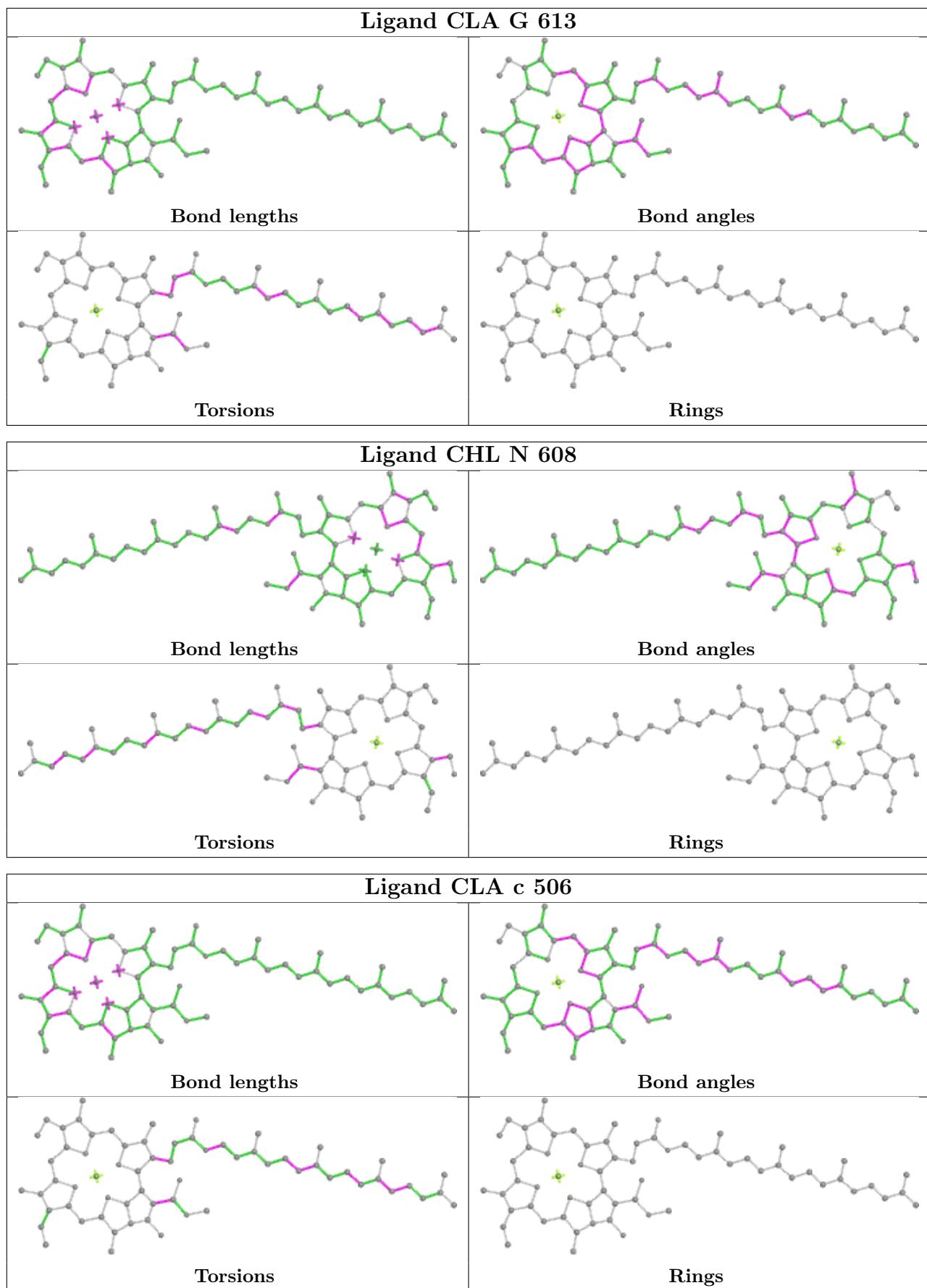


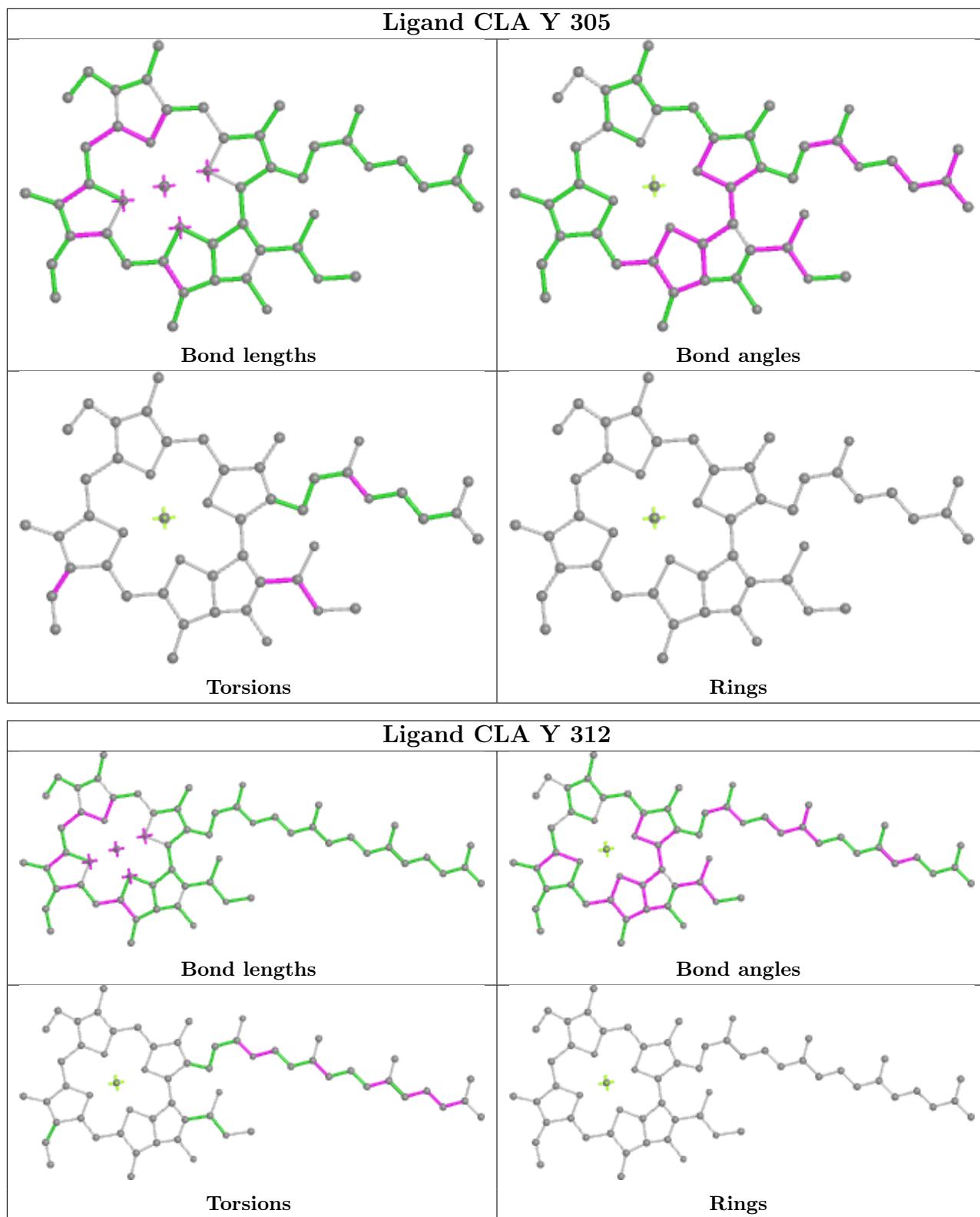


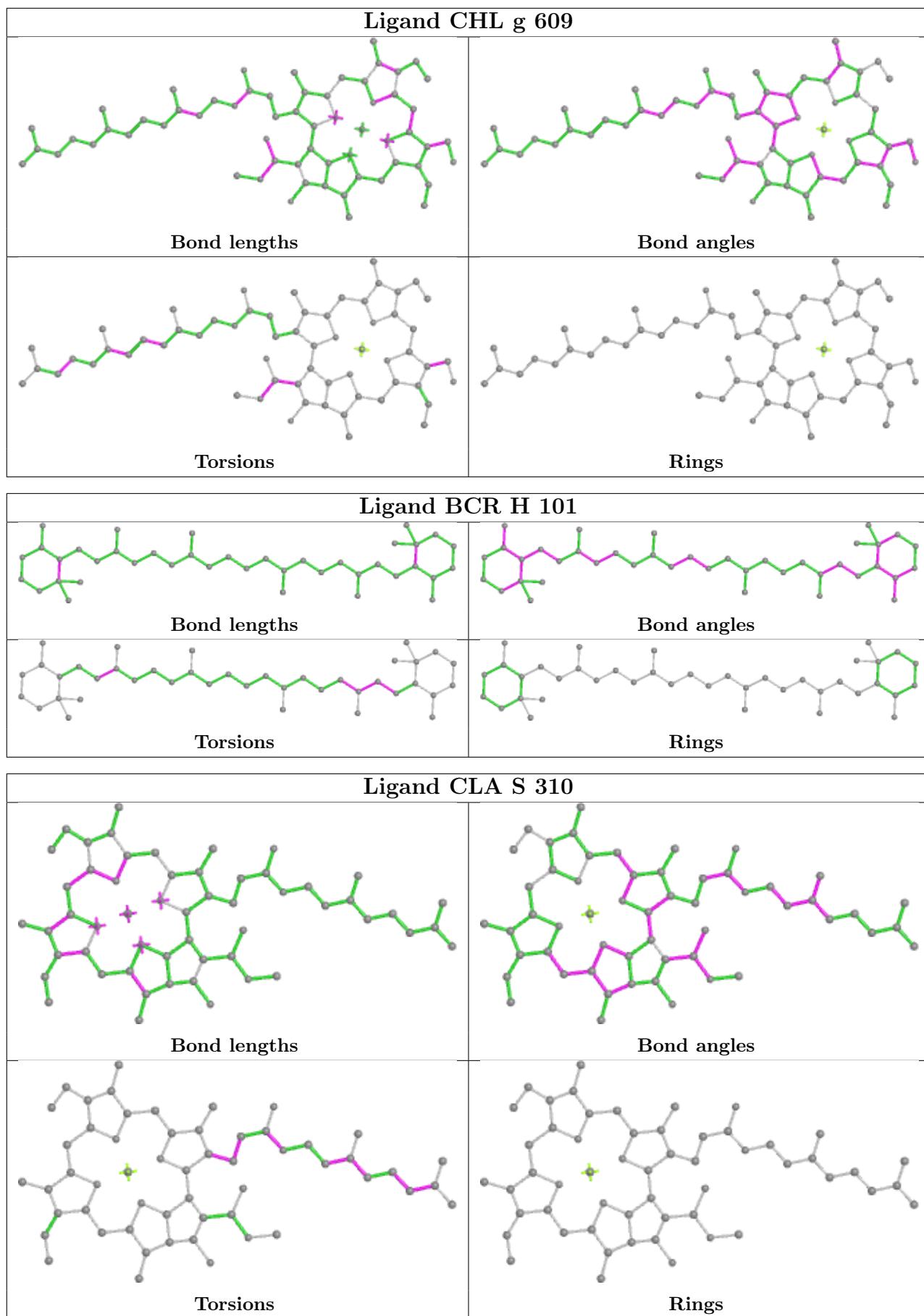


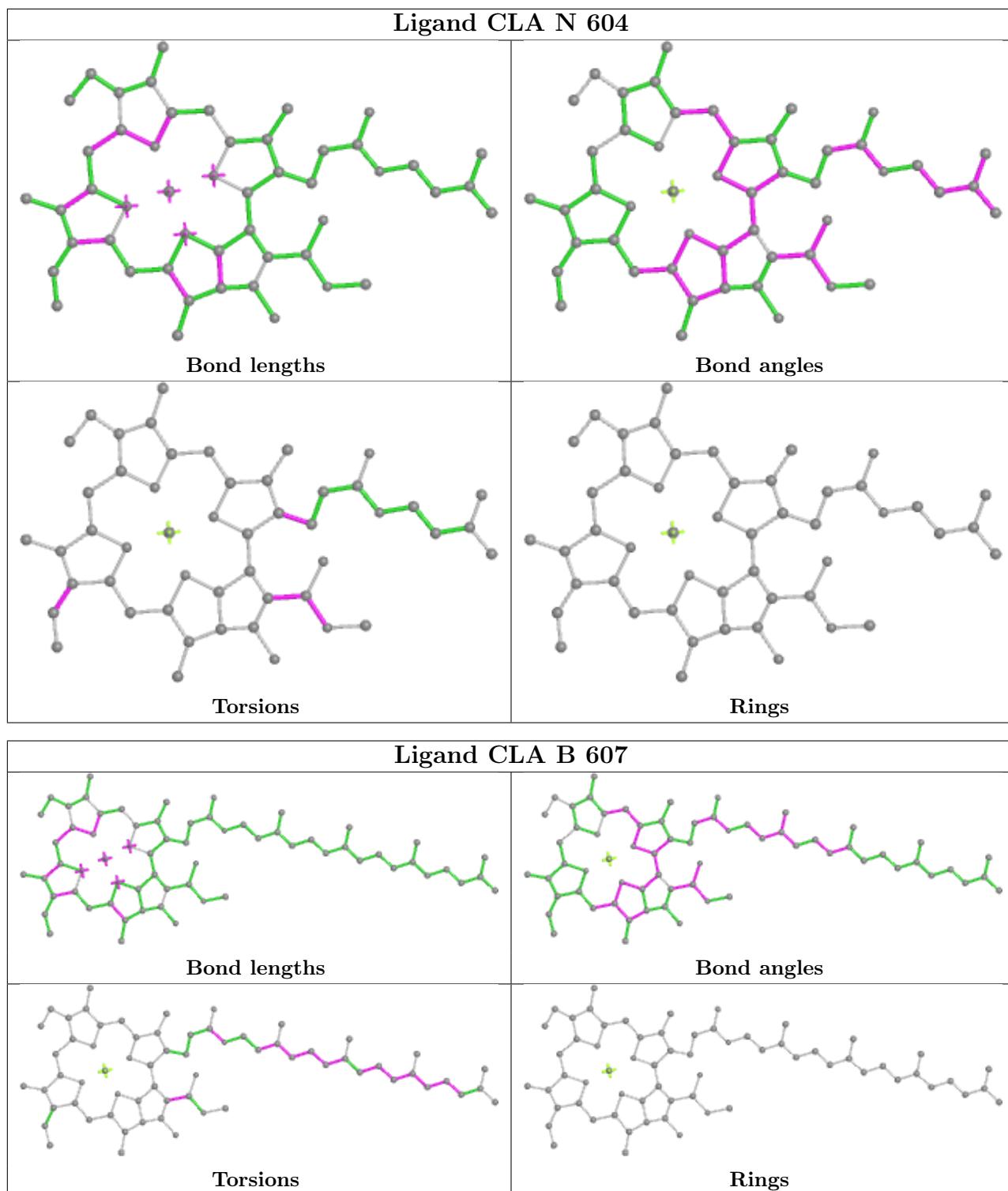


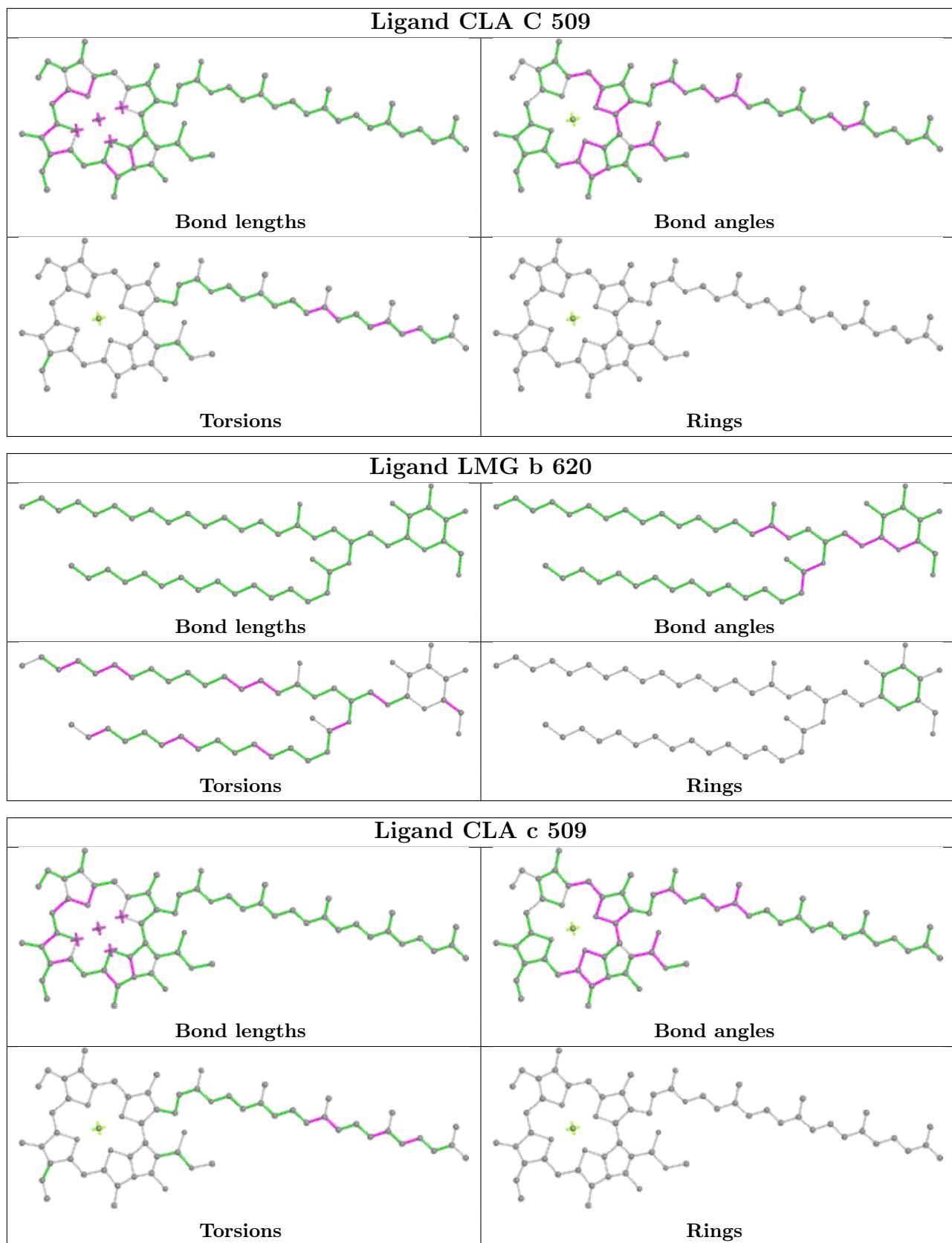


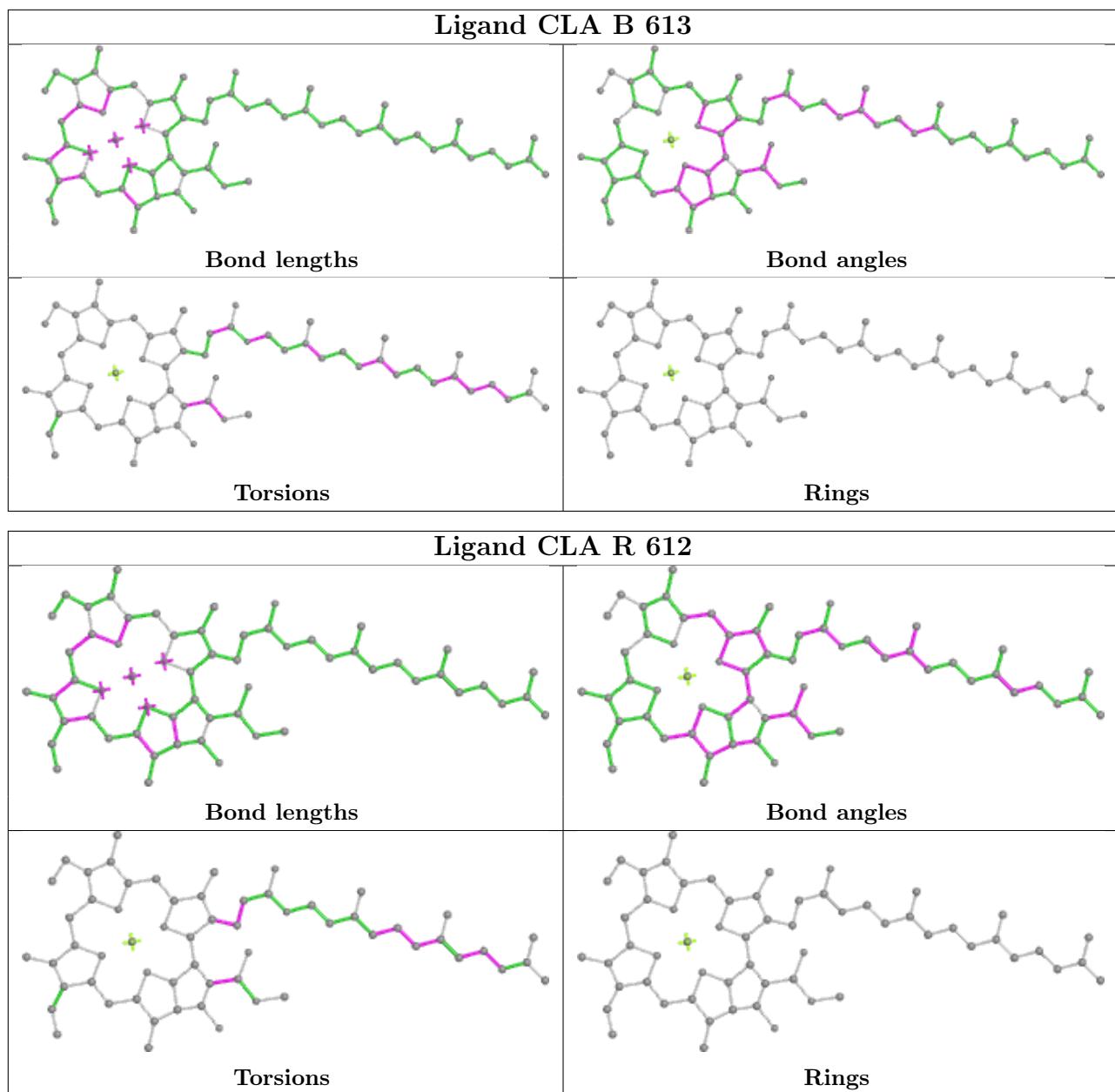


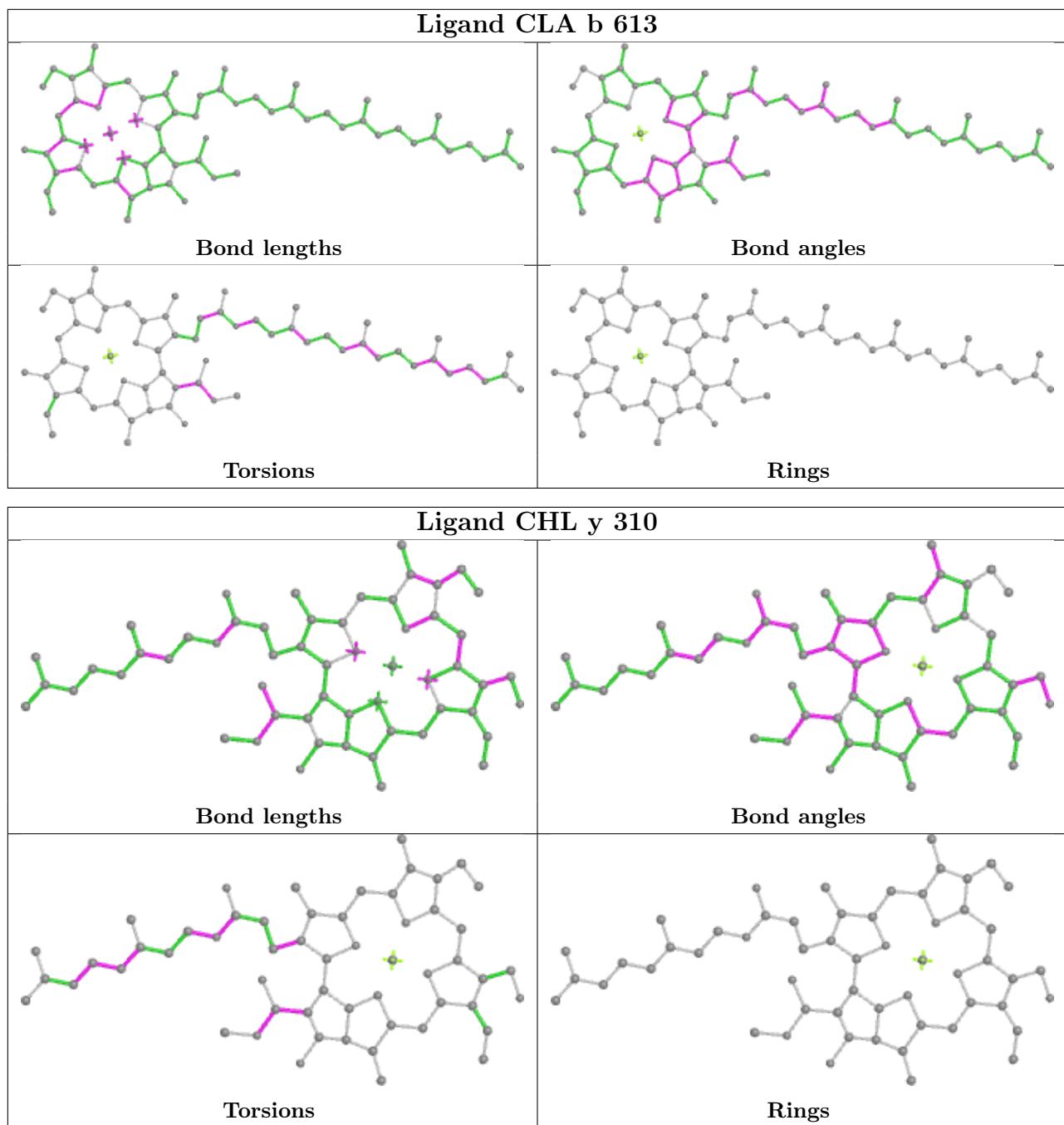


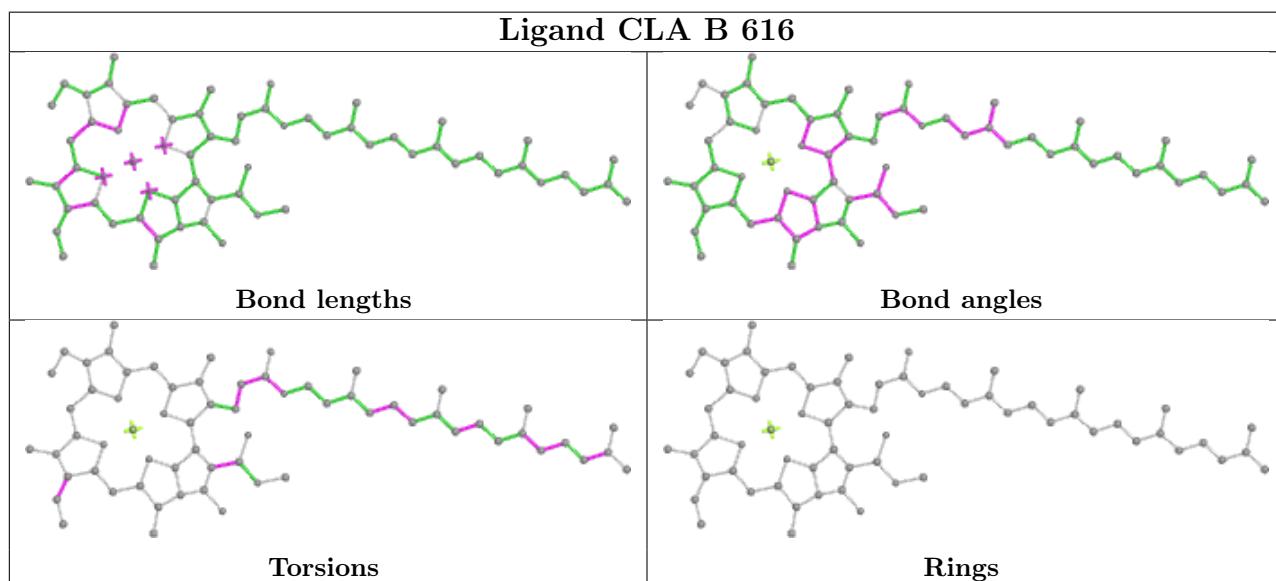
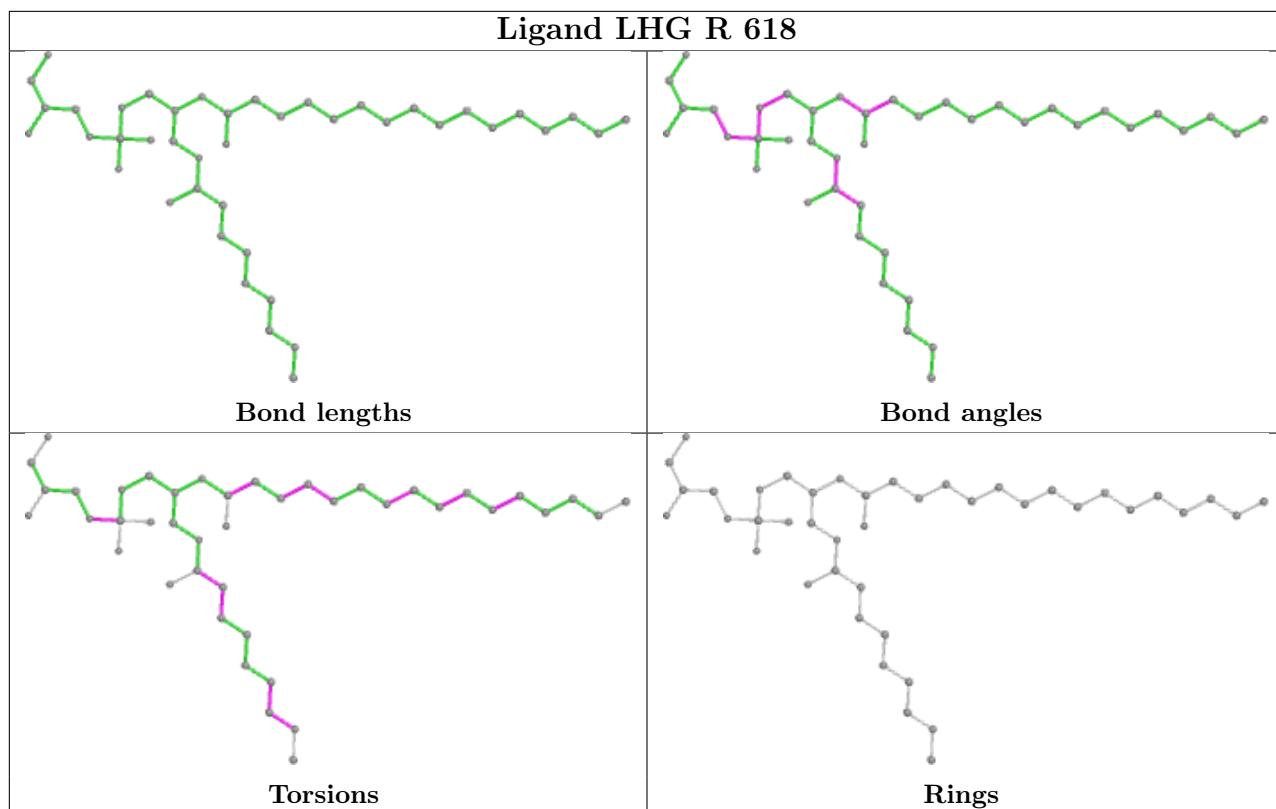


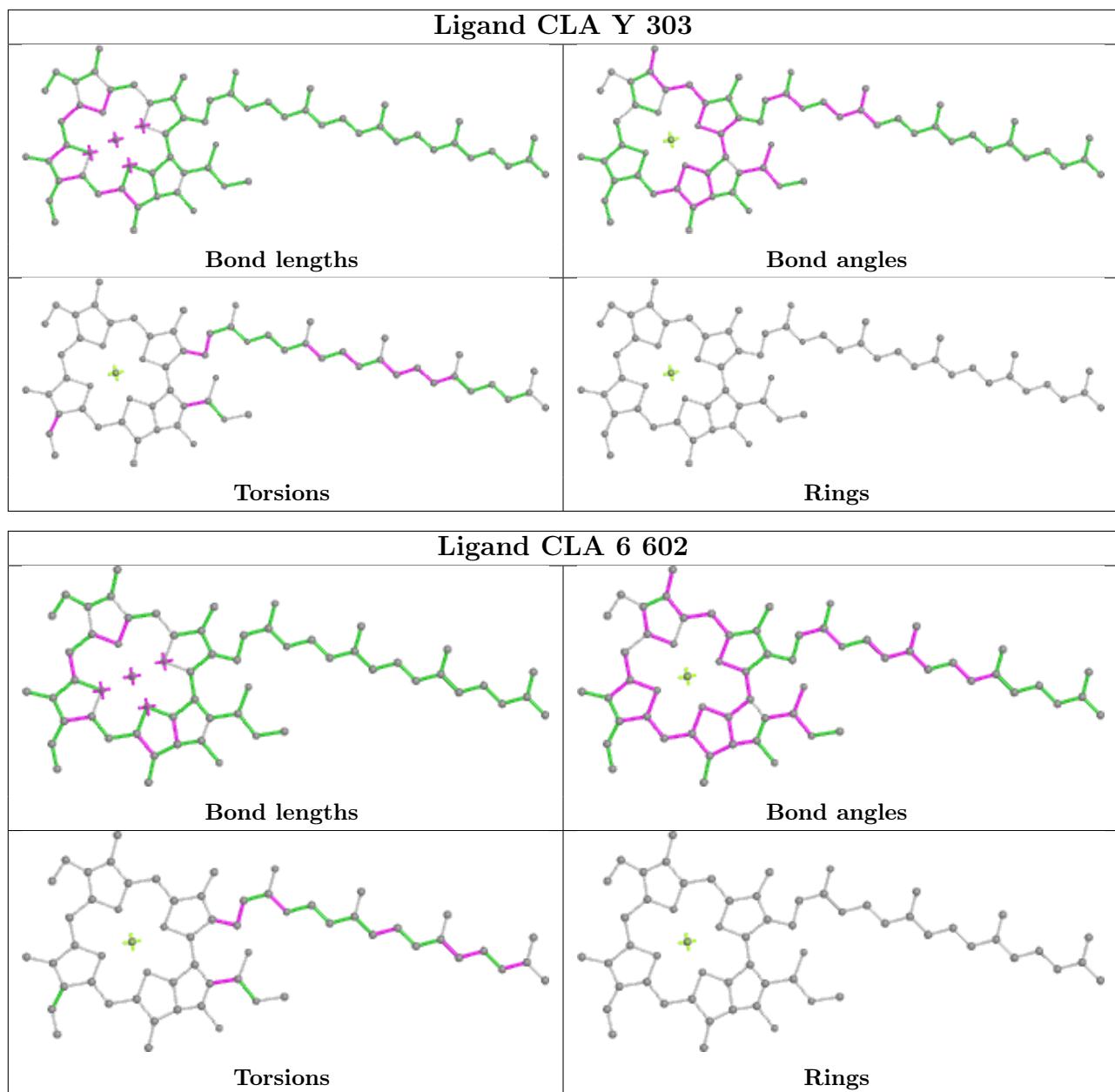


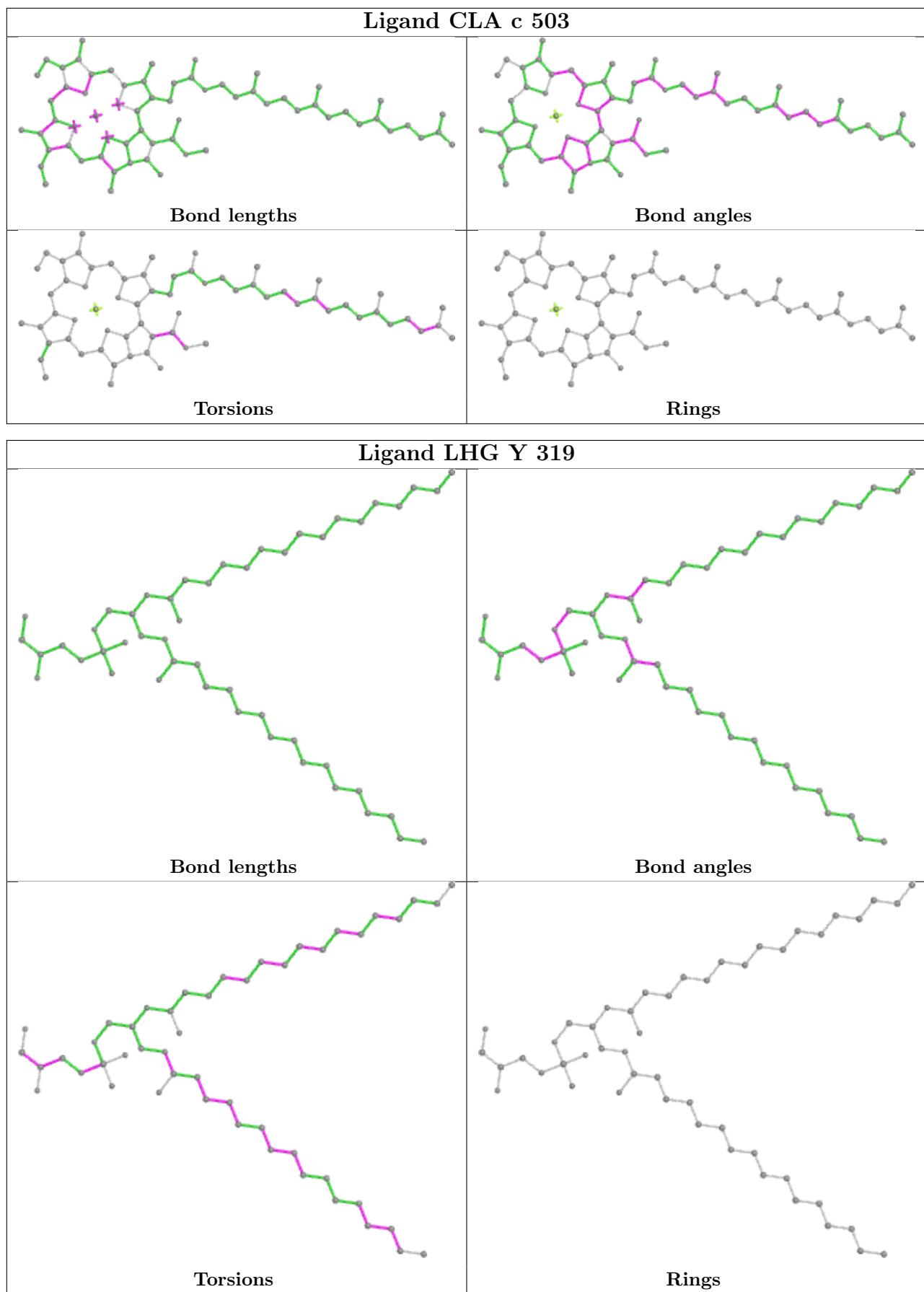


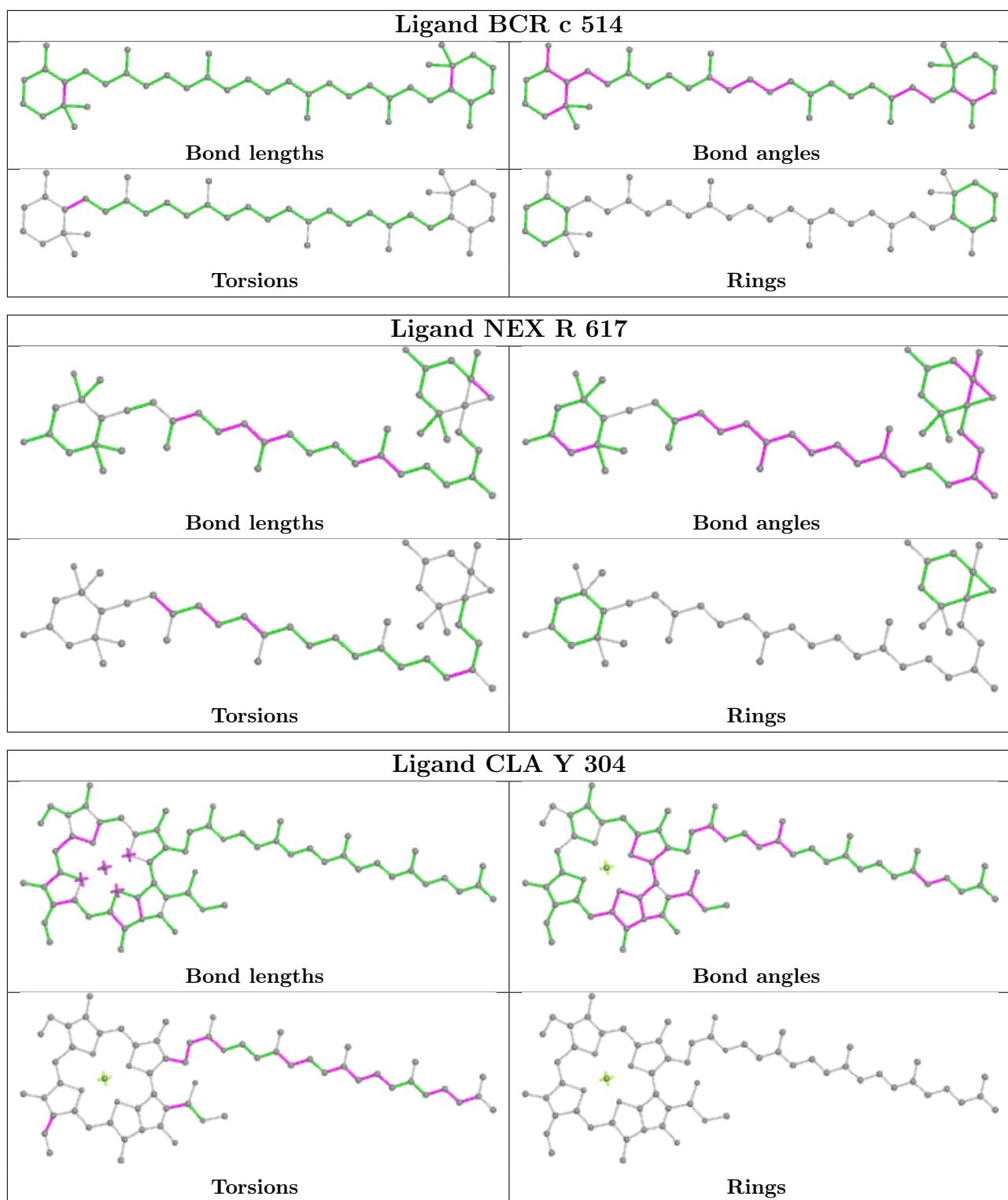


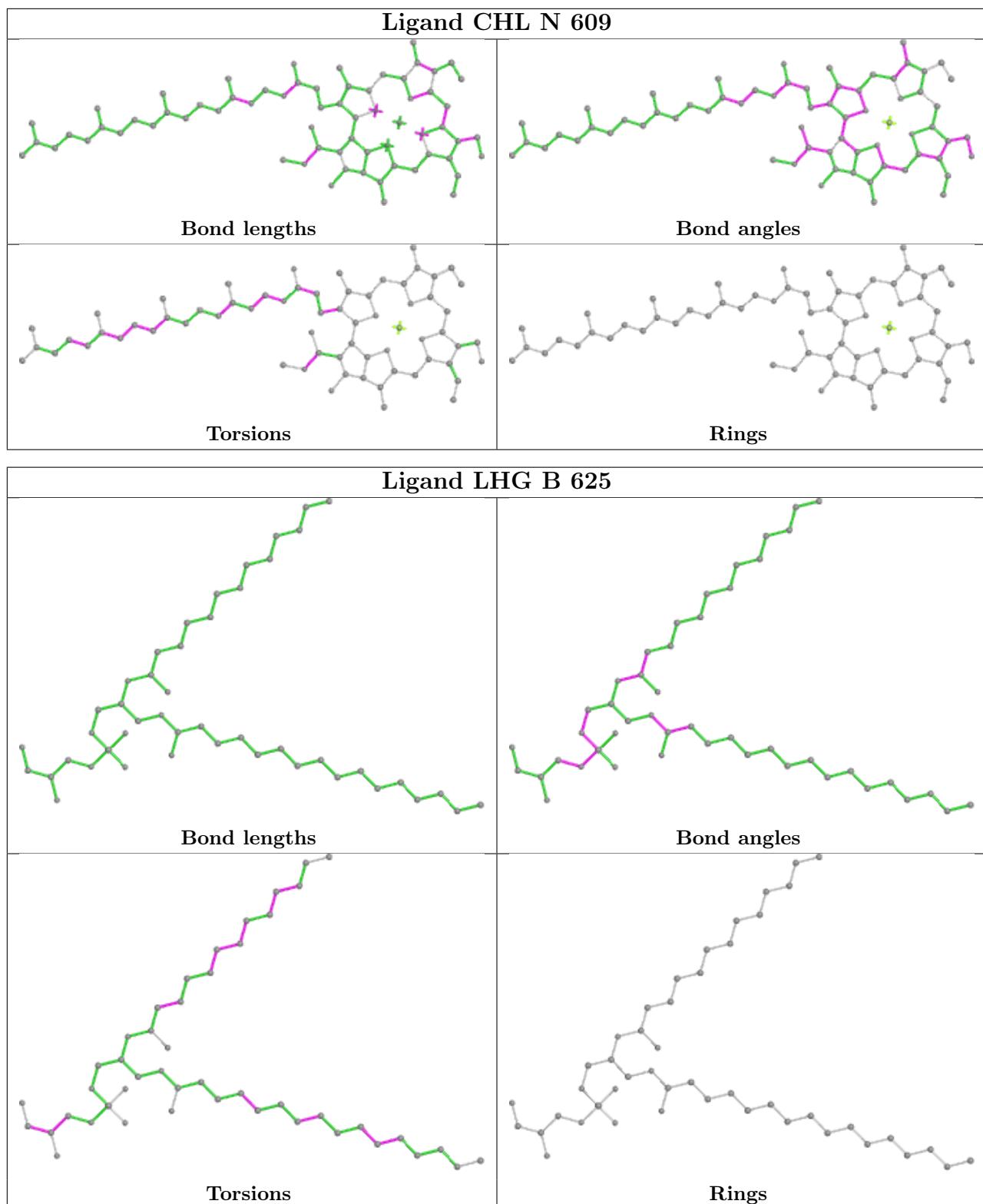


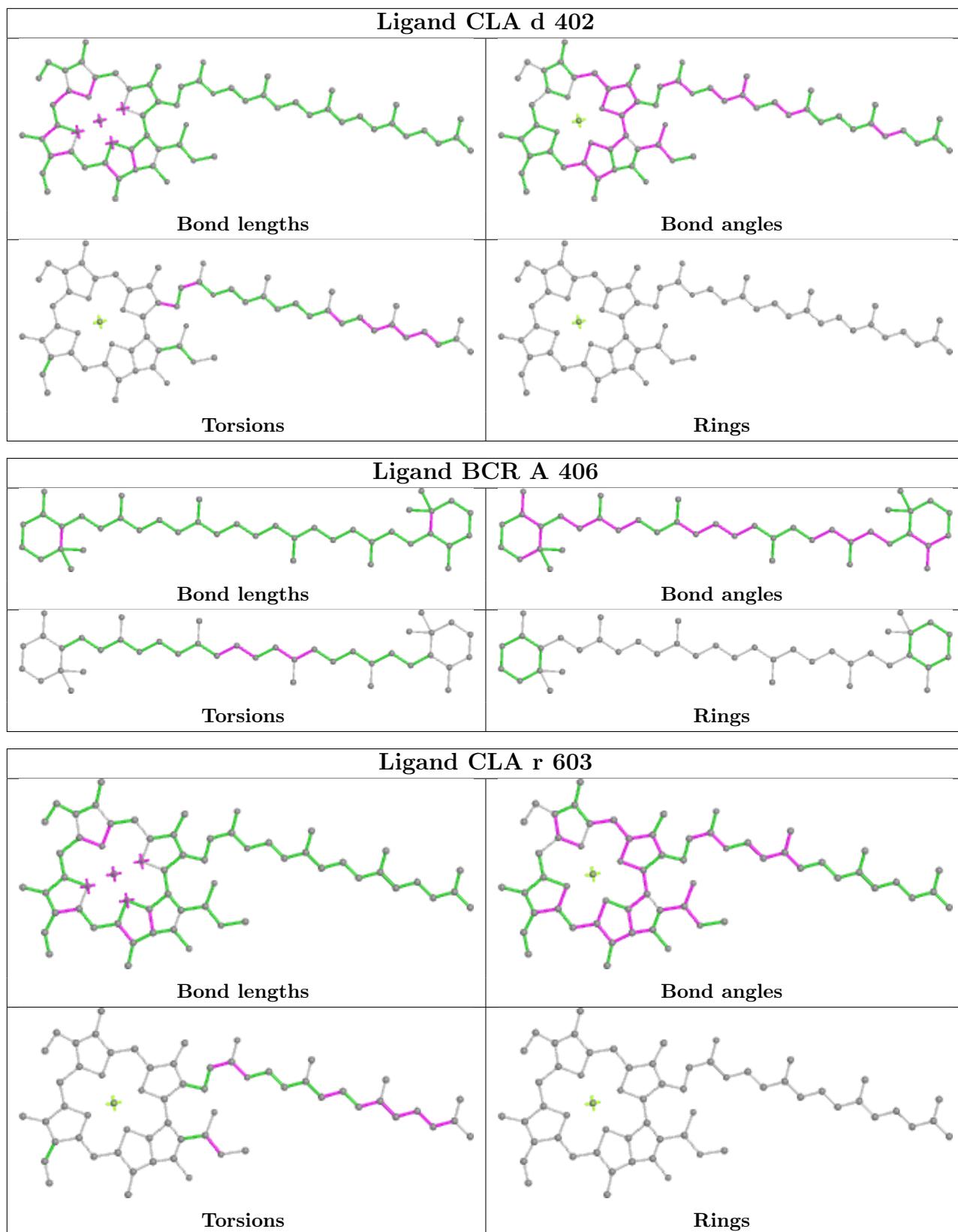


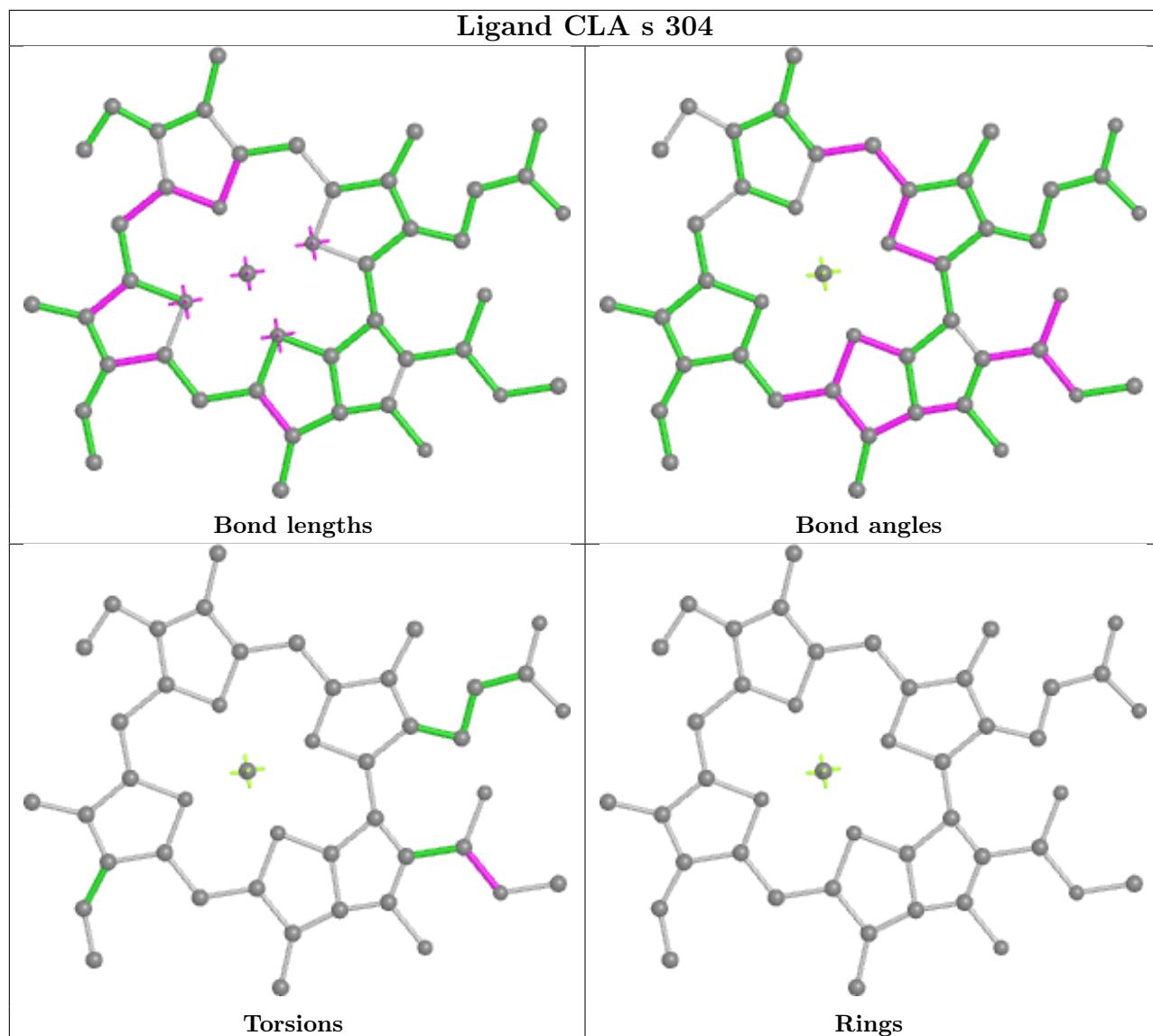


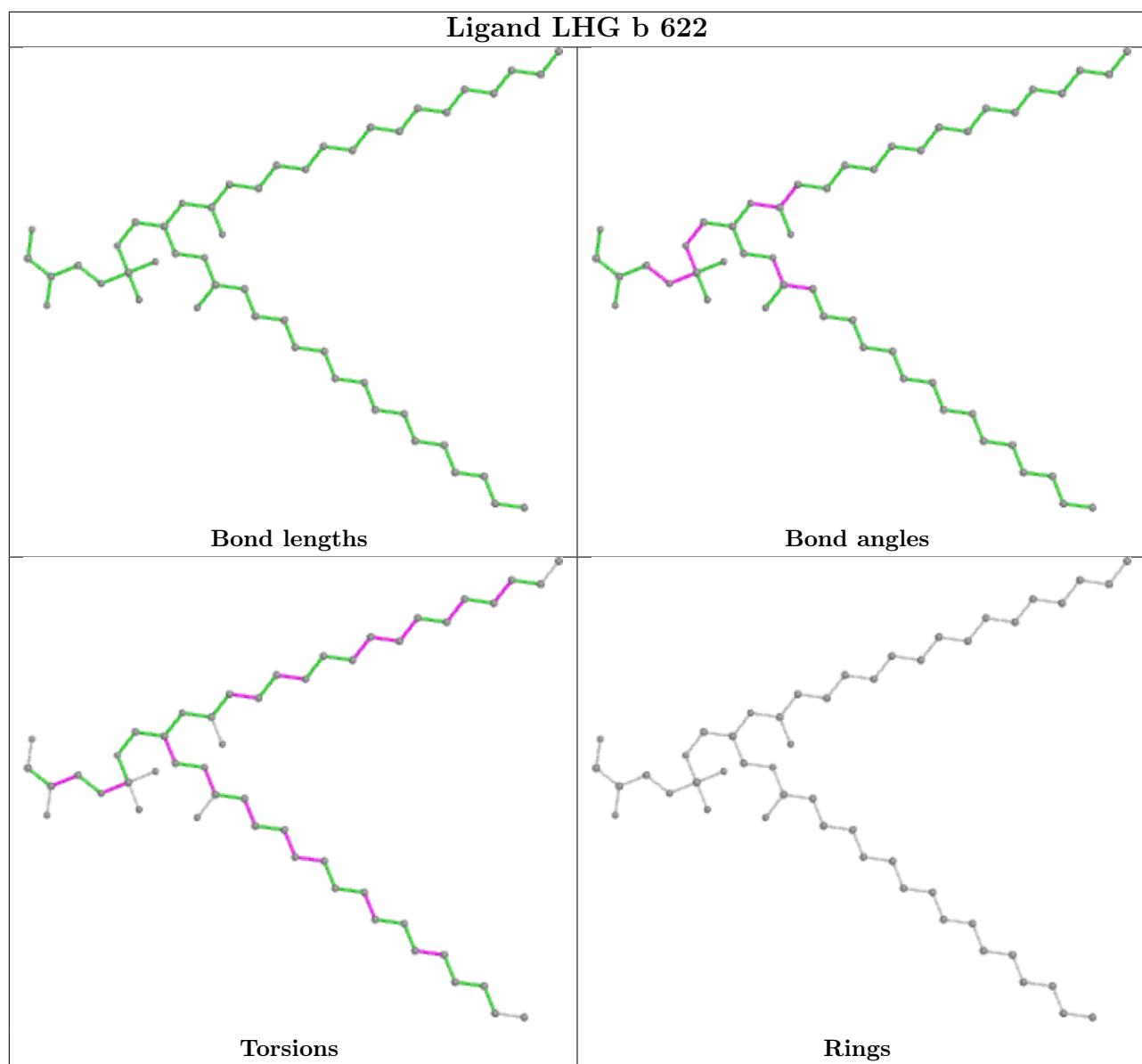


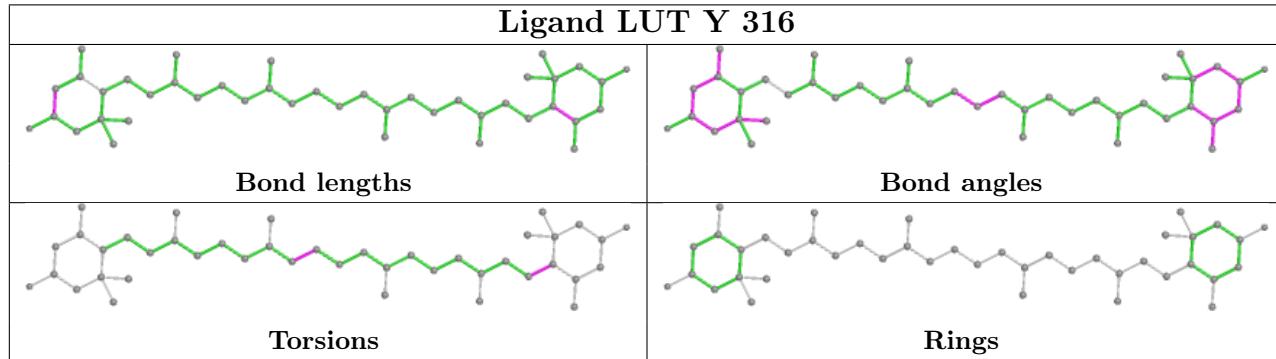
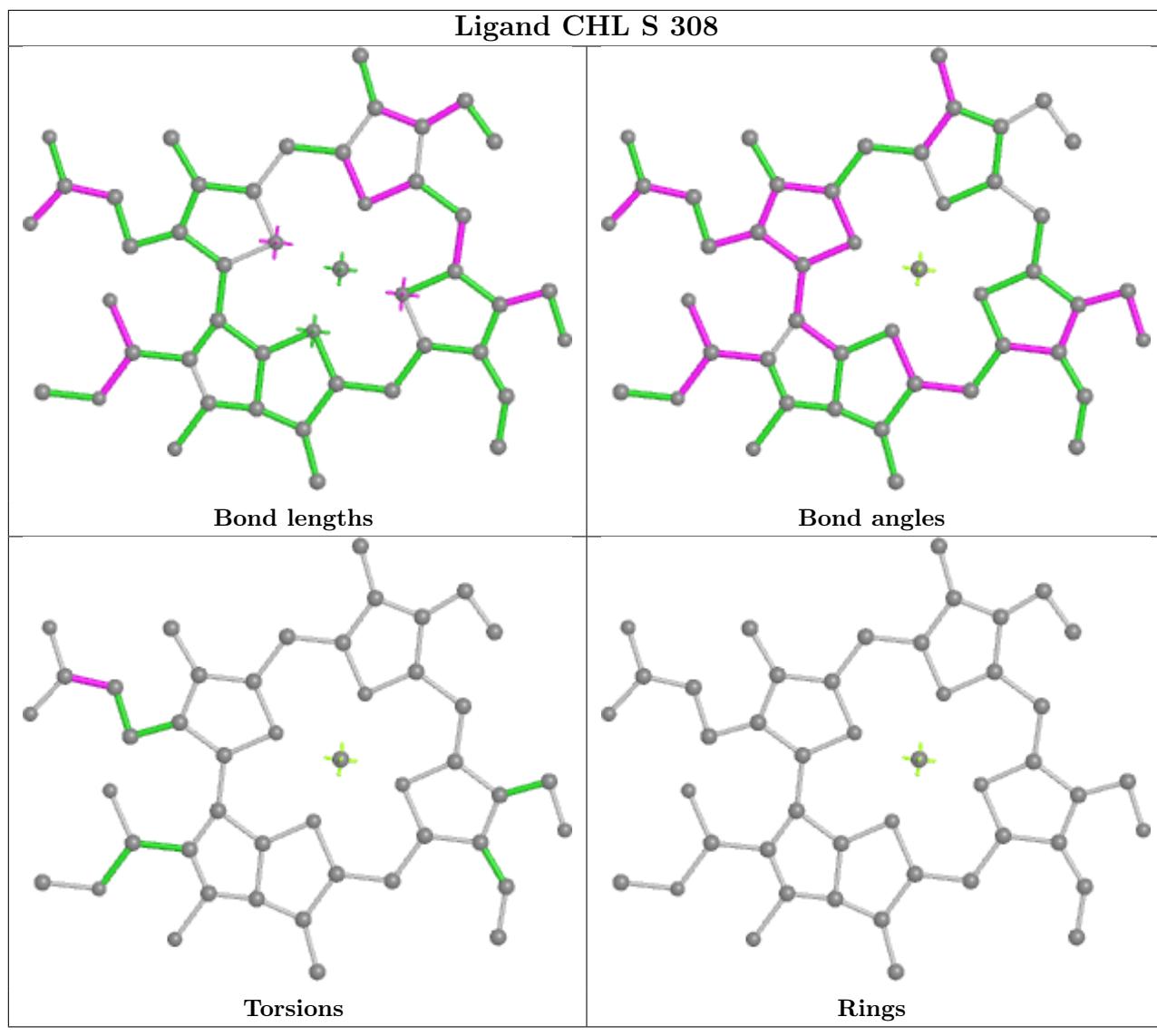


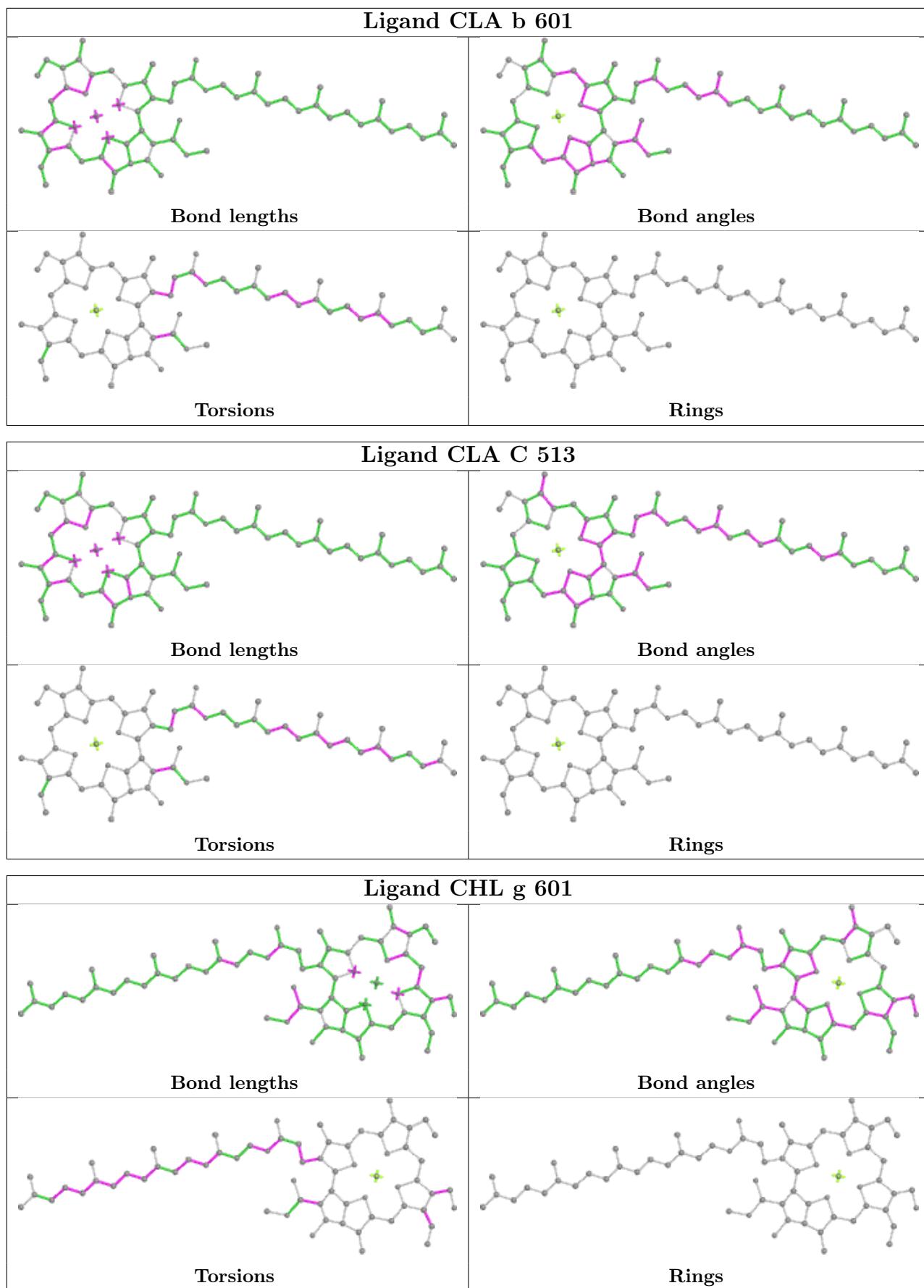


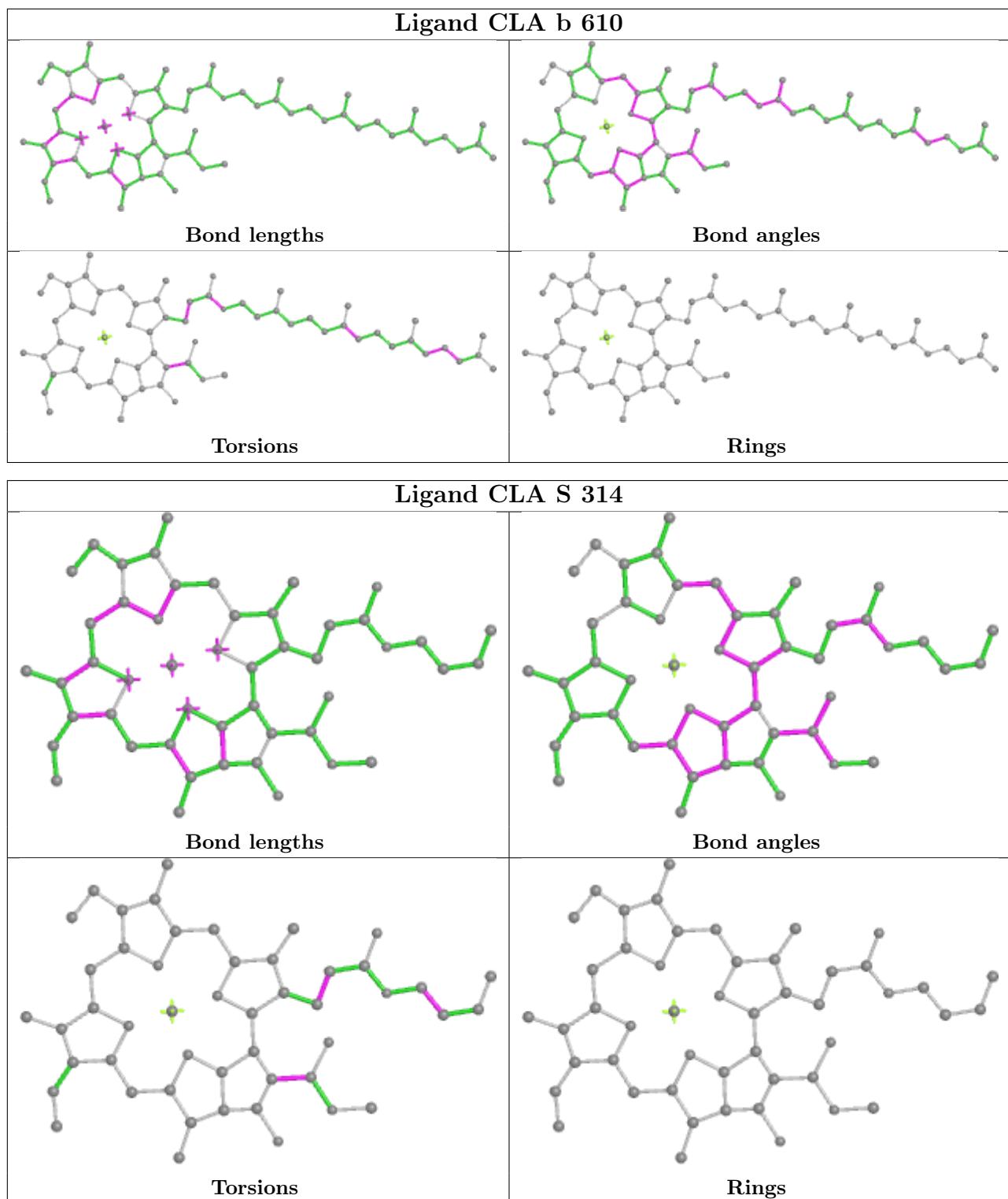


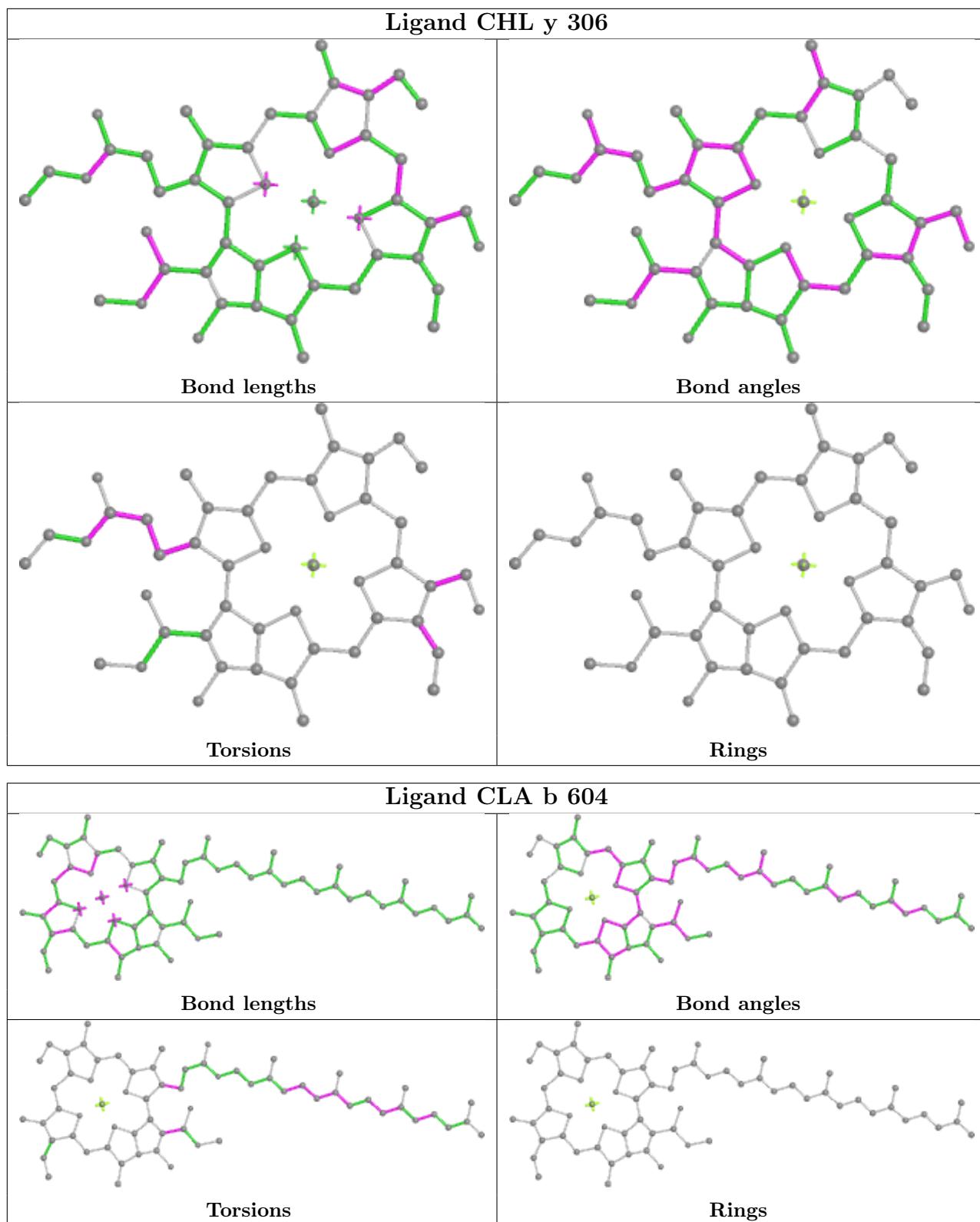


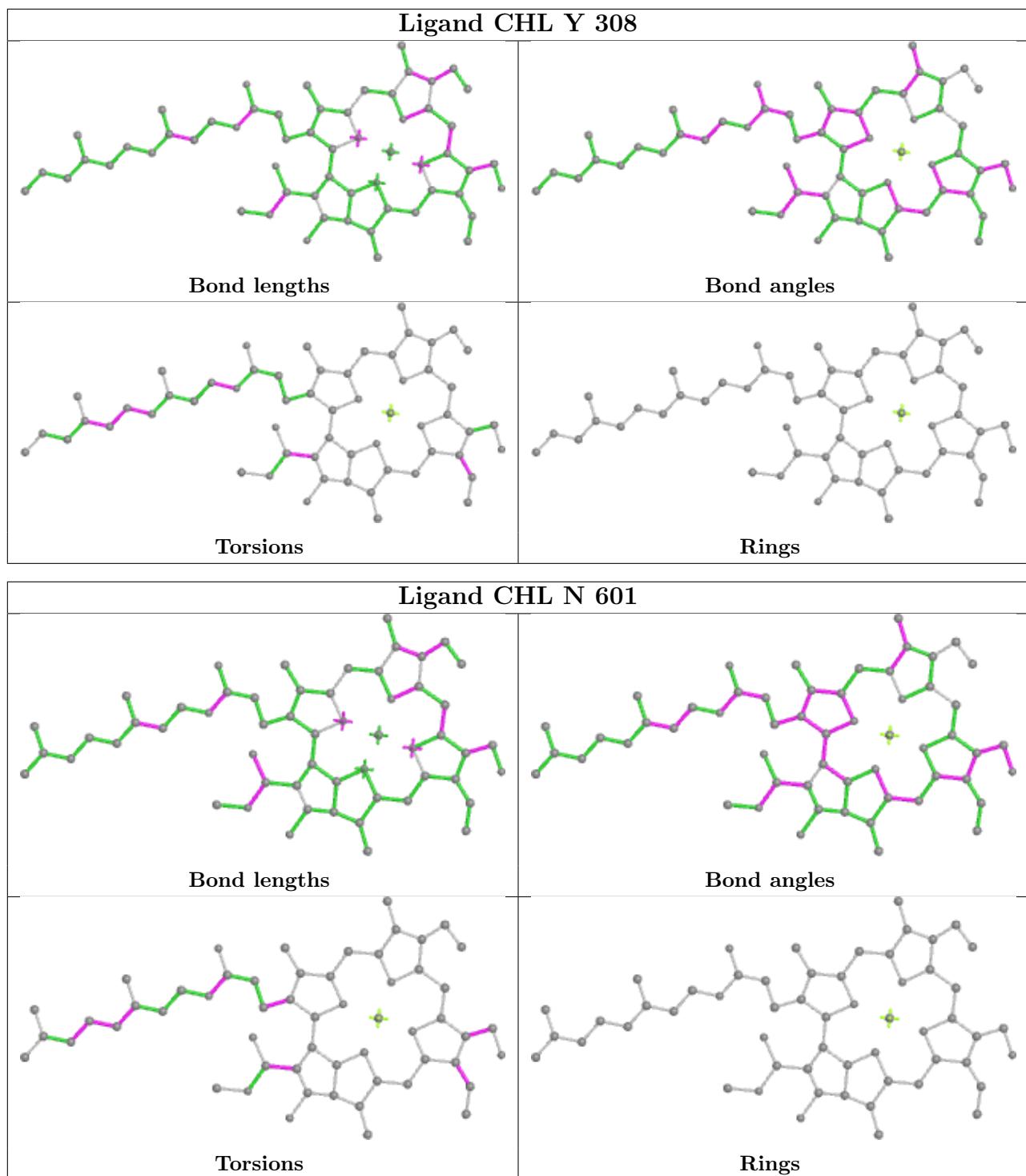


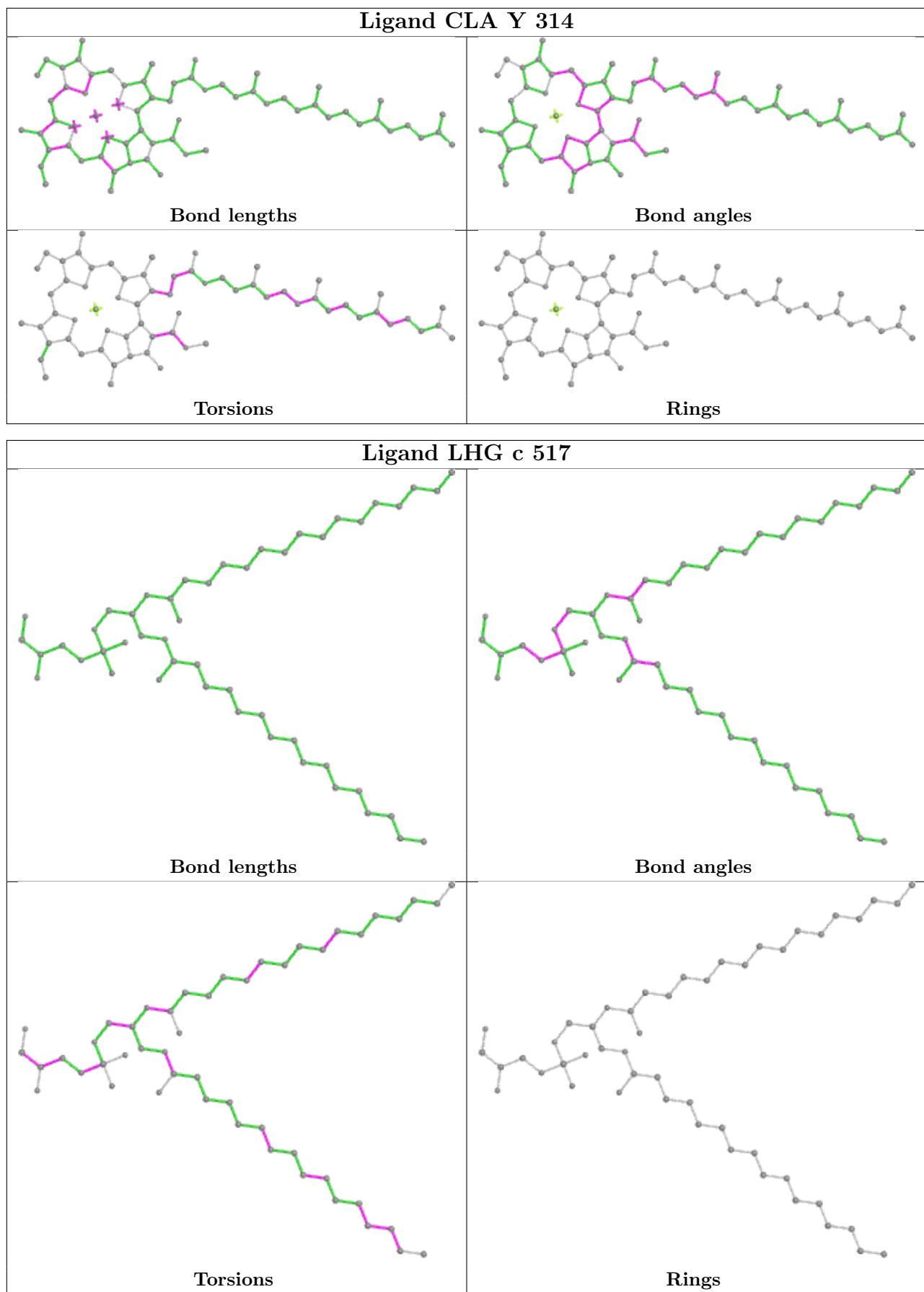


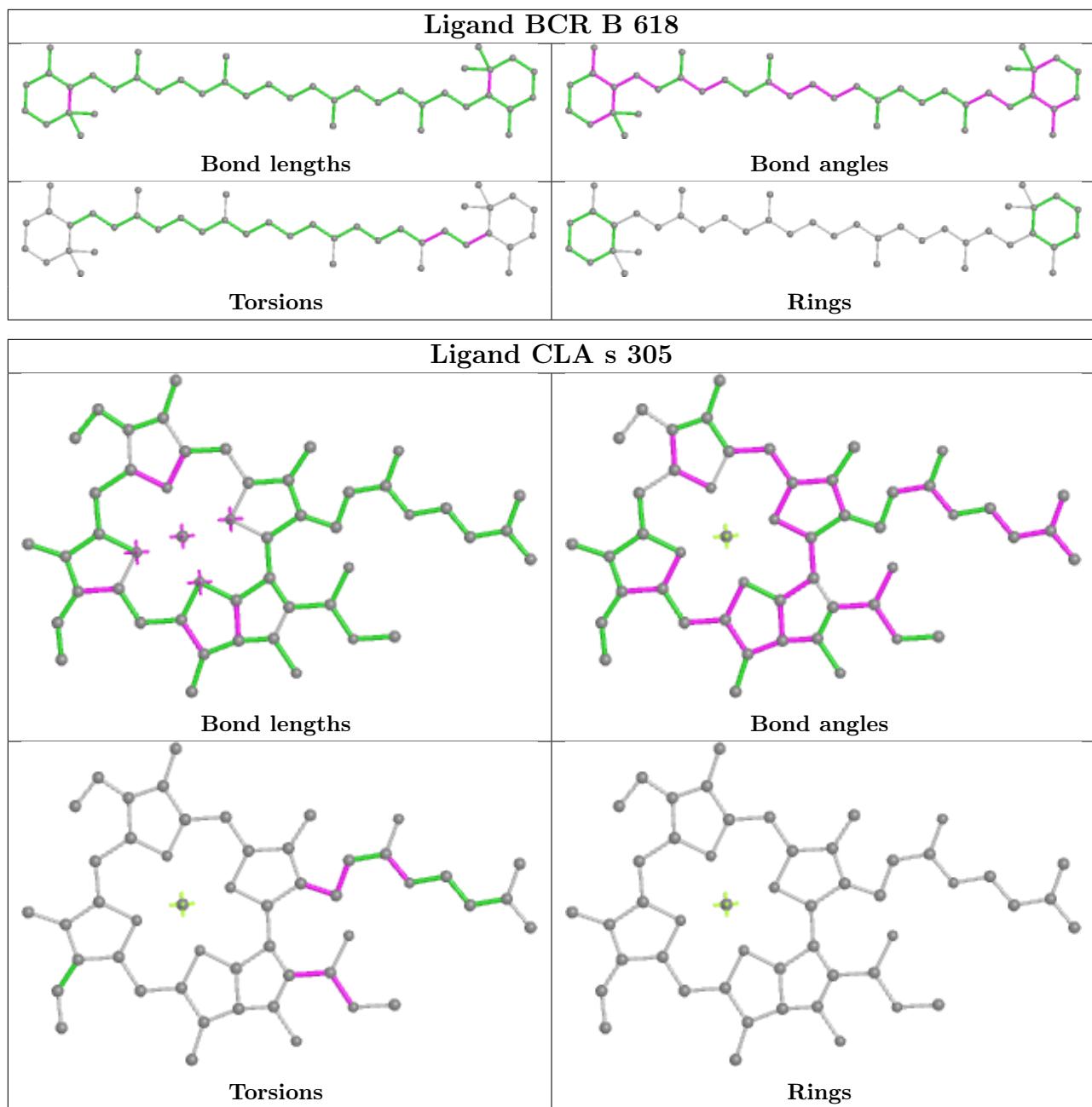


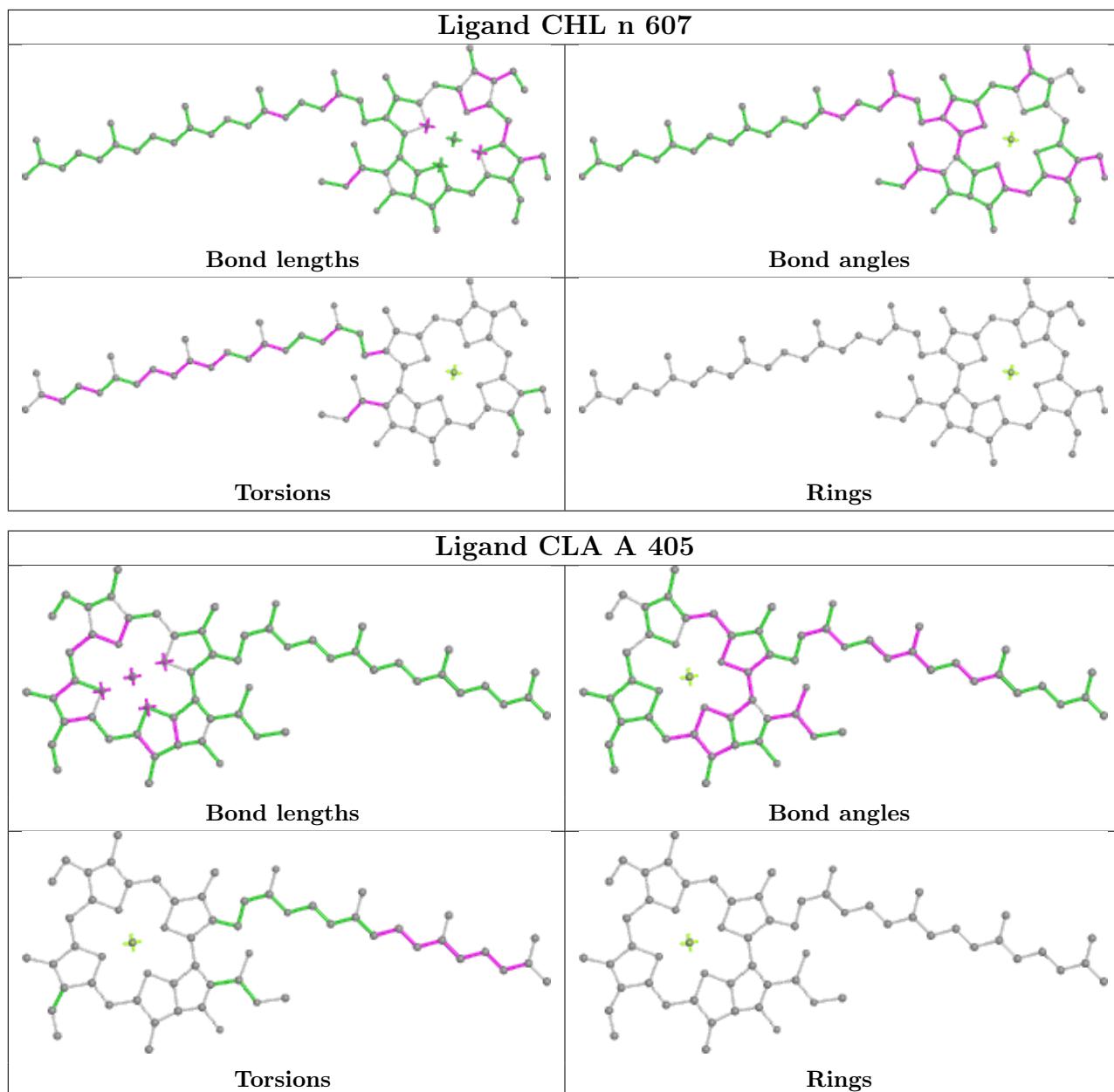


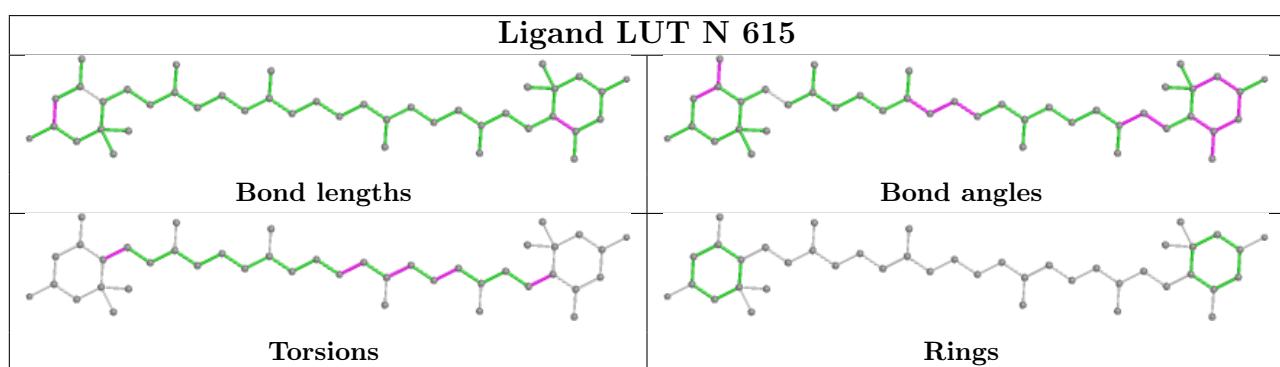
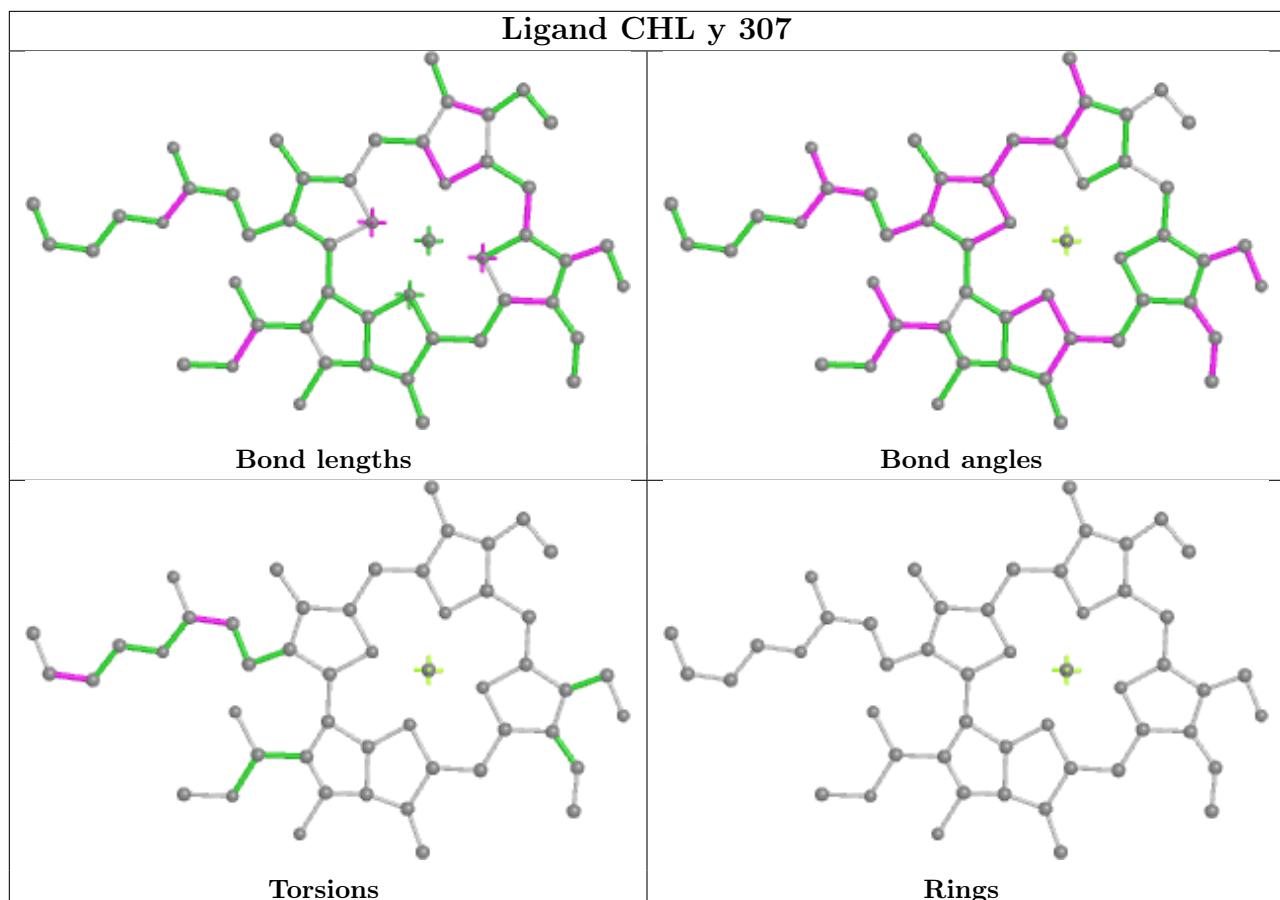


