



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:44 PM UTC

PDB ID : 7OUI / pdb_00007oui
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

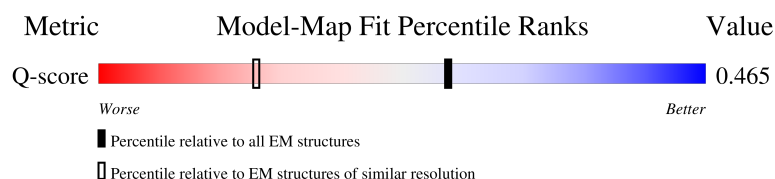
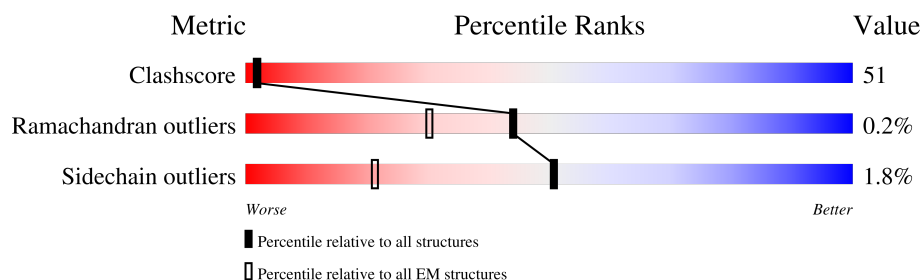
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.79 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	266	76% 30% 43% 24%
1	3	266	76% 30% 43% 24%
1	5	266	76% 30% 43% 24%
1	7	266	76% 30% 43% 24%

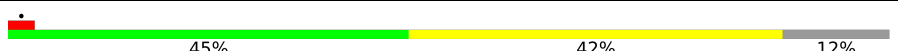
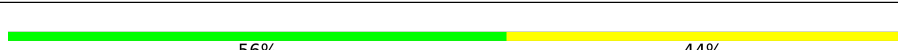
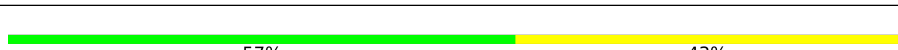
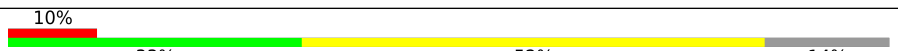
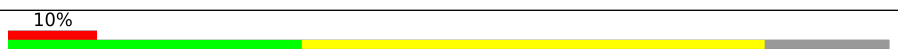
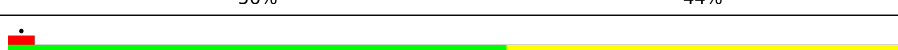
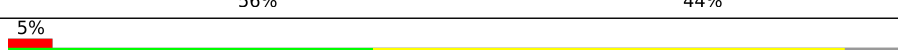
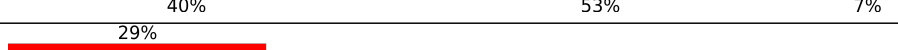
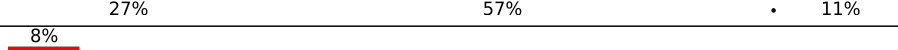
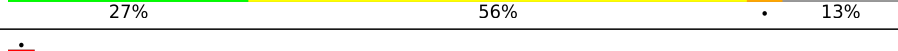
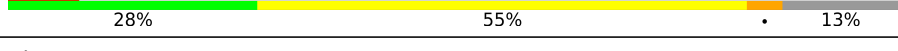
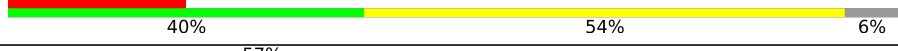
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Mol	Chain	Length	Quality of chain
2	2	243	
2	6	243	
3	4	212	
3	8	212	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	459	
6	c	459	
7	D	352	
7	d	352	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	72	
10	h	72	
11	I	36	
11	i	36	
12	K	37	
12	k	37	
13	L	38	
13	l	38	
14	M	34	

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Mol	Chain	Length	Quality of chain
14	m	34	
15	O	247	
15	o	247	
16	T	33	
16	t	33	
17	W	54	
17	w	54	
18	X	42	
18	x	42	
19	Z	62	
19	z	62	
20	S	232	
20	s	232	
21	G	232	
21	N	232	
21	Y	232	
21	g	232	
21	n	232	
21	y	232	
22	R	250	
22	r	250	
23	U	28	
23	u	28	

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	-	X	-
24	CHL	5	301	X	-	-	-
24	CHL	5	302	X	-	-	-
24	CHL	6	601	X	-	-	-
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	-	X	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	n	607	X	-	X	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	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	-	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	-	X	-
25	CLA	N	603	X	-	X	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	X	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	X	-
25	CLA	Y	304	X	-	X	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	311	X	-	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	-	-	-

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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	-	X	-
25	CLA	c	511	X	-	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	-	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	-	X	-
25	CLA	n	603	X	-	X	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	X	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	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	-	X	-
25	CLA	y	304	X	-	-	-
25	CLA	y	305	X	-	-	-
25	CLA	y	311	X	-	X	-
25	CLA	y	312	X	-	-	-
25	CLA	y	313	X	-	-	-
25	CLA	y	314	X	-	-	-
25	CLA	y	315	X	-	-	-
28	BCR	t	101	-	-	X	-
32	AJP	A	412	X	-	-	-
32	AJP	B	624	X	-	-	-
32	AJP	G	618	X	-	-	-
32	AJP	N	619	X	-	-	-
32	AJP	N	620	X	-	-	-
32	AJP	S	319	X	-	-	-
32	AJP	Y	320	X	-	-	-
32	AJP	Y	321	X	-	-	-
32	AJP	Y	322	X	-	-	-
32	AJP	Y	323	X	-	-	-
32	AJP	Y	324	X	-	-	-
32	AJP	a	413	X	-	-	-
32	AJP	b	624	X	-	-	-
32	AJP	g	618	X	-	-	-
32	AJP	n	619	X	-	-	-
32	AJP	n	620	X	-	-	-
32	AJP	s	319	X	-	-	-
32	AJP	y	320	X	-	-	-
32	AJP	y	321	X	-	-	-
32	AJP	y	322	X	-	-	-
32	AJP	y	323	X	-	-	-
32	AJP	y	324	X	-	-	-
33	BCT	A	413	-	-	X	-
39	LUT	s	316	-	-	X	-
41	XAT	r	616	-	-	X	-

2 Entry composition

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 Chlorophyll a-b binding protein, chloroplastic.

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 Chlorophyll a-b binding protein 3, chloroplastic.

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
5	B	487	Total	C	N	O	S	0	0
			3810	2495	644	659	12		
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
6	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
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
7	D	342	Total	C	N	O	S	0	0
			2722	1800	445	465	12		
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
8	E	66	Total	C	N	O	0	0
			543	357	88	98		
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
9	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
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	0	0
			446	293	70	81	2		
10	h	60	Total	C	N	O	S	0	0
			446	293	70	81	2		

- 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	0	0
			286	195	44	46	1		
11	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

- 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	0	0
			301	211	44	45	1		
12	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

- 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	S	0	0
			302	200	47	55			
13	l	36	Total	C	N	O	S	0	0
			302	200	47	55			

- 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	0	0
			250	173	35	41	1		
14	m	32	Total	C	N	O	S	0	0
			250	173	35	41	1		

- 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	0	0
			1516	969	241	302	4		

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

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

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

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

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

- Molecule 18 is a protein called (thale cress) hypothetical protein.

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

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

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

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

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

- 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	0	0
			1562	1010	255	292	5		
21	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	Y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		
21	g	206	Total	C	N	O	S	0	0
			1562	1010	255	292	5		
21	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
21	y	213	Total	C	N	O	S	0	0
			1621	1048	266	302	5		

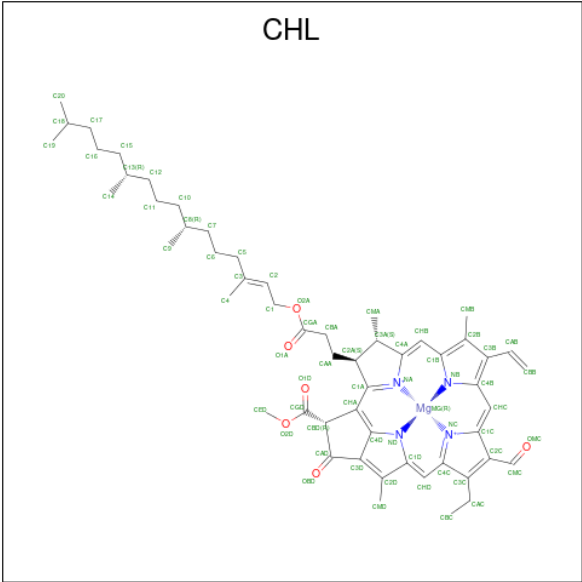
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

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

- Molecule 23 is a protein called Photosystem II 5 kDa protein, chloroplastic.

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

- Molecule 24 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	2	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	G	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	G	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
24	N	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 48	C 37	Mg 1	N 4	O 6	0
24	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
24	Y	1	Total 58	C 47	Mg 1	N 4	O 6	0
24	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
24	Y	1	Total 56	C 45	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	R	1	Total 61	C 50	Mg 1	N 4	O 6	0
24	R	1	Total 42	C 33	Mg 1	N 4	O 4	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	6	1	Total 64	C 53	Mg 1	N 4	O 6	0
24	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
24	s	1	Total 46	C 35	Mg 1	N 4	O 6	0

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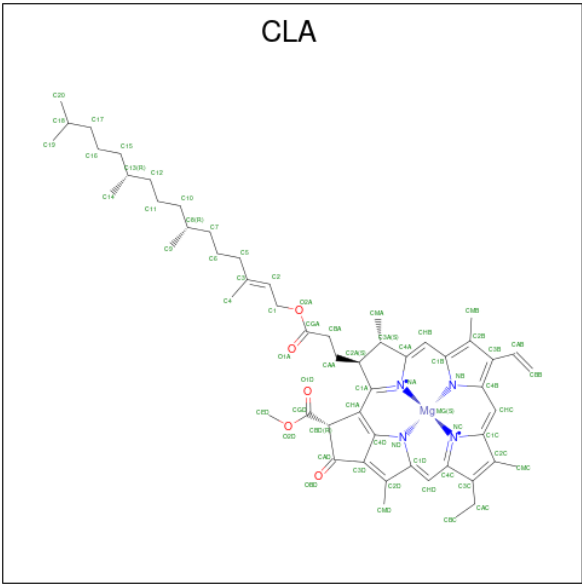
Mol	Chain	Residues	Atoms					AltConf
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
24	y	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
24	r	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	R	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	s	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	s	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	g	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0

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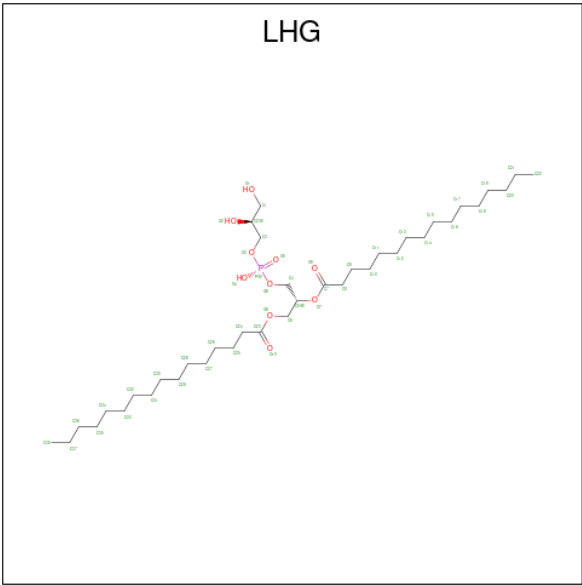
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	g	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	n	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	r	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
26	2	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			47	36	10	1	
26	B	1	Total	C	O	P	0
			49	38	10	1	

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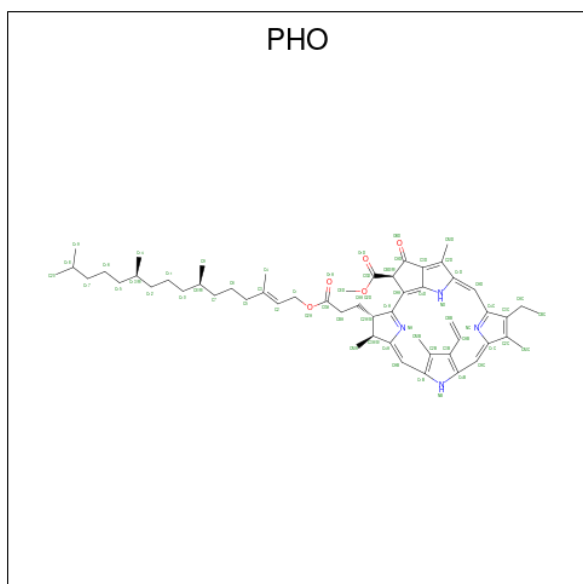
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 46	C 35	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 49	C 38	O 10	P 1	0	
26	C	1	Total 123	C 38	H 74	O 10 P 1	0	
26	D	1	Total 49	C 38	O 10	P 1	0	
26	L	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	S	1	Total 49	C 38	O 10	P 1	0	
26	N	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	Y	1	Total 49	C 38	O 10	P 1	0	
26	R	1	Total 42	C 31	O 10	P 1	0	
26	6	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 47	C 36	O 10	P 1	0	
26	b	1	Total 49	C 38	O 10	P 1	0	
26	b	1	Total 46	C 35	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 49	C 38	O 10	P 1	0	
26	c	1	Total 123	C 38	H 74	O 10 P 1	0	
26	d	1	Total 49	C 38	O 10	P 1	0	
26	l	1	Total 49	C 38	O 10	P 1	0	

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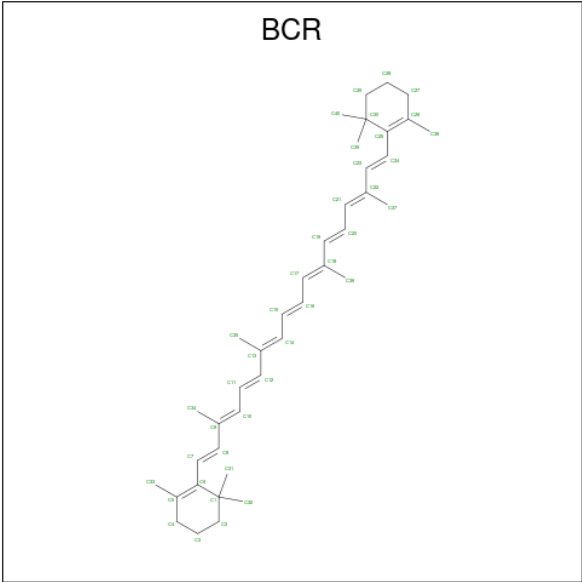
Mol	Chain	Residues	Atoms				AltConf
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	s	1	Total	C	O	P	0
			49	38	10	1	
26	n	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	y	1	Total	C	O	P	0
			49	38	10	1	
26	r	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



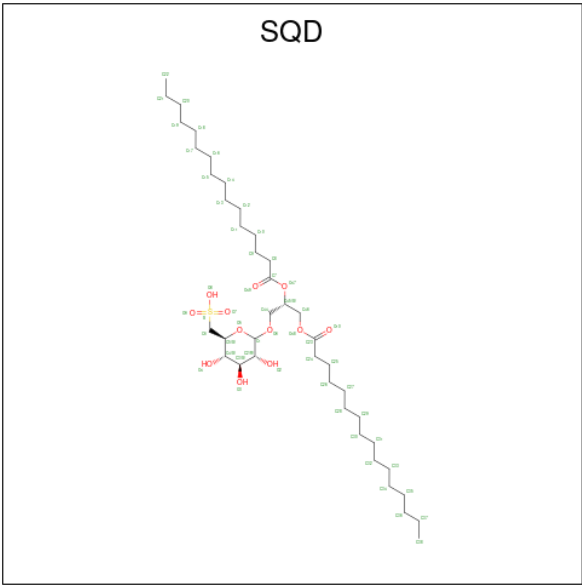
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	D	1	Total	C	0
			40	40	
28	H	1	Total	C	0
			40	40	
28	I	1	Total	C	0
			40	40	
28	K	1	Total	C	0
			40	40	
28	T	1	Total	C	0
			40	40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

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Mol	Chain	Residues	Atoms	AltConf
28	b	1	Total C 40 40	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-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



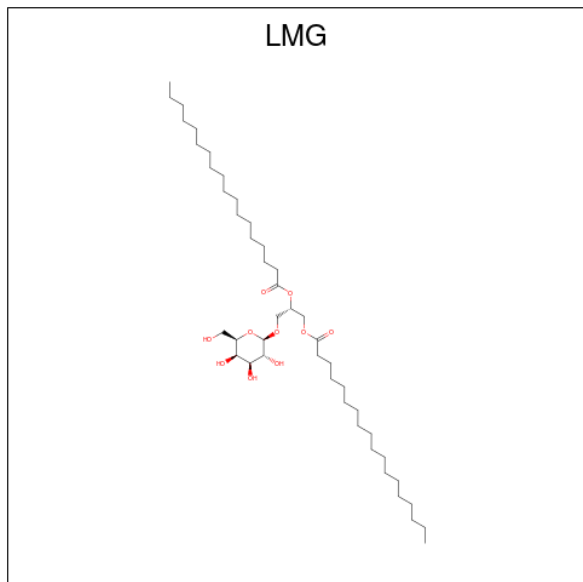
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O S 50 37 12 1	0
29	A	1	Total C O S 54 41 12 1	0
29	L	1	Total C O S 42 29 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	L	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			54	41	12	1	
29	l	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



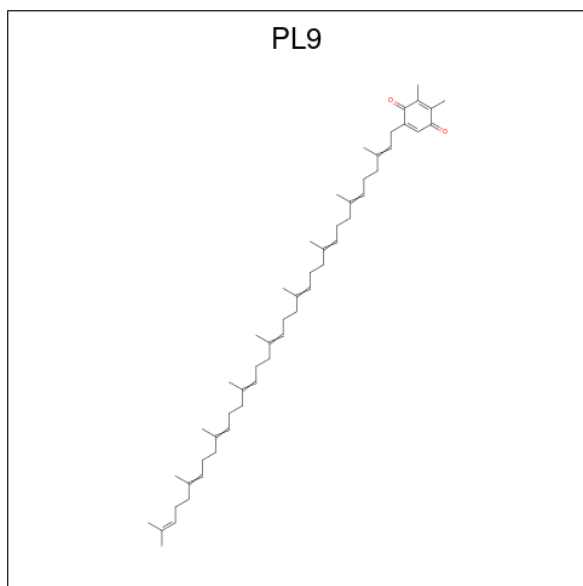
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O		0
			48	38	10		
30	A	1	Total	C	O		0
			40	30	10		
30	B	1	Total	C	O		0
			51	41	10		
30	B	1	Total	C	O		0
			55	45	10		
30	C	1	Total	C	O		0
			51	41	10		
30	D	1	Total	C	O		0
			46	36	10		

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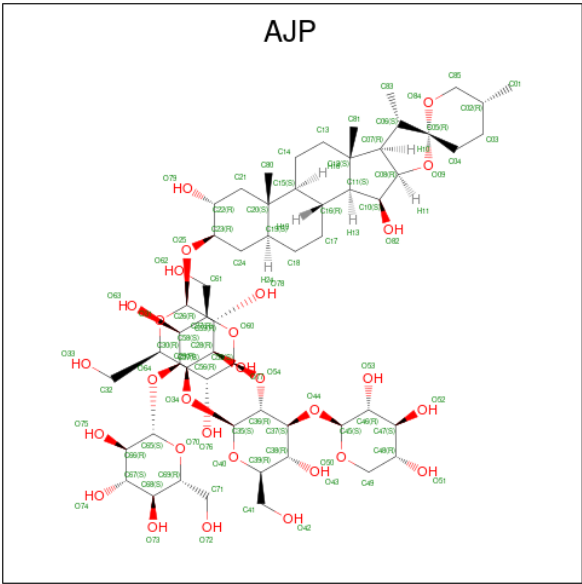
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			48	38	10	
30	a	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			55	45	10	
30	c	1	Total	C	O	0
			51	41	10	
30	d	1	Total	C	O	0
			46	36	10	

- 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 32 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉) (labeled as "Ligand of Interest" by depositor).



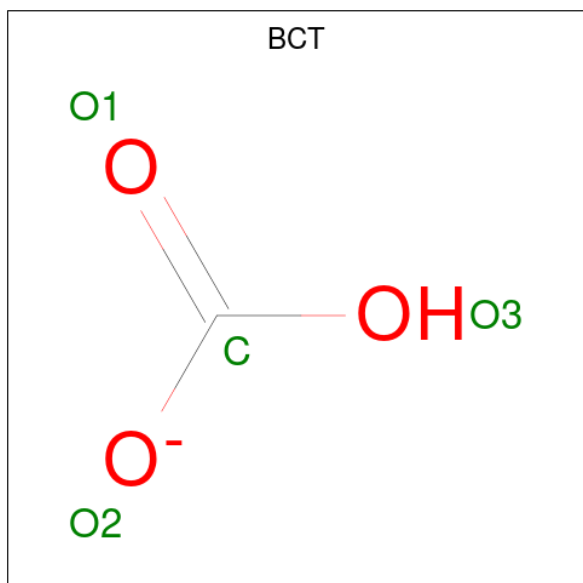
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	H	O	0
			177	56	92	29	
32	B	1	Total	C	H	O	0
			177	56	92	29	
32	S	1	Total	C	H	O	0
			95	33	53	9	
32	G	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	N	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	Y	1	Total	C	H	O	0
			95	33	53	9	
32	a	1	Total	C	H	O	0
			177	56	92	29	

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Mol	Chain	Residues	Atoms				AltConf
32	b	1	Total	C	H	O	0
			177	56	92	29	
32	s	1	Total	C	H	O	0
			95	33	53	9	
32	g	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	n	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	
32	y	1	Total	C	H	O	0
			95	33	53	9	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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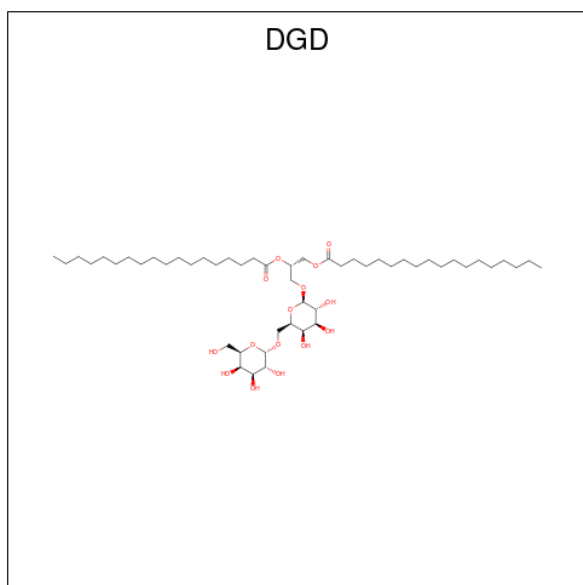
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Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	C	O	0
			4	1	3	

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



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
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	a	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			62	47	15	

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Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	

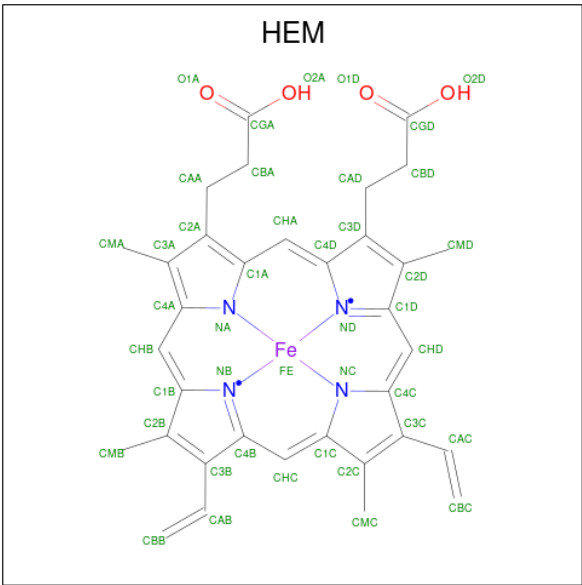
- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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 (CCD ID: CL) (formula: Cl).

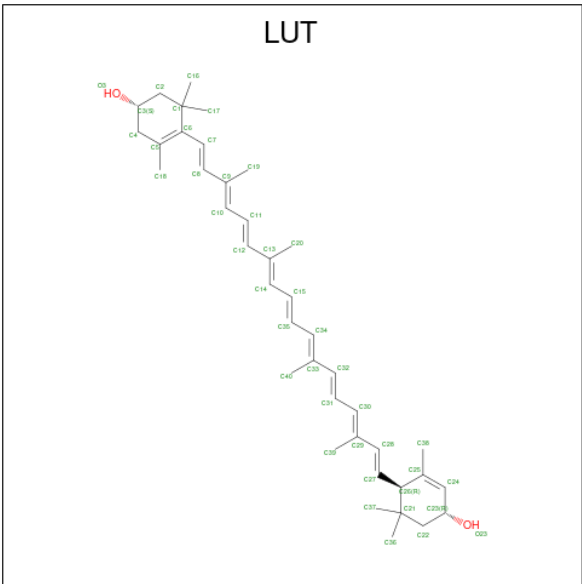
Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Cl	0
			1	1	
37	d	1	Total	Cl	0
			1	1	

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
38	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
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 (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



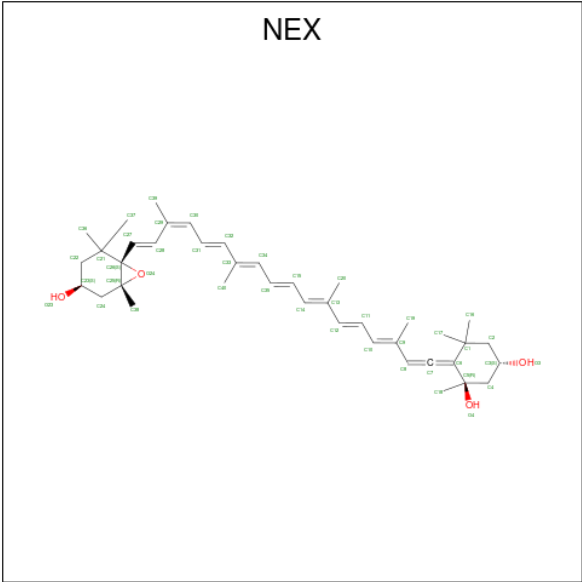
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	

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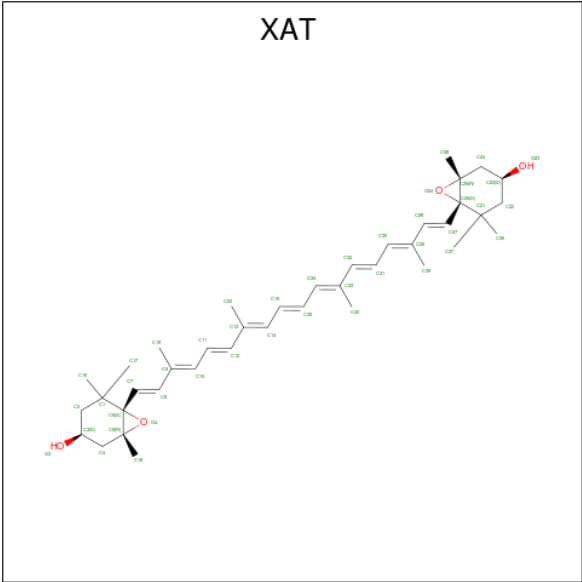
Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	G	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	N	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	Y	1	Total	C	O	0
			42	40	2	
39	R	1	Total	C	O	0
			42	40	2	
39	s	1	Total	C	O	0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

- 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-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



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

- 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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
41	R	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	23	Total	O	0
			23	23	
42	B	10	Total	O	0
			10	10	
42	C	14	Total	O	0
			14	14	
42	D	14	Total	O	0
			14	14	
42	H	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	L	3	Total	O	0
			3	3	
42	M	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	W	1	Total	O	0
			1	1	

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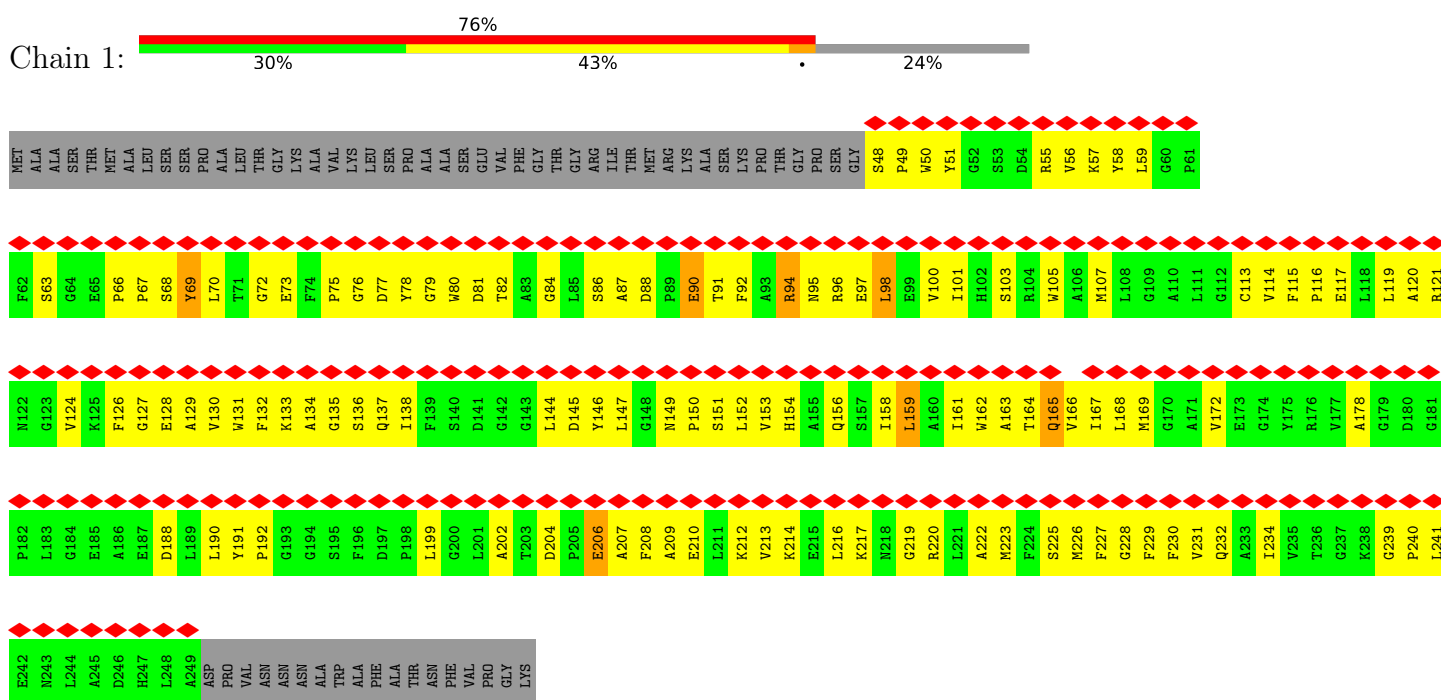
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Mol	Chain	Residues	Atoms		AltConf
42	a	23	Total 23	O 23	0
42	b	10	Total 10	O 10	0
42	c	14	Total 14	O 14	0
42	d	14	Total 14	O 14	0
42	h	1	Total 1	O 1	0
42	i	1	Total 1	O 1	0
42	l	3	Total 3	O 3	0
42	m	2	Total 2	O 2	0
42	t	1	Total 1	O 1	0
42	w	1	Total 1	O 1	0

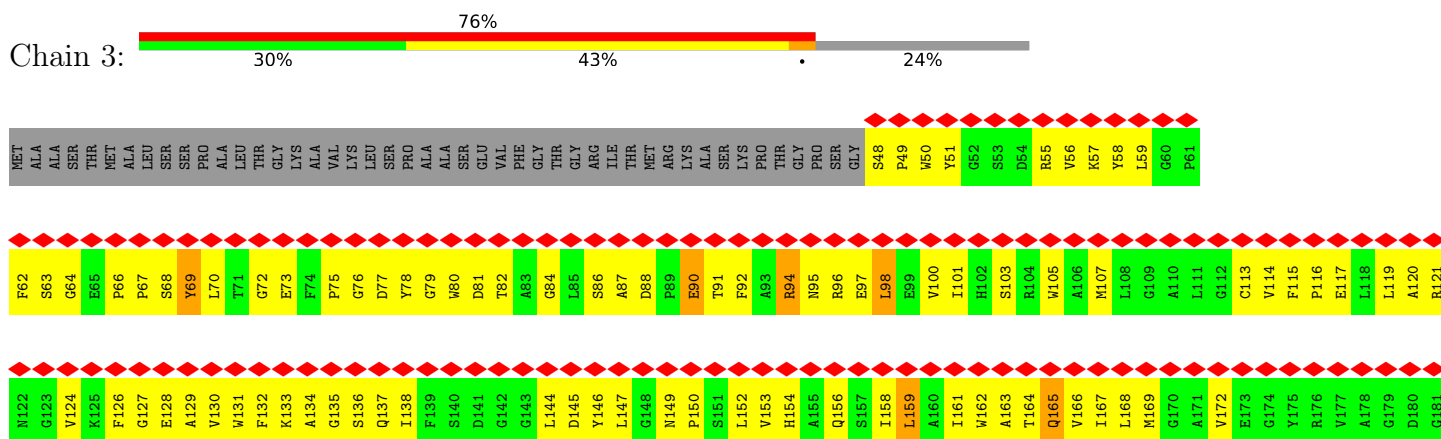
3 Residue-property plots [i](#)

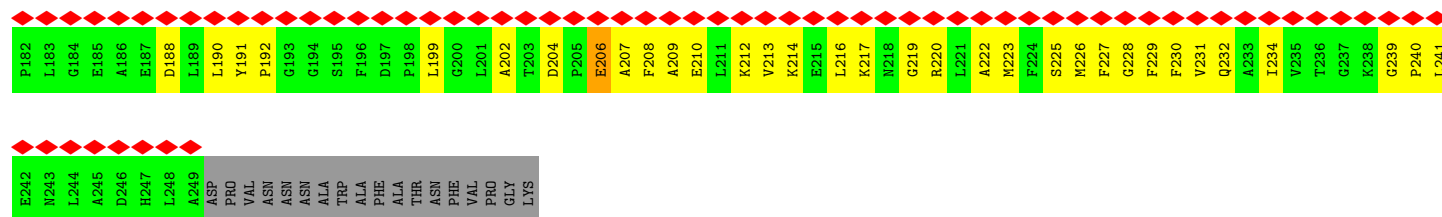
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

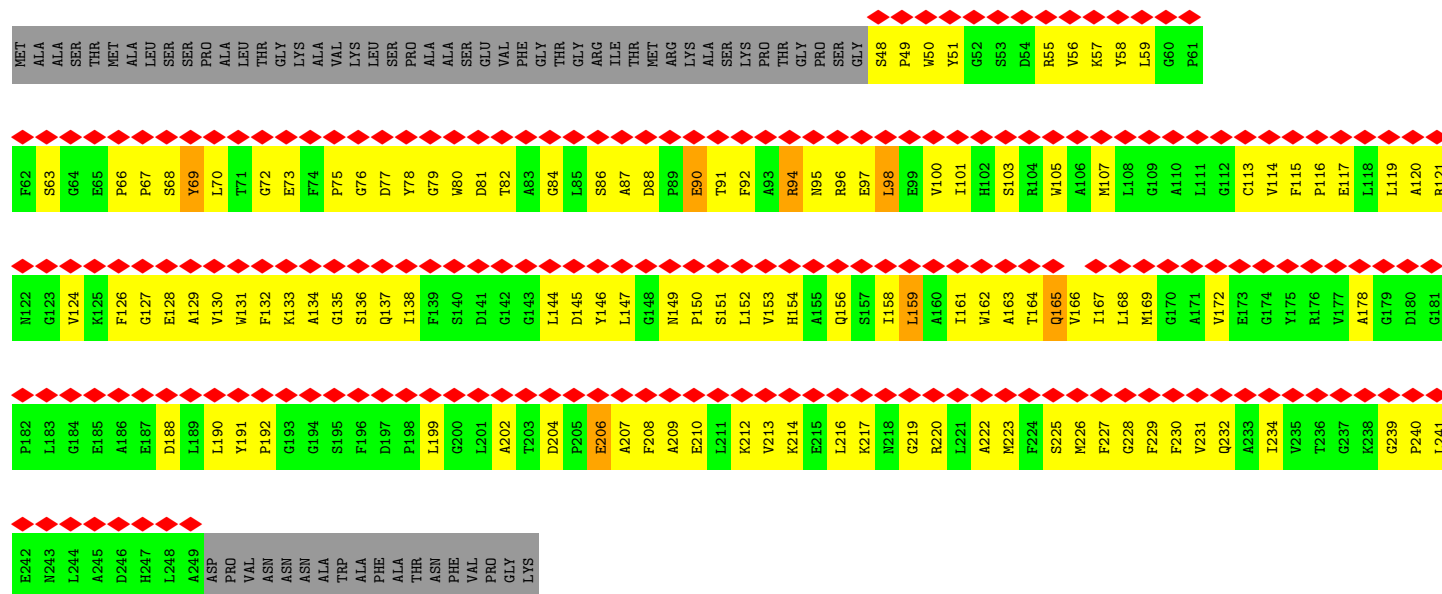
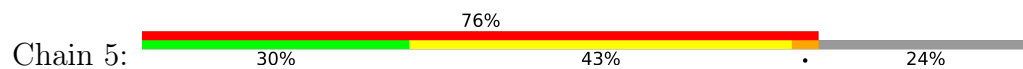


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

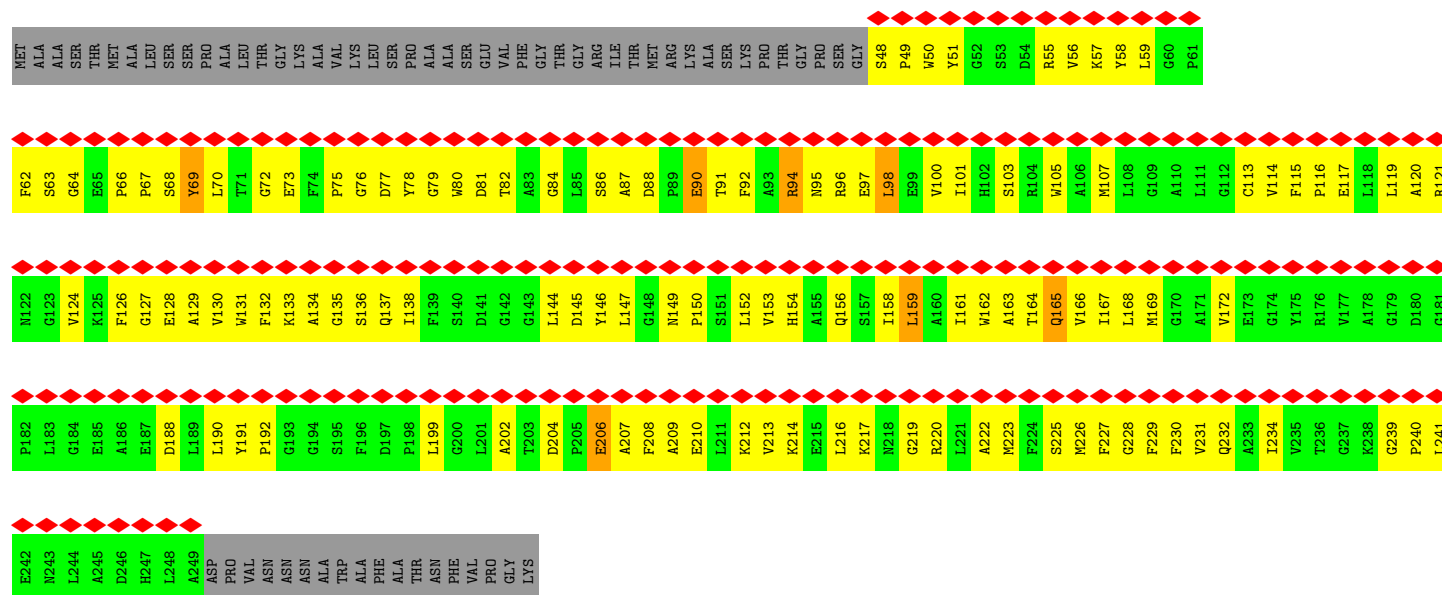
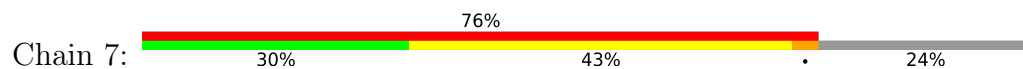




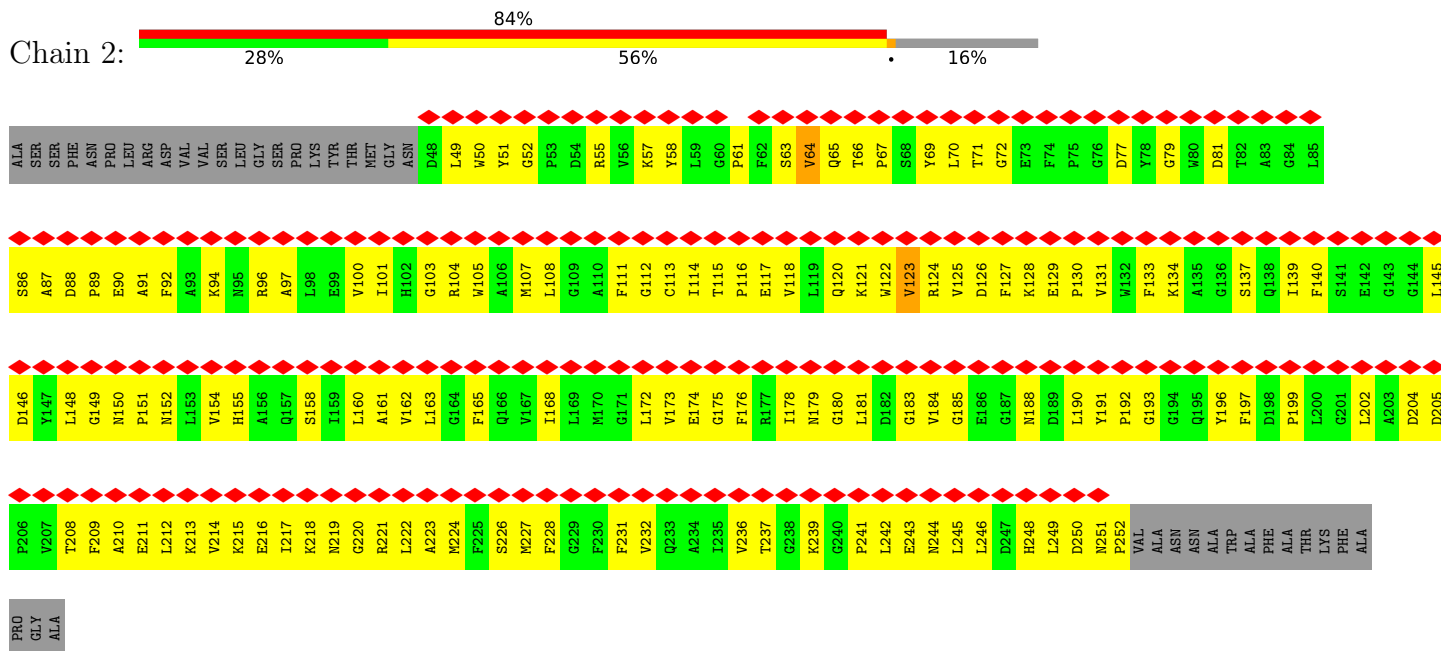
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



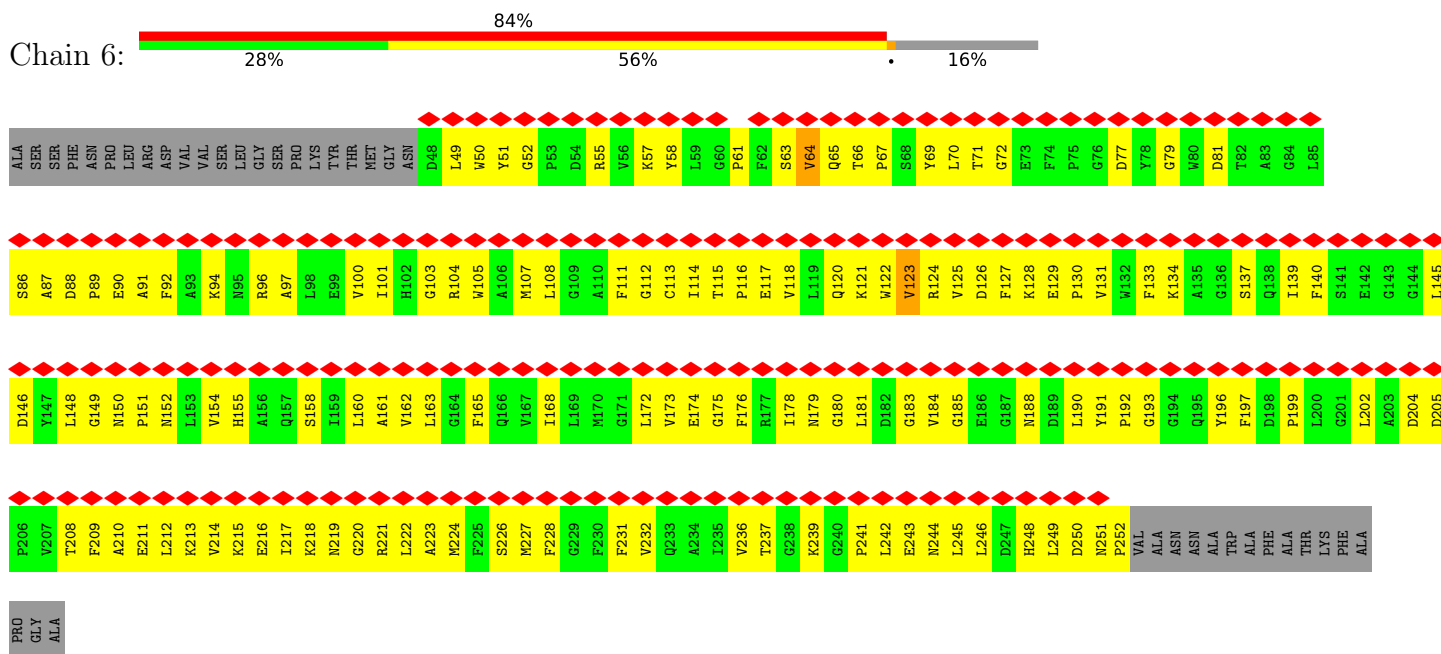
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



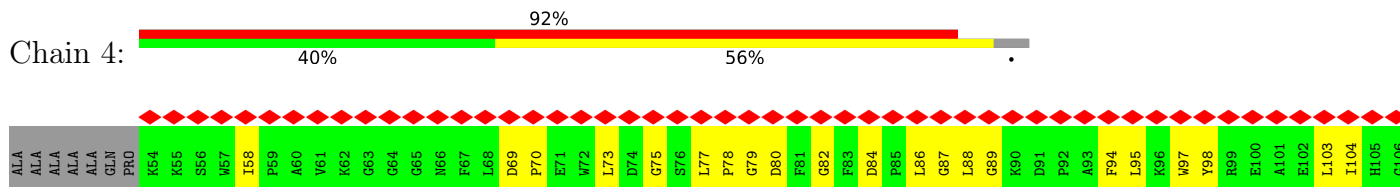
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

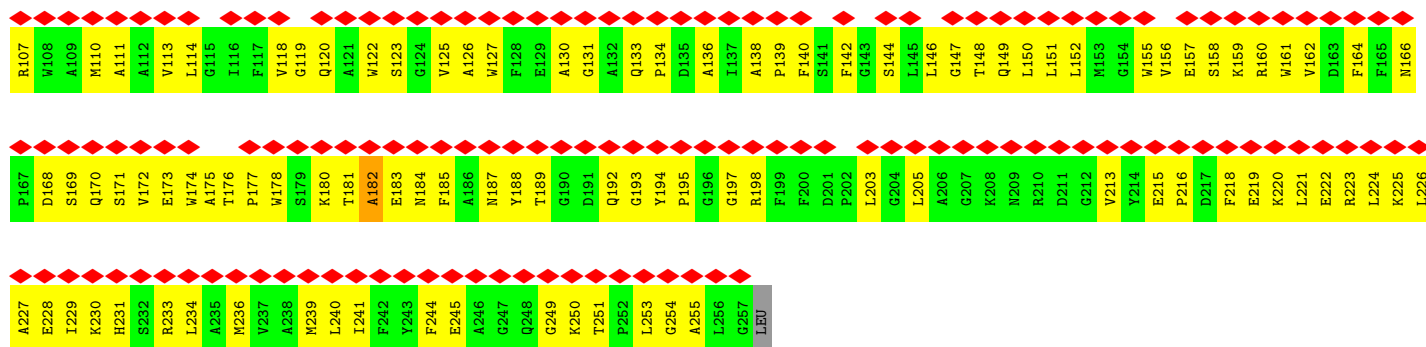


- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

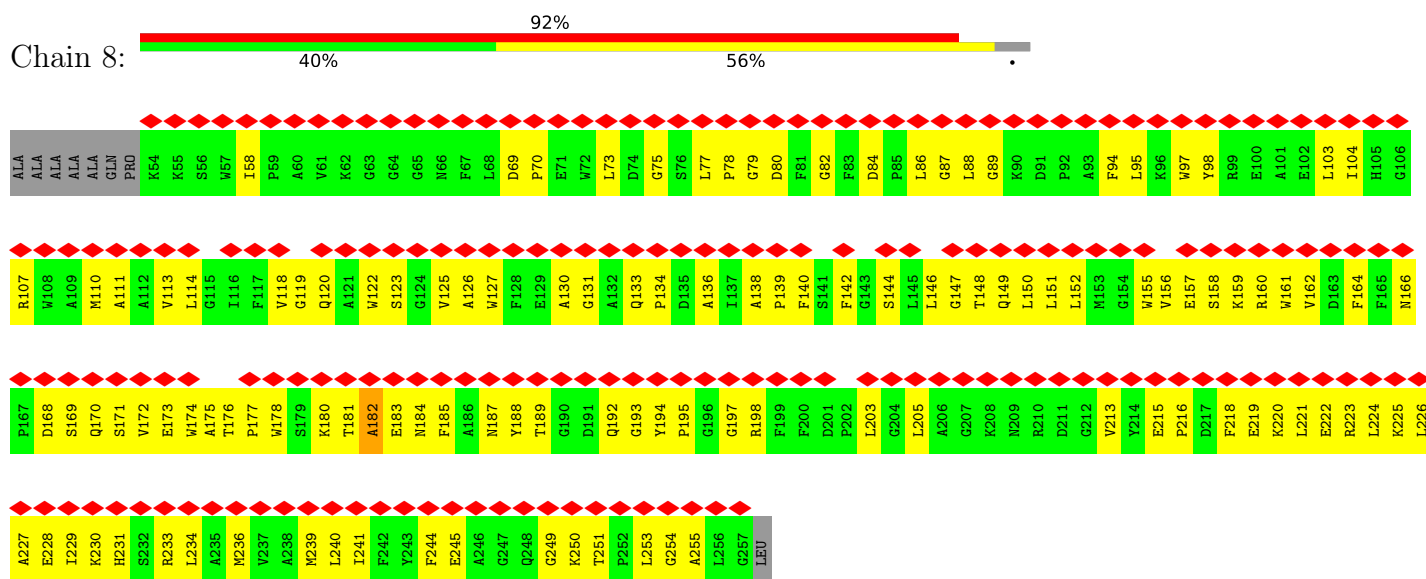


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

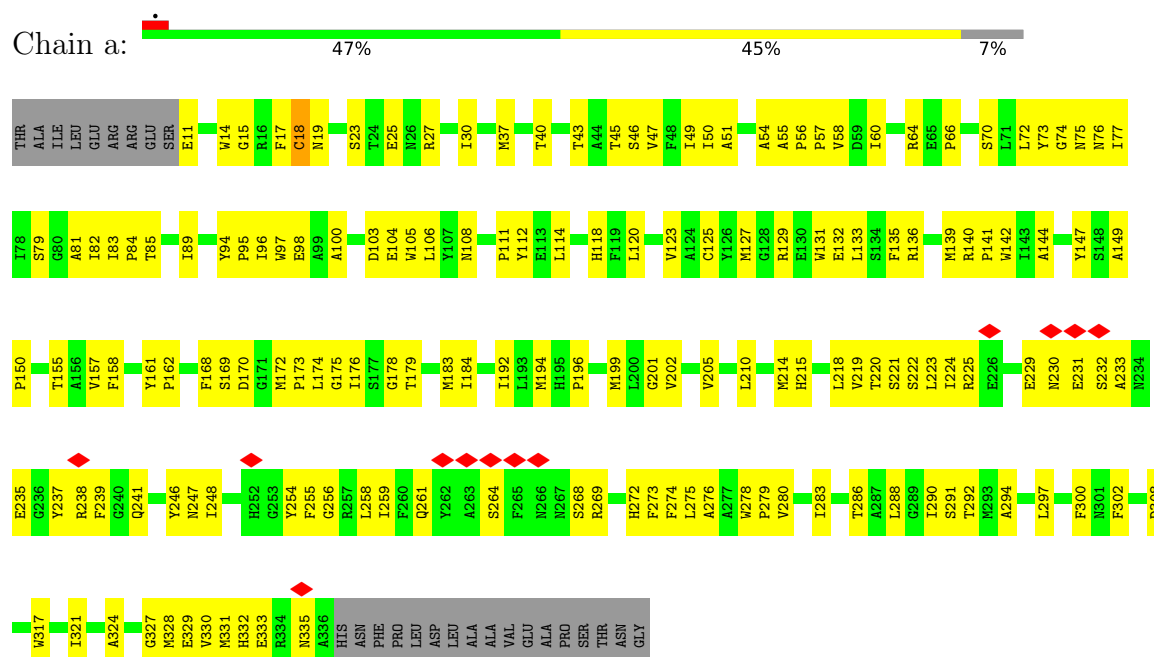




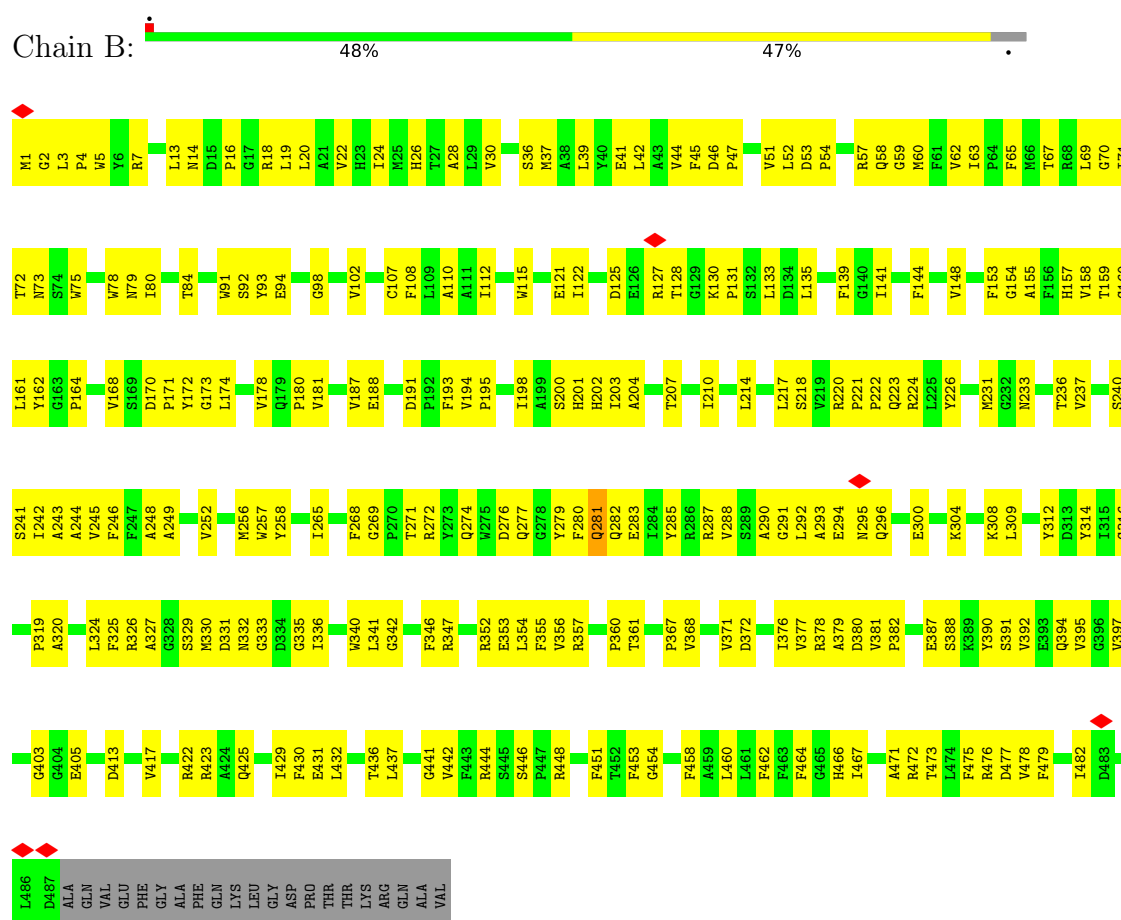
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic



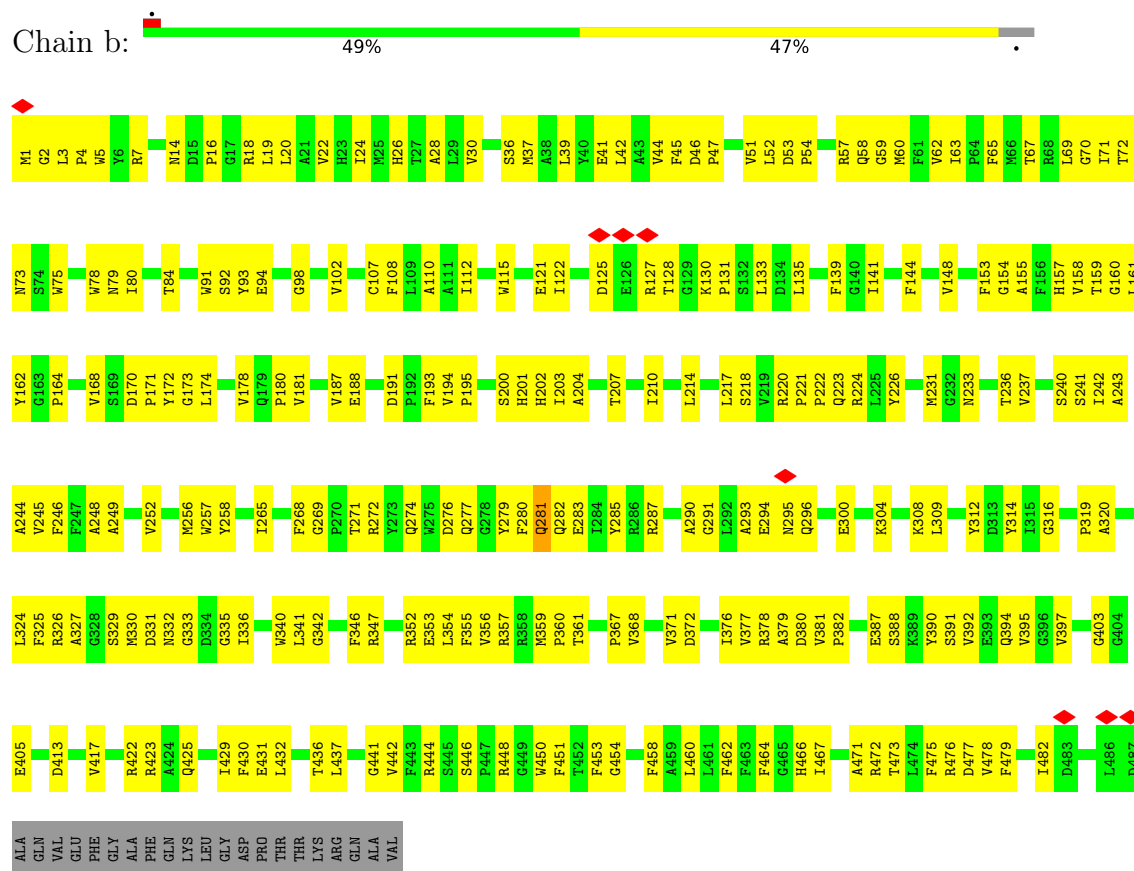
- Molecule 4: Photosystem II protein D1



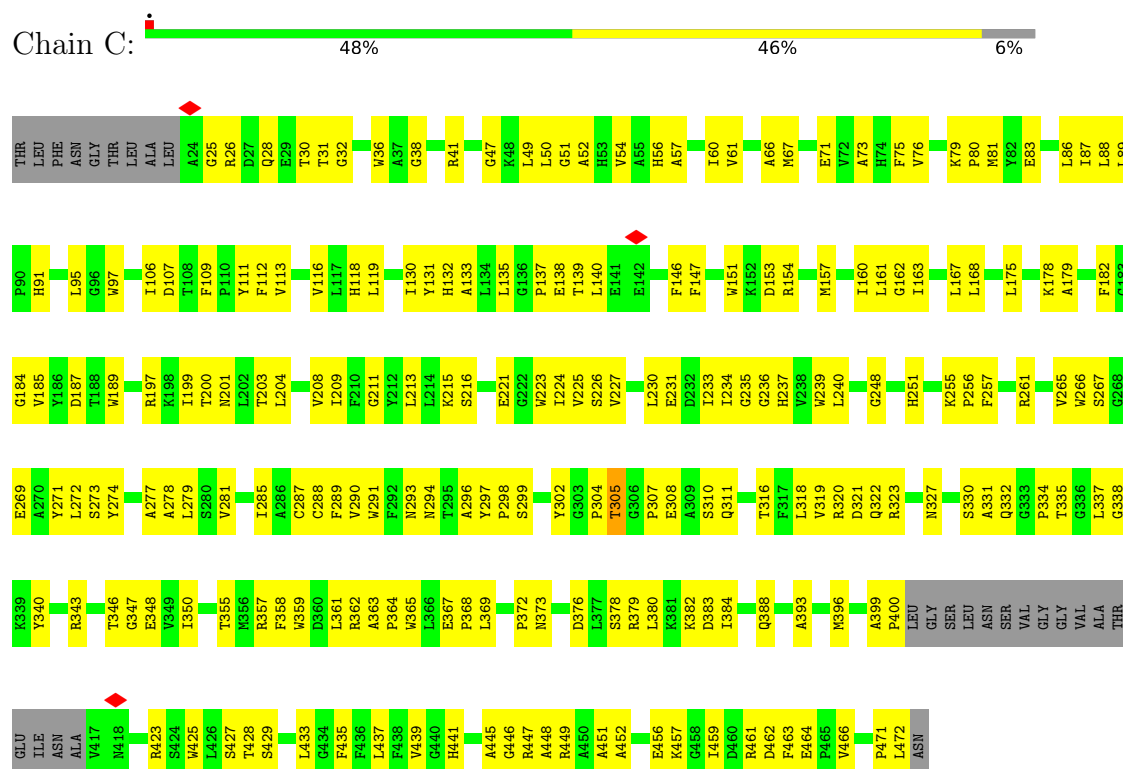
- Molecule 5: Photosystem II CP47 reaction center protein



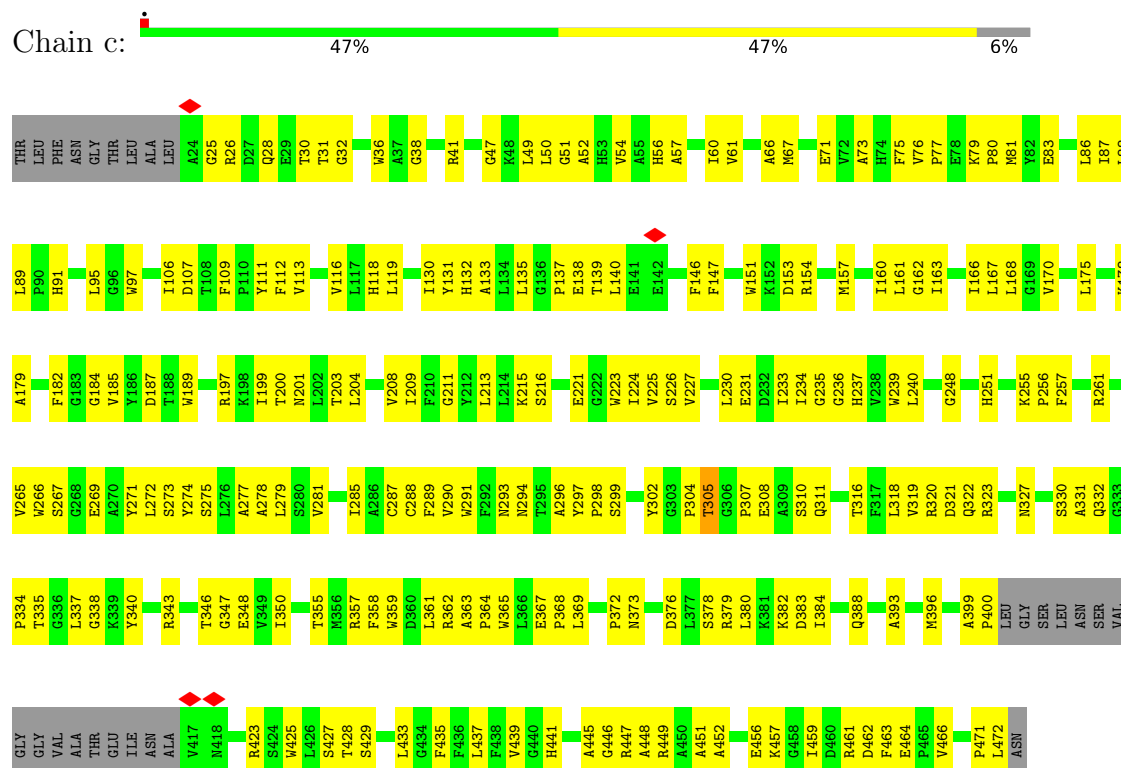
- Molecule 5: Photosystem II CP47 reaction center protein



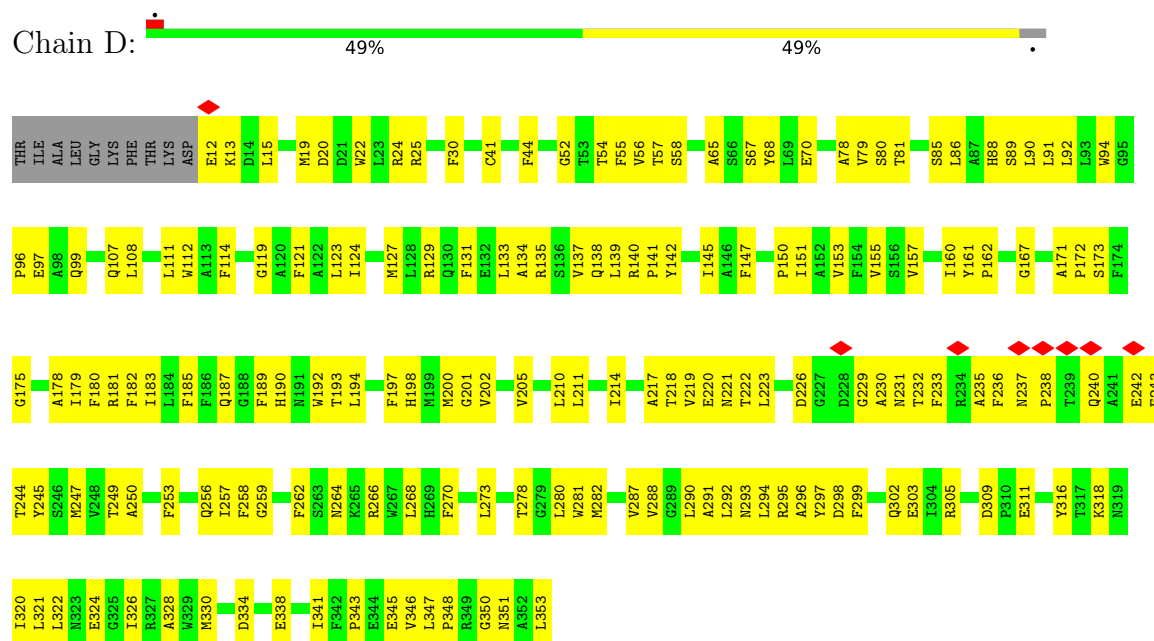
• Molecule 6: Photosystem II CP43 reaction center protein



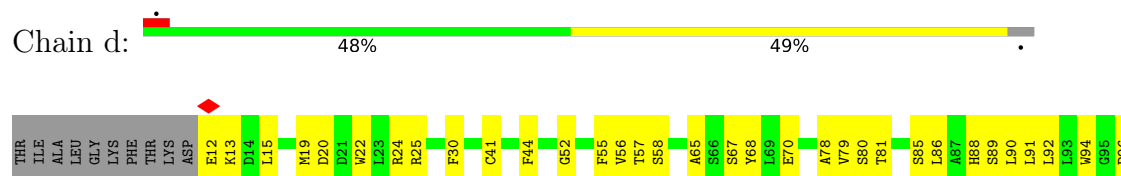
• Molecule 6: Photosystem II CP43 reaction center protein

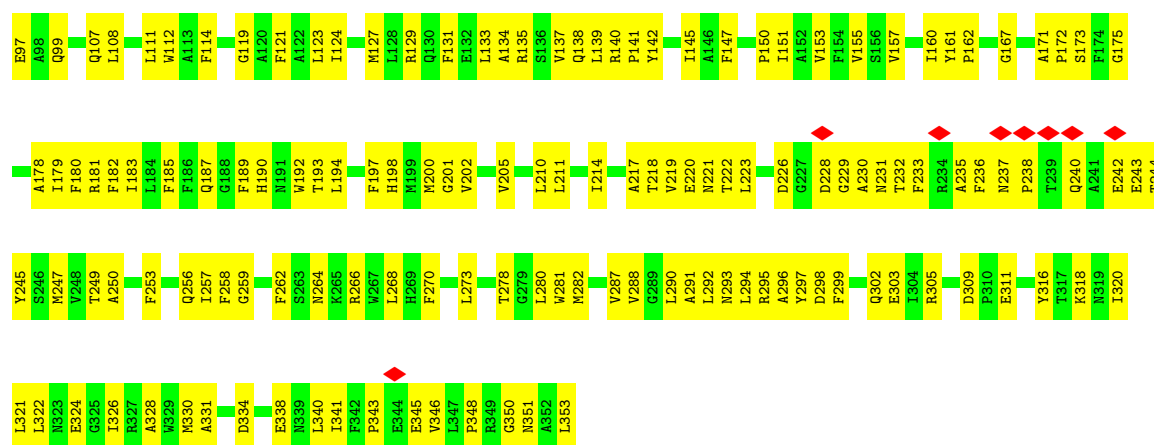


• Molecule 7: Photosystem II D2 protein

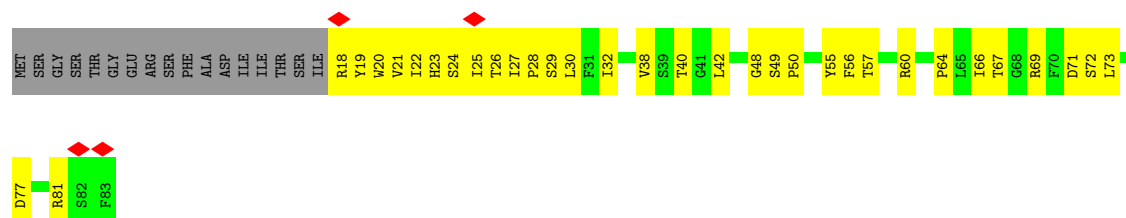
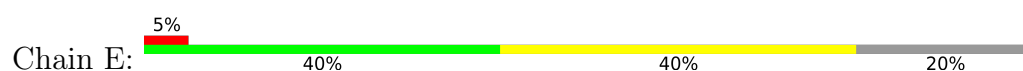


• Molecule 7: Photosystem II D2 protein

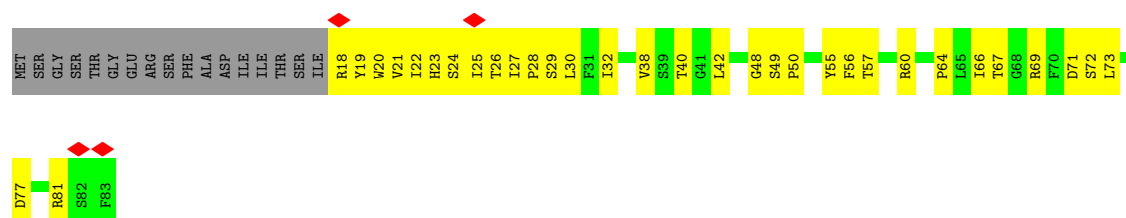




• Molecule 8: Cytochrome b559 subunit alpha



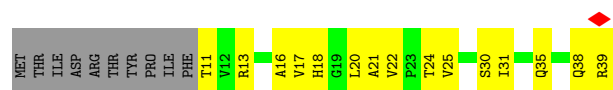
• Molecule 8: Cytochrome b559 subunit alpha



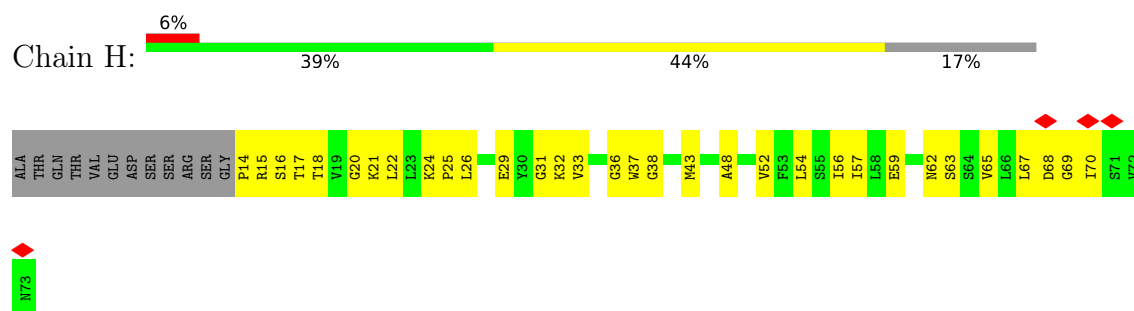
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



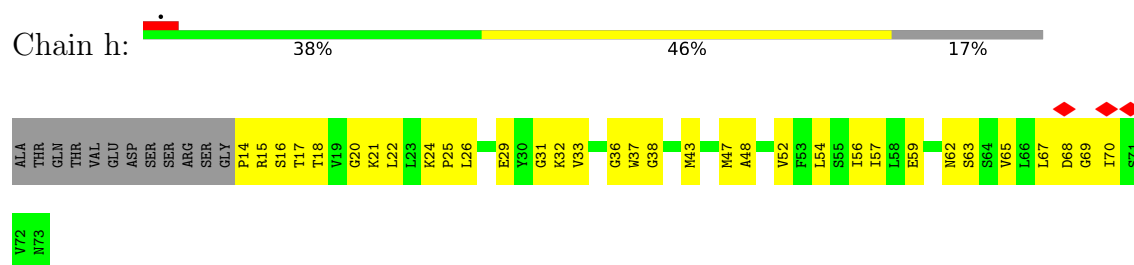
• Molecule 9: Cytochrome b559 subunit beta (PsbF)



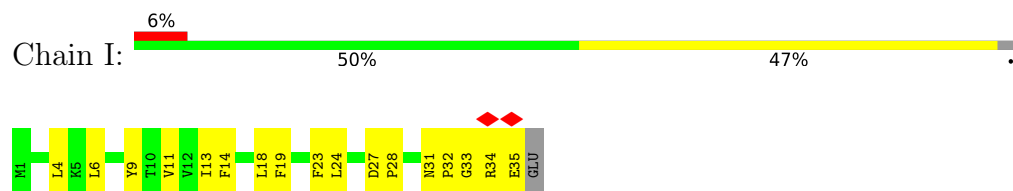
- Molecule 10: Photosystem II reaction center protein H



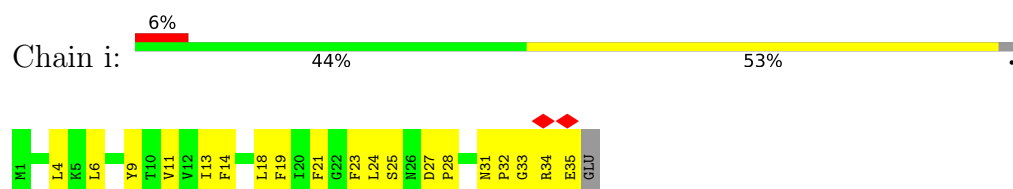
- Molecule 10: Photosystem II reaction center protein H



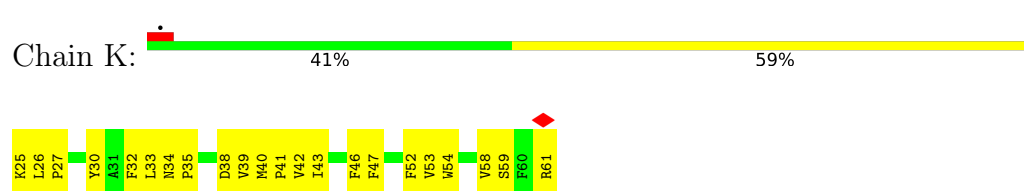
- Molecule 11: Photosystem II reaction center protein I



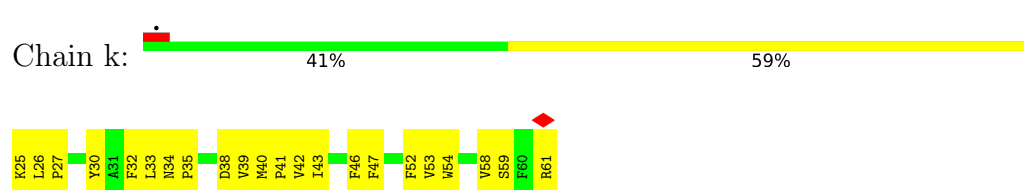
- Molecule 11: Photosystem II reaction center protein I



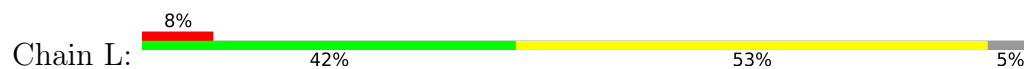
- Molecule 12: Photosystem II reaction center protein K



- Molecule 12: Photosystem II reaction center protein K



- Molecule 13: Photosystem II reaction center protein L



- Molecule 13: Photosystem II reaction center protein L



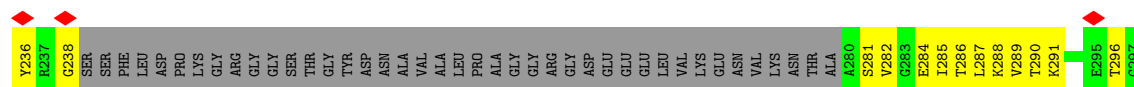
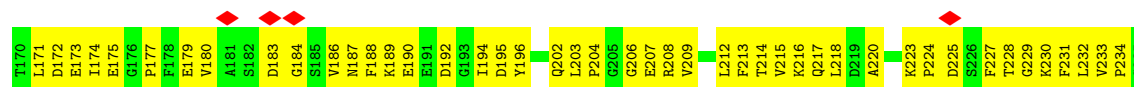
- Molecule 14: Photosystem II reaction center protein M



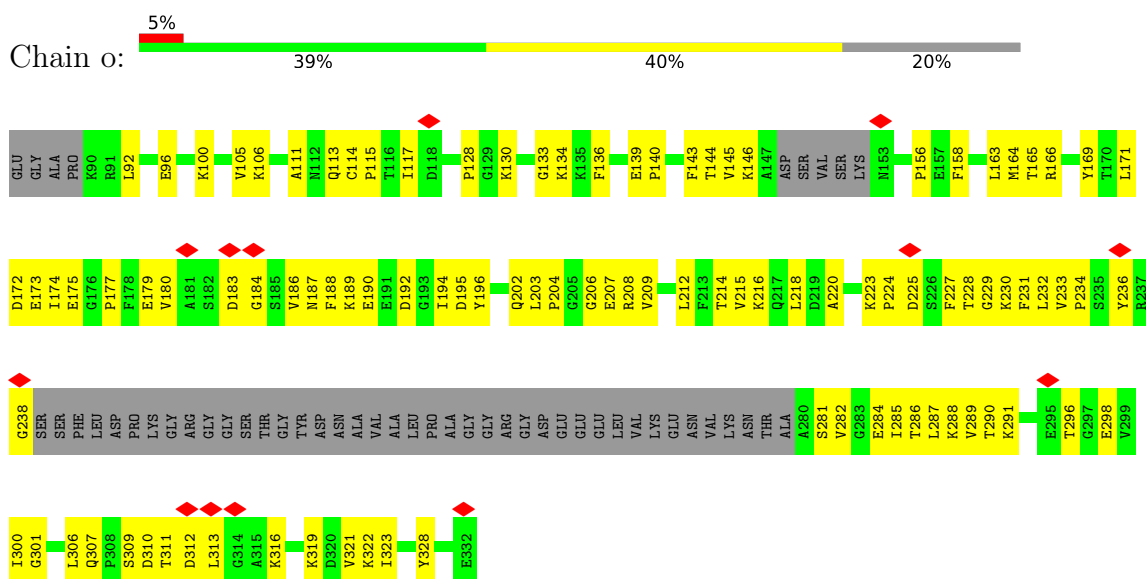
- Molecule 14: Photosystem II reaction center protein M



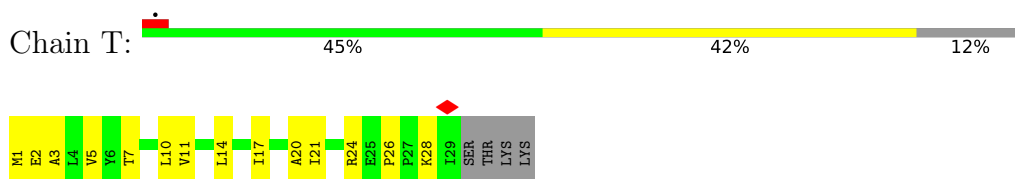
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



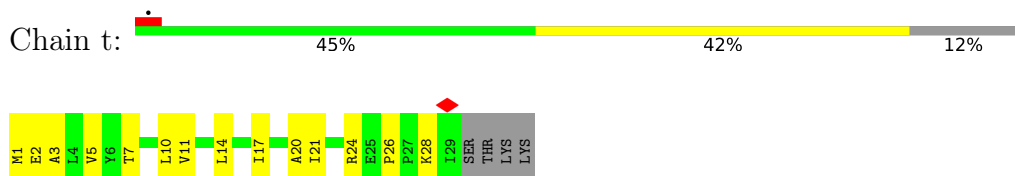
- Molecule 15: Oxygen-evolving enhancer protein 1-1, chloroplastic



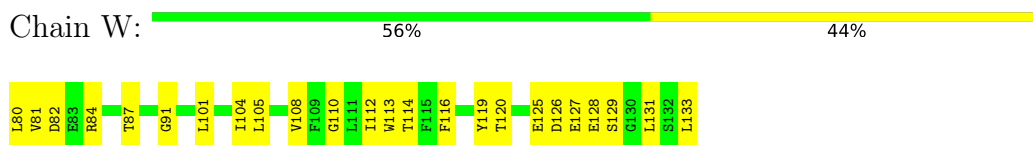
- Molecule 16: Photosystem II reaction center protein T



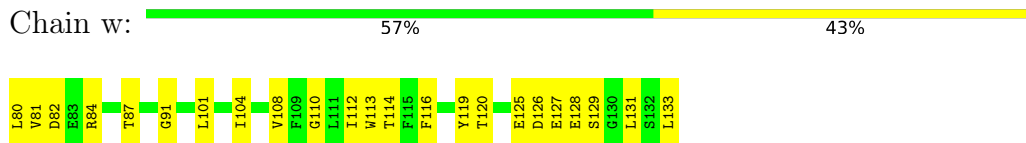
- Molecule 16: Photosystem II reaction center protein T



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



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



- Molecule 18: (thale cress) hypothetical protein





- Molecule 18: (thale cress) hypothetical protein



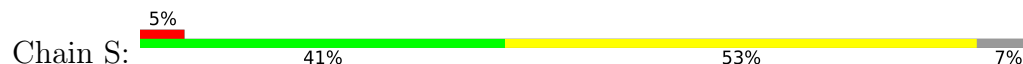
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z

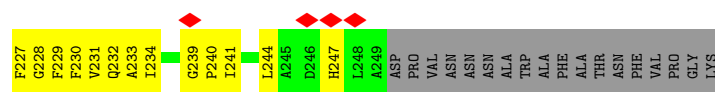


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

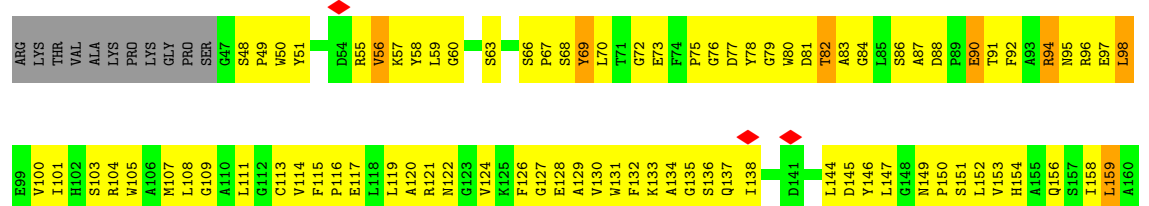
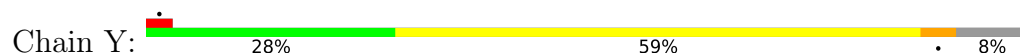


- Molecule 20: Chlorophyll a-b binding protein CP26, chloroplastic

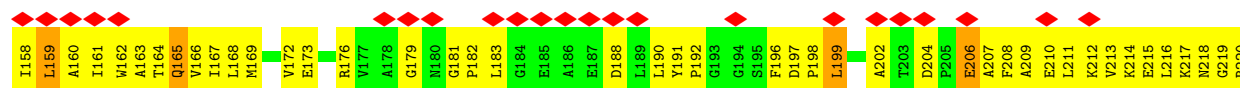




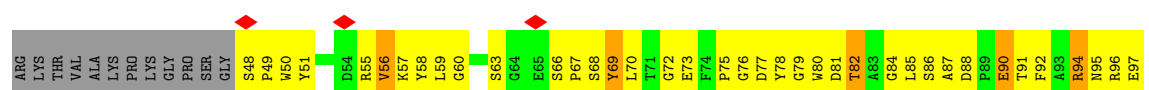
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

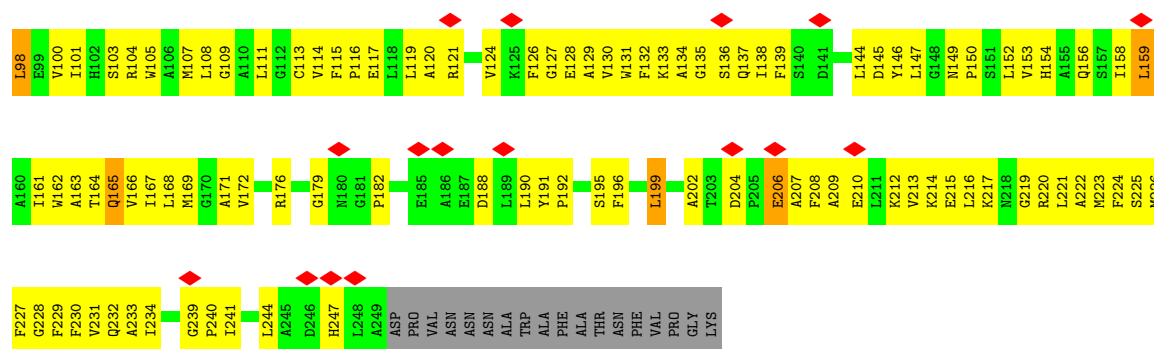


- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic



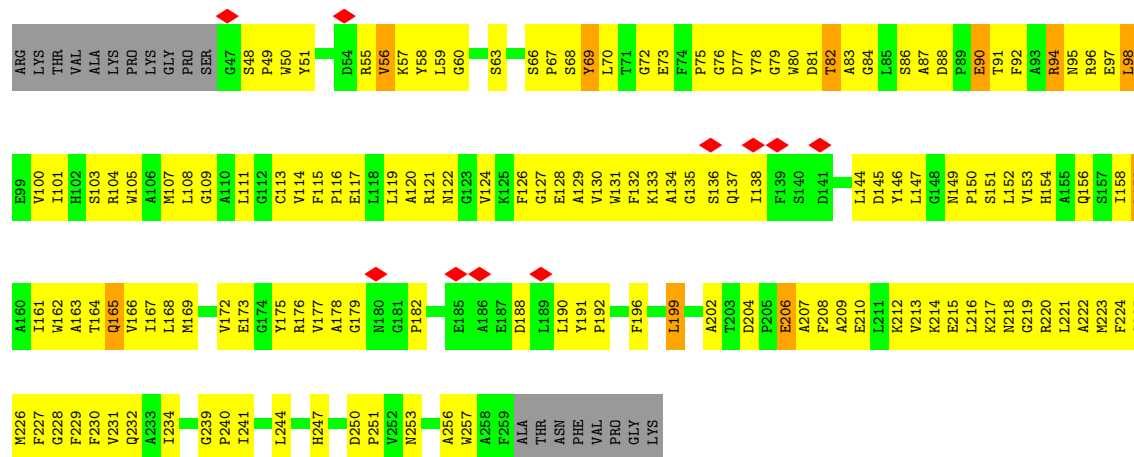
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic





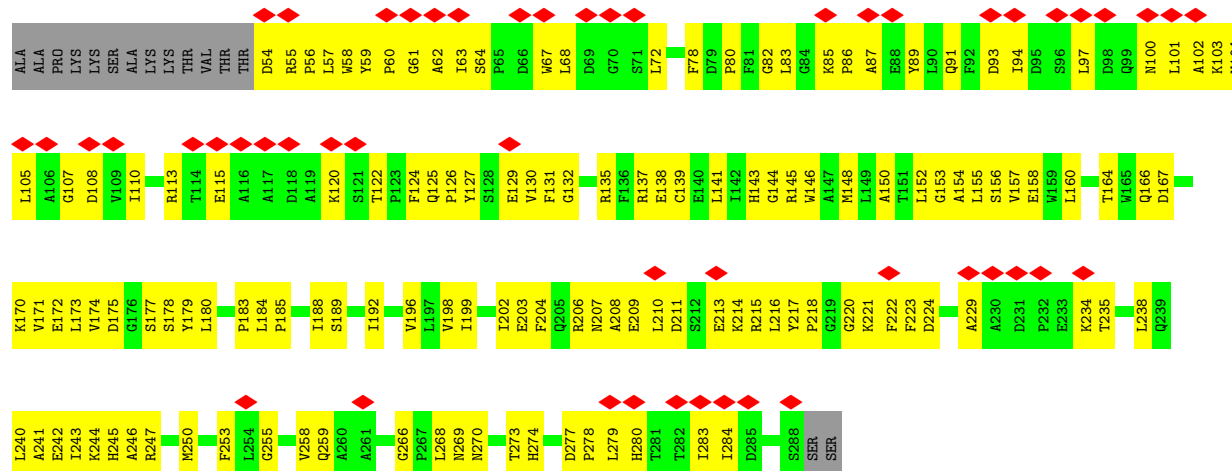
- Molecule 21: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 29% 59% 8%

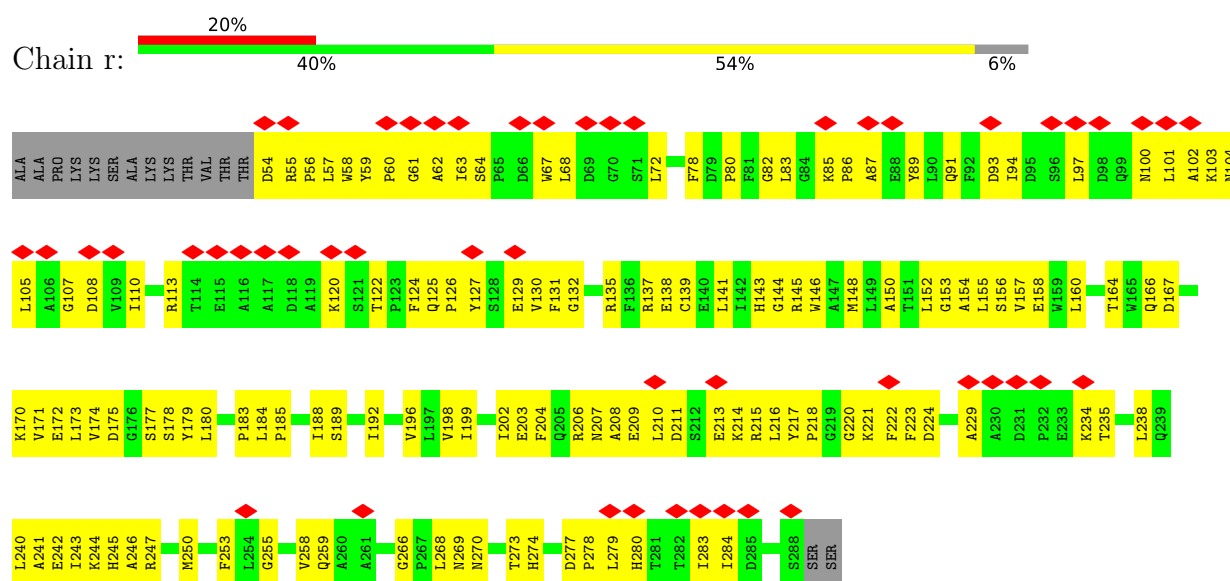


- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

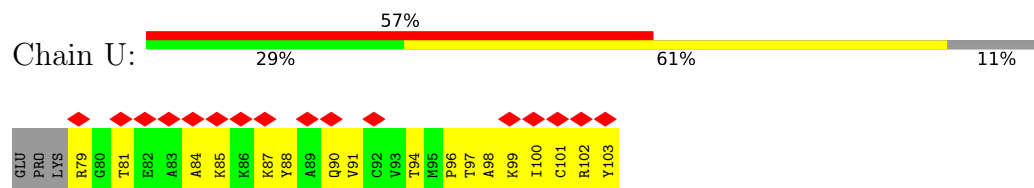
Chain R: 20% 39% 55% 6%



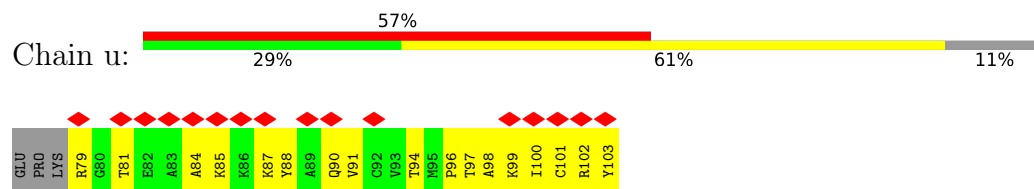
- Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic



• Molecule 23: Photosystem II 5 kDa protein, chloroplastic



• Molecule 23: Photosystem II 5 kDa protein, chloroplastic



4 Experimental information

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	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.19	0/1582	0.45	0/2150
1	3	0.19	0/1582	0.45	0/2150
1	5	0.19	0/1582	0.45	0/2150
1	7	0.19	0/1582	0.45	0/2150
2	2	0.17	0/1640	0.42	0/2229
2	6	0.17	0/1640	0.42	0/2229
3	4	0.17	0/1652	0.43	0/2242
3	8	0.17	0/1652	0.43	0/2242
4	A	0.12	0/2626	0.34	0/3580
4	a	0.12	0/2626	0.34	0/3580
5	B	0.12	0/3940	0.29	0/5368
5	b	0.12	0/3940	0.29	0/5368
6	C	0.11	0/3487	0.26	0/4750
6	c	0.11	0/3487	0.26	0/4750
7	D	0.12	0/2815	0.28	0/3837
7	d	0.12	0/2815	0.28	0/3837
8	E	0.10	0/561	0.29	0/763
8	e	0.10	0/561	0.29	0/763
9	F	0.09	0/229	0.24	0/311
9	f	0.09	0/229	0.24	0/311
10	H	0.10	0/455	0.36	0/619
10	h	0.10	0/455	0.35	0/619
11	I	0.13	0/294	0.38	0/397
11	i	0.12	0/294	0.38	0/397
12	K	0.10	0/312	0.27	0/428
12	k	0.10	0/312	0.27	0/428
13	L	0.09	0/310	0.20	0/421
13	l	0.09	0/310	0.20	0/421
14	M	0.11	0/254	0.28	0/347
14	m	0.11	0/254	0.28	0/347
15	O	0.10	0/1548	0.31	0/2091

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	o	0.10	0/1548	0.31	0/2091
16	T	0.09	0/246	0.22	0/333
16	t	0.09	0/246	0.22	0/333
17	W	0.10	0/438	0.26	0/594
17	w	0.10	0/438	0.26	0/594
18	X	0.09	0/250	0.23	0/339
18	x	0.10	0/250	0.23	0/339
19	Z	0.15	0/474	0.30	0/649
19	z	0.15	0/474	0.30	0/649
20	S	0.12	0/1715	0.29	0/2328
20	s	0.12	0/1715	0.30	0/2328
21	G	0.19	0/1607	0.44	0/2184
21	N	0.19	0/1580	0.44	0/2146
21	Y	0.19	0/1669	0.44	0/2270
21	g	0.19	0/1607	0.44	0/2184
21	n	0.19	0/1580	0.44	0/2146
21	y	0.19	0/1669	0.44	0/2270
22	R	0.15	0/1878	0.34	0/2561
22	r	0.15	0/1878	0.34	0/2561
23	U	0.08	0/196	0.27	0/261
23	u	0.09	0/196	0.27	0/261
All	All	0.14	0/66680	0.35	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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1537	0	1480	181	0
1	3	1537	0	1480	182	0
1	5	1537	0	1480	179	0
1	7	1537	0	1480	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	1593	0	1543	287	0
2	6	1593	0	1543	292	0
3	4	1597	0	1534	197	0
3	8	1597	0	1534	200	0
4	A	2548	0	2460	229	0
4	a	2548	0	2460	233	0
5	B	3810	0	3688	326	0
5	b	3810	0	3688	327	0
6	C	3373	0	3302	277	0
6	c	3373	0	3302	284	0
7	D	2722	0	2615	251	0
7	d	2722	0	2615	255	0
8	E	543	0	519	38	0
8	e	543	0	519	37	0
9	F	224	0	233	14	0
9	f	224	0	233	14	0
10	H	446	0	471	58	0
10	h	446	0	471	60	0
11	I	286	0	295	32	0
11	i	286	0	295	32	0
12	K	301	0	313	28	0
12	k	301	0	313	28	0
13	L	302	0	291	29	0
13	l	302	0	291	30	0
14	M	250	0	279	41	0
14	m	250	0	279	41	0
15	O	1516	0	1494	133	0
15	o	1516	0	1494	131	0
16	T	239	0	255	19	0
16	t	239	0	255	20	0
17	W	427	0	405	33	0
17	w	427	0	405	34	0
18	X	248	0	266	43	0
18	x	248	0	266	43	0
19	Z	464	0	495	38	0
19	z	464	0	495	40	0
20	S	1670	0	1647	186	0
20	s	1670	0	1647	188	0
21	G	1562	0	1501	302	0
21	N	1536	0	1478	293	0
21	Y	1621	0	1546	306	0
21	g	1562	0	1501	300	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	n	1536	0	1478	295	0
21	y	1621	0	1546	307	0
22	R	1827	0	1777	212	0
22	r	1827	0	1777	211	0
23	U	194	0	206	36	0
23	u	194	0	206	35	0
24	1	92	0	62	18	0
24	2	110	0	91	29	0
24	5	92	0	62	17	0
24	6	110	0	91	30	0
24	G	335	0	296	78	0
24	N	348	0	321	117	0
24	R	195	0	146	23	0
24	S	184	0	124	28	0
24	Y	344	0	308	94	0
24	g	335	0	296	77	0
24	n	348	0	321	116	0
24	r	195	0	146	24	0
24	s	184	0	124	33	0
24	y	344	0	308	93	0
25	2	163	0	142	33	0
25	6	163	0	142	37	0
25	A	190	0	203	39	0
25	B	1040	0	1150	147	0
25	C	840	0	923	145	0
25	D	180	0	183	41	0
25	G	472	0	464	110	0
25	N	473	0	468	139	0
25	R	543	0	490	113	0
25	S	465	0	393	90	0
25	Y	470	0	465	123	0
25	a	190	0	203	39	0
25	b	1040	0	1150	149	0
25	c	840	0	923	157	0
25	d	180	0	183	42	0
25	g	472	0	464	115	0
25	n	473	0	468	136	0
25	r	543	0	490	121	0
25	s	465	0	393	92	0
25	y	470	0	465	120	0
26	2	47	0	67	14	0
26	6	47	0	67	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	142	0	206	18	0
26	C	147	74	222	10	0
26	D	49	0	74	10	0
26	L	49	0	74	5	0
26	N	49	0	74	11	0
26	R	42	0	56	14	0
26	S	98	0	148	13	0
26	Y	98	0	146	20	0
26	b	142	0	206	18	0
26	c	147	74	222	10	0
26	d	49	0	74	10	0
26	l	49	0	74	5	0
26	n	49	0	74	10	0
26	r	42	0	56	16	0
26	s	98	0	148	15	0
26	y	98	0	146	20	0
27	A	128	0	148	27	0
27	a	128	0	148	28	0
28	A	40	0	56	4	0
28	B	120	0	168	18	0
28	C	40	0	56	7	0
28	D	40	0	56	3	0
28	H	40	0	56	6	0
28	I	40	0	56	20	0
28	K	40	0	56	7	0
28	T	40	0	54	20	0
28	Z	40	0	56	5	0
28	a	40	0	56	5	0
28	b	120	0	168	19	0
28	c	40	0	56	7	0
28	d	40	0	56	3	0
28	h	40	0	56	8	0
28	i	40	0	56	20	0
28	k	40	0	56	9	0
28	t	40	0	54	21	0
28	z	40	0	56	5	0
29	A	104	0	145	13	0
29	L	96	0	126	25	0
29	a	104	0	145	12	0
29	l	96	0	126	25	0
30	A	88	0	116	6	0
30	B	106	0	158	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C	51	0	72	4	0
30	D	46	0	62	3	0
30	a	88	0	116	6	0
30	b	106	0	158	10	0
30	c	51	0	72	4	0
30	d	46	0	62	3	0
31	A	13	0	7	2	0
31	D	55	0	80	6	0
31	a	13	0	7	2	0
31	d	55	0	80	6	0
32	A	85	92	0	0	0
32	B	85	92	0	0	0
32	G	42	53	0	0	0
32	N	84	106	0	3	0
32	S	42	53	0	2	0
32	Y	210	265	0	7	0
32	a	85	92	0	0	0
32	b	85	92	0	0	0
32	g	42	53	0	0	0
32	n	84	106	0	3	0
32	s	42	53	0	2	0
32	y	210	265	0	7	0
33	A	4	0	1	2	0
33	a	4	0	1	1	0
34	A	1	0	0	0	0
34	a	1	0	0	0	0
35	A	59	0	76	3	0
35	B	62	0	82	5	0
35	C	117	0	150	18	0
35	a	59	0	76	3	0
35	b	62	0	82	6	0
35	c	117	0	150	17	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
37	D	1	0	0	1	0
37	d	1	0	0	1	0
38	F	43	0	30	7	0
38	f	43	0	30	8	0
39	G	84	0	112	30	0
39	N	84	0	112	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	R	42	0	56	6	0
39	S	84	0	112	27	0
39	Y	84	0	112	25	0
39	g	84	0	112	30	0
39	n	84	0	112	27	0
39	r	42	0	56	8	0
39	s	84	0	112	29	0
39	y	84	0	112	25	0
40	G	44	0	56	15	0
40	N	44	0	56	15	0
40	R	44	0	56	8	0
40	S	44	0	56	6	0
40	Y	44	0	56	7	0
40	g	44	0	56	15	0
40	n	44	0	56	13	0
40	r	44	0	56	10	0
40	s	44	0	56	5	0
40	y	44	0	56	10	0
41	R	44	0	56	20	0
41	r	44	0	56	22	0
42	A	23	0	0	0	0
42	B	10	0	0	3	0
42	C	14	0	0	1	0
42	D	14	0	0	0	0
42	H	1	0	0	0	0
42	I	1	0	0	0	0
42	L	3	0	0	2	0
42	M	1	0	0	0	0
42	T	1	0	0	0	0
42	W	1	0	0	0	0
42	a	23	0	0	1	0
42	b	10	0	0	3	0
42	c	14	0	0	1	0
42	d	14	0	0	0	0
42	h	1	0	0	0	0
42	i	1	0	0	0	0
42	l	3	0	0	2	0
42	m	2	0	0	0	0
42	t	1	0	0	0	0
42	w	1	0	0	0	0
All	All	84427	1470	83152	8481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 51.

The worst 5 of 8481 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:196:TYR:HB2	15:O:212:LEU:HD21	1.21	1.19
10:h:56:ILE:HD13	18:x:84:LYS:HE3	1.25	1.17
21:n:138:ILE:HG21	24:n:606:CHL:HBC1	1.23	1.17
22:r:144:GLY:HA3	22:r:246:ALA:HB1	1.28	1.16
22:R:144:GLY:HA3	22:R:246:ALA:HB1	1.28	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	12	38
2	6	203/243 (84%)	181 (89%)	20 (10%)	2 (1%)	12	38
3	4	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
3	8	202/212 (95%)	183 (91%)	18 (9%)	1 (0%)	24	55
4	A	324/352 (92%)	309 (95%)	14 (4%)	1 (0%)	36	66
4	a	324/352 (92%)	308 (95%)	15 (5%)	1 (0%)	36	66
5	B	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
5	b	485/508 (96%)	466 (96%)	18 (4%)	1 (0%)	43	72
6	C	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	429/459 (94%)	417 (97%)	11 (3%)	1 (0%)	43	72
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%)	3	11
14	m	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	11
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	44	72

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 ⓘ

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%)	142 (92%)	12 (8%)	11	35
1	3	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	5	154/201 (77%)	142 (92%)	12 (8%)	11	35
1	7	154/201 (77%)	142 (92%)	12 (8%)	11	35
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%)	156 (100%)	0	100	100
3	8	156/159 (98%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	384 (100%)	0	100	100
5	b	384/402 (96%)	384 (100%)	0	100	100
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
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%)	167 (100%)	0	100	100
15	o	167/204 (82%)	167 (100%)	0	100	100
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%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	54/54 (100%)	54 (100%)	0	100	100
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%)	145 (92%)	12 (8%)	12	36
21	N	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	Y	162/177 (92%)	150 (93%)	12 (7%)	13	37
21	g	157/177 (89%)	145 (92%)	12 (8%)	12	36
21	n	154/177 (87%)	142 (92%)	12 (8%)	11	35
21	y	162/177 (92%)	150 (93%)	12 (7%)	13	37
22	R	189/201 (94%)	189 (100%)	0	100	100
22	r	189/201 (94%)	189 (100%)	0	100	100
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%)	6520 (98%)	120 (2%)	51	82

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	Y	165	GLN
21	y	68	SER
1	5	206	GLU
21	y	56	VAL
21	y	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	6	150	ASN
6	c	237	HIS
20	s	135	ASN
5	b	73	ASN
5	b	296	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 374 ligands modelled in this entry, 8 are monoatomic - leaving 366 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$
24	CHL	g	605	21	40,54,74	2.32	13 (32%)	34,90,114	3.20	16 (47%)
30	LMG	a	409	-	48,48,55	0.44	0	56,56,63	1.19	4 (7%)
28	BCR	D	404	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	5 (8%)
30	LMG	B	620	-	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
28	BCR	t	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	9 (16%)
26	LHG	2	606	25	46,46,48	0.44	0	49,52,54	1.20	4 (8%)
24	CHL	Y	308	-	52,66,74	2.10	12 (23%)	48,104,114	2.75	18 (37%)
26	LHG	y	319	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
32	AJP	B	624	-	95,95,95	0.62	0	144,149,149	3.58	58 (40%)
24	CHL	l	302	1	40,54,74	2.34	14 (35%)	34,90,114	3.28	15 (44%)
28	BCR	h	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
24	CHL	R	606	-	40,54,74	2.32	12 (30%)	34,90,114	3.22	16 (47%)
26	LHG	n	618	25	48,48,48	0.43	0	51,54,54	1.16	4 (7%)
25	CLA	b	614	5	69,73,73	1.35	11 (15%)	82,113,113	1.72	14 (17%)
26	LHG	S	318	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
28	BCR	k	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	9 (16%)
25	CLA	b	613	5	69,73,73	1.36	11 (15%)	82,113,113	1.55	15 (18%)
24	CHL	s	307	-	40,54,74	2.31	12 (30%)	34,90,114	3.17	17 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	S	306	-	40,54,74	2.31	12 (30%)	34,90,114	3.15	18 (52%)
24	CHL	s	308	-	40,54,74	2.32	13 (32%)	34,90,114	3.17	16 (47%)
25	CLA	n	614	21	52,56,73	1.60	8 (15%)	61,92,113	1.98	16 (26%)
25	CLA	B	609	5	69,73,73	1.37	11 (15%)	82,113,113	1.71	17 (20%)
39	LUT	Y	316	-	42,43,43	0.82	2 (4%)	51,60,60	1.55	7 (13%)
25	CLA	S	313	20	59,63,73	1.50	9 (15%)	70,101,113	2.19	16 (22%)
25	CLA	s	310	20	59,63,73	1.49	10 (16%)	70,101,113	1.61	12 (17%)
25	CLA	B	602	5	69,73,73	1.35	11 (15%)	82,113,113	1.62	17 (20%)
25	CLA	S	314	20	53,57,73	1.55	12 (22%)	61,93,113	1.66	13 (21%)
25	CLA	b	602	5	69,73,73	1.36	10 (14%)	82,113,113	1.62	18 (21%)
24	CHL	N	607	-	60,74,74	1.92	12 (20%)	58,114,114	2.46	17 (29%)
25	CLA	d	403	-	69,73,73	1.54	8 (11%)	82,113,113	2.61	21 (25%)
28	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
32	AJP	G	618	-	48,48,95	0.90	0	72,78,149	5.61	37 (51%)
24	CHL	n	605	21	42,56,74	2.22	11 (26%)	36,92,114	3.11	16 (44%)
26	LHG	c	517	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	n	612	21	64,68,73	1.44	12 (18%)	76,107,113	1.72	14 (18%)
25	CLA	r	612	22	64,68,73	1.45	9 (14%)	76,107,113	1.91	17 (22%)
24	CHL	N	606	-	40,54,74	2.29	12 (30%)	34,90,114	3.25	17 (50%)
24	CHL	g	609	21	55,69,74	2.02	12 (21%)	52,108,114	2.78	18 (34%)
32	AJP	n	619	-	48,48,95	0.73	0	72,78,149	4.33	34 (47%)
30	LMG	C	520	-	51,51,55	0.45	0	59,59,63	1.22	4 (6%)
25	CLA	N	603	-	69,73,73	1.37	11 (15%)	82,113,113	1.64	15 (18%)
25	CLA	C	501	-	69,73,73	1.50	7 (10%)	82,113,113	2.42	21 (25%)
31	PL9	A	409	-	13,13,55	0.89	0	17,17,69	0.76	0
25	CLA	B	612	5	69,73,73	1.37	11 (15%)	82,113,113	1.66	16 (19%)
24	CHL	5	301	1	40,54,74	2.33	13 (32%)	34,90,114	3.11	17 (50%)
26	LHG	c	519	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
26	LHG	S	301	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
25	CLA	R	612	22	64,68,73	1.45	9 (14%)	76,107,113	1.91	17 (22%)
25	CLA	D	402	7	69,73,73	1.39	11 (15%)	82,113,113	1.69	18 (21%)
25	CLA	s	311	26	60,64,73	1.46	10 (16%)	71,102,113	2.04	13 (18%)
30	LMG	A	408	-	48,48,55	0.44	0	56,56,63	1.19	4 (7%)
24	CHL	y	310	21	50,64,74	2.10	13 (26%)	46,102,114	2.83	18 (39%)
25	CLA	C	507	-	69,73,73	1.39	11 (15%)	82,113,113	1.55	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LHG	b	622	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
24	CHL	1	301	1	40,54,74	2.33	13 (32%)	34,90,114	3.08	17 (50%)
26	LHG	6	606	25	46,46,48	0.44	0	49,52,54	1.20	4 (8%)
31	PL9	a	410	-	13,13,55	0.89	0	17,17,69	0.75	0
26	LHG	c	518	-	48,48,48	0.43	0	51,54,54	1.20	4 (7%)
24	CHL	G	605	21	40,54,74	2.32	13 (32%)	34,90,114	3.21	16 (47%)
24	CHL	y	308	-	52,66,74	2.10	12 (23%)	48,104,114	2.76	18 (37%)
25	CLA	S	304	-	49,53,73	1.60	11 (22%)	58,89,113	1.91	10 (17%)
25	CLA	S	311	26	60,64,73	1.46	10 (16%)	71,102,113	2.04	13 (18%)
38	HEM	F	101	9	50,50,50	2.51	9 (18%)	67,82,82	1.65	11 (16%)
40	NEX	y	318	-	40,46,46	1.36	8 (20%)	50,70,70	2.11	17 (34%)
32	AJP	N	620	-	48,48,95	0.73	0	72,78,149	4.40	31 (43%)
25	CLA	y	312	26	64,68,73	1.43	12 (18%)	76,107,113	1.63	15 (19%)
31	PL9	D	405	-	55,55,55	0.47	0	68,69,69	0.75	0
24	CHL	y	306	21	42,56,74	2.23	11 (26%)	36,92,114	3.14	17 (47%)
25	CLA	b	605	5	69,73,73	1.36	9 (13%)	82,113,113	1.78	14 (17%)
24	CHL	N	605	21	42,56,74	2.22	11 (26%)	36,92,114	3.11	16 (44%)
25	CLA	B	608	5	69,73,73	1.35	12 (17%)	82,113,113	1.68	15 (18%)
40	NEX	S	317	-	40,46,46	1.33	6 (15%)	50,70,70	2.05	14 (28%)
39	LUT	y	316	-	42,43,43	0.82	2 (4%)	51,60,60	1.55	7 (13%)
39	LUT	s	316	-	42,43,43	0.90	3 (7%)	51,60,60	1.54	8 (15%)
24	CHL	y	302	21	60,74,74	1.91	12 (20%)	58,114,114	2.51	19 (32%)
24	CHL	Y	302	21	60,74,74	1.91	12 (20%)	58,114,114	2.51	19 (32%)
25	CLA	B	605	5	69,73,73	1.36	11 (15%)	82,113,113	1.78	14 (17%)
25	CLA	C	510	-	69,73,73	1.35	11 (15%)	82,113,113	1.64	14 (17%)
25	CLA	N	611	26	64,68,73	1.43	11 (17%)	76,107,113	1.62	16 (21%)
25	CLA	g	613	21	69,73,73	1.41	10 (14%)	82,113,113	1.83	16 (19%)
25	CLA	b	612	5	69,73,73	1.37	11 (15%)	82,113,113	1.66	16 (19%)
25	CLA	N	610	21	69,73,73	1.37	10 (14%)	82,113,113	1.63	15 (18%)
25	CLA	c	504	-	64,68,73	1.59	7 (10%)	76,107,113	2.60	20 (26%)
26	LHG	R	618	25	41,41,48	0.45	0	44,47,54	1.24	4 (9%)
26	LHG	C	519	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
25	CLA	R	608	22	62,66,73	1.42	11 (17%)	73,104,113	1.71	16 (21%)
28	BCR	K	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	9 (16%)
25	CLA	b	607	-	69,73,73	1.35	11 (15%)	82,113,113	1.67	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	R	602	22	64,68,73	1.42	10 (15%)	76,107,113	1.76	17 (22%)
35	DGD	c	515	-	56,56,67	0.49	0	70,70,81	1.21	6 (8%)
25	CLA	2	604	26	59,63,73	1.60	8 (13%)	70,101,113	2.11	20 (28%)
25	CLA	C	503	6	69,73,73	1.35	12 (17%)	82,113,113	1.72	15 (18%)
24	CHL	N	608	-	60,74,74	1.92	12 (20%)	58,114,114	2.44	17 (29%)
26	LHG	D	406	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
25	CLA	r	609	22	69,73,73	1.39	10 (14%)	82,113,113	1.60	15 (18%)
40	NEX	s	317	-	40,46,46	1.33	6 (15%)	50,70,70	2.05	14 (28%)
25	CLA	B	607	-	69,73,73	1.35	11 (15%)	82,113,113	1.66	15 (18%)
40	NEX	n	617	-	40,46,46	1.32	6 (15%)	50,70,70	2.25	17 (34%)
25	CLA	g	603	-	64,68,73	1.43	10 (15%)	76,107,113	1.72	16 (21%)
39	LUT	G	615	-	42,43,43	0.87	2 (4%)	51,60,60	1.48	7 (13%)
40	NEX	r	617	-	40,46,46	1.34	6 (15%)	50,70,70	2.95	17 (34%)
25	CLA	a	406	4	64,68,73	1.41	12 (18%)	76,107,113	1.72	16 (21%)
26	LHG	B	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	G	603	-	64,68,73	1.43	10 (15%)	76,107,113	1.72	16 (21%)
38	HEM	f	101	9	50,50,50	2.51	9 (18%)	67,82,82	1.64	11 (16%)
26	LHG	y	301	-	48,48,48	0.44	0	51,54,54	1.19	4 (7%)
25	CLA	c	506	6	69,73,73	1.37	11 (15%)	82,113,113	1.58	16 (19%)
28	BCR	d	404	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	5 (8%)
24	CHL	2	603	-	40,54,74	2.67	16 (40%)	34,90,114	3.67	21 (61%)
26	LHG	N	618	25	48,48,48	0.43	0	51,54,54	1.16	4 (7%)
25	CLA	s	313	20	59,63,73	1.49	9 (15%)	70,101,113	2.19	16 (22%)
28	BCR	z	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
35	DGD	A	415	-	60,60,67	0.49	0	74,74,81	1.20	6 (8%)
40	NEX	R	617	-	40,46,46	1.33	6 (15%)	50,70,70	2.95	17 (34%)
25	CLA	b	608	5	69,73,73	1.35	12 (17%)	82,113,113	1.68	15 (18%)
25	CLA	B	601	-	69,73,73	1.38	7 (10%)	82,113,113	1.80	16 (19%)
32	AJP	Y	322	-	48,48,95	0.73	0	72,78,149	4.34	33 (45%)
24	CHL	n	607	-	60,74,74	1.92	12 (20%)	58,114,114	2.46	17 (29%)
25	CLA	2	605	-	52,56,73	1.57	11 (21%)	61,92,113	1.81	12 (19%)
29	SQD	a	412	-	52,54,54	0.79	1 (1%)	62,65,65	0.90	2 (3%)
27	PHO	A	403	-	58,69,69	0.52	0	55,99,99	1.76	6 (10%)
25	CLA	c	508	6	69,73,73	1.37	10 (14%)	82,113,113	1.77	17 (20%)
26	LHG	Y	301	-	48,48,48	0.44	0	51,54,54	1.20	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	b	623	-	55,55,55	0.43	0	63,63,63	1.22	4 (6%)
30	LMG	A	410	-	40,40,55	0.48	0	48,48,63	1.27	4 (8%)
25	CLA	a	403	-	69,73,73	1.37	10 (14%)	82,113,113	1.70	15 (18%)
35	DGD	b	626	-	63,63,67	0.49	0	77,77,81	1.27	6 (7%)
26	LHG	C	518	-	48,48,48	0.43	0	51,54,54	1.20	4 (7%)
25	CLA	s	305	-	54,58,73	1.74	7 (12%)	64,95,113	3.16	19 (29%)
25	CLA	b	616	5	69,73,73	1.35	11 (15%)	82,113,113	1.60	14 (17%)
25	CLA	y	314	21	69,73,73	1.36	9 (13%)	82,113,113	1.80	14 (17%)
26	LHG	B	622	-	48,48,48	0.44	0	51,54,54	1.16	4 (7%)
25	CLA	r	603	22	64,68,73	1.59	7 (10%)	76,107,113	2.65	20 (26%)
24	CHL	g	601	21	60,74,74	1.92	13 (21%)	58,114,114	2.52	19 (32%)
25	CLA	C	511	6	69,73,73	1.38	9 (13%)	82,113,113	2.05	16 (19%)
25	CLA	Y	311	21	64,68,73	1.42	10 (15%)	76,107,113	1.68	16 (21%)
25	CLA	c	510	-	69,73,73	1.35	11 (15%)	82,113,113	1.64	14 (17%)
25	CLA	g	611	-	64,68,73	1.49	8 (12%)	76,107,113	1.74	21 (27%)
25	CLA	R	603	22	64,68,73	1.60	7 (10%)	76,107,113	2.64	20 (26%)
32	AJP	Y	320	-	48,48,95	0.82	1 (2%)	72,78,149	4.36	32 (44%)
25	CLA	G	613	21	69,73,73	1.41	9 (13%)	82,113,113	1.82	17 (20%)
25	CLA	G	614	21	52,56,73	1.54	11 (21%)	61,92,113	1.67	14 (22%)
25	CLA	Y	313	21	64,68,73	1.44	12 (18%)	76,107,113	1.65	13 (17%)
28	BCR	Z	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	7 (12%)
24	CHL	r	607	-	55,69,74	2.01	13 (23%)	52,108,114	2.72	19 (36%)
39	LUT	n	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.59	8 (15%)
39	LUT	r	615	-	42,43,43	0.96	5 (11%)	51,60,60	1.54	8 (15%)
25	CLA	C	504	-	64,68,73	1.59	7 (10%)	76,107,113	2.60	20 (26%)
25	CLA	c	503	6	69,73,73	1.35	12 (17%)	82,113,113	1.73	15 (18%)
25	CLA	n	603	-	69,73,73	1.37	11 (15%)	82,113,113	1.64	15 (18%)
25	CLA	b	603	-	69,73,73	1.36	11 (15%)	82,113,113	1.61	16 (19%)
25	CLA	c	513	6	69,73,73	1.36	12 (17%)	82,113,113	1.69	17 (20%)
25	CLA	b	604	5	69,73,73	1.37	11 (15%)	82,113,113	1.68	15 (18%)
28	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	10 (17%)
28	BCR	C	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	Y	303	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	14 (17%)
25	CLA	N	602	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	16 (19%)
33	BCT	a	414	34	3,3,3	1.08	0	2,3,3	4.37	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	B	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	11 (19%)
27	PHO	a	404	-	58,69,69	0.52	0	55,99,99	1.76	6 (10%)
25	CLA	S	310	20	59,63,73	1.49	10 (16%)	70,101,113	1.62	12 (17%)
25	CLA	c	507	-	69,73,73	1.39	11 (15%)	82,113,113	1.56	15 (18%)
25	CLA	n	613	21	64,68,73	1.44	9 (14%)	76,107,113	1.82	17 (22%)
25	CLA	r	614	22	49,53,73	1.61	9 (18%)	58,89,113	1.59	13 (22%)
24	CHL	s	306	-	40,54,74	2.31	12 (30%)	34,90,114	3.15	18 (52%)
29	SQD	A	411	-	52,54,54	0.79	1 (1%)	62,65,65	0.90	2 (3%)
25	CLA	Y	305	-	54,58,73	1.53	11 (20%)	64,95,113	1.70	15 (23%)
24	CHL	Y	306	21	42,56,74	2.23	11 (26%)	36,92,114	3.14	17 (47%)
28	BCR	a	407	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	10 (17%)
25	CLA	B	611	5	69,73,73	1.35	10 (14%)	82,113,113	1.71	15 (18%)
25	CLA	R	614	22	49,53,73	1.60	9 (18%)	58,89,113	1.59	13 (22%)
25	CLA	C	506	6	69,73,73	1.37	11 (15%)	82,113,113	1.58	16 (19%)
25	CLA	B	614	5	69,73,73	1.35	11 (15%)	82,113,113	1.72	14 (17%)
25	CLA	b	606	5	69,73,73	1.35	8 (11%)	82,113,113	1.66	16 (19%)
40	NEX	G	617	25	40,46,46	1.31	5 (12%)	50,70,70	2.61	13 (26%)
32	AJP	n	620	-	48,48,95	0.74	0	72,78,149	4.40	31 (43%)
29	SQD	l	101	-	52,54,54	0.80	1 (1%)	62,65,65	0.92	3 (4%)
28	BCR	i	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
24	CHL	R	613	22	36,50,74	2.37	11 (30%)	29,85,114	3.47	15 (51%)
33	BCT	A	413	34	3,3,3	1.08	0	2,3,3	4.37	2 (100%)
39	LUT	g	616	-	42,43,43	0.91	3 (7%)	51,60,60	1.39	3 (5%)
25	CLA	s	303	20	65,69,73	1.40	11 (16%)	77,108,113	1.62	15 (19%)
32	AJP	y	324	-	48,48,95	0.73	0	72,78,149	4.51	32 (44%)
40	NEX	g	617	25	40,46,46	1.32	7 (17%)	50,70,70	2.62	15 (30%)
25	CLA	N	612	21	64,68,73	1.43	12 (18%)	76,107,113	1.72	14 (18%)
39	LUT	G	616	-	42,43,43	0.92	3 (7%)	51,60,60	1.39	3 (5%)
25	CLA	Y	304	-	69,73,73	1.38	12 (17%)	82,113,113	1.67	15 (18%)
32	AJP	N	619	-	48,48,95	0.72	0	72,78,149	4.33	34 (47%)
32	AJP	y	322	-	48,48,95	0.73	0	72,78,149	4.34	33 (45%)
25	CLA	c	512	-	69,73,73	1.36	11 (15%)	82,113,113	1.64	16 (19%)
32	AJP	g	618	-	48,48,95	0.90	0	72,78,149	5.61	37 (51%)
24	CHL	G	606	-	44,58,74	2.21	11 (25%)	37,94,114	3.13	17 (45%)
41	XAT	R	616	-	41,47,47	1.09	4 (9%)	54,74,74	2.23	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	AJP	Y	324	-	48,48,95	0.72	0	72,78,149	4.51	32 (44%)
24	CHL	r	613	22	36,50,74	2.35	11 (30%)	29,85,114	3.47	15 (51%)
40	NEX	Y	318	-	40,46,46	1.36	8 (20%)	50,70,70	2.12	17 (34%)
24	CHL	r	606	-	40,54,74	2.32	12 (30%)	34,90,114	3.22	16 (47%)
39	LUT	g	615	-	42,43,43	0.86	2 (4%)	51,60,60	1.48	7 (13%)
25	CLA	s	314	20	53,57,73	1.55	12 (22%)	61,93,113	1.66	13 (21%)
25	CLA	D	401	42	54,58,73	1.54	10 (18%)	64,95,113	1.92	14 (21%)
27	PHO	A	404	-	58,69,69	0.52	0	55,99,99	1.75	6 (10%)
25	CLA	C	513	6	69,73,73	1.36	12 (17%)	82,113,113	1.69	17 (20%)
25	CLA	S	303	20	65,69,73	1.40	12 (18%)	77,108,113	1.63	15 (19%)
24	CHL	g	607	-	40,54,74	2.29	12 (30%)	34,90,114	3.22	18 (52%)
32	AJP	A	412	-	95,95,95	0.64	0	144,149,149	3.81	66 (45%)
25	CLA	s	309	20	49,53,73	1.64	10 (20%)	58,89,113	1.90	13 (22%)
25	CLA	y	311	21	64,68,73	1.43	10 (15%)	76,107,113	1.68	15 (19%)
24	CHL	G	607	-	40,54,74	2.30	12 (30%)	34,90,114	3.22	18 (52%)
25	CLA	Y	315	21	49,53,73	1.61	11 (22%)	58,89,113	1.66	12 (20%)
25	CLA	s	304	-	49,53,73	1.60	10 (20%)	58,89,113	1.92	10 (17%)
31	PL9	d	405	-	55,55,55	0.47	0	68,69,69	0.75	0
25	CLA	c	502	6	69,73,73	1.37	10 (14%)	82,113,113	1.73	14 (17%)
41	XAT	r	616	-	41,47,47	1.08	4 (9%)	54,74,74	2.23	15 (27%)
26	LHG	l	103	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
24	CHL	2	601	2	58,72,74	2.02	13 (22%)	55,111,114	2.48	18 (32%)
25	CLA	G	610	-	68,72,73	1.43	8 (11%)	80,111,113	1.94	16 (20%)
25	CLA	y	313	21	64,68,73	1.44	12 (18%)	76,107,113	1.65	13 (17%)
26	LHG	C	517	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
32	AJP	y	321	-	48,48,95	0.77	0	72,78,149	4.39	30 (41%)
30	LMG	D	407	-	46,46,55	0.44	0	54,54,63	1.20	4 (7%)
25	CLA	S	309	20	49,53,73	1.64	10 (20%)	58,89,113	1.90	13 (22%)
30	LMG	d	407	-	46,46,55	0.44	0	54,54,63	1.20	4 (7%)
26	LHG	d	406	-	48,48,48	0.43	0	51,54,54	1.19	4 (7%)
24	CHL	n	606	-	40,54,74	2.29	13 (32%)	34,90,114	3.26	17 (50%)
25	CLA	N	613	21	64,68,73	1.44	9 (14%)	76,107,113	1.82	17 (22%)
25	CLA	2	602	2	64,68,73	1.64	7 (10%)	76,107,113	2.54	27 (35%)
25	CLA	S	312	20	53,57,73	1.59	10 (18%)	61,93,113	1.70	15 (24%)
29	SQD	L	103	-	52,54,54	0.80	1 (1%)	62,65,65	0.92	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	a	408	-	48,50,54	0.81	1 (2%)	58,61,65	0.88	2 (3%)
24	CHL	r	605	-	40,54,74	2.31	13 (32%)	34,90,114	3.22	18 (52%)
25	CLA	G	611	-	64,68,73	1.49	8 (12%)	76,107,113	1.74	21 (27%)
25	CLA	R	609	22	69,73,73	1.39	10 (14%)	82,113,113	1.60	15 (18%)
24	CHL	Y	309	-	60,74,74	1.92	12 (20%)	58,114,114	2.43	19 (32%)
32	AJP	b	624	-	95,95,95	0.62	0	144,149,149	3.58	58 (40%)
26	LHG	s	318	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
32	AJP	y	320	-	48,48,95	0.82	1 (2%)	72,78,149	4.36	32 (44%)
25	CLA	B	616	5	69,73,73	1.35	11 (15%)	82,113,113	1.60	14 (17%)
25	CLA	Y	314	21	69,73,73	1.35	9 (13%)	82,113,113	1.79	14 (17%)
26	LHG	s	301	-	48,48,48	0.44	0	51,54,54	1.17	4 (7%)
25	CLA	B	613	5	69,73,73	1.36	11 (15%)	82,113,113	1.55	15 (18%)
24	CHL	R	607	-	55,69,74	2.01	13 (23%)	52,108,114	2.72	19 (36%)
24	CHL	G	608	-	60,74,74	1.93	13 (21%)	58,114,114	2.43	18 (31%)
39	LUT	N	616	-	42,43,43	0.92	3 (7%)	51,60,60	1.45	5 (9%)
24	CHL	N	609	21	60,74,74	1.93	12 (20%)	58,114,114	2.64	18 (31%)
25	CLA	g	614	21	52,56,73	1.54	11 (21%)	61,92,113	1.67	14 (22%)
35	DGD	C	516	-	63,63,67	0.52	0	77,77,81	1.23	6 (7%)
40	NEX	N	617	-	40,46,46	1.33	6 (15%)	50,70,70	2.25	17 (34%)
25	CLA	A	405	4	64,68,73	1.41	12 (18%)	76,107,113	1.72	16 (21%)
25	CLA	n	611	26	64,68,73	1.43	11 (17%)	76,107,113	1.62	16 (21%)
39	LUT	S	315	-	42,43,43	0.94	4 (9%)	51,60,60	1.47	7 (13%)
25	CLA	D	403	-	69,73,73	1.54	8 (11%)	82,113,113	2.61	21 (25%)
35	DGD	B	626	-	63,63,67	0.49	0	77,77,81	1.27	6 (7%)
39	LUT	Y	317	-	42,43,43	0.93	3 (7%)	51,60,60	1.42	5 (9%)
32	AJP	s	319	-	48,48,95	0.79	0	72,78,149	4.40	30 (41%)
28	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	l	102	-	40,42,54	0.88	1 (2%)	50,53,65	1.05	3 (6%)
24	CHL	n	601	21	50,64,74	2.12	12 (24%)	46,102,114	2.84	17 (36%)
24	CHL	6	603	-	40,54,74	2.67	16 (40%)	34,90,114	3.67	21 (61%)
25	CLA	r	601	-	53,57,73	1.76	8 (15%)	61,93,113	3.04	17 (27%)
24	CHL	g	608	-	60,74,74	1.94	13 (21%)	58,114,114	2.43	18 (31%)
25	CLA	y	303	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	14 (17%)
25	CLA	r	610	26	53,57,73	1.80	7 (13%)	61,93,113	2.95	16 (26%)
25	CLA	N	604	-	54,58,73	1.52	11 (20%)	64,95,113	1.96	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	y	305	-	54,58,73	1.53	11 (20%)	64,95,113	1.71	15 (23%)
30	LMG	c	520	-	51,51,55	0.45	0	59,59,63	1.22	4 (6%)
25	CLA	R	611	-	53,57,73	1.85	8 (15%)	61,93,113	3.32	22 (36%)
25	CLA	B	606	5	69,73,73	1.35	8 (11%)	82,113,113	1.66	16 (19%)
26	LHG	b	621	-	46,46,48	0.45	0	49,52,54	1.19	4 (8%)
25	CLA	c	505	6	69,73,73	1.35	11 (15%)	82,113,113	1.64	15 (18%)
30	LMG	B	623	-	55,55,55	0.43	0	63,63,63	1.22	4 (6%)
25	CLA	R	610	26	53,57,73	1.80	7 (13%)	61,93,113	2.95	16 (26%)
32	AJP	S	319	-	48,48,95	0.79	0	72,78,149	4.40	30 (41%)
25	CLA	B	603	-	69,73,73	1.36	11 (15%)	82,113,113	1.60	16 (19%)
32	AJP	a	413	-	95,95,95	0.64	0	144,149,149	3.81	66 (45%)
25	CLA	G	604	40	54,58,73	1.54	11 (20%)	64,95,113	1.84	15 (23%)
39	LUT	R	615	-	42,43,43	0.97	5 (11%)	51,60,60	1.53	8 (15%)
26	LHG	Y	319	25	48,48,48	0.42	0	51,54,54	1.20	4 (7%)
28	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	11 (19%)
24	CHL	N	601	21	50,64,74	2.12	12 (24%)	46,102,114	2.85	17 (36%)
25	CLA	6	602	2	64,68,73	1.64	7 (10%)	76,107,113	2.54	27 (35%)
25	CLA	A	401	4	69,73,73	1.36	11 (15%)	82,113,113	1.63	17 (20%)
28	BCR	B	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
24	CHL	s	302	20	40,54,74	2.32	12 (30%)	34,90,114	3.33	16 (47%)
24	CHL	y	307	21	44,58,74	2.15	10 (22%)	37,94,114	2.69	17 (45%)
30	LMG	a	411	-	40,40,55	0.48	0	48,48,63	1.27	4 (8%)
25	CLA	b	611	5	69,73,73	1.35	10 (14%)	82,113,113	1.71	15 (18%)
25	CLA	r	611	-	53,57,73	1.85	7 (13%)	61,93,113	3.31	22 (36%)
25	CLA	y	304	-	69,73,73	1.38	12 (17%)	82,113,113	1.67	15 (18%)
25	CLA	B	615	5	69,73,73	1.39	10 (14%)	82,113,113	1.61	16 (19%)
25	CLA	b	610	-	69,73,73	1.39	10 (14%)	82,113,113	1.55	13 (15%)
25	CLA	C	512	-	69,73,73	1.36	11 (15%)	82,113,113	1.64	16 (19%)
25	CLA	c	509	6	69,73,73	1.37	12 (17%)	82,113,113	1.67	12 (14%)
25	CLA	d	401	42	54,58,73	1.54	10 (18%)	64,95,113	1.93	14 (21%)
24	CHL	G	609	21	55,69,74	2.03	13 (23%)	52,108,114	2.78	18 (34%)
25	CLA	6	604	26	59,63,73	1.60	8 (13%)	70,101,113	2.11	20 (28%)
25	CLA	g	604	40	54,58,73	1.54	11 (20%)	64,95,113	1.84	15 (23%)
30	LMG	b	620	-	51,51,55	0.44	0	59,59,63	1.20	4 (6%)
25	CLA	c	511	6	69,73,73	1.38	9 (13%)	82,113,113	2.04	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	S	305	-	54,58,73	1.74	7 (12%)	64,95,113	3.16	19 (29%)
25	CLA	B	610	-	69,73,73	1.39	10 (14%)	82,113,113	1.55	13 (15%)
28	BCR	B	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	7 (12%)
32	AJP	Y	321	-	48,48,95	0.77	0	72,78,149	4.39	30 (41%)
24	CHL	S	307	-	40,54,74	2.31	12 (30%)	34,90,114	3.19	17 (50%)
39	LUT	N	615	-	42,43,43	0.89	2 (4%)	51,60,60	1.59	9 (17%)
25	CLA	n	604	-	54,58,73	1.53	11 (20%)	64,95,113	1.96	15 (23%)
24	CHL	6	601	2	58,72,74	2.02	13 (22%)	55,111,114	2.48	17 (30%)
24	CHL	n	608	-	60,74,74	1.92	12 (20%)	58,114,114	2.44	17 (29%)
25	CLA	6	605	-	52,56,73	1.56	10 (19%)	61,92,113	1.81	11 (18%)
29	SQD	L	101	-	40,42,54	0.87	1 (2%)	50,53,65	1.05	3 (6%)
25	CLA	b	609	5	69,73,73	1.37	11 (15%)	82,113,113	1.71	17 (20%)
25	CLA	y	315	21	49,53,73	1.62	11 (22%)	58,89,113	1.66	12 (20%)
25	CLA	C	502	6	69,73,73	1.37	10 (14%)	82,113,113	1.73	15 (18%)
39	LUT	y	317	-	42,43,43	0.93	3 (7%)	51,60,60	1.42	5 (9%)
25	CLA	c	501	-	69,73,73	1.50	7 (10%)	82,113,113	2.43	21 (25%)
25	CLA	r	608	22	62,66,73	1.43	11 (17%)	73,104,113	1.72	16 (21%)
25	CLA	s	312	20	53,57,73	1.59	10 (18%)	61,93,113	1.70	15 (24%)
25	CLA	B	604	5	69,73,73	1.37	12 (17%)	82,113,113	1.67	15 (18%)
39	LUT	n	616	-	42,43,43	0.92	2 (4%)	51,60,60	1.45	5 (9%)
24	CHL	n	609	21	60,74,74	1.92	12 (20%)	58,114,114	2.64	19 (32%)
24	CHL	S	308	-	40,54,74	2.32	13 (32%)	34,90,114	3.18	16 (47%)
25	CLA	a	402	4	69,73,73	1.36	11 (15%)	82,113,113	1.63	17 (20%)
24	CHL	Y	310	21	50,64,74	2.10	12 (24%)	46,102,114	2.83	18 (39%)
24	CHL	y	309	-	60,74,74	1.92	12 (20%)	58,114,114	2.43	19 (32%)
25	CLA	A	402	-	69,73,73	1.38	10 (14%)	82,113,113	1.70	16 (19%)
32	AJP	y	323	-	48,48,95	0.76	0	72,78,149	4.59	32 (44%)
25	CLA	d	402	7	69,73,73	1.39	11 (15%)	82,113,113	1.69	18 (21%)
25	CLA	n	602	21	69,73,73	1.34	11 (15%)	82,113,113	1.65	16 (19%)
25	CLA	N	614	21	52,56,73	1.60	8 (15%)	61,92,113	1.99	16 (26%)
28	BCR	T	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	9 (16%)
25	CLA	r	604	-	52,56,73	1.58	8 (15%)	61,92,113	1.81	16 (26%)
24	CHL	G	601	21	60,74,74	1.91	13 (21%)	58,114,114	2.52	19 (32%)
39	LUT	S	316	-	42,43,43	0.89	3 (7%)	51,60,60	1.54	8 (15%)
26	LHG	B	621	-	46,46,48	0.45	0	49,52,54	1.19	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	AJP	Y	323	-	48,48,95	0.76	0	72,78,149	4.59	32 (44%)
25	CLA	Y	312	26	64,68,73	1.43	12 (18%)	76,107,113	1.62	15 (19%)
28	BCR	b	617	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	7 (12%)
24	CHL	g	606	-	44,58,74	2.20	11 (25%)	37,94,114	3.13	17 (45%)
29	SQD	A	407	-	48,50,54	0.81	1 (2%)	58,61,65	0.88	2 (3%)
25	CLA	R	601	-	53,57,73	1.76	8 (15%)	61,93,113	3.02	17 (27%)
25	CLA	R	604	-	52,56,73	1.59	9 (17%)	61,92,113	1.81	16 (26%)
25	CLA	C	508	6	69,73,73	1.37	10 (14%)	82,113,113	1.76	17 (20%)
35	DGD	a	401	-	60,60,67	0.49	0	74,74,81	1.20	6 (8%)
24	CHL	S	302	20	40,54,74	2.31	12 (30%)	34,90,114	3.33	16 (47%)
26	LHG	r	618	25	41,41,48	0.45	0	44,47,54	1.23	4 (9%)
28	BCR	H	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
27	PHO	a	405	-	58,69,69	0.52	0	55,99,99	1.74	6 (10%)
25	CLA	C	505	6	69,73,73	1.35	11 (15%)	82,113,113	1.64	15 (18%)
39	LUT	s	315	-	42,43,43	0.94	4 (9%)	51,60,60	1.47	7 (13%)
26	LHG	L	102	-	48,48,48	0.44	0	51,54,54	1.18	4 (7%)
25	CLA	G	602	21	69,73,73	1.35	12 (17%)	82,113,113	1.70	16 (19%)
25	CLA	b	601	-	69,73,73	1.38	7 (10%)	82,113,113	1.79	16 (19%)
26	LHG	b	625	-	45,45,48	0.44	0	48,51,54	1.19	4 (8%)
25	CLA	G	612	21	64,68,73	1.41	10 (15%)	76,107,113	1.57	12 (15%)
35	DGD	C	515	-	56,56,67	0.49	0	70,70,81	1.21	6 (8%)
25	CLA	r	602	22	64,68,73	1.42	11 (17%)	76,107,113	1.76	17 (22%)
25	CLA	g	610	-	68,72,73	1.44	8 (11%)	80,111,113	1.94	16 (20%)
28	BCR	I	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.30	9 (16%)
25	CLA	C	509	6	69,73,73	1.37	12 (17%)	82,113,113	1.67	12 (14%)
24	CHL	Y	307	21	44,58,74	2.15	10 (22%)	37,94,114	2.69	17 (45%)
35	DGD	c	516	-	63,63,67	0.52	0	77,77,81	1.22	6 (7%)
24	CHL	R	605	-	40,54,74	2.31	13 (32%)	34,90,114	3.23	18 (52%)
25	CLA	b	615	5	69,73,73	1.39	9 (13%)	82,113,113	1.61	16 (19%)
25	CLA	g	602	21	69,73,73	1.35	12 (17%)	82,113,113	1.70	16 (19%)
24	CHL	5	302	1	40,54,74	2.35	14 (35%)	34,90,114	3.27	16 (47%)
25	CLA	n	610	21	69,73,73	1.38	10 (14%)	82,113,113	1.63	15 (18%)
25	CLA	g	612	21	64,68,73	1.42	10 (15%)	76,107,113	1.58	12 (15%)