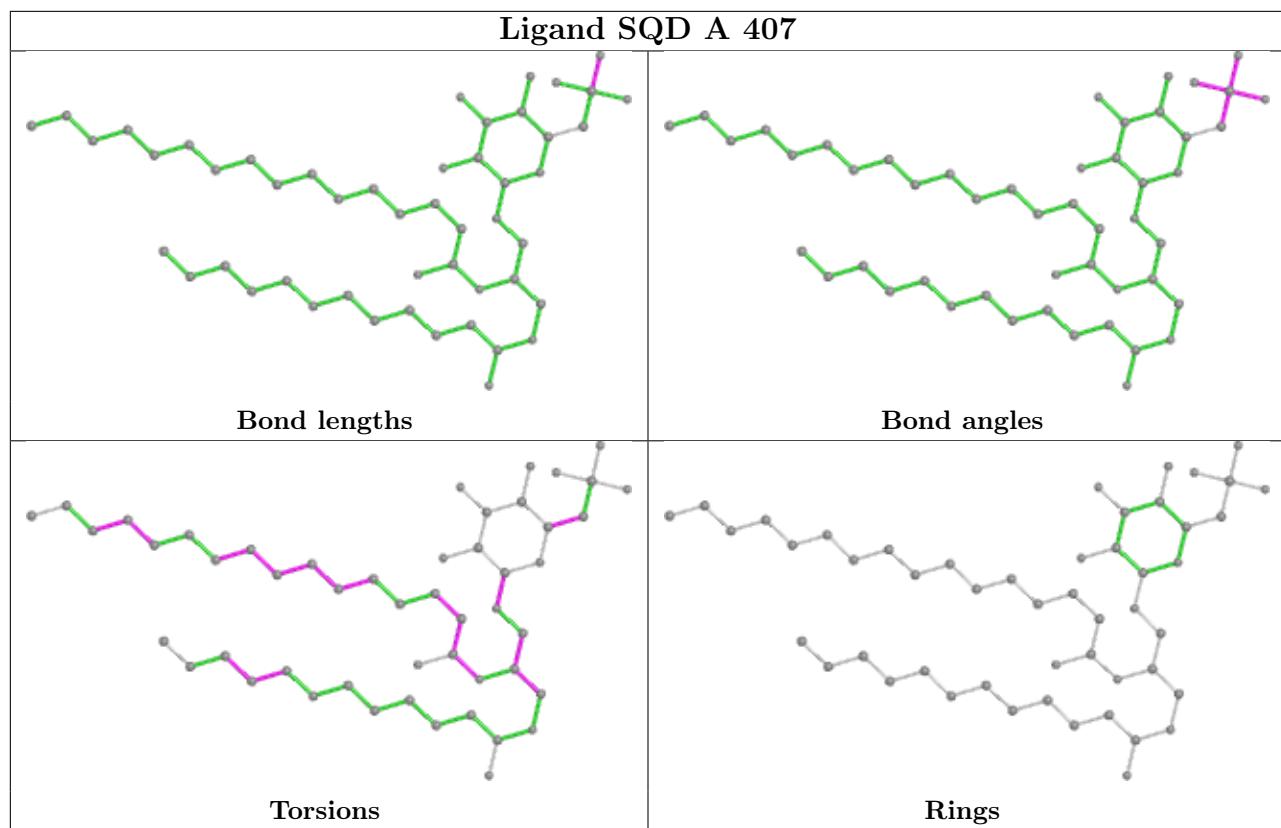


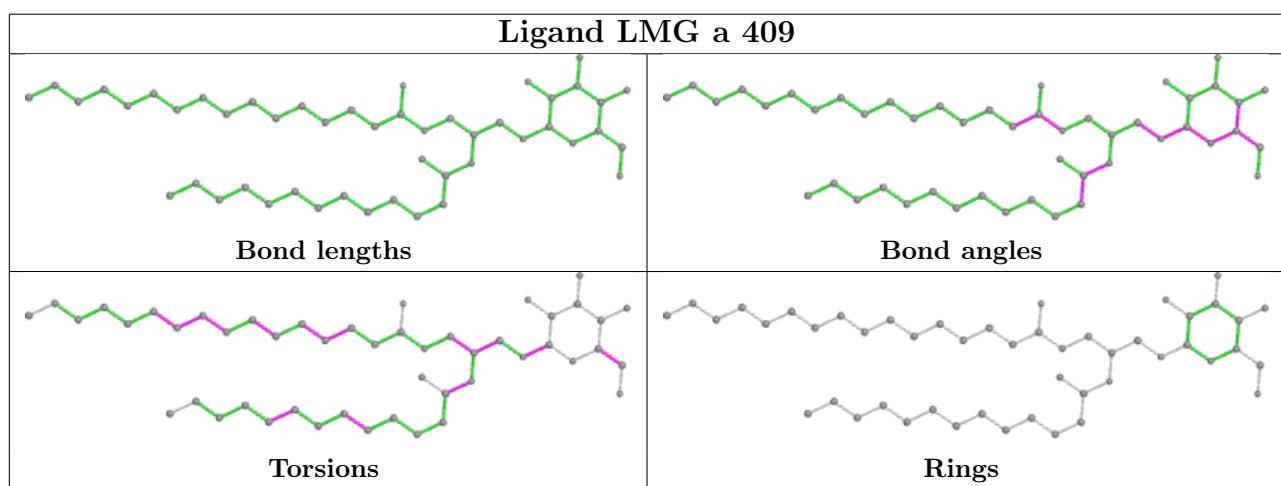
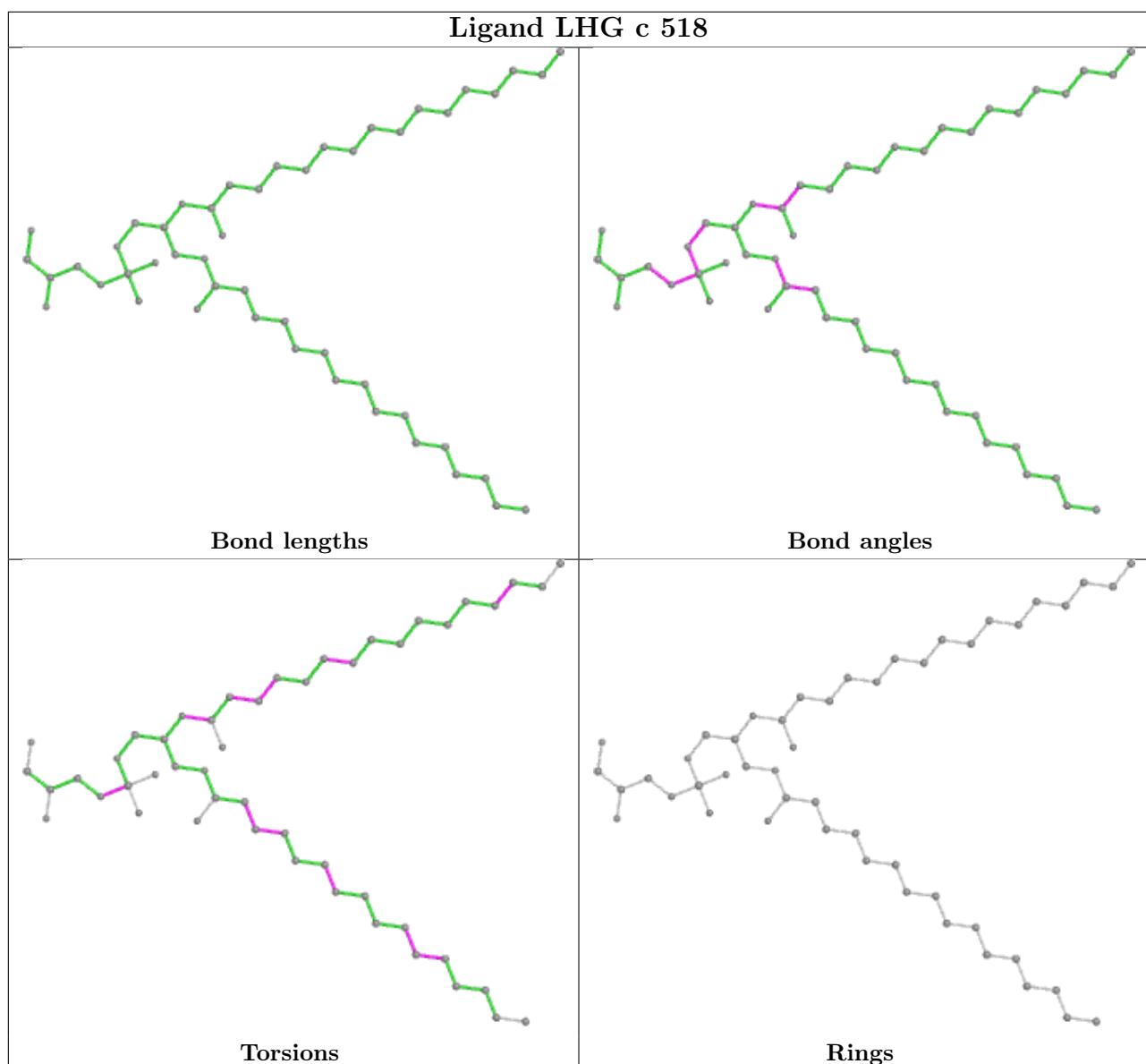


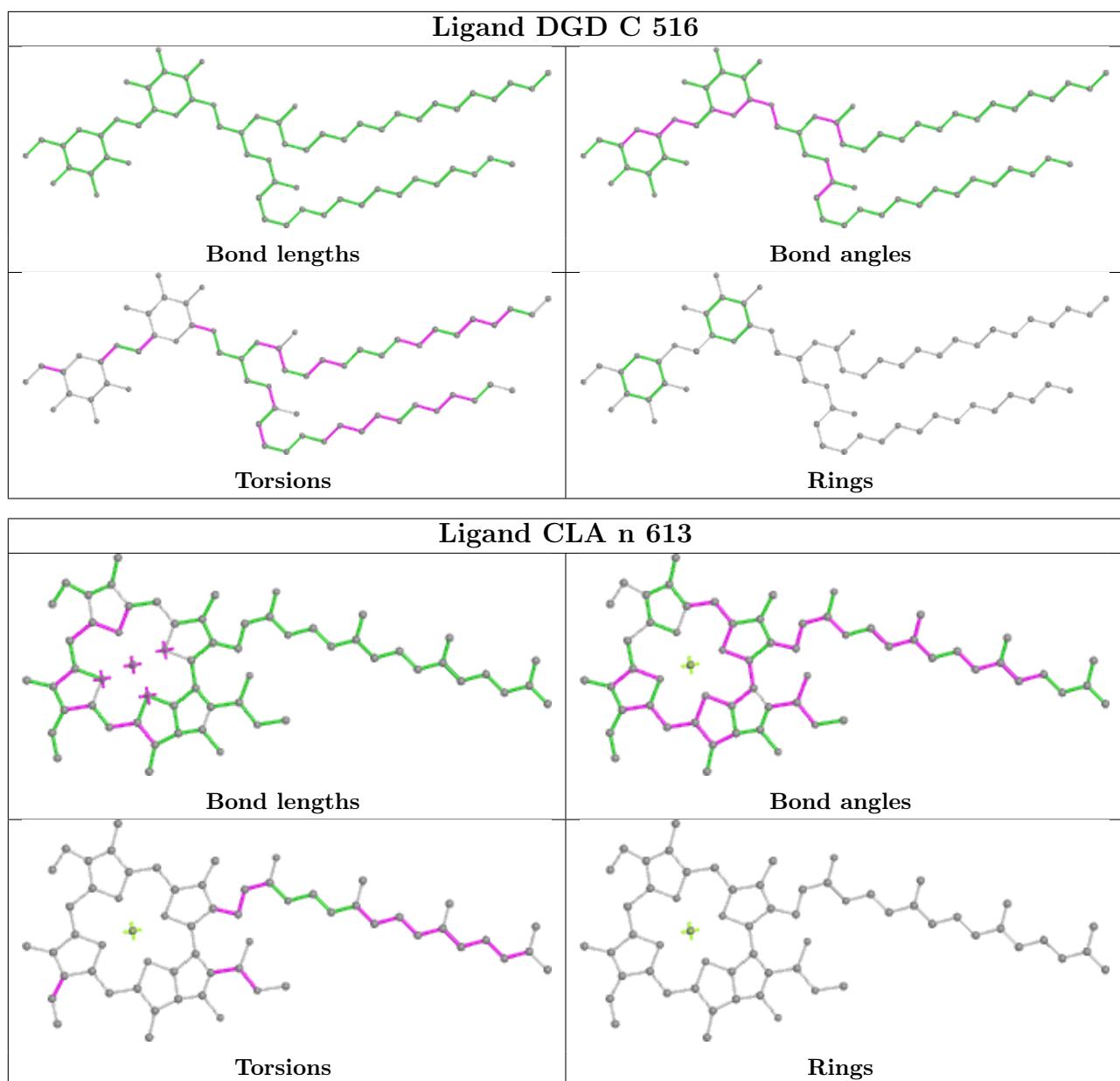


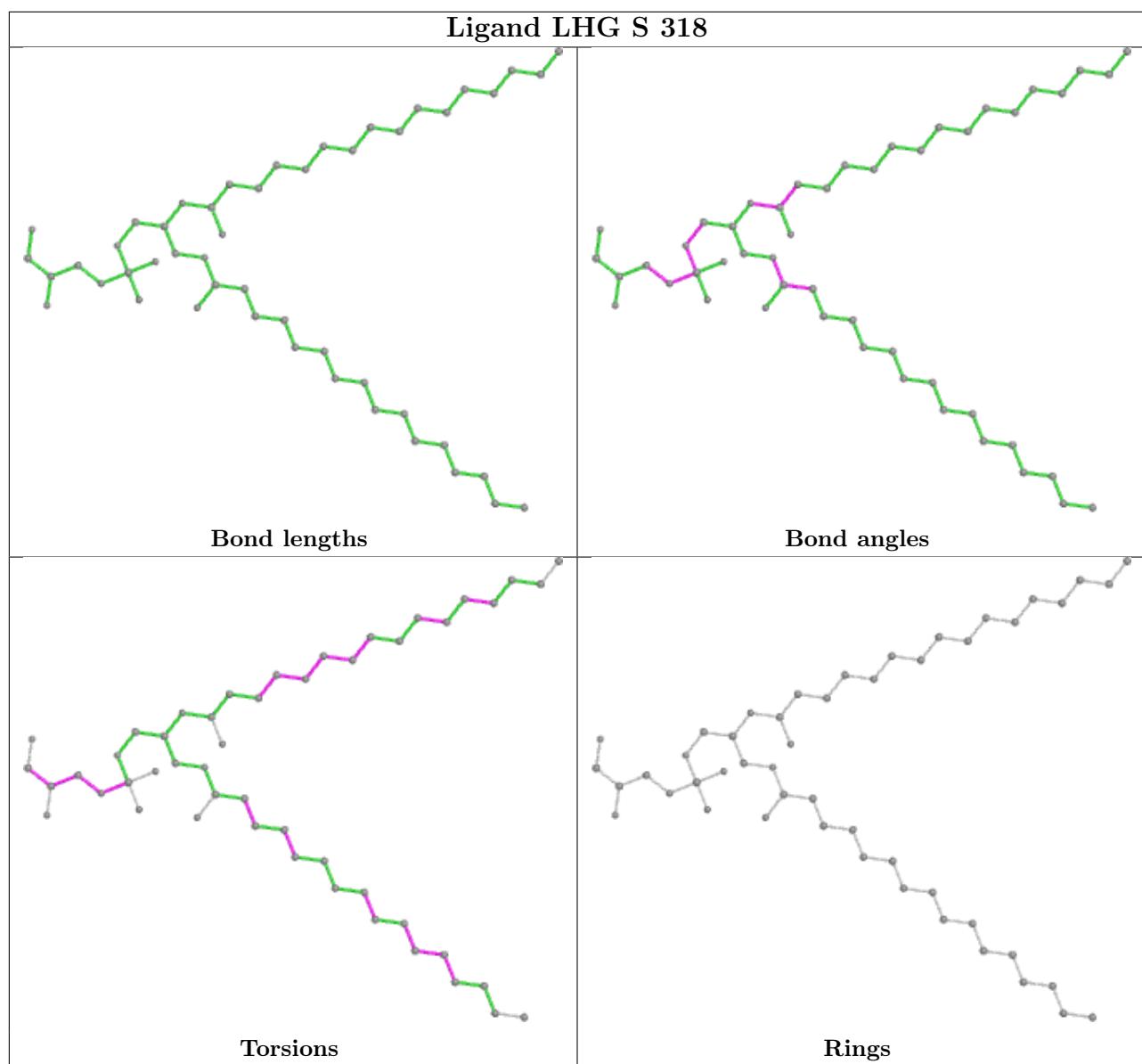


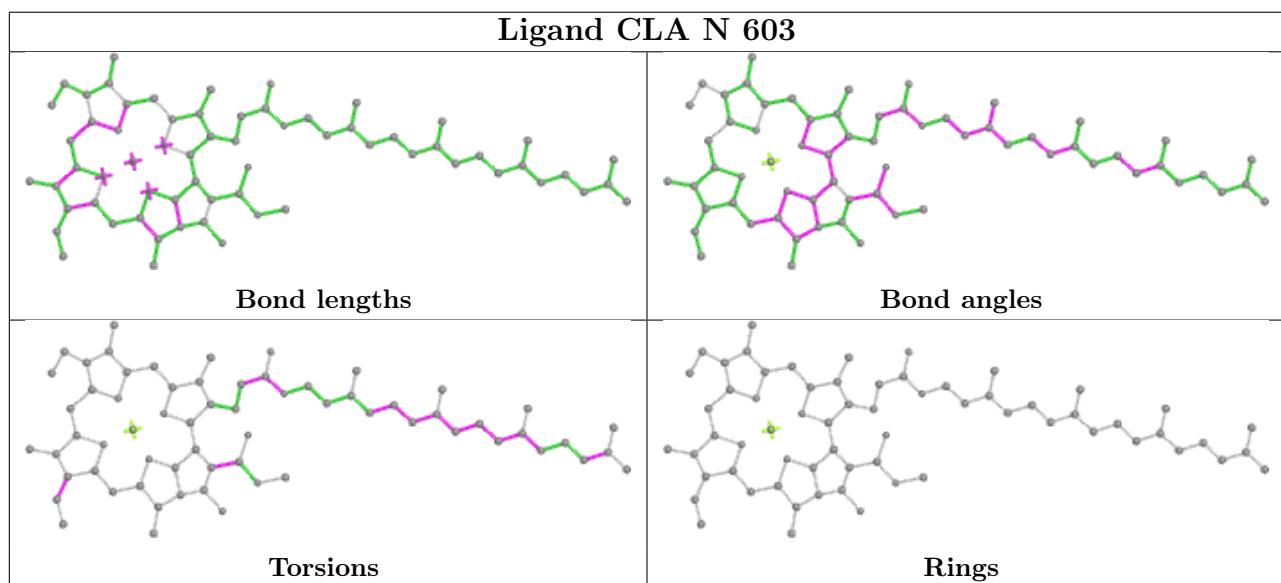
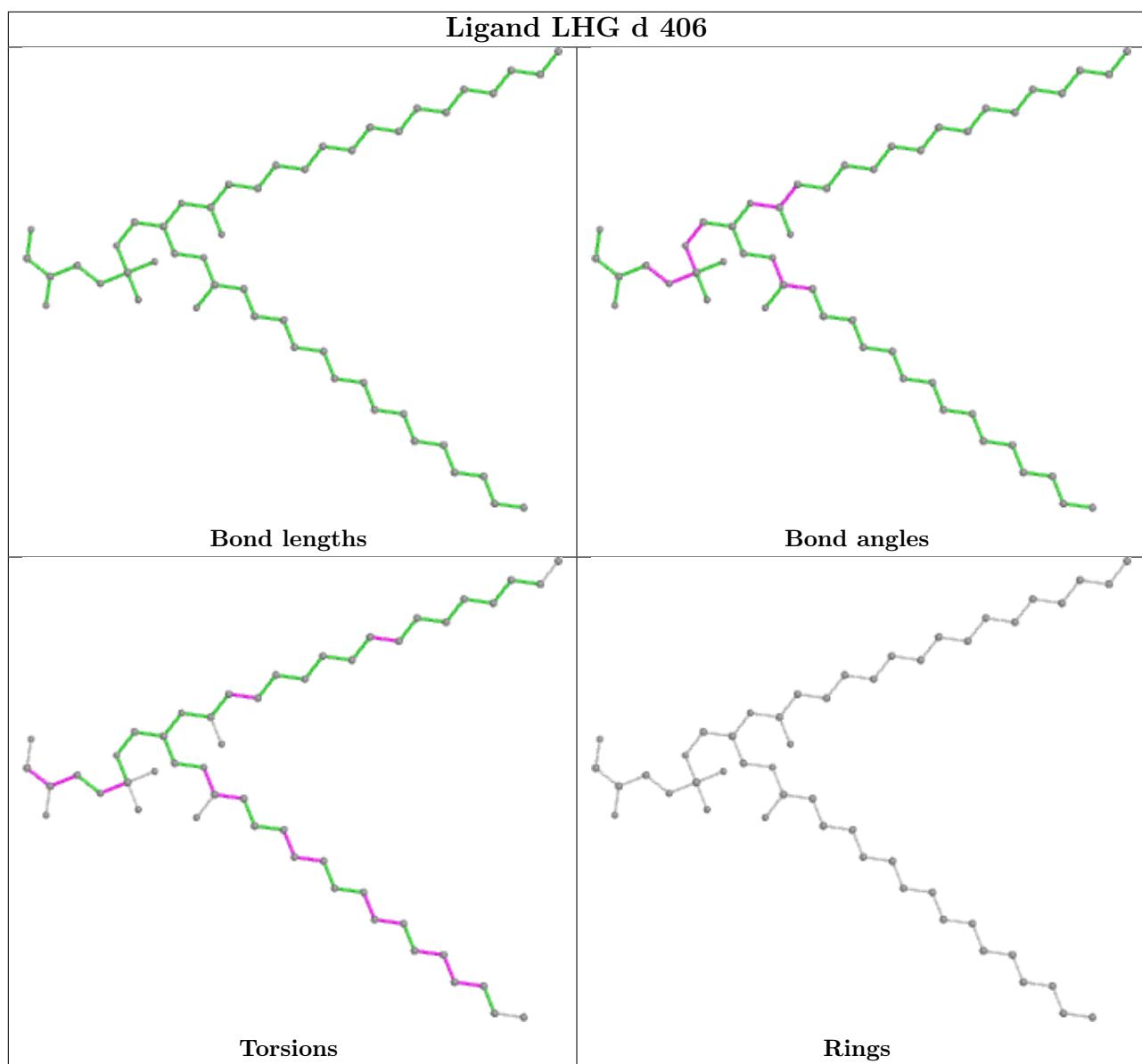


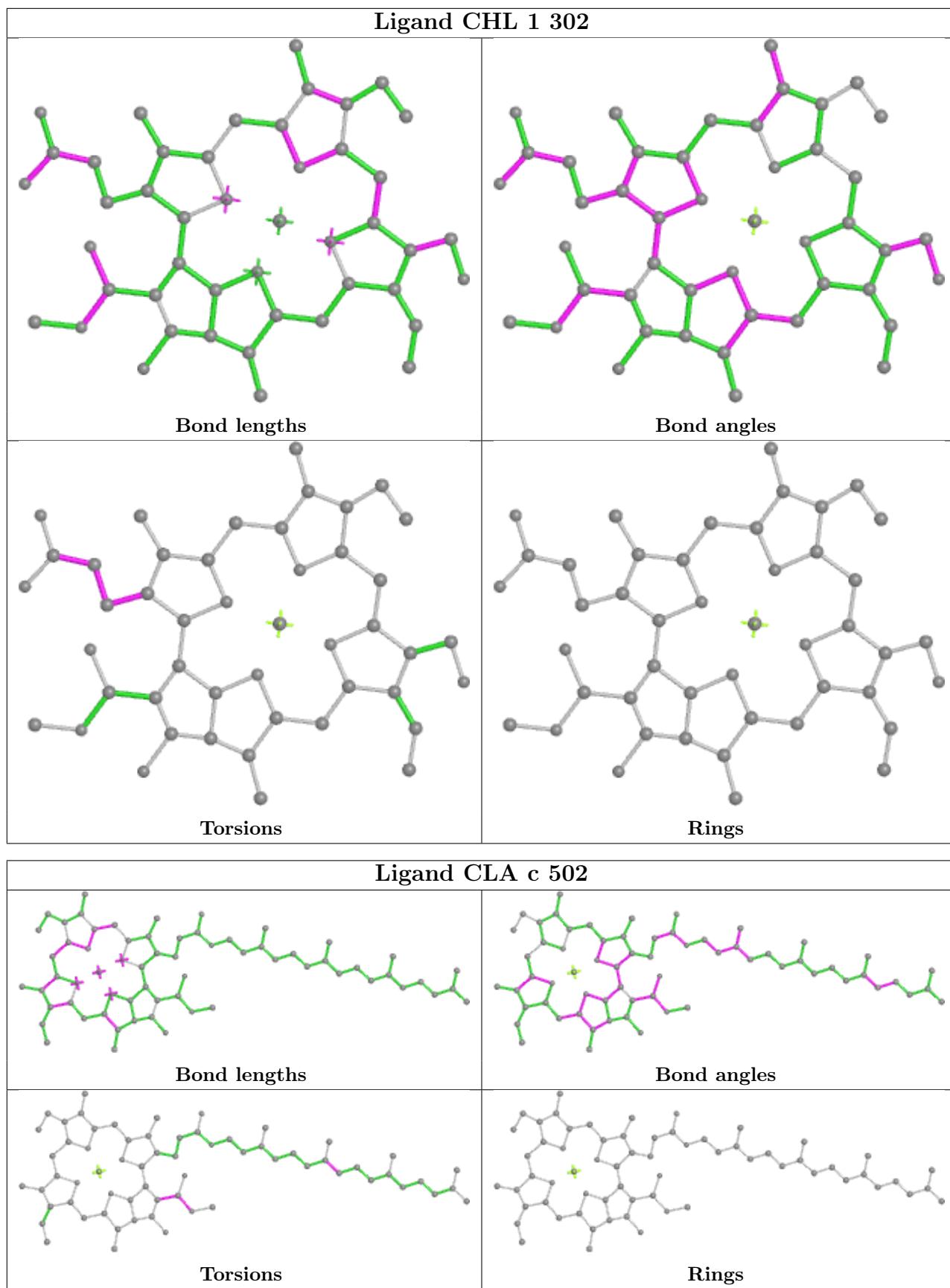


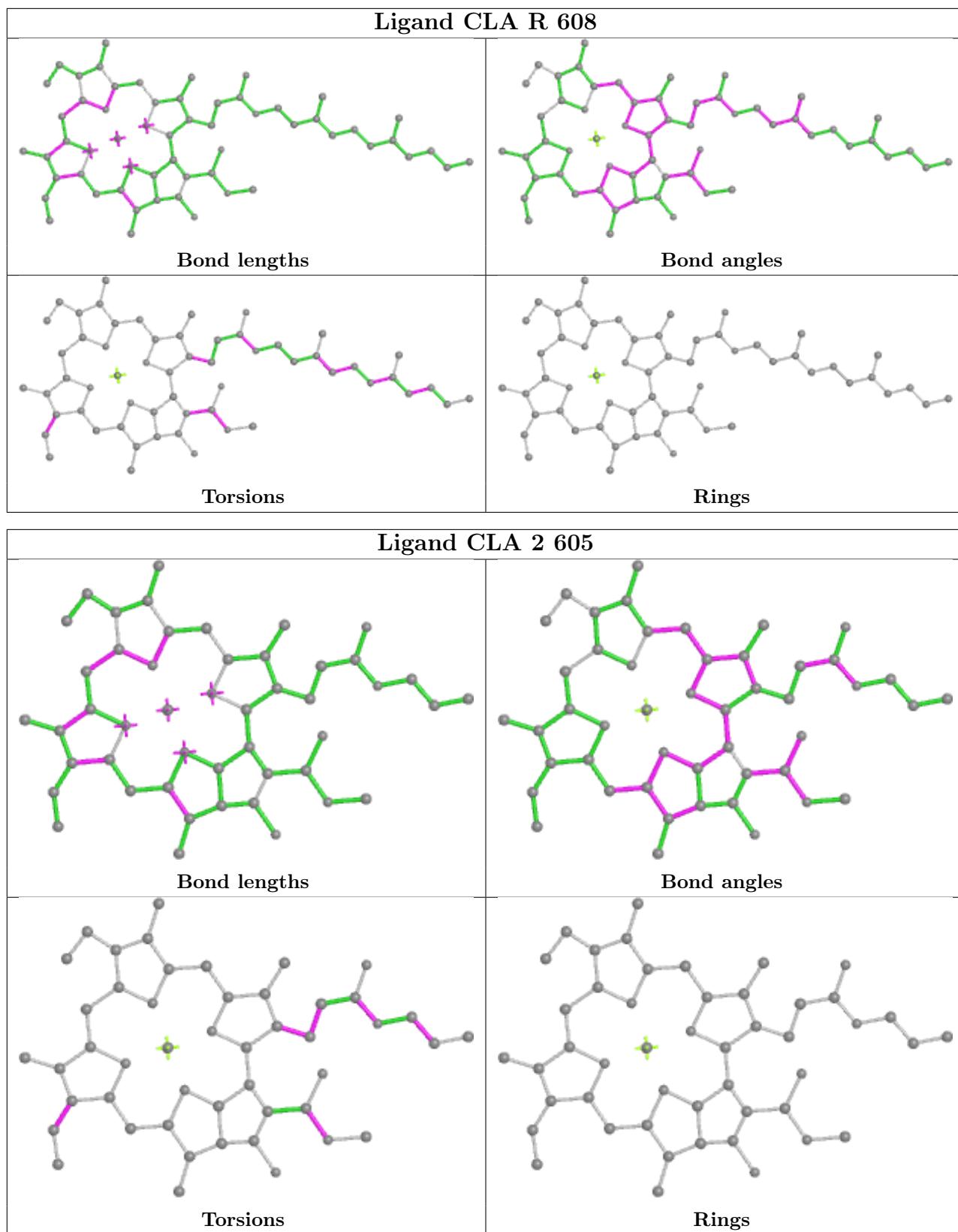


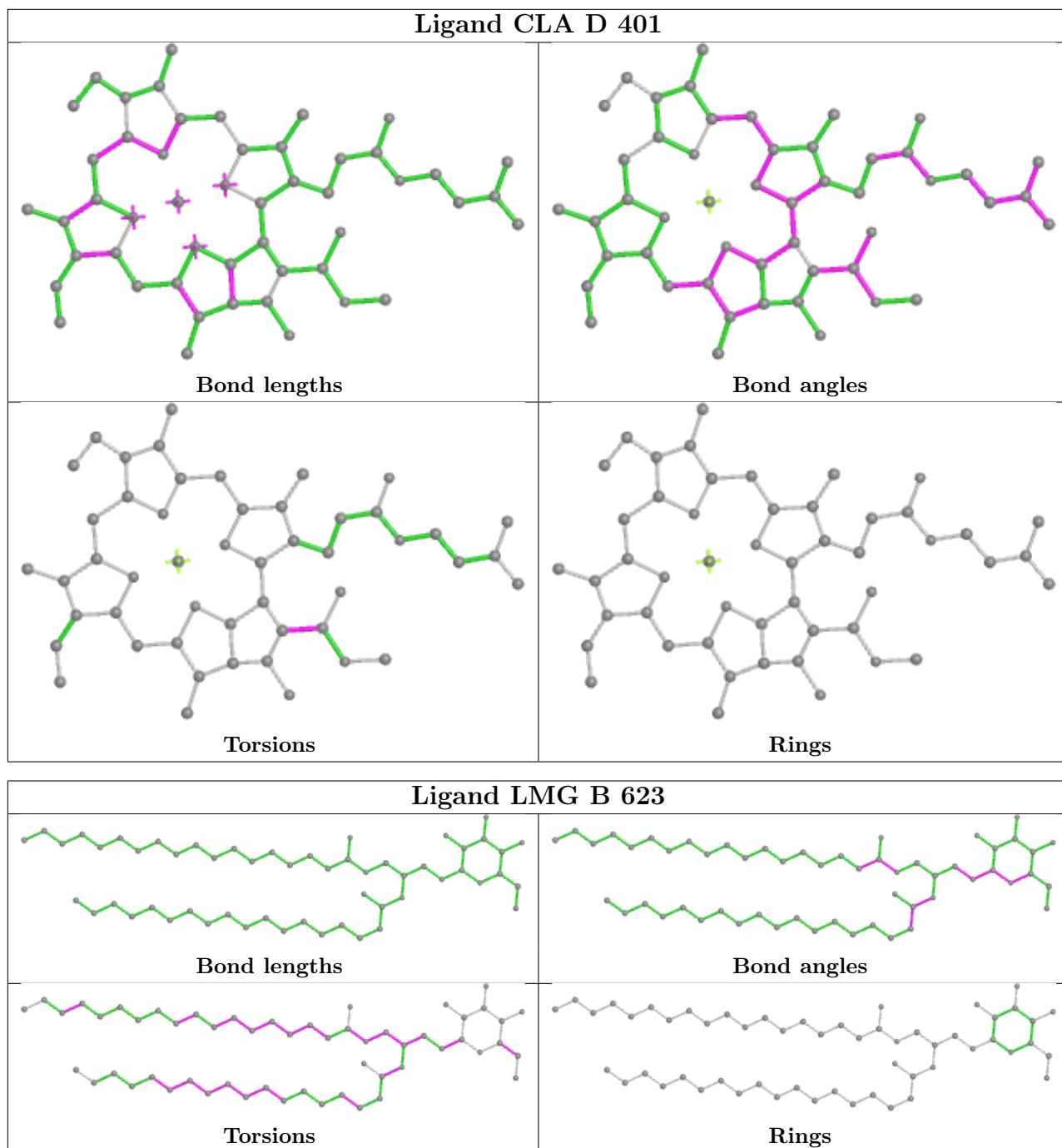


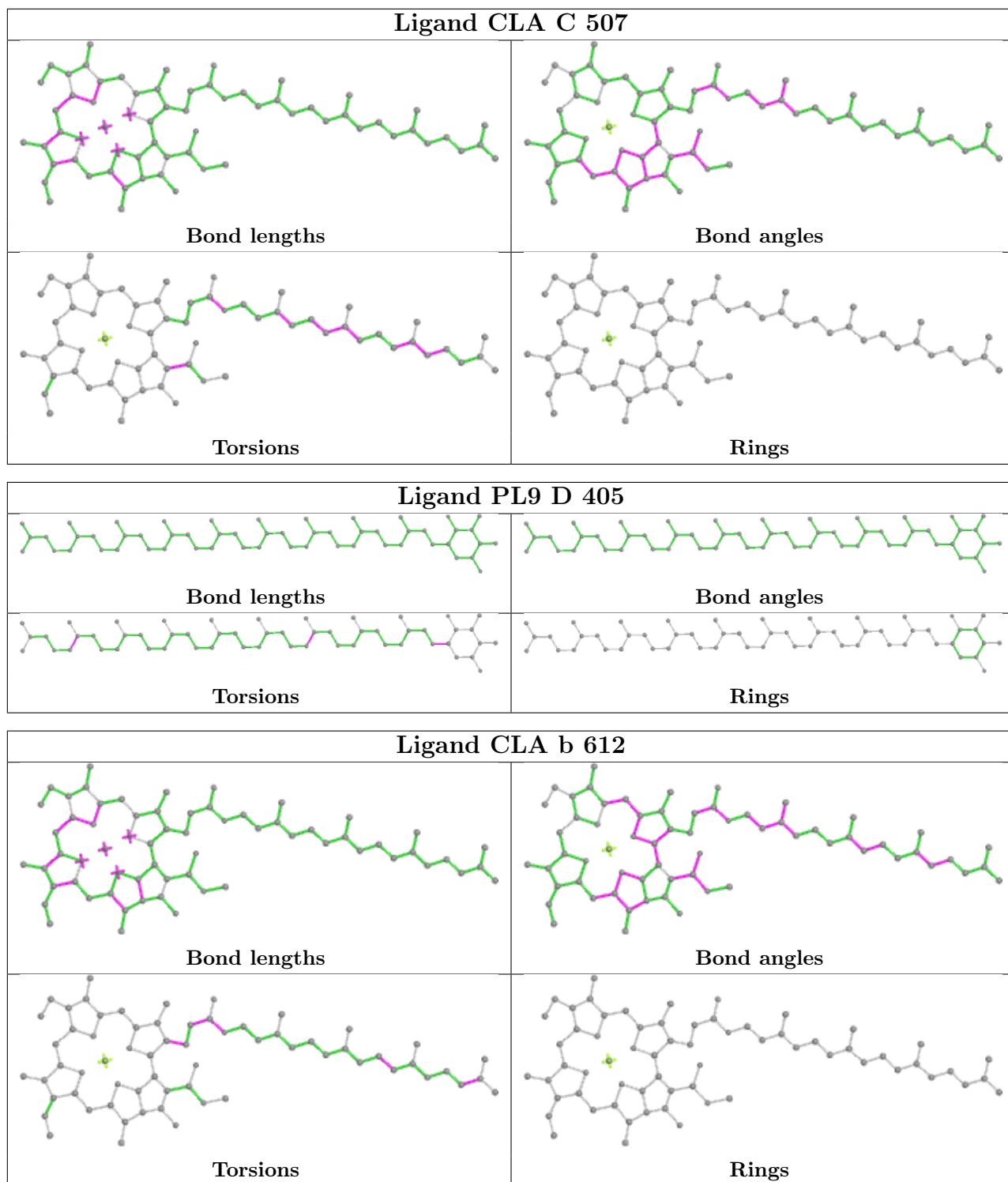


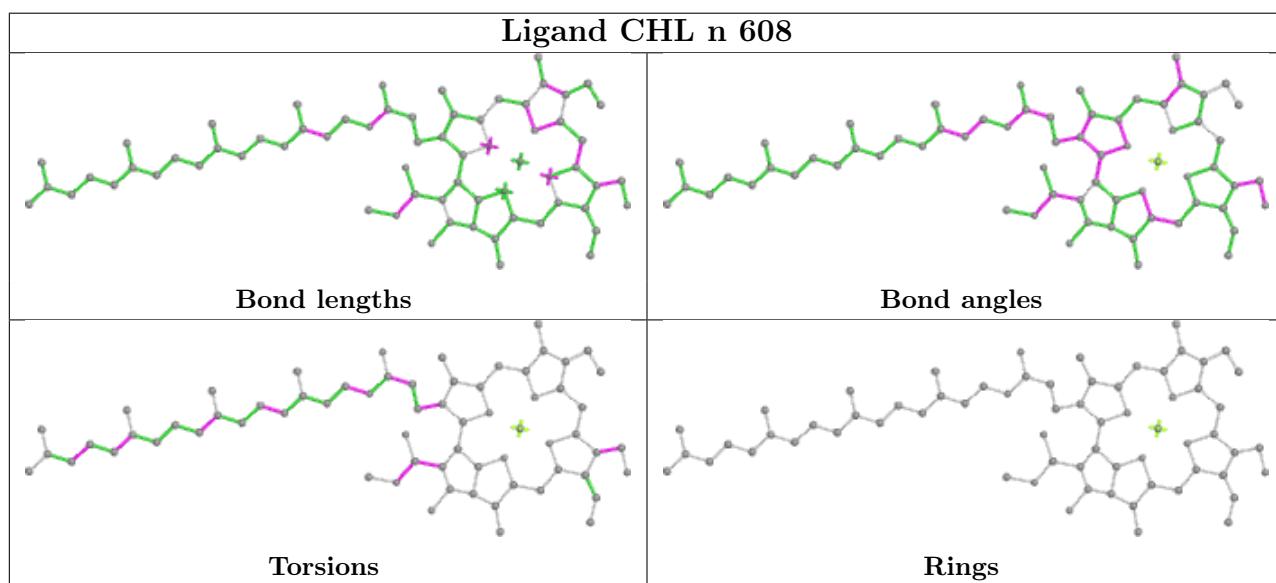
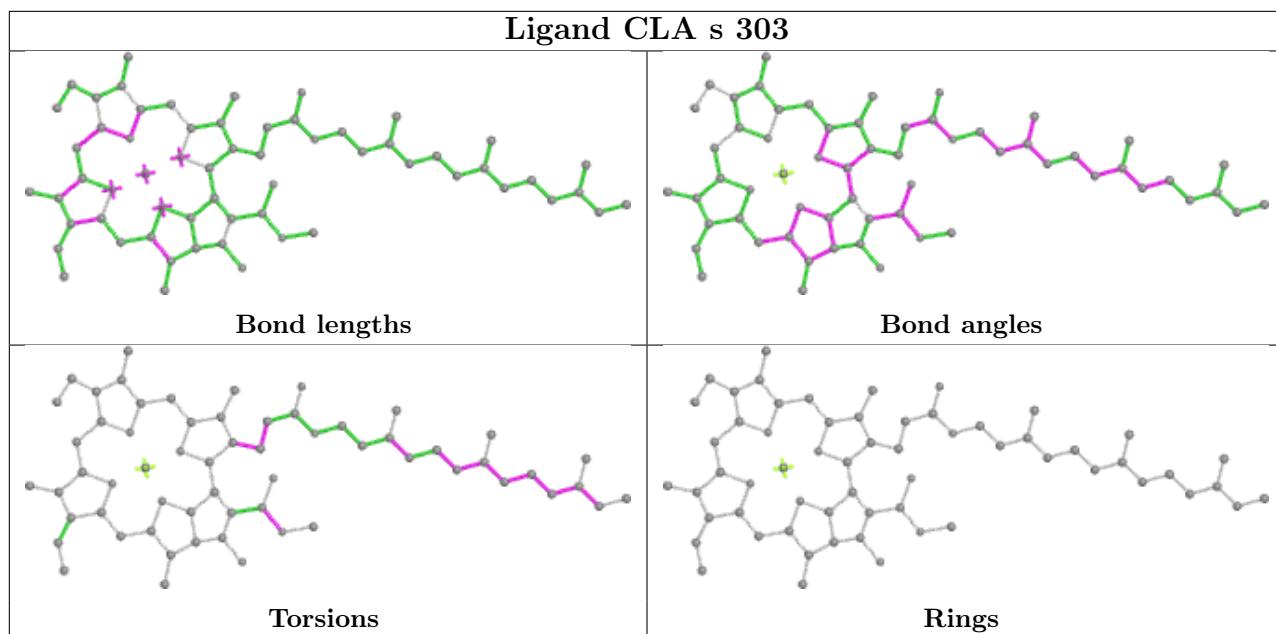


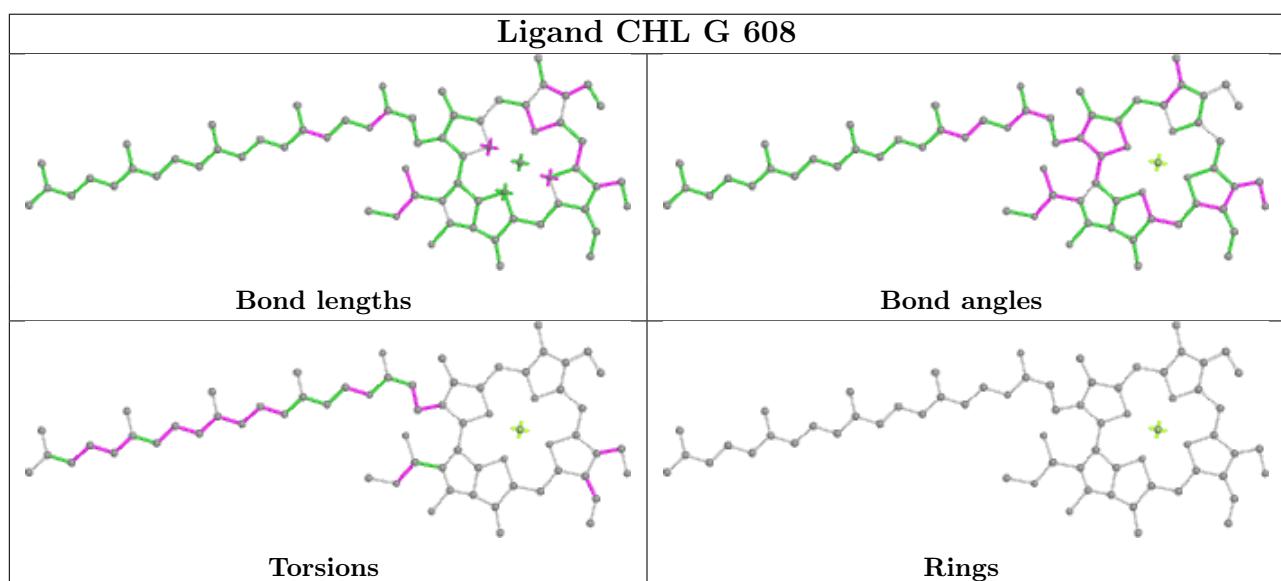
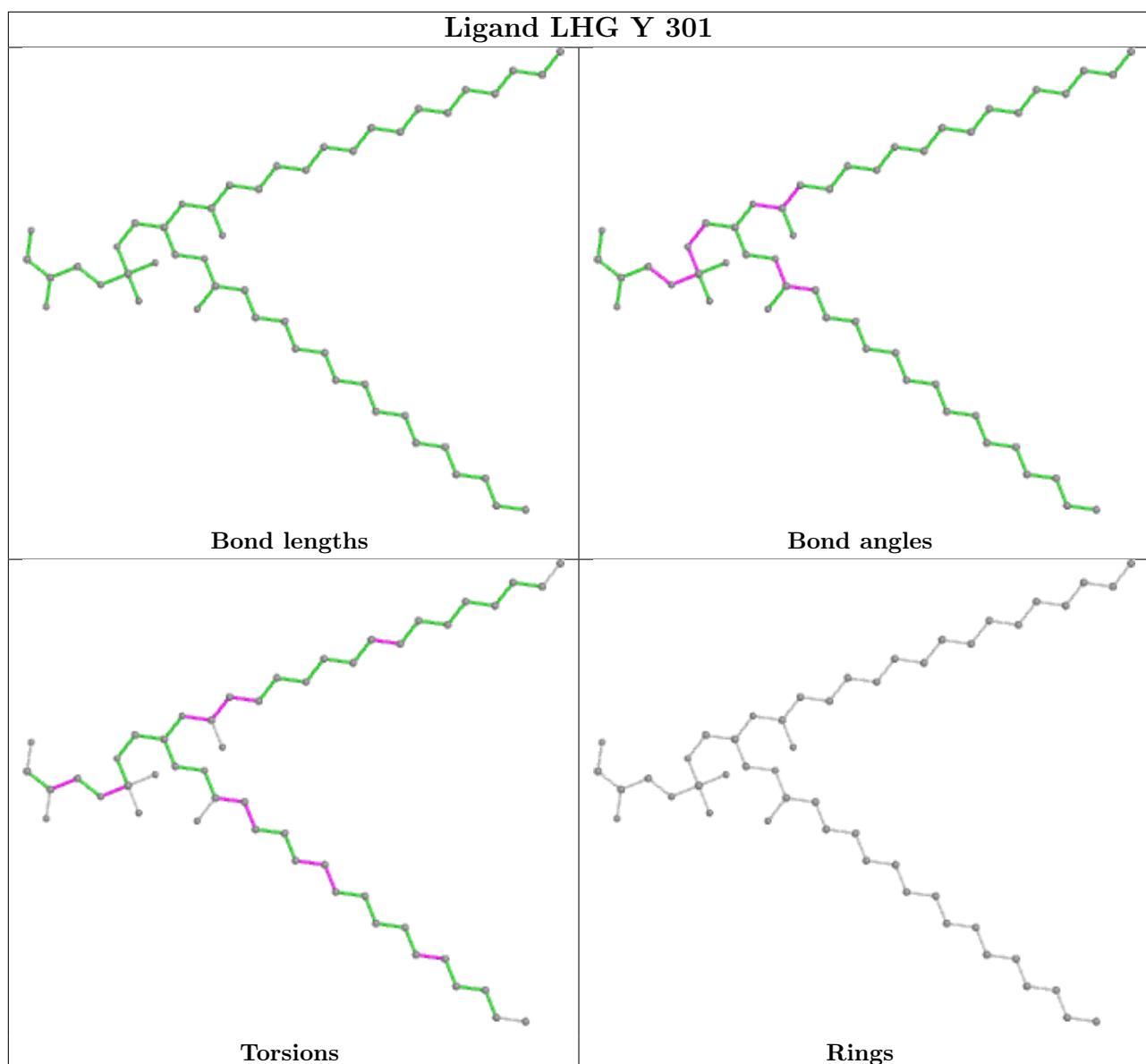


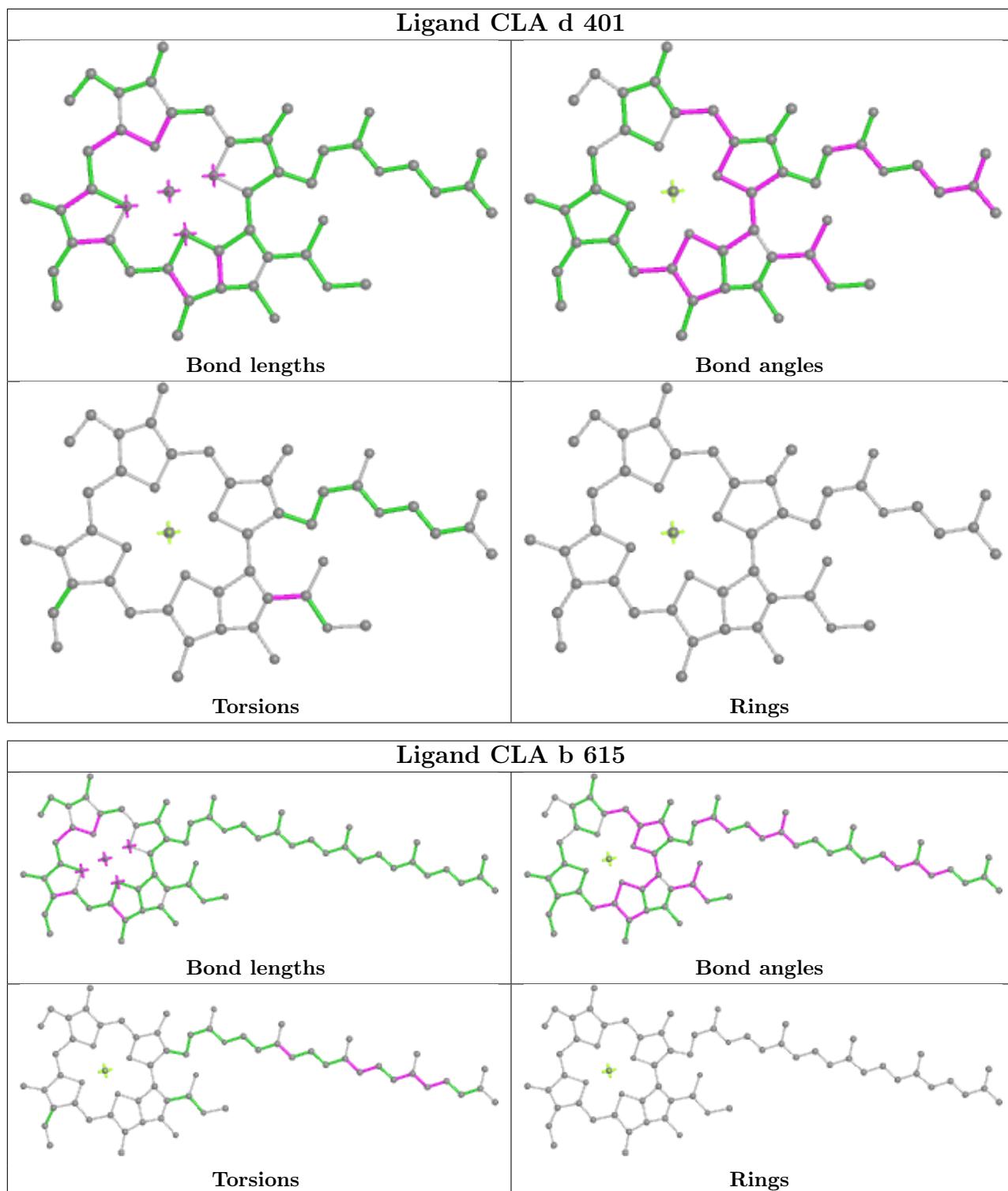


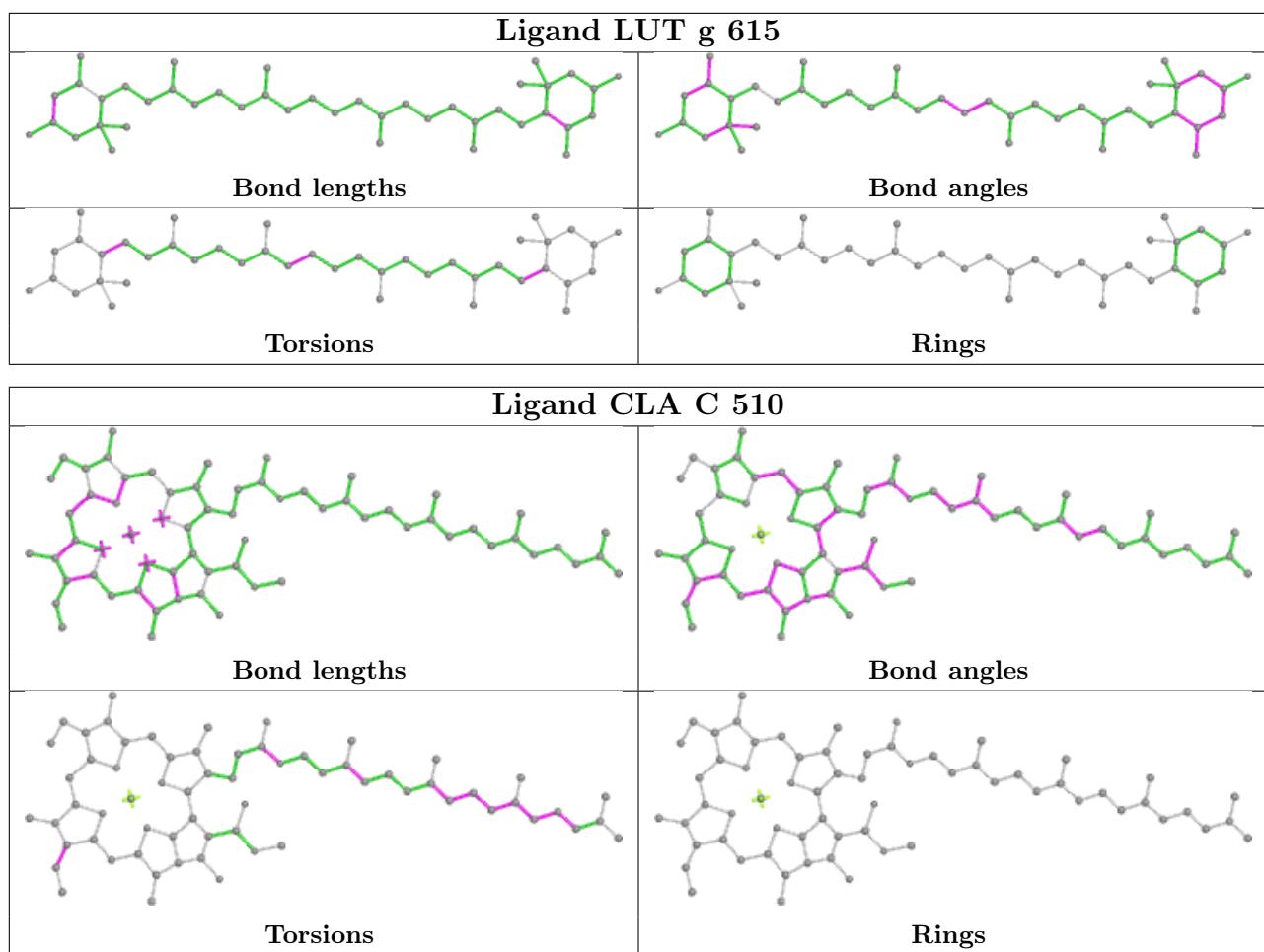


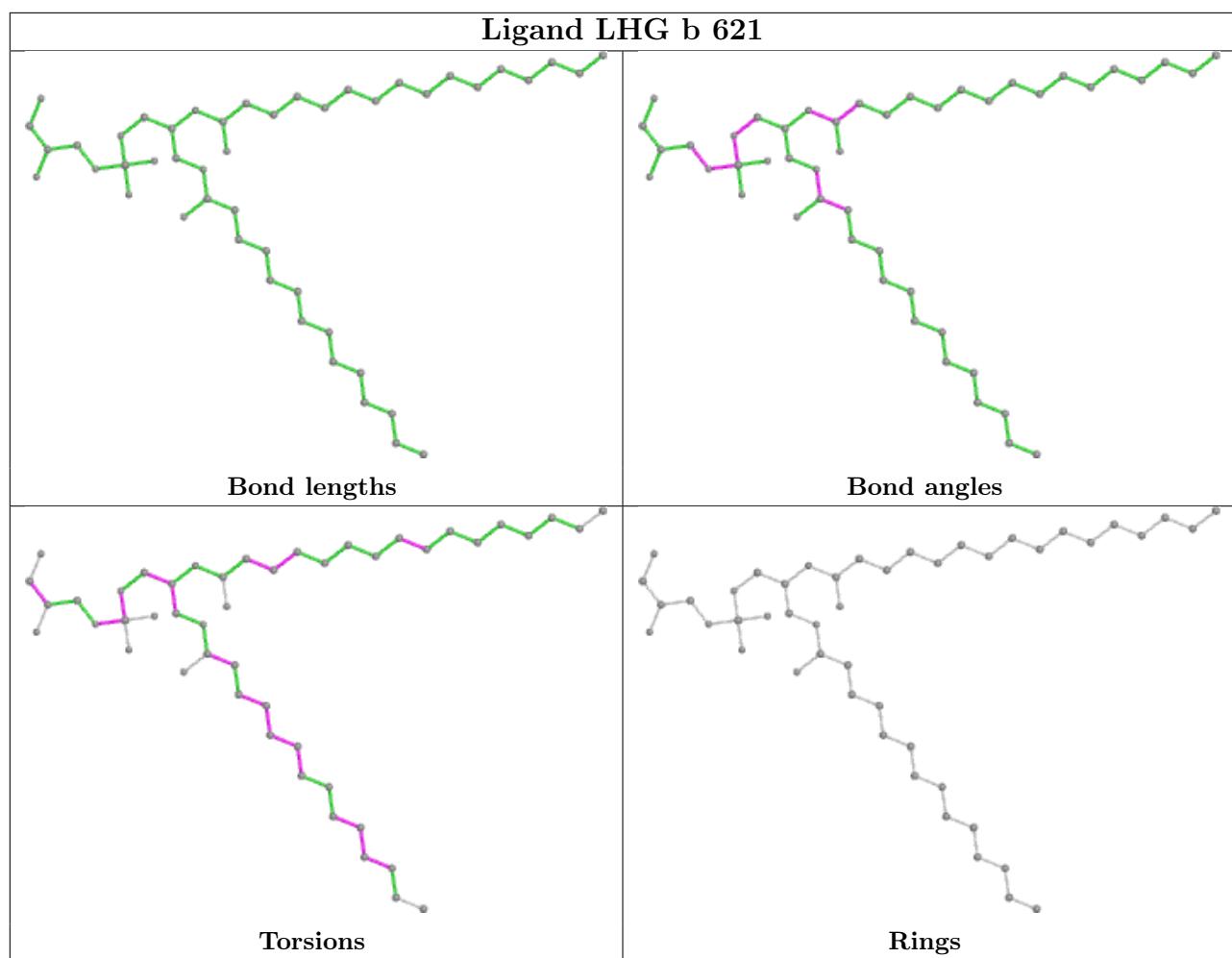


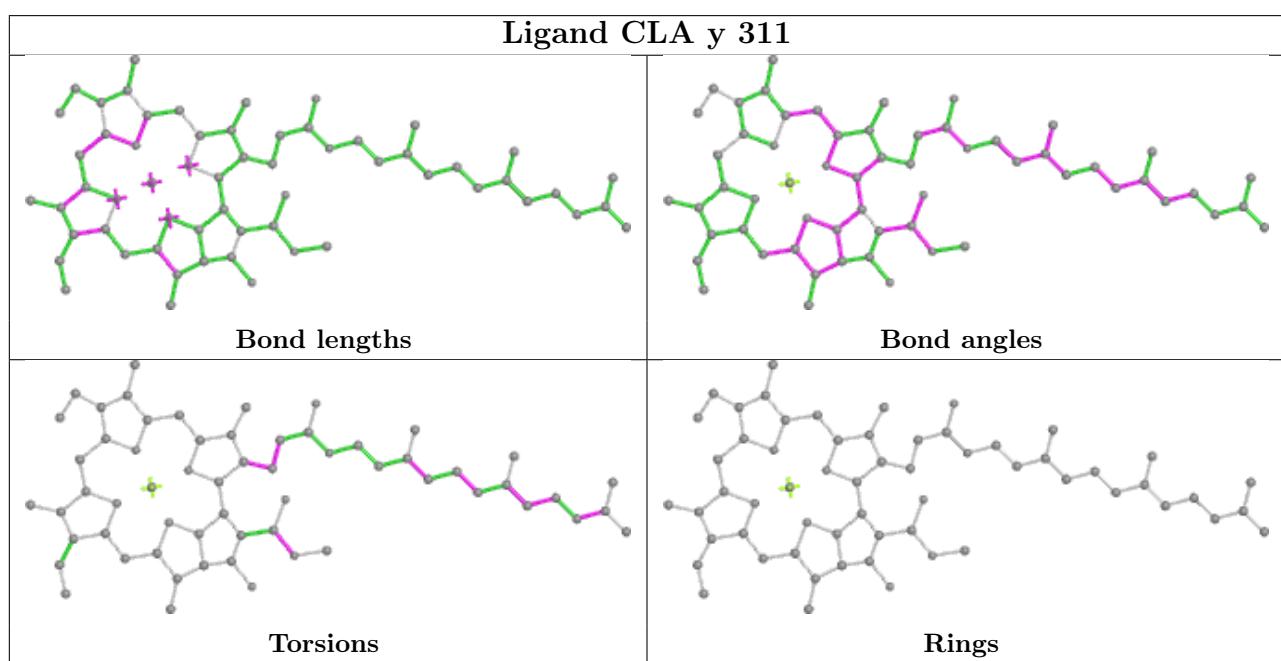
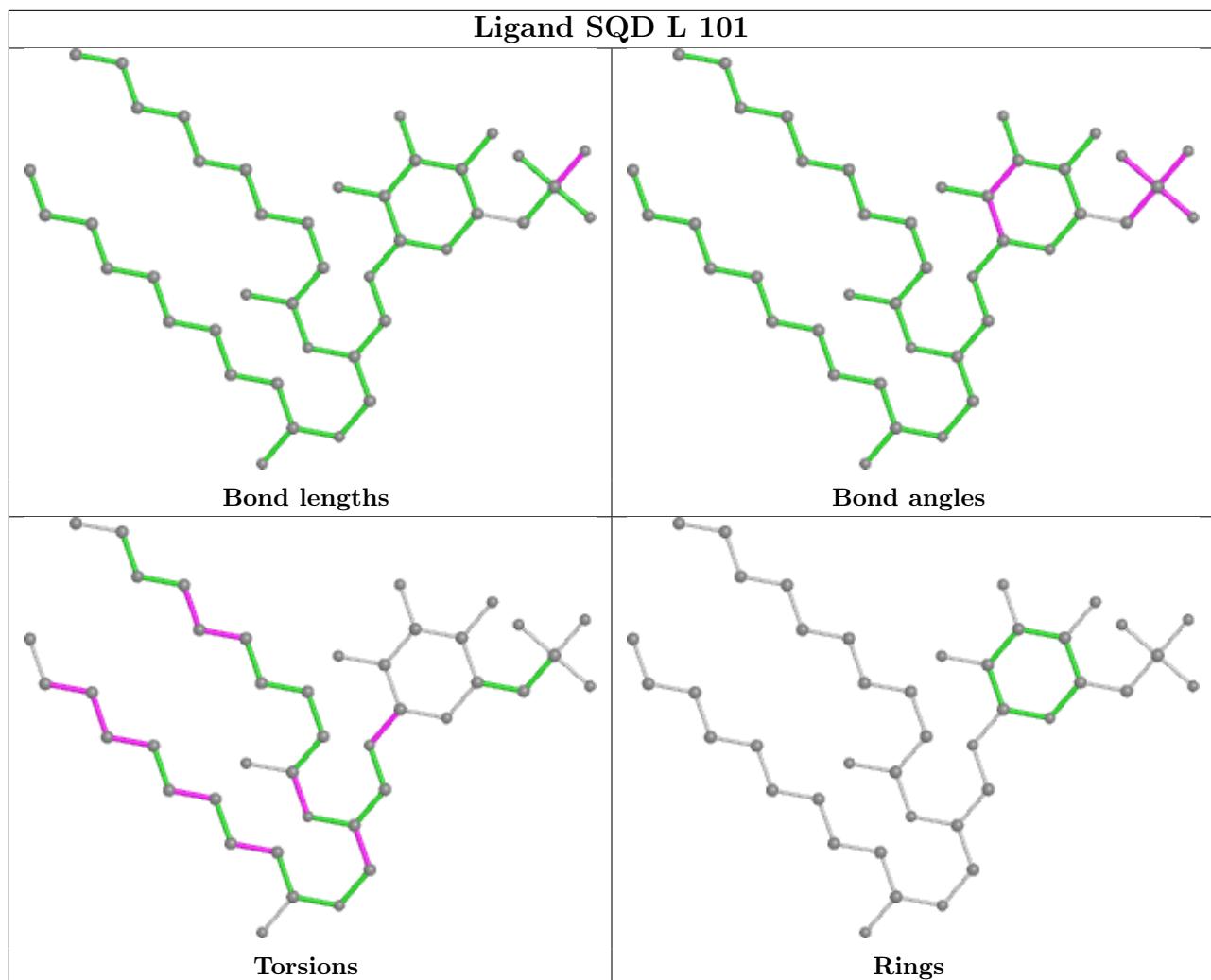


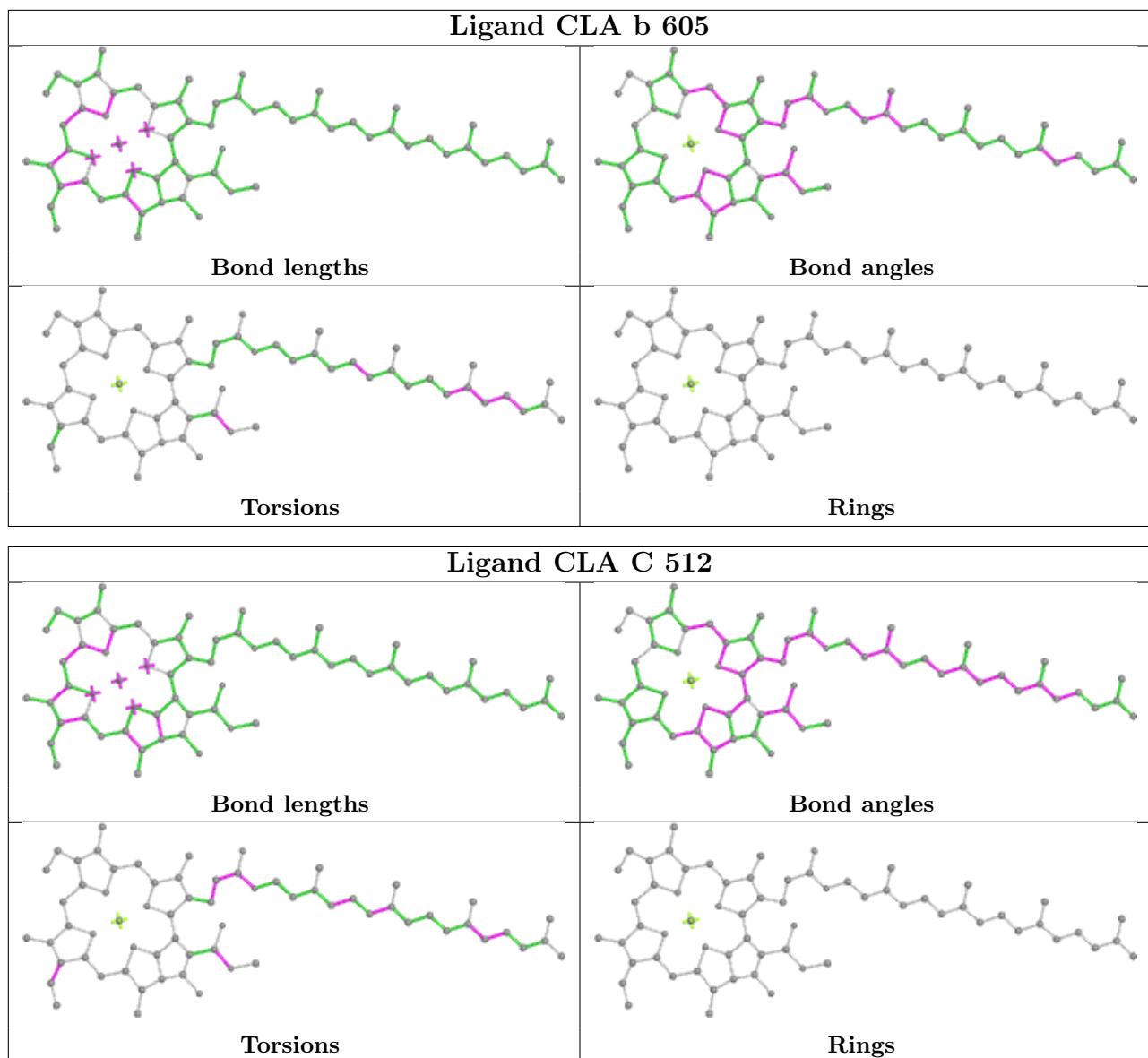


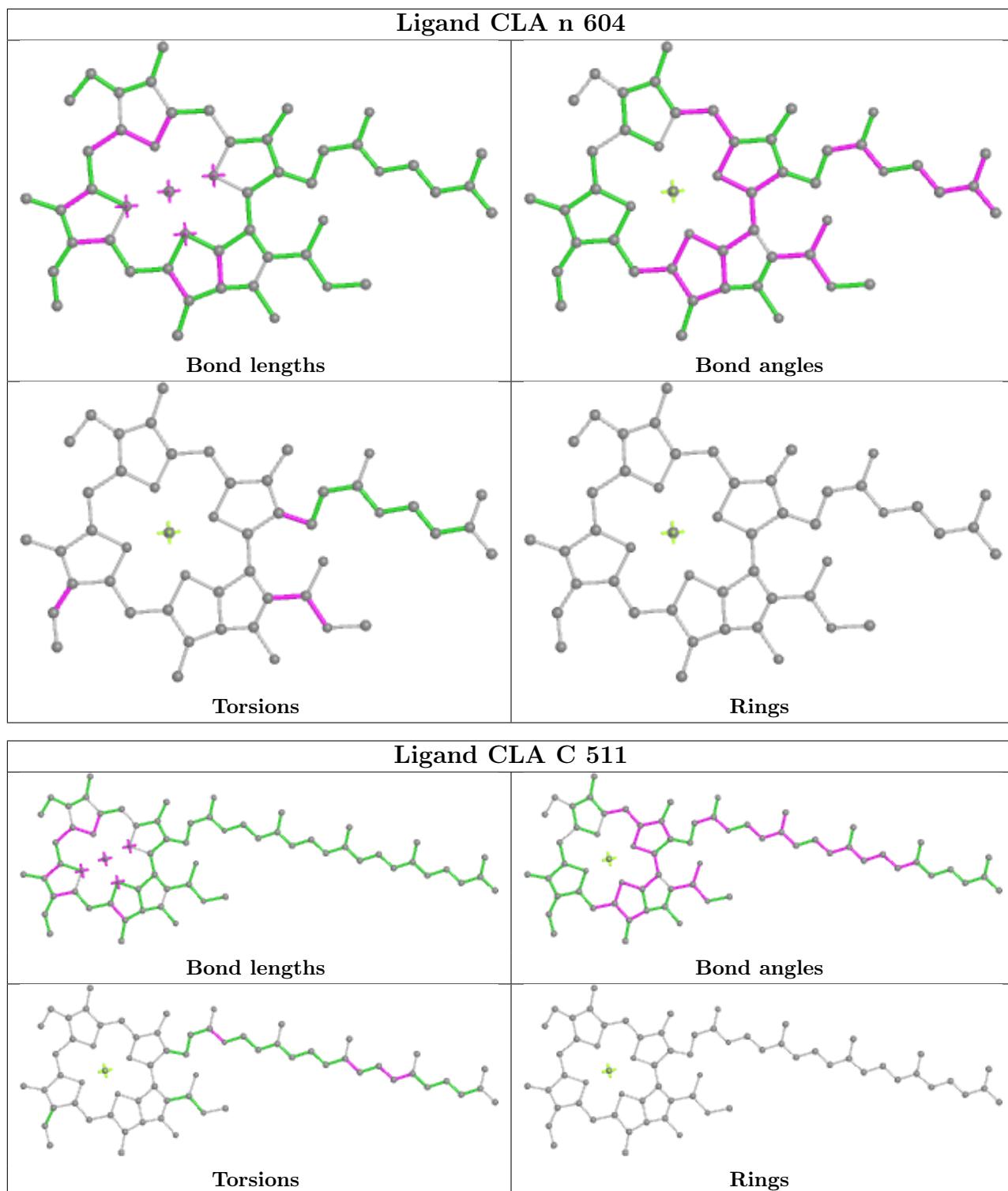


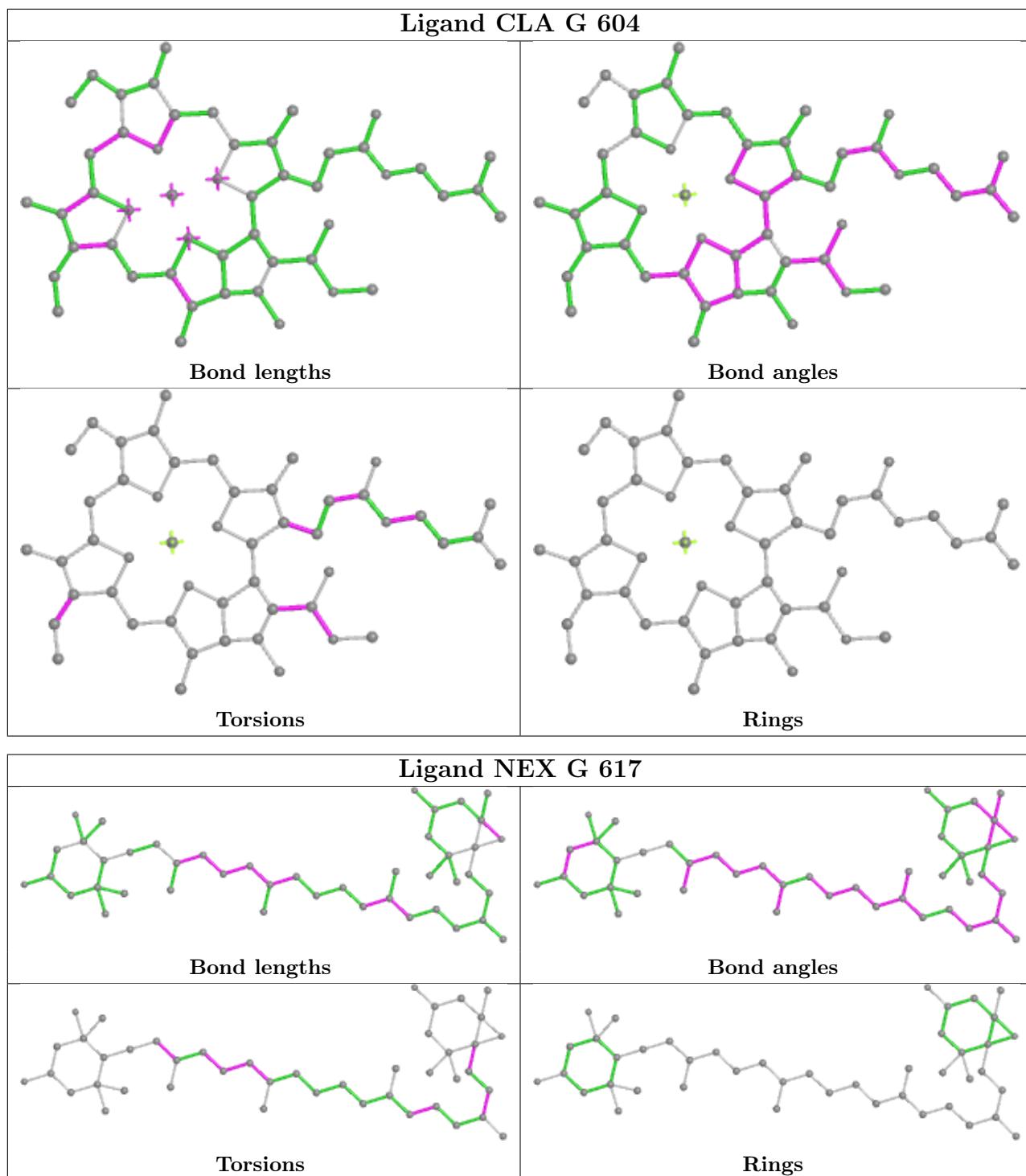


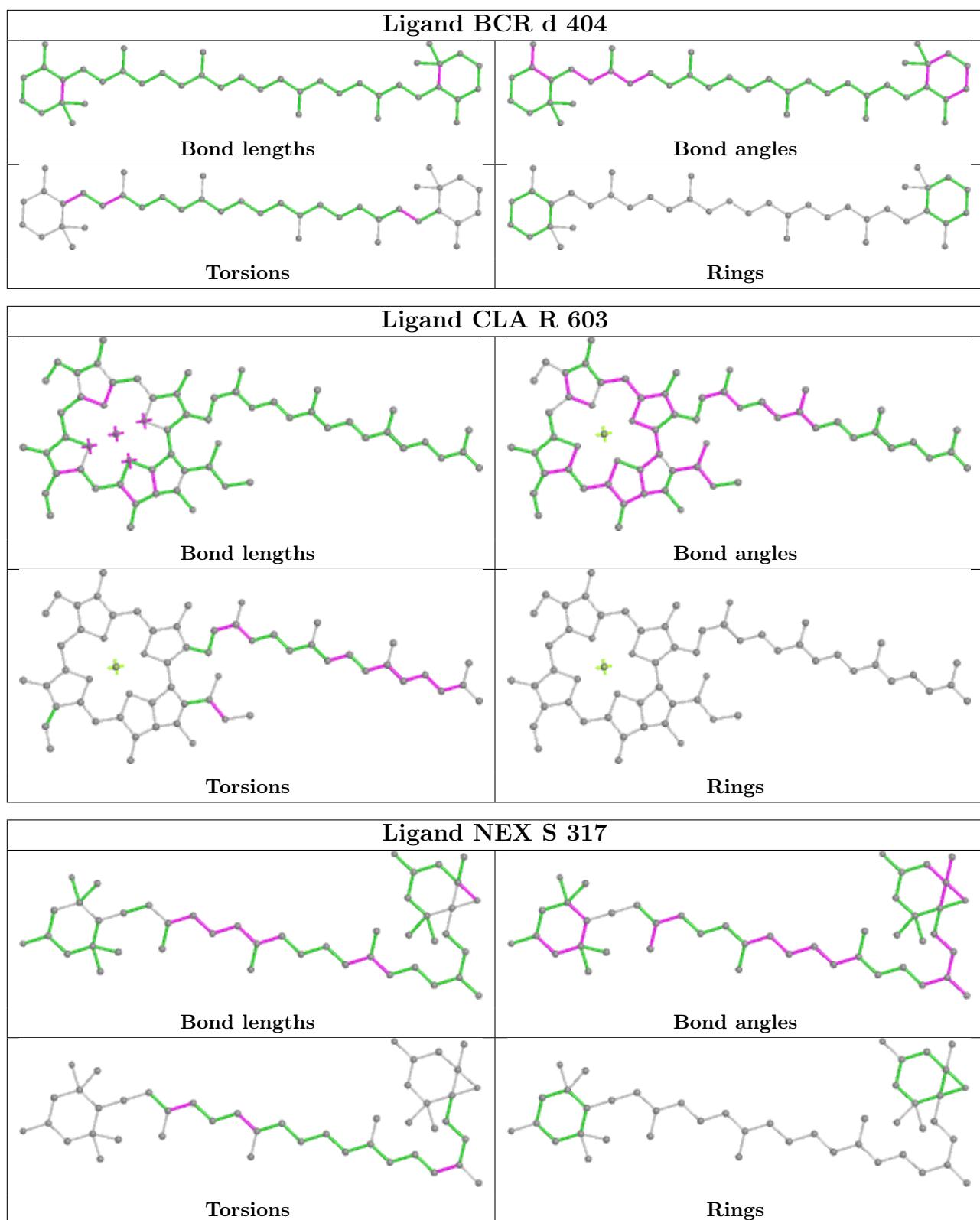


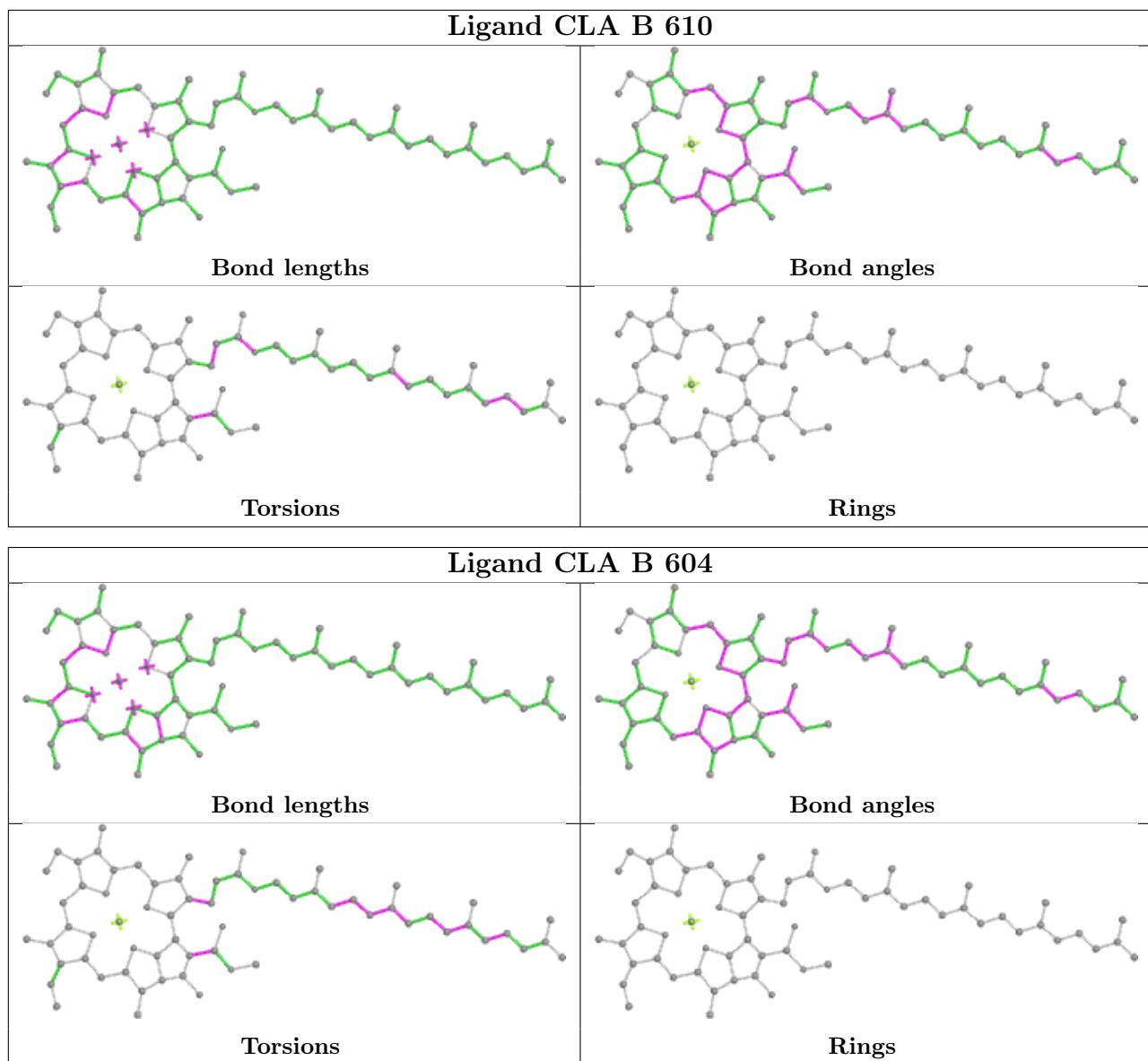


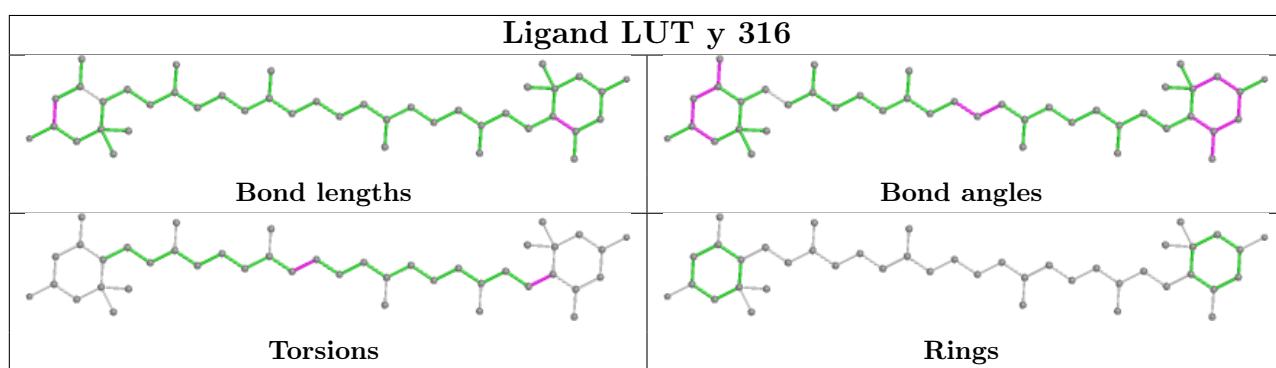
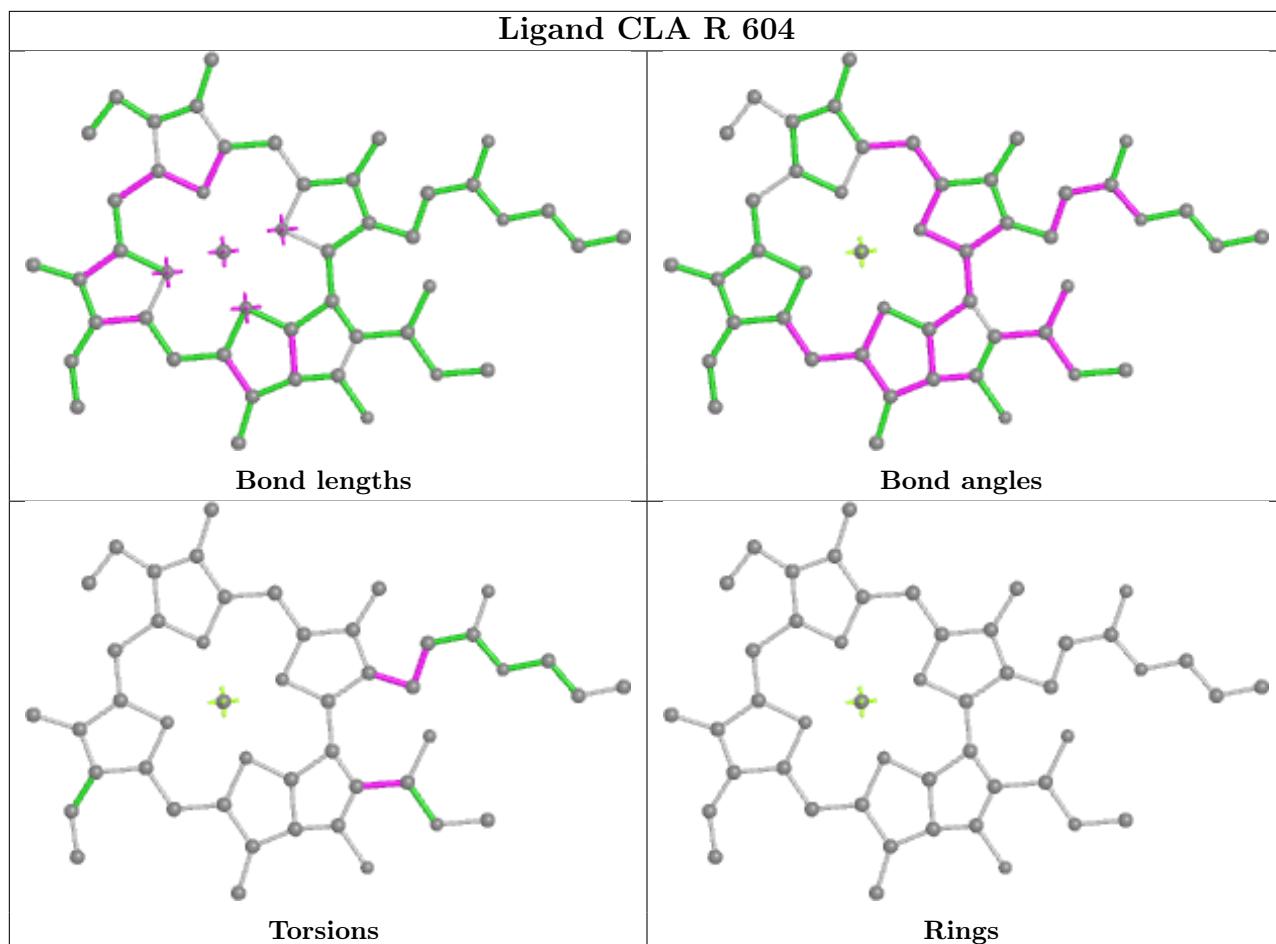


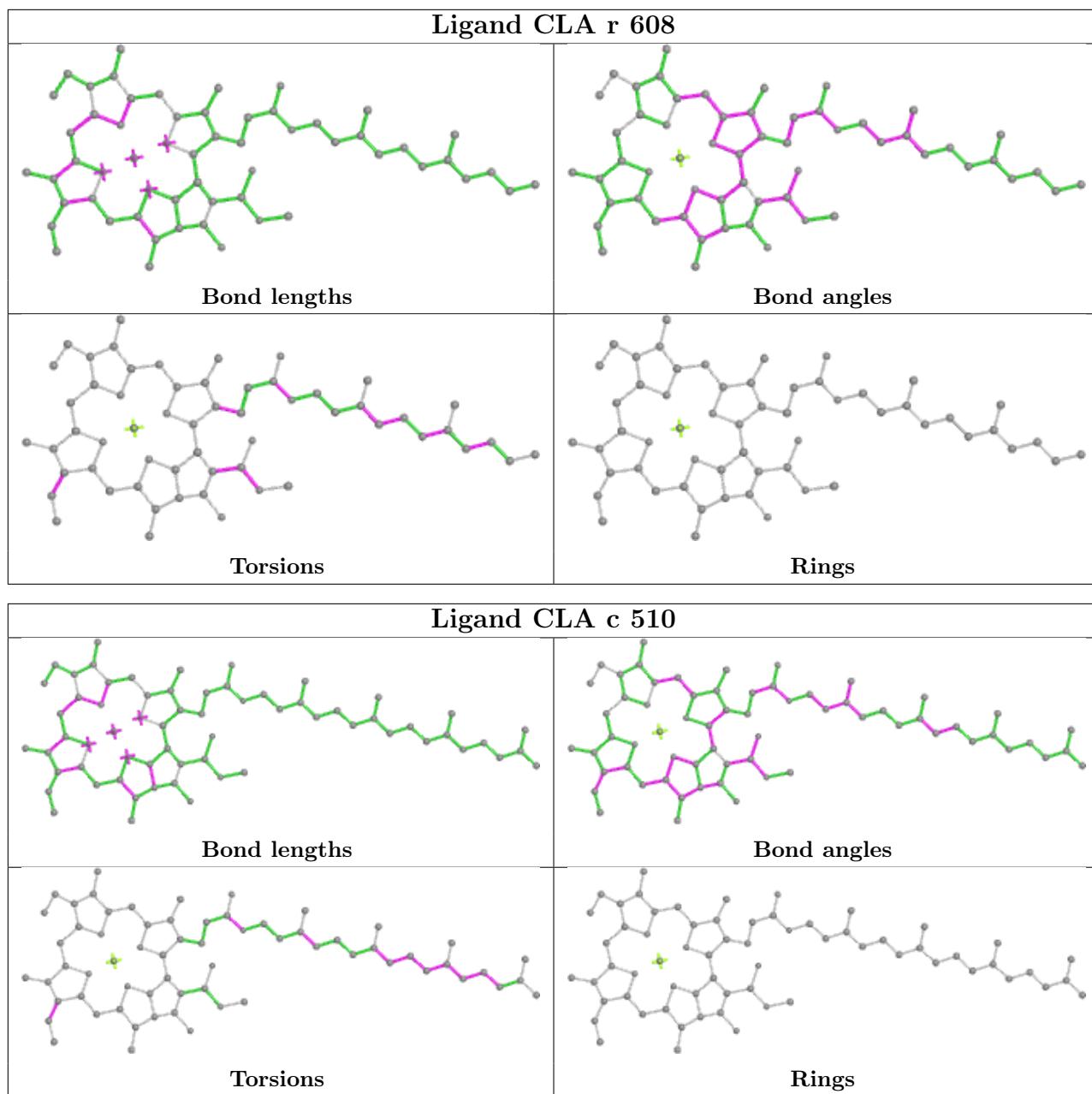


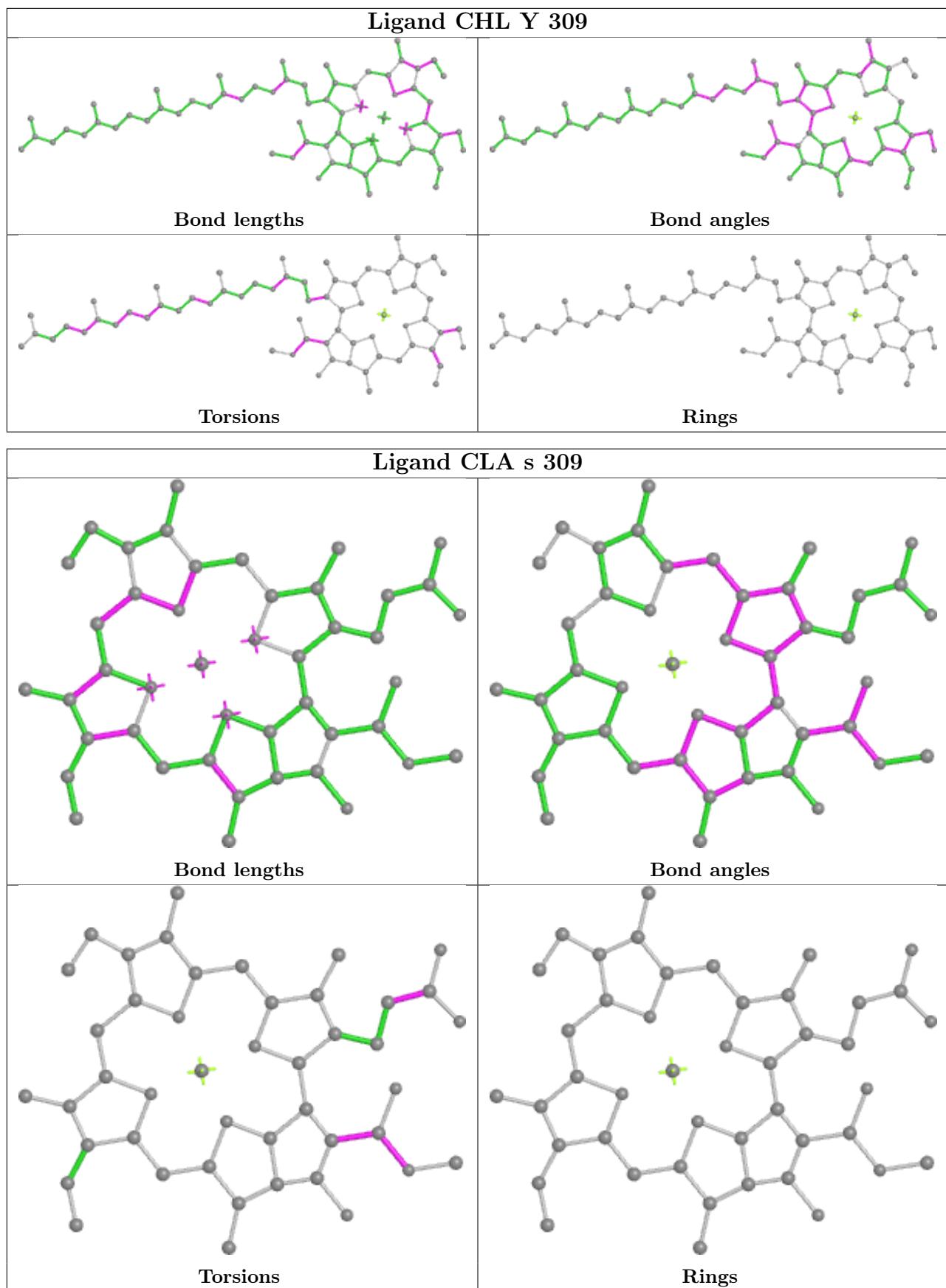


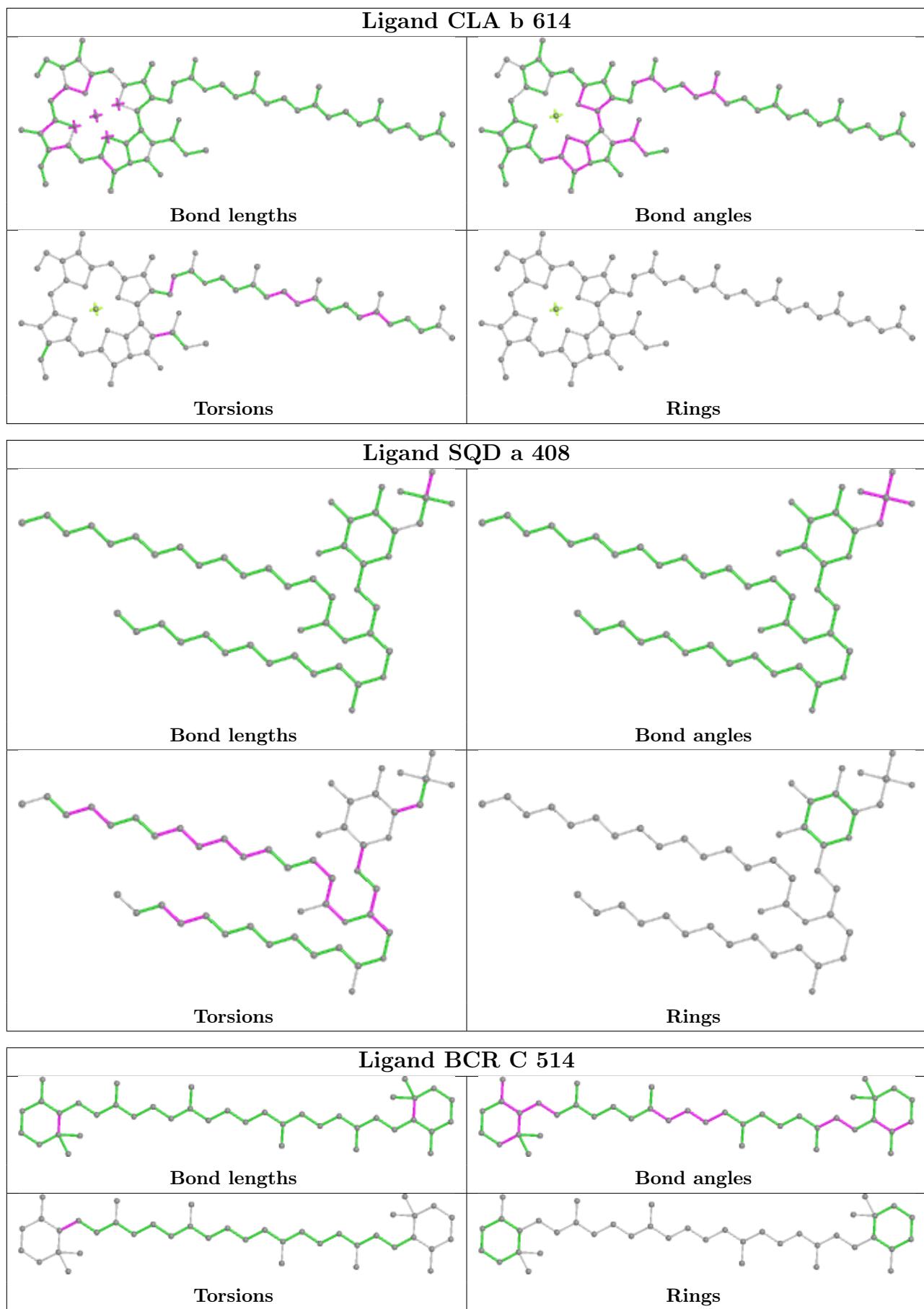


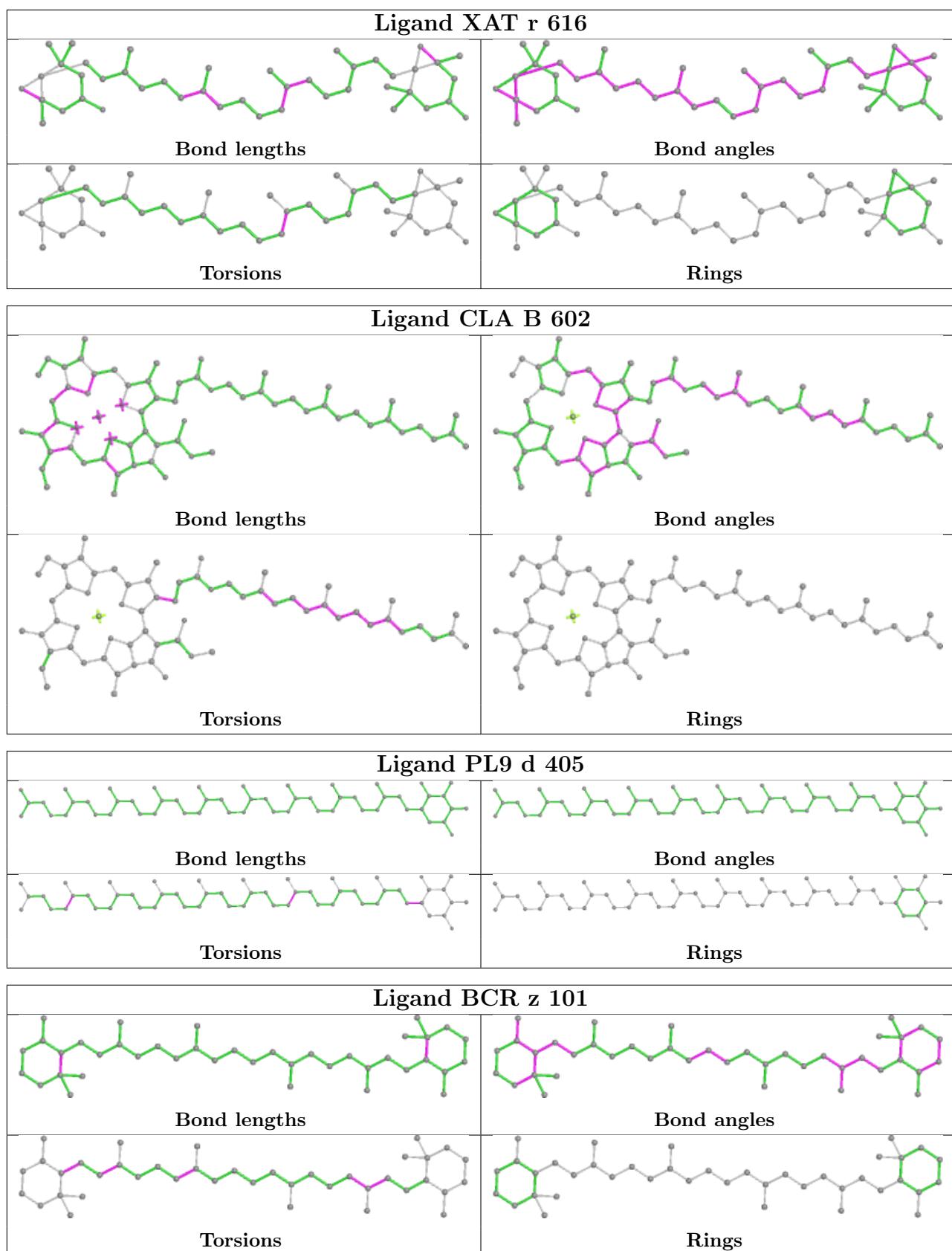


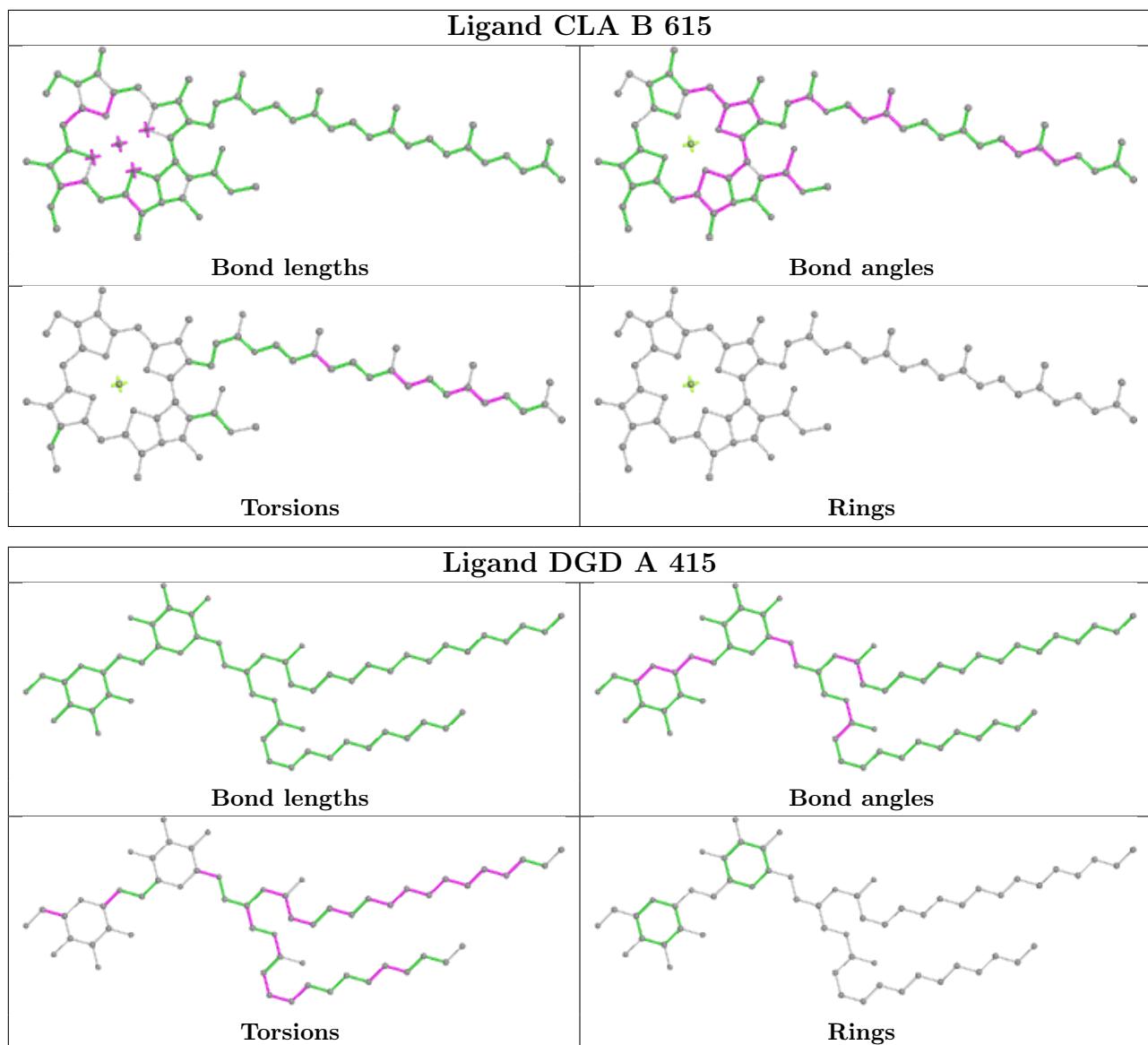


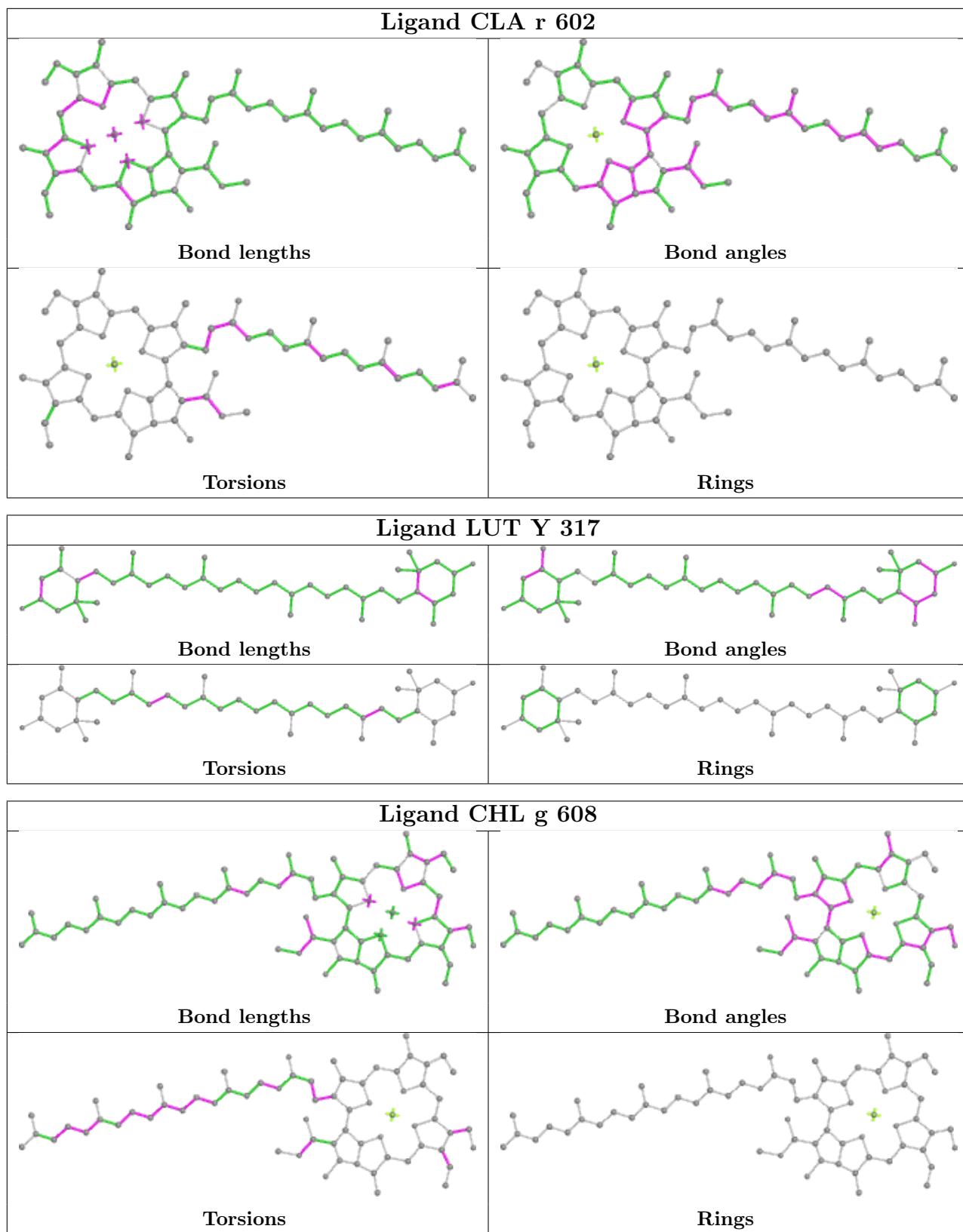


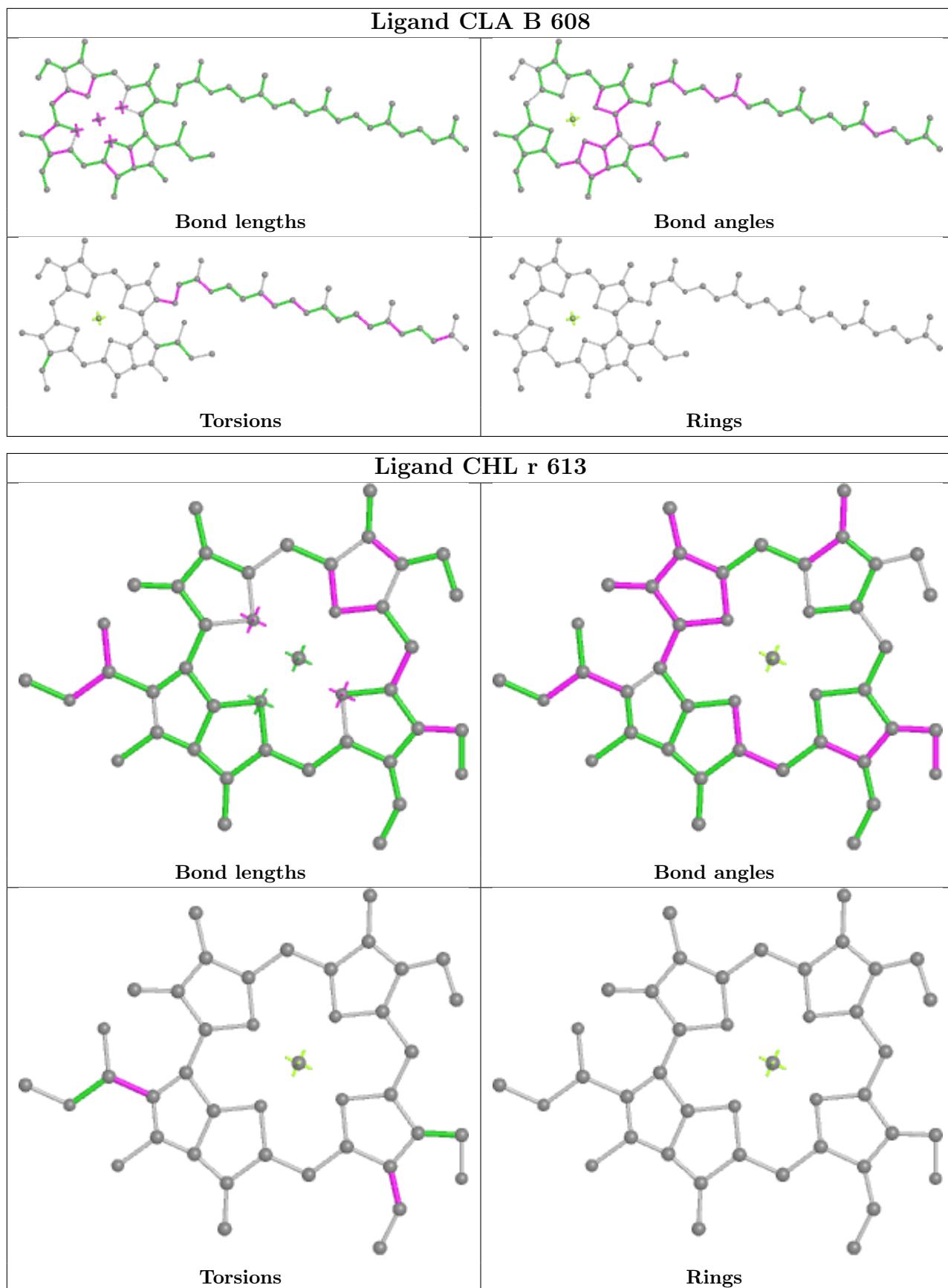


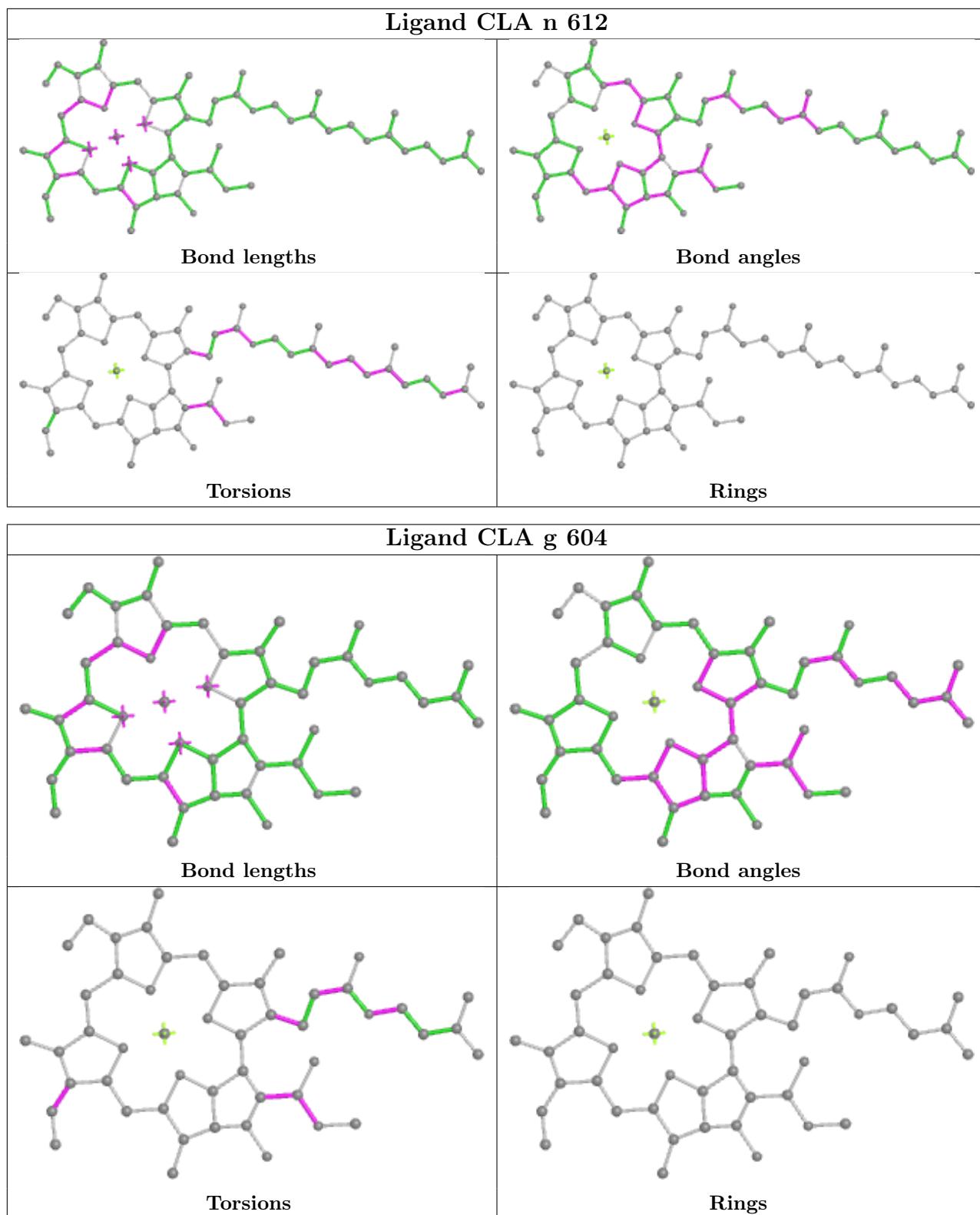


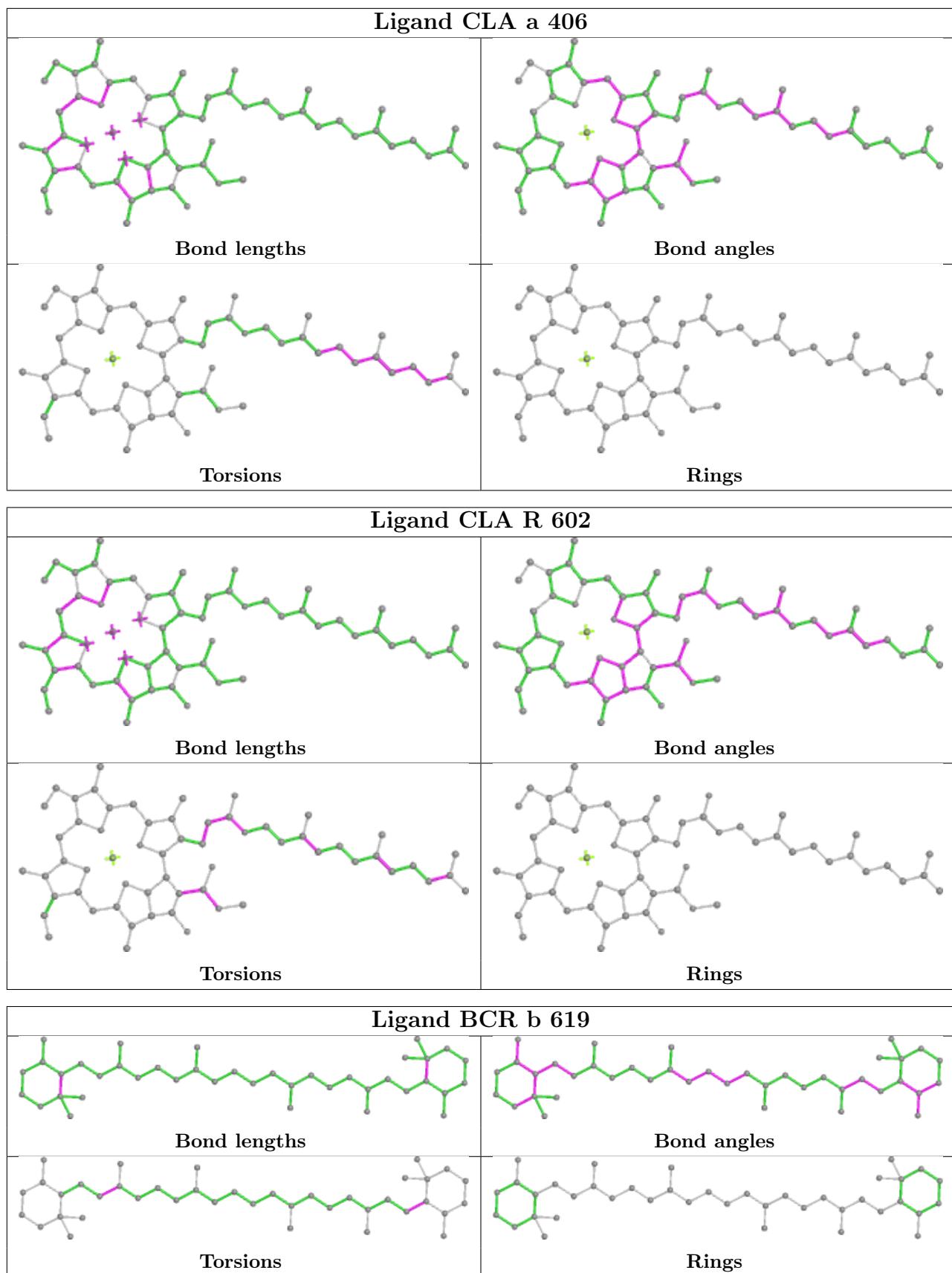


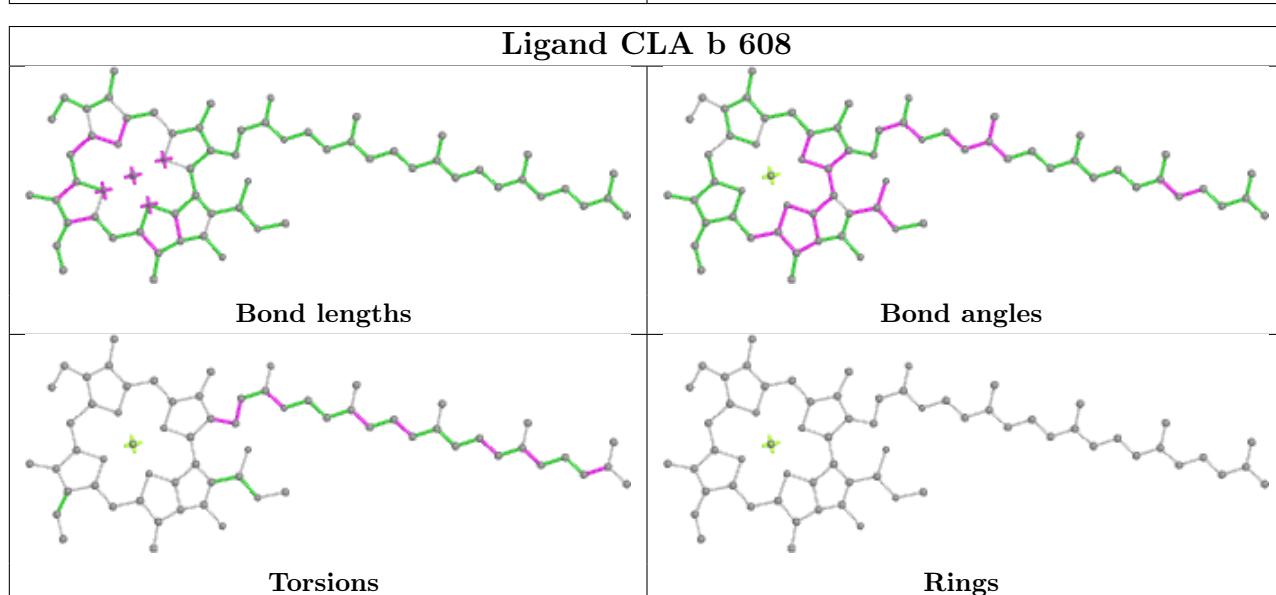
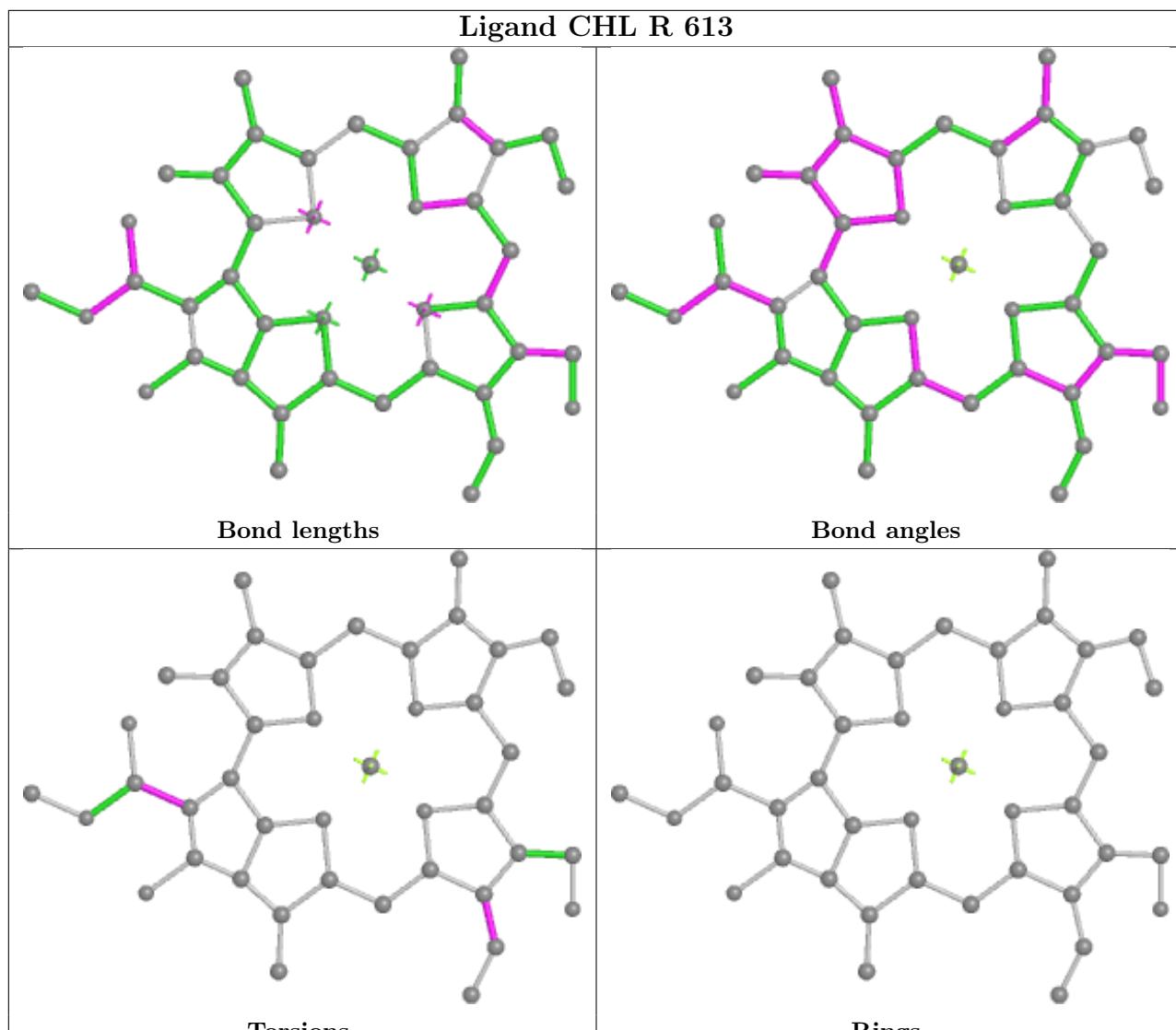


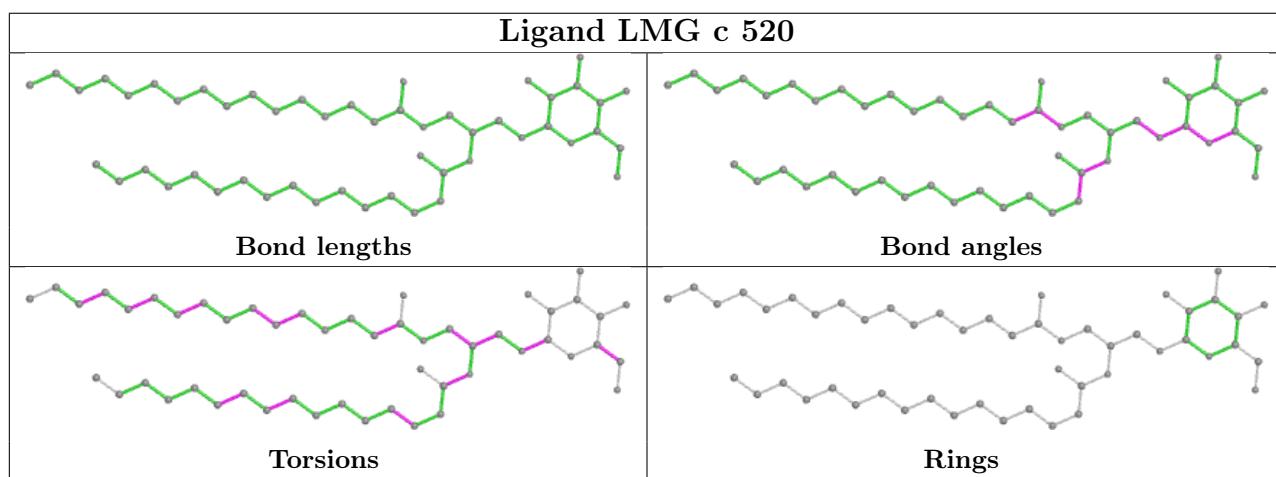
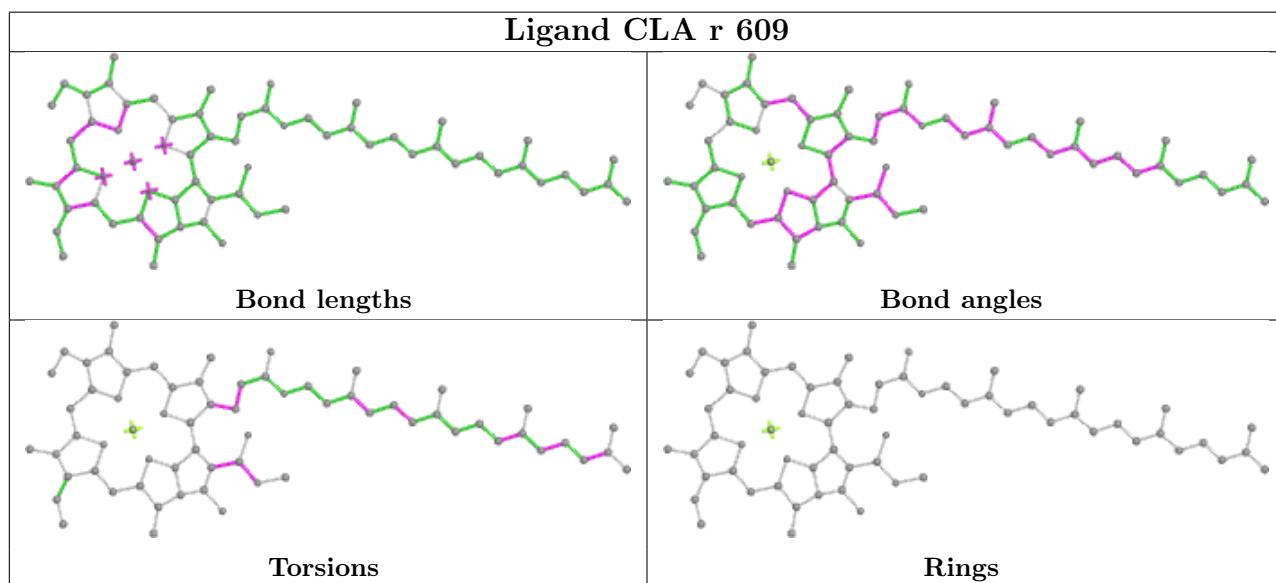
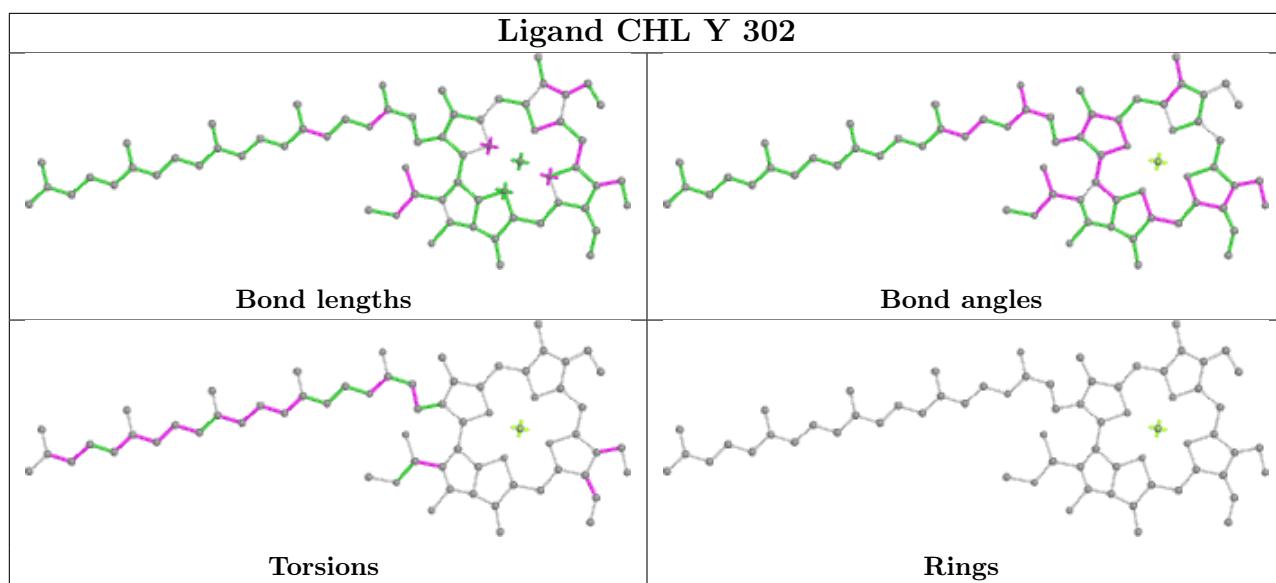


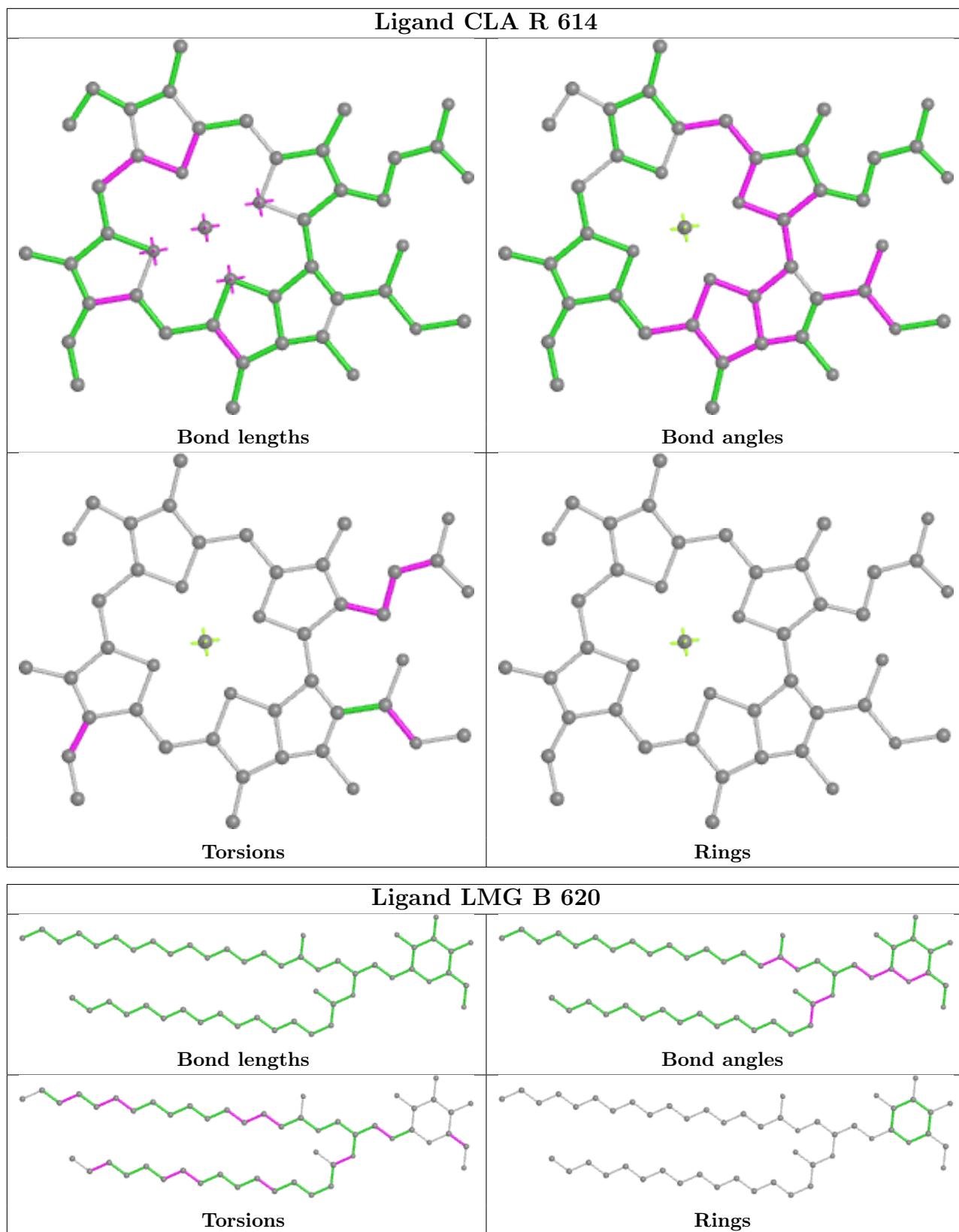


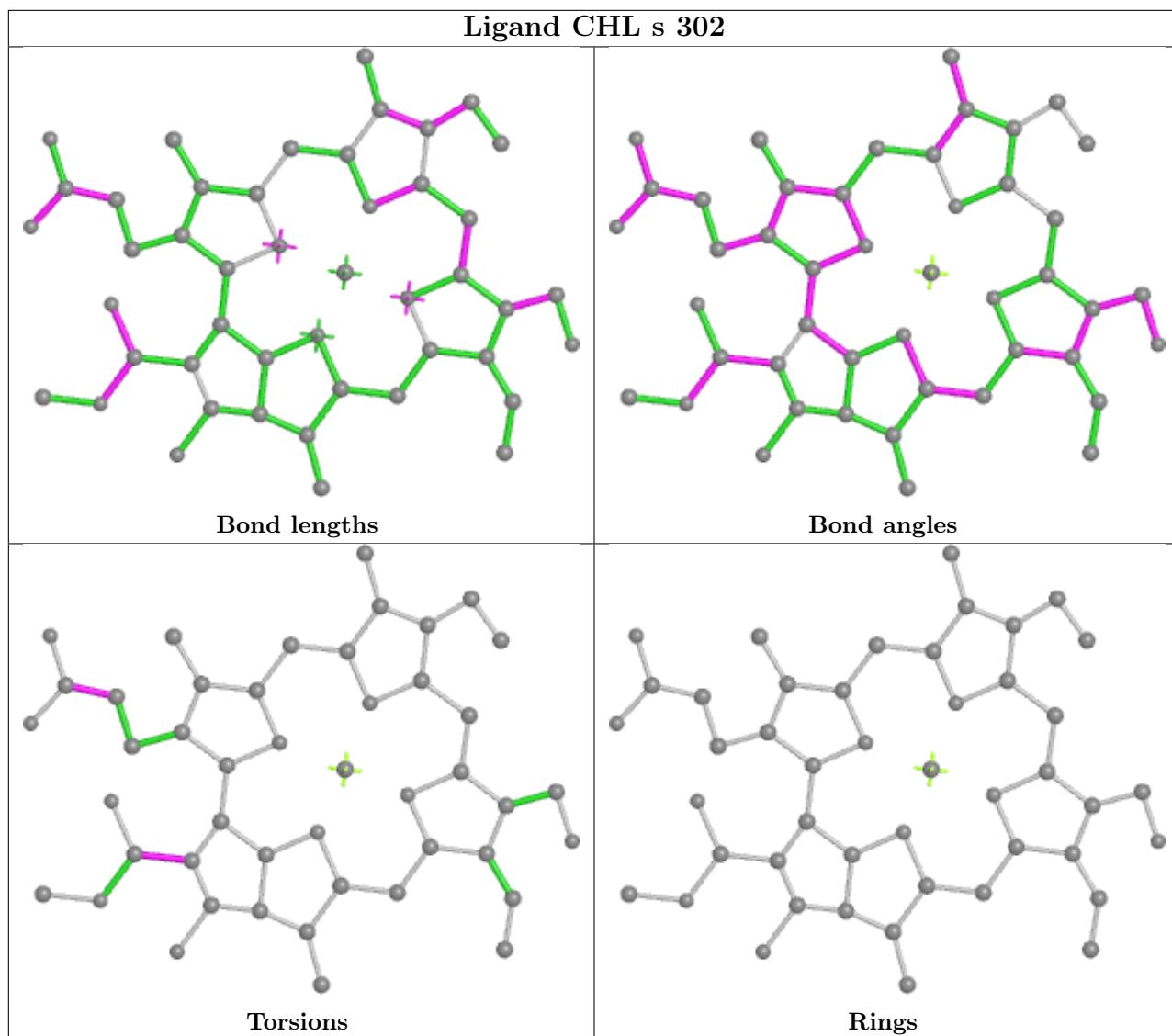


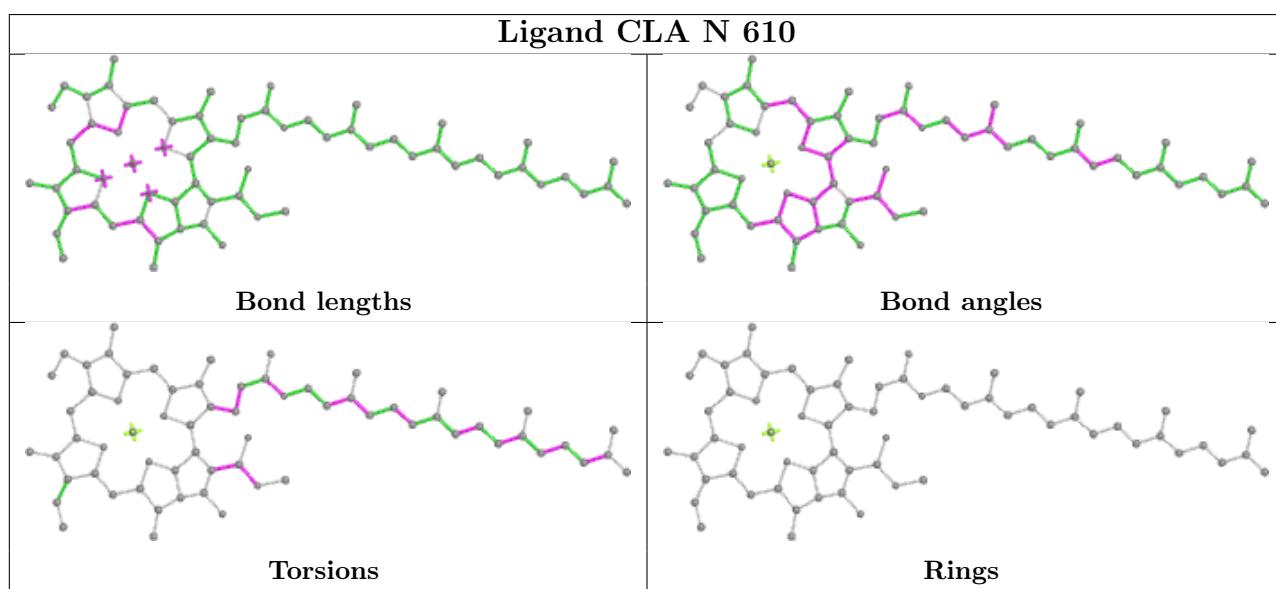
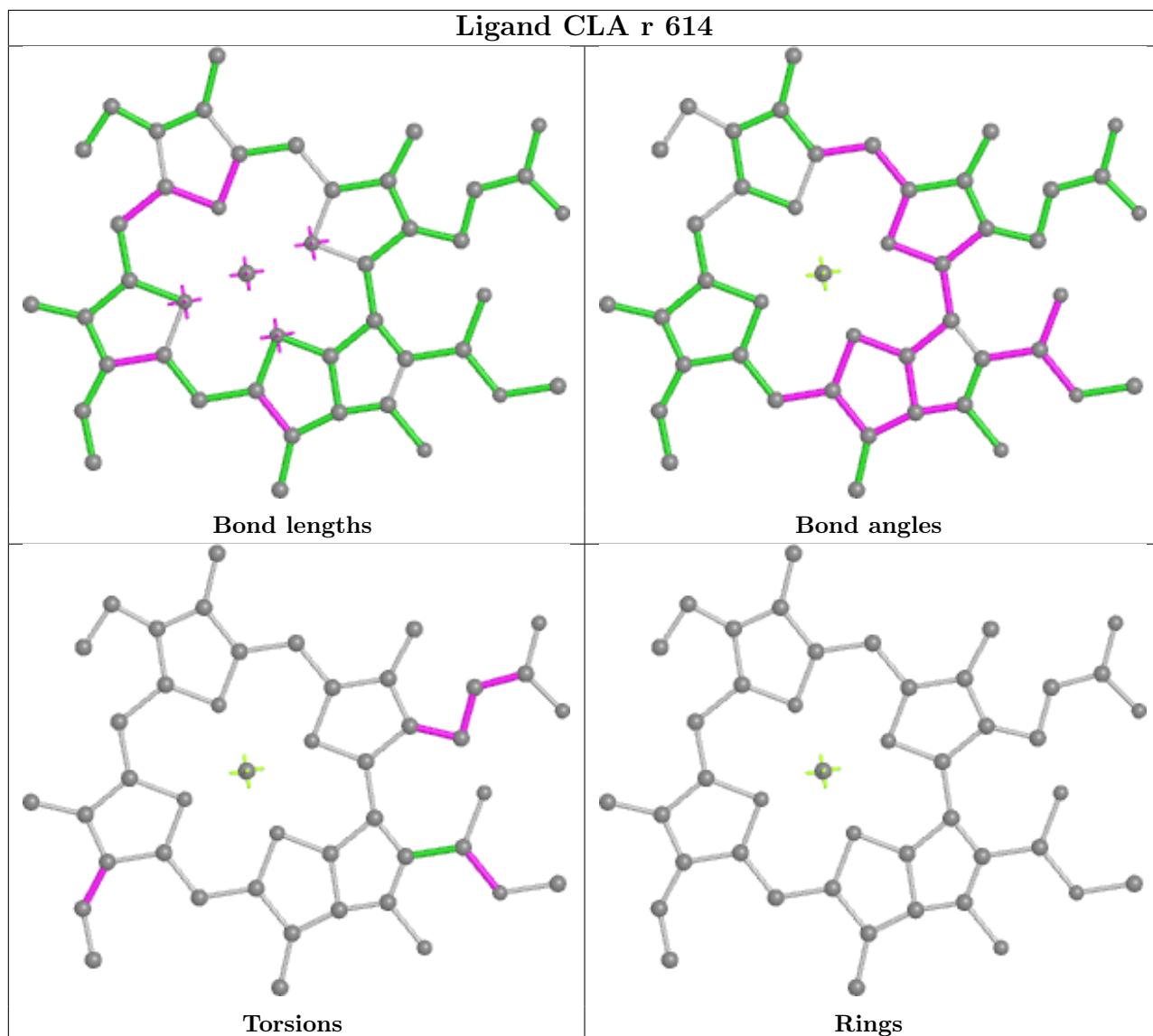