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
24	CHL	g	605	21	3/3/16/26	7/15/113/137	-
30	LMG	a	409	-	-	18/43/63/70	0/1/1/1
28	BCR	D	404	-	-	5/29/63/63	0/2/2/2
30	LMG	B	620	-	-	15/46/66/70	0/1/1/1
28	BCR	t	101	-	-	17/29/63/63	0/2/2/2
26	LHG	2	606	25	-	25/51/51/53	-
24	CHL	Y	308	-	2/2/18/26	7/30/128/137	-
26	LHG	y	319	25	-	23/53/53/53	-
32	AJP	B	624	-	34/34/38/38	13/28/220/220	0/11/11/11
24	CHL	l	302	1	3/3/16/26	6/15/113/137	-
28	BCR	h	101	-	-	6/29/63/63	0/2/2/2
24	CHL	R	606	-	3/3/16/26	9/15/113/137	-
26	LHG	n	618	25	-	28/53/53/53	-
25	CLA	b	614	5	1/1/15/20	13/39/115/115	-
26	LHG	S	318	25	-	20/53/53/53	-
28	BCR	k	101	-	-	4/29/63/63	0/2/2/2
25	CLA	b	613	5	1/1/15/20	13/39/115/115	-
24	CHL	s	307	-	3/3/16/26	7/15/113/137	-
24	CHL	S	306	-	3/3/16/26	6/15/113/137	-
24	CHL	s	308	-	3/3/16/26	3/15/113/137	-
25	CLA	n	614	21	1/1/11/20	3/19/95/115	-
25	CLA	B	609	5	1/1/15/20	11/39/115/115	-
39	LUT	Y	316	-	-	4/29/67/67	0/2/2/2
25	CLA	S	313	20	1/1/13/20	11/27/103/115	-
25	CLA	s	310	20	1/1/13/20	11/27/103/115	-
25	CLA	B	602	5	1/1/15/20	13/39/115/115	-
25	CLA	S	314	20	1/1/11/20	2/20/96/115	-
25	CLA	b	602	5	1/1/15/20	13/39/115/115	-
24	CHL	N	607	-	2/2/20/26	17/39/137/137	-
25	CLA	d	403	-	1/1/15/20	11/39/115/115	-
32	AJP	G	618	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	b	619	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	n	605	21	3/3/16/26	9/18/116/137	-
26	LHG	c	517	-	-	15/53/53/53	-
25	CLA	n	612	21	1/1/14/20	18/33/109/115	-
25	CLA	r	612	22	1/1/14/20	11/33/109/115	-
24	CHL	N	606	-	2/2/16/26	5/15/113/137	-
24	CHL	g	609	21	3/3/19/26	10/33/131/137	-
32	AJP	n	619	-	15/15/19/38	1/6/117/220	0/7/7/11
30	LMG	C	520	-	-	18/46/66/70	0/1/1/1
25	CLA	N	603	-	1/1/15/20	20/39/115/115	-
25	CLA	C	501	-	1/1/15/20	7/39/115/115	-
31	PL9	A	409	-	-	2/5/18/73	0/1/1/1
25	CLA	B	612	5	1/1/15/20	10/39/115/115	-
24	CHL	5	301	1	3/3/16/26	3/15/113/137	-
26	LHG	c	519	-	-	21/53/53/53	-
26	LHG	S	301	-	-	21/53/53/53	-
25	CLA	R	612	22	1/1/14/20	11/33/109/115	-
25	CLA	D	402	7	1/1/15/20	10/39/115/115	-
25	CLA	s	311	26	1/1/13/20	10/29/105/115	-
30	LMG	A	408	-	-	18/43/63/70	0/1/1/1
24	CHL	y	310	21	3/3/18/26	9/27/125/137	-
25	CLA	C	507	-	1/1/15/20	17/39/115/115	-
26	LHG	b	622	-	-	17/53/53/53	-
24	CHL	1	301	1	3/3/16/26	3/15/113/137	-
26	LHG	6	606	25	-	25/51/51/53	-
31	PL9	a	410	-	-	2/5/18/73	0/1/1/1
26	LHG	c	518	-	-	12/53/53/53	-
24	CHL	G	605	21	3/3/16/26	7/15/113/137	-
24	CHL	y	308	-	2/2/18/26	7/30/128/137	-
25	CLA	S	304	-	1/1/11/20	4/15/91/115	-
25	CLA	S	311	26	1/1/13/20	10/29/105/115	-
38	HEM	F	101	9	-	3/14/54/54	-
40	NEX	y	318	-	-	7/27/83/83	1/3/3/3
32	AJP	N	620	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	y	312	26	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	D	405	-	-	5/53/73/73	0/1/1/1
24	CHL	y	306	21	3/3/16/26	9/18/116/137	-
25	CLA	b	605	5	1/1/15/20	8/39/115/115	-
24	CHL	N	605	21	3/3/16/26	9/18/116/137	-
25	CLA	B	608	5	1/1/15/20	13/39/115/115	-
40	NEX	S	317	-	-	6/27/83/83	0/3/3/3
39	LUT	y	316	-	-	4/29/67/67	0/2/2/2
39	LUT	s	316	-	-	4/29/67/67	0/2/2/2
24	CHL	y	302	21	2/2/20/26	22/39/137/137	-
24	CHL	Y	302	21	2/2/20/26	22/39/137/137	-
25	CLA	B	605	5	1/1/15/20	8/39/115/115	-
25	CLA	C	510	-	1/1/15/20	13/39/115/115	-
25	CLA	N	611	26	1/1/14/20	14/33/109/115	-
25	CLA	g	613	21	1/1/15/20	15/39/115/115	-
25	CLA	b	612	5	1/1/15/20	10/39/115/115	-
25	CLA	N	610	21	1/1/15/20	16/39/115/115	-
25	CLA	c	504	-	1/1/14/20	13/33/109/115	-
26	LHG	R	618	25	-	11/46/46/53	-
26	LHG	C	519	-	-	21/53/53/53	-
25	CLA	R	608	22	1/1/13/20	16/31/107/115	-
28	BCR	K	101	-	-	4/29/63/63	0/2/2/2
25	CLA	b	607	-	1/1/15/20	16/39/115/115	-
25	CLA	R	602	22	1/1/14/20	8/33/109/115	-
35	DGD	c	515	-	-	17/44/84/95	0/2/2/2
25	CLA	2	604	26	1/1/13/20	11/27/103/115	-
25	CLA	C	503	6	1/1/15/20	11/39/115/115	-
24	CHL	N	608	-	3/3/20/26	14/39/137/137	-
26	LHG	D	406	-	-	17/53/53/53	-
25	CLA	r	609	22	1/1/15/20	15/39/115/115	-
40	NEX	s	317	-	-	6/27/83/83	0/3/3/3
25	CLA	B	607	-	1/1/15/20	16/39/115/115	-
40	NEX	n	617	-	-	10/27/83/83	0/3/3/3
25	CLA	g	603	-	1/1/14/20	12/33/109/115	-
39	LUT	G	615	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	NEX	r	617	-	-	6/27/83/83	0/3/3/3
25	CLA	a	406	4	1/1/14/20	11/33/109/115	-
26	LHG	B	625	-	-	14/50/50/53	-
25	CLA	G	603	-	1/1/14/20	13/33/109/115	-
38	HEM	f	101	9	-	3/14/54/54	-
26	LHG	y	301	-	-	14/53/53/53	-
25	CLA	c	506	6	1/1/15/20	11/39/115/115	-
28	BCR	d	404	-	-	5/29/63/63	0/2/2/2
24	CHL	2	603	-	3/3/16/26	10/15/113/137	-
26	LHG	N	618	25	-	28/53/53/53	-
25	CLA	s	313	20	1/1/13/20	11/27/103/115	-
28	BCR	z	101	-	-	8/29/63/63	0/2/2/2
35	DGD	A	415	-	-	26/48/88/95	0/2/2/2
40	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	b	608	5	1/1/15/20	13/39/115/115	-
25	CLA	B	601	-	1/1/15/20	15/39/115/115	-
32	AJP	Y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	n	607	-	2/2/20/26	17/39/137/137	-
25	CLA	2	605	-	1/1/11/20	10/19/95/115	-
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
27	PHO	A	403	-	-	11/37/103/103	0/5/6/6
25	CLA	c	508	6	1/1/15/20	12/39/115/115	-
26	LHG	Y	301	-	-	14/53/53/53	-
30	LMG	b	623	-	-	28/50/70/70	0/1/1/1
30	LMG	A	410	-	-	14/35/55/70	0/1/1/1
25	CLA	a	403	-	1/1/15/20	8/39/115/115	-
35	DGD	b	626	-	-	22/51/91/95	0/2/2/2
26	LHG	C	518	-	-	12/53/53/53	-
25	CLA	s	305	-	1/1/12/20	8/21/97/115	-
25	CLA	b	616	5	1/1/15/20	18/39/115/115	-
25	CLA	y	314	21	1/1/15/20	13/39/115/115	-
26	LHG	B	622	-	-	17/53/53/53	-
25	CLA	r	603	22	1/1/14/20	12/33/109/115	-
24	CHL	g	601	21	2/2/20/26	23/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	511	6	1/1/15/20	9/39/115/115	-
25	CLA	Y	311	21	1/1/14/20	11/33/109/115	-
25	CLA	c	510	-	1/1/15/20	13/39/115/115	-
25	CLA	g	611	-	1/1/14/20	15/33/109/115	-
25	CLA	R	603	22	1/1/14/20	12/33/109/115	-
32	AJP	Y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	G	613	21	1/1/15/20	15/39/115/115	-
25	CLA	G	614	21	1/1/11/20	10/19/95/115	-
25	CLA	Y	313	21	1/1/14/20	12/33/109/115	-
28	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
24	CHL	r	607	-	3/3/19/26	12/33/131/137	-
39	LUT	n	615	-	-	7/29/67/67	0/2/2/2
39	LUT	r	615	-	-	4/29/67/67	0/2/2/2
25	CLA	C	504	-	1/1/14/20	13/33/109/115	-
25	CLA	c	503	6	1/1/15/20	11/39/115/115	-
25	CLA	n	603	-	1/1/15/20	20/39/115/115	-
25	CLA	b	603	-	1/1/15/20	12/39/115/115	-
25	CLA	c	513	6	1/1/15/20	10/39/115/115	-
25	CLA	b	604	5	1/1/15/20	16/39/115/115	-
28	BCR	A	406	-	-	5/29/63/63	0/2/2/2
28	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	CLA	Y	303	21	1/1/15/20	12/39/115/115	-
25	CLA	N	602	21	1/1/15/20	15/39/115/115	-
28	BCR	B	618	-	-	2/29/63/63	0/2/2/2
27	PHO	a	404	-	-	11/37/103/103	0/5/6/6
25	CLA	S	310	20	1/1/13/20	11/27/103/115	-
25	CLA	c	507	-	1/1/15/20	17/39/115/115	-
25	CLA	n	613	21	1/1/14/20	20/33/109/115	-
25	CLA	r	614	22	1/1/11/20	8/15/91/115	-
24	CHL	s	306	-	3/3/16/26	6/15/113/137	-
29	SQD	A	411	-	-	22/49/69/69	0/1/1/1
25	CLA	Y	305	-	1/1/12/20	6/21/97/115	-
24	CHL	Y	306	21	3/3/16/26	9/18/116/137	-
28	BCR	a	407	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	611	5	1/1/15/20	11/39/115/115	-
25	CLA	R	614	22	1/1/11/20	8/15/91/115	-
25	CLA	C	506	6	1/1/15/20	11/39/115/115	-
25	CLA	B	614	5	1/1/15/20	13/39/115/115	-
25	CLA	b	606	5	1/1/15/20	13/39/115/115	-
40	NEX	G	617	25	-	11/27/83/83	0/3/3/3
32	AJP	n	620	-	16/16/19/38	4/6/117/220	0/7/7/11
29	SQD	l	101	-	-	27/49/69/69	0/1/1/1
28	BCR	i	101	-	-	3/29/63/63	0/2/2/2
24	CHL	R	613	22	3/3/15/26	5/10/108/137	-
39	LUT	g	616	-	-	0/29/67/67	0/2/2/2
25	CLA	s	303	20	1/1/14/20	20/35/111/115	-
32	AJP	y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
40	NEX	g	617	25	-	11/27/83/83	0/3/3/3
25	CLA	N	612	21	1/1/14/20	18/33/109/115	-
39	LUT	G	616	-	-	0/29/67/67	0/2/2/2
25	CLA	Y	304	-	1/1/15/20	22/39/115/115	-
32	AJP	N	619	-	15/15/19/38	1/6/117/220	0/7/7/11
32	AJP	y	322	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	c	512	-	1/1/15/20	13/39/115/115	-
32	AJP	g	618	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	G	606	-	3/3/16/26	3/20/118/137	-
41	XAT	R	616	-	-	2/31/93/93	0/4/4/4
32	AJP	Y	324	-	15/15/19/38	3/6/117/220	0/7/7/11
24	CHL	r	613	22	3/3/15/26	5/10/108/137	-
40	NEX	Y	318	-	-	7/27/83/83	1/3/3/3
24	CHL	r	606	-	3/3/16/26	9/15/113/137	-
39	LUT	g	615	-	-	4/29/67/67	0/2/2/2
25	CLA	s	314	20	1/1/11/20	2/20/96/115	-
25	CLA	D	401	42	1/1/12/20	2/21/97/115	-
27	PHO	A	404	-	-	2/37/103/103	0/5/6/6
25	CLA	C	513	6	1/1/15/20	10/39/115/115	-
25	CLA	S	303	20	1/1/14/20	20/35/111/115	-
24	CHL	g	607	-	2/2/16/26	5/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	AJP	A	412	-	34/34/38/38	9/28/220/220	0/11/11/11
25	CLA	s	309	20	1/1/11/20	6/15/91/115	-
25	CLA	y	311	21	1/1/14/20	11/33/109/115	-
24	CHL	G	607	-	2/2/16/26	5/15/113/137	-
25	CLA	Y	315	21	1/1/11/20	9/15/91/115	-
25	CLA	s	304	-	1/1/11/20	4/15/91/115	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
25	CLA	c	502	6	1/1/15/20	6/39/115/115	-
41	XAT	r	616	-	-	2/31/93/93	0/4/4/4
26	LHG	l	103	-	-	28/53/53/53	-
24	CHL	2	601	2	3/3/19/26	14/37/135/137	-
25	CLA	G	610	-	1/1/14/20	14/38/114/115	-
25	CLA	y	313	21	1/1/14/20	12/33/109/115	-
26	LHG	C	517	-	-	15/53/53/53	-
32	AJP	y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
25	CLA	S	309	20	1/1/11/20	6/15/91/115	-
30	LMG	D	407	-	-	16/41/61/70	0/1/1/1
30	LMG	d	407	-	-	16/41/61/70	0/1/1/1
26	LHG	d	406	-	-	17/53/53/53	-
24	CHL	n	606	-	2/2/16/26	5/15/113/137	-
25	CLA	N	613	21	1/1/14/20	20/33/109/115	-
25	CLA	2	602	2	1/1/14/20	14/33/109/115	-
25	CLA	S	312	20	1/1/11/20	8/20/96/115	-
29	SQD	L	103	-	-	27/49/69/69	0/1/1/1
29	SQD	a	408	-	-	21/45/65/69	0/1/1/1
24	CHL	r	605	-	3/3/16/26	3/15/113/137	-
25	CLA	G	611	-	1/1/14/20	15/33/109/115	-
25	CLA	R	609	22	1/1/15/20	15/39/115/115	-
24	CHL	Y	309	-	3/3/20/26	19/39/137/137	-
32	AJP	b	624	-	34/34/38/38	13/28/220/220	0/11/11/11
26	LHG	s	318	25	-	20/53/53/53	-
32	AJP	y	320	-	15/15/19/38	2/6/117/220	0/7/7/11
25	CLA	B	616	5	1/1/15/20	18/39/115/115	-
25	CLA	Y	314	21	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	s	301	-	-	21/53/53/53	-
25	CLA	B	613	5	1/1/15/20	13/39/115/115	-
24	CHL	R	607	-	3/3/19/26	12/33/131/137	-
24	CHL	G	608	-	3/3/20/26	23/39/137/137	-
39	LUT	N	616	-	-	4/29/67/67	0/2/2/2
24	CHL	N	609	21	2/2/20/26	13/39/137/137	-
25	CLA	g	614	21	1/1/11/20	10/19/95/115	-
35	DGD	C	516	-	-	27/51/91/95	0/2/2/2
40	NEX	N	617	-	-	10/27/83/83	0/3/3/3
25	CLA	A	405	4	1/1/14/20	11/33/109/115	-
25	CLA	n	611	26	1/1/14/20	14/33/109/115	-
39	LUT	S	315	-	-	3/29/67/67	0/2/2/2
25	CLA	D	403	-	1/1/15/20	11/39/115/115	-
35	DGD	B	626	-	-	22/51/91/95	0/2/2/2
39	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
32	AJP	s	319	-	15/15/19/38	3/6/117/220	0/7/7/11
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
29	SQD	l	102	-	-	13/37/57/69	0/1/1/1
24	CHL	n	601	21	2/2/18/26	11/27/125/137	-
24	CHL	6	603	-	3/3/16/26	10/15/113/137	-
25	CLA	r	601	-	1/1/11/20	11/20/96/115	-
24	CHL	g	608	-	3/3/20/26	23/39/137/137	-
25	CLA	y	303	21	1/1/15/20	12/39/115/115	-
25	CLA	r	610	26	1/1/11/20	10/20/96/115	-
25	CLA	N	604	-	1/1/12/20	5/21/97/115	-
25	CLA	y	305	-	1/1/12/20	6/21/97/115	-
30	LMG	c	520	-	-	18/46/66/70	0/1/1/1
25	CLA	R	611	-	1/1/11/20	11/20/96/115	-
25	CLA	B	606	5	1/1/15/20	13/39/115/115	-
26	LHG	b	621	-	-	17/51/51/53	-
25	CLA	c	505	6	1/1/15/20	9/39/115/115	-
30	LMG	B	623	-	-	28/50/70/70	0/1/1/1
25	CLA	R	610	26	1/1/11/20	10/20/96/115	-
32	AJP	S	319	-	15/15/19/38	3/6/117/220	0/7/7/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	603	-	1/1/15/20	12/39/115/115	-
32	AJP	a	413	-	34/34/38/38	9/28/220/220	0/11/11/11
25	CLA	G	604	40	1/1/12/20	10/21/97/115	-
39	LUT	R	615	-	-	4/29/67/67	0/2/2/2
26	LHG	Y	319	25	-	23/53/53/53	-
28	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CHL	N	601	21	2/2/18/26	11/27/125/137	-
25	CLA	6	602	2	1/1/14/20	14/33/109/115	-
25	CLA	A	401	4	1/1/15/20	7/39/115/115	-
28	BCR	B	619	-	-	3/29/63/63	0/2/2/2
24	CHL	s	302	20	2/2/16/26	3/15/113/137	-
24	CHL	y	307	21	3/3/16/26	4/20/118/137	-
30	LMG	a	411	-	-	14/35/55/70	0/1/1/1
25	CLA	b	611	5	1/1/15/20	11/39/115/115	-
25	CLA	r	611	-	1/1/11/20	11/20/96/115	-
25	CLA	y	304	-	1/1/15/20	22/39/115/115	-
25	CLA	B	615	5	1/1/15/20	10/39/115/115	-
25	CLA	b	610	-	1/1/15/20	7/39/115/115	-
25	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	CLA	c	509	6	1/1/15/20	10/39/115/115	-
25	CLA	d	401	42	1/1/12/20	2/21/97/115	-
24	CHL	G	609	21	3/3/19/26	10/33/131/137	-
25	CLA	6	604	26	1/1/13/20	11/27/103/115	-
25	CLA	g	604	40	1/1/12/20	10/21/97/115	-
30	LMG	b	620	-	-	15/46/66/70	0/1/1/1
25	CLA	c	511	6	1/1/15/20	9/39/115/115	-
25	CLA	S	305	-	1/1/12/20	8/21/97/115	-
25	CLA	B	610	-	1/1/15/20	7/39/115/115	-
28	BCR	B	617	-	-	3/29/63/63	0/2/2/2
32	AJP	Y	321	-	16/16/19/38	4/6/117/220	0/7/7/11
24	CHL	S	307	-	3/3/16/26	7/15/113/137	-
39	LUT	N	615	-	-	7/29/67/67	0/2/2/2
25	CLA	n	604	-	1/1/12/20	5/21/97/115	-
24	CHL	6	601	2	3/3/19/26	14/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	n	608	-	3/3/20/26	15/39/137/137	-
25	CLA	6	605	-	1/1/11/20	10/19/95/115	-
29	SQD	L	101	-	-	13/37/57/69	0/1/1/1
25	CLA	b	609	5	1/1/15/20	11/39/115/115	-
25	CLA	y	315	21	1/1/11/20	9/15/91/115	-
25	CLA	C	502	6	1/1/15/20	6/39/115/115	-
39	LUT	y	317	-	-	4/29/67/67	0/2/2/2
25	CLA	c	501	-	1/1/15/20	7/39/115/115	-
25	CLA	r	608	22	1/1/13/20	16/31/107/115	-
25	CLA	s	312	20	1/1/11/20	8/20/96/115	-
25	CLA	B	604	5	1/1/15/20	16/39/115/115	-
39	LUT	n	616	-	-	4/29/67/67	0/2/2/2
24	CHL	n	609	21	2/2/20/26	13/39/137/137	-
24	CHL	S	308	-	3/3/16/26	3/15/113/137	-
25	CLA	a	402	4	1/1/15/20	7/39/115/115	-
24	CHL	Y	310	21	3/3/18/26	9/27/125/137	-
24	CHL	y	309	-	3/3/20/26	19/39/137/137	-
25	CLA	A	402	-	1/1/15/20	8/39/115/115	-
32	AJP	y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	d	402	7	1/1/15/20	10/39/115/115	-
25	CLA	n	602	21	1/1/15/20	15/39/115/115	-
25	CLA	N	614	21	1/1/11/20	3/19/95/115	-
28	BCR	T	101	-	-	17/29/63/63	0/2/2/2
25	CLA	r	604	-	1/1/11/20	7/19/95/115	-
24	CHL	G	601	21	2/2/20/26	23/39/137/137	-
39	LUT	S	316	-	-	4/29/67/67	0/2/2/2
26	LHG	B	621	-	-	17/51/51/53	-
32	AJP	Y	323	-	15/15/19/38	3/6/117/220	0/7/7/11
25	CLA	Y	312	26	1/1/14/20	12/33/109/115	-
28	BCR	b	617	-	-	3/29/63/63	0/2/2/2
24	CHL	g	606	-	3/3/16/26	3/20/118/137	-
29	SQD	A	407	-	-	21/45/65/69	0/1/1/1
25	CLA	R	601	-	1/1/11/20	11/20/96/115	-
25	CLA	R	604	-	1/1/11/20	7/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	508	6	1/1/15/20	12/39/115/115	-
35	DGD	a	401	-	-	26/48/88/95	0/2/2/2
24	CHL	S	302	20	2/2/16/26	3/15/113/137	-
26	LHG	r	618	25	-	11/46/46/53	-
28	BCR	H	101	-	-	6/29/63/63	0/2/2/2
27	PHO	a	405	-	-	2/37/103/103	0/5/6/6
25	CLA	C	505	6	1/1/15/20	9/39/115/115	-
39	LUT	s	315	-	-	3/29/67/67	0/2/2/2
26	LHG	L	102	-	-	28/53/53/53	-
25	CLA	G	602	21	1/1/15/20	14/39/115/115	-
25	CLA	b	601	-	1/1/15/20	15/39/115/115	-
26	LHG	b	625	-	-	14/50/50/53	-
25	CLA	G	612	21	1/1/14/20	12/33/109/115	-
35	DGD	C	515	-	-	17/44/84/95	0/2/2/2
25	CLA	r	602	22	1/1/14/20	8/33/109/115	-
25	CLA	g	610	-	1/1/14/20	14/38/114/115	-
28	BCR	I	101	-	-	4/29/63/63	0/2/2/2
25	CLA	C	509	6	1/1/15/20	10/39/115/115	-
24	CHL	Y	307	21	3/3/16/26	4/20/118/137	-
35	DGD	c	516	-	-	27/51/91/95	0/2/2/2
24	CHL	R	605	-	3/3/16/26	3/15/113/137	-
25	CLA	b	615	5	1/1/15/20	10/39/115/115	-
25	CLA	g	602	21	1/1/15/20	14/39/115/115	-
24	CHL	5	302	1	3/3/16/26	6/15/113/137	-
25	CLA	n	610	21	1/1/15/20	16/39/115/115	-
25	CLA	g	612	21	1/1/14/20	12/33/109/115	-

The worst 5 of 2571 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	F	101	HEM	FE-NB	14.55	2.39	1.94
38	f	101	HEM	FE-NB	14.55	2.39	1.94
24	2	603	CHL	C1D-C2D	7.93	1.48	1.39
24	6	603	CHL	C1D-C2D	7.93	1.48	1.39
25	R	611	CLA	MG-ND	-6.76	1.92	2.05

The worst 5 of 5192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	305	CLA	C4A-NA-C1A	-18.47	98.25	106.68
25	S	305	CLA	C4A-NA-C1A	-18.41	98.28	106.68
32	Y	320	AJP	O09-C08-C10	17.50	145.62	110.20
32	y	320	AJP	O09-C08-C10	17.50	145.62	110.20
25	r	601	CLA	C4A-NA-C1A	-16.99	98.93	106.68

5 of 734 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 3970 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	CBD-CGD-O2D-CED
24	2	601	CHL	C6-C7-C8-C10

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

356 monomers are involved in 3261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	g	605	CHL	4	0
30	a	409	LMG	3	0
28	D	404	BCR	3	0
30	B	620	LMG	5	0
28	t	101	BCR	21	0
26	2	606	LHG	14	0
24	Y	308	CHL	17	0
26	y	319	LHG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	l	302	CHL	9	0
28	h	101	BCR	8	0
24	R	606	CHL	2	0
26	n	618	LHG	10	0
25	b	614	CLA	10	0
26	S	318	LHG	5	0
28	k	101	BCR	9	0
25	b	613	CLA	14	0
24	s	307	CHL	7	0
24	S	306	CHL	10	0
24	s	308	CHL	9	0
25	n	614	CLA	6	0
25	B	609	CLA	11	0
39	Y	316	LUT	12	0
25	S	313	CLA	12	0
25	s	310	CLA	15	0
25	B	602	CLA	8	0
25	S	314	CLA	10	0
25	b	602	CLA	9	0
24	N	607	CHL	48	0
25	d	403	CLA	15	0
28	b	619	BCR	4	0
24	n	605	CHL	5	0
26	c	517	LHG	3	0
25	n	612	CLA	10	0
25	r	612	CLA	19	0
24	N	606	CHL	18	0
24	g	609	CHL	10	0
32	n	619	AJP	2	0
30	C	520	LMG	4	0
25	N	603	CLA	33	0
25	C	501	CLA	18	0
31	A	409	PL9	2	0
25	B	612	CLA	6	0
24	5	301	CHL	9	0
26	c	519	LHG	4	0
26	S	301	LHG	8	0
25	R	612	CLA	19	0
25	D	402	CLA	19	0
25	s	311	CLA	9	0
30	A	408	LMG	3	0
24	y	310	CHL	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	507	CLA	6	0
26	b	622	LHG	8	0
24	1	301	CHL	9	0
26	6	606	LHG	14	0
31	a	410	PL9	2	0
26	c	518	LHG	3	0
24	G	605	CHL	4	0
24	y	308	CHL	14	0
25	S	304	CLA	12	0
25	S	311	CLA	8	0
38	F	101	HEM	7	0
40	y	318	NEX	10	0
32	N	620	AJP	1	0
25	y	312	CLA	11	0
31	D	405	PL9	6	0
24	y	306	CHL	5	0
25	b	605	CLA	9	0
24	N	605	CHL	5	0
25	B	608	CLA	8	0
40	S	317	NEX	6	0
39	y	316	LUT	13	0
39	s	316	LUT	22	0
24	y	302	CHL	31	0
24	Y	302	CHL	30	0
25	B	605	CLA	7	0
25	C	510	CLA	23	0
25	N	611	CLA	7	0
25	g	613	CLA	17	0
25	b	612	CLA	7	0
25	N	610	CLA	34	0
25	c	504	CLA	15	0
26	R	618	LHG	14	0
26	C	519	LHG	4	0
25	R	608	CLA	18	0
28	K	101	BCR	7	0
25	b	607	CLA	14	0
25	R	602	CLA	15	0
35	c	515	DGD	7	0
25	2	604	CLA	19	0
25	C	503	CLA	4	0
24	N	608	CHL	11	0
26	D	406	LHG	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	r	609	CLA	7	0
40	s	317	NEX	5	0
25	B	607	CLA	15	0
40	n	617	NEX	13	0
25	g	603	CLA	14	0
39	G	615	LUT	15	0
40	r	617	NEX	10	0
25	a	406	CLA	9	0
26	B	625	LHG	7	0
25	G	603	CLA	12	0
38	f	101	HEM	8	0
26	y	301	LHG	12	0
25	c	506	CLA	10	0
28	d	404	BCR	3	0
24	2	603	CHL	21	0
26	N	618	LHG	11	0
25	s	313	CLA	9	0
28	z	101	BCR	5	0
35	A	415	DGD	3	0
40	R	617	NEX	8	0
25	b	608	CLA	9	0
25	B	601	CLA	10	0
32	Y	322	AJP	2	0
24	n	607	CHL	50	0
25	2	605	CLA	6	0
29	a	412	SQD	6	0
27	A	403	PHO	13	0
25	c	508	CLA	12	0
26	Y	301	LHG	13	0
30	b	623	LMG	5	0
30	A	410	LMG	3	0
25	a	403	CLA	13	0
35	b	626	DGD	6	0
26	C	518	LHG	3	0
25	s	305	CLA	15	0
25	b	616	CLA	15	0
25	y	314	CLA	17	0
26	B	622	LHG	8	0
25	r	603	CLA	17	0
24	g	601	CHL	15	0
25	C	511	CLA	20	0
25	Y	311	CLA	25	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	510	CLA	24	0
25	g	611	CLA	14	0
25	R	603	CLA	17	0
32	Y	320	AJP	3	0
25	G	613	CLA	18	0
25	G	614	CLA	5	0
25	Y	313	CLA	9	0
28	Z	101	BCR	5	0
24	r	607	CHL	9	0
39	n	615	LUT	12	0
39	r	615	LUT	8	0
25	C	504	CLA	14	0
25	c	503	CLA	5	0
25	n	603	CLA	33	0
25	b	603	CLA	6	0
25	c	513	CLA	17	0
25	b	604	CLA	14	0
28	A	406	BCR	4	0
28	C	514	BCR	7	0
25	Y	303	CLA	26	0
25	N	602	CLA	22	0
33	a	414	BCT	1	0
28	B	618	BCR	7	0
27	a	404	PHO	14	0
25	S	310	CLA	14	0
25	c	507	CLA	7	0
25	n	613	CLA	28	0
25	r	614	CLA	13	0
24	s	306	CHL	11	0
29	A	411	SQD	5	0
25	Y	305	CLA	4	0
24	Y	306	CHL	6	0
28	a	407	BCR	5	0
25	B	611	CLA	7	0
25	R	614	CLA	11	0
25	C	506	CLA	8	0
25	B	614	CLA	12	0
25	b	606	CLA	16	0
40	G	617	NEX	15	0
32	n	620	AJP	1	0
29	l	101	SQD	5	0
28	i	101	BCR	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	R	613	CHL	4	0
33	A	413	BCT	2	0
39	g	616	LUT	15	0
25	s	303	CLA	15	0
40	g	617	NEX	15	0
25	N	612	CLA	10	0
39	G	616	LUT	15	0
25	Y	304	CLA	23	0
32	N	619	AJP	2	0
32	y	322	AJP	2	0
25	c	512	CLA	12	0
24	G	606	CHL	19	0
41	R	616	XAT	20	0
24	r	613	CHL	4	0
40	Y	318	NEX	7	0
24	r	606	CHL	2	0
39	g	615	LUT	15	0
25	s	314	CLA	10	0
25	D	401	CLA	8	0
27	A	404	PHO	14	0
25	C	513	CLA	15	0
25	S	303	CLA	14	0
24	g	607	CHL	11	0
25	s	309	CLA	3	0
25	y	311	CLA	24	0
24	G	607	CHL	11	0
25	Y	315	CLA	17	0
25	s	304	CLA	12	0
31	d	405	PL9	6	0
25	c	502	CLA	12	0
41	r	616	XAT	22	0
26	l	103	LHG	5	0
24	2	601	CHL	8	0
25	G	610	CLA	37	0
25	y	313	CLA	9	0
26	C	517	LHG	3	0
32	y	321	AJP	2	0
30	D	407	LMG	3	0
25	S	309	CLA	3	0
30	d	407	LMG	3	0
26	d	406	LHG	10	0
24	n	606	CHL	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	613	CLA	30	0
25	2	602	CLA	8	0
25	S	312	CLA	9	0
29	L	103	SQD	6	0
29	a	408	SQD	6	0
24	r	605	CHL	9	0
25	G	611	CLA	12	0
25	R	609	CLA	5	0
24	Y	309	CHL	14	0
26	s	318	LHG	6	0
32	y	320	AJP	3	0
25	B	616	CLA	14	0
25	Y	314	CLA	15	0
26	s	301	LHG	9	0
25	B	613	CLA	16	0
24	R	607	CHL	9	0
24	G	608	CHL	19	0
39	N	616	LUT	15	0
24	N	609	CHL	26	0
25	g	614	CLA	4	0
35	C	516	DGD	10	0
40	N	617	NEX	15	0
25	A	405	CLA	9	0
25	n	611	CLA	7	0
39	S	315	LUT	7	0
25	D	403	CLA	15	0
35	B	626	DGD	5	0
39	Y	317	LUT	13	0
32	s	319	AJP	2	0
28	c	514	BCR	7	0
29	l	102	SQD	20	0
24	n	601	CHL	16	0
24	6	603	CHL	20	0
25	r	601	CLA	17	0
24	g	608	CHL	20	0
25	y	303	CLA	24	0
25	r	610	CLA	11	0
25	N	604	CLA	9	0
25	y	305	CLA	4	0
30	c	520	LMG	4	0
25	R	611	CLA	3	0
25	B	606	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	b	621	LHG	3	0
25	c	505	CLA	10	0
30	B	623	LMG	5	0
25	R	610	CLA	11	0
32	S	319	AJP	2	0
25	B	603	CLA	6	0
25	G	604	CLA	12	0
39	R	615	LUT	6	0
26	Y	319	LHG	7	0
28	b	618	BCR	8	0
24	N	601	CHL	18	0
25	6	602	CLA	10	0
25	A	401	CLA	19	0
28	B	619	BCR	4	0
24	s	302	CHL	7	0
24	y	307	CHL	15	0
30	a	411	LMG	3	0
25	b	611	CLA	7	0
25	r	611	CLA	4	0
25	y	304	CLA	20	0
25	B	615	CLA	15	0
25	b	610	CLA	14	0
25	C	512	CLA	12	0
25	c	509	CLA	9	0
25	d	401	CLA	9	0
24	G	609	CHL	10	0
25	6	604	CLA	19	0
25	g	604	CLA	12	0
30	b	620	LMG	5	0
25	c	511	CLA	21	0
25	S	305	CLA	14	0
25	B	610	CLA	14	0
28	B	617	BCR	7	0
32	Y	321	AJP	2	0
24	S	307	CHL	6	0
39	N	615	LUT	12	0
25	n	604	CLA	8	0
24	6	601	CHL	10	0
24	n	608	CHL	9	0
25	6	605	CLA	8	0
29	L	101	SQD	19	0
25	b	609	CLA	11	0

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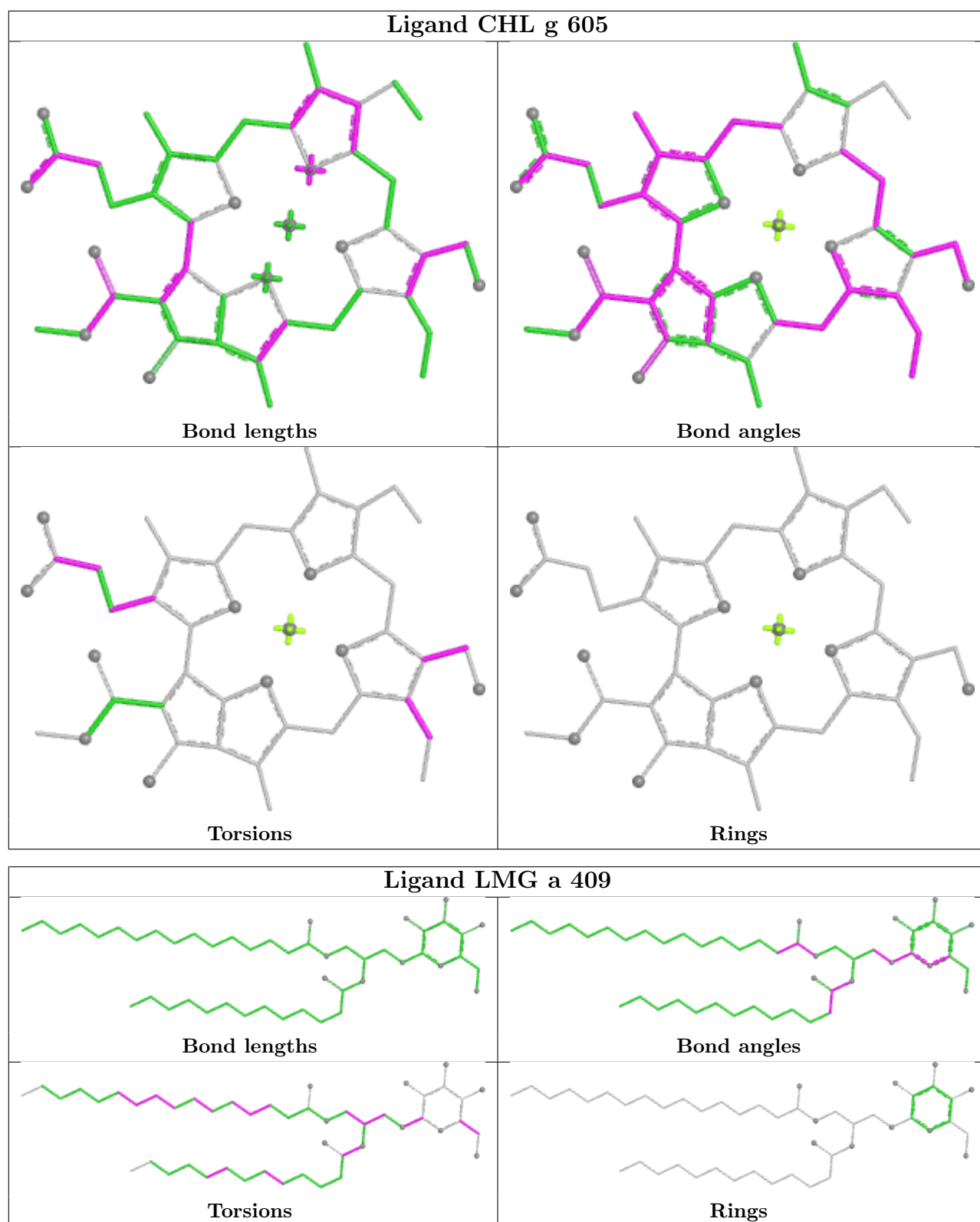
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	y	315	CLA	17	0
25	C	502	CLA	12	0
39	y	317	LUT	12	0
25	c	501	CLA	19	0
25	r	608	CLA	17	0
25	s	312	CLA	10	0
25	B	604	CLA	14	0
39	n	616	LUT	15	0
24	n	609	CHL	29	0
24	S	308	CHL	9	0
25	a	402	CLA	19	0
24	Y	310	CHL	17	0
24	y	309	CHL	14	0
25	A	402	CLA	13	0
25	d	402	CLA	19	0
25	n	602	CLA	23	0
25	N	614	CLA	6	0
28	T	101	BCR	20	0
25	r	604	CLA	10	0
24	G	601	CHL	17	0
39	S	316	LUT	20	0
26	B	621	LHG	3	0
25	Y	312	CLA	10	0
28	b	617	BCR	7	0
24	g	606	CHL	19	0
29	A	407	SQD	8	0
25	R	601	CLA	15	0
25	R	604	CLA	8	0
25	C	508	CLA	10	0
35	a	401	DGD	3	0
24	S	302	CHL	4	0
26	r	618	LHG	16	0
28	H	101	BCR	6	0
27	a	405	PHO	14	0
25	C	505	CLA	10	0
39	s	315	LUT	7	0
26	L	102	LHG	5	0
25	G	602	CLA	12	0
25	b	601	CLA	9	0
26	b	625	LHG	7	0
25	G	612	CLA	8	0
35	C	515	DGD	8	0

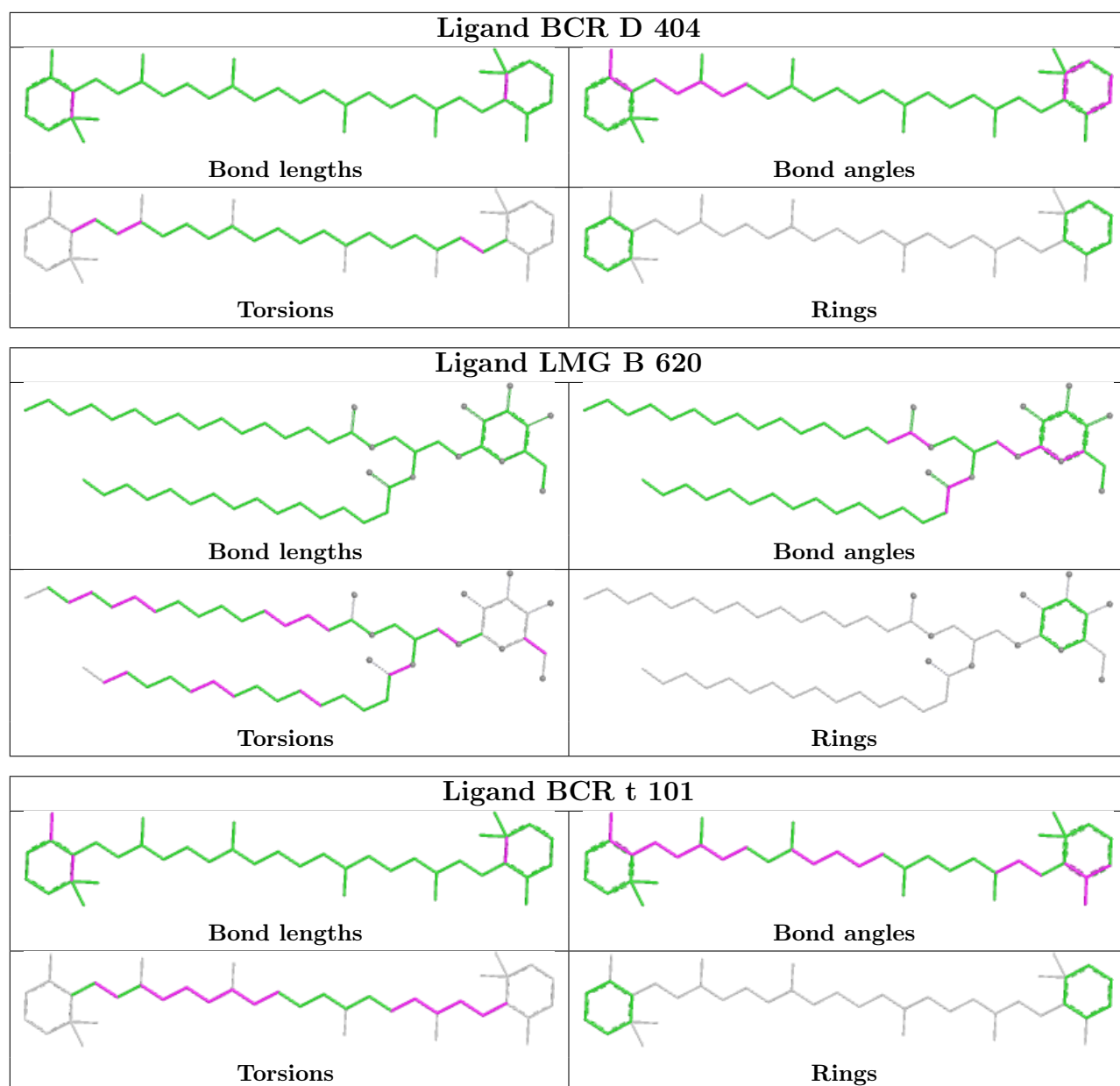
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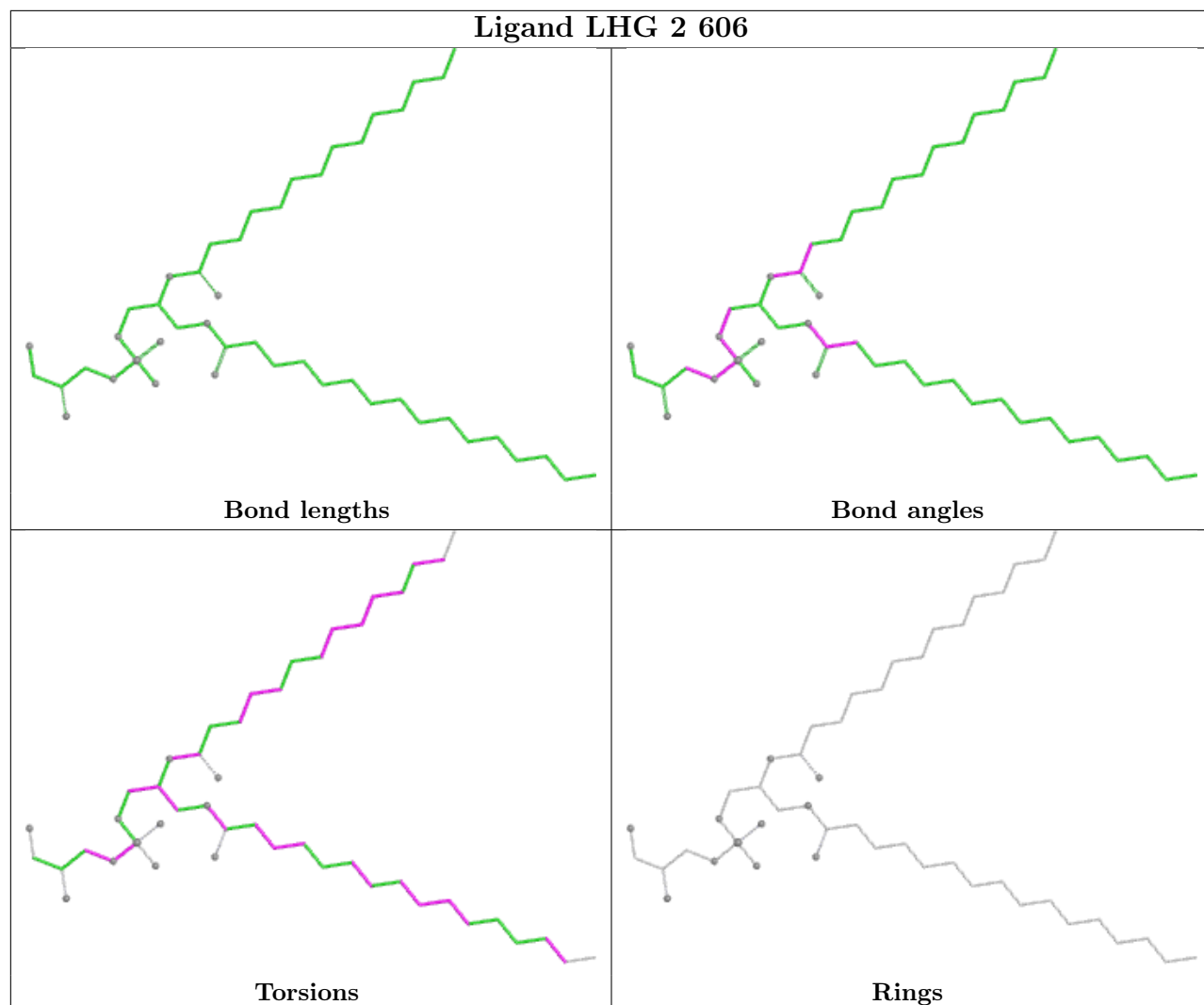
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	r	602	CLA	14	0
25	g	610	CLA	40	0
28	I	101	BCR	20	0
25	C	509	CLA	7	0
24	Y	307	CHL	14	0
35	c	516	DGD	10	0
24	R	605	CHL	8	0
25	b	615	CLA	16	0
25	g	602	CLA	11	0
24	5	302	CHL	8	0
25	n	610	CLA	33	0
25	g	612	CLA	9	0

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

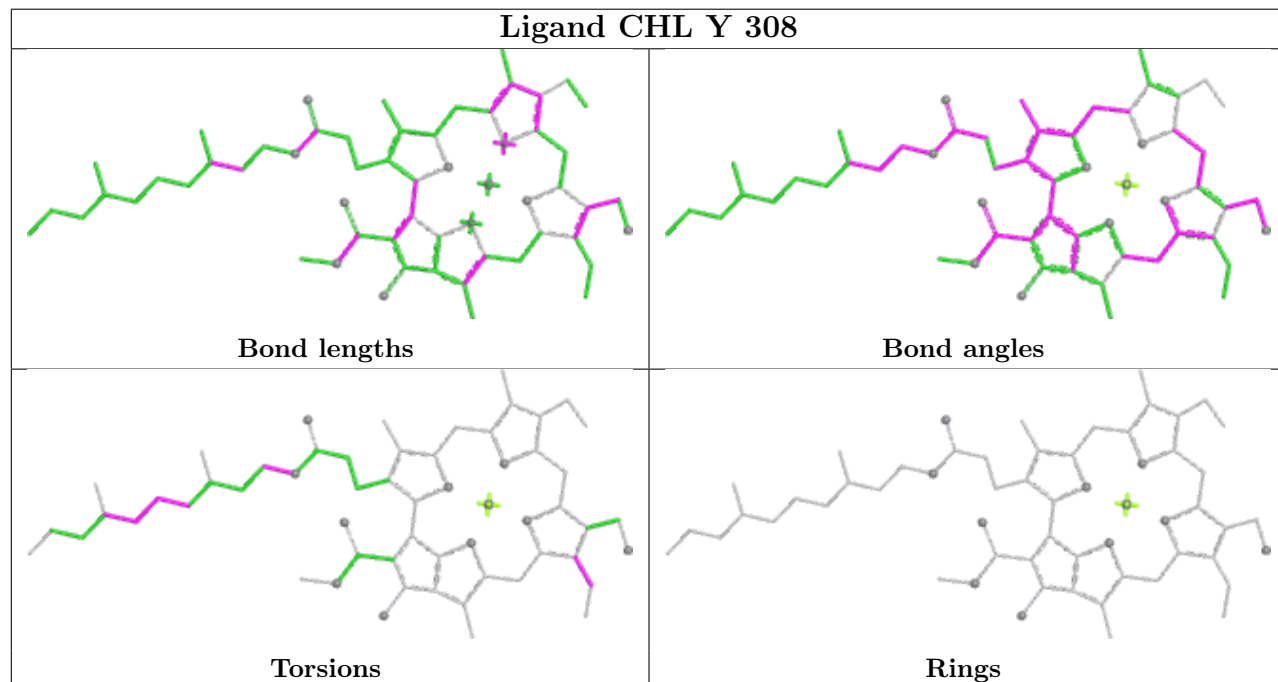


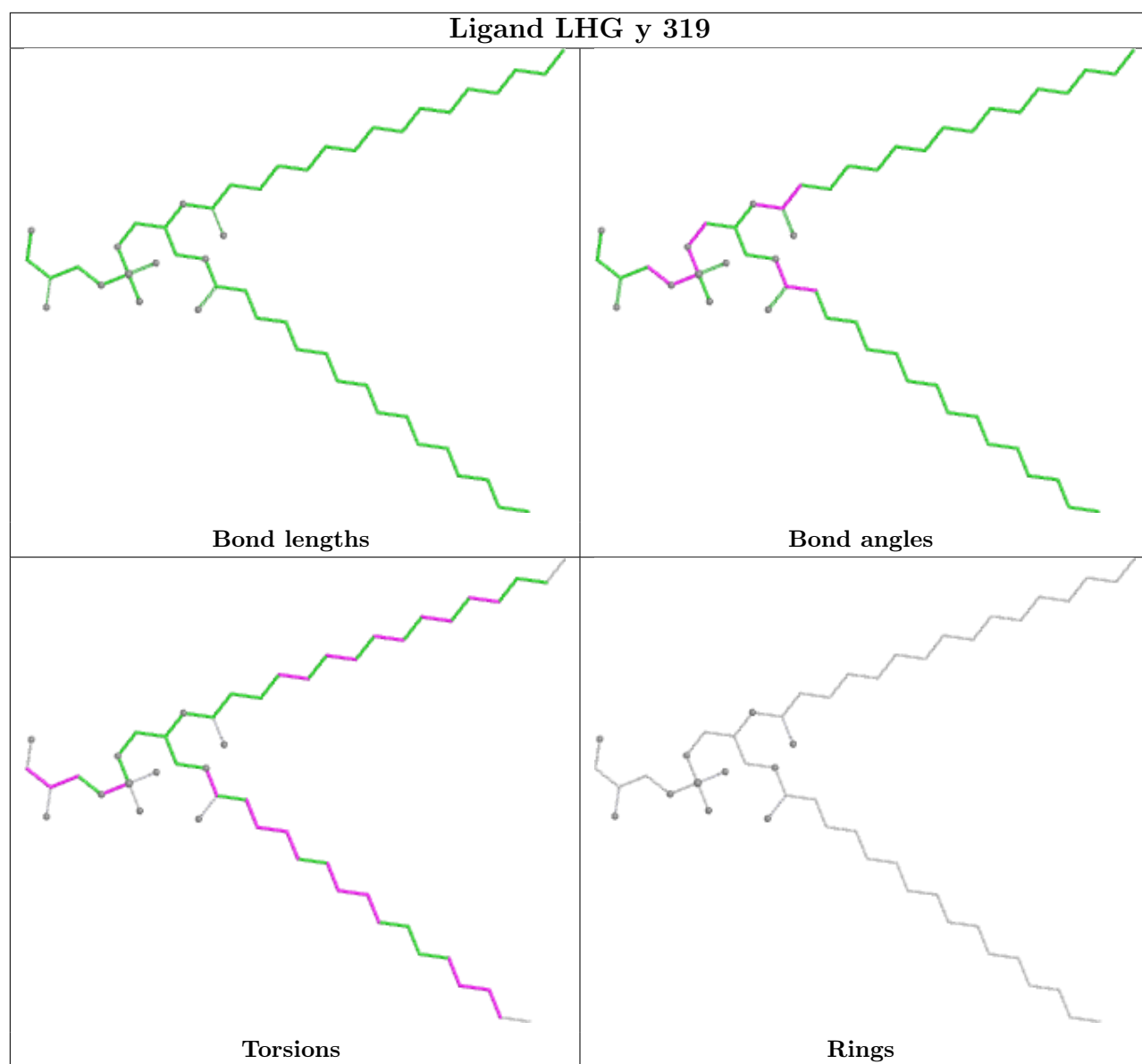


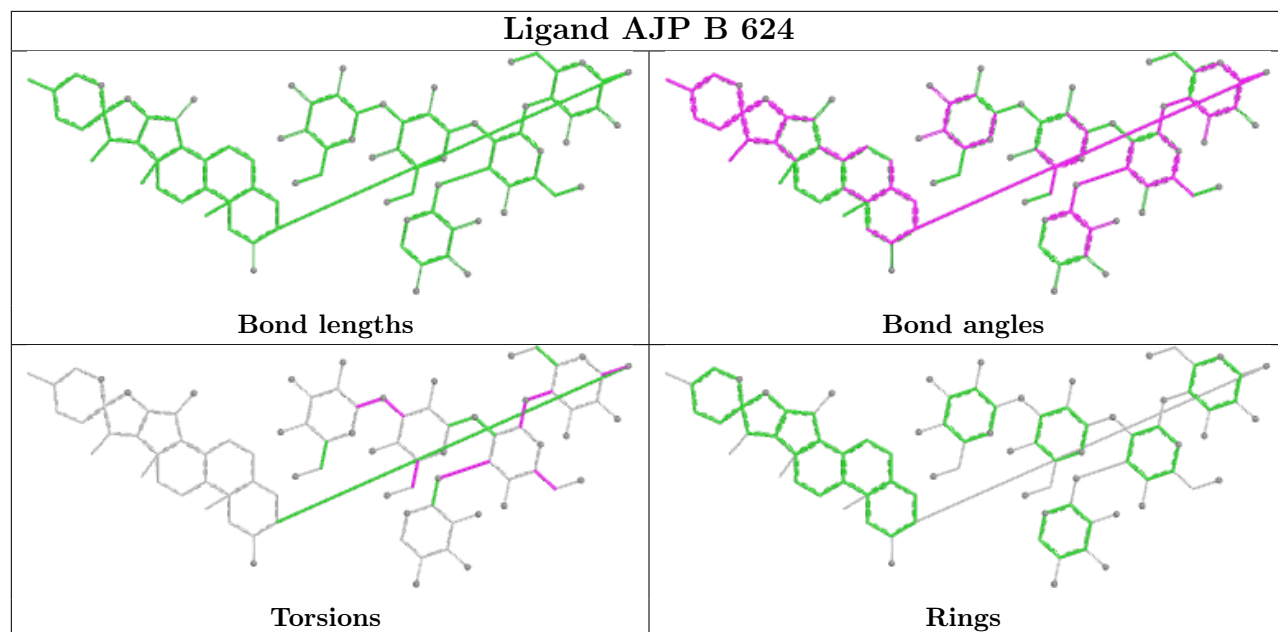
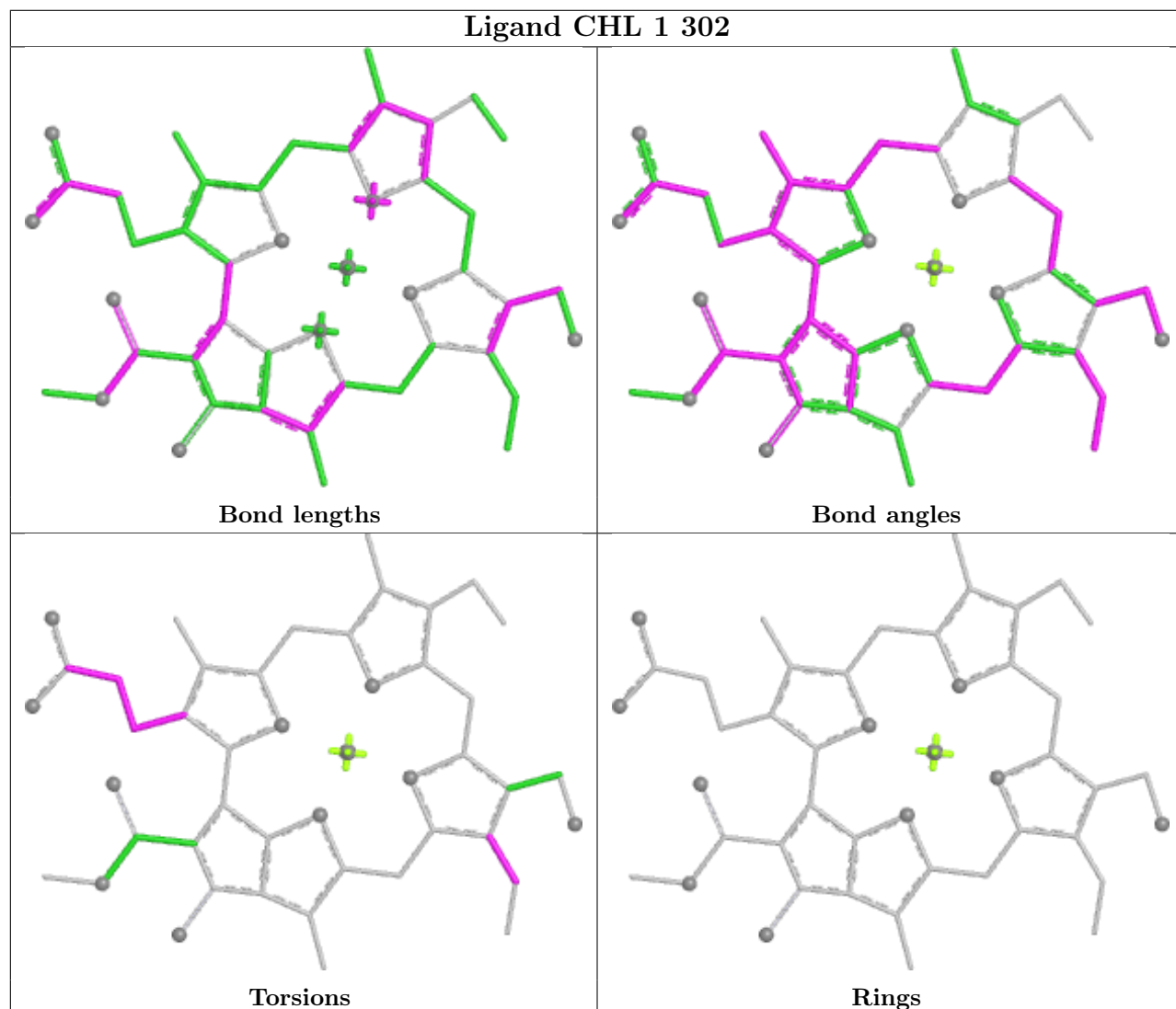
Ligand LHG 2 606

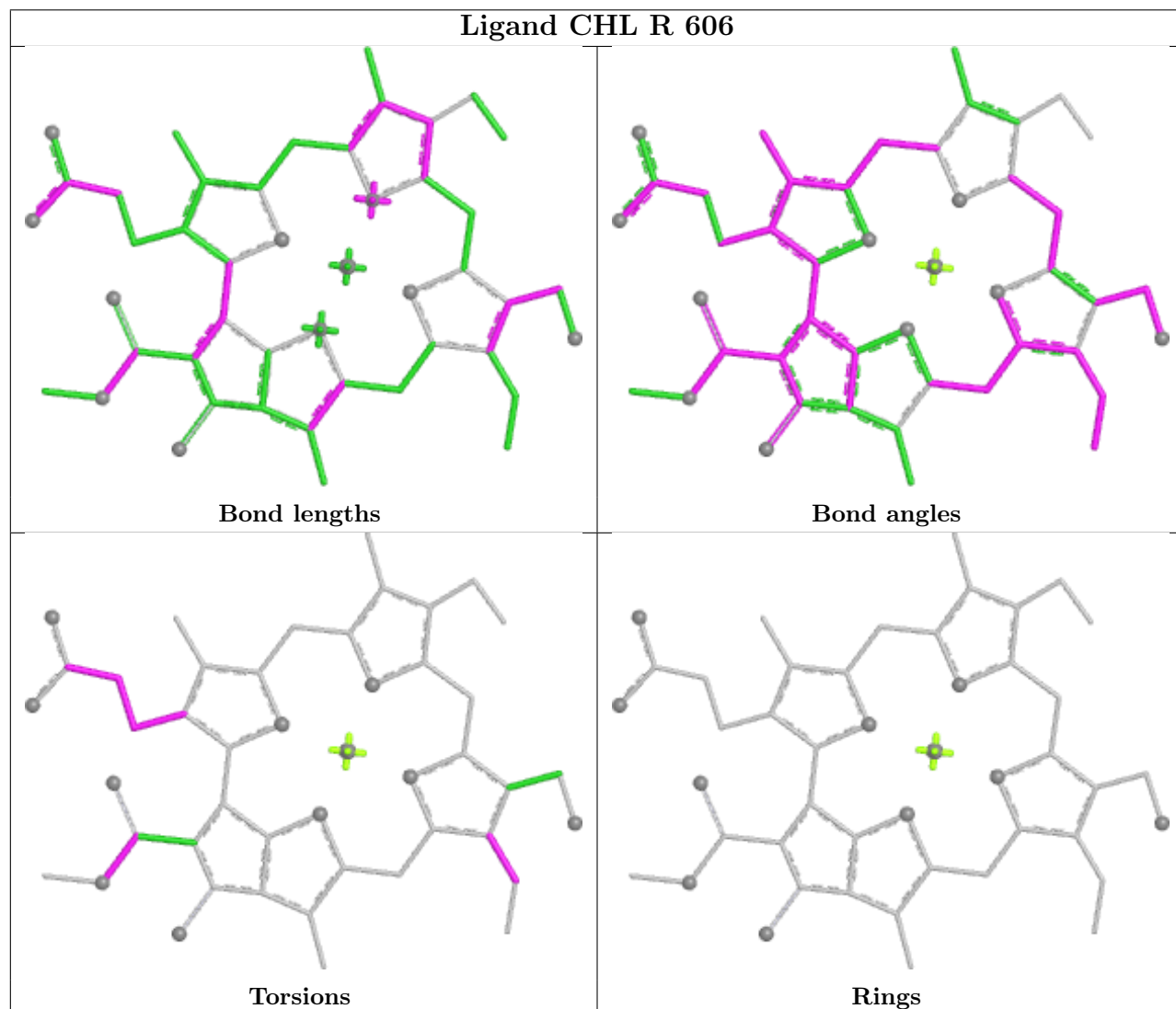
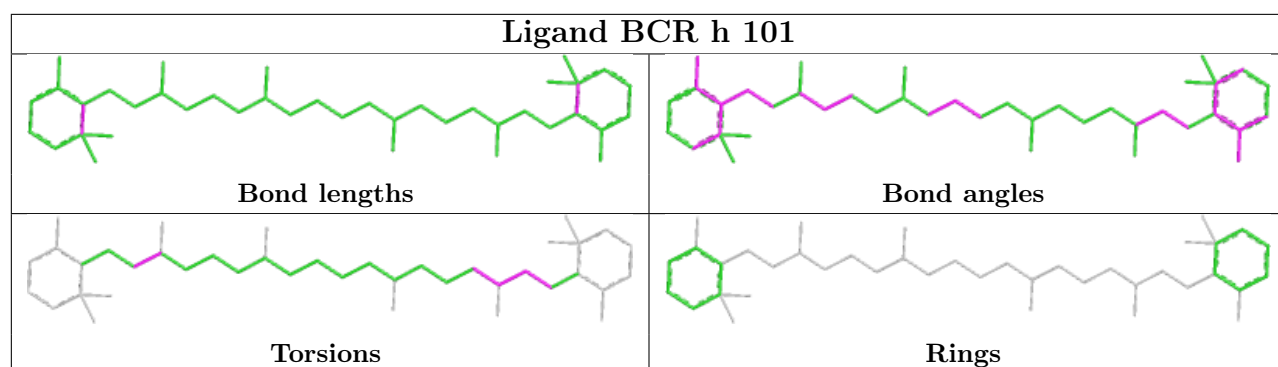


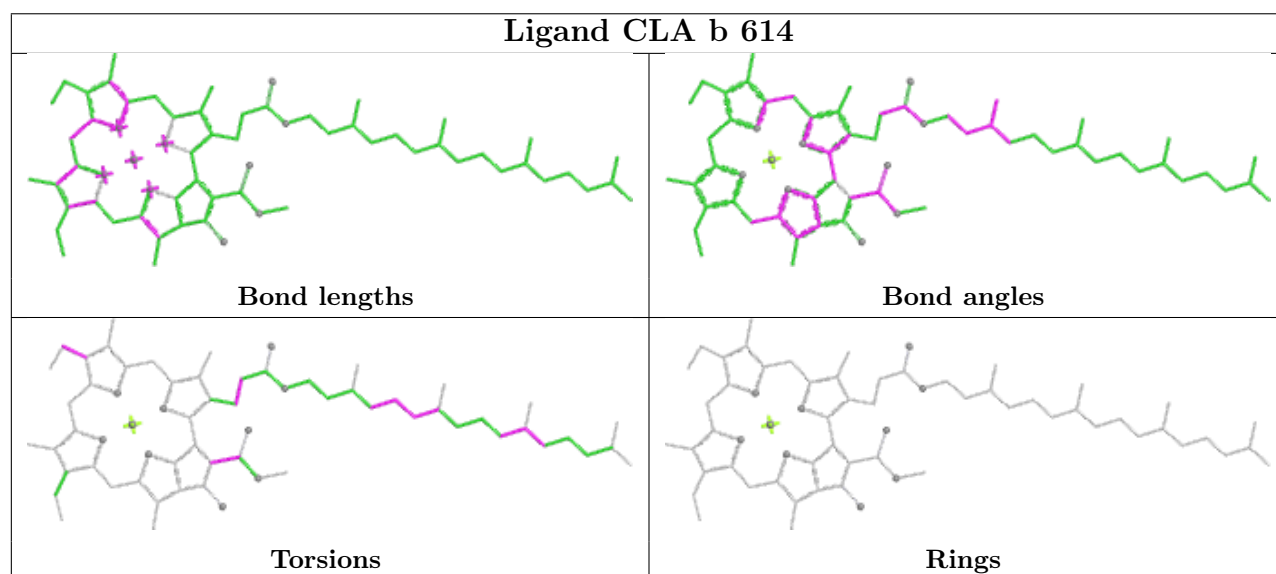
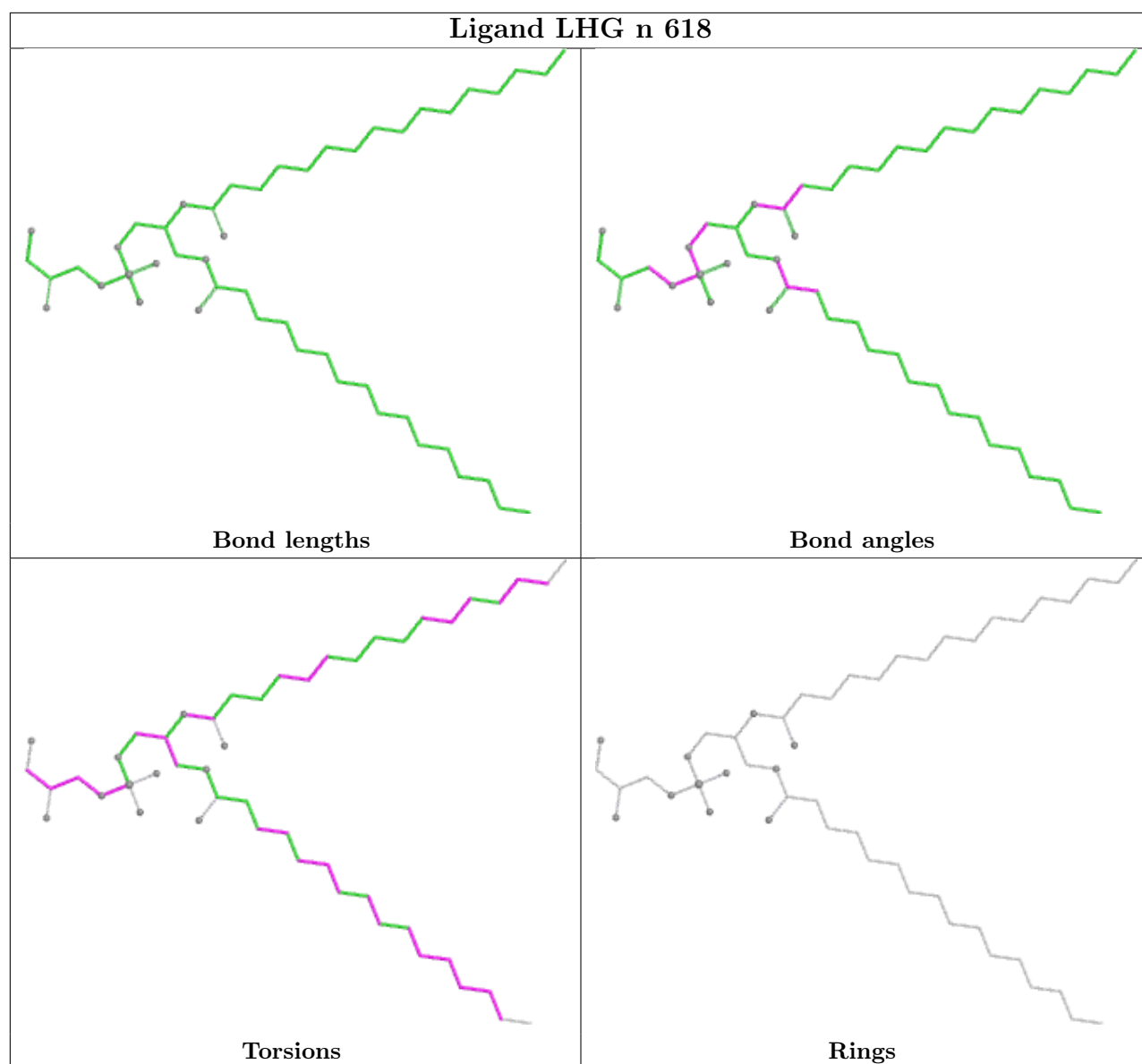
Ligand CHL Y 308

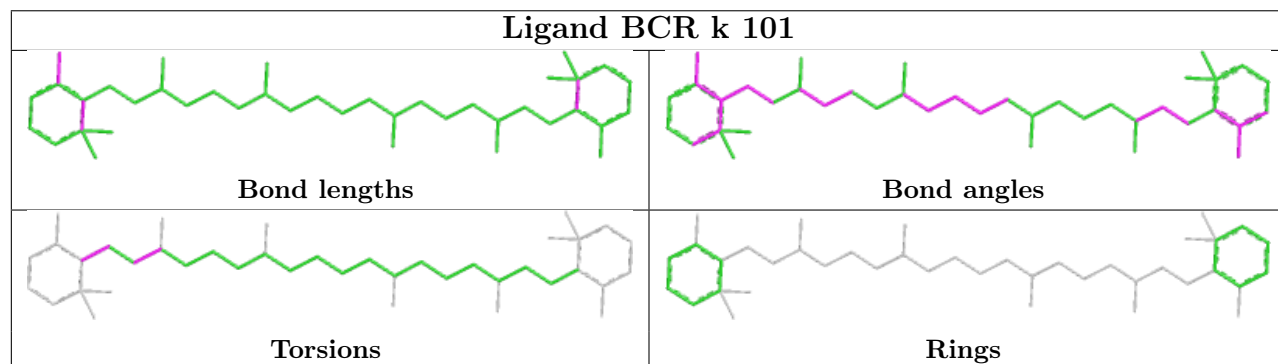
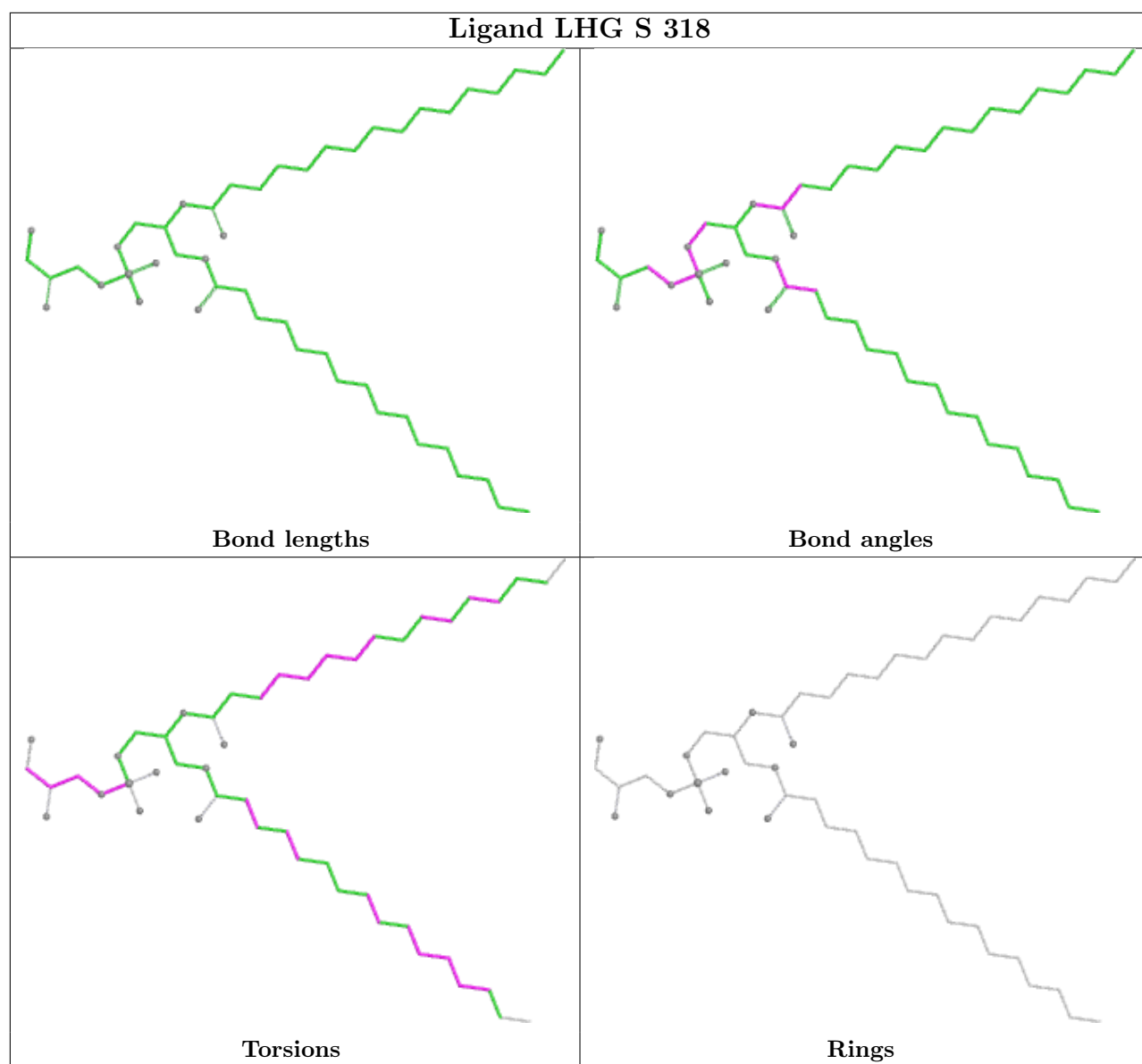




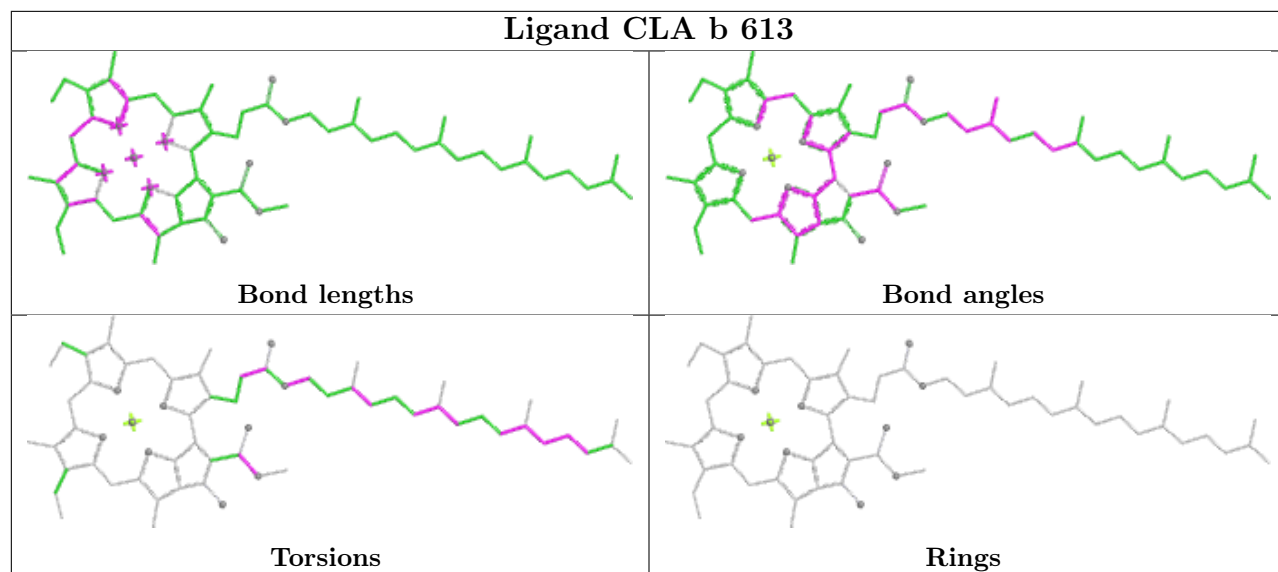
Ligand AJP B 624**Ligand CHL 1 302**



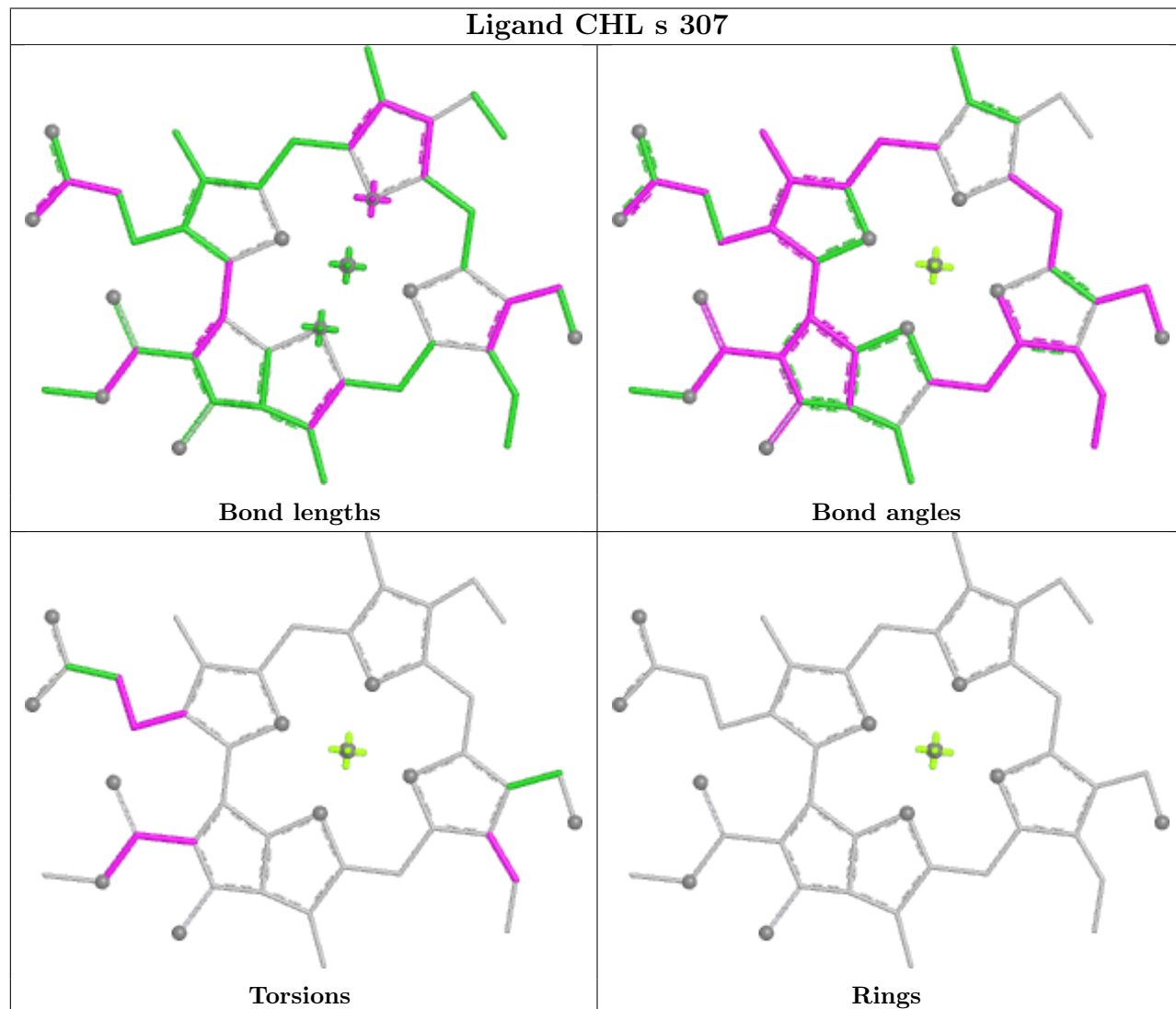




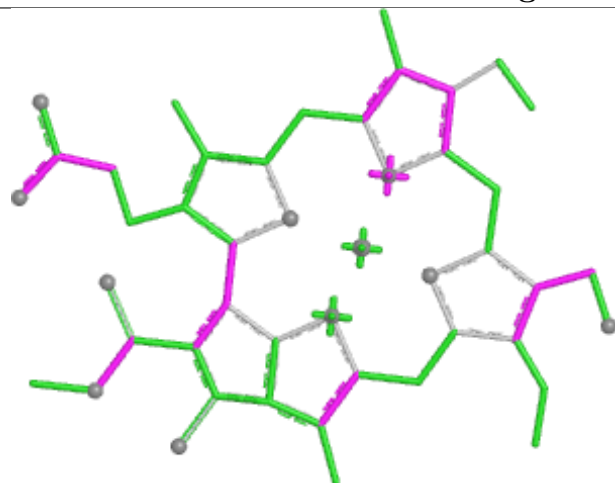
Ligand CLA b 613



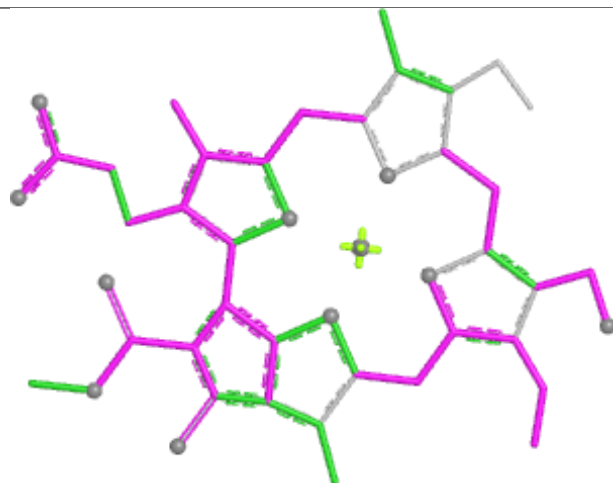
Ligand CHL s 307



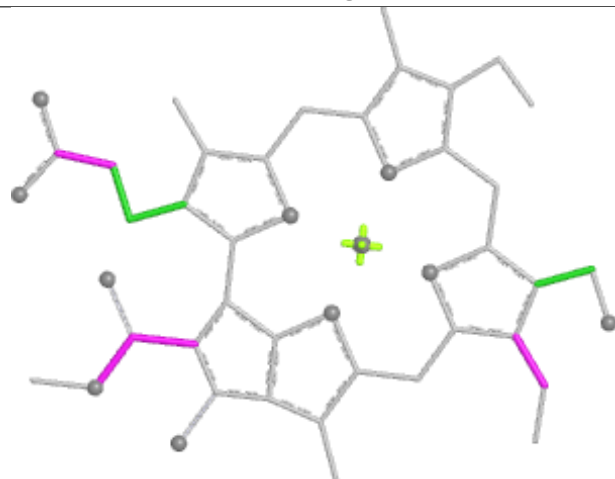
Ligand CHL S 306



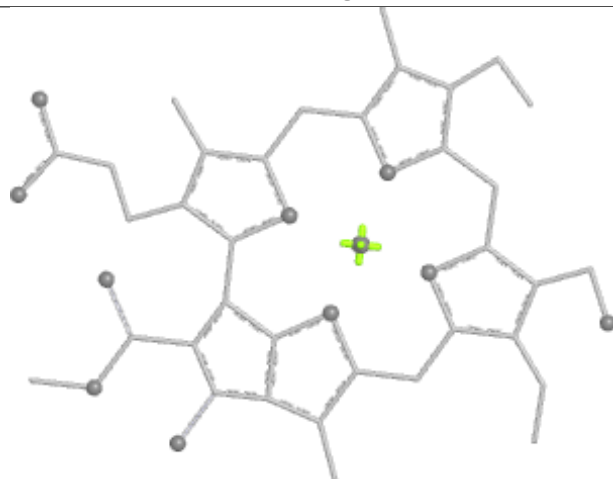
Bond lengths



Bond angles

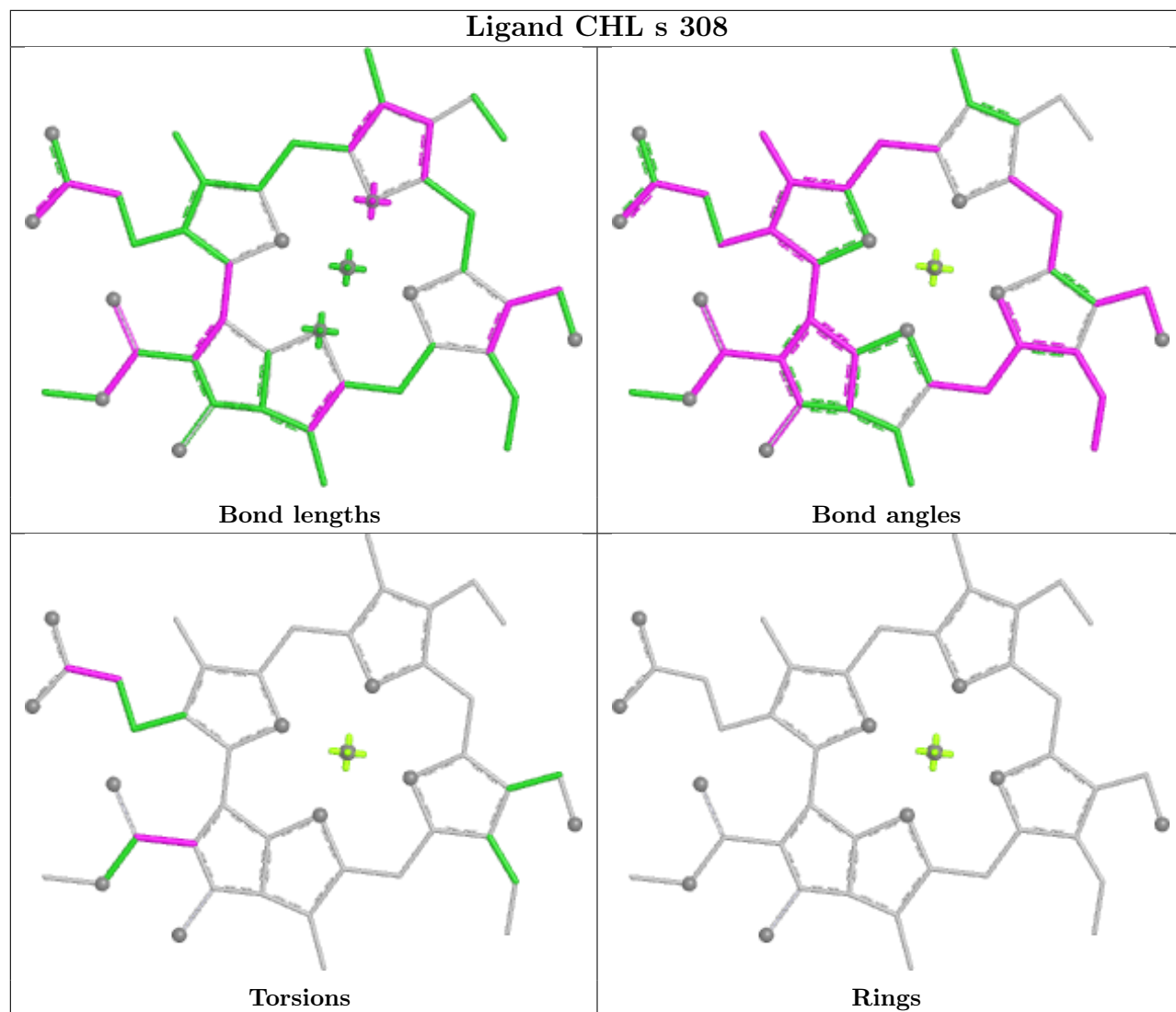


Torsions

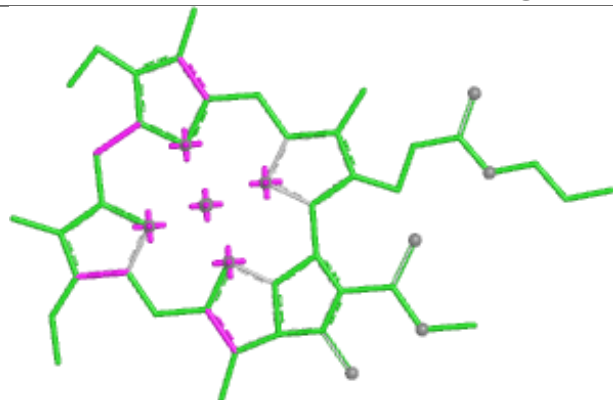


Rings

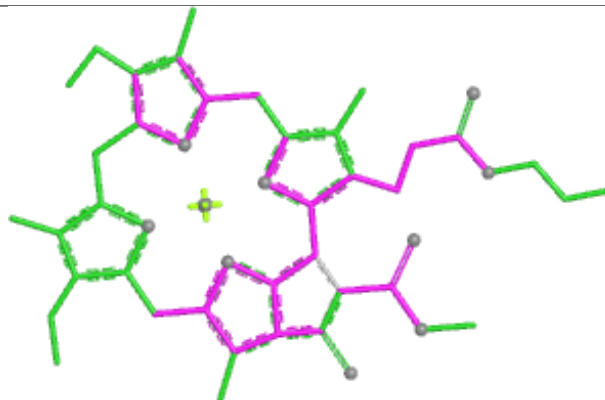
Ligand CHL s 308



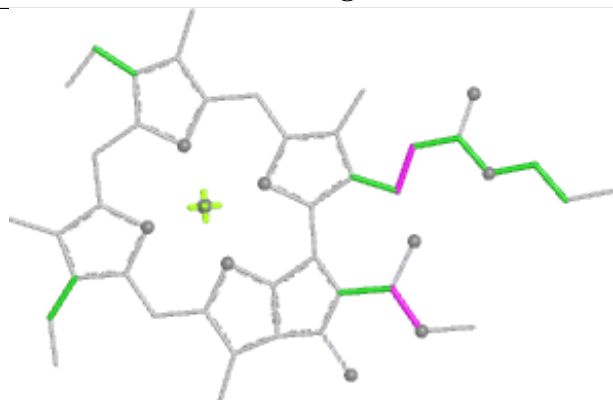
Ligand CLA n 614



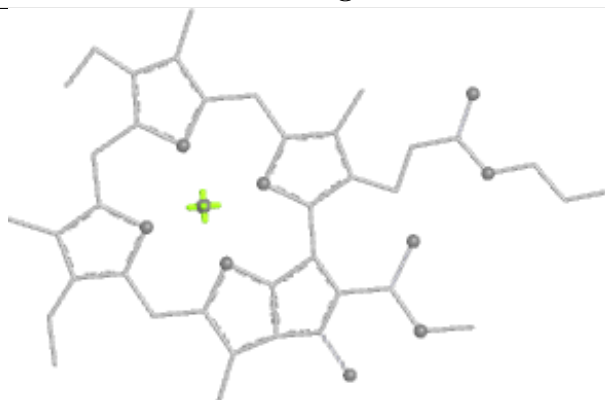
Bond lengths



Bond angles

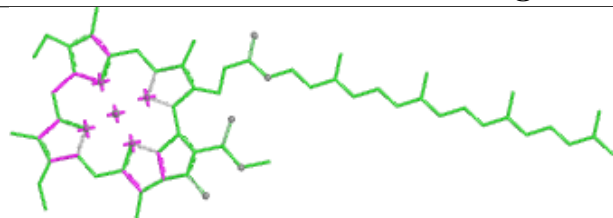


Torsions

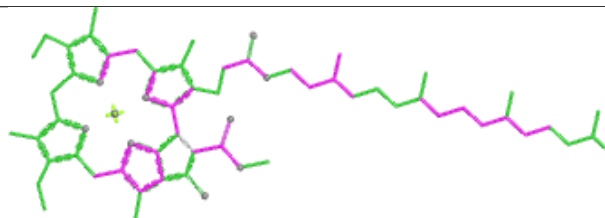


Rings

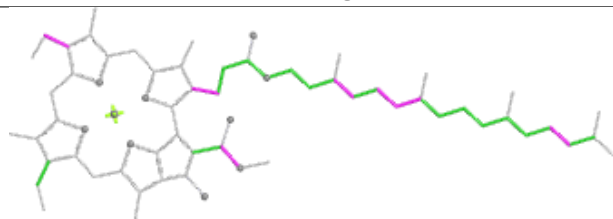
Ligand CLA B 609



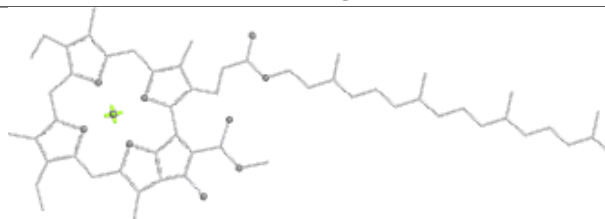
Bond lengths



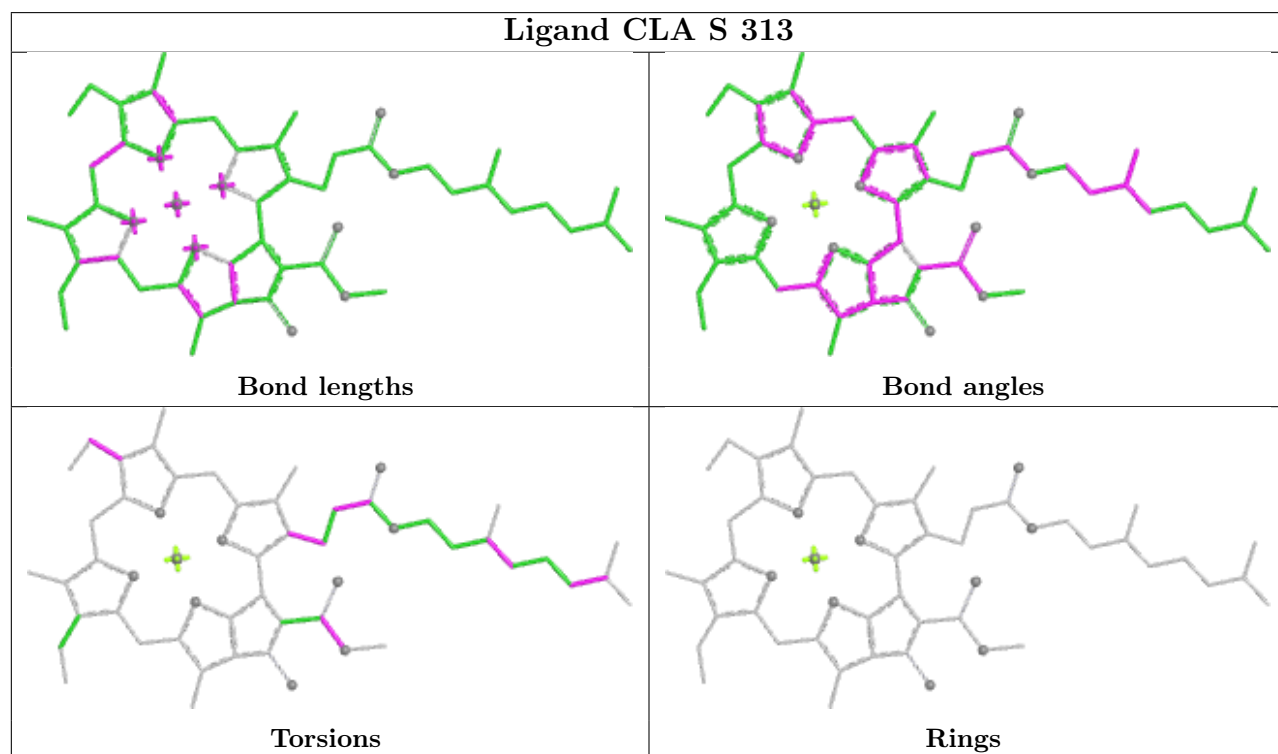
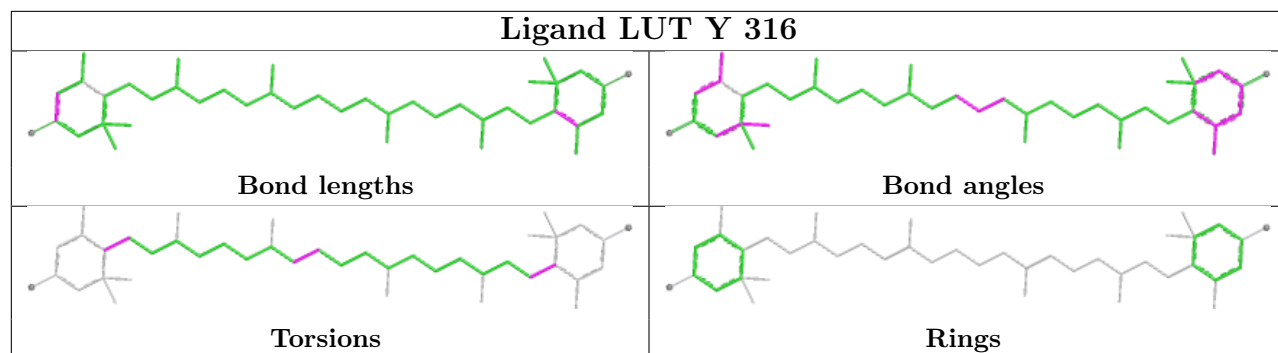
Bond angles

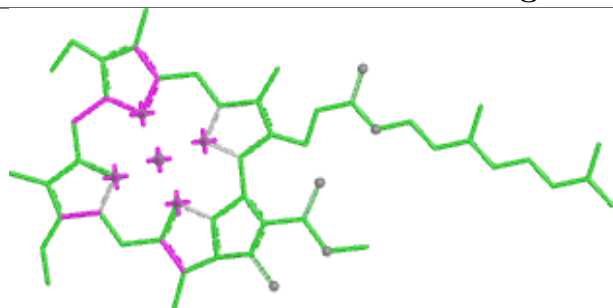


Torsions

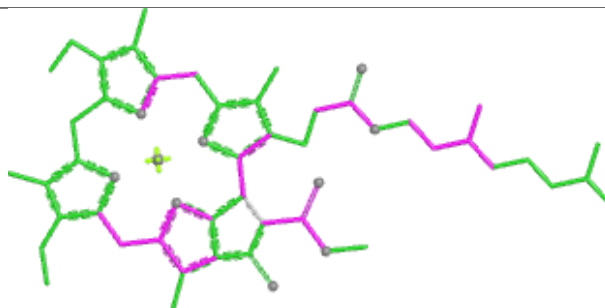


Rings

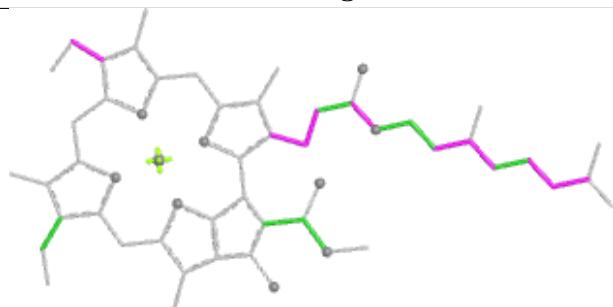


Ligand CLA s 310

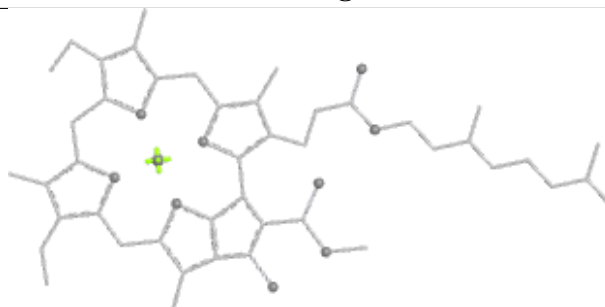
Bond lengths



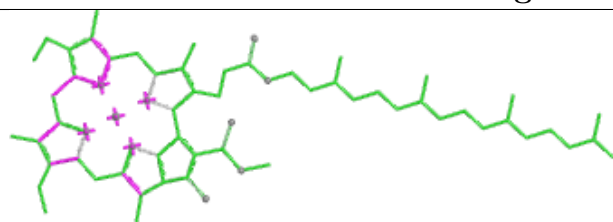
Bond angles



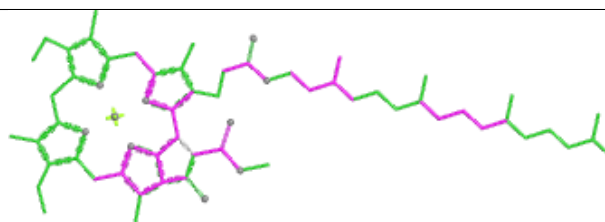
Torsions



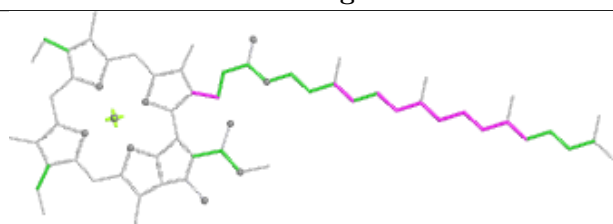
Rings

Ligand CLA B 602

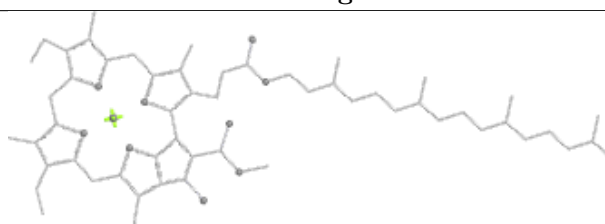
Bond lengths



Bond angles

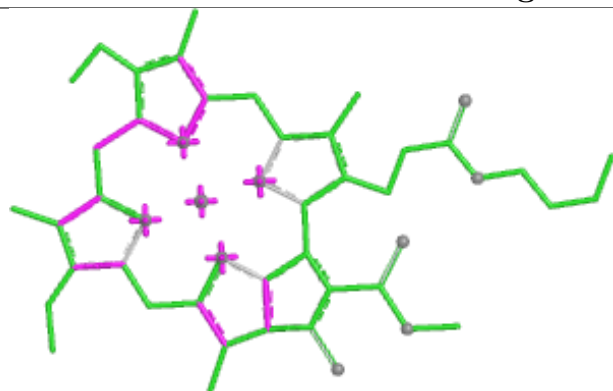


Torsions

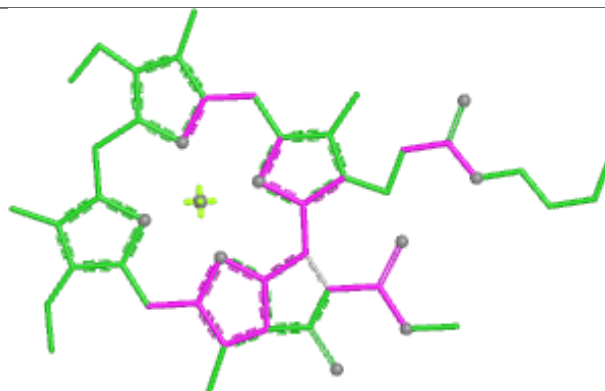


Rings

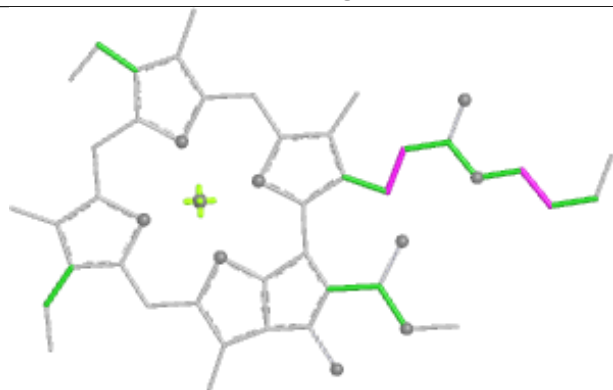
Ligand CLA S 314



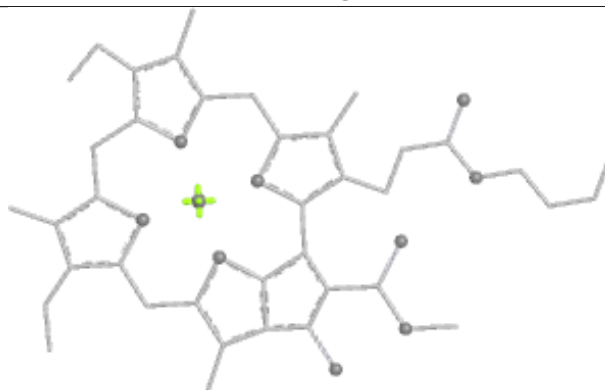
Bond lengths



Bond angles

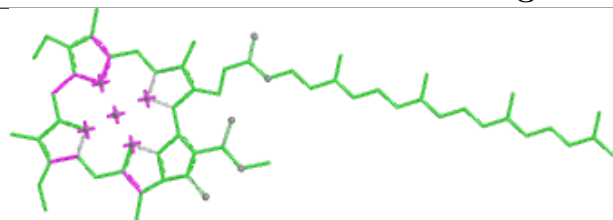


Torsions

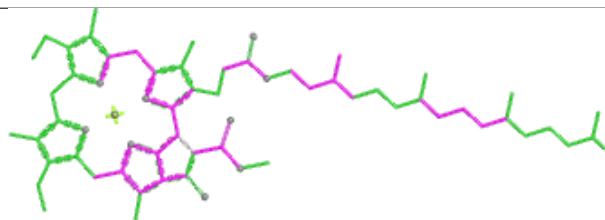


Rings

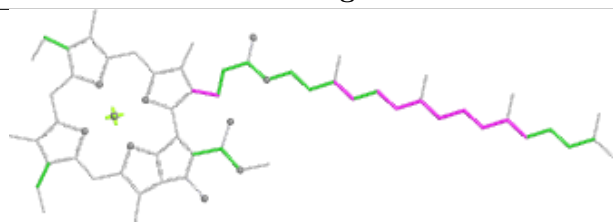
Ligand CLA b 602



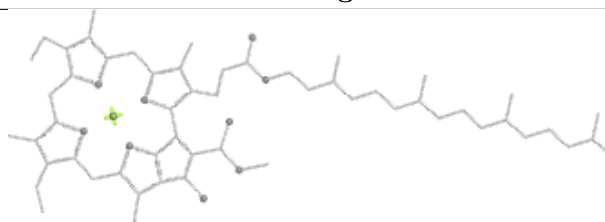
Bond lengths



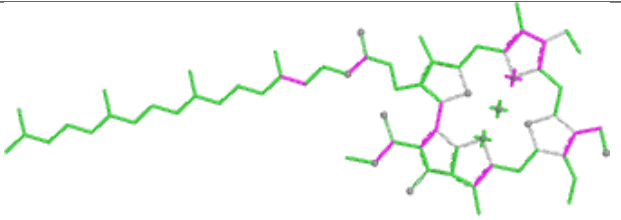
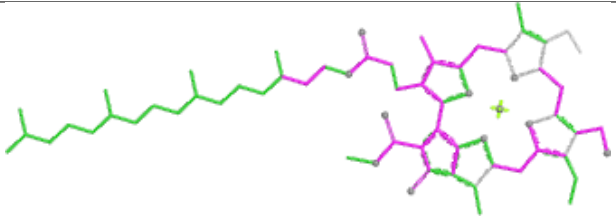
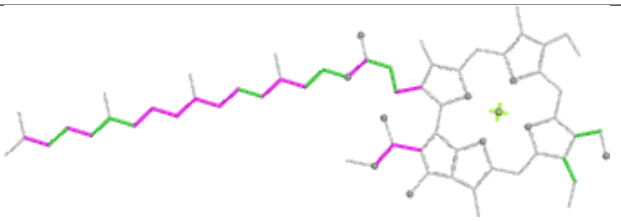
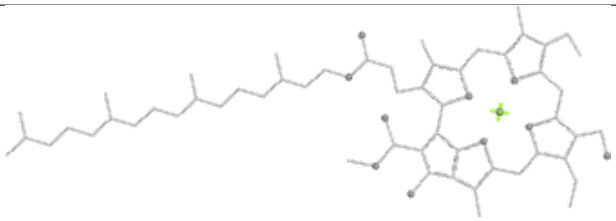
Bond angles

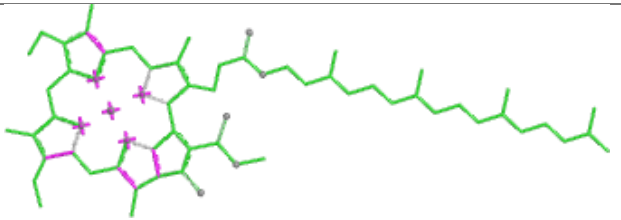
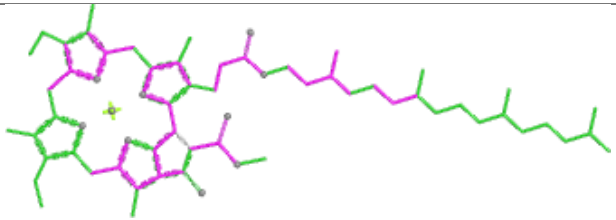
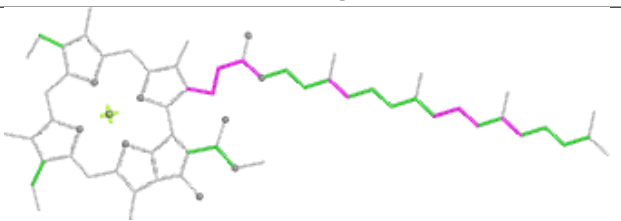
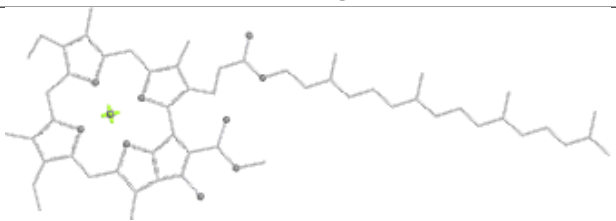


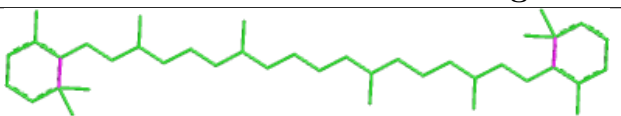
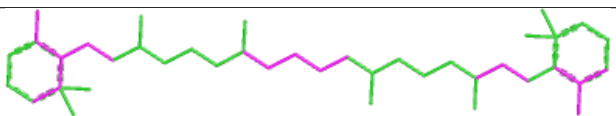
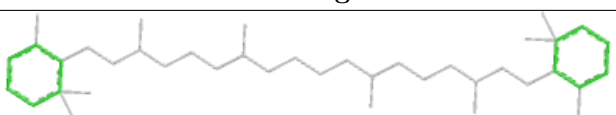
Torsions

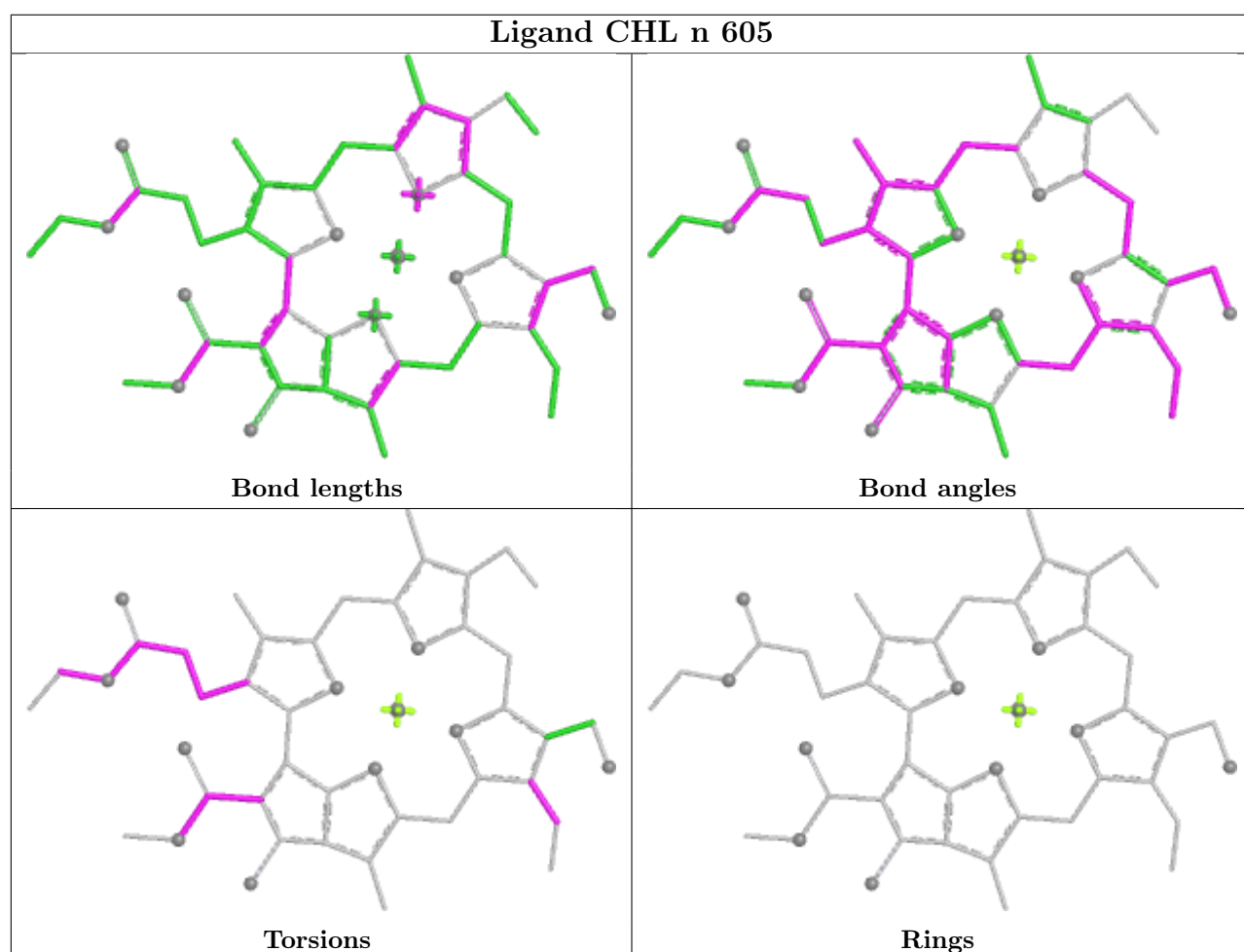
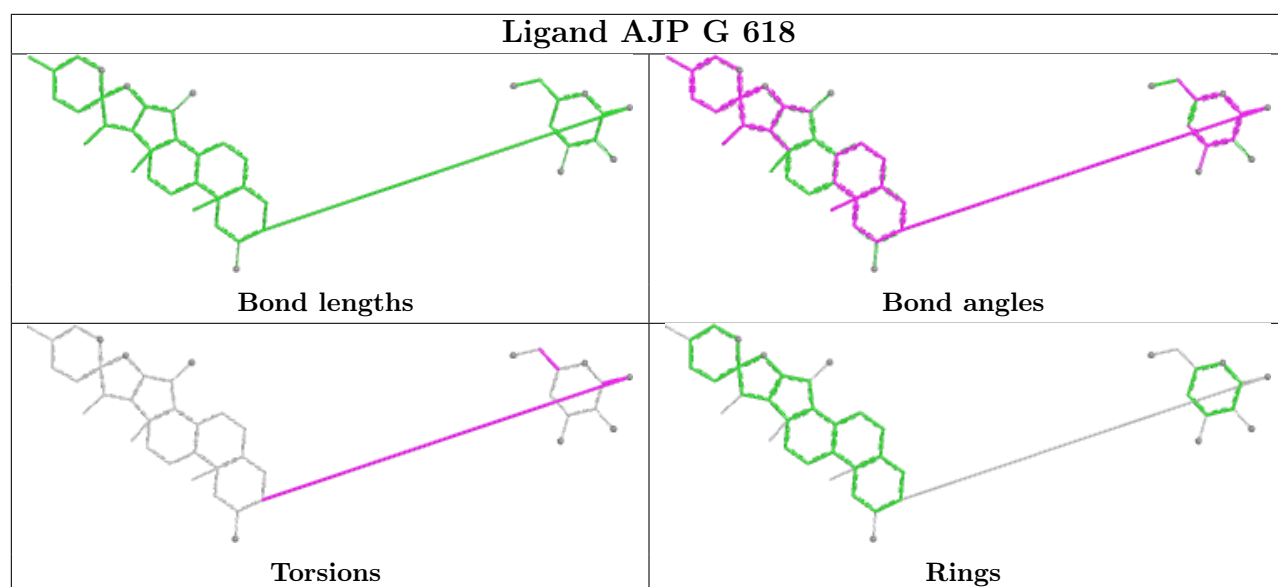


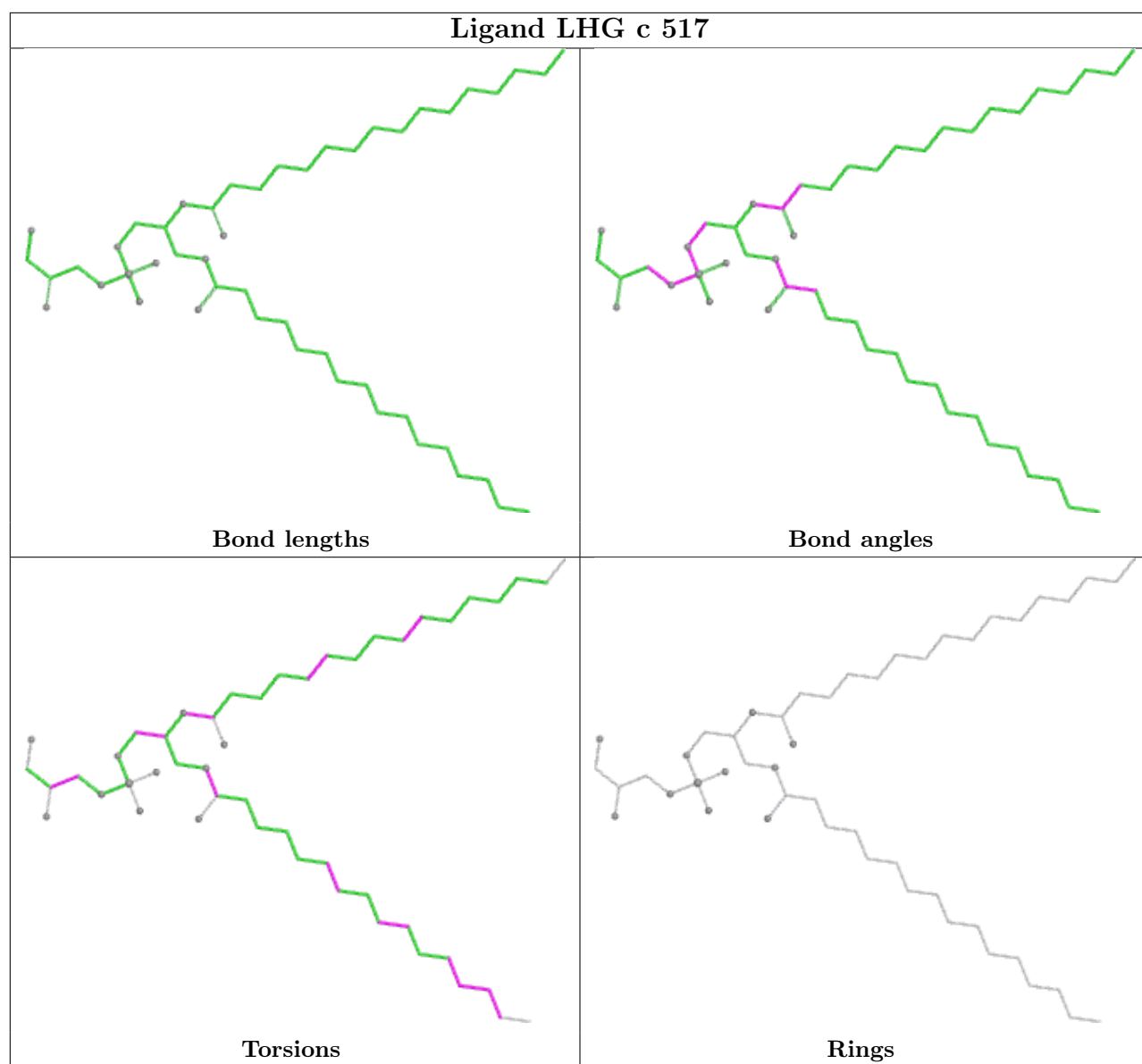
Rings

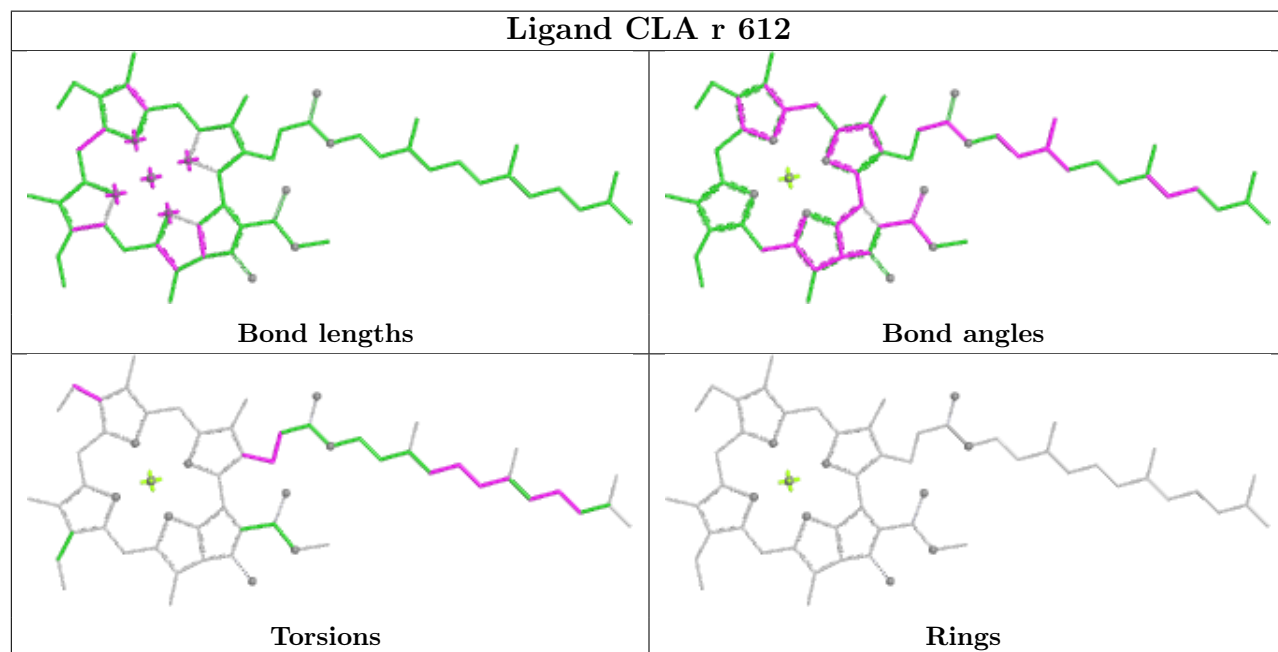
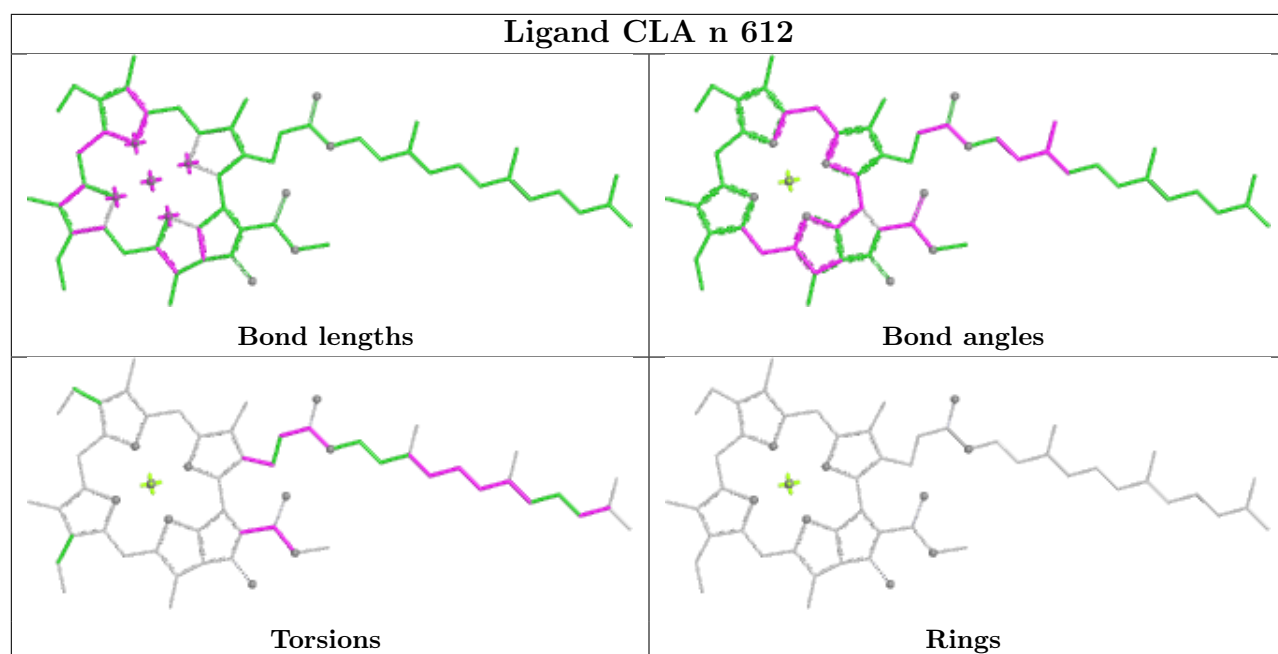
Ligand CHL N 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