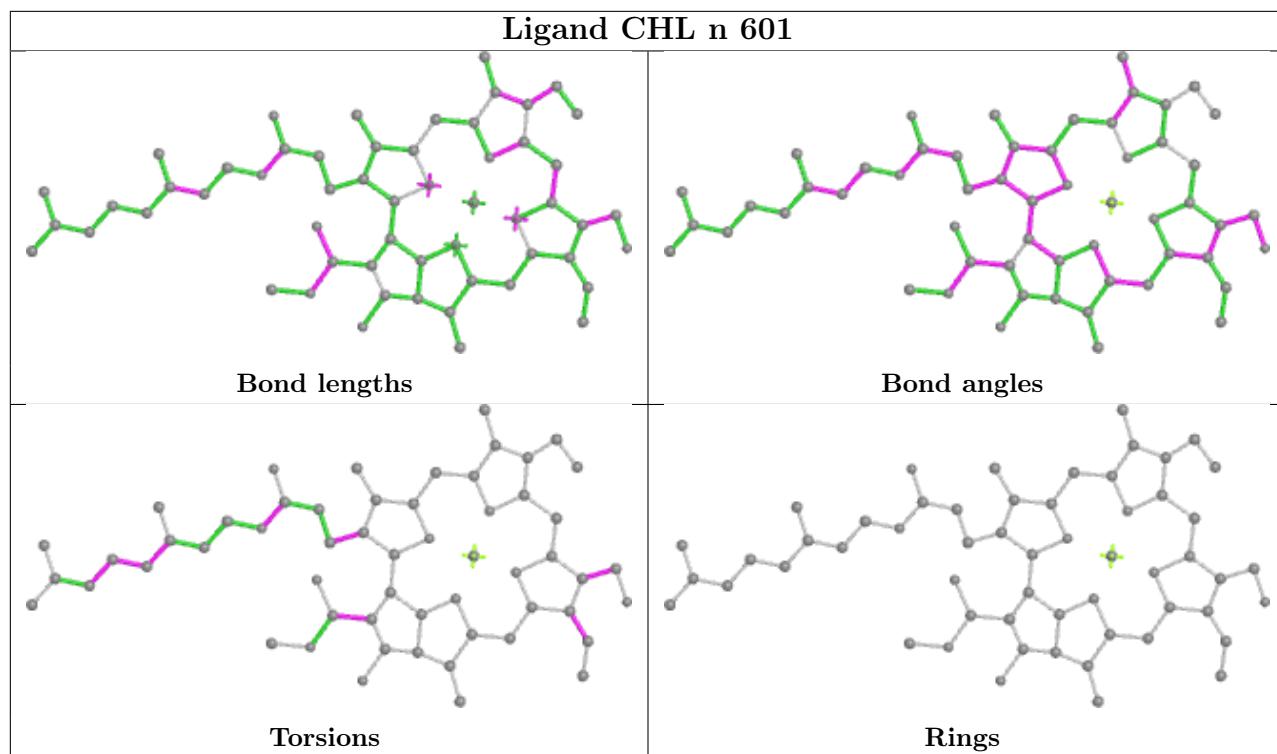


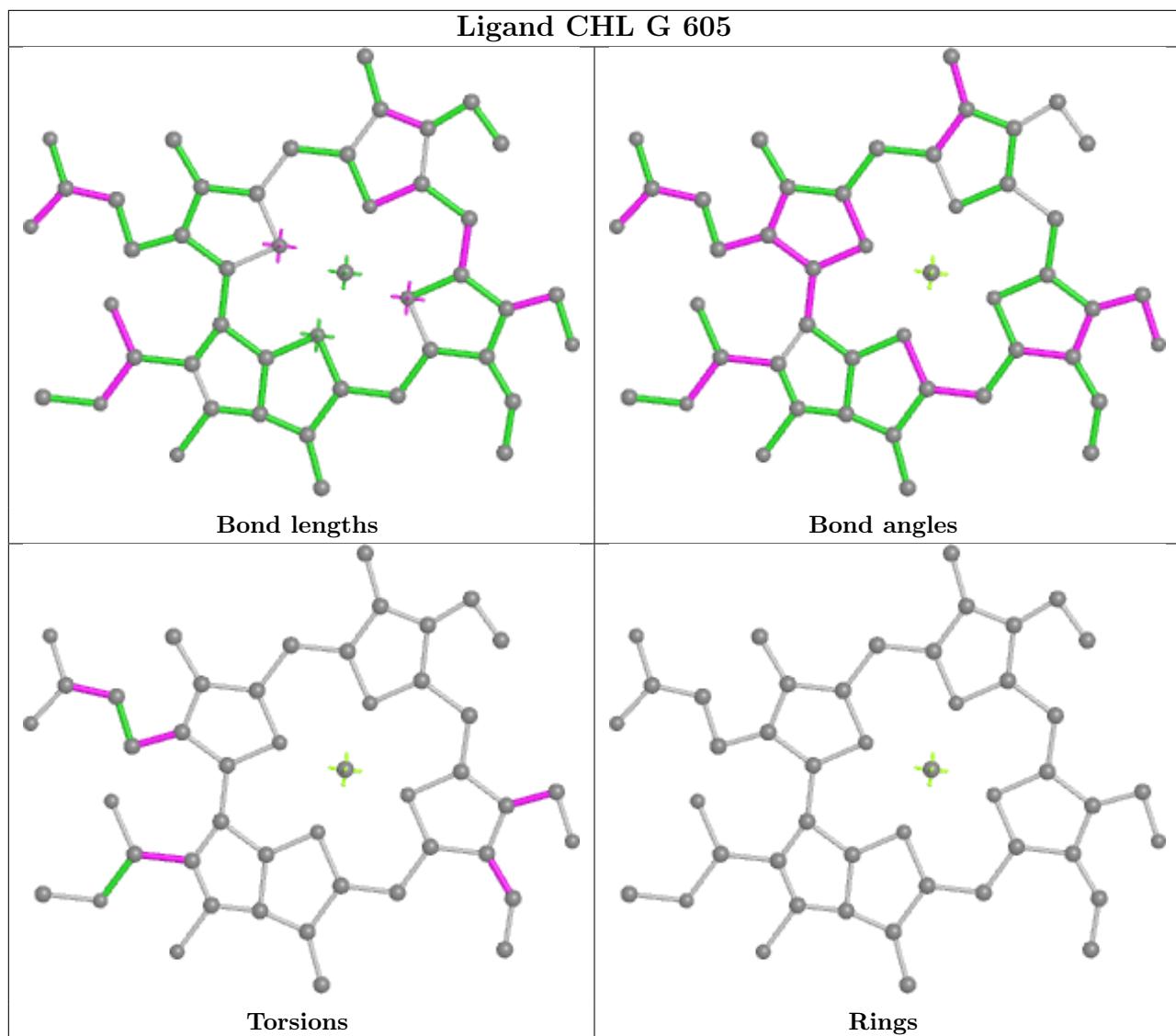


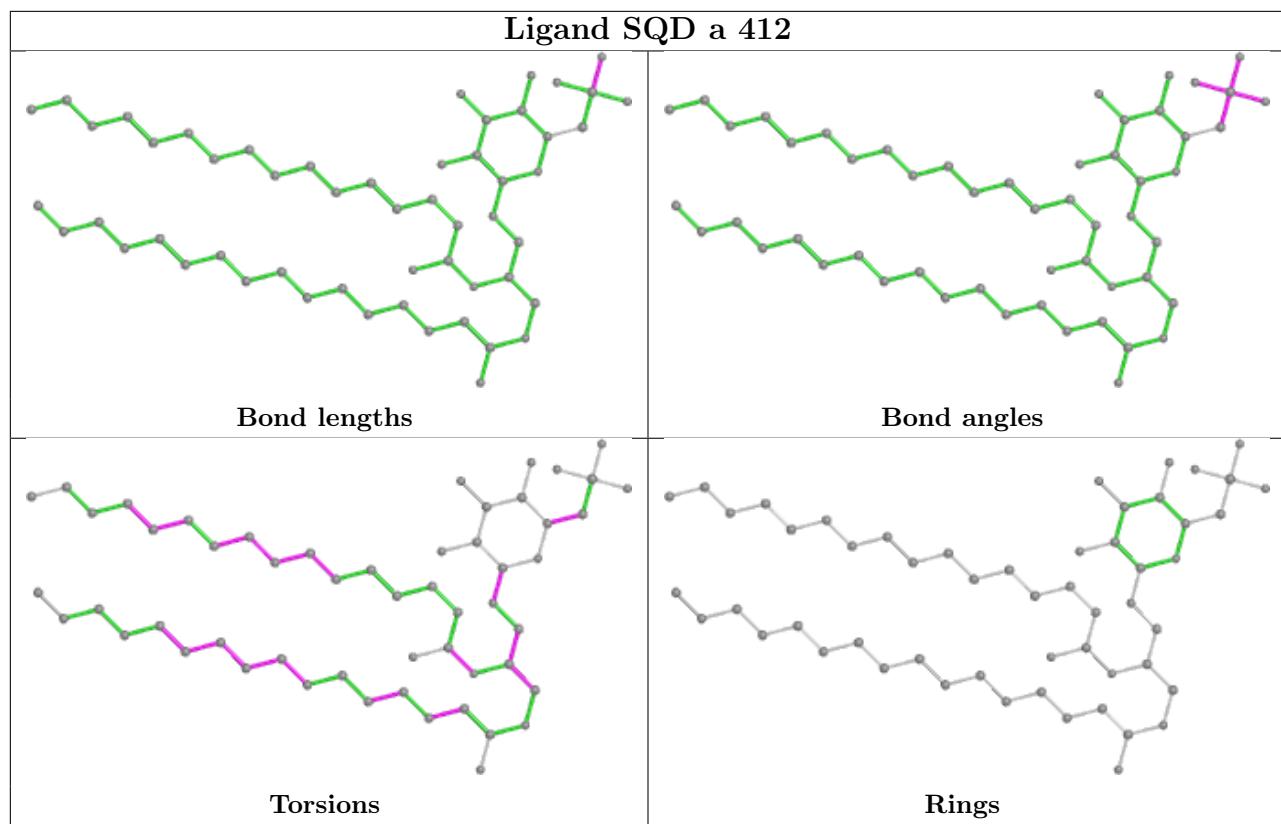


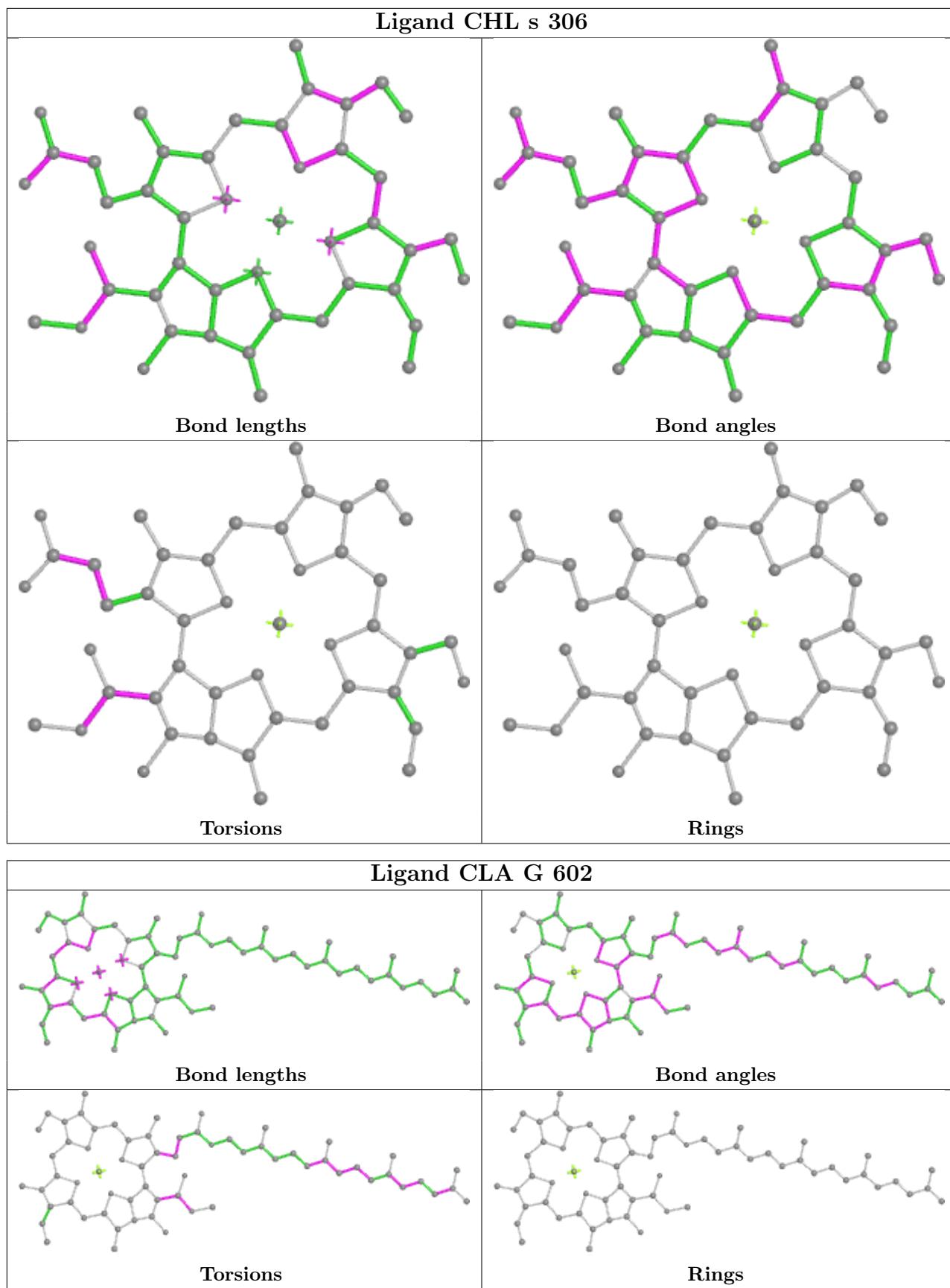


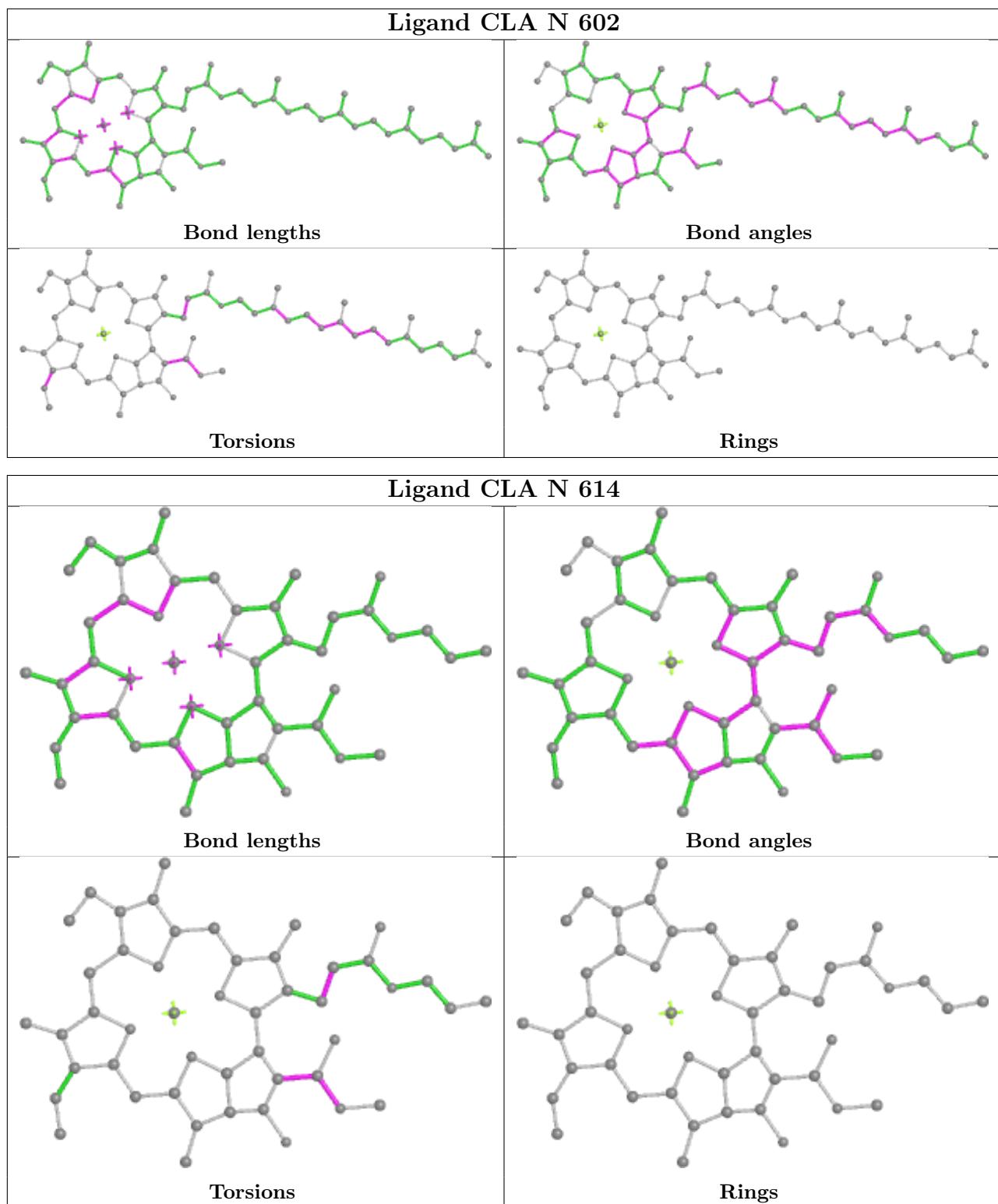


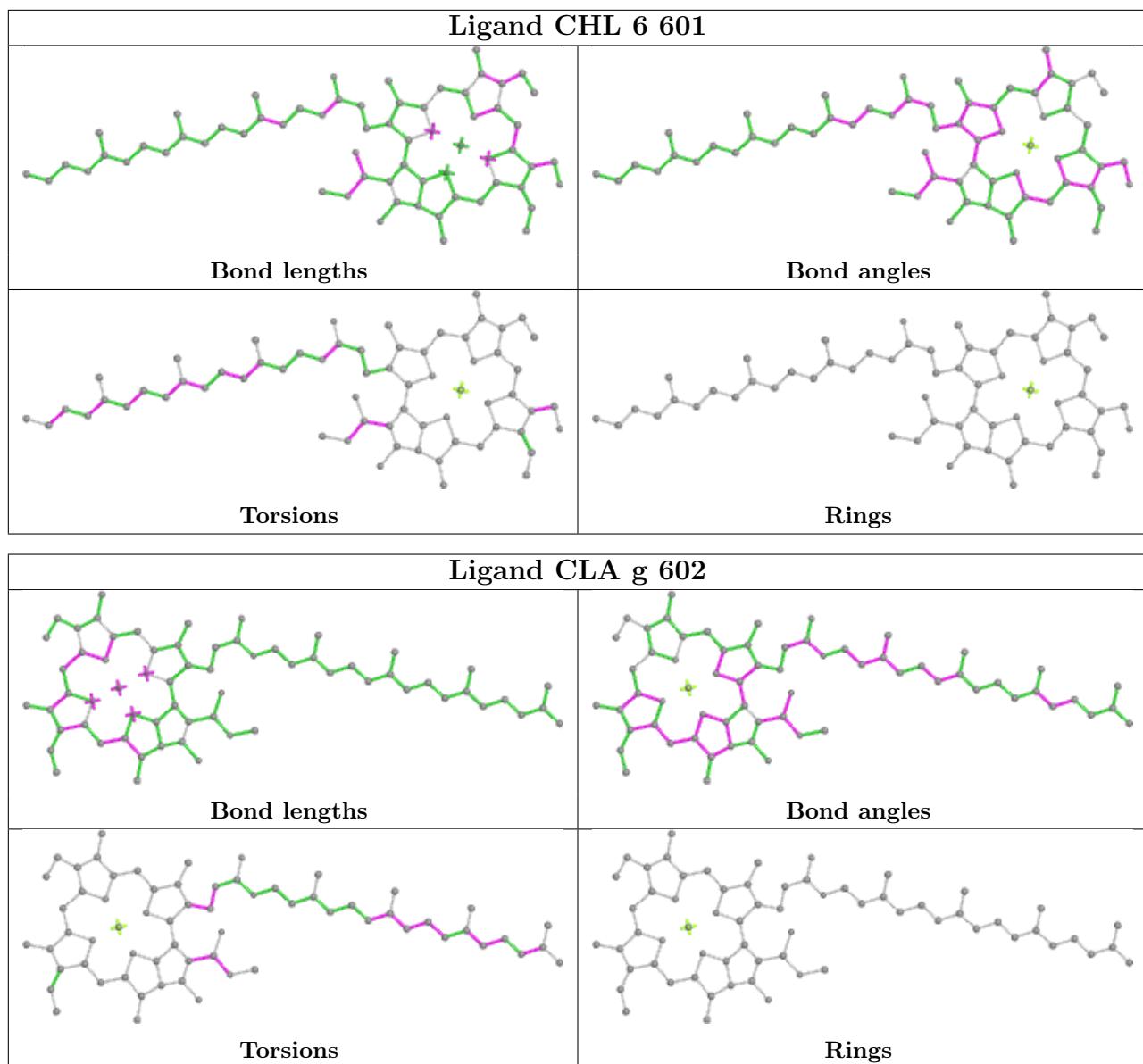


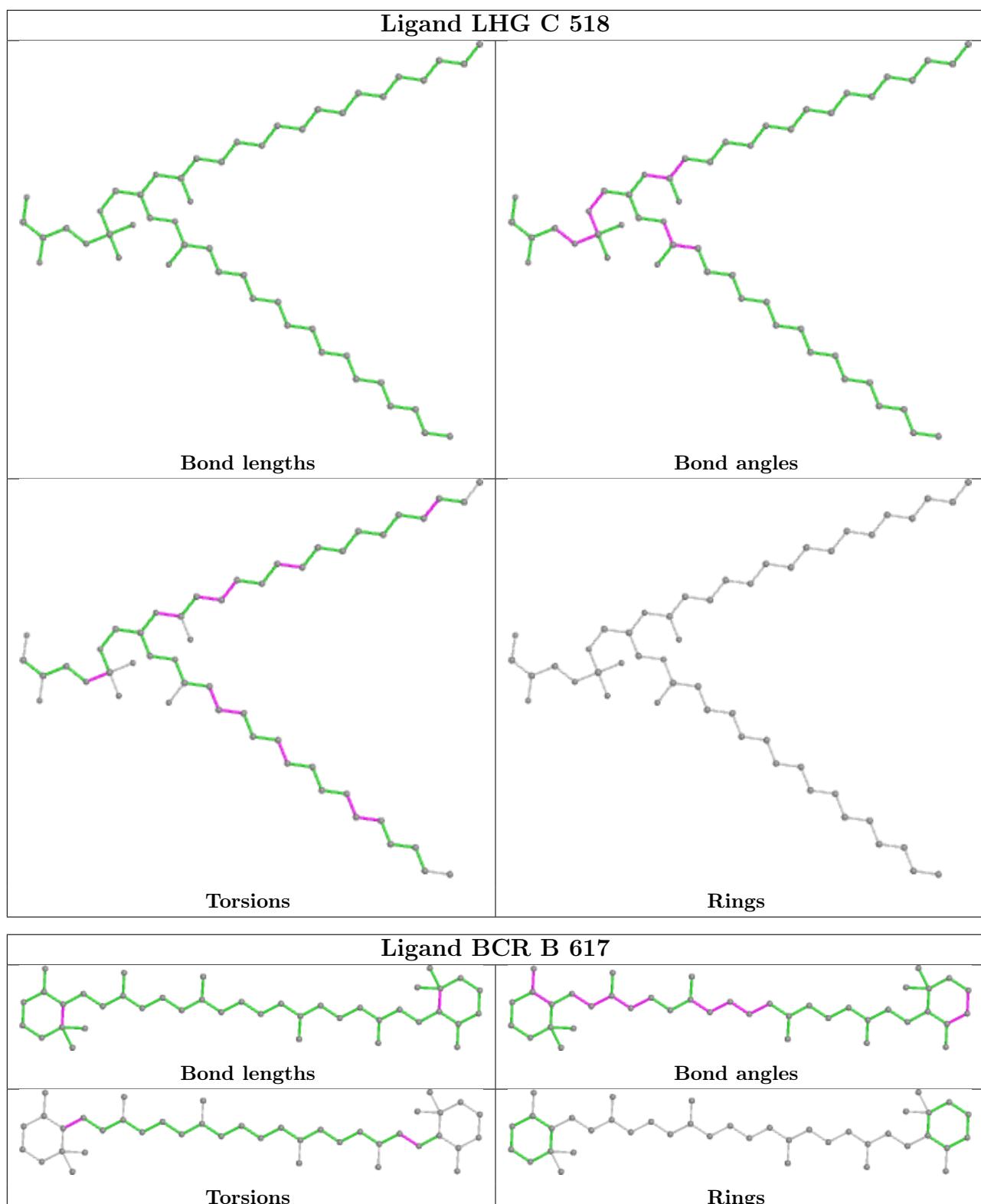


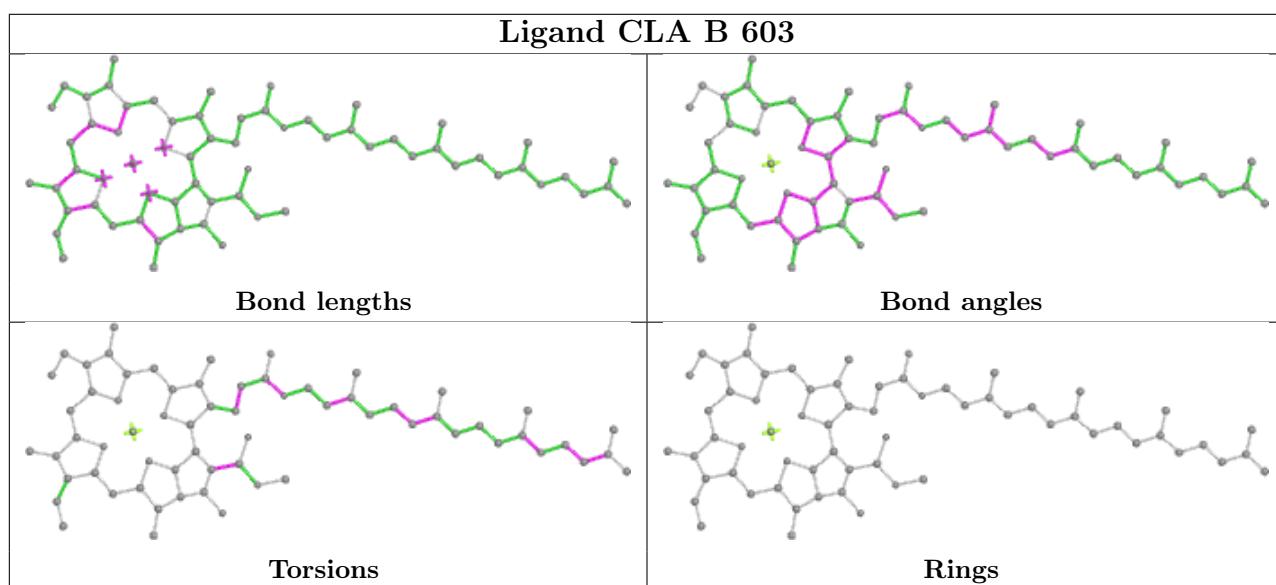
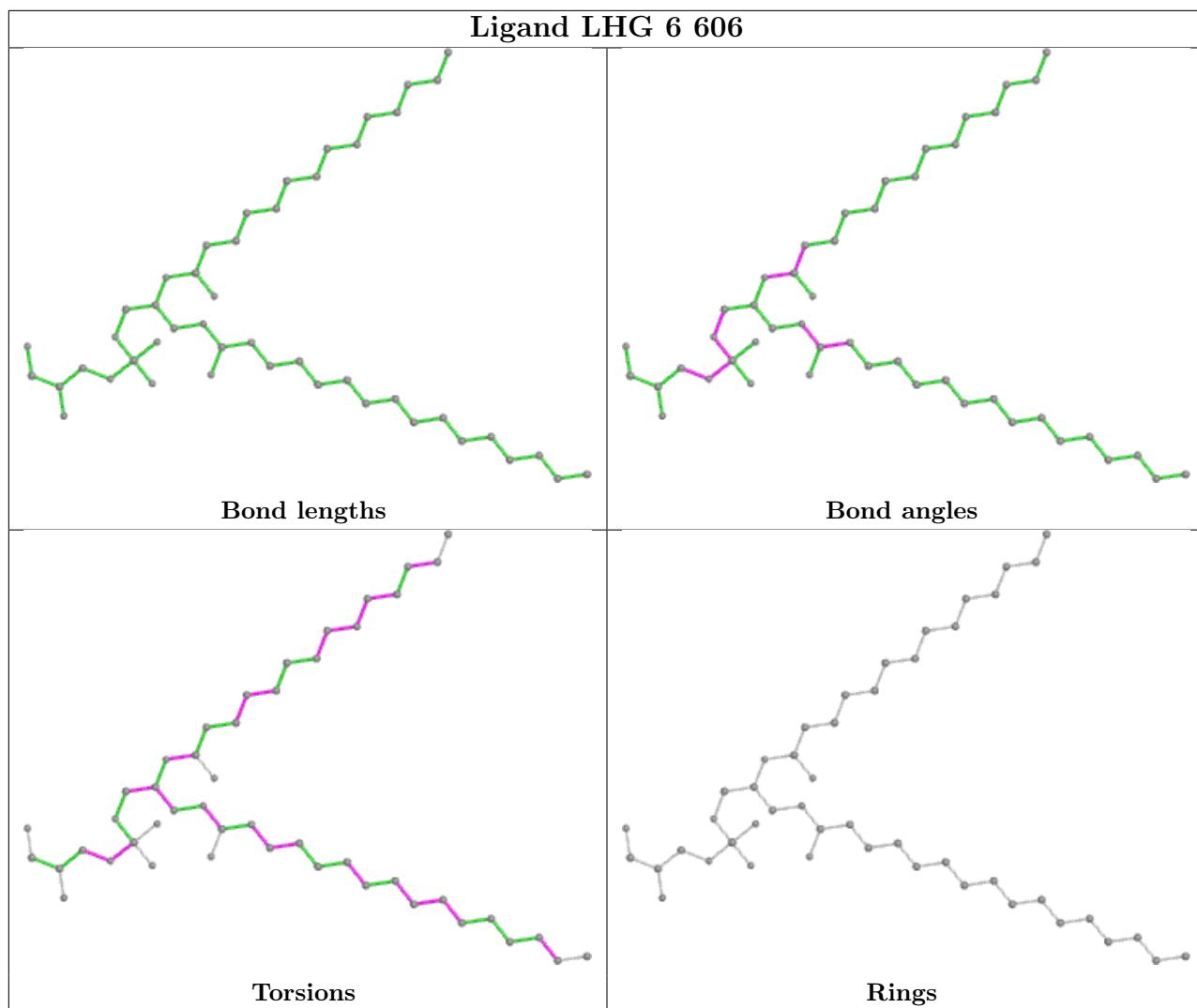


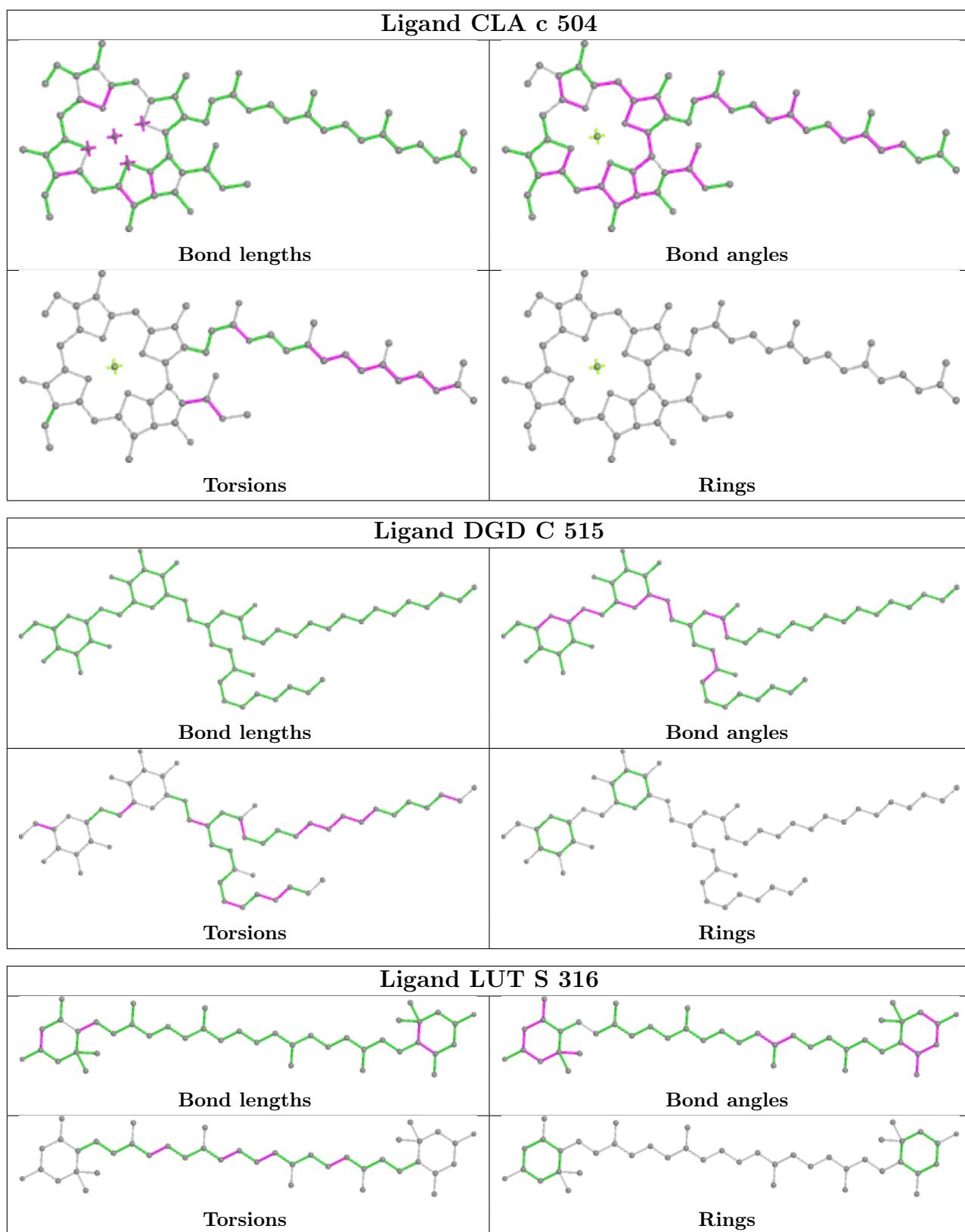


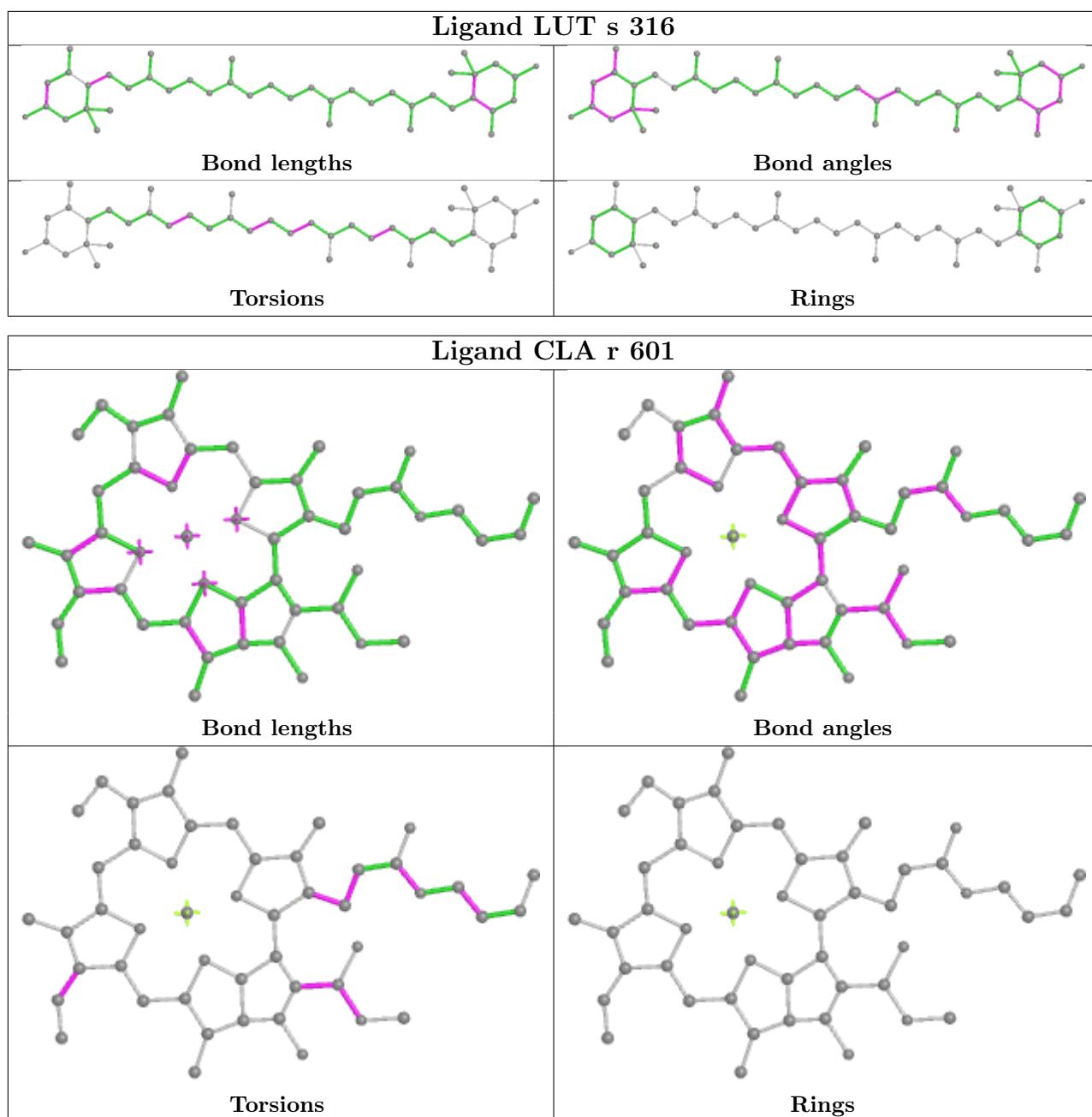


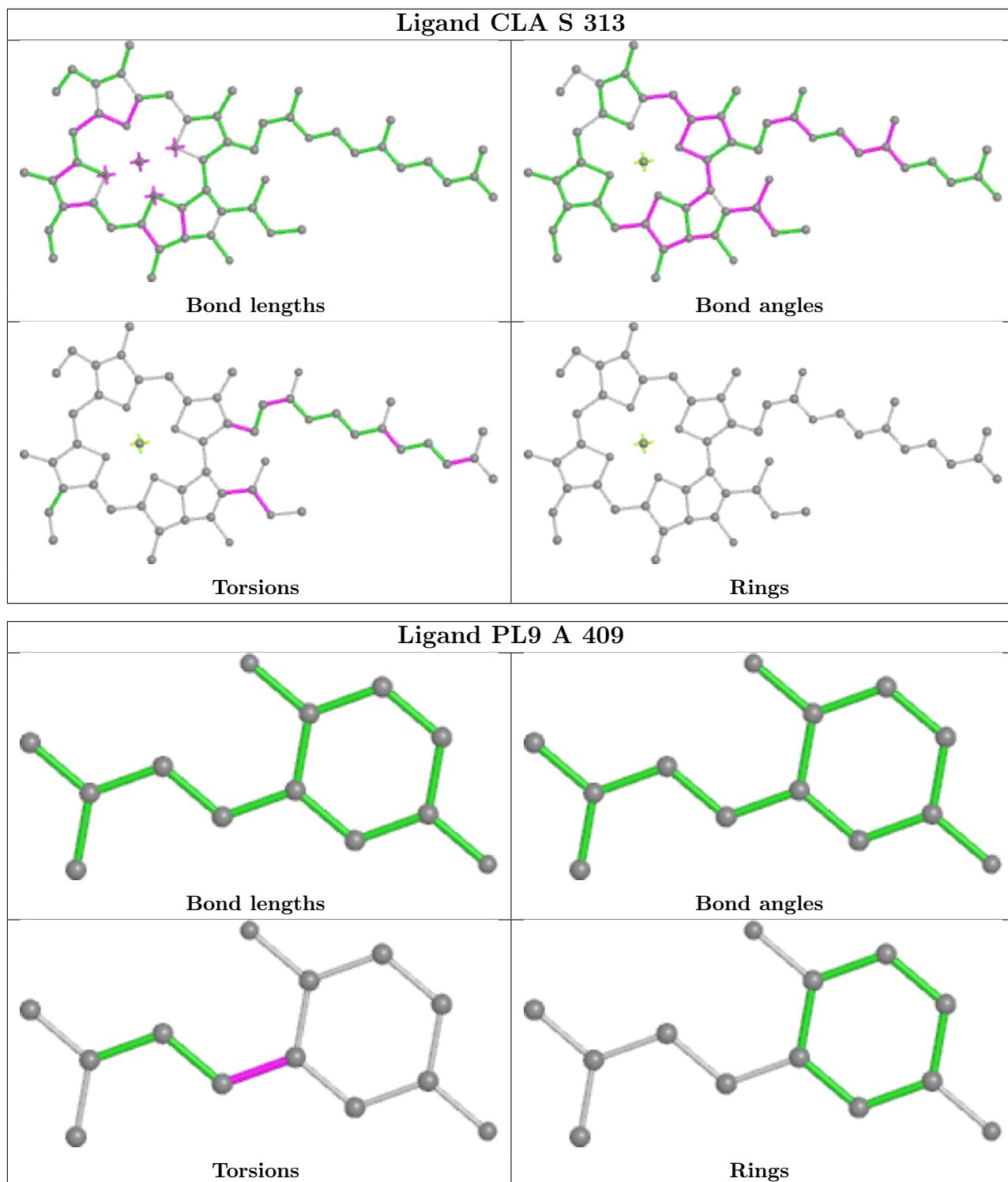


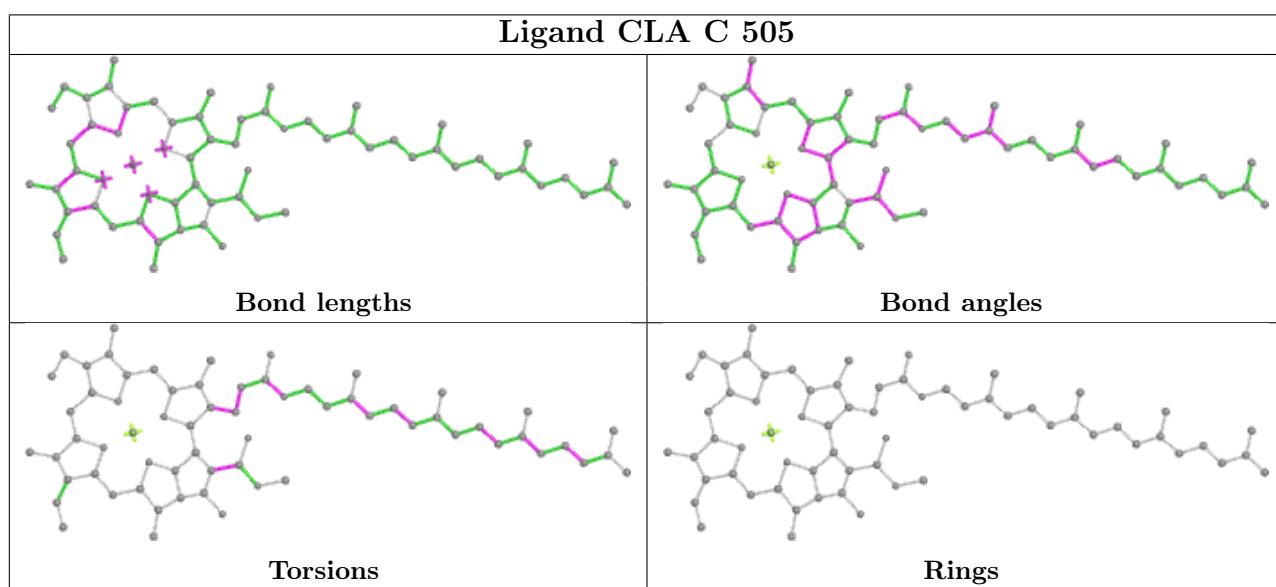
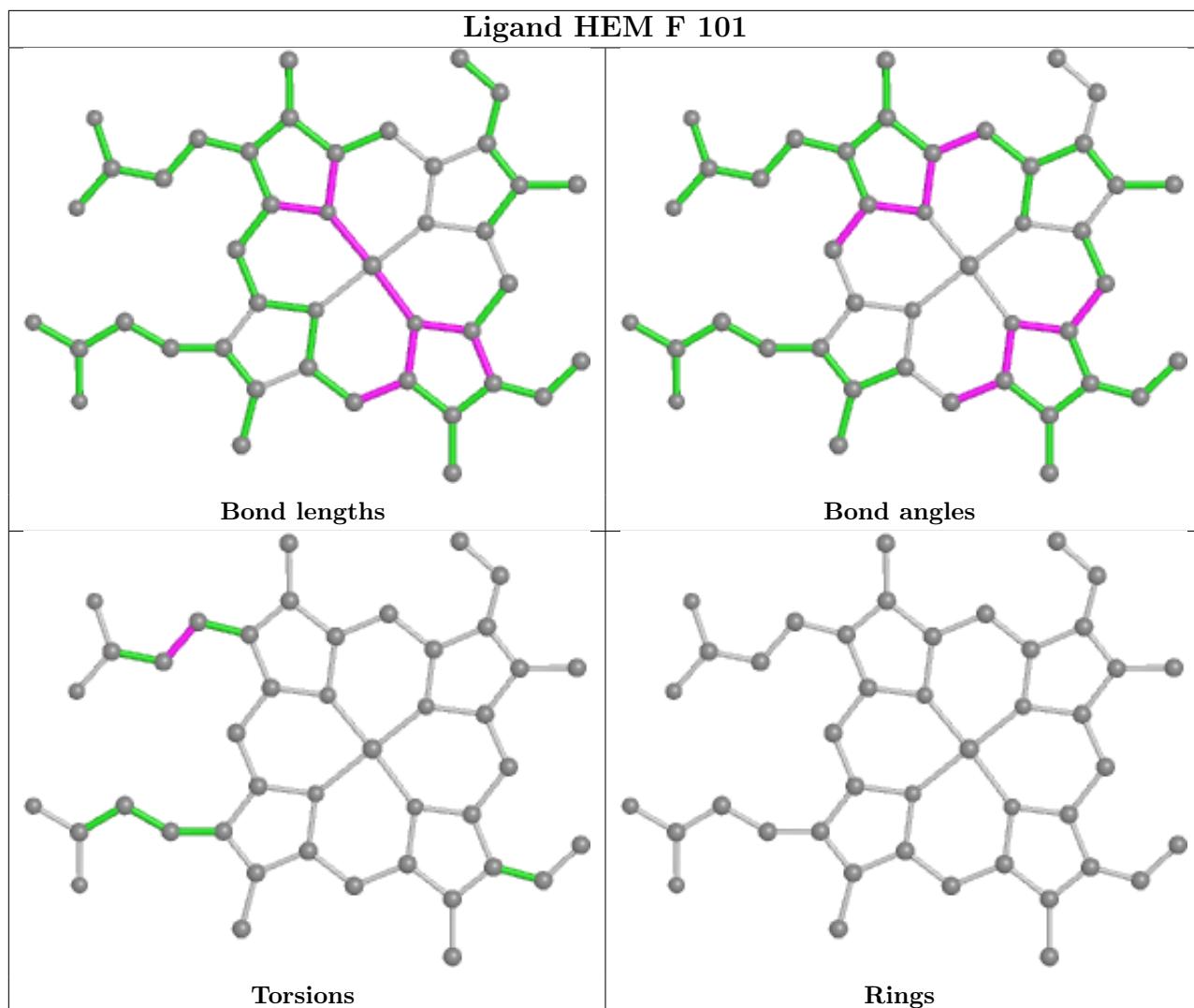


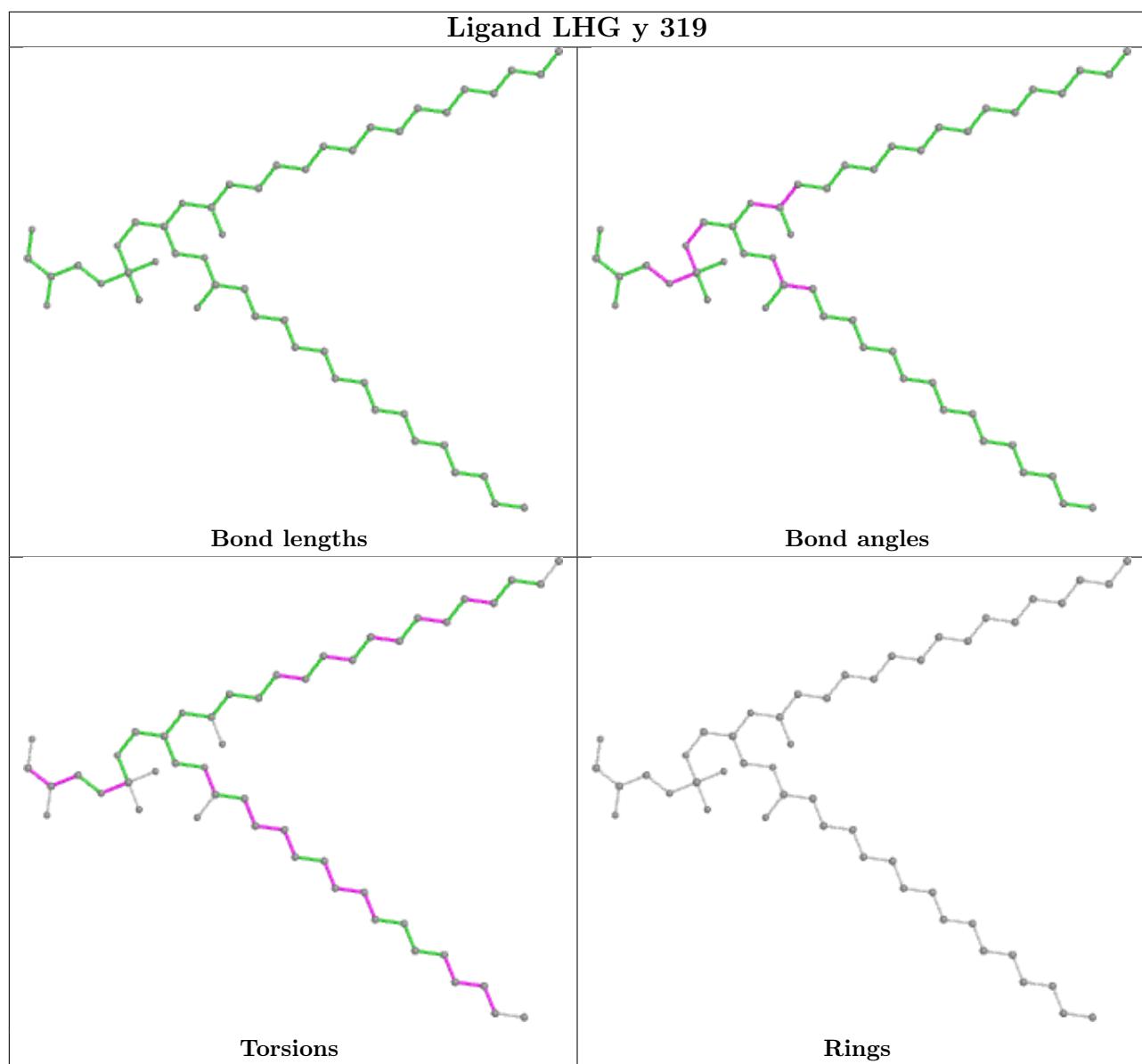


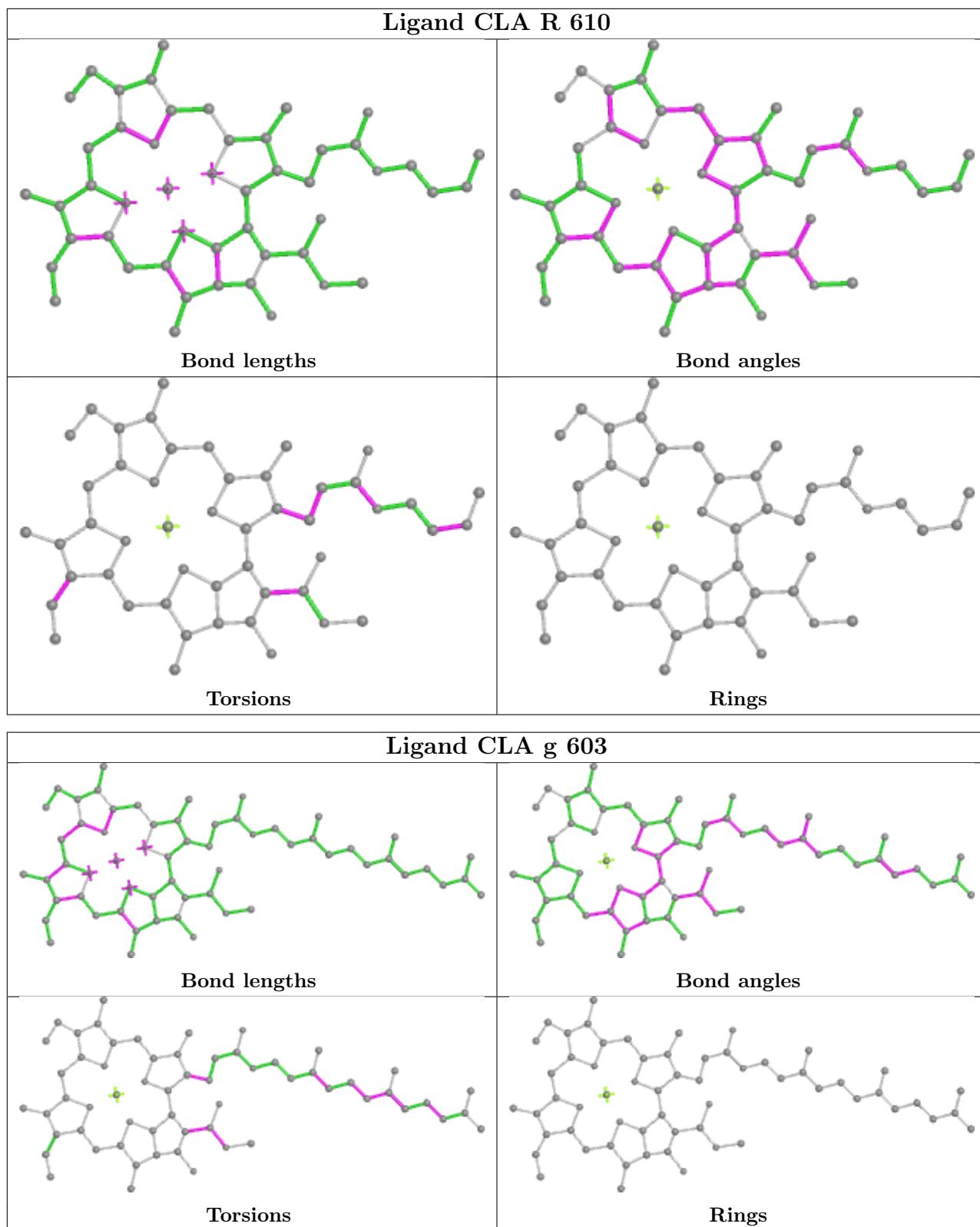


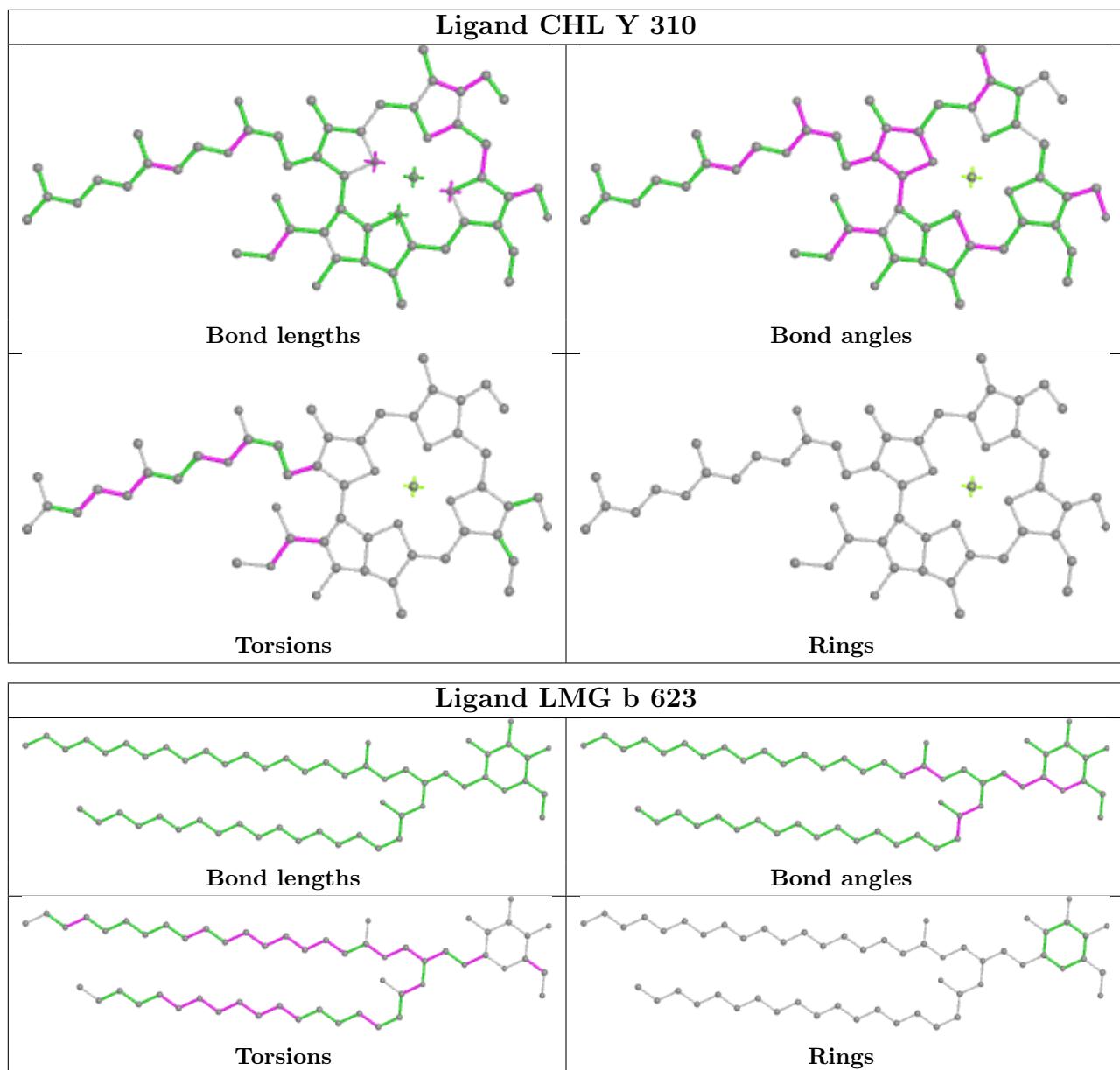


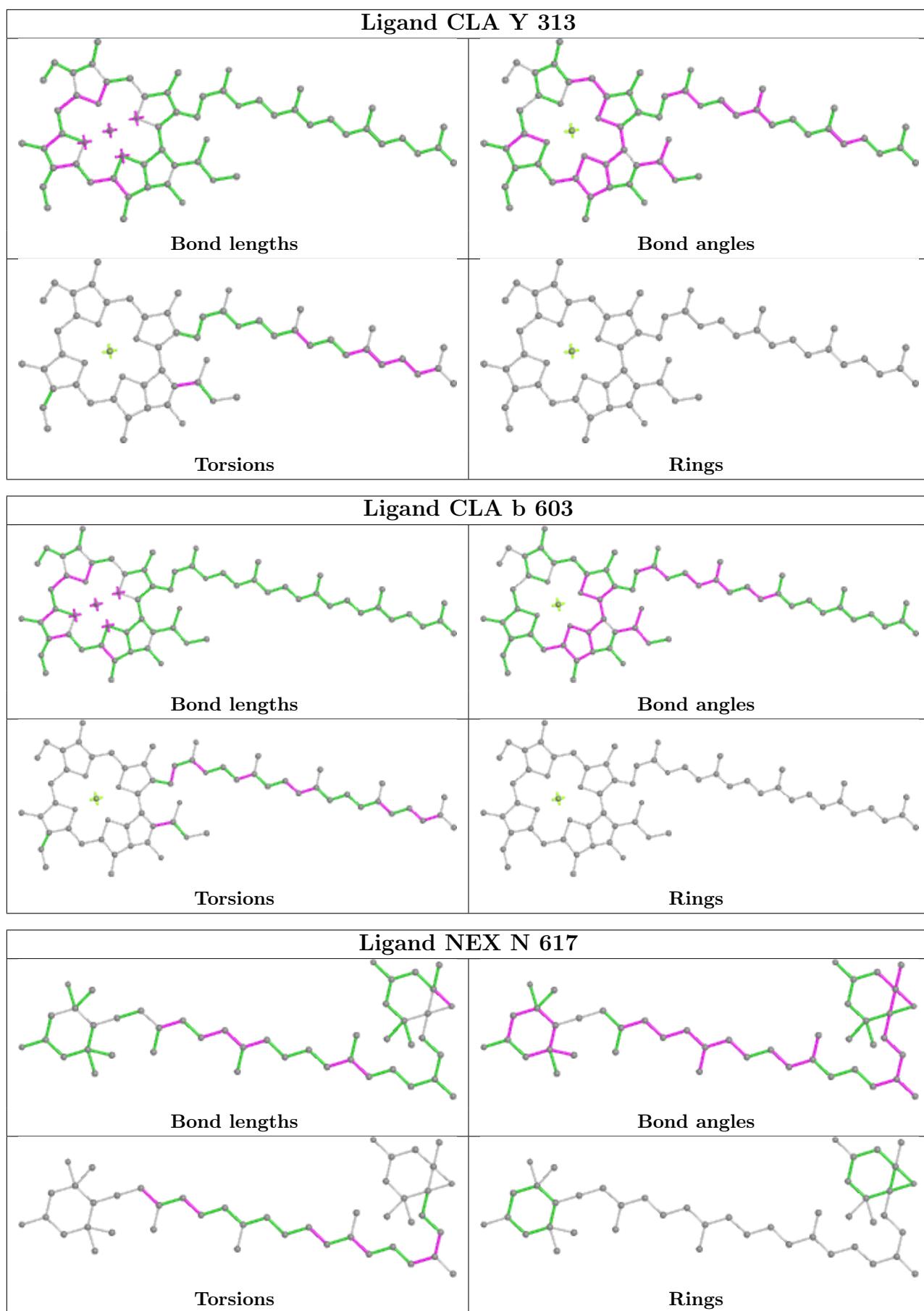


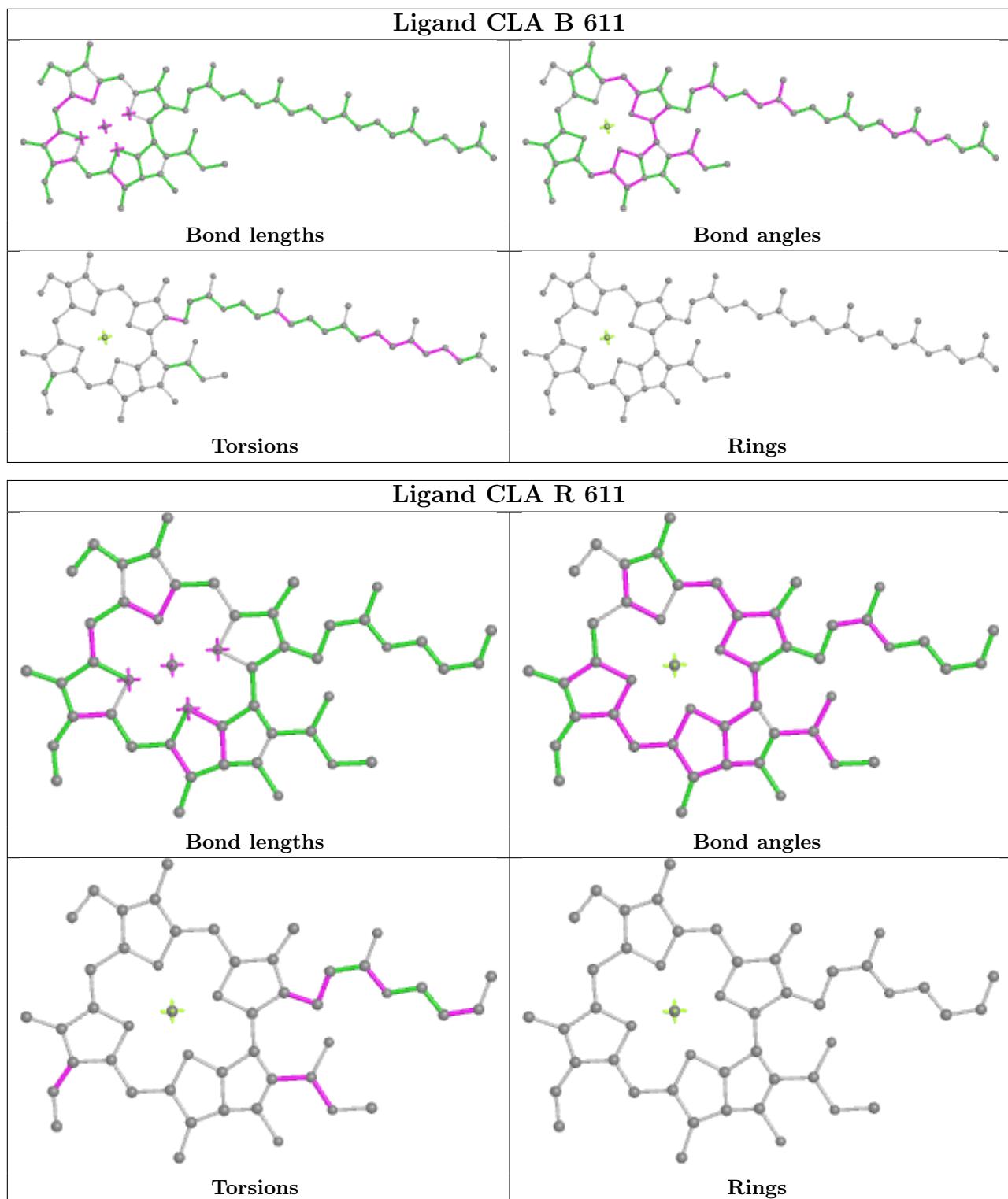


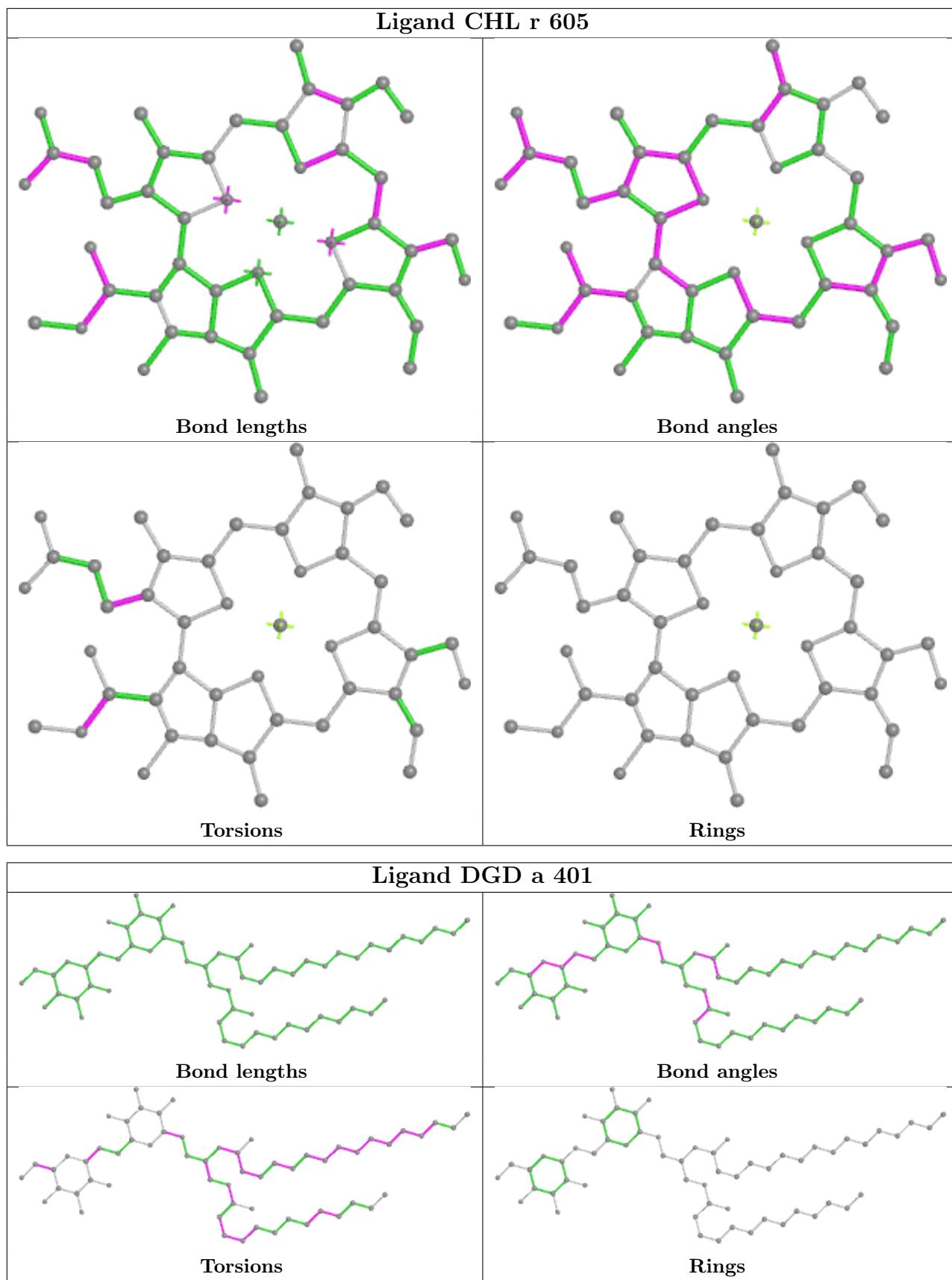


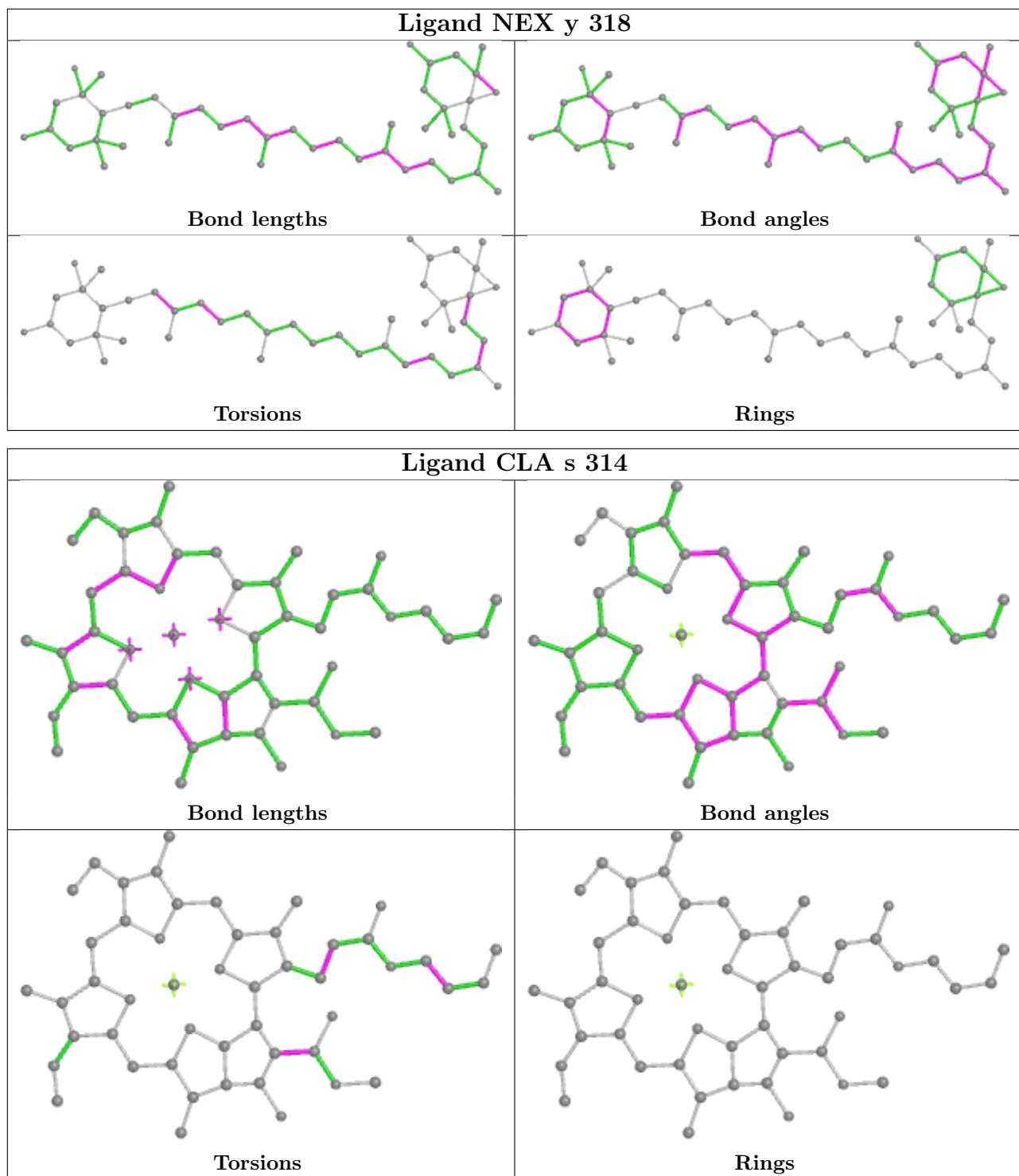


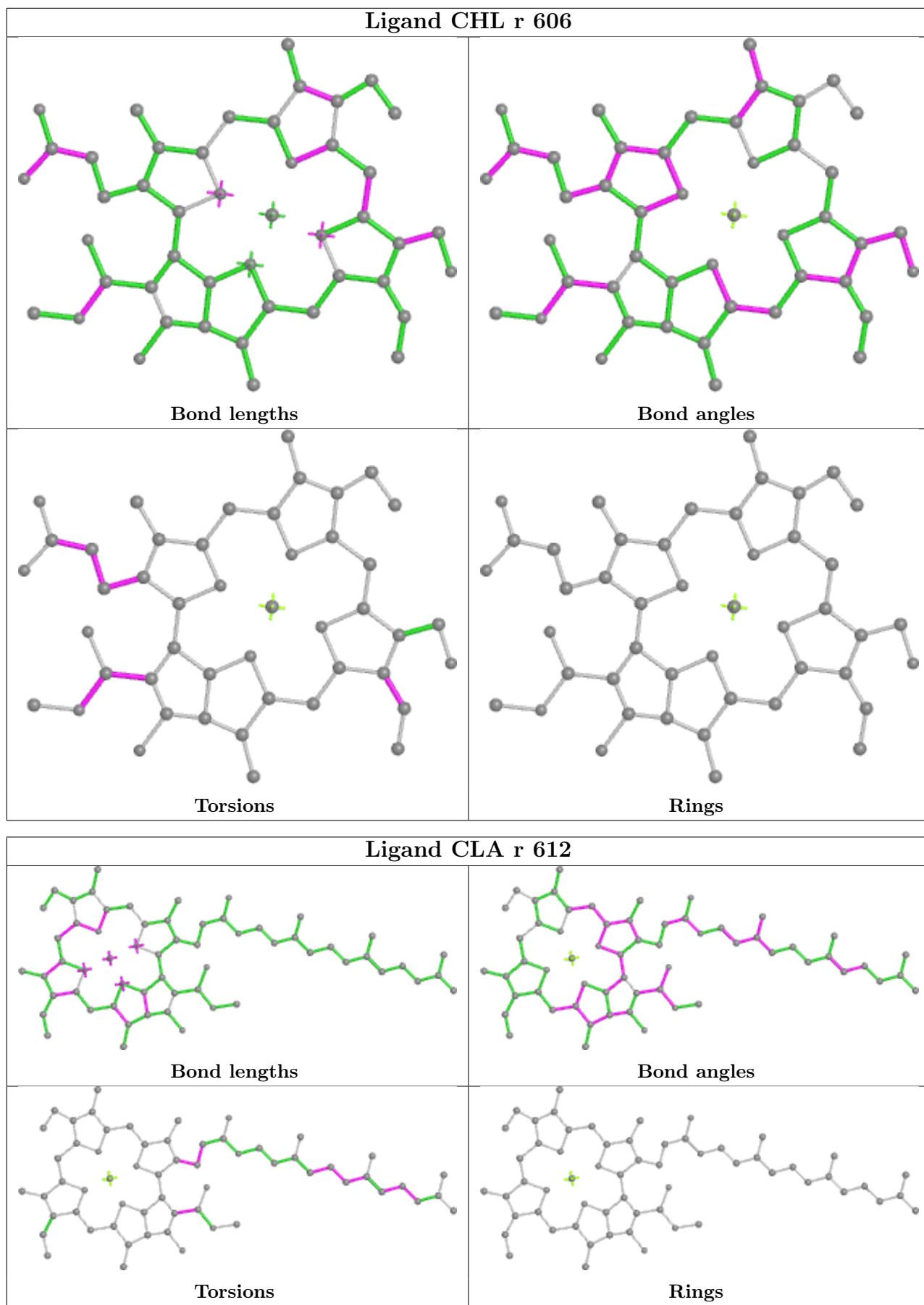


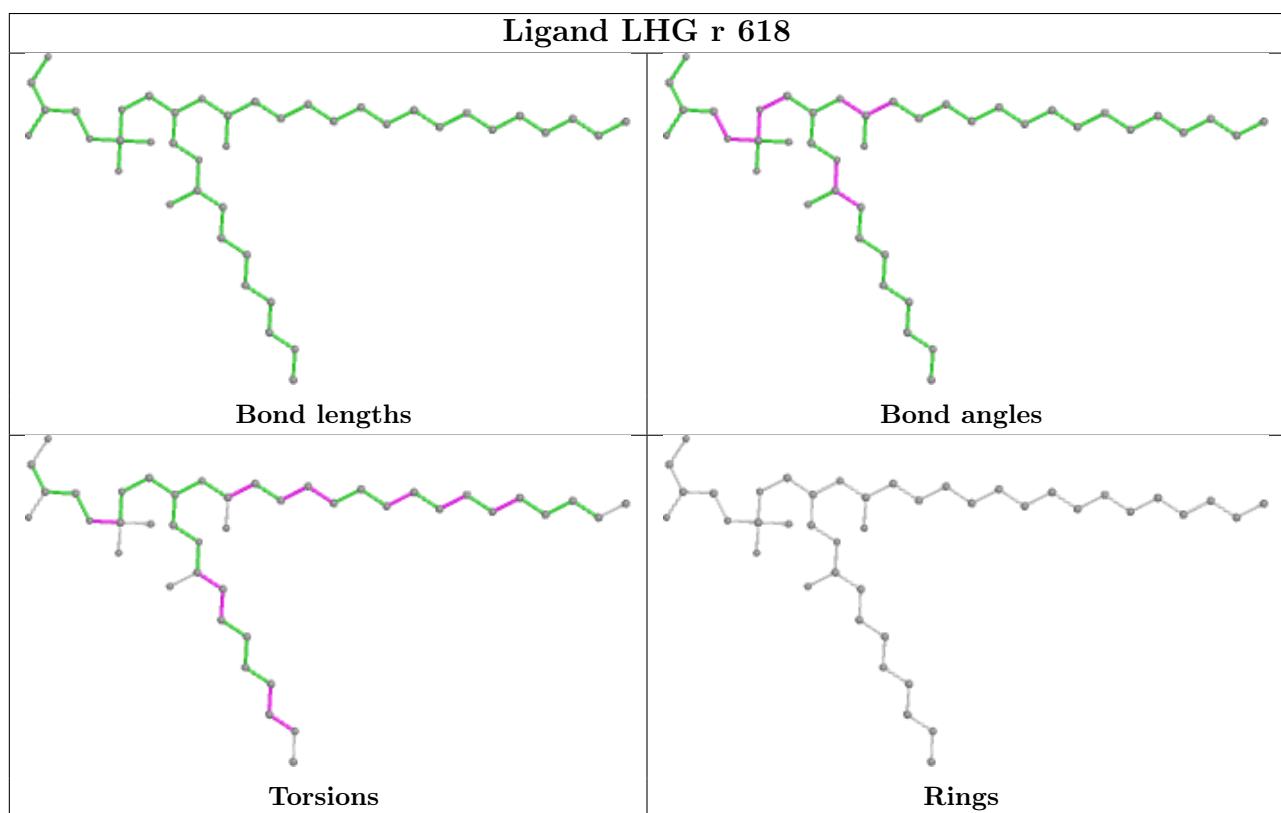
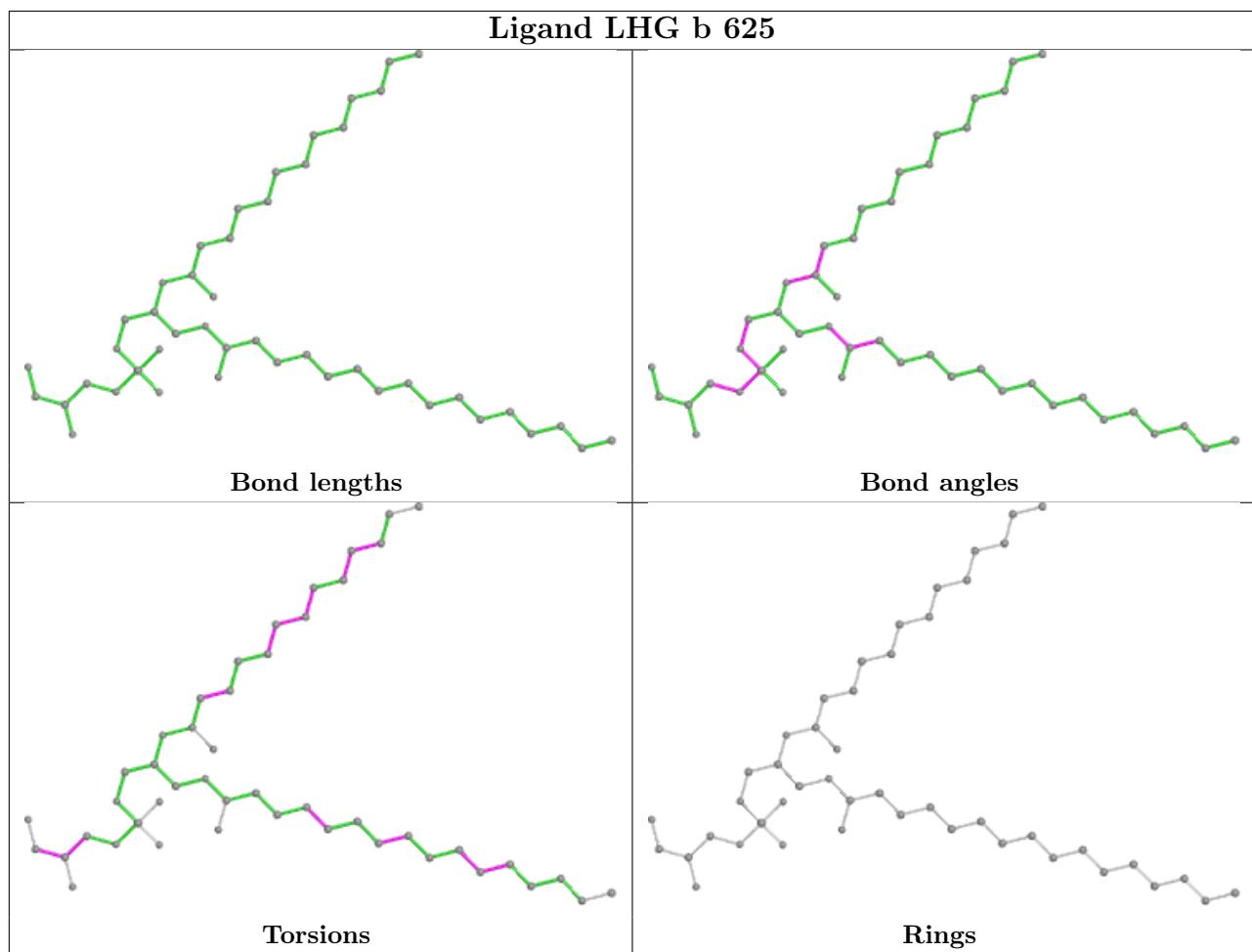


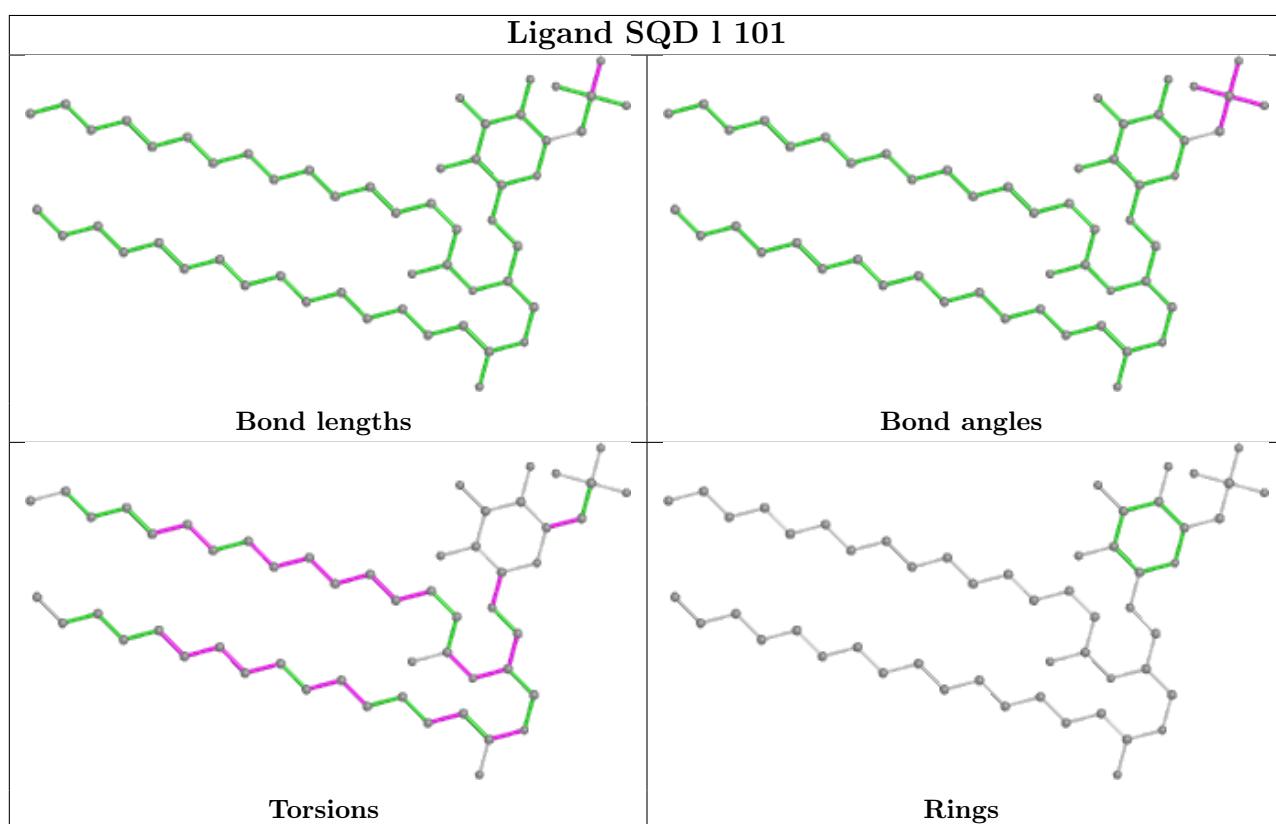
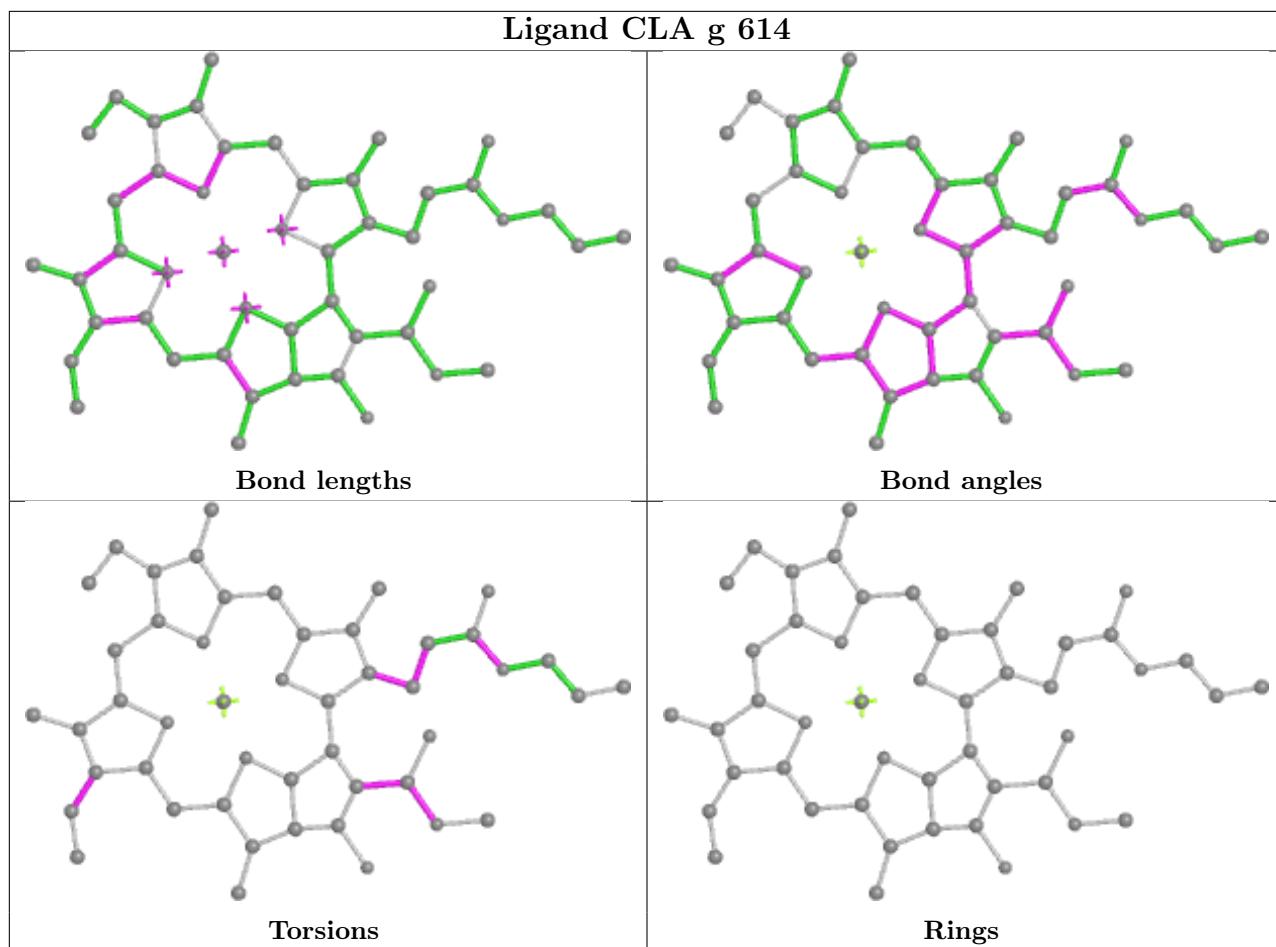


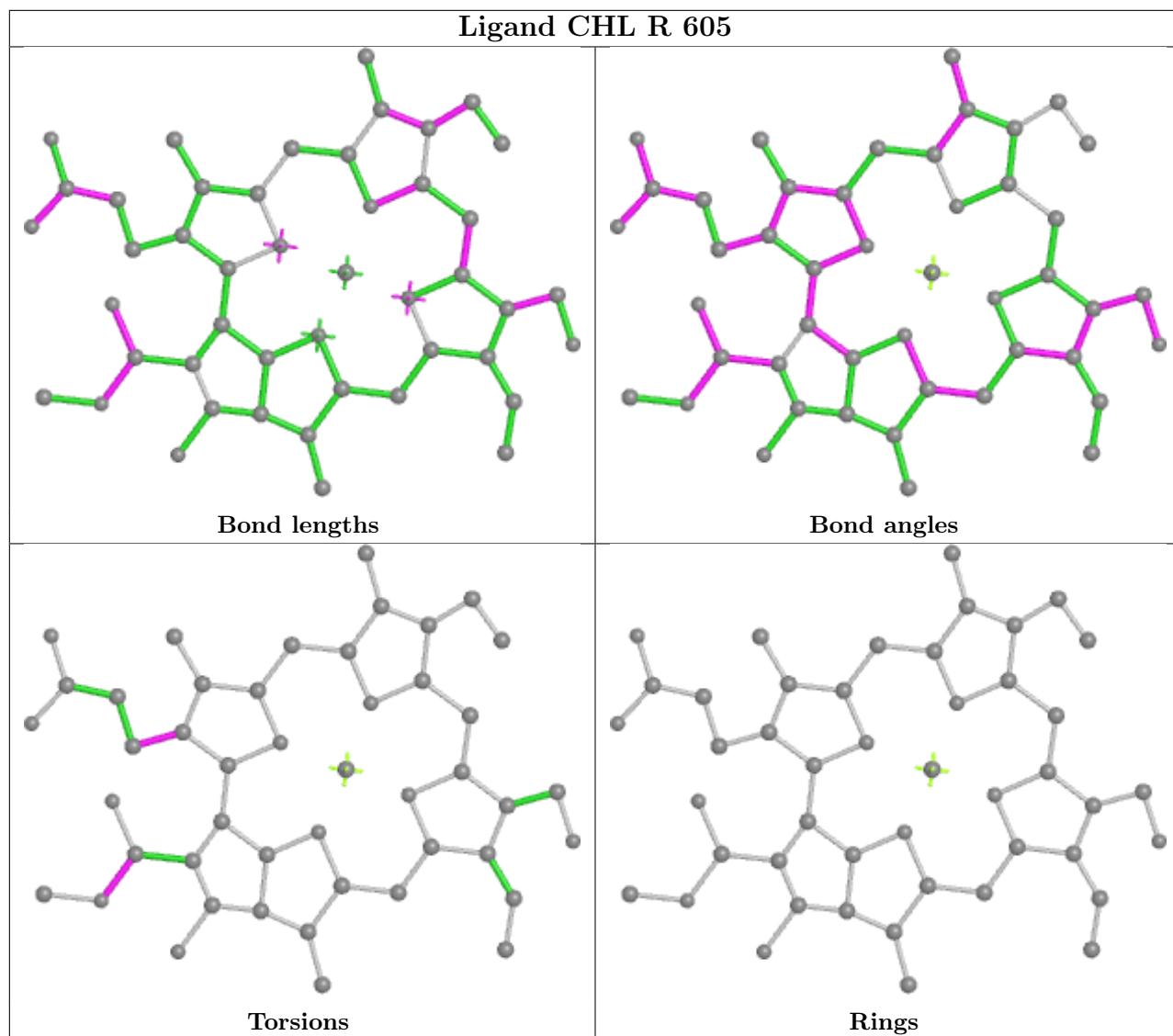


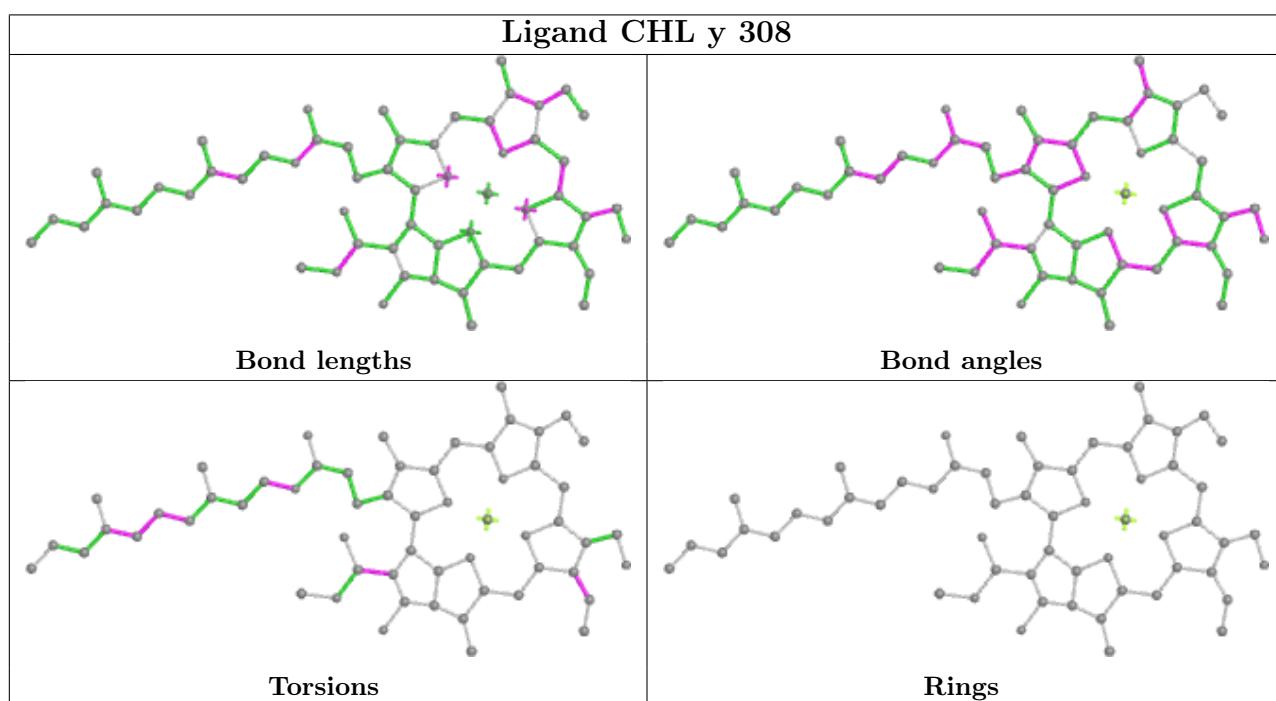
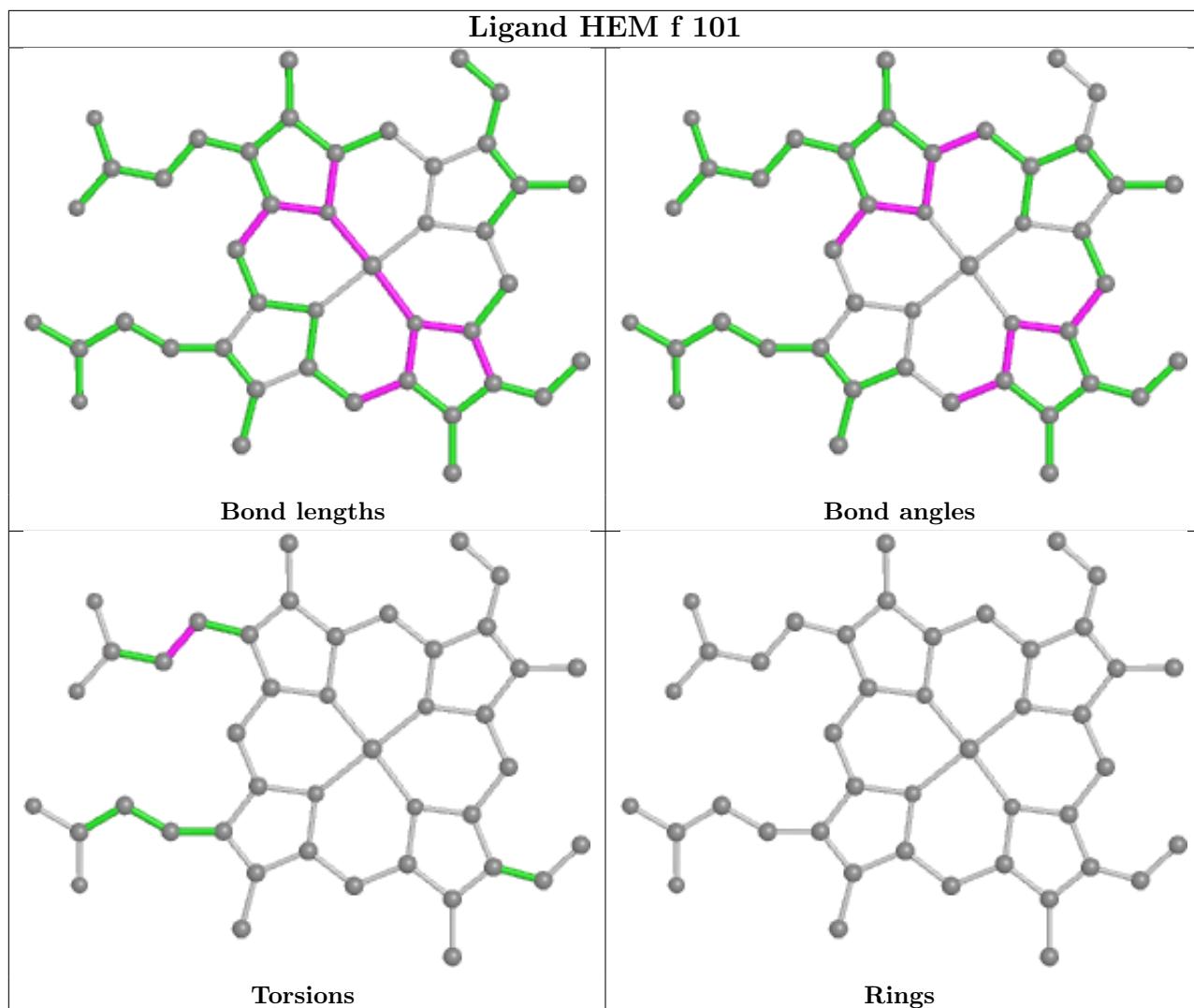


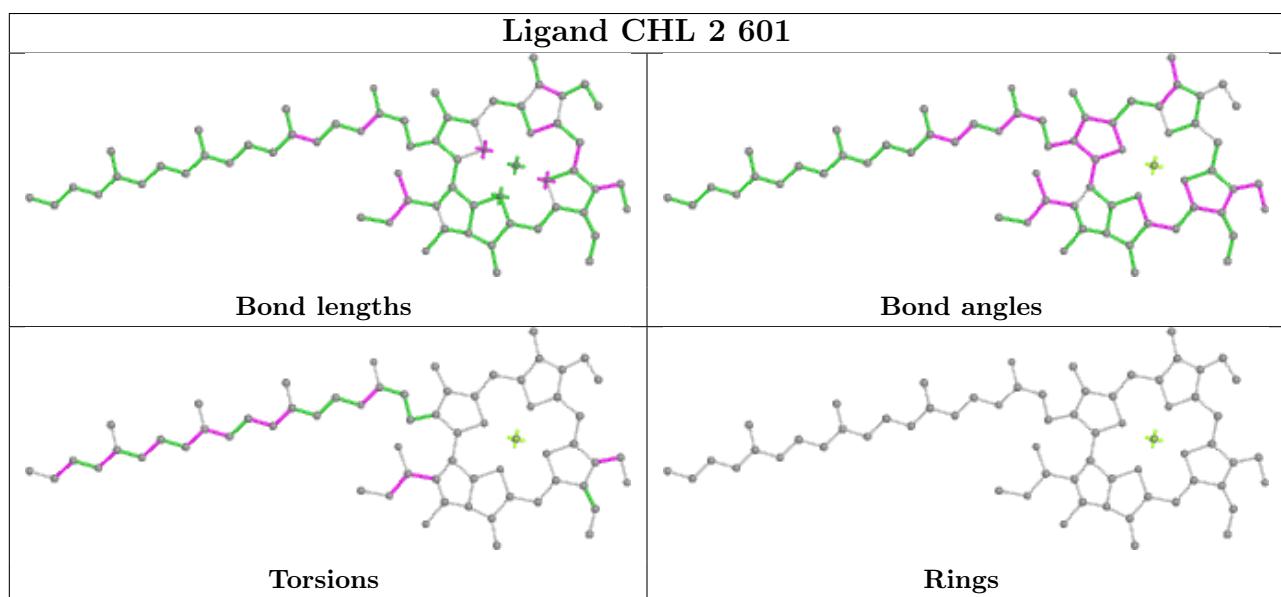
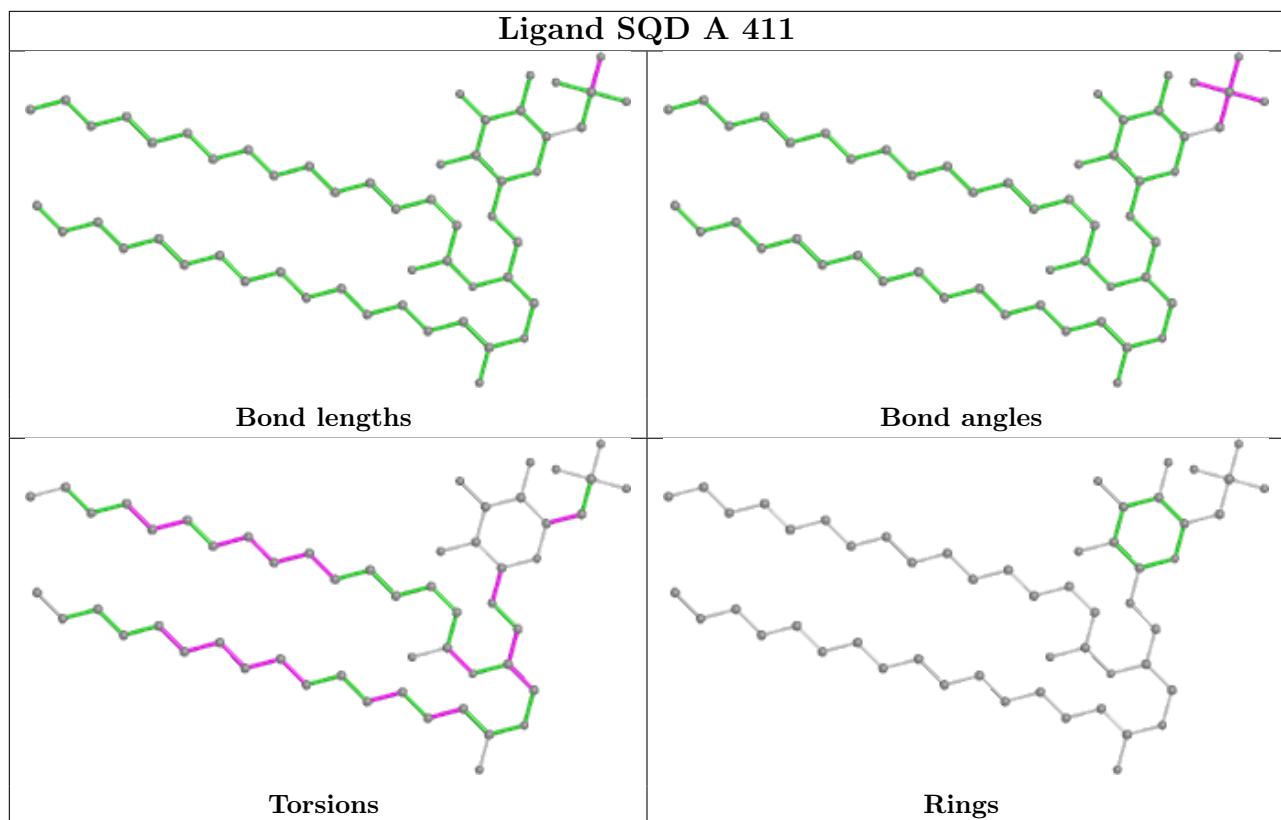


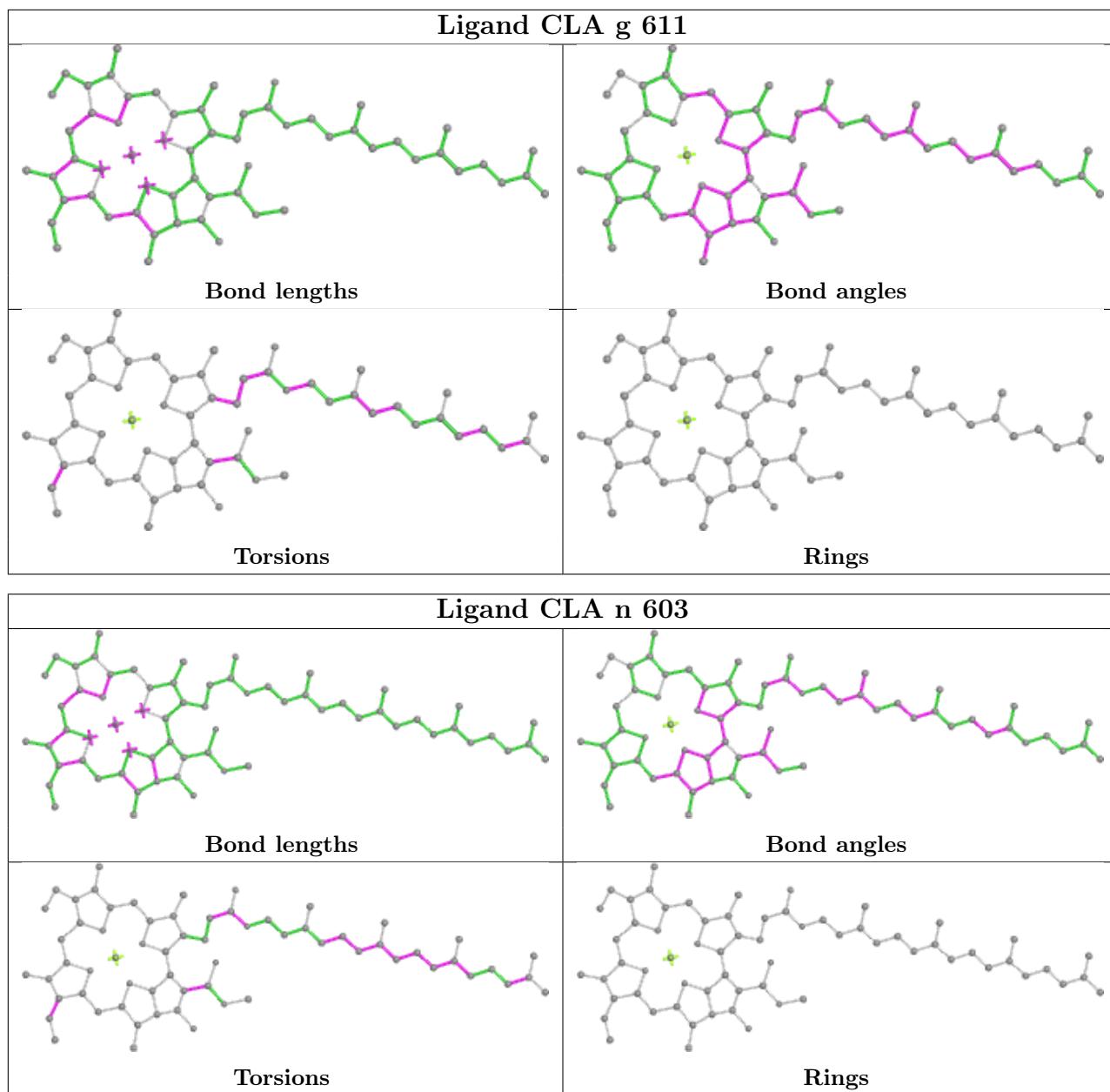


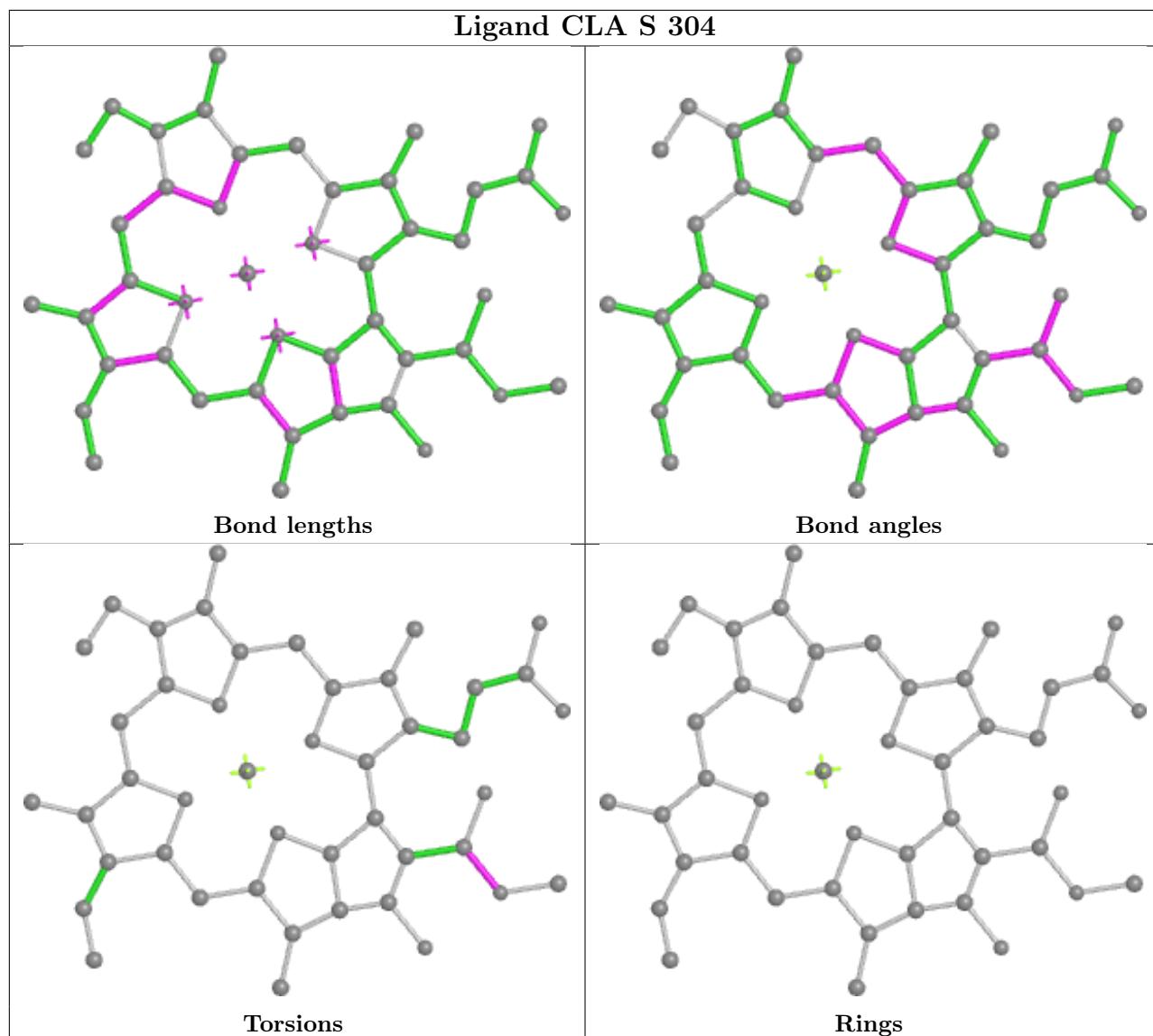


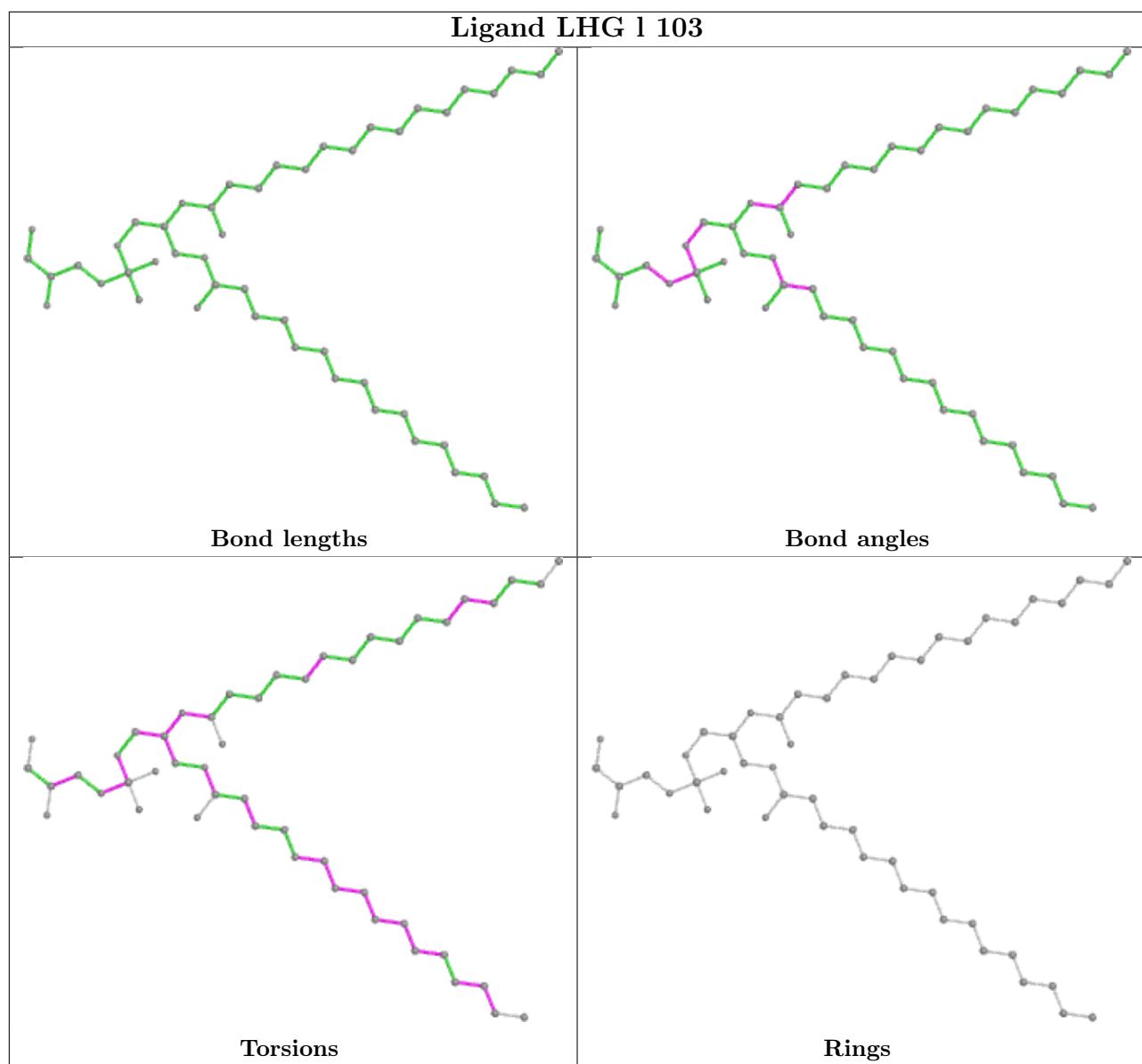


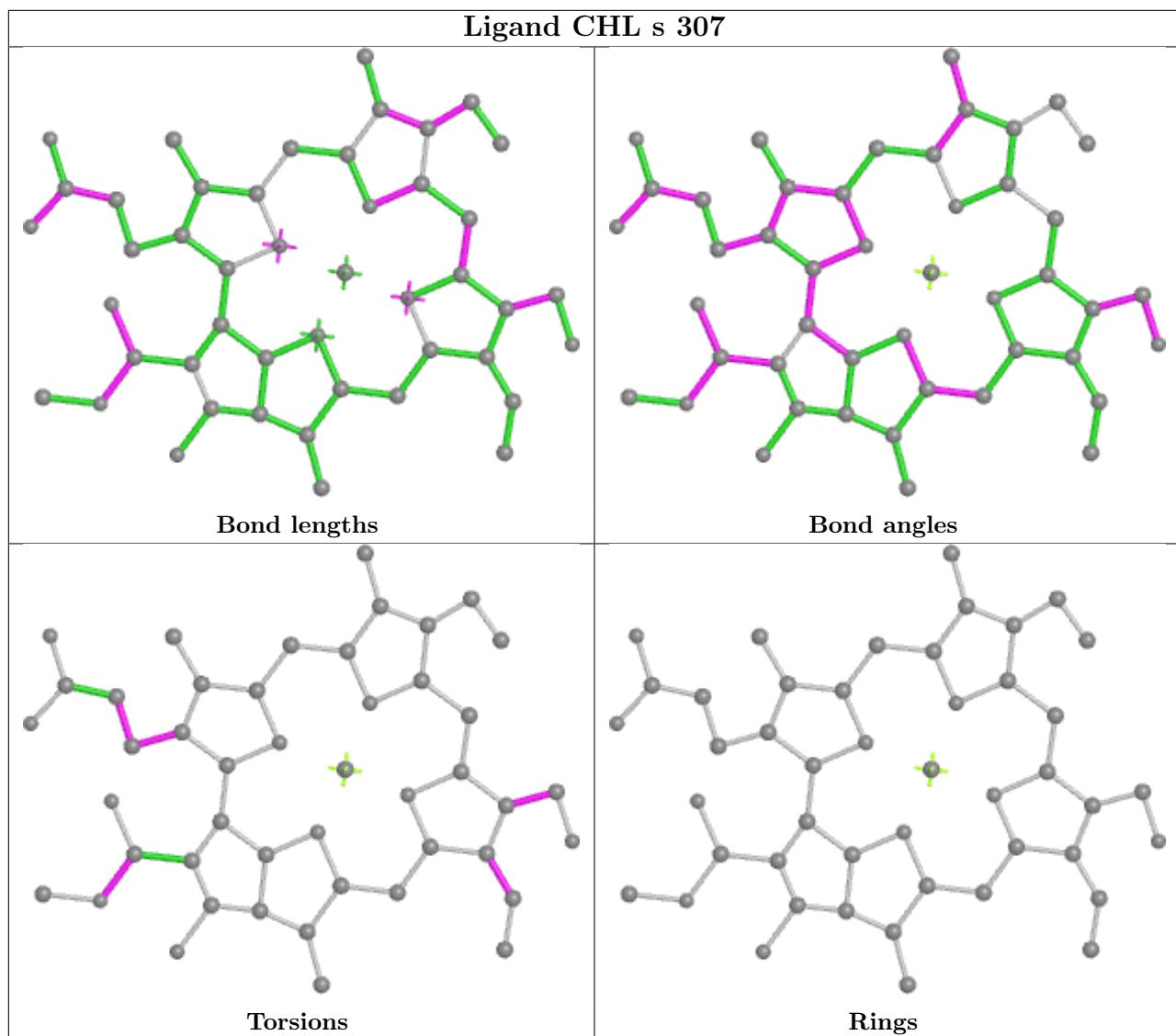


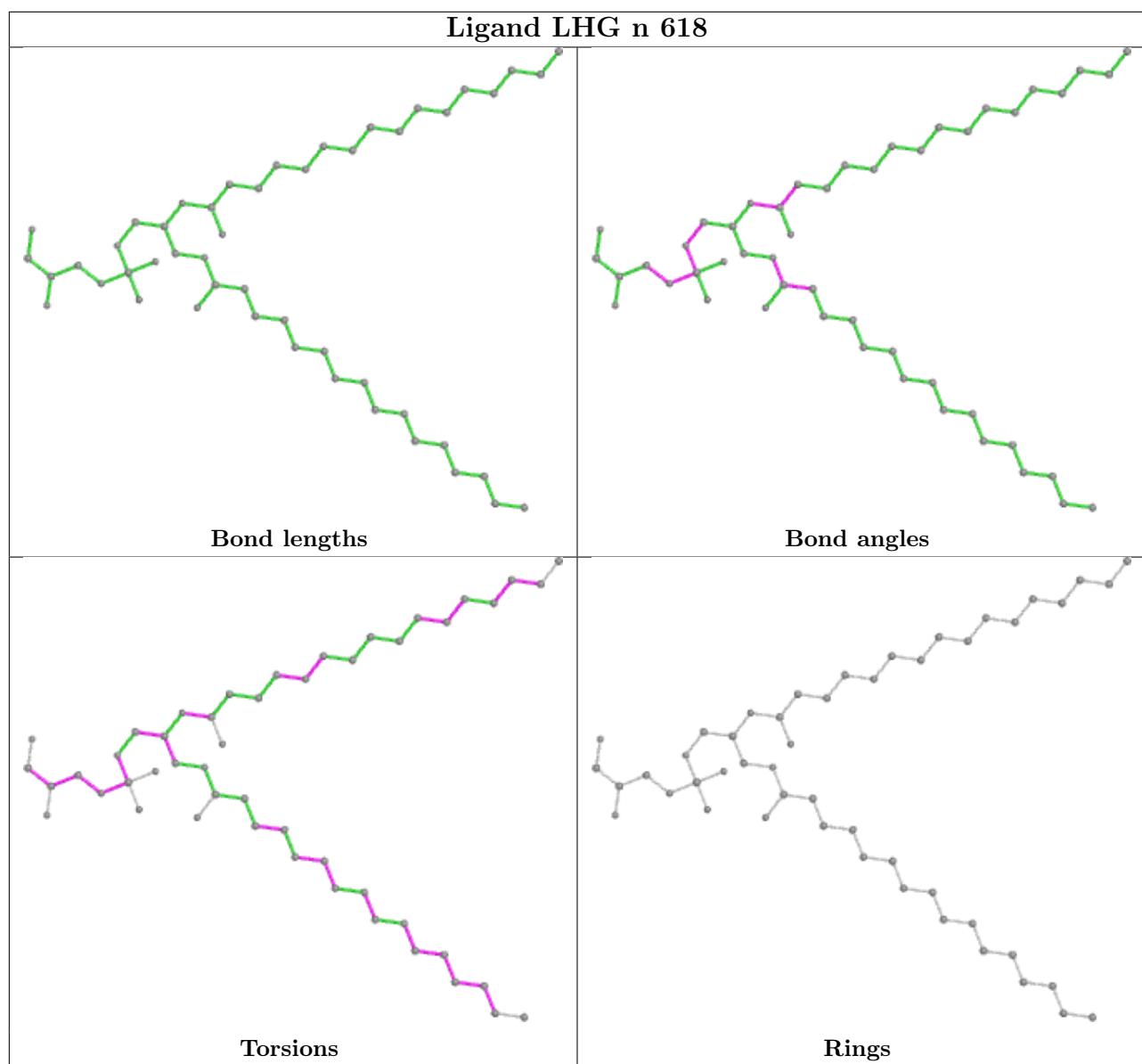


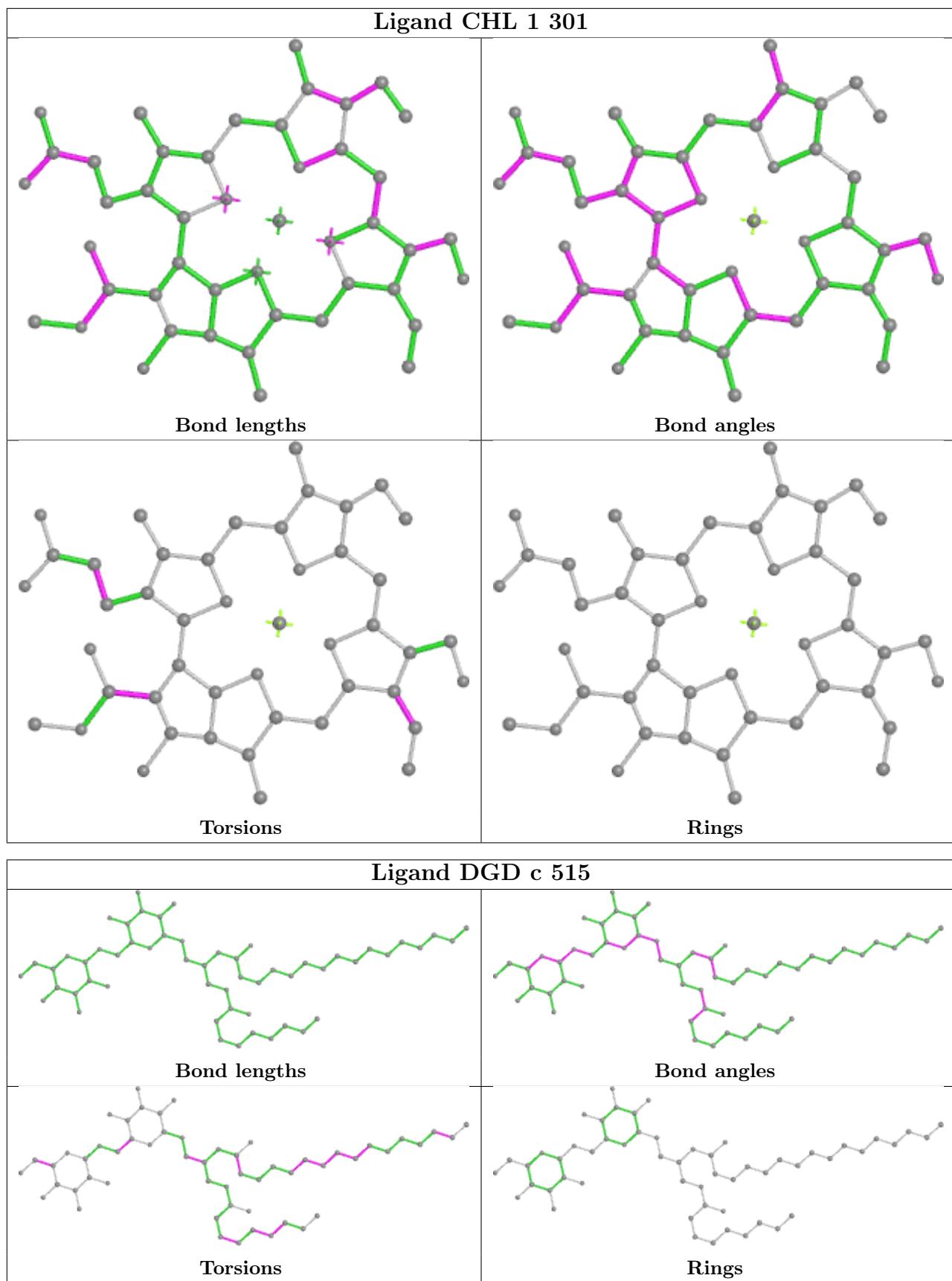


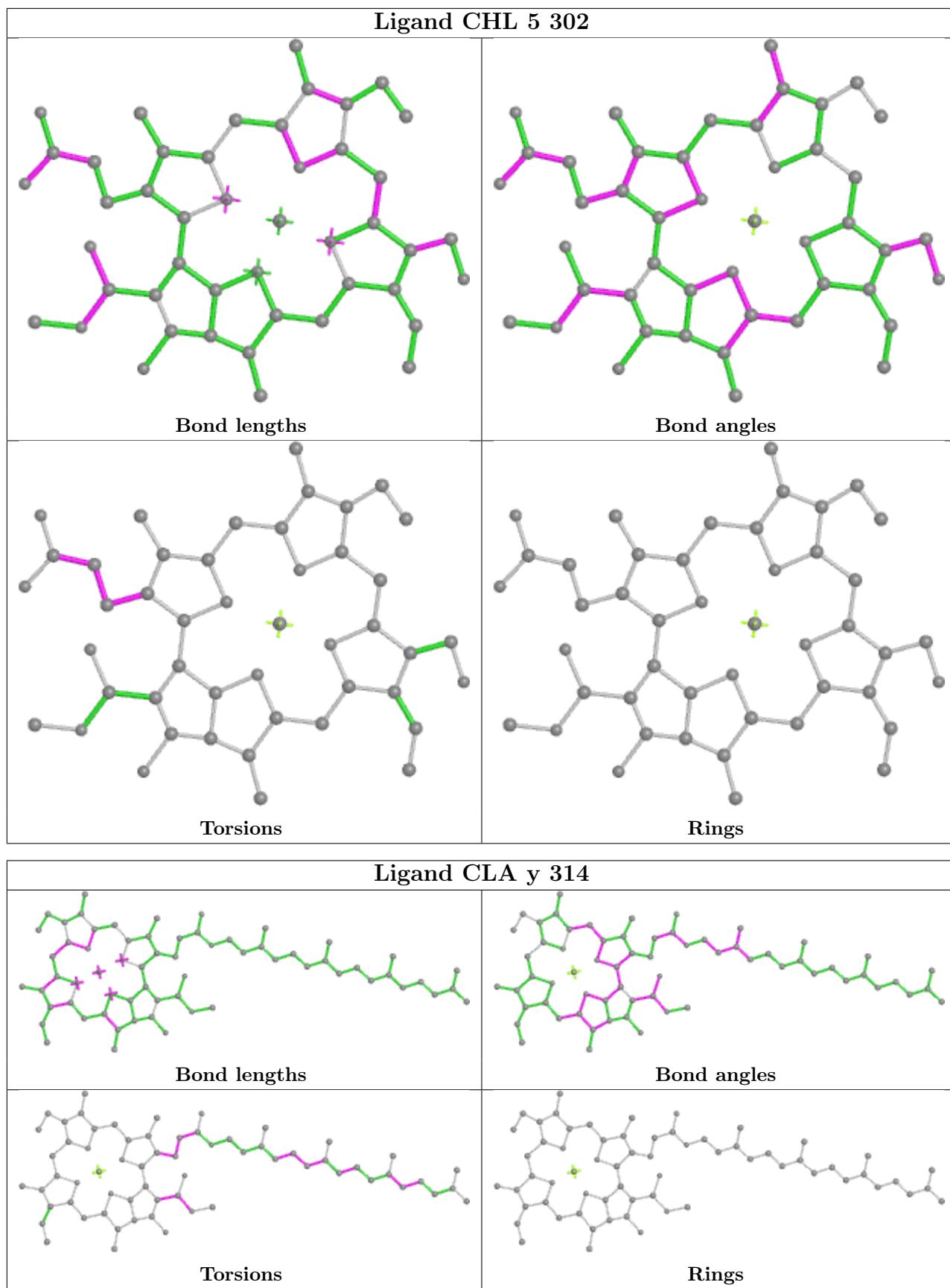


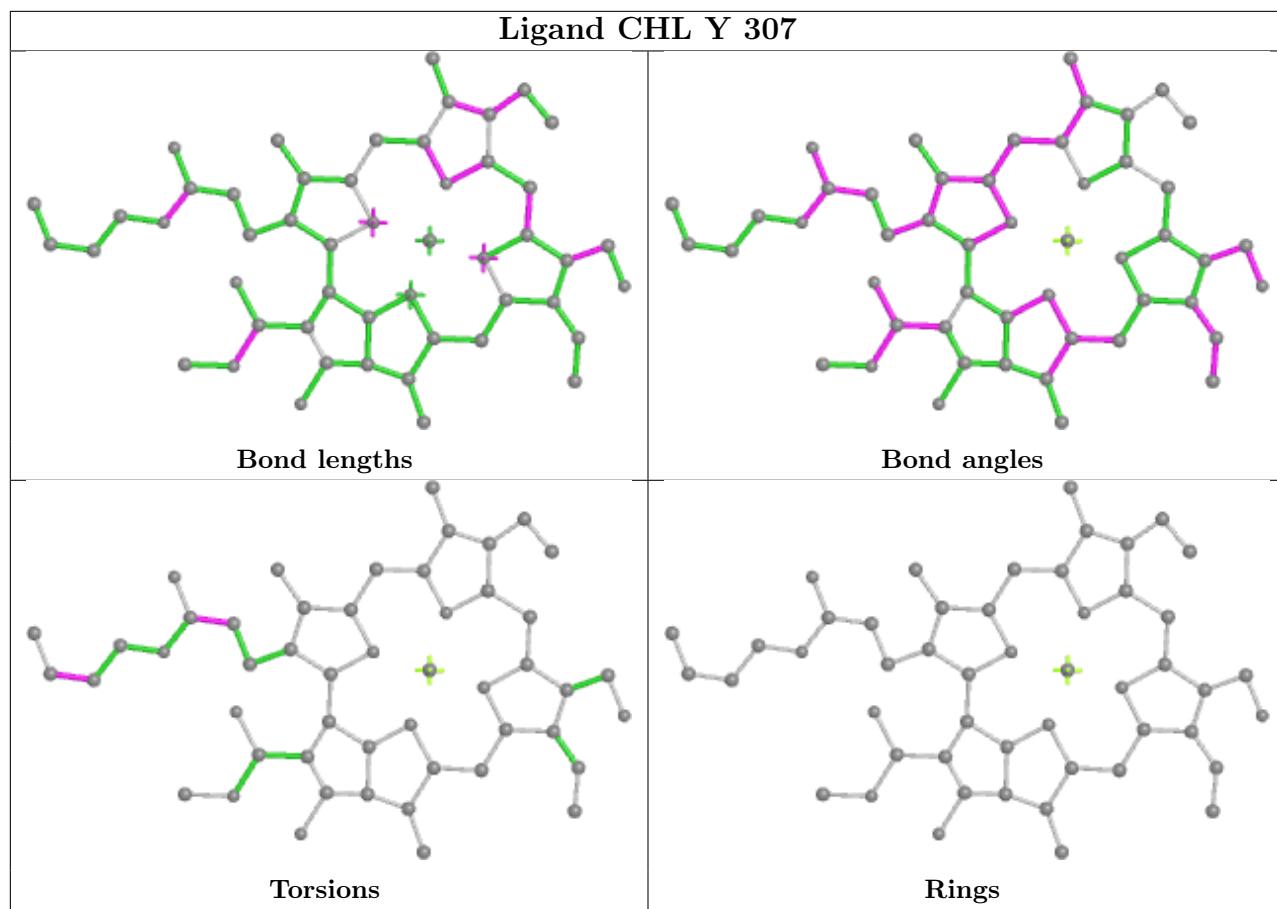


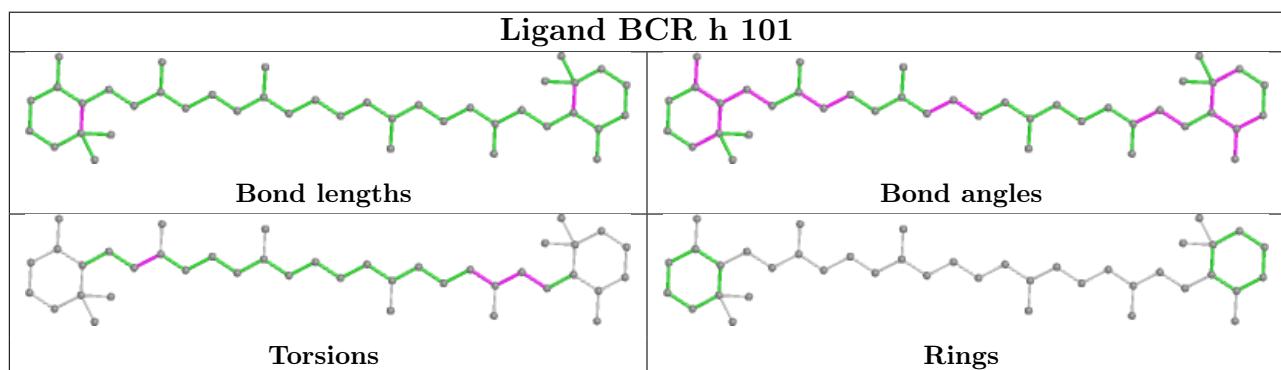
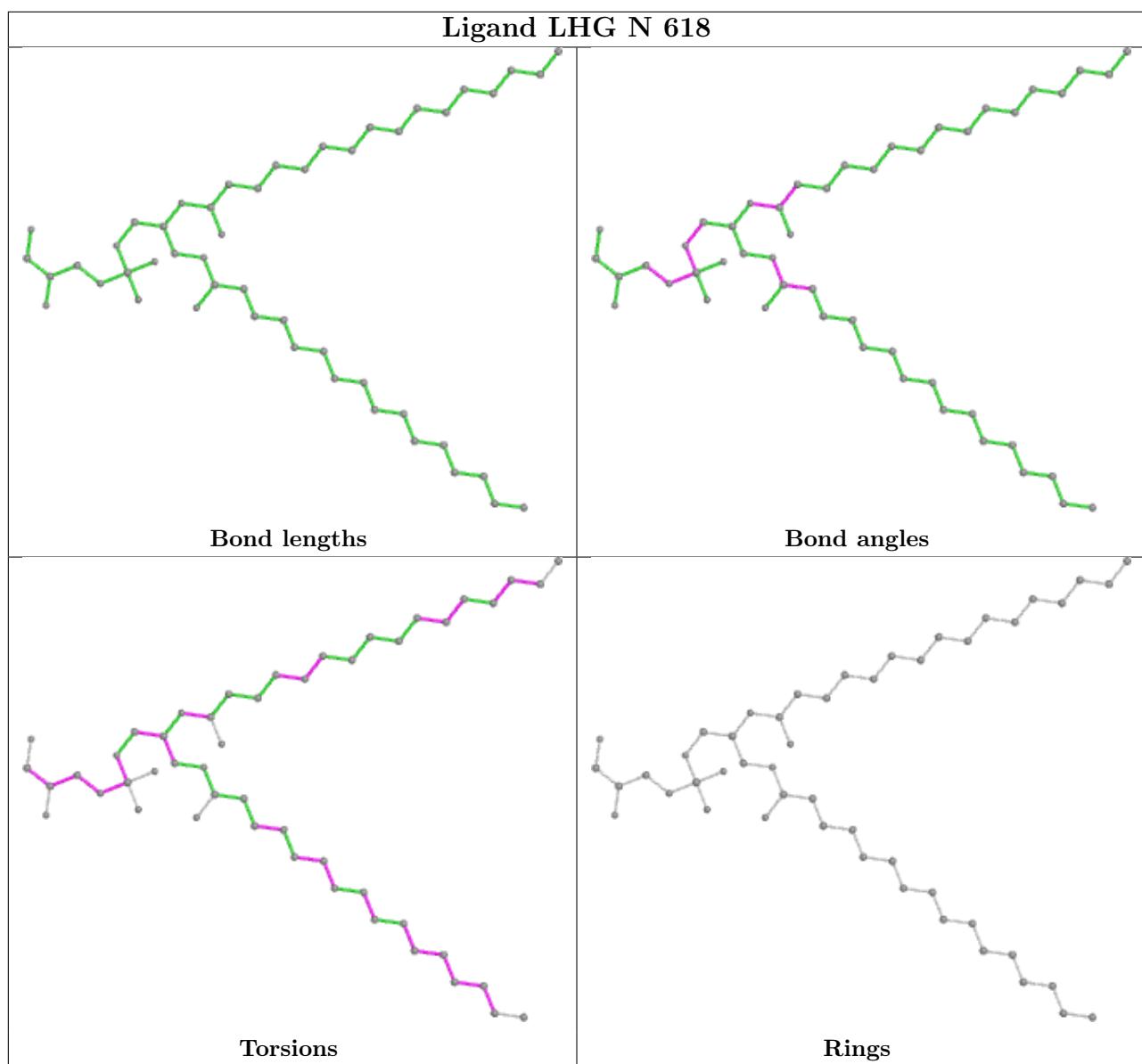


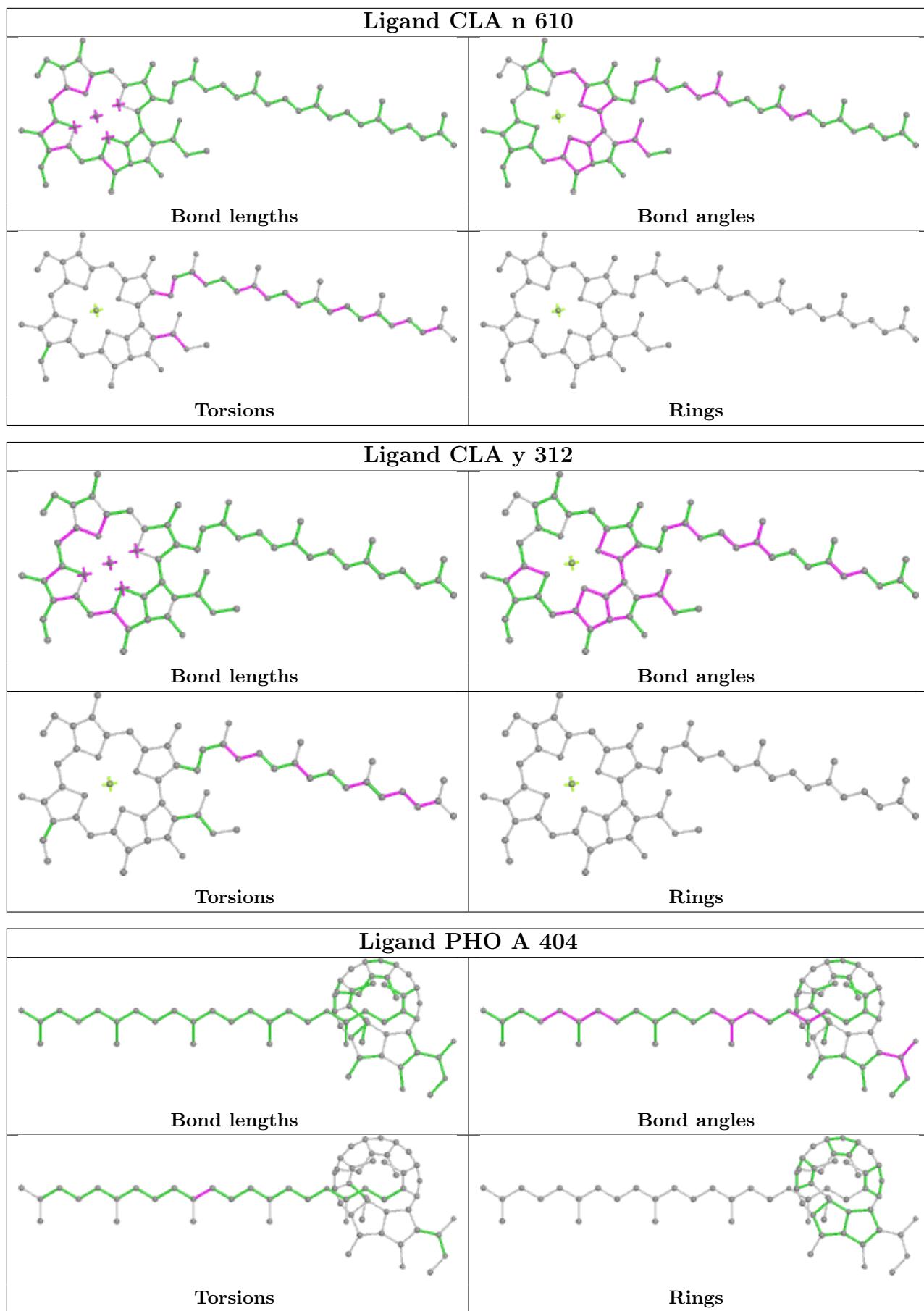


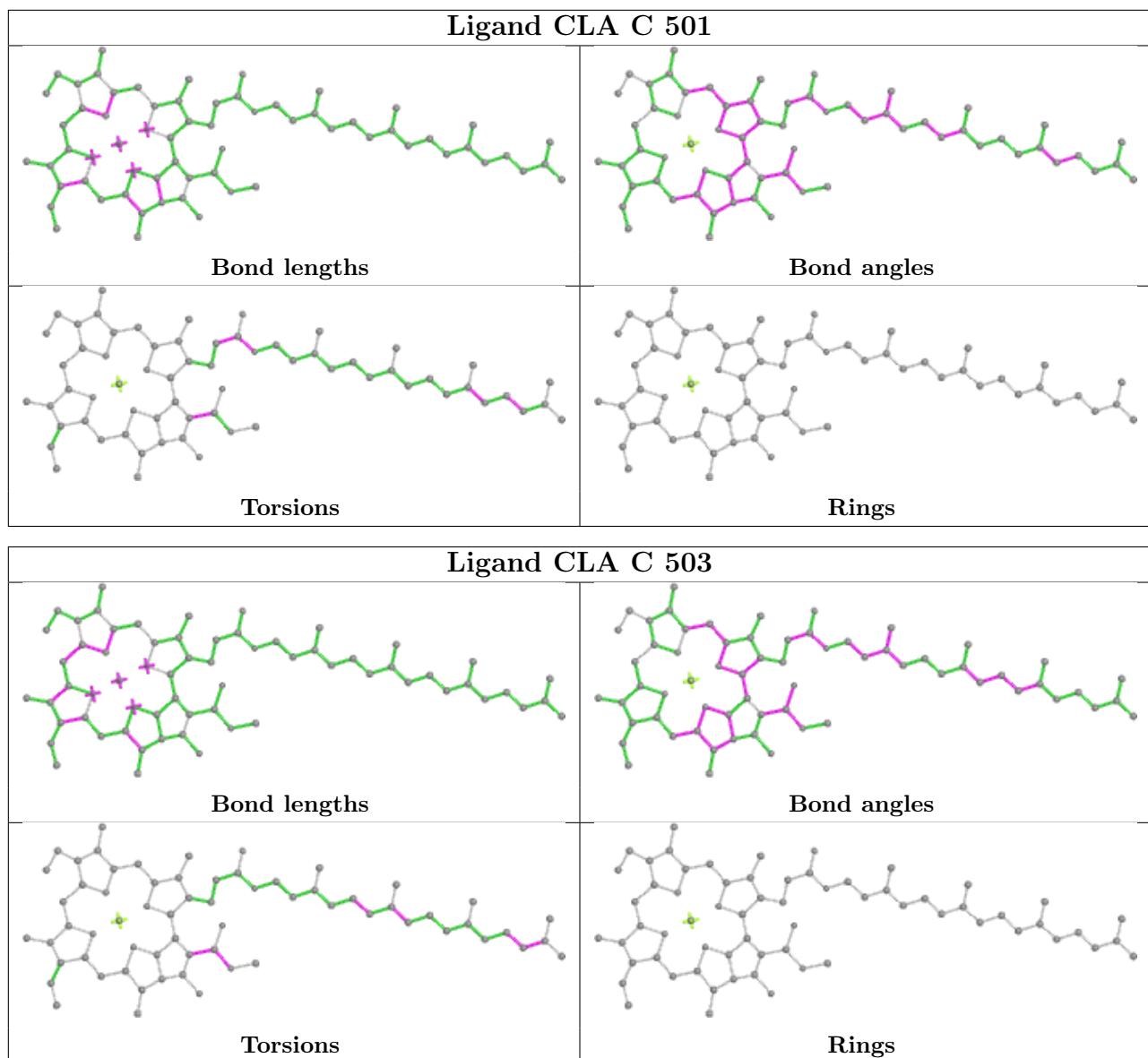


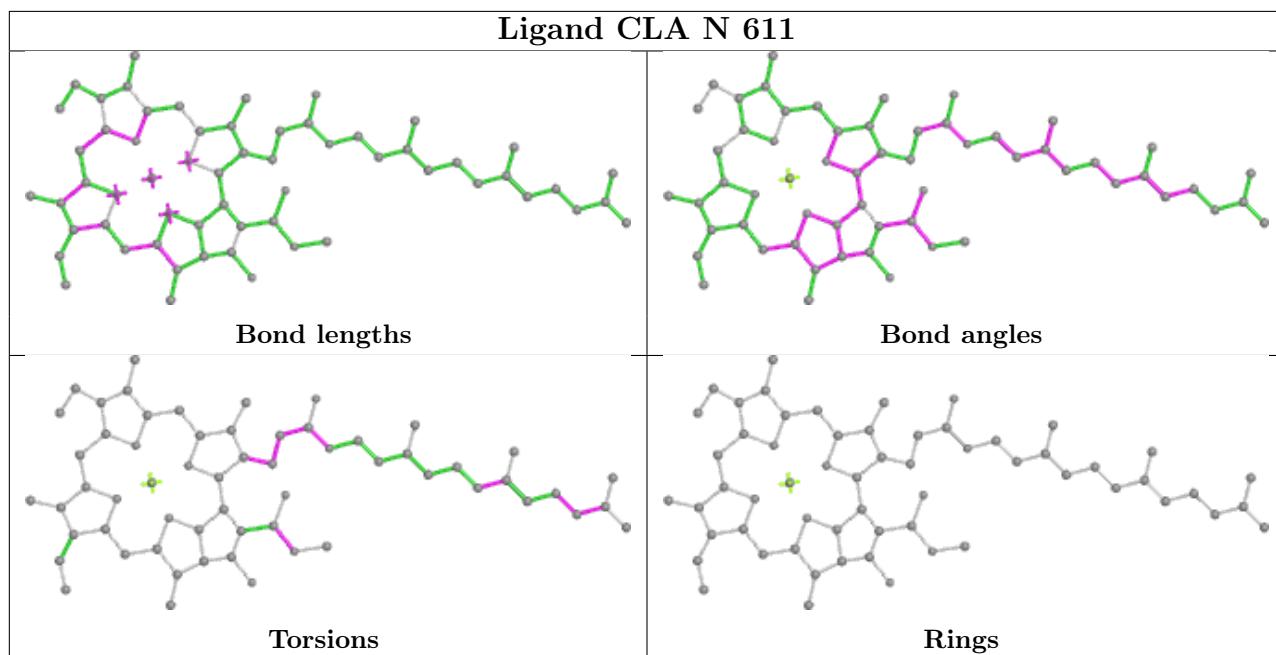
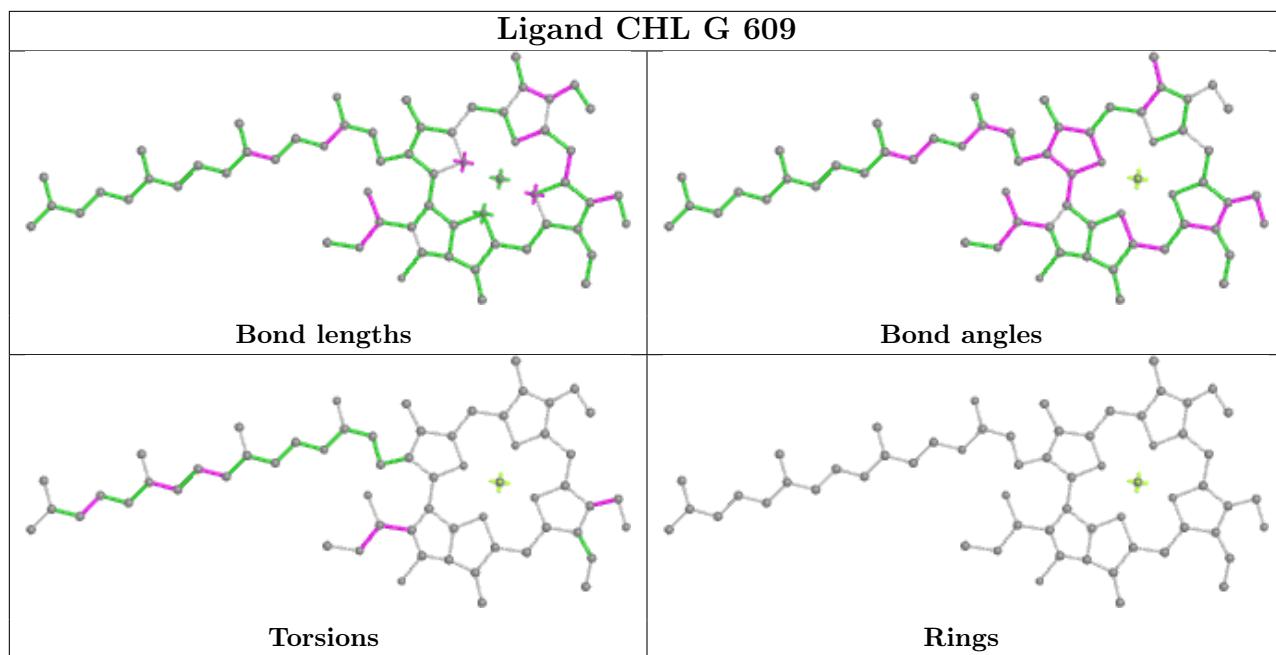


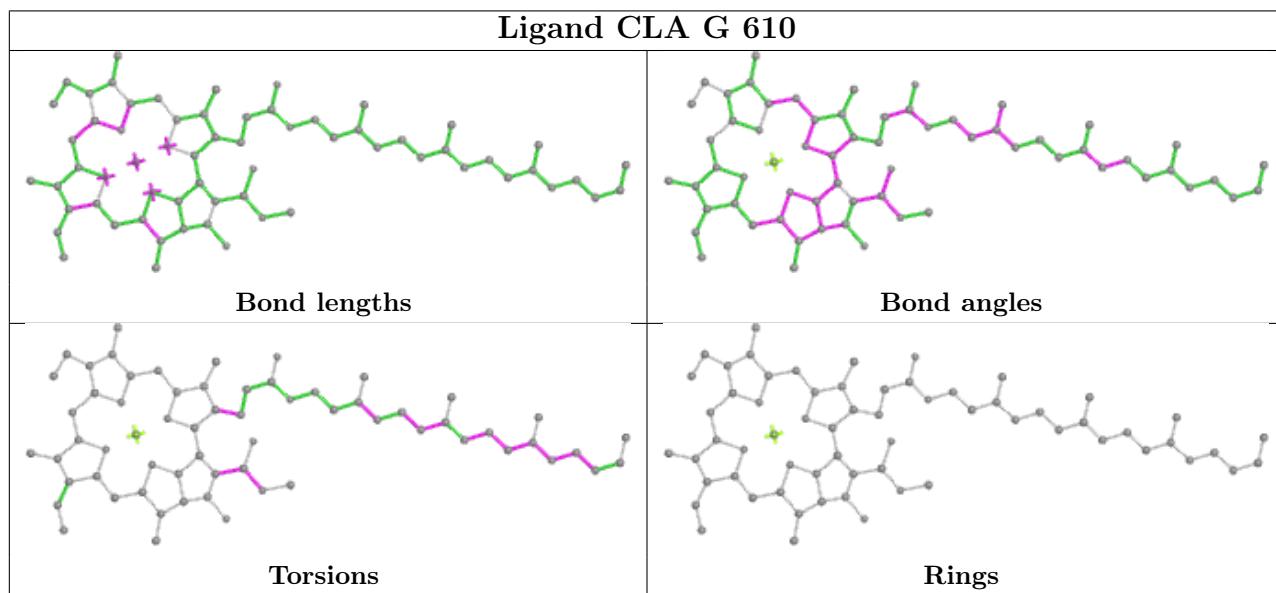
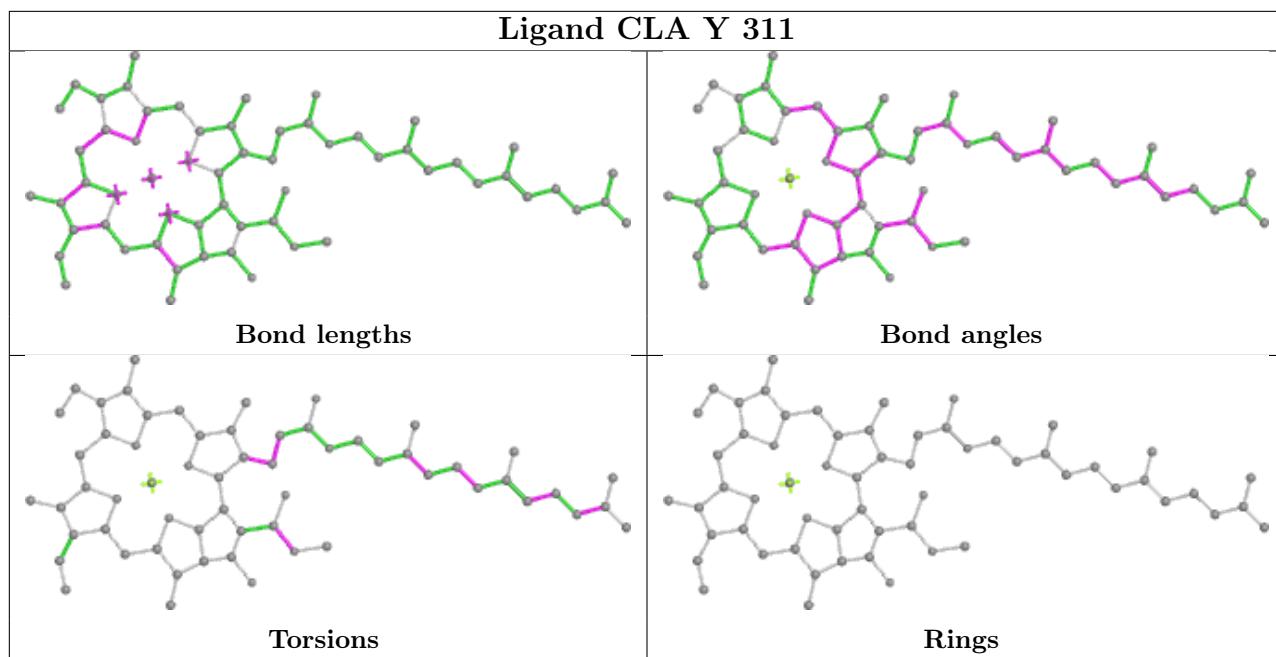


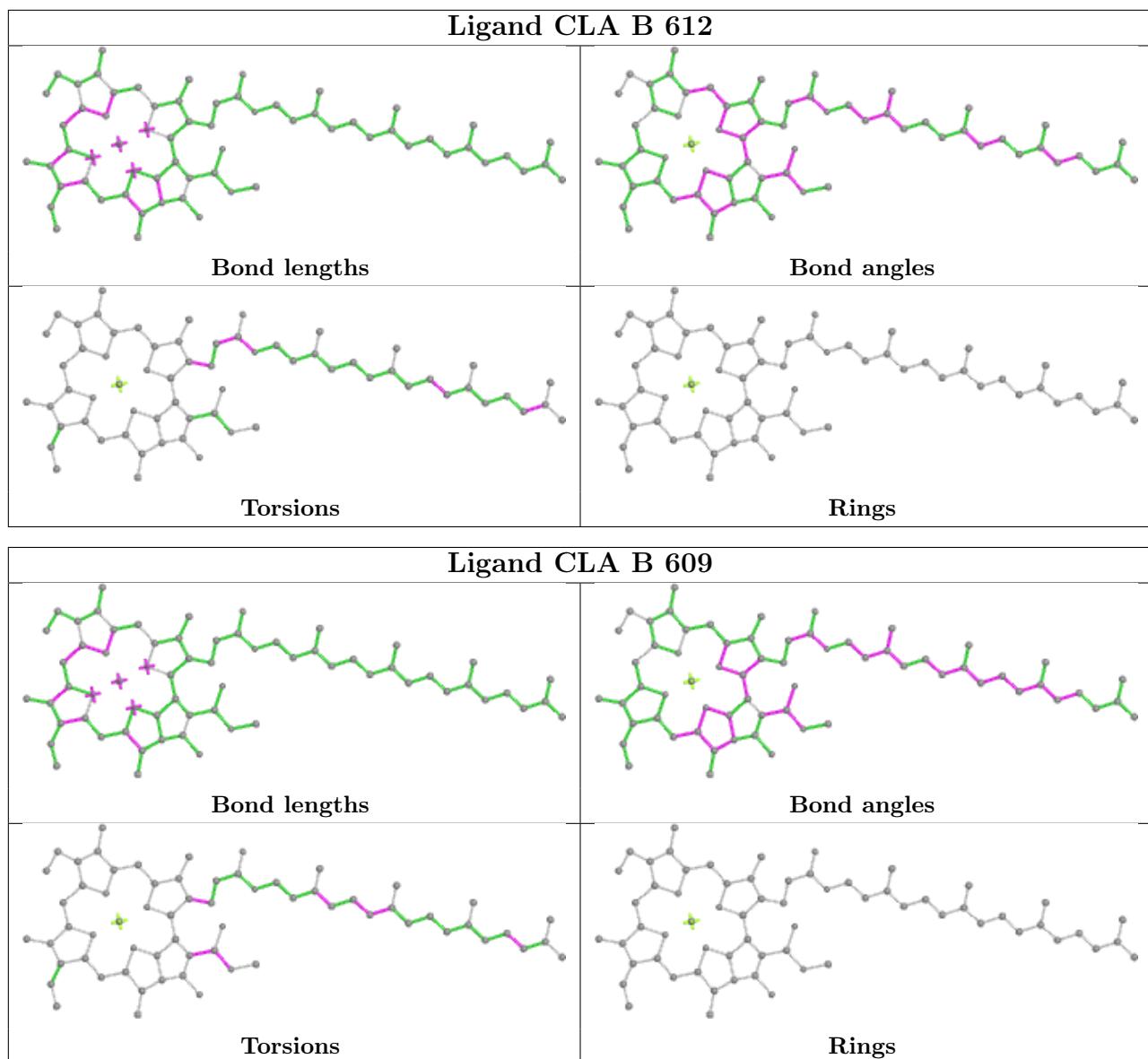


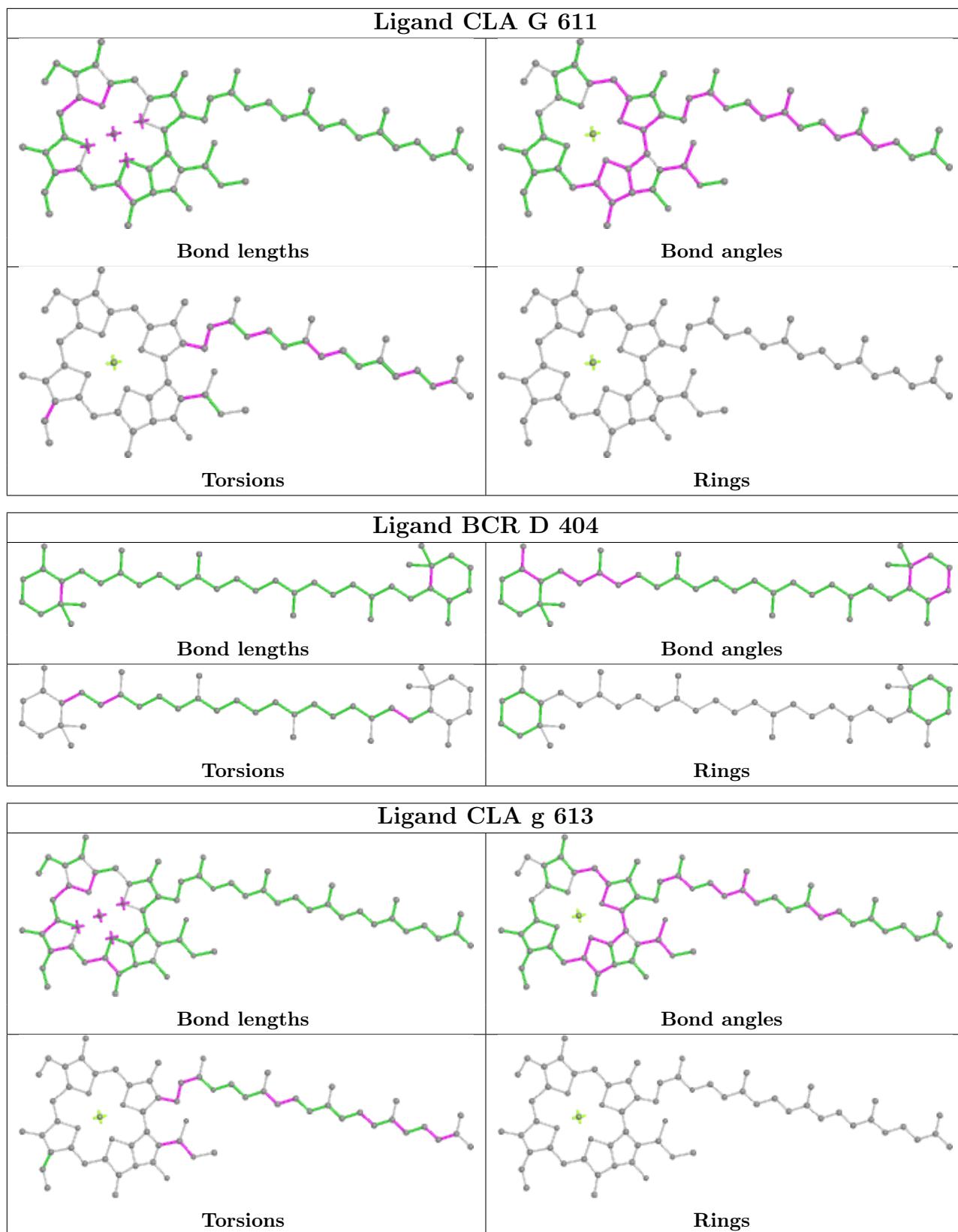


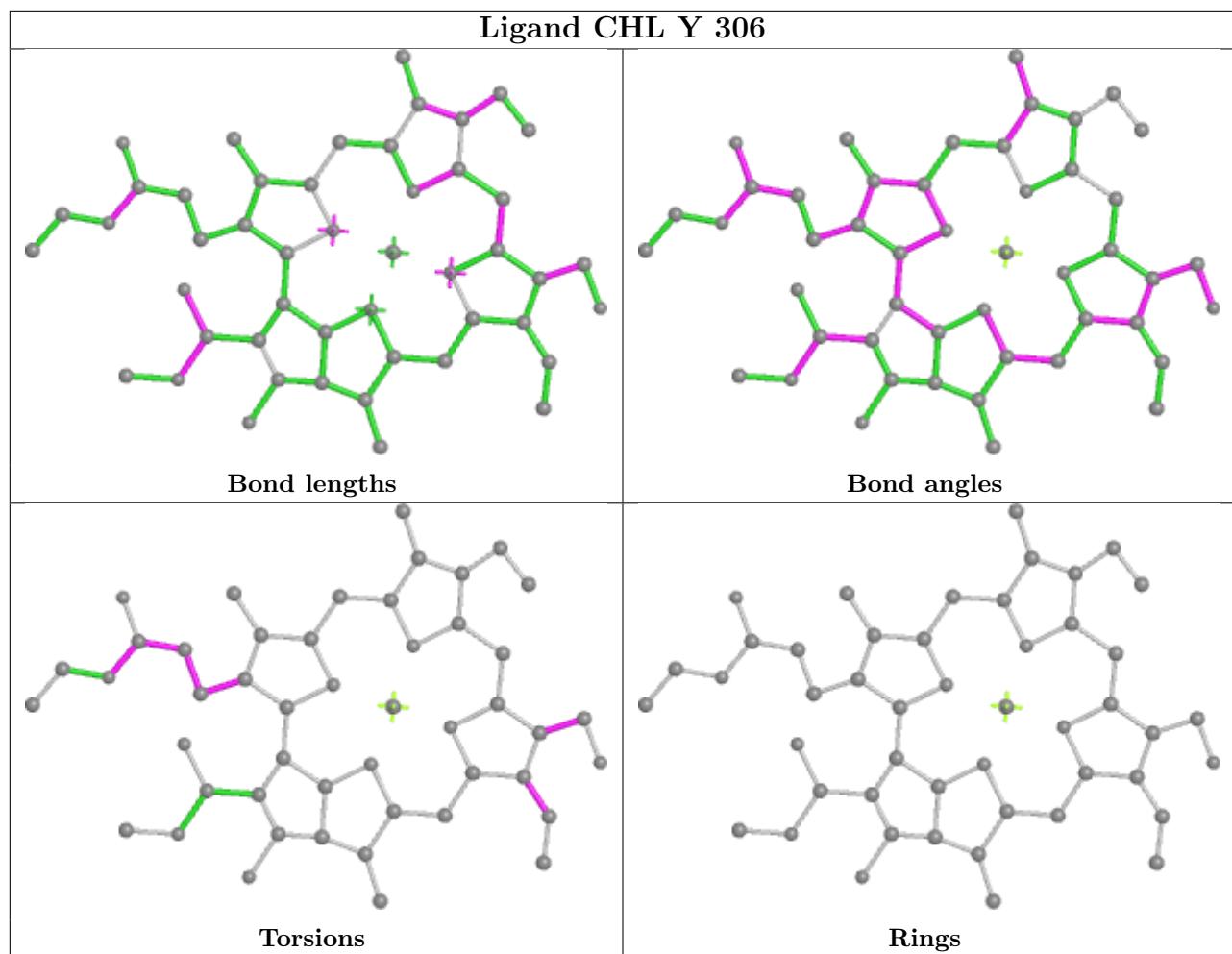


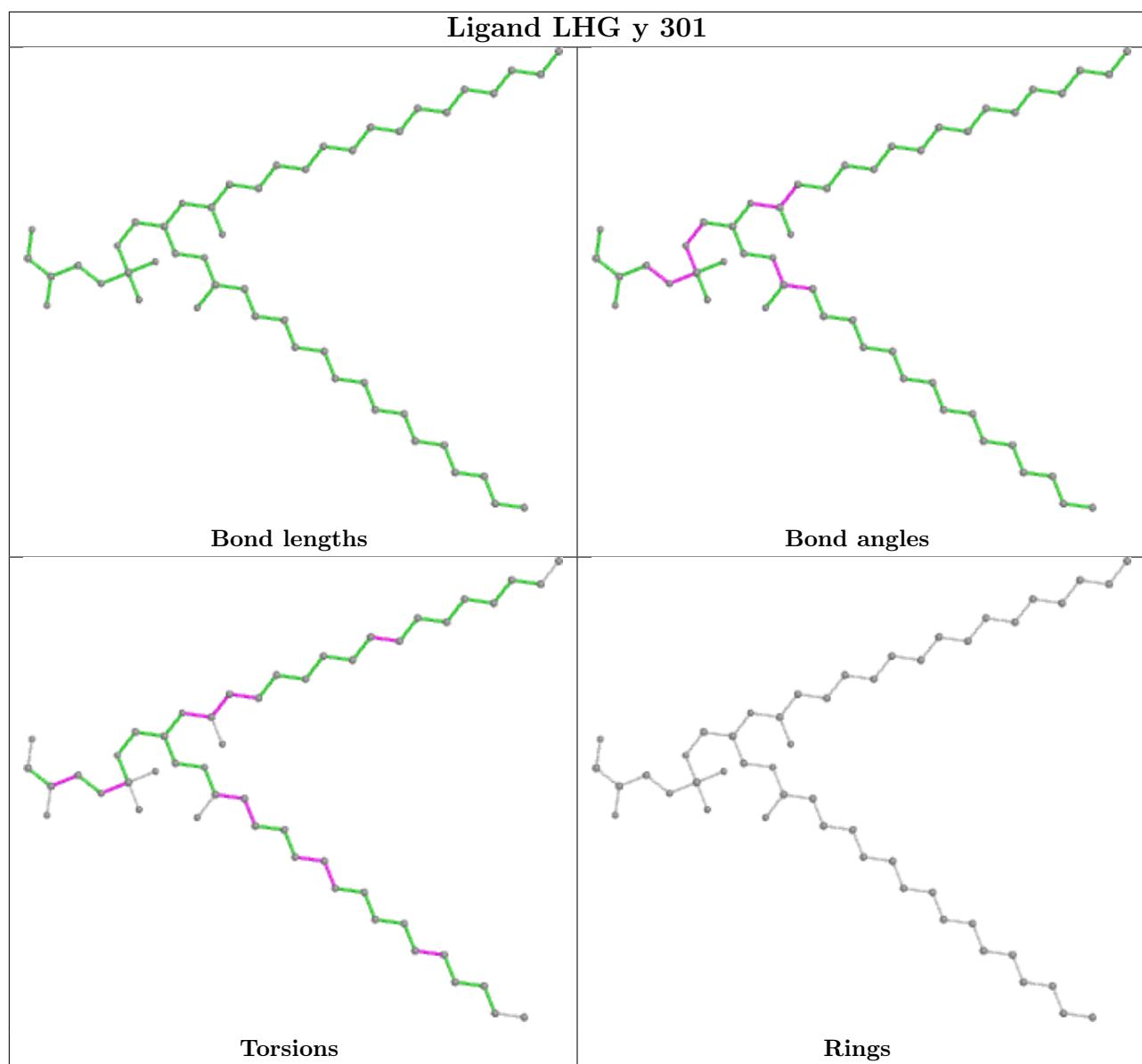


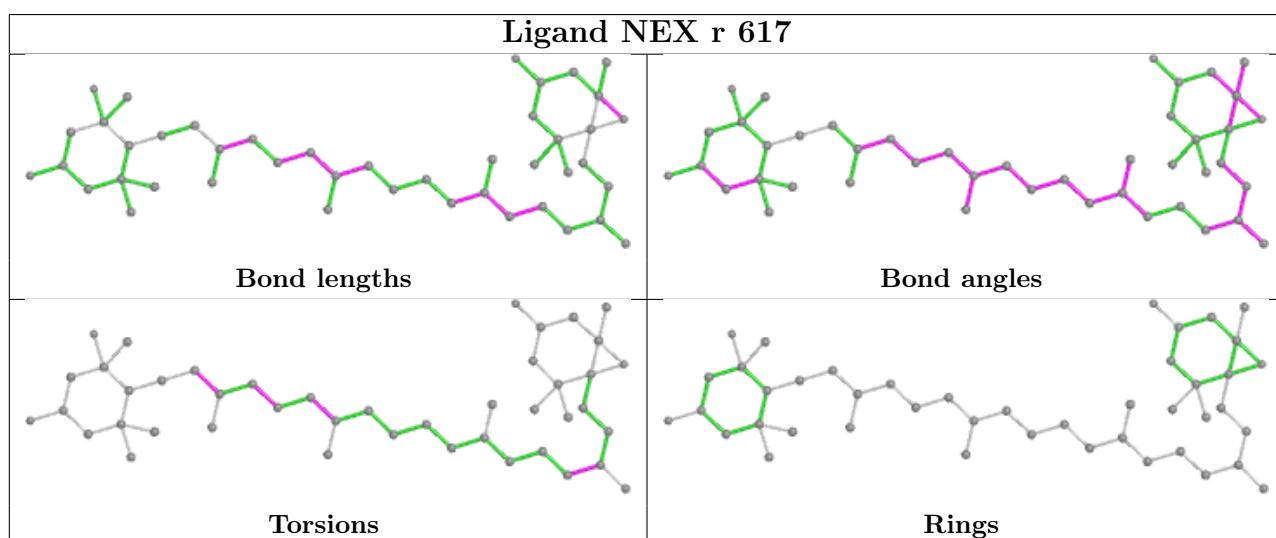
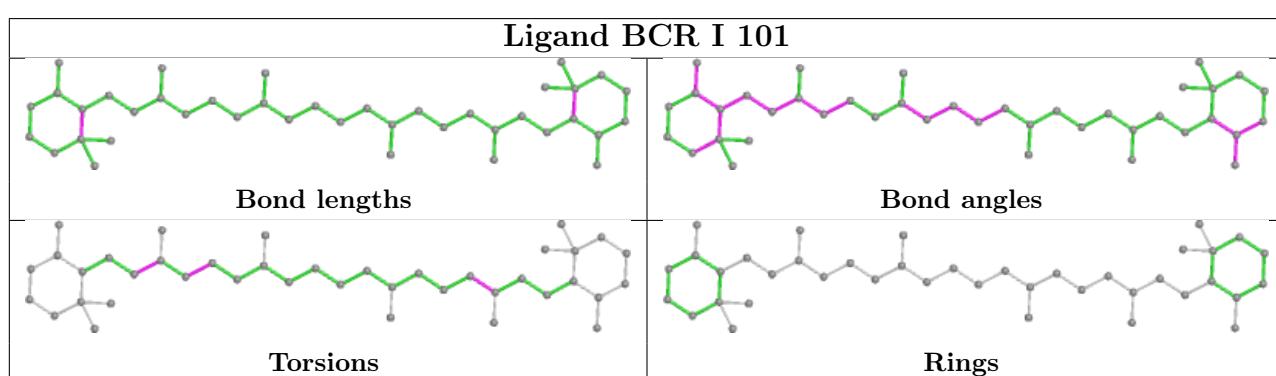
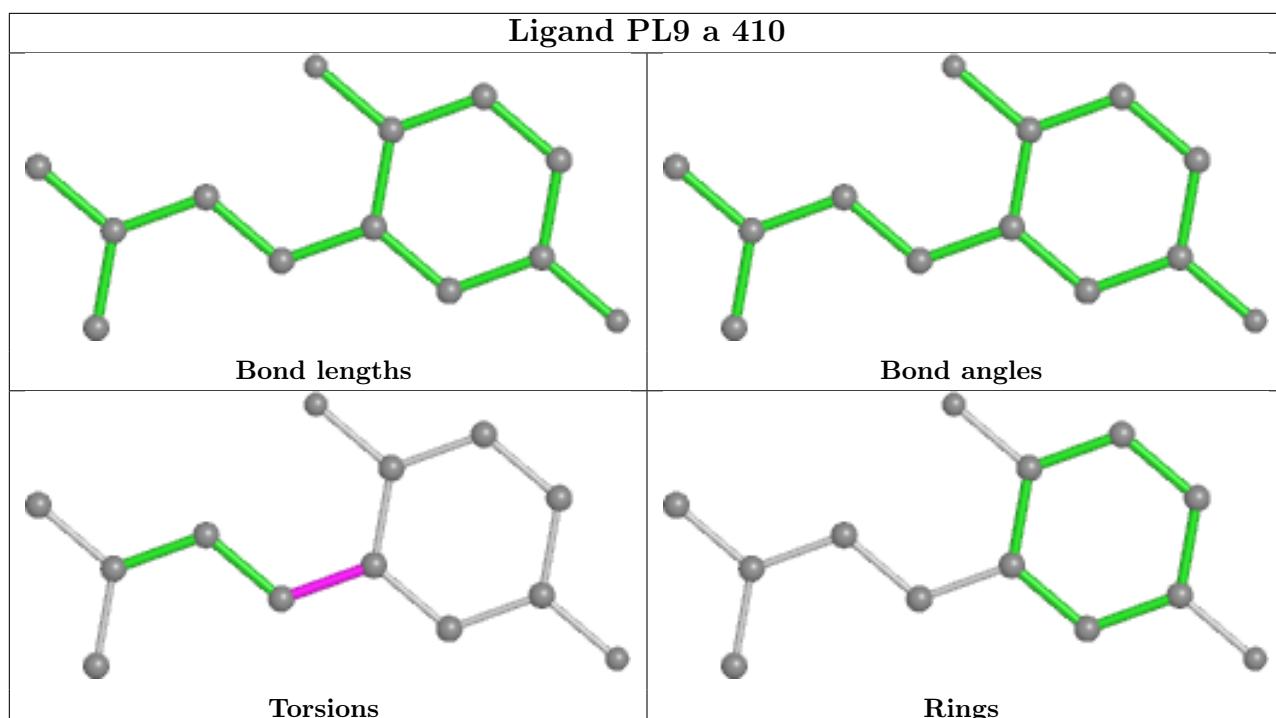