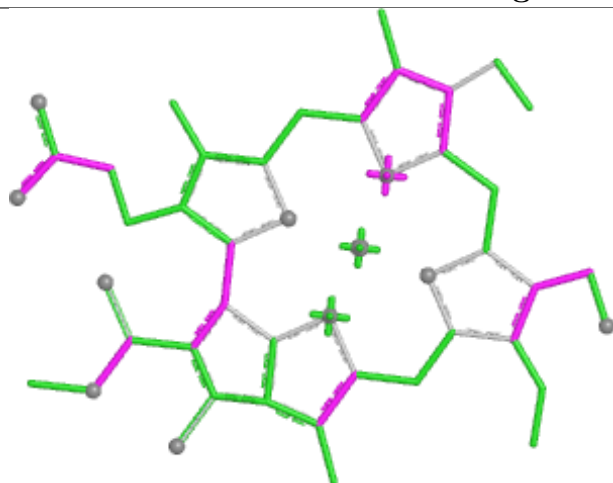
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings



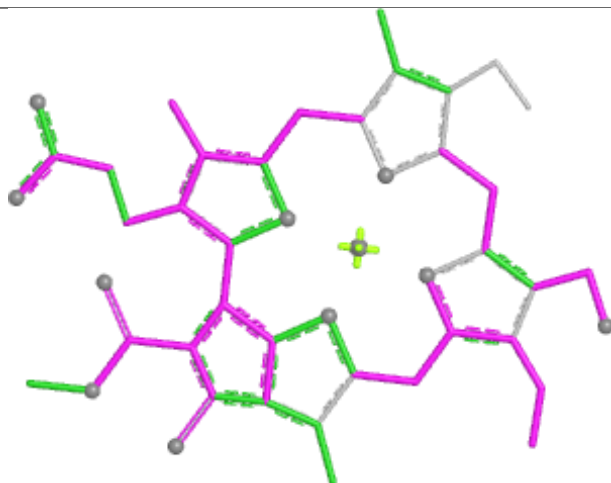




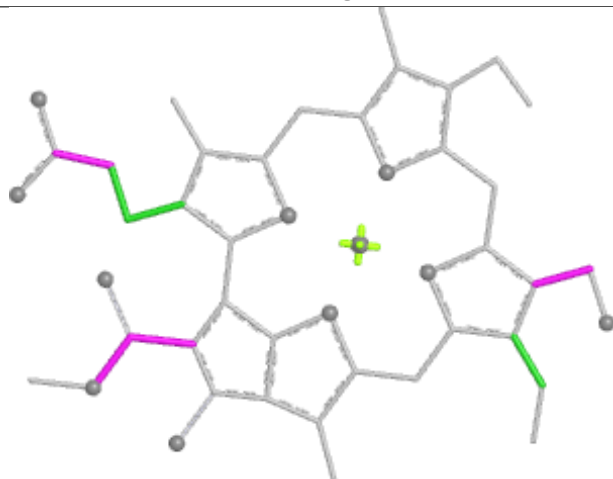
Ligand CHL N 606



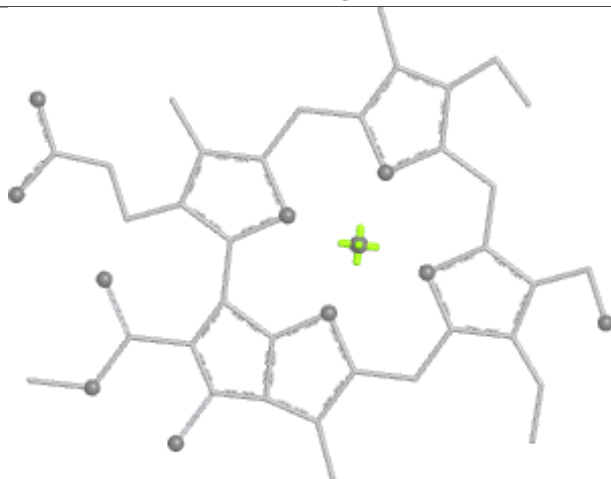
Bond lengths



Bond angles

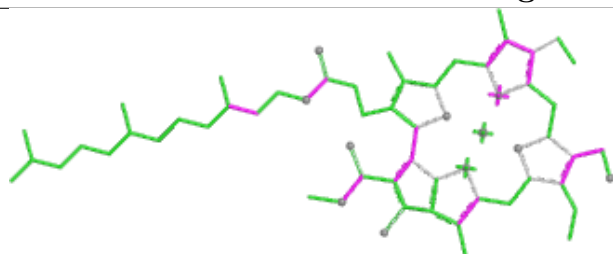


Torsions

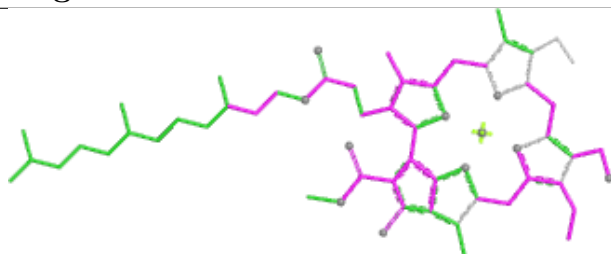


Rings

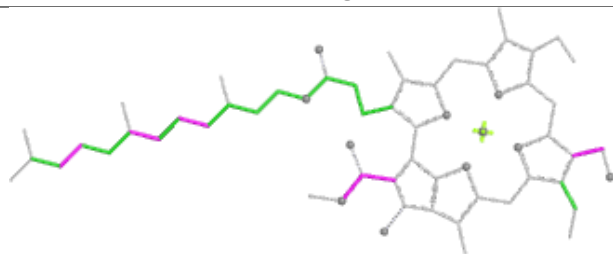
Ligand CHL g 609



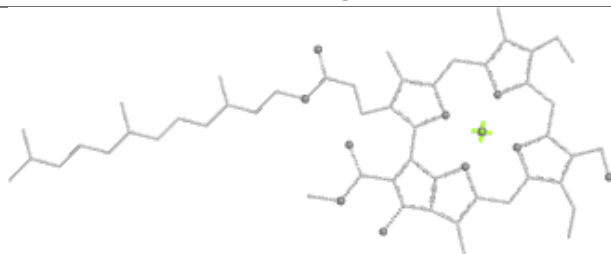
Bond lengths



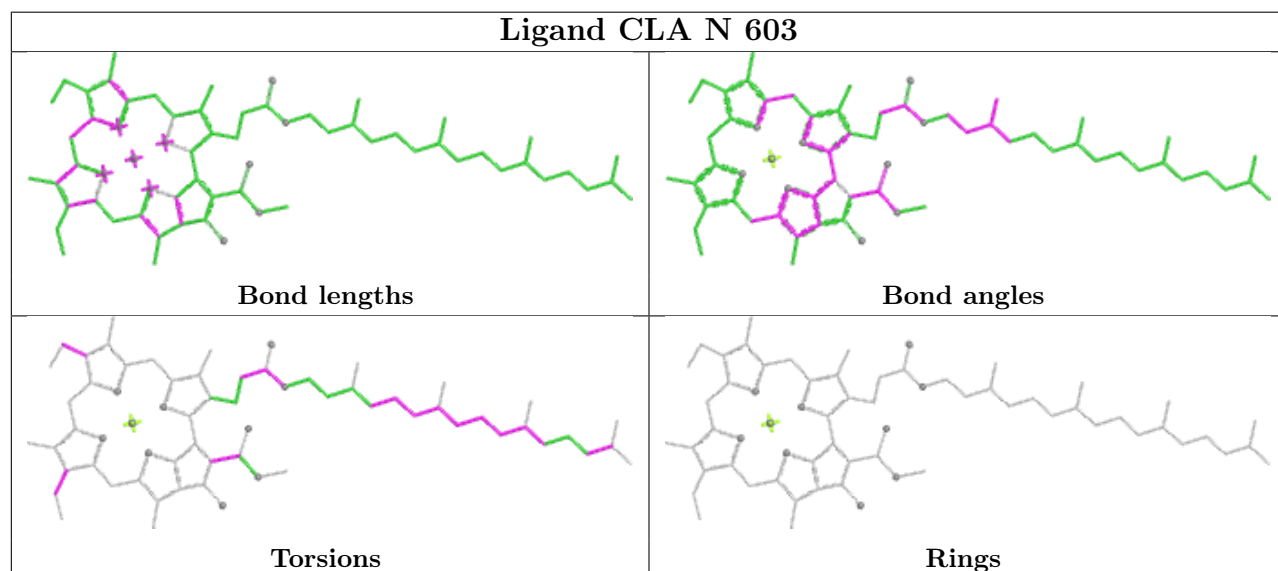
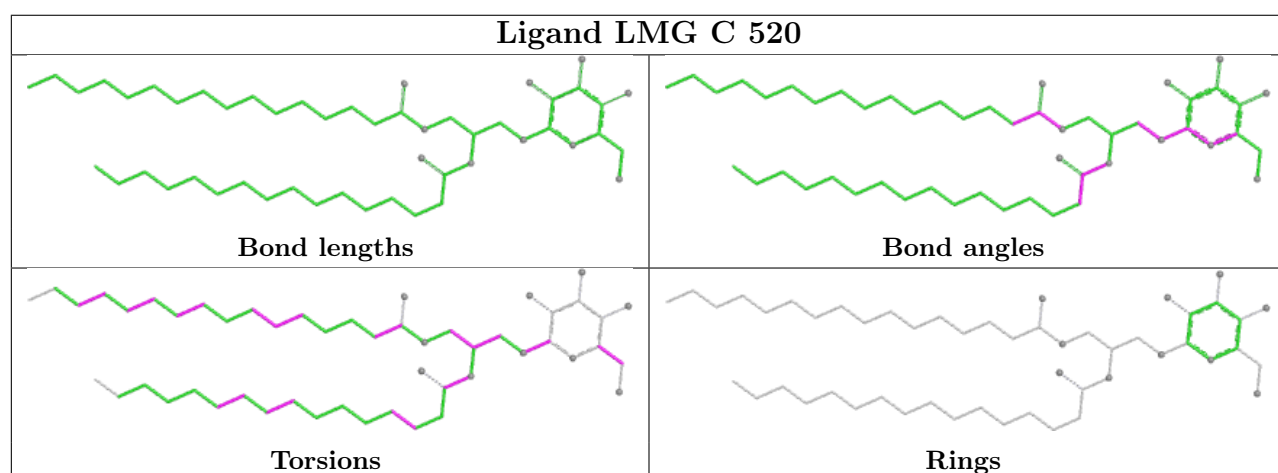
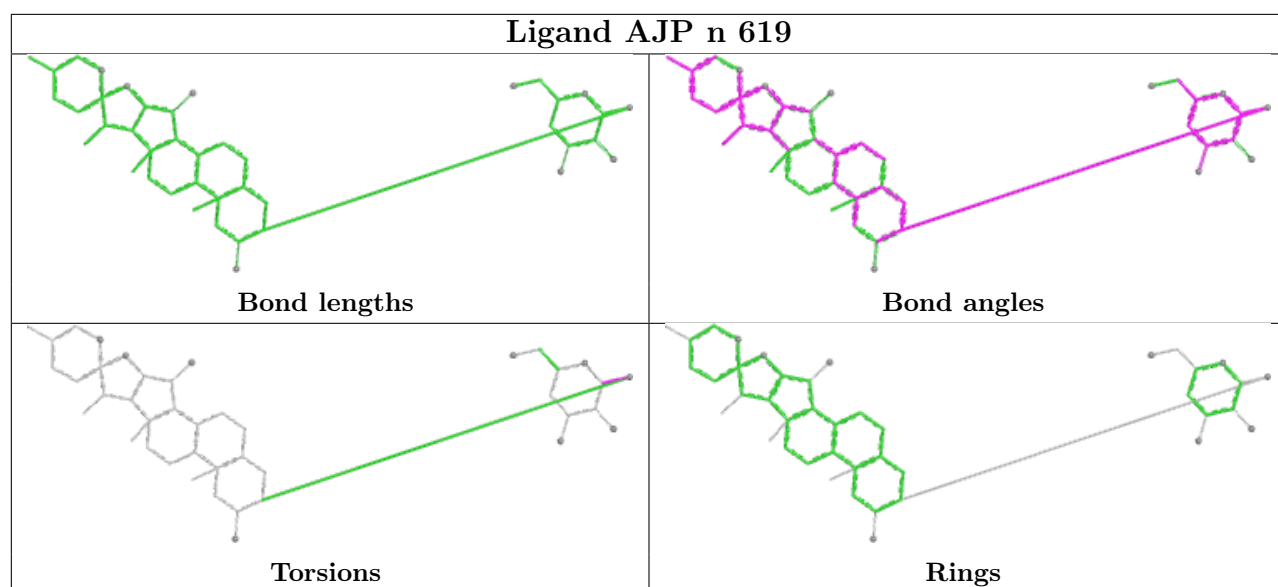
Bond angles

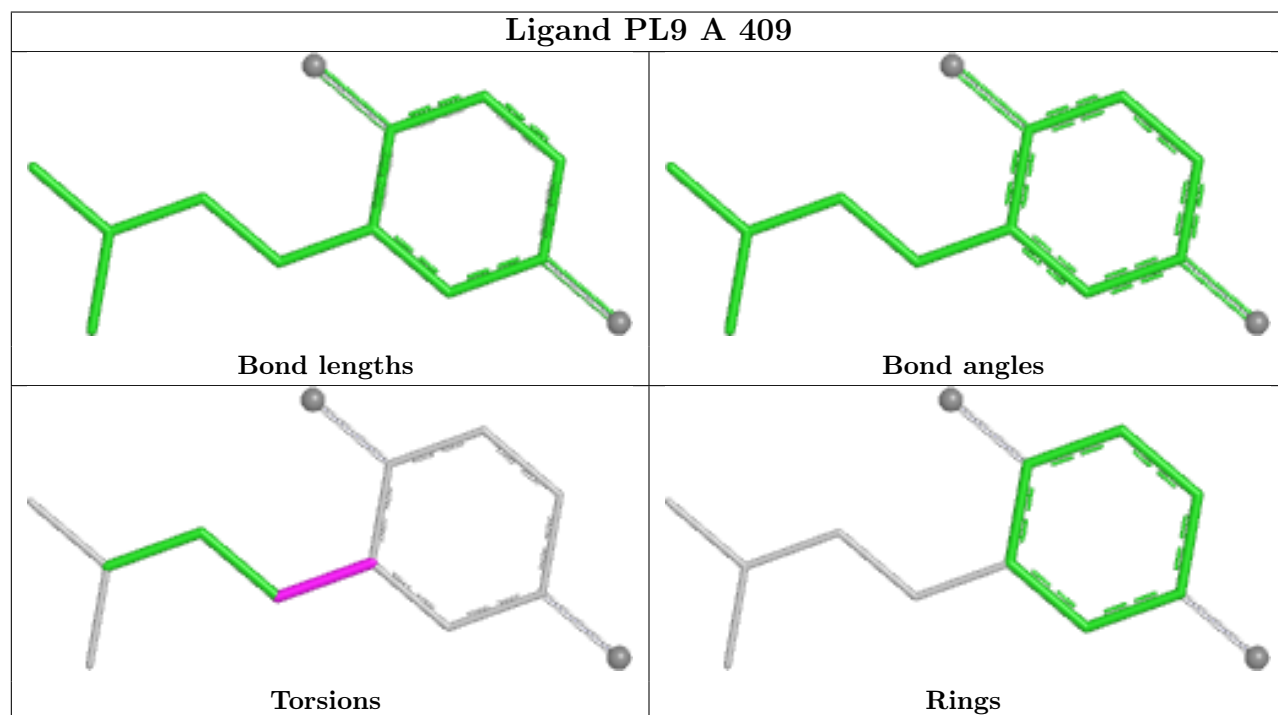
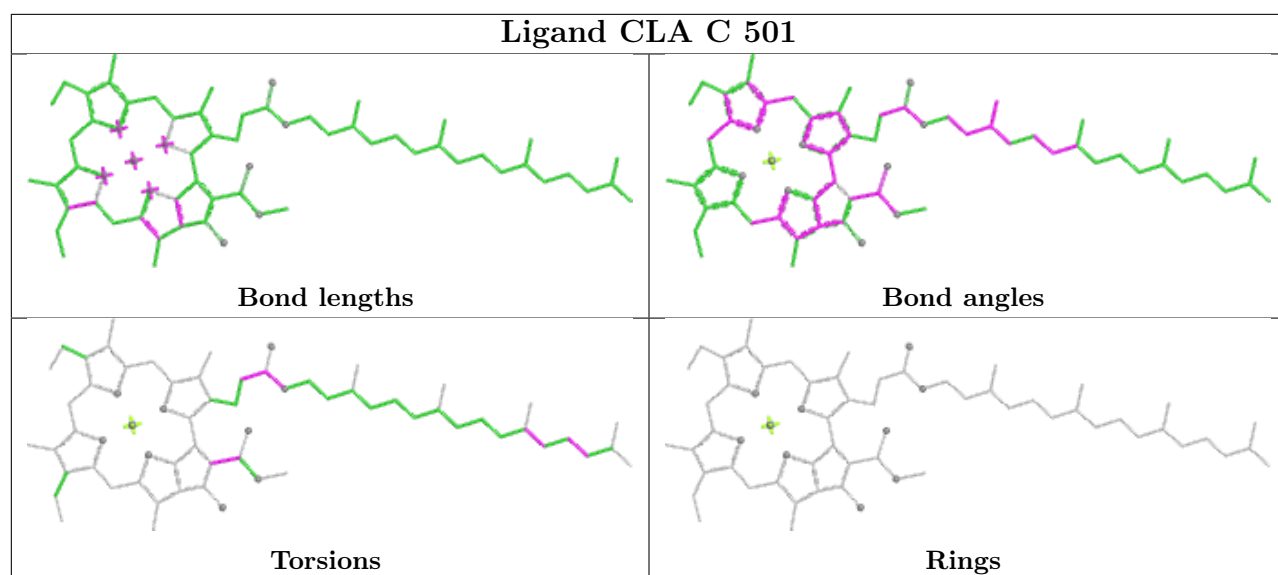


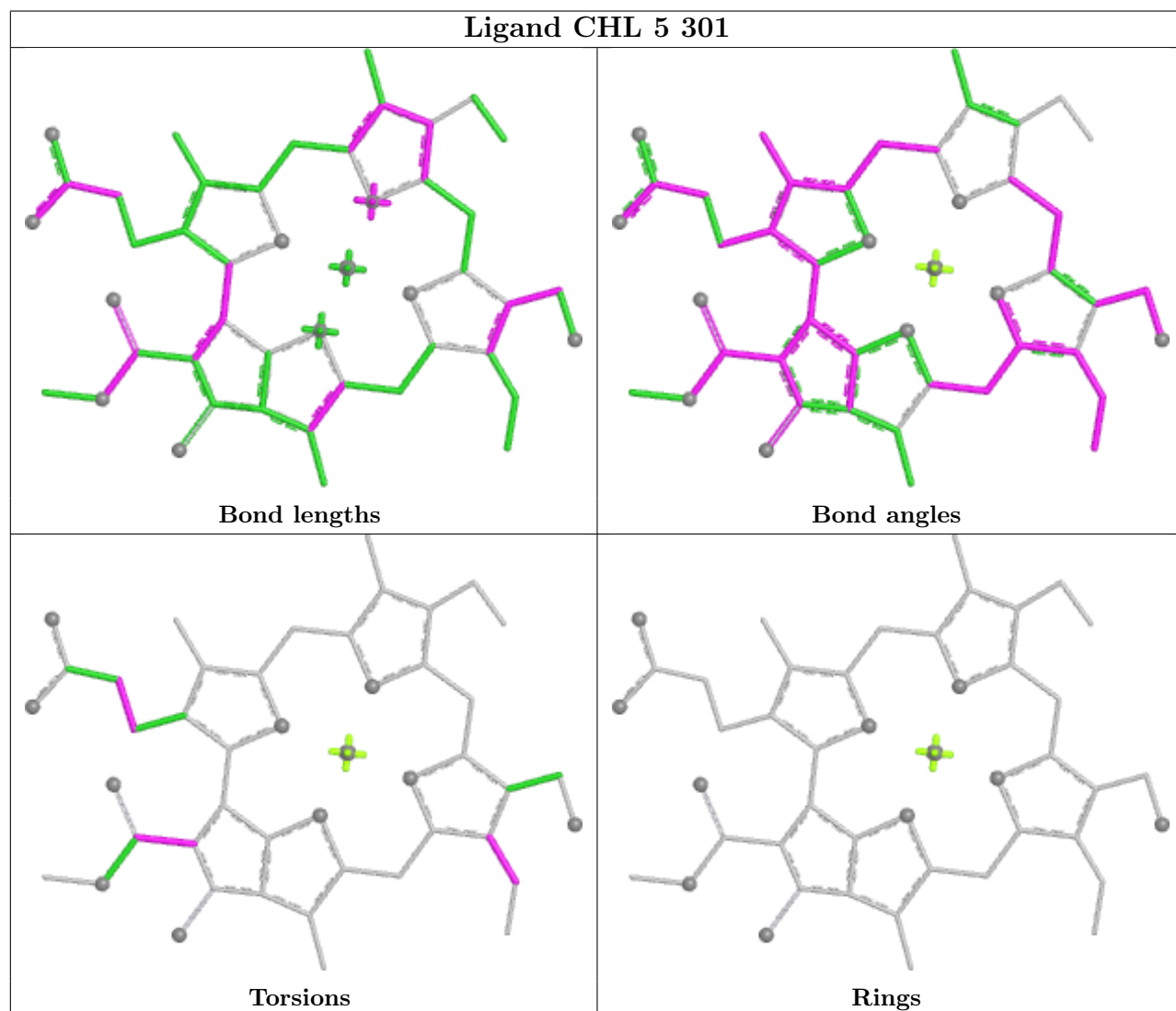
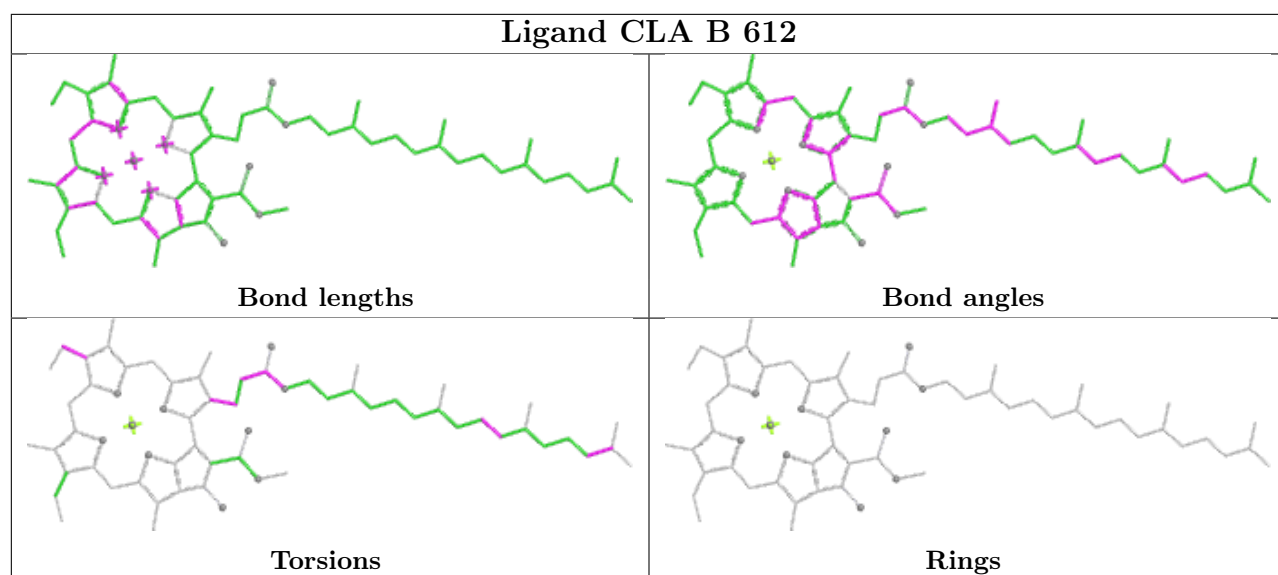
Torsions

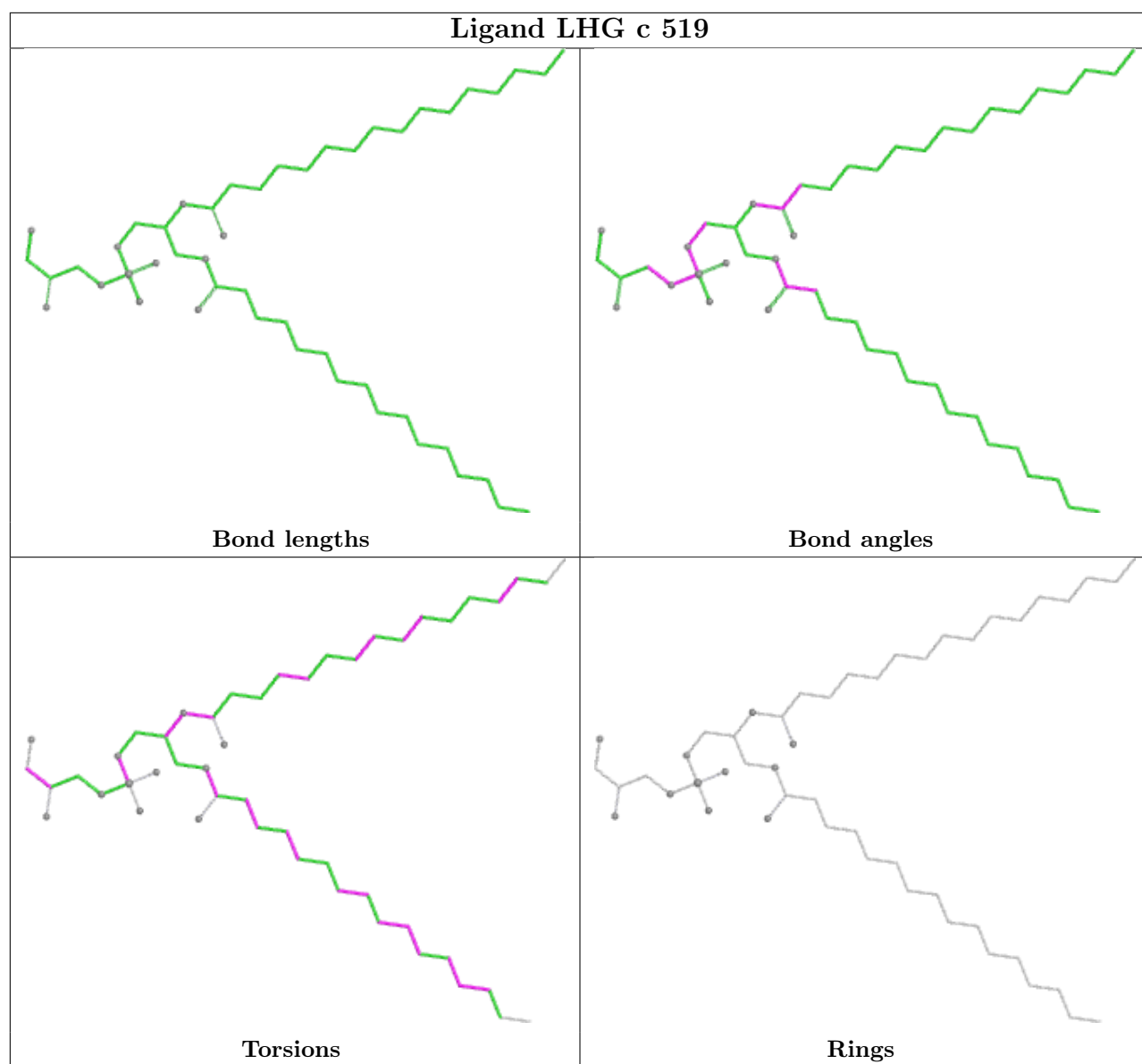


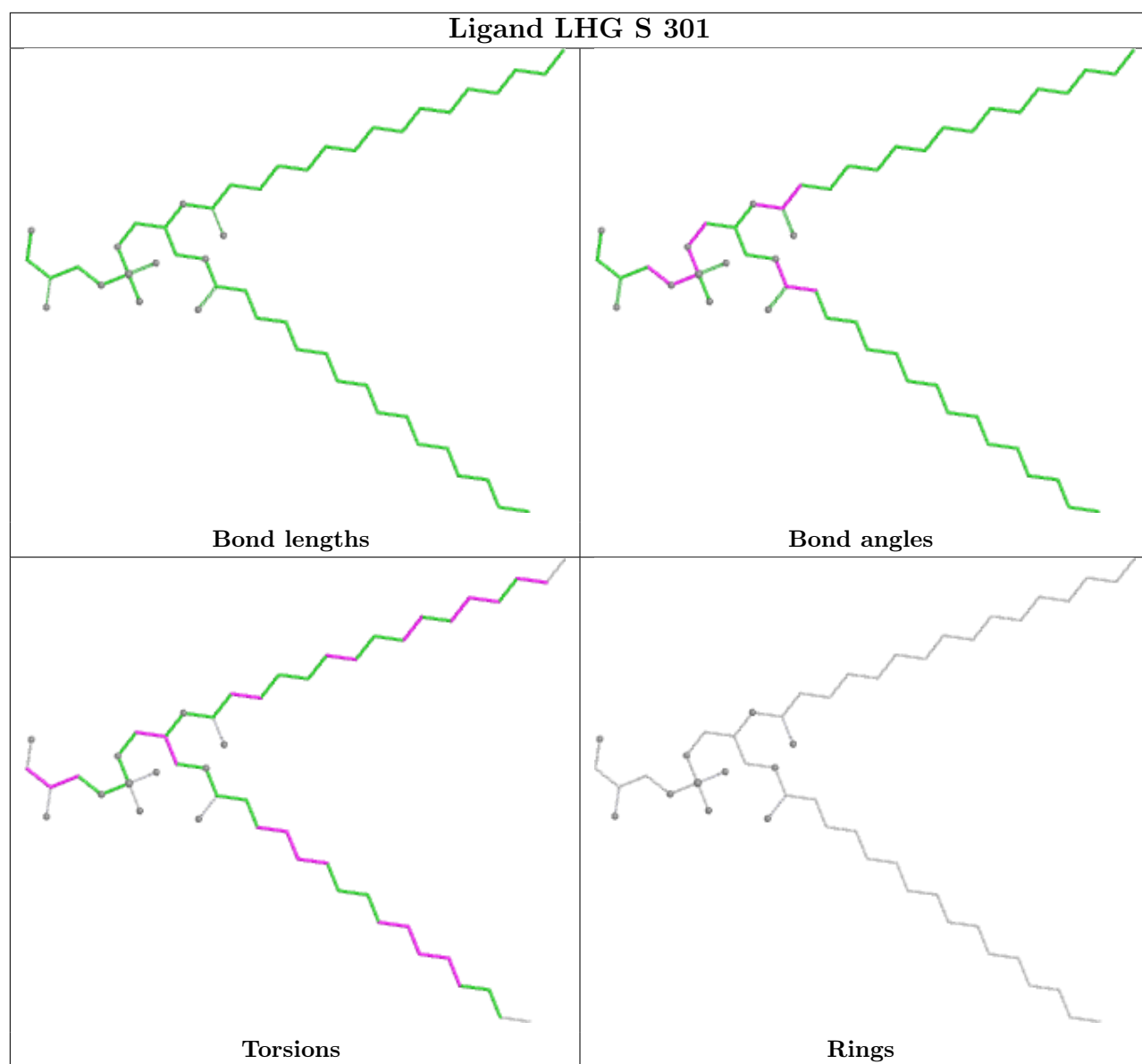
Rings

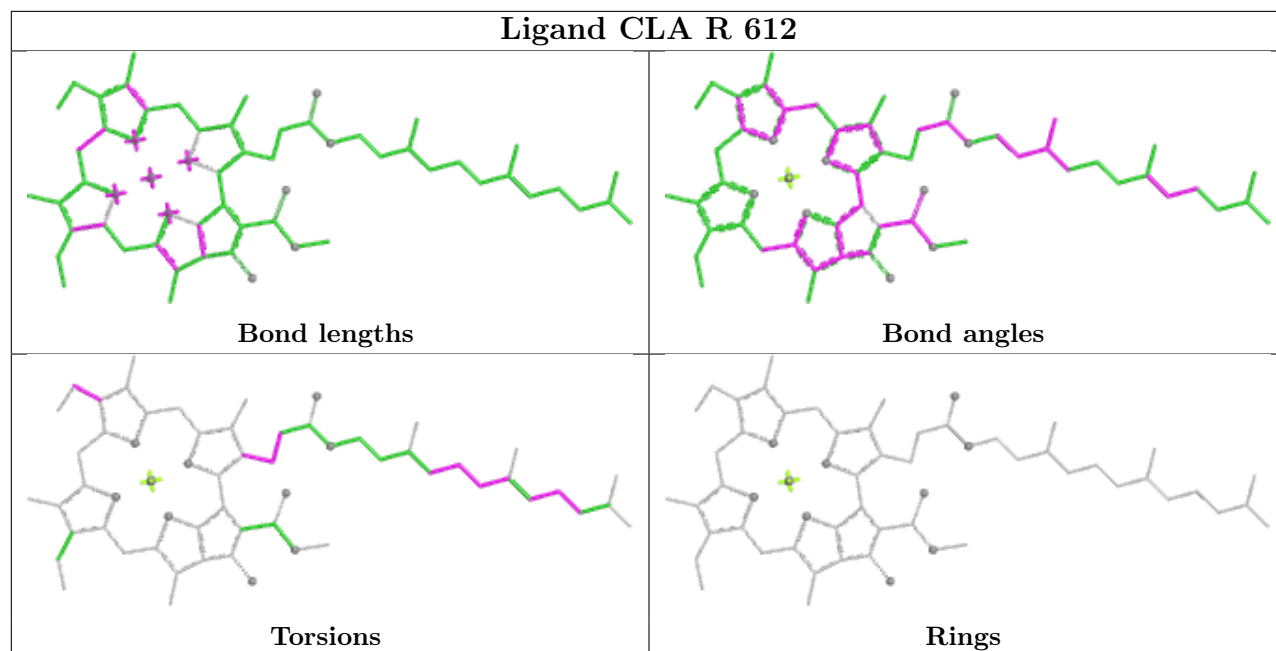
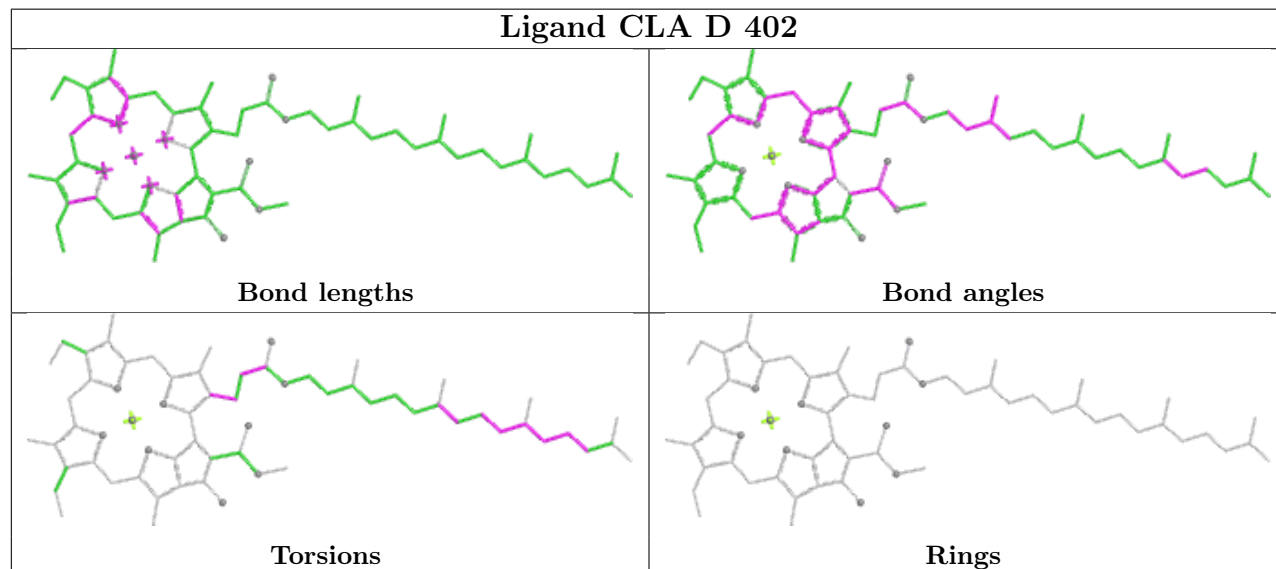


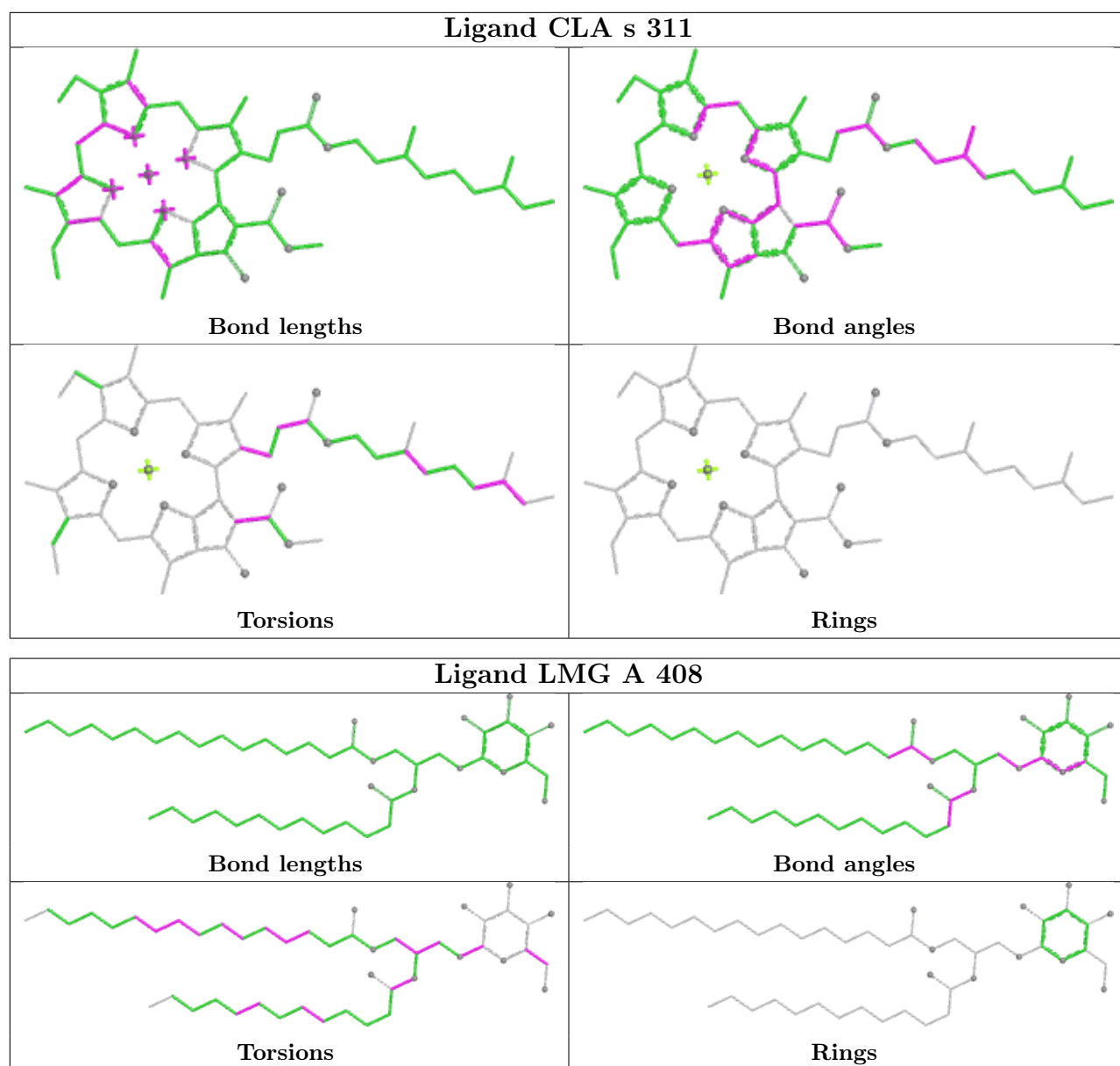


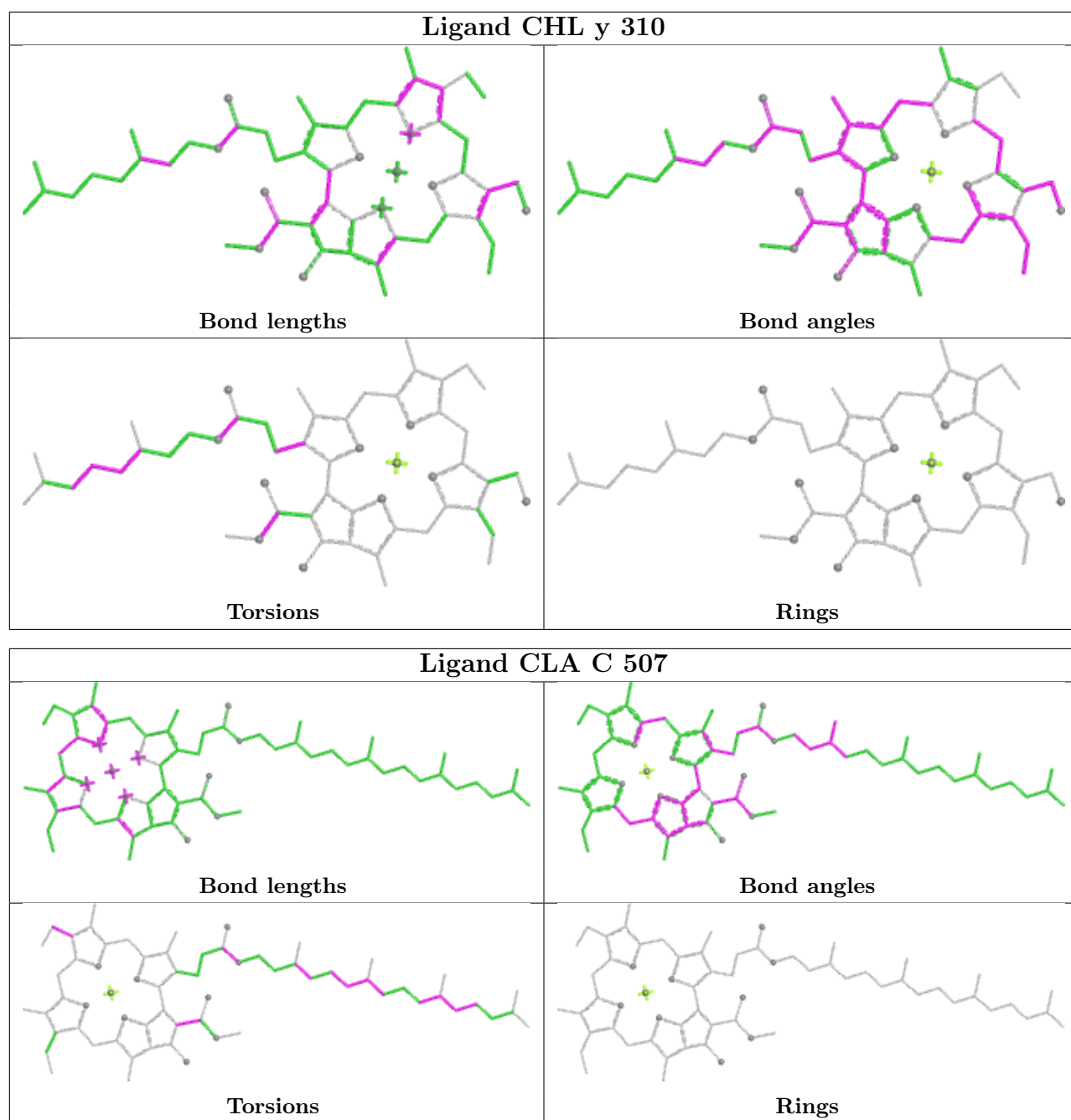


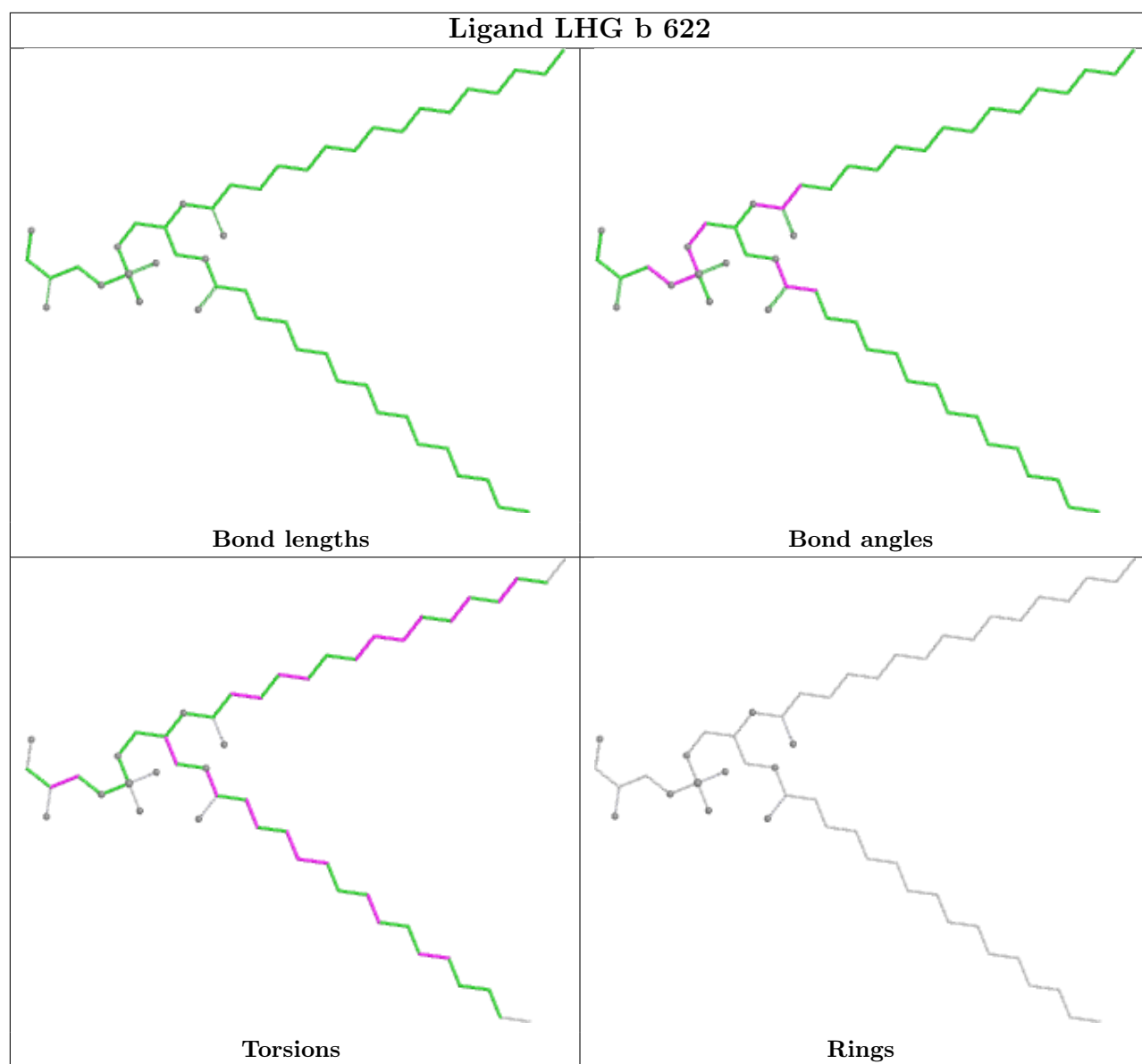




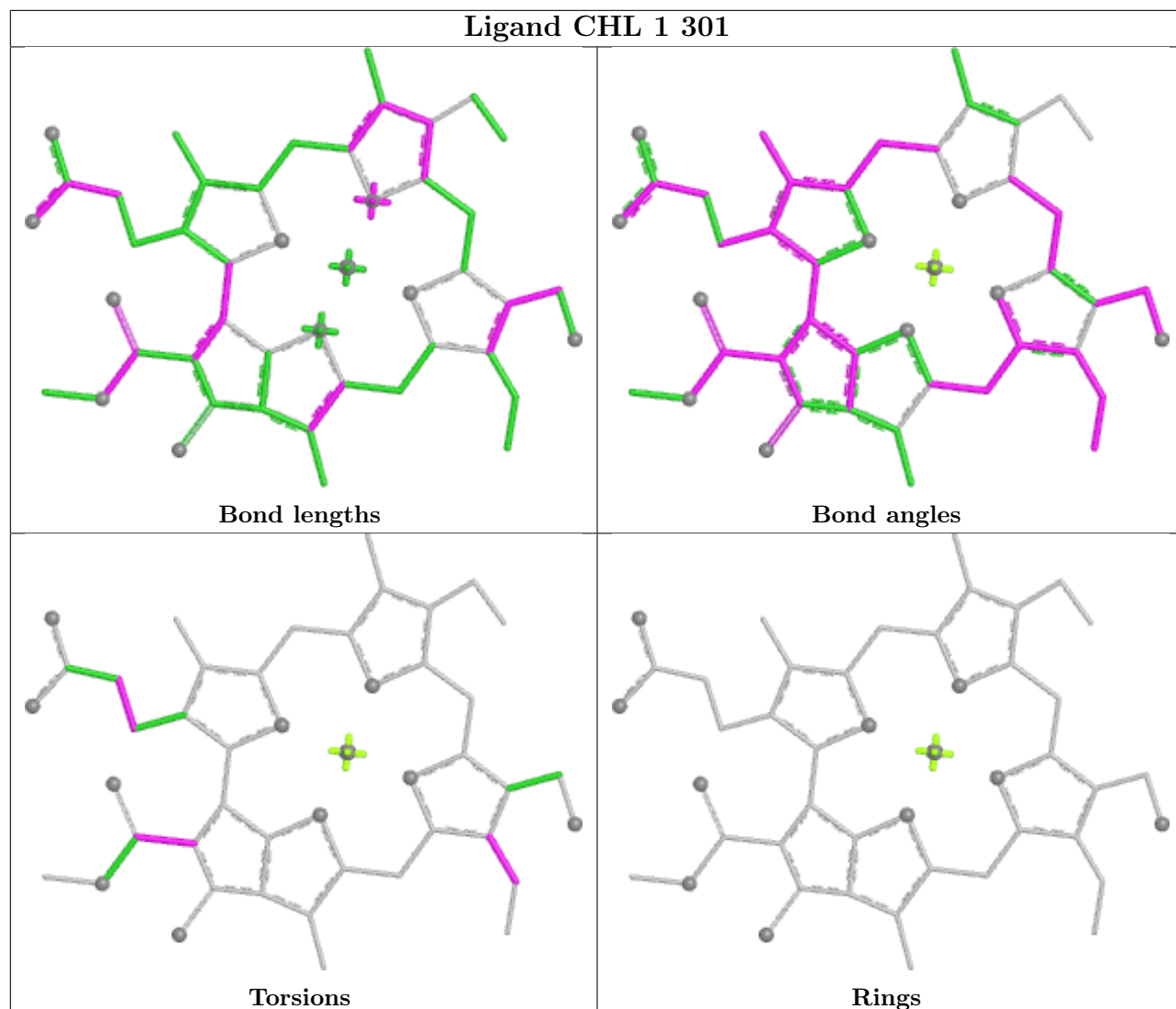
Ligand CLA R 612**Ligand CLA D 402**

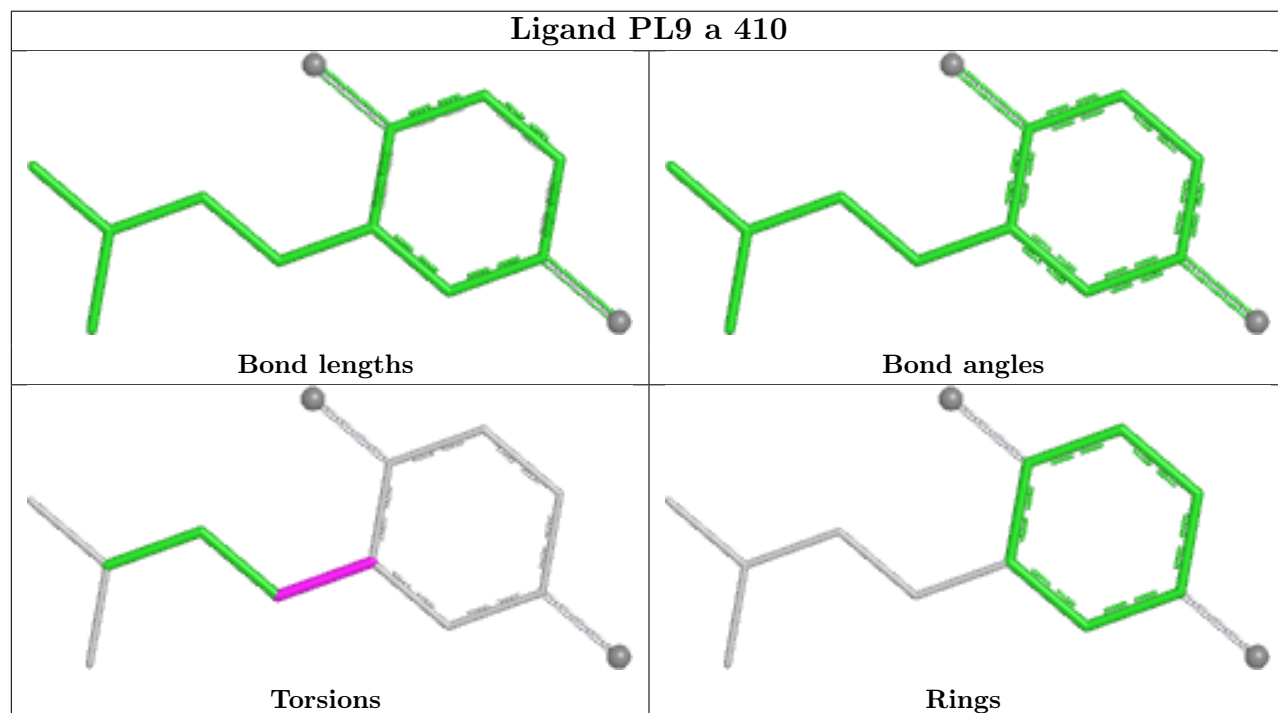
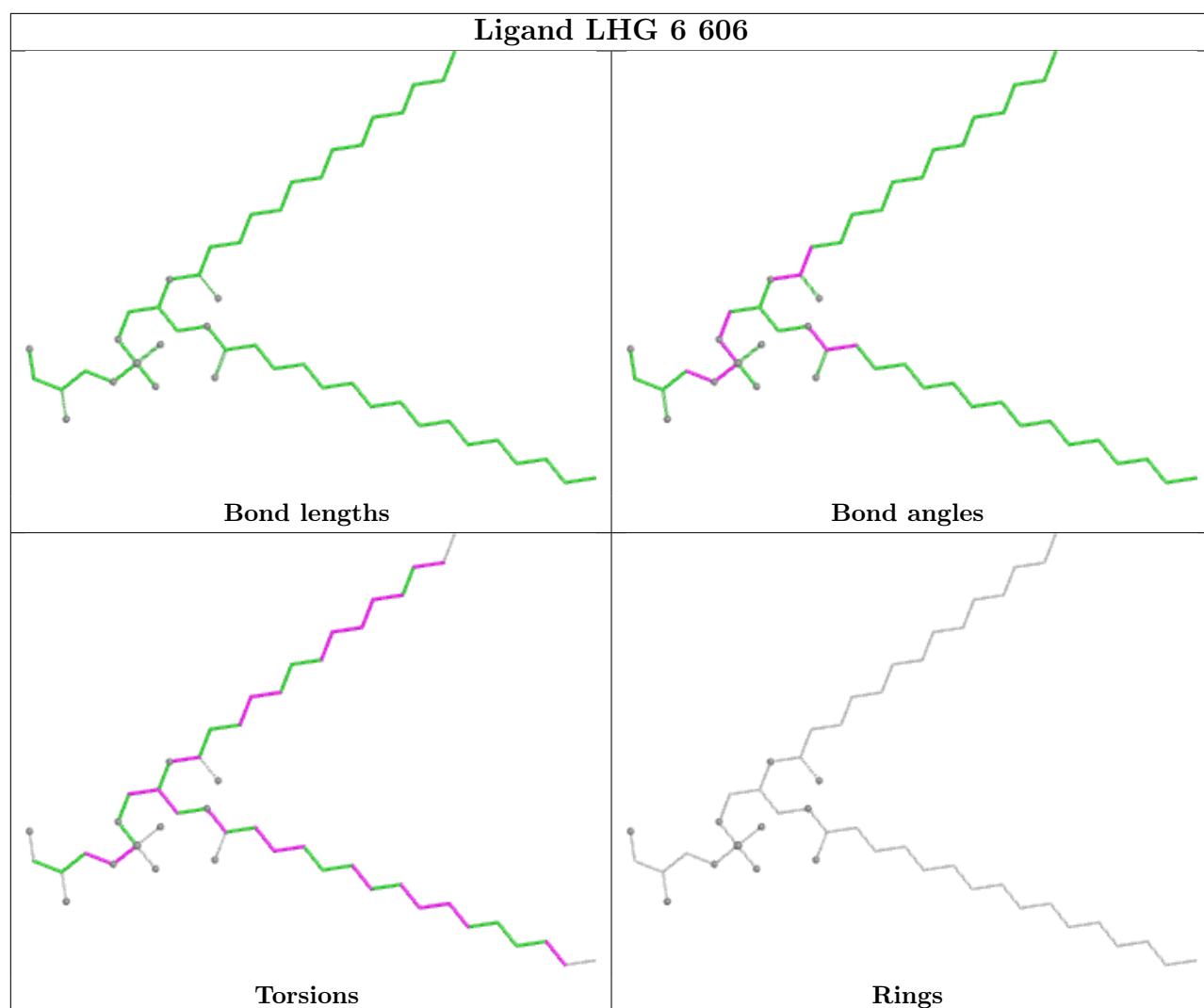


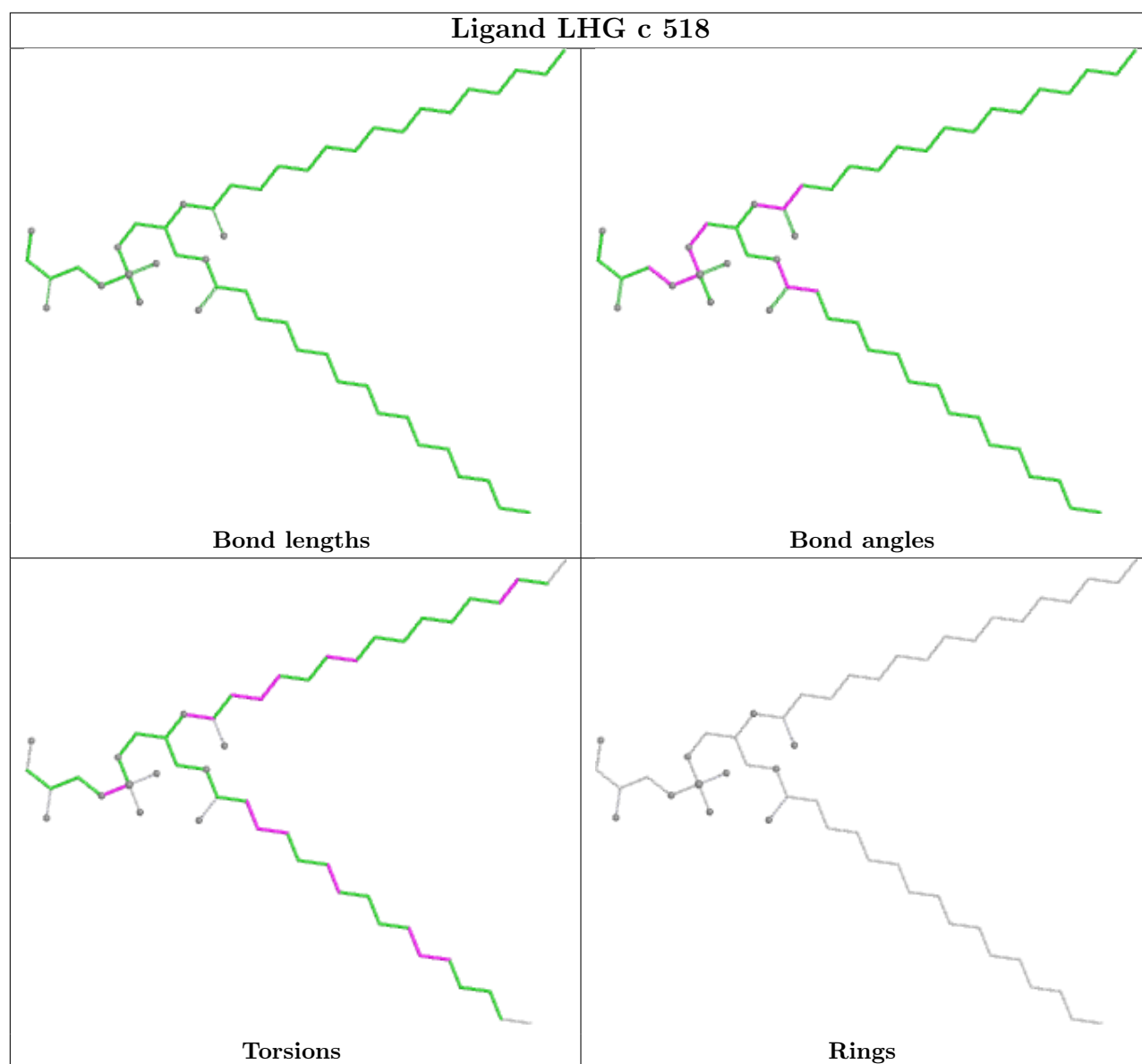


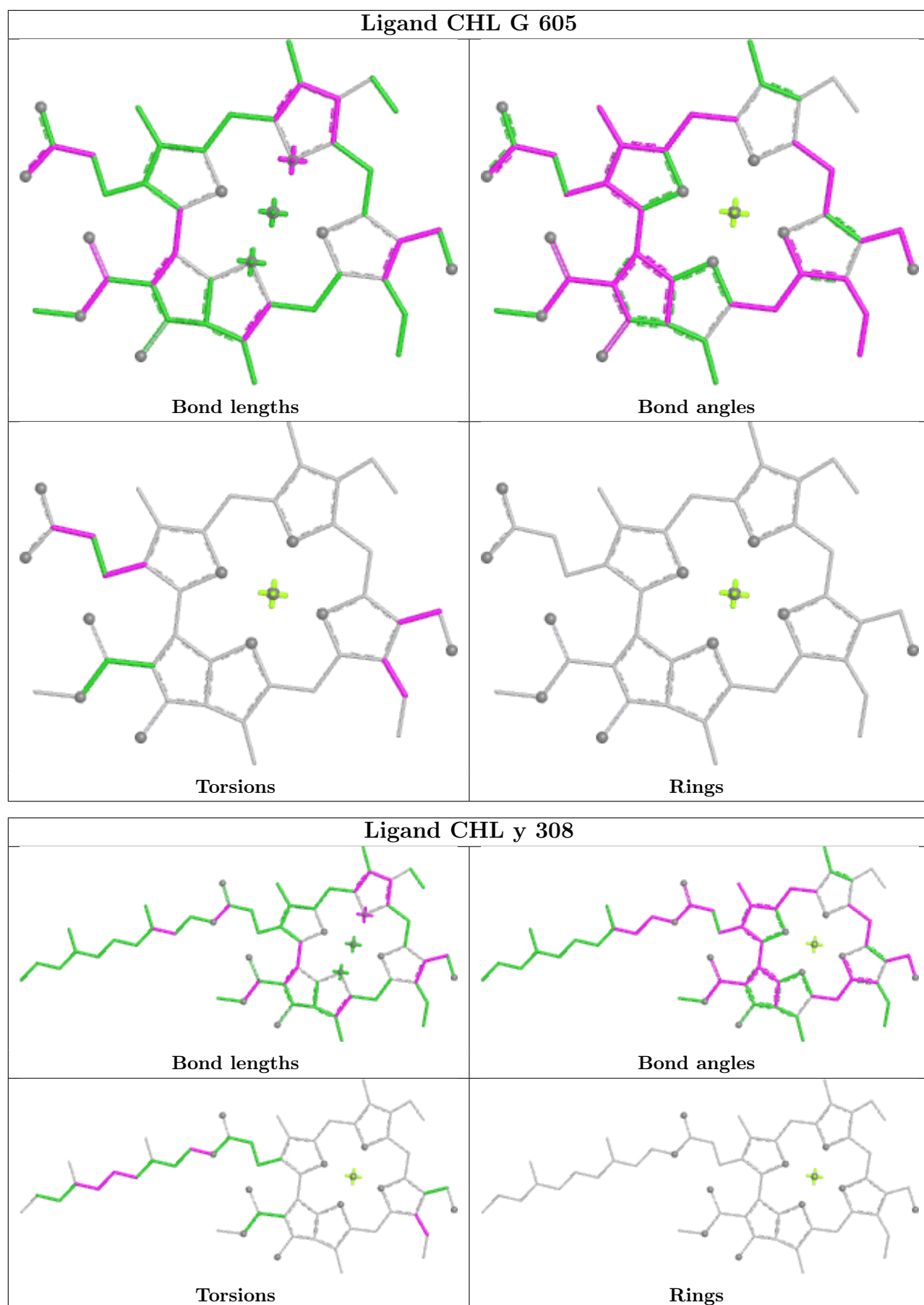


Ligand CHL 1 301

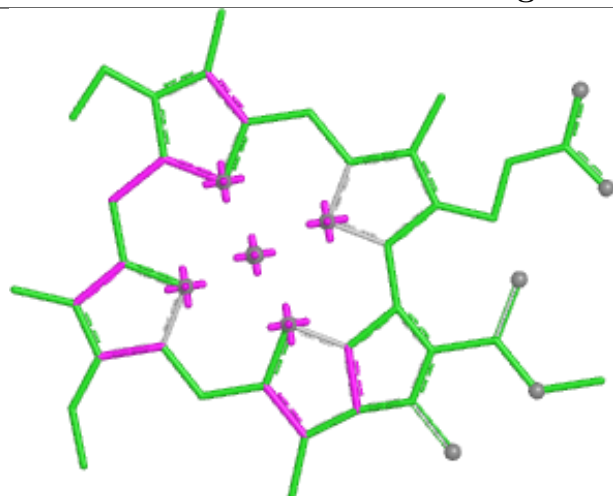




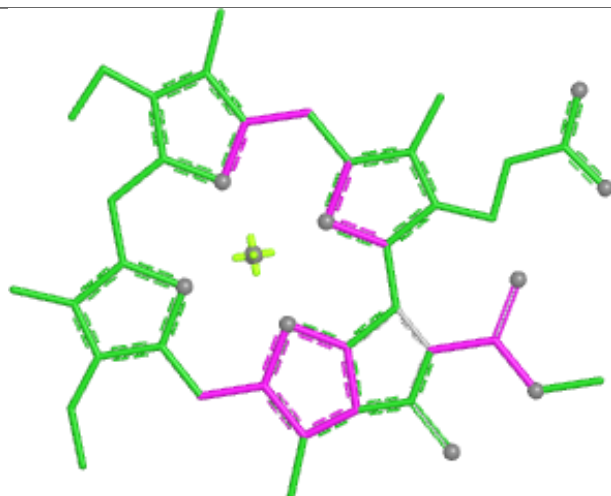




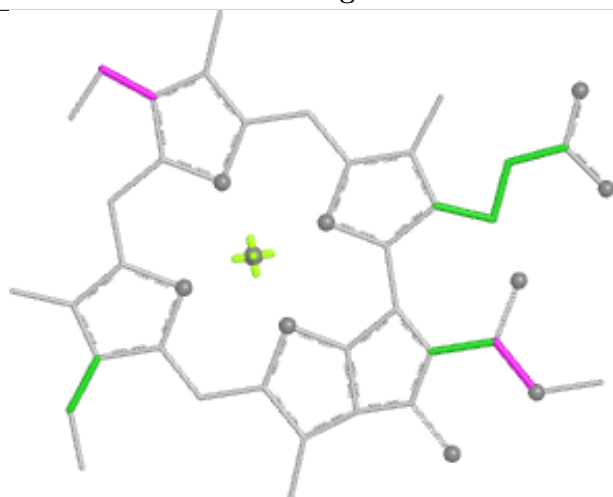
Ligand CLA S 304



Bond lengths



Bond angles

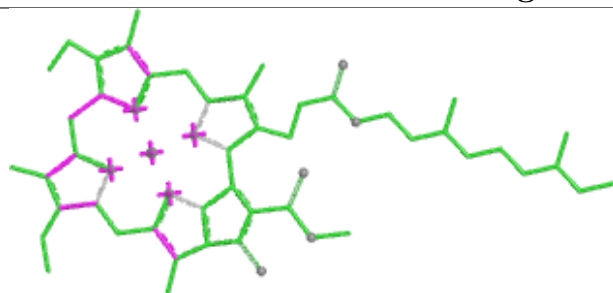


Torsions

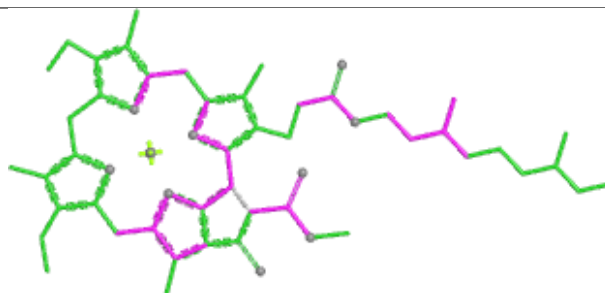


Rings

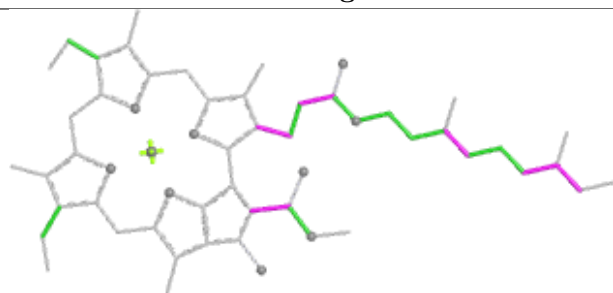
Ligand CLA S 311



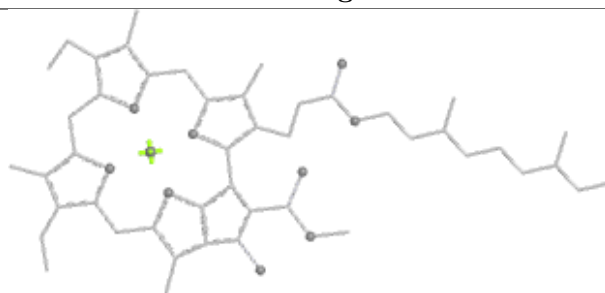
Bond lengths



Bond angles

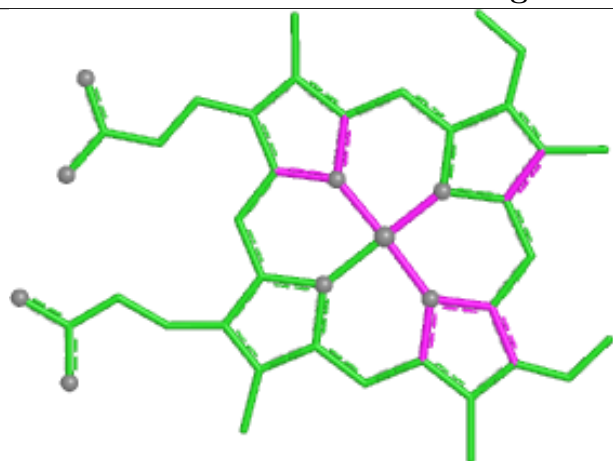


Torsions

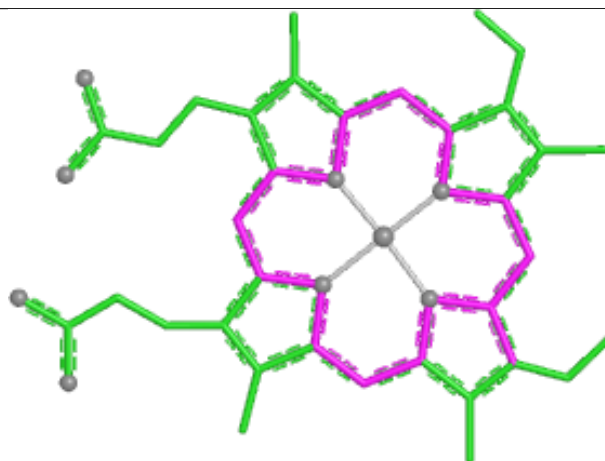


Rings

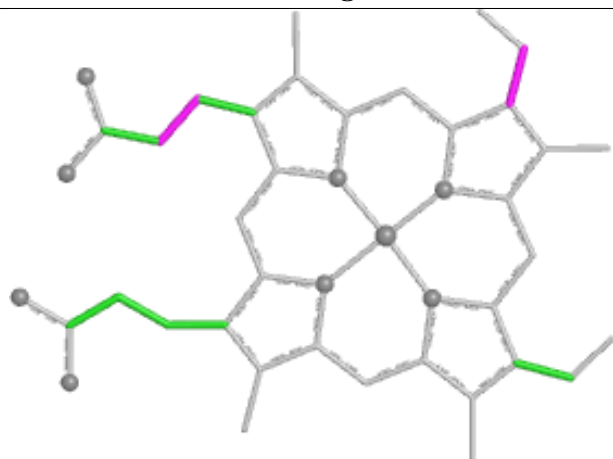
Ligand HEM F 101



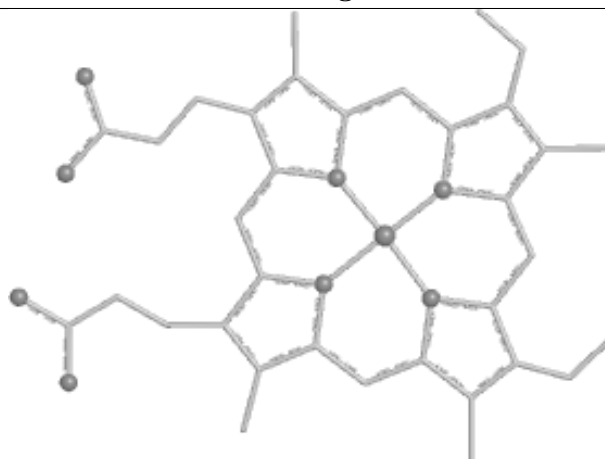
Bond lengths



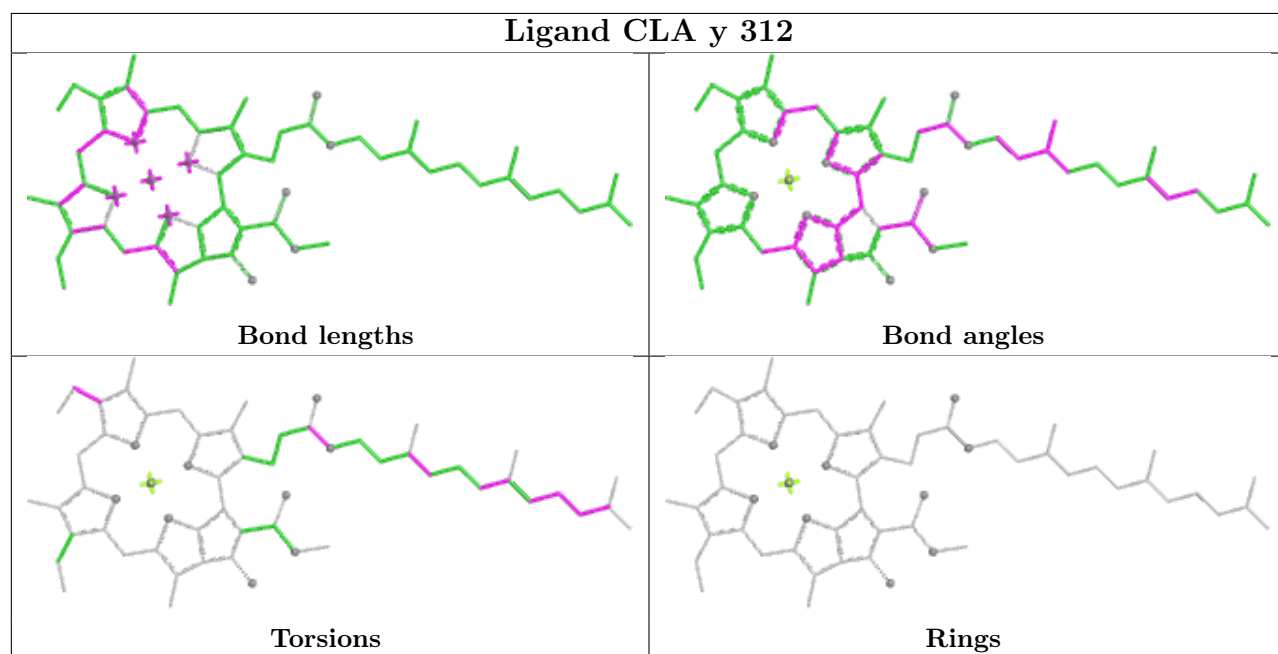
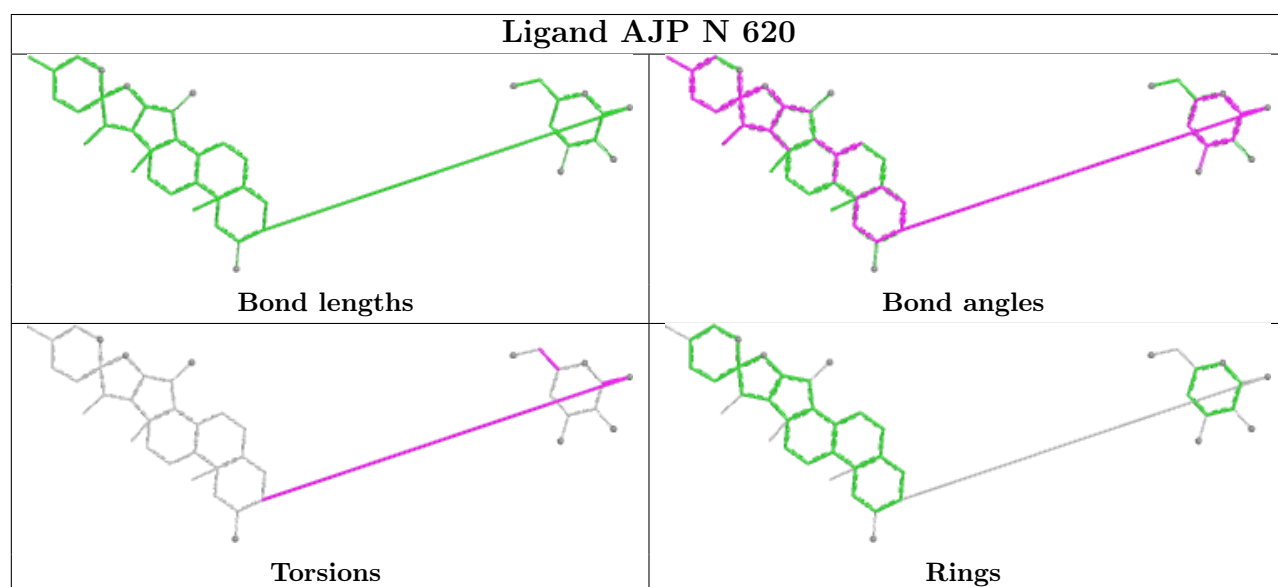
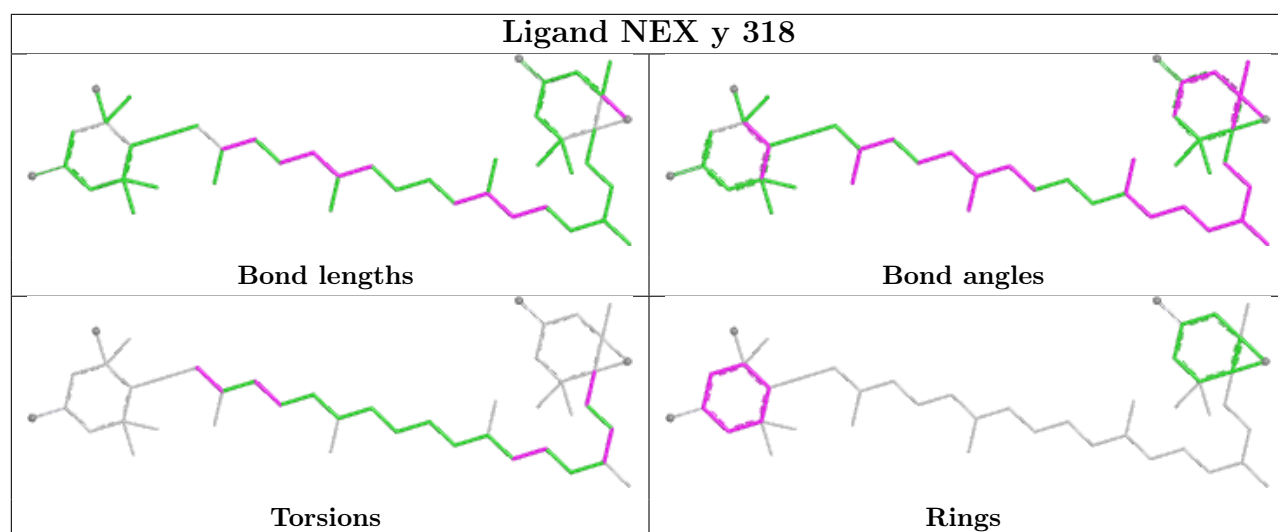
Bond angles

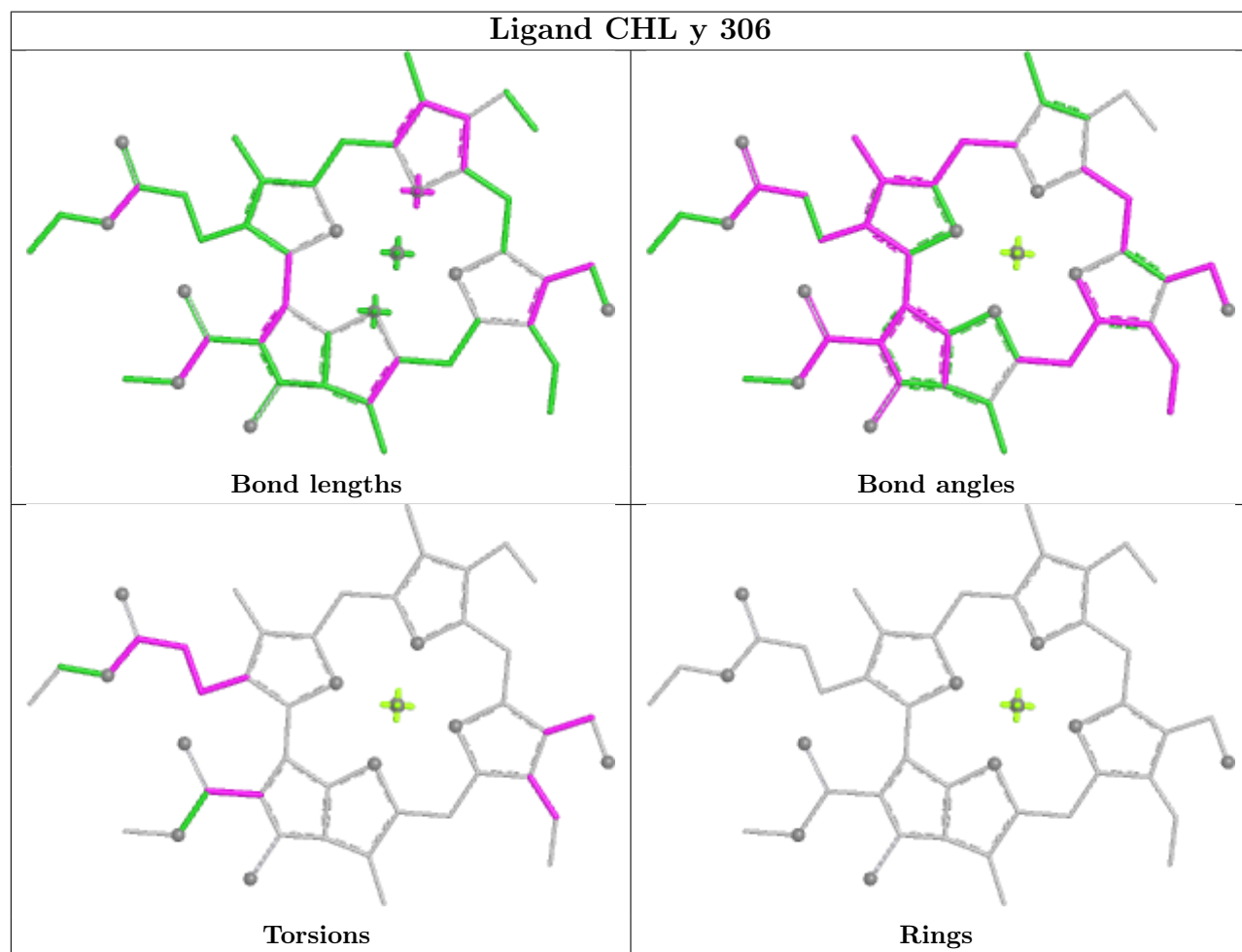
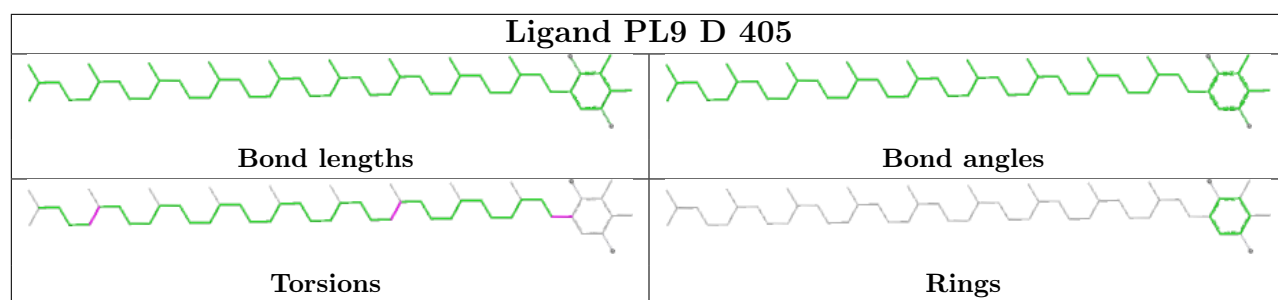


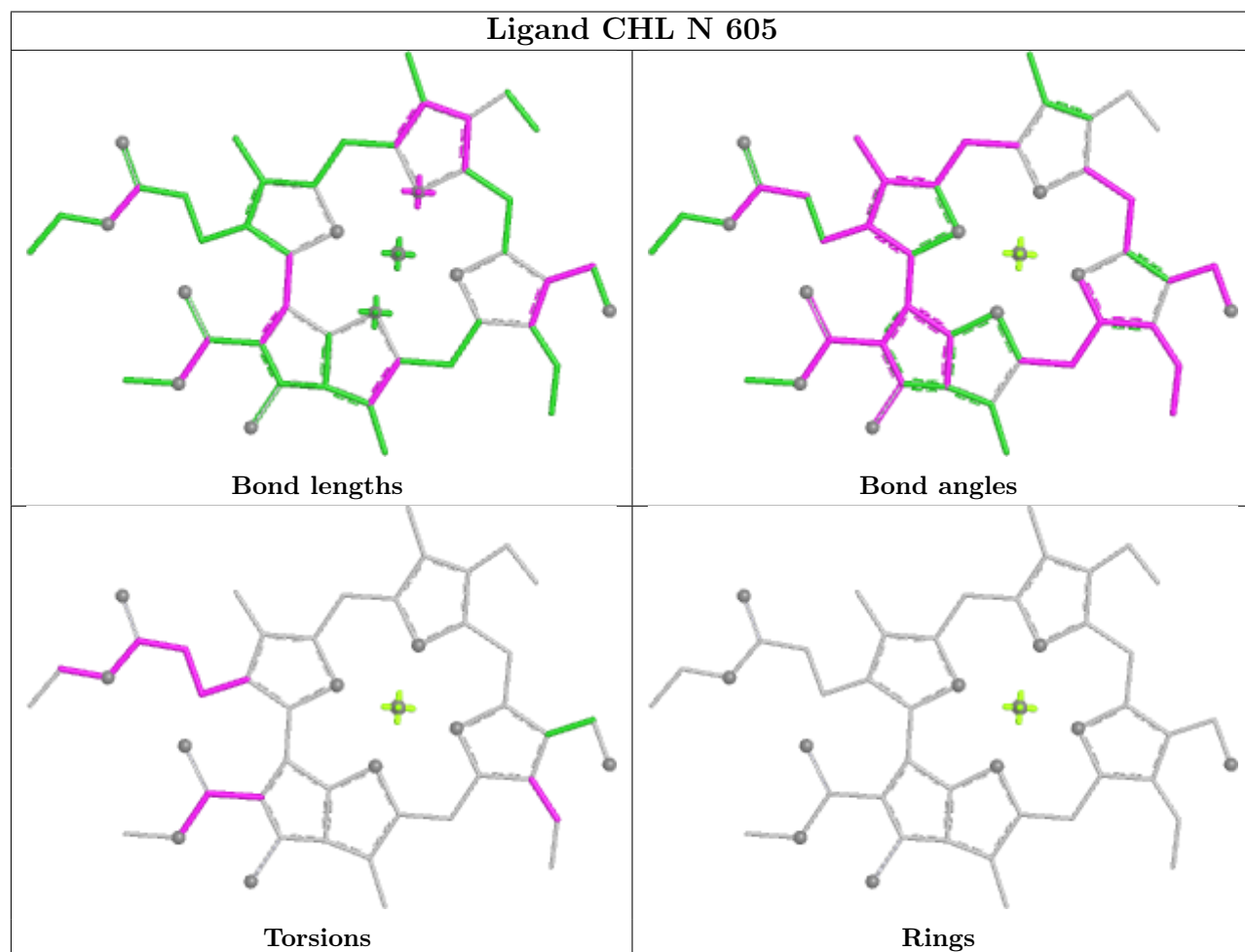
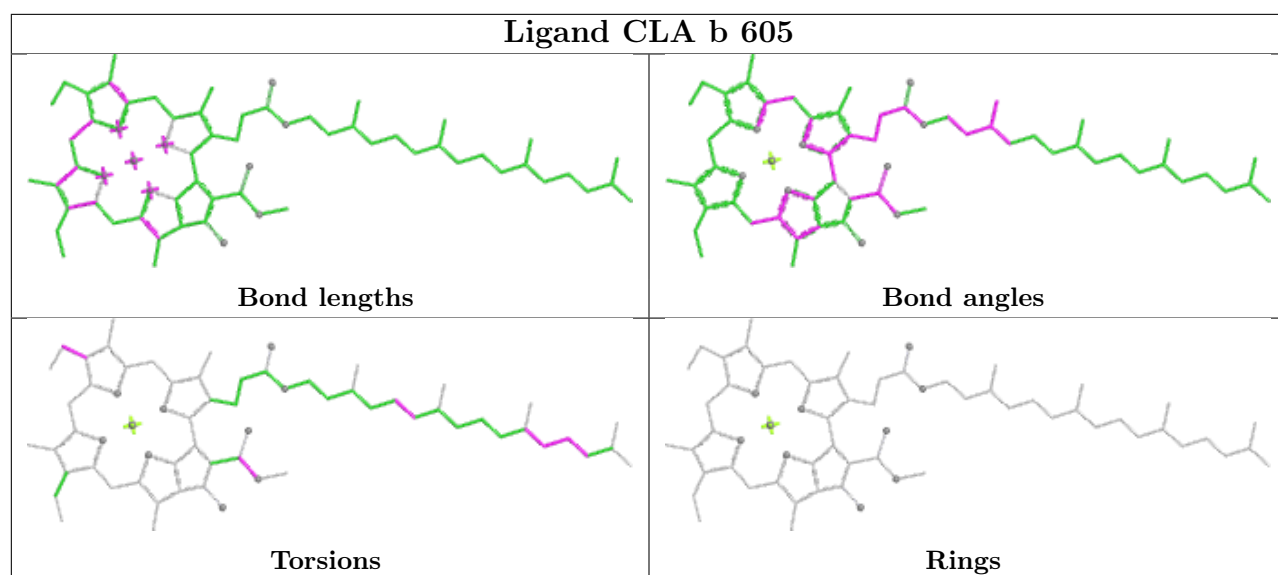
Torsions

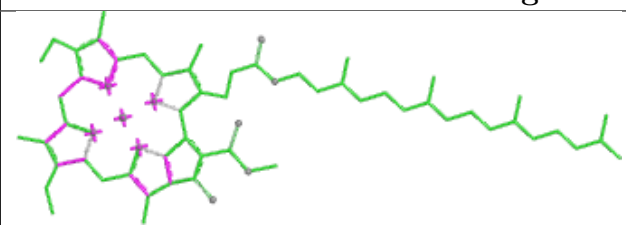
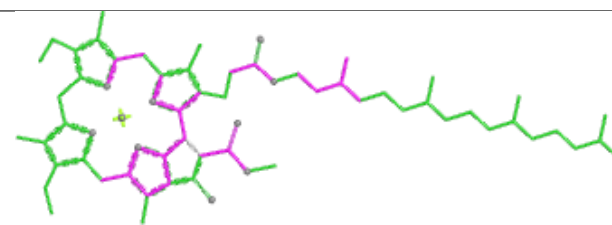
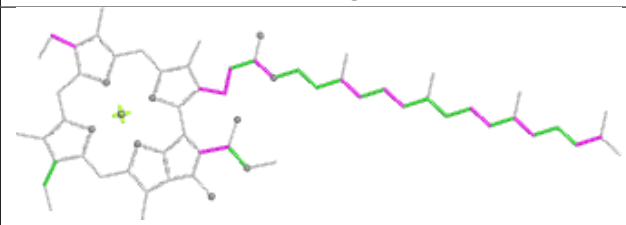
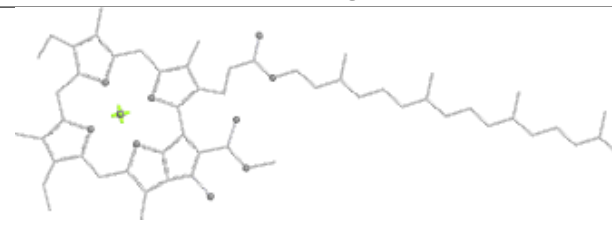


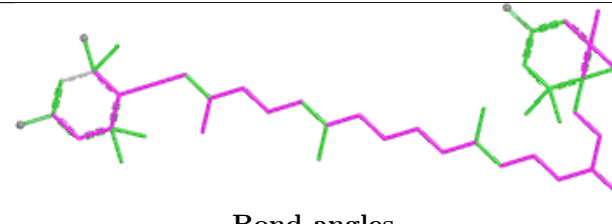
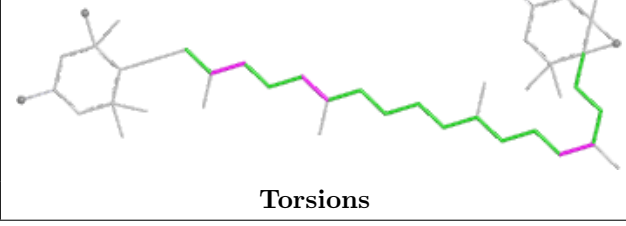
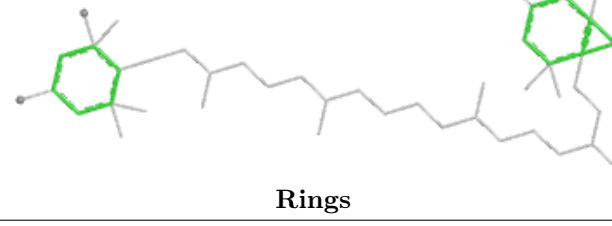
Rings

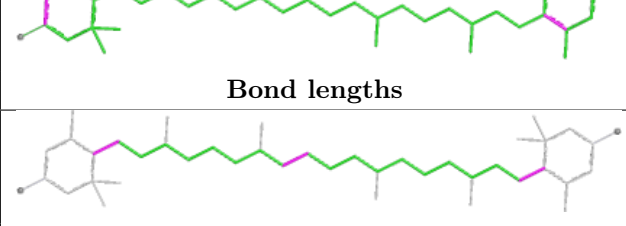
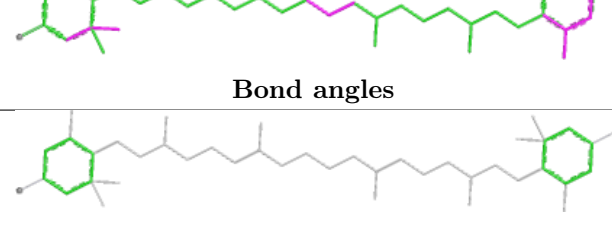
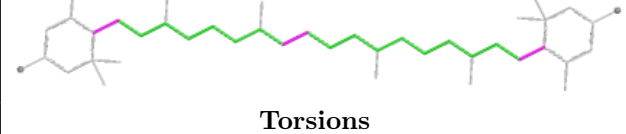
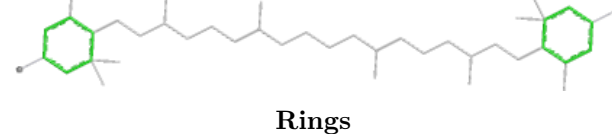


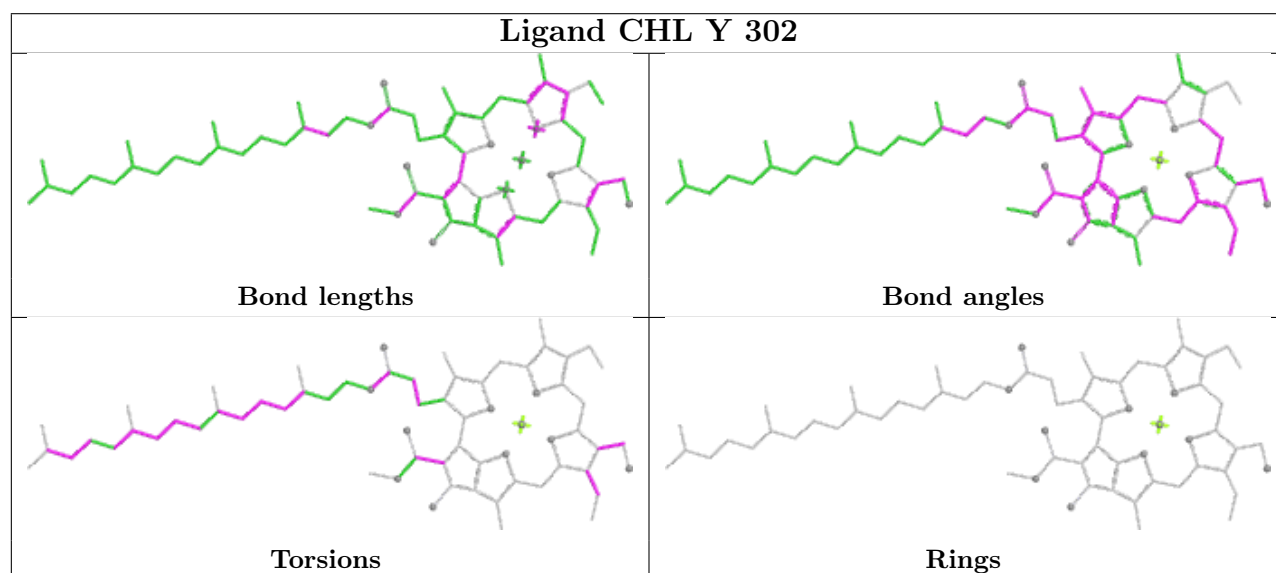
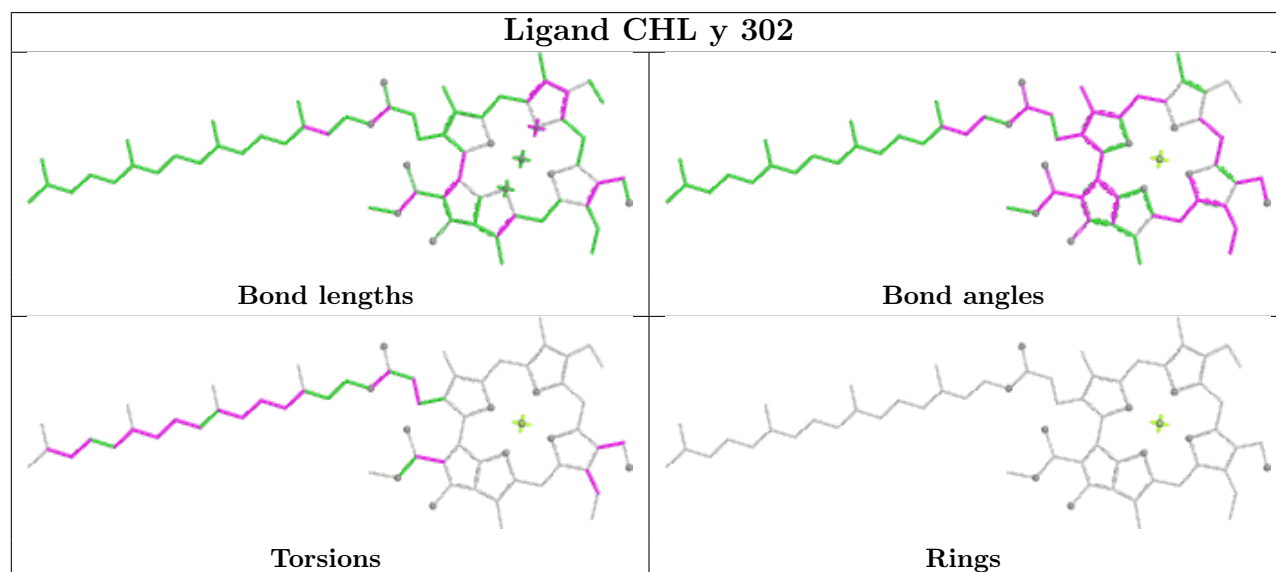
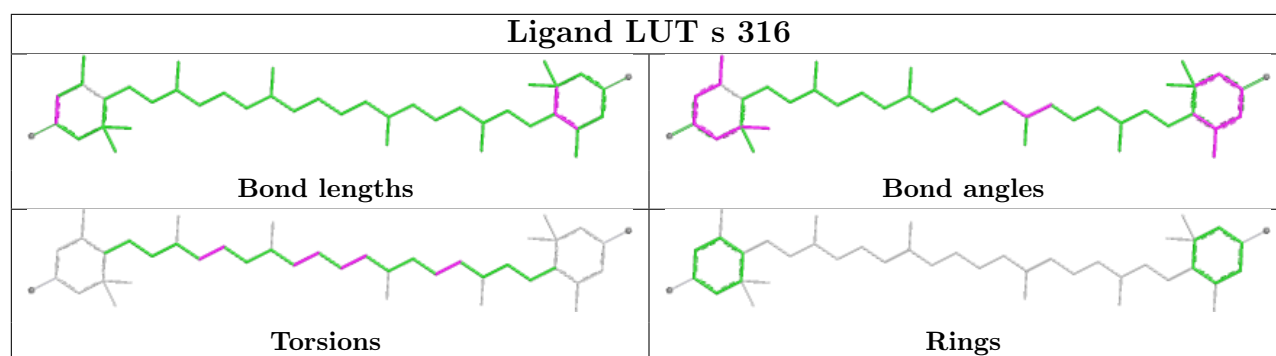


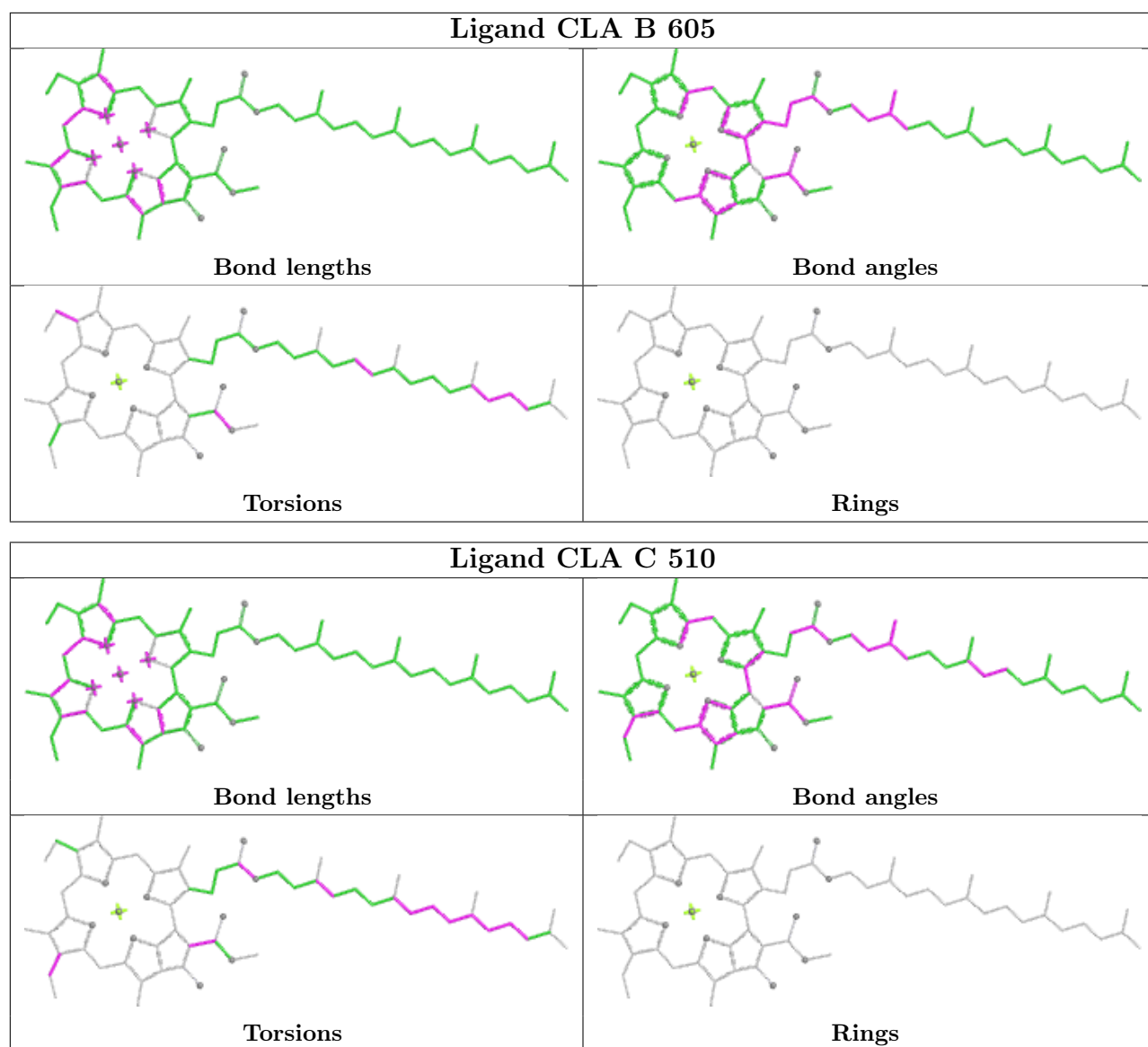


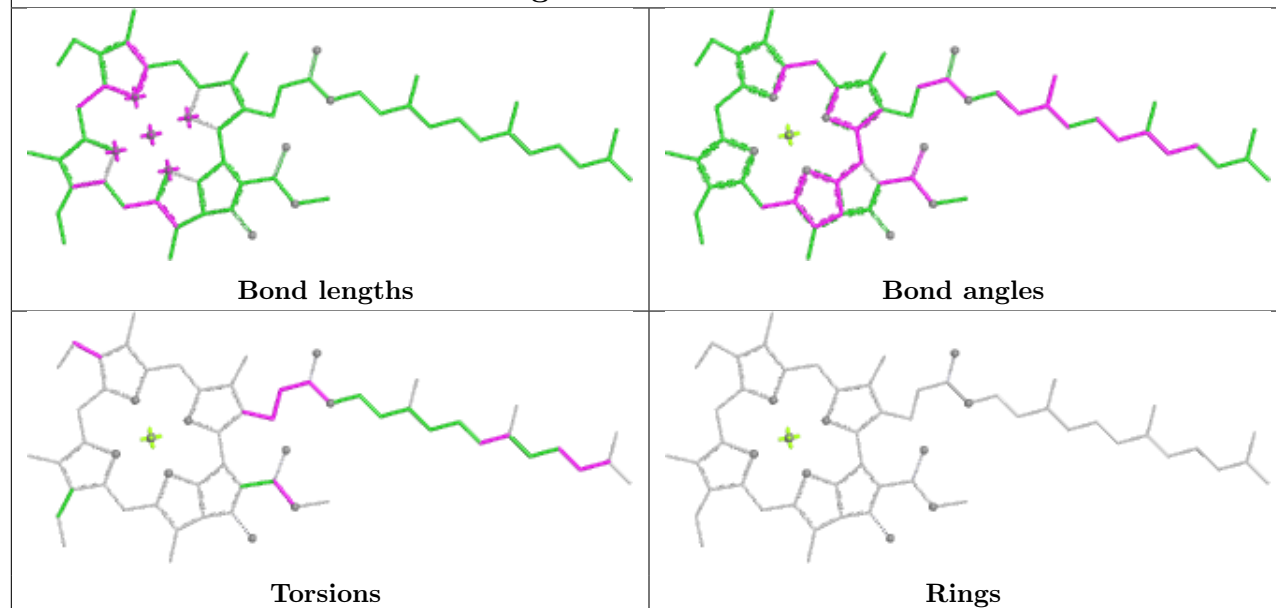
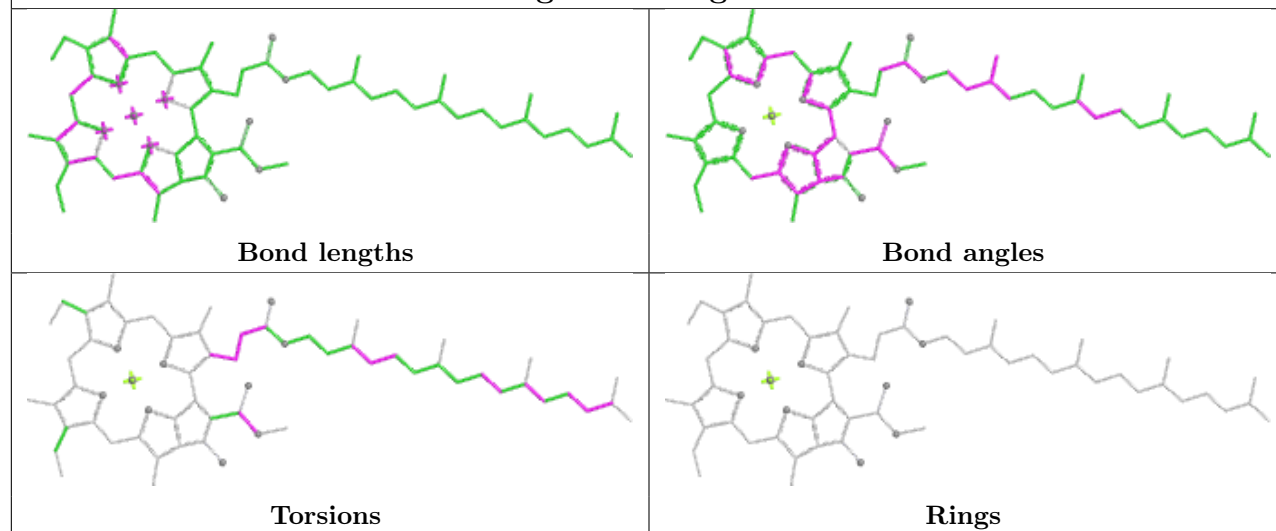
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

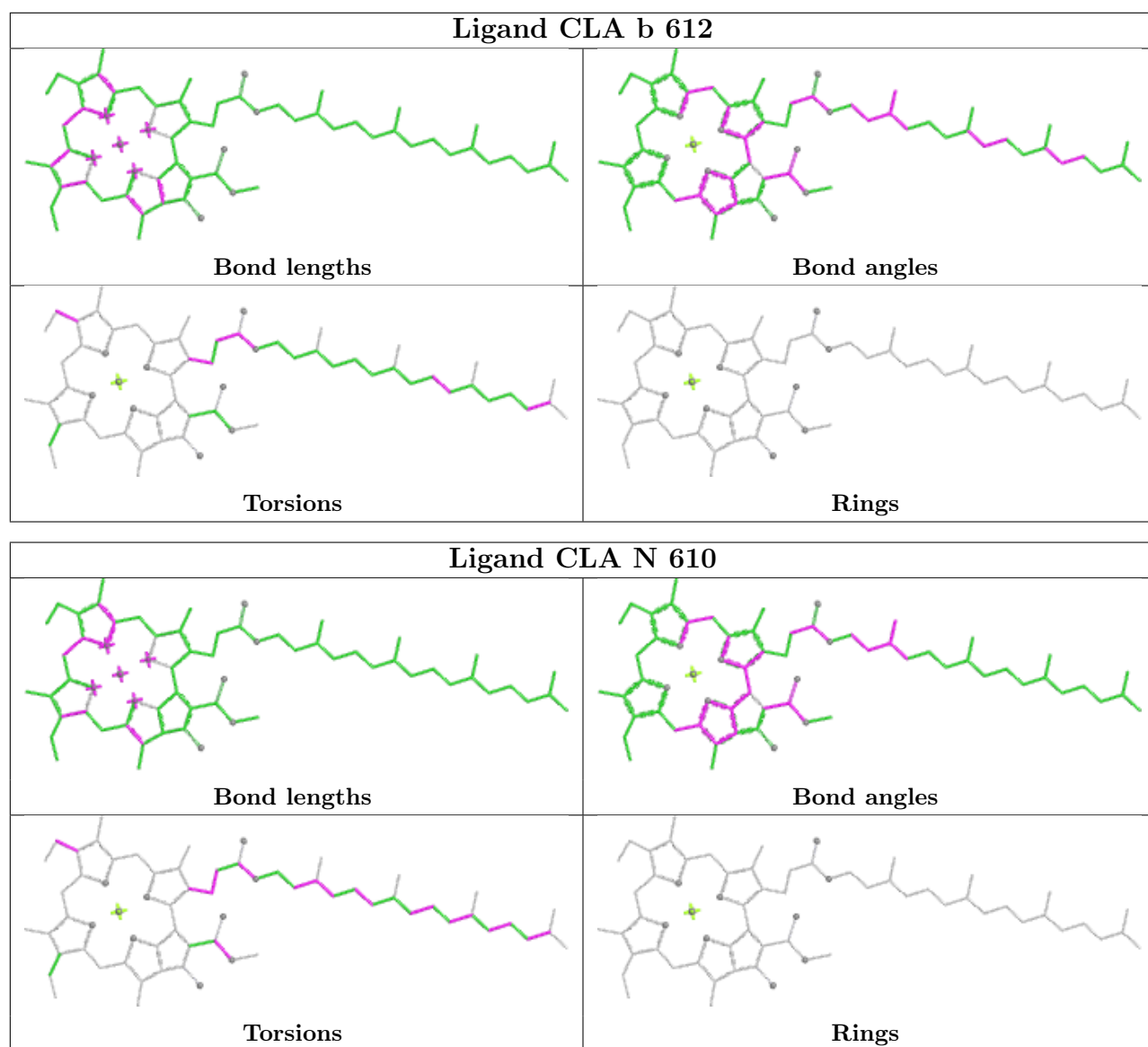
Ligand NEX S 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

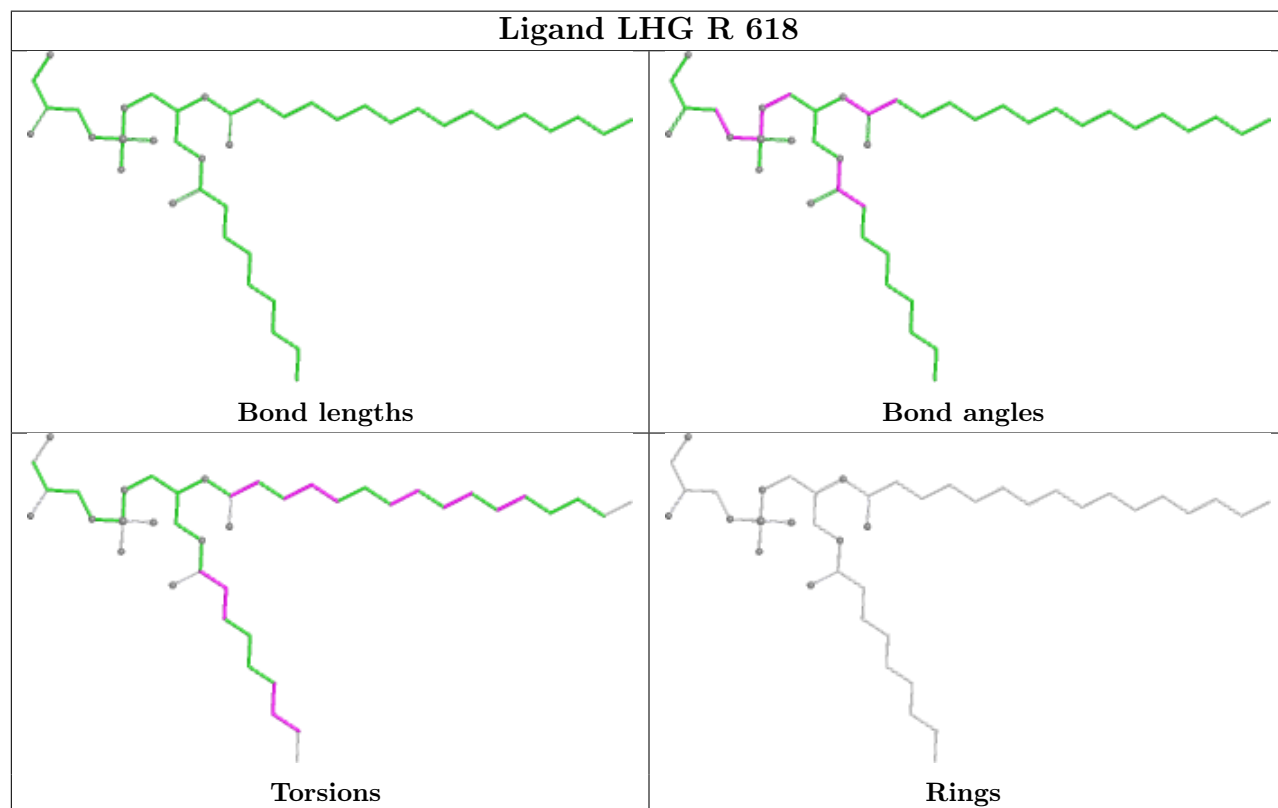
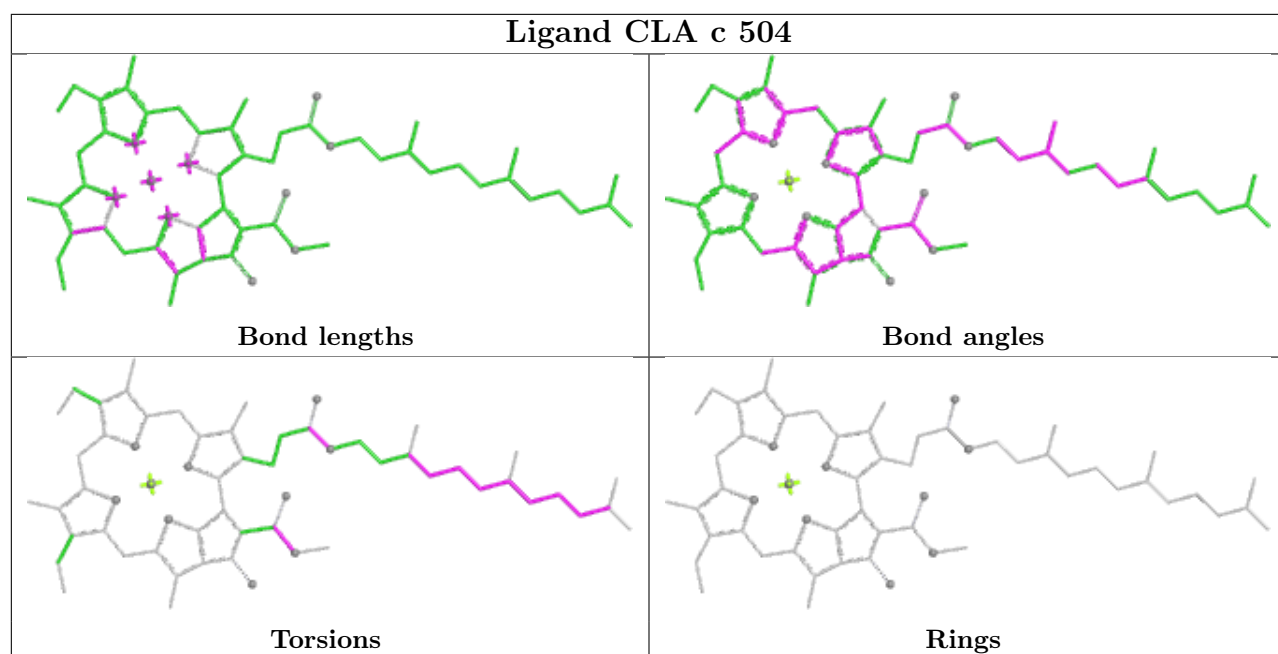
Ligand LUT y 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

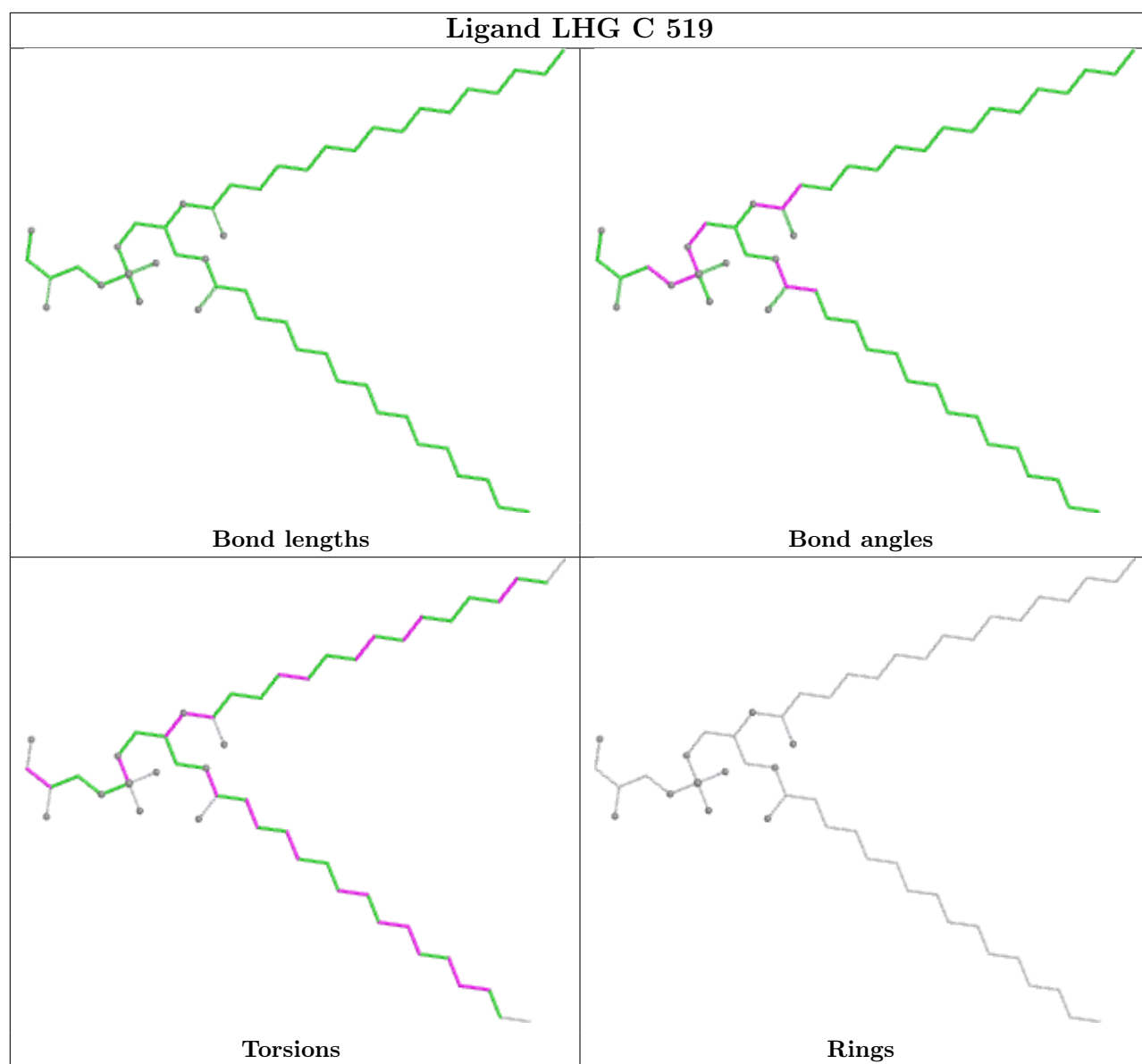


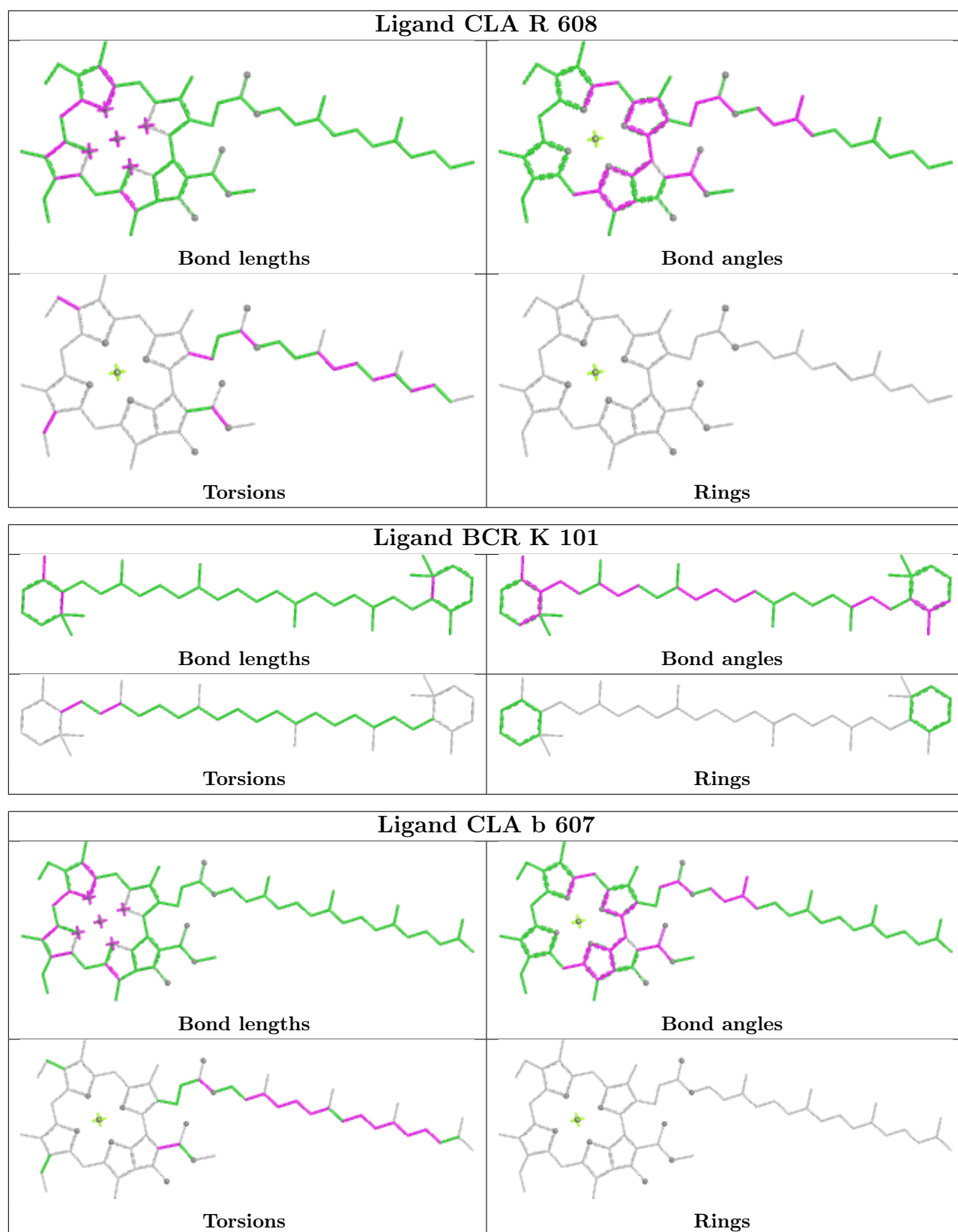


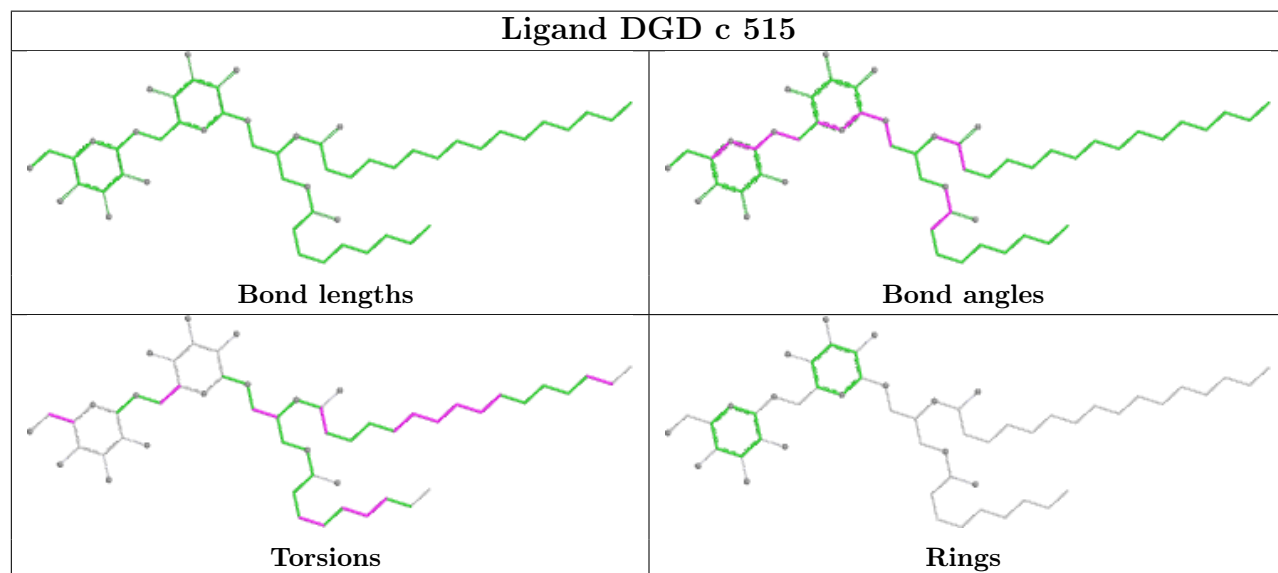
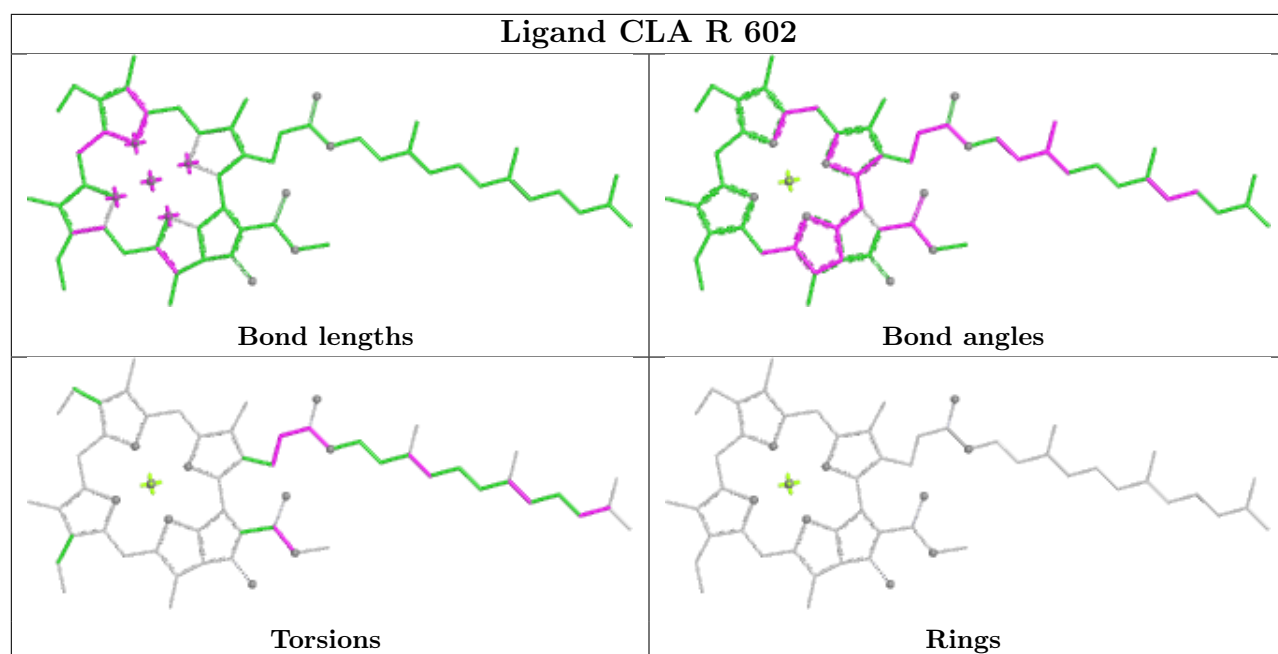
Ligand CLA N 611**Ligand CLA g 613**