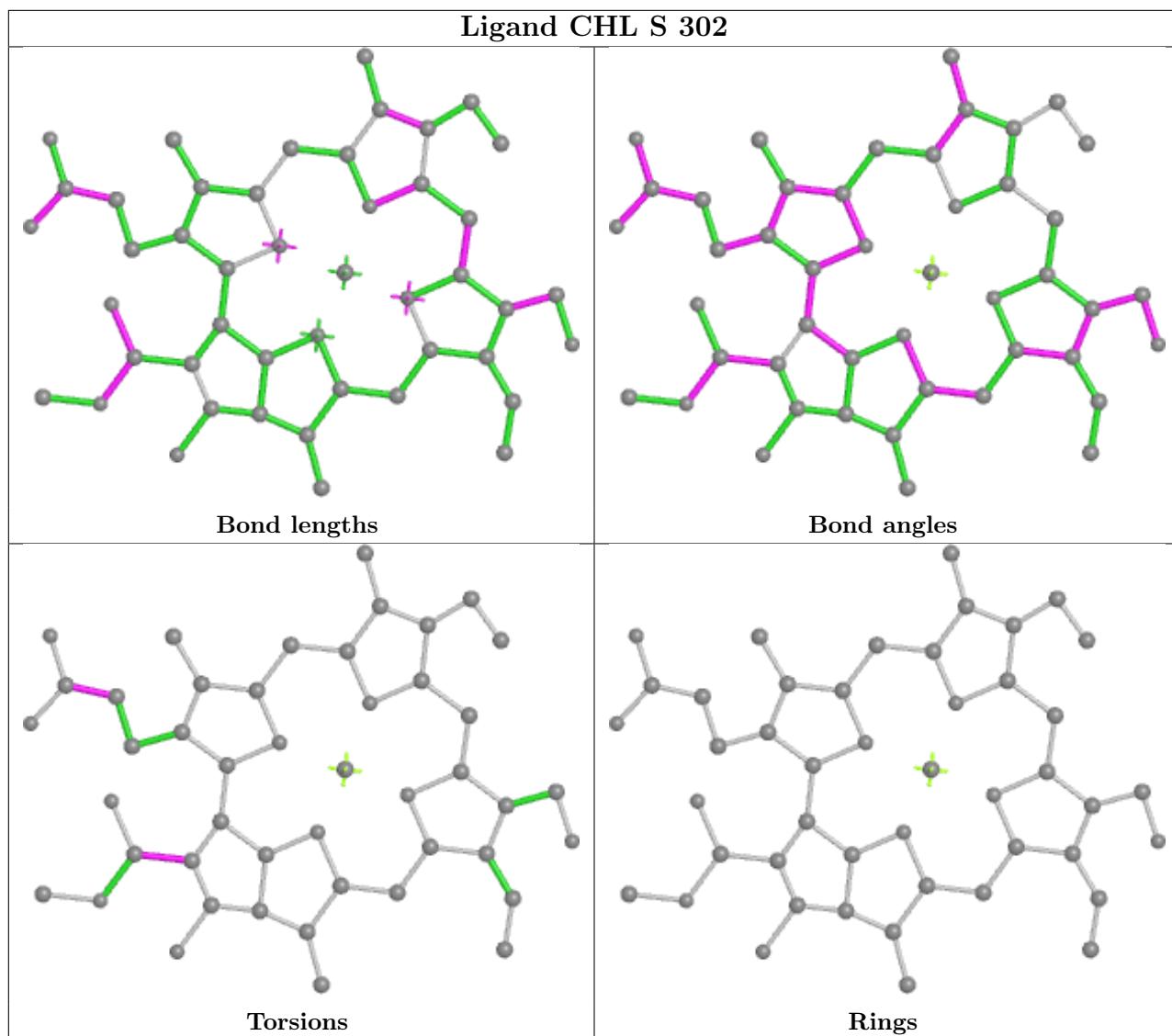


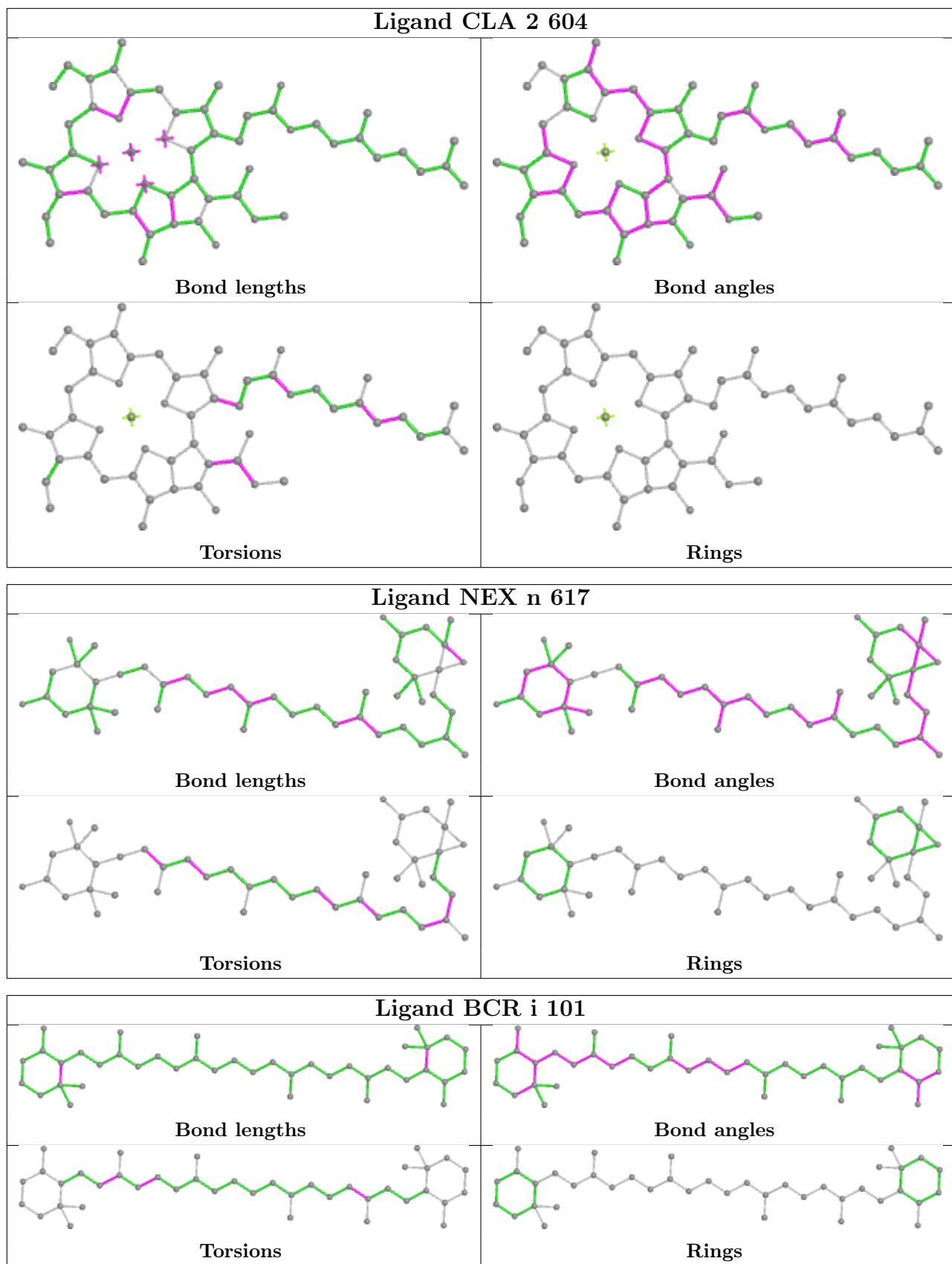


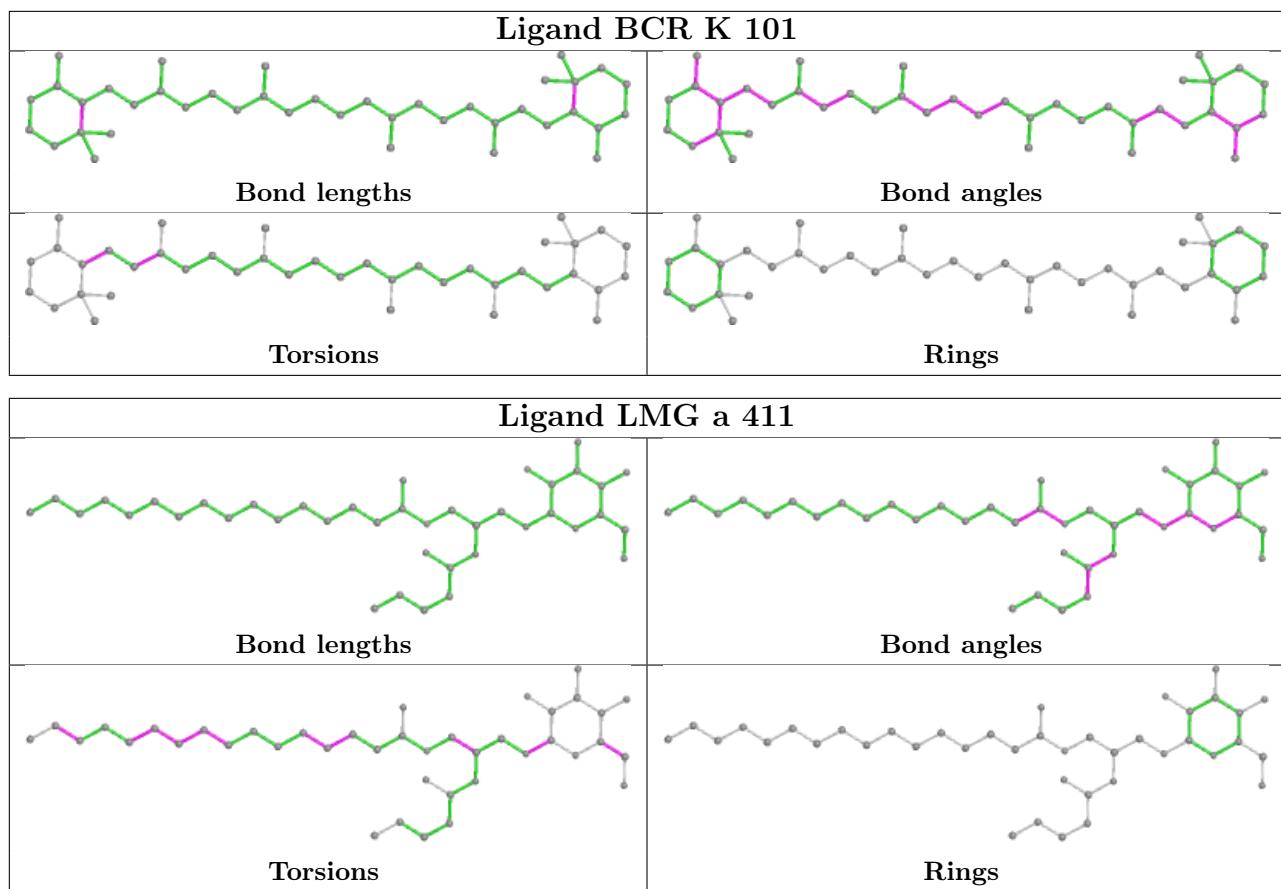


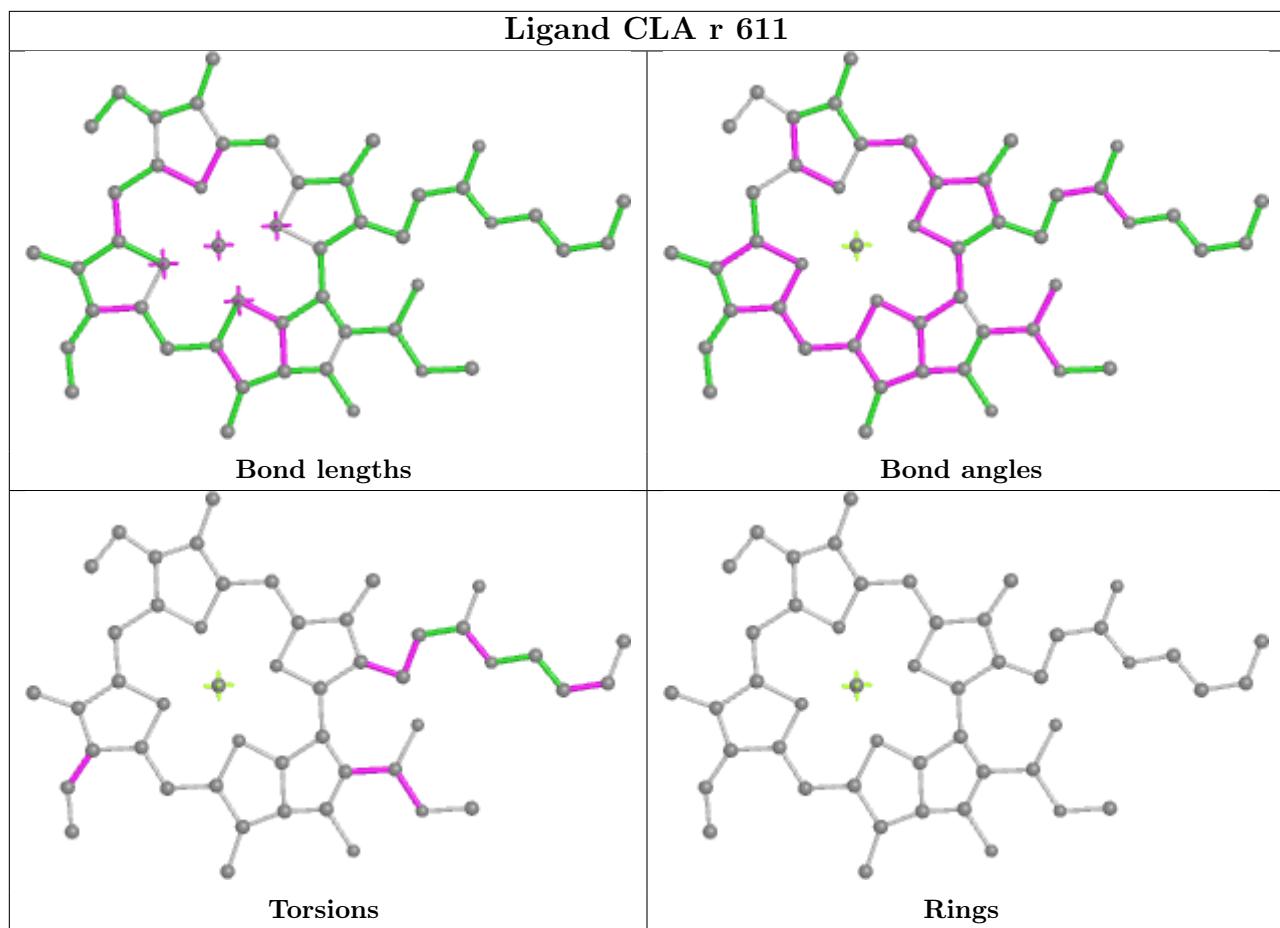


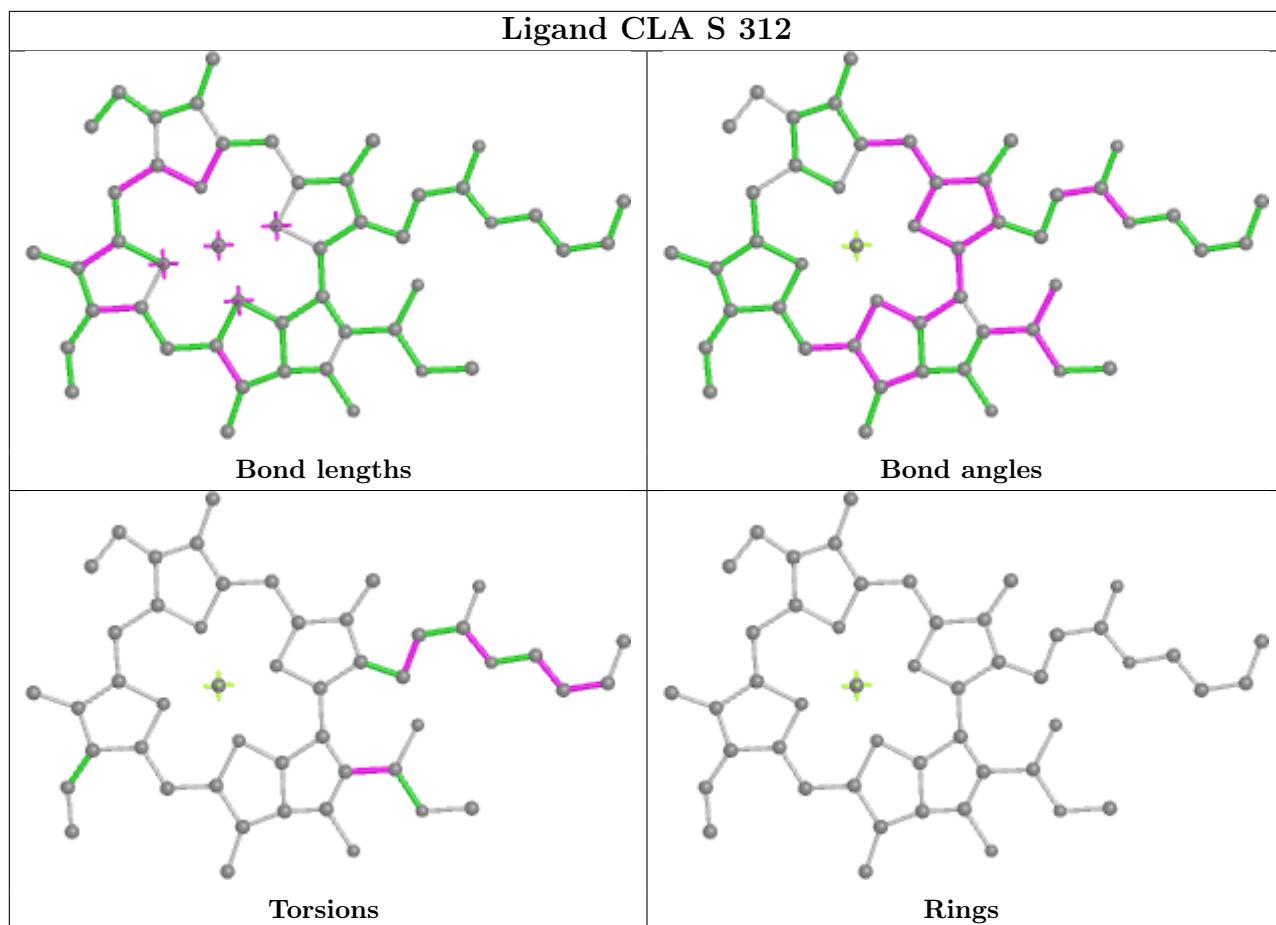


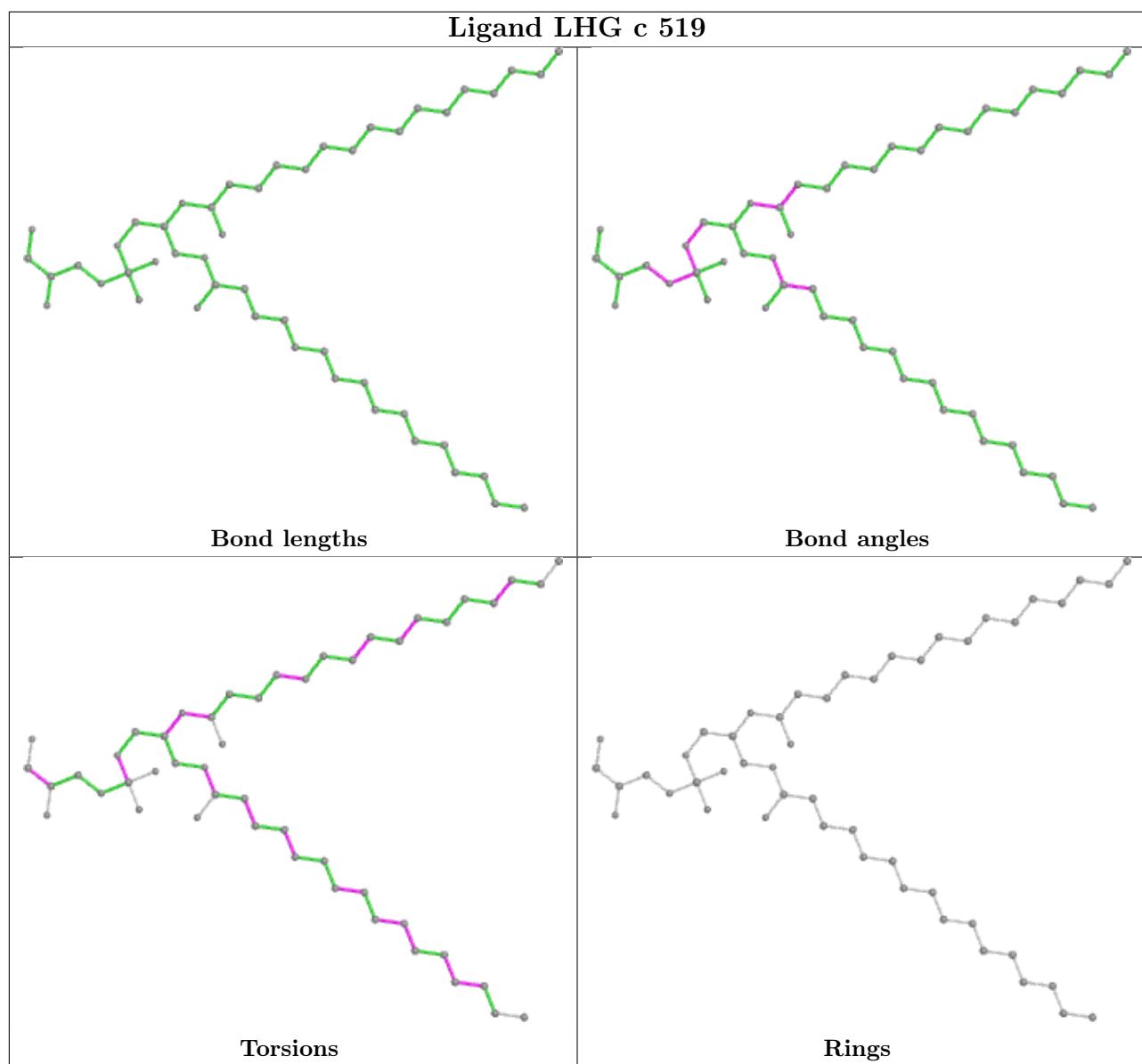


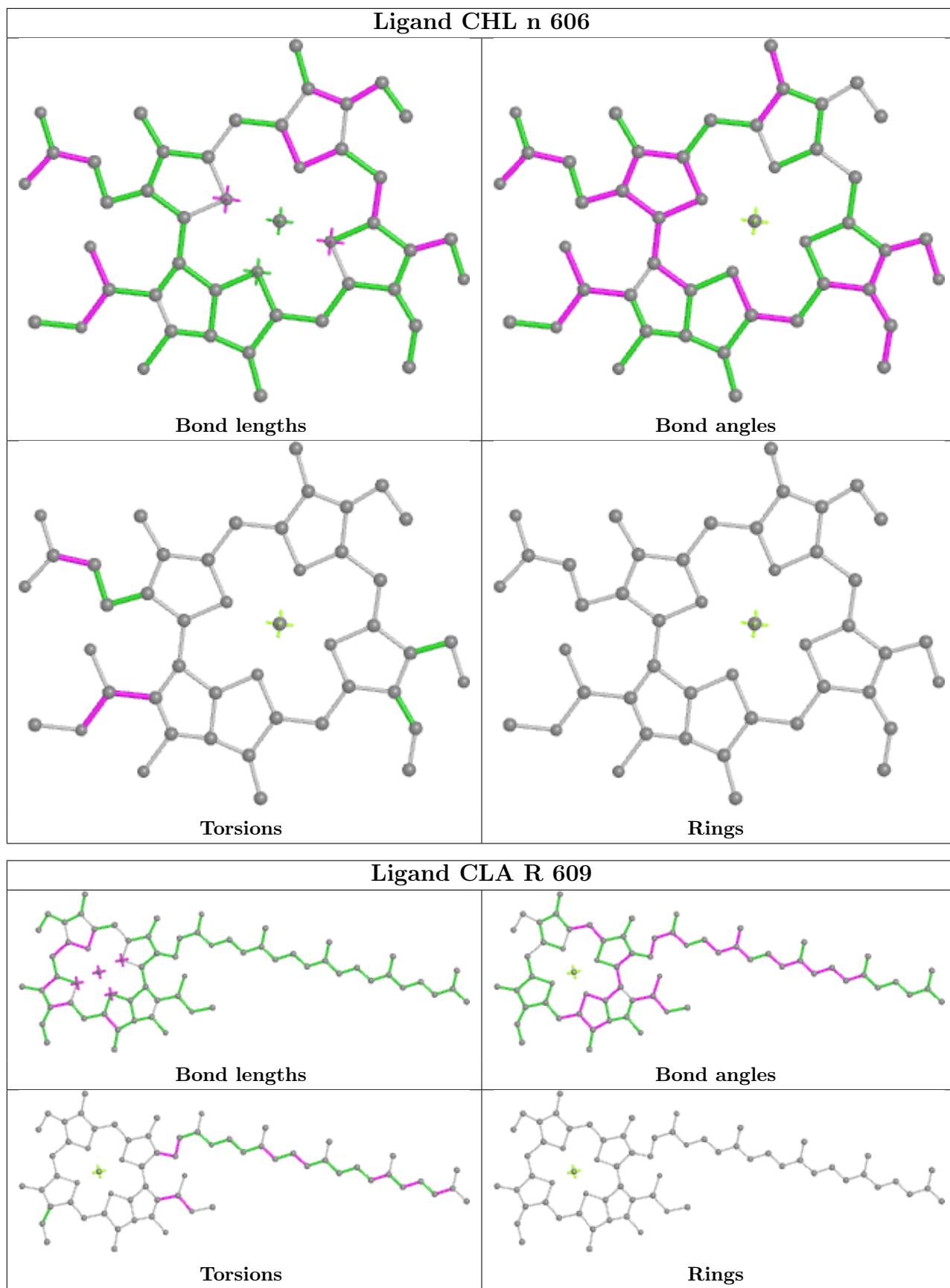


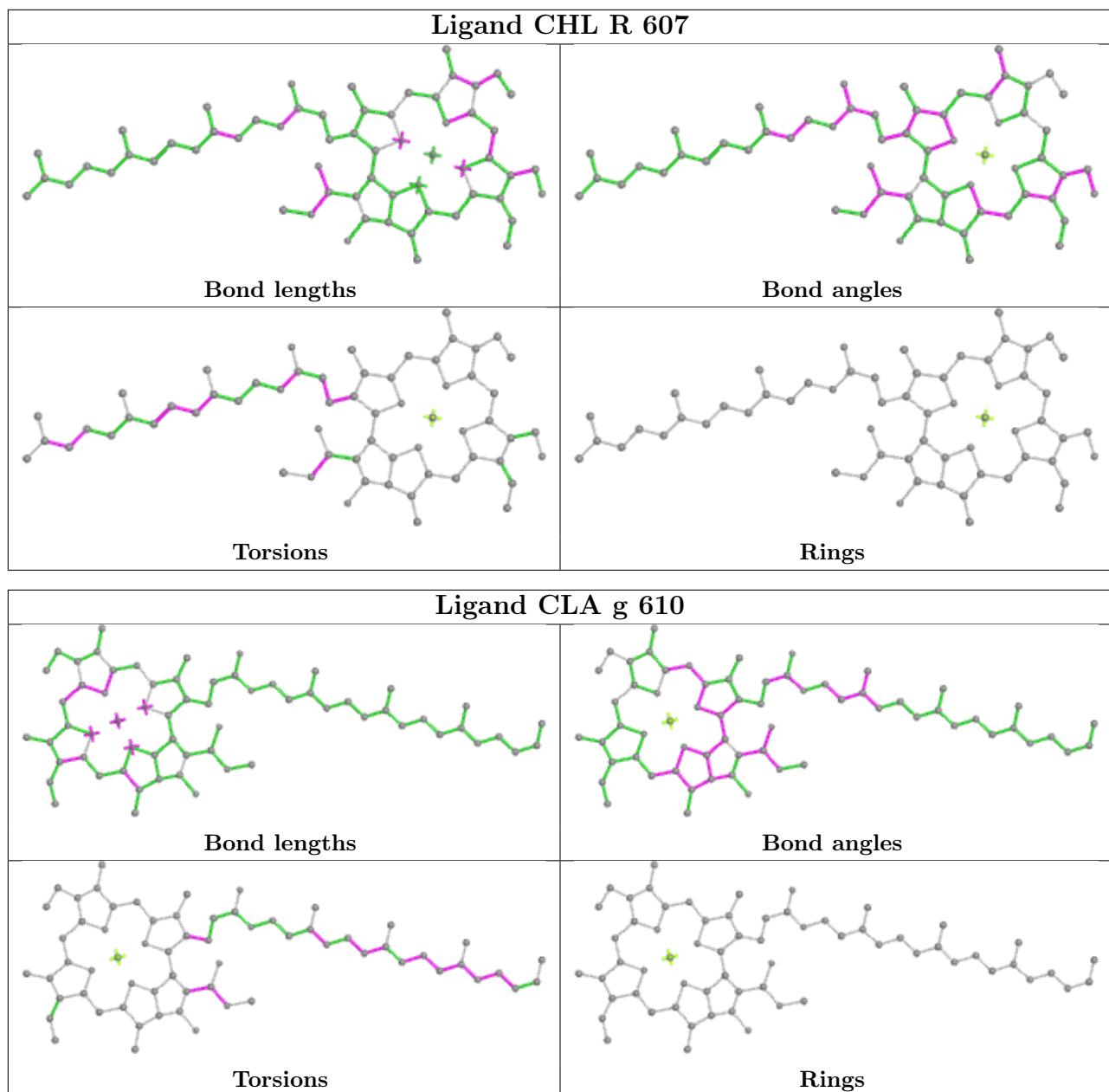


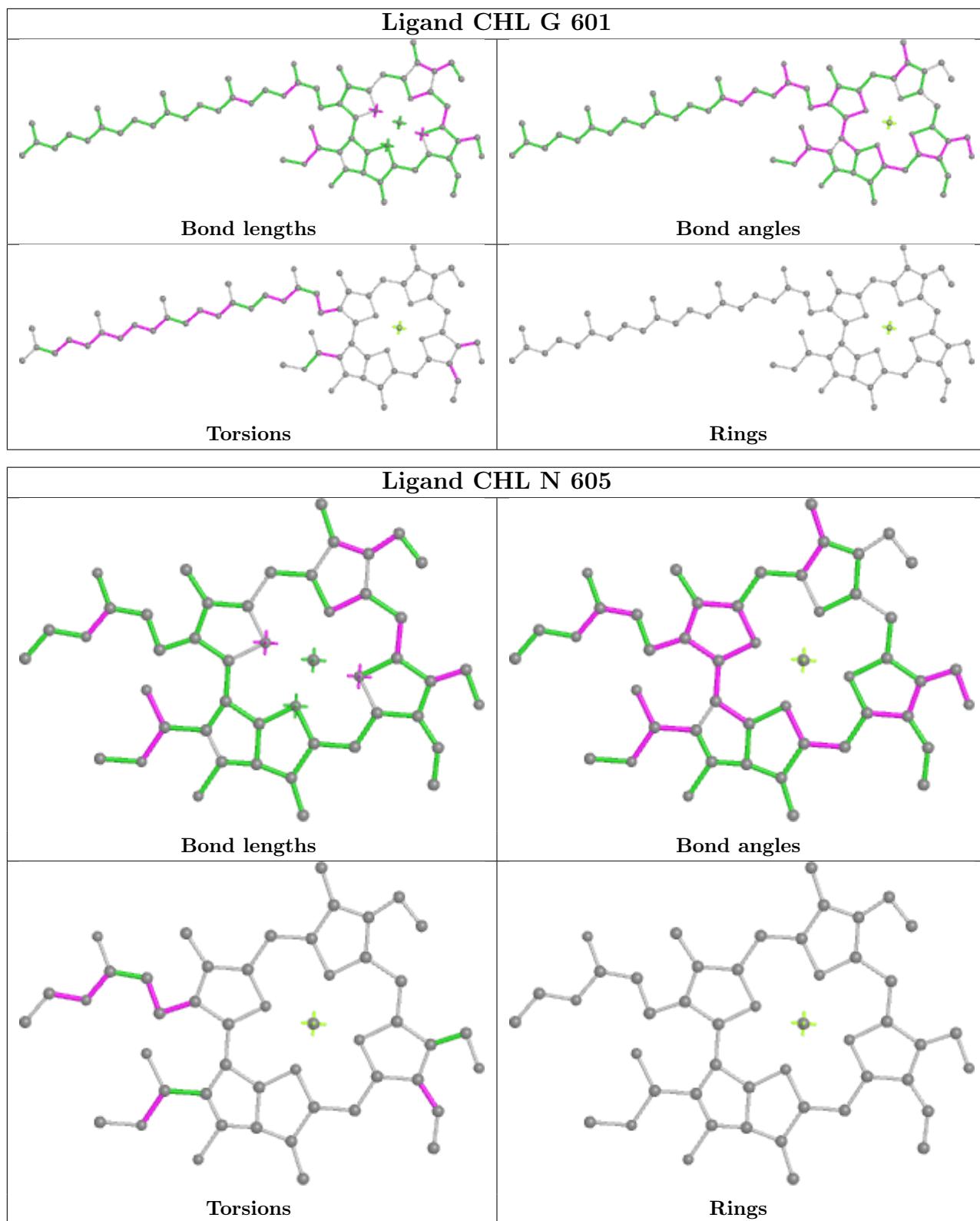


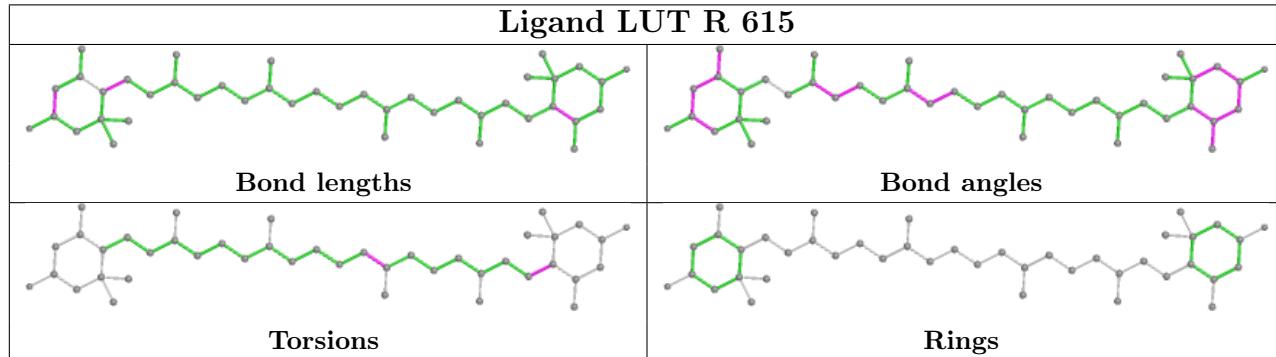
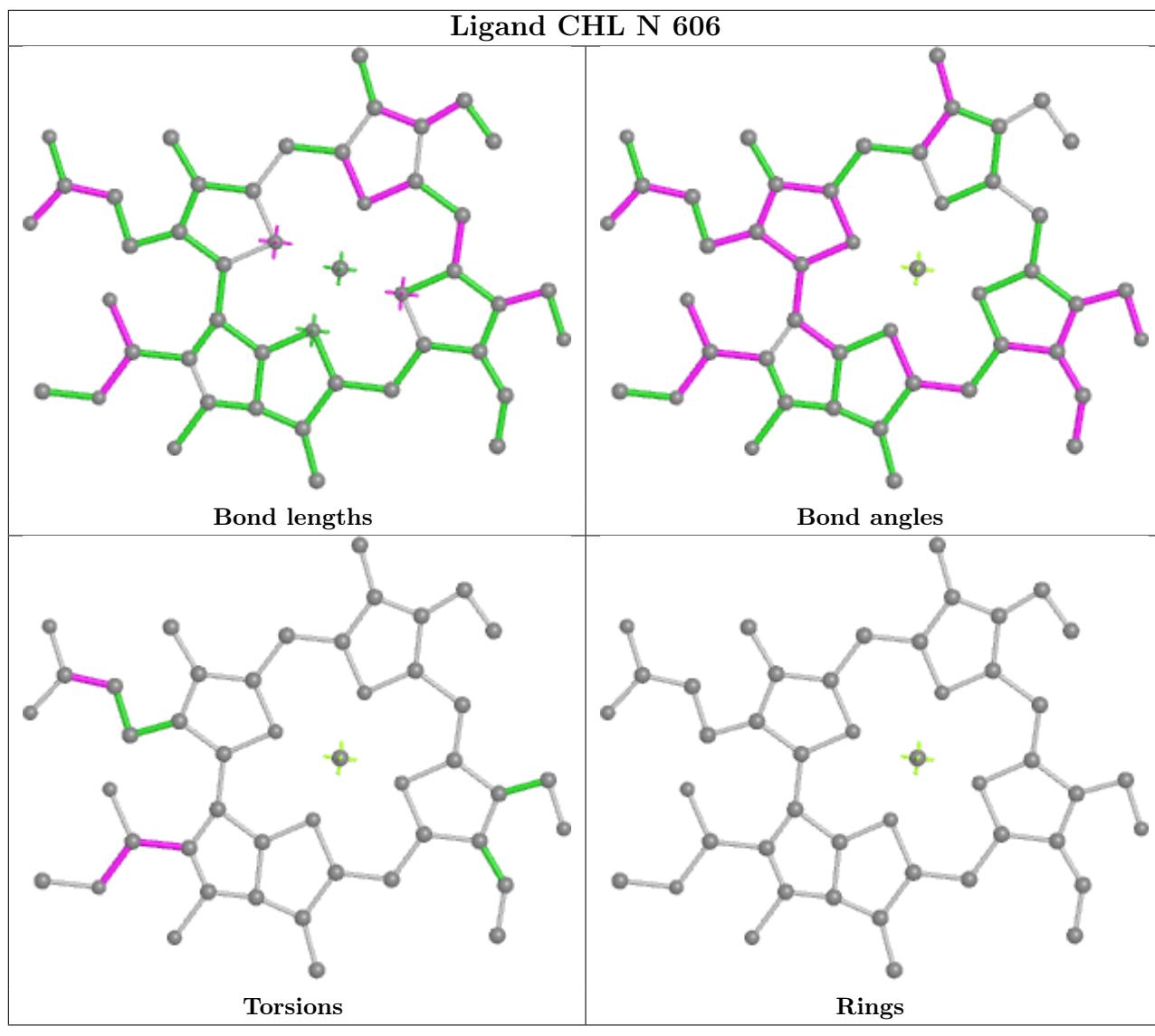


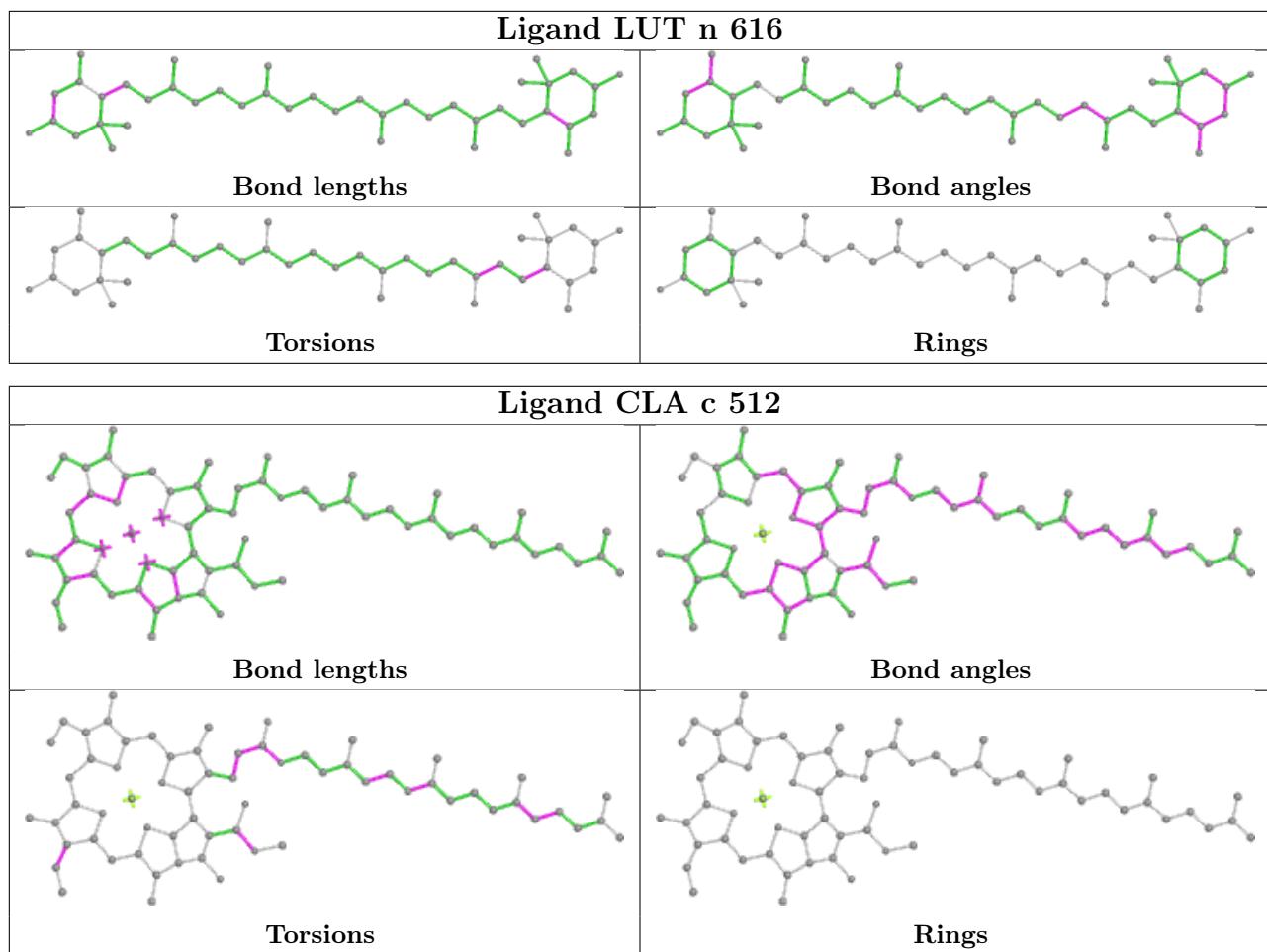


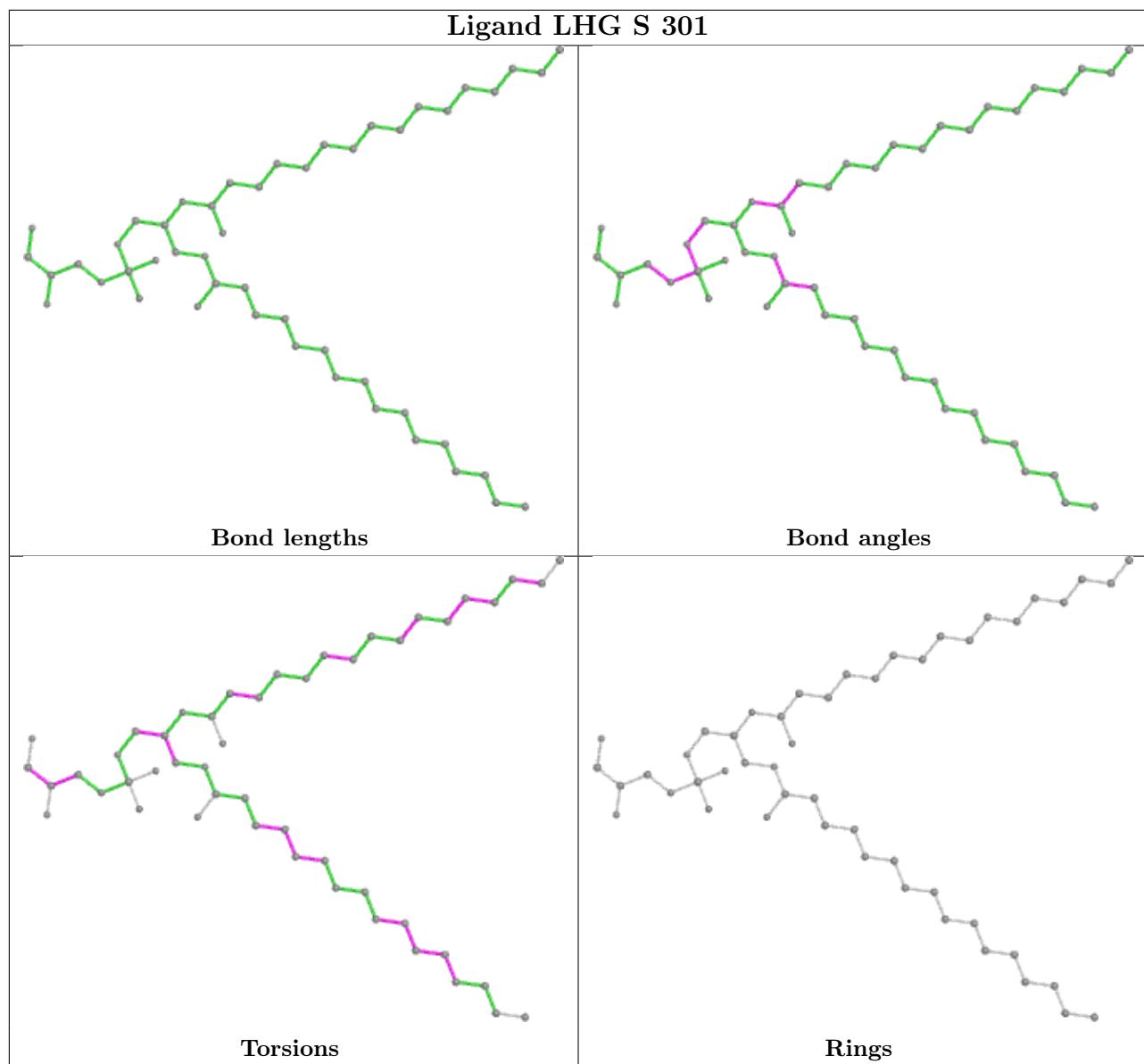


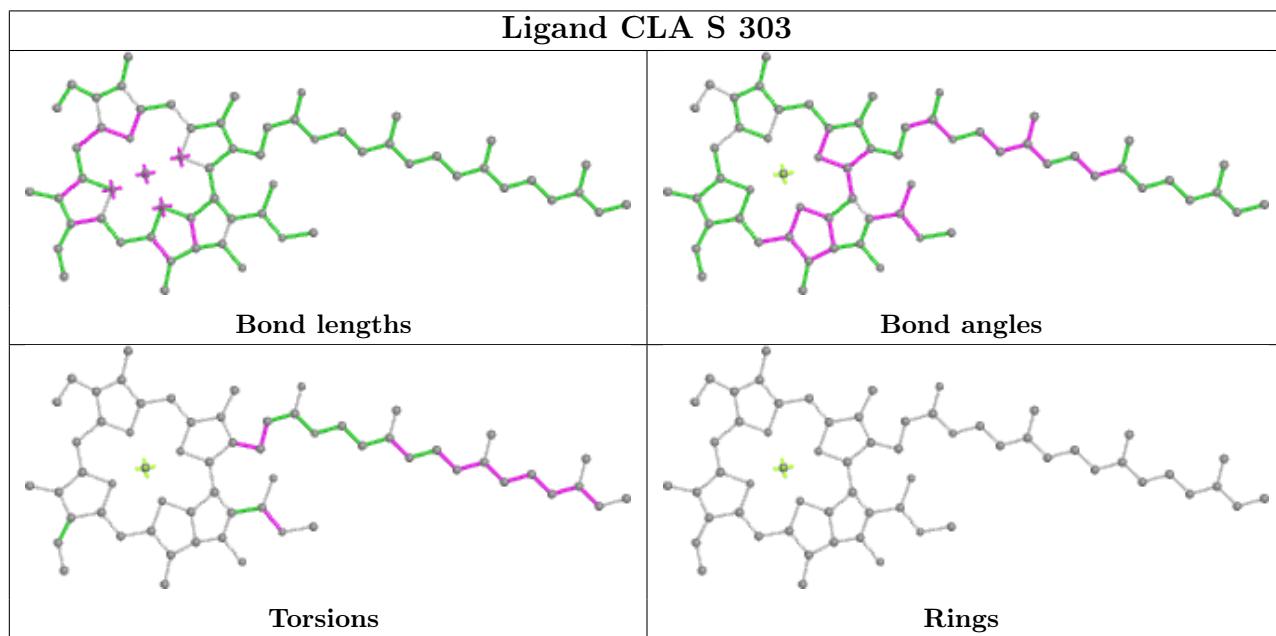
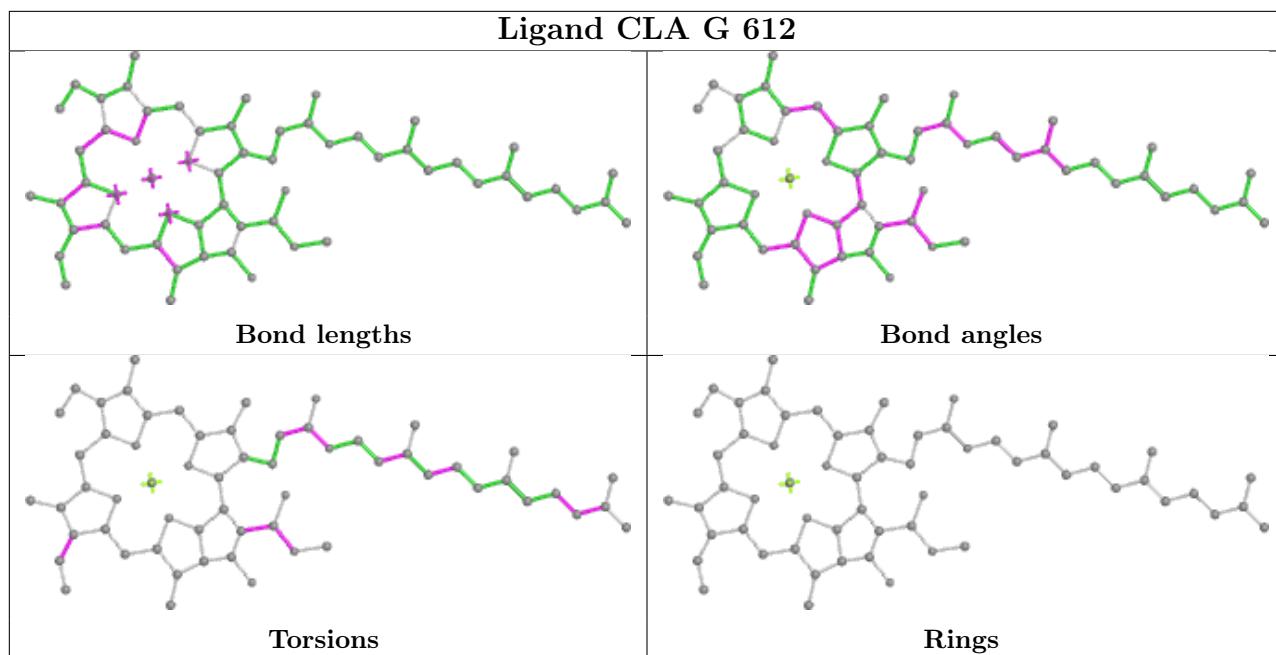


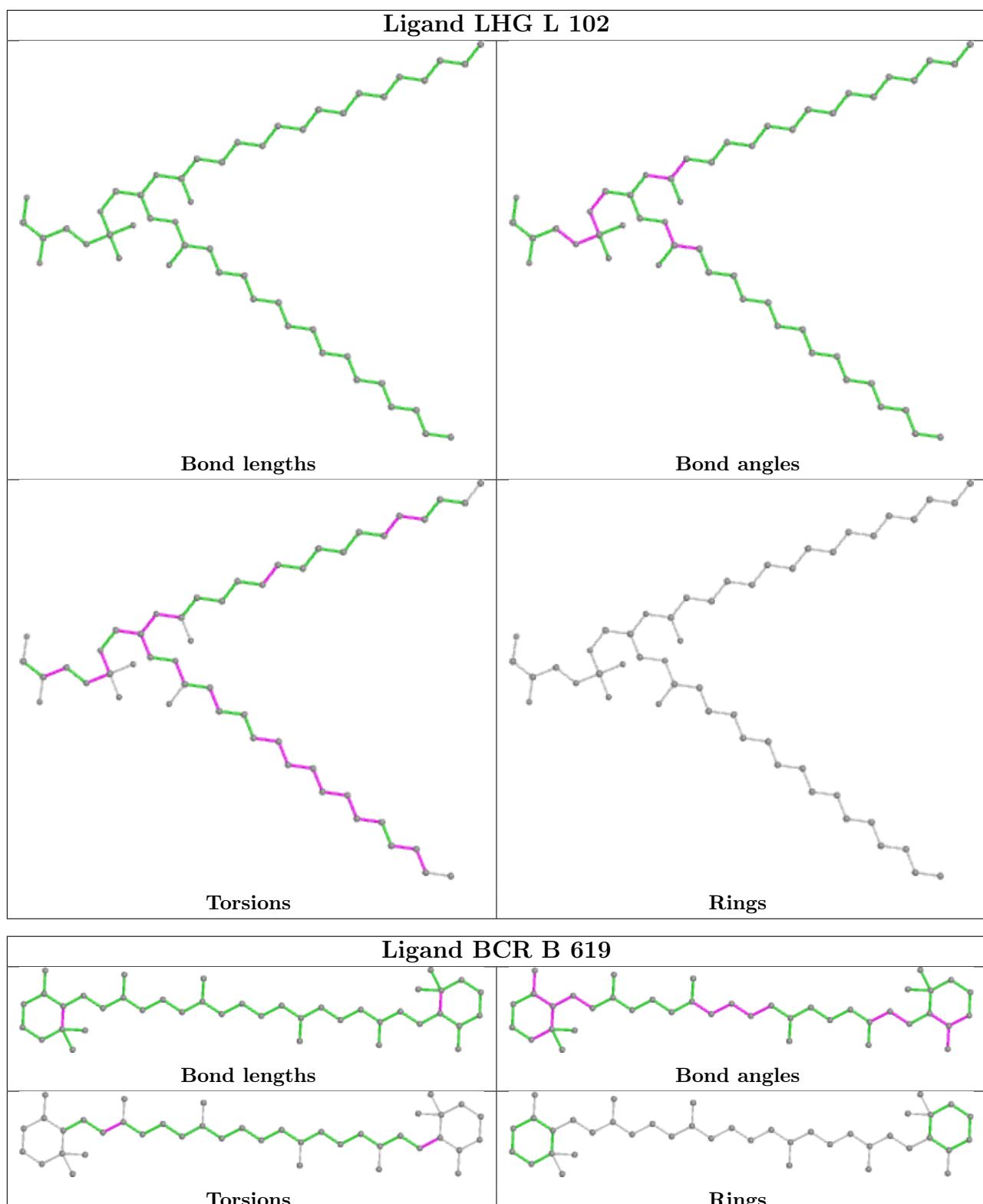


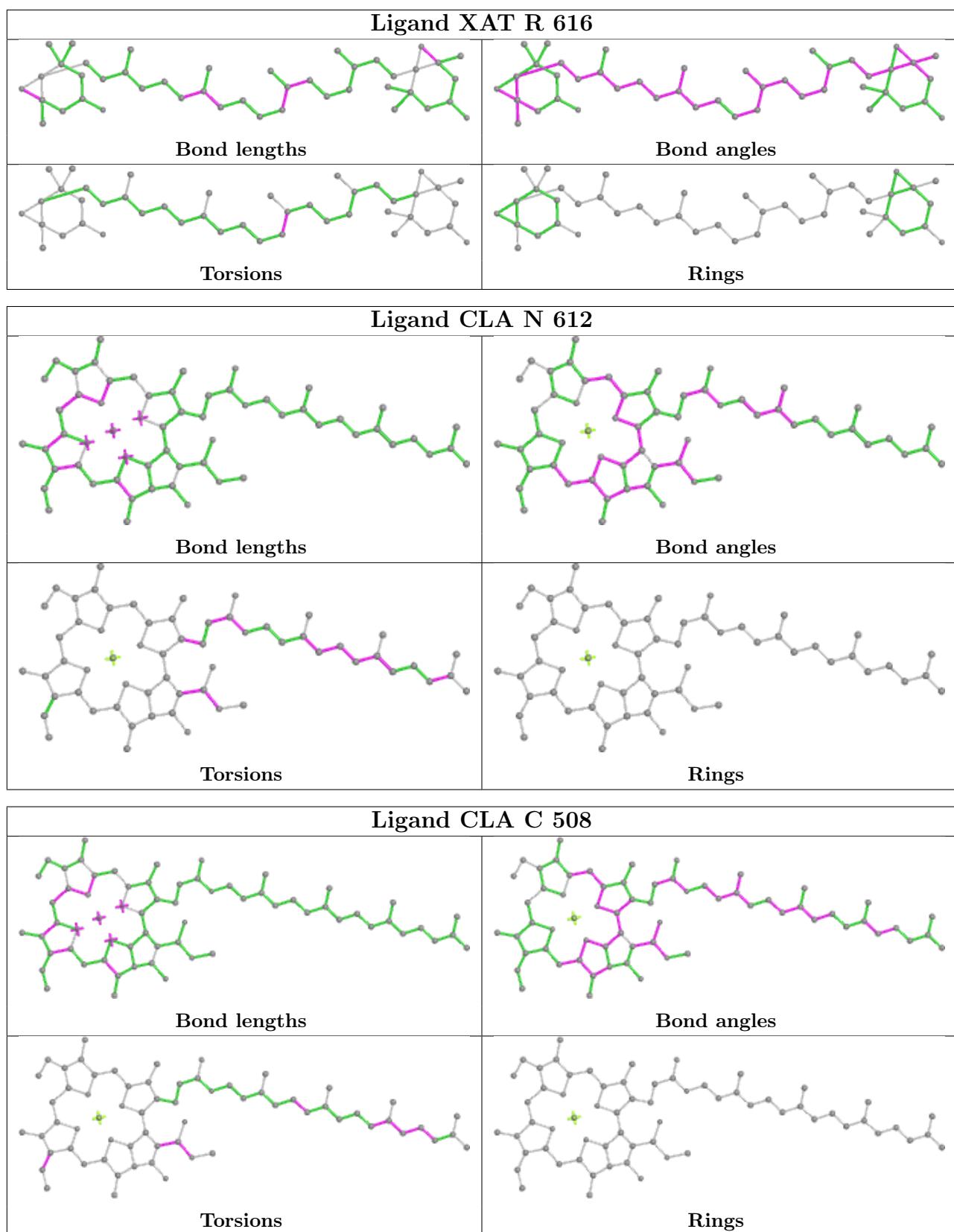


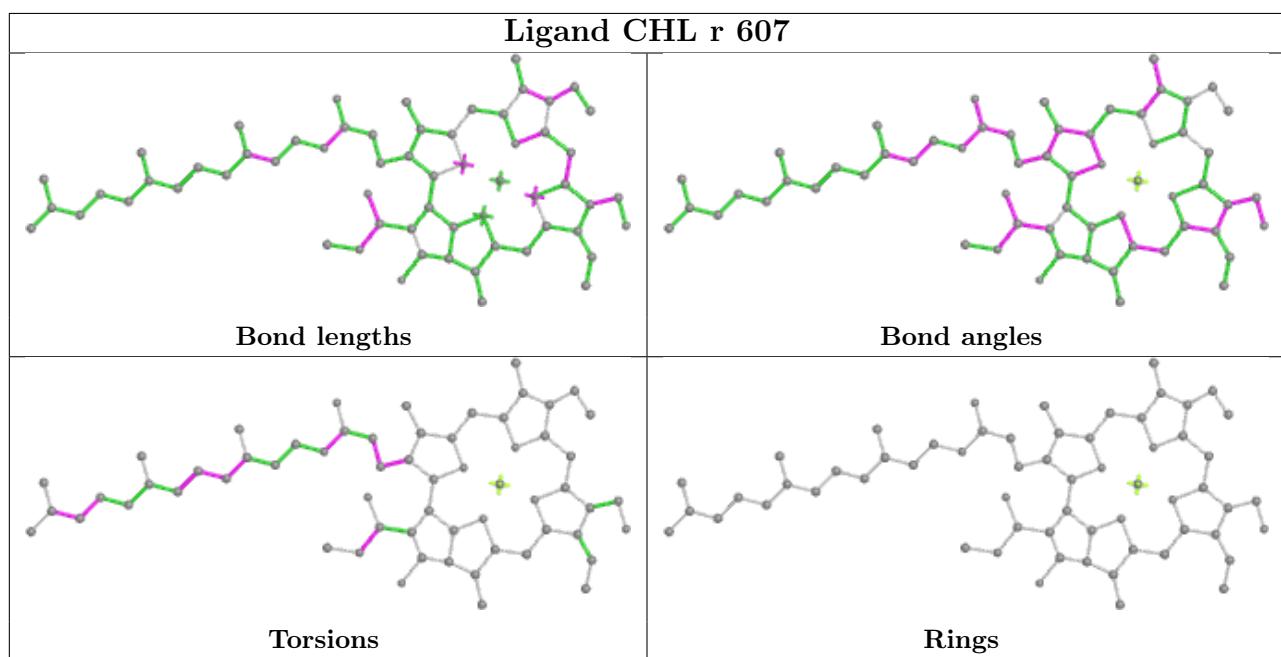
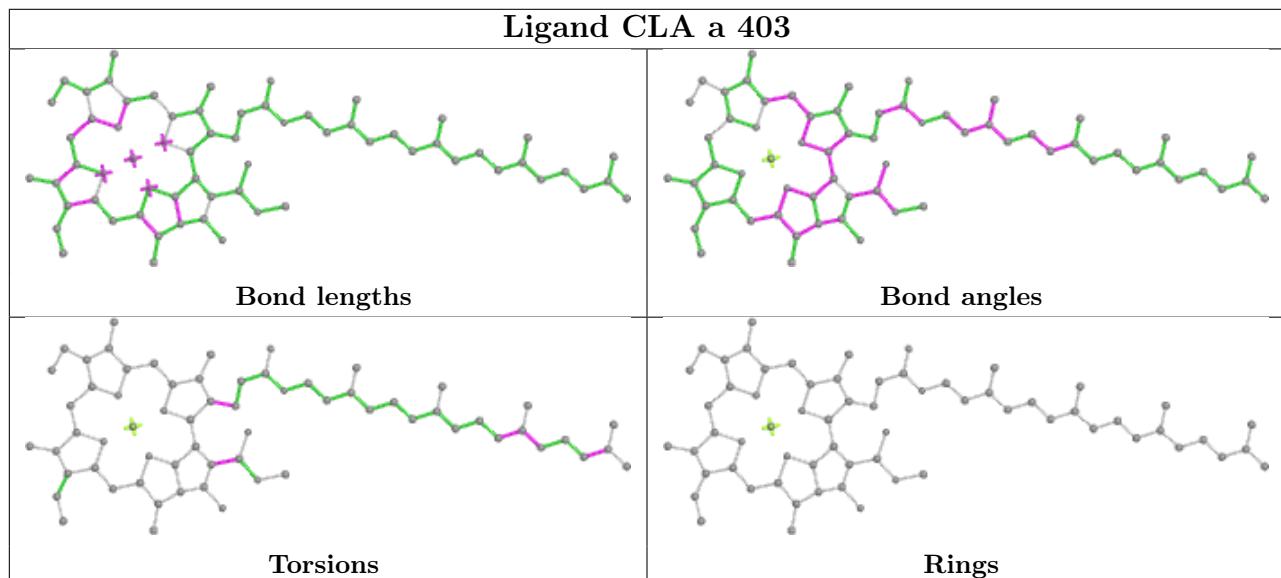
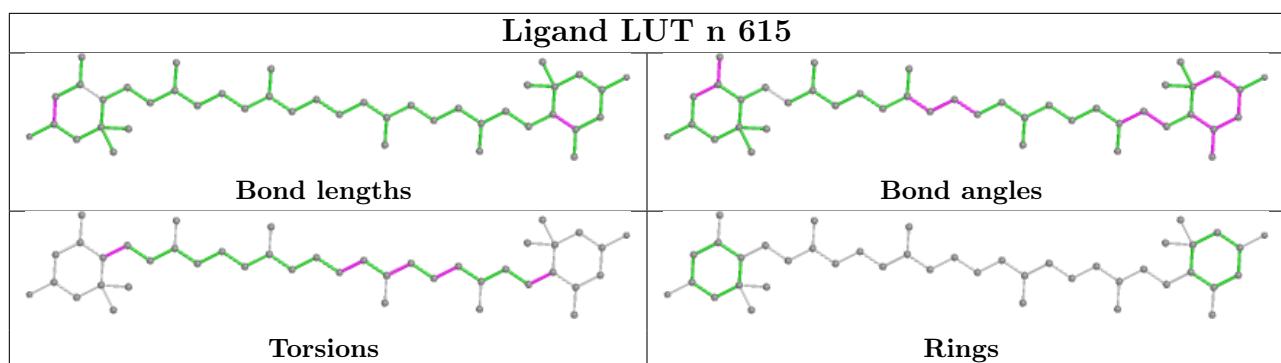


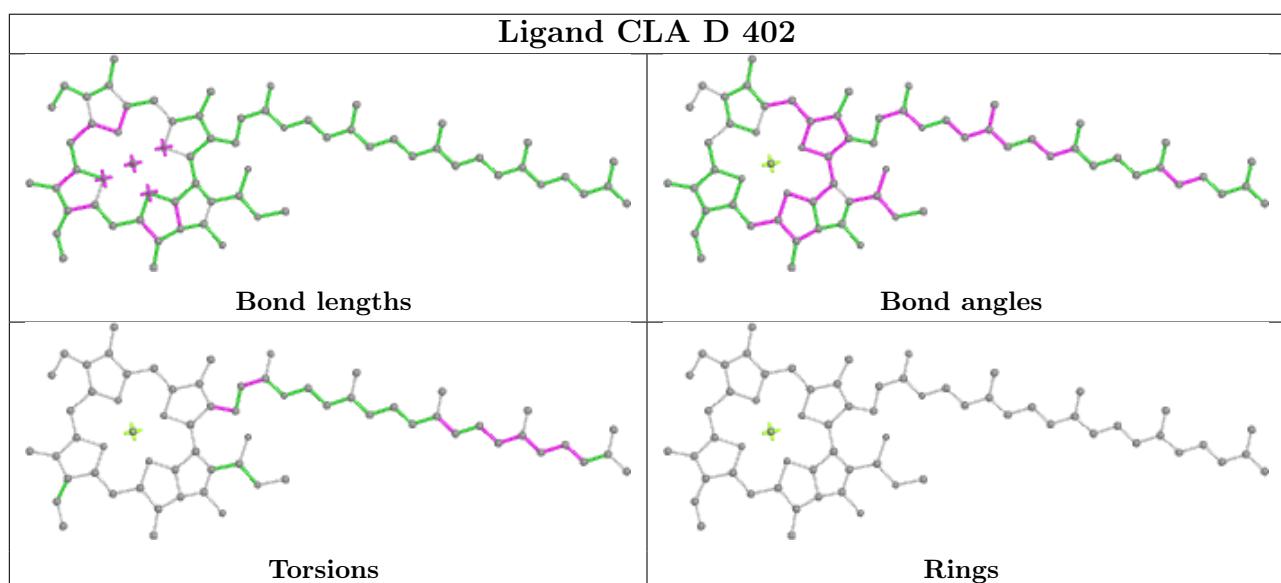
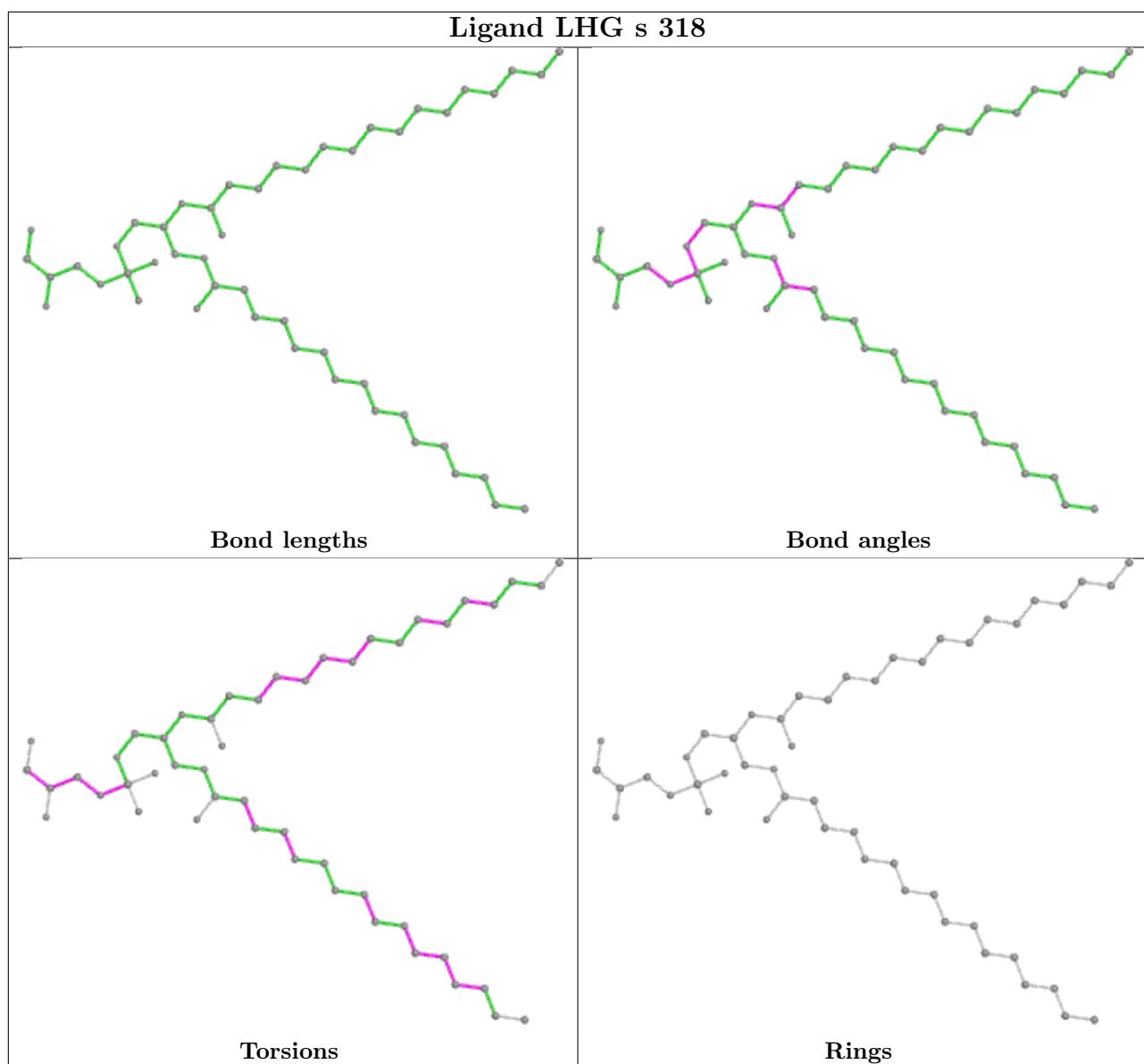


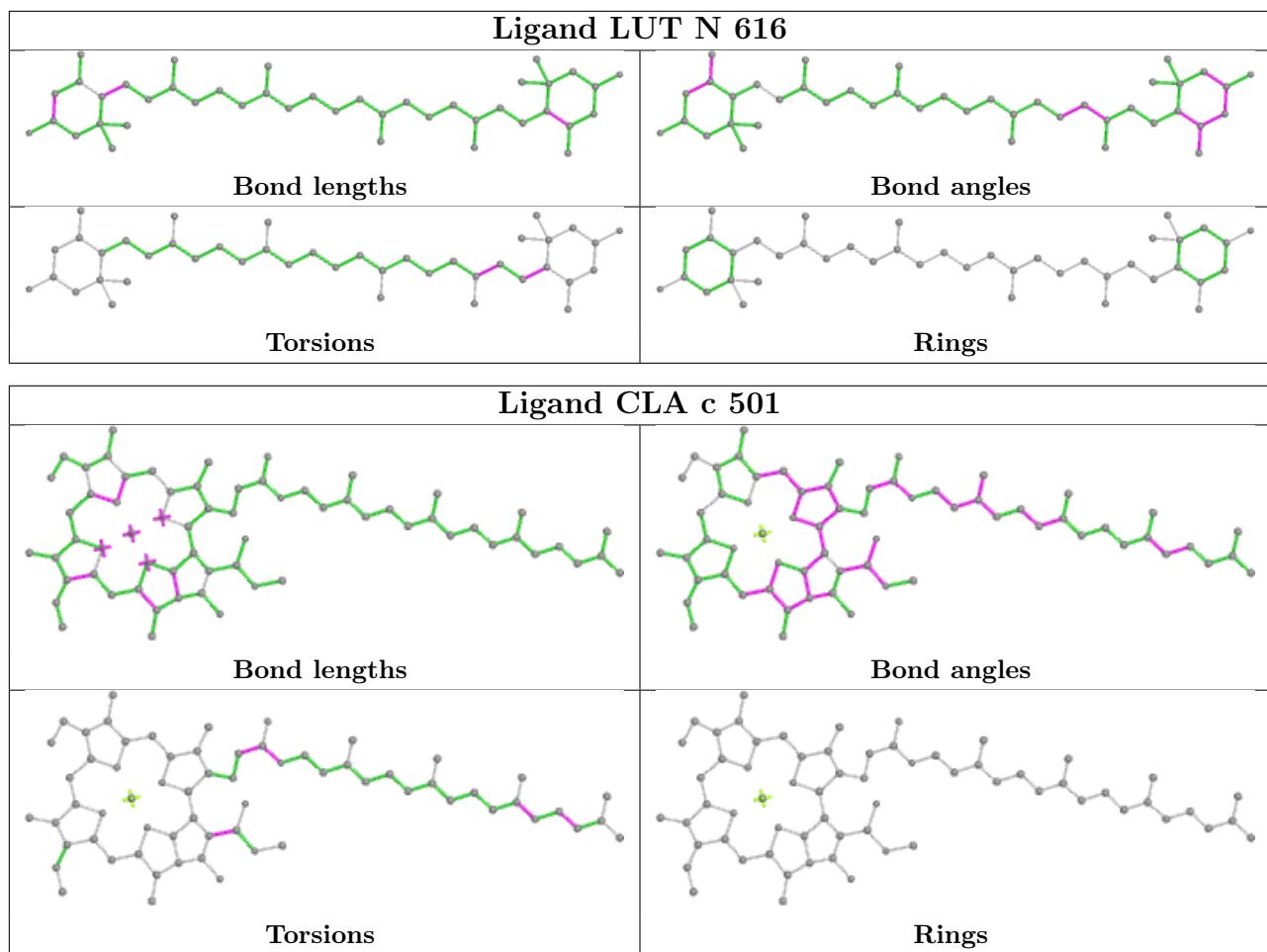


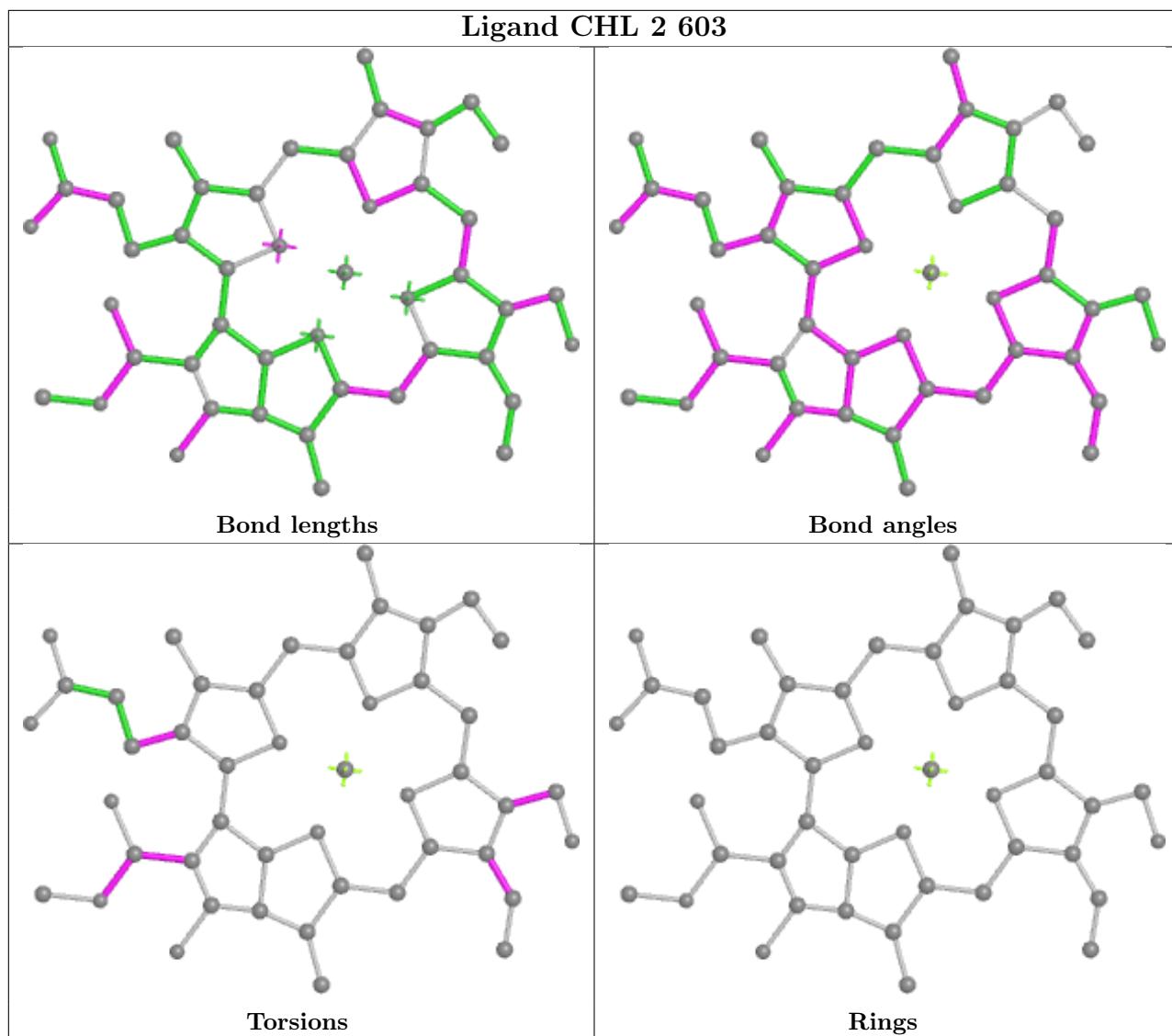


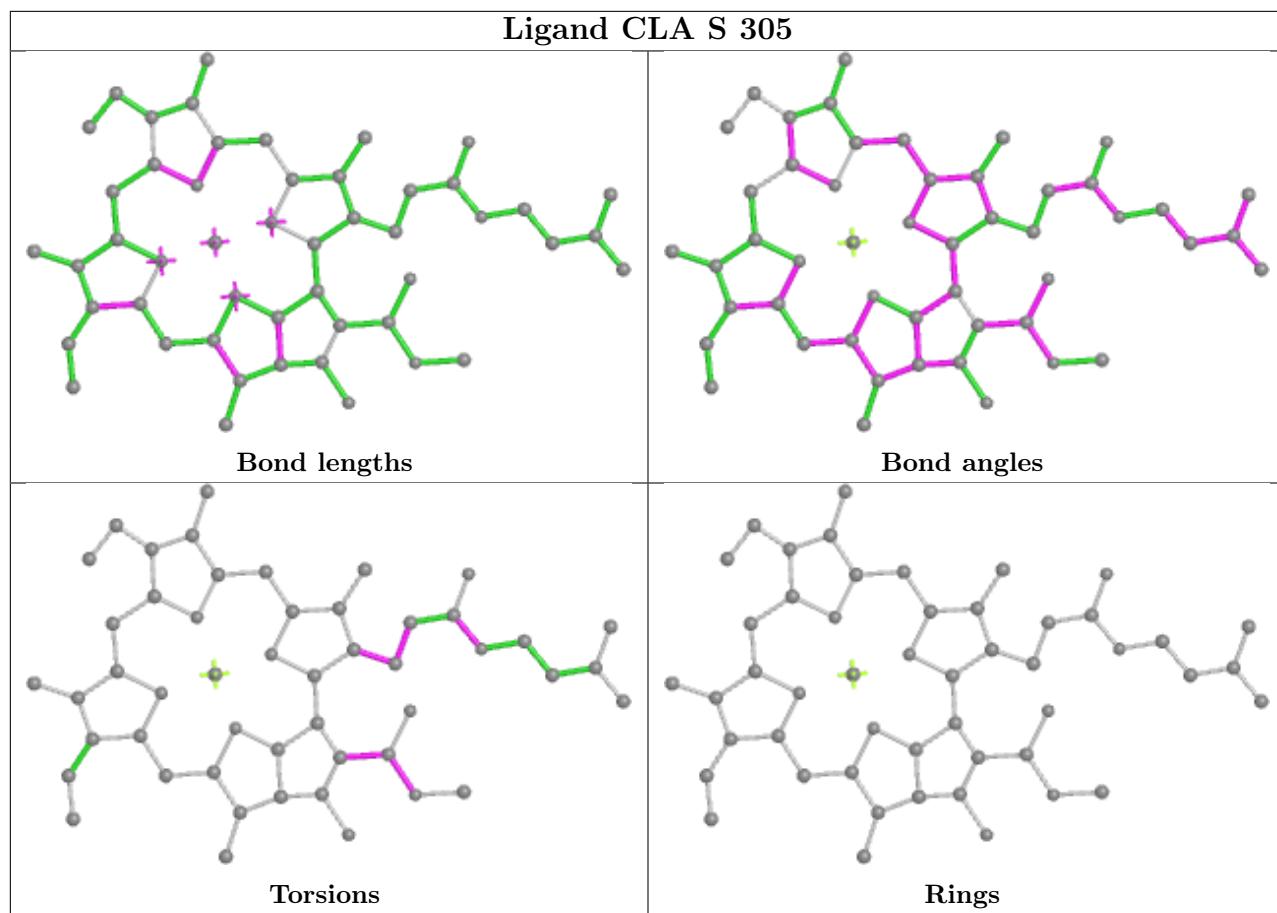


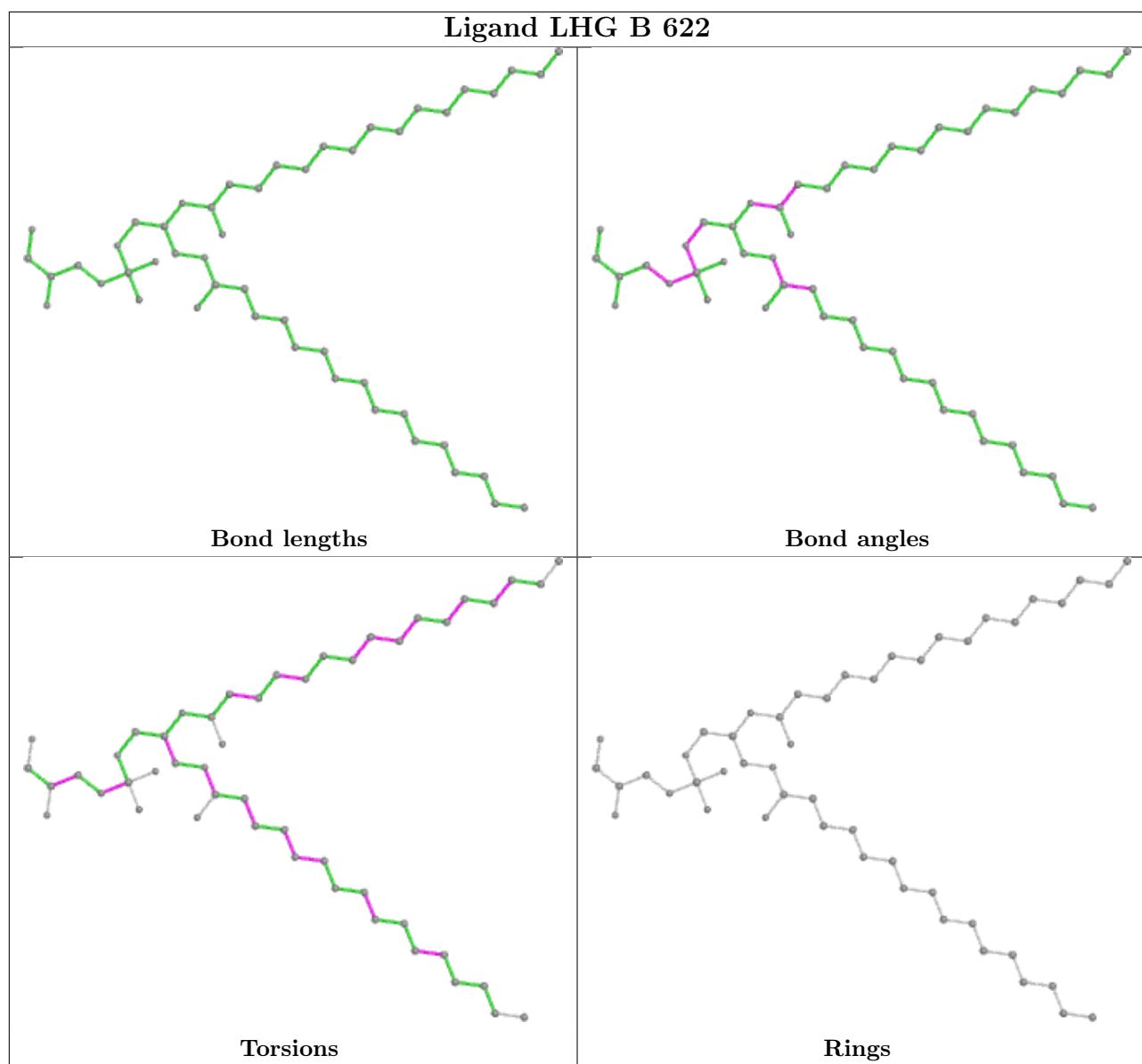


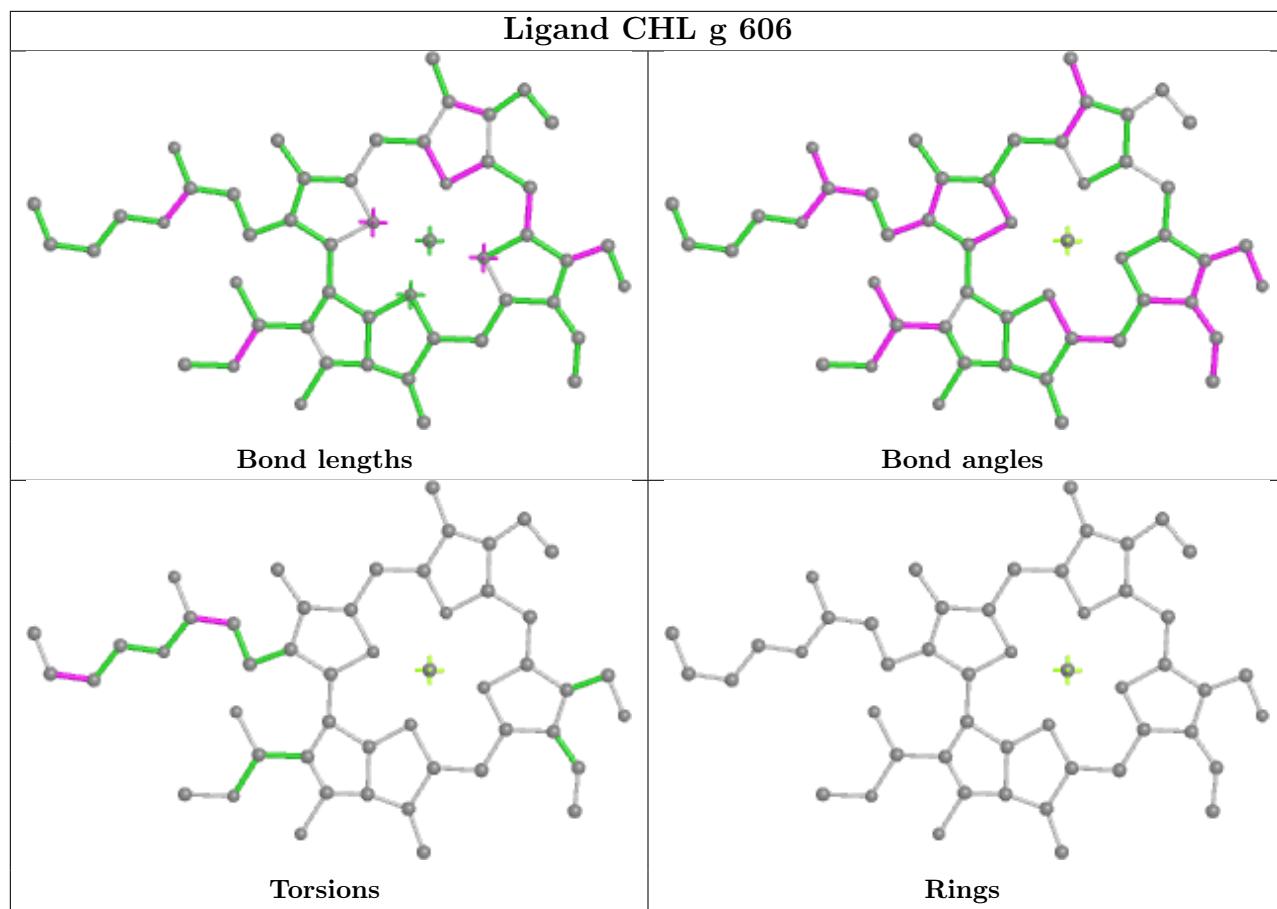


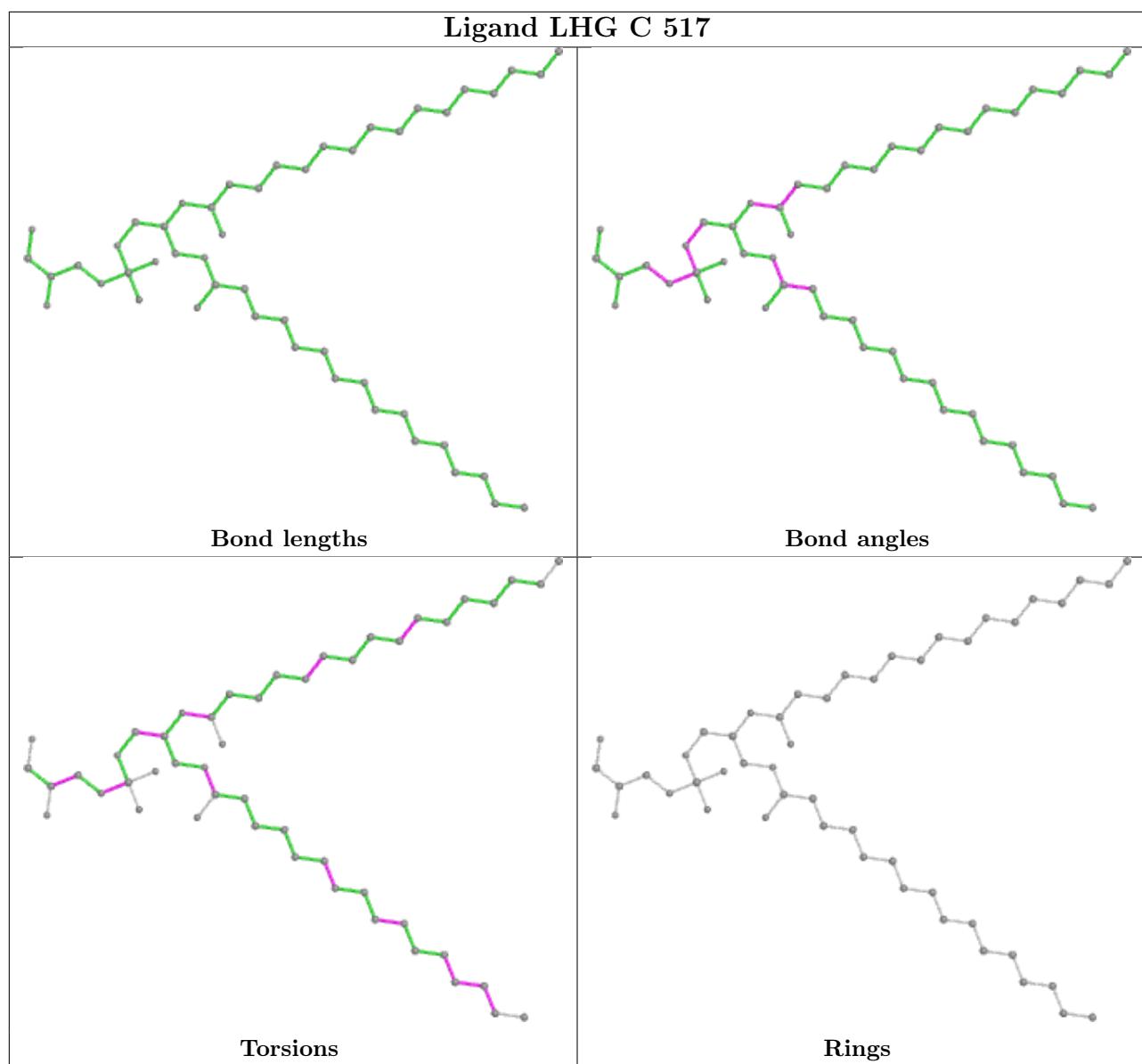


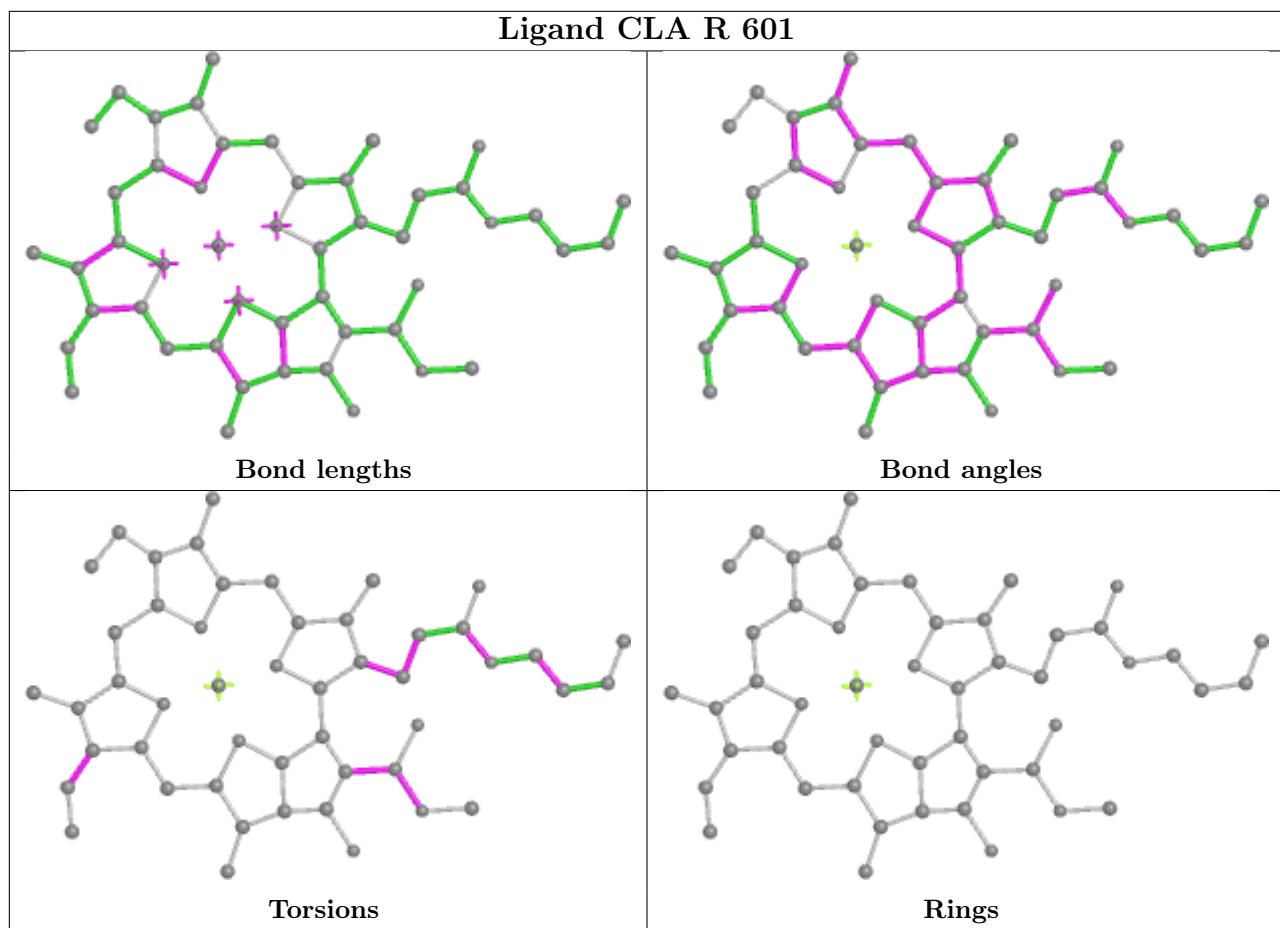


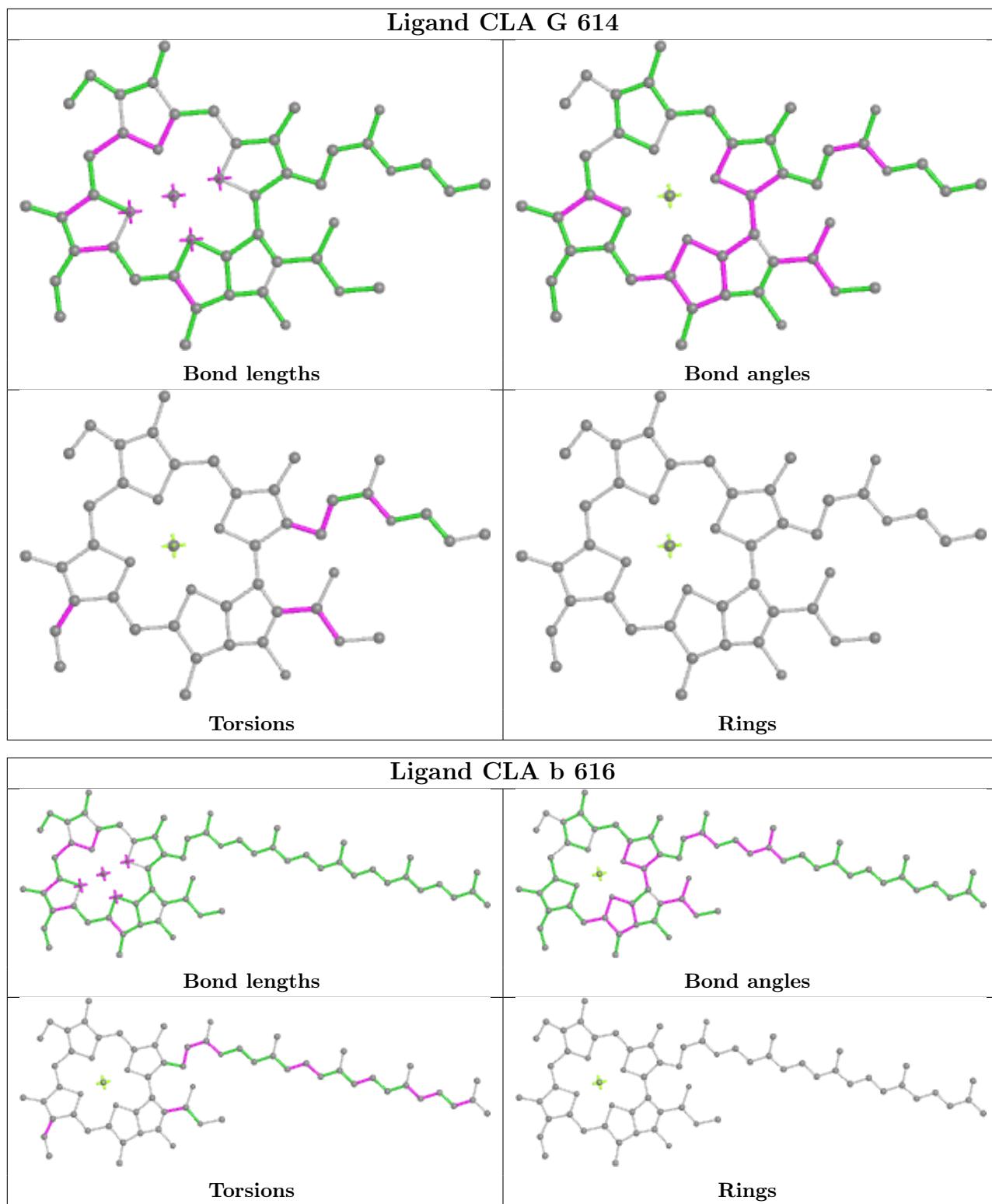


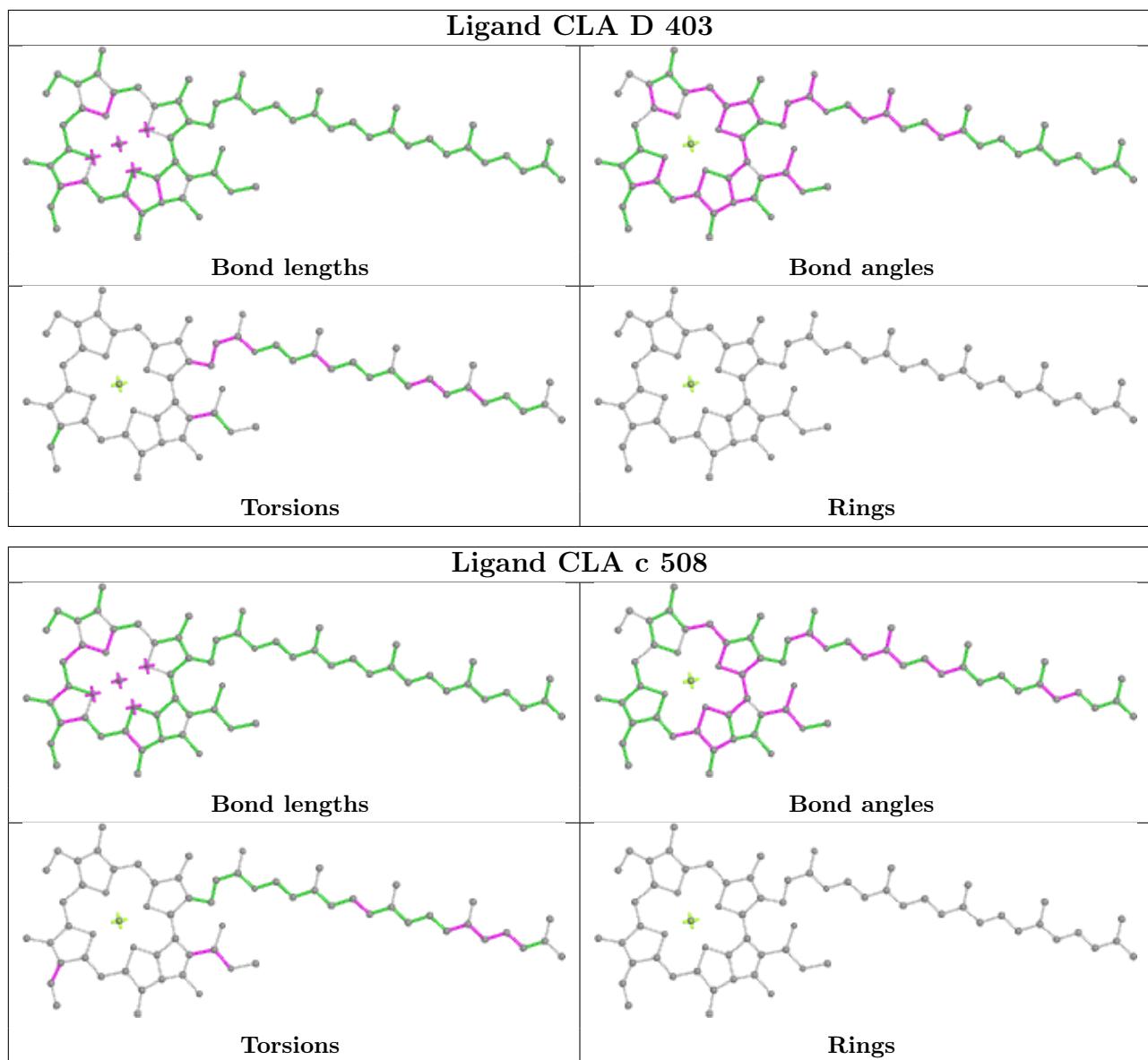


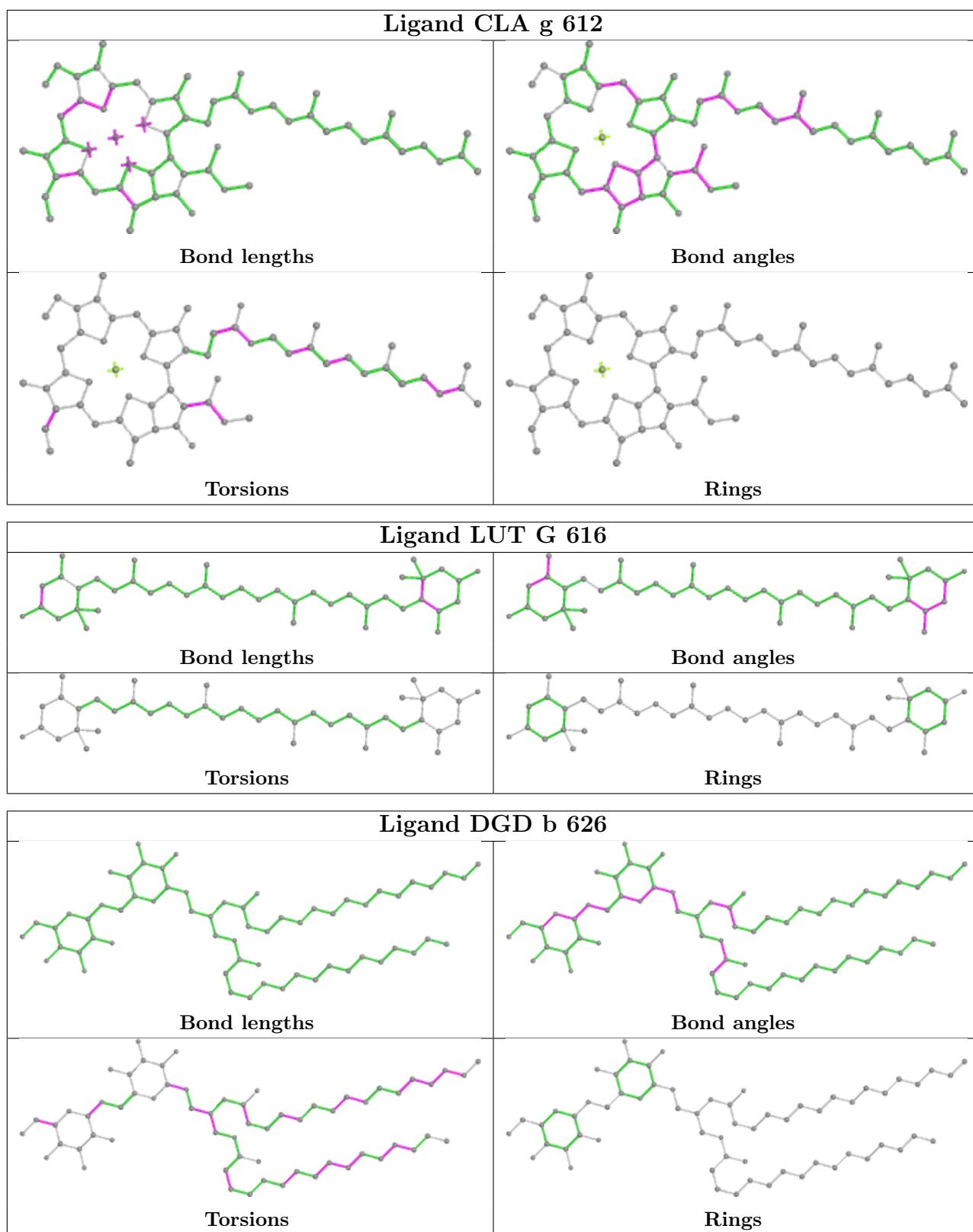


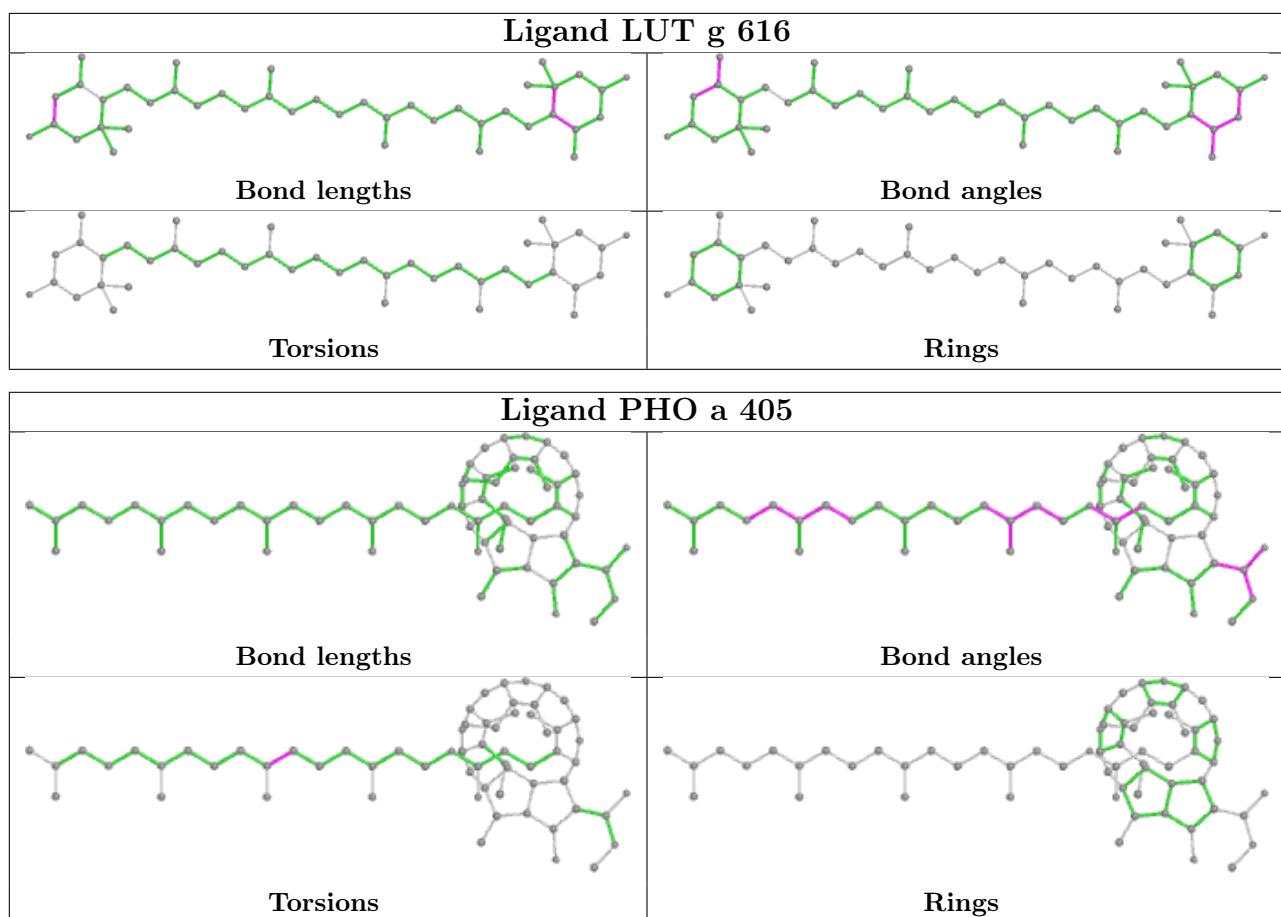


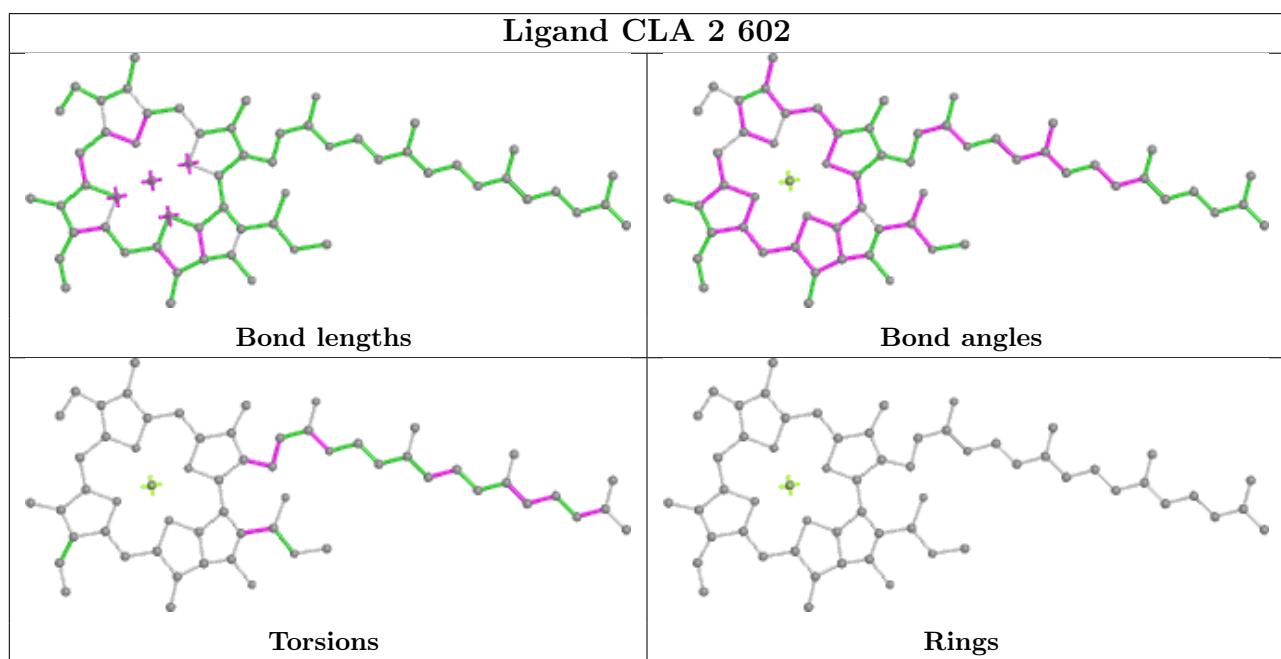
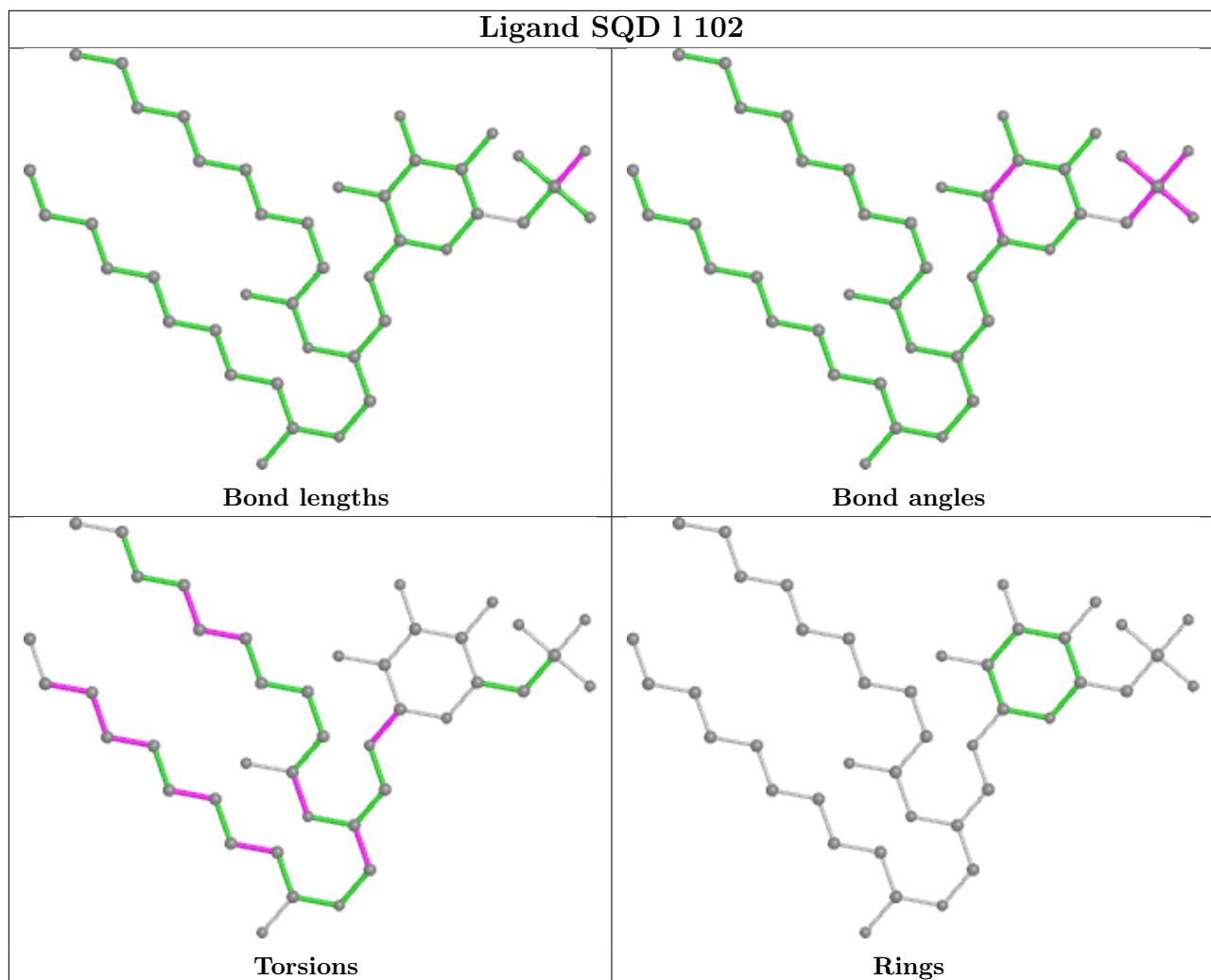


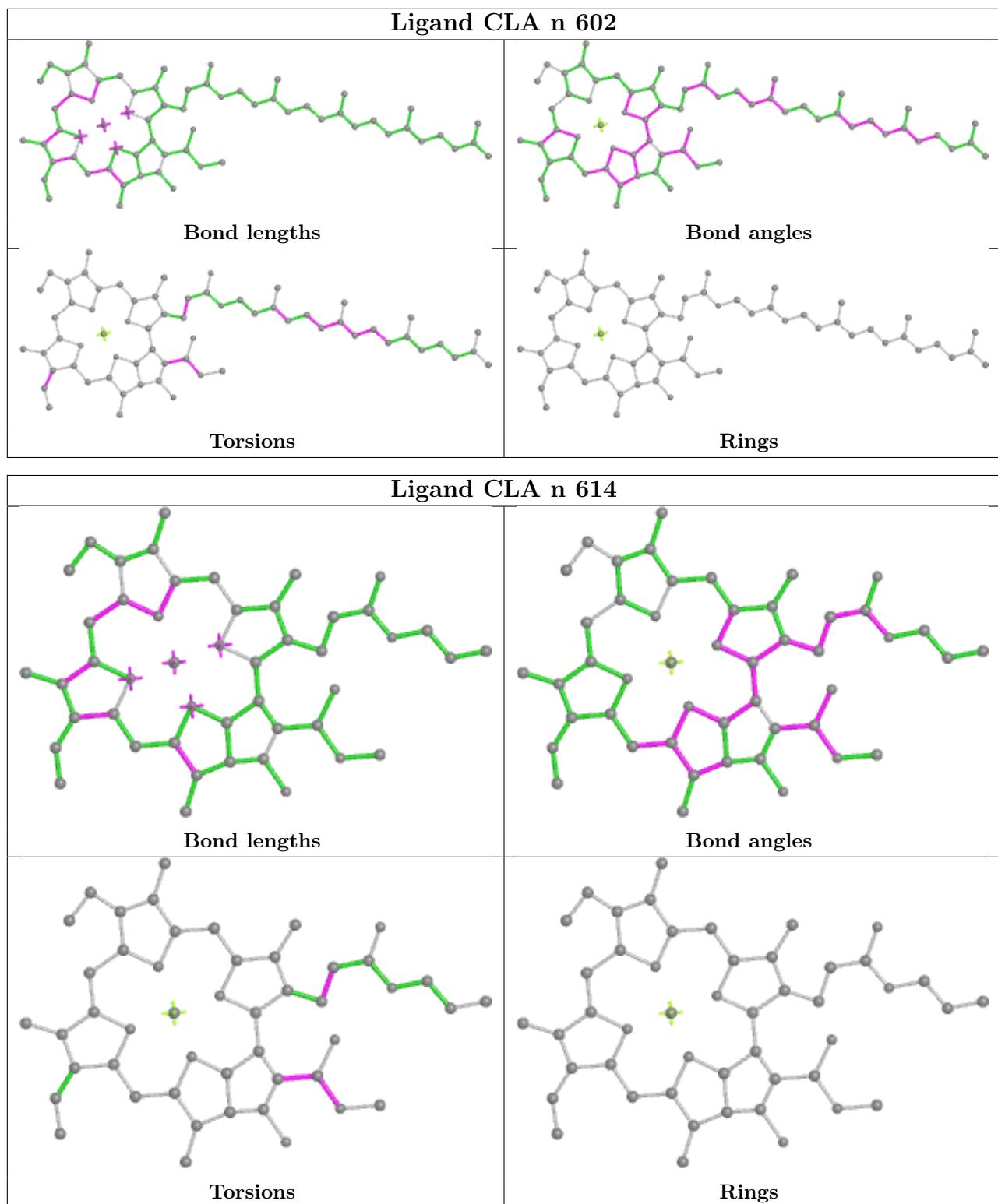


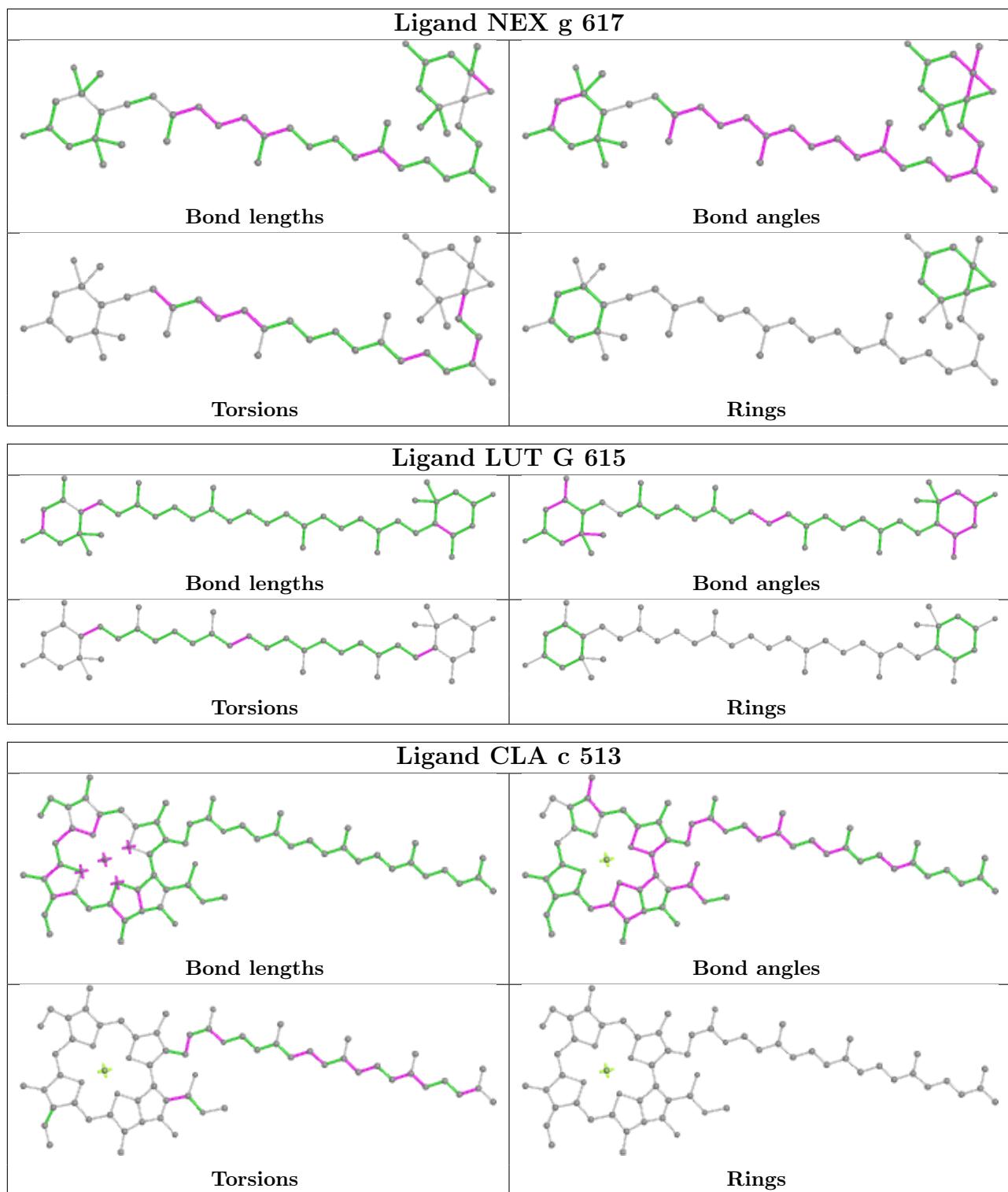


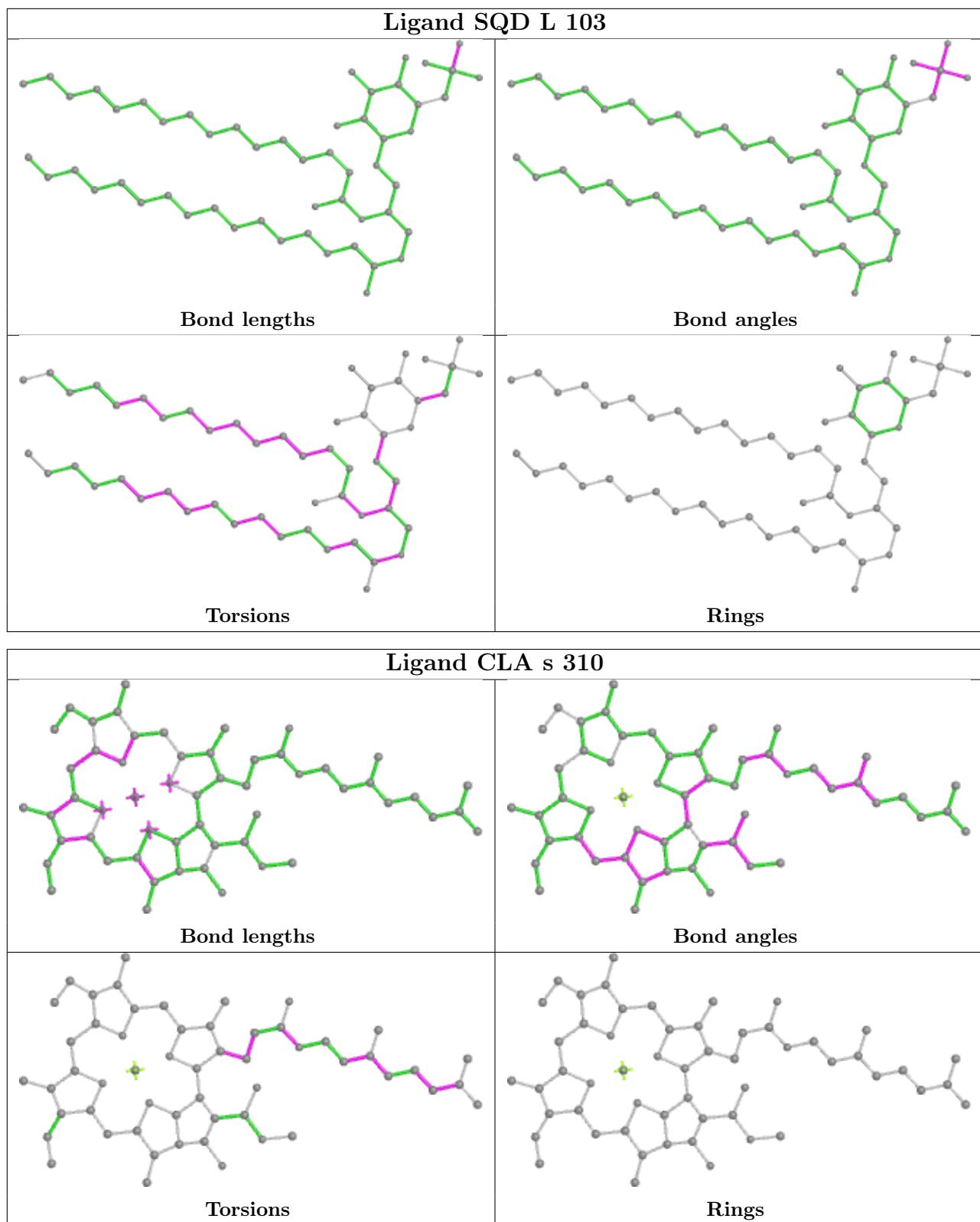


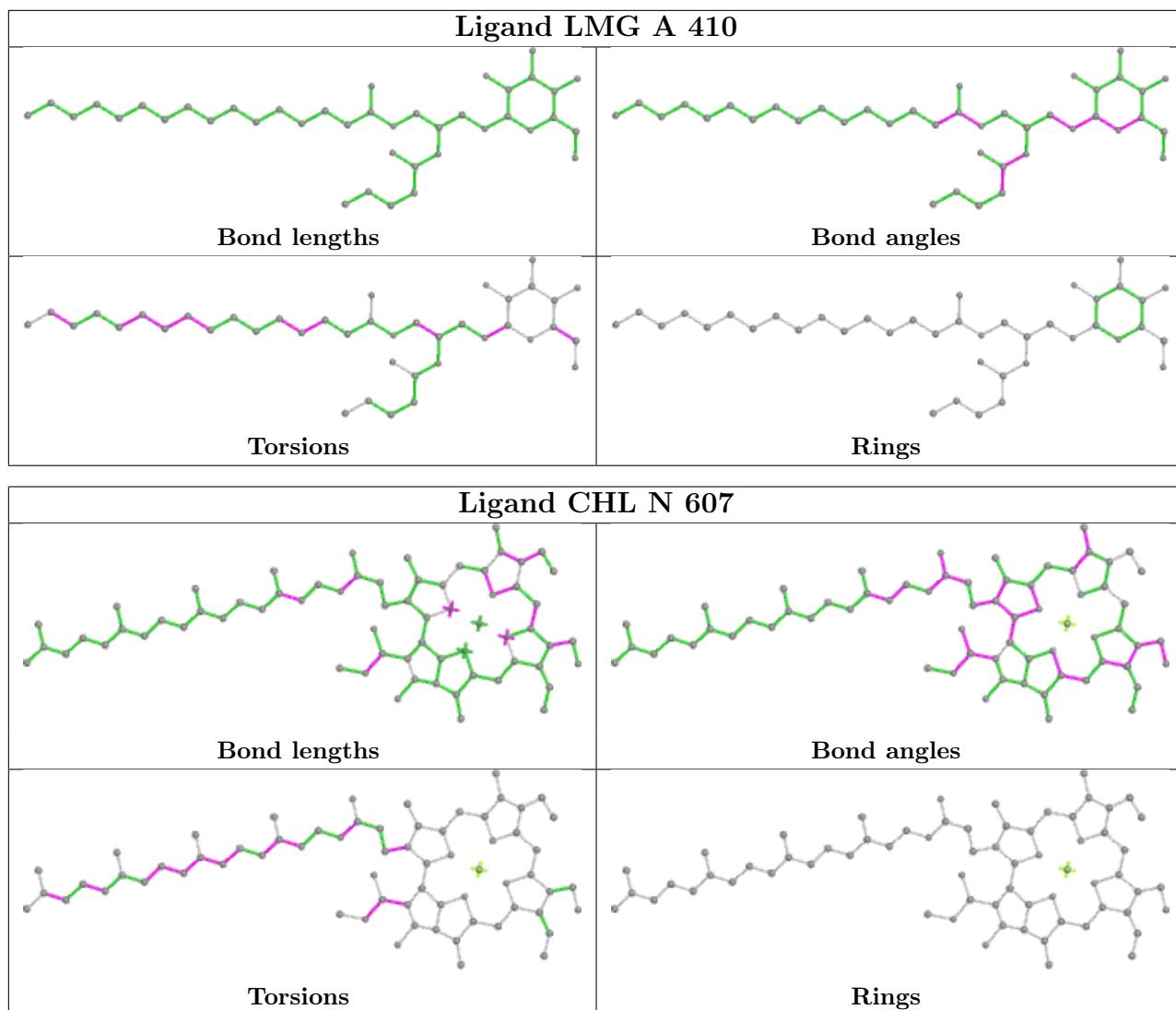


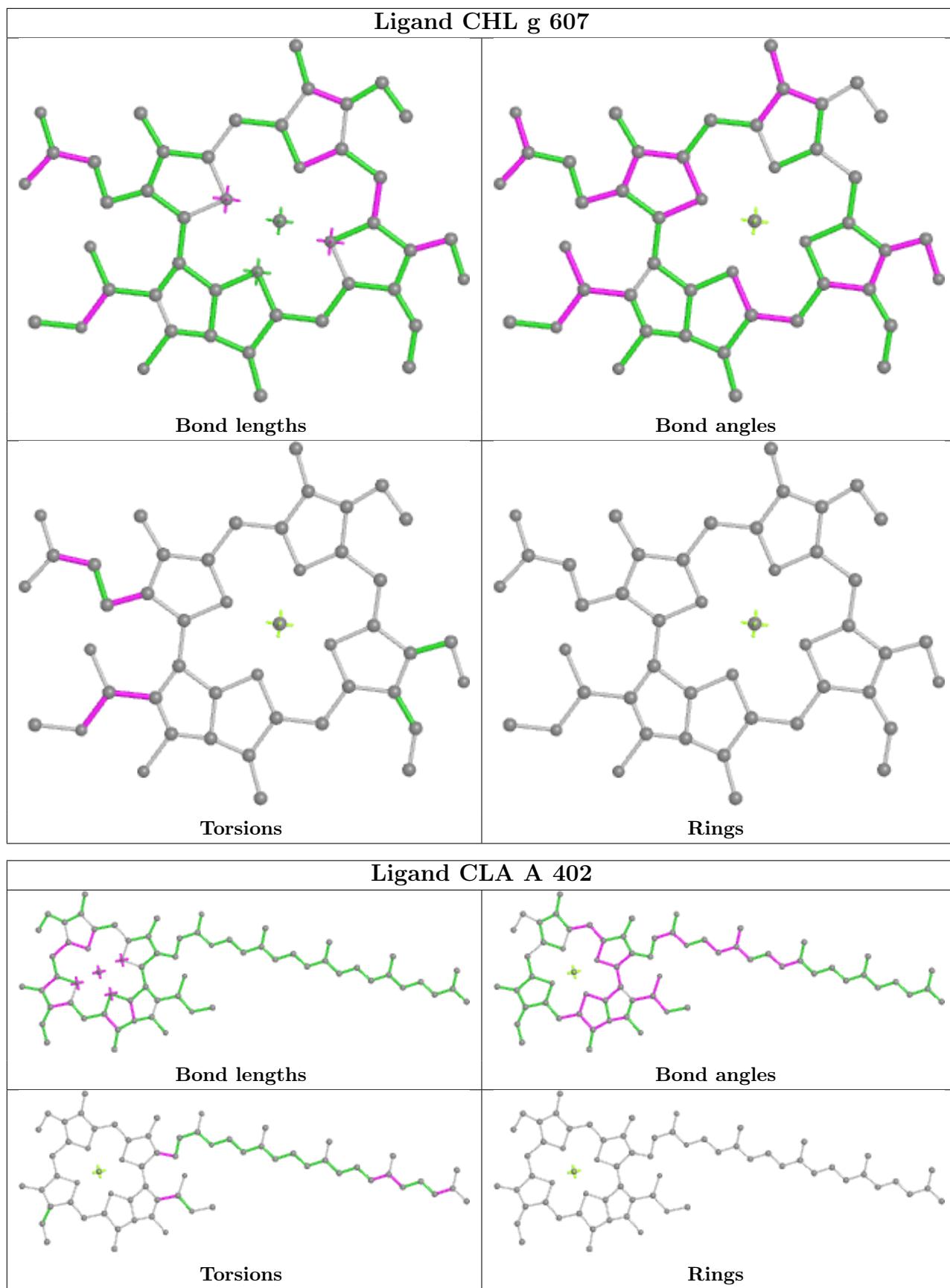


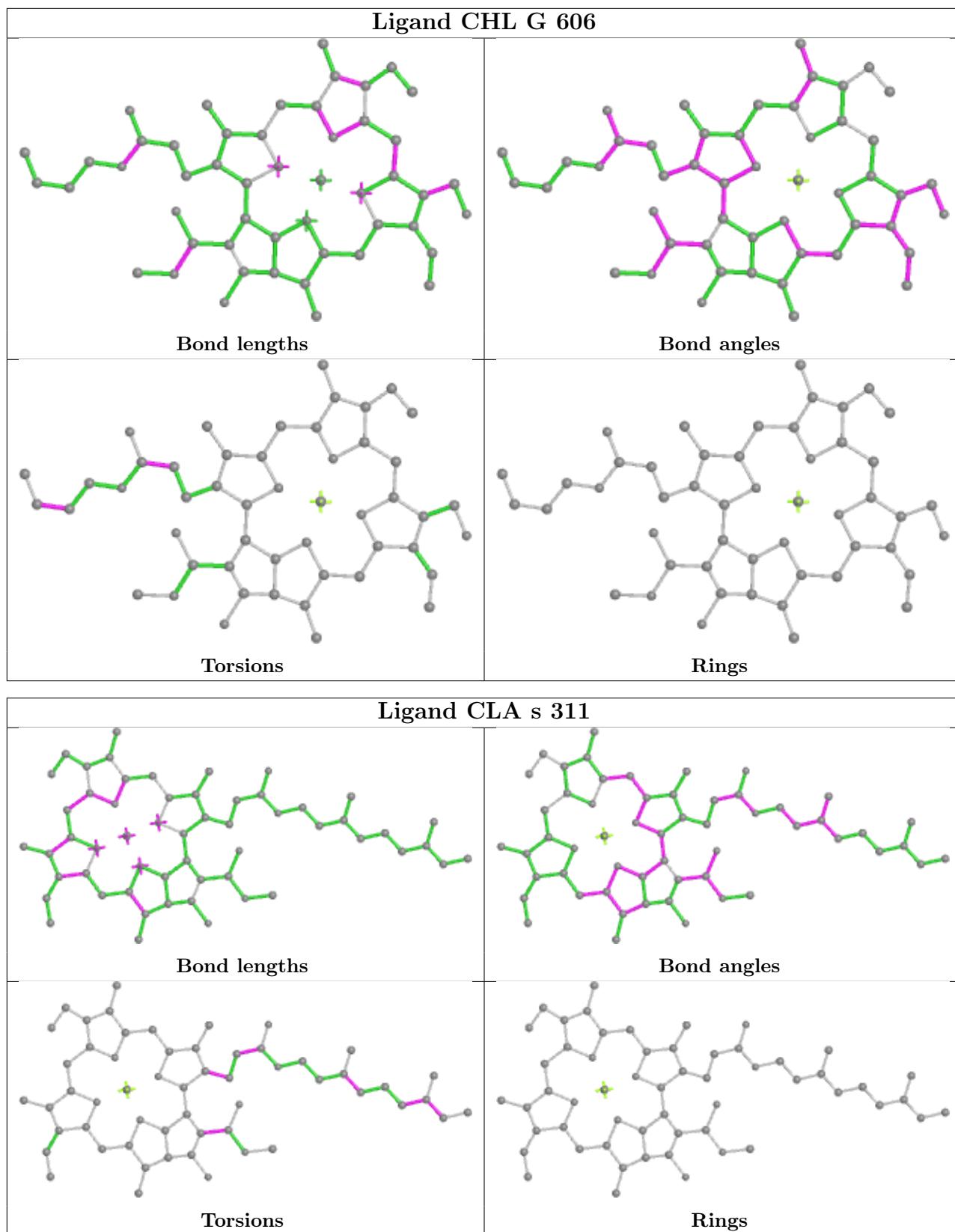


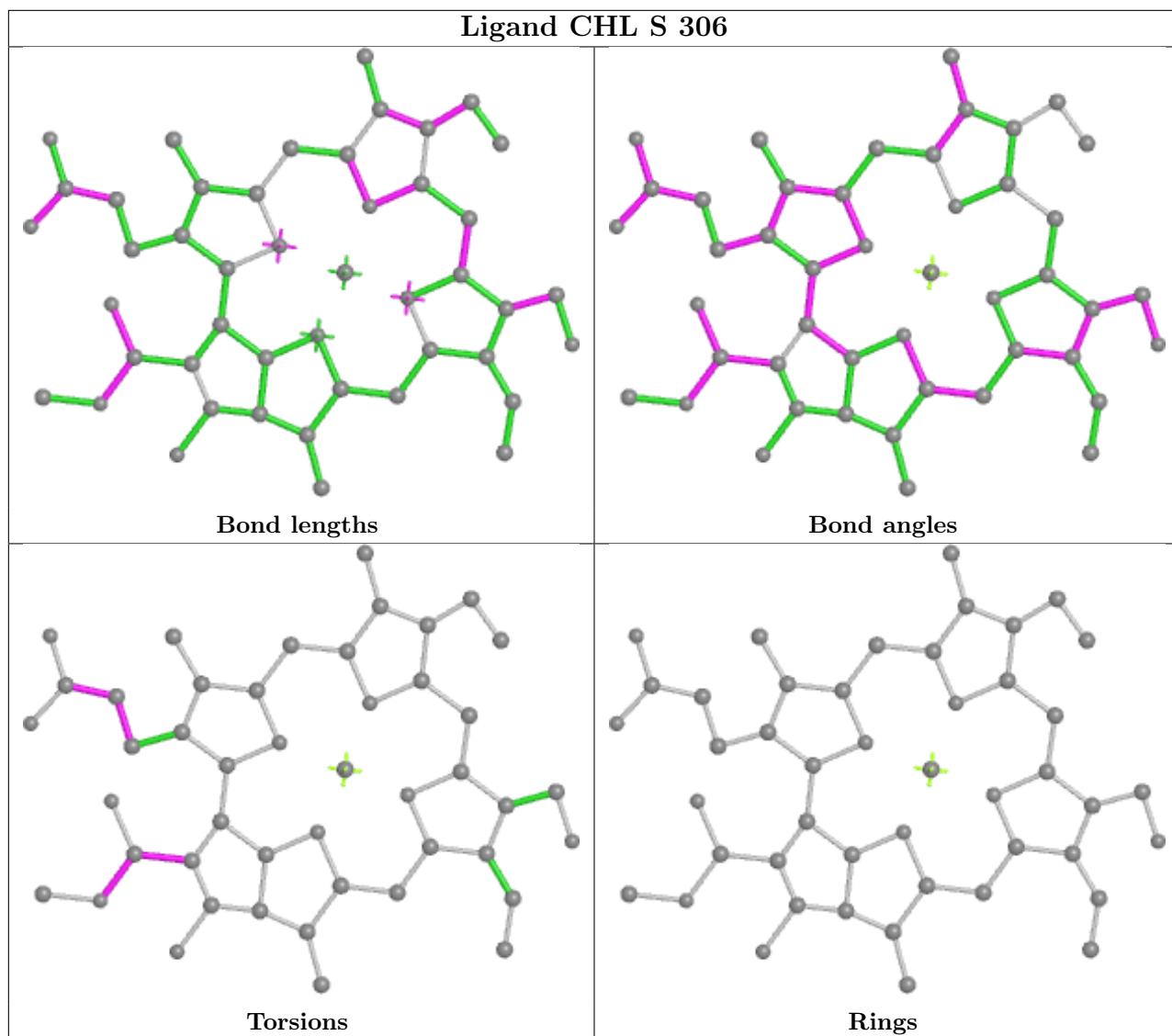


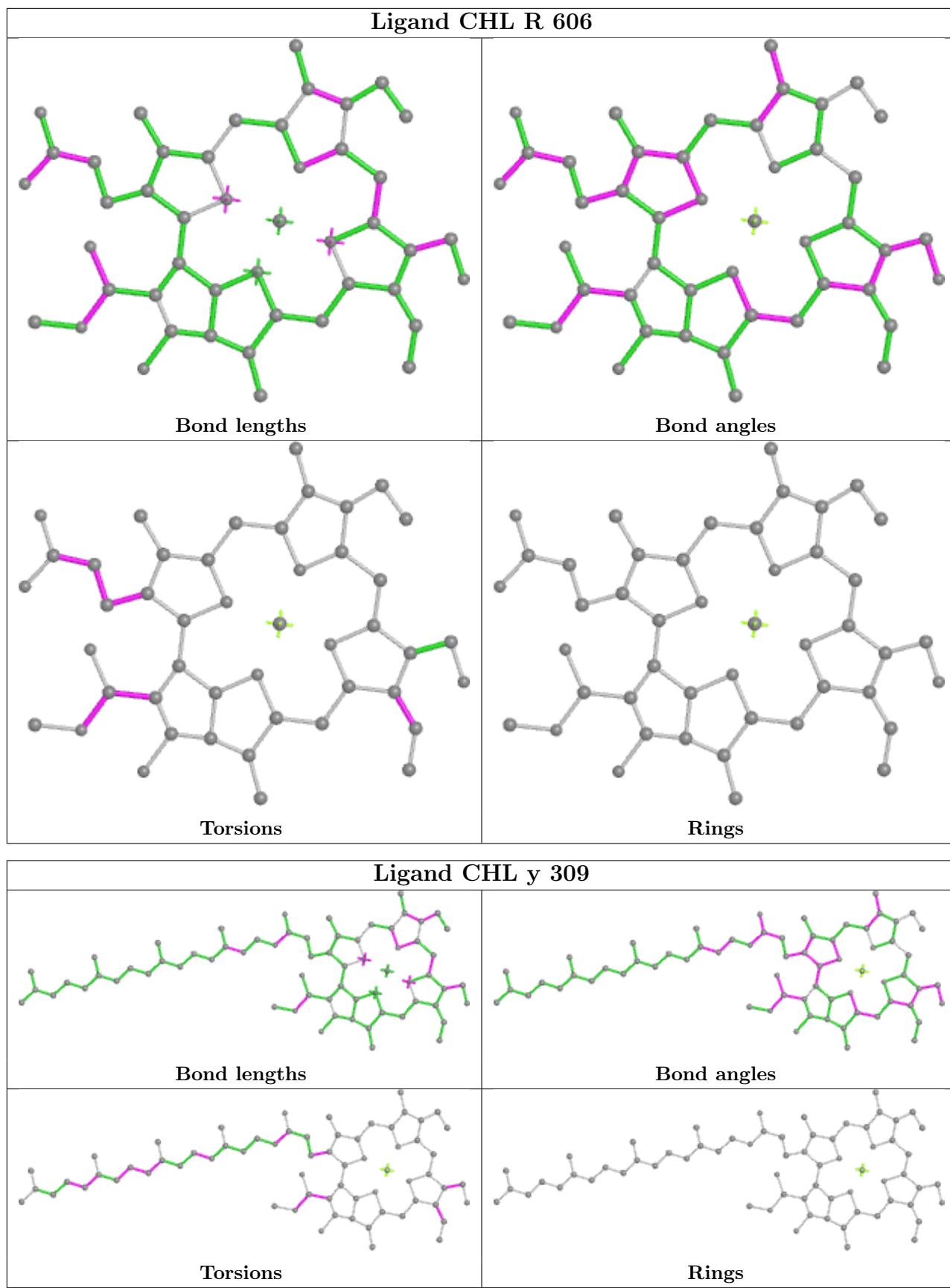


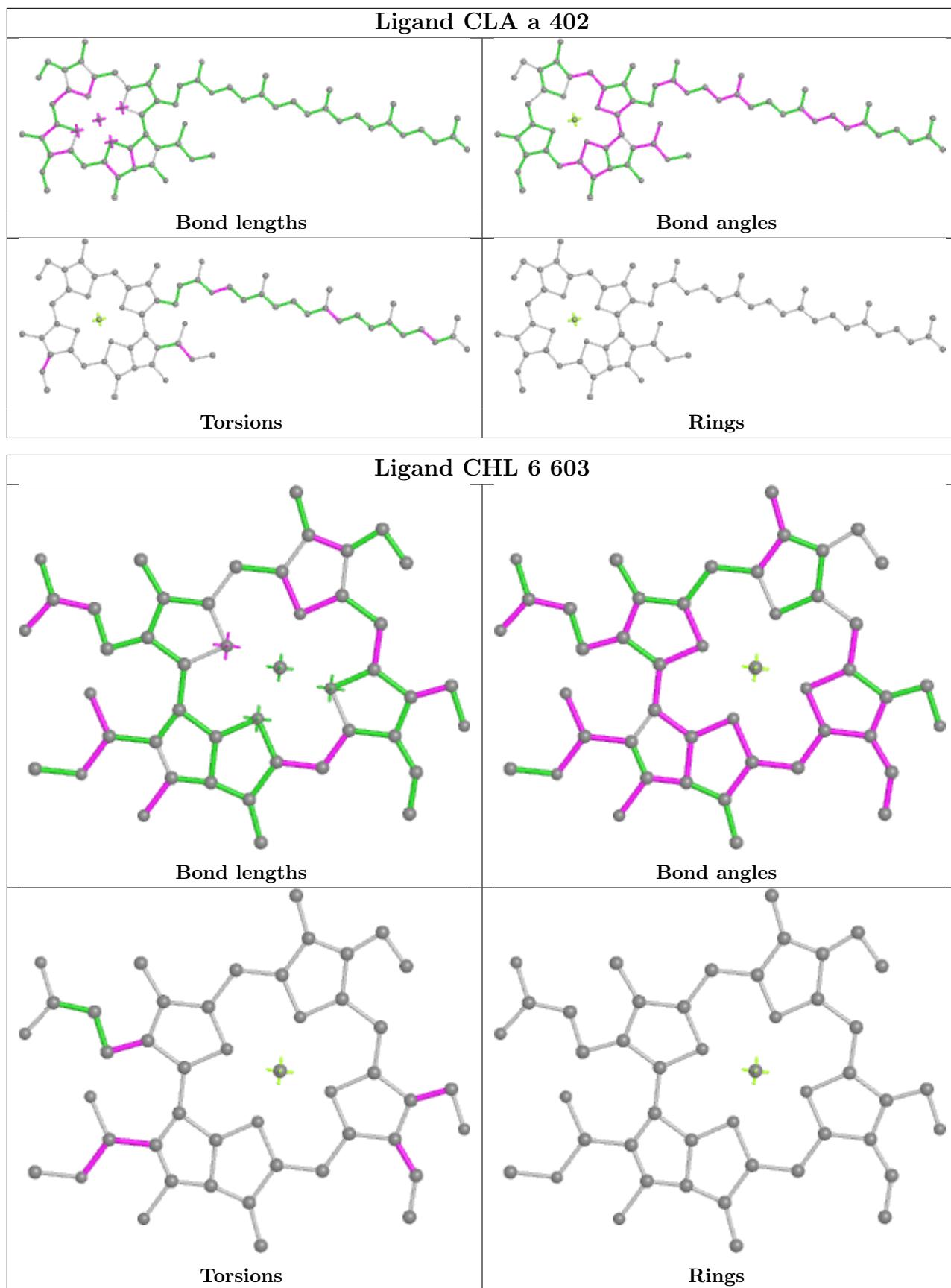


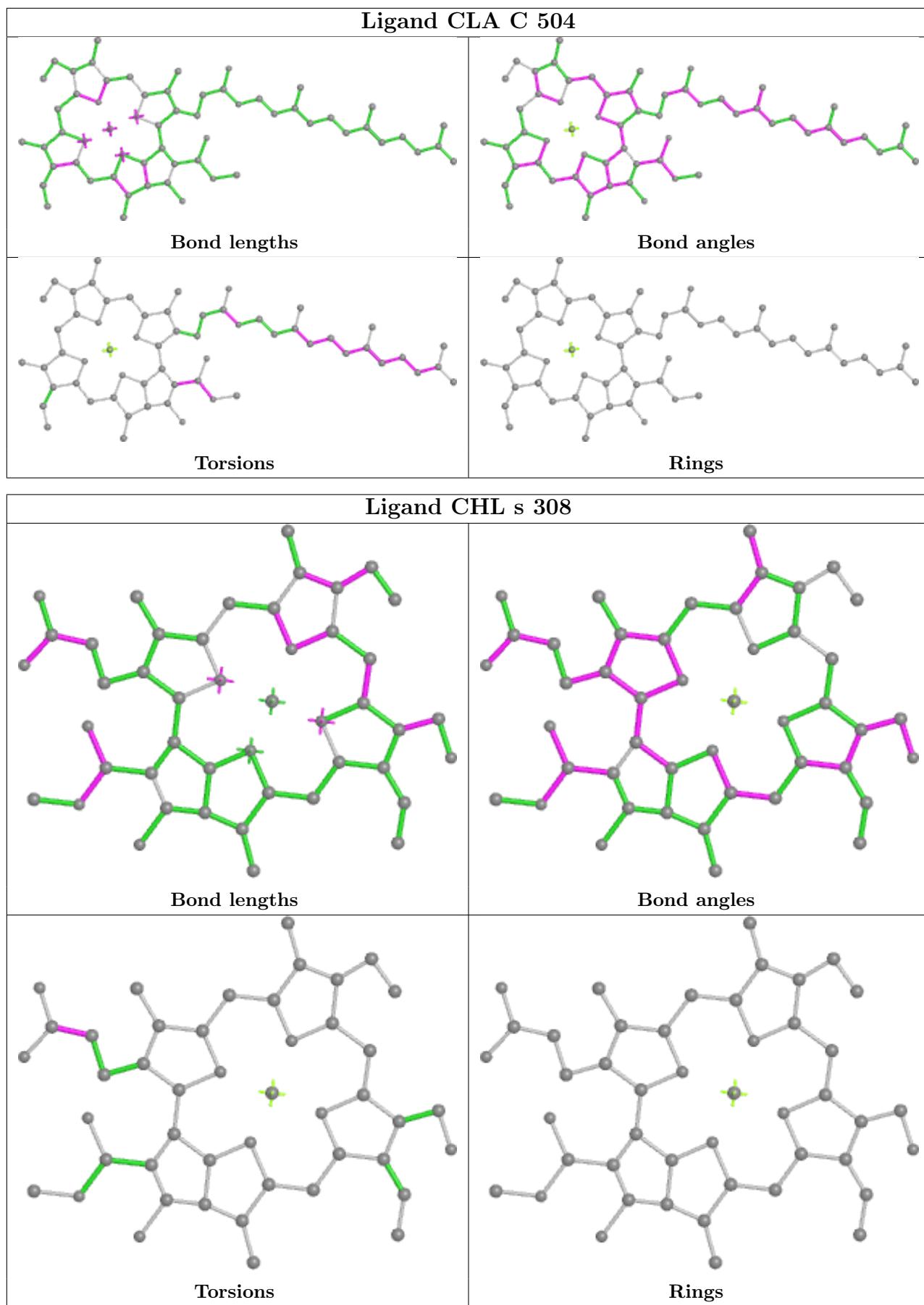


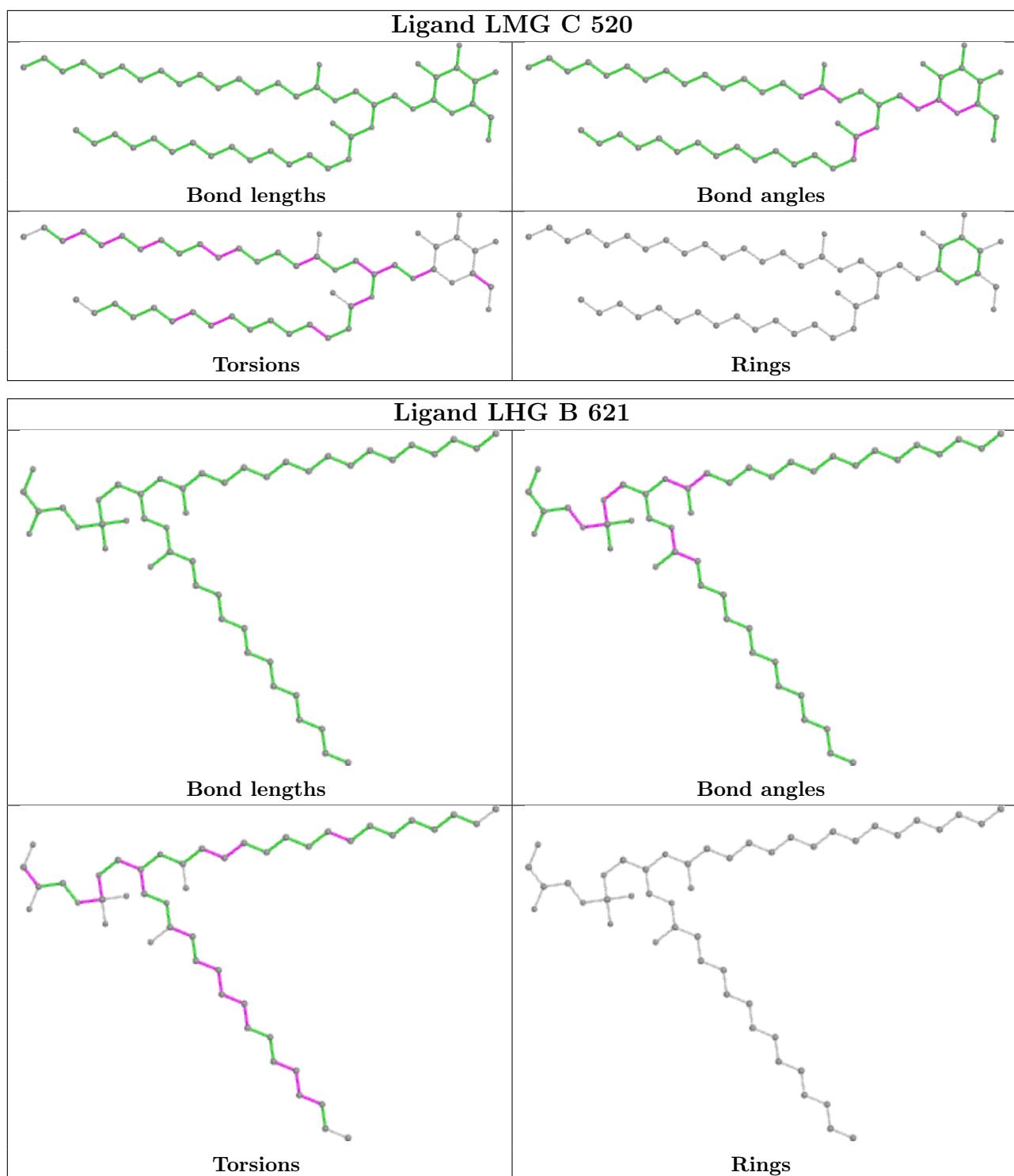


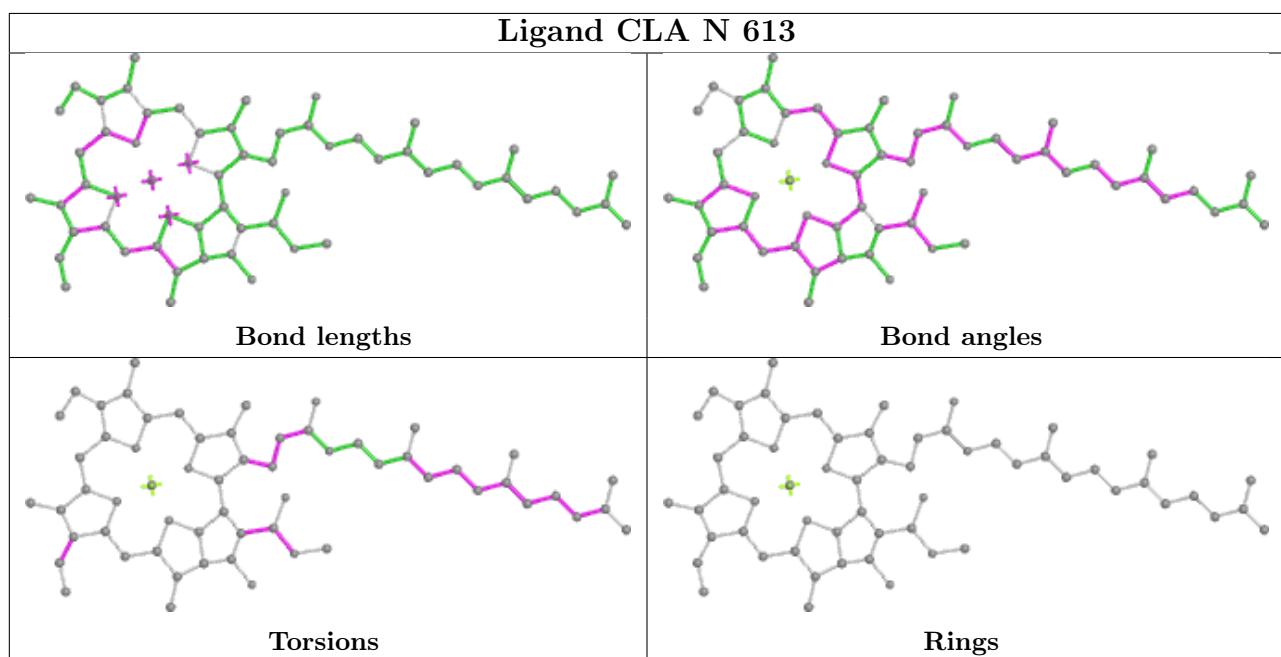
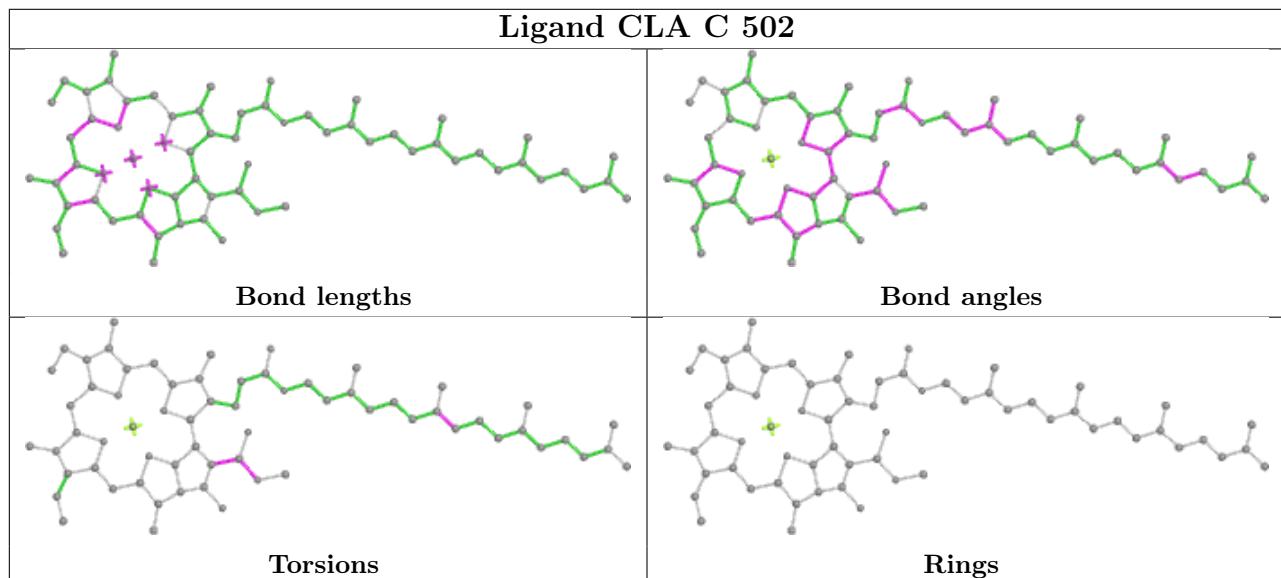
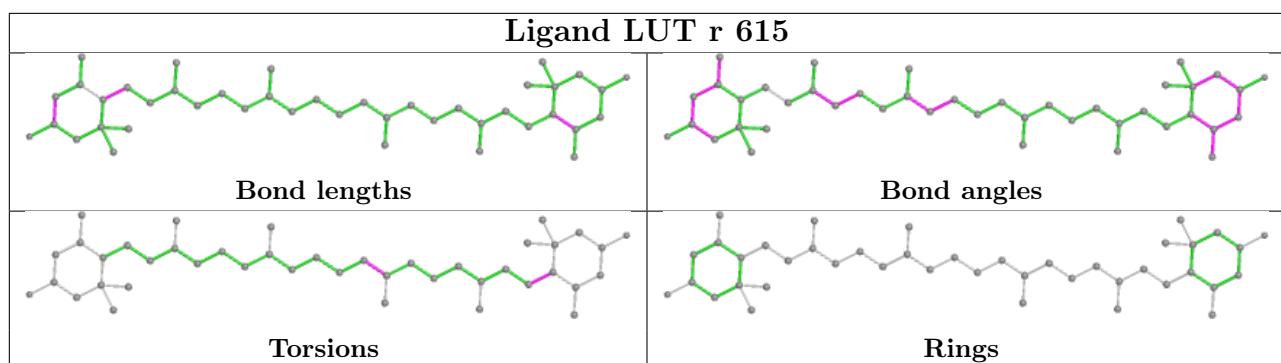