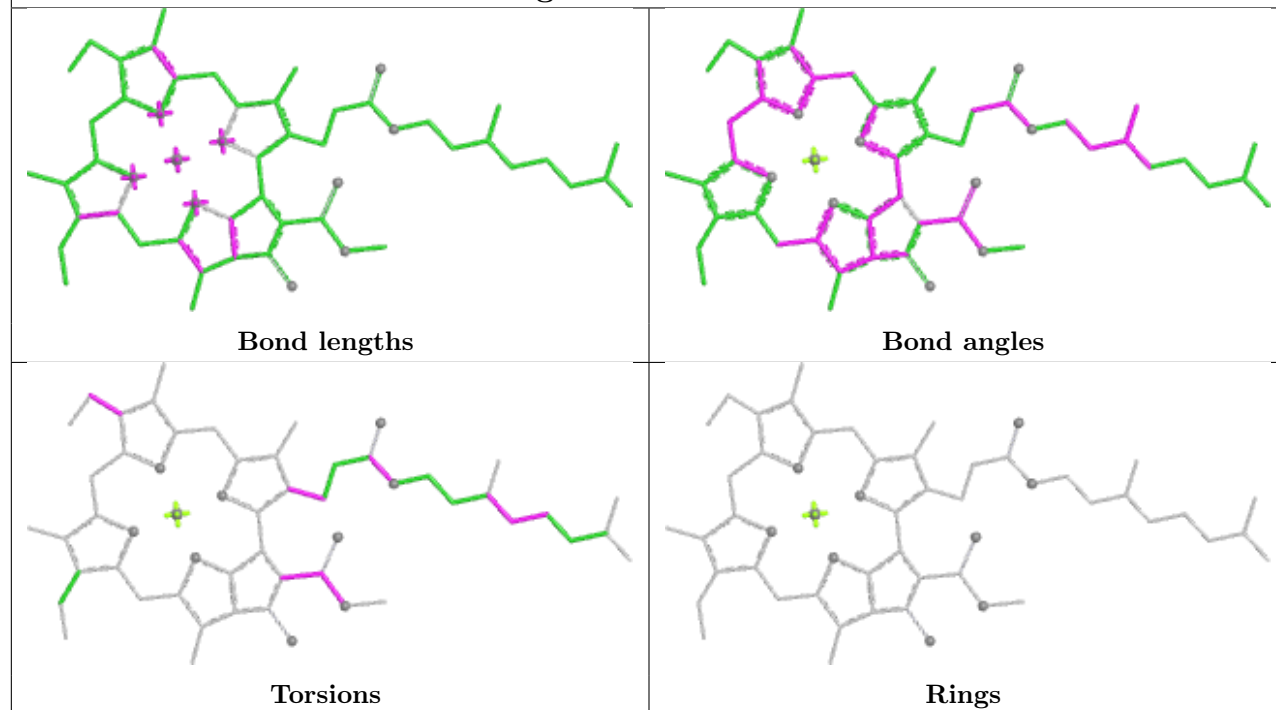
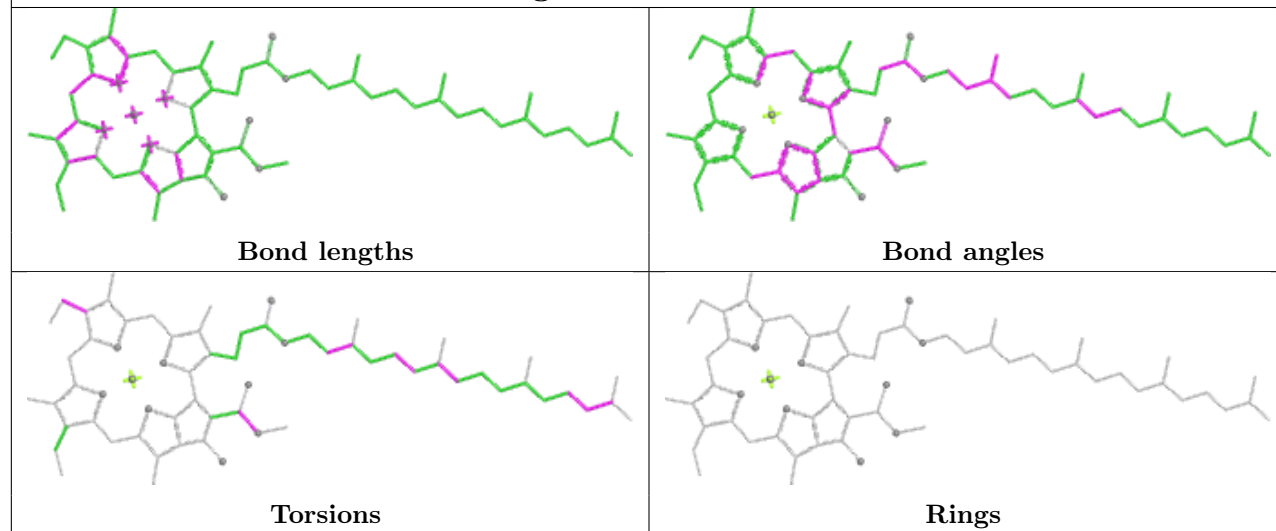


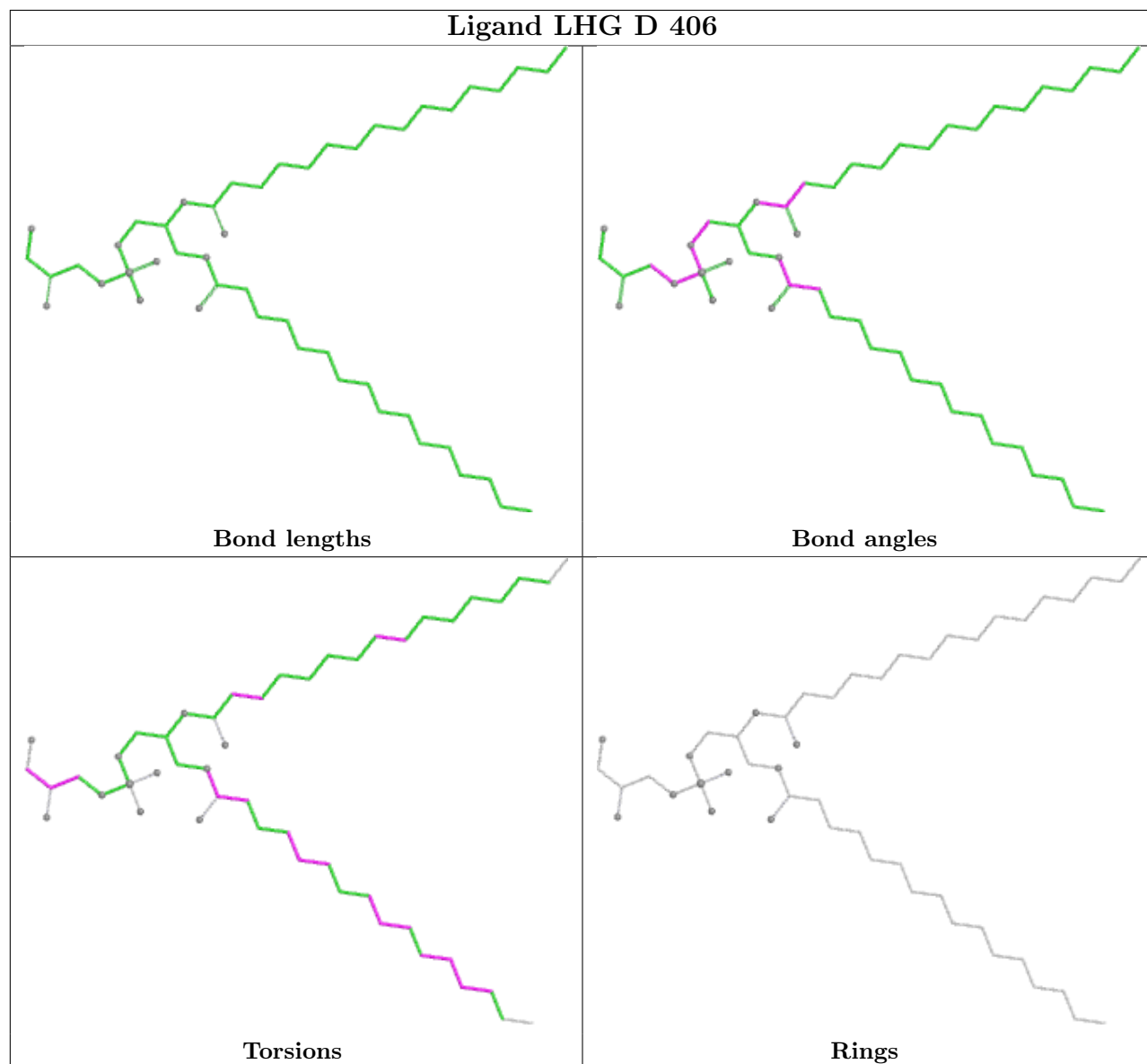
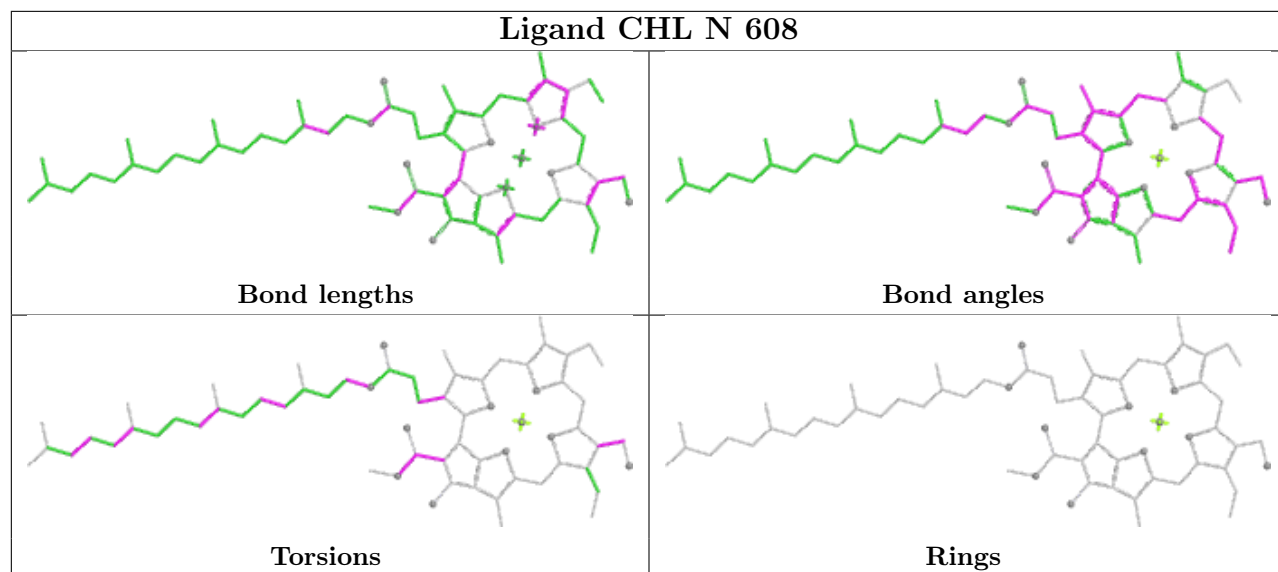


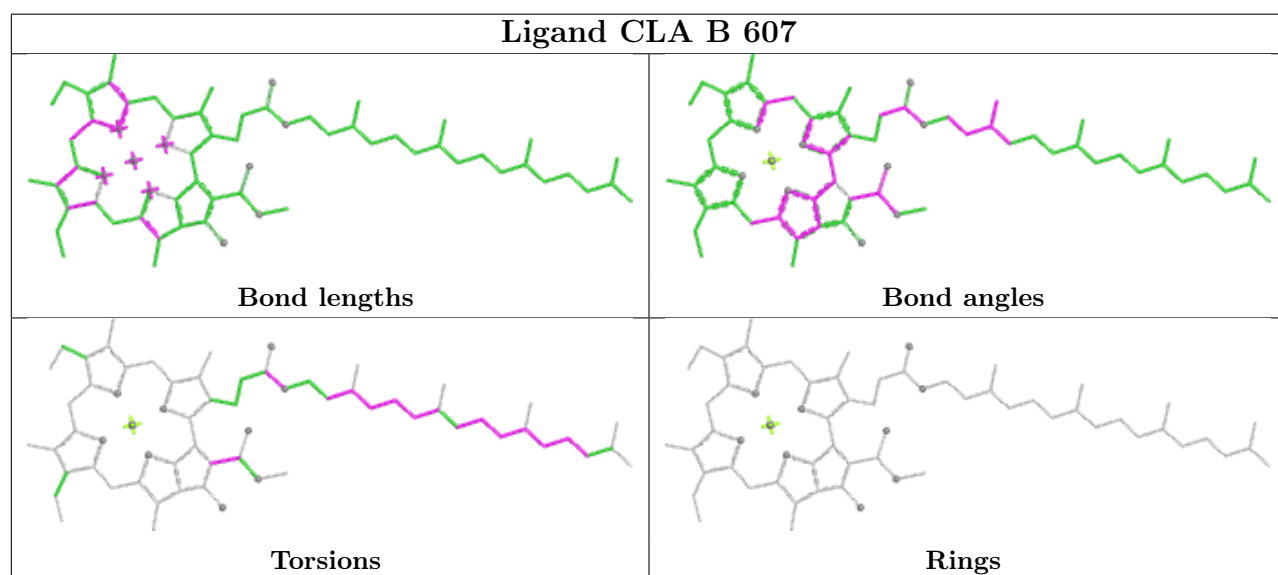
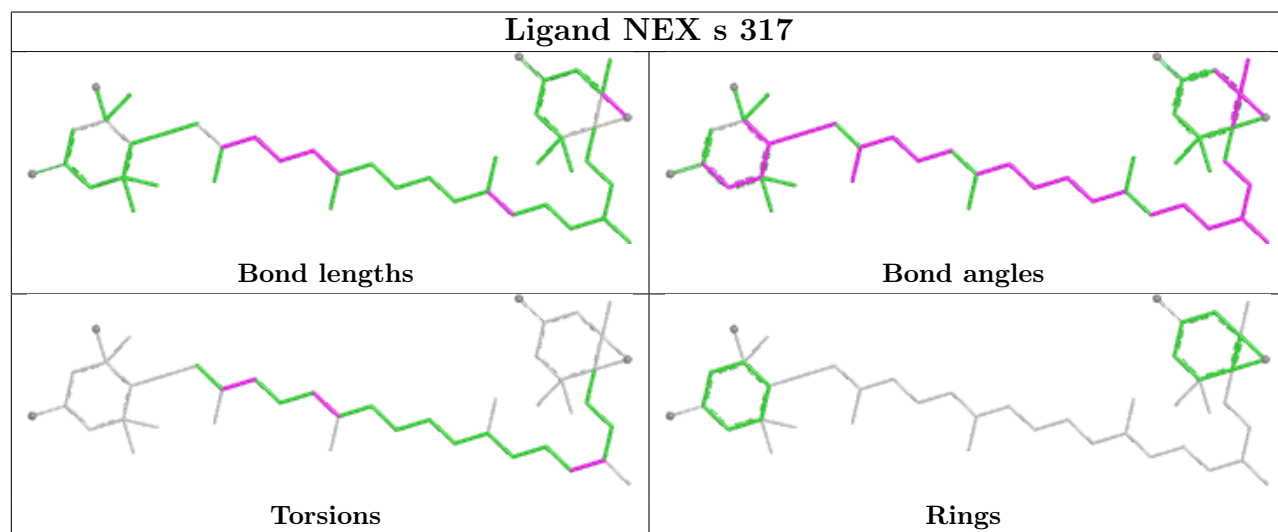
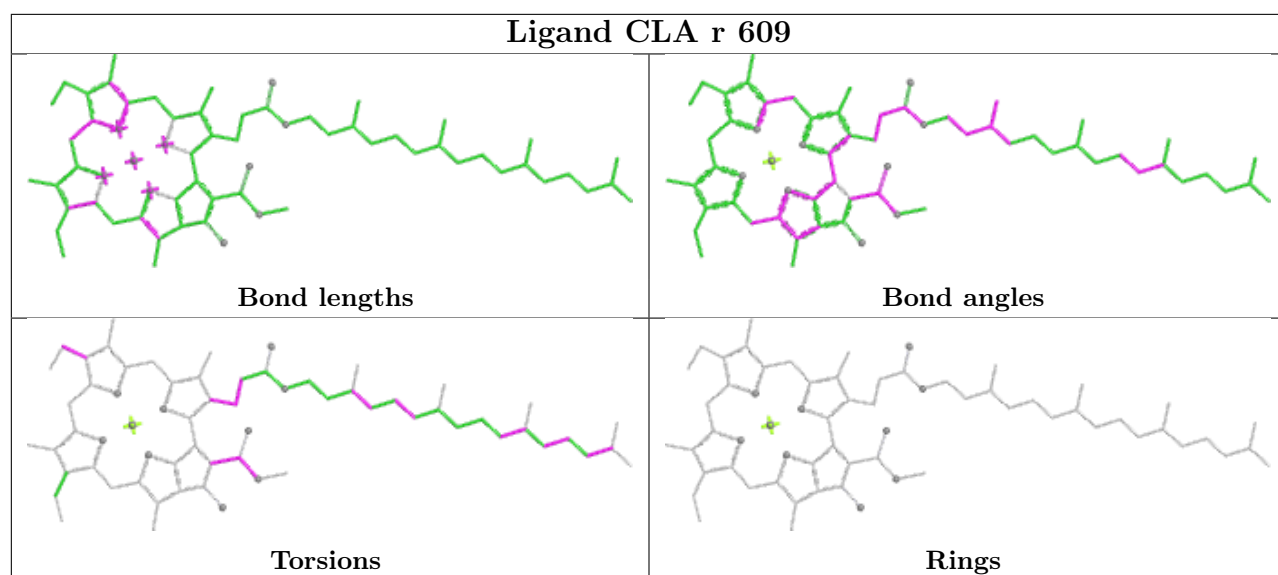


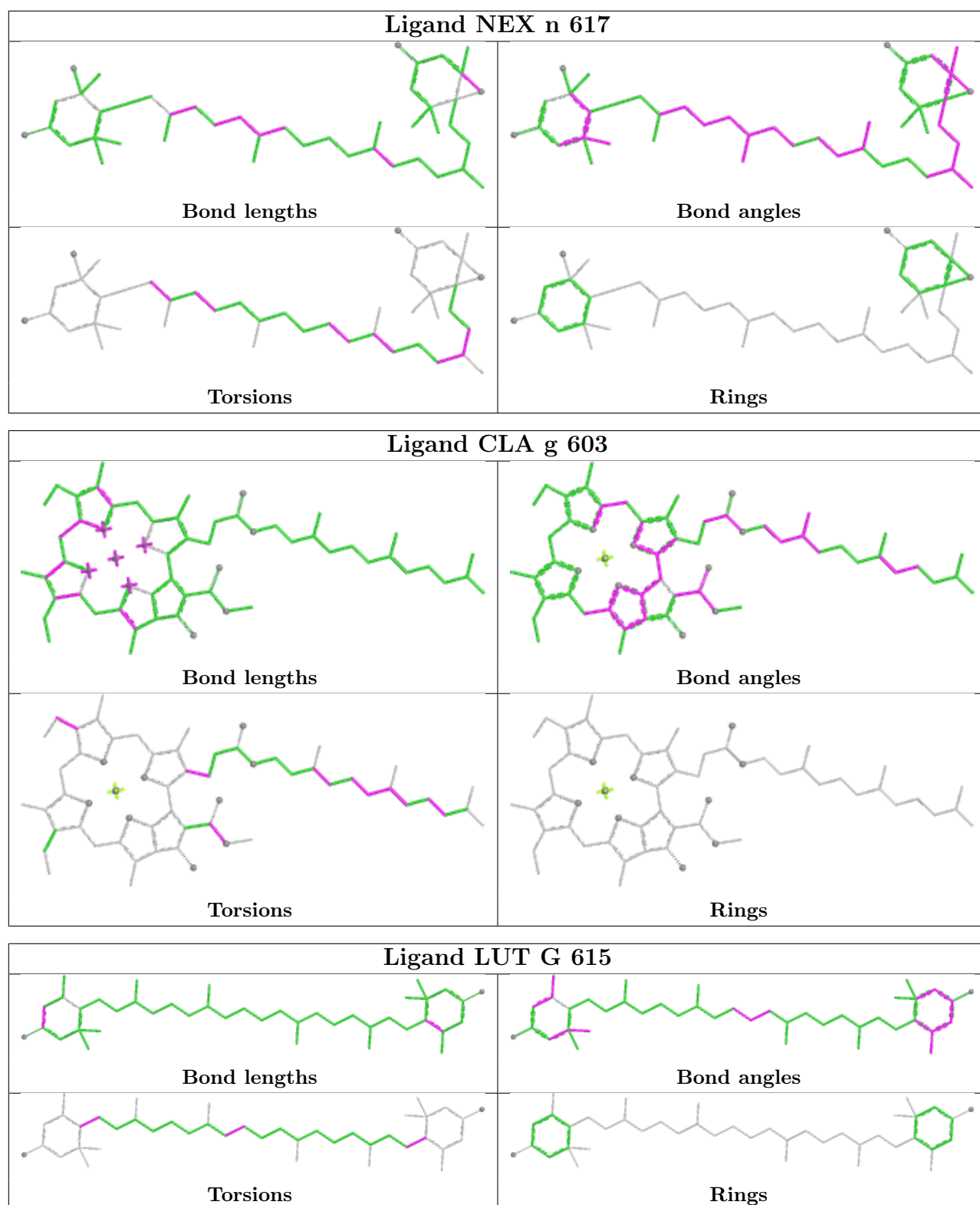


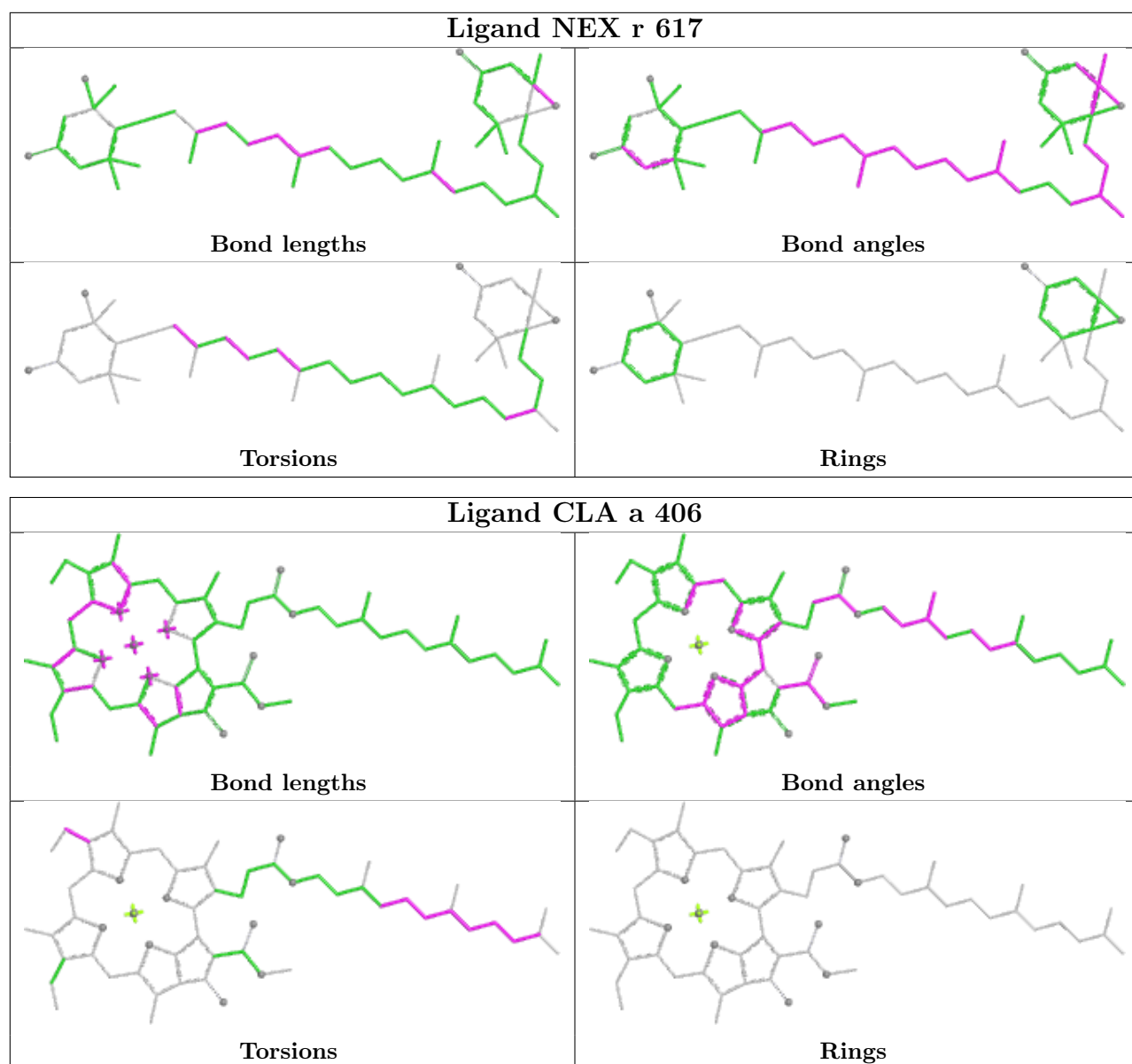


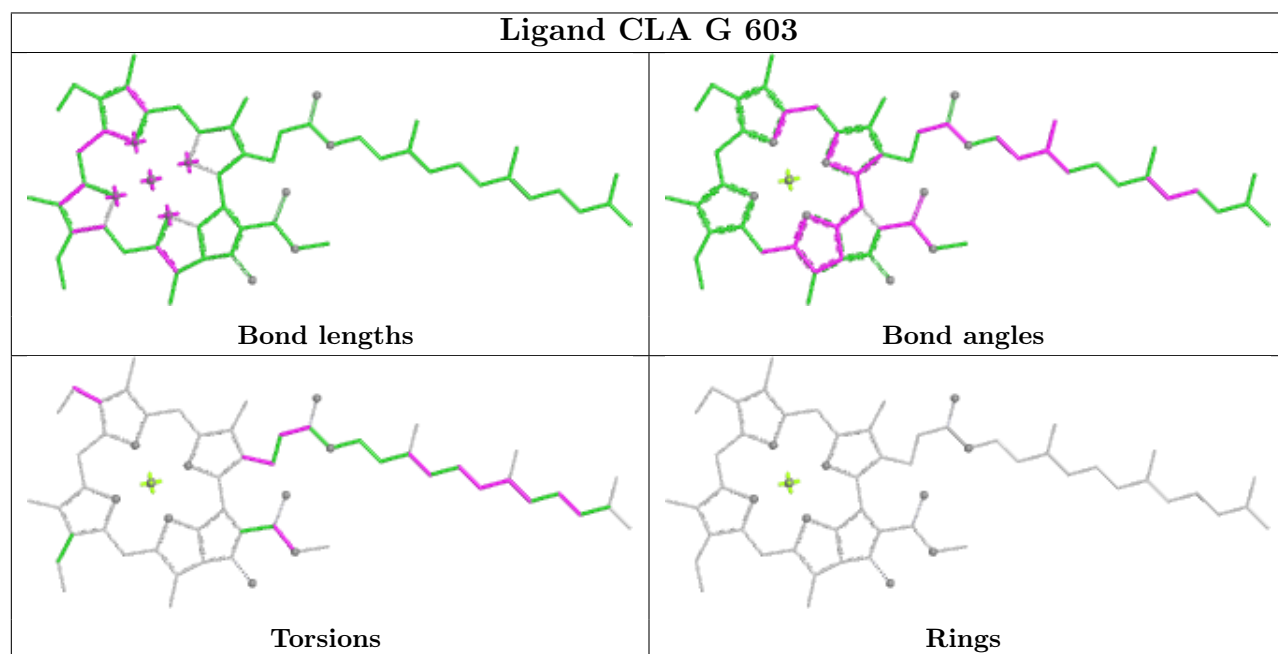
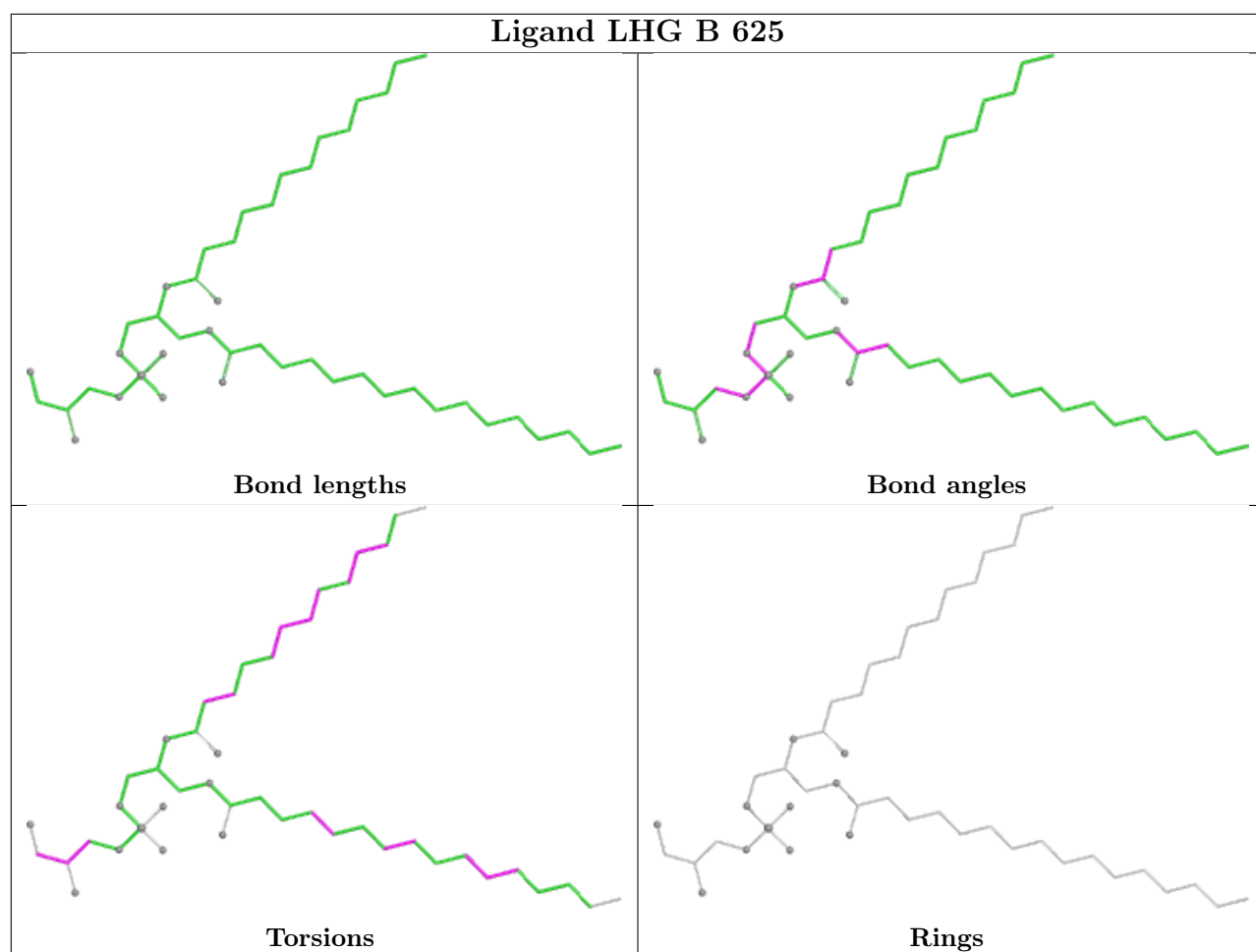
Ligand CLA 2 604**Ligand CLA C 503**

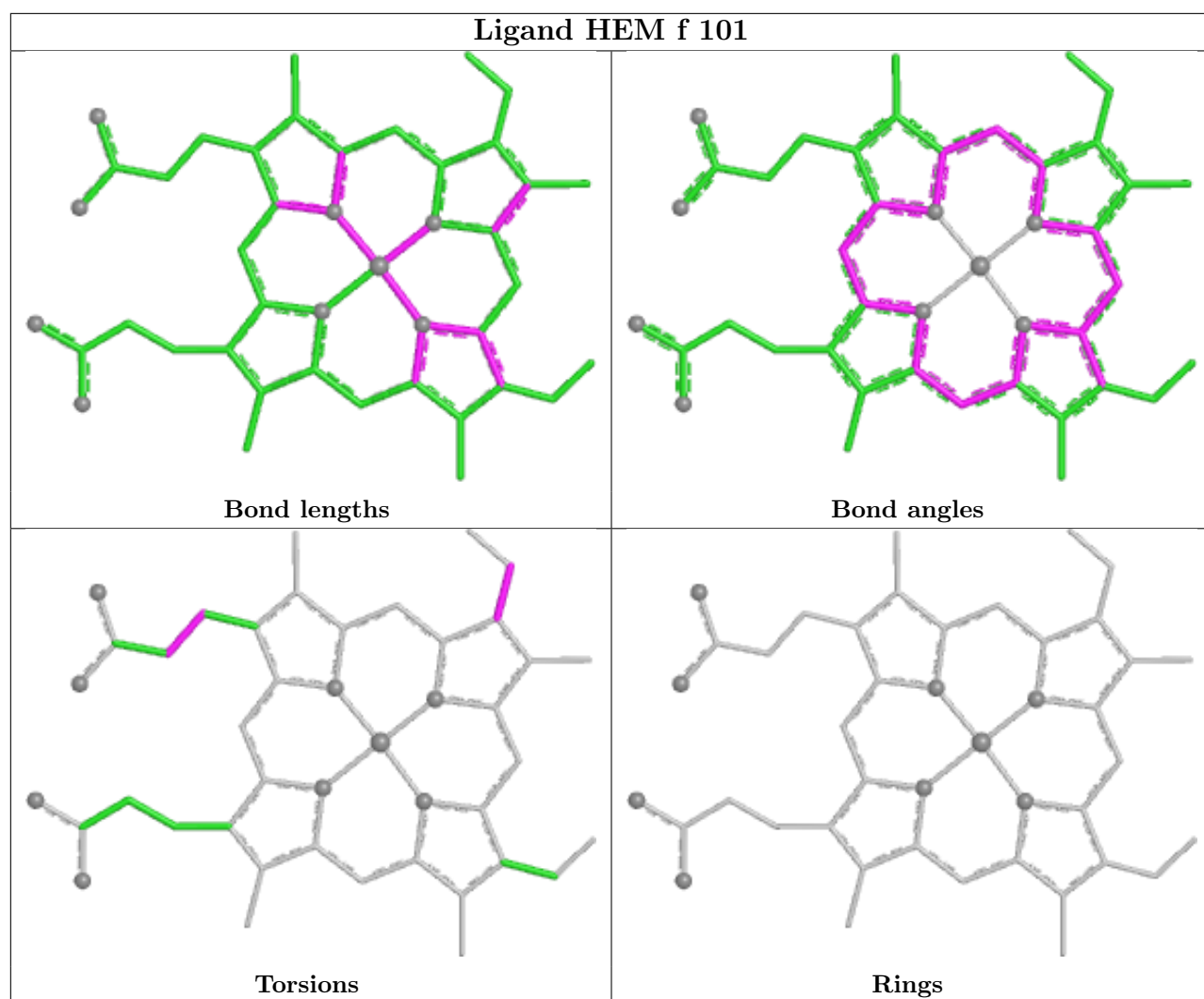


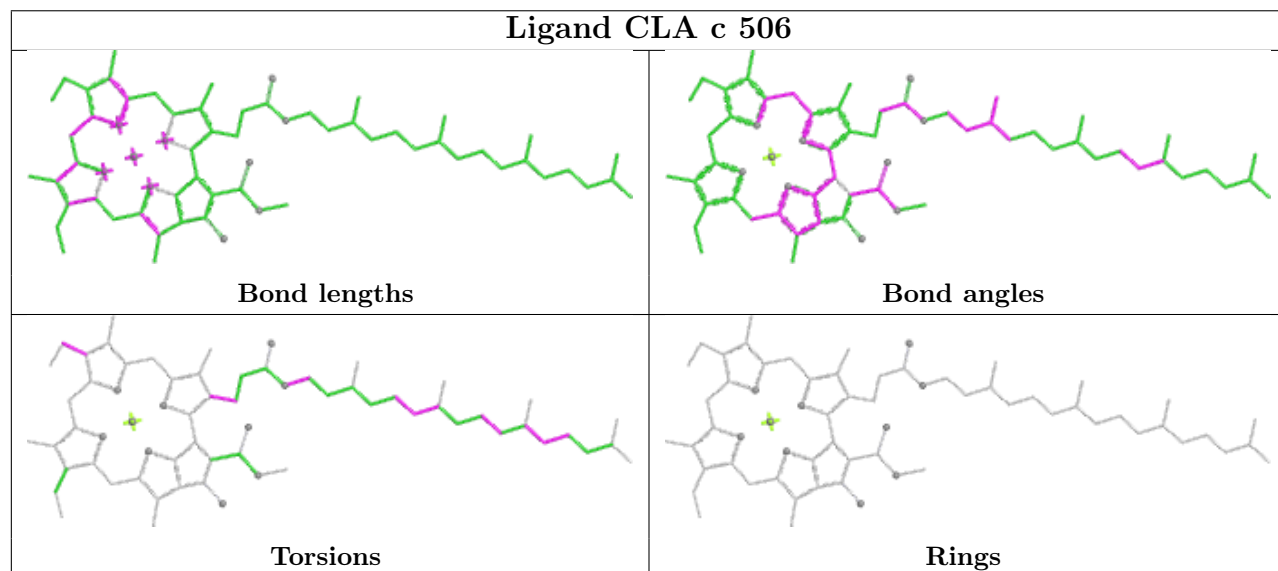
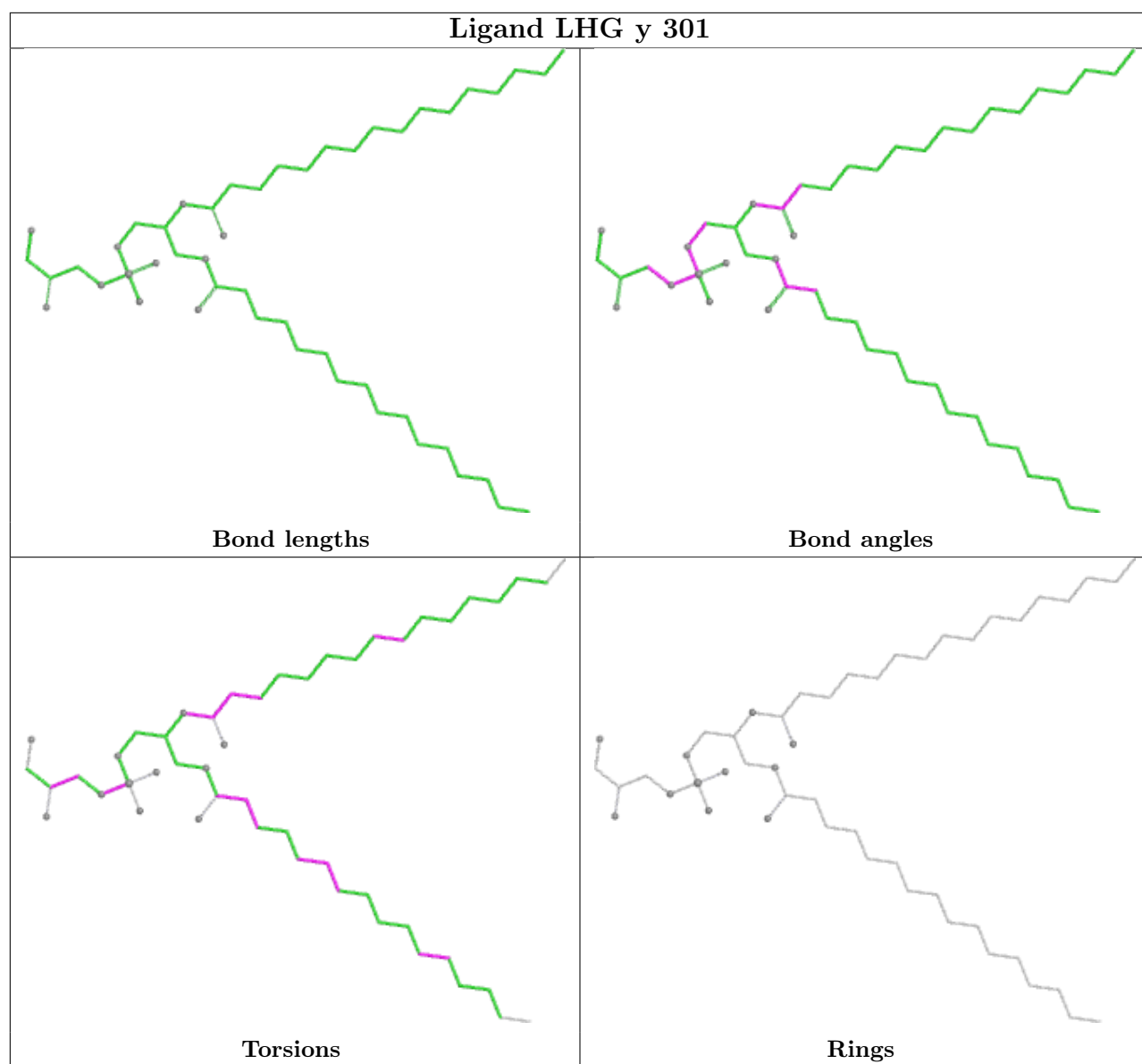


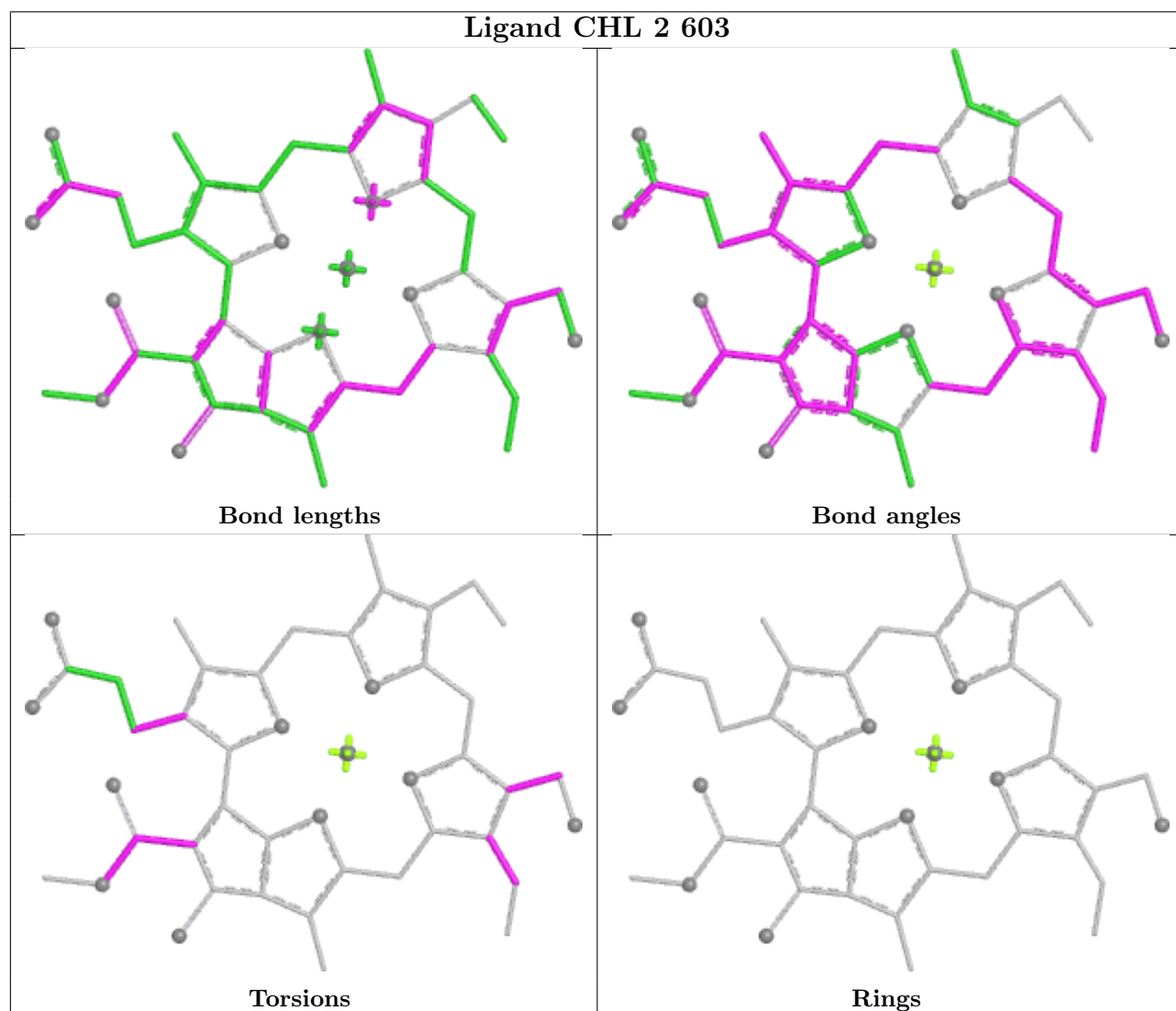
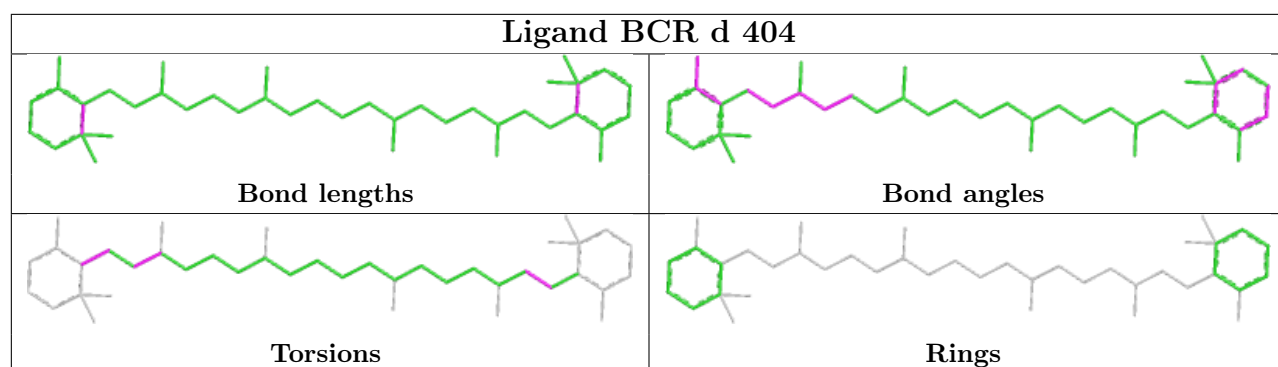


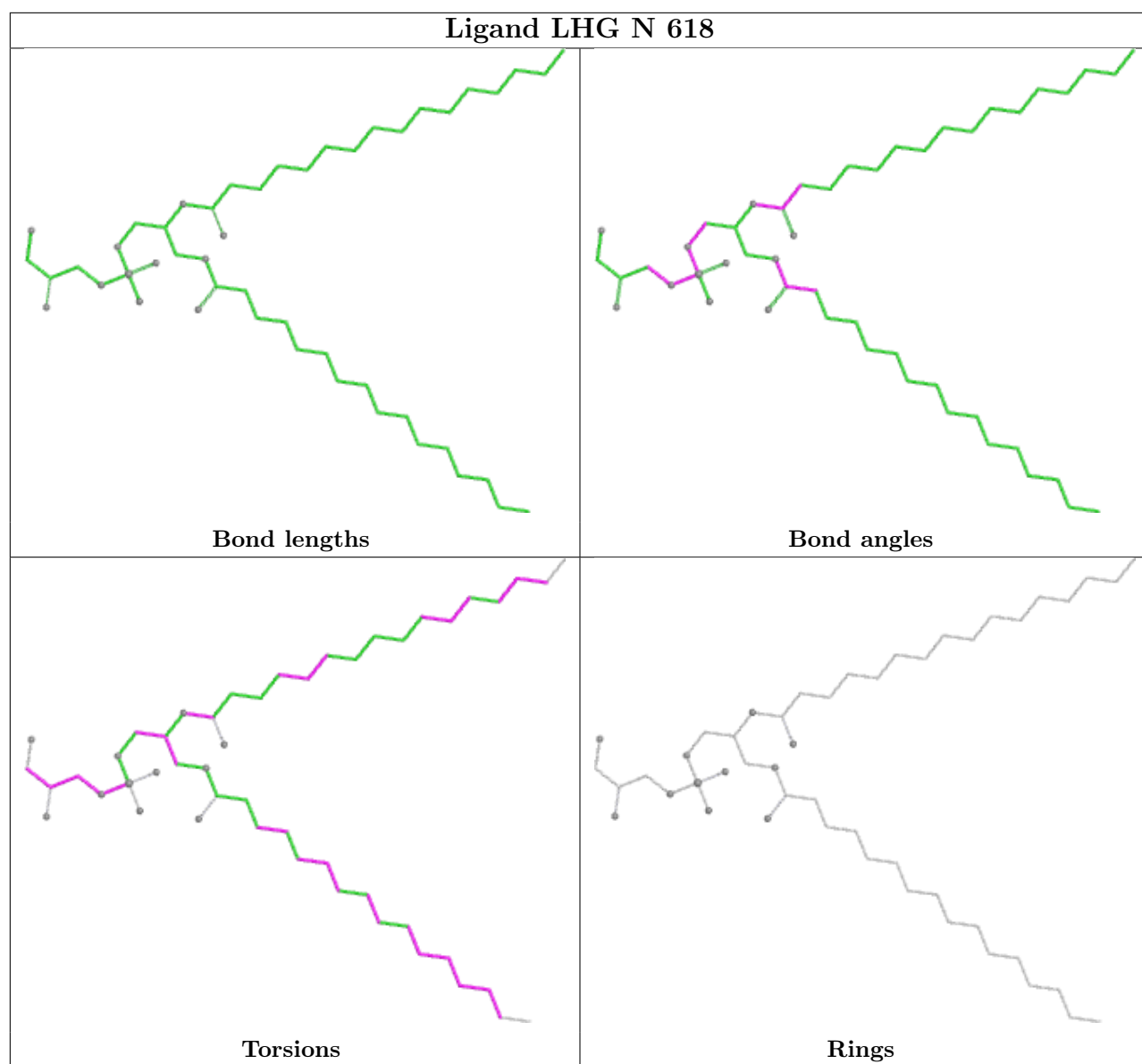


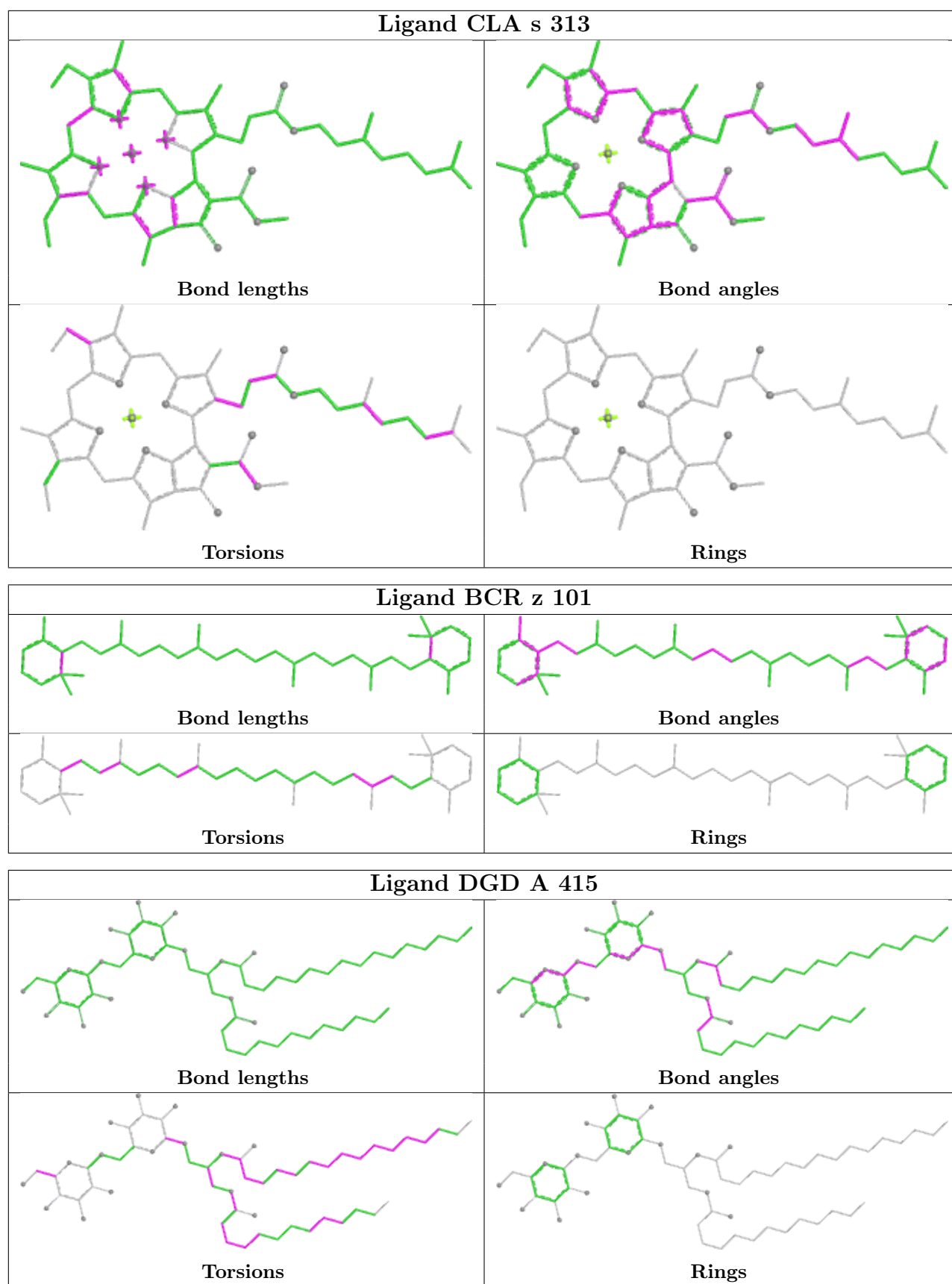


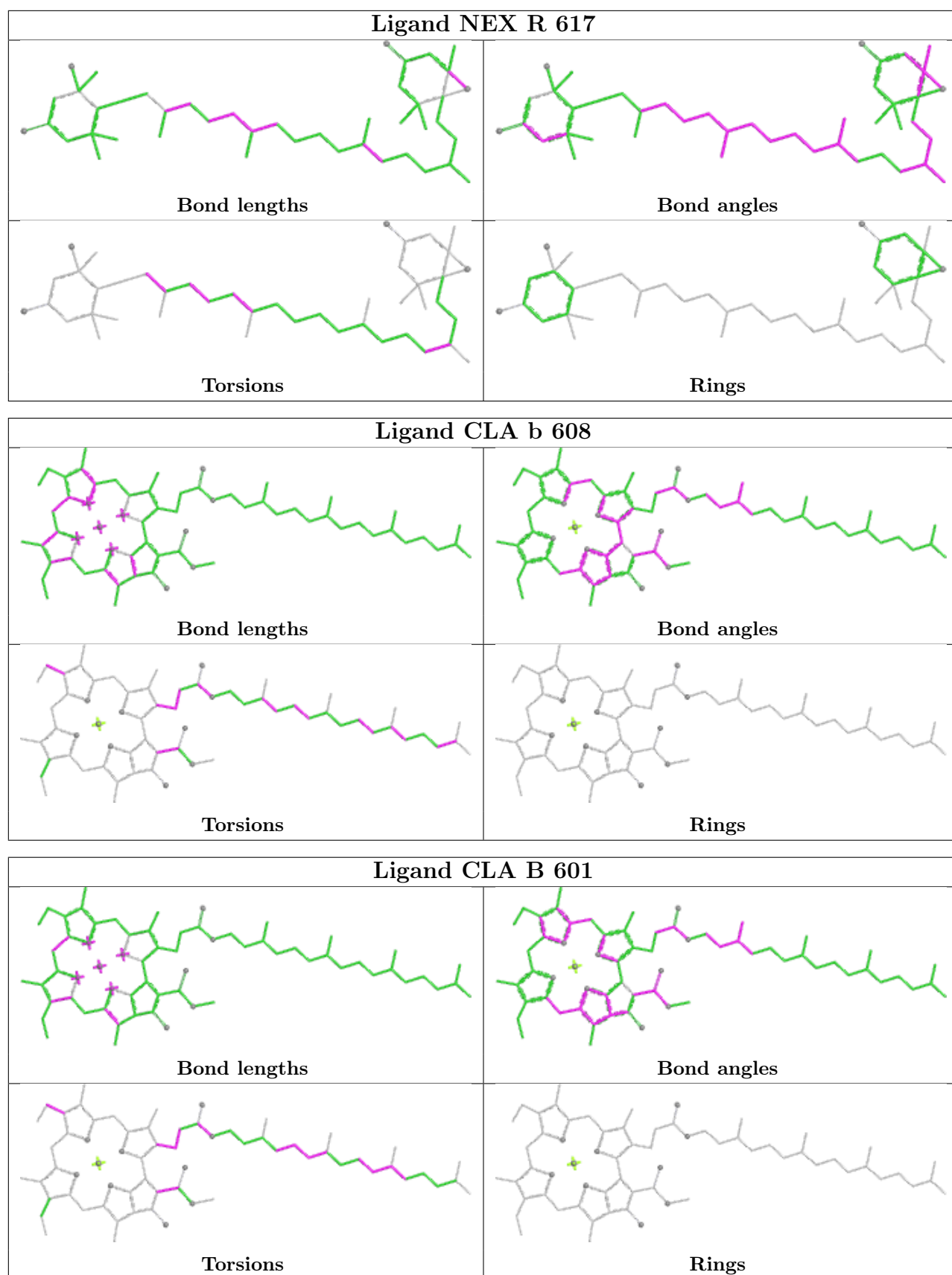


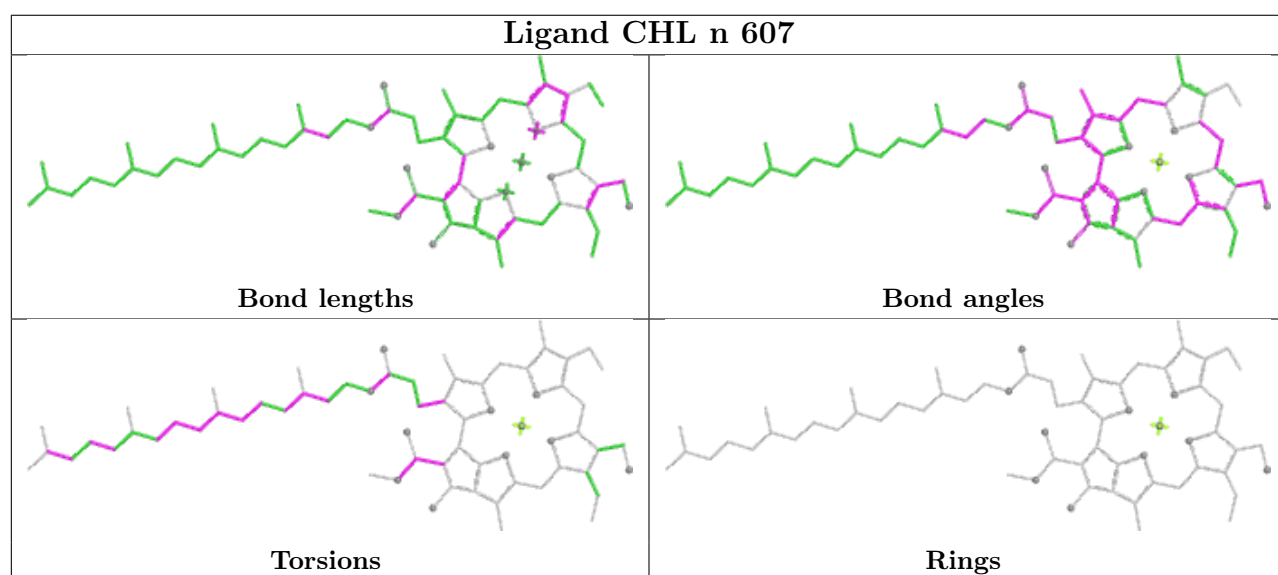
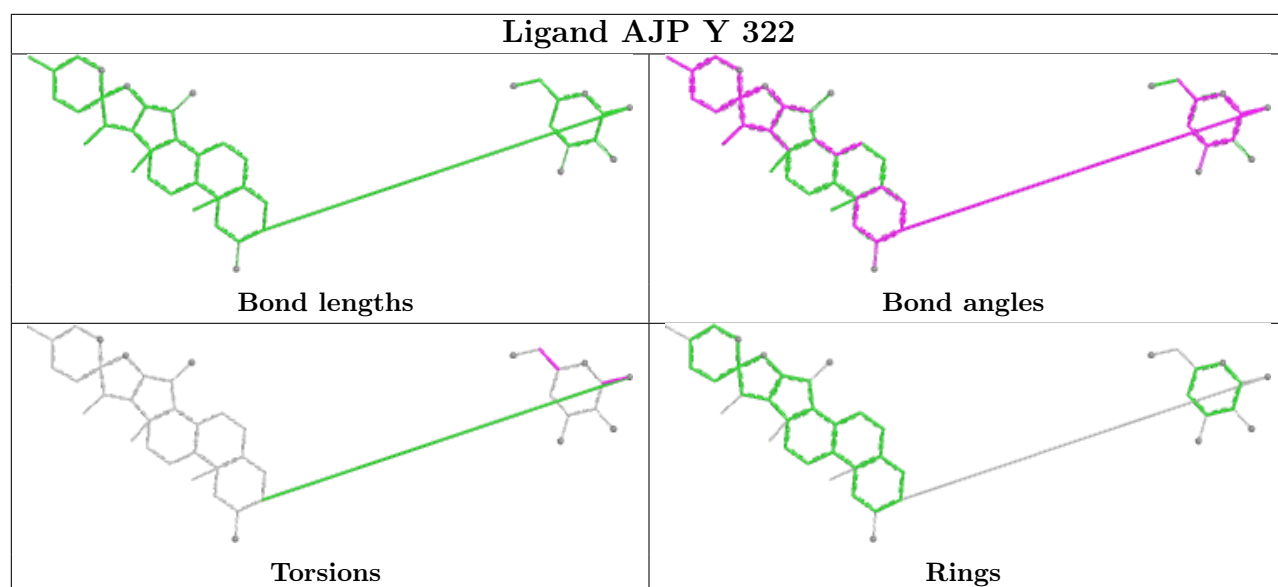




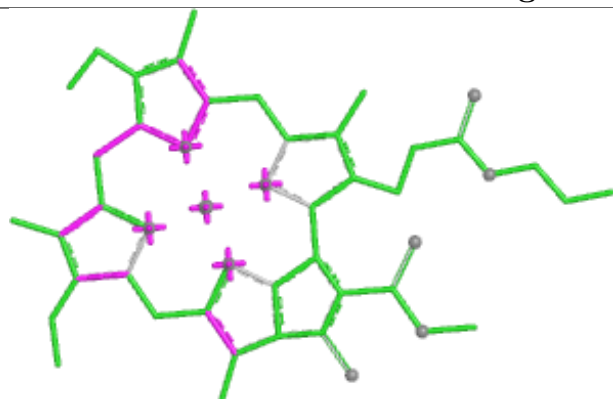




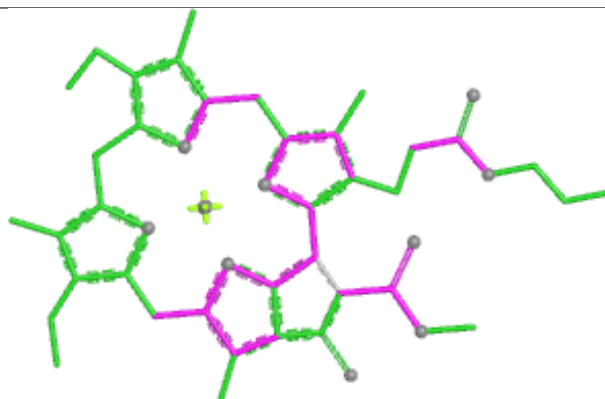




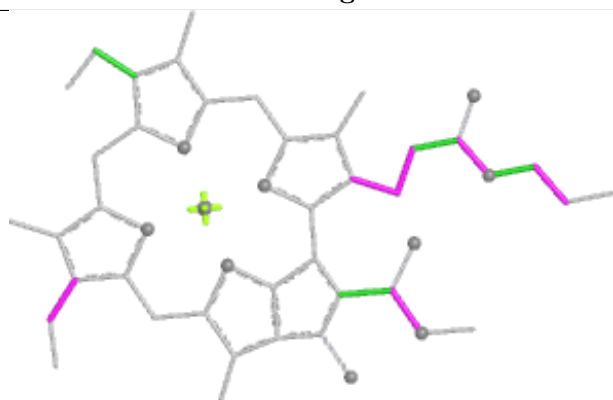
Ligand CLA 2 605



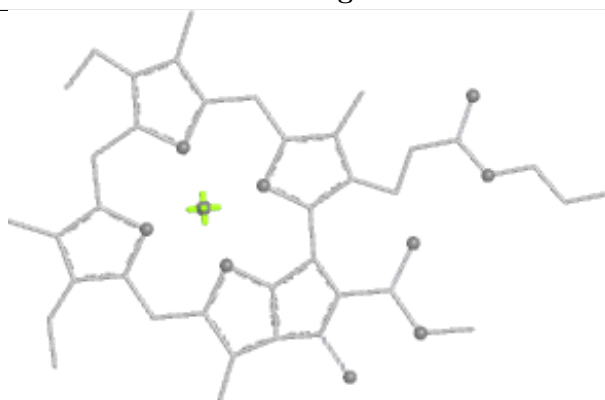
Bond lengths



Bond angles

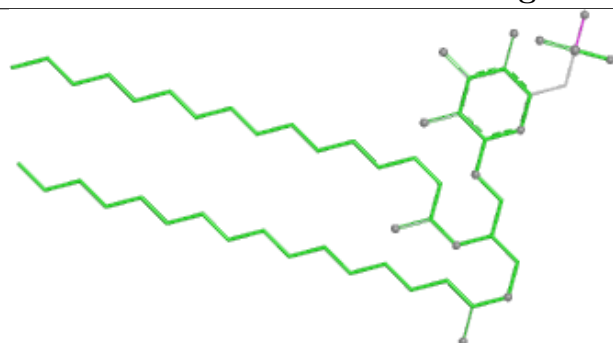


Torsions

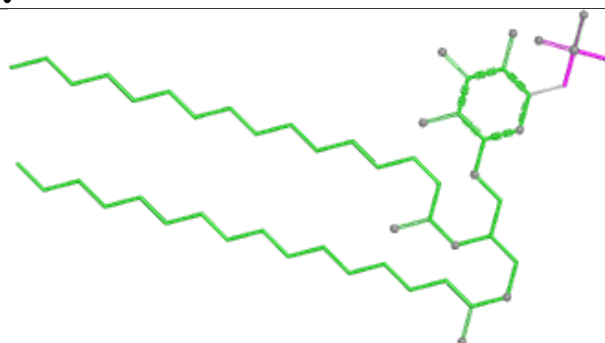


Rings

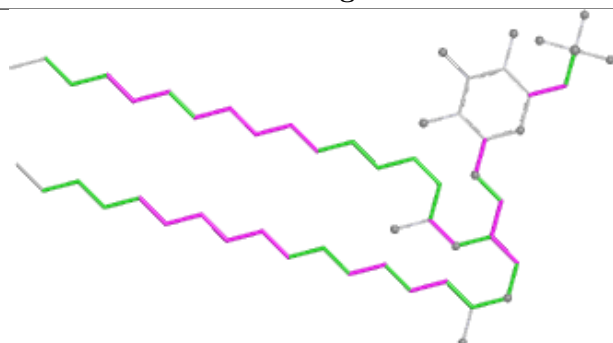
Ligand SQD a 412



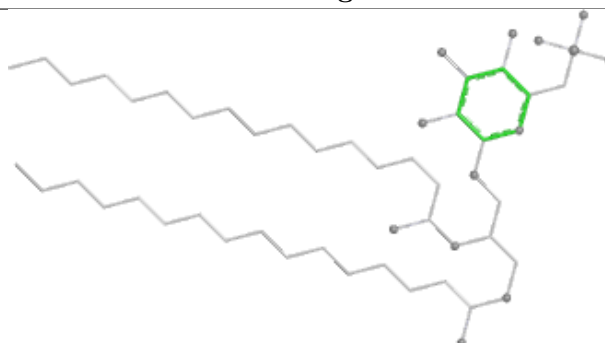
Bond lengths



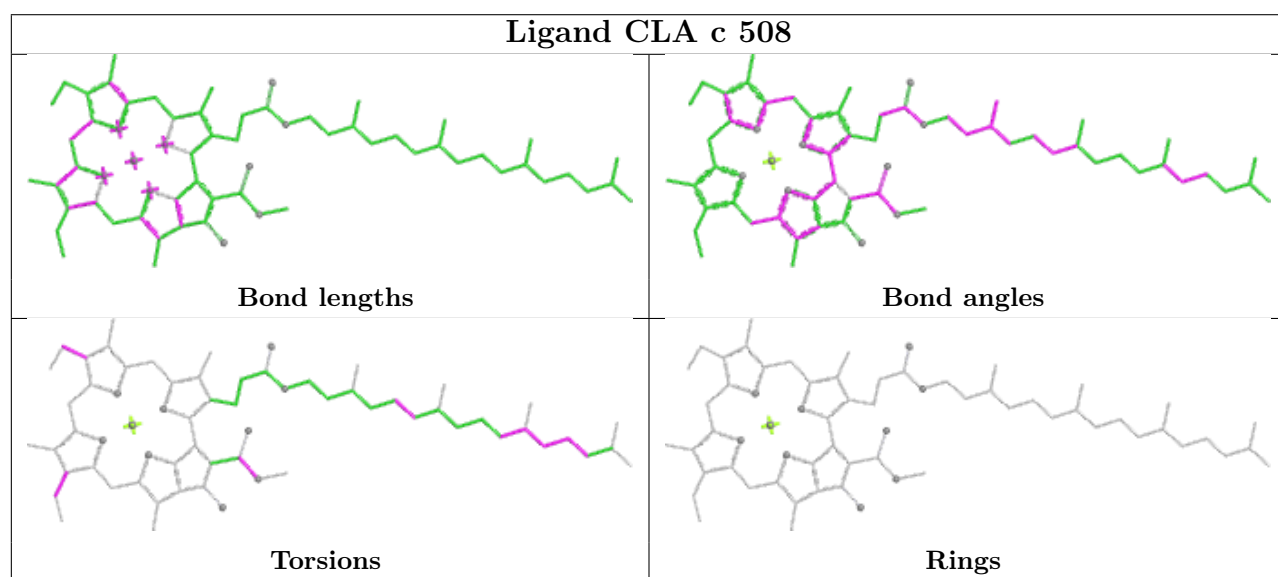
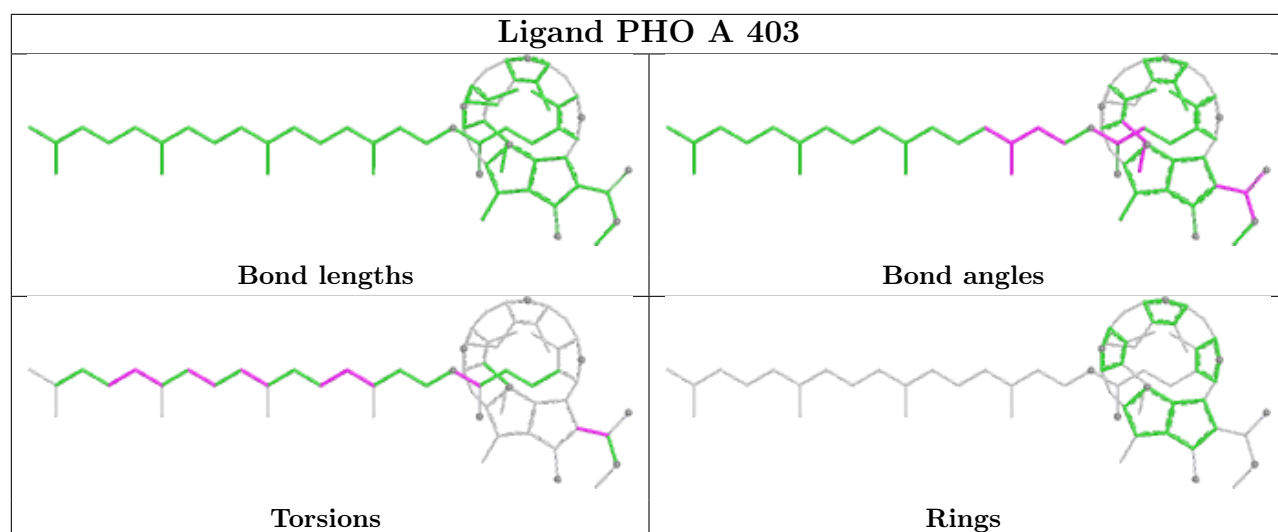
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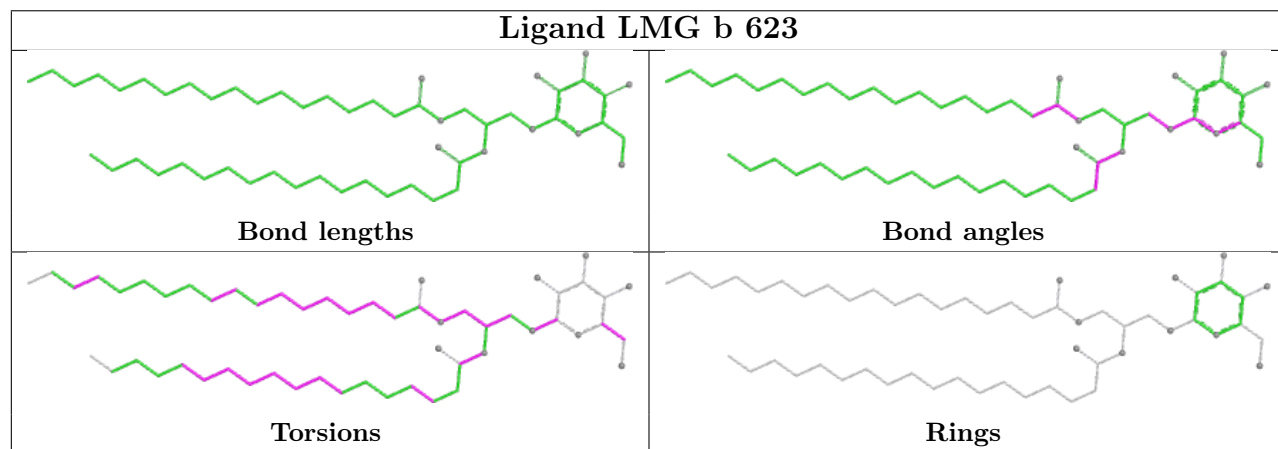
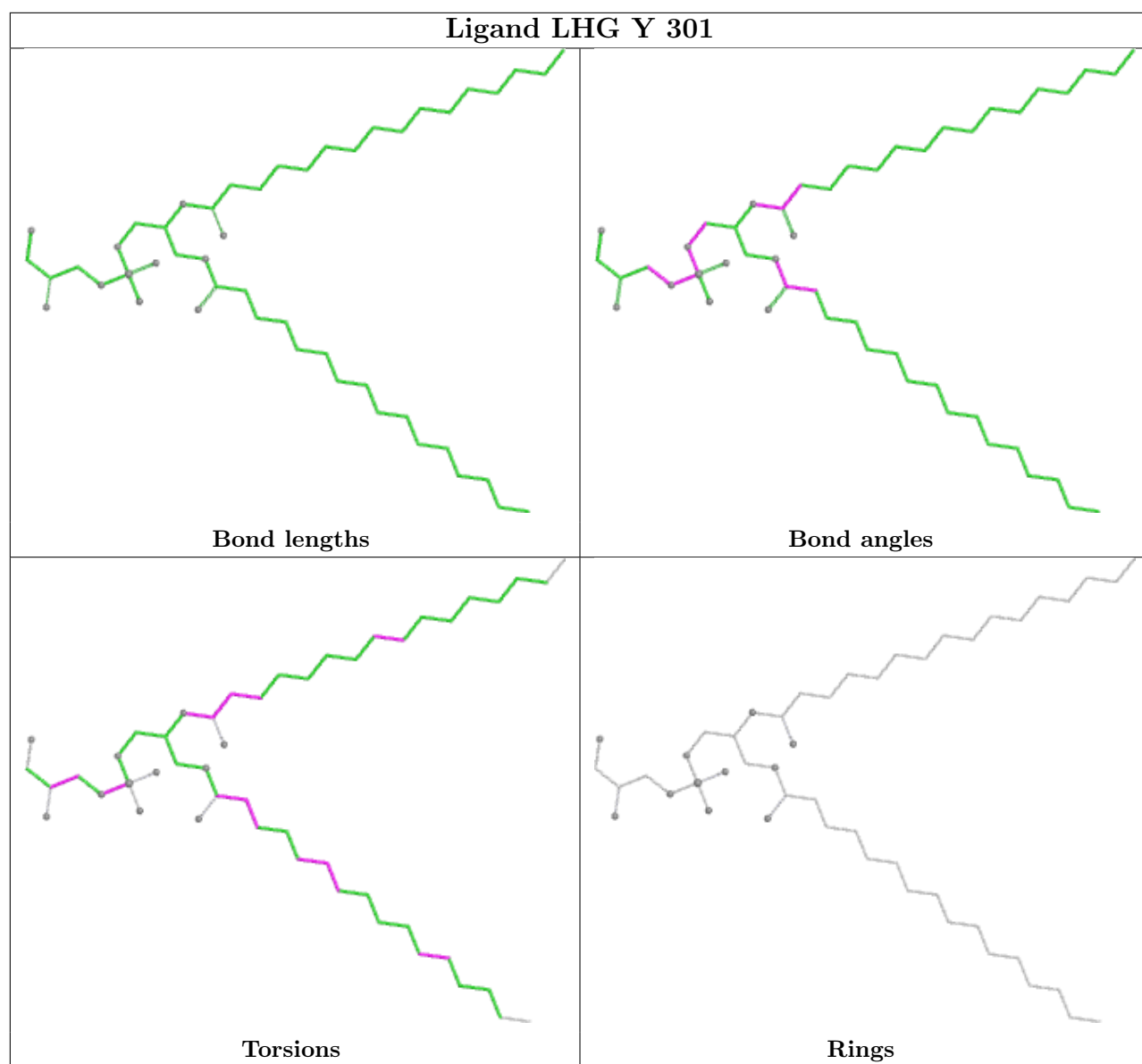


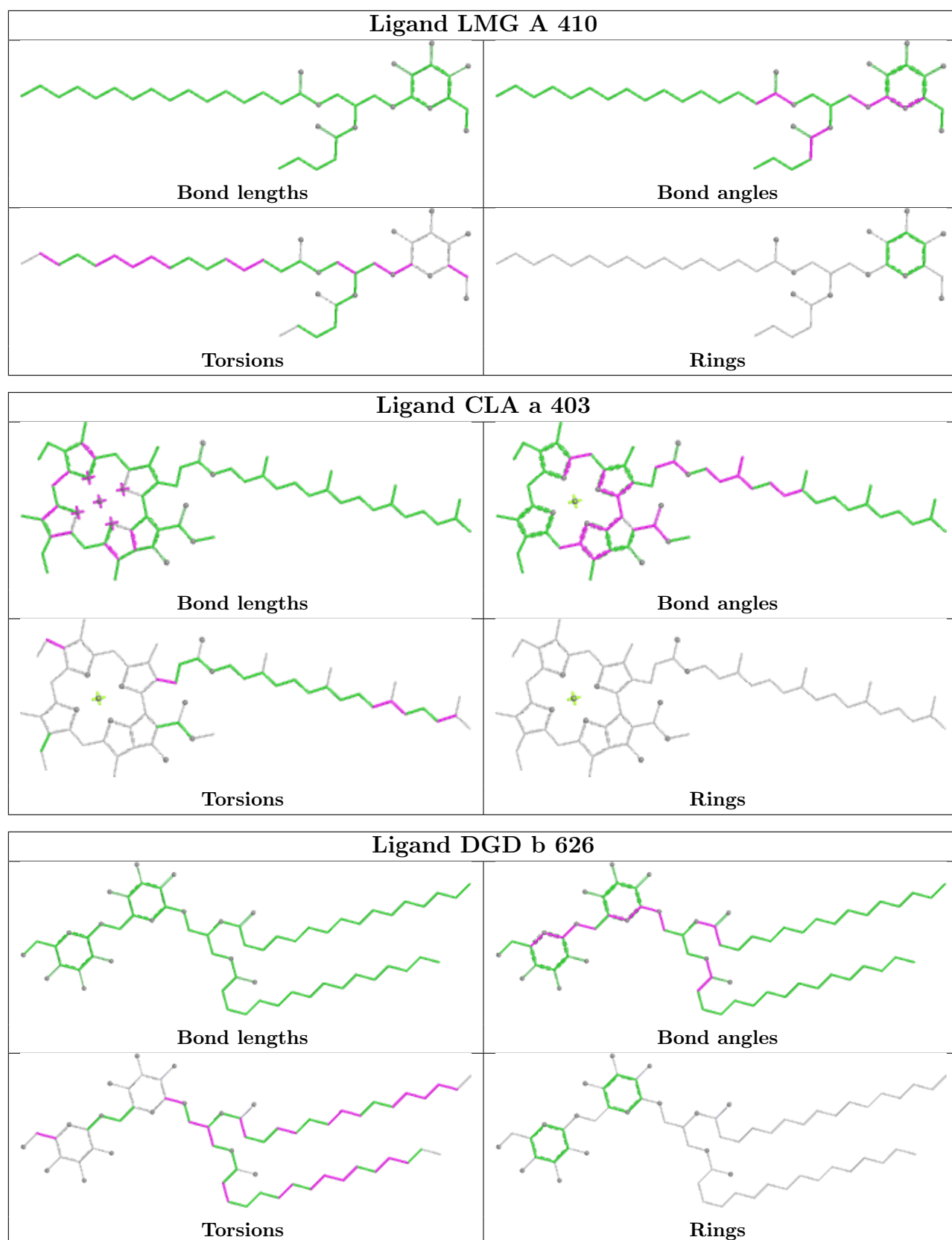
Torsions

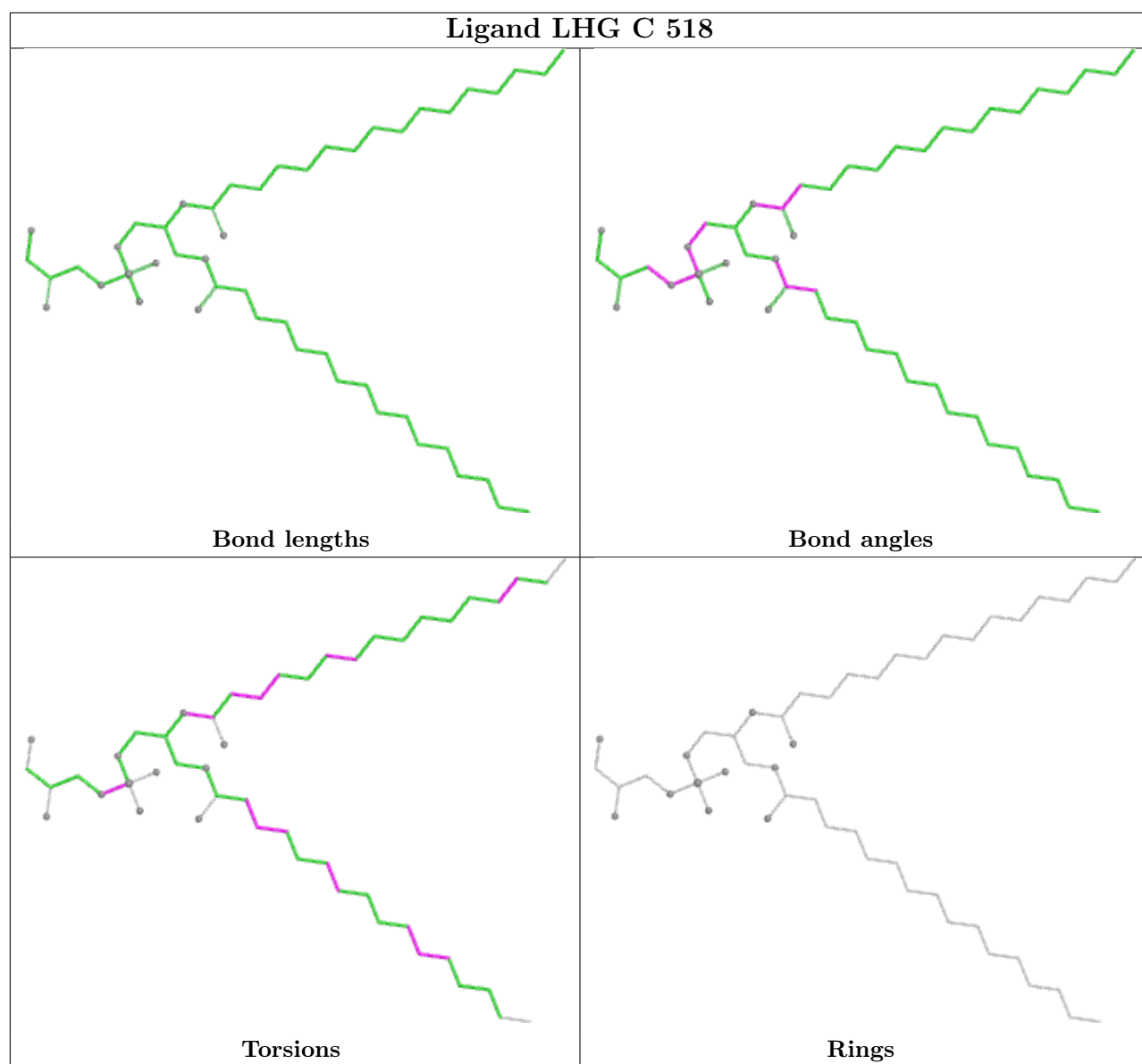


Rings

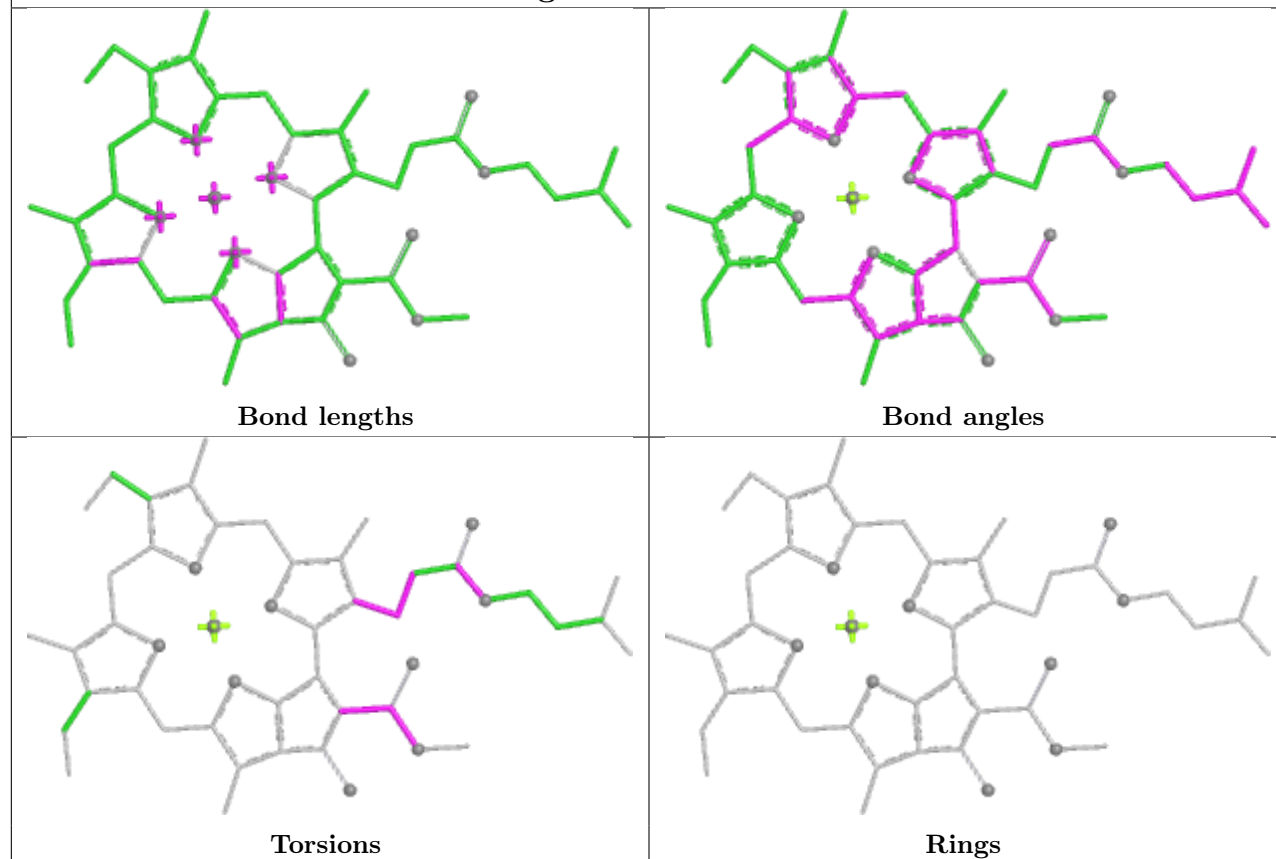




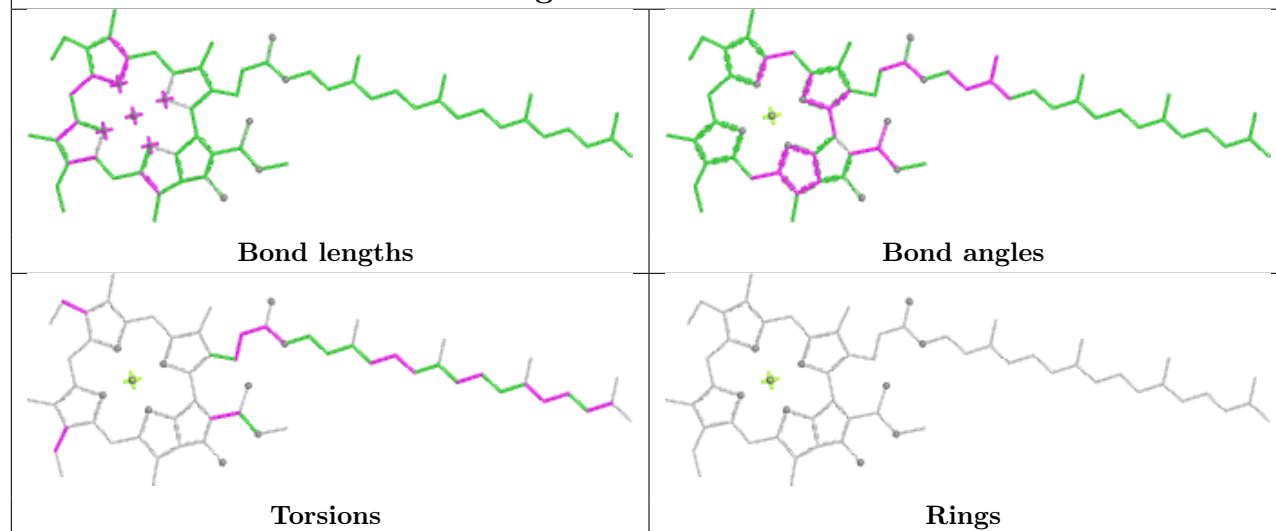


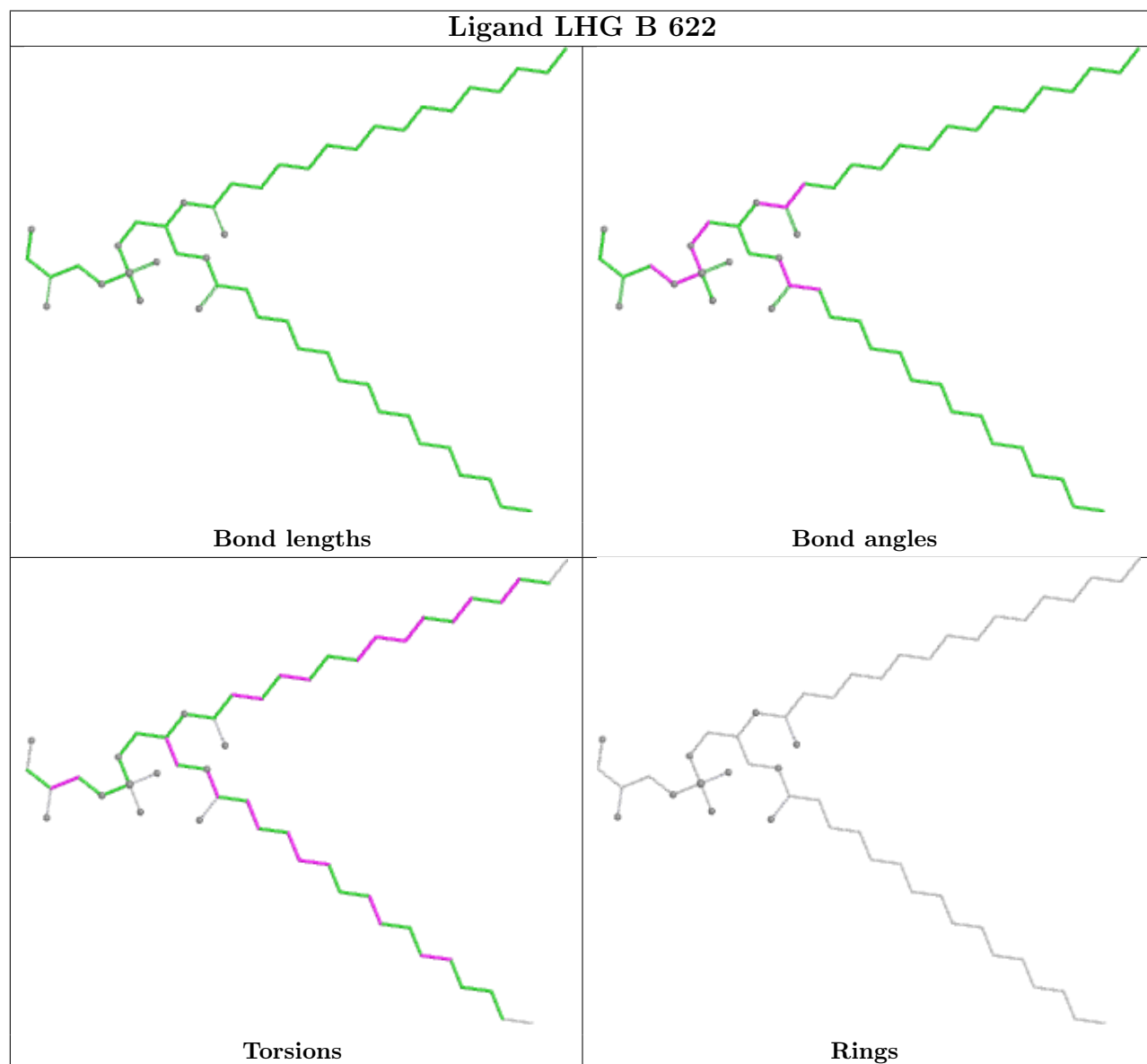
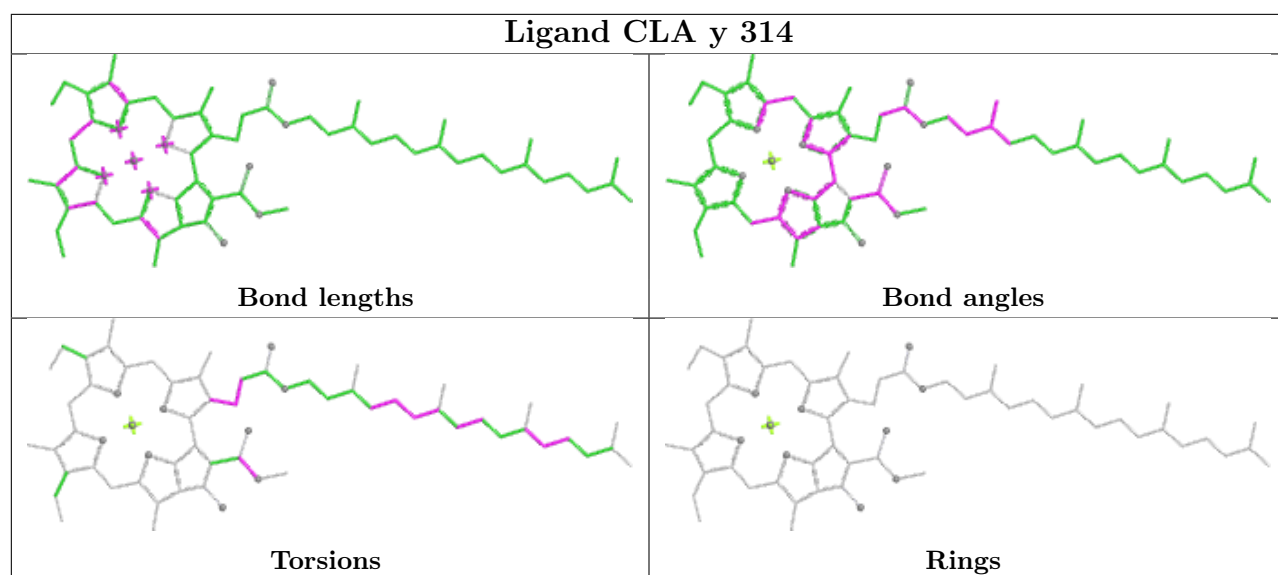


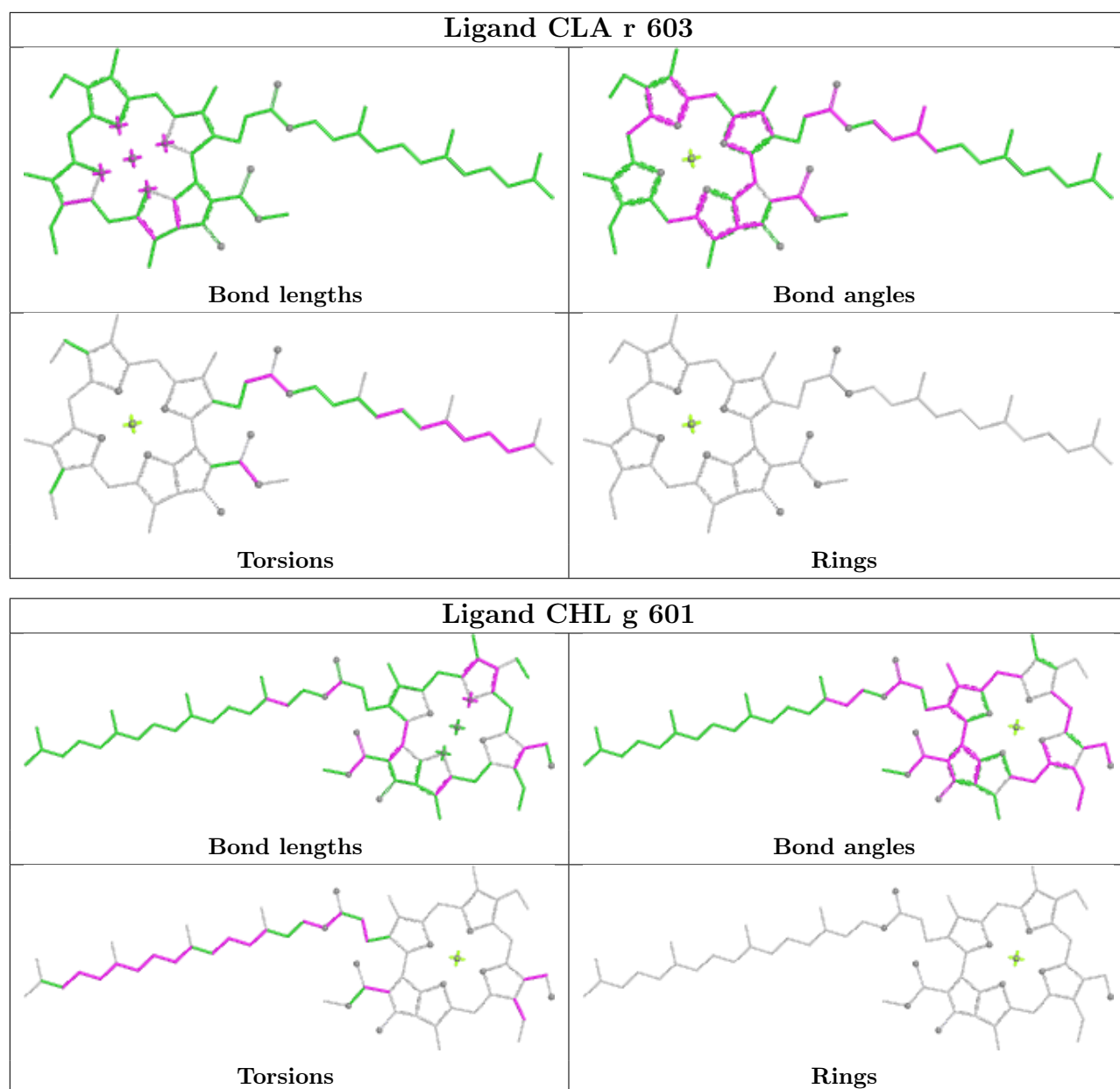
Ligand CLA s 305

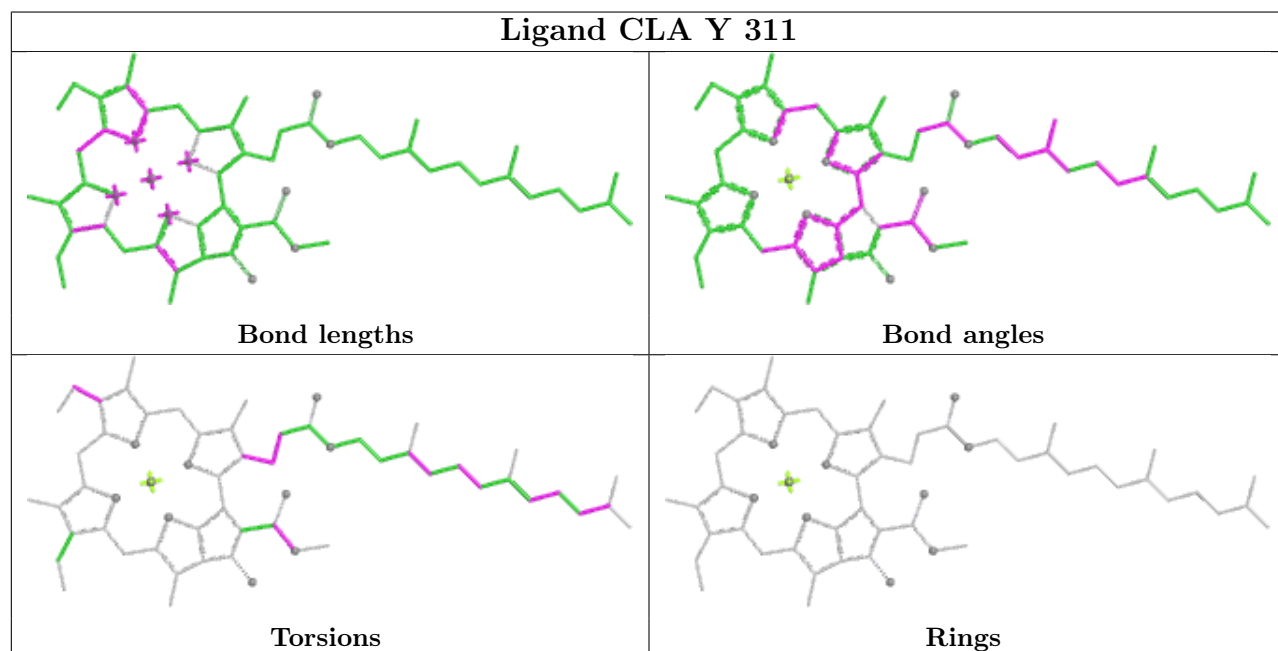
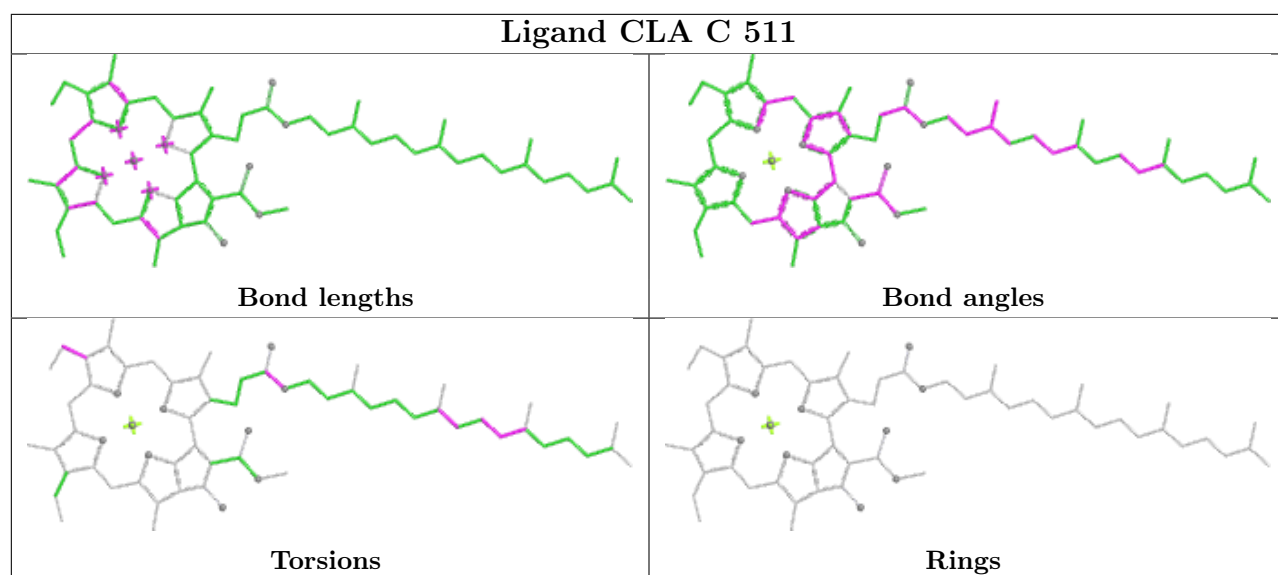


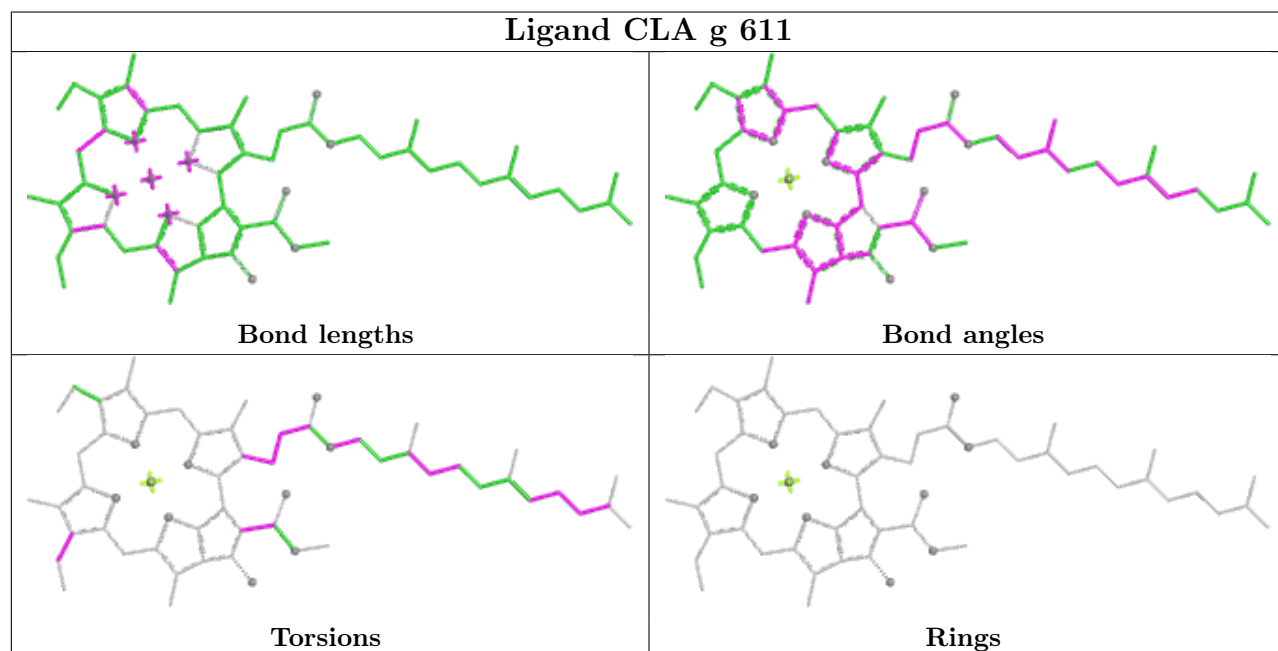
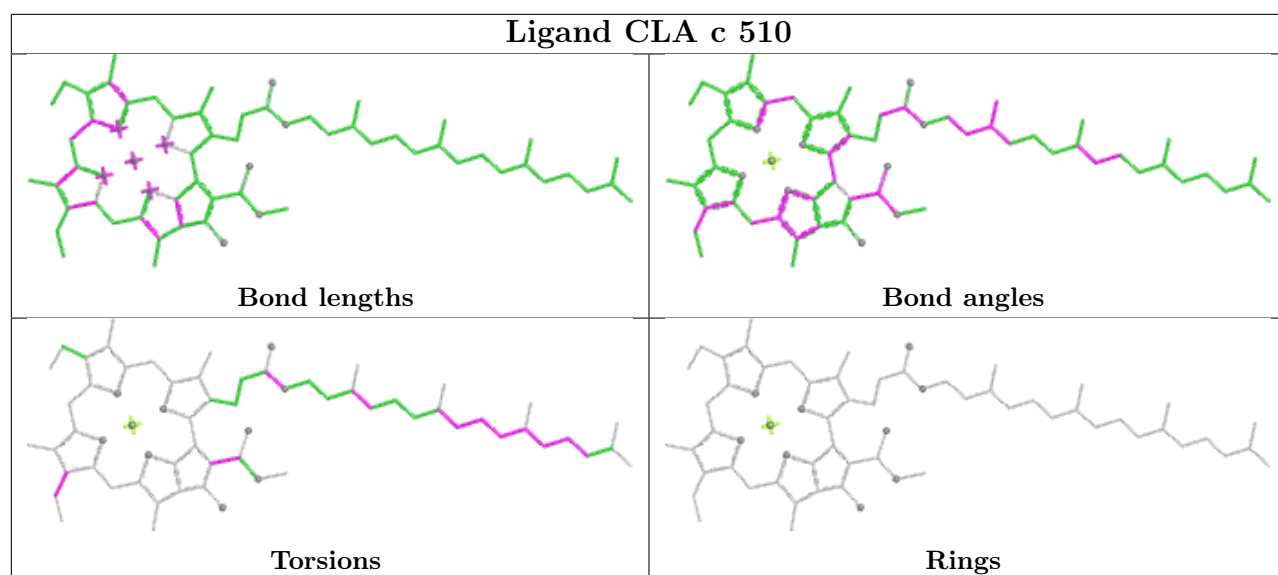
Ligand CLA b 616

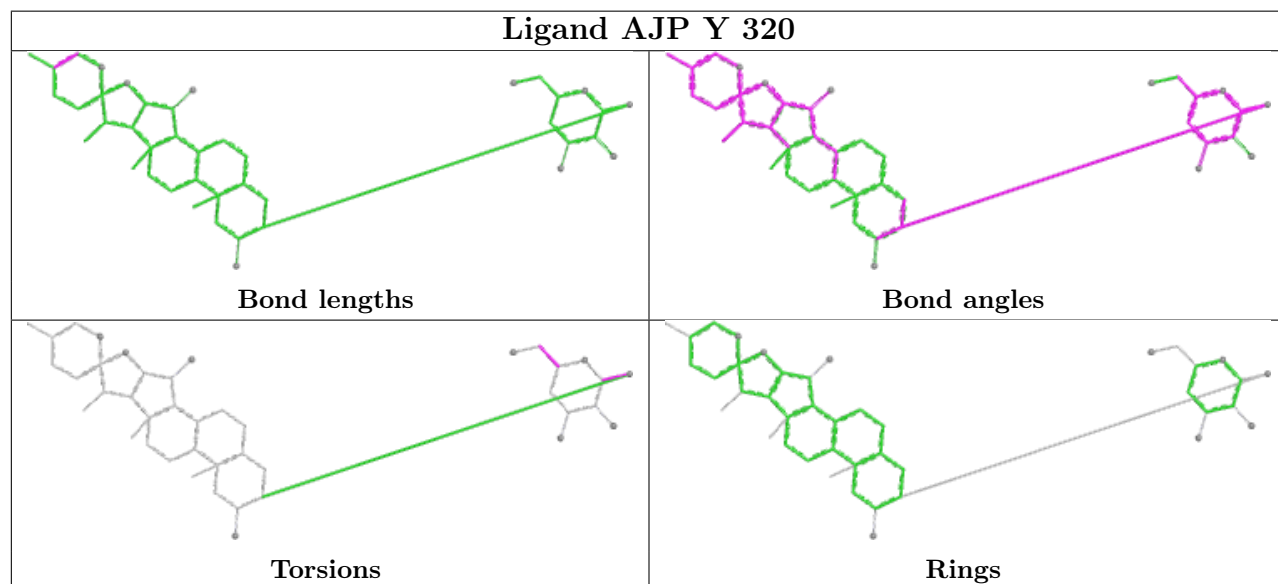
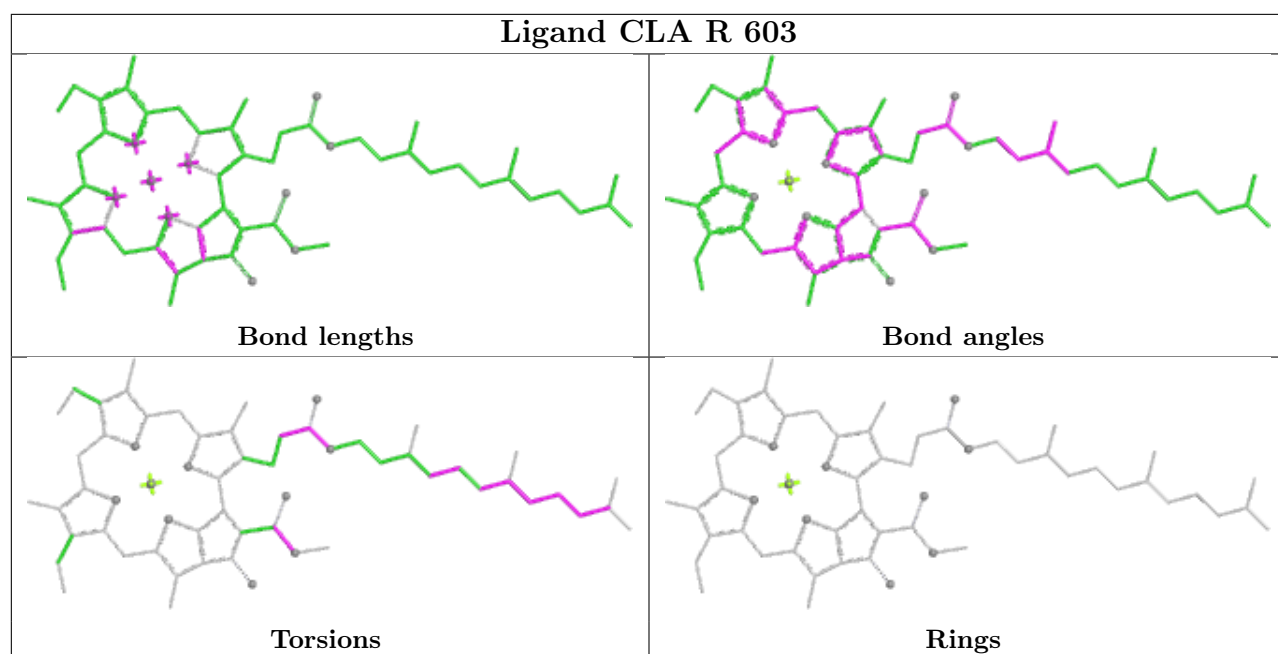


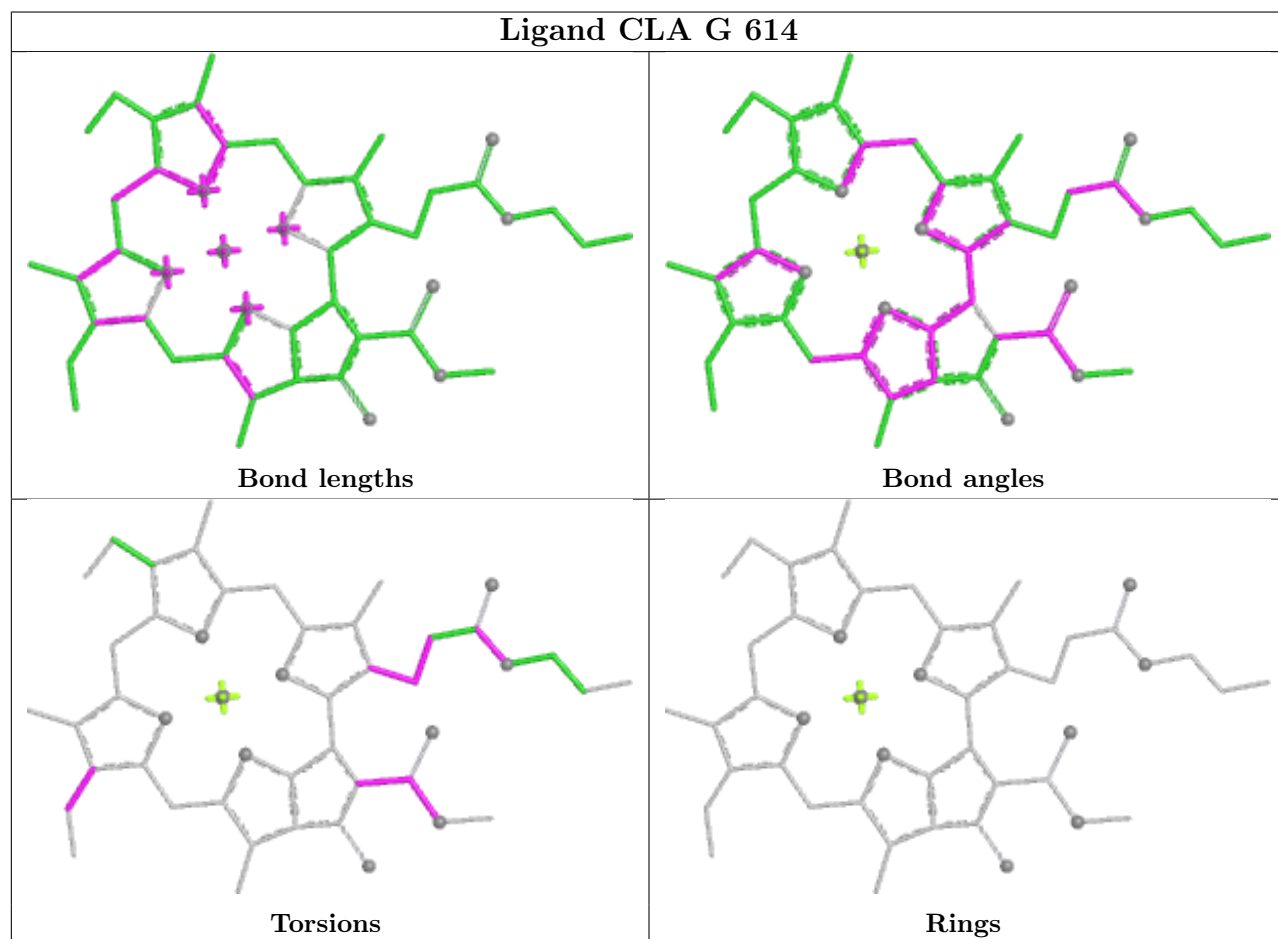
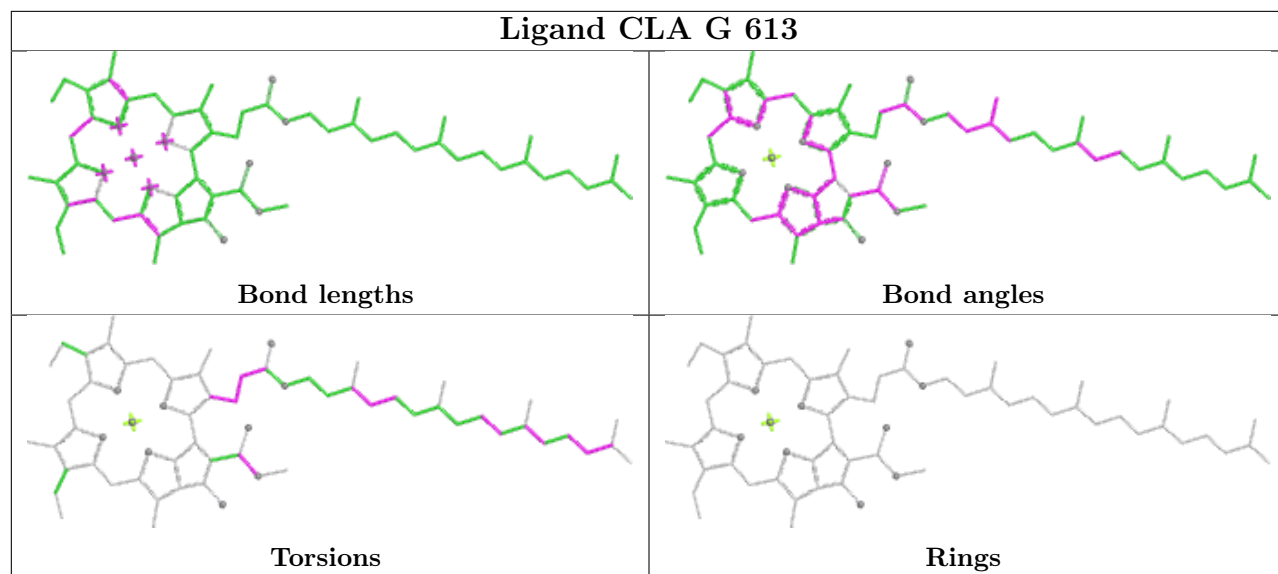


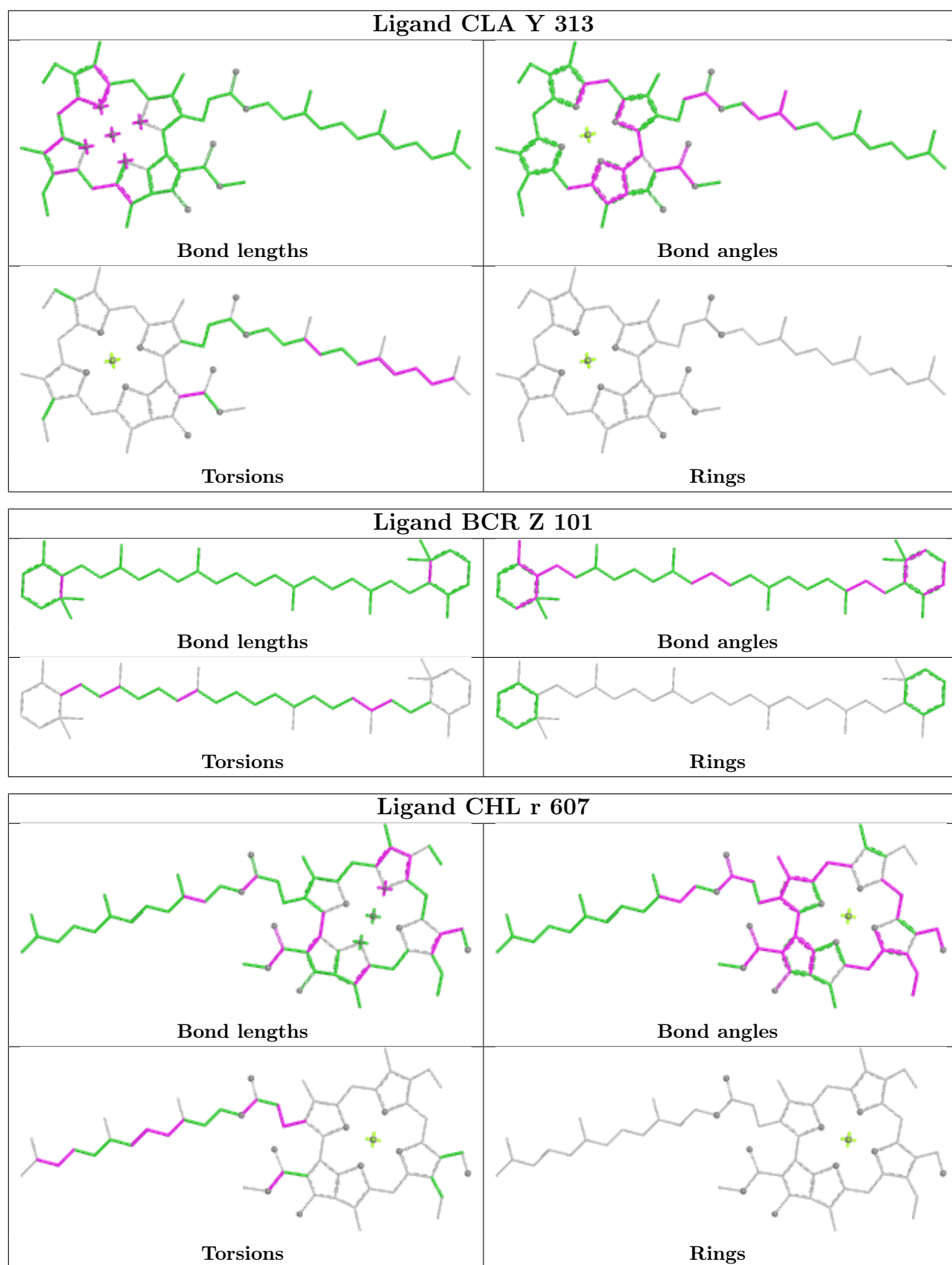


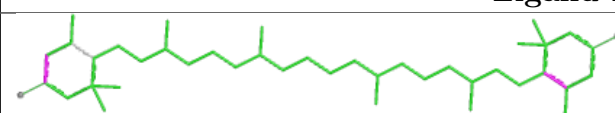
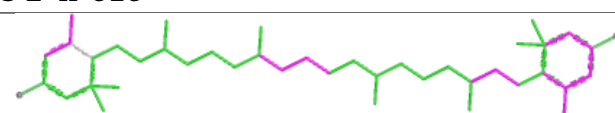
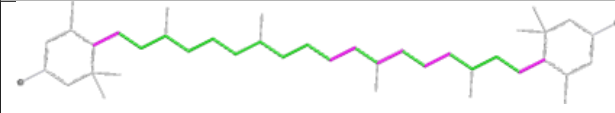
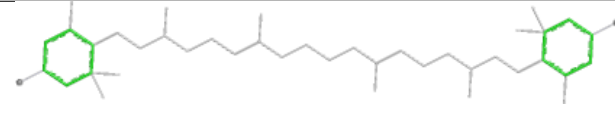


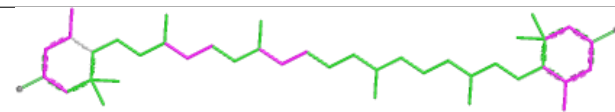
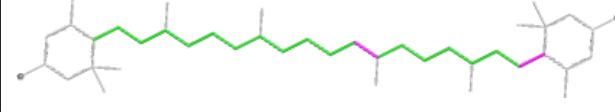
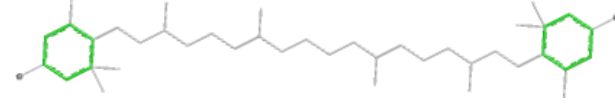


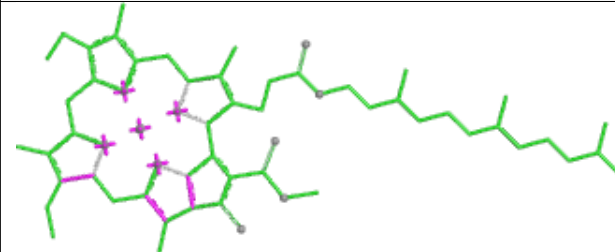
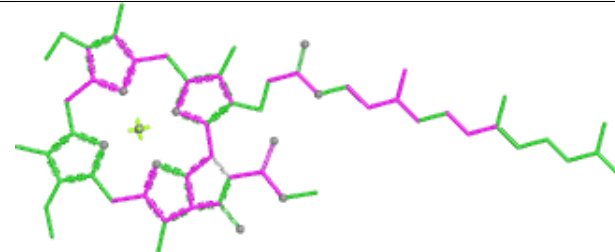
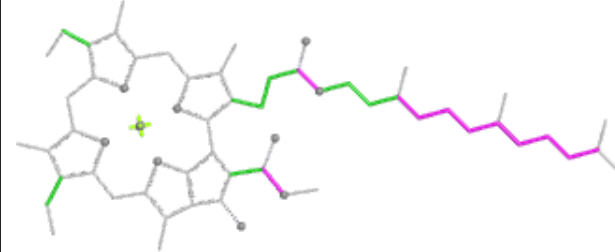
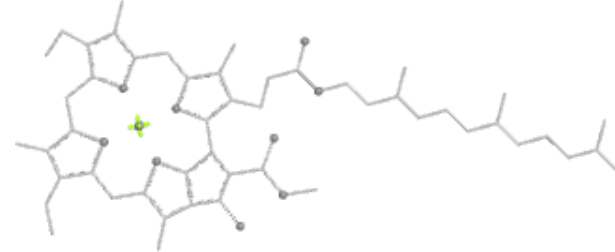


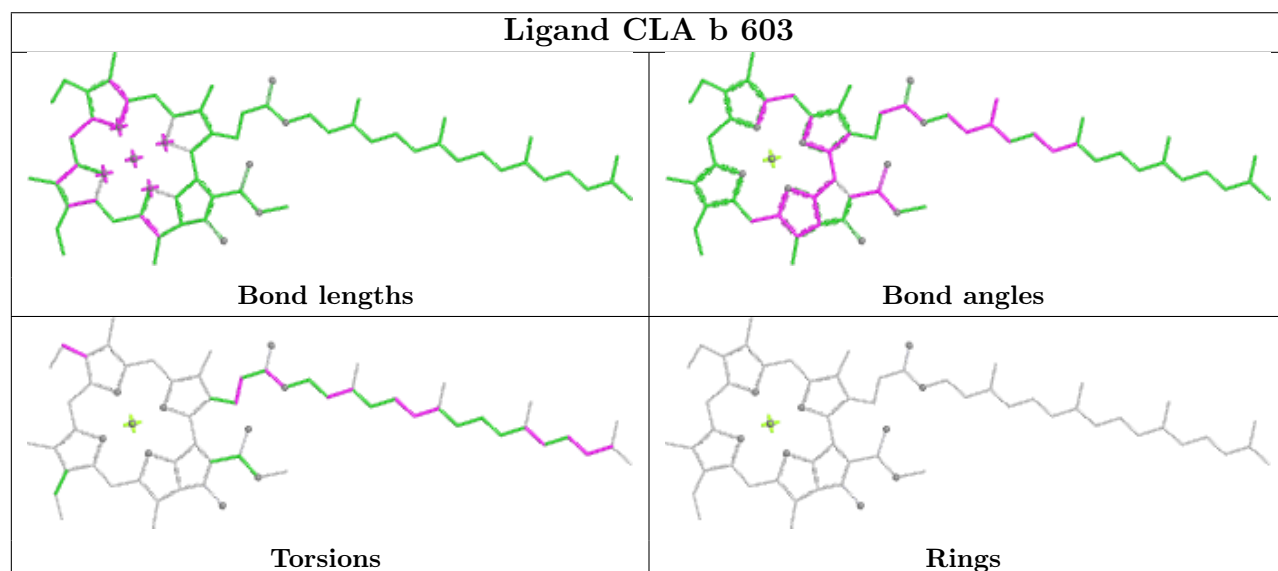
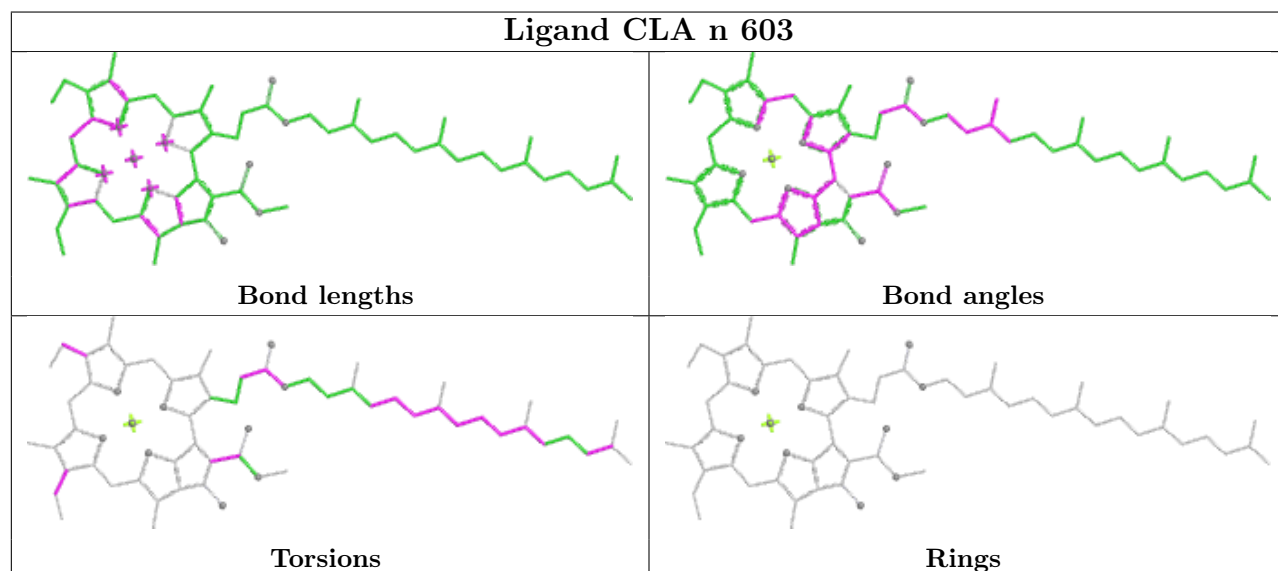
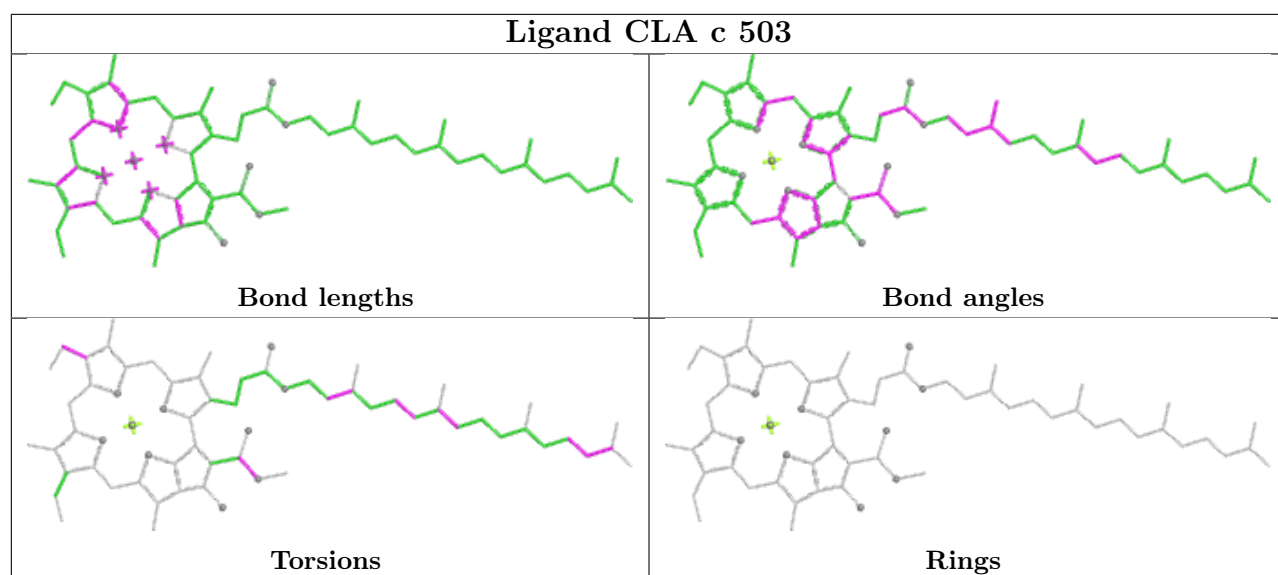


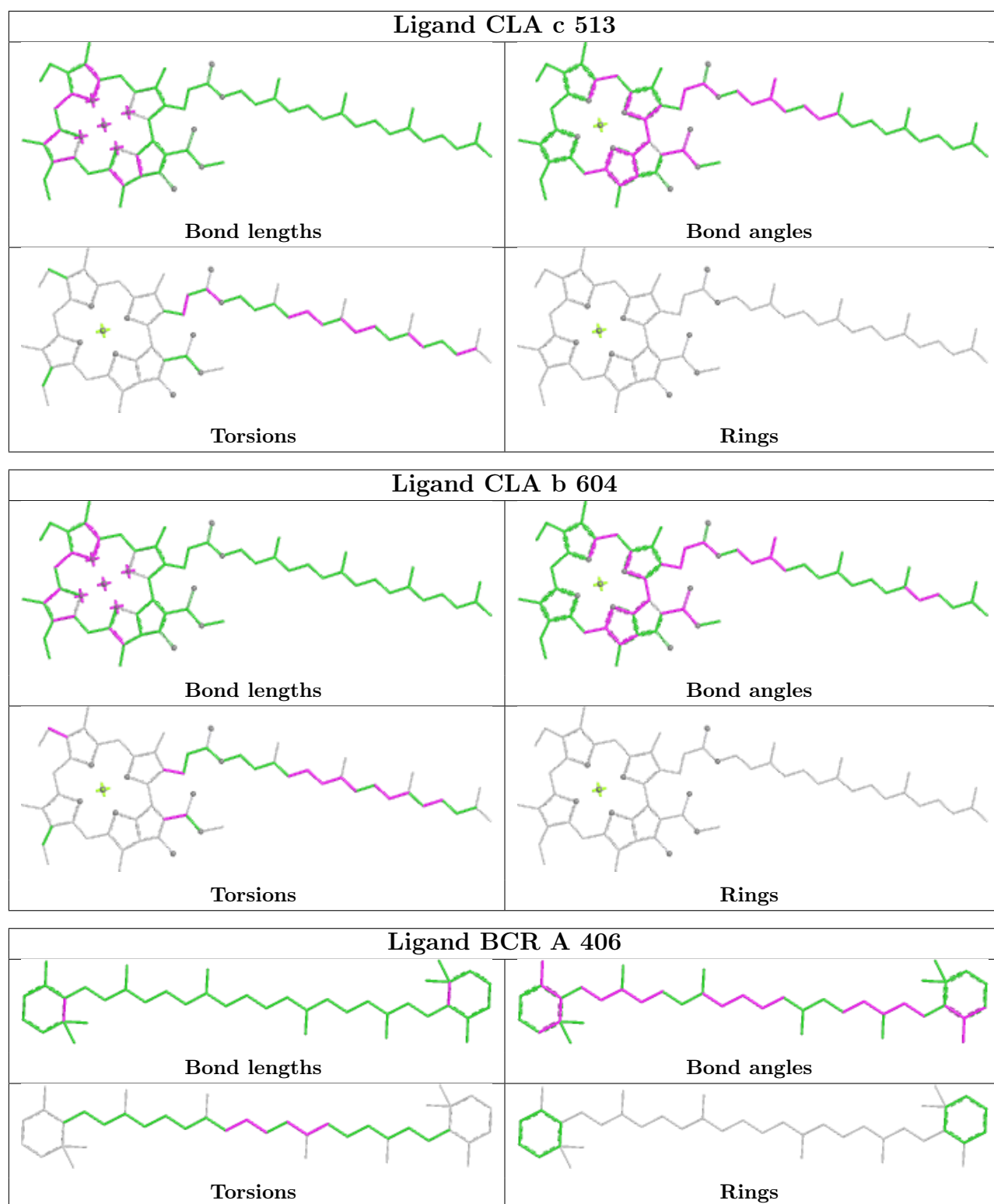


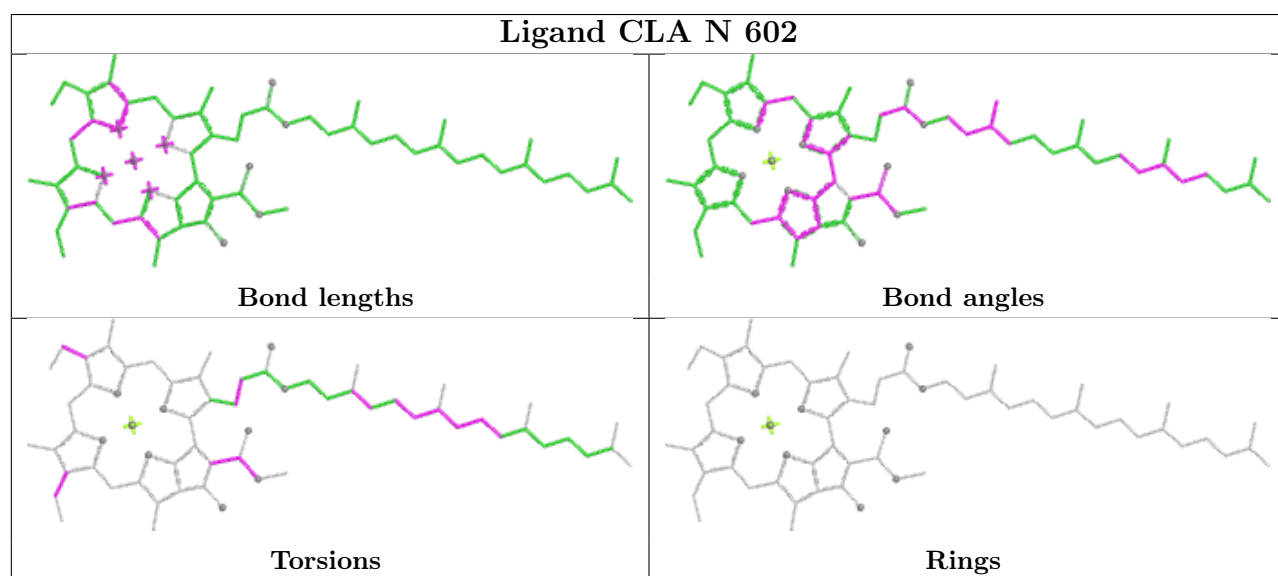
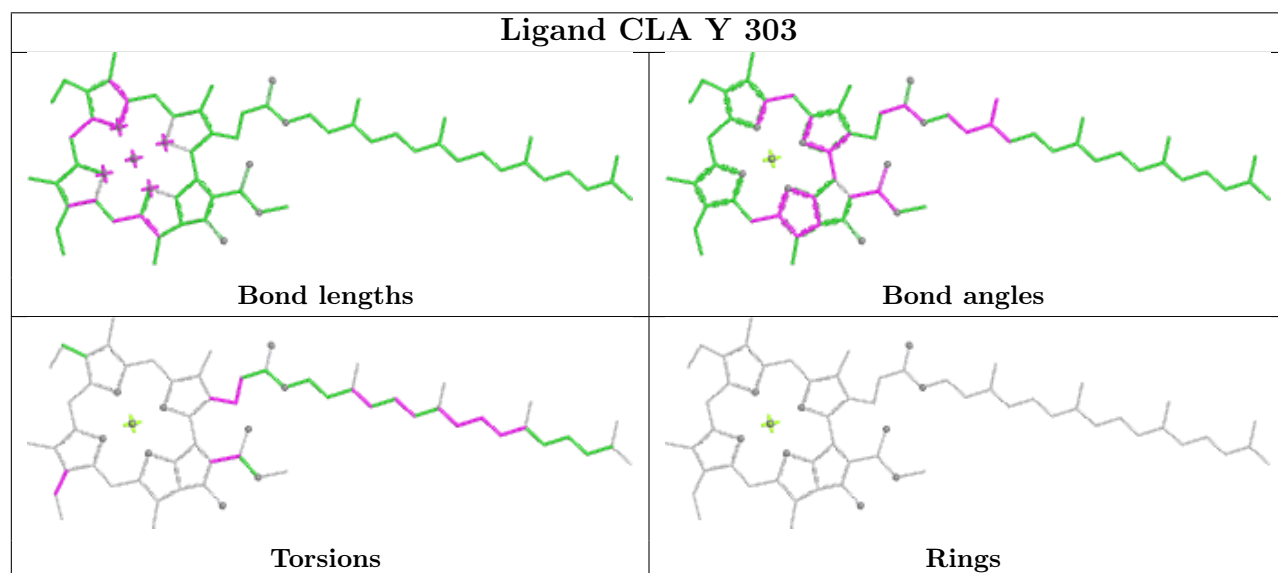
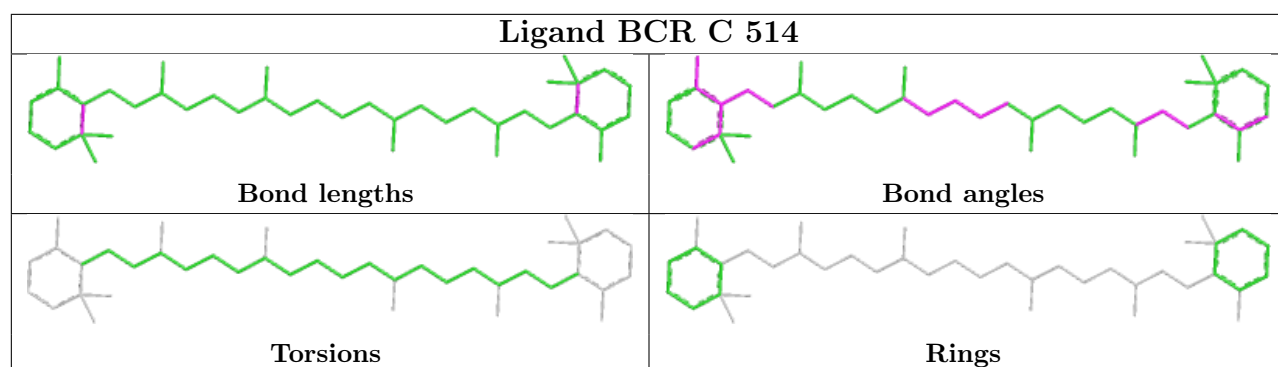
Ligand LUT n 615	
	Bond lengths
	Bond angles
	Torsions
	Rings

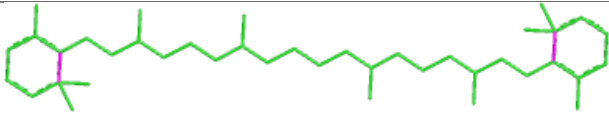
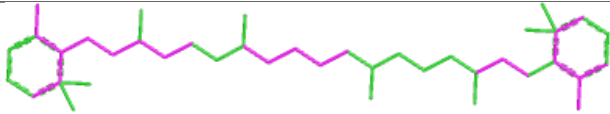
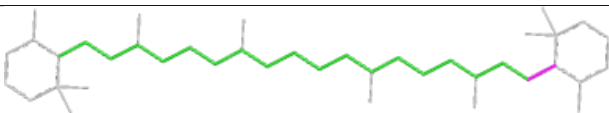
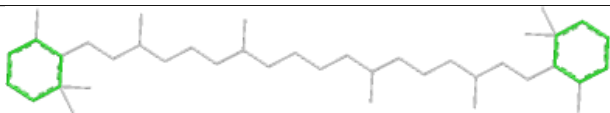
Ligand LUT r 615	
	Bond lengths
	Bond angles
	Torsions
	Rings

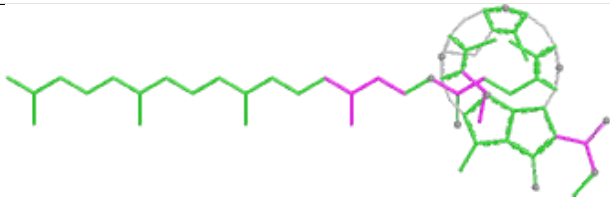
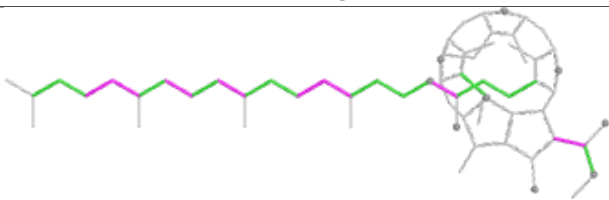
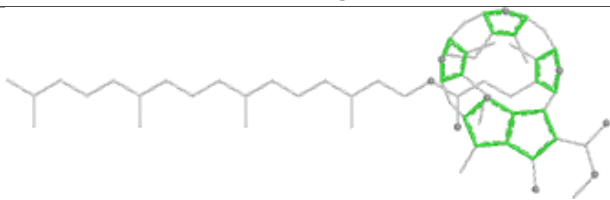
Ligand CLA C 504	
	Bond lengths
	Bond angles
	Torsions
	Rings

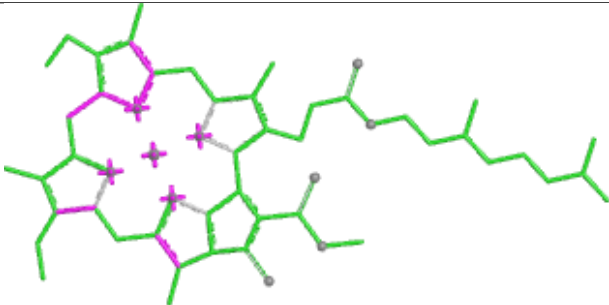
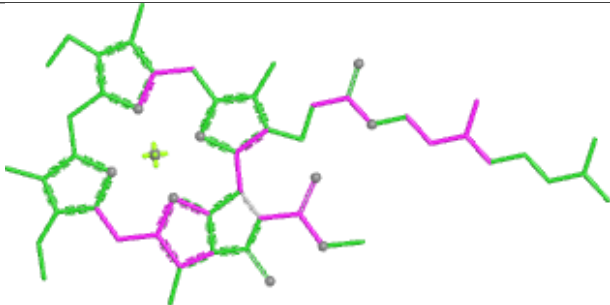
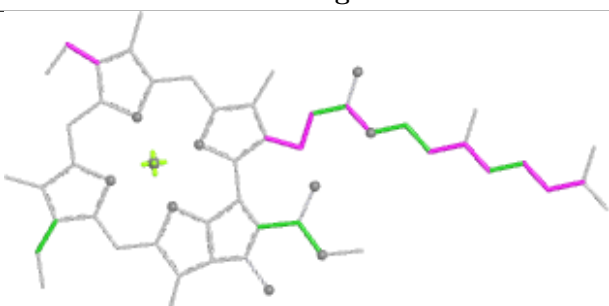
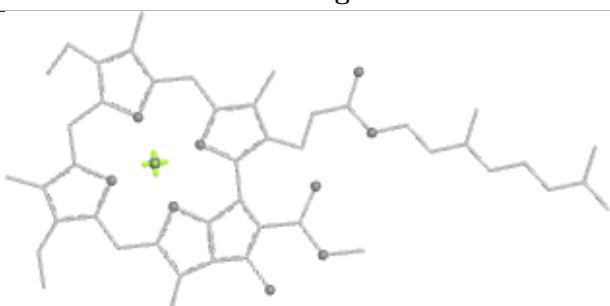


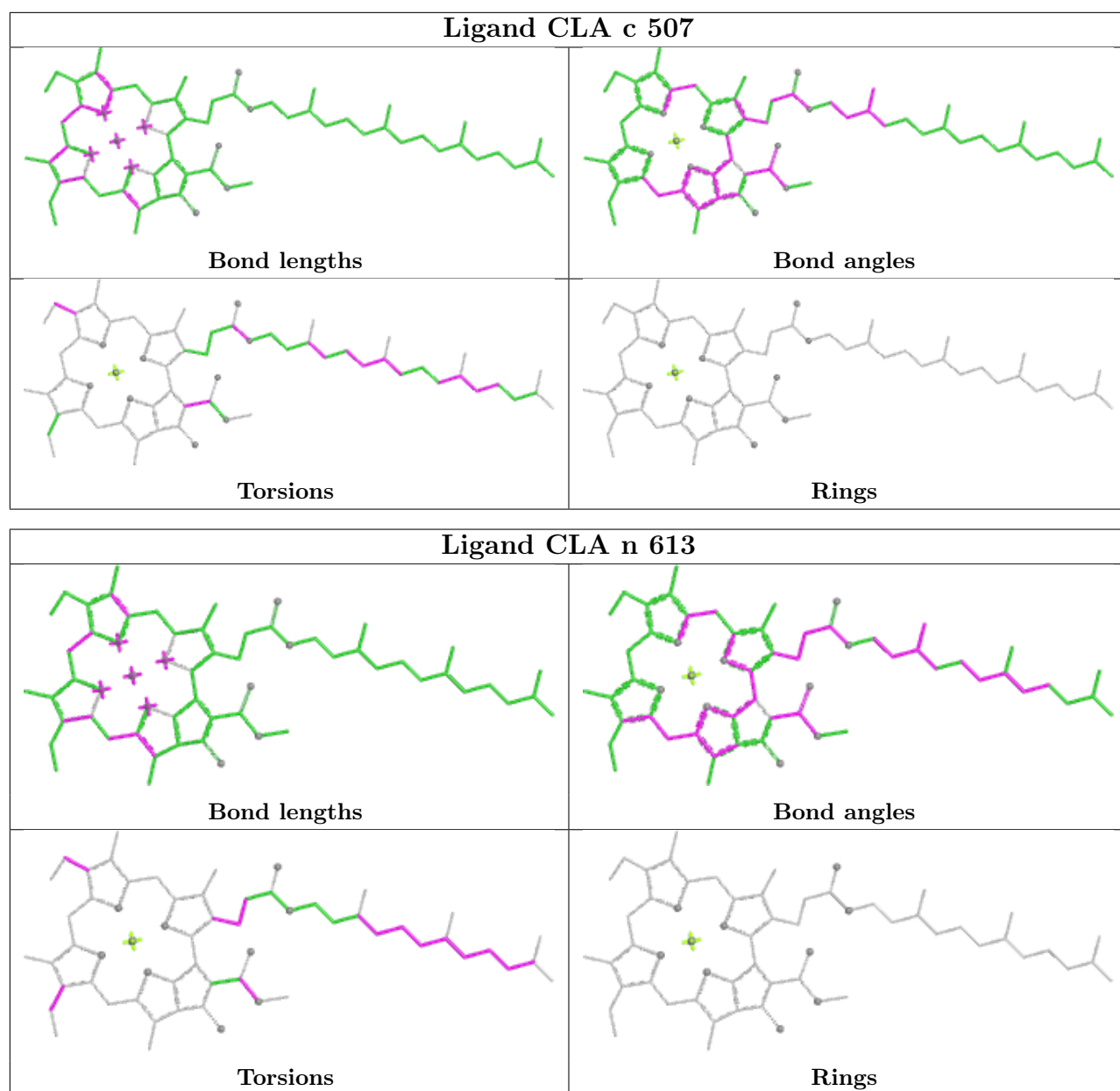




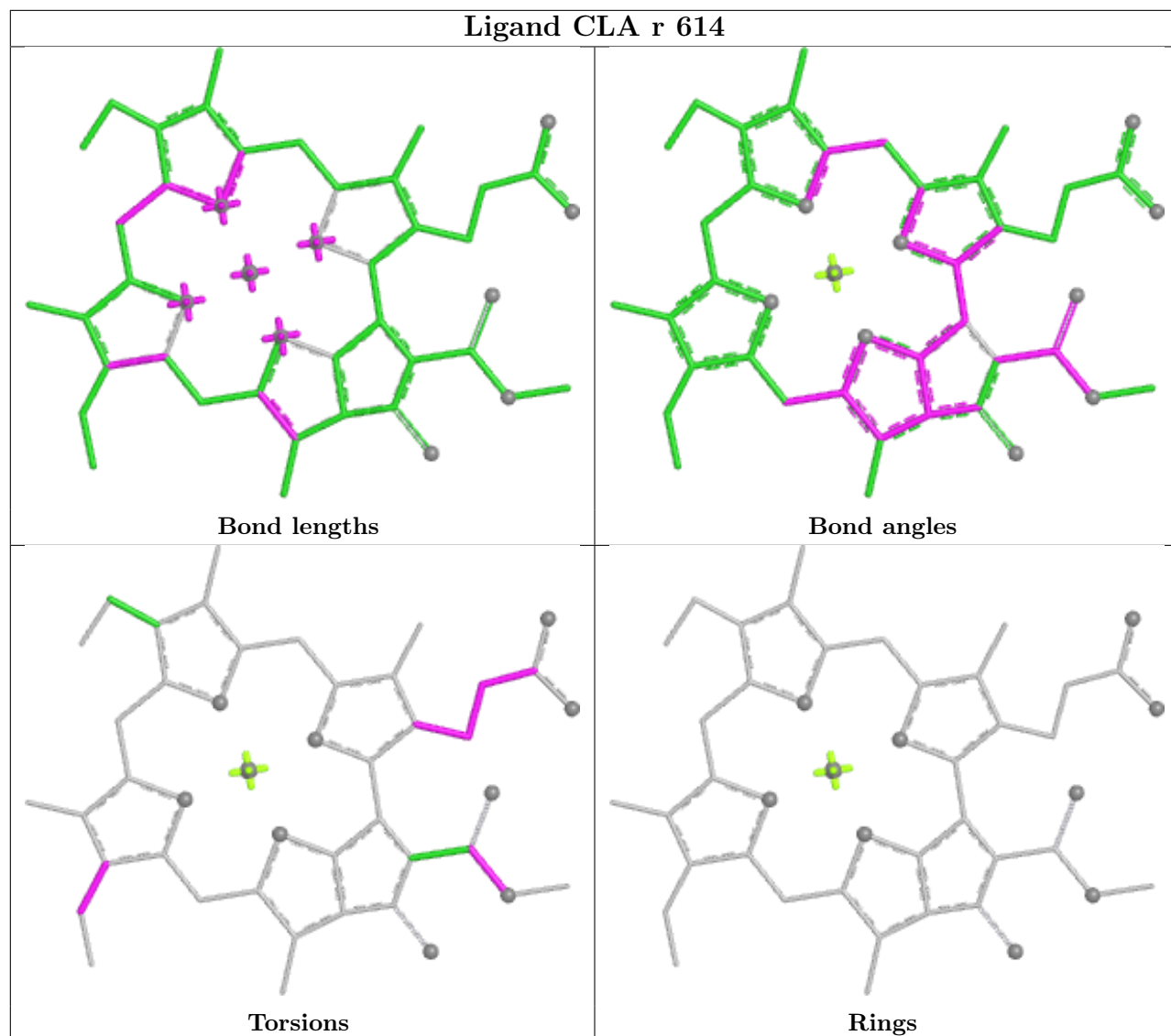
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

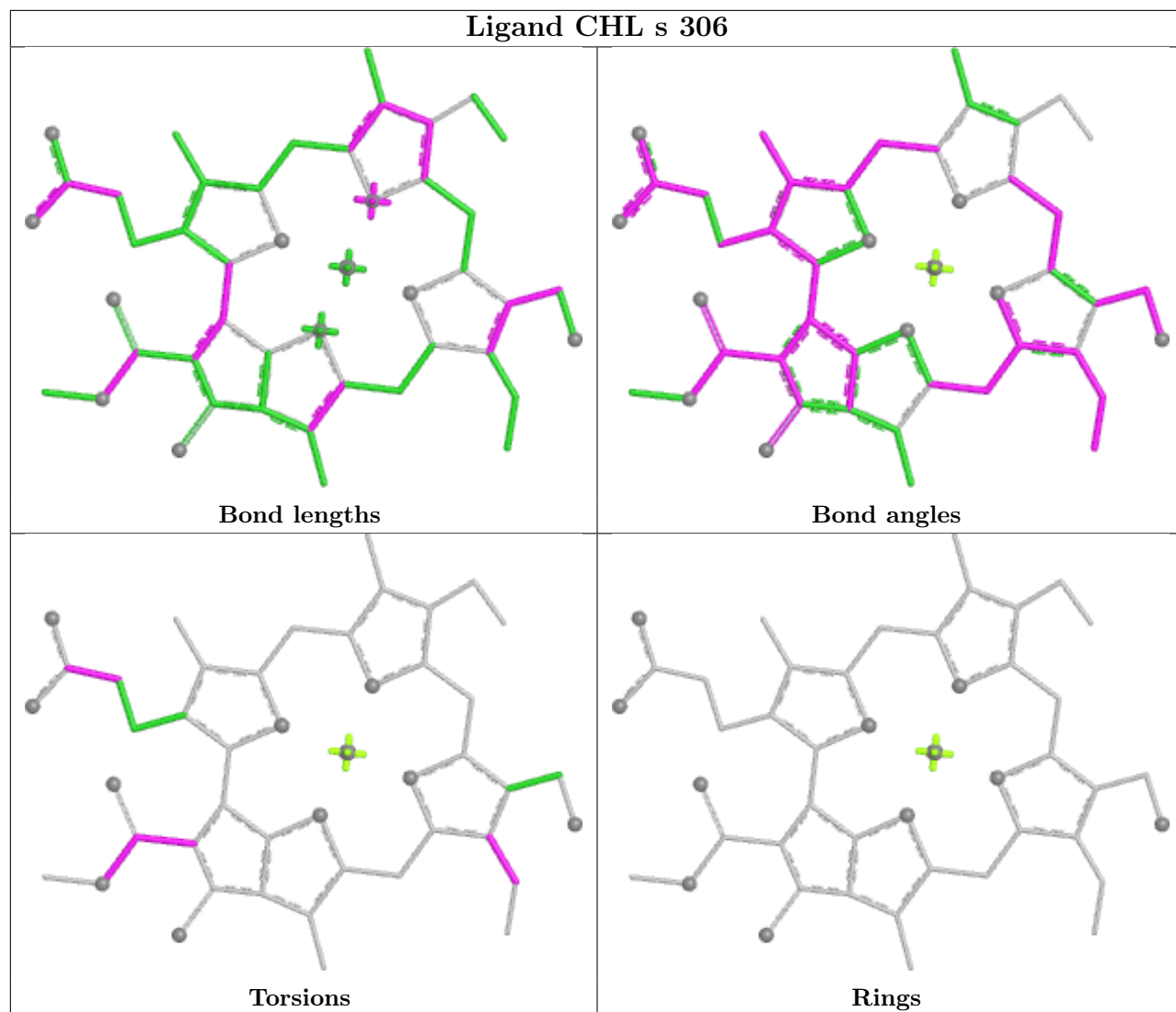
Ligand CLA S 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

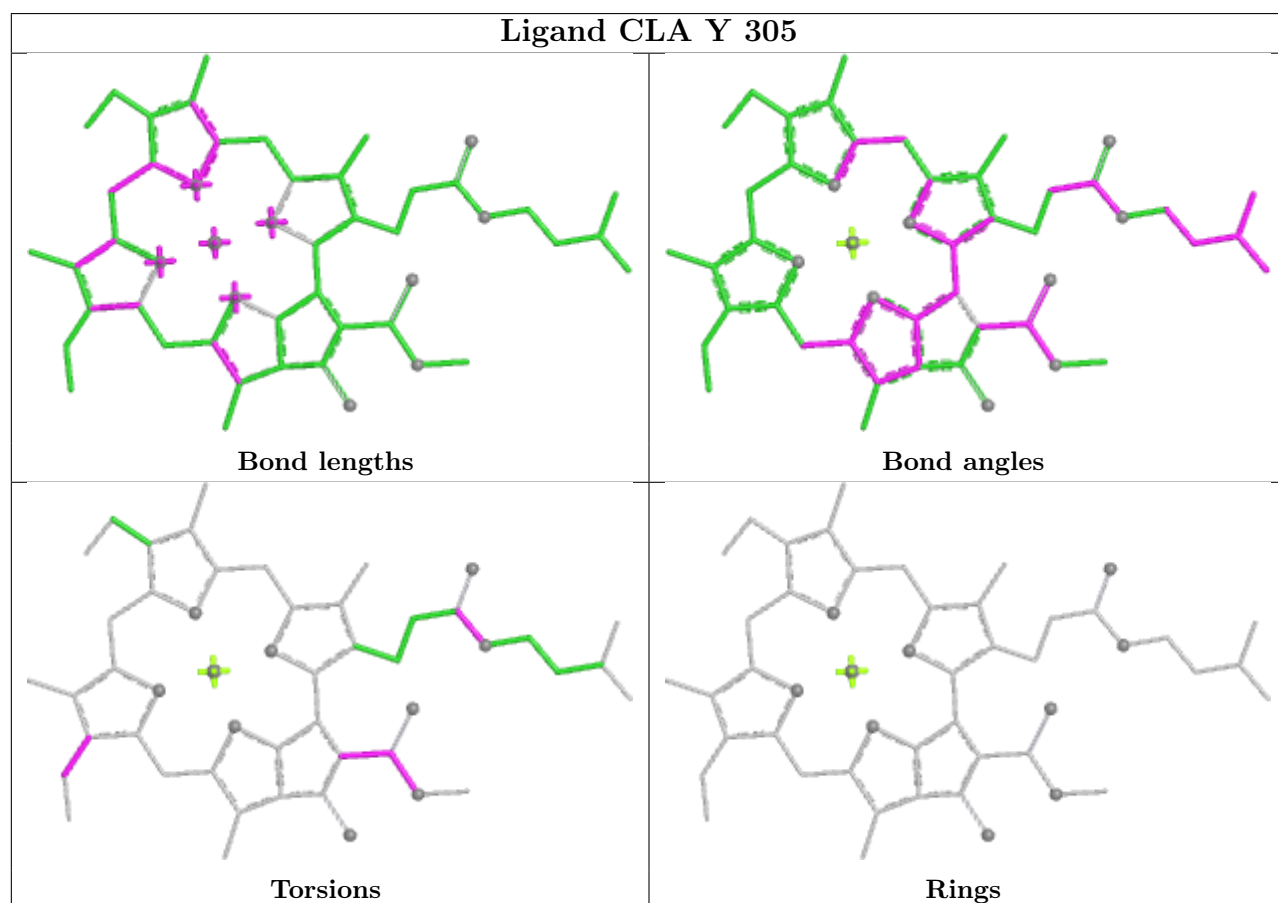
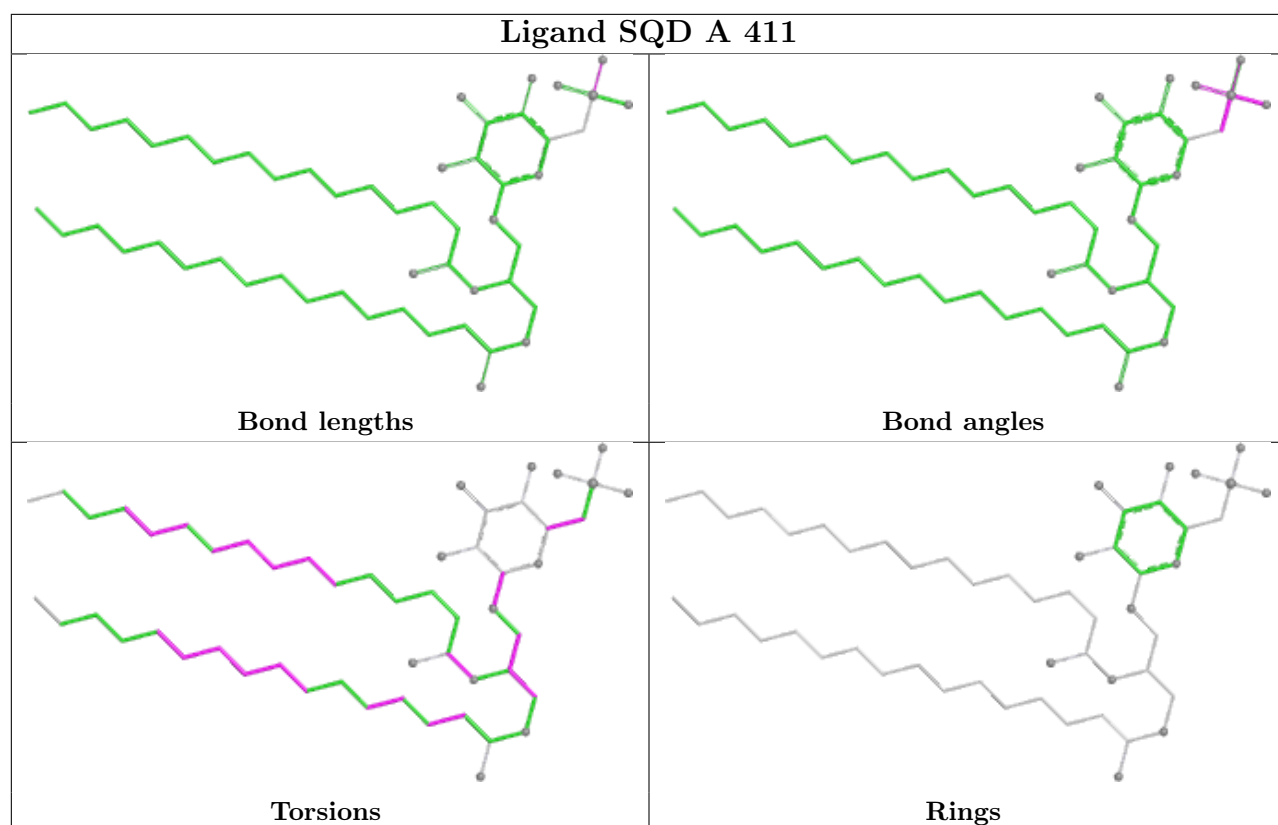


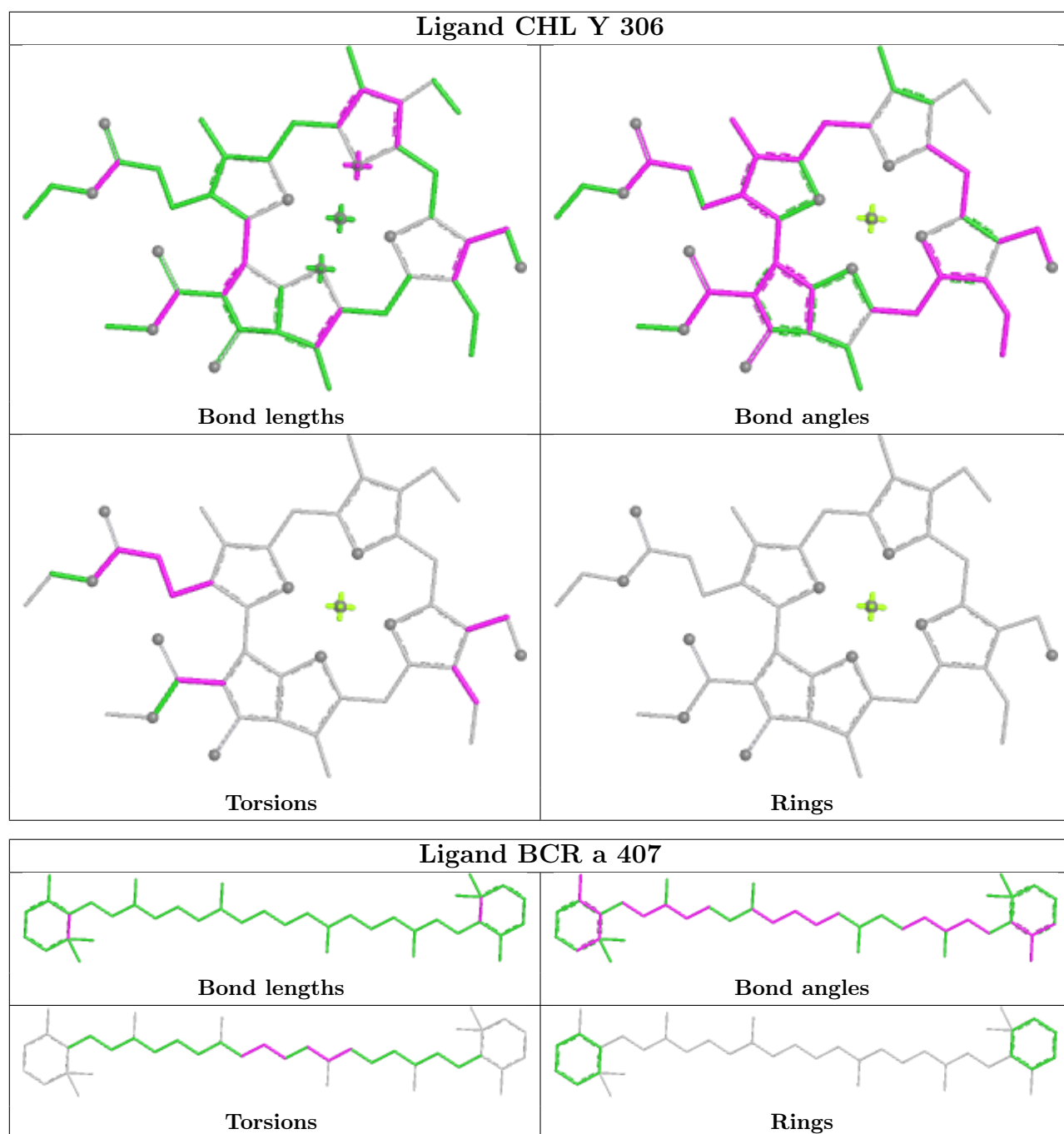
Ligand CLA r 614

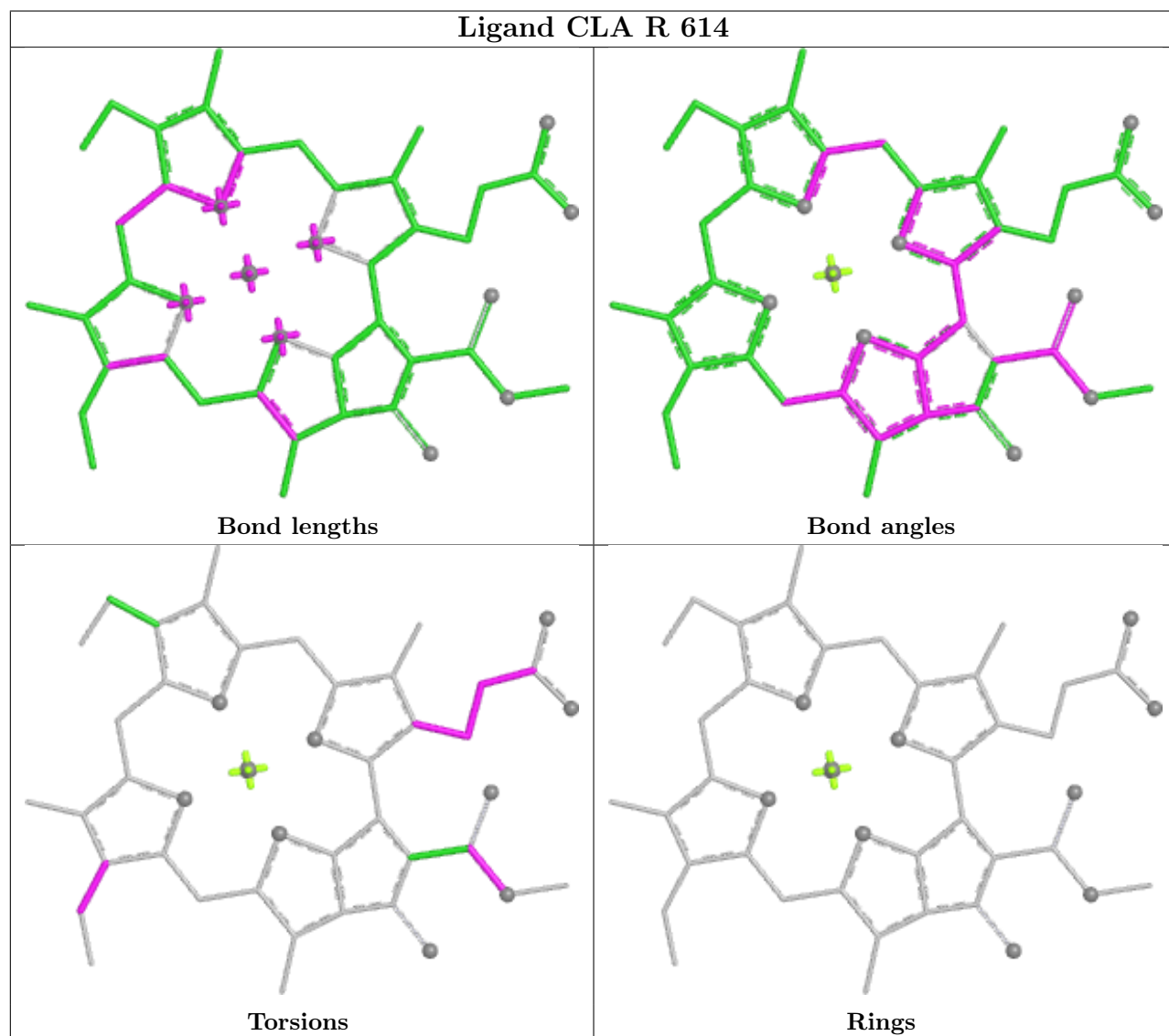
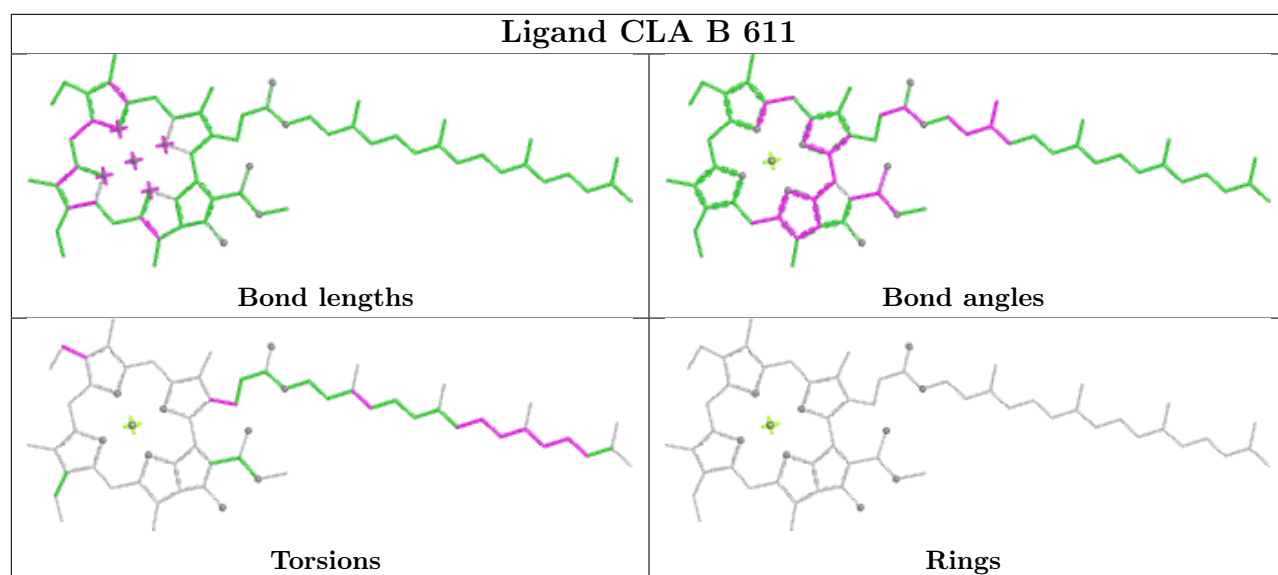


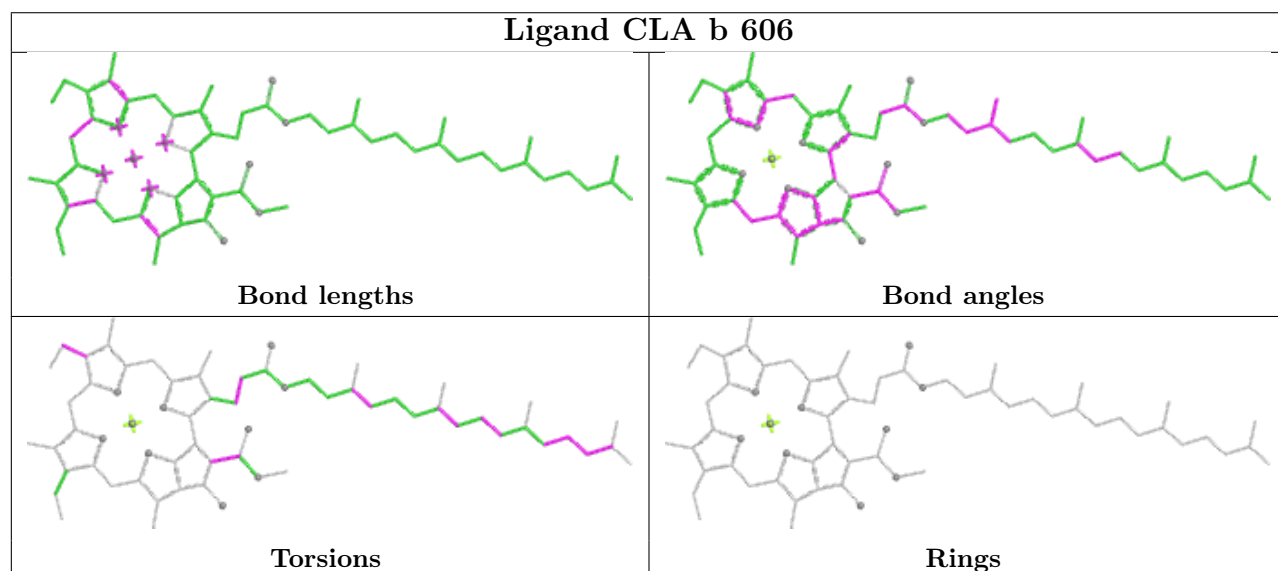
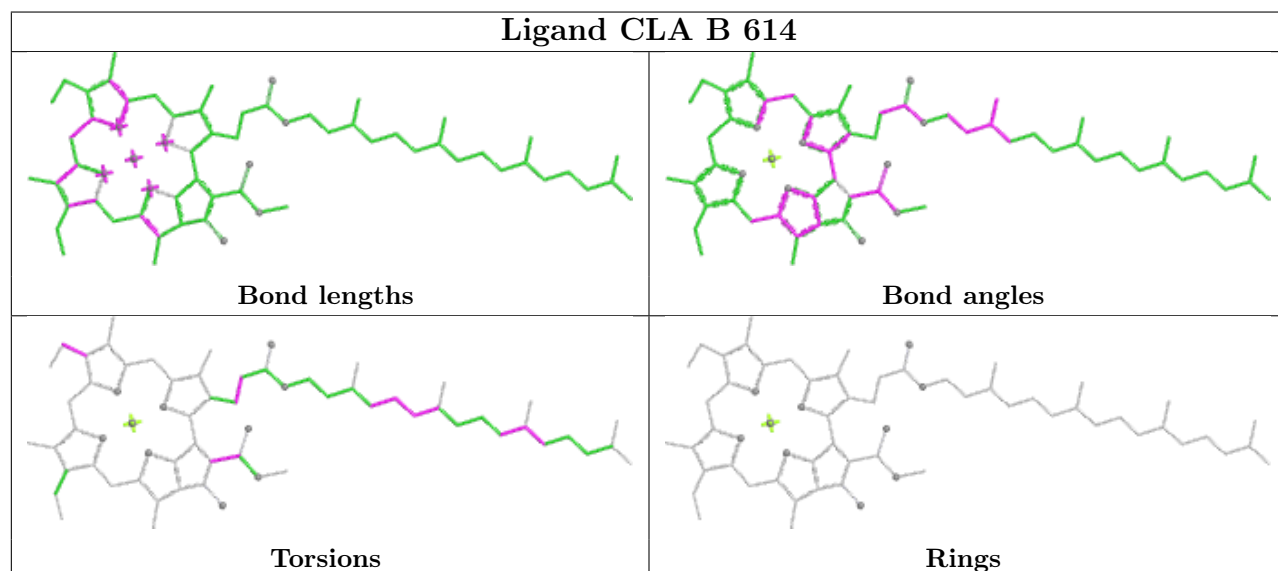
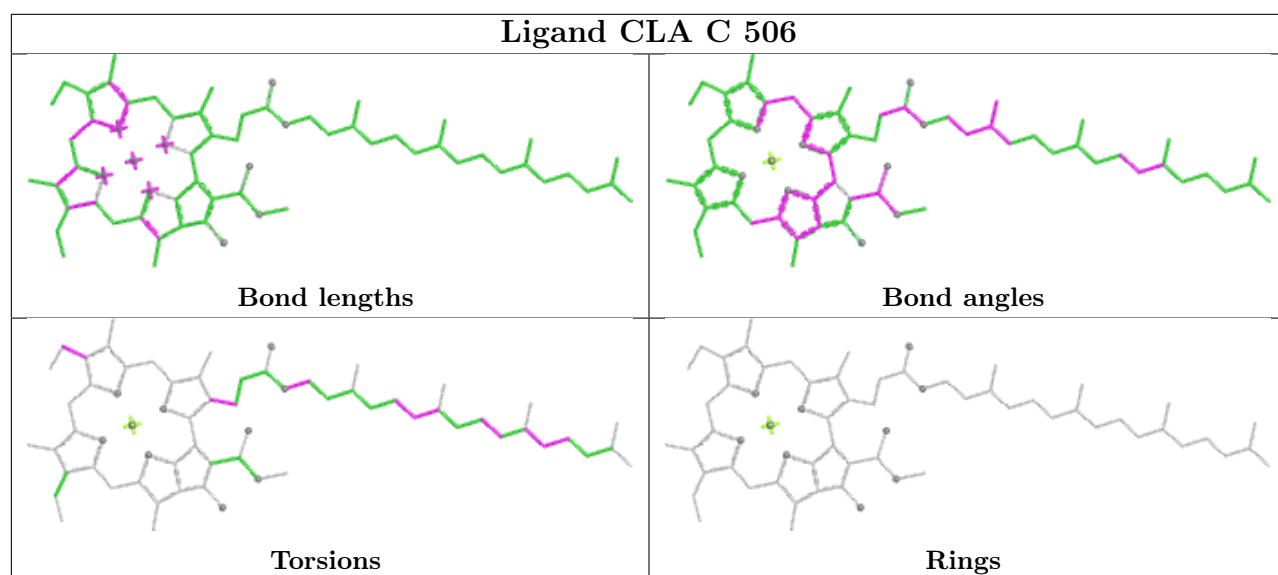
Ligand CHL s 306

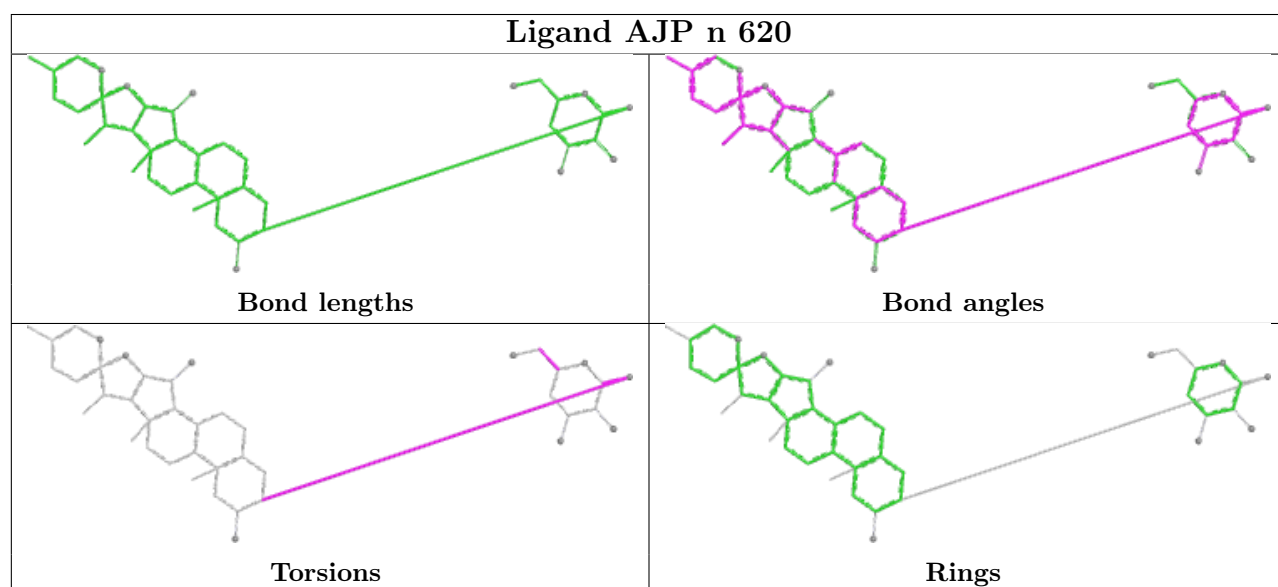
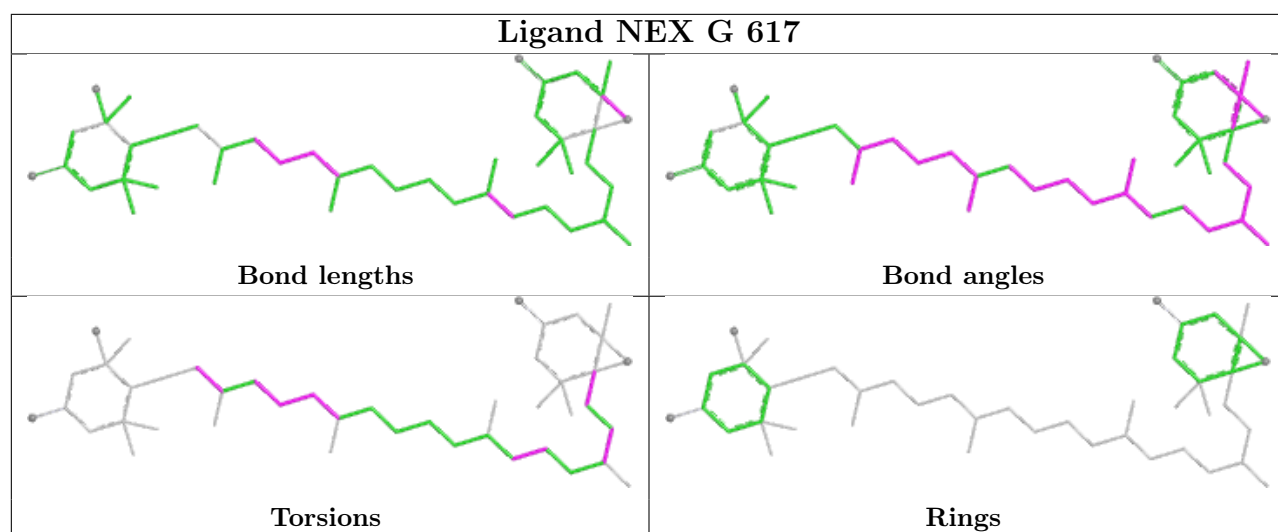


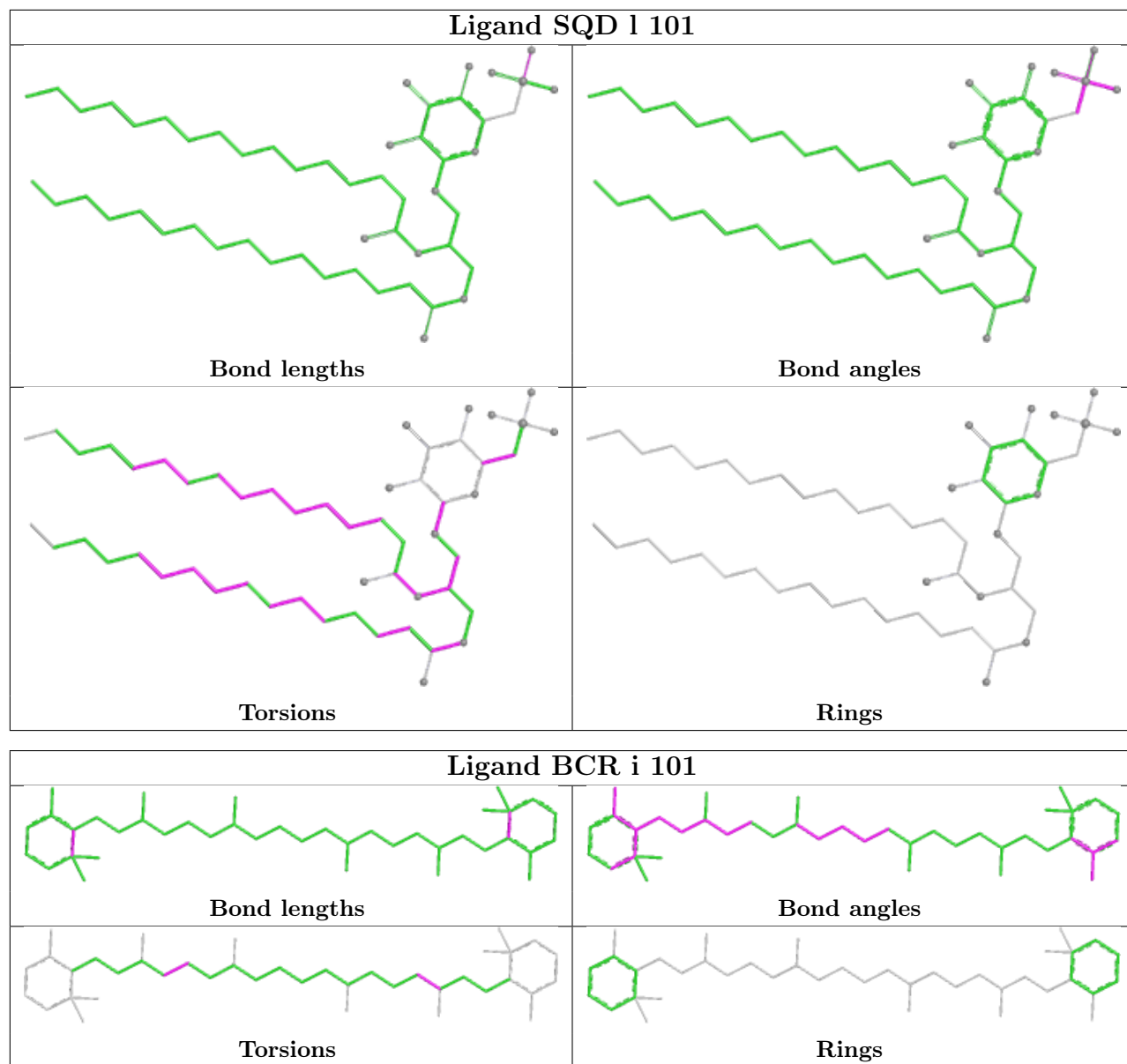




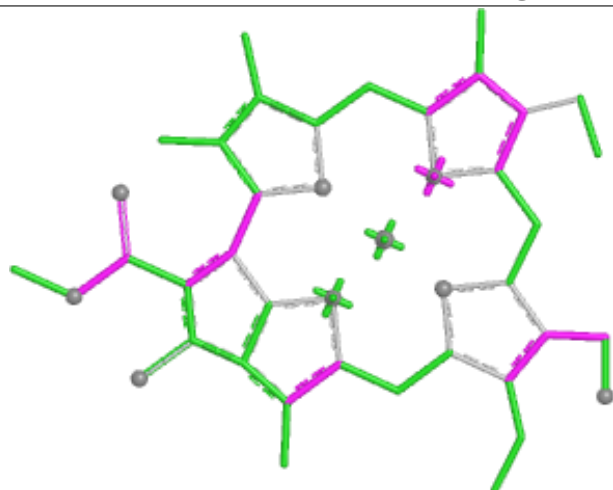




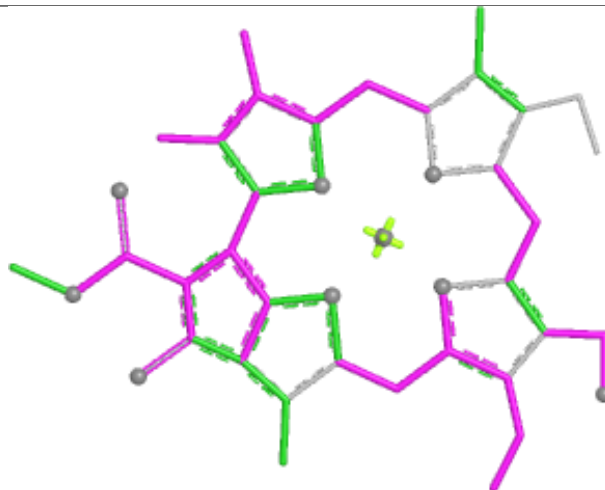




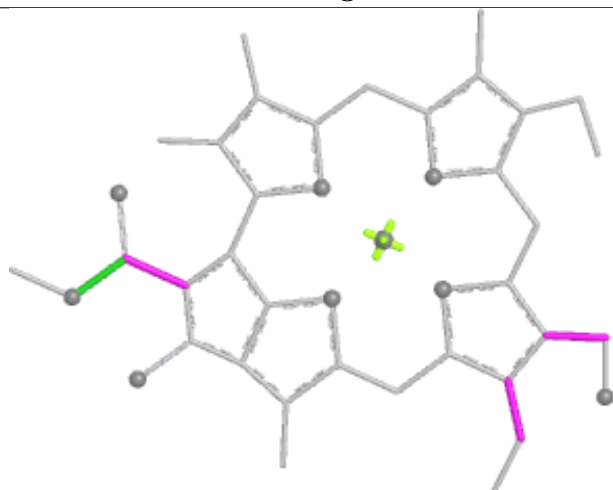
Ligand CHL R 613



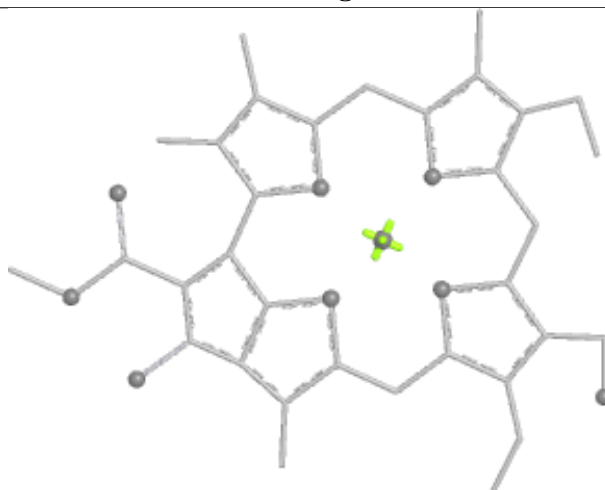
Bond lengths



Bond angles

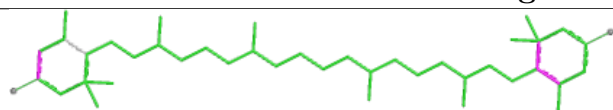


Torsions

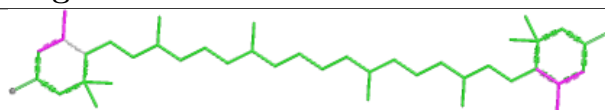


Rings

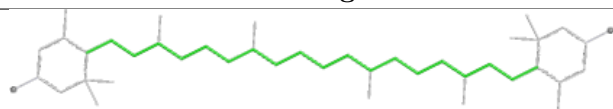
Ligand LUT g 616



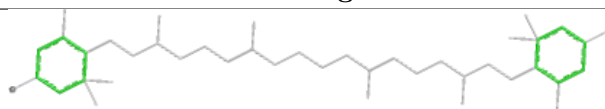
Bond lengths



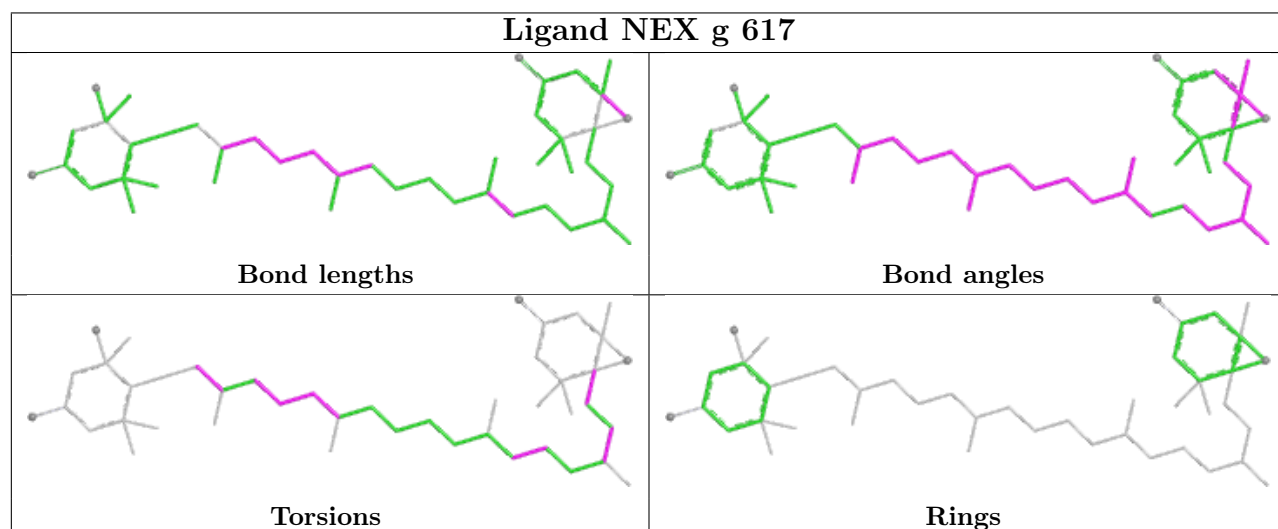
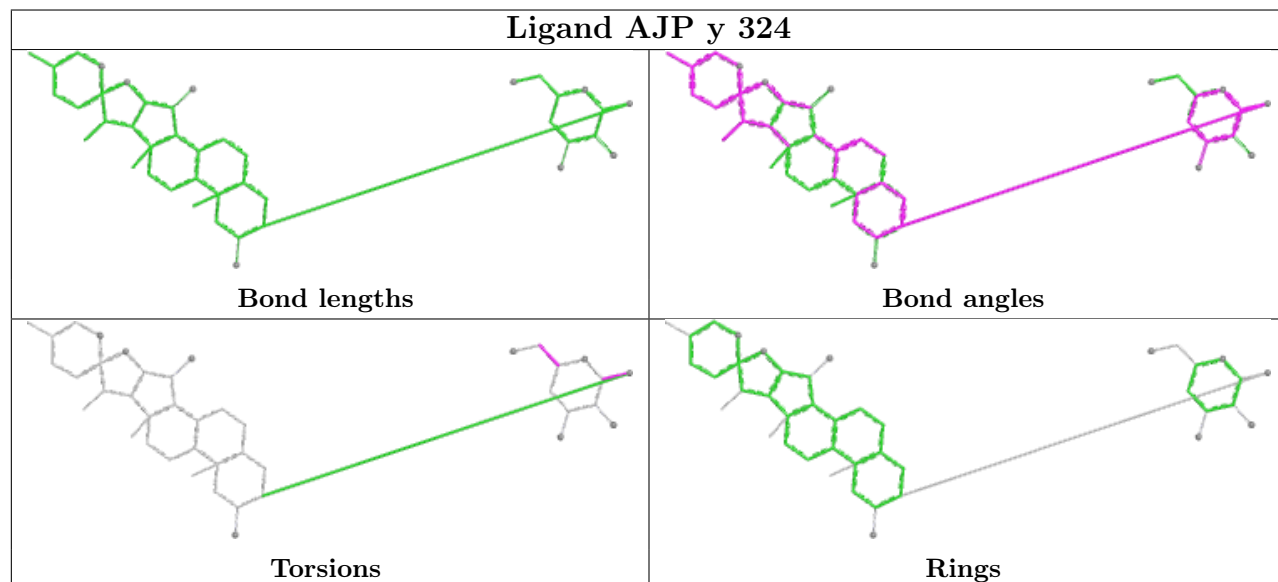
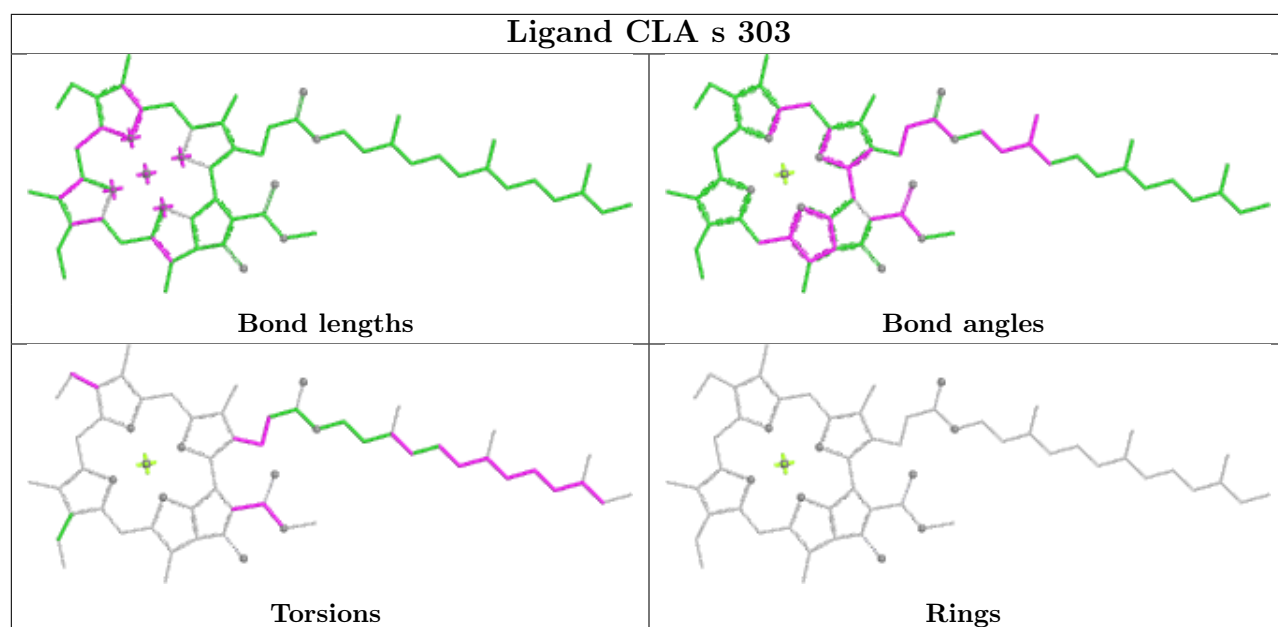
Bond angles

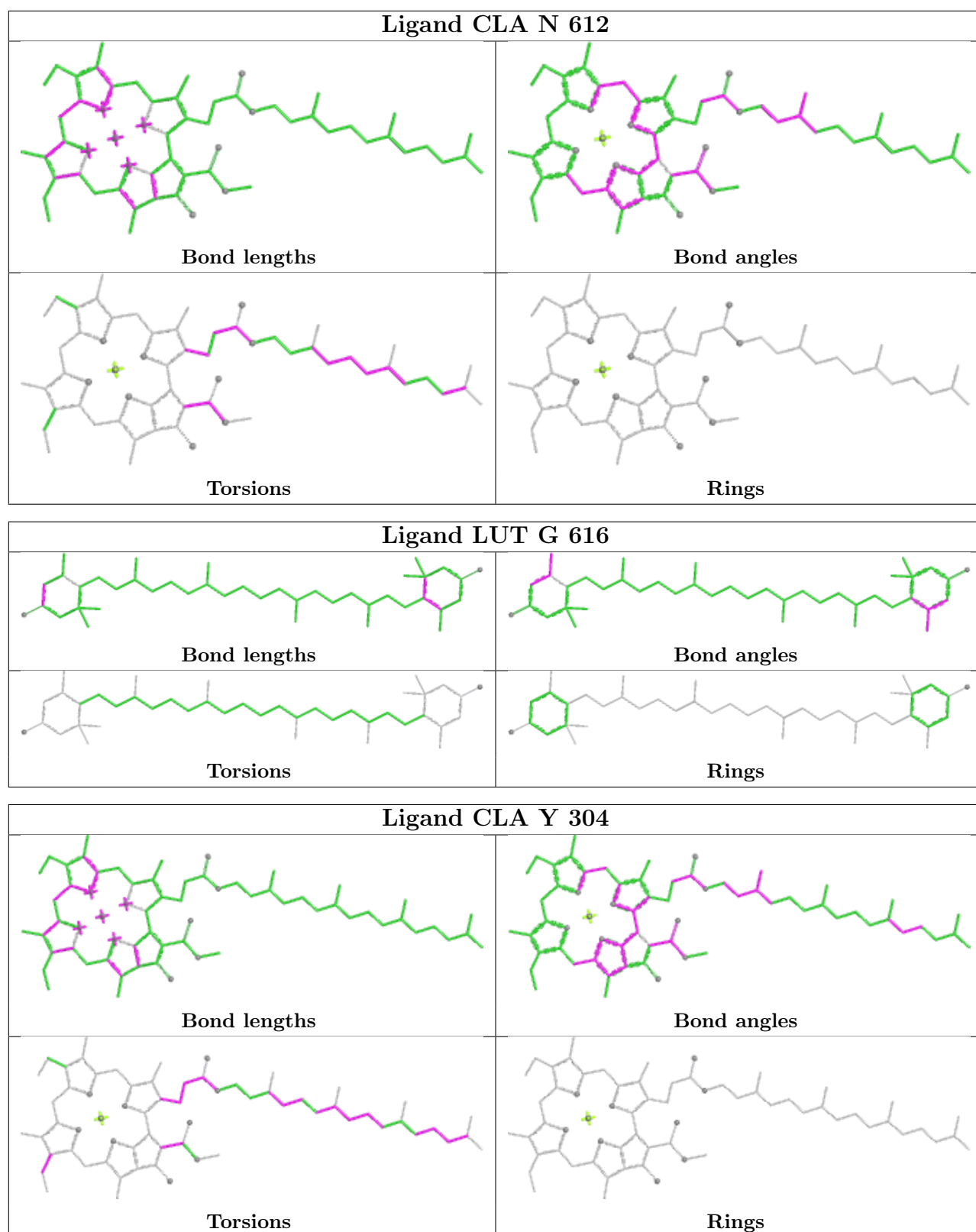


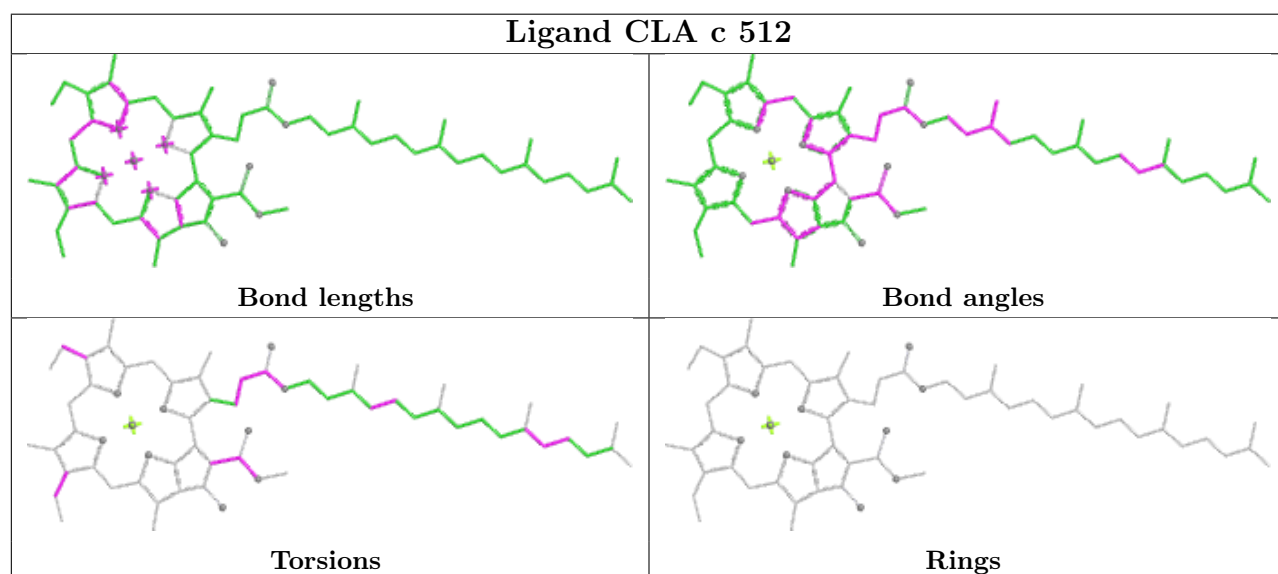
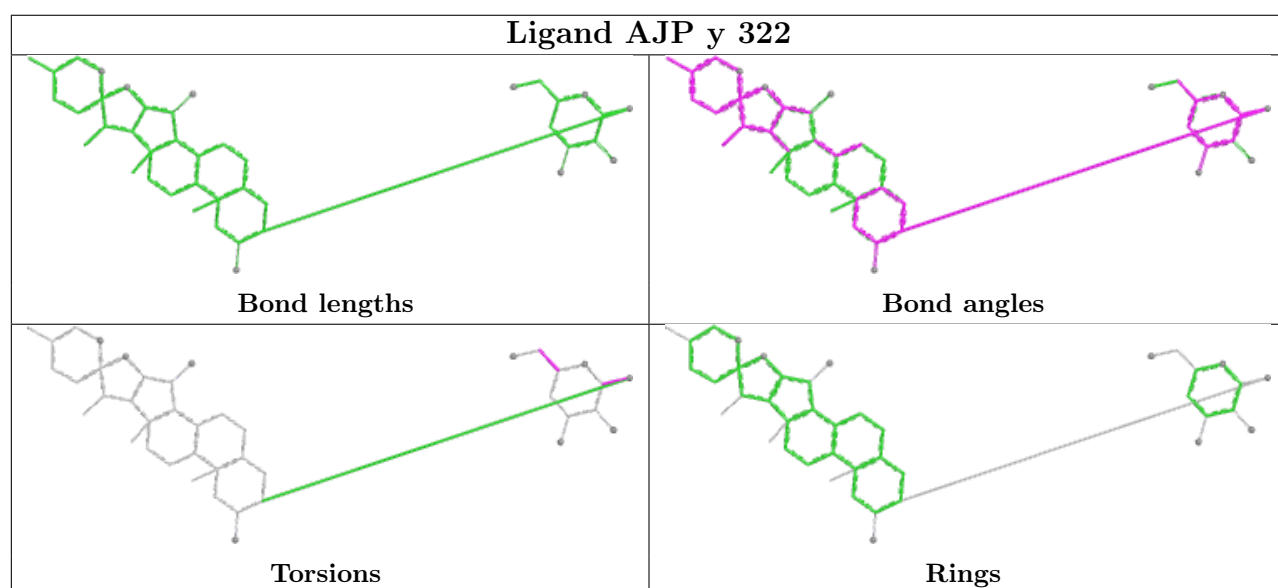
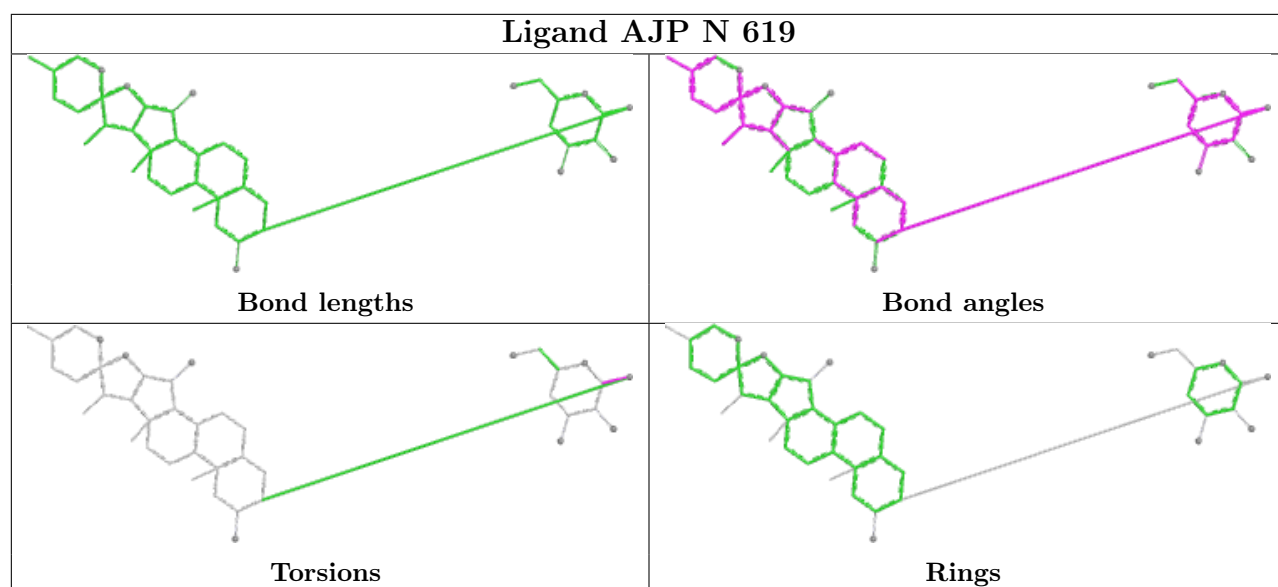
Torsions

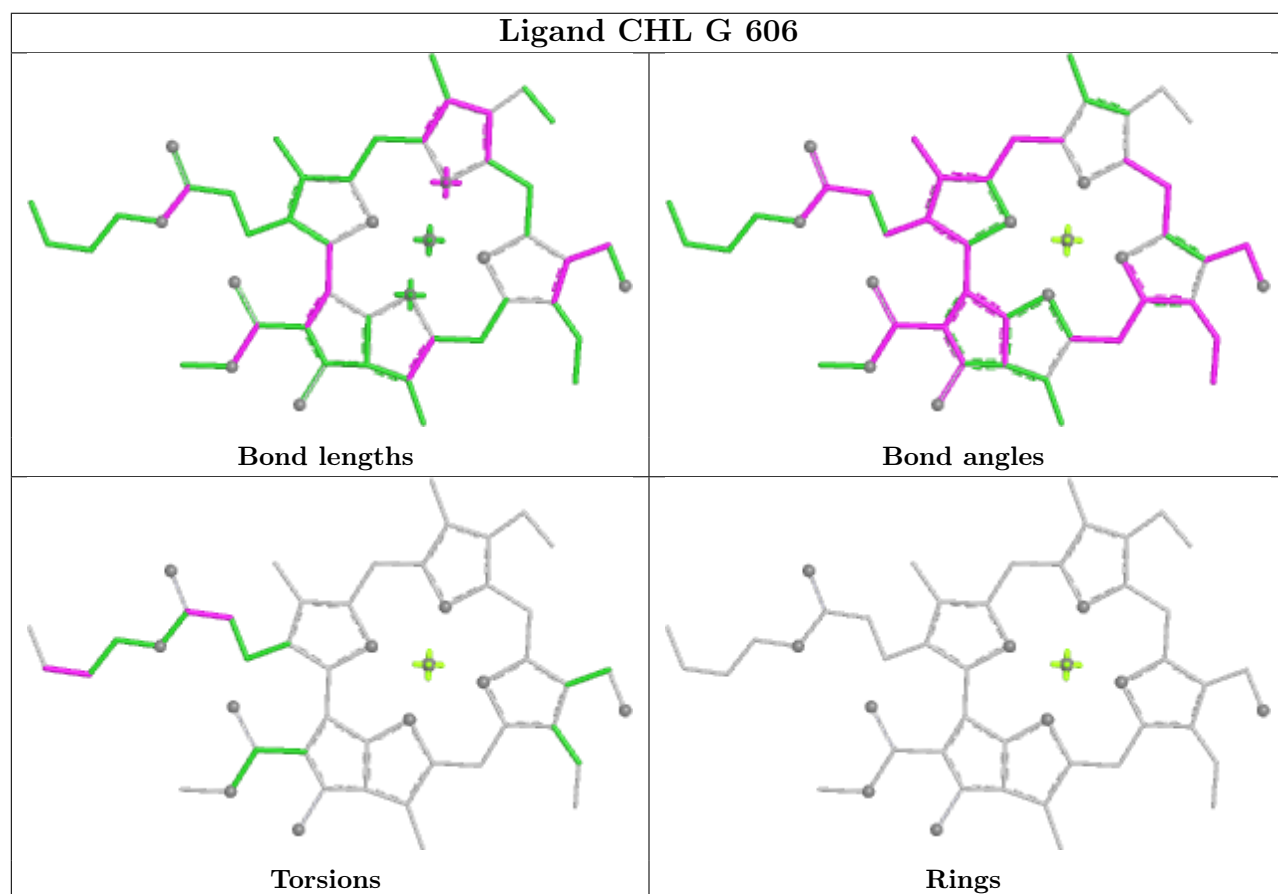
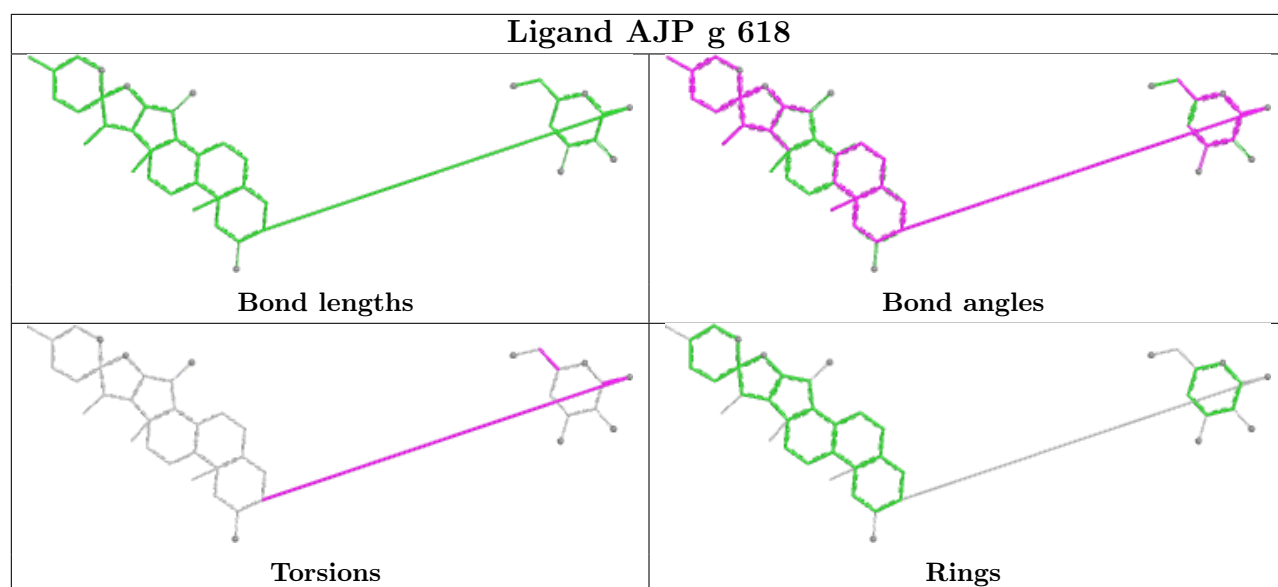


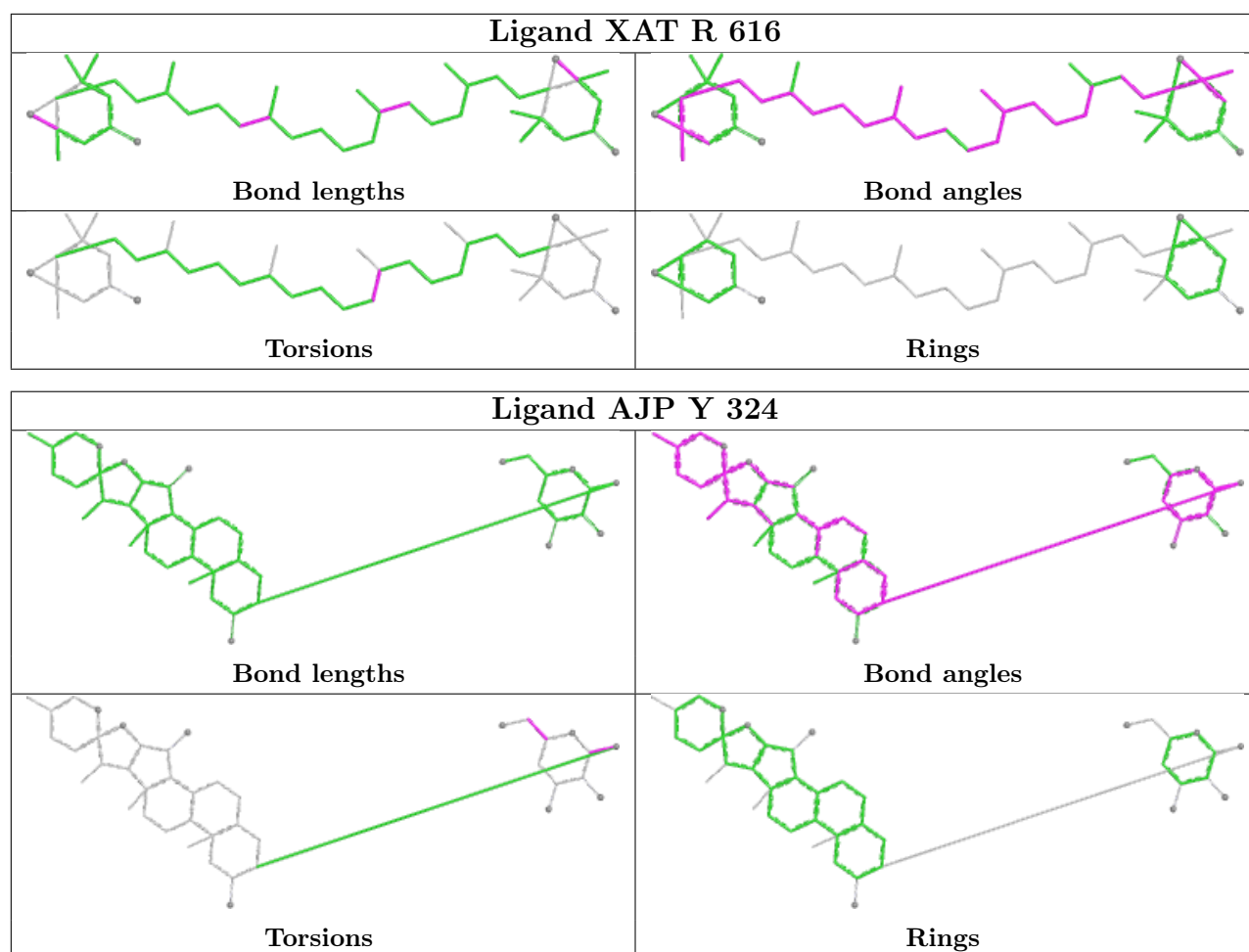
Rings



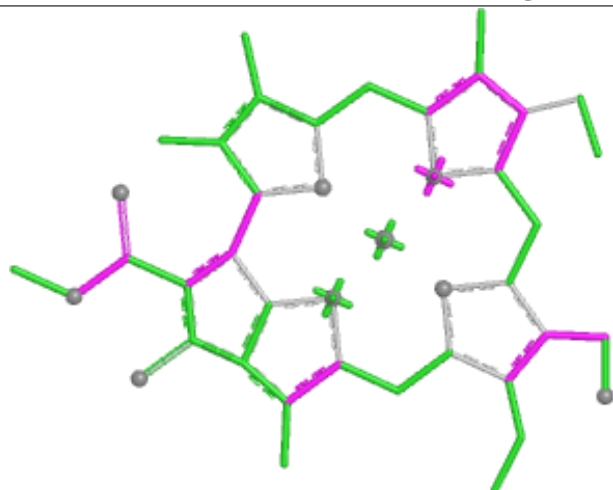




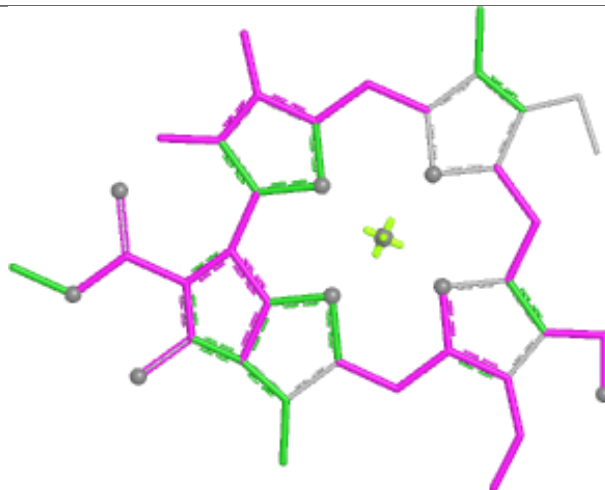




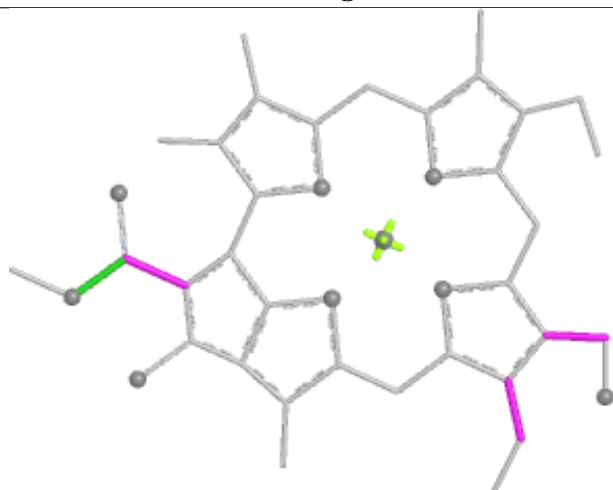
Ligand CHL r 613



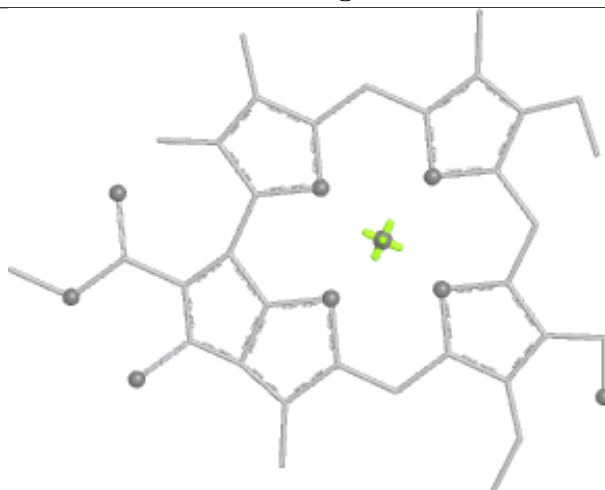
Bond lengths



Bond angles

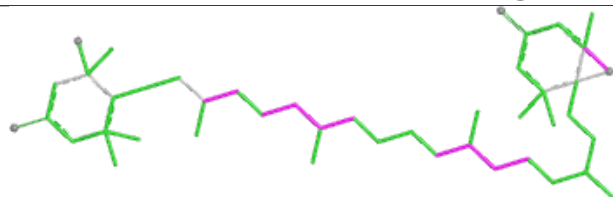


Torsions

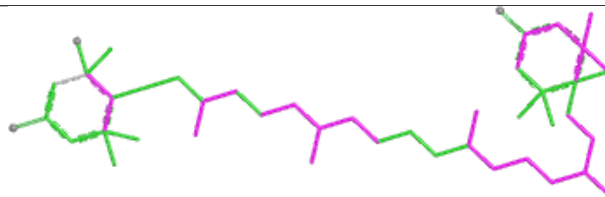


Rings

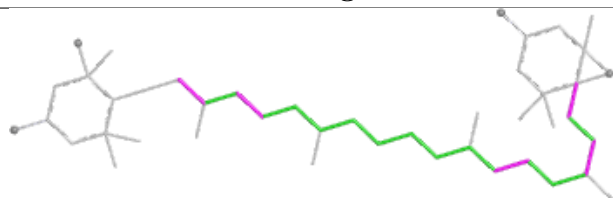
Ligand NEX Y 318



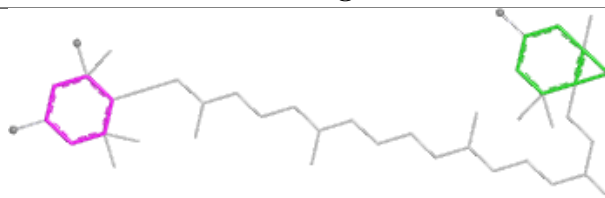
Bond lengths



Bond angles

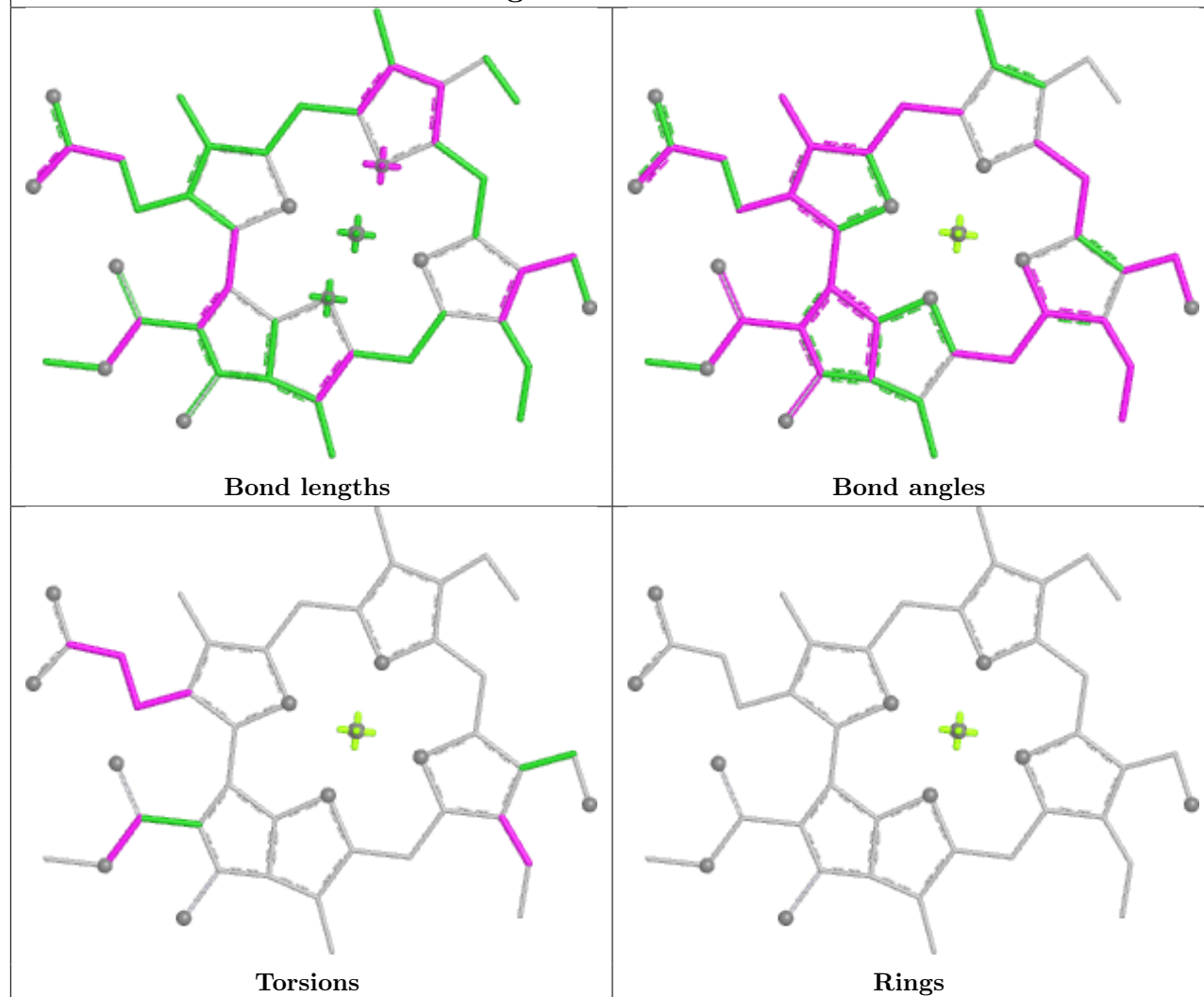


Torsions

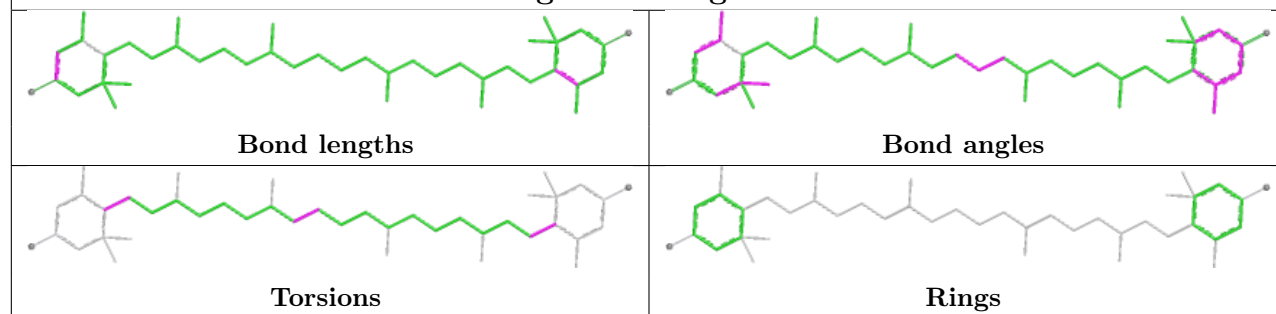


Rings

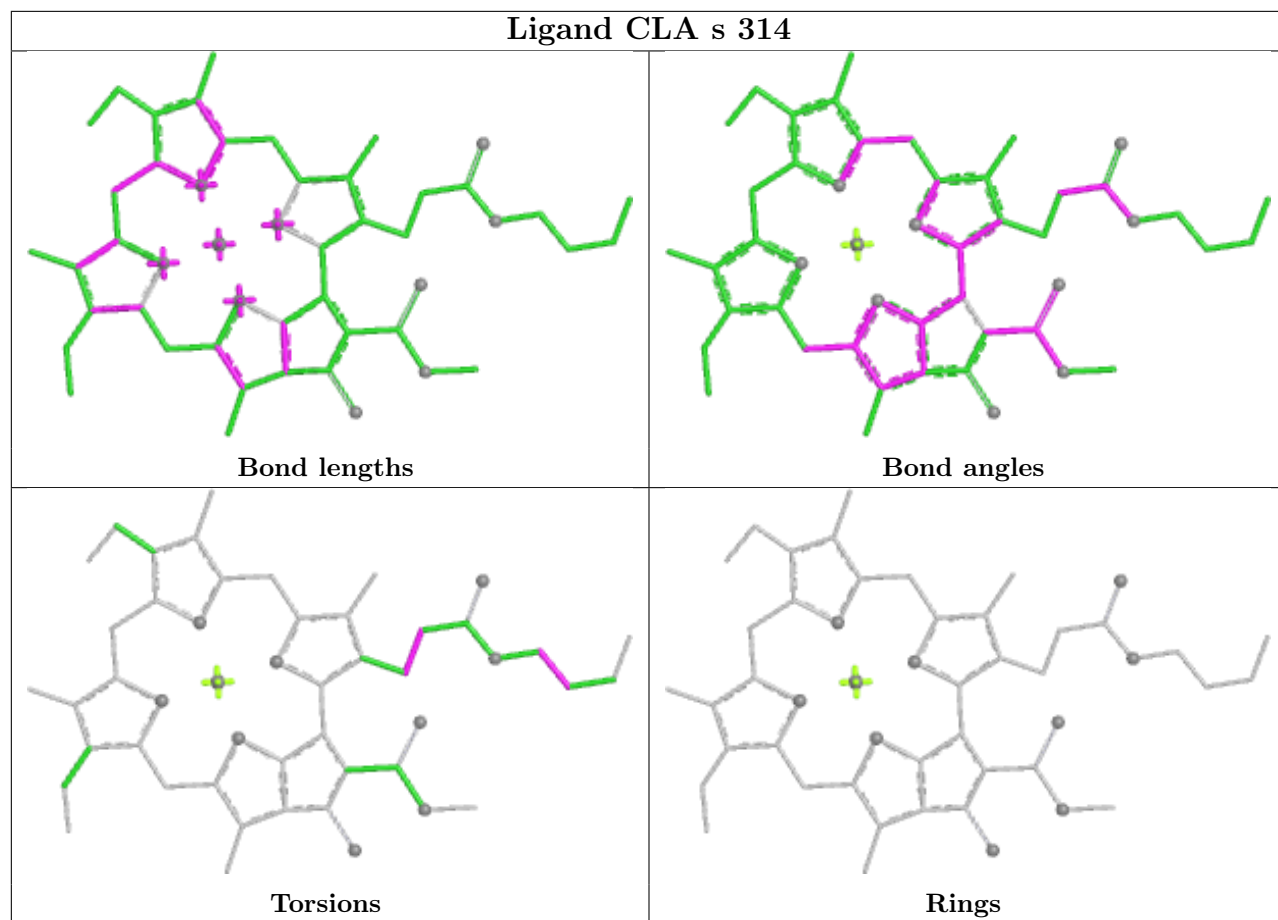
Ligand CHL r 606

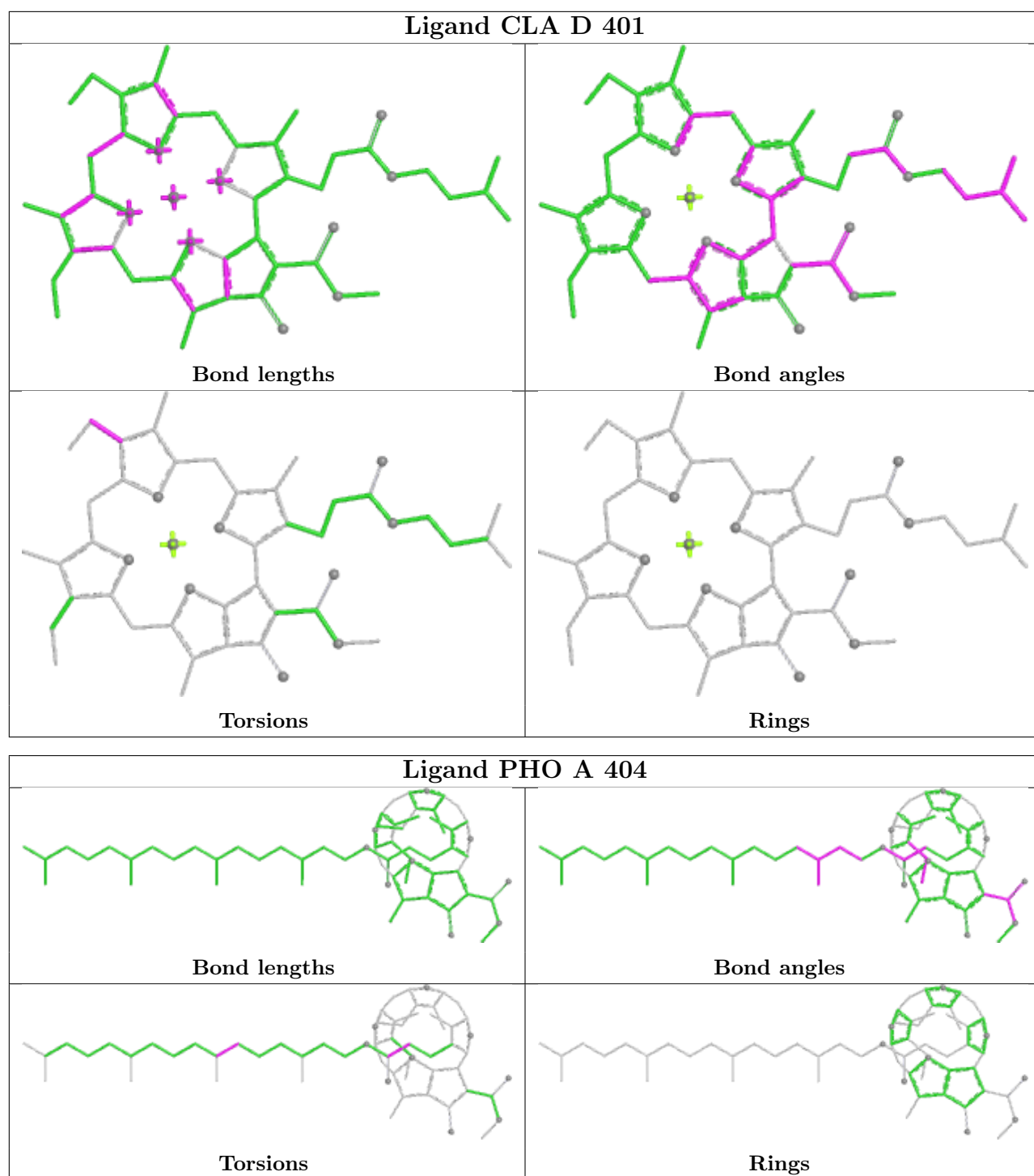


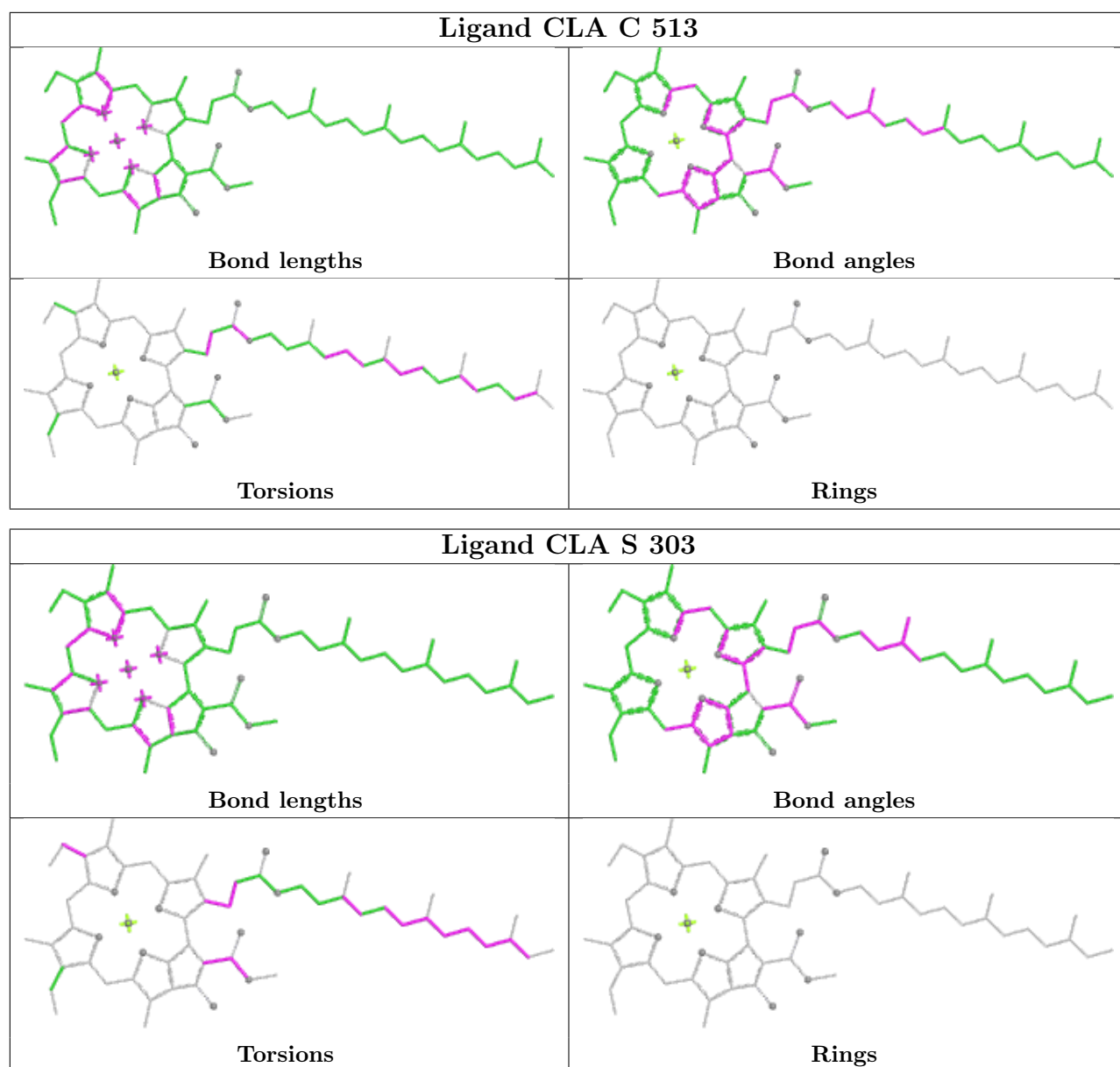
Ligand LUT g 615



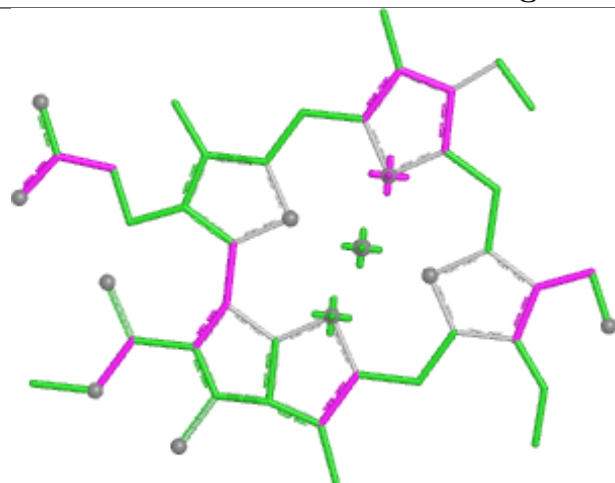
Ligand CLA s 314



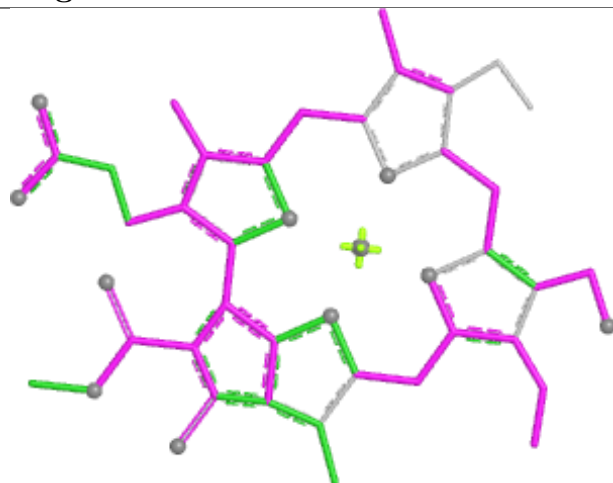




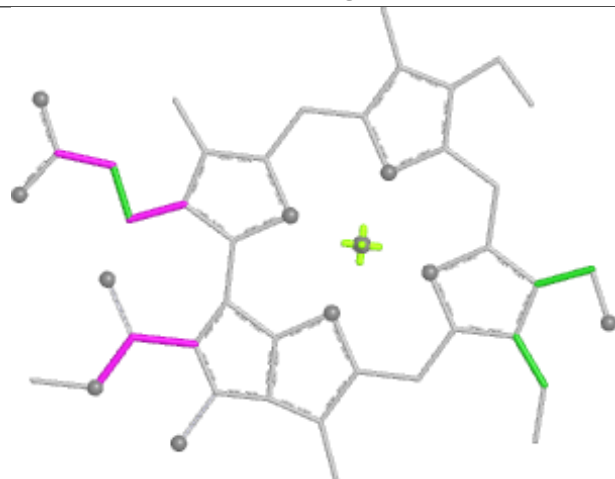
Ligand CHL g 607



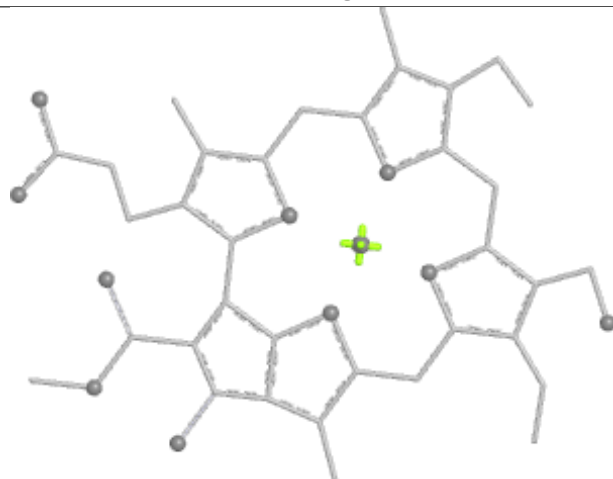
Bond lengths



Bond angles

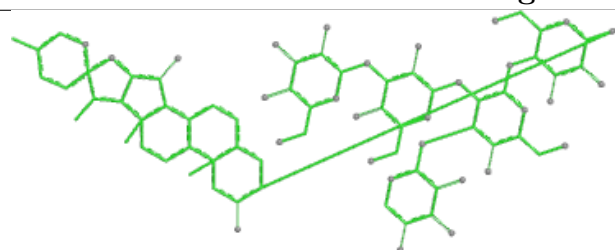


Torsions

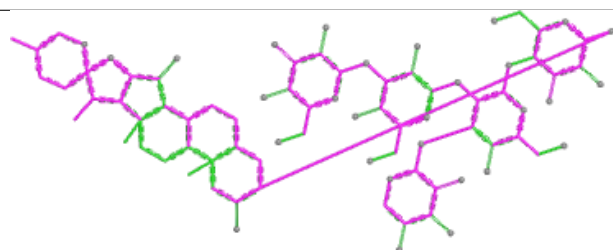


Rings

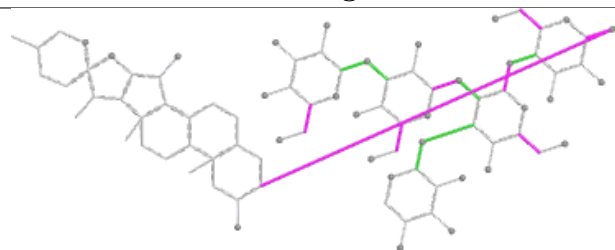
Ligand AJP A 412



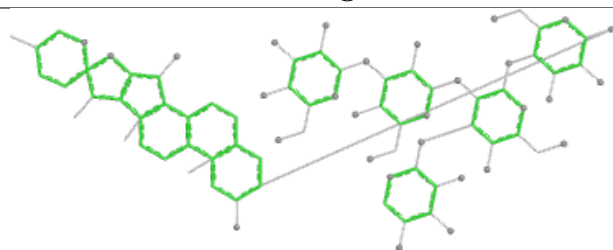
Bond lengths



Bond angles

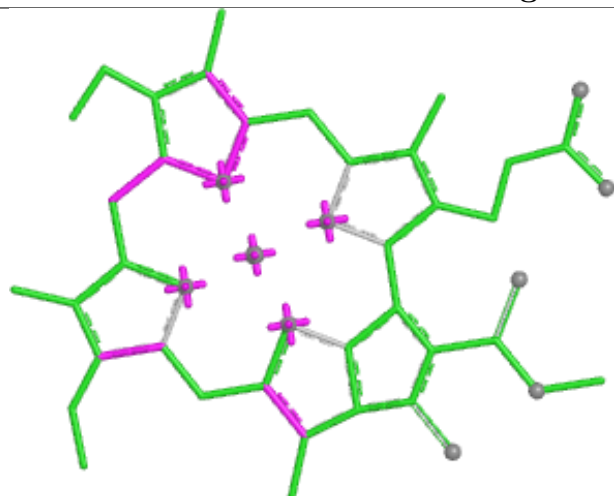


Torsions

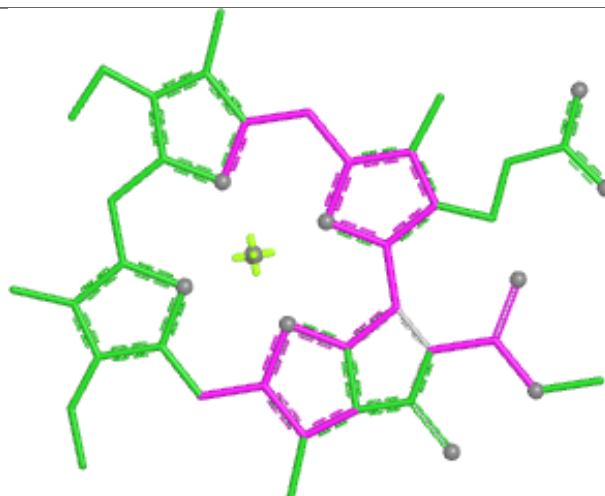


Rings

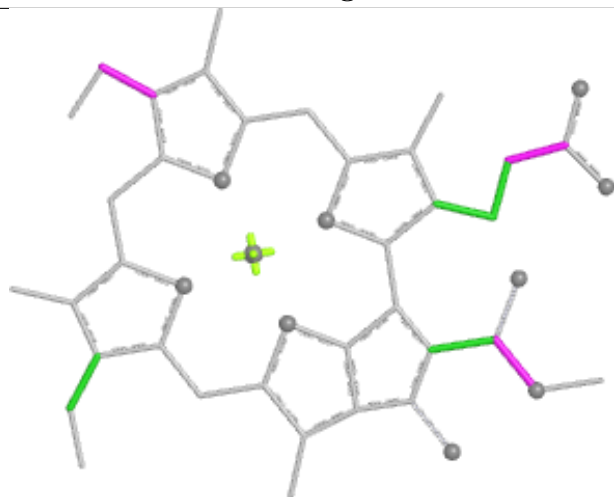
Ligand CLA s 309



Bond lengths



Bond angles

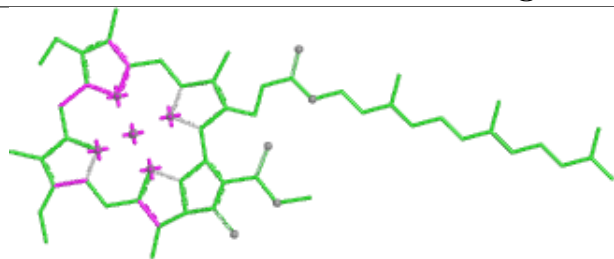


Torsions

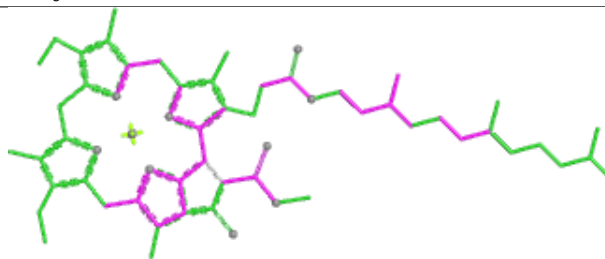


Rings

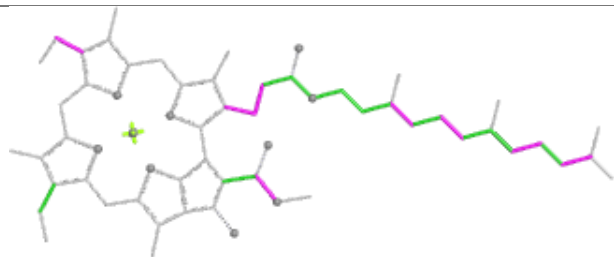
Ligand CLA y 311



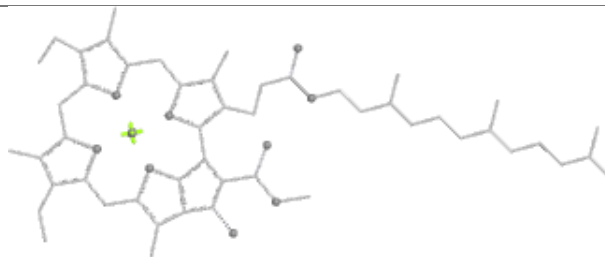
Bond lengths



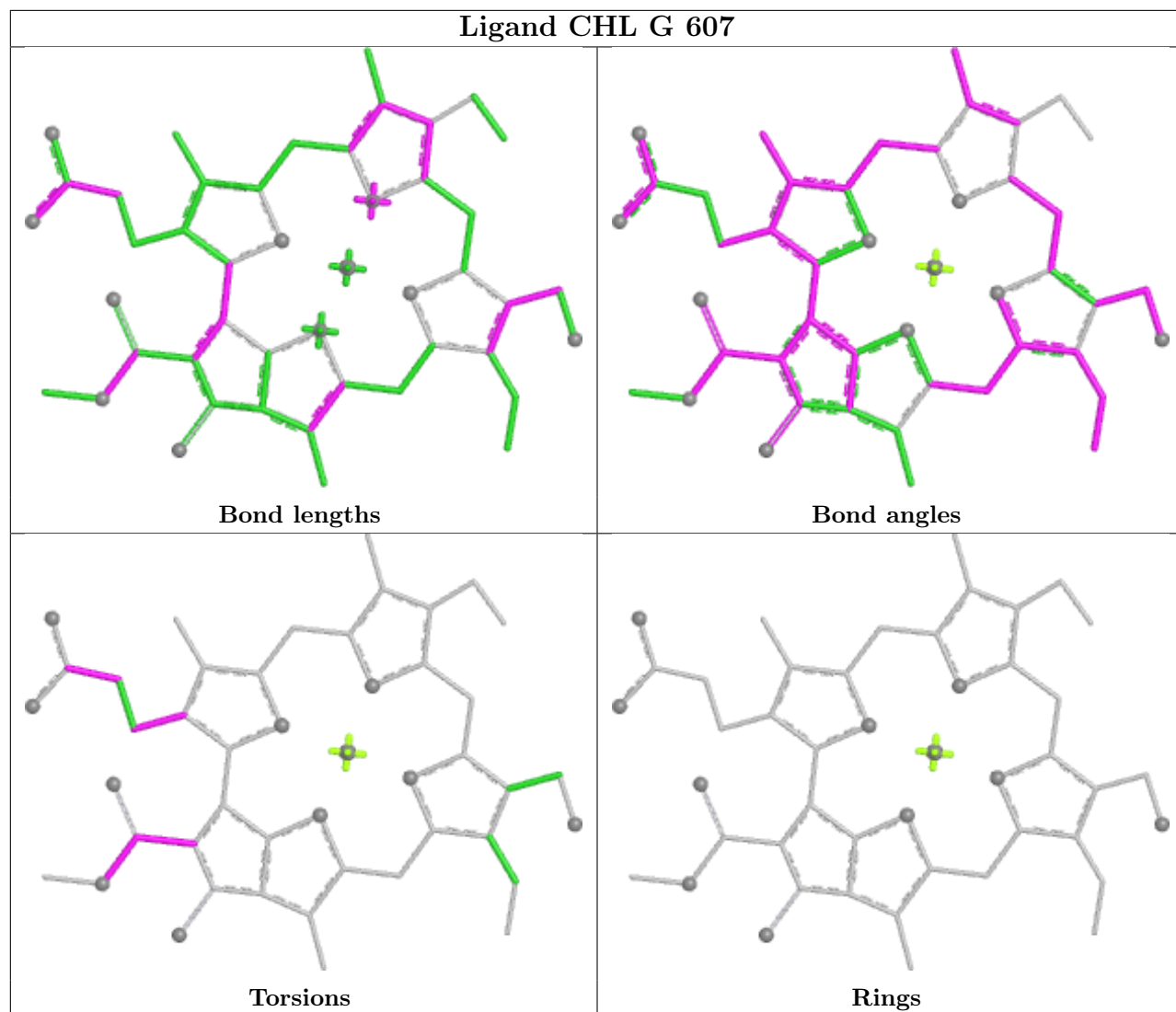
Bond angles



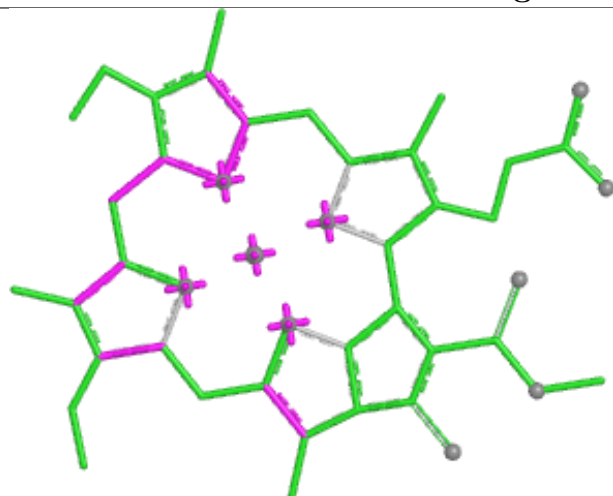
Torsions



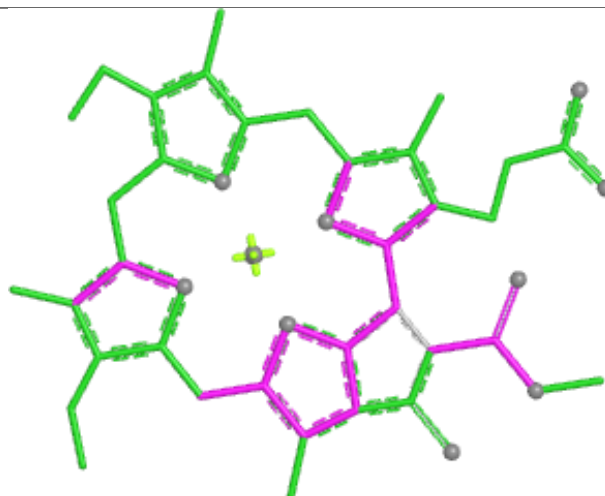
Rings



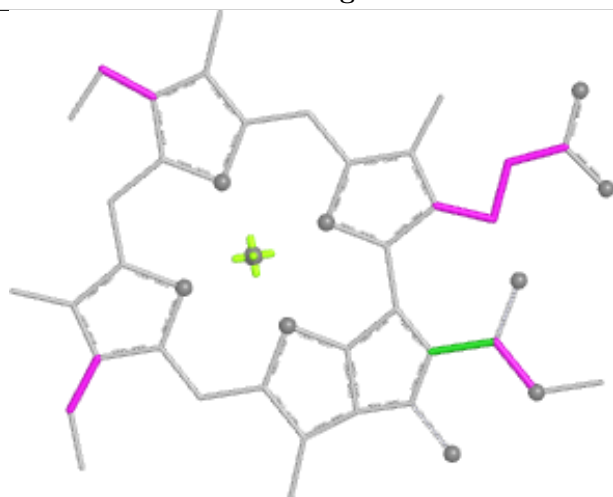
Ligand CLA Y 315



Bond lengths



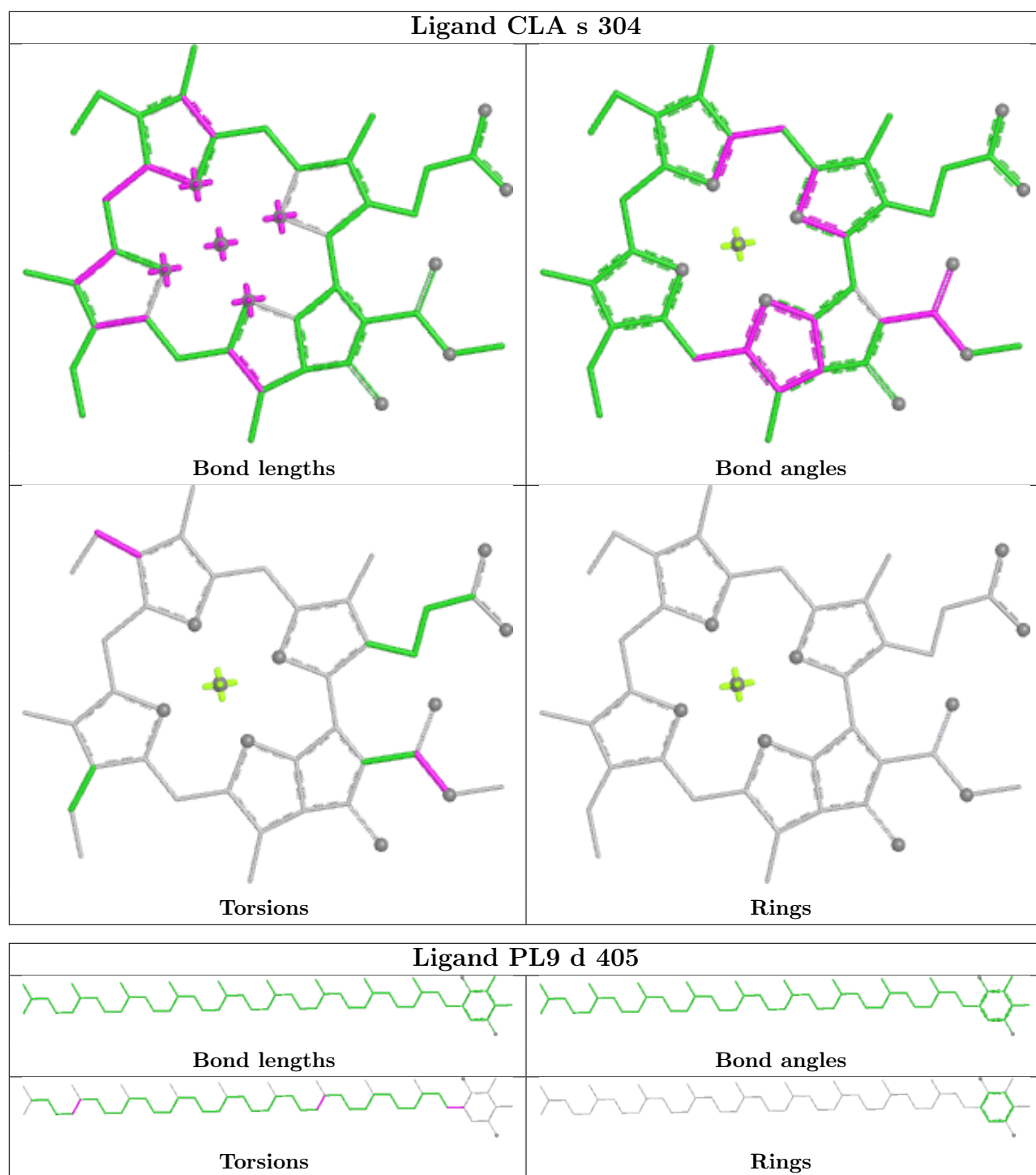
Bond angles

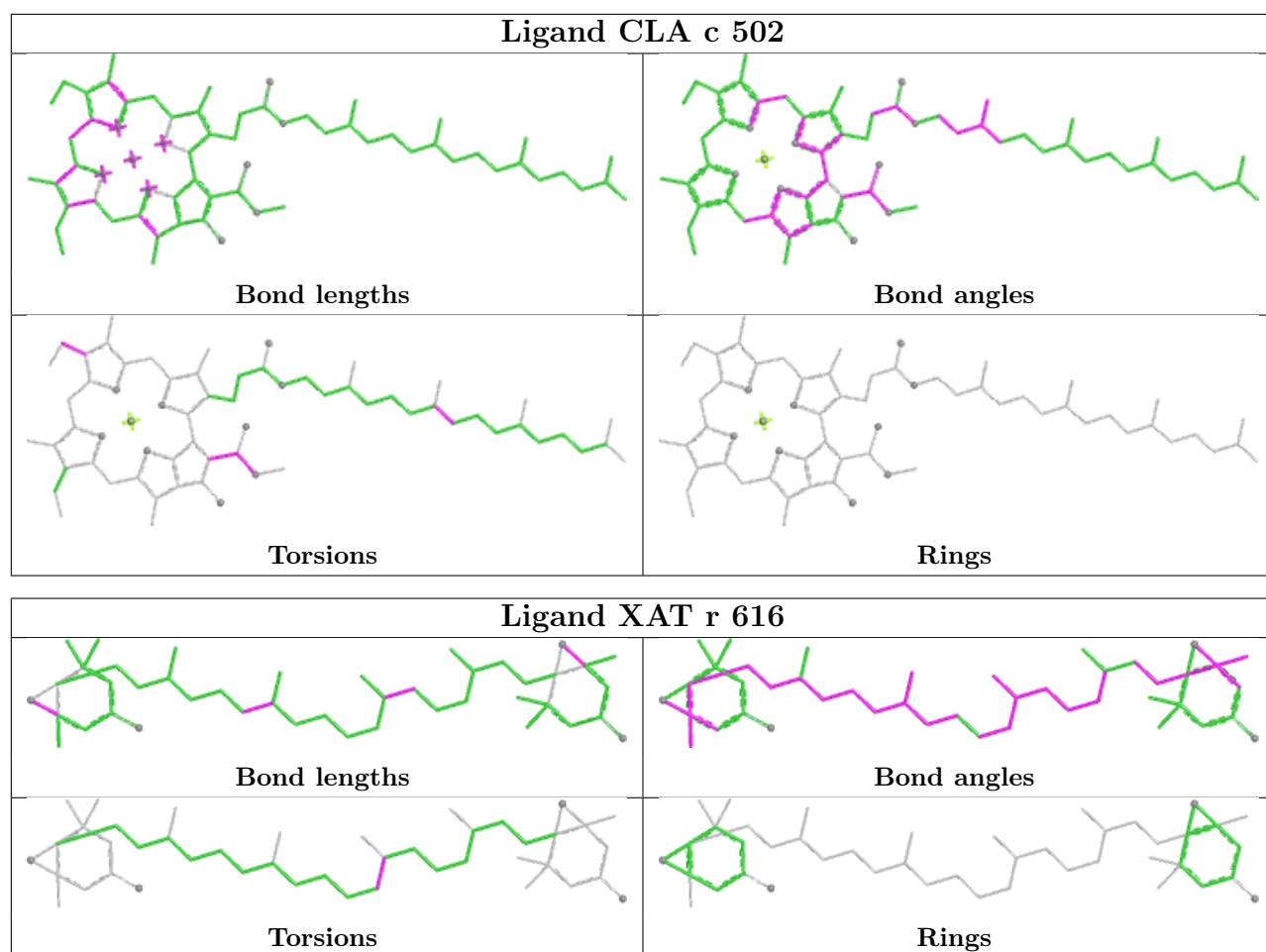


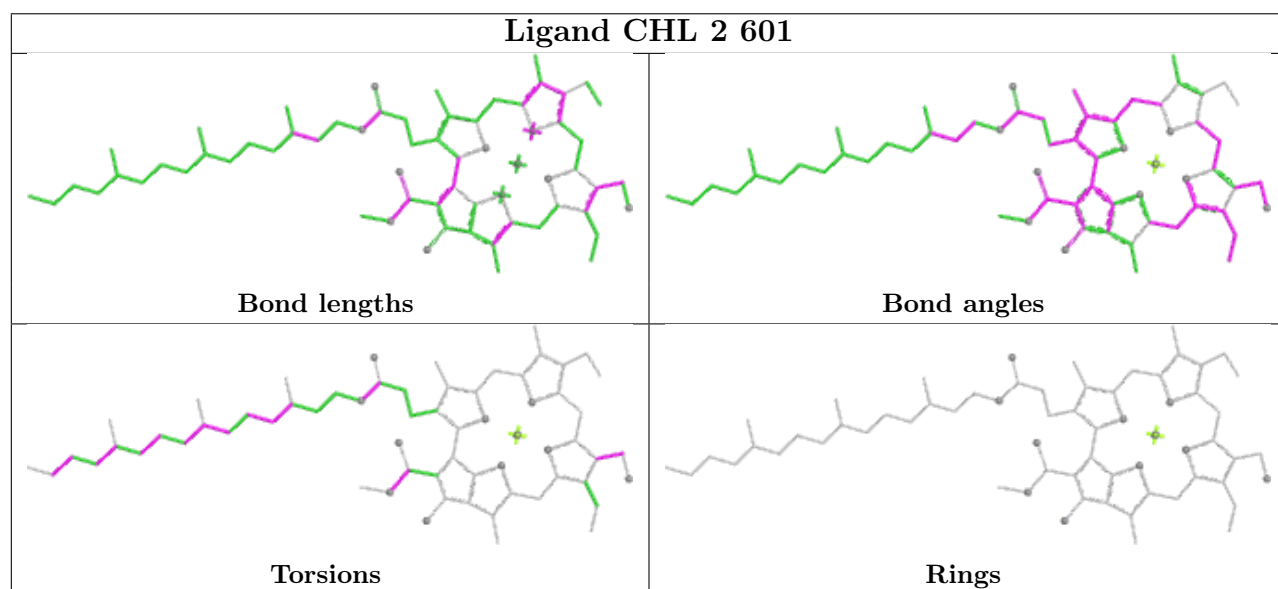
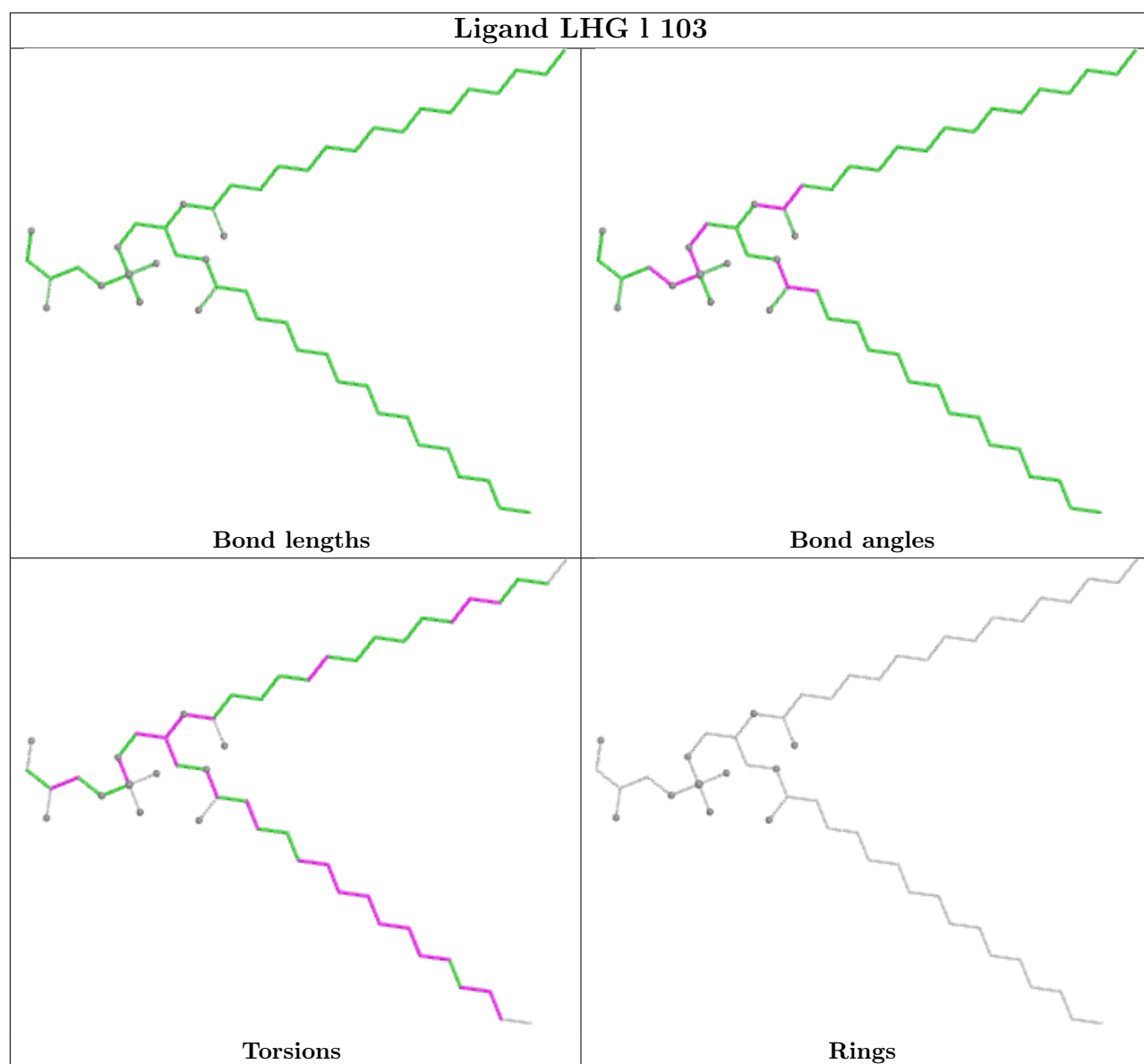
Torsions