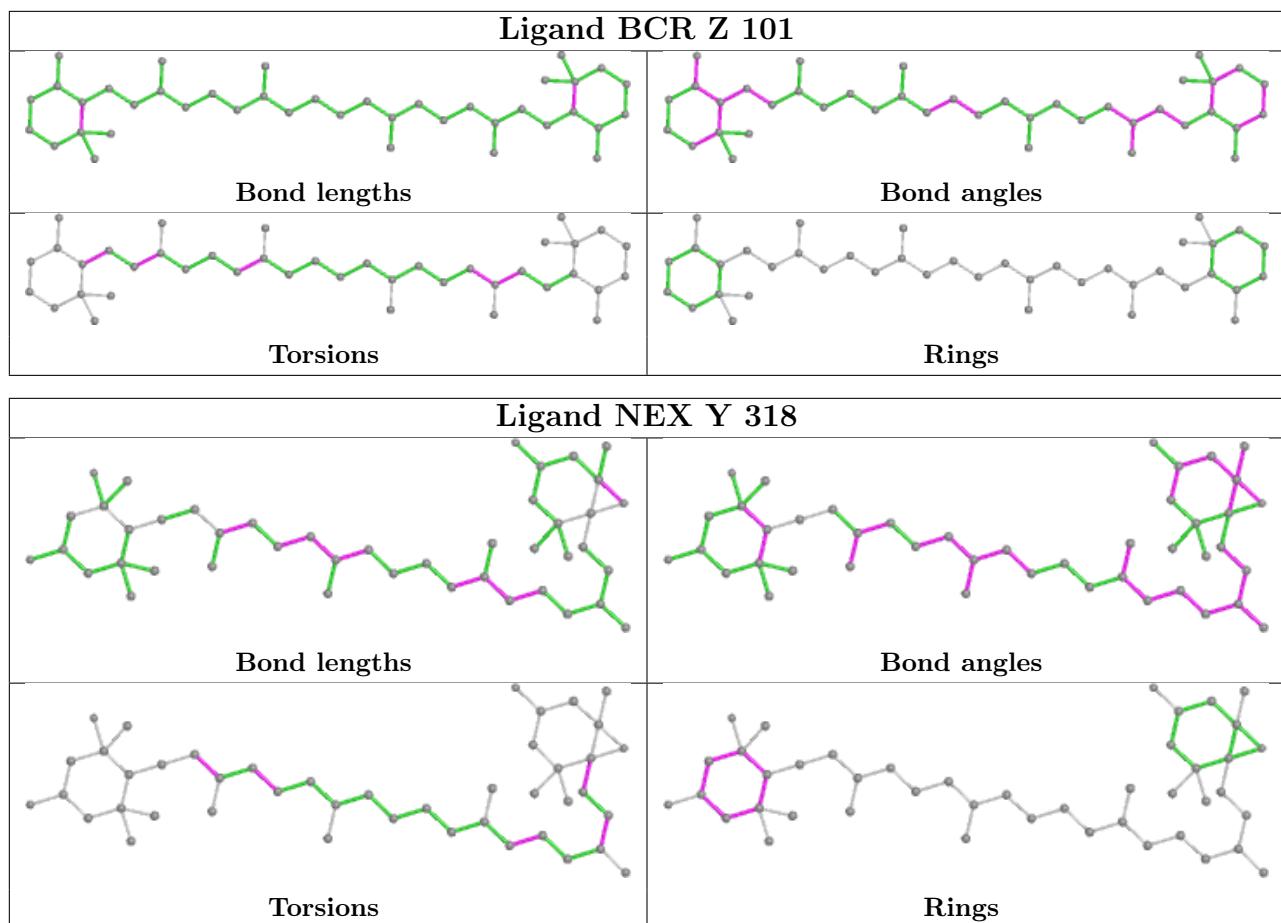


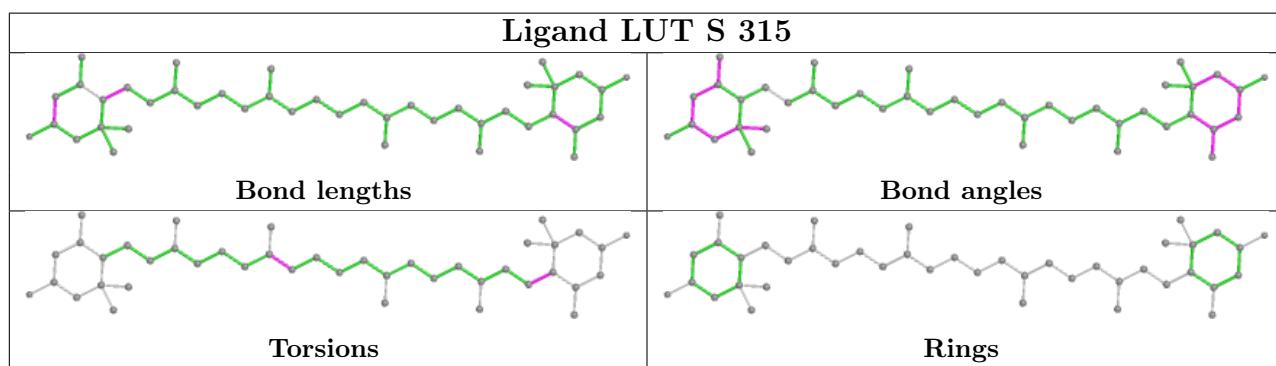
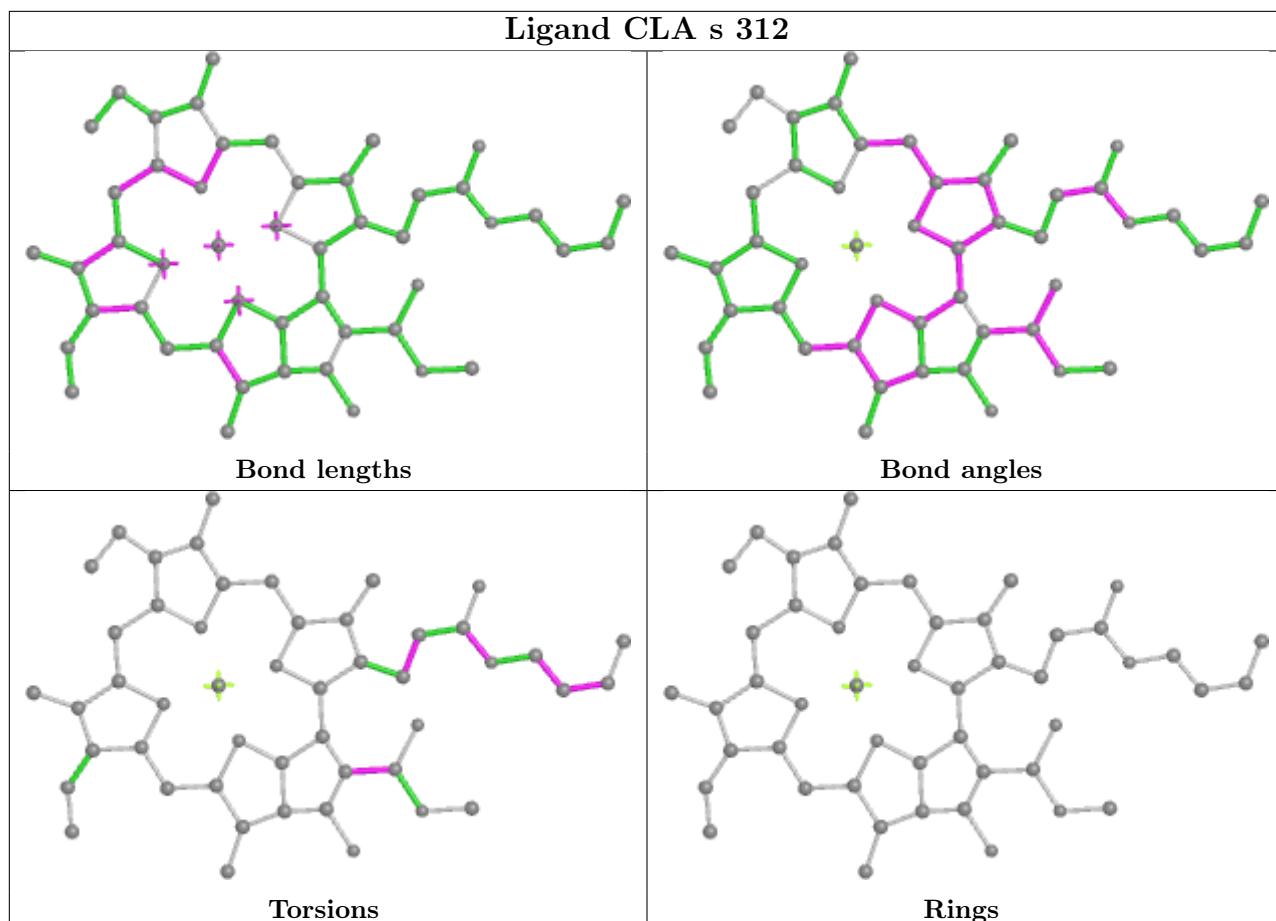


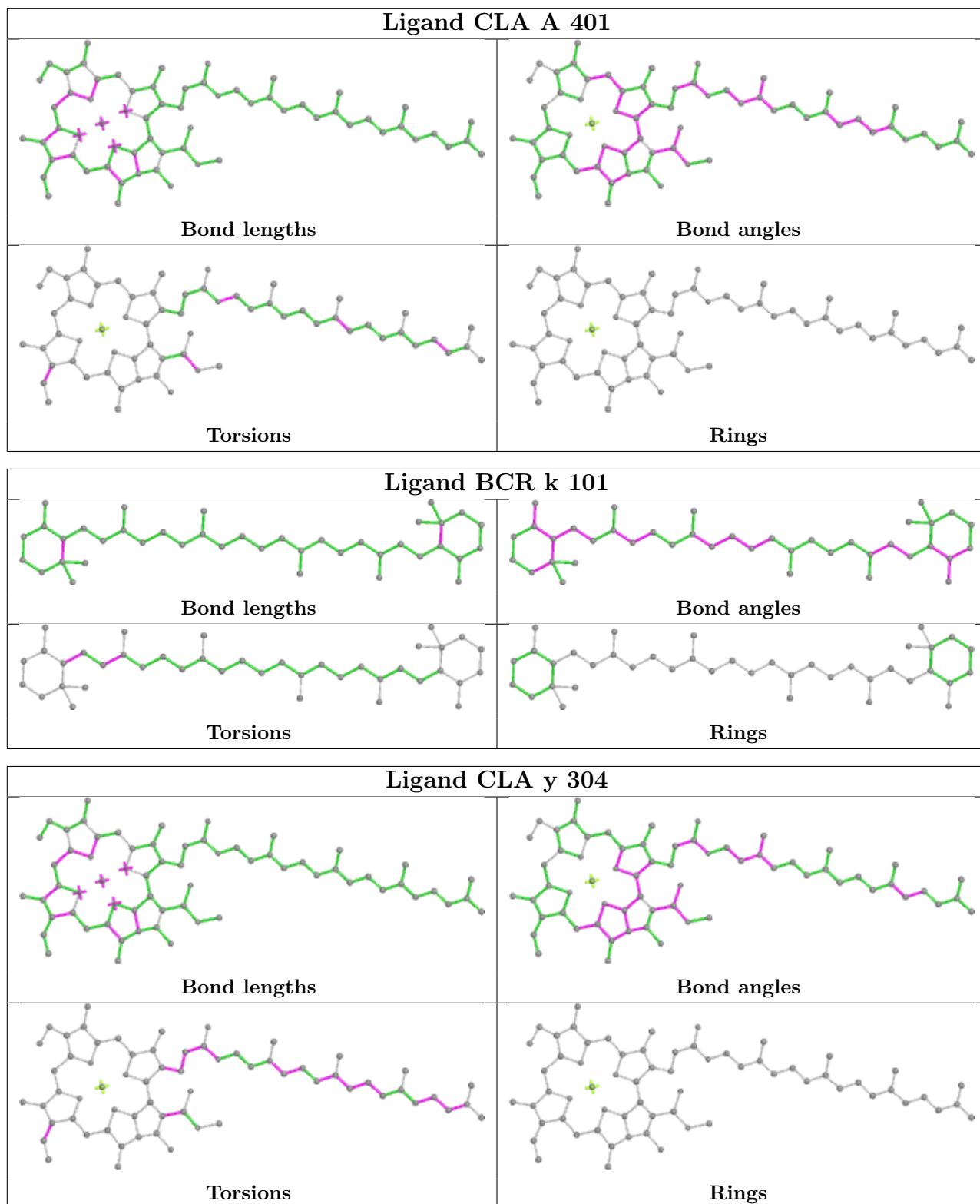


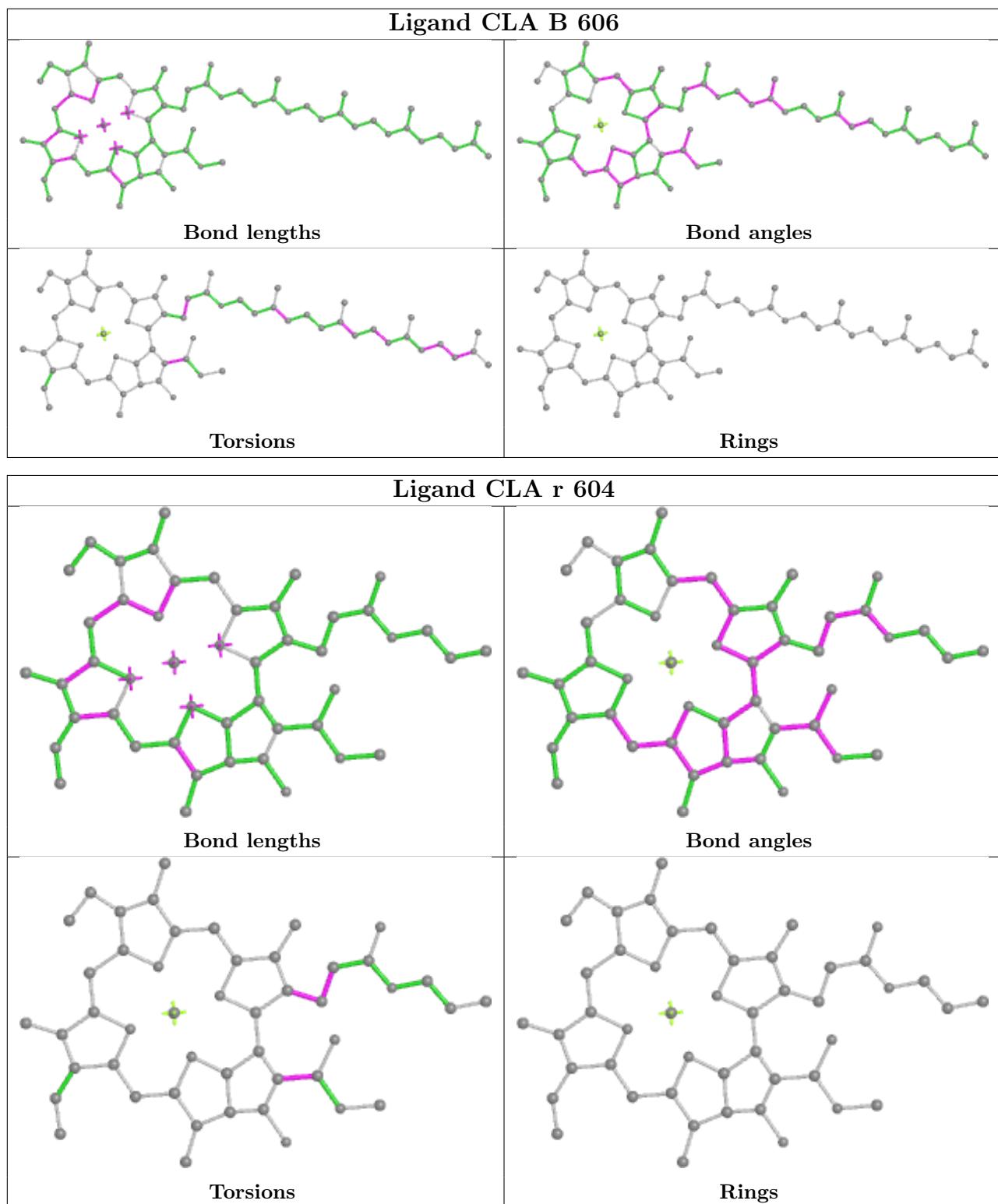


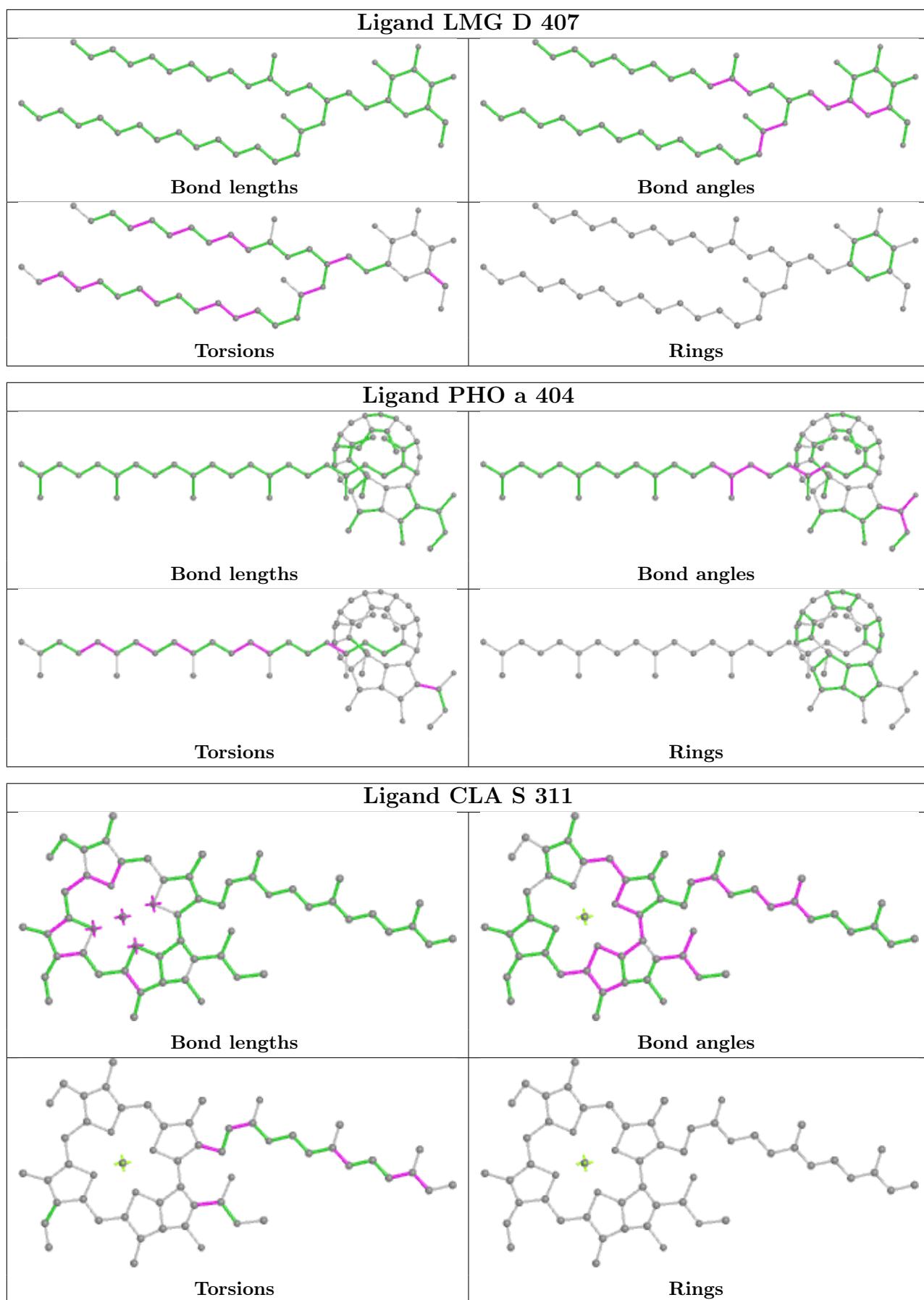


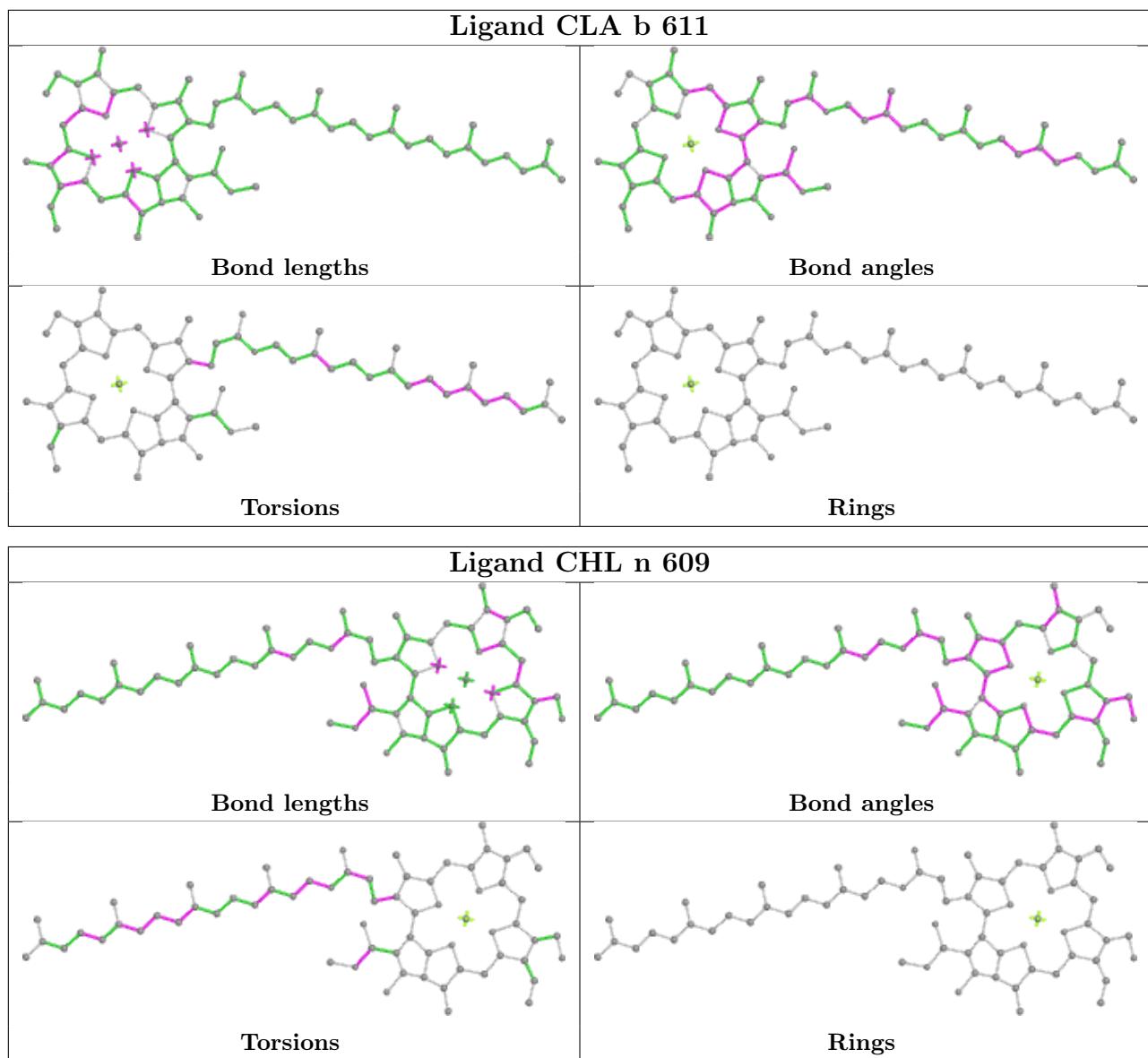


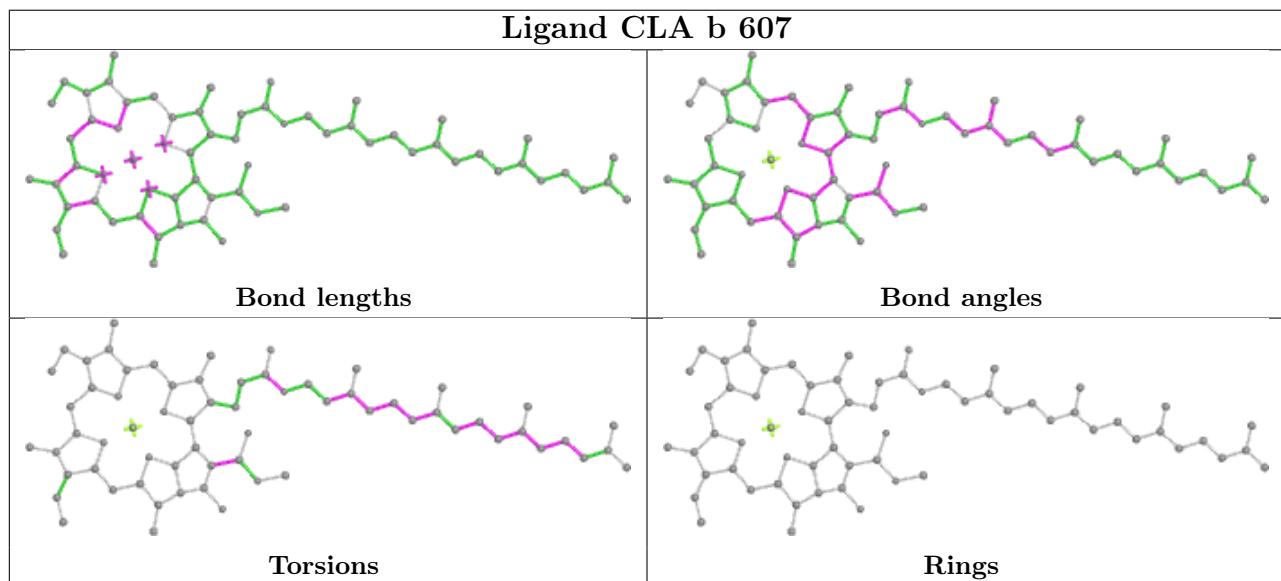
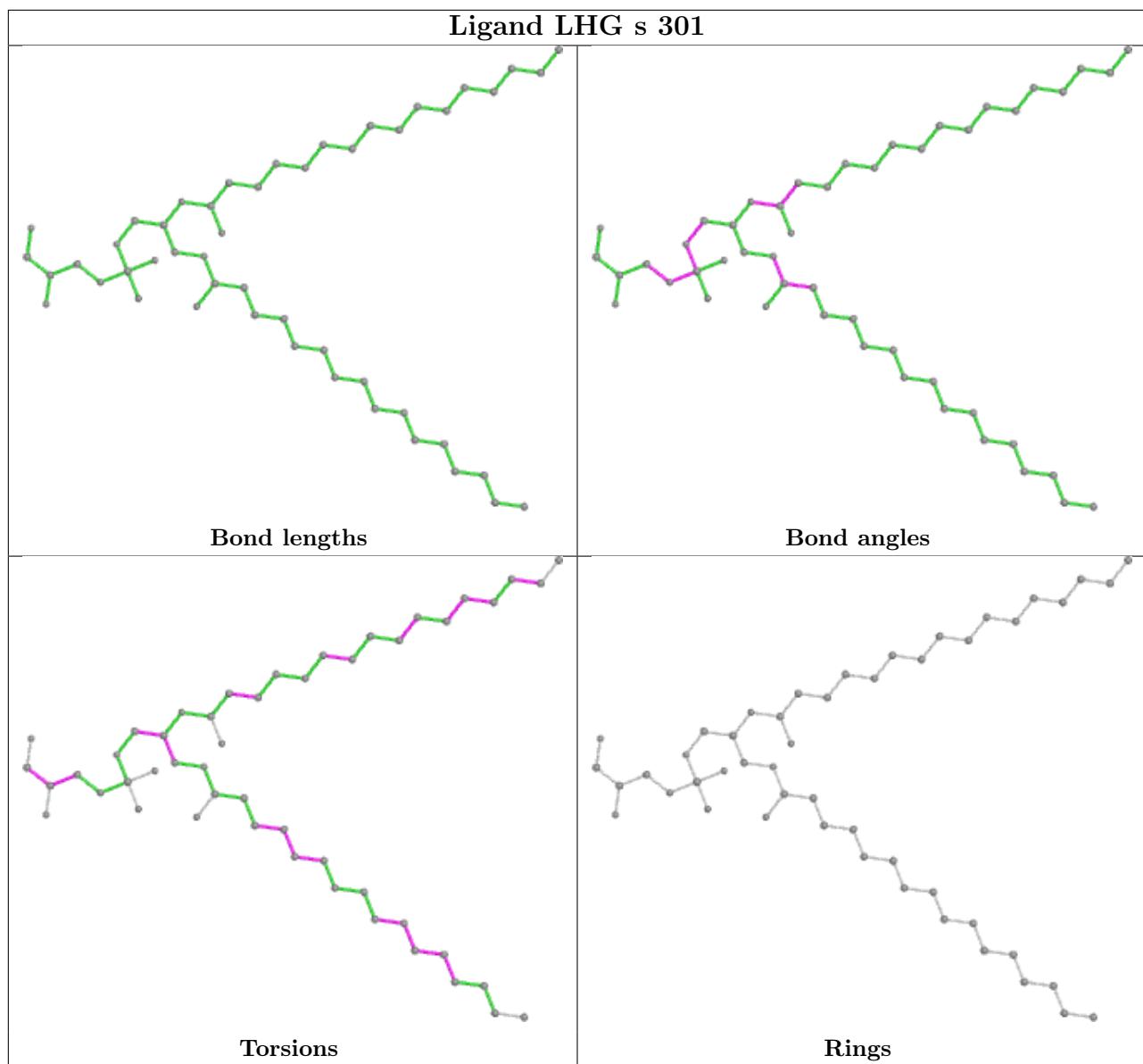


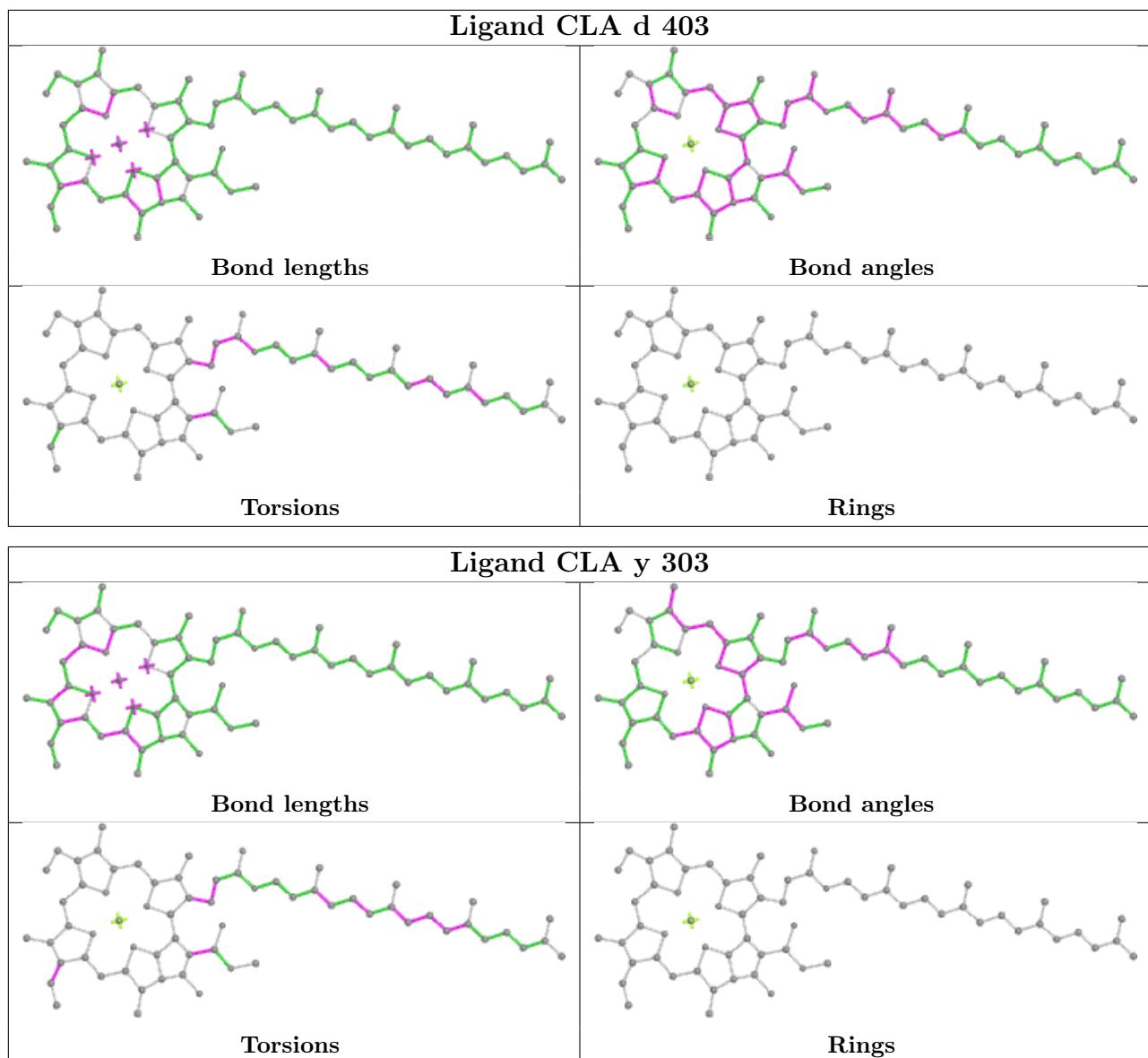


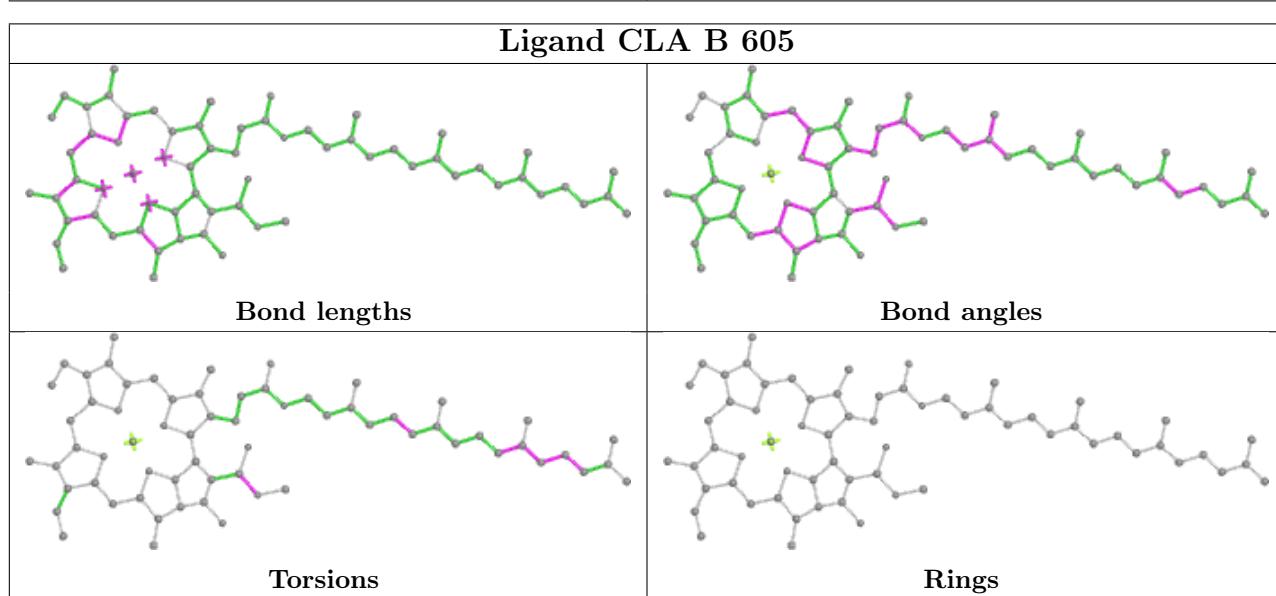
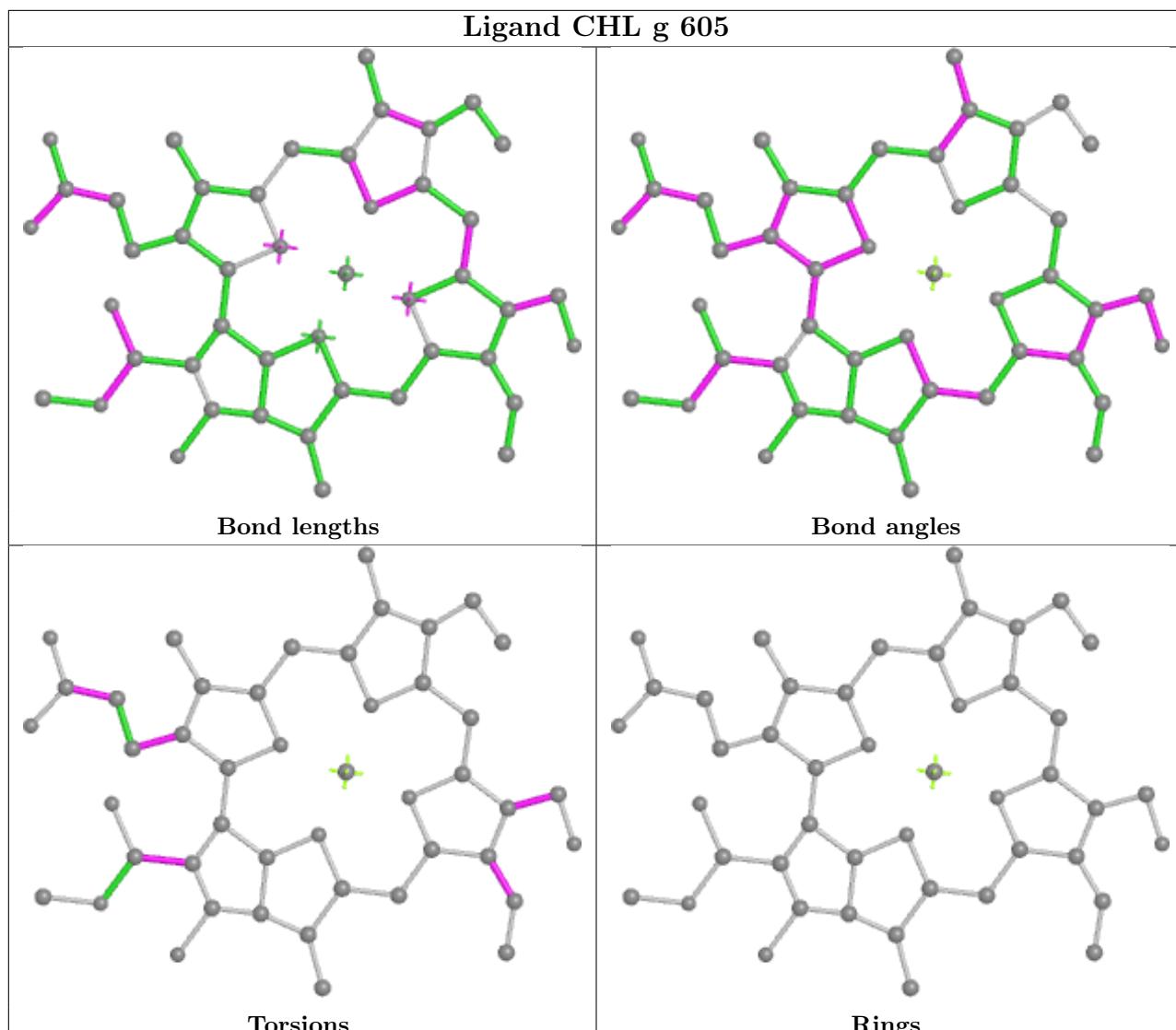


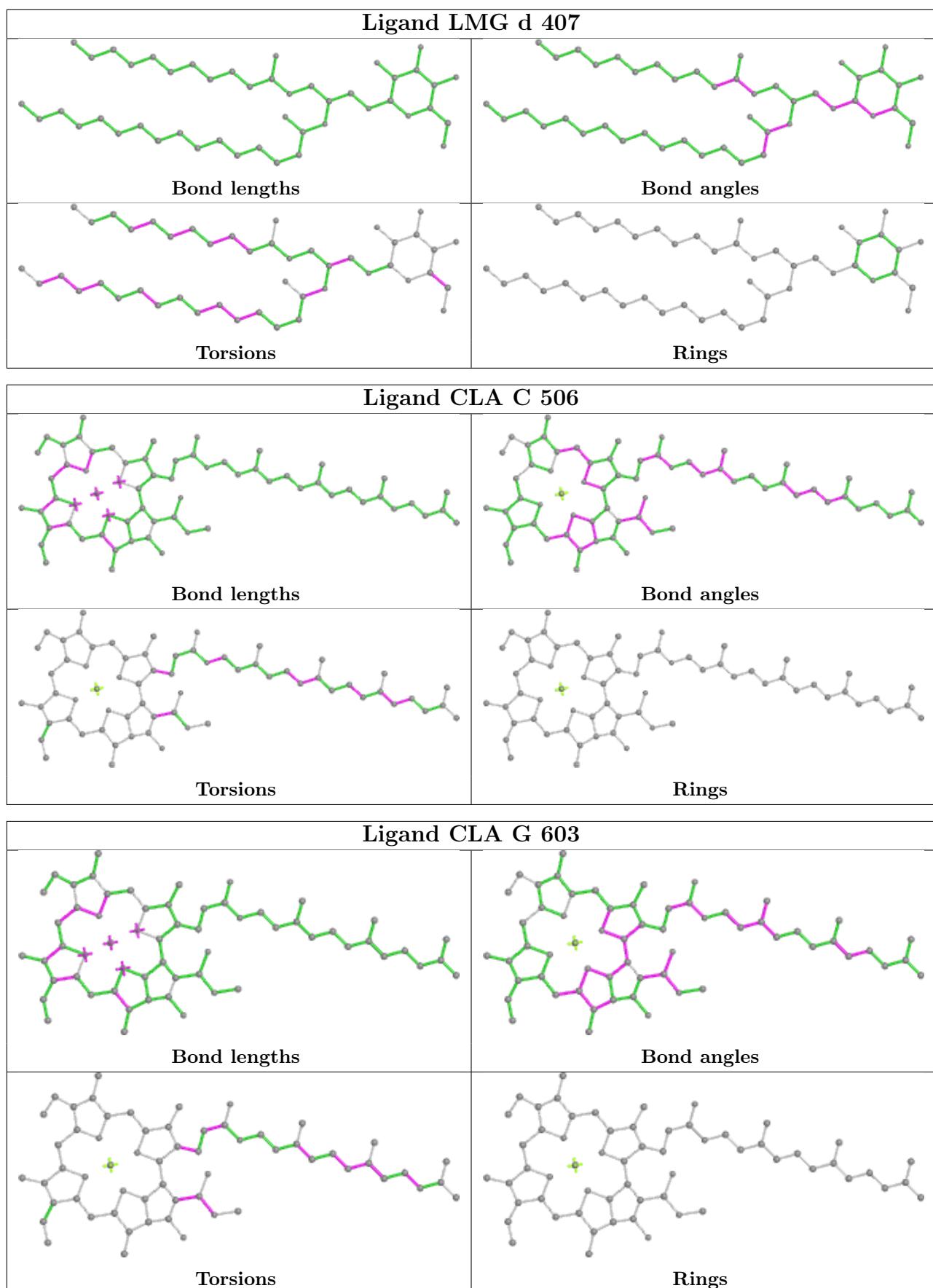


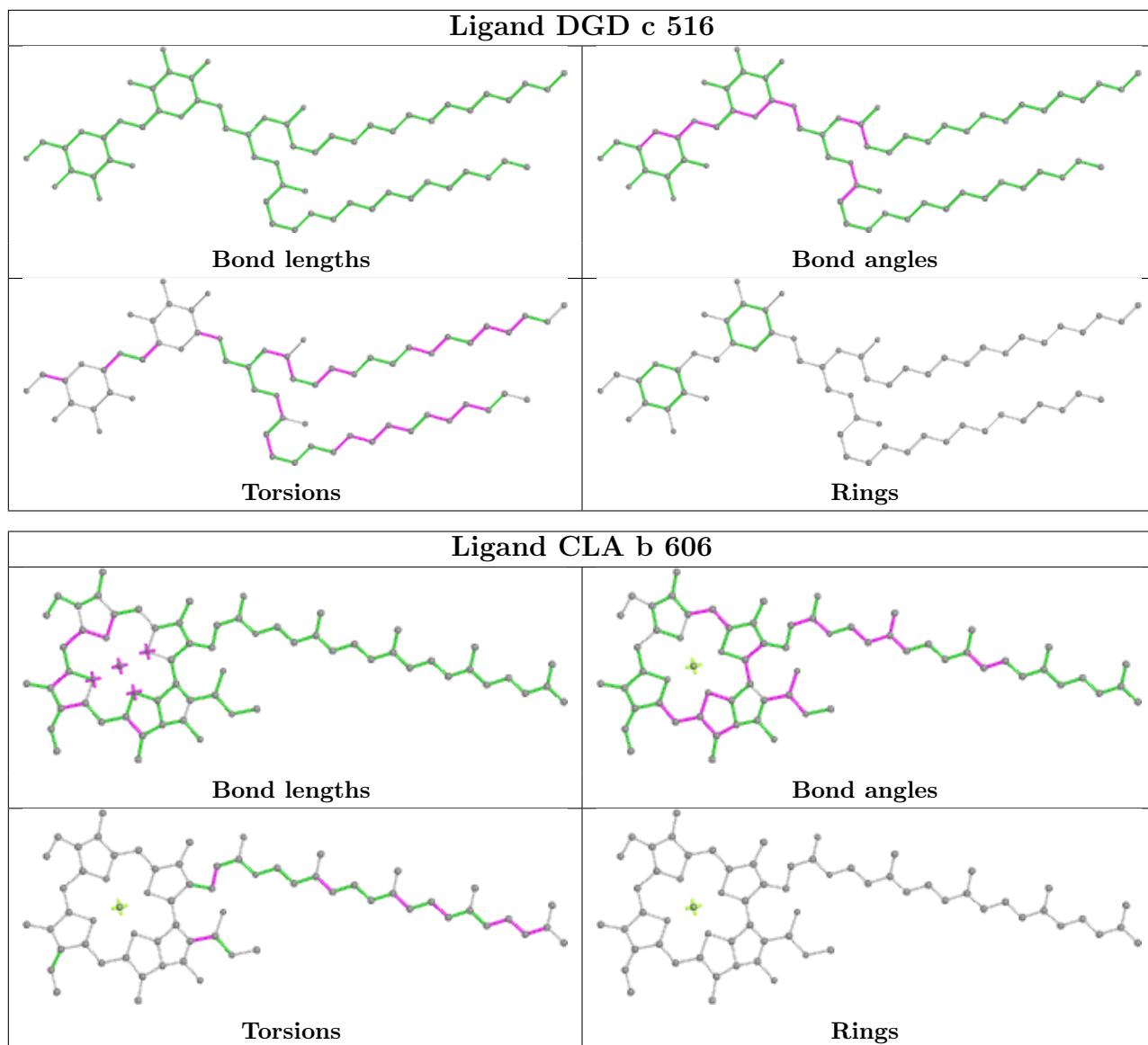


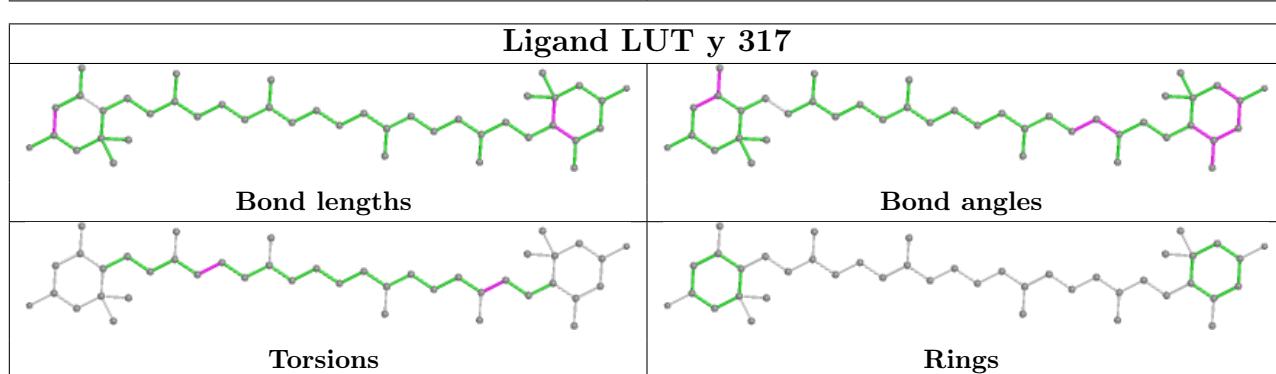
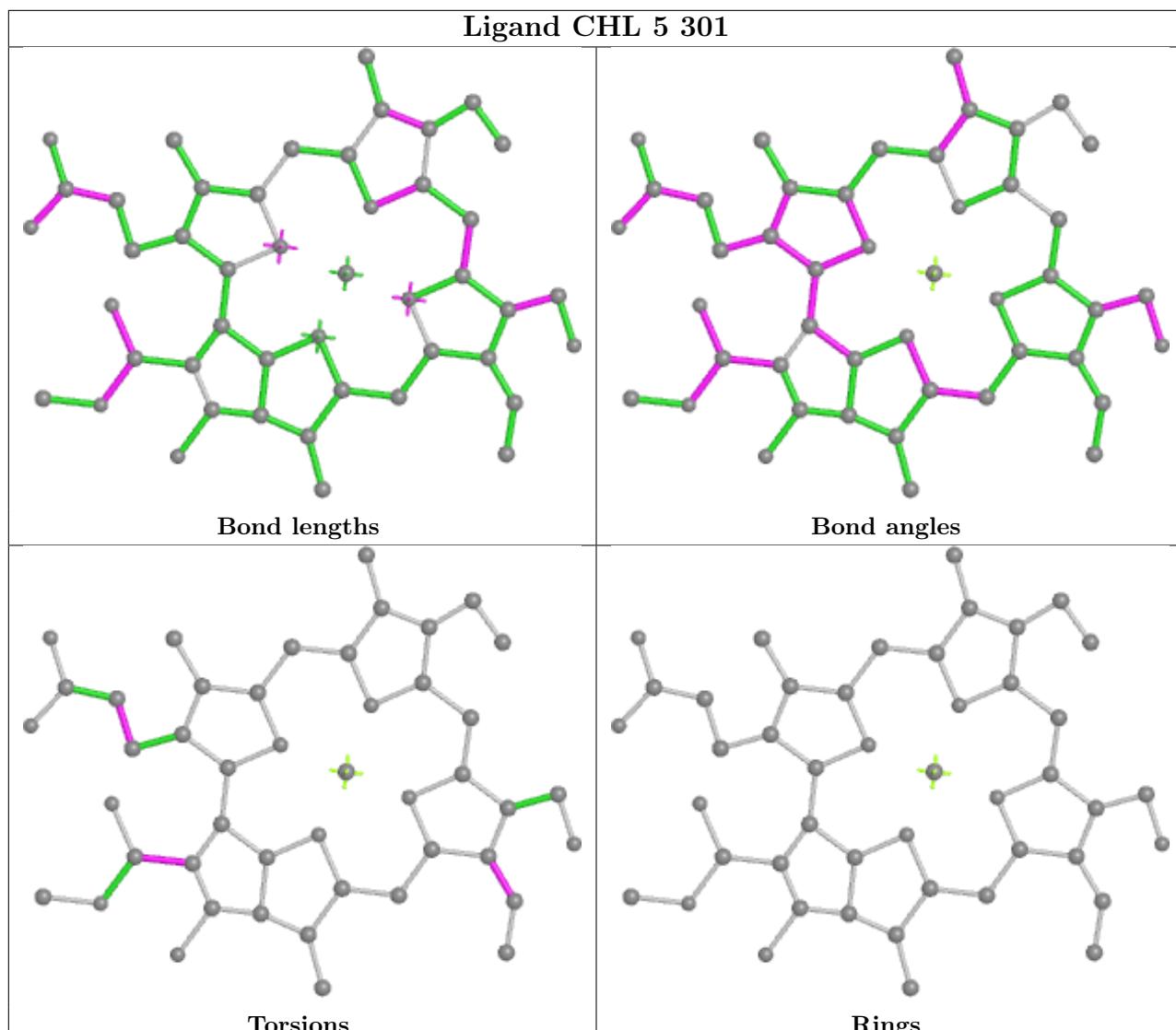


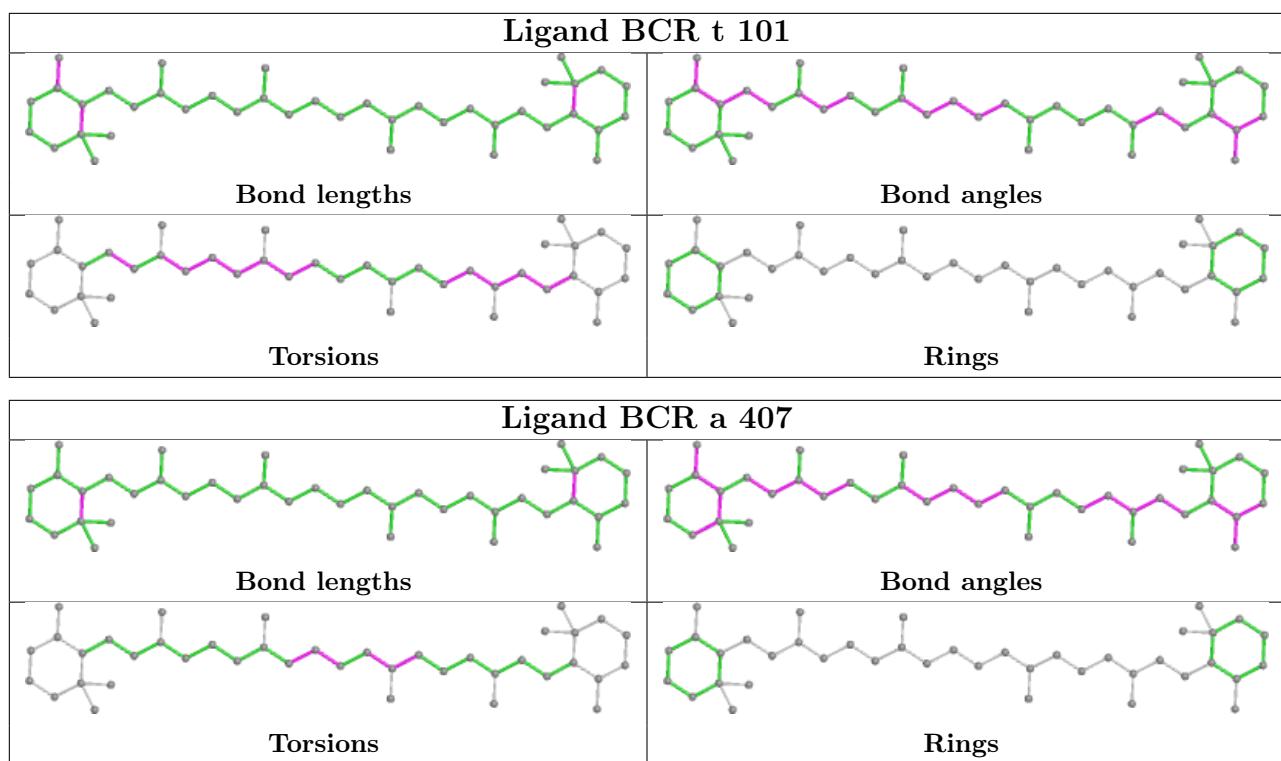












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

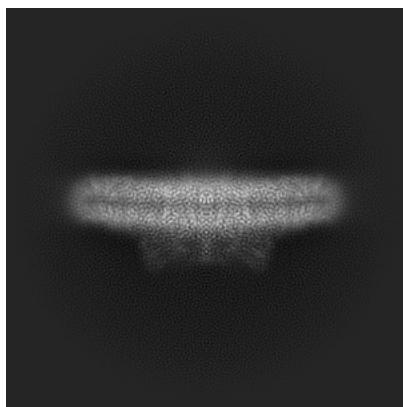
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13078. These allow visual inspection of the internal detail of the map and identification of artifacts.

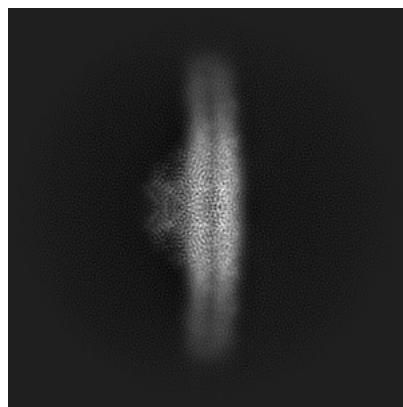
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

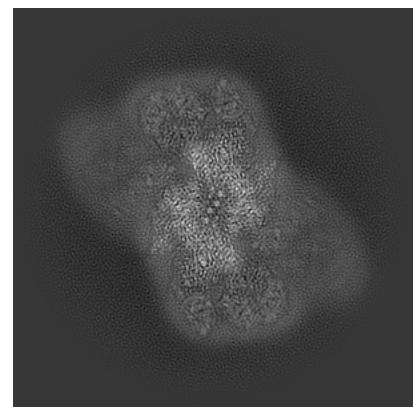
6.1.1 Primary map



X



Y

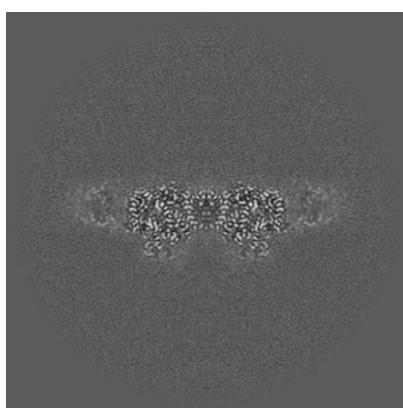


Z

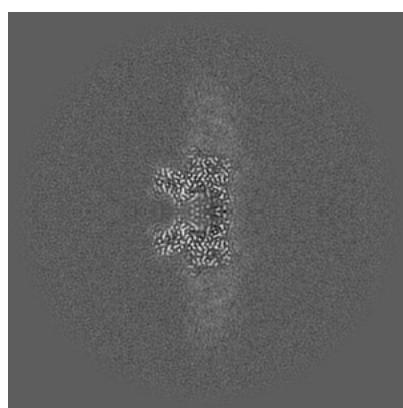
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

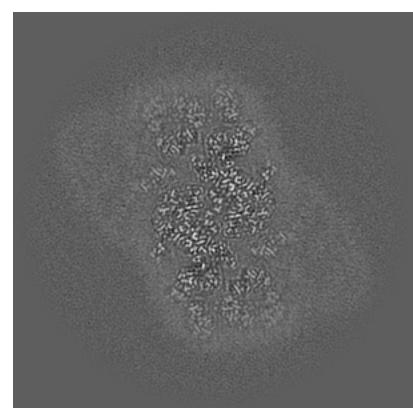
6.2.1 Primary map



X Index: 250



Y Index: 250

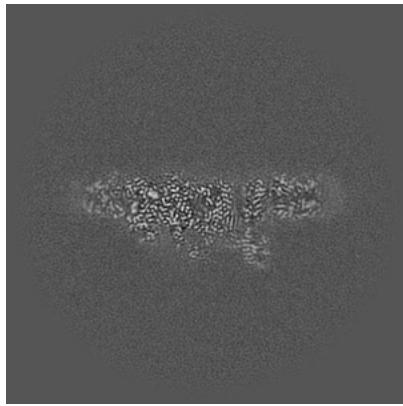


Z Index: 250

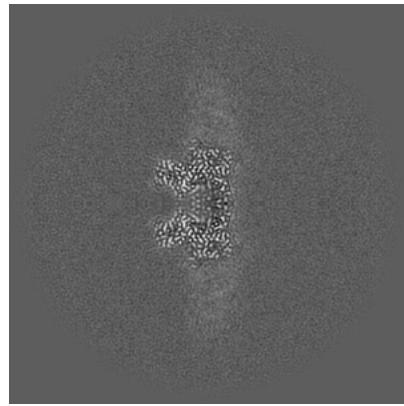
The images above show central slices of the map in three orthogonal directions.

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

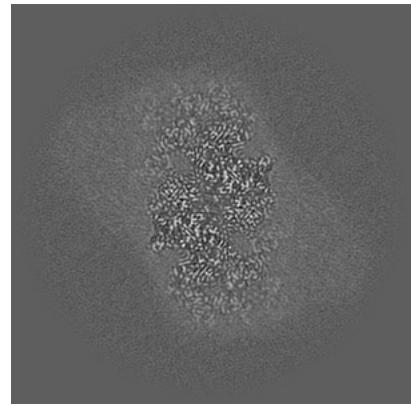
6.3.1 Primary map



X Index: 228



Y Index: 250



Z Index: 239

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

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

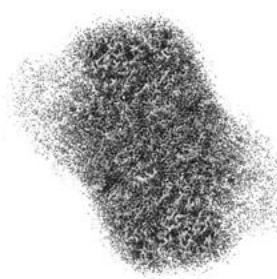
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

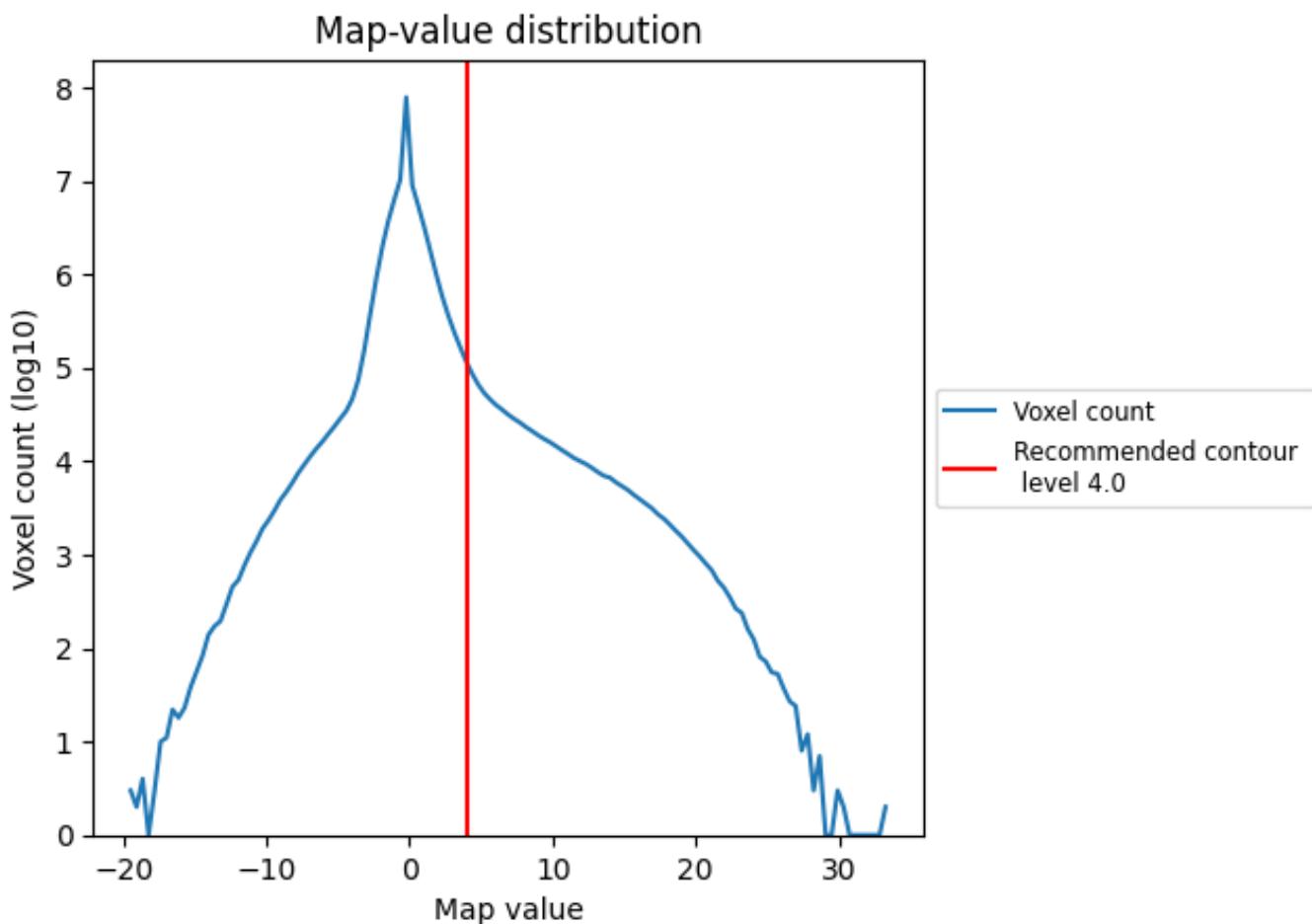
6.5 Mask visualisation

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

7 Map analysis (i)

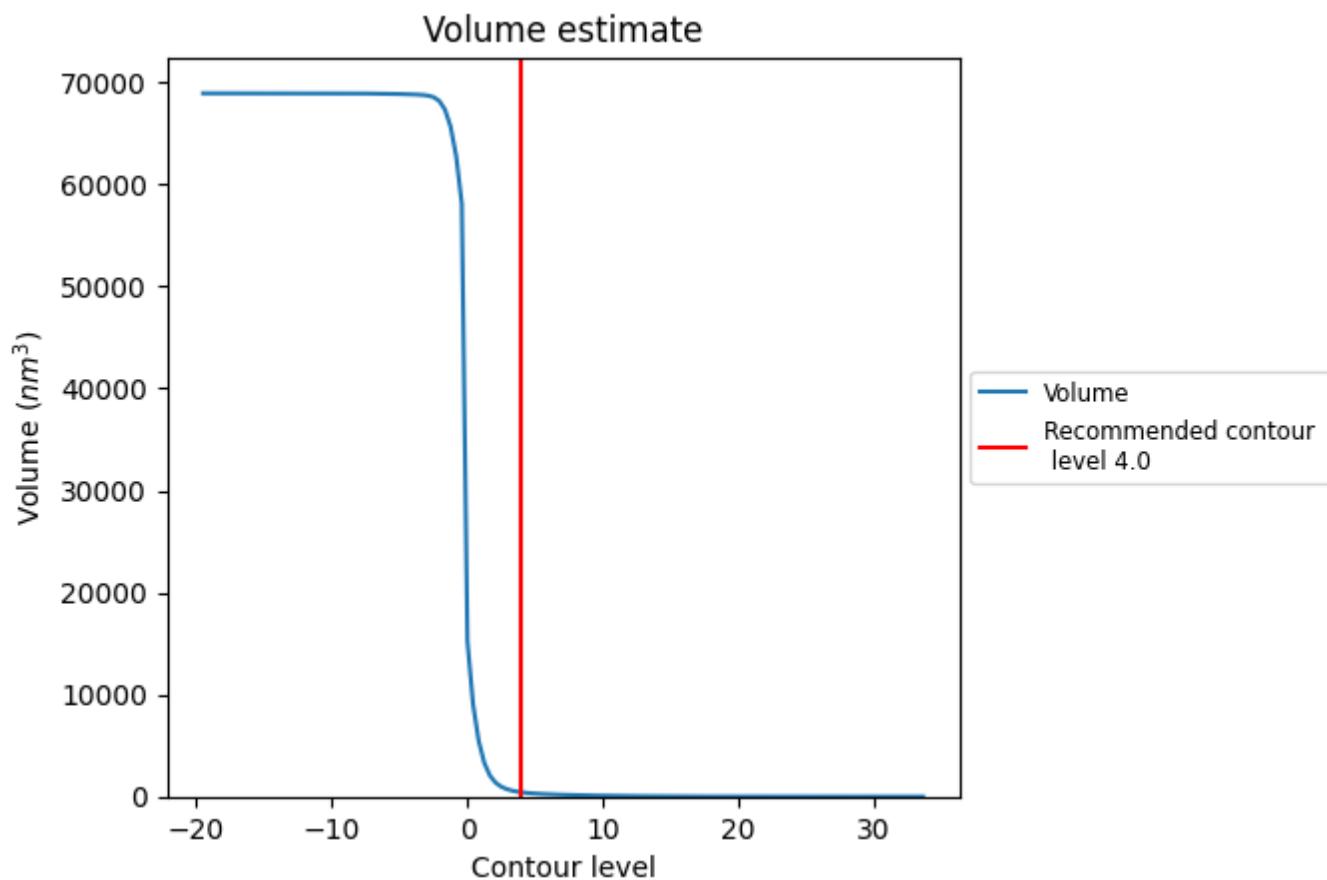
This section contains the results of statistical analysis of the map.

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.

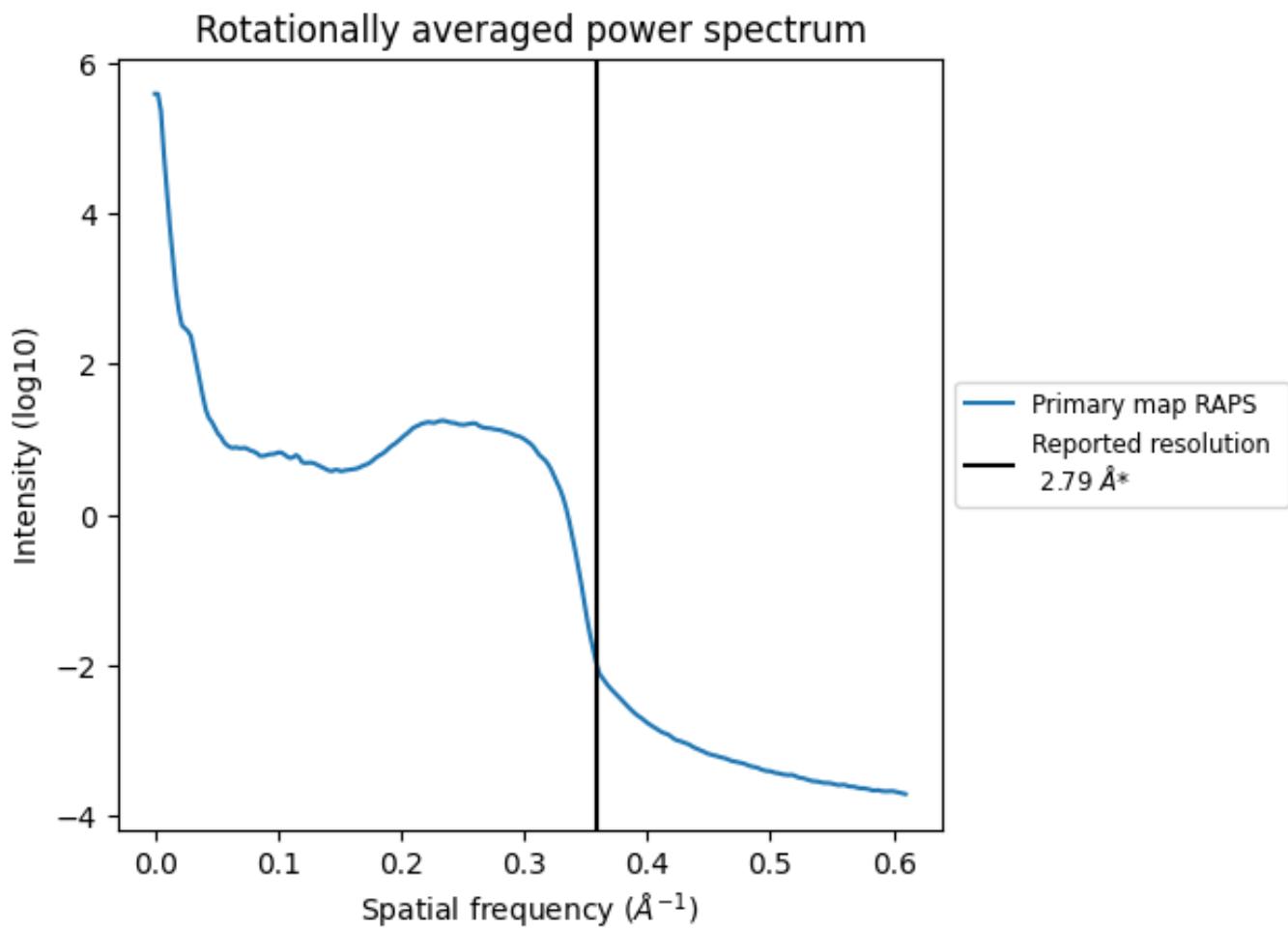
7.2 Volume estimate (i)



The volume at the recommended contour level is 423 nm³; this corresponds to an approximate mass of 382 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 0.358 \AA^{-1}

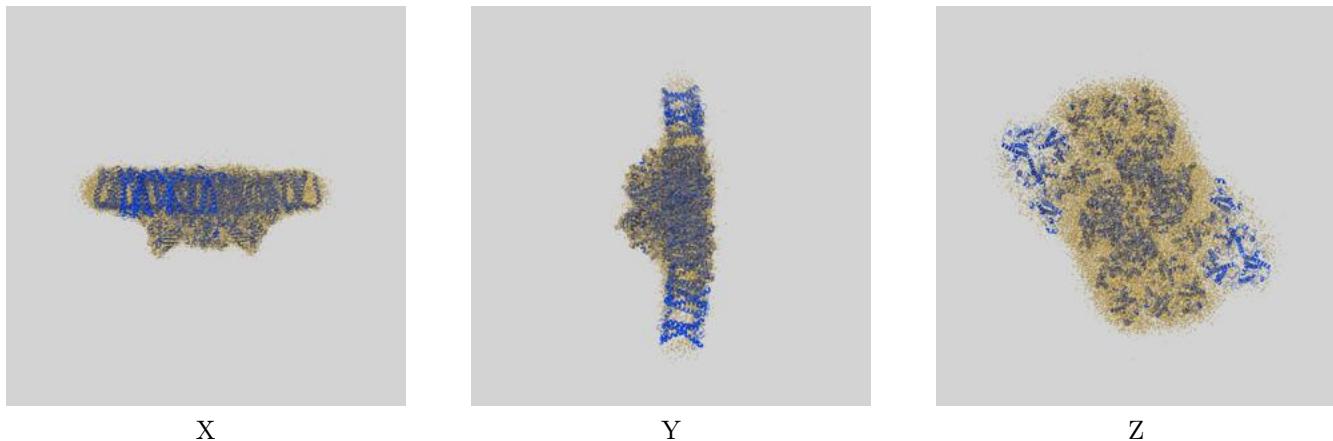
8 Fourier-Shell correlation

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

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

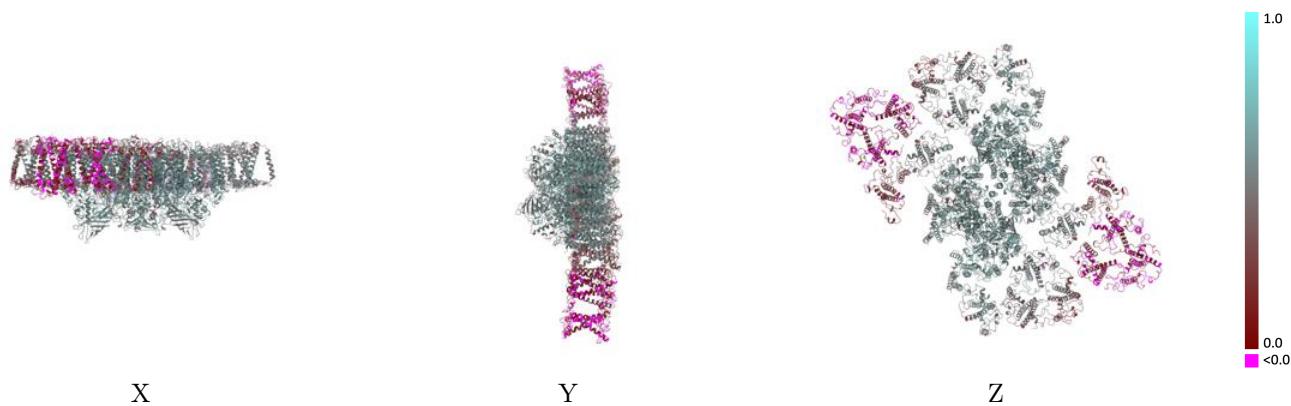
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section 3 on page [42](#).

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



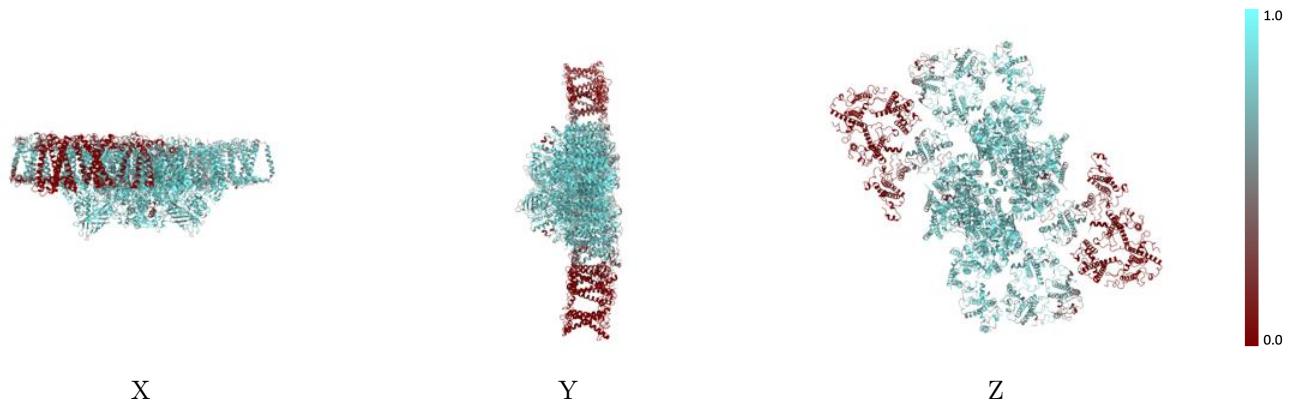
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



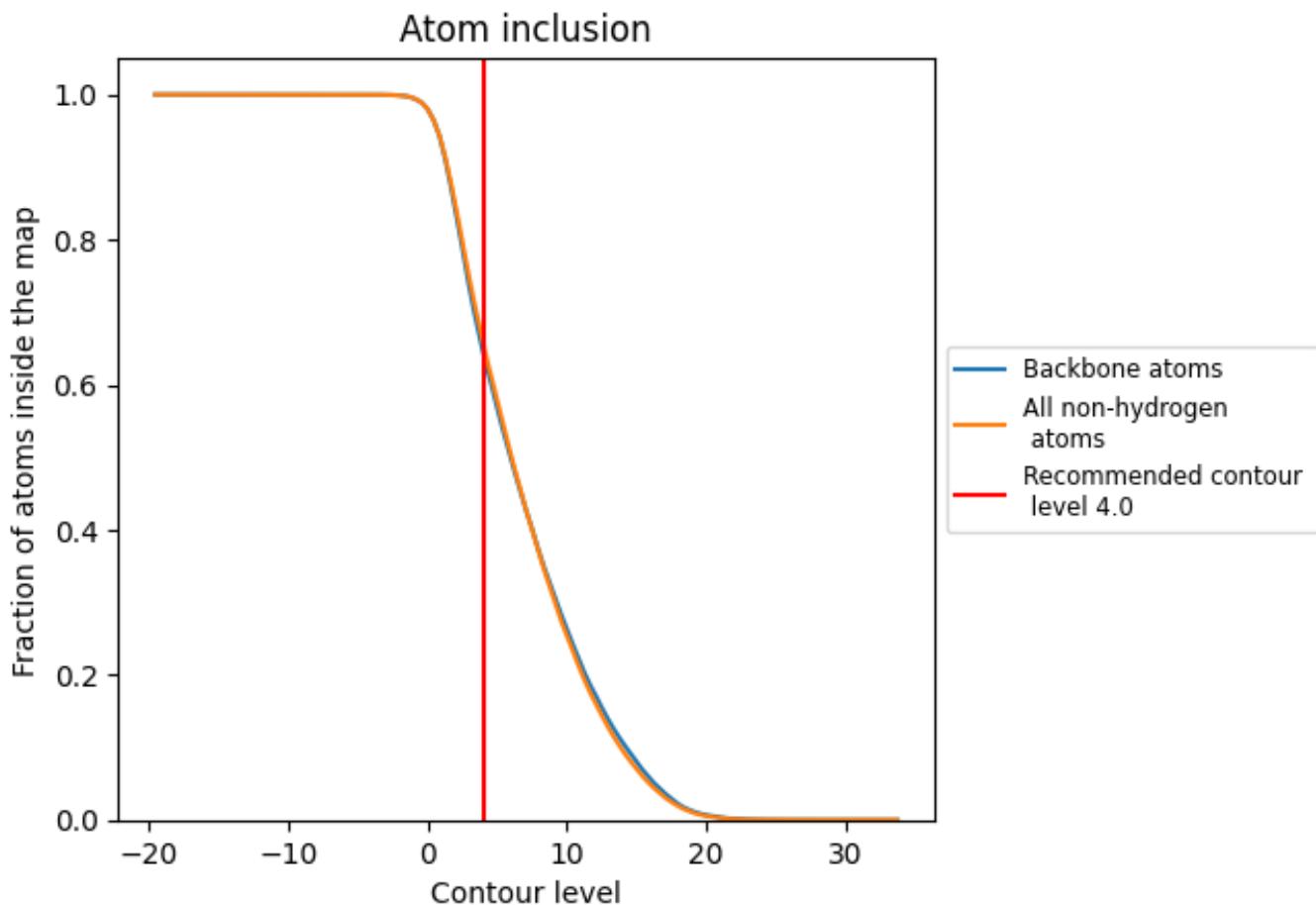
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).

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



At the recommended contour level, 64% of all backbone atoms, 66% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6566	0.4650
1	0.0339	0.0670
2	0.0321	0.1050
3	0.0060	0.0400
4	0.0874	0.2440
5	0.0339	0.0680
6	0.0321	0.1040
7	0.0060	0.0410
8	0.0874	0.2450
A	0.8546	0.5740
B	0.8684	0.5810
C	0.8729	0.5820
D	0.8802	0.5890
E	0.7936	0.5260
F	0.7713	0.5100
G	0.5246	0.3940
H	0.7942	0.5510
I	0.8816	0.6010
K	0.8249	0.5570
L	0.8348	0.5430
M	0.8313	0.5620
N	0.6501	0.4540
O	0.7367	0.5090
R	0.6277	0.4770
S	0.7301	0.5110
T	0.8007	0.5660
U	0.2766	0.4110
W	0.8341	0.5810
X	0.6210	0.4490
Y	0.7790	0.5100
Z	0.7271	0.5140
a	0.8555	0.5750
b	0.8677	0.5800
c	0.8696	0.5820
d	0.8762	0.5900



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Chain	Atom inclusion	Q-score
e	0.7917	0.5240
f	0.7752	0.5080
g	0.5271	0.3930
h	0.7921	0.5510
i	0.8941	0.5980
k	0.8398	0.5590
l	0.8348	0.5420
m	0.8233	0.5660
n	0.6505	0.4530
o	0.7360	0.5130
r	0.6250	0.4760
s	0.7257	0.5110
t	0.8080	0.5700
u	0.2819	0.4040
w	0.8341	0.5760
x	0.6250	0.4400
y	0.7772	0.5080
z	0.7151	0.5110