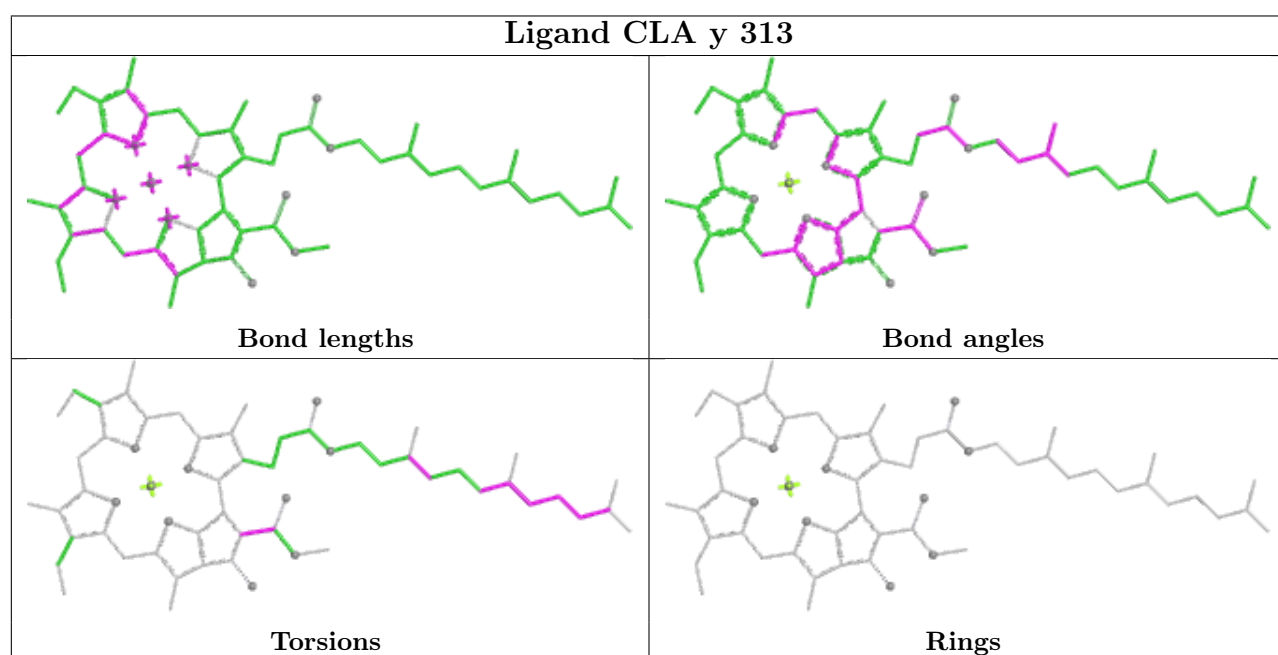
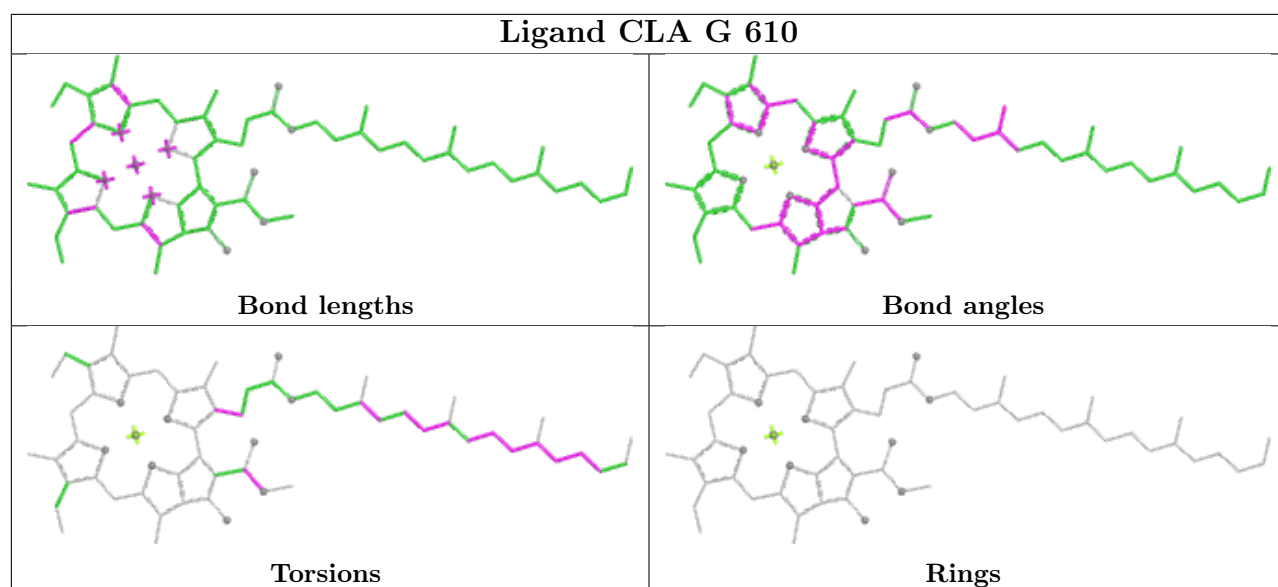


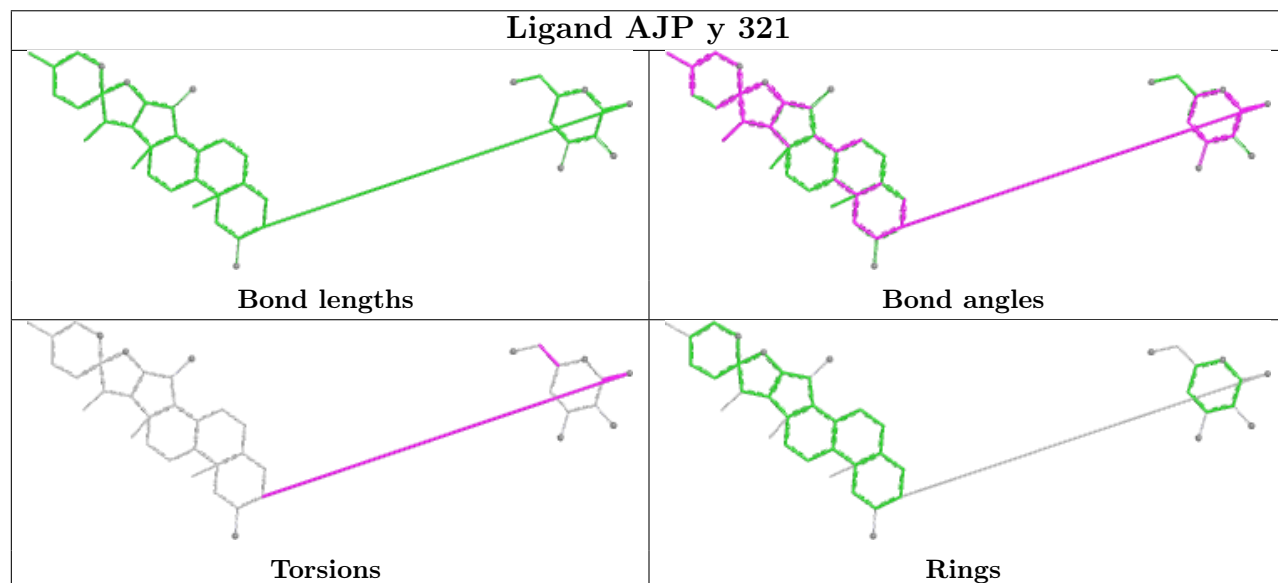
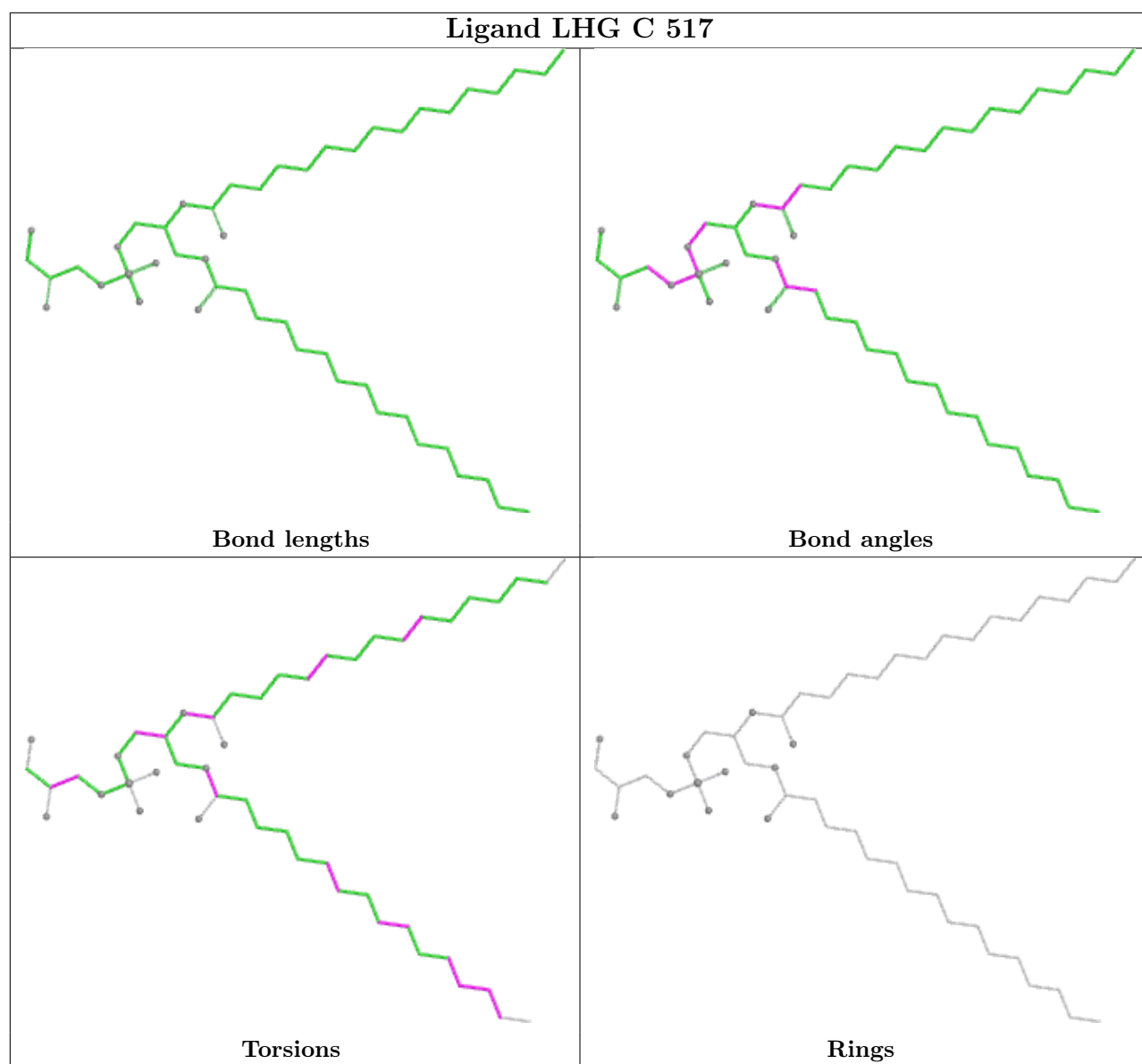
Rings

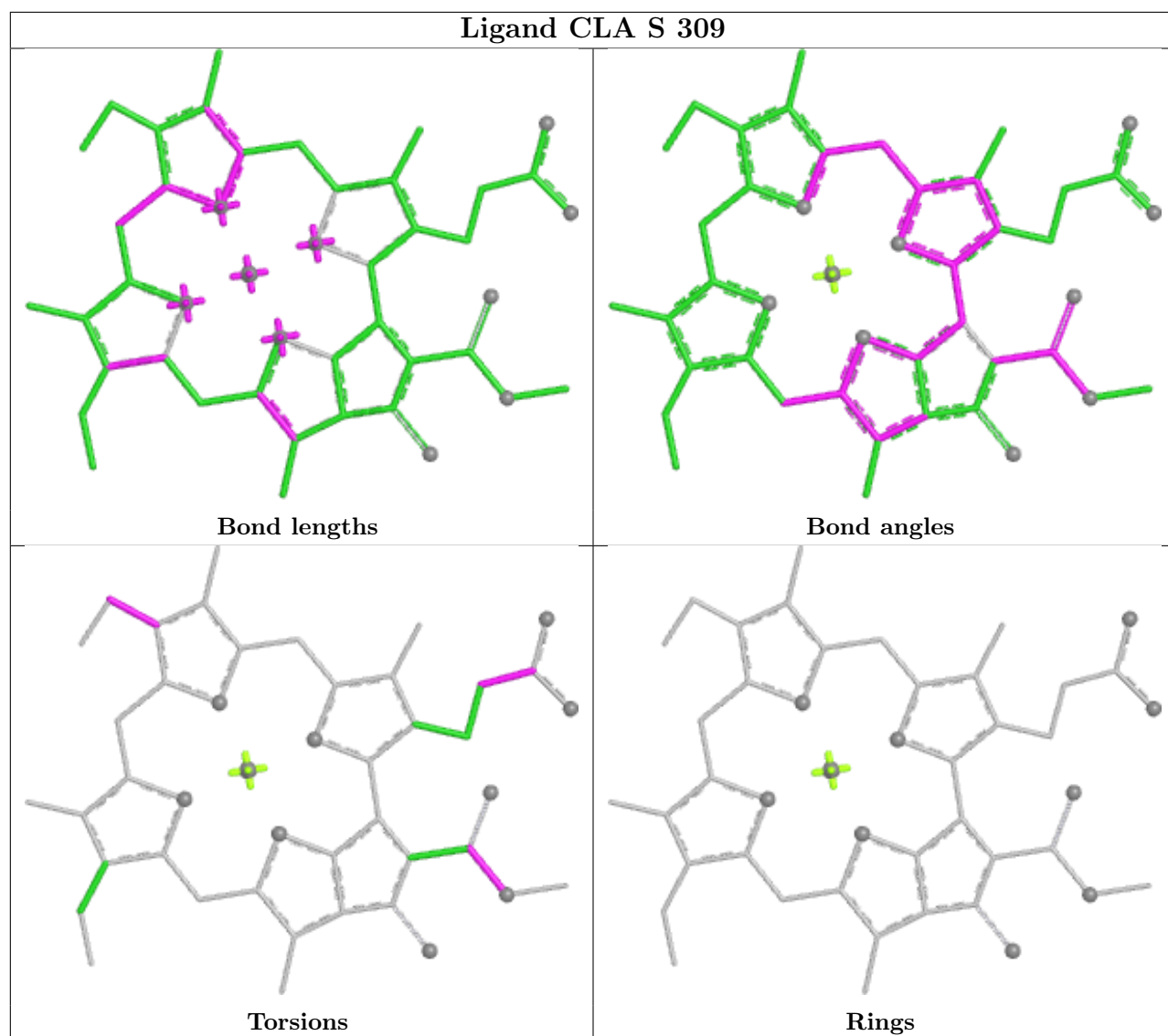
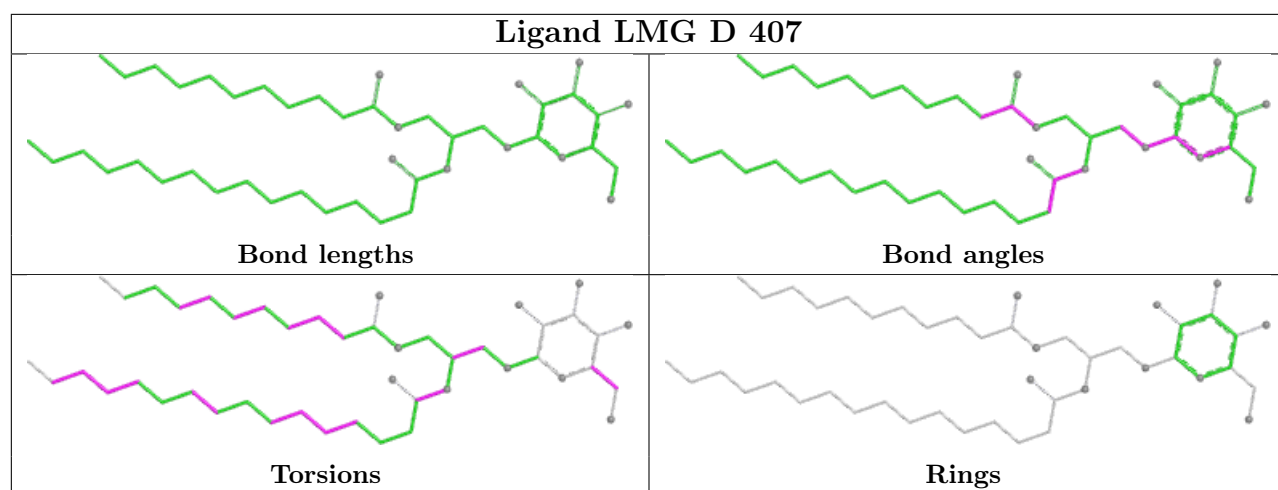


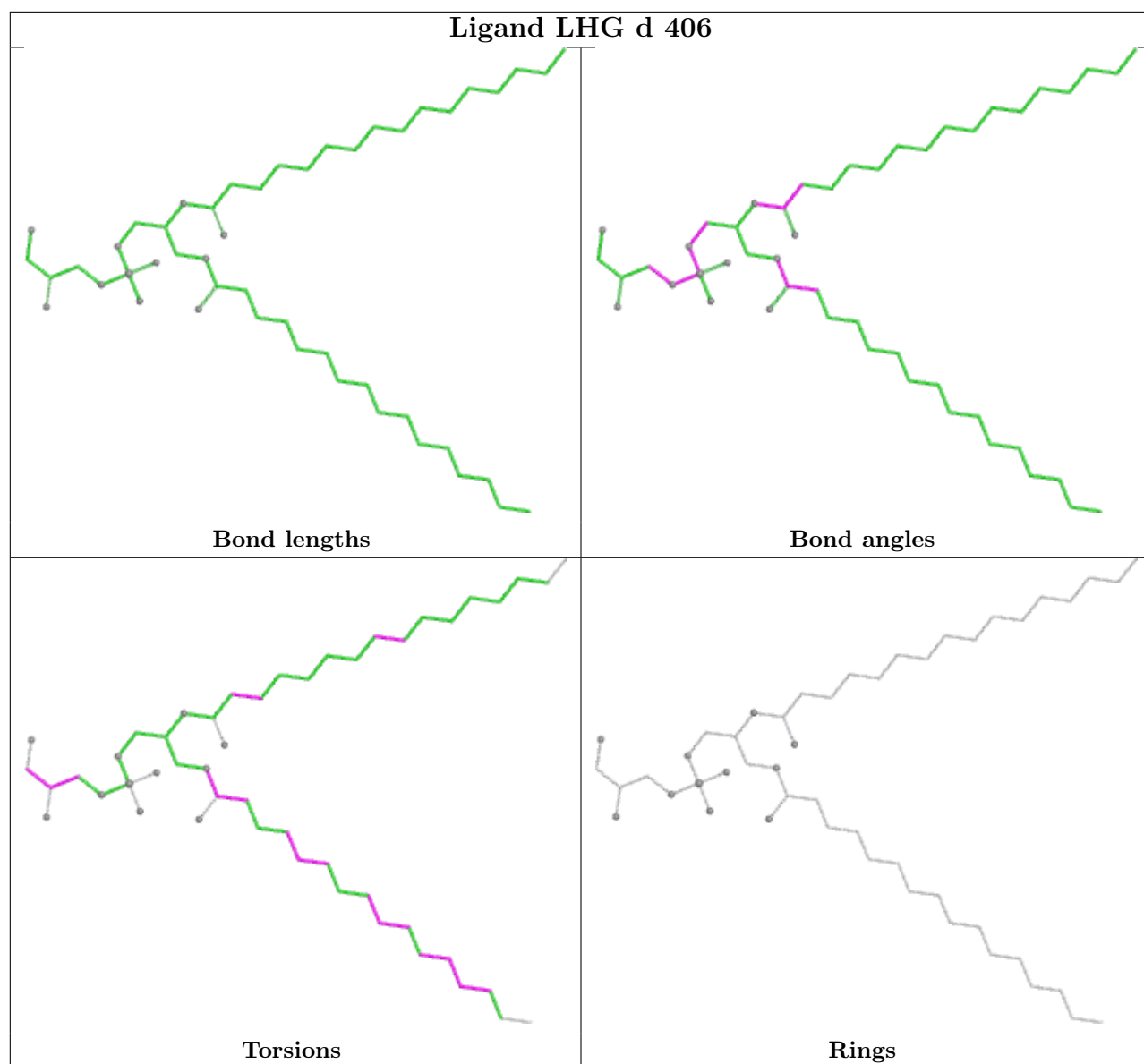
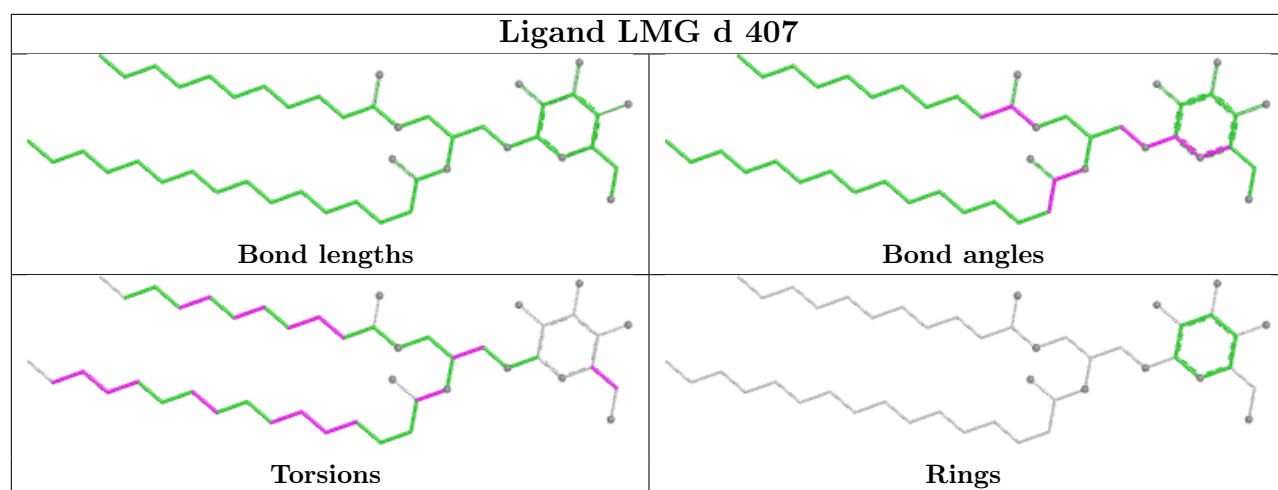




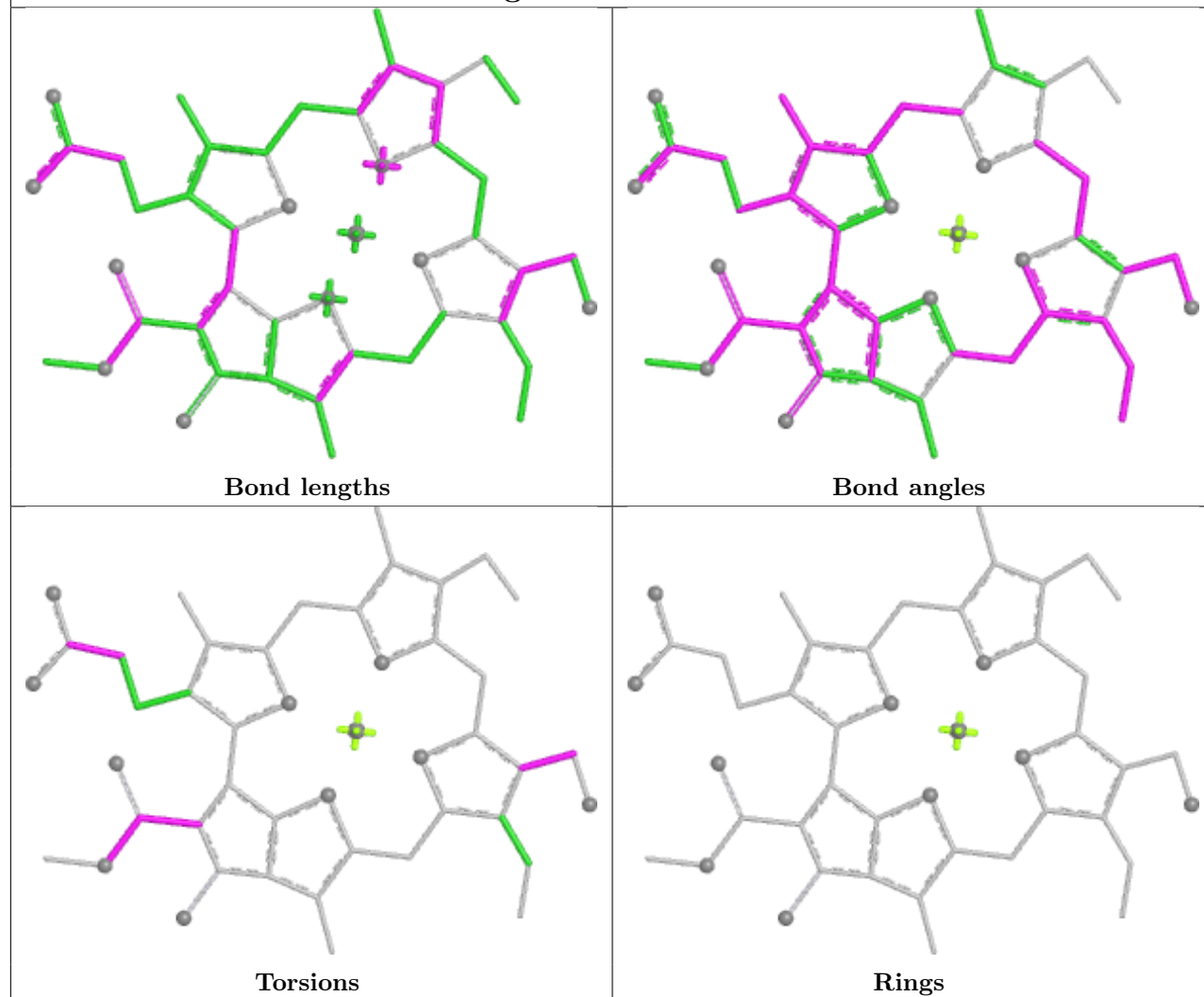




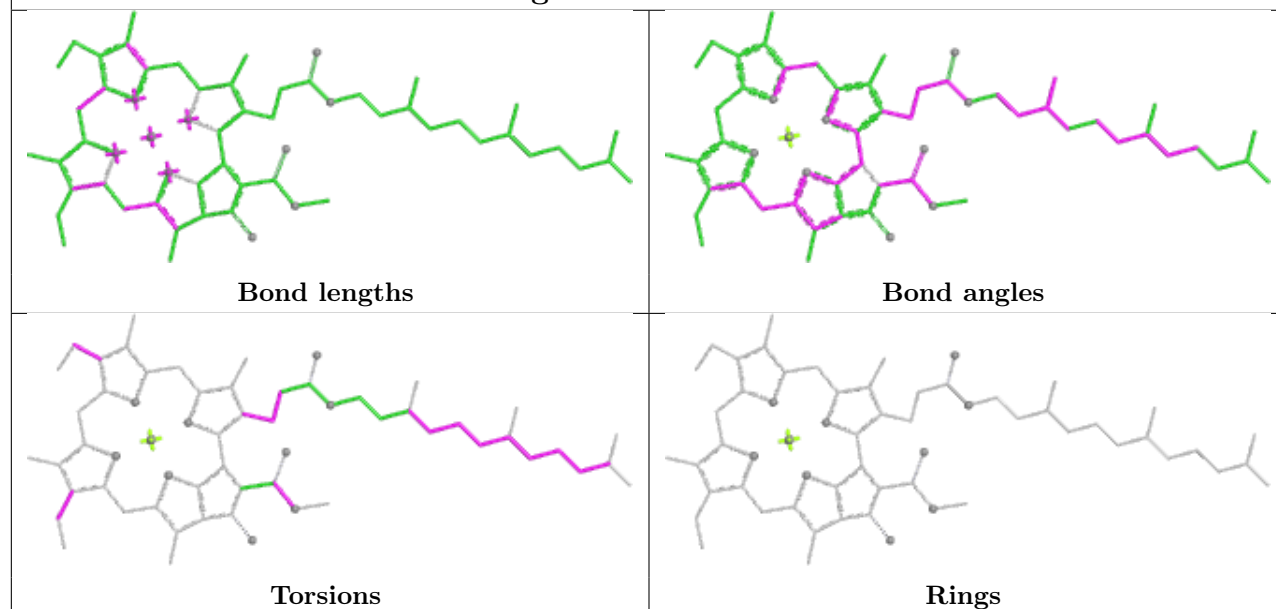




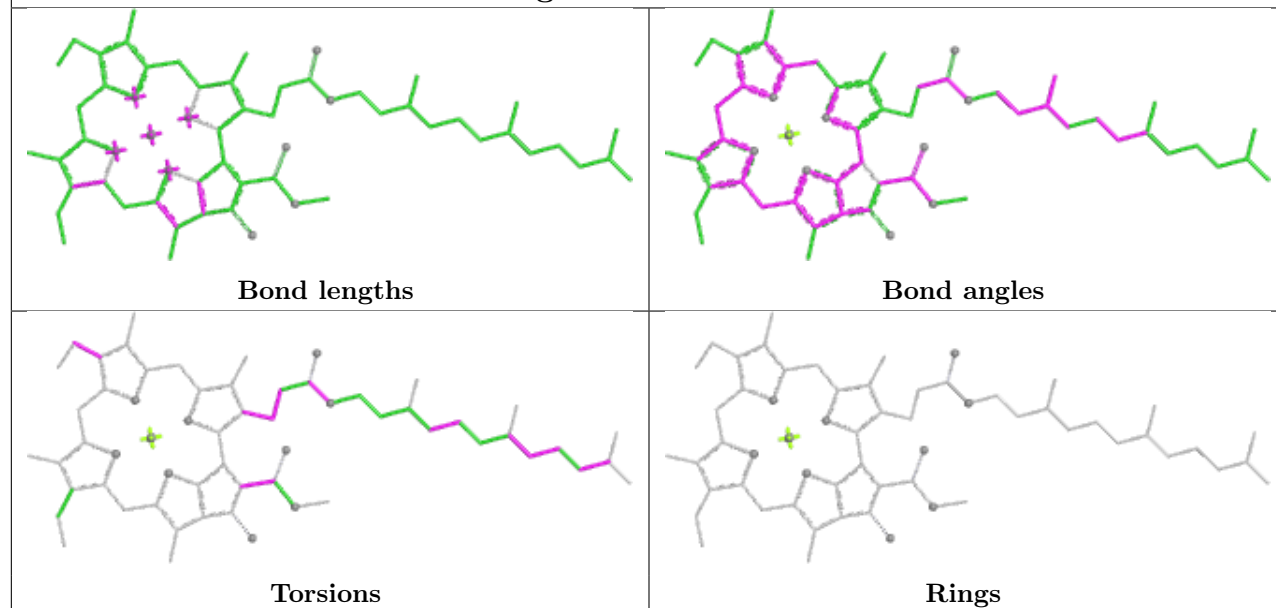
Ligand CHL n 606



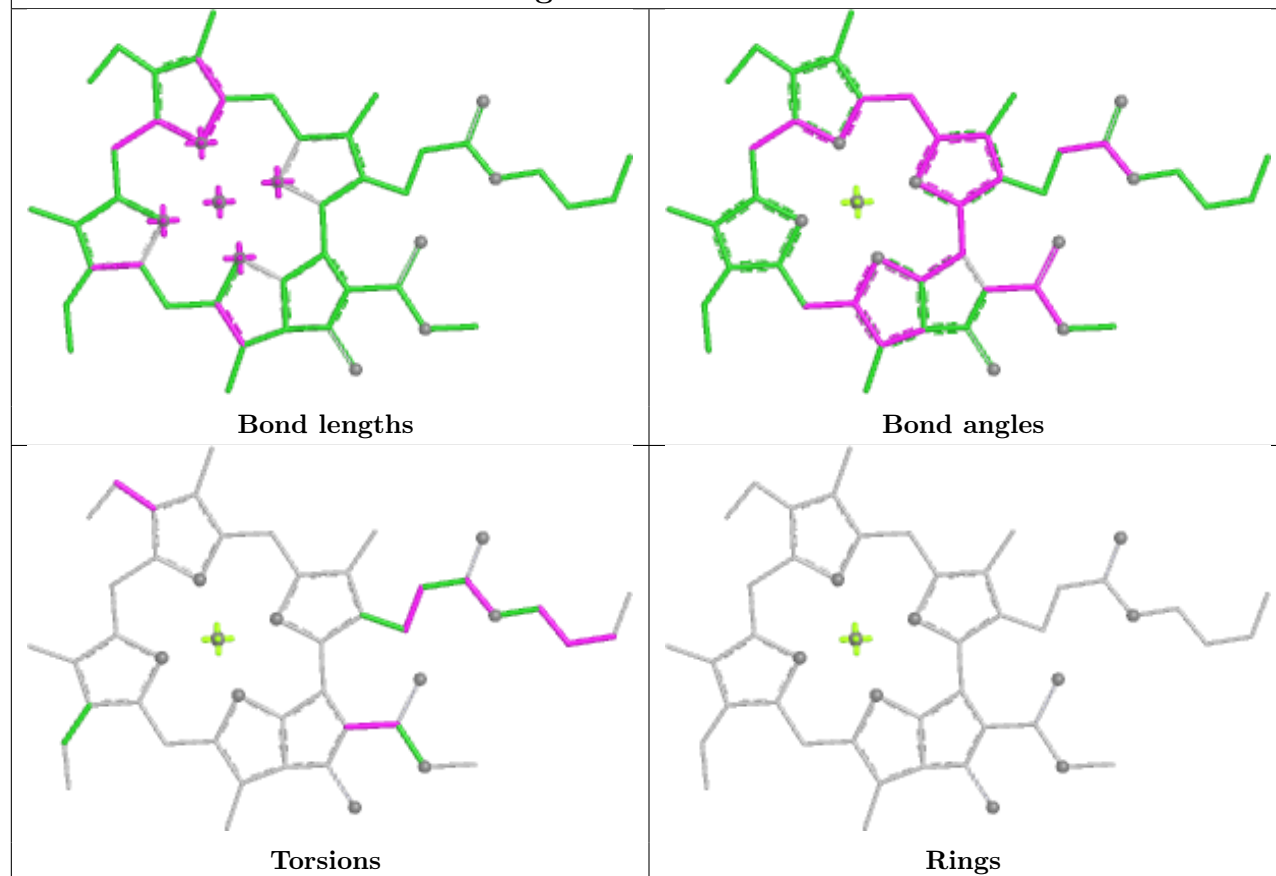
Ligand CLA N 613

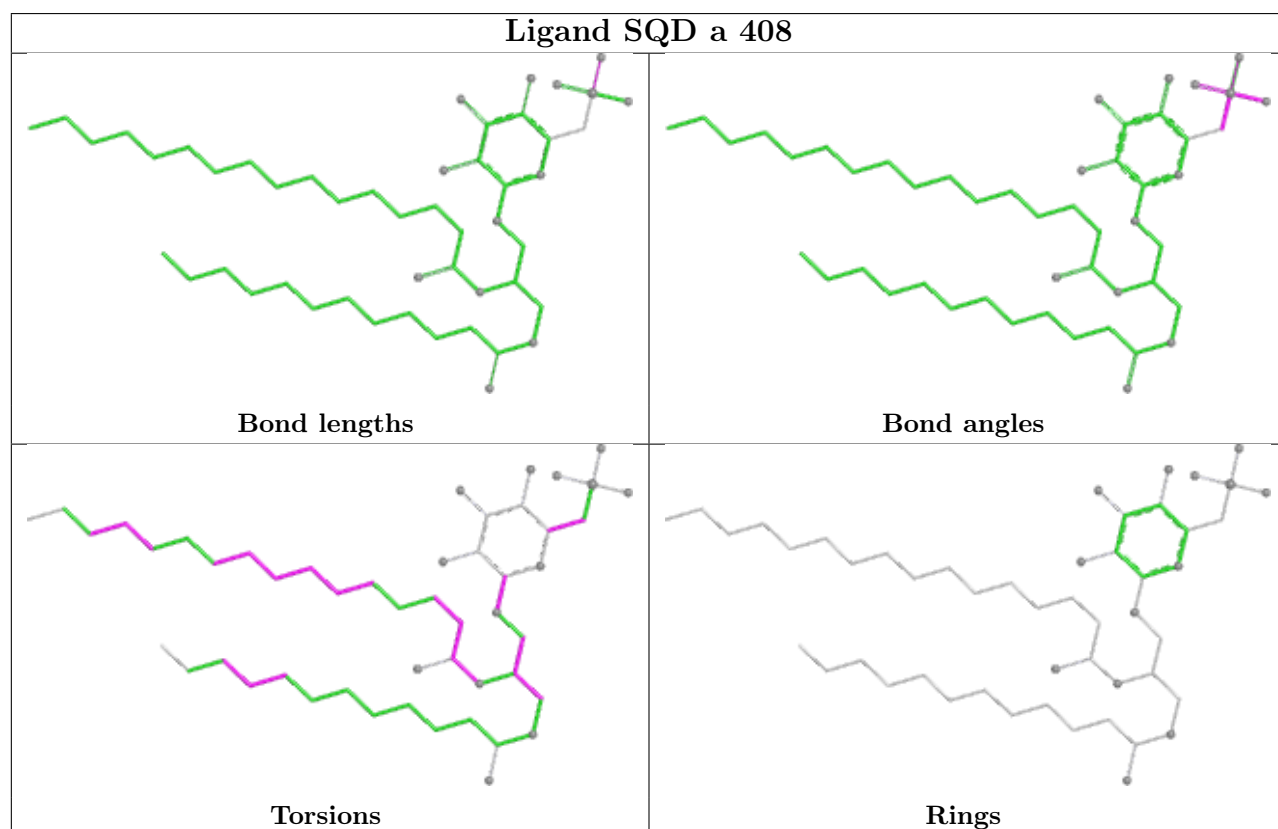
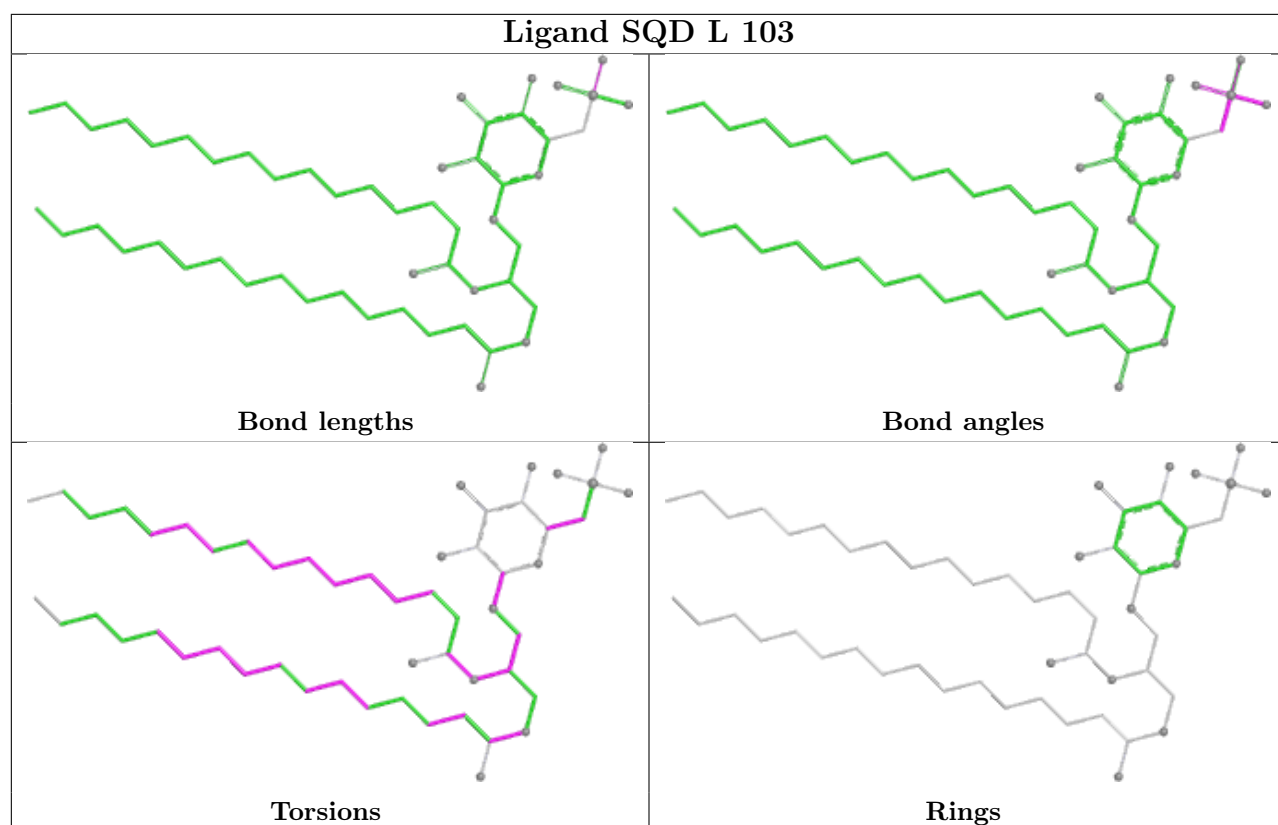


Ligand CLA 2 602

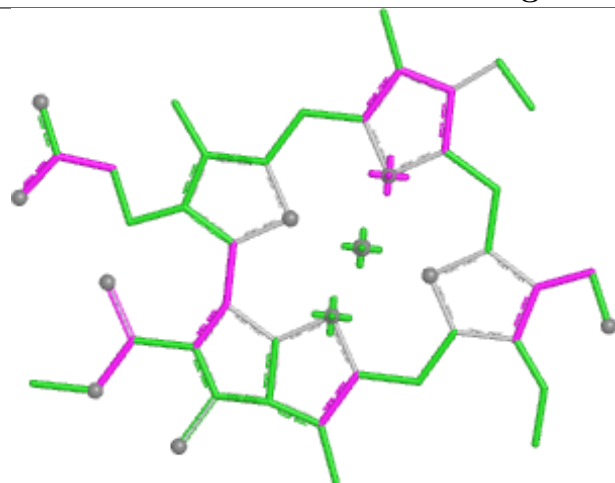


Ligand CLA S 312

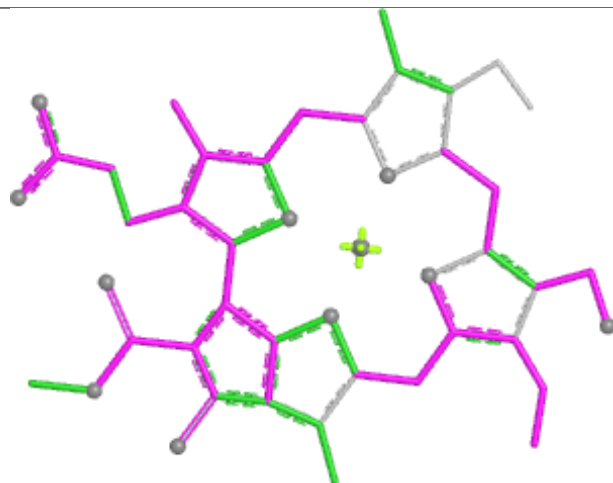




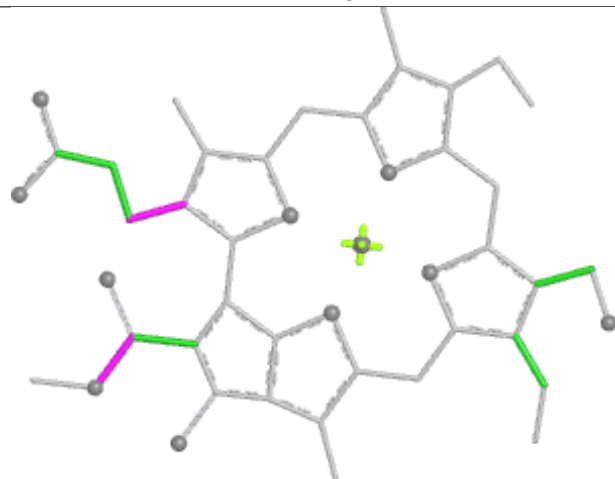
Ligand CHL r 605



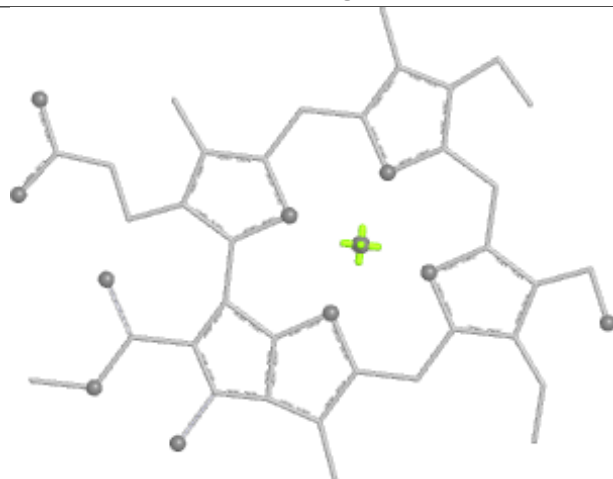
Bond lengths



Bond angles

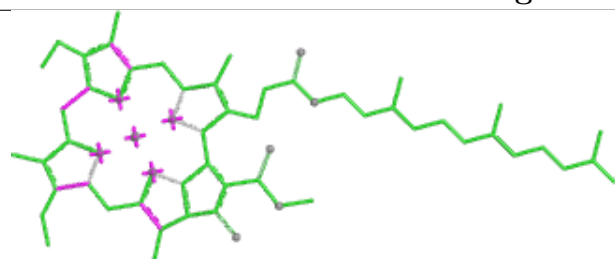


Torsions

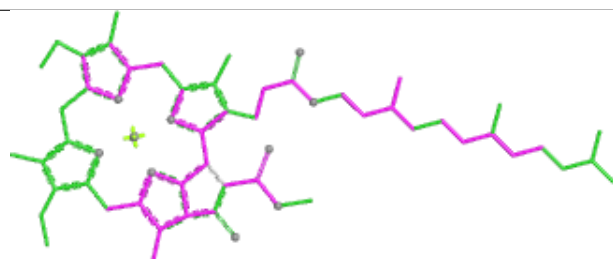


Rings

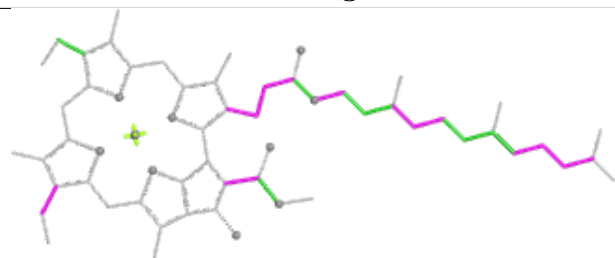
Ligand CLA G 611



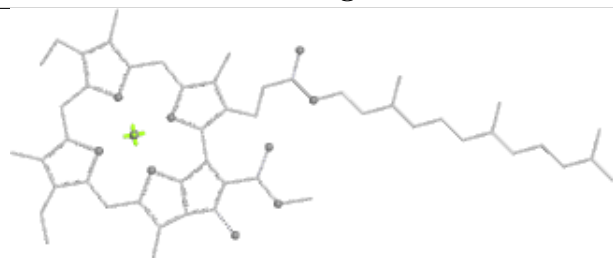
Bond lengths



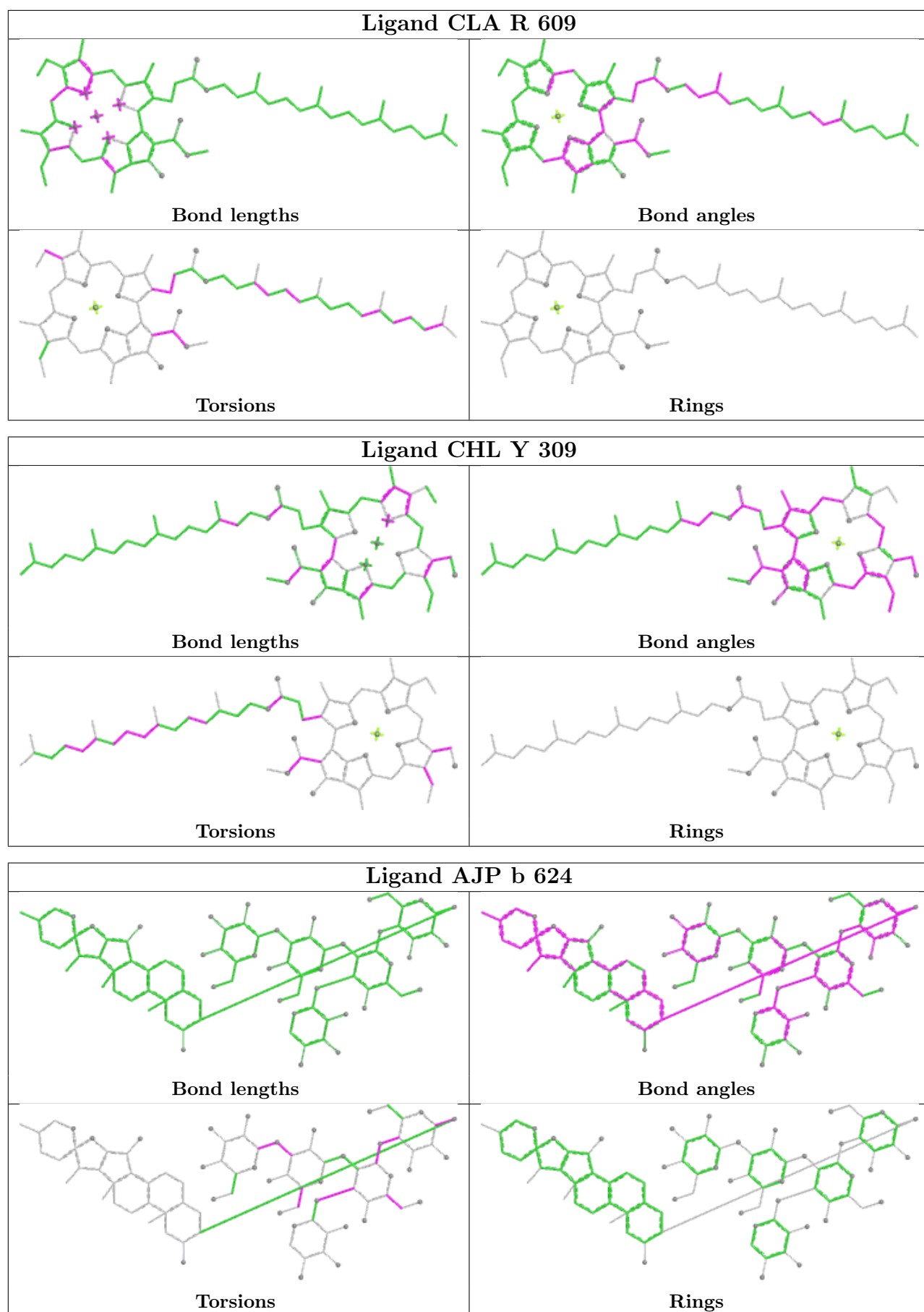
Bond angles

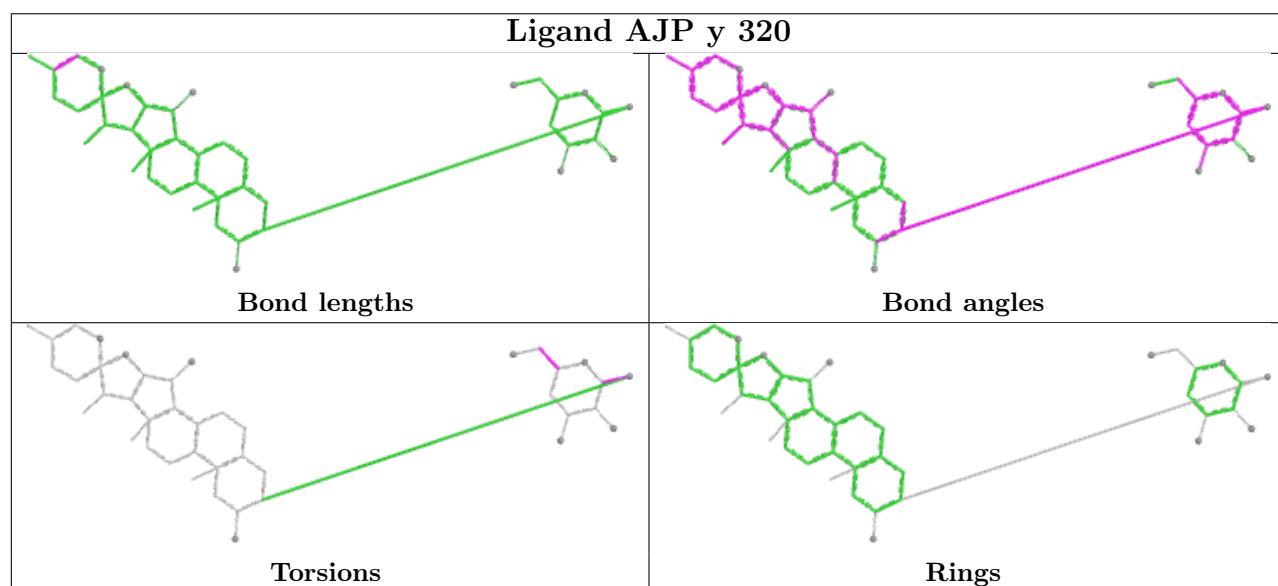
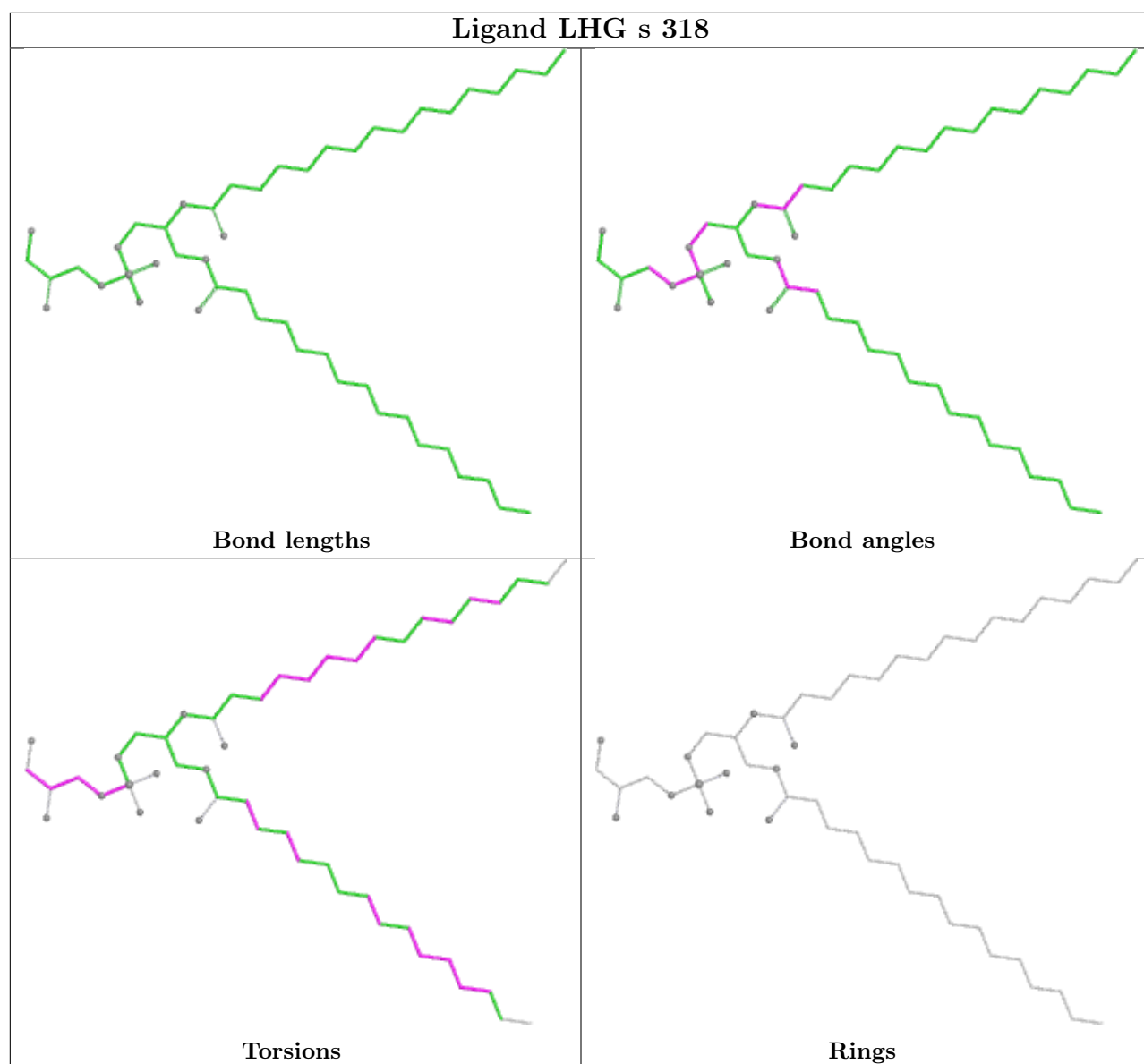


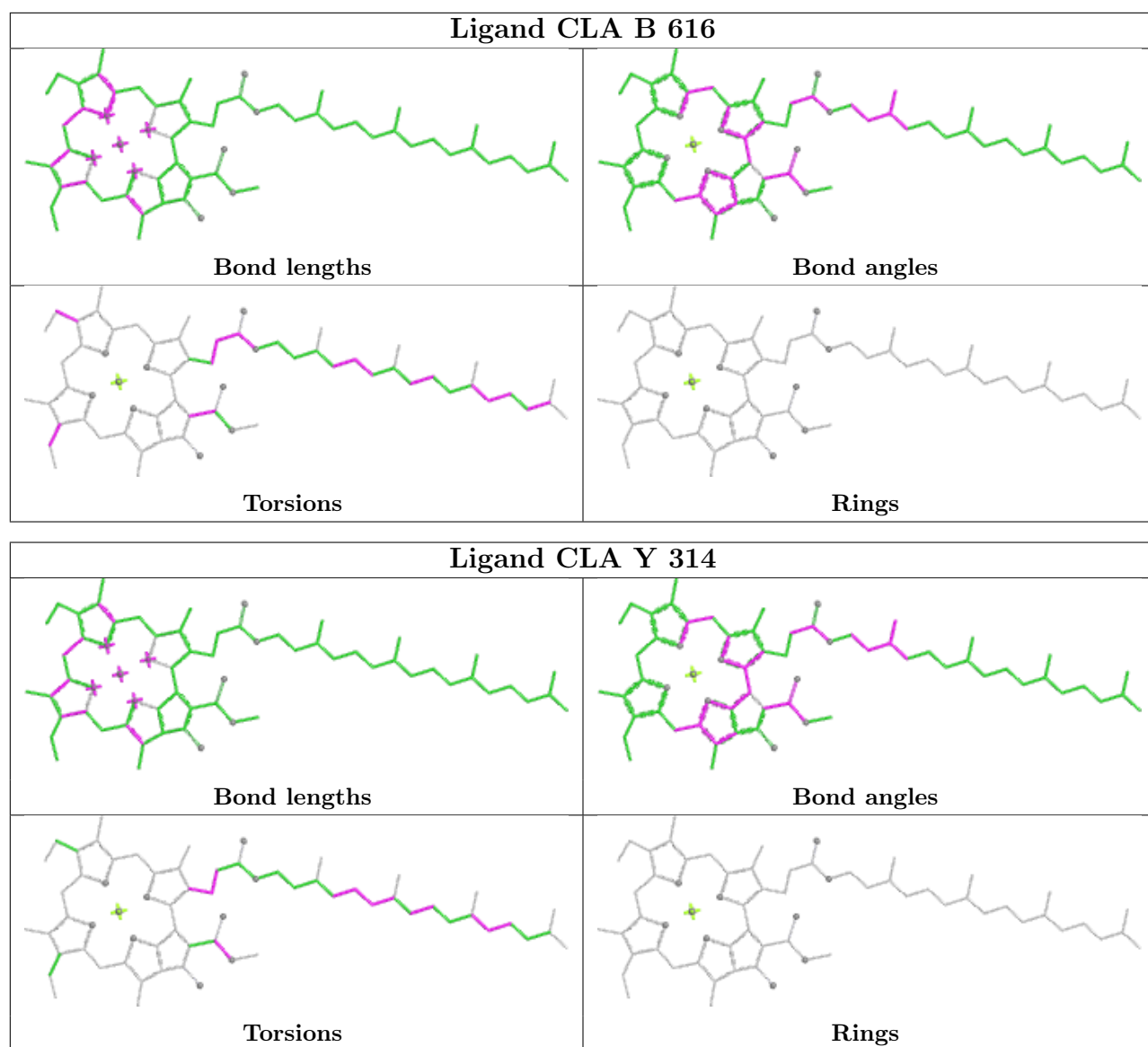
Torsions

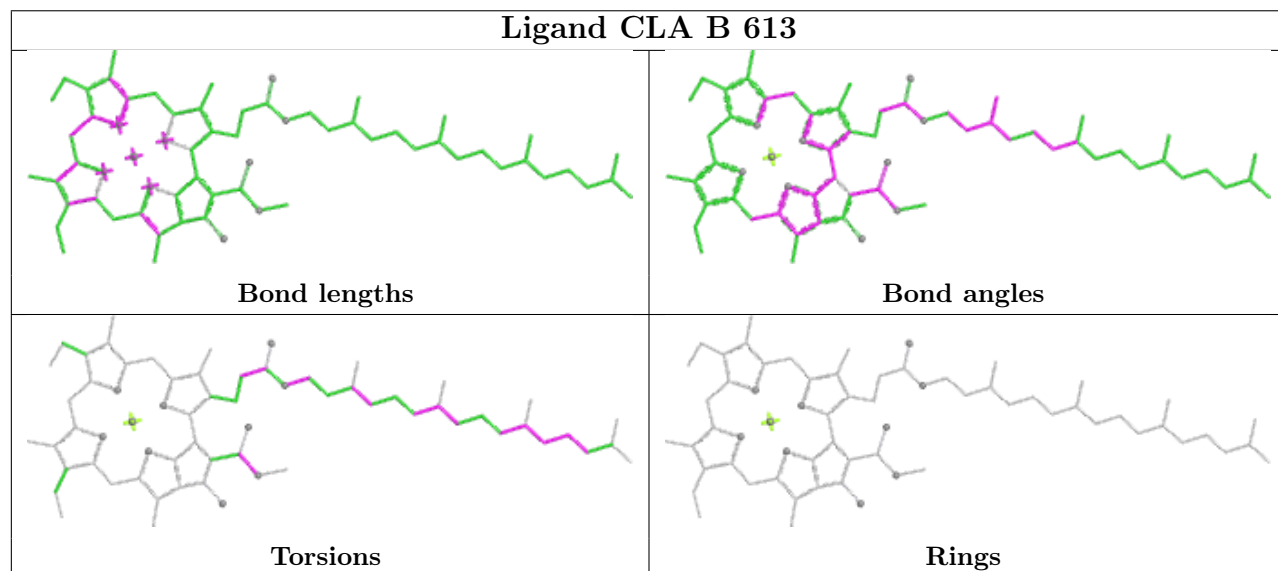
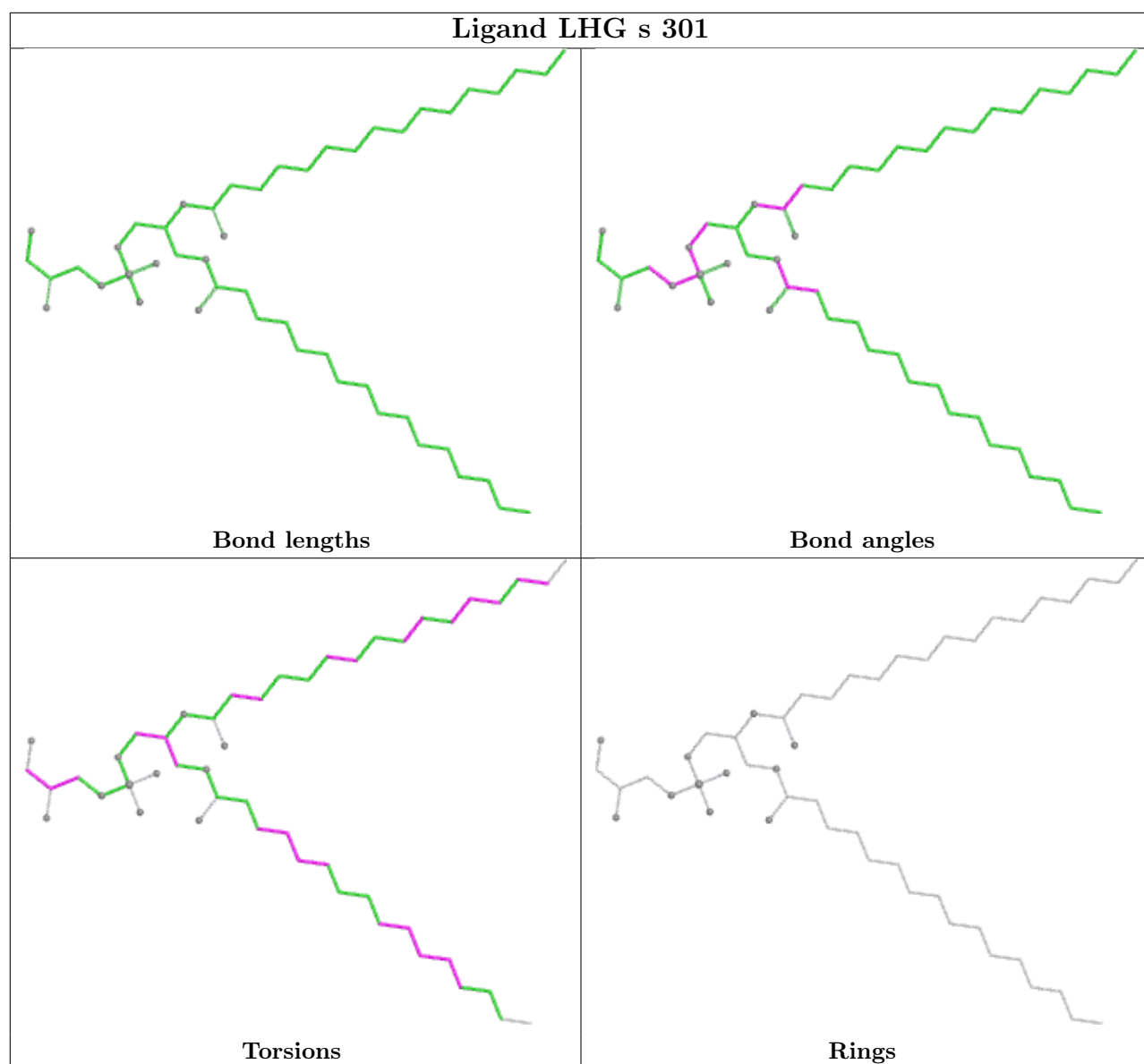


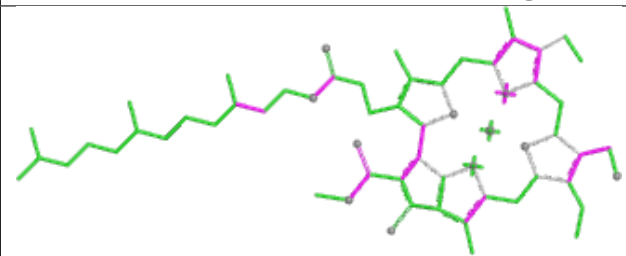
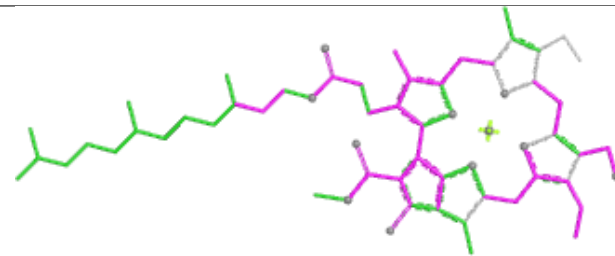
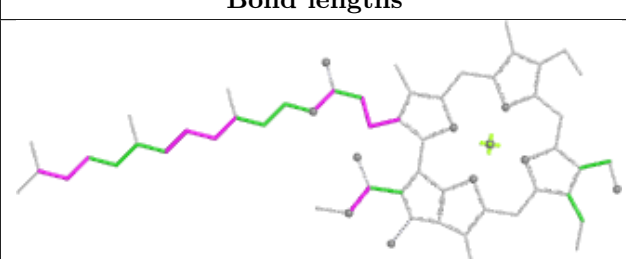
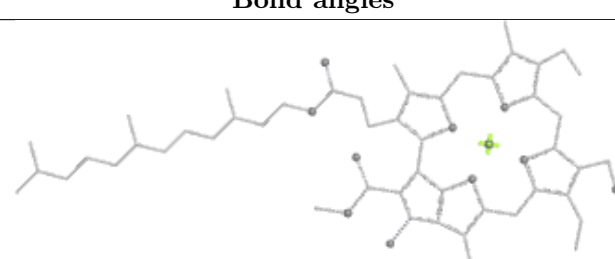
Rings

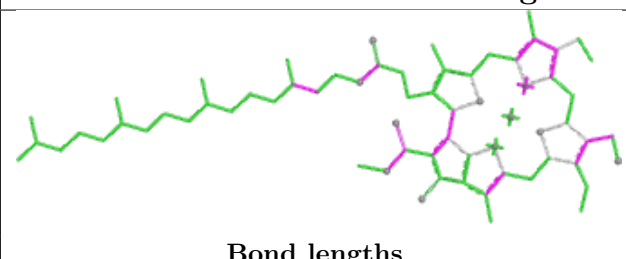
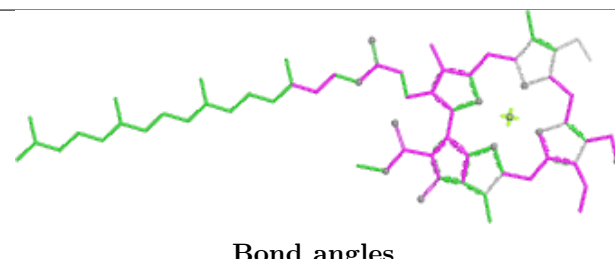
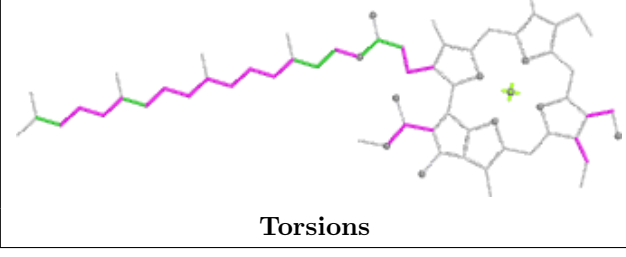
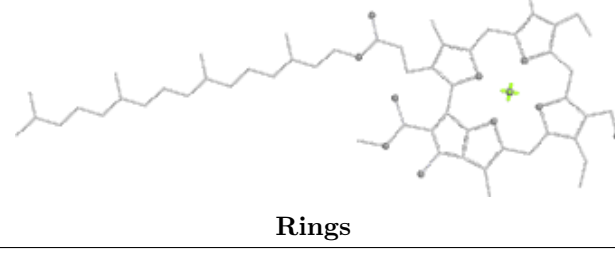


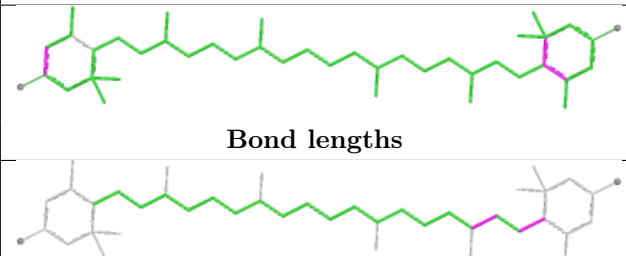
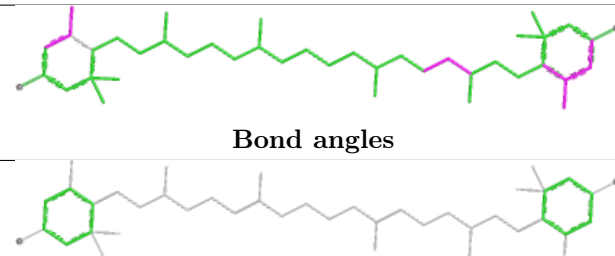


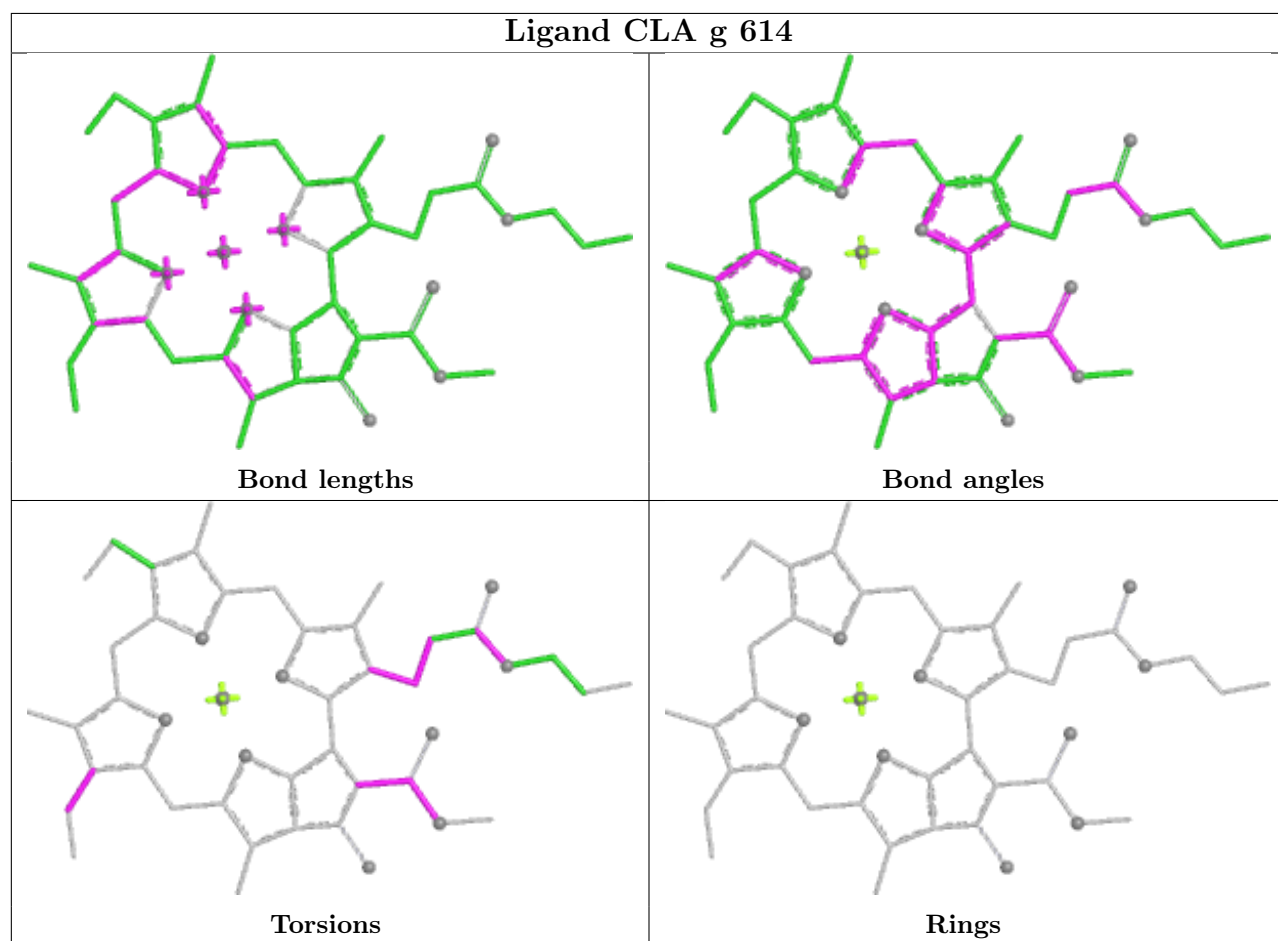
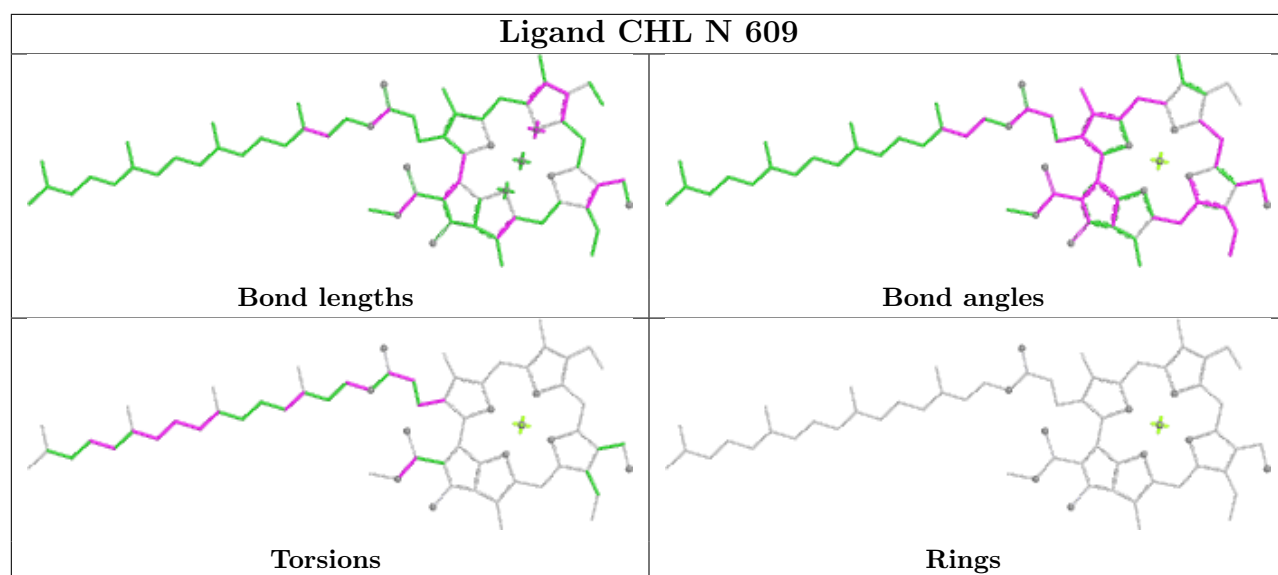


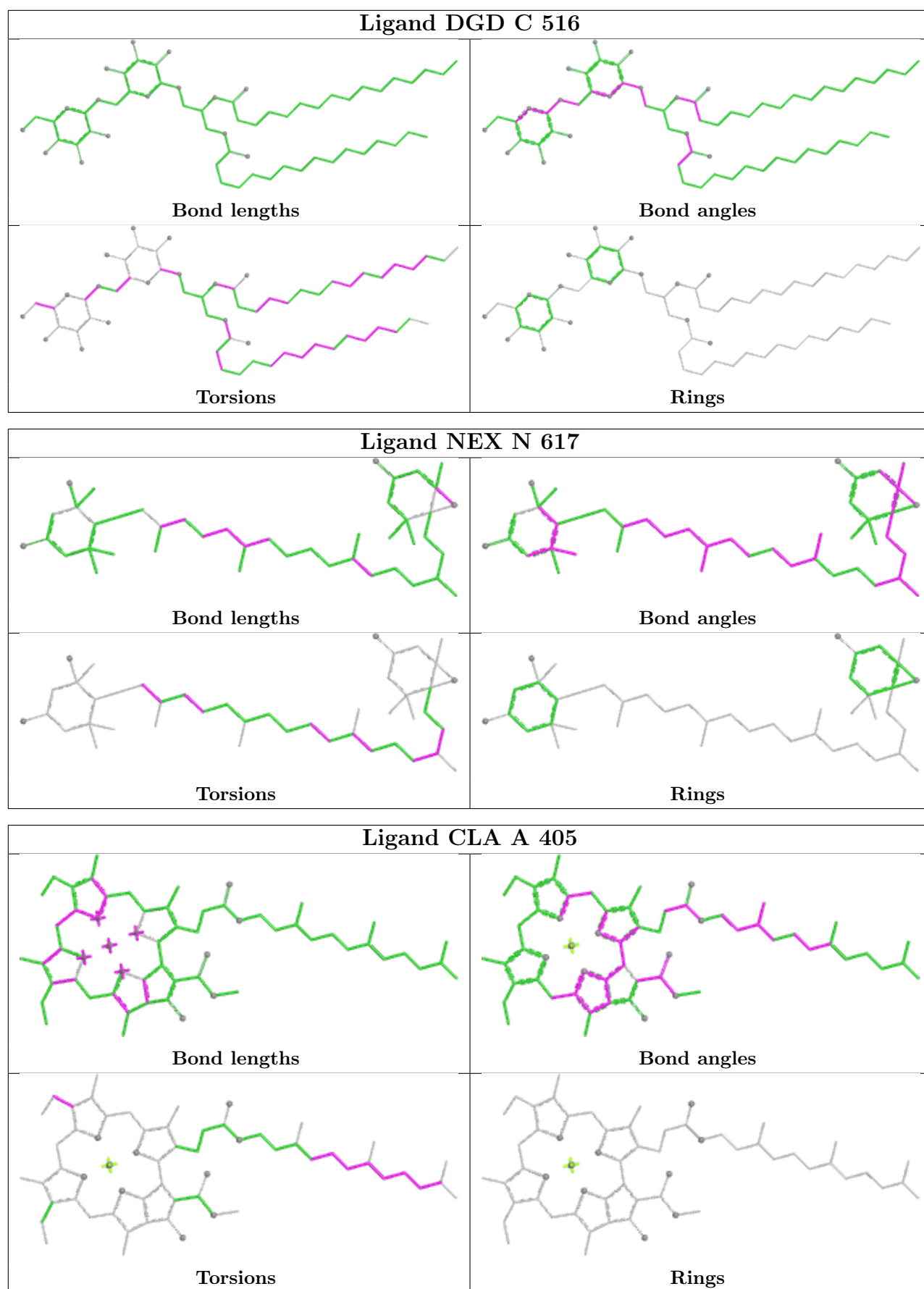


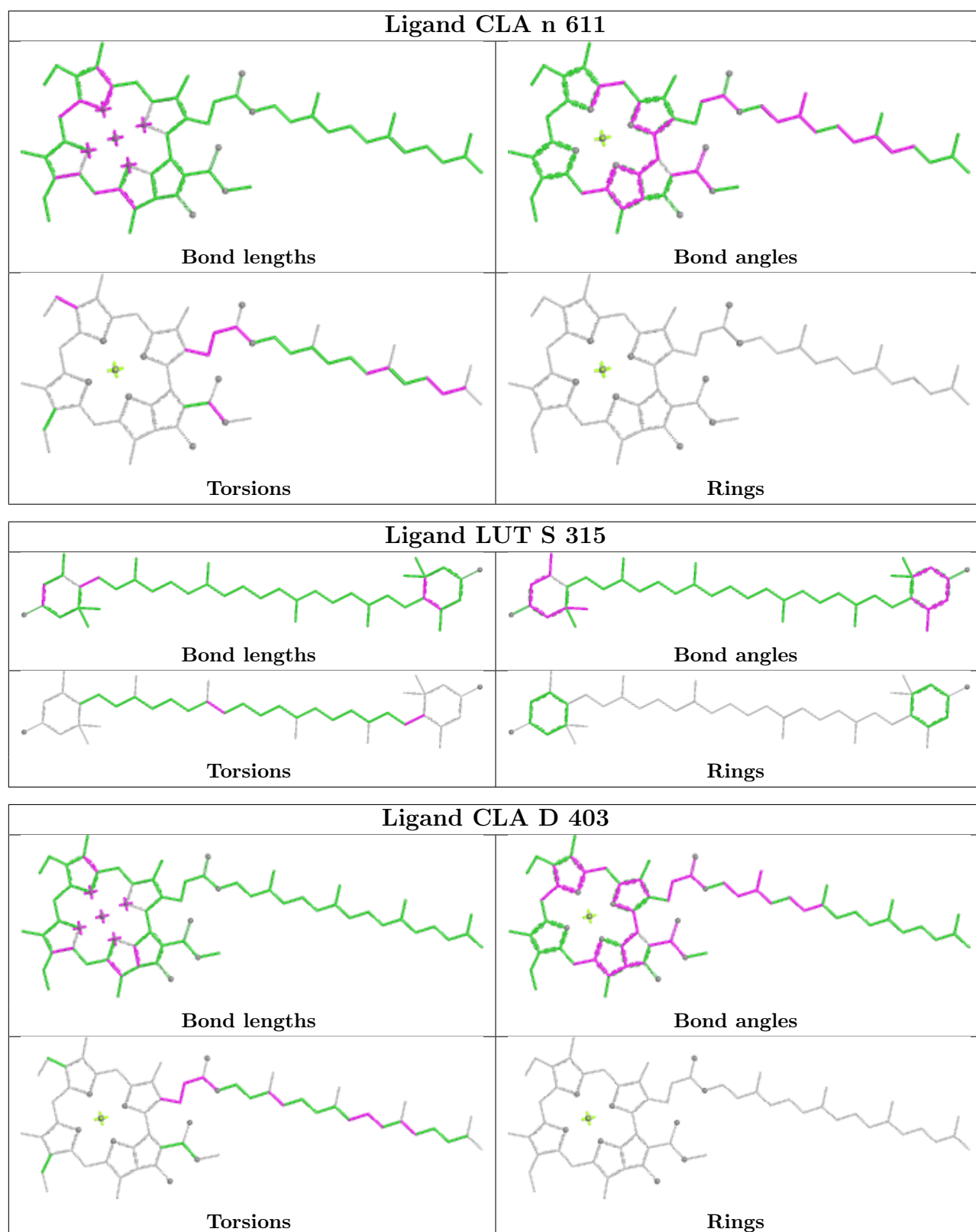
Ligand CHL R 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

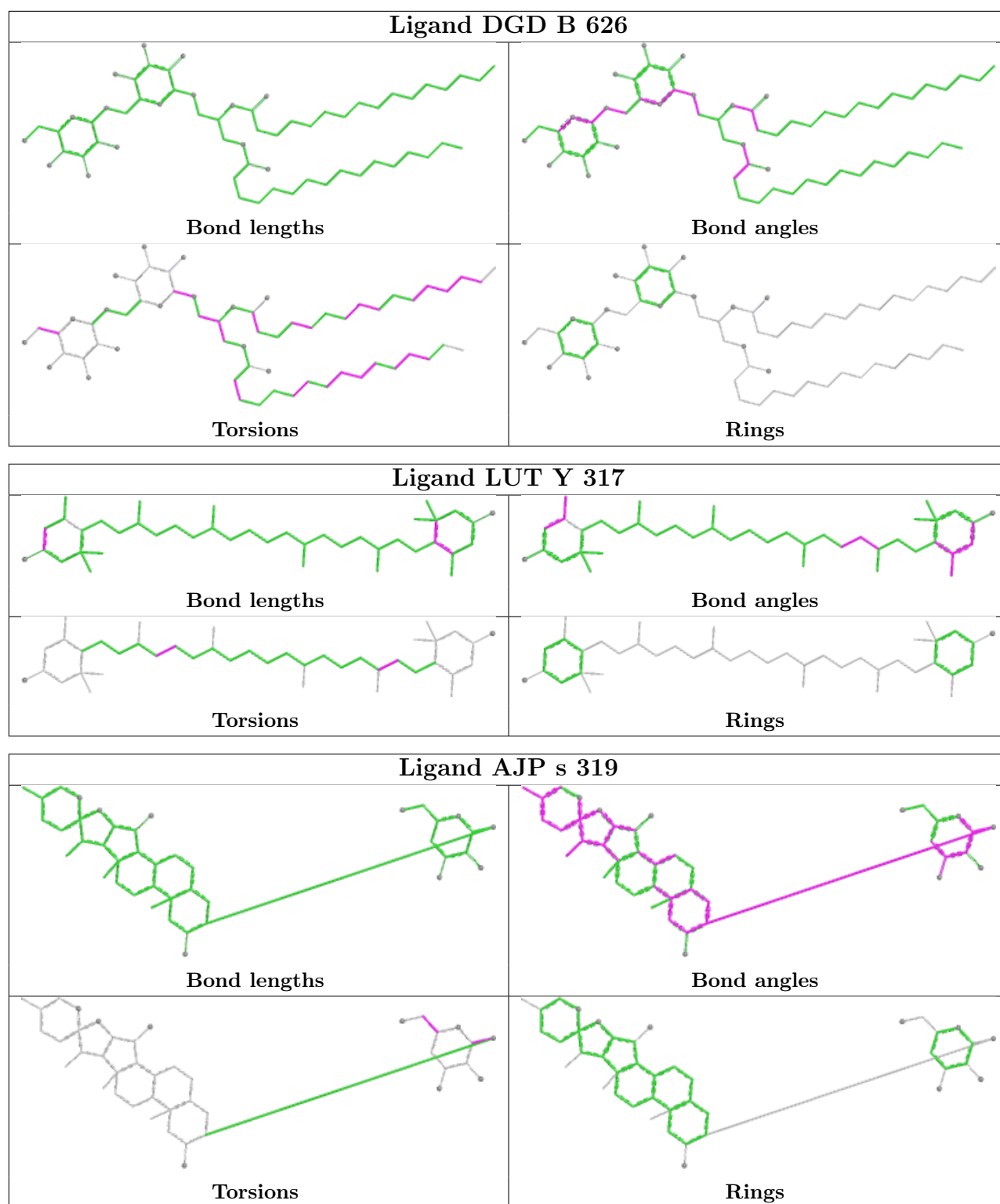
Ligand CHL G 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

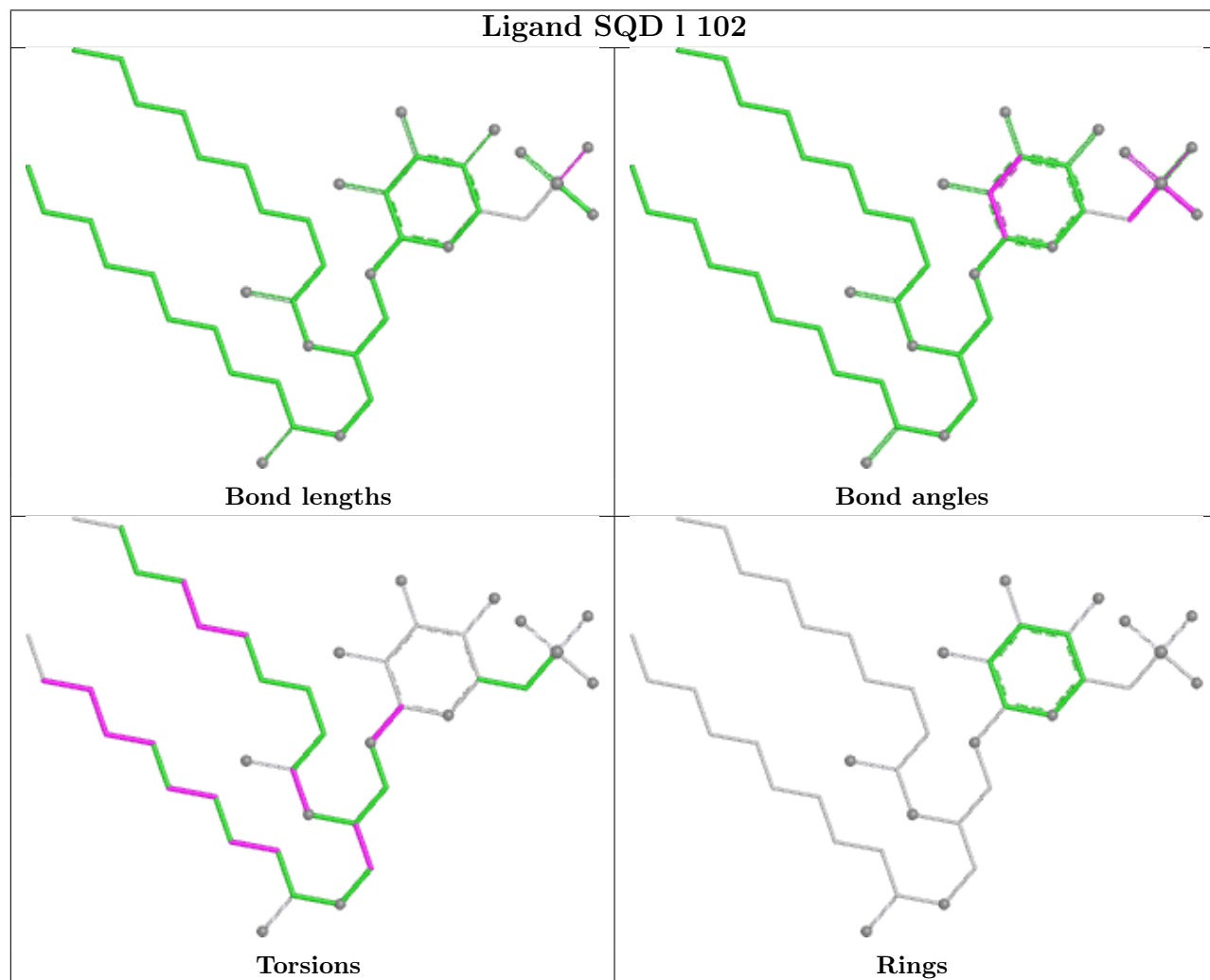
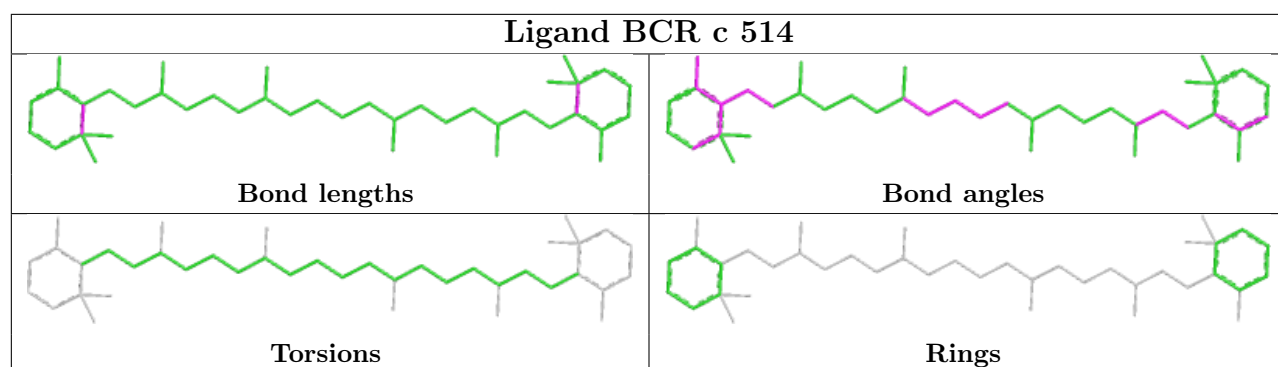
Ligand LUT N 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

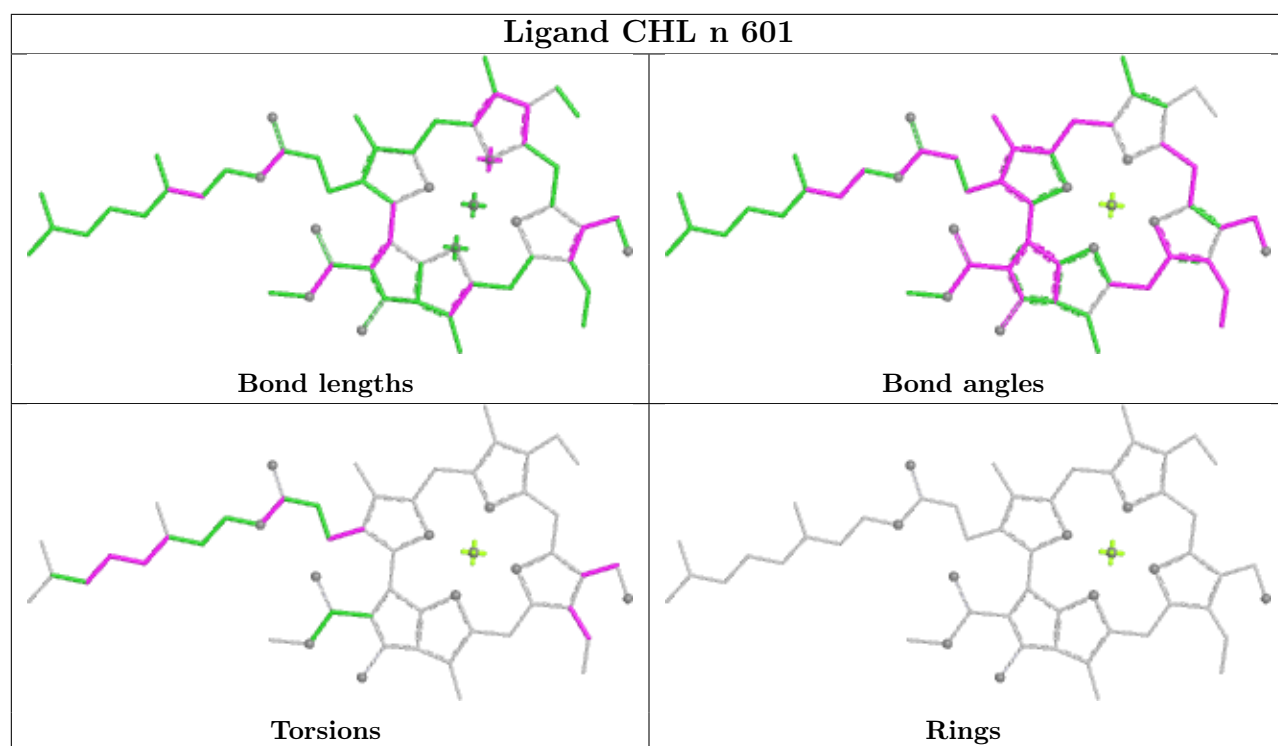




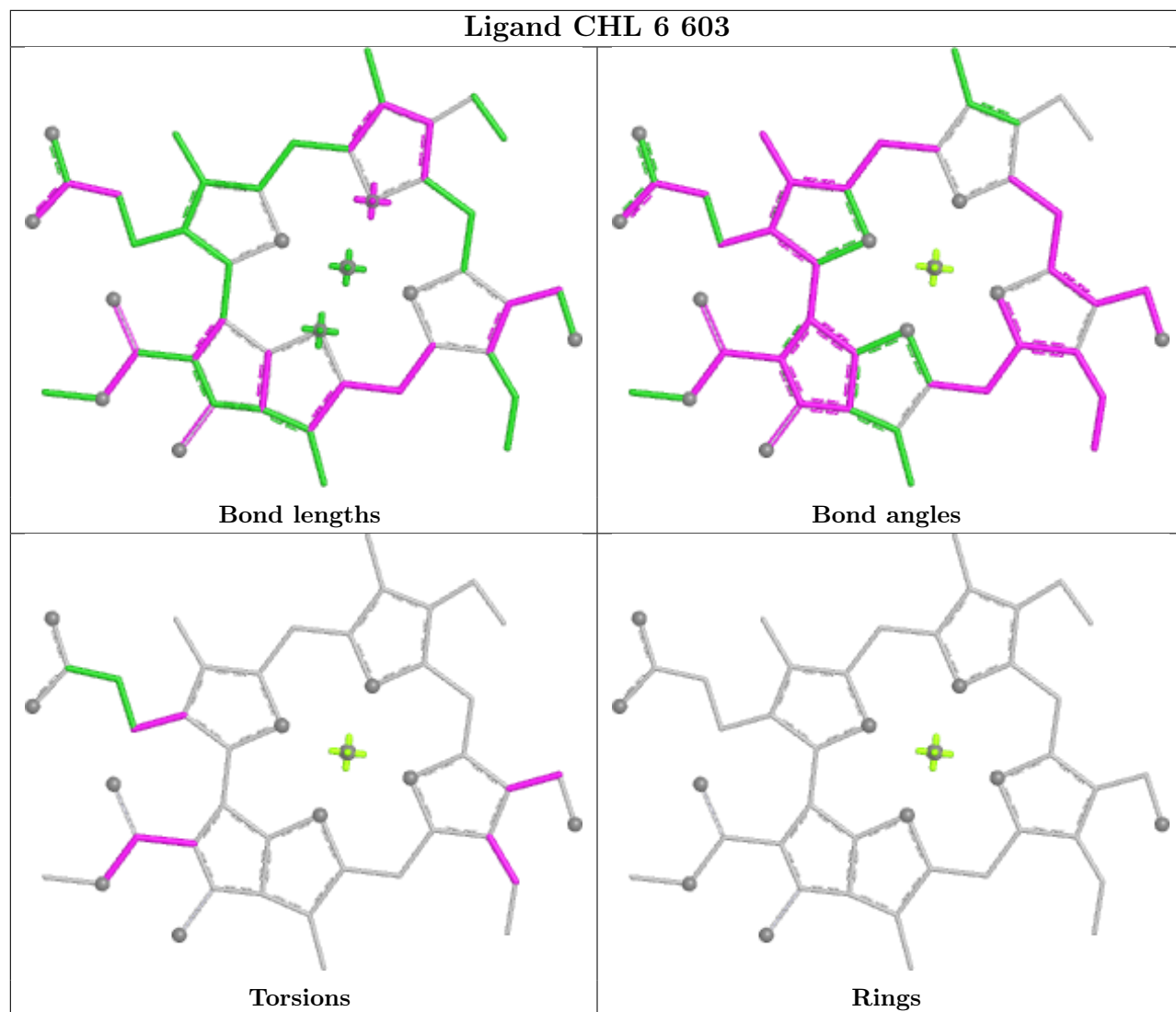




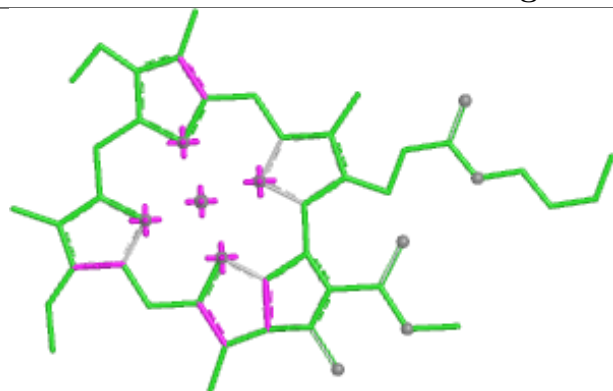




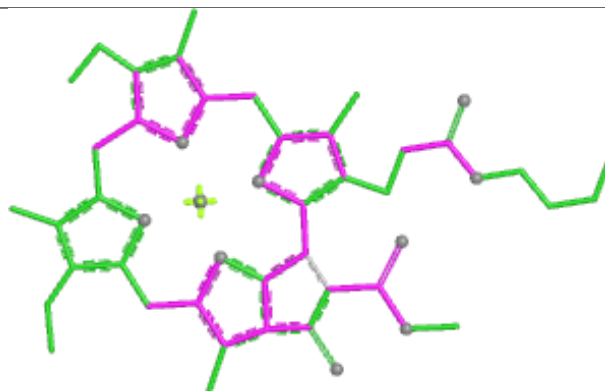
Ligand CHL 6 603



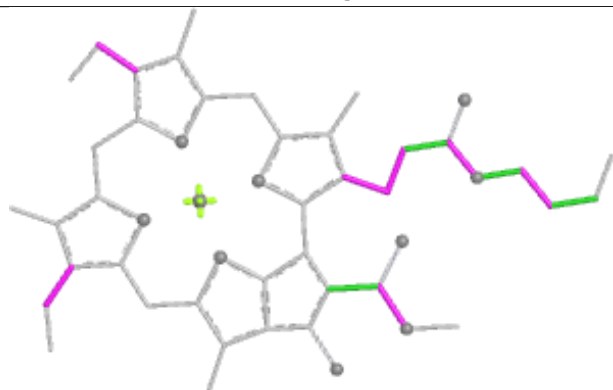
Ligand CLA r 601



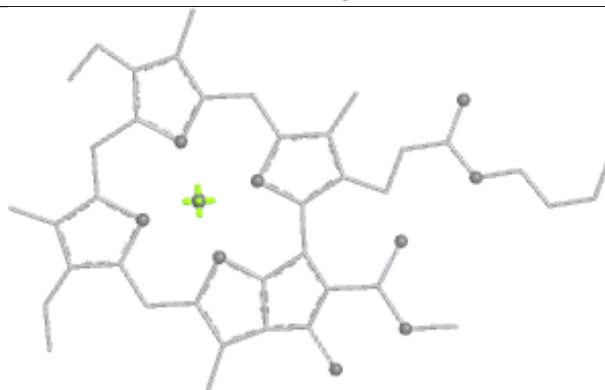
Bond lengths



Bond angles

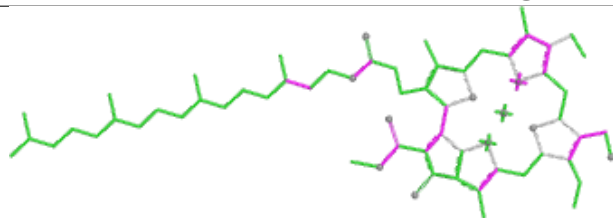


Torsions

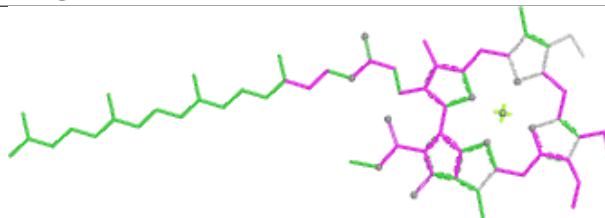


Rings

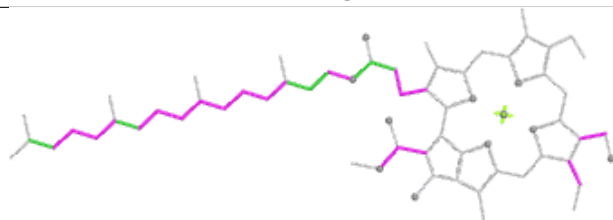
Ligand CHL g 608



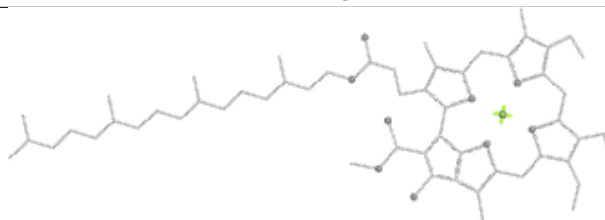
Bond lengths



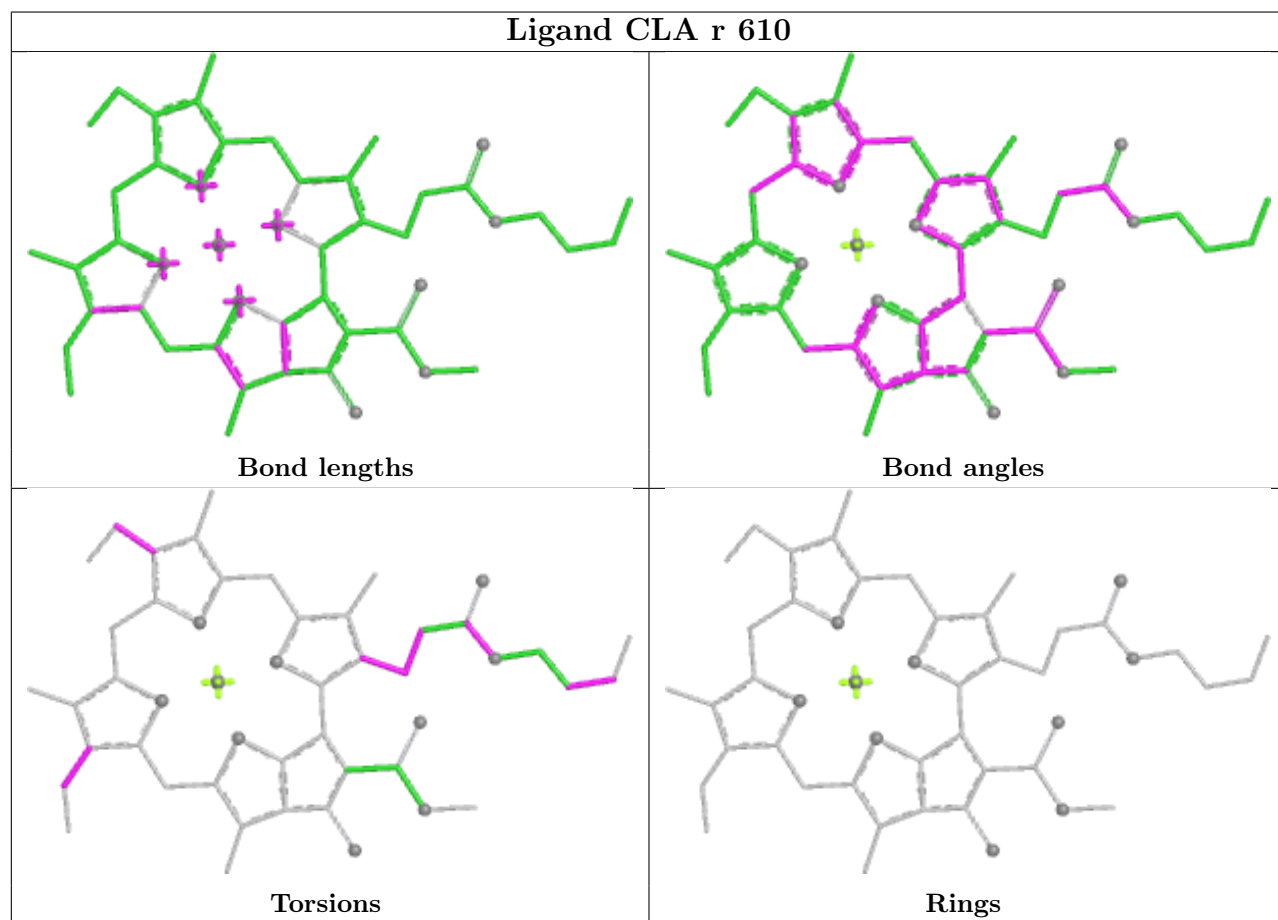
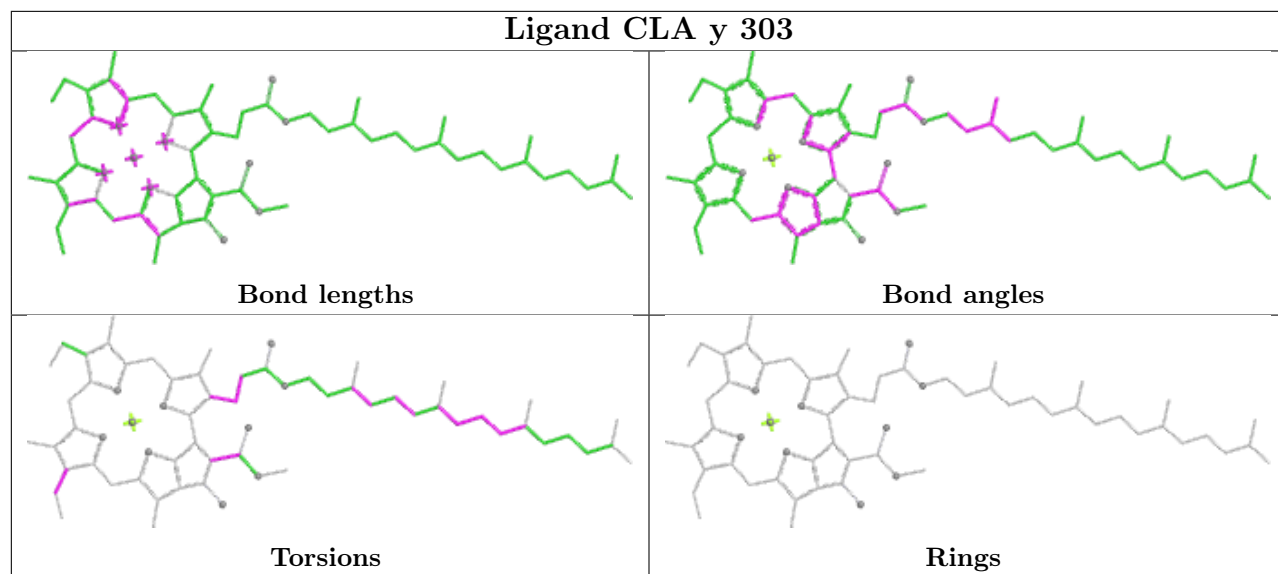
Bond angles

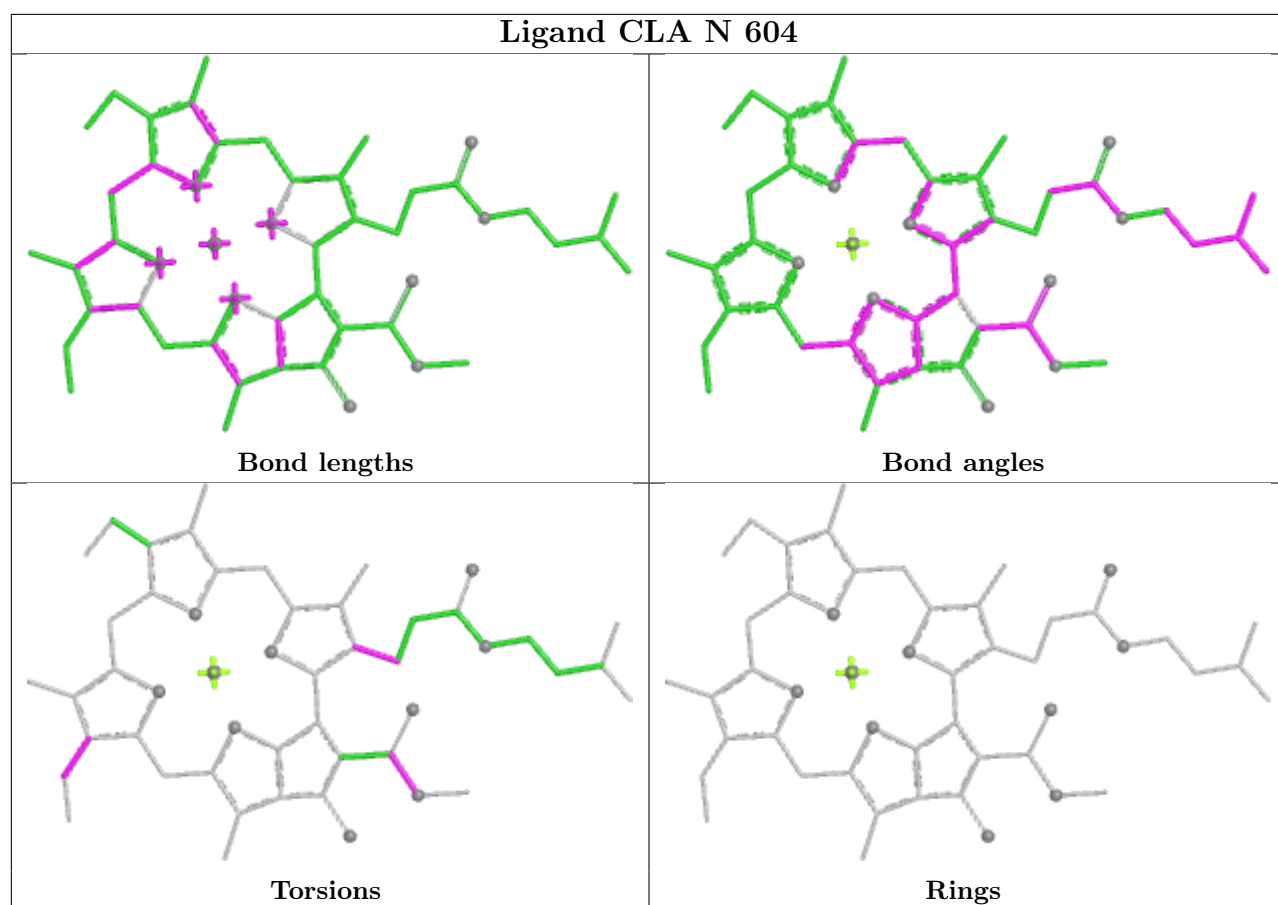


Torsions

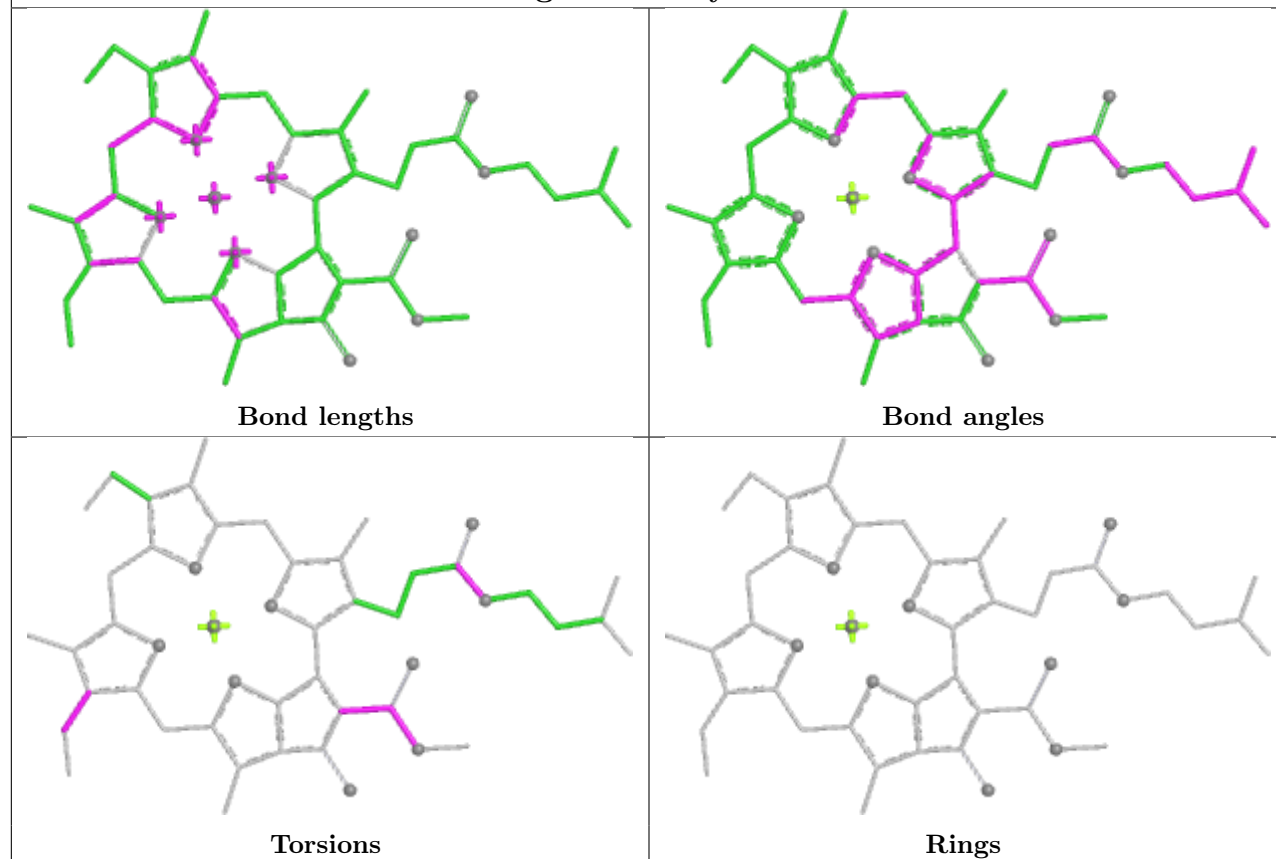


Rings

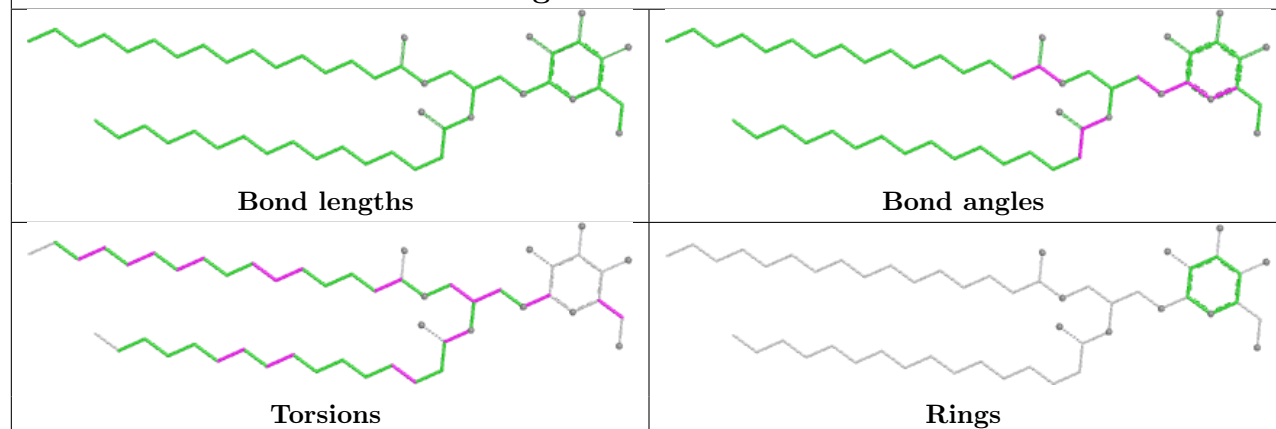




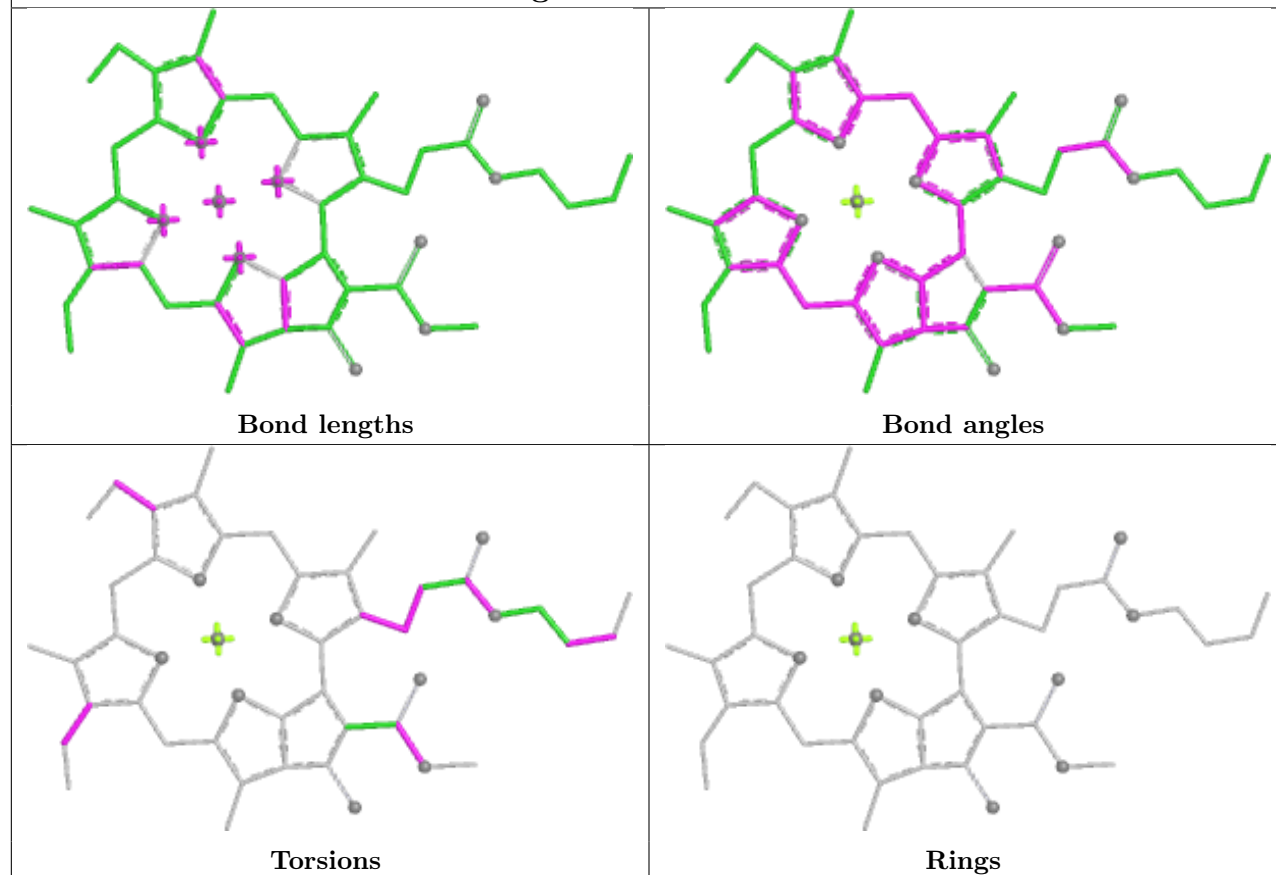
Ligand CLA y 305



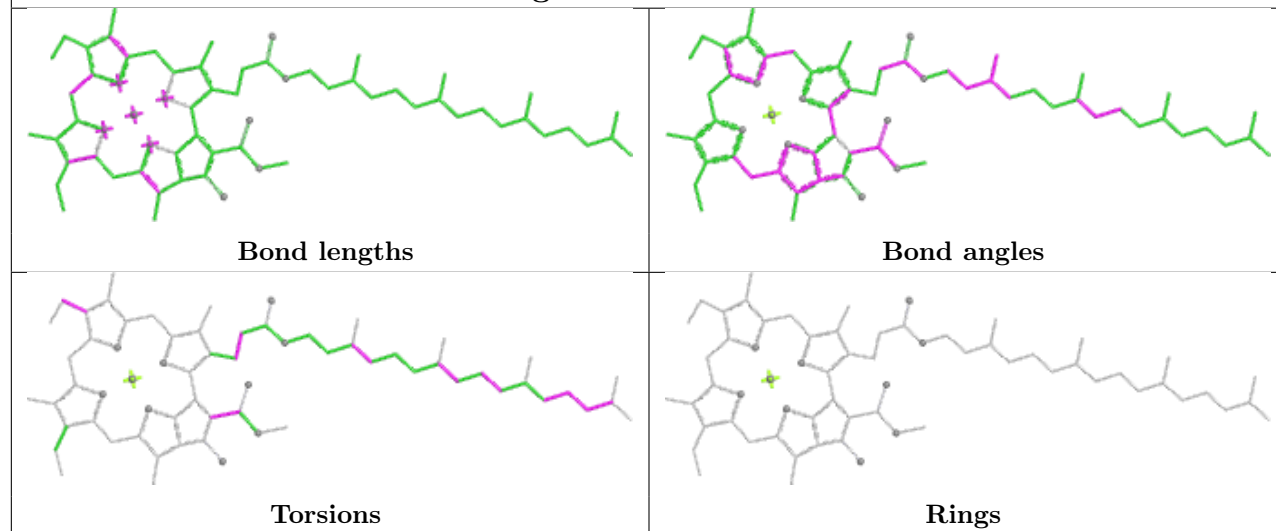
Ligand LMG c 520

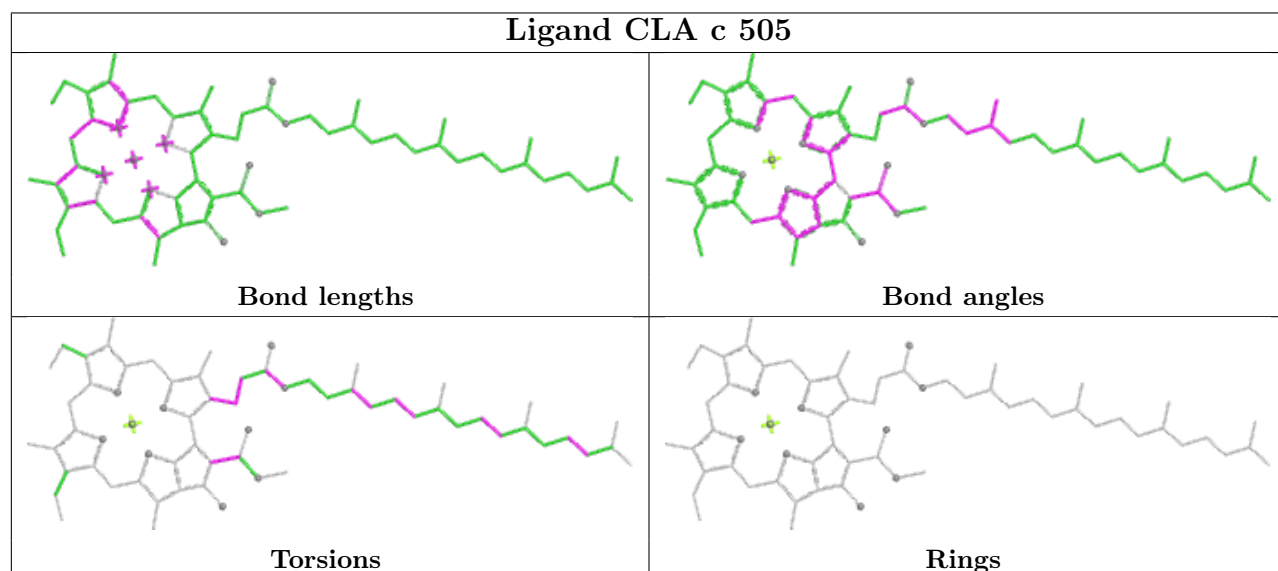
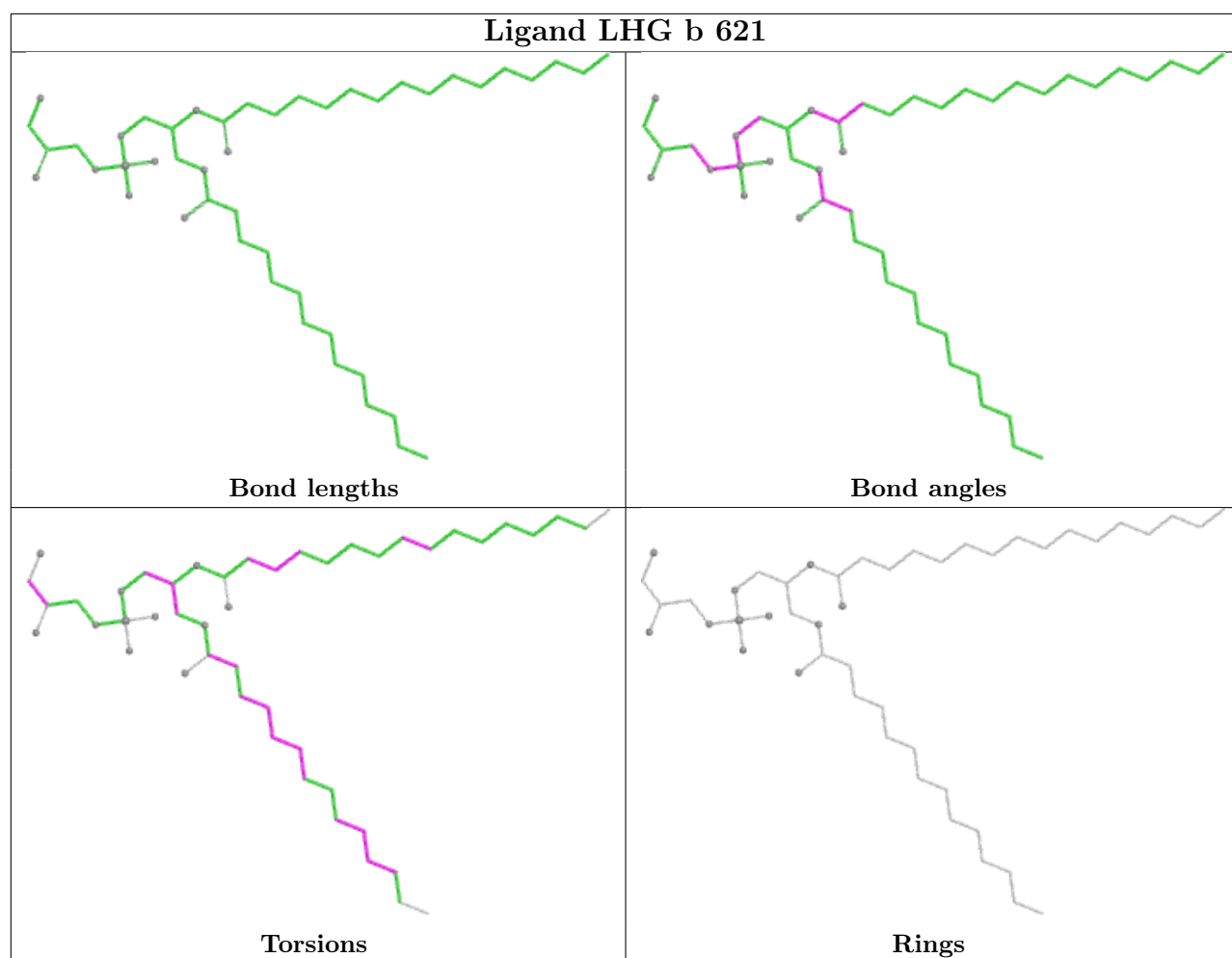


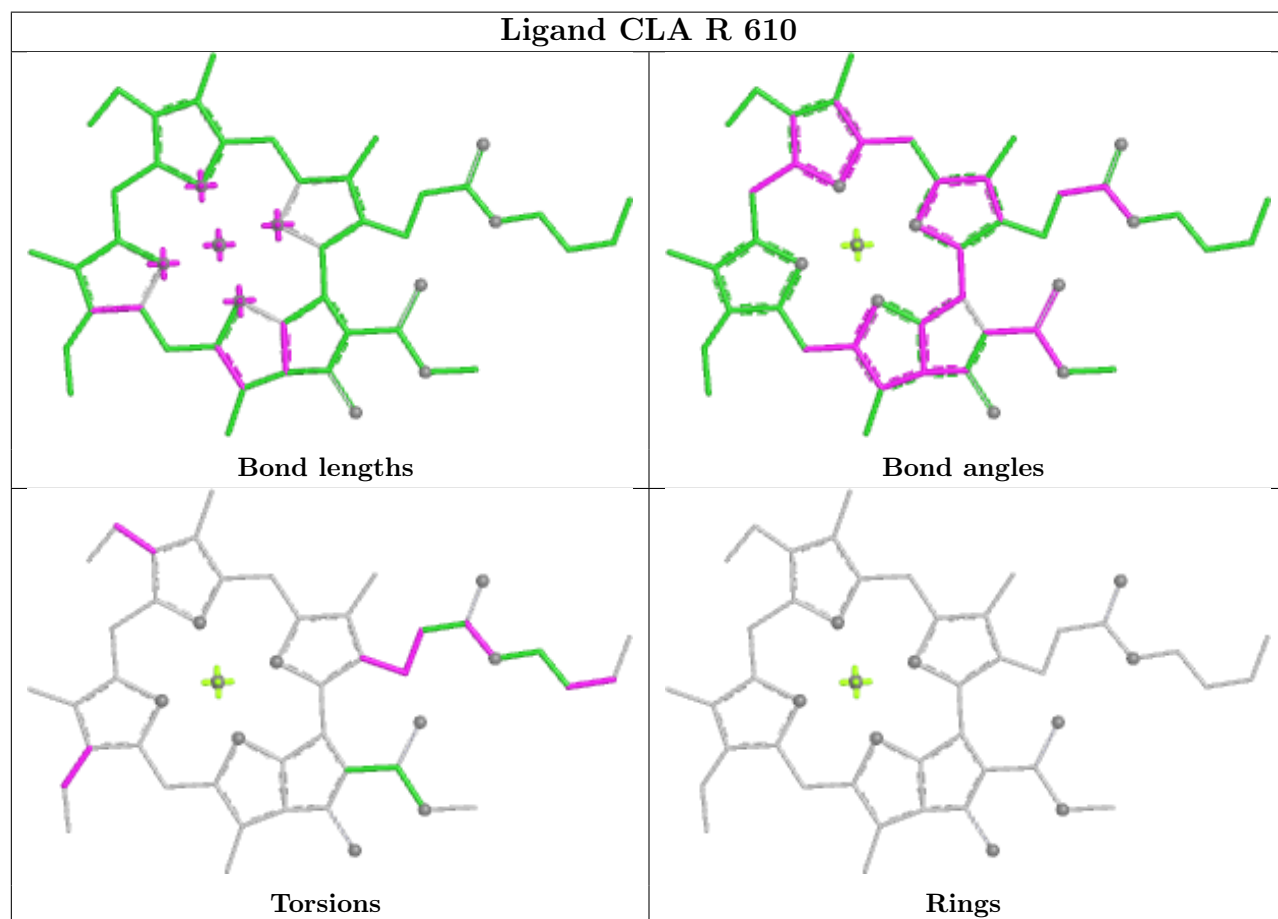
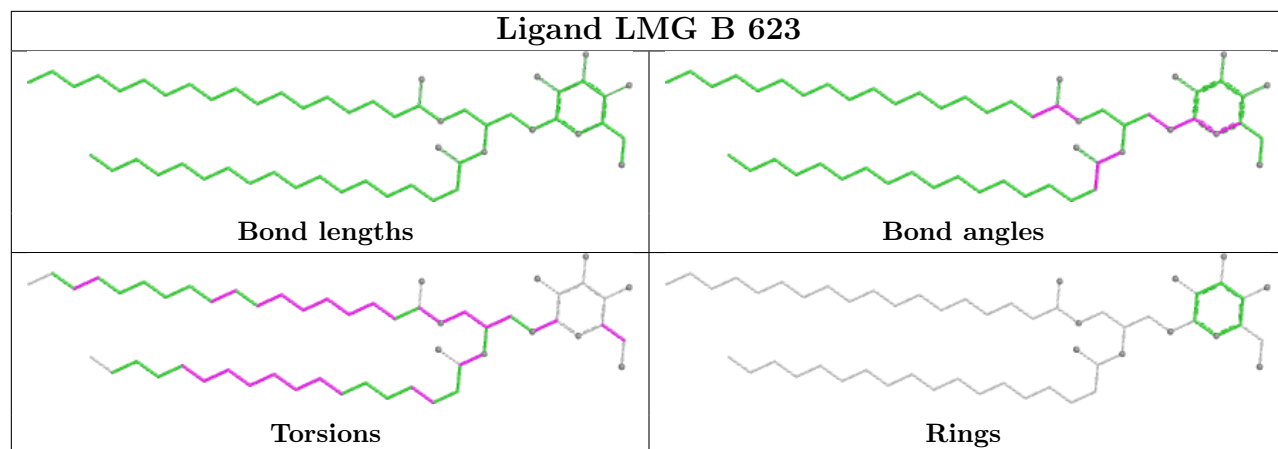
Ligand CLA R 611

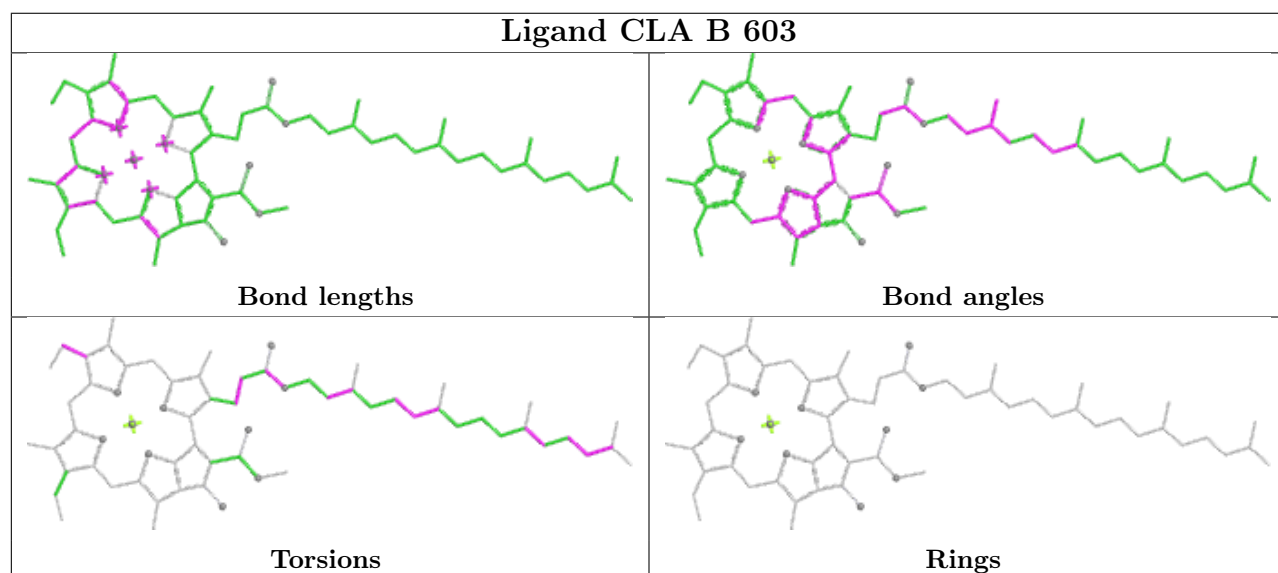
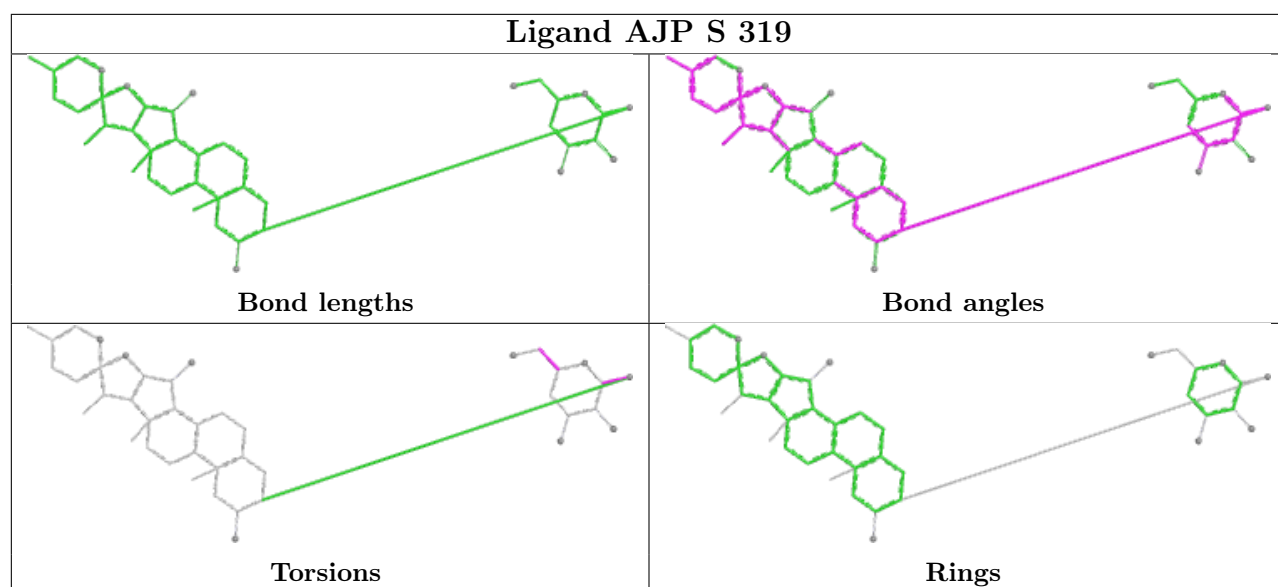


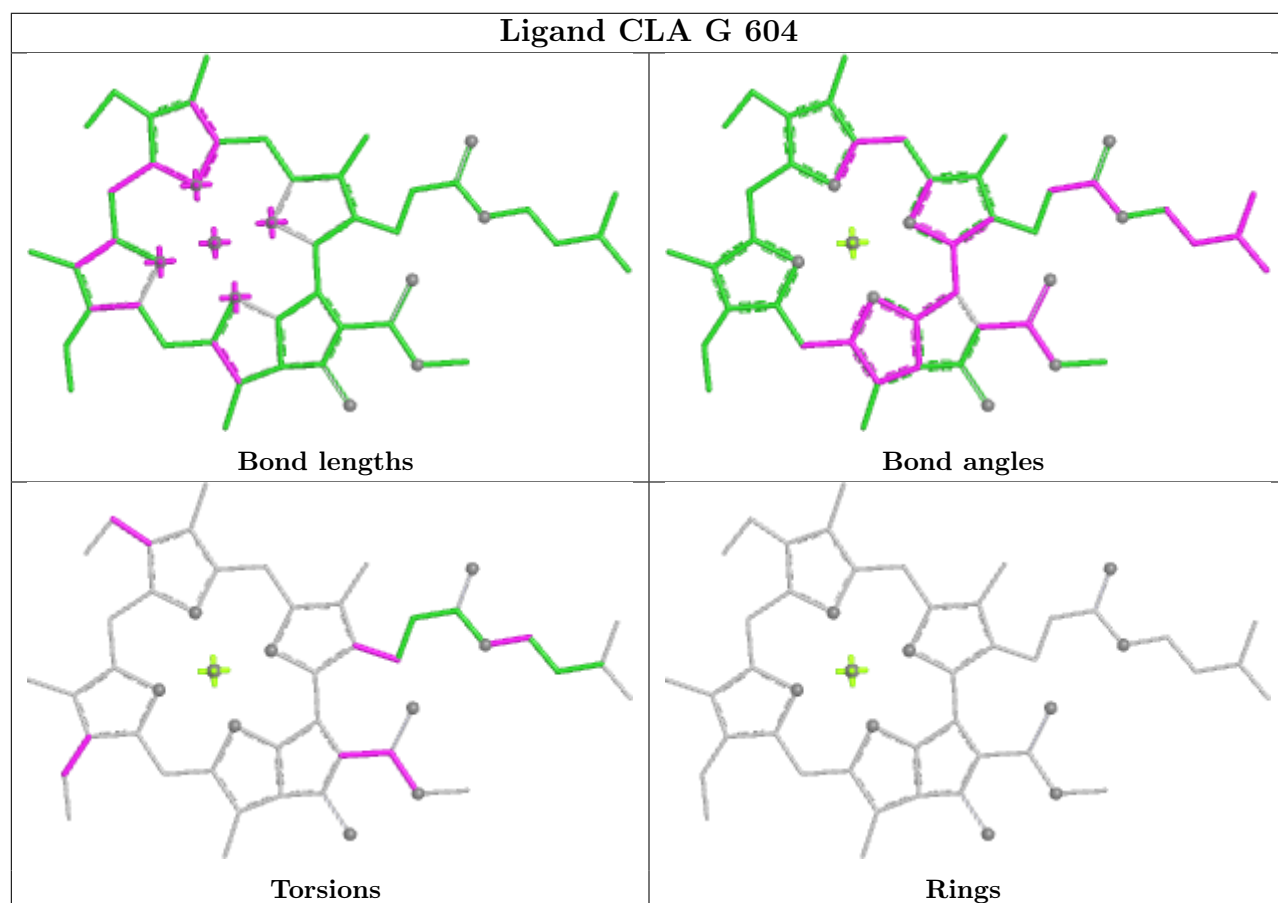
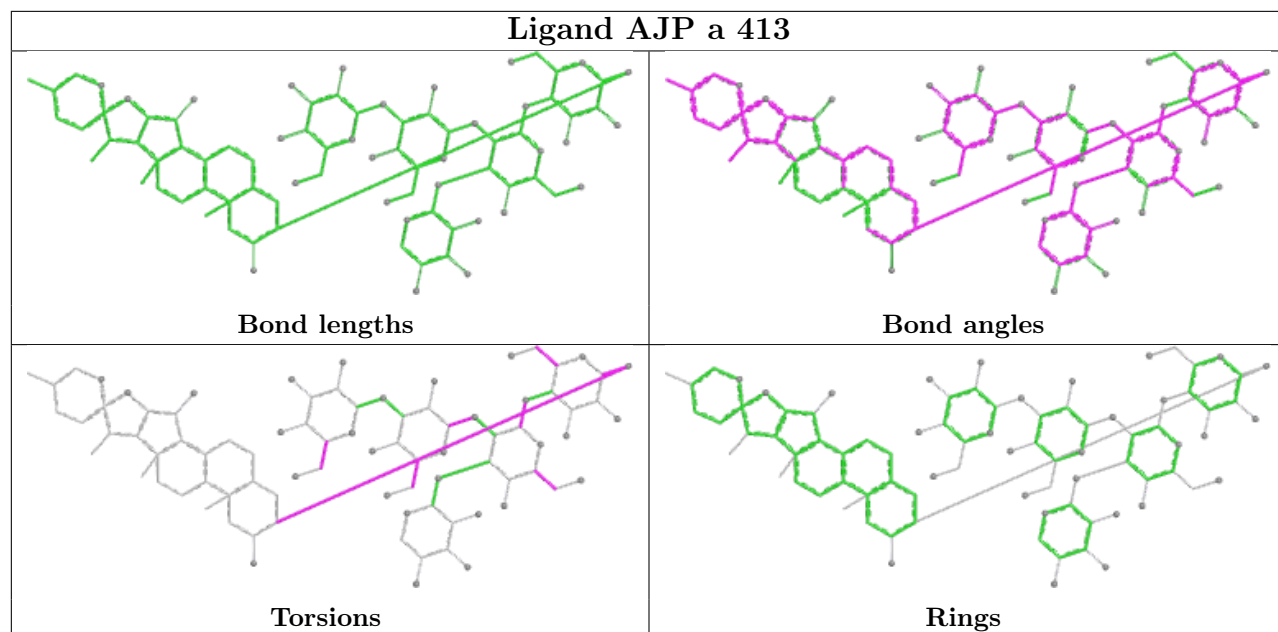
Ligand CLA B 606

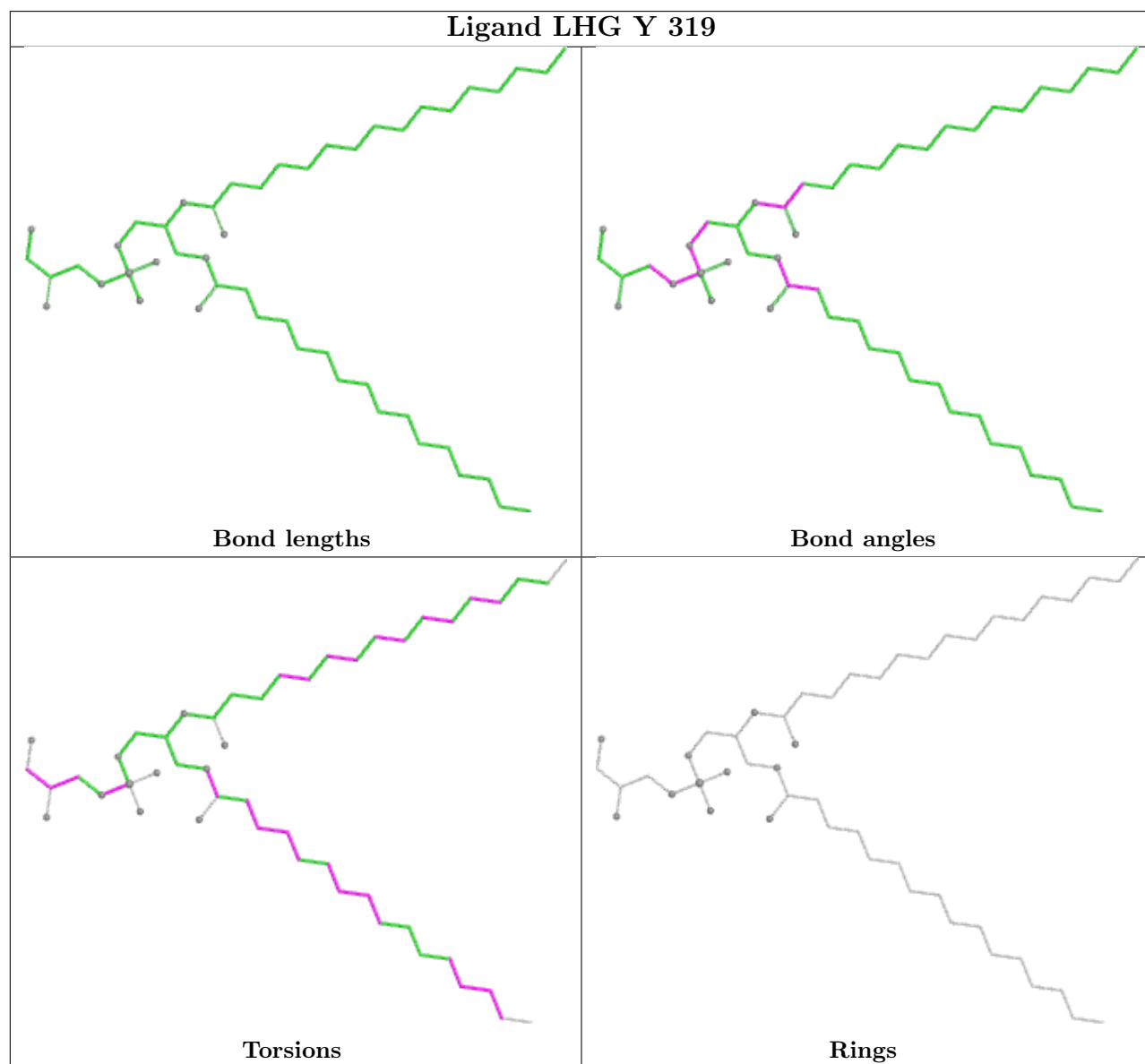
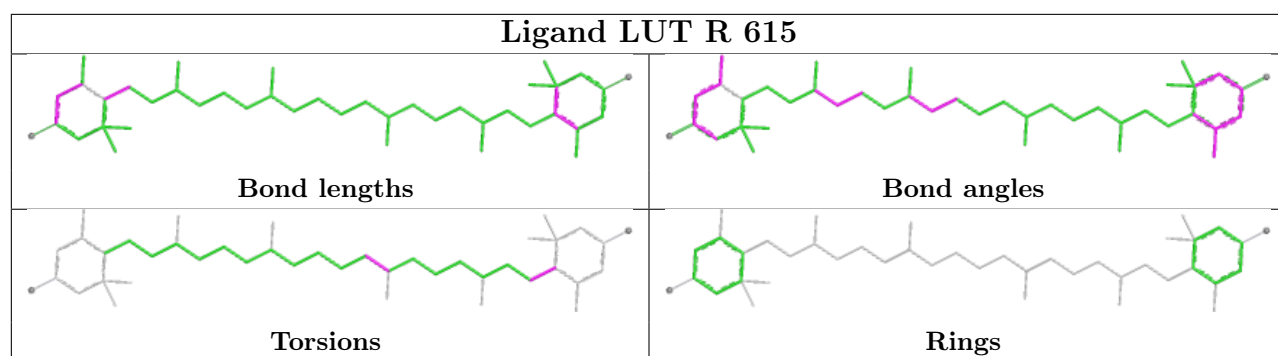


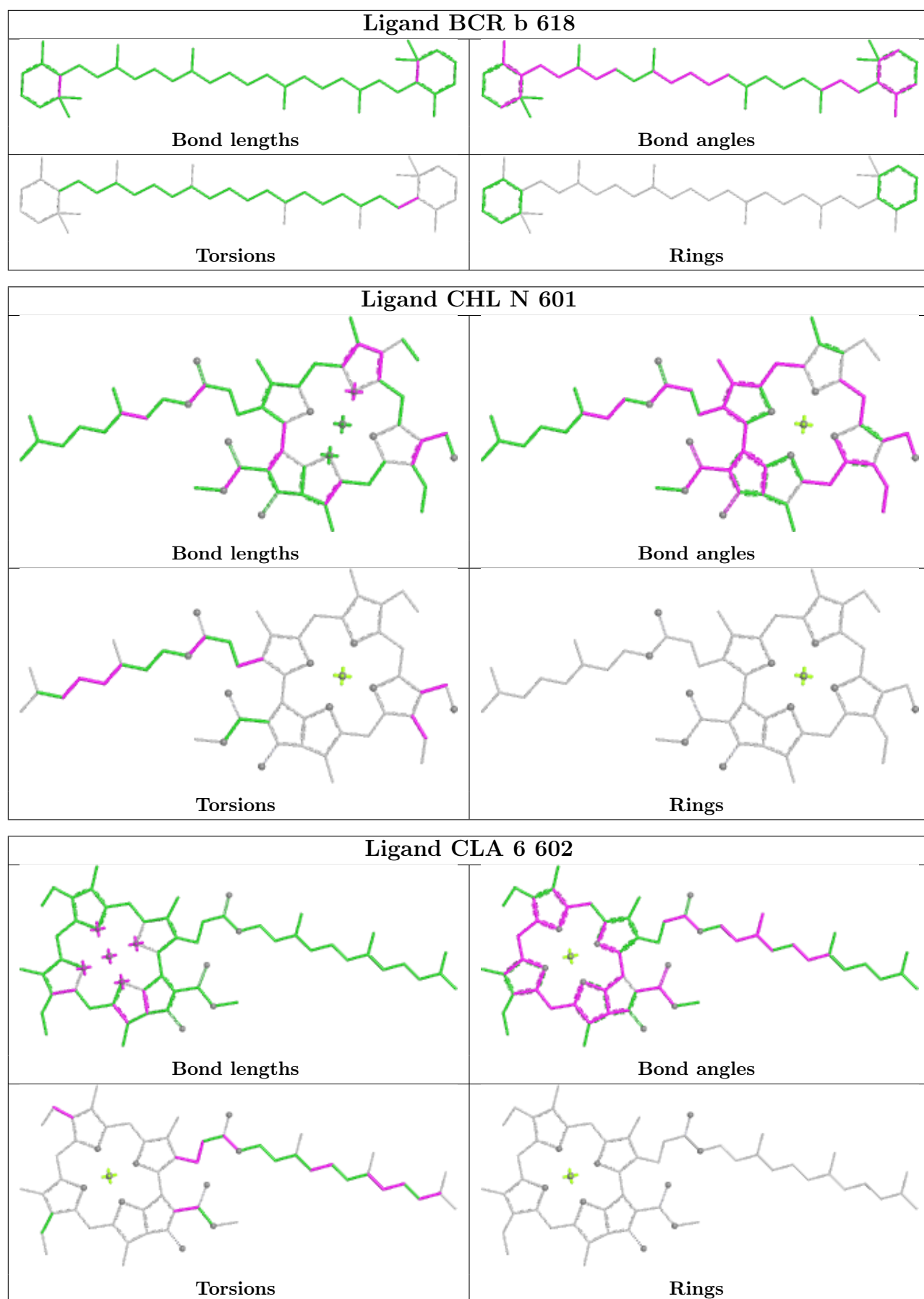


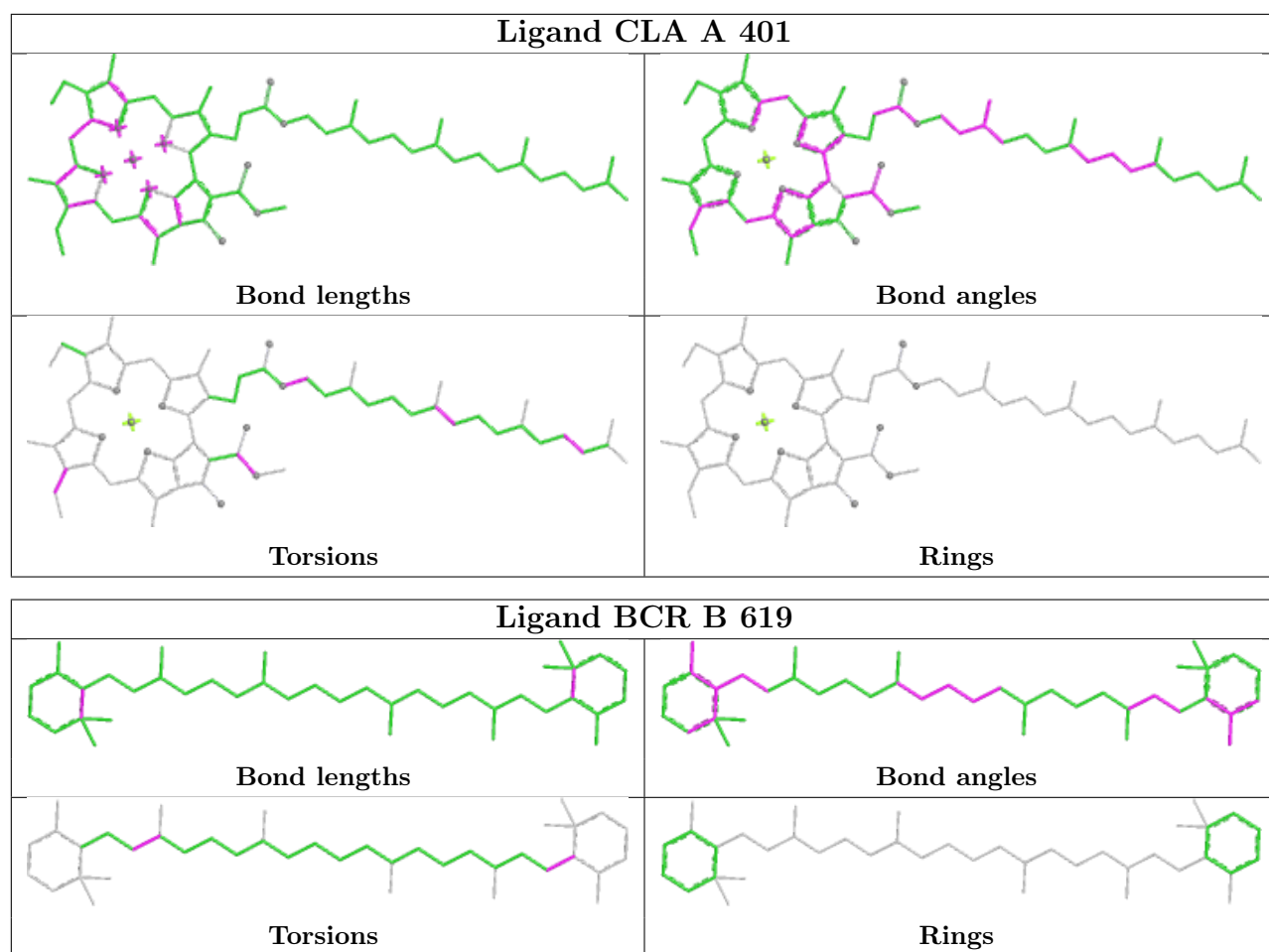




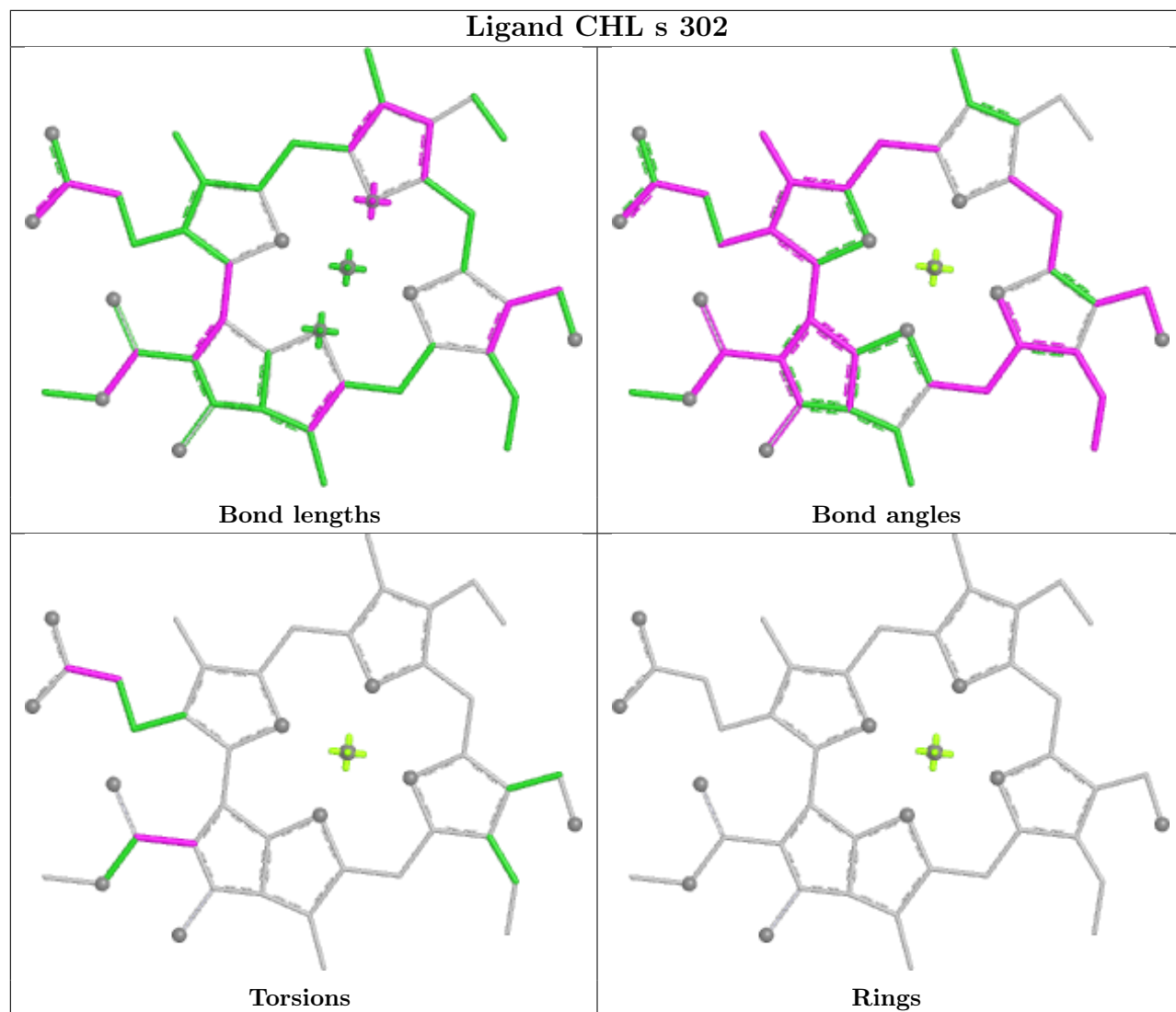


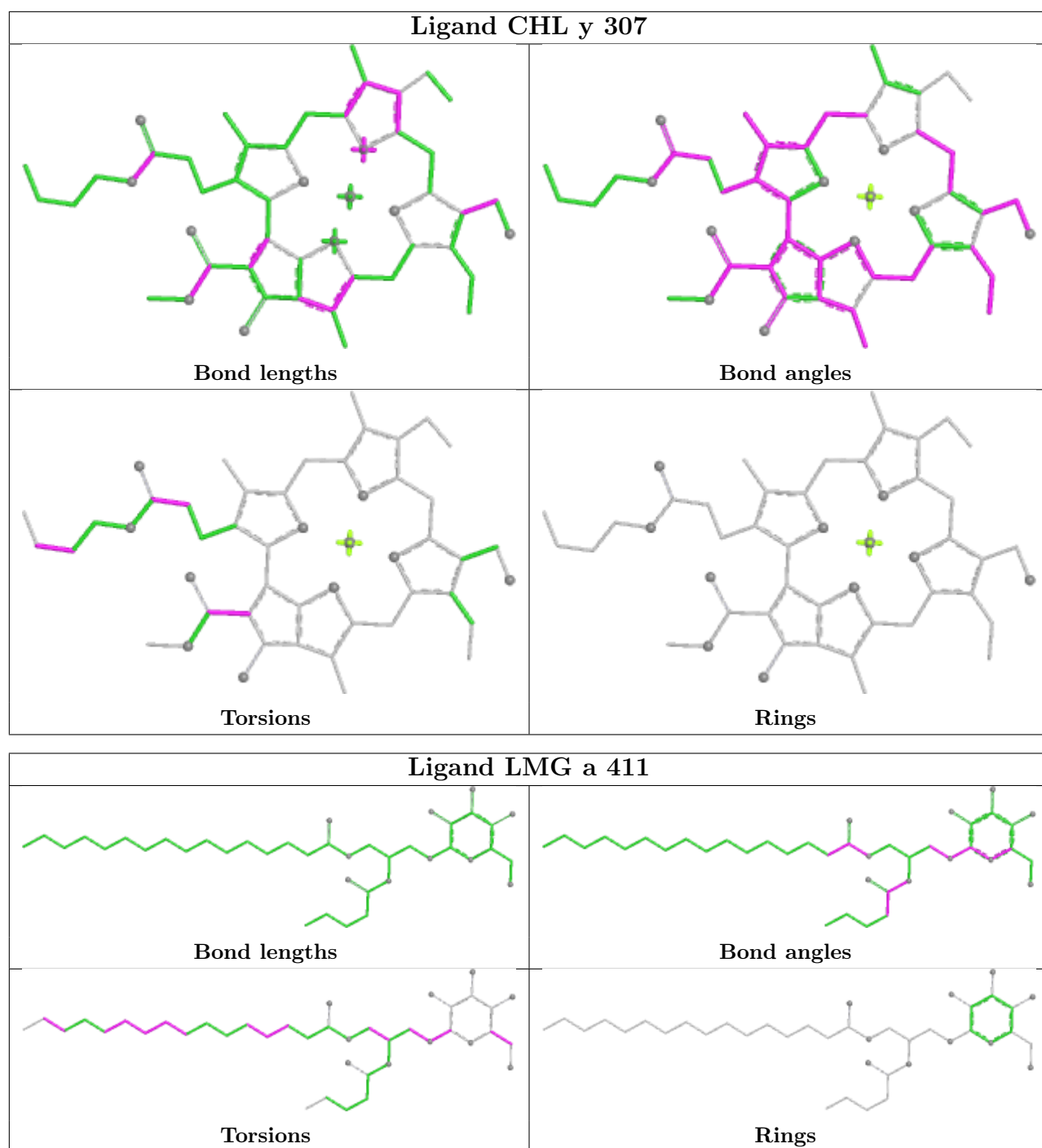


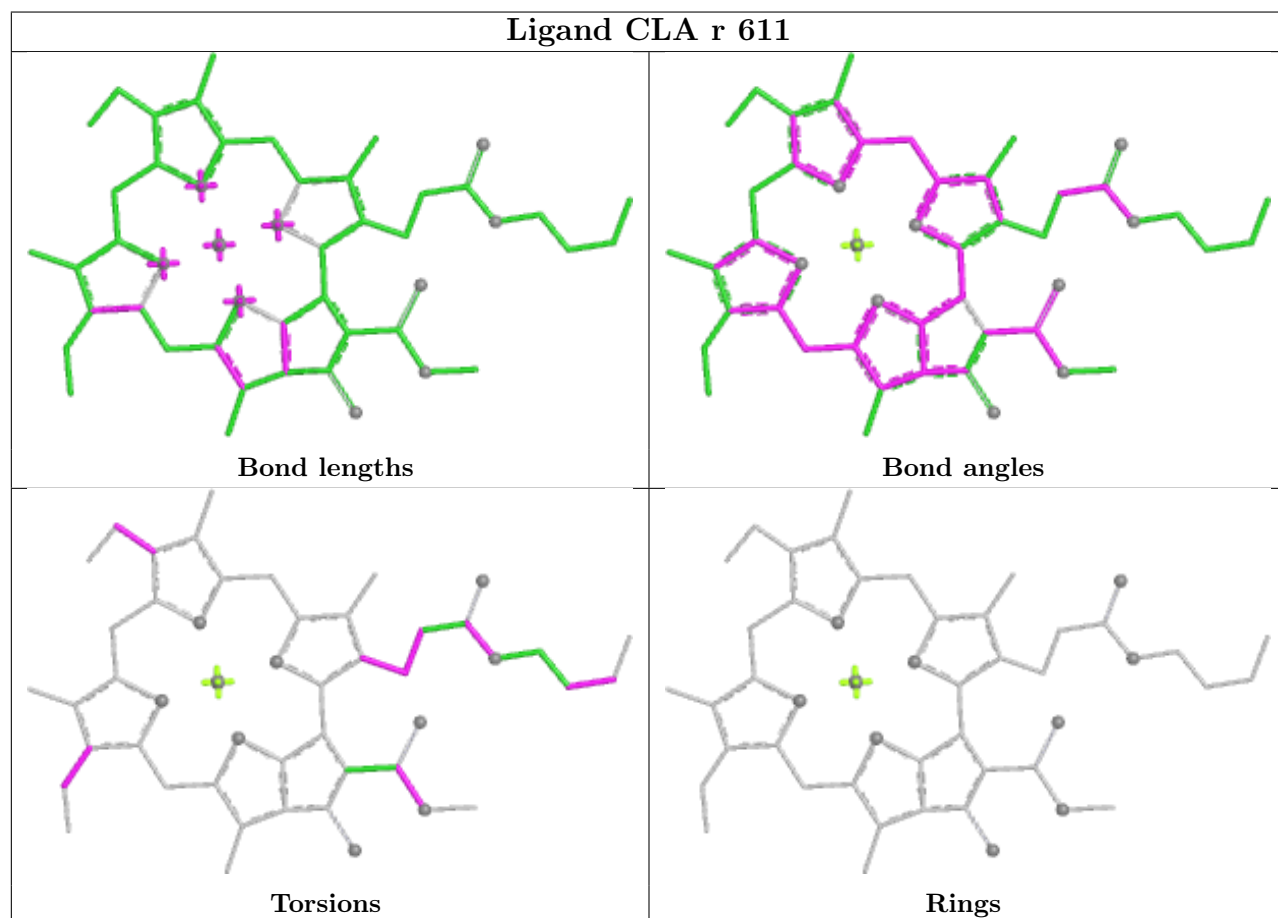
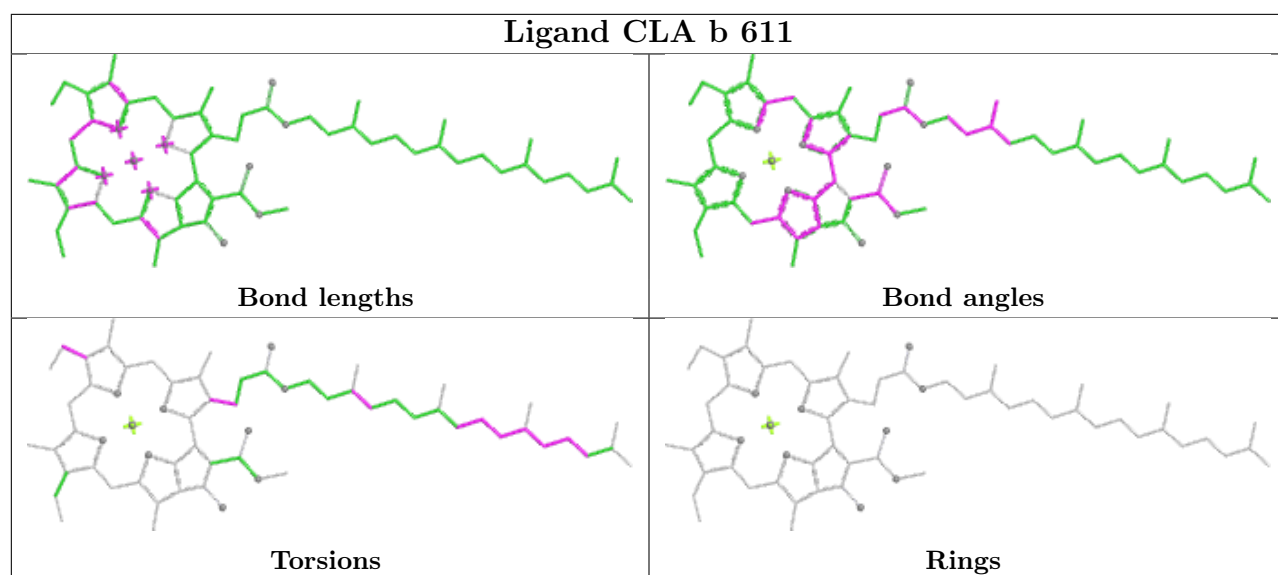


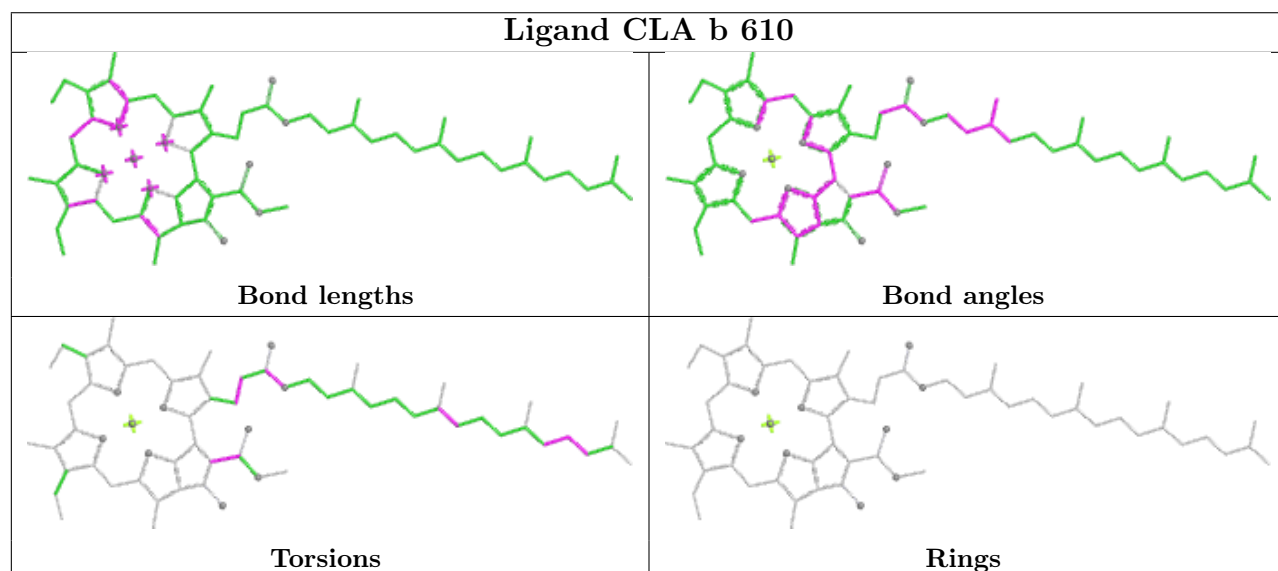
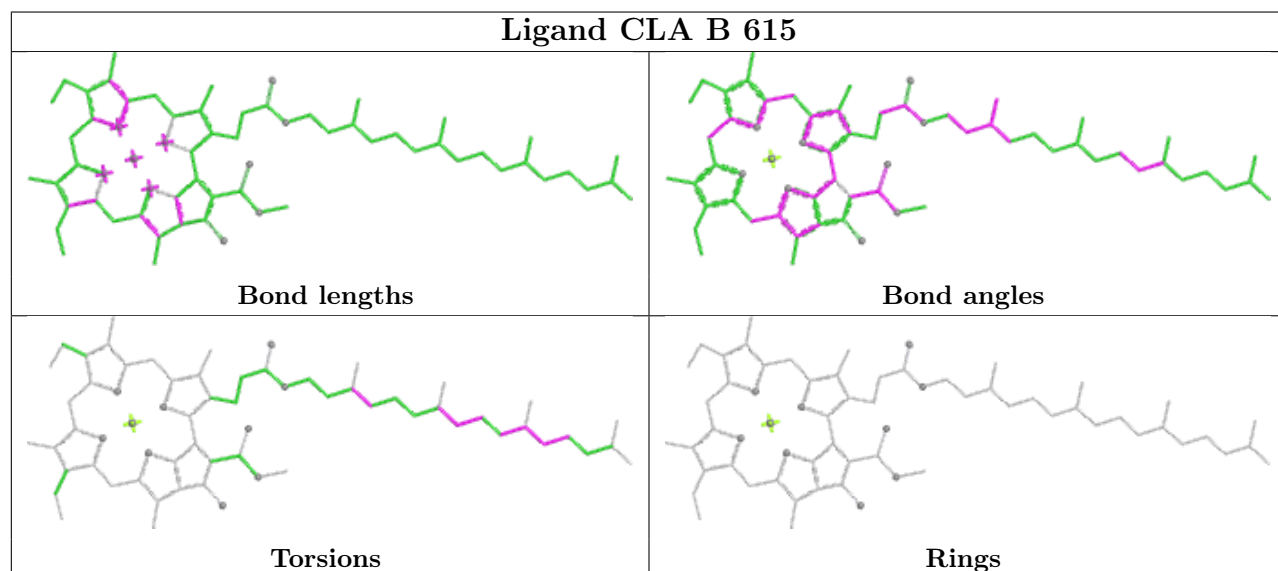
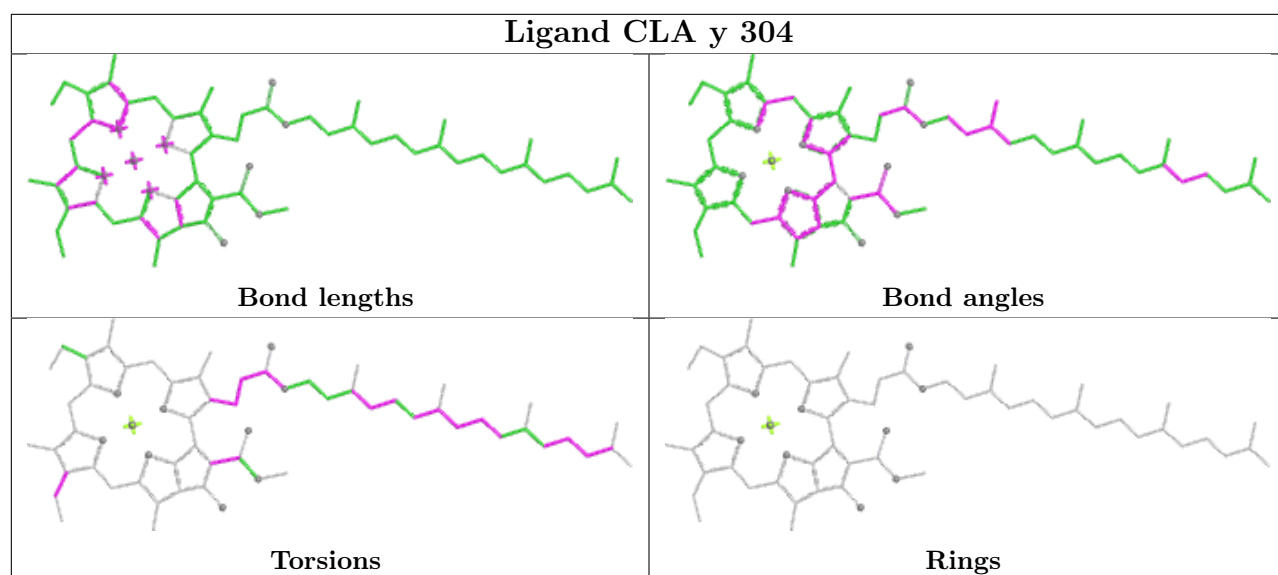


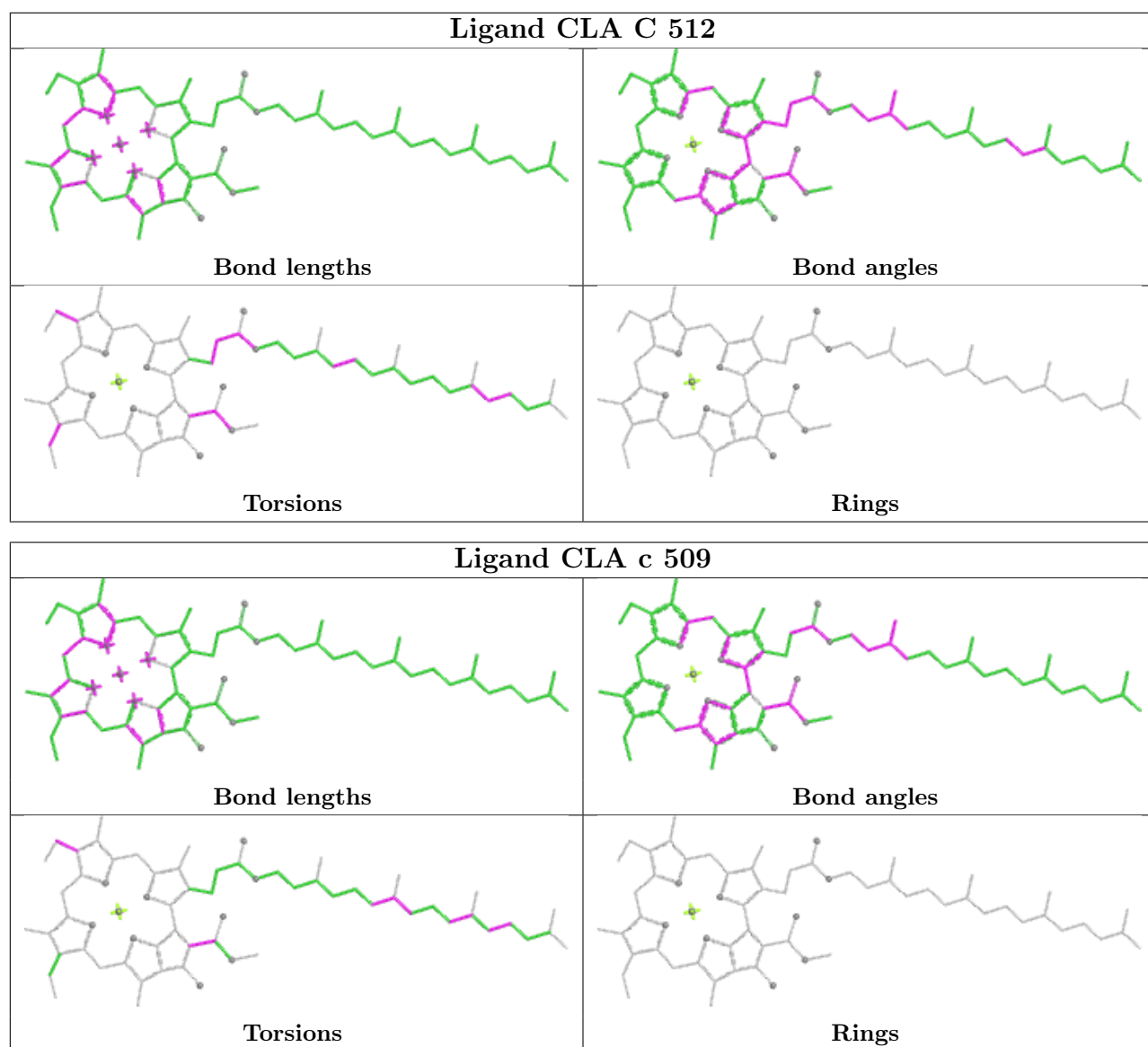
Ligand CHL s 302



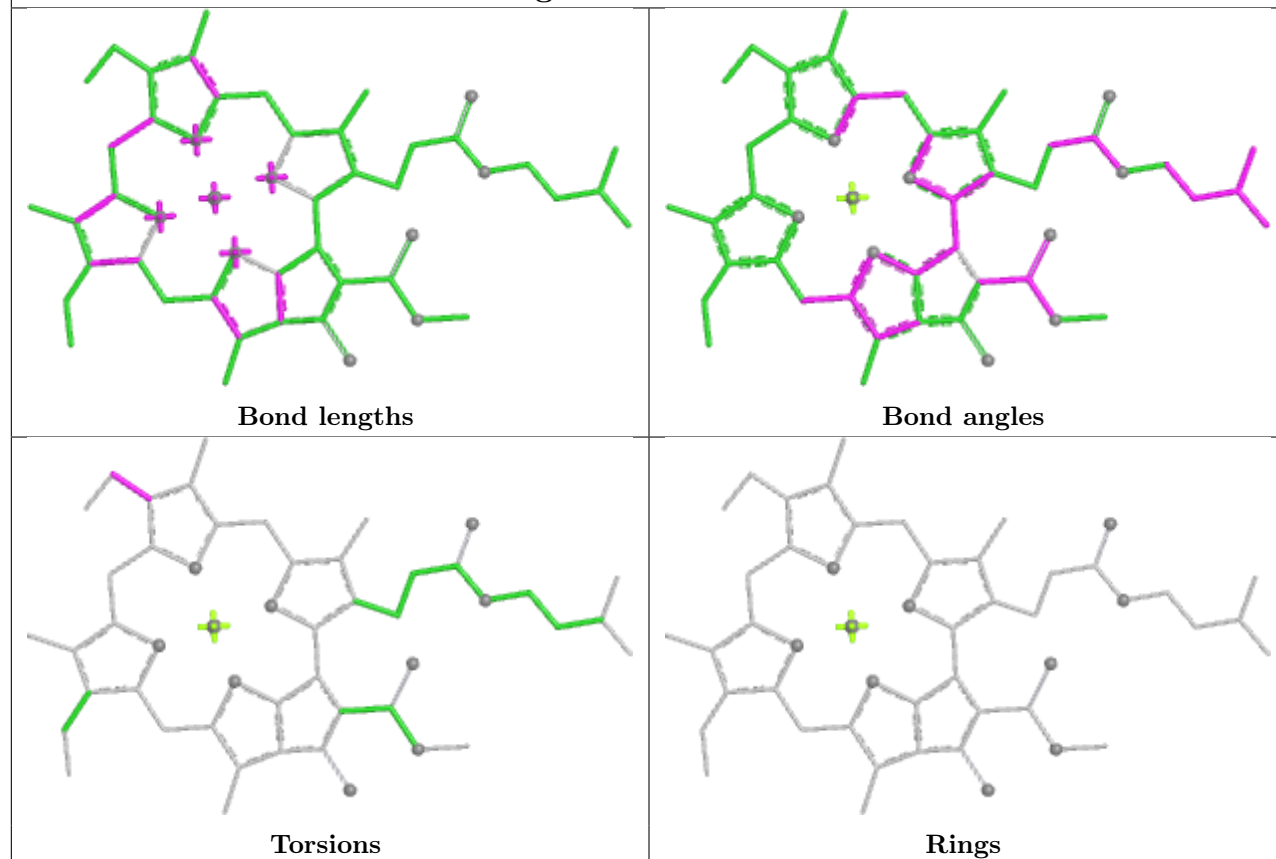




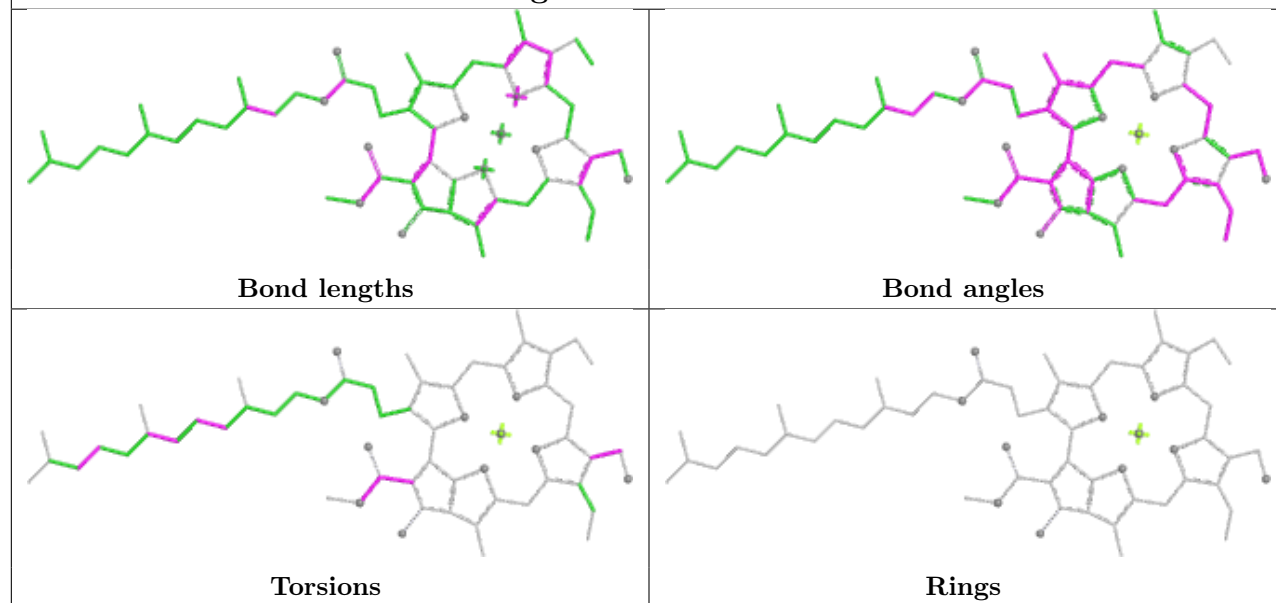


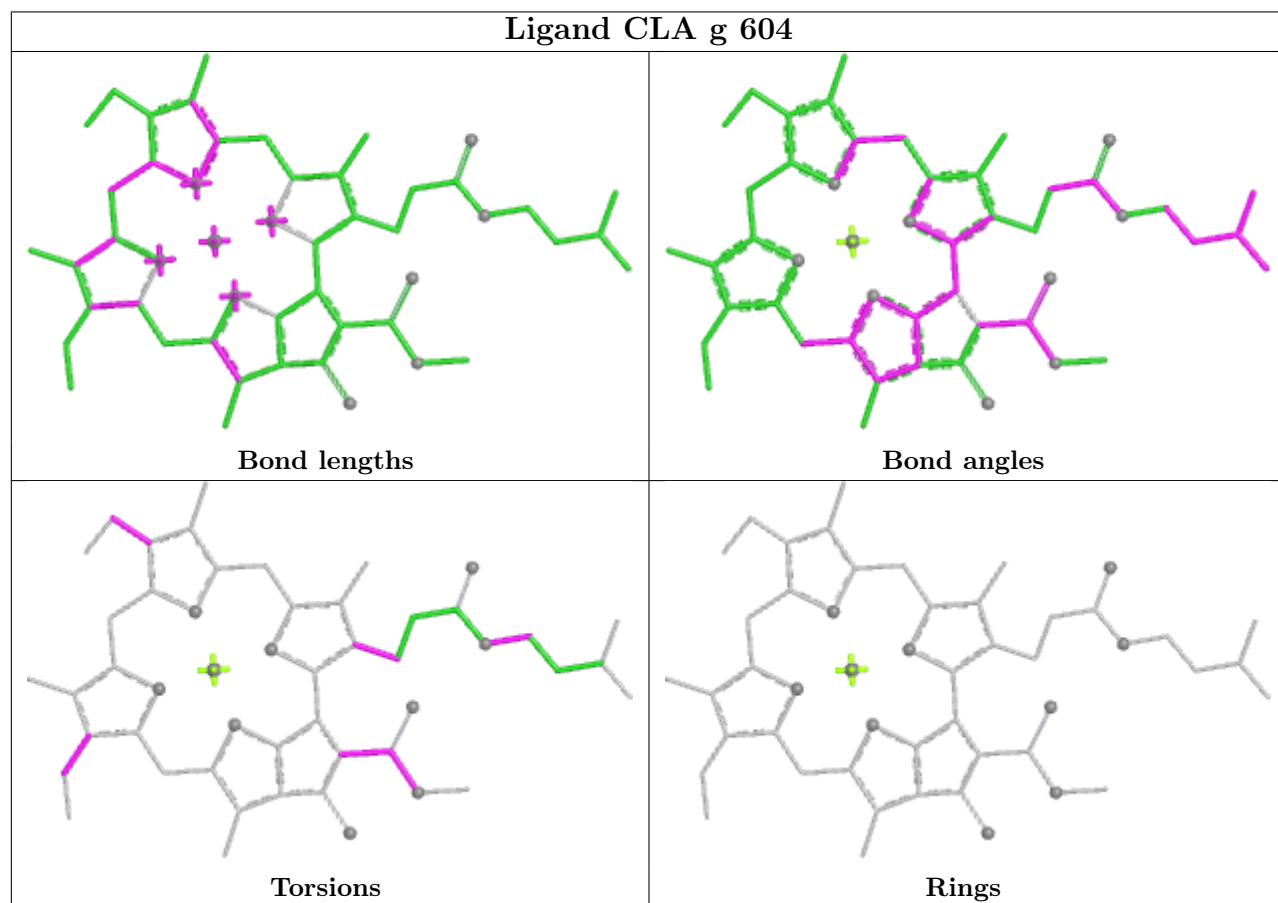
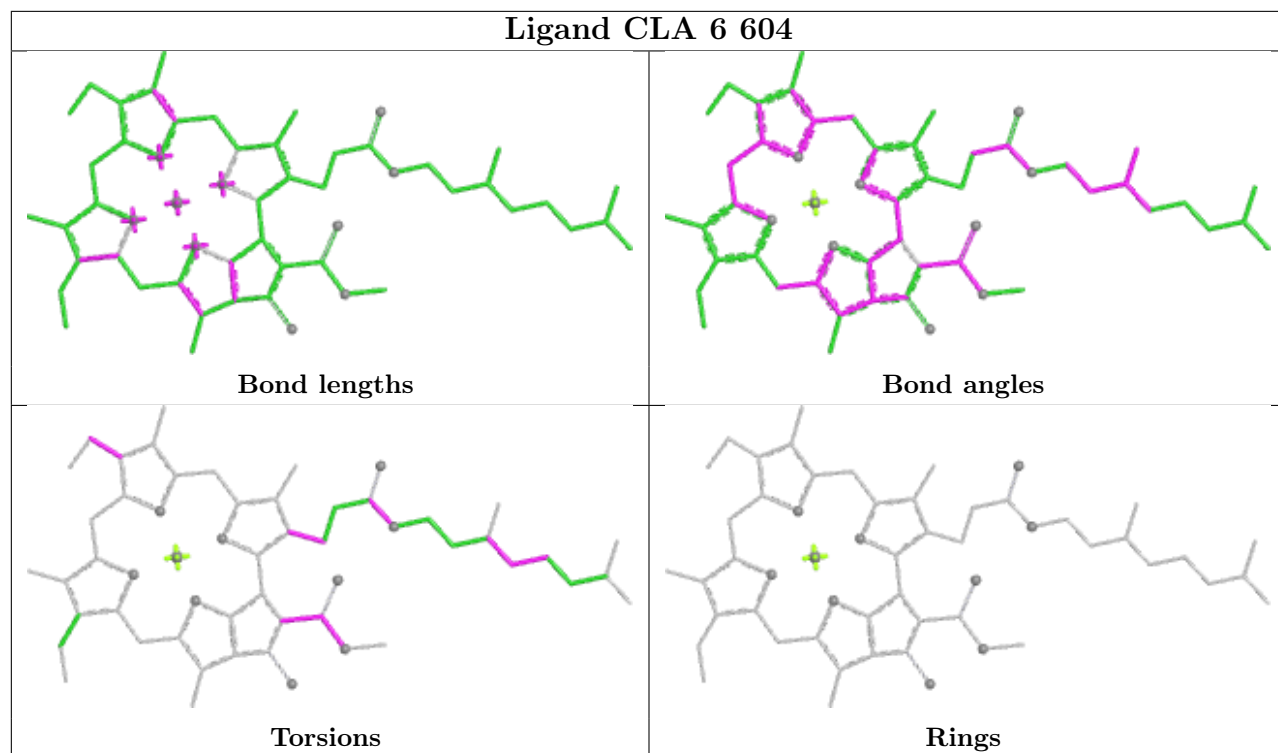


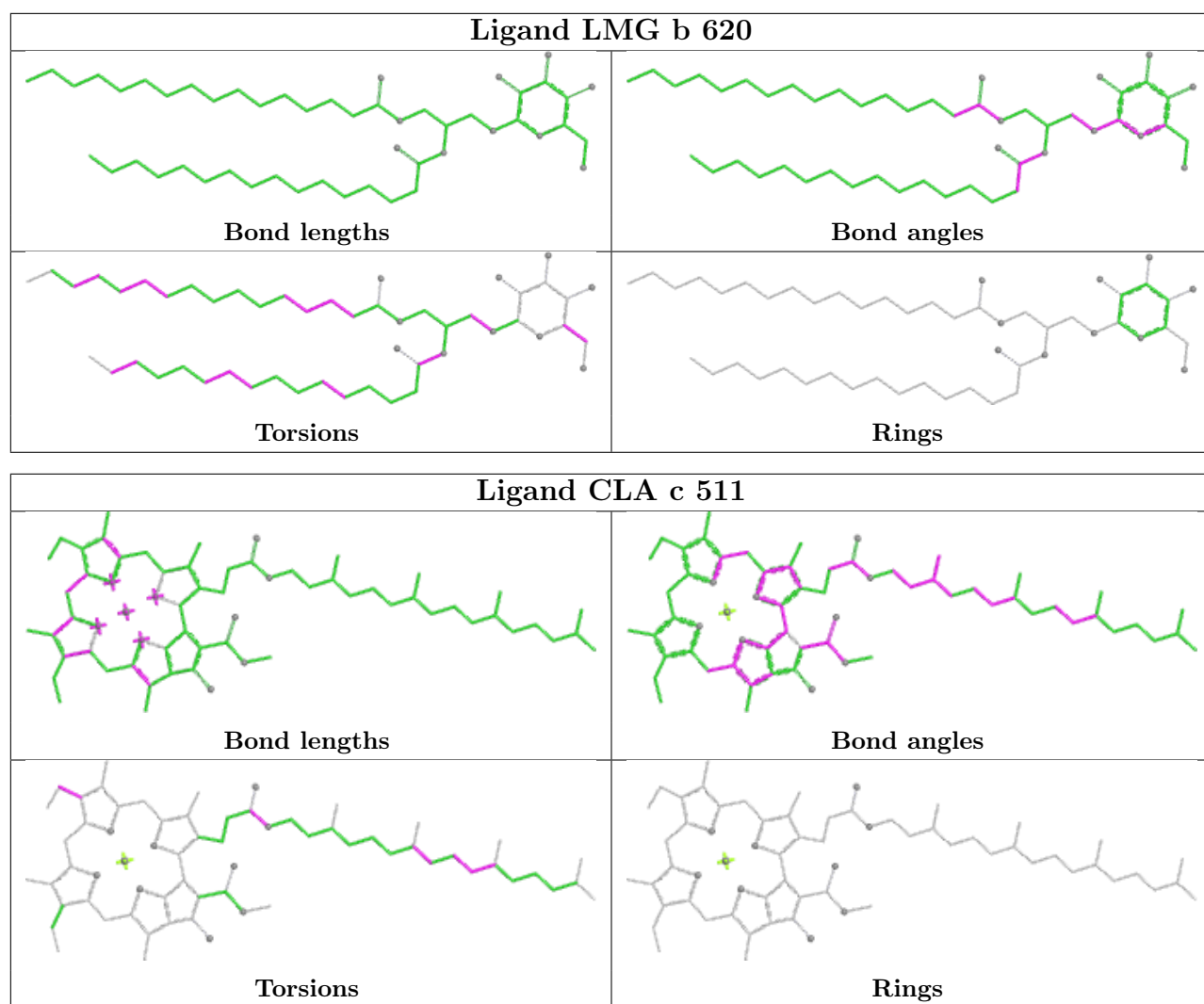
Ligand CLA d 401



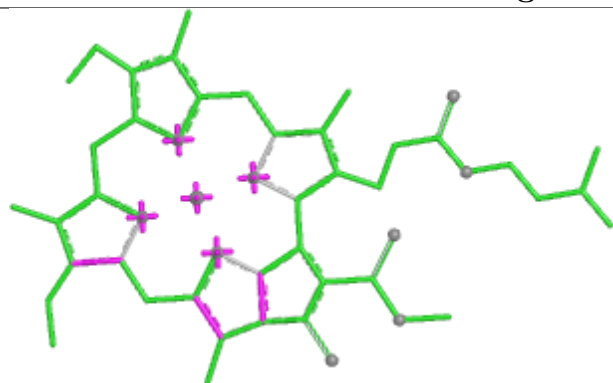
Ligand CHL G 609



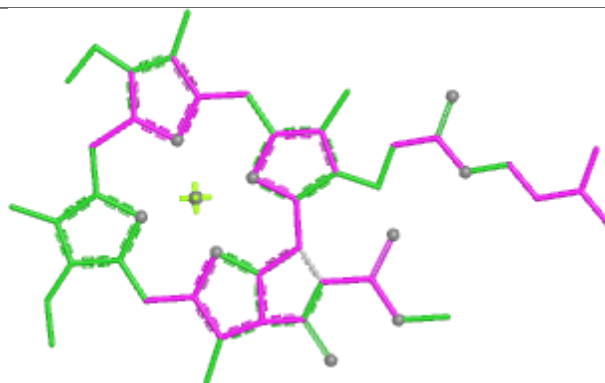




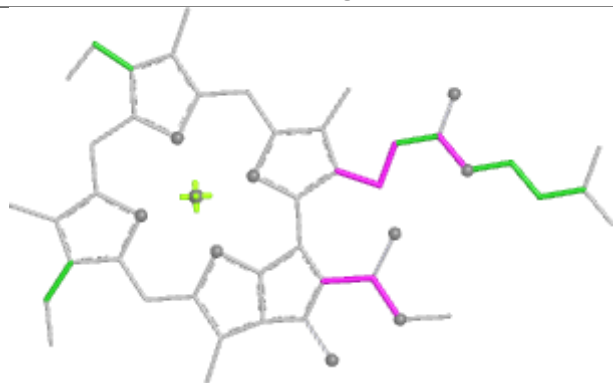
Ligand CLA S 305



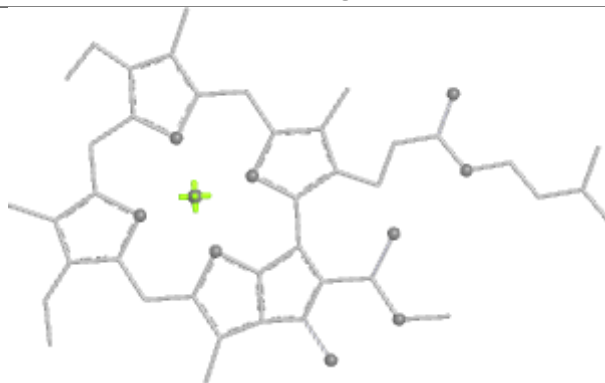
Bond lengths



Bond angles

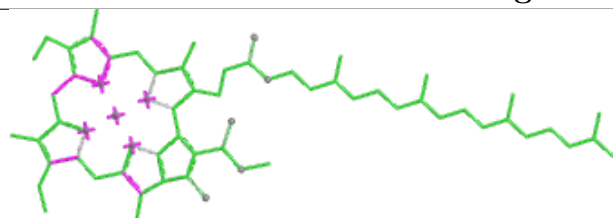


Torsions

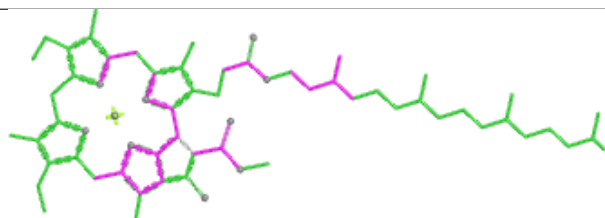


Rings

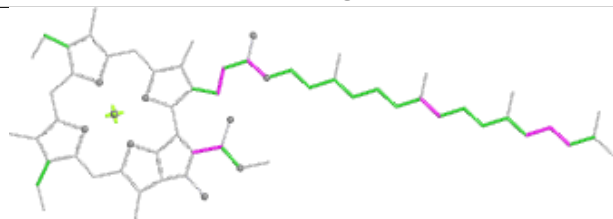
Ligand CLA B 610



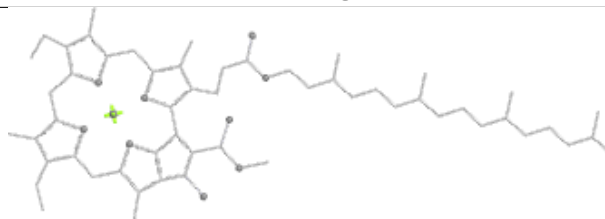
Bond lengths



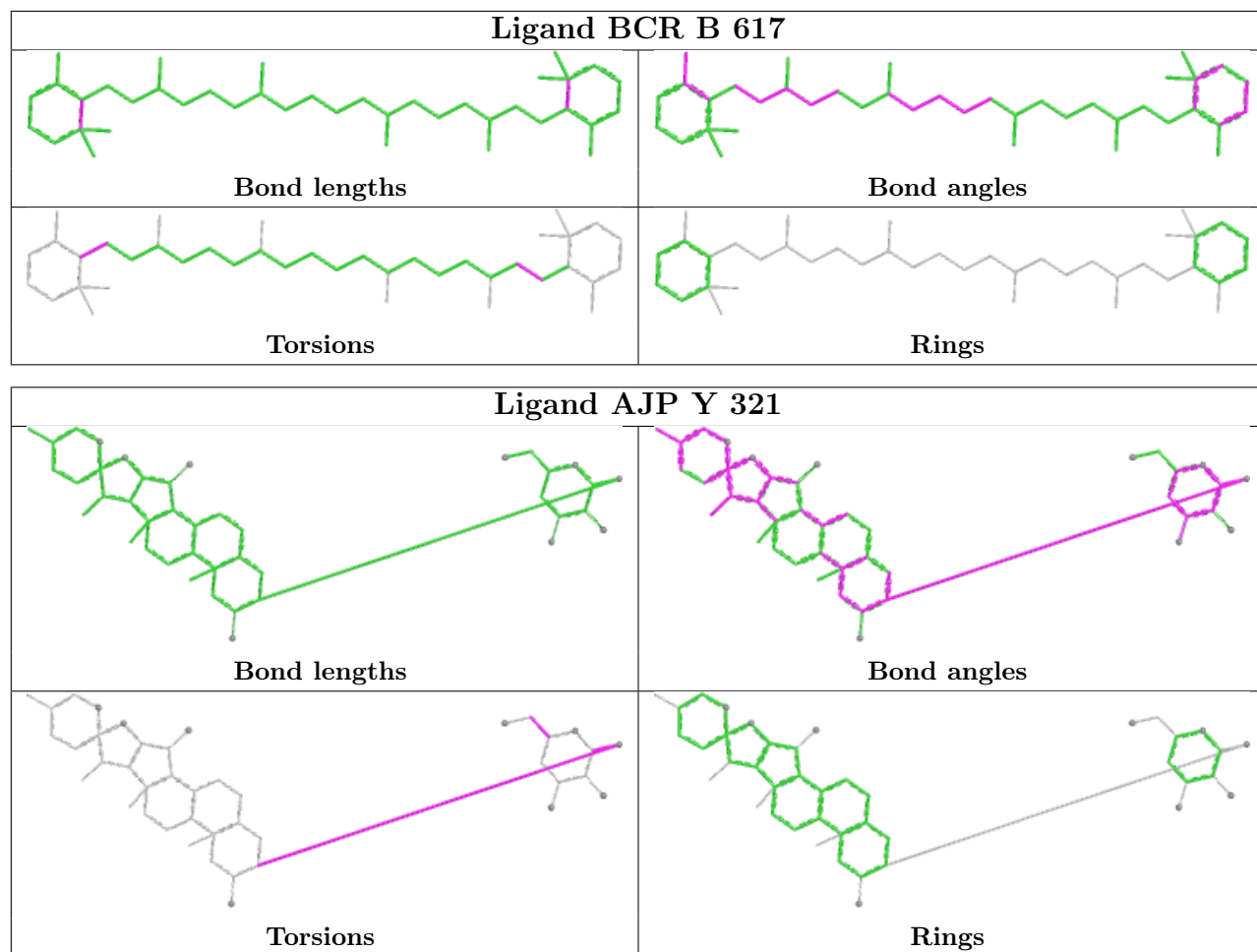
Bond angles



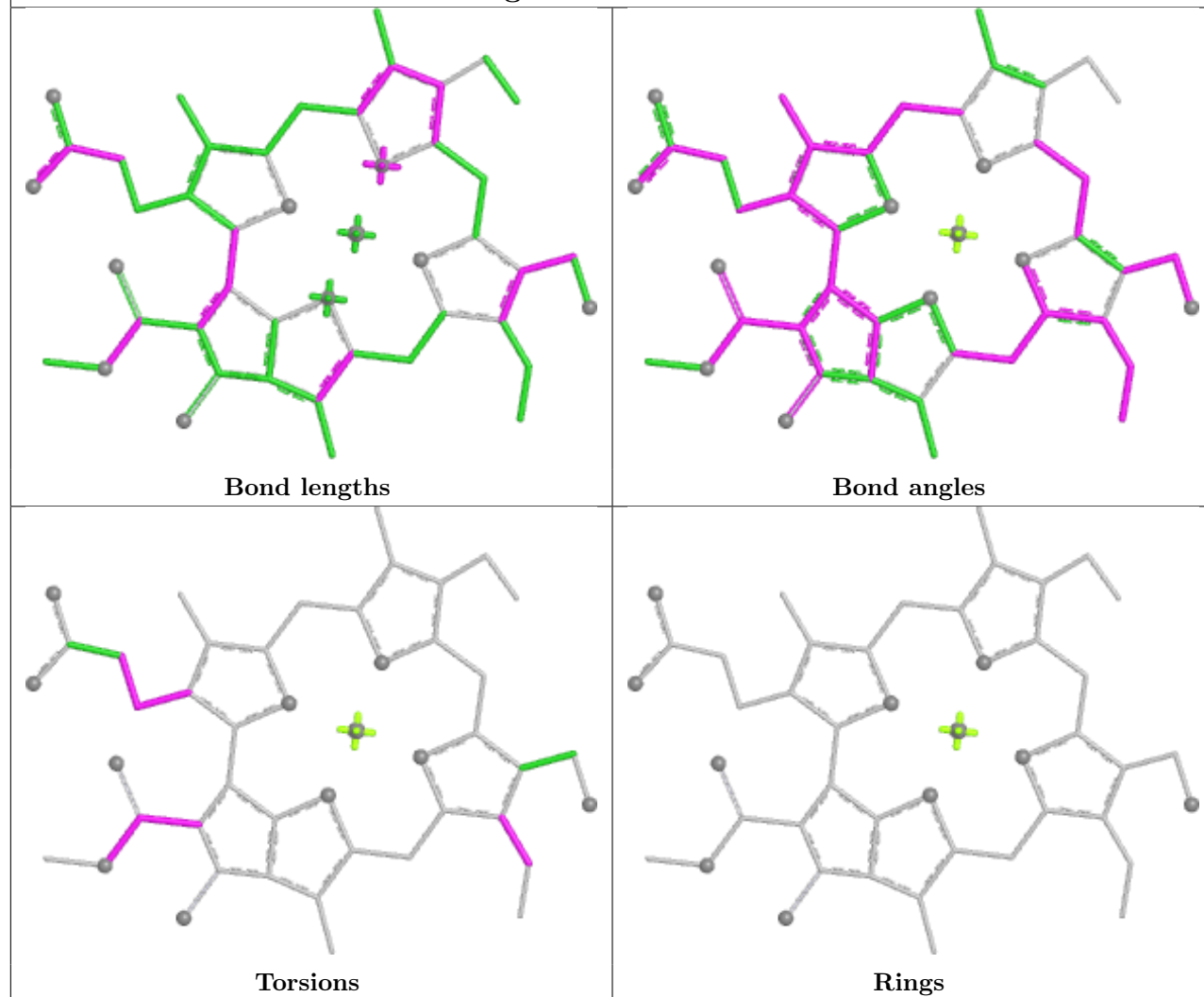
Torsions



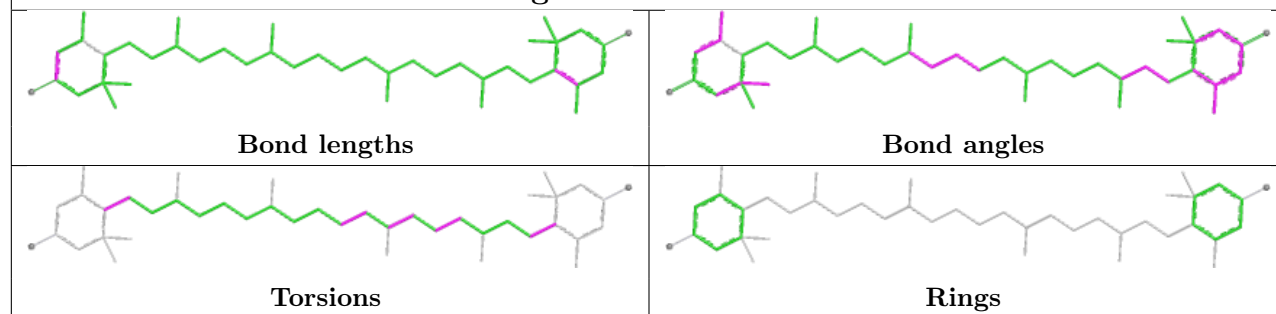
Rings



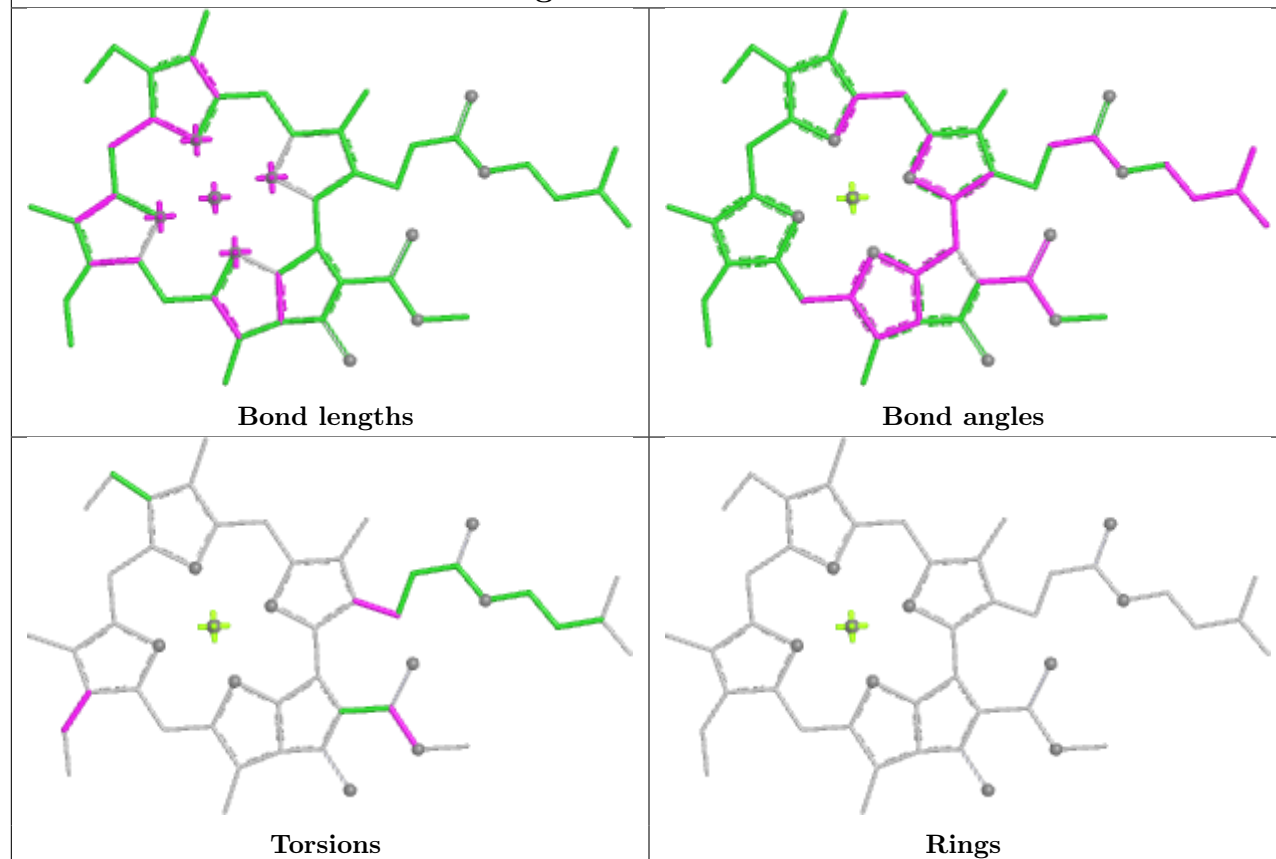
Ligand CHL S 307



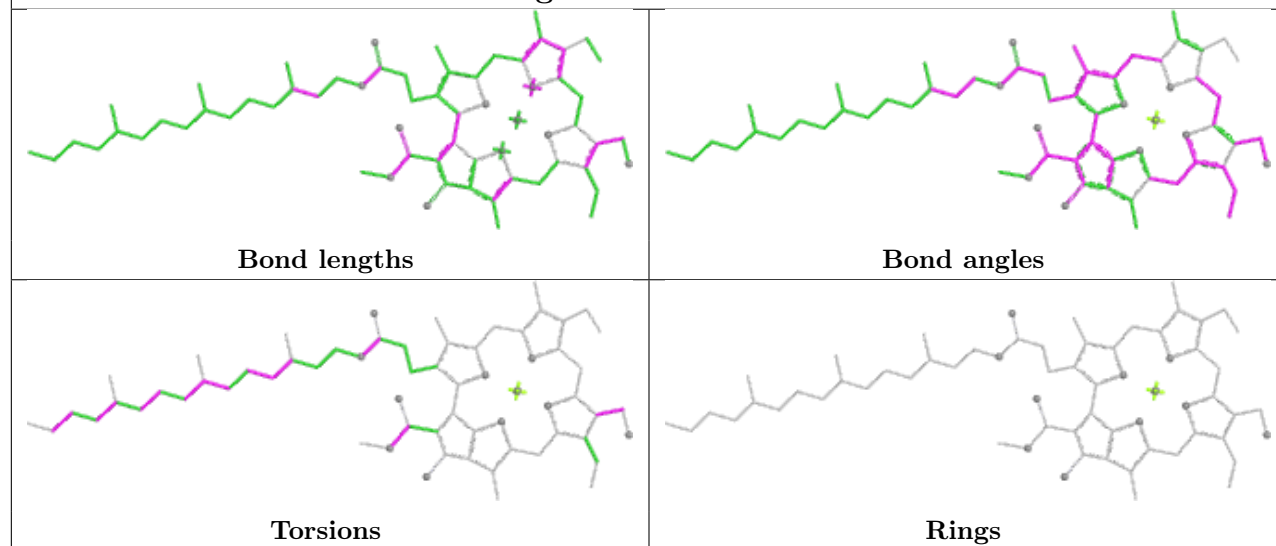
Ligand LUT N 615

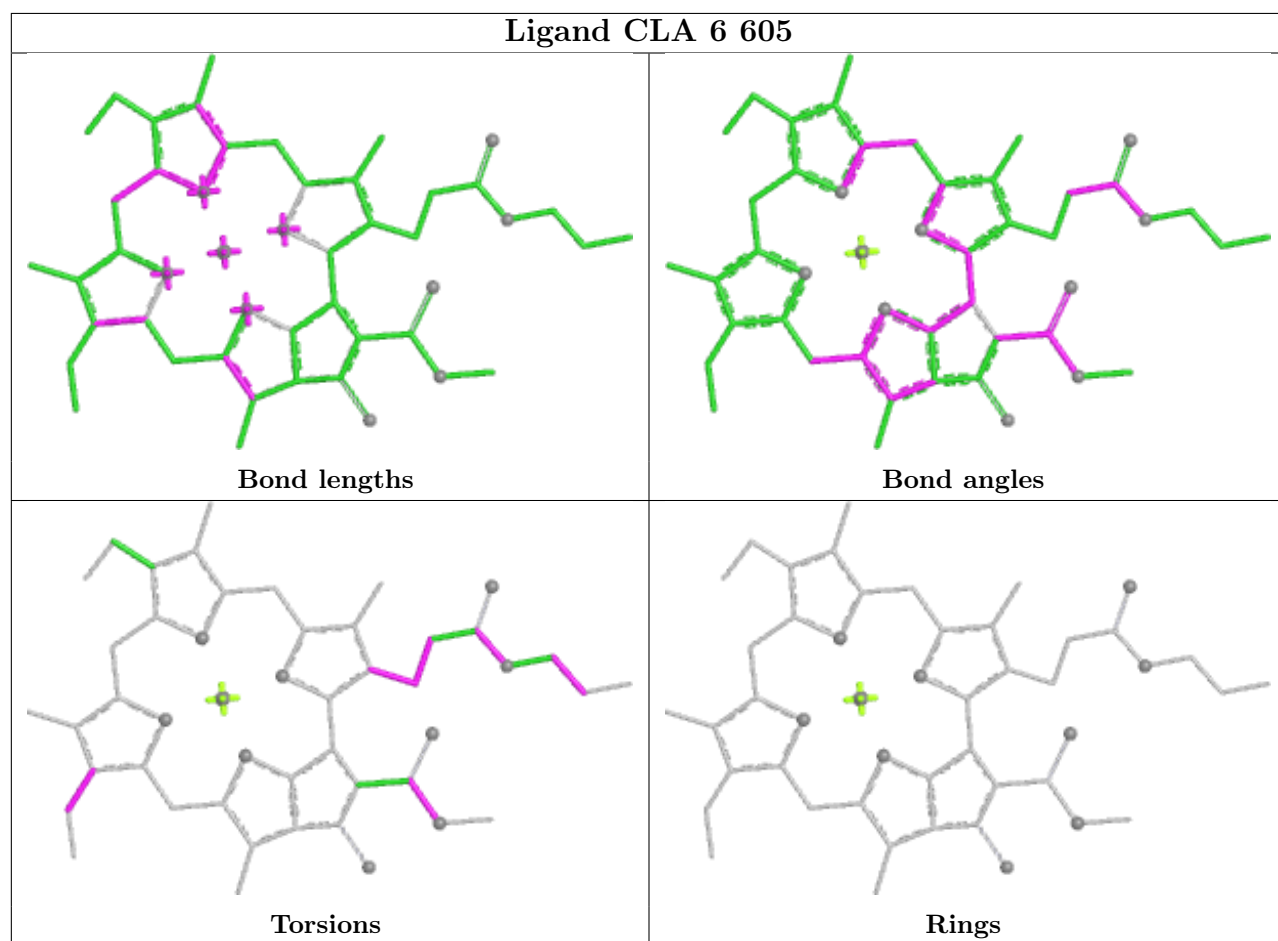
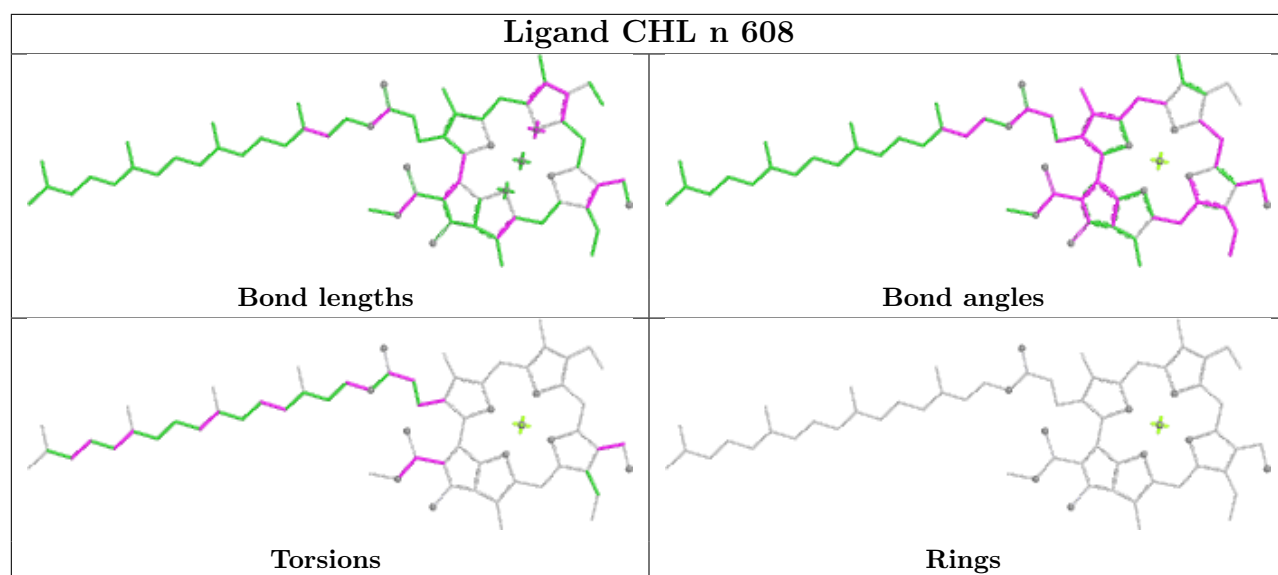


Ligand CLA n 604

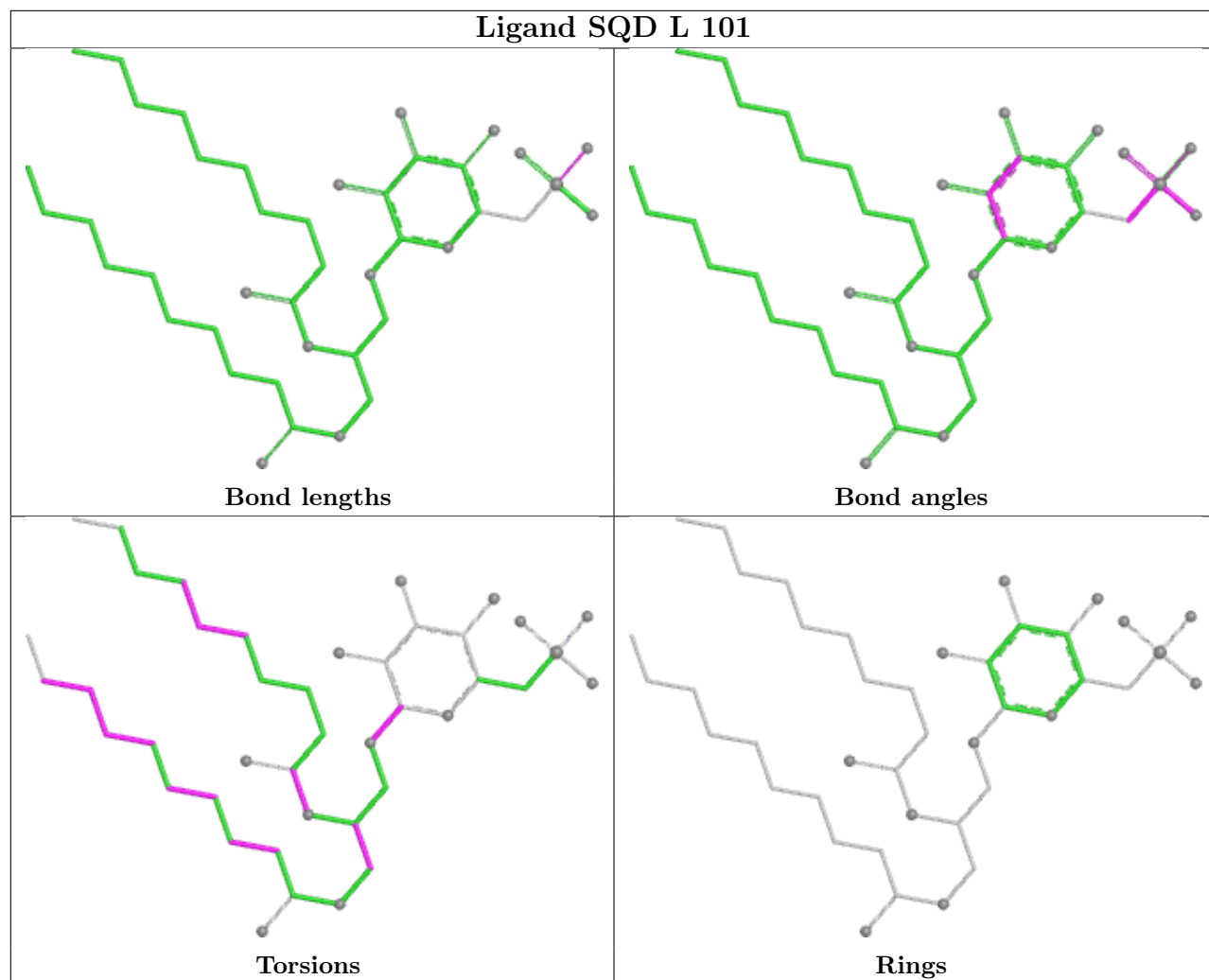


Ligand CHL 6 601

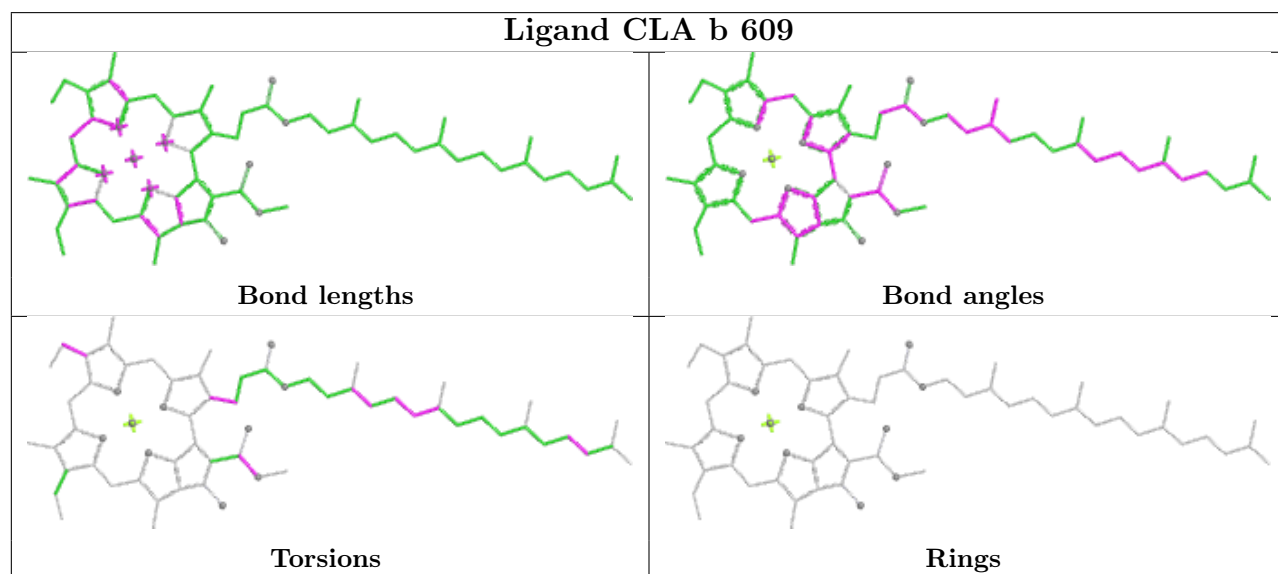




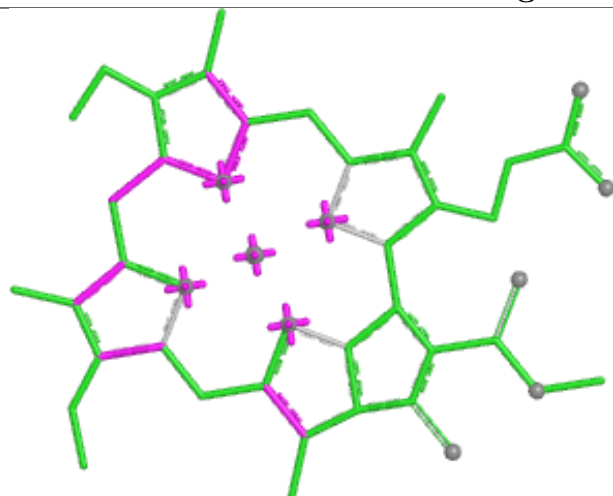
Ligand SQD L 101



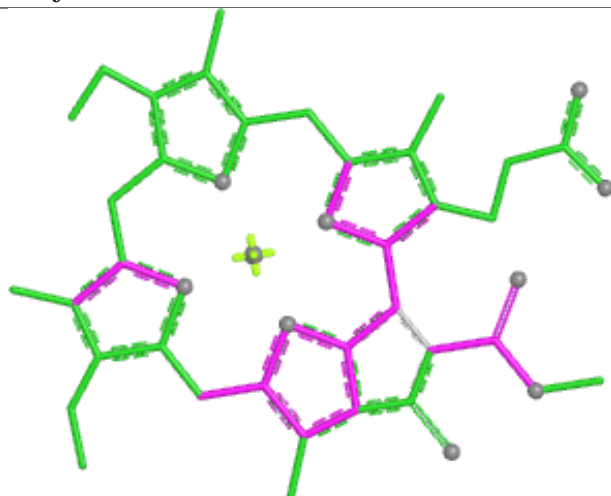
Ligand CLA b 609



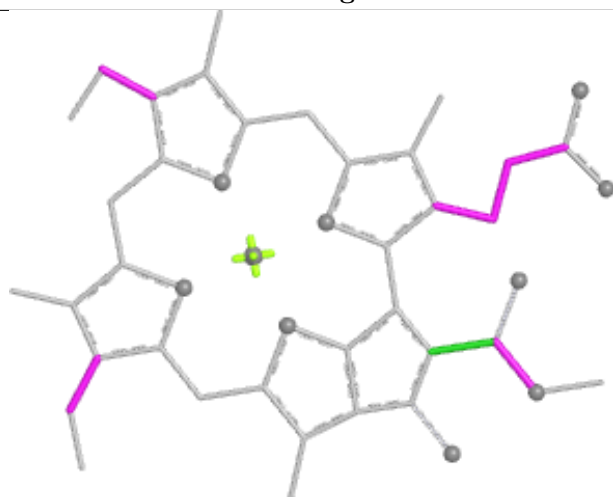
Ligand CLA y 315



Bond lengths



Bond angles

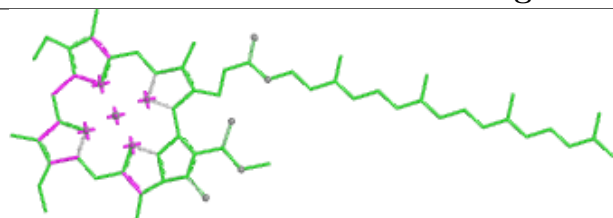


Torsions

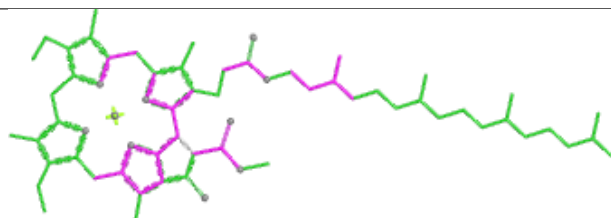


Rings

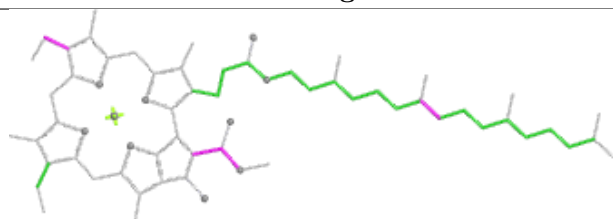
Ligand CLA C 502



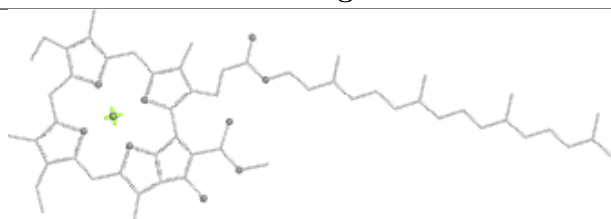
Bond lengths



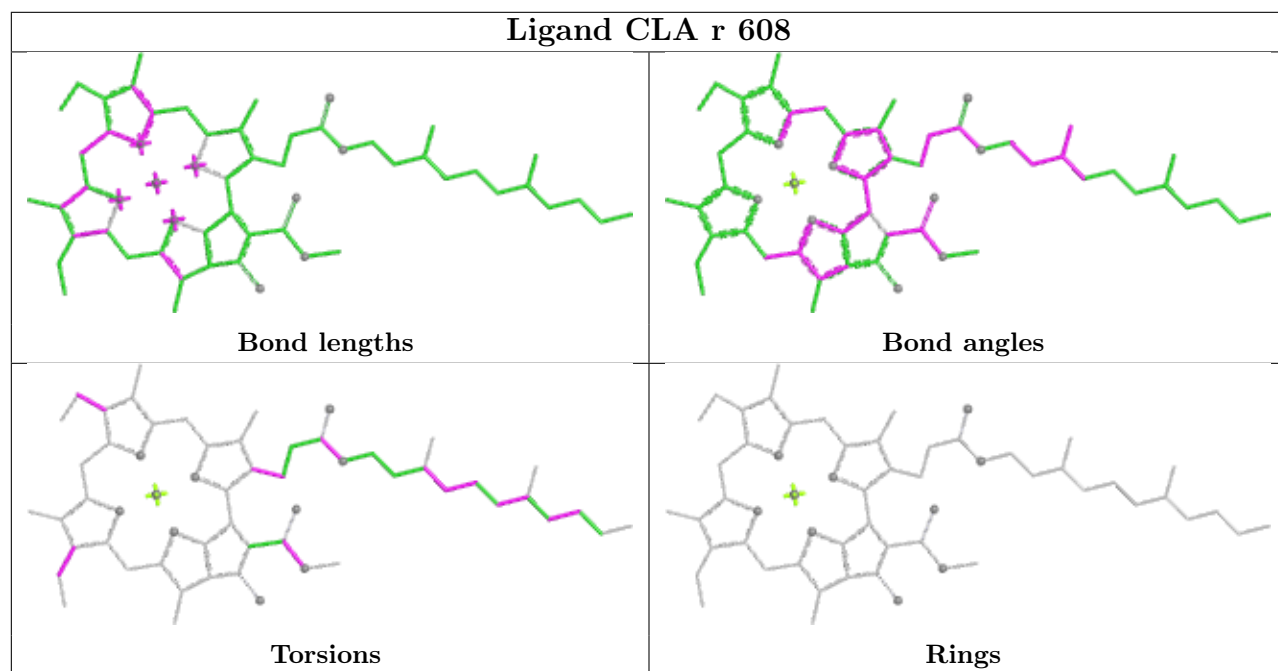
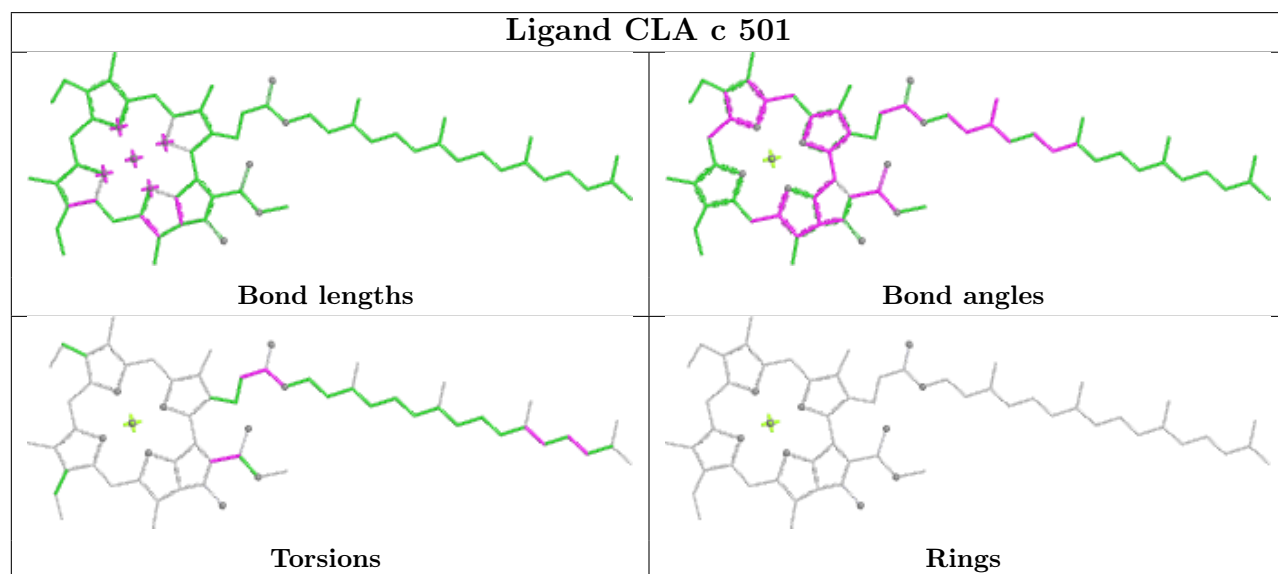
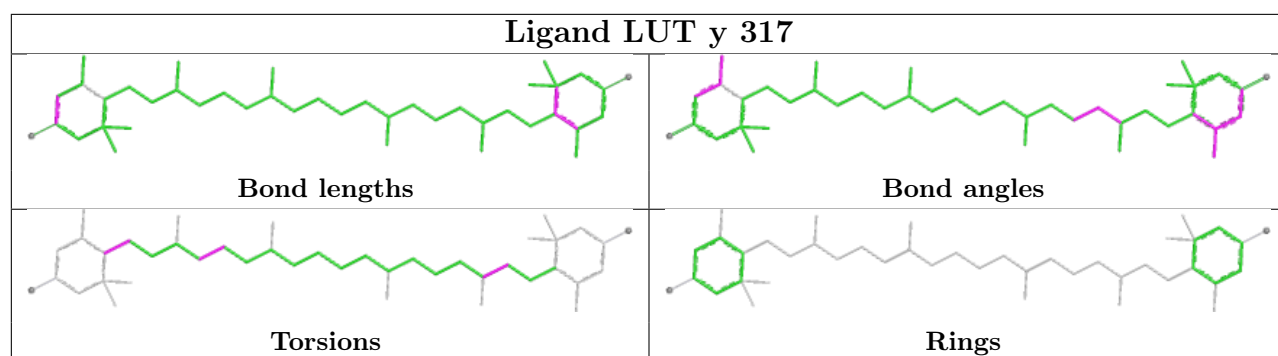
Bond angles



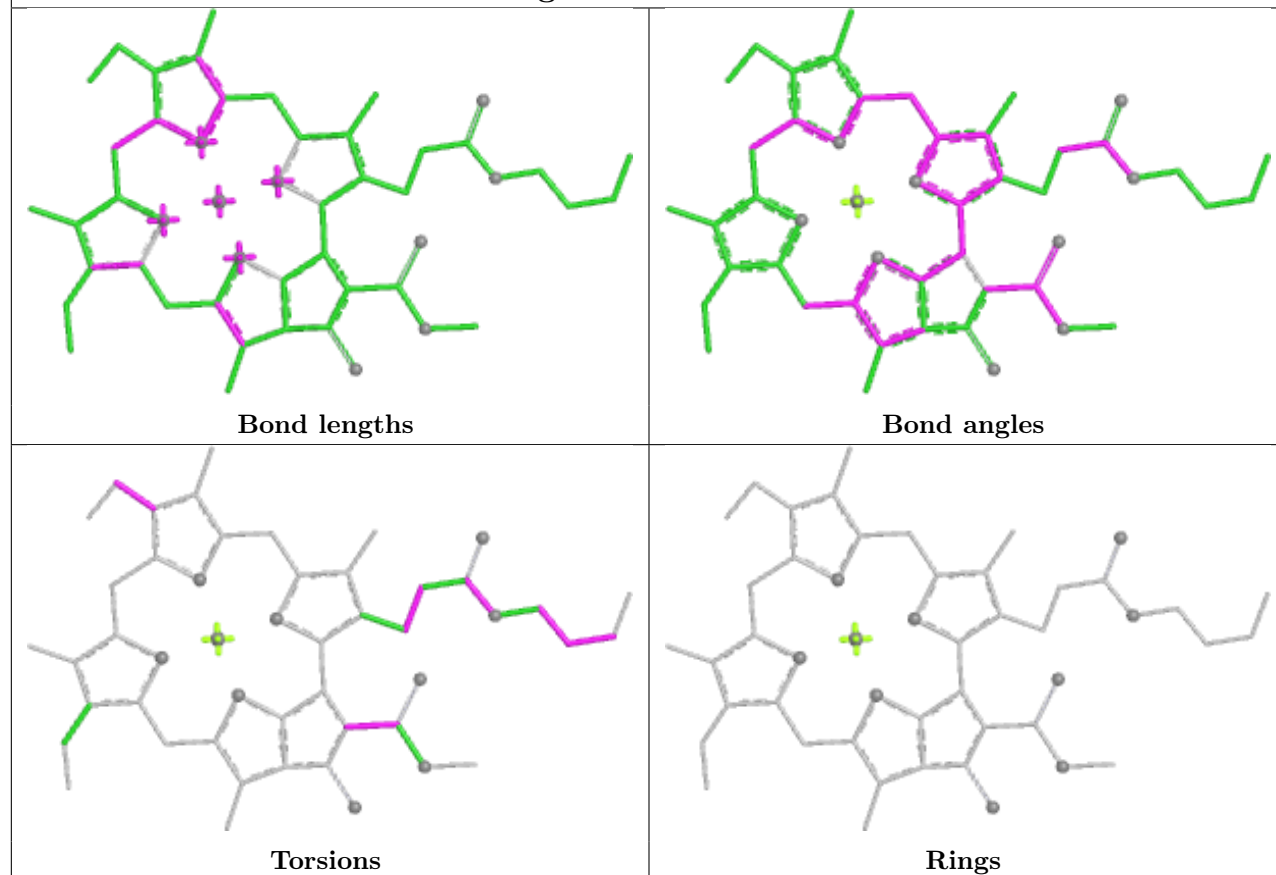
Torsions



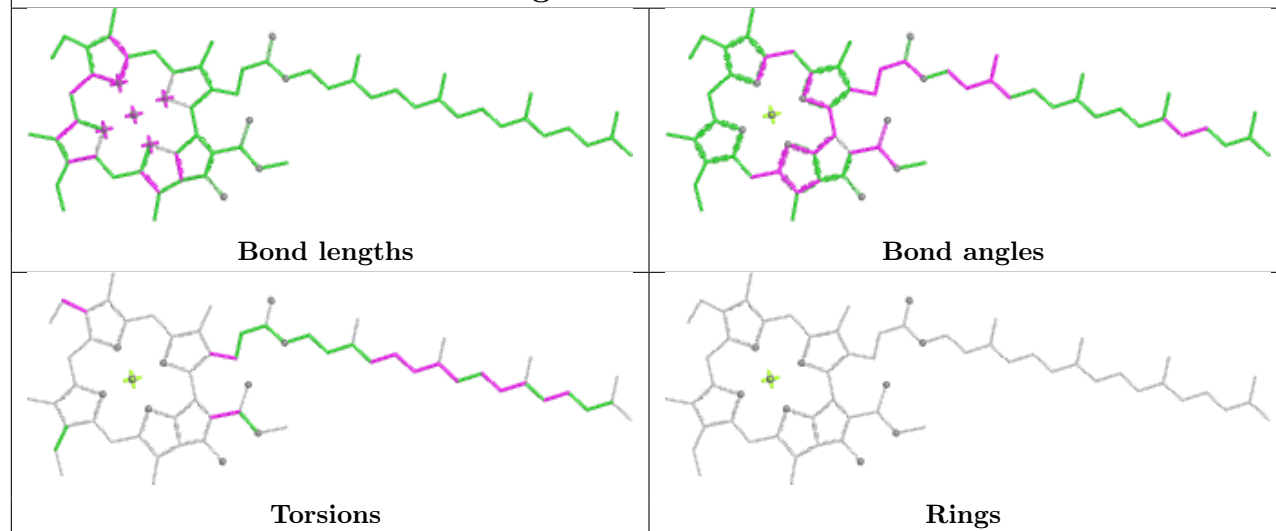
Rings

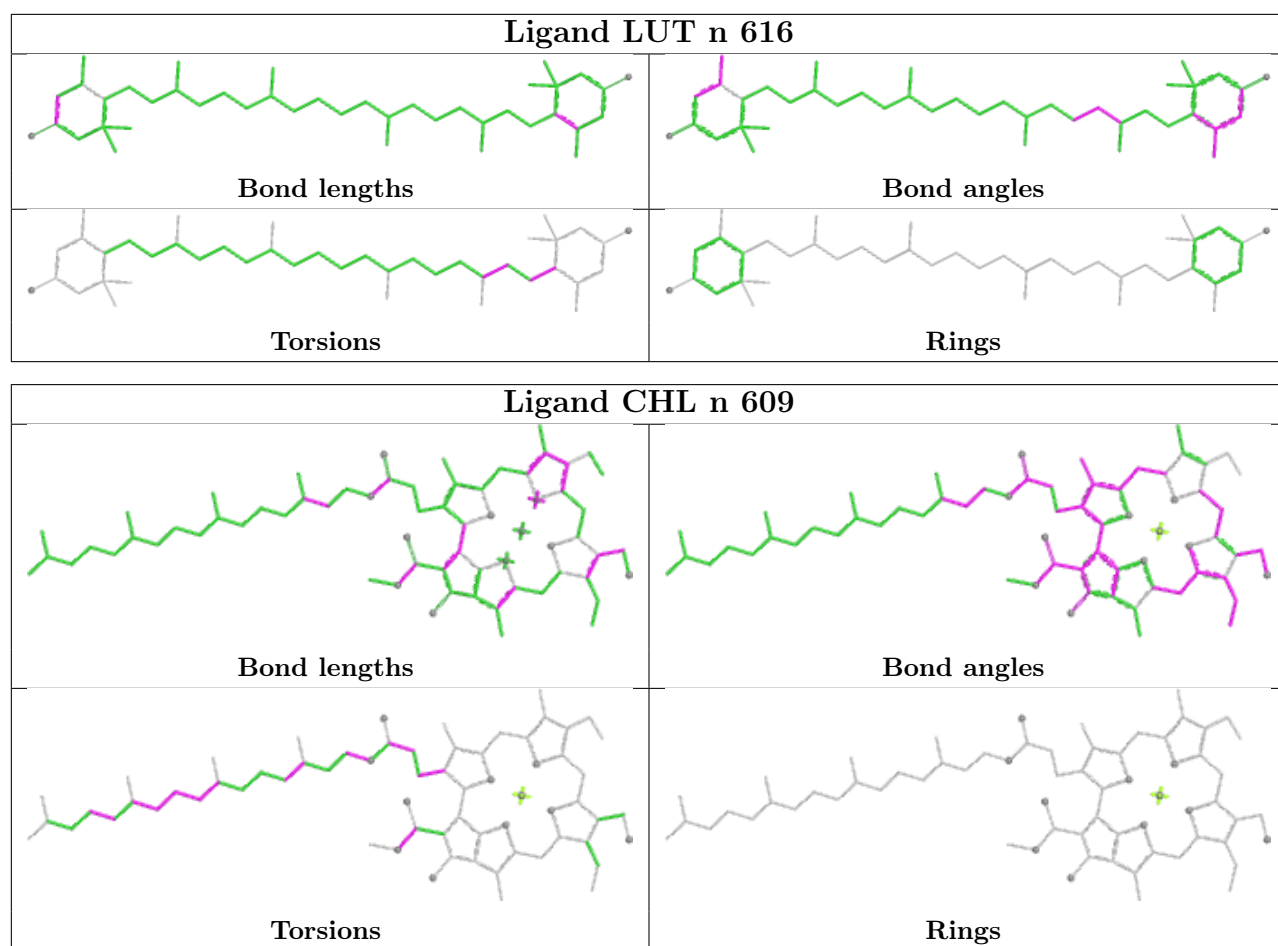


Ligand CLA s 312

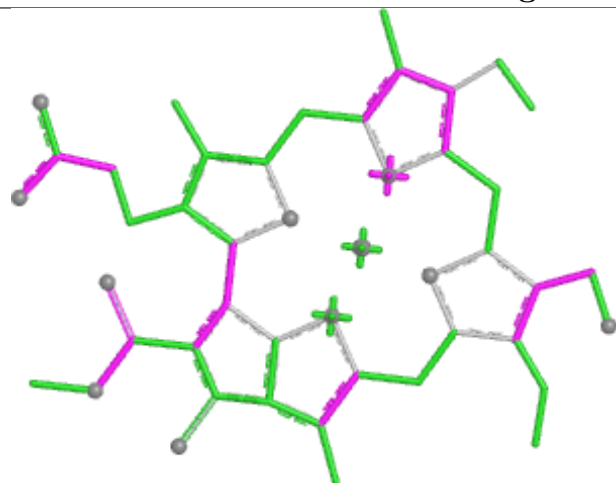


Ligand CLA B 604

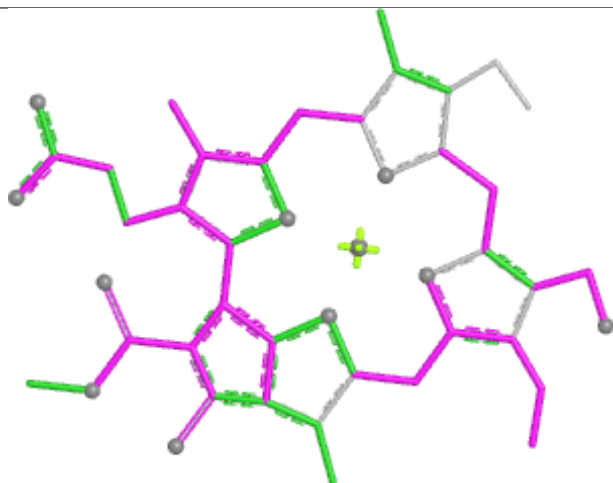




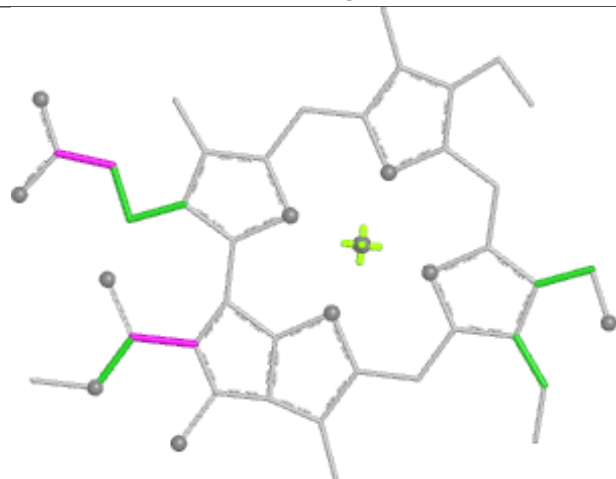
Ligand CHL S 308



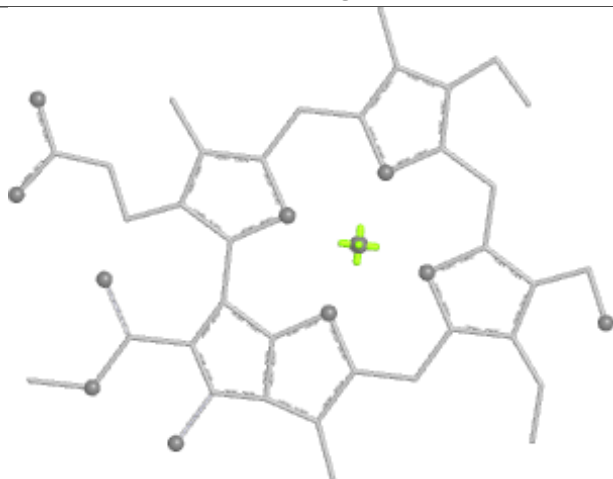
Bond lengths



Bond angles

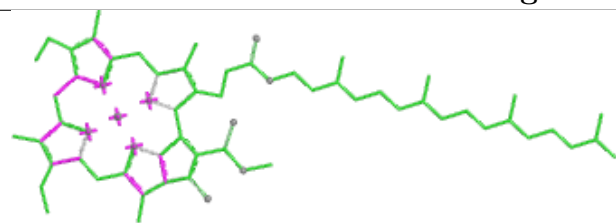


Torsions

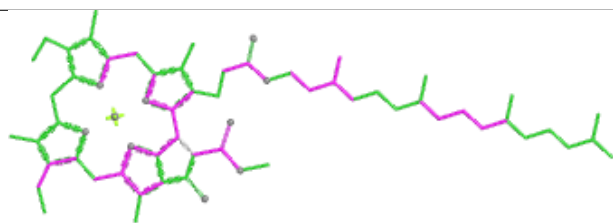


Rings

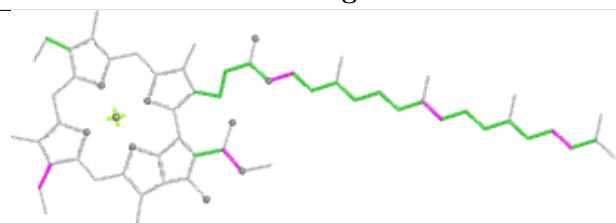
Ligand CLA a 402



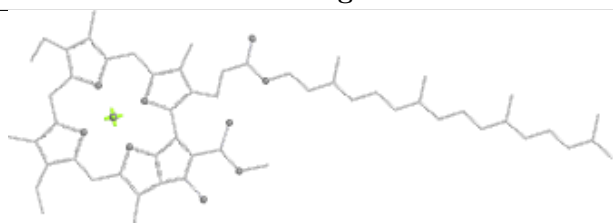
Bond lengths



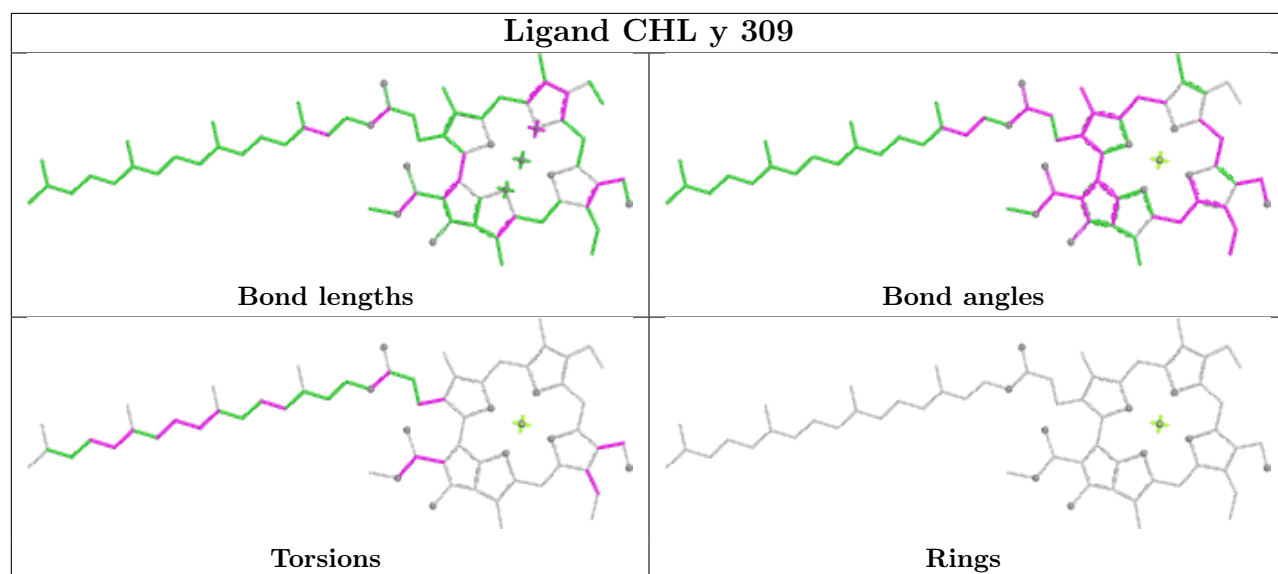
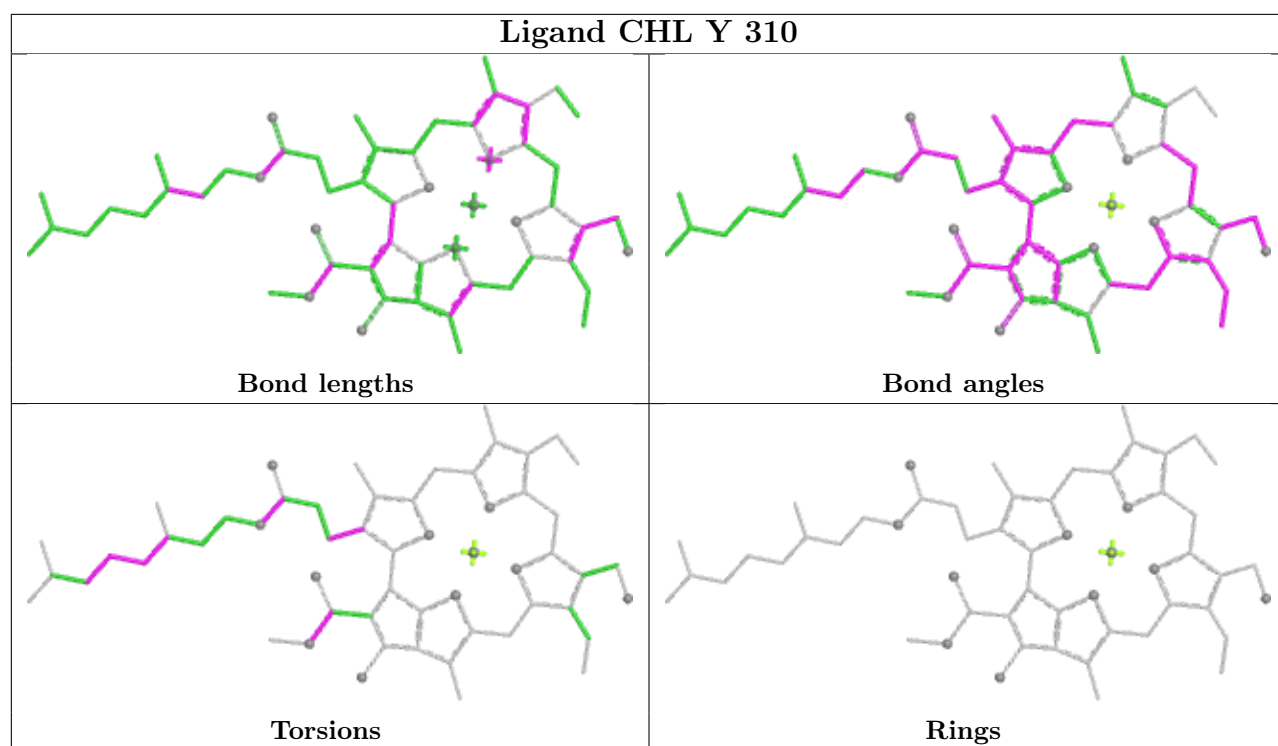
Bond angles

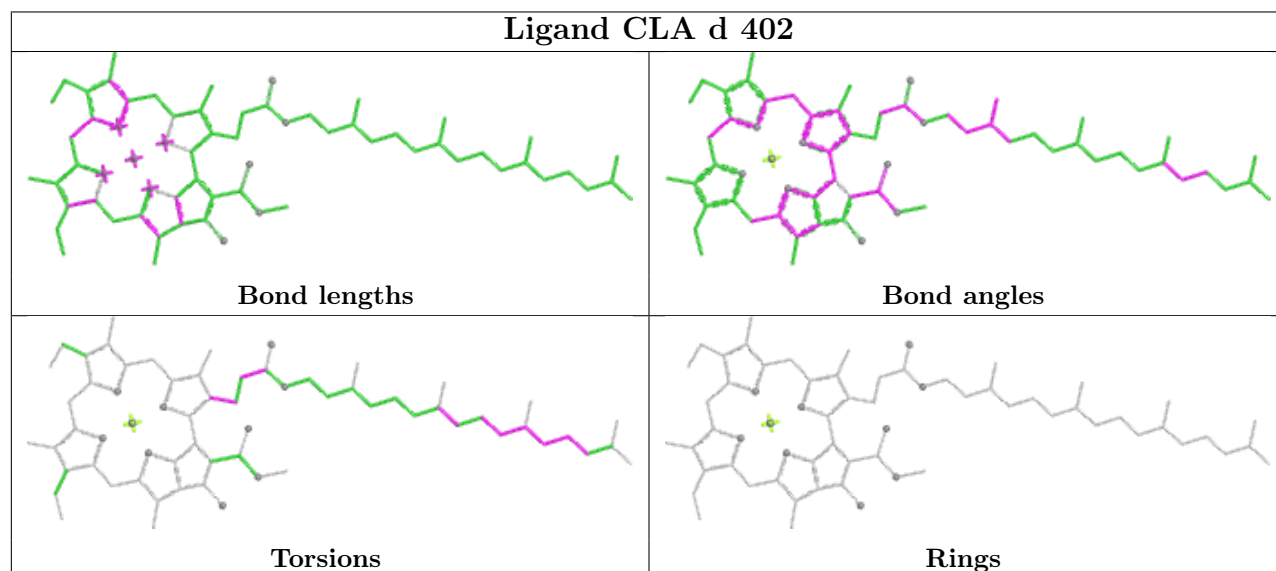
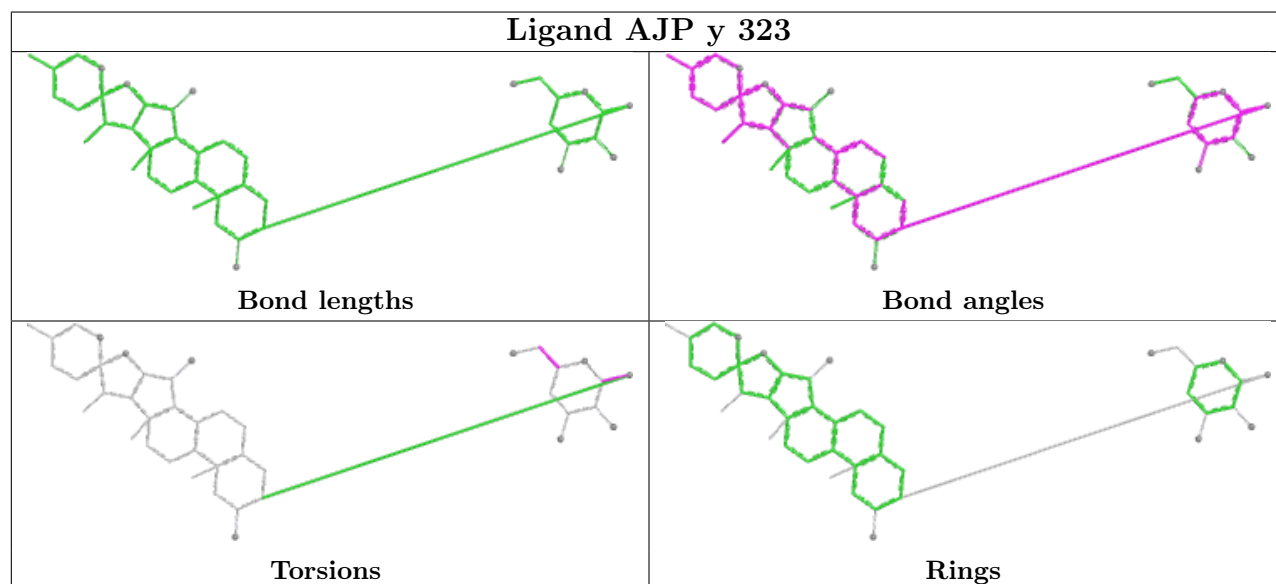
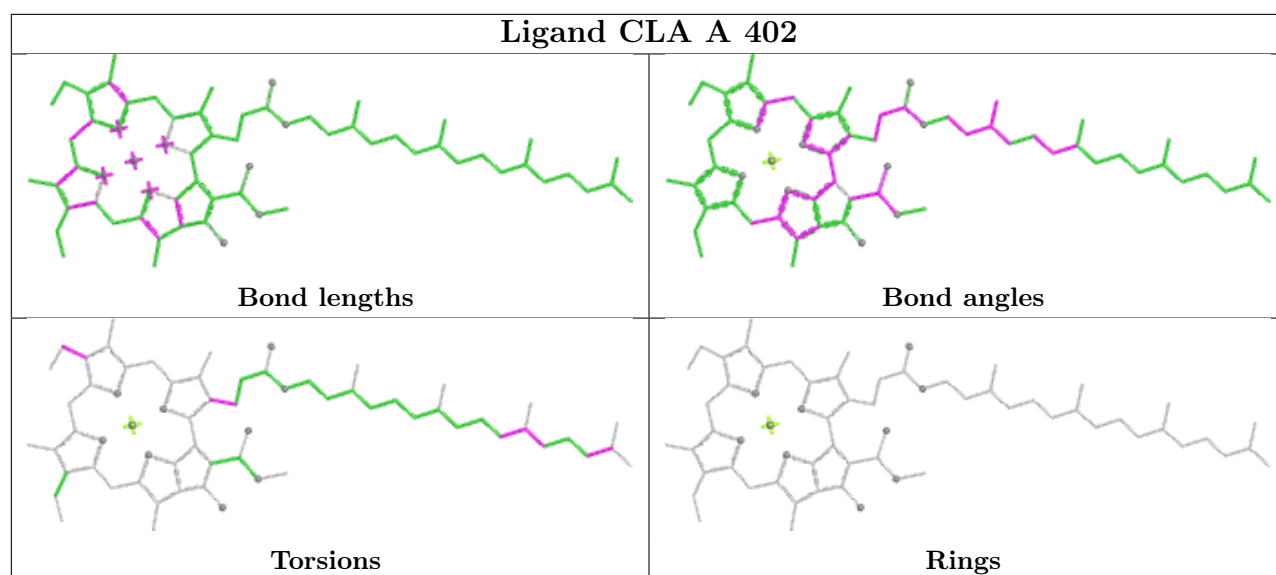


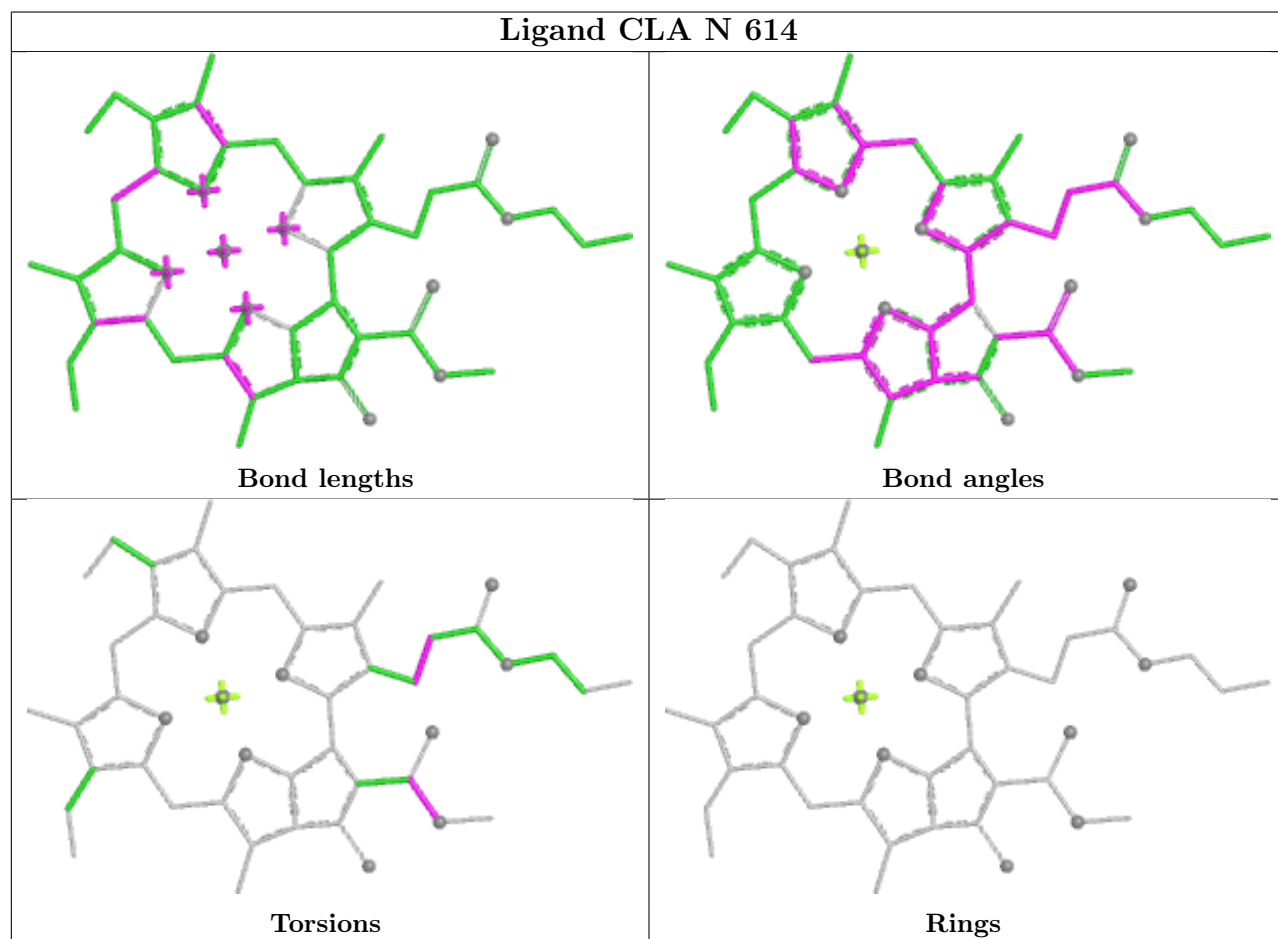
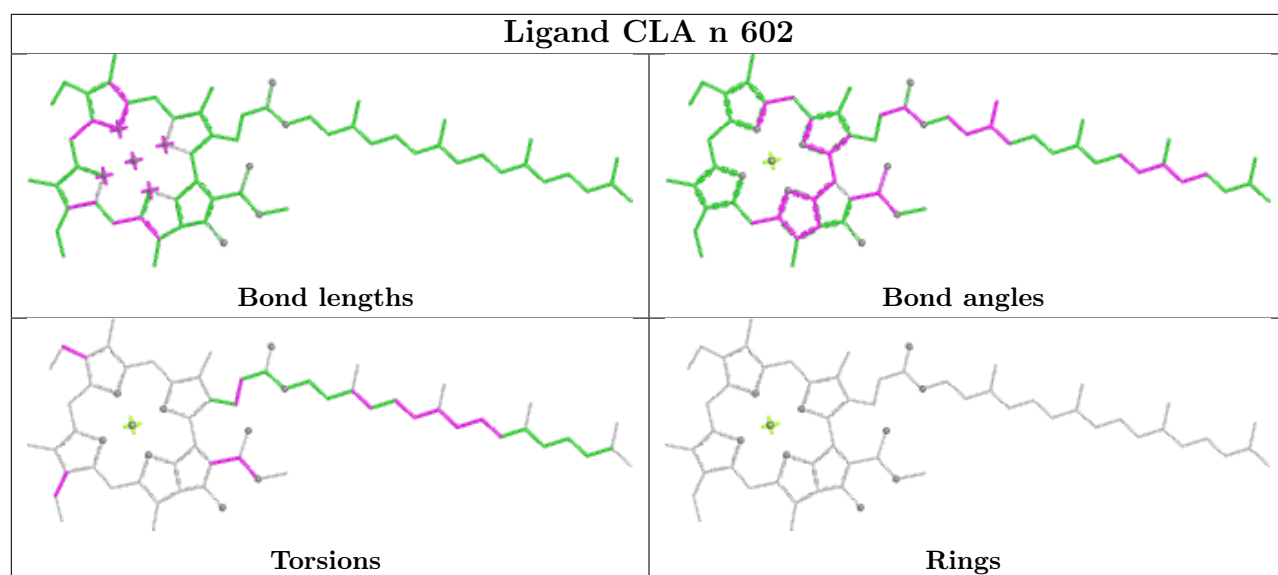
Torsions

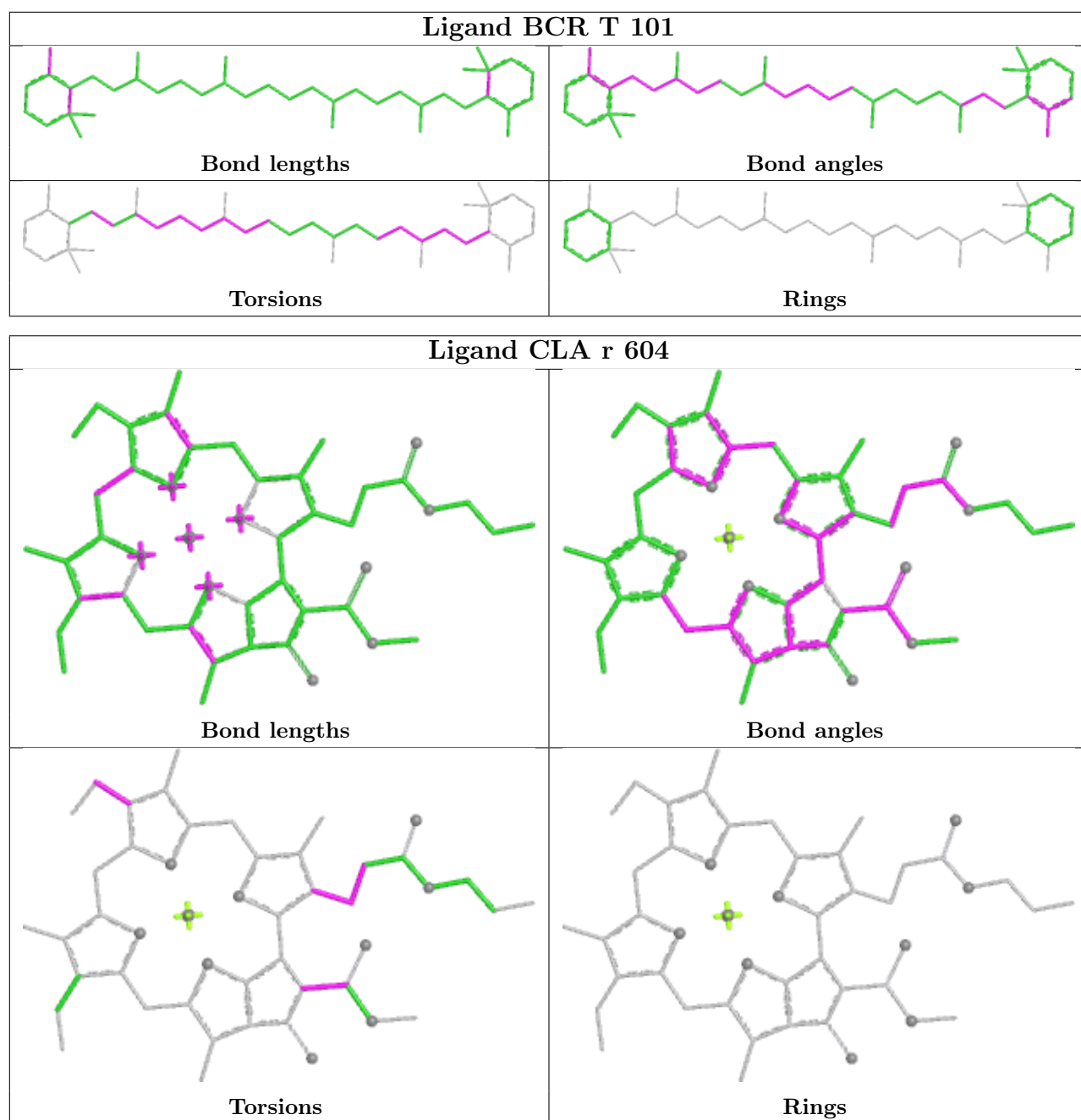


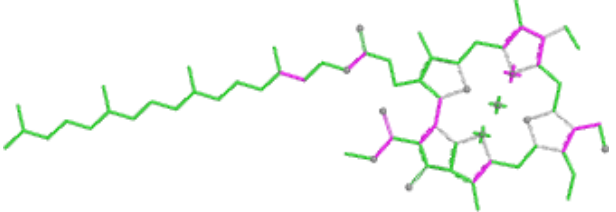
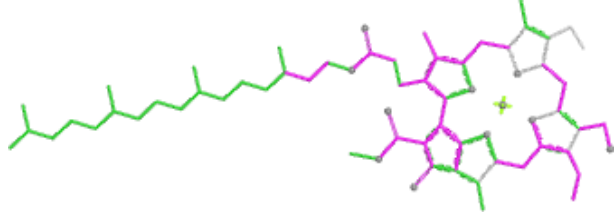
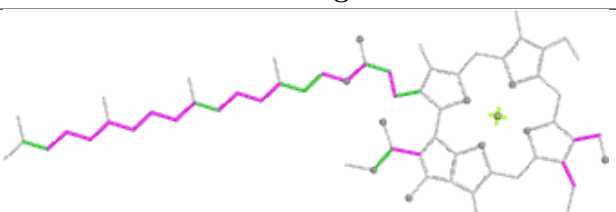
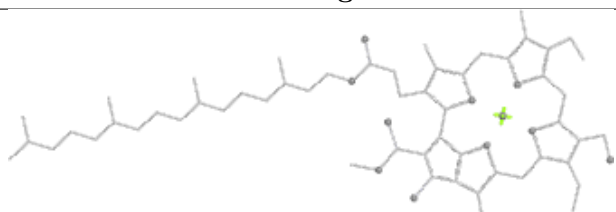
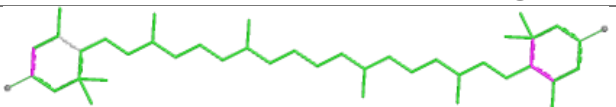
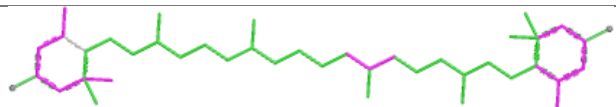
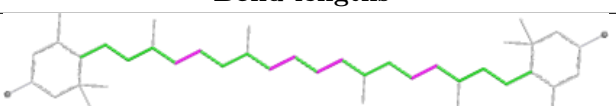
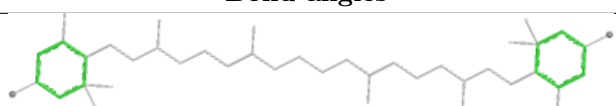
Rings

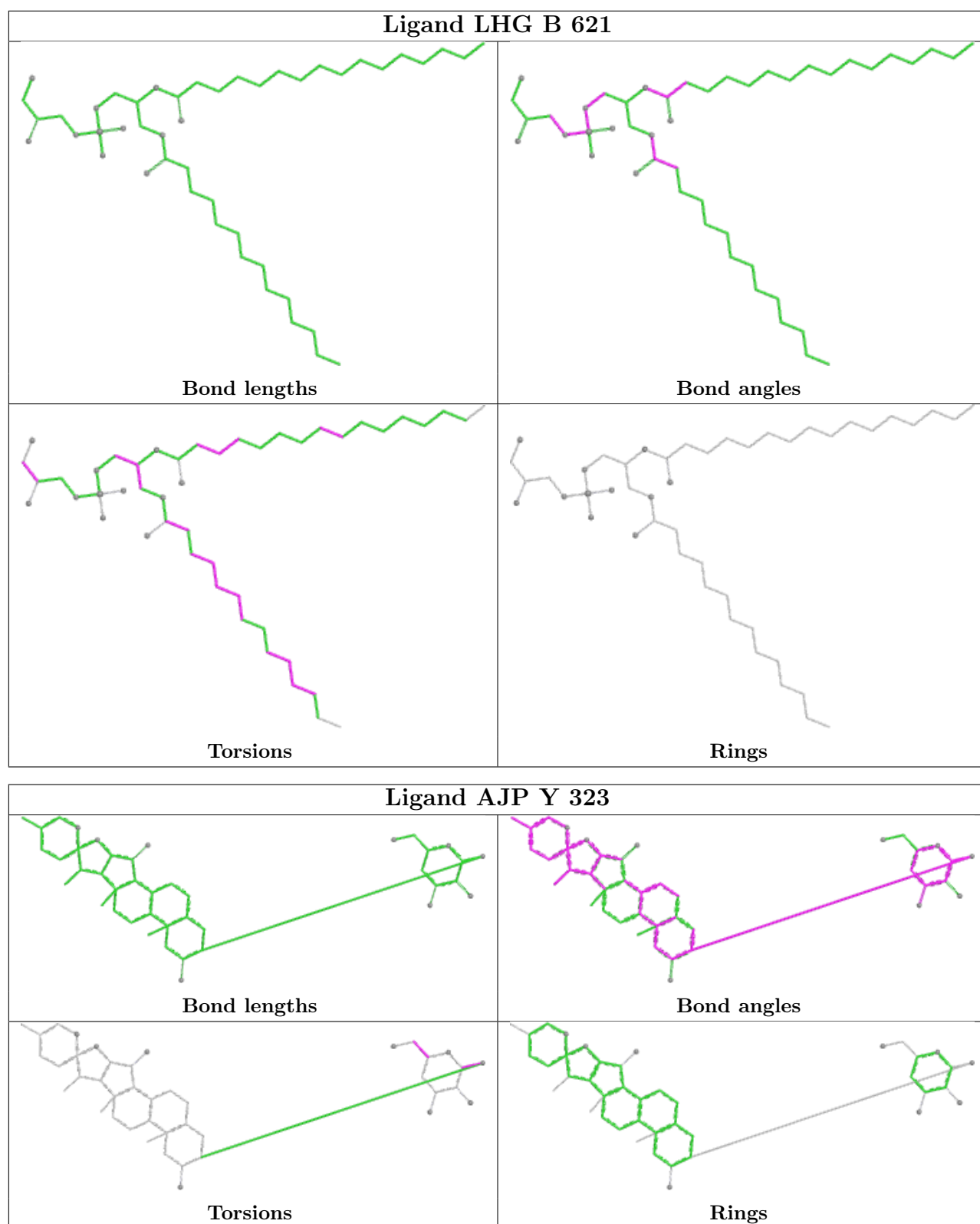


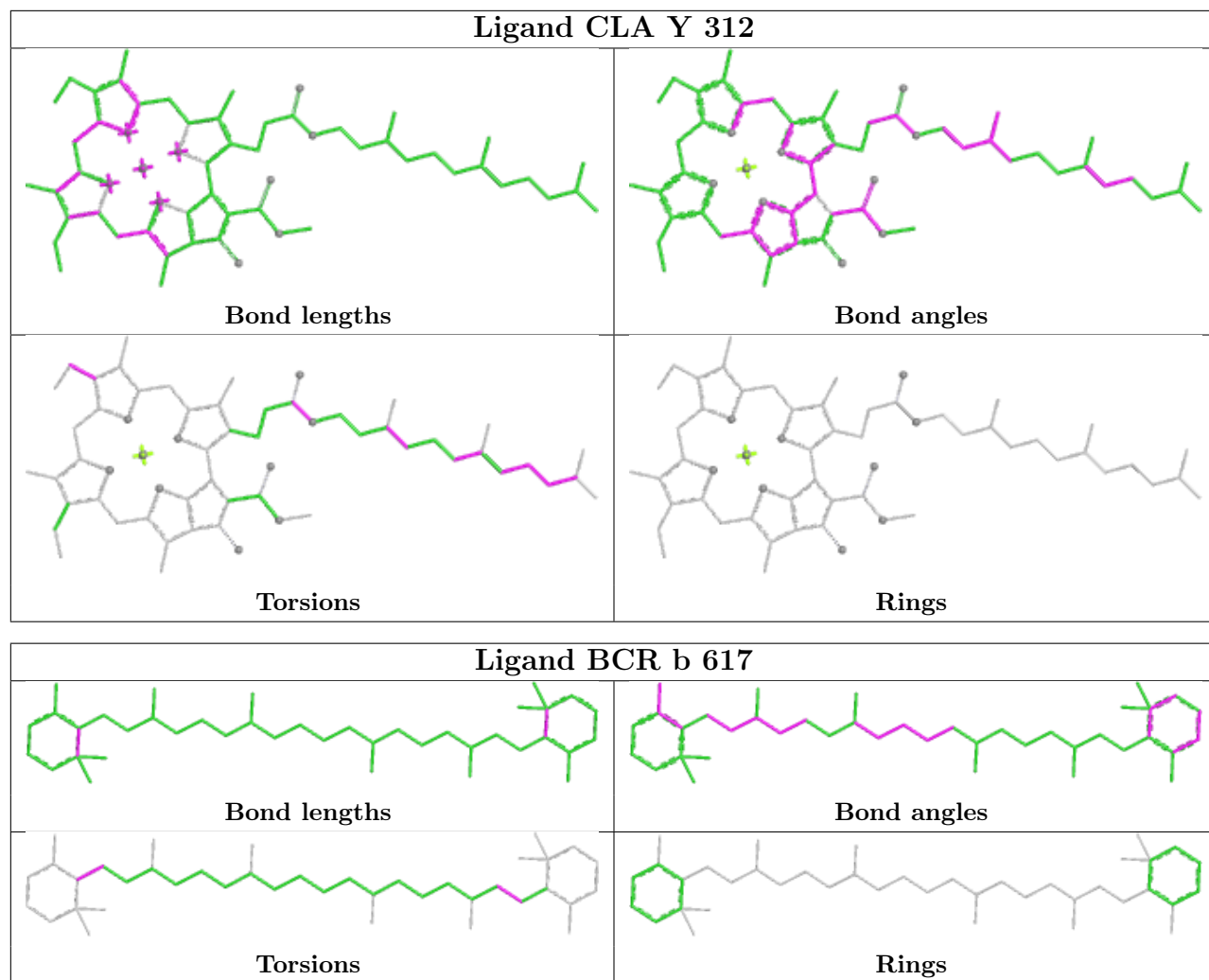


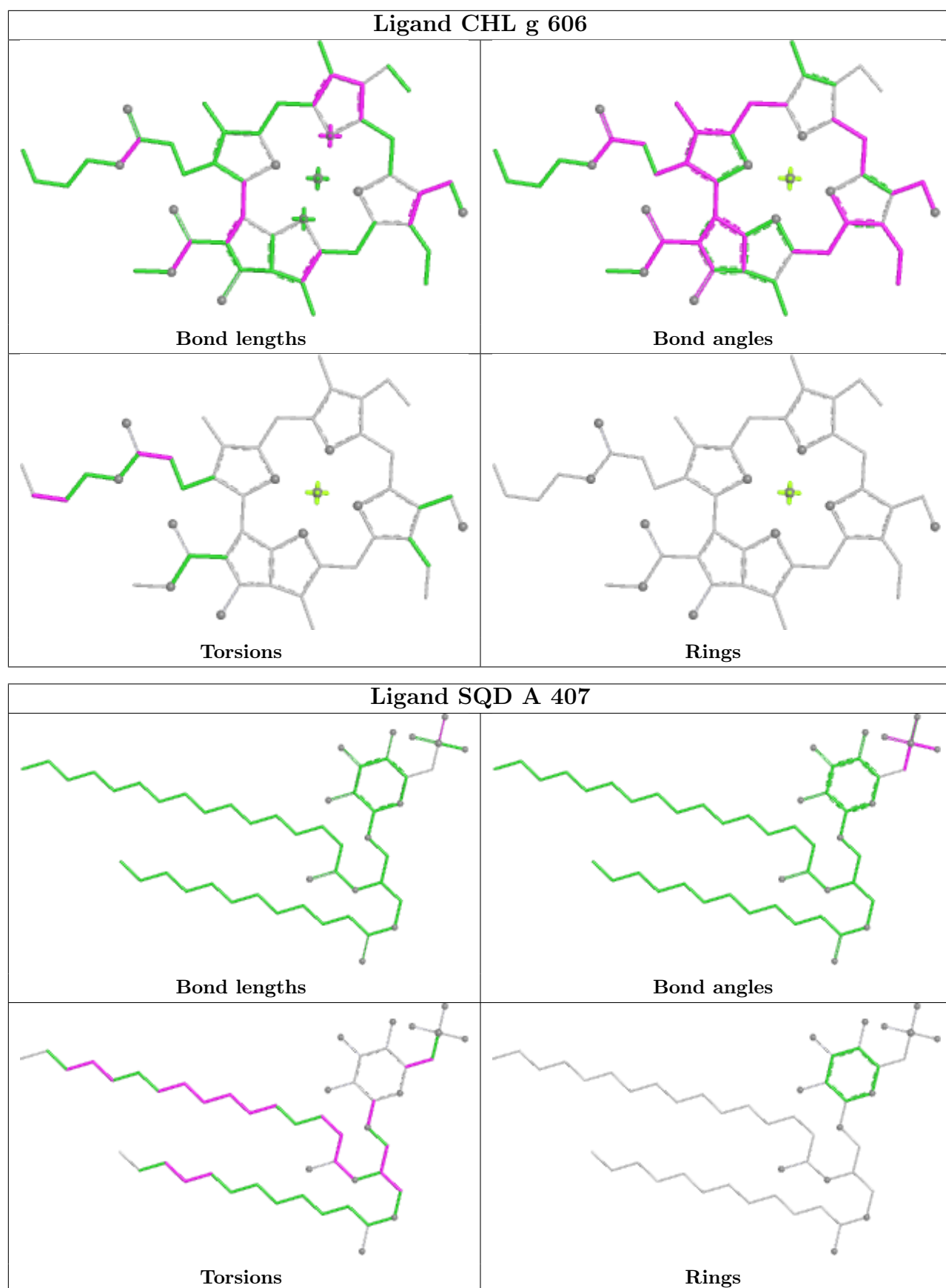


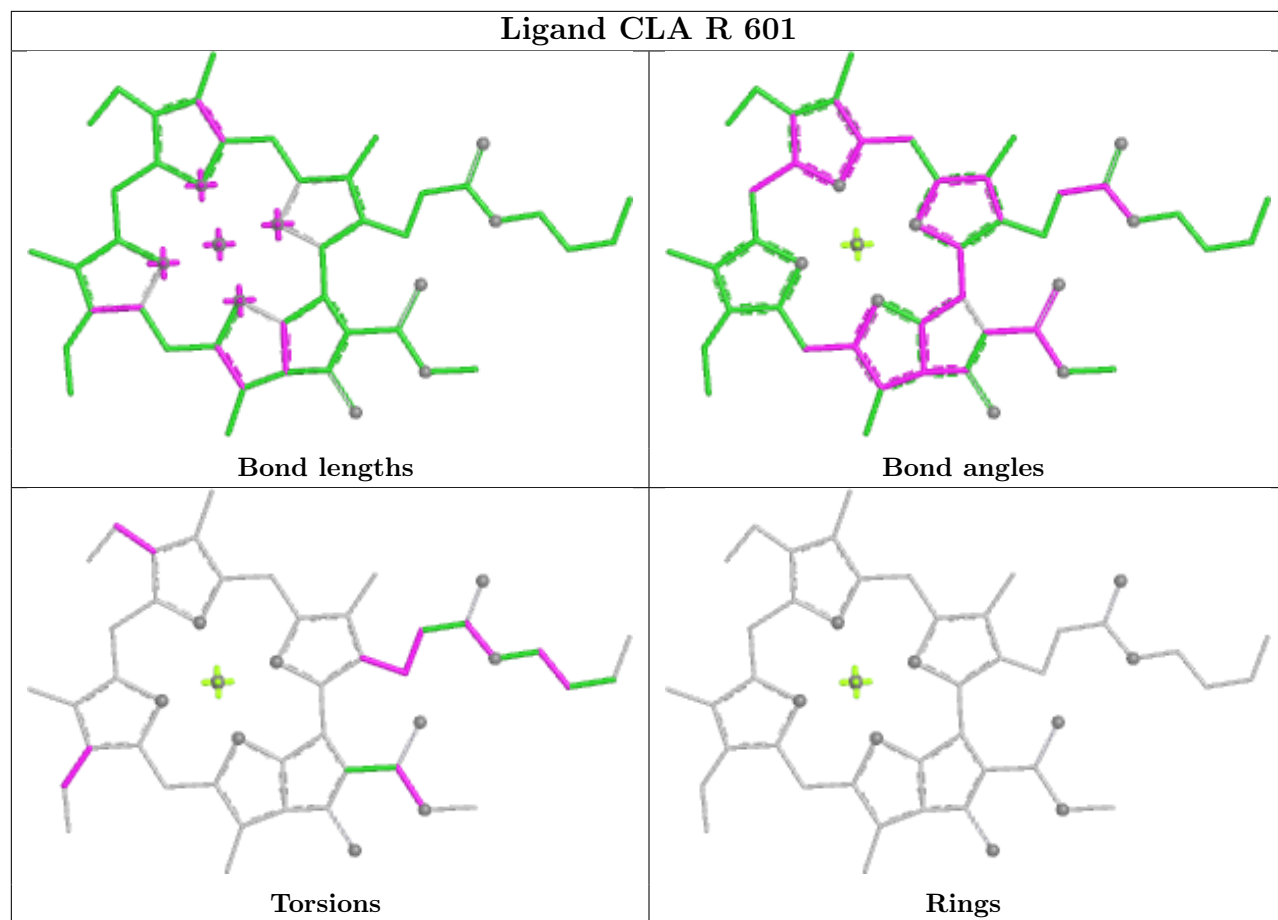


Ligand CHL G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT S 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

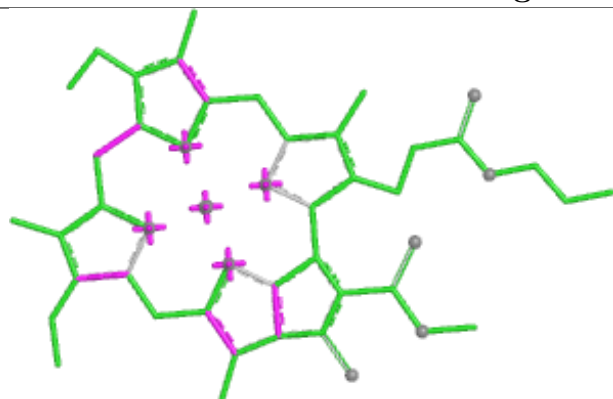




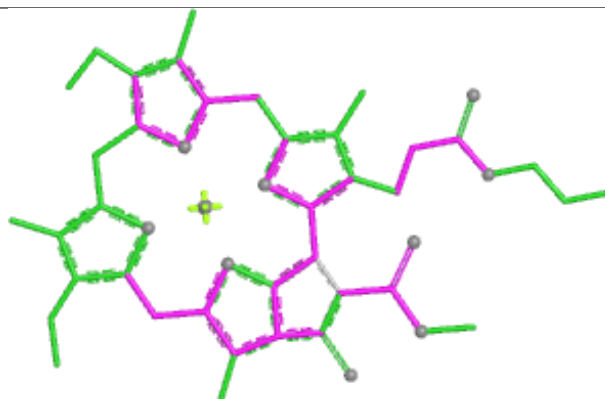




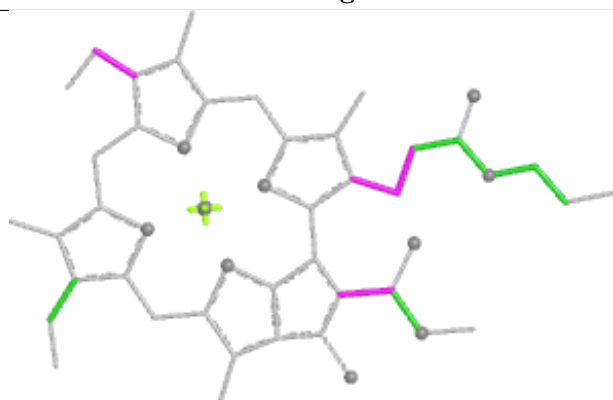
Ligand CLA R 604



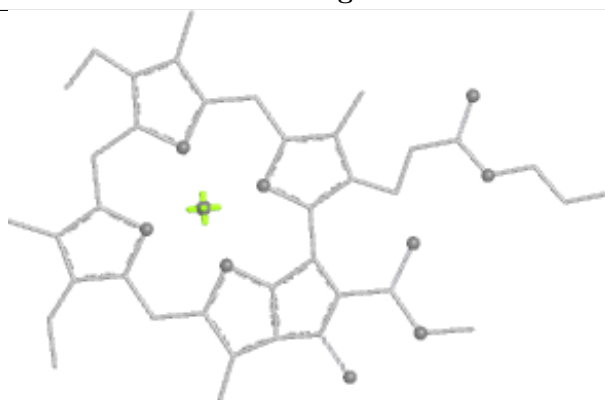
Bond lengths



Bond angles

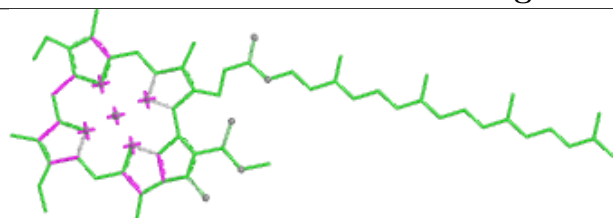


Torsions

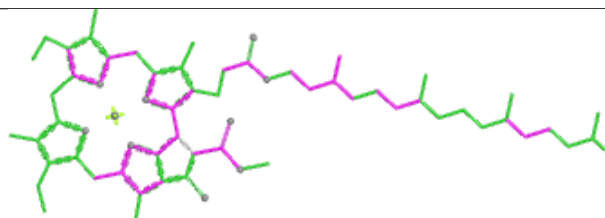


Rings

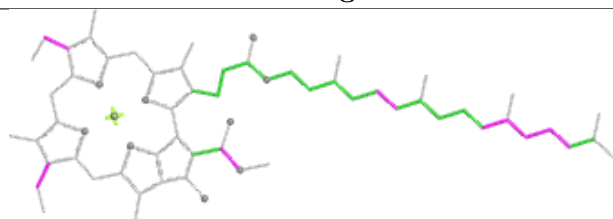
Ligand CLA C 508



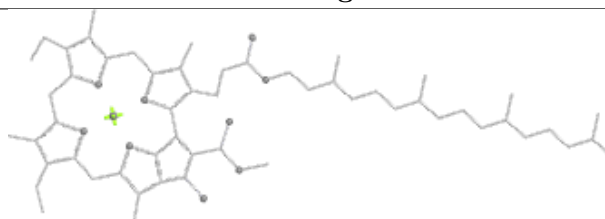
Bond lengths



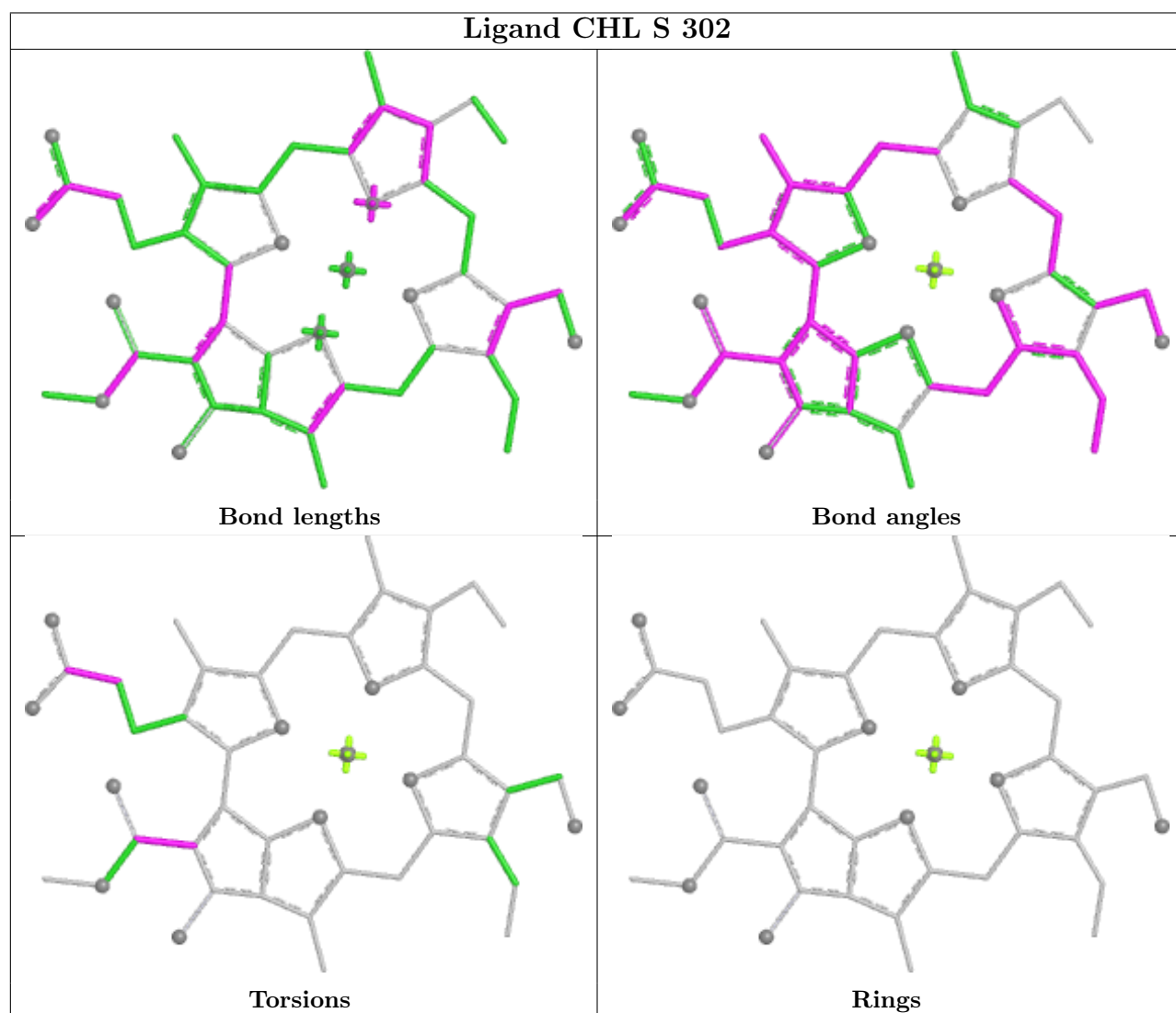
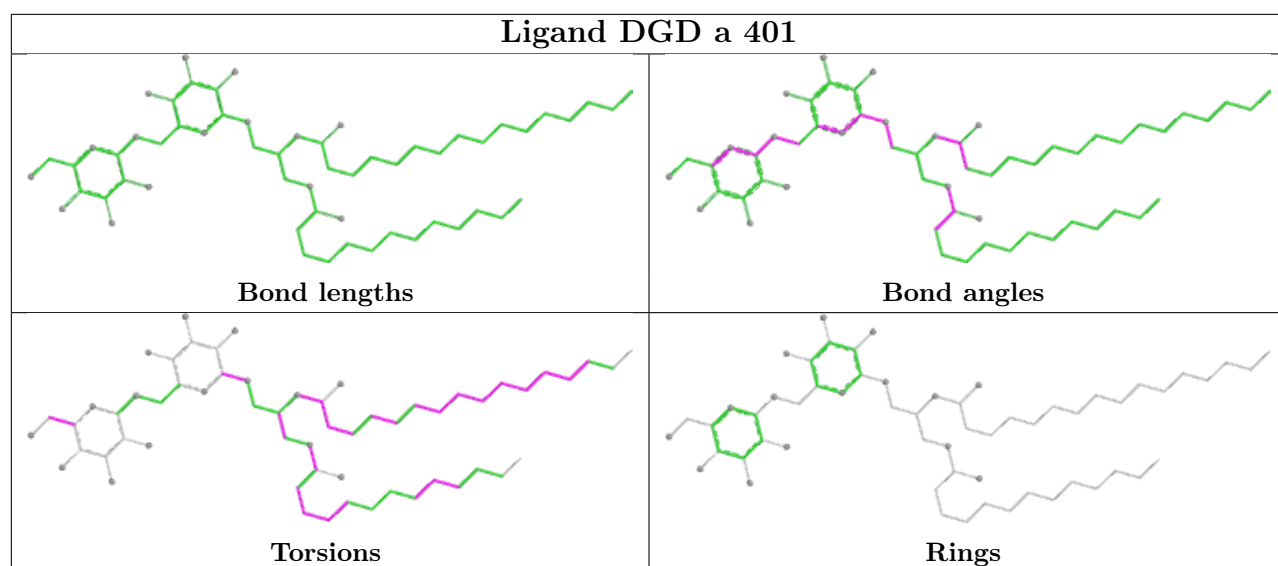
Bond angles

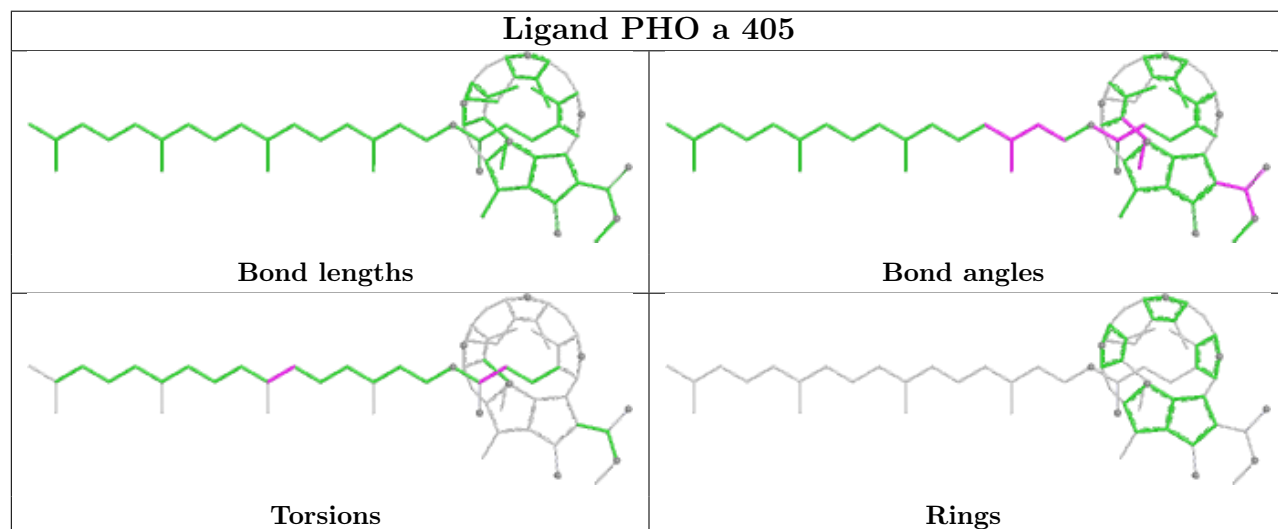
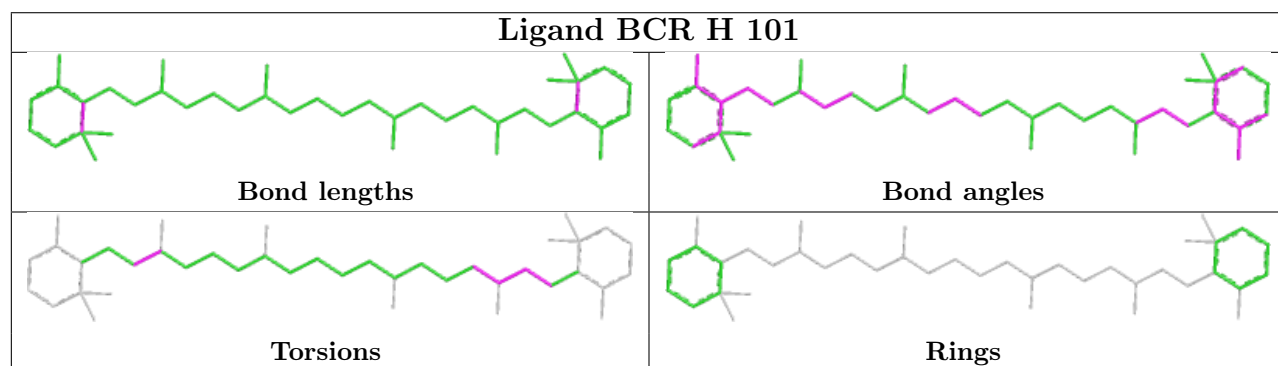
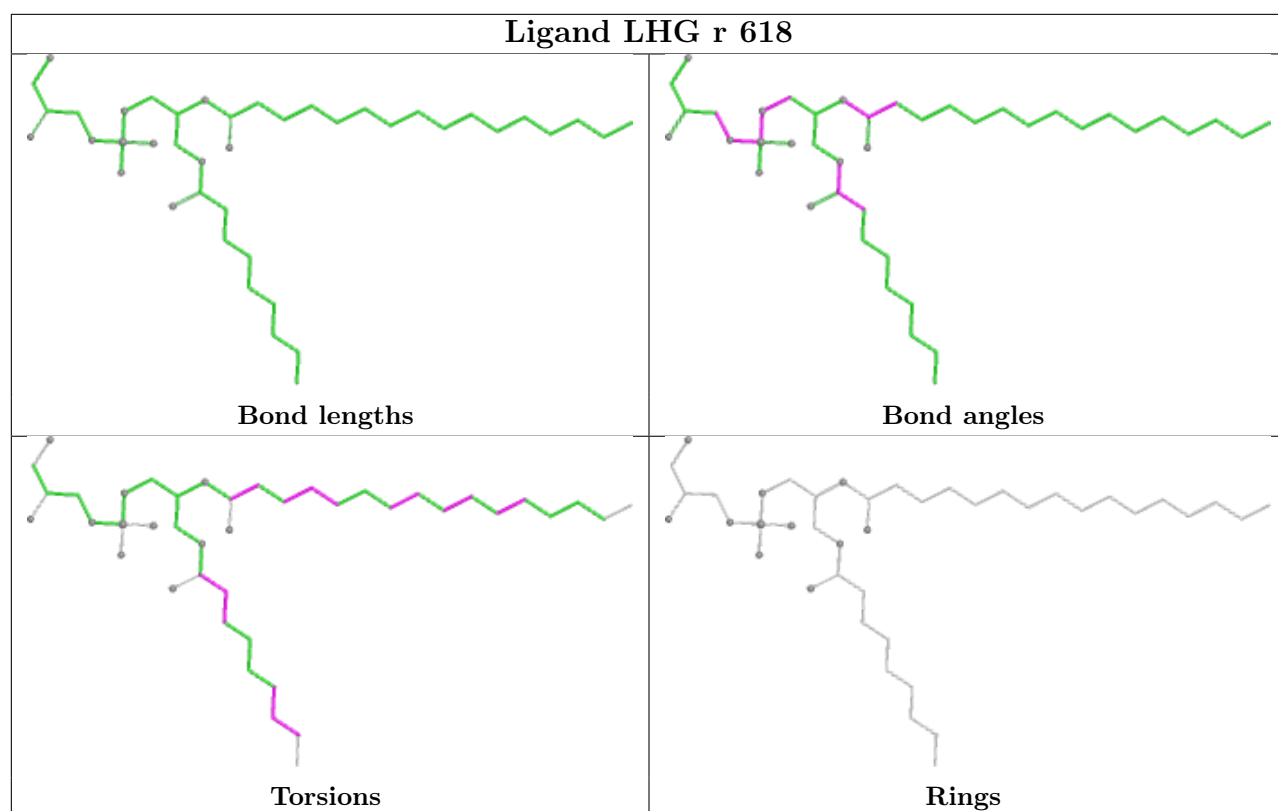


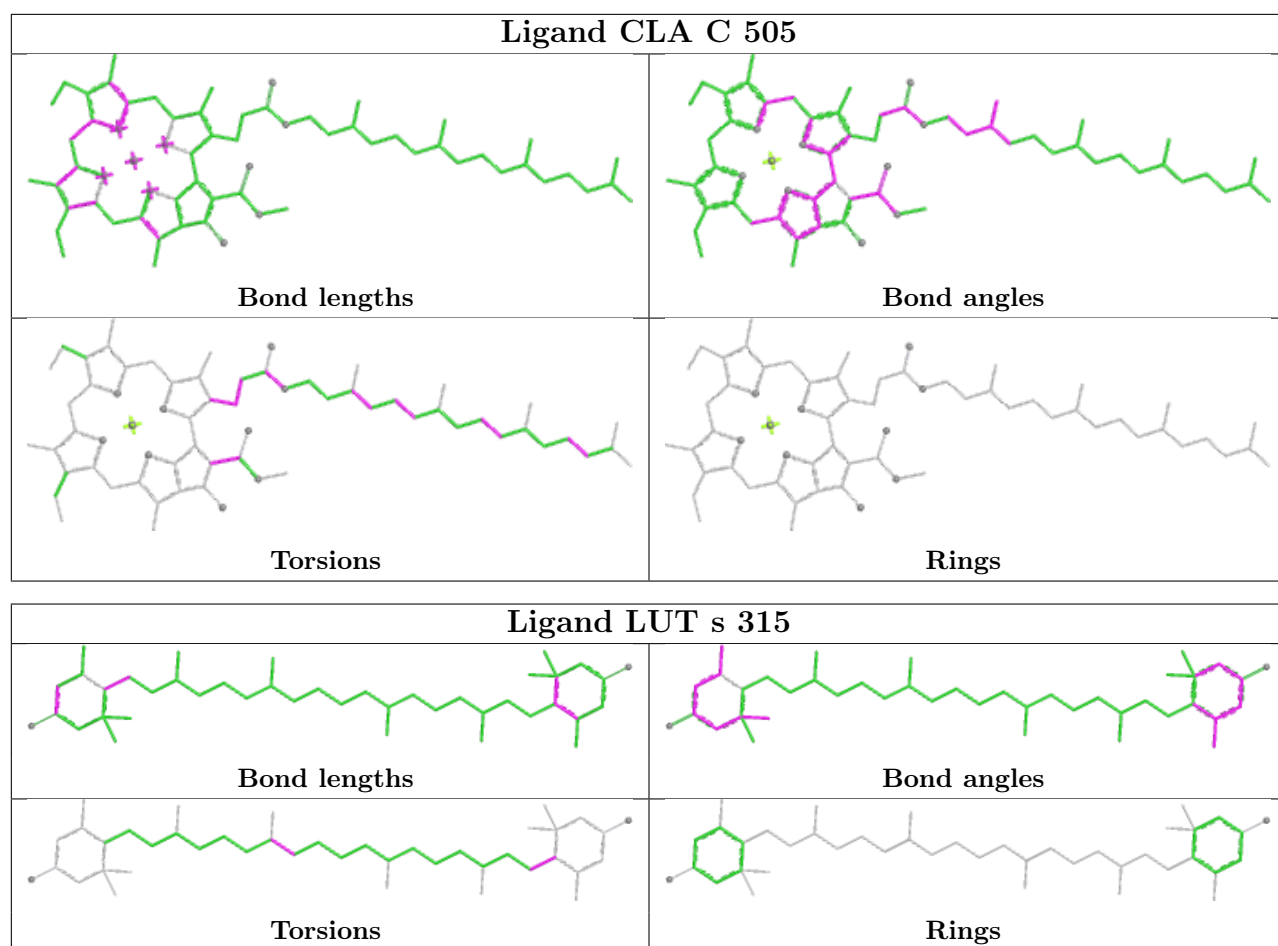
Torsions

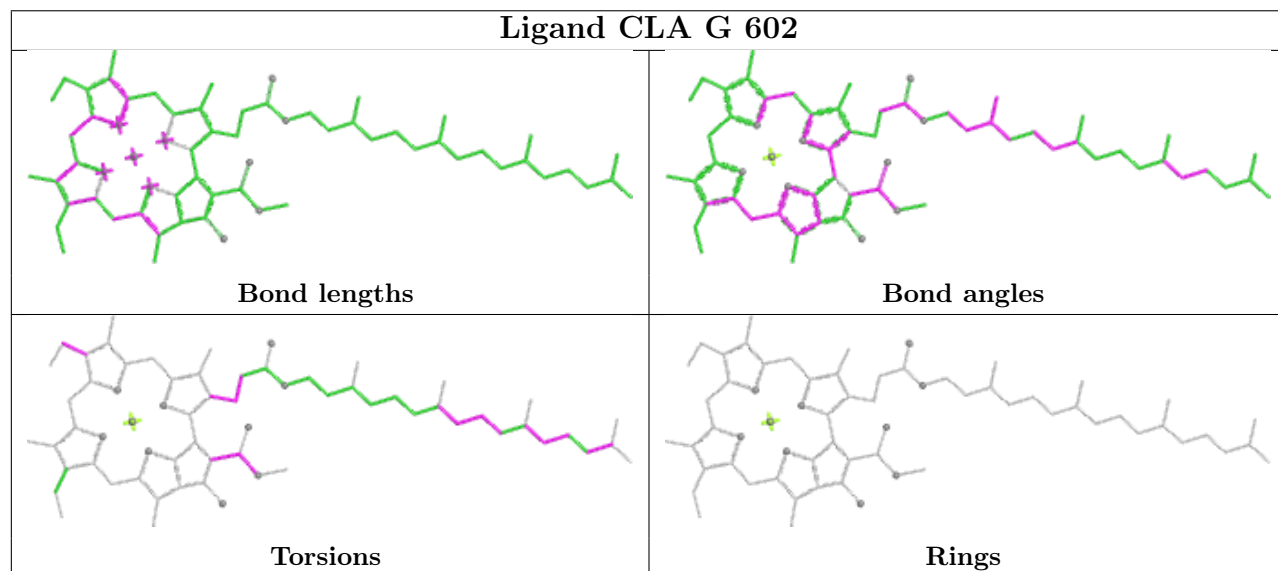
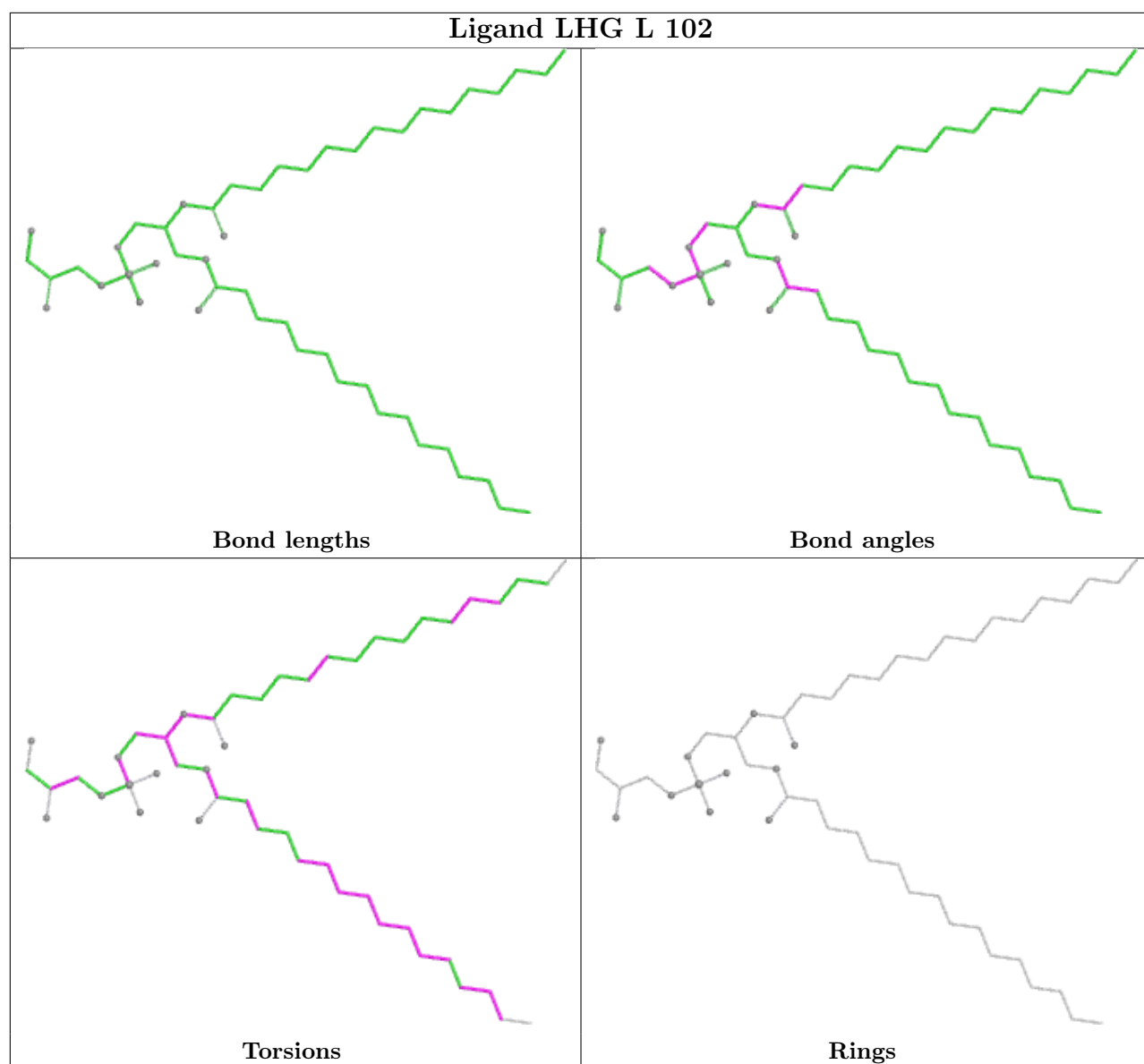


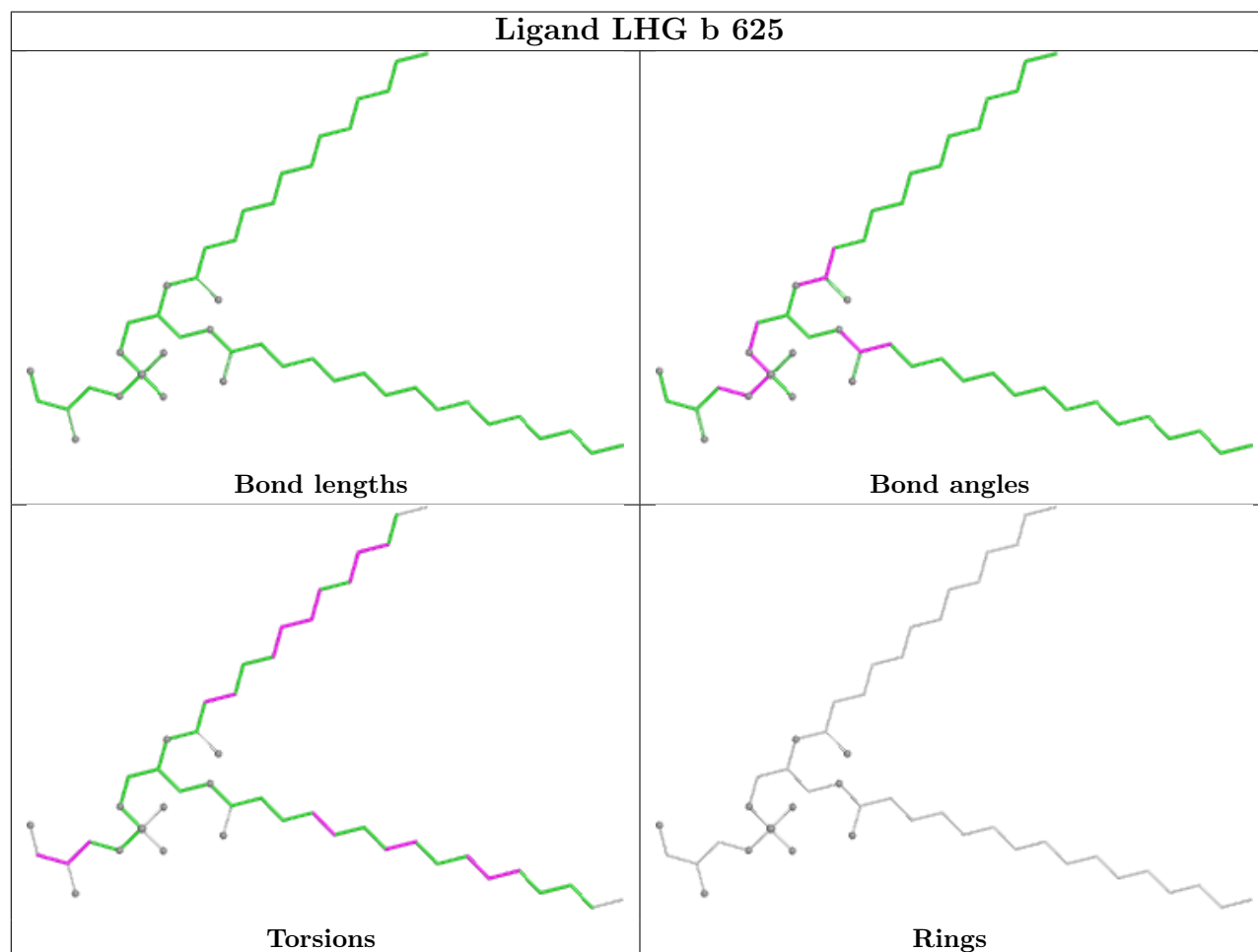
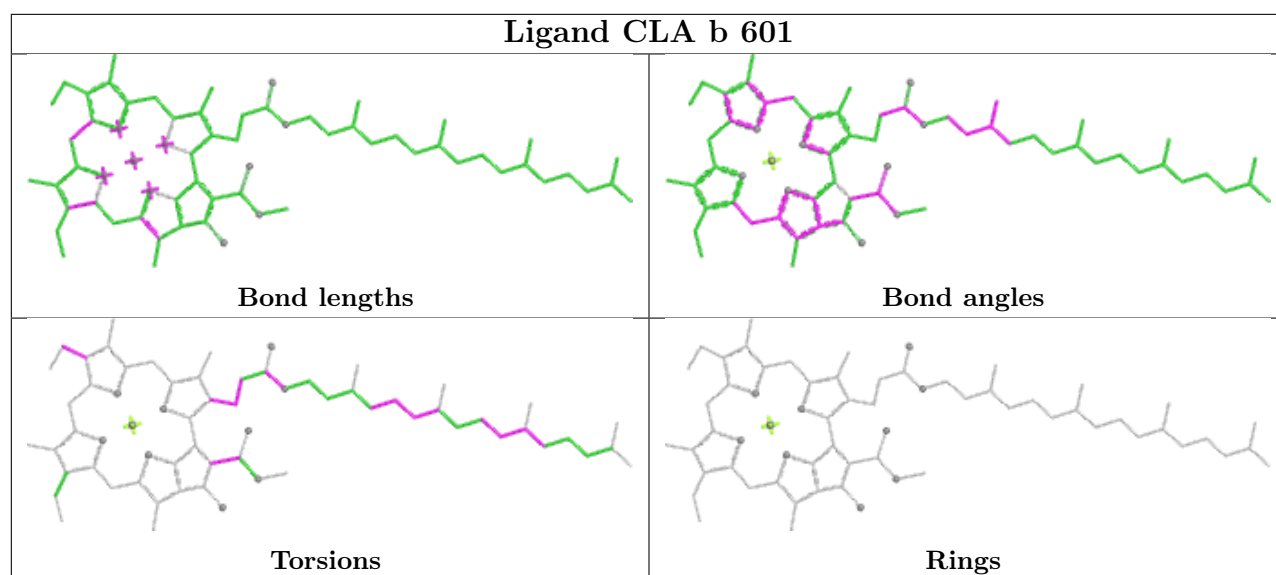
Rings

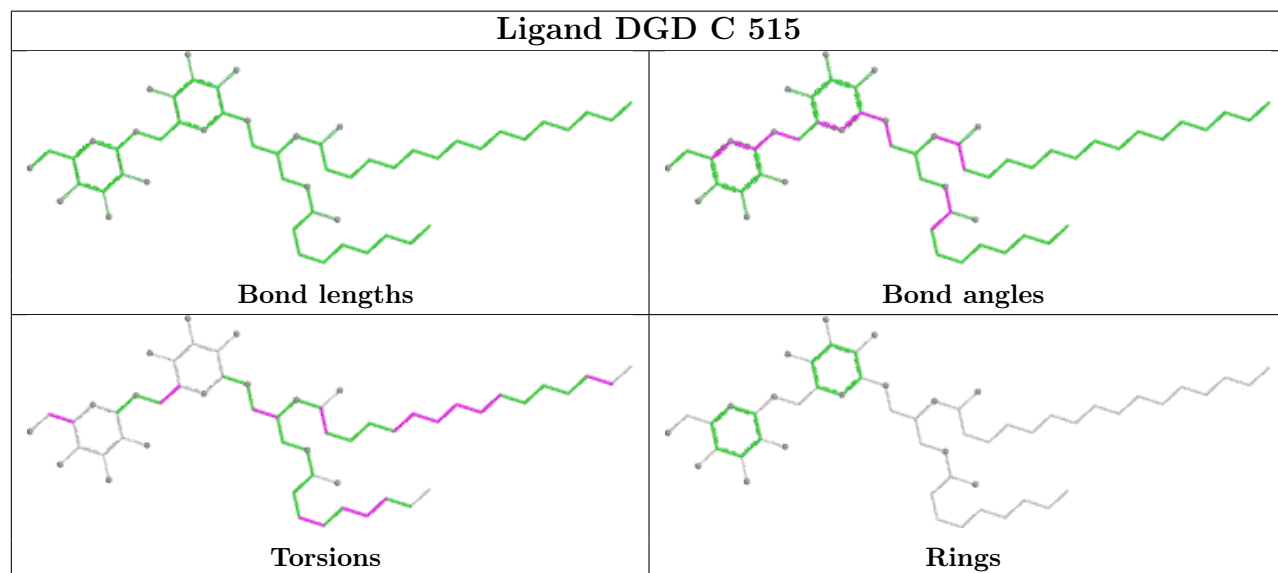
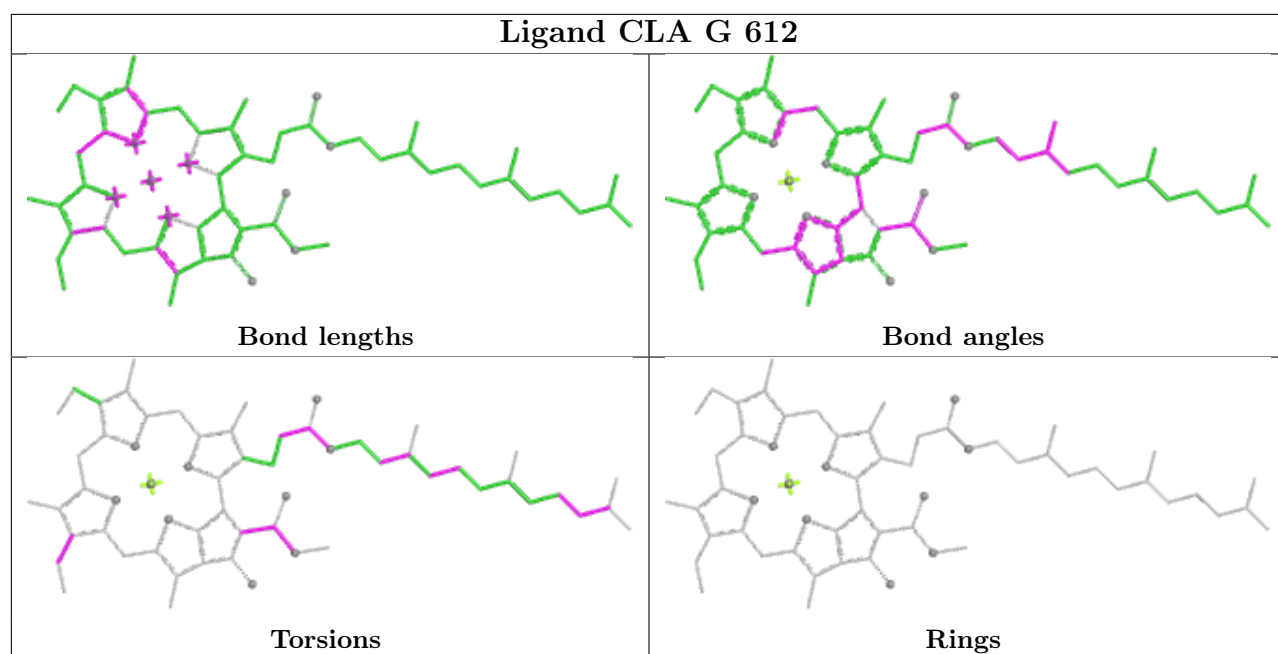


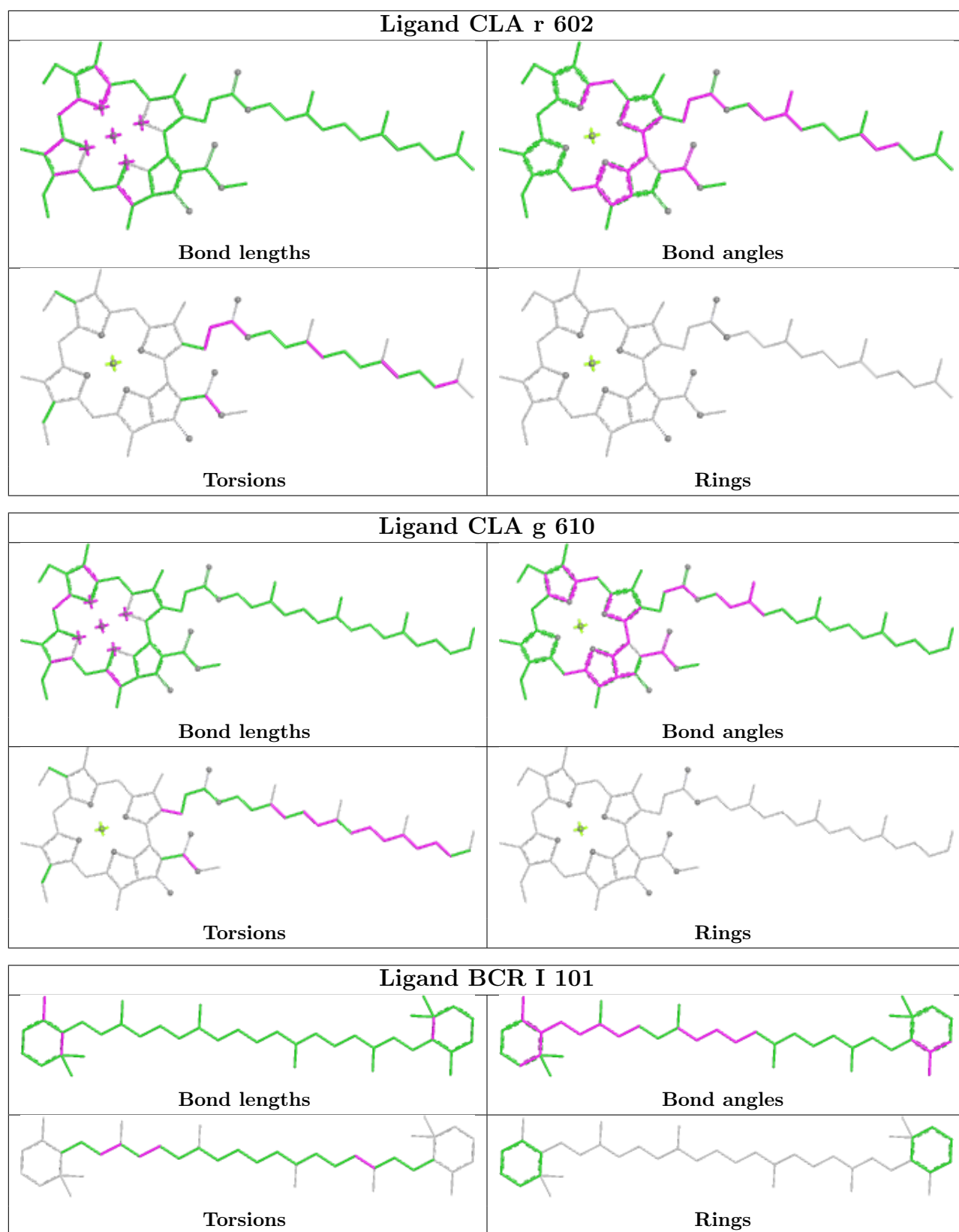


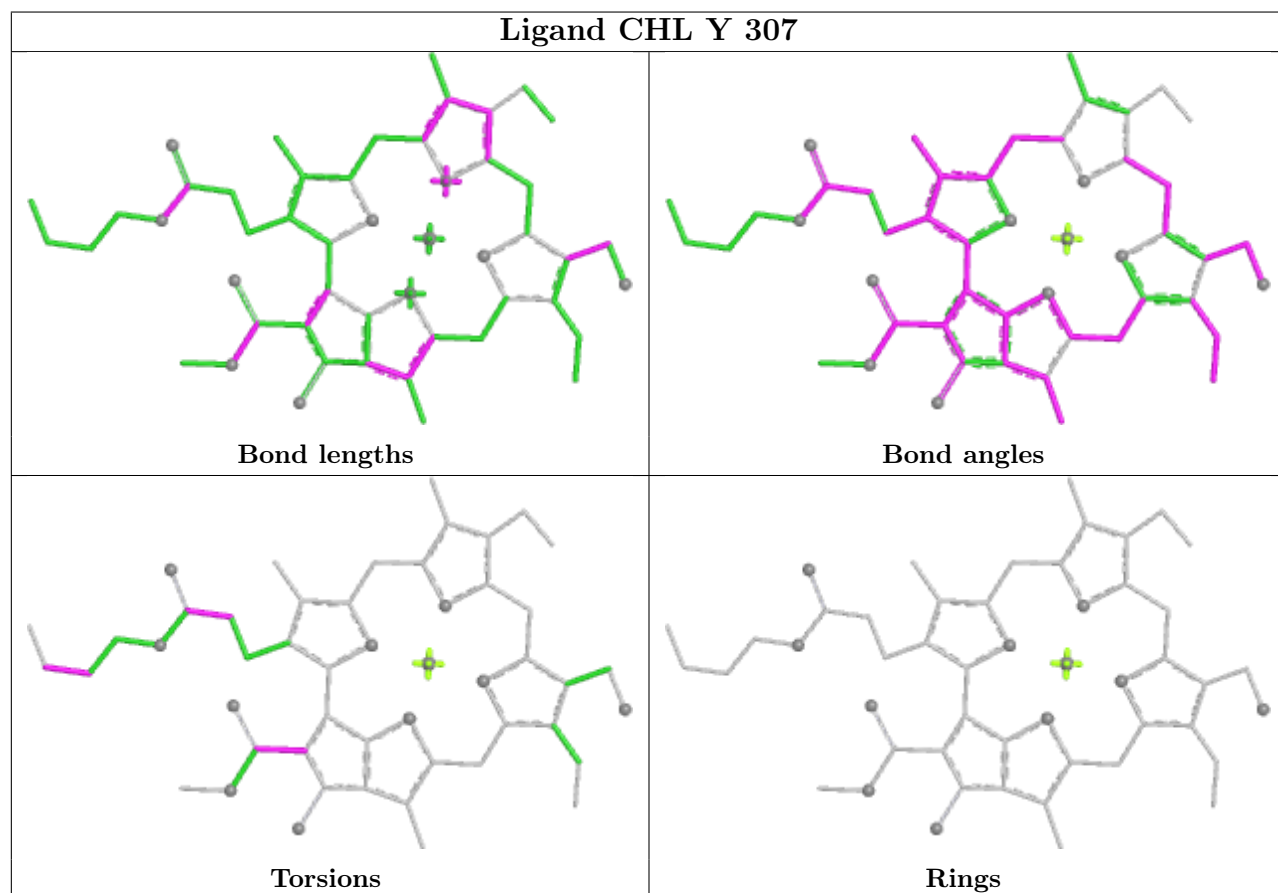
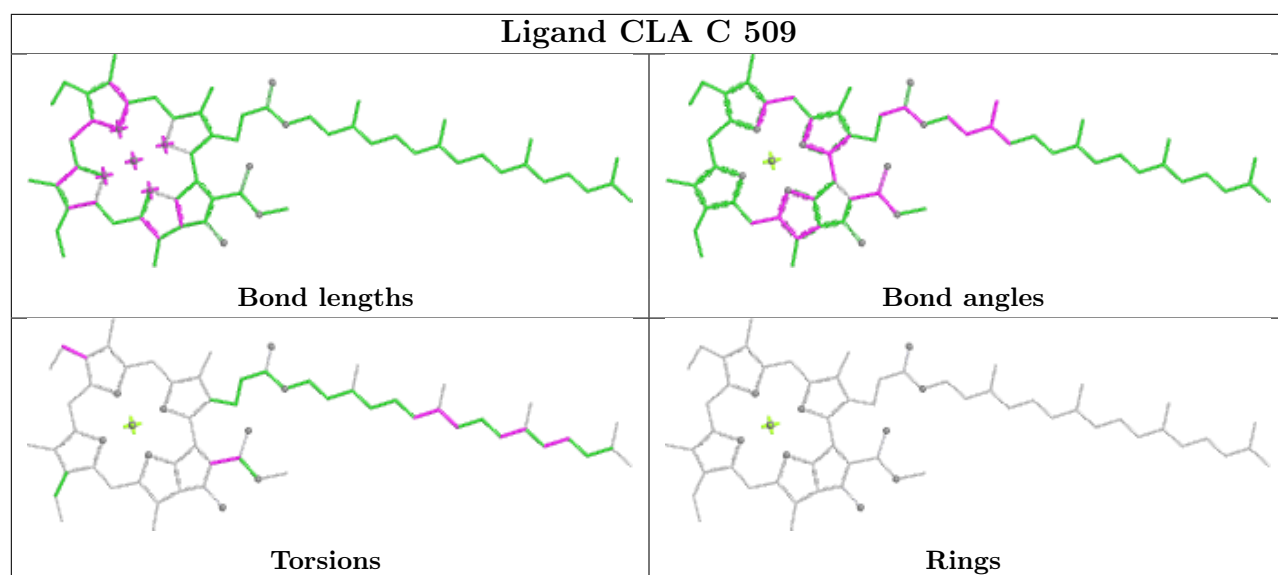


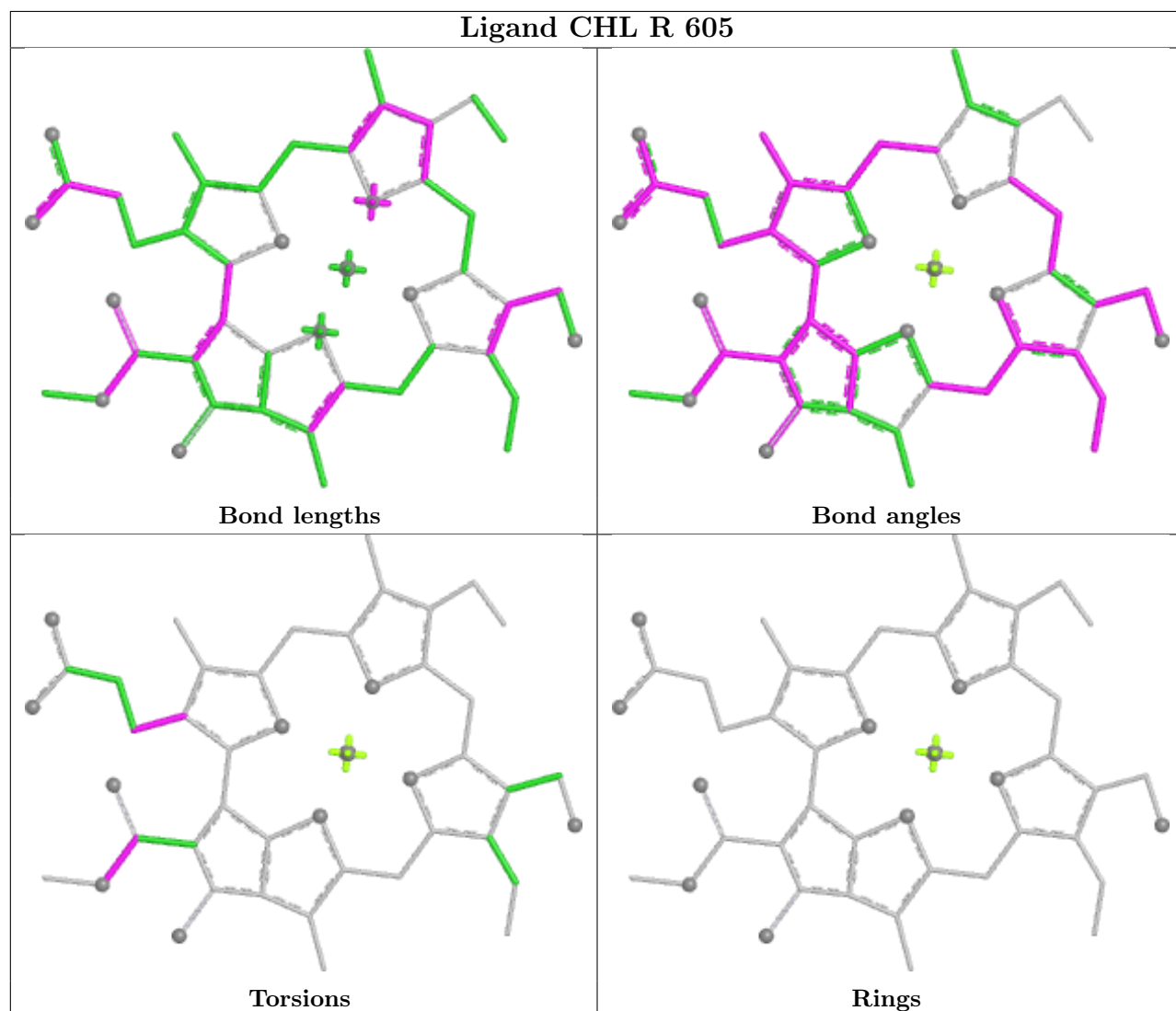
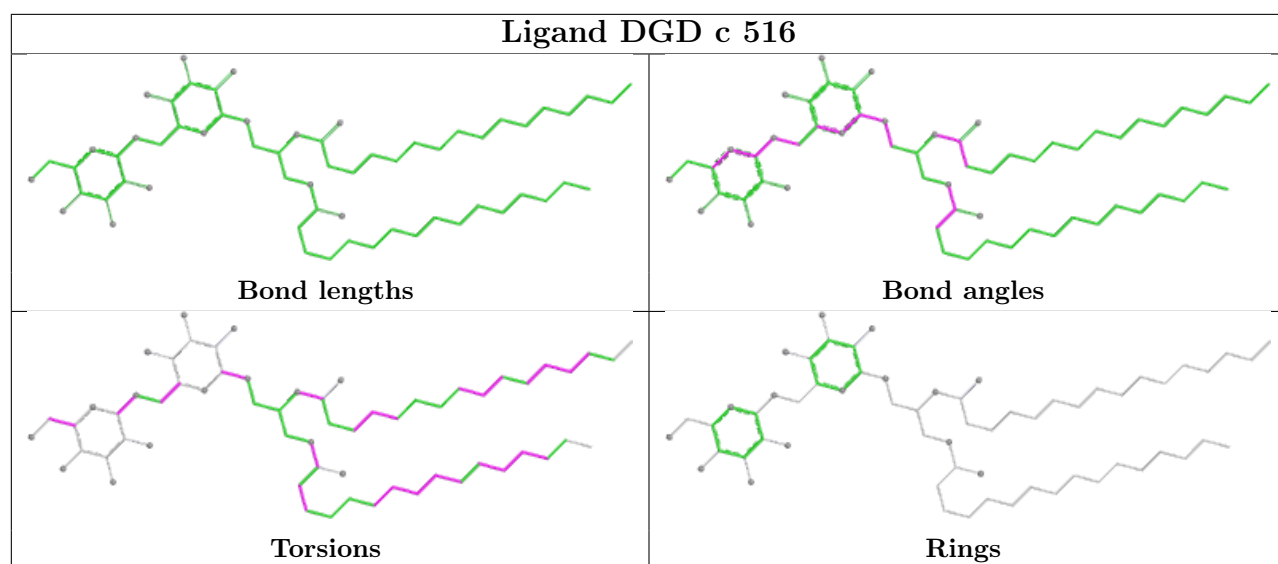


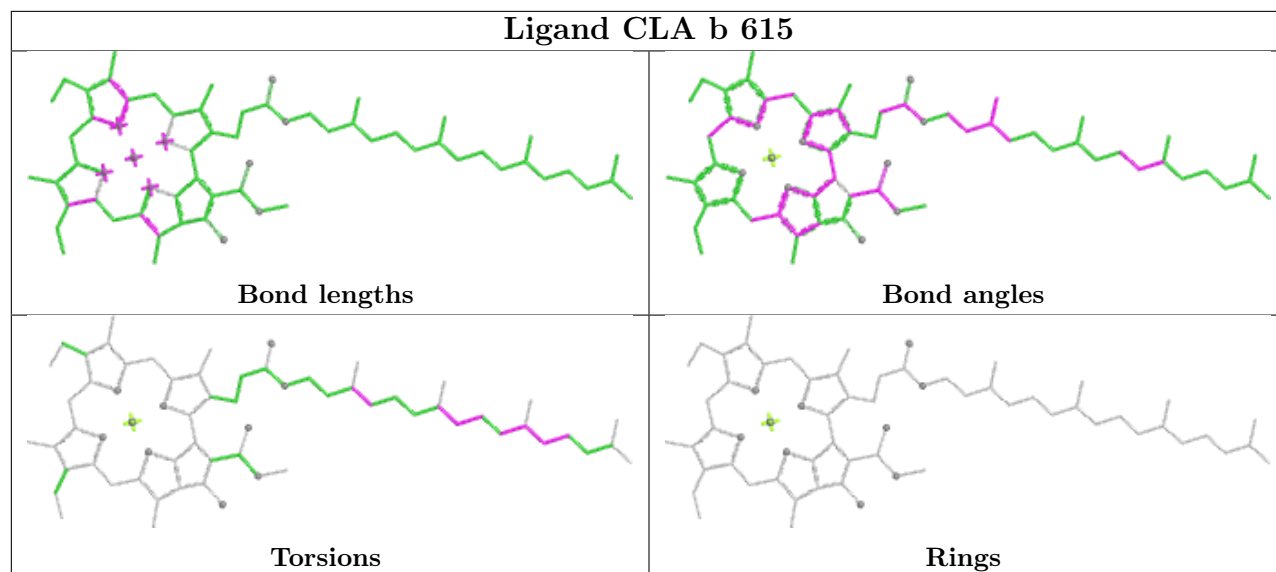
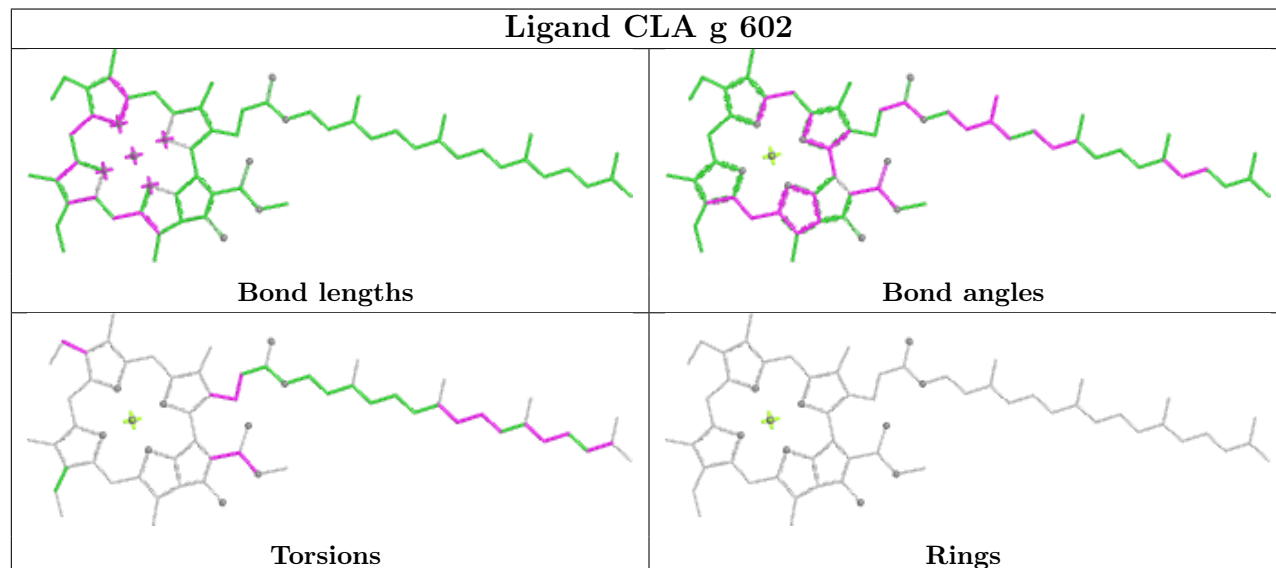




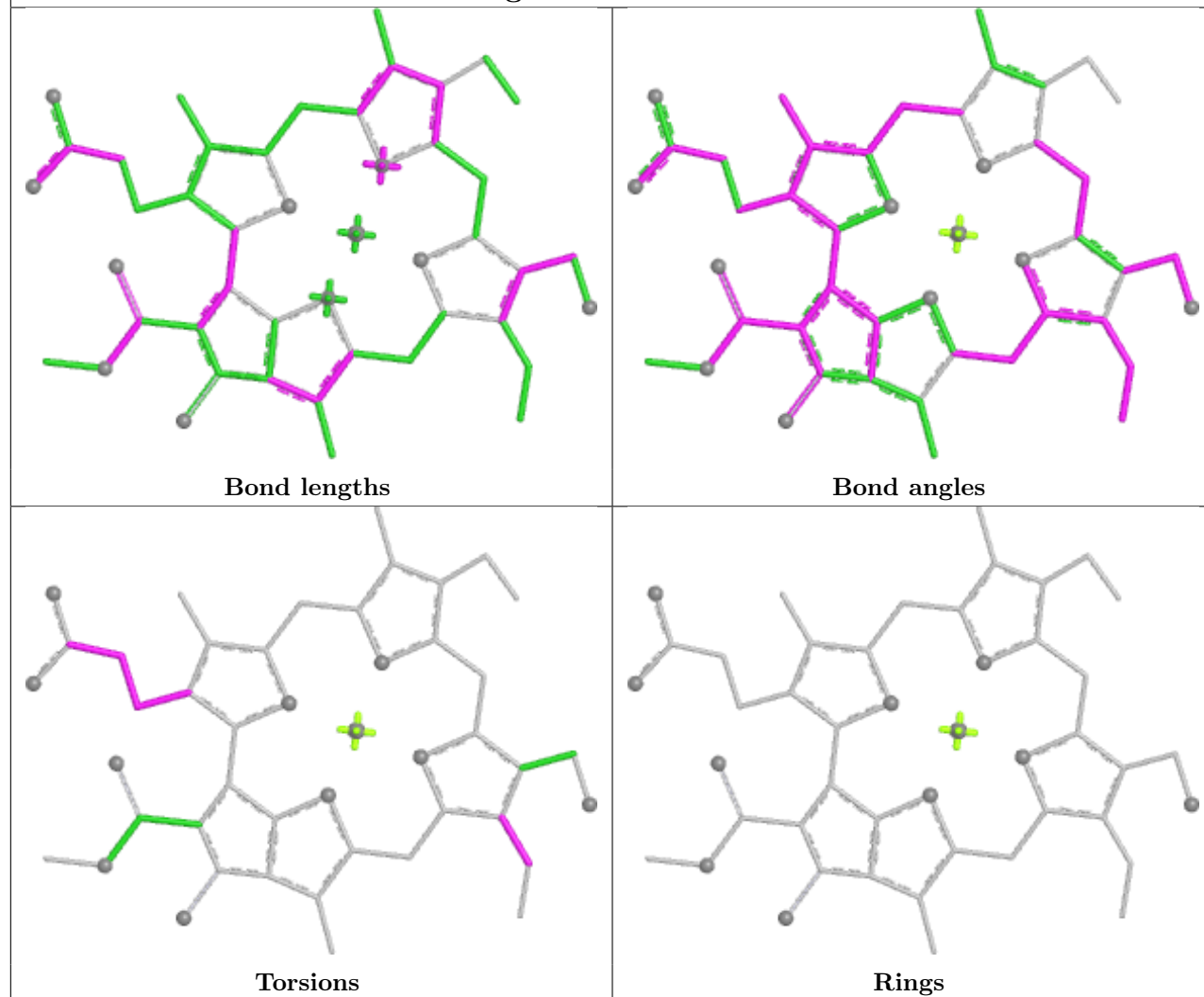




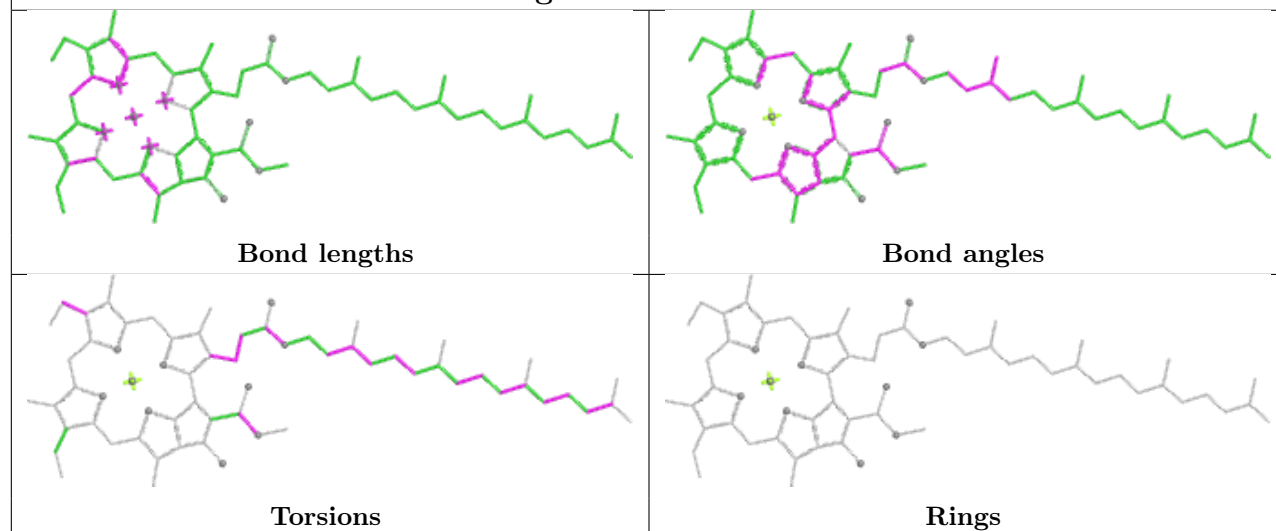


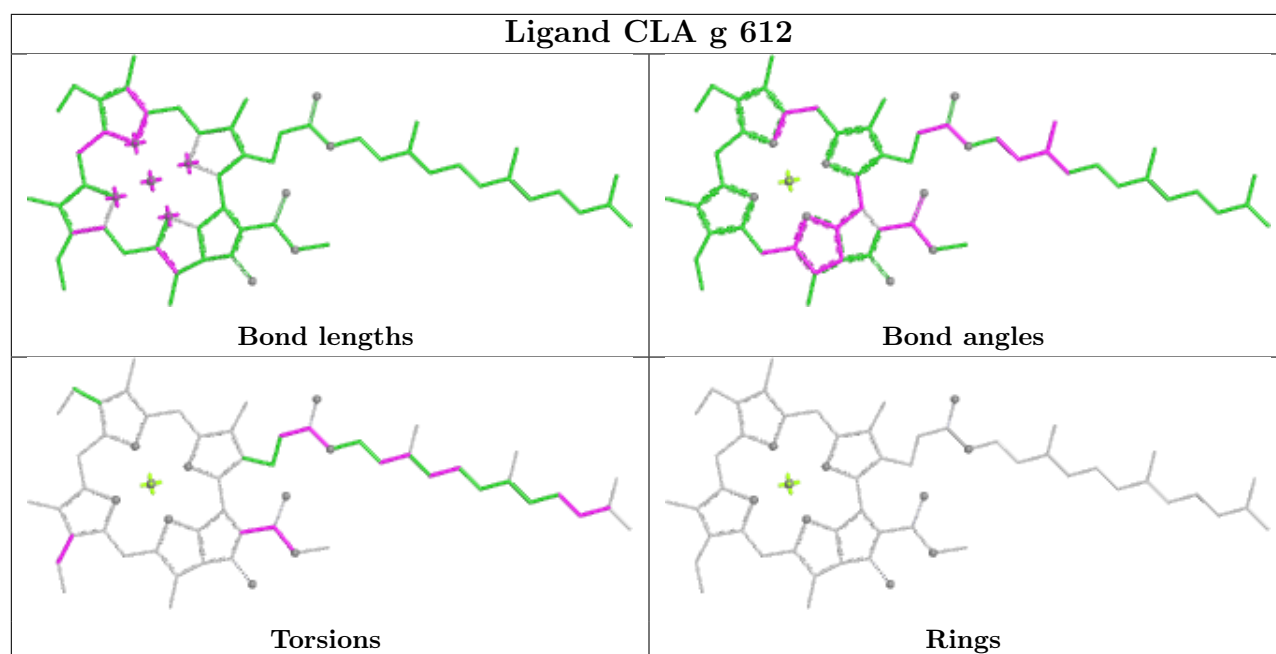
Ligand CLA b 615**Ligand CLA g 602**

Ligand CHL 5 302



Ligand CLA n 610





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.

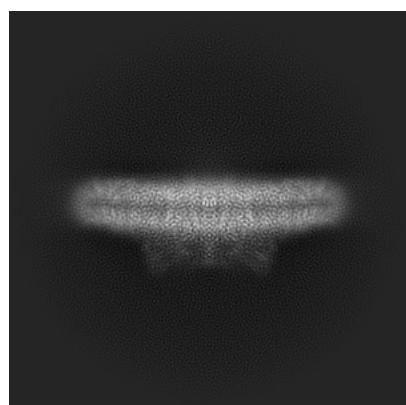
6 Map visualisation [i](#)

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.

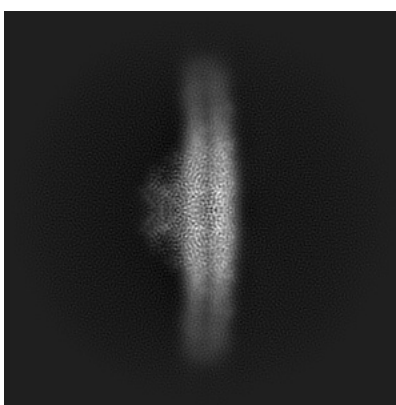
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

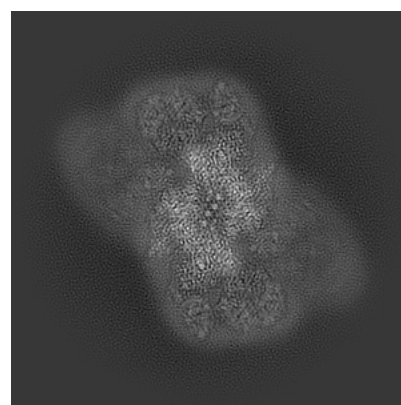
6.1.1 Primary map



X



Y

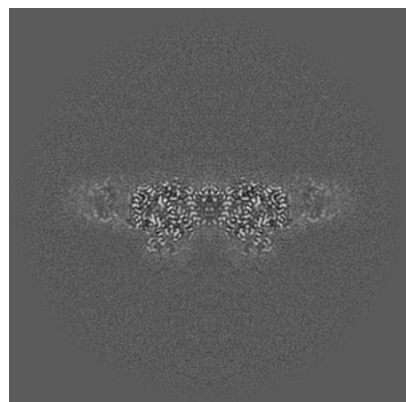


Z

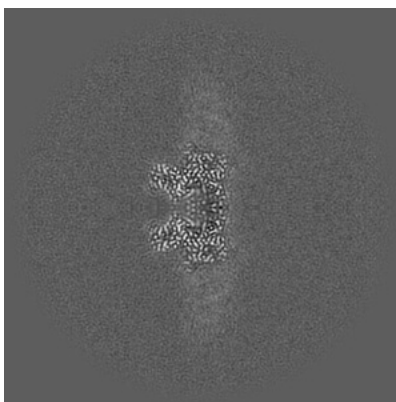
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

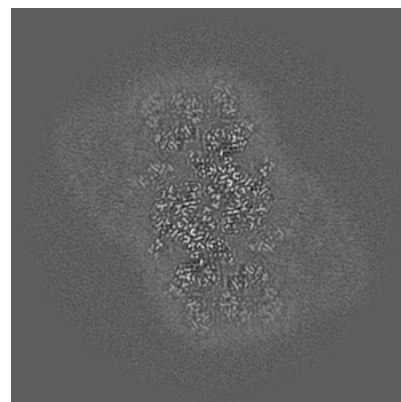
6.2.1 Primary map



X Index: 250



Y Index: 250

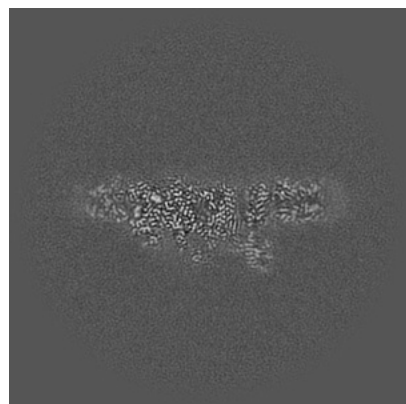


Z Index: 250

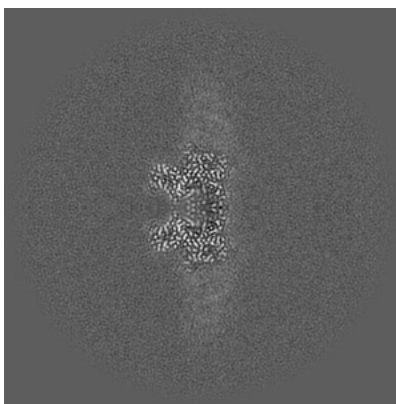
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

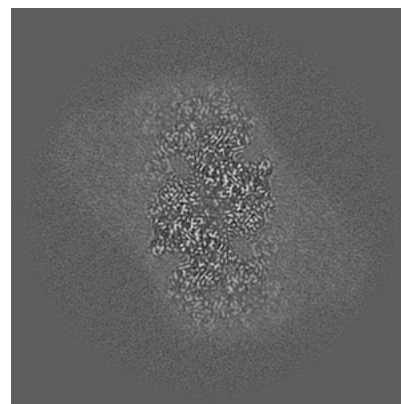
6.3.1 Primary map



X Index: 228



Y Index: 250

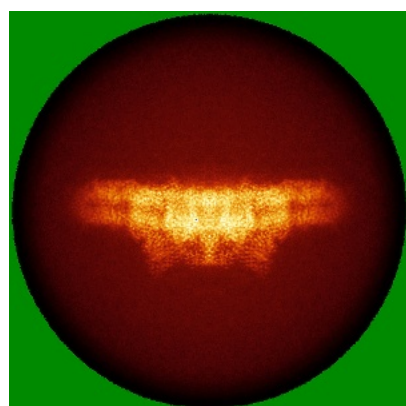


Z Index: 239

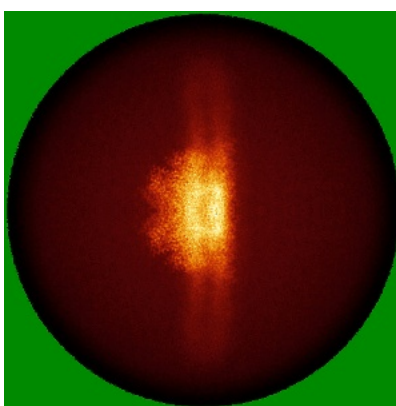
The images above show the largest variance slices of the map in three orthogonal directions.

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

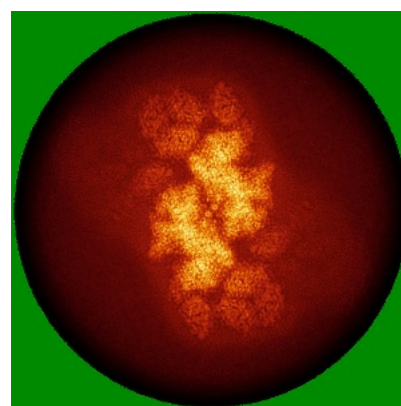
6.4.1 Primary map



X



Y

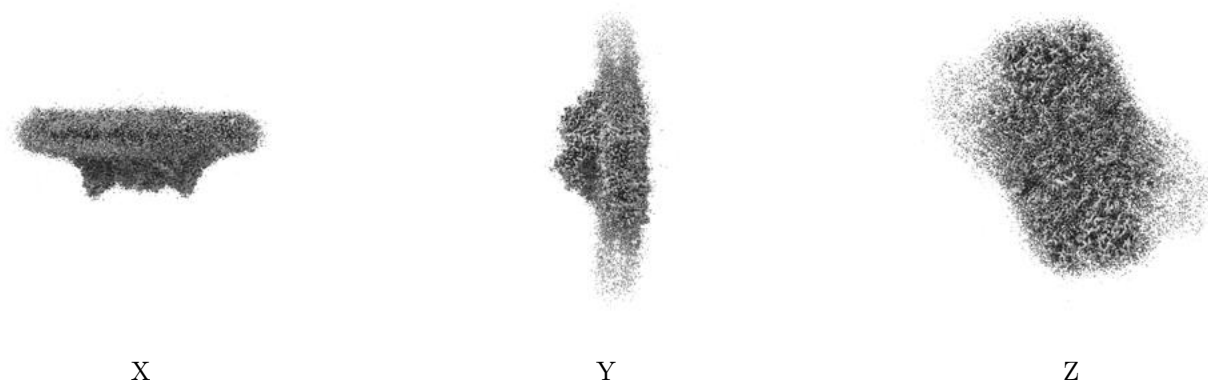


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

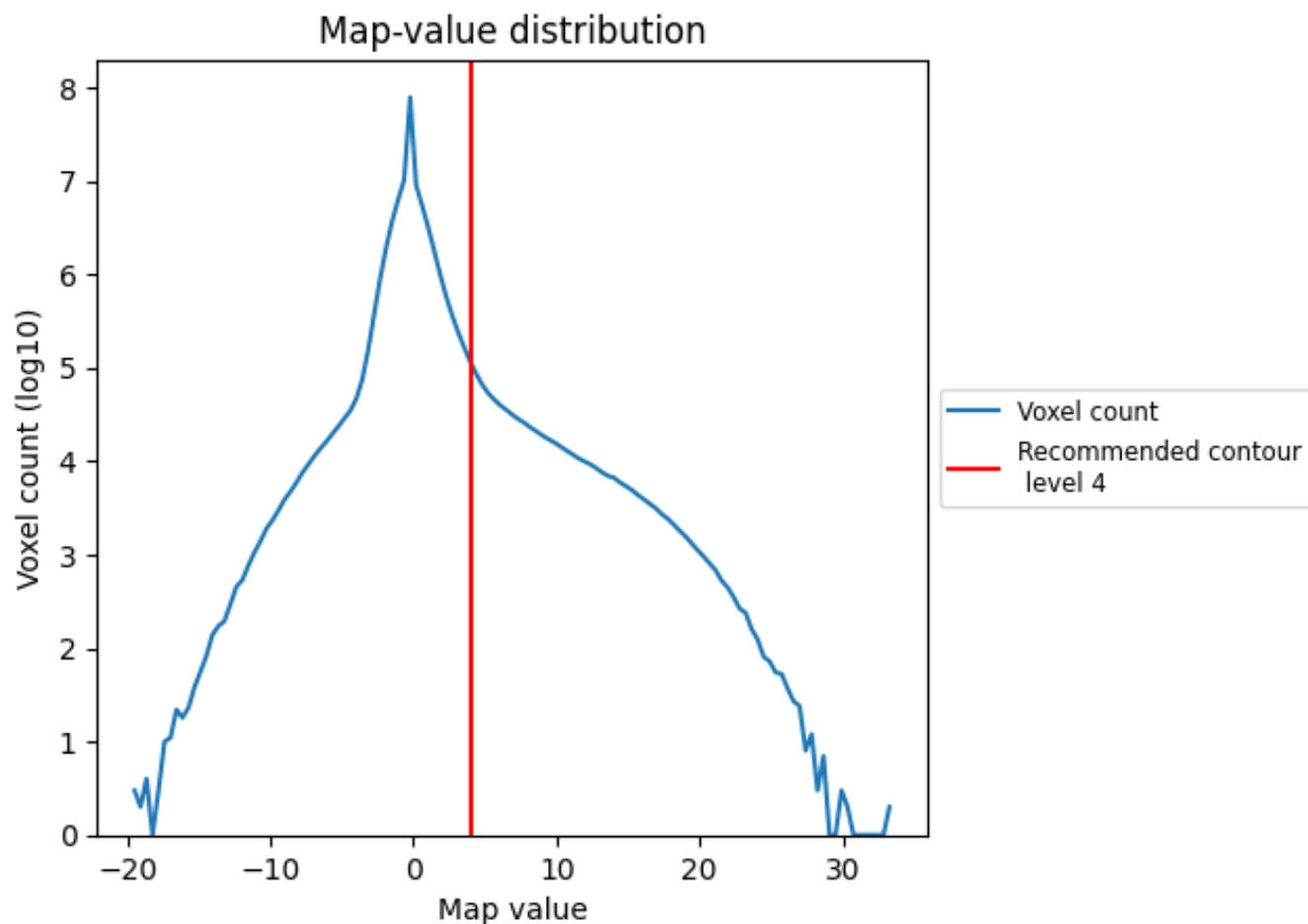
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

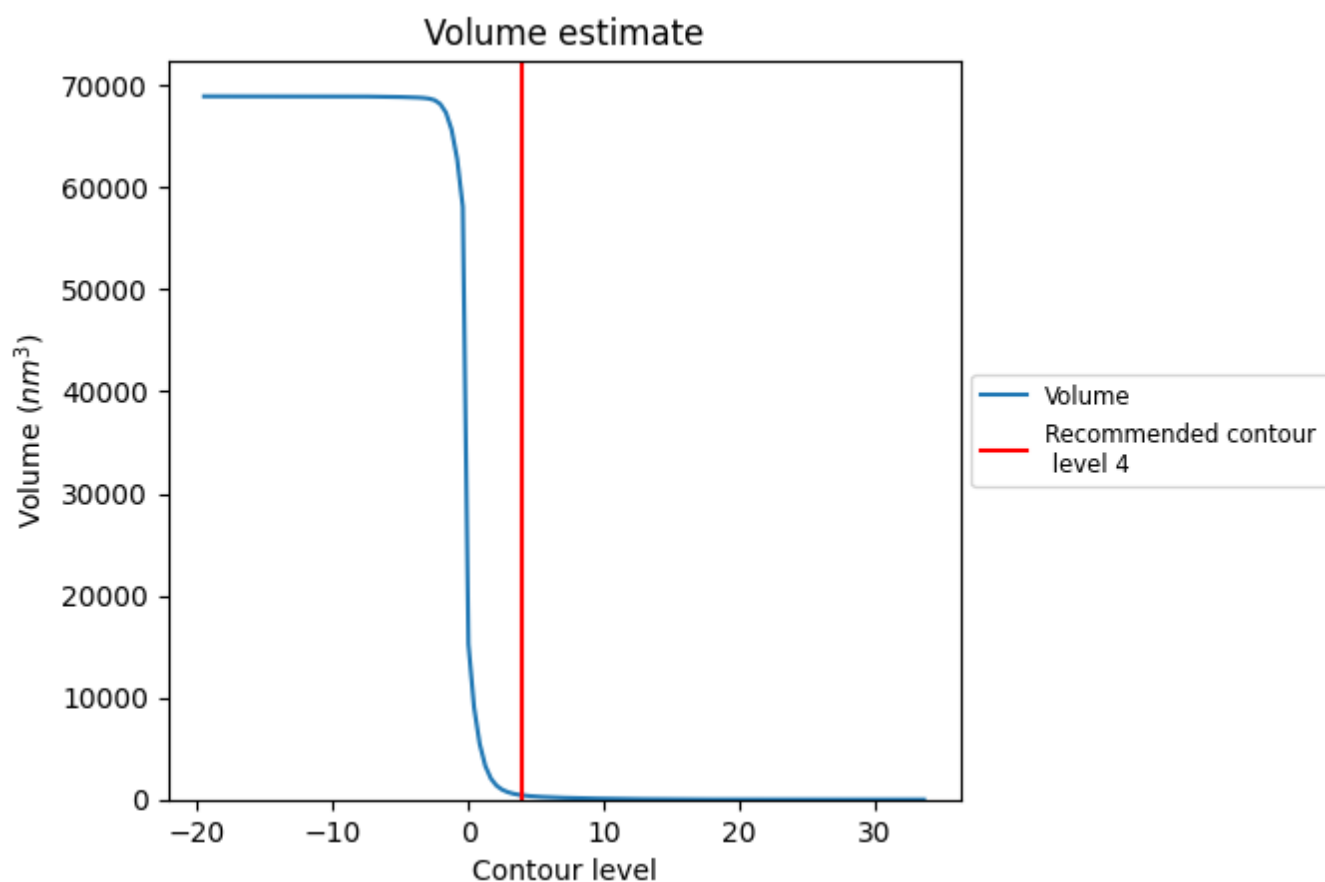
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

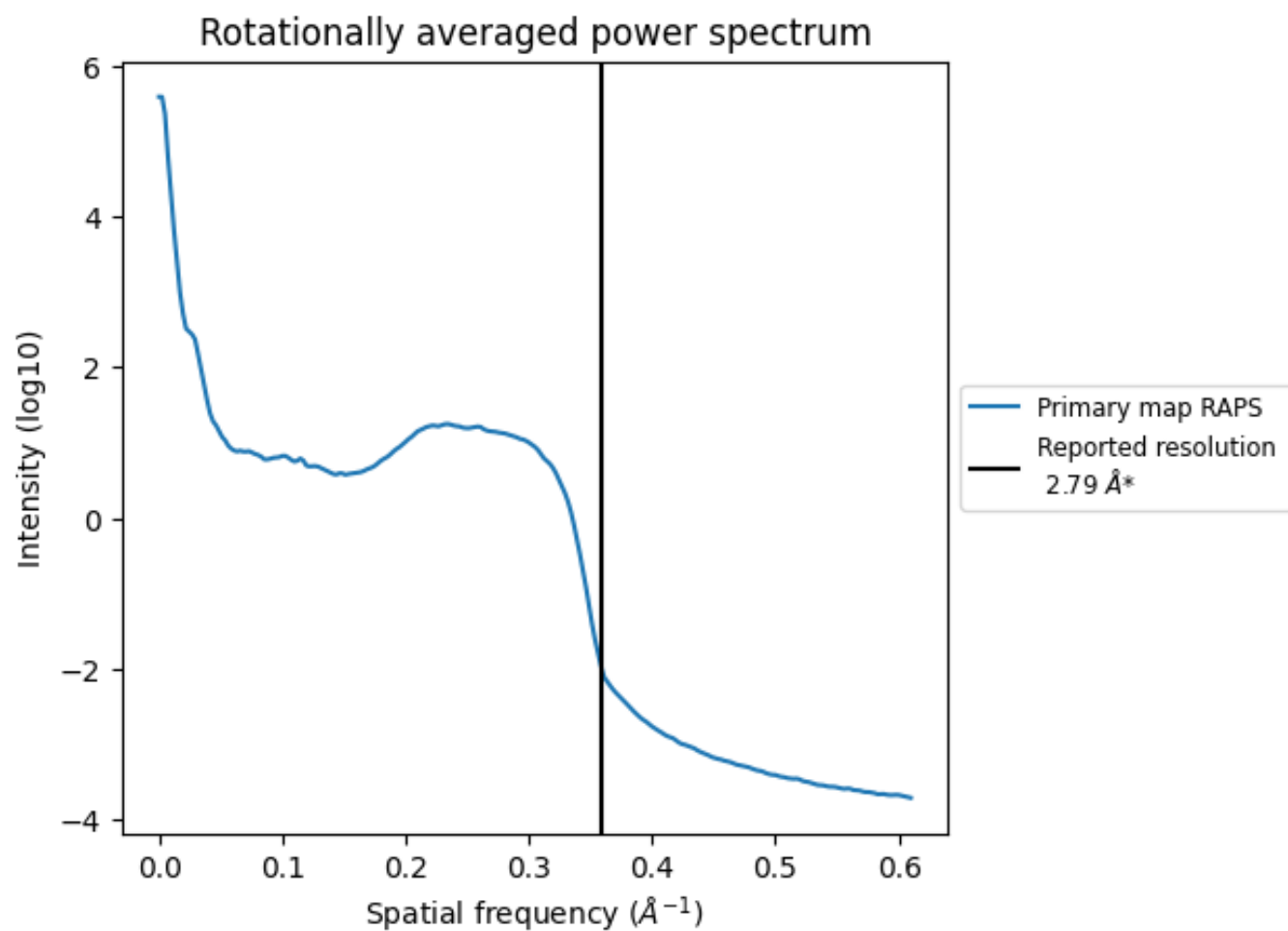
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

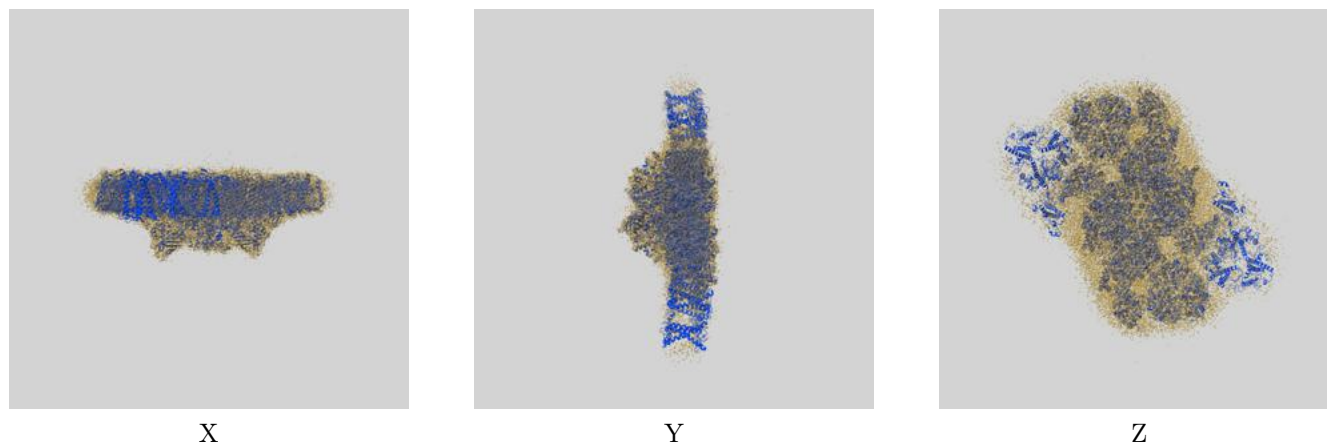
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

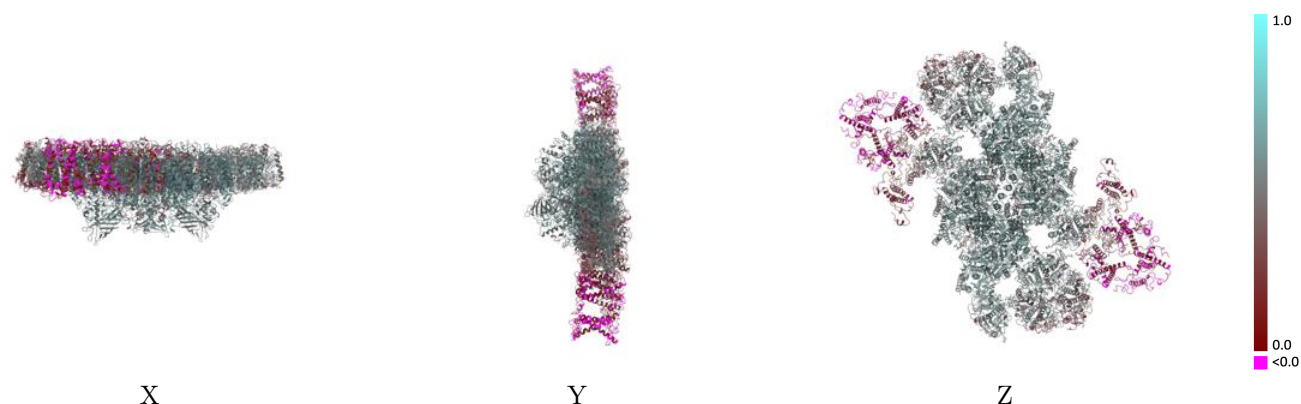
This section contains information regarding the fit between EMDB map EMD-13078 and PDB model 7OUI. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



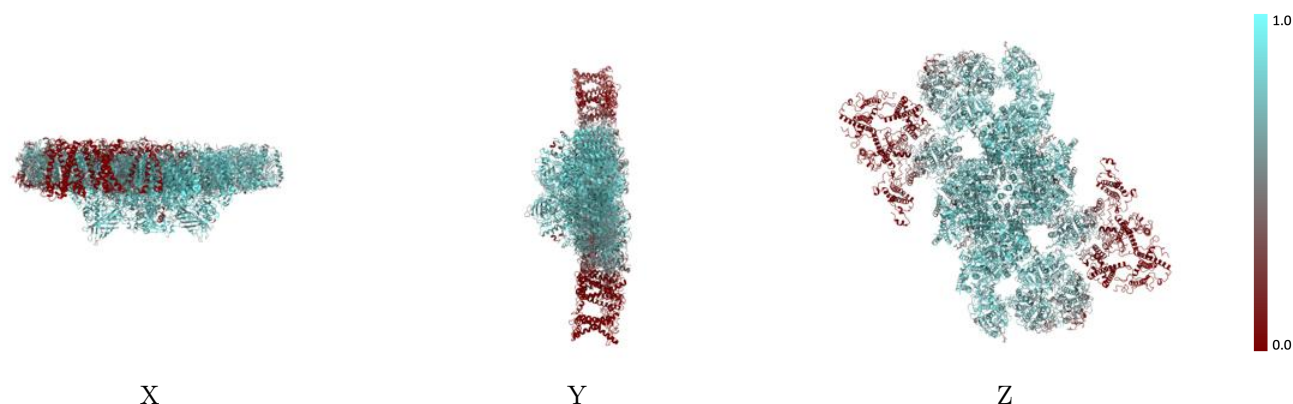
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



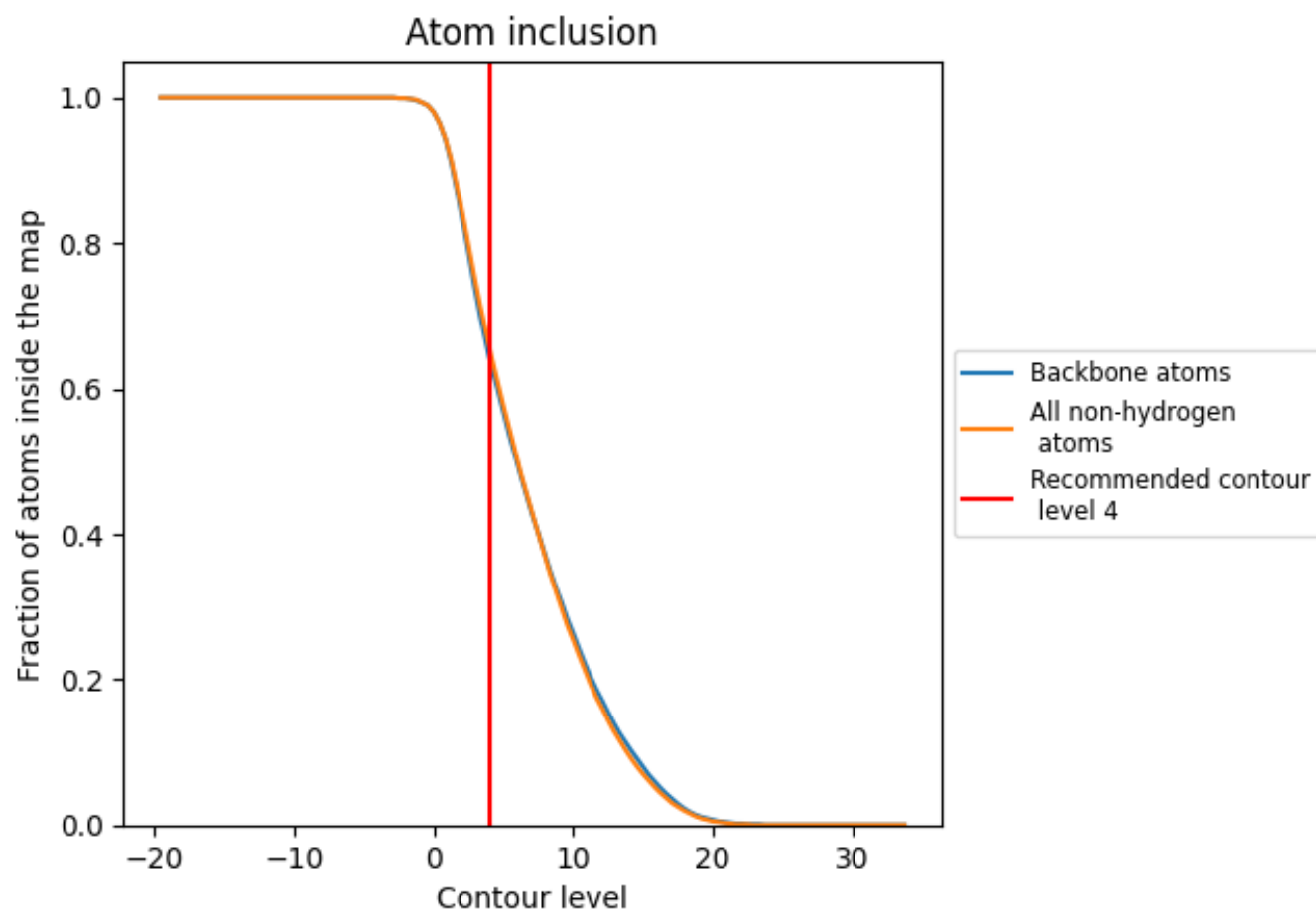
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6570	 0.4650
1	 0.0340	 0.0670
2	 0.0320	 0.1050
3	 0.0060	 0.0400
4	 0.0870	 0.2440
5	 0.0340	 0.0680
6	 0.0320	 0.1040
7	 0.0060	 0.0410
8	 0.0870	 0.2450
A	 0.8540	 0.5740
B	 0.8690	 0.5810
C	 0.8730	 0.5820
D	 0.8800	 0.5890
E	 0.7940	 0.5260
F	 0.7710	 0.5100
G	 0.5250	 0.3940
H	 0.7940	 0.5510
I	 0.8820	 0.6010
K	 0.8250	 0.5570
L	 0.8350	 0.5430
M	 0.8310	 0.5620
N	 0.6500	 0.4540
O	 0.7370	 0.5090
R	 0.6280	 0.4770
S	 0.7300	 0.5110
T	 0.8010	 0.5660
U	 0.2770	 0.4110
W	 0.8340	 0.5810
X	 0.6210	 0.4490
Y	 0.7790	 0.5100
Z	 0.7270	 0.5140
a	 0.8550	 0.5750
b	 0.8680	 0.5800
c	 0.8700	 0.5820
d	 0.8760	 0.5900



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Chain	Atom inclusion	Q-score
e	 0.7920	 0.5240
f	 0.7750	 0.5080
g	 0.5270	 0.3930
h	 0.7920	 0.5510
i	 0.8940	 0.5980
k	 0.8400	 0.5590
l	 0.8350	 0.5420
m	 0.8230	 0.5660
n	 0.6500	 0.4530
o	 0.7360	 0.5130
r	 0.6250	 0.4760
s	 0.7260	 0.5110
t	 0.8080	 0.5700
u	 0.2820	 0.4040
w	 0.8340	 0.5760
x	 0.6250	 0.4400
y	 0.7770	 0.5080
z	 0.7150	 0.5